



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 2, 2025 – 03:23 am BST

PDB ID : 2WSC / pdb_00002wsc
Title : Improved Model of Plant Photosystem I
Authors : Amunts, A.; Toporik, H.; Borovikov, A.; Nelson, N.
Deposited on : 2009-09-04
Resolution : 3.30 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

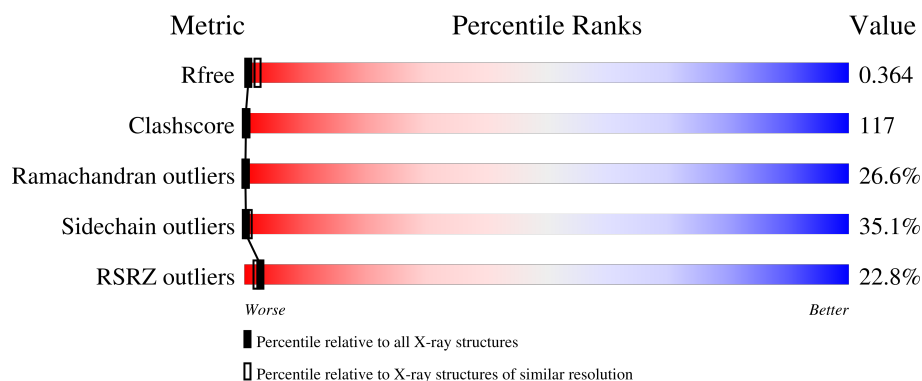
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	164625	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)

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

Mol	Chain	Length	Quality of chain
1	1	241	
2	2	269	
3	3	276	
4	4	251	
5	A	758	

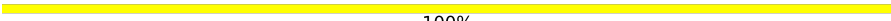
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Mol	Chain	Length	Quality of chain
6	B	734	
7	C	81	
8	D	212	
9	E	143	
10	F	231	
11	G	167	
12	H	144	
13	I	40	
14	J	44	
15	K	131	
16	L	216	
17	N	170	
18	R	53	
19	M	2	
19	O	2	
19	P	2	
19	Q	2	
19	S	2	
19	T	2	
19	U	2	
19	V	2	
19	W	2	
19	X	2	
19	Y	2	
19	Z	2	

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Mol	Chain	Length	Quality of chain
19	a	2	 100%

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
19	GLC	M	1	-	-	X	-
19	FRU	M	2	X	-	X	-
19	FRU	O	2	X	-	X	-
19	FRU	P	2	X	-	-	-
19	GLC	Q	1	-	-	X	-
19	FRU	Q	2	X	-	X	-
19	FRU	S	2	X	-	-	-
19	GLC	T	1	-	-	X	-
19	FRU	T	2	X	-	X	-
19	GLC	U	1	-	-	X	-
19	FRU	U	2	X	-	X	-
19	FRU	V	2	X	-	-	-
19	GLC	W	1	-	-	X	-
19	FRU	W	2	X	-	X	-
19	GLC	X	1	-	-	X	-
19	FRU	X	2	X	-	X	-
19	FRU	Y	2	X	-	-	-
19	GLC	Z	1	-	-	X	-
19	FRU	Z	2	X	-	X	-
19	FRU	a	2	X	-	-	-
20	CLA	1	1187	X	-	-	-
20	CLA	1	1188	X	-	-	-
20	CLA	1	1189	X	-	-	-
20	CLA	1	1190	X	-	-	-
20	CLA	1	1191	X	-	-	-
20	CLA	1	1192	X	-	-	-
20	CLA	1	1193	X	-	-	-
20	CLA	1	1194	X	-	-	-
20	CLA	1	1195	X	-	-	-
20	CLA	1	1196	X	-	-	-
20	CLA	1	1197	X	-	-	-
20	CLA	1	1198	X	-	-	-
20	CLA	1	1199	X	-	-	-
20	CLA	1	1200	X	-	-	-
20	CLA	1	1201	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	2	1212	X	-	-	-
20	CLA	2	1213	X	-	-	-
20	CLA	2	1214	X	-	-	-
20	CLA	2	1215	X	-	X	-
20	CLA	2	1216	X	-	-	-
20	CLA	2	1217	X	-	-	-
20	CLA	2	1218	X	-	-	-
20	CLA	2	1219	X	-	-	-
20	CLA	2	1220	X	-	X	-
20	CLA	2	1221	X	-	-	-
20	CLA	2	1222	X	-	-	-
20	CLA	2	1223	X	-	-	-
20	CLA	2	1224	X	-	-	-
20	CLA	2	1227	X	-	-	-
20	CLA	2	2010	X	-	-	-
20	CLA	3	1212	X	-	-	-
20	CLA	3	1213	X	-	-	-
20	CLA	3	1214	X	-	-	-
20	CLA	3	1215	X	-	-	-
20	CLA	3	1216	X	-	-	-
20	CLA	3	1217	X	-	-	-
20	CLA	3	1218	X	-	X	-
20	CLA	3	1219	X	-	-	-
20	CLA	3	3001	X	-	-	-
20	CLA	3	3002	X	-	-	-
20	CLA	3	3007	X	-	-	-
20	CLA	3	3008	X	-	-	-
20	CLA	3	3011	X	-	-	-
20	CLA	3	3014	X	-	-	-
20	CLA	3	3015	X	-	-	-
20	CLA	4	1196	X	-	X	-
20	CLA	4	1197	X	-	-	-
20	CLA	4	1198	X	-	X	-
20	CLA	4	1199	X	-	X	-
20	CLA	4	1200	X	-	-	-
20	CLA	4	1201	X	-	X	-
20	CLA	4	1202	X	-	-	-
20	CLA	4	1203	X	-	-	-
20	CLA	4	1204	X	-	-	-
20	CLA	4	1205	X	-	-	-
20	CLA	4	1206	X	-	-	-
20	CLA	4	1207	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	4	1208	X	-	-	-
20	CLA	4	1209	X	-	-	-
20	CLA	4	4003	X	-	-	-
20	CLA	4	4007	X	-	-	-
20	CLA	4	4014	X	-	-	-
20	CLA	A	1759	X	-	-	-
20	CLA	A	1760	X	-	X	-
20	CLA	A	1761	X	-	X	-
20	CLA	A	1762	X	-	-	-
20	CLA	A	1763	X	-	X	-
20	CLA	A	1764	X	-	X	-
20	CLA	A	1765	X	-	X	-
20	CLA	A	1766	X	-	-	-
20	CLA	A	1767	X	-	X	-
20	CLA	A	1768	X	-	-	-
20	CLA	A	1769	X	-	X	-
20	CLA	A	1770	X	-	X	-
20	CLA	A	1771	X	-	-	-
20	CLA	A	1772	X	-	X	-
20	CLA	A	1773	X	-	-	-
20	CLA	A	1774	X	-	X	-
20	CLA	A	1775	X	-	-	-
20	CLA	A	1776	X	-	X	-
20	CLA	A	1777	X	-	-	-
20	CLA	A	1778	X	-	-	-
20	CLA	A	1779	X	-	X	-
20	CLA	A	1780	X	-	-	-
20	CLA	A	1781	X	-	X	-
20	CLA	A	1782	X	-	X	-
20	CLA	A	1783	X	-	X	-
20	CLA	A	1784	X	-	-	-
20	CLA	A	1785	X	-	-	-
20	CLA	A	1786	X	-	-	-
20	CLA	A	1787	X	-	X	-
20	CLA	A	1788	X	-	X	-
20	CLA	A	1789	X	-	-	-
20	CLA	A	1790	X	-	-	-
20	CLA	A	1791	X	-	X	-
20	CLA	A	1792	X	-	X	-
20	CLA	A	1793	X	-	X	-
20	CLA	A	1794	X	-	X	-
20	CLA	A	1795	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	1796	X	-	X	-
20	CLA	A	1797	X	-	X	-
20	CLA	A	1798	X	-	X	-
20	CLA	A	1799	X	-	-	-
20	CLA	A	1800	X	-	X	-
20	CLA	A	1801	X	-	-	-
20	CLA	A	1811	X	-	-	-
20	CLA	A	1812	X	-	X	-
20	CLA	A	1813	X	-	X	-
20	CLA	A	1815	X	-	-	-
20	CLA	A	1816	X	-	X	-
20	CLA	A	1817	X	-	-	-
20	CLA	B	1735	X	-	X	-
20	CLA	B	1736	X	-	-	-
20	CLA	B	1737	X	-	X	-
20	CLA	B	1738	X	-	-	-
20	CLA	B	1739	X	-	X	-
20	CLA	B	1740	X	-	-	-
20	CLA	B	1741	X	-	-	-
20	CLA	B	1742	X	-	-	-
20	CLA	B	1743	X	-	X	-
20	CLA	B	1744	X	-	-	-
20	CLA	B	1745	X	-	-	-
20	CLA	B	1746	X	-	X	-
20	CLA	B	1747	X	-	X	-
20	CLA	B	1748	X	-	-	-
20	CLA	B	1749	X	-	-	-
20	CLA	B	1750	X	-	-	-
20	CLA	B	1751	X	-	-	-
20	CLA	B	1752	X	-	-	-
20	CLA	B	1753	X	-	X	-
20	CLA	B	1754	X	-	X	-
20	CLA	B	1755	X	-	X	-
20	CLA	B	1756	X	-	X	-
20	CLA	B	1757	X	-	X	-
20	CLA	B	1758	X	-	X	-
20	CLA	B	1759	X	-	X	-
20	CLA	B	1760	X	-	-	-
20	CLA	B	1761	X	-	-	-
20	CLA	B	1762	X	-	X	-
20	CLA	B	1763	X	-	-	-
20	CLA	B	1764	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	1765	X	-	-	-
20	CLA	B	1766	X	-	-	-
20	CLA	B	1767	X	-	-	-
20	CLA	B	1768	X	-	X	-
20	CLA	B	1769	X	-	X	-
20	CLA	B	1770	X	-	X	-
20	CLA	B	1771	X	-	X	-
20	CLA	B	1772	X	-	-	-
20	CLA	B	1785	X	-	X	-
20	CLA	B	1786	X	-	X	-
20	CLA	B	1787	X	-	X	-
20	CLA	F	1155	X	-	-	-
20	CLA	F	1156	X	-	-	-
20	CLA	F	1157	X	-	-	-
20	CLA	G	1099	X	-	-	-
20	CLA	H	1079	X	-	-	-
20	CLA	I	1031	X	-	-	-
20	CLA	I	1033	X	-	-	-
20	CLA	J	1043	X	-	X	-
20	CLA	J	1044	X	-	X	-
20	CLA	J	1045	X	-	X	-
20	CLA	J	1046	X	-	-	-
20	CLA	K	1085	X	-	X	-
20	CLA	K	1142	X	-	X	-
20	CLA	K	1146	X	-	-	-
20	CLA	K	3009	X	-	-	-
20	CLA	L	1166	X	-	-	-
20	CLA	L	1167	X	-	-	-
20	CLA	L	1168	X	-	-	-
20	CLA	L	1505	X	-	-	-
20	CLA	R	1054	X	-	-	-
20	CLA	R	1055	X	-	-	-
21	LMU	A	7016	-	-	X	-
21	LMU	A	7020	-	-	X	-
21	LMU	A	7021	-	-	X	-
21	LMU	A	7023	-	-	X	-
21	LMU	A	7026	-	-	X	-
21	LMU	A	7032	-	-	X	-
21	LMU	A	7037	-	-	X	-
21	LMU	A	7042	-	-	X	-
21	LMU	R	1057	X	-	-	-
22	BCR	3	1220	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	BCR	A	1803	-	-	X	-
22	BCR	A	1804	-	-	X	-
22	BCR	A	1805	-	-	X	-
22	BCR	A	1806	-	-	X	-
22	BCR	A	1807	-	-	X	-
22	BCR	A	1808	-	-	X	-
22	BCR	B	1777	-	-	X	-
22	BCR	B	1778	-	-	X	-
22	BCR	B	1779	-	-	X	-
22	BCR	B	1780	-	-	X	-
22	BCR	I	1032	-	-	X	-
22	BCR	L	1169	-	-	X	-
23	PQN	A	1802	X	-	-	-
23	PQN	B	1773	X	-	X	-
24	LMG	B	1783	-	-	X	-
25	SF4	B	1784	-	-	X	-
25	SF4	C	1082	-	-	X	-
25	SF4	C	1083	-	-	X	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 36379 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 AT3G54890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	165	Total	C	N	O	S	0	0	0
			1264	822	208	230	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-33	ILE	LYS	conflict	UNP Q9C5R7
1	-1	ARG	LYS	conflict	UNP Q9C5R7

- Molecule 2 is a protein called TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	176	Total	C	N	O	S	0	0	0
			1374	899	226	245	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	195	ALA	-	insertion	UNP Q41038
2	?	-	GLY	deletion	UNP Q41038

- Molecule 3 is a protein called LHCA3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	162	Total	C	N	O	S	0	0	0
			1254	826	203	220	5			

- Molecule 4 is a protein called CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	166	Total	C	N	O	S	0	0	0
			1319	861	219	236	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	?	-	ALA	deletion	UNP Q9SQL2

- Molecule 5 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	730	Total	C	N	O	S	0	0	0
			5745	3766	974	987	18			

- Molecule 6 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	733	Total	C	N	O	S	0	0	0
			5848	3843	997	995	13			

- Molecule 7 is a protein called PHOTOSYSTEM I IRON-SULFUR CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	C	81	Total	C	N	O	S	0	0	0
			619	384	108	115	12			

- Molecule 8 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-52	GLY	ALA	conflict	UNP P12353
D	-50	PRO	GLN	conflict	UNP P12353
D	-44	ARG	PRO	conflict	UNP P12353
D	-34	GLU	ASP	conflict	UNP P12353
D	-11	LEU	HIS	conflict	UNP P12353

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	THR	SER	conflict	UNP P12353
D	12	THR	PRO	conflict	UNP P12353
D	14	ALA	GLY	conflict	UNP P12353

- Molecule 9 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	E	65	Total	C	N	O	0	0	0
			520	332	93	95			

- Molecule 10 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC.

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

- Molecule 11 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	G	95	Total	C	N	O	S	0	0	0
			740	481	120	137	2			

- Molecule 12 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	H	69	Total	C	N	O	0	0	0
			529	344	82	103			

- Molecule 13 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII.

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

- Molecule 14 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	J	42	Total	C	N	O	S	0	0	0
			338	230	51	56	1			

- Molecule 15 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	K	84	Total	C	N	O	S	0	0	0
			593	374	102	113	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	47	ILE	LEU	conflict	UNP P36886

- Molecule 16 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	L	161	Total	C	N	O	S	0	0	0
			1203	791	193	214	5			

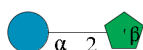
- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

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

- Molecule 18 is a protein called PHOTOSYSTEM I-N SUBUNIT.

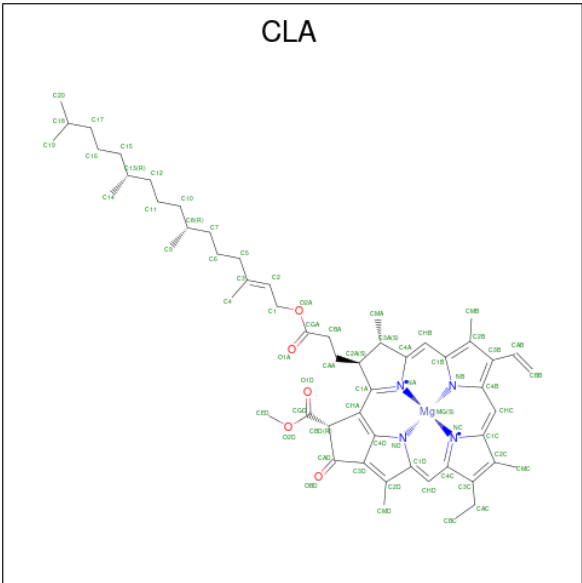
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	53	Total	C	N	O	0	0	0
			265	159	53	53			

- Molecule 19 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
19	M	2	Total	C	O	0	0	0
			22	12	10			
19	O	2	Total	C	O	0	0	0
			23	12	11			
19	P	2	Total	C	O	0	0	0
			23	12	11			
19	Q	2	Total	C	O	0	0	0
			23	12	11			
19	S	2	Total	C	O	0	0	0
			23	12	11			
19	T	2	Total	C	O	0	0	0
			23	12	11			
19	U	2	Total	C	O	0	0	0
			23	12	11			
19	V	2	Total	C	O	0	0	0
			23	12	11			
19	W	2	Total	C	O	0	0	0
			23	12	11			
19	X	2	Total	C	O	0	0	0
			23	12	11			
19	Y	2	Total	C	O	0	0	0
			23	12	11			
19	Z	2	Total	C	O	0	0	0
			23	12	11			
19	a	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	2	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	2	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
20	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	2	1	Total 25	C 20	Mg 1	N 4	0	0
20	2	1	Total 56	C 46	Mg 1	N 4 O 5	0	0
20	2	1	Total 25	C 20	Mg 1	N 4	0	0
20	2	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
20	2	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
20	2	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
20	2	1	Total 25	C 20	Mg 1	N 4	0	0
20	2	1	Total 25	C 20	Mg 1	N 4	0	0
20	3	1	Total 36	C 30	Mg 1	N 4 O 1	0	0
20	3	1	Total 25	C 20	Mg 1	N 4	0	0
20	3	1	Total 25	C 20	Mg 1	N 4	0	0
20	3	1	Total 25	C 20	Mg 1	N 4	0	0
20	3	1	Total 25	C 20	Mg 1	N 4	0	0
20	3	1	Total 25	C 20	Mg 1	N 4	0	0
20	3	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
20	3	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
20	3	1	Total 25	C 20	Mg 1	N 4	0	0
20	3	1	Total 25	C 20	Mg 1	N 4	0	0
20	3	1	Total 42	C 34	Mg 1	N 4 O 3	0	0
20	3	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
20	3	1	Total 65	C 55	Mg 1	N 4 O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	3	1	Total 25	C 20	Mg 1	N 4		0	0
20	3	1	Total 25	C 20	Mg 1	N 4		0	0
20	4	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	4	1	Total 36	C 30	Mg 1	N 4	O 1	0	0
20	4	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	4	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	4	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
20	4	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
20	4	1	Total 25	C 20	Mg 1	N 4		0	0
20	4	1	Total 25	C 20	Mg 1	N 4		0	0
20	4	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	4	1	Total 25	C 20	Mg 1	N 4		0	0
20	4	1	Total 25	C 20	Mg 1	N 4		0	0
20	4	1	Total 36	C 30	Mg 1	N 4	O 1	0	0
20	4	1	Total 25	C 20	Mg 1	N 4		0	0
20	4	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
20	4	1	Total 25	C 20	Mg 1	N 4		0	0
20	4	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
20	4	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
20	A	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	A	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
20	B	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
20	B	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
20	B	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
20	B	1	Total 50	C 40	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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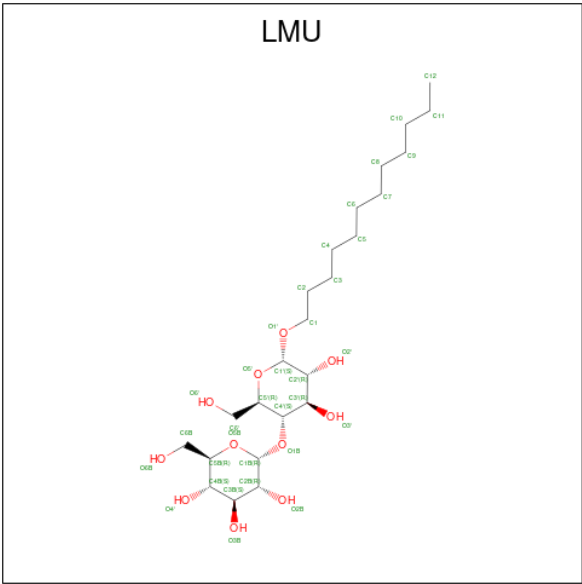
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	F	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	F	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
20	F	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
20	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	I	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	I	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	J	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	J	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	R	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
20	R	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 21 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	1	1	Total	C	O	0	0
			35	24	11		
21	1	1	Total	C	O	0	0
			35	24	11		
21	2	1	Total	C	O	0	0
			35	24	11		
21	2	1	Total	C	O	0	0
			35	24	11		
21	2	1	Total	C	O	0	0
			35	24	11		
21	3	1	Total	C	O	0	0
			35	24	11		
21	4	1	Total	C	O	0	0
			35	24	11		

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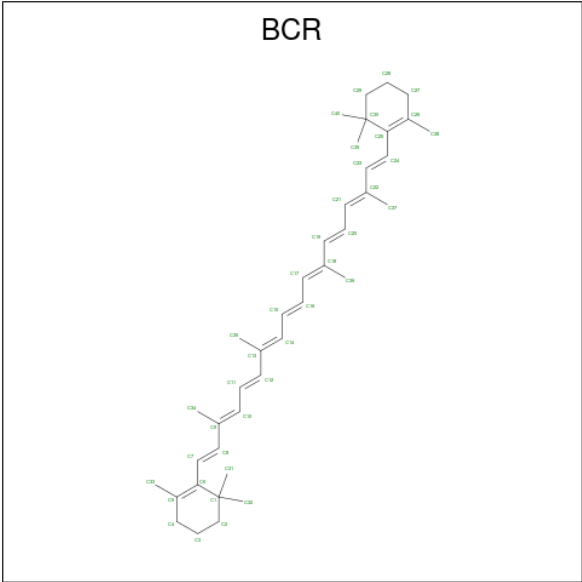
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			34	23	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			34	23	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	B	1	Total	C	O	0	0
			25	14	11		
21	K	1	Total	C	O	0	0
			35	24	11		
21	L	1	Total	C	O	0	0
			35	24	11		
21	R	1	Total	C	O	0	0
			35	24	11		
21	R	1	Total	C	O	0	0
			35	24	11		

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



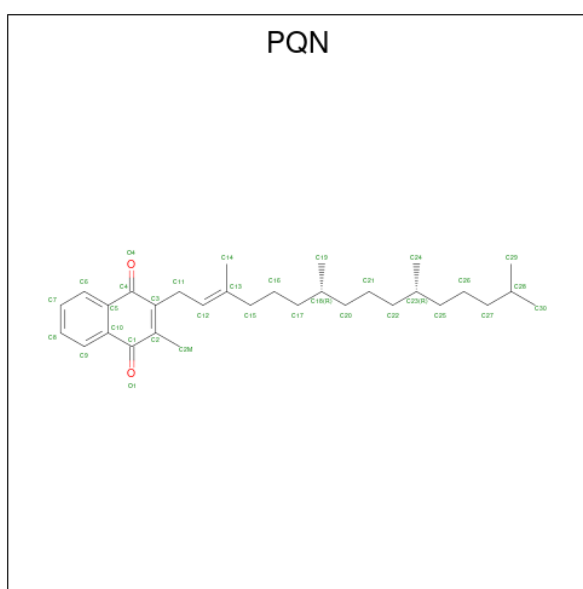
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	3	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0

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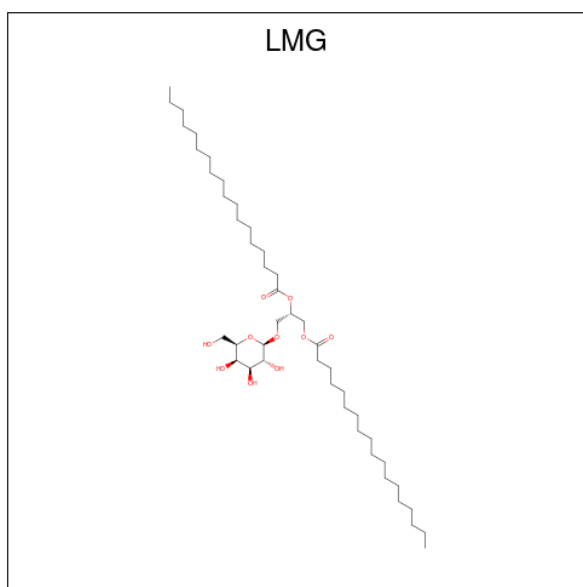
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C 40 40	0	0
22	I	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0

- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



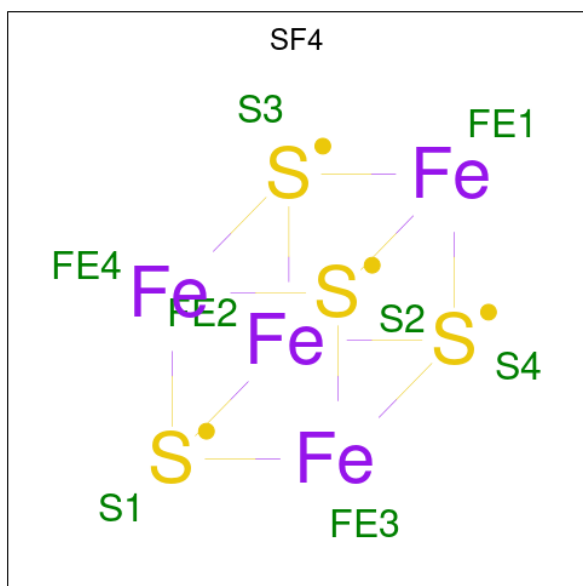
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 33 31 2	0	0
23	B	1	Total C O 33 31 2	0	0

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total	C	O	0	0
			49	39	10		

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

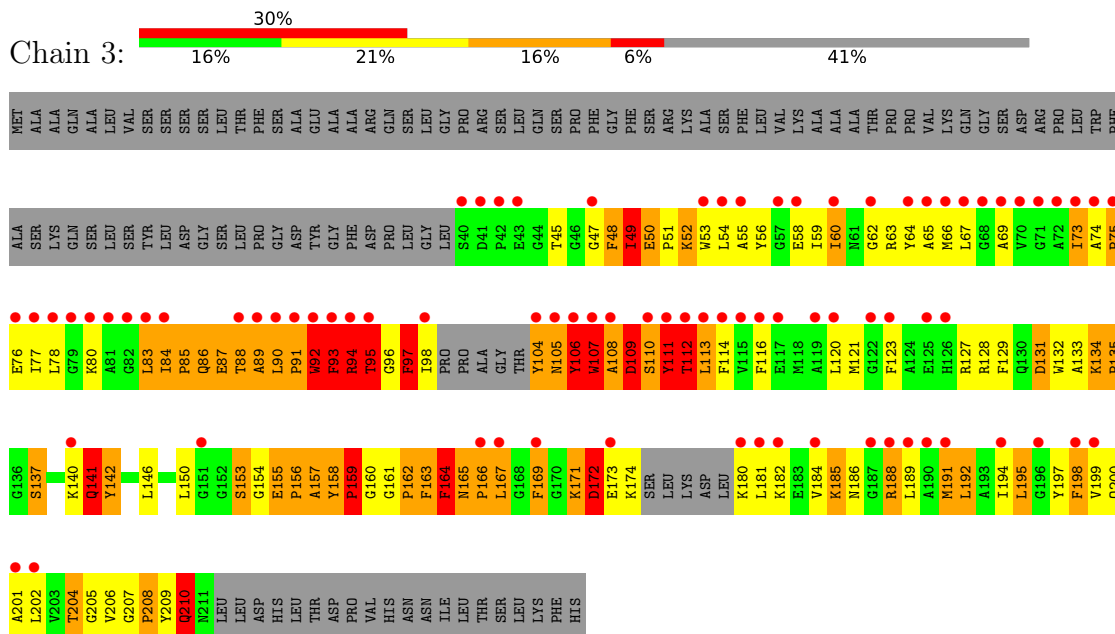


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	Fe	S	0	0
			8	4	4		
25	C	1	Total	Fe	S	0	0
			8	4	4		
25	C	1	Total	Fe	S	0	0
			8	4	4		

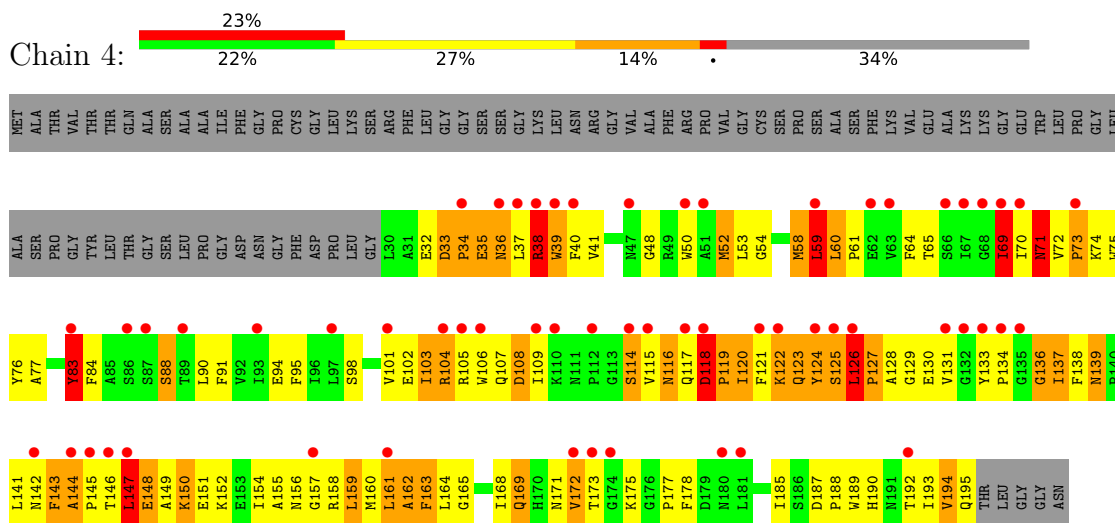
- Molecule 26 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	B	1	Total	C	O	0	0
			23	12	11		

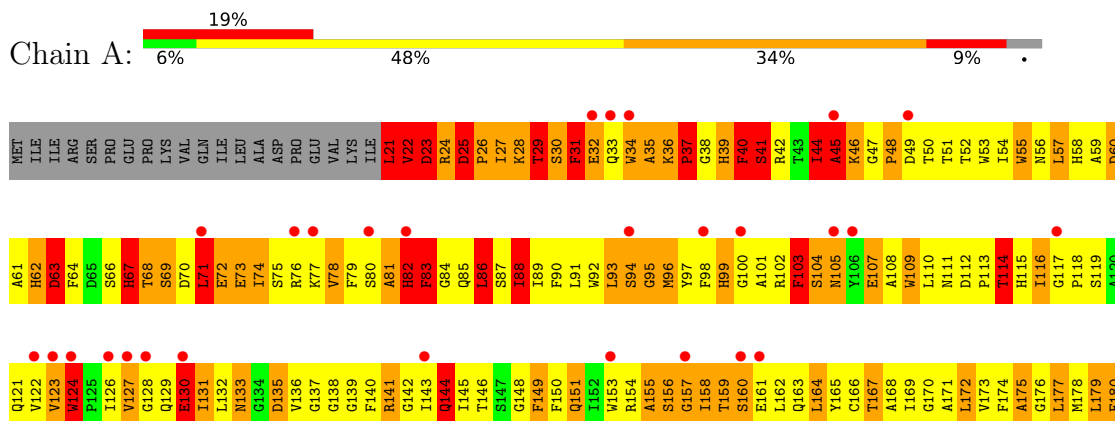
- Molecule 3: LHCA3

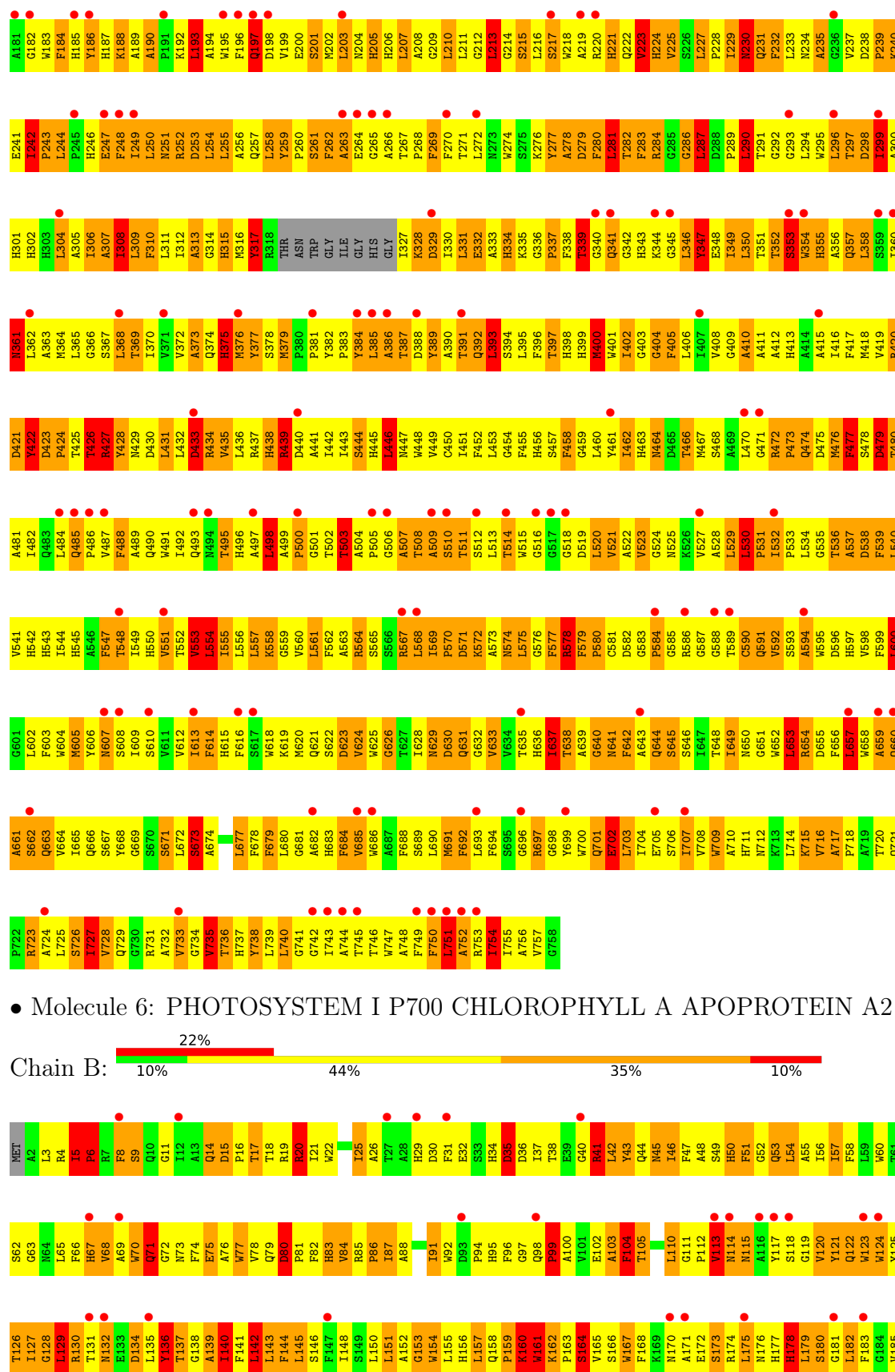


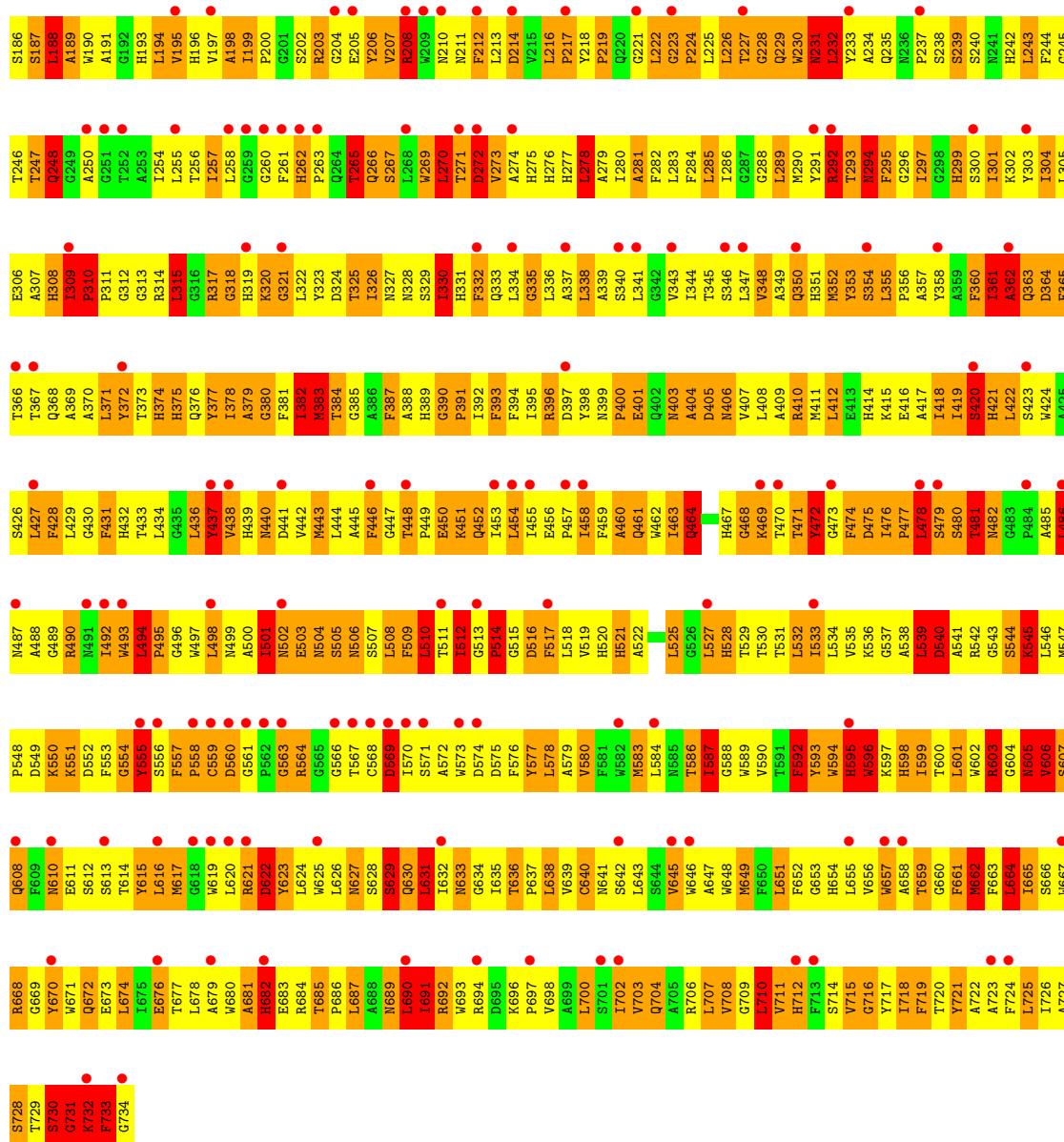
- Molecule 4: CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC

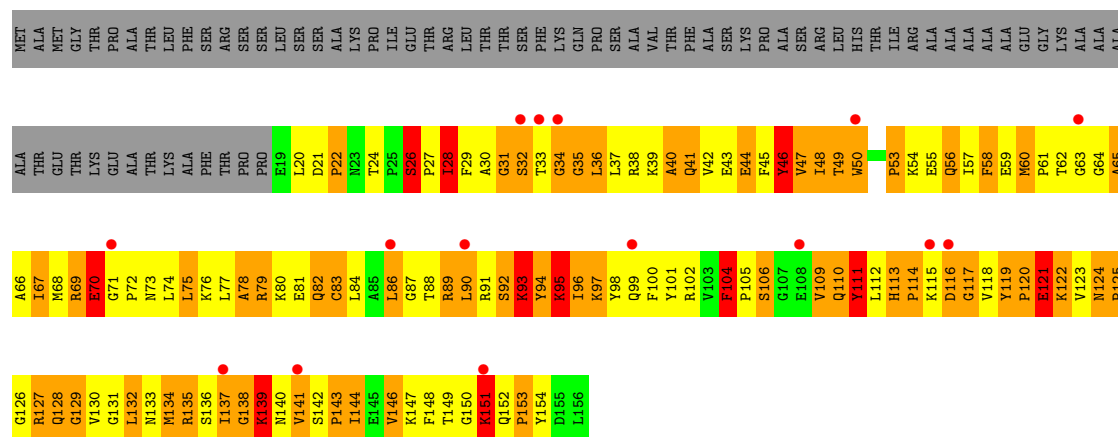


- Molecule 5: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1

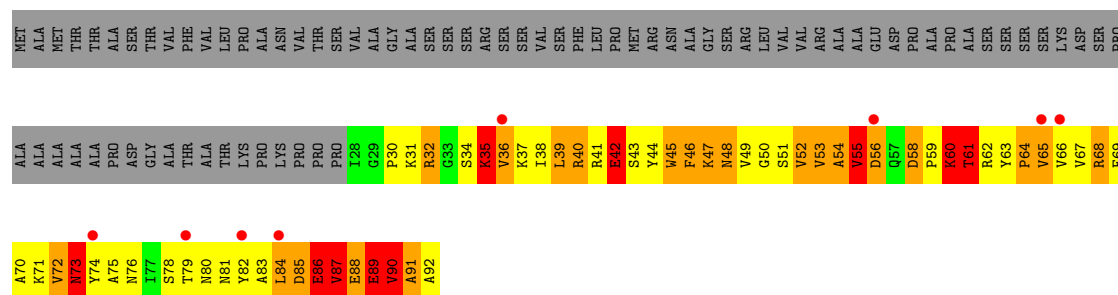
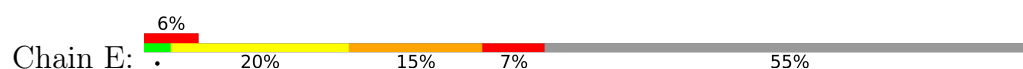




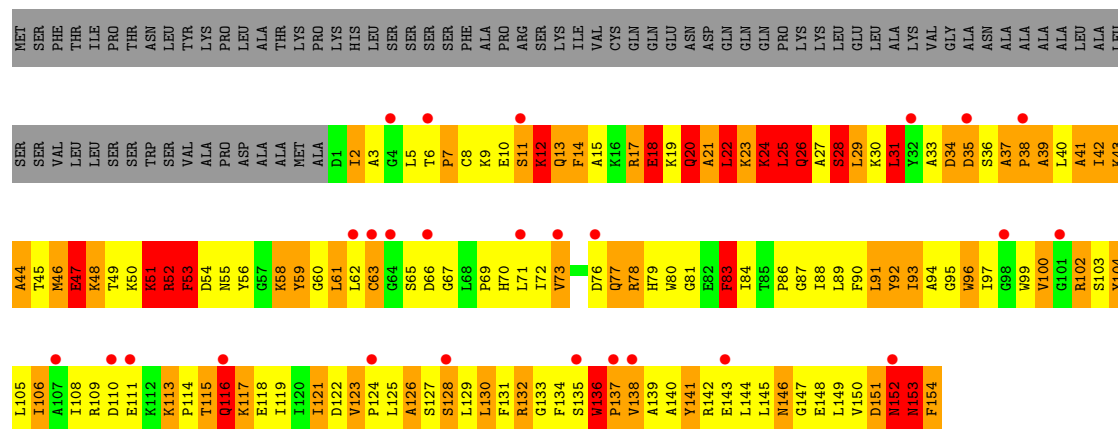




• Molecule 9: PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC

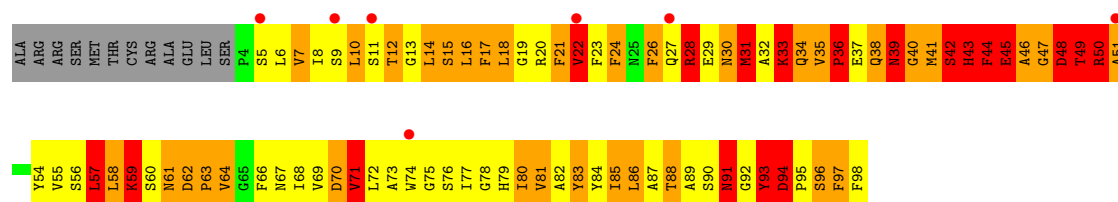


• Molecule 10: PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC

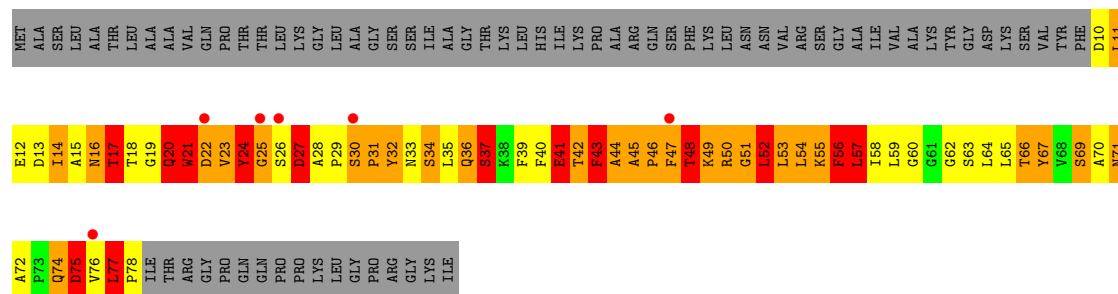
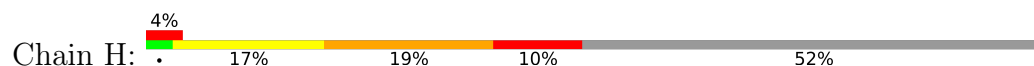


• Molecule 11: PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC

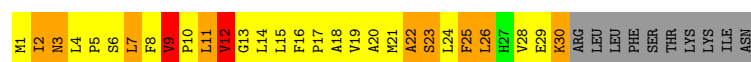




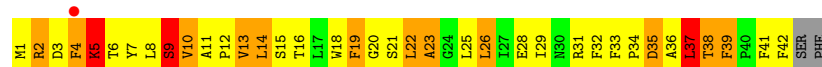
• Molecule 12: PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC



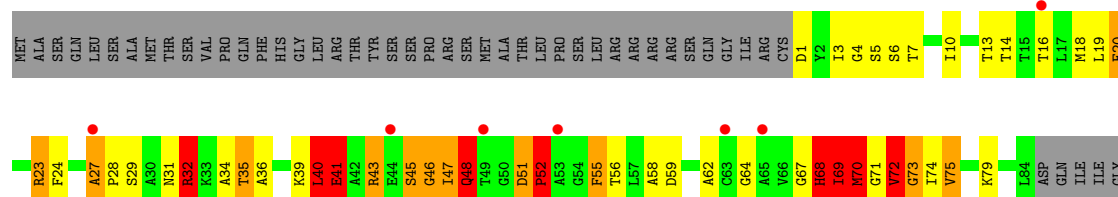
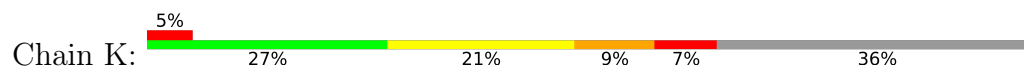
• Molecule 13: PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII



• Molecule 14: PHOTOSYSTEM I REACTION CENTER SUBUNIT IX

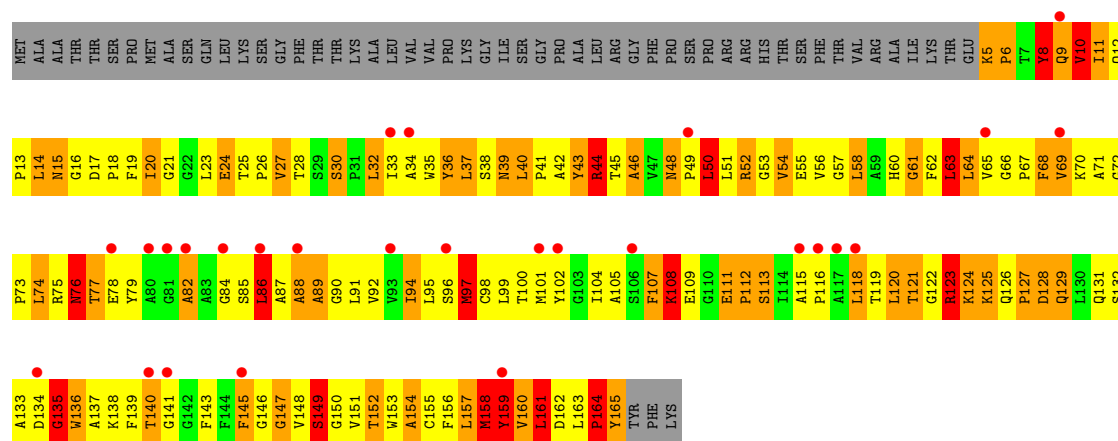


• Molecule 15: PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC

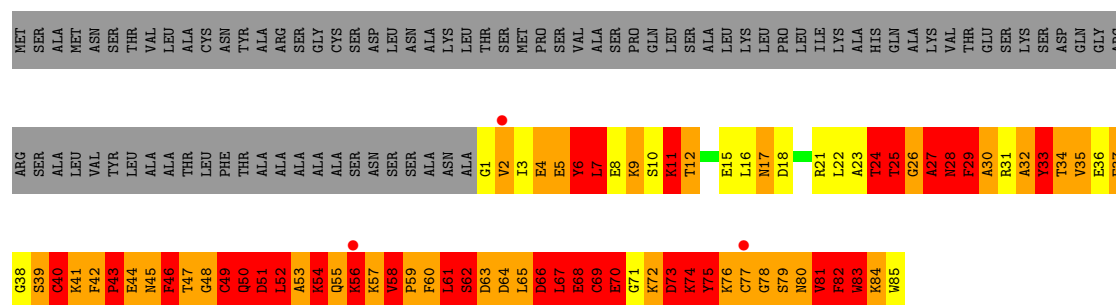
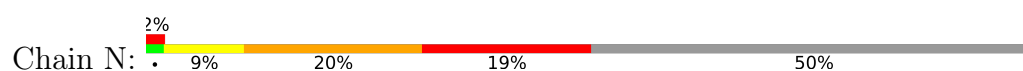


• Molecule 16: PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC

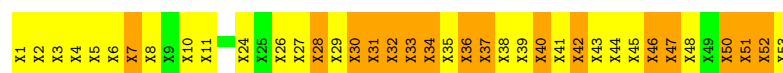




• Molecule 17: PHOTOSYSTEM I-N SUBUNIT



• Molecule 18: PHOTOSYSTEM I-N SUBUNIT



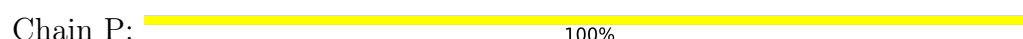
• Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



• Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



• Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



GLC1
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain Q:  100%GLC1
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain S:  50% 50%GLC1
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain T:  100%GLC1
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain U:  100%GLC1
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain V:  100%GLC1
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain W:  100%GLC1
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain X:  100%GLC1
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain Y:  100%

GLC1
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain Z:  100%

GLC1
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain a:  100%

GLC1
FRU2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.66Å 189.09Å 129.39Å 90.00° 91.24° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 30.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-3.30) 99.3 (30.00-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.363 , 0.366 0.359 , 0.364	Depositor DCC
R_{free} test set	4345 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	78.5	Xtriage
Anisotropy	0.655	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.13 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	36379	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: UNL, SF4, FRU, BCR, CLA, GLC, LMG, PQN, LMU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.48	0/1303	0.72	3/1774 (0.2%)
2	2	0.45	0/1420	0.71	0/1943
3	3	0.87	6/1292 (0.5%)	0.96	3/1743 (0.2%)
4	4	0.49	0/1359	0.75	2/1851 (0.1%)
5	A	0.95	3/5938 (0.1%)	1.04	11/8104 (0.1%)
6	B	0.95	2/6058 (0.0%)	1.02	14/8278 (0.2%)
7	C	1.43	7/632 (1.1%)	1.33	4/856 (0.5%)
8	D	1.10	0/1122	1.05	0/1514
9	E	1.15	0/530	1.17	2/718 (0.3%)
10	F	1.10	1/1250 (0.1%)	1.07	2/1687 (0.1%)
11	G	1.07	0/760	1.28	9/1031 (0.9%)
12	H	1.16	0/543	1.19	3/741 (0.4%)
13	I	1.00	0/235	0.97	0/320
14	J	1.02	0/349	1.09	1/475 (0.2%)
15	K	0.55	0/599	0.83	1/810 (0.1%)
16	L	1.08	0/1238	1.10	5/1691 (0.3%)
17	N	1.23	1/699 (0.1%)	1.33	7/936 (0.7%)
All	All	0.94	20/25327 (0.1%)	1.02	67/34472 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	3
2	2	0	1
3	3	0	19
5	A	0	28
6	B	0	20
7	C	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	D	0	6
9	E	0	6
10	F	0	12
11	G	1	16
12	H	0	9
15	K	0	2
16	L	0	3
17	N	0	21
18	R	0	17
All	All	1	166

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	92	TRP	CB-CG	16.88	1.80	1.50
3	3	93	PHE	CE1-CZ	8.69	1.53	1.37
6	B	640	CYS	CB-SG	7.67	1.95	1.82
7	C	72	GLU	CD-OE1	-7.43	1.17	1.25
3	3	93	PHE	CD2-CE2	7.38	1.54	1.39

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	732	LYS	N-CA-C	-8.11	89.10	111.00
5	A	93	LEU	CA-CB-CG	8.06	133.84	115.30
5	A	530	LEU	CA-CB-CG	7.27	132.02	115.30
6	B	486	LEU	CA-CB-CG	7.27	132.01	115.30
6	B	315	LEU	CA-CB-CG	7.21	131.88	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	G	21	PHE	CA

5 of 166 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	182	ALA	Peptide
1	1	183	ASP	Peptide
1	1	184	PRO	Peptide
2	2	120	ASN	Peptide
3	3	49	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1264	0	1230	91	1
2	2	1374	0	1329	142	0
3	3	1254	0	1221	333	1
4	4	1319	0	1283	201	13
5	A	5745	0	5595	1661	0
6	B	5848	0	5655	1449	1
7	C	619	0	608	236	0
8	D	1095	0	1112	226	0
9	E	520	0	528	150	0
10	F	1221	0	1246	289	0
11	G	740	0	709	297	7
12	H	529	0	514	117	0
13	I	229	0	252	58	0
14	J	338	0	340	80	0
15	K	593	0	619	65	1
16	L	1203	0	1213	326	13
17	N	685	0	671	448	7
18	R	265	0	67	77	0
19	M	22	0	18	11	0
19	O	23	0	21	14	0
19	P	23	0	21	0	0
19	Q	23	0	21	11	0
19	S	23	0	20	1	0
19	T	23	0	21	8	0
19	U	23	0	21	9	0
19	V	23	0	21	3	0
19	W	23	0	21	17	0
19	X	23	0	21	7	0
19	Y	23	0	21	1	0
19	Z	23	0	20	20	0
19	a	23	0	19	0	0
20	1	644	0	429	113	2
20	2	658	0	480	160	0
20	3	548	0	326	115	0
20	4	699	0	454	157	0
20	A	2777	0	2599	1120	1
20	B	2372	0	2285	808	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	F	130	0	86	27	0
20	G	51	0	40	6	0
20	H	65	0	71	19	0
20	I	115	0	106	26	0
20	J	202	0	169	99	0
20	K	210	0	177	44	2
20	L	202	0	158	40	0
20	R	122	0	123	17	0
21	1	70	0	92	15	0
21	2	105	0	138	15	1
21	3	35	0	46	3	0
21	4	35	0	46	0	0
21	A	1153	0	1505	397	0
21	B	25	0	23	1	0
21	K	35	0	45	6	0
21	L	35	0	46	3	0
21	R	70	0	91	24	0
22	3	40	0	54	21	0
22	A	240	0	323	250	0
22	B	320	0	432	225	0
22	I	40	0	54	47	0
22	L	80	0	105	61	0
23	A	33	0	46	12	0
23	B	33	0	46	33	0
24	B	49	0	71	30	0
25	B	8	0	0	18	0
25	C	16	0	0	9	0
26	B	23	0	0	2	0
All	All	36379	0	35124	8371	25

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 117.

The worst 5 of 8371 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)
4:4:160:MET:SD	20:4:1201:CLA:HBB1	1.28	1.66
20:A:1776:CLA:H92	22:A:1805:BCR:C37	1.17	1.58
6:B:25:ILE:HG21	22:L:1169:BCR:C29	1.11	1.58
5:A:51:THR:HG21	20:A:1795:CLA:CBB	1.24	1.57
21:A:7036:LMU:H82	21:A:7036:LMU:C2	1.34	1.57

The worst 5 of 25 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:31:MET:CE	17:N:85:TRP:NE1[2_546]	0.92	1.28
4:4:130:GLU:C	16:L:159:TYR:OH[1_655]	1.18	1.02
11:G:31:MET:CE	17:N:85:TRP:CE2[2_546]	1.19	1.01
20:1:1193:CLA:O2D	20:K:1142:CLA:O2A[1_654]	1.34	0.86
4:4:130:GLU:CA	16:L:159:TYR:OH[1_655]	1.43	0.77

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	161/241 (67%)	83 (52%)	43 (27%)	35 (22%)	0	0
2	2	174/269 (65%)	88 (51%)	56 (32%)	30 (17%)	0	1
3	3	156/276 (56%)	78 (50%)	43 (28%)	35 (22%)	0	0
4	4	164/251 (65%)	79 (48%)	47 (29%)	38 (23%)	0	0
5	A	726/758 (96%)	334 (46%)	200 (28%)	192 (26%)	0	0
6	B	731/734 (100%)	361 (49%)	189 (26%)	181 (25%)	0	0
7	C	79/81 (98%)	23 (29%)	29 (37%)	27 (34%)	0	0
8	D	136/212 (64%)	48 (35%)	42 (31%)	46 (34%)	0	0
9	E	63/143 (44%)	29 (46%)	14 (22%)	20 (32%)	0	0
10	F	152/231 (66%)	67 (44%)	44 (29%)	41 (27%)	0	0
11	G	93/167 (56%)	35 (38%)	28 (30%)	30 (32%)	0	0
12	H	67/144 (46%)	28 (42%)	15 (22%)	24 (36%)	0	0
13	I	28/40 (70%)	10 (36%)	11 (39%)	7 (25%)	0	0
14	J	40/44 (91%)	19 (48%)	11 (28%)	10 (25%)	0	0
15	K	82/131 (63%)	49 (60%)	15 (18%)	18 (22%)	0	0
16	L	159/216 (74%)	66 (42%)	47 (30%)	46 (29%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	N	83/170 (49%)	22 (26%)	19 (23%)	42 (51%)	0	0
All	All	3094/4108 (75%)	1419 (46%)	853 (28%)	822 (27%)	0	0

5 of 822 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	25	ASP
1	1	29	LEU
1	1	30	GLY
1	1	35	ASN
1	1	58	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	127/190 (67%)	102 (80%)	25 (20%)	1	5
2	2	140/216 (65%)	107 (76%)	33 (24%)	0	3
3	3	120/215 (56%)	82 (68%)	38 (32%)	0	1
4	4	138/201 (69%)	103 (75%)	35 (25%)	0	2
5	A	592/618 (96%)	392 (66%)	200 (34%)	0	1
6	B	598/600 (100%)	367 (61%)	231 (39%)	0	0
7	C	70/70 (100%)	40 (57%)	30 (43%)	0	0
8	D	118/173 (68%)	75 (64%)	43 (36%)	0	0
9	E	56/114 (49%)	37 (66%)	19 (34%)	0	1
10	F	127/190 (67%)	73 (58%)	54 (42%)	0	0
11	G	79/144 (55%)	46 (58%)	33 (42%)	0	0
12	H	57/115 (50%)	26 (46%)	31 (54%)	0	0
13	I	26/36 (72%)	18 (69%)	8 (31%)	0	1
14	J	36/39 (92%)	25 (69%)	11 (31%)	0	1
15	K	61/102 (60%)	43 (70%)	18 (30%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	L	124/169 (73%)	81 (65%)	43 (35%)	0	1
17	N	74/139 (53%)	33 (45%)	41 (55%)	0	0
All	All	2543/3331 (76%)	1650 (65%)	893 (35%)	0	1

5 of 893 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	440	ASN
17	N	73	ASP
7	C	37	LYS
17	N	62	SER
15	K	41	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 111 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	277	HIS
17	N	55	GLN
6	B	595	HIS
17	N	45	ASN
12	H	33	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

26 monosaccharides 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$
19	GLC	M	1	19	10,10,12	1.46	3 (30%)	14,14,17	3.31	10 (71%)
19	FRU	M	2	19	11,12,12	1.06	1 (9%)	10,18,18	2.33	3 (30%)
19	GLC	O	1	19	11,11,12	0.92	0	15,15,17	3.54	8 (53%)
19	FRU	O	2	19	11,12,12	1.08	1 (9%)	10,18,18	1.70	2 (20%)
19	GLC	P	1	19	11,11,12	0.99	0	15,15,17	2.44	3 (20%)
19	FRU	P	2	19	11,12,12	1.16	2 (18%)	10,18,18	0.96	0
19	GLC	Q	1	19	11,11,12	1.19	1 (9%)	15,15,17	2.20	5 (33%)
19	FRU	Q	2	19	11,12,12	1.00	1 (9%)	10,18,18	1.76	4 (40%)
19	GLC	S	1	19	11,11,12	0.44	0	15,15,17	1.12	2 (13%)
19	FRU	S	2	19,21	11,12,12	0.67	0	10,18,18	1.12	0
19	GLC	T	1	19	11,11,12	1.07	0	15,15,17	1.64	3 (20%)
19	FRU	T	2	19	11,12,12	2.01	4 (36%)	10,18,18	2.89	4 (40%)
19	GLC	U	1	19	11,11,12	1.06	1 (9%)	15,15,17	2.67	5 (33%)
19	FRU	U	2	19	11,12,12	0.96	0	10,18,18	1.53	2 (20%)
19	GLC	V	1	19	11,11,12	1.54	2 (18%)	15,15,17	1.98	5 (33%)
19	FRU	V	2	19	11,12,12	0.90	0	10,18,18	2.00	5 (50%)
19	GLC	W	1	19	11,11,12	1.30	1 (9%)	15,15,17	2.89	9 (60%)
19	FRU	W	2	19	11,12,12	1.17	2 (18%)	10,18,18	2.10	2 (20%)
19	GLC	X	1	19	11,11,12	1.22	1 (9%)	15,15,17	1.83	4 (26%)
19	FRU	X	2	19	11,12,12	1.56	2 (18%)	10,18,18	2.32	4 (40%)
19	GLC	Y	1	19	11,11,12	1.09	0	15,15,17	3.55	7 (46%)
19	FRU	Y	2	19	11,12,12	1.15	0	10,18,18	2.27	4 (40%)
19	GLC	Z	1	19	11,11,12	1.75	2 (18%)	15,15,17	4.50	8 (53%)
19	FRU	Z	2	19,21	11,12,12	1.06	1 (9%)	10,18,18	2.34	3 (30%)
19	GLC	a	1	19	11,11,12	1.06	1 (9%)	15,15,17	1.52	3 (20%)
19	FRU	a	2	19,12	11,12,12	1.07	0	10,18,18	2.15	3 (30%)

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
19	GLC	M	1	19	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	FRU	M	2	19	1/1/4/4	0/5/24/24	0/1/1/1
19	GLC	O	1	19	-	1/2/19/22	0/1/1/1
19	FRU	O	2	19	1/1/4/4	4/5/24/24	0/1/1/1
19	GLC	P	1	19	-	2/2/19/22	0/1/1/1
19	FRU	P	2	19	1/1/4/4	2/5/24/24	0/1/1/1
19	GLC	Q	1	19	-	2/2/19/22	0/1/1/1
19	FRU	Q	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	S	1	19	-	1/2/19/22	0/1/1/1
19	FRU	S	2	19,21	1/1/4/4	0/5/24/24	0/1/1/1
19	GLC	T	1	19	-	2/2/19/22	0/1/1/1
19	FRU	T	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	U	1	19	-	2/2/19/22	0/1/1/1
19	FRU	U	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	V	1	19	-	0/2/19/22	0/1/1/1
19	FRU	V	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	W	1	19	-	1/2/19/22	0/1/1/1
19	FRU	W	2	19	1/1/4/4	2/5/24/24	0/1/1/1
19	GLC	X	1	19	-	2/2/19/22	0/1/1/1
19	FRU	X	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	Y	1	19	-	2/2/19/22	0/1/1/1
19	FRU	Y	2	19	1/1/4/4	1/5/24/24	0/1/1/1
19	GLC	Z	1	19	-	0/2/19/22	0/1/1/1
19	FRU	Z	2	19,21	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	a	1	19	-	2/2/19/22	0/1/1/1
19	FRU	a	2	19,12	1/1/4/4	2/5/24/24	0/1/1/1

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Z	1	GLC	O5-C1	-4.10	1.37	1.43
19	T	2	FRU	O5-C2	-3.74	1.37	1.43
19	T	2	FRU	C1-C2	-3.01	1.47	1.52
19	V	1	GLC	O5-C1	-2.83	1.39	1.43
19	X	2	FRU	O2-C2	-2.70	1.36	1.40

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	1	GLC	C1-O5-C5	-11.46	96.66	112.19
19	M	1	GLC	C1-C2-C3	7.92	119.40	109.67
19	P	1	GLC	C1-O5-C5	7.71	122.64	112.19
19	Y	1	GLC	C1-O5-C5	7.50	122.35	112.19
19	Z	1	GLC	O5-C1-C2	-7.29	99.52	110.77

5 of 13 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	M	2	FRU	C2
19	O	2	FRU	C2
19	P	2	FRU	C2
19	Q	2	FRU	C2
19	S	2	FRU	C2

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	O	2	FRU	O1-C1-C2-C3
19	O	2	FRU	O1-C1-C2-O2
19	Q	2	FRU	O1-C1-C2-C3
19	Q	2	FRU	O1-C1-C2-O2
19	Q	2	FRU	O1-C1-C2-O5

There are no ring outliers.

21 monomers are involved in 102 short contacts:

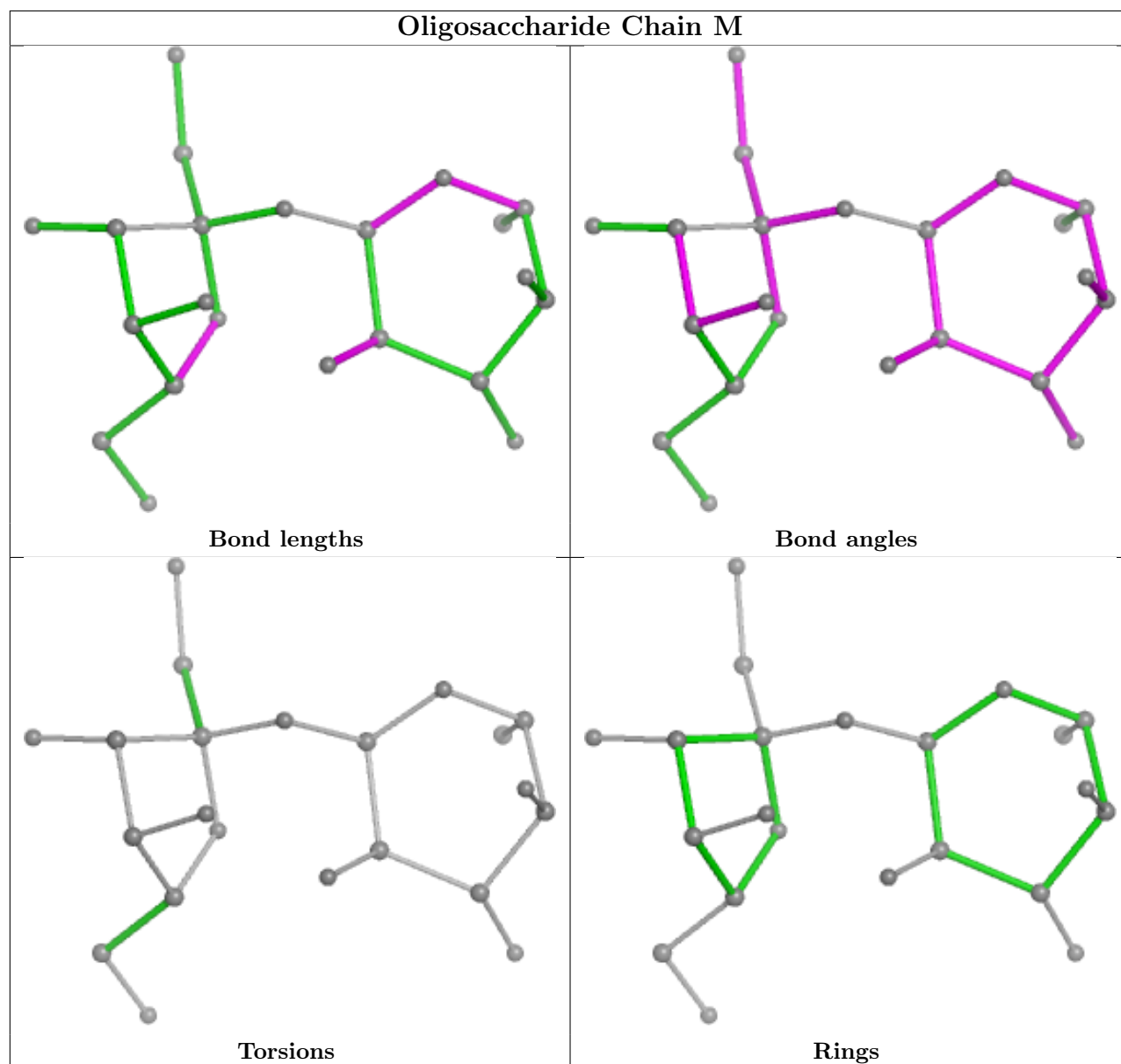
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	M	2	FRU	7	0
19	S	1	GLC	1	0
19	V	1	GLC	3	0
19	Y	2	FRU	1	0
19	Y	1	GLC	1	0
19	O	2	FRU	14	0
19	U	2	FRU	9	0
19	W	1	GLC	13	0
19	U	1	GLC	6	0
19	V	2	FRU	3	0
19	Z	1	GLC	7	0
19	T	2	FRU	8	0
19	X	2	FRU	7	0
19	Q	1	GLC	10	0
19	O	1	GLC	5	0

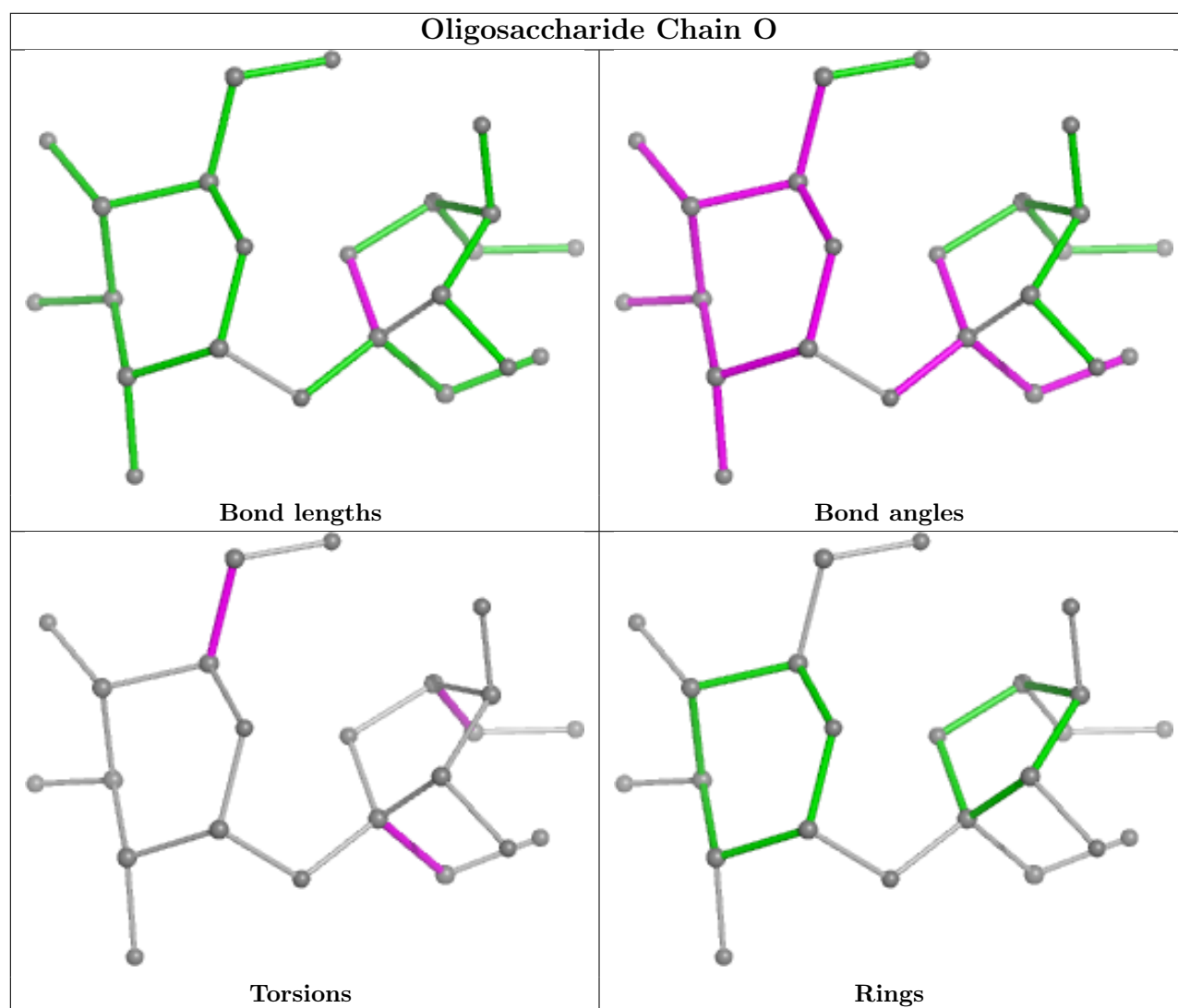
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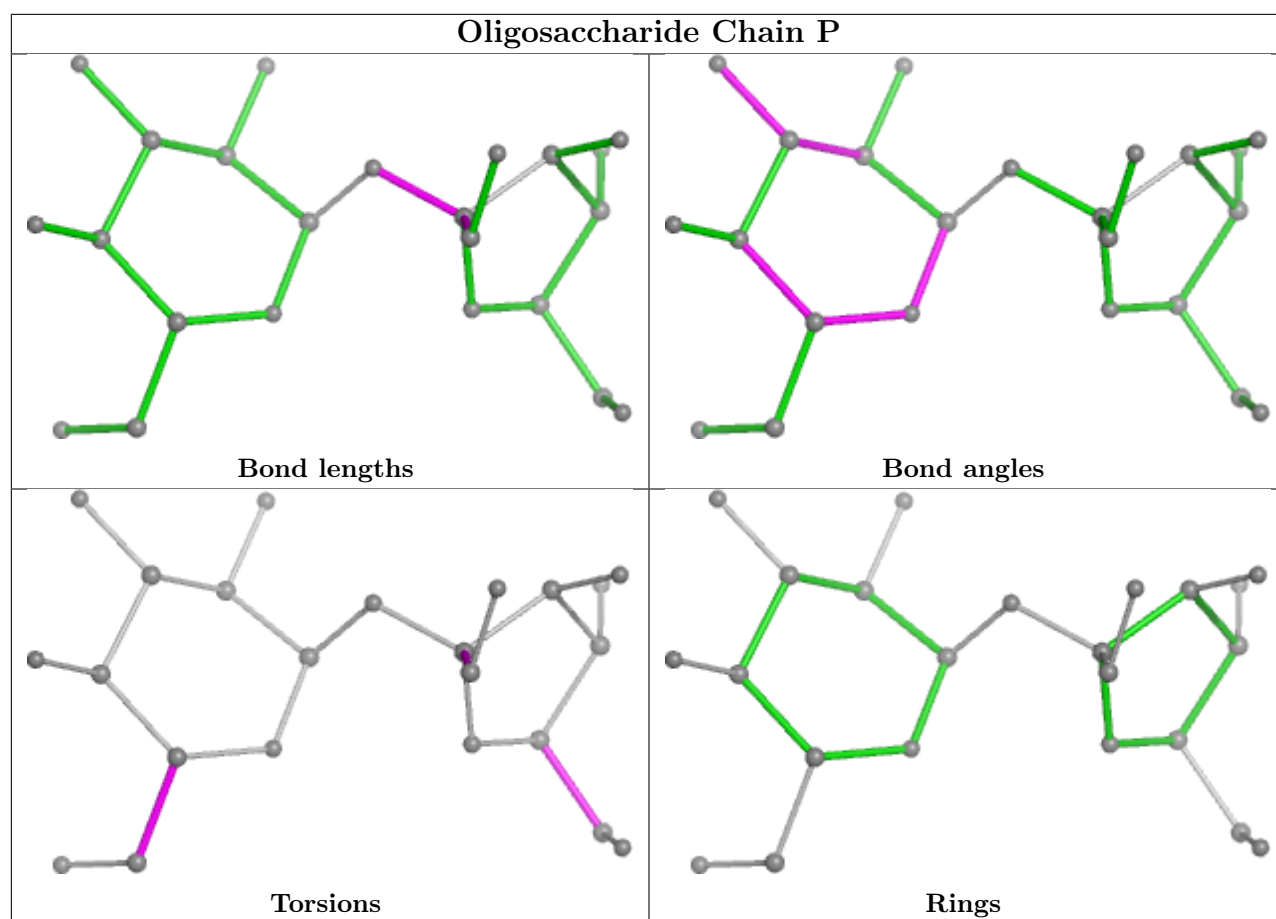
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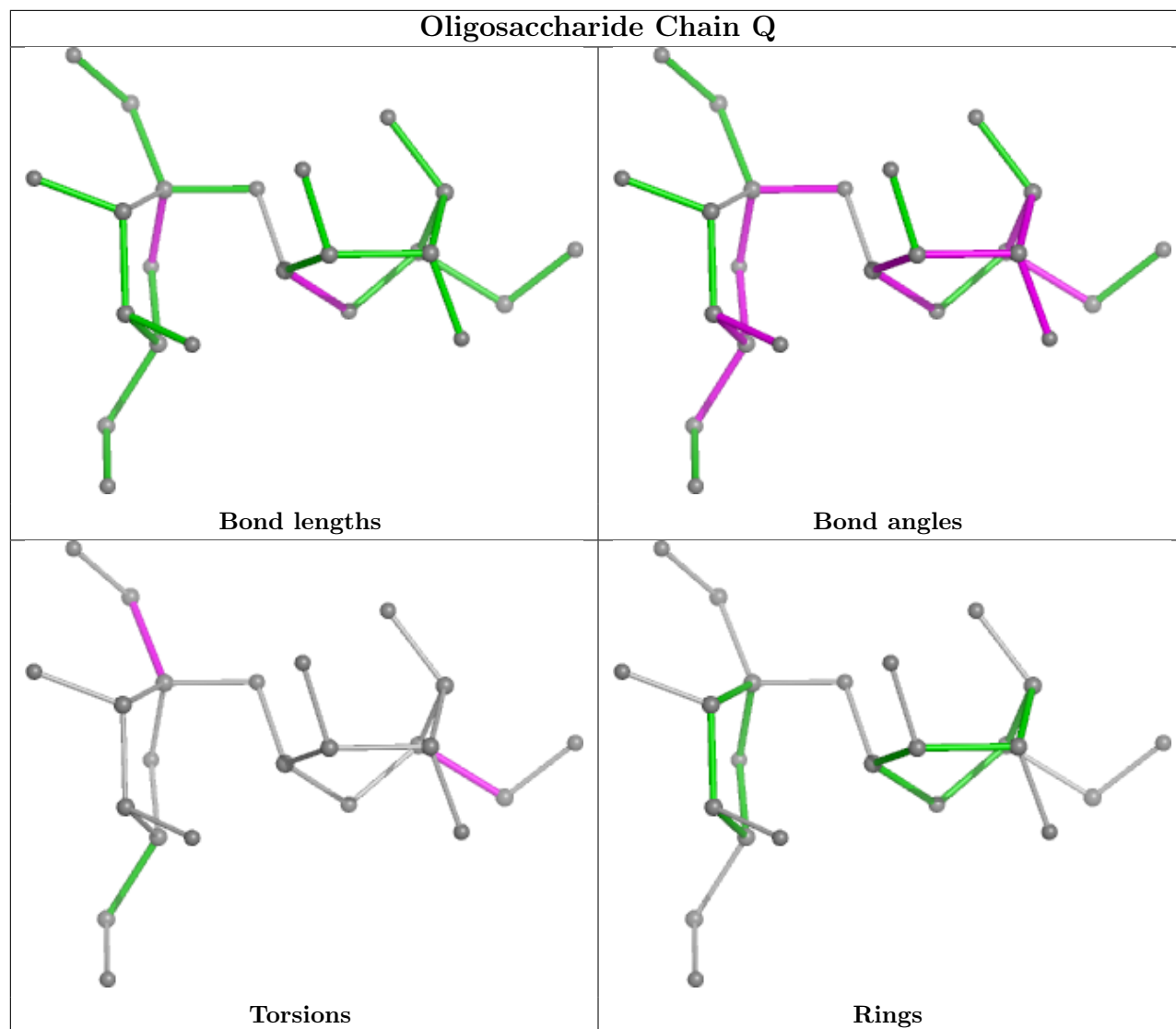
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	Z	2	FRU	18	0
19	T	1	GLC	7	0
19	W	2	FRU	15	0
19	M	1	GLC	10	0
19	X	1	GLC	7	0
19	Q	2	FRU	9	0

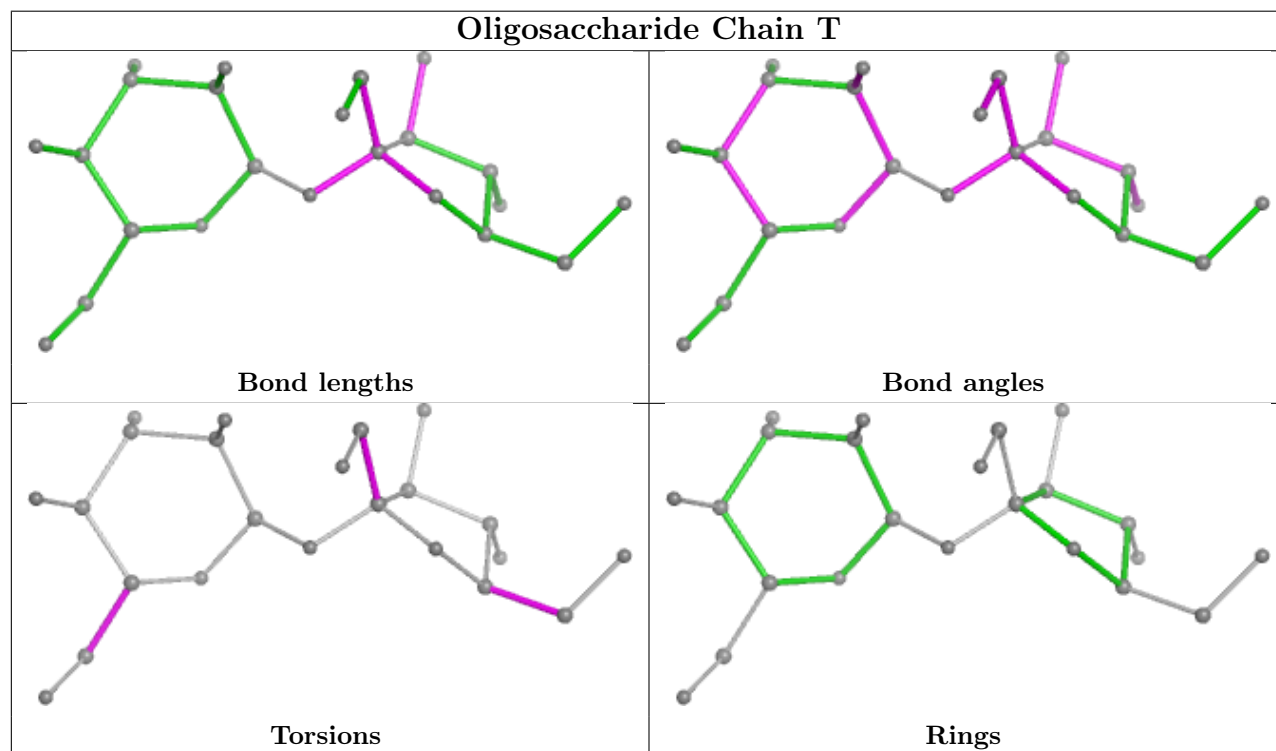
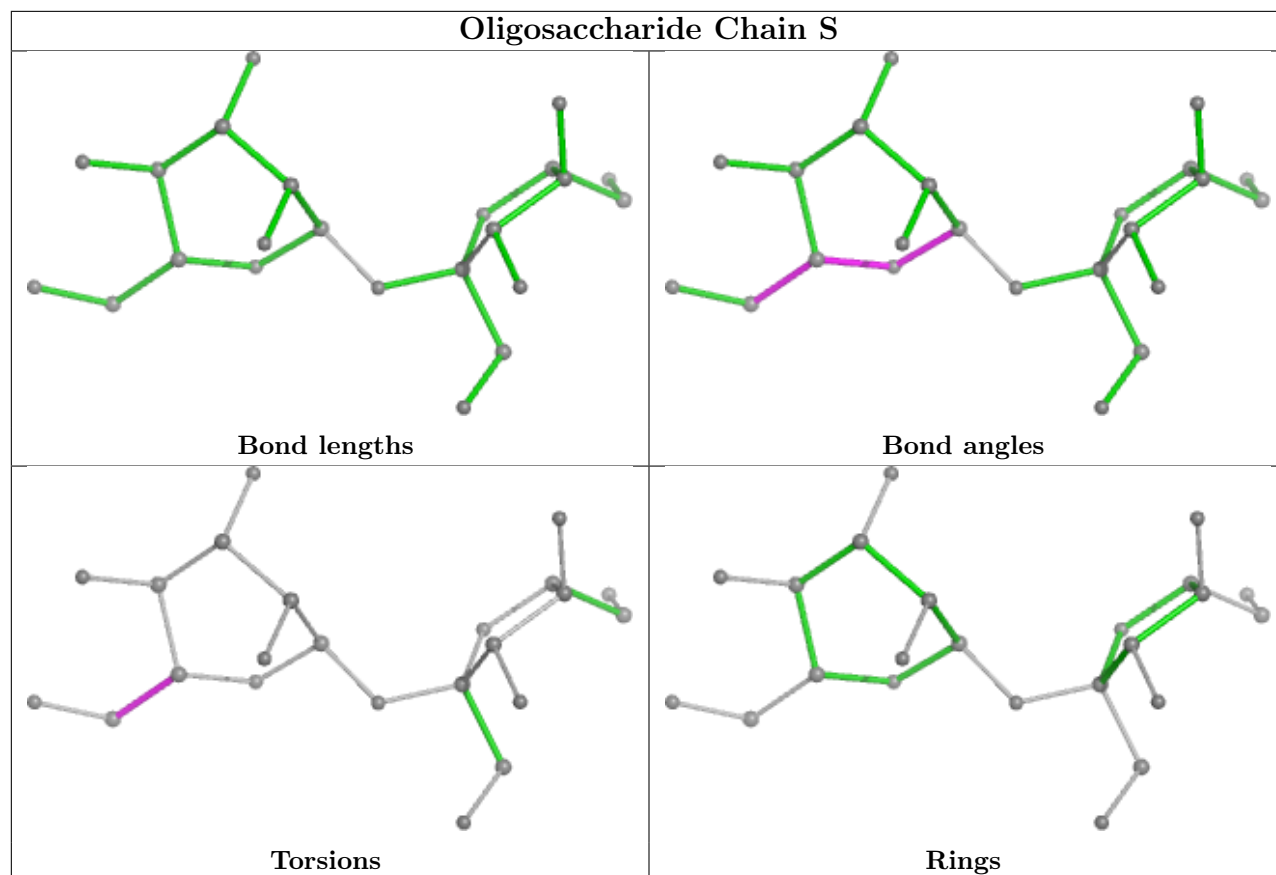
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

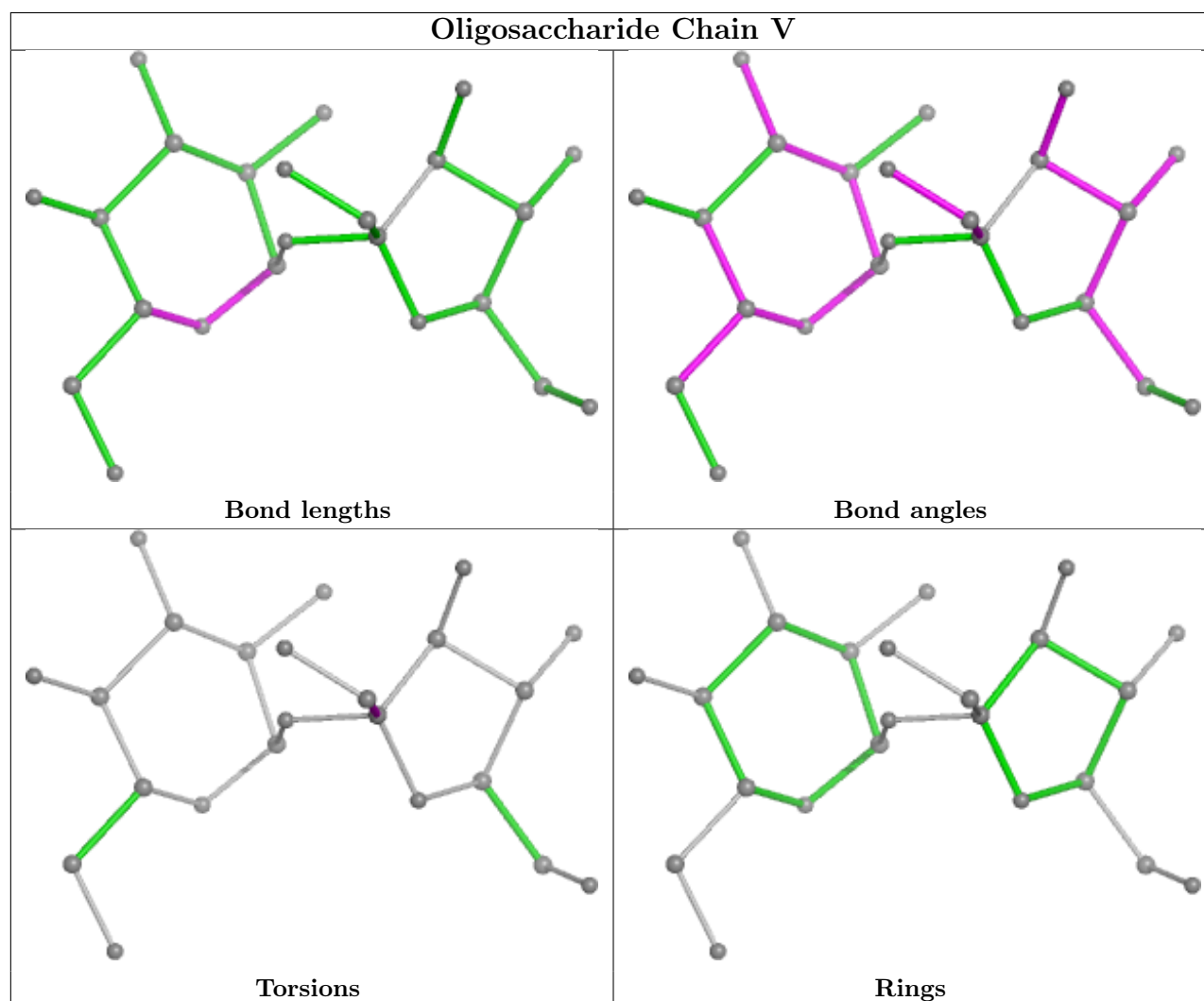
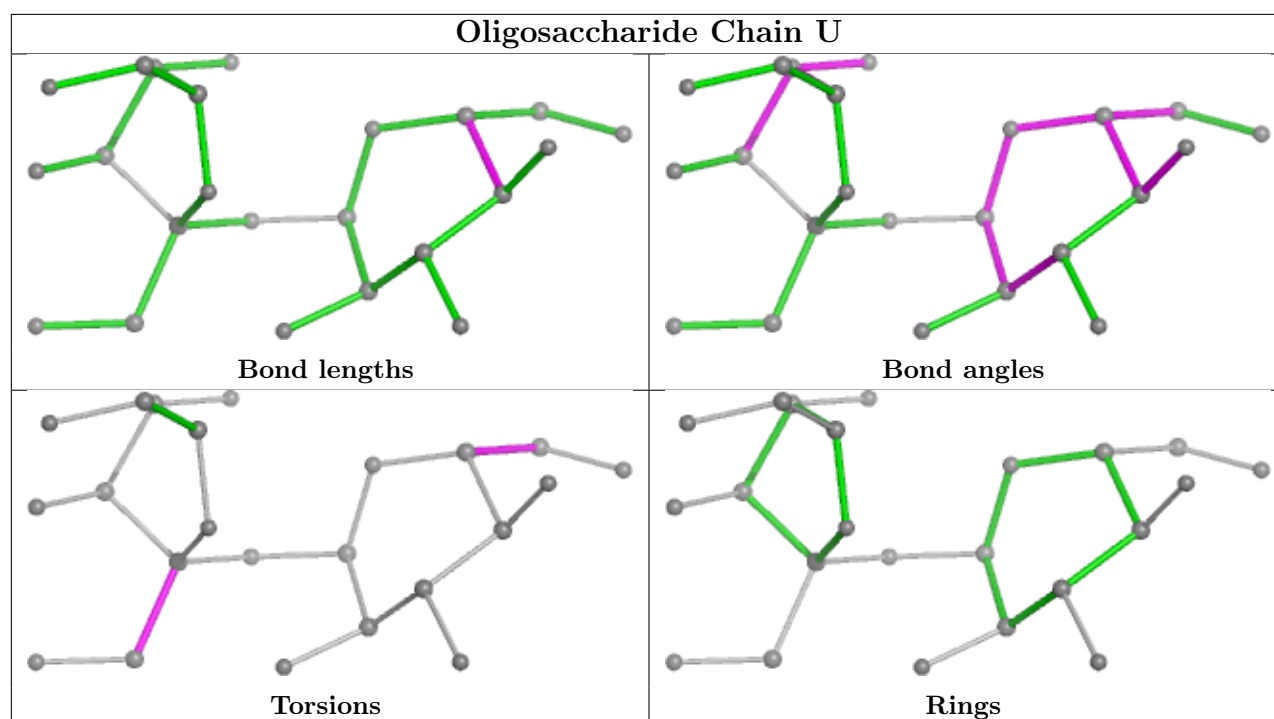




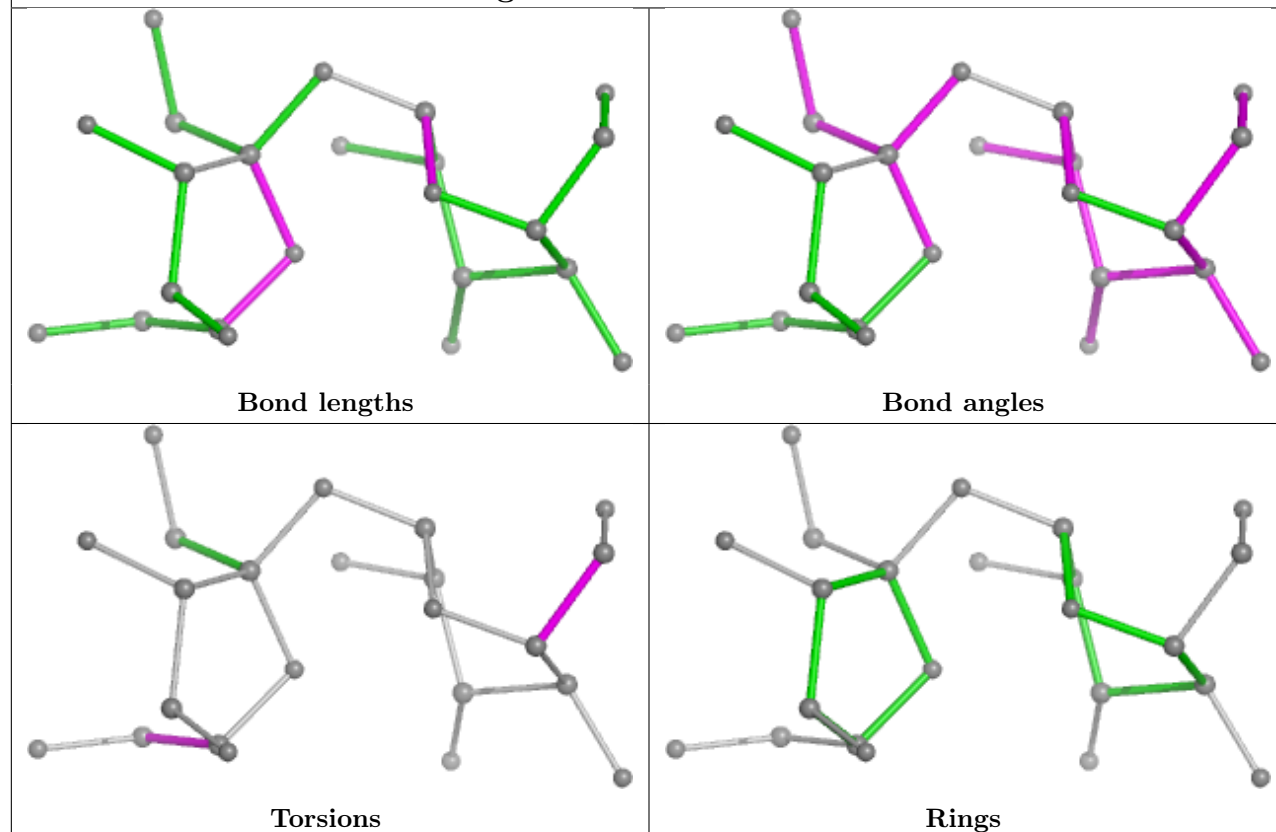




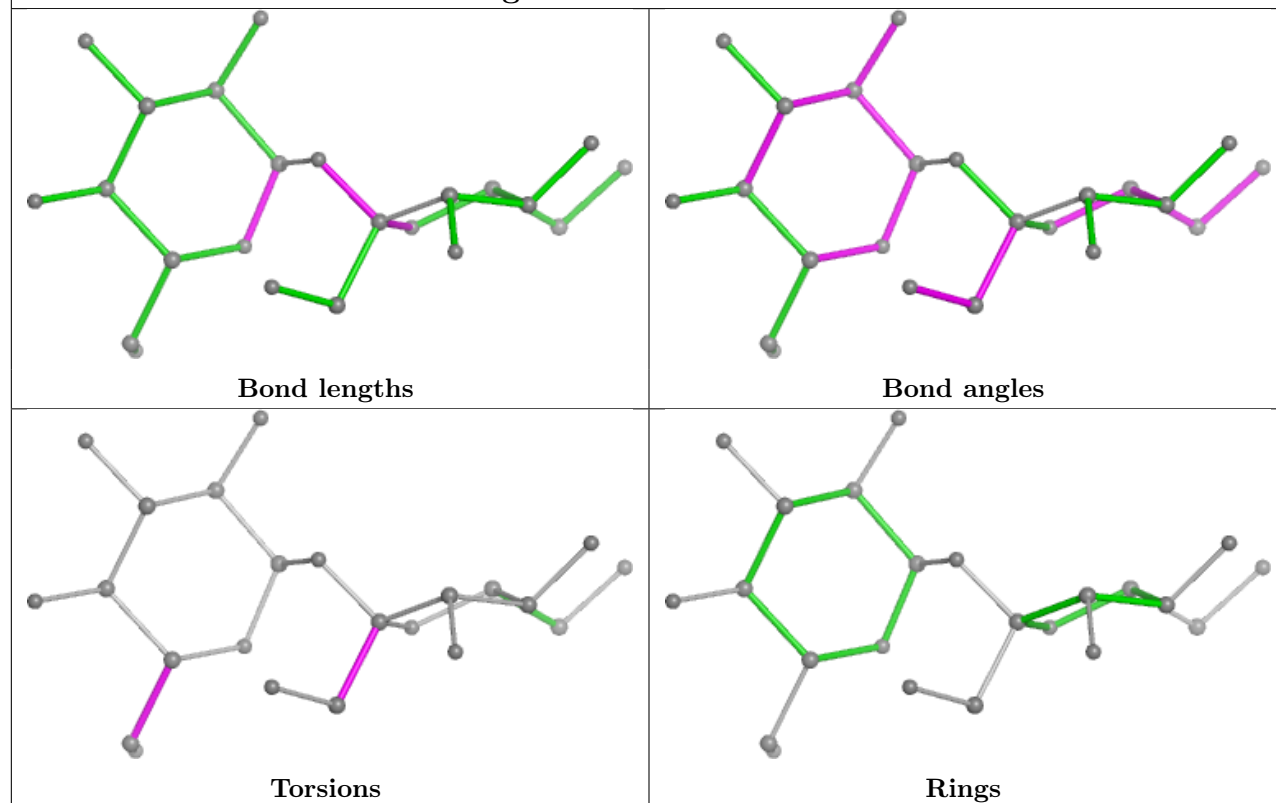


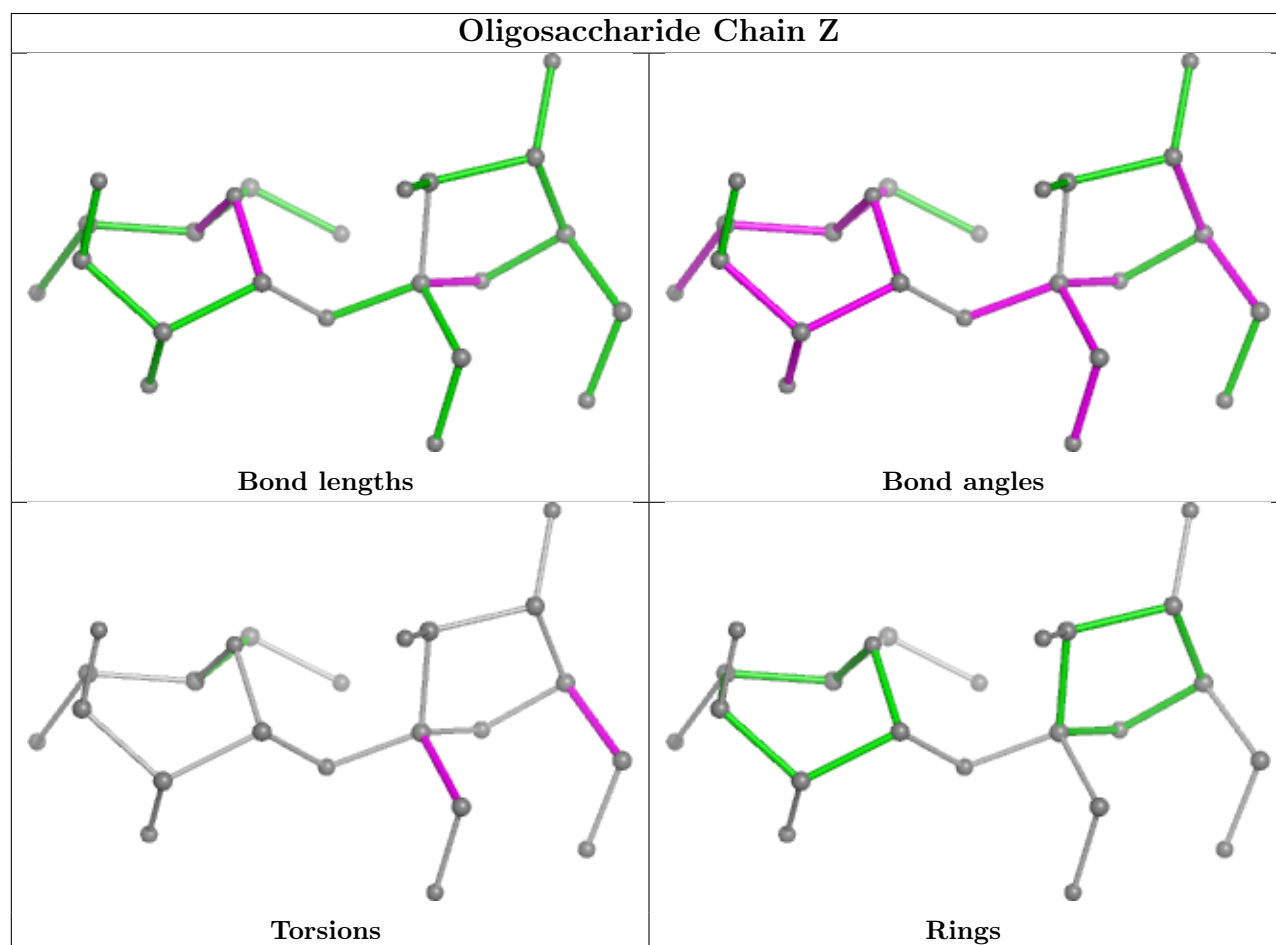
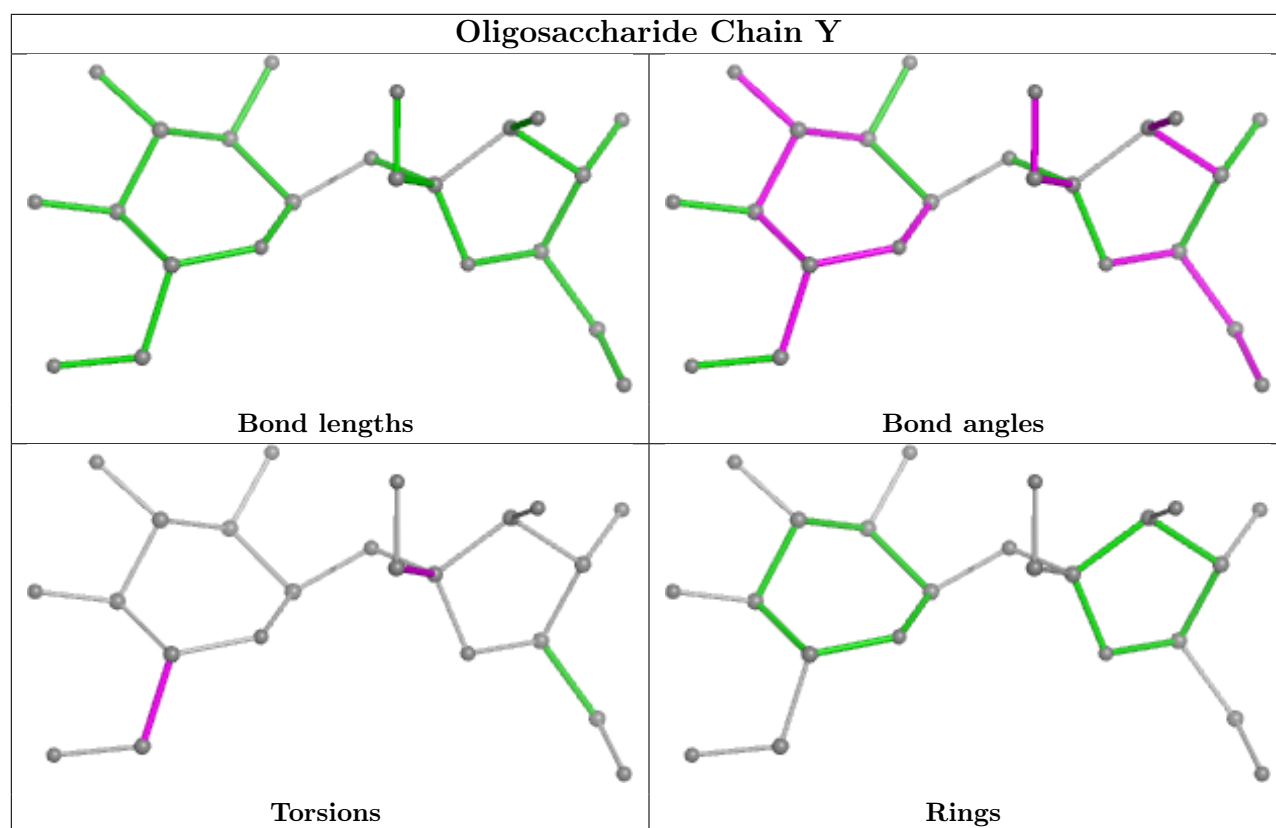


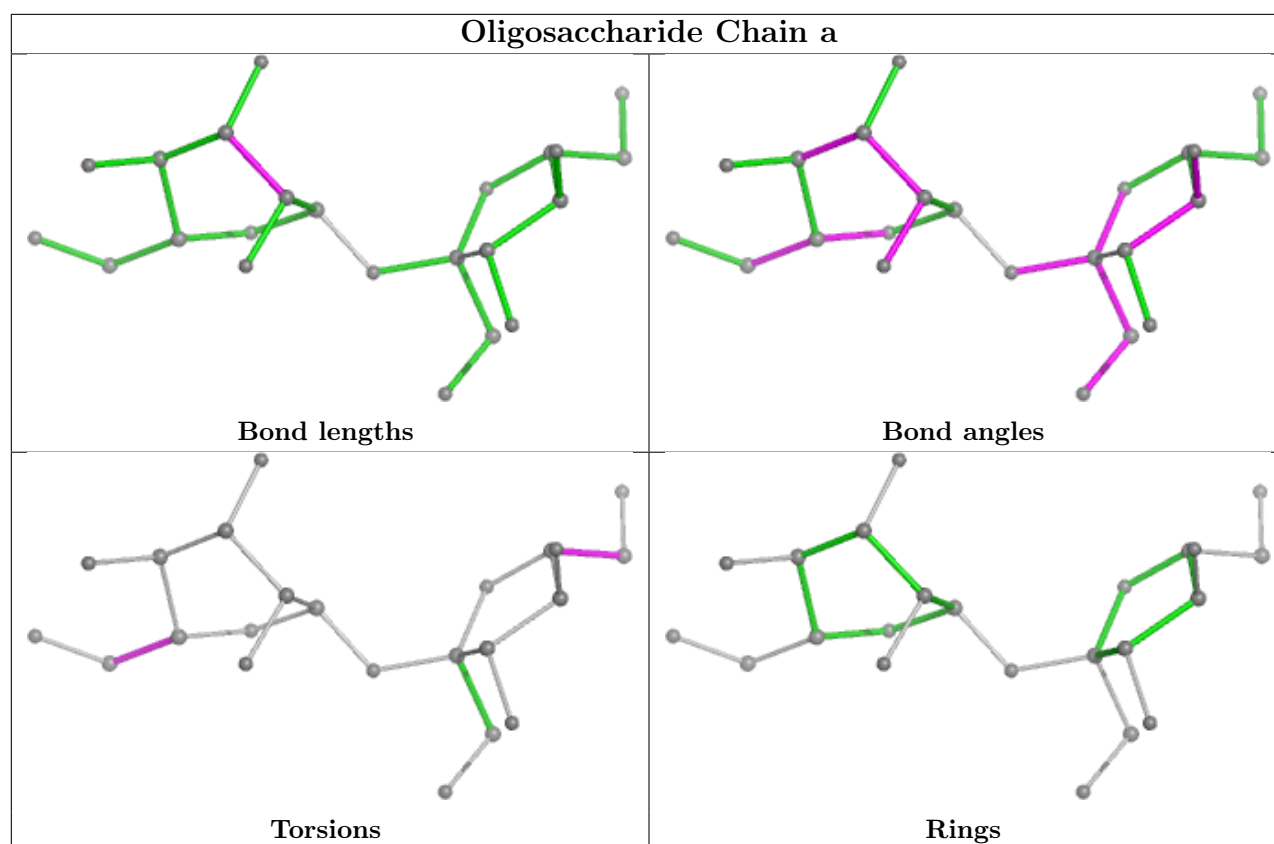
Oligosaccharide Chain W



Oligosaccharide Chain X







5.6 Ligand geometry [i](#)

Of 243 ligands modelled in this entry, 1 is unknown - leaving 242 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	CLA	3	3007	-	42,50,73	2.56	10 (23%)	48,85,113	2.73	19 (39%)
20	CLA	3	3011	-	65,73,73	2.13	11 (16%)	76,113,113	2.12	21 (27%)
21	LMU	A	7010	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
21	LMU	L	1171	-	36,36,36	0.99	3 (8%)	47,47,47	1.48	8 (17%)
20	CLA	A	1766	-	45,53,73	2.76	13 (28%)	52,89,113	2.81	19 (36%)
20	CLA	I	1031	-	60,68,73	2.30	12 (20%)	70,107,113	2.45	18 (25%)
20	CLA	1	1192	-	61,69,73	2.30	14 (22%)	71,108,113	2.34	23 (32%)
20	CLA	2	1224	-	65,73,73	2.24	15 (23%)	76,113,113	2.51	22 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	3	1213	-	27,32,73	2.59	13 (48%)	30,54,113	3.54	17 (56%)
20	CLA	4	4007	-	52,60,73	2.49	12 (23%)	60,97,113	2.60	20 (33%)
20	CLA	A	1800	-	65,73,73	2.18	13 (20%)	76,113,113	2.41	23 (30%)
21	LMU	3	7005	-	36,36,36	0.41	0	47,47,47	0.68	1 (2%)
25	SF4	C	1083	7	0,12,12	-	-	-	-	-
20	CLA	B	1748	-	60,68,73	2.22	14 (23%)	70,107,113	2.33	22 (31%)
20	CLA	2	1214	-	27,32,73	2.14	11 (40%)	30,54,113	3.14	18 (60%)
20	CLA	A	1787	-	65,73,73	2.23	12 (18%)	76,113,113	2.24	21 (27%)
20	CLA	B	1764	20	45,53,73	2.78	14 (31%)	52,89,113	2.77	18 (34%)
22	BCR	L	1169	-	41,41,41	2.47	8 (19%)	56,56,56	5.72	20 (35%)
20	CLA	1	1187	1	46,54,73	2.91	21 (45%)	53,90,113	3.85	29 (54%)
20	CLA	A	1790	20	50,58,73	2.46	12 (24%)	58,95,113	2.51	19 (32%)
20	CLA	I	1033	-	55,63,73	2.45	11 (20%)	64,101,113	2.54	22 (34%)
20	CLA	4	4014	21	47,55,73	2.58	13 (27%)	54,91,113	2.57	16 (29%)
22	BCR	B	1776	-	41,41,41	1.87	5 (12%)	56,56,56	5.04	24 (42%)
20	CLA	B	1745	-	60,68,73	2.26	12 (20%)	70,107,113	2.14	19 (27%)
21	LMU	A	7009	-	35,35,36	0.41	0	46,46,47	0.70	1 (2%)
20	CLA	2	1221	-	27,32,73	2.10	8 (29%)	30,54,113	3.17	19 (63%)
21	LMU	A	7015	-	36,36,36	0.94	1 (2%)	47,47,47	1.35	7 (14%)
20	CLA	B	1735	-	65,73,73	2.19	13 (20%)	76,113,113	2.29	18 (23%)
20	CLA	B	1786	-	65,73,73	2.19	14 (21%)	76,113,113	2.50	24 (31%)
20	CLA	3	1212	-	35,44,73	2.78	10 (28%)	46,78,113	3.16	17 (36%)
20	CLA	B	1737	-	65,73,73	2.21	13 (20%)	76,113,113	2.68	29 (38%)
20	CLA	2	1212	-	51,59,73	2.47	13 (25%)	59,96,113	2.56	18 (30%)
21	LMU	2	7006	-	36,36,36	0.39	0	47,47,47	0.69	1 (2%)
20	CLA	B	1736	-	45,53,73	2.64	12 (26%)	52,89,113	2.83	17 (32%)
21	LMU	4	1210	-	36,36,36	0.86	1 (2%)	47,47,47	1.18	3 (6%)
20	CLA	3	1219	-	65,73,73	2.18	13 (20%)	76,113,113	2.29	18 (23%)
20	CLA	A	1775	-	35,44,73	2.81	10 (28%)	46,78,113	3.48	16 (34%)
22	BCR	B	1779	-	41,41,41	2.79	13 (31%)	56,56,56	6.08	31 (55%)
20	CLA	1	1191	-	35,44,73	2.95	10 (28%)	46,78,113	3.34	18 (39%)
20	CLA	A	1799	-	50,58,73	2.53	10 (20%)	58,95,113	2.43	19 (32%)
20	CLA	B	1750	-	50,58,73	2.43	12 (24%)	58,95,113	2.67	20 (34%)
20	CLA	B	1769	-	47,55,73	2.52	15 (31%)	54,91,113	2.55	17 (31%)
20	CLA	2	1215	-	50,58,73	2.49	13 (26%)	58,95,113	2.36	19 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	1785	-	65,73,73	2.20	15 (23%)	76,113,113	2.47	25 (32%)
20	CLA	A	1801	-	55,63,73	2.47	11 (20%)	64,101,113	2.50	20 (31%)
22	BCR	B	1774	-	41,41,41	1.95	4 (9%)	56,56,56	5.90	21 (37%)
20	CLA	A	1767	-	65,73,73	2.26	12 (18%)	76,113,113	2.50	24 (31%)
20	CLA	F	1156	20	41,49,73	2.71	13 (31%)	47,84,113	2.74	15 (31%)
20	CLA	3	1214	-	27,32,73	2.17	9 (33%)	30,54,113	3.19	19 (63%)
21	LMU	A	7031	-	36,36,36	1.09	1 (2%)	47,47,47	1.28	6 (12%)
20	CLA	B	1743	-	65,73,73	2.28	15 (23%)	76,113,113	2.27	22 (28%)
20	CLA	B	1746	-	46,54,73	2.58	12 (26%)	53,90,113	2.68	17 (32%)
21	LMU	A	7043	19	36,36,36	0.76	0	47,47,47	2.25	17 (36%)
20	CLA	4	1196	-	55,63,73	2.38	13 (23%)	64,101,113	2.46	19 (29%)
22	BCR	3	1220	-	41,41,41	2.06	5 (12%)	56,56,56	5.90	22 (39%)
20	CLA	F	1155	-	35,44,73	2.80	10 (28%)	46,78,113	3.13	23 (50%)
21	LMU	1	1202	-	36,36,36	0.40	0	47,47,47	0.69	1 (2%)
20	CLA	4	1207	-	35,44,73	2.70	10 (28%)	46,78,113	3.61	20 (43%)
21	LMU	2	1225	-	36,36,36	0.89	1 (2%)	47,47,47	0.92	2 (4%)
20	CLA	B	1741	-	54,62,73	2.61	12 (22%)	67,100,113	2.90	24 (35%)
20	CLA	A	1763	-	46,54,73	2.54	11 (23%)	53,90,113	2.50	19 (35%)
20	CLA	3	1215	-	27,32,73	2.14	9 (33%)	30,54,113	3.20	19 (63%)
20	CLA	A	1783	-	65,73,73	2.19	12 (18%)	76,113,113	2.44	25 (32%)
20	CLA	R	1055	-	65,73,73	2.32	13 (20%)	76,113,113	2.33	24 (31%)
22	BCR	A	1808	-	41,41,41	1.93	4 (9%)	56,56,56	5.91	21 (37%)
20	CLA	1	1189	-	47,55,73	2.60	11 (23%)	54,91,113	2.97	20 (37%)
20	CLA	A	1791	5	45,53,73	2.62	13 (28%)	52,89,113	2.62	15 (28%)
20	CLA	3	1218	-	65,73,73	2.55	22 (33%)	76,113,113	2.92	23 (30%)
20	CLA	B	1738	-	65,73,73	2.28	16 (24%)	76,113,113	2.64	31 (40%)
20	CLA	R	1054	-	57,65,73	2.39	12 (21%)	66,103,113	2.61	23 (34%)
20	CLA	B	1763	-	50,58,73	2.64	17 (34%)	58,95,113	2.85	22 (37%)
20	CLA	1	1200	-	51,59,73	2.96	22 (43%)	59,96,113	3.27	29 (49%)
21	LMU	A	7030	-	36,36,36	0.91	1 (2%)	47,47,47	2.29	15 (31%)
20	CLA	A	1760	-	55,63,73	2.43	12 (21%)	64,101,113	2.28	21 (32%)
20	CLA	B	1747	-	59,67,73	2.32	13 (22%)	68,105,113	2.14	21 (30%)
20	CLA	1	1196	1	35,44,73	2.84	10 (28%)	46,78,113	3.31	17 (36%)
20	CLA	A	1777	-	51,59,73	2.51	13 (25%)	59,96,113	2.57	19 (32%)
22	BCR	A	1807	-	41,41,41	1.94	3 (7%)	56,56,56	5.91	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	2	1216	-	27,32,73	2.23	11 (40%)	30,54,113	3.29	18 (60%)
21	LMU	B	1782	-	26,26,36	1.04	1 (3%)	37,37,47	1.42	6 (16%)
20	CLA	B	1758	-	65,73,73	2.27	17 (26%)	76,113,113	2.57	23 (30%)
20	CLA	B	1755	-	58,66,73	2.31	13 (22%)	67,104,113	2.42	19 (28%)
21	LMU	A	7040	-	36,36,36	0.97	3 (8%)	47,47,47	2.46	13 (27%)
20	CLA	A	1788	-	65,73,73	2.28	15 (23%)	76,113,113	2.29	20 (26%)
20	CLA	A	1769	-	54,62,73	2.25	12 (22%)	62,99,113	2.50	22 (35%)
20	CLA	B	1759	-	65,73,73	2.21	15 (23%)	76,113,113	2.57	20 (26%)
20	CLA	B	1770	-	65,73,73	2.22	13 (20%)	76,113,113	2.45	23 (30%)
21	LMU	R	1057	-	36,36,36	1.16	2 (5%)	47,47,47	2.44	14 (29%)
20	CLA	G	1099	-	51,59,73	2.55	12 (23%)	59,96,113	2.57	23 (38%)
20	CLA	4	1203	-	27,32,73	2.17	9 (33%)	30,54,113	3.27	17 (56%)
22	BCR	A	1804	-	41,41,41	1.93	3 (7%)	56,56,56	5.91	21 (37%)
20	CLA	3	1217	-	27,32,73	2.36	10 (37%)	30,54,113	3.33	18 (60%)
20	CLA	A	1811	-	65,73,73	2.20	15 (23%)	76,113,113	2.30	21 (27%)
20	CLA	A	1813	-	65,73,73	2.39	14 (21%)	76,113,113	2.47	21 (27%)
20	CLA	4	1206	-	27,32,73	2.29	7 (25%)	30,54,113	3.31	18 (60%)
20	CLA	B	1753	-	65,73,73	3.07	27 (41%)	76,113,113	2.58	21 (27%)
20	CLA	1	1198	-	61,69,73	2.37	19 (31%)	71,108,113	2.51	24 (33%)
20	CLA	B	1787	-	65,73,73	2.32	14 (21%)	76,113,113	2.38	23 (30%)
20	CLA	A	1759	-	50,58,73	2.41	12 (24%)	58,95,113	2.85	22 (37%)
21	LMU	A	7041	-	36,36,36	0.62	0	47,47,47	1.90	13 (27%)
21	LMU	K	1086	20	36,36,36	0.75	0	47,47,47	2.27	12 (25%)
20	CLA	K	1146	-	50,58,73	2.92	20 (40%)	58,95,113	2.99	24 (41%)
20	CLA	L	1505	-	55,63,73	2.40	11 (20%)	64,101,113	2.59	17 (26%)
20	CLA	A	1789	-	65,73,73	2.27	12 (18%)	76,113,113	2.57	26 (34%)
20	CLA	1	1199	-	27,32,73	2.20	9 (33%)	30,54,113	3.21	19 (63%)
20	CLA	4	1200	-	50,58,73	2.60	13 (26%)	58,95,113	2.55	16 (27%)
20	CLA	4	1198	-	65,73,73	2.57	23 (35%)	76,113,113	3.36	33 (43%)
20	CLA	1	1188	-	47,55,73	2.57	11 (23%)	54,91,113	2.70	19 (35%)
20	CLA	2	1218	20	65,73,73	2.21	11 (16%)	76,113,113	2.34	22 (28%)
20	CLA	B	1751	-	46,54,73	2.52	10 (21%)	53,90,113	2.95	17 (32%)
21	LMU	A	7032	-	36,36,36	0.99	3 (8%)	47,47,47	2.76	19 (40%)
21	LMU	A	7047	-	36,36,36	1.11	1 (2%)	47,47,47	1.34	3 (6%)
20	CLA	J	1046	-	27,32,73	2.13	11 (40%)	30,54,113	2.99	16 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	BCR	A	1803	-	41,41,41	1.93	4 (9%)	56,56,56	5.91	20 (35%)
22	BCR	I	1032	-	41,41,41	2.67	8 (19%)	56,56,56	6.54	28 (50%)
20	CLA	2	1223	-	50,58,73	2.58	13 (26%)	58,95,113	2.77	19 (32%)
20	CLA	H	1079	-	65,73,73	2.27	12 (18%)	76,113,113	2.39	22 (28%)
20	CLA	1	1201	-	27,32,73	2.46	9 (33%)	30,54,113	3.65	18 (60%)
20	CLA	B	1754	-	54,62,73	2.46	16 (29%)	62,99,113	2.47	25 (40%)
22	BCR	A	1805	-	41,41,41	1.94	4 (9%)	56,56,56	5.91	21 (37%)
20	CLA	B	1766	-	51,59,73	2.57	11 (21%)	59,96,113	2.62	19 (32%)
22	BCR	B	1778	-	41,41,41	1.94	3 (7%)	56,56,56	5.91	21 (37%)
20	CLA	B	1771	-	65,73,73	2.15	12 (18%)	76,113,113	2.19	22 (28%)
21	LMU	A	7017	-	36,36,36	0.70	2 (5%)	47,47,47	2.40	15 (31%)
22	BCR	A	1806	-	41,41,41	1.94	3 (7%)	56,56,56	5.91	21 (37%)
20	CLA	A	1796	-	65,73,73	2.18	13 (20%)	76,113,113	2.28	18 (23%)
20	CLA	2	1227	-	27,32,73	2.51	14 (51%)	30,54,113	3.29	19 (63%)
20	CLA	B	1785	-	65,73,73	2.20	15 (23%)	76,113,113	2.39	28 (36%)
20	CLA	L	1167	22	47,55,73	2.51	11 (23%)	54,91,113	3.01	24 (44%)
21	LMU	A	7034	20	36,36,36	0.85	1 (2%)	47,47,47	1.23	4 (8%)
21	LMU	A	7019	-	36,36,36	1.03	1 (2%)	47,47,47	1.41	8 (17%)
20	CLA	A	1762	-	57,65,73	2.35	13 (22%)	66,103,113	2.49	20 (30%)
20	CLA	J	1044	20	61,69,73	2.44	23 (37%)	71,108,113	2.68	28 (39%)
21	LMU	2	7003	-	36,36,36	0.39	0	47,47,47	0.69	1 (2%)
20	CLA	A	1798	-	55,63,73	2.38	12 (21%)	64,101,113	2.51	19 (29%)
21	LMU	A	7028	-	36,36,36	0.74	2 (5%)	47,47,47	1.89	17 (36%)
20	CLA	4	1209	-	46,54,73	2.79	20 (43%)	53,90,113	2.70	20 (37%)
21	LMU	A	7016	-	36,36,36	0.63	1 (2%)	47,47,47	1.89	11 (23%)
23	PQN	B	1773	-	34,34,34	1.66	2 (5%)	42,45,45	1.59	6 (14%)
20	CLA	L	1166	16	50,58,73	2.50	11 (22%)	58,95,113	2.48	18 (31%)
20	CLA	3	1216	-	27,32,73	2.20	10 (37%)	30,54,113	3.04	17 (56%)
20	CLA	4	1204	-	55,63,73	2.45	12 (21%)	64,101,113	2.54	20 (31%)
20	CLA	J	1043	-	61,69,73	2.25	13 (21%)	71,108,113	2.35	18 (25%)
21	LMU	A	7027	-	36,36,36	1.12	1 (2%)	47,47,47	1.91	14 (29%)
20	CLA	1	1193	-	51,59,73	2.58	14 (27%)	59,96,113	3.19	27 (45%)
20	CLA	4	1208	4	27,32,73	2.05	9 (33%)	30,54,113	2.88	16 (53%)
20	CLA	A	1776	-	65,73,73	2.17	12 (18%)	76,113,113	2.36	21 (27%)
20	CLA	B	1757	-	65,73,73	2.35	13 (20%)	76,113,113	2.59	23 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	1765	-	55,63,73	2.38	11 (20%)	64,101,113	2.67	24 (37%)
20	CLA	F	1157	20	53,61,73	2.87	21 (39%)	61,98,113	2.57	23 (37%)
20	CLA	4	1205	-	27,32,73	2.15	9 (33%)	30,54,113	3.23	19 (63%)
20	CLA	2	1217	-	65,73,73	2.21	12 (18%)	76,113,113	2.44	20 (26%)
20	CLA	3	3014	-	27,32,73	2.33	10 (37%)	30,54,113	3.39	20 (66%)
20	CLA	B	1762	-	65,73,73	2.29	16 (24%)	76,113,113	2.59	23 (30%)
22	BCR	B	1777	-	41,41,41	1.95	4 (9%)	56,56,56	5.90	21 (37%)
20	CLA	A	1793	-	65,73,73	2.19	13 (20%)	76,113,113	2.29	18 (23%)
25	SF4	C	1082	7	0,12,12	-	-	-	-	-
20	CLA	4	1202	-	27,32,73	2.18	9 (33%)	30,54,113	3.22	19 (63%)
21	LMU	R	1056	-	36,36,36	0.39	0	47,47,47	0.69	1 (2%)
20	CLA	4	1197	-	35,44,73	3.02	13 (37%)	46,78,113	3.85	21 (45%)
21	LMU	A	7039	-	36,36,36	0.99	2 (5%)	47,47,47	2.57	12 (25%)
20	CLA	3	3002	-	27,32,73	2.20	9 (33%)	30,54,113	3.08	16 (53%)
20	CLA	4	1201	-	52,60,73	3.09	26 (50%)	60,97,113	3.72	37 (61%)
20	CLA	B	1772	-	35,44,73	2.85	12 (34%)	46,78,113	3.56	21 (45%)
20	CLA	A	1773	-	52,60,73	2.50	12 (23%)	60,97,113	2.66	20 (33%)
20	CLA	3	3008	-	50,58,73	2.55	17 (34%)	58,95,113	2.87	24 (41%)
20	CLA	B	1767	-	60,68,73	2.24	11 (18%)	70,107,113	2.72	15 (21%)
20	CLA	B	1742	-	55,63,73	2.29	14 (25%)	64,101,113	2.49	19 (29%)
20	CLA	A	1816	-	55,63,73	2.95	22 (40%)	64,101,113	3.52	27 (42%)
20	CLA	A	1774	-	65,73,73	2.19	13 (20%)	76,113,113	2.21	22 (28%)
20	CLA	B	1749	-	61,69,73	2.19	13 (21%)	71,108,113	2.47	23 (32%)
20	CLA	2	1220	20	56,64,73	2.48	17 (30%)	65,102,113	2.60	23 (35%)
20	CLA	2	1219	-	27,32,73	2.12	8 (29%)	30,54,113	3.13	18 (60%)
22	BCR	L	1170	20	41,41,41	3.29	19 (46%)	56,56,56	6.44	27 (48%)
20	CLA	B	1756	-	65,73,73	2.19	13 (20%)	76,113,113	2.29	18 (23%)
20	CLA	A	1792	-	51,59,73	2.48	13 (25%)	59,96,113	2.56	18 (30%)
20	CLA	A	1768	-	54,62,73	2.37	12 (22%)	62,99,113	2.30	16 (25%)
20	CLA	3	3001	-	27,32,73	2.23	9 (33%)	30,54,113	3.18	18 (60%)
20	CLA	A	1781	-	65,73,73	2.19	13 (20%)	76,113,113	2.29	18 (23%)
20	CLA	A	1786	-	50,58,73	2.52	11 (22%)	58,95,113	2.72	23 (39%)
21	LMU	A	1809	-	36,36,36	0.94	0	47,47,47	1.38	7 (14%)
24	LMG	B	1783	-	49,49,55	0.95	2 (4%)	57,57,63	1.01	3 (5%)
20	CLA	K	1142	-	45,53,73	2.61	13 (28%)	52,89,113	2.62	15 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	LMU	A	7035	-	36,36,36	0.84	1 (2%)	47,47,47	1.58	8 (17%)
20	CLA	2	1222	2	50,58,73	2.54	11 (22%)	58,95,113	2.71	19 (32%)
20	CLA	4	1199	-	55,63,73	2.36	11 (20%)	64,101,113	2.55	20 (31%)
20	CLA	B	1739	-	65,73,73	2.29	13 (20%)	76,113,113	2.43	22 (28%)
20	CLA	B	1740	6	65,73,73	2.14	13 (20%)	76,113,113	2.40	21 (27%)
20	CLA	K	1085	21	50,58,73	2.50	13 (26%)	58,95,113	2.58	18 (31%)
22	BCR	B	1780	-	41,41,41	1.93	3 (7%)	56,56,56	5.92	21 (37%)
20	CLA	1	1194	-	27,32,73	2.07	9 (33%)	30,54,113	3.15	20 (66%)
20	CLA	A	1764	5	65,73,73	2.27	13 (20%)	76,113,113	2.56	25 (32%)
20	CLA	B	1765	20	45,53,73	2.69	12 (26%)	52,89,113	2.72	18 (34%)
20	CLA	3	3015	-	27,32,73	2.14	8 (29%)	30,54,113	3.01	18 (60%)
20	CLA	A	1771	-	50,58,73	2.61	12 (24%)	58,95,113	2.42	22 (37%)
20	CLA	A	1770	-	45,53,73	2.69	12 (26%)	52,89,113	2.37	16 (30%)
20	CLA	A	1779	-	55,63,73	2.40	12 (21%)	64,101,113	2.48	20 (31%)
20	CLA	2	2010	-	27,32,73	2.24	10 (37%)	30,54,113	2.90	17 (56%)
20	CLA	A	1815	-	55,63,73	2.46	12 (21%)	64,101,113	2.68	24 (37%)
20	CLA	A	1794	-	47,55,73	2.57	13 (27%)	54,91,113	2.58	16 (29%)
20	CLA	B	1760	-	50,58,73	2.70	13 (26%)	58,95,113	2.34	21 (36%)
20	CLA	B	1768	-	65,73,73	2.17	12 (18%)	76,113,113	2.31	17 (22%)
22	BCR	B	1775	-	41,41,41	1.94	4 (9%)	56,56,56	5.90	21 (37%)
20	CLA	L	1168	-	50,58,73	2.65	17 (34%)	58,95,113	2.95	20 (34%)
21	LMU	A	1810	-	36,36,36	0.94	1 (2%)	47,47,47	1.65	10 (21%)
21	LMU	A	7023	-	36,36,36	0.68	1 (2%)	47,47,47	1.97	17 (36%)
20	CLA	J	1045	20	55,63,73	2.54	18 (32%)	64,101,113	2.67	21 (32%)
20	CLA	A	1784	-	55,63,73	2.39	13 (23%)	64,101,113	2.39	20 (31%)
20	CLA	B	1752	-	55,63,73	2.53	14 (25%)	64,101,113	2.40	19 (29%)
21	LMU	A	7033	-	36,36,36	1.02	2 (5%)	47,47,47	2.25	13 (27%)
21	LMU	A	7037	-	36,36,36	0.90	2 (5%)	47,47,47	3.08	22 (46%)
20	CLA	A	1761	-	65,73,73	2.21	13 (20%)	76,113,113	2.34	21 (27%)
20	CLA	A	1817	-	46,54,73	2.80	14 (30%)	57,90,113	4.09	29 (50%)
20	CLA	B	1744	-	65,73,73	2.28	11 (16%)	76,113,113	2.15	21 (27%)
20	CLA	A	1772	-	65,73,73	2.28	16 (24%)	76,113,113	2.44	24 (31%)
20	CLA	1	1197	-	51,59,73	3.04	25 (49%)	59,96,113	3.90	27 (45%)
20	CLA	2	1213	-	56,64,73	2.37	12 (21%)	65,102,113	2.66	25 (38%)
20	CLA	A	1780	-	65,73,73	2.10	10 (15%)	76,113,113	2.16	21 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	K	3009	-	65,73,73	2.23	12 (18%)	76,113,113	2.17	22 (28%)
21	LMU	A	7042	-	36,36,36	0.48	0	47,47,47	2.05	16 (34%)
21	LMU	A	7013	-	36,36,36	0.45	0	47,47,47	1.62	9 (19%)
20	CLA	B	1761	-	50,58,73	2.40	11 (22%)	58,95,113	2.65	21 (36%)
21	LMU	A	7020	-	36,36,36	0.41	0	47,47,47	1.75	12 (25%)
21	LMU	A	7036	-	35,35,36	1.21	5 (14%)	46,46,47	2.34	15 (32%)
20	CLA	A	1778	5	42,50,73	2.66	12 (28%)	48,85,113	2.93	16 (33%)
21	LMU	1	7004	-	36,36,36	0.40	0	47,47,47	0.69	1 (2%)
22	BCR	B	1781	-	41,41,41	2.68	17 (41%)	56,56,56	5.37	31 (55%)
20	CLA	1	1190	-	46,54,73	2.69	13 (28%)	53,90,113	2.47	18 (33%)
21	LMU	A	7026	19	36,36,36	1.23	3 (8%)	47,47,47	3.10	22 (46%)
23	PQN	A	1802	-	34,34,34	1.77	3 (8%)	42,45,45	1.49	6 (14%)
20	CLA	4	4003	-	27,32,73	2.15	10 (37%)	30,54,113	2.89	17 (56%)
21	LMU	A	7022	-	36,36,36	0.70	0	47,47,47	2.16	16 (34%)
21	LMU	A	7025	-	36,36,36	0.96	1 (2%)	47,47,47	1.58	10 (21%)
21	LMU	A	7021	-	36,36,36	0.76	0	47,47,47	2.07	14 (29%)
25	SF4	B	1784	6,5	0,12,12	-	-	-	-	-
20	CLA	A	1795	-	51,59,73	2.47	13 (25%)	59,96,113	2.56	18 (30%)
20	CLA	A	1797	-	65,73,73	2.19	13 (20%)	76,113,113	2.29	18 (23%)
20	CLA	1	1195	-	35,44,73	3.61	19 (54%)	46,78,113	4.32	19 (41%)
20	CLA	A	1812	-	65,73,73	2.24	15 (23%)	76,113,113	2.24	19 (25%)
21	LMU	A	7038	-	36,36,36	0.65	0	47,47,47	2.41	15 (31%)
21	LMU	A	7024	-	36,36,36	0.97	2 (5%)	47,47,47	1.63	10 (21%)
20	CLA	A	1782	20	65,73,73	2.18	13 (20%)	76,113,113	2.29	18 (23%)

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
20	CLA	3	3007	-	1/1/10/20	5/10/88/115	-
20	CLA	3	3011	-	2/2/15/20	20/37/115/115	-
21	LMU	A	7010	-	-	19/21/61/61	0/2/2/2
21	LMU	L	1171	-	-	14/21/61/61	0/2/2/2
20	CLA	A	1766	-	1/1/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	I	1031	-	2/2/14/20	13/31/109/115	-
20	CLA	1	1192	-	2/2/14/20	20/33/111/115	-
20	CLA	2	1224	-	2/2/15/20	17/37/115/115	-
20	CLA	3	1213	-	1/1/4/20	-	-
20	CLA	4	4007	-	1/1/12/20	8/22/100/115	-
20	CLA	A	1800	-	2/2/15/20	16/37/115/115	-
21	LMU	3	7005	-	-	18/21/61/61	0/2/2/2
25	SF4	C	1083	7	-	-	0/6/5/5
20	CLA	B	1748	-	2/2/14/20	13/31/109/115	-
20	CLA	2	1214	-	1/1/4/20	-	-
20	CLA	A	1787	-	2/2/15/20	15/37/115/115	-
20	CLA	B	1764	20	1/1/11/20	11/13/91/115	-
22	BCR	L	1169	-	-	12/29/63/63	0/2/2/2
20	CLA	1	1187	1	1/1/11/20	10/15/93/115	-
20	CLA	A	1790	20	1/1/12/20	12/19/97/115	-
20	CLA	I	1033	-	2/2/13/20	9/25/103/115	-
20	CLA	4	4014	21	1/1/11/20	9/16/94/115	-
22	BCR	B	1776	-	-	11/29/63/63	0/2/2/2
20	CLA	B	1745	-	2/2/14/20	14/31/109/115	-
21	LMU	A	7009	-	-	15/20/60/61	0/2/2/2
20	CLA	2	1221	-	1/1/4/20	-	-
21	LMU	A	7015	-	-	14/21/61/61	0/2/2/2
20	CLA	B	1735	-	2/2/15/20	23/37/115/115	-
20	CLA	B	1786	-	2/2/15/20	15/37/115/115	-
20	CLA	3	1212	-	1/1/9/20	-	-
20	CLA	B	1737	-	2/2/15/20	22/37/115/115	-
20	CLA	2	1212	-	1/1/12/20	11/21/99/115	-
21	LMU	2	7006	-	-	14/21/61/61	0/2/2/2
20	CLA	B	1736	-	1/1/11/20	6/13/91/115	-
21	LMU	4	1210	-	-	13/21/61/61	0/2/2/2
20	CLA	3	1219	-	2/2/15/20	21/37/115/115	-
20	CLA	A	1775	-	1/1/9/20	-	-
22	BCR	B	1779	-	-	12/29/63/63	0/2/2/2
20	CLA	1	1191	-	1/1/9/20	-	-
20	CLA	A	1799	-	1/1/12/20	10/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	1750	-	1/1/12/20	6/19/97/115	-
20	CLA	B	1769	-	1/1/11/20	6/16/94/115	-
20	CLA	2	1215	-	1/1/12/20	9/19/97/115	-
20	CLA	A	1785	-	2/2/15/20	18/37/115/115	-
20	CLA	A	1801	-	2/2/13/20	7/25/103/115	-
22	BCR	B	1774	-	-	10/29/63/63	0/2/2/2
20	CLA	A	1767	-	2/2/15/20	25/37/115/115	-
20	CLA	F	1156	20	1/1/10/20	5/8/86/115	-
20	CLA	3	1214	-	1/1/4/20	-	-
21	LMU	A	7031	-	-	13/21/61/61	0/2/2/2
20	CLA	B	1743	-	2/2/15/20	22/37/115/115	-
20	CLA	B	1746	-	1/1/11/20	9/15/93/115	-
21	LMU	A	7043	19	-	11/21/61/61	0/2/2/2
20	CLA	4	1196	-	2/2/13/20	14/25/103/115	-
22	BCR	3	1220	-	-	13/29/63/63	0/2/2/2
20	CLA	F	1155	-	1/1/9/20	-	-
21	LMU	1	1202	-	-	13/21/61/61	0/2/2/2
20	CLA	4	1207	-	1/1/9/20	-	-
21	LMU	2	1225	-	-	16/21/61/61	0/2/2/2
20	CLA	B	1741	-	2/2/13/20	11/25/101/115	-
20	CLA	A	1763	-	1/1/11/20	7/15/93/115	-
20	CLA	3	1215	-	1/1/4/20	-	-
20	CLA	A	1783	-	2/2/15/20	16/37/115/115	-
20	CLA	R	1055	-	2/2/15/20	20/37/115/115	-
22	BCR	A	1808	-	-	12/29/63/63	0/2/2/2
20	CLA	1	1189	-	1/1/11/20	8/16/94/115	-
20	CLA	A	1791	5	1/1/11/20	7/13/91/115	-
20	CLA	3	1218	-	2/2/15/20	19/37/115/115	-
20	CLA	B	1738	-	2/2/15/20	17/37/115/115	-
20	CLA	R	1054	-	2/2/13/20	13/28/106/115	-
20	CLA	B	1763	-	1/1/12/20	6/19/97/115	-
20	CLA	1	1200	-	3/3/12/20	12/21/99/115	-
21	LMU	A	7030	-	-	16/21/61/61	0/2/2/2
20	CLA	A	1760	-	2/2/13/20	12/25/103/115	-
20	CLA	B	1747	-	2/2/13/20	12/30/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	1	1196	1	1/1/9/20	-	-
20	CLA	A	1777	-	1/1/12/20	9/21/99/115	-
22	BCR	A	1807	-	-	10/29/63/63	0/2/2/2
20	CLA	2	1216	-	1/1/4/20	-	-
21	LMU	B	1782	-	-	4/11/51/61	0/2/2/2
20	CLA	B	1758	-	2/2/15/20	16/37/115/115	-
20	CLA	B	1755	-	2/2/13/20	17/29/107/115	-
21	LMU	A	7040	-	-	11/21/61/61	0/2/2/2
20	CLA	A	1788	-	2/2/15/20	21/37/115/115	-
20	CLA	A	1769	-	1/1/12/20	10/24/102/115	-
20	CLA	B	1759	-	2/2/15/20	27/37/115/115	-
20	CLA	B	1770	-	2/2/15/20	20/37/115/115	-
21	LMU	R	1057	-	1/1/10/10	11/21/61/61	0/2/2/2
20	CLA	G	1099	-	1/1/12/20	10/21/99/115	-
20	CLA	4	1203	-	1/1/4/20	-	-
22	BCR	A	1804	-	-	13/29/63/63	0/2/2/2
20	CLA	3	1217	-	1/1/4/20	-	-
20	CLA	A	1811	-	2/2/15/20	25/37/115/115	-
20	CLA	A	1813	-	2/2/15/20	24/37/115/115	-
20	CLA	4	1206	-	1/1/4/20	-	-
20	CLA	B	1753	-	1/1/15/20	19/37/115/115	-
20	CLA	1	1198	-	2/2/14/20	16/33/111/115	-
20	CLA	B	1787	-	2/2/15/20	18/37/115/115	-
20	CLA	A	1759	-	1/1/12/20	5/19/97/115	-
21	LMU	A	7041	-	-	12/21/61/61	0/2/2/2
21	LMU	K	1086	20	-	12/21/61/61	0/2/2/2
20	CLA	K	1146	-	1/1/12/20	9/19/97/115	-
20	CLA	L	1505	-	2/2/13/20	14/25/103/115	-
20	CLA	A	1789	-	2/2/15/20	22/37/115/115	-
20	CLA	1	1199	-	1/1/4/20	-	-
20	CLA	4	1200	-	1/1/12/20	6/19/97/115	-
20	CLA	4	1198	-	3/3/15/20	20/37/115/115	-
20	CLA	1	1188	-	1/1/11/20	8/16/94/115	-
20	CLA	2	1218	20	2/2/15/20	15/37/115/115	-
20	CLA	B	1751	-	1/1/11/20	13/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMU	A	7032	-	-	13/21/61/61	0/2/2/2
21	LMU	A	7047	-	-	8/21/61/61	0/2/2/2
20	CLA	J	1046	-	1/1/4/20	-	-
22	BCR	A	1803	-	-	12/29/63/63	0/2/2/2
22	BCR	I	1032	-	-	13/29/63/63	0/2/2/2
20	CLA	2	1223	-	1/1/12/20	11/19/97/115	-
20	CLA	H	1079	-	2/2/15/20	19/37/115/115	-
20	CLA	1	1201	-	1/1/4/20	-	-
20	CLA	B	1754	-	1/1/12/20	8/24/102/115	-
22	BCR	A	1805	-	-	17/29/63/63	0/2/2/2
20	CLA	B	1766	-	1/1/12/20	9/21/99/115	-
22	BCR	B	1778	-	-	12/29/63/63	0/2/2/2
20	CLA	B	1771	-	2/2/15/20	18/37/115/115	-
21	LMU	A	7017	-	-	14/21/61/61	0/2/2/2
22	BCR	A	1806	-	-	15/29/63/63	0/2/2/2
20	CLA	A	1796	-	2/2/15/20	18/37/115/115	-
20	CLA	2	1227	-	1/1/4/20	-	-
20	CLA	B	1785	-	2/2/15/20	21/37/115/115	-
20	CLA	L	1167	22	1/1/11/20	9/16/94/115	-
21	LMU	A	7034	20	-	14/21/61/61	0/2/2/2
21	LMU	A	7019	-	-	15/21/61/61	0/2/2/2
20	CLA	A	1762	-	2/2/13/20	7/28/106/115	-
20	CLA	J	1044	20	2/2/14/20	21/33/111/115	-
21	LMU	2	7003	-	-	11/21/61/61	0/2/2/2
20	CLA	A	1798	-	2/2/13/20	6/25/103/115	-
21	LMU	A	7028	-	-	14/21/61/61	0/2/2/2
20	CLA	4	1209	-	1/1/11/20	10/15/93/115	-
23	PQN	B	1773	-	1/1/8/9	10/23/43/43	0/2/2/2
21	LMU	A	7016	-	-	11/21/61/61	0/2/2/2
20	CLA	L	1166	16	1/1/12/20	8/19/97/115	-
20	CLA	3	1216	-	1/1/4/20	-	-
20	CLA	4	1204	-	2/2/13/20	13/25/103/115	-
20	CLA	J	1043	-	2/2/14/20	24/33/111/115	-
21	LMU	A	7027	-	-	13/21/61/61	0/2/2/2
20	CLA	1	1193	-	2/2/12/20	9/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	1208	4	1/1/4/20	-	-
20	CLA	A	1776	-	2/2/15/20	16/37/115/115	-
20	CLA	B	1757	-	2/2/15/20	16/37/115/115	-
20	CLA	A	1765	-	2/2/13/20	11/25/103/115	-
20	CLA	F	1157	20	4/4/12/20	9/23/101/115	-
20	CLA	4	1205	-	1/1/4/20	-	-
20	CLA	2	1217	-	2/2/15/20	17/37/115/115	-
20	CLA	3	3014	-	1/1/4/20	-	-
20	CLA	B	1762	-	2/2/15/20	20/37/115/115	-
22	BCR	B	1777	-	-	15/29/63/63	0/2/2/2
20	CLA	A	1793	-	2/2/15/20	16/37/115/115	-
25	SF4	C	1082	7	-	-	0/6/5/5
20	CLA	4	1202	-	1/1/4/20	-	-
21	LMU	R	1056	-	-	16/21/61/61	0/2/2/2
20	CLA	4	1197	-	1/1/9/20	-	-
21	LMU	A	7039	-	-	15/21/61/61	0/2/2/2
20	CLA	3	3002	-	1/1/4/20	-	-
20	CLA	4	1201	-	2/2/12/20	7/22/100/115	-
20	CLA	B	1772	-	1/1/9/20	-	-
20	CLA	A	1773	-	1/1/12/20	14/22/100/115	-
20	CLA	3	3008	-	1/1/12/20	6/19/97/115	-
20	CLA	B	1767	-	2/2/14/20	15/31/109/115	-
20	CLA	B	1742	-	2/2/13/20	12/25/103/115	-
20	CLA	A	1816	-	3/3/13/20	12/25/103/115	-
20	CLA	A	1774	-	2/2/15/20	19/37/115/115	-
20	CLA	B	1749	-	2/2/14/20	17/33/111/115	-
20	CLA	2	1220	20	2/2/13/20	14/27/105/115	-
20	CLA	2	1219	-	1/1/4/20	-	-
22	BCR	L	1170	20	-	12/29/63/63	0/2/2/2
20	CLA	B	1756	-	2/2/15/20	21/37/115/115	-
20	CLA	A	1792	-	1/1/12/20	11/21/99/115	-
20	CLA	A	1768	-	1/1/12/20	13/24/102/115	-
20	CLA	3	3001	-	1/1/4/20	-	-
20	CLA	A	1781	-	2/2/15/20	17/37/115/115	-
20	CLA	A	1786	-	1/1/12/20	3/19/97/115	-
21	LMU	A	1809	-	-	16/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMG	B	1783	-	-	23/44/64/70	0/1/1/1
20	CLA	K	1142	-	1/1/11/20	5/13/91/115	-
21	LMU	A	7035	-	-	14/21/61/61	0/2/2/2
20	CLA	2	1222	2	1/1/12/20	7/19/97/115	-
20	CLA	4	1199	-	2/2/13/20	12/25/103/115	-
20	CLA	B	1739	-	2/2/15/20	9/37/115/115	-
20	CLA	B	1740	6	2/2/15/20	19/37/115/115	-
20	CLA	K	1085	21	1/1/12/20	5/19/97/115	-
22	BCR	B	1780	-	-	14/29/63/63	0/2/2/2
20	CLA	1	1194	-	1/1/4/20	-	-
20	CLA	A	1764	5	2/2/15/20	21/37/115/115	-
20	CLA	B	1765	20	1/1/11/20	8/13/91/115	-
20	CLA	3	3015	-	1/1/4/20	-	-
20	CLA	A	1771	-	1/1/12/20	11/19/97/115	-
20	CLA	A	1770	-	1/1/11/20	9/13/91/115	-
20	CLA	A	1779	-	2/2/13/20	9/25/103/115	-
20	CLA	2	2010	-	1/1/4/20	-	-
20	CLA	A	1815	-	3/3/13/20	12/25/103/115	-
20	CLA	A	1794	-	1/1/11/20	8/16/94/115	-
20	CLA	B	1760	-	1/1/12/20	9/19/97/115	-
20	CLA	B	1768	-	2/2/15/20	16/37/115/115	-
22	BCR	B	1775	-	-	8/29/63/63	0/2/2/2
20	CLA	L	1168	-	2/2/12/20	10/19/97/115	-
21	LMU	A	1810	-	-	13/21/61/61	0/2/2/2
21	LMU	A	7023	-	-	14/21/61/61	0/2/2/2
20	CLA	J	1045	20	2/2/13/20	15/25/103/115	-
20	CLA	A	1784	-	2/2/13/20	10/25/103/115	-
20	CLA	B	1752	-	2/2/13/20	8/25/103/115	-
21	LMU	A	7033	-	-	13/21/61/61	0/2/2/2
21	LMU	A	7037	-	-	14/21/61/61	0/2/2/2
20	CLA	A	1761	-	2/2/15/20	22/37/115/115	-
20	CLA	A	1817	-	3/3/11/20	12/16/92/115	-
20	CLA	B	1744	-	2/2/15/20	24/37/115/115	-
20	CLA	A	1772	-	2/2/15/20	17/37/115/115	-
20	CLA	1	1197	-	2/2/12/20	9/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	2	1213	-	2/2/13/20	11/27/105/115	-
20	CLA	A	1780	-	2/2/15/20	20/37/115/115	-
20	CLA	K	3009	-	2/2/15/20	21/37/115/115	-
21	LMU	A	7042	-	-	18/21/61/61	0/2/2/2
21	LMU	A	7013	-	-	10/21/61/61	0/2/2/2
20	CLA	B	1761	-	1/1/12/20	12/19/97/115	-
21	LMU	A	7020	-	-	11/21/61/61	0/2/2/2
21	LMU	A	7036	-	-	14/20/60/61	0/2/2/2
20	CLA	A	1778	5	1/1/10/20	2/10/88/115	-
21	LMU	1	7004	-	-	13/21/61/61	0/2/2/2
22	BCR	B	1781	-	-	7/29/63/63	0/2/2/2
20	CLA	1	1190	-	1/1/11/20	6/15/93/115	-
21	LMU	A	7026	19	-	14/21/61/61	0/2/2/2
23	PQN	A	1802	-	1/1/8/9	11/23/43/43	0/2/2/2
20	CLA	4	4003	-	1/1/4/20	-	-
21	LMU	A	7022	-	-	17/21/61/61	0/2/2/2
21	LMU	A	7025	-	-	13/21/61/61	0/2/2/2
21	LMU	A	7021	-	-	13/21/61/61	0/2/2/2
25	SF4	B	1784	6,5	-	-	0/6/5/5
20	CLA	A	1795	-	1/1/12/20	11/21/99/115	-
20	CLA	A	1797	-	2/2/15/20	19/37/115/115	-
20	CLA	1	1195	-	1/1/9/20	-	-
20	CLA	A	1812	-	2/2/15/20	18/37/115/115	-
21	LMU	A	7038	-	-	16/21/61/61	0/2/2/2
21	LMU	A	7024	-	-	15/21/61/61	0/2/2/2
20	CLA	A	1782	20	2/2/15/20	23/37/115/115	-

The worst 5 of 2423 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	1170	BCR	C21-C22	-11.03	1.21	1.35
20	1	1195	CLA	CAB-C3B	-10.23	1.30	1.51
22	B	1781	BCR	C21-C22	-10.00	1.22	1.35
22	L	1170	BCR	C20-C21	-9.90	1.12	1.43
22	B	1779	BCR	C21-C22	-9.40	1.23	1.35

The worst 5 of 4431 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1780	BCR	C20-C21-C22	36.92	179.99	127.31
22	A	1808	BCR	C20-C21-C22	36.90	179.97	127.31
22	A	1805	BCR	C20-C21-C22	36.89	179.95	127.31
22	A	1806	BCR	C20-C21-C22	36.88	179.95	127.31
22	A	1804	BCR	C20-C21-C22	36.87	179.93	127.31

5 of 271 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	1	1187	CLA	ND
20	1	1188	CLA	ND
20	1	1189	CLA	ND
20	1	1190	CLA	ND
20	1	1191	CLA	ND

5 of 2727 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	1	1187	CLA	C1A-C2A-CAA-CBA
20	1	1187	CLA	C3A-C2A-CAA-CBA
20	1	1187	CLA	CBA-CGA-O2A-C1
20	1	1187	CLA	CHA-CBD-CGD-O1D
20	1	1187	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

222 monomers are involved in 3478 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	3	3007	CLA	2	0
20	3	3011	CLA	17	0
21	A	7010	LMU	8	0
21	L	1171	LMU	3	0
20	A	1766	CLA	5	0
20	I	1031	CLA	11	0
20	1	1192	CLA	9	0
20	2	1224	CLA	7	0
20	3	1213	CLA	1	0
20	A	1800	CLA	31	0
21	3	7005	LMU	3	0
25	C	1083	SF4	4	0
20	B	1748	CLA	14	0
20	2	1214	CLA	7	0
20	A	1787	CLA	26	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	1764	CLA	21	0
22	L	1169	BCR	48	0
20	1	1187	CLA	11	0
20	A	1790	CLA	16	0
20	I	1033	CLA	15	0
20	4	4014	CLA	11	0
22	B	1776	BCR	20	0
20	B	1745	CLA	12	0
21	A	7009	LMU	9	0
20	B	1735	CLA	33	0
20	B	1786	CLA	43	0
20	3	1212	CLA	9	0
20	B	1737	CLA	24	0
20	2	1212	CLA	18	0
21	2	7006	LMU	11	0
20	B	1736	CLA	9	0
20	3	1219	CLA	18	0
22	B	1779	BCR	46	0
20	1	1191	CLA	10	0
20	A	1799	CLA	7	0
20	B	1750	CLA	9	0
20	B	1769	CLA	25	0
20	2	1215	CLA	24	0
20	A	1785	CLA	17	0
20	A	1801	CLA	15	0
22	B	1774	BCR	8	0
20	A	1767	CLA	23	0
20	F	1156	CLA	13	0
20	3	1214	CLA	3	0
21	A	7031	LMU	4	0
20	B	1743	CLA	29	0
20	B	1746	CLA	23	0
21	A	7043	LMU	16	0
20	4	1196	CLA	34	0
22	3	1220	BCR	21	0
20	F	1155	CLA	1	0
21	1	1202	LMU	5	0
20	4	1207	CLA	5	0
21	2	1225	LMU	1	1
20	B	1741	CLA	6	0
20	A	1763	CLA	31	0
20	3	1215	CLA	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	1783	CLA	61	0
20	R	1055	CLA	6	0
22	A	1808	BCR	43	0
20	1	1189	CLA	11	0
20	A	1791	CLA	24	1
20	3	1218	CLA	25	0
20	B	1738	CLA	19	0
20	R	1054	CLA	11	0
20	B	1763	CLA	13	0
20	1	1200	CLA	11	0
21	A	7030	LMU	12	0
20	A	1760	CLA	29	0
20	B	1747	CLA	23	0
20	1	1196	CLA	6	0
20	A	1777	CLA	13	0
22	A	1807	BCR	62	0
21	B	1782	LMU	1	0
20	B	1758	CLA	34	0
20	B	1755	CLA	62	0
21	A	7040	LMU	4	0
20	A	1788	CLA	40	0
20	A	1769	CLA	22	0
20	B	1759	CLA	34	0
20	B	1770	CLA	24	0
21	R	1057	LMU	5	0
20	G	1099	CLA	6	0
22	A	1804	BCR	22	0
20	3	1217	CLA	8	0
20	A	1811	CLA	20	0
20	A	1813	CLA	33	0
20	4	1206	CLA	2	0
20	B	1753	CLA	40	0
20	1	1198	CLA	20	0
20	B	1787	CLA	50	0
20	A	1759	CLA	20	0
21	A	7041	LMU	9	0
21	K	1086	LMU	6	0
20	K	1146	CLA	11	0
20	L	1505	CLA	3	0
20	A	1789	CLA	20	0
20	1	1199	CLA	2	0
20	4	1200	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	4	1198	CLA	25	0
20	1	1188	CLA	7	0
20	2	1218	CLA	7	0
20	B	1751	CLA	16	0
21	A	7032	LMU	28	0
22	A	1803	BCR	41	0
22	I	1032	BCR	47	0
20	2	1223	CLA	4	0
20	H	1079	CLA	19	0
20	B	1754	CLA	23	0
22	A	1805	BCR	48	0
20	B	1766	CLA	3	0
22	B	1778	BCR	30	0
20	B	1771	CLA	24	0
21	A	7017	LMU	3	0
22	A	1806	BCR	36	0
20	A	1796	CLA	63	0
20	B	1785	CLA	22	0
20	L	1167	CLA	18	0
21	A	7034	LMU	1	0
21	A	7019	LMU	2	0
20	A	1762	CLA	18	0
20	J	1044	CLA	41	0
21	2	7003	LMU	3	0
20	A	1798	CLA	29	0
21	A	7028	LMU	4	0
20	4	1209	CLA	5	0
21	A	7016	LMU	42	0
23	B	1773	PQN	33	0
20	L	1166	CLA	7	0
20	3	1216	CLA	7	0
20	4	1204	CLA	8	0
20	J	1043	CLA	29	0
21	A	7027	LMU	6	0
20	1	1193	CLA	6	2
20	4	1208	CLA	8	0
20	A	1776	CLA	47	0
20	B	1757	CLA	21	0
20	A	1765	CLA	25	0
20	F	1157	CLA	13	0
20	4	1205	CLA	3	0
20	2	1217	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	1762	CLA	28	0
22	B	1777	BCR	31	0
20	A	1793	CLA	35	0
25	C	1082	SF4	5	0
20	4	1202	CLA	4	0
21	R	1056	LMU	19	0
20	4	1197	CLA	2	0
21	A	7039	LMU	19	0
20	4	1201	CLA	25	0
20	B	1772	CLA	2	0
20	A	1773	CLA	11	0
20	3	3008	CLA	17	0
20	B	1767	CLA	15	0
20	B	1742	CLA	9	0
20	A	1816	CLA	35	0
20	A	1774	CLA	31	0
20	B	1749	CLA	18	0
20	2	1220	CLA	74	0
22	L	1170	BCR	13	0
20	B	1756	CLA	46	0
20	A	1792	CLA	22	0
20	A	1768	CLA	4	0
20	A	1781	CLA	85	0
20	A	1786	CLA	9	0
21	A	1809	LMU	4	0
24	B	1783	LMG	30	0
20	K	1142	CLA	20	2
20	2	1222	CLA	14	0
20	4	1199	CLA	22	0
20	B	1739	CLA	22	0
20	B	1740	CLA	20	0
20	K	1085	CLA	26	0
22	B	1780	BCR	53	0
20	1	1194	CLA	5	0
20	A	1764	CLA	26	0
20	B	1765	CLA	20	0
20	A	1771	CLA	13	0
20	A	1770	CLA	27	0
20	A	1779	CLA	35	0
20	A	1815	CLA	19	0
20	A	1794	CLA	21	0
20	B	1760	CLA	10	0

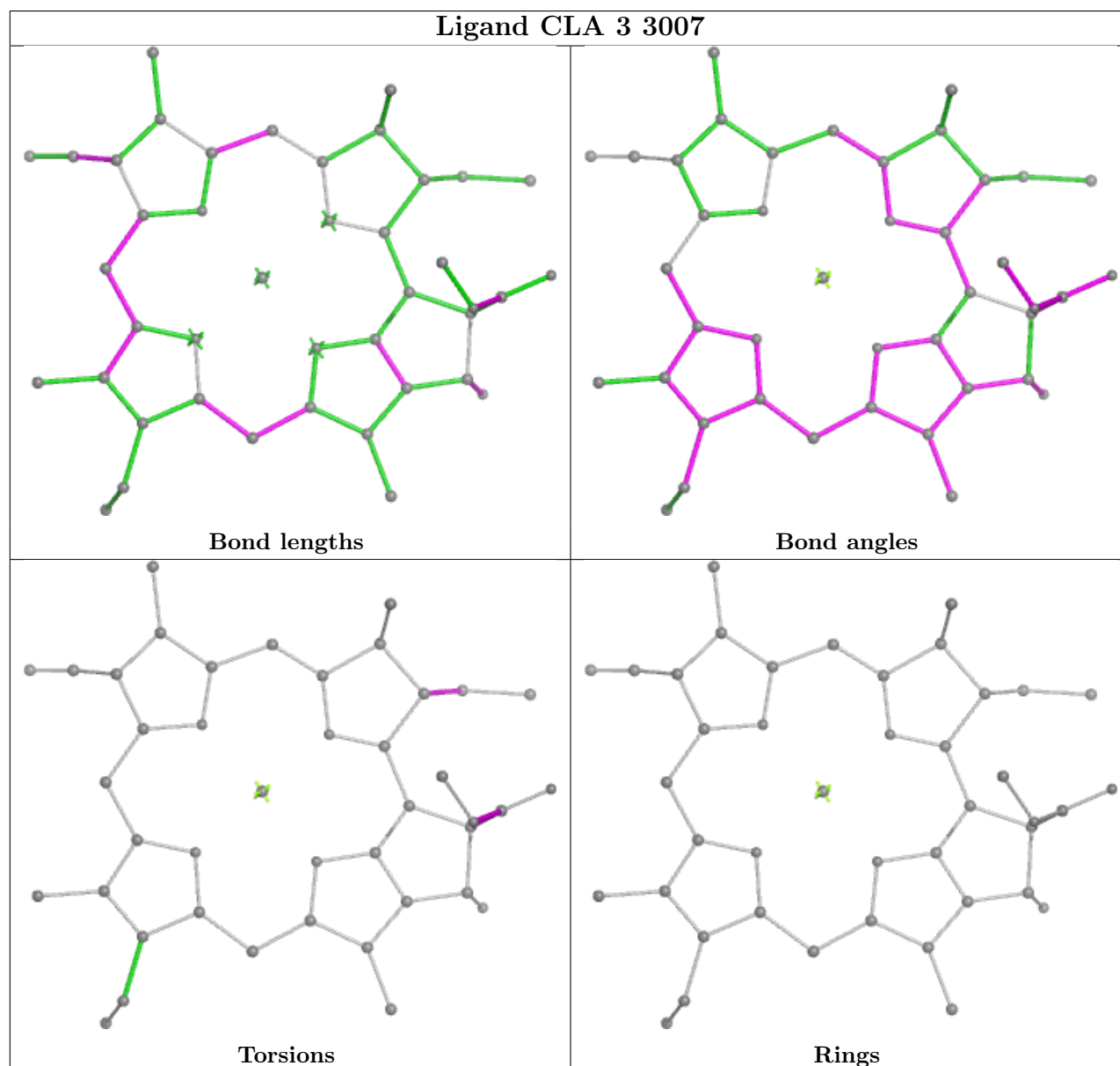
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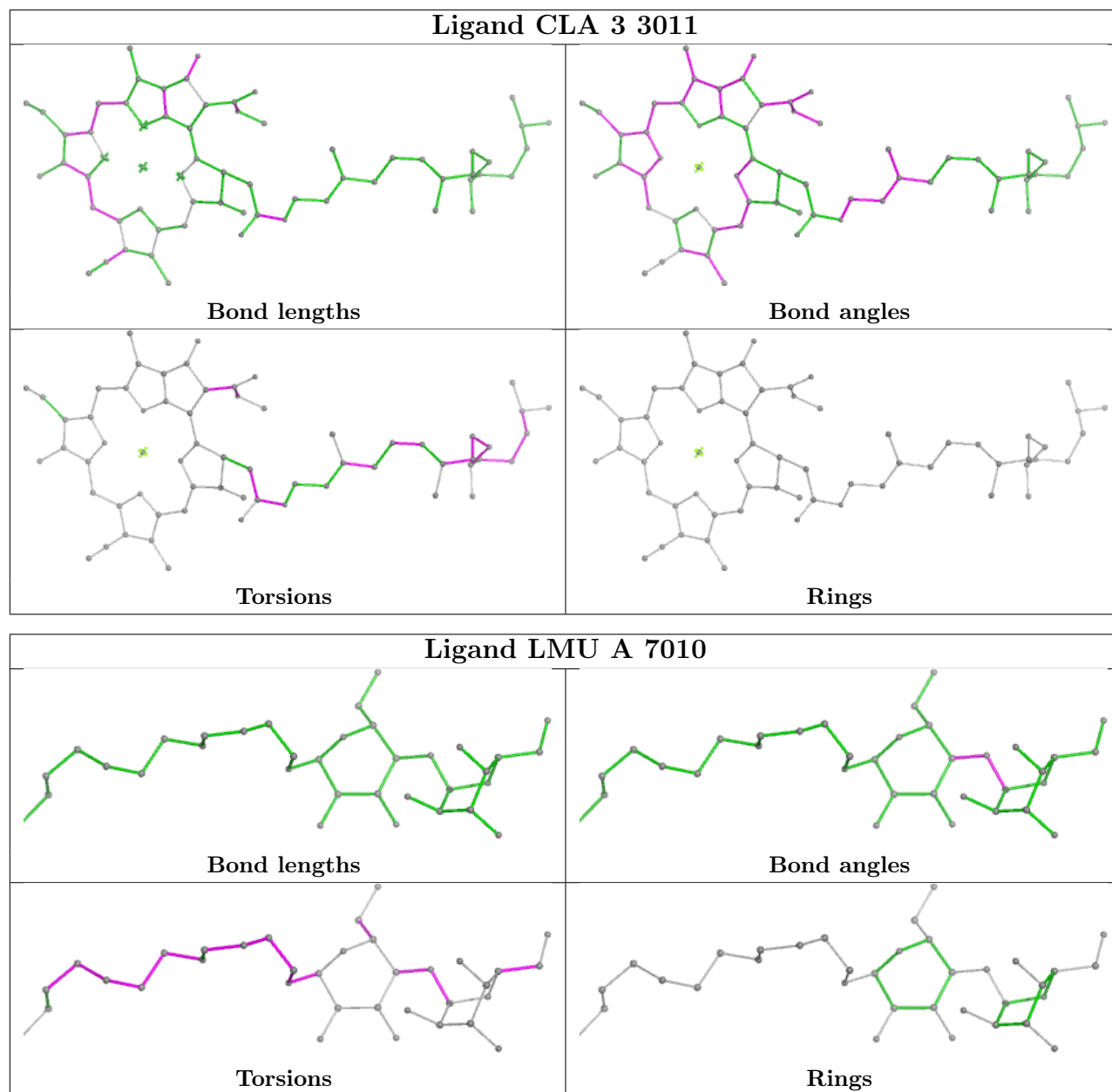
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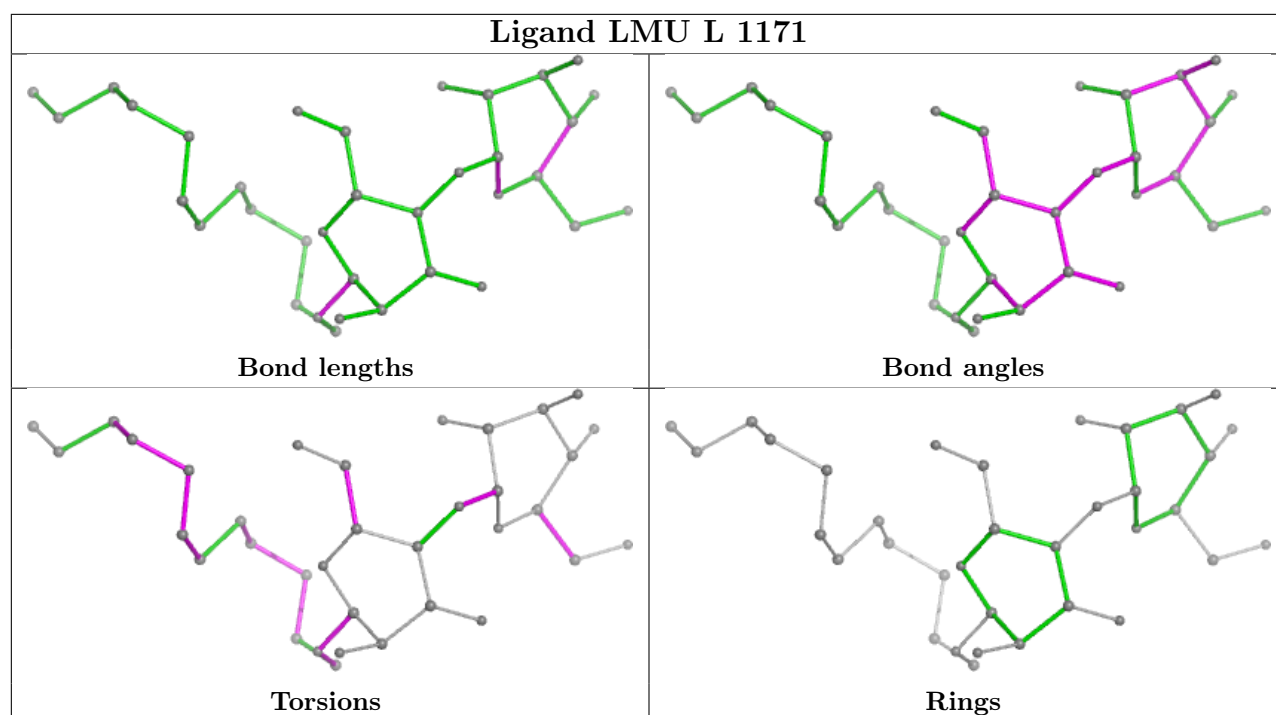
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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22	B	1775	BCR	20	0
20	L	1168	CLA	12	0
21	A	1810	LMU	4	0
21	A	7023	LMU	26	0
20	J	1045	CLA	45	0
20	A	1784	CLA	18	0
20	B	1752	CLA	14	0
21	A	7033	LMU	19	0
21	A	7037	LMU	24	0
20	A	1761	CLA	32	0
20	A	1817	CLA	9	0
20	B	1744	CLA	20	0
20	A	1772	CLA	35	0
20	1	1197	CLA	20	0
20	2	1213	CLA	13	0
20	A	1780	CLA	17	0
20	K	3009	CLA	3	0
21	A	7042	LMU	35	0
21	A	7013	LMU	9	0
20	B	1761	CLA	12	0
21	A	7020	LMU	21	0
21	A	7036	LMU	19	0
20	A	1778	CLA	11	0
21	1	7004	LMU	10	0
22	B	1781	BCR	17	0
20	1	1190	CLA	5	0
21	A	7026	LMU	21	0
23	A	1802	PQN	12	0
21	A	7022	LMU	11	0
21	A	7025	LMU	1	0
21	A	7021	LMU	24	0
25	B	1784	SF4	18	0
20	A	1795	CLA	40	0
20	A	1797	CLA	35	0
20	1	1195	CLA	4	0
20	A	1812	CLA	35	0
21	A	7038	LMU	13	0
20	A	1782	CLA	81	0

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

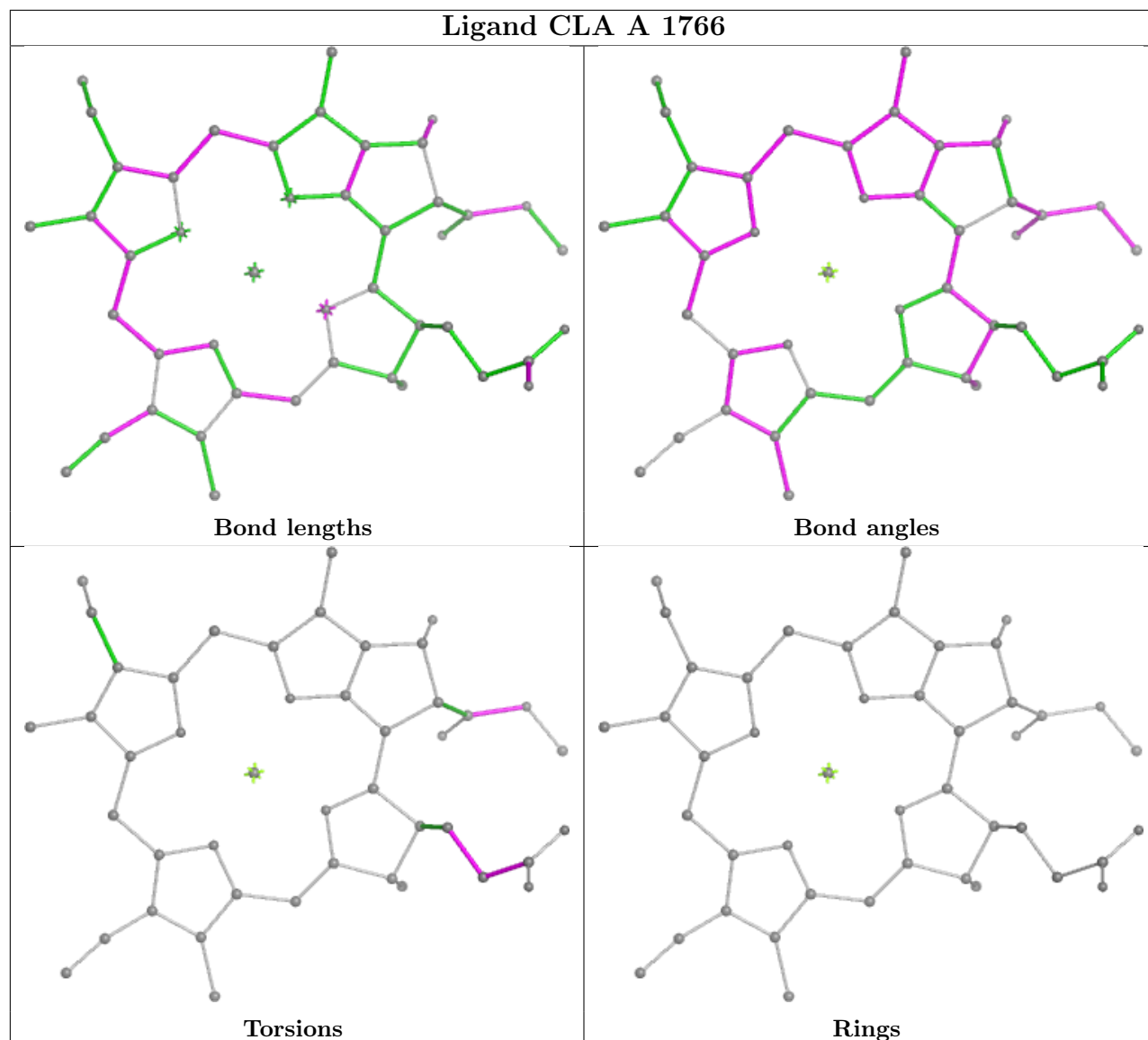
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

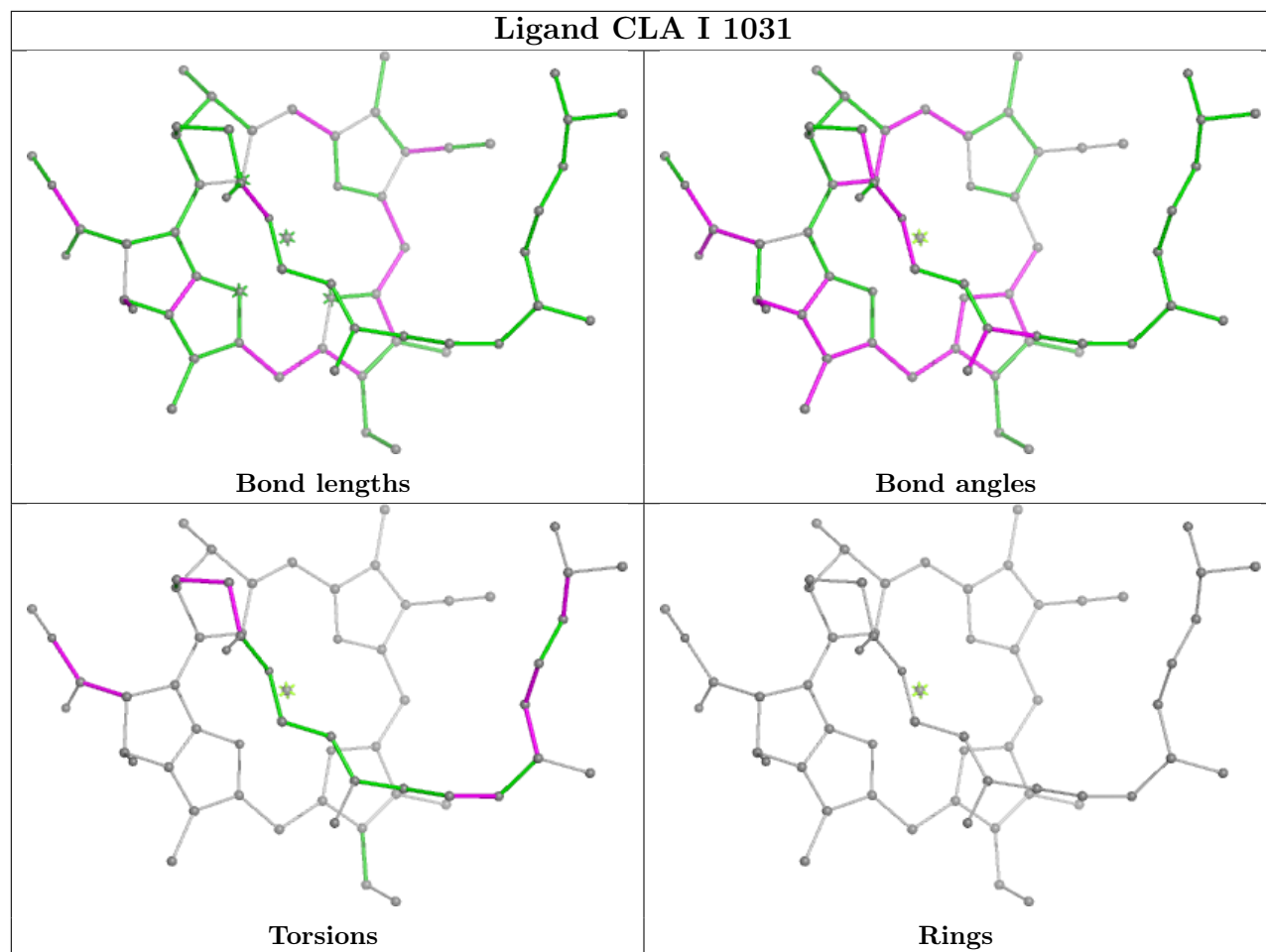


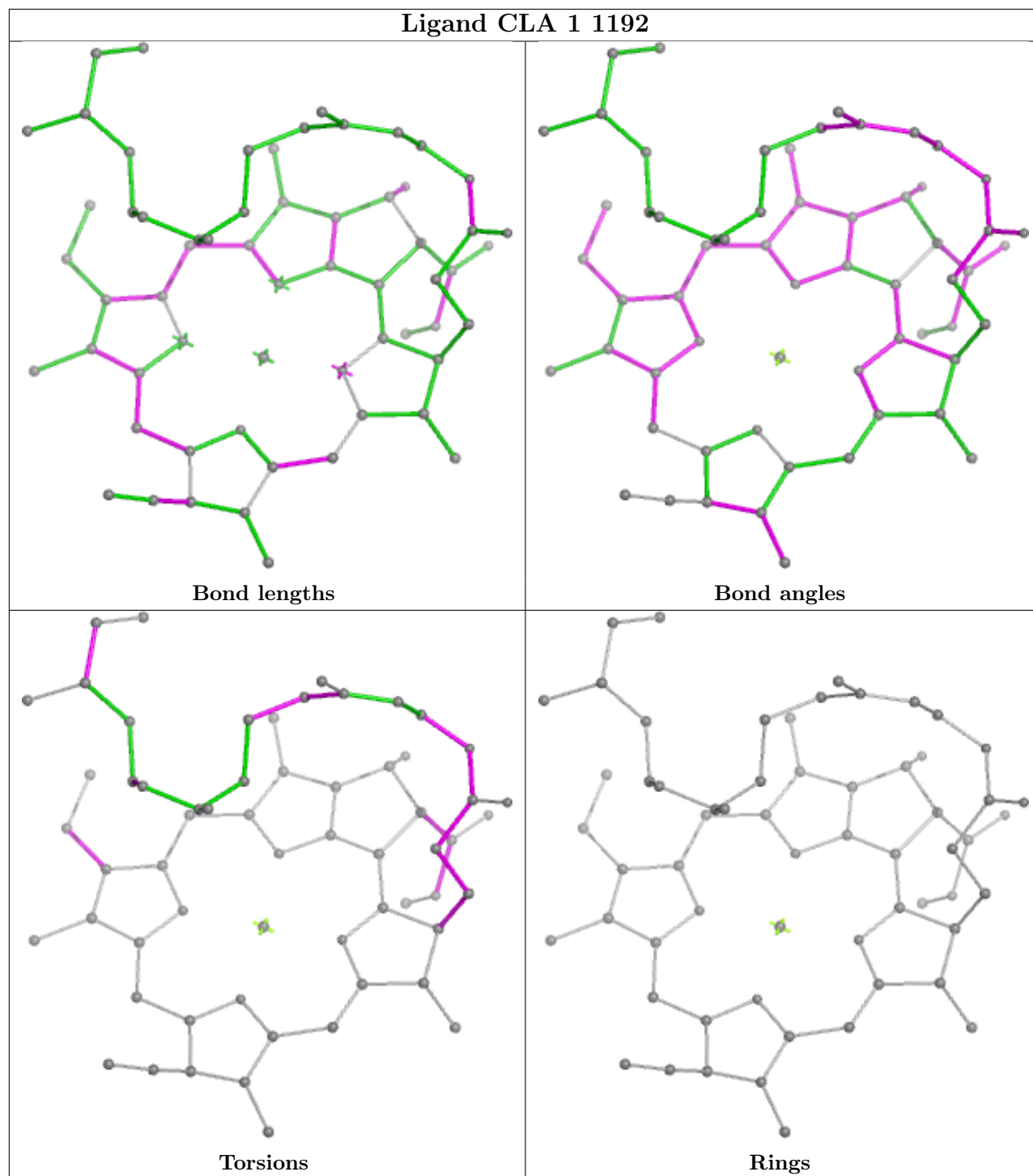


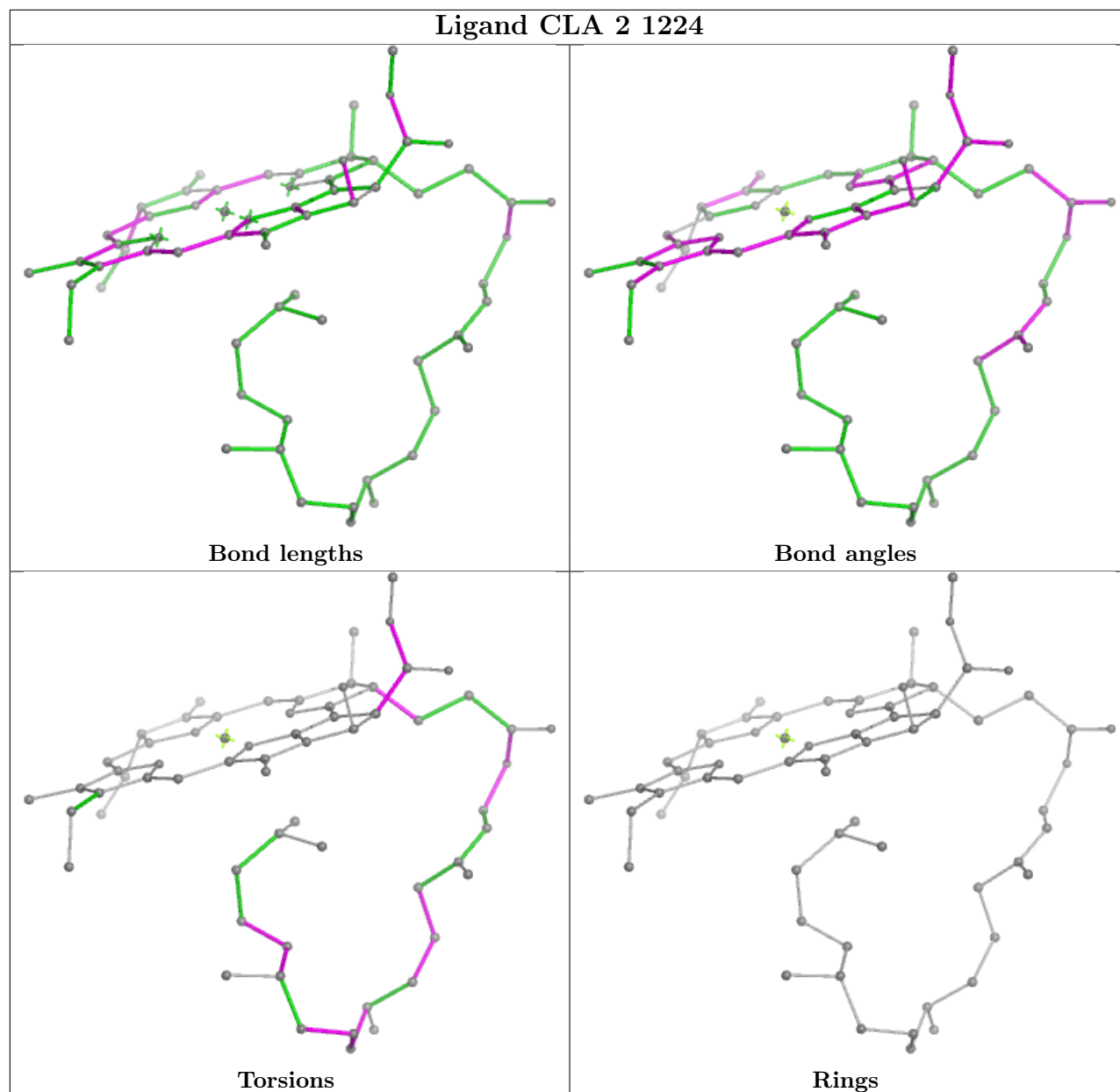


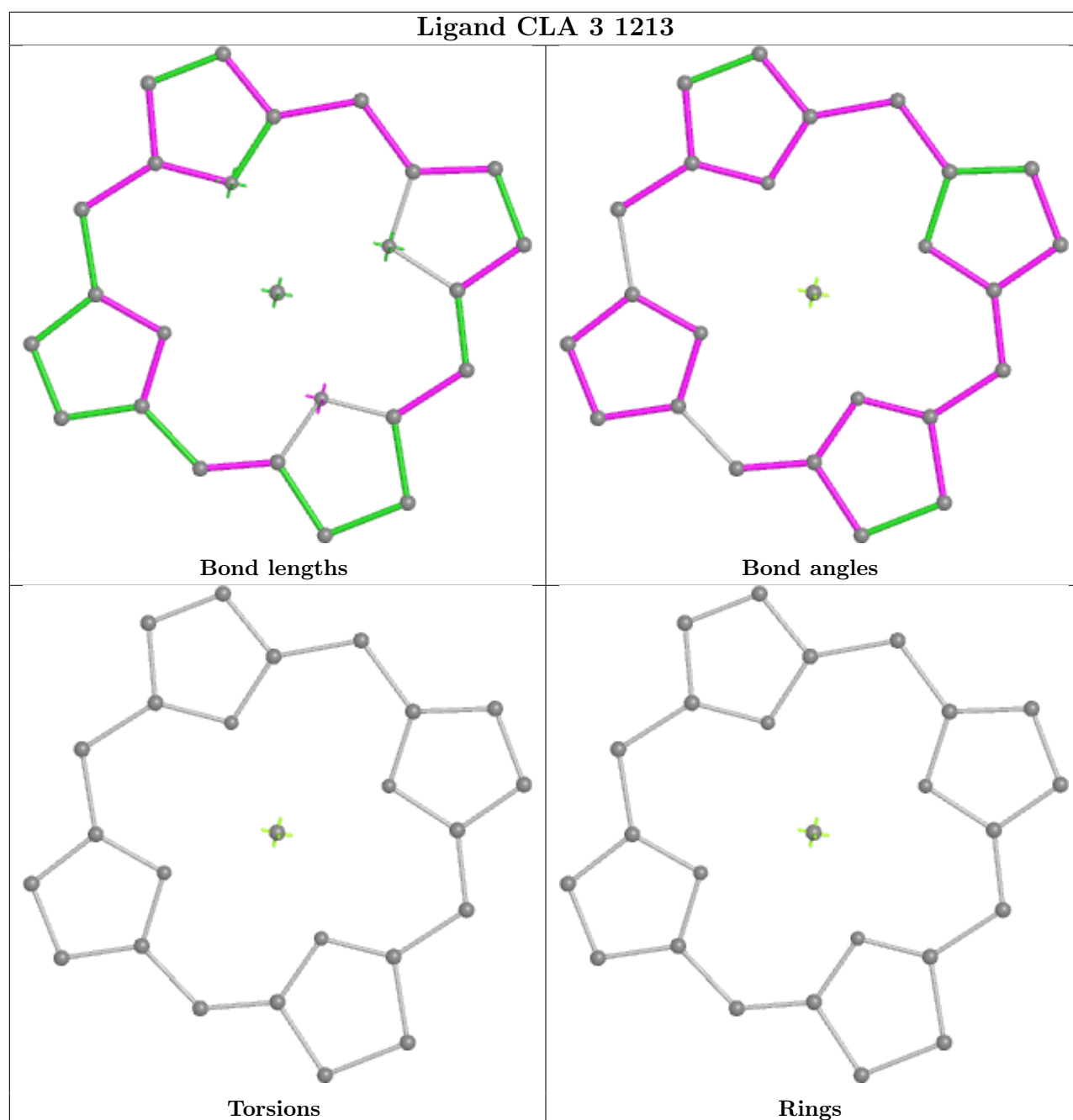
Ligand CLA A 1766

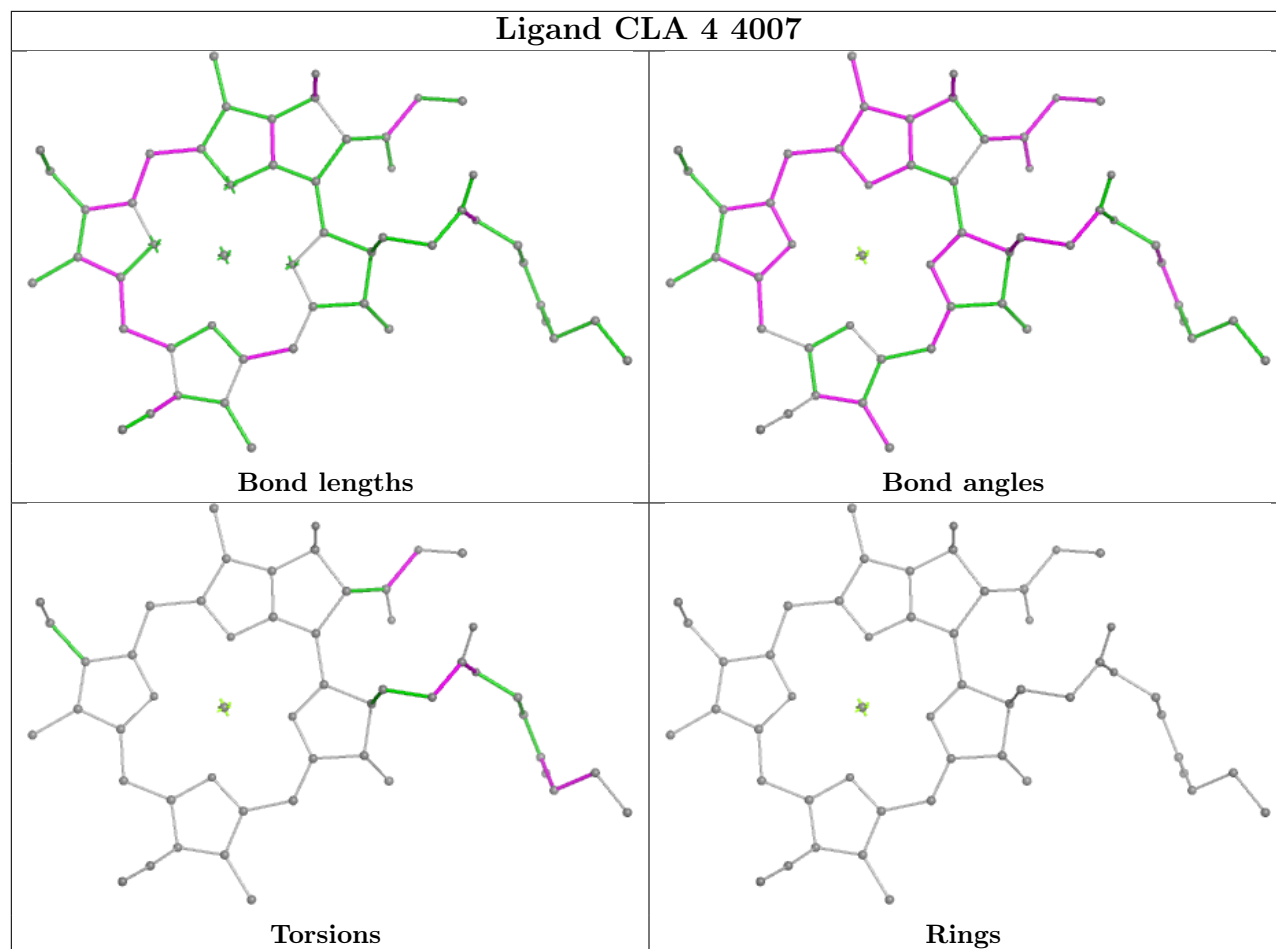


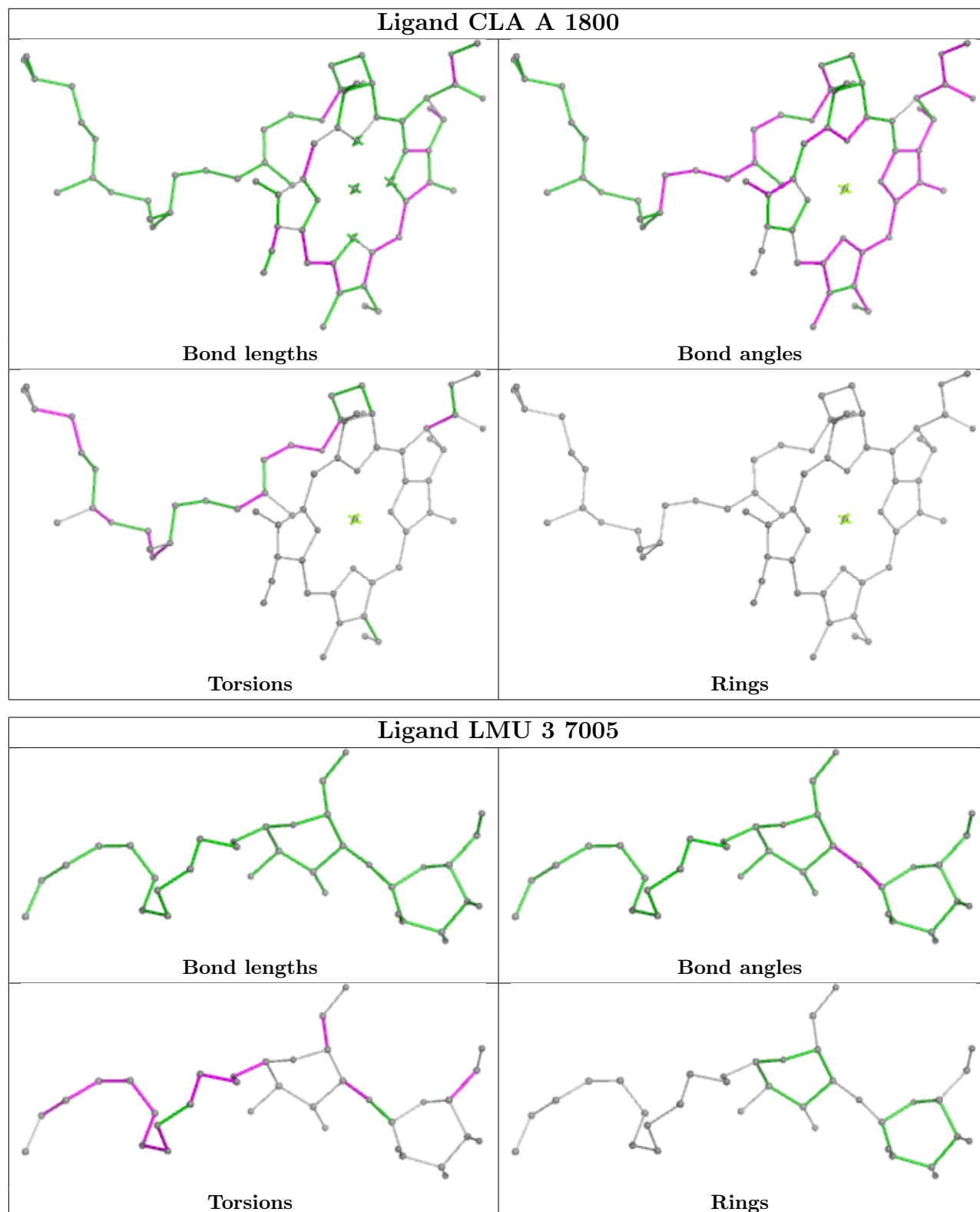


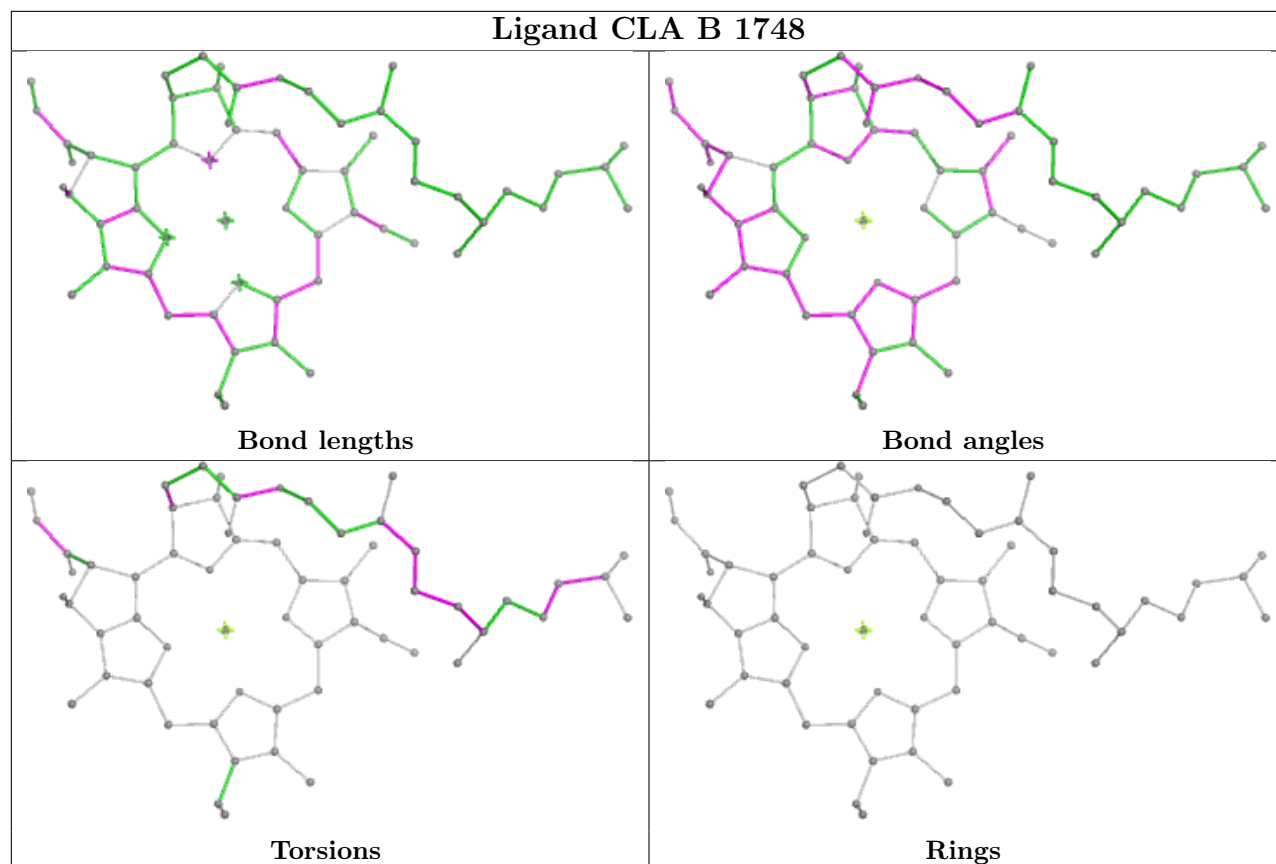


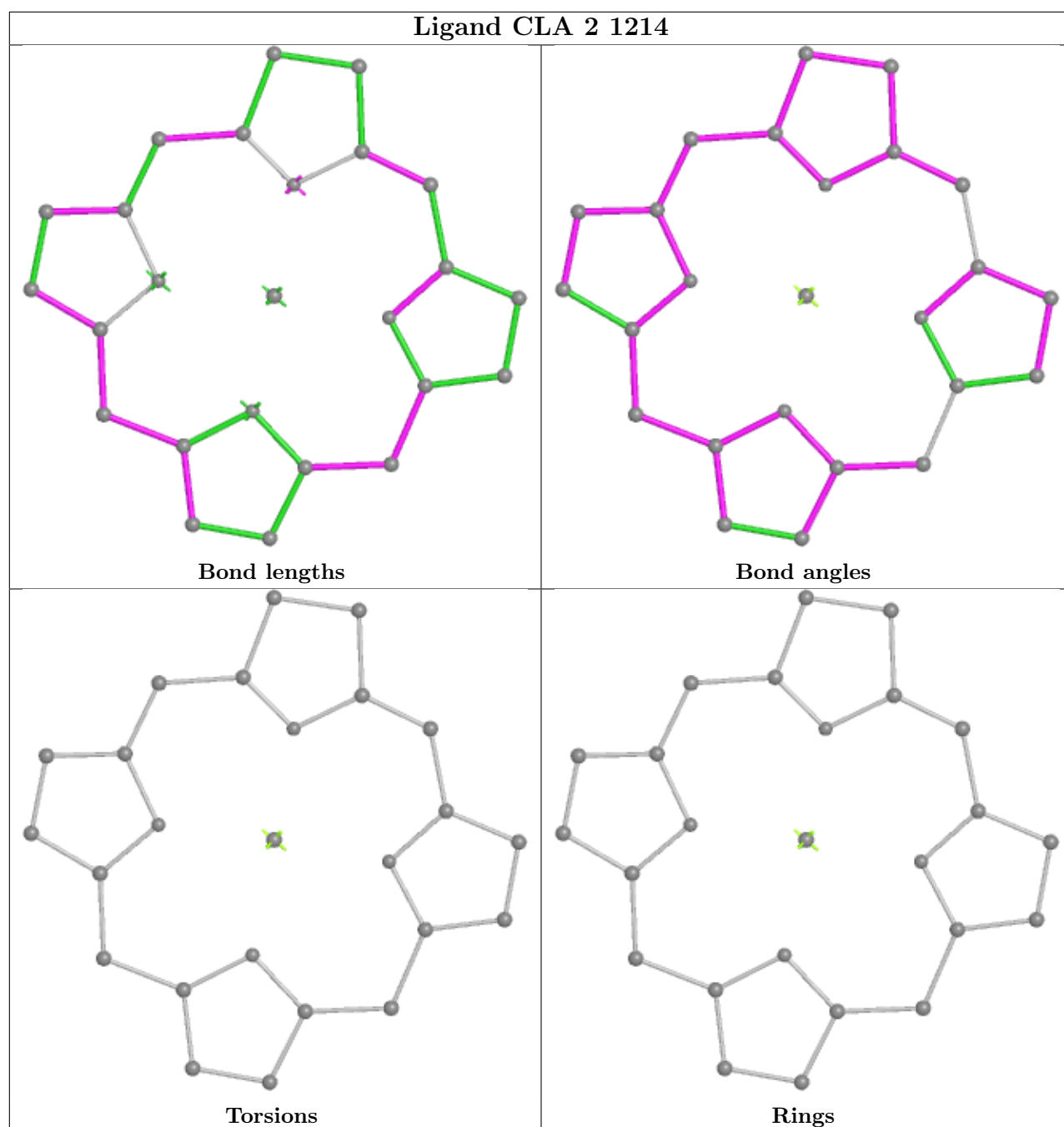


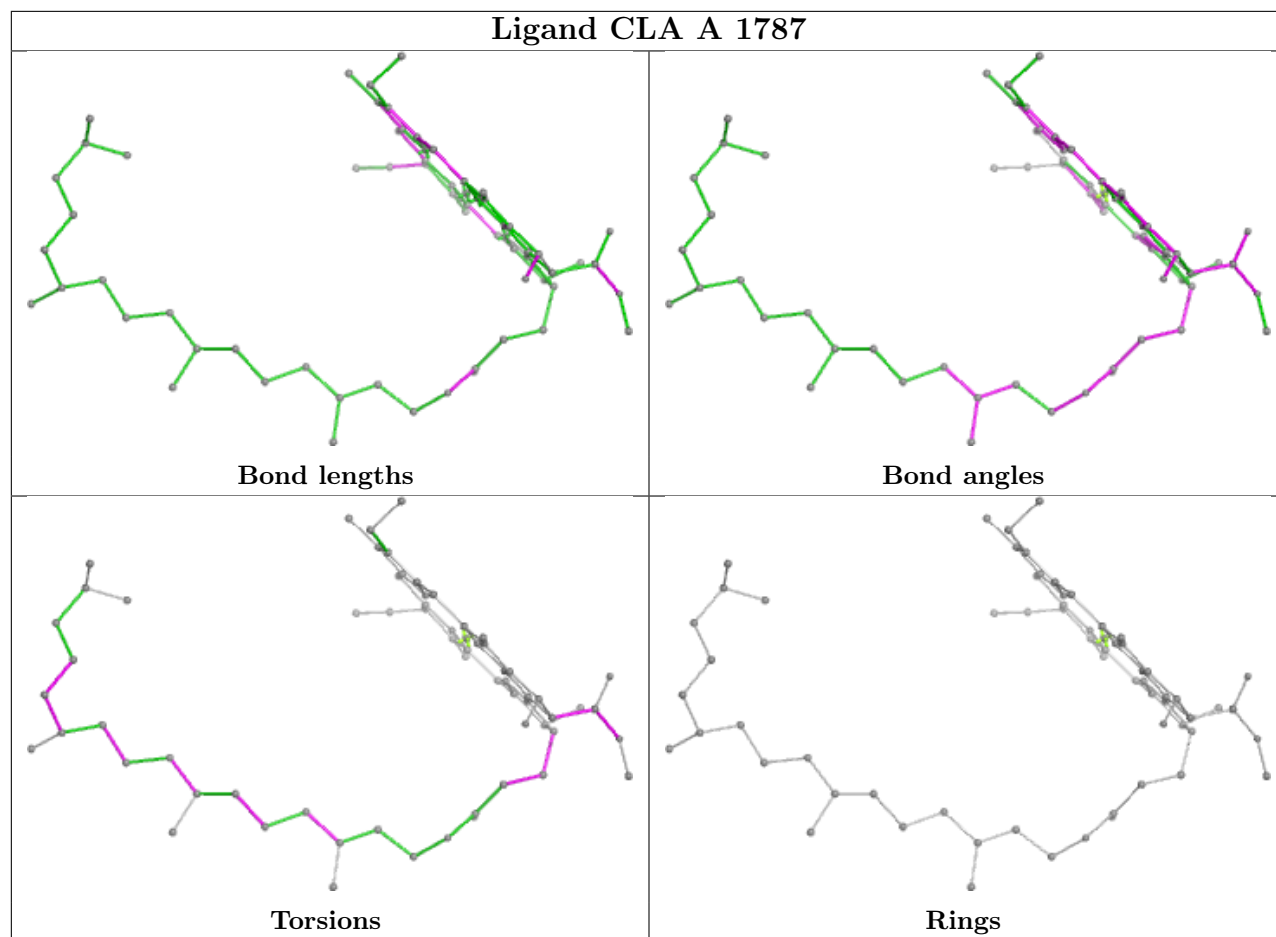




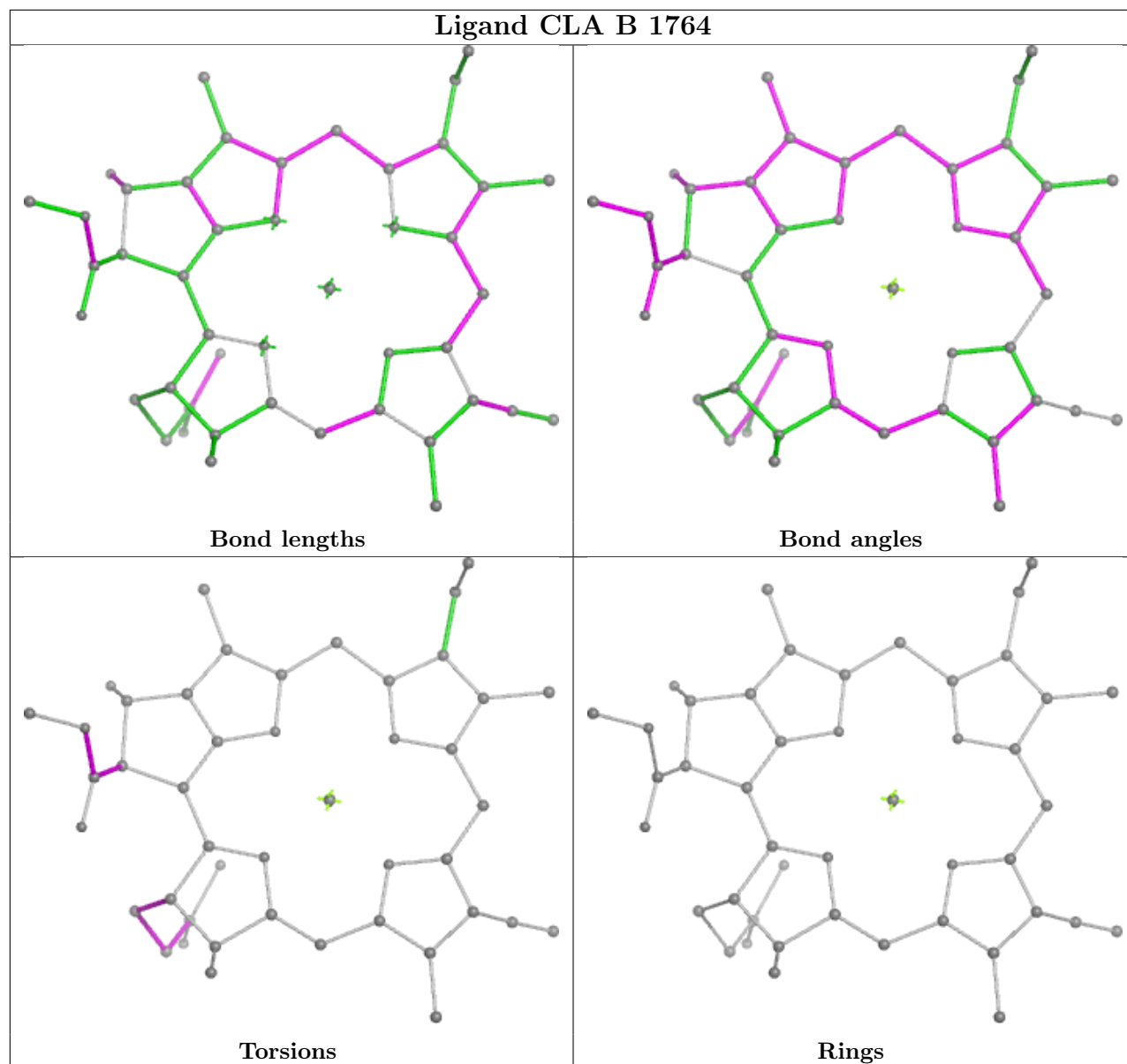




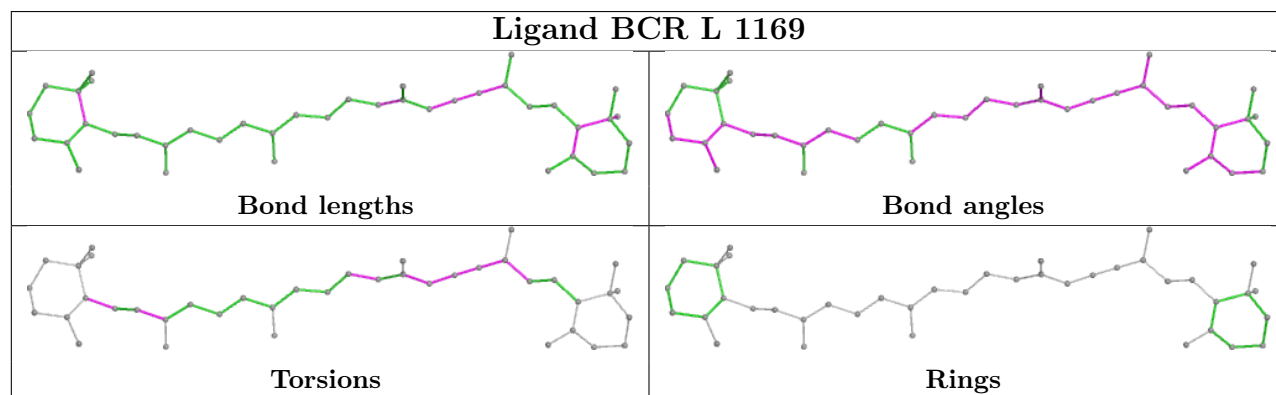


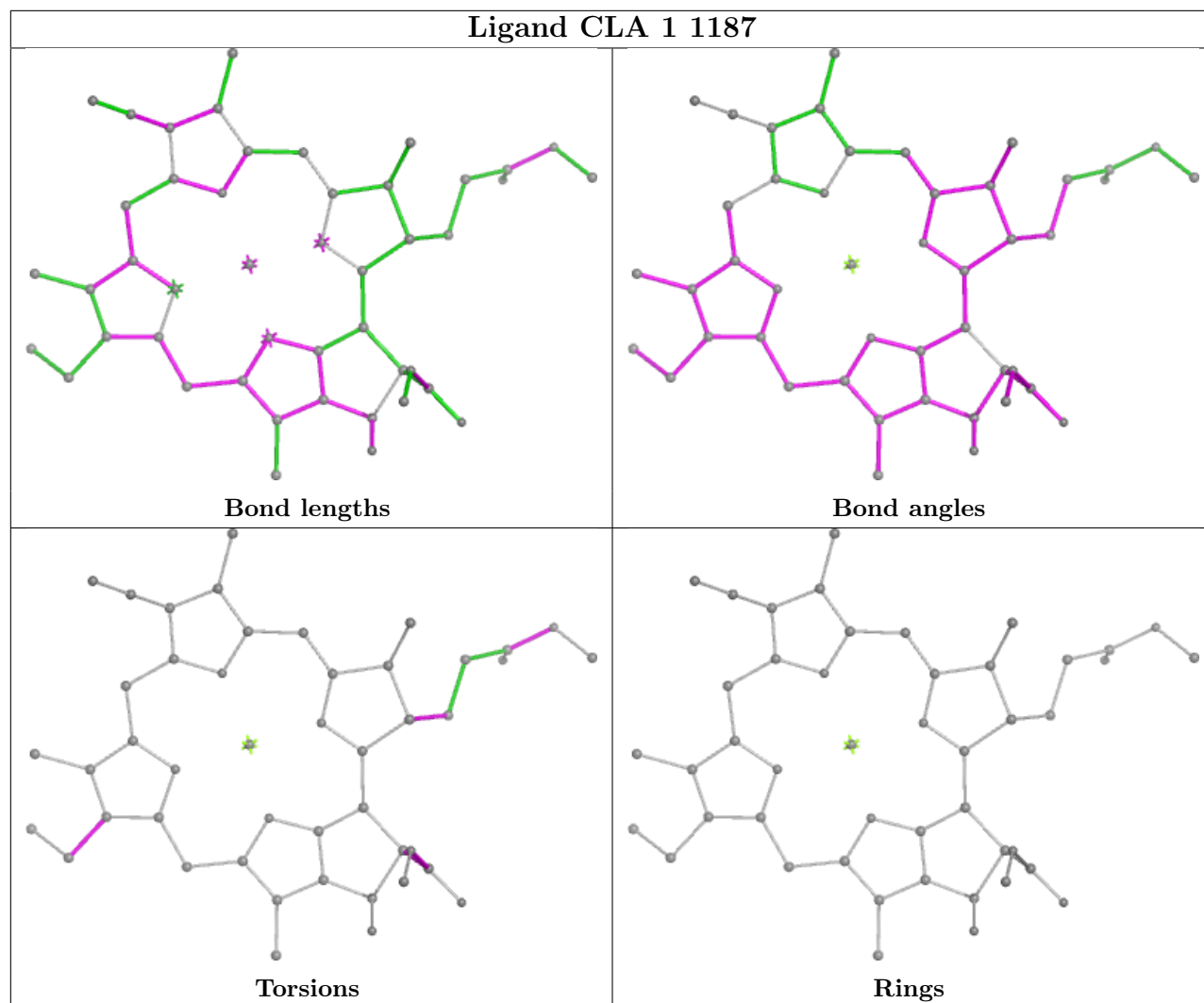


Ligand CLA B 1764

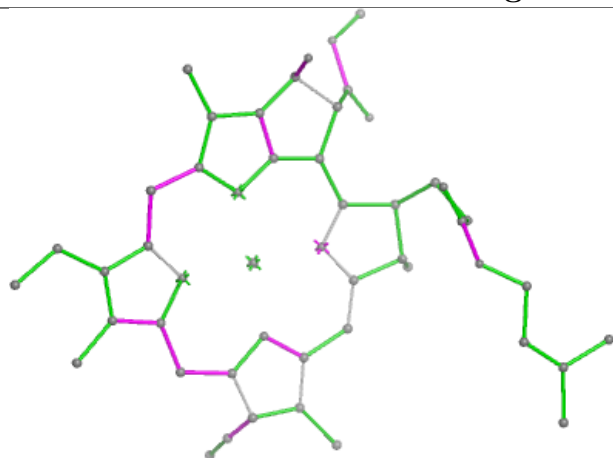


Ligand BCR L 1169

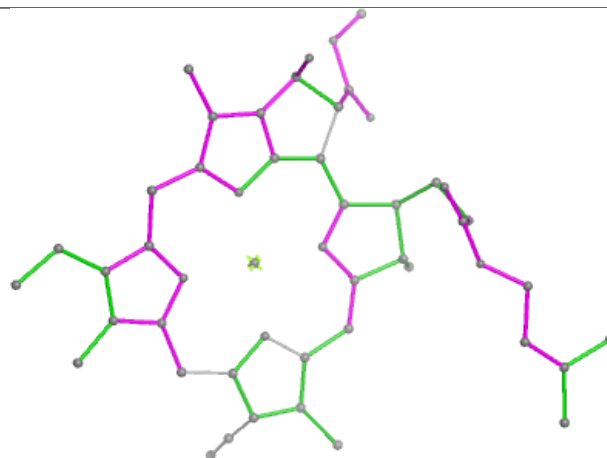




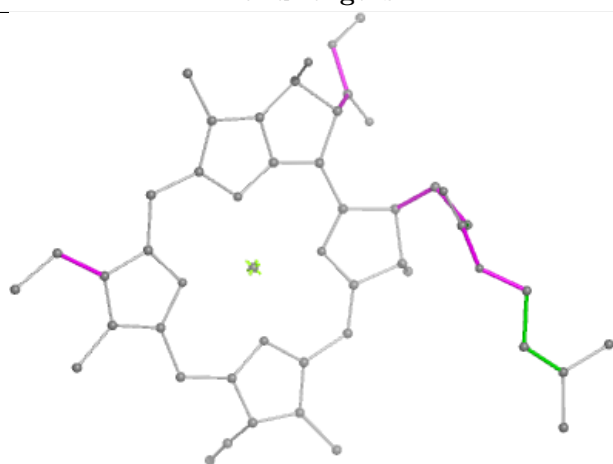
Ligand CLA A 1790



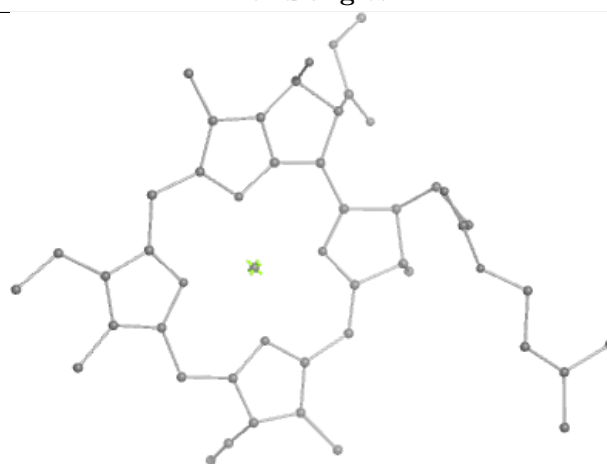
Bond lengths



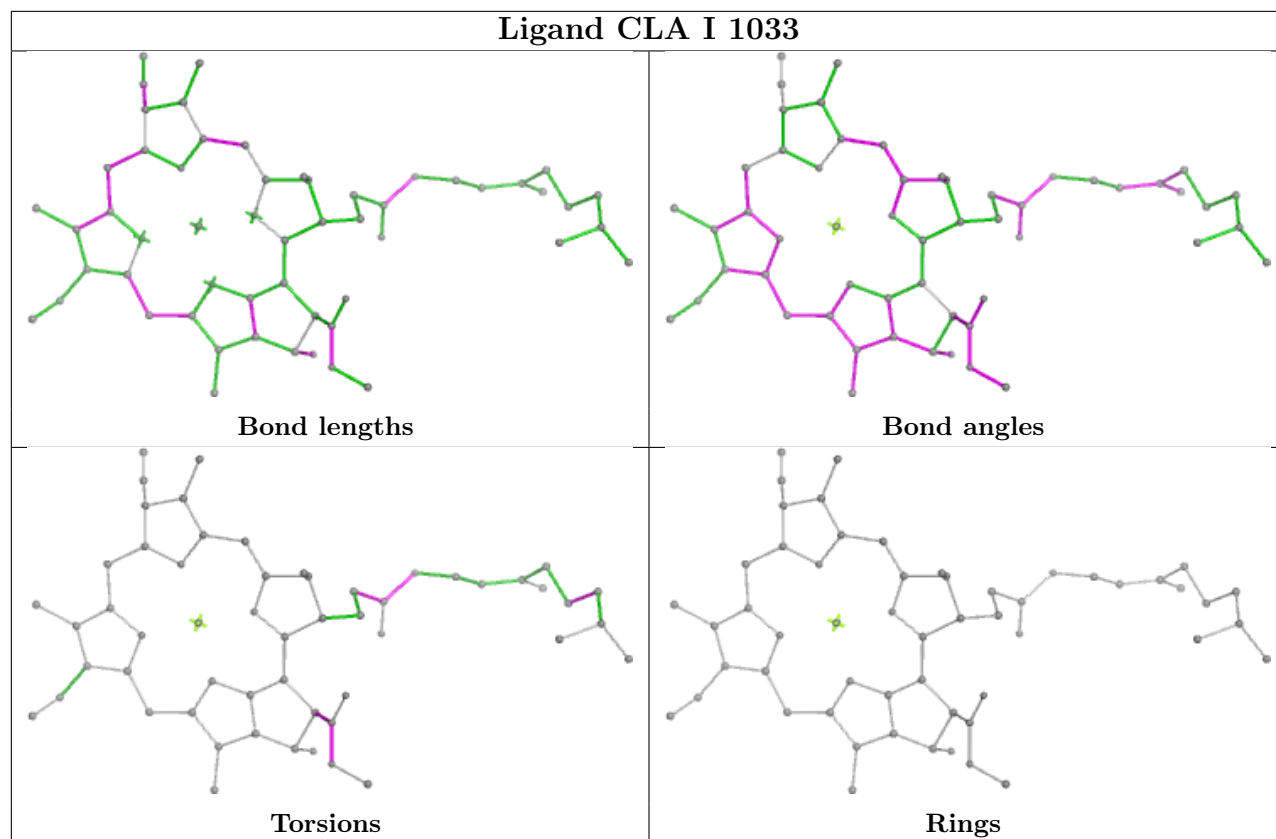
Bond angles

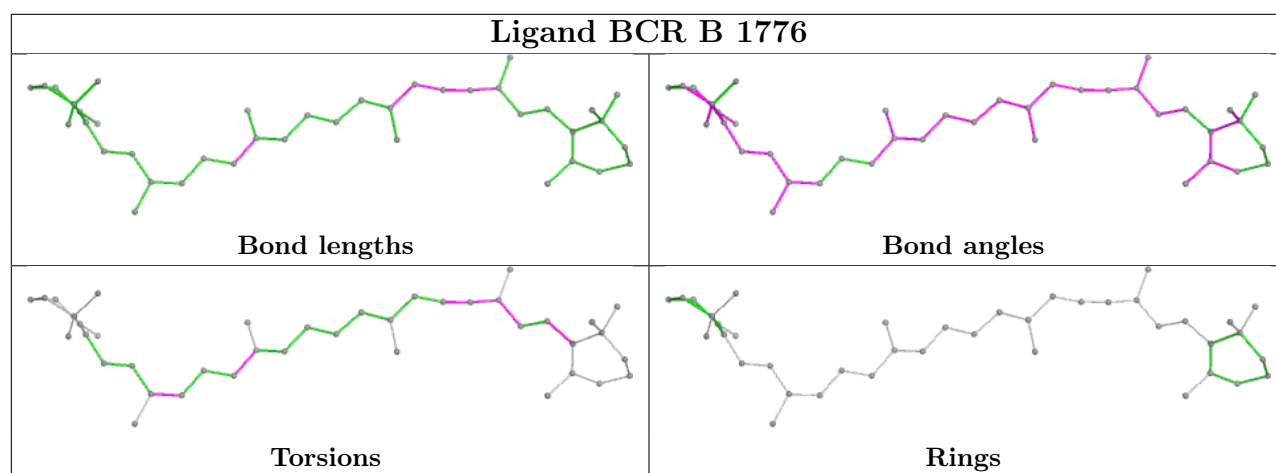
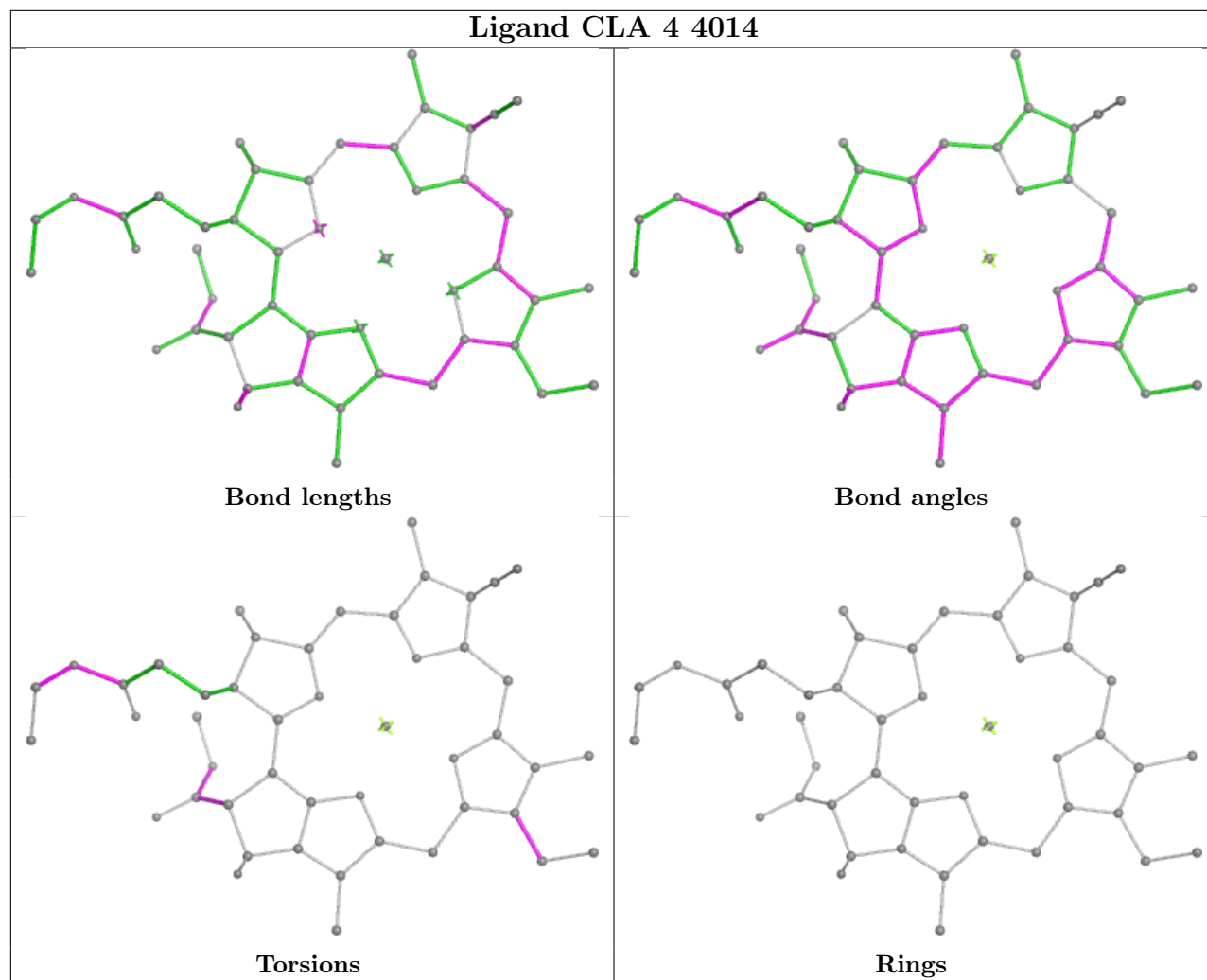


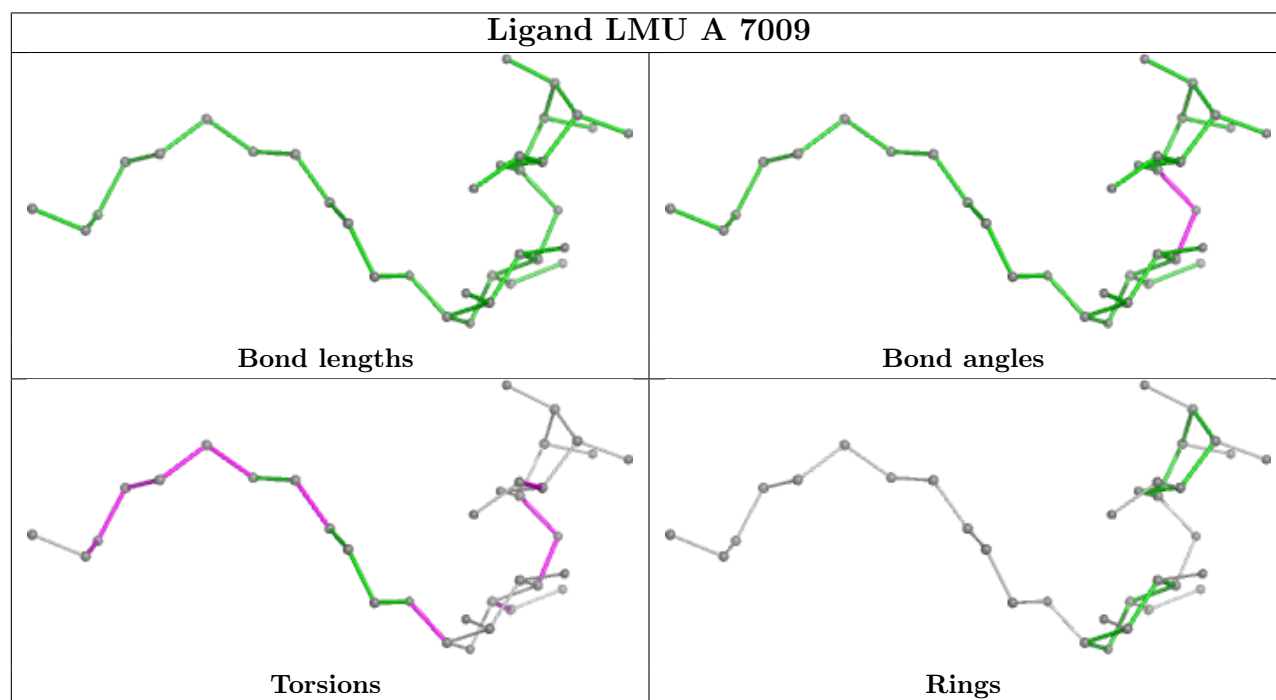
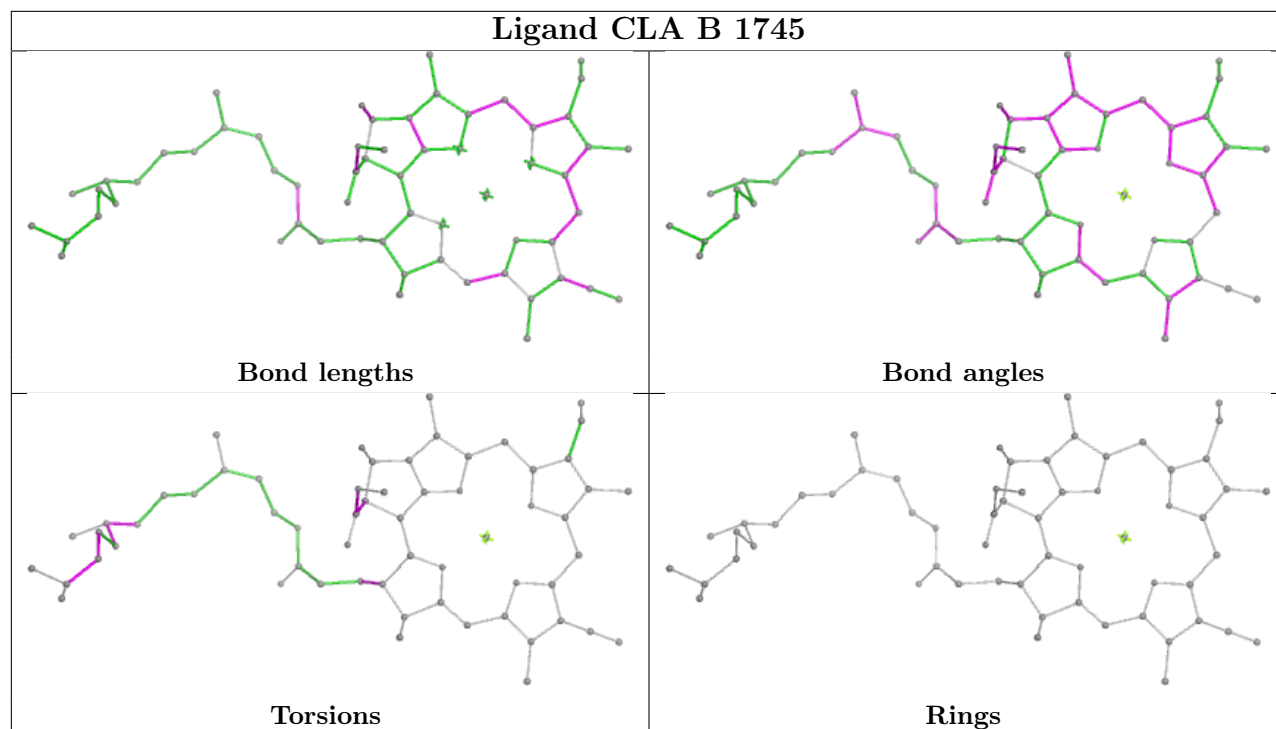
Torsions

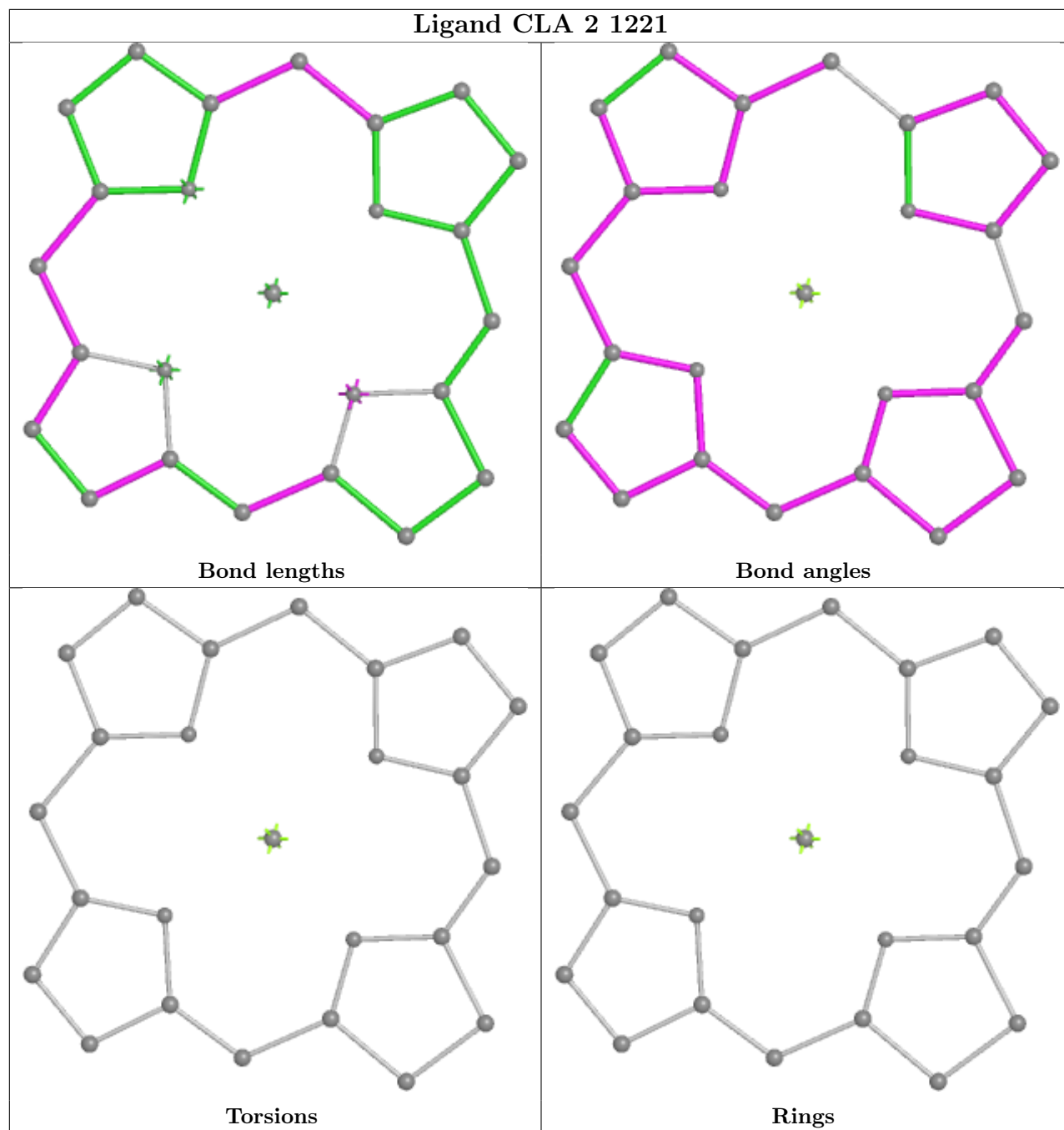


Rings

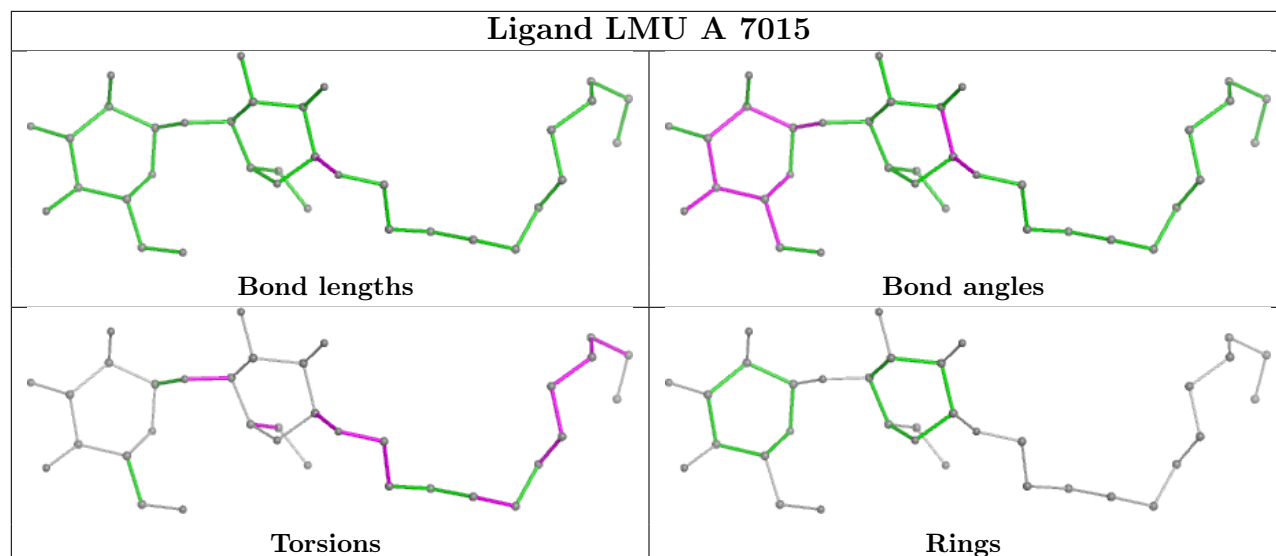




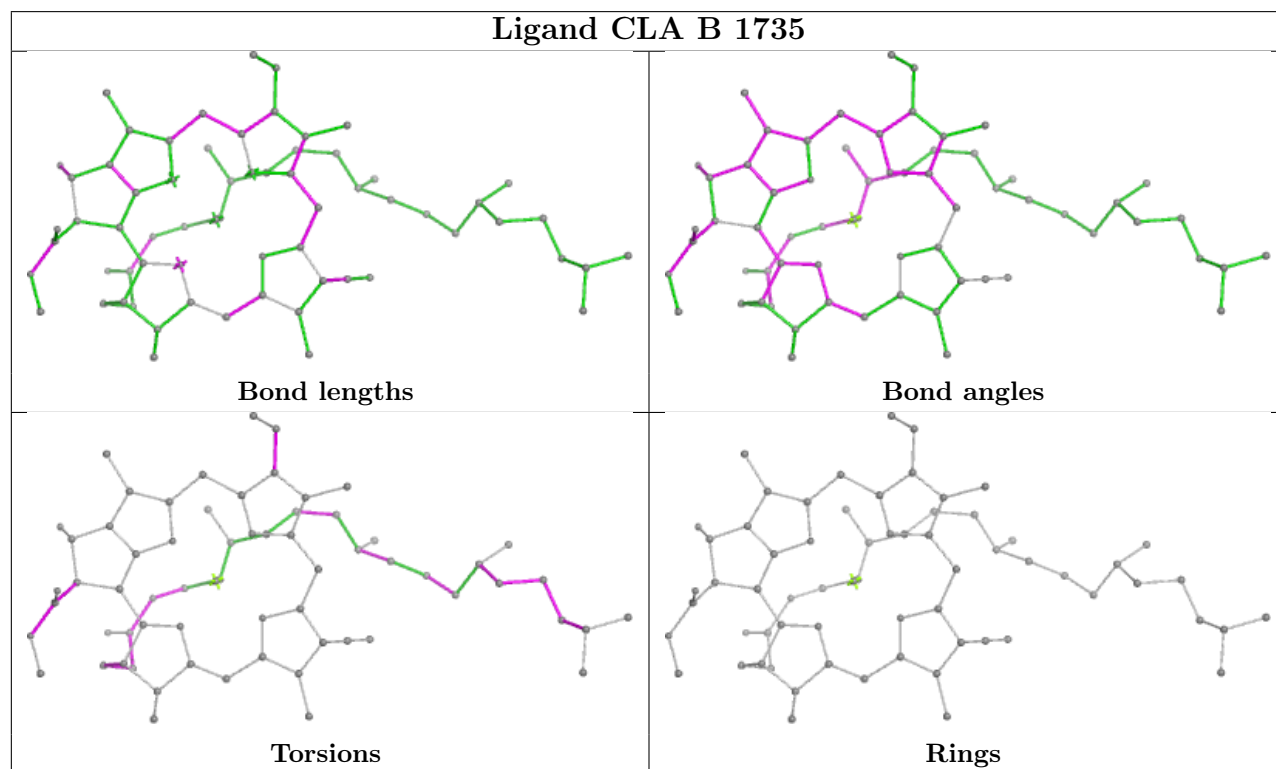


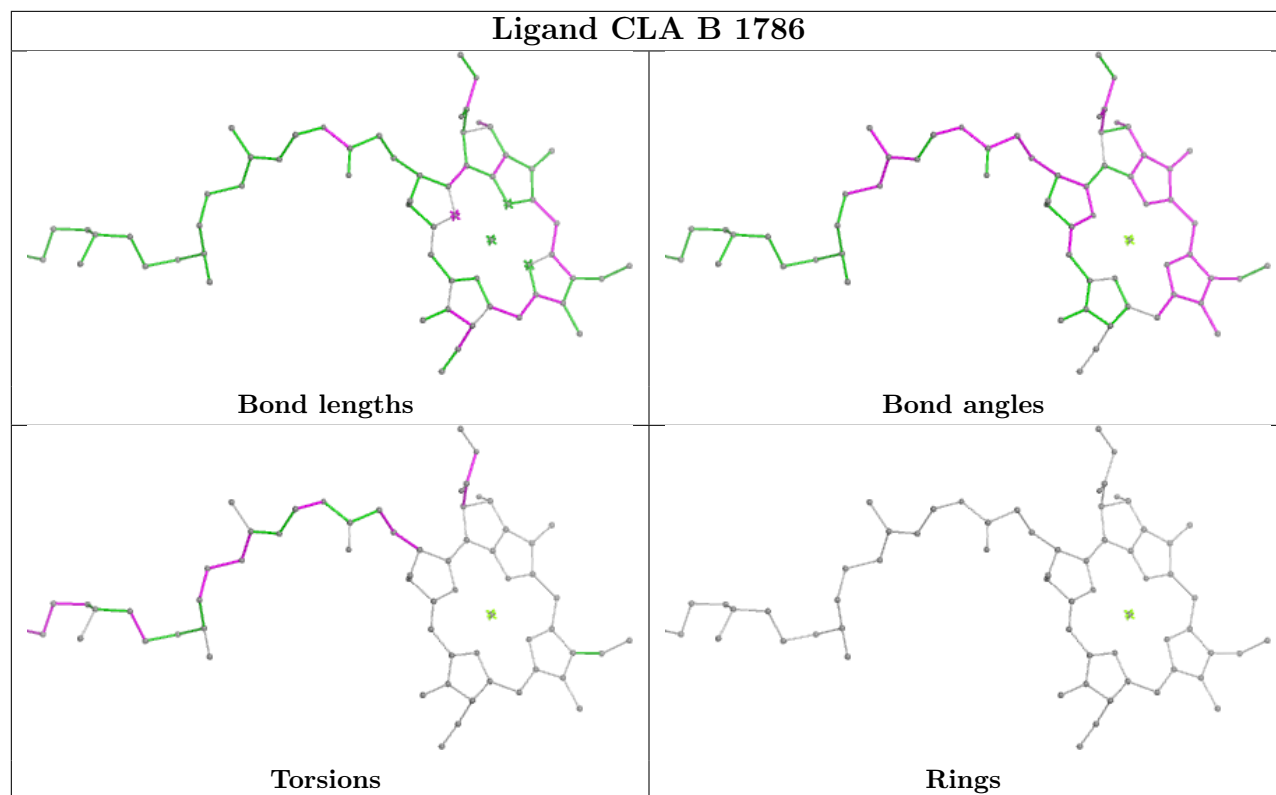


Ligand LMU A 7015

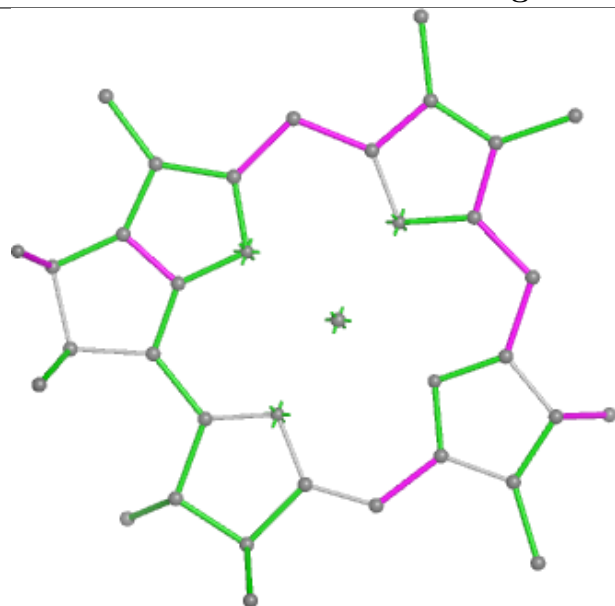


Ligand CLA B 1735

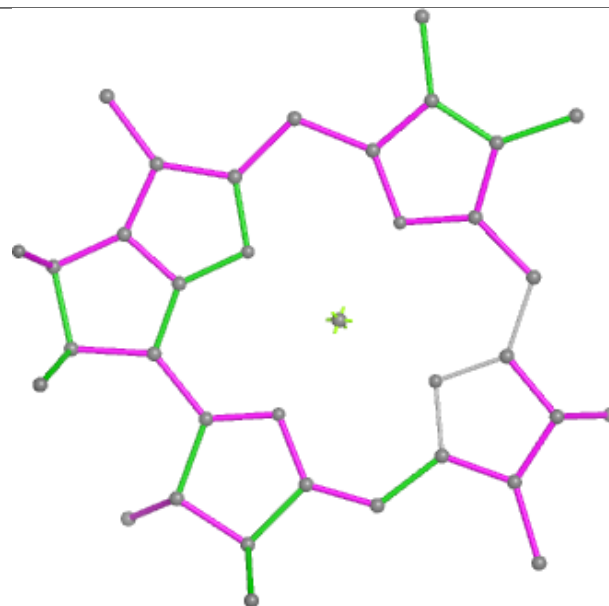




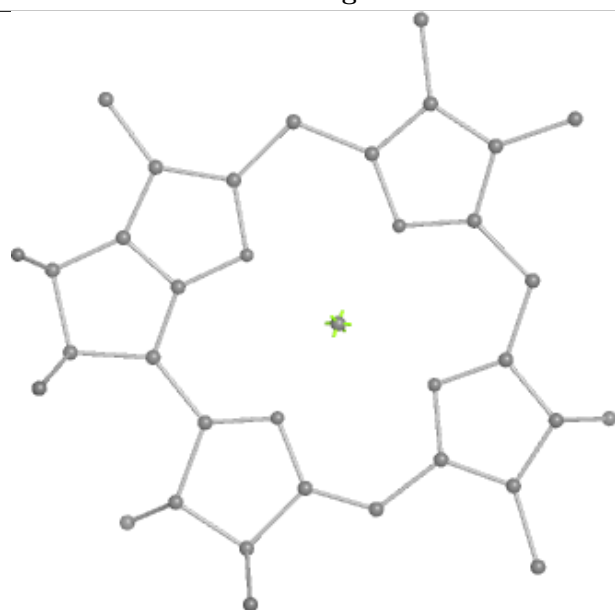
Ligand CLA 3 1212



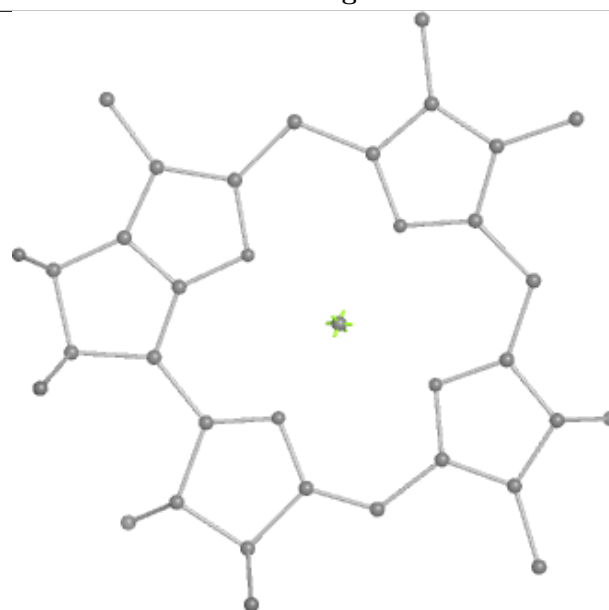
Bond lengths



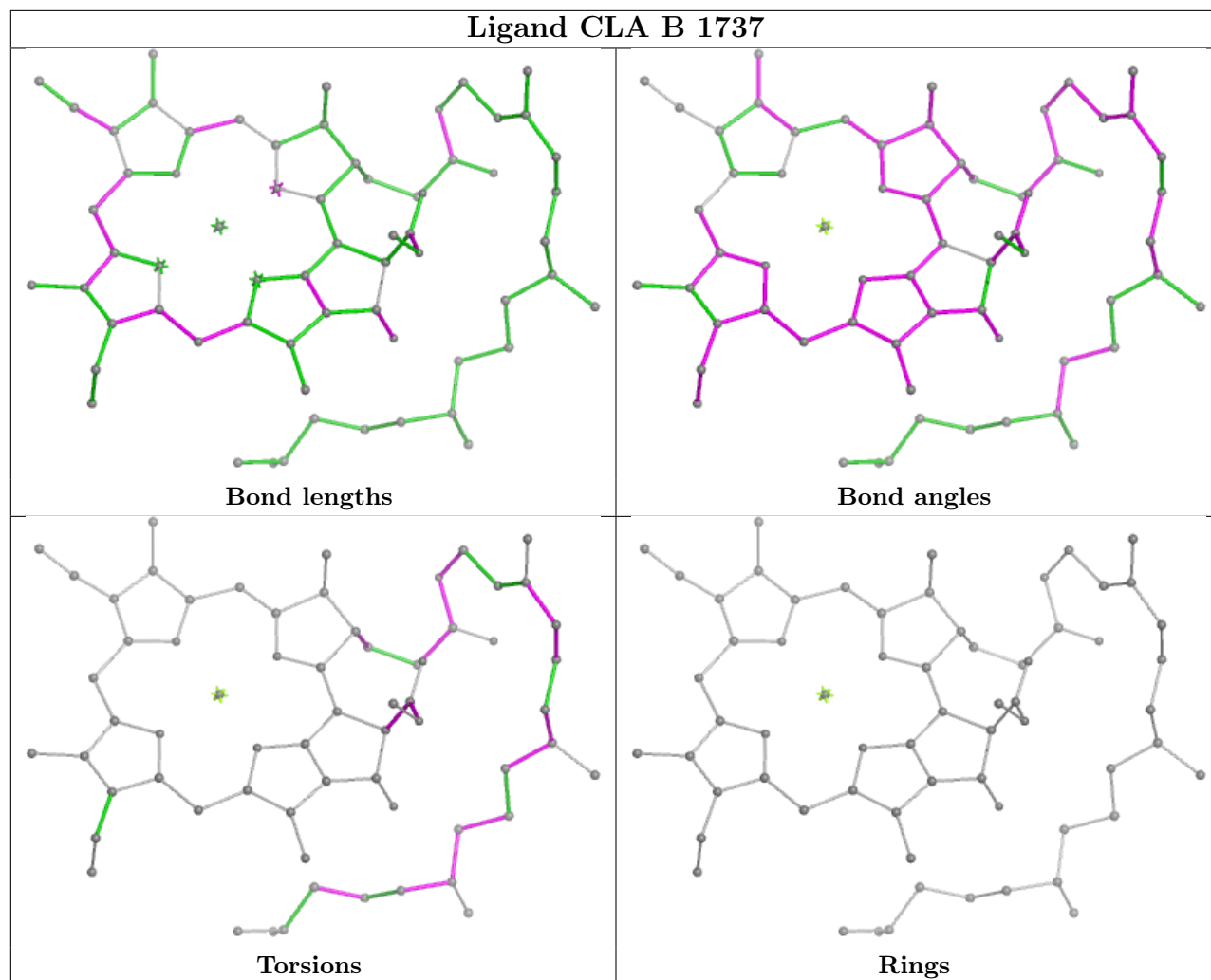
Bond angles



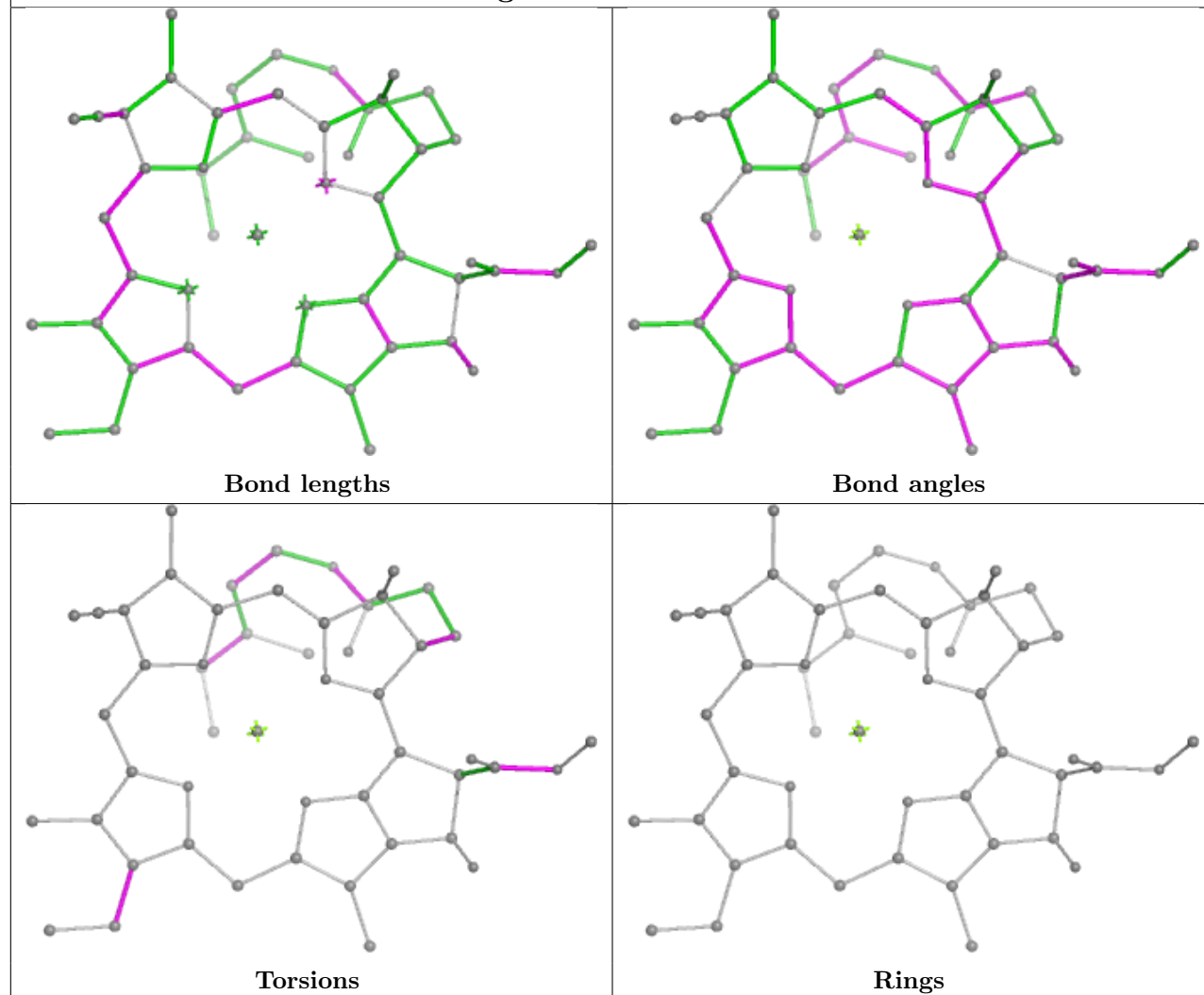
Torsions

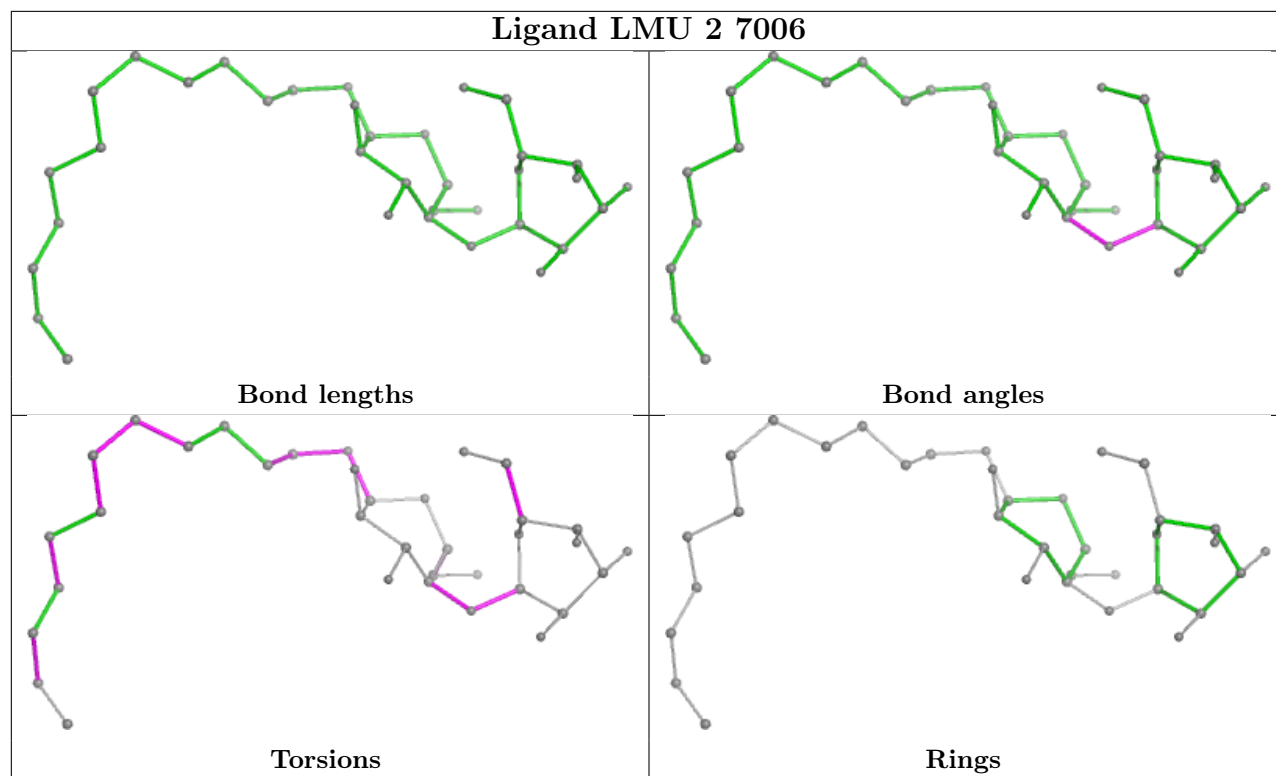


Rings

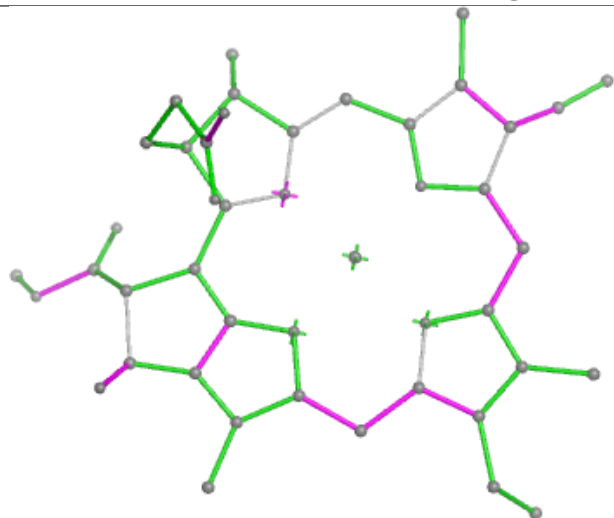


Ligand CLA 2 1212

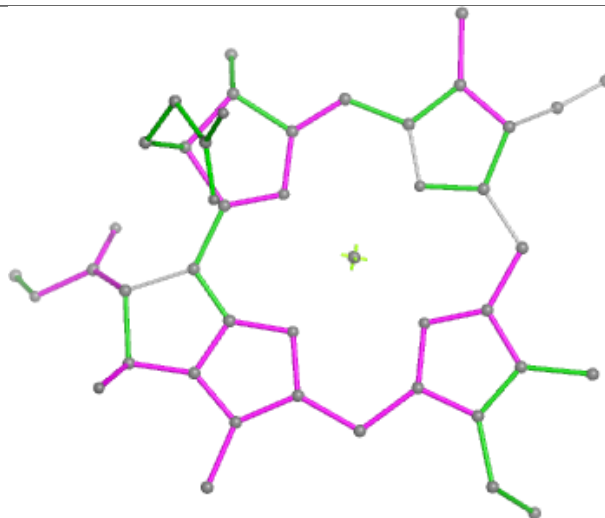




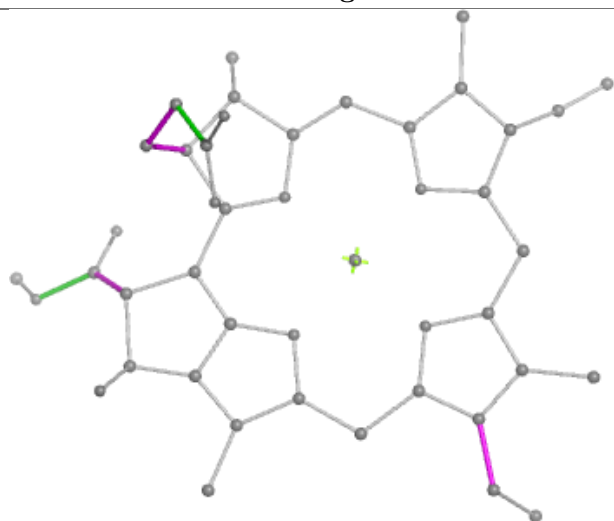
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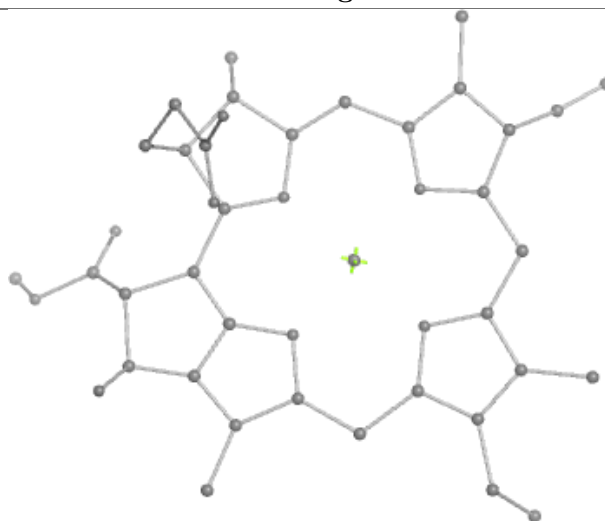
Bond lengths



Bond angles

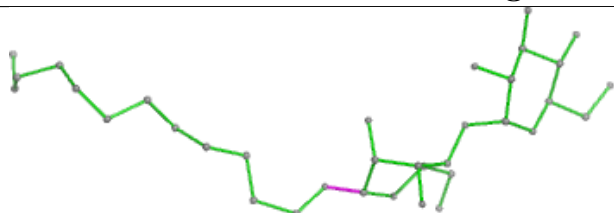


Torsions

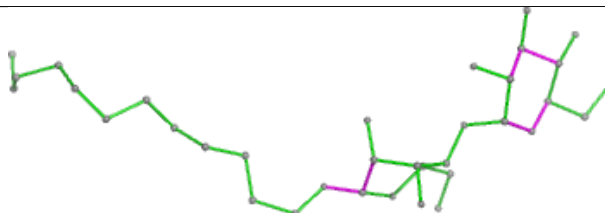


Rings

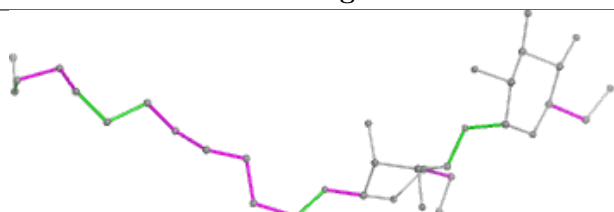
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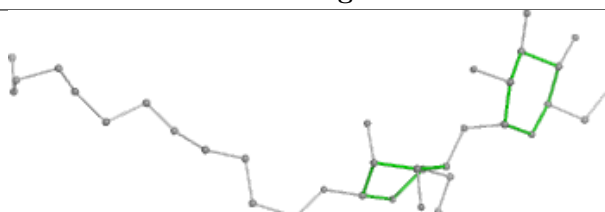
Bond lengths



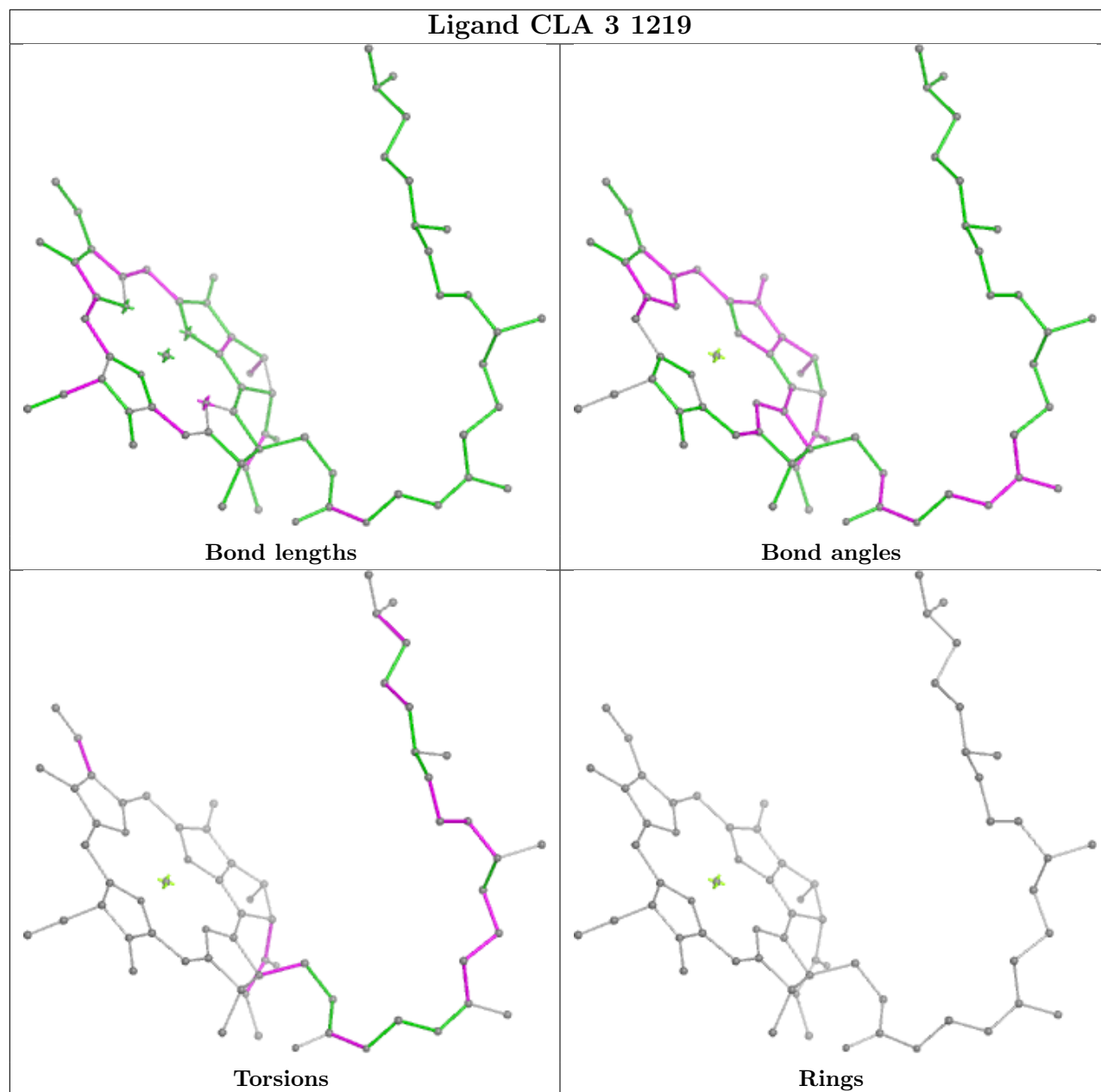
Bond angles



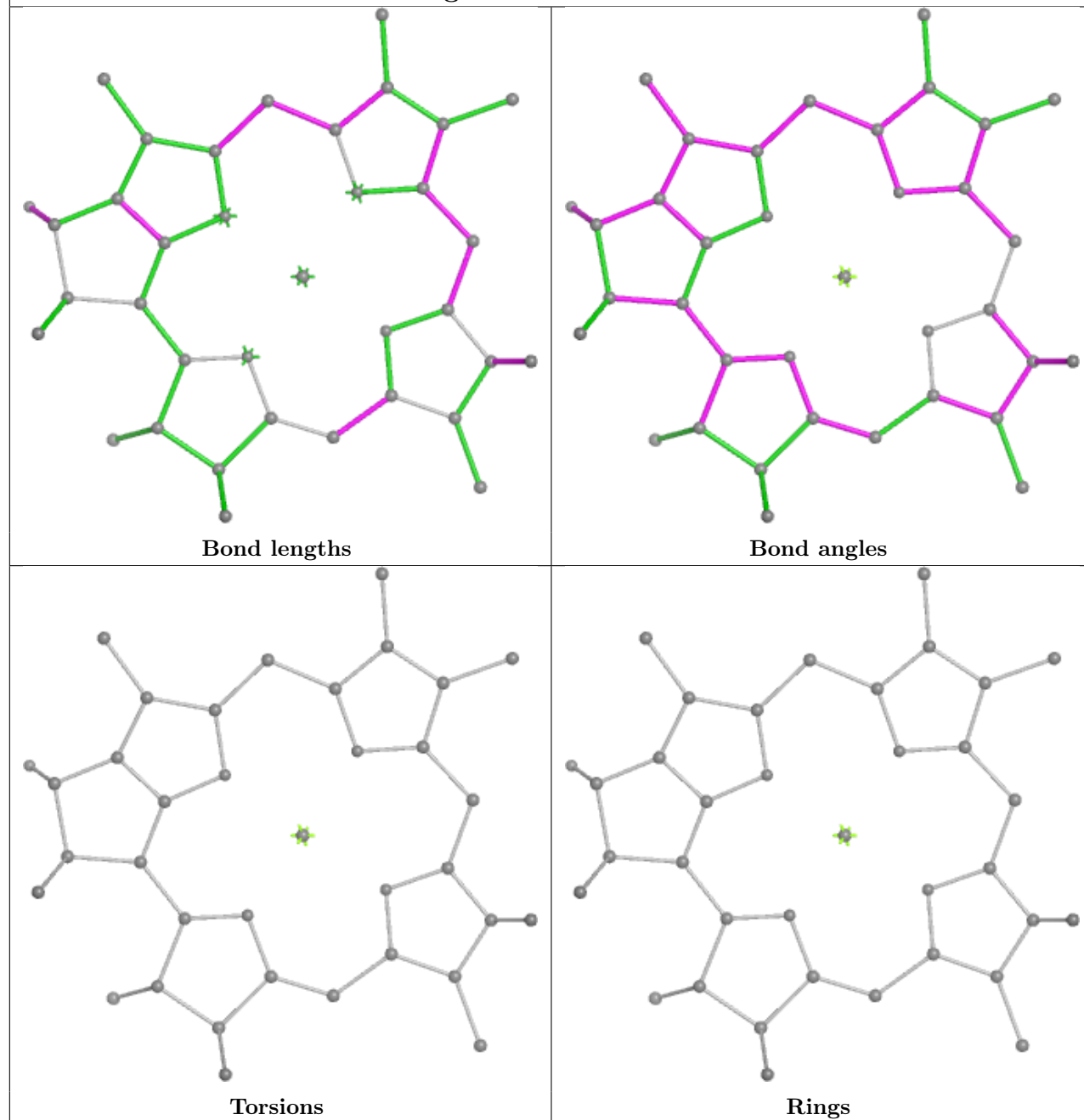
Torsions

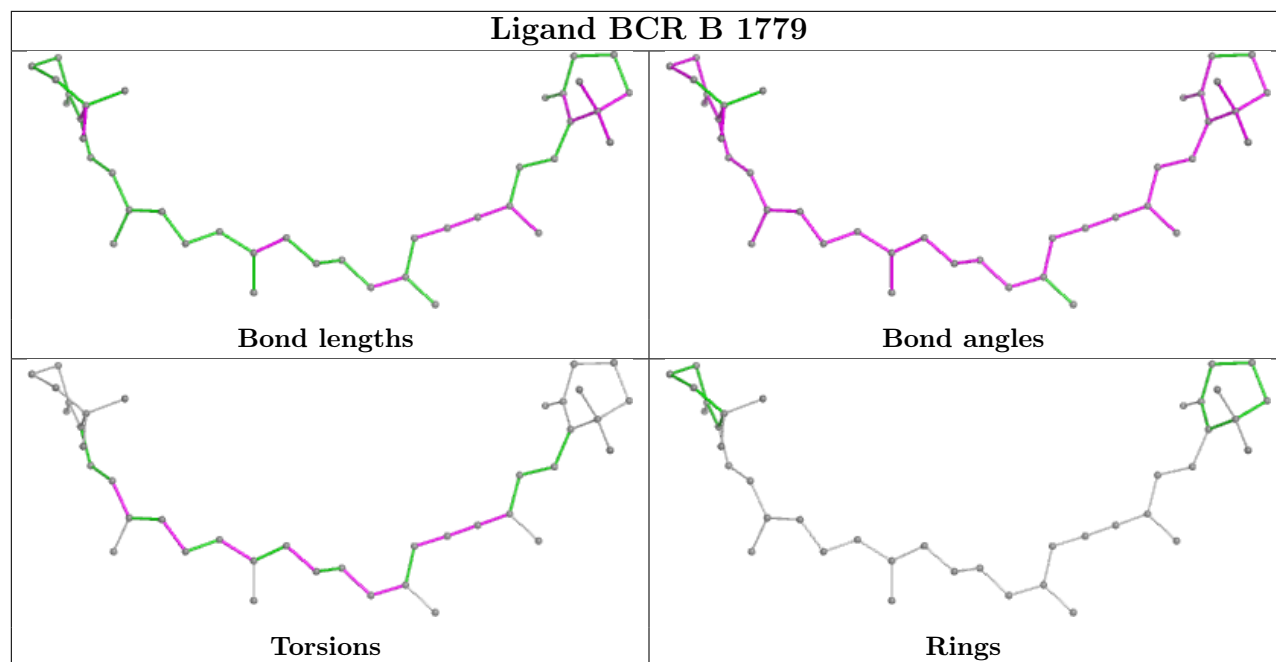


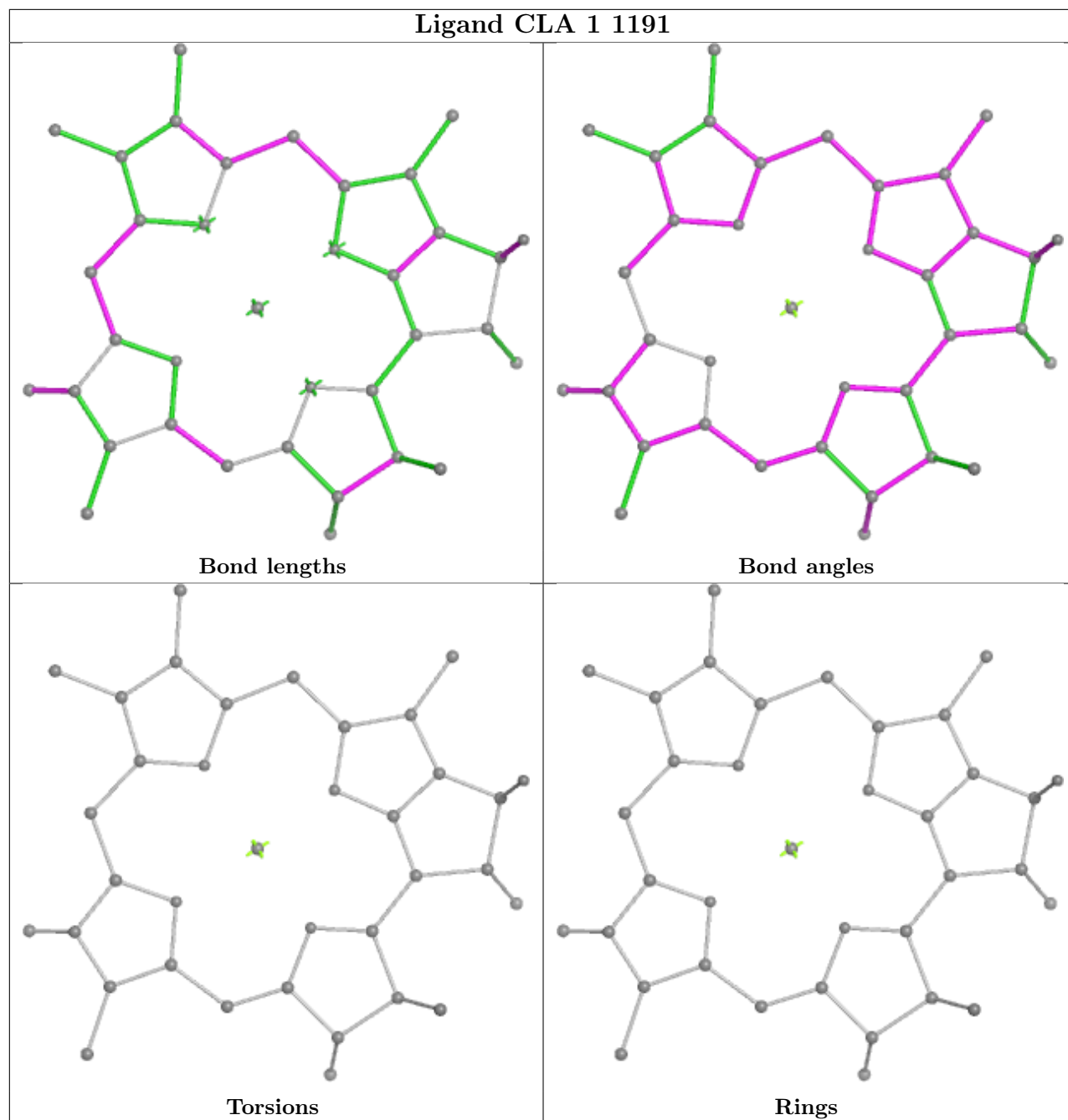
Rings

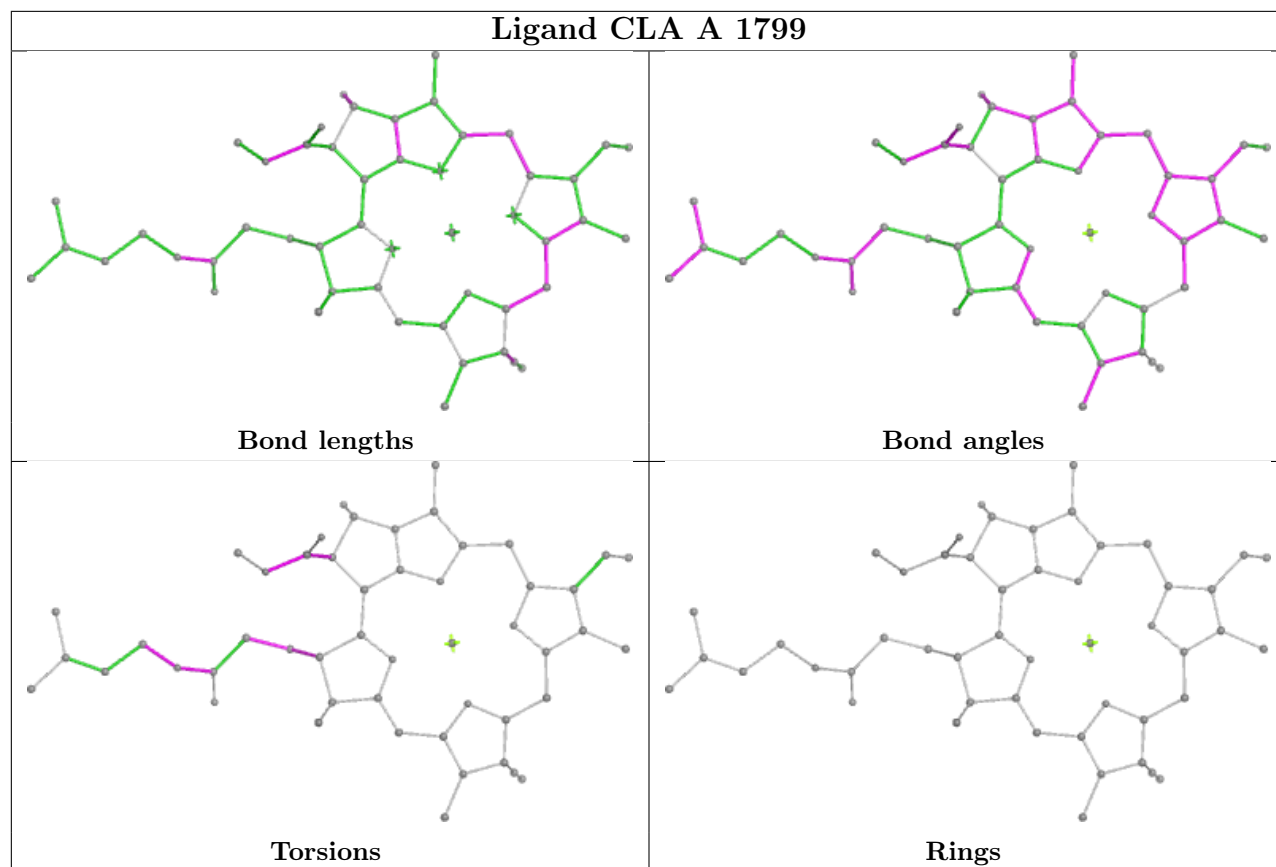


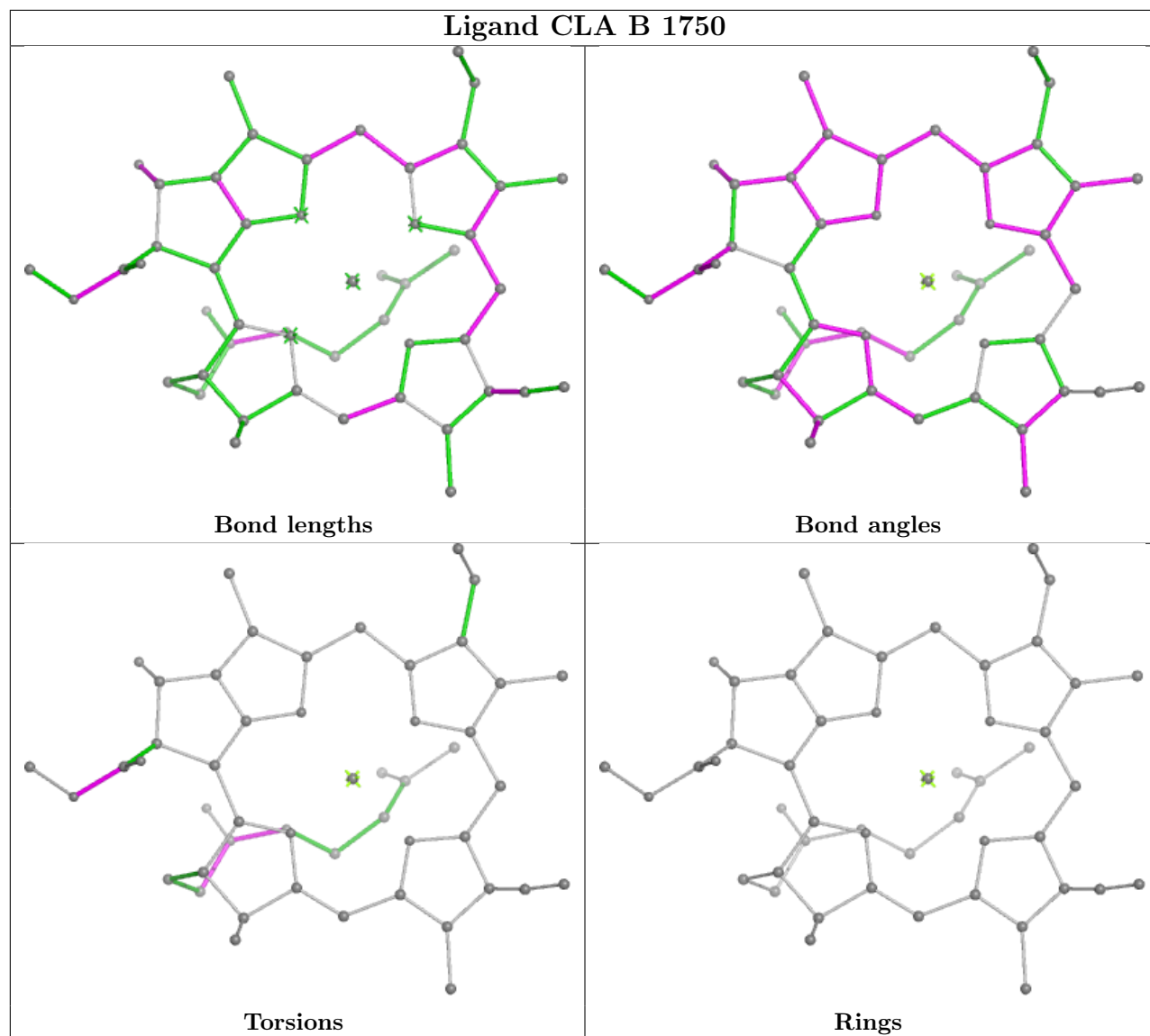
Ligand CLA A 1775



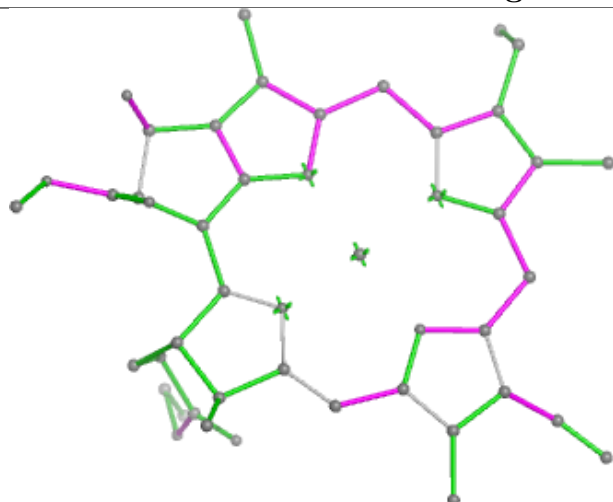




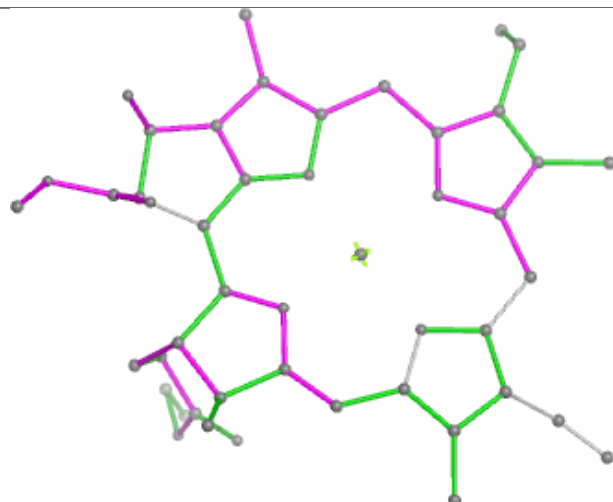




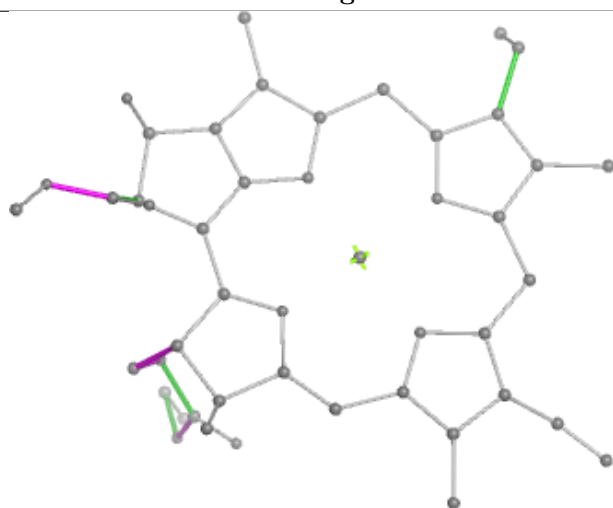
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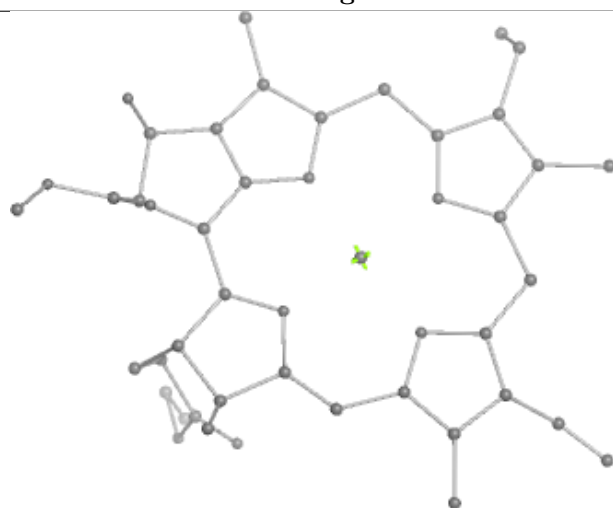
Bond lengths



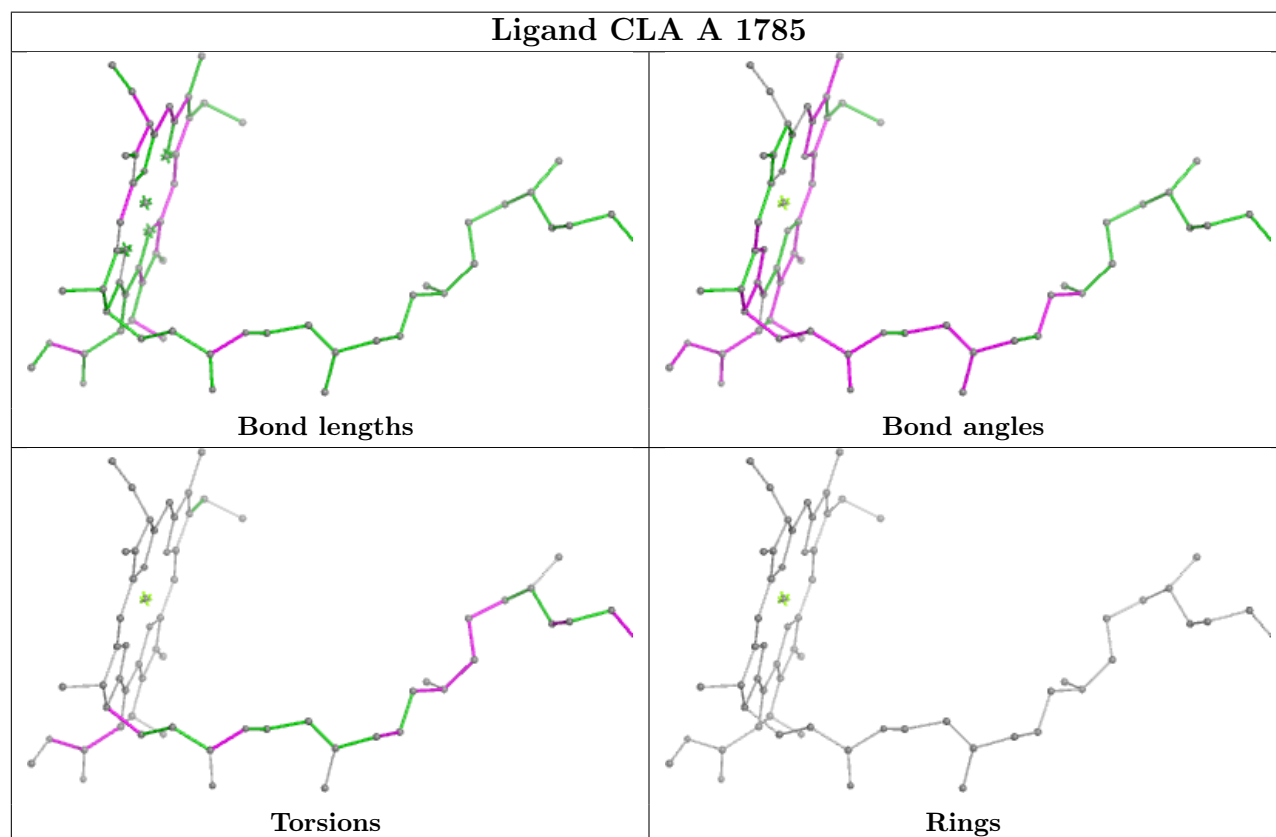
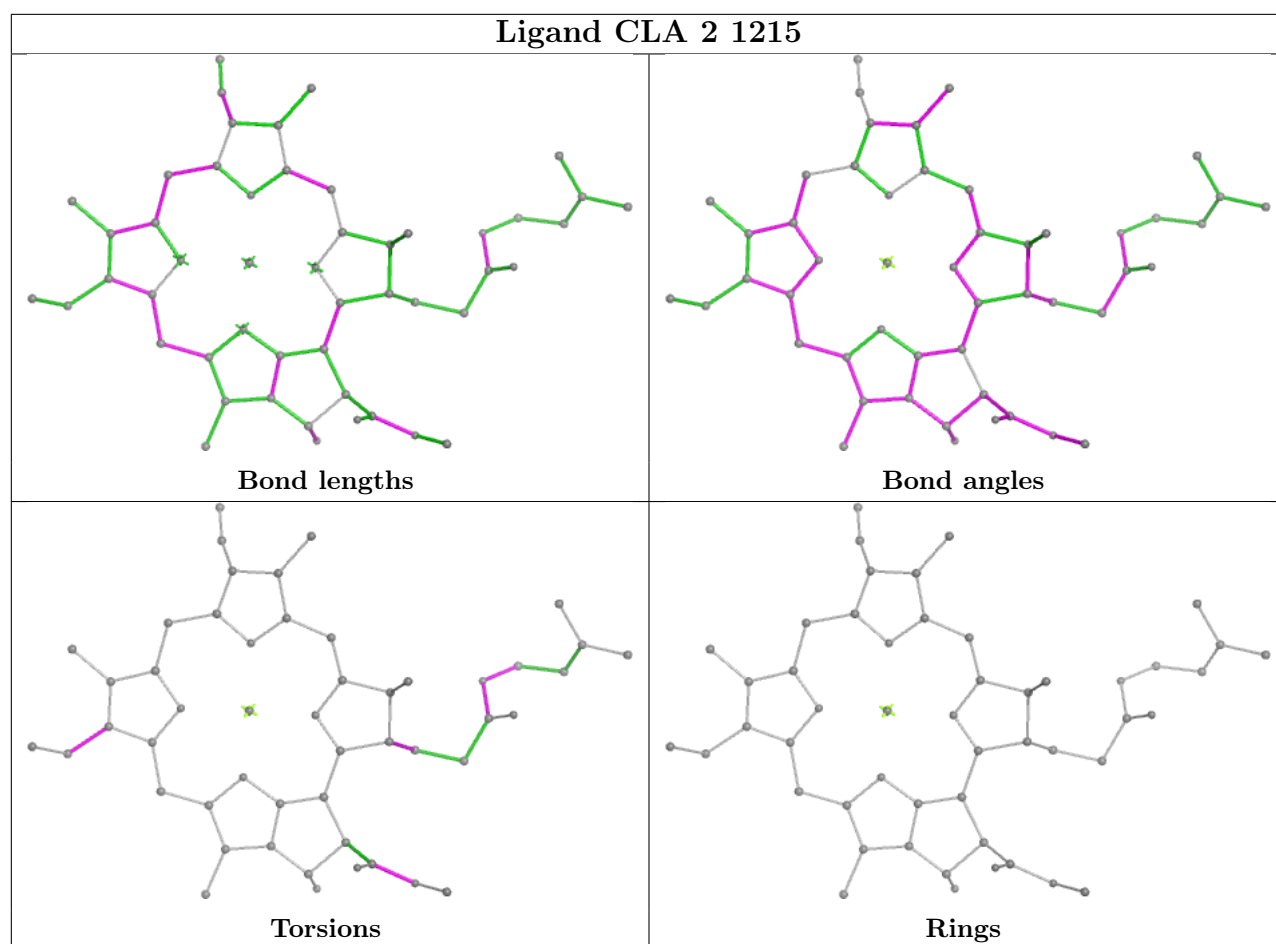
Bond angles

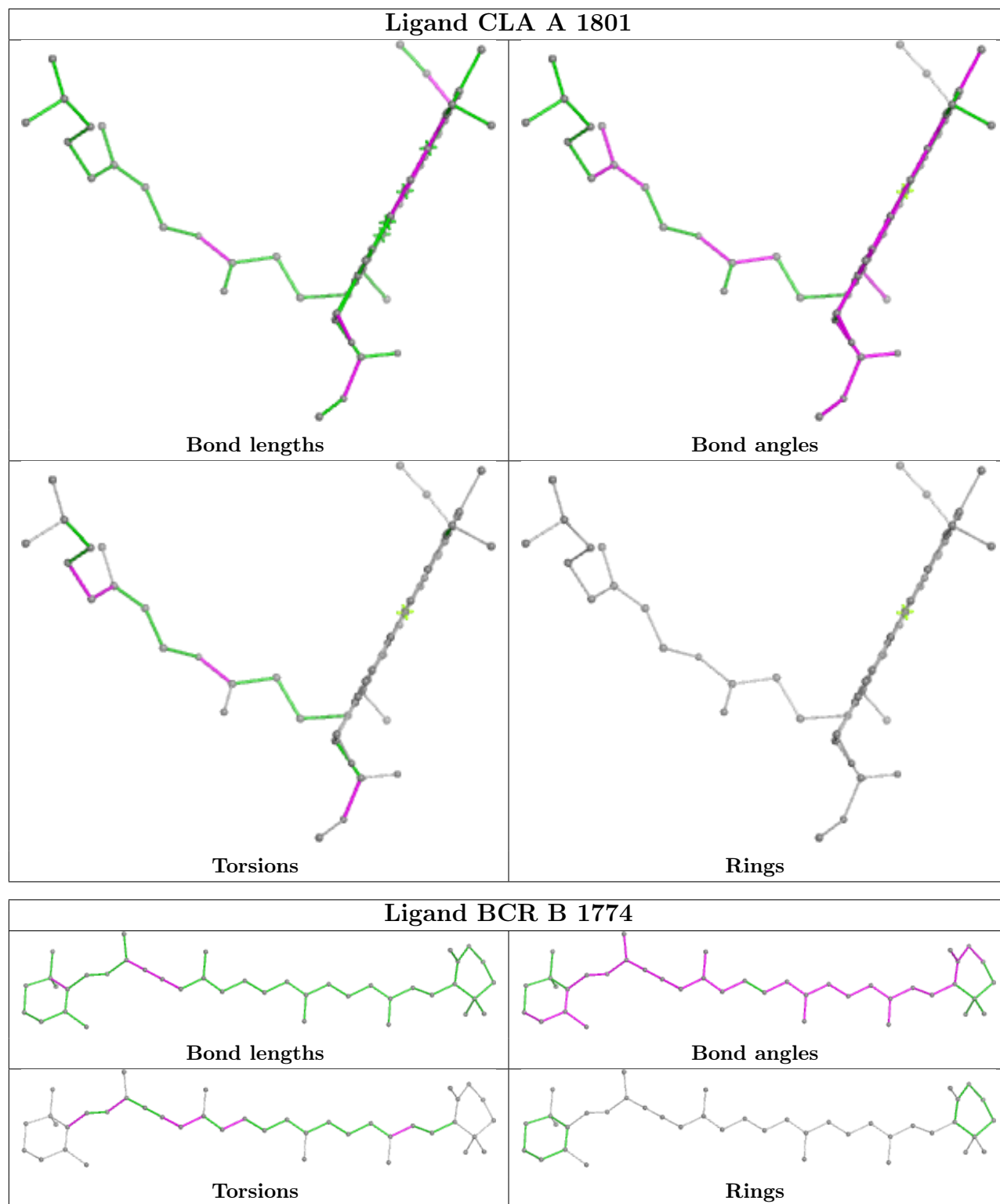


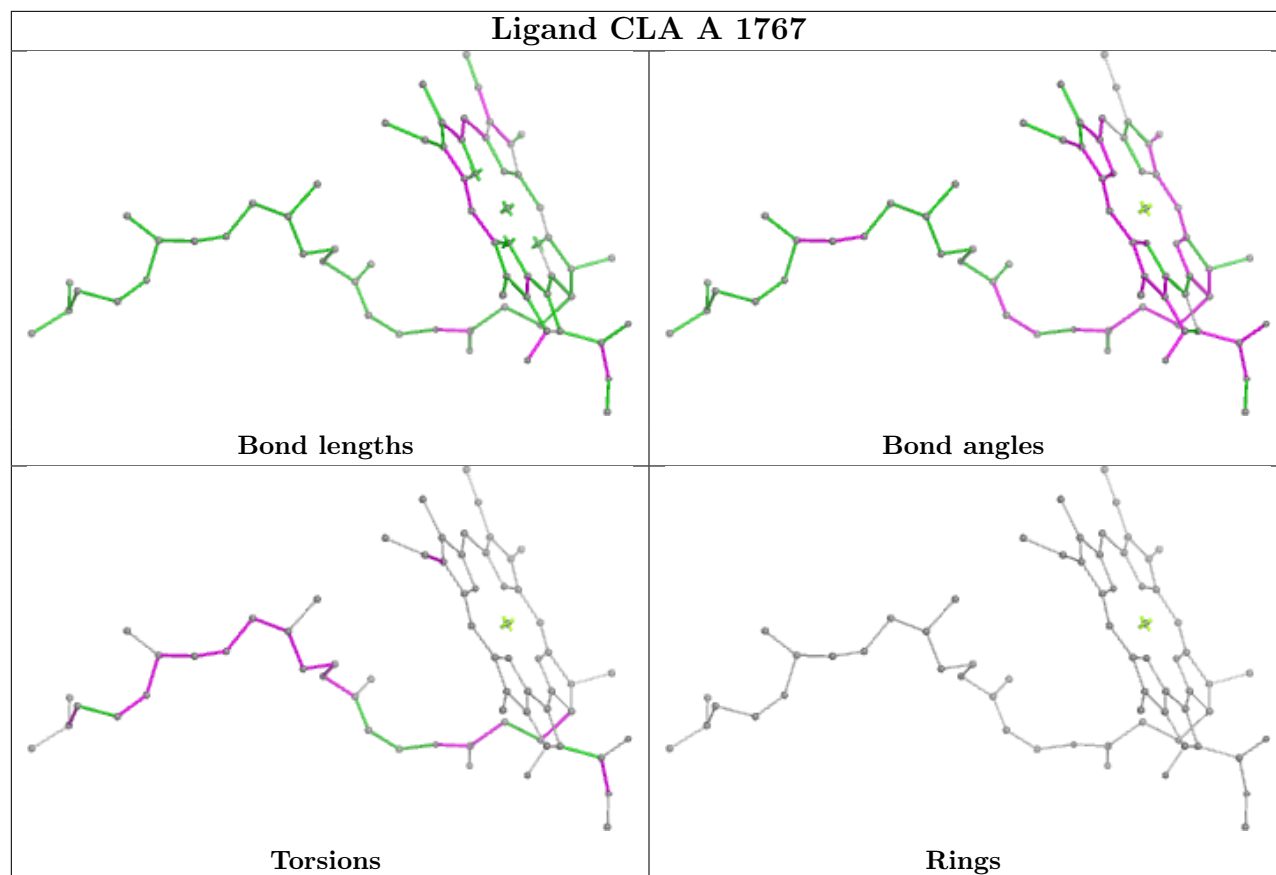
Torsions

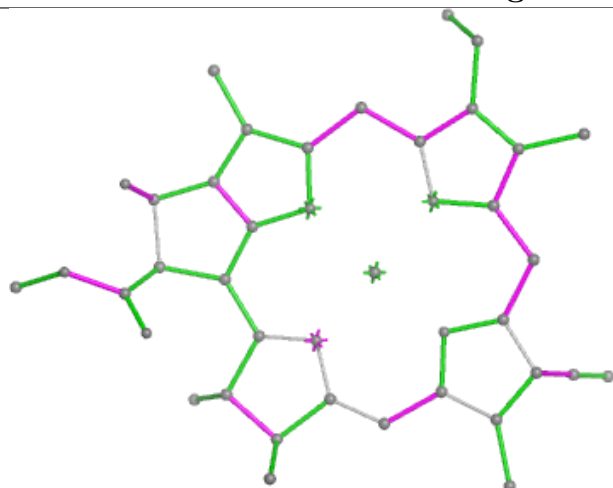


Rings

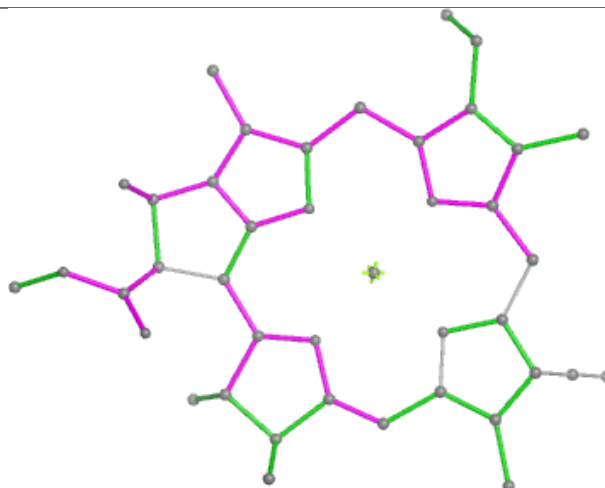




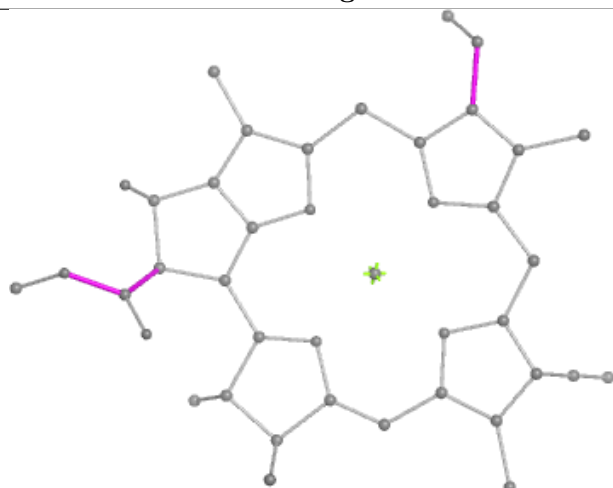


Ligand CLA F 1156

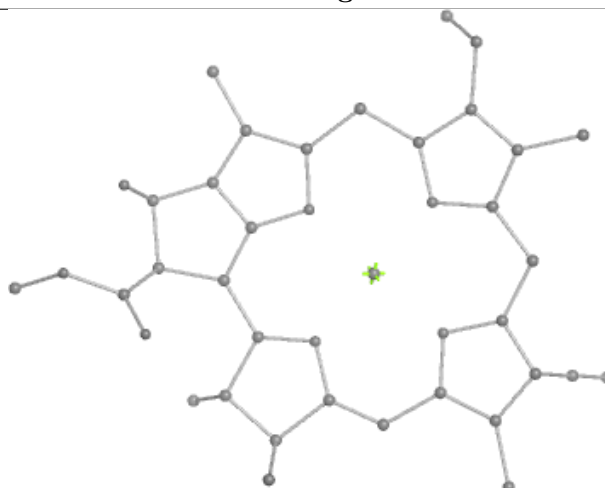
Bond lengths



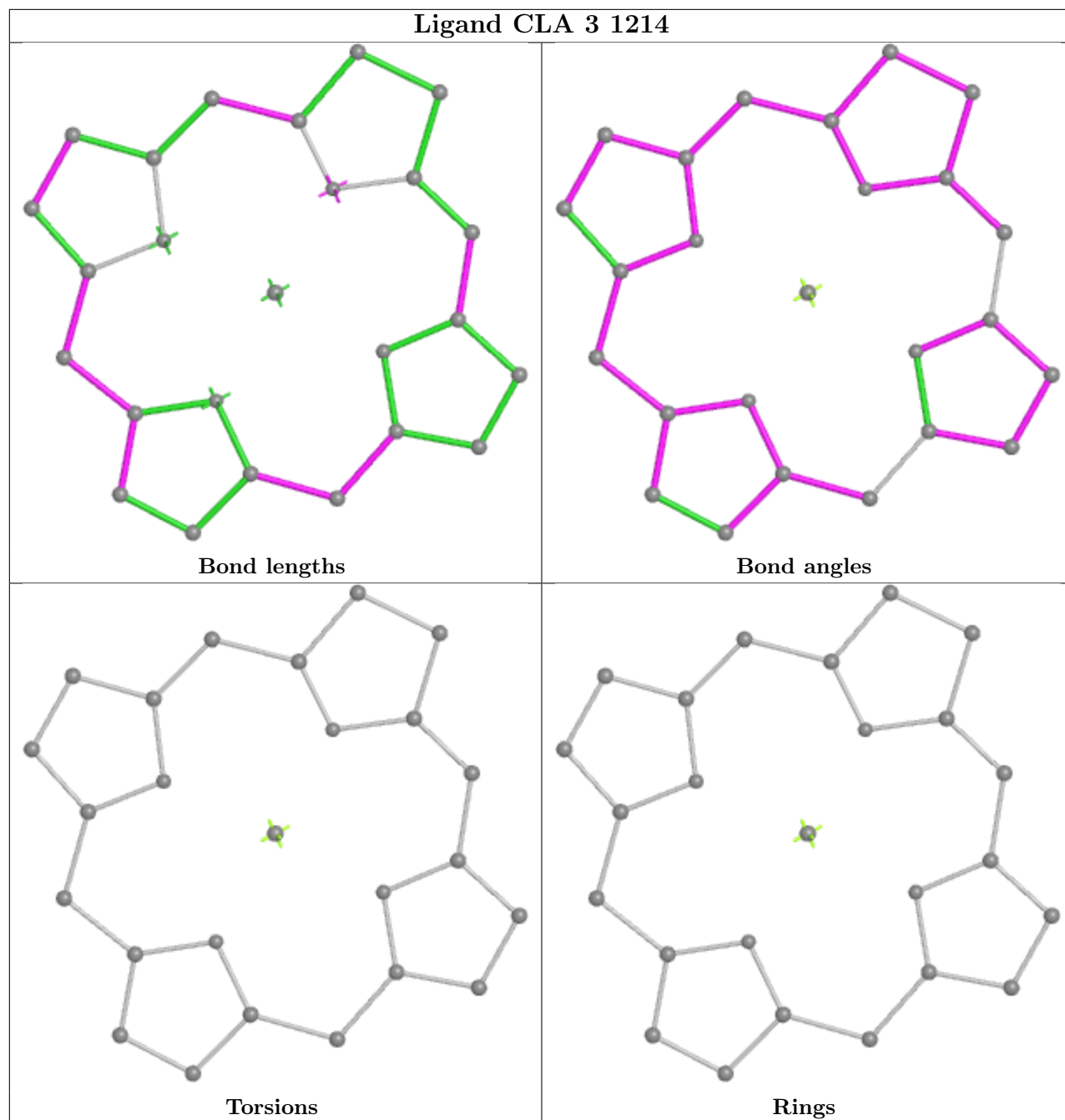
Bond angles



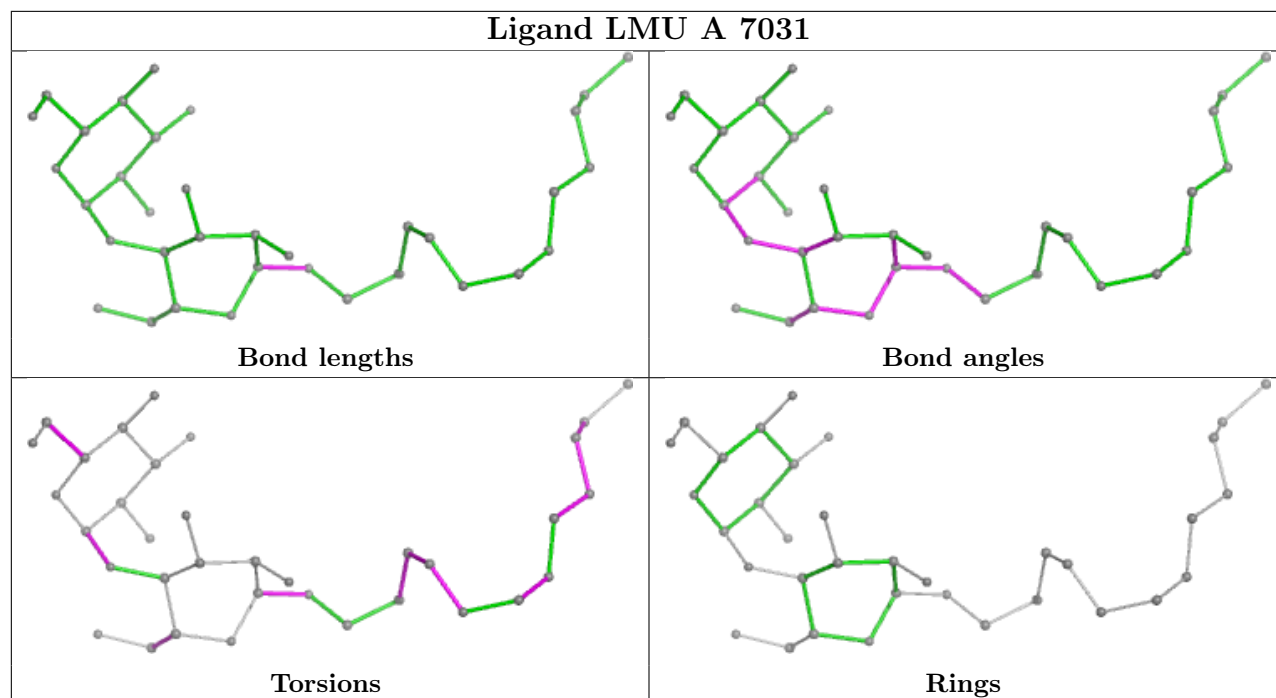
Torsions



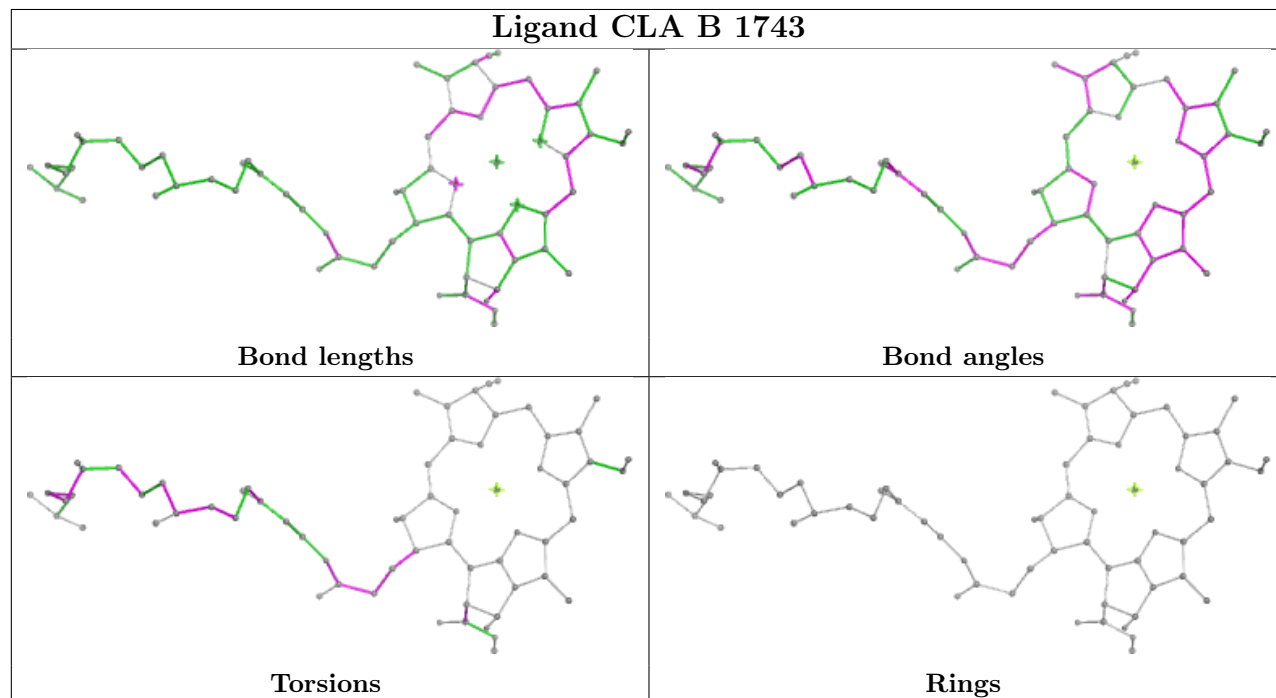
Rings



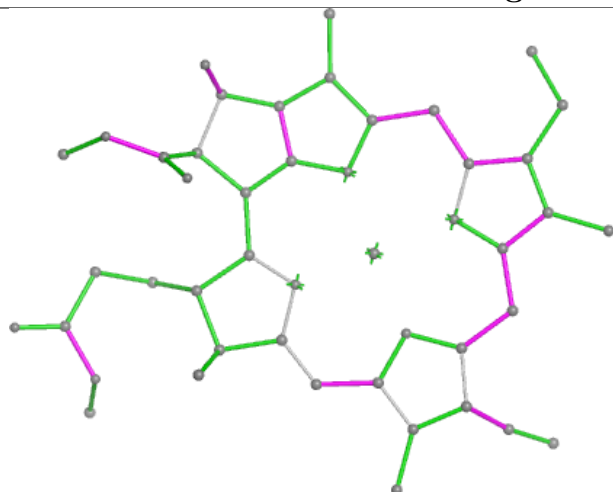
Ligand LMU A 7031



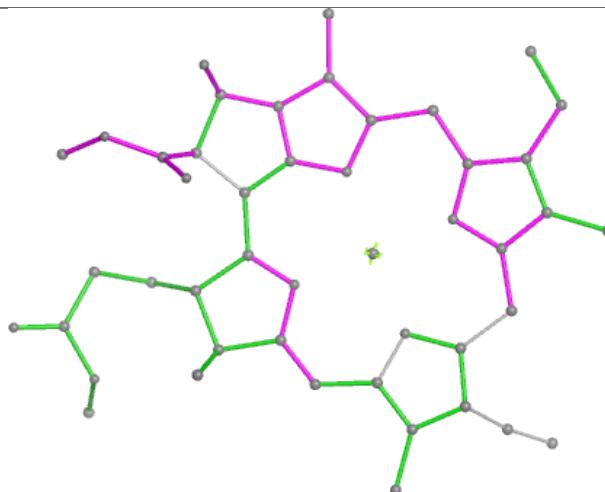
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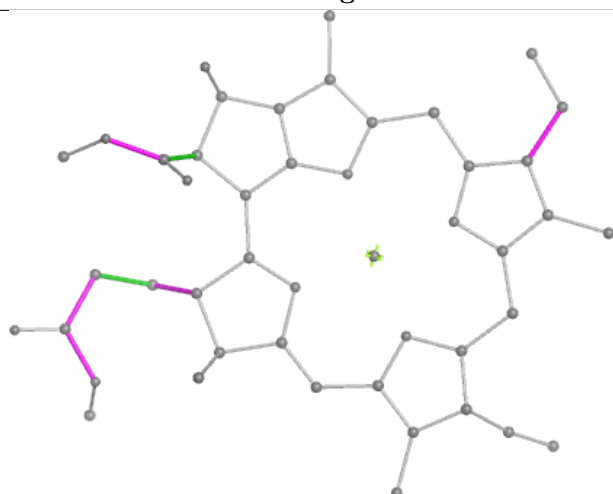
Ligand CLA B 1746



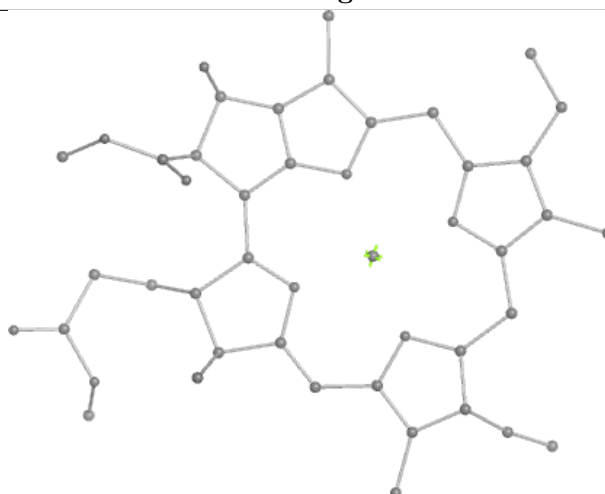
Bond lengths



Bond angles



Torsions

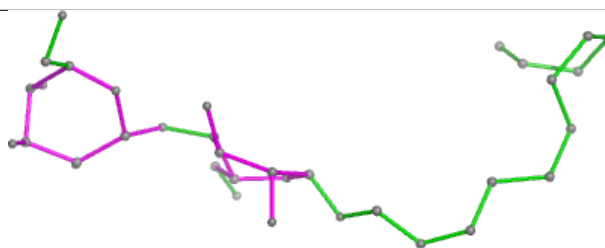


Rings

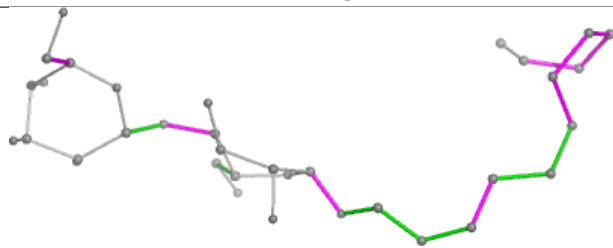
Ligand LMU A 7043



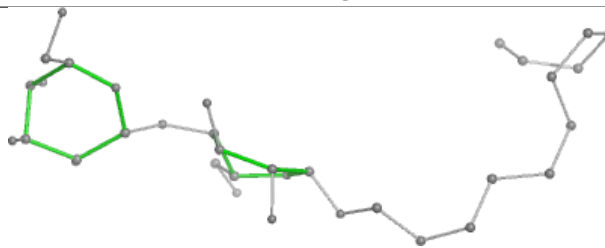
Bond lengths



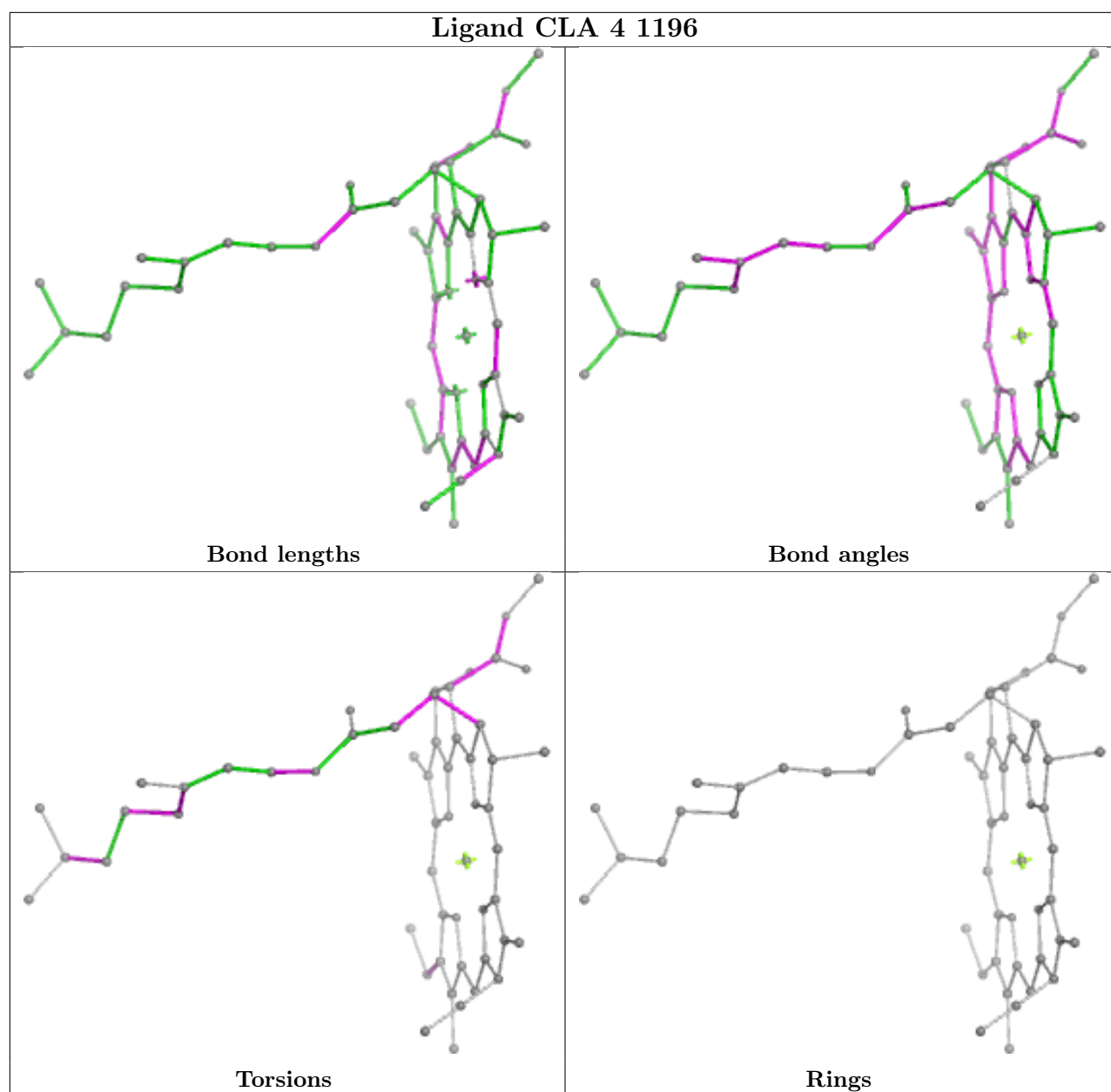
Bond angles

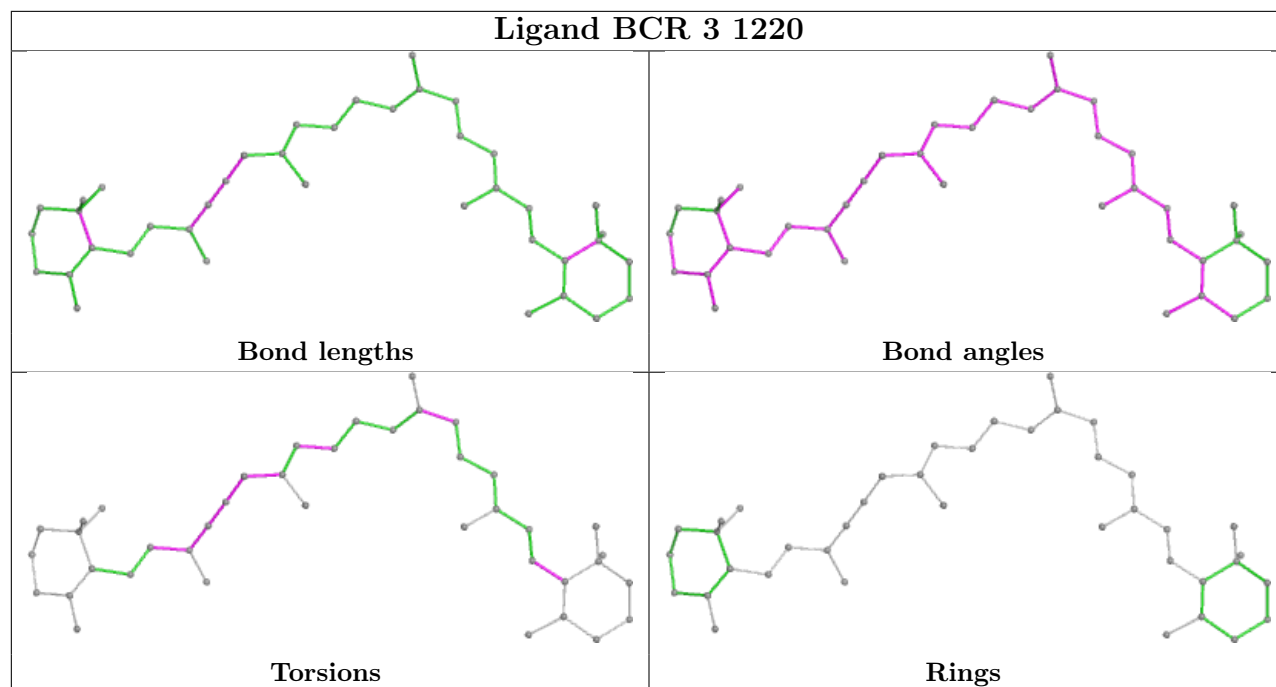


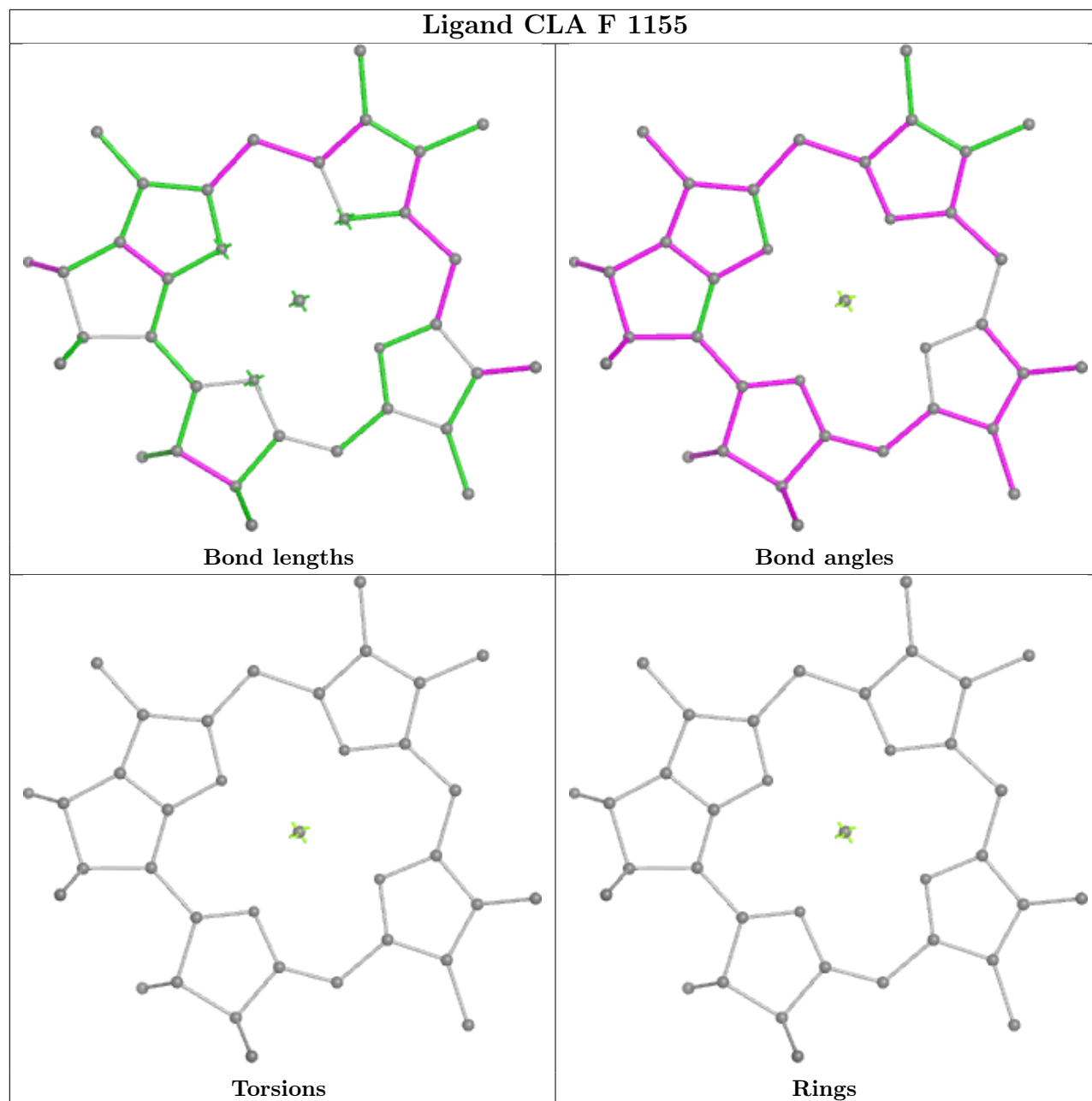
Torsions

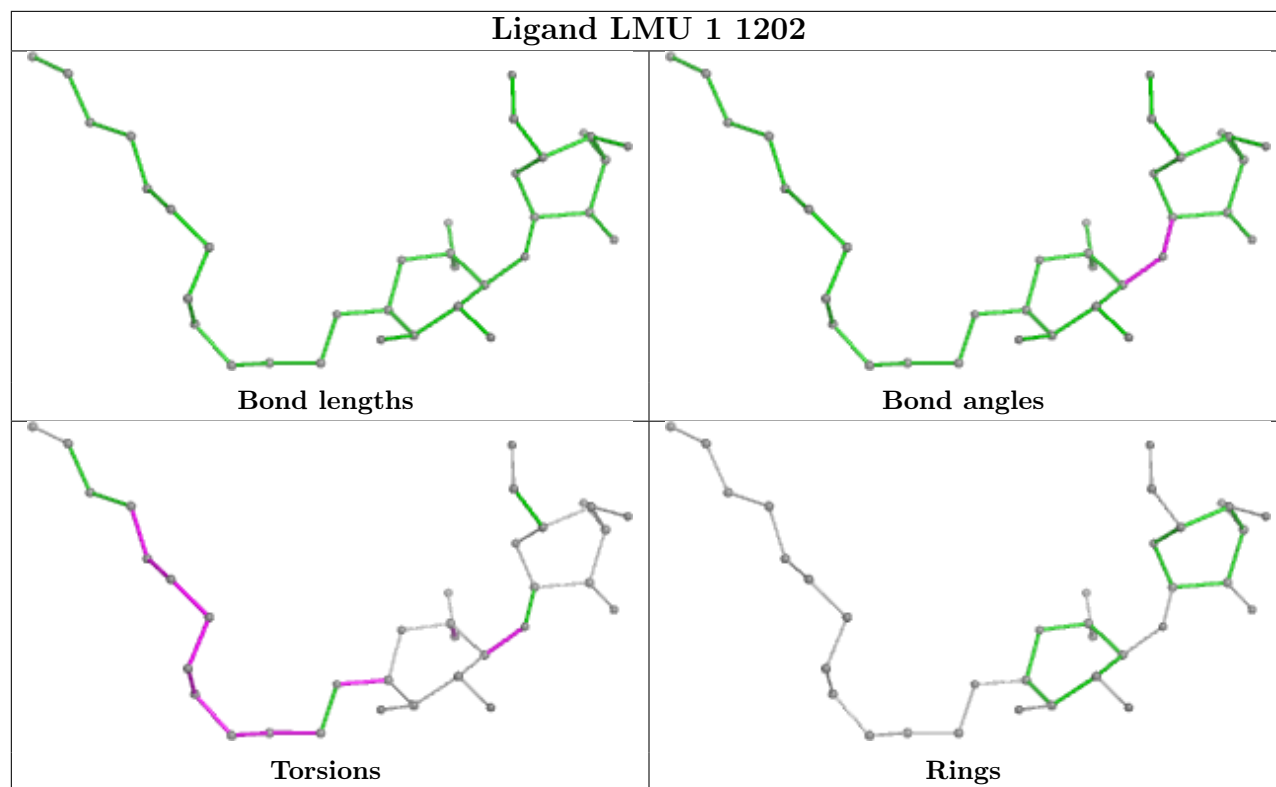


Rings

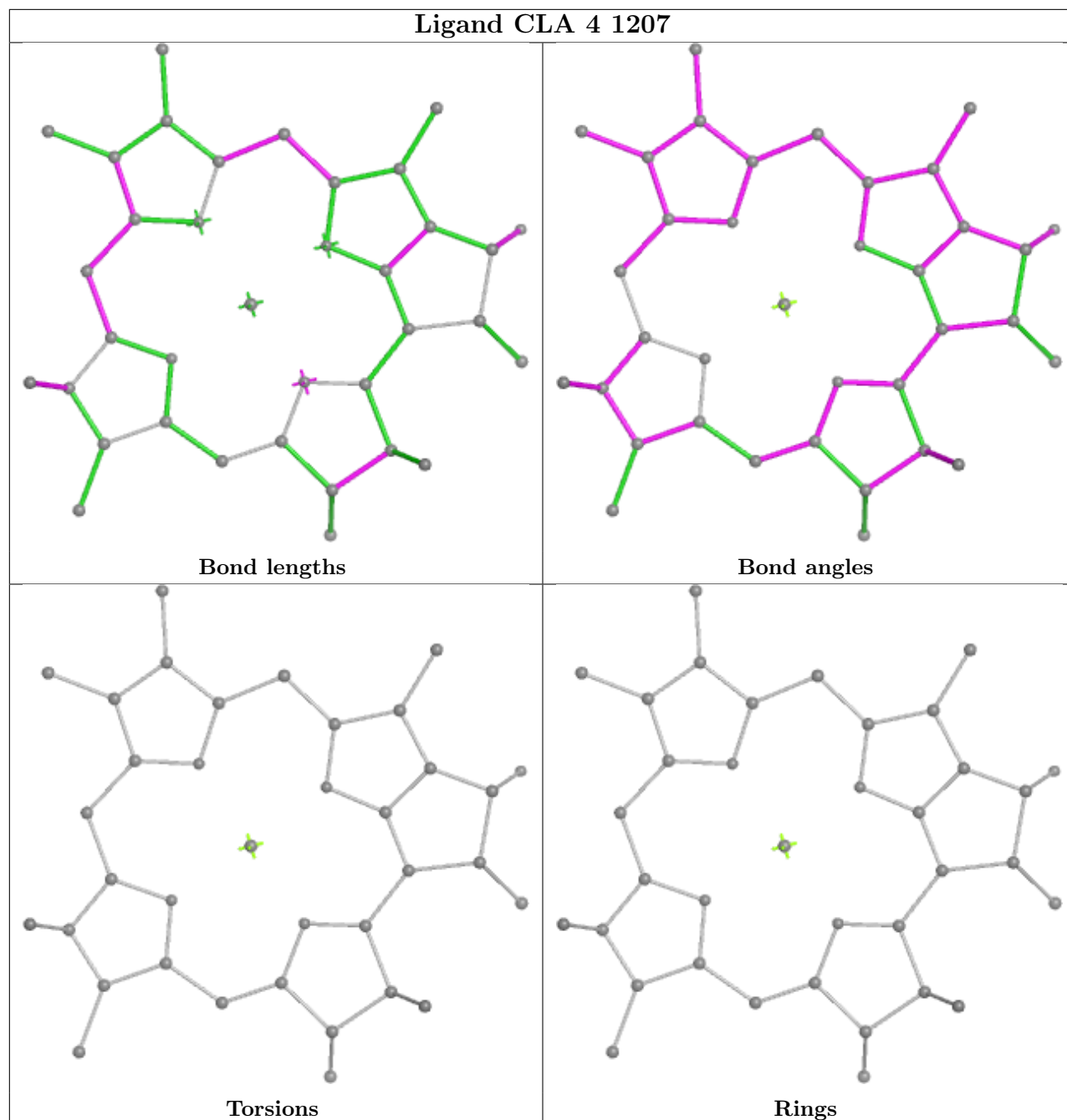


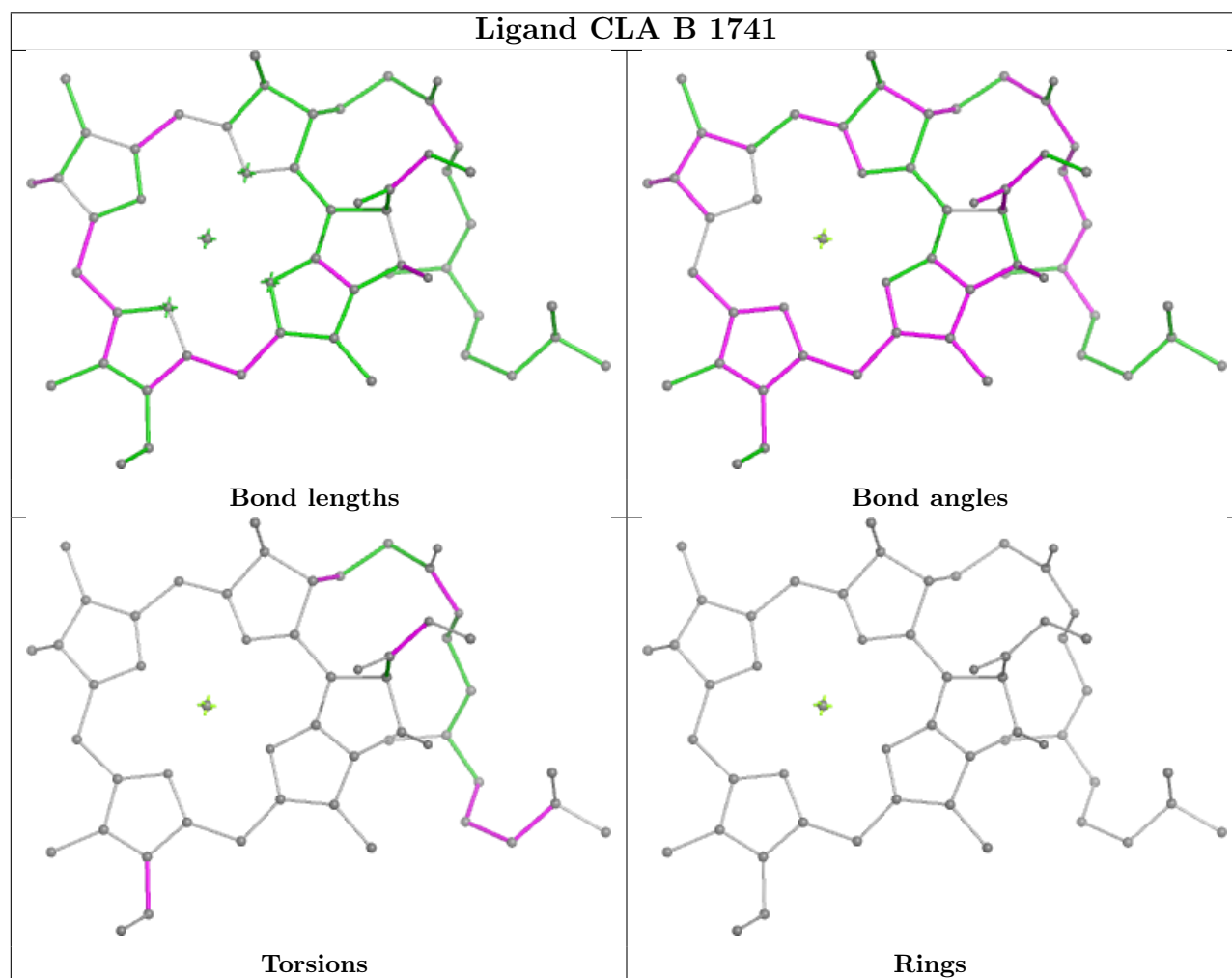
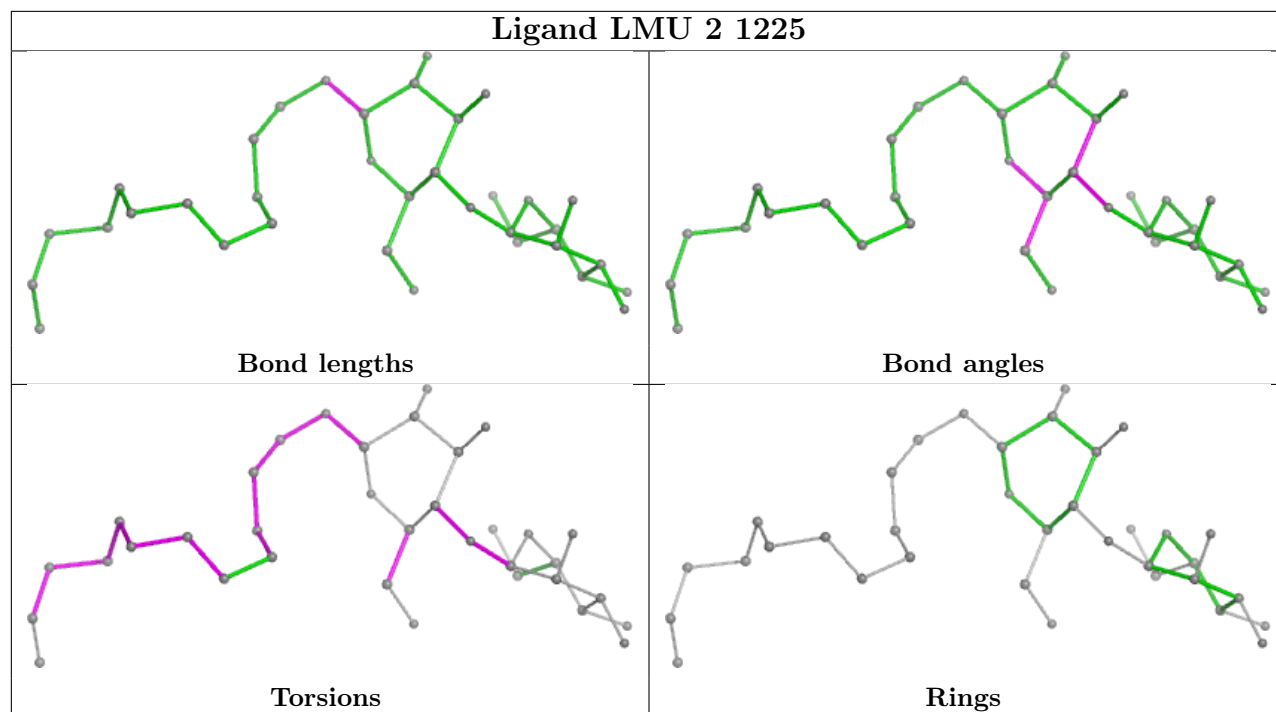




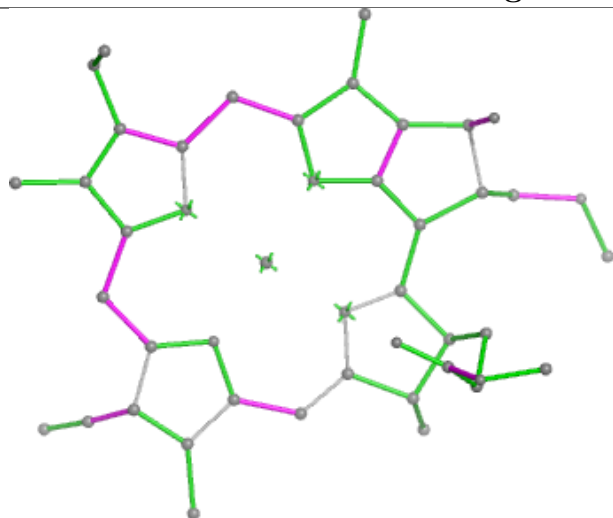


Ligand CLA 4 1207

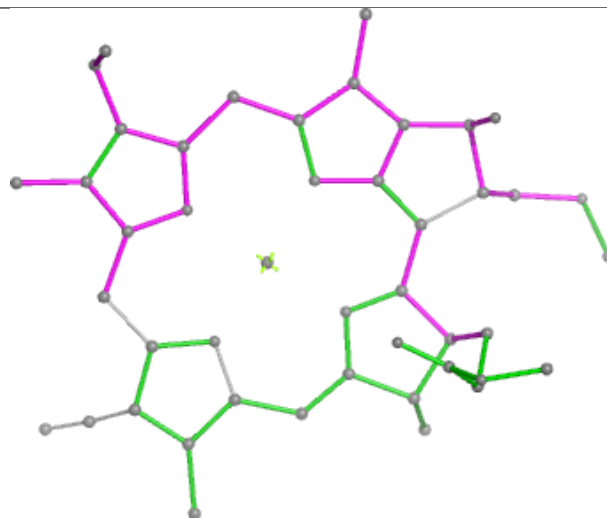




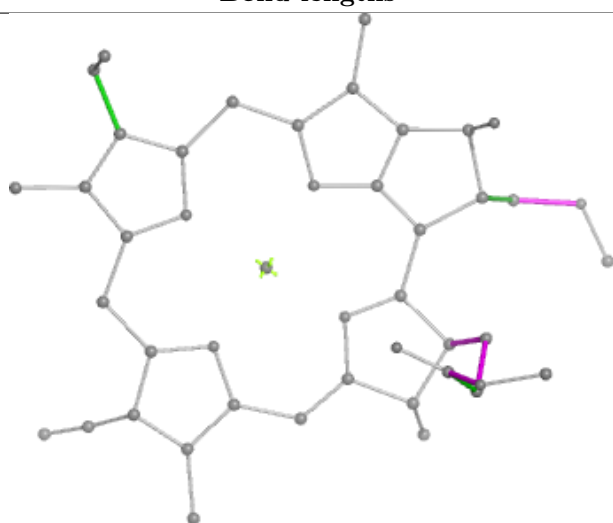
Ligand CLA A 1763



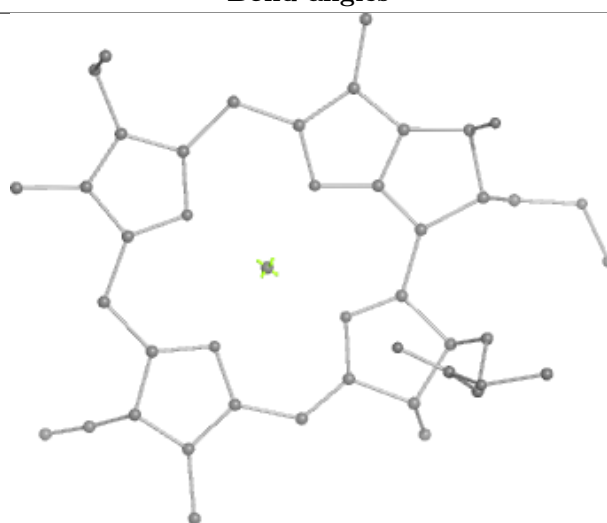
Bond lengths



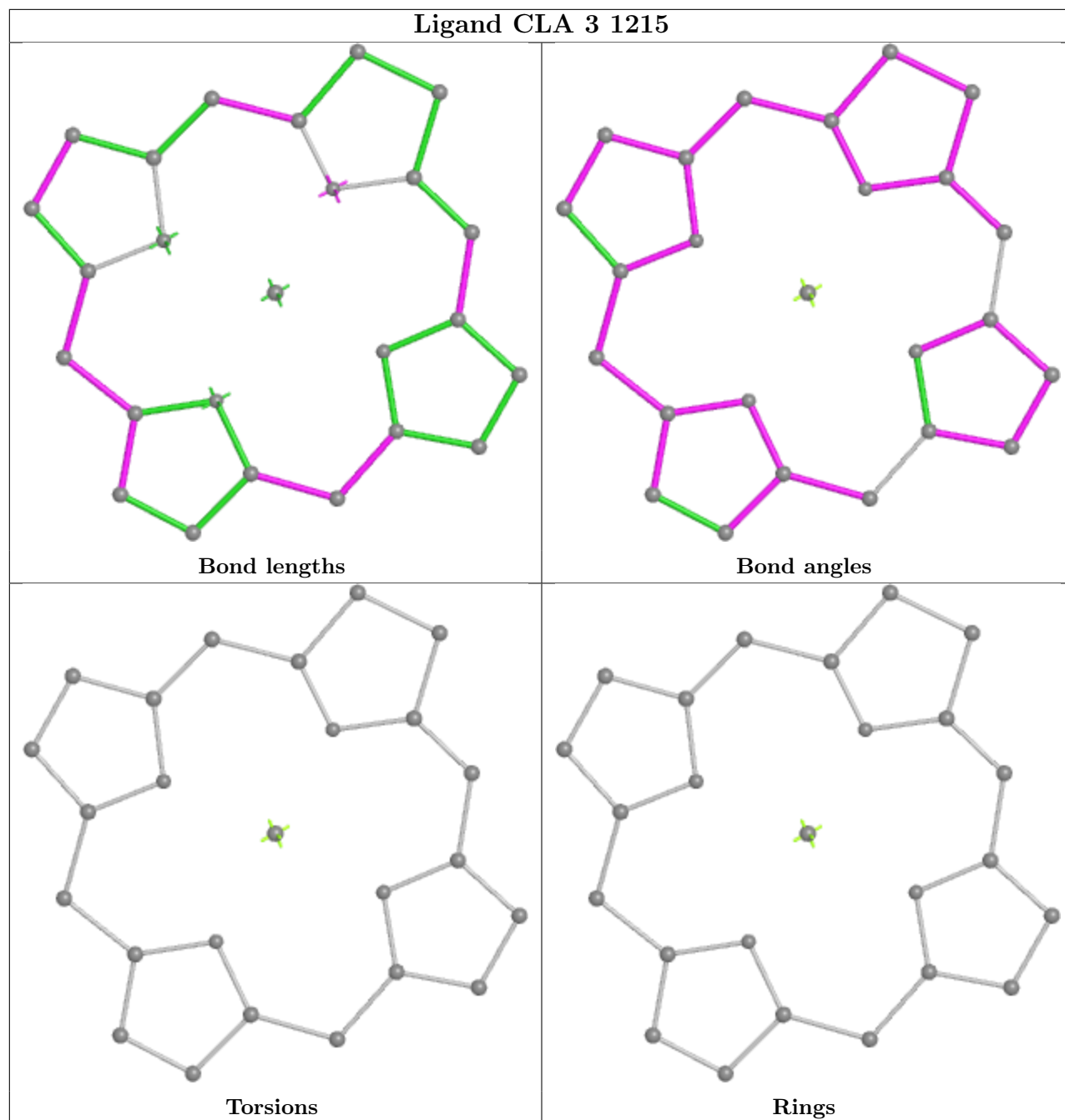
Bond angles

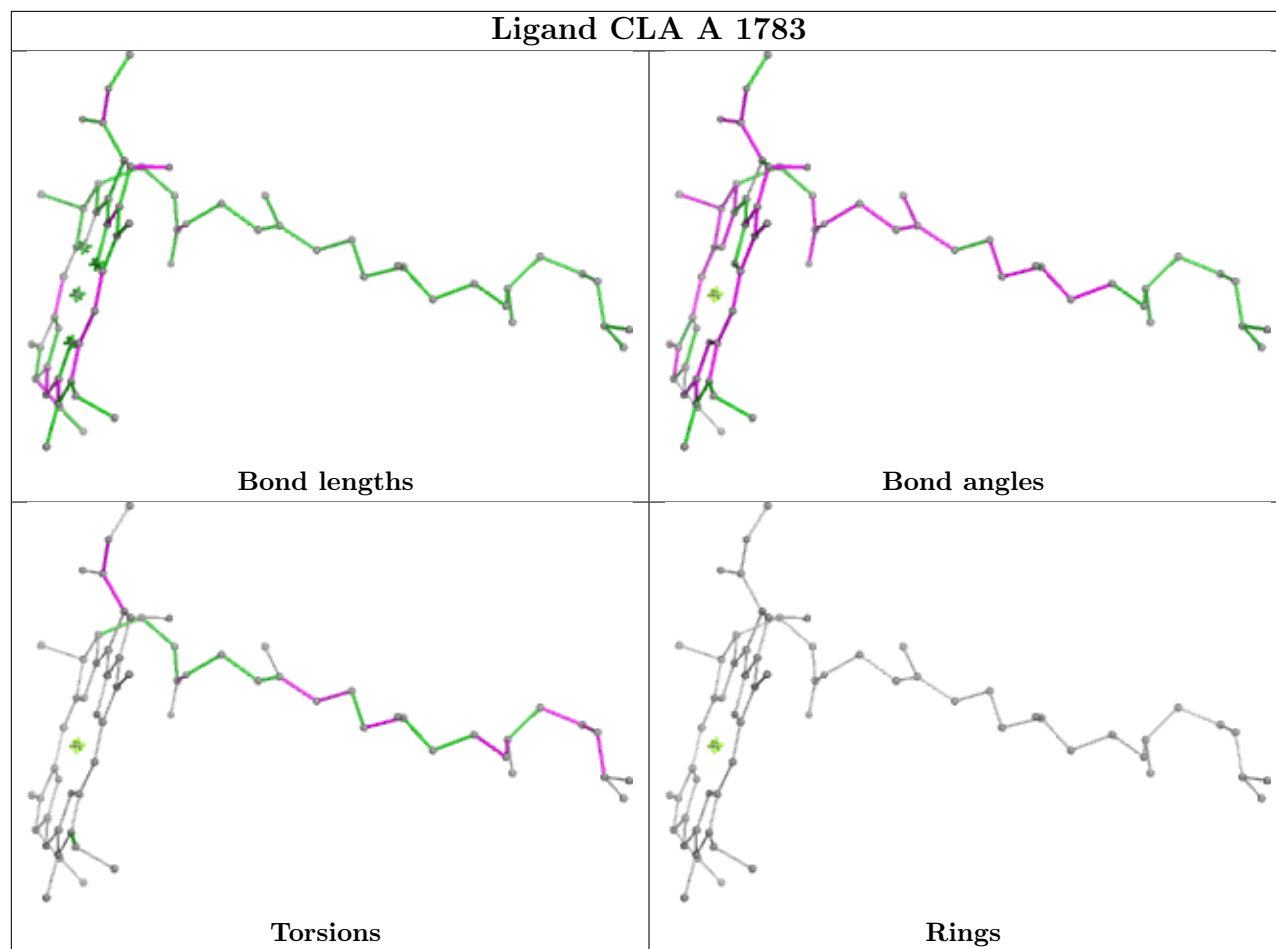


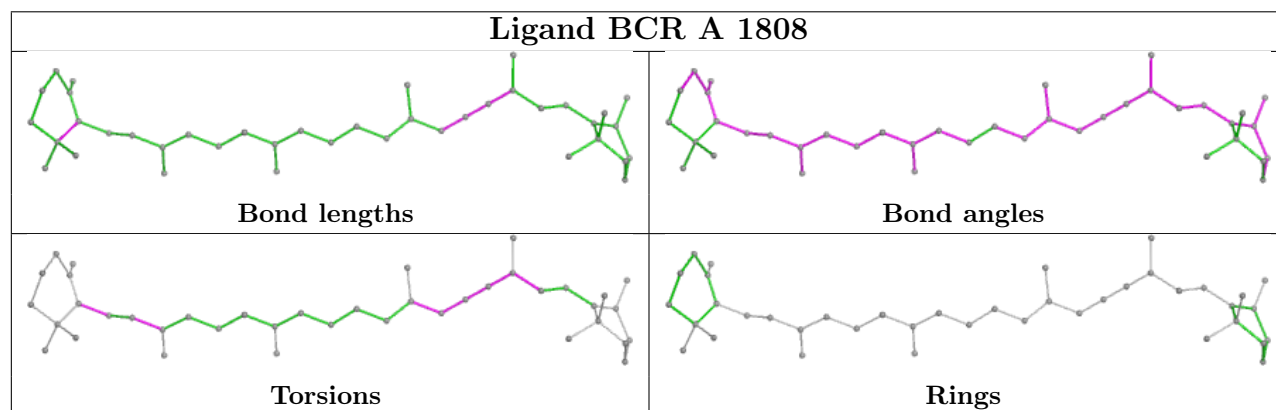
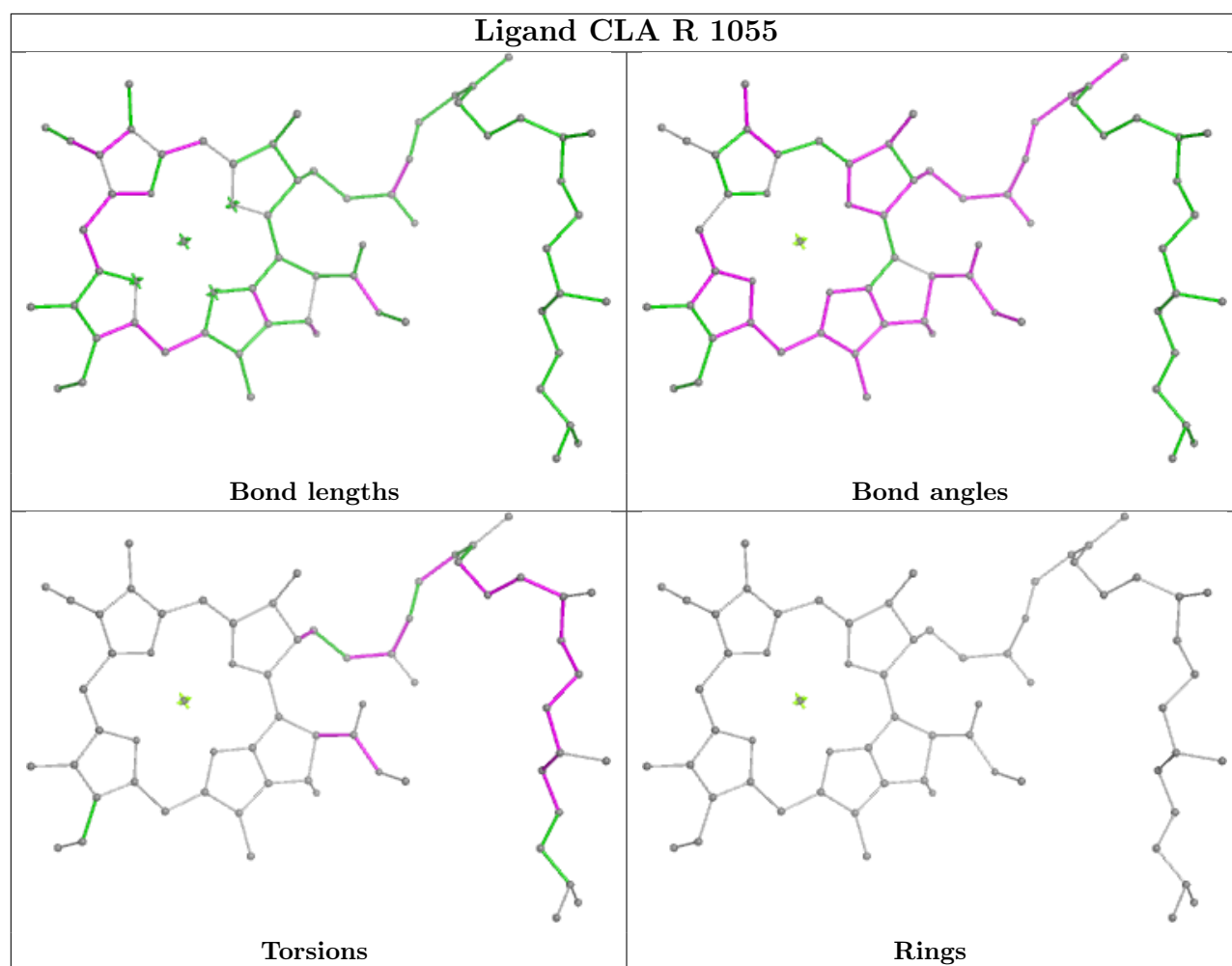
Torsions



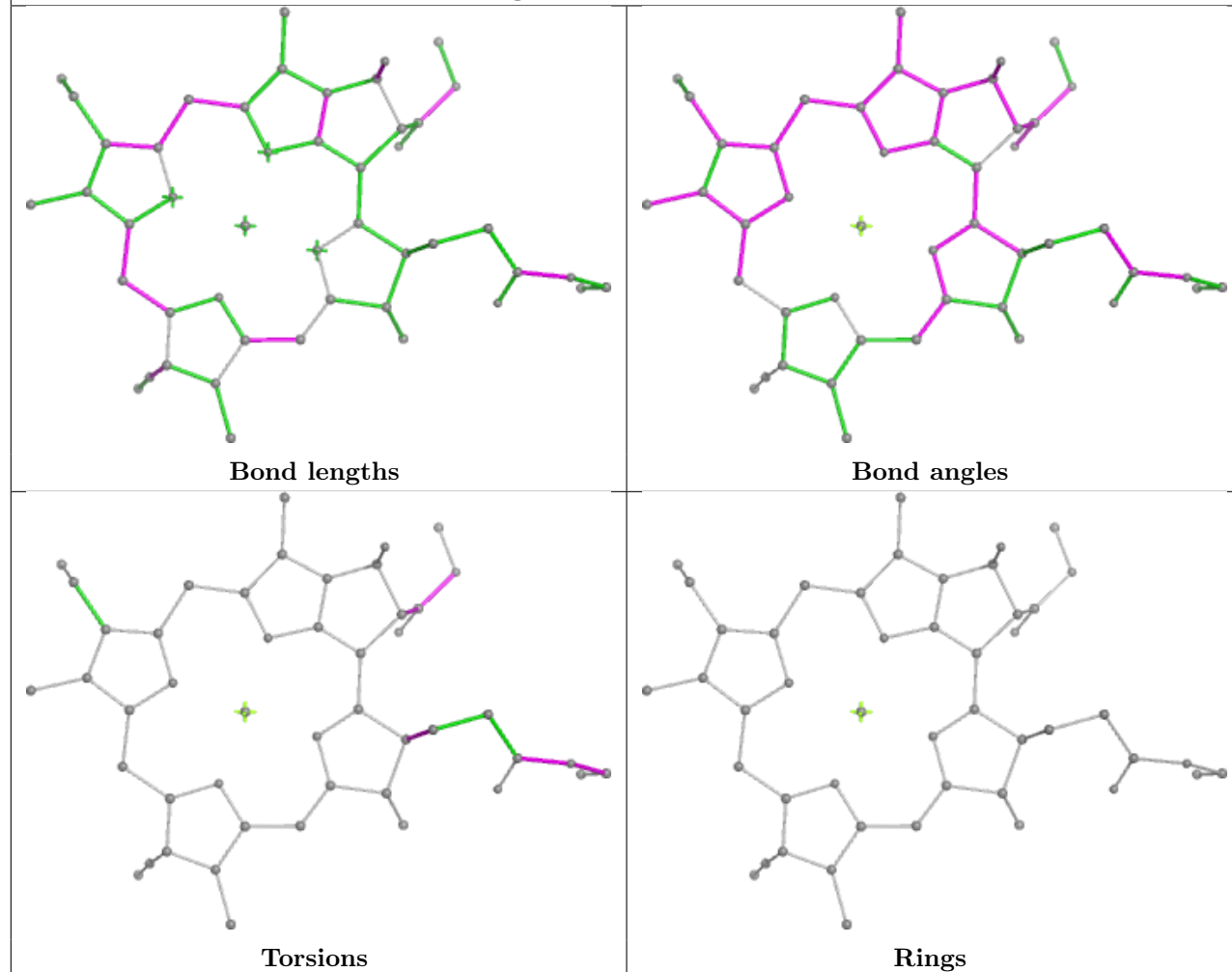
Rings



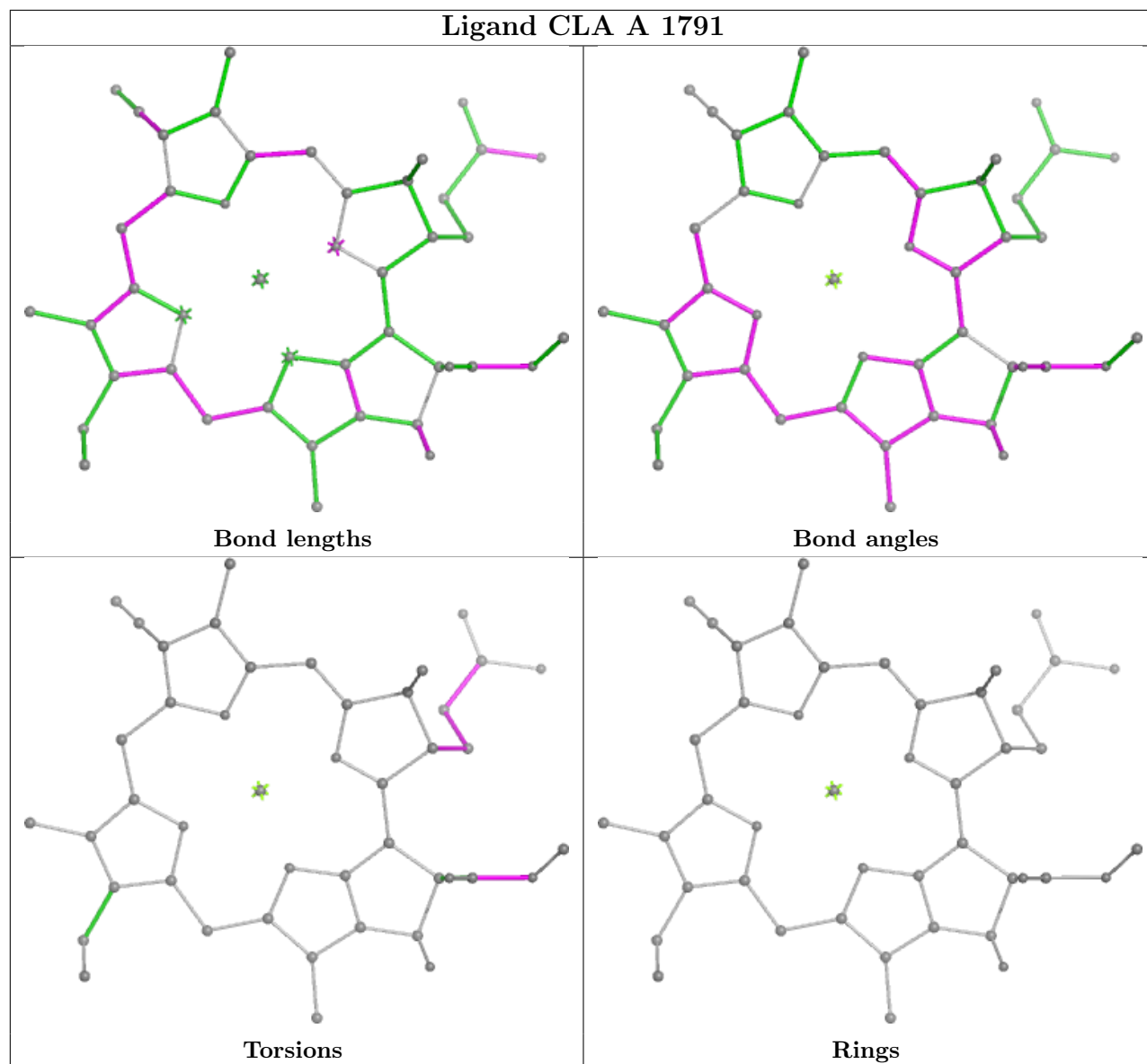


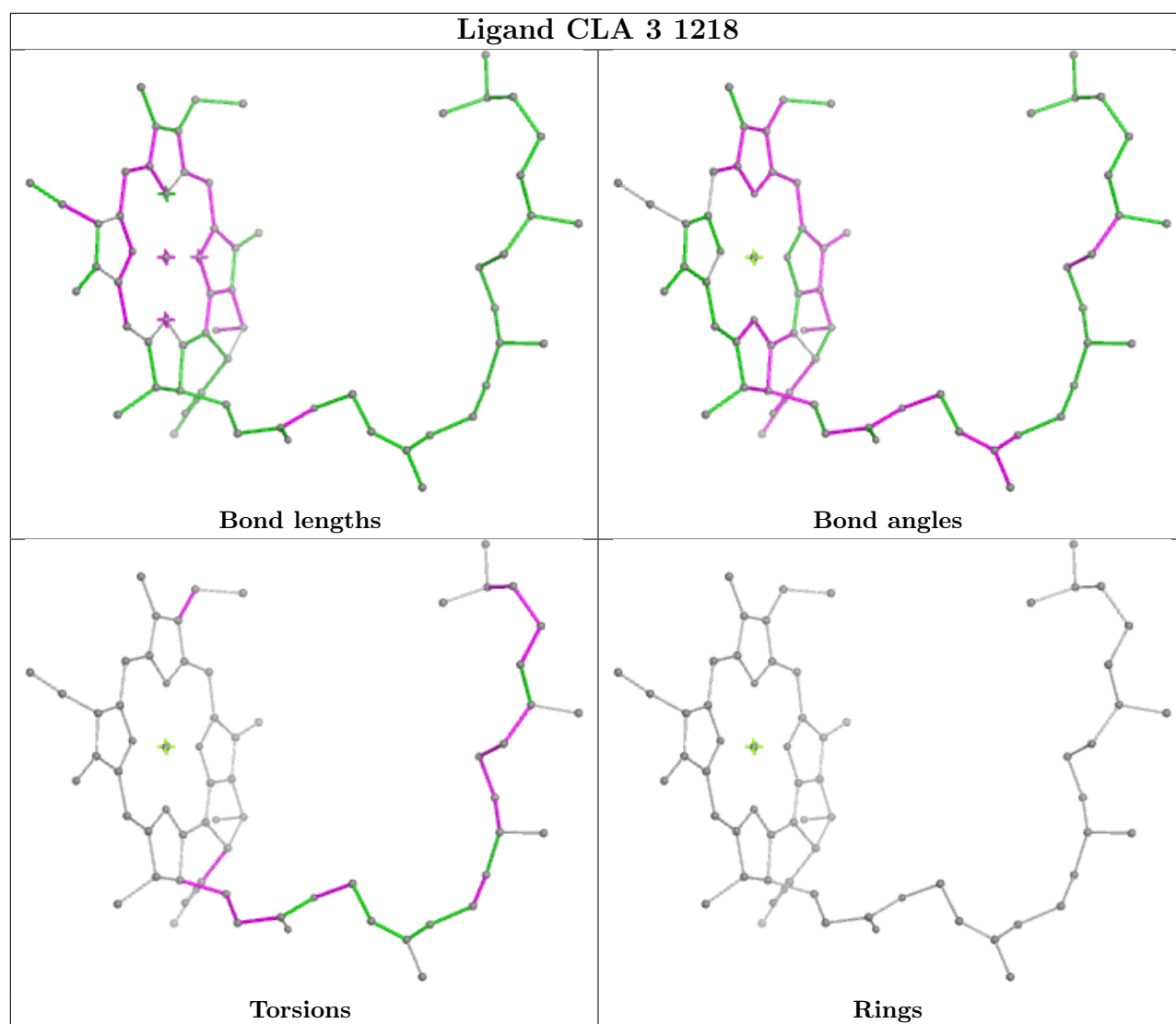


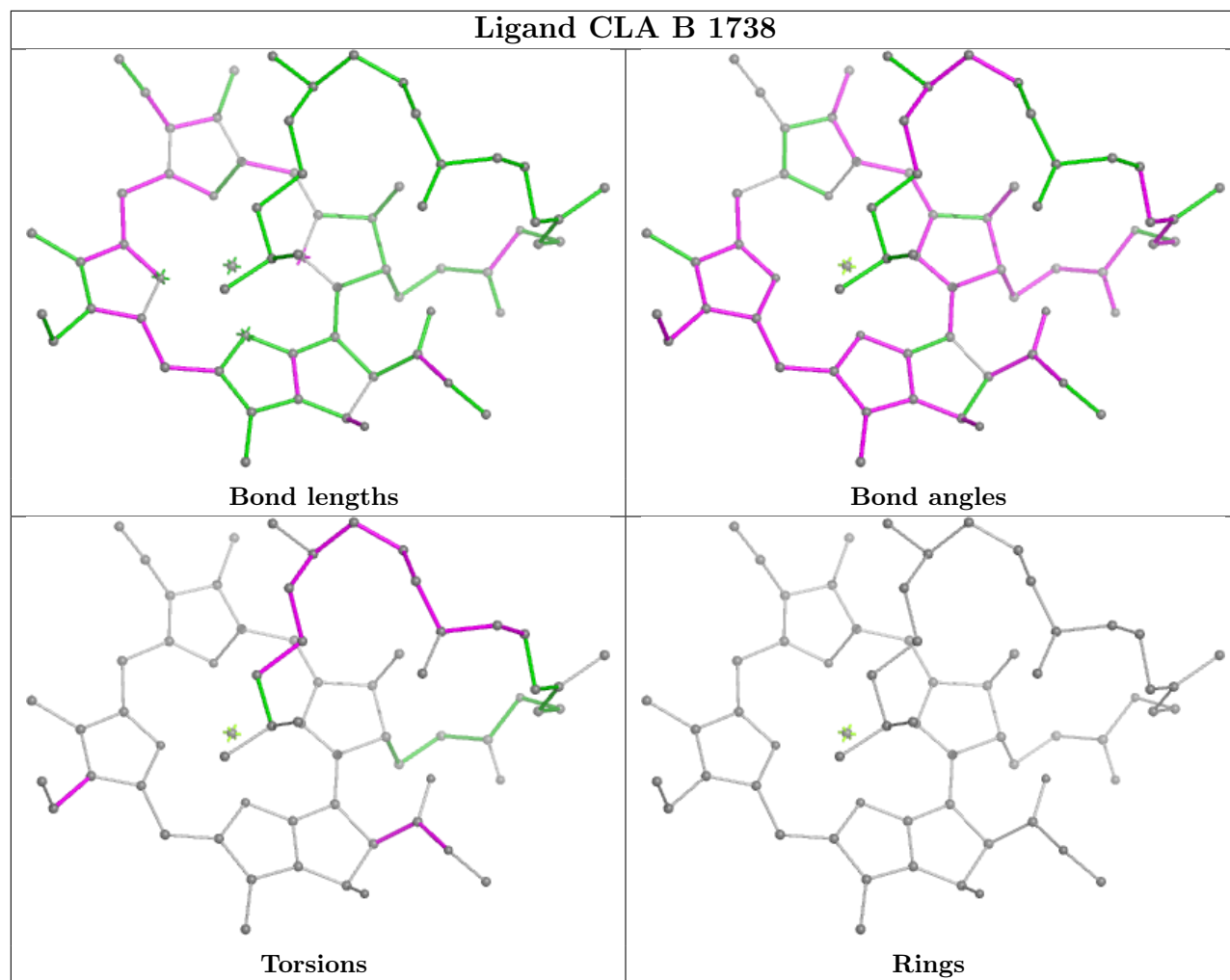
Ligand CLA 1 1189



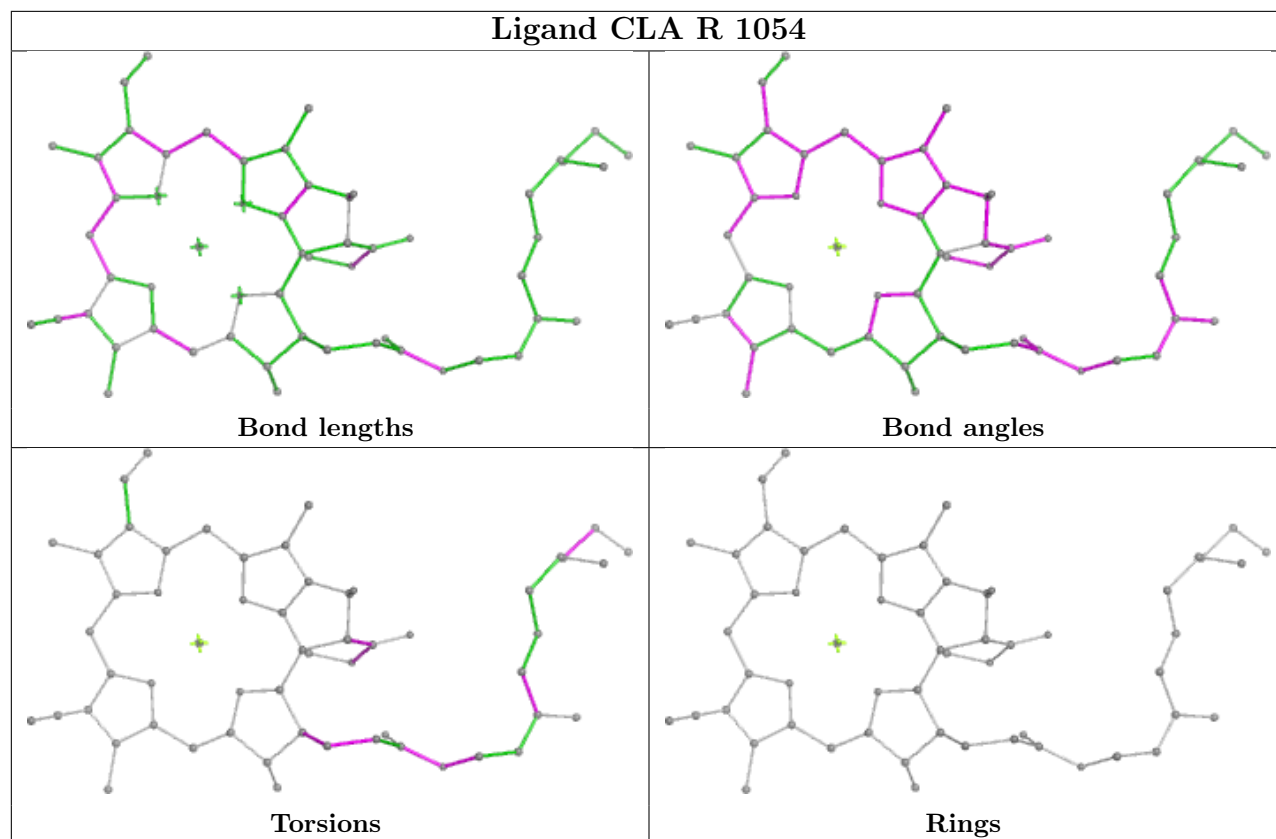
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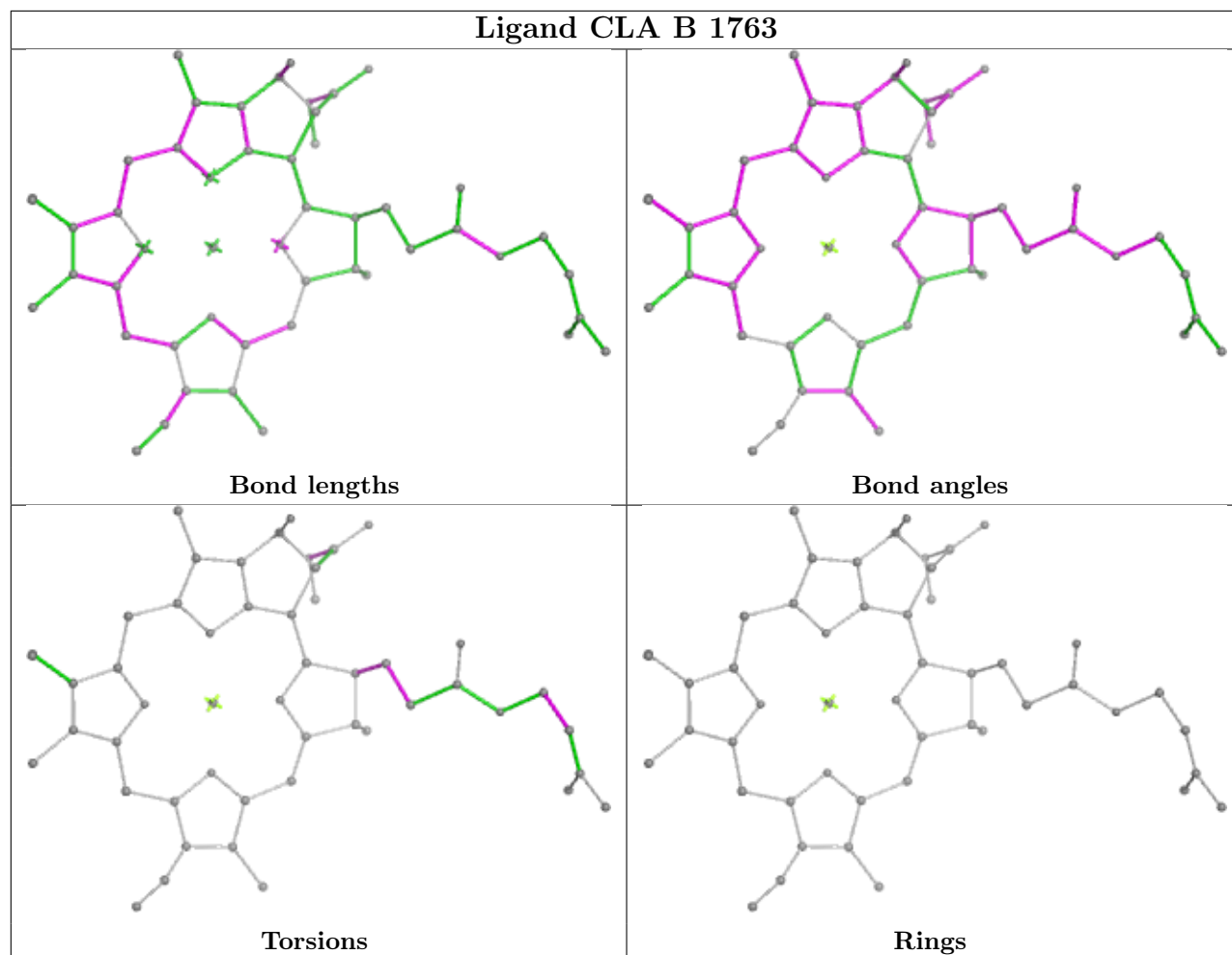


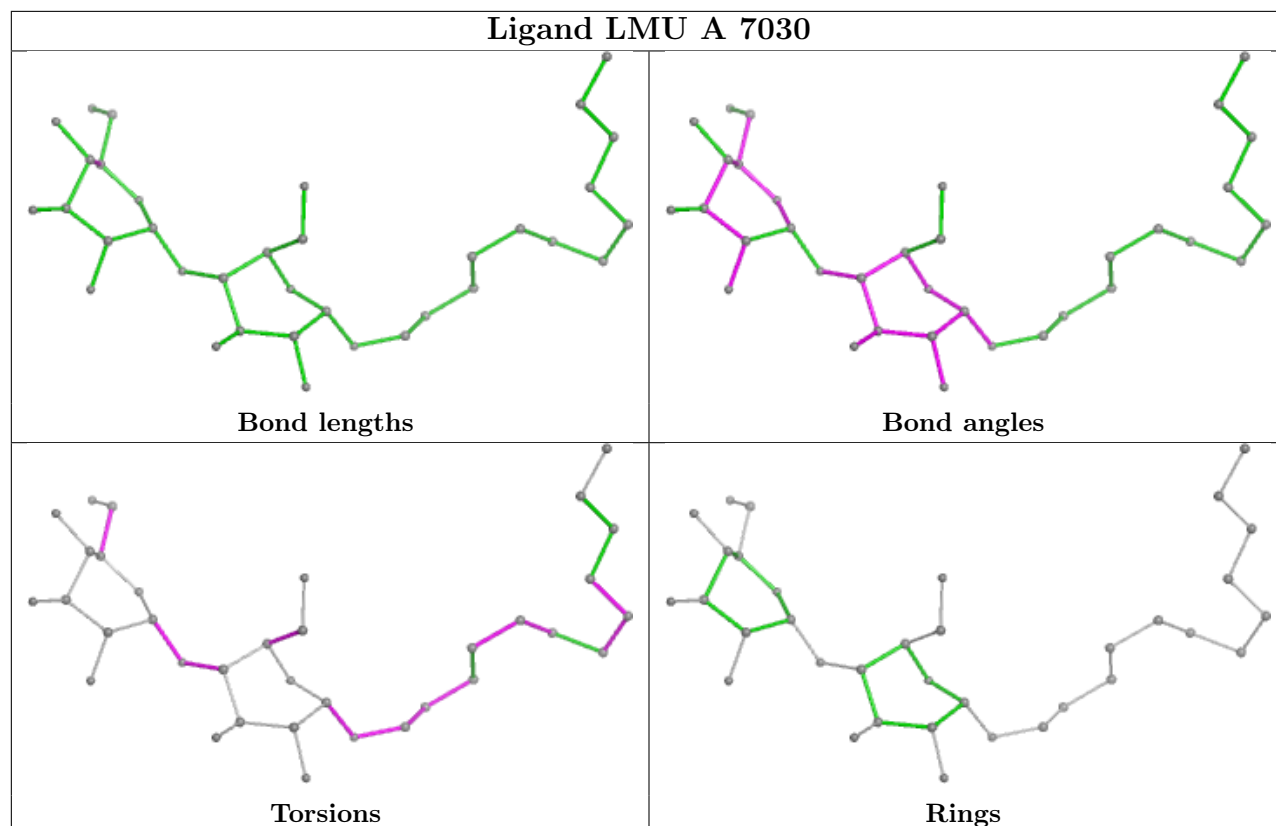
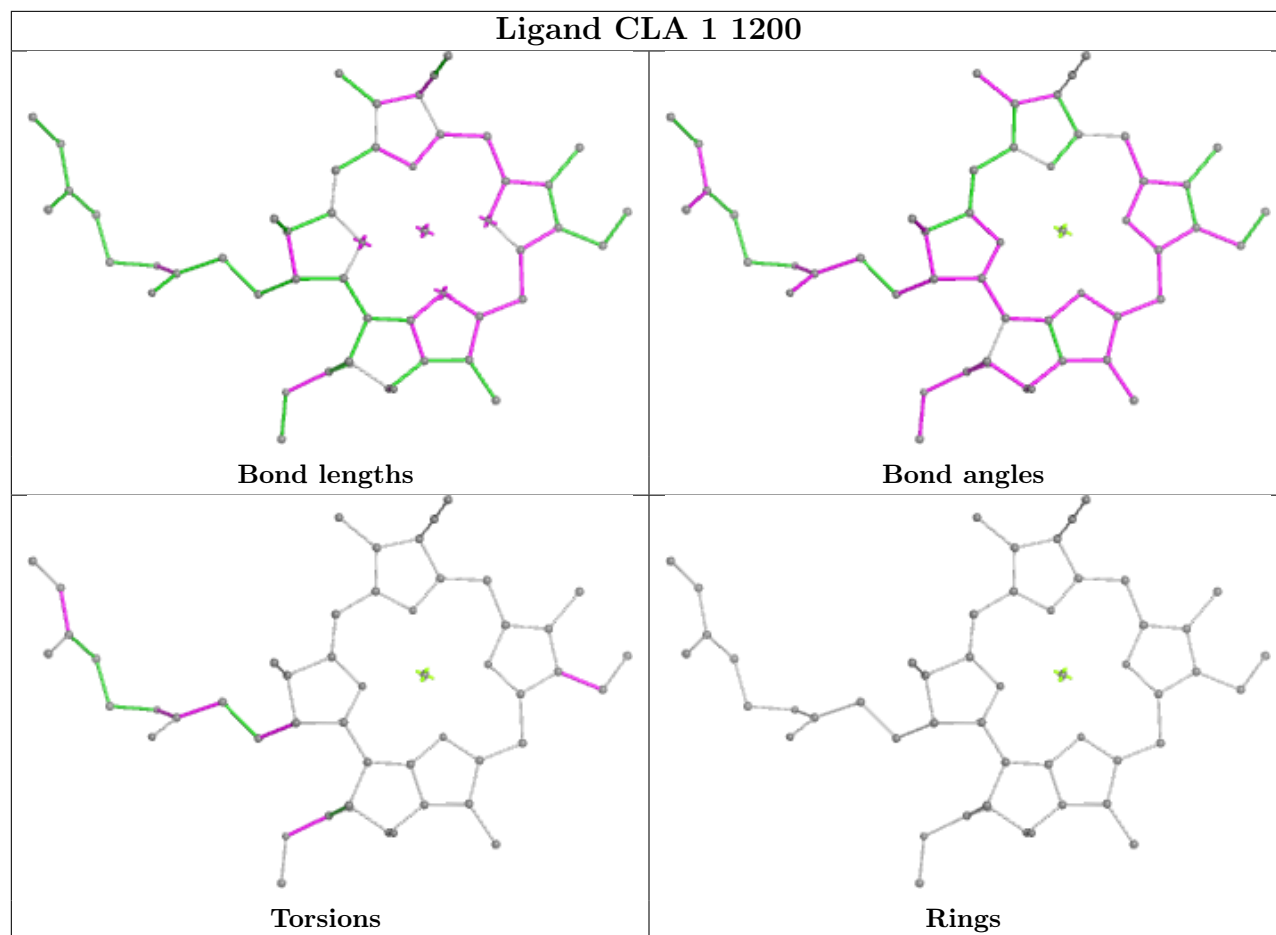


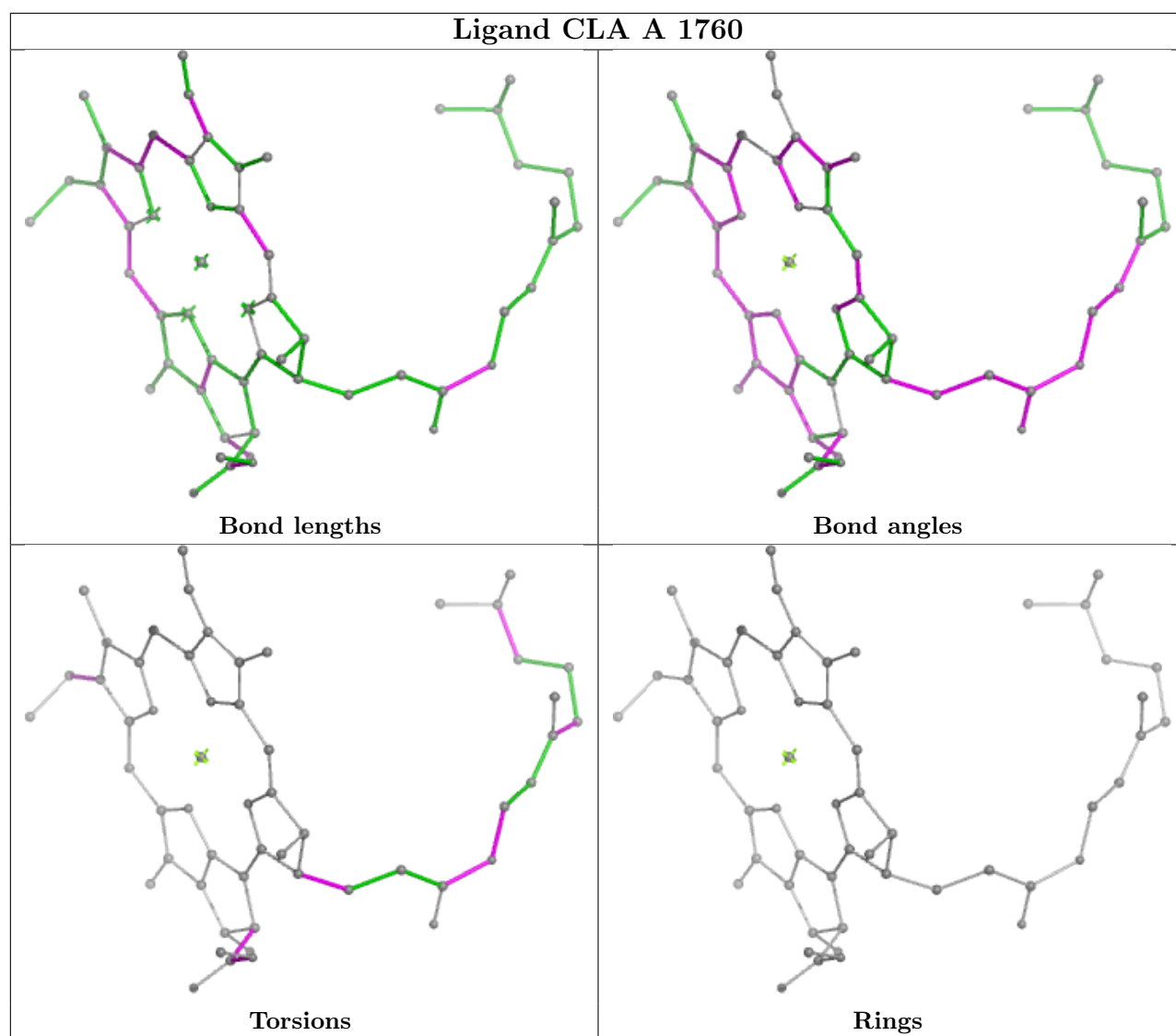


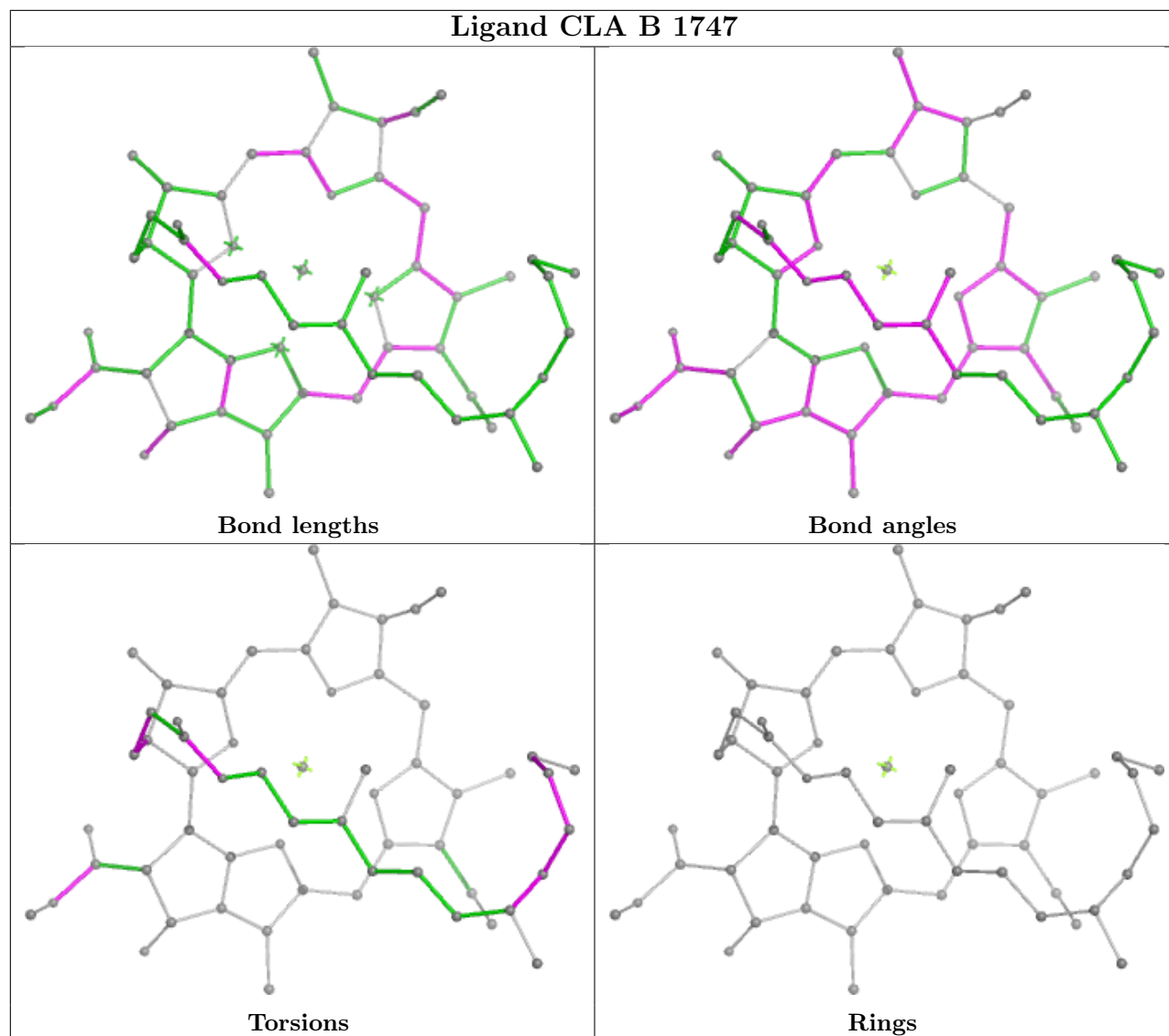
Ligand CLA R 1054



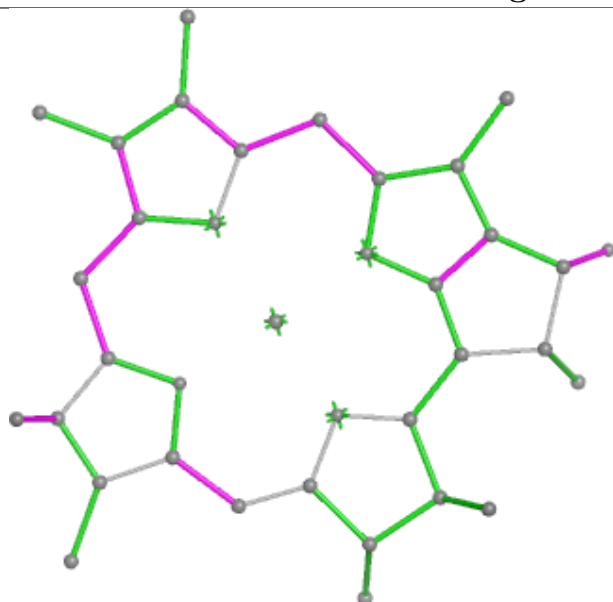




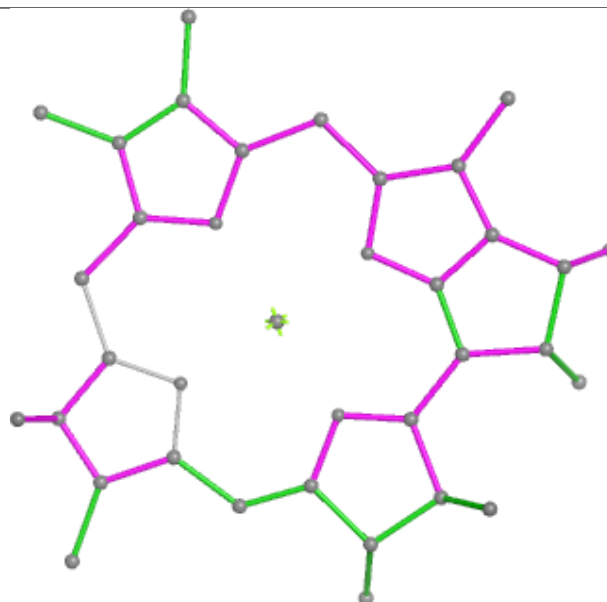




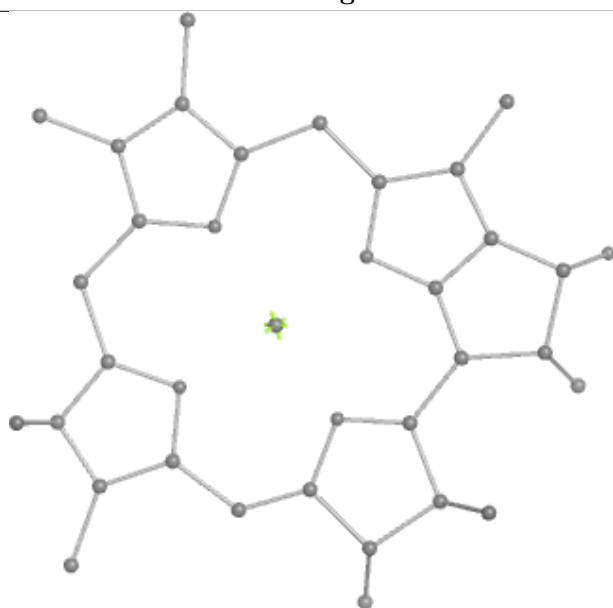
Ligand CLA 1 1196



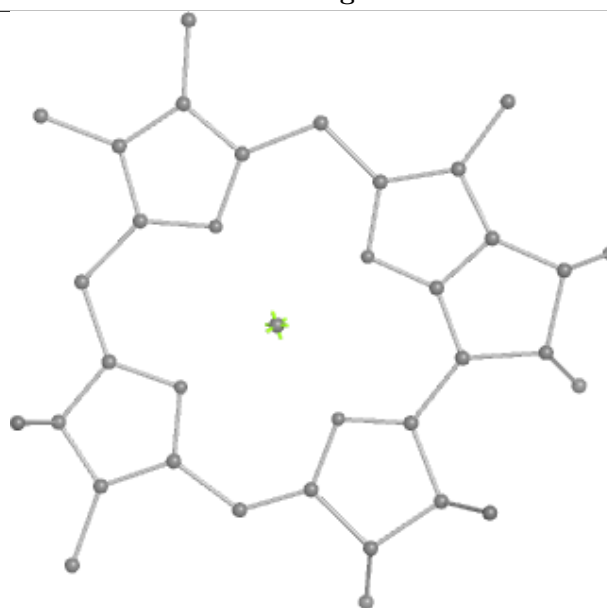
Bond lengths



Bond angles

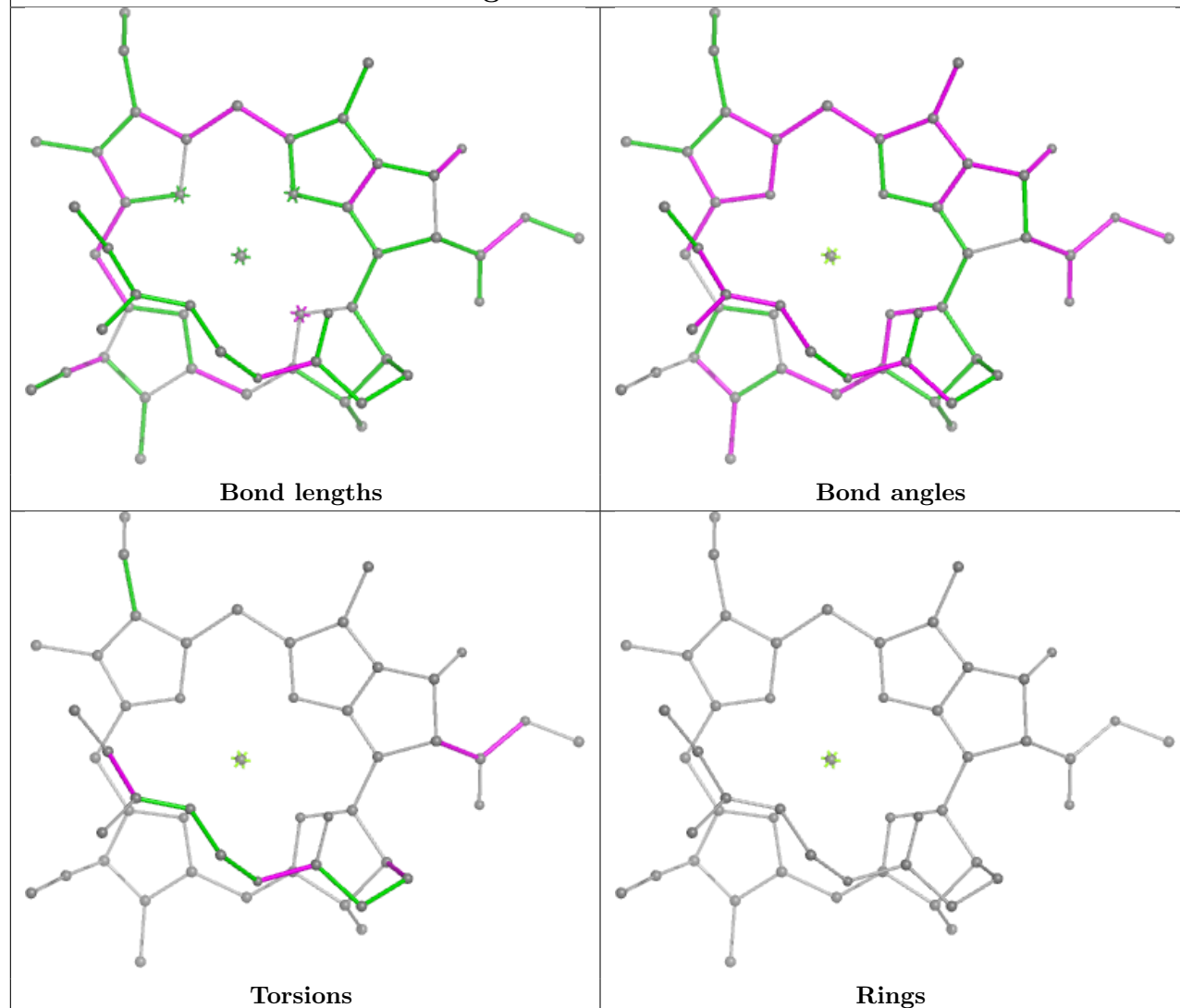


Torsions

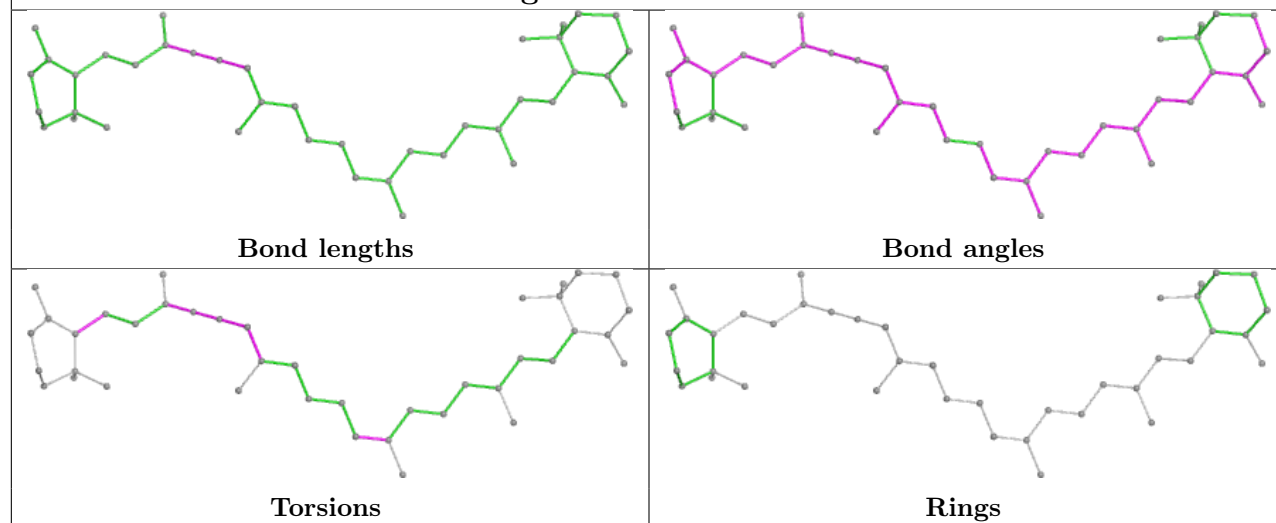


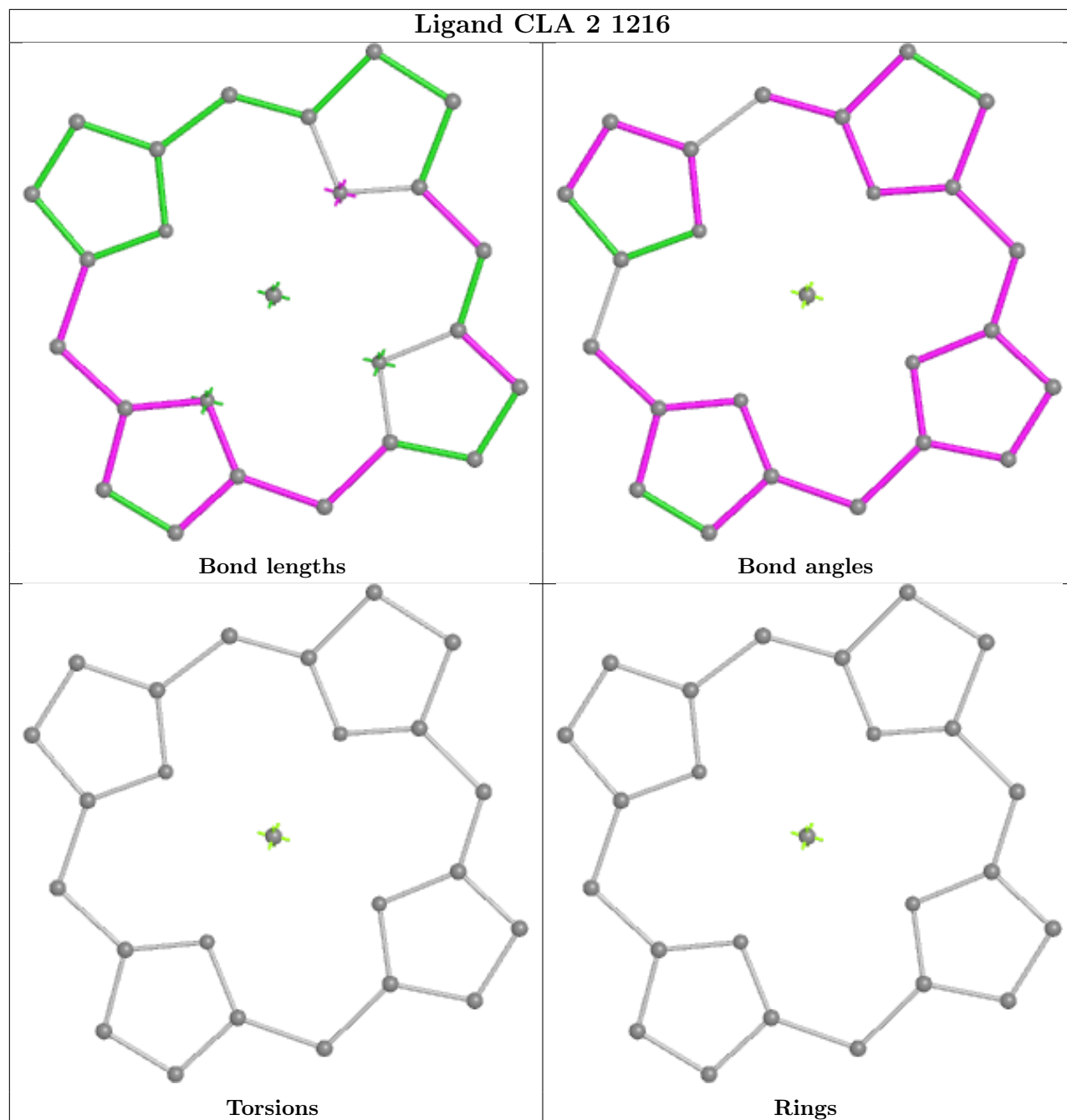
Rings

Ligand CLA A 1777

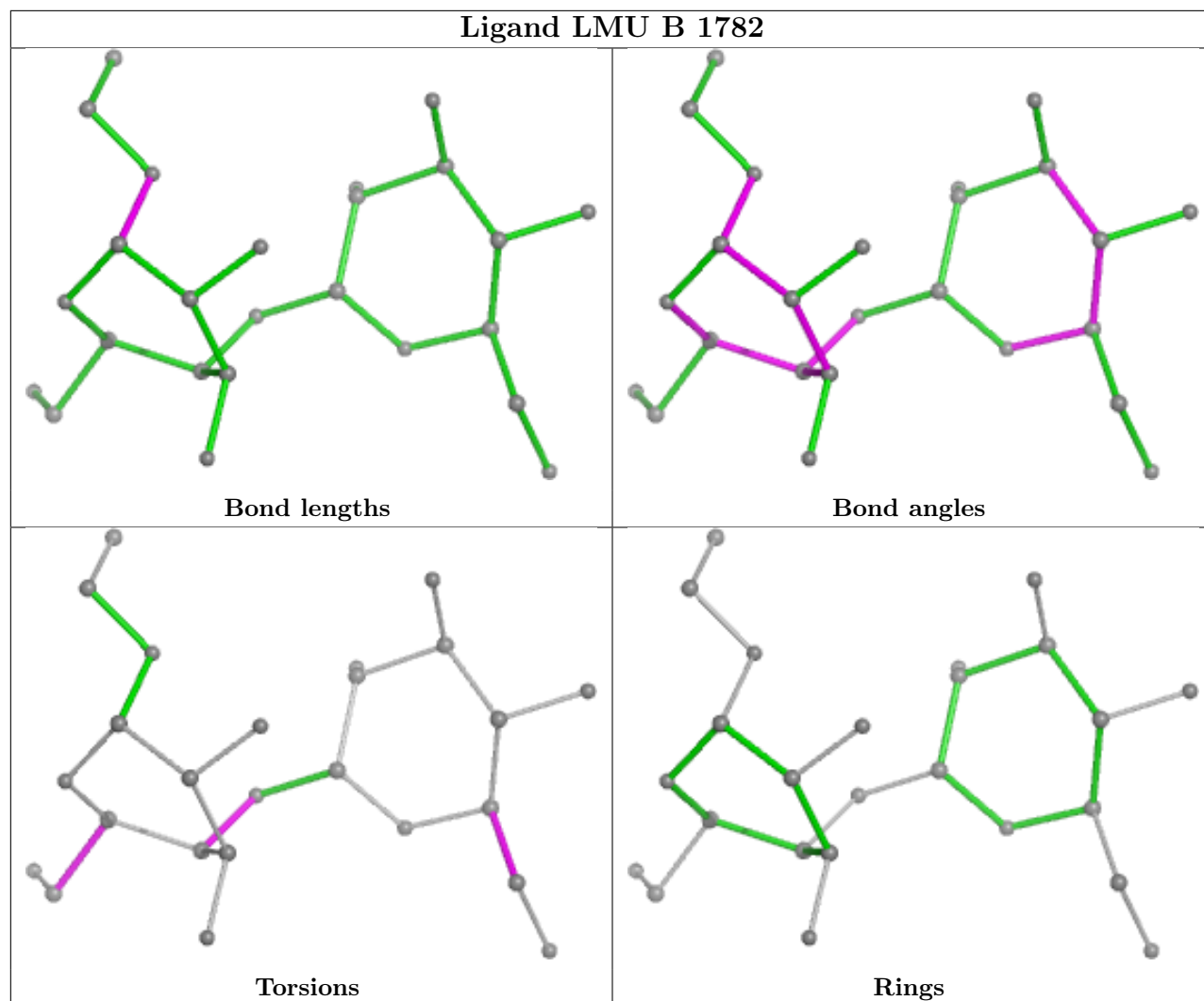


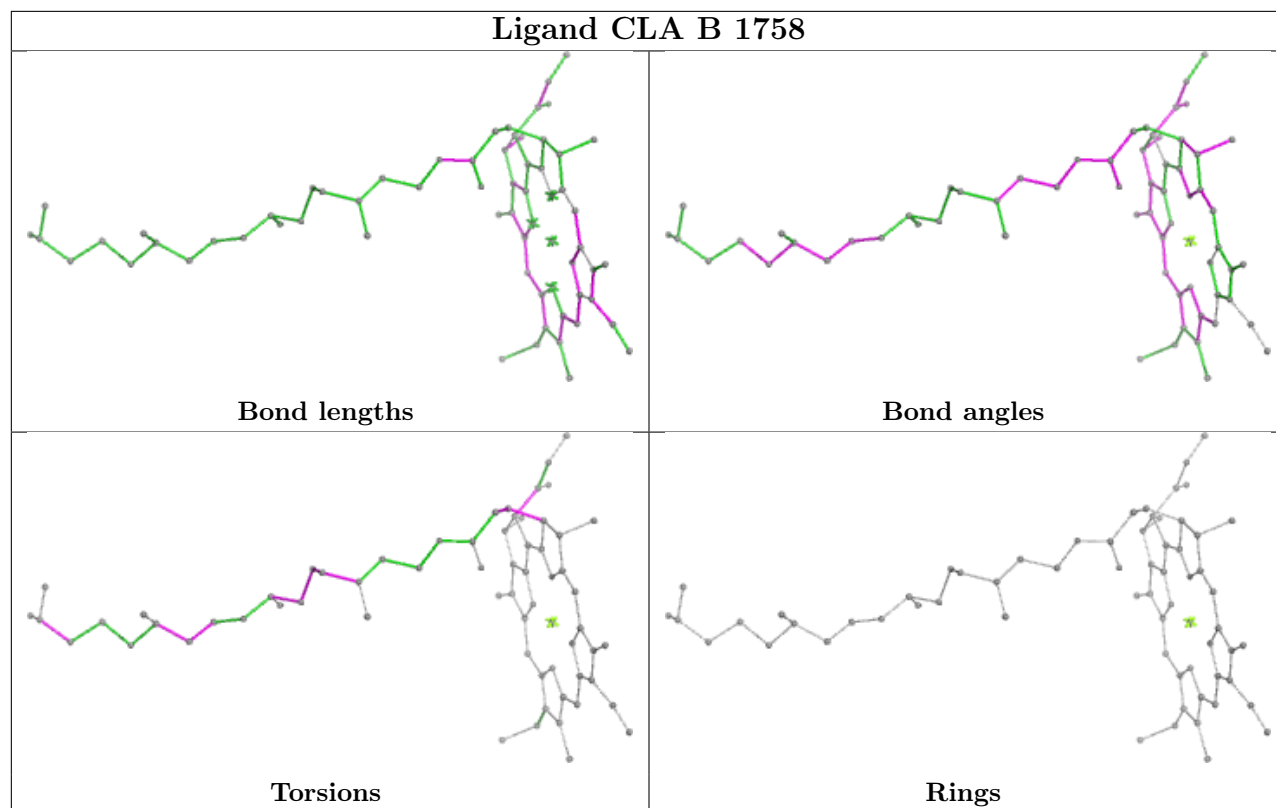
Ligand BCR A 1807

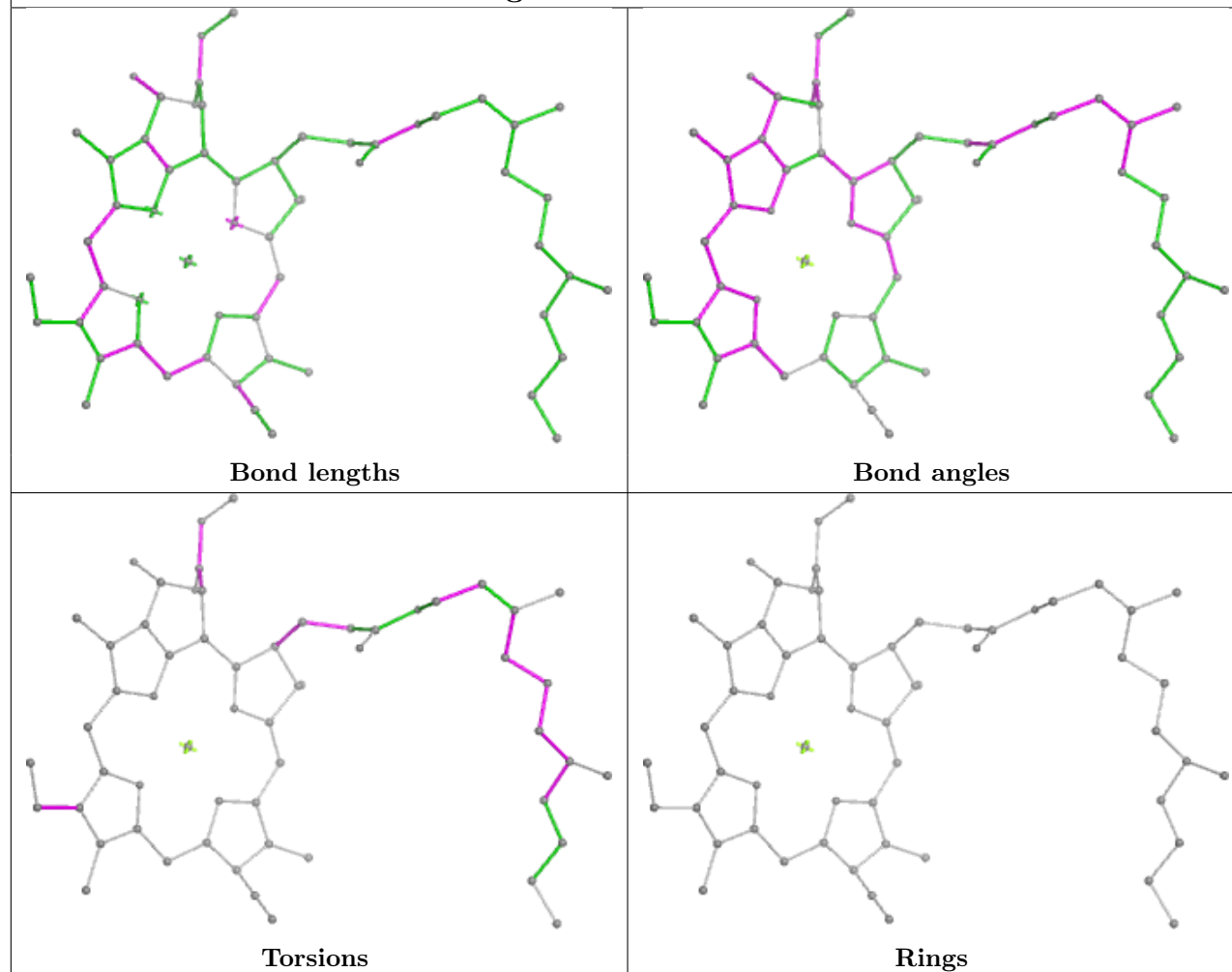
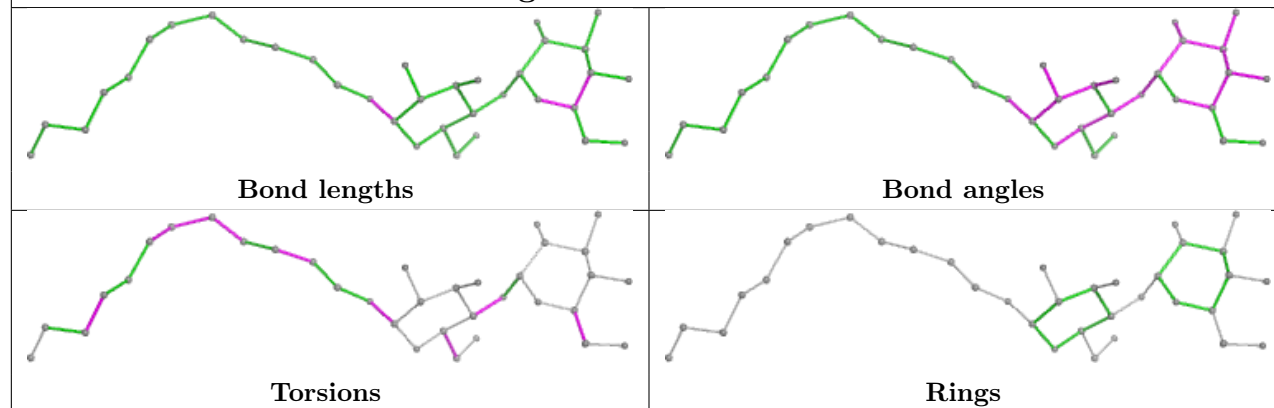


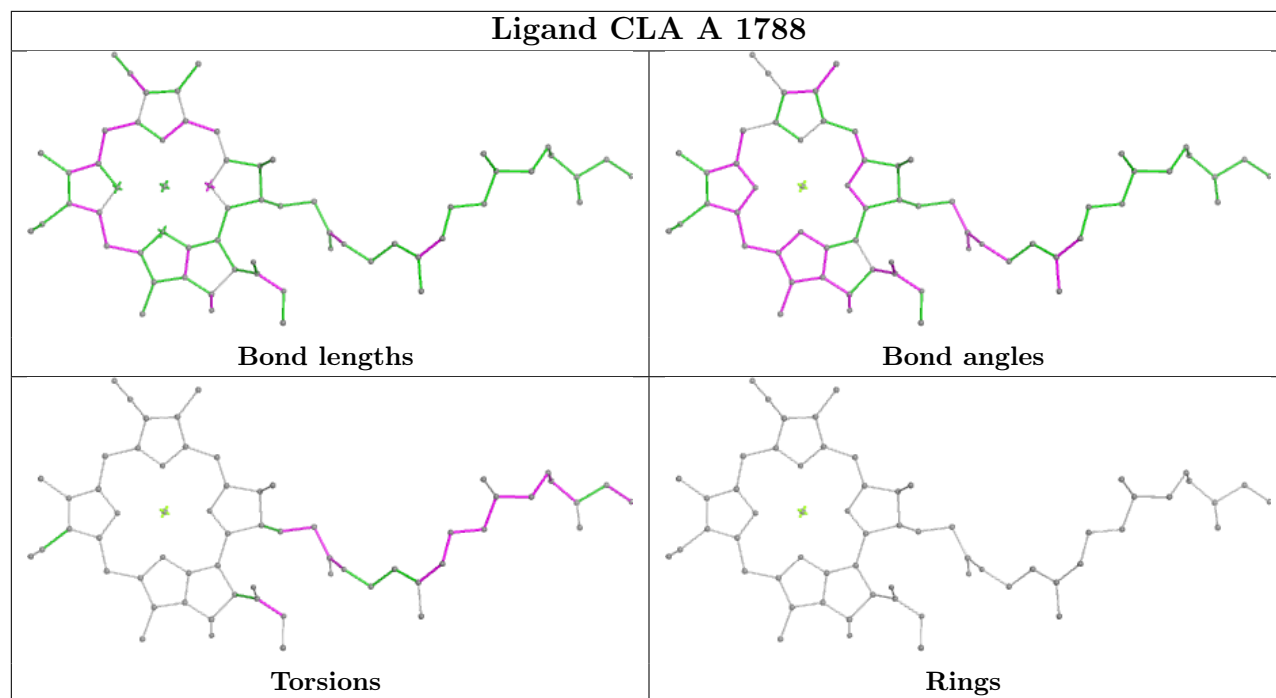


Ligand LMU B 1782

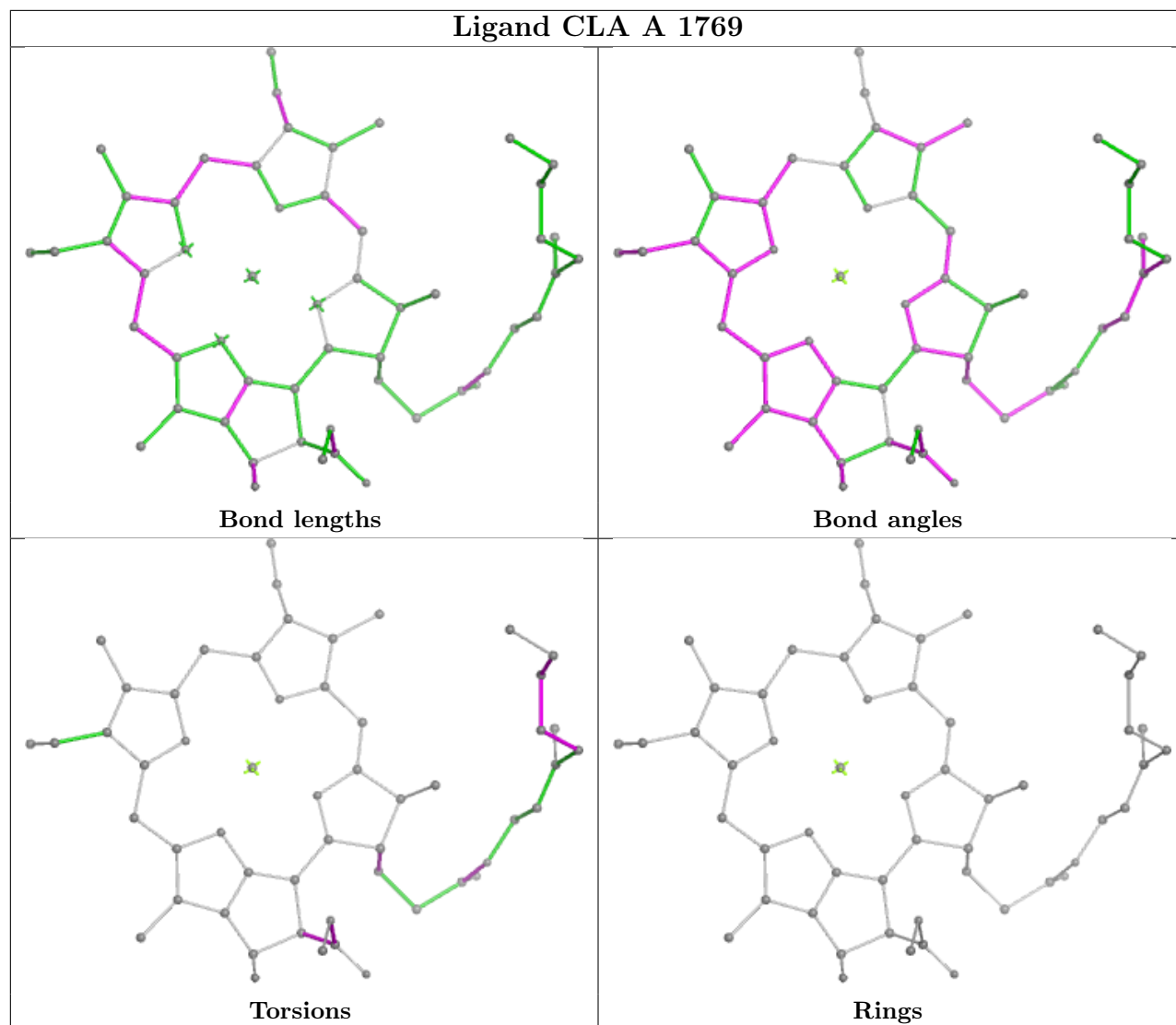


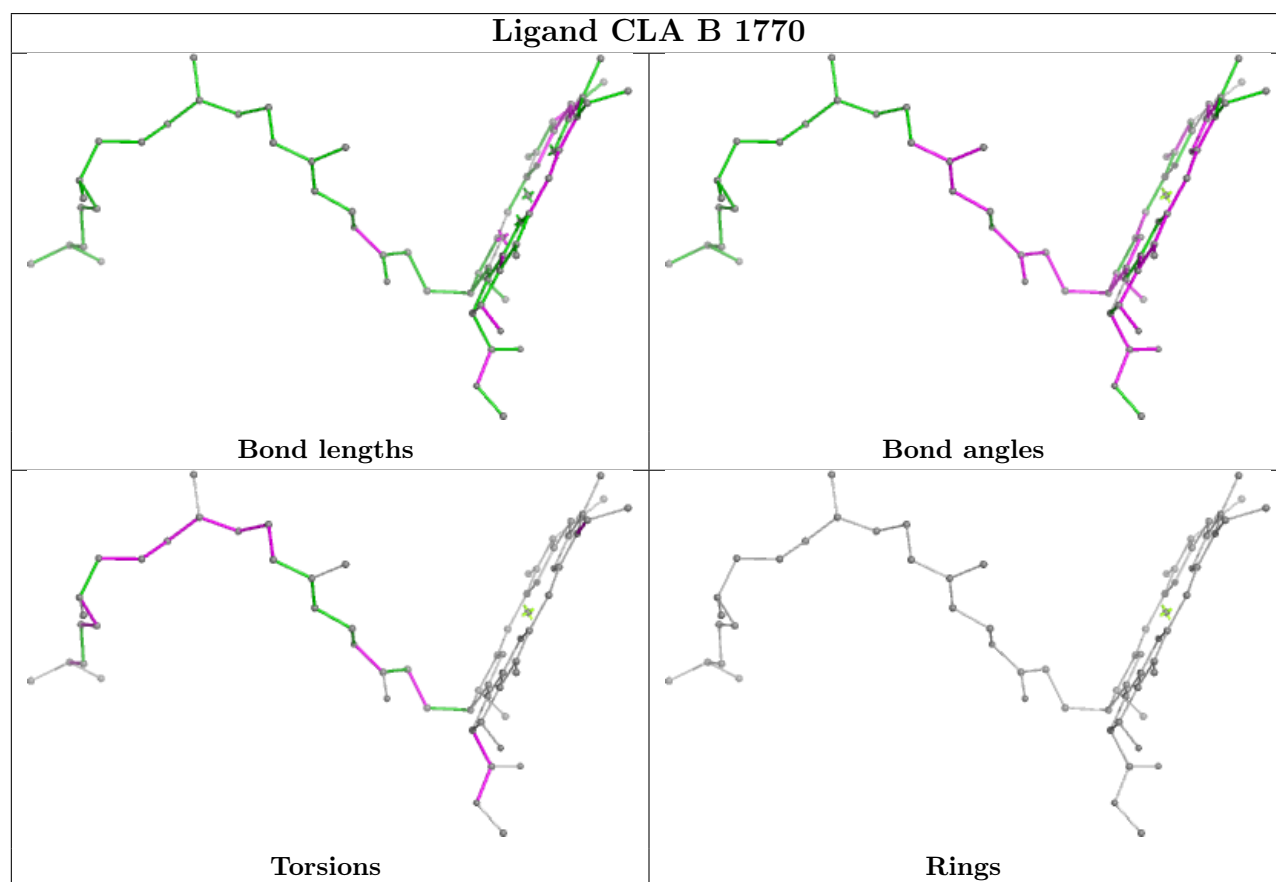
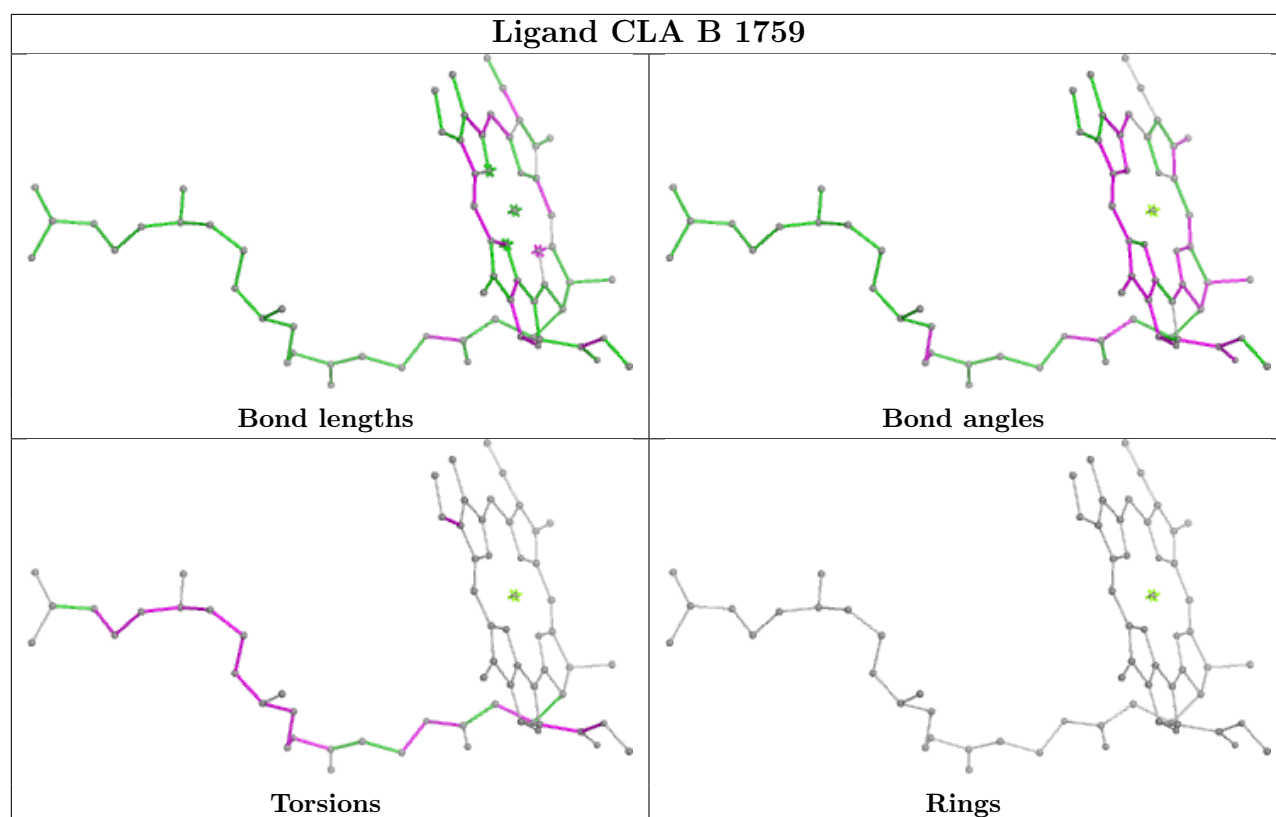


Ligand CLA B 1755**Ligand LMU A 7040**

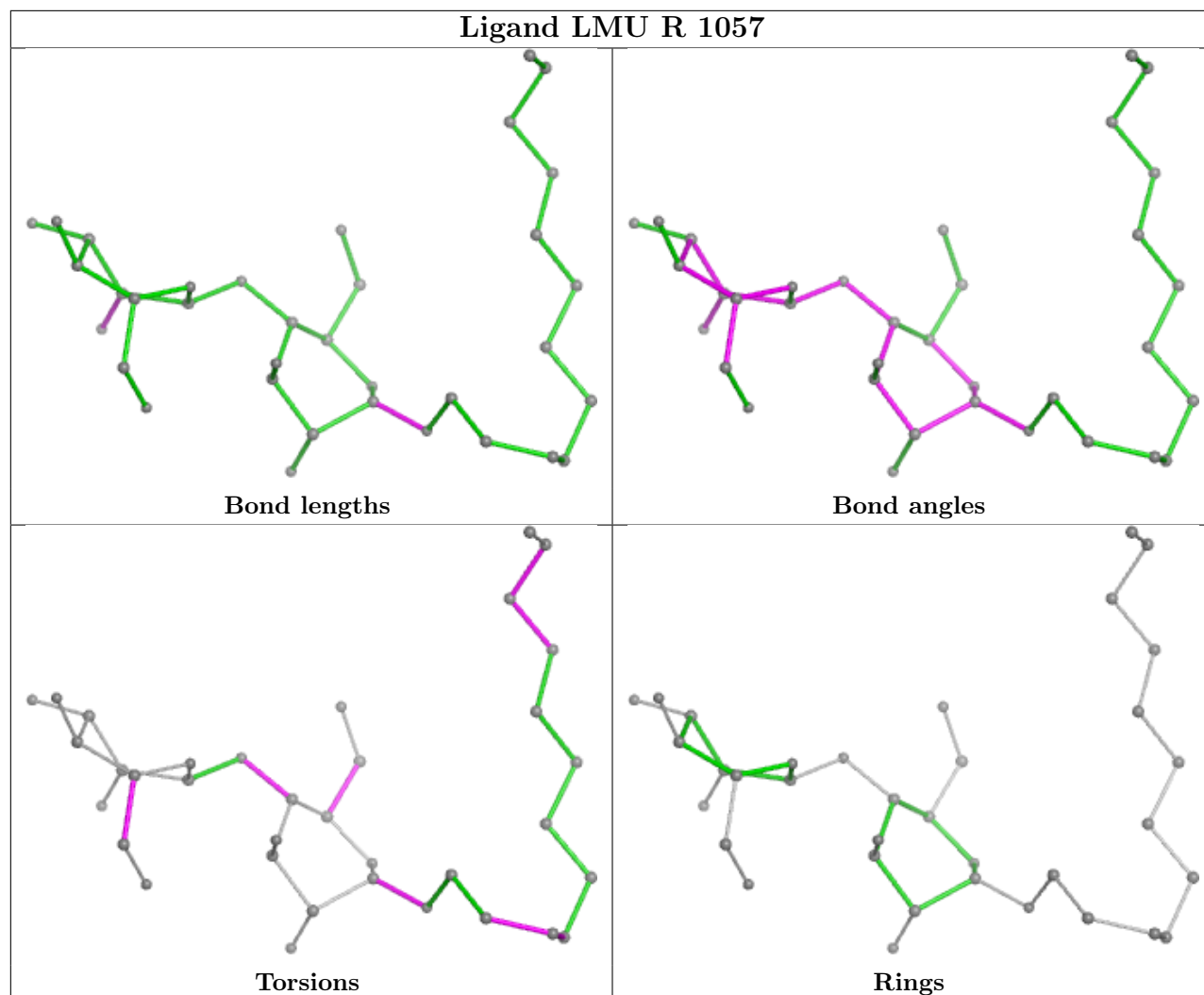


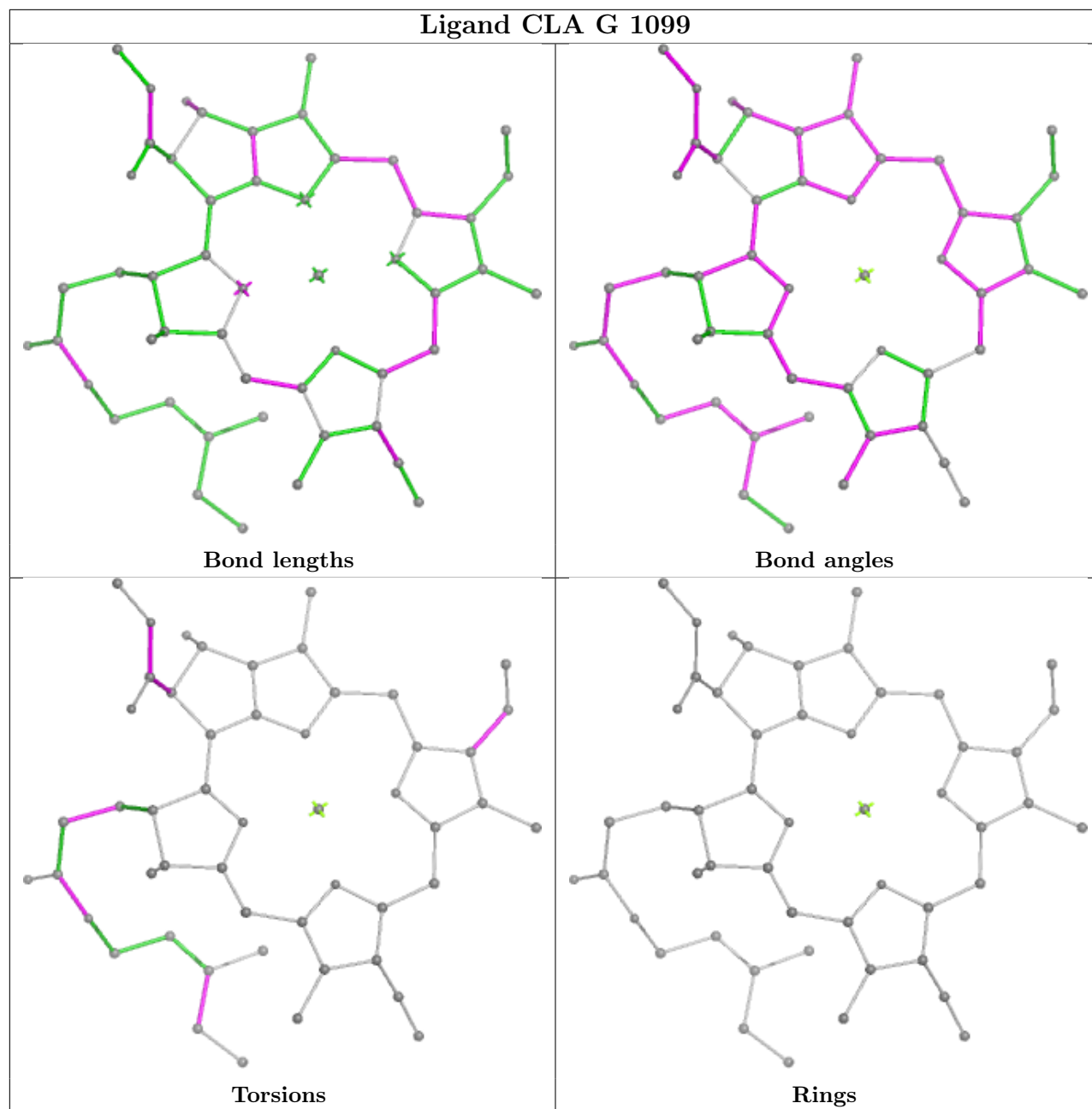
Ligand CLA A 1769

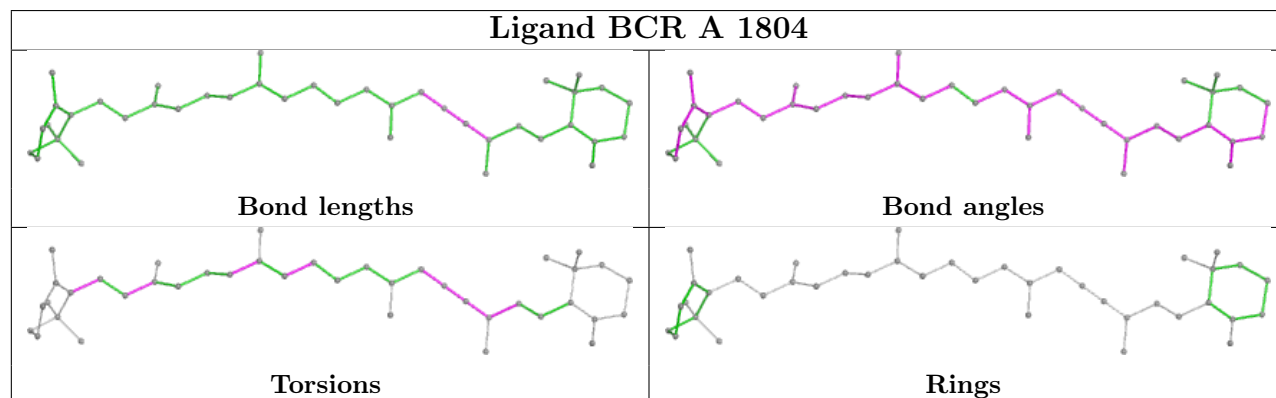
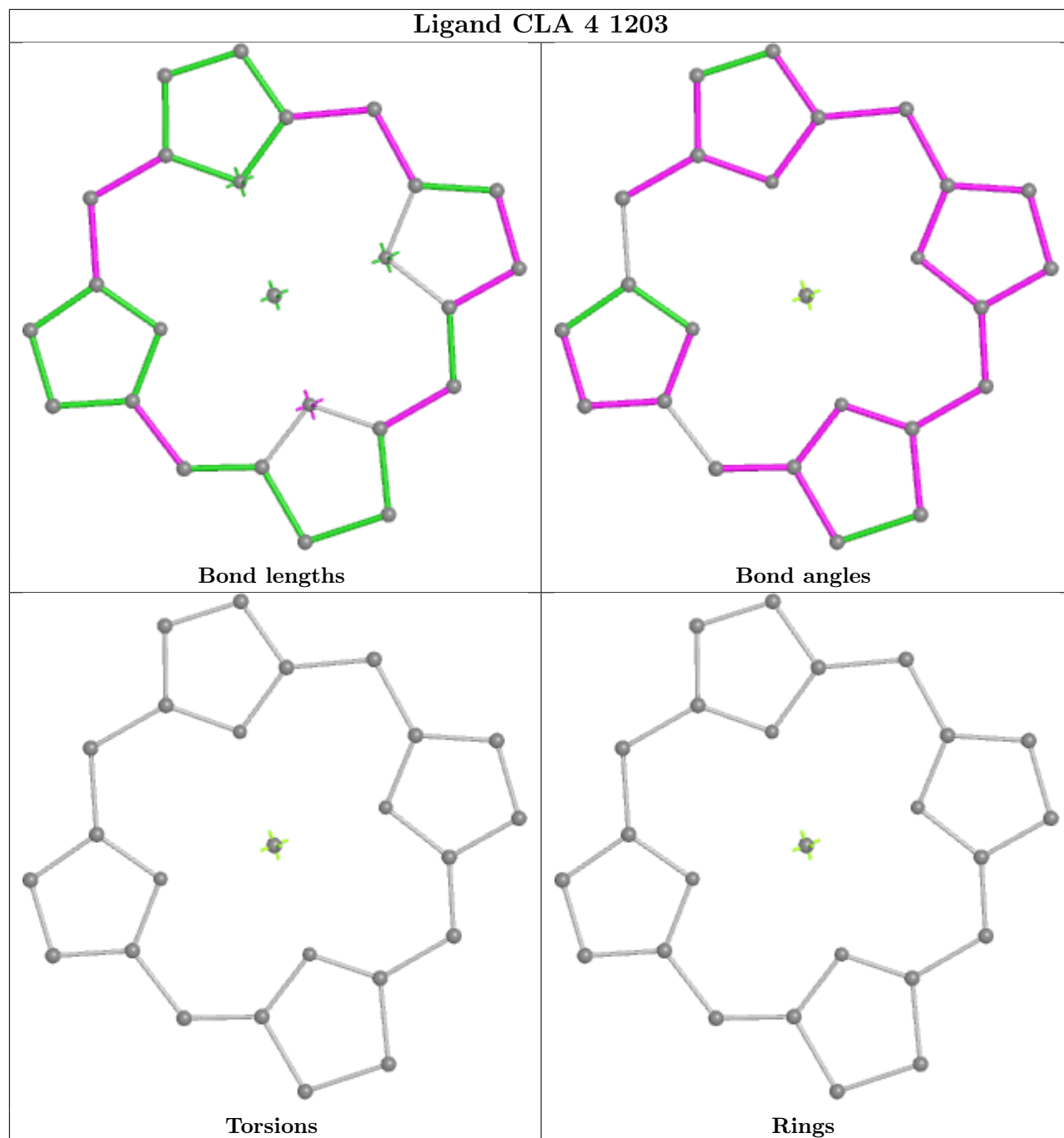


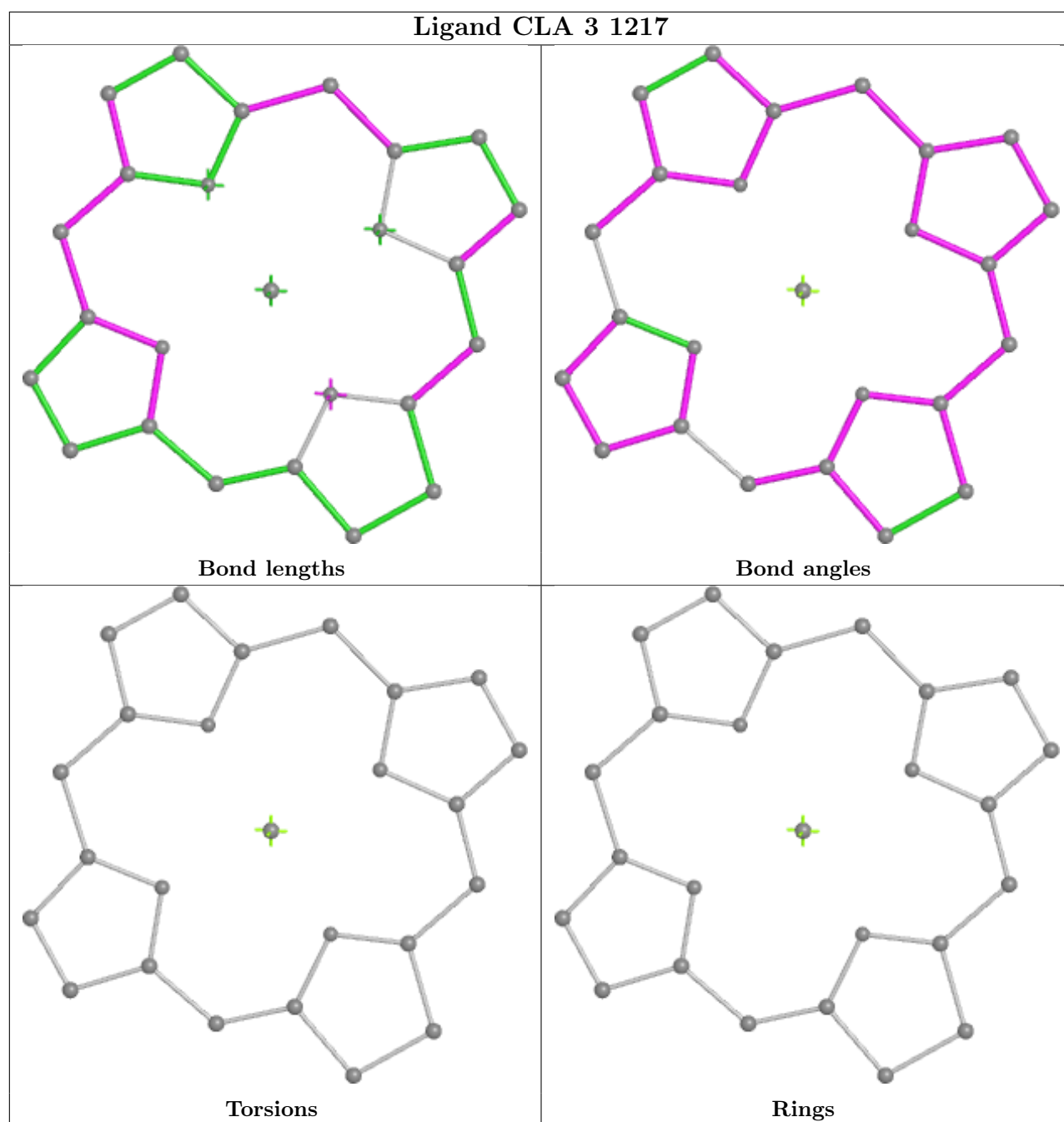


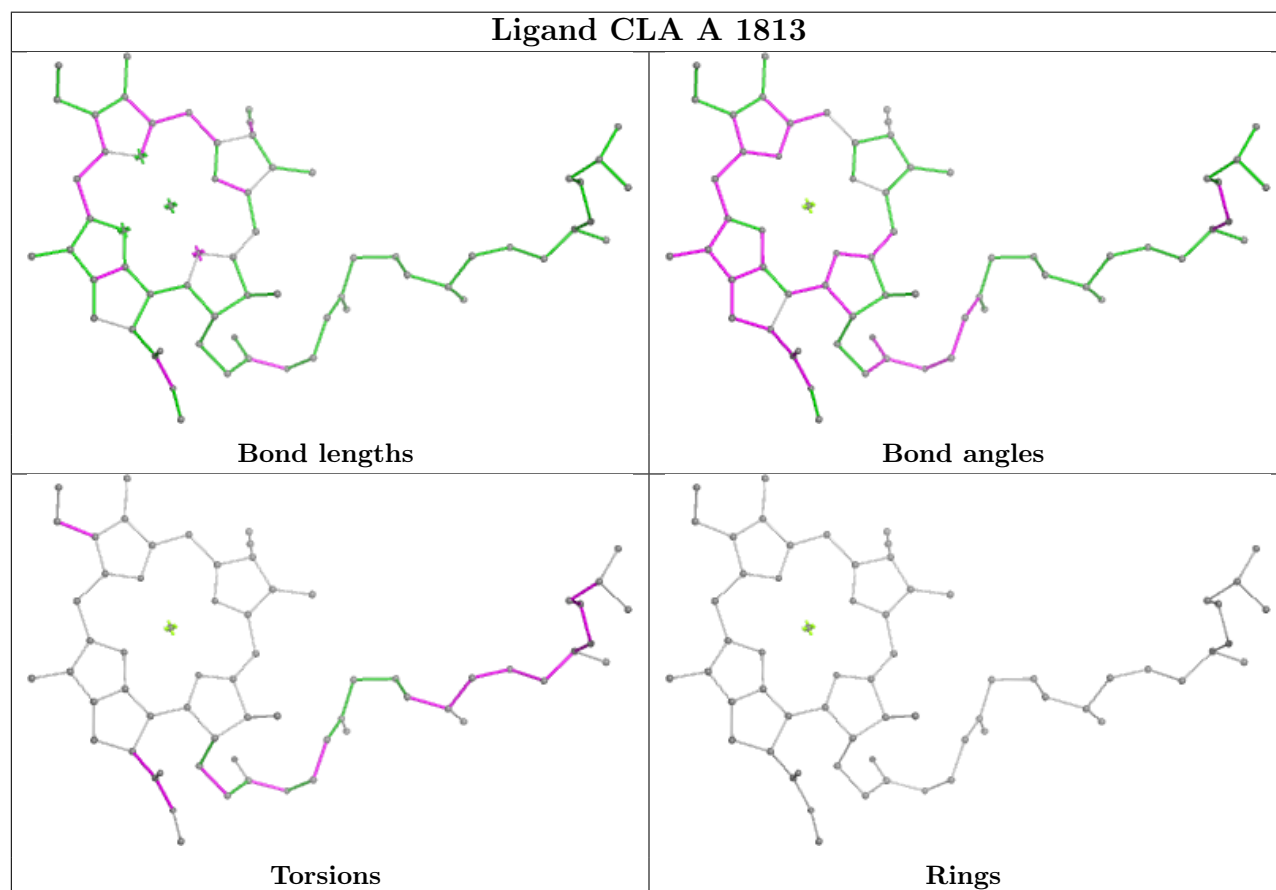
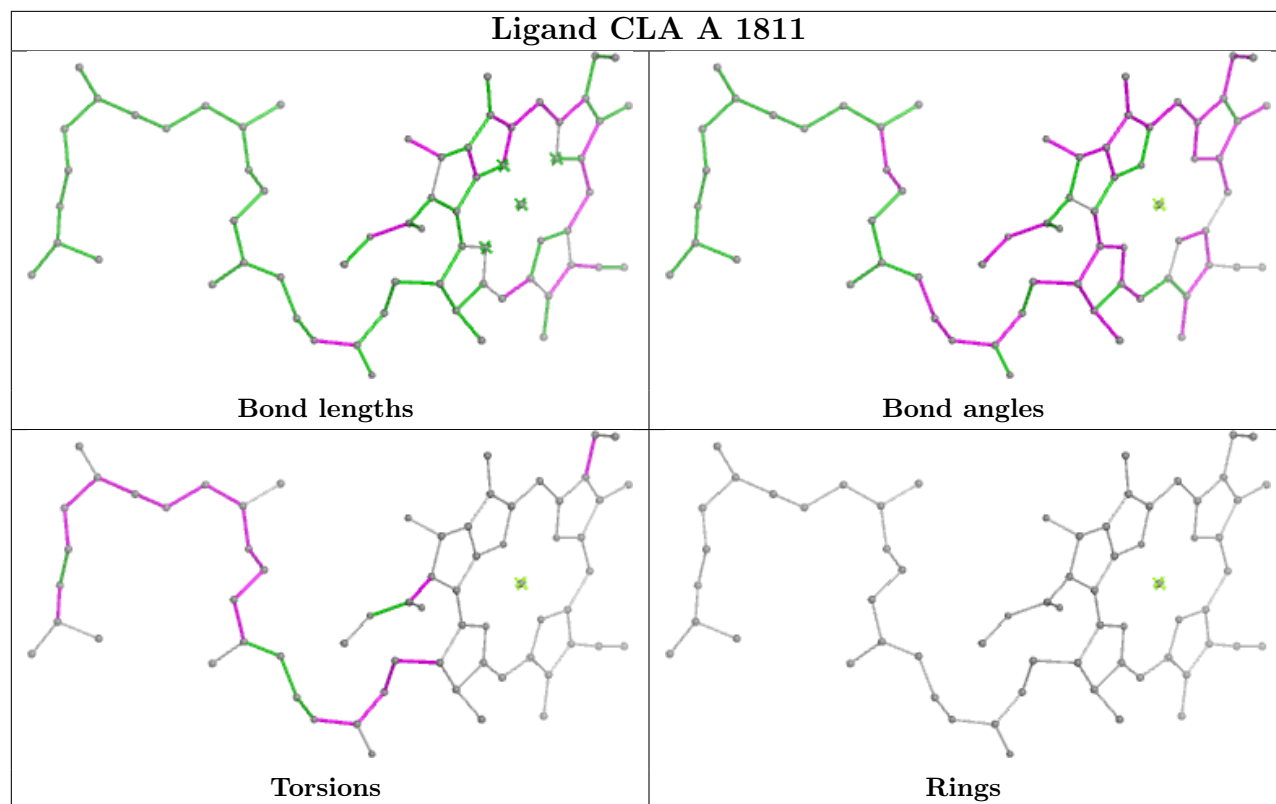
Ligand LMU R 1057



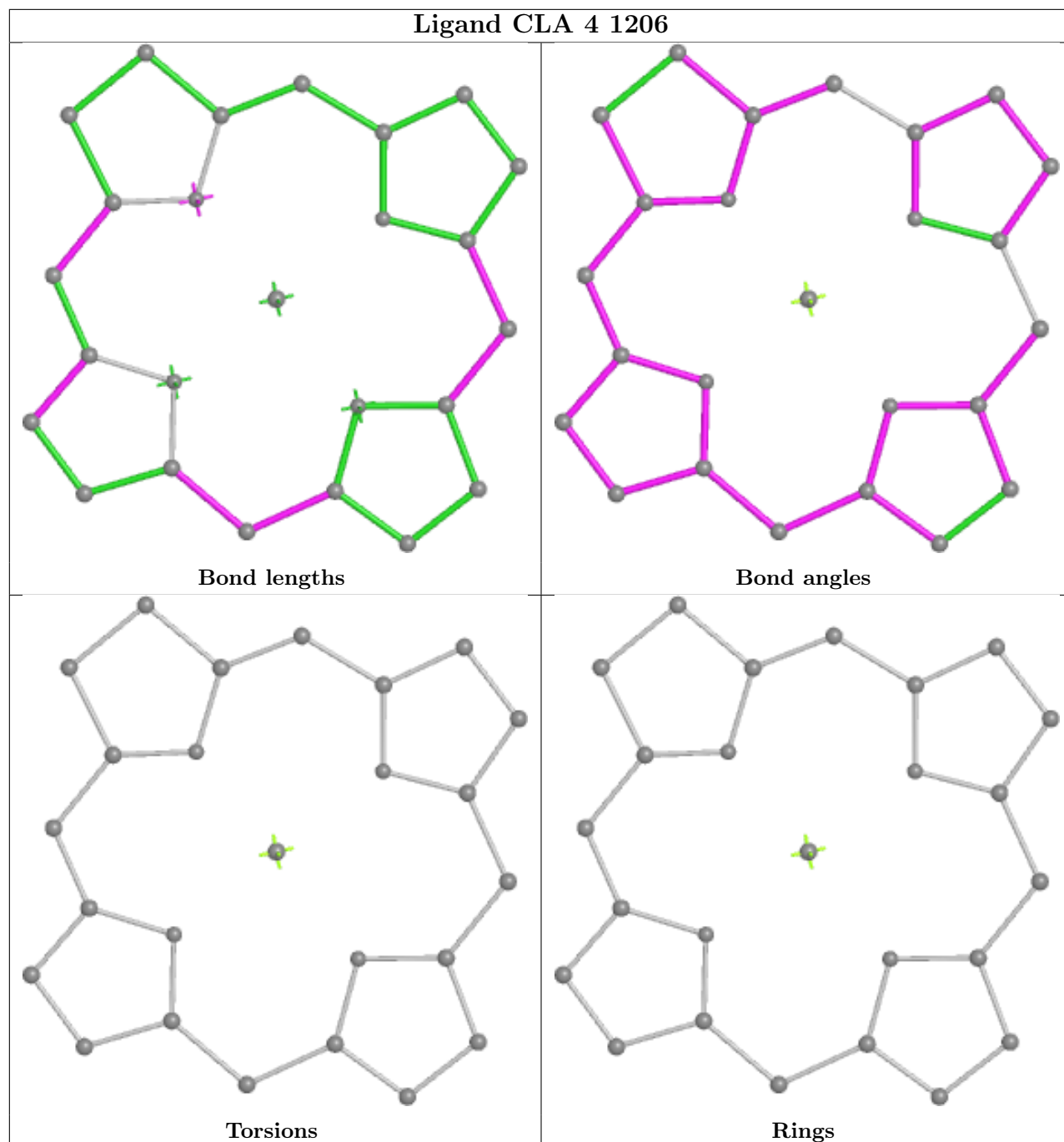




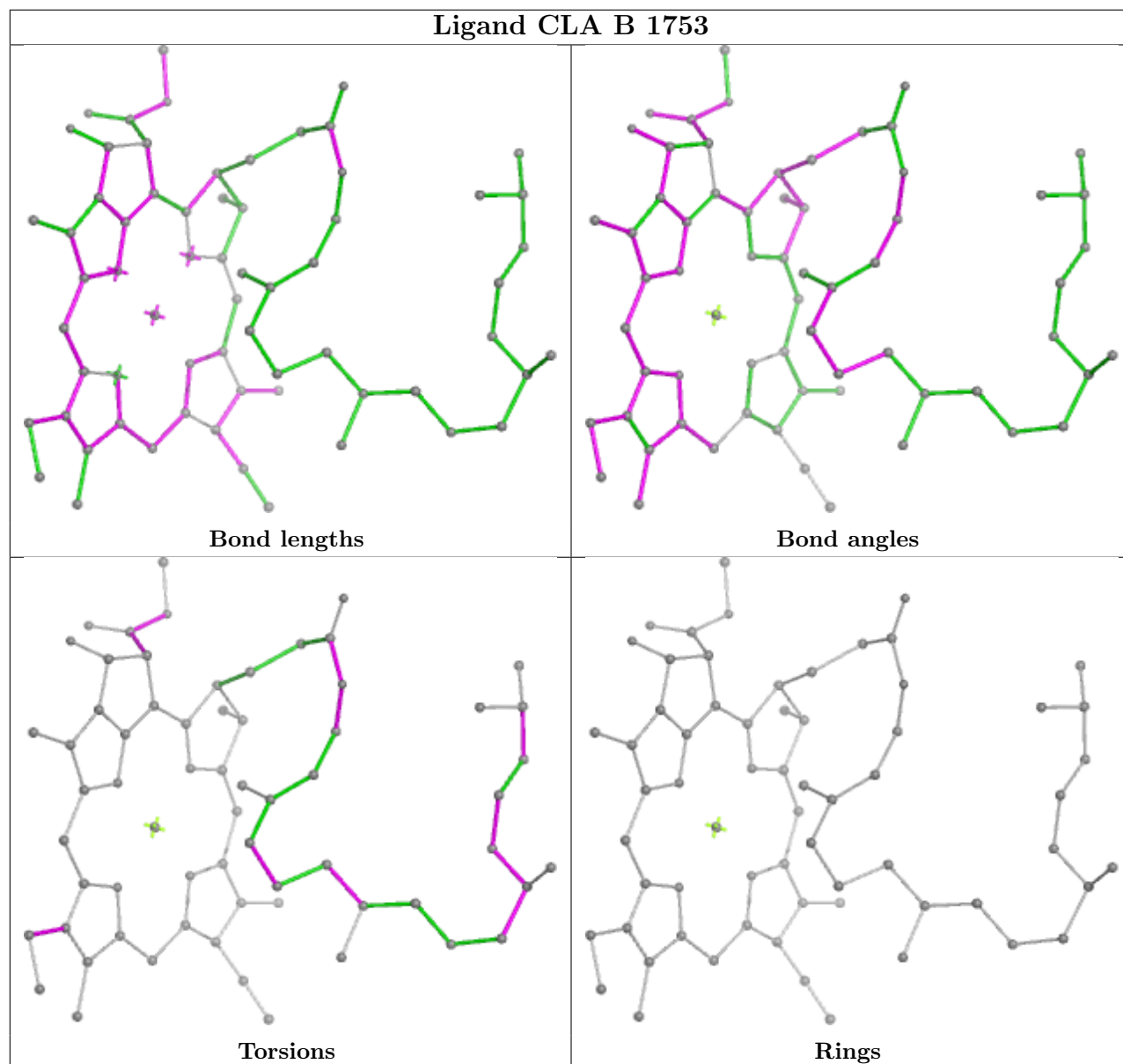


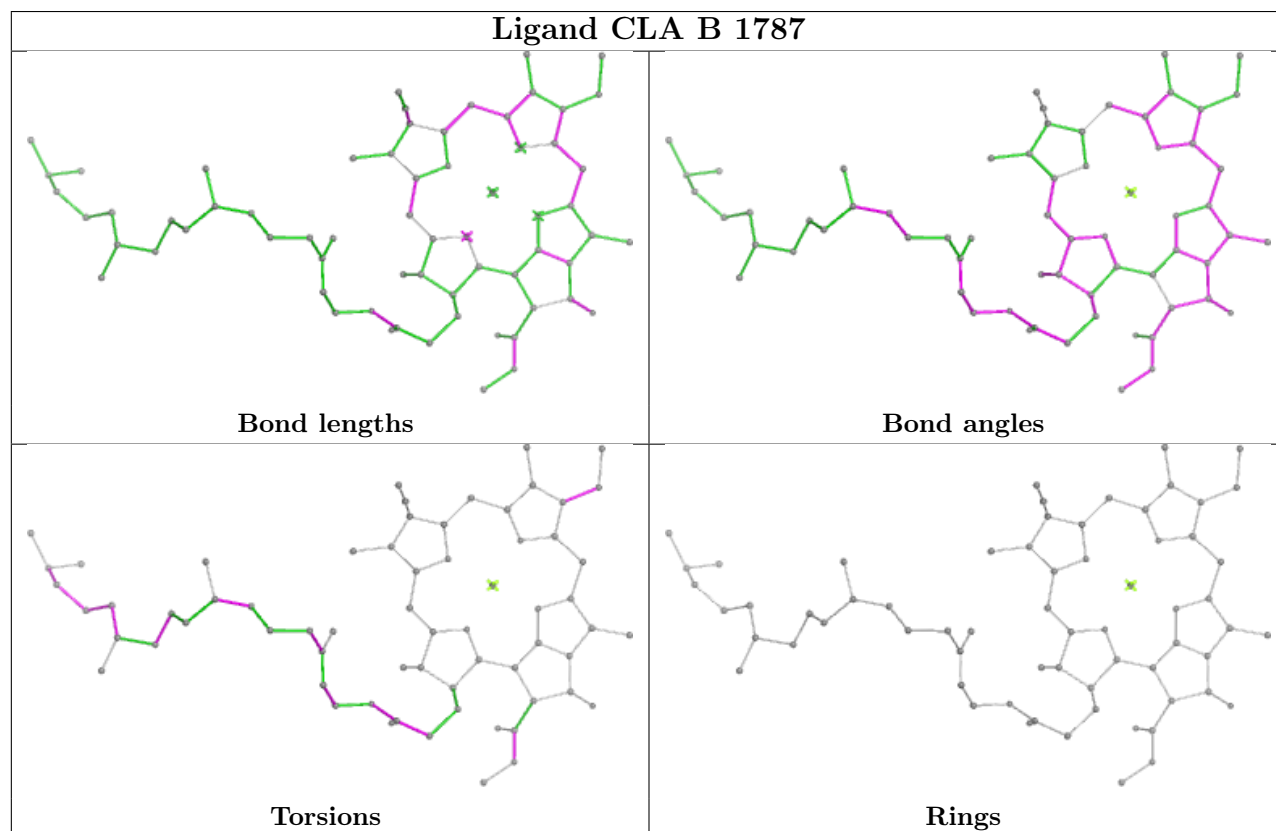
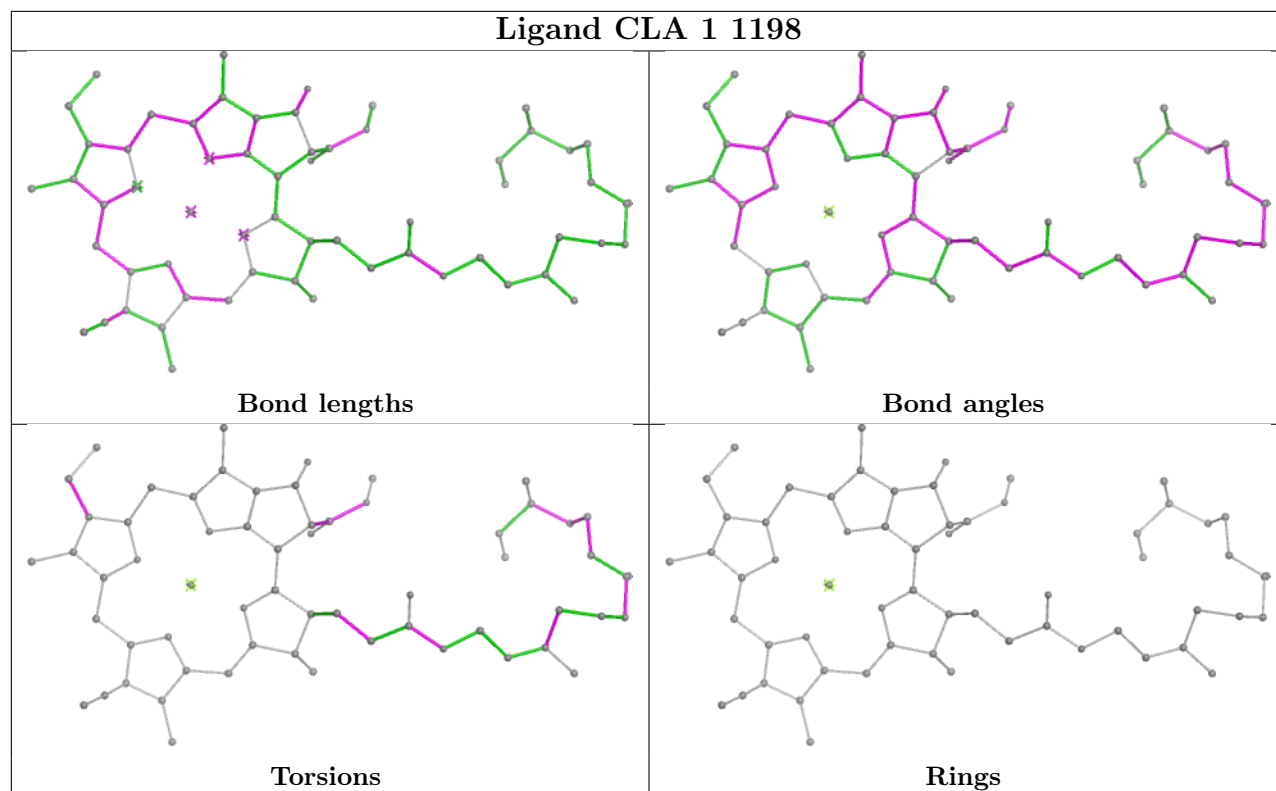


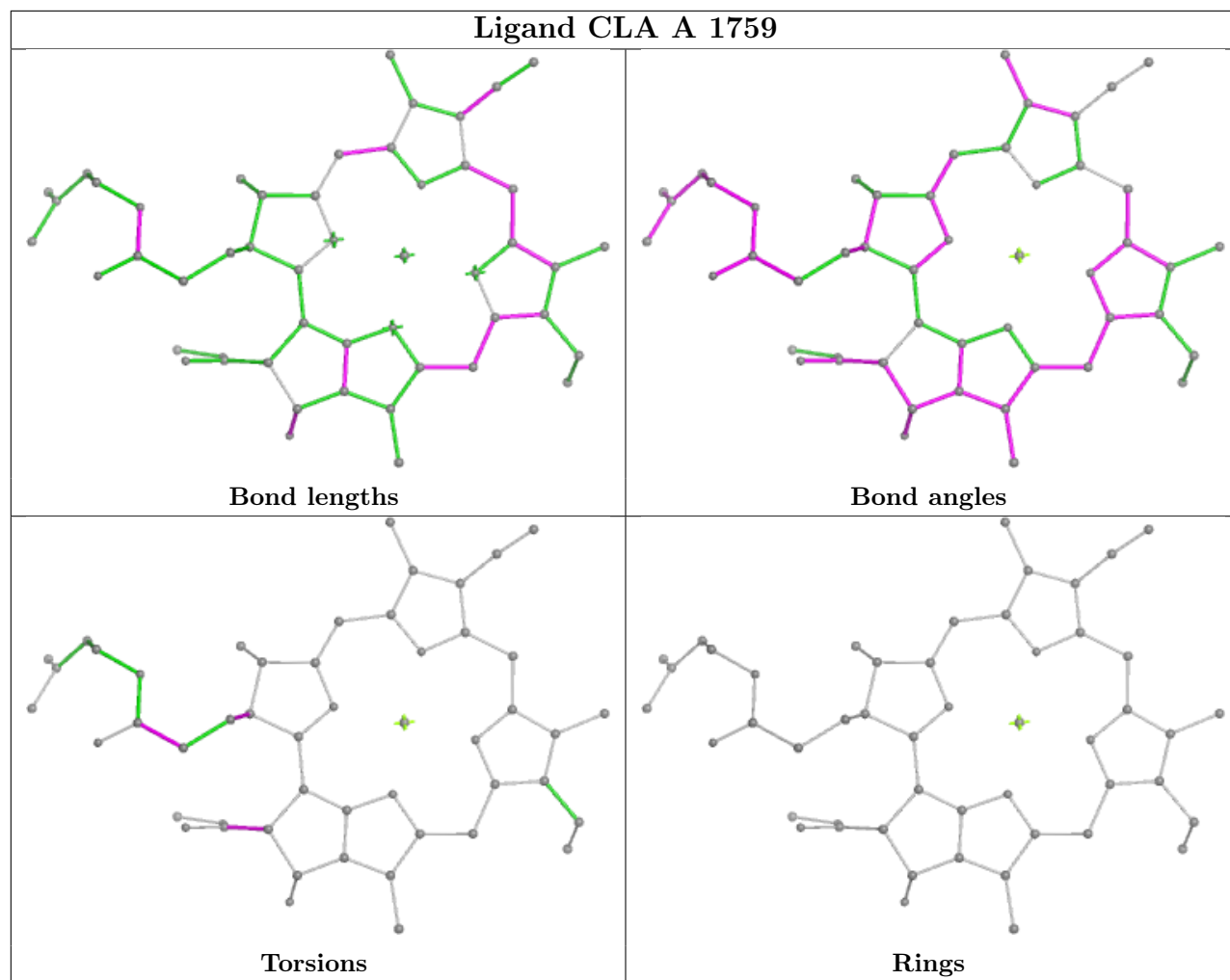
Ligand CLA 4 1206



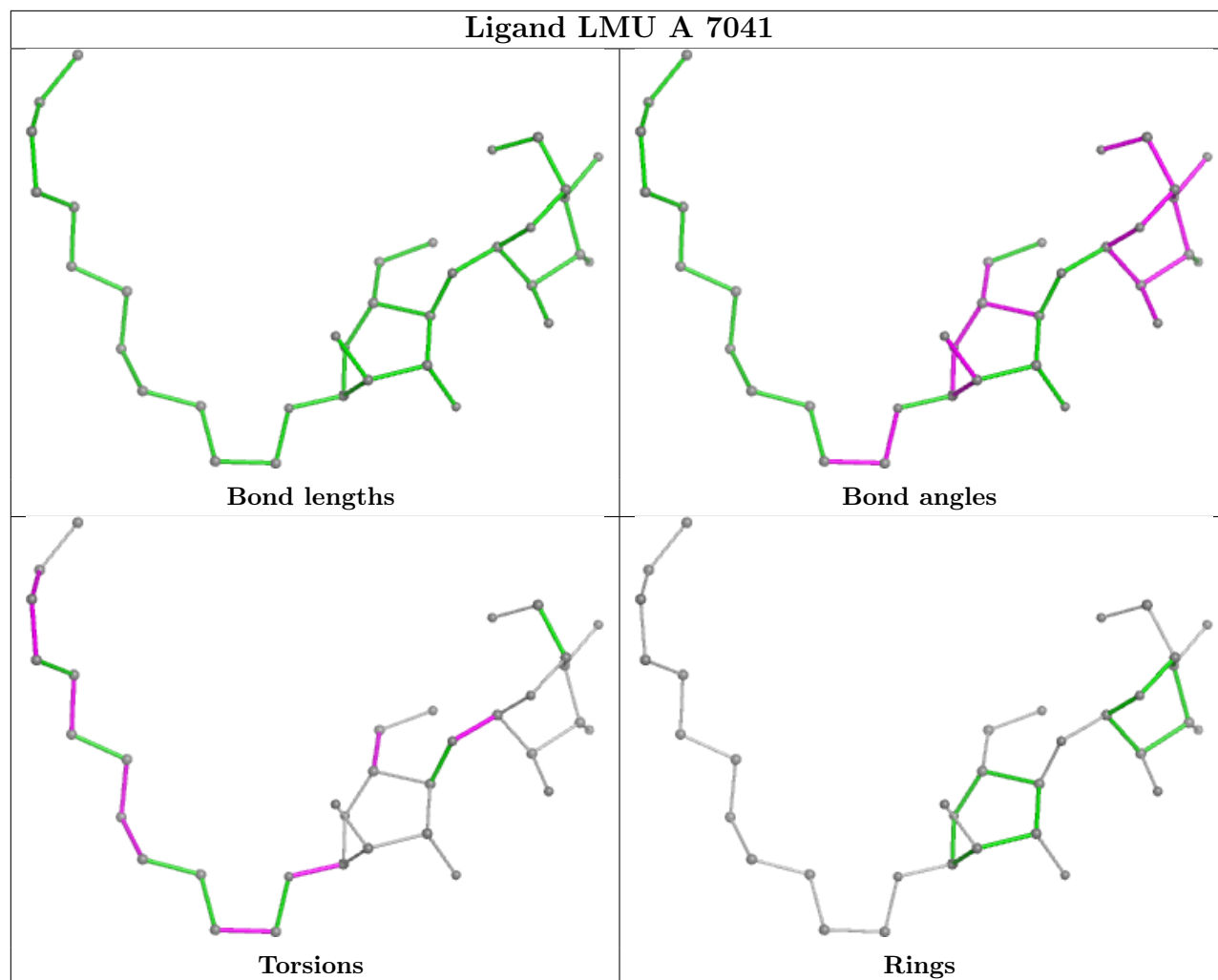
Ligand CLA B 1753

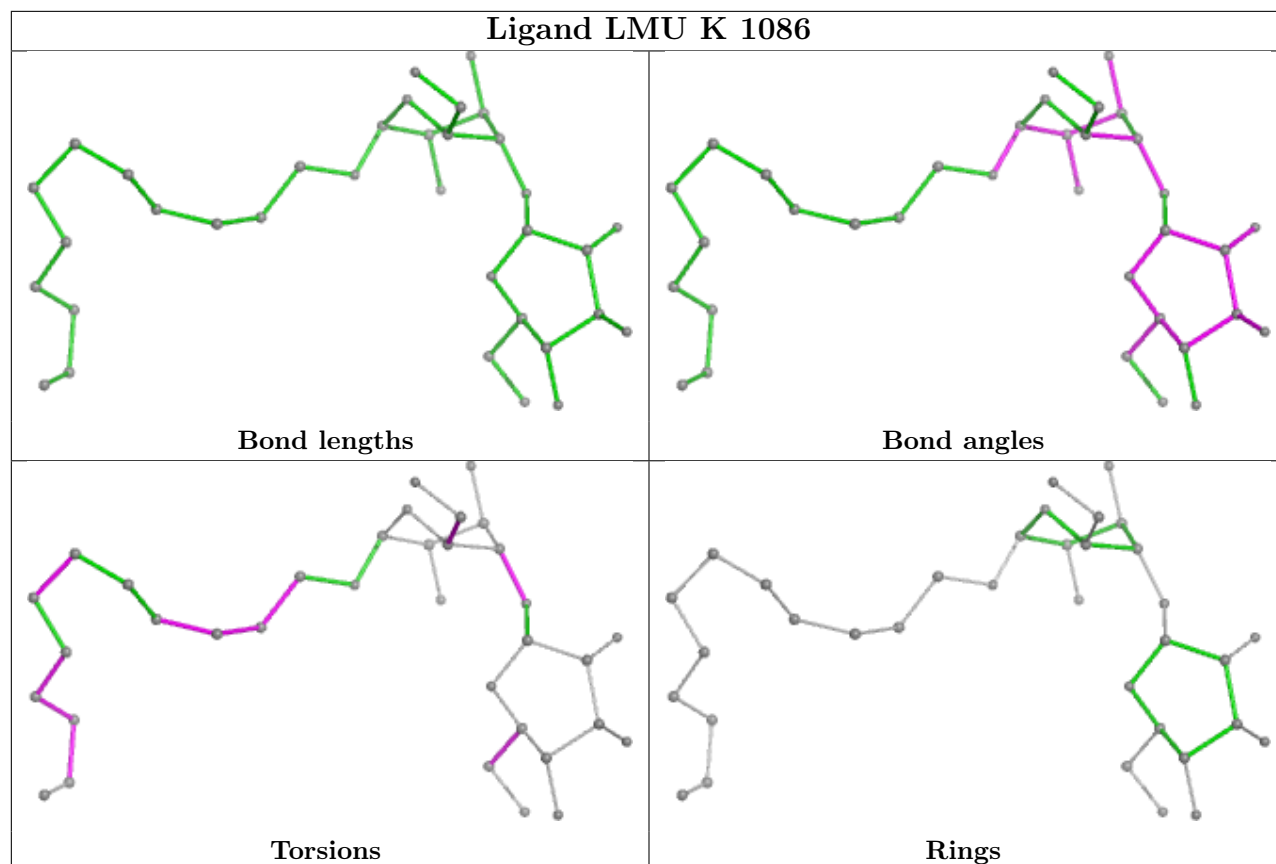


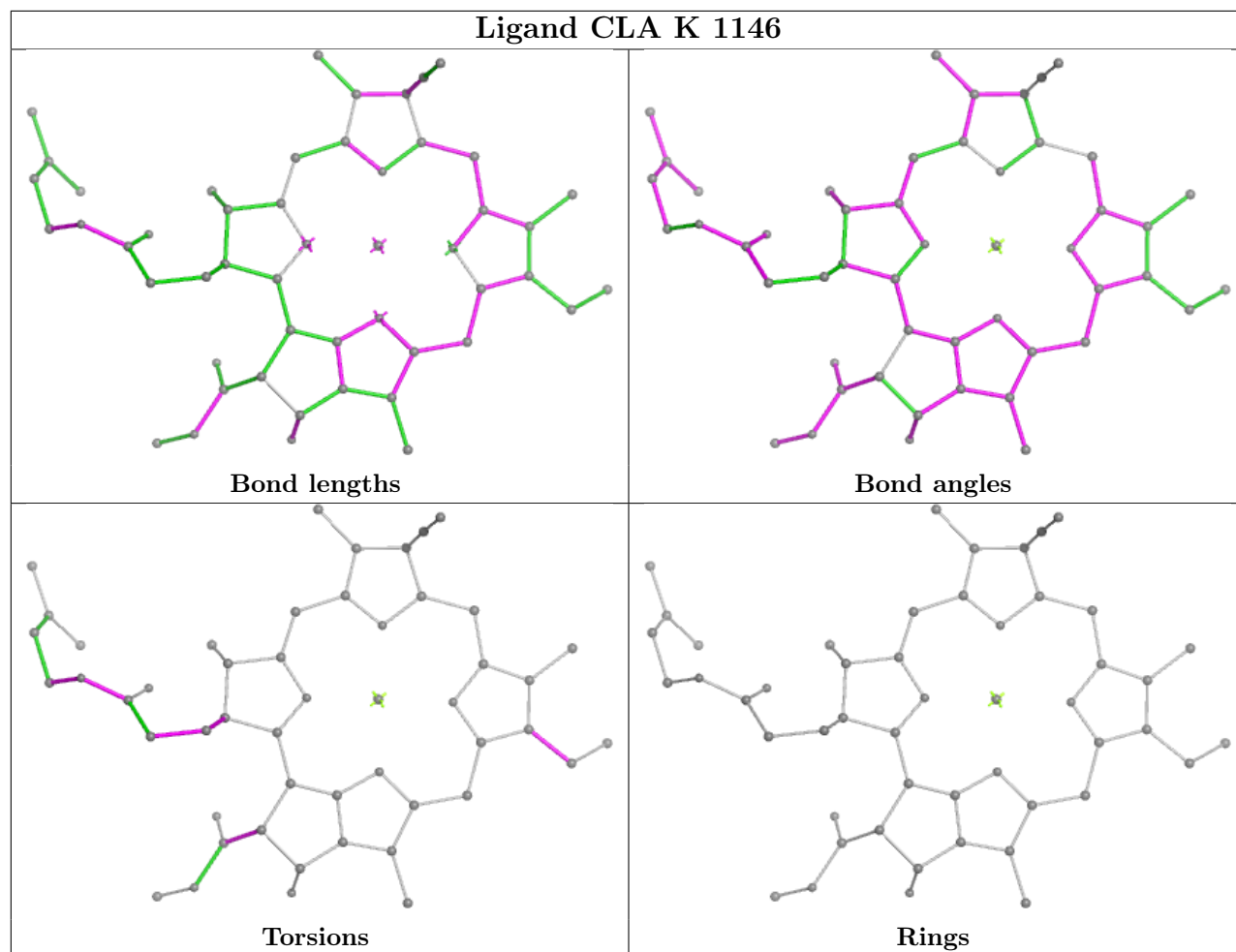


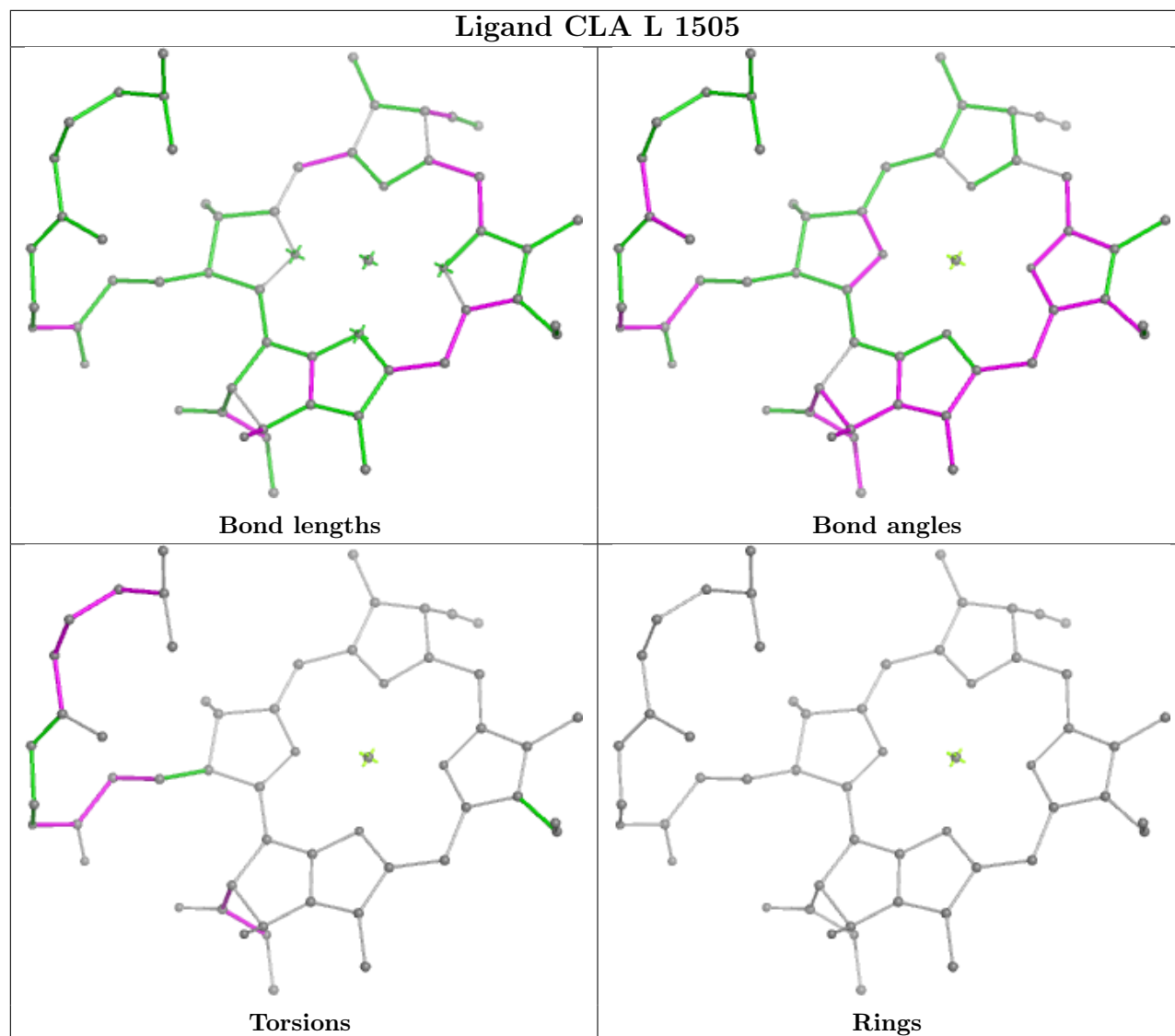


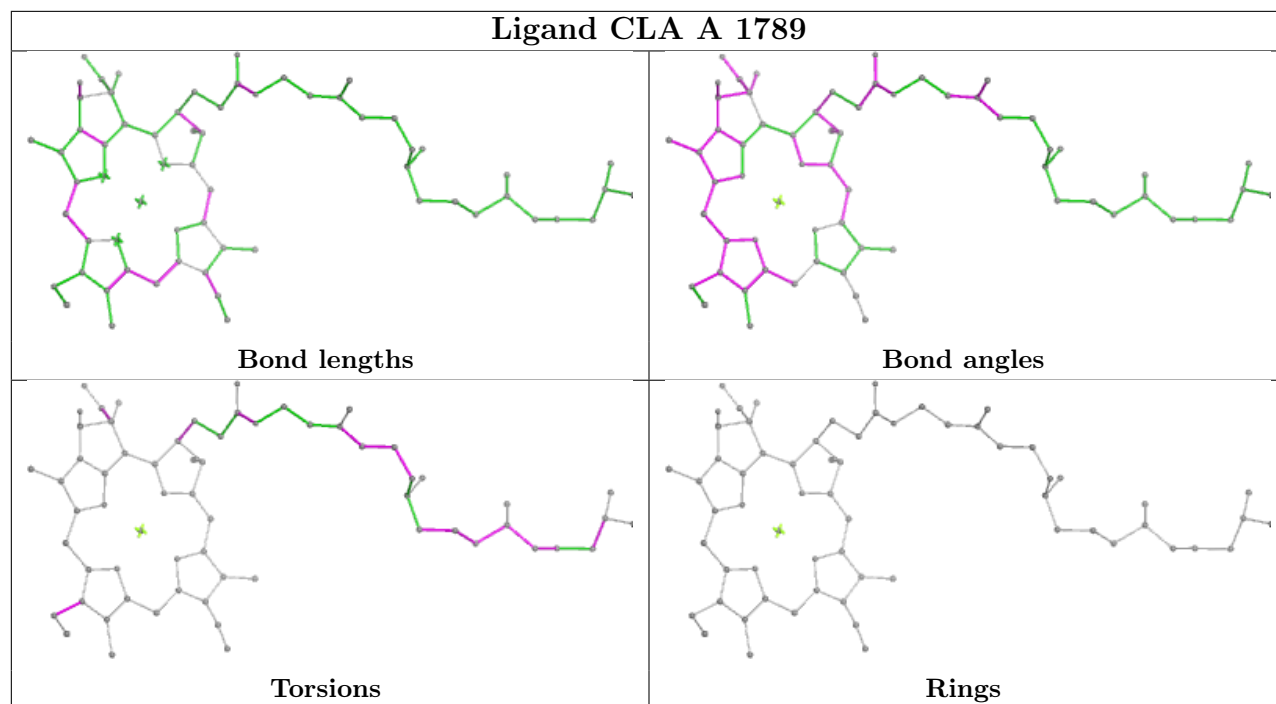
Ligand LMU A 7041

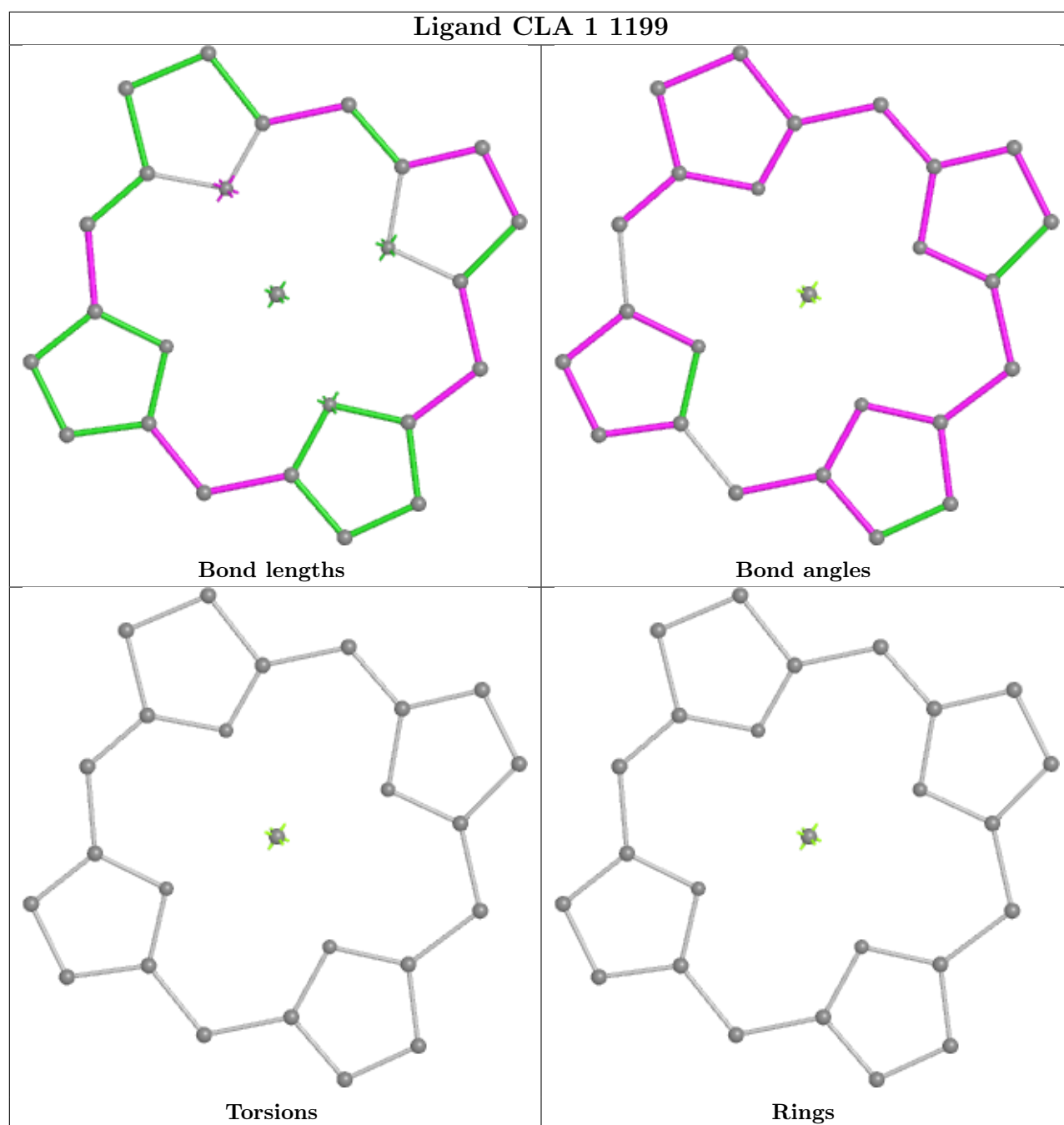


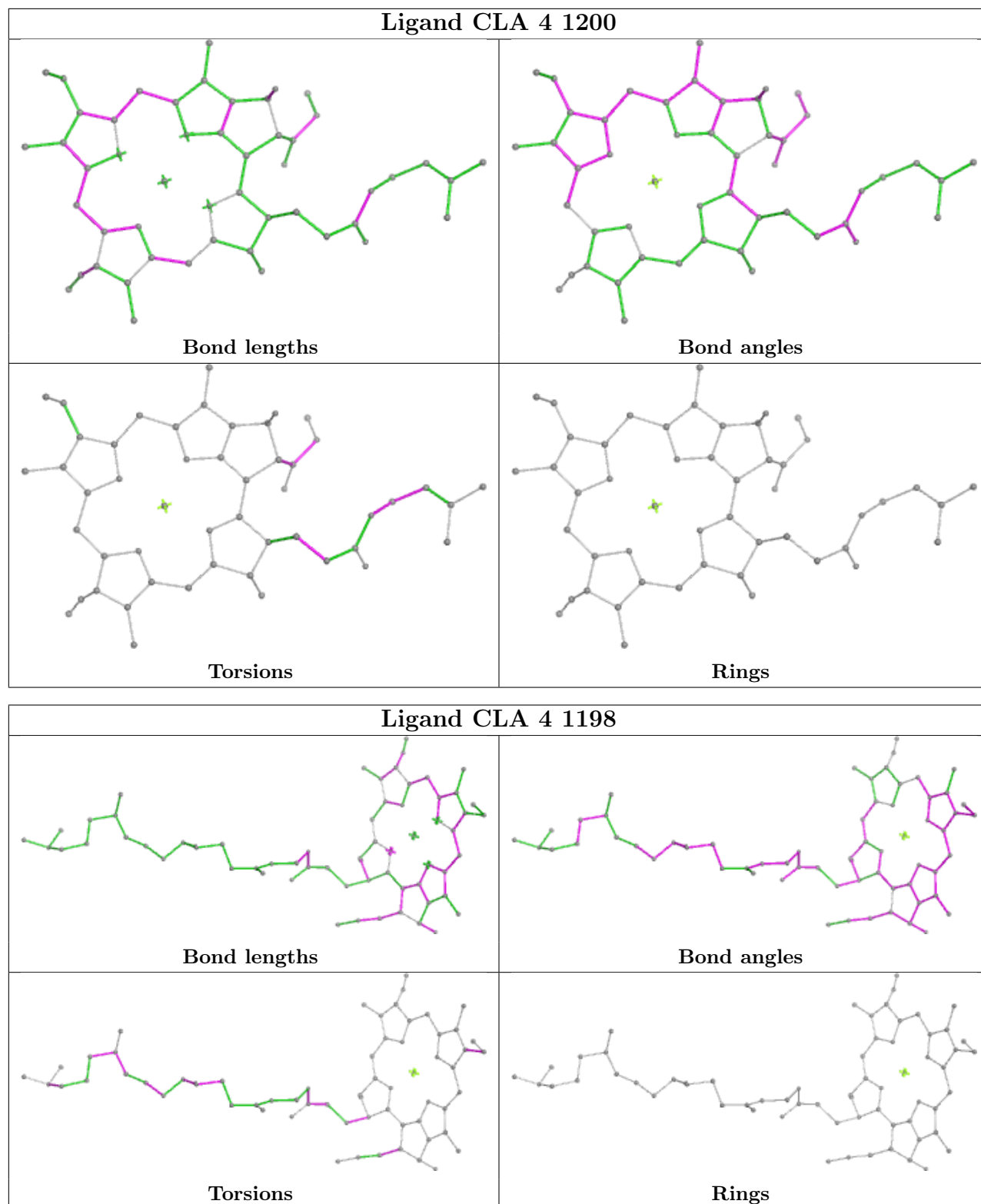


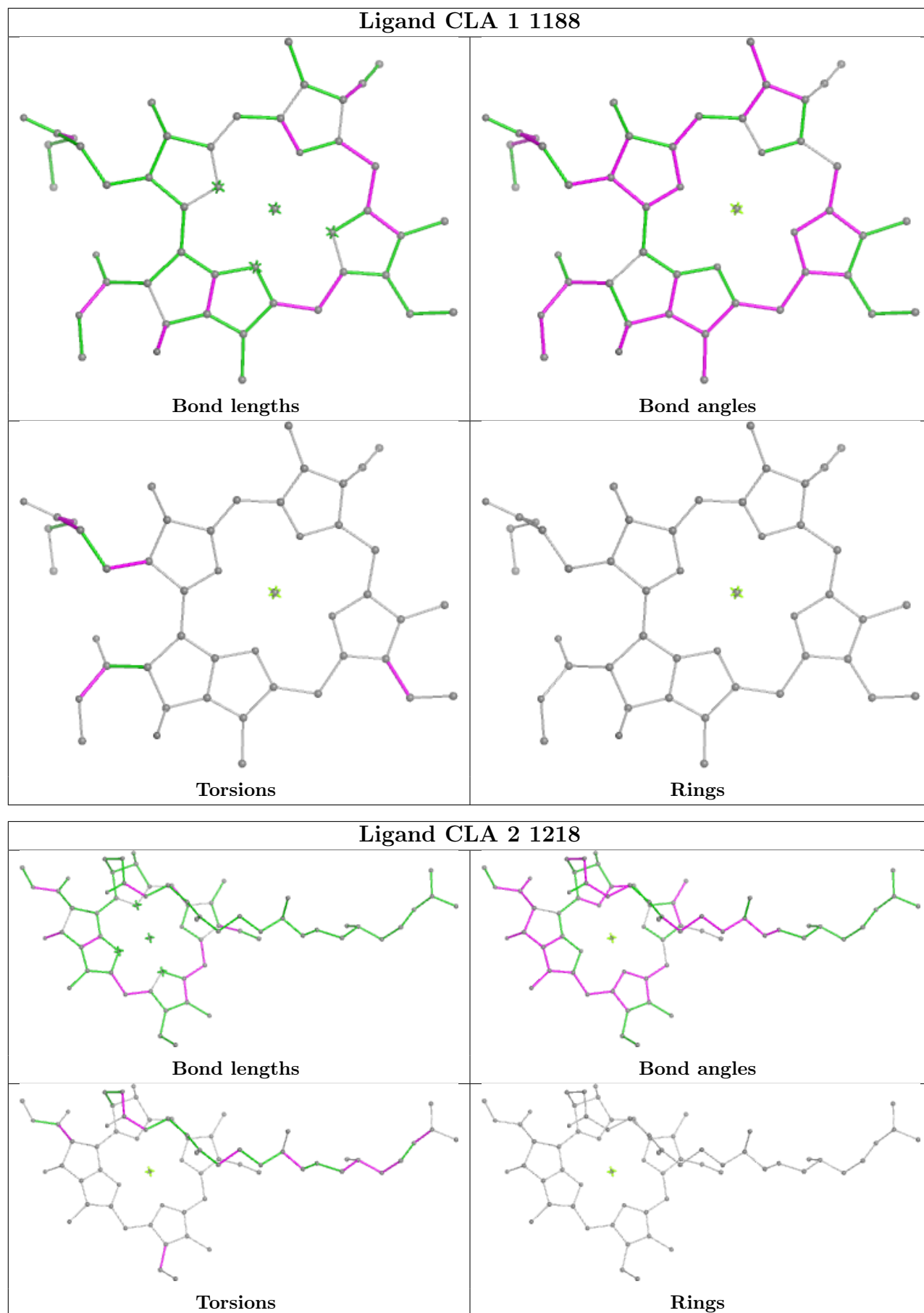


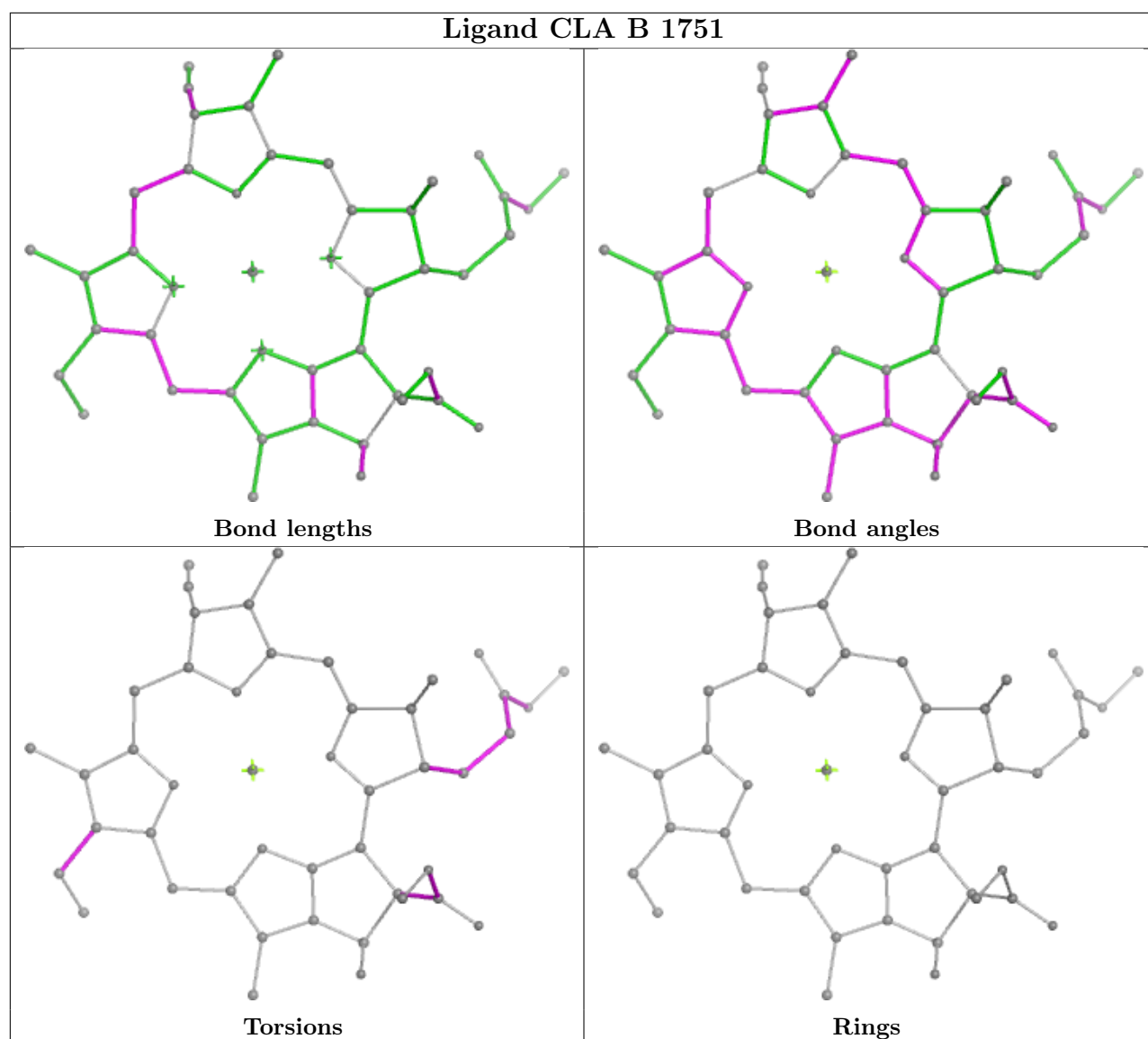




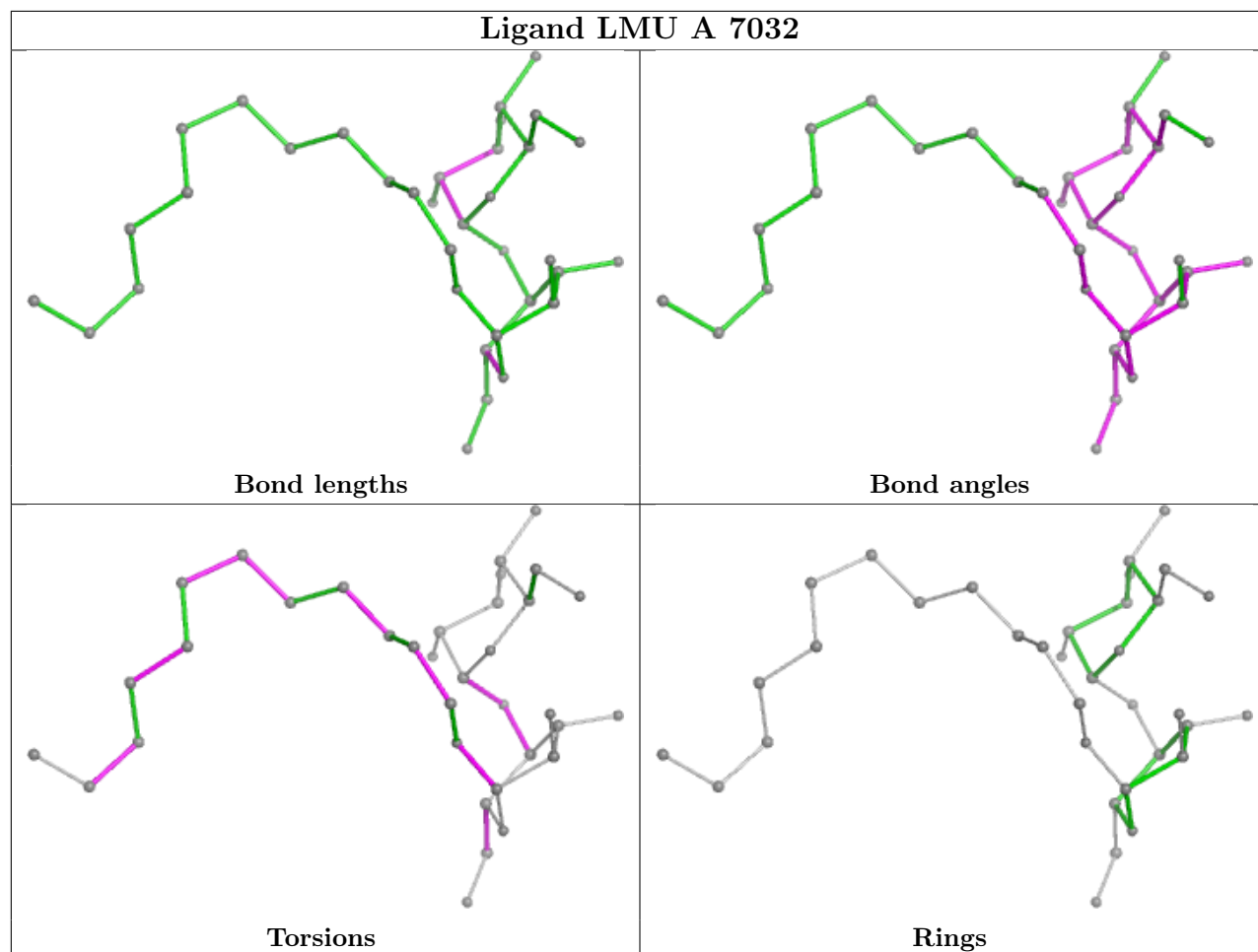




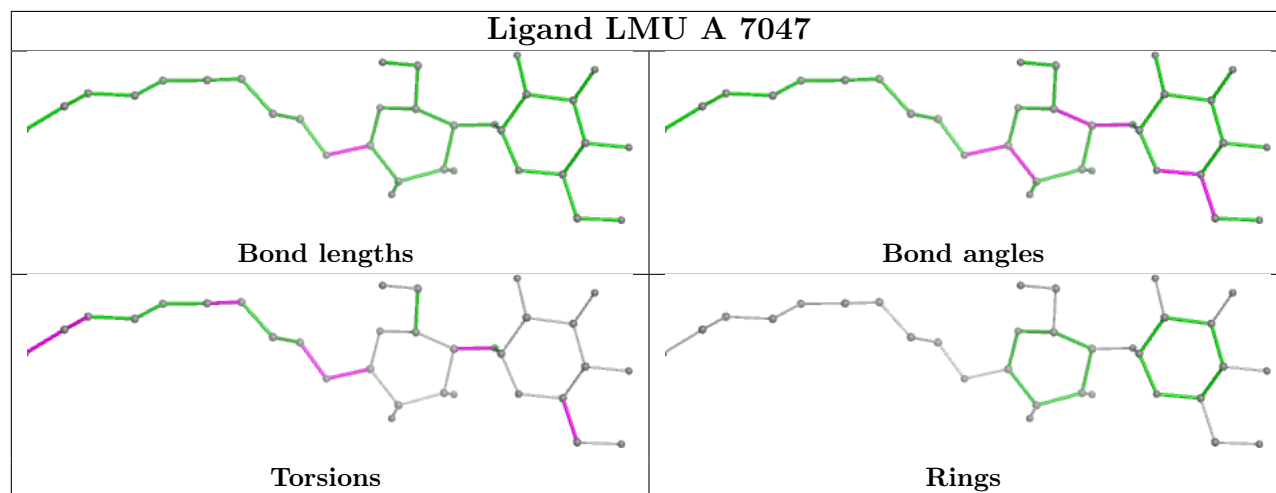


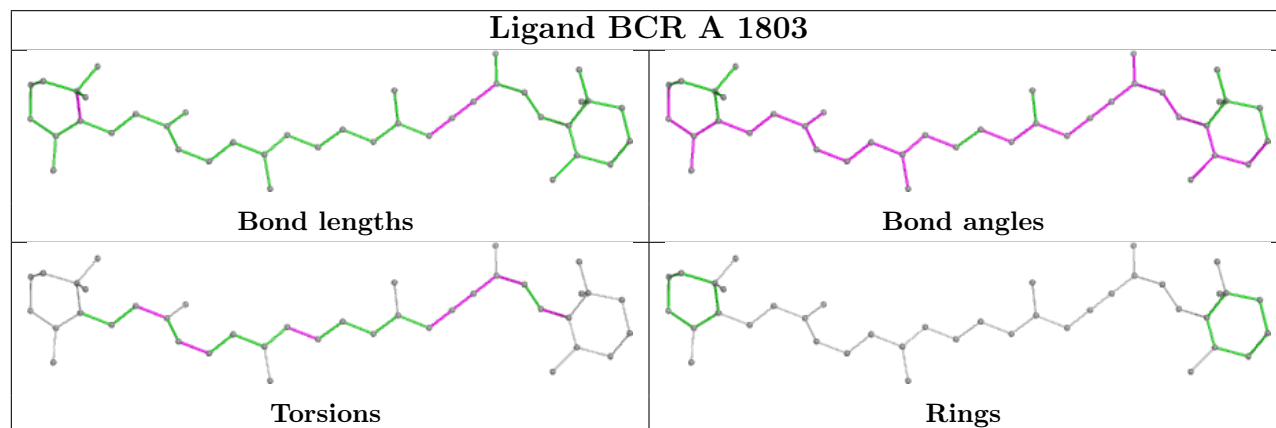
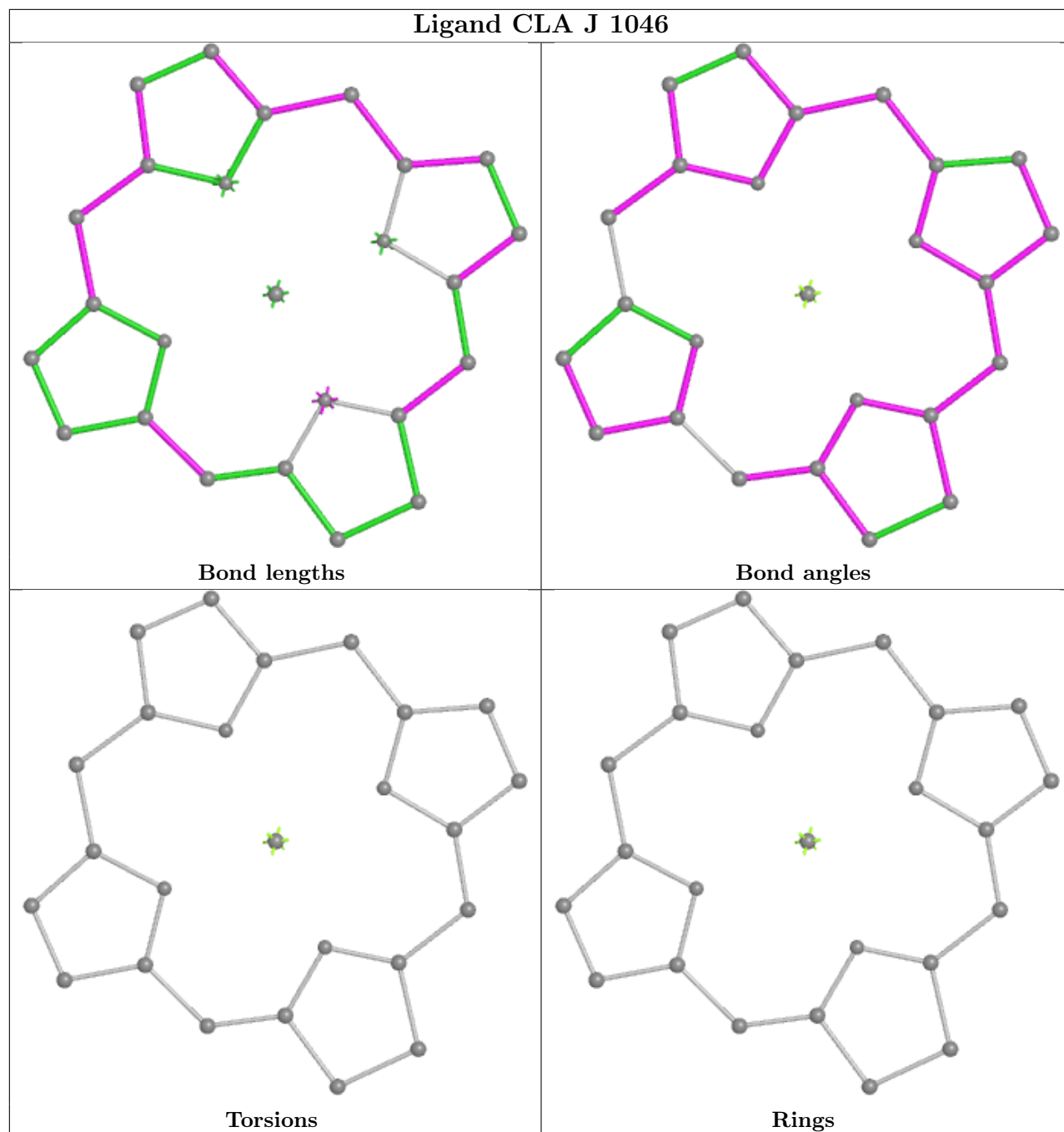


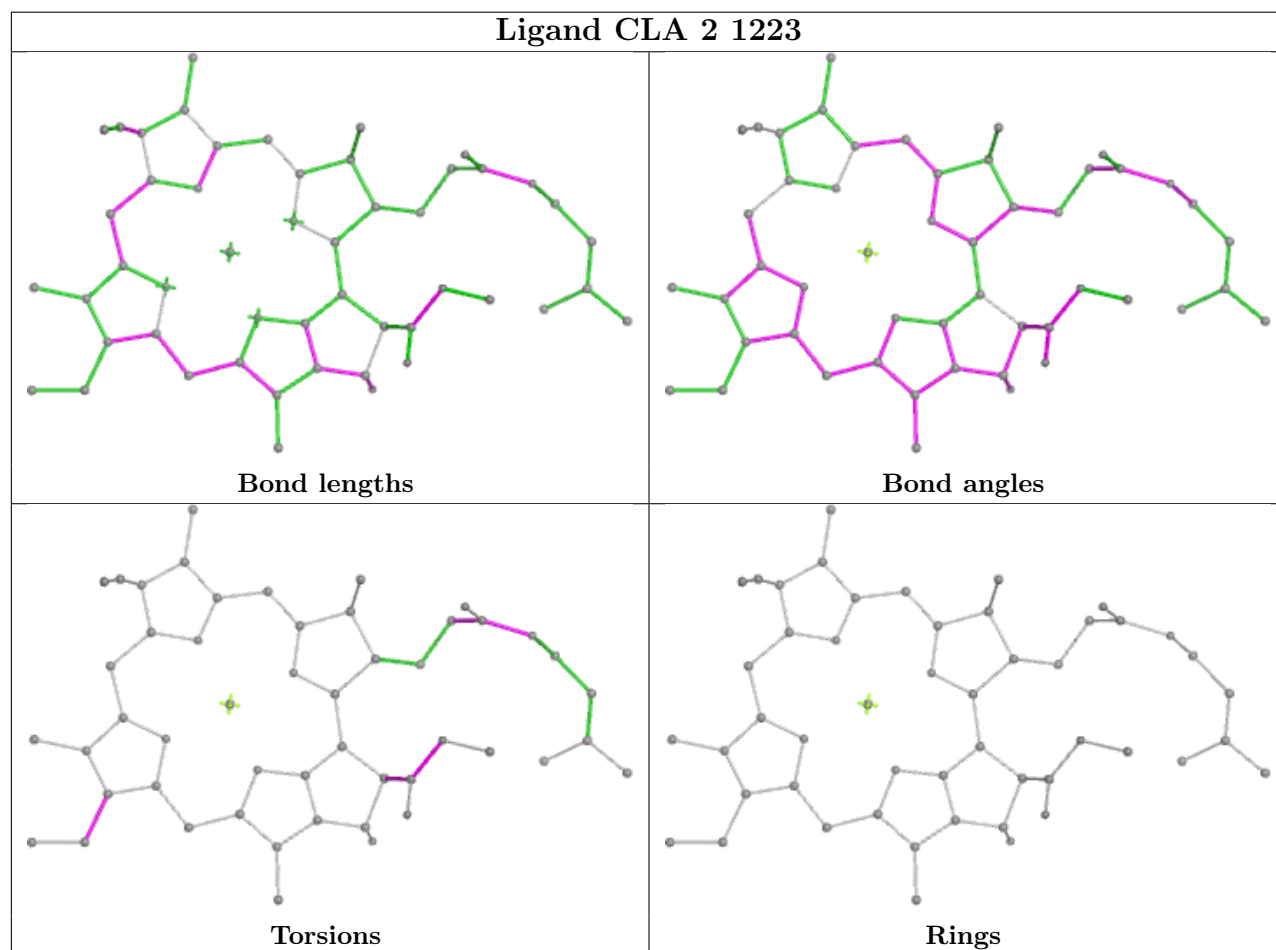
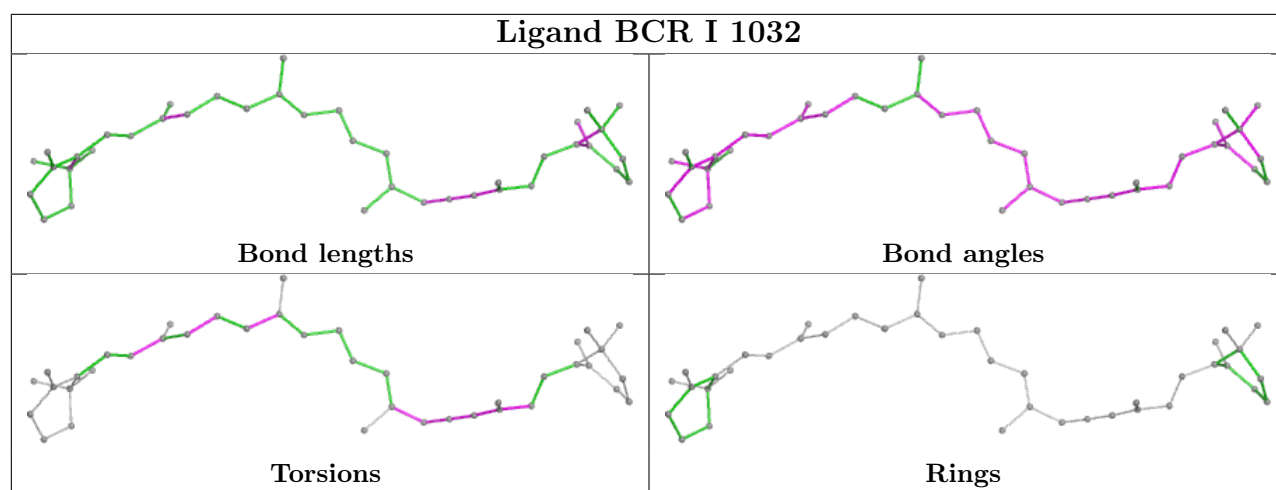
Ligand LMU A 7032

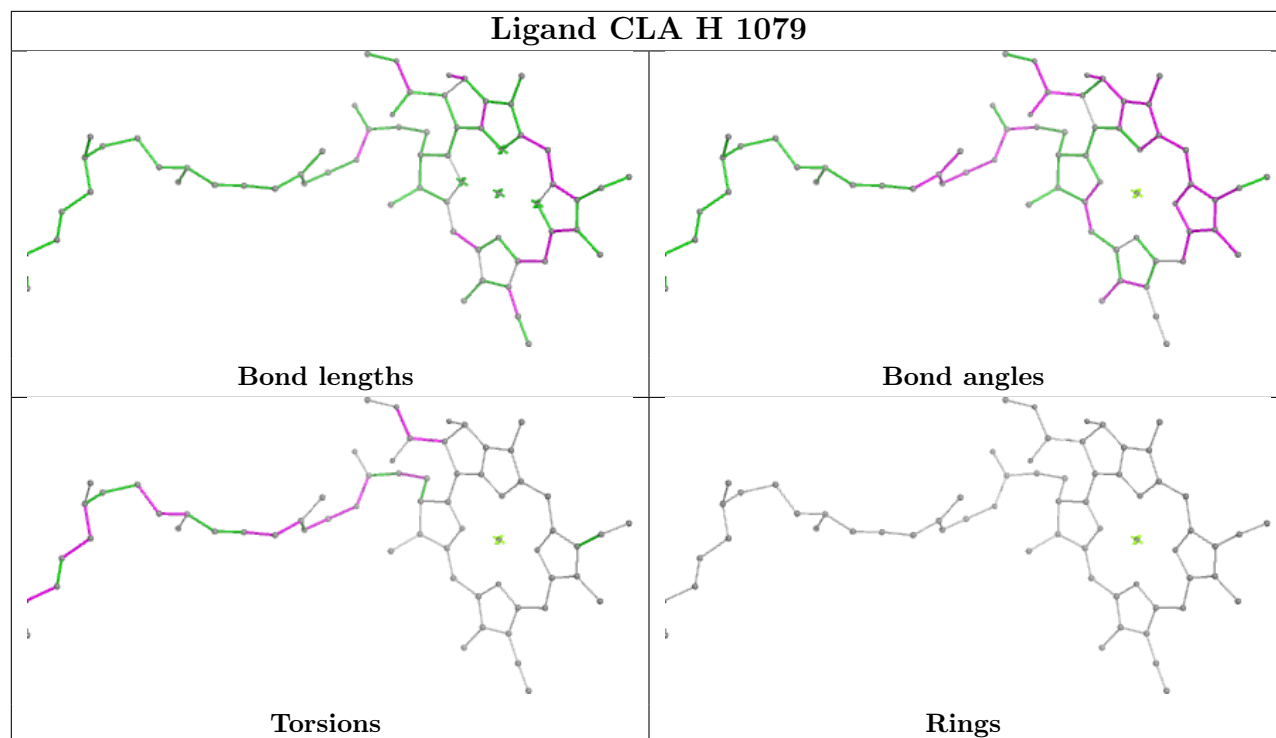


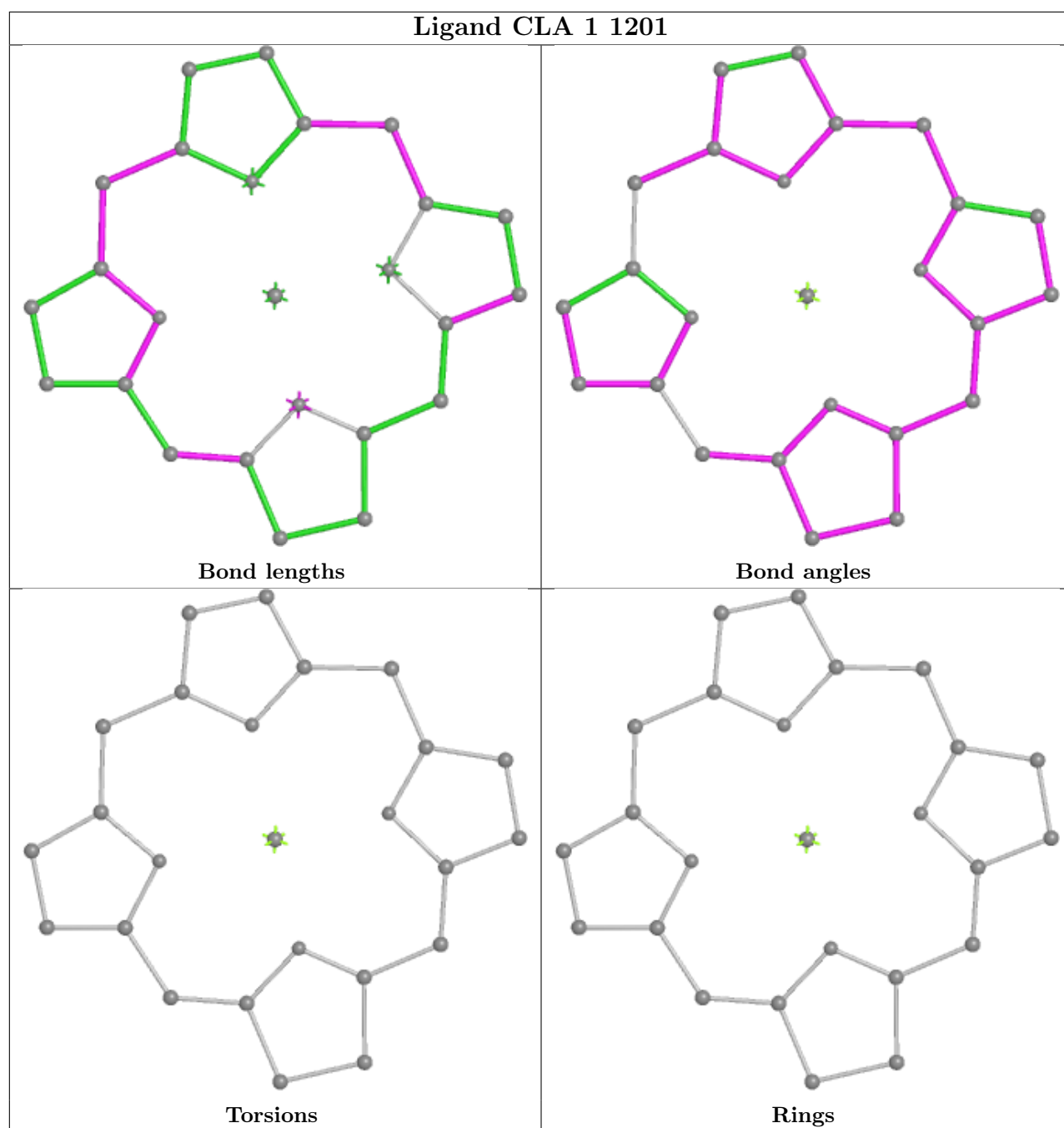
Ligand LMU A 7047



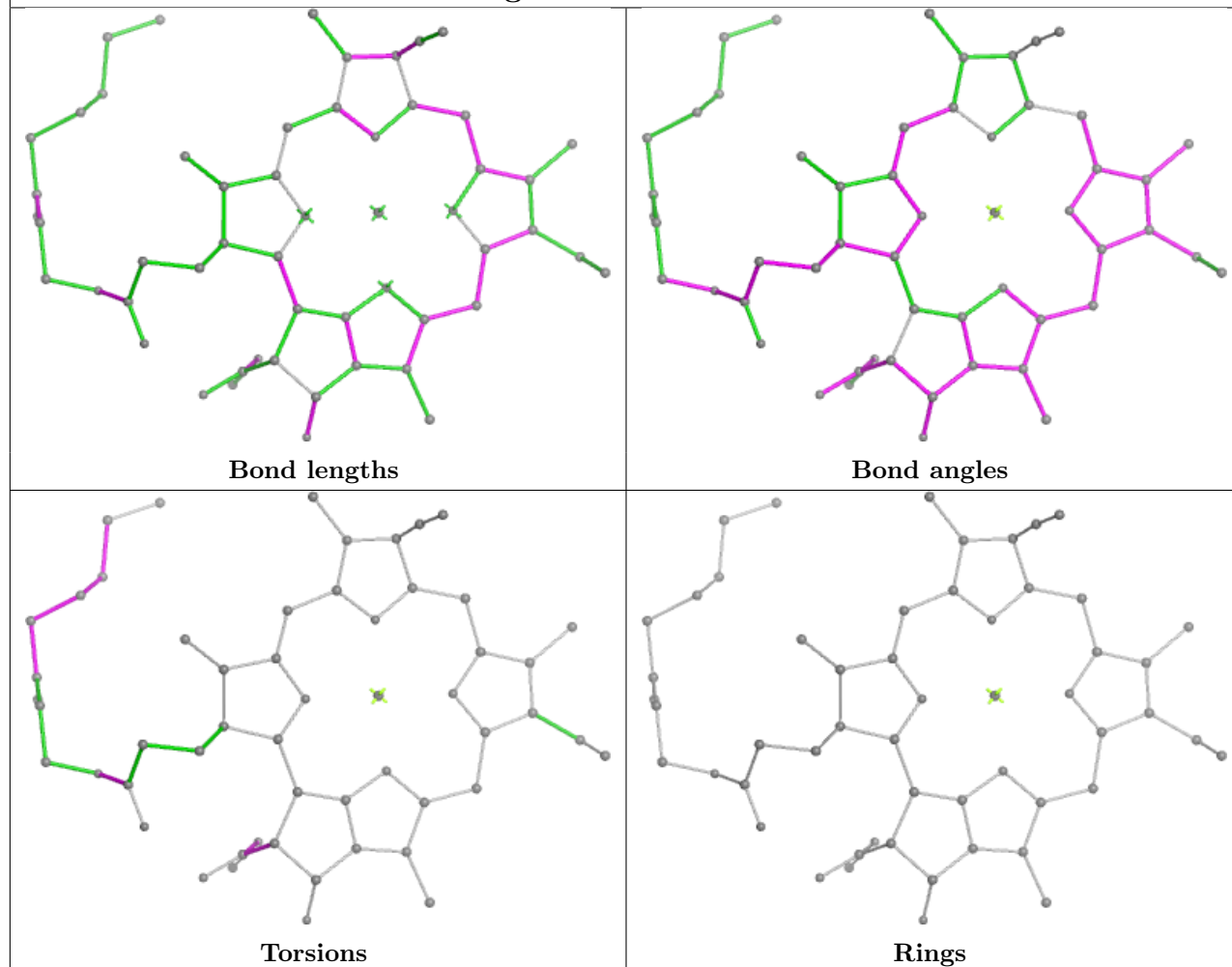




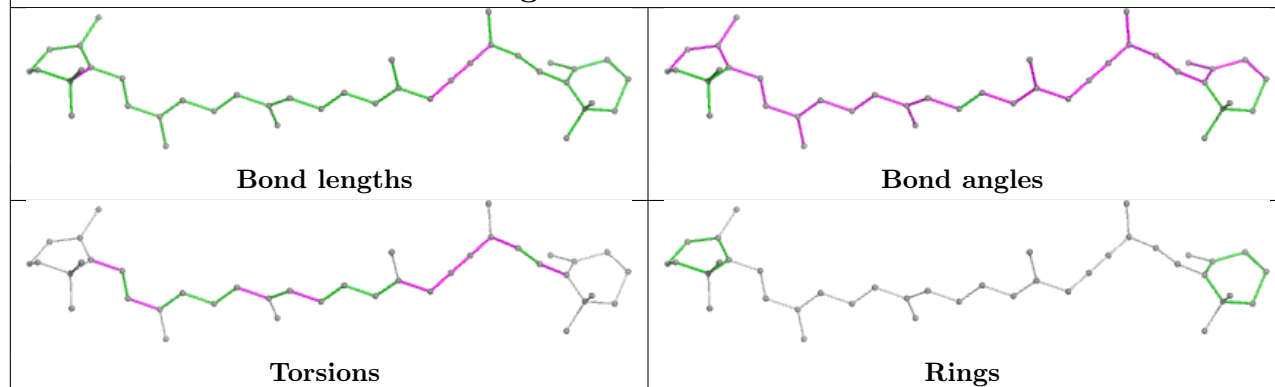




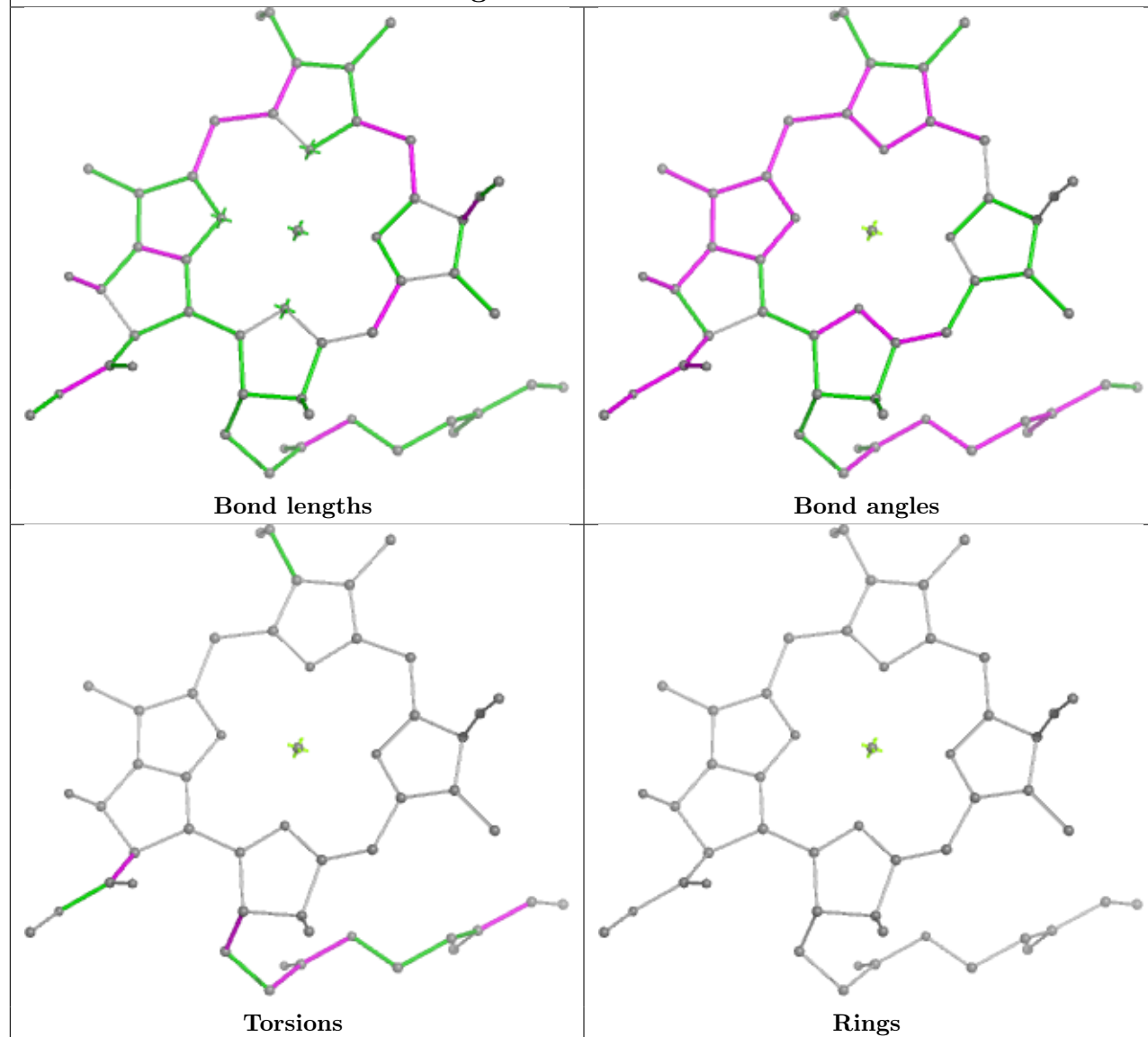
Ligand CLA B 1754



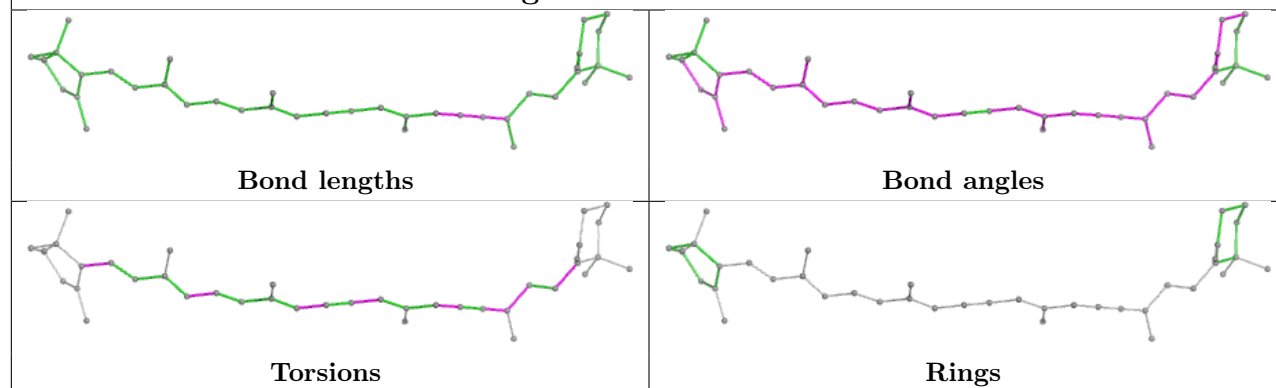
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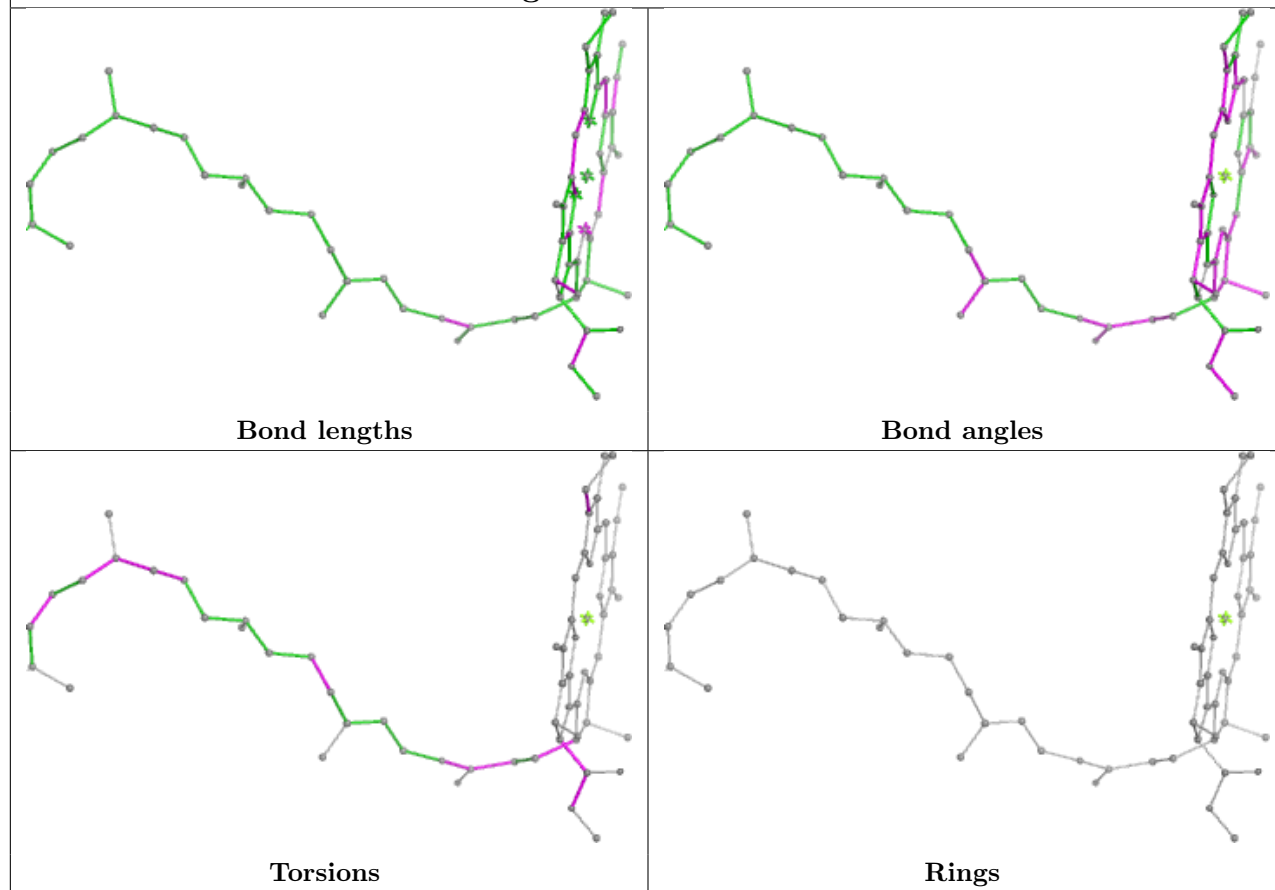
Ligand CLA B 1766



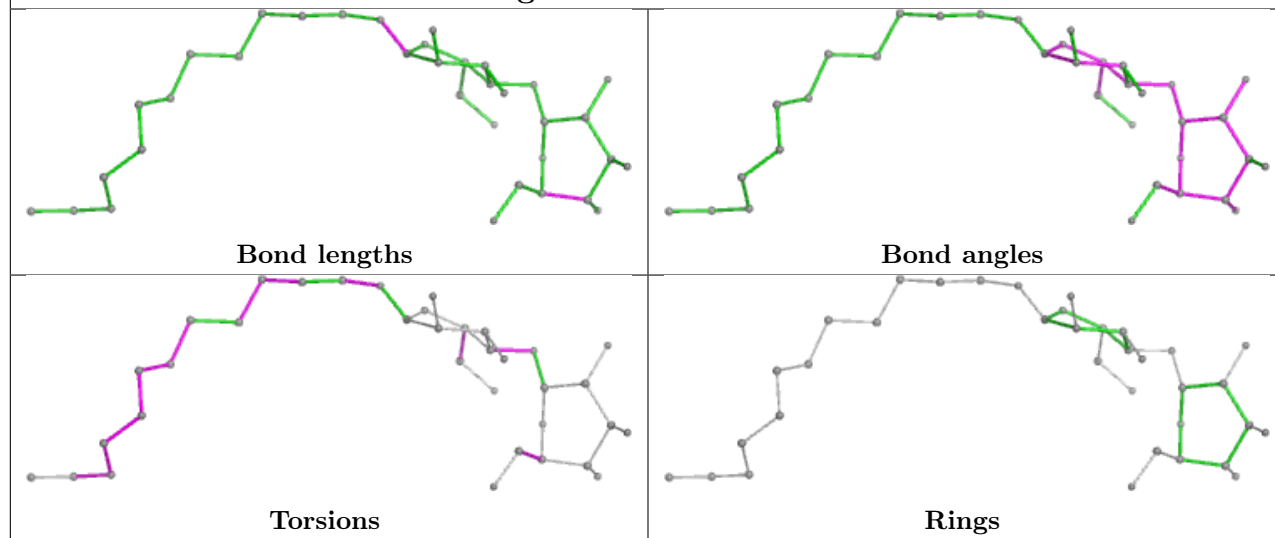
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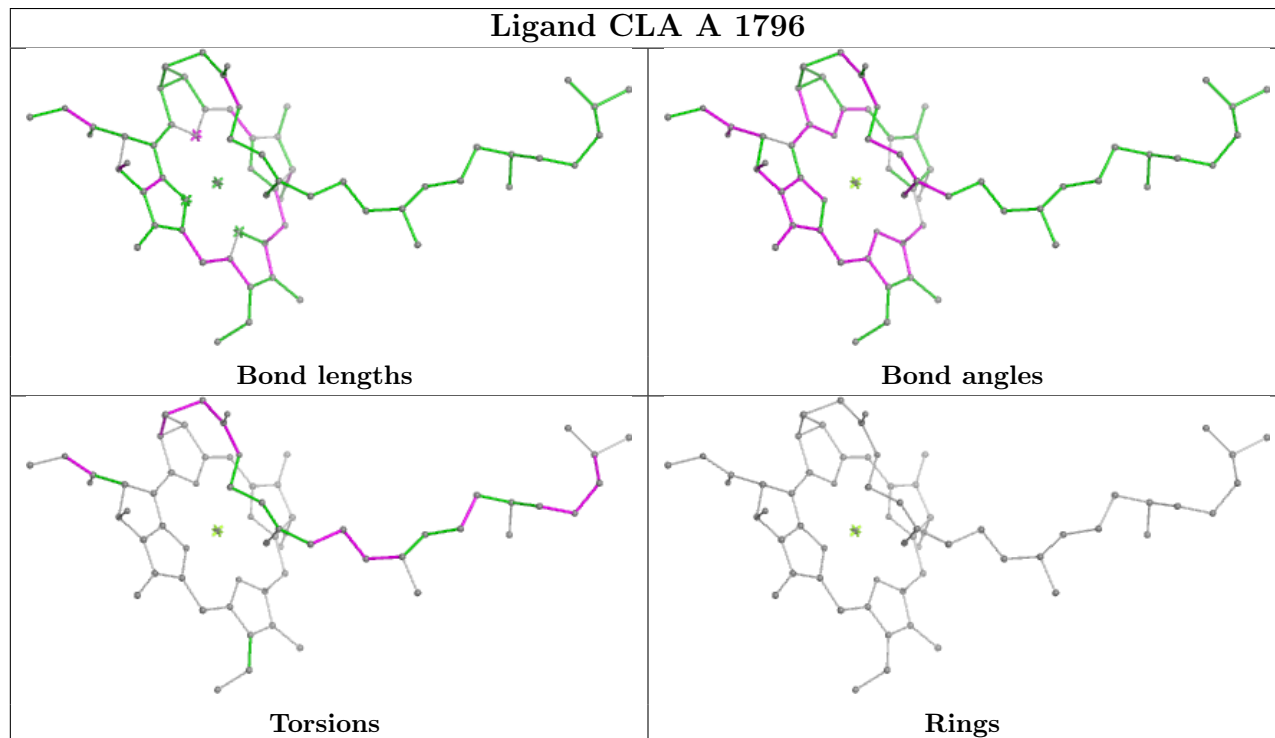
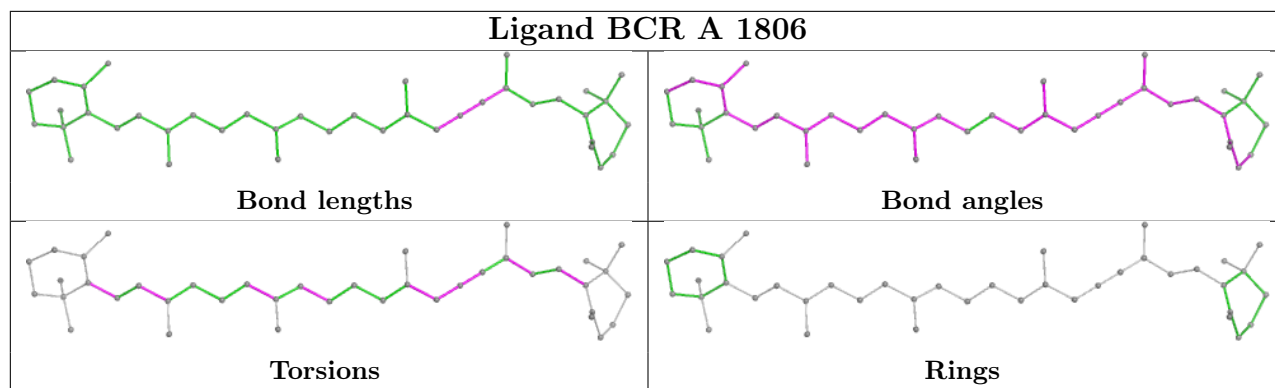


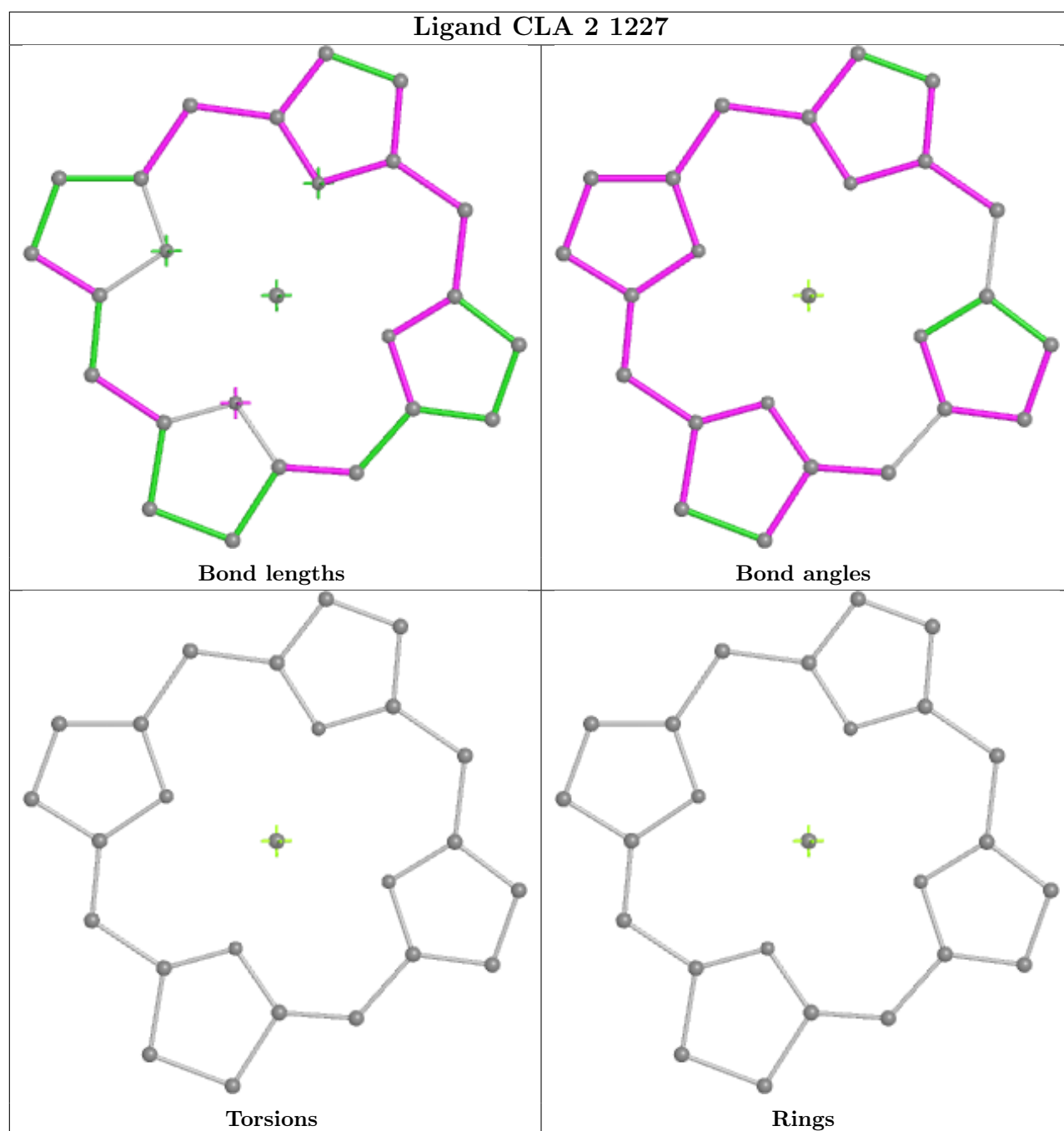
Ligand CLA B 1771

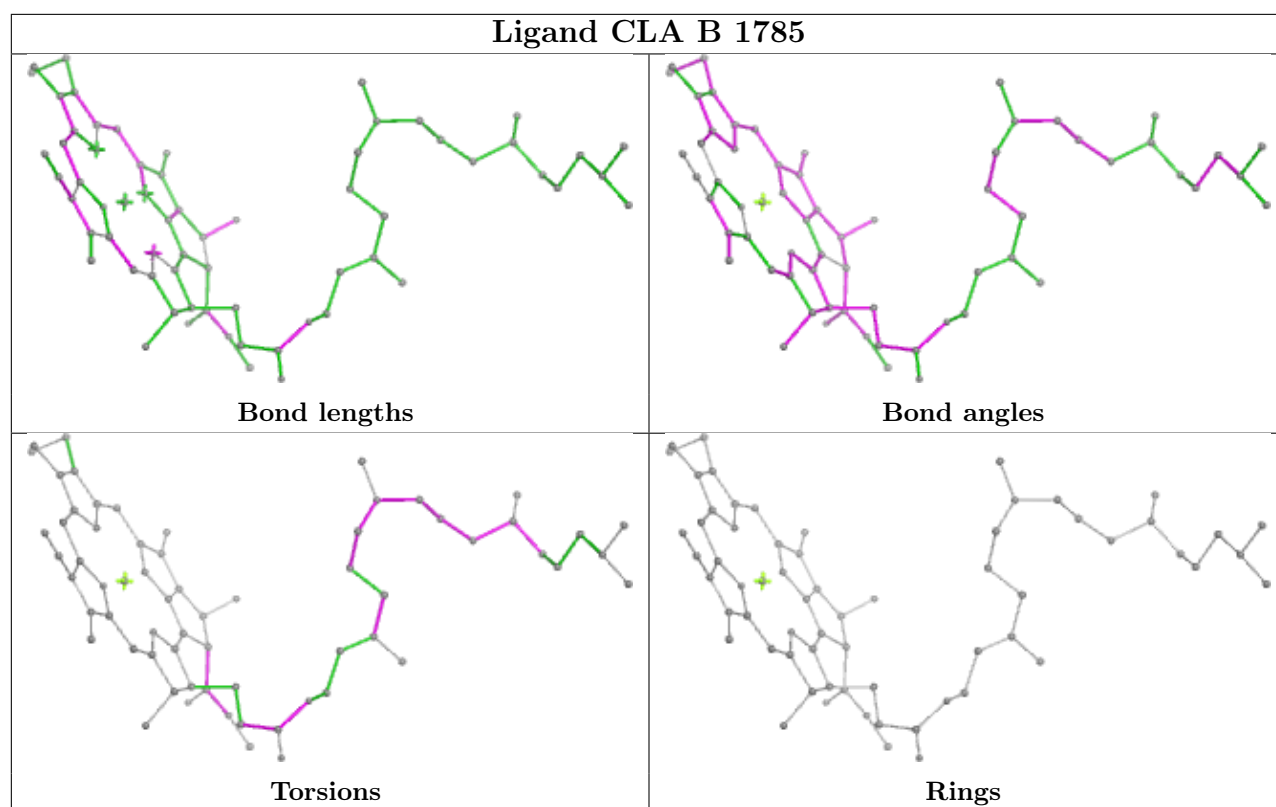


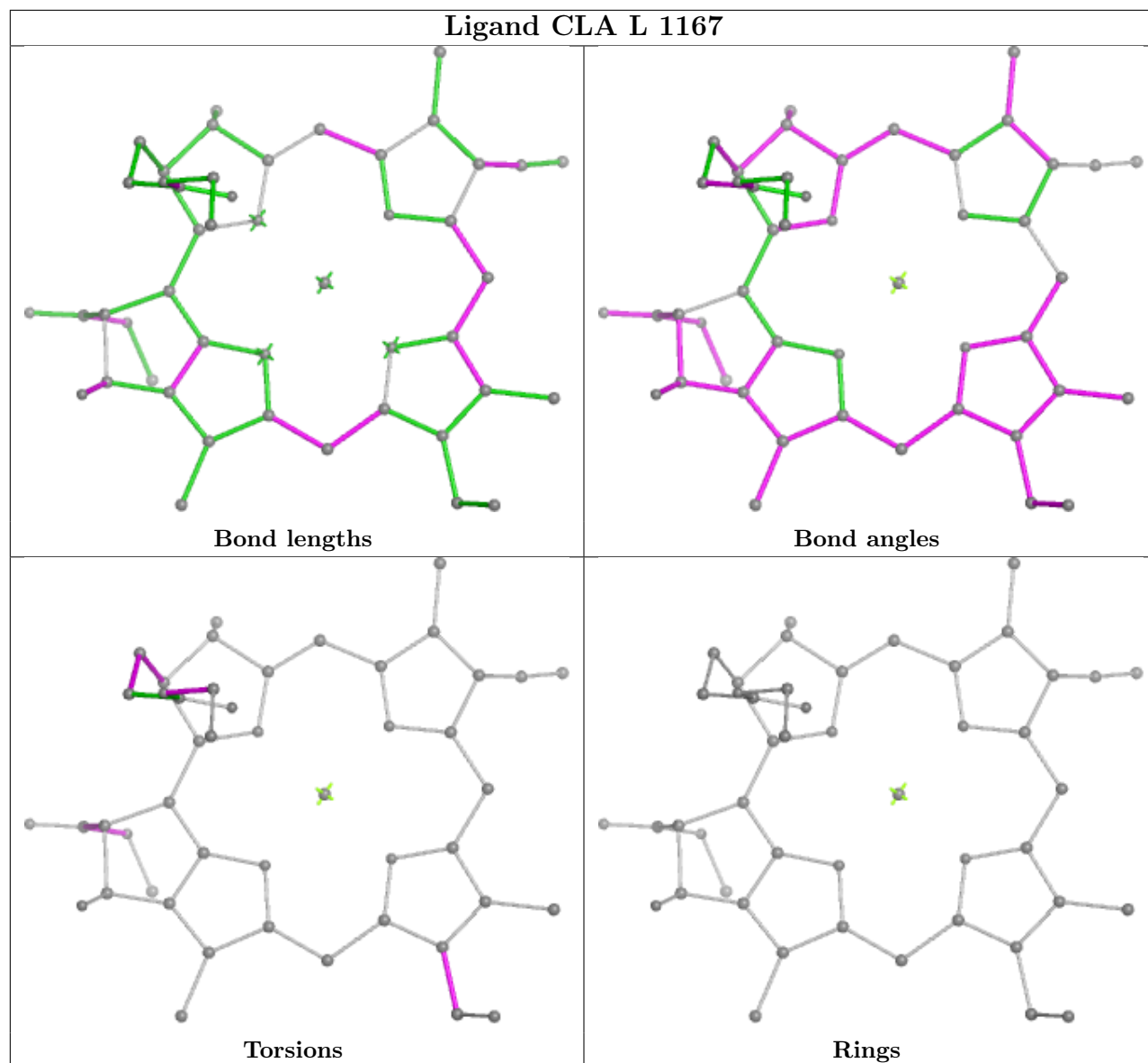
Ligand LMU A 7017



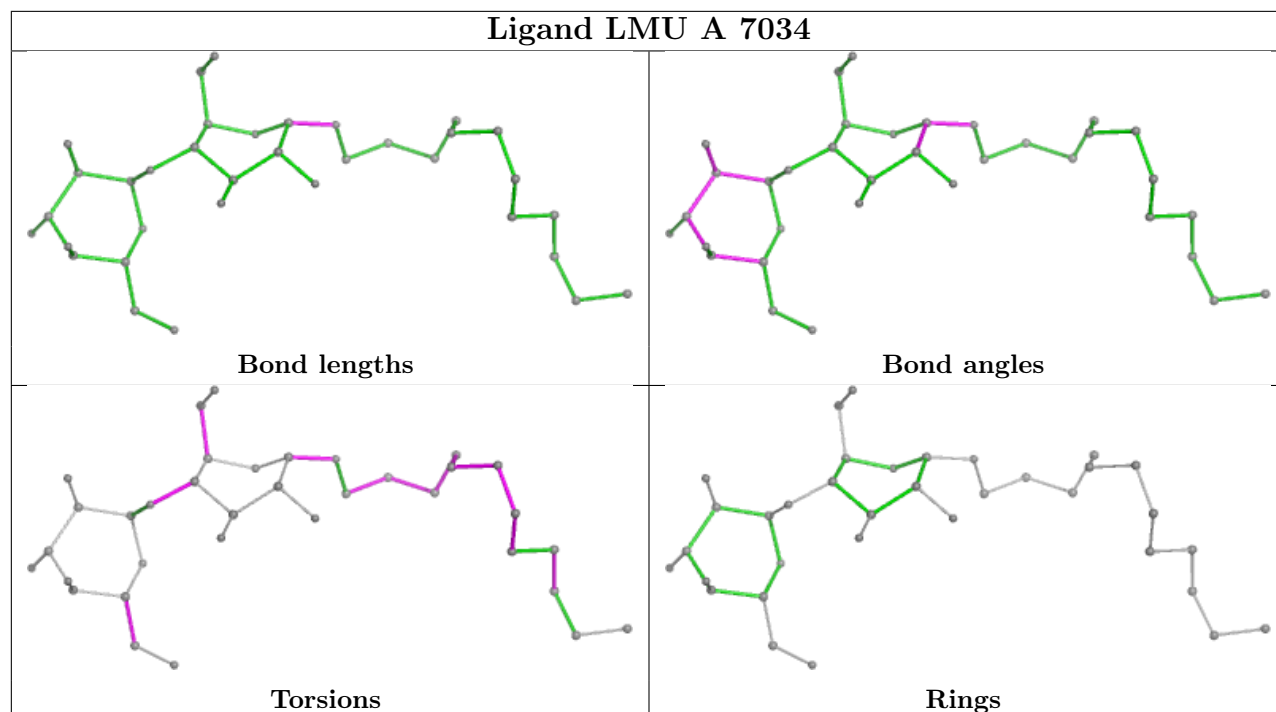




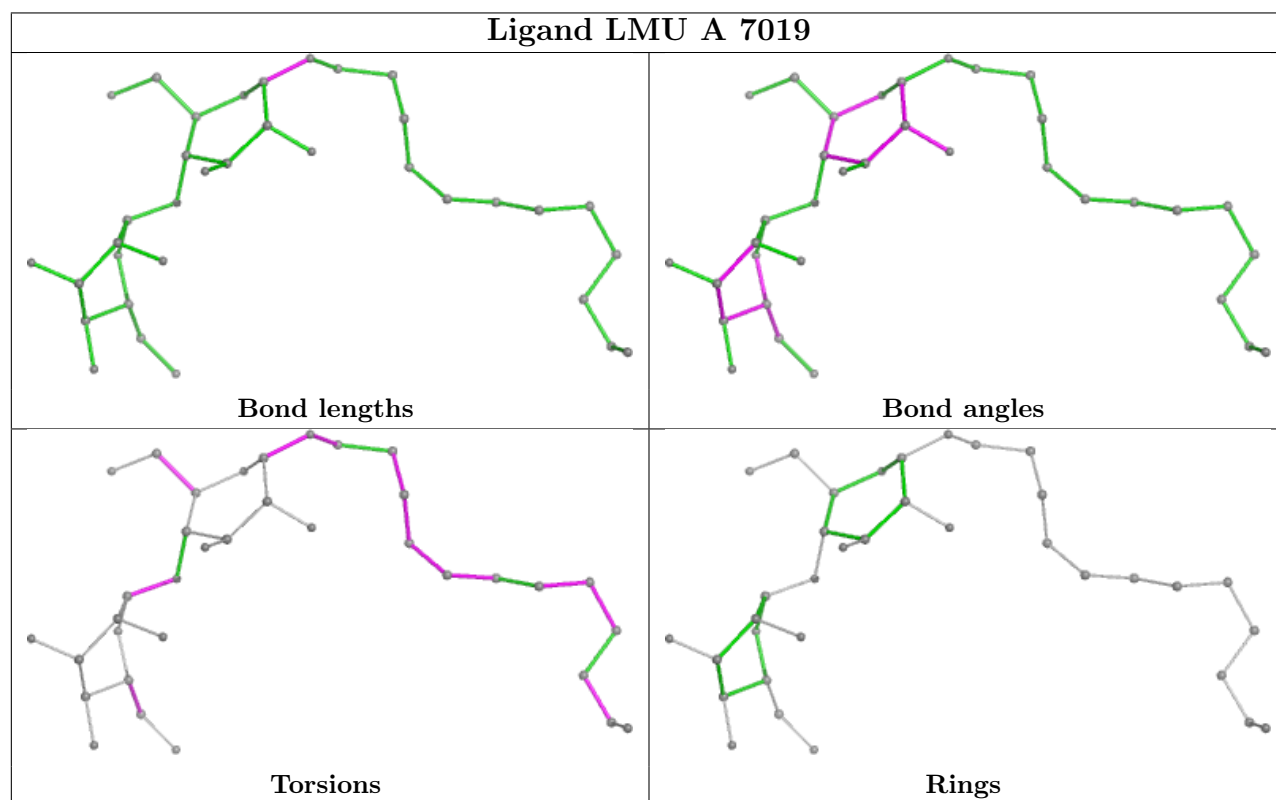




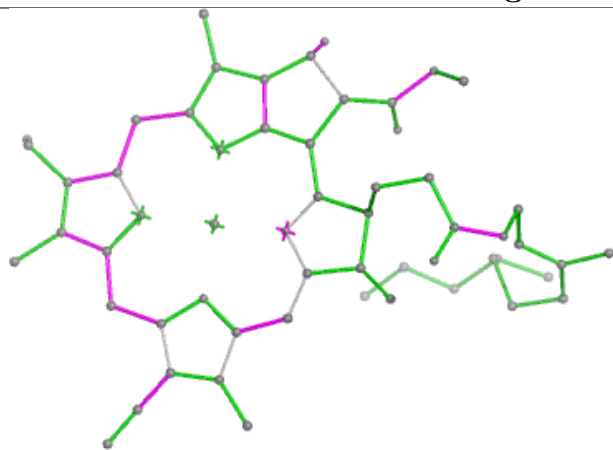
Ligand LMU A 7034



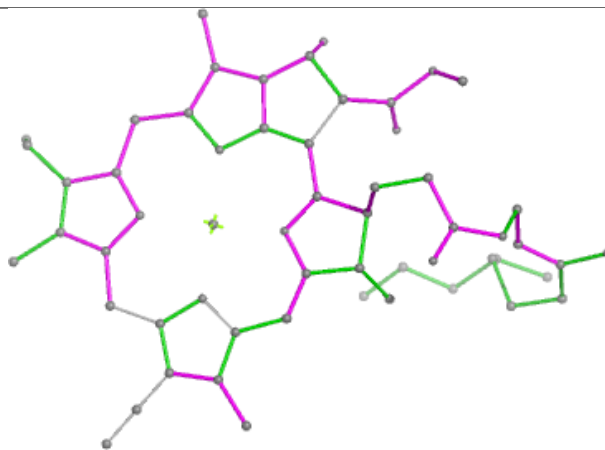
Ligand LMU A 7019



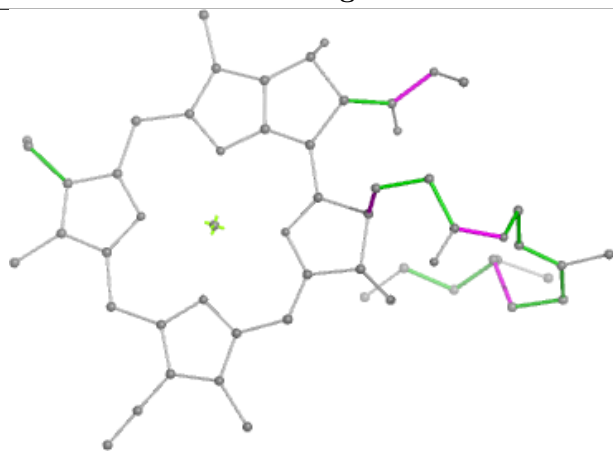
Ligand CLA A 1762



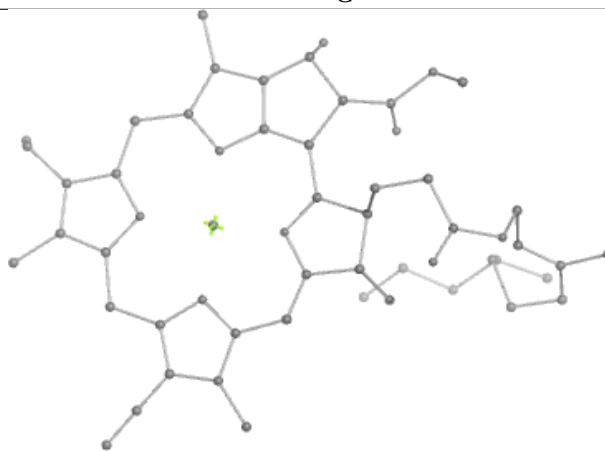
Bond lengths



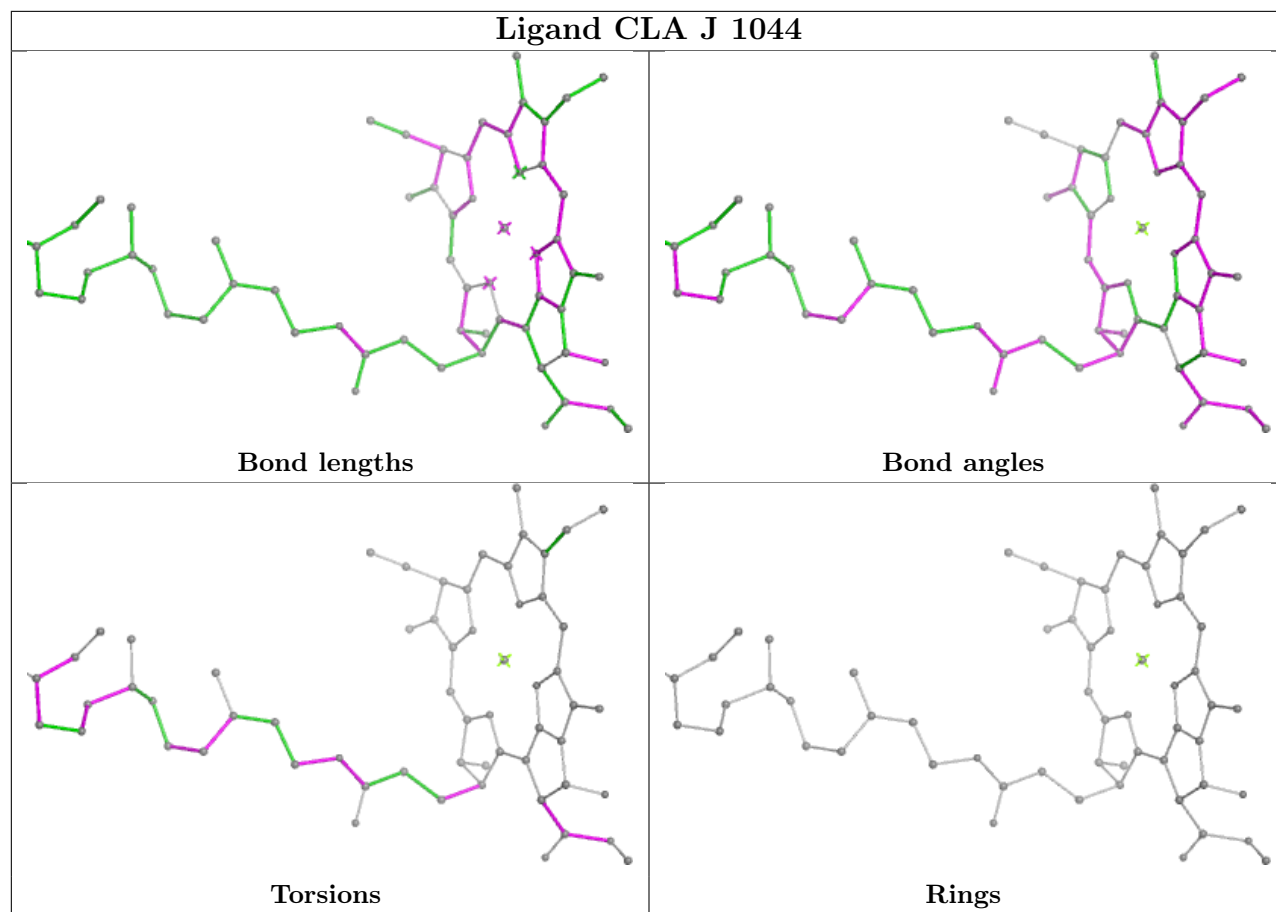
Bond angles

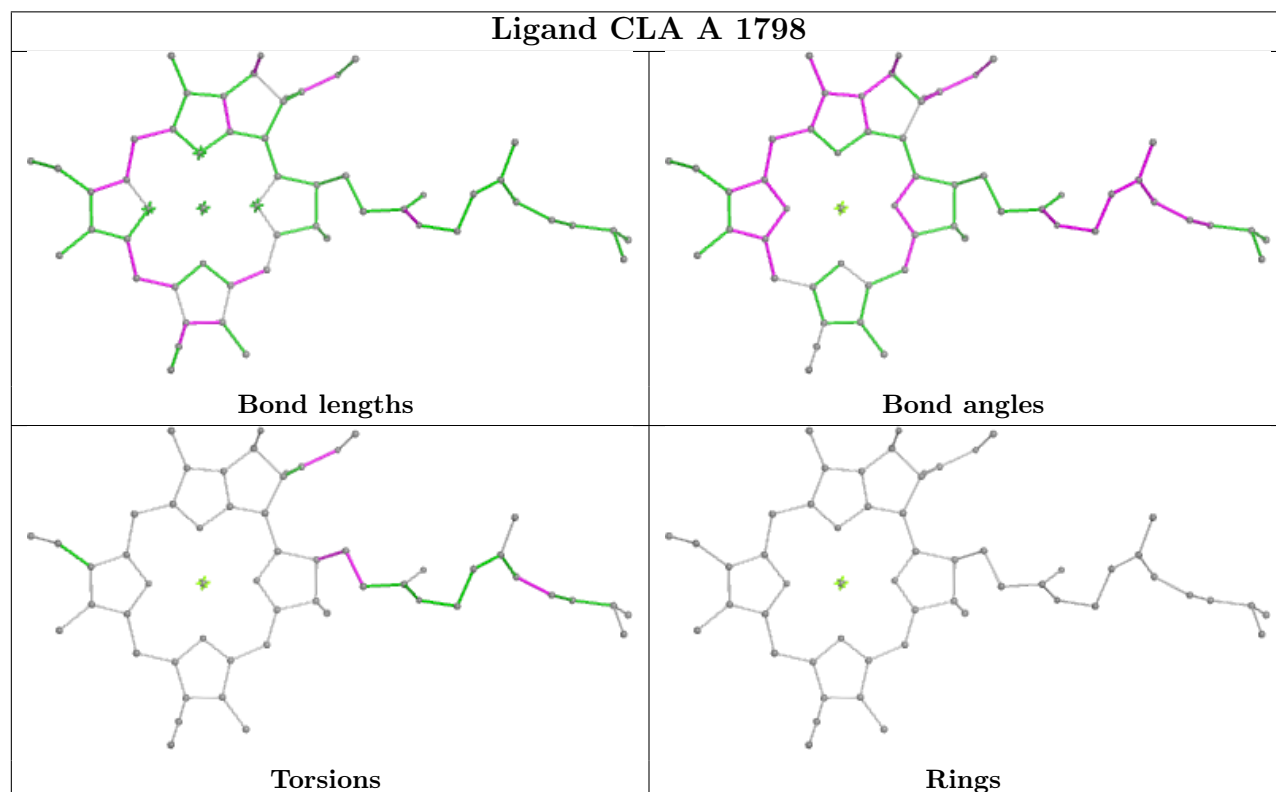
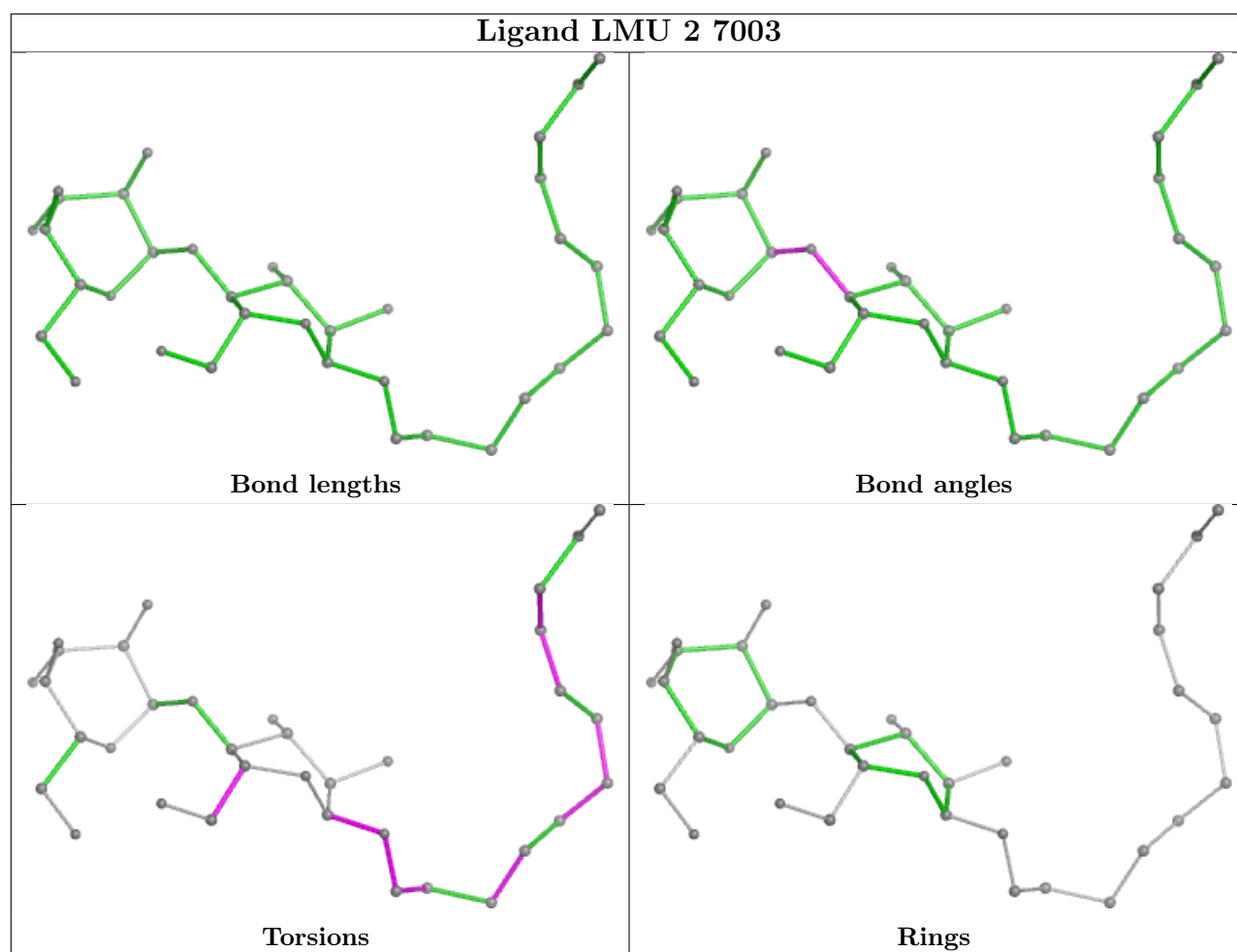


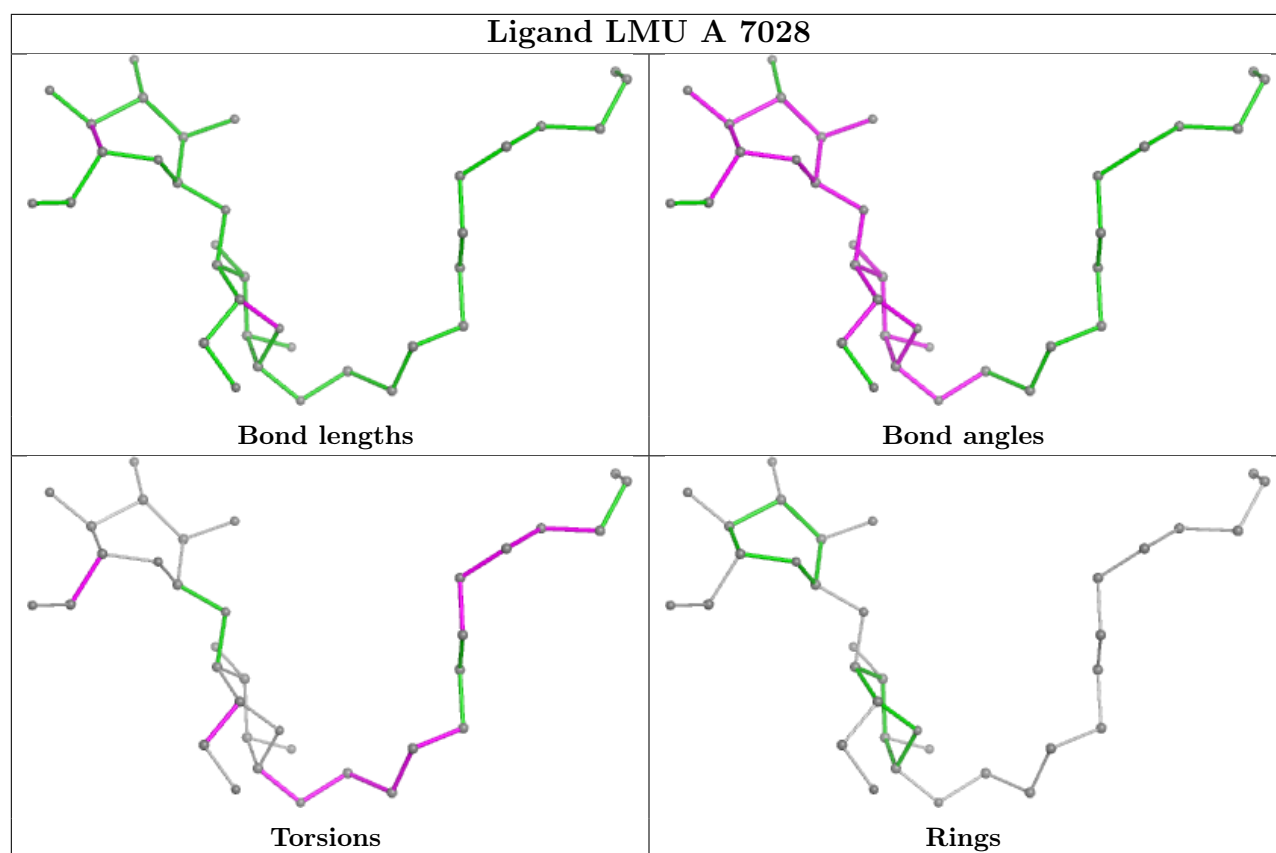
Torsions

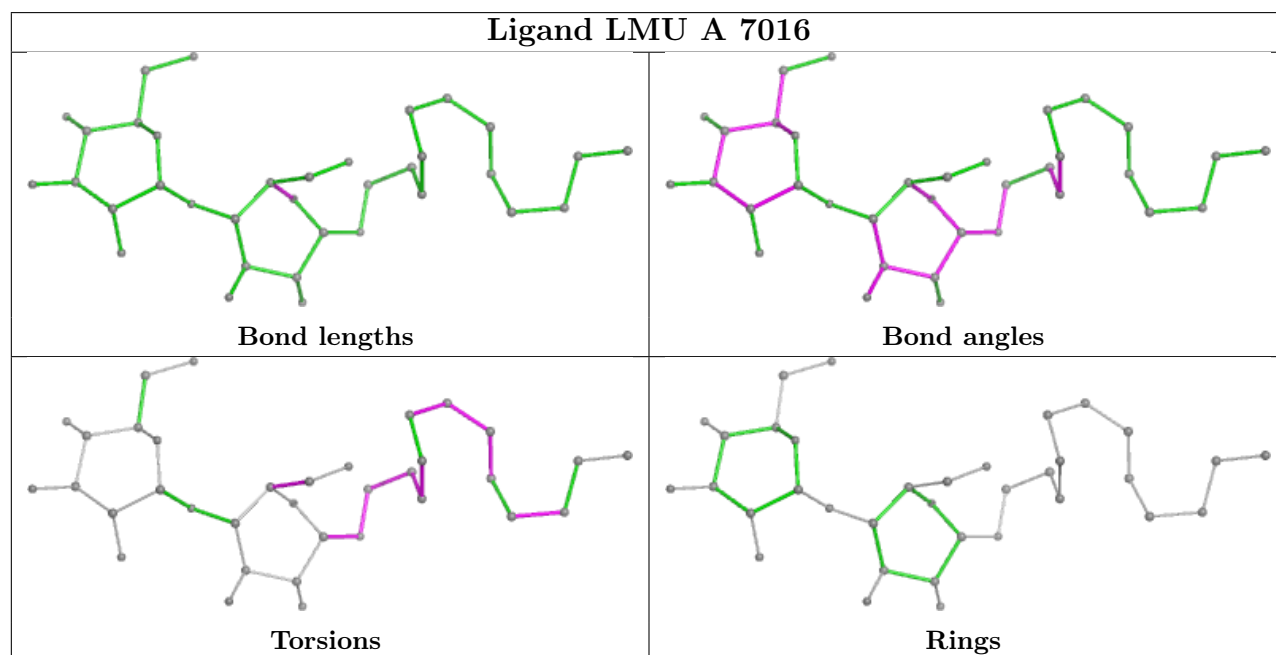
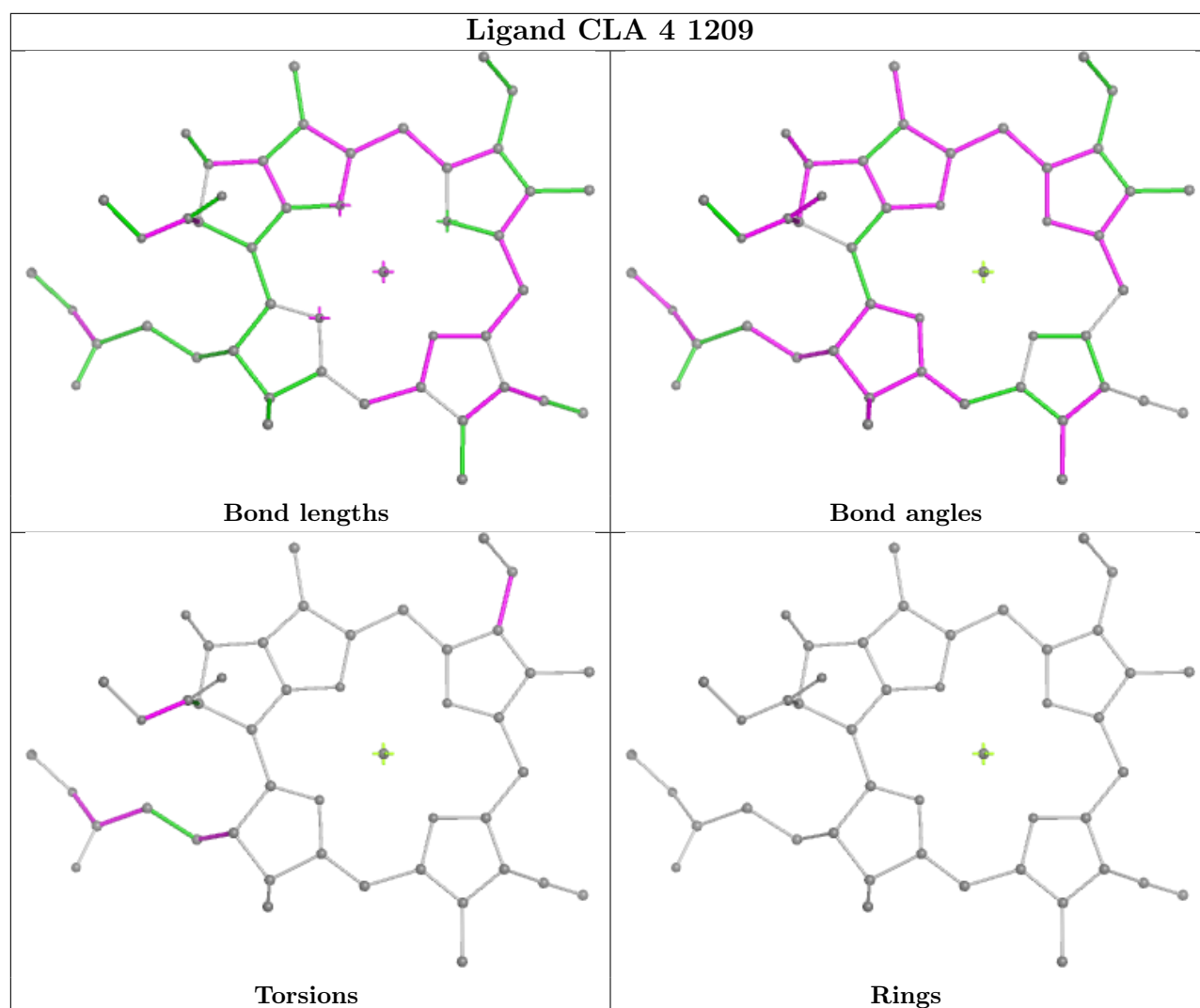


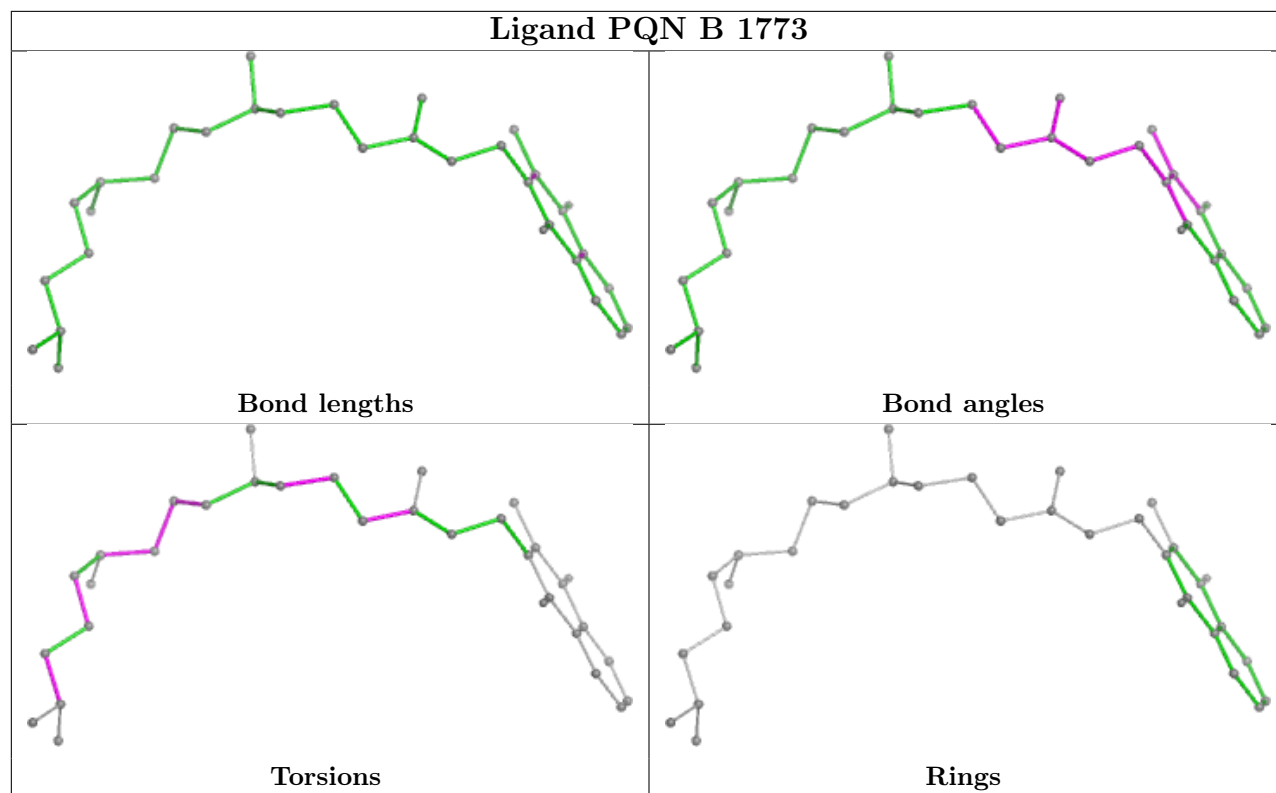
Rings

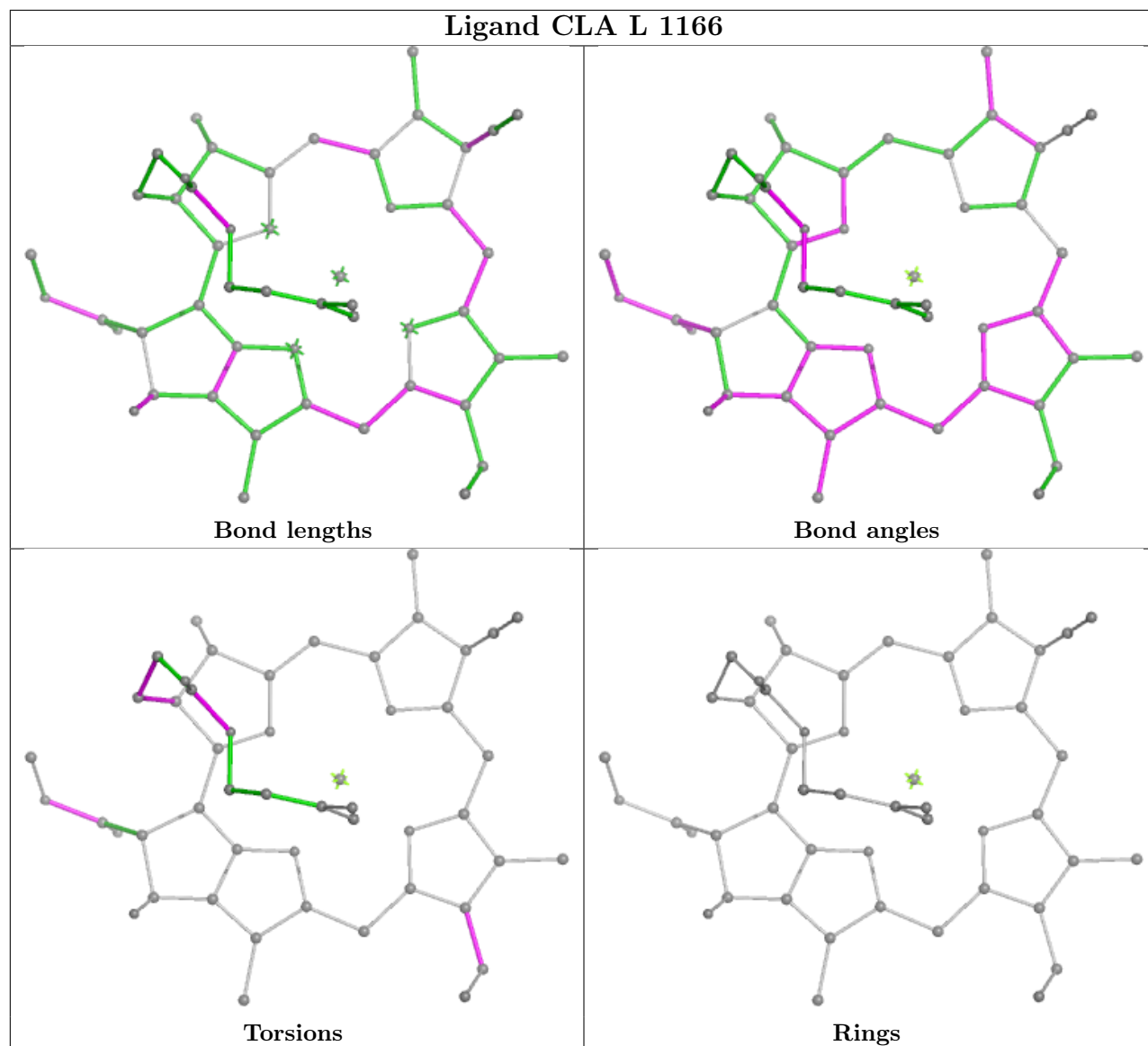


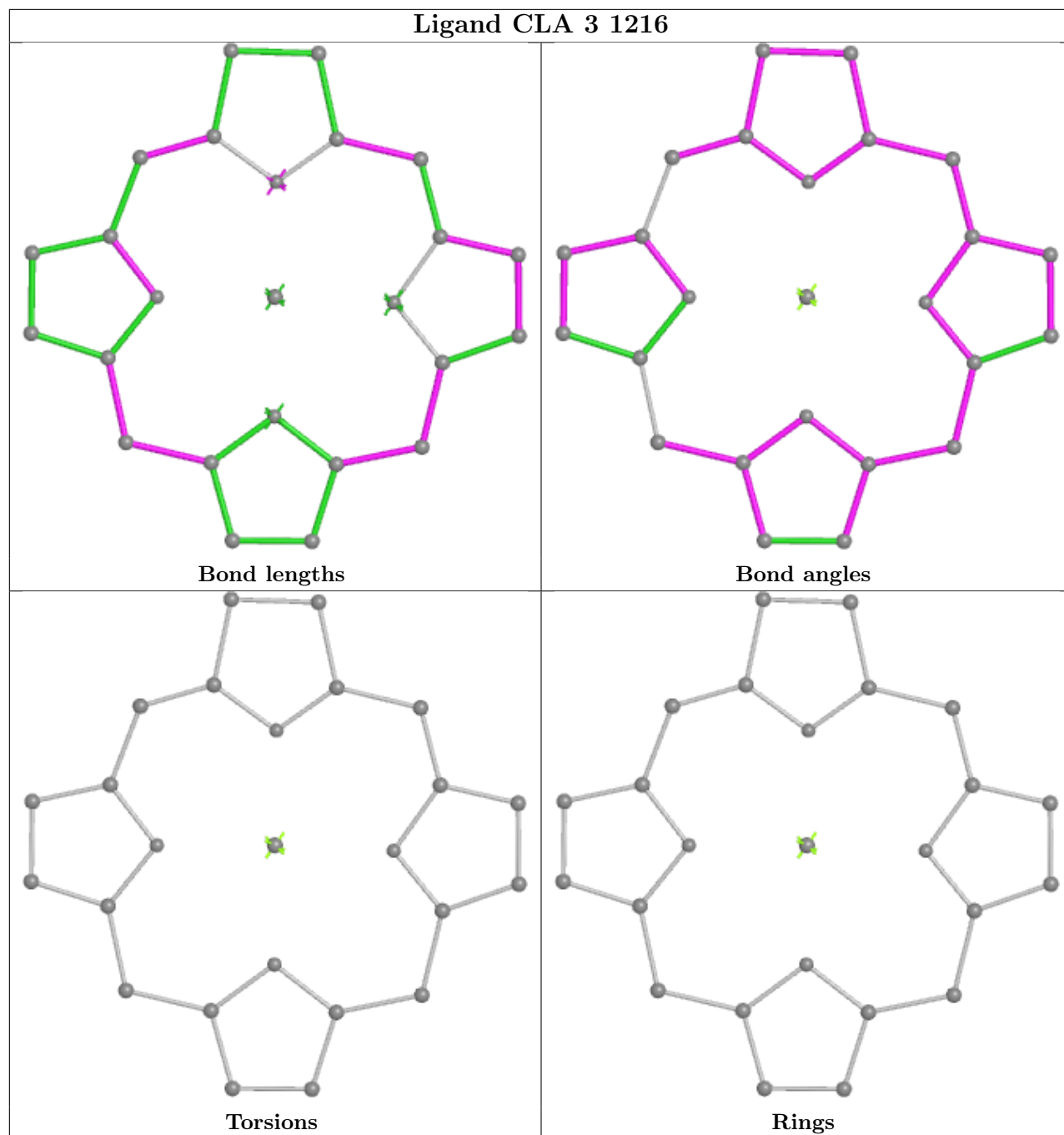


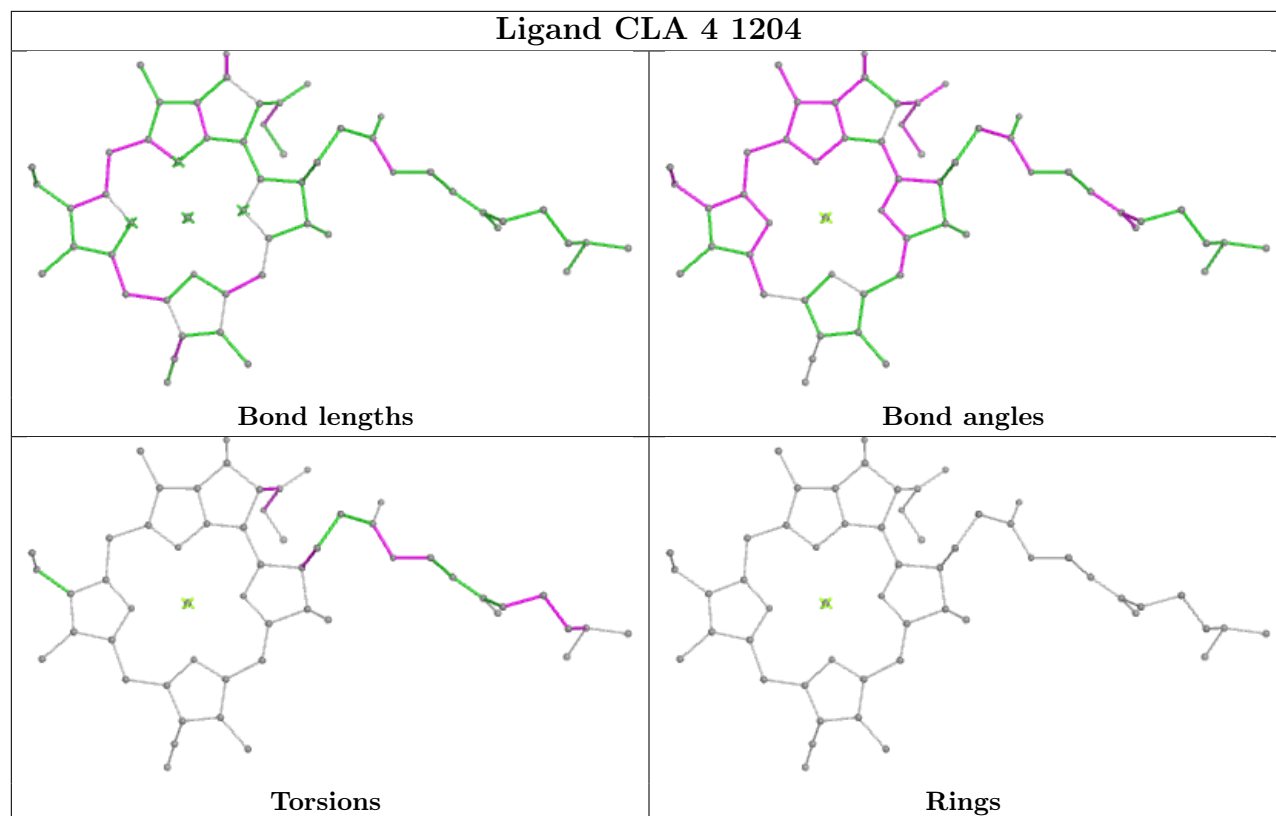




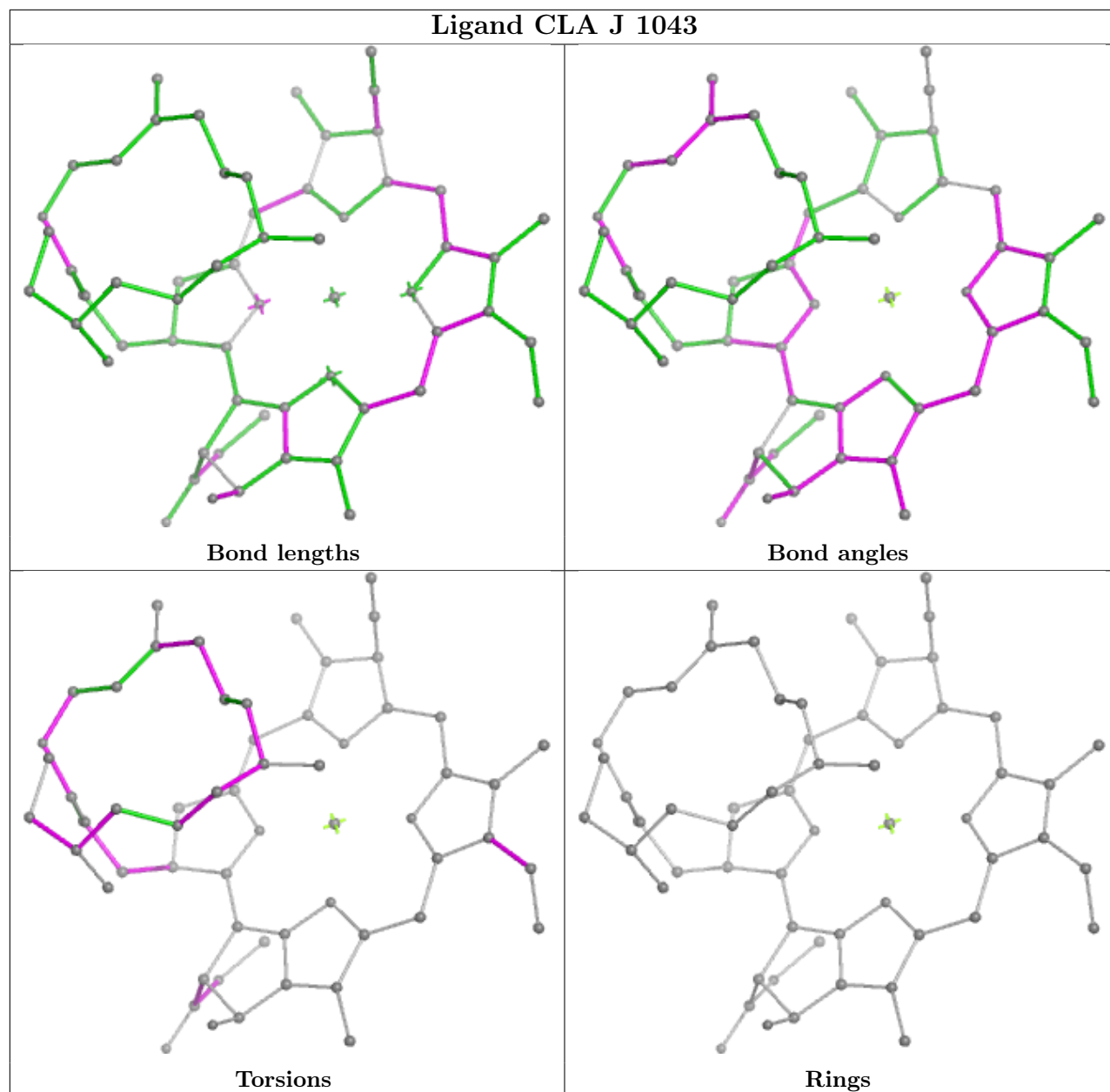




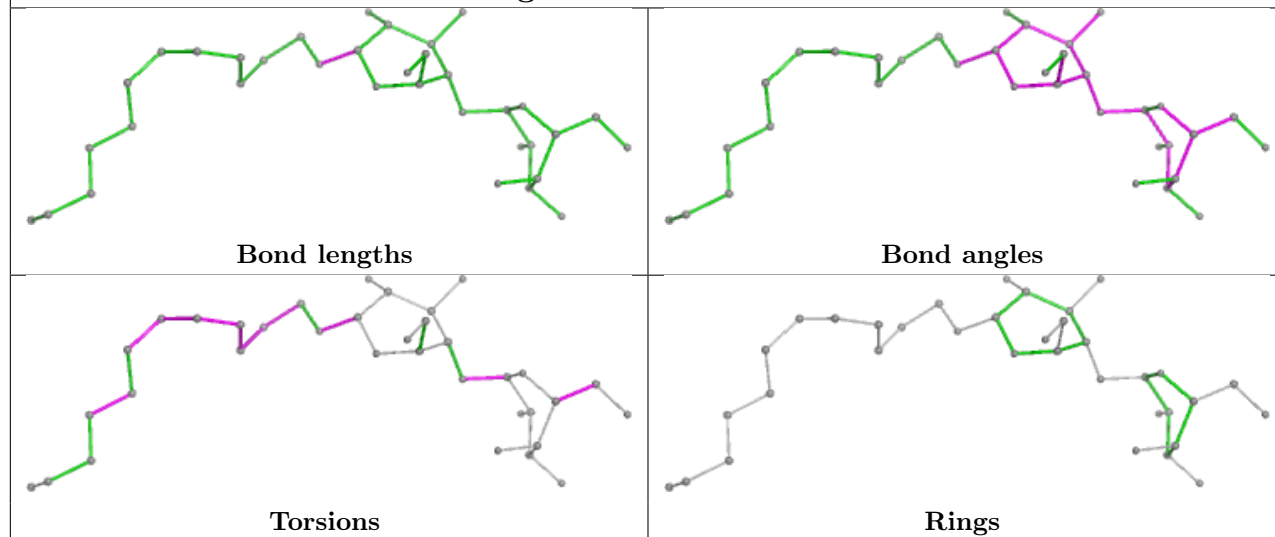




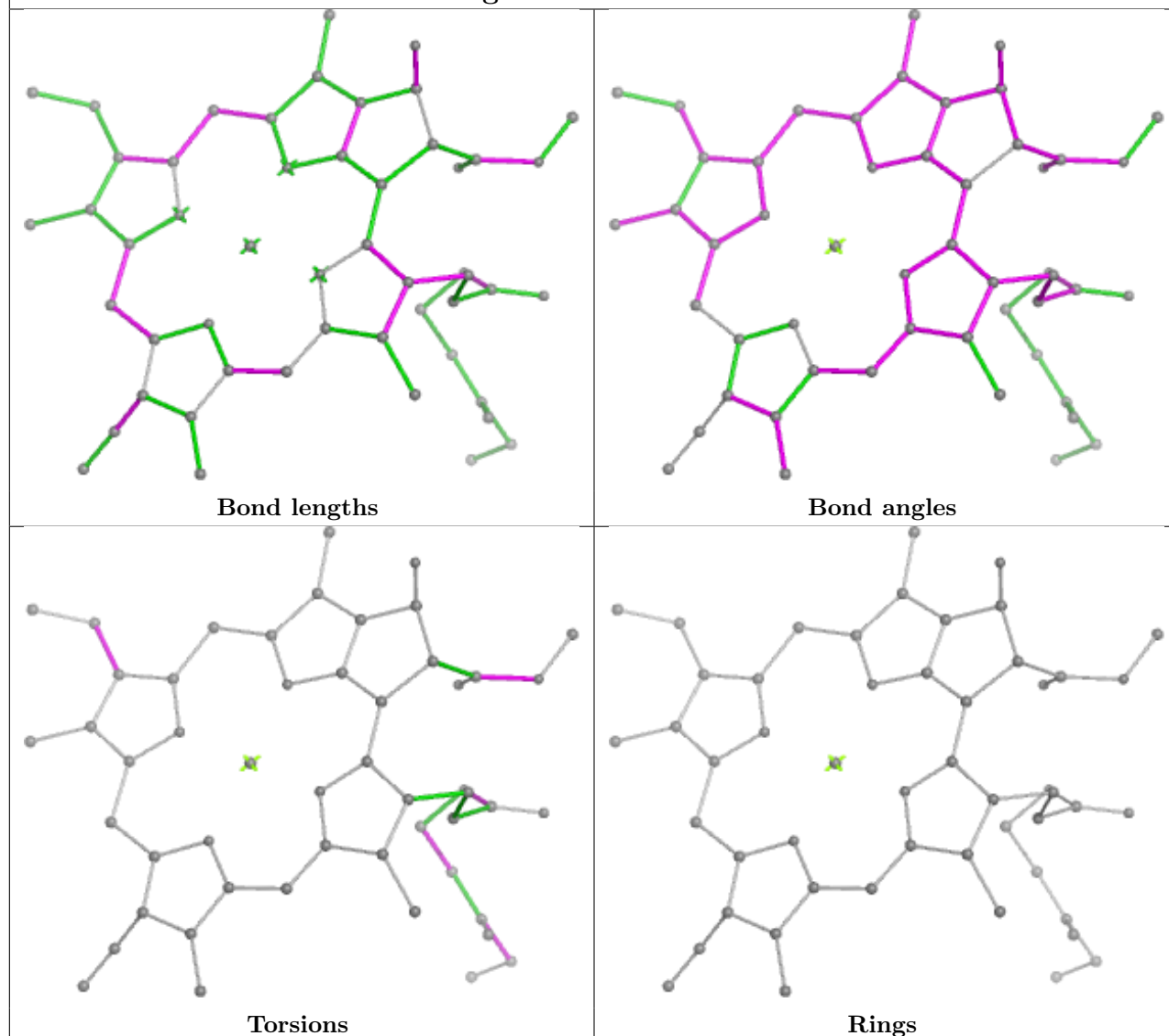
Ligand CLA J 1043

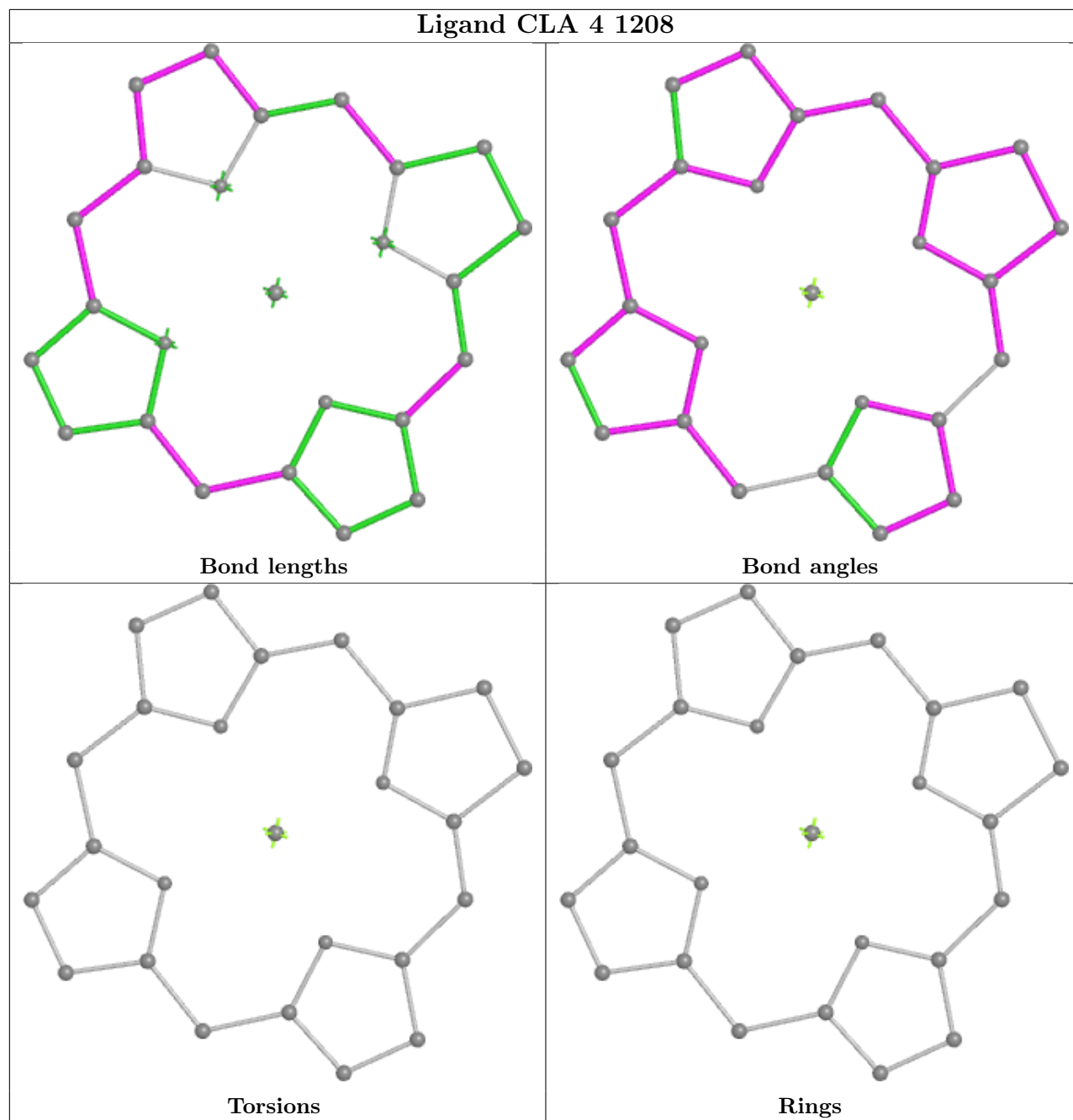


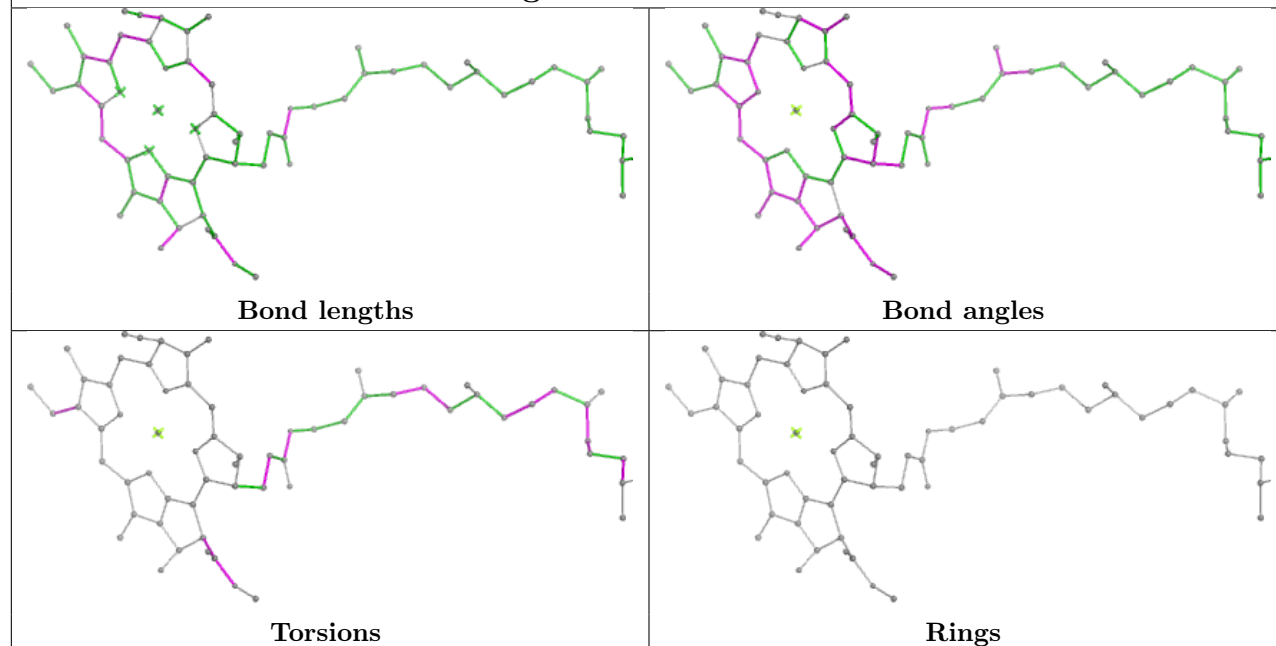
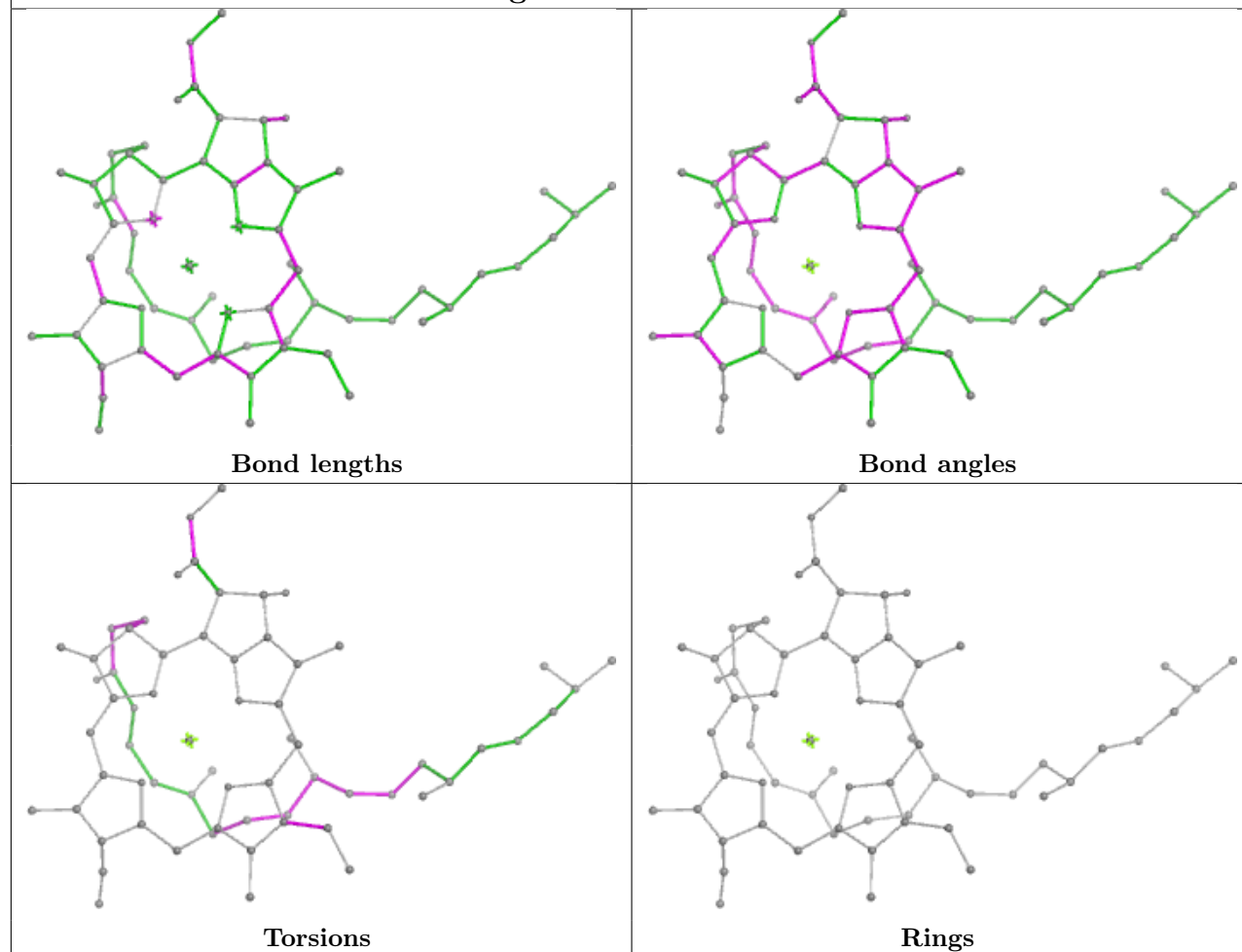
Ligand LMU A 7027

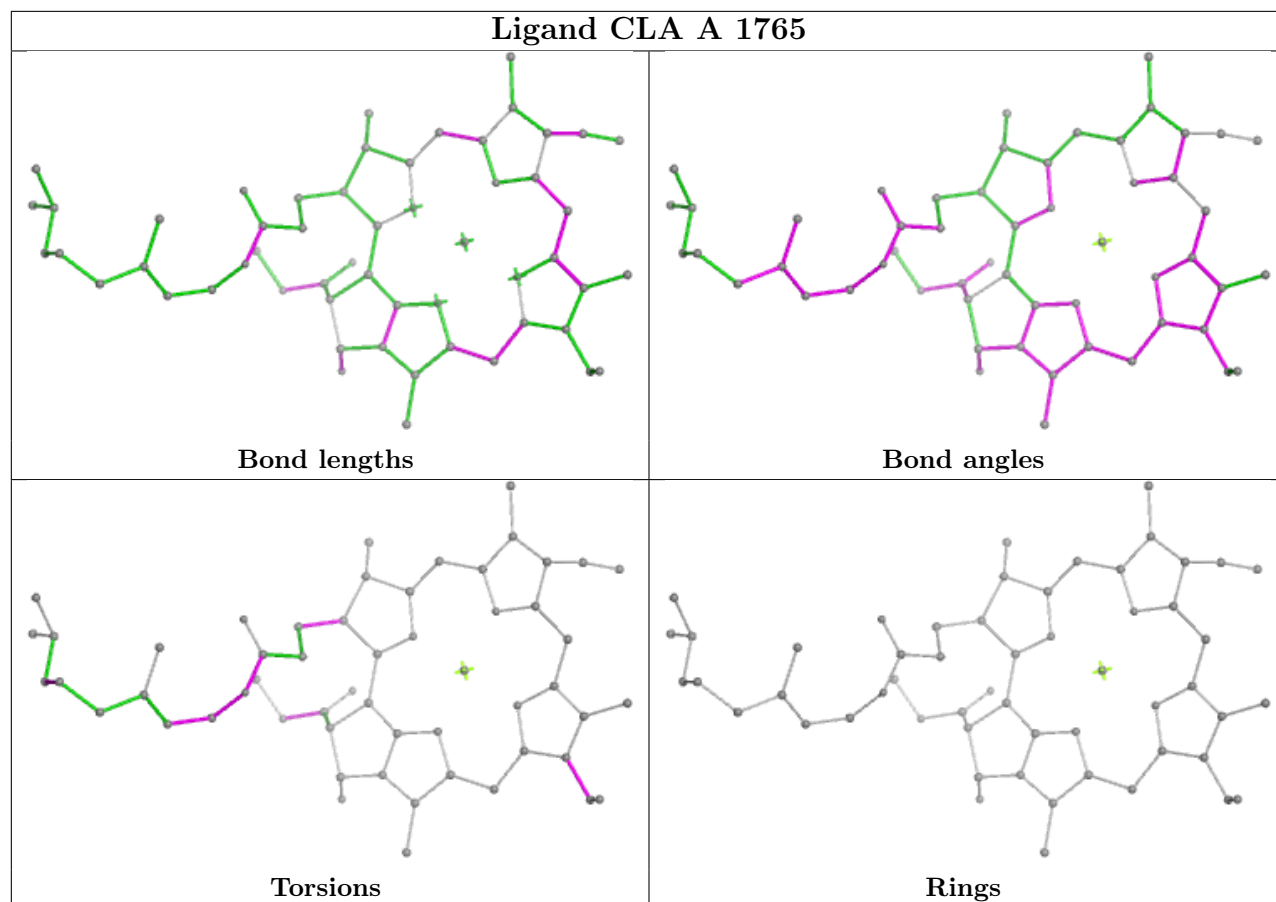


Ligand CLA 1 1193

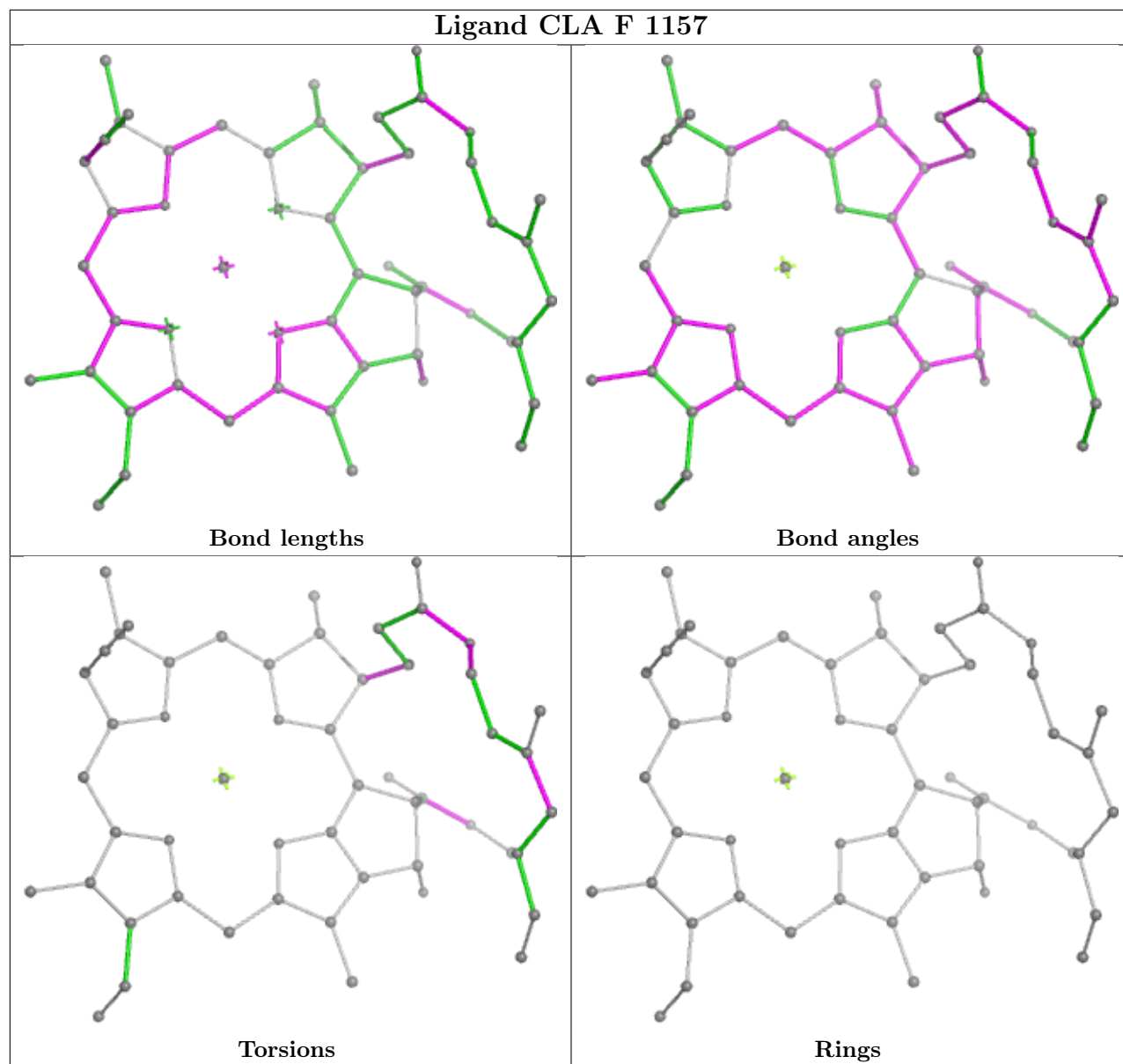


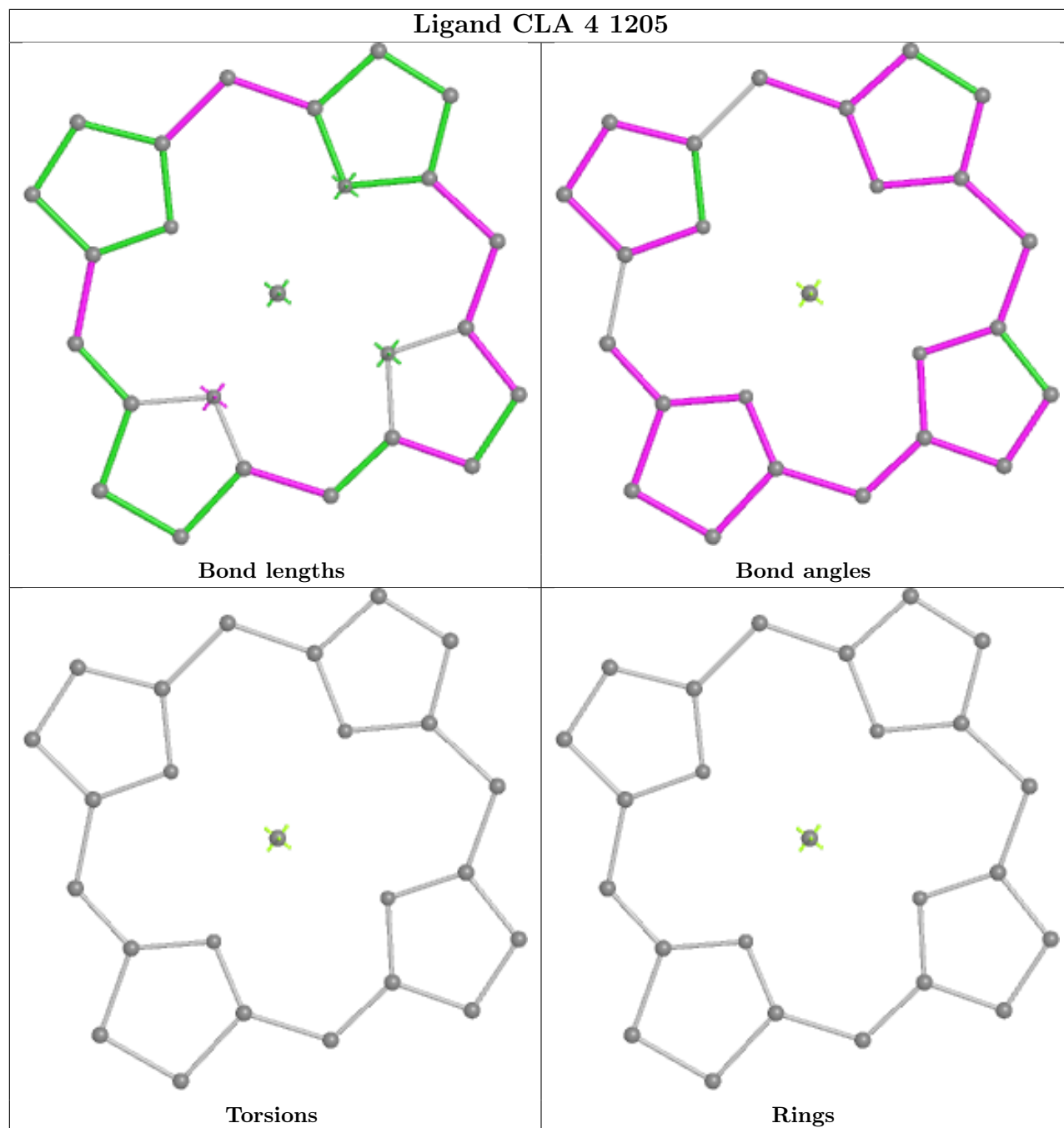


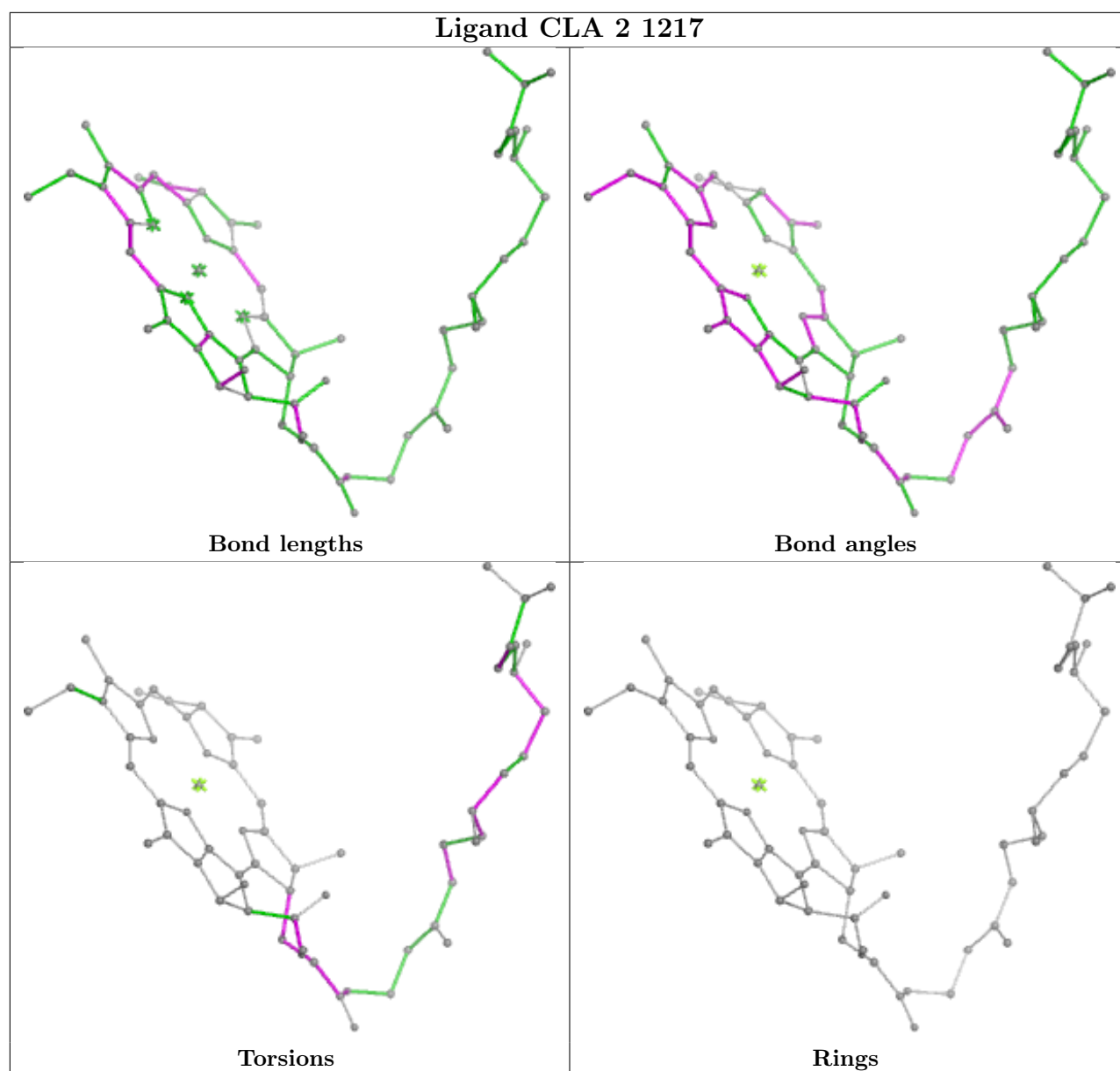
Ligand CLA A 1776**Ligand CLA B 1757**

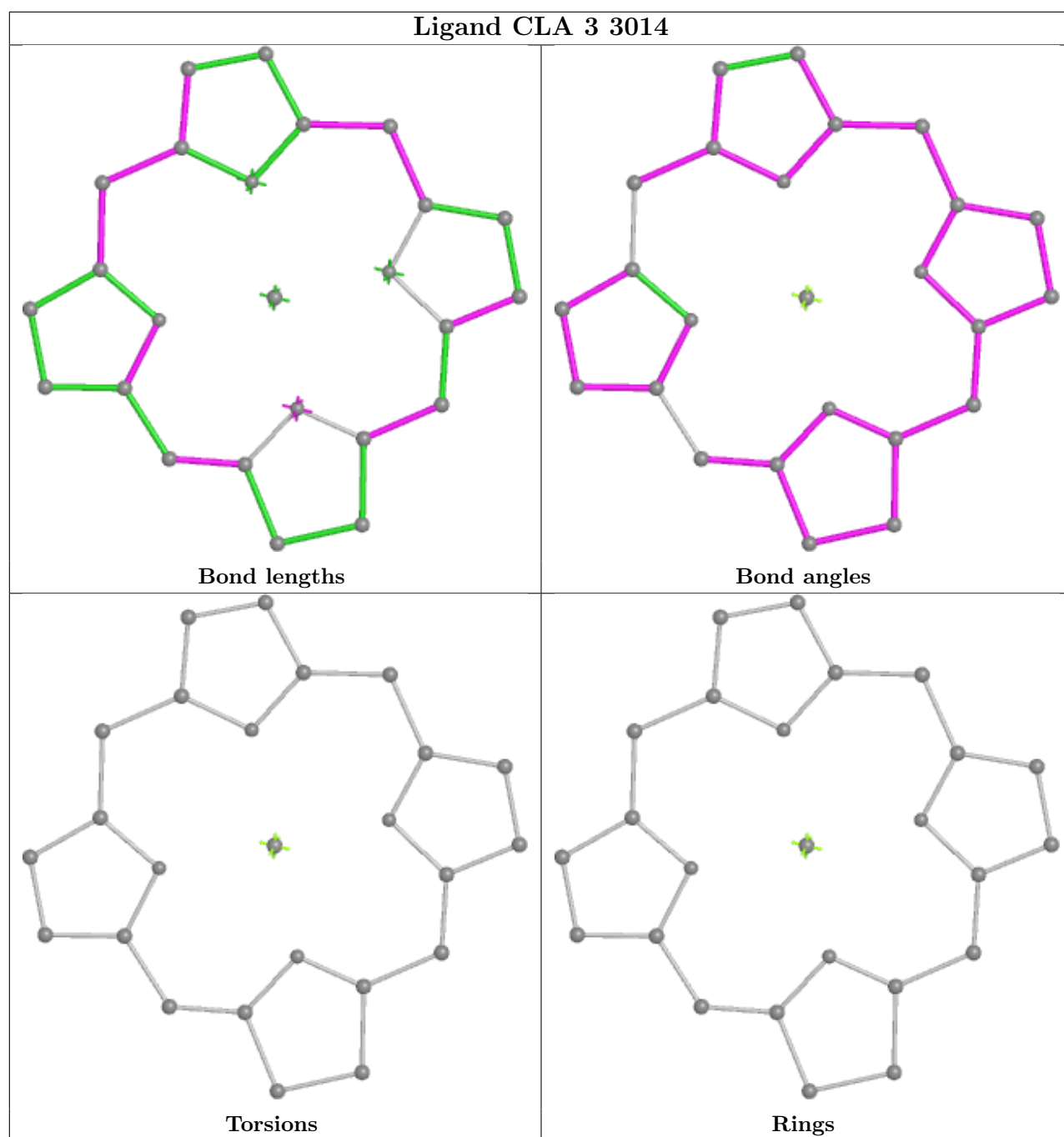


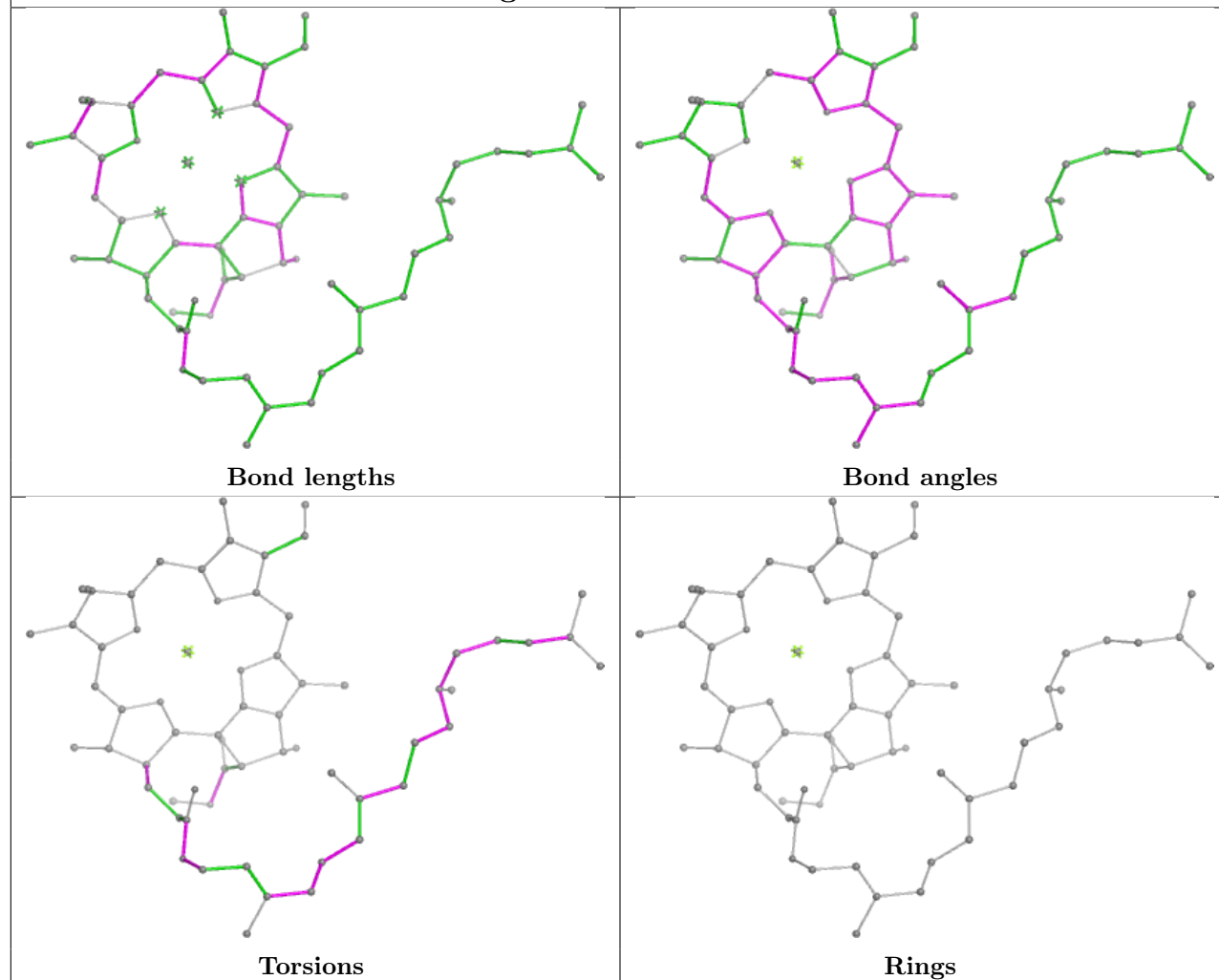
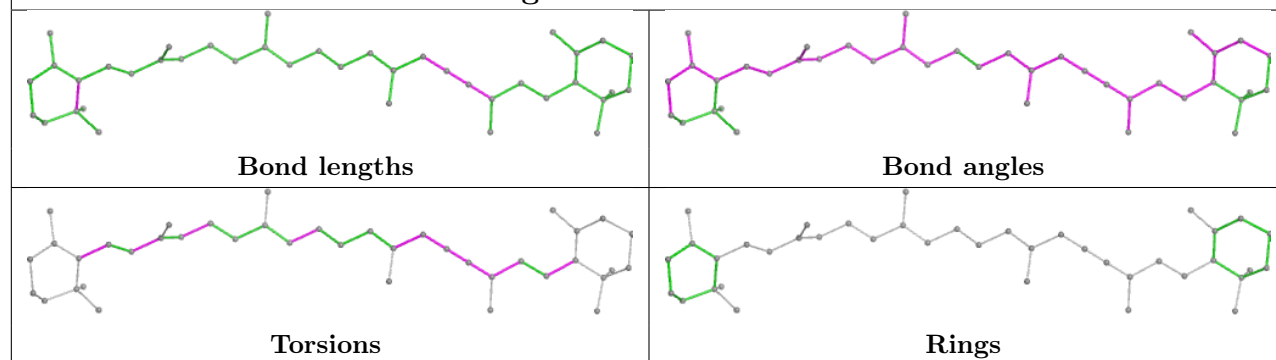
Ligand CLA F 1157

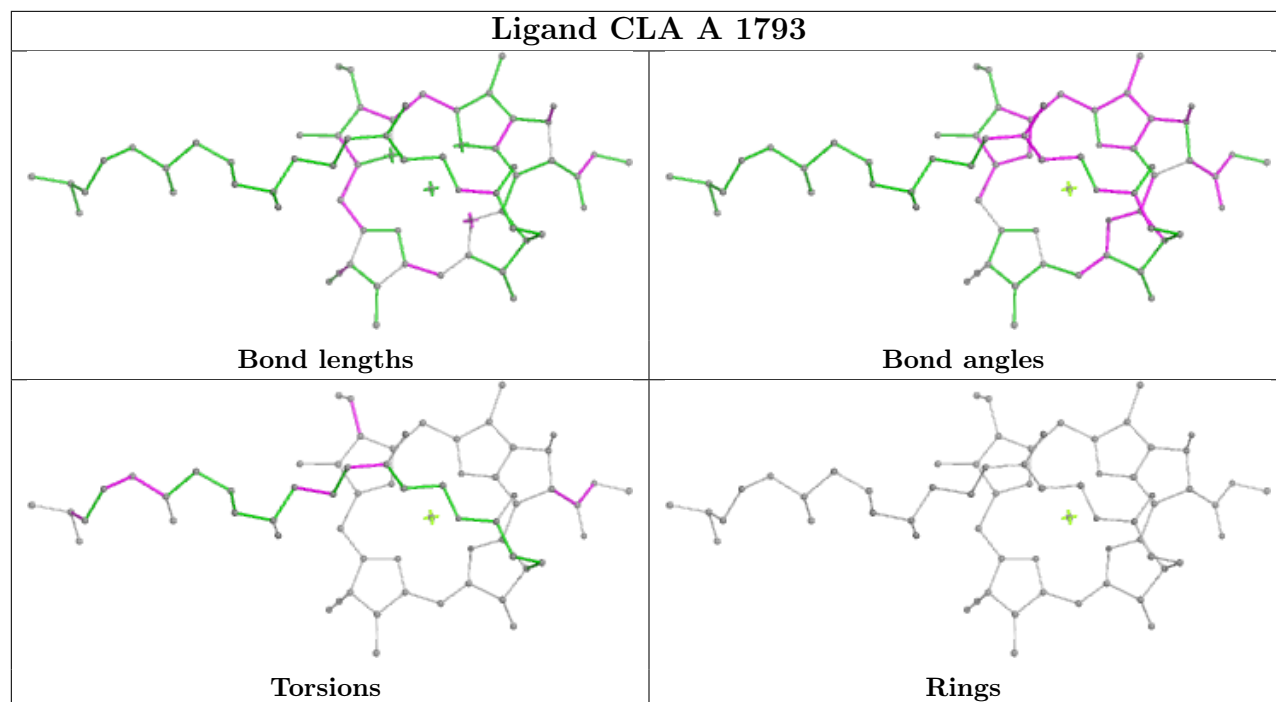


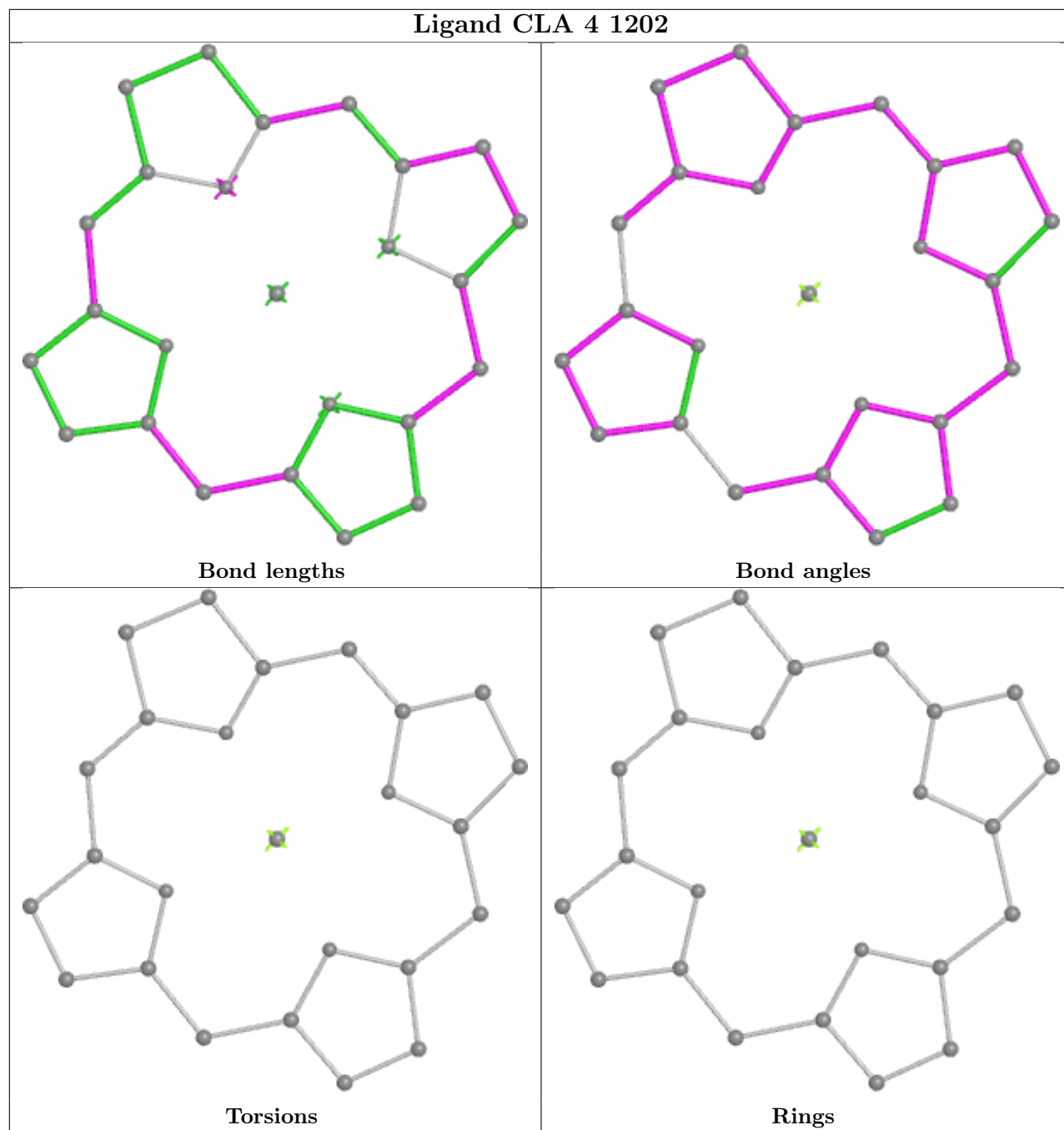


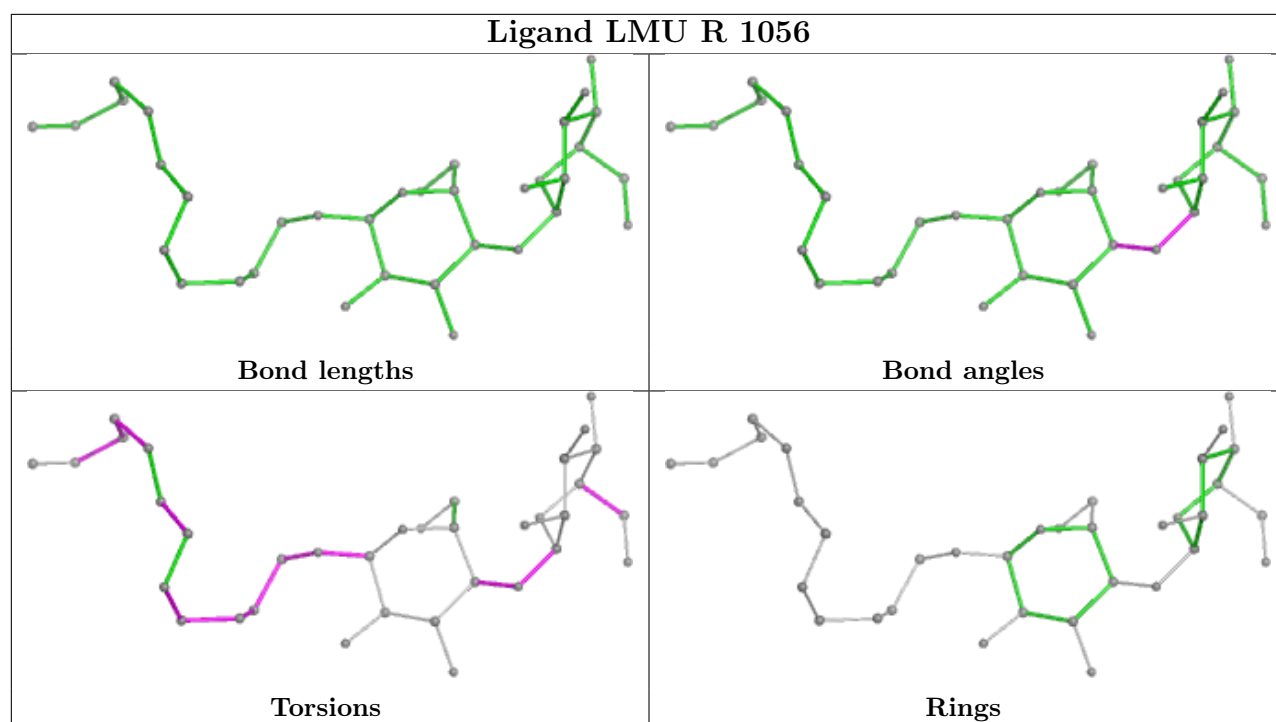




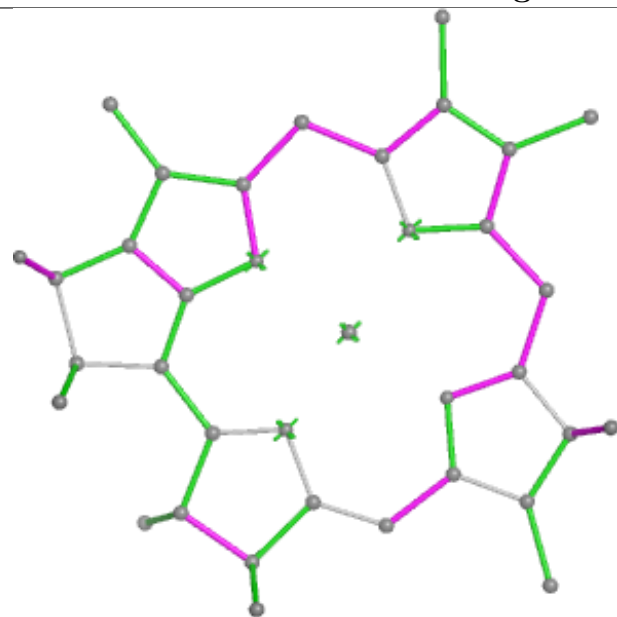
Ligand CLA B 1762**Ligand BCR B 1777**



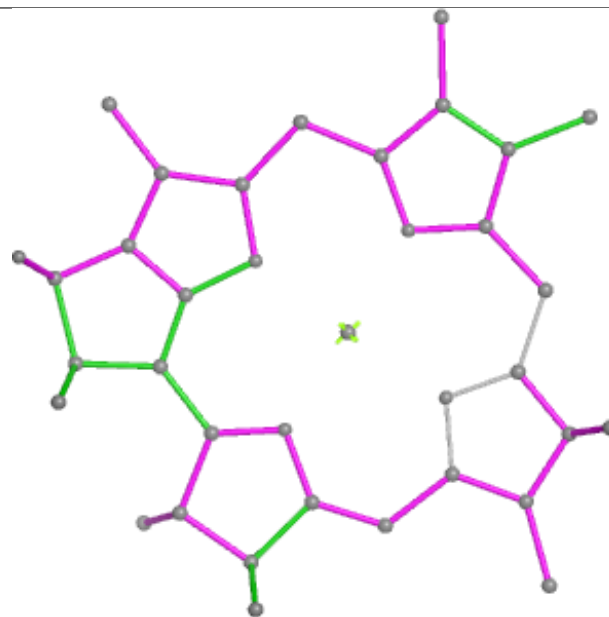




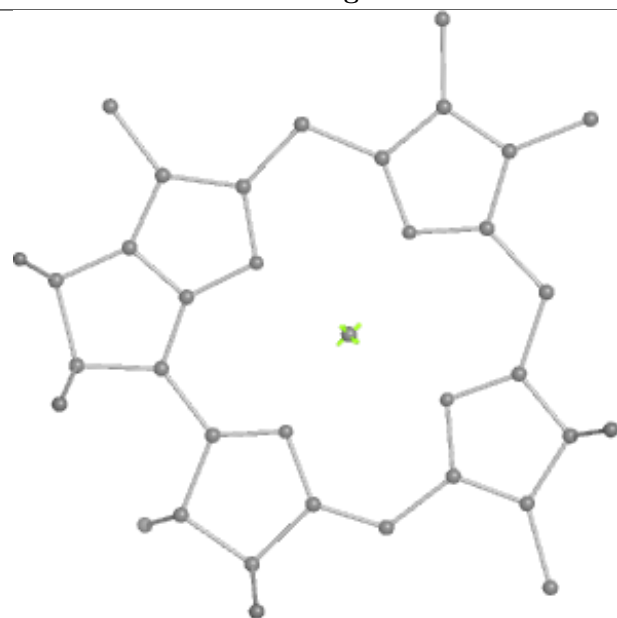
Ligand CLA 4 1197



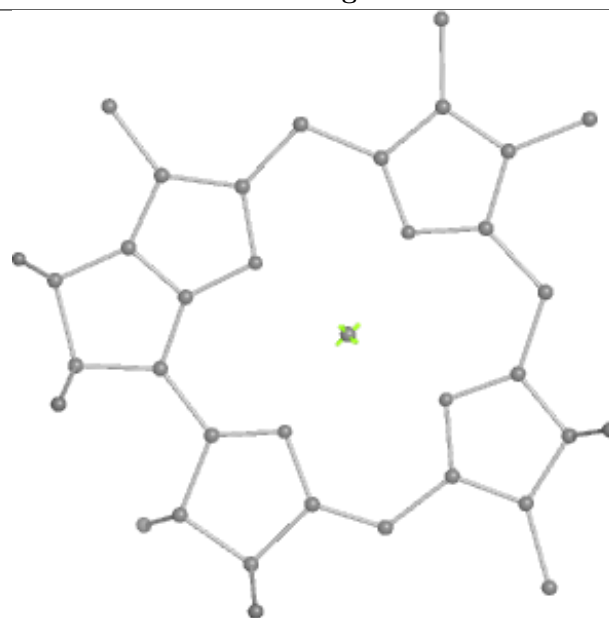
Bond lengths



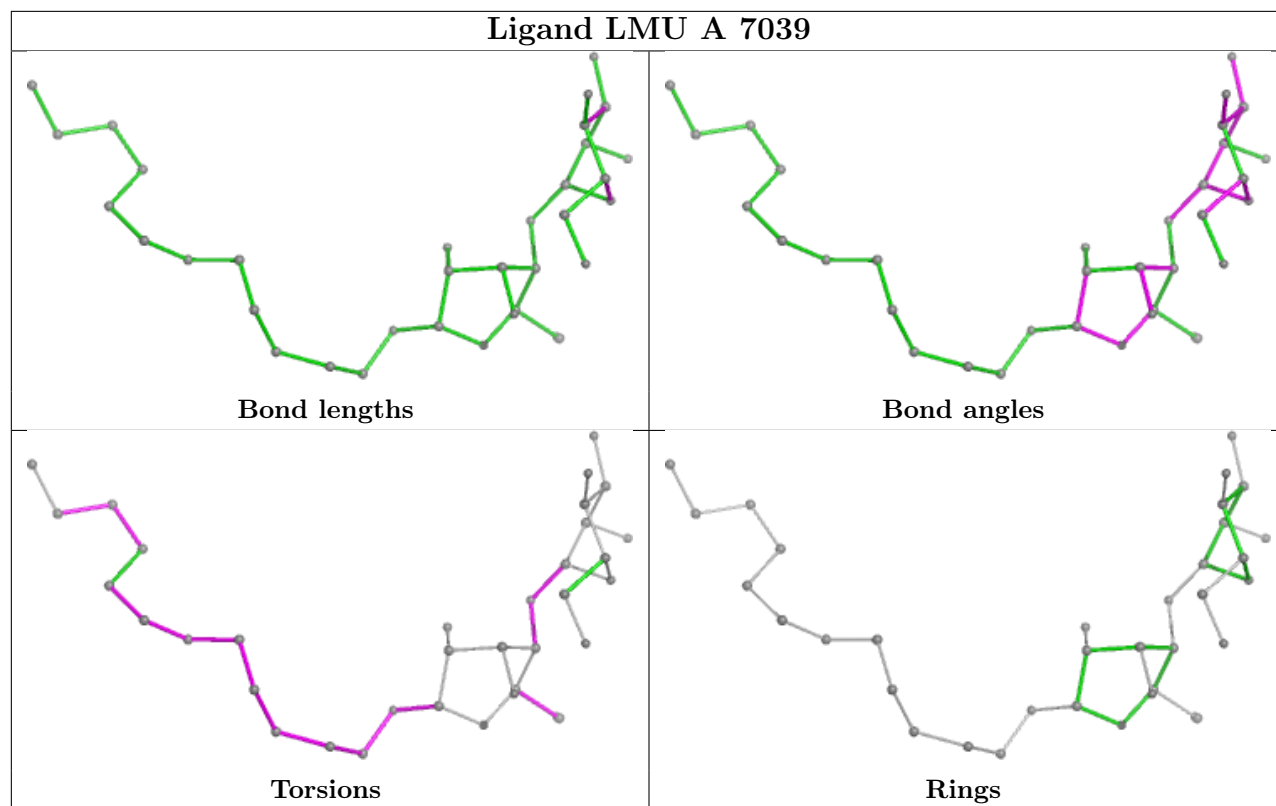
Bond angles

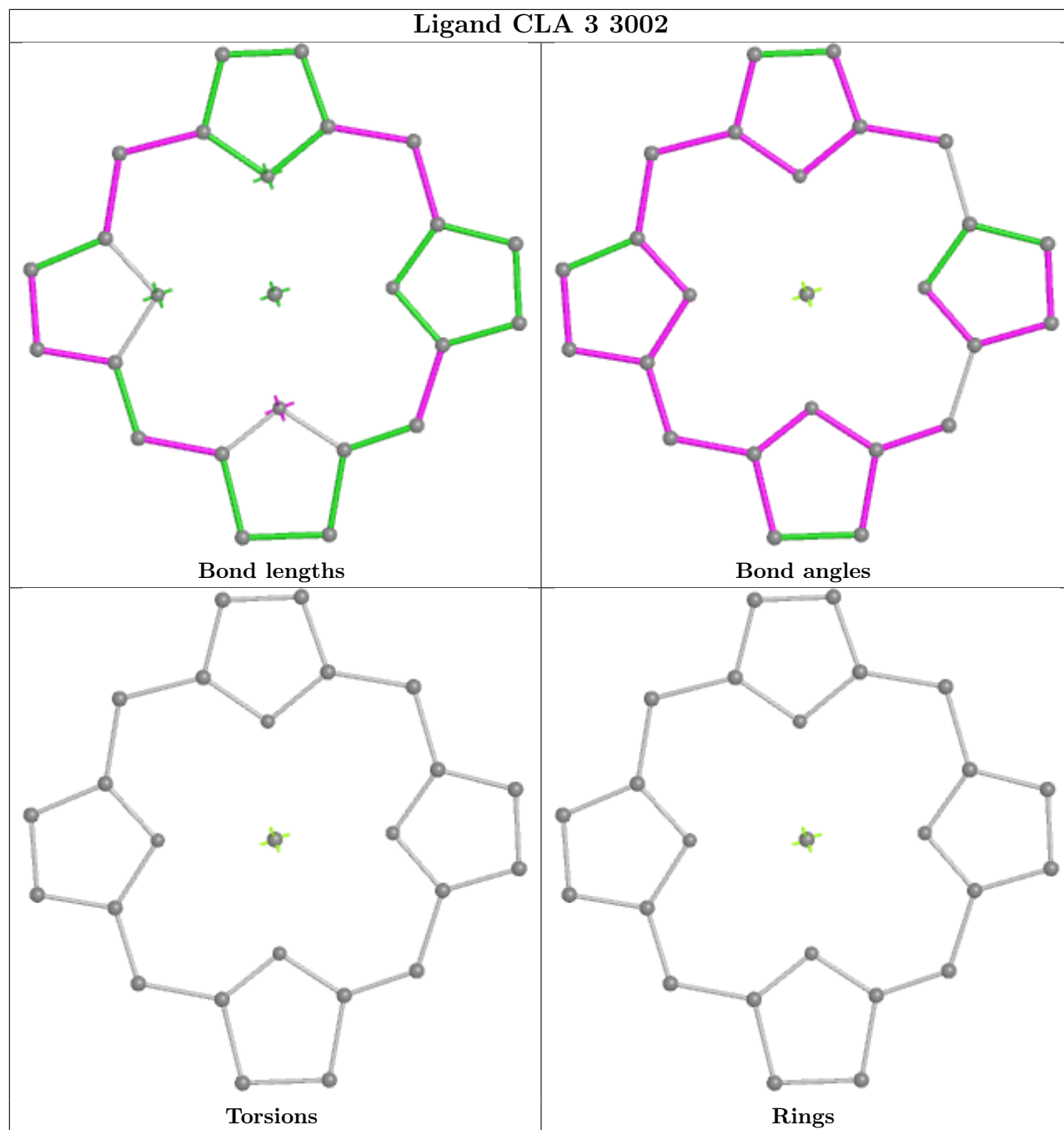


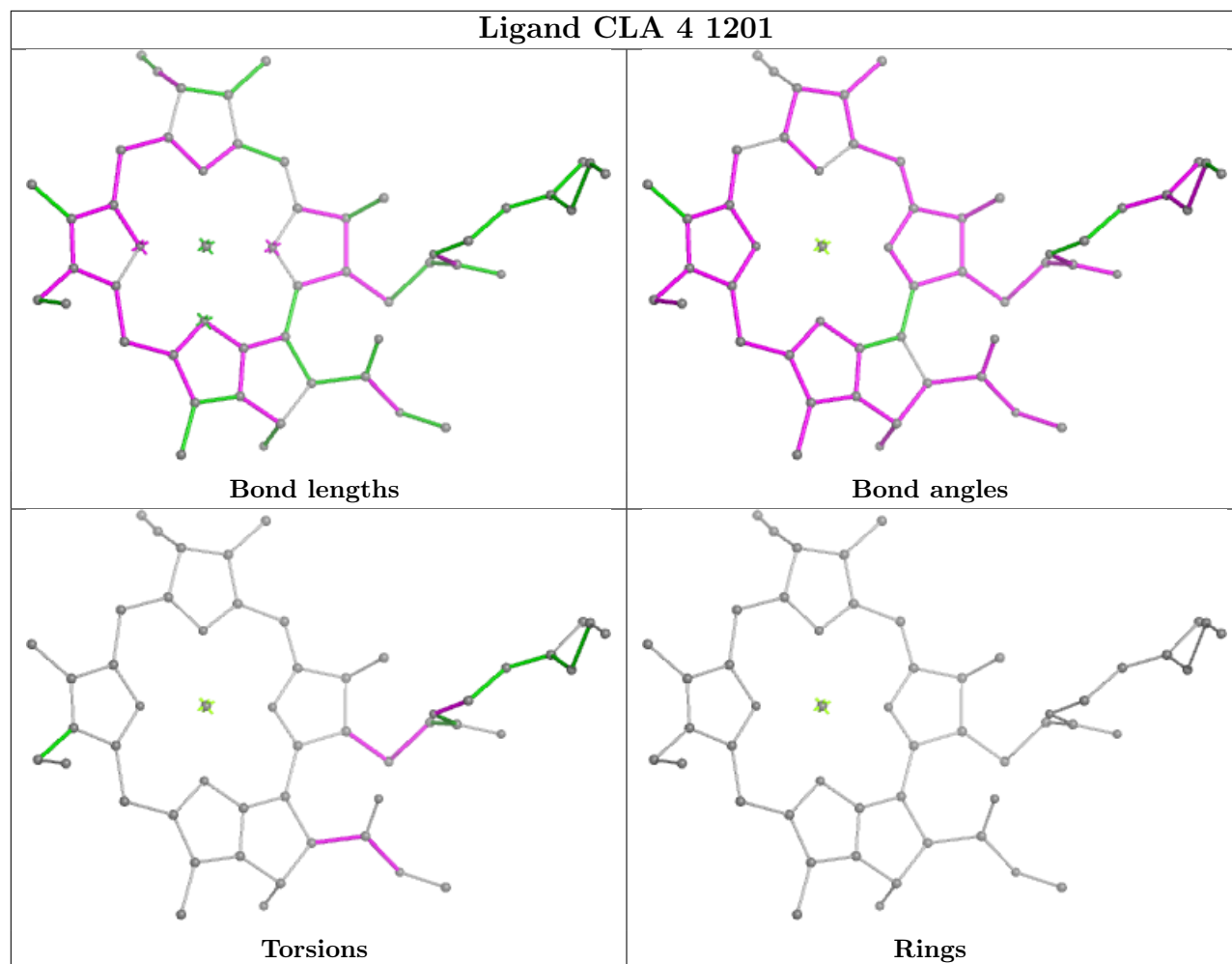
Torsions



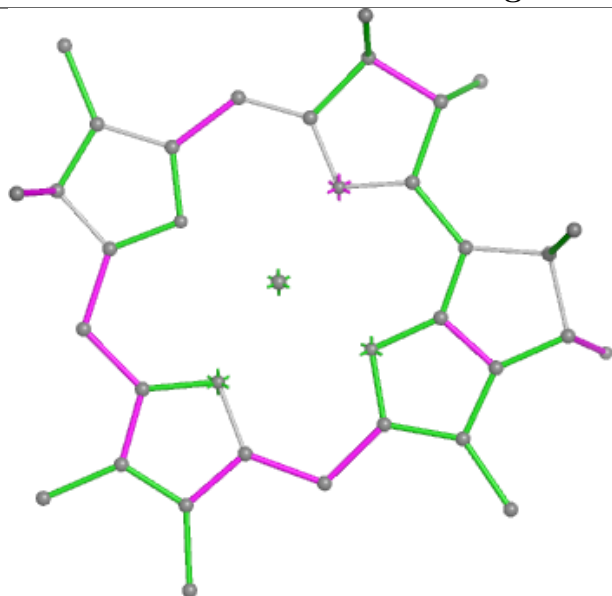
Rings



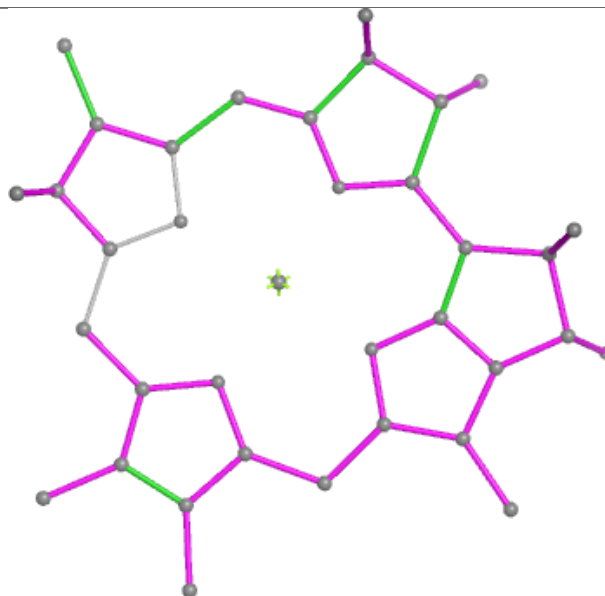




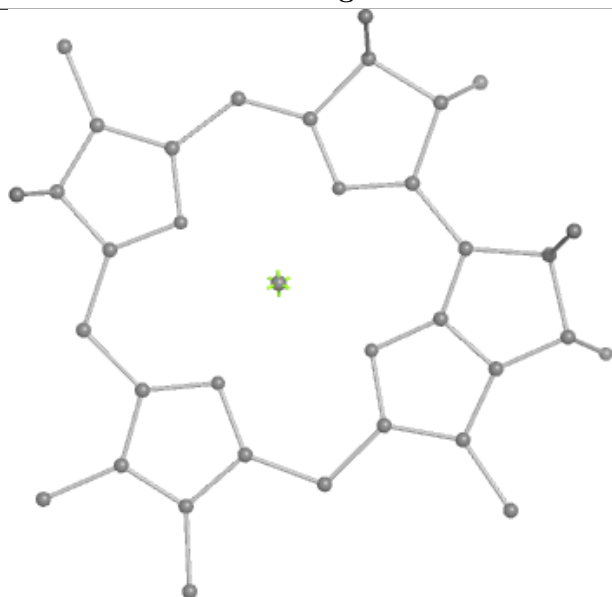
Ligand CLA B 1772



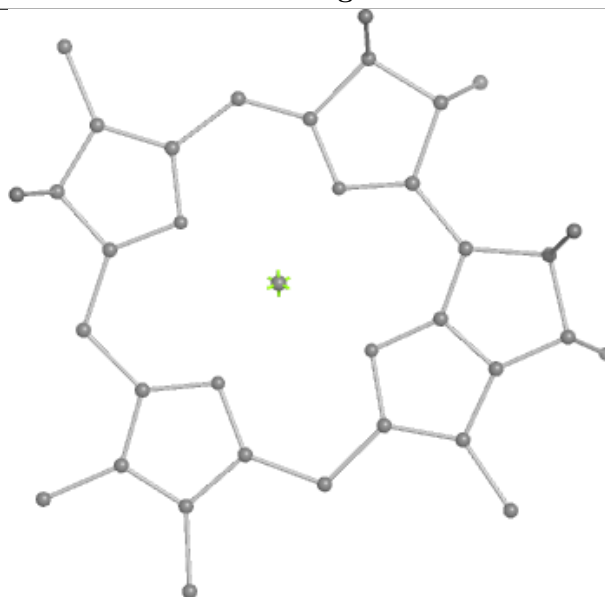
Bond lengths



Bond angles

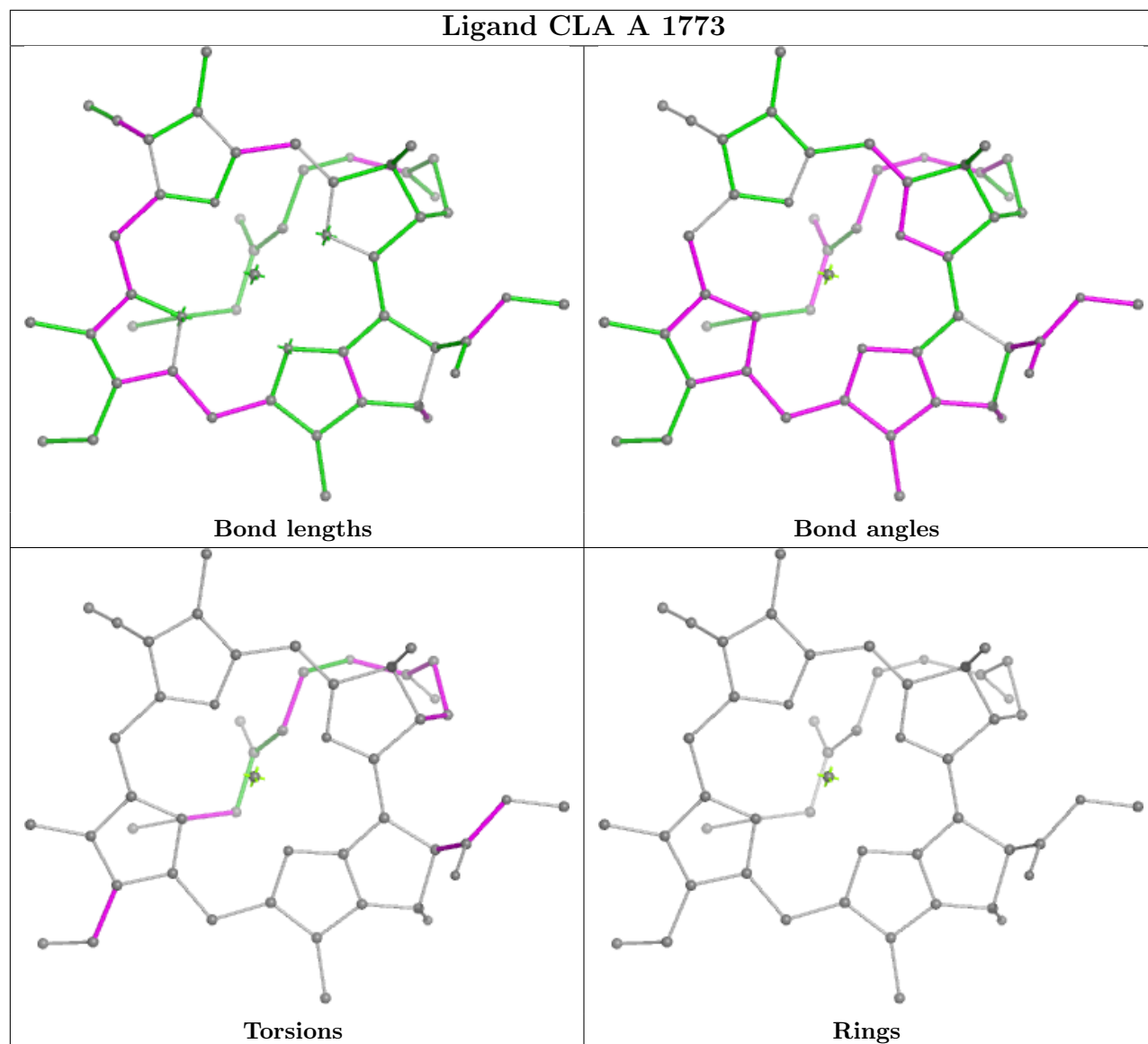


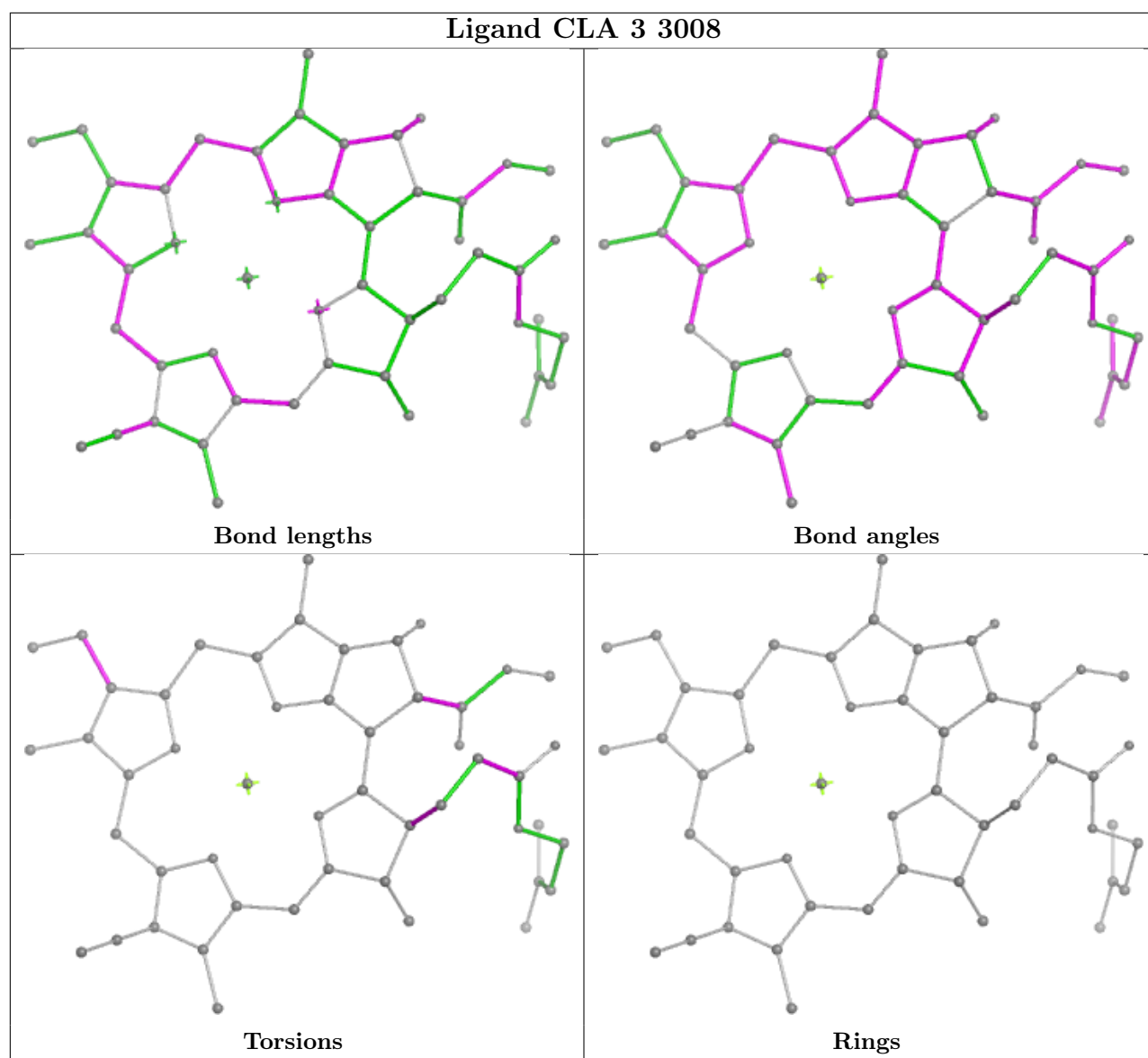
Torsions



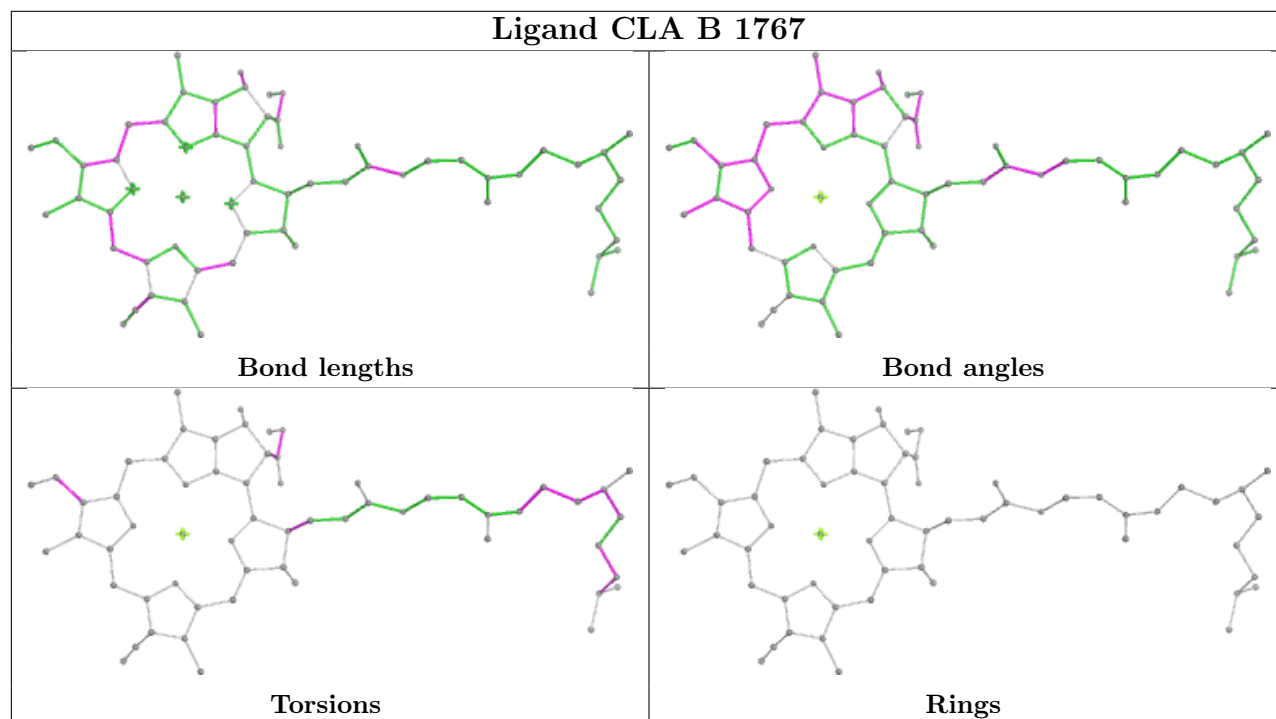
Rings

Ligand CLA A 1773

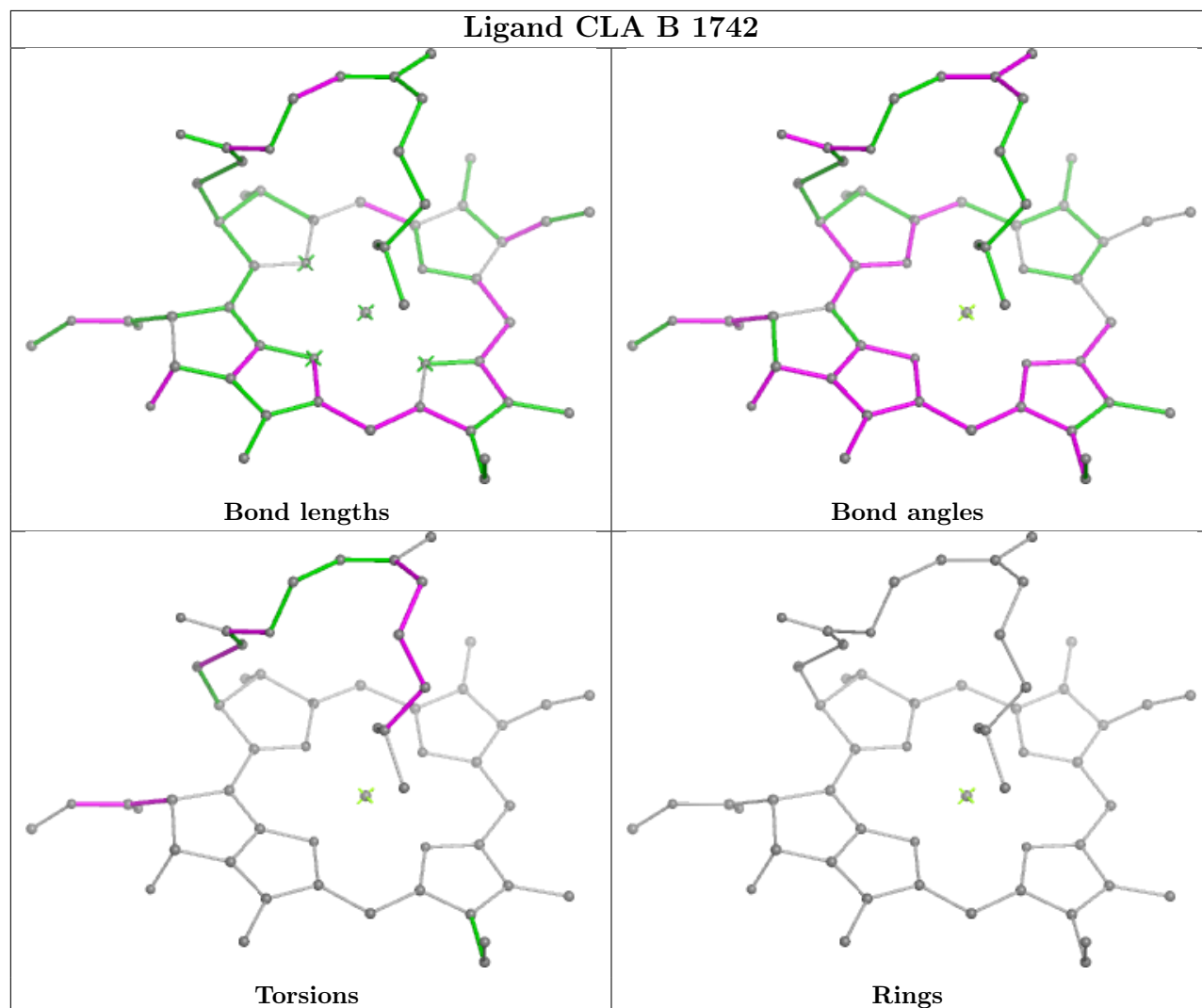




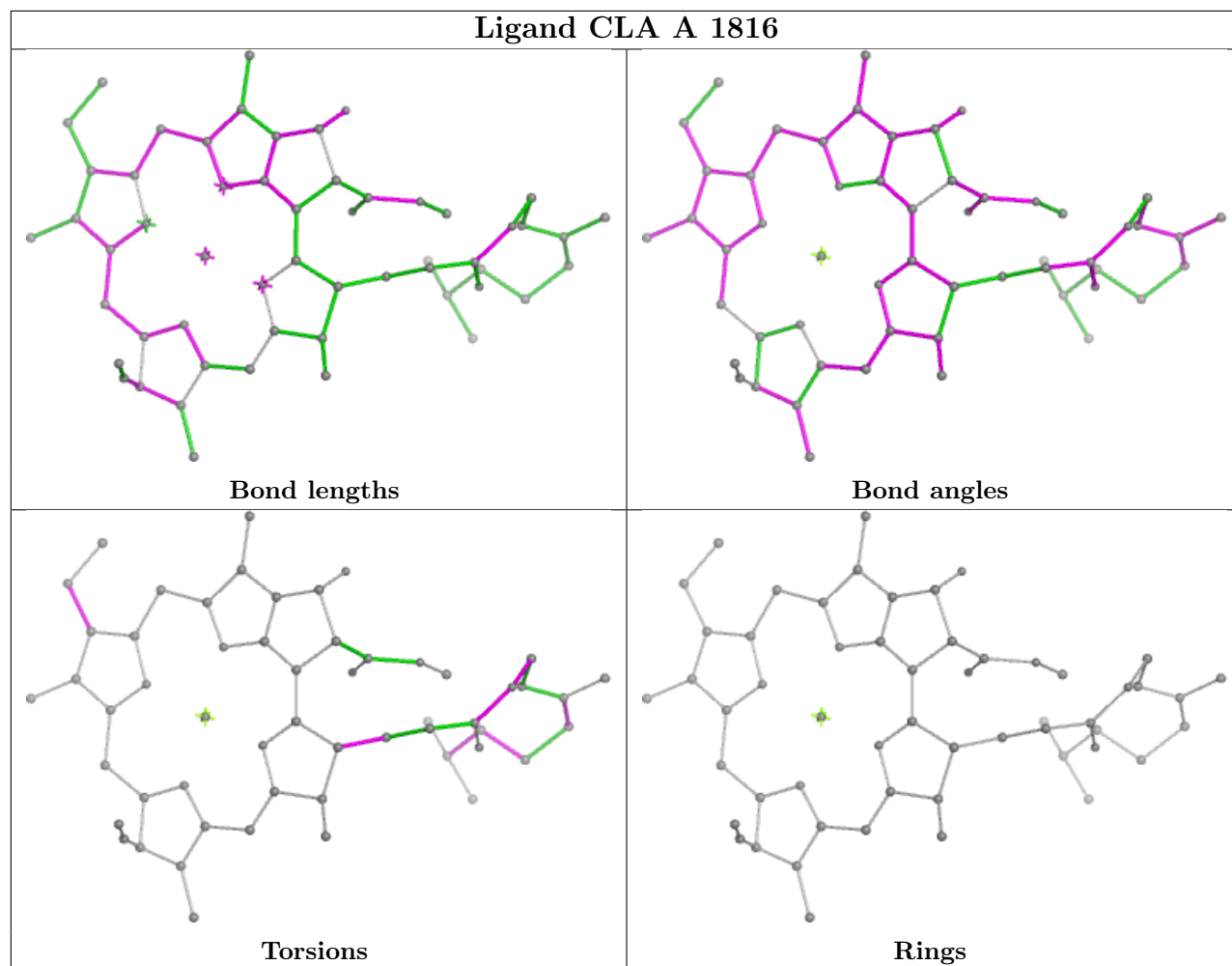
Ligand CLA B 1767

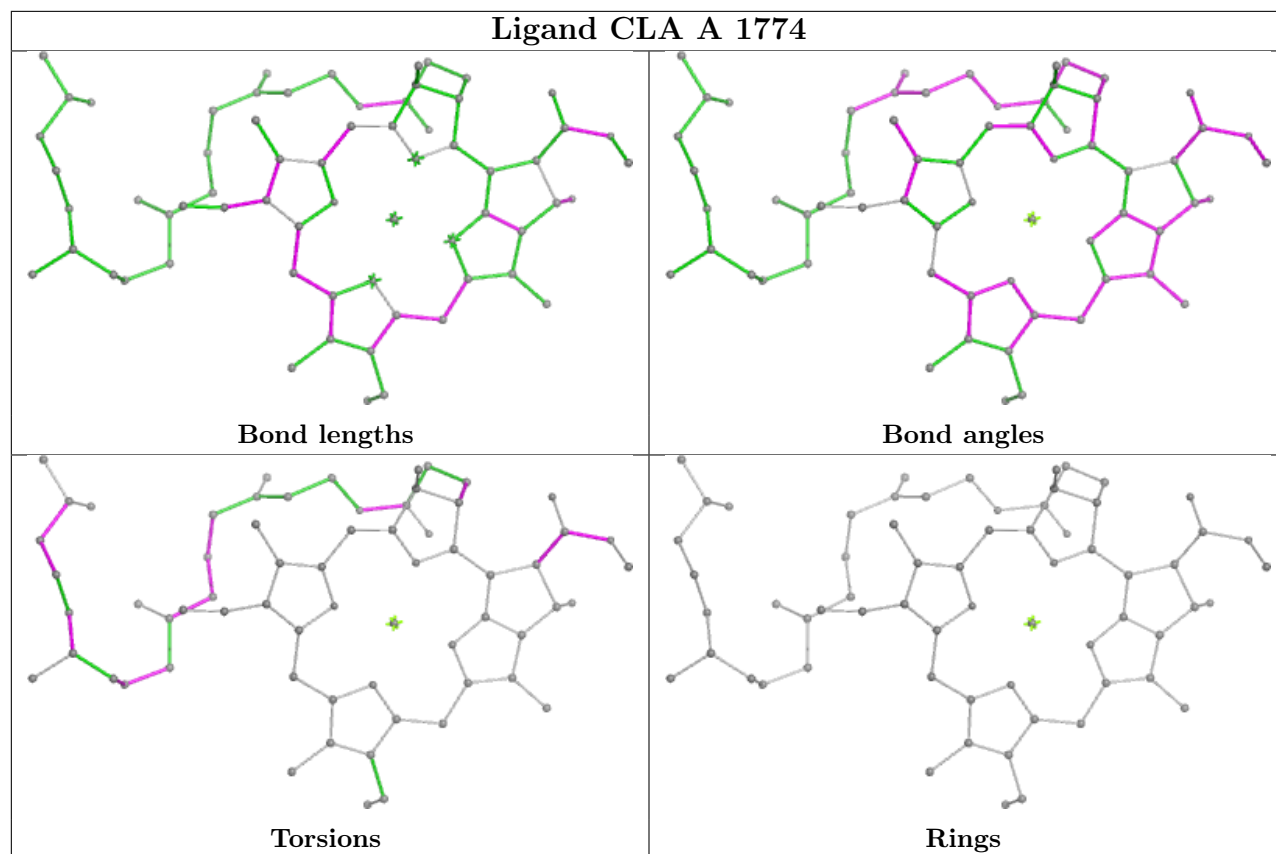


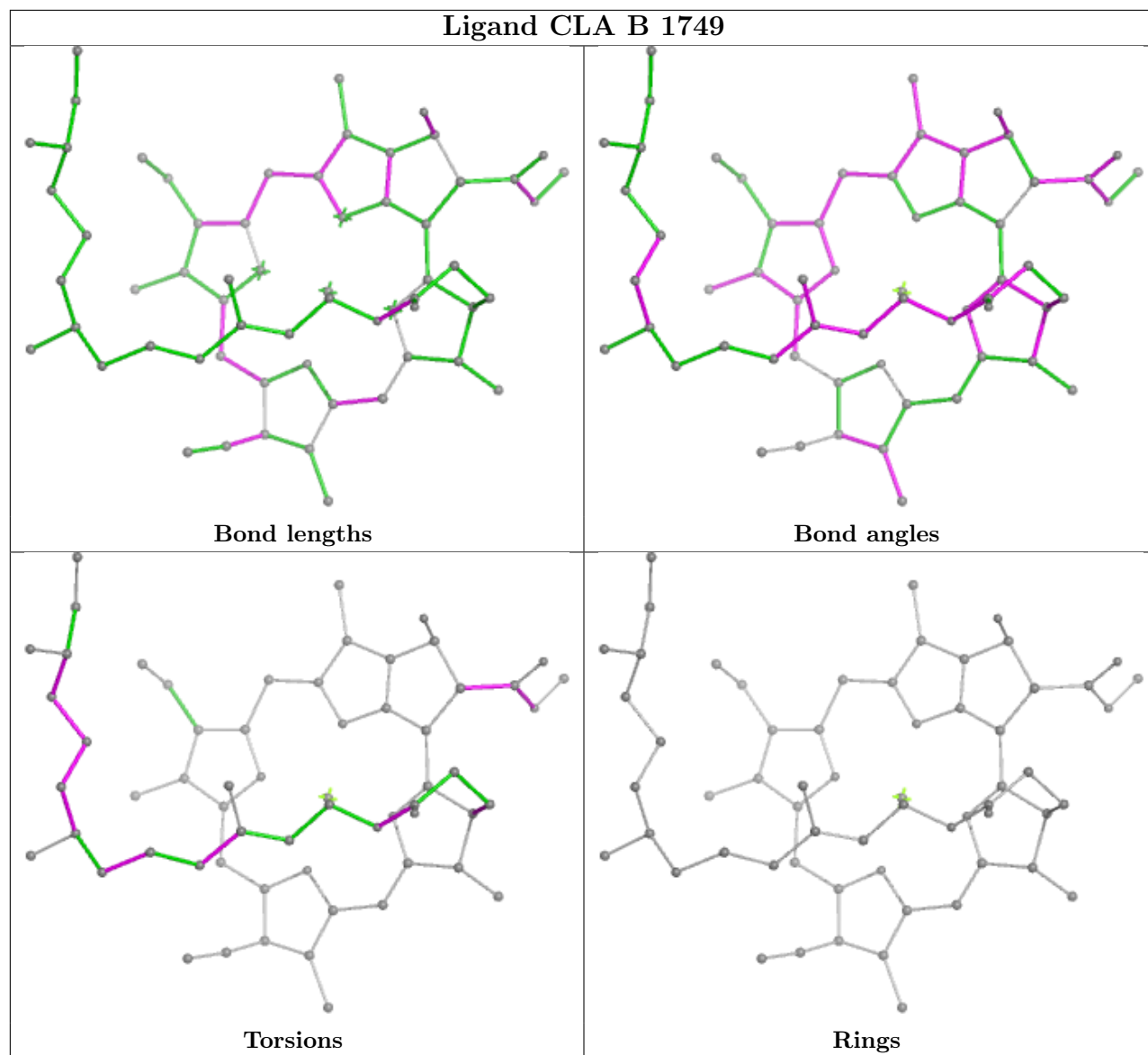
Ligand CLA B 1742

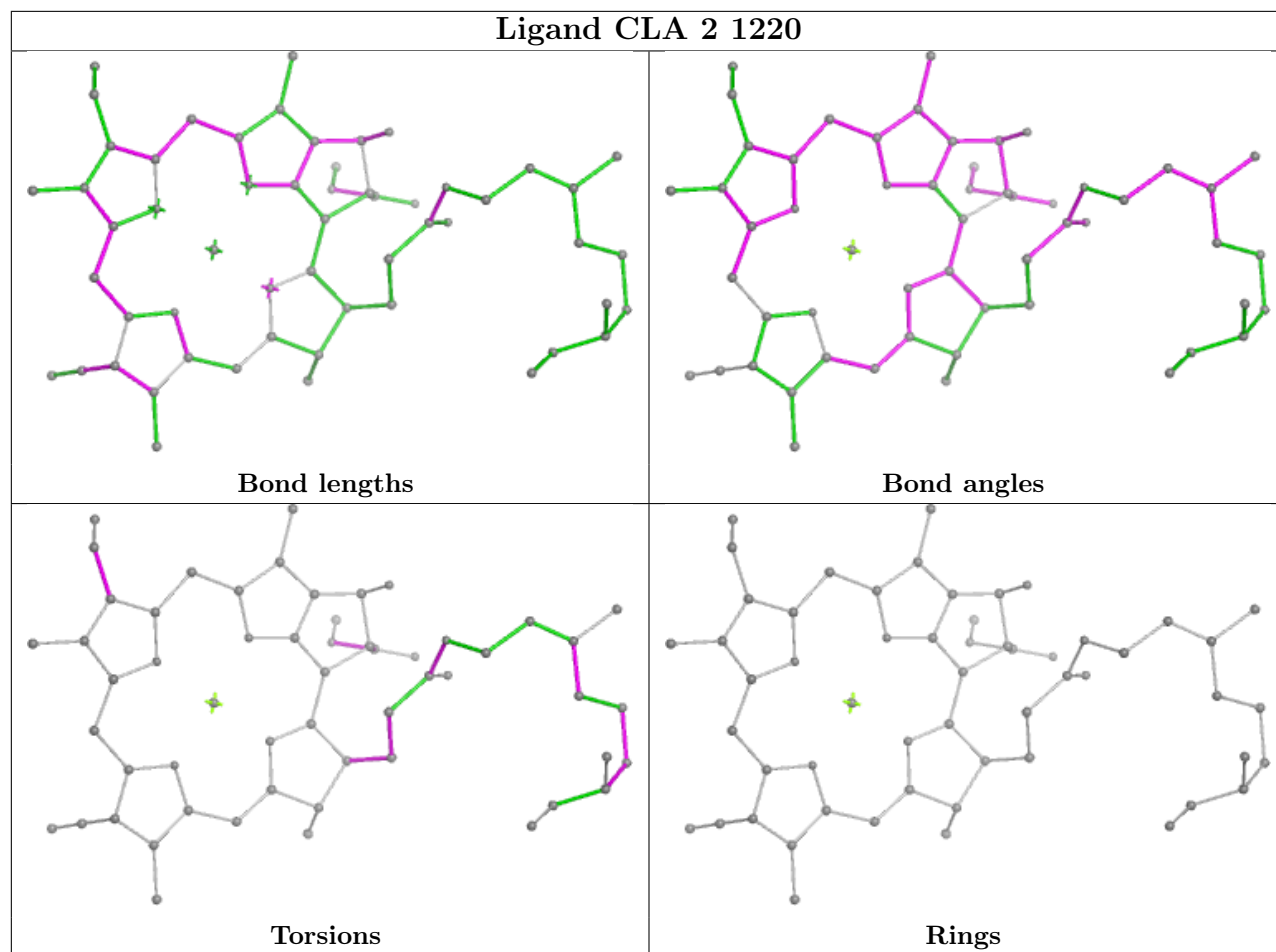


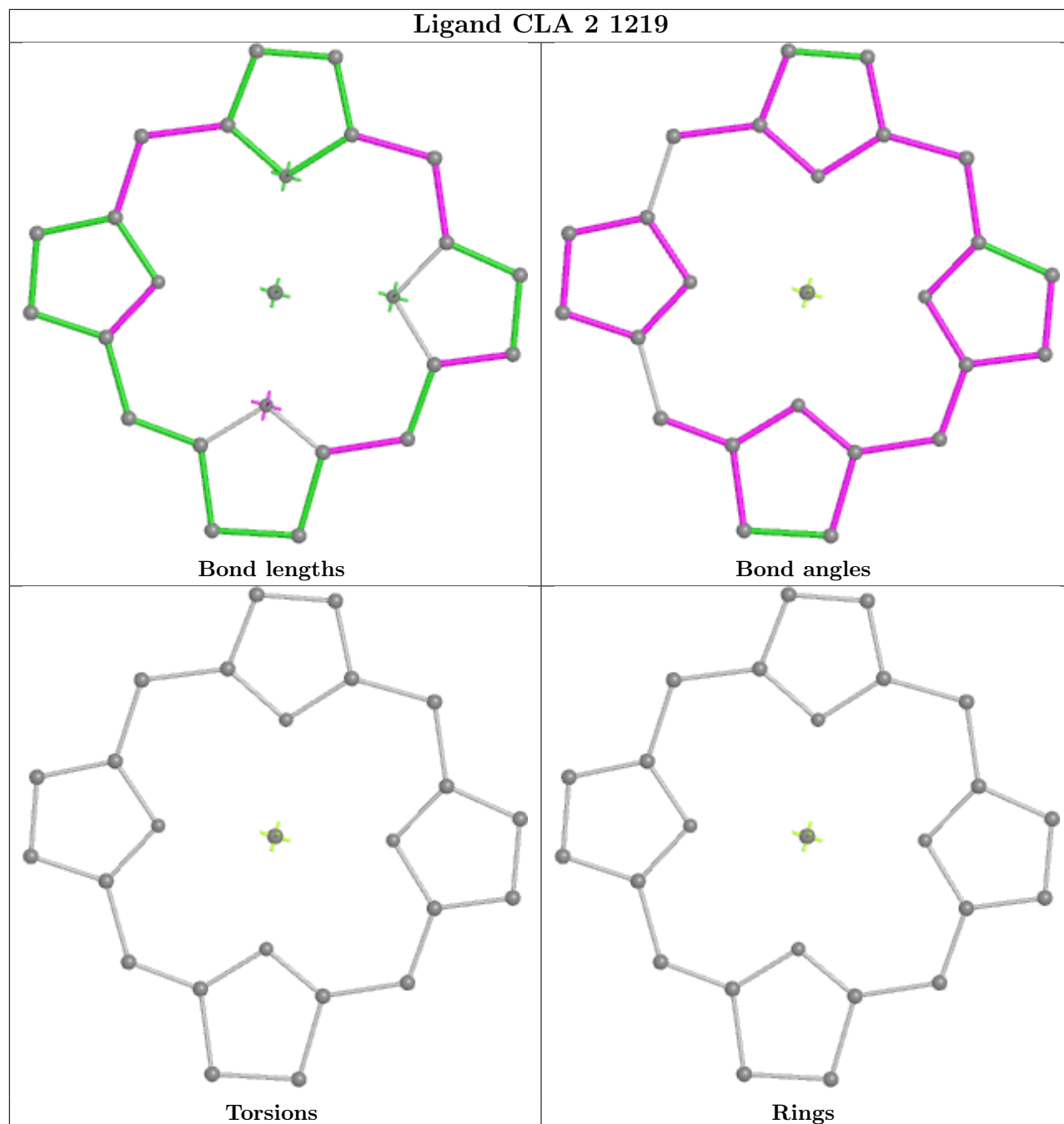
Ligand CLA A 1816

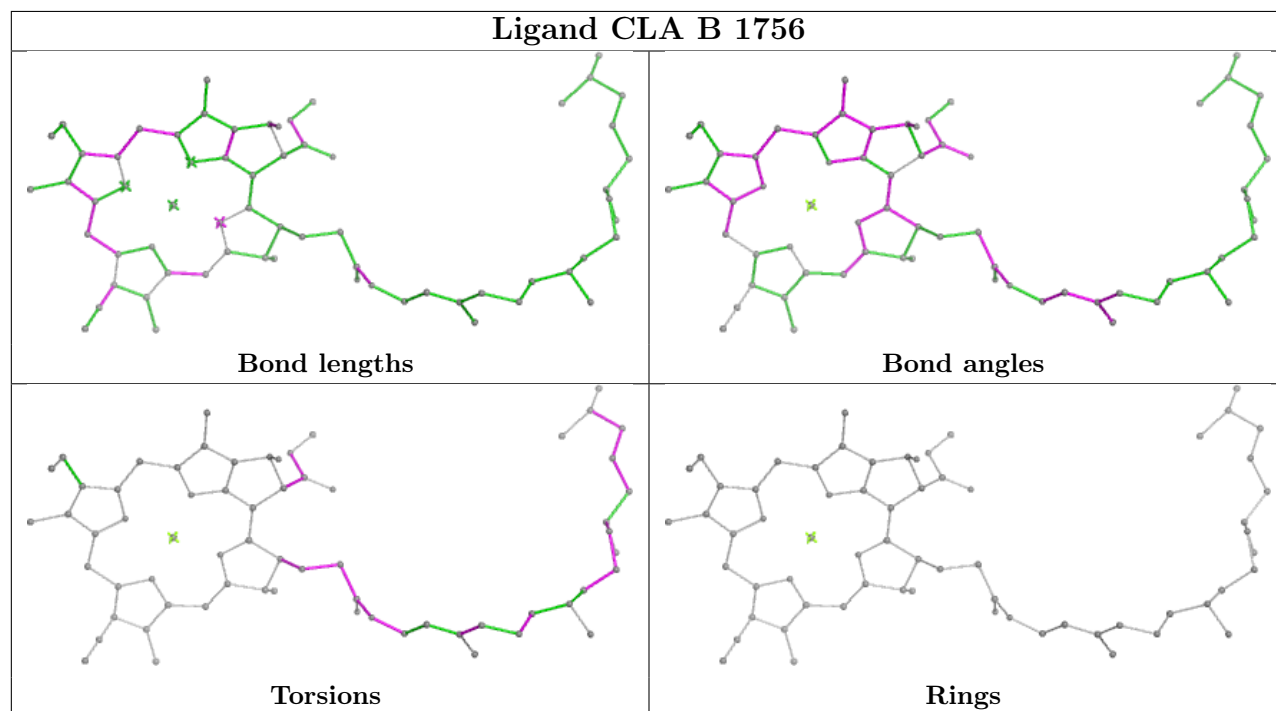
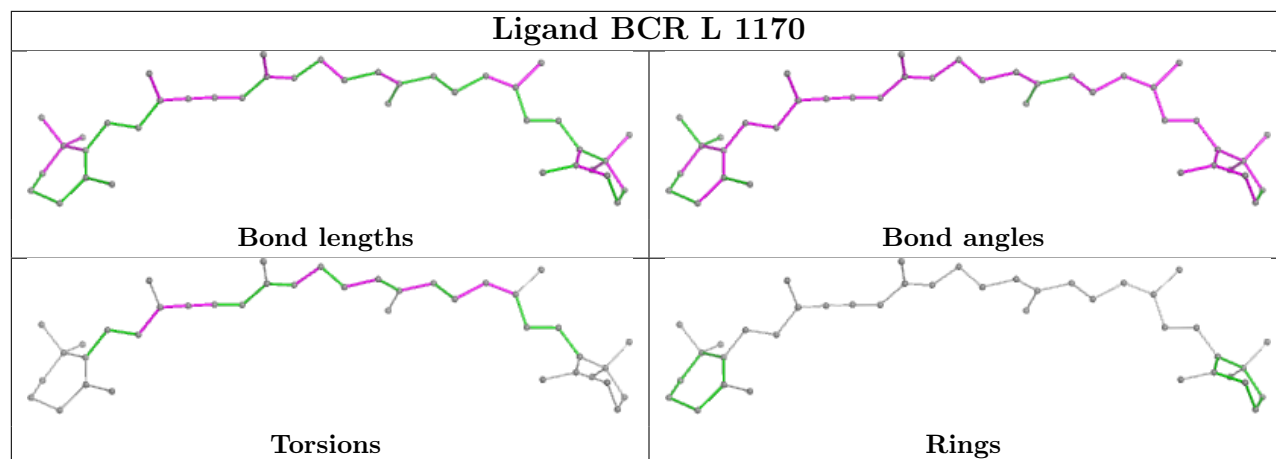


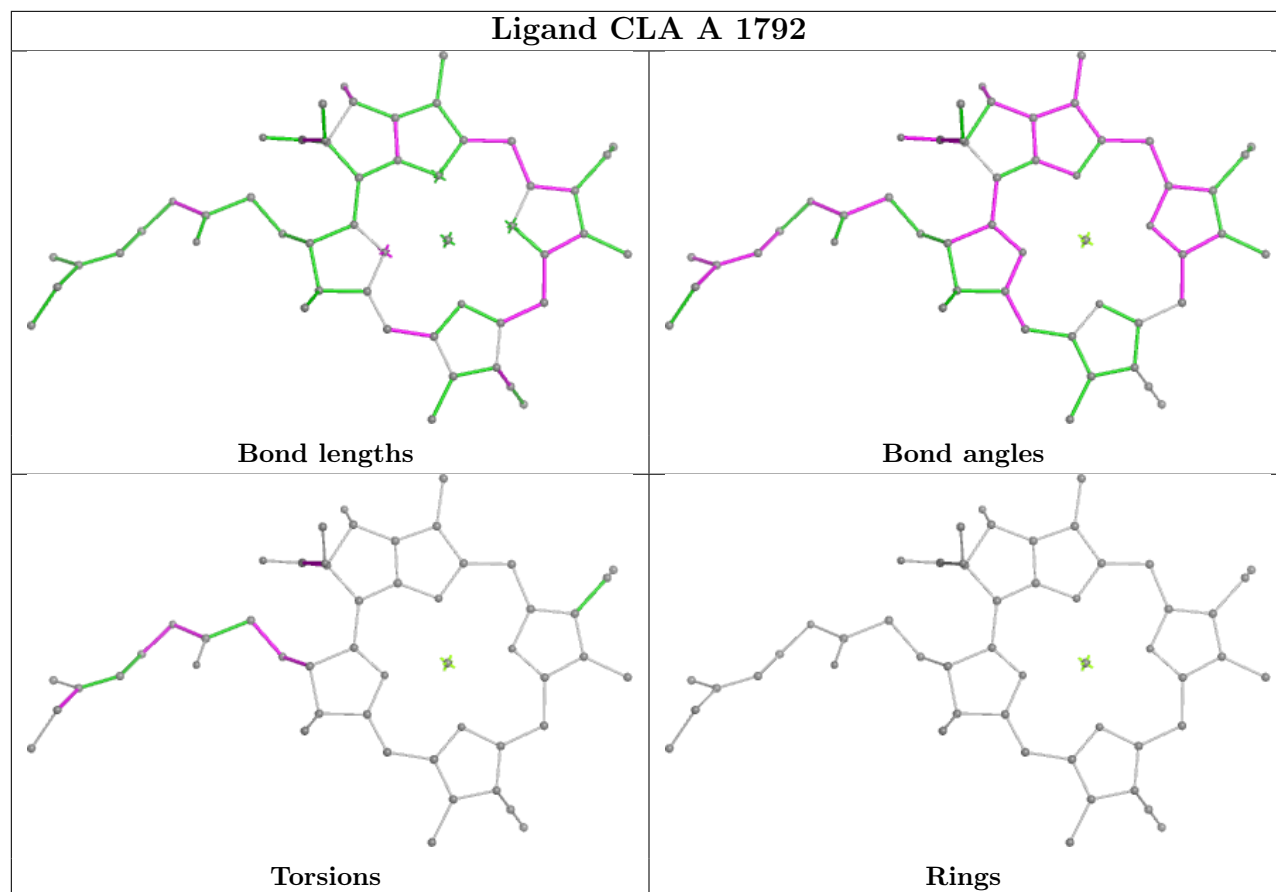




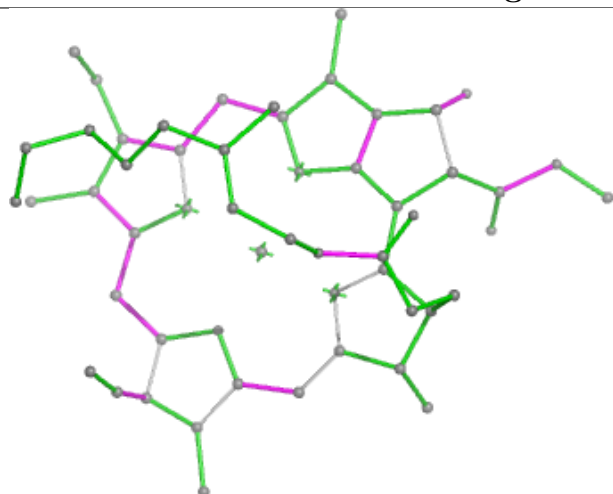




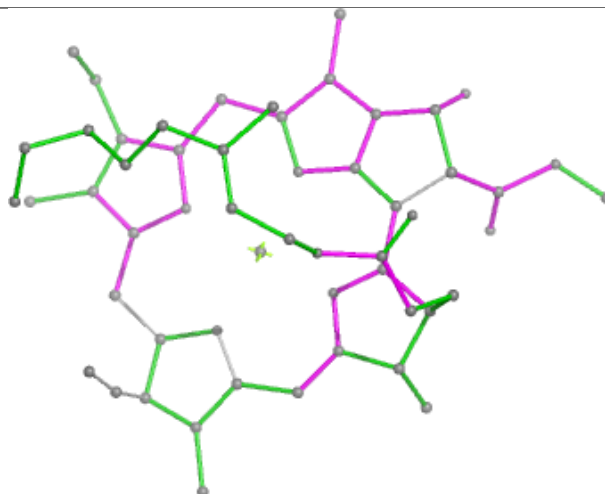




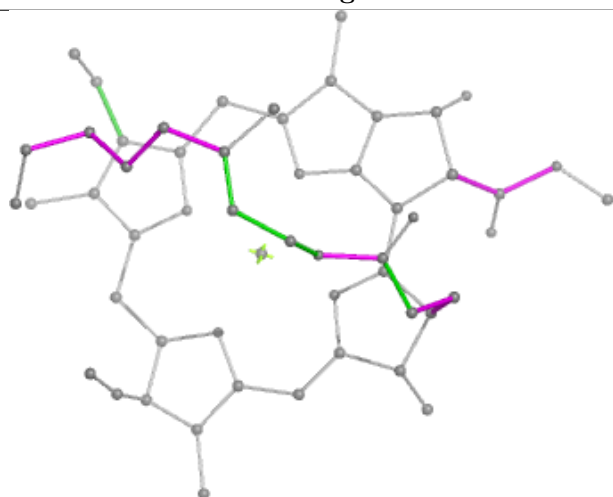
Ligand CLA A 1768



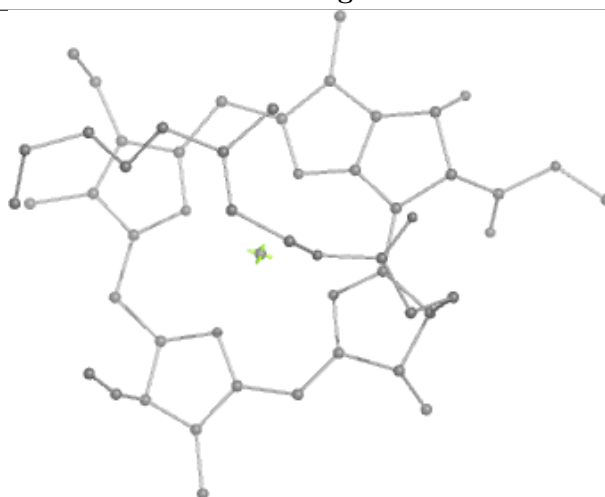
Bond lengths



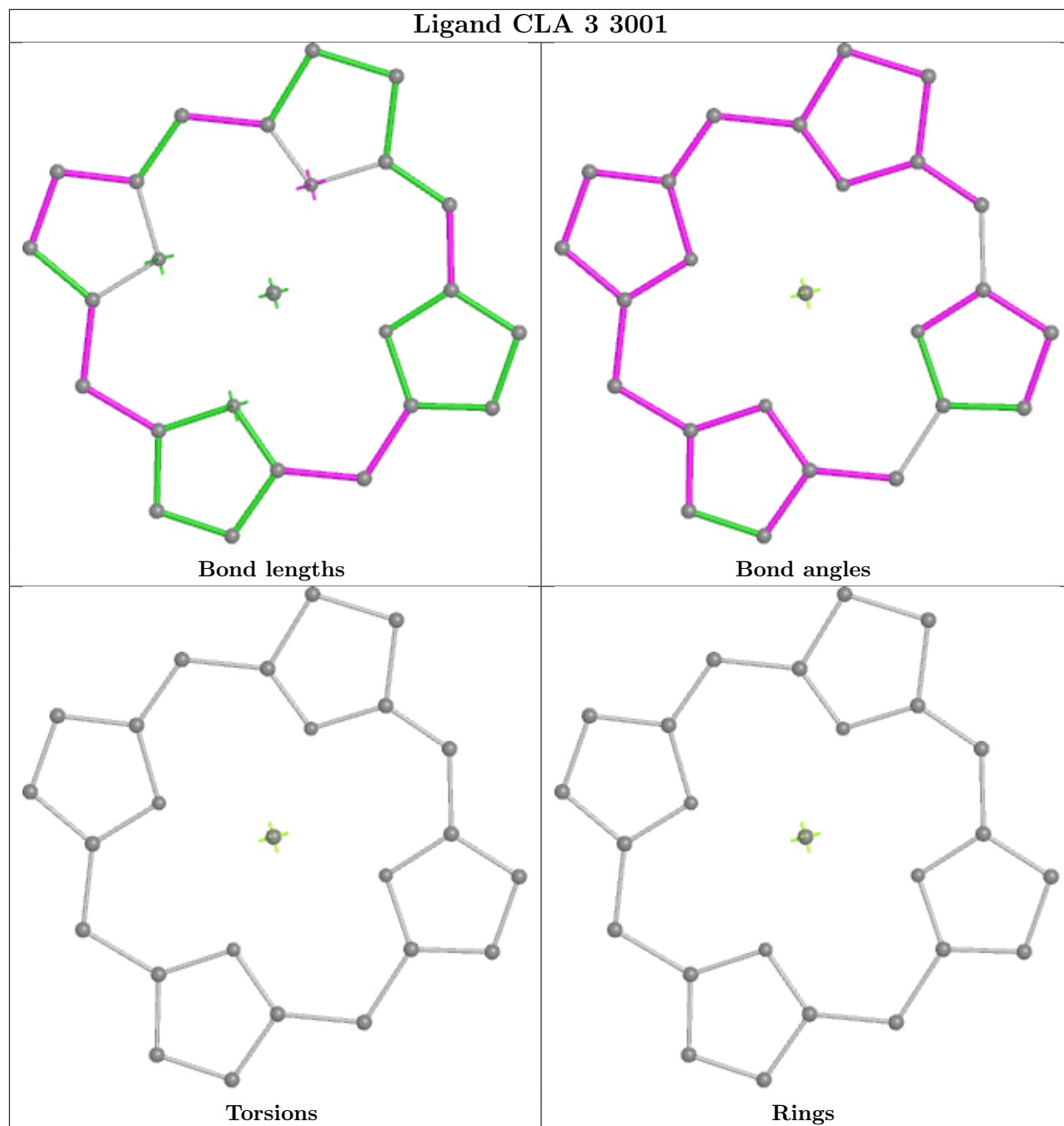
Bond angles

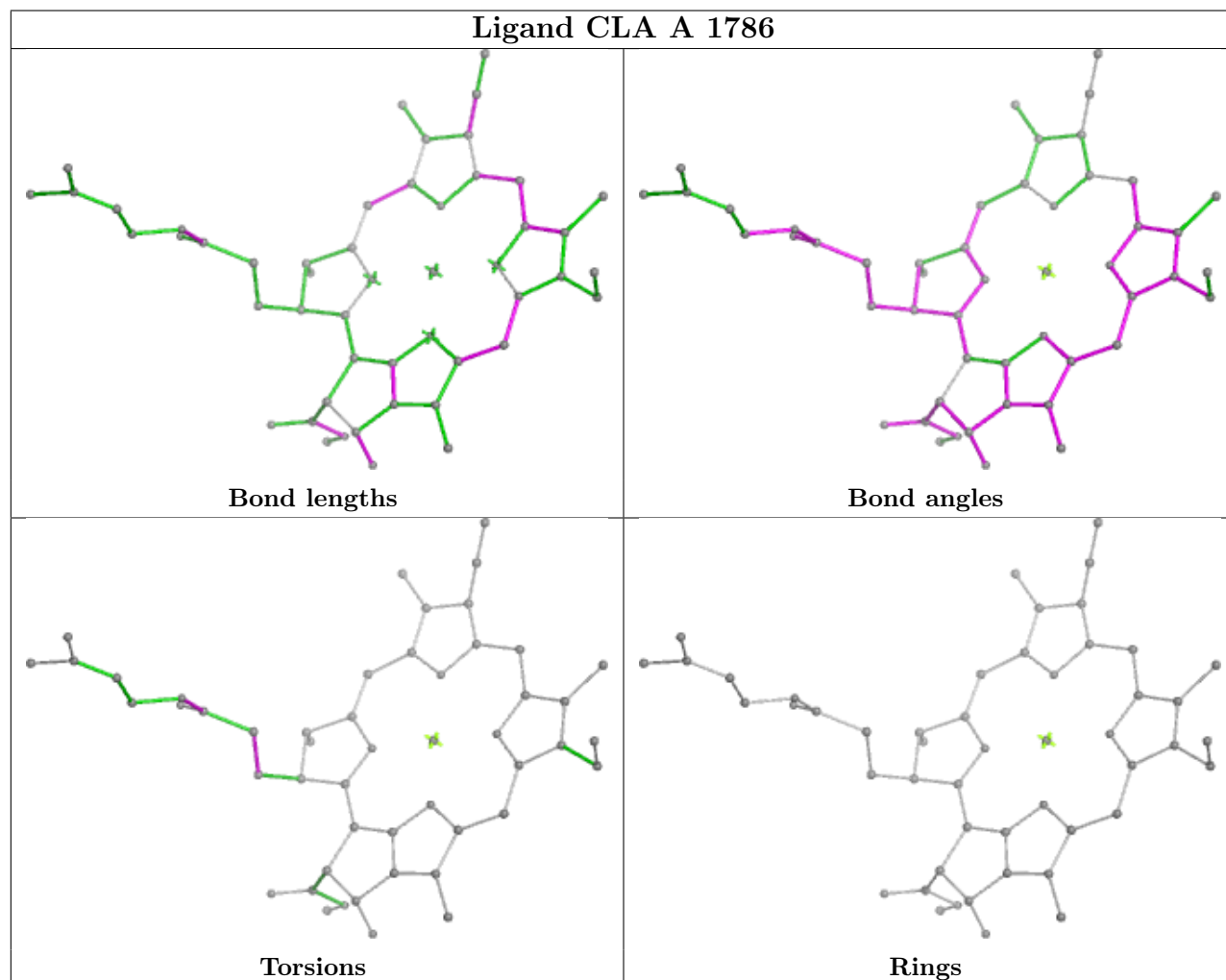
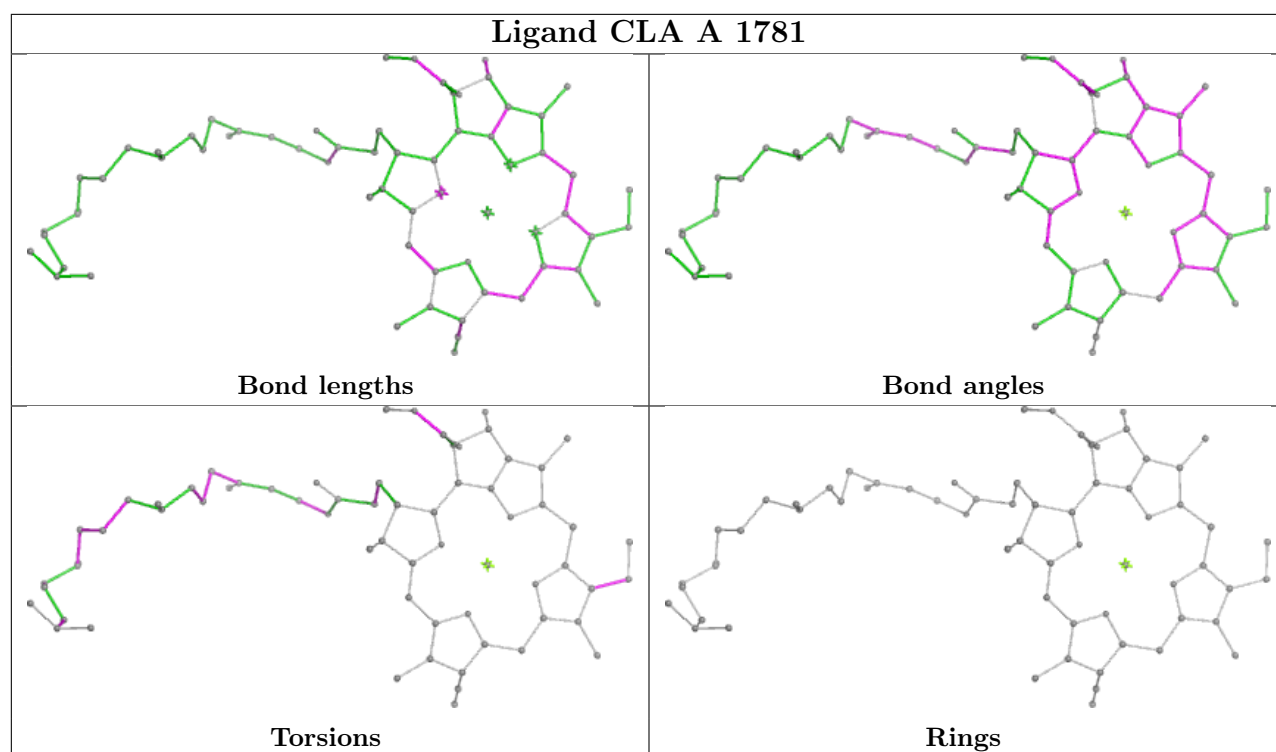


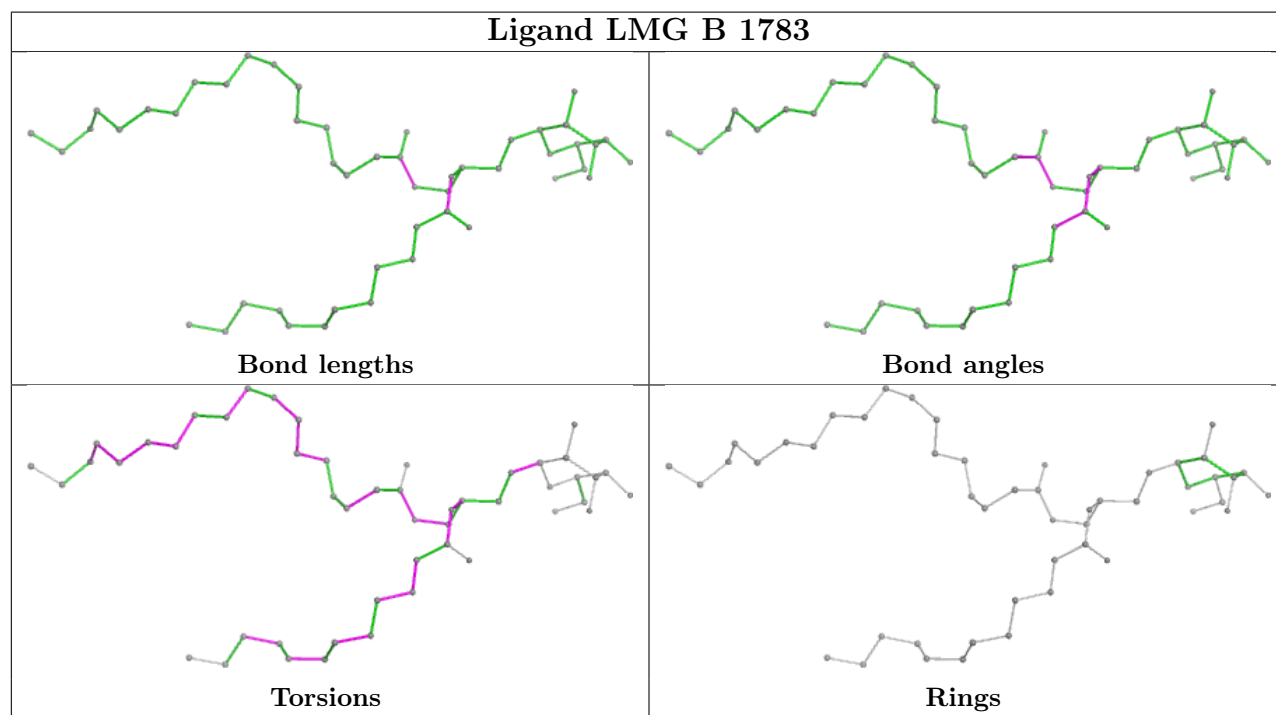
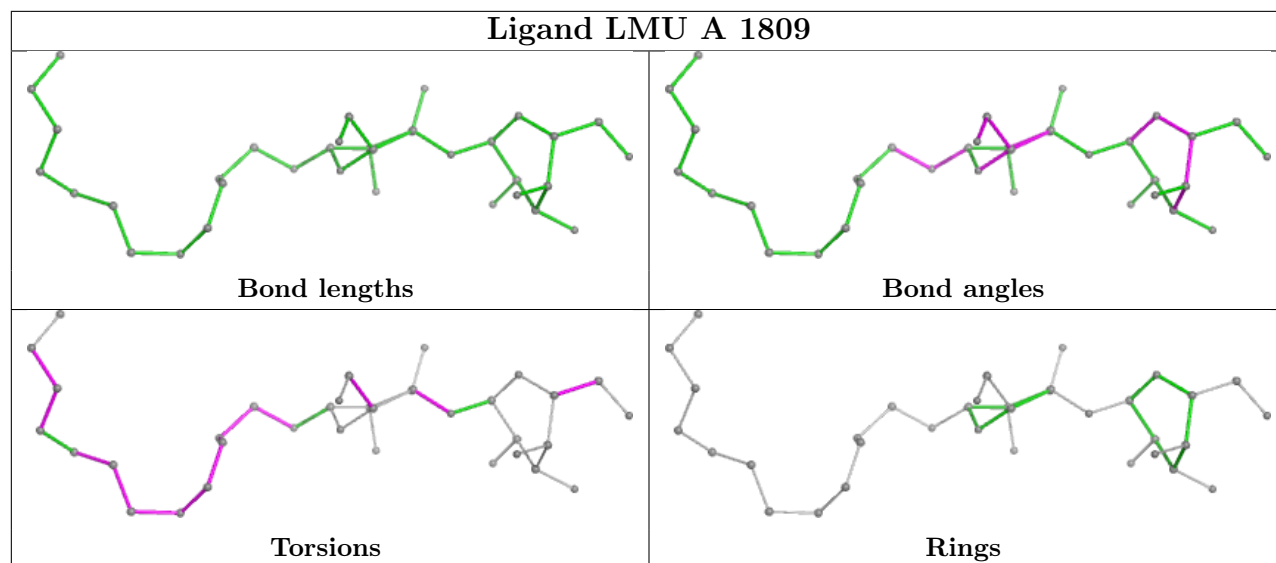
Torsions



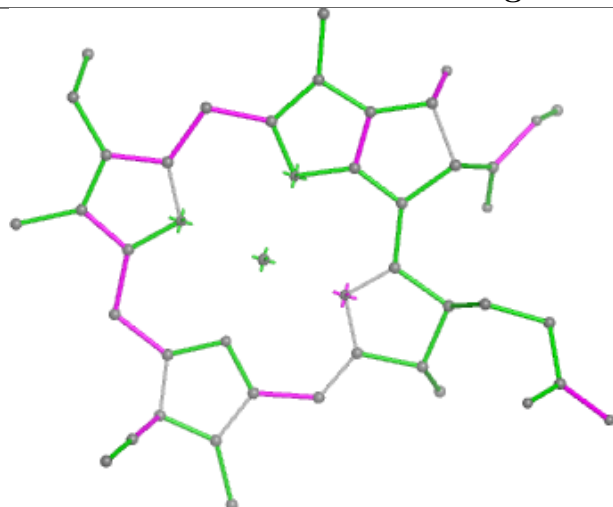
Rings



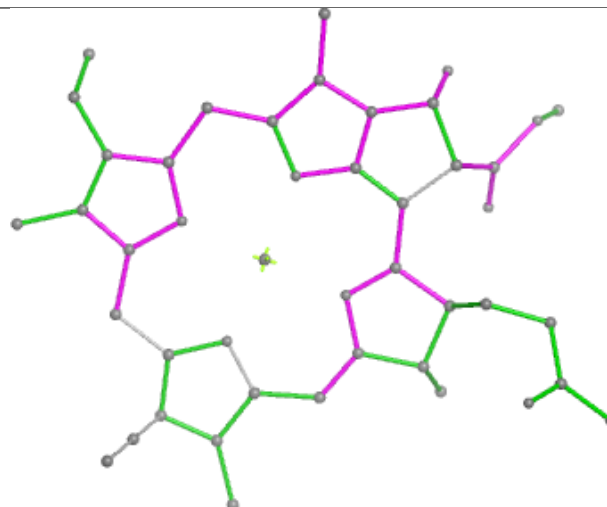




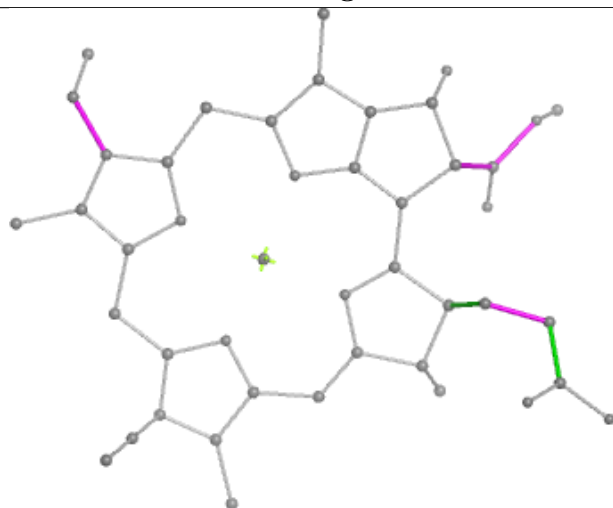
Ligand CLA K 1142



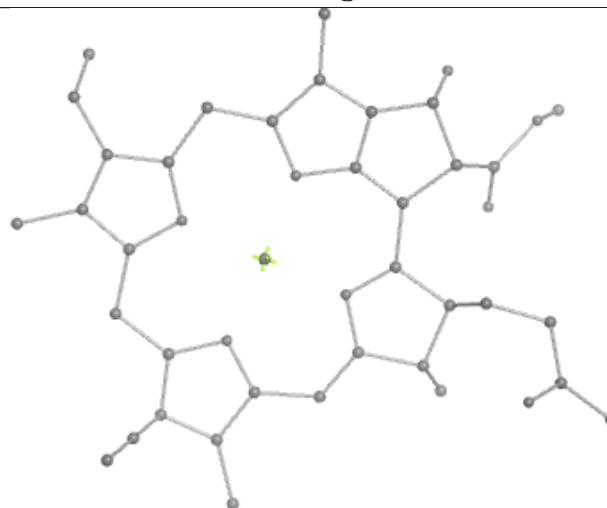
Bond lengths



Bond angles

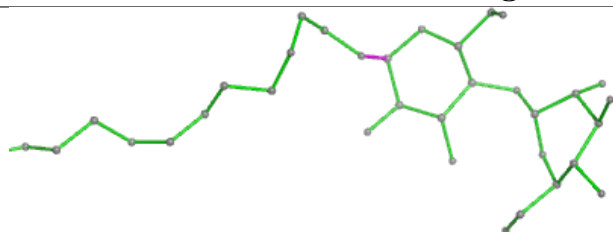


Torsions

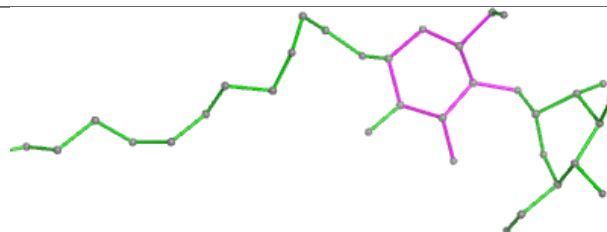


Rings

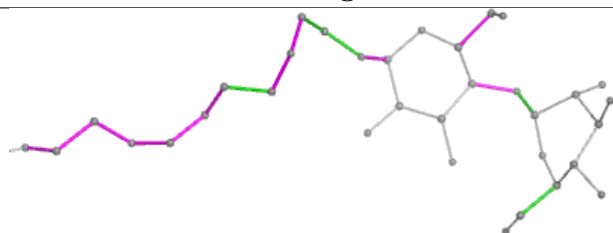
Ligand LMU A 7035



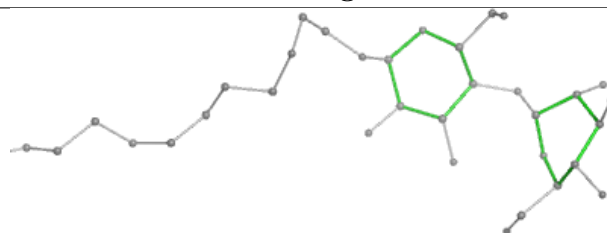
Bond lengths



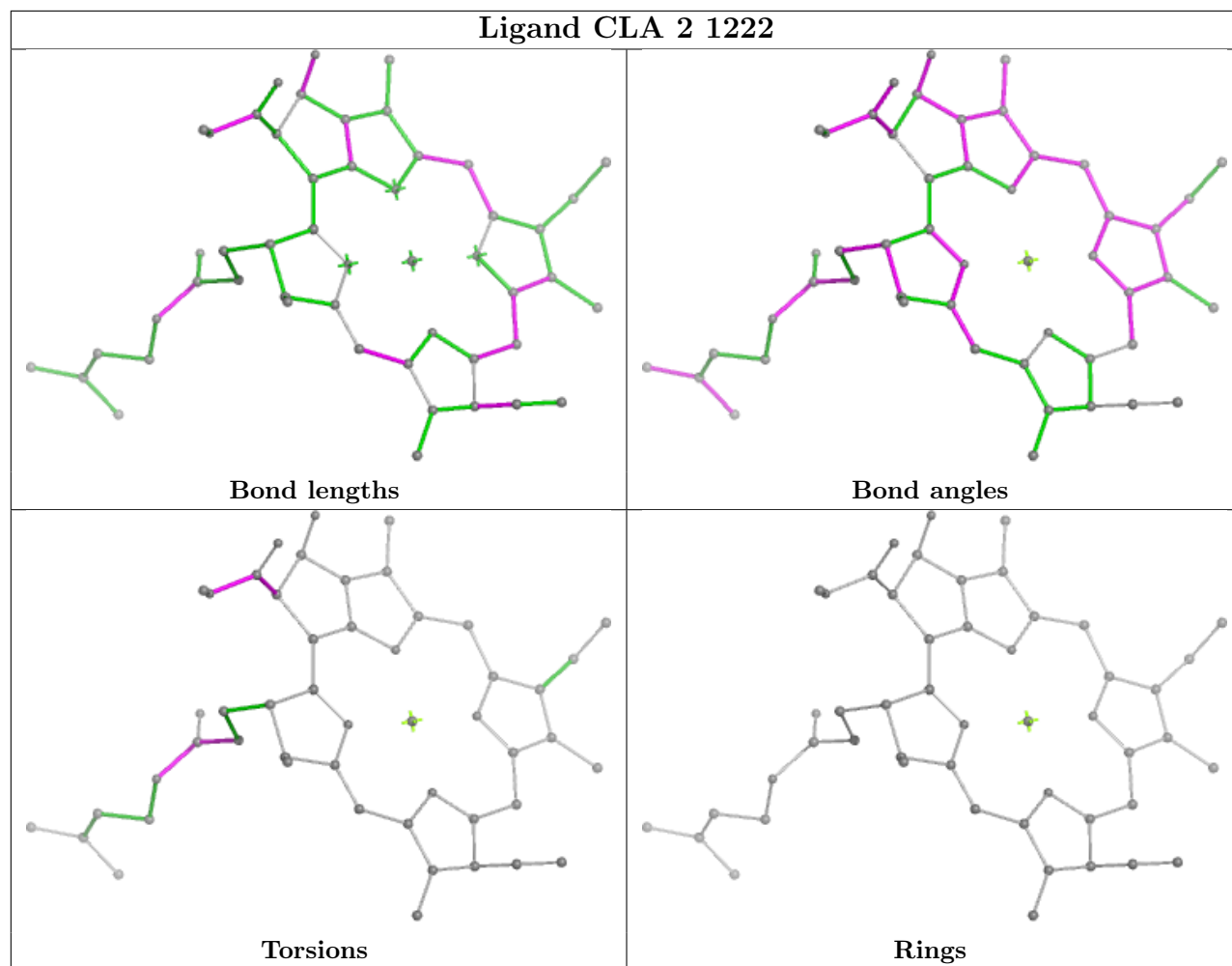
Bond angles

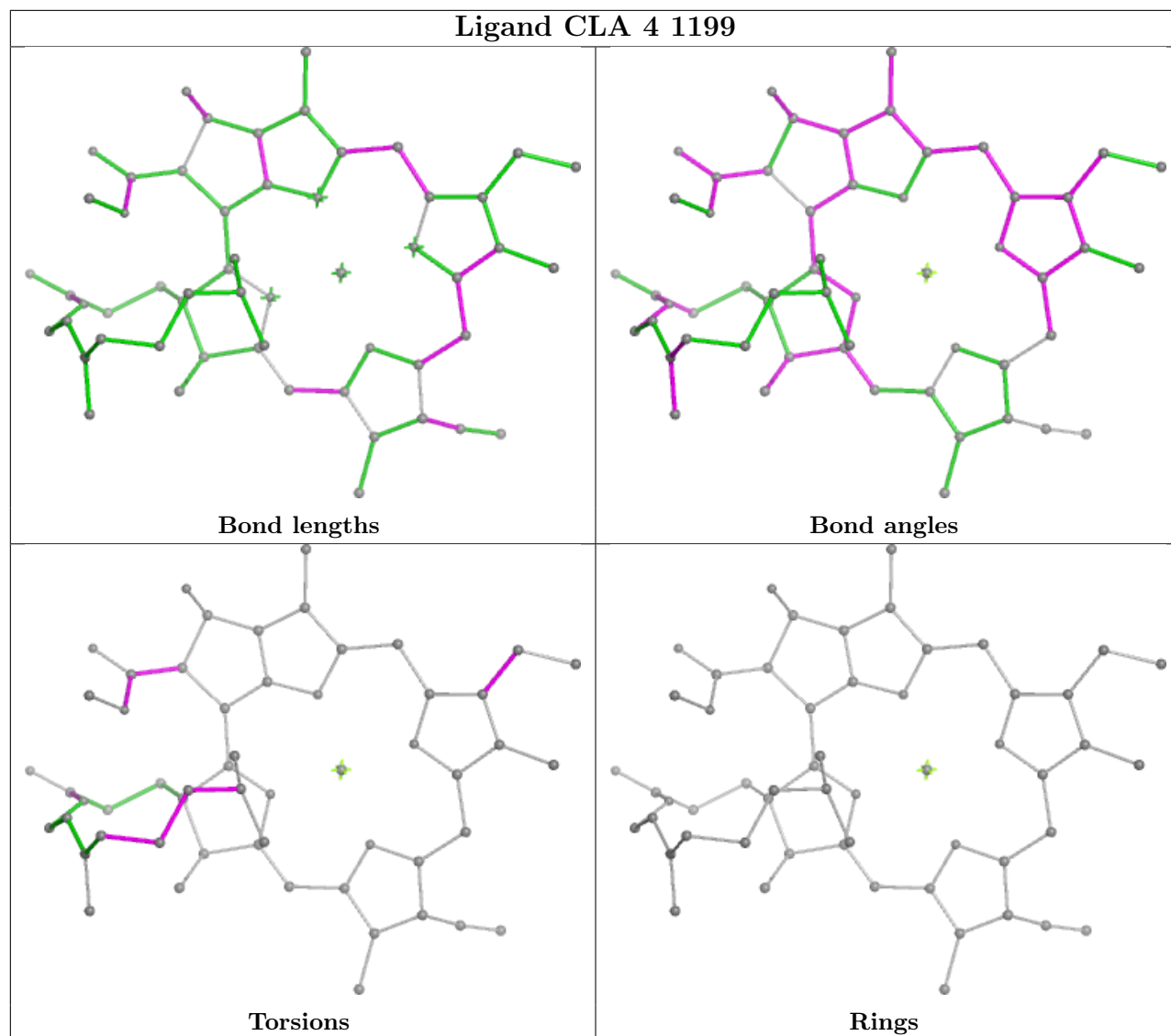


Torsions

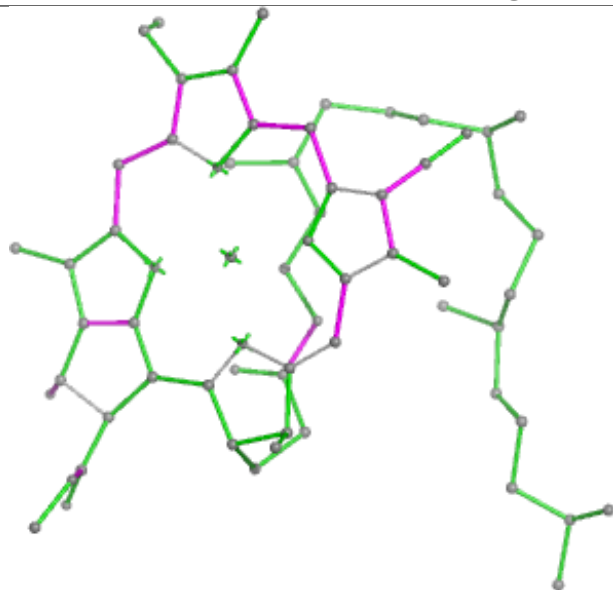


Rings

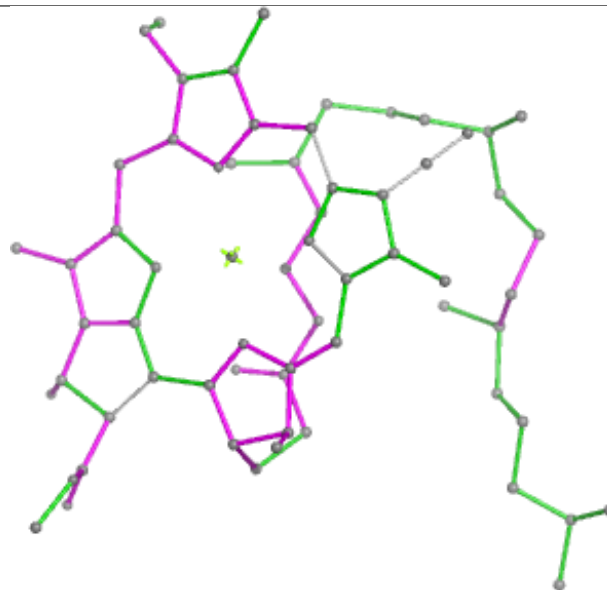




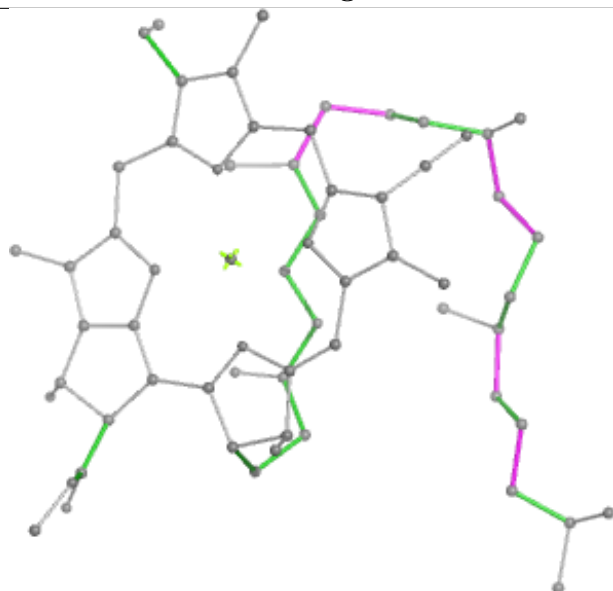
Ligand CLA B 1739



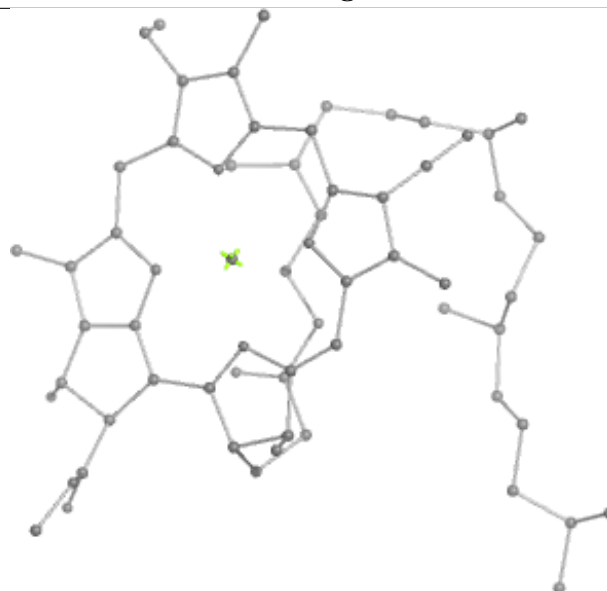
Bond lengths



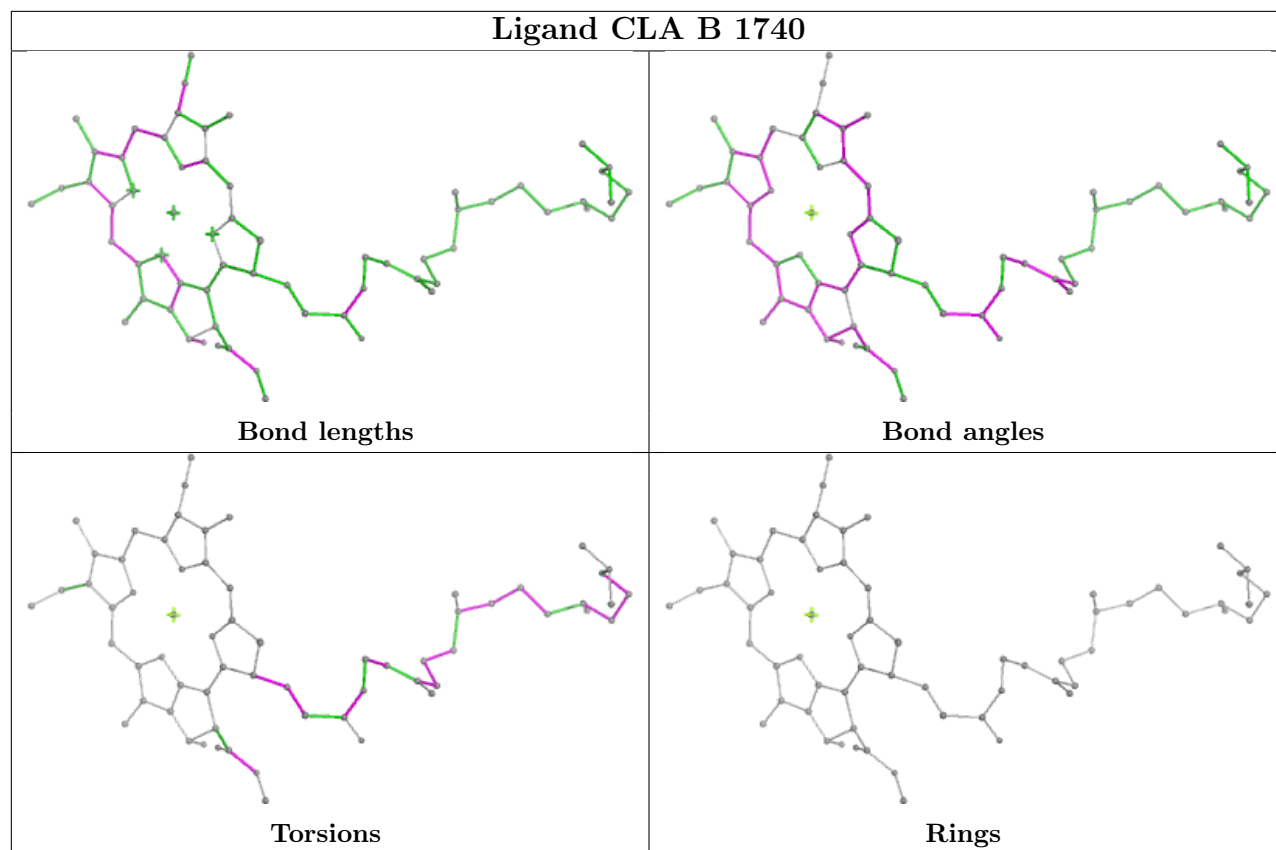
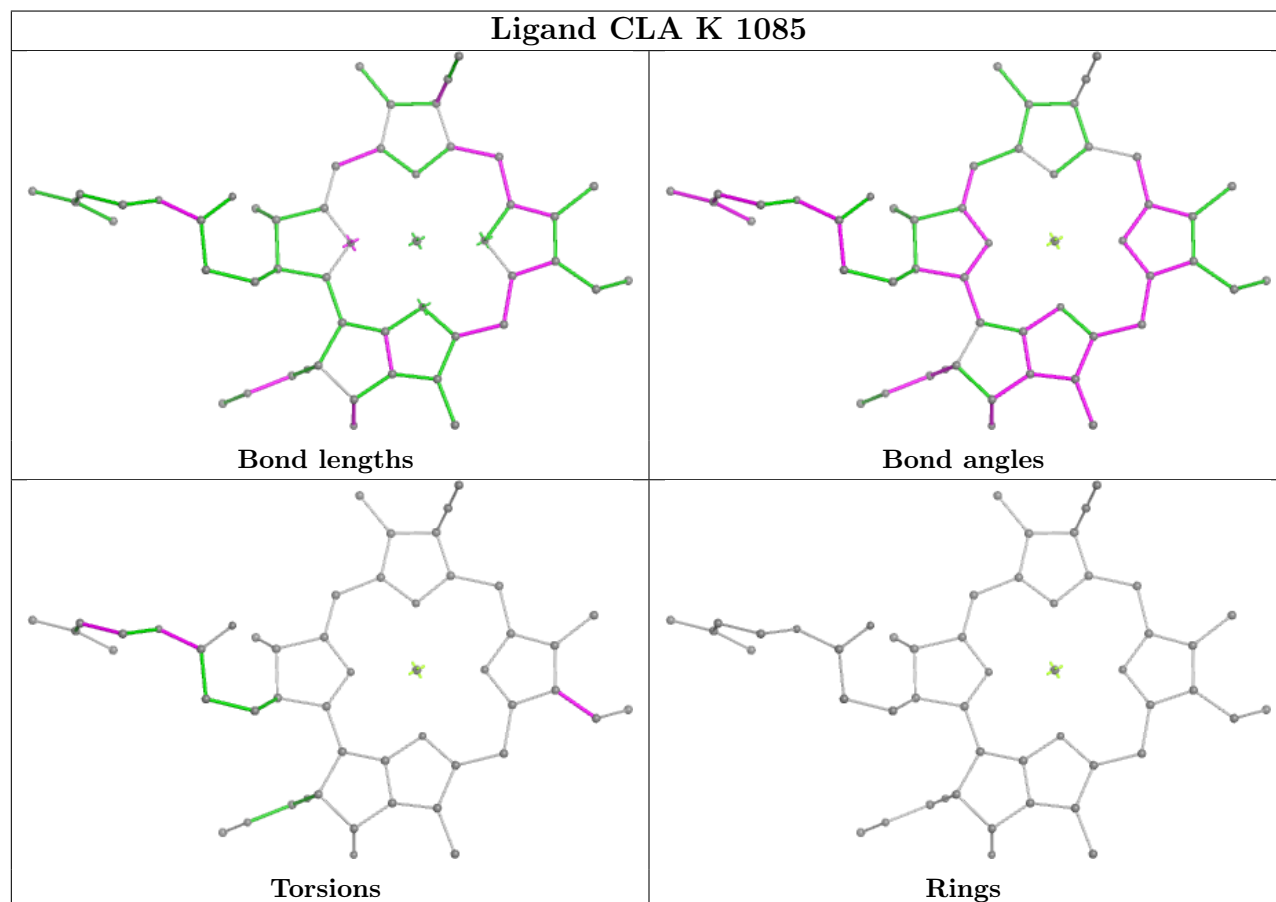
Bond angles

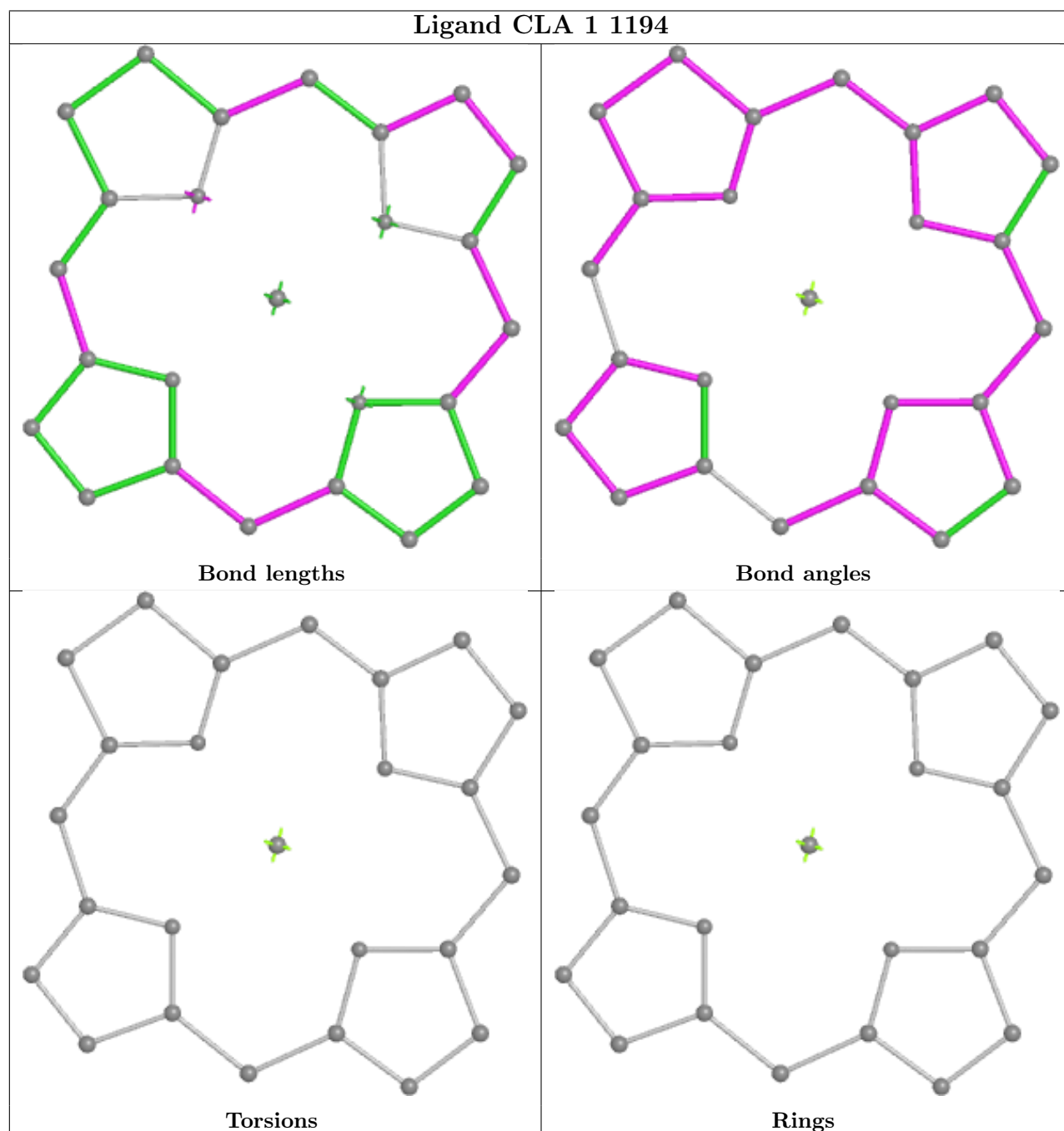
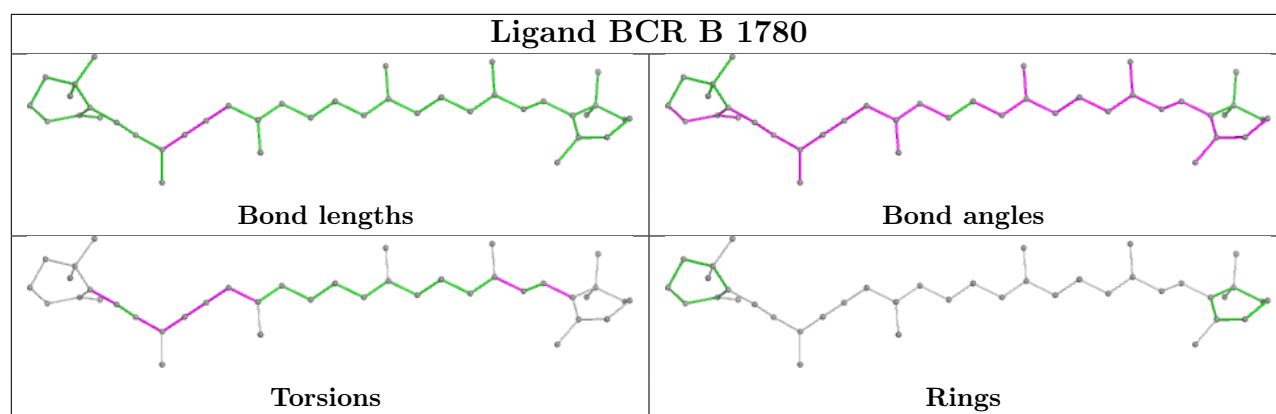


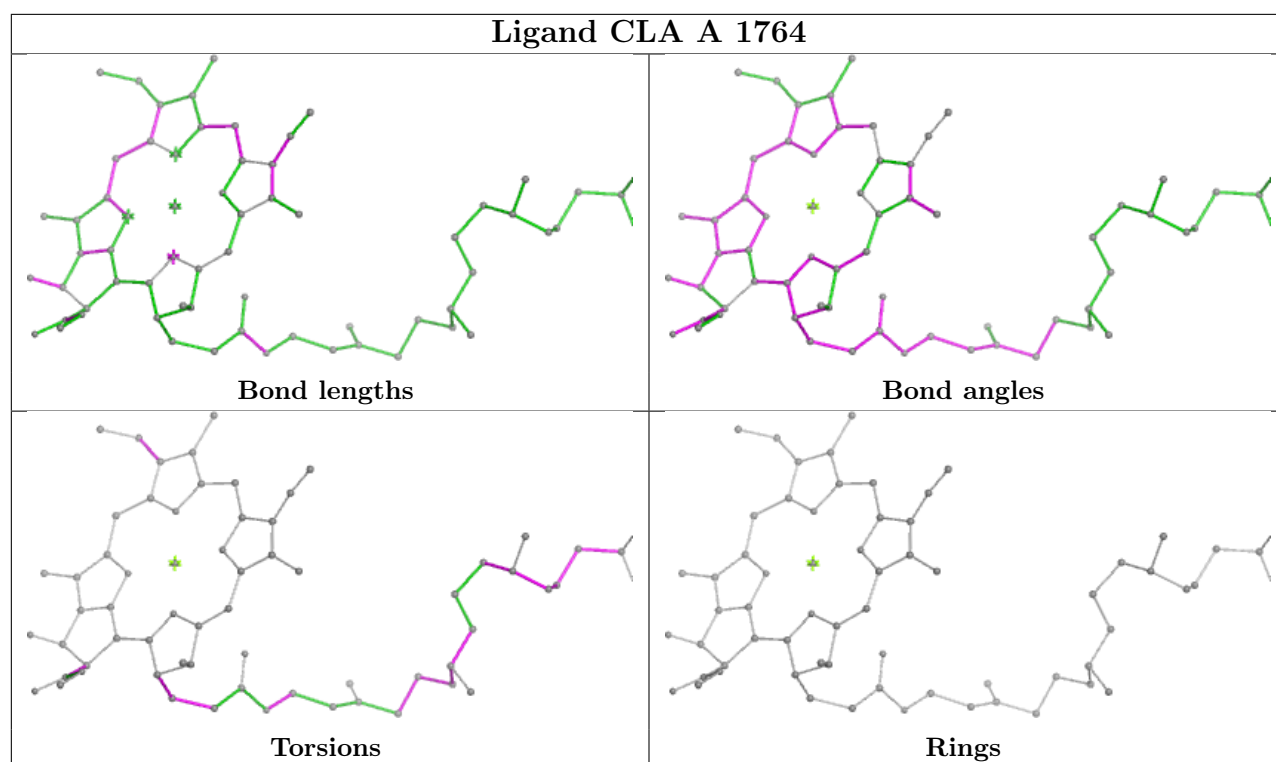
Torsions

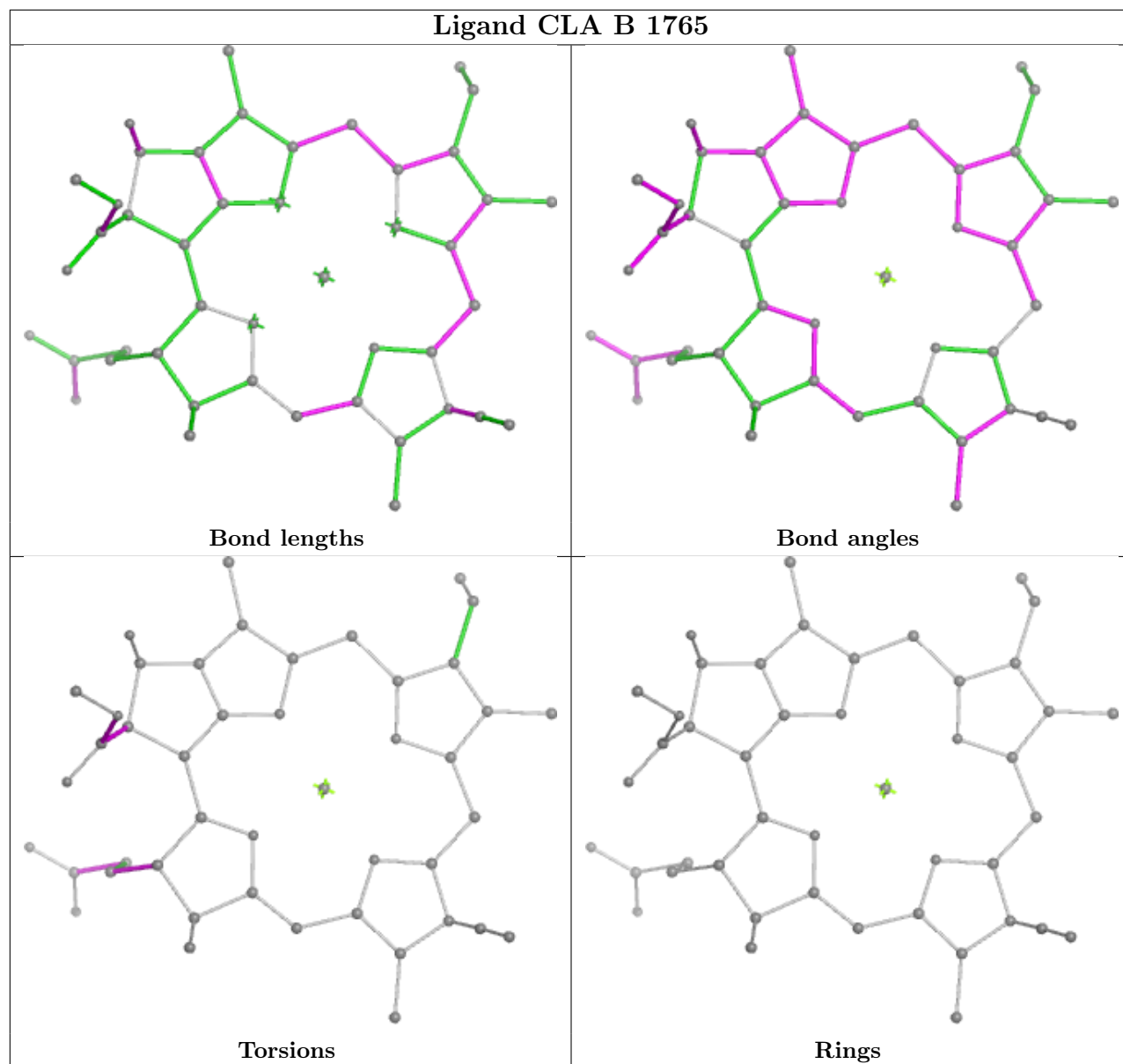


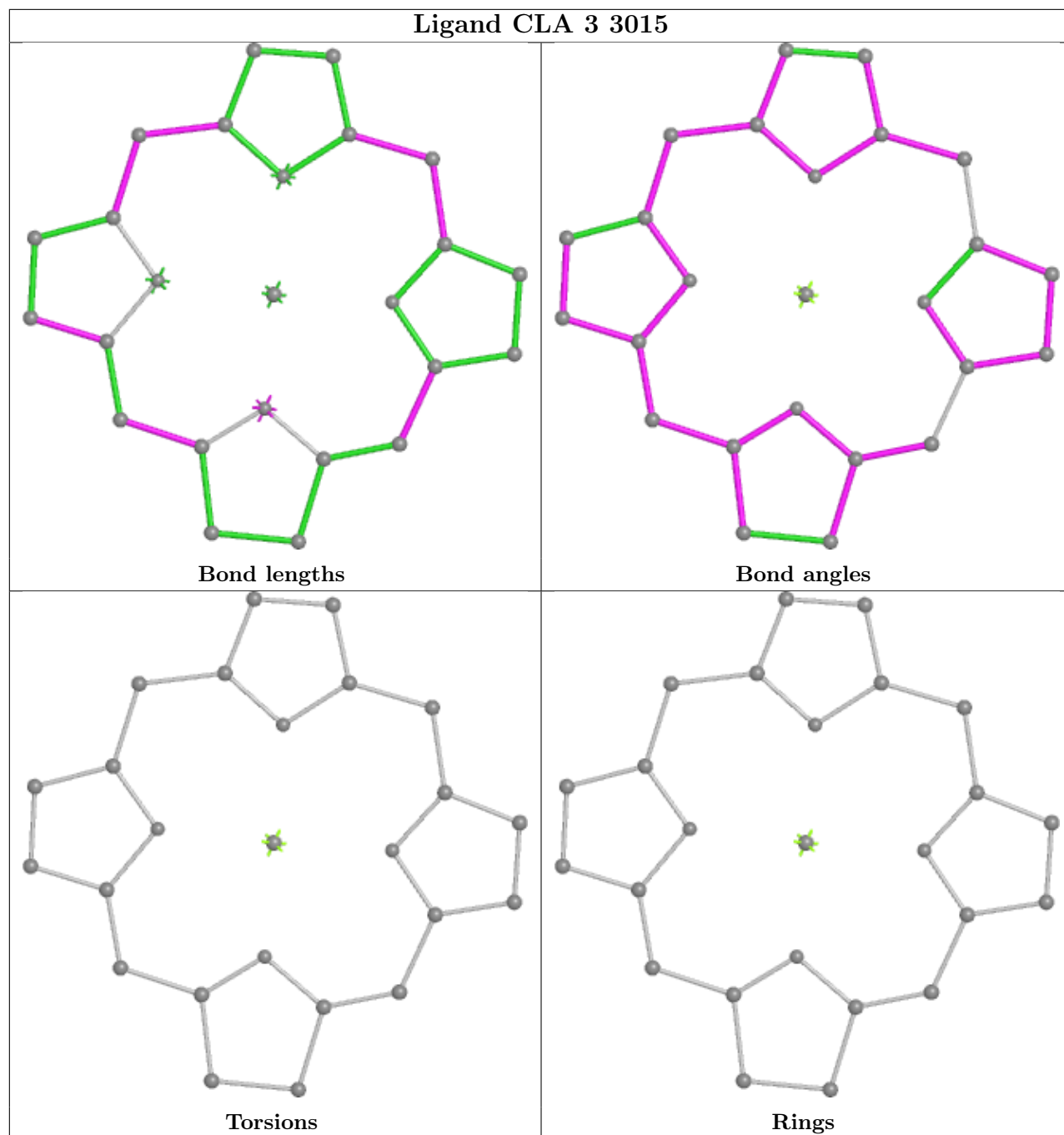
Rings

Ligand CLA B 1740**Ligand CLA K 1085**

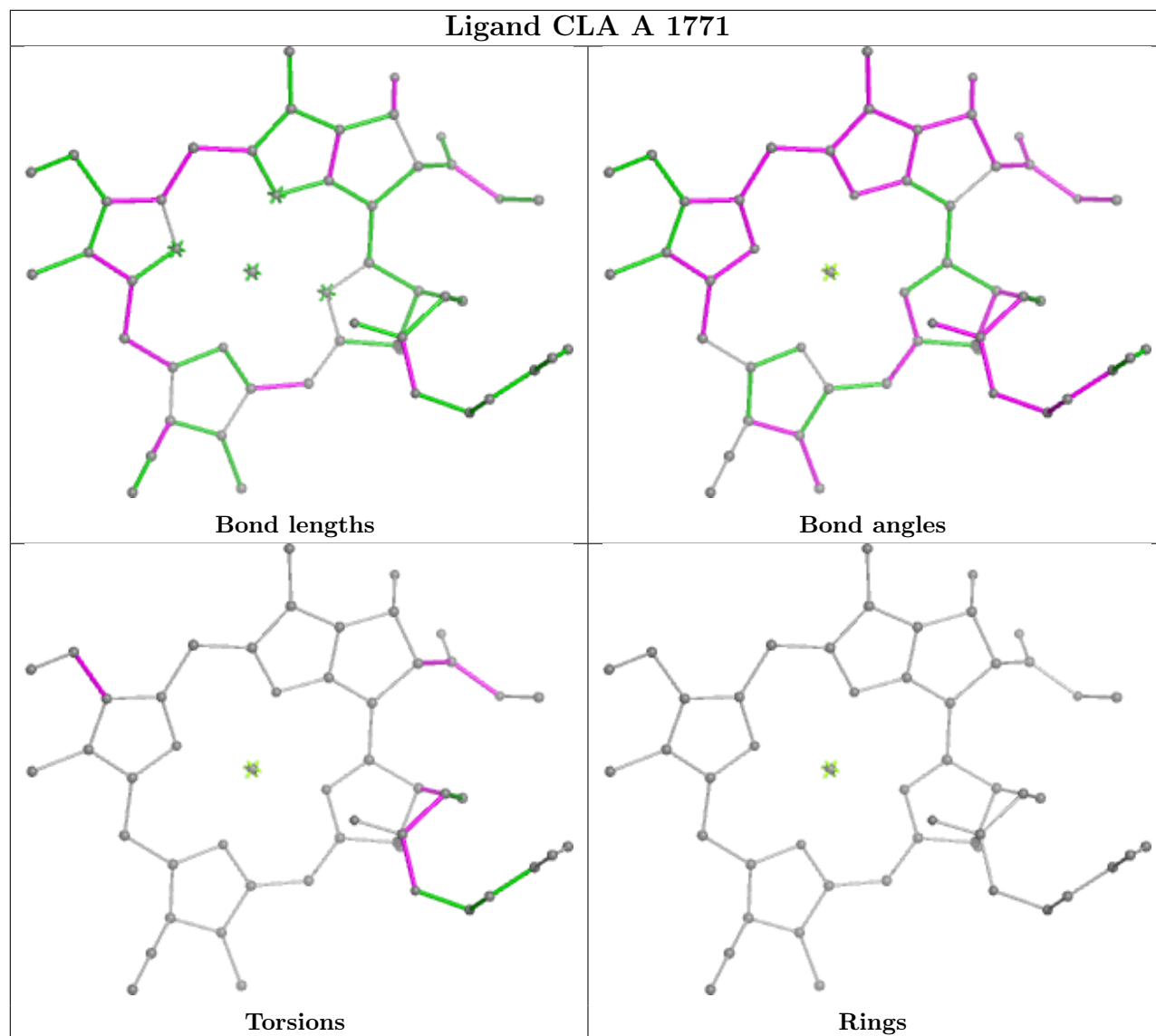




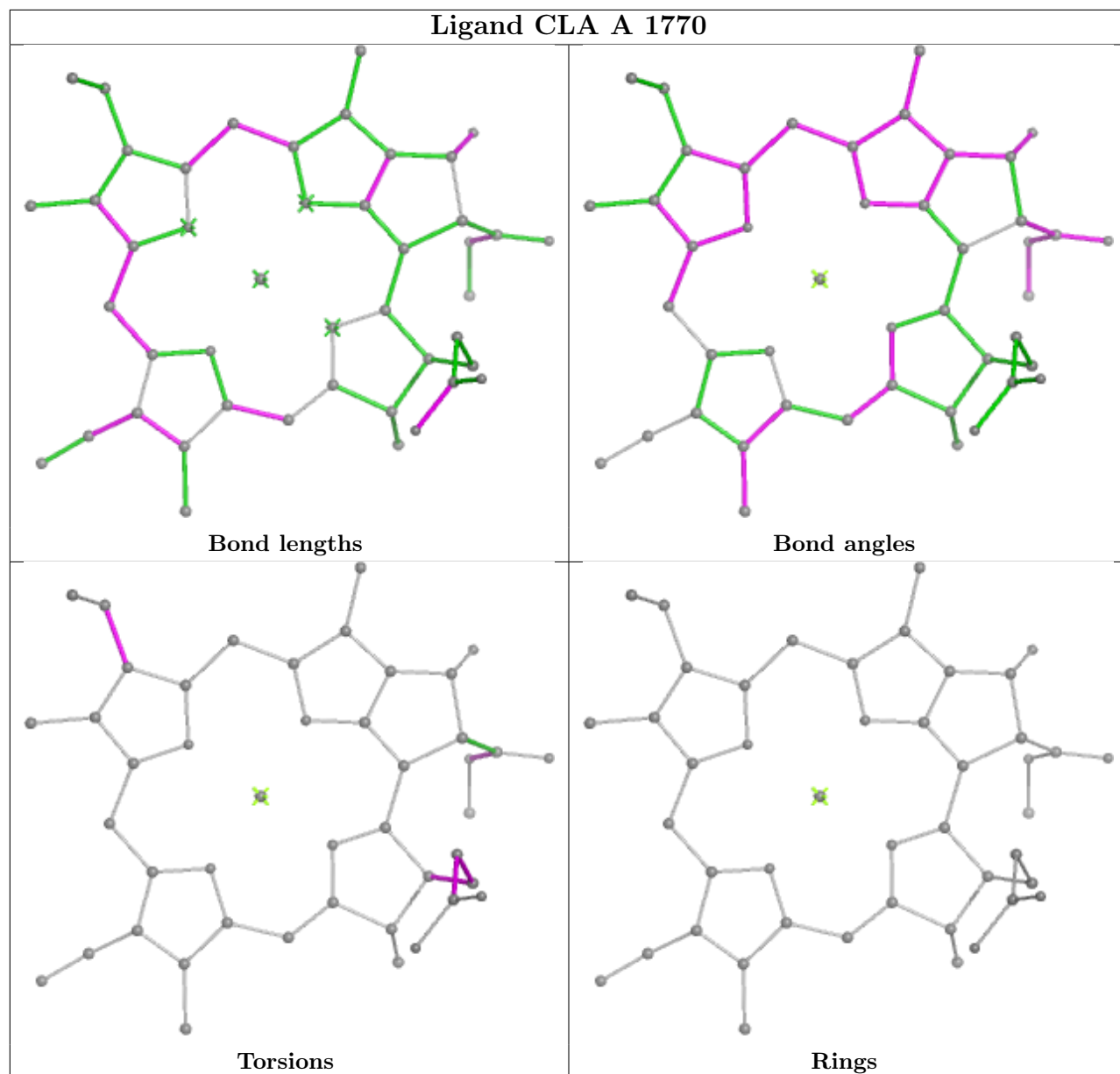


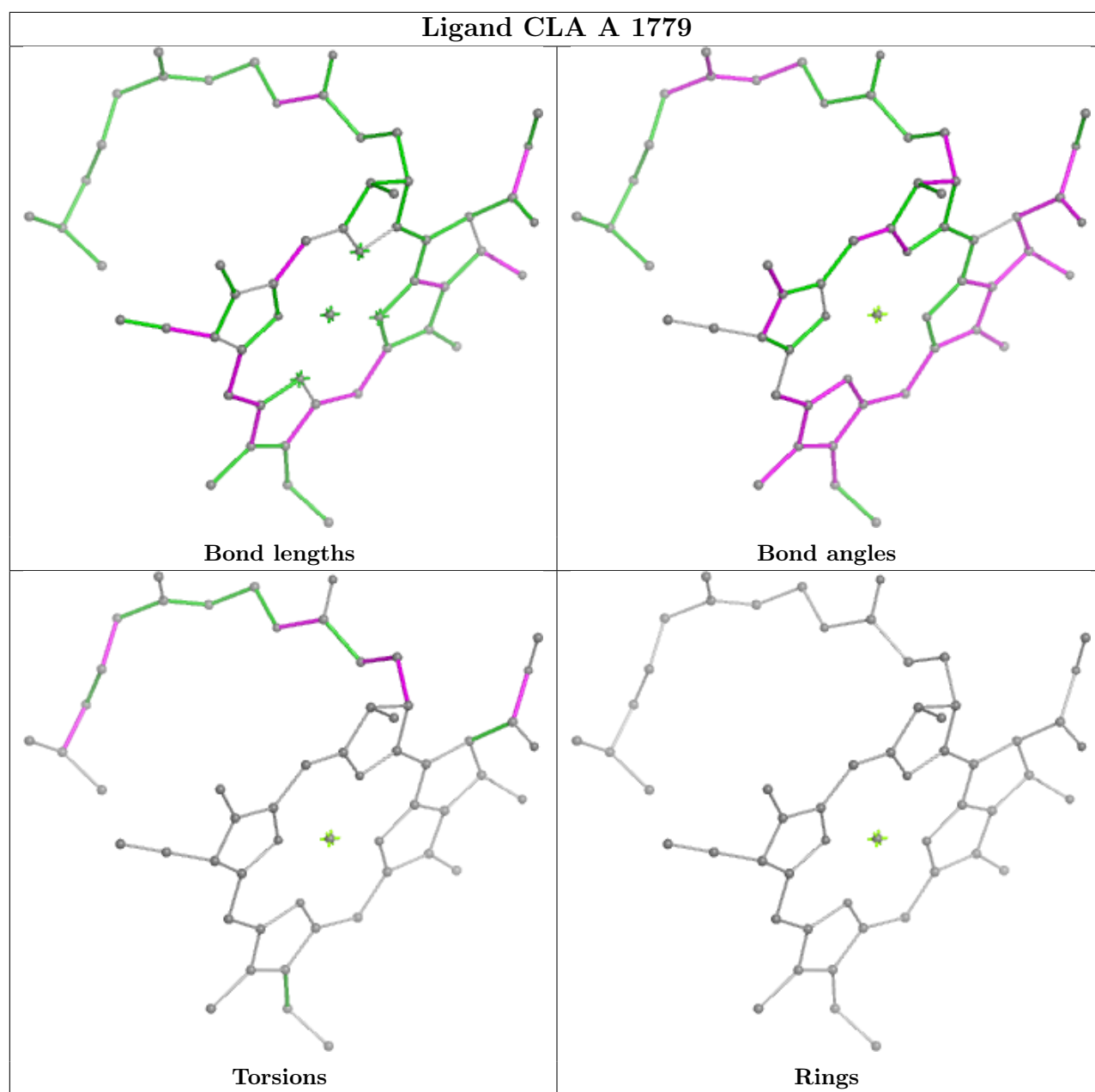


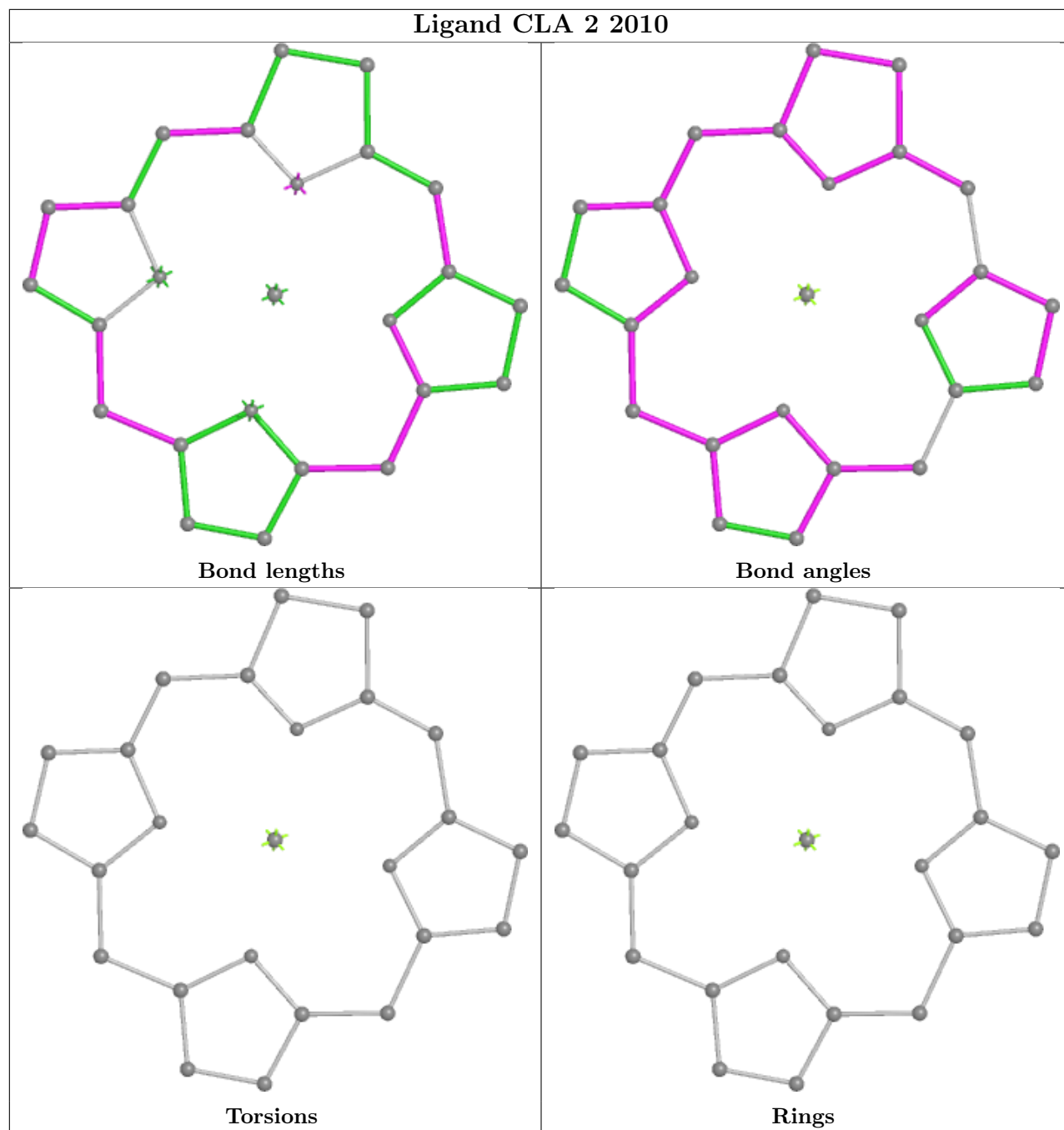
Ligand CLA A 1771



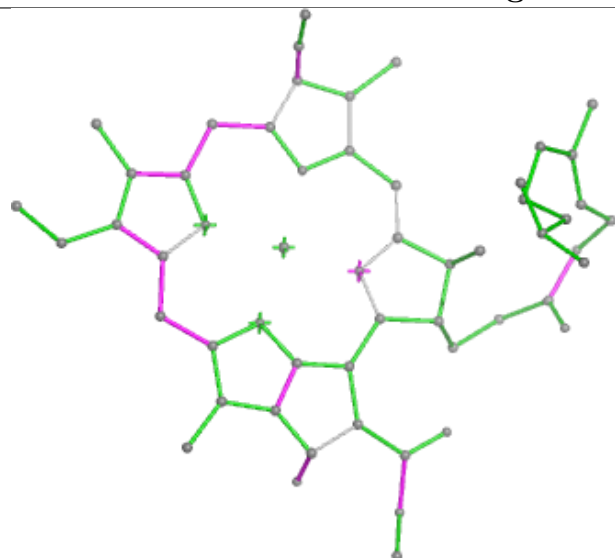
Ligand CLA A 1770



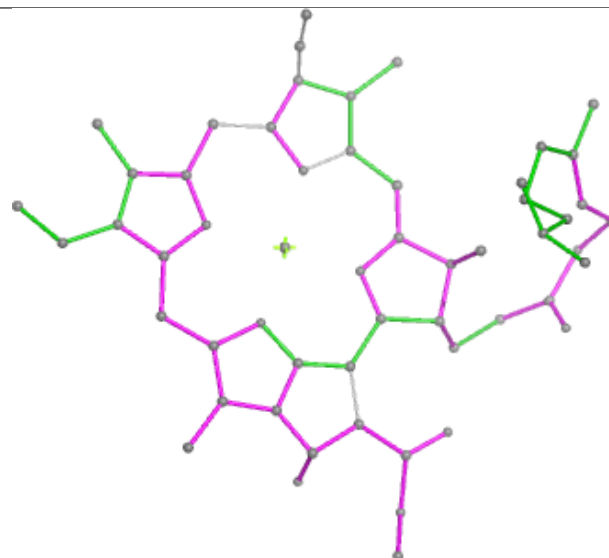




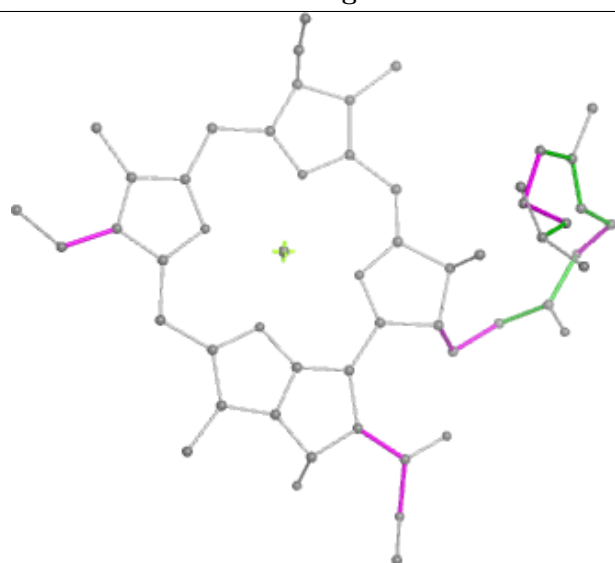
Ligand CLA A 1815



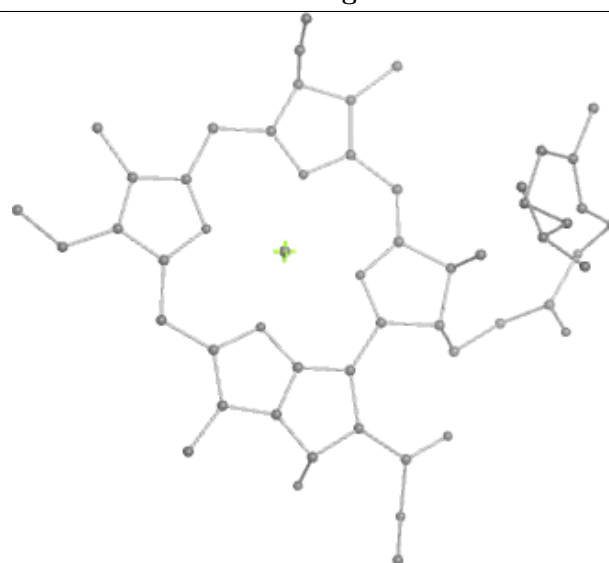
Bond lengths



Bond angles

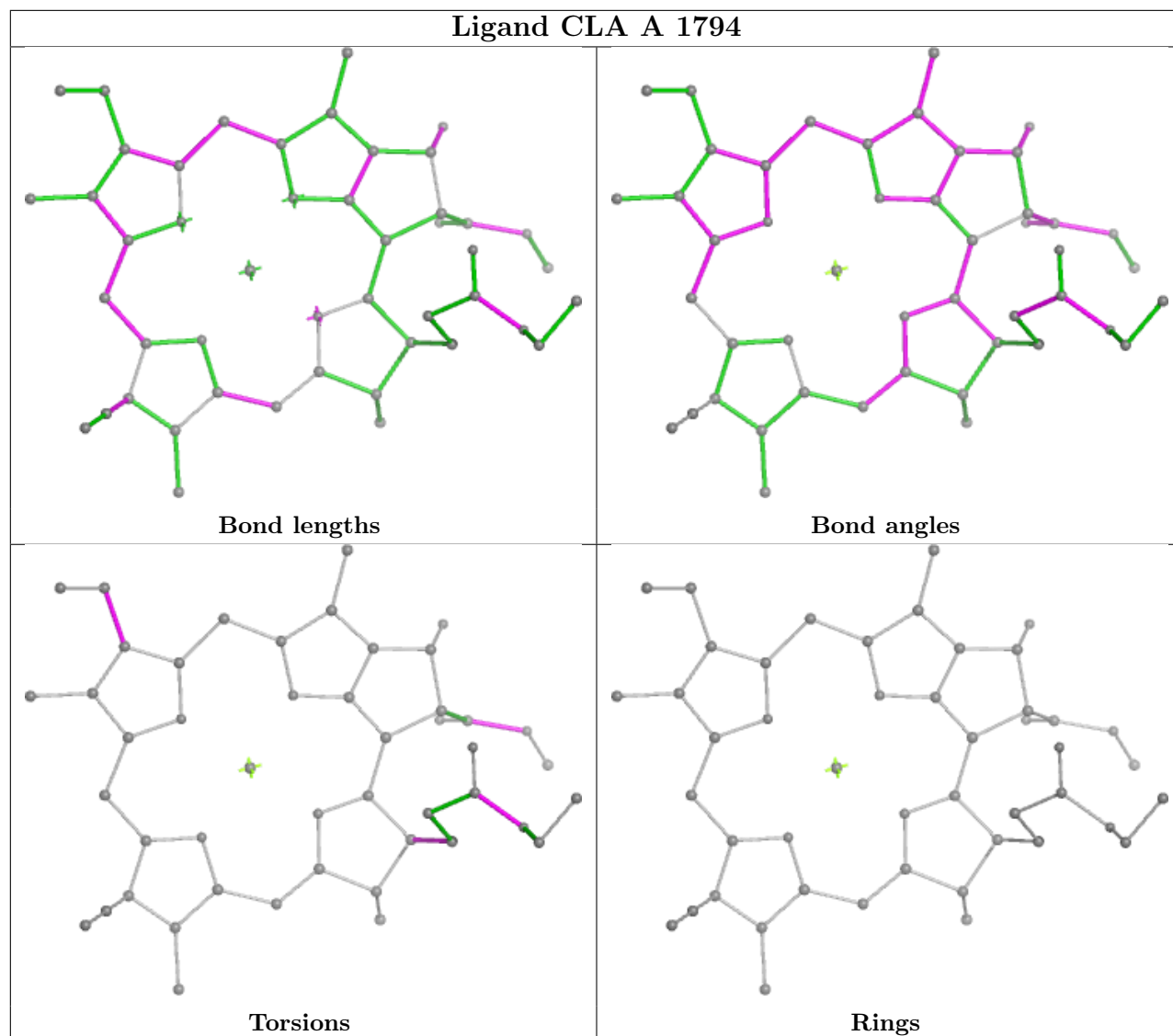


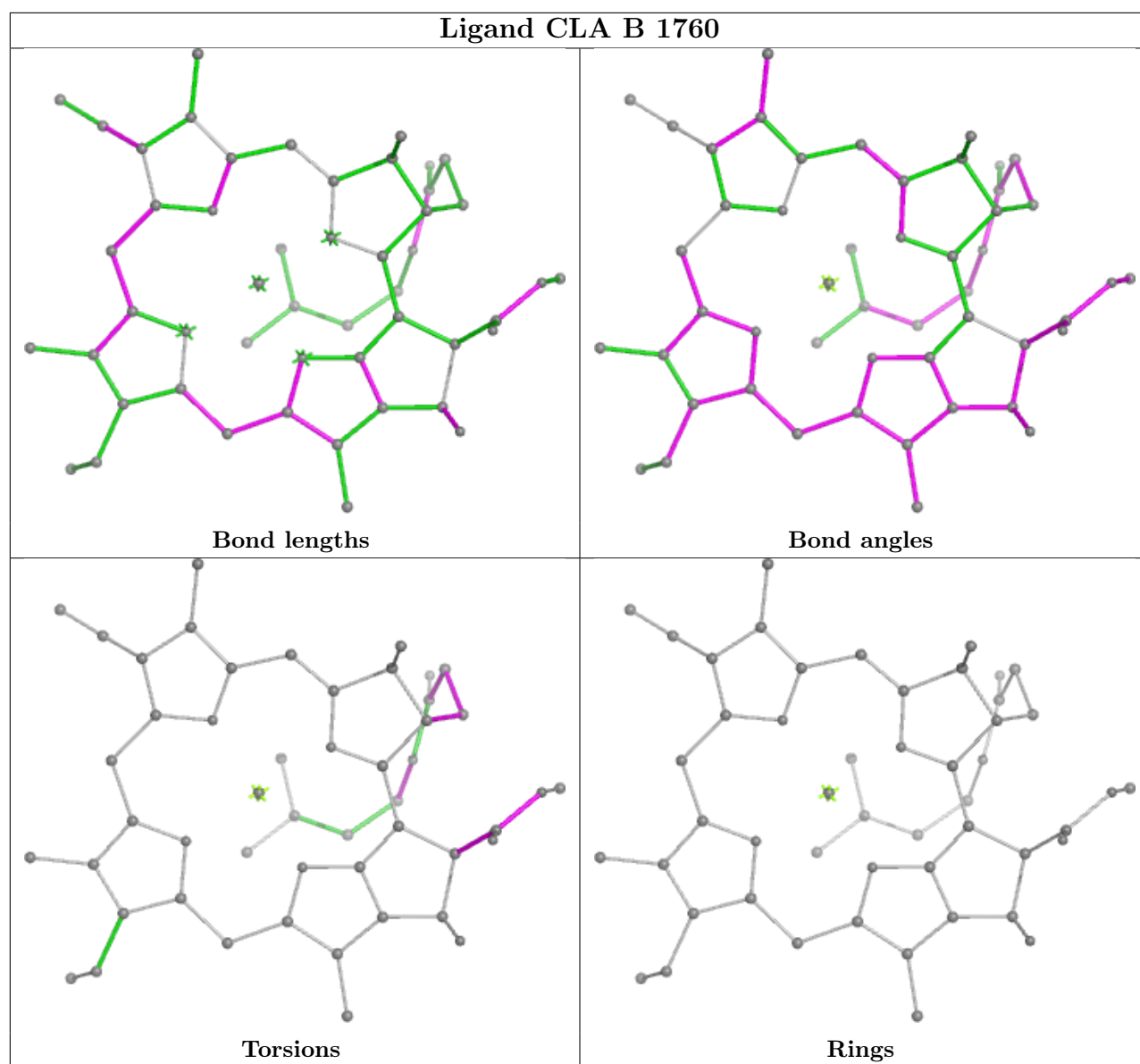
Torsions

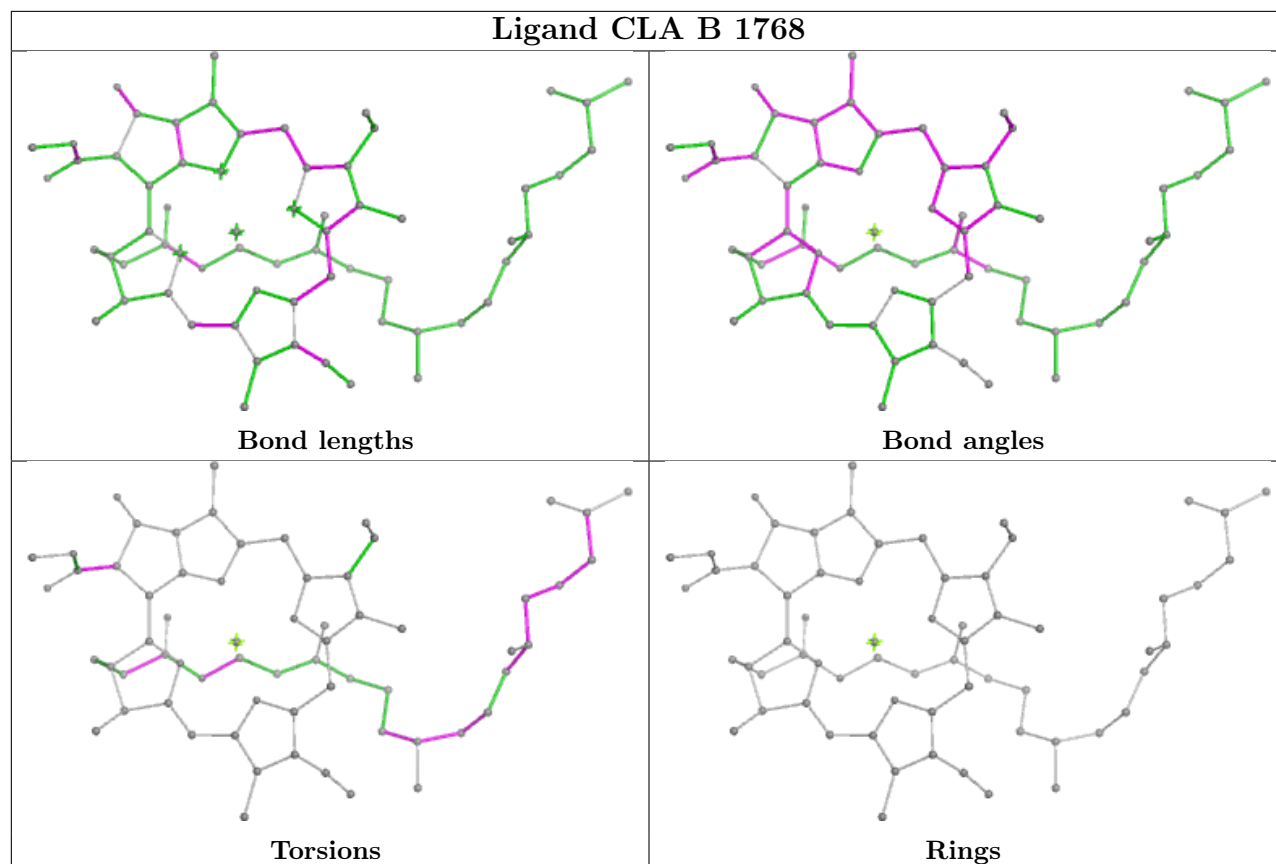
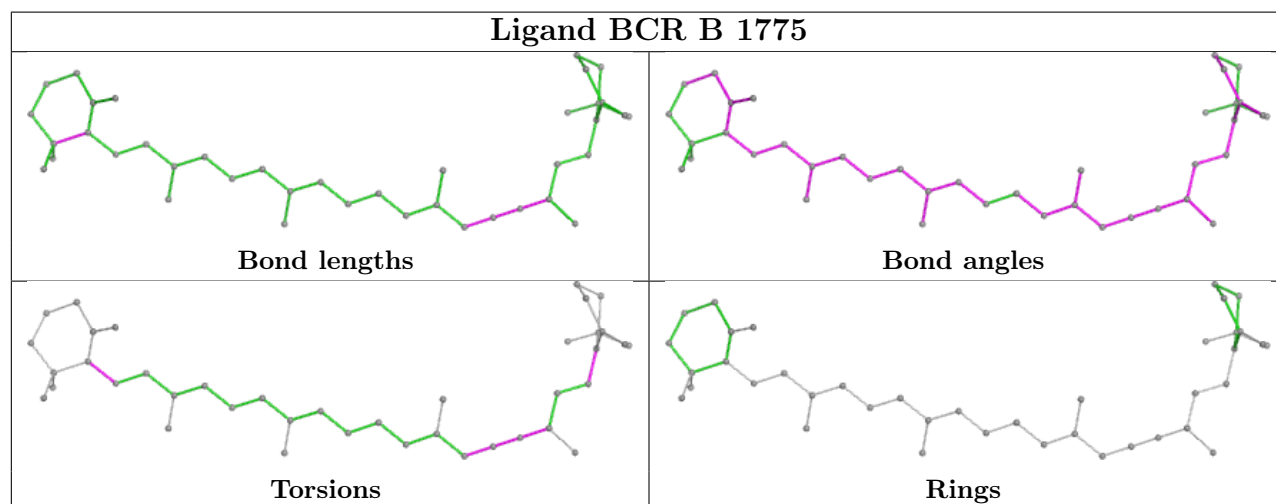


Rings

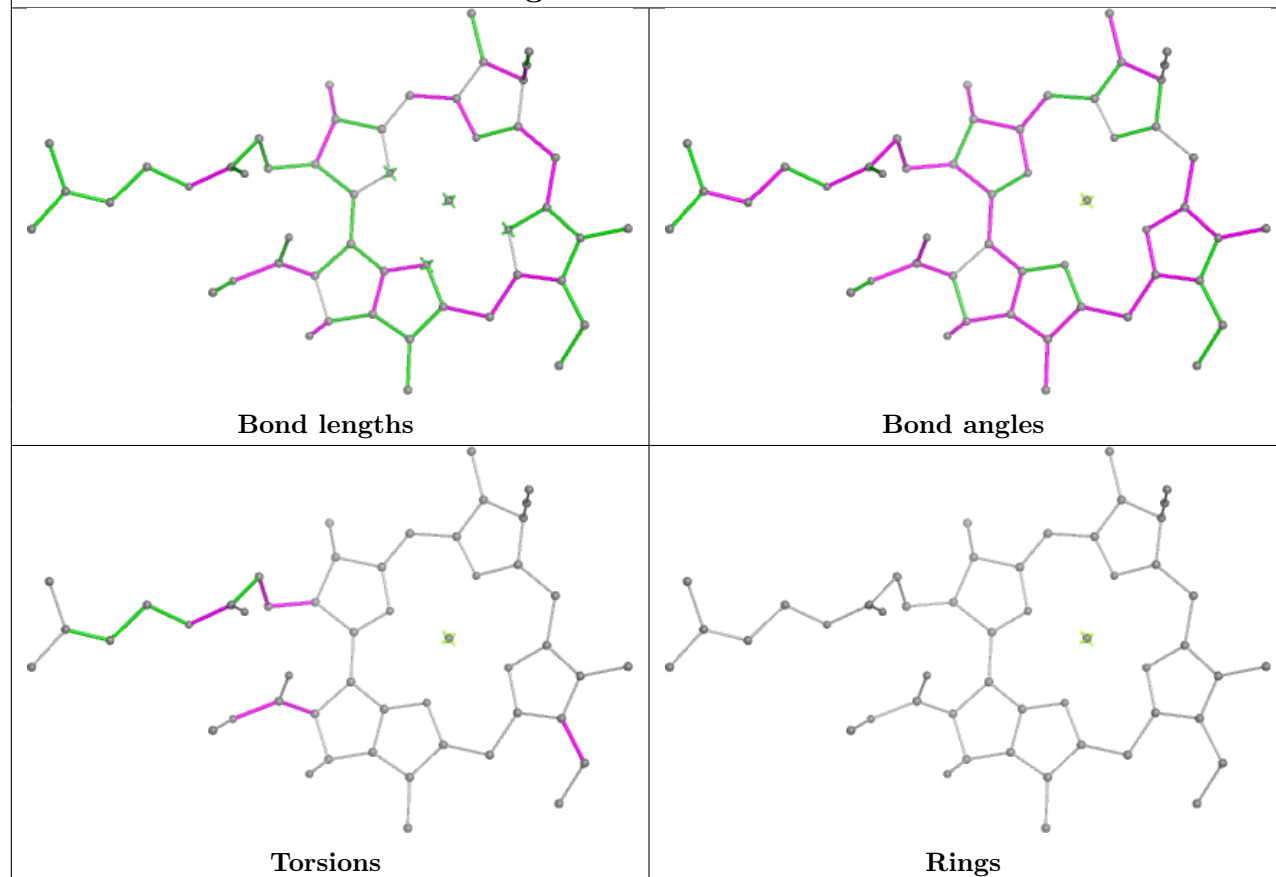
Ligand CLA A 1794



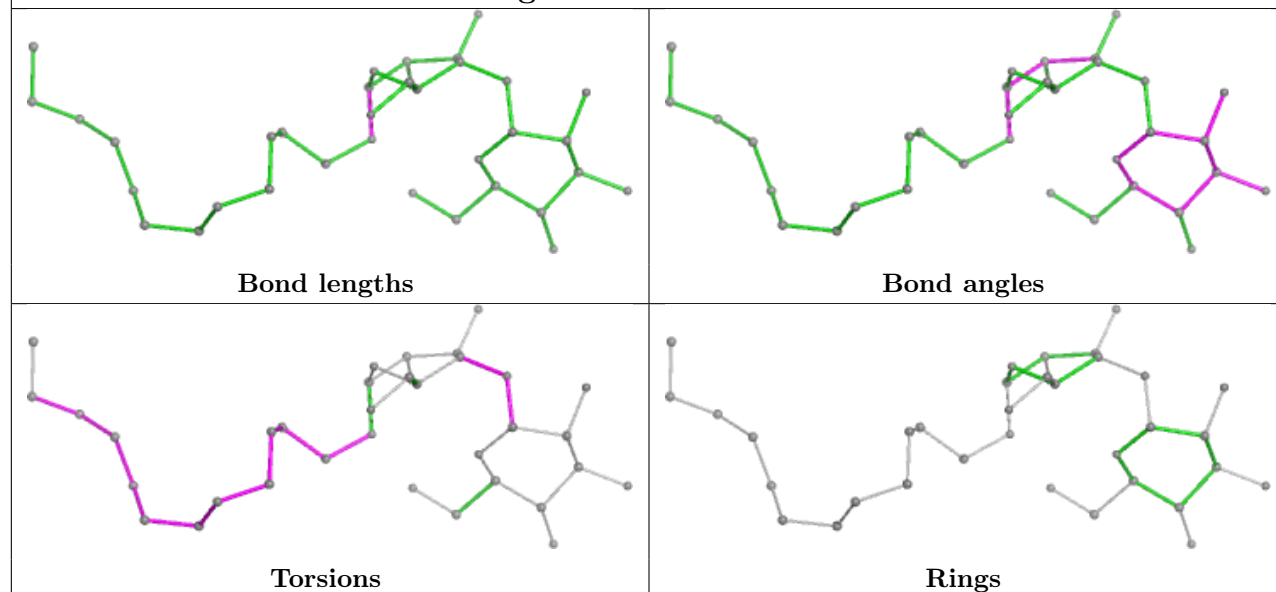


Ligand CLA B 1768**Ligand BCR B 1775**

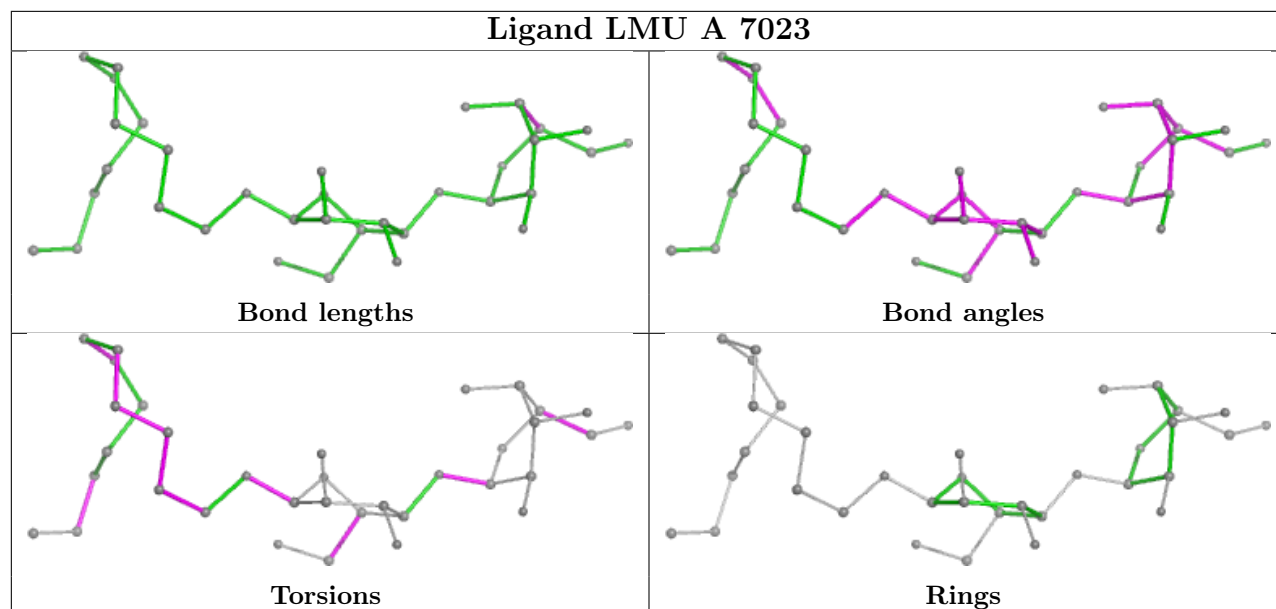
Ligand CLA L 1168



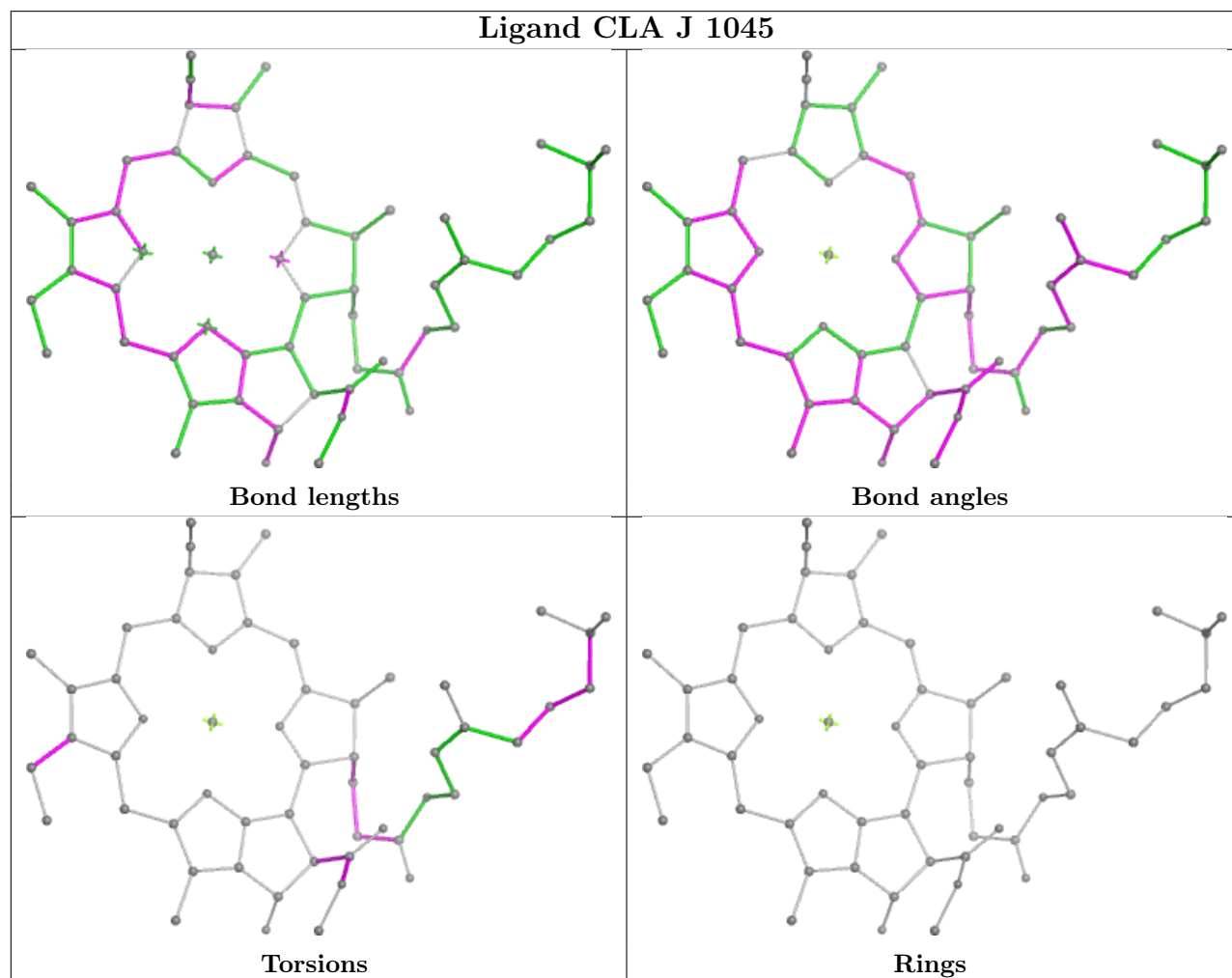
Ligand LMU A 1810



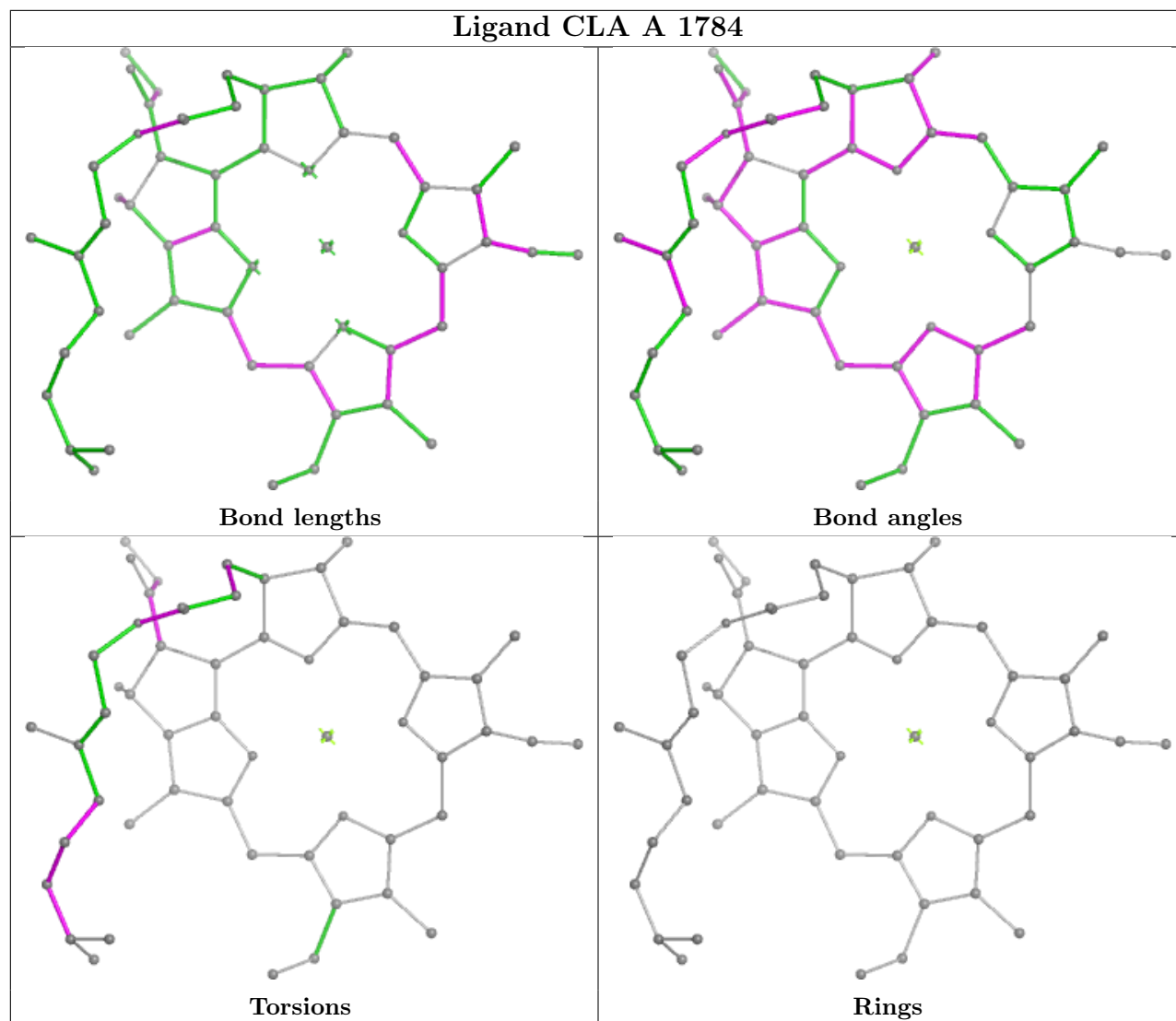
Ligand LMU A 7023



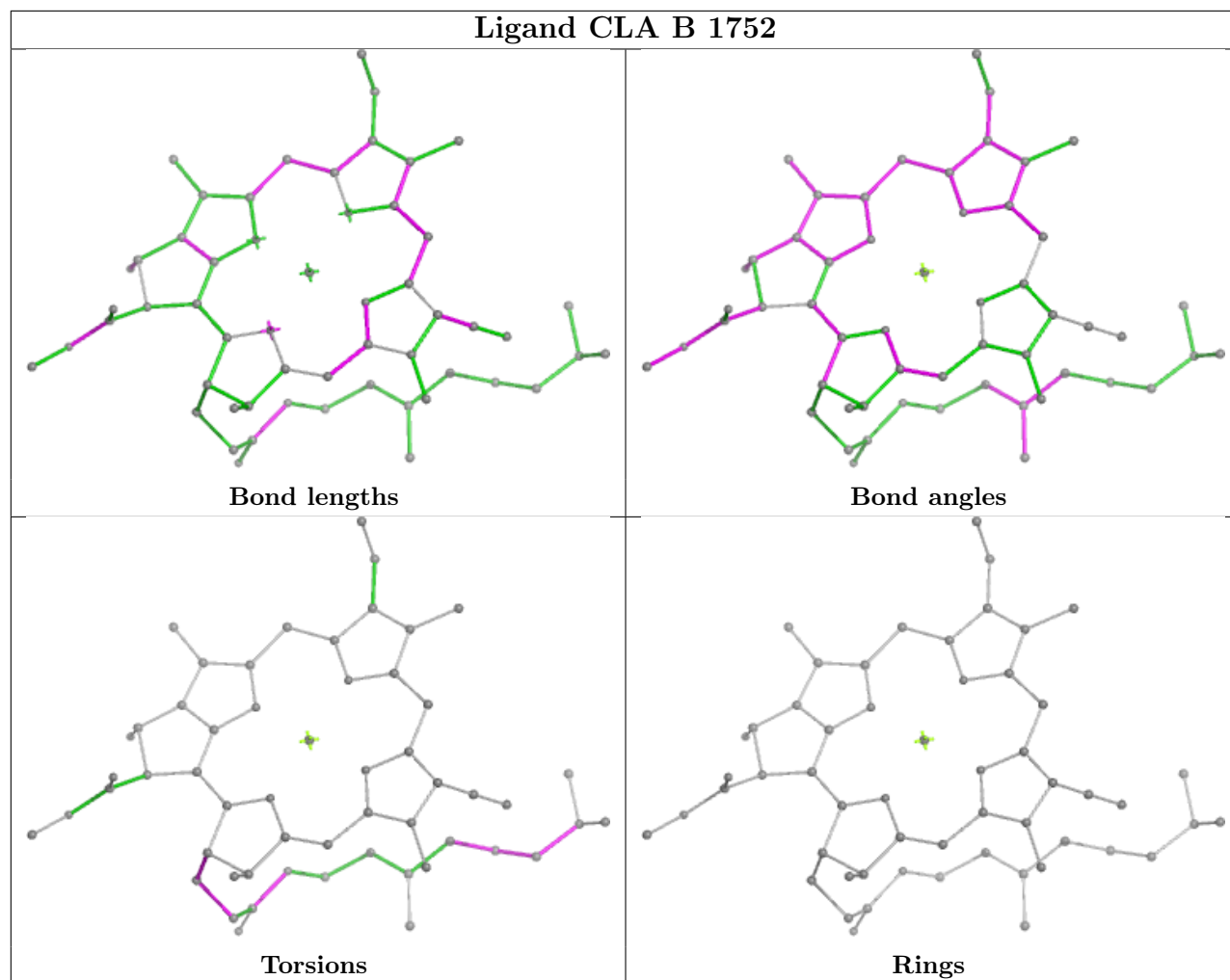
Ligand CLA J 1045



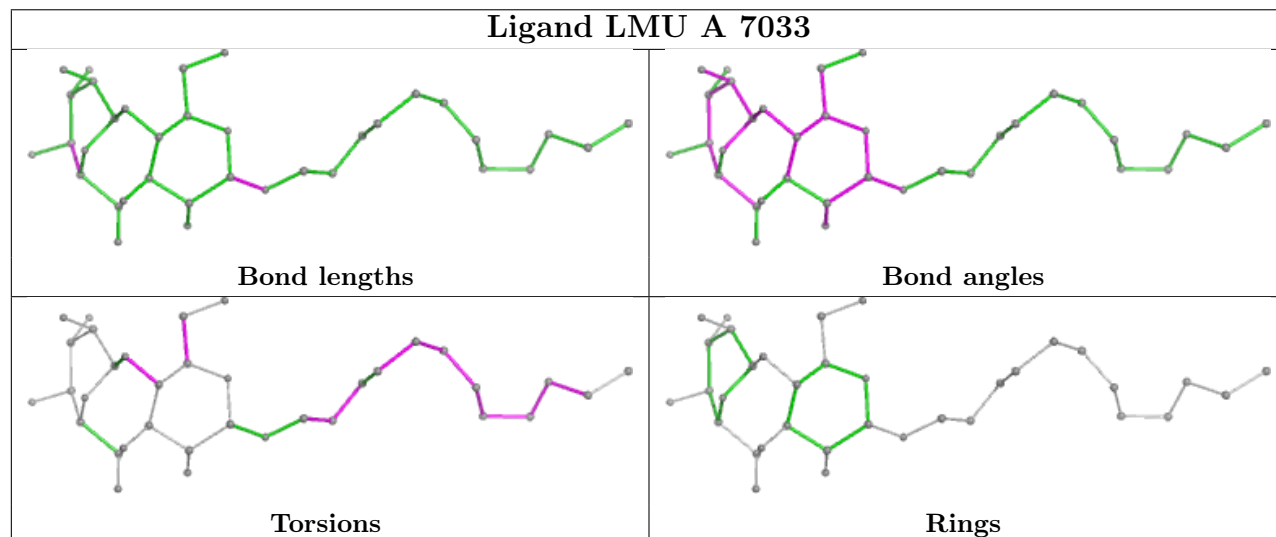
Ligand CLA A 1784



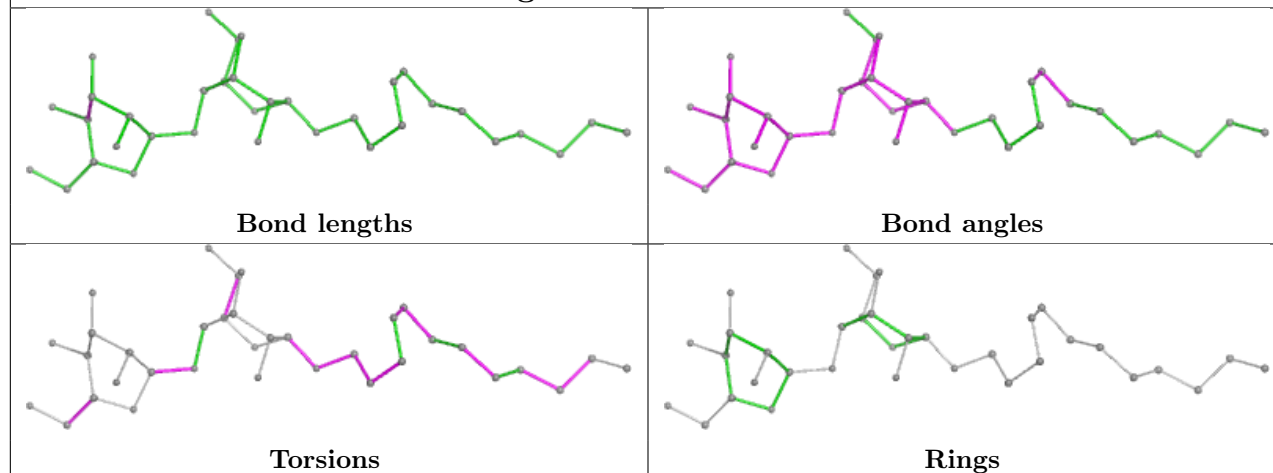
Ligand CLA B 1752



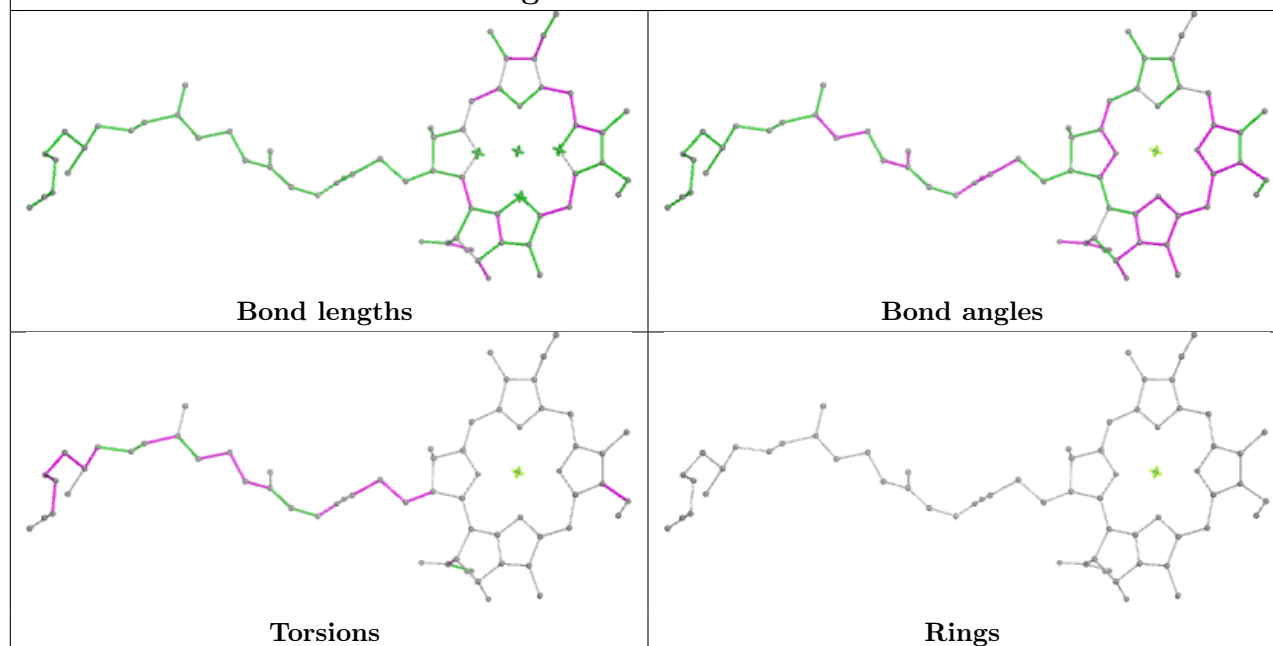
Ligand LMU A 7033



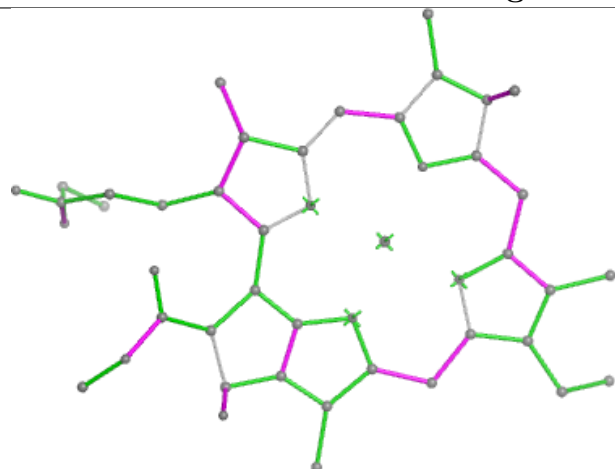
Ligand LMU A 7037



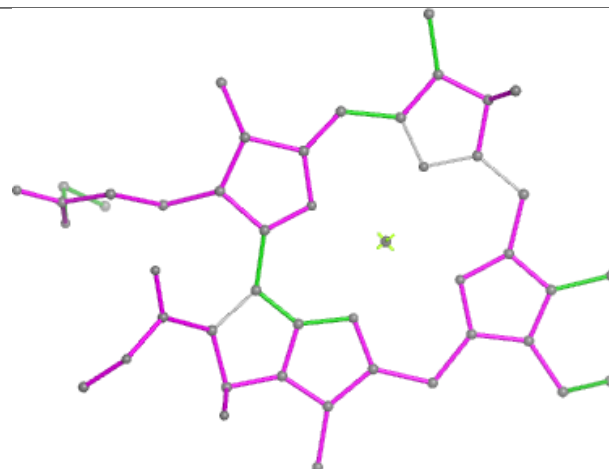
Ligand CLA A 1761



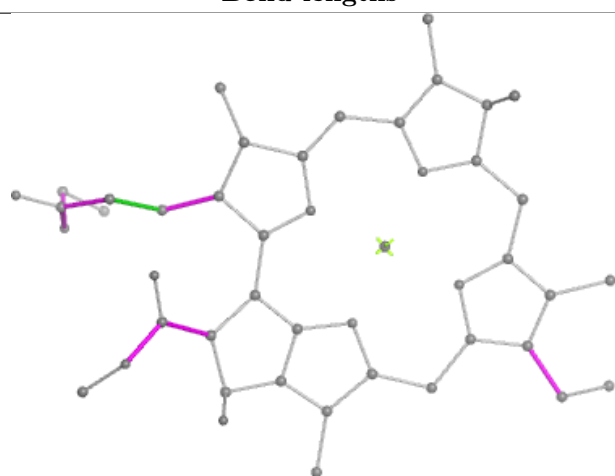
Ligand CLA A 1817



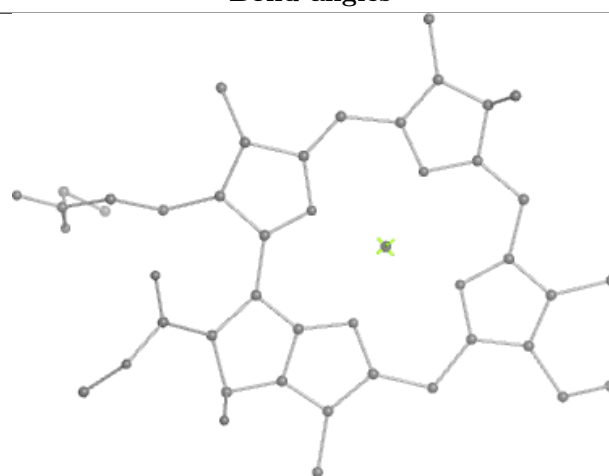
Bond lengths



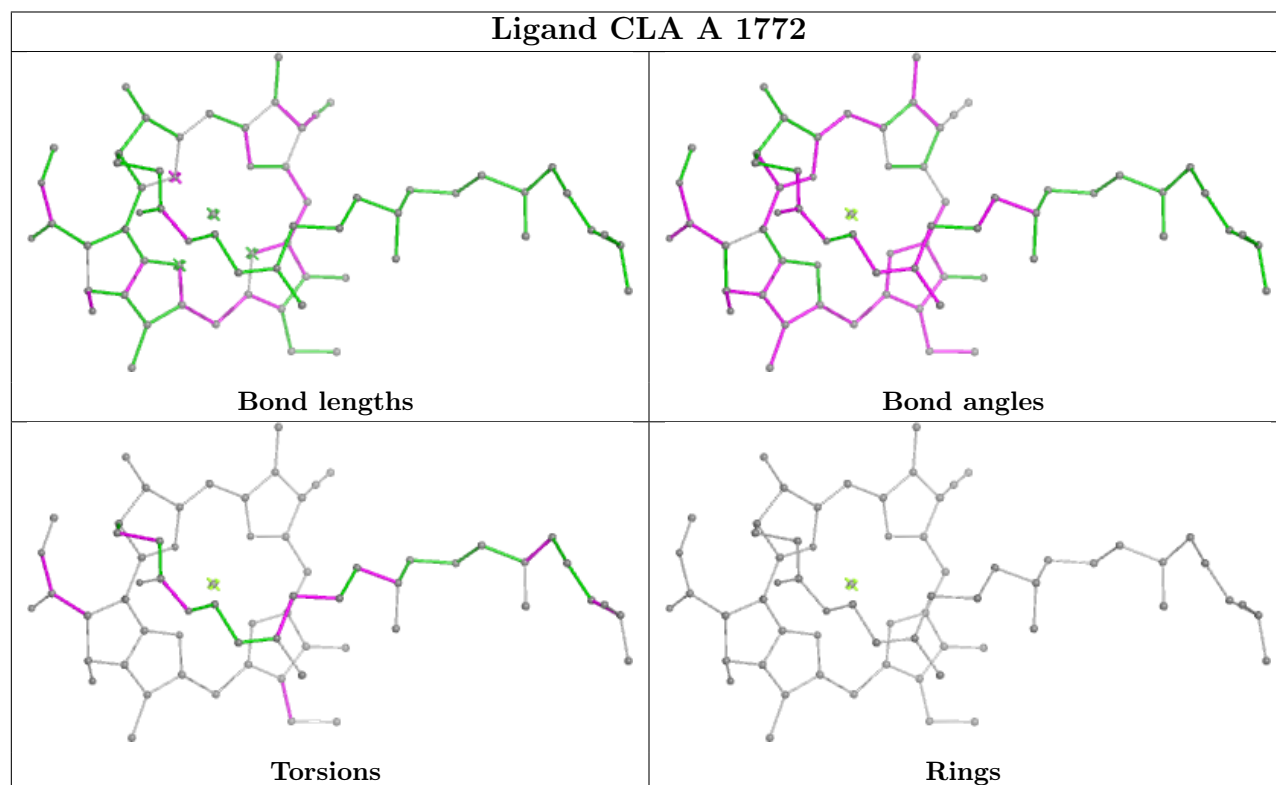
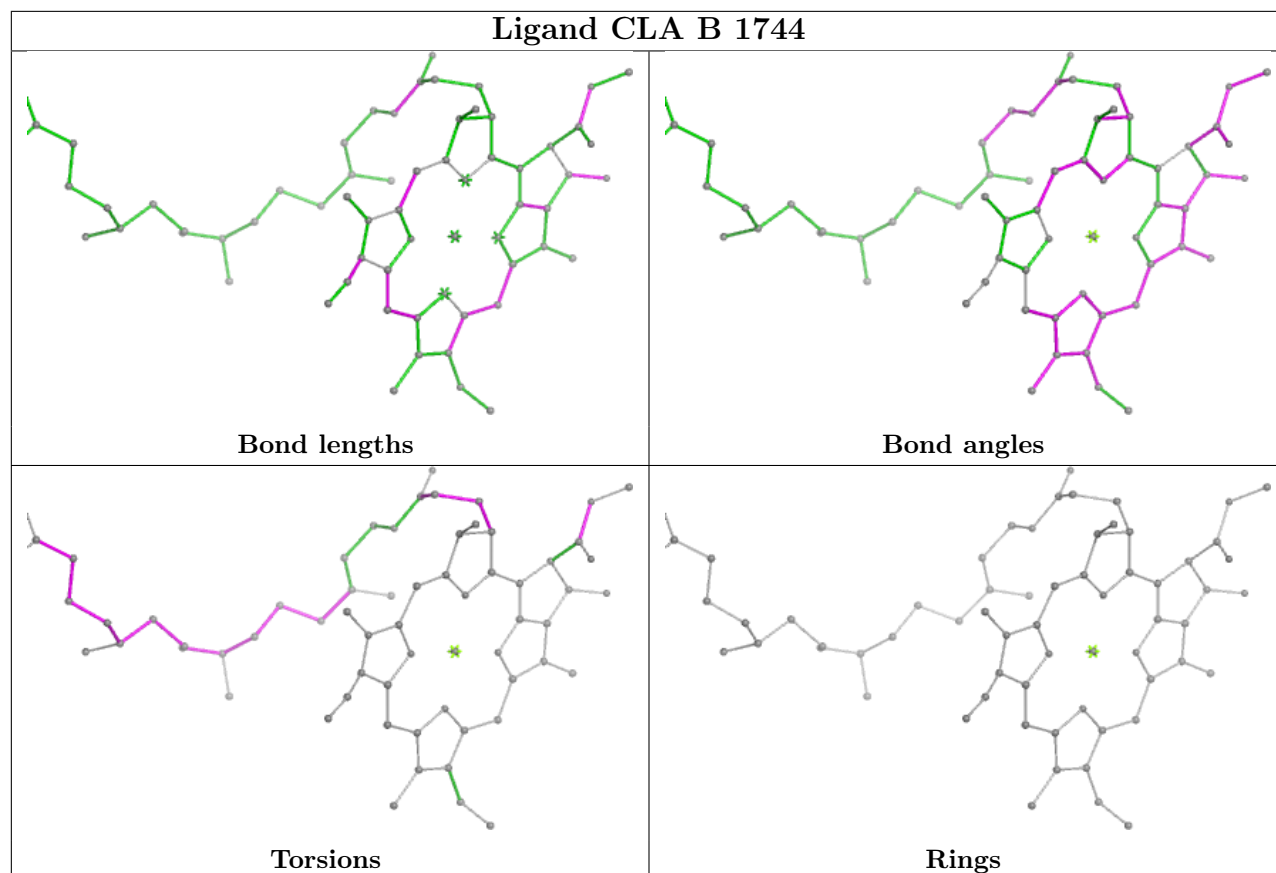
Bond angles

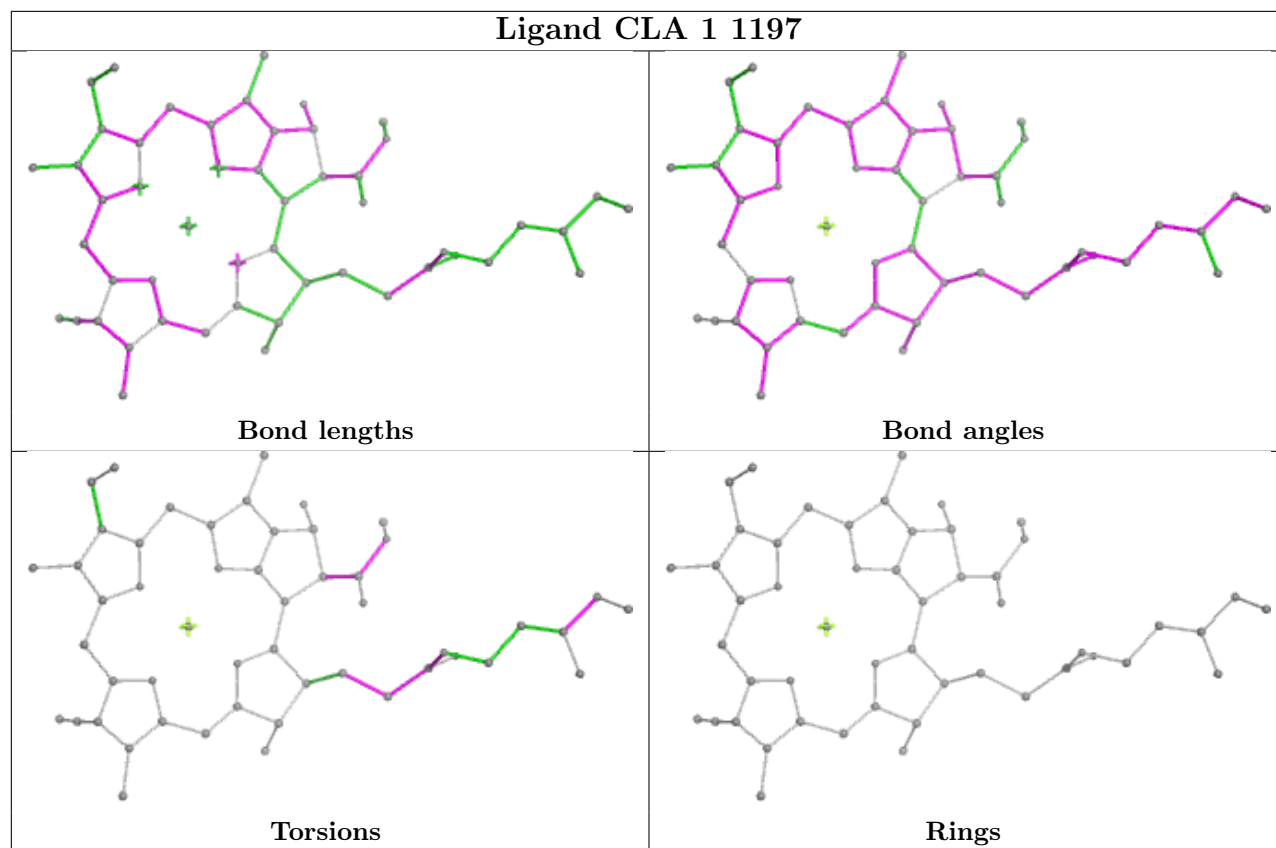


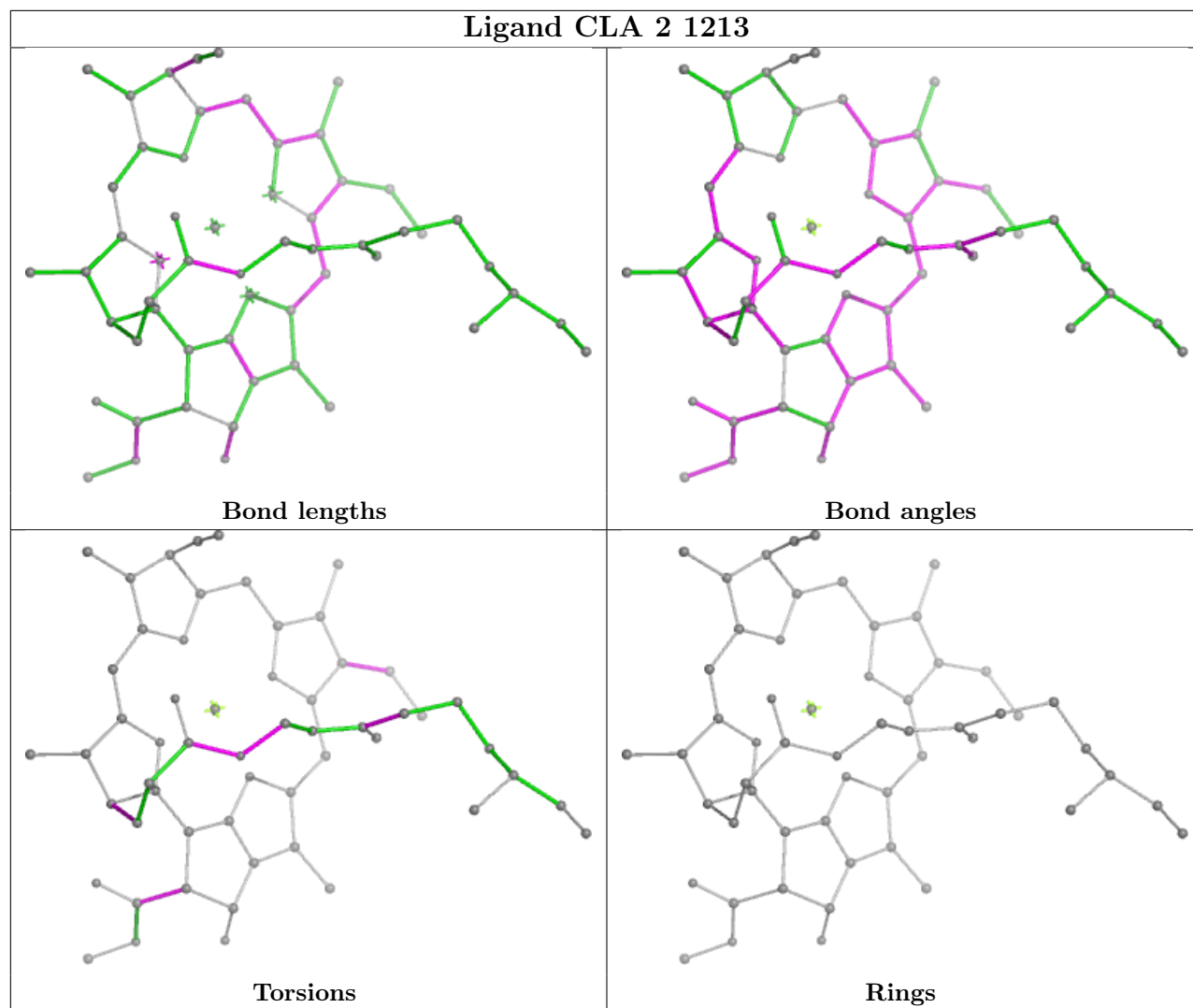
Torsions



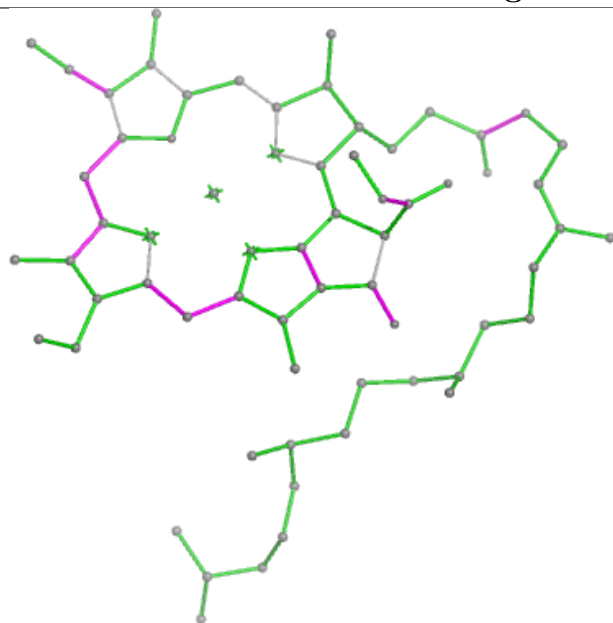
Rings



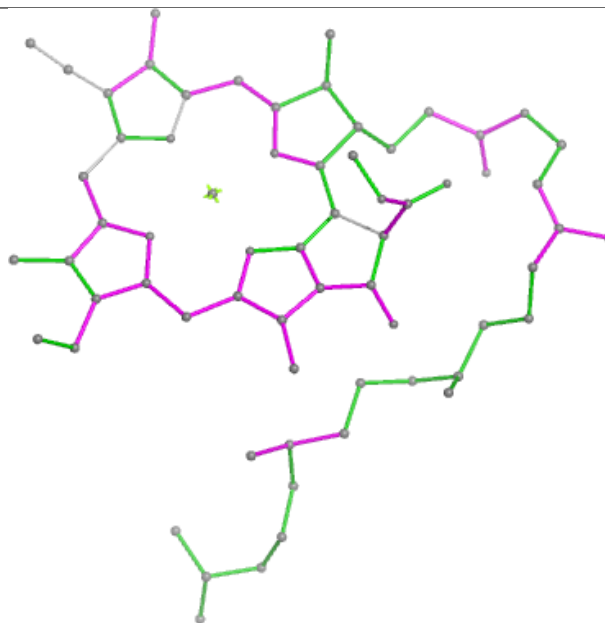




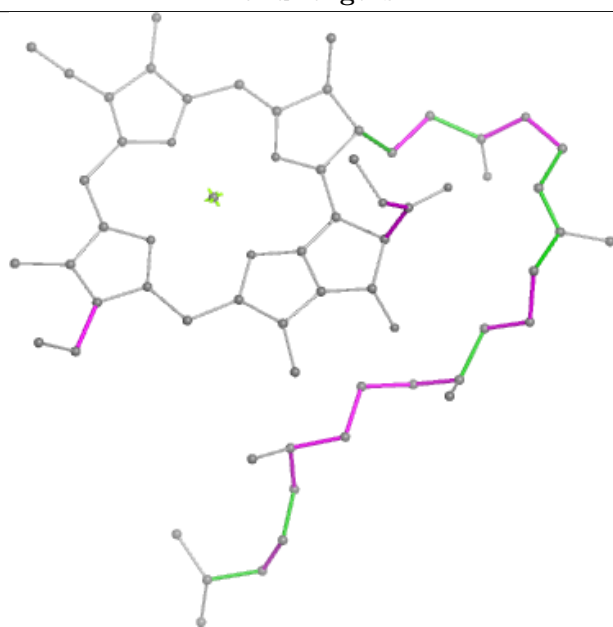
Ligand CLA A 1780



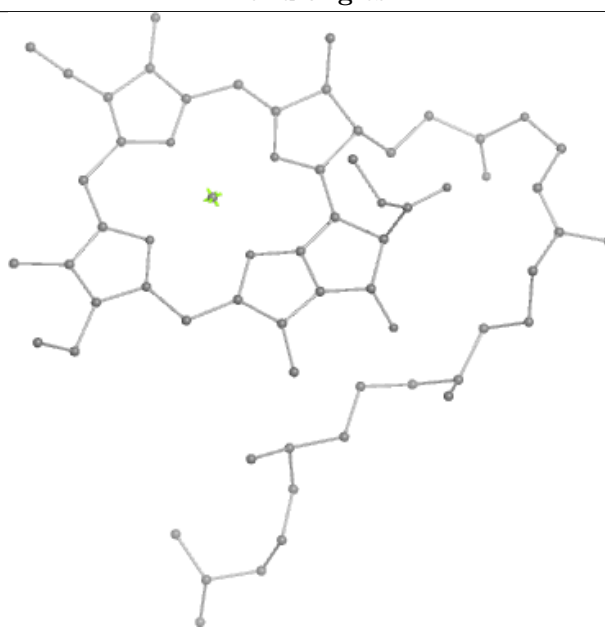
Bond lengths



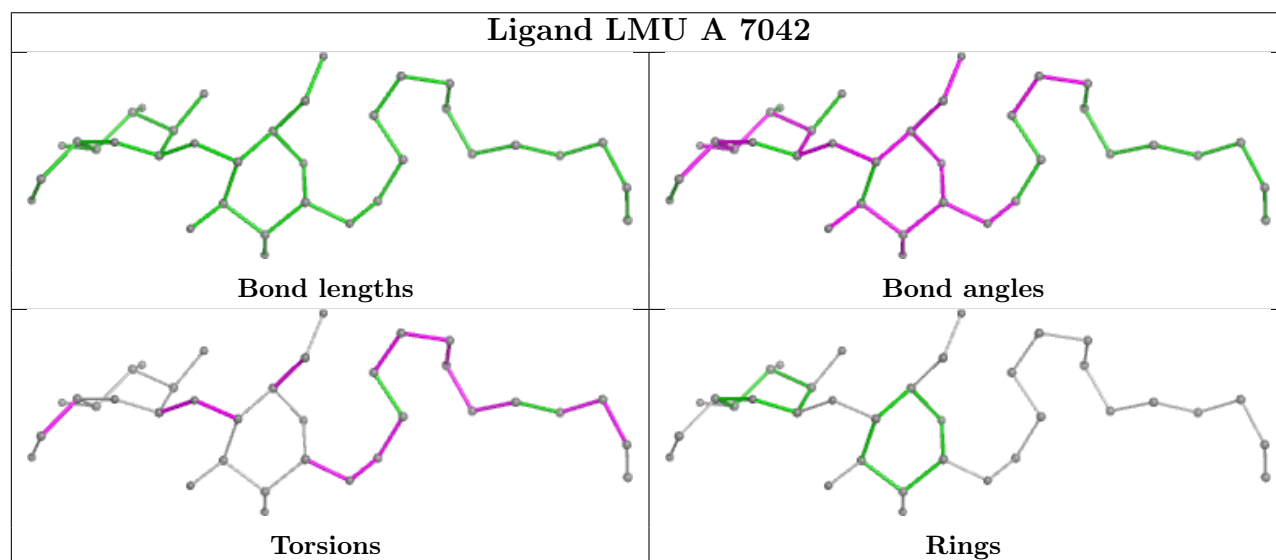
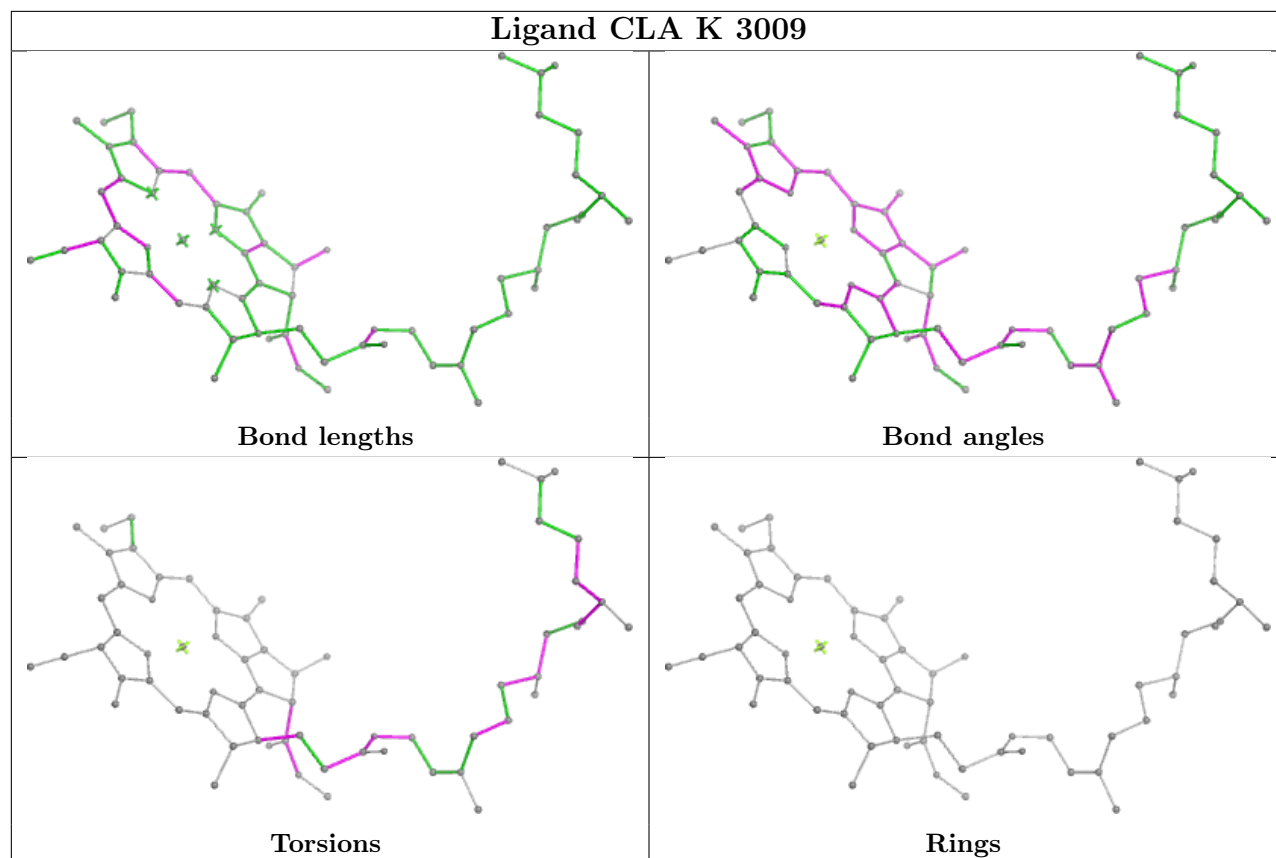
Bond angles

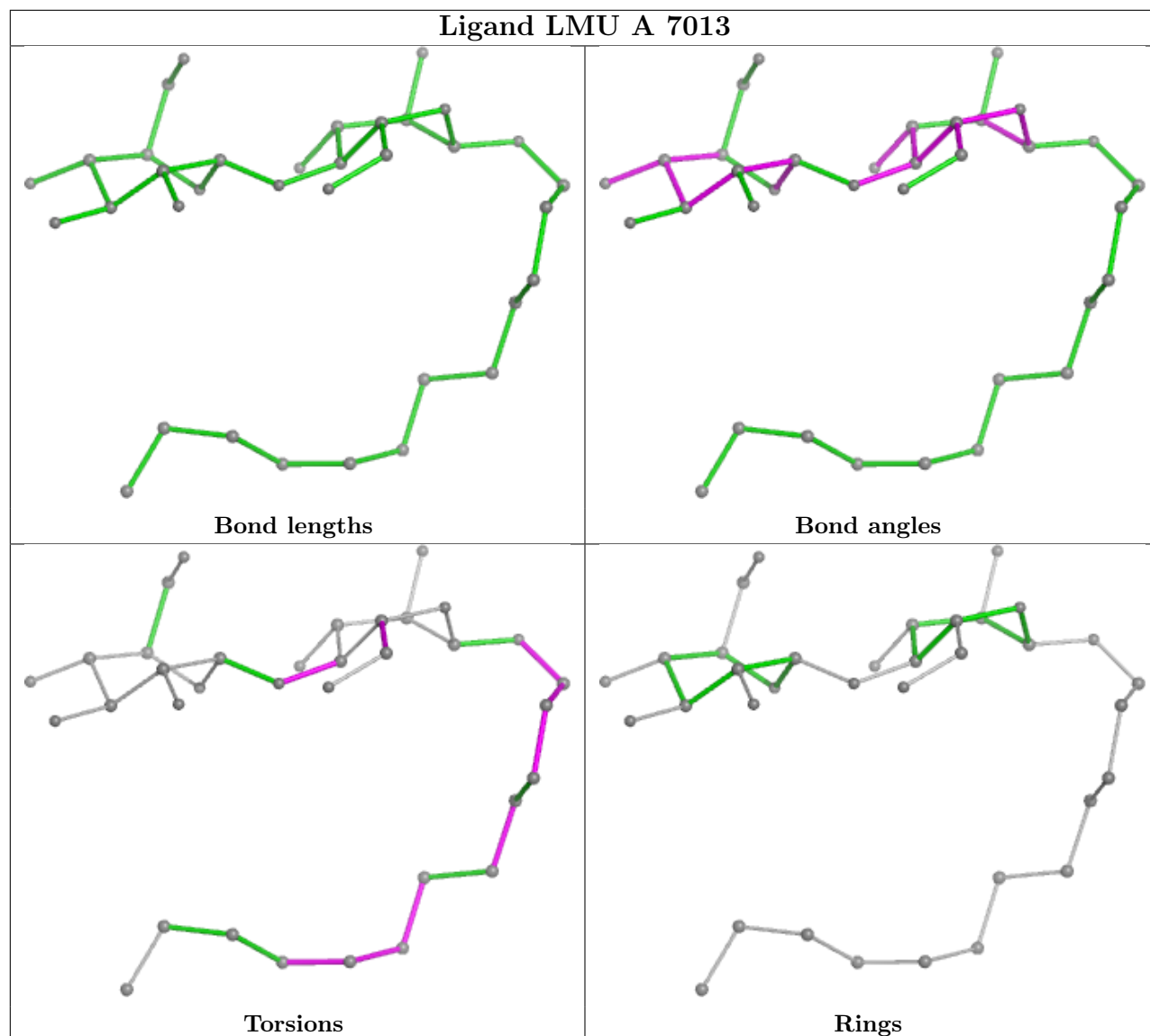


Torsions

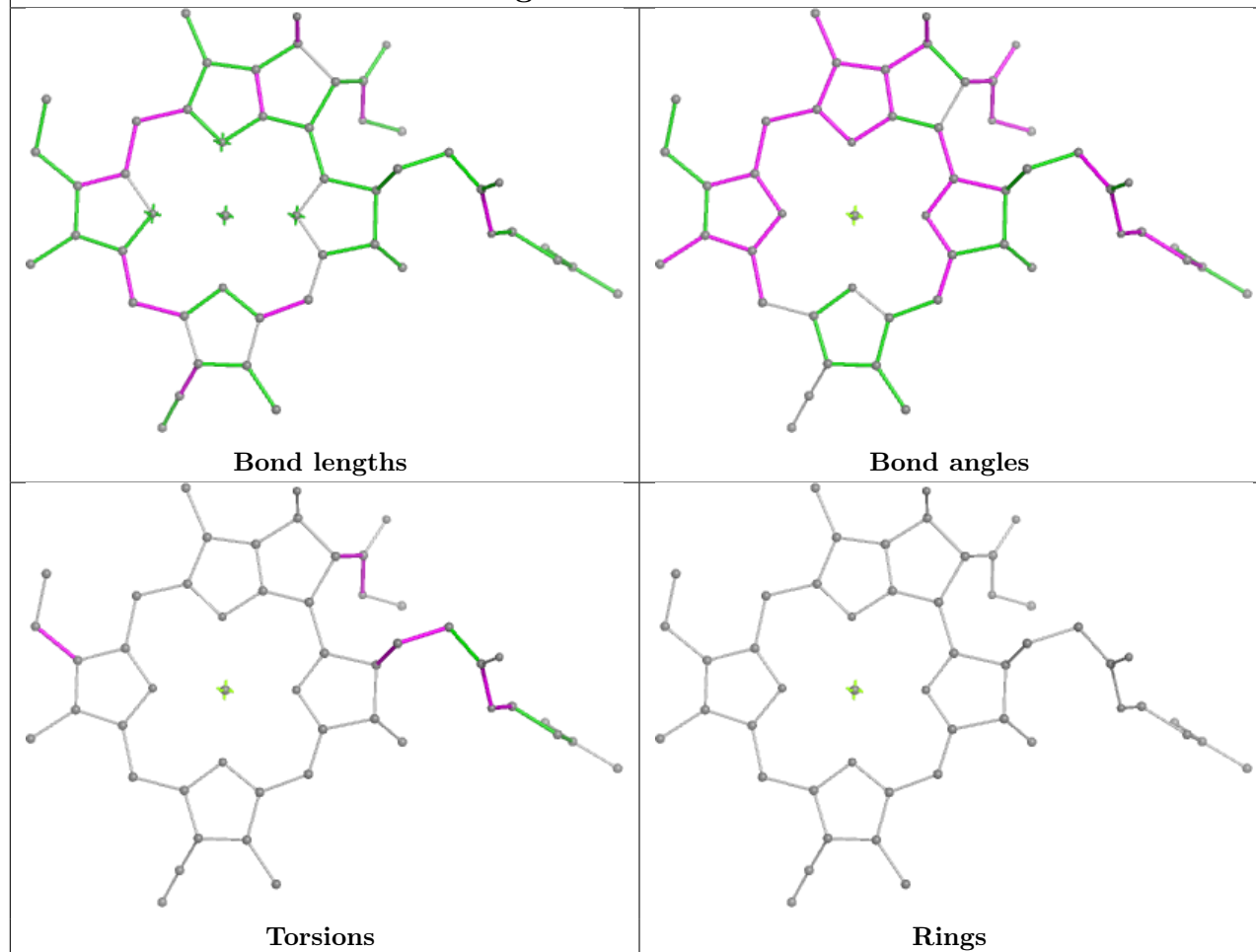


Rings

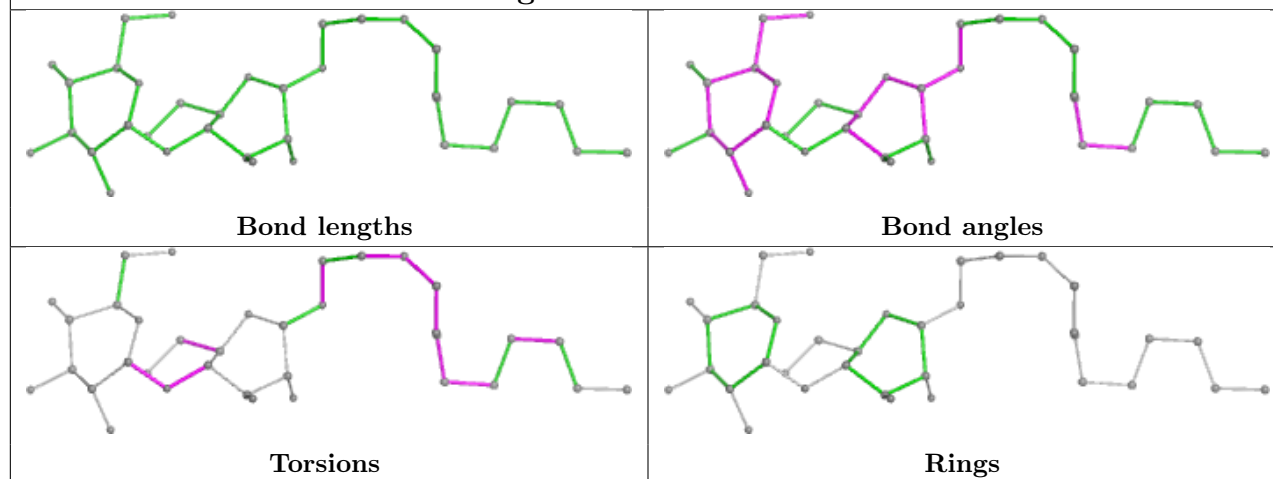


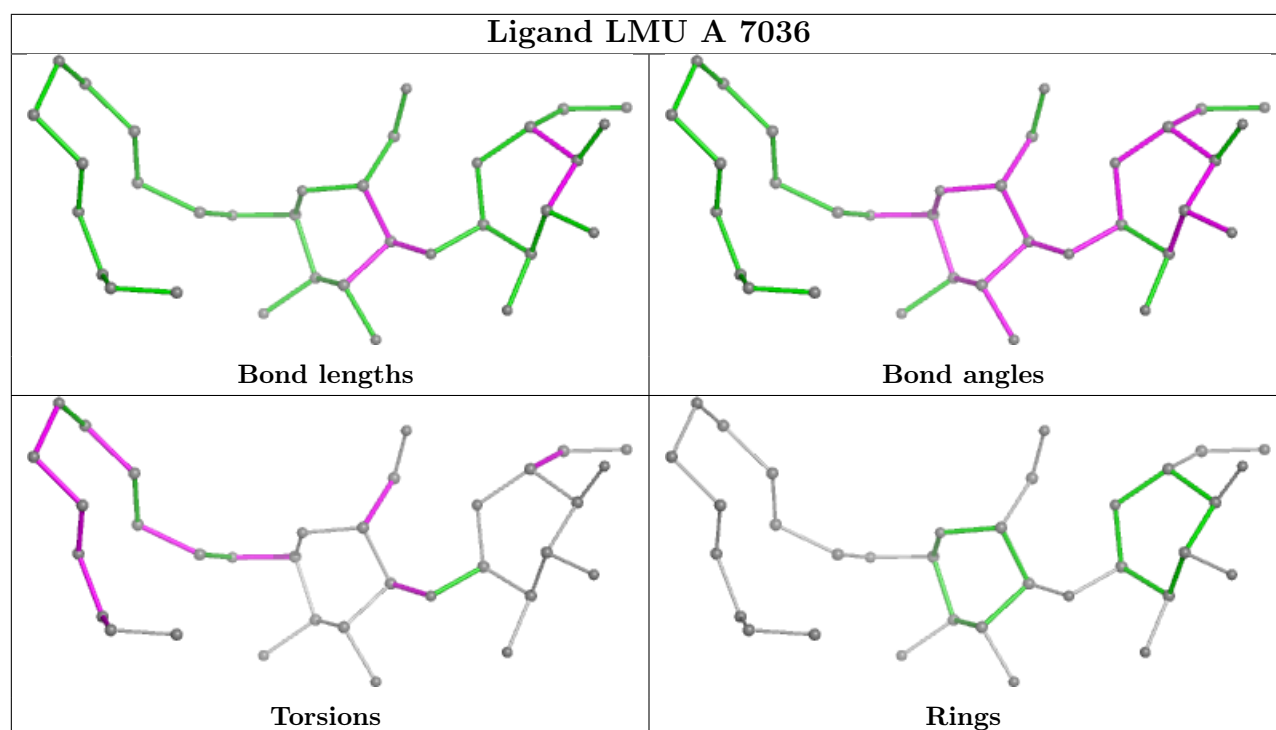


Ligand CLA B 1761

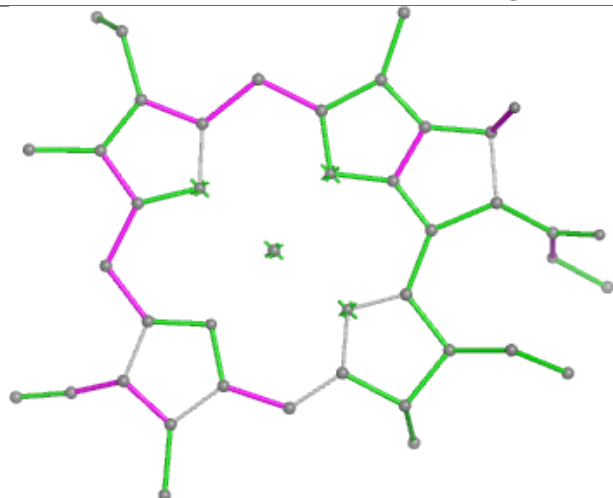


Ligand LMU A 7020

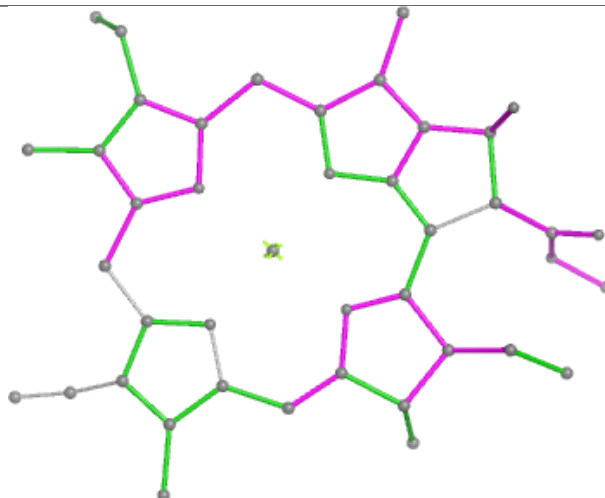




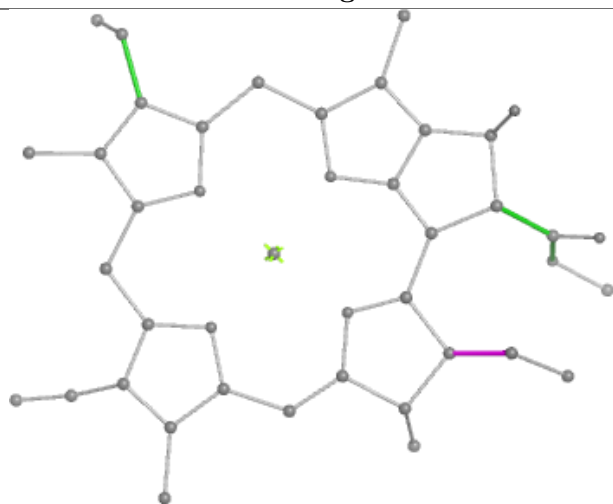
Ligand CLA A 1778



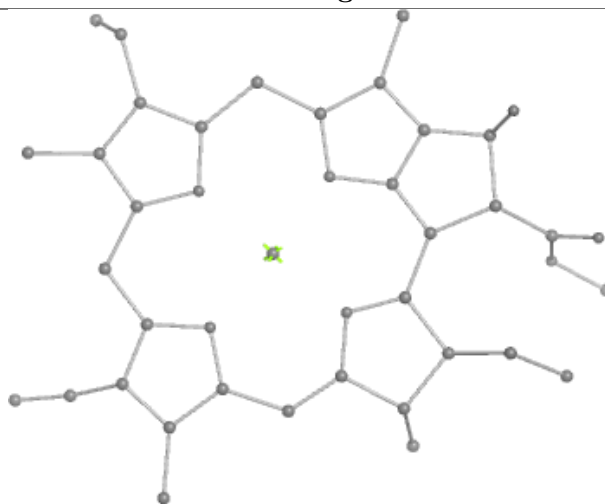
Bond lengths



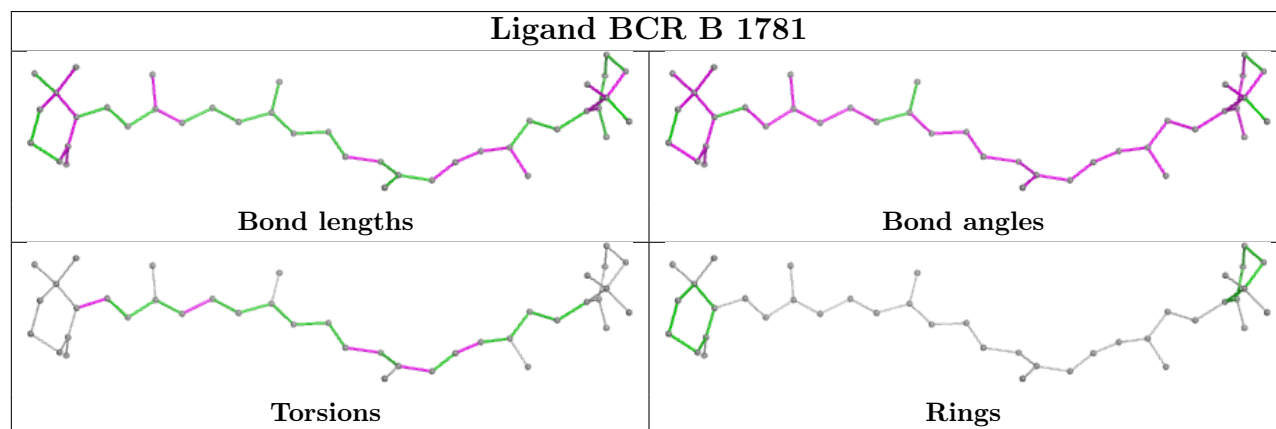
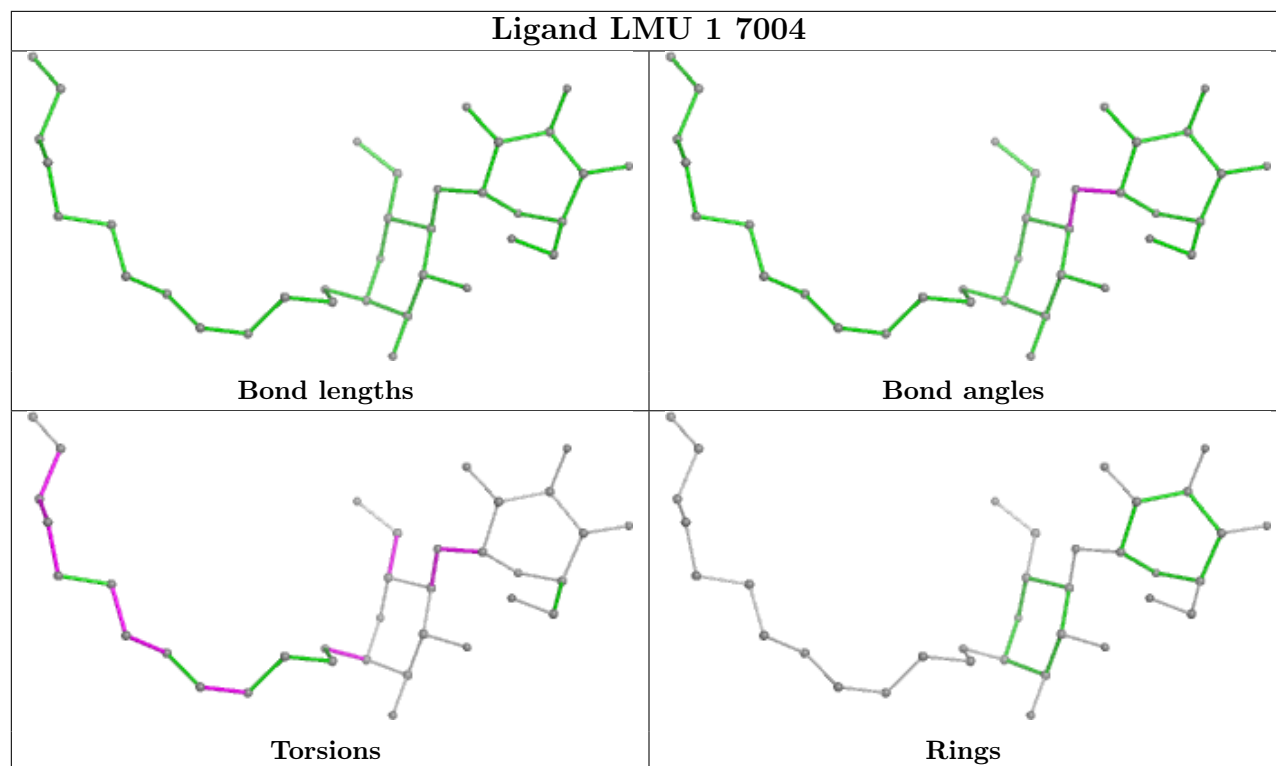
Bond angles

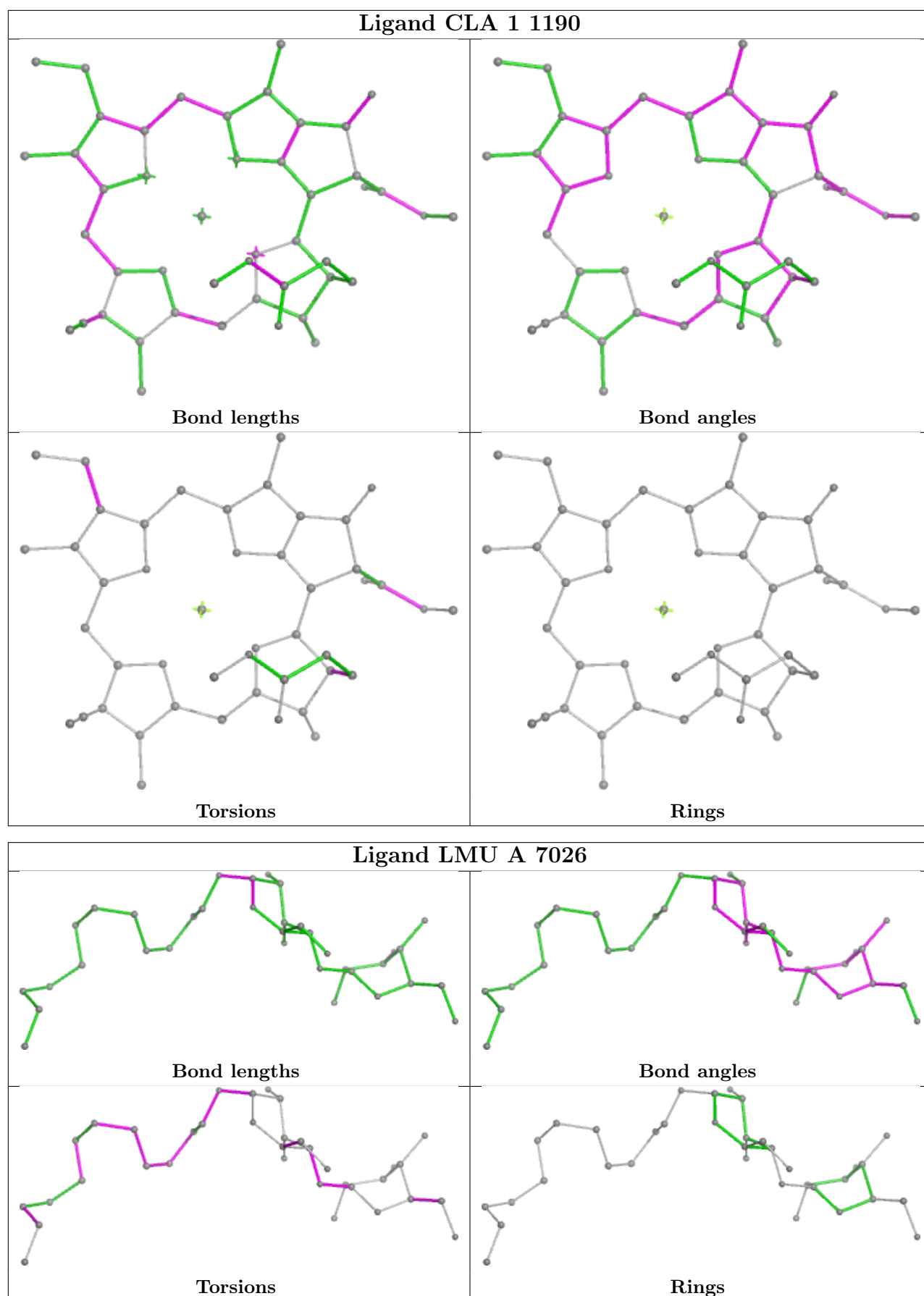


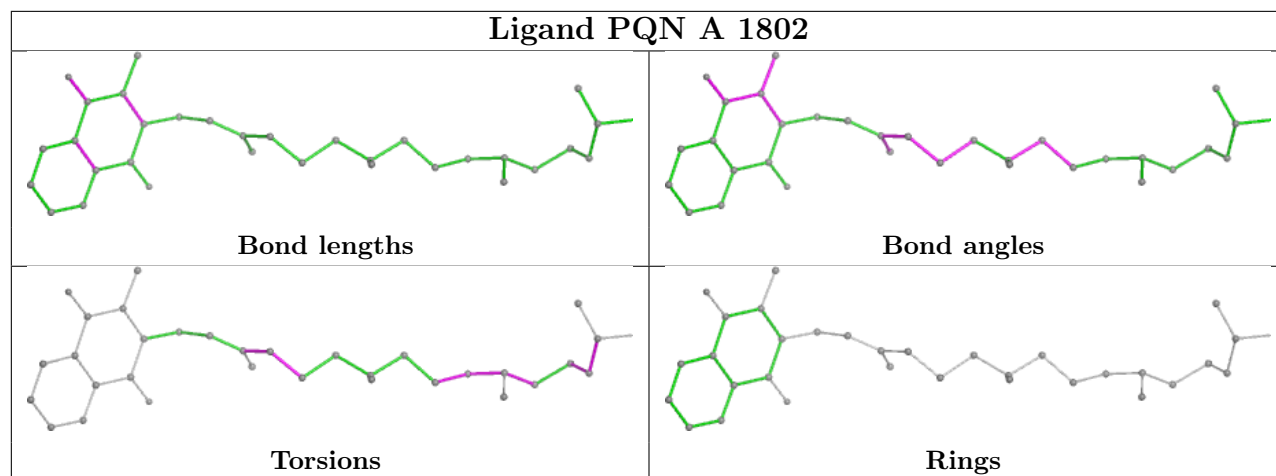
Torsions



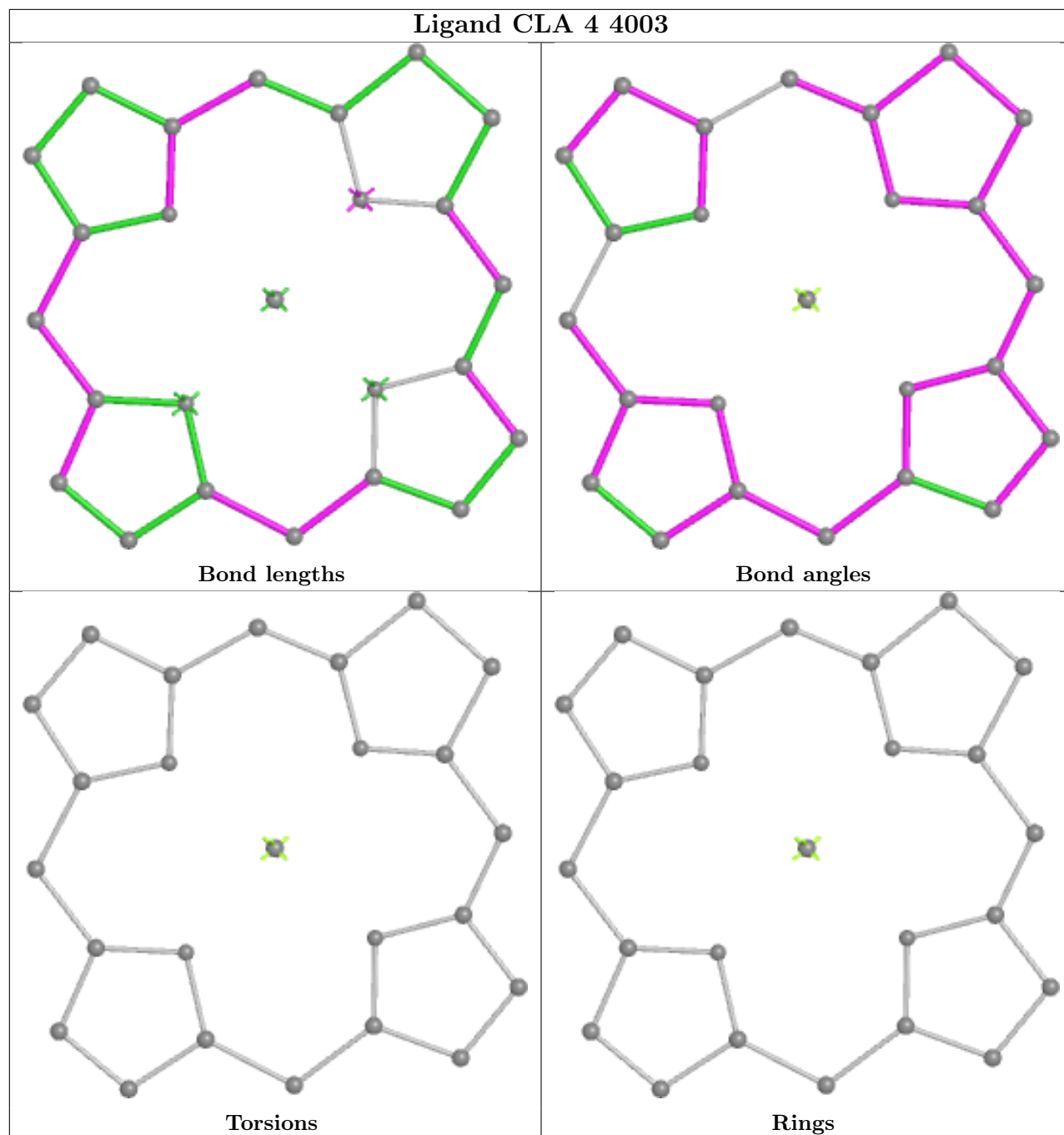
Rings

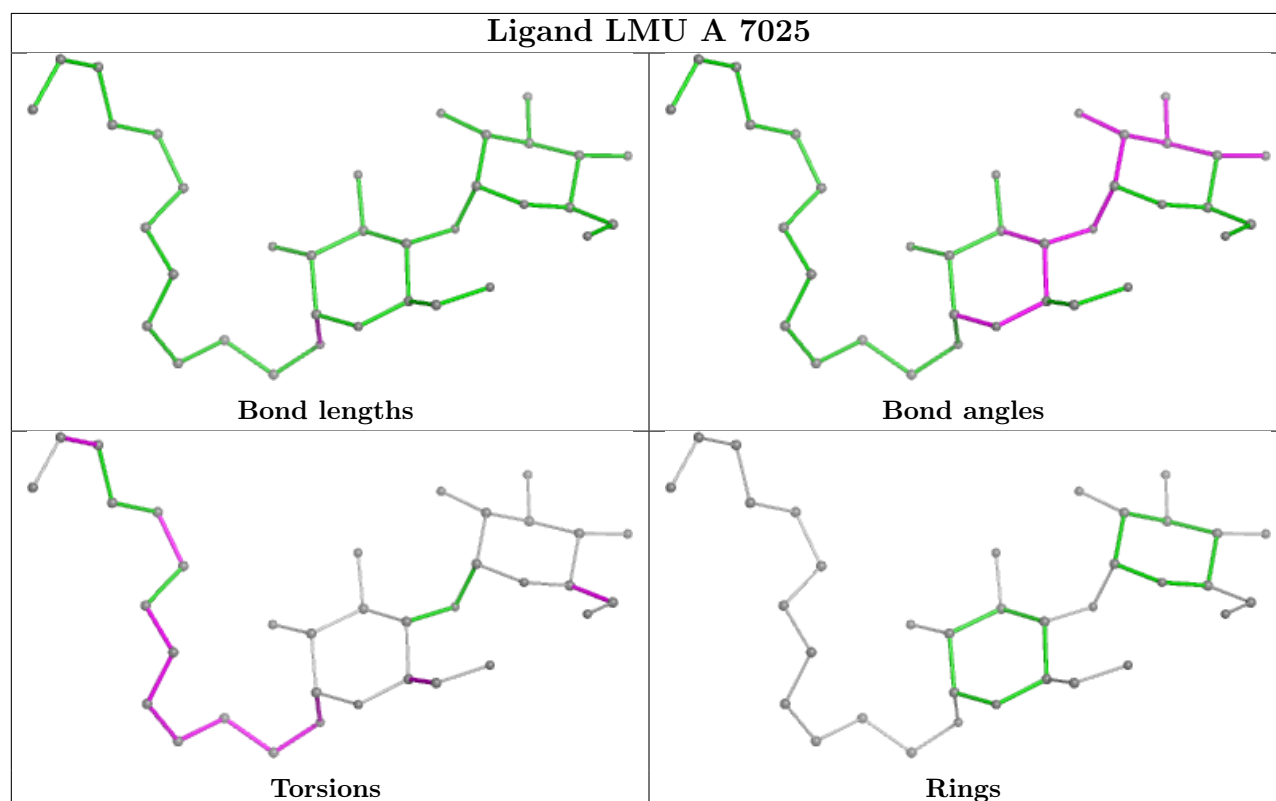
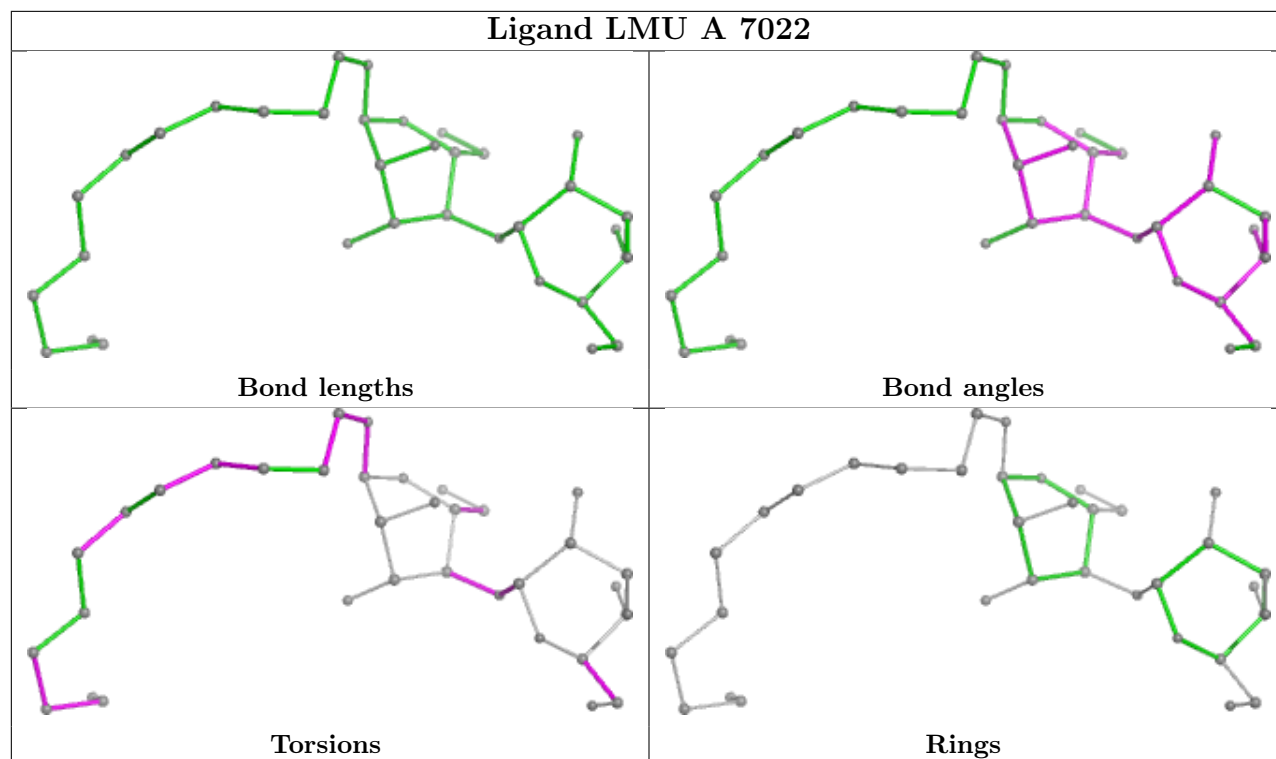




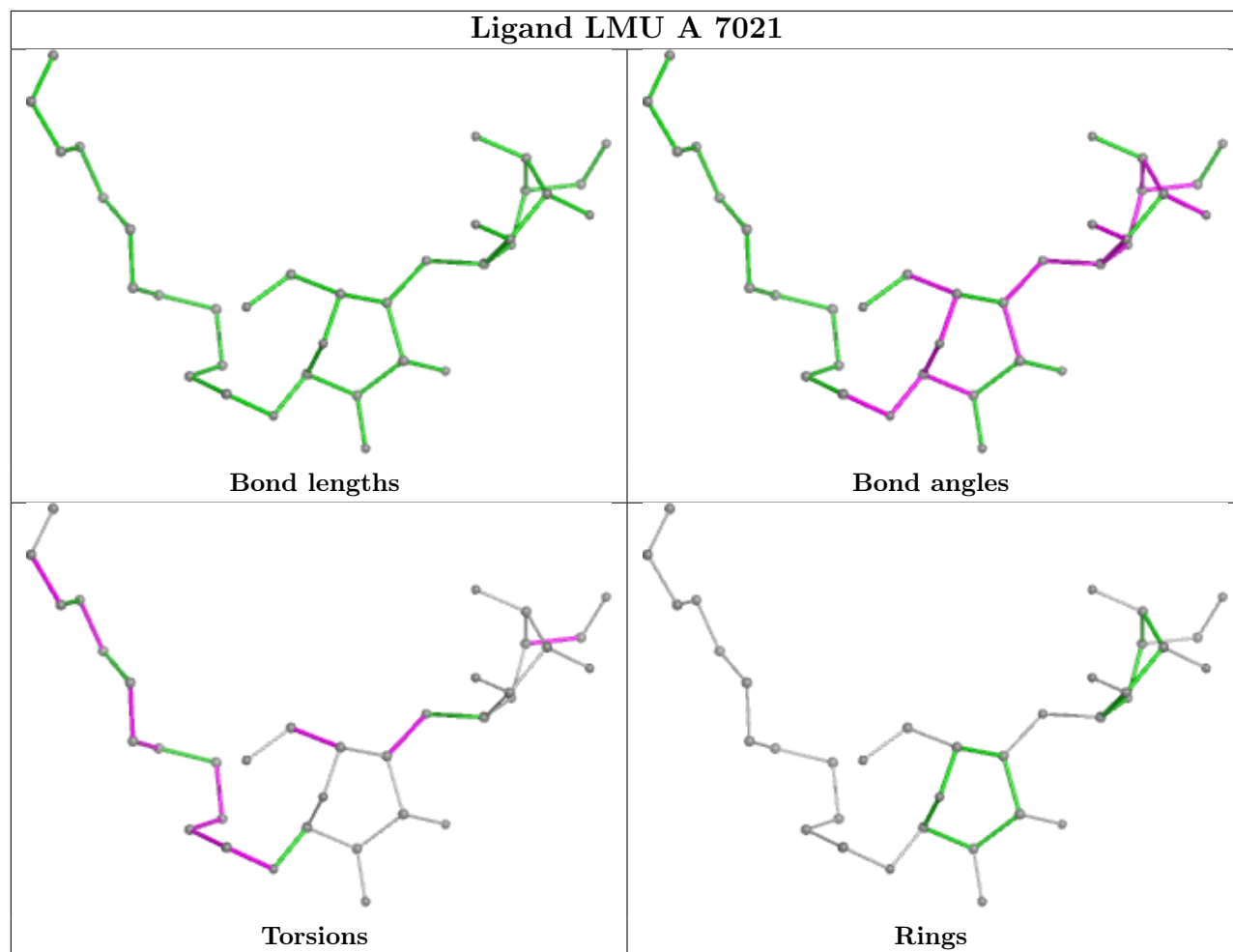


Ligand CLA 4 4003

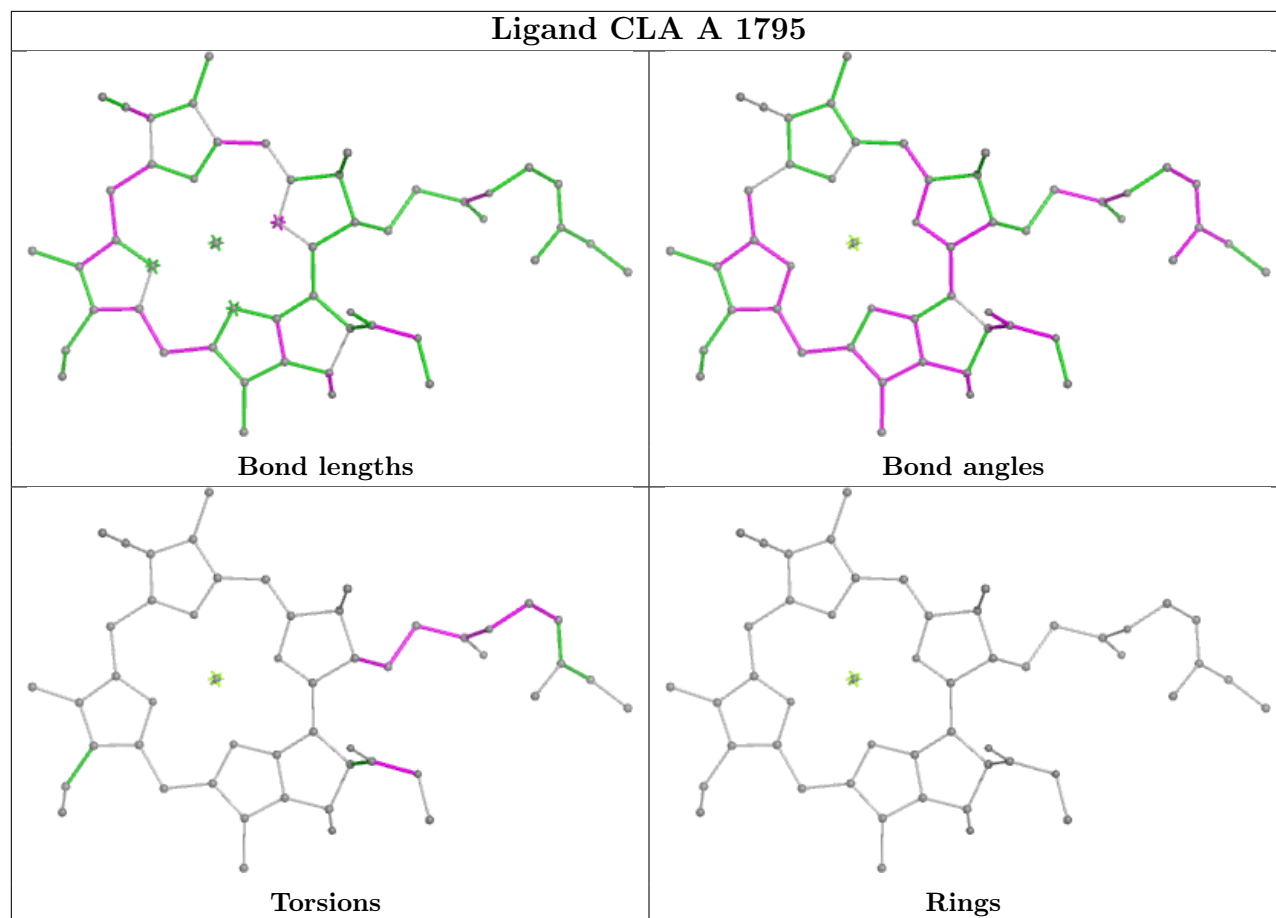


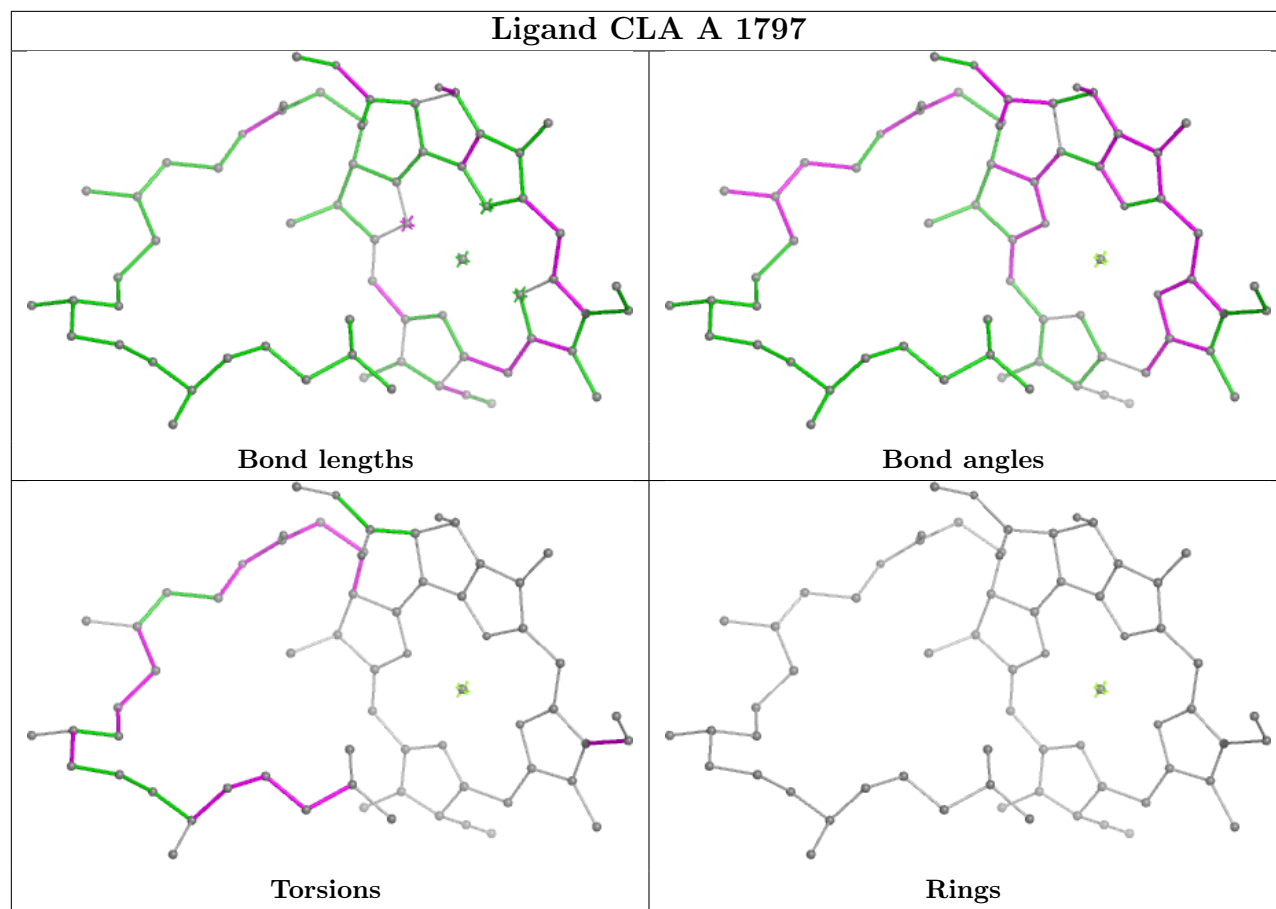


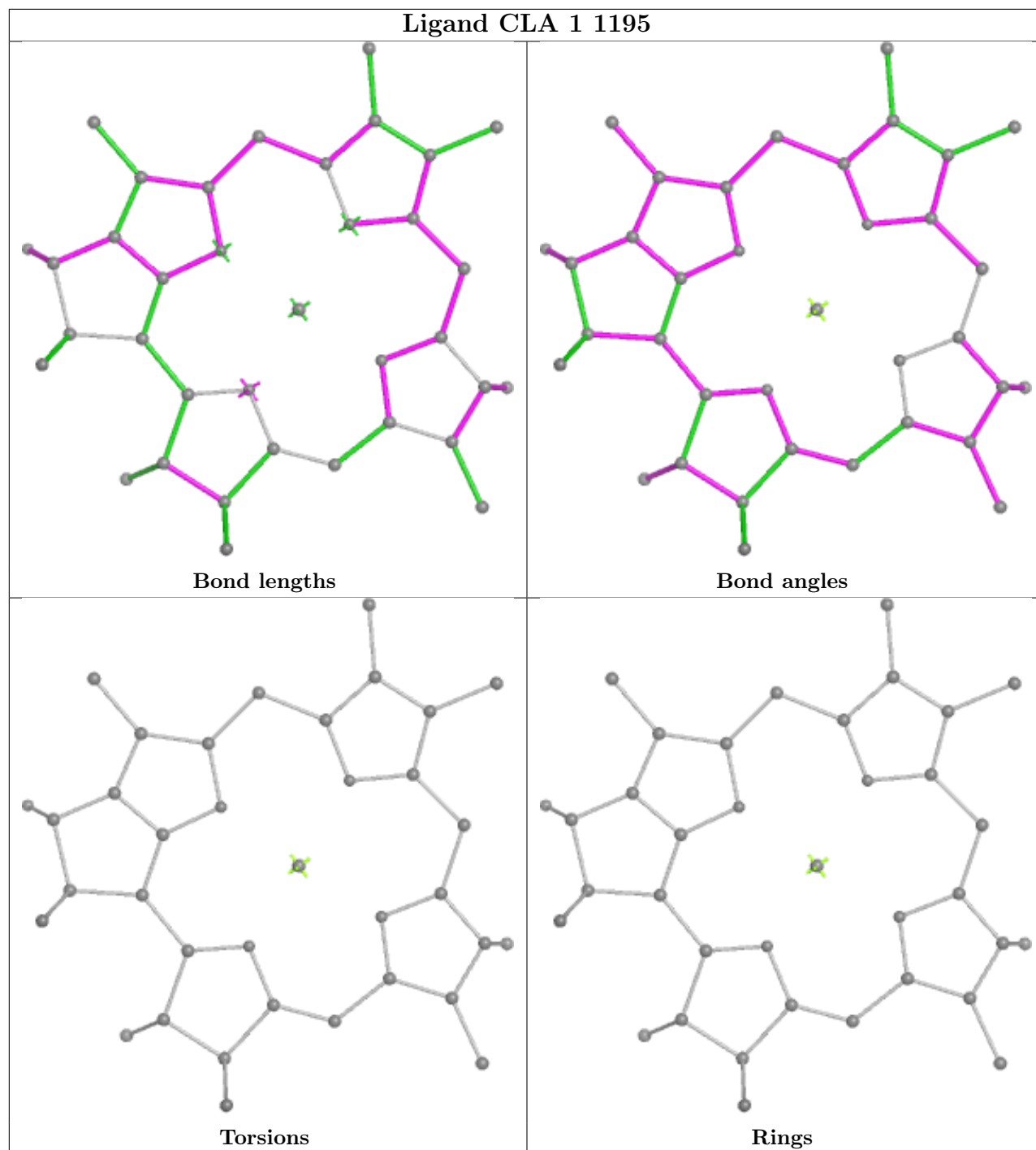
Ligand LMU A 7021

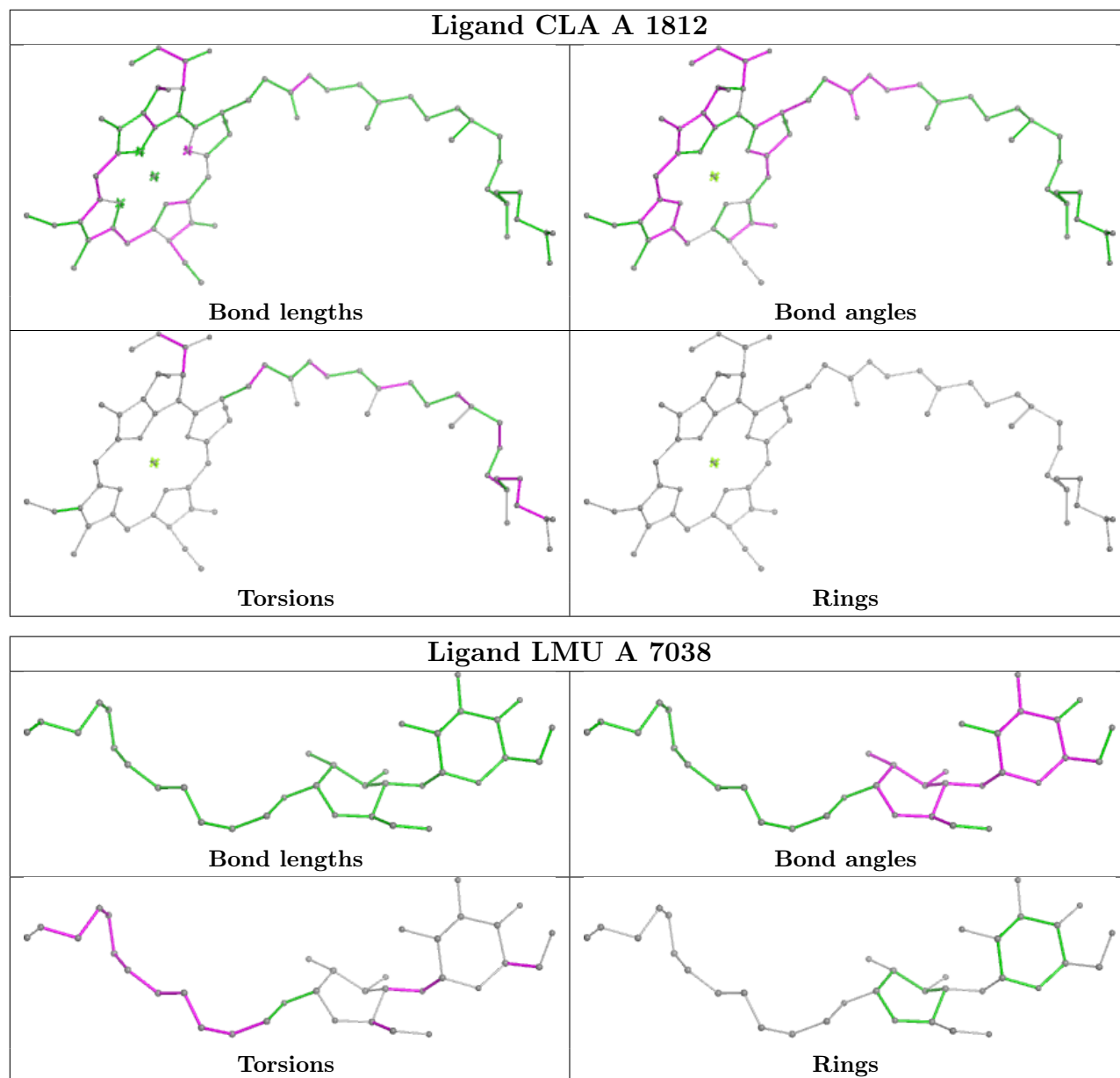


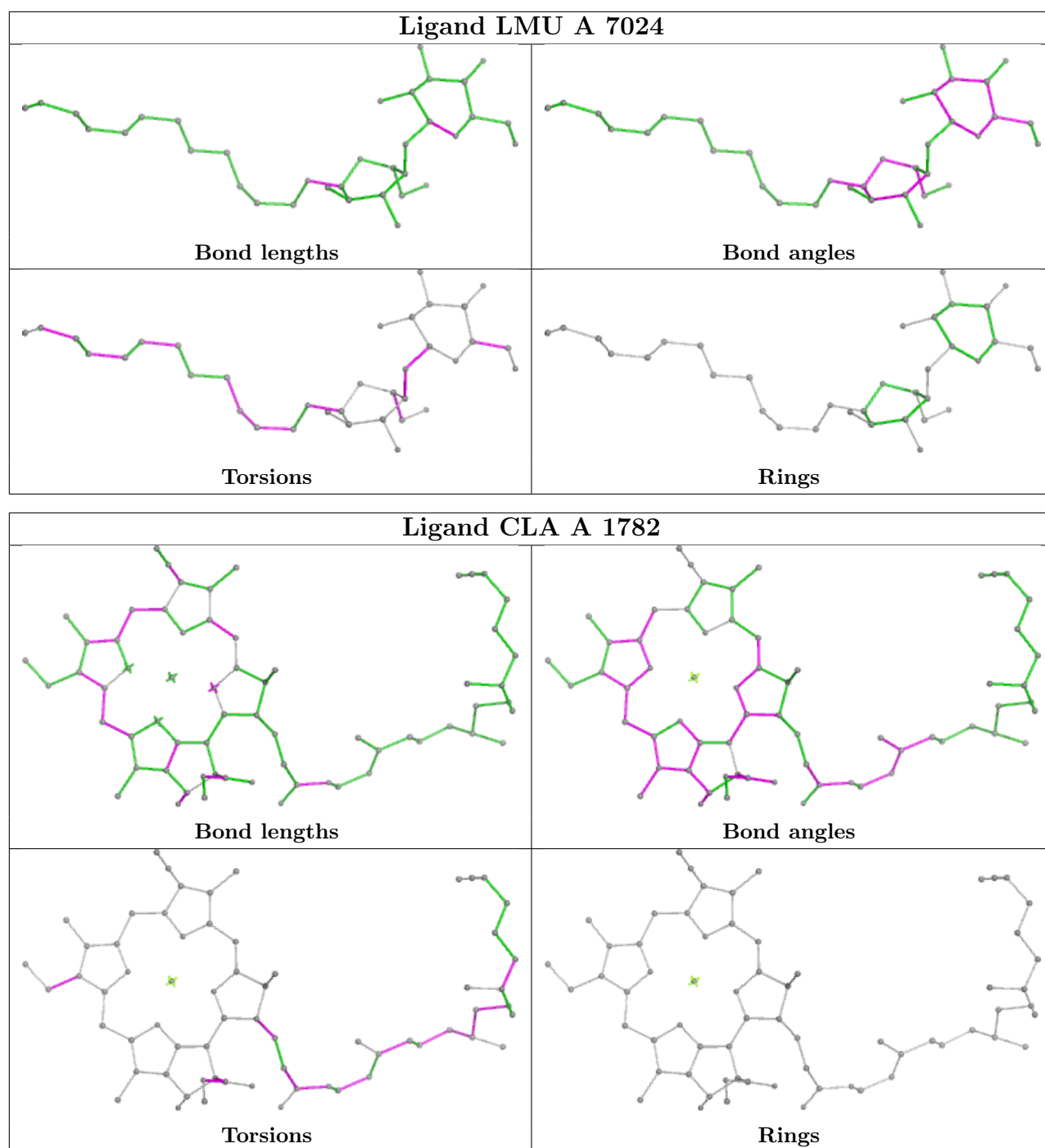
Ligand CLA A 1795











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	317:TYR	C	318:ARG	N	1.17

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	165/241 (68%)	2.32	86 (52%) 0 0	31, 61, 71, 72	0
2	2	176/269 (65%)	1.82	60 (34%) 1 1	33, 52, 64, 68	0
3	3	162/276 (58%)	2.26	82 (50%) 0 0	49, 79, 110, 112	0
4	4	166/251 (66%)	1.81	58 (34%) 1 1	21, 44, 57, 58	0
5	A	730/758 (96%)	1.29	141 (19%) 4 3	20, 20, 20, 20	0
6	B	733/734 (99%)	1.36	160 (21%) 3 2	20, 20, 20, 20	0
7	C	81/81 (100%)	1.71	27 (33%) 1 1	20, 20, 20, 20	0
8	D	138/212 (65%)	1.00	15 (10%) 12 12	20, 20, 20, 20	0
9	E	65/143 (45%)	0.98	8 (12%) 9 9	20, 20, 20, 20	0
10	F	154/231 (66%)	1.01	26 (16%) 5 4	20, 20, 20, 20	0
11	G	95/167 (56%)	0.76	7 (7%) 22 19	20, 20, 20, 20	0
12	H	69/144 (47%)	0.88	6 (8%) 17 16	20, 20, 20, 20	0
13	I	30/40 (75%)	0.42	0 100 100	20, 20, 20, 20	0
14	J	42/44 (95%)	0.79	1 (2%) 59 44	20, 20, 20, 20	0
15	K	84/131 (64%)	0.93	7 (8%) 19 17	20, 20, 20, 20	0
16	L	161/216 (74%)	1.01	27 (16%) 5 4	20, 20, 20, 20	0
17	N	85/170 (50%)	0.35	3 (3%) 47 35	20, 20, 20, 20	0
18	R	0/53	-	-	-	-
All	All	3136/4161 (75%)	1.36	714 (22%) 2 2	20, 20, 65, 112	0

The worst 5 of 714 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	B	491	ASN	11.1
2	2	123	PRO	10.7
1	1	92	GLY	9.6

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Mol	Chain	Res	Type	RSRZ
1	1	75	ALA	8.5
1	1	113	SER	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](#)

SUGAR-RSR INFOmissingINFO

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
20	CLA	J	1046	25/65	0.43	0.17	5,42,60,60	0
22	BCR	A	1803	40/40	0.50	0.24	20,20,20,20	0
21	LMU	A	7013	35/35	0.57	0.16	20,20,20,20	0
20	CLA	L	1505	55/65	0.58	0.17	20,20,20,20	0
20	CLA	3	1217	25/65	0.58	0.19	20,20,20,20	0
20	CLA	1	1199	25/65	0.58	0.22	20,20,20,20	0
20	CLA	2	1218	65/65	0.59	0.18	20,20,20,20	0
22	BCR	A	1808	40/40	0.59	0.22	20,20,20,20	0
21	LMU	A	7037	35/35	0.60	0.18	20,20,20,20	0
20	CLA	2	1212	51/65	0.61	0.20	20,20,20,20	0
22	BCR	3	1220	40/40	0.61	0.19	20,20,20,20	0
20	CLA	4	4003	25/65	0.61	0.17	20,20,20,20	0
20	CLA	I	1033	55/65	0.61	0.16	20,20,20,20	0
21	LMU	2	1225	35/35	0.62	0.16	20,20,20,20	0
20	CLA	A	1797	65/65	0.62	0.17	20,20,20,20	0
20	CLA	B	1746	46/65	0.63	0.21	20,20,20,20	0
20	CLA	B	1766	51/65	0.63	0.17	20,20,20,20	0
20	CLA	3	1214	25/65	0.63	0.19	20,20,20,20	0
21	LMU	A	7041	35/35	0.63	0.16	20,20,20,20	0
20	CLA	3	1219	65/65	0.63	0.17	20,20,20,20	0
20	CLA	K	1142	45/65	0.63	0.16	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	A	1801	55/65	0.63	0.19	20,20,20,20	0
20	CLA	B	1745	60/65	0.64	0.18	20,20,20,20	0
21	LMU	1	7004	35/35	0.65	0.15	20,20,20,20	0
20	CLA	2	1216	25/65	0.65	0.17	20,20,20,20	0
20	CLA	4	4007	52/65	0.65	0.16	20,20,20,20	0
20	CLA	1	1191	36/65	0.65	0.15	20,20,20,20	0
20	CLA	J	1044	61/65	0.65	0.17	20,20,20,20	0
20	CLA	A	1799	50/65	0.65	0.15	20,20,20,20	0
20	CLA	2	1220	56/65	0.65	0.16	2,36,60,60	0
20	CLA	4	1200	50/65	0.65	0.19	20,20,20,20	0
20	CLA	3	3007	42/65	0.66	0.16	20,20,20,20	0
20	CLA	K	3009	65/65	0.67	0.17	20,20,20,20	0
21	LMU	A	7010	35/35	0.67	0.15	20,20,20,20	0
20	CLA	3	1218	65/65	0.67	0.17	20,20,20,20	0
20	CLA	4	4014	47/65	0.67	0.17	20,20,20,20	0
21	LMU	A	7017	35/35	0.68	0.13	20,20,20,20	0
20	CLA	B	1755	58/65	0.68	0.23	20,20,20,20	0
20	CLA	A	1816	55/65	0.68	0.14	20,20,20,20	0
21	LMU	A	7009	34/35	0.68	0.15	20,20,20,20	0
20	CLA	4	1196	55/65	0.68	0.17	20,20,20,20	0
22	BCR	A	1805	40/40	0.68	0.21	20,20,20,20	0
20	CLA	1	1198	61/65	0.68	0.15	2,35,60,60	0
20	CLA	R	1054	57/65	0.69	0.16	20,20,20,20	0
20	CLA	A	1815	55/65	0.69	0.14	20,20,20,20	0
21	LMU	A	7015	35/35	0.69	0.14	20,20,20,20	0
20	CLA	1	1197	51/65	0.69	0.15	20,20,20,20	0
20	CLA	F	1156	41/65	0.69	0.17	20,20,20,20	0
20	CLA	B	1765	45/65	0.70	0.15	20,20,20,20	0
20	CLA	J	1043	61/65	0.70	0.15	20,20,20,20	0
21	LMU	A	7043	35/35	0.70	0.13	20,20,20,20	0
20	CLA	4	1198	65/65	0.70	0.17	20,20,20,20	0
20	CLA	4	1199	55/65	0.70	0.16	20,20,20,20	0
20	CLA	G	1099	51/65	0.70	0.14	20,20,20,20	0
21	LMU	A	7034	35/35	0.70	0.15	20,20,20,20	0
21	LMU	A	1809	35/35	0.71	0.14	20,20,20,20	0
21	LMU	A	1810	35/35	0.71	0.14	20,20,20,20	0
21	LMU	A	7038	35/35	0.71	0.13	20,20,20,20	0
20	CLA	A	1766	45/65	0.71	0.16	20,20,20,20	0
20	CLA	A	1770	45/65	0.71	0.19	20,20,20,20	0
20	CLA	A	1791	45/65	0.71	0.16	20,20,20,20	0
20	CLA	1	1193	51/65	0.71	0.14	20,20,20,20	0
20	CLA	1	1200	51/65	0.71	0.15	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	LMU	A	7030	35/35	0.71	0.12	20,20,20,20	0
20	CLA	3	1213	25/65	0.72	0.15	20,20,20,20	0
20	CLA	K	1146	50/65	0.72	0.14	20,20,20,20	0
21	LMU	A	7025	35/35	0.72	0.15	20,20,20,20	0
21	LMU	A	7027	35/35	0.72	0.13	20,20,20,20	0
20	CLA	A	1798	55/65	0.72	0.17	20,20,20,20	0
21	LMU	A	7031	35/35	0.72	0.13	20,20,20,20	0
20	CLA	2	1215	50/65	0.72	0.17	20,20,20,20	0
20	CLA	A	1763	46/65	0.72	0.17	20,20,20,20	0
20	CLA	F	1157	53/65	0.72	0.14	20,20,20,20	0
20	CLA	3	3001	25/65	0.72	0.15	20,20,20,20	0
20	CLA	2	1223	50/65	0.72	0.20	20,20,20,20	0
20	CLA	A	1775	36/65	0.72	0.15	20,20,20,20	0
20	CLA	3	3014	25/65	0.72	0.15	20,20,20,20	0
20	CLA	B	1751	46/65	0.72	0.19	20,20,20,20	0
20	CLA	K	1085	50/65	0.72	0.15	20,20,20,20	0
22	BCR	I	1032	40/40	0.72	0.15	20,20,20,20	0
20	CLA	2	1213	56/65	0.73	0.16	20,20,20,20	0
21	LMU	3	7005	35/35	0.73	0.14	20,20,20,20	0
21	LMU	A	7020	35/35	0.73	0.13	20,20,20,20	0
20	CLA	1	1187	46/65	0.73	0.14	20,20,20,20	0
21	LMU	A	7047	35/35	0.73	0.13	20,20,20,20	0
20	CLA	A	1780	65/65	0.73	0.24	20,20,20,20	0
21	LMU	A	7028	35/35	0.73	0.13	20,20,20,20	0
20	CLA	3	1215	25/65	0.73	0.15	20,20,20,20	0
20	CLA	3	3002	25/65	0.73	0.14	20,20,20,20	0
22	BCR	B	1776	40/40	0.73	0.18	20,20,20,20	0
22	BCR	B	1780	40/40	0.73	0.27	20,20,20,20	0
20	CLA	2	1227	25/65	0.73	0.13	20,20,20,20	0
20	CLA	2	1217	65/65	0.74	0.15	20,20,20,20	0
21	LMU	K	1086	35/35	0.74	0.12	20,20,20,20	0
20	CLA	4	1204	55/65	0.74	0.17	20,20,20,20	0
20	CLA	A	1778	42/65	0.74	0.14	20,20,20,20	0
20	CLA	4	1208	25/65	0.74	0.14	20,20,20,20	0
20	CLA	1	1194	25/65	0.74	0.15	20,20,20,20	0
20	CLA	R	1055	65/65	0.74	0.14	20,20,20,20	0
21	LMU	A	7042	35/35	0.74	0.14	20,20,20,20	0
21	LMU	1	1202	35/35	0.74	0.12	20,20,20,20	0
20	CLA	H	1079	65/65	0.75	0.20	20,20,20,20	0
20	CLA	L	1168	50/65	0.75	0.18	20,20,20,20	0
21	LMU	2	7003	35/35	0.75	0.13	20,20,20,20	0
22	BCR	A	1806	40/40	0.75	0.20	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	LMU	2	7006	35/35	0.75	0.13	20,20,20,20	0
21	LMU	A	7036	34/35	0.75	0.13	20,20,20,20	0
20	CLA	1	1192	61/65	0.75	0.14	20,20,20,20	0
21	LMU	R	1057	35/35	0.75	0.12	20,20,20,20	0
21	LMU	A	7019	35/35	0.76	0.12	20,20,20,20	0
20	CLA	1	1188	47/65	0.76	0.15	20,20,20,20	0
20	CLA	A	1817	46/65	0.76	0.13	20,20,20,20	0
21	LMU	B	1782	25/35	0.76	0.12	20,20,20,20	0
21	LMU	4	1210	35/35	0.76	0.12	20,20,20,20	0
20	CLA	3	1212	36/65	0.76	0.13	20,20,20,20	0
20	CLA	1	1189	47/65	0.76	0.14	20,20,20,20	0
24	LMG	B	1783	49/55	0.76	0.22	20,20,20,20	0
20	CLA	4	1203	25/65	0.77	0.15	20,20,20,20	0
20	CLA	3	3008	50/65	0.77	0.13	20,20,20,20	0
20	CLA	2	1224	65/65	0.77	0.15	20,20,20,20	0
20	CLA	L	1166	50/65	0.77	0.16	20,20,20,20	0
22	BCR	A	1804	40/40	0.77	0.18	20,20,20,20	0
20	CLA	B	1764	45/65	0.77	0.17	20,20,20,20	0
20	CLA	4	1209	46/65	0.77	0.13	20,20,20,20	0
22	BCR	A	1807	40/40	0.77	0.22	20,20,20,20	0
21	LMU	A	7021	35/35	0.77	0.12	20,20,20,20	0
22	BCR	B	1774	40/40	0.77	0.20	20,20,20,20	0
22	BCR	B	1775	40/40	0.77	0.20	20,20,20,20	0
21	LMU	A	7023	35/35	0.77	0.12	20,20,20,20	0
20	CLA	A	1767	65/65	0.77	0.18	20,20,20,20	0
20	CLA	B	1772	36/65	0.77	0.13	20,20,20,20	0
20	CLA	4	1202	25/65	0.77	0.15	20,20,20,20	0
20	CLA	A	1776	65/65	0.78	0.18	20,20,20,20	0
20	CLA	J	1045	55/65	0.78	0.13	2,33,60,60	0
20	CLA	B	1762	65/65	0.78	0.20	20,20,20,20	0
20	CLA	A	1771	50/65	0.78	0.15	20,20,20,20	0
20	CLA	A	1772	65/65	0.78	0.17	2,35,60,60	0
22	BCR	B	1779	40/40	0.78	0.18	20,20,20,20	0
20	CLA	A	1787	65/65	0.78	0.18	20,20,20,20	0
20	CLA	1	1195	36/65	0.78	0.14	20,20,20,20	0
22	BCR	L	1169	40/40	0.78	0.18	20,20,20,20	0
21	LMU	A	7033	35/35	0.78	0.12	20,20,20,20	0
20	CLA	1	1196	36/65	0.79	0.16	20,20,20,20	0
20	CLA	1	1201	25/65	0.79	0.13	20,20,20,20	0
20	CLA	2	1219	25/65	0.79	0.14	20,20,20,20	0
21	LMU	A	7022	35/35	0.79	0.13	20,20,20,20	0
21	LMU	A	7040	35/35	0.79	0.12	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	3	1216	25/65	0.79	0.12	20,20,20,20	0
20	CLA	2	2010	25/65	0.79	0.15	20,20,20,20	0
21	LMU	A	7026	35/35	0.79	0.12	20,20,20,20	0
20	CLA	3	3011	65/65	0.79	0.13	20,20,20,20	0
20	CLA	1	1190	46/65	0.79	0.14	20,20,20,20	0
20	CLA	B	1741	54/65	0.79	0.17	20,20,20,20	0
21	LMU	R	1056	35/35	0.79	0.12	20,20,20,20	0
20	CLA	B	1742	55/65	0.79	0.18	20,20,20,20	0
20	CLA	3	3015	25/65	0.79	0.13	20,20,20,20	0
20	CLA	A	1782	65/65	0.80	0.16	20,20,20,20	0
20	CLA	2	1221	25/65	0.80	0.15	20,20,20,20	0
20	CLA	B	1756	65/65	0.80	0.18	20,20,20,20	0
20	CLA	4	1197	36/65	0.80	0.17	20,20,20,20	0
20	CLA	B	1735	65/65	0.80	0.22	20,20,20,20	0
20	CLA	A	1769	54/65	0.80	0.17	20,20,20,20	0
20	CLA	A	1761	65/65	0.80	0.21	20,20,20,20	0
20	CLA	B	1744	65/65	0.80	0.17	20,20,20,20	0
20	CLA	4	1205	25/65	0.80	0.18	20,20,20,20	0
20	CLA	A	1781	65/65	0.80	0.17	20,20,20,20	0
20	CLA	A	1760	55/65	0.81	0.17	20,20,20,20	0
20	CLA	A	1768	54/65	0.81	0.13	20,20,20,20	0
20	CLA	B	1736	45/65	0.81	0.17	20,20,20,20	0
20	CLA	B	1740	65/65	0.81	0.19	20,20,20,20	0
20	CLA	B	1761	50/65	0.81	0.16	20,20,20,20	0
20	CLA	A	1777	51/65	0.81	0.14	20,20,20,20	0
21	LMU	L	1171	35/35	0.81	0.11	20,20,20,20	0
22	BCR	B	1777	40/40	0.81	0.22	20,20,20,20	0
22	BCR	B	1778	40/40	0.81	0.22	20,20,20,20	0
21	LMU	A	7035	35/35	0.81	0.13	20,20,20,20	0
20	CLA	B	1763	50/65	0.81	0.20	20,20,20,20	0
20	CLA	A	1813	65/65	0.81	0.19	20,20,20,20	0
20	CLA	4	1207	36/65	0.81	0.17	20,20,20,20	0
20	CLA	A	1774	65/65	0.81	0.21	20,20,20,20	0
20	CLA	2	1214	25/65	0.82	0.12	20,20,20,20	0
20	CLA	B	1753	65/65	0.82	0.16	20,20,20,20	0
20	CLA	A	1786	50/65	0.82	0.15	20,20,20,20	0
20	CLA	2	1222	50/65	0.82	0.15	20,20,20,20	0
20	CLA	4	1201	52/65	0.82	0.12	20,20,20,20	0
20	CLA	I	1031	60/65	0.82	0.17	20,20,20,20	0
20	CLA	A	1792	51/65	0.83	0.17	20,20,20,20	0
20	CLA	A	1812	65/65	0.83	0.20	20,20,20,20	0
20	CLA	A	1773	52/65	0.83	0.17	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	A	1789	65/65	0.83	0.18	20,20,20,20	0
20	CLA	F	1155	36/65	0.83	0.15	20,20,20,20	0
20	CLA	B	1747	59/65	0.83	0.16	20,20,20,20	0
20	CLA	L	1167	47/65	0.83	0.16	20,20,20,20	0
20	CLA	A	1765	55/65	0.83	0.18	20,20,20,20	0
23	PQN	A	1802	33/33	0.83	0.23	20,20,20,20	0
21	LMU	A	7016	35/35	0.83	0.10	20,20,20,20	0
20	CLA	A	1784	55/65	0.84	0.18	20,20,20,20	0
20	CLA	B	1759	65/65	0.84	0.19	20,20,20,20	0
20	CLA	A	1793	65/65	0.84	0.18	20,20,20,20	0
20	CLA	A	1795	51/65	0.84	0.20	20,20,20,20	0
20	CLA	A	1796	65/65	0.84	0.16	20,20,20,20	0
20	CLA	A	1785	65/65	0.84	0.18	20,20,20,20	0
20	CLA	4	1206	25/65	0.84	0.15	20,20,20,20	0
20	CLA	B	1743	65/65	0.84	0.17	20,20,20,20	0
20	CLA	B	1767	60/65	0.84	0.19	20,20,20,20	0
21	LMU	A	7024	35/35	0.84	0.10	20,20,20,20	0
21	LMU	A	7039	35/35	0.84	0.10	20,20,20,20	0
20	CLA	B	1769	47/65	0.84	0.20	20,20,20,20	0
20	CLA	B	1770	65/65	0.84	0.18	20,20,20,20	0
20	CLA	B	1749	61/65	0.85	0.17	20,20,20,20	0
20	CLA	B	1750	50/65	0.85	0.16	20,20,20,20	0
20	CLA	A	1790	50/65	0.85	0.15	20,20,20,20	0
20	CLA	B	1752	55/65	0.85	0.14	20,20,20,20	0
20	CLA	A	1759	50/65	0.85	0.14	20,20,20,20	0
20	CLA	A	1764	65/65	0.85	0.22	20,20,20,20	0
20	CLA	A	1788	65/65	0.85	0.15	20,20,20,20	0
22	BCR	B	1781	40/40	0.85	0.16	20,20,20,20	0
20	CLA	A	1762	57/65	0.85	0.16	20,20,20,20	0
21	LMU	A	7032	35/35	0.85	0.10	20,20,20,20	0
20	CLA	B	1748	60/65	0.85	0.21	20,20,20,20	0
20	CLA	B	1787	65/65	0.85	0.20	20,20,20,20	0
22	BCR	L	1170	40/40	0.86	0.18	20,20,20,20	0
20	CLA	B	1758	65/65	0.86	0.21	20,20,20,20	0
20	CLA	A	1800	65/65	0.86	0.15	20,20,20,20	0
26	UNL	B	8057	23/-	0.86	0.09	20,20,20,20	0
20	CLA	B	1737	65/65	0.87	0.18	20,20,20,20	0
20	CLA	A	1779	55/65	0.87	0.16	20,20,20,20	0
20	CLA	B	1768	65/65	0.87	0.18	20,20,20,20	0
20	CLA	B	1757	65/65	0.87	0.18	20,20,20,20	0
20	CLA	A	1794	47/65	0.87	0.17	20,20,20,20	0
20	CLA	B	1771	65/65	0.87	0.17	20,20,20,20	0

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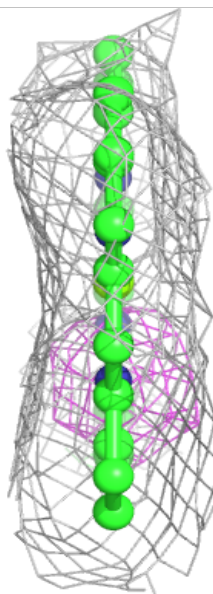
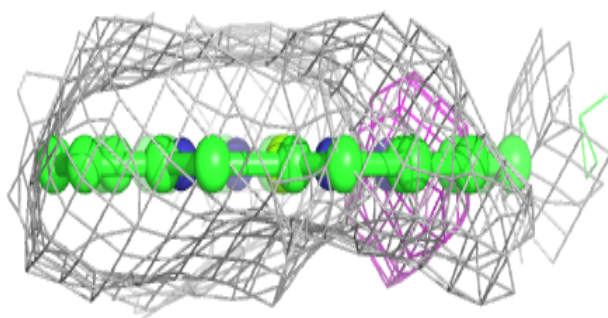
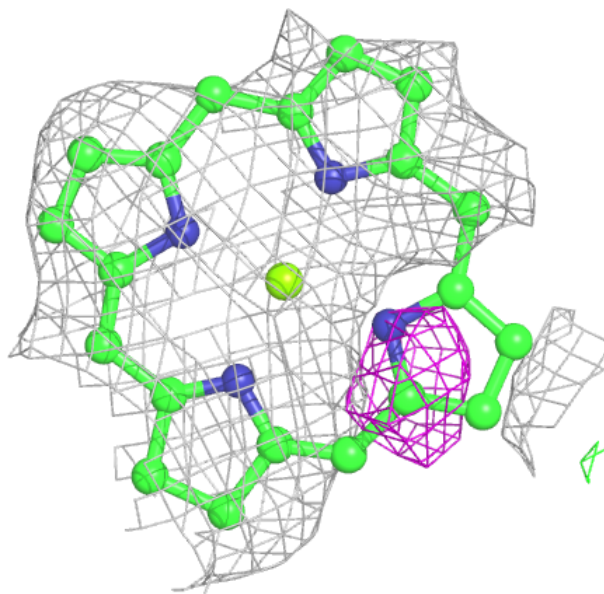
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	B	1754	54/65	0.87	0.18	20,20,20,20	0
20	CLA	B	1785	65/65	0.87	0.20	20,20,20,20	0
23	PQN	B	1773	33/33	0.88	0.18	20,20,20,20	0
20	CLA	B	1738	65/65	0.88	0.17	20,20,20,20	0
20	CLA	B	1786	65/65	0.88	0.18	20,20,20,20	0
20	CLA	B	1760	50/65	0.89	0.14	20,20,20,20	0
20	CLA	B	1739	65/65	0.89	0.20	20,20,20,20	0
20	CLA	A	1811	65/65	0.89	0.23	20,20,20,20	0
20	CLA	A	1783	65/65	0.89	0.18	20,20,20,20	0
25	SF4	C	1082	8/8	0.98	0.06	20,20,20,20	0
25	SF4	C	1083	8/8	0.99	0.05	20,20,20,20	0
25	SF4	B	1784	8/8	0.99	0.05	20,20,20,20	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.

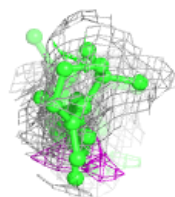
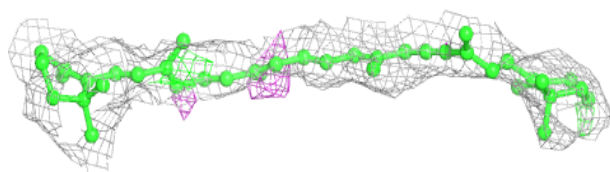
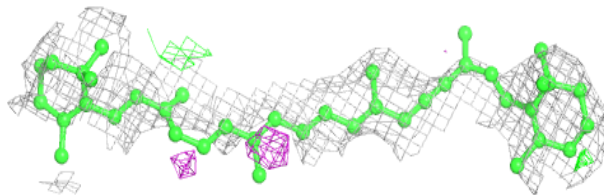
Electron density around CLA J 1046:

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



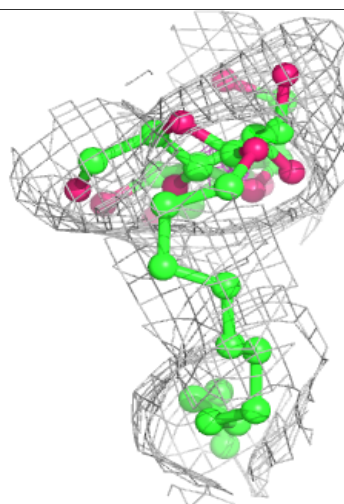
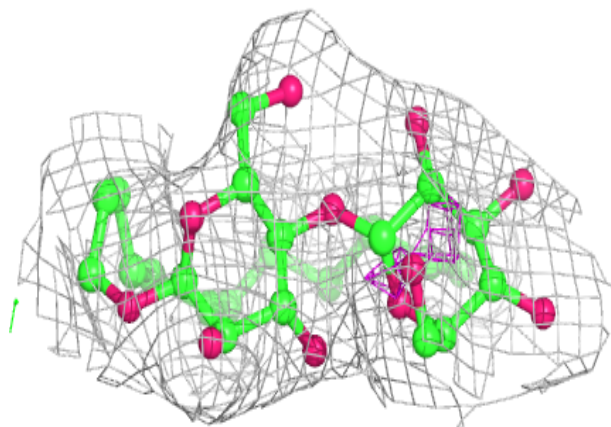
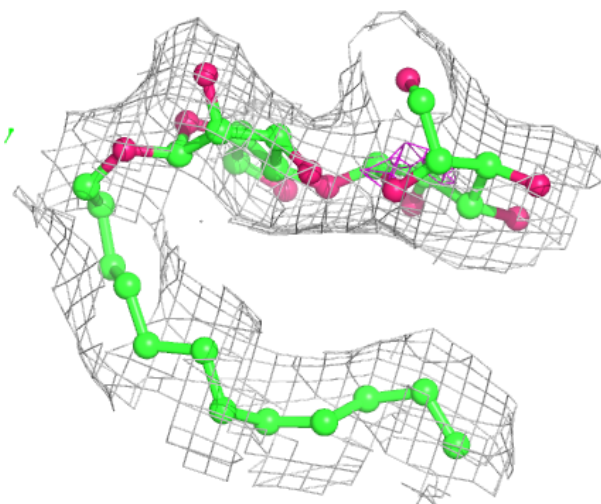
Electron density around BCR A 1803:

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



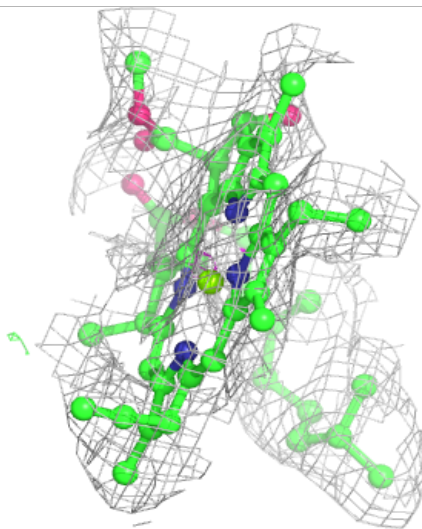
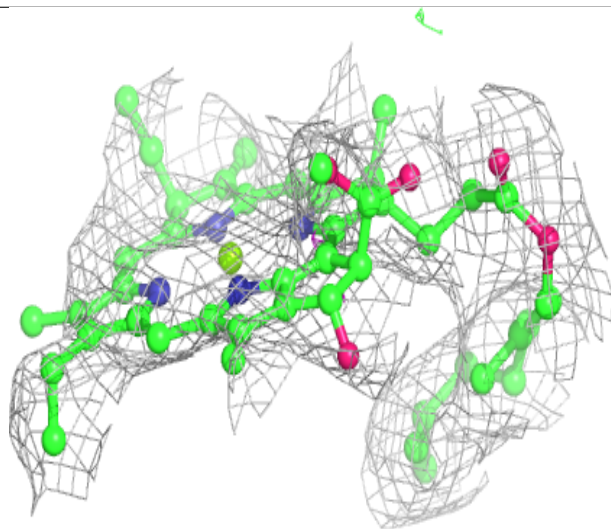
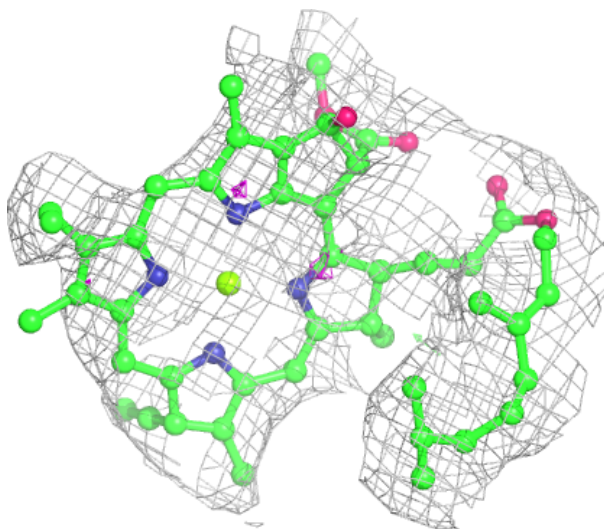
Electron density around LMU A 7013:

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



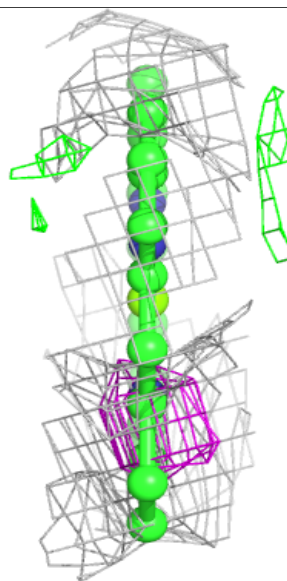
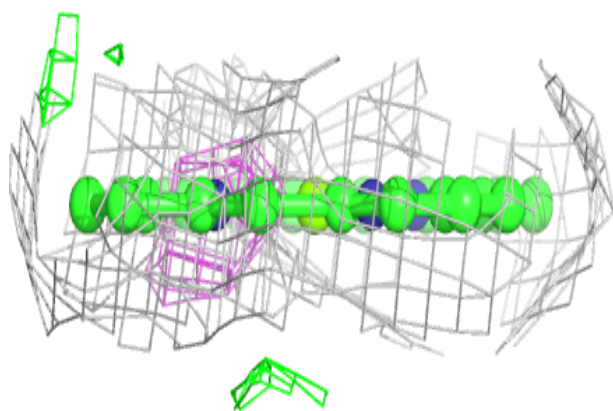
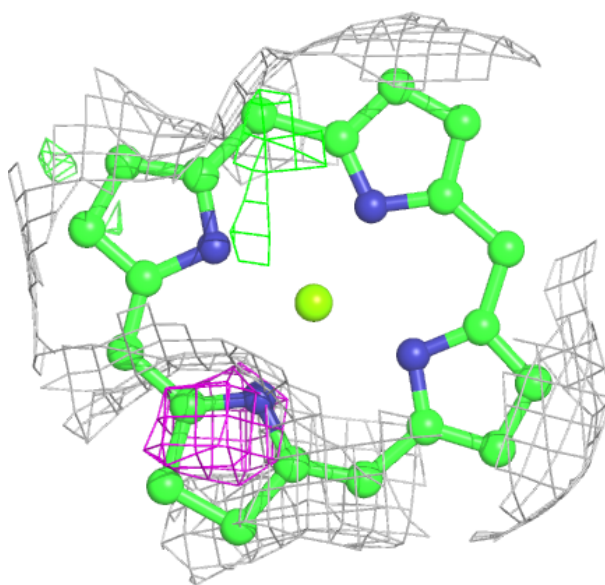
Electron density around CLA L 1505:

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



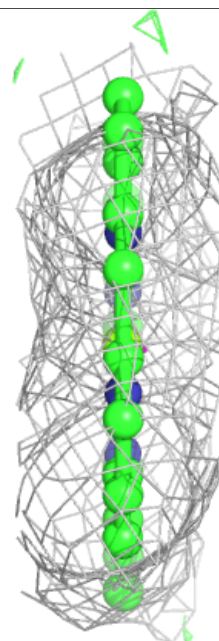
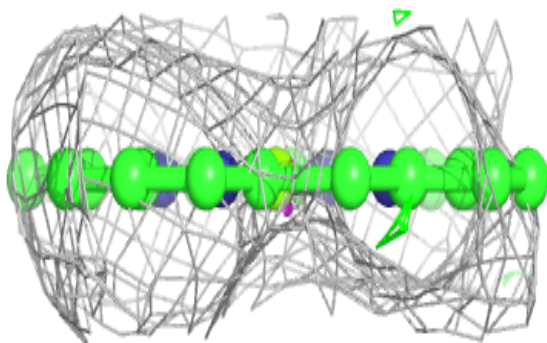
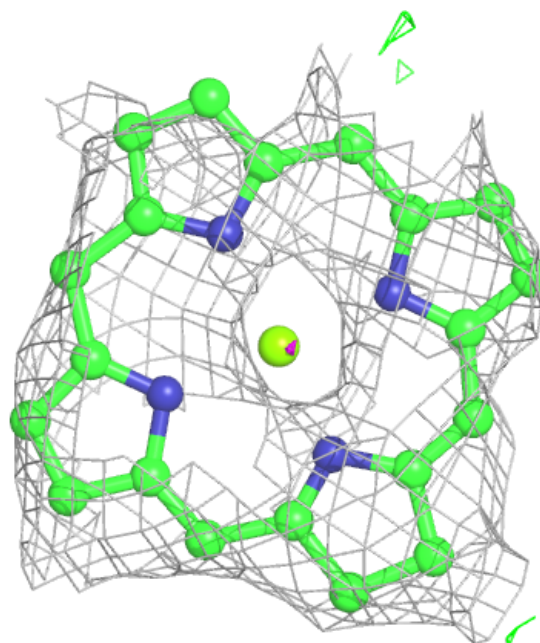
Electron density around CLA 3 1217:

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



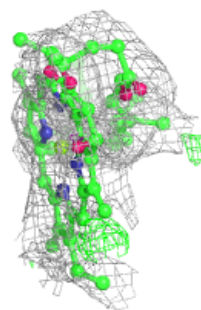
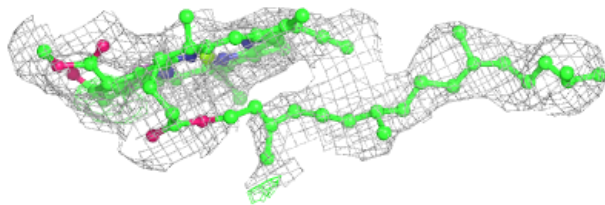
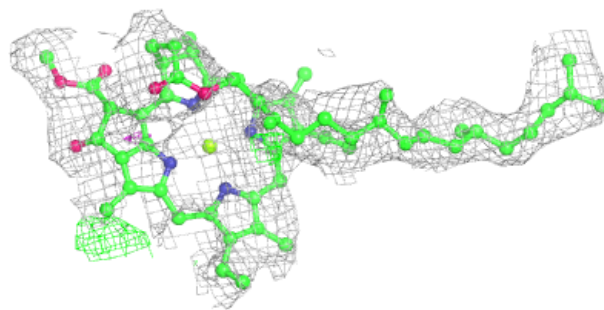
Electron density around CLA 1 1199:

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

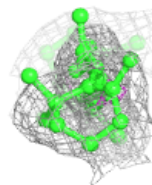
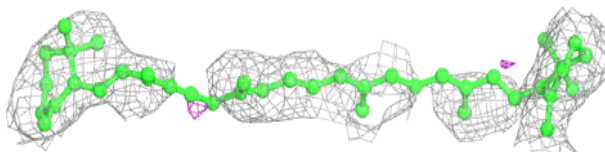
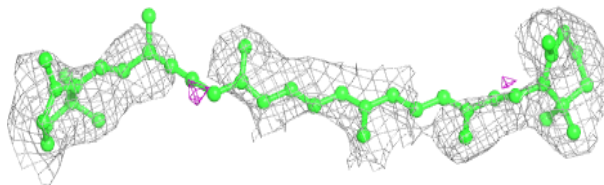


Electron density around CLA 2 1218:

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

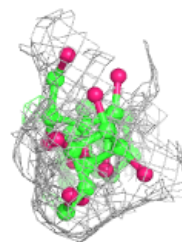
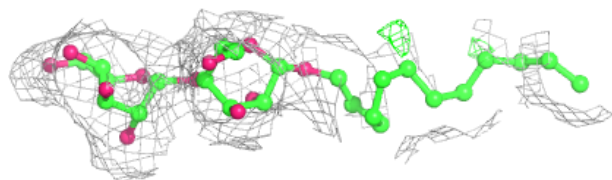
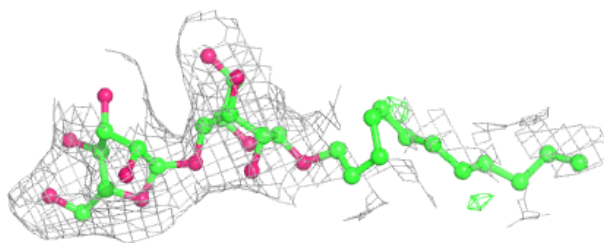
**Electron density around BCR A 1808:**

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



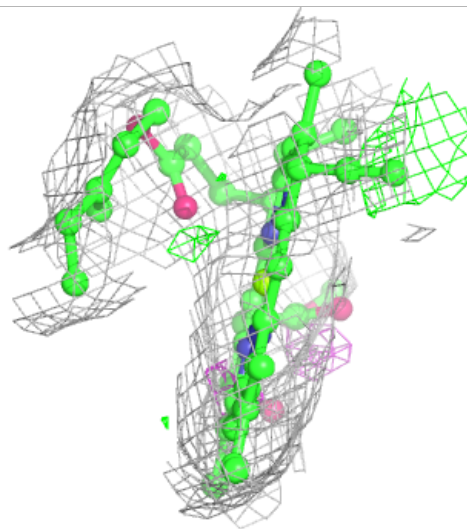
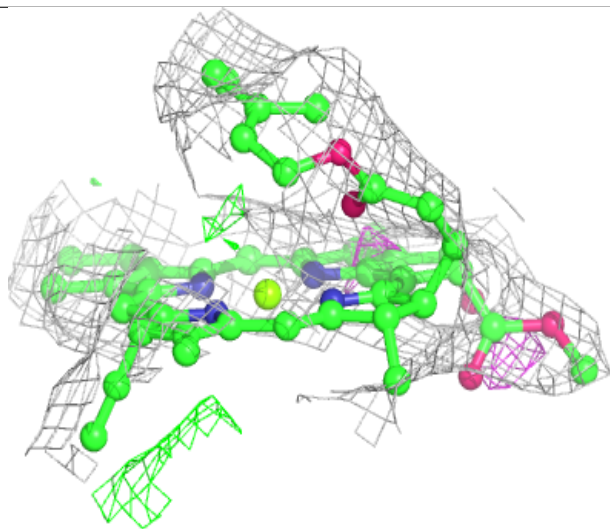
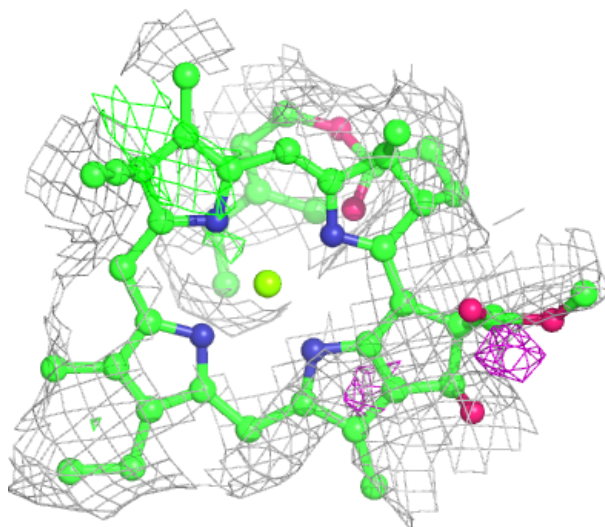
Electron density around LMU A 7037:

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



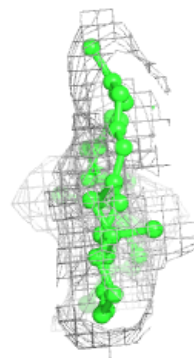
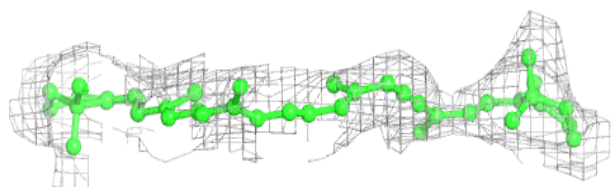
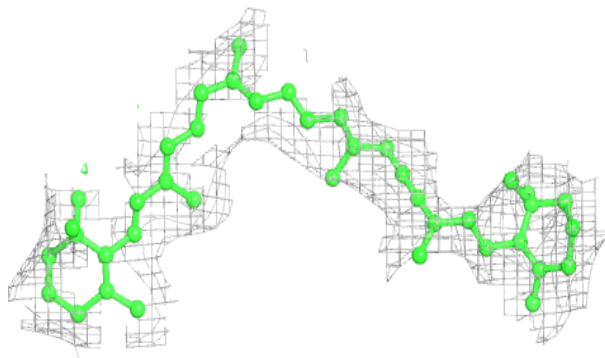
Electron density around CLA 2 1212:

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



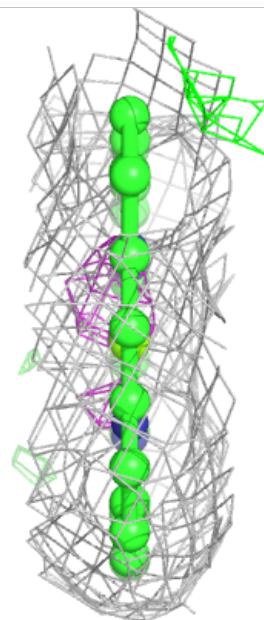
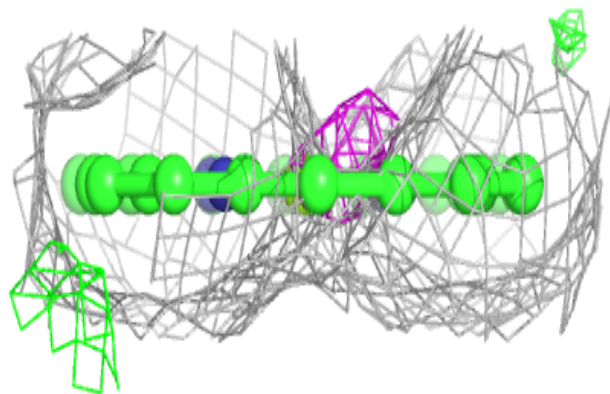
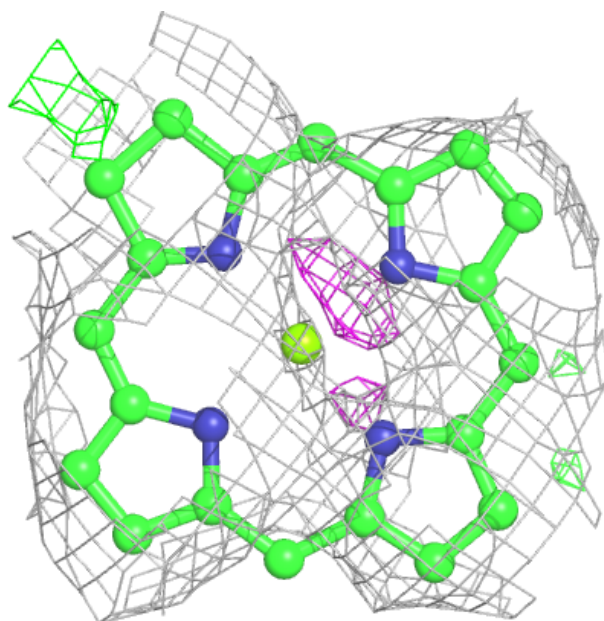
Electron density around BCR 3 1220:

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



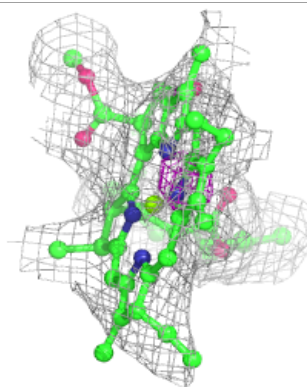
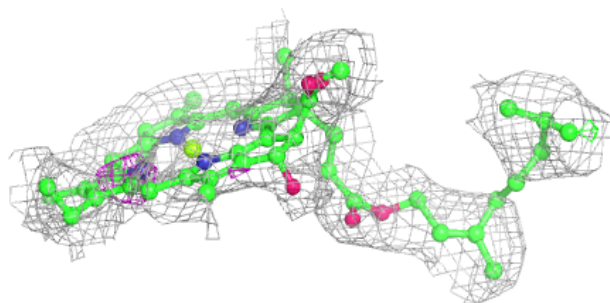
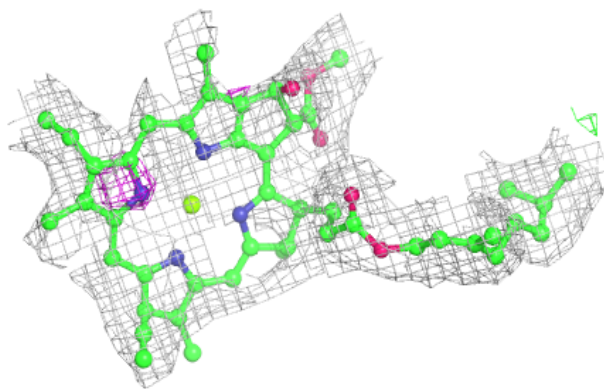
Electron density around CLA 4 4003:

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

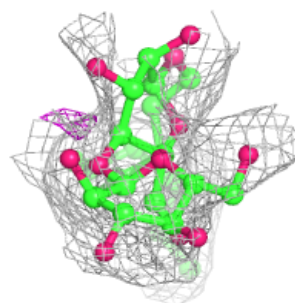
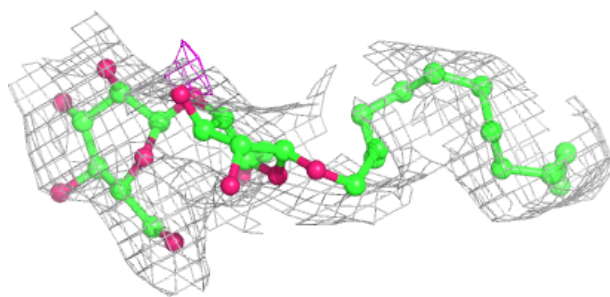
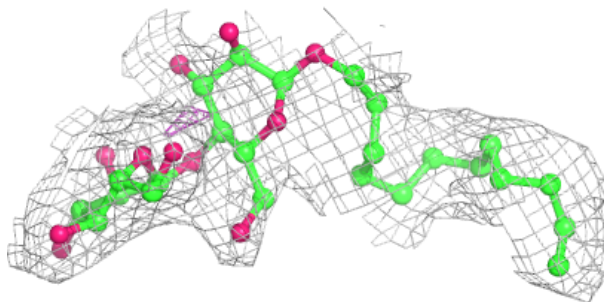


Electron density around CLA I 1033:

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

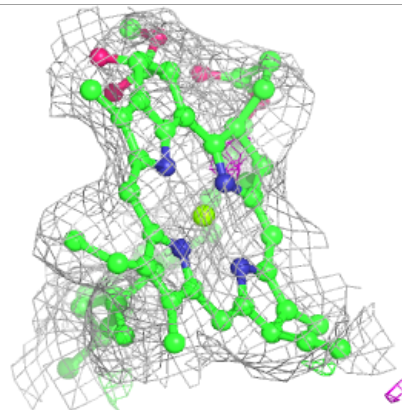
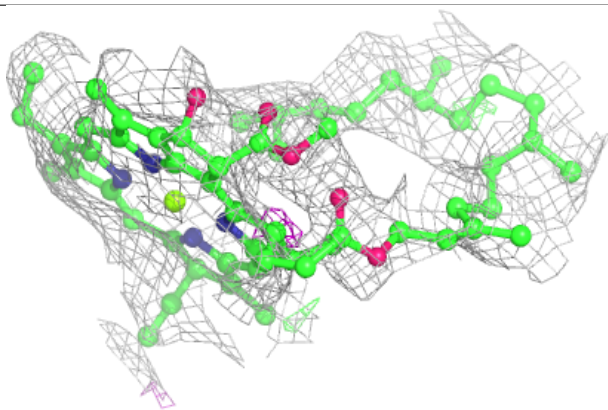
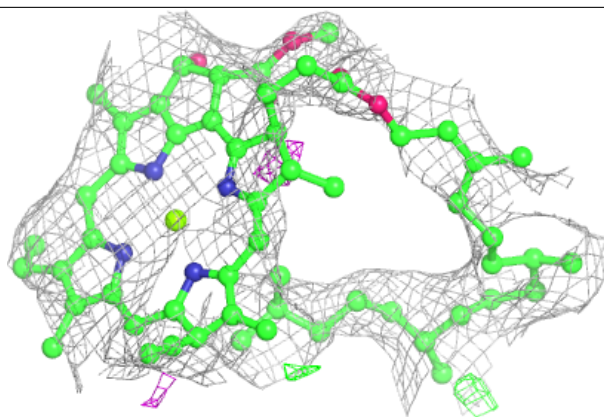
**Electron density around LMU 2 1225:**

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



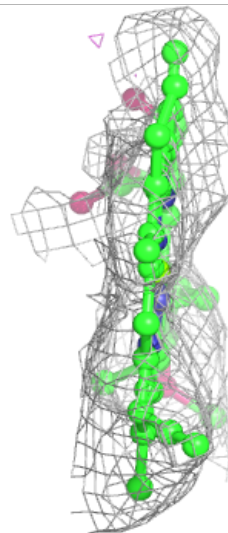
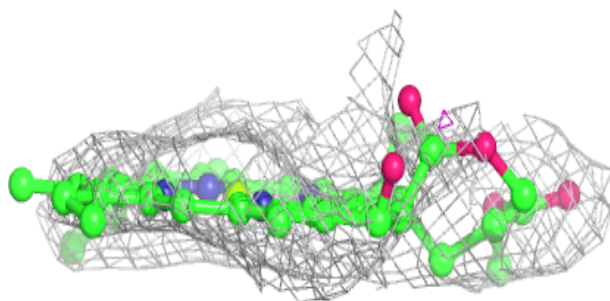
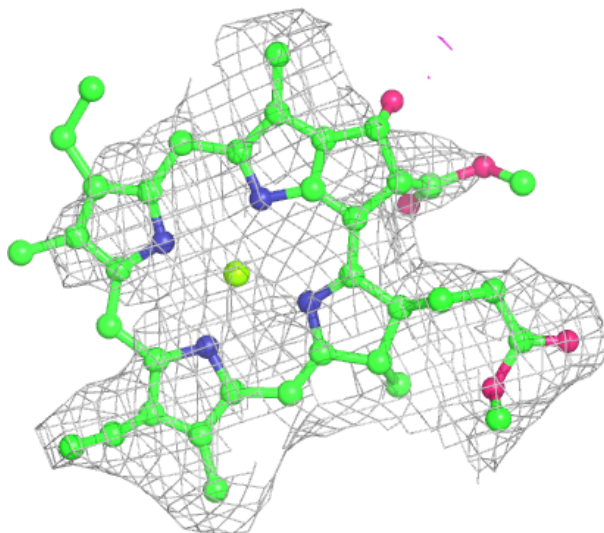
Electron density around CLA A 1797:

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



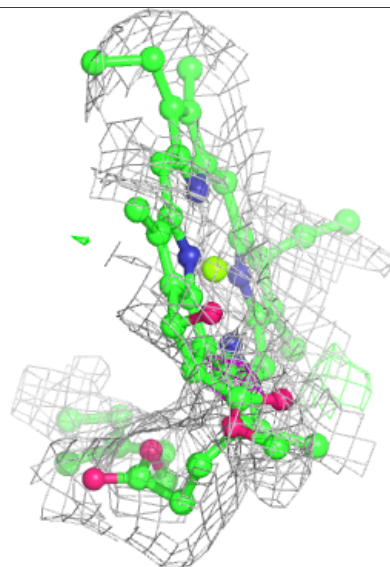
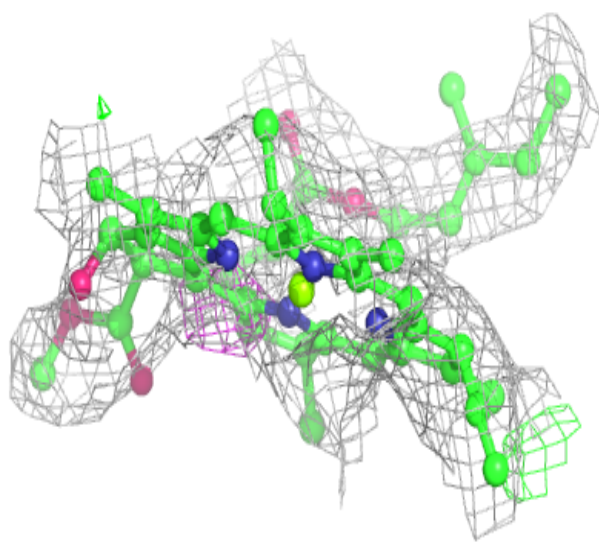
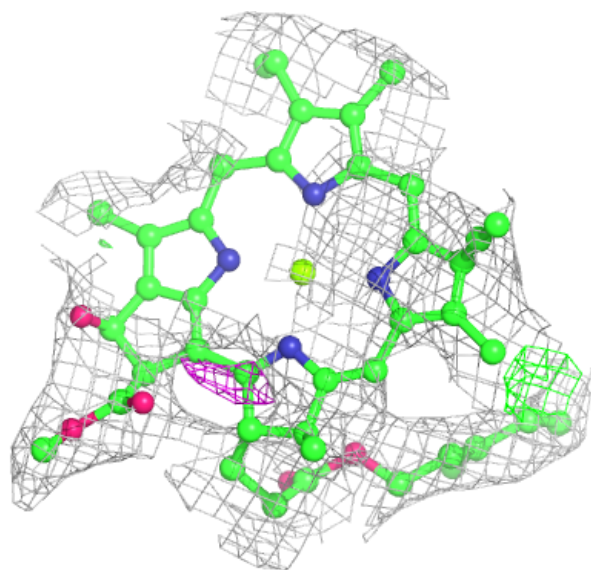
Electron density around CLA B 1746:

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



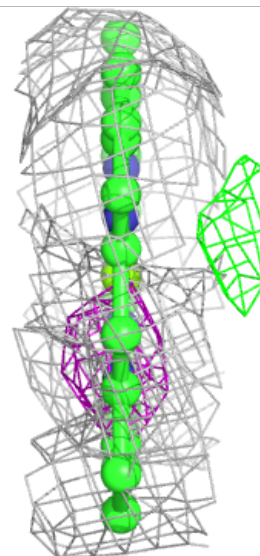
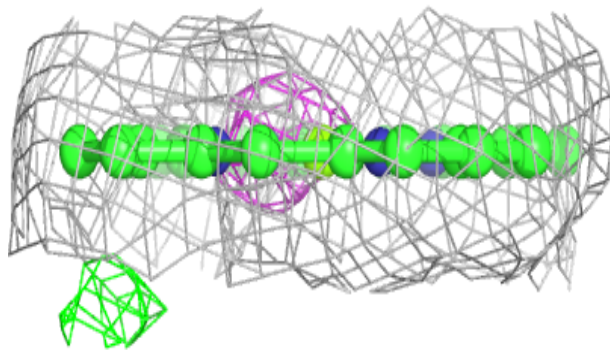
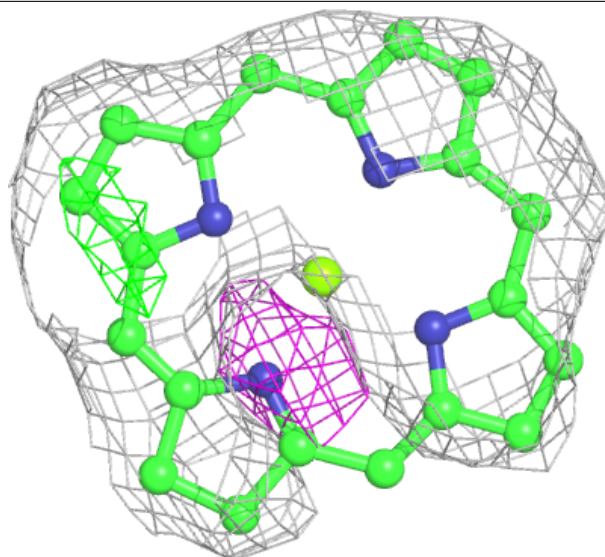
Electron density around CLA B 1766:

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



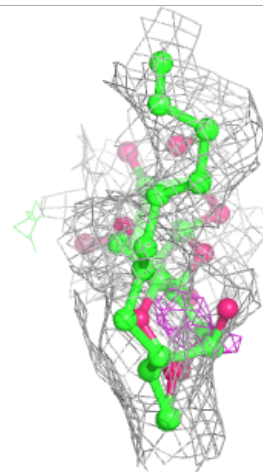
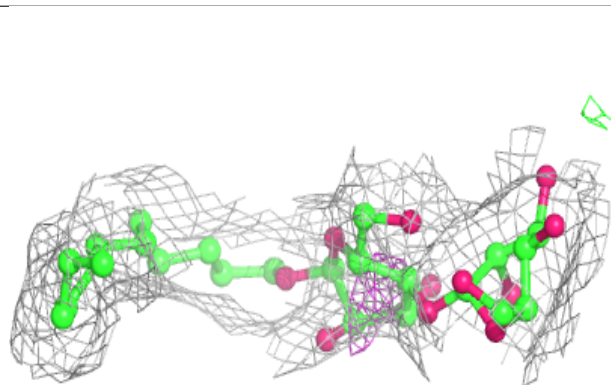
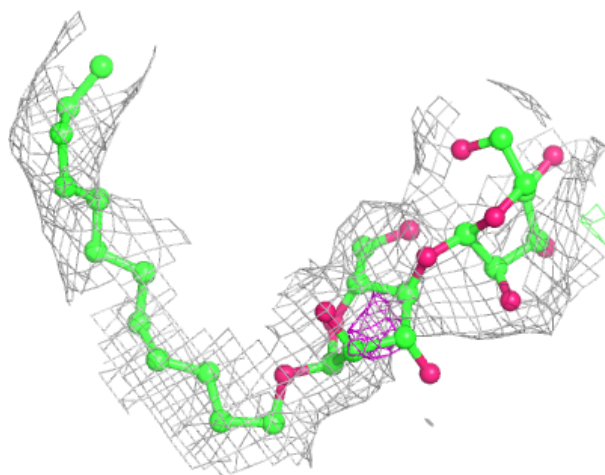
Electron density around CLA 3 1214:

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



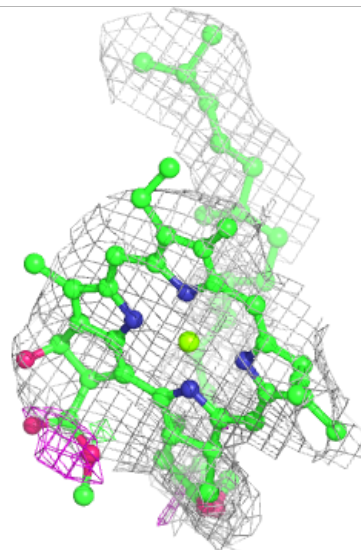
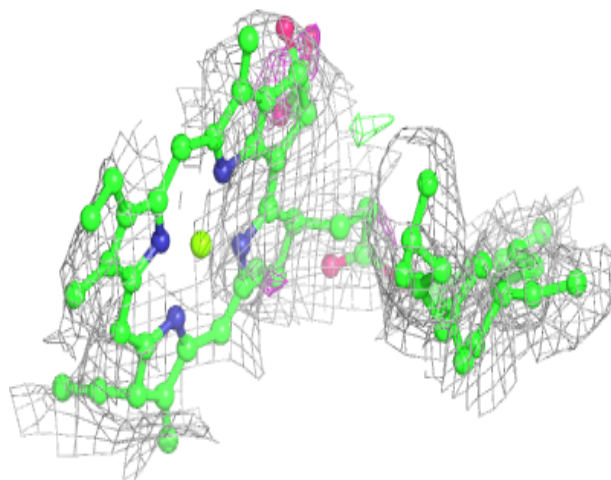
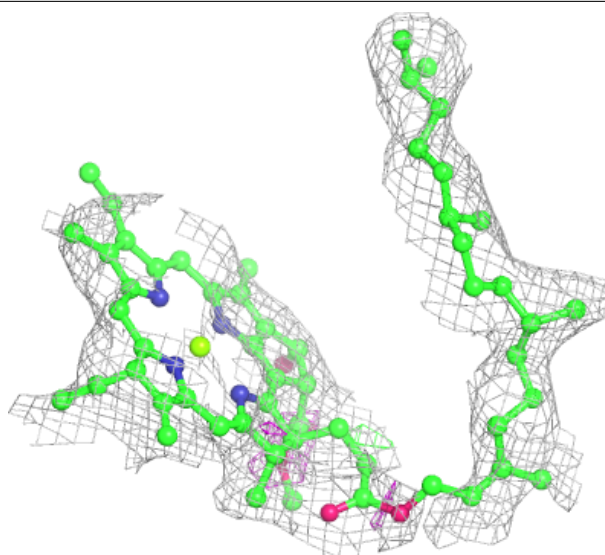
Electron density around LMU A 7041:

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



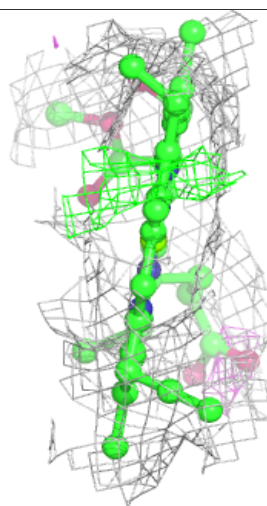
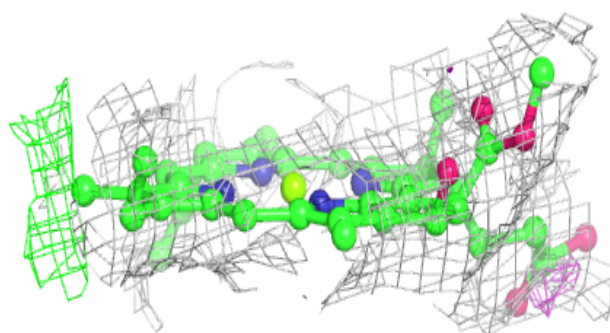
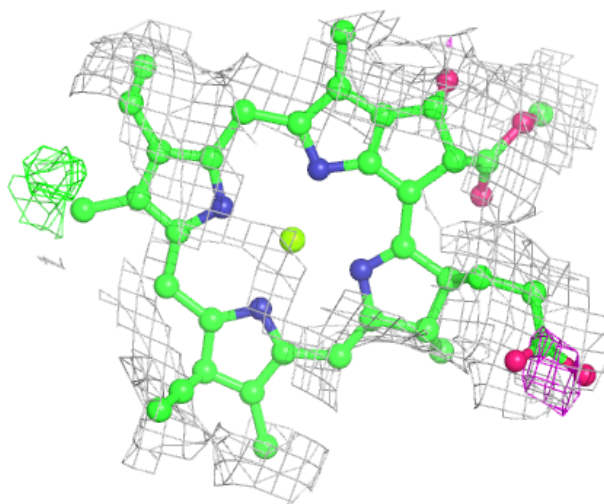
Electron density around CLA 3 1219:

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



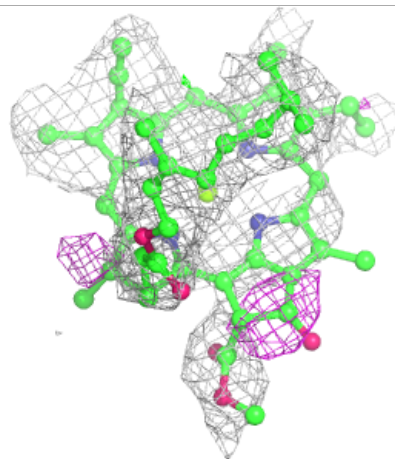
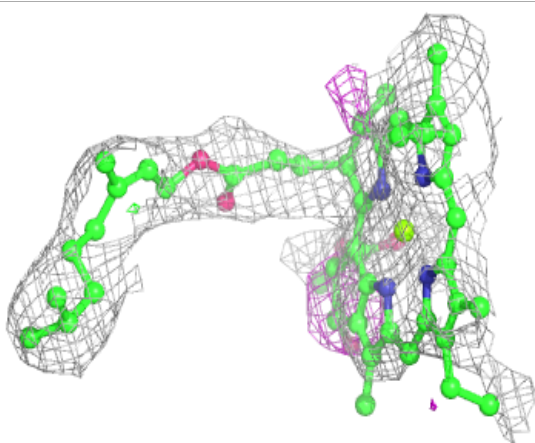
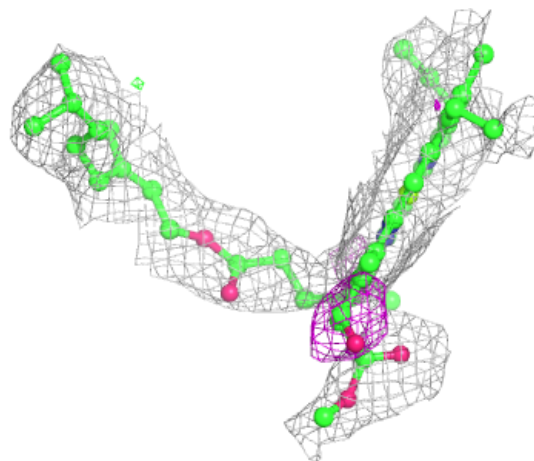
Electron density around CLA K 1142:

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



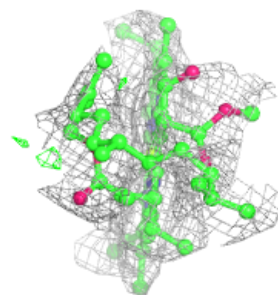
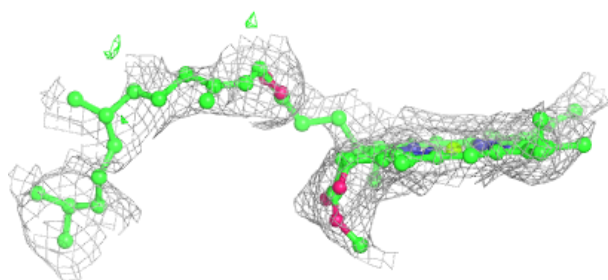
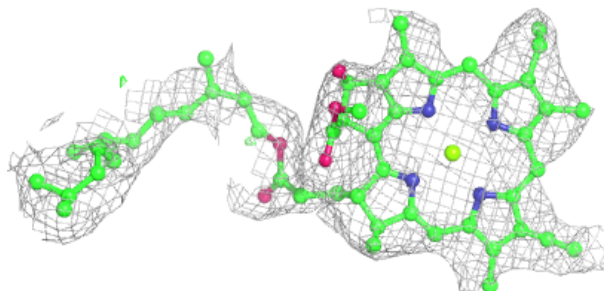
Electron density around CLA A 1801:

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

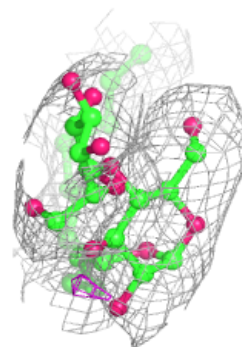
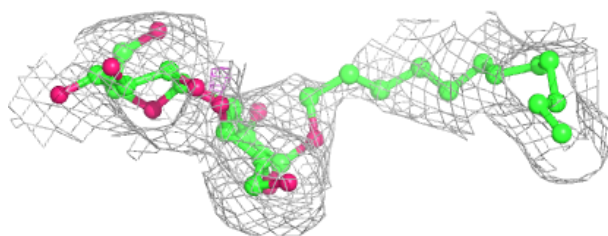
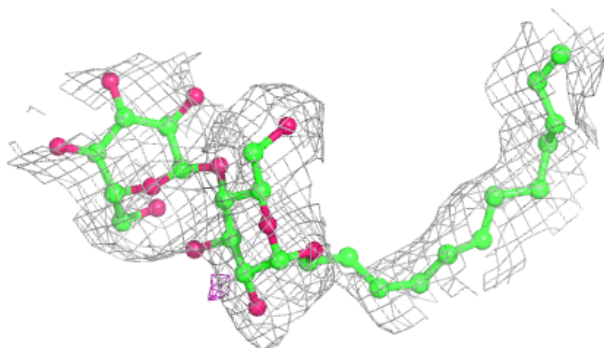


Electron density around CLA B 1745:

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

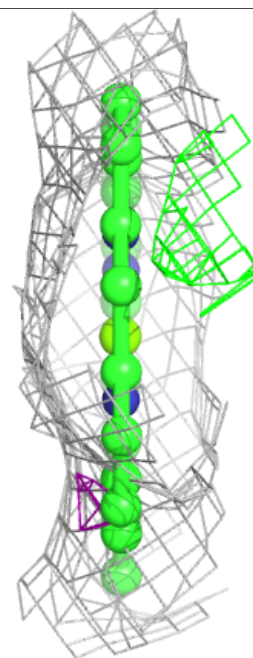
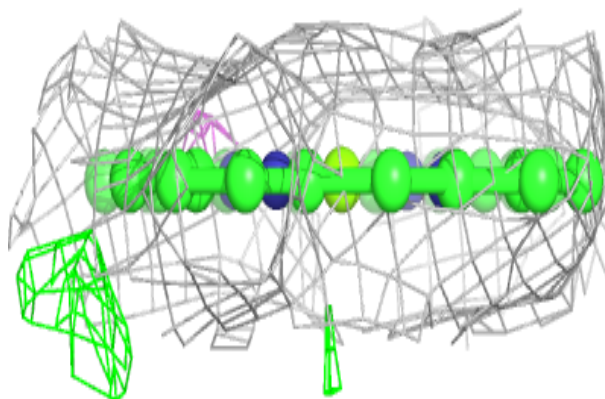
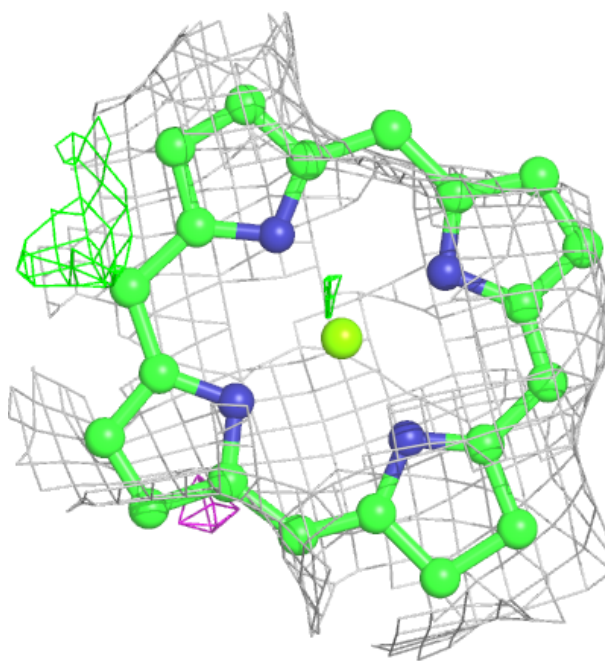
**Electron density around LMU 1 7004:**

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



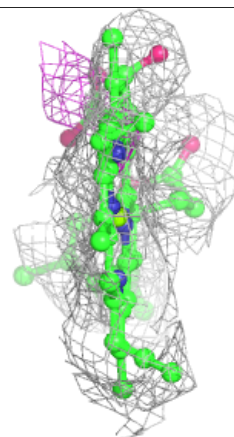
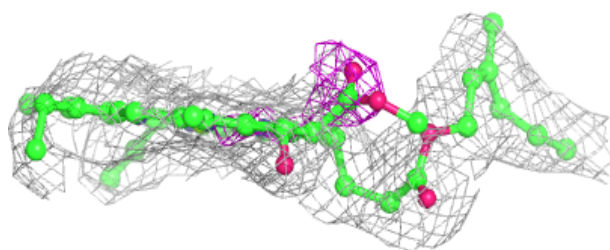
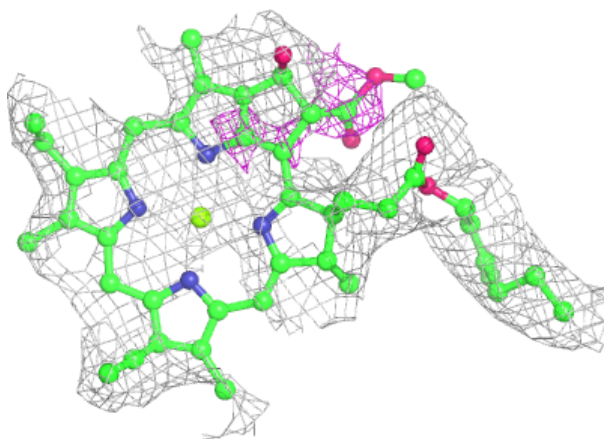
Electron density around CLA 2 1216:

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



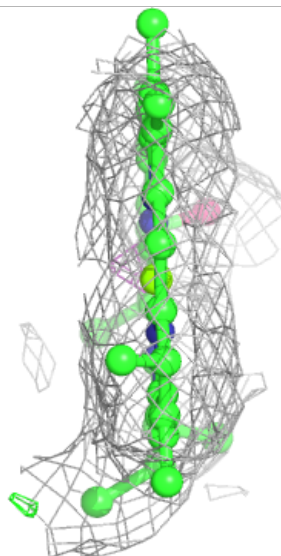
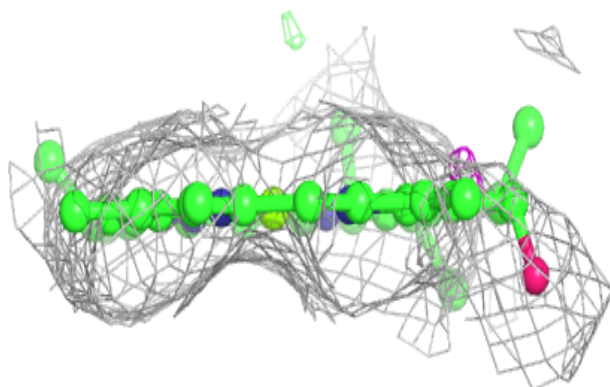
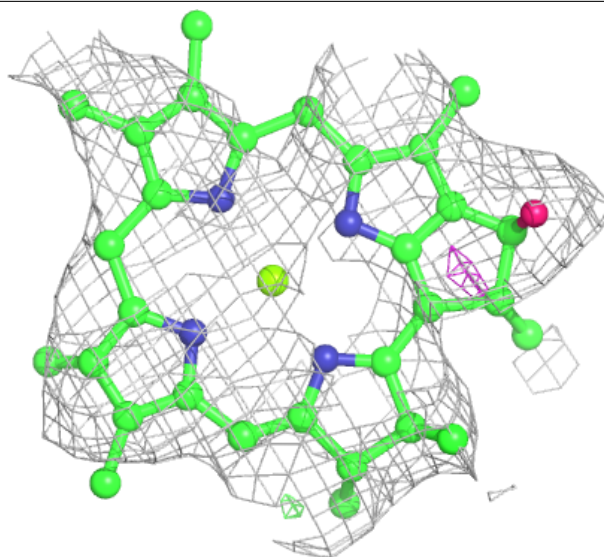
Electron density around CLA 4 4007:

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



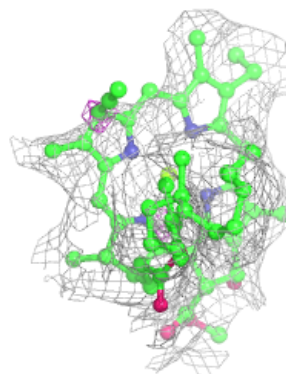
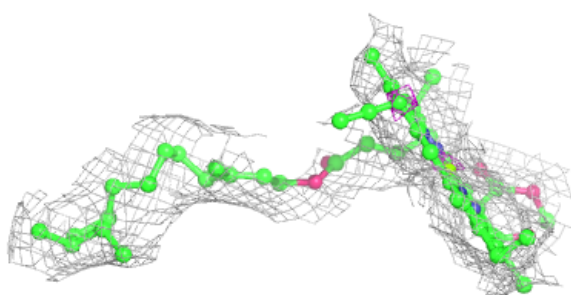
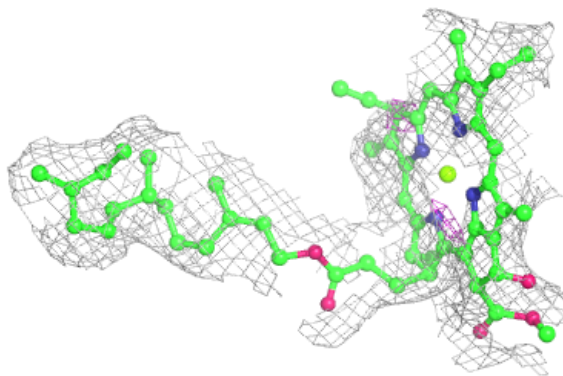
Electron density around CLA 1 1191:

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

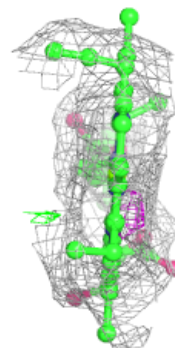
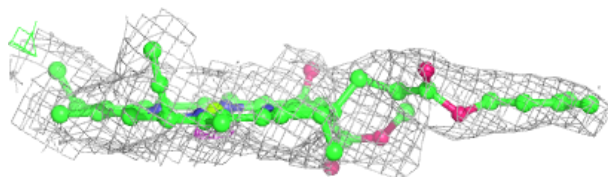
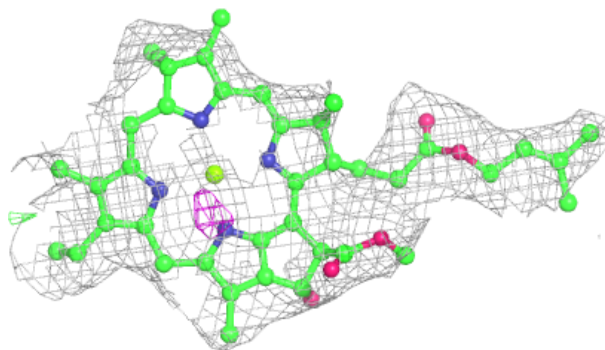


Electron density around CLA J 1044:

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

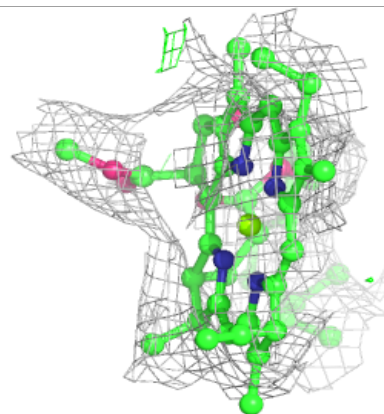
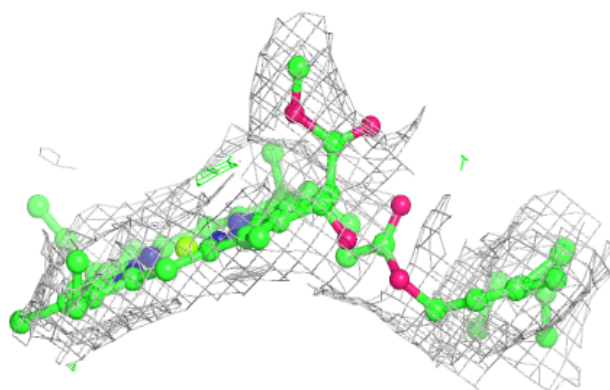
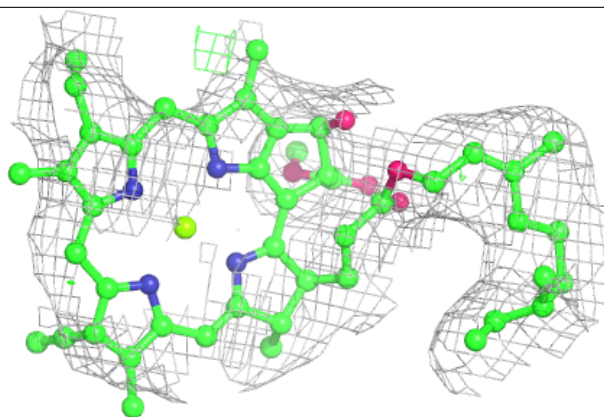
**Electron density around CLA A 1799:**

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

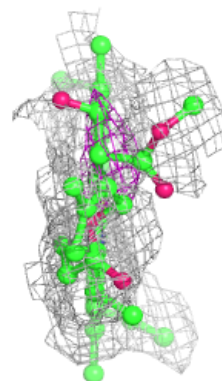
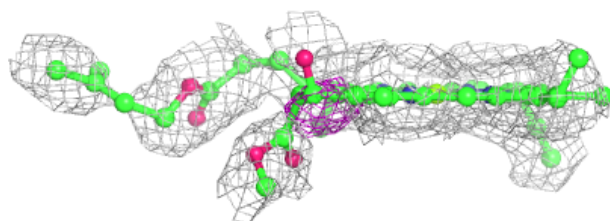
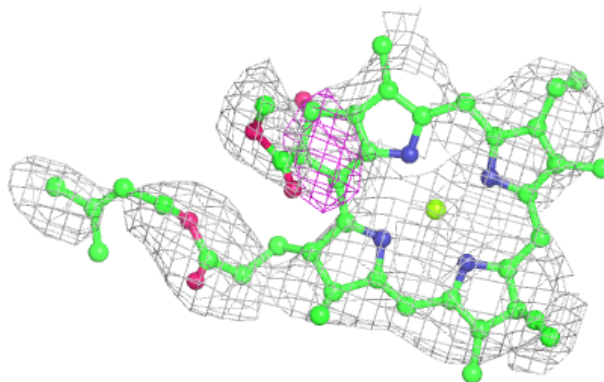


Electron density around CLA 2 1220:

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

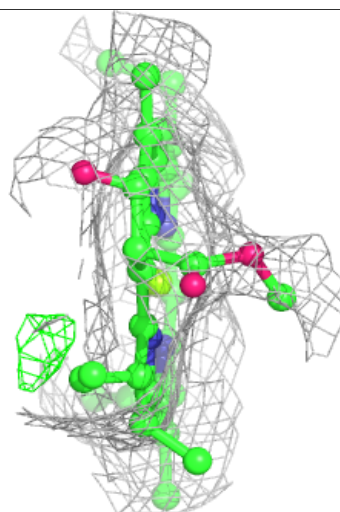
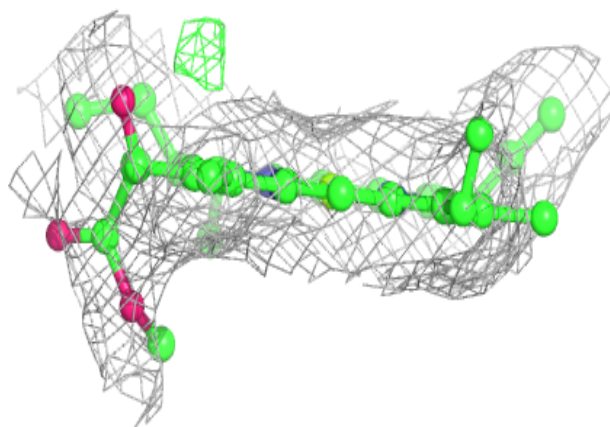
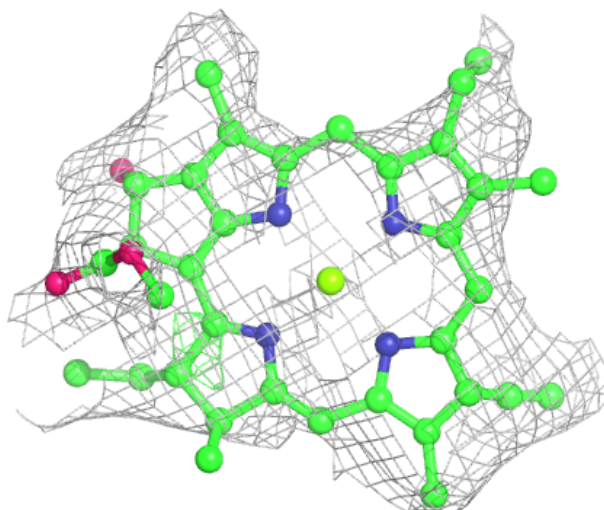
**Electron density around CLA 4 1200:**

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



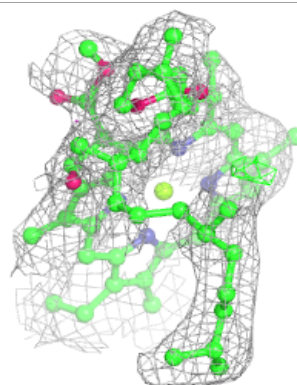
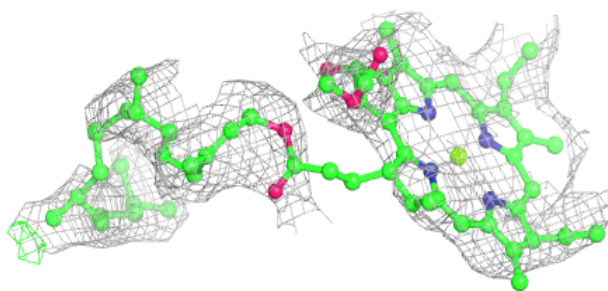
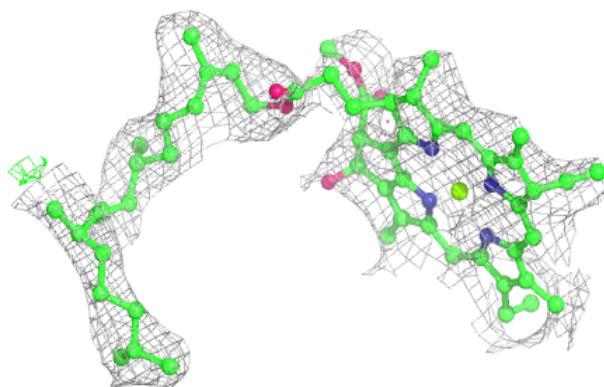
Electron density around CLA 3 3007:

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

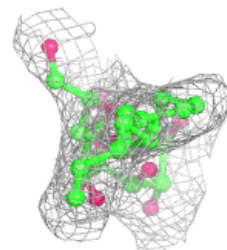
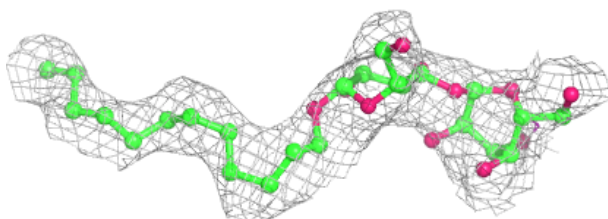
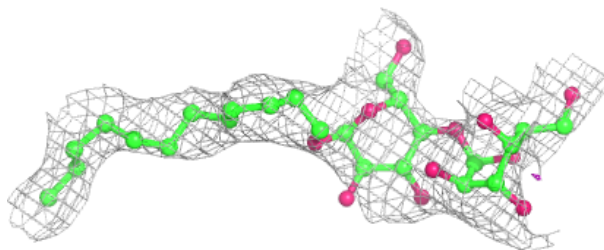


Electron density around CLA K 3009:

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

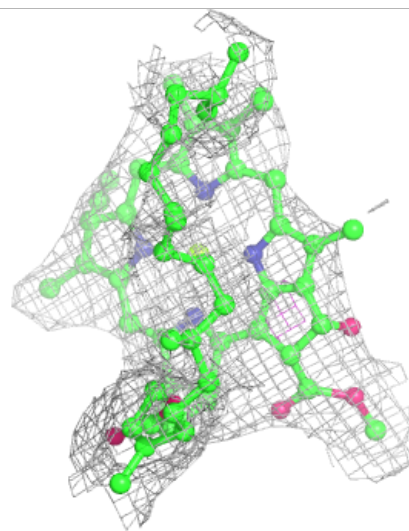
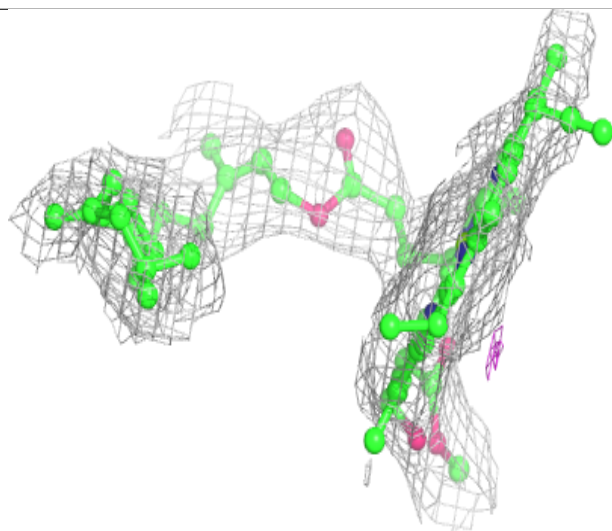
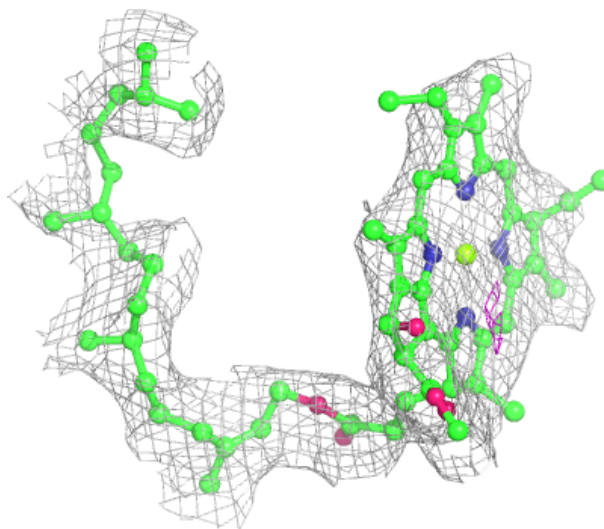
**Electron density around LMU A 7010:**

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



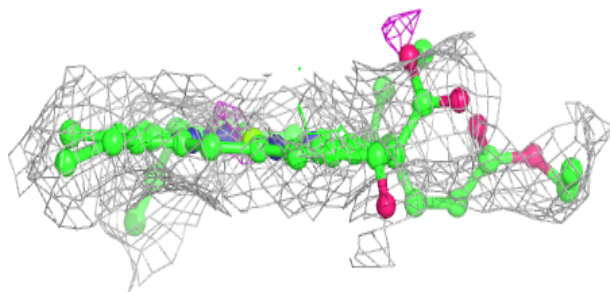
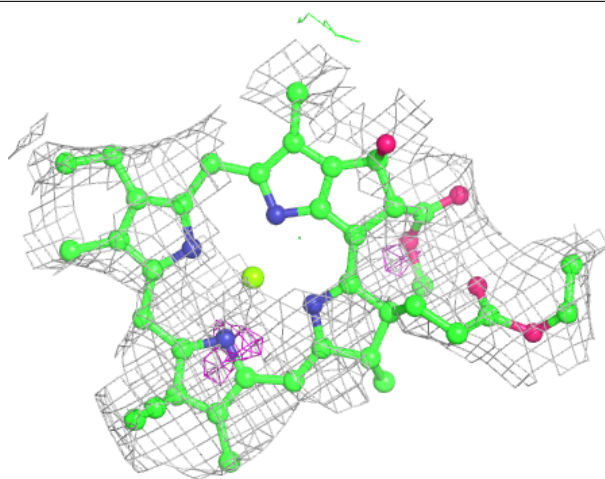
Electron density around CLA 3 1218:

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



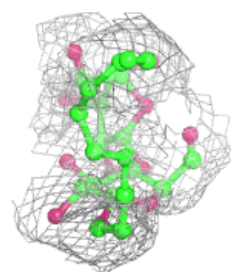
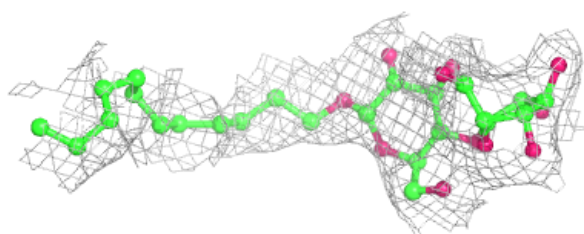
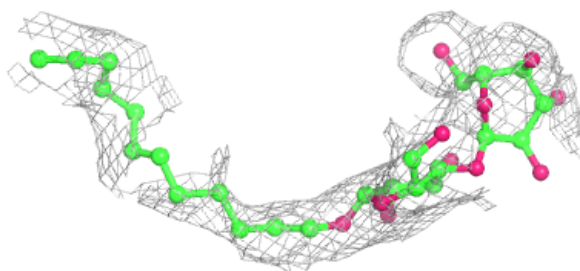
Electron density around CLA 4 4014:

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



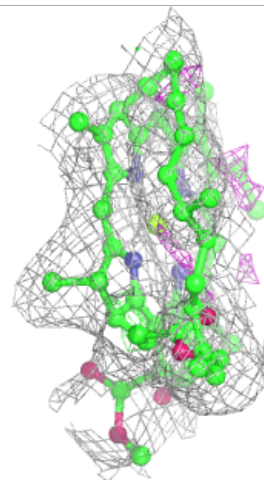
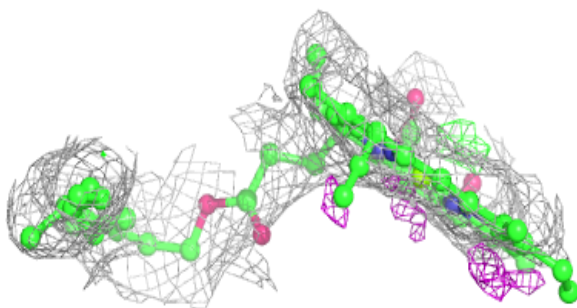
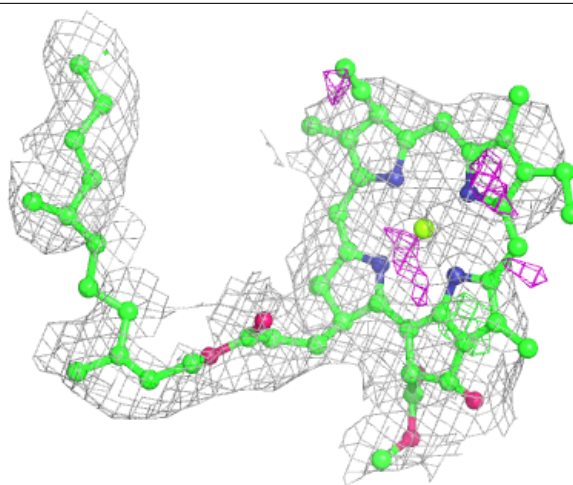
Electron density around LMU A 7017:

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



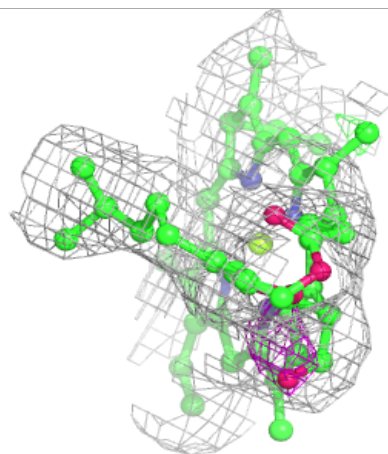
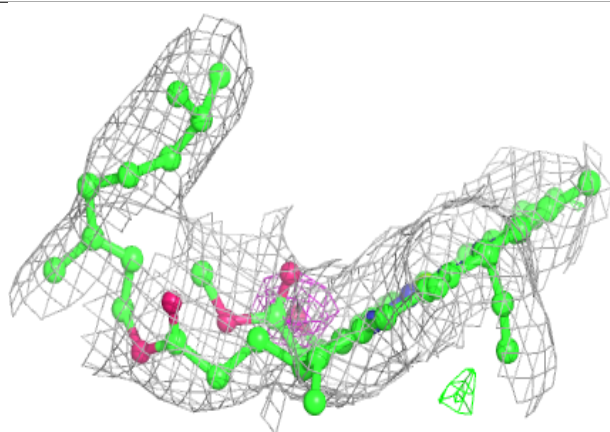
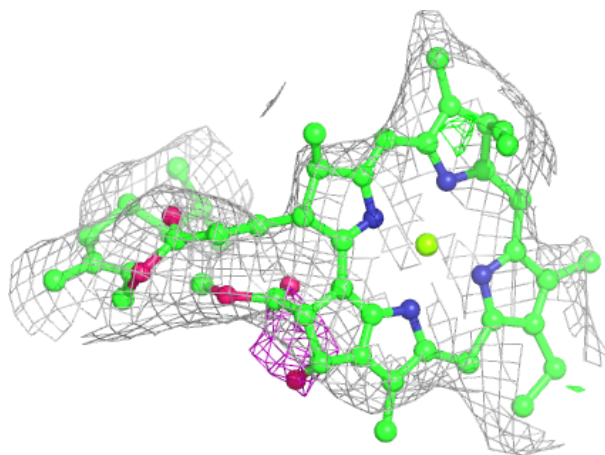
Electron density around CLA B 1755:

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



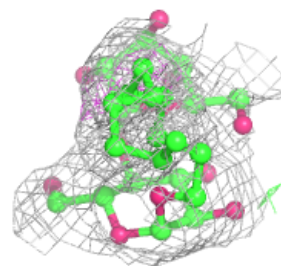
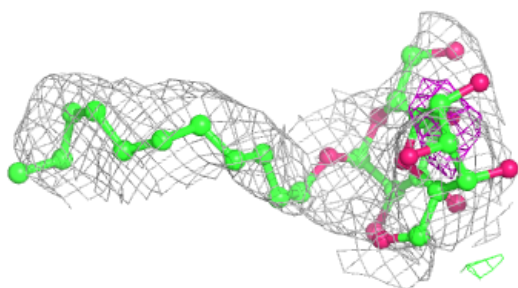
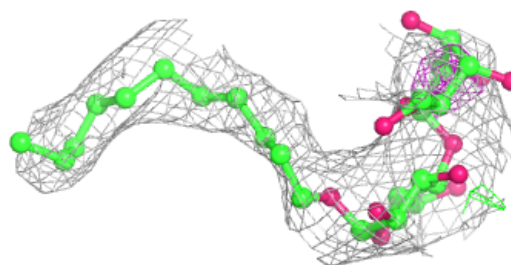
Electron density around CLA A 1816:

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



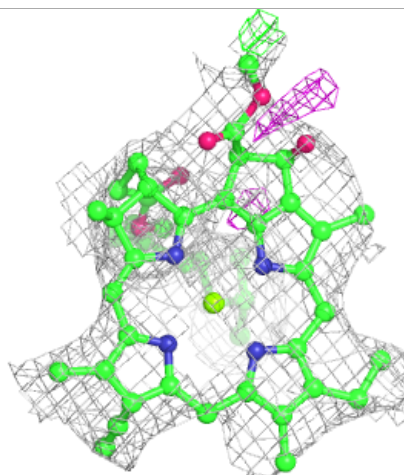
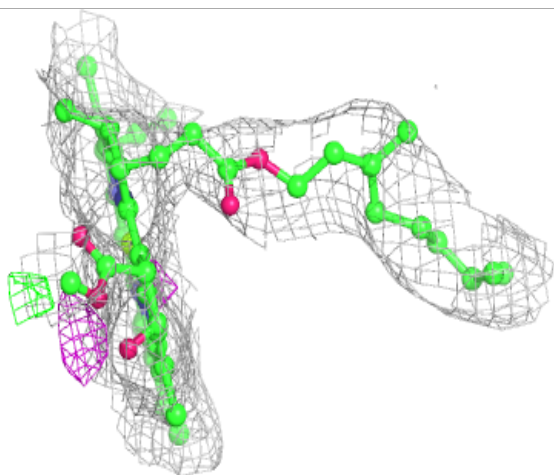
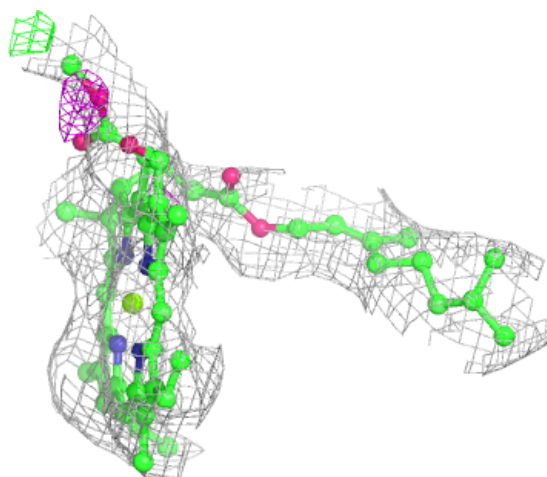
Electron density around LMU A 7009:

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



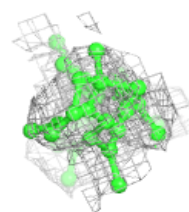
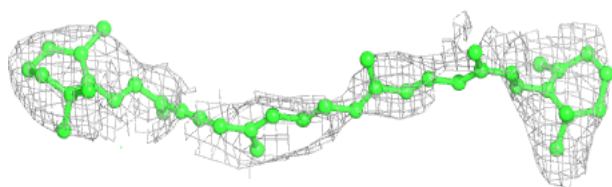
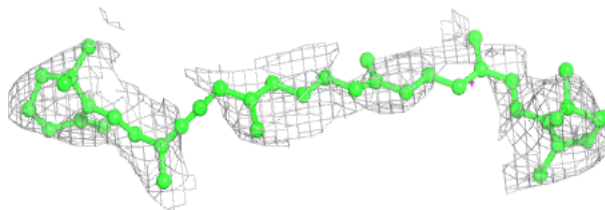
Electron density around CLA 4 1196:

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

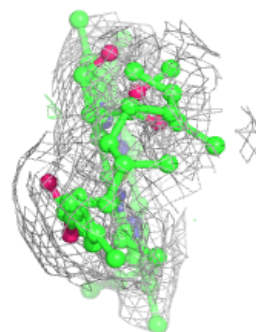
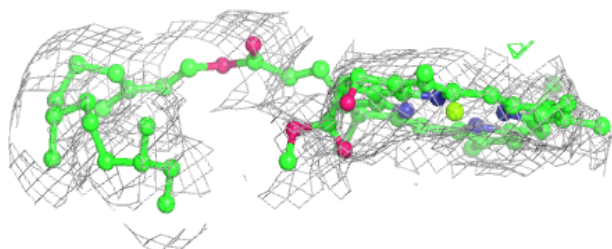
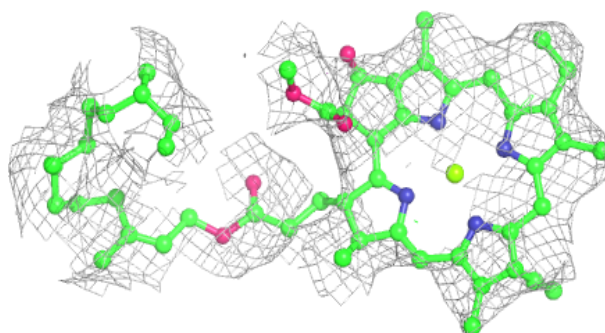


Electron density around BCR A 1805:

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

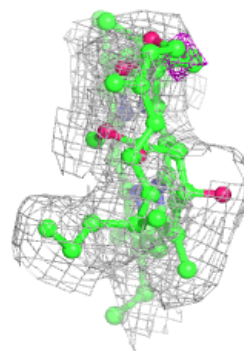
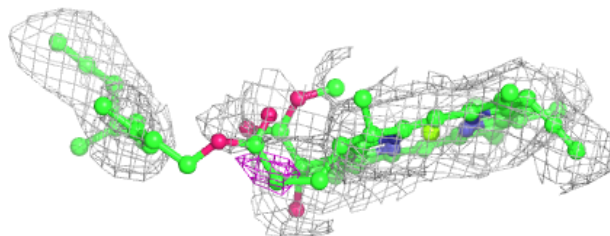
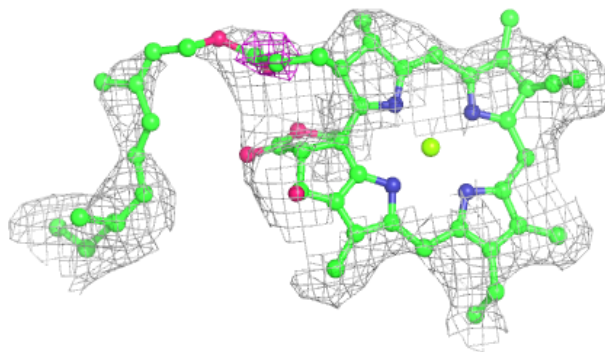
**Electron density around CLA 1 1198:**

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



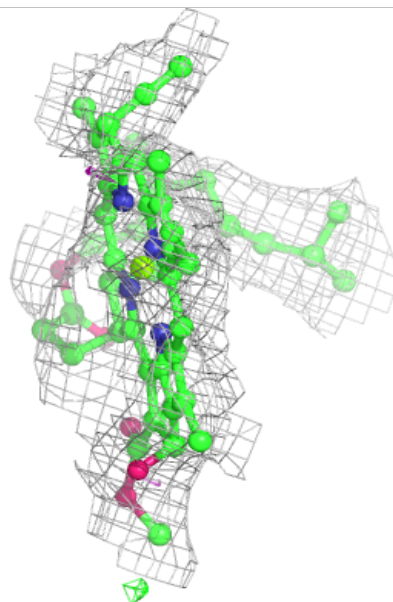
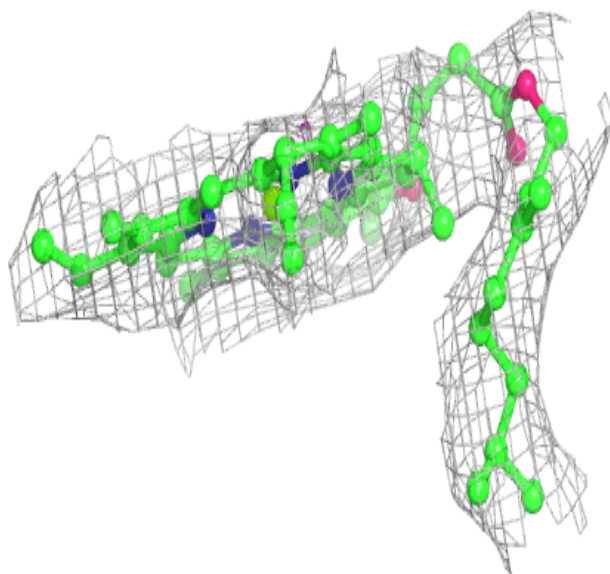
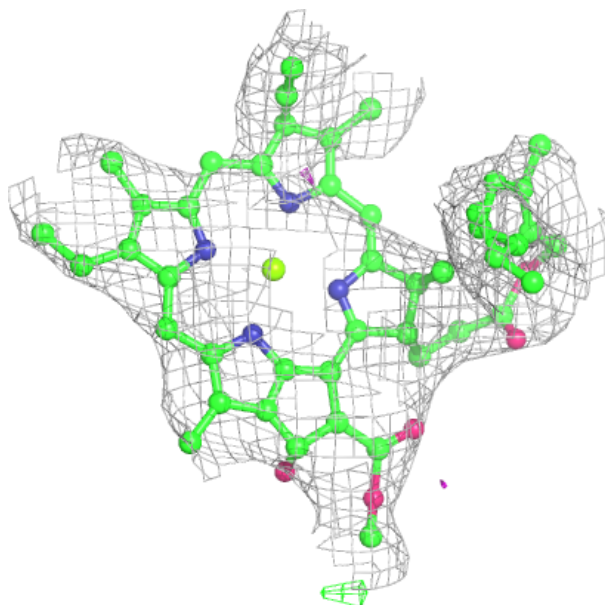
Electron density around CLA R 1054:

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



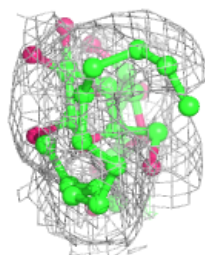
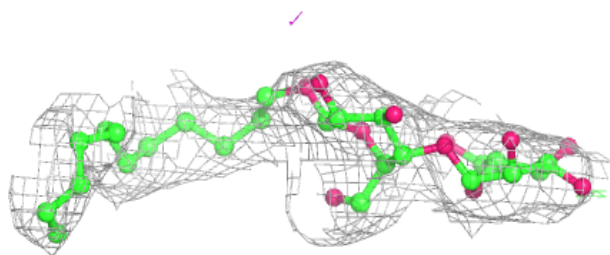
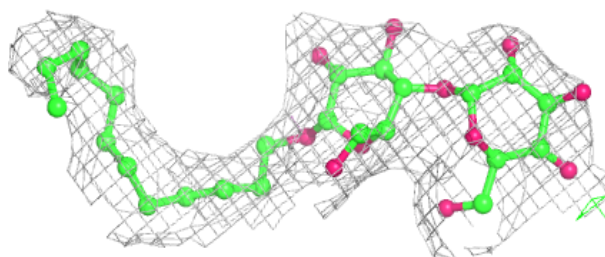
Electron density around CLA A 1815:

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

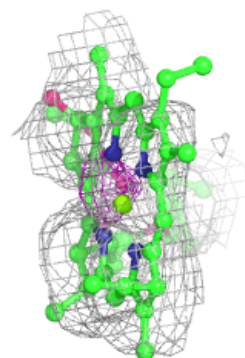
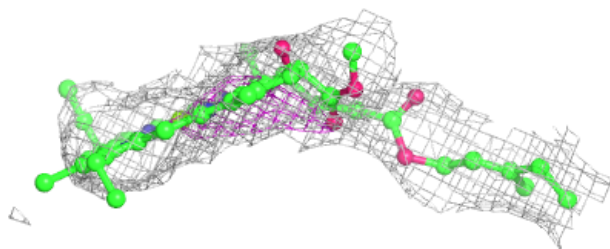
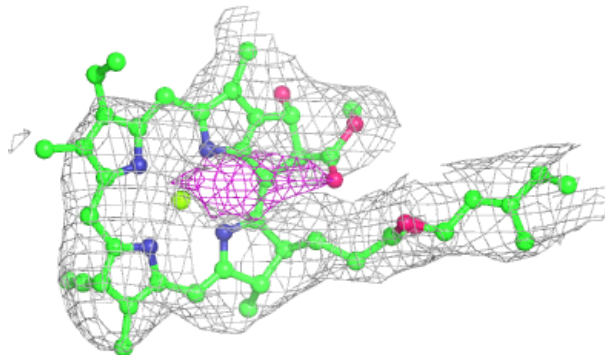


Electron density around LMU A 7015:

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

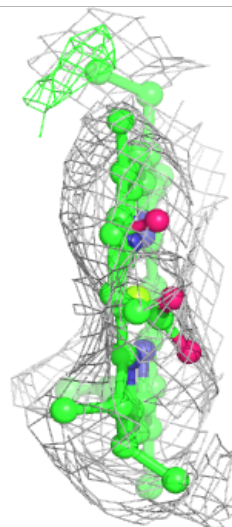
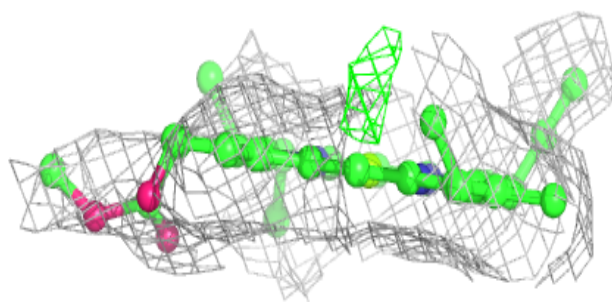
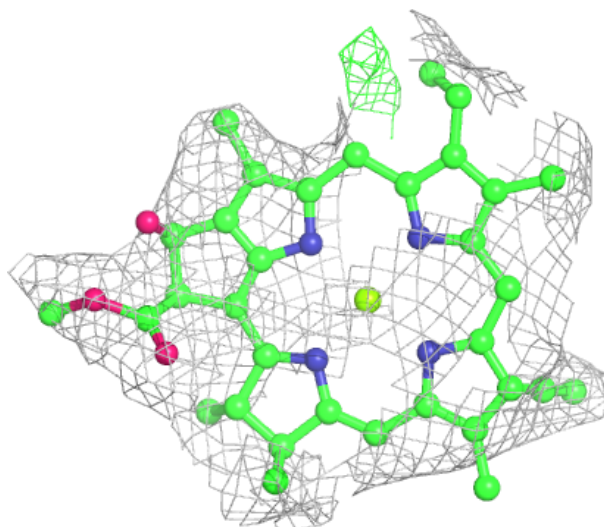
**Electron density around CLA 1 1197:**

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



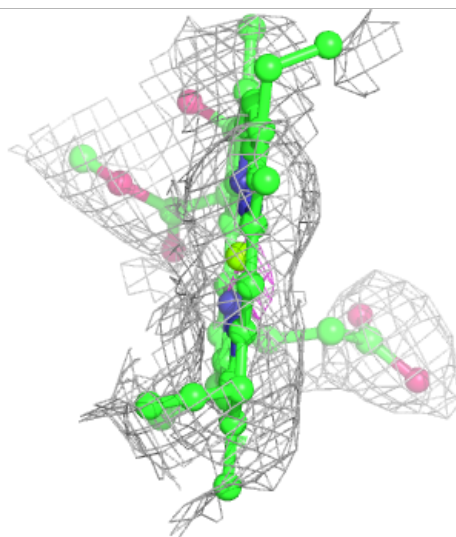
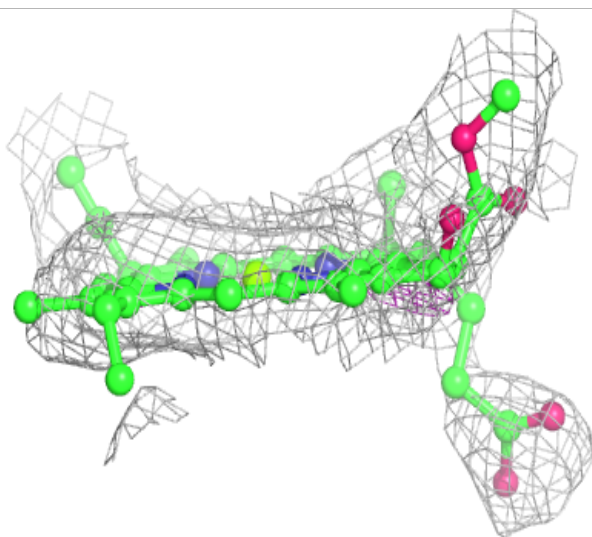
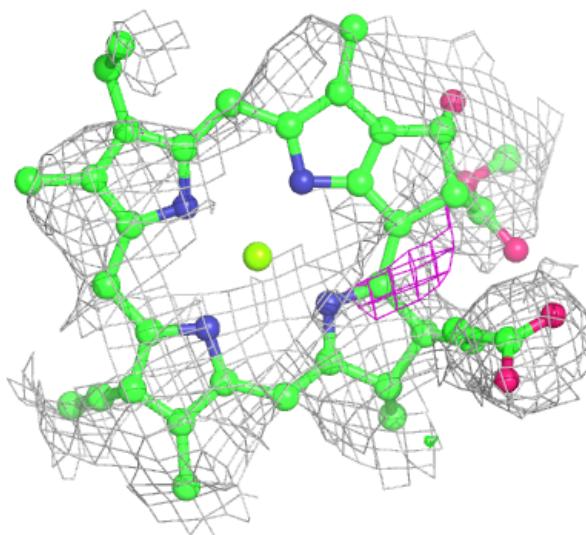
Electron density around CLA F 1156:

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



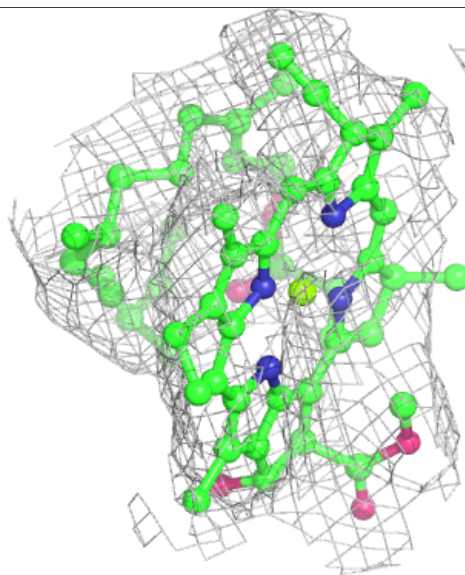
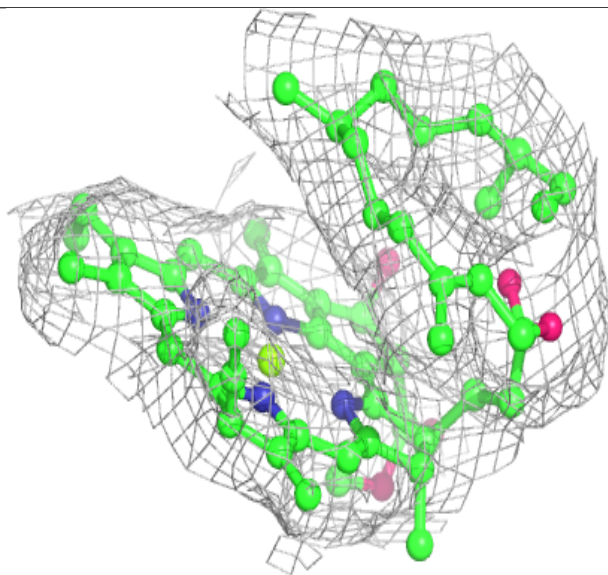
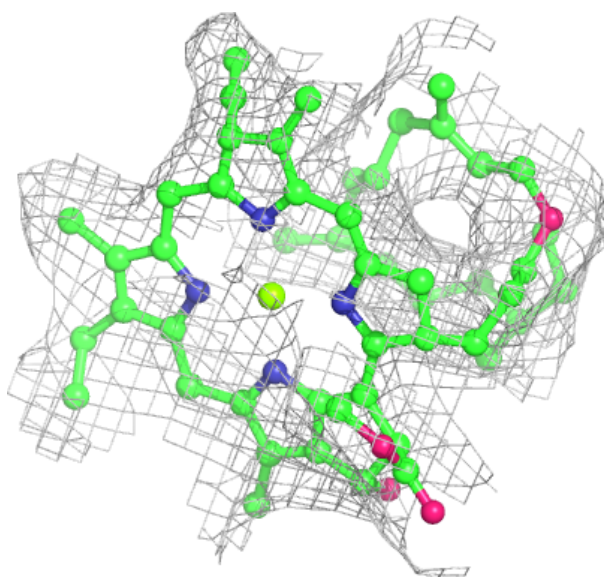
Electron density around CLA B 1765:

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



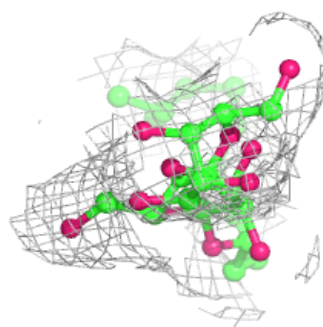
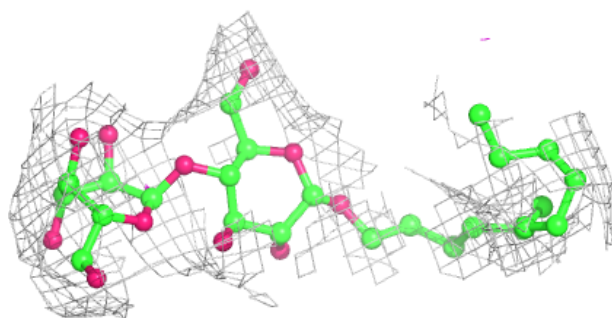
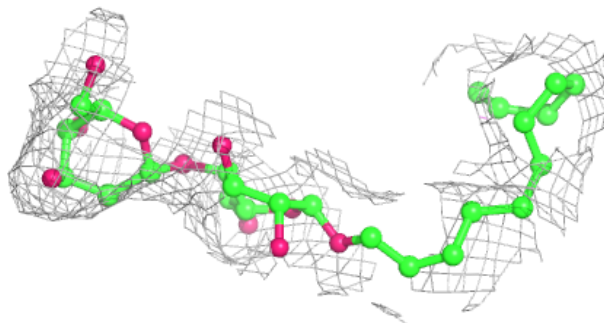
Electron density around CLA J 1043:

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

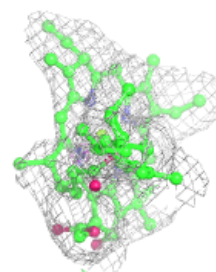
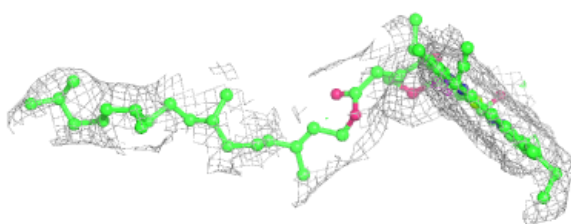
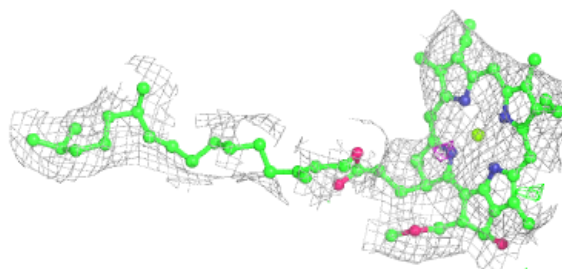


Electron density around LMU A 7043:

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

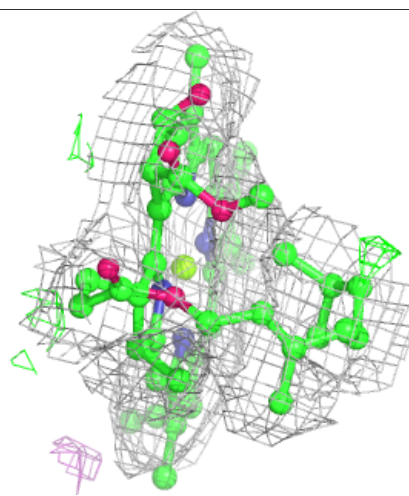
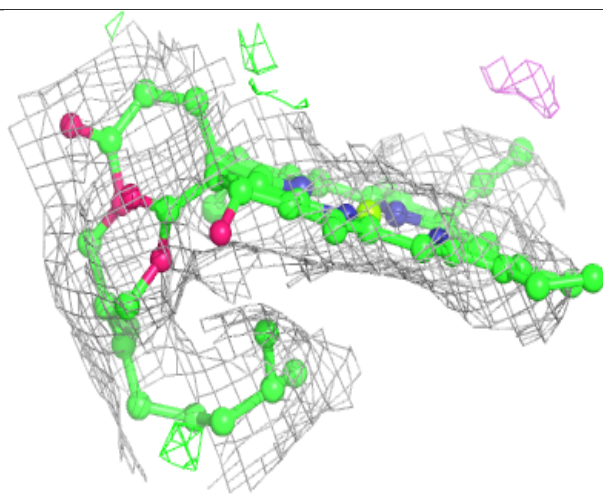
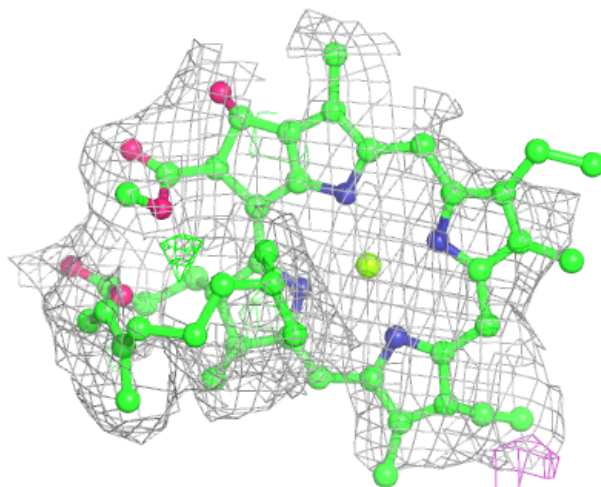
**Electron density around CLA 4 1198:**

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



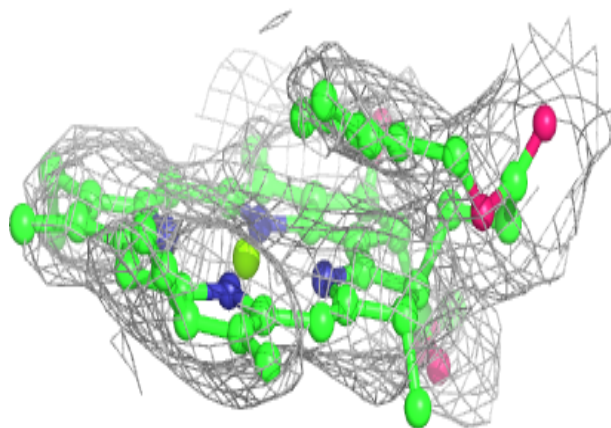
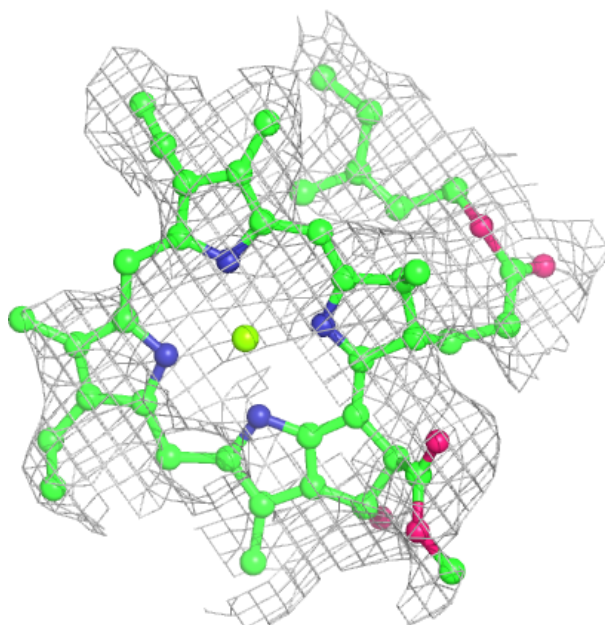
Electron density around CLA 4 1199:

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



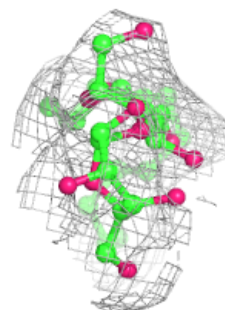
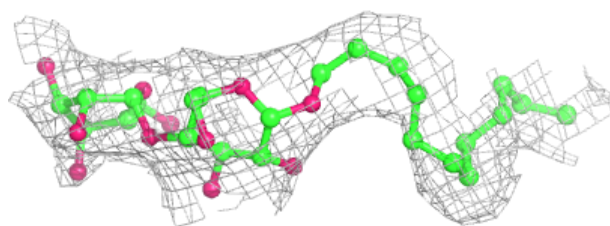
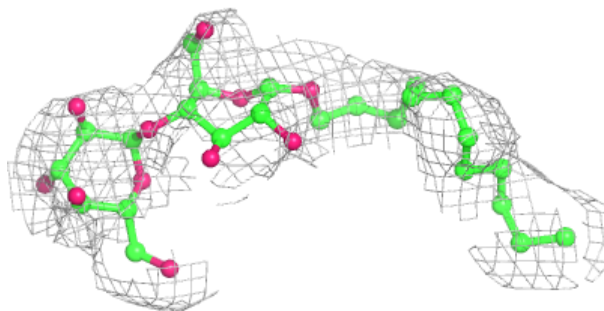
Electron density around CLA G 1099:

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

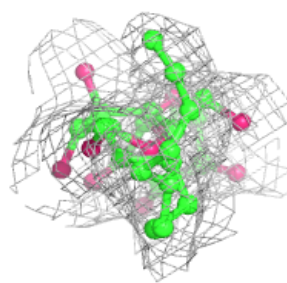
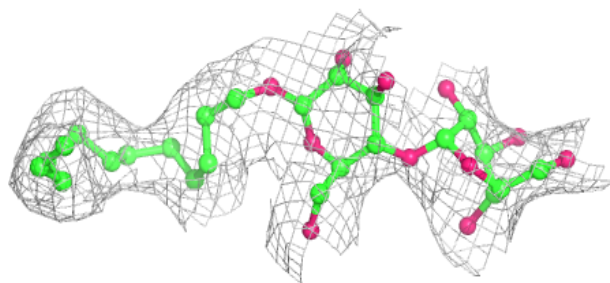
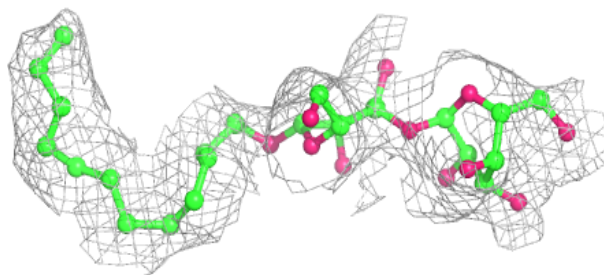


Electron density around LMU A 7034:

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

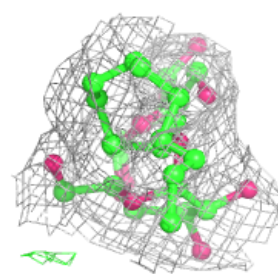
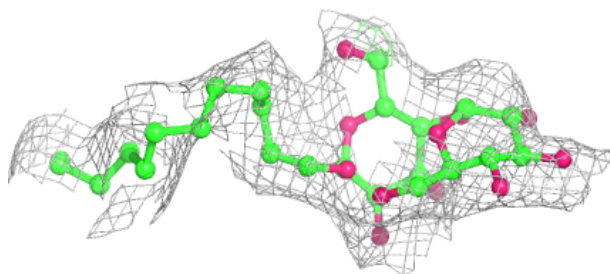
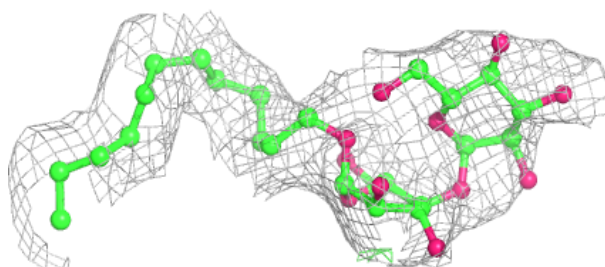
**Electron density around LMU A 1809:**

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

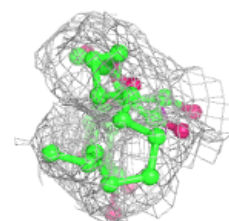
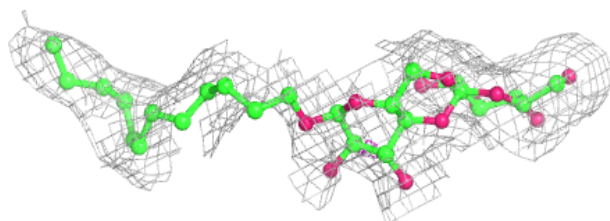
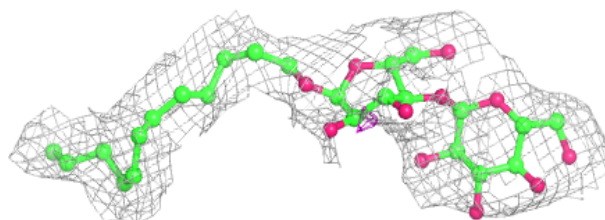


Electron density around LMU A 1810:

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

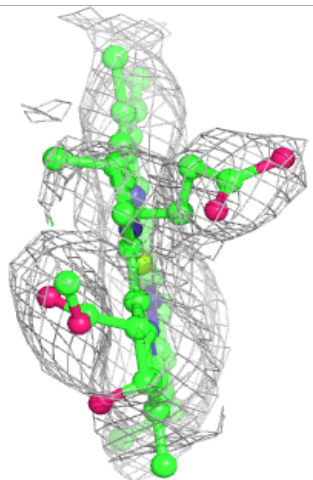
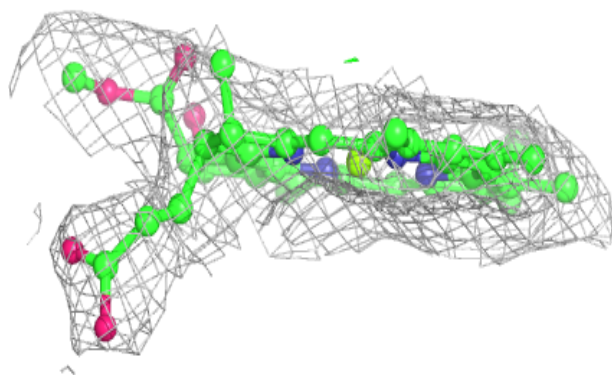
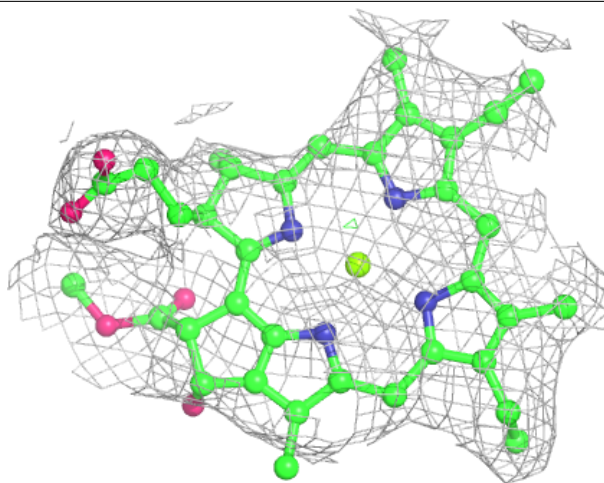
**Electron density around LMU A 7038:**

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



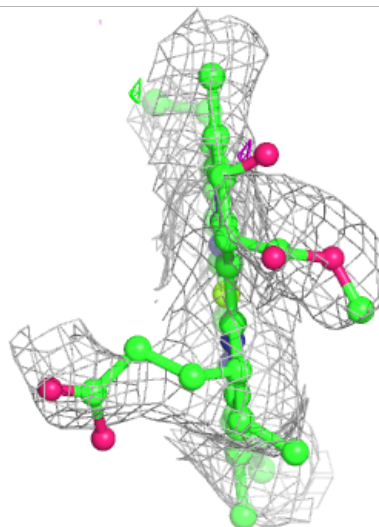
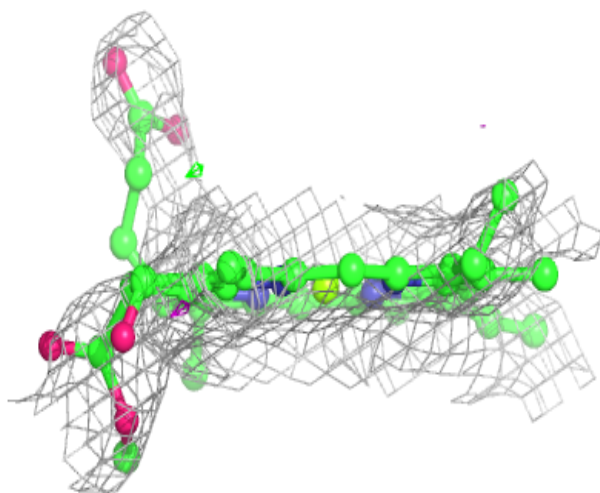
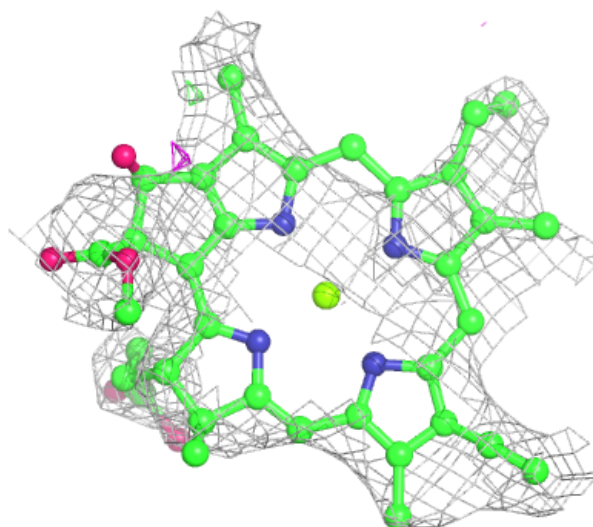
Electron density around CLA A 1766:

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



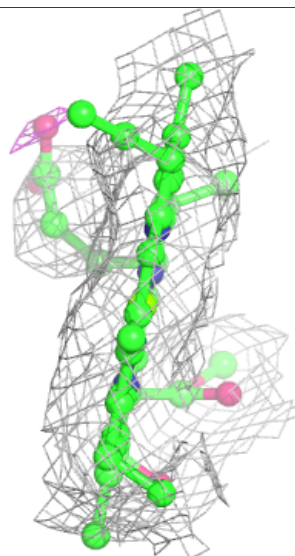
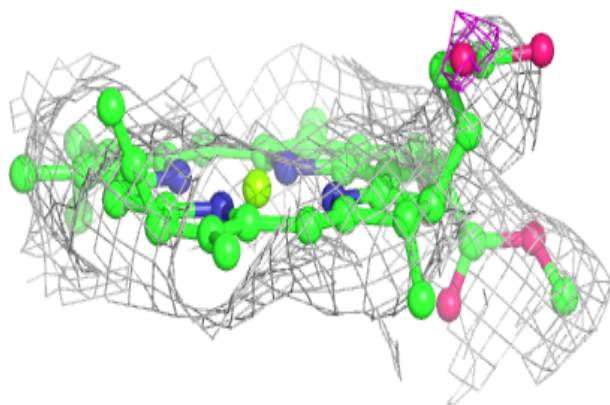
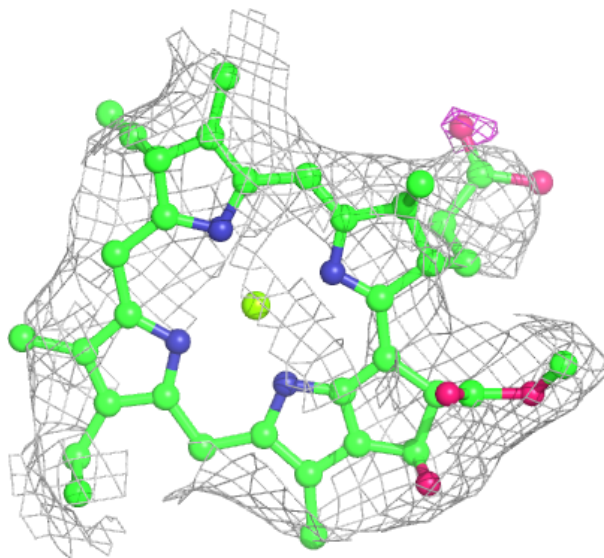
Electron density around CLA A 1770:

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



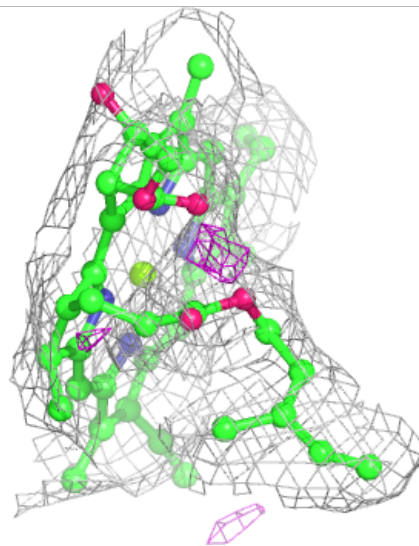
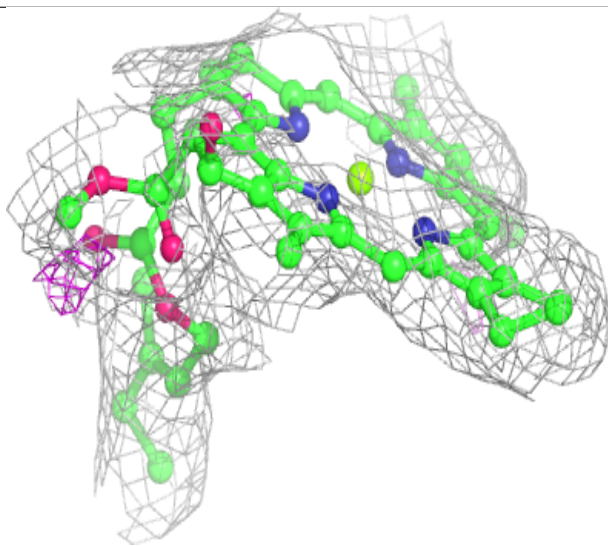
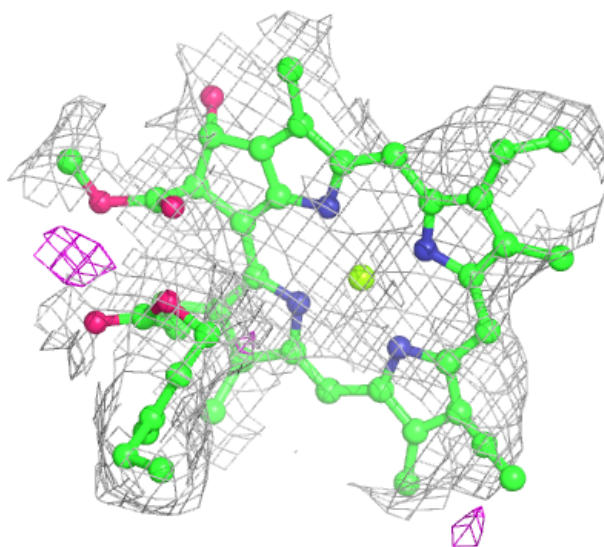
Electron density around CLA A 1791:

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



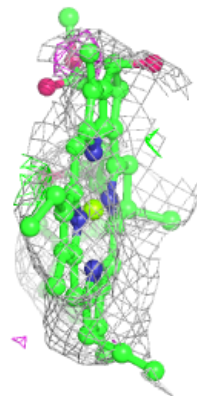
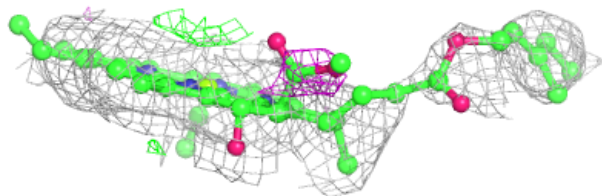
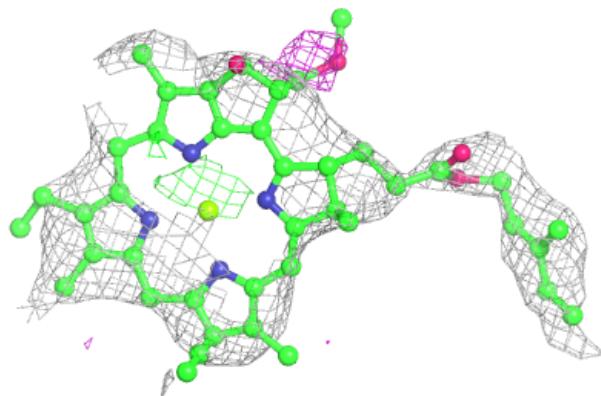
Electron density around CLA 1 1193:

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

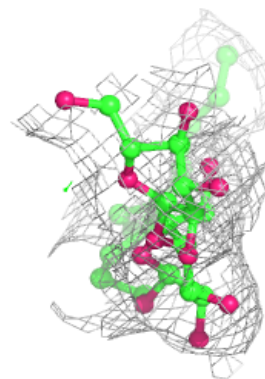
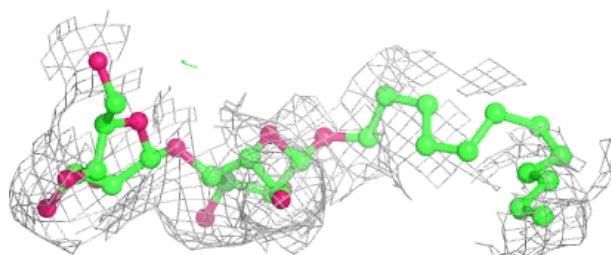
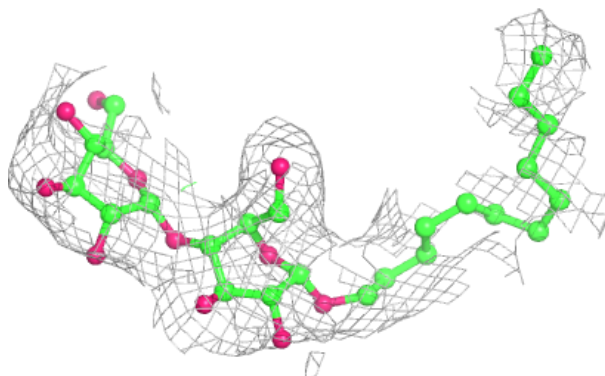


Electron density around CLA 1 1200:

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

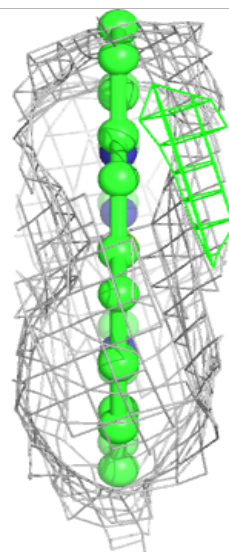
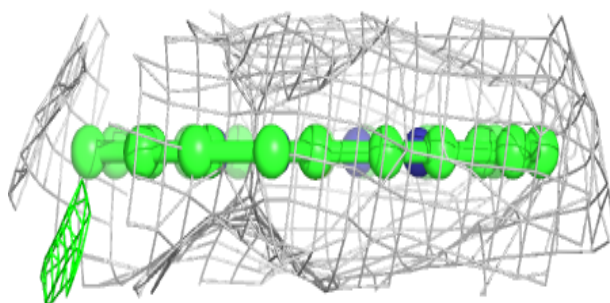
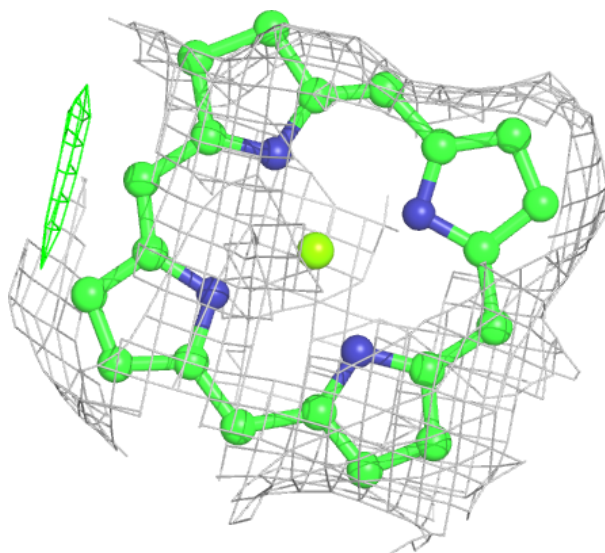
**Electron density around LMU A 7030:**

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



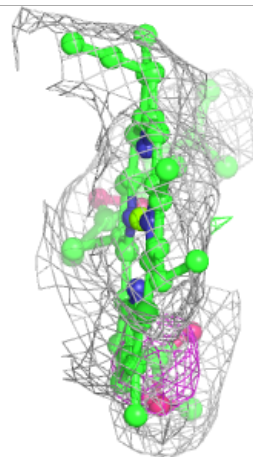
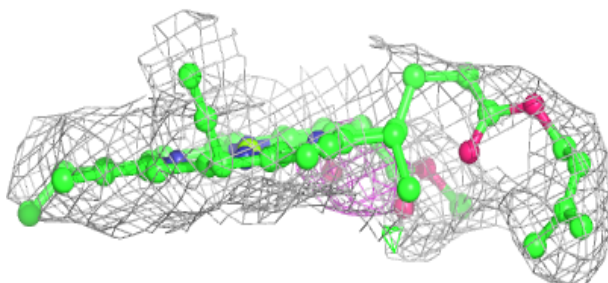
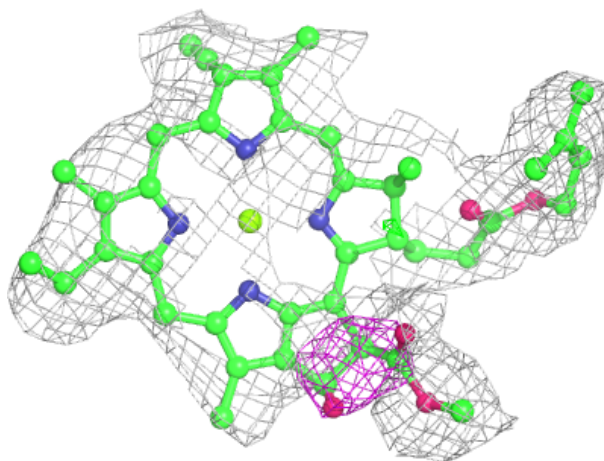
Electron density around CLA 3 1213:

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



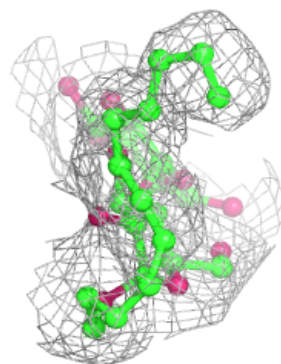
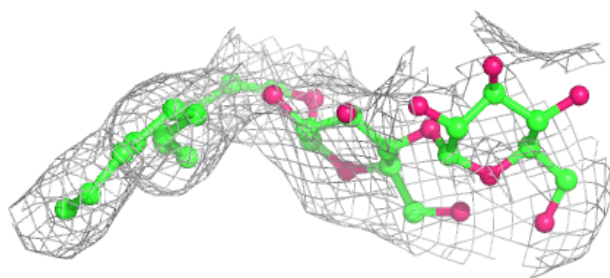
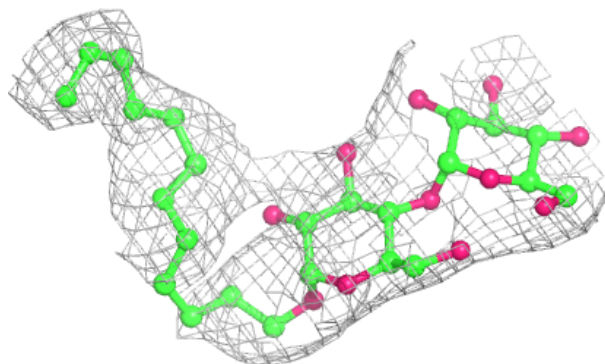
Electron density around CLA K 1146:

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

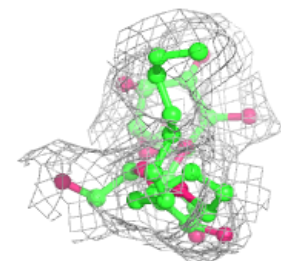
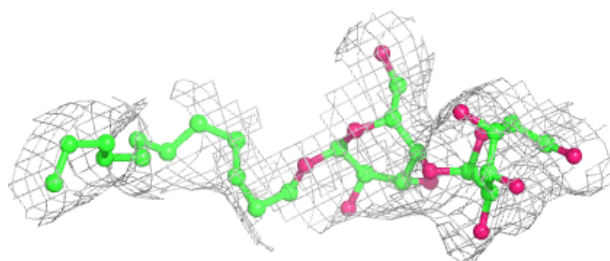
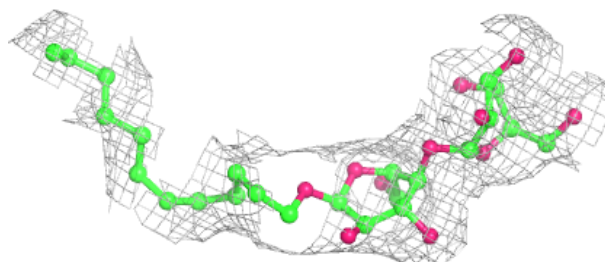


Electron density around LMU A 7025:

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

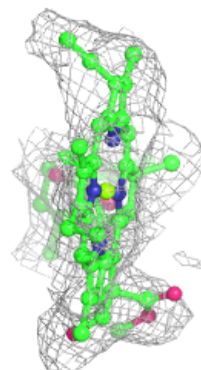
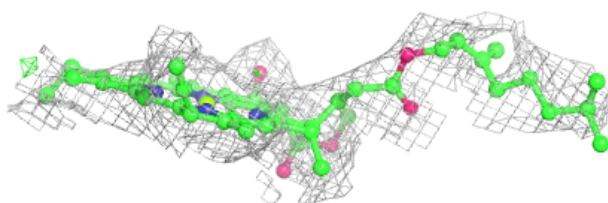
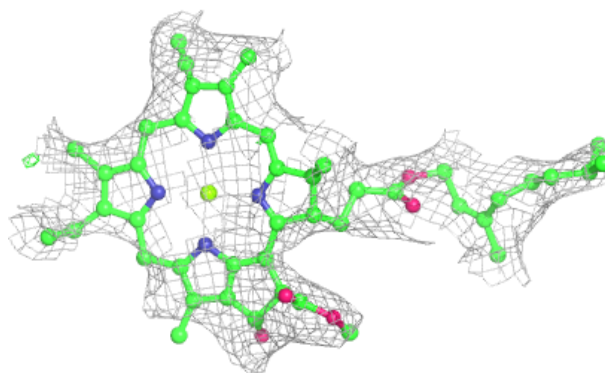
**Electron density around LMU A 7027:**

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

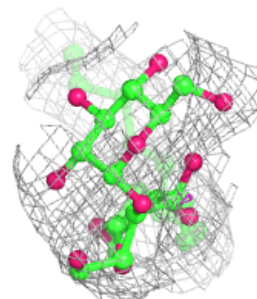
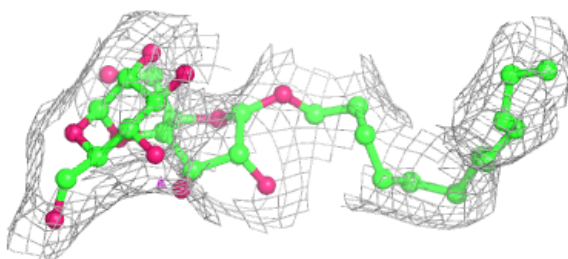
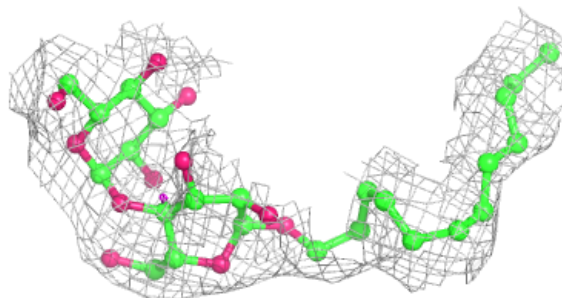


Electron density around CLA A 1798:

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

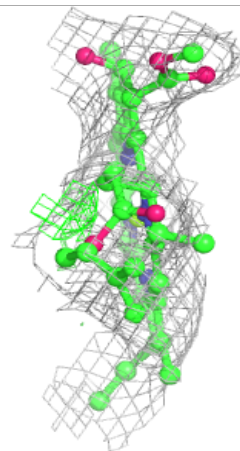
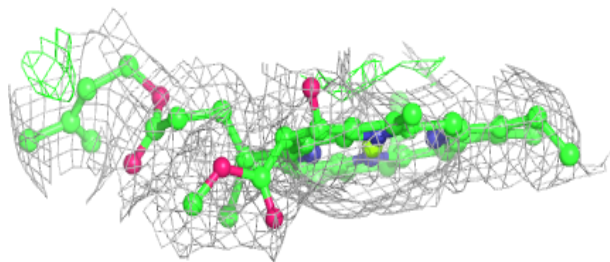
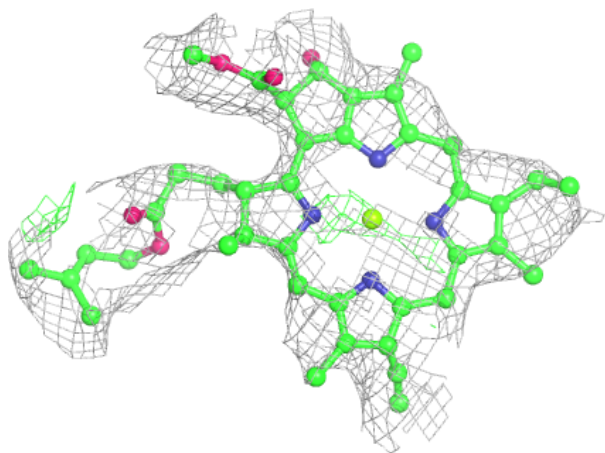
**Electron density around LMU A 7031:**

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



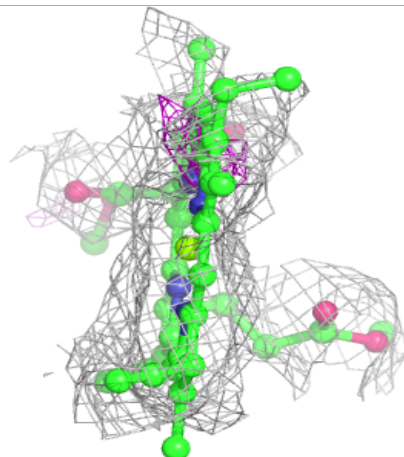
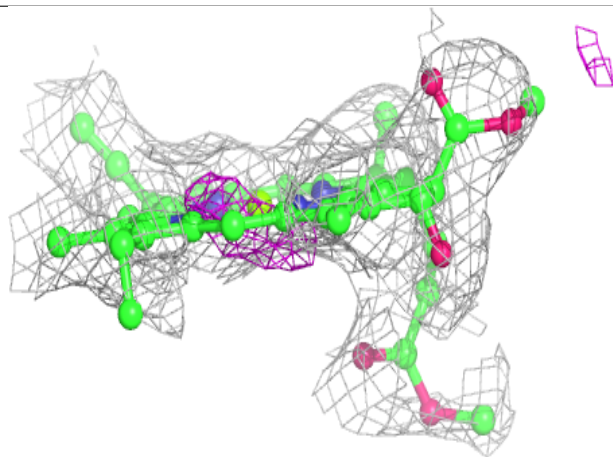
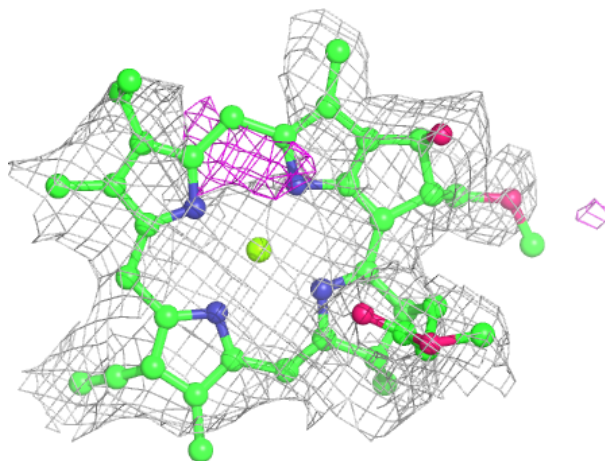
Electron density around CLA 2 1215:

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



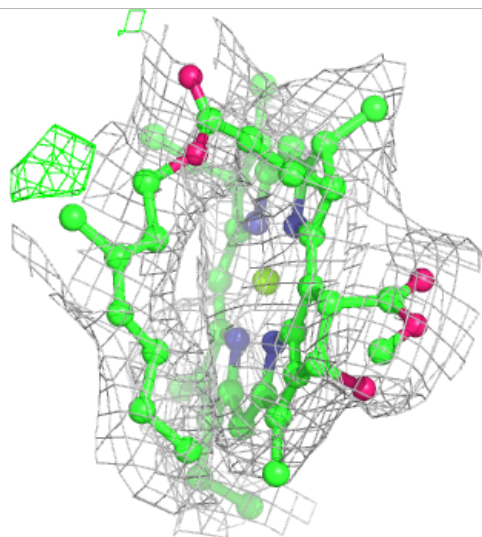
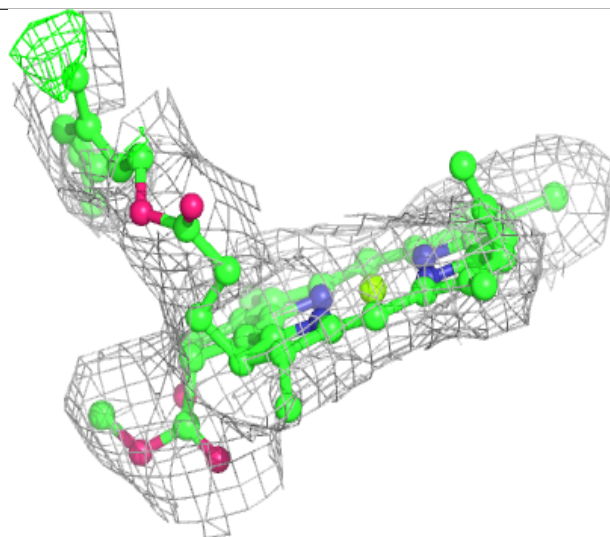
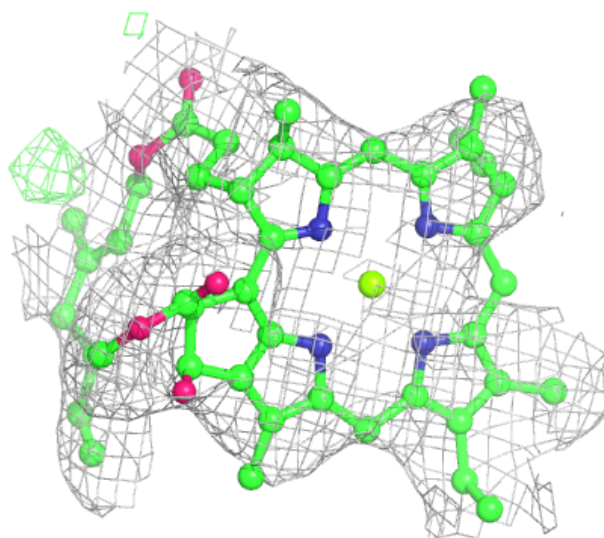
Electron density around CLA A 1763:

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



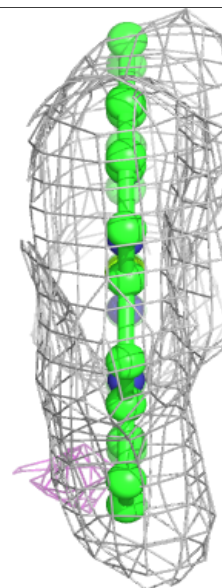
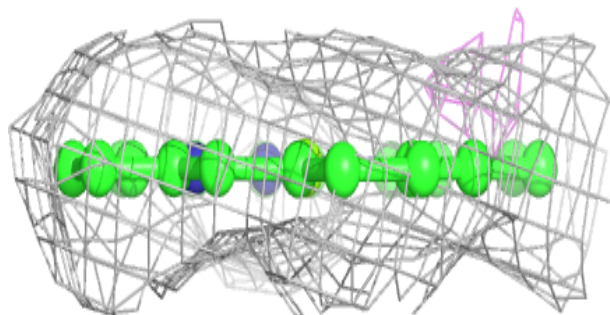
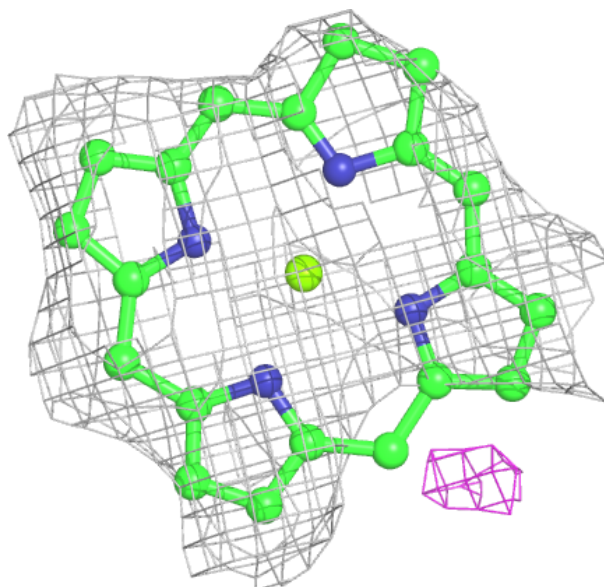
Electron density around CLA F 1157:

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



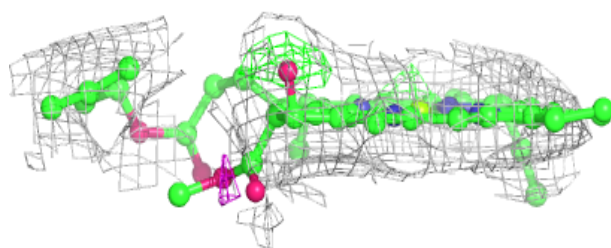
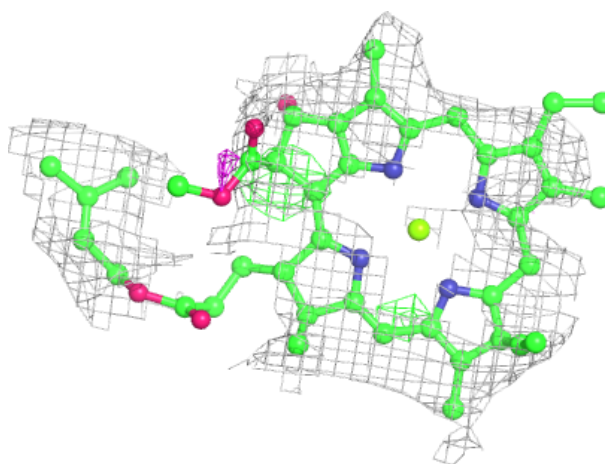
Electron density around CLA 3 3001:

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



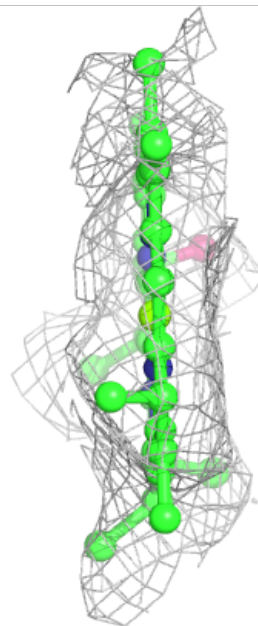
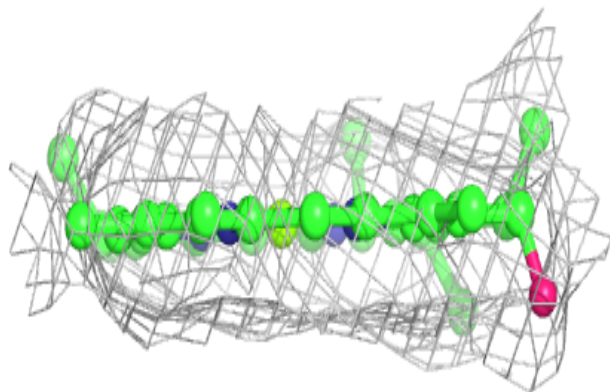
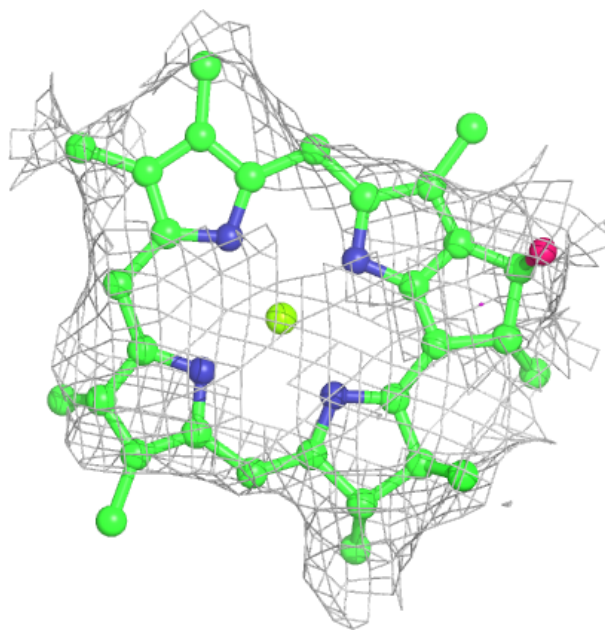
Electron density around CLA 2 1223:

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



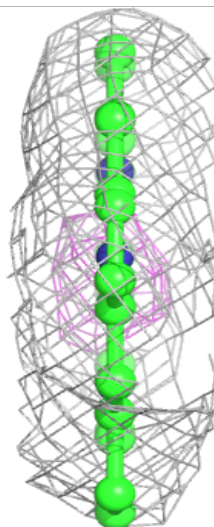
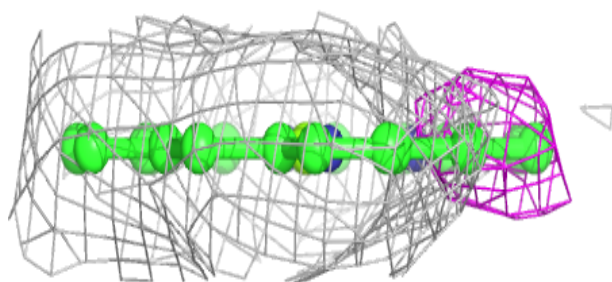
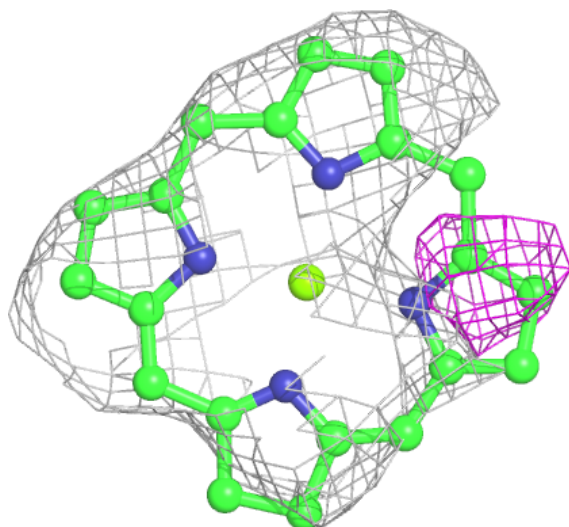
Electron density around CLA A 1775:

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



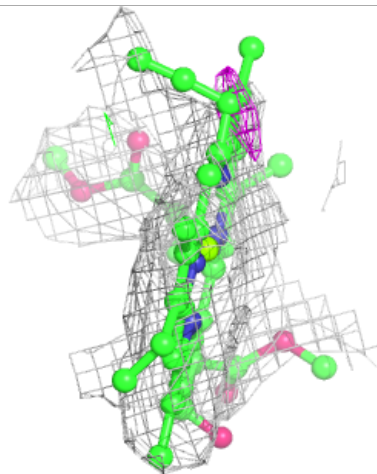
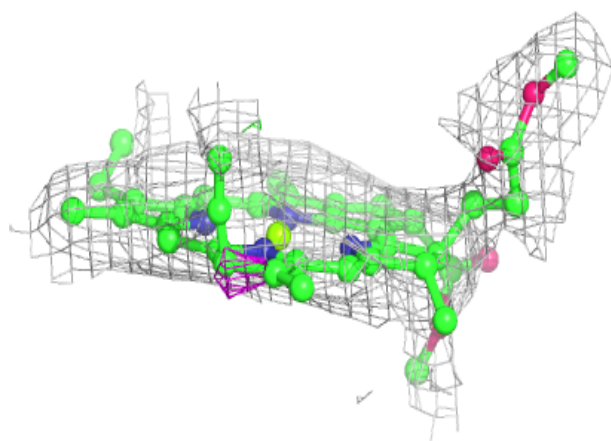
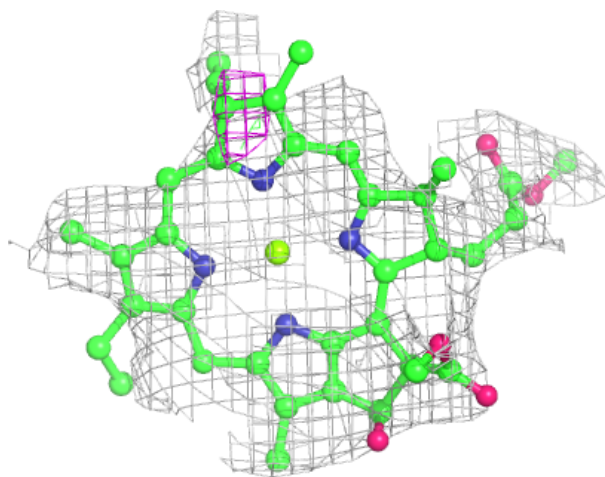
Electron density around CLA 3 3014:

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



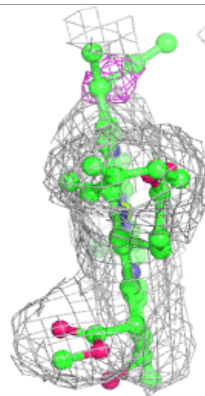
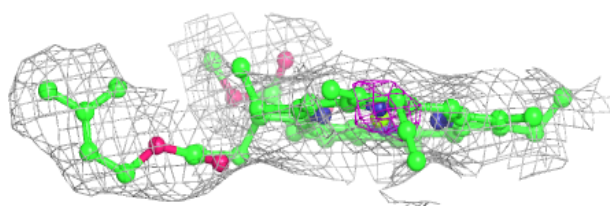
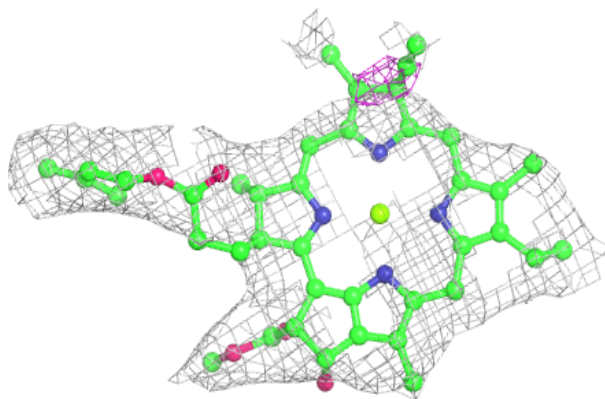
Electron density around CLA B 1751:

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

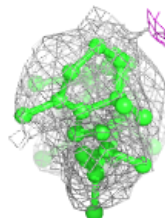
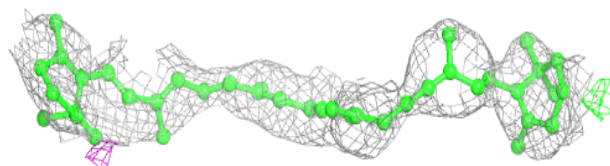
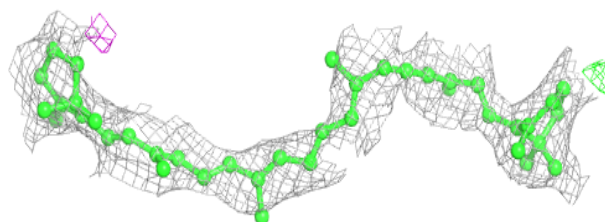


Electron density around CLA K 1085:

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

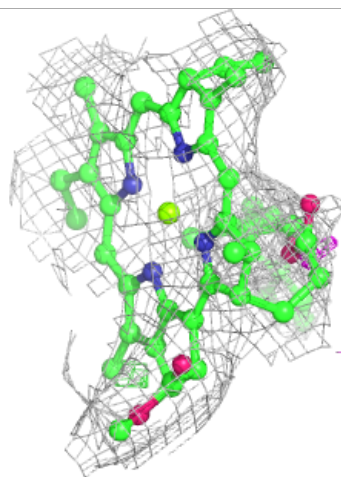
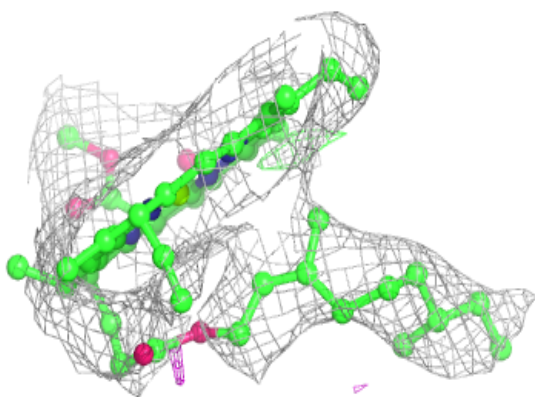
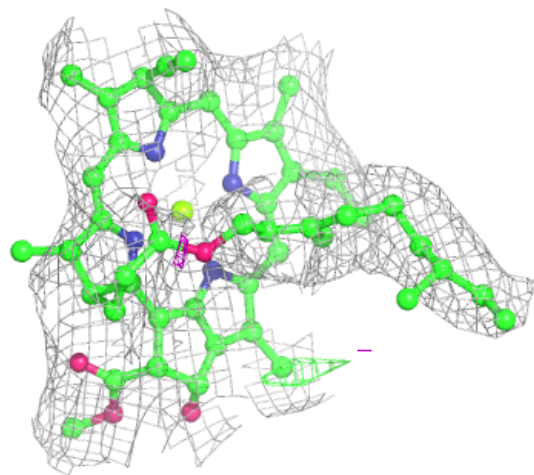
**Electron density around BCR I 1032:**

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



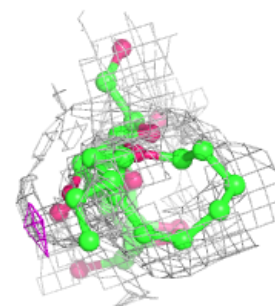
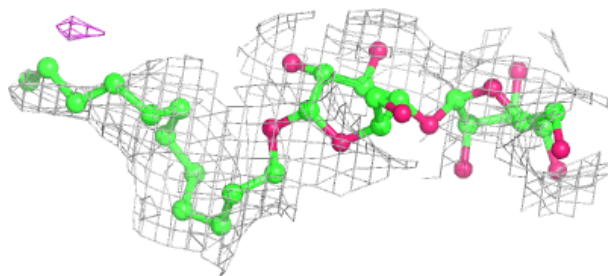
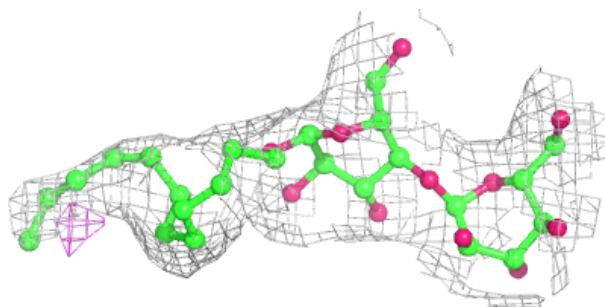
Electron density around CLA 2 1213:

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

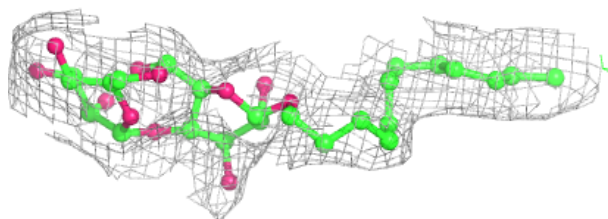
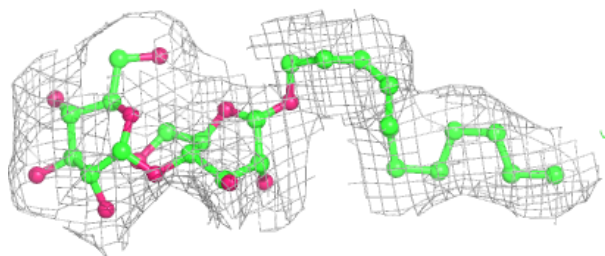


Electron density around LMU 3 7005:

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

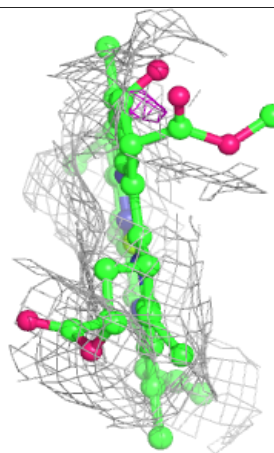
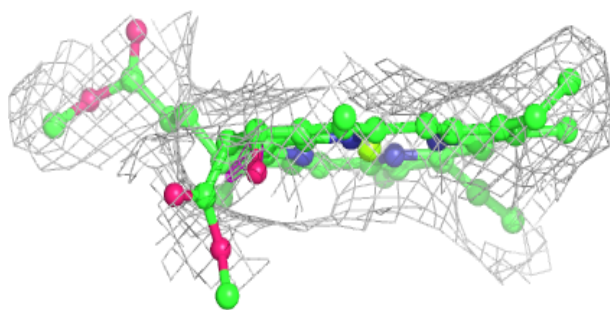
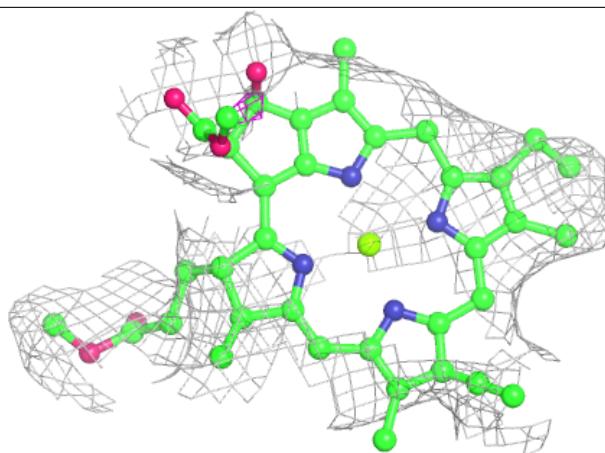
**Electron density around LMU A 7020:**

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

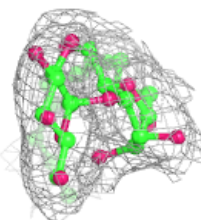
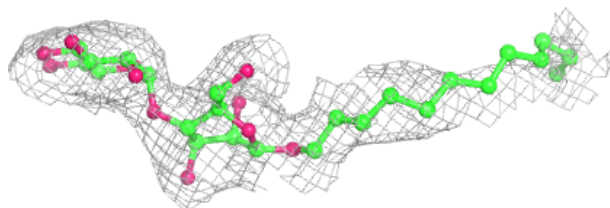
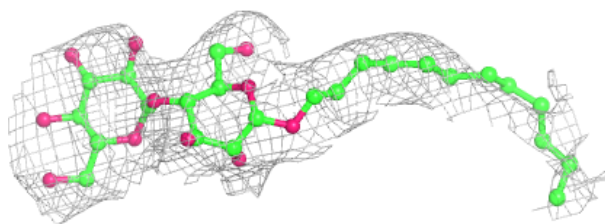


Electron density around CLA 1 1187:

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

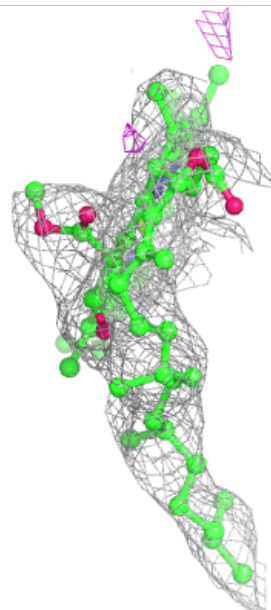
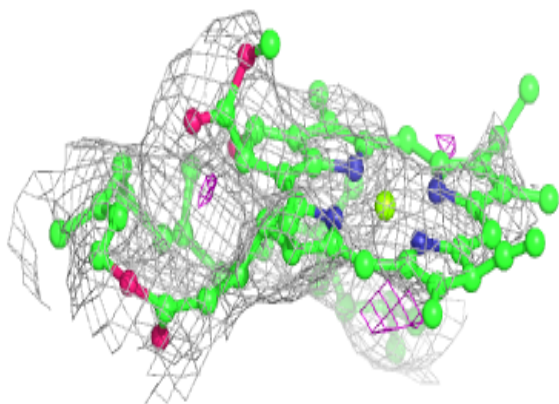
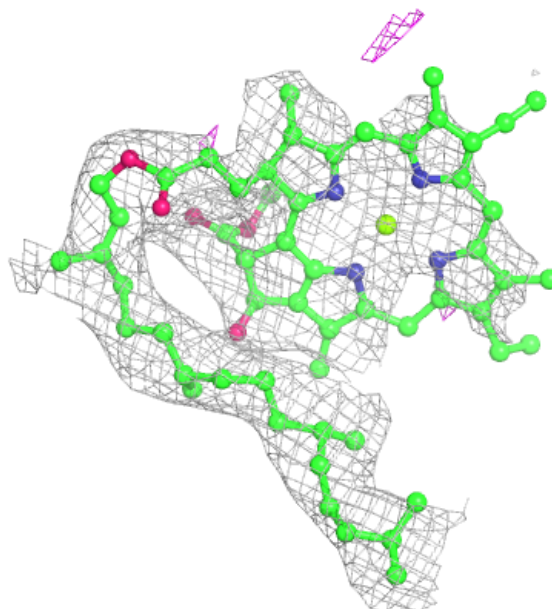
**Electron density around LMU A 7047:**

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



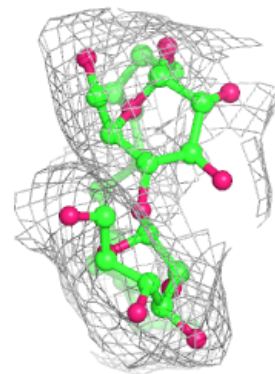
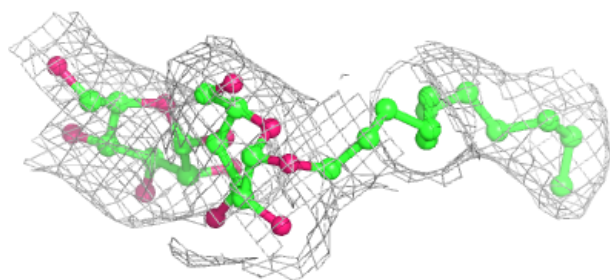
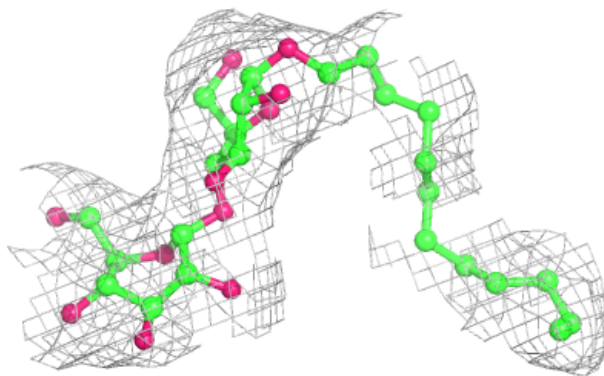
Electron density around CLA A 1780:

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



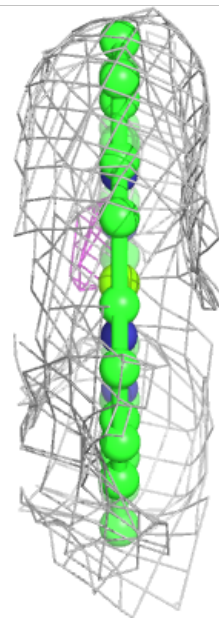
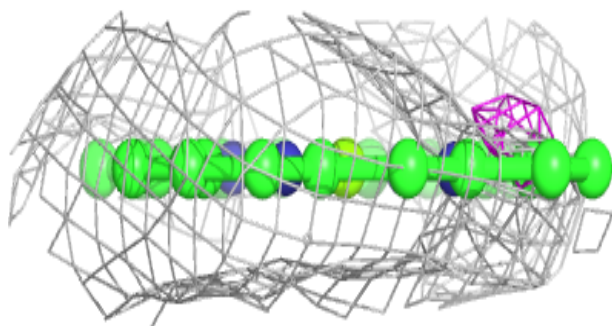
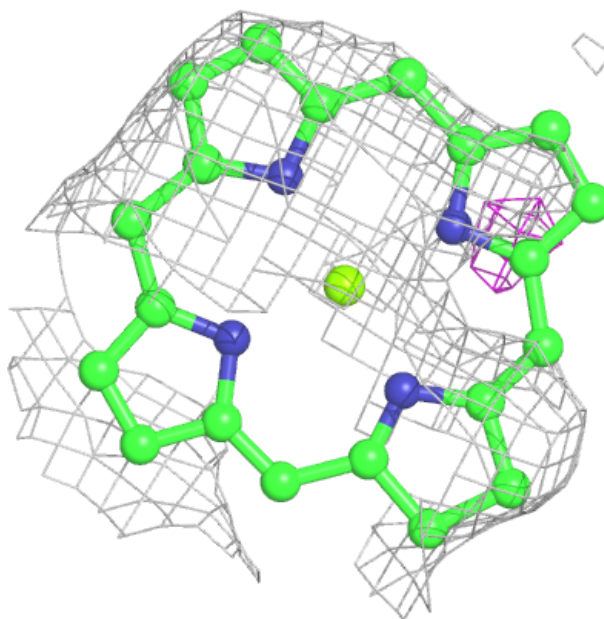
Electron density around LMU A 7028:

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



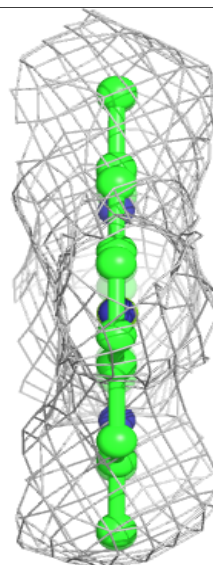
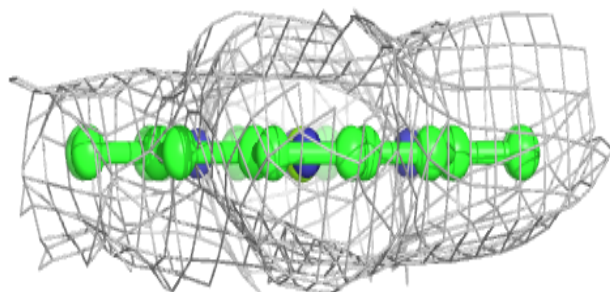
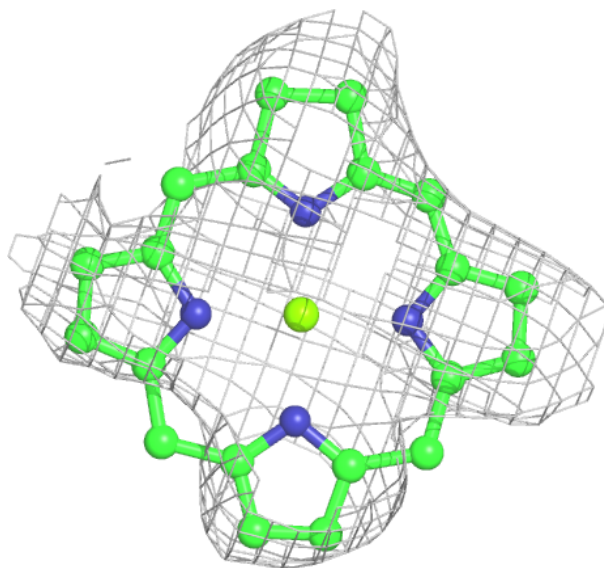
Electron density around CLA 3 1215:

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



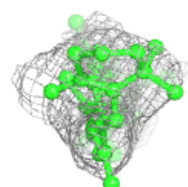
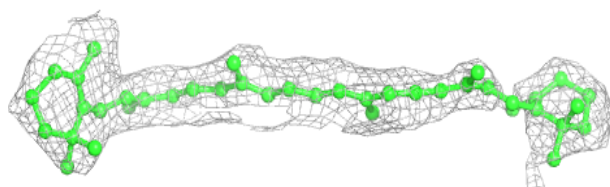
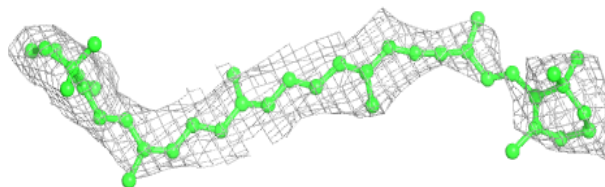
Electron density around CLA 3 3002:

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

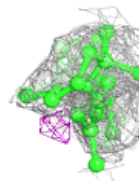
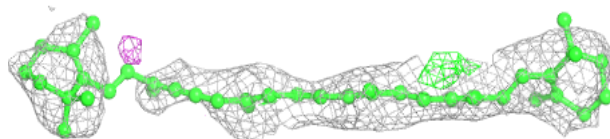
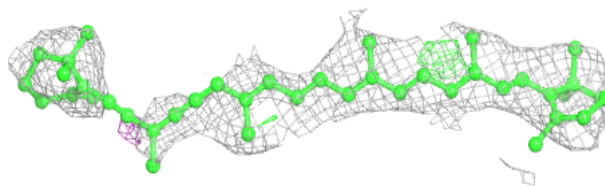


Electron density around BCR B 1776:

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

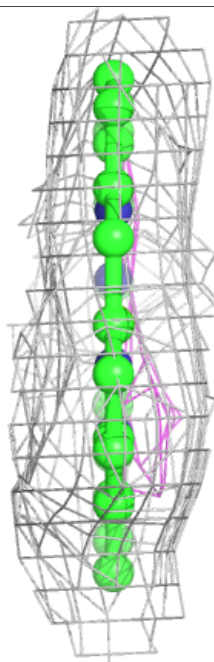
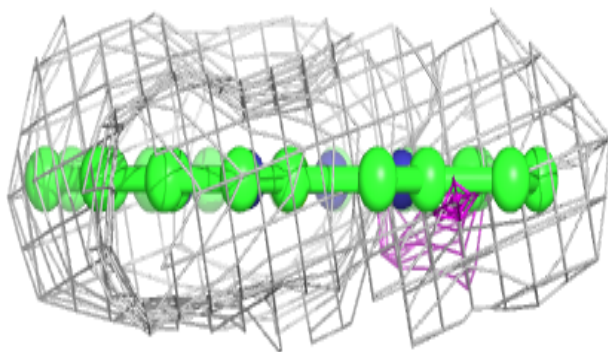
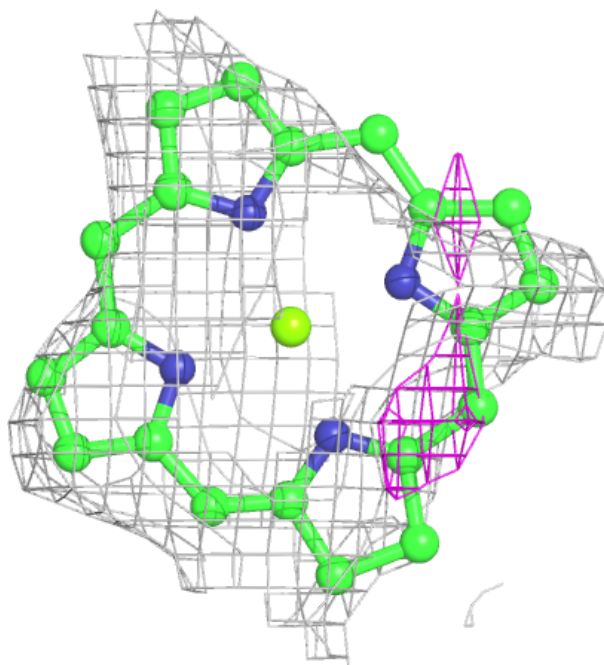
**Electron density around BCR B 1780:**

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



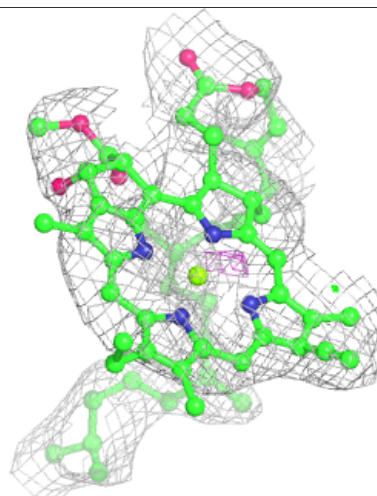
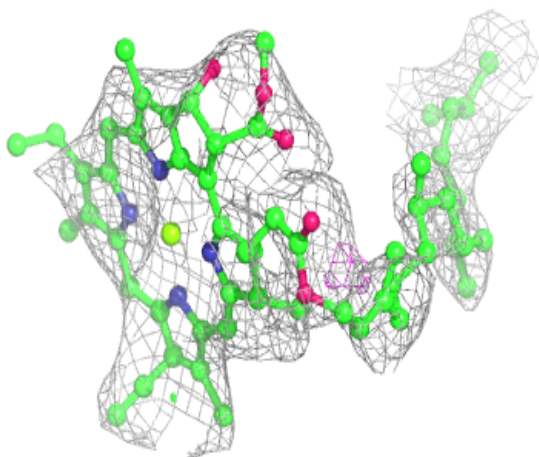
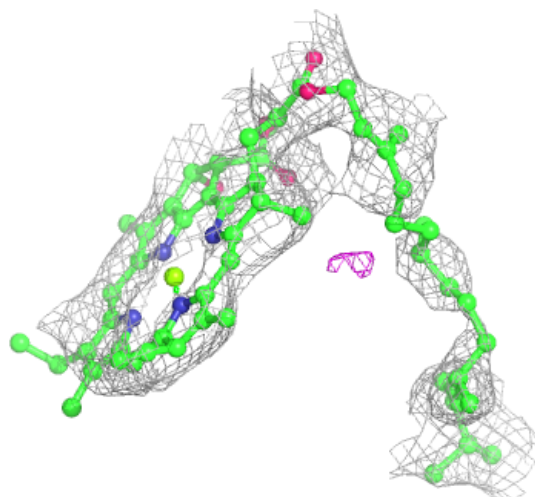
Electron density around CLA 2 1227:

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



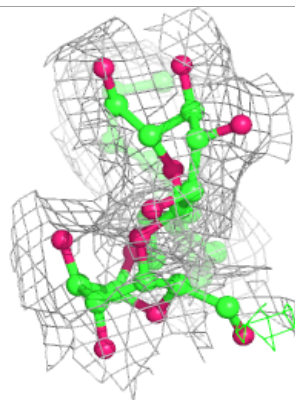
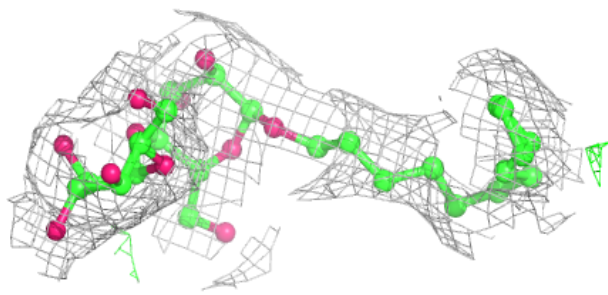
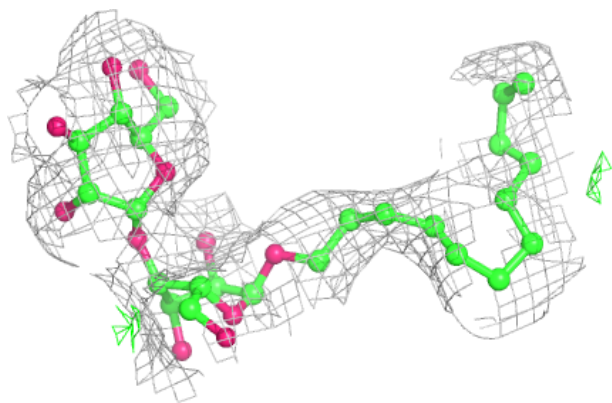
Electron density around CLA 2 1217:

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

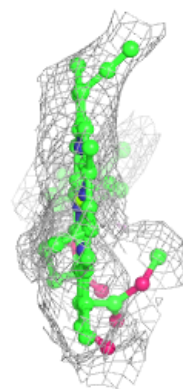
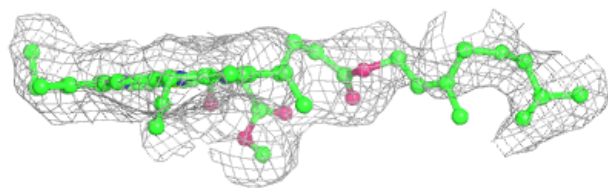
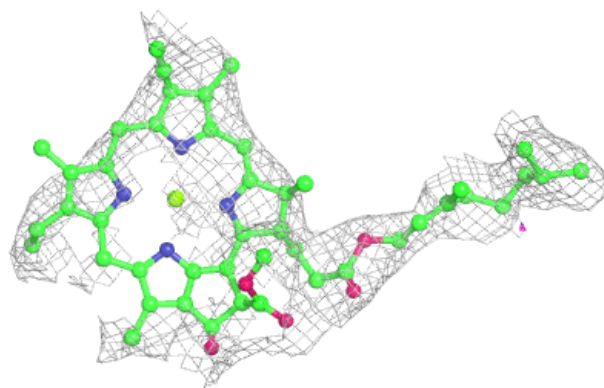


Electron density around LMU K 1086:

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

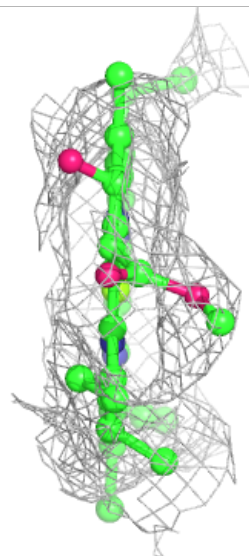
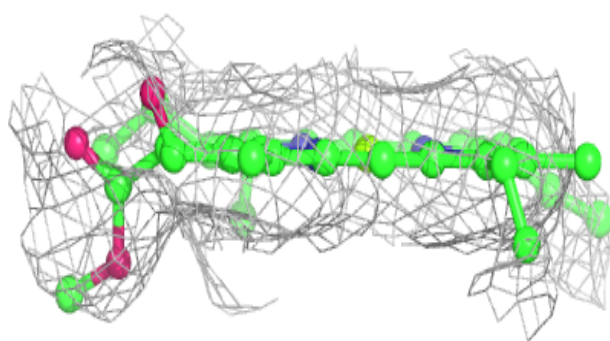
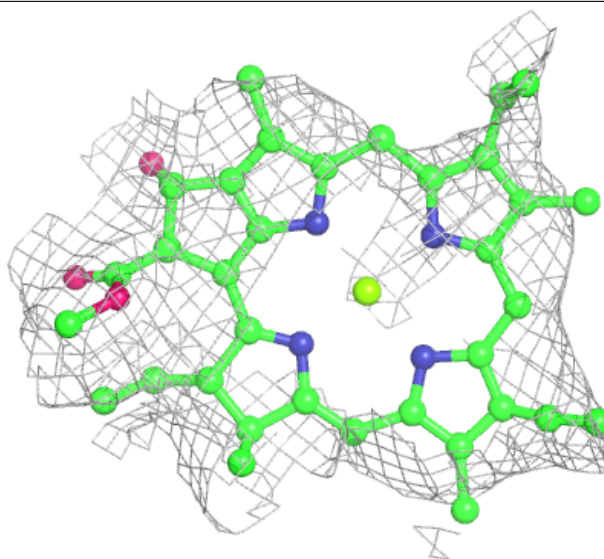
**Electron density around CLA 4 1204:**

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



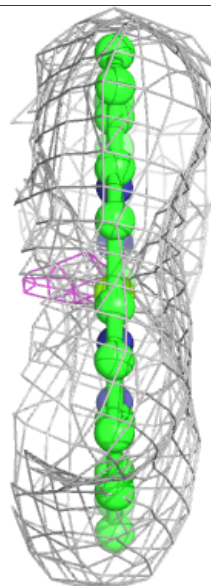
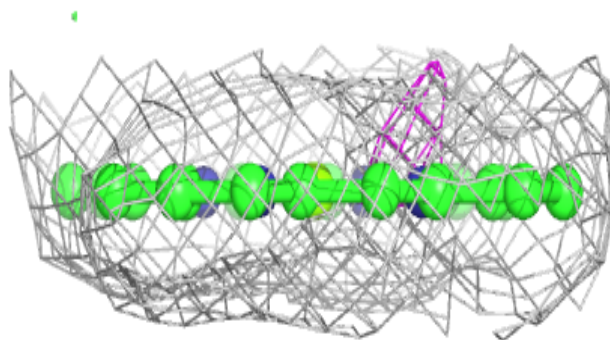
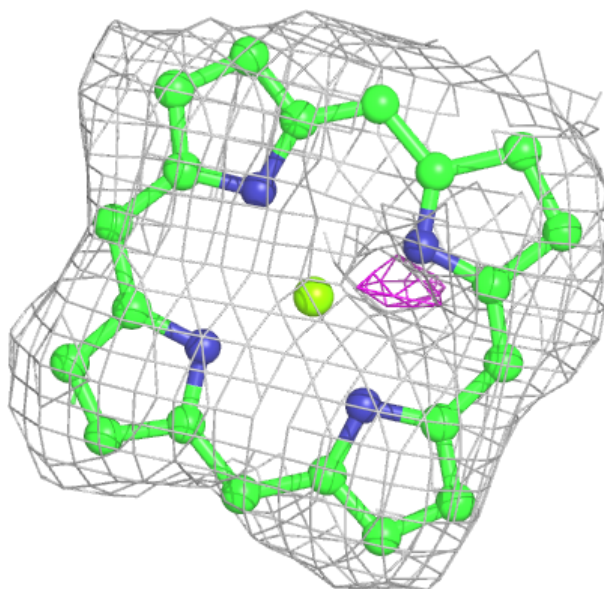
Electron density around CLA A 1778:

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



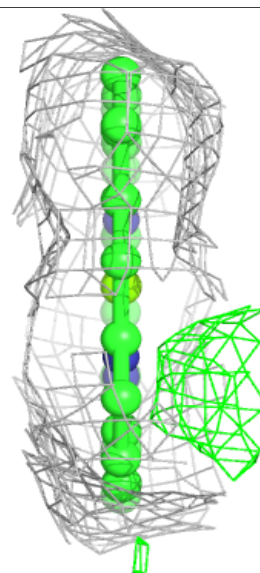
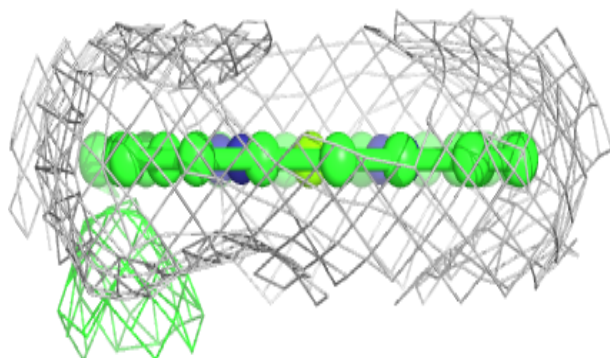
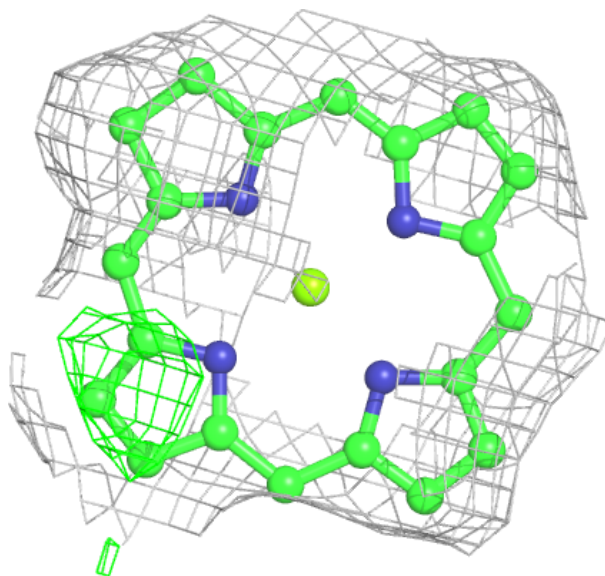
Electron density around CLA 4 1208:

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



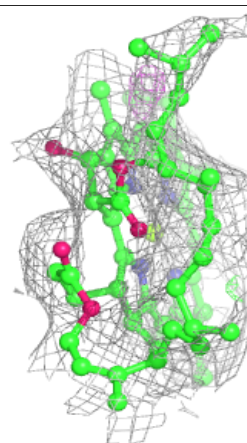
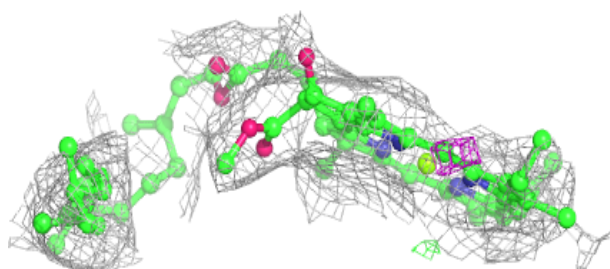
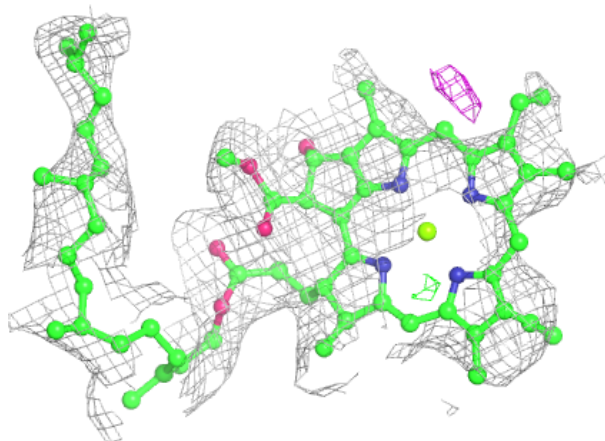
Electron density around CLA 1 1194:

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

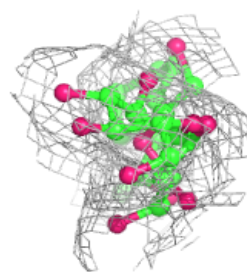
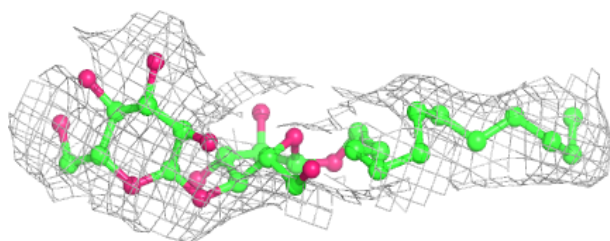
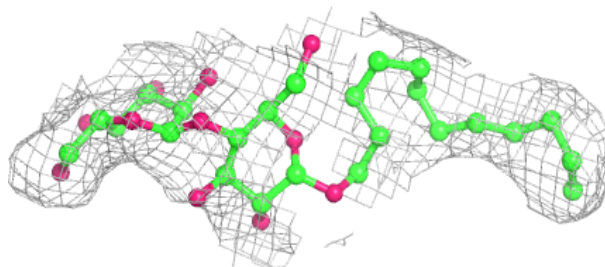


Electron density around CLA R 1055:

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

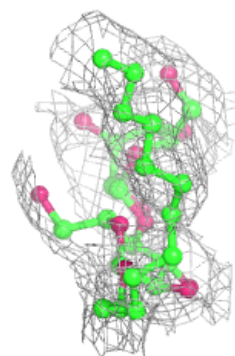
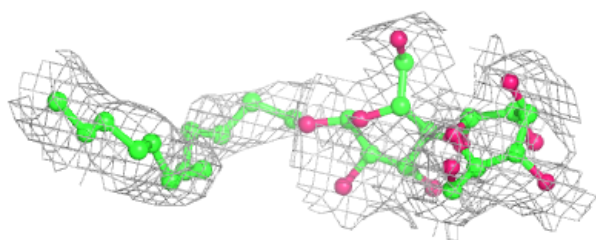
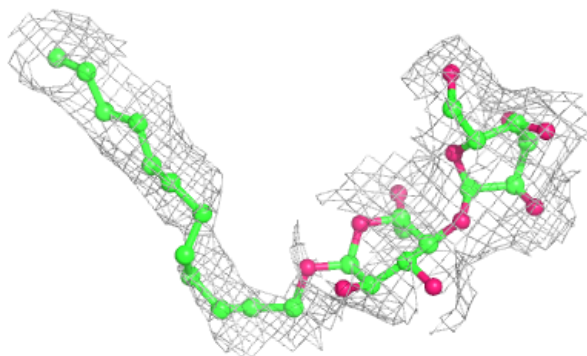
**Electron density around LMU A 7042:**

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

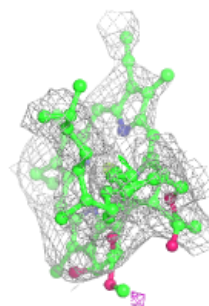
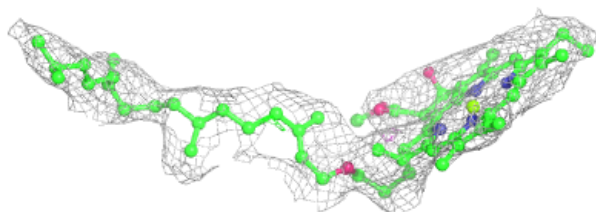
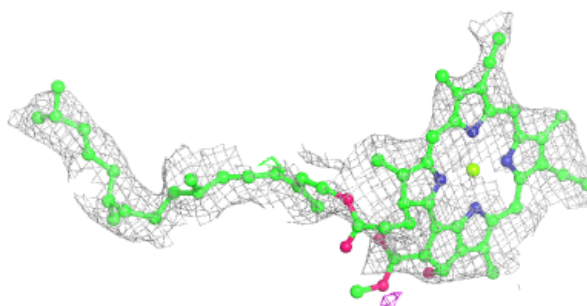


Electron density around LMU 1 1202:

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

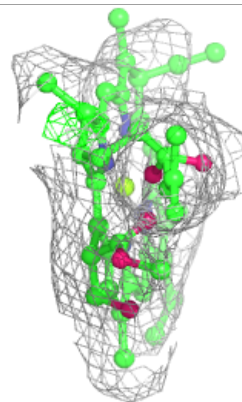
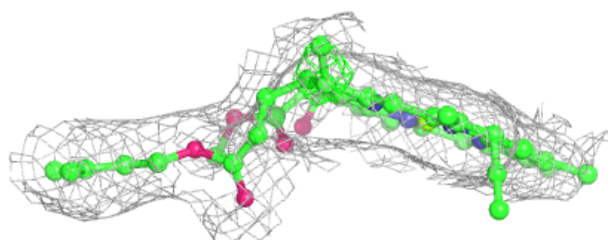
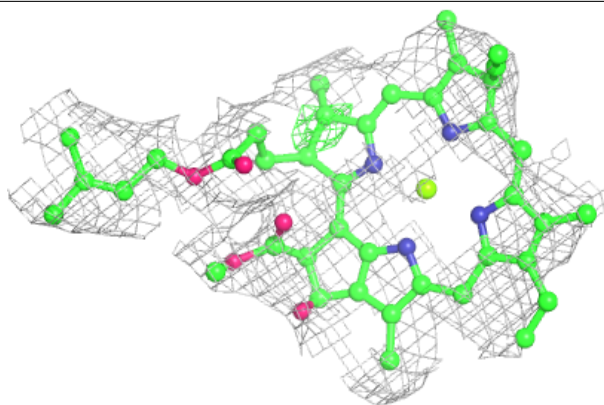
**Electron density around CLA H 1079:**

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

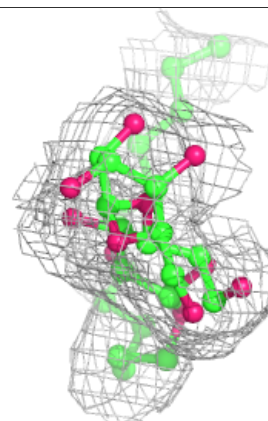
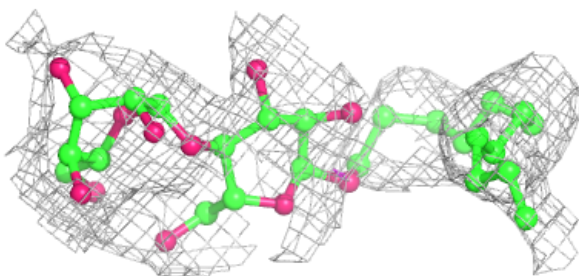
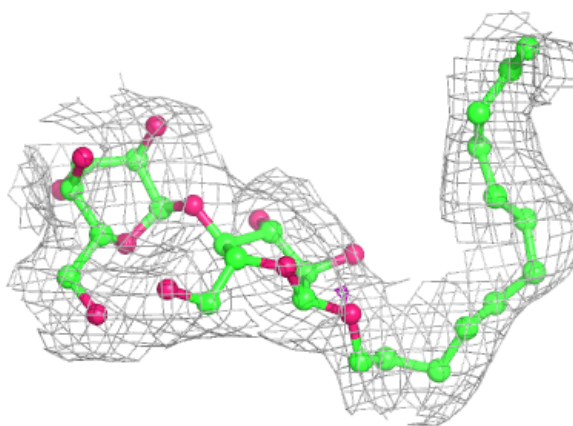


Electron density around CLA L 1168:

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

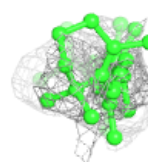
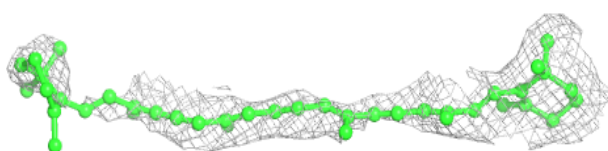
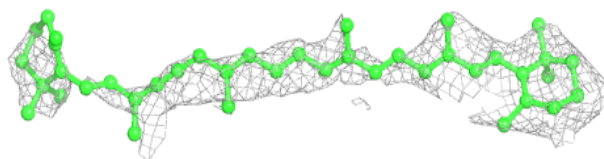
**Electron density around LMU 2 7003:**

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

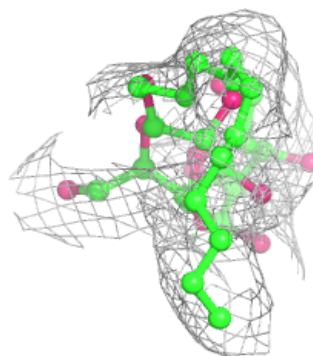
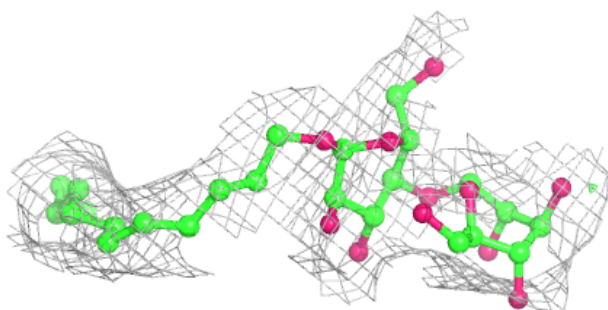
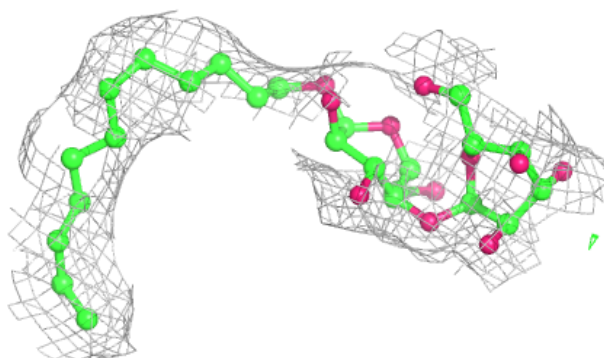


Electron density around BCR A 1806:

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

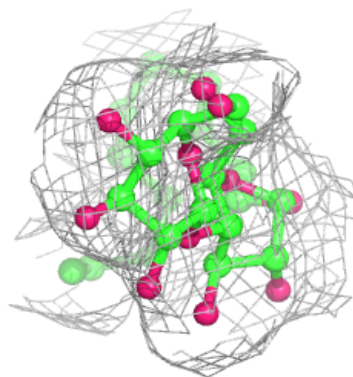
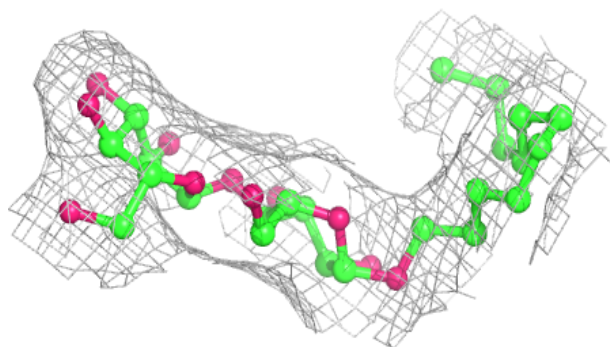
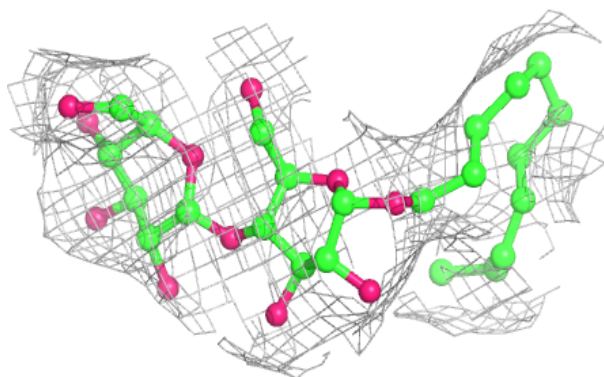
**Electron density around LMU 2 7006:**

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



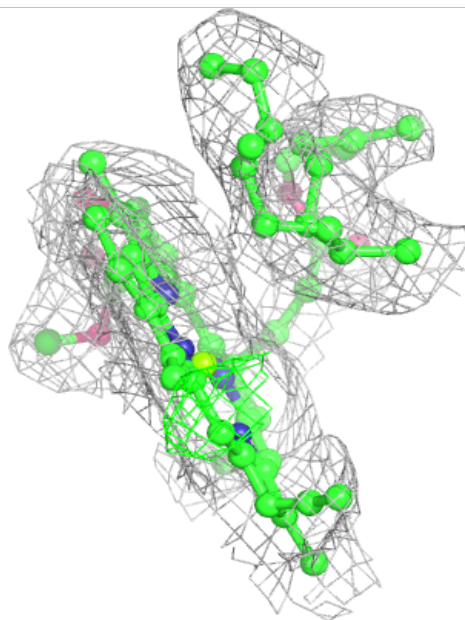
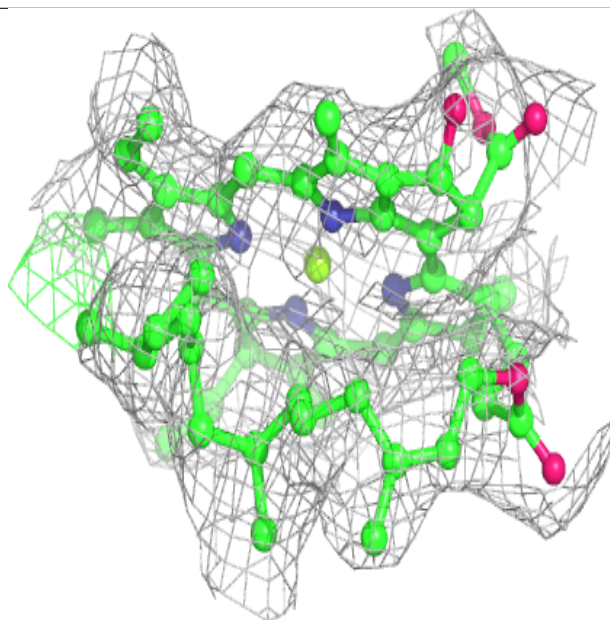
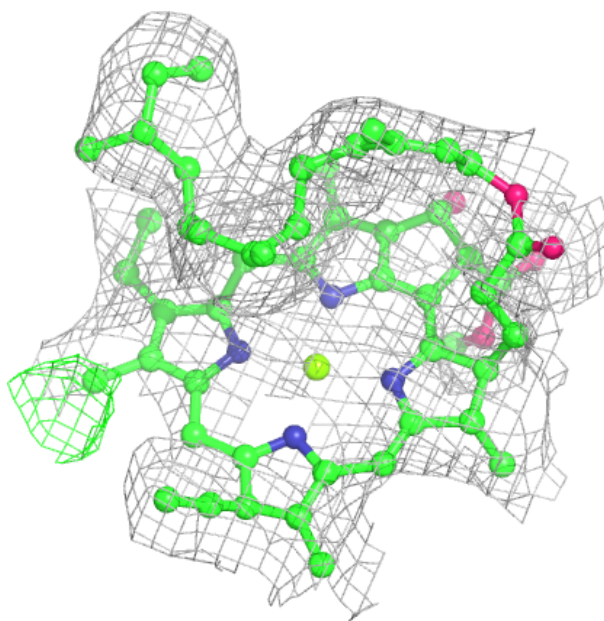
Electron density around LMU A 7036:

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



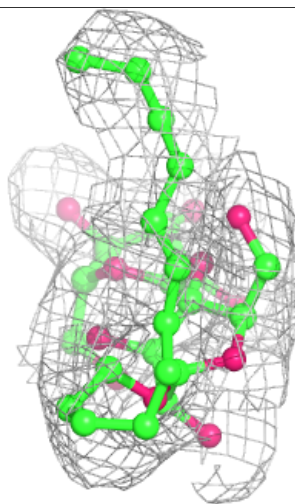
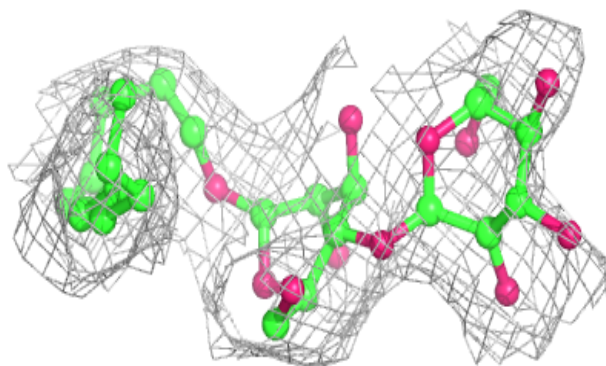
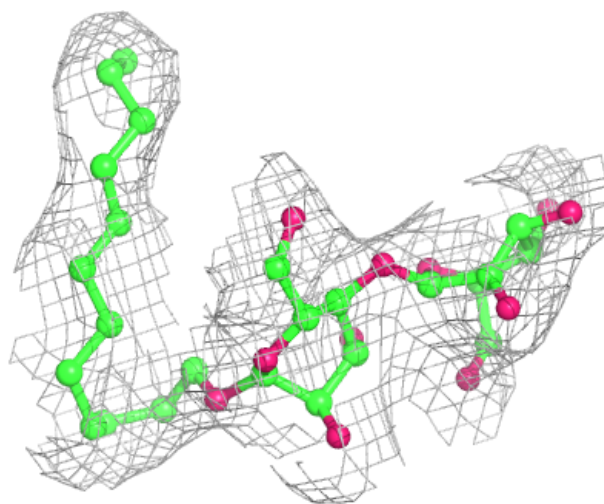
Electron density around CLA 1 1192:

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



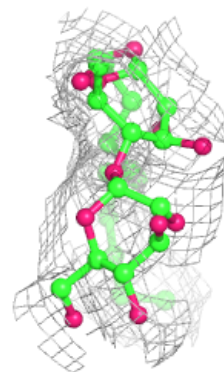
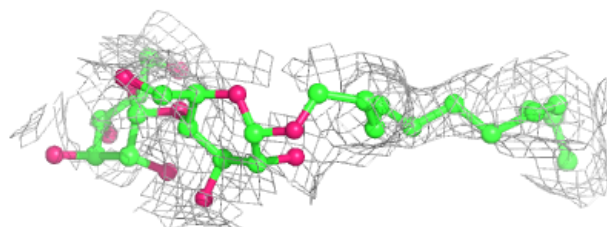
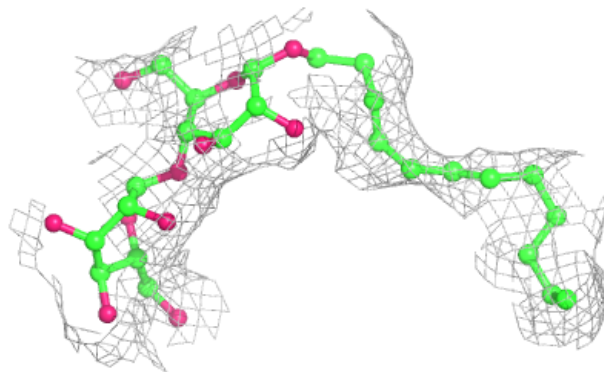
Electron density around LMU R 1057:

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



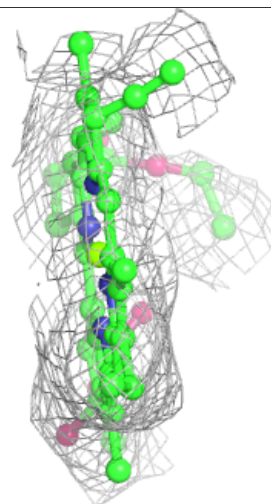
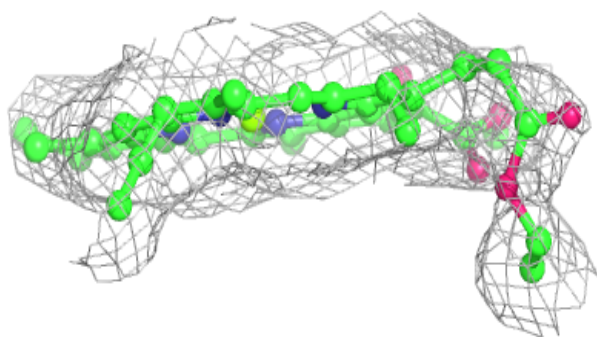
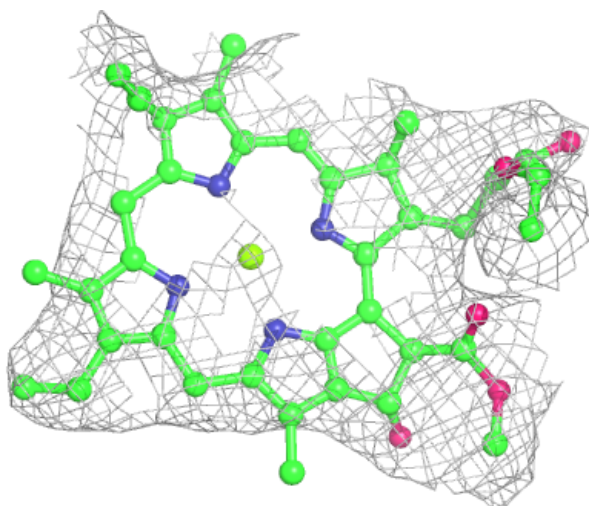
Electron density around LMU A 7019:

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



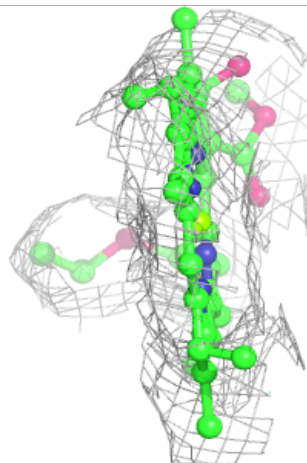
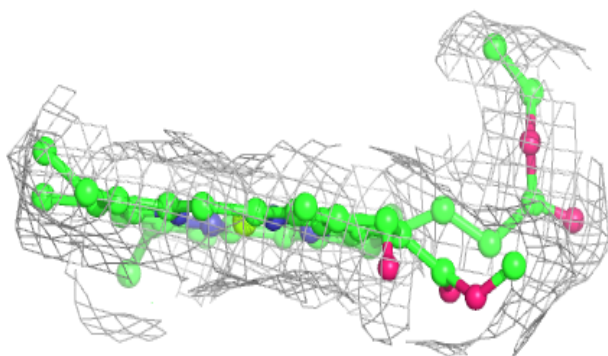
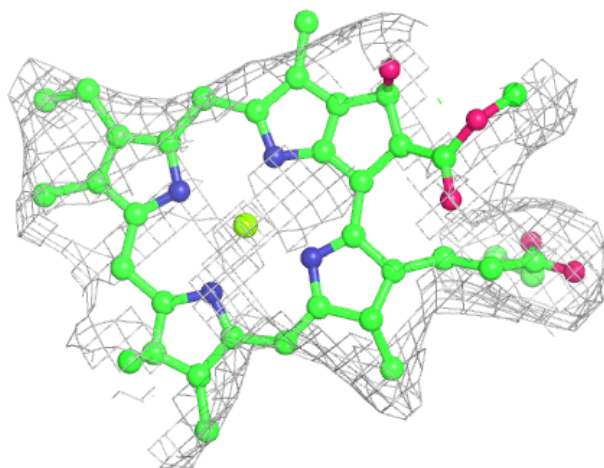
Electron density around CLA 1 1188:

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



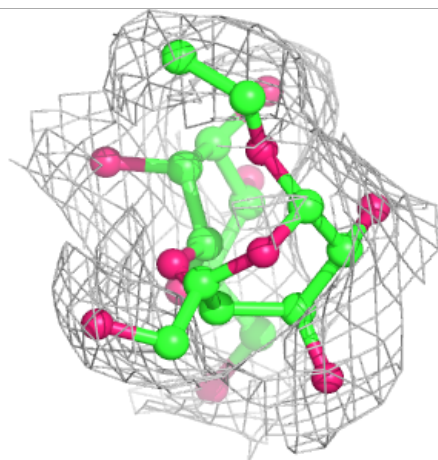
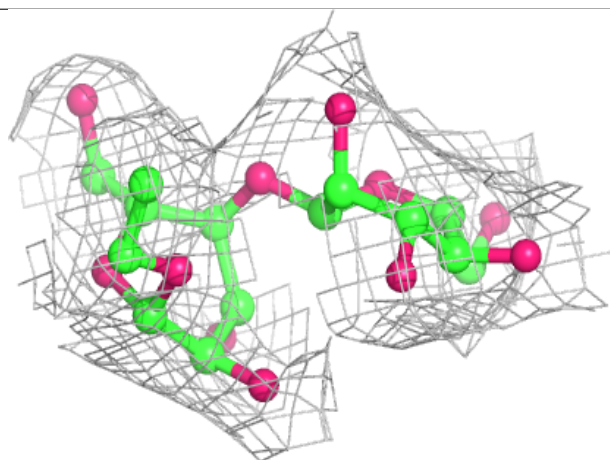
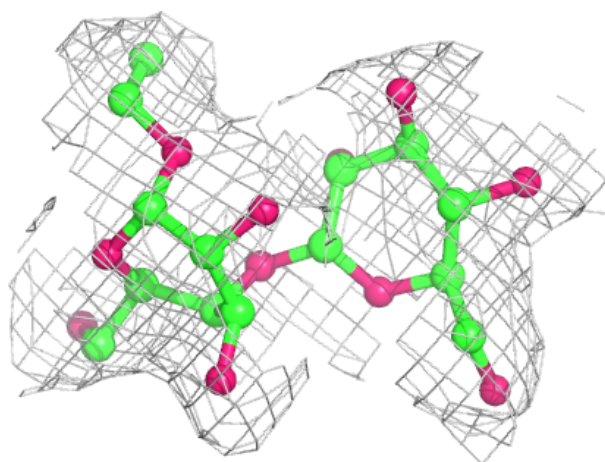
Electron density around CLA A 1817:

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



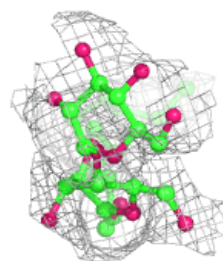
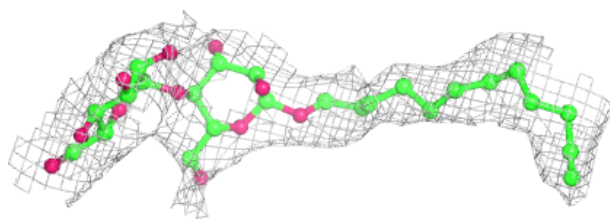
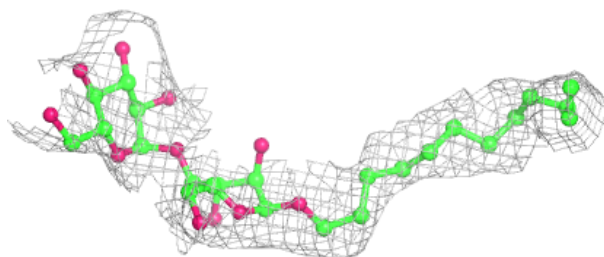
Electron density around LMU B 1782:

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



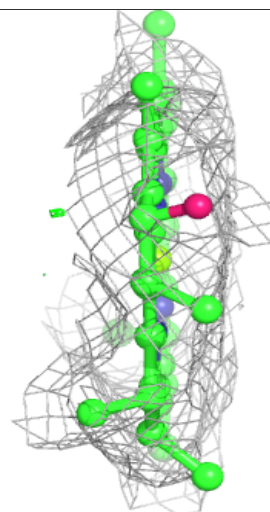
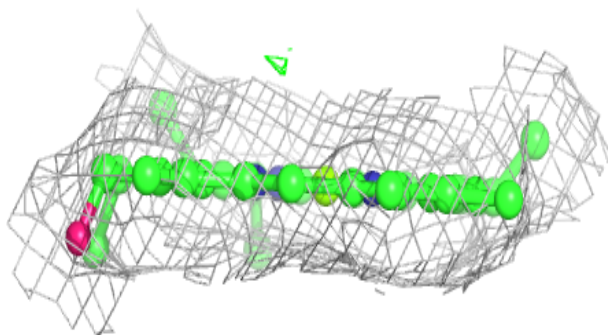
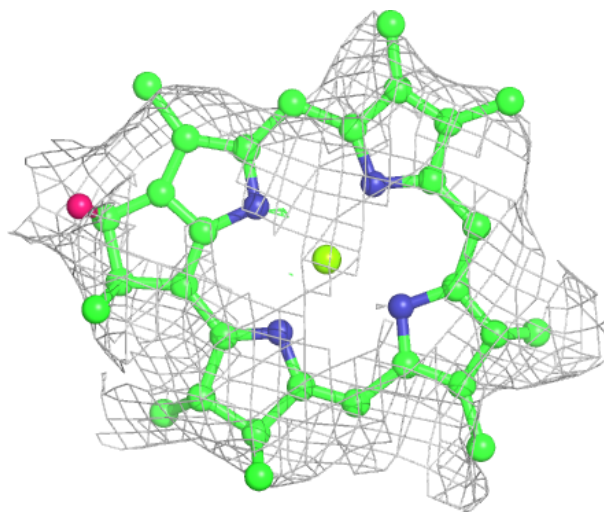
Electron density around LMU 4 1210:

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



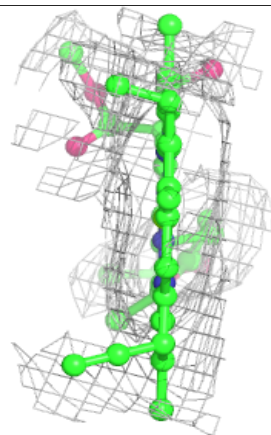
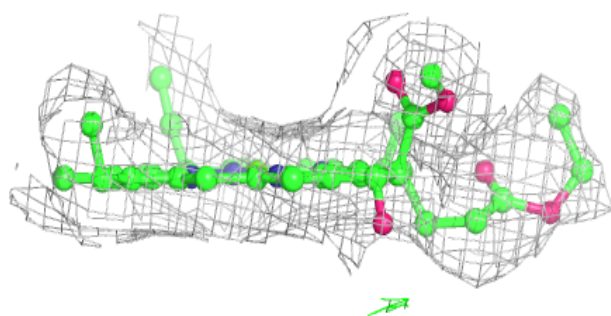
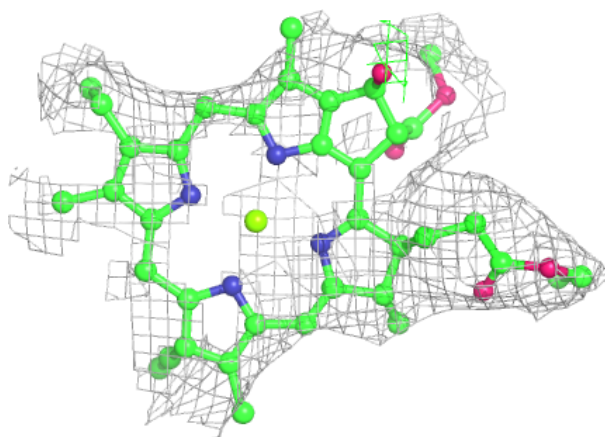
Electron density around CLA 3 1212:

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

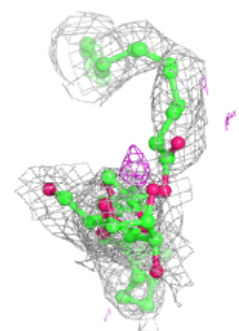
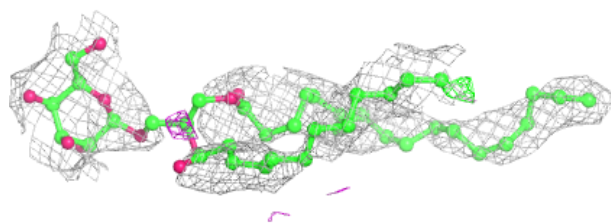
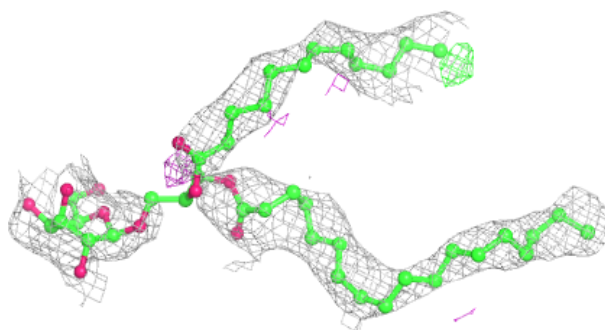


Electron density around CLA 1 1189:

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

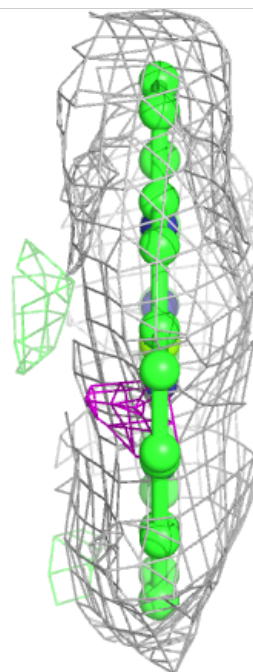
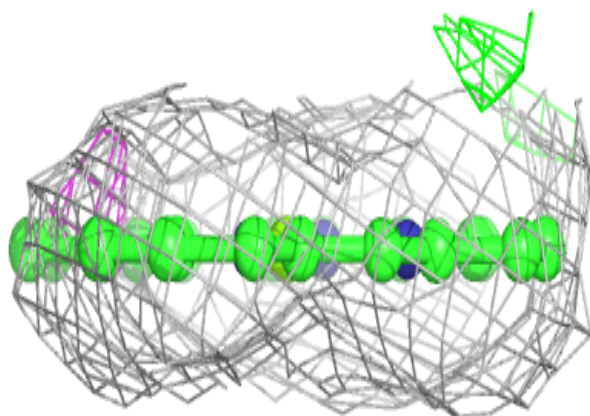
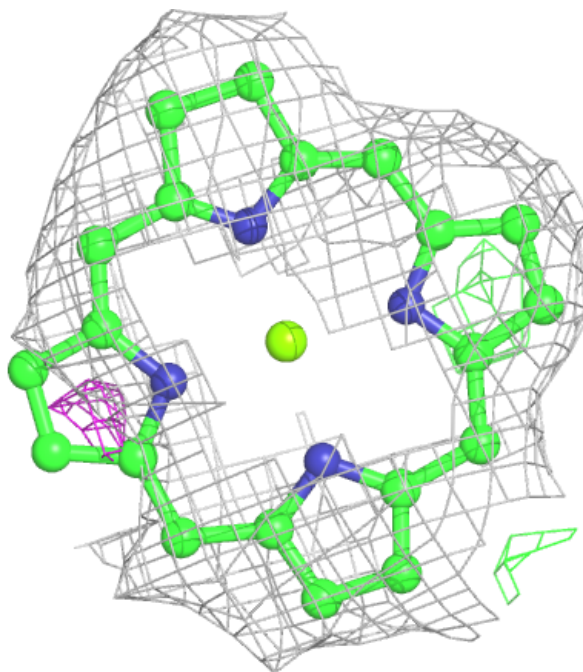
**Electron density around LMG B 1783:**

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



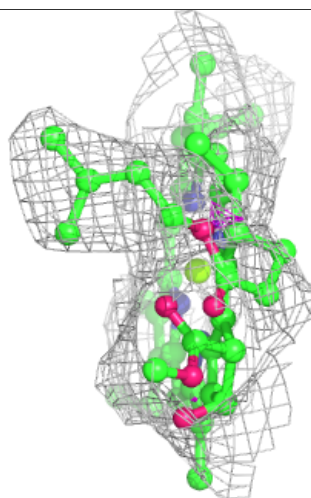
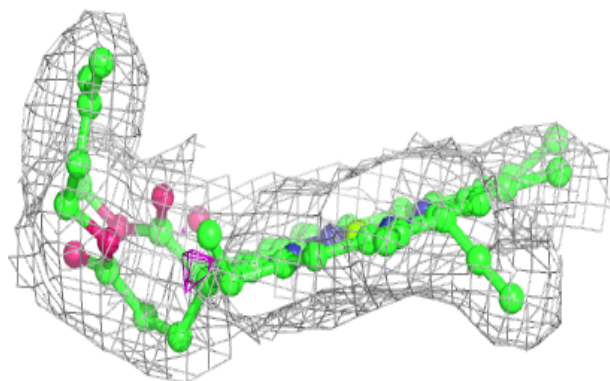
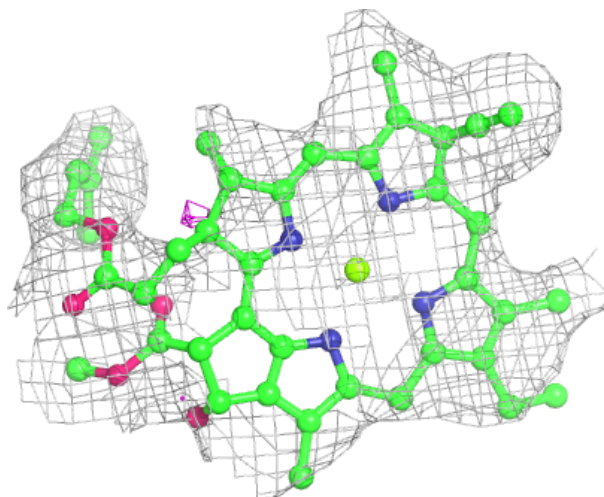
Electron density around CLA 4 1203:

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



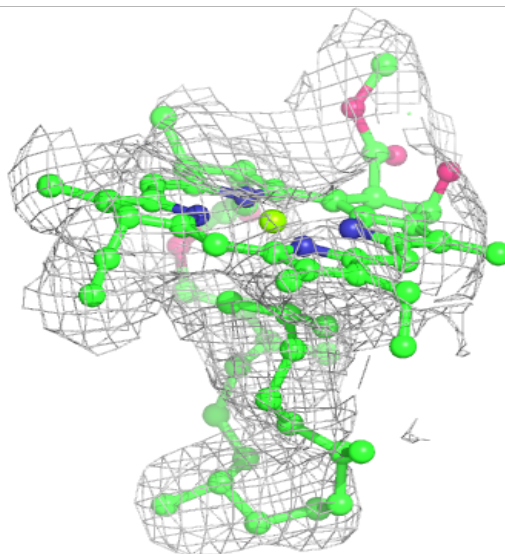
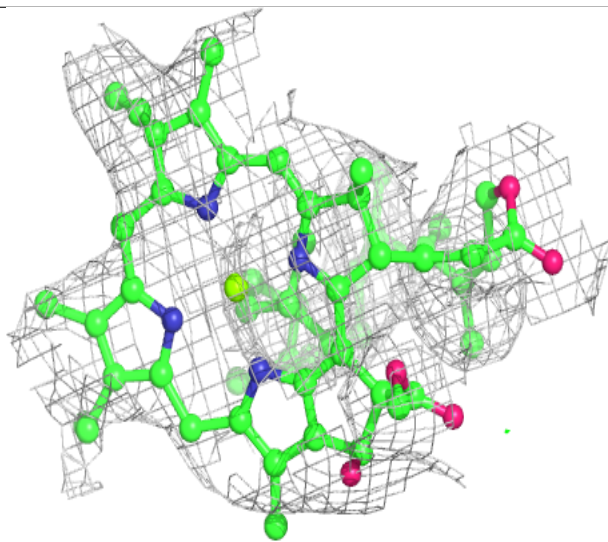
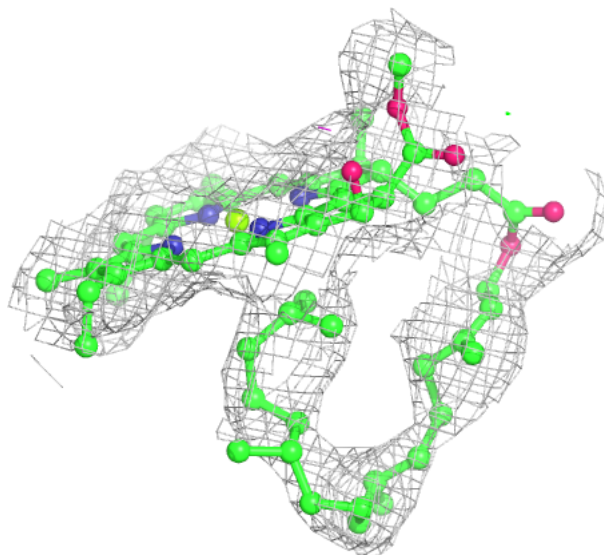
Electron density around CLA 3 3008:

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



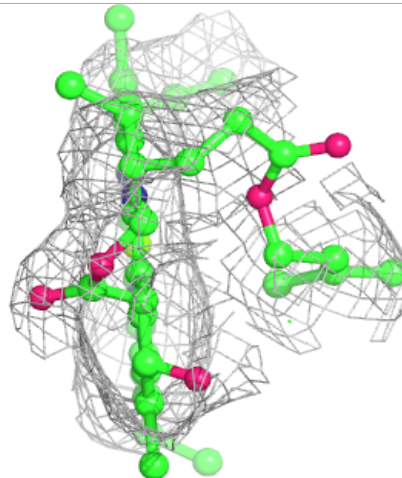
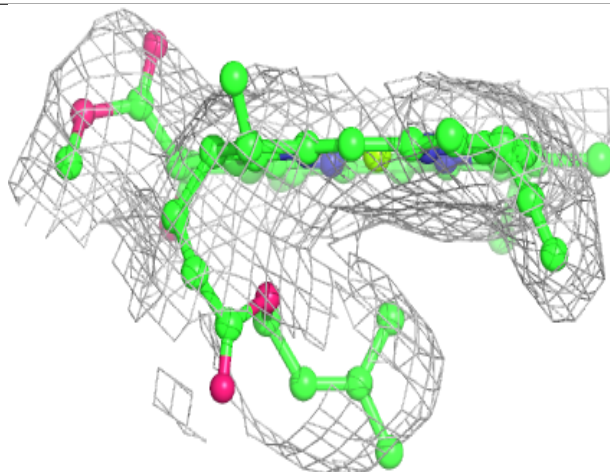
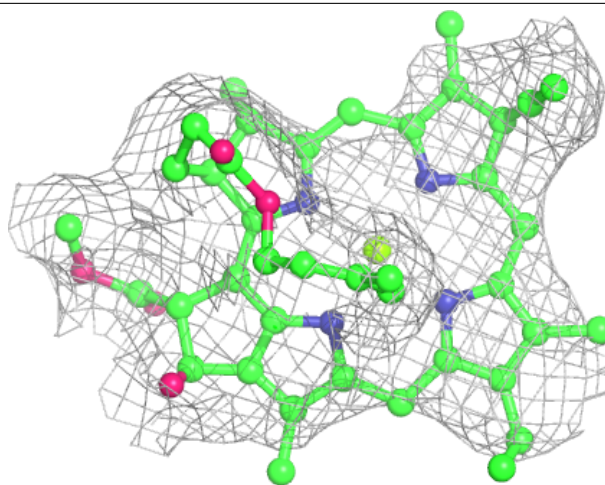
Electron density around CLA 2 1224:

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



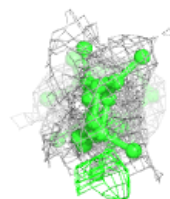
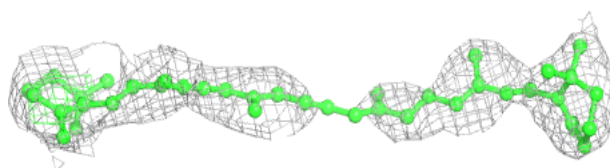
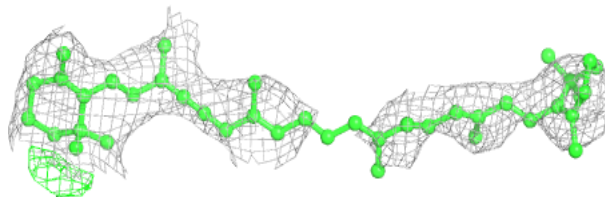
Electron density around CLA L 1166:

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



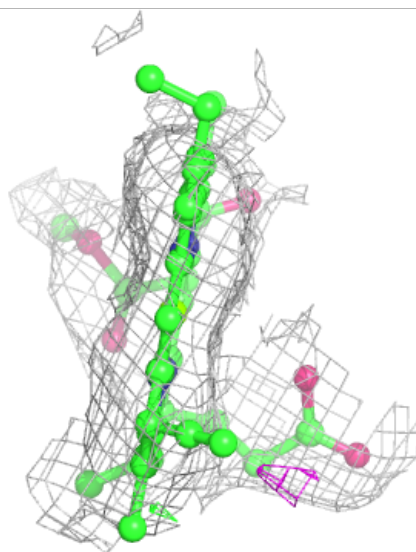
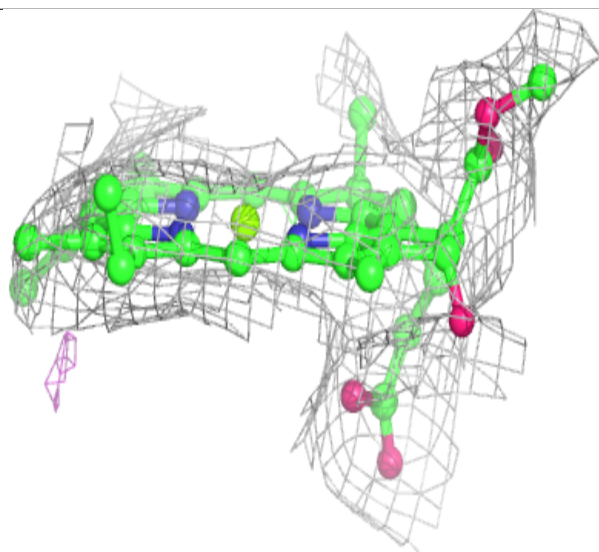
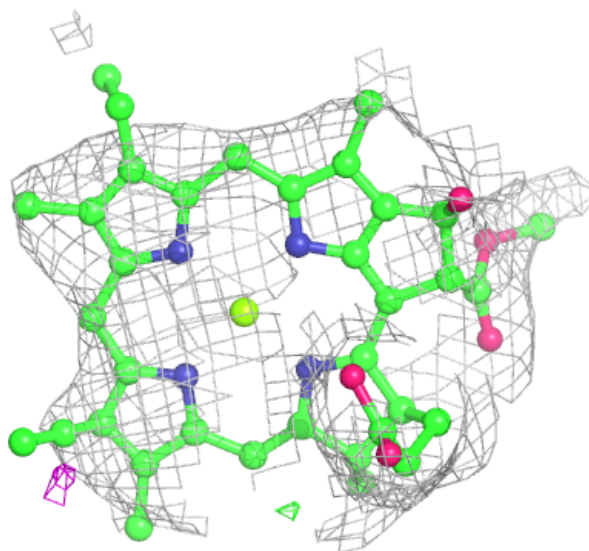
Electron density around BCR A 1804:

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



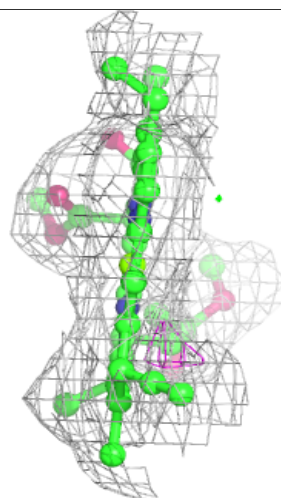
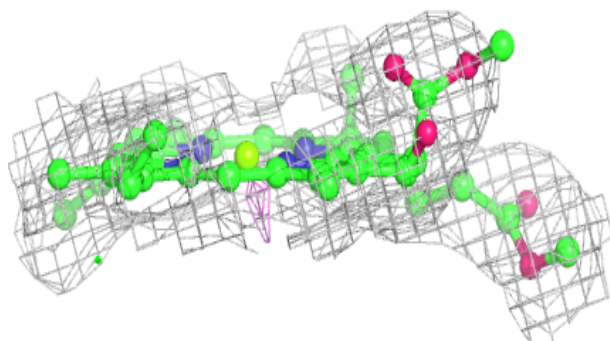
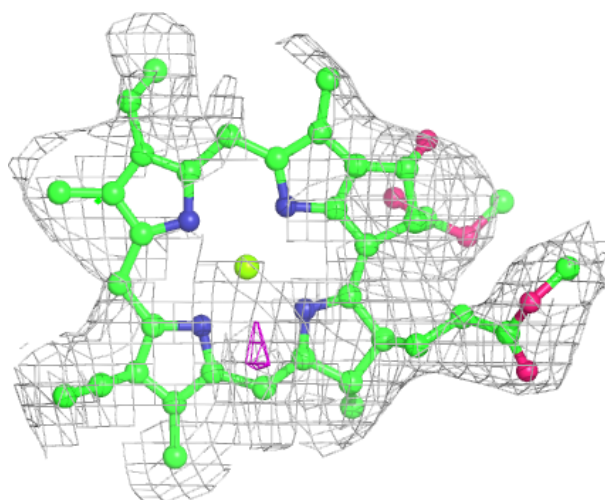
Electron density around CLA B 1764:

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



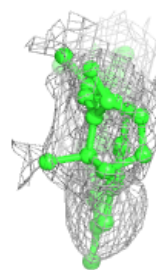
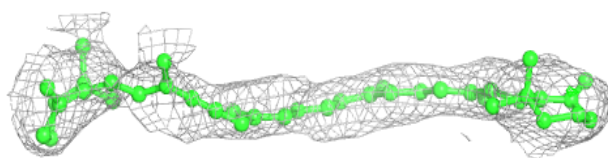
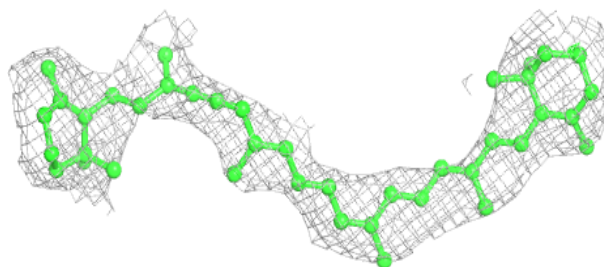
Electron density around CLA 4 1209:

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

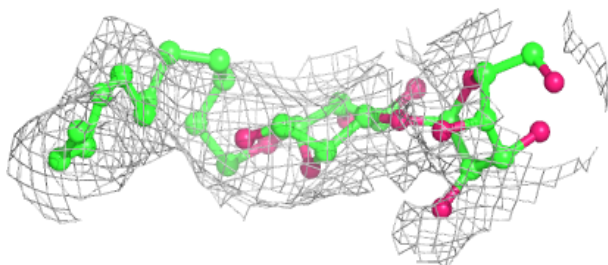
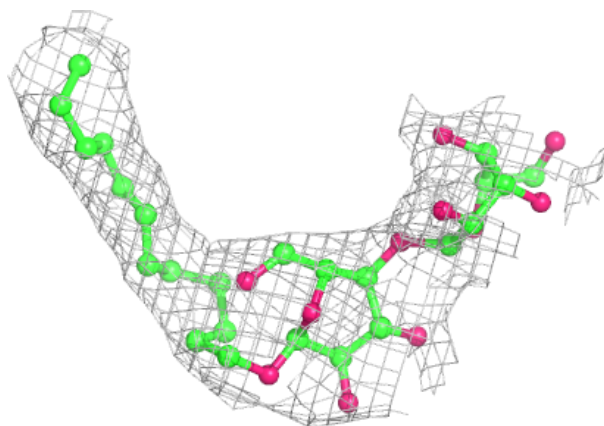


Electron density around BCR A 1807:

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

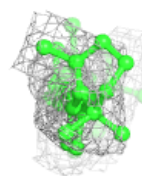
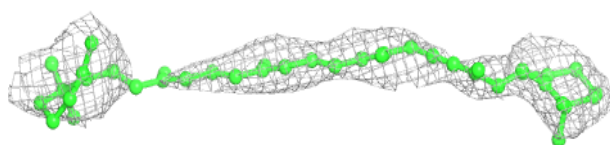
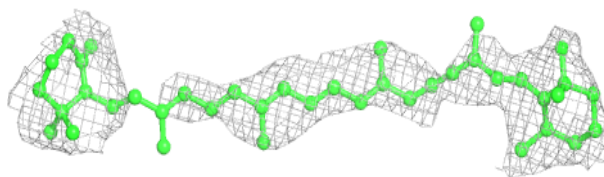
**Electron density around LMU A 7021:**

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

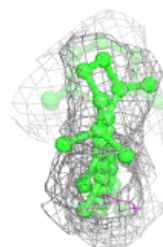
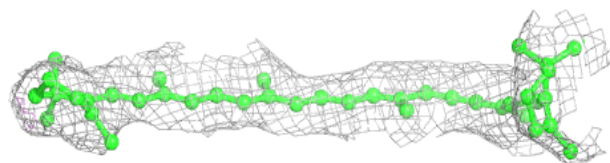
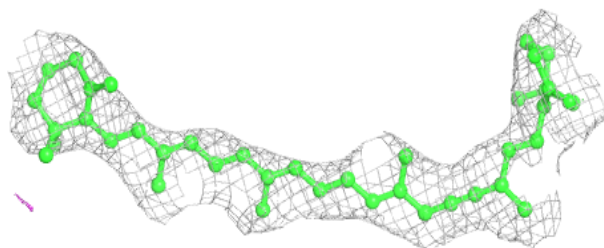


Electron density around BCR B 1774:

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

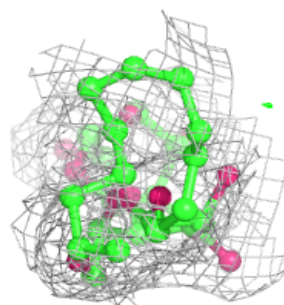
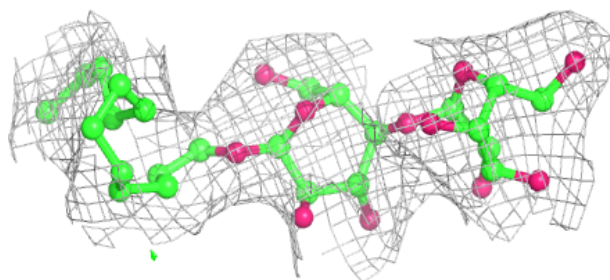
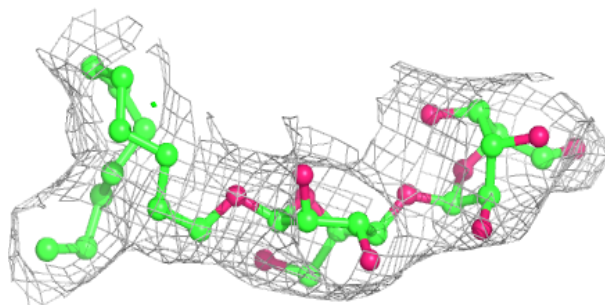
**Electron density around BCR B 1775:**

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

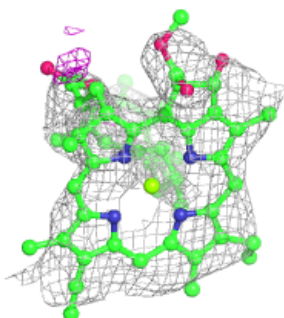
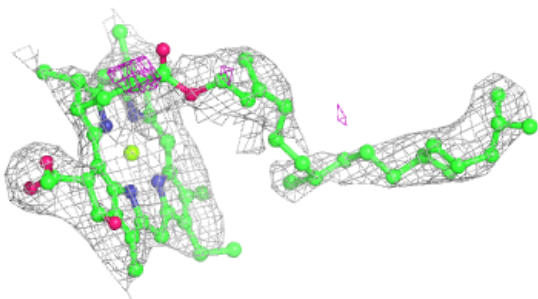
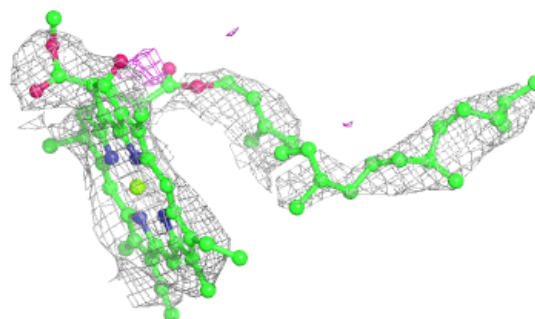


Electron density around LMU A 7023:

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

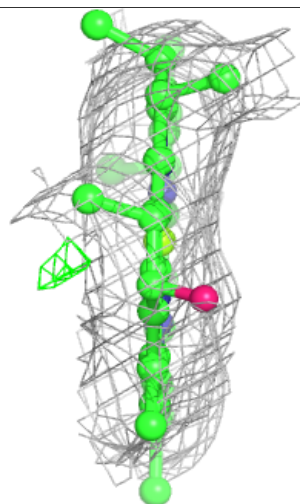
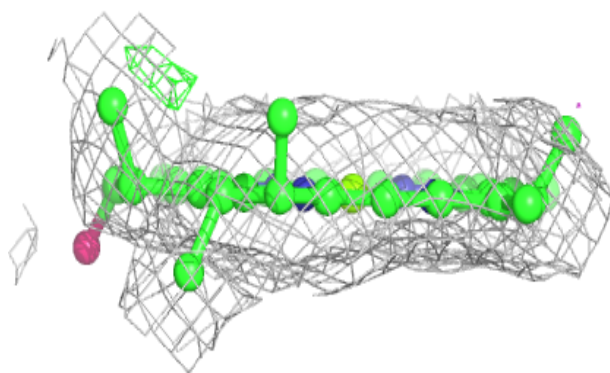
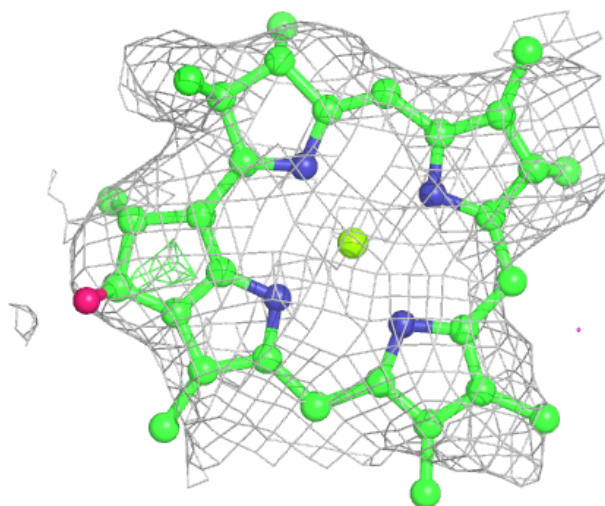
**Electron density around CLA A 1767:**

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



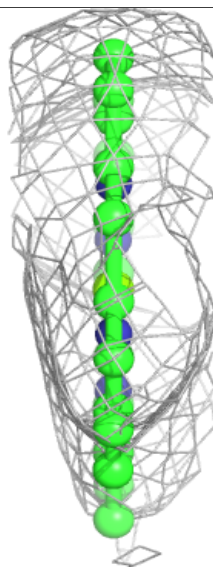
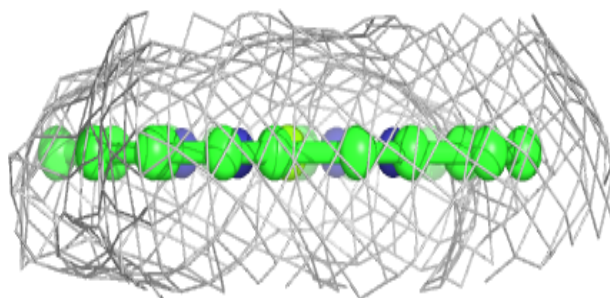
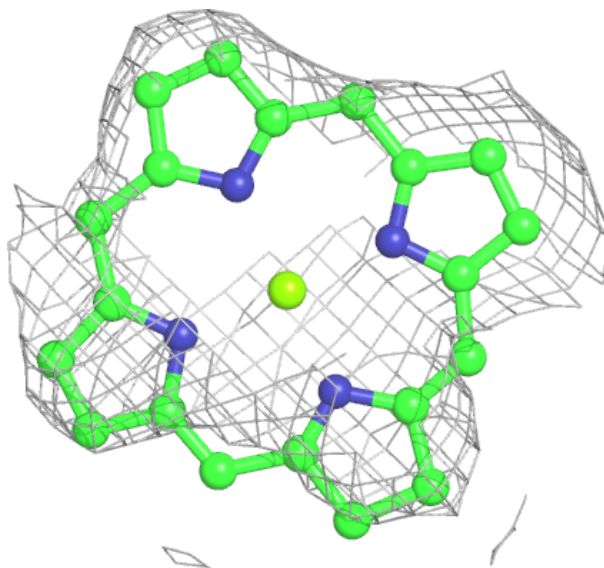
Electron density around CLA B 1772:

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



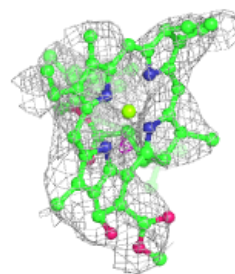
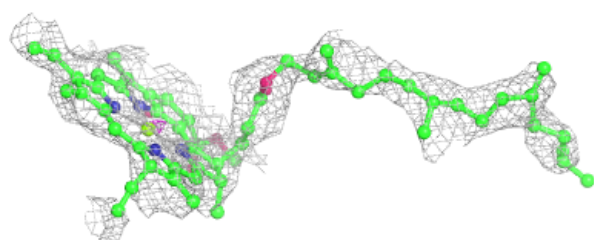
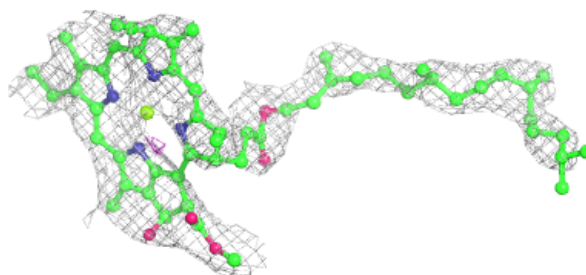
Electron density around CLA 4 1202:

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



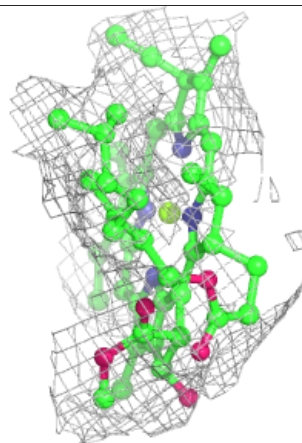
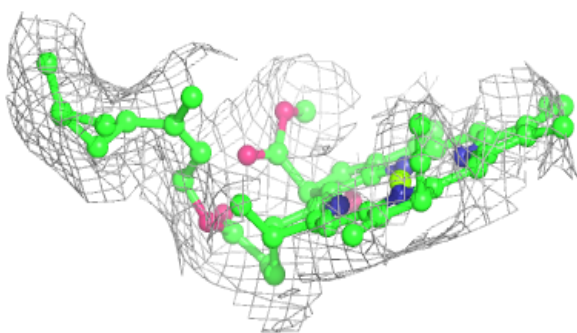
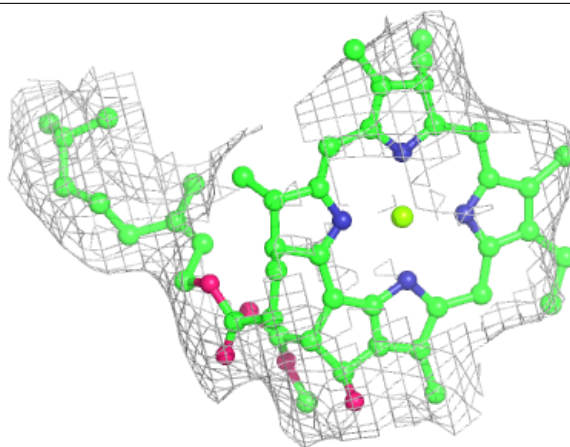
Electron density around CLA A 1776:

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



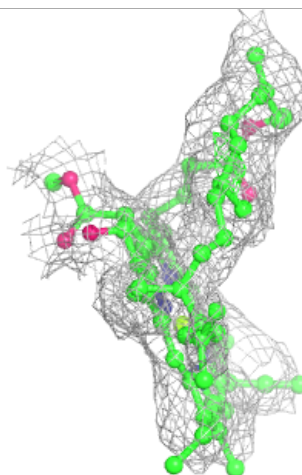
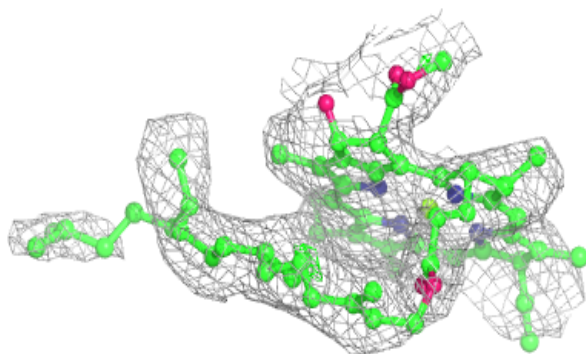
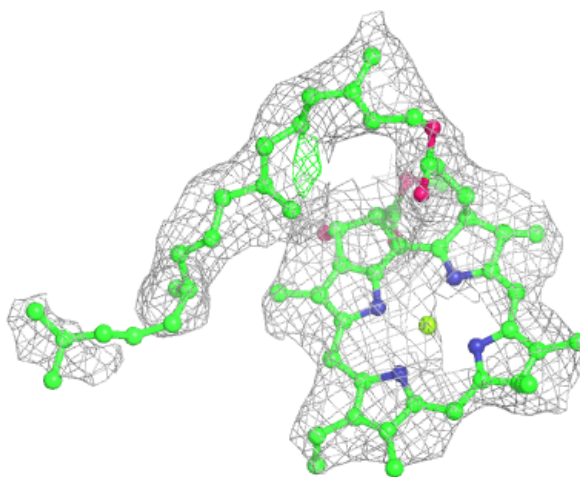
Electron density around CLA J 1045:

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



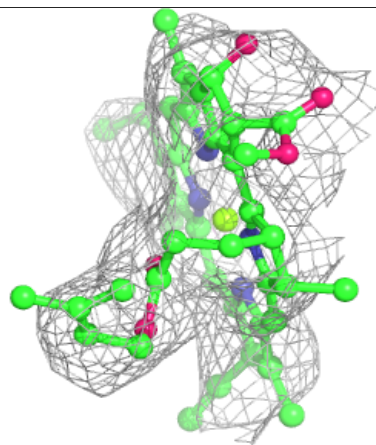
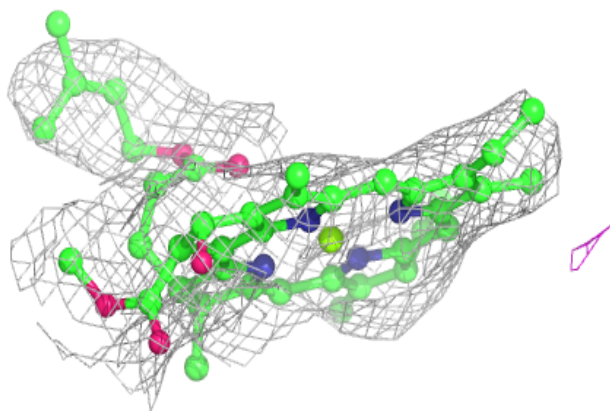
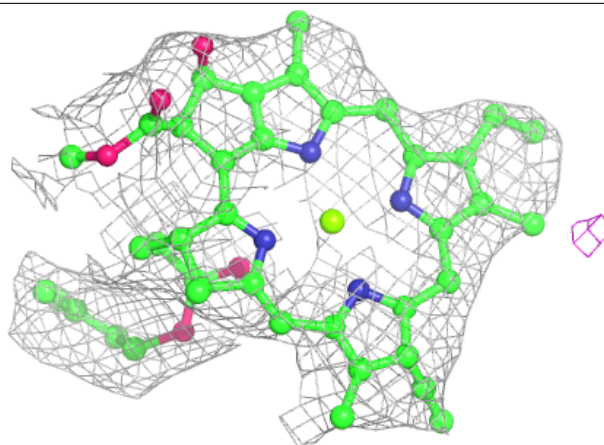
Electron density around CLA B 1762:

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



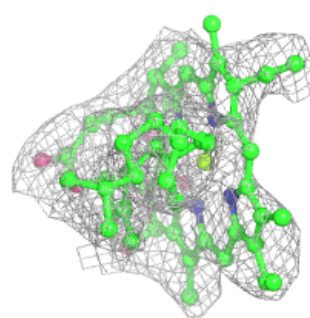
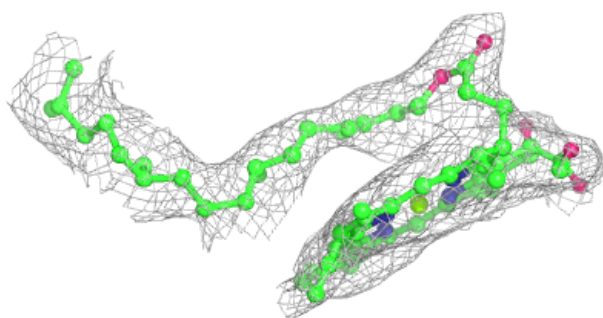
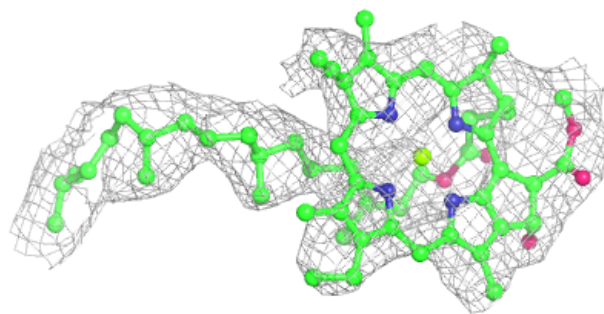
Electron density around CLA A 1771:

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

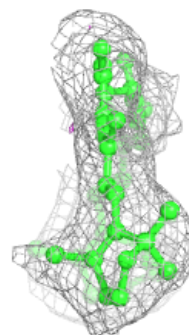
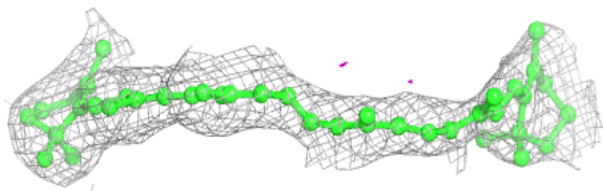
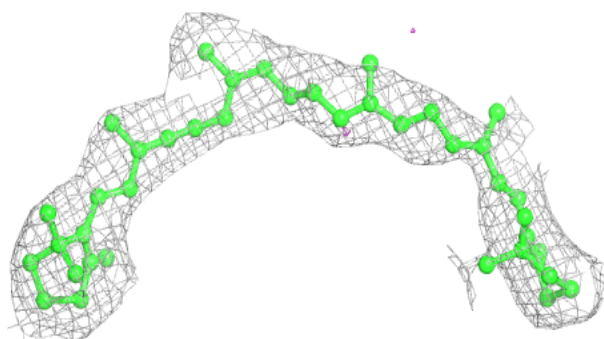


Electron density around CLA A 1772:

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

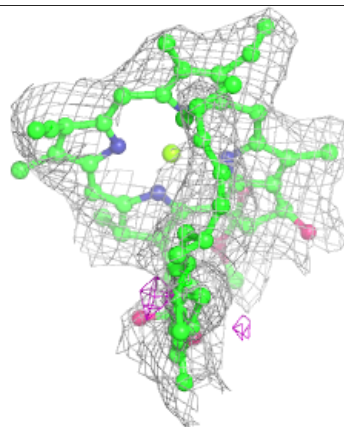
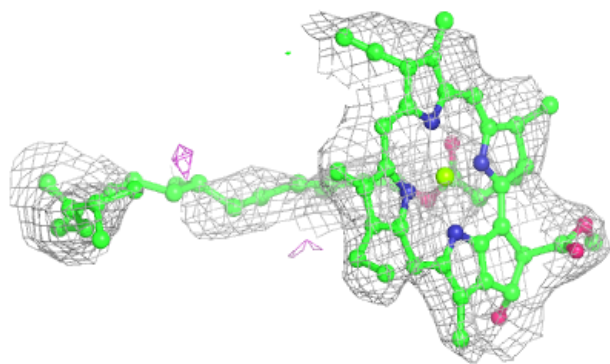
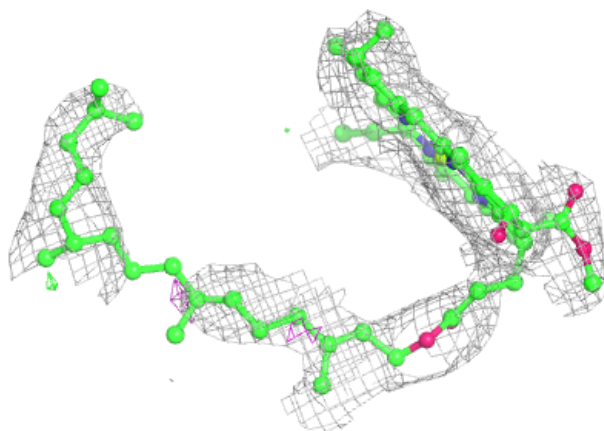
**Electron density around BCR B 1779:**

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



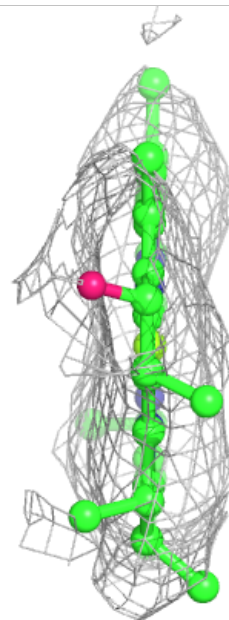
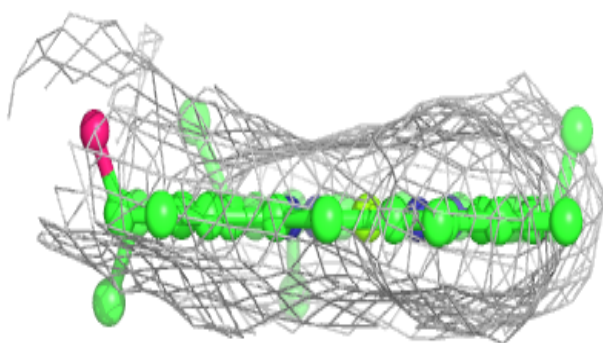
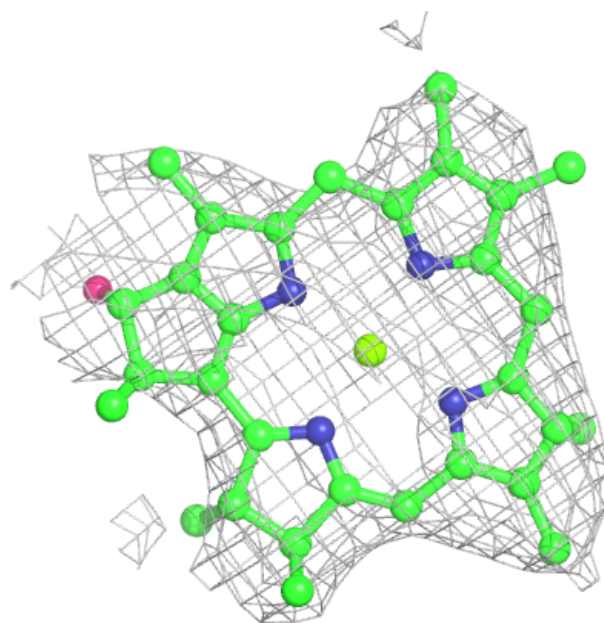
Electron density around CLA A 1787:

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



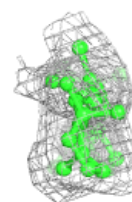
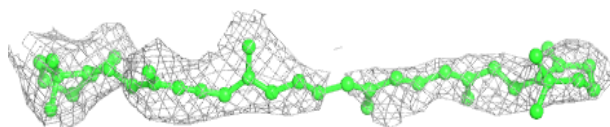
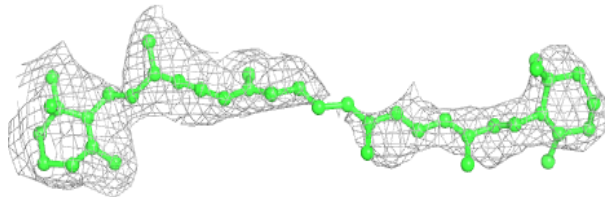
Electron density around CLA 1 1195:

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

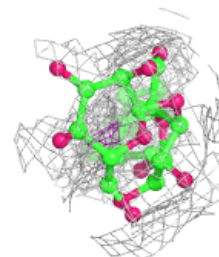
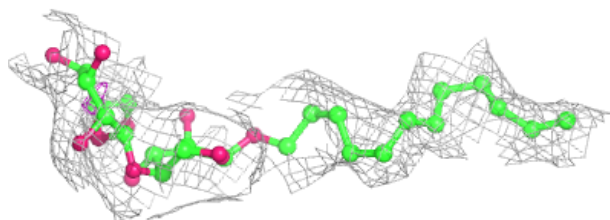
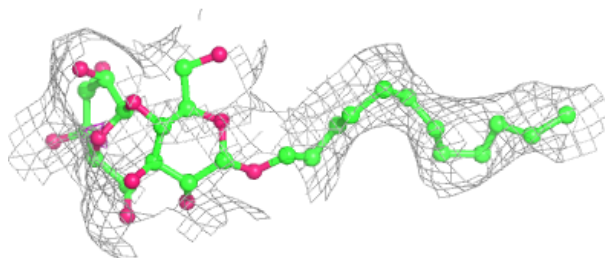


Electron density around BCR L 1169:

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

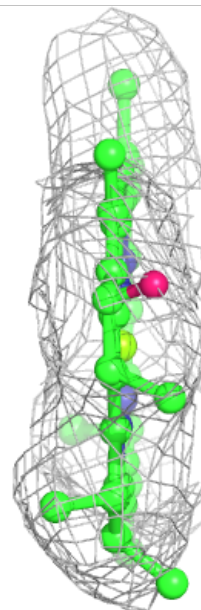
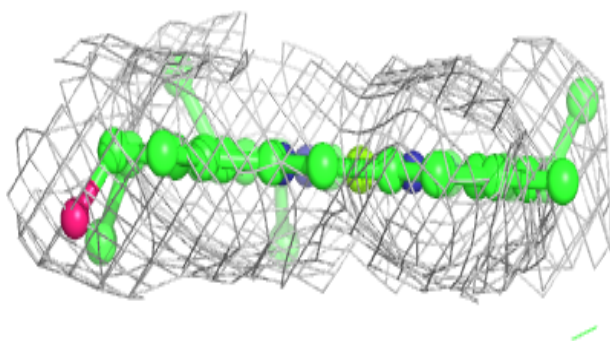
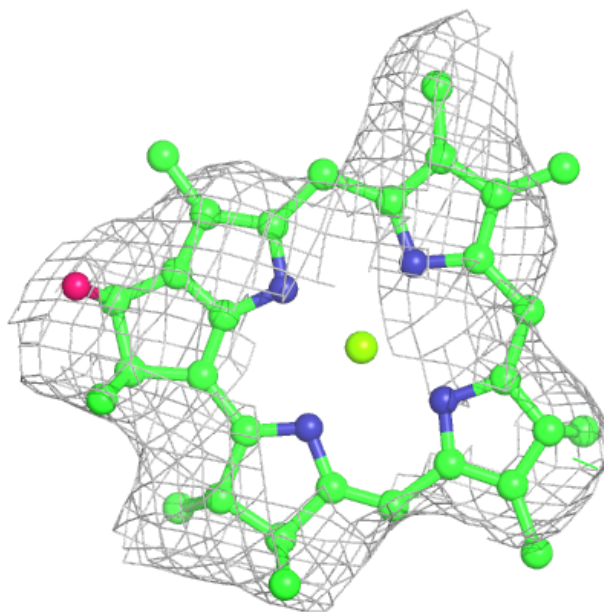
**Electron density around LMU A 7033:**

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



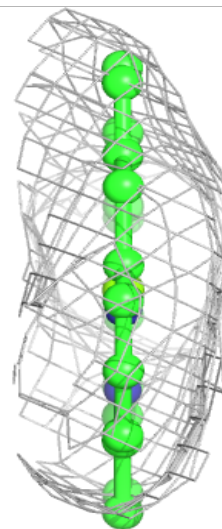
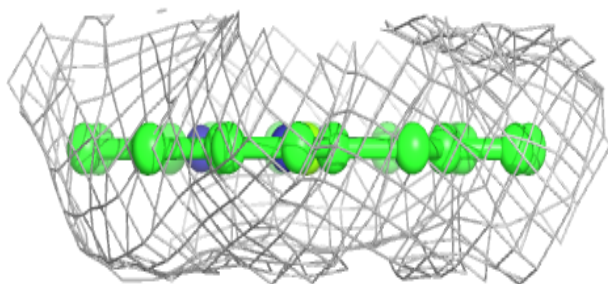
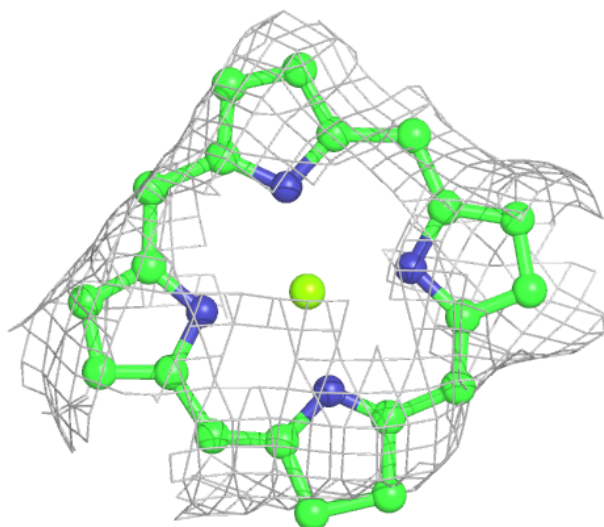
Electron density around CLA 1 1196:

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



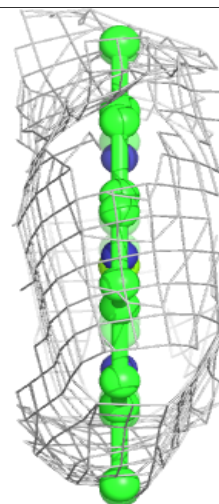
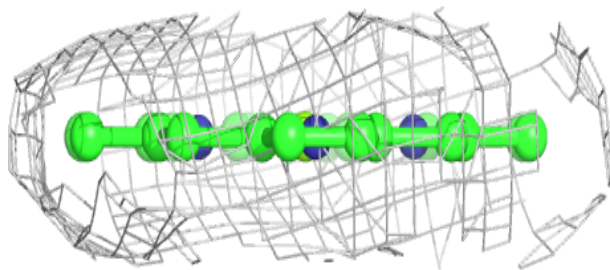
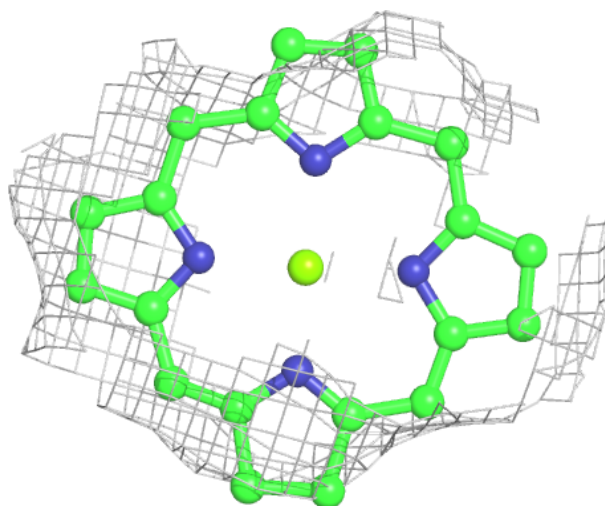
Electron density around CLA 1 1201:

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



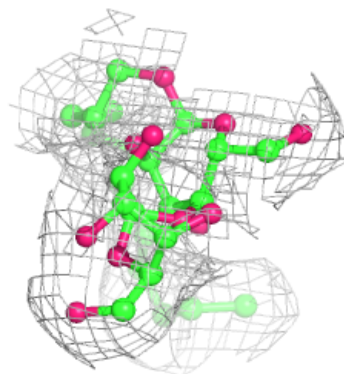
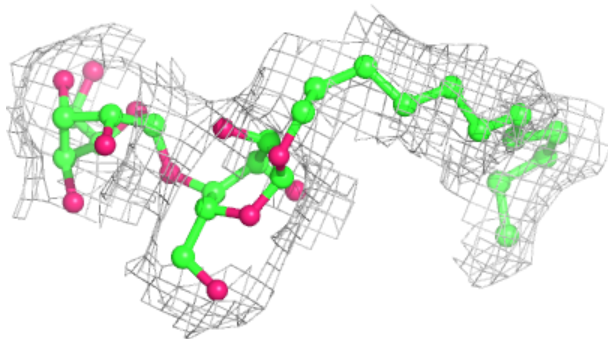
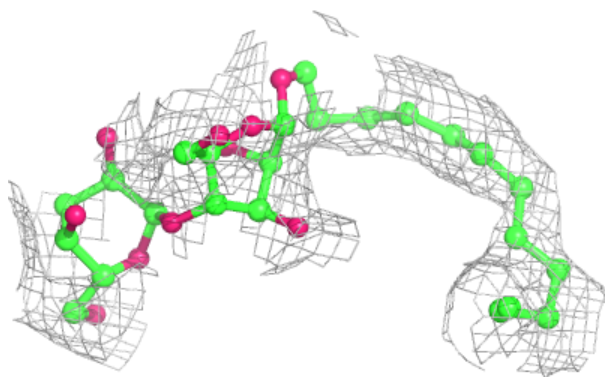
Electron density around CLA 2 1219:

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

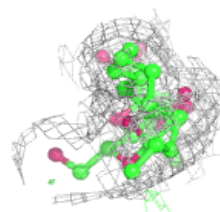
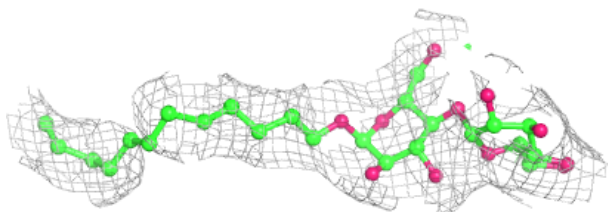
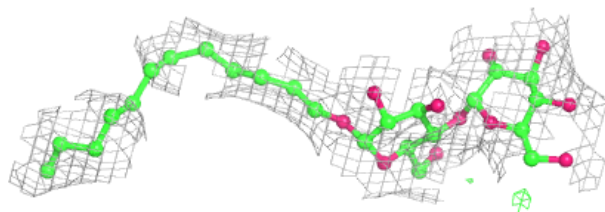


Electron density around LMU A 7022:

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

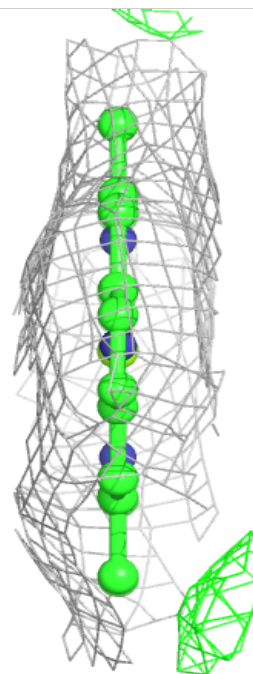
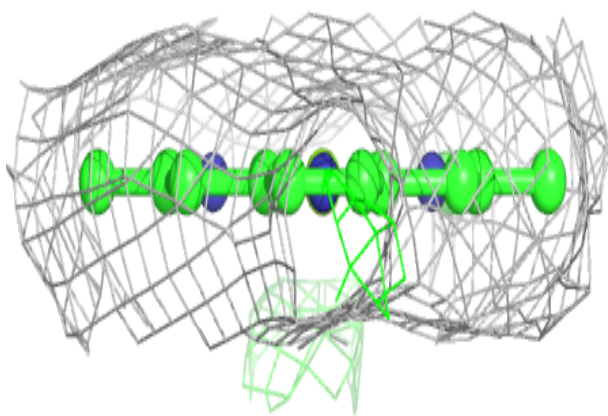
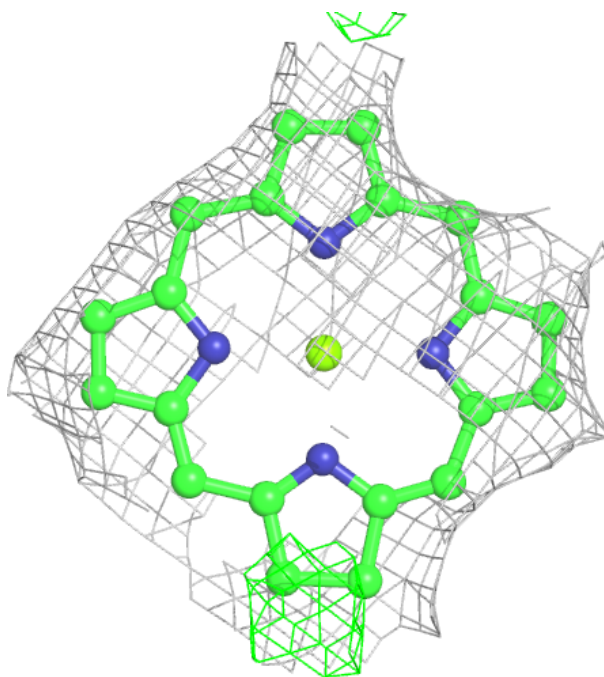
**Electron density around LMU A 7040:**

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



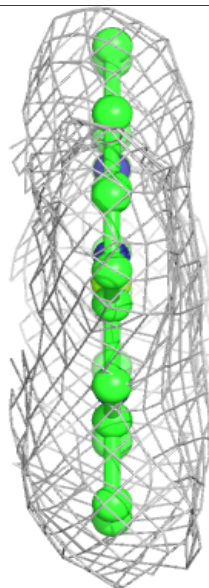
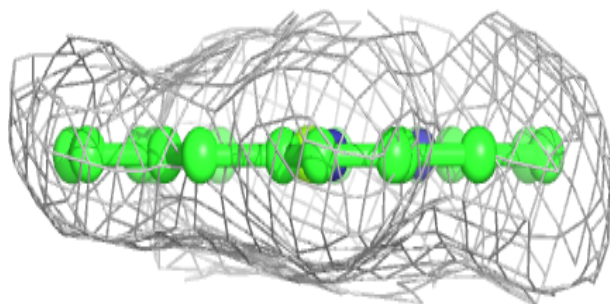
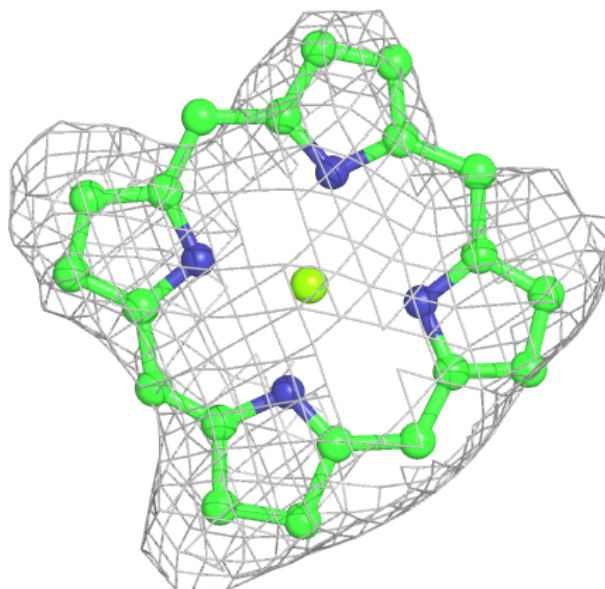
Electron density around CLA 3 1216:

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



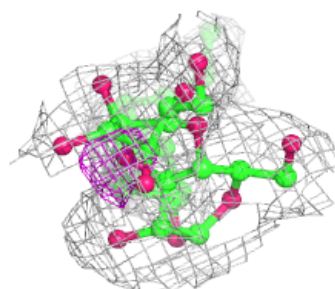
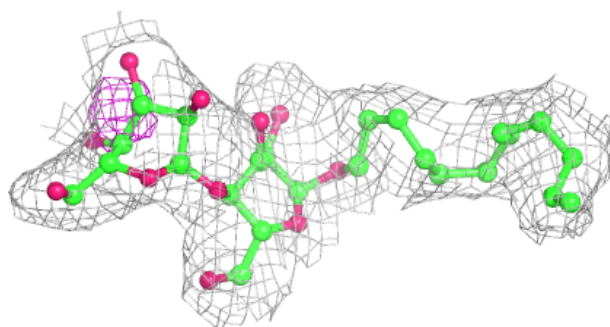
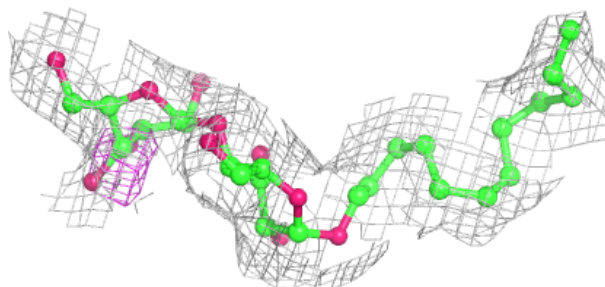
Electron density around CLA 2 2010:

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

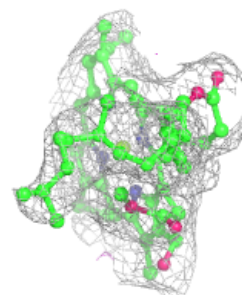
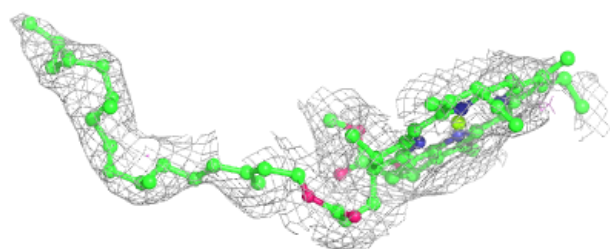
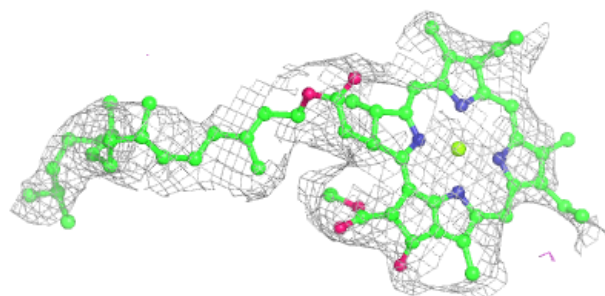


Electron density around LMU A 7026:

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

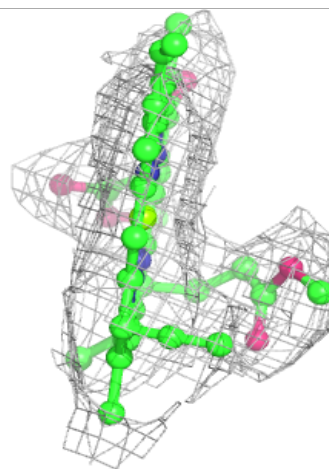
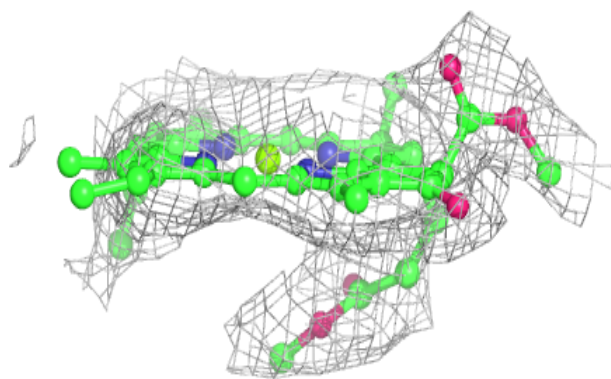
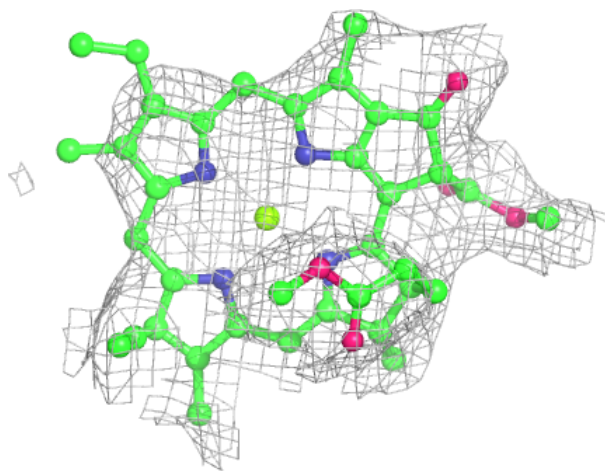
**Electron density around CLA 3 3011:**

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



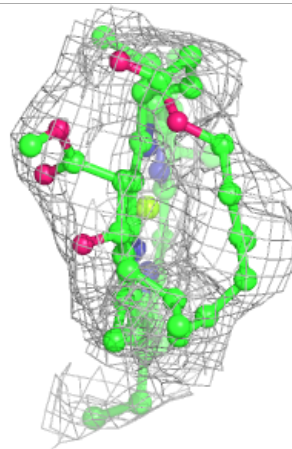
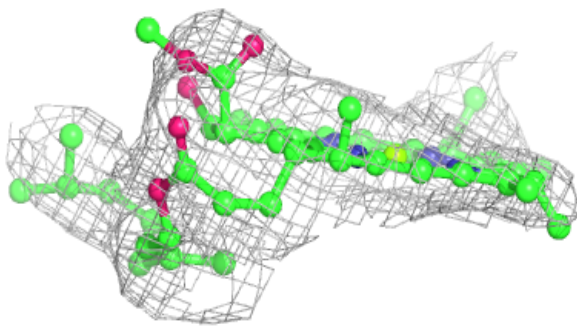
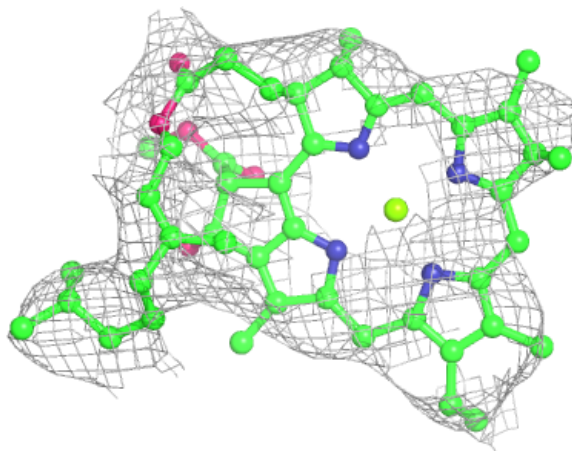
Electron density around CLA 1 1190:

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



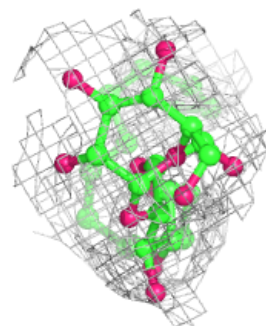
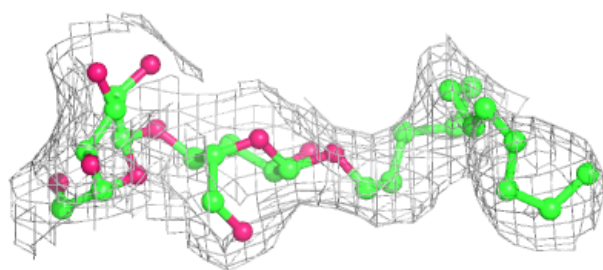
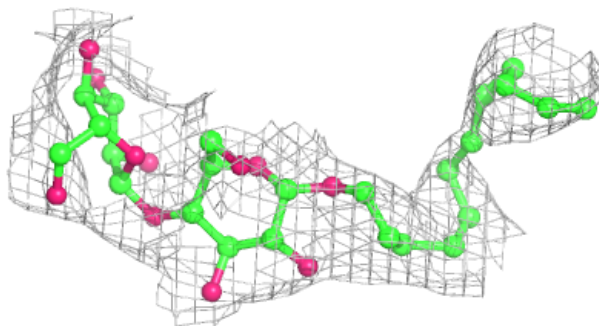
Electron density around CLA B 1741:

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



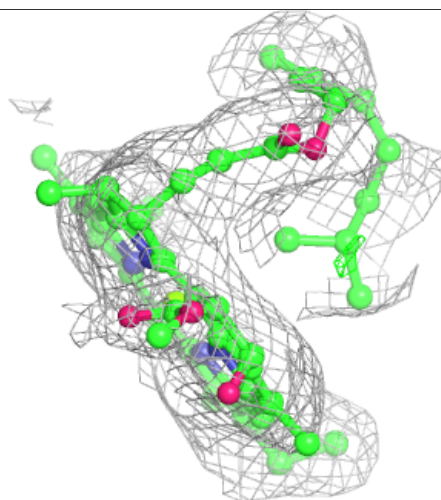
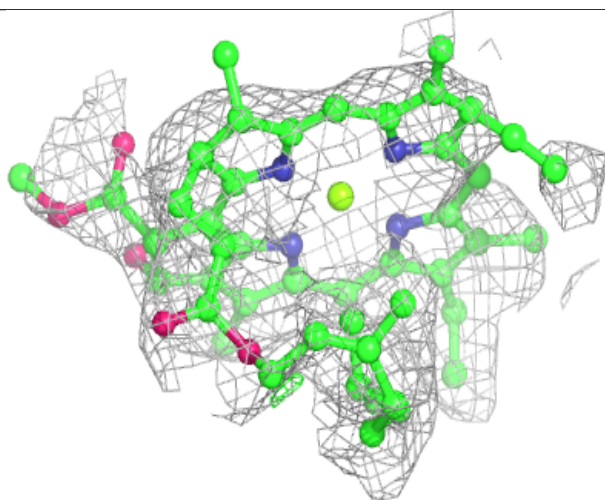
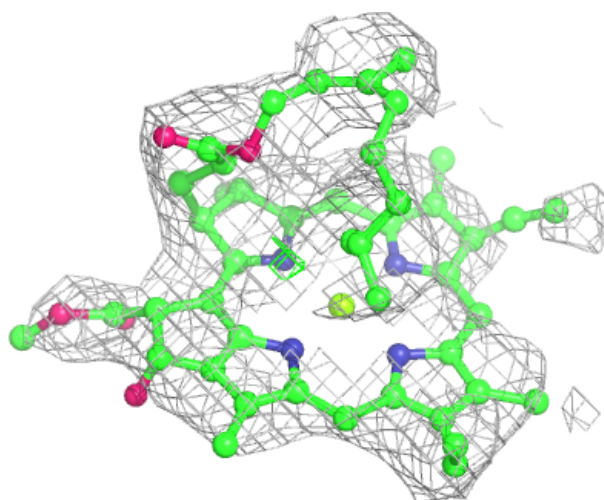
Electron density around LMU R 1056:

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



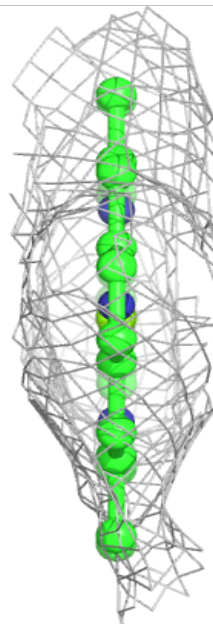
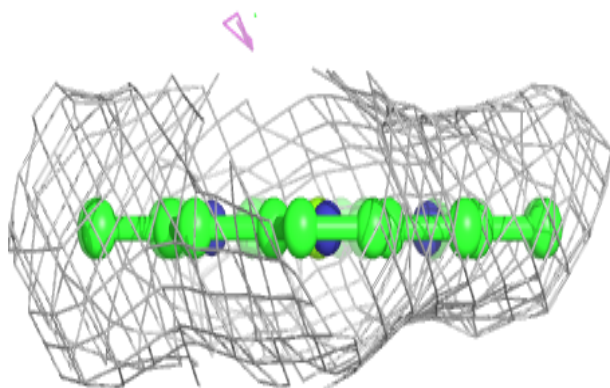
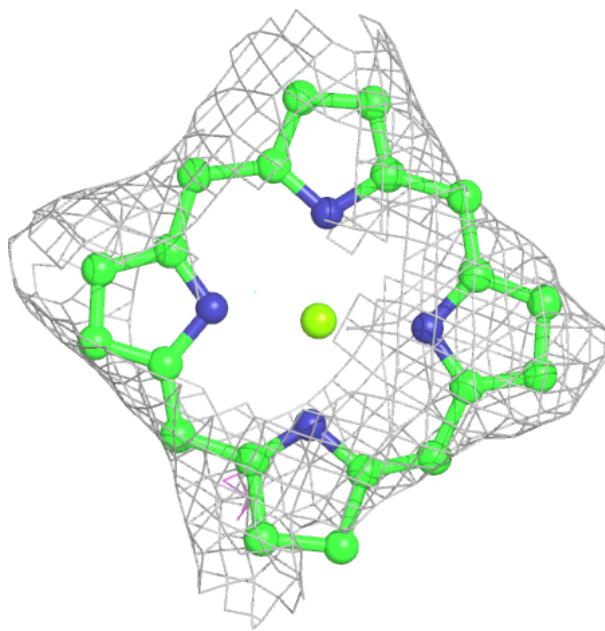
Electron density around CLA B 1742:

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



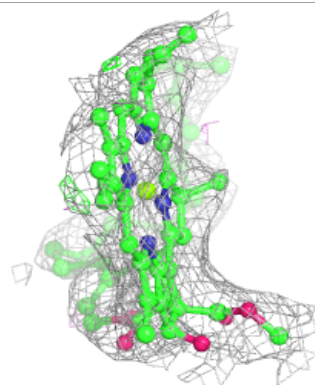
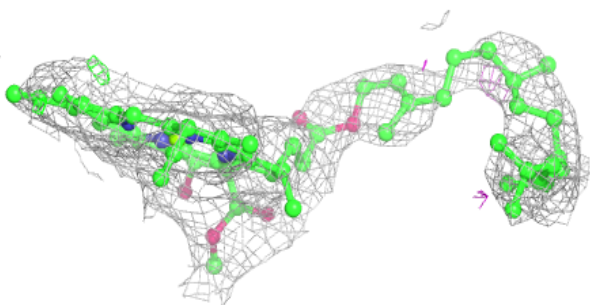
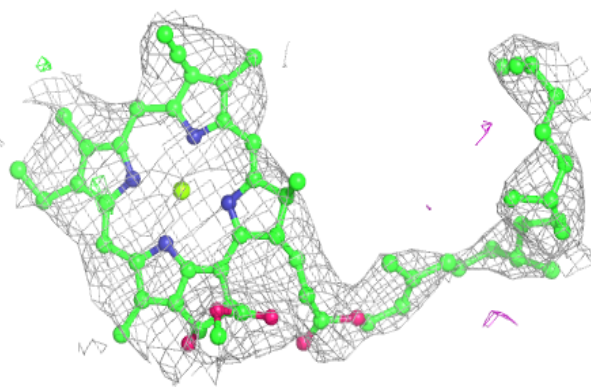
Electron density around CLA 3 3015:

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



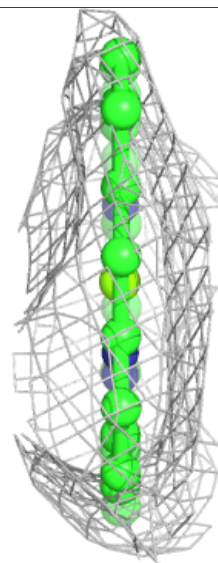
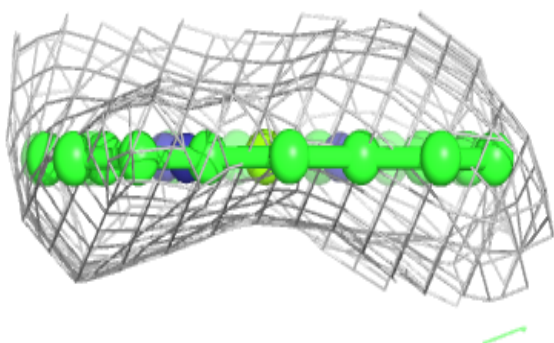
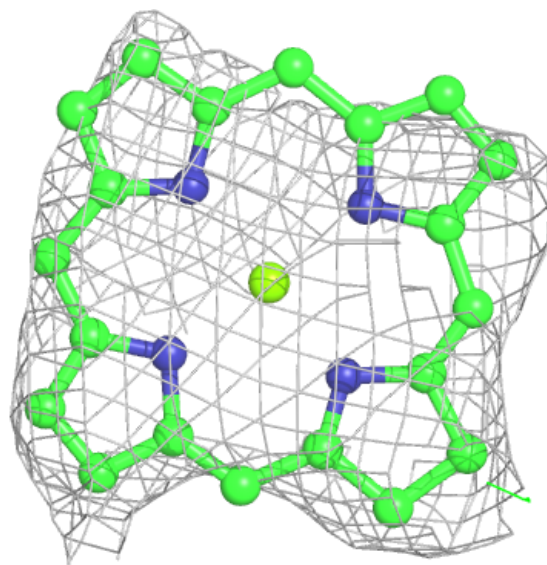
Electron density around CLA A 1782:

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



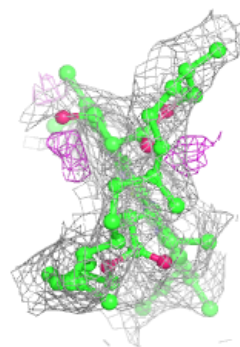
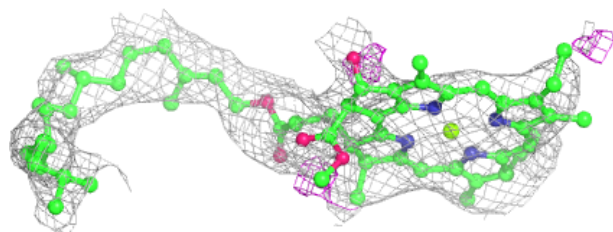
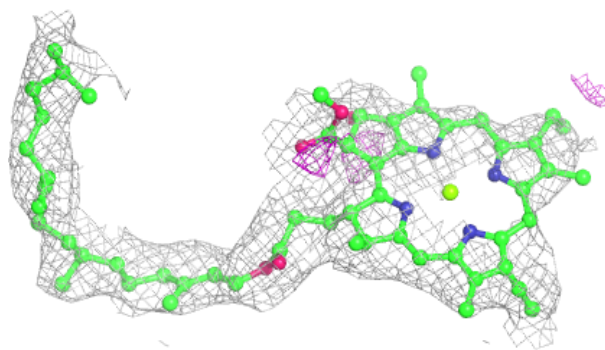
Electron density around CLA 2 1221:

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



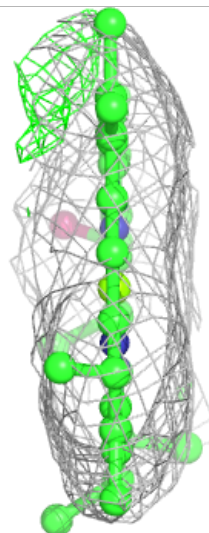
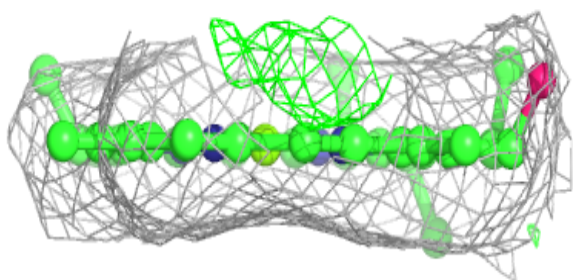
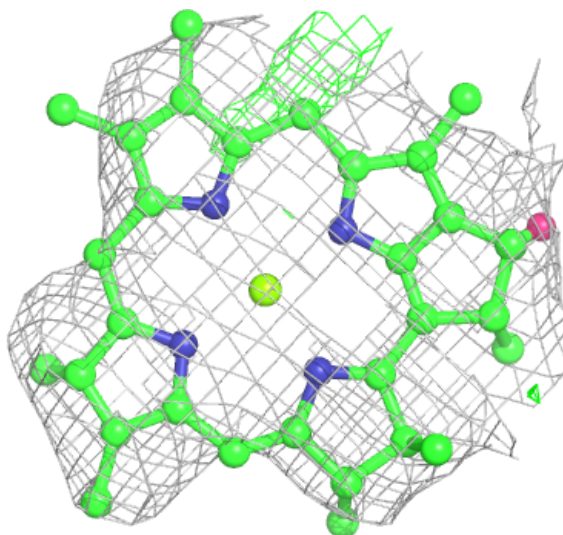
Electron density around CLA B 1756:

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



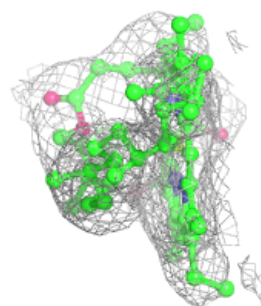
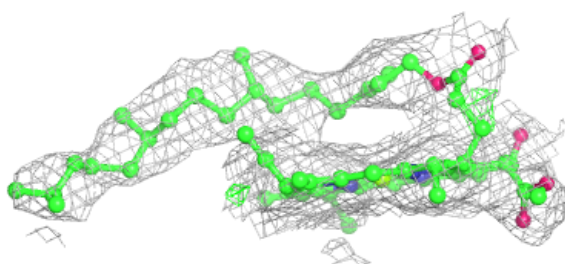
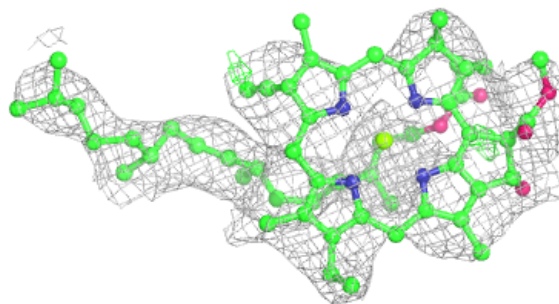
Electron density around CLA 4 1197:

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



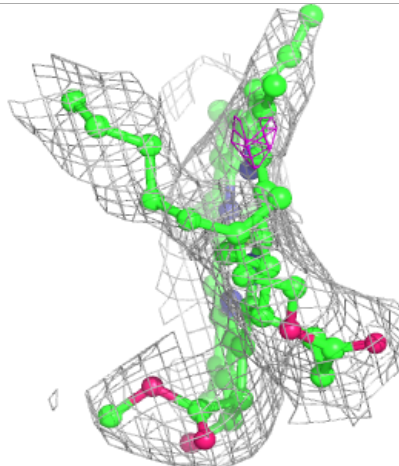
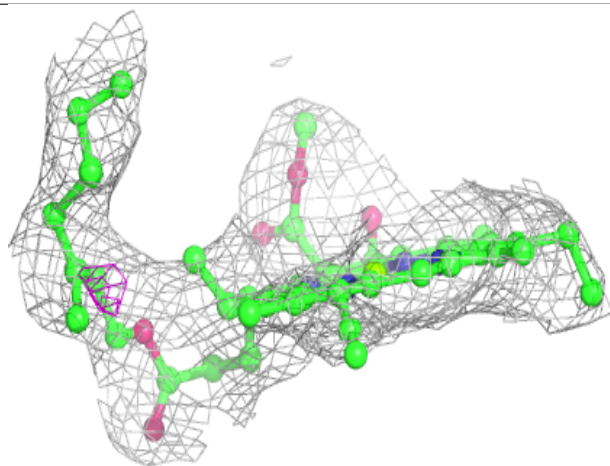
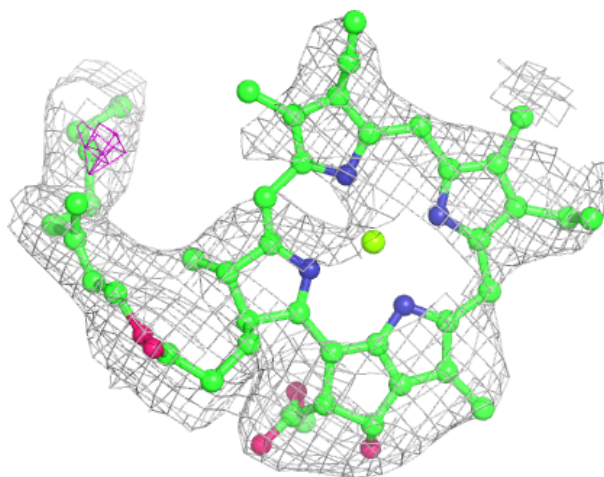
Electron density around CLA B 1735:

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



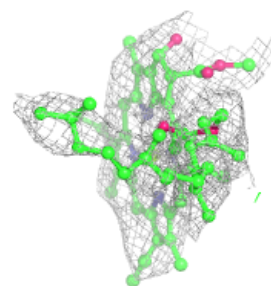
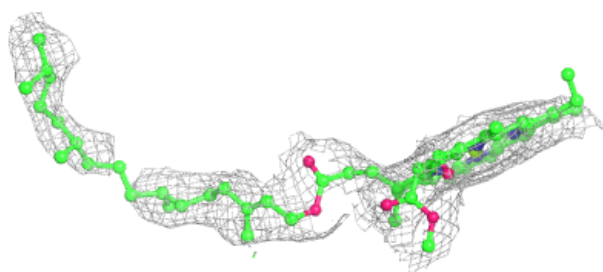
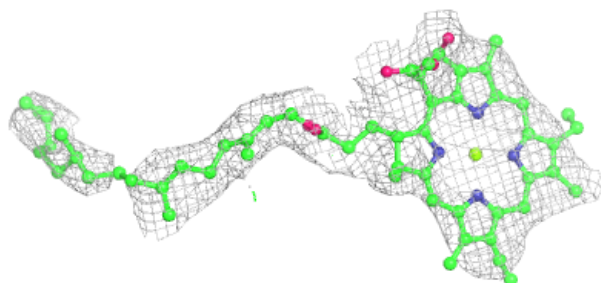
Electron density around CLA A 1769:

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

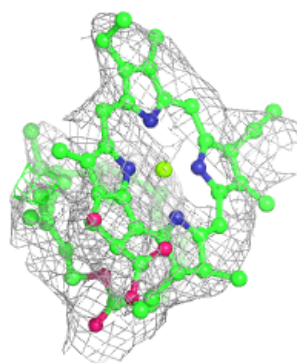
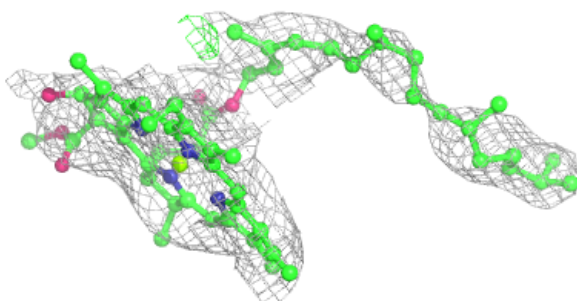
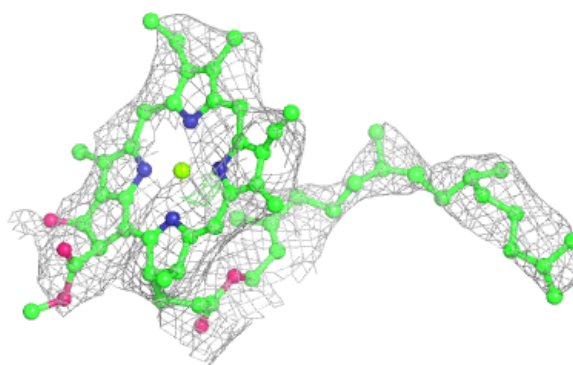


Electron density around CLA A 1761:

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

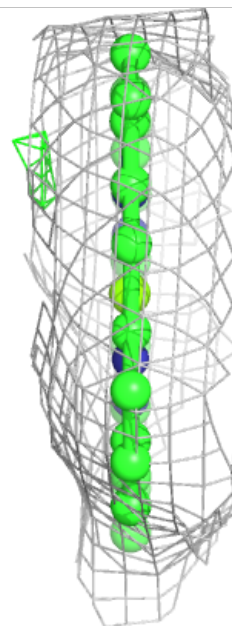
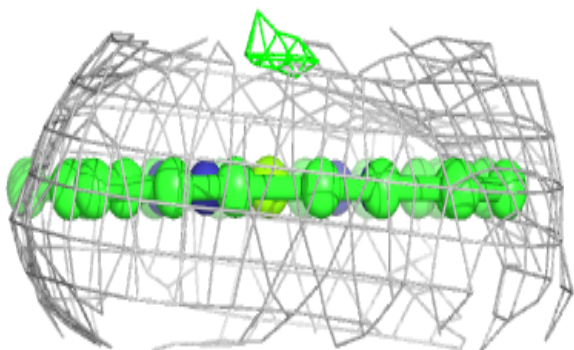
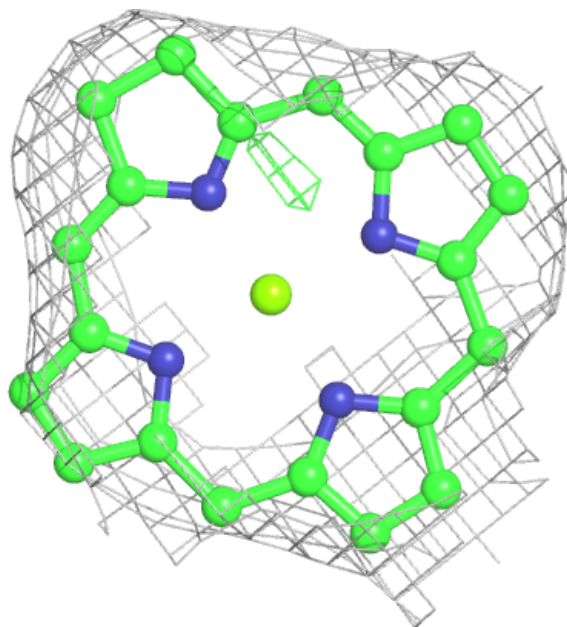
**Electron density around CLA B 1744:**

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



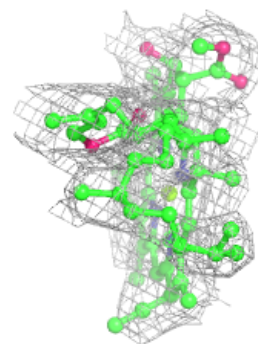
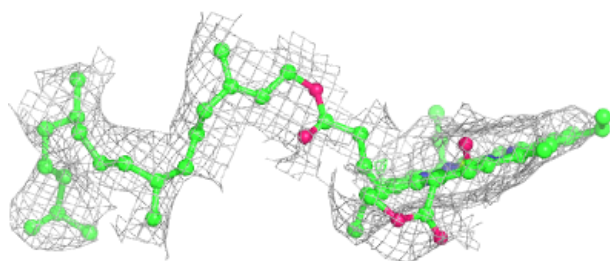
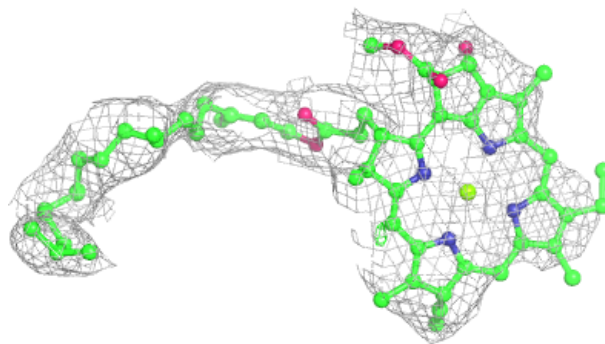
Electron density around CLA 4 1205:

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



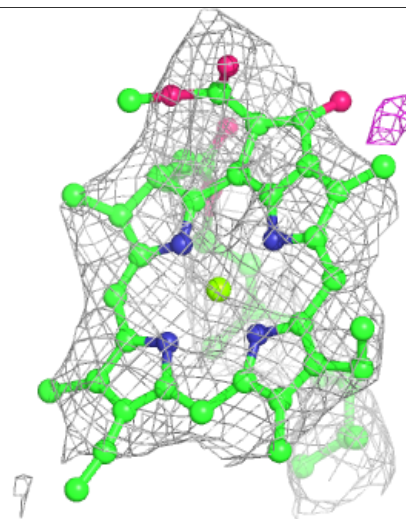
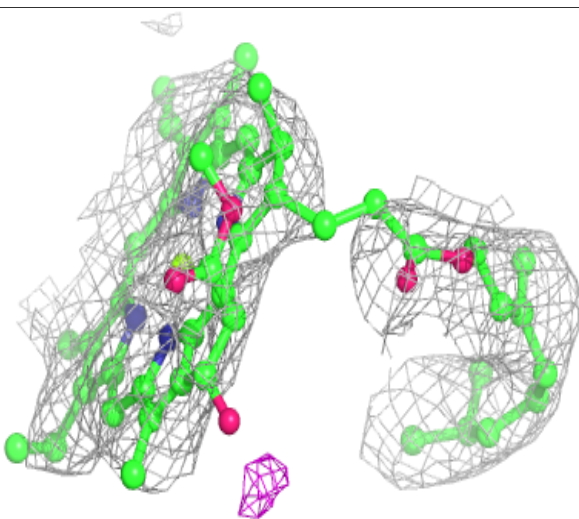
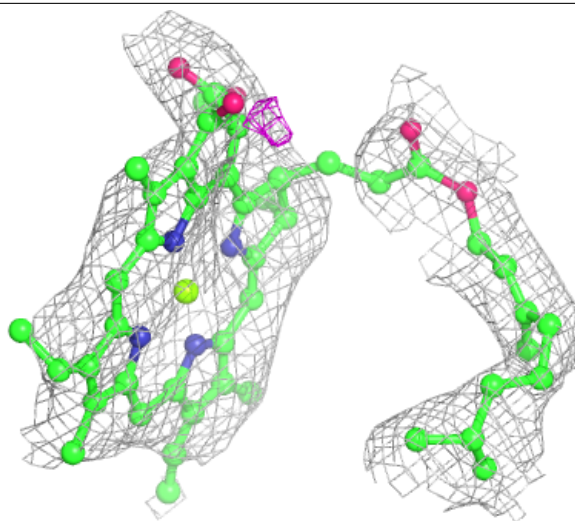
Electron density around CLA A 1781:

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



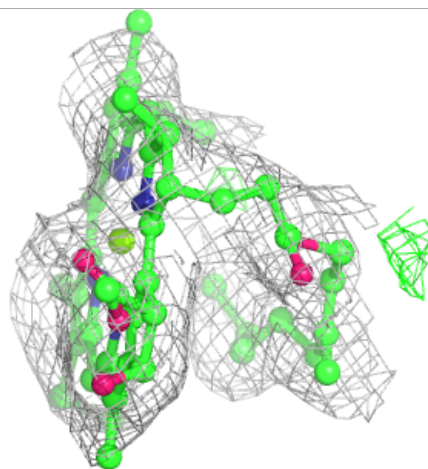
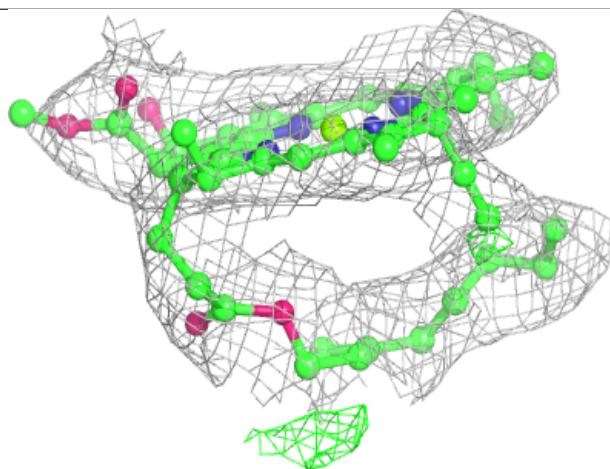
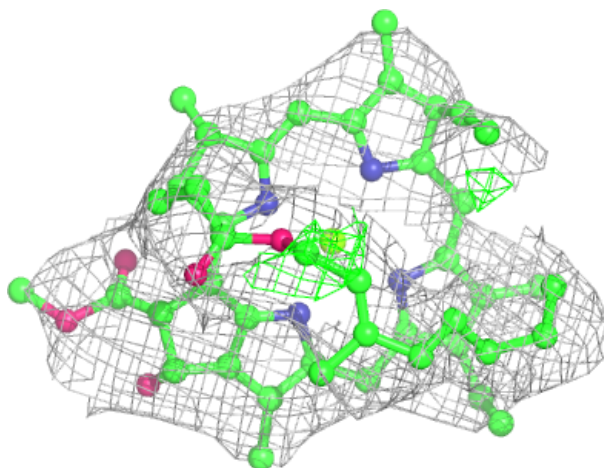
Electron density around CLA A 1760:

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



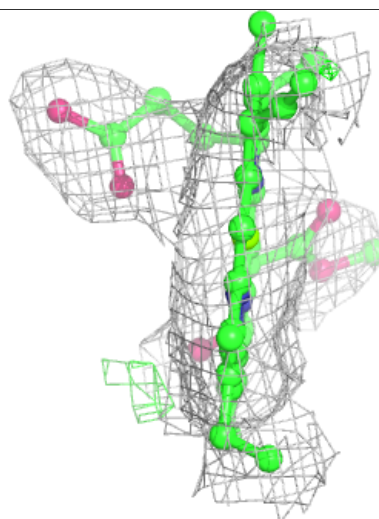
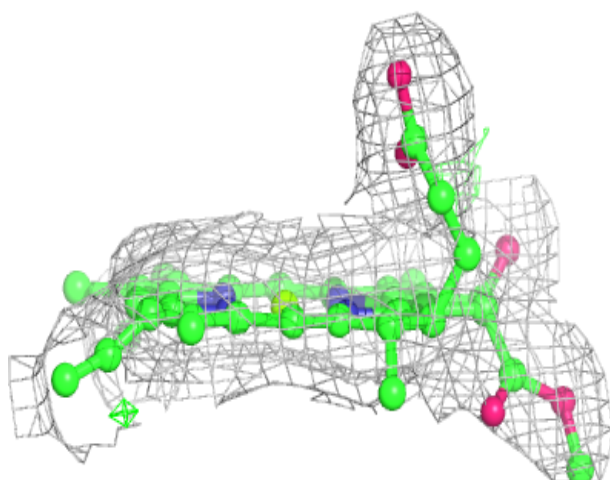
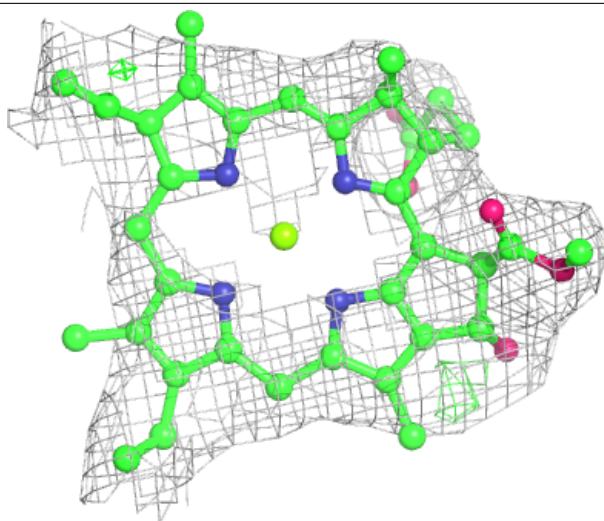
Electron density around CLA A 1768:

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



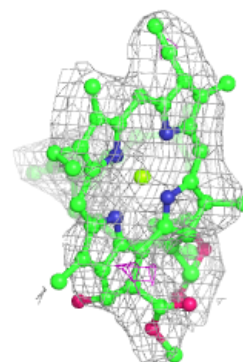
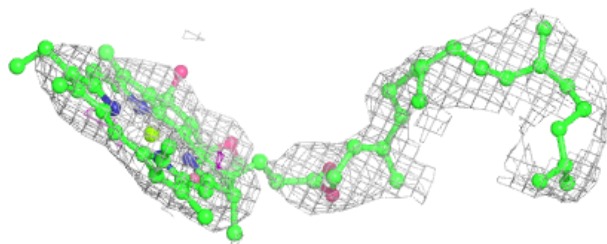
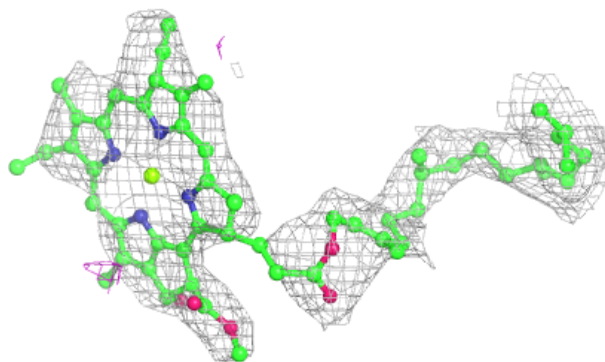
Electron density around CLA B 1736:

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

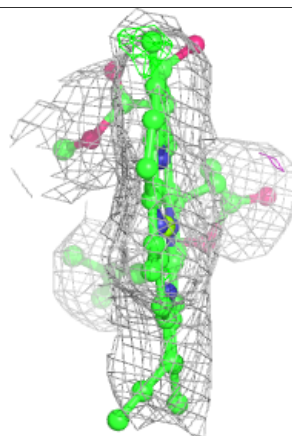
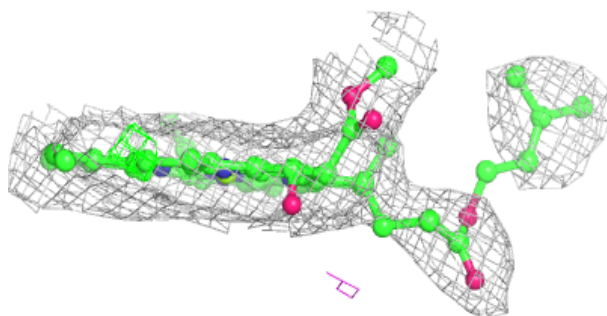
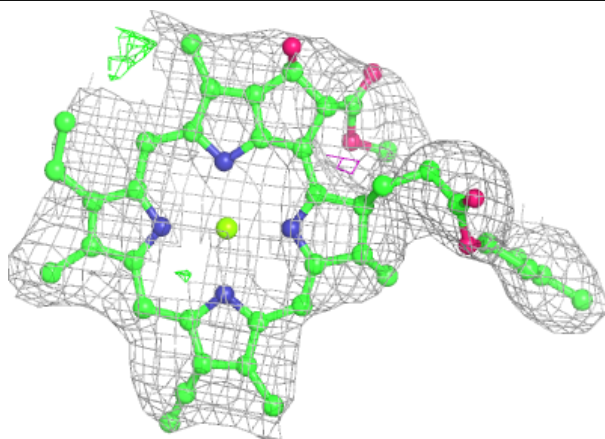


Electron density around CLA B 1740:

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

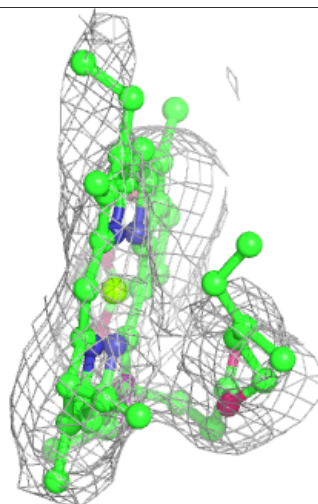
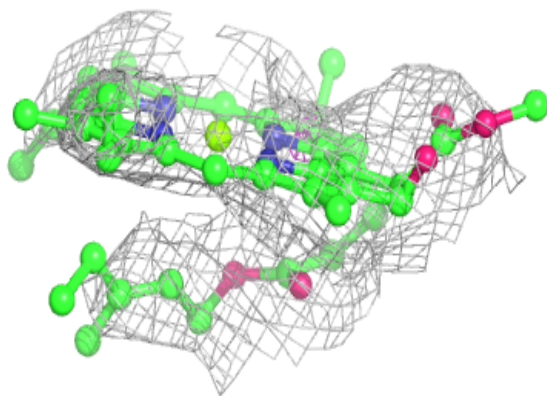
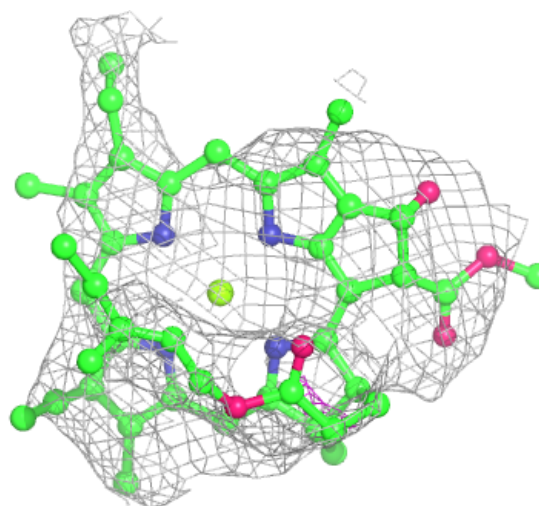
**Electron density around CLA B 1761:**

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



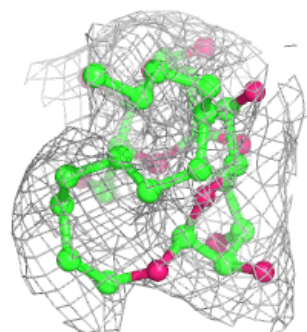
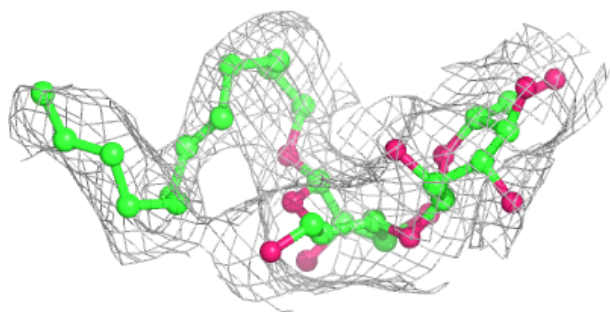
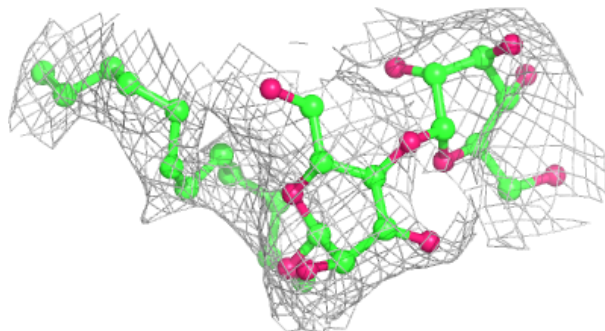
Electron density around CLA A 1777:

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

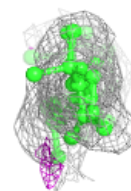
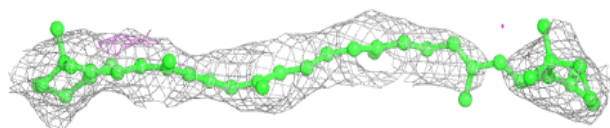
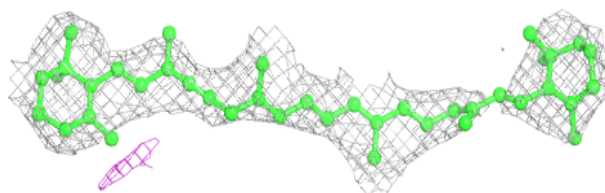


Electron density around LMU L 1171:

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

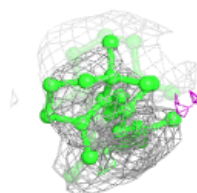
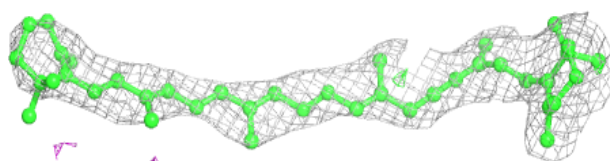
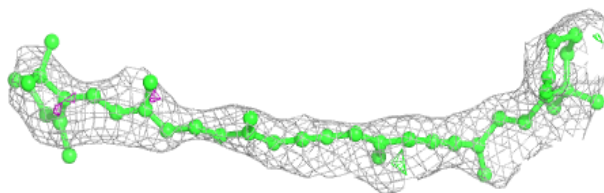
**Electron density around BCR B 1777:**

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

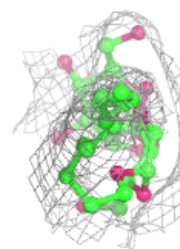
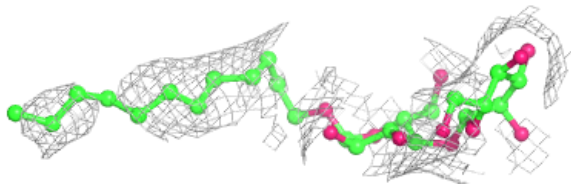
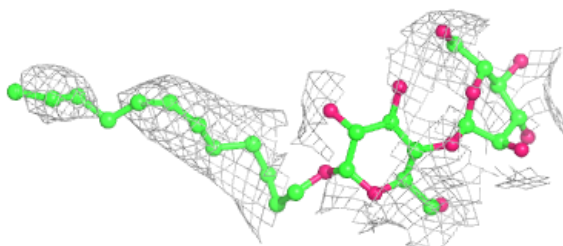


Electron density around BCR B 1778:

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

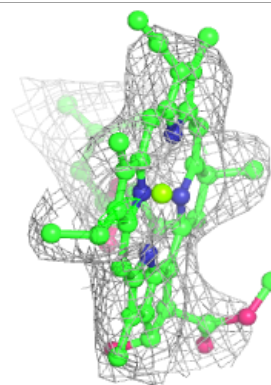
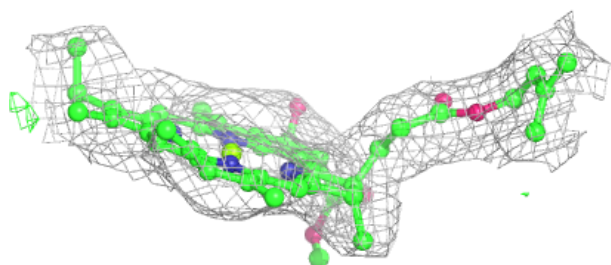
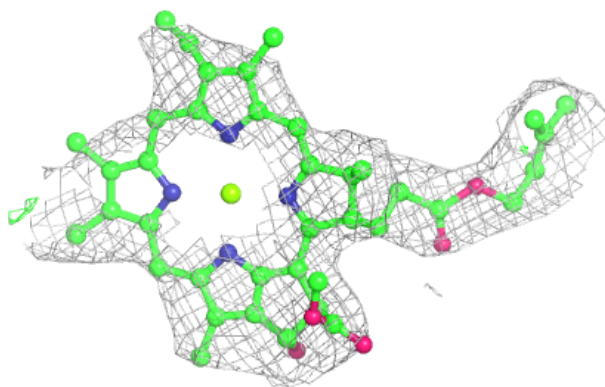
**Electron density around LMU A 7035:**

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

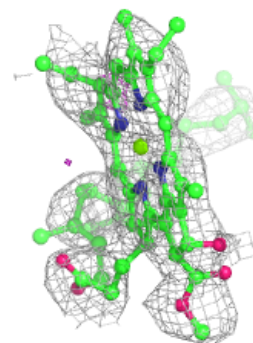
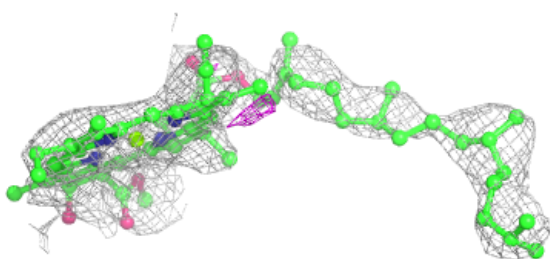
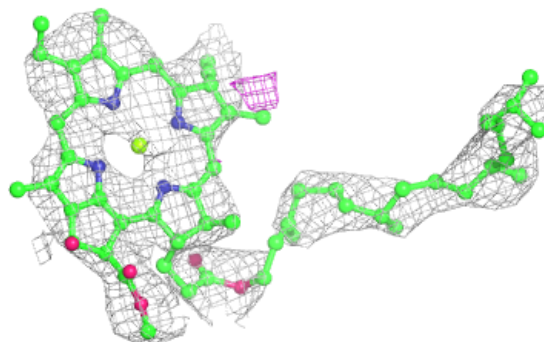


Electron density around CLA B 1763:

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

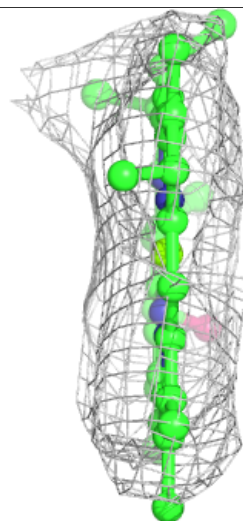
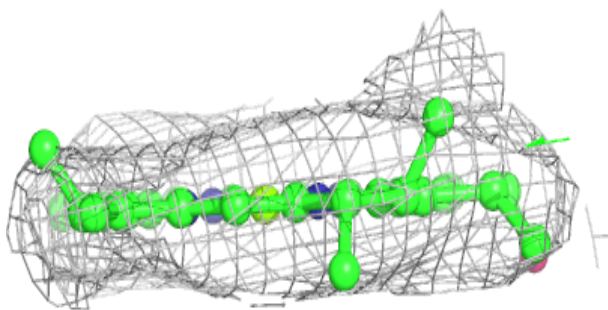
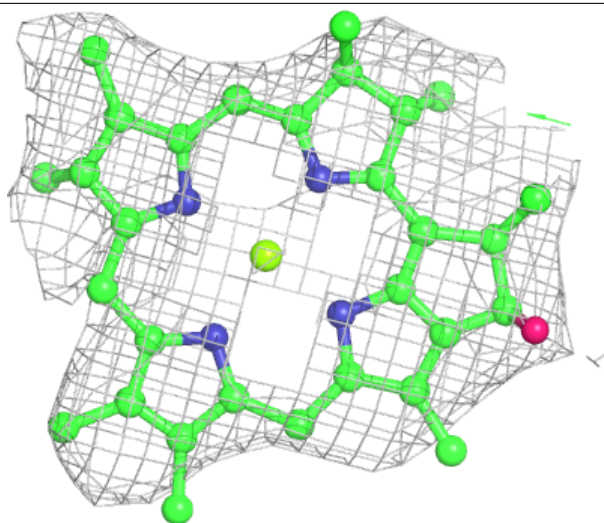
**Electron density around CLA A 1813:**

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



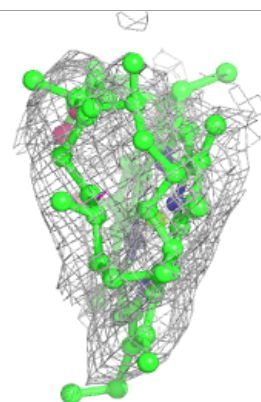
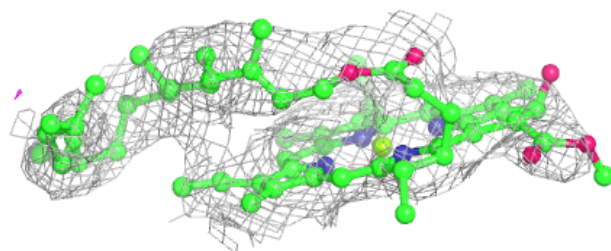
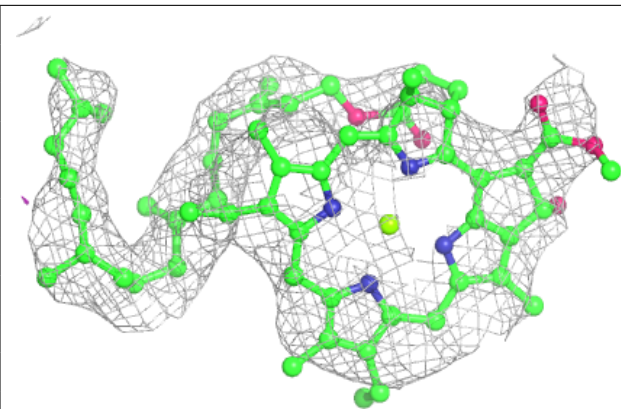
Electron density around CLA 4 1207:

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



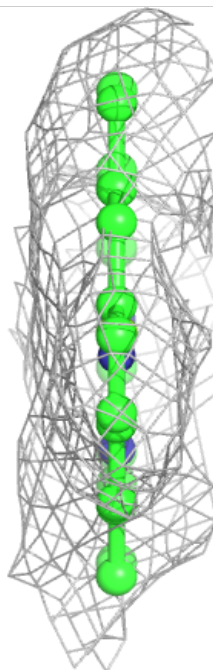
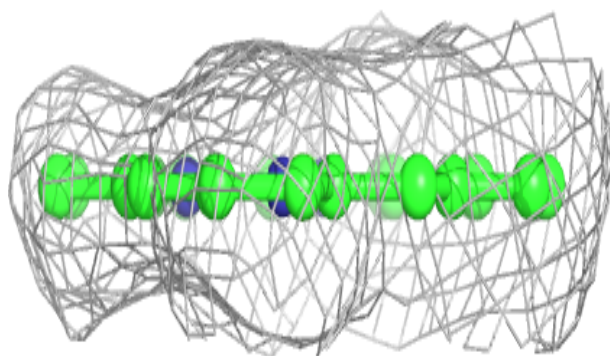
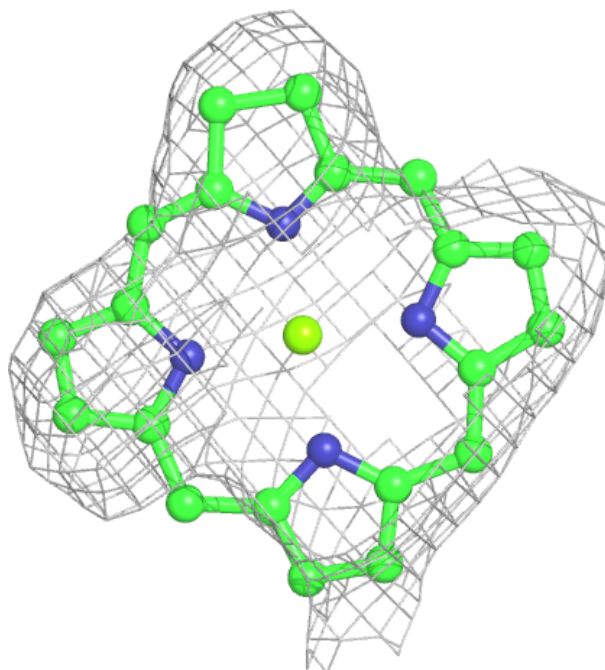
Electron density around CLA A 1774:

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



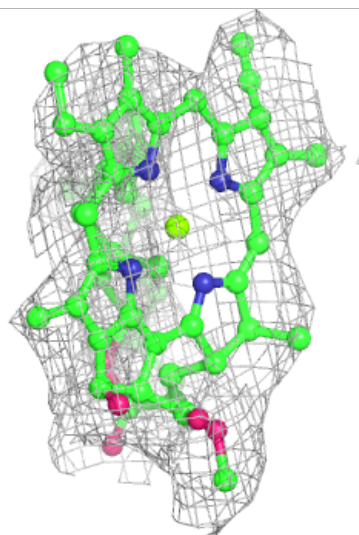
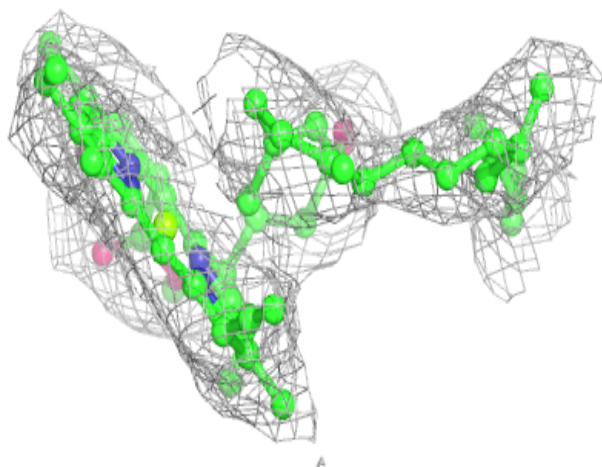
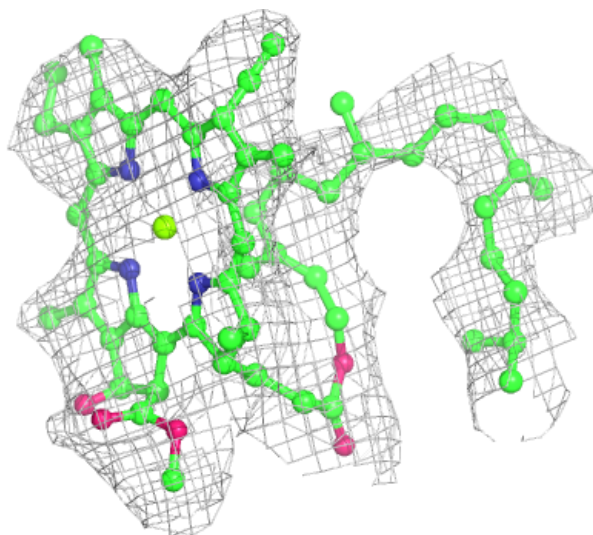
Electron density around CLA 2 1214:

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



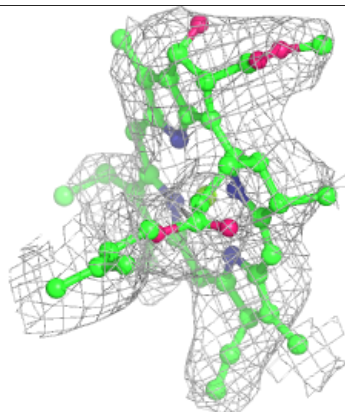
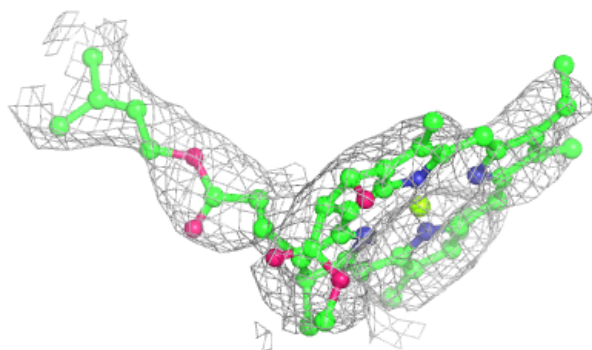
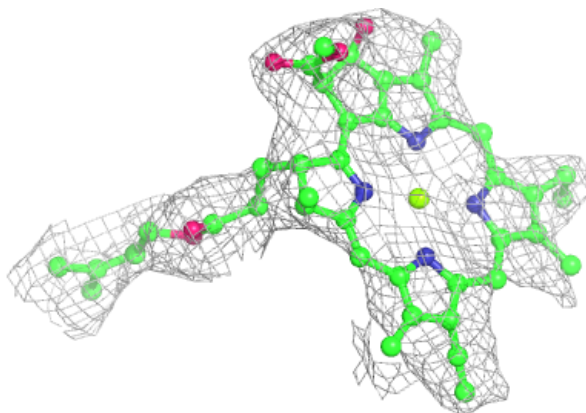
Electron density around CLA B 1753:

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

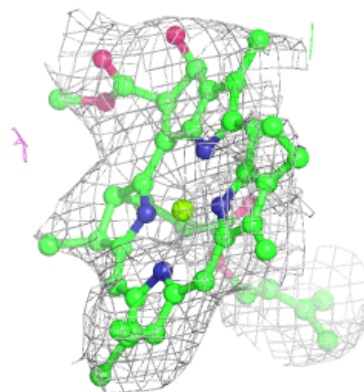
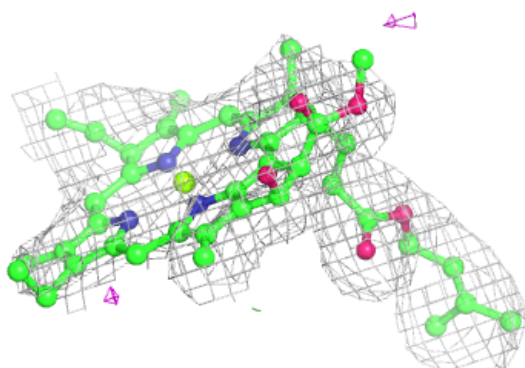
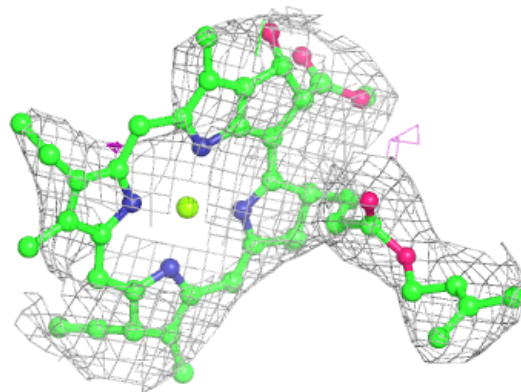


Electron density around CLA A 1786:

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

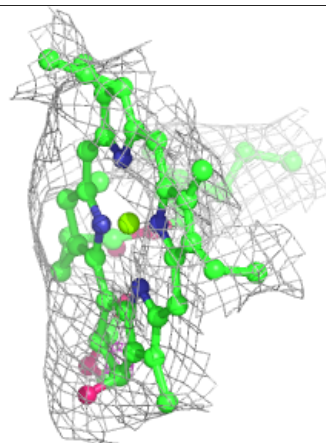
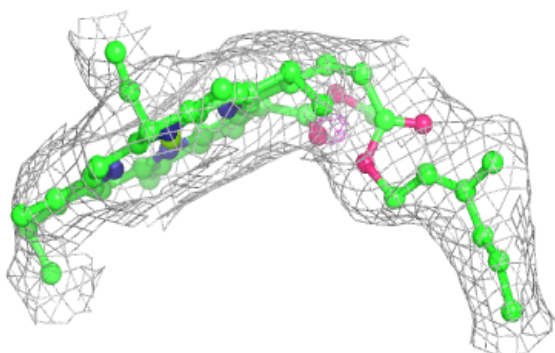
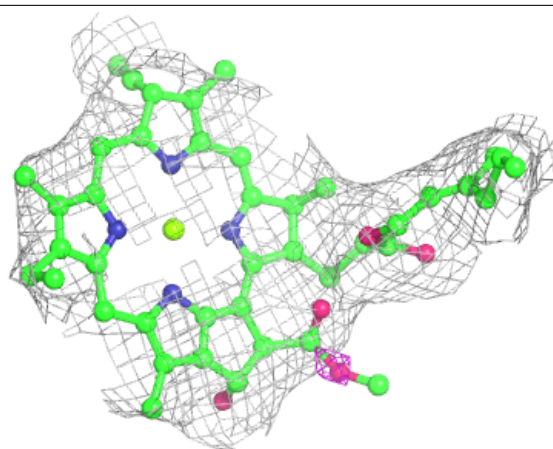
**Electron density around CLA 2 1222:**

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

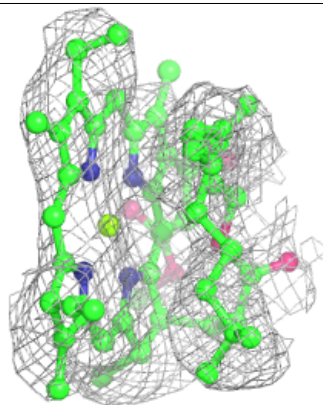
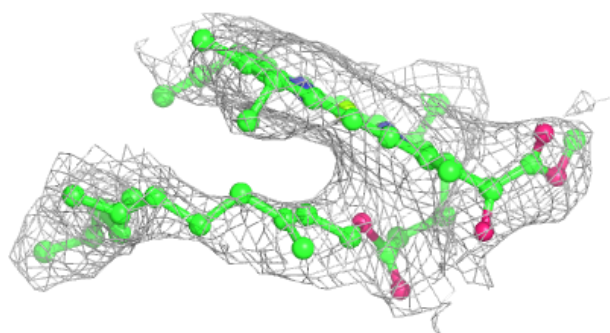
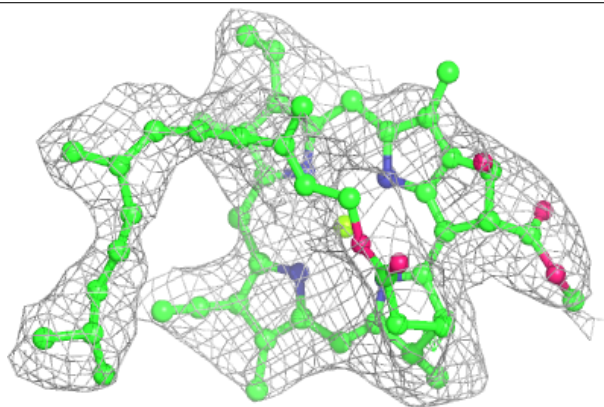


Electron density around CLA 4 1201:

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

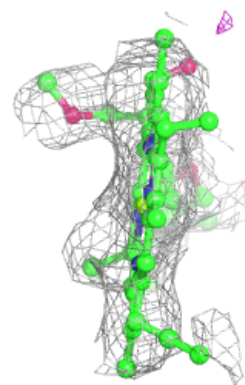
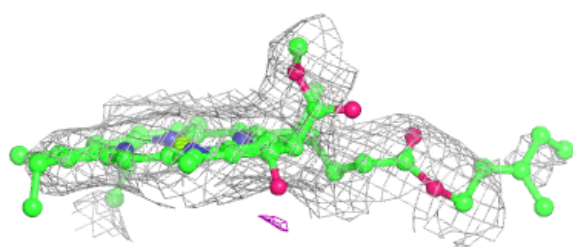
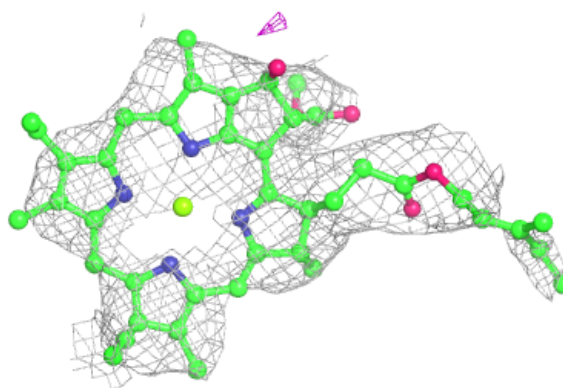
**Electron density around CLA I 1031:**

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

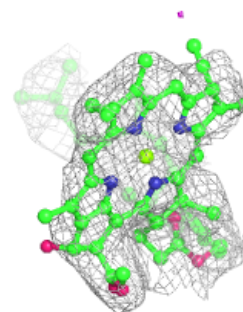
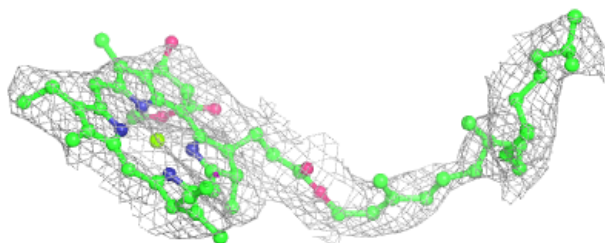
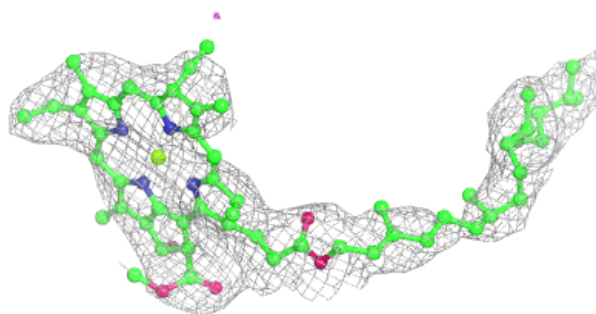


Electron density around CLA A 1792:

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

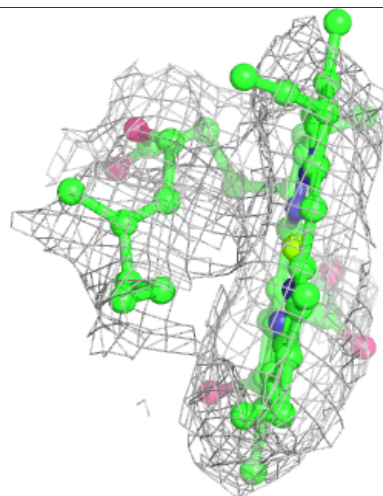
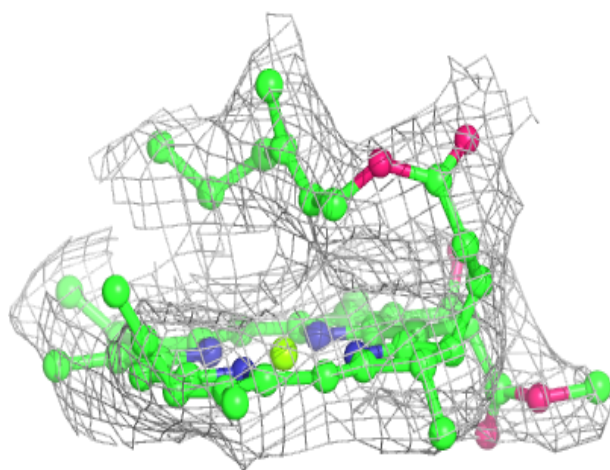
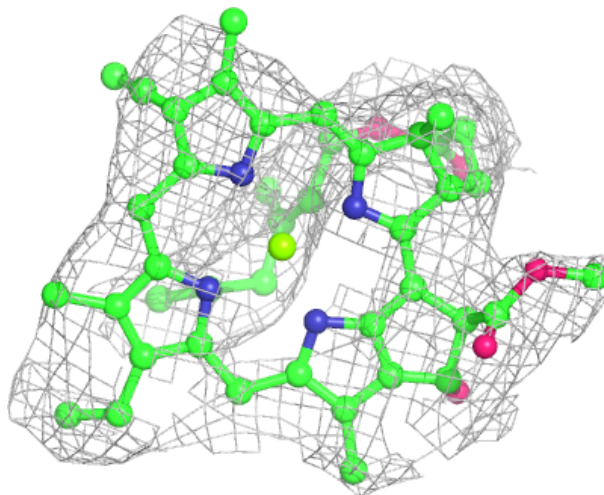
**Electron density around CLA A 1812:**

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



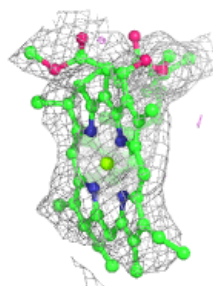
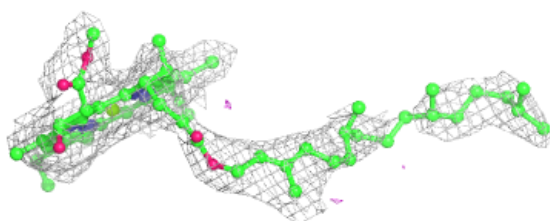
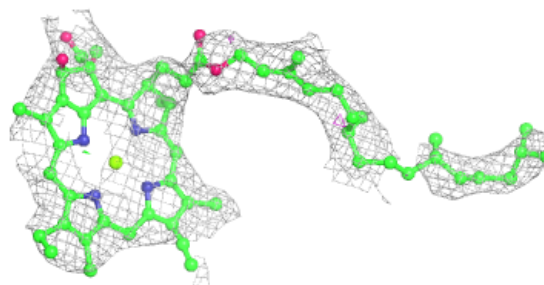
Electron density around CLA A 1773:

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



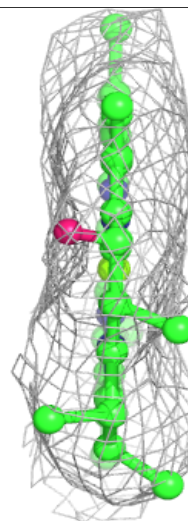
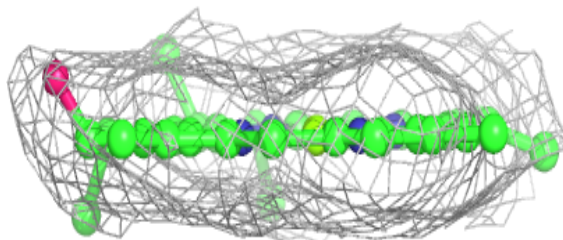
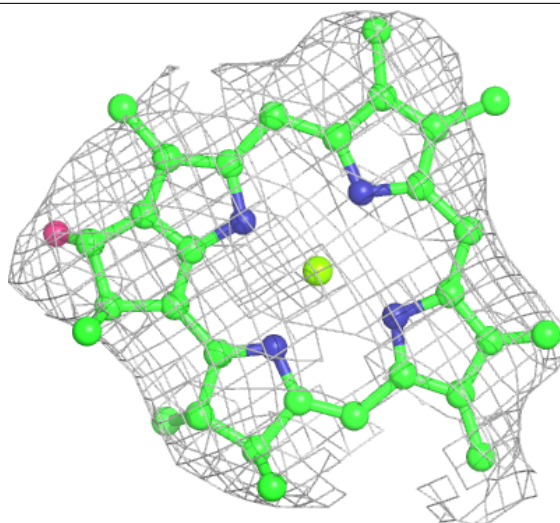
Electron density around CLA A 1789:

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



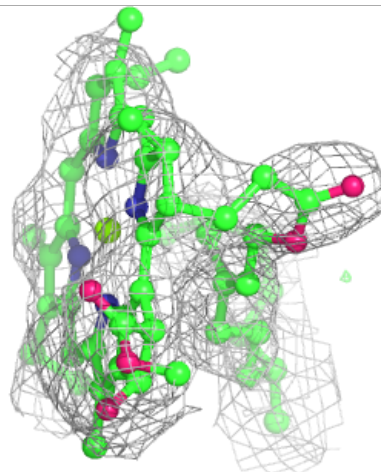
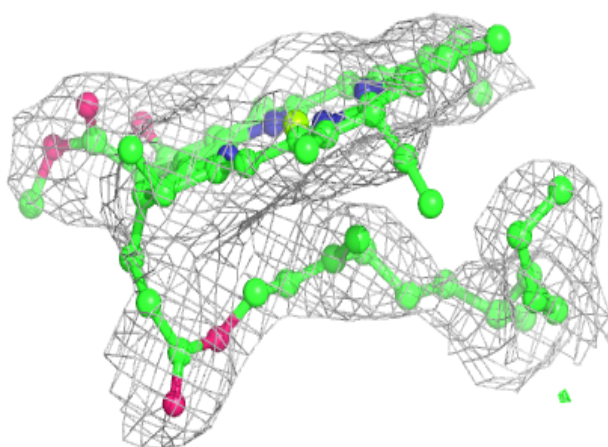
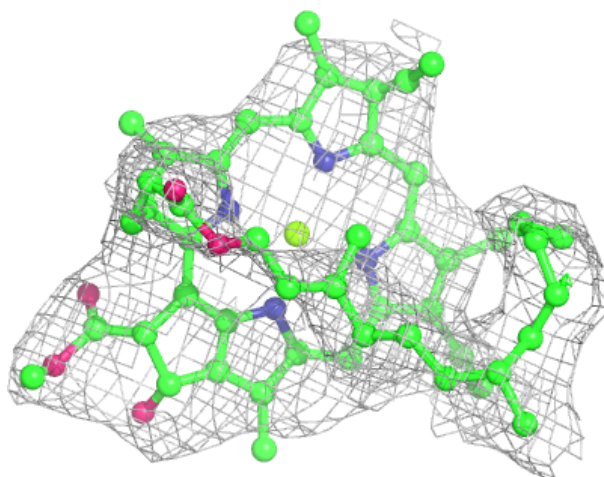
Electron density around CLA F 1155:

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



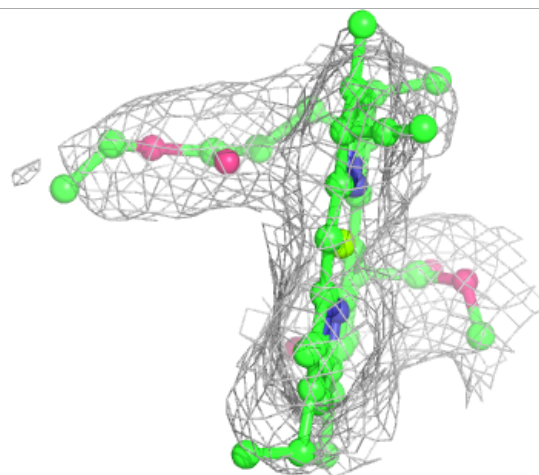
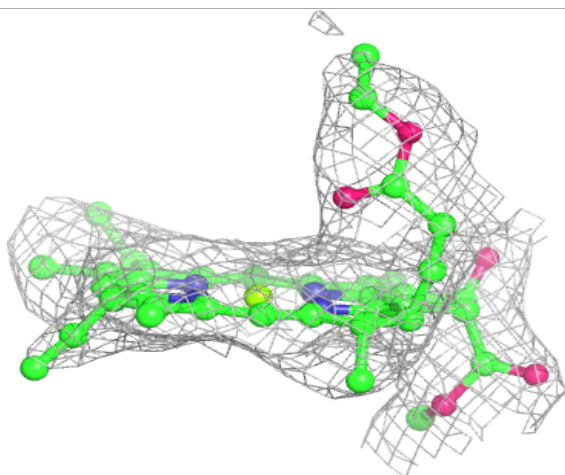
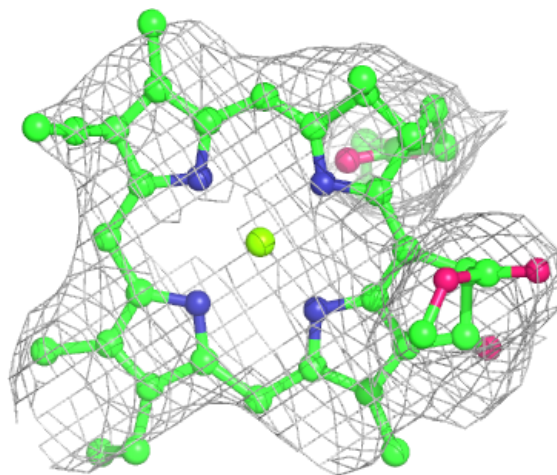
Electron density around CLA B 1747:

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



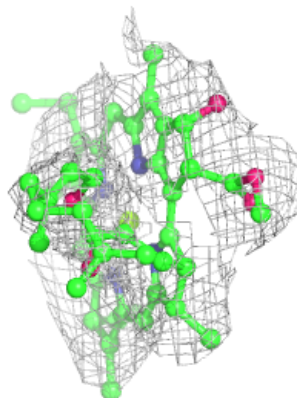
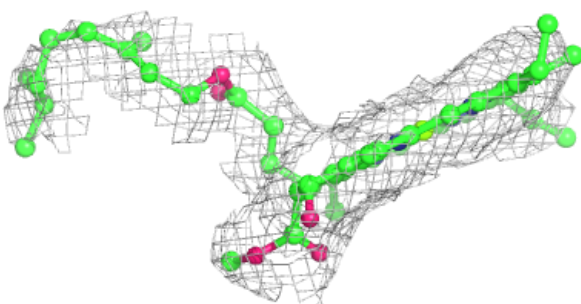
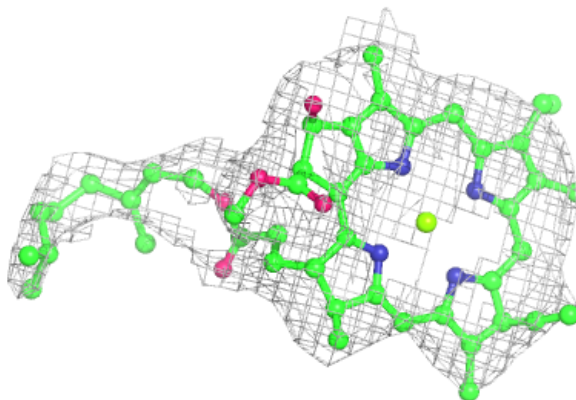
Electron density around CLA L 1167:

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

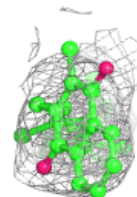
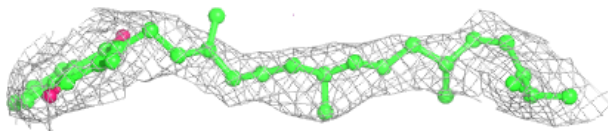
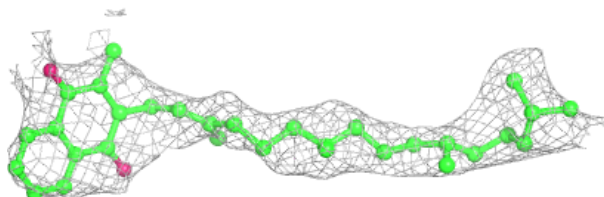


Electron density around CLA A 1765:

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

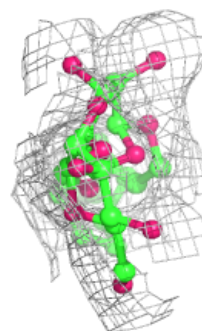
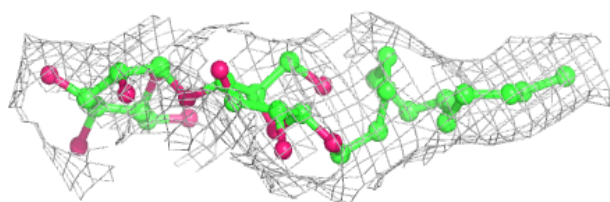
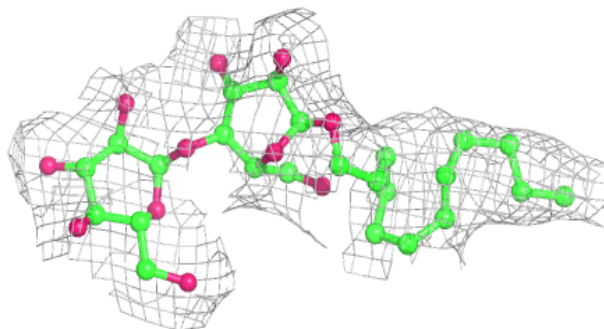
**Electron density around PQN A 1802:**

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



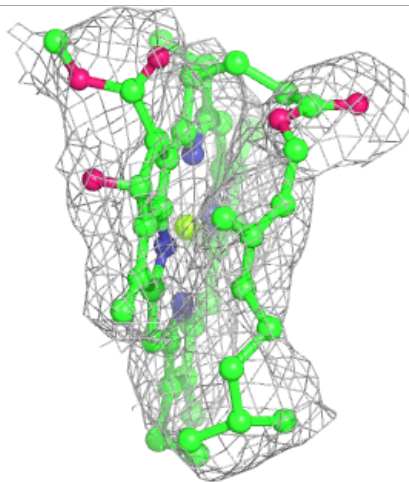
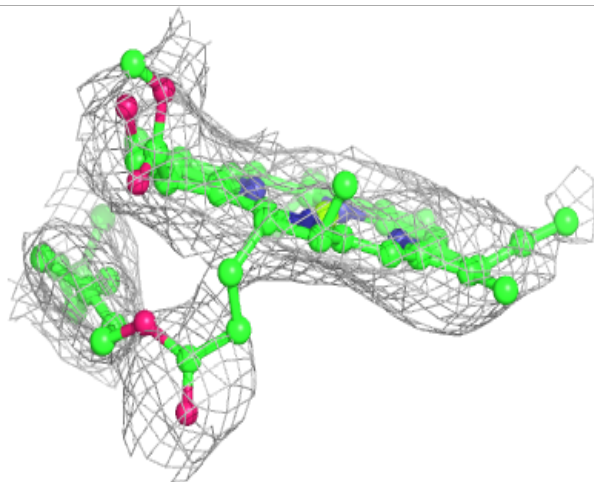
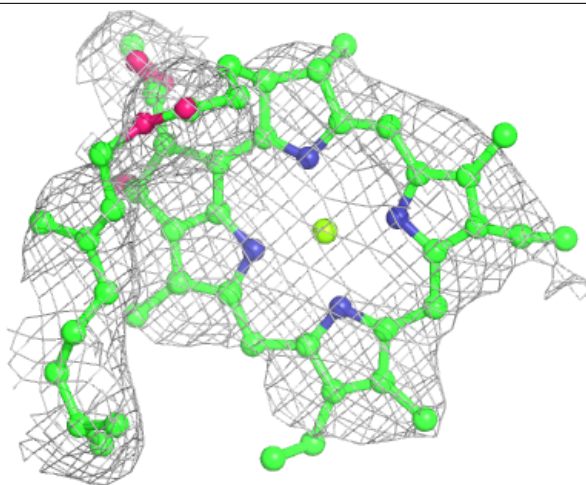
Electron density around LMU A 7016:

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



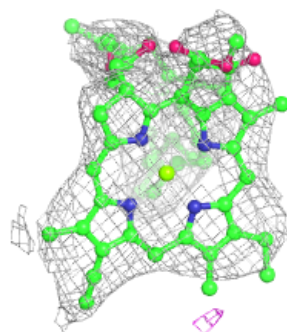
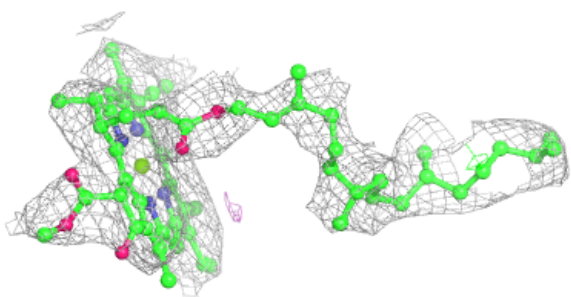
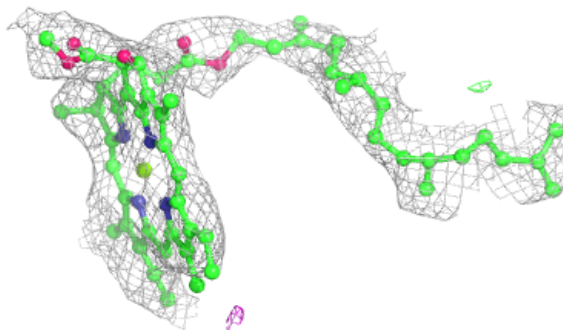
Electron density around CLA A 1784:

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

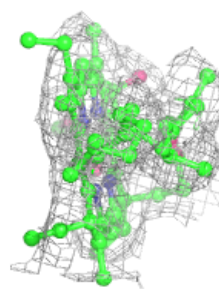
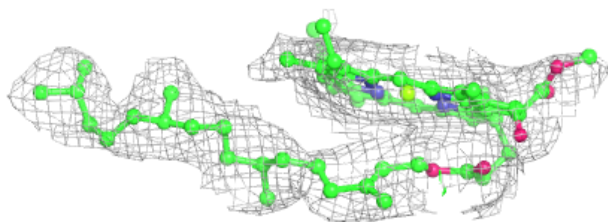
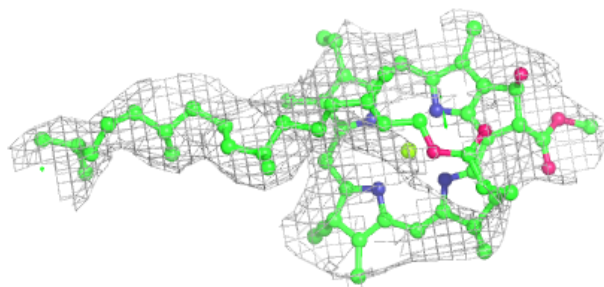


Electron density around CLA B 1759:

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

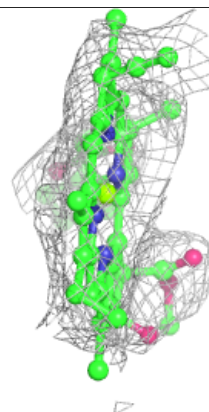
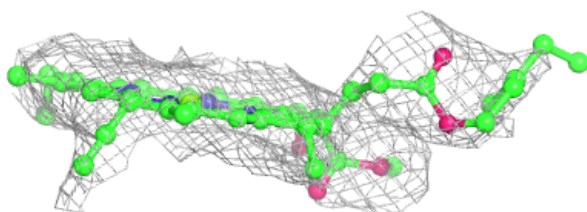
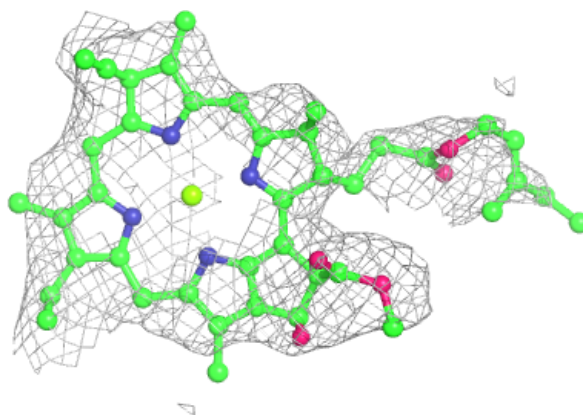
**Electron density around CLA A 1793:**

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

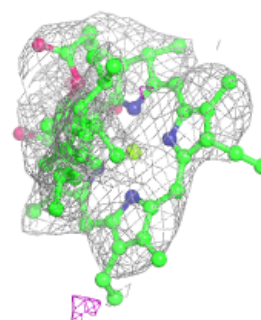
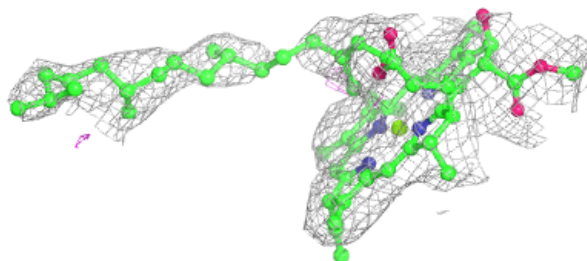
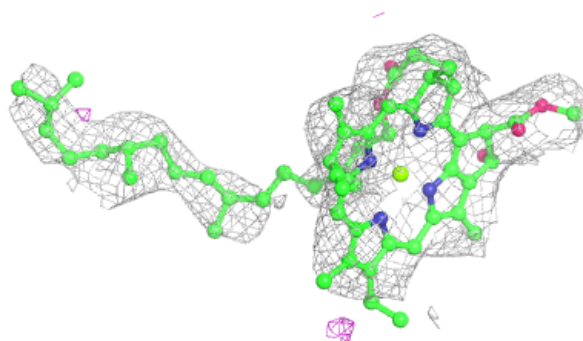


Electron density around CLA A 1795:

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

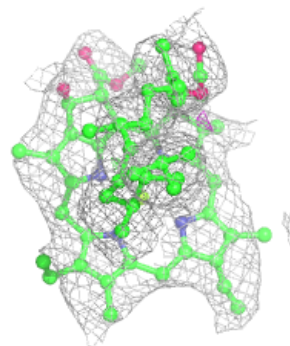
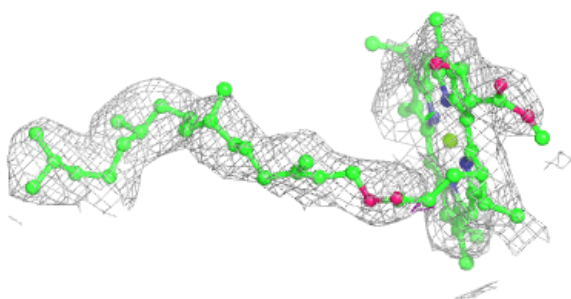
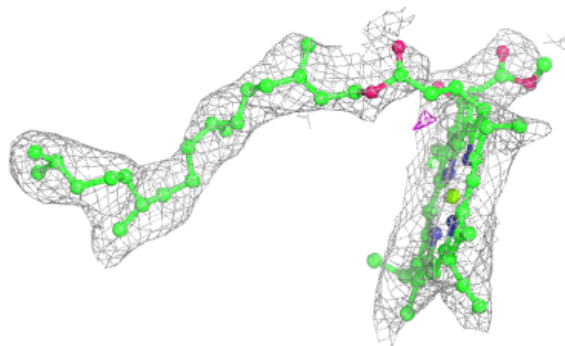
**Electron density around CLA A 1796:**

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



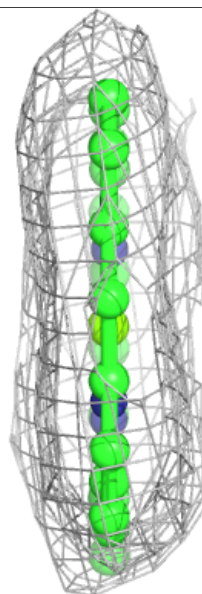
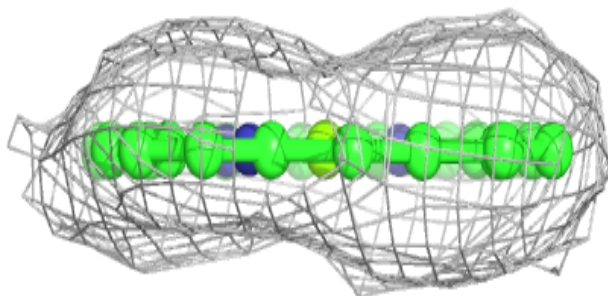
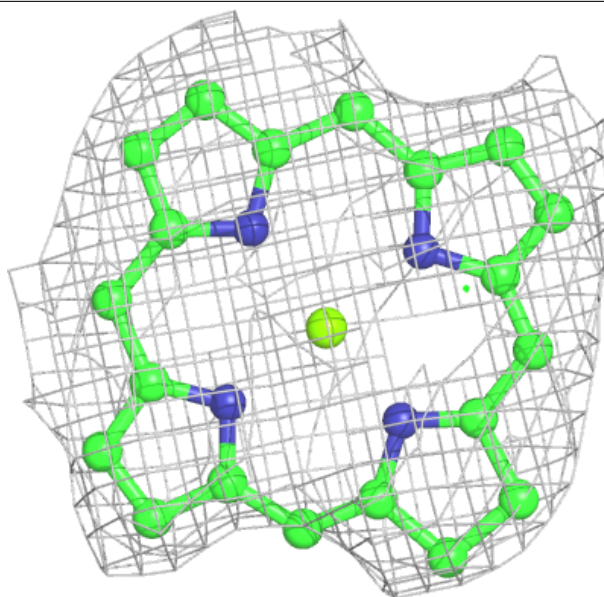
Electron density around CLA A 1785:

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



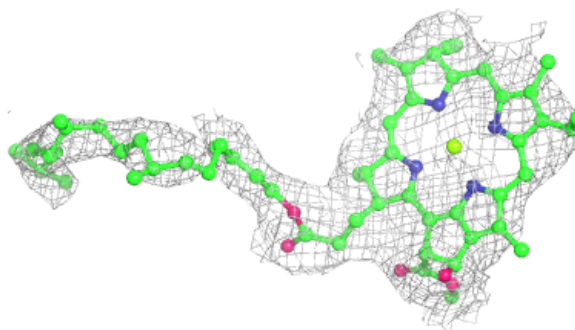
Electron density around CLA 4 1206:

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

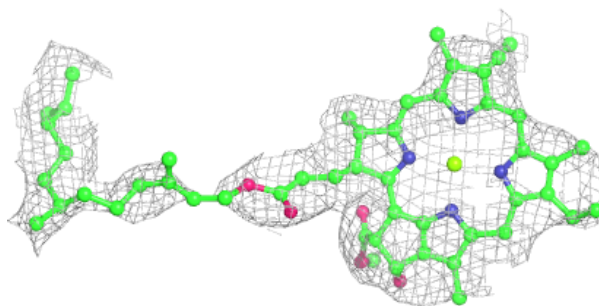


Electron density around CLA B 1743:

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

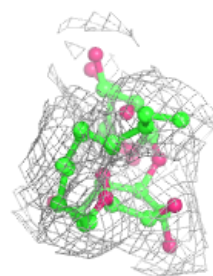
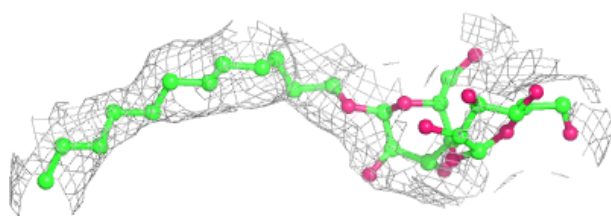
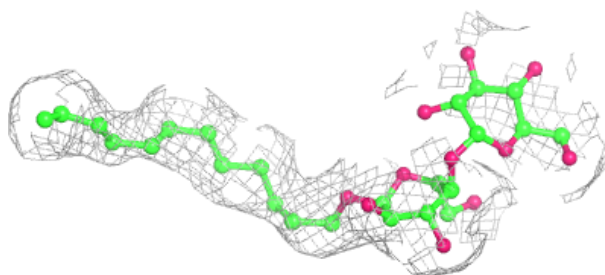
**Electron density around CLA B 1767:**

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

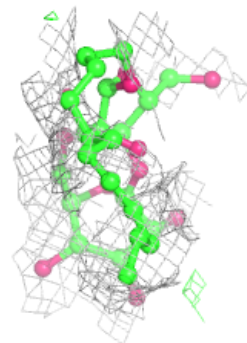
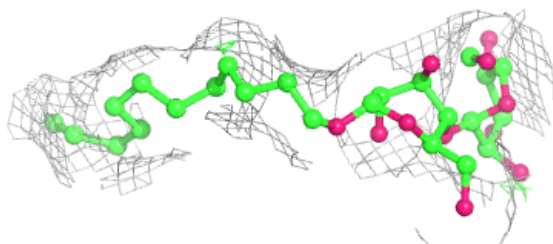
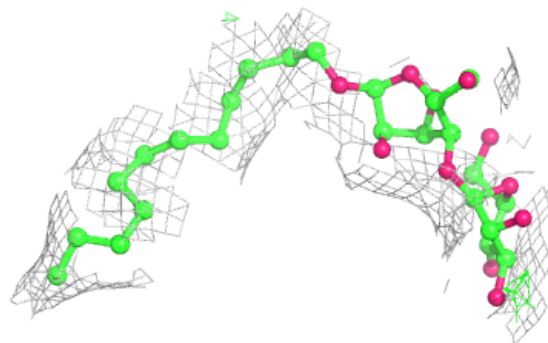


Electron density around LMU A 7024:

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

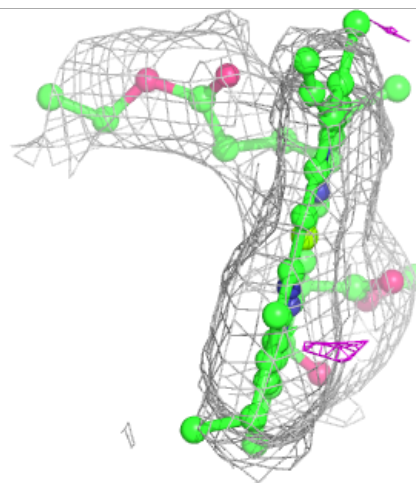
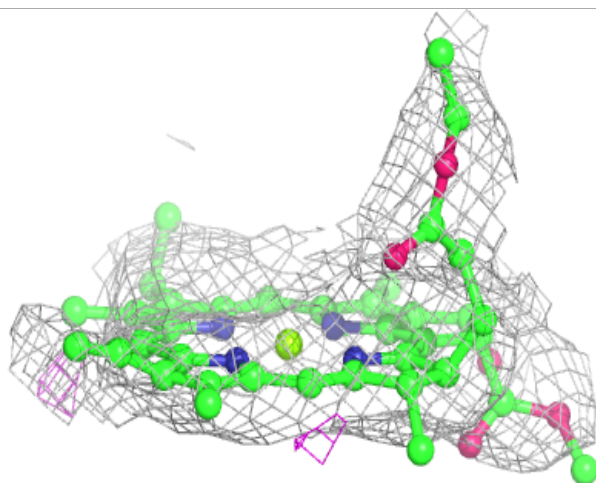
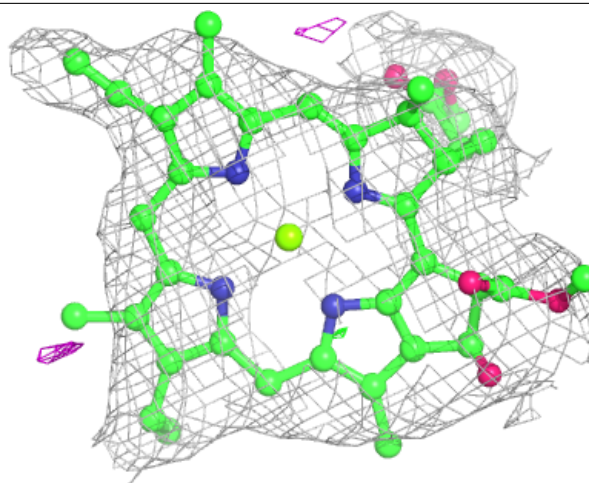
**Electron density around LMU A 7039:**

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



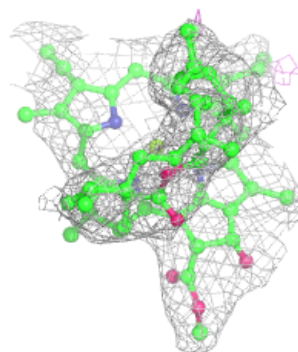
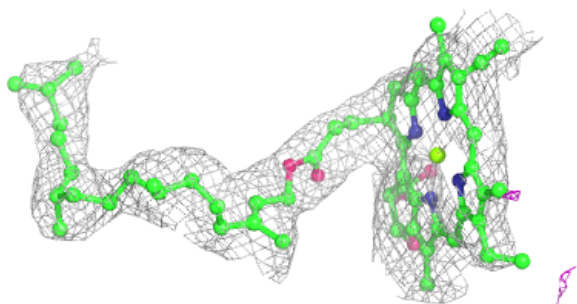
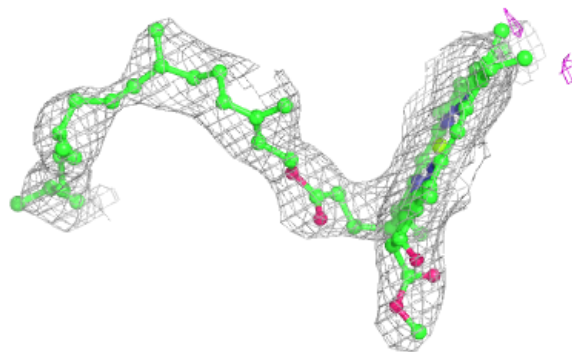
Electron density around CLA B 1769:

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



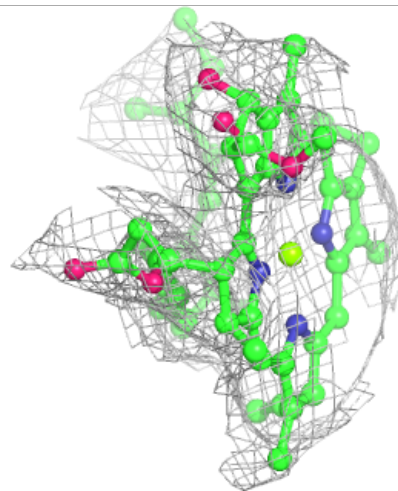
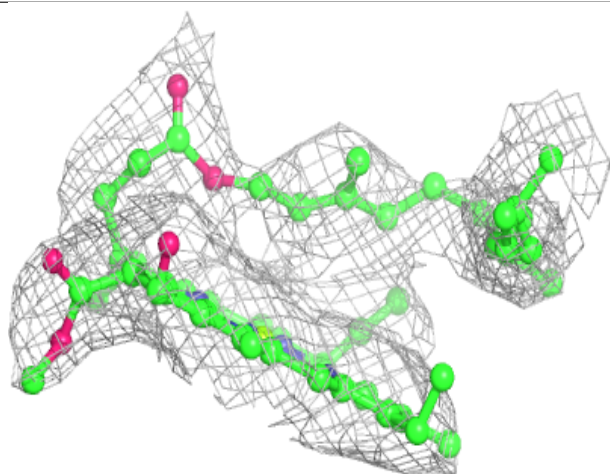
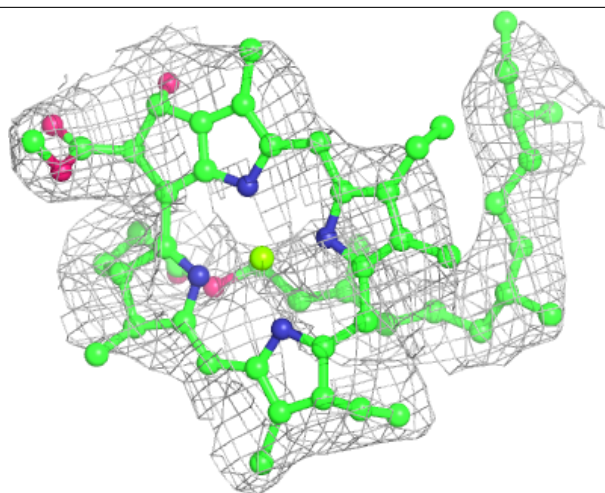
Electron density around CLA B 1770:

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



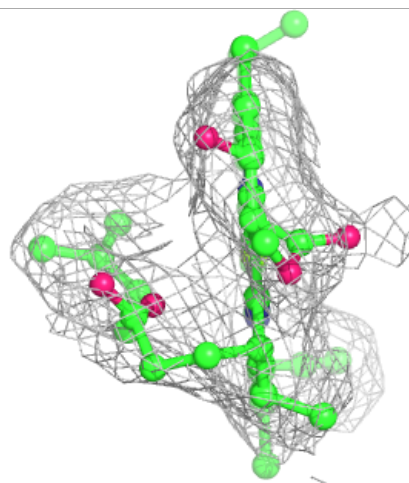
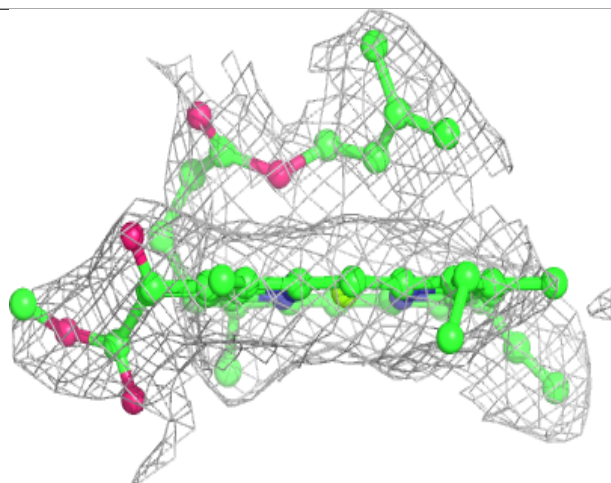
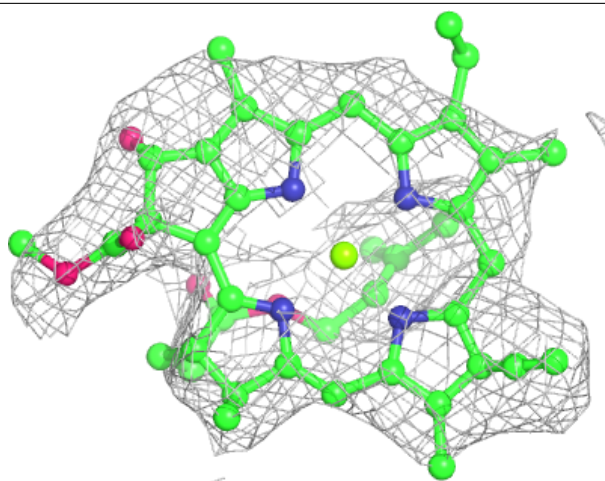
Electron density around CLA B 1749:

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



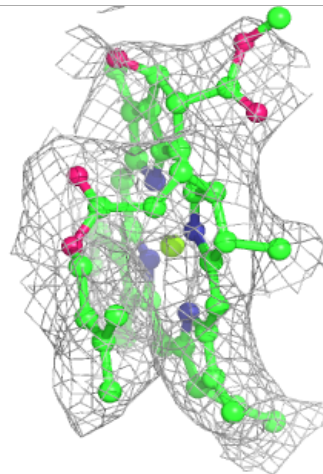
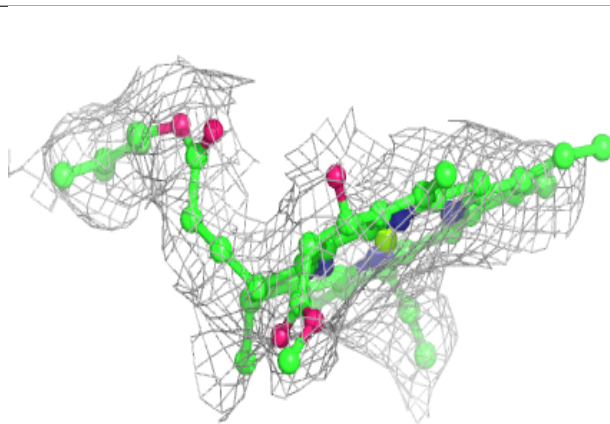
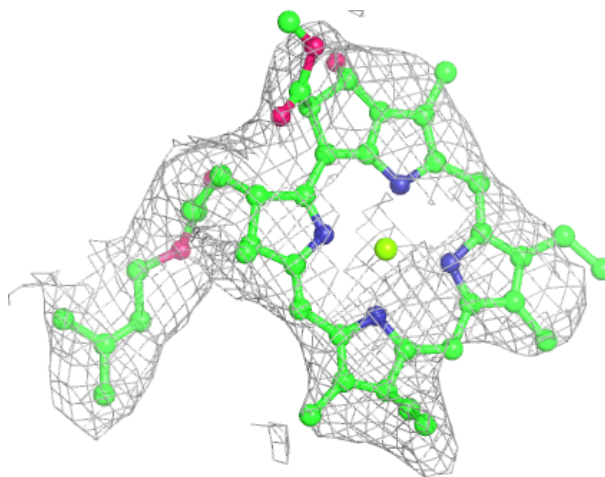
Electron density around CLA B 1750:

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



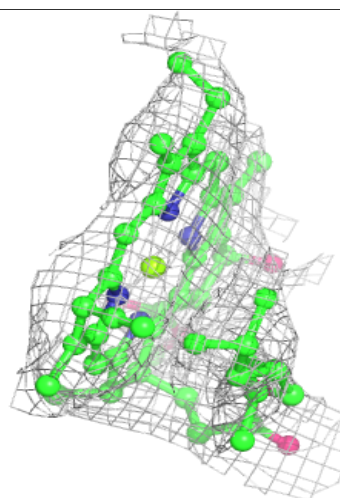
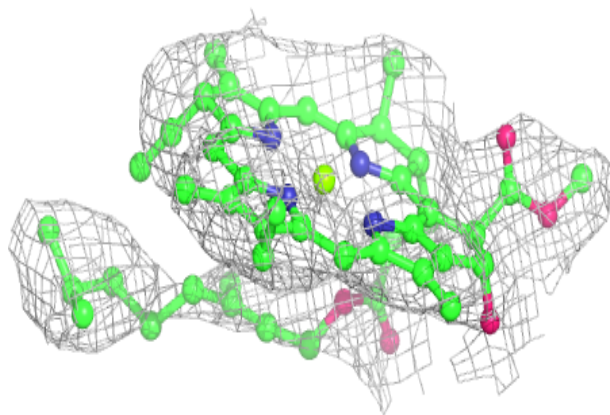
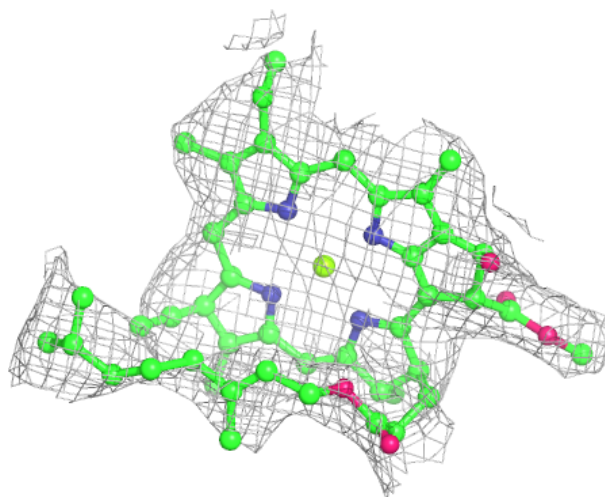
Electron density around CLA A 1790:

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



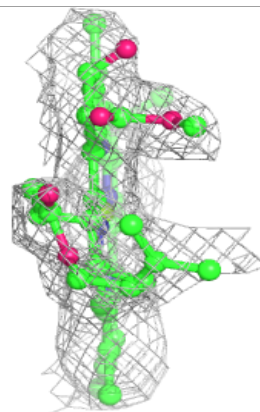
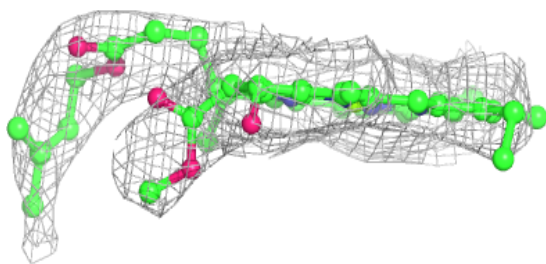
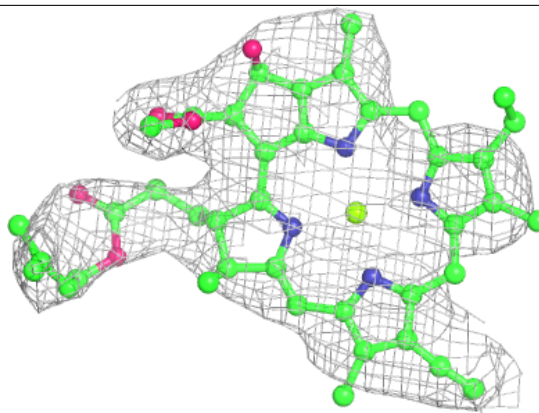
Electron density around CLA B 1752:

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

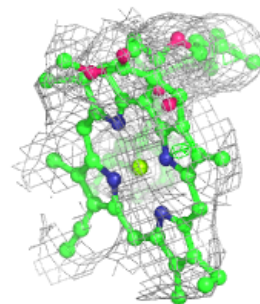
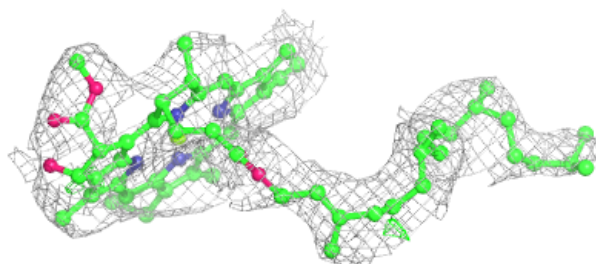
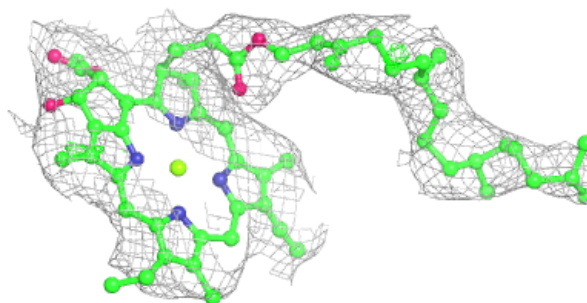


Electron density around CLA A 1759:

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

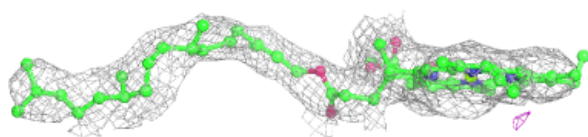
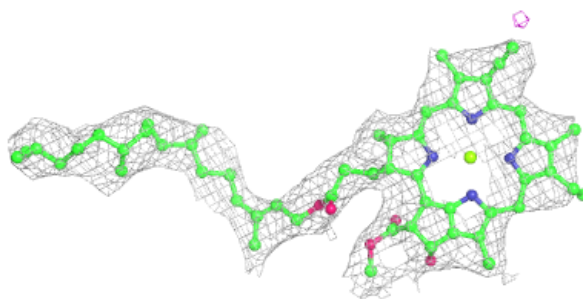
**Electron density around CLA A 1764:**

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

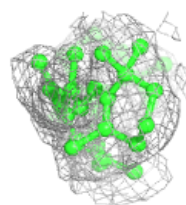
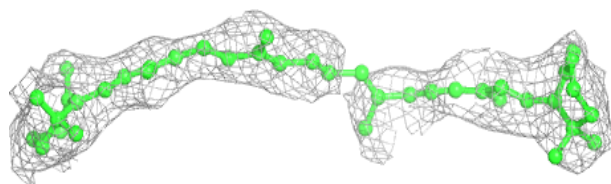
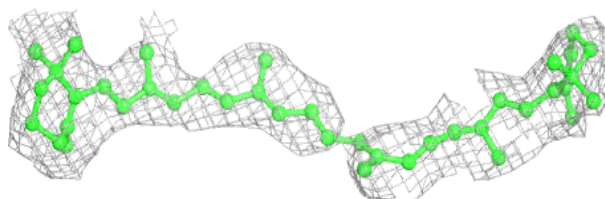


Electron density around CLA A 1788:

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

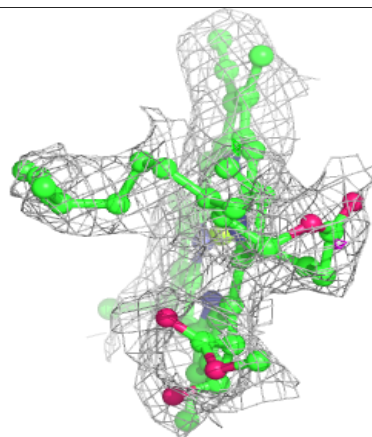
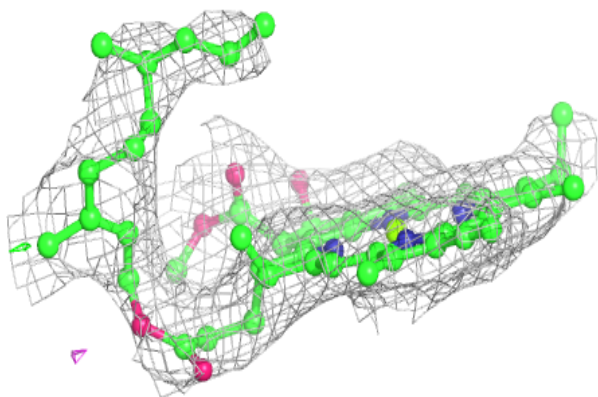
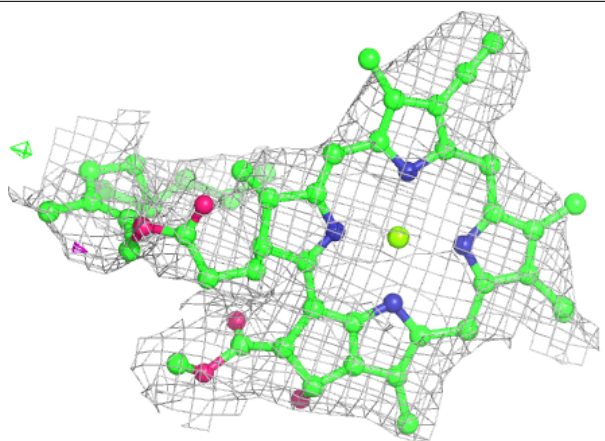
**Electron density around BCR B 1781:**

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



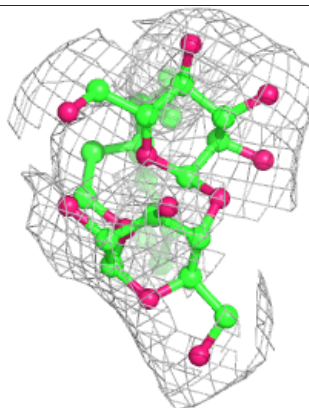
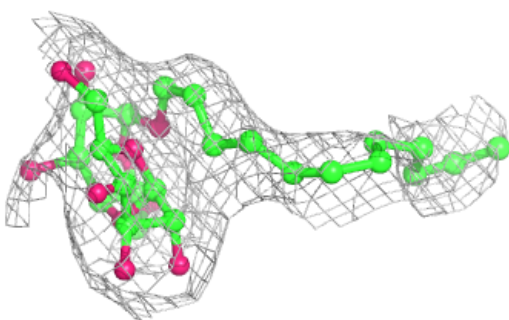
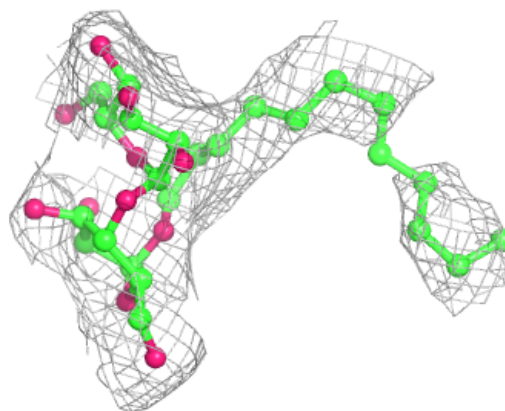
Electron density around CLA A 1762:

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

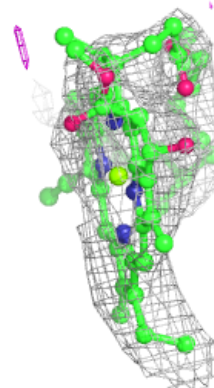
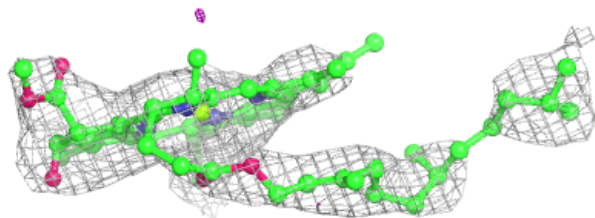
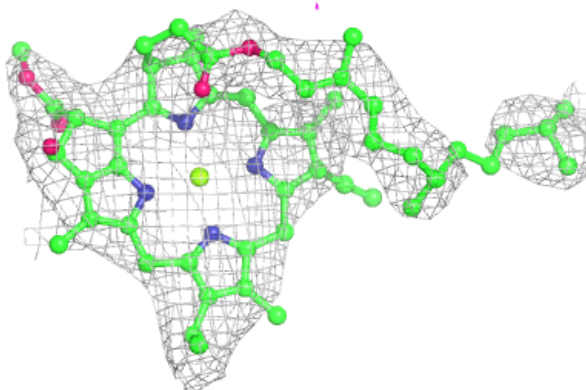


Electron density around LMU A 7032:

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

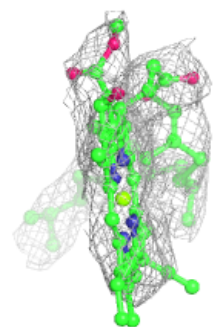
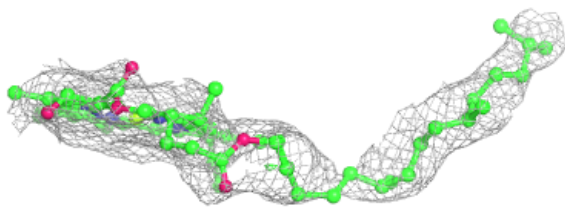
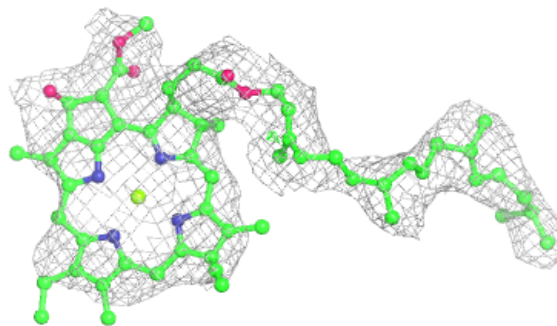
**Electron density around CLA B 1748:**

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

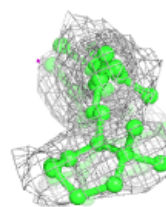
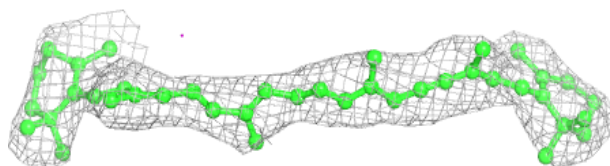
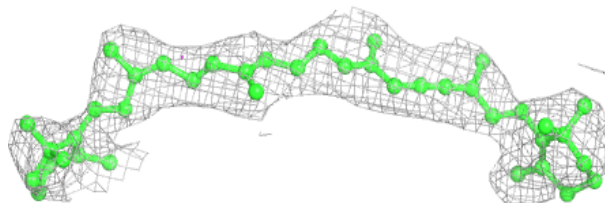


Electron density around CLA B 1787:

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

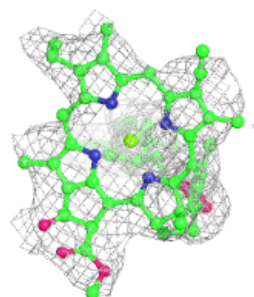
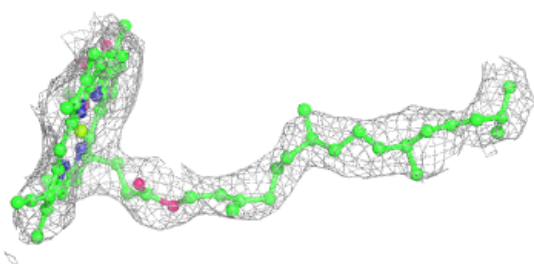
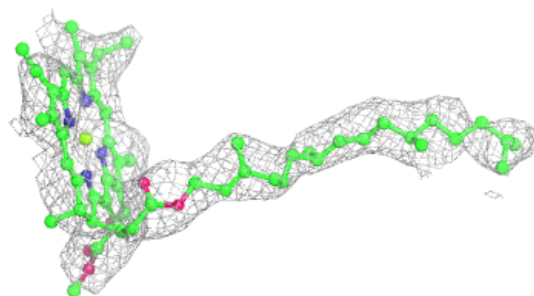
**Electron density around BCR L 1170:**

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

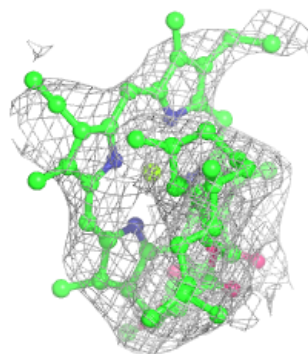
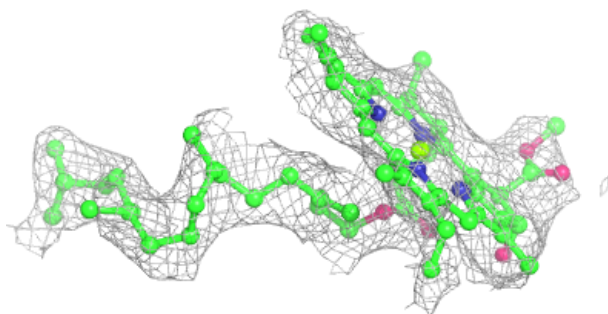
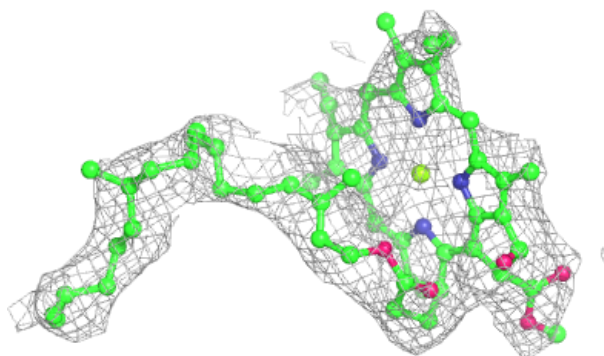


Electron density around CLA B 1758:

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

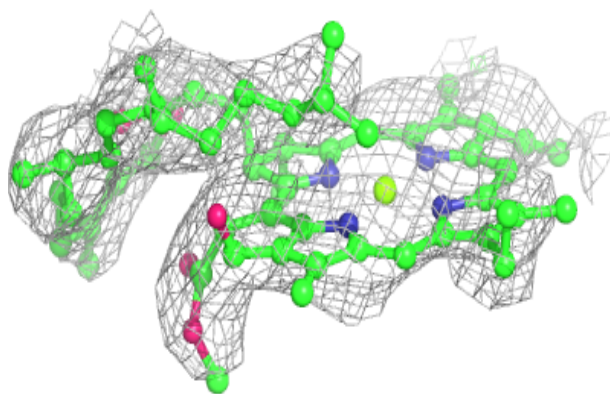
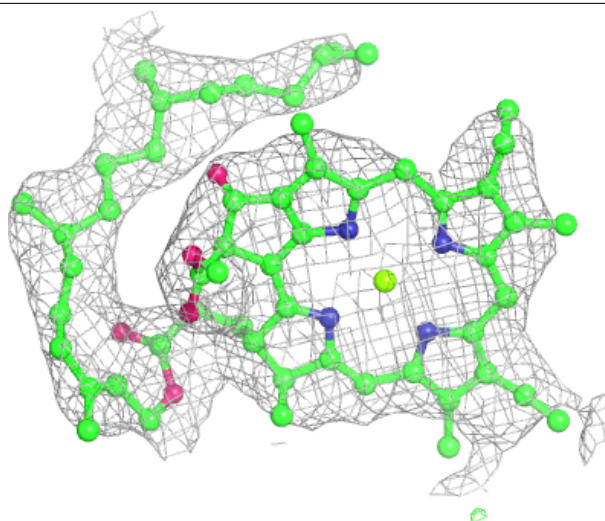
**Electron density around CLA A 1800:**

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



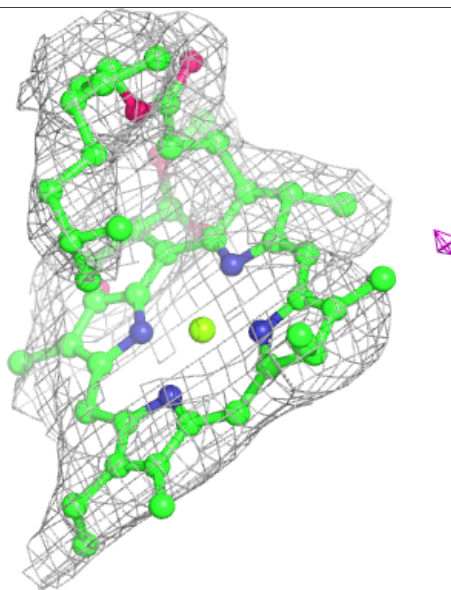
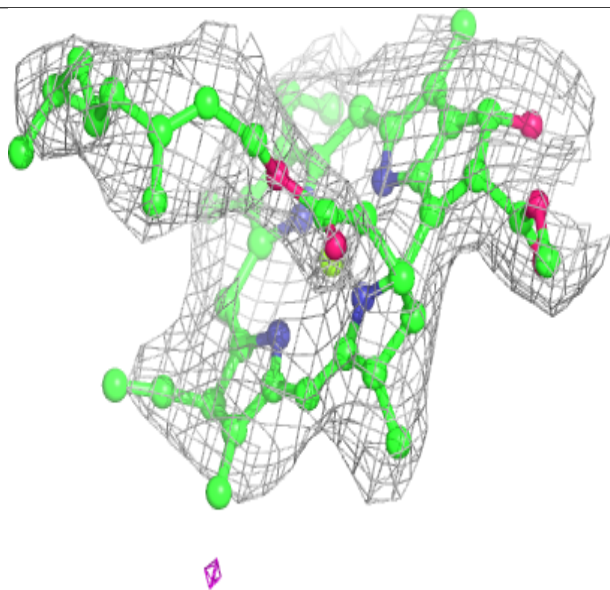
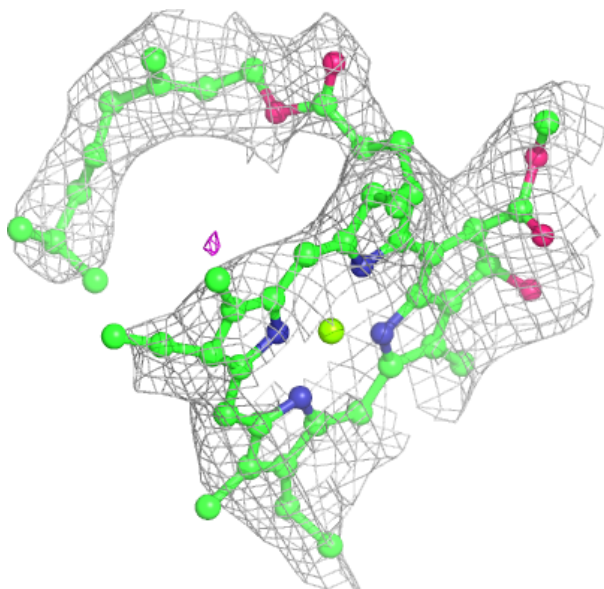
Electron density around CLA B 1737:

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



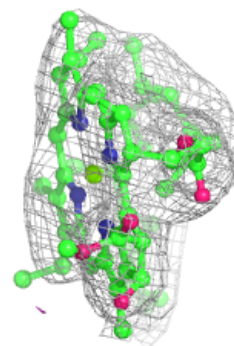
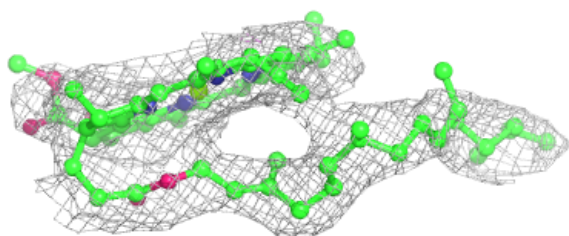
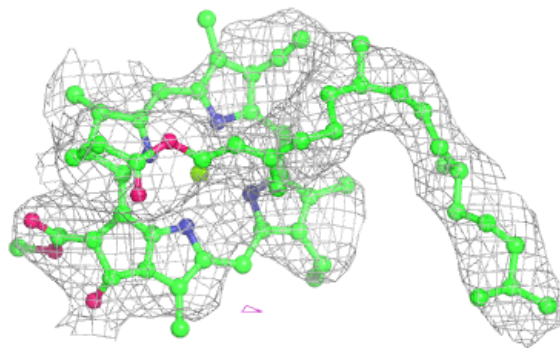
Electron density around CLA A 1779:

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

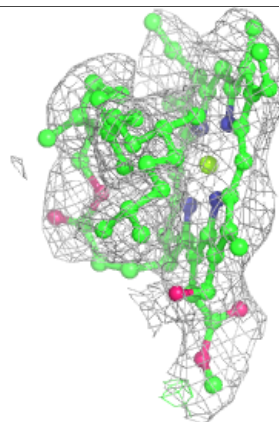
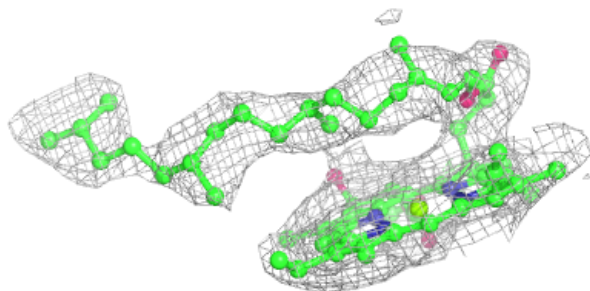
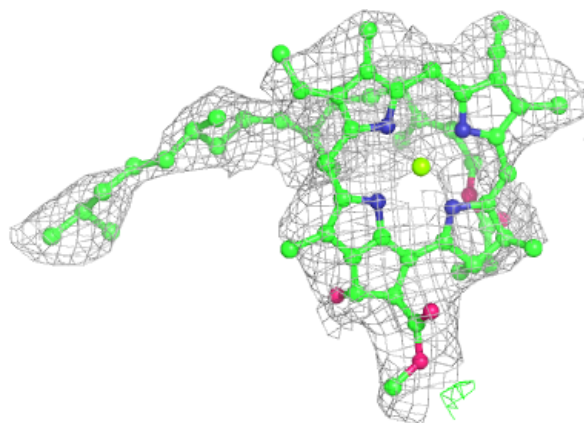


Electron density around CLA B 1768:

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

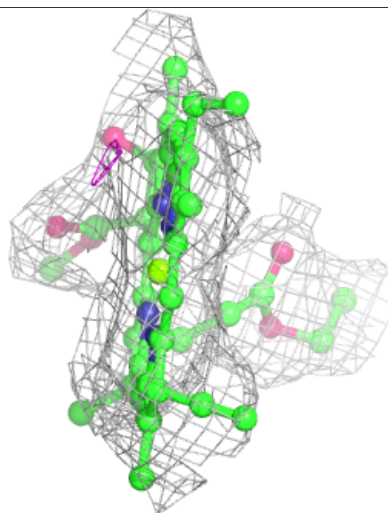
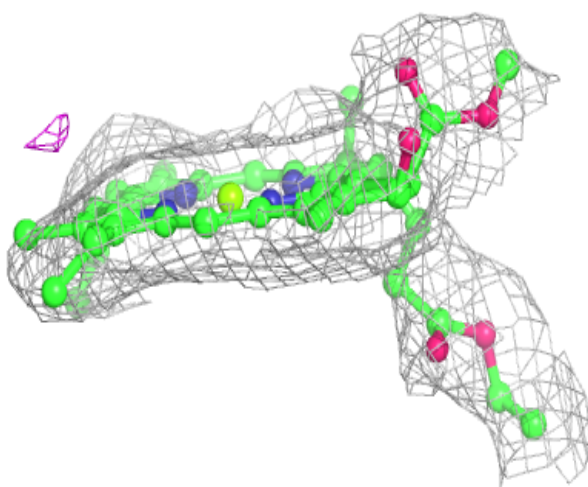
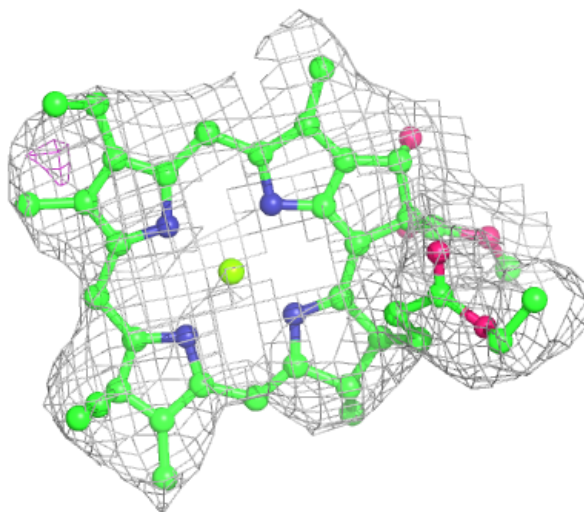
**Electron density around CLA B 1757:**

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



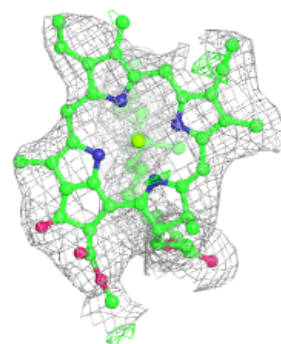
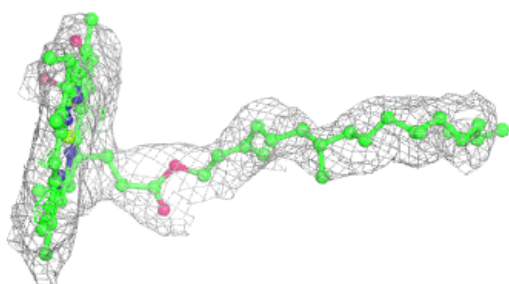
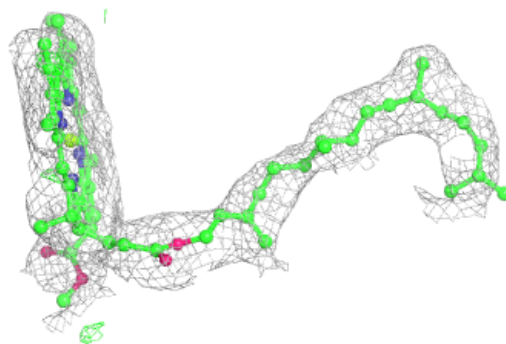
Electron density around CLA A 1794:

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



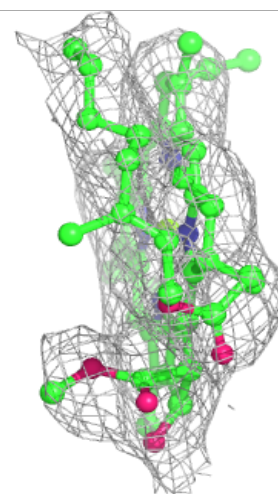
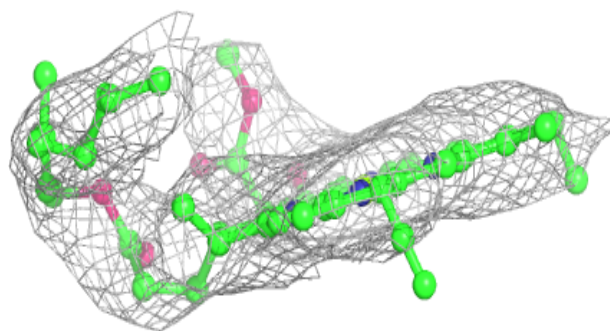
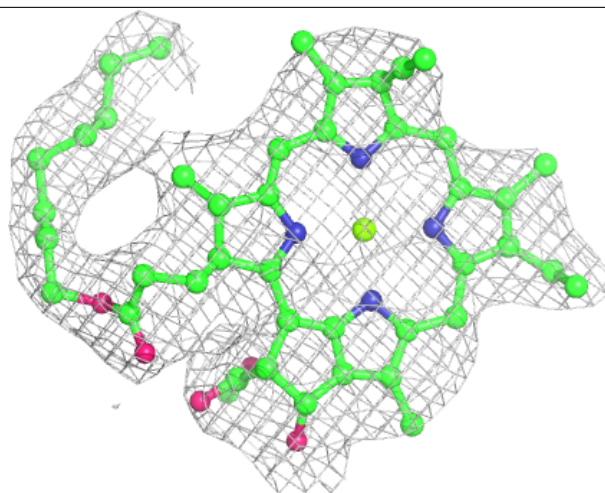
Electron density around CLA B 1771:

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



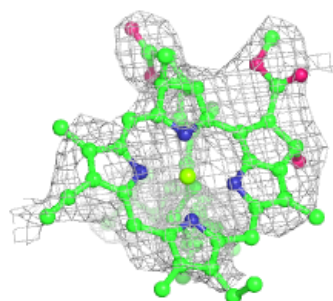
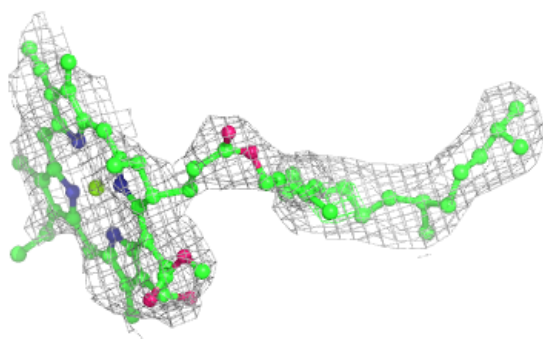
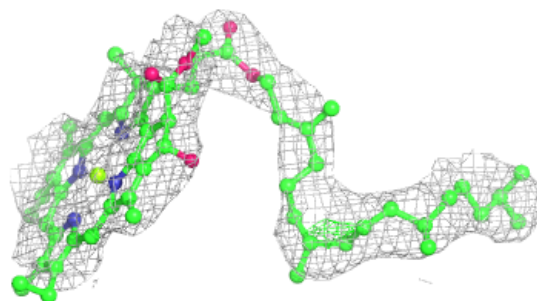
Electron density around CLA B 1754:

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

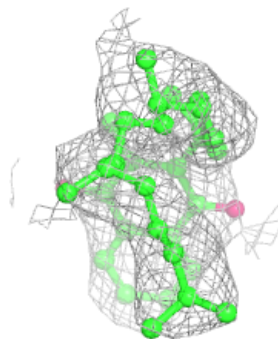
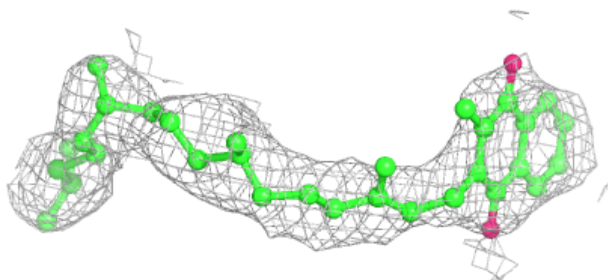
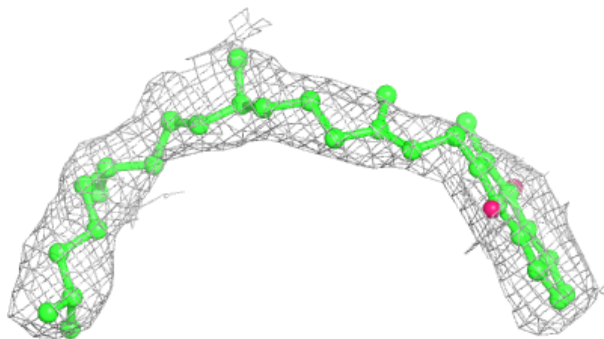


Electron density around CLA B 1785:

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

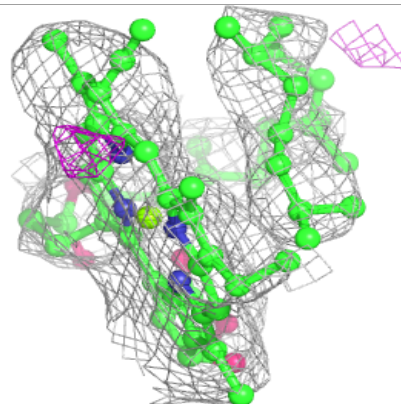
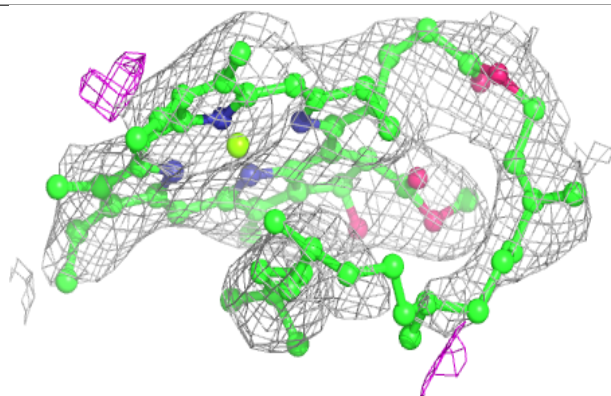
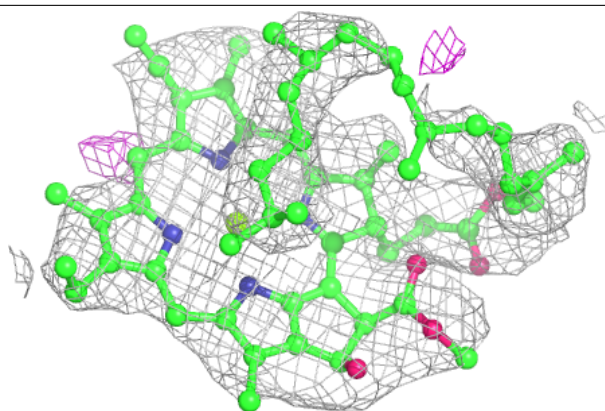
**Electron density around PQN B 1773:**

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

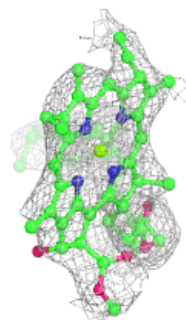
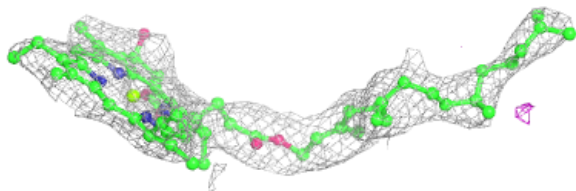
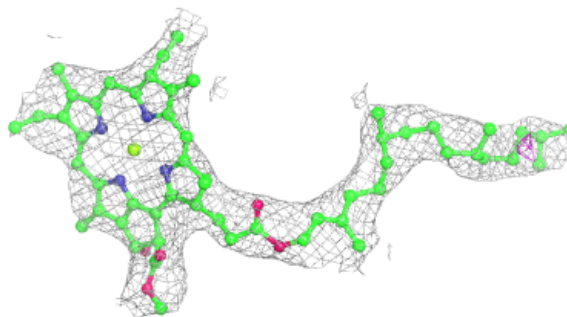


Electron density around CLA B 1738:

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

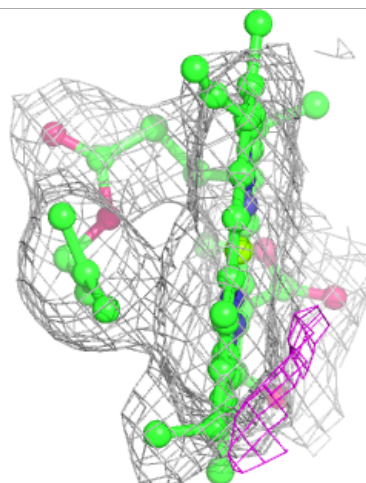
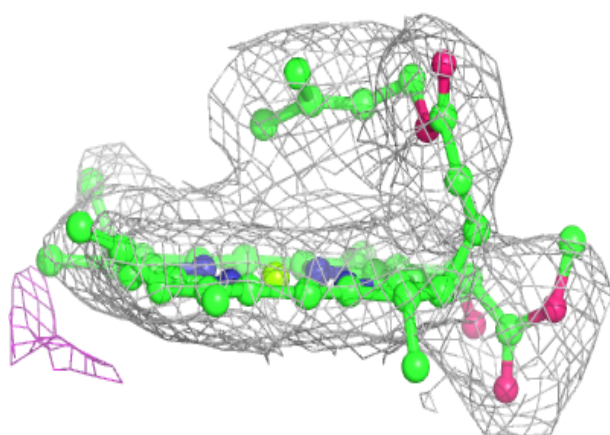
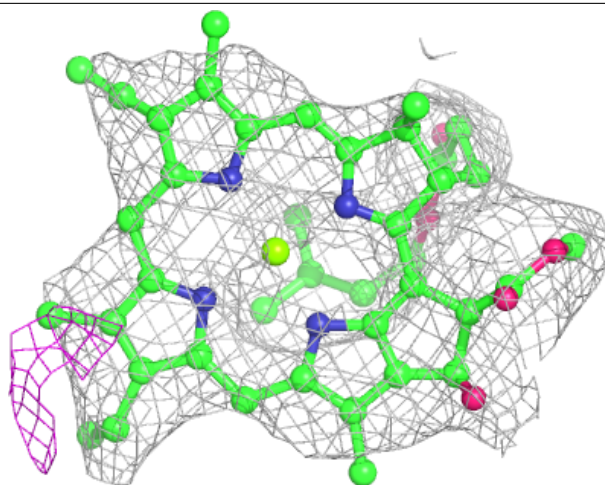
**Electron density around CLA B 1786:**

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



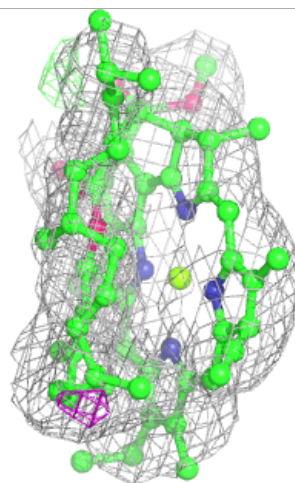
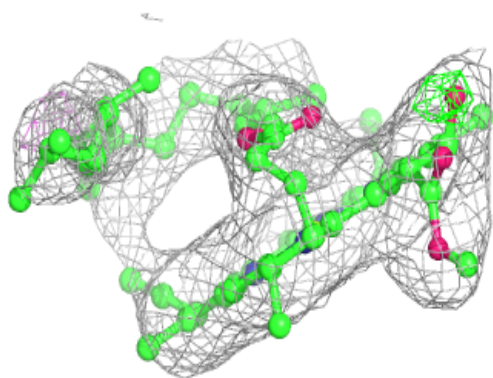
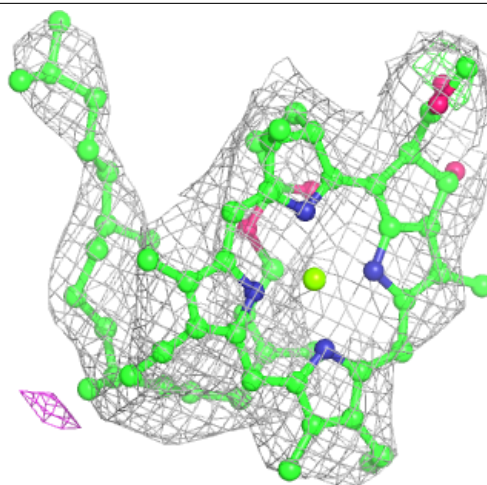
Electron density around CLA B 1760:

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



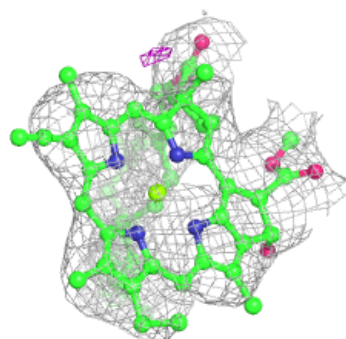
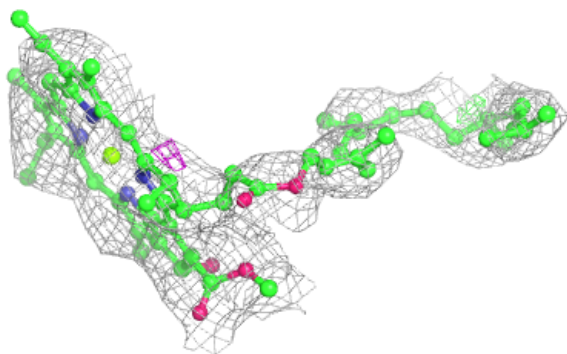
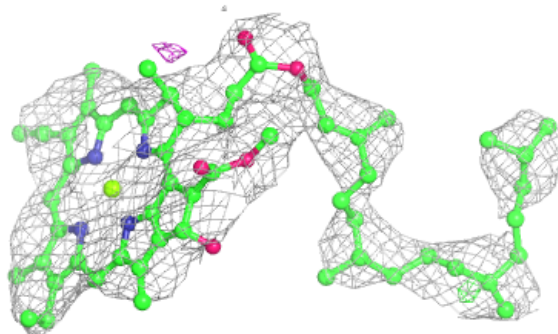
Electron density around CLA B 1739:

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

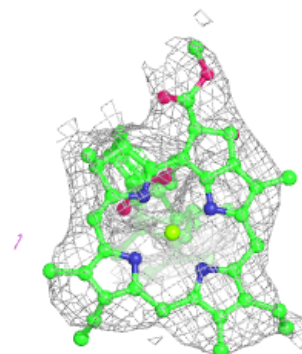
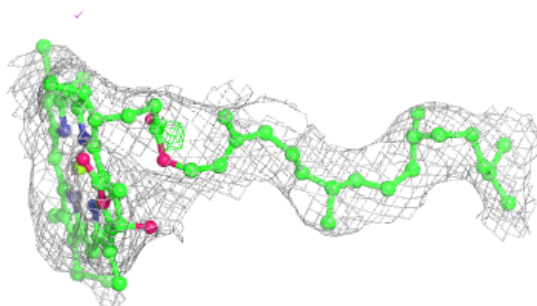
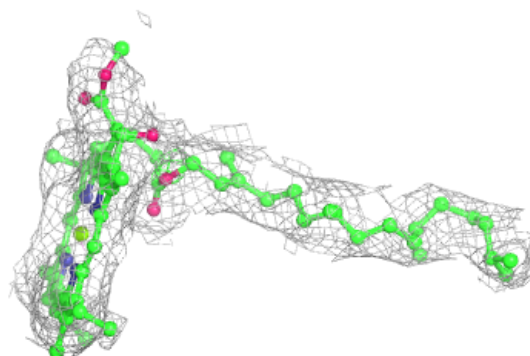


Electron density around CLA A 1811:

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

**Electron density around CLA A 1783:**

$2mF_o-DF_c$ (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.