



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 10:20 AM BST

PDB ID : 2WSE
Title : Improved Model of Plant Photosystem I
Authors : Amunts, A.; Toporik, H.; Borovikov, A.; Nelson, N.
Deposited on : 2009-09-05
Resolution : 3.49 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

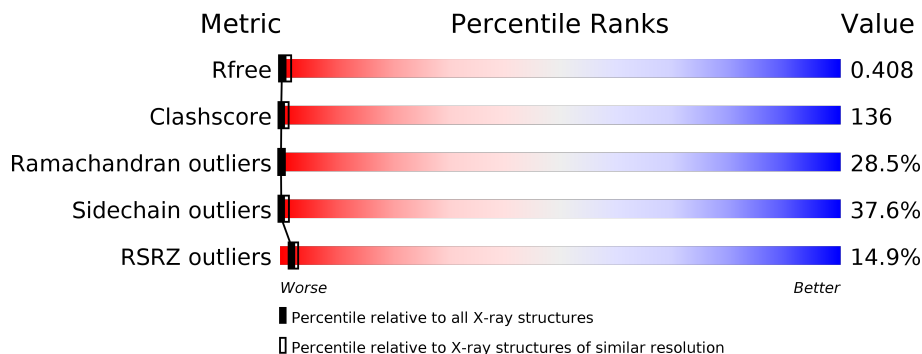
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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

Mol	Chain	Length	Quality of chain
1	1	241	
2	2	269	
3	3	276	
4	4	251	
5	A	758	
6	B	734	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
19	a	2	

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	GLC	O	1	-	-	X	-
19	FRU	O	2	X	-	X	X
19	GLC	P	1	-	-	X	-
19	FRU	P	2	X	-	X	X
19	GLC	Q	1	-	-	-	X
19	FRU	Q	2	X	-	X	X
19	GLC	S	1	-	-	X	-
19	FRU	S	2	X	-	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	FRU	W	2	X	-	-	-
19	GLC	X	1	-	-	X	-
19	FRU	X	2	X	-	X	X
19	GLC	Y	1	-	-	X	-
19	FRU	Y	2	X	-	X	-
19	GLC	Z	1	-	-	X	-
19	FRU	Z	2	X	-	X	-
19	GLC	a	1	-	-	-	X
19	FRU	a	2	X	-	-	-
20	CLA	1	201	X	-	-	-
20	CLA	1	202	X	-	X	-
20	CLA	1	203	X	-	-	-
20	CLA	1	204	X	-	-	-
20	CLA	1	205	X	-	-	-
20	CLA	1	206	X	-	-	-
20	CLA	1	207	X	-	-	-
20	CLA	1	208	X	-	-	-
20	CLA	1	209	X	-	-	-
20	CLA	1	210	X	-	-	-
20	CLA	1	211	X	-	-	-
20	CLA	1	212	X	-	-	-
20	CLA	1	214	X	-	-	-
20	CLA	1	215	X	-	X	-
20	CLA	1	216	X	-	-	-
20	CLA	2	301	X	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	2	302	X	-	-	-
20	CLA	2	303	X	-	-	-
20	CLA	2	304	X	-	-	-
20	CLA	2	305	X	-	-	-
20	CLA	2	306	X	-	-	-
20	CLA	2	307	X	-	-	-
20	CLA	2	308	X	-	-	X
20	CLA	2	309	X	-	-	-
20	CLA	2	310	X	-	-	X
20	CLA	2	311	X	-	-	-
20	CLA	2	312	X	-	-	-
20	CLA	2	315	X	-	-	-
20	CLA	2	316	X	-	-	-
20	CLA	2	322	X	-	X	-
20	CLA	3	301	X	-	-	X
20	CLA	3	302	X	-	X	-
20	CLA	3	303	X	-	-	-
20	CLA	3	304	X	-	-	-
20	CLA	3	305	X	-	-	-
20	CLA	3	306	X	-	-	X
20	CLA	3	307	X	-	-	-
20	CLA	3	308	X	-	-	-
20	CLA	3	309	X	-	-	X
20	CLA	3	310	X	-	-	X
20	CLA	3	311	X	-	-	-
20	CLA	3	312	X	-	-	-
20	CLA	3	313	X	-	X	X
20	CLA	3	316	X	-	-	-
20	CLA	3	317	X	-	-	-
20	CLA	3	318	X	-	-	-
20	CLA	3	319	X	-	-	-
20	CLA	3	320	X	-	-	-
20	CLA	4	302	X	-	X	-
20	CLA	4	303	X	-	-	-
20	CLA	4	304	X	-	X	-
20	CLA	4	305	X	-	-	-
20	CLA	4	306	X	-	-	X
20	CLA	4	307	X	-	-	-
20	CLA	4	308	X	-	-	-
20	CLA	4	309	X	-	-	-
20	CLA	4	310	X	-	-	-
20	CLA	4	311	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	4	312	X	-	-	-
20	CLA	4	313	X	-	-	-
20	CLA	4	314	X	-	-	-
20	CLA	4	315	X	-	-	-
20	CLA	4	316	X	-	-	-
20	CLA	4	318	X	-	-	-
20	CLA	4	319	X	-	-	-
20	CLA	A	801	X	-	-	-
20	CLA	A	802	X	-	-	X
20	CLA	A	803	X	-	-	-
20	CLA	A	804	X	-	X	-
20	CLA	A	805	X	-	X	-
20	CLA	A	806	X	-	X	-
20	CLA	A	807	X	-	X	X
20	CLA	A	808	X	-	X	-
20	CLA	A	809	X	-	X	-
20	CLA	A	810	X	-	-	X
20	CLA	A	811	X	-	X	X
20	CLA	A	812	X	-	-	-
20	CLA	A	813	X	-	-	-
20	CLA	A	814	X	-	X	X
20	CLA	A	815	X	-	X	-
20	CLA	A	816	X	-	X	-
20	CLA	A	817	X	-	-	-
20	CLA	A	818	X	-	X	X
20	CLA	A	819	X	-	X	X
20	CLA	A	820	X	-	-	X
20	CLA	A	821	X	-	-	-
20	CLA	A	822	X	-	X	-
20	CLA	A	823	X	-	-	X
20	CLA	A	824	X	-	X	-
20	CLA	A	825	X	-	X	-
20	CLA	A	826	X	-	X	X
20	CLA	A	827	X	-	X	-
20	CLA	A	828	X	-	-	-
20	CLA	A	829	X	-	-	X
20	CLA	A	830	X	-	X	-
20	CLA	A	831	X	-	-	-
20	CLA	A	832	X	-	-	-
20	CLA	A	833	X	-	-	-
20	CLA	A	834	X	-	-	-
20	CLA	A	835	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	836	X	-	-	-
20	CLA	A	837	X	-	-	-
20	CLA	A	838	X	-	X	-
20	CLA	A	839	X	-	X	X
20	CLA	A	840	X	-	-	-
20	CLA	A	841	X	-	X	-
20	CLA	A	850	X	-	-	-
20	CLA	A	851	X	-	X	-
20	CLA	A	852	X	-	X	-
20	CLA	B	803	X	-	X	X
20	CLA	B	804	X	-	-	-
20	CLA	B	805	X	-	-	-
20	CLA	B	806	X	-	-	-
20	CLA	B	807	X	-	X	-
20	CLA	B	808	X	-	X	-
20	CLA	B	809	X	-	-	-
20	CLA	B	810	X	-	-	-
20	CLA	B	811	X	-	X	-
20	CLA	B	812	X	-	-	-
20	CLA	B	813	X	-	-	-
20	CLA	B	814	X	-	X	X
20	CLA	B	815	X	-	X	-
20	CLA	B	816	X	-	-	-
20	CLA	B	817	X	-	-	-
20	CLA	B	818	X	-	-	-
20	CLA	B	819	X	-	X	-
20	CLA	B	820	X	-	-	-
20	CLA	B	821	X	-	X	-
20	CLA	B	822	X	-	X	-
20	CLA	B	823	X	-	X	-
20	CLA	B	824	X	-	X	-
20	CLA	B	825	X	-	X	-
20	CLA	B	826	X	-	X	-
20	CLA	B	827	X	-	X	-
20	CLA	B	828	X	-	-	-
20	CLA	B	829	X	-	-	-
20	CLA	B	830	X	-	X	-
20	CLA	B	831	X	-	-	-
20	CLA	B	832	X	-	X	-
20	CLA	B	833	X	-	X	X
20	CLA	B	834	X	-	-	X
20	CLA	B	835	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	836	X	-	X	-
20	CLA	B	837	X	-	X	-
20	CLA	B	838	X	-	X	X
20	CLA	B	839	X	-	X	-
20	CLA	B	840	X	-	-	X
20	CLA	B	849	X	-	X	-
20	CLA	B	850	X	-	X	-
20	CLA	B	851	X	-	X	-
20	CLA	F	204	X	-	-	-
20	CLA	F	205	X	-	-	-
20	CLA	F	206	X	-	-	-
20	CLA	G	102	X	-	-	-
20	CLA	H	101	X	-	X	-
20	CLA	H	102	X	-	-	-
20	CLA	H	103	X	-	-	X
20	CLA	H	109	X	-	-	-
20	CLA	I	102	X	-	-	-
20	CLA	J	101	X	-	X	-
20	CLA	J	103	X	-	X	-
20	CLA	K	101	X	-	-	-
20	CLA	K	102	X	-	-	X
20	CLA	K	103	X	-	-	X
20	CLA	K	108	X	-	X	X
20	CLA	L	201	X	-	X	-
20	CLA	L	202	X	-	X	-
20	CLA	L	203	X	-	-	X
20	CLA	L	207	X	-	-	-
20	CLA	L	208	X	-	X	-
20	CLA	L	209	X	-	-	-
20	CLA	R	107	X	-	-	X
20	CLA	R	108	X	-	-	-
21	LMU	1	217	-	-	-	X
21	LMU	1	218	-	-	-	X
21	LMU	2	313	-	-	-	X
21	LMU	2	320	-	-	-	X
21	LMU	4	320	-	-	-	X
21	LMU	A	848	-	-	-	X
21	LMU	A	849	-	-	-	X
21	LMU	A	853	-	-	-	X
21	LMU	A	854	-	-	X	-
21	LMU	A	855	-	-	X	-
21	LMU	B	801	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	LMU	B	847	-	-	X	-
21	LMU	E	101	-	-	X	-
21	LMU	H	104	-	-	X	-
21	LMU	H	106	-	-	X	-
21	LMU	H	108	-	-	X	-
21	LMU	K	104	-	-	-	X
21	LMU	K	105	-	-	X	-
21	LMU	K	106	-	-	X	-
21	LMU	L	204	-	-	-	X
21	LMU	N	101	-	-	X	-
21	LMU	R	101	X	-	-	-
21	LMU	R	102	-	-	-	X
21	LMU	R	103	-	-	X	-
21	LMU	R	109	-	-	X	-
22	BCR	3	314	-	-	X	-
22	BCR	A	843	-	-	X	X
22	BCR	A	844	-	-	X	X
22	BCR	A	845	-	-	X	-
22	BCR	A	846	-	-	X	-
22	BCR	A	847	-	-	X	X
22	BCR	B	845	-	-	X	-
22	BCR	B	846	-	-	X	X
22	BCR	F	202	-	-	X	X
22	BCR	F	203	-	-	X	-
22	BCR	I	103	-	-	X	X
22	BCR	J	102	-	-	X	X
22	BCR	L	210	-	-	X	X
23	PQN	A	842	X	-	-	X
23	PQN	B	841	X	-	X	X
24	SF4	A	857	-	-	X	-
24	SF4	C	102	-	-	X	-
24	SF4	C	103	-	-	X	-
25	LMG	B	848	-	-	X	X

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 36461 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
			Total	C	N	O	S			
1	1	164	1255	817	206	228	4	0	0	0

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
			Total	C	N	O	S			
2	2	176	1380	902	229	245	4	0	0	0

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
			Total	C	N	O	S			
3	3	160	1233	811	200	217	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	4	166	1322	864	219	236	3	0	0	0

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
			Total	C	N	O	S			
5	A	730	5745	3766	974	987	18	0	0	0

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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
			Total	C	N	O			
9	E	65	520	332	93	95	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S			
16	L	161	1203	791	193	214	5	0	0	0

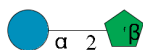
- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

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

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

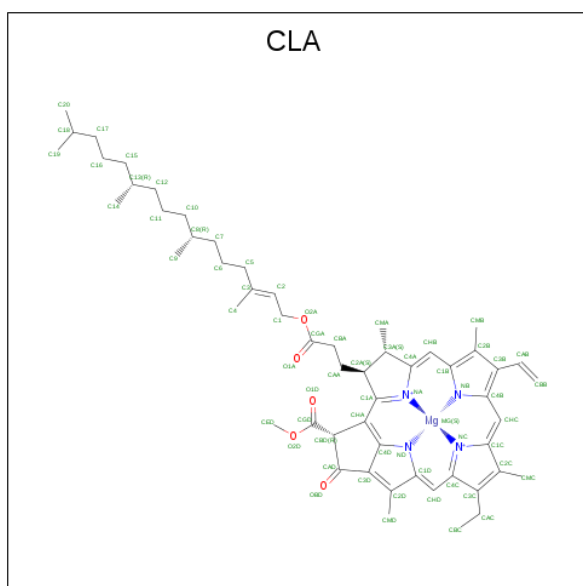
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	R	53	265	159	53	53	0	0	0

- 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
			23	12	11			
19	O	2	Total	C	O	0	0	0
			22	12	10			
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 (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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
			57	47	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		0	0
			25	20	1	4			
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
			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		0	0
			25	20	1	4			
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	2	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
			65	55	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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
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	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
			61	51	1	4	5		
20	3	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	3	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	3	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
20	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	4	1	Total	C	Mg	N	O	0	0
			47	37	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		0	0
			25	20	1	4			
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
			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
			55	45	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
			52	42	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
			54	44	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
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
20	A	1	42	34	1	4	3	0	0
20	A	1	55	45	1	4	5	0	0
20	A	1	65	55	1	4	5	0	0
20	A	1	65	55	1	4	5	0	0
20	A	1	65	55	1	4	5	0	0
20	A	1	65	55	1	4	5	0	0
20	A	1	55	45	1	4	5	0	0
20	A	1	65	55	1	4	5	0	0
20	A	1	50	40	1	4	5	0	0
20	A	1	65	55	1	4	5	0	0
20	A	1	55	45	1	4	5	0	0
20	A	1	50	40	1	4	5	0	0
20	A	1	45	35	1	4	5	0	0
20	A	1	49	39	1	4	5	0	0
20	A	1	65	55	1	4	5	0	0
20	A	1	47	37	1	4	5	0	0
20	A	1	47	37	1	4	5	0	0
20	A	1	65	55	1	4	5	0	0
20	A	1	65	55	1	4	5	0	0
20	A	1	50	40	1	4	5	0	0
20	A	1	65	55	1	4	5	0	0

Continued on next page...

Continued from previous page...

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
			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
			45	35	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
			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
			54	44	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
			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
			60	50	1	4	5		
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
			59	49	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
			61	51	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
			46	36	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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
			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		
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		

Continued on next page...

Continued from previous page...

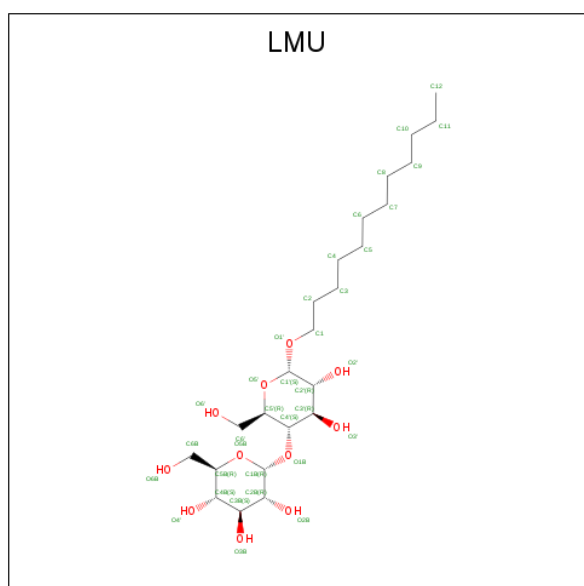
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	F	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	F	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
20	F	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
20	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	I	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	J	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
20	J	1	Total	C	Mg	N	O	0	0
			61	51	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	K	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	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	L	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			50	40	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
			58	48	1	4	5		

- Molecule 21 is DODECYL-ALPHA-D-MALTOSE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



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	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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	3	1	Total	C	O	0	0
			35	24	11		
21	4	1	Total	C	O	0	0
			35	24	11		
21	4	1	Total	C	O	0	0
			35	24	11		
21	4	1	Total	C	O	0	0
			34	23	11		
21	4	1	Total	C	O	0	0
			35	24	11		
21	4	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	B	1	Total	C	O	0	0
			35	24	11		
21	B	1	Total	C	O	0	0
			35	24	11		
21	B	1	Total	C	O	0	0
			35	24	11		
21	C	1	Total	C	O	0	0
			35	24	11		
21	D	1	Total	C	O	0	0
			35	24	11		

Continued on next page...

Continued from previous page...

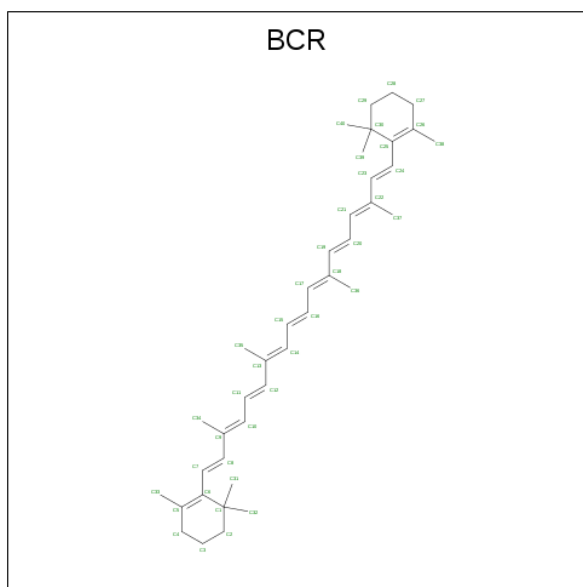
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	E	1	Total	C	O	0	0
			35	24	11		
21	F	1	Total	C	O	0	0
			34	23	11		
21	G	1	Total	C	O	0	0
			35	24	11		
21	H	1	Total	C	O	0	0
			35	24	11		
21	H	1	Total	C	O	0	0
			35	24	11		
21	H	1	Total	C	O	0	0
			35	24	11		
21	H	1	Total	C	O	0	0
			35	24	11		
21	H	1	Total	C	O	0	0
			35	24	11		
21	K	1	Total	C	O	0	0
			35	24	11		
21	K	1	Total	C	O	0	0
			35	24	11		
21	K	1	Total	C	O	0	0
			35	24	11		
21	K	1	Total	C	O	0	0
			35	24	11		
21	L	1	Total	C	O	0	0
			35	24	11		
21	L	1	Total	C	O	0	0
			35	24	11		
21	L	1	Total	C	O	0	0
			35	24	11		
21	N	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		
21	R	1	Total	C	O	0	0
			35	24	11		
21	R	1	Total	C	O	0	0
			35	24	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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 (three-letter code: BCR) (formula: C₄₀H₅₆).



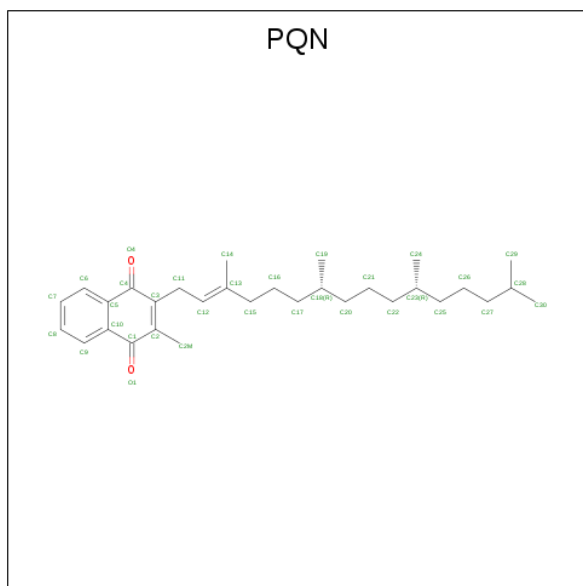
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	3	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	A	1	Total	C	0	0
			40	40		
22	B	1	Total	C	0	0
			40	40		
22	B	1	Total	C	0	0
			40	40		
22	B	1	Total	C	0	0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

Continued on next page...

Continued from previous page...

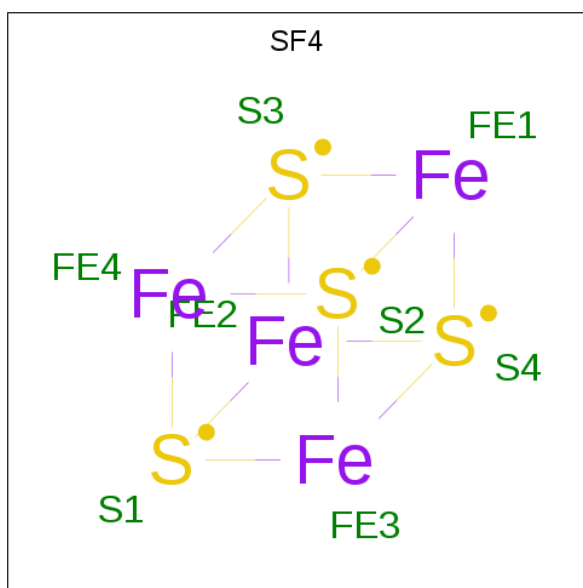
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	I	1	Total C 40 40	0	0
22	I	1	Total C 40 40	0	0
22	J	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0

- Molecule 23 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



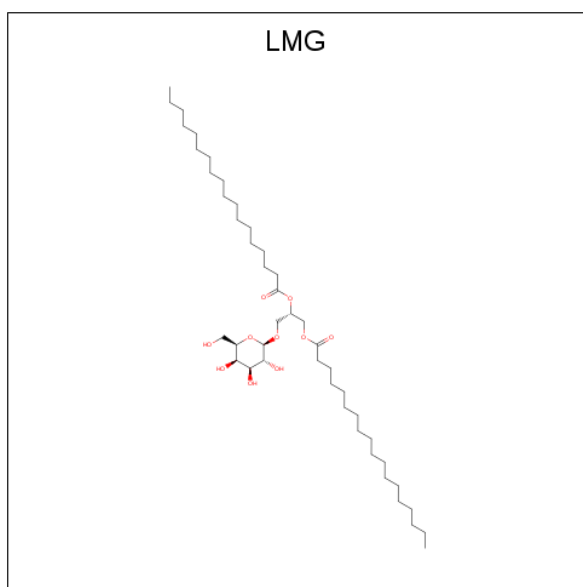
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 33 31 2	0	0
23	B	1	Total C O 33 31 2	0	0

- Molecule 24 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

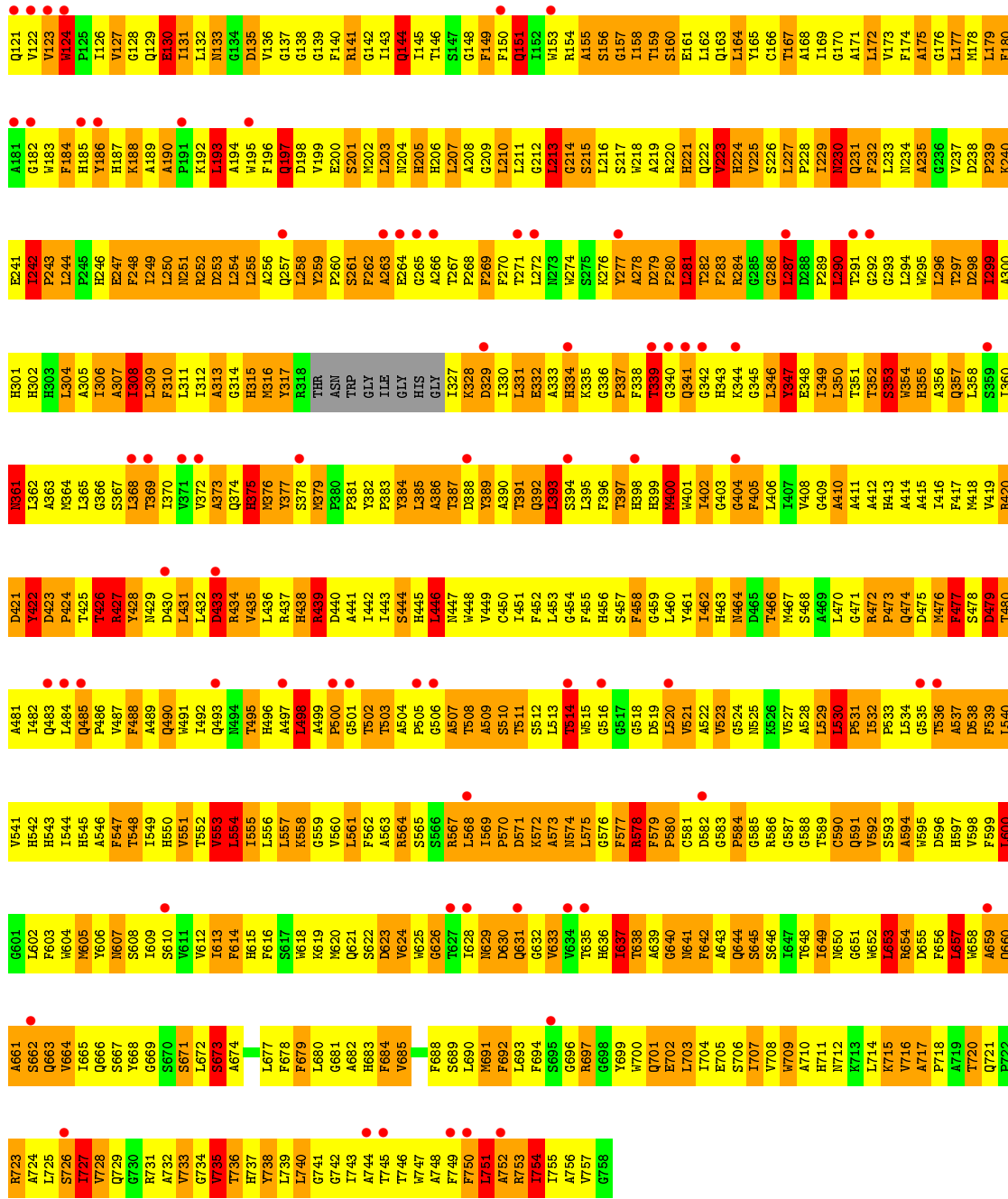
- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



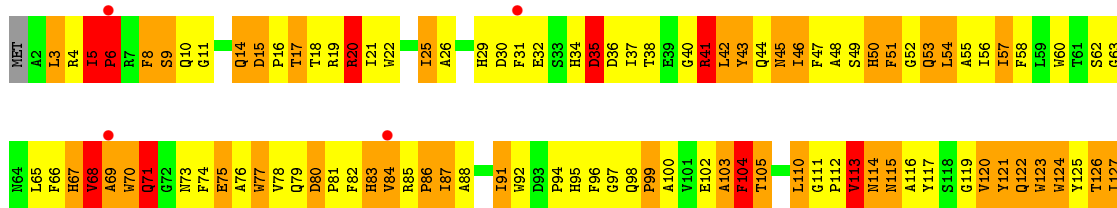
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			49	39	10		

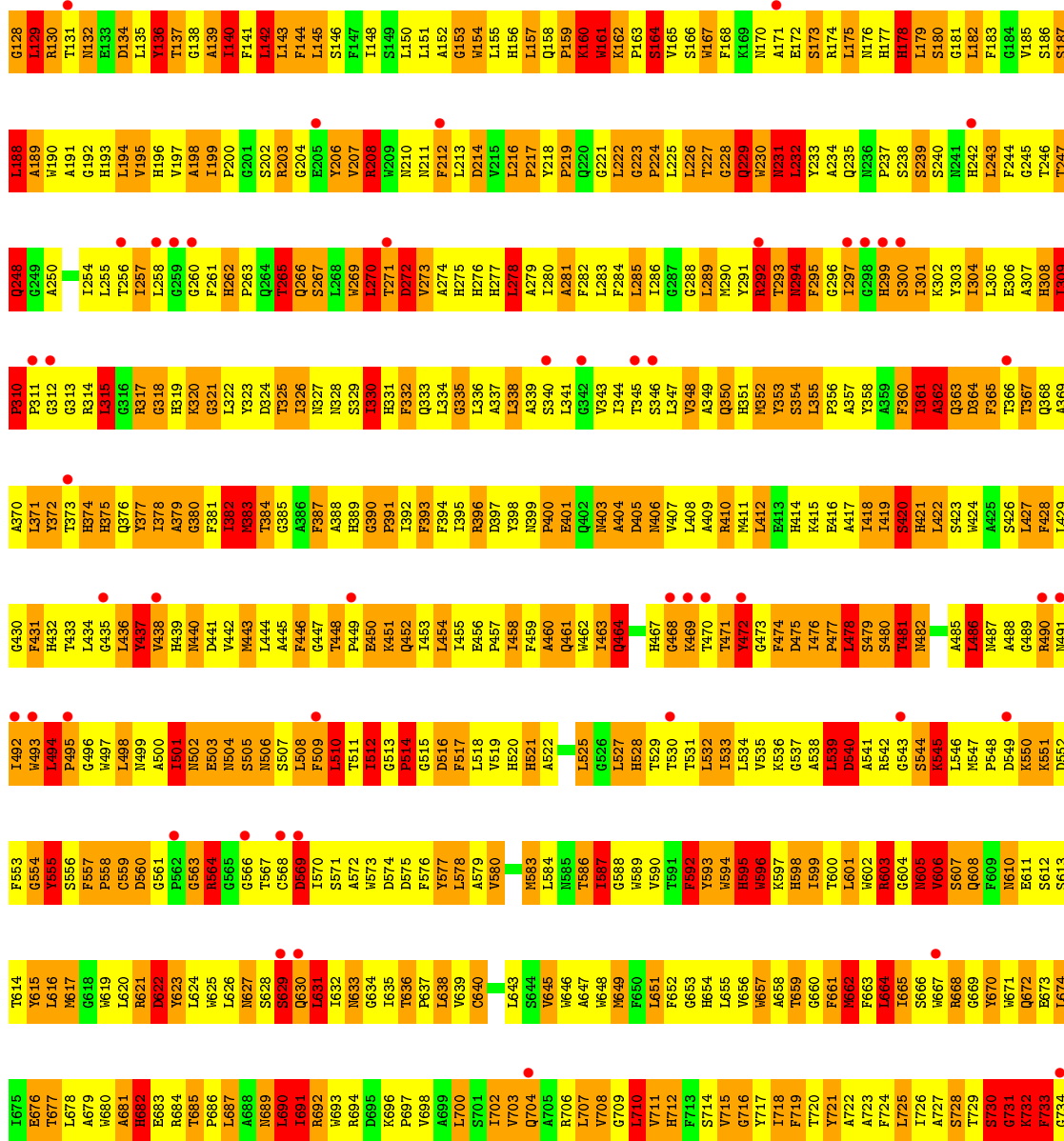
- Molecule 26 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

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

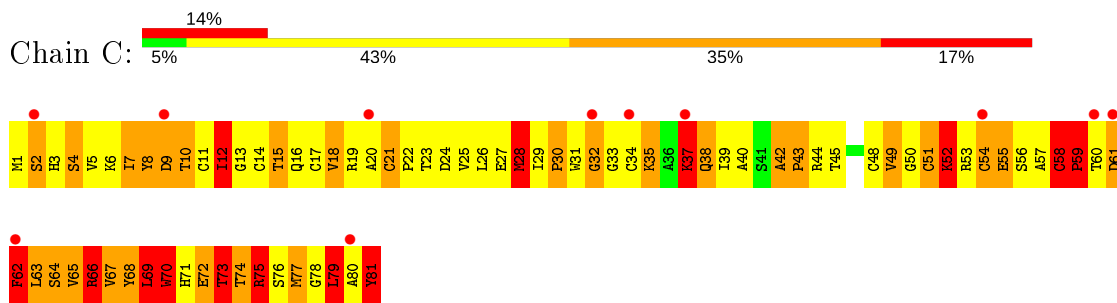


● Molecule 6: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2

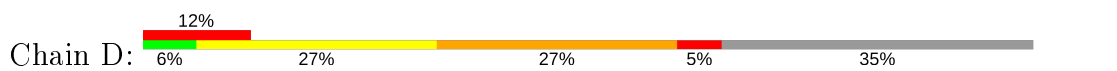


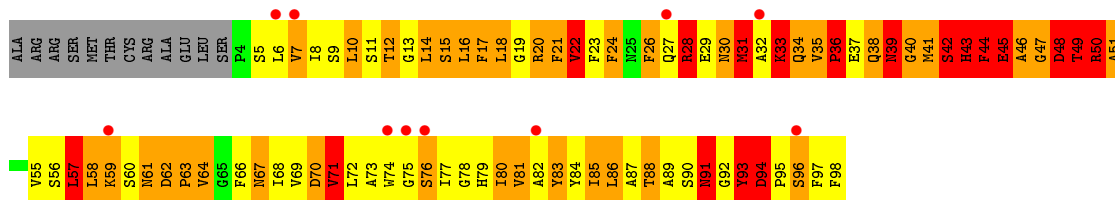


● Molecule 7: PHOTOSYSTEM I IRON-SULFUR CENTER

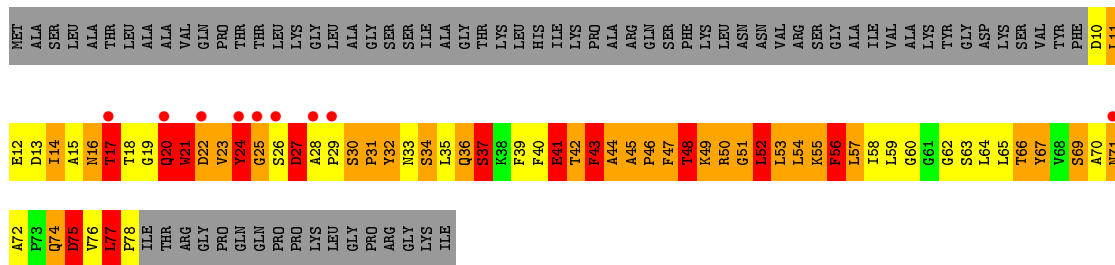
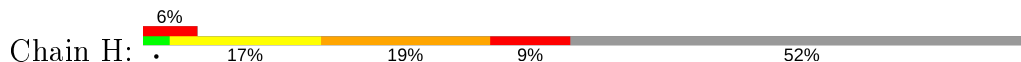


● Molecule 8: PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC





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



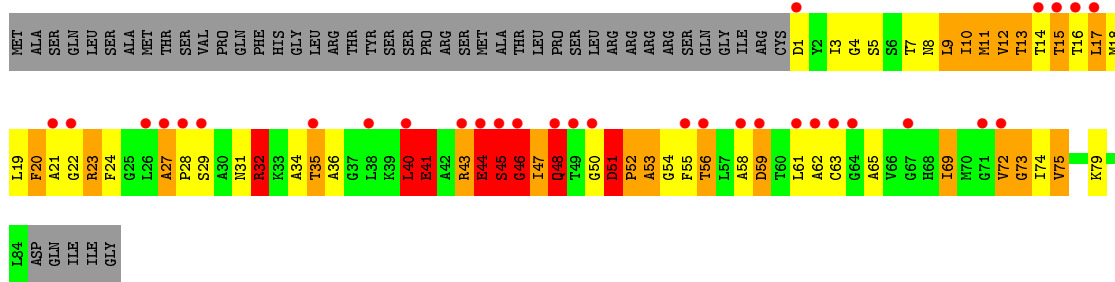
• Molecule 13: PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII



• Molecule 14: PHOTOSYSTEM I REACTION CENTER SUBUNIT IX

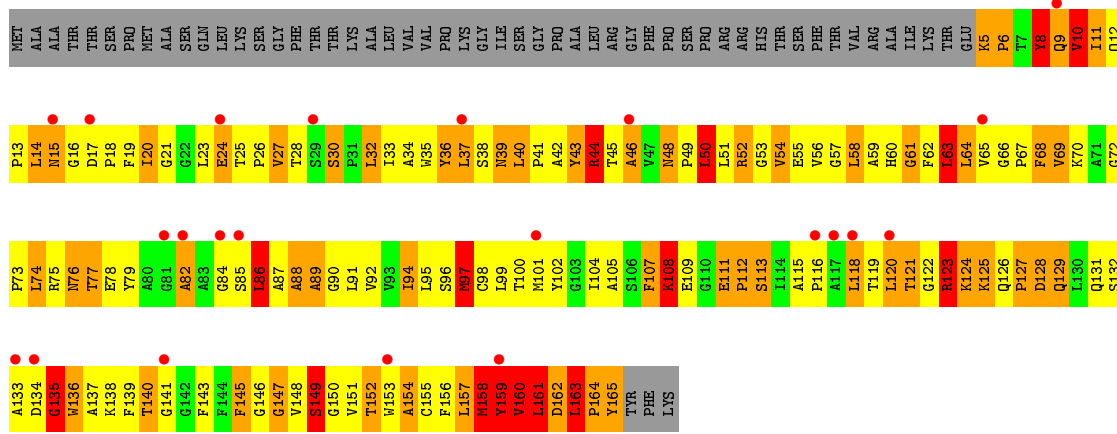


• Molecule 15: PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC

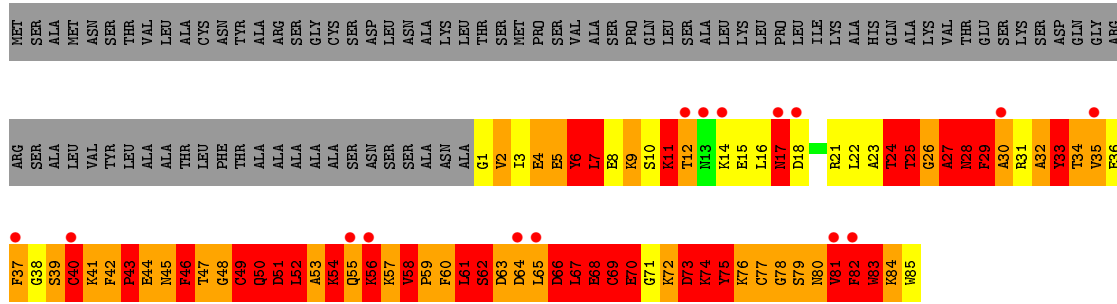
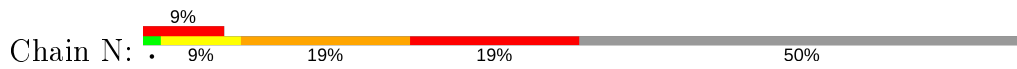


• Molecule 16: PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC

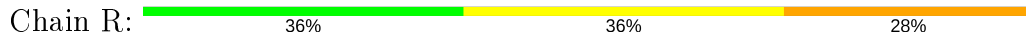




• Molecule 17: PHOTOSYSTEM I-N SUBUNIT



• 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:  100%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 – 3.49 39.96 – 3.49	Depositor EDS
% Data completeness (in resolution range)	91.2 (30.00-3.49) 90.6 (39.96-3.49)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 3.48Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.369 , 0.375 0.387 , 0.408	Depositor DCC
R_{free} test set	1334 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	90.9	Xtrriage
Anisotropy	0.544	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 113.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.71	EDS
Total number of atoms	36461	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, GLC, CLA, PQN, LMU, FRU, UNL, BCR, LMG

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	0.62	0/1294	0.89	5/1762 (0.3%)
2	2	1.05	1/1426 (0.1%)	1.32	15/1950 (0.8%)
3	3	0.88	6/1270 (0.5%)	0.96	4/1714 (0.2%)
4	4	1.27	9/1362 (0.7%)	1.35	17/1855 (0.9%)
5	A	0.89	0/5938	1.06	15/8104 (0.2%)
6	B	0.89	2/6058 (0.0%)	1.03	13/8278 (0.2%)
7	C	1.42	7/632 (1.1%)	1.34	5/856 (0.6%)
8	D	1.00	0/1122	1.06	0/1514
9	E	1.10	0/530	1.17	2/718 (0.3%)
10	F	1.05	1/1250 (0.1%)	1.07	3/1687 (0.2%)
11	G	1.04	0/760	1.27	10/1031 (1.0%)
12	H	1.10	0/543	1.20	2/741 (0.3%)
13	I	0.89	0/235	0.98	0/320
14	J	0.93	0/349	1.09	1/475 (0.2%)
15	K	0.63	0/599	1.16	6/810 (0.7%)
16	L	1.02	0/1238	1.14	6/1691 (0.4%)
17	N	1.28	1/699 (0.1%)	1.32	7/936 (0.7%)
All	All	0.97	27/25305 (0.1%)	1.11	111/34442 (0.3%)

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	6
2	2	3	22
3	3	0	19
4	4	0	22
5	A	0	30
6	B	0	20

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
7	C	0	3
8	D	0	6
9	E	0	6
10	F	0	12
11	G	1	16
12	H	0	9
15	K	0	3
16	L	0	5
17	N	0	21
18	R	0	17
All	All	4	217

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	92	TRP	CB-CG	16.89	1.80	1.50
3	3	93	PHE	CE1-CZ	8.69	1.53	1.37
7	C	72	GLU	CD-OE1	-7.90	1.17	1.25
4	4	83	TYR	CE1-CZ	-7.46	1.28	1.38
3	3	93	PHE	CD2-CE2	7.39	1.54	1.39

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	57	ILE	N-CA-C	9.01	135.32	111.00
5	A	93	LEU	CA-CB-CG	8.09	133.90	115.30
6	B	732	LYS	N-CA-C	-8.08	89.19	111.00
16	L	160	VAL	CB-CA-C	-7.79	96.61	111.40
4	4	39	TRP	C-N-CA	-7.68	102.51	121.70

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	2	67	PHE	CA
2	2	101	PHE	CA
2	2	174	VAL	CA
11	G	21	PHE	CA

5 of 217 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	184	PRO	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	1	56	GLY	Peptide
1	1	57	ILE	Peptide
1	1	60	PRO	Peptide
1	1	63	LEU	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1255	0	1222	206	0
2	2	1380	0	1341	486	0
3	3	1233	0	1199	283	12
4	4	1322	0	1287	744	8
5	A	5745	0	5595	1666	0
6	B	5848	0	5653	1490	13
7	C	619	0	608	234	0
8	D	1095	0	1112	222	0
9	E	520	0	528	154	0
10	F	1221	0	1246	306	1
11	G	740	0	709	304	11
12	H	529	0	514	122	0
13	I	229	0	252	63	0
14	J	338	0	340	78	0
15	K	593	0	618	120	0
16	L	1203	0	1213	369	8
17	N	685	0	670	447	11
18	R	265	0	65	65	0
19	M	23	0	21	0	0
19	O	22	0	18	11	0
19	P	23	0	21	19	0
19	Q	23	0	21	14	0
19	S	23	0	21	7	0
19	T	23	0	21	7	0
19	U	23	0	21	21	0
19	V	23	0	21	2	0
19	W	23	0	18	5	0
19	X	23	0	21	10	0
19	Y	23	0	20	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Z	23	0	21	13	0
19	a	23	0	21	0	0
20	1	606	0	376	166	1
20	2	672	0	513	141	0
20	3	659	0	382	132	0
20	4	710	0	463	175	0
20	A	2449	0	2260	988	1
20	B	2360	0	2255	834	0
20	F	130	0	86	31	0
20	G	51	0	40	20	0
20	H	225	0	201	66	0
20	I	60	0	58	12	0
20	J	109	0	95	55	0
20	K	210	0	177	43	1
20	L	322	0	277	113	0
20	R	115	0	106	22	0
21	1	175	0	230	46	0
21	2	175	0	230	25	3
21	3	70	0	92	12	0
21	4	174	0	224	23	5
21	A	210	0	276	84	0
21	B	105	0	138	45	30
21	C	35	0	46	0	0
21	D	35	0	40	12	0
21	E	35	0	41	30	0
21	F	34	0	41	19	0
21	G	35	0	46	19	0
21	H	175	0	230	110	0
21	K	140	0	183	95	0
21	L	105	0	138	10	0
21	N	35	0	45	36	0
21	R	245	0	321	84	5
22	3	40	0	54	19	28
22	A	200	0	269	214	0
22	B	240	0	321	144	0
22	F	80	0	108	76	0
22	I	80	0	108	64	0
22	J	40	0	52	41	0
22	L	40	0	54	51	0
23	A	33	0	46	15	0
23	B	33	0	46	32	0
24	A	8	0	0	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	C	16	0	0	8	0
25	B	49	0	71	30	0
26	H	23	0	0	2	0
All	All	36461	0	35177	9737	69

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 136.

The worst 5 of 9737 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)
2:2:43:TRP:CZ3	2:2:125:PHE:CG	1.81	1.63
4:4:69:ILE:CD1	4:4:175:LYS:HG2	1.30	1.61
2:2:43:TRP:CH2	2:2:125:PHE:CE1	1.88	1.61
4:4:69:ILE:HD11	4:4:175:LYS:CG	1.24	1.61
2:2:43:TRP:CH2	2:2:125:PHE:CZ	1.85	1.60

The worst 5 of 69 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)
22:3:314:BCR:C28	21:B:847:LMU:C5[2_556]	0.48	1.72
22:3:314:BCR:C40	21:B:847:LMU:C8[2_556]	0.57	1.63
4:4:130:GLU:O	16:L:159:TYR:OH[1_655]	0.69	1.51
3:3:181:LEU:CG	6:B:490:ARG:NH2[1_556]	0.72	1.48
11:G:31:MET:CE	17:N:85:TRP:NE1[2_546]	0.72	1.48

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	160/241 (66%)	83 (52%)	47 (29%)	30 (19%)	0	2
2	2	174/269 (65%)	62 (36%)	48 (28%)	64 (37%)	0	0
3	3	154/276 (56%)	77 (50%)	42 (27%)	35 (23%)	0	1
4	4	164/251 (65%)	56 (34%)	47 (29%)	61 (37%)	0	0
5	A	726/758 (96%)	333 (46%)	198 (27%)	195 (27%)	0	0
6	B	731/734 (100%)	362 (50%)	186 (25%)	183 (25%)	0	0
7	C	79/81 (98%)	23 (29%)	29 (37%)	27 (34%)	0	0
8	D	136/212 (64%)	49 (36%)	41 (30%)	46 (34%)	0	0
9	E	63/143 (44%)	28 (44%)	15 (24%)	20 (32%)	0	0
10	F	152/231 (66%)	69 (45%)	41 (27%)	42 (28%)	0	0
11	G	93/167 (56%)	37 (40%)	25 (27%)	31 (33%)	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%)	54 (66%)	12 (15%)	16 (20%)	0	2
16	L	159/216 (74%)	65 (41%)	46 (29%)	48 (30%)	0	0
17	N	83/170 (49%)	22 (26%)	19 (23%)	42 (51%)	0	0
All	All	3091/4108 (75%)	1377 (44%)	833 (27%)	881 (28%)	0	0

5 of 881 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	25	ASP
1	1	30	GLY
1	1	35	ASN
1	1	90	PRO
1	1	130	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	126/190 (66%)	99 (79%)	27 (21%)	1	5
2	2	141/216 (65%)	78 (55%)	63 (45%)	0	0
3	3	118/215 (55%)	78 (66%)	40 (34%)	0	1
4	4	139/201 (69%)	73 (52%)	66 (48%)	0	0
5	A	592/618 (96%)	395 (67%)	197 (33%)	0	1
6	B	598/600 (100%)	369 (62%)	229 (38%)	0	1
7	C	70/70 (100%)	40 (57%)	30 (43%)	0	0
8	D	118/173 (68%)	75 (64%)	43 (36%)	0	1
9	E	56/114 (49%)	36 (64%)	20 (36%)	0	1
10	F	127/190 (67%)	74 (58%)	53 (42%)	0	0
11	G	79/144 (55%)	47 (60%)	32 (40%)	0	1
12	H	57/115 (50%)	26 (46%)	31 (54%)	0	0
13	I	26/36 (72%)	18 (69%)	8 (31%)	0	2
14	J	36/39 (92%)	24 (67%)	12 (33%)	0	1
15	K	61/102 (60%)	39 (64%)	22 (36%)	0	1
16	L	124/169 (73%)	81 (65%)	43 (35%)	0	1
17	N	74/139 (53%)	33 (45%)	41 (55%)	0	0
All	All	2542/3331 (76%)	1585 (62%)	957 (38%)	0	1

5 of 957 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	136	TYR
6	B	481	THR
16	L	40	LEU
6	B	175	LEU
6	B	325	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 109 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	95	HIS
6	B	403	ASN
14	J	30	ASN
6	B	122	GLN
6	B	266	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	11,11,12	0.86	0	15,15,17	2.46	4 (26%)
19	FRU	M	2	19	11,12,12	1.15	2 (18%)	10,18,18	0.97	0
19	GLC	O	1	19	10,10,12	1.48	3 (30%)	14,14,17	3.32	9 (64%)
19	FRU	O	2	19	11,12,12	1.11	1 (9%)	10,18,18	2.31	3 (30%)
19	GLC	P	1	19	11,11,12	1.51	2 (18%)	15,15,17	2.88	10 (66%)
19	FRU	P	2	19	11,12,12	1.38	2 (18%)	10,18,18	2.17	2 (20%)
19	GLC	Q	1	19	11,11,12	1.02	0	15,15,17	3.55	8 (53%)
19	FRU	Q	2	19	11,12,12	1.29	1 (9%)	10,18,18	1.71	2 (20%)
19	GLC	S	1	19	11,11,12	1.19	1 (9%)	15,15,17	1.61	3 (20%)
19	FRU	S	2	19	11,12,12	2.16	4 (36%)	10,18,18	2.83	4 (40%)
19	GLC	T	1	19	11,11,12	1.36	2 (18%)	15,15,17	1.81	3 (20%)
19	FRU	T	2	19	11,12,12	1.74	2 (18%)	10,18,18	2.33	4 (40%)
19	GLC	U	1	19	11,11,12	1.37	1 (9%)	15,15,17	1.56	3 (20%)
19	FRU	U	2	19	11,12,12	1.25	1 (9%)	10,18,18	1.61	2 (20%)
19	GLC	V	1	19	11,11,12	1.15	1 (9%)	15,15,17	3.47	6 (40%)
19	FRU	V	2	19	11,12,12	1.16	0	10,18,18	2.27	4 (40%)
19	GLC	W	1	19	11,11,12	1.16	1 (9%)	15,15,17	1.60	3 (20%)
19	FRU	W	2	19	11,12,12	1.23	1 (9%)	10,18,18	2.21	3 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	GLC	X	1	19	11,11,12	1.29	1 (9%)	15,15,17	2.17	4 (26%)
19	FRU	X	2	19	11,12,12	1.17	1 (9%)	10,18,18	1.83	4 (40%)
19	GLC	Y	1	19	11,11,12	1.95	3 (27%)	15,15,17	4.48	8 (53%)
19	FRU	Y	2	19	11,12,12	1.17	2 (18%)	10,18,18	2.41	3 (30%)
19	GLC	Z	1	19	11,11,12	1.08	0	15,15,17	2.04	5 (33%)
19	FRU	Z	2	19	11,12,12	0.70	0	10,18,18	1.67	4 (40%)
19	GLC	a	1	19	11,11,12	1.73	2 (18%)	15,15,17	2.10	5 (33%)
19	FRU	a	2	19	11,12,12	1.06	0	10,18,18	2.02	5 (50%)

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	-	2/2/19/22	0/1/1/1
19	FRU	M	2	19	1/1/4/4	2/5/24/24	0/1/1/1
19	GLC	O	1	19	-	-	0/1/1/1
19	FRU	O	2	19	1/1/4/4	0/5/24/24	0/1/1/1
19	GLC	P	1	19	-	1/2/19/22	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	-	1/2/19/22	0/1/1/1
19	FRU	Q	2	19	1/1/4/4	4/5/24/24	0/1/1/1
19	GLC	S	1	19	-	2/2/19/22	0/1/1/1
19	FRU	S	2	19	1/1/4/4	3/5/24/24	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	5/5/24/24	0/1/1/1
19	GLC	V	1	19	-	2/2/19/22	0/1/1/1
19	FRU	V	2	19	1/1/4/4	1/5/24/24	0/1/1/1
19	GLC	W	1	19	-	2/2/19/22	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	-	0/2/19/22	0/1/1/1
19	FRU	Y	2	19	1/1/4/4	3/5/24/24	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	GLC	Z	1	19	-	2/2/19/22	0/1/1/1
19	FRU	Z	2	19	1/1/4/4	1/5/24/24	0/1/1/1
19	GLC	a	1	19	-	0/2/19/22	0/1/1/1
19	FRU	a	2	19	1/1/4/4	3/5/24/24	0/1/1/1

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Y	1	GLC	O5-C1	-4.80	1.36	1.43
19	S	2	FRU	O5-C2	-3.61	1.37	1.43
19	U	2	FRU	O5-C2	-3.34	1.38	1.43
19	Q	2	FRU	O5-C2	-3.19	1.38	1.43
19	T	2	FRU	O5-C2	-3.14	1.38	1.43

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Y	1	GLC	C1-O5-C5	-11.22	97.00	112.19
19	M	1	GLC	C1-O5-C5	7.92	122.92	112.19
19	O	1	GLC	C1-C2-C3	7.69	119.11	109.67
19	V	1	GLC	C1-O5-C5	7.47	122.31	112.19
19	Y	1	GLC	O5-C1-C2	-7.39	99.37	110.77

5 of 13 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	a	2	FRU	C2
19	S	2	FRU	C2
19	O	2	FRU	C2
19	Z	2	FRU	C2
19	U	2	FRU	C2

5 of 50 torsion outliers are listed below:

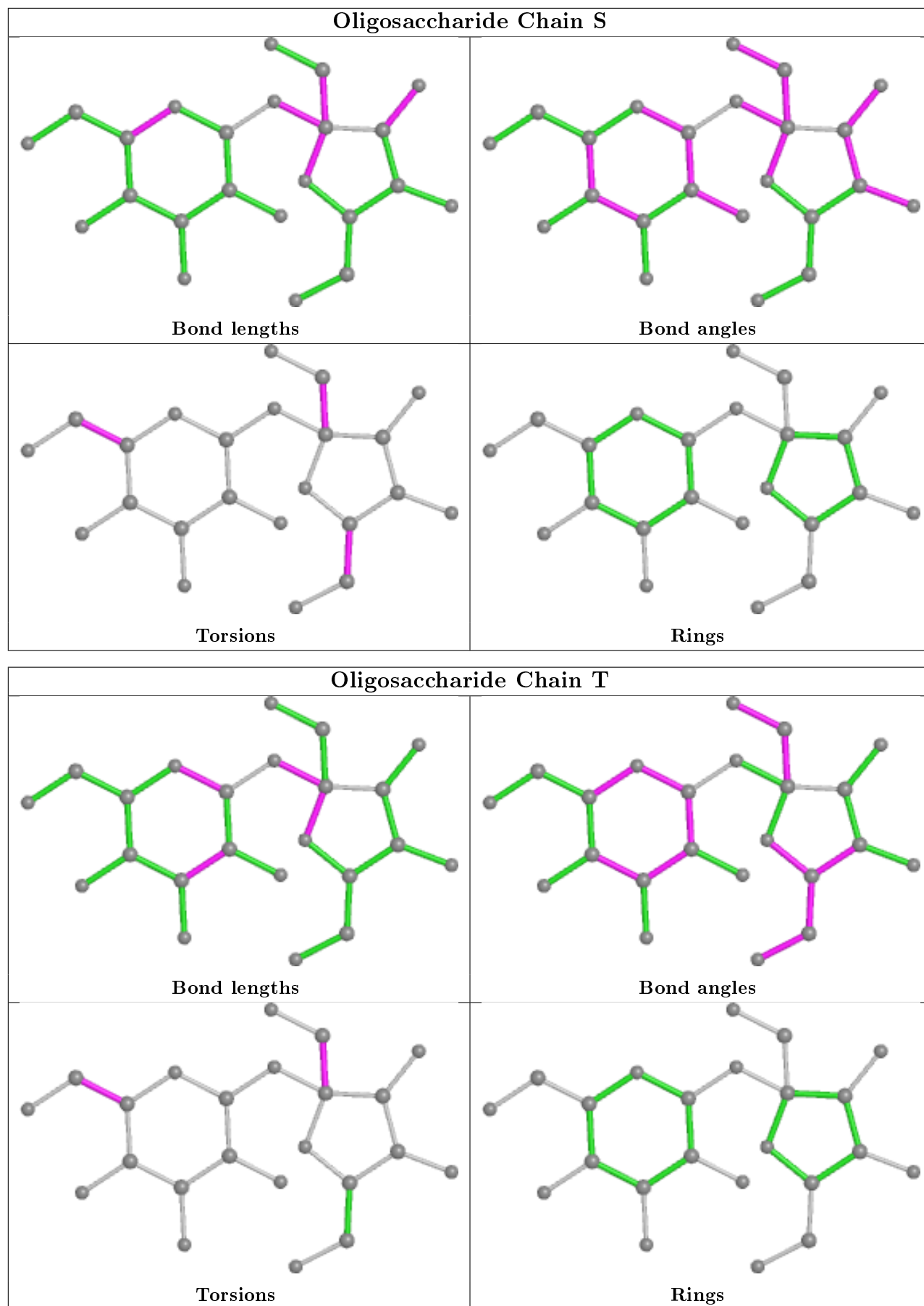
Mol	Chain	Res	Type	Atoms
19	U	2	FRU	O1-C1-C2-C3
19	U	2	FRU	O1-C1-C2-O2
19	U	2	FRU	C4-C5-C6-O6
19	X	2	FRU	O1-C1-C2-C3
19	X	2	FRU	O1-C1-C2-O2

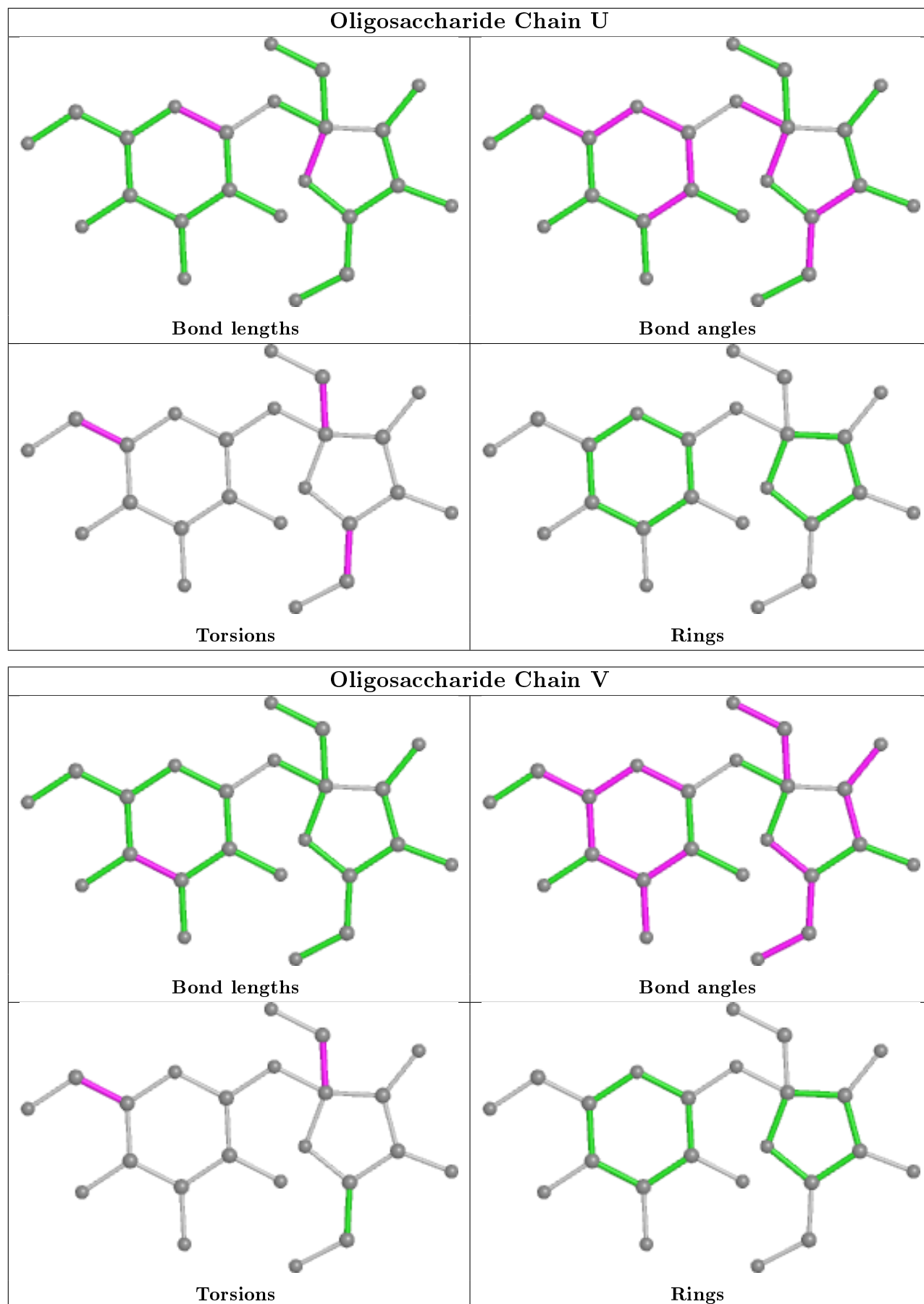
There are no ring outliers.

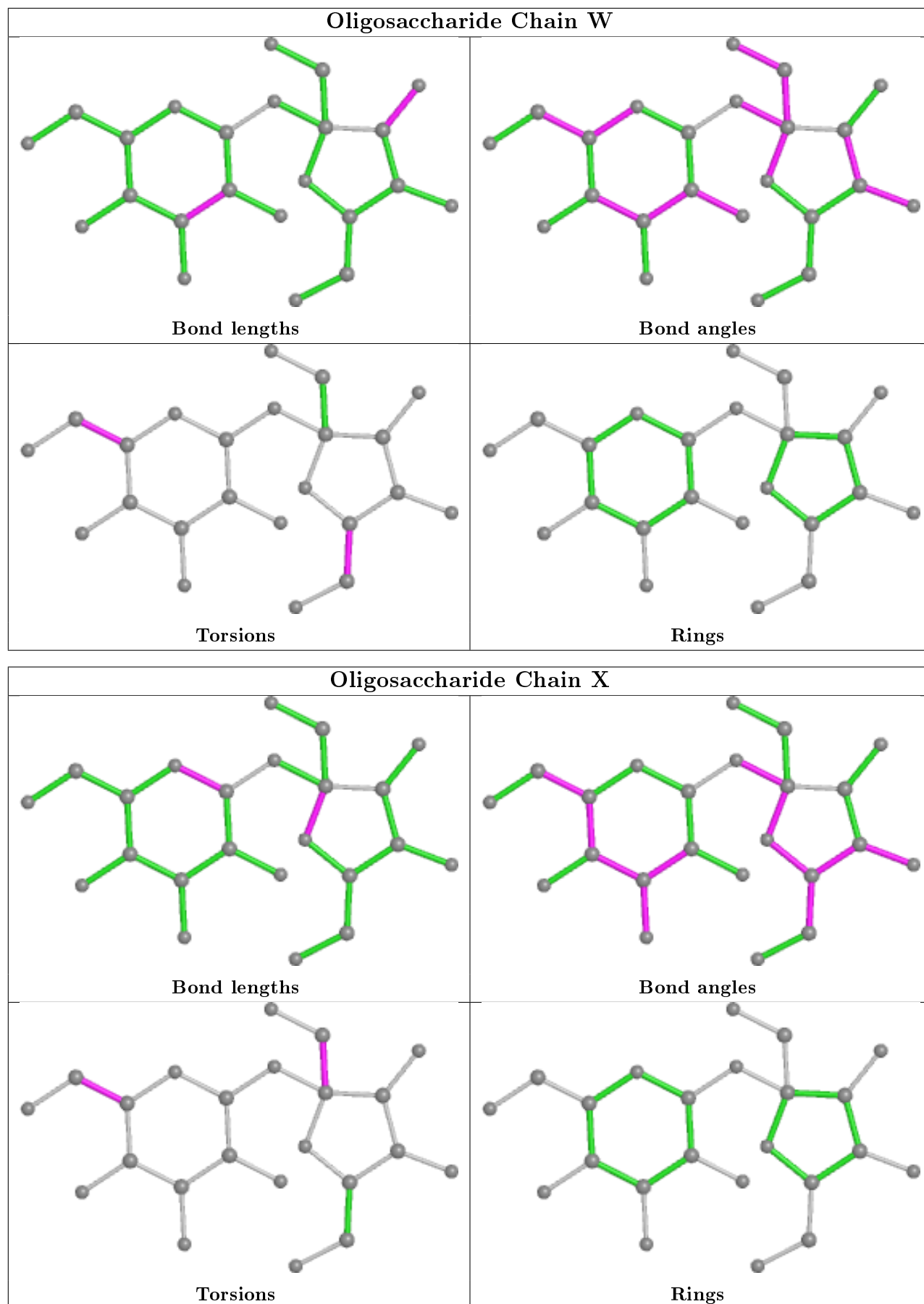
22 monomers are involved in 129 short contacts:

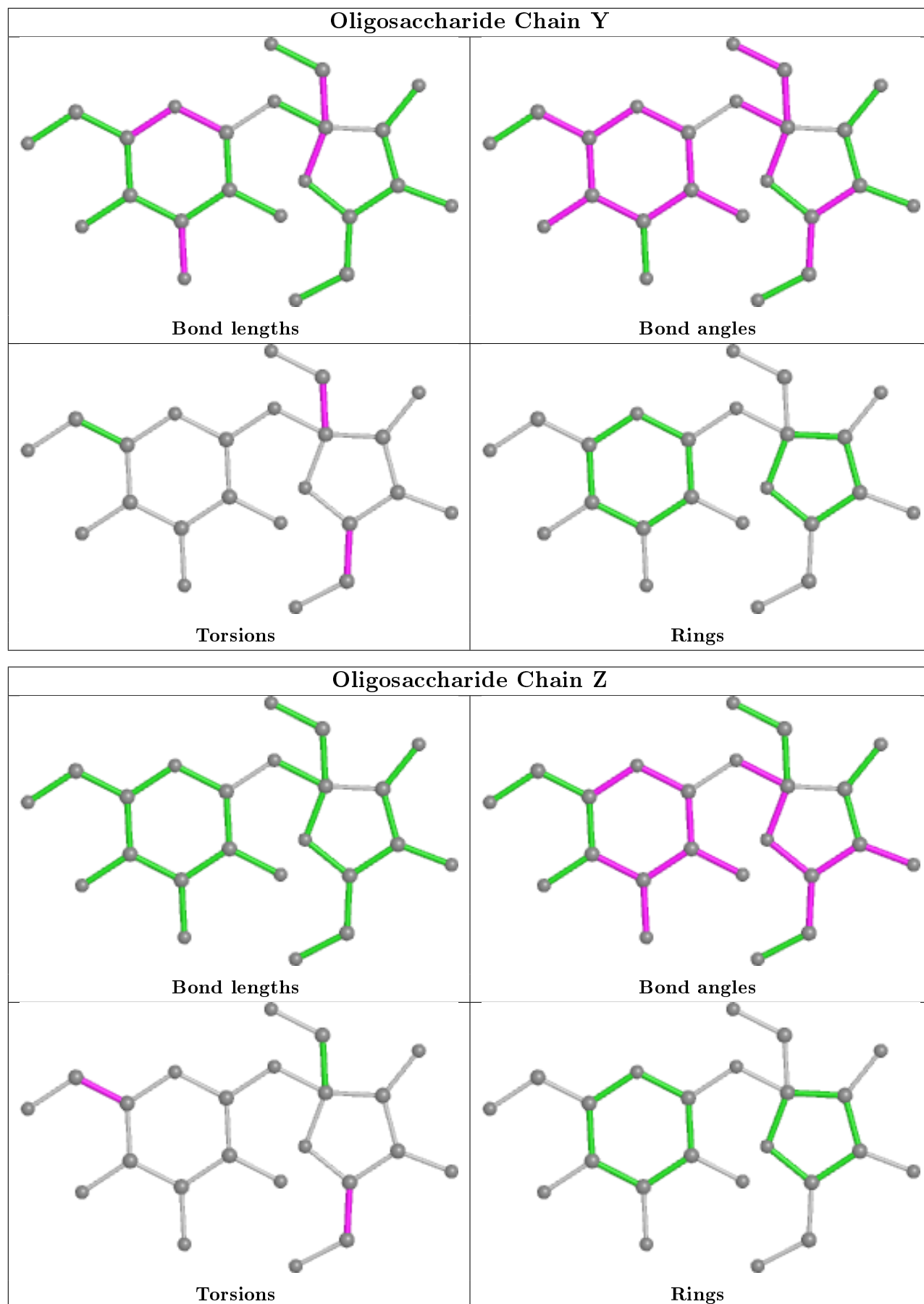
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	S	2	FRU	7	0
19	O	2	FRU	7	0
19	S	1	GLC	6	0
19	Z	2	FRU	9	0
19	O	1	GLC	10	0
19	U	2	FRU	20	0
19	T	2	FRU	7	0
19	W	1	GLC	2	0
19	U	1	GLC	11	0
19	T	1	GLC	7	0
19	Z	1	GLC	13	0
19	P	1	GLC	13	0
19	P	2	FRU	17	0
19	X	1	GLC	9	0
19	Q	1	GLC	5	0
19	Y	1	GLC	7	0
19	X	2	FRU	8	0
19	V	1	GLC	1	0
19	W	2	FRU	3	0
19	Y	2	FRU	18	0
19	V	2	FRU	2	0
19	Q	2	FRU	14	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.









5.6 Ligand geometry

Of 249 ligands modelled in this entry, 1 is unknown - leaving 248 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	J	103	-	55,69,73	2.11	12 (21%)	62,108,113	3.35	18 (29%)
22	BCR	B	852	-	41,41,41	3.47	21 (51%)	56,56,56	6.45	26 (46%)
20	CLA	4	316	-	40,54,73	2.83	17 (42%)	44,90,113	3.46	19 (43%)
20	CLA	A	809	-	46,60,73	2.20	14 (30%)	51,97,113	3.42	24 (47%)
20	CLA	3	303	-	22,32,73	2.82	11 (50%)	26,54,113	3.22	15 (57%)
20	CLA	B	825	-	59,73,73	2.13	12 (20%)	67,113,113	3.71	24 (35%)
20	CLA	B	806	-	59,73,73	2.12	14 (23%)	67,113,113	3.30	29 (43%)
20	CLA	B	851	-	59,73,73	2.06	12 (20%)	67,113,113	3.02	23 (34%)
20	CLA	A	851	-	59,73,73	2.07	13 (22%)	67,113,113	3.09	21 (31%)
20	CLA	2	303	-	59,73,73	2.05	11 (18%)	67,113,113	2.94	25 (37%)
20	CLA	B	836	-	59,73,73	1.94	12 (20%)	67,113,113	2.87	17 (25%)
20	CLA	3	308	-	36,50,73	2.42	10 (27%)	39,85,113	4.23	20 (51%)
20	CLA	4	304	-	59,73,73	2.51	20 (33%)	67,113,113	4.08	29 (43%)
20	CLA	4	302	-	49,63,73	2.30	13 (26%)	55,101,113	3.57	18 (32%)
20	CLA	A	827	-	49,63,73	2.26	12 (24%)	55,101,113	3.43	20 (36%)
20	CLA	A	816	-	48,62,73	2.62	16 (33%)	53,99,113	3.83	22 (41%)
20	CLA	1	203	-	41,55,73	2.43	10 (24%)	45,91,113	4.23	19 (42%)
20	CLA	2	305	-	44,58,73	2.30	13 (29%)	49,95,113	3.73	20 (40%)
20	CLA	1	209	1	30,44,73	2.66	9 (30%)	35,78,113	3.98	13 (37%)
22	BCR	B	843	-	41,41,41	2.11	5 (12%)	56,56,56	5.92	21 (37%)
21	LMU	4	317	-	36,36,36	0.75	1 (2%)	47,47,47	1.15	3 (6%)
20	CLA	2	322	-	55,69,73	2.22	17 (30%)	62,108,113	3.53	28 (45%)
20	CLA	A	818	-	59,73,73	2.01	12 (20%)	67,113,113	3.11	25 (37%)
22	BCR	B	844	-	41,41,41	1.91	4 (9%)	56,56,56	5.05	24 (42%)
22	BCR	I	101	-	41,41,41	2.84	17 (41%)	56,56,56	5.37	31 (55%)
20	CLA	A	841	-	59,73,73	2.03	13 (22%)	67,113,113	3.61	21 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	F	206	-	47,61,73	2.69	16 (34%)	52,98,113	3.57	21 (40%)
21	LMU	1	217	-	36,36,36	0.38	0	47,47,47	0.70	1 (2%)
21	LMU	2	313	-	36,36,36	0.82	1 (2%)	47,47,47	0.91	2 (4%)
20	CLA	4	305	-	49,63,73	2.14	12 (24%)	55,101,113	3.23	20 (36%)
21	LMU	4	320	-	35,35,36	0.30	0	46,46,47	0.72	1 (2%)
20	CLA	B	811	-	52,66,73	2.67	18 (34%)	58,104,113	4.27	27 (46%)
20	CLA	3	310	-	22,32,73	2.27	9 (40%)	26,54,113	3.59	14 (53%)
20	CLA	B	814	-	40,54,73	2.46	11 (27%)	44,90,113	3.71	17 (38%)
22	BCR	A	847	-	41,41,41	2.06	5 (12%)	56,56,56	5.93	22 (39%)
21	LMU	N	101	-	36,36,36	0.55	1 (2%)	47,47,47	2.05	13 (27%)
20	CLA	2	310	-	22,32,73	1.89	5 (22%)	26,54,113	3.05	17 (65%)
20	CLA	4	306	-	44,58,73	2.71	15 (34%)	49,95,113	4.89	21 (42%)
21	LMU	4	322	-	36,36,36	0.75	1 (2%)	47,47,47	1.26	4 (8%)
22	BCR	F	203	-	41,41,41	3.03	14 (34%)	56,56,56	6.09	31 (55%)
22	BCR	A	845	-	41,41,41	2.00	5 (12%)	56,56,56	5.92	23 (41%)
20	CLA	A	812	-	48,62,73	2.16	10 (20%)	53,99,113	3.40	16 (30%)
21	LMU	L	205	-	36,36,36	0.80	2 (5%)	47,47,47	1.89	16 (34%)
21	LMU	H	107	-	36,36,36	0.77	0	47,47,47	2.24	14 (29%)
20	CLA	2	308	-	59,73,73	2.03	9 (15%)	67,113,113	3.04	23 (34%)
20	CLA	A	805	-	59,73,73	2.01	12 (20%)	67,113,113	3.04	21 (31%)
20	CLA	B	829	-	44,58,73	2.20	10 (22%)	49,95,113	3.44	20 (40%)
20	CLA	K	102	-	44,58,73	2.69	19 (43%)	49,95,113	4.06	22 (44%)
20	CLA	2	316	-	59,73,73	2.07	12 (20%)	67,113,113	3.89	21 (31%)
20	CLA	B	834	-	45,59,73	2.43	12 (26%)	50,96,113	3.88	19 (38%)
20	CLA	1	211	-	22,32,73	1.94	6 (27%)	26,54,113	3.28	17 (65%)
20	CLA	A	833	5	36,53,73	2.42	11 (30%)	39,89,113	4.73	21 (53%)
20	CLA	A	814	-	36,53,73	2.63	11 (30%)	39,89,113	3.80	16 (41%)
20	CLA	F	205	-	35,49,73	2.55	13 (37%)	38,84,113	4.05	18 (47%)
20	CLA	G	102	-	45,59,73	2.61	16 (35%)	50,96,113	4.15	20 (40%)
20	CLA	4	313	-	22,32,73	1.88	4 (18%)	26,54,113	3.18	18 (69%)
20	CLA	B	826	-	59,73,73	2.12	13 (22%)	67,113,113	3.29	22 (32%)
20	CLA	3	305	-	22,32,73	2.69	9 (40%)	26,54,113	3.50	16 (61%)
20	CLA	A	824	-	59,73,73	1.99	13 (22%)	67,113,113	3.22	19 (28%)
20	CLA	B	804	-	36,53,73	2.41	12 (33%)	39,89,113	3.81	16 (41%)
20	CLA	R	107	-	51,65,73	2.15	11 (21%)	57,103,113	3.85	22 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	812	-	59,73,73	2.10	11 (18%)	67,113,113	2.67	21 (31%)
20	CLA	3	306	-	22,32,73	1.94	7 (31%)	26,54,113	3.27	16 (61%)
20	CLA	B	818	-	44,58,73	2.27	12 (27%)	49,95,113	3.68	18 (36%)
21	LMU	L	204	-	36,36,36	0.69	2 (5%)	47,47,47	2.38	14 (29%)
21	LMU	R	101	-	36,36,36	1.04	2 (5%)	47,47,47	2.44	13 (27%)
20	CLA	B	820	-	49,63,73	2.28	13 (26%)	55,101,113	3.51	18 (32%)
20	CLA	4	308	-	30,44,73	2.70	13 (43%)	35,78,113	4.37	14 (40%)
20	CLA	A	825	-	59,73,73	2.01	13 (22%)	67,113,113	3.22	18 (26%)
20	CLA	B	807	-	59,73,73	2.18	11 (18%)	67,113,113	3.17	23 (34%)
20	CLA	A	838	-	59,73,73	2.10	10 (16%)	67,113,113	3.31	23 (34%)
20	CLA	4	314	-	30,44,73	2.60	9 (30%)	35,78,113	4.59	18 (51%)
20	CLA	A	837	-	41,55,73	2.59	12 (29%)	45,91,113	3.92	20 (44%)
20	CLA	1	201	-	40,54,73	2.76	17 (42%)	44,90,113	4.80	27 (61%)
20	CLA	B	850	-	59,73,73	2.02	13 (22%)	67,113,113	3.32	24 (35%)
24	SF4	C	103	7	0,12,12	0.00	-	-	-	-
20	CLA	1	208	-	22,32,73	3.08	11 (50%)	26,54,113	3.96	17 (65%)
20	CLA	2	307	-	59,73,73	2.39	19 (32%)	67,113,113	3.74	22 (32%)
22	BCR	B	845	-	41,41,41	2.16	5 (12%)	56,56,56	5.93	23 (41%)
20	CLA	A	801	-	40,54,73	2.59	13 (32%)	48,90,113	5.54	29 (60%)
21	LMU	B	801	-	36,36,36	0.67	0	47,47,47	2.44	16 (34%)
20	CLA	3	309	-	22,32,73	2.00	7 (31%)	26,54,113	2.94	16 (61%)
20	CLA	B	816	-	54,68,73	2.01	11 (20%)	61,107,113	3.69	22 (36%)
20	CLA	B	830	-	59,73,73	2.10	13 (22%)	67,113,113	3.37	23 (34%)
20	CLA	1	207	-	45,59,73	2.43	14 (31%)	50,96,113	4.08	25 (50%)
20	CLA	3	313	-	59,73,73	2.55	18 (30%)	67,113,113	4.36	25 (37%)
22	BCR	A	844	-	41,41,41	2.03	4 (9%)	56,56,56	5.93	20 (35%)
20	CLA	3	311	-	59,73,73	2.29	18 (30%)	67,113,113	4.53	24 (35%)
20	CLA	3	316	-	22,32,73	2.01	6 (27%)	26,54,113	3.24	15 (57%)
20	CLA	A	811	-	59,73,73	2.09	11 (18%)	67,113,113	3.05	24 (35%)
21	LMU	H	108	-	36,36,36	1.03	3 (8%)	47,47,47	2.76	19 (40%)
20	CLA	2	315	-	22,32,73	1.92	6 (27%)	26,54,113	2.82	14 (53%)
21	LMU	E	101	-	36,36,36	0.93	2 (5%)	47,47,47	3.05	25 (53%)
20	CLA	H	102	-	49,63,73	2.27	10 (20%)	55,101,113	3.86	23 (41%)
21	LMU	R	105	-	36,36,36	0.86	1 (2%)	47,47,47	1.64	11 (23%)
21	LMU	A	848	-	36,36,36	0.87	0	47,47,47	1.41	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	L	202	-	59,73,73	2.03	10 (16%)	67,113,113	2.66	21 (31%)
22	BCR	F	202	-	41,41,41	1.99	4 (9%)	56,56,56	5.89	20 (35%)
20	CLA	A	810	-	36,53,73	2.51	12 (33%)	39,89,113	4.25	19 (48%)
20	CLA	B	849	-	59,73,73	2.00	13 (22%)	67,113,113	3.37	25 (37%)
21	LMU	K	109	-	36,36,36	0.79	1 (2%)	47,47,47	2.27	12 (25%)
22	BCR	L	210	-	41,41,41	2.56	11 (26%)	56,56,56	5.71	20 (35%)
21	LMU	R	102	-	36,36,36	0.43	0	47,47,47	1.74	12 (25%)
21	LMU	K	104	-	36,36,36	0.67	1 (2%)	47,47,47	1.90	13 (27%)
20	CLA	3	302	-	44,58,73	3.14	14 (31%)	49,95,113	3.73	21 (42%)
20	CLA	4	311	-	49,63,73	2.26	9 (18%)	55,101,113	3.31	20 (36%)
20	CLA	B	805	-	54,68,73	2.11	10 (18%)	61,107,113	3.92	26 (42%)
21	LMU	1	219	-	36,36,36	1.02	2 (5%)	47,47,47	2.24	13 (27%)
21	LMU	B	802	-	36,36,36	1.02	4 (11%)	47,47,47	2.47	13 (27%)
22	BCR	J	102	-	41,41,41	1.93	4 (9%)	56,56,56	5.92	19 (33%)
20	CLA	A	850	-	59,73,73	2.12	12 (20%)	67,113,113	3.60	22 (32%)
20	CLA	K	103	-	59,73,73	2.05	10 (16%)	67,113,113	2.90	21 (31%)
21	LMU	H	106	-	36,36,36	1.05	4 (11%)	47,47,47	2.75	19 (40%)
20	CLA	J	101	-	42,56,73	2.44	13 (30%)	46,92,113	3.80	16 (34%)
21	LMU	3	322	-	36,36,36	0.71	0	47,47,47	1.91	11 (23%)
23	PQN	B	841	-	34,34,34	1.67	2 (5%)	42,45,45	1.60	6 (14%)
20	CLA	A	802	-	22,32,73	2.36	9 (40%)	26,54,113	3.99	14 (53%)
20	CLA	B	822	-	48,62,73	2.32	14 (29%)	53,99,113	2.87	24 (45%)
20	CLA	A	852	-	59,73,73	2.19	12 (20%)	67,113,113	3.33	21 (31%)
20	CLA	A	819	-	59,73,73	1.96	10 (16%)	67,113,113	3.28	21 (31%)
20	CLA	A	813	-	48,62,73	2.12	11 (22%)	53,99,113	3.49	22 (41%)
20	CLA	1	204	-	40,54,73	2.59	11 (27%)	44,90,113	2.67	18 (40%)
21	LMU	A	854	-	36,36,36	0.69	1 (2%)	47,47,47	1.89	11 (23%)
20	CLA	B	824	-	59,73,73	1.99	12 (20%)	67,113,113	3.15	18 (26%)
20	CLA	A	808	5	59,73,73	2.15	13 (22%)	67,113,113	3.35	25 (37%)
21	LMU	K	106	-	36,36,36	0.46	0	47,47,47	2.20	17 (36%)
20	CLA	A	803	-	44,58,73	2.38	13 (29%)	49,95,113	3.76	22 (44%)
20	CLA	B	821	-	59,73,73	2.92	21 (35%)	67,113,113	3.62	20 (29%)
20	CLA	B	833	20	36,53,73	2.52	10 (27%)	39,89,113	3.96	16 (41%)
20	CLA	3	318	-	59,73,73	1.92	11 (18%)	67,113,113	2.58	22 (32%)
21	LMU	H	104	-	36,36,36	1.13	4 (11%)	47,47,47	3.11	22 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	LMU	R	103	-	36,36,36	0.78	0	47,47,47	2.05	14 (29%)
20	CLA	1	205	-	22,32,73	2.26	10 (45%)	26,54,113	4.03	16 (61%)
20	CLA	4	315	-	22,32,73	1.84	5 (22%)	26,54,113	2.61	15 (57%)
20	CLA	B	815	-	53,67,73	2.09	12 (22%)	59,105,113	2.60	18 (30%)
20	CLA	2	306	-	22,32,73	2.06	10 (45%)	26,54,113	3.48	15 (57%)
20	CLA	2	311	2	44,58,73	2.31	10 (22%)	49,95,113	3.67	19 (38%)
22	BCR	I	103	-	41,41,41	2.82	11 (26%)	56,56,56	6.56	29 (51%)
20	CLA	A	832	-	44,58,73	2.30	11 (25%)	49,95,113	3.50	19 (38%)
20	CLA	A	817	-	46,60,73	2.35	12 (26%)	51,97,113	3.83	19 (37%)
20	CLA	R	108	-	52,66,73	2.70	16 (30%)	58,104,113	3.51	25 (43%)
20	CLA	1	215	-	55,69,73	2.24	16 (29%)	62,108,113	3.57	27 (43%)
20	CLA	2	304	-	22,32,73	2.48	11 (50%)	26,54,113	3.56	17 (65%)
20	CLA	H	101	-	49,63,73	2.54	17 (34%)	55,101,113	4.84	26 (47%)
20	CLA	A	821	5	36,50,73	2.45	10 (27%)	39,85,113	4.26	17 (43%)
20	CLA	A	839	-	59,73,73	2.47	16 (27%)	67,113,113	3.86	27 (40%)
20	CLA	3	317	-	44,58,73	2.36	10 (22%)	49,95,113	2.88	19 (38%)
21	LMU	R	104	-	36,36,36	0.77	1 (2%)	47,47,47	2.17	18 (38%)
20	CLA	3	320	-	22,32,73	1.87	5 (22%)	26,54,113	2.79	11 (42%)
21	LMU	A	849	-	36,36,36	0.86	1 (2%)	47,47,47	1.67	10 (21%)
20	CLA	B	817	-	55,69,73	2.02	12 (21%)	62,108,113	3.60	23 (37%)
20	CLA	4	319	-	41,55,73	2.35	12 (29%)	45,91,113	3.75	16 (35%)
20	CLA	L	209	-	44,58,73	2.47	14 (31%)	49,95,113	4.24	20 (40%)
20	CLA	B	823	-	52,66,73	2.19	12 (23%)	58,104,113	3.45	18 (31%)
24	SF4	A	857	5,6	0,12,12	0.00	-	-	-	-
20	CLA	B	827	-	59,73,73	2.02	13 (22%)	67,113,113	3.08	19 (28%)
24	SF4	C	102	7	0,12,12	0.00	-	-	-	-
21	LMU	4	321	-	36,36,36	0.95	1 (2%)	47,47,47	1.40	8 (17%)
20	CLA	I	102	-	54,68,73	2.08	10 (18%)	61,107,113	3.74	19 (31%)
21	LMU	3	321	-	36,36,36	0.40	0	47,47,47	0.71	1 (2%)
21	LMU	2	320	-	36,36,36	1.04	1 (2%)	47,47,47	1.37	3 (6%)
20	CLA	B	810	-	49,63,73	2.08	11 (22%)	55,101,113	3.52	21 (38%)
20	CLA	L	207	16	44,58,73	2.37	12 (27%)	49,95,113	3.74	20 (40%)
20	CLA	3	307	-	22,32,73	1.91	7 (31%)	26,54,113	3.27	17 (65%)
21	LMU	H	105	-	36,36,36	0.98	1 (2%)	47,47,47	2.33	16 (34%)
21	LMU	2	318	-	36,36,36	1.06	1 (2%)	47,47,47	1.93	15 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	1	216	-	22,32,73	2.27	11 (50%)	26,54,113	2.91	16 (61%)
20	CLA	4	307	-	46,60,73	3.13	22 (47%)	51,97,113	5.12	36 (70%)
21	LMU	1	218	-	36,36,36	0.44	0	47,47,47	1.61	9 (19%)
20	CLA	4	310	-	22,32,73	2.75	11 (50%)	26,54,113	3.05	14 (53%)
21	LMU	D	201	-	36,36,36	0.40	0	47,47,47	0.69	1 (2%)
21	LMU	1	213	-	36,36,36	0.81	0	47,47,47	2.10	16 (34%)
20	CLA	B	840	-	30,44,73	2.72	11 (36%)	35,78,113	4.39	19 (54%)
20	CLA	B	828	-	44,58,73	2.42	9 (20%)	49,95,113	3.42	23 (46%)
21	LMU	K	105	-	36,36,36	0.53	0	47,47,47	2.04	15 (31%)
20	CLA	A	804	-	49,63,73	2.34	11 (22%)	55,101,113	2.78	19 (34%)
20	CLA	A	836	-	41,55,73	2.34	11 (26%)	45,91,113	2.38	17 (37%)
20	CLA	A	822	-	49,63,73	2.24	11 (22%)	55,101,113	3.60	22 (40%)
20	CLA	1	210	-	45,59,73	3.09	19 (42%)	50,96,113	4.84	26 (52%)
20	CLA	K	108	-	44,58,73	2.31	13 (29%)	49,95,113	3.70	18 (36%)
21	LMU	L	211	-	36,36,36	0.87	1 (2%)	47,47,47	1.50	9 (19%)
21	LMU	B	847	-	36,36,36	1.00	1 (2%)	47,47,47	2.37	16 (34%)
22	BCR	B	846	-	41,41,41	2.10	4 (9%)	56,56,56	5.93	21 (37%)
20	CLA	B	809	-	48,62,73	2.43	10 (20%)	58,100,113	3.39	24 (41%)
20	CLA	A	829	-	44,58,73	2.27	10 (22%)	49,95,113	3.80	23 (46%)
20	CLA	A	834	-	43,57,73	2.40	11 (25%)	46,93,113	3.83	19 (41%)
20	CLA	A	820	-	45,59,73	2.34	12 (26%)	50,96,113	3.55	20 (40%)
20	CLA	B	831	-	44,58,73	2.43	14 (31%)	49,95,113	4.01	22 (44%)
20	CLA	B	803	-	59,73,73	2.15	13 (22%)	67,113,113	2.62	25 (37%)
20	CLA	B	808	6	59,73,73	1.94	11 (18%)	67,113,113	3.43	20 (29%)
21	LMU	2	317	-	36,36,36	0.39	0	47,47,47	0.71	1 (2%)
21	LMU	A	855	-	36,36,36	0.78	1 (2%)	47,47,47	1.95	17 (36%)
20	CLA	3	301	-	30,44,73	2.50	9 (30%)	35,78,113	4.52	19 (54%)
20	CLA	B	837	-	41,55,73	2.33	12 (29%)	45,91,113	3.65	18 (40%)
21	LMU	A	856	-	36,36,36	0.78	1 (2%)	47,47,47	1.59	8 (17%)
20	CLA	1	214	-	22,32,73	1.80	5 (22%)	26,54,113	3.10	17 (65%)
22	BCR	B	842	-	41,41,41	1.97	4 (9%)	56,56,56	5.89	20 (35%)
20	CLA	4	303	-	30,44,73	2.92	12 (40%)	35,78,113	4.79	18 (51%)
20	CLA	H	103	-	49,63,73	2.23	13 (26%)	55,101,113	3.63	20 (36%)
21	LMU	A	853	-	36,36,36	0.40	0	47,47,47	0.72	1 (2%)
20	CLA	K	101	-	36,53,73	2.56	12 (33%)	39,89,113	4.10	15 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	835	-	54,68,73	2.00	10 (18%)	61,107,113	3.57	16 (26%)
20	CLA	3	319	-	22,32,73	2.50	10 (45%)	26,54,113	3.64	16 (61%)
20	CLA	B	839	-	59,73,73	1.98	14 (23%)	67,113,113	2.96	21 (31%)
20	CLA	B	838	-	59,73,73	2.08	13 (22%)	67,113,113	3.00	24 (35%)
20	CLA	2	301	-	22,32,73	3.15	11 (50%)	26,54,113	3.74	17 (65%)
21	LMU	4	301	-	36,36,36	0.41	0	47,47,47	0.72	1 (2%)
20	CLA	1	202	-	51,65,73	2.46	18 (35%)	57,103,113	4.16	27 (47%)
25	LMG	B	848	-	49,49,55	0.96	2 (4%)	57,57,63	1.02	3 (5%)
21	LMU	G	101	-	36,36,36	1.02	2 (5%)	47,47,47	2.58	13 (27%)
20	CLA	1	206	-	55,69,73	2.15	11 (20%)	62,108,113	3.06	20 (32%)
20	CLA	A	807	-	40,54,73	2.92	19 (47%)	44,90,113	5.25	24 (54%)
20	CLA	B	832	20	36,53,73	2.72	11 (30%)	39,89,113	4.13	17 (43%)
20	CLA	B	813	-	54,68,73	2.10	12 (22%)	61,107,113	2.92	19 (31%)
21	LMU	C	101	-	36,36,36	0.85	1 (2%)	47,47,47	1.37	7 (14%)
20	CLA	A	830	-	59,73,73	2.05	13 (22%)	67,113,113	3.30	19 (28%)
20	CLA	3	304	-	30,44,73	2.55	9 (30%)	35,78,113	3.93	15 (42%)
23	PQN	A	842	-	34,34,34	1.73	3 (8%)	42,45,45	1.52	7 (16%)
20	CLA	A	831	-	49,63,73	2.14	11 (22%)	55,101,113	3.54	22 (40%)
20	CLA	A	815	-	44,58,73	3.02	21 (47%)	49,95,113	4.96	31 (63%)
20	CLA	A	840	-	44,58,73	2.30	10 (22%)	49,95,113	3.83	19 (38%)
20	CLA	2	309	-	22,32,73	1.98	6 (27%)	26,54,113	3.15	15 (57%)
20	CLA	4	309	-	22,32,73	3.09	13 (59%)	26,54,113	4.03	17 (65%)
20	CLA	A	826	-	59,73,73	2.00	11 (18%)	67,113,113	3.61	26 (38%)
22	BCR	A	846	-	41,41,41	2.08	4 (9%)	56,56,56	5.92	22 (39%)
21	LMU	R	106	-	36,36,36	0.88	1 (2%)	47,47,47	1.57	10 (21%)
20	CLA	4	312	-	22,32,73	1.93	6 (27%)	26,54,113	3.25	15 (57%)
22	BCR	3	314	-	41,41,41	2.06	5 (12%)	56,56,56	5.89	21 (37%)
20	CLA	F	204	-	30,44,73	2.56	8 (26%)	35,78,113	3.84	21 (60%)
20	CLA	3	312	-	22,32,73	2.86	9 (40%)	26,54,113	4.43	19 (73%)
21	LMU	1	220	-	36,36,36	0.59	1 (2%)	47,47,47	1.36	7 (14%)
20	CLA	H	109	-	54,68,73	2.09	12 (22%)	61,107,113	3.55	22 (36%)
20	CLA	1	212	-	22,32,73	2.44	9 (40%)	26,54,113	3.71	16 (61%)
20	CLA	L	203	-	49,63,73	2.32	10 (20%)	55,101,113	2.96	21 (38%)
21	LMU	R	109	-	36,36,36	0.37	0	47,47,47	0.70	1 (2%)
20	CLA	L	201	-	49,63,73	2.64	16 (32%)	55,101,113	4.50	24 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	819	-	40,54,73	2.38	9 (22%)	44,90,113	4.14	18 (40%)
20	CLA	2	302	-	45,59,73	2.31	12 (26%)	50,96,113	3.64	17 (34%)
20	CLA	A	823	-	59,73,73	1.87	10 (16%)	67,113,113	2.59	21 (31%)
20	CLA	A	828	-	59,73,73	1.99	12 (20%)	67,113,113	3.50	24 (35%)
20	CLA	2	312	-	44,58,73	2.42	10 (22%)	49,95,113	4.29	19 (38%)
20	CLA	L	208	-	41,55,73	2.34	9 (21%)	45,91,113	4.05	25 (55%)
20	CLA	4	318	-	46,60,73	2.83	16 (34%)	51,97,113	4.57	25 (49%)
22	BCR	A	843	-	41,41,41	1.93	4 (9%)	56,56,56	5.89	19 (33%)
21	LMU	F	201	-	35,35,36	1.30	4 (11%)	46,46,47	2.37	15 (32%)
21	LMU	2	319	-	36,36,36	1.01	1 (2%)	47,47,47	1.28	6 (12%)
20	CLA	A	806	-	49,63,73	2.22	11 (22%)	55,101,113	3.61	21 (38%)
20	CLA	A	835	-	59,73,73	2.10	12 (20%)	67,113,113	3.29	24 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	J	103	-	4/4/19/25	24/33/131/135	-
22	BCR	B	852	-	-	12/29/63/63	0/2/2/2
20	CLA	4	316	-	3/3/16/25	10/15/113/135	-
20	CLA	A	809	-	3/3/17/25	10/22/120/135	-
20	CLA	3	303	-	3/3/7/25	-	-
20	CLA	B	825	-	4/4/20/25	16/37/135/135	-
20	CLA	B	806	-	4/4/20/25	17/37/135/135	-
20	CLA	B	851	-	4/4/20/25	18/37/135/135	-
20	CLA	A	851	-	4/4/20/25	18/37/135/135	-
20	CLA	2	303	-	4/4/20/25	17/37/135/135	-
20	CLA	B	836	-	4/4/20/25	17/37/135/135	-
20	CLA	3	308	-	3/3/15/25	5/10/108/135	-
20	CLA	4	304	-	5/5/20/25	20/37/135/135	-
20	CLA	4	302	-	4/4/18/25	14/25/123/135	-
20	CLA	A	827	-	4/4/18/25	11/25/123/135	-
20	CLA	A	816	-	3/3/17/25	11/24/122/135	-
20	CLA	1	203	-	3/3/16/25	8/16/114/135	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	2	305	-	3/3/17/25	9/19/117/135	-
20	CLA	1	209	1	3/3/14/25	-	-
22	BCR	B	843	-	-	7/29/63/63	0/2/2/2
21	LMU	4	317	-	-	13/21/61/61	0/2/2/2
20	CLA	2	322	-	4/4/19/25	21/33/131/135	-
20	CLA	A	818	-	4/4/20/25	18/37/135/135	-
22	BCR	B	844	-	-	11/29/63/63	0/2/2/2
22	BCR	I	101	-	-	7/29/63/63	0/2/2/2
20	CLA	A	841	-	4/4/20/25	16/37/135/135	-
20	CLA	F	206	-	6/6/17/25	9/23/121/135	-
21	LMU	1	217	-	-	14/21/61/61	0/2/2/2
21	LMU	2	313	-	-	16/21/61/61	0/2/2/2
20	CLA	4	305	-	4/4/18/25	12/25/123/135	-
21	LMU	4	320	-	-	15/20/60/61	0/2/2/2
20	CLA	B	811	-	4/4/18/25	17/29/127/135	-
20	CLA	3	310	-	3/3/7/25	-	-
21	LMU	A	848	-	-	16/21/61/61	0/2/2/2
20	CLA	B	814	-	3/3/16/25	9/15/113/135	-
22	BCR	A	847	-	-	10/29/63/63	0/2/2/2
21	LMU	N	101	-	-	15/21/61/61	0/2/2/2
20	CLA	2	310	-	3/3/7/25	-	-
20	CLA	4	306	-	3/3/17/25	9/19/117/135	-
21	LMU	4	322	-	-	14/21/61/61	0/2/2/2
22	BCR	F	203	-	-	12/29/63/63	0/2/2/2
22	BCR	A	845	-	-	14/29/63/63	0/2/2/2
20	CLA	A	812	-	3/3/17/25	13/24/122/135	-
21	LMU	L	205	-	-	14/21/61/61	0/2/2/2
21	LMU	H	107	-	-	12/21/61/61	0/2/2/2
20	CLA	2	308	-	4/4/20/25	15/37/135/135	-
20	CLA	A	805	-	4/4/20/25	23/37/135/135	-
20	CLA	B	829	-	3/3/17/25	12/19/117/135	-
20	CLA	K	102	-	3/3/17/25	9/19/117/135	-
21	LMU	L	204	-	-	14/21/61/61	0/2/2/2
20	CLA	2	316	-	4/4/20/25	17/37/135/135	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	834	-	3/3/17/25	9/21/119/135	-
20	CLA	1	211	-	3/3/7/25	-	-
20	CLA	A	833	5	3/3/16/25	5/11/111/135	-
20	CLA	A	814	-	3/3/16/25	7/11/111/135	-
20	CLA	F	205	-	3/3/15/25	5/8/106/135	-
20	CLA	G	102	-	3/3/17/25	8/21/119/135	-
20	CLA	4	313	-	3/3/7/25	-	-
20	CLA	B	826	-	4/4/20/25	17/37/135/135	-
20	CLA	3	305	-	3/3/7/25	-	-
20	CLA	A	824	-	4/4/20/25	17/37/135/135	-
20	CLA	B	804	-	3/3/16/25	6/11/111/135	-
20	CLA	R	107	-	4/4/18/25	13/28/126/135	-
20	CLA	B	812	-	4/4/20/25	24/37/135/135	-
20	CLA	3	306	-	3/3/7/25	-	-
20	CLA	B	818	-	3/3/17/25	6/19/117/135	-
20	CLA	2	306	-	3/3/7/25	-	-
21	LMU	R	101	-	1/1/10/10	11/21/61/61	0/2/2/2
21	LMU	K	105	-	-	18/21/61/61	0/2/2/2
20	CLA	B	820	-	4/4/18/25	9/25/123/135	-
20	CLA	4	308	-	3/3/14/25	-	-
20	CLA	A	825	-	4/4/20/25	22/37/135/135	-
20	CLA	B	807	-	4/4/20/25	9/37/135/135	-
20	CLA	A	838	-	4/4/20/25	19/37/135/135	-
20	CLA	4	314	-	3/3/14/25	-	-
21	LMU	A	853	-	-	19/21/61/61	0/2/2/2
20	CLA	A	837	-	3/3/16/25	11/16/114/135	-
20	CLA	1	201	-	3/3/16/25	10/15/113/135	-
20	CLA	B	850	-	4/4/20/25	15/37/135/135	-
24	SF4	C	103	7	-	-	0/6/5/5
20	CLA	1	208	-	3/3/7/25	-	-
20	CLA	2	307	-	4/4/20/25	20/37/135/135	-
22	BCR	B	845	-	-	14/29/63/63	0/2/2/2
20	CLA	A	801	-	5/5/16/25	12/16/112/135	-
21	LMU	B	801	-	-	16/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	3	309	-	3/3/7/25	-	-
20	CLA	B	816	-	4/4/19/25	13/31/129/135	-
20	CLA	B	830	-	4/4/20/25	21/37/135/135	-
20	CLA	1	207	-	4/4/17/25	9/21/119/135	-
20	CLA	3	313	-	4/4/20/25	18/37/135/135	-
22	BCR	A	844	-	-	12/29/63/63	0/2/2/2
20	CLA	3	316	-	3/3/7/25	-	-
20	CLA	A	811	-	4/4/20/25	25/37/135/135	-
21	LMU	H	108	-	-	14/21/61/61	0/2/2/2
21	LMU	B	802	-	-	11/21/61/61	0/2/2/2
20	CLA	2	315	-	3/3/7/25	-	-
21	LMU	E	101	-	-	14/21/61/61	0/2/2/2
21	LMU	3	322	-	-	15/21/61/61	0/2/2/2
20	CLA	L	202	-	4/4/20/25	15/37/135/135	-
21	LMU	R	105	-	-	15/21/61/61	0/2/2/2
20	CLA	4	319	-	3/3/16/25	9/16/114/135	-
20	CLA	B	815	-	4/4/18/25	12/30/128/135	-
22	BCR	F	202	-	-	12/29/63/63	0/2/2/2
20	CLA	A	810	-	3/3/16/25	3/11/111/135	-
20	CLA	B	849	-	4/4/20/25	21/37/135/135	-
21	LMU	K	109	-	-	12/21/61/61	0/2/2/2
22	BCR	L	210	-	-	10/29/63/63	0/2/2/2
21	LMU	R	102	-	-	11/21/61/61	0/2/2/2
21	LMU	K	104	-	-	12/21/61/61	0/2/2/2
20	CLA	3	302	-	3/3/17/25	3/19/117/135	-
20	CLA	4	311	-	4/4/18/25	13/25/123/135	-
20	CLA	B	805	-	4/4/19/25	21/31/129/135	-
20	CLA	A	822	-	4/4/18/25	9/25/123/135	-
20	CLA	1	214	-	3/3/7/25	-	-
22	BCR	J	102	-	-	12/29/63/63	0/2/2/2
20	CLA	A	850	-	4/4/20/25	25/37/135/135	-
20	CLA	K	103	-	4/4/20/25	21/37/135/135	-
21	LMU	H	106	-	-	13/21/61/61	0/2/2/2
20	CLA	J	101	-	3/3/16/25	10/17/115/135	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	838	-	4/4/20/25	20/37/135/135	-
23	PQN	B	841	-	1/1/8/9	10/23/43/43	0/2/2/2
20	CLA	A	802	-	3/3/7/25	-	-
20	CLA	B	822	-	3/3/17/25	8/24/122/135	-
20	CLA	A	852	-	4/4/20/25	24/37/135/135	-
20	CLA	A	819	-	4/4/20/25	16/37/135/135	-
20	CLA	A	813	-	3/3/17/25	11/24/122/135	-
20	CLA	1	204	-	3/3/16/25	6/15/113/135	-
21	LMU	A	854	-	-	11/21/61/61	0/2/2/2
20	CLA	B	824	-	4/4/20/25	21/37/135/135	-
20	CLA	A	808	5	4/4/20/25	21/37/135/135	-
21	LMU	K	106	-	-	15/21/61/61	0/2/2/2
20	CLA	A	803	-	3/3/17/25	5/19/117/135	-
20	CLA	B	821	-	3/3/20/25	19/37/135/135	-
20	CLA	B	833	20	3/3/16/25	6/11/111/135	-
20	CLA	3	318	-	4/4/20/25	19/37/135/135	-
21	LMU	H	104	-	-	14/21/61/61	0/2/2/2
21	LMU	R	103	-	-	13/21/61/61	0/2/2/2
20	CLA	1	205	-	3/3/7/25	-	-
20	CLA	4	315	-	3/3/7/25	-	-
20	CLA	3	311	-	4/4/20/25	22/37/135/135	-
21	LMU	R	106	-	-	13/21/61/61	0/2/2/2
20	CLA	2	311	2	3/3/17/25	6/19/117/135	-
22	BCR	I	103	-	-	13/29/63/63	0/2/2/2
20	CLA	A	832	-	3/3/17/25	12/19/117/135	-
20	CLA	A	817	-	3/3/17/25	14/22/120/135	-
20	CLA	R	108	-	4/4/18/25	17/29/127/135	-
20	CLA	2	304	-	3/3/7/25	-	-
20	CLA	H	101	-	4/4/18/25	16/25/123/135	-
20	CLA	A	821	5	3/3/15/25	2/10/108/135	-
20	CLA	A	839	-	4/4/20/25	22/37/135/135	-
20	CLA	3	317	-	3/3/17/25	9/19/117/135	-
21	LMU	R	104	-	-	17/21/61/61	0/2/2/2
20	CLA	3	320	-	3/3/7/25	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMU	A	849	-	-	13/21/61/61	0/2/2/2
20	CLA	B	817	-	4/4/19/25	17/33/131/135	-
20	CLA	L	209	-	4/4/17/25	10/19/117/135	-
24	SF4	A	857	5,6	-	-	0/6/5/5
20	CLA	B	827	-	4/4/20/25	27/37/135/135	-
24	SF4	C	102	7	-	-	0/6/5/5
21	LMU	4	321	-	-	15/21/61/61	0/2/2/2
20	CLA	I	102	-	4/4/19/25	13/31/129/135	-
21	LMU	3	321	-	-	11/21/61/61	0/2/2/2
21	LMU	2	320	-	-	8/21/61/61	0/2/2/2
20	CLA	B	810	-	4/4/18/25	12/25/123/135	-
20	CLA	L	207	16	3/3/17/25	8/19/117/135	-
20	CLA	3	307	-	3/3/7/25	-	-
21	LMU	H	105	-	-	17/21/61/61	0/2/2/2
21	LMU	2	318	-	-	13/21/61/61	0/2/2/2
20	CLA	1	216	-	3/3/7/25	-	-
20	CLA	4	307	-	4/4/17/25	7/22/120/135	-
21	LMU	1	218	-	-	10/21/61/61	0/2/2/2
20	CLA	4	310	-	3/3/7/25	-	-
21	LMU	D	201	-	-	14/21/61/61	0/2/2/2
21	LMU	1	213	-	-	13/21/61/61	0/2/2/2
20	CLA	B	840	-	3/3/14/25	-	-
20	CLA	B	828	-	3/3/17/25	9/19/117/135	-
20	CLA	B	823	-	4/4/18/25	17/29/127/135	-
20	CLA	A	804	-	4/4/18/25	13/25/123/135	-
20	CLA	A	836	-	3/3/16/25	8/16/114/135	-
20	CLA	1	215	-	4/4/19/25	21/33/131/135	-
20	CLA	1	210	-	4/4/17/25	9/21/119/135	-
20	CLA	K	108	-	3/3/17/25	5/19/117/135	-
21	LMU	L	211	-	-	14/21/61/61	0/2/2/2
21	LMU	B	847	-	-	10/21/61/61	0/2/2/2
22	BCR	B	846	-	-	12/29/63/63	0/2/2/2
20	CLA	B	809	-	4/4/18/25	11/25/121/135	-
20	CLA	A	829	-	3/3/17/25	3/19/117/135	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	834	-	3/3/16/25	9/18/116/135	-
20	CLA	A	820	-	3/3/17/25	9/21/119/135	-
20	CLA	B	831	-	3/3/17/25	6/19/117/135	-
20	CLA	B	803	-	4/4/20/25	21/37/135/135	-
20	CLA	B	808	6	4/4/20/25	19/37/135/135	-
21	LMU	2	317	-	-	14/21/61/61	0/2/2/2
21	LMU	A	855	-	-	14/21/61/61	0/2/2/2
20	CLA	3	301	-	3/3/14/25	-	-
20	CLA	B	837	-	3/3/16/25	6/16/114/135	-
21	LMU	A	856	-	-	14/21/61/61	0/2/2/2
22	BCR	B	842	-	-	13/29/63/63	0/2/2/2
20	CLA	4	303	-	3/3/14/25	-	-
20	CLA	H	103	-	4/4/18/25	14/25/123/135	-
21	LMU	1	219	-	-	13/21/61/61	0/2/2/2
20	CLA	K	101	-	3/3/16/25	5/11/111/135	-
20	CLA	B	835	-	4/4/19/25	15/31/129/135	-
20	CLA	3	319	-	3/3/7/25	-	-
20	CLA	B	839	-	4/4/20/25	18/37/135/135	-
20	CLA	2	301	-	3/3/7/25	-	-
21	LMU	4	301	-	-	13/21/61/61	0/2/2/2
20	CLA	1	202	-	4/4/18/25	16/28/126/135	-
25	LMG	B	848	-	-	23/44/64/70	0/1/1/1
21	LMU	G	101	-	-	15/21/61/61	0/2/2/2
20	CLA	1	206	-	4/4/19/25	20/33/131/135	-
20	CLA	A	807	-	3/3/16/25	6/15/113/135	-
20	CLA	B	832	20	3/3/16/25	9/11/111/135	-
20	CLA	B	813	-	4/4/19/25	14/31/129/135	-
21	LMU	C	101	-	-	14/21/61/61	0/2/2/2
20	CLA	A	830	-	4/4/20/25	21/37/135/135	-
20	CLA	3	304	-	3/3/14/25	-	-
23	PQN	A	842	-	1/1/8/9	11/23/43/43	0/2/2/2
20	CLA	A	831	-	4/4/18/25	14/25/123/135	-
20	CLA	A	815	-	3/3/17/25	8/19/117/135	-
20	CLA	A	840	-	3/3/17/25	11/19/117/135	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	2	309	-	3/3/7/25	-	-
20	CLA	4	309	-	3/3/7/25	-	-
20	CLA	A	826	-	4/4/20/25	16/37/135/135	-
22	BCR	A	846	-	-	17/29/63/63	0/2/2/2
20	CLA	4	312	-	3/3/7/25	-	-
22	BCR	3	314	-	-	13/29/63/63	0/2/2/2
20	CLA	F	204	-	3/3/14/25	-	-
20	CLA	3	312	-	3/3/7/25	-	-
21	LMU	1	220	-	-	13/21/61/61	0/2/2/2
20	CLA	H	109	-	4/4/19/25	13/31/129/135	-
20	CLA	1	212	-	3/3/7/25	-	-
20	CLA	L	203	-	4/4/18/25	7/25/123/135	-
21	LMU	R	109	-	-	16/21/61/61	0/2/2/2
20	CLA	L	201	-	5/5/18/25	12/25/123/135	-
20	CLA	B	819	-	3/3/16/25	13/15/113/135	-
20	CLA	2	302	-	3/3/17/25	11/21/119/135	-
20	CLA	A	823	-	4/4/20/25	20/37/135/135	-
20	CLA	A	828	-	4/4/20/25	18/37/135/135	-
20	CLA	2	312	-	3/3/17/25	11/19/117/135	-
20	CLA	H	102	-	4/4/18/25	9/25/123/135	-
20	CLA	L	208	-	3/3/16/25	9/16/114/135	-
20	CLA	4	318	-	3/3/17/25	12/22/120/135	-
22	BCR	A	843	-	-	11/29/63/63	0/2/2/2
21	LMU	F	201	-	-	14/20/60/61	0/2/2/2
21	LMU	2	319	-	-	13/21/61/61	0/2/2/2
20	CLA	A	806	-	4/4/18/25	7/25/123/135	-
20	CLA	A	835	-	4/4/20/25	17/37/135/135	-

The worst 5 of 2242 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	852	BCR	C21-C22	-11.54	1.20	1.35
22	I	101	BCR	C21-C22	-10.73	1.21	1.35
22	F	203	BCR	C21-C22	-10.22	1.22	1.35
22	B	852	BCR	C20-C21	-10.12	1.12	1.43
20	F	206	CLA	C3B-CAB	-9.63	1.28	1.47

The worst 5 of 4484 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	102	BCR	C20-C21-C22	36.89	179.96	127.31
22	A	846	BCR	C20-C21-C22	36.89	179.96	127.31
22	B	846	BCR	C20-C21-C22	36.87	179.93	127.31
22	A	845	BCR	C20-C21-C22	36.86	179.91	127.31
22	A	844	BCR	C20-C21-C22	36.84	179.89	127.31

5 of 610 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	J	103	CLA	C8
20	J	103	CLA	NC
20	J	103	CLA	ND
20	J	103	CLA	NA
20	4	316	CLA	NC

5 of 2773 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	J	103	CLA	C3A-C2A-CAA-CBA
20	J	103	CLA	C2A-CAA-CBA-CGA
20	J	103	CLA	CHA-CBD-CGD-O1D
20	J	103	CLA	CHA-CBD-CGD-O2D
20	J	103	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

227 monomers are involved in 3721 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	J	103	CLA	28	0
22	B	852	BCR	13	0
20	4	316	CLA	6	0
20	A	809	CLA	26	0
20	B	825	CLA	25	0
20	B	806	CLA	20	0
20	B	851	CLA	51	0
20	A	851	CLA	36	0
20	2	303	CLA	13	0
20	B	836	CLA	44	0
20	3	308	CLA	2	0
20	4	304	CLA	24	0
20	4	302	CLA	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	827	CLA	21	0
20	A	816	CLA	36	0
20	1	203	CLA	13	0
20	2	305	CLA	13	0
20	1	209	CLA	11	0
22	B	843	BCR	17	0
21	4	317	LMU	4	0
20	2	322	CLA	35	0
20	A	818	CLA	29	0
22	B	844	BCR	20	0
22	I	101	BCR	19	0
20	A	841	CLA	30	0
20	F	206	CLA	15	0
21	1	217	LMU	10	0
21	2	313	LMU	3	1
20	4	305	CLA	20	0
21	4	320	LMU	9	5
20	B	811	CLA	29	0
20	3	310	CLA	7	0
20	B	814	CLA	24	0
22	A	847	BCR	63	0
21	N	101	LMU	36	0
20	4	306	CLA	9	0
21	4	322	LMU	1	0
22	F	203	BCR	45	0
22	A	845	BCR	45	0
20	A	812	CLA	4	0
21	L	205	LMU	4	0
21	H	107	LMU	11	0
20	2	308	CLA	9	0
20	A	805	CLA	28	0
20	B	829	CLA	13	0
20	K	102	CLA	11	0
20	2	316	CLA	6	0
20	B	834	CLA	4	0
20	1	211	CLA	5	0
20	A	833	CLA	18	1
20	A	814	CLA	35	0
20	F	205	CLA	15	0
20	G	102	CLA	20	0
20	4	313	CLA	5	0
20	B	826	CLA	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	3	305	CLA	1	0
20	A	824	CLA	86	0
20	B	804	CLA	9	0
20	R	107	CLA	10	0
20	B	812	CLA	20	0
20	3	306	CLA	3	0
20	B	818	CLA	9	0
21	L	204	LMU	3	0
21	R	101	LMU	6	0
20	B	820	CLA	15	0
20	A	825	CLA	79	0
20	B	807	CLA	23	0
20	A	838	CLA	42	0
20	4	314	CLA	7	0
20	A	837	CLA	18	0
20	1	201	CLA	13	0
20	B	850	CLA	41	0
24	C	103	SF4	4	0
20	2	307	CLA	18	0
22	B	845	BCR	32	0
20	A	801	CLA	9	0
21	B	801	LMU	13	0
20	3	309	CLA	5	0
20	B	816	CLA	15	0
20	B	830	CLA	29	0
20	1	207	CLA	6	1
20	3	313	CLA	25	0
22	A	844	BCR	24	0
20	3	311	CLA	20	0
20	A	811	CLA	22	0
21	H	108	LMU	38	0
21	E	101	LMU	30	0
20	H	102	CLA	15	0
21	A	848	LMU	3	0
20	L	202	CLA	26	0
22	F	202	BCR	31	0
20	A	810	CLA	4	0
20	B	849	CLA	22	0
21	K	109	LMU	6	0
22	L	210	BCR	51	0
21	R	102	LMU	20	0
21	K	104	LMU	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	3	302	CLA	28	0
20	4	311	CLA	17	0
20	B	805	CLA	19	0
21	1	219	LMU	20	0
21	B	802	LMU	4	0
22	J	102	BCR	41	0
20	A	850	CLA	20	0
20	K	103	CLA	3	0
21	H	106	LMU	29	0
20	J	101	CLA	27	0
21	3	322	LMU	8	0
23	B	841	PQN	32	0
20	B	822	CLA	25	0
20	A	852	CLA	27	0
20	A	819	CLA	45	0
20	A	813	CLA	20	0
20	1	204	CLA	5	0
21	A	854	LMU	42	0
20	B	824	CLA	50	0
20	A	808	CLA	26	0
21	K	106	LMU	47	0
20	A	803	CLA	14	0
20	B	821	CLA	39	0
20	B	833	CLA	23	0
20	3	318	CLA	17	0
21	H	104	LMU	21	0
21	R	103	LMU	25	0
20	4	315	CLA	3	0
20	B	815	CLA	24	0
20	2	311	CLA	18	0
22	I	103	BCR	46	0
20	A	832	CLA	16	0
20	A	817	CLA	12	0
20	R	108	CLA	12	0
20	1	215	CLA	52	0
20	2	304	CLA	5	0
20	H	101	CLA	31	0
20	A	821	CLA	10	0
20	A	839	CLA	42	0
20	3	317	CLA	3	0
21	R	104	LMU	11	0
21	A	849	LMU	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	817	CLA	19	0
20	4	319	CLA	11	0
20	L	209	CLA	13	0
20	B	823	CLA	62	0
24	A	857	SF4	19	0
20	B	827	CLA	32	0
24	C	102	SF4	4	0
21	4	321	LMU	2	0
20	I	102	CLA	12	0
21	3	321	LMU	4	0
21	2	320	LMU	0	2
20	B	810	CLA	17	0
20	L	207	CLA	9	0
20	3	307	CLA	16	0
21	H	105	LMU	12	0
21	2	318	LMU	6	0
20	4	307	CLA	15	0
21	1	218	LMU	8	0
20	4	310	CLA	3	0
21	D	201	LMU	12	0
21	1	213	LMU	8	0
20	B	840	CLA	2	0
20	B	828	CLA	11	0
21	K	105	LMU	35	0
20	A	804	CLA	28	0
20	A	836	CLA	19	0
20	A	822	CLA	34	0
20	1	210	CLA	9	0
20	K	108	CLA	25	0
21	L	211	LMU	3	0
21	B	847	LMU	28	30
22	B	846	BCR	52	0
20	B	809	CLA	6	0
20	A	829	CLA	11	0
20	A	834	CLA	10	0
20	A	820	CLA	17	0
20	B	831	CLA	16	0
20	B	803	CLA	28	0
20	B	808	CLA	21	0
21	2	317	LMU	12	0
21	A	855	LMU	27	0
20	3	301	CLA	1	0

Continued on next page...

Continued from previous page...

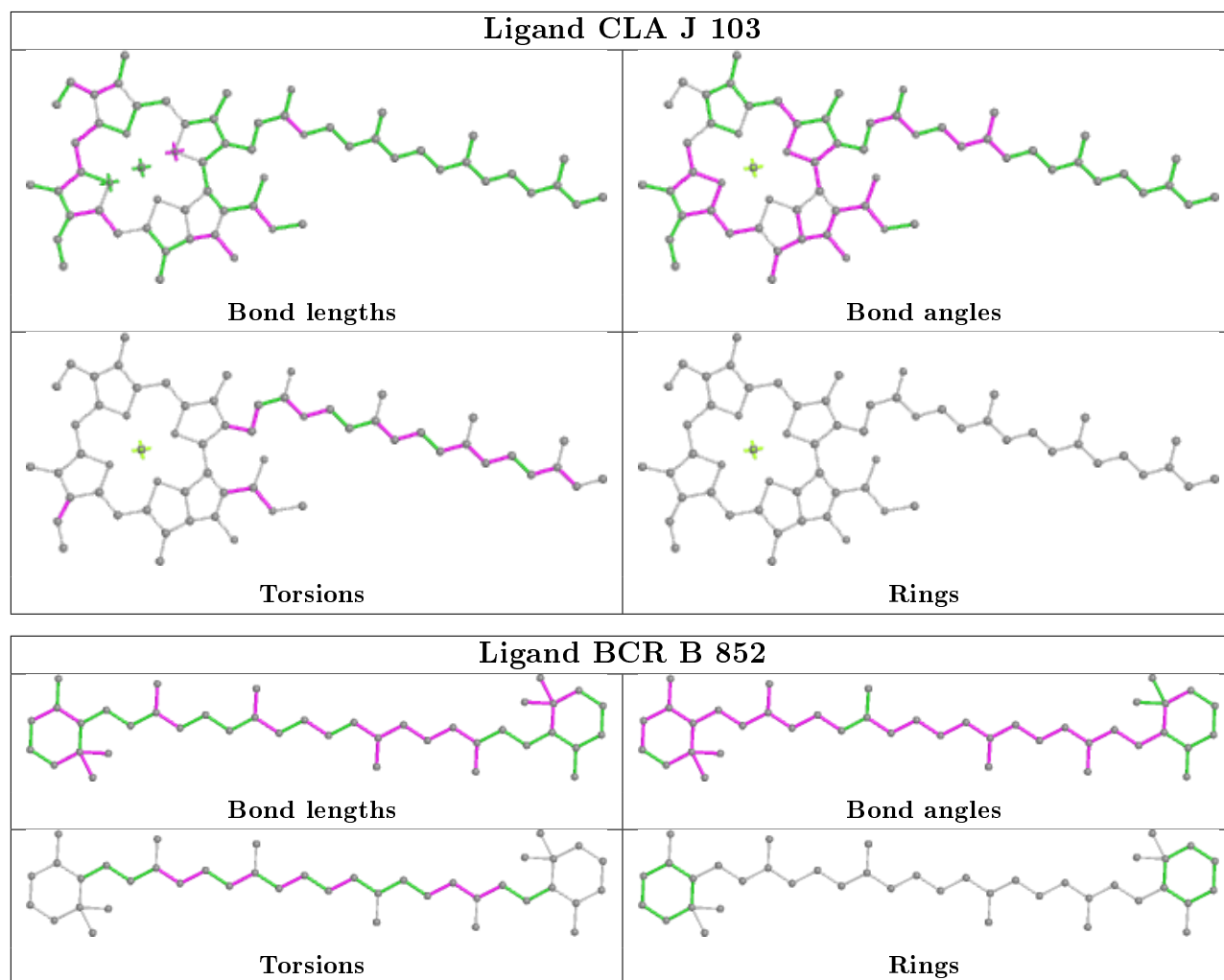
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	837	CLA	25	0
22	B	842	BCR	10	0
20	4	303	CLA	6	0
20	H	103	CLA	3	0
21	A	853	LMU	8	0
20	K	101	CLA	19	1
20	B	835	CLA	16	0
20	B	839	CLA	26	0
20	B	838	CLA	28	0
21	4	301	LMU	7	0
20	1	202	CLA	40	0
25	B	848	LMG	30	0
21	G	101	LMU	19	0
20	1	206	CLA	16	0
20	A	807	CLA	29	0
20	B	832	CLA	22	0
20	B	813	CLA	13	0
20	A	830	CLA	38	0
20	3	304	CLA	14	0
23	A	842	PQN	15	0
20	A	831	CLA	16	0
20	A	815	CLA	44	0
20	A	840	CLA	8	0
20	4	309	CLA	1	0
20	A	826	CLA	63	0
22	A	846	BCR	37	0
21	R	106	LMU	2	0
20	4	312	CLA	4	0
22	3	314	BCR	19	28
20	F	204	CLA	1	0
20	H	109	CLA	17	0
20	L	203	CLA	17	0
21	R	109	LMU	20	5
20	L	201	CLA	35	0
20	B	819	CLA	21	0
20	2	302	CLA	17	0
20	A	823	CLA	18	0
20	A	828	CLA	17	0
20	2	312	CLA	10	0
20	L	208	CLA	22	0
20	4	318	CLA	19	0
22	A	843	BCR	45	0

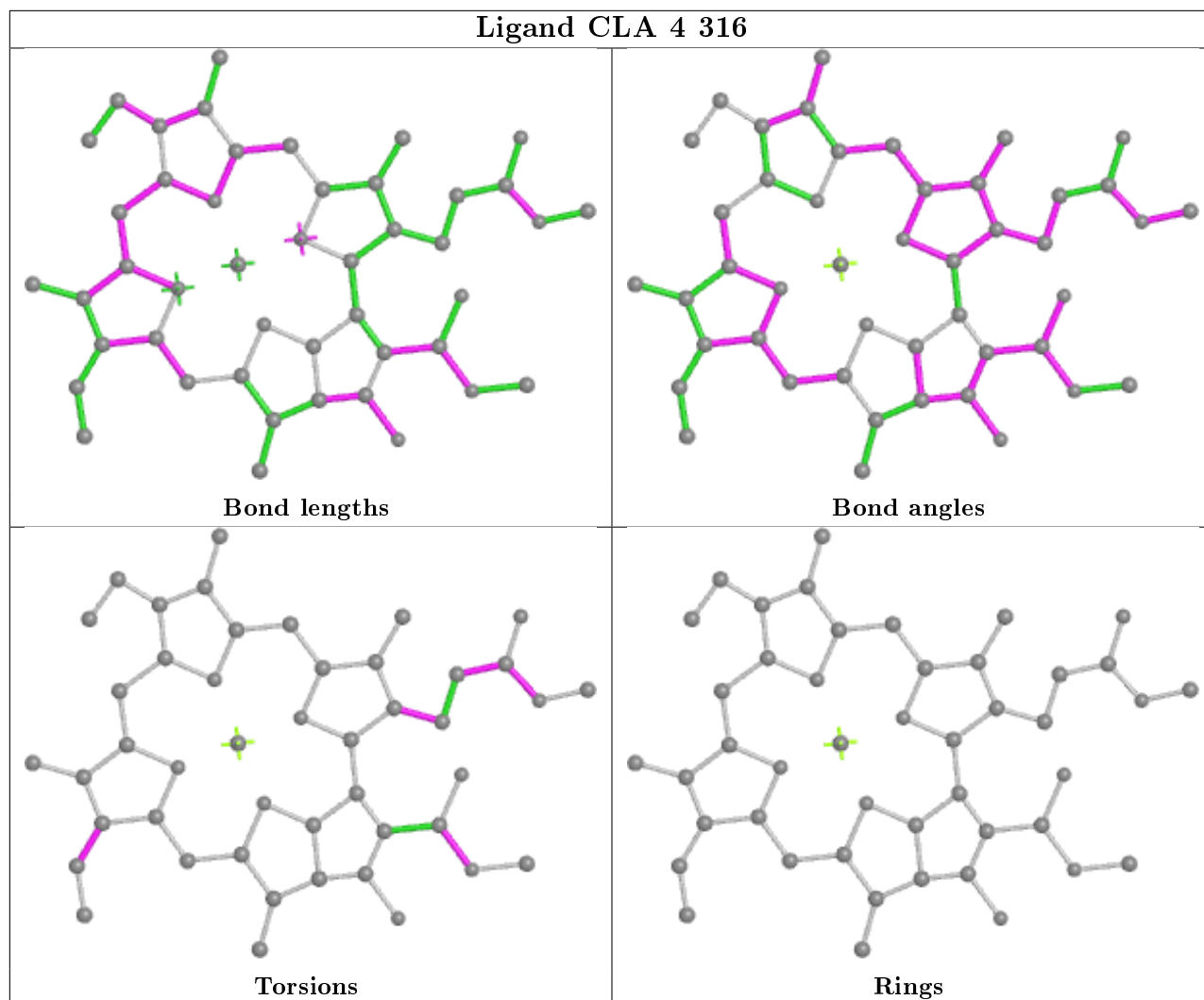
Continued on next page...

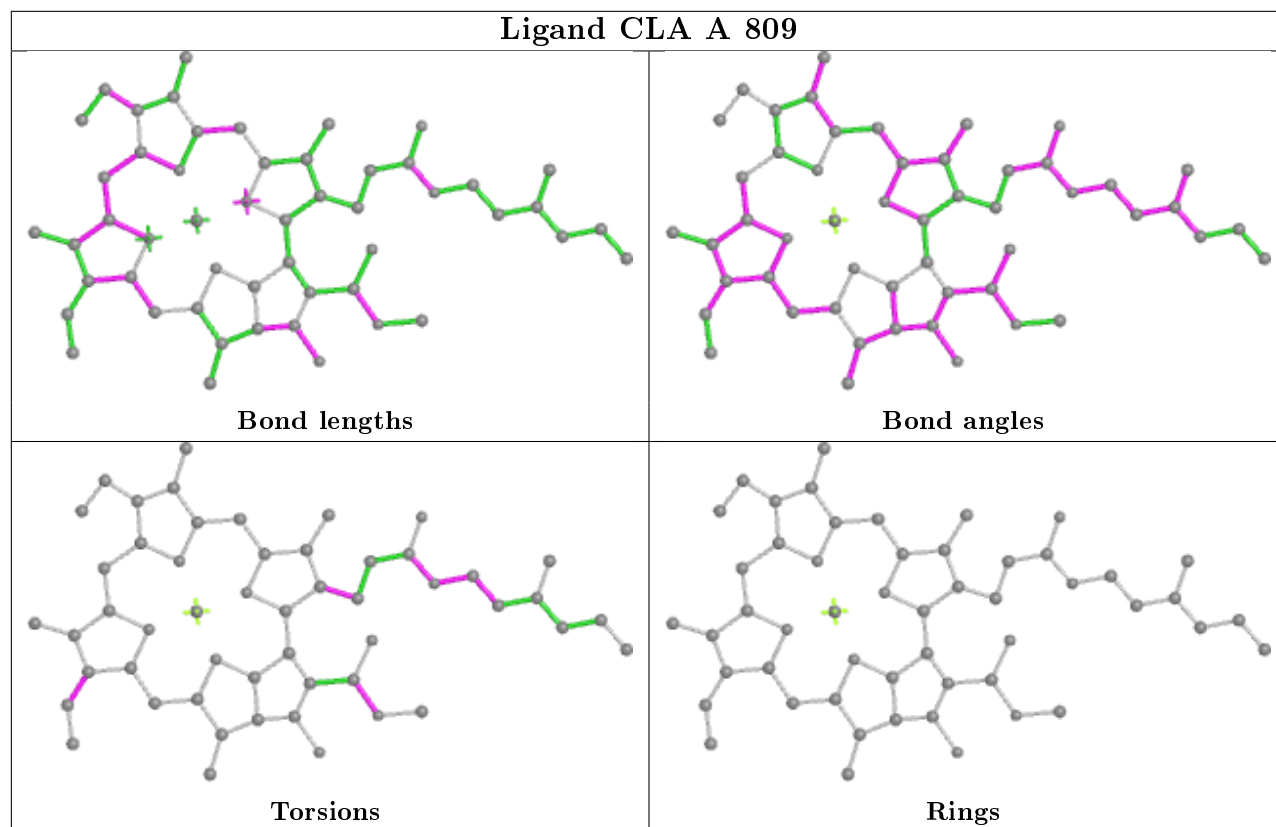
Continued from previous page...

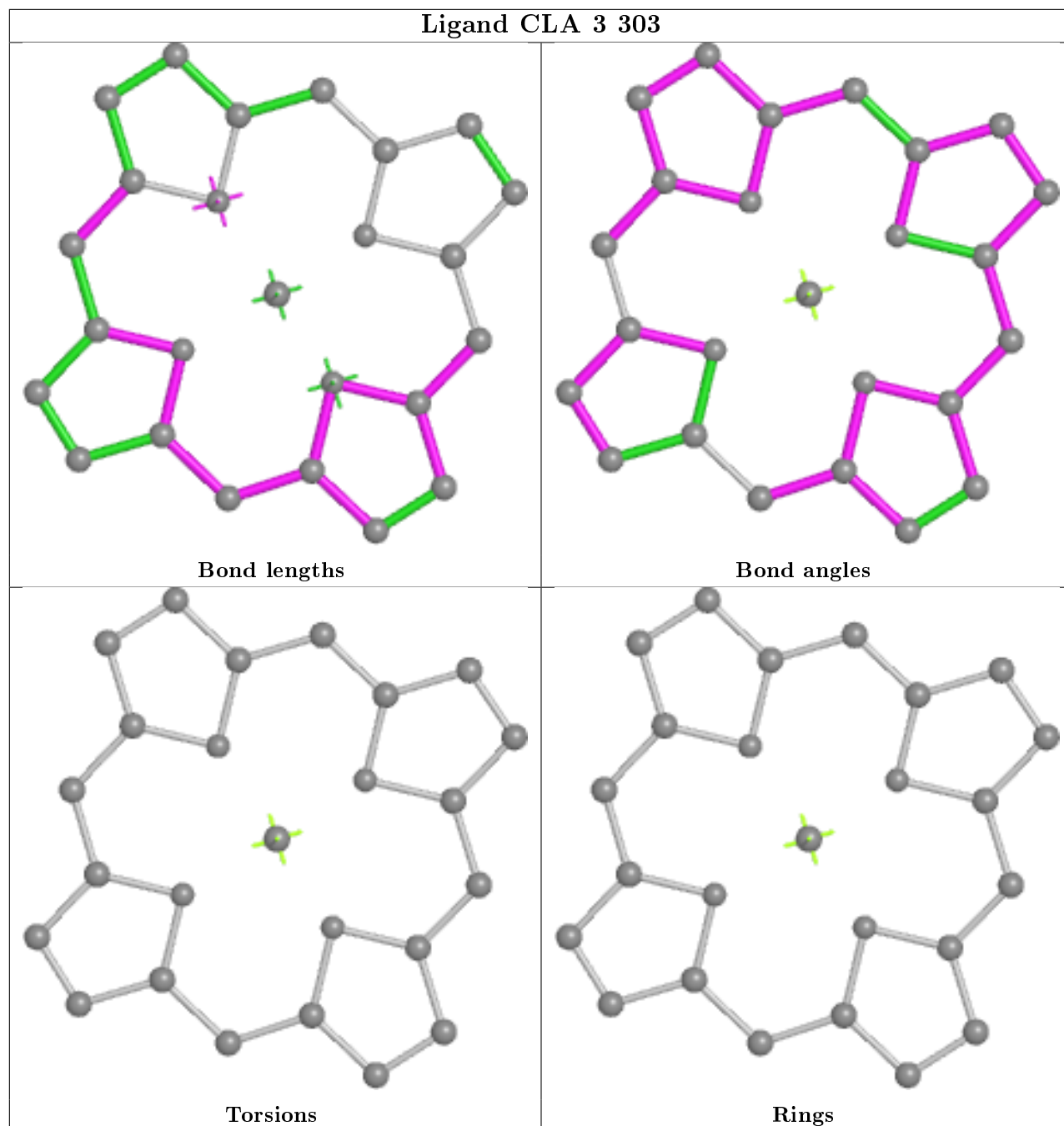
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	F	201	LMU	19	0
21	2	319	LMU	4	0
20	A	806	CLA	21	0
20	A	835	CLA	19	0

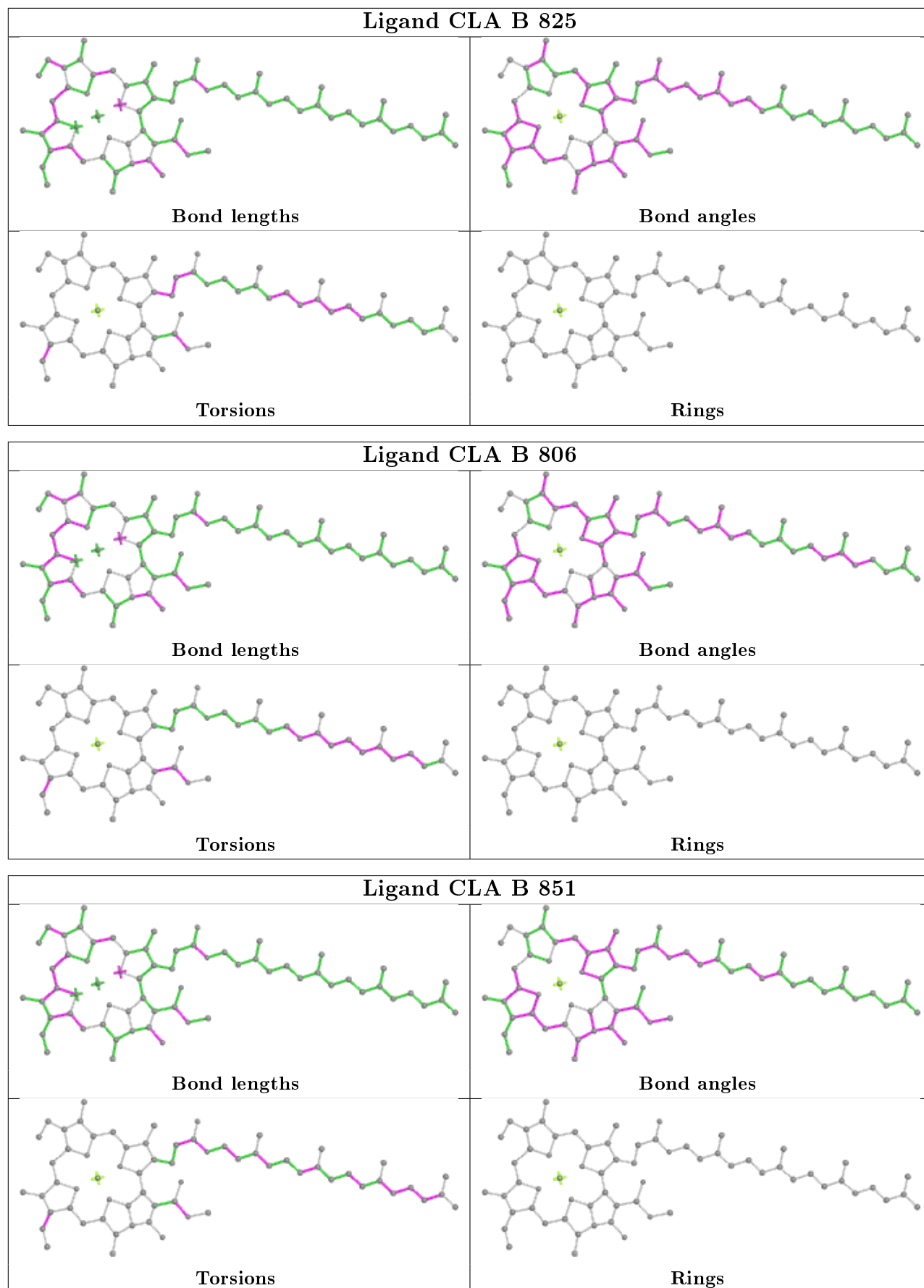
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

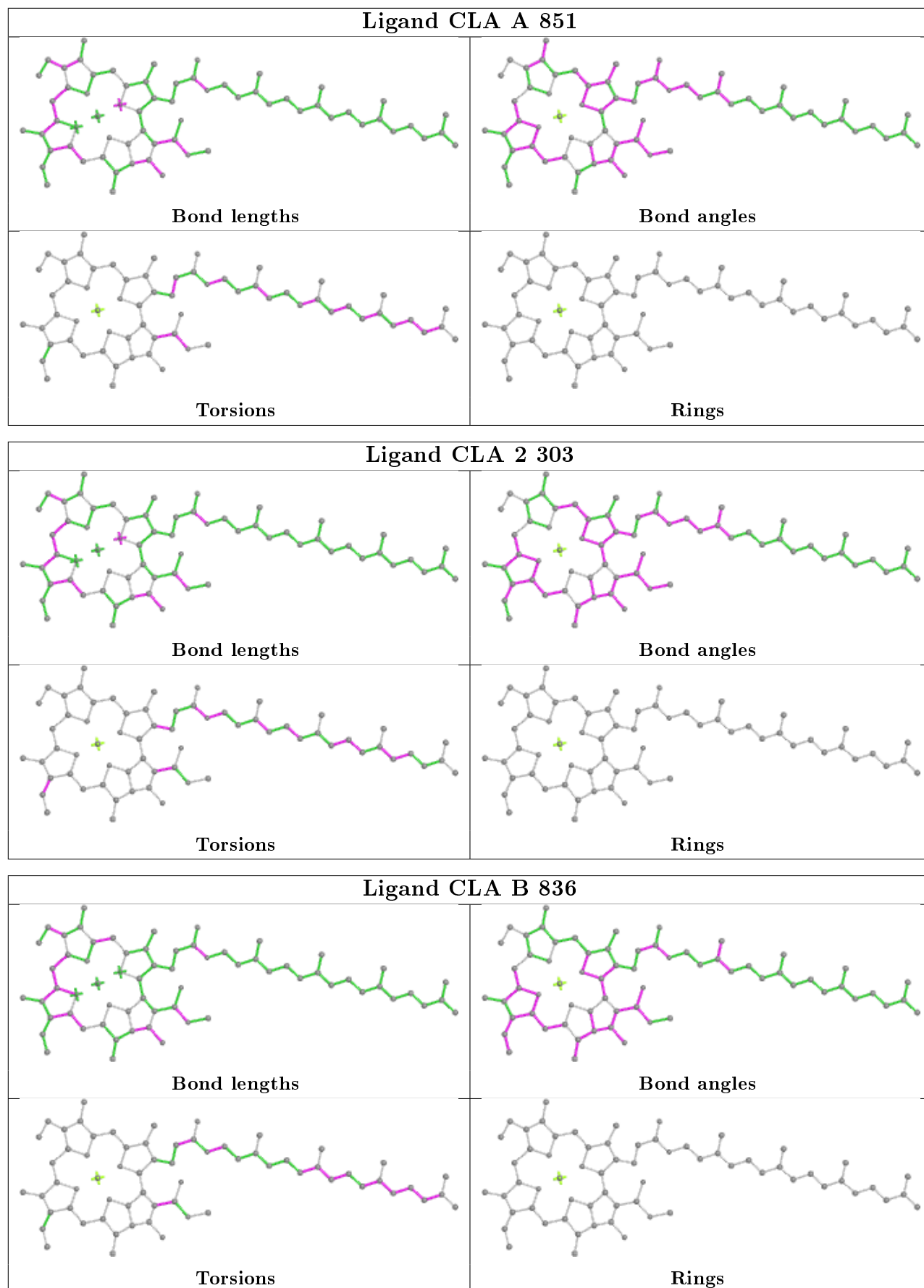




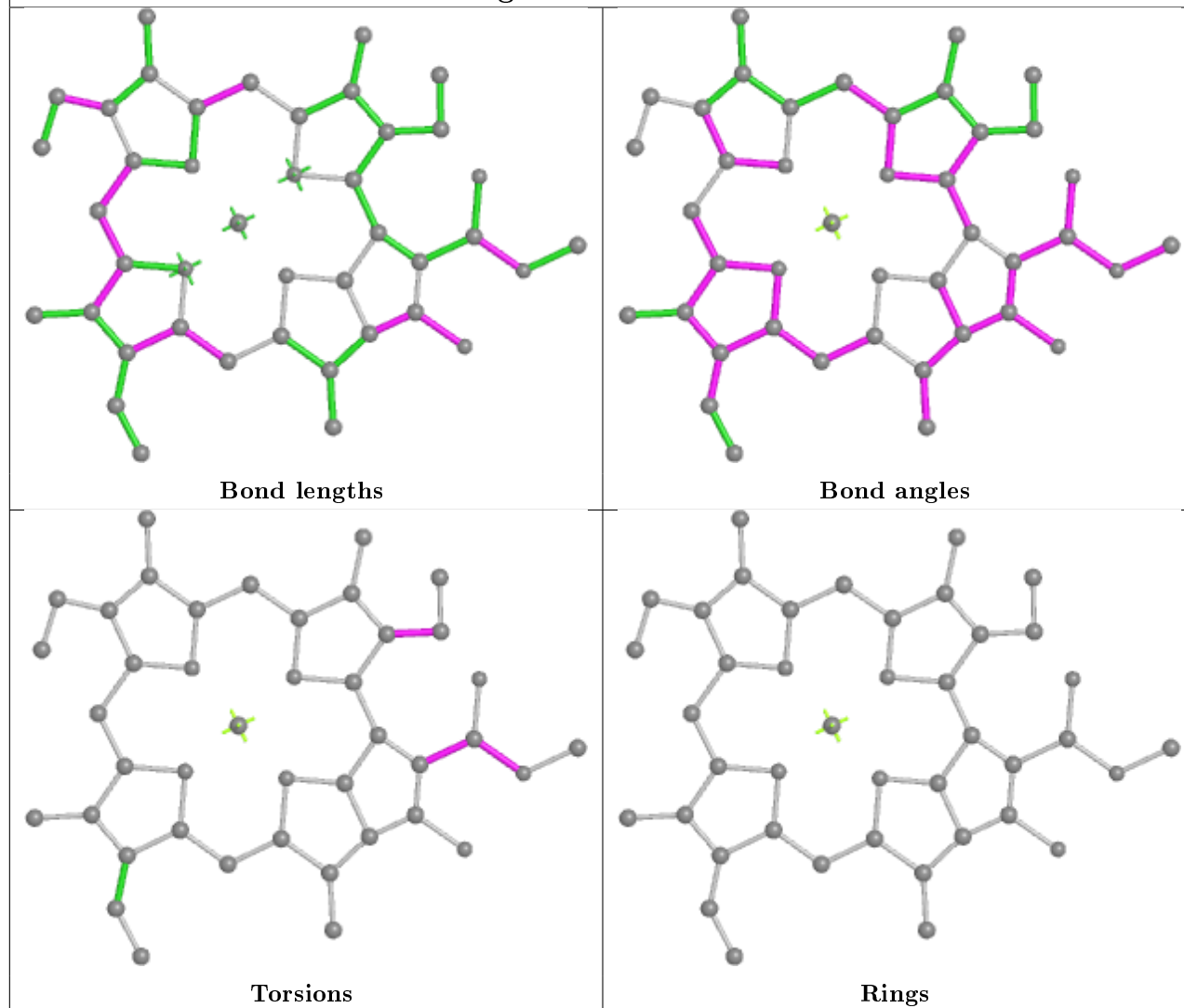




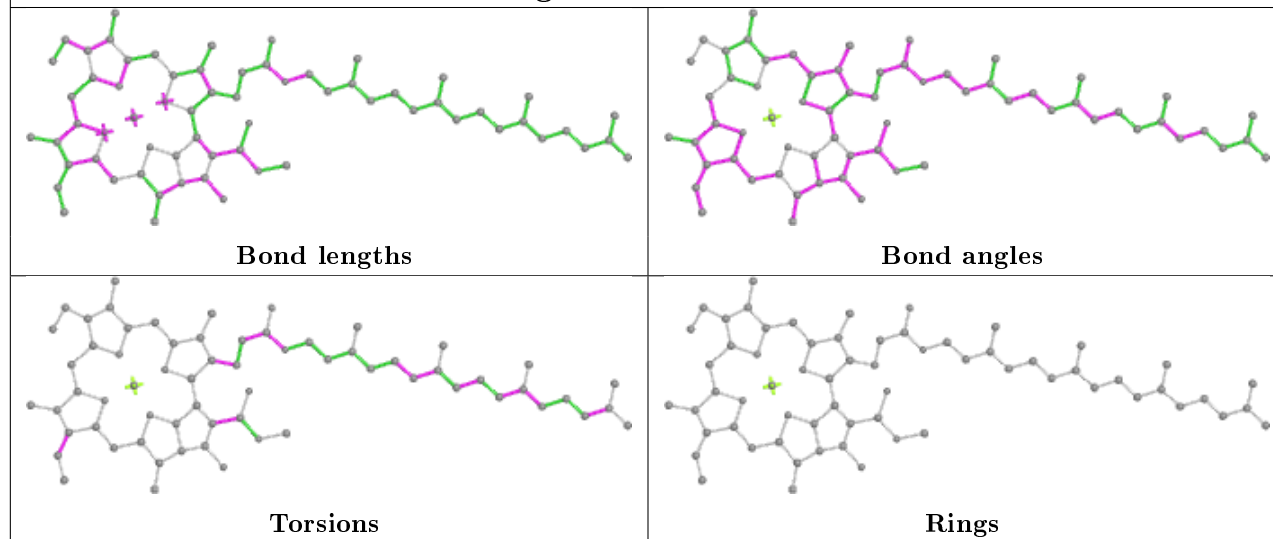


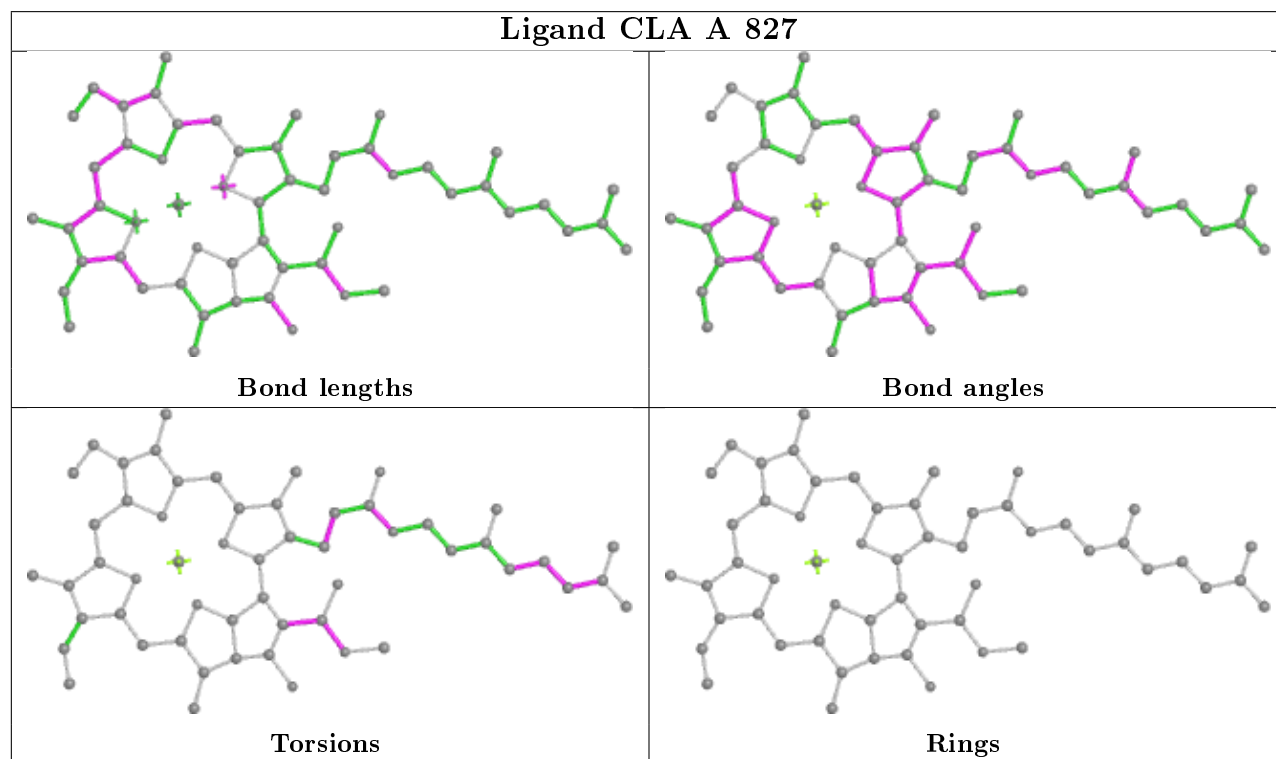
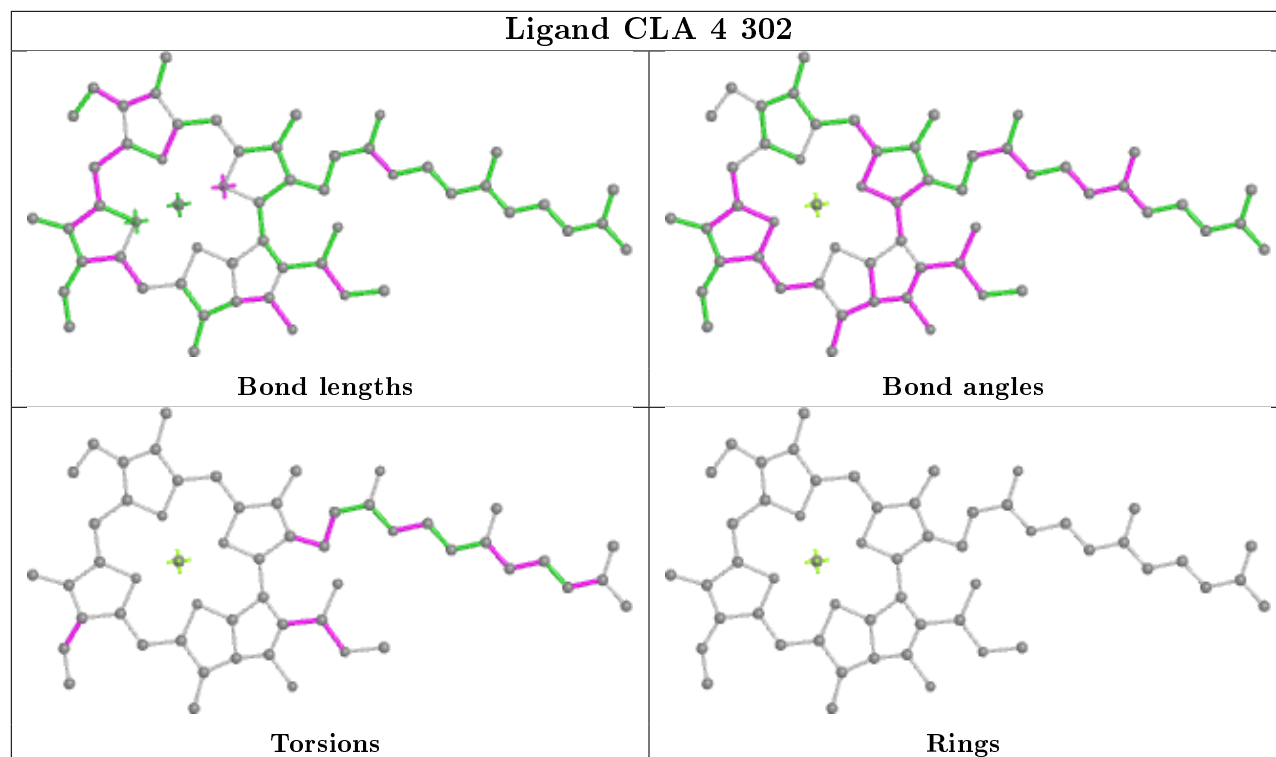


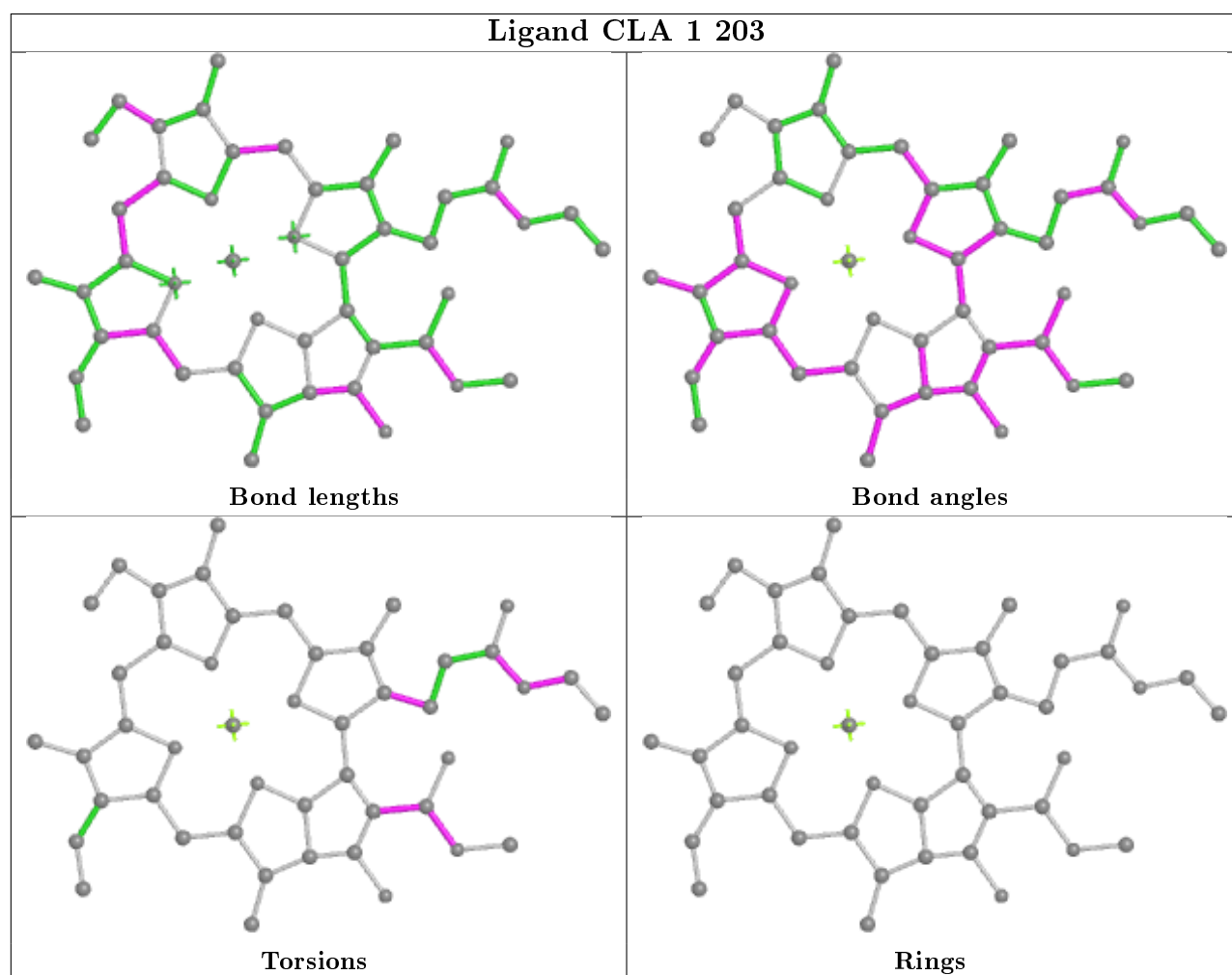
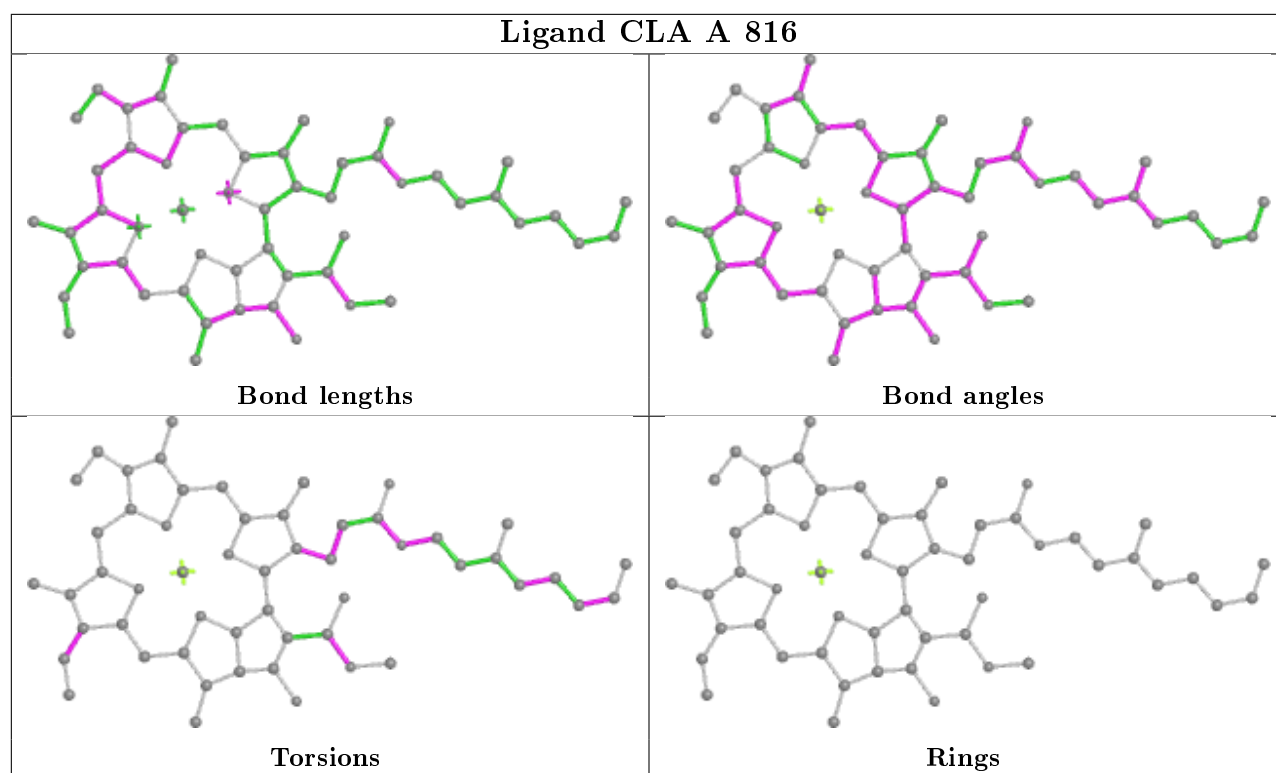
Ligand CLA 3 308

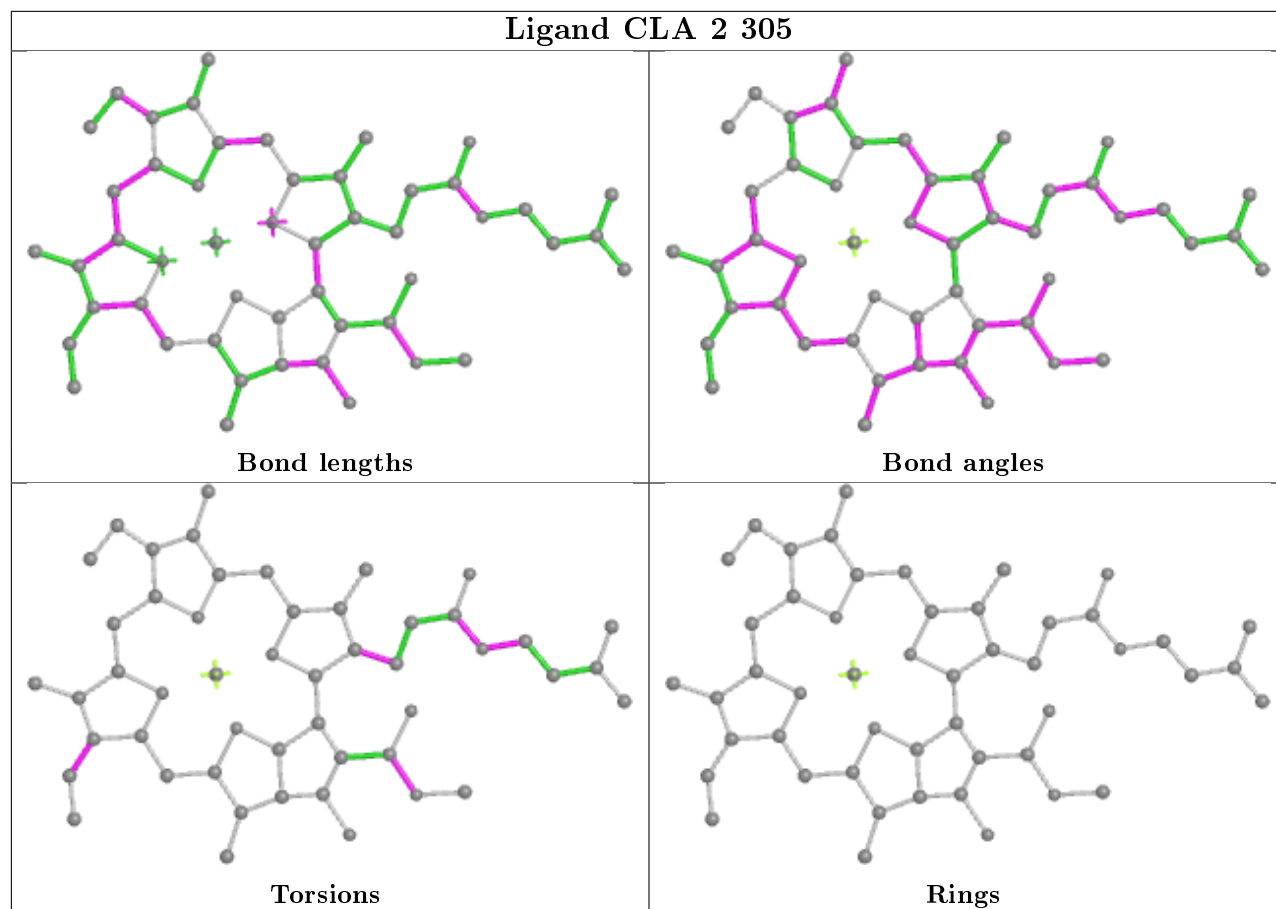


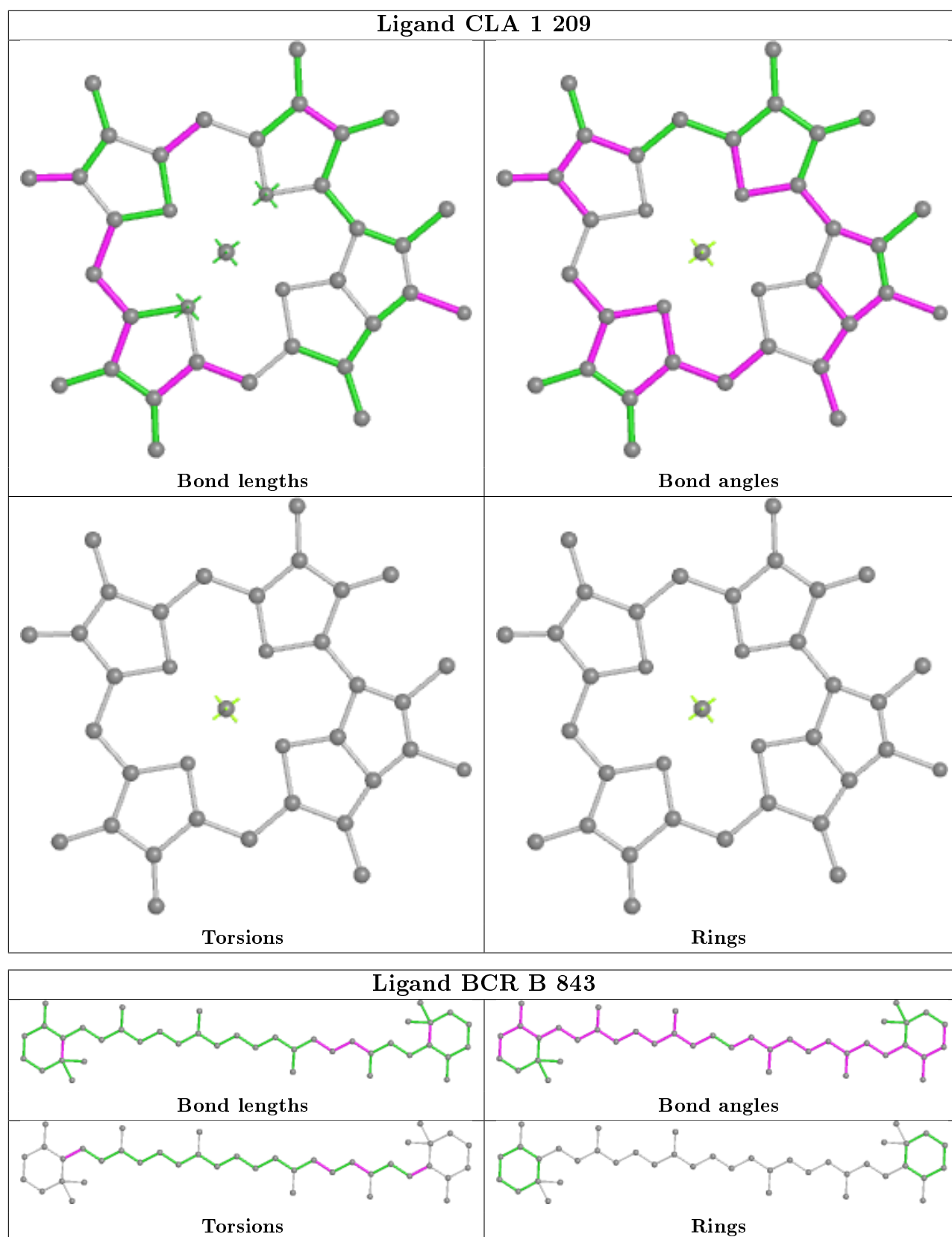
Ligand CLA 4 304

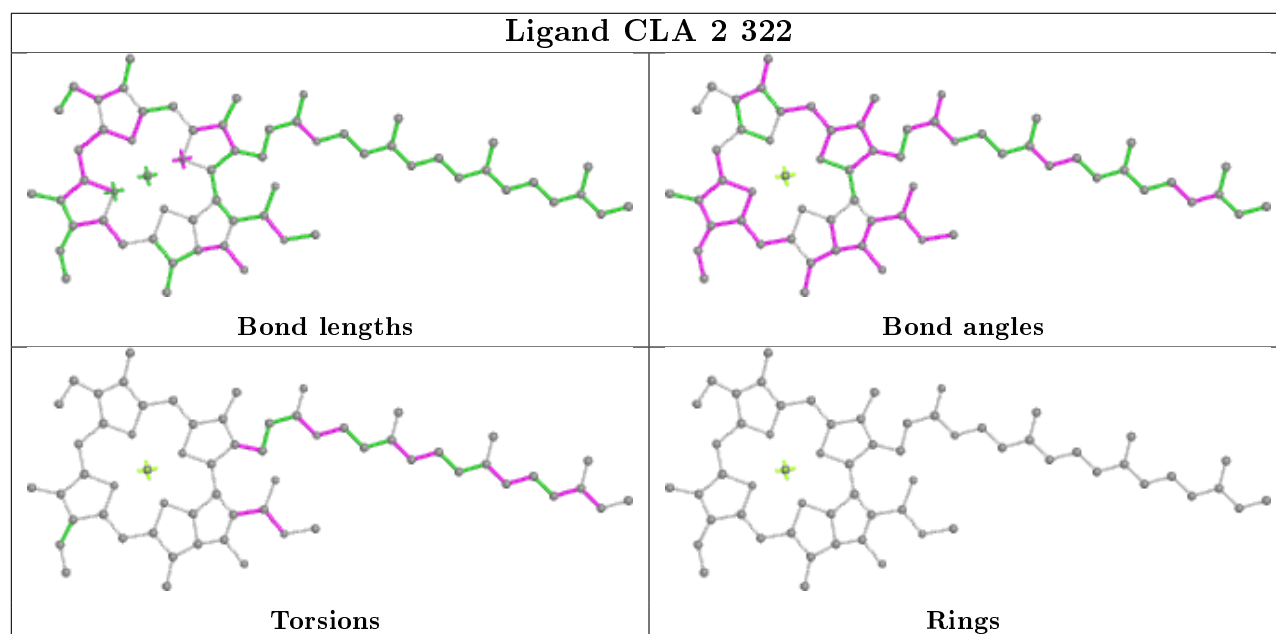
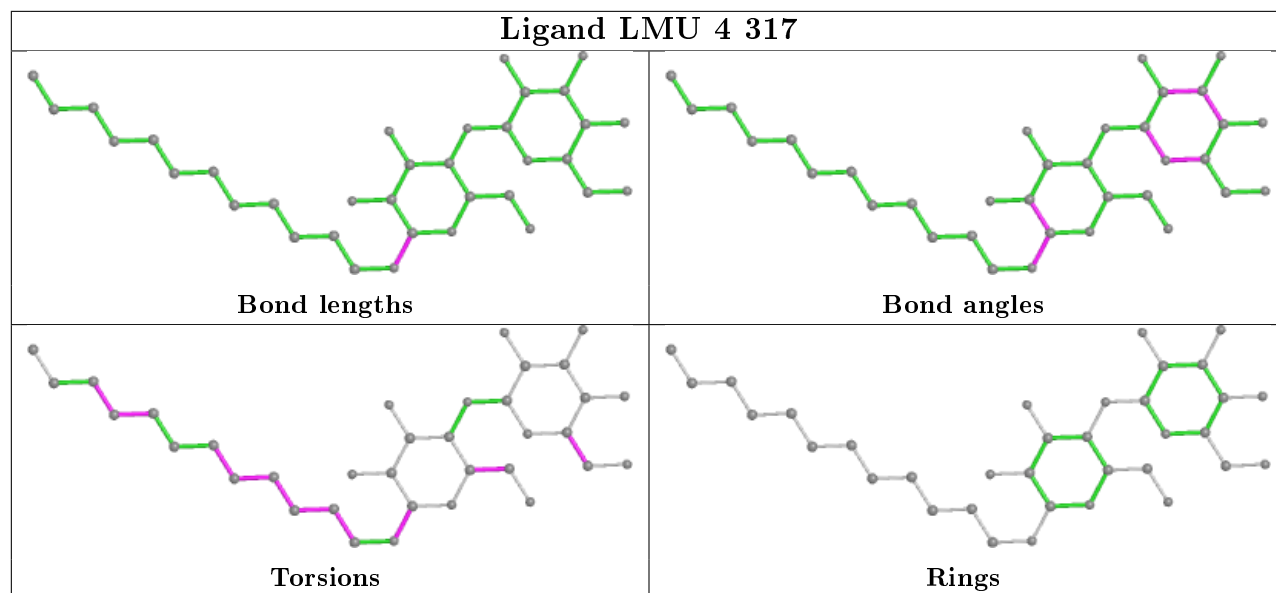


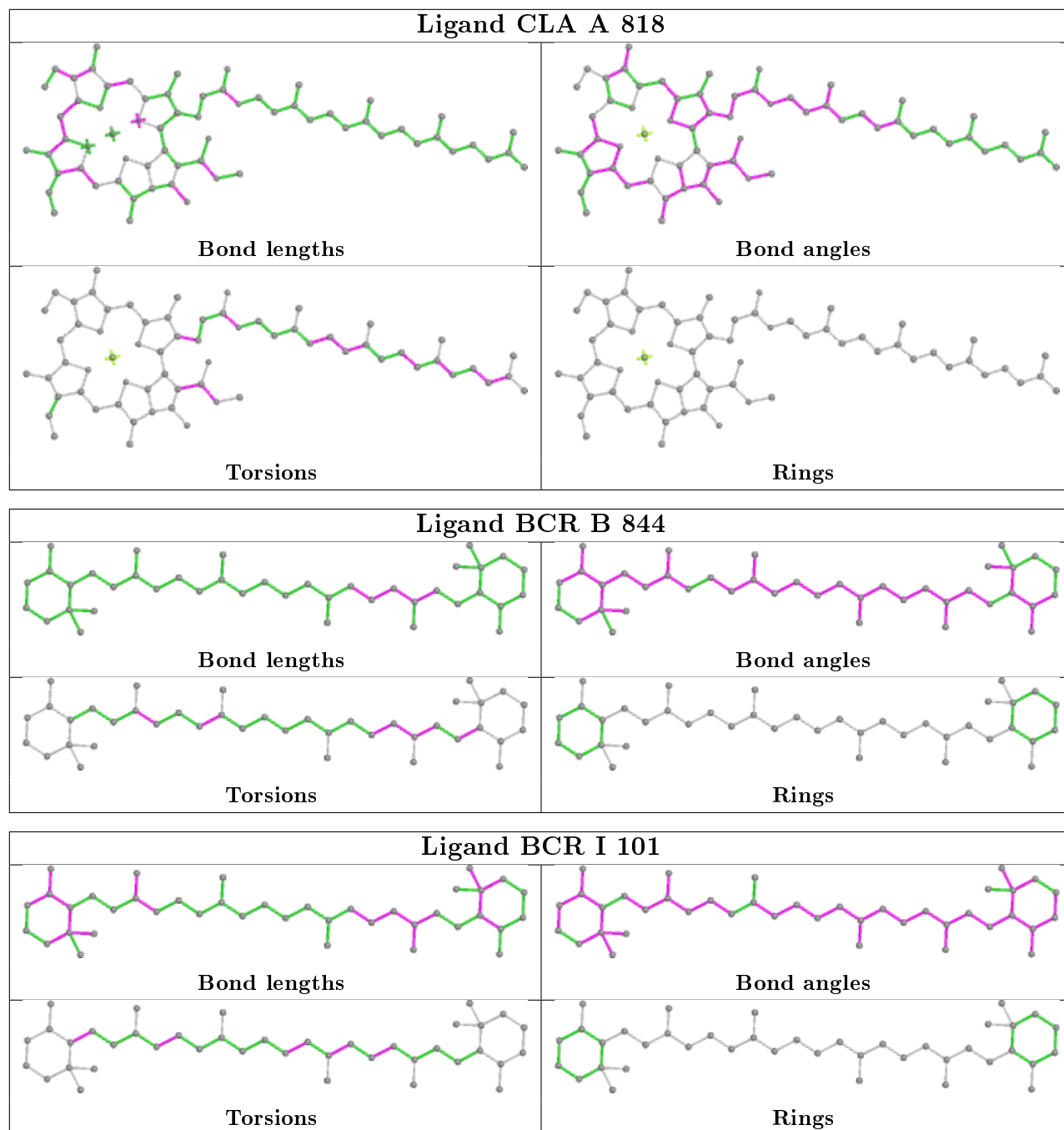


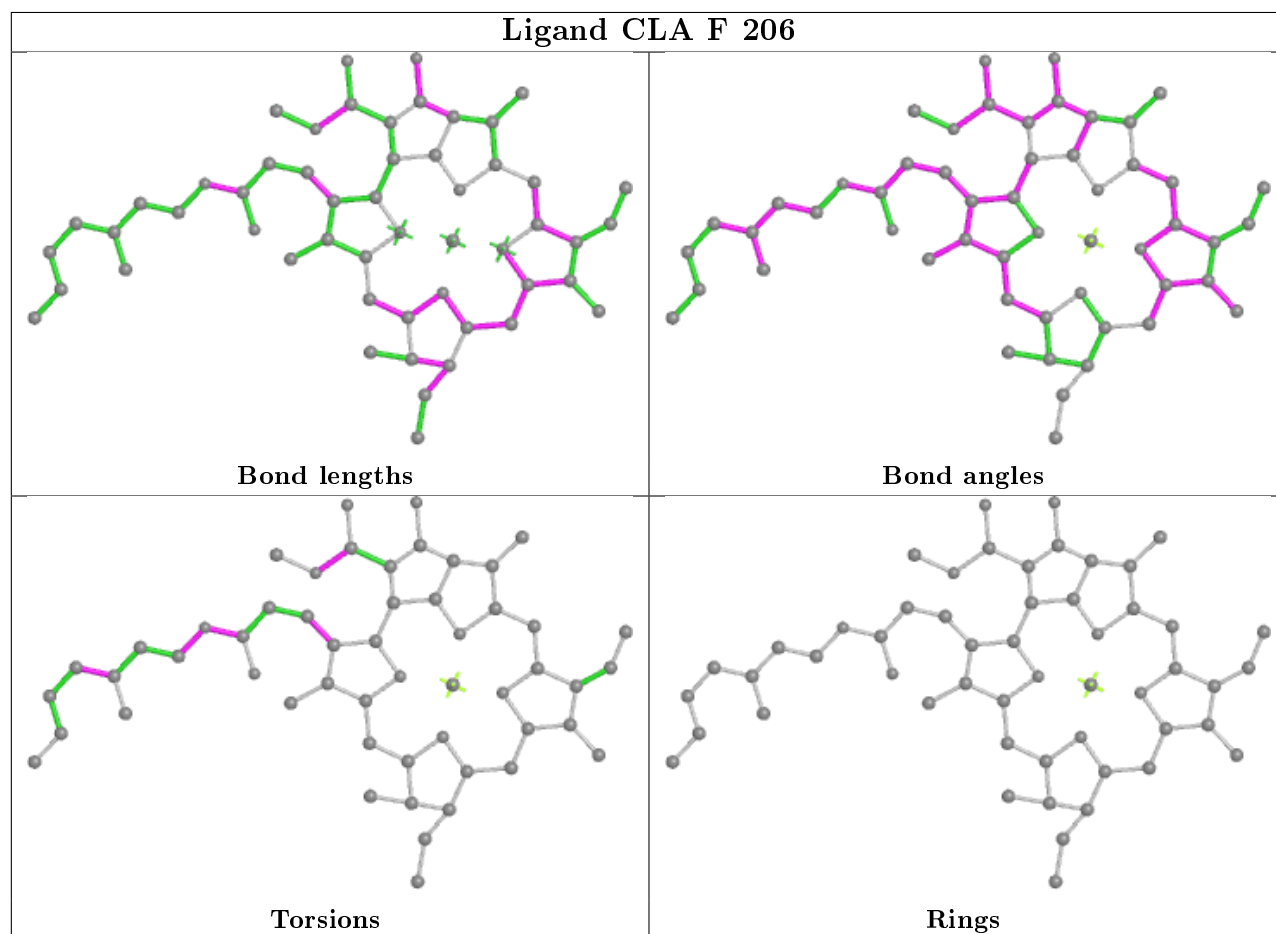
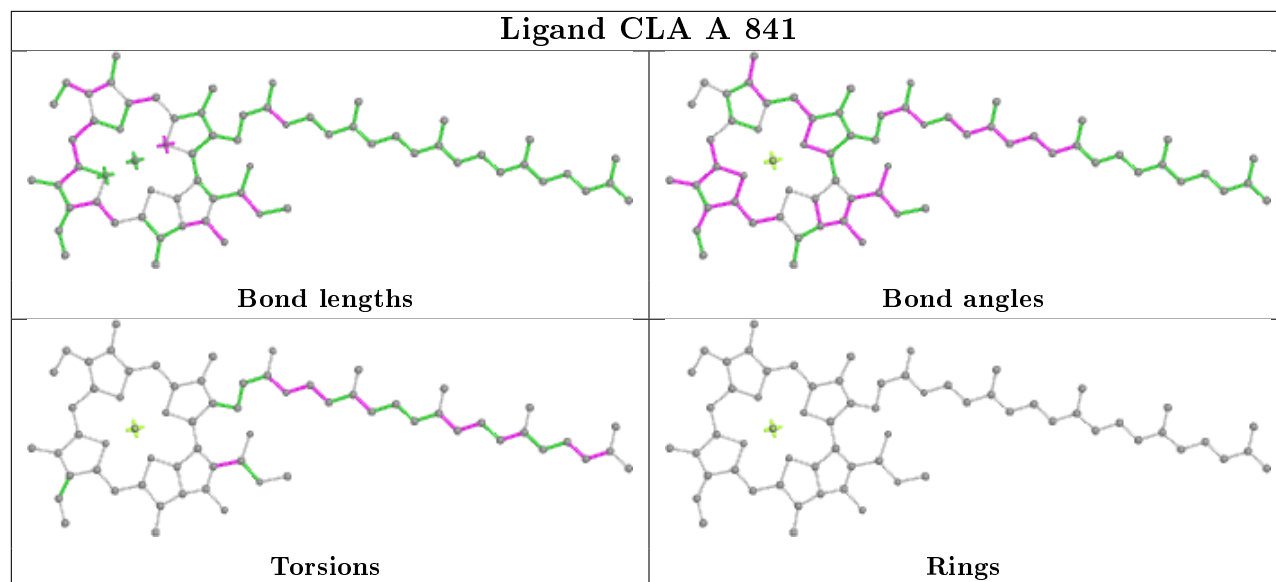


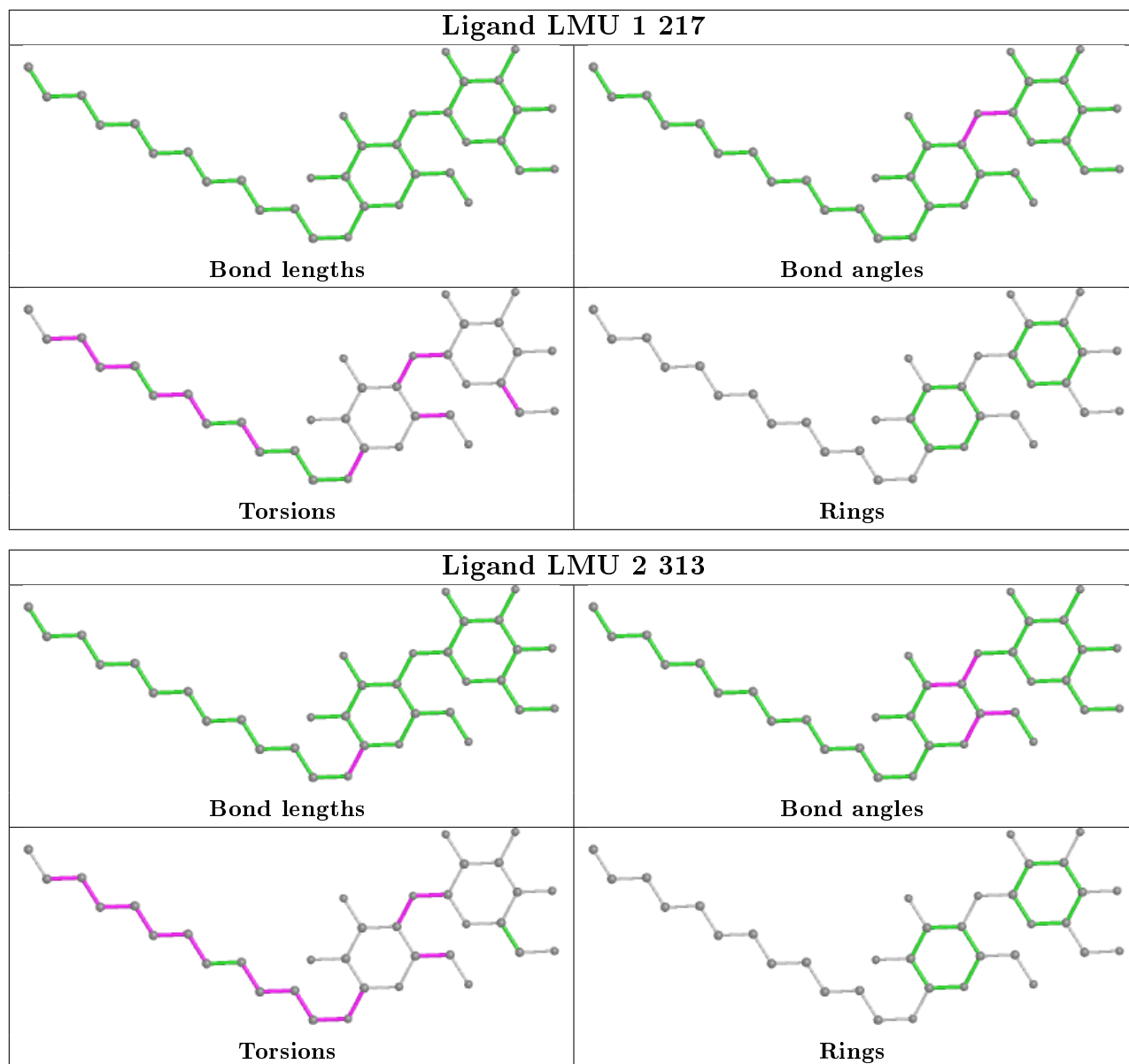


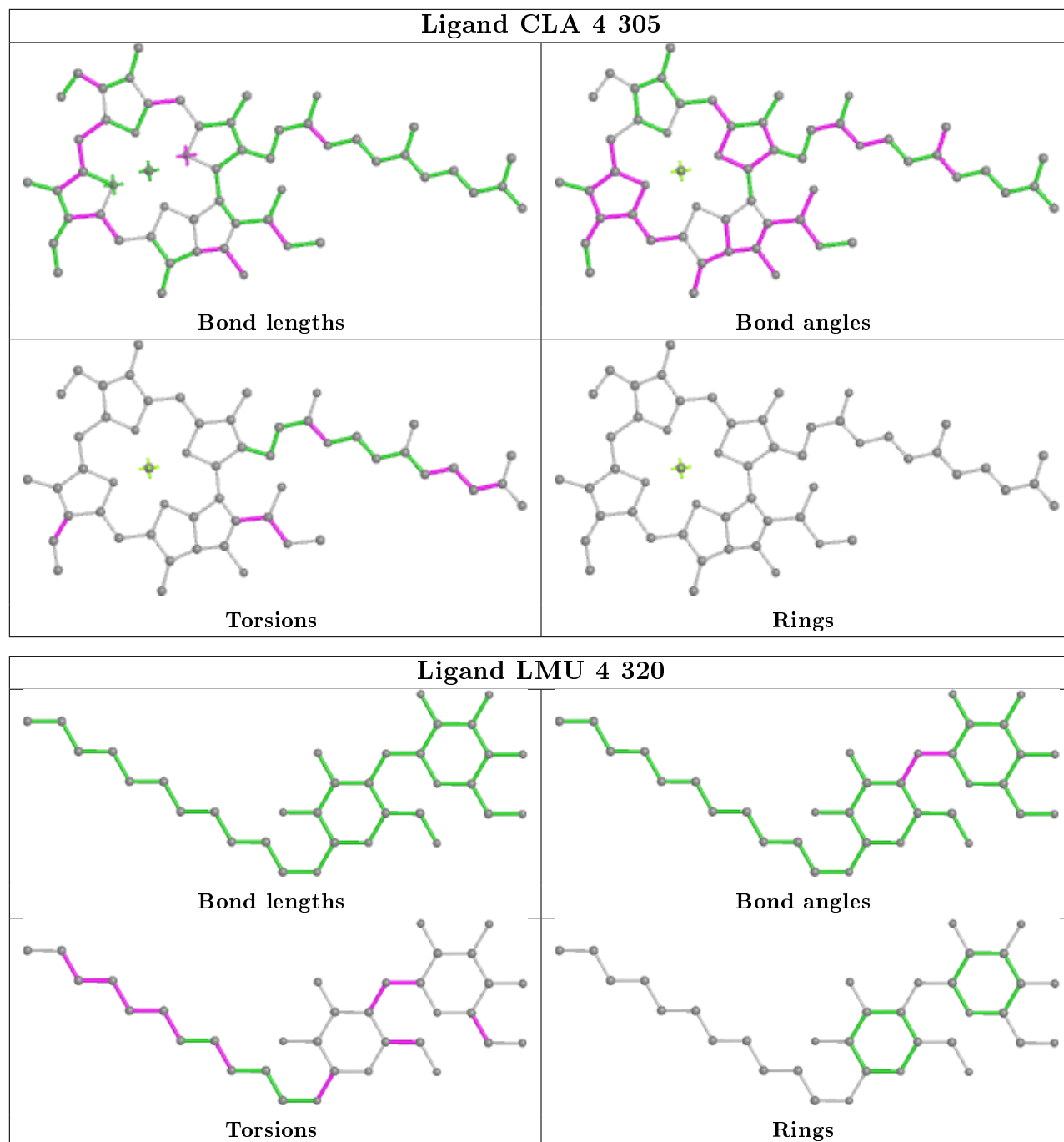


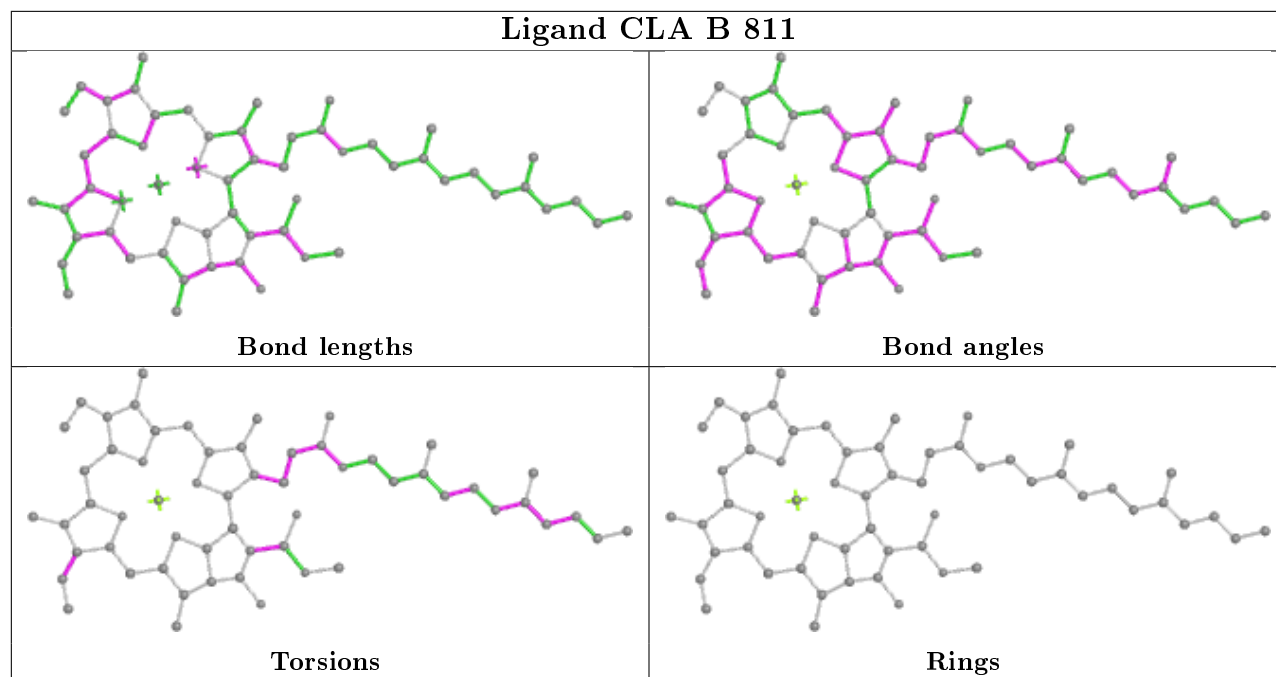


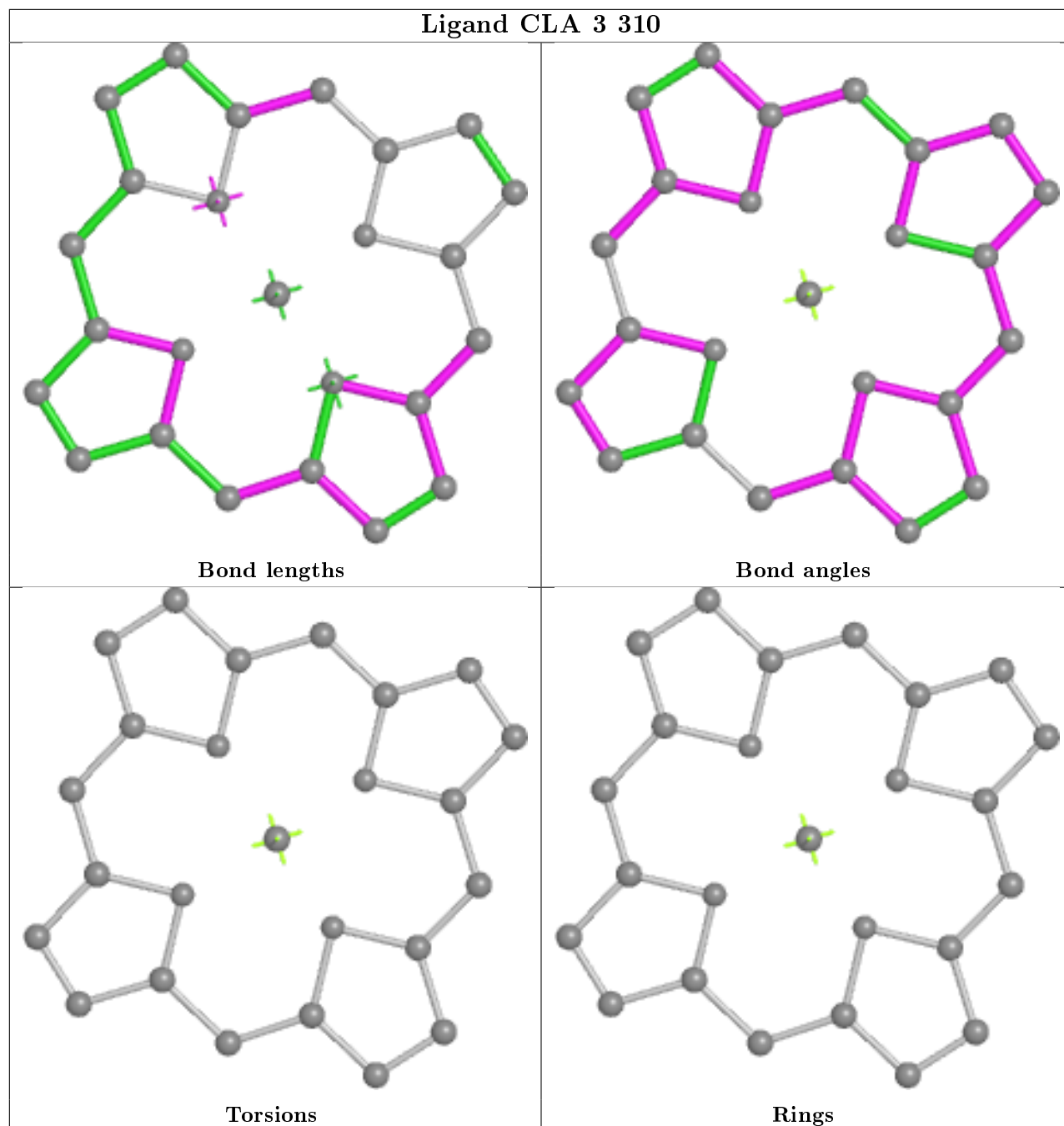


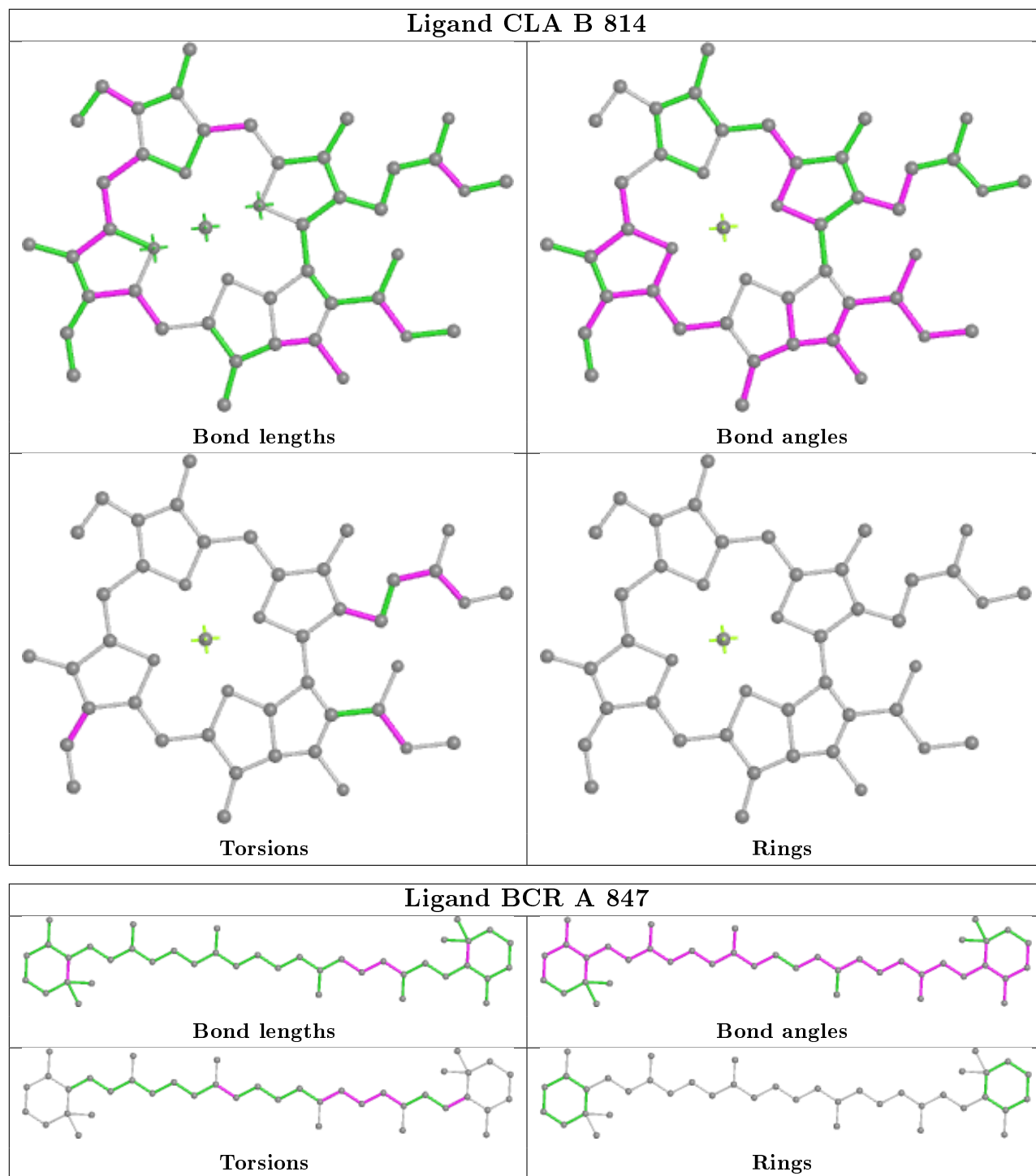


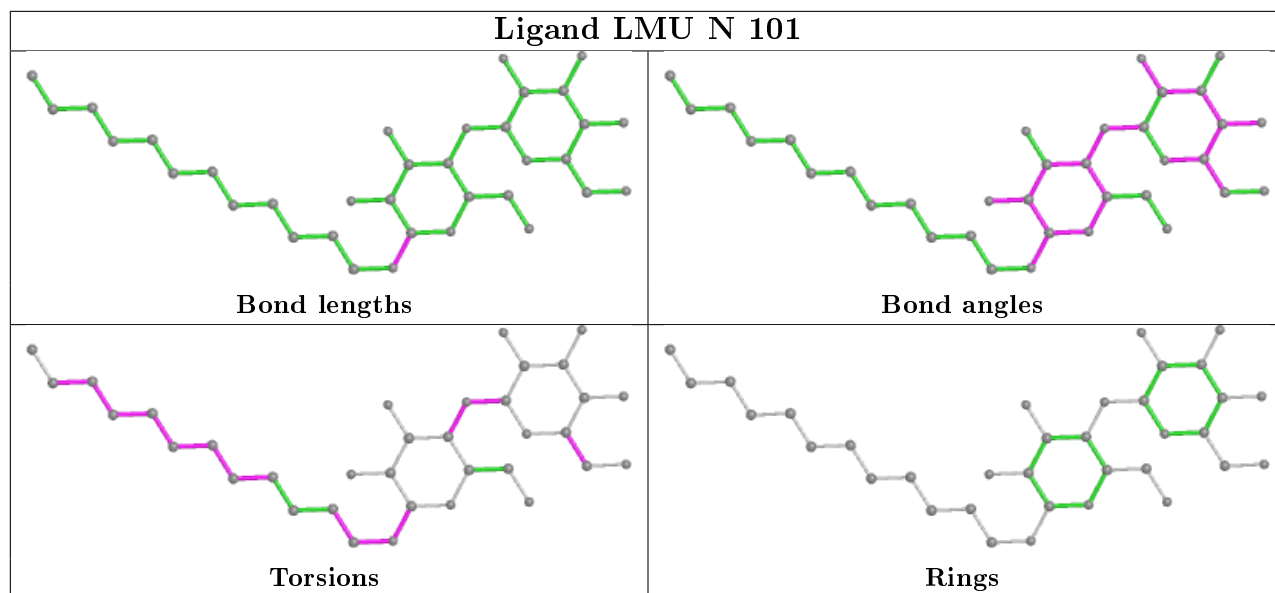


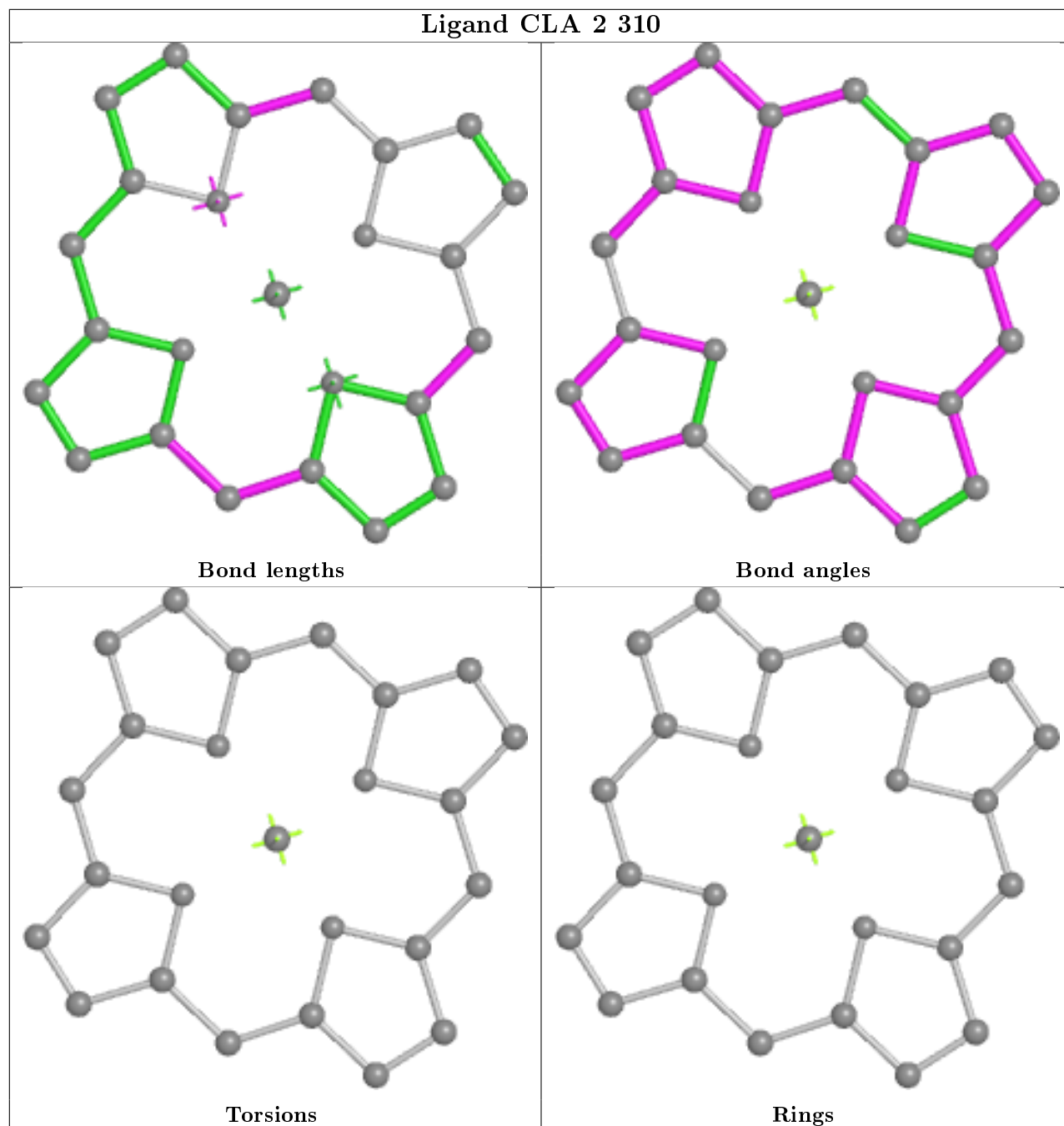


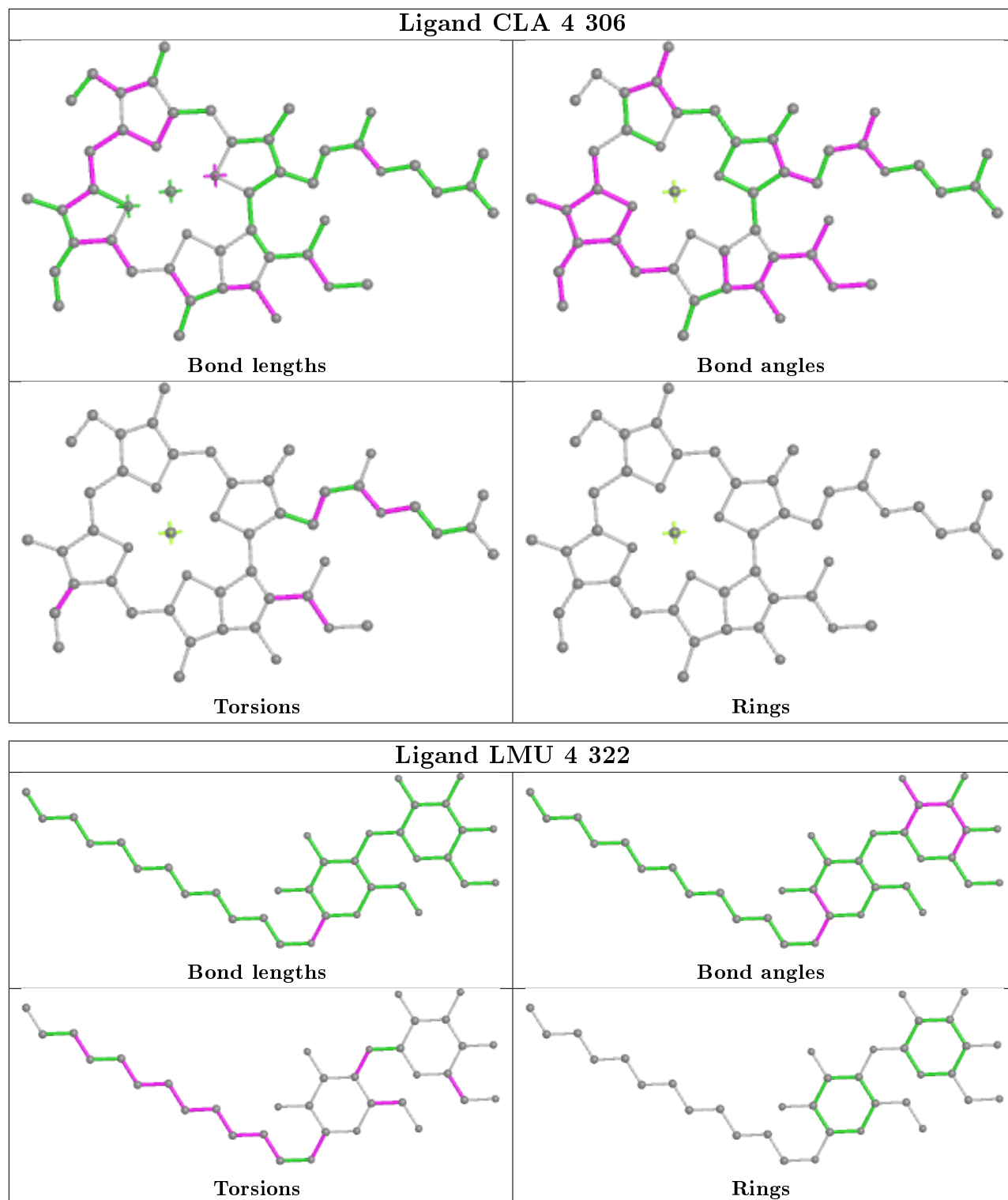


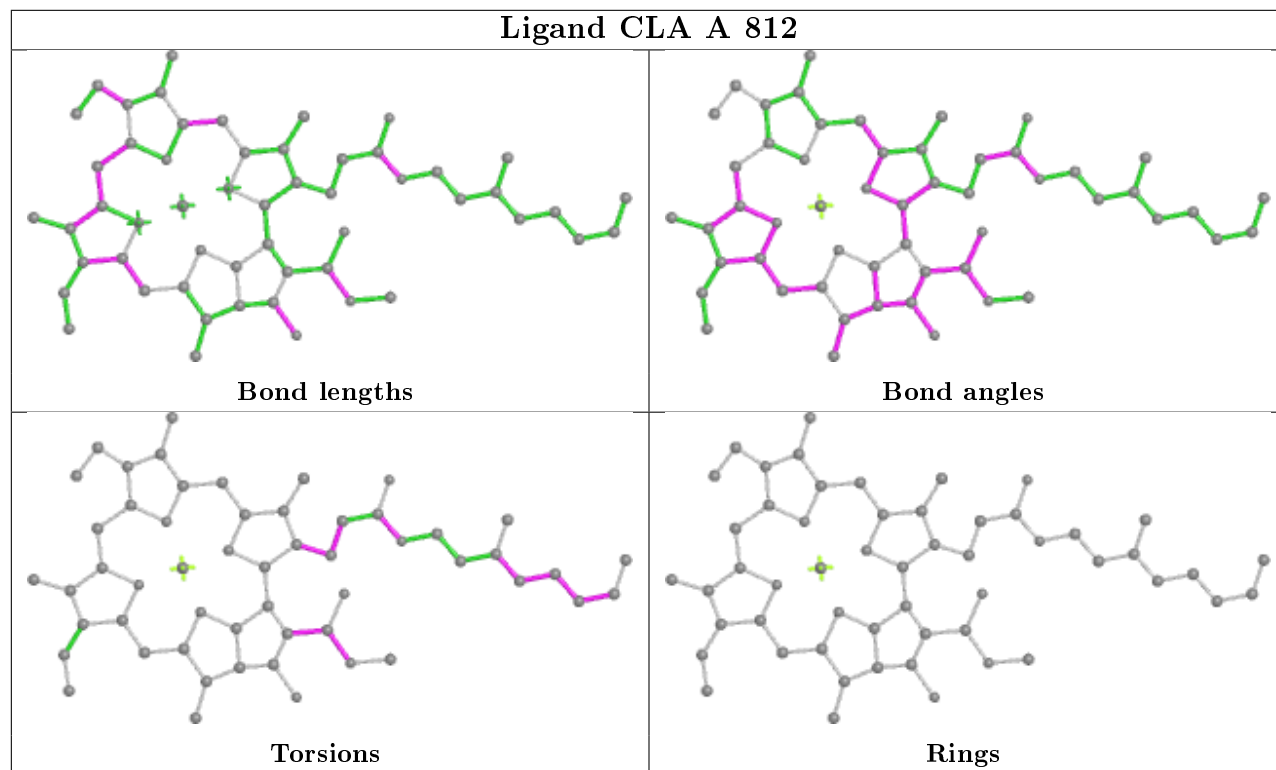
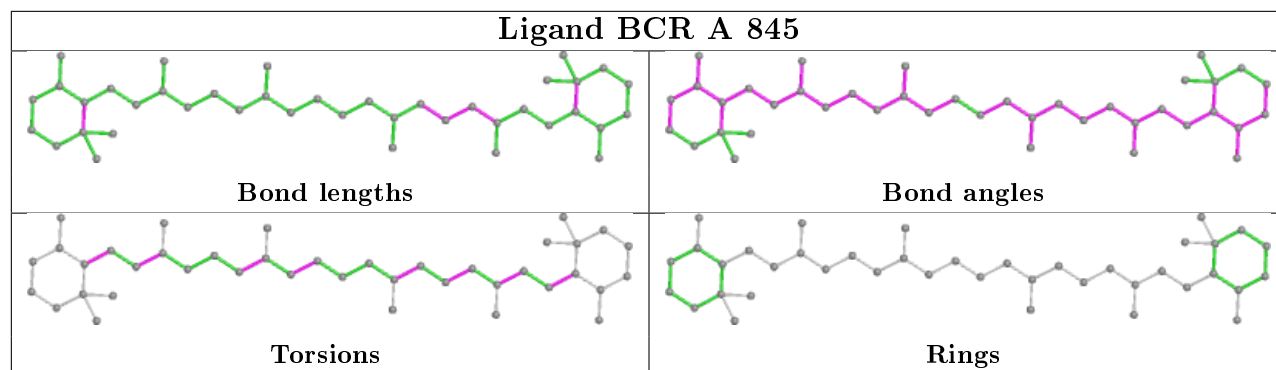
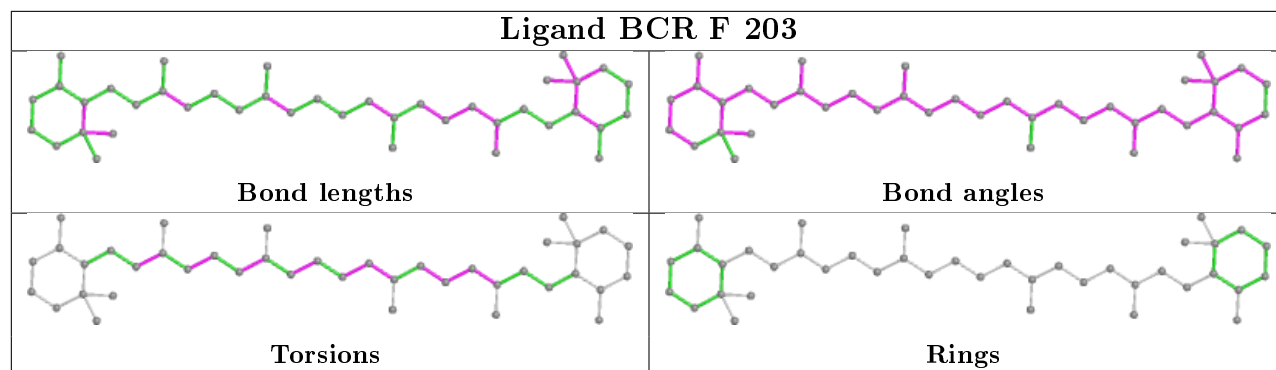


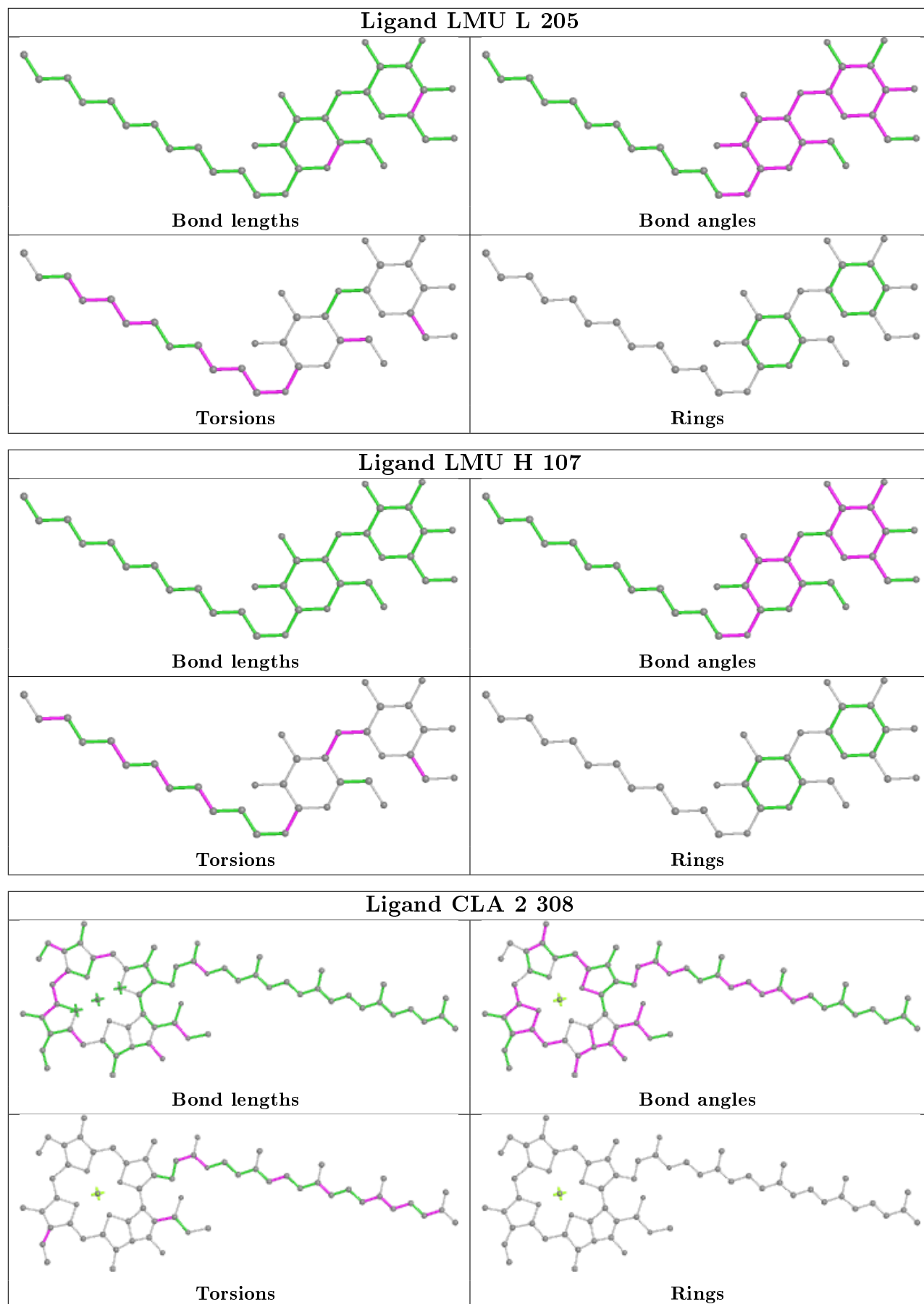


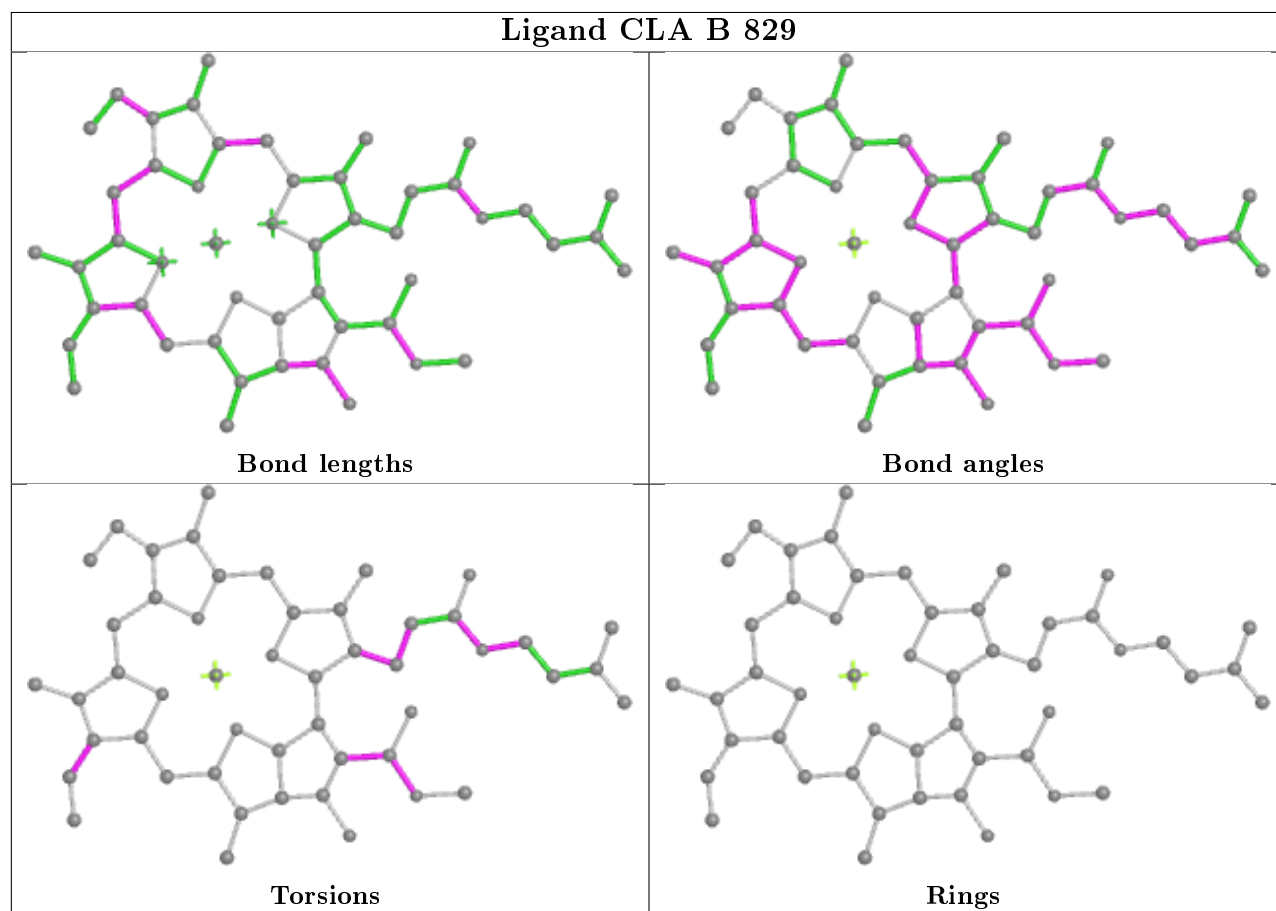
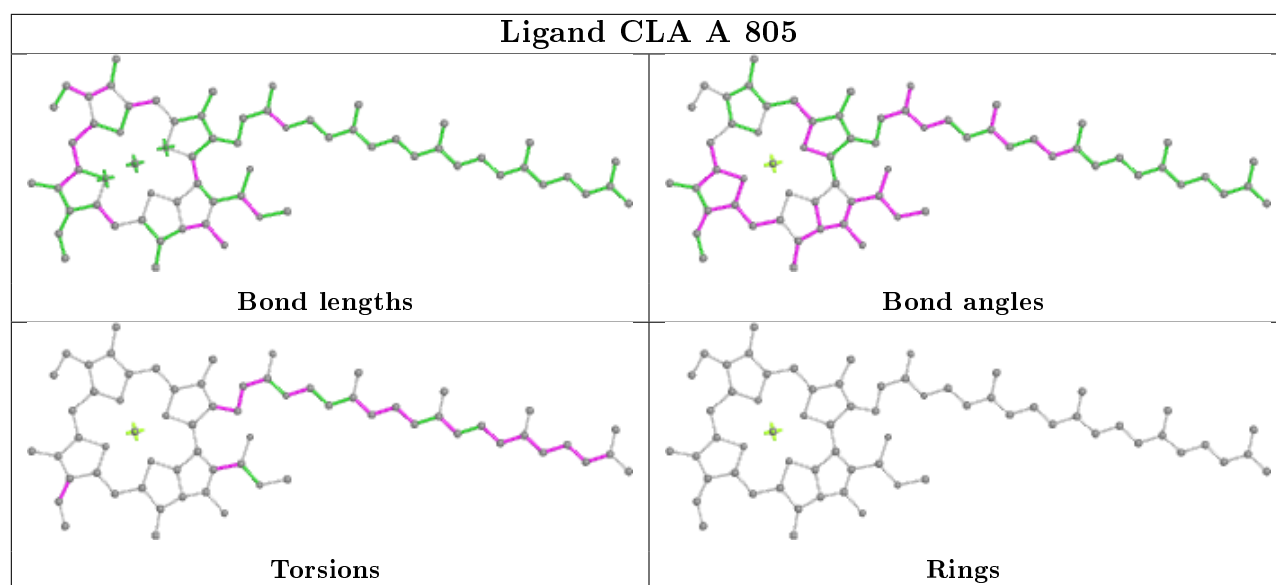


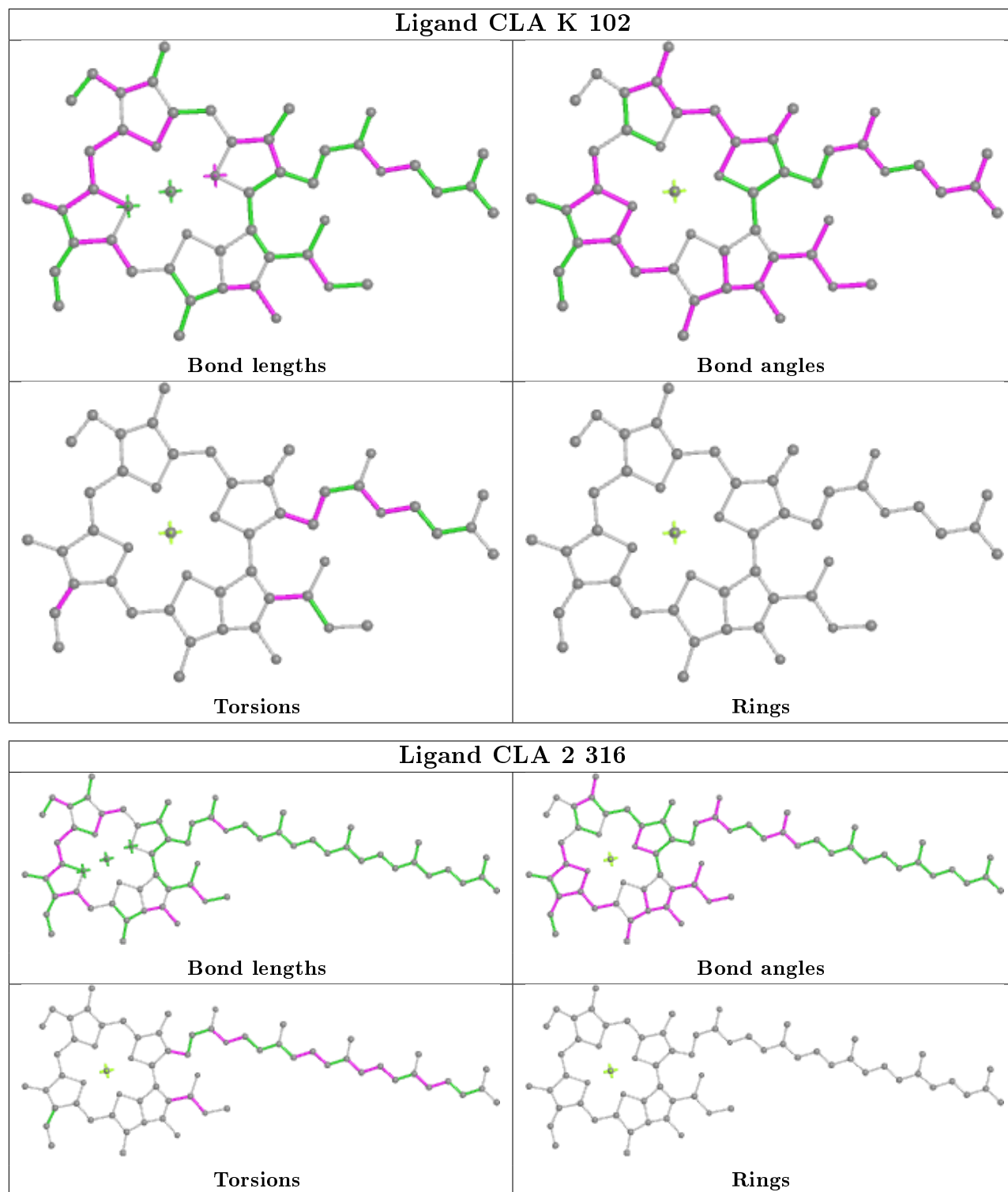


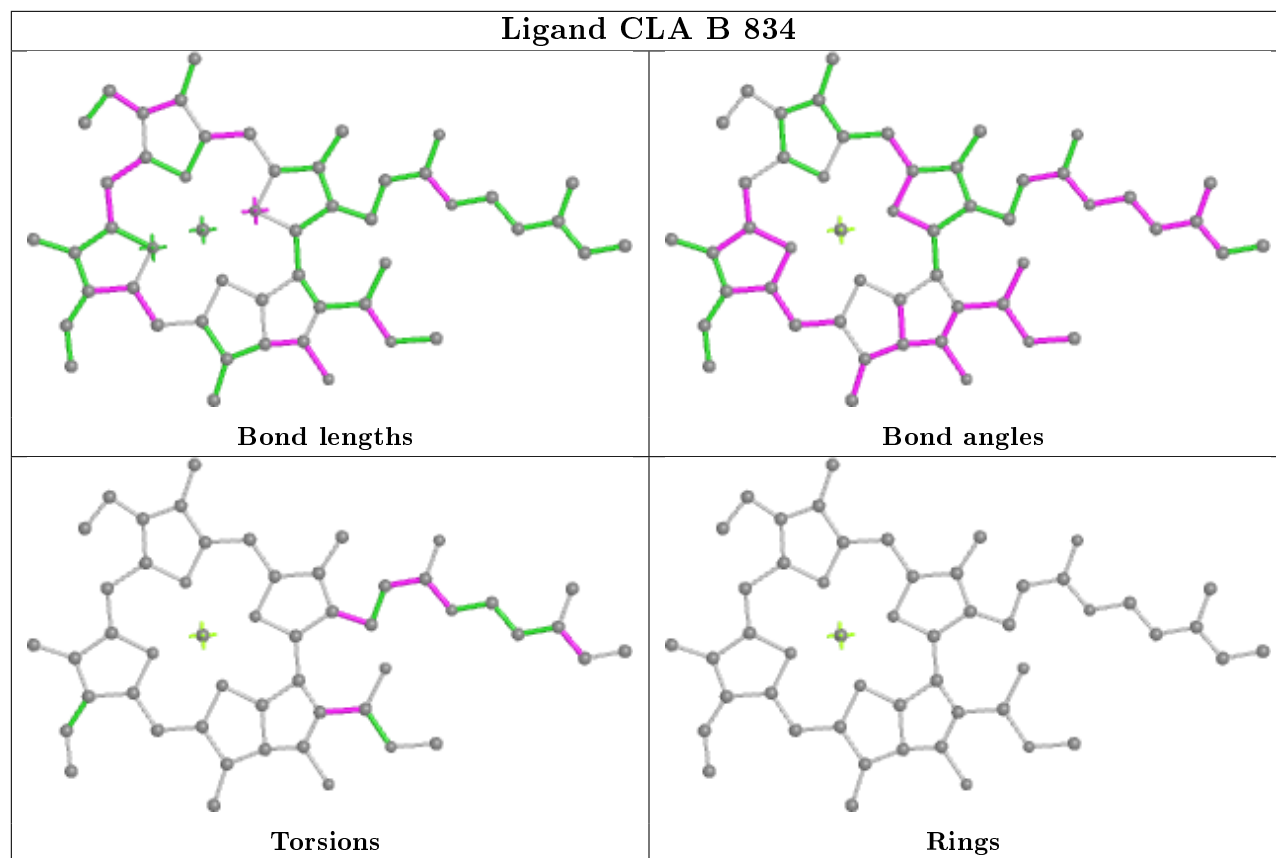


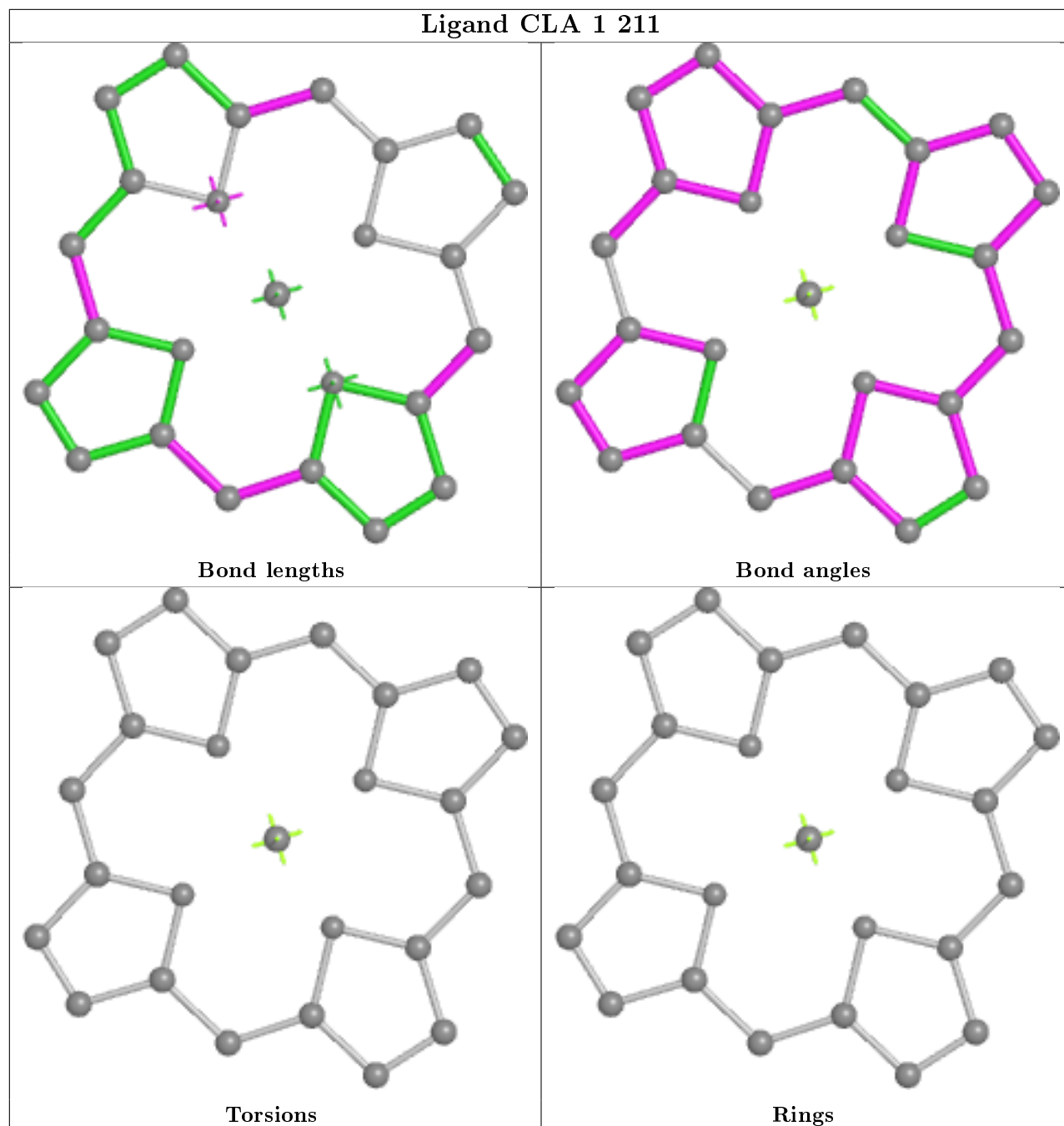


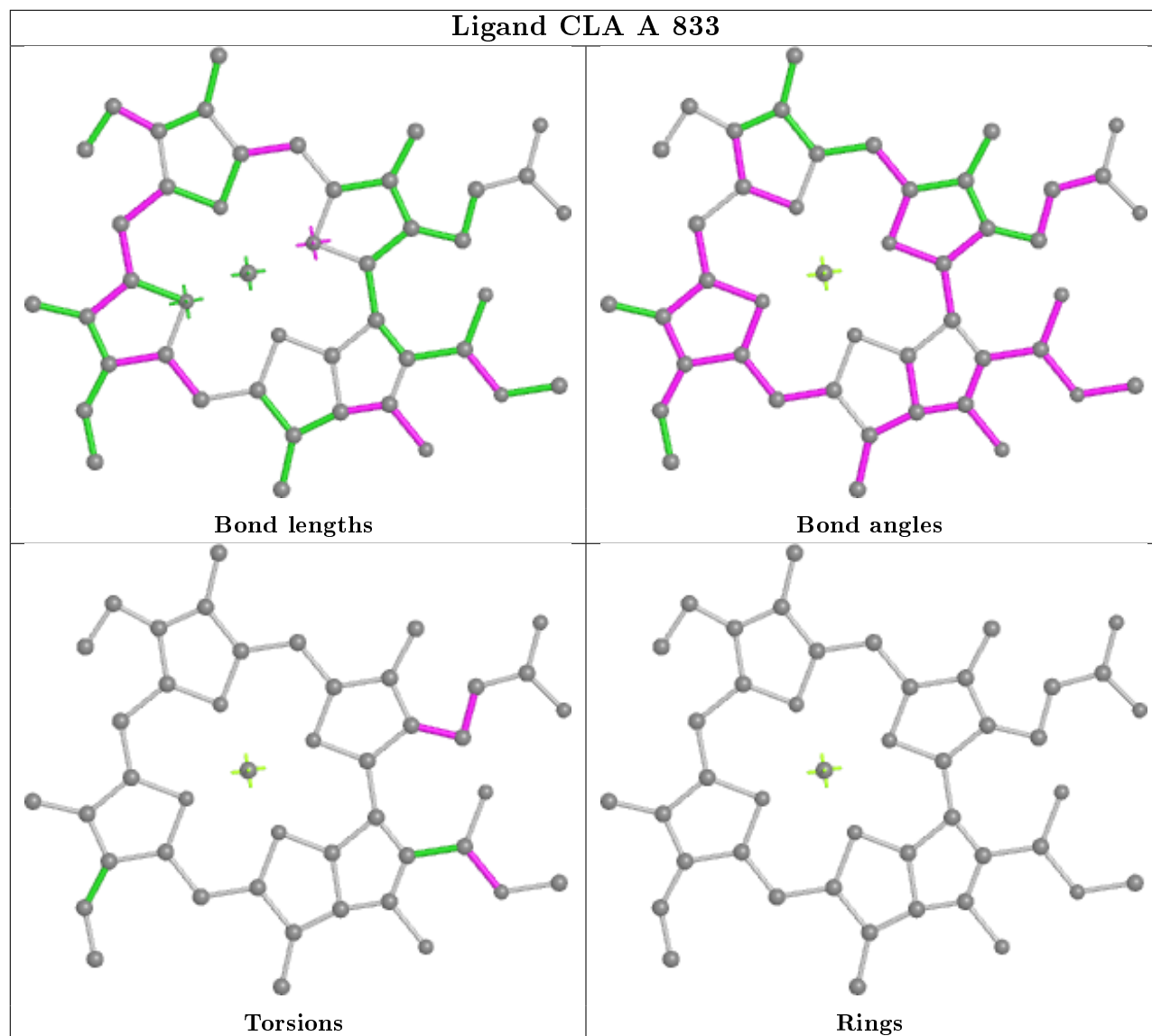


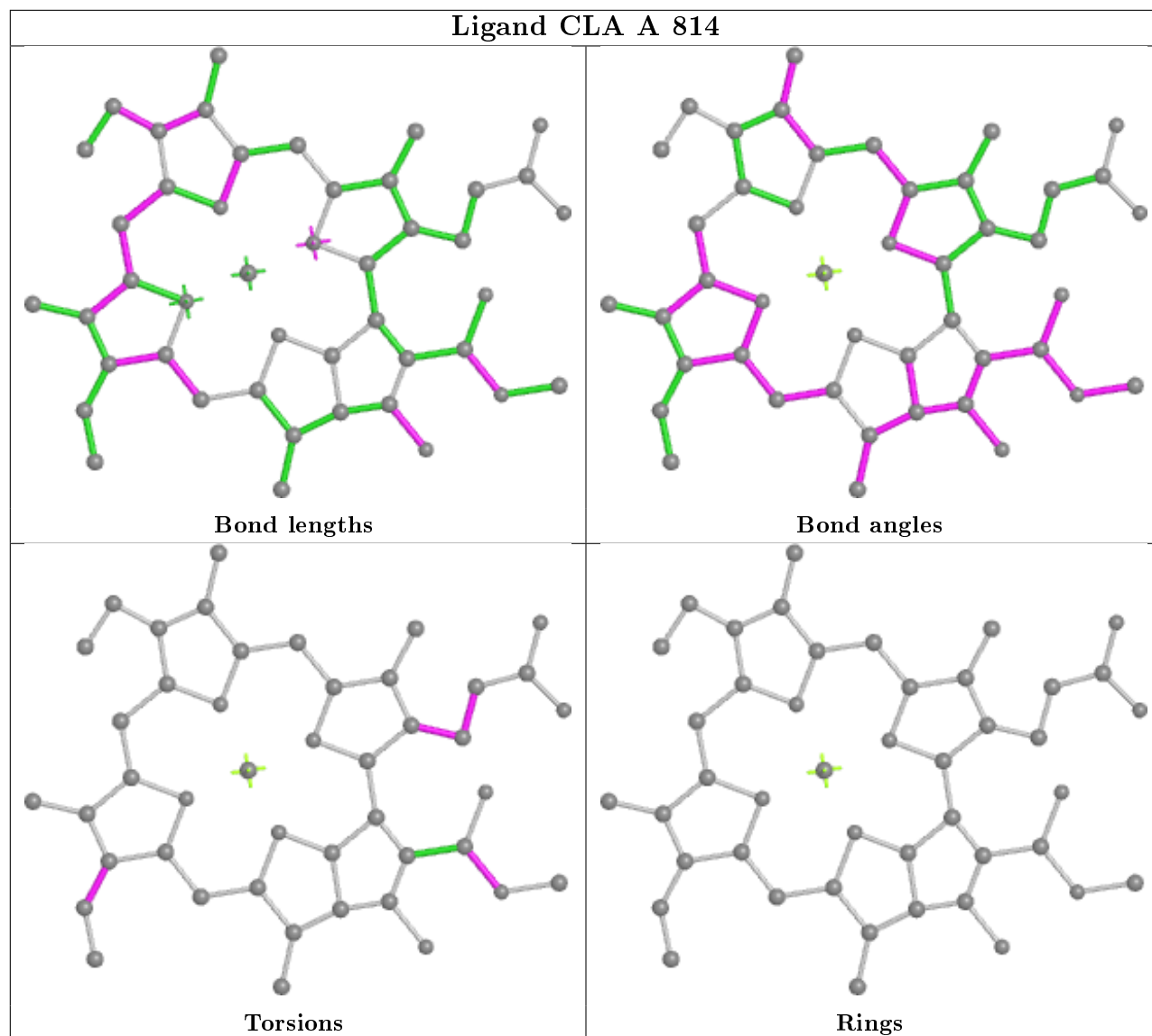


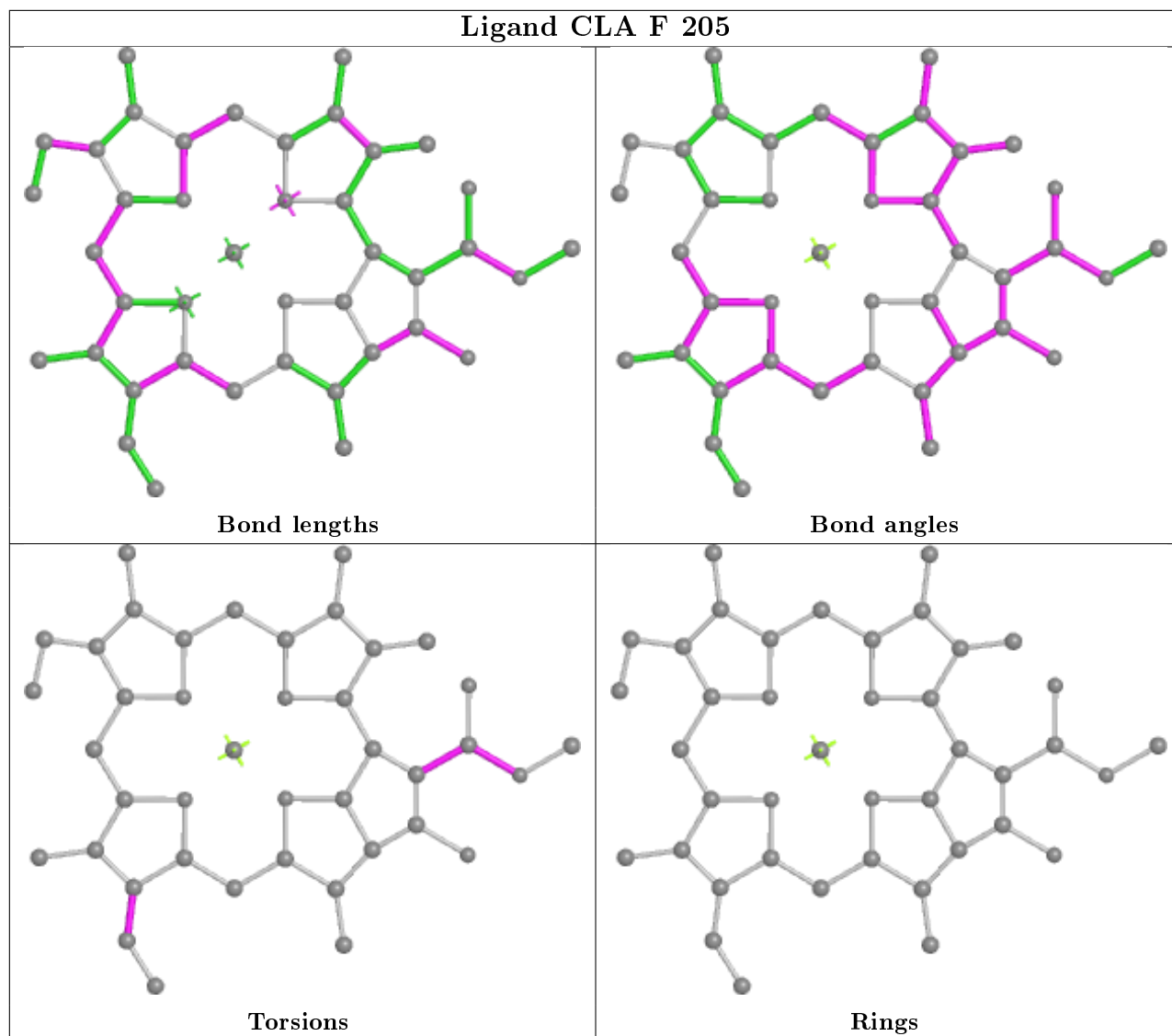


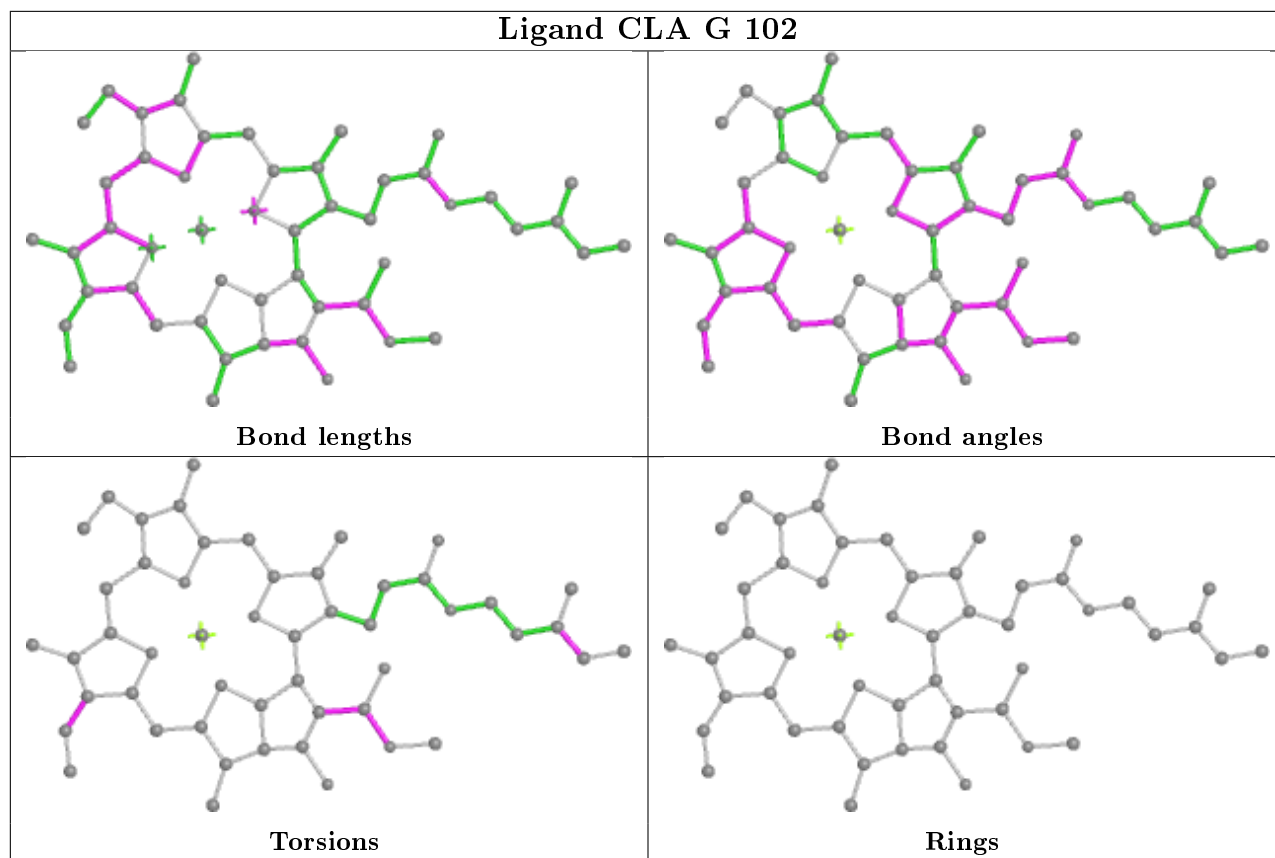


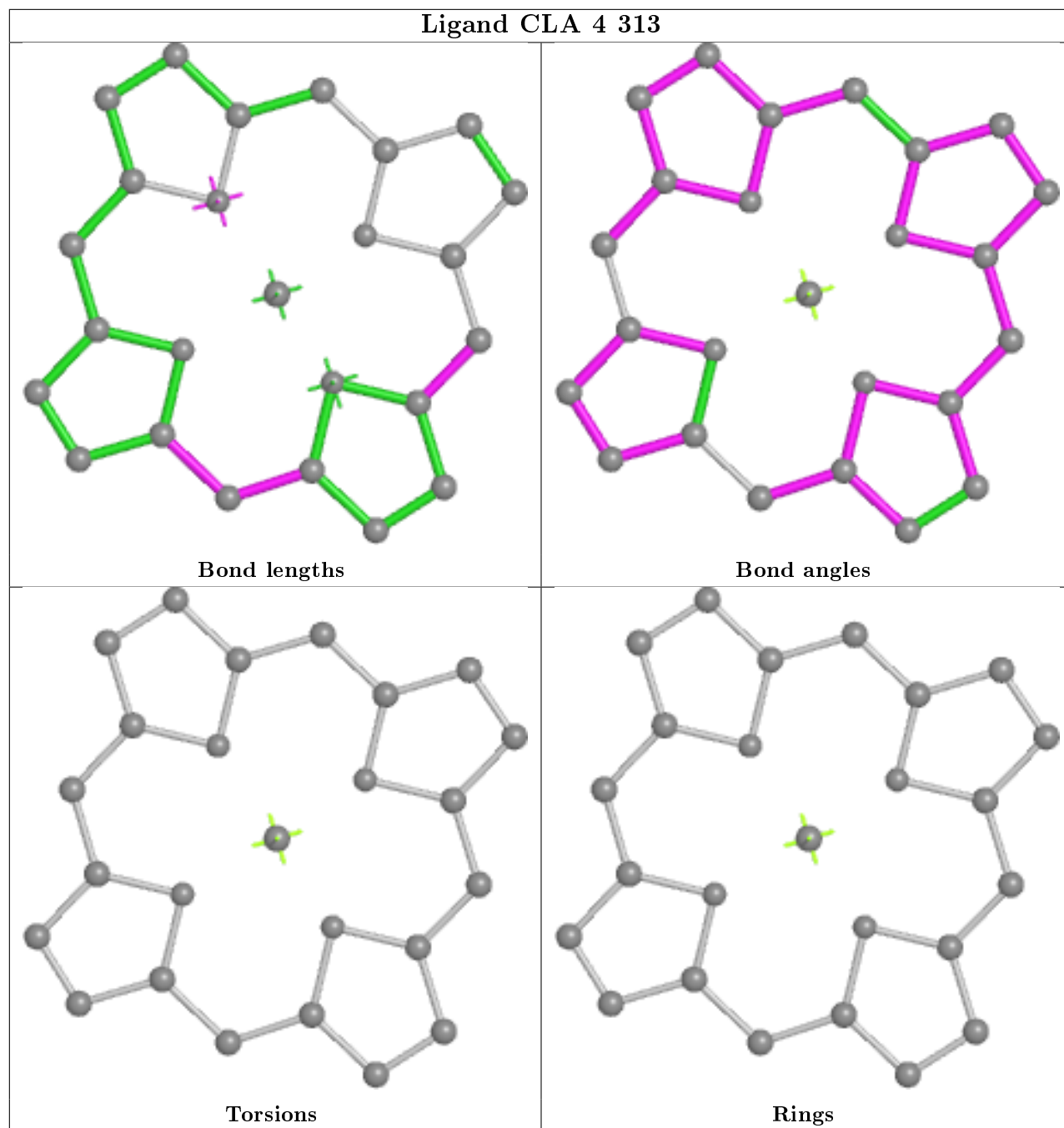


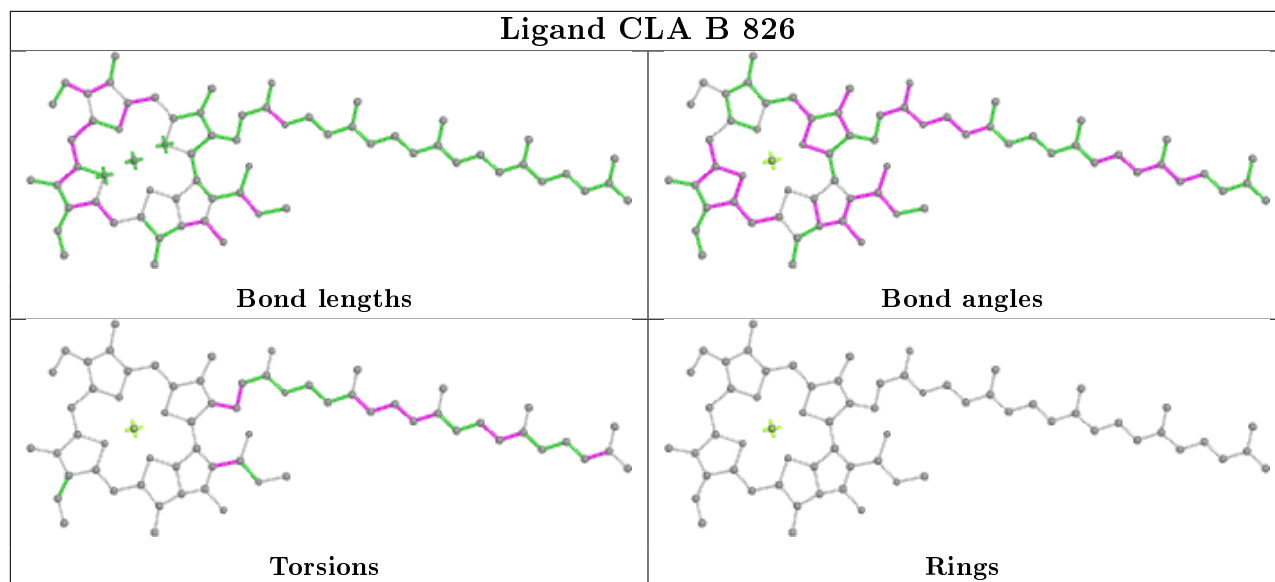


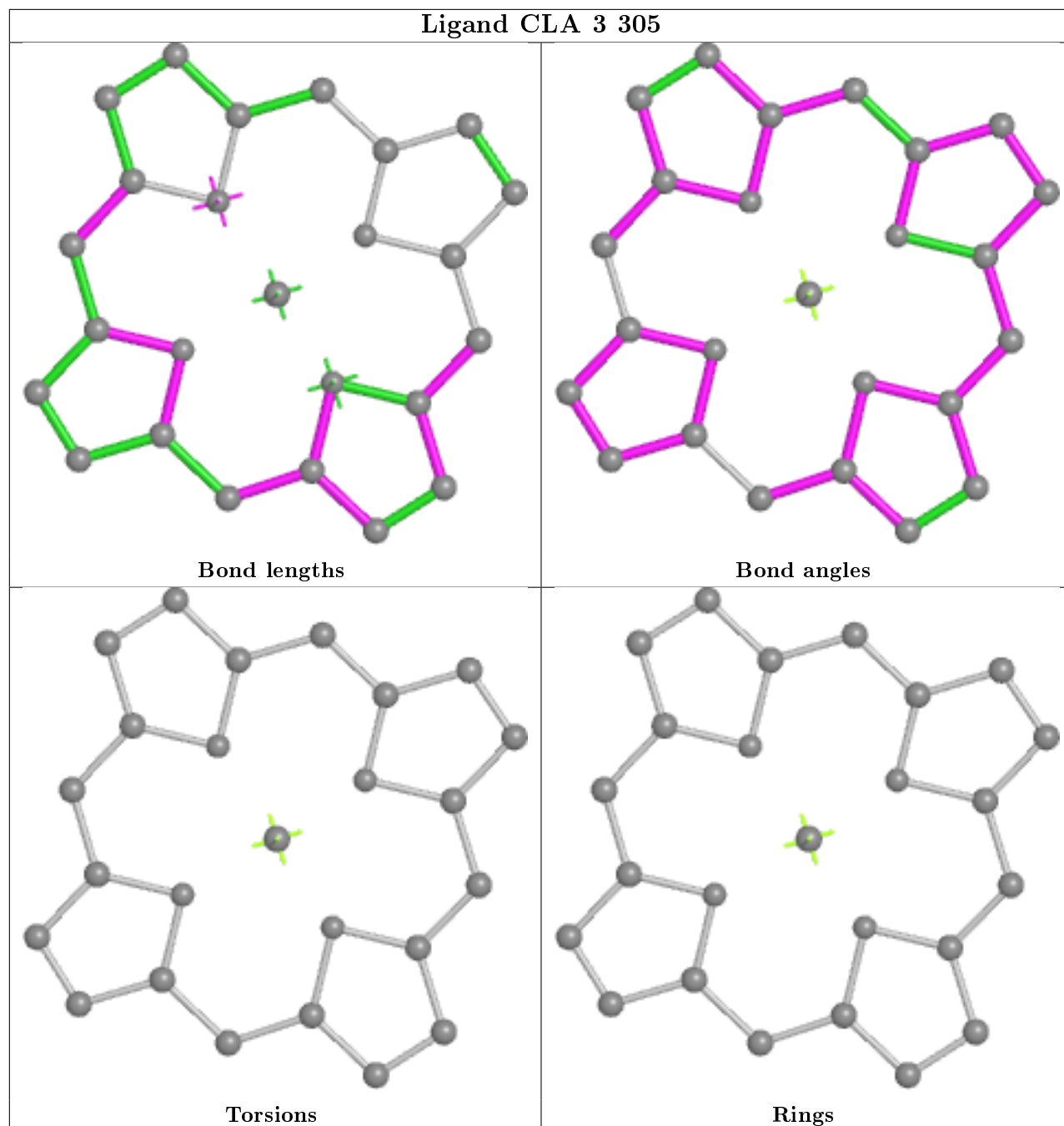


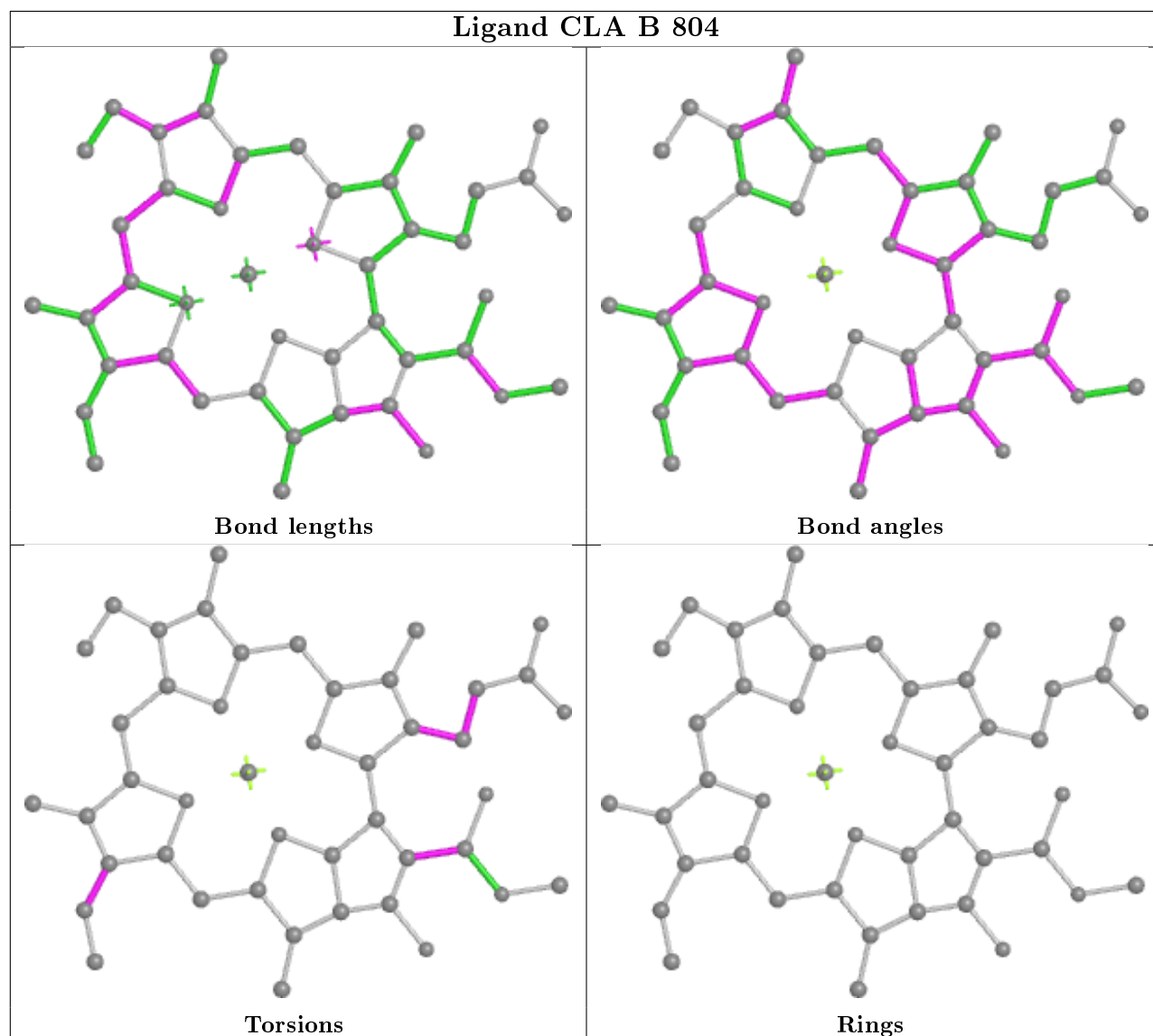
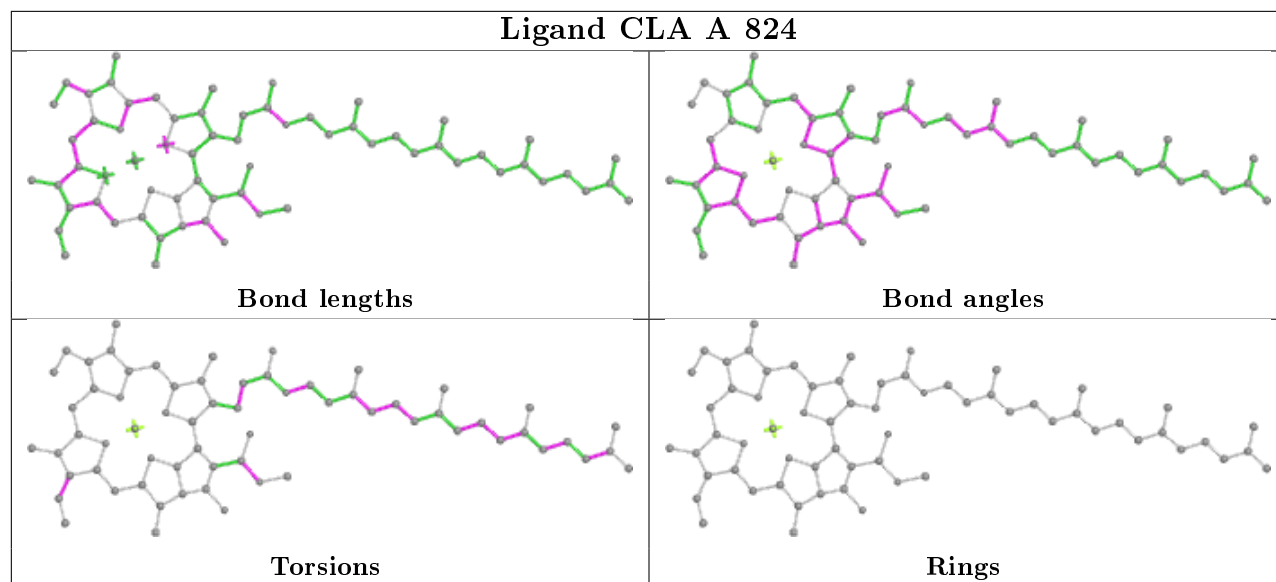


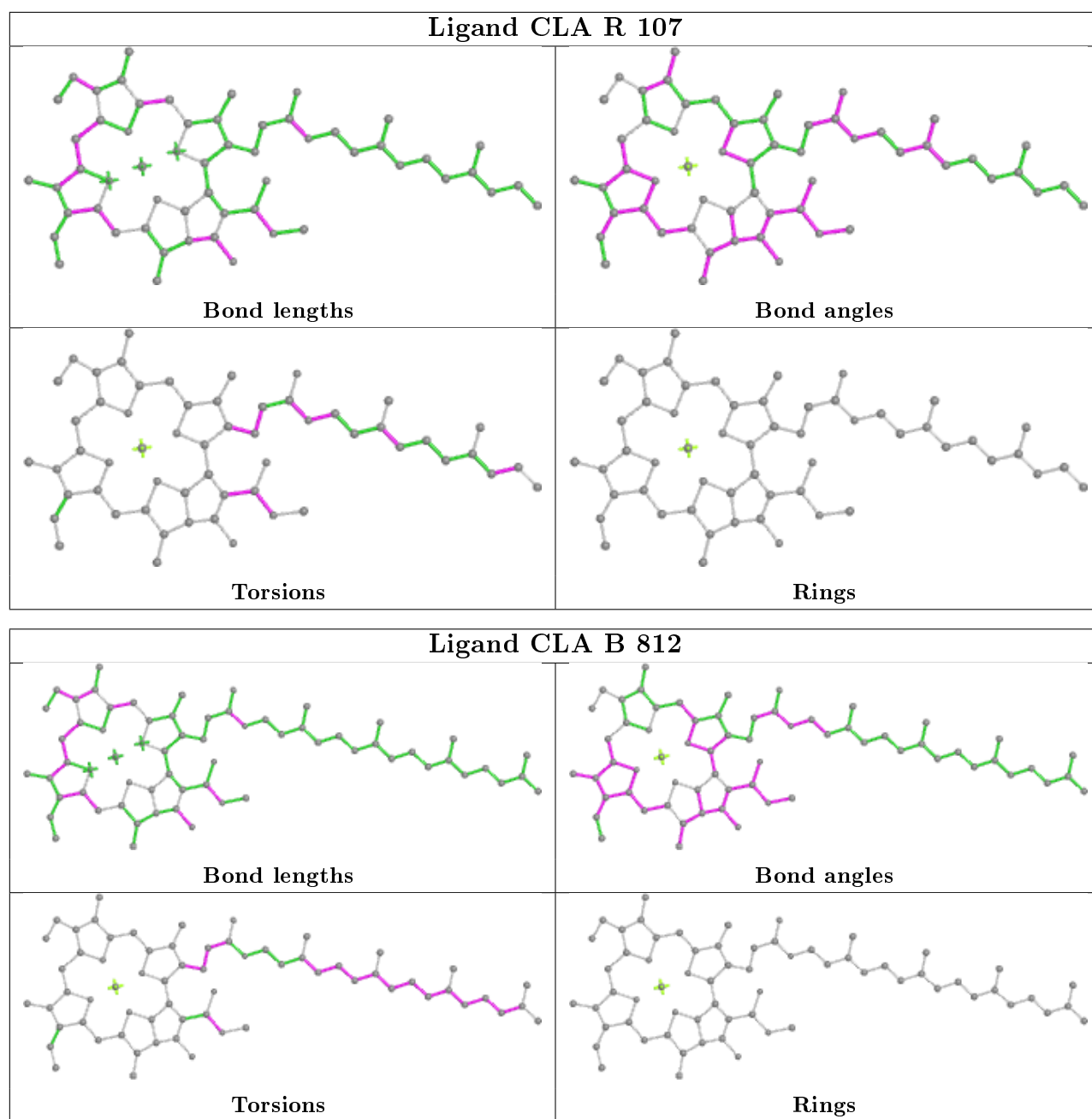


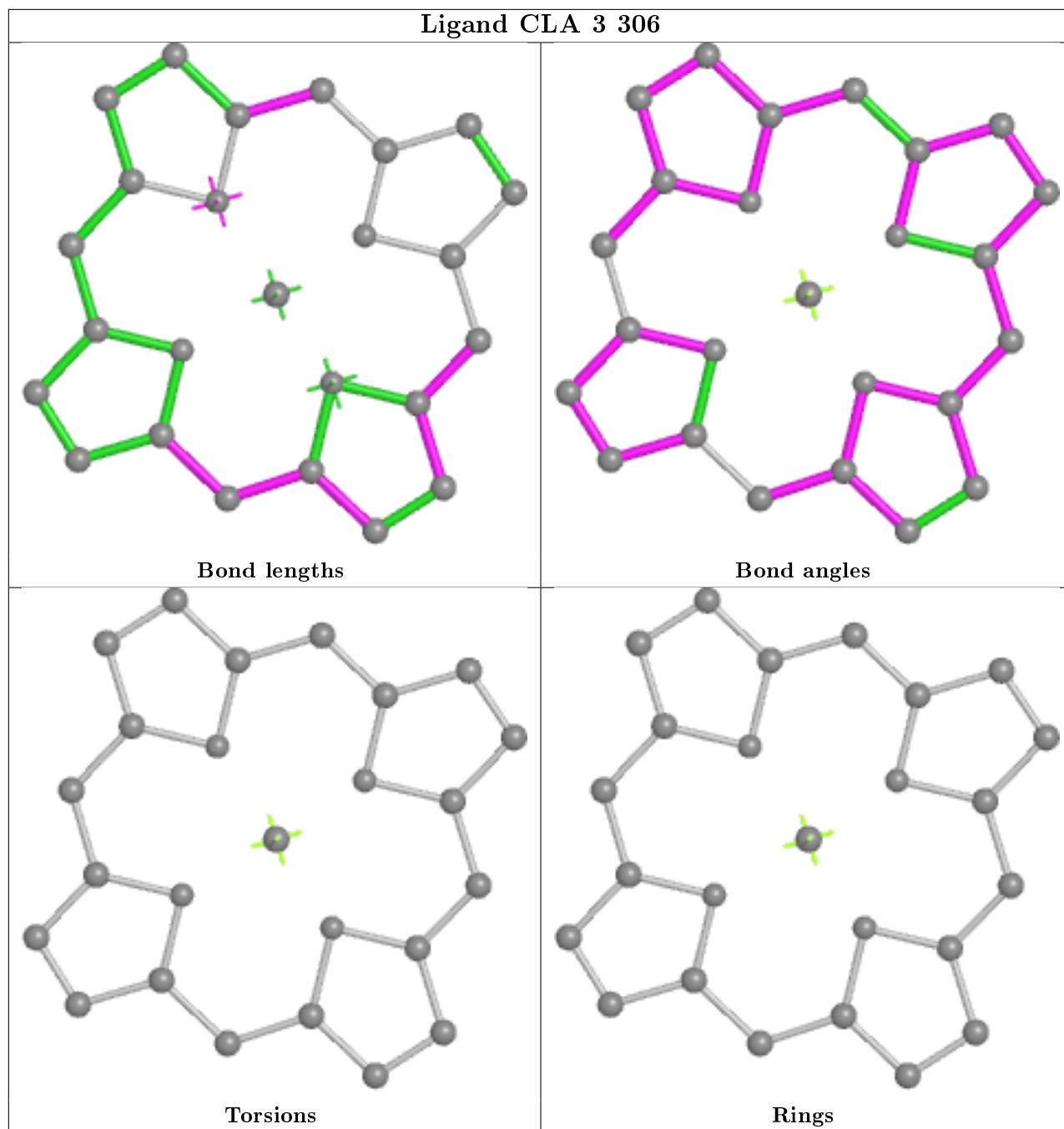


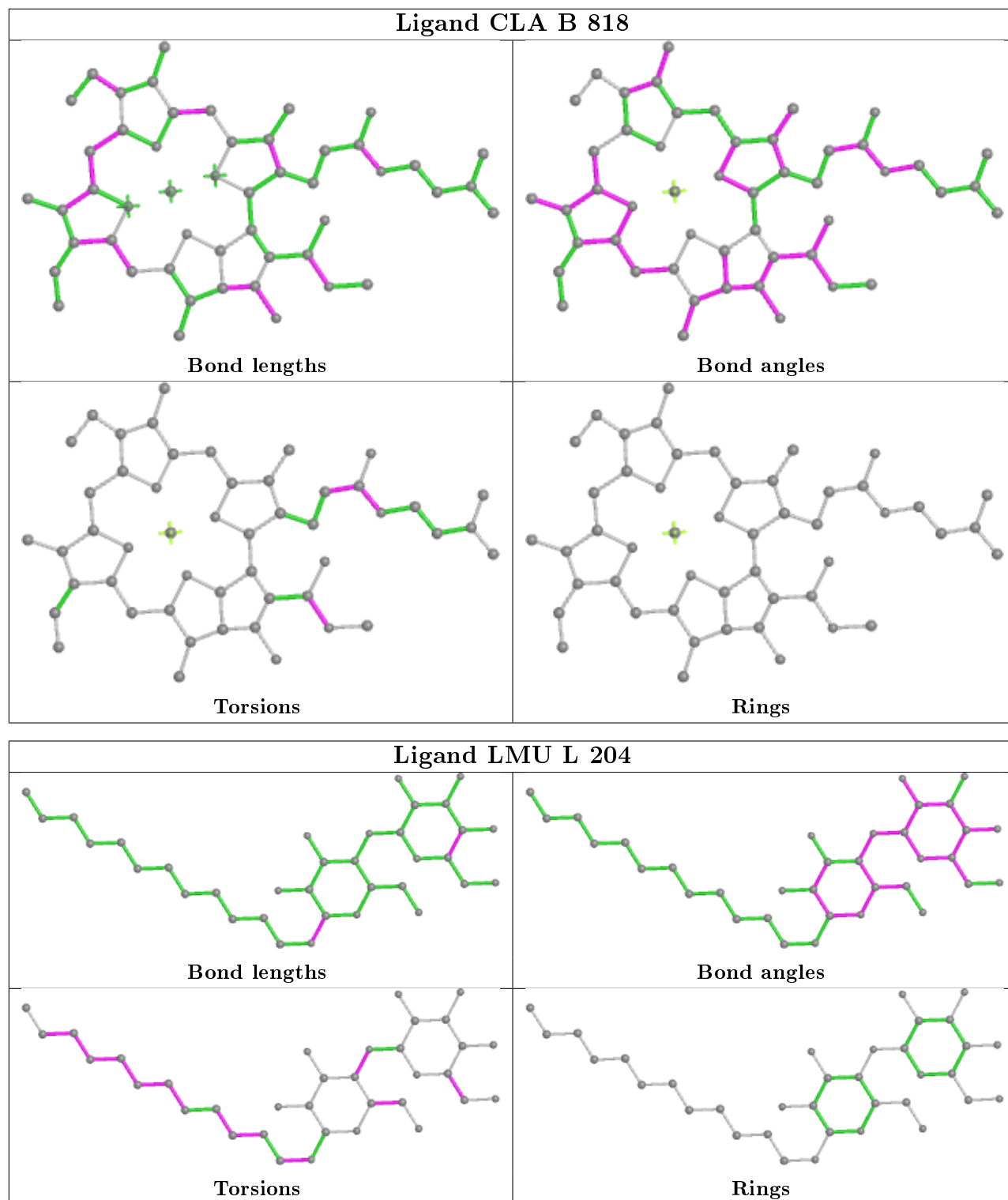


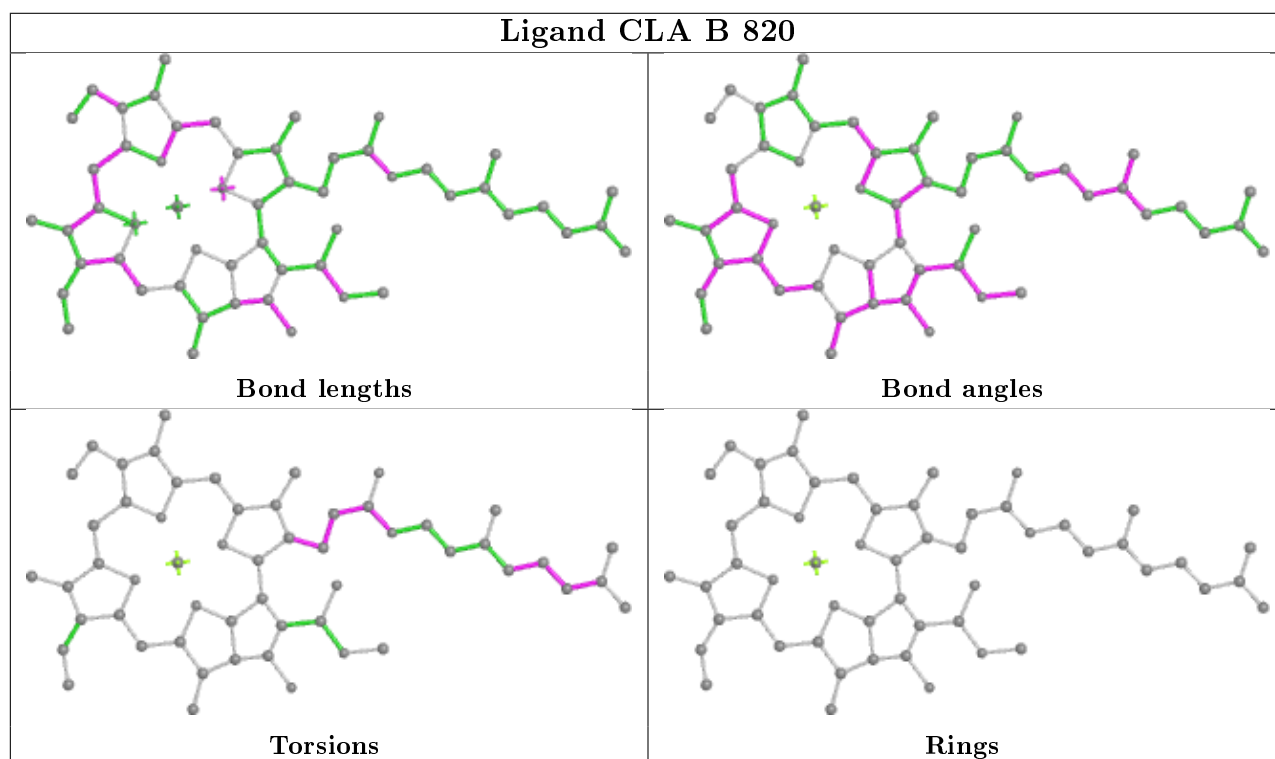
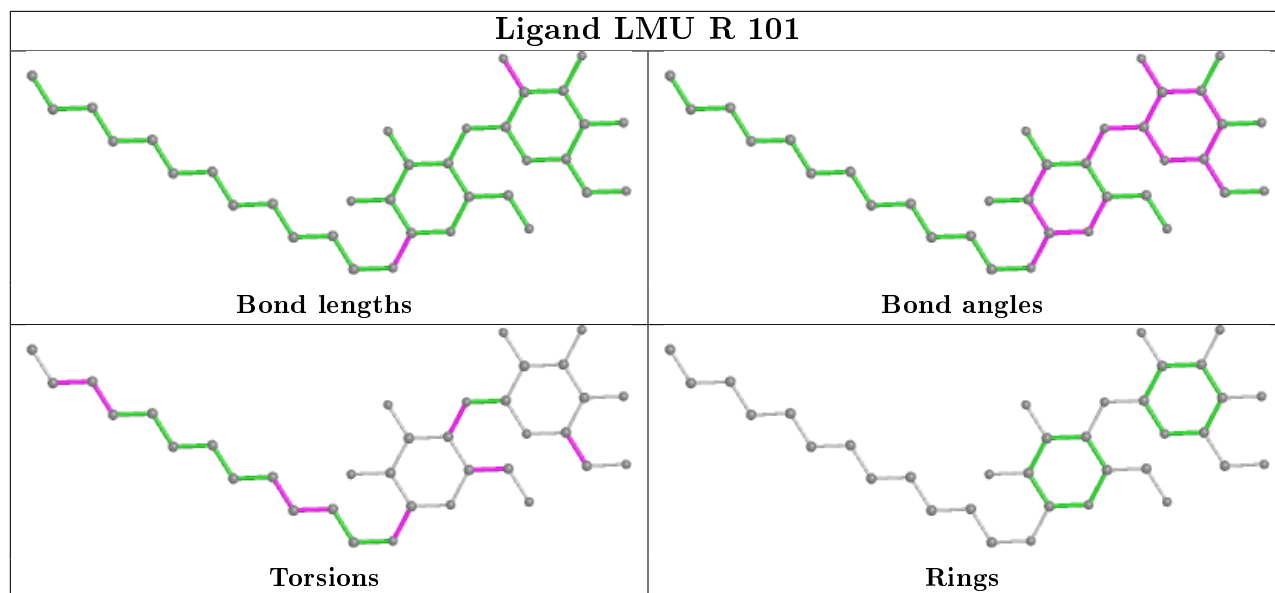




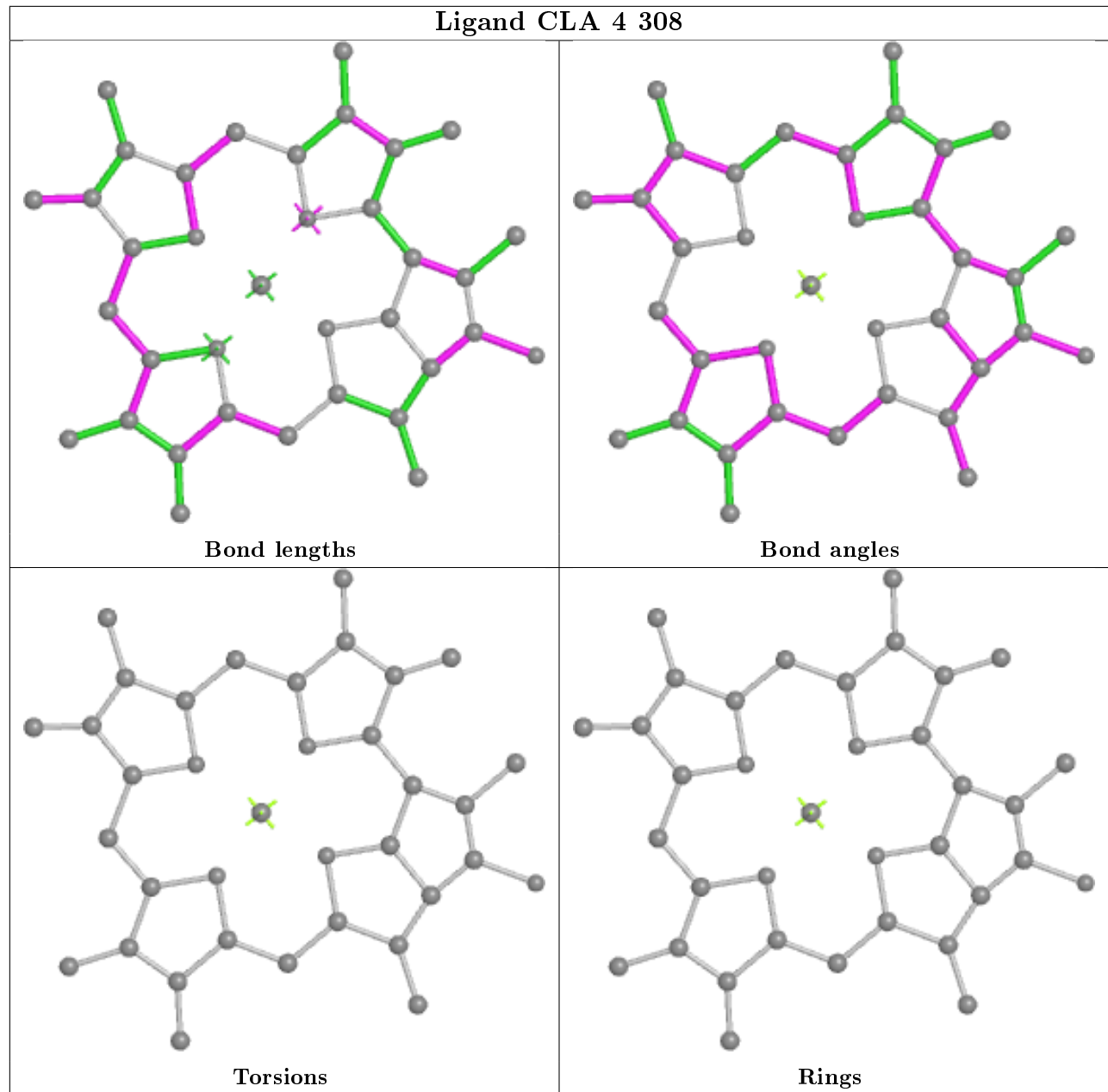


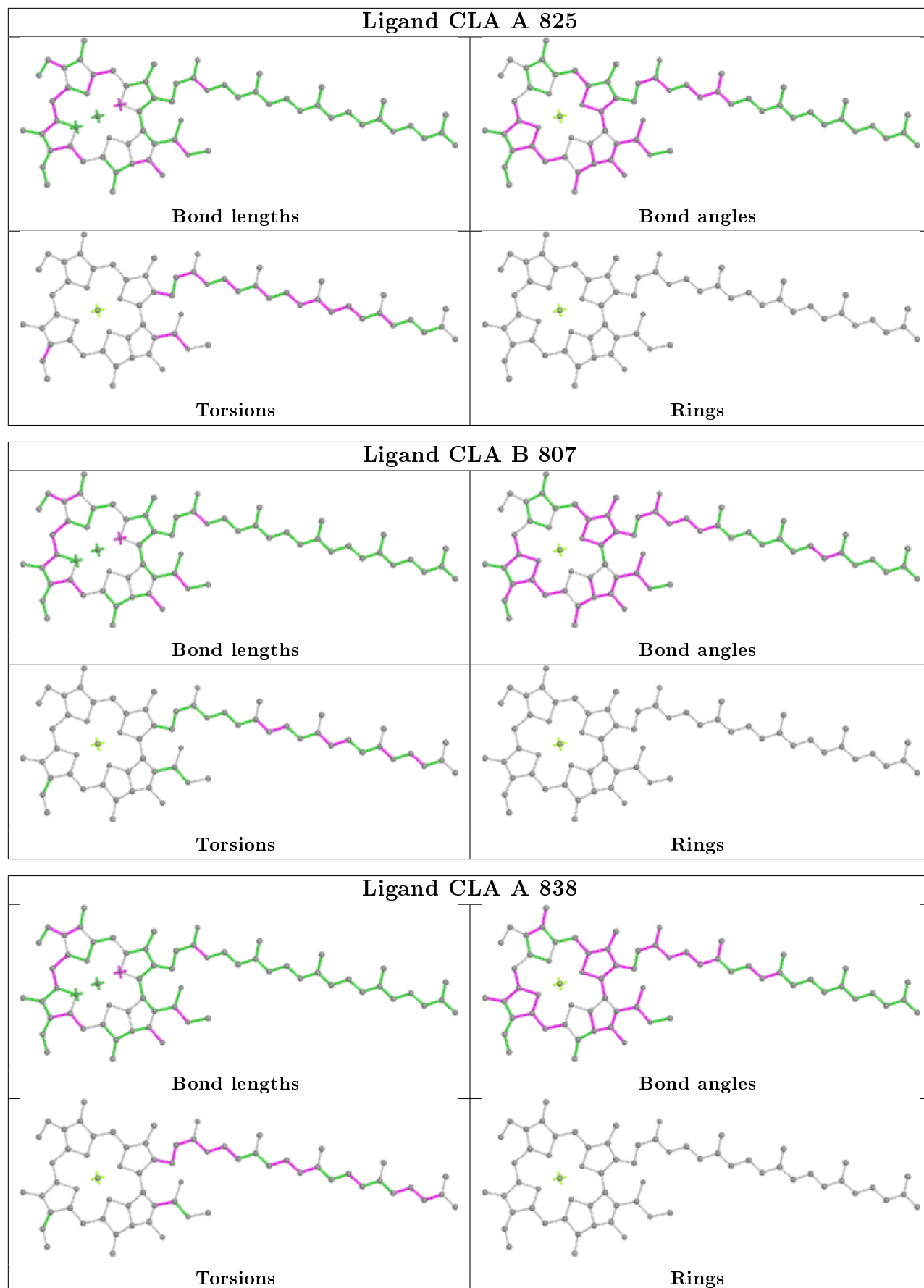


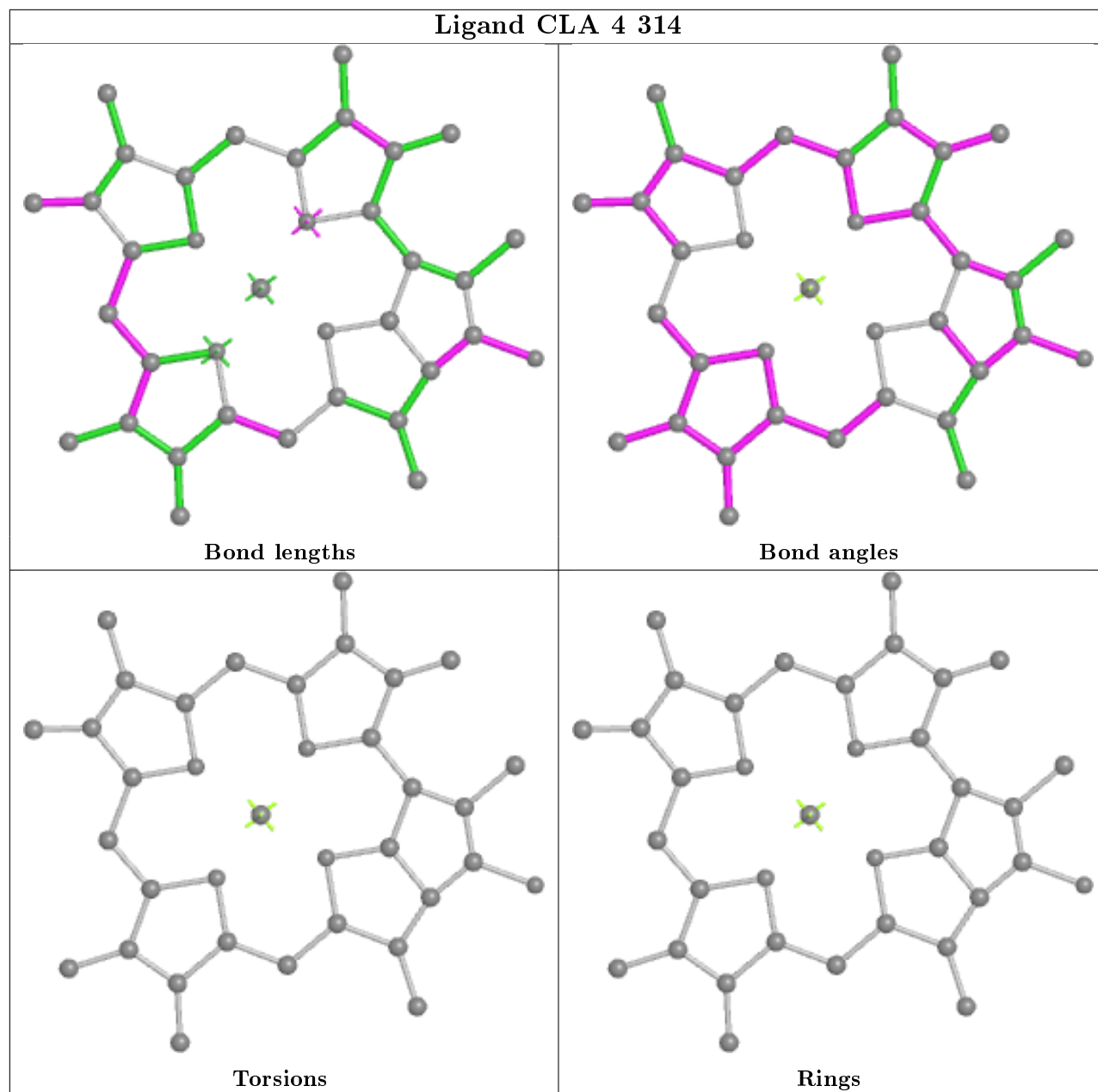


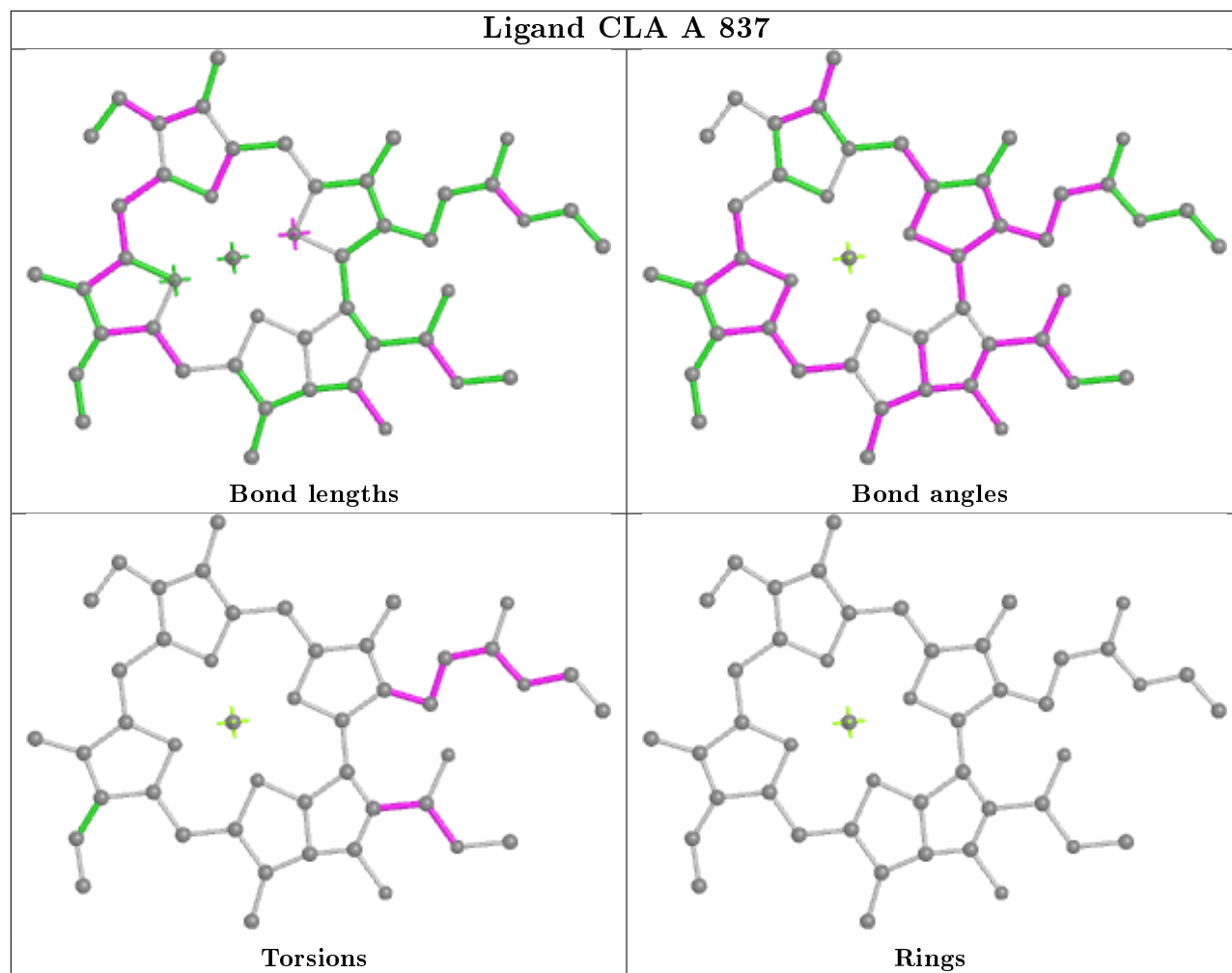


Ligand CLA 4 308

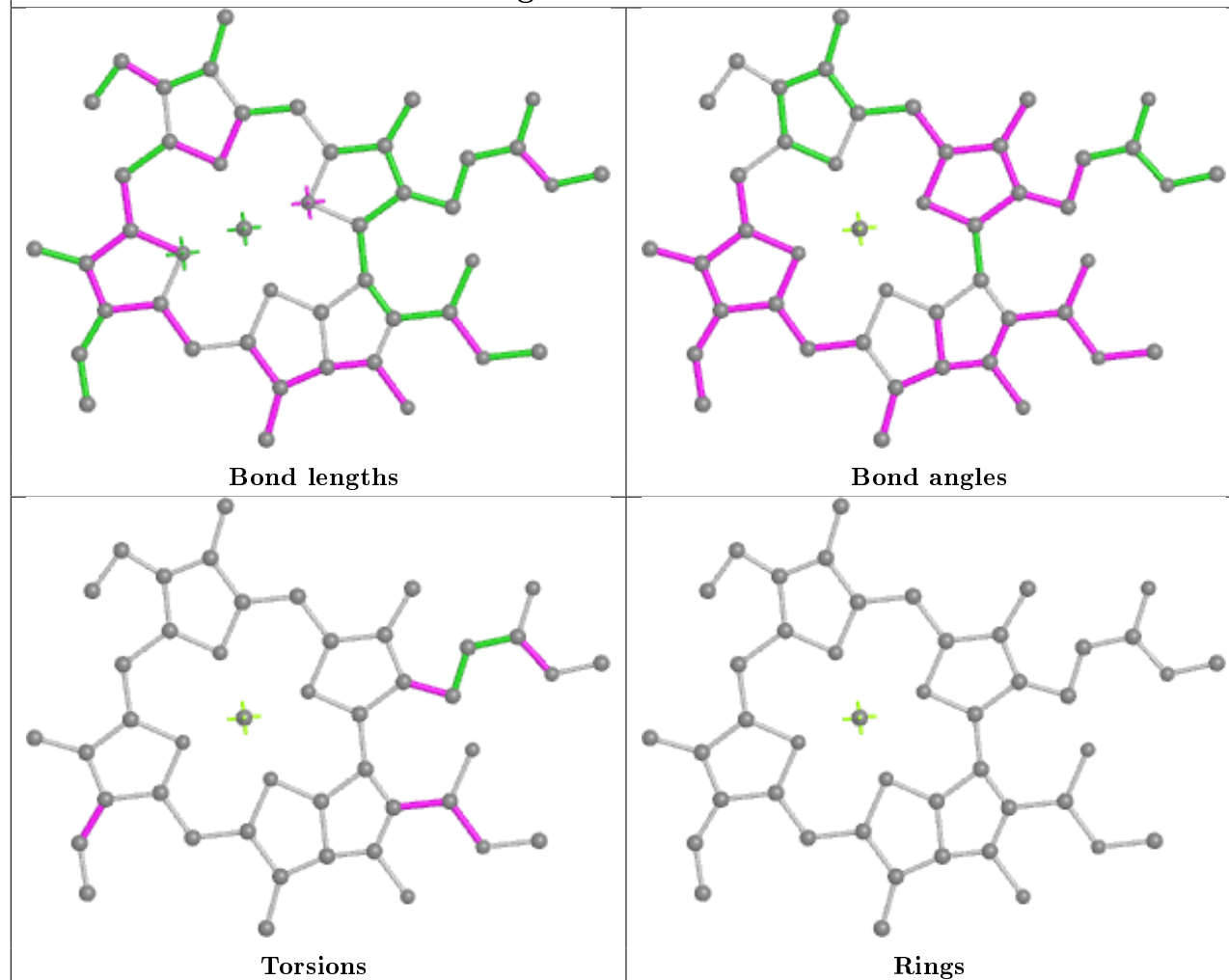




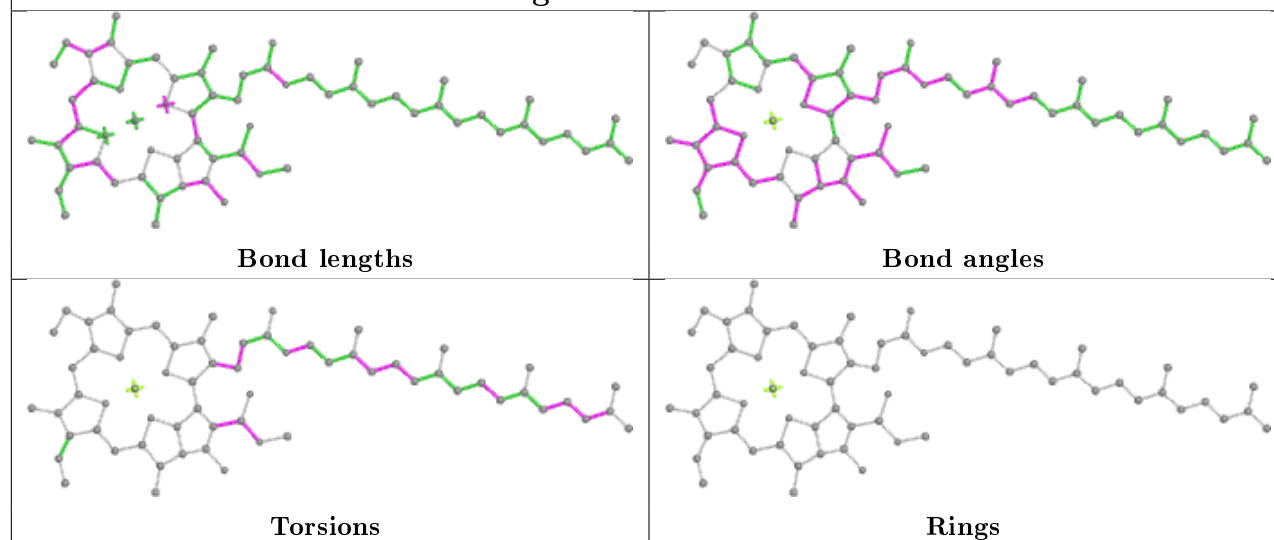


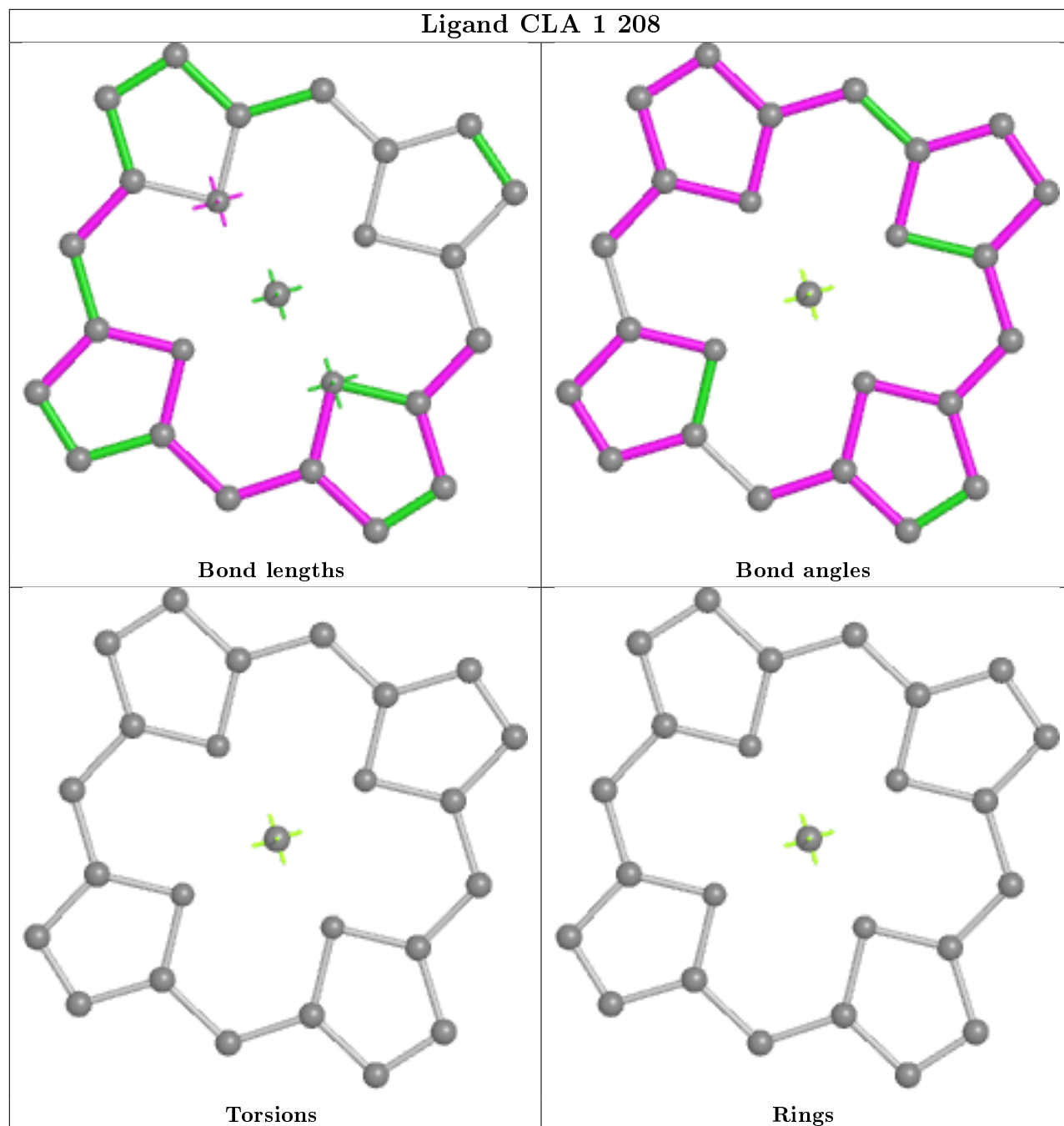


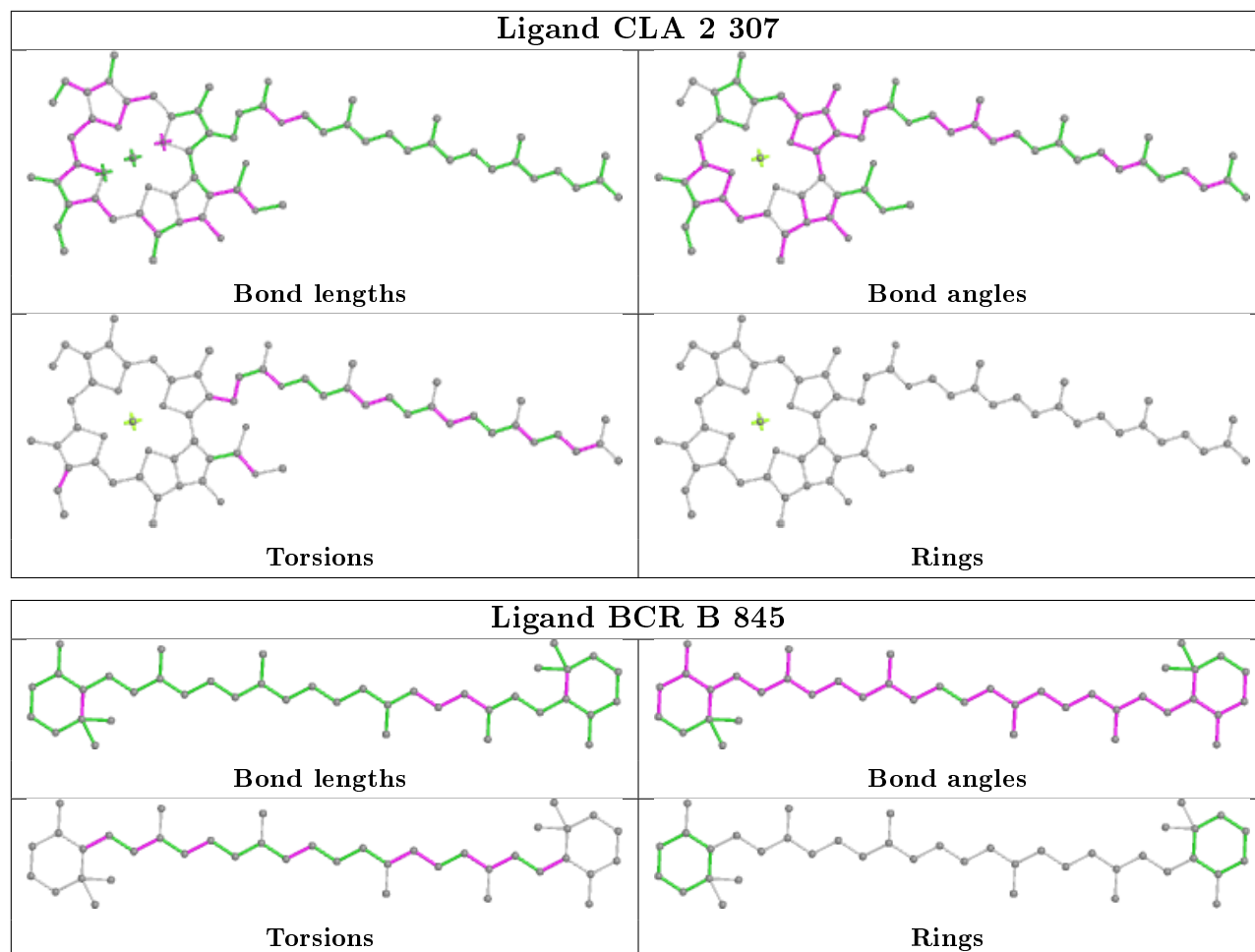
Ligand CLA 1 201

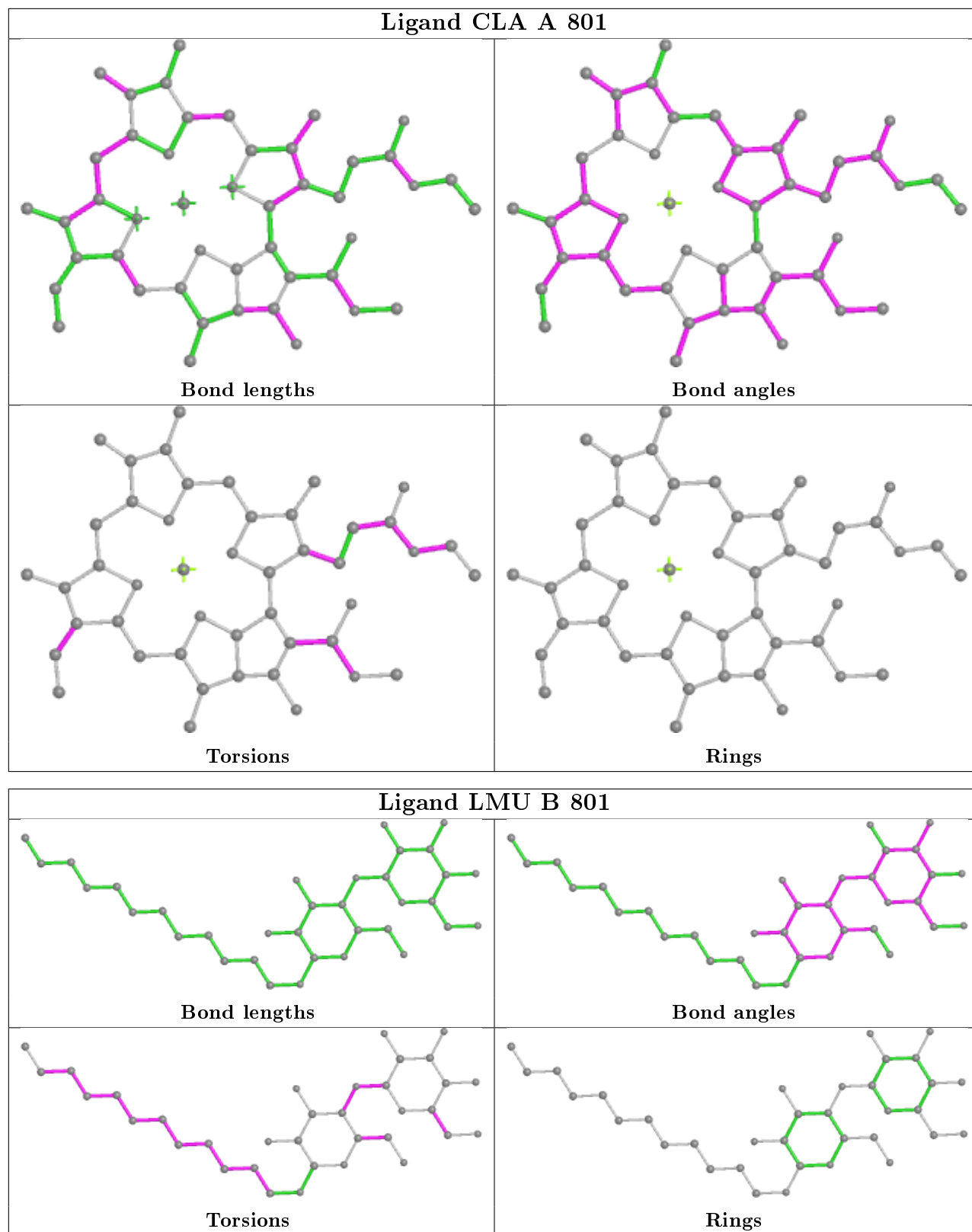


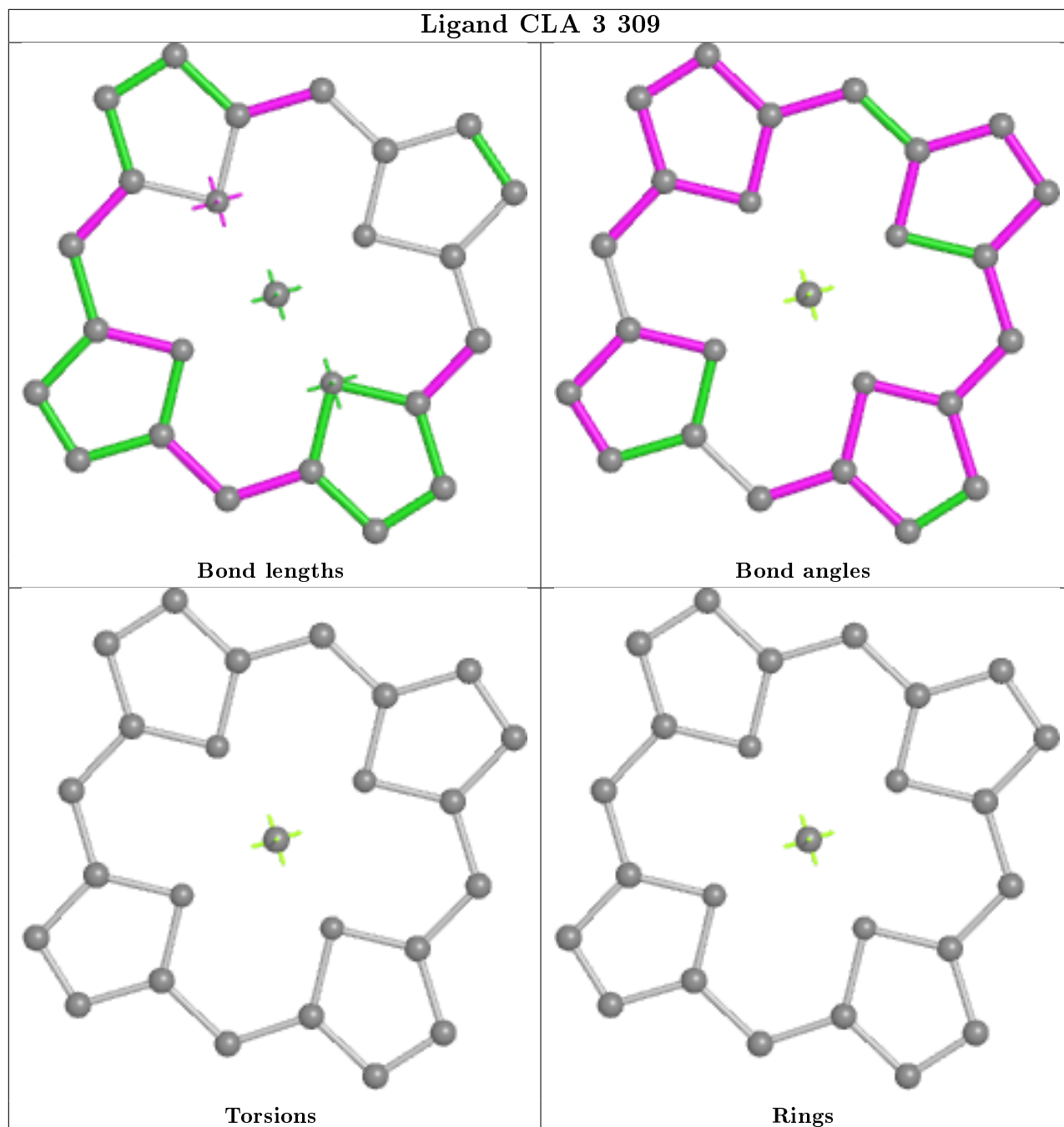
Ligand CLA B 850

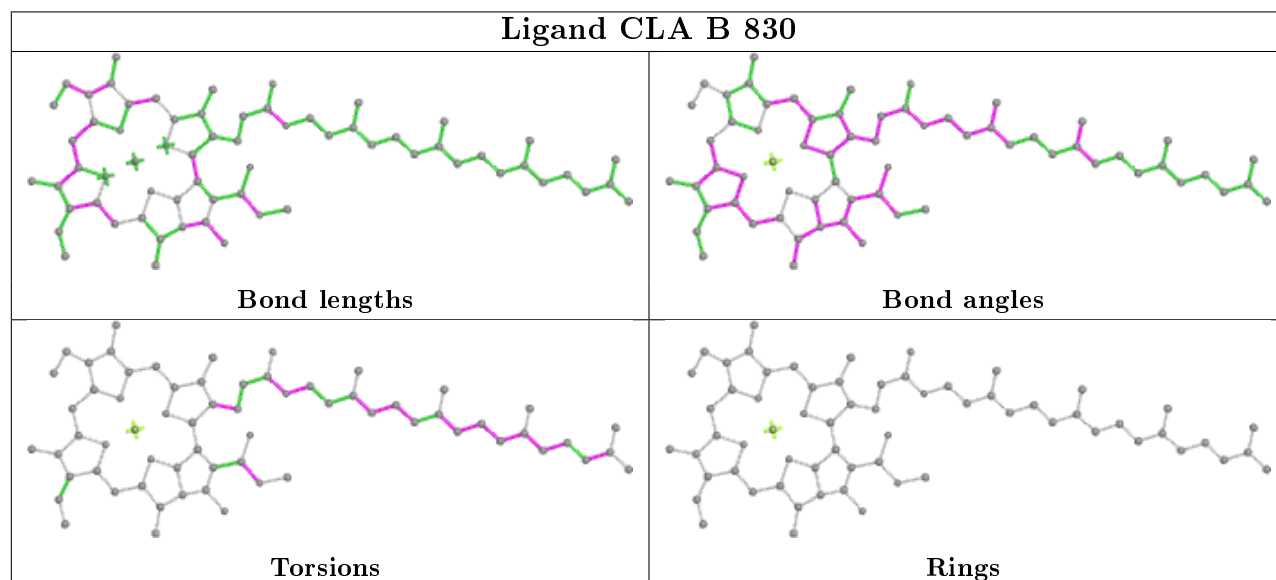
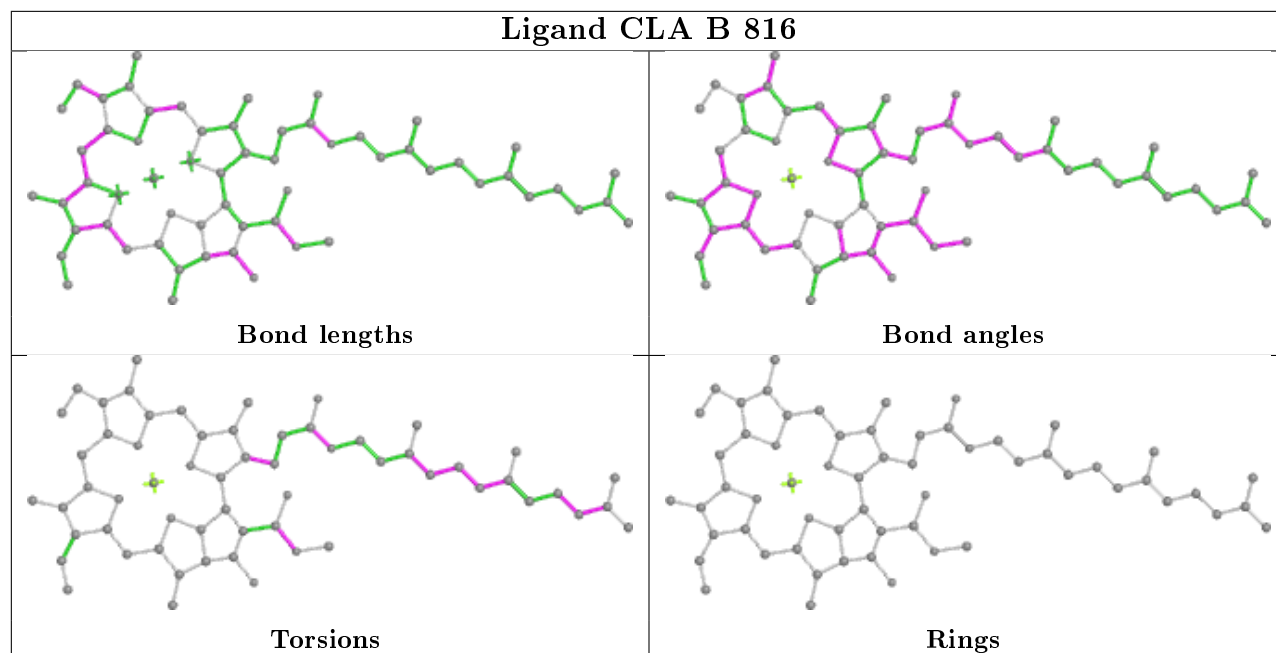


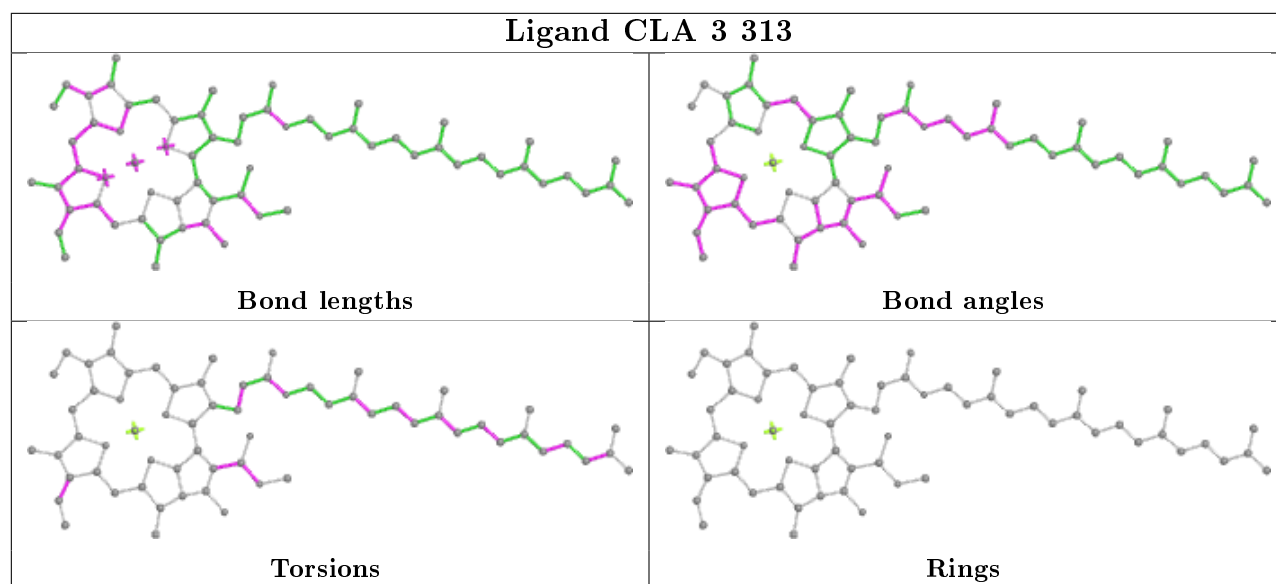
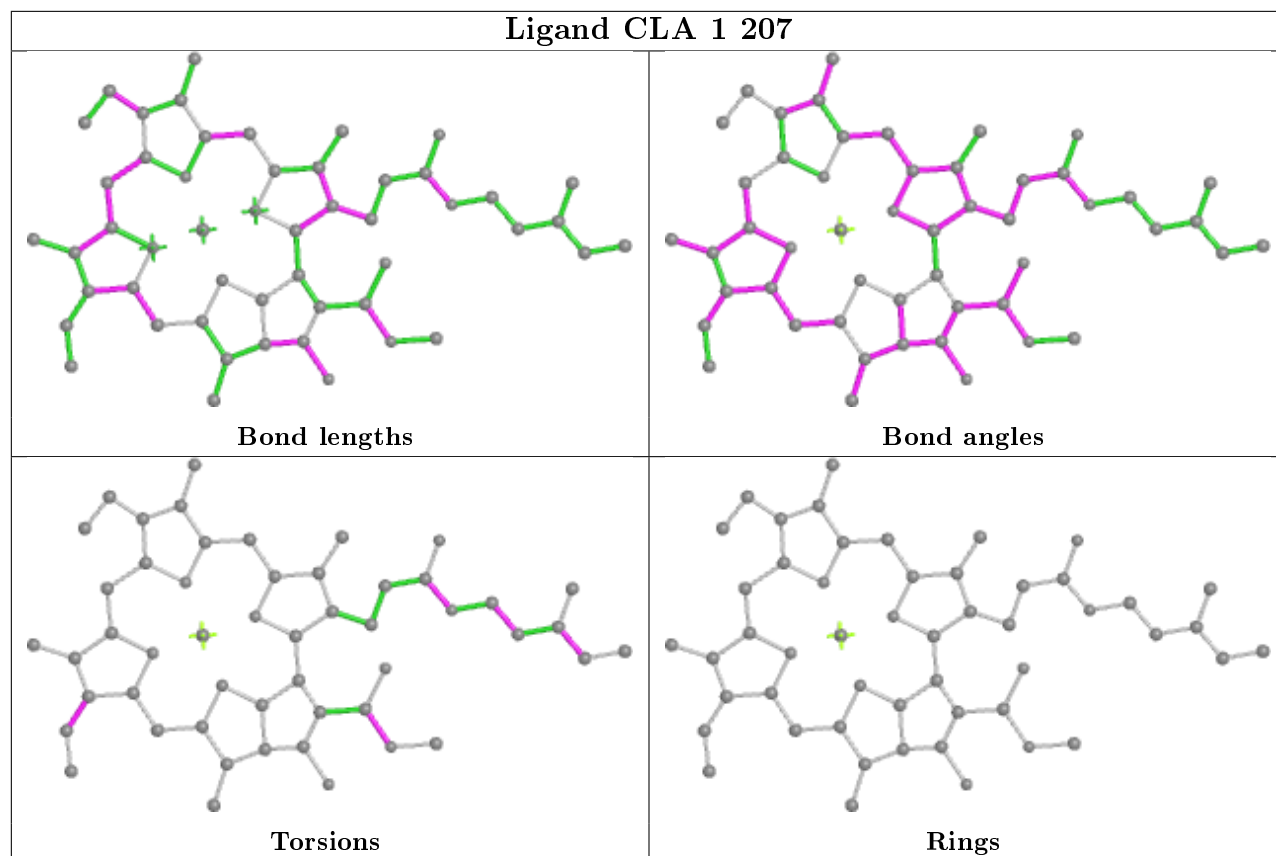


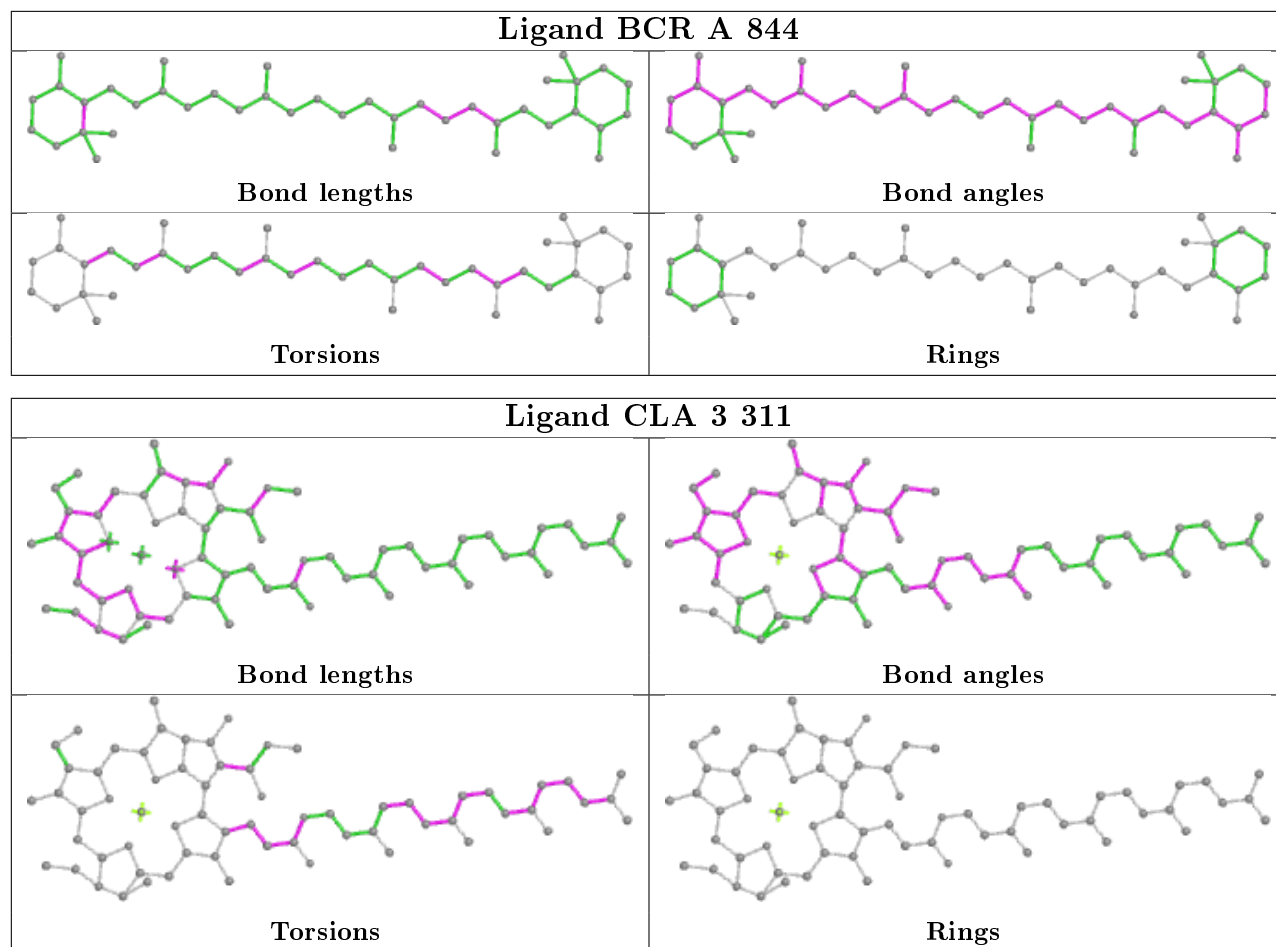


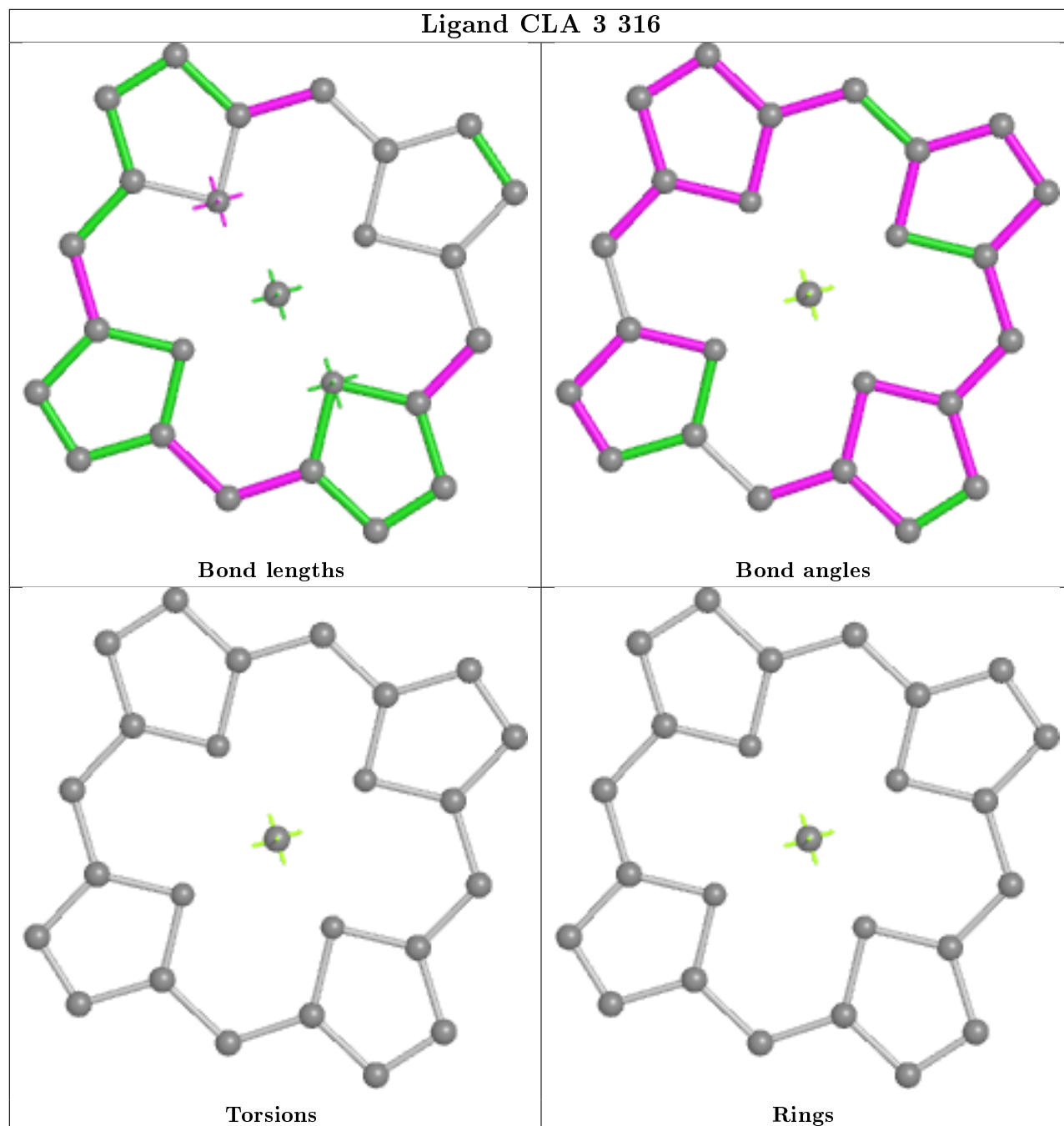


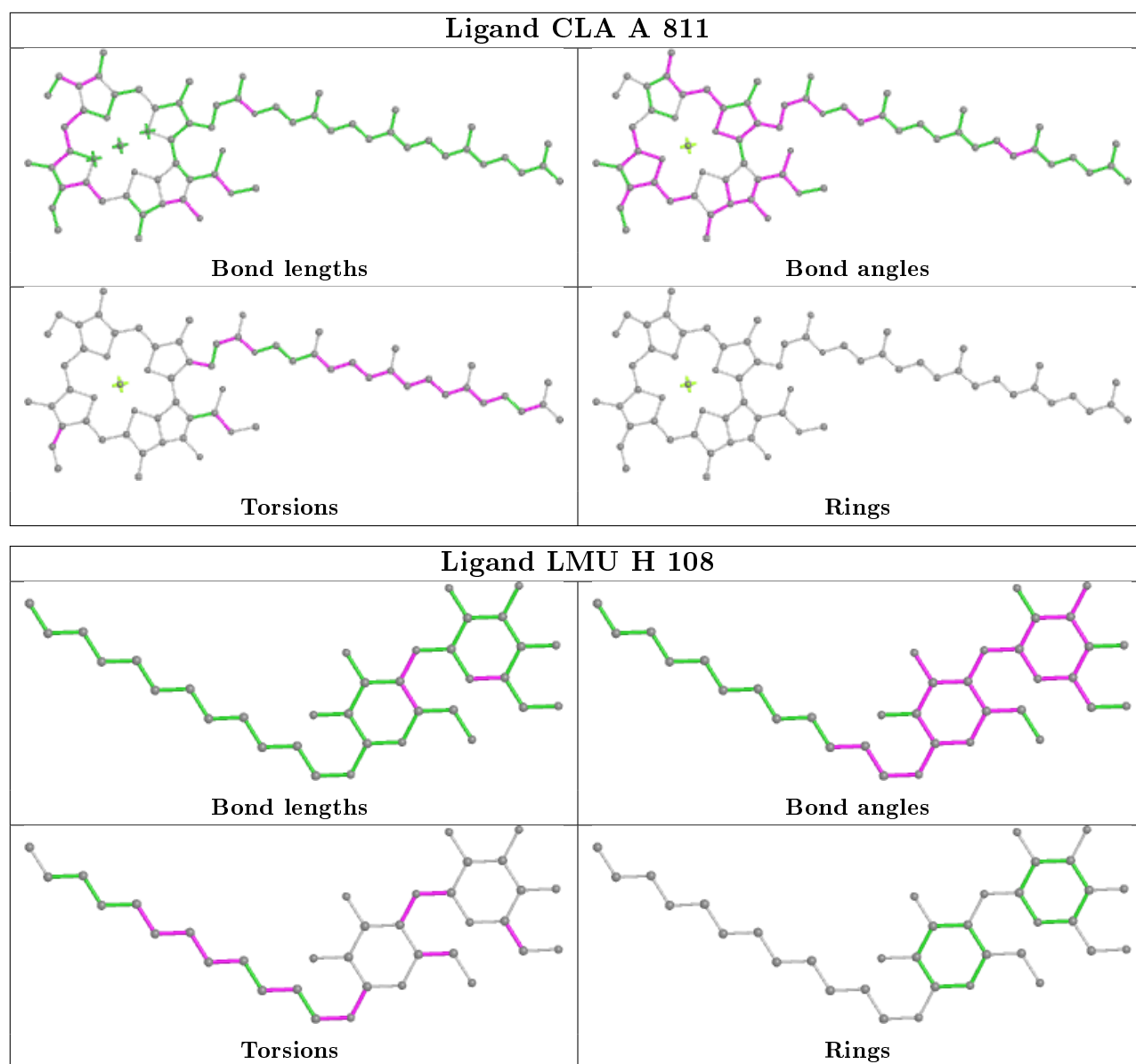


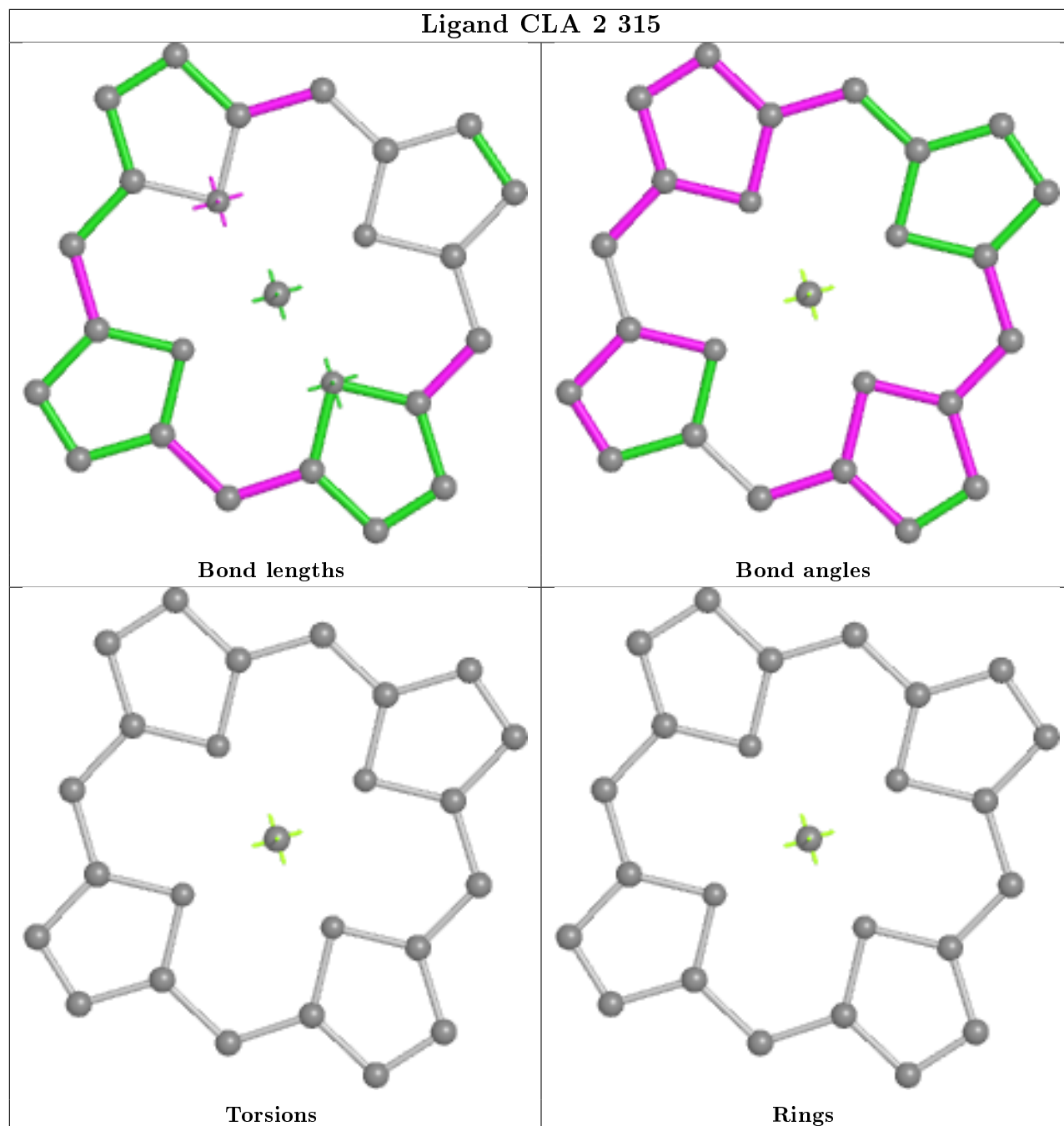


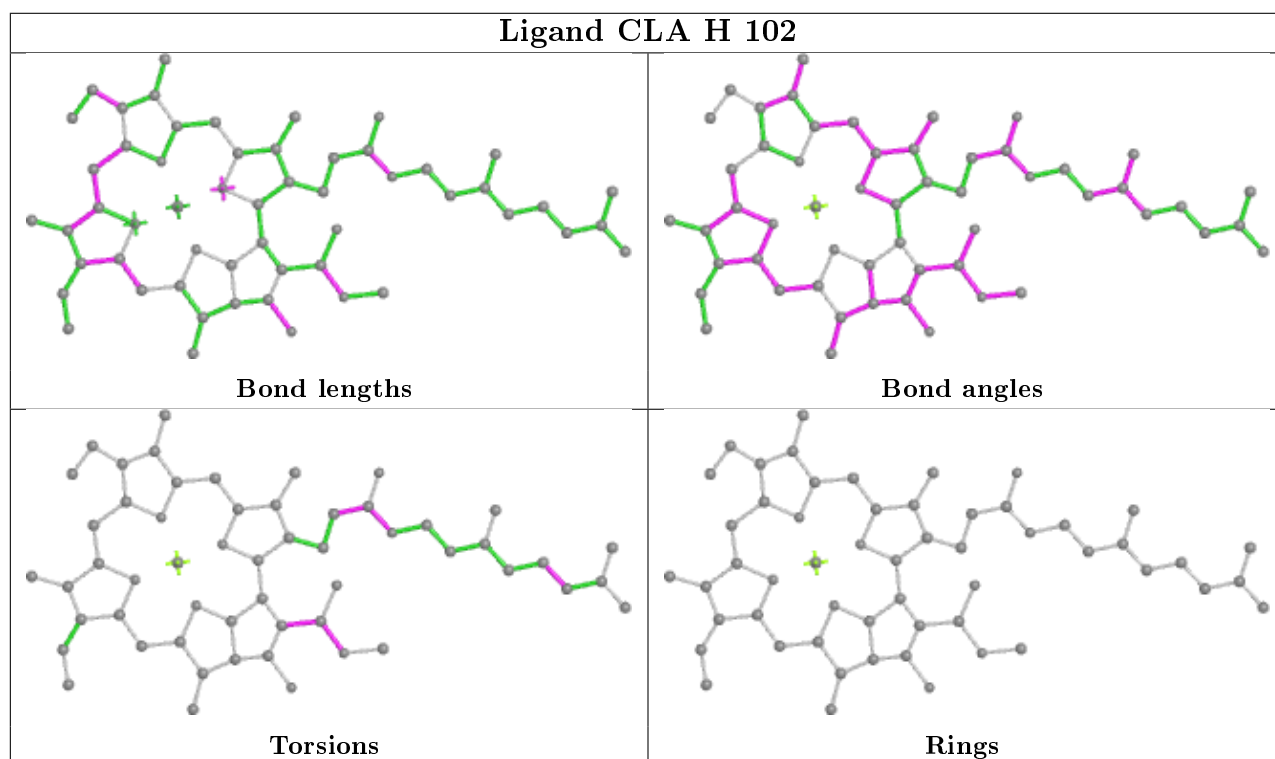
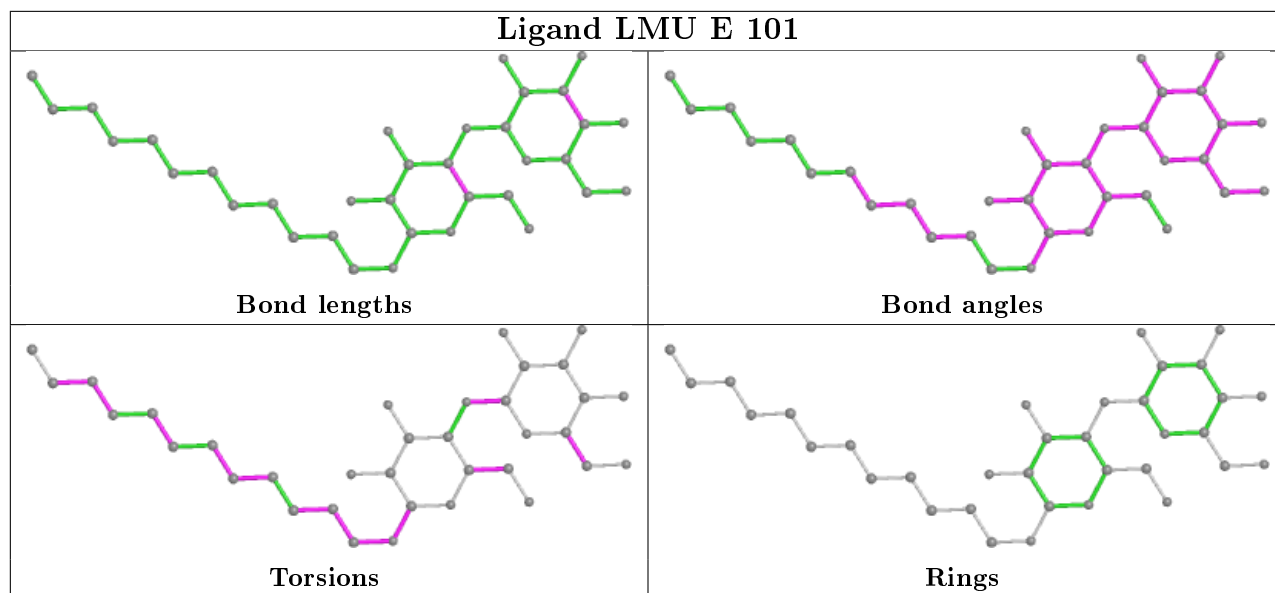


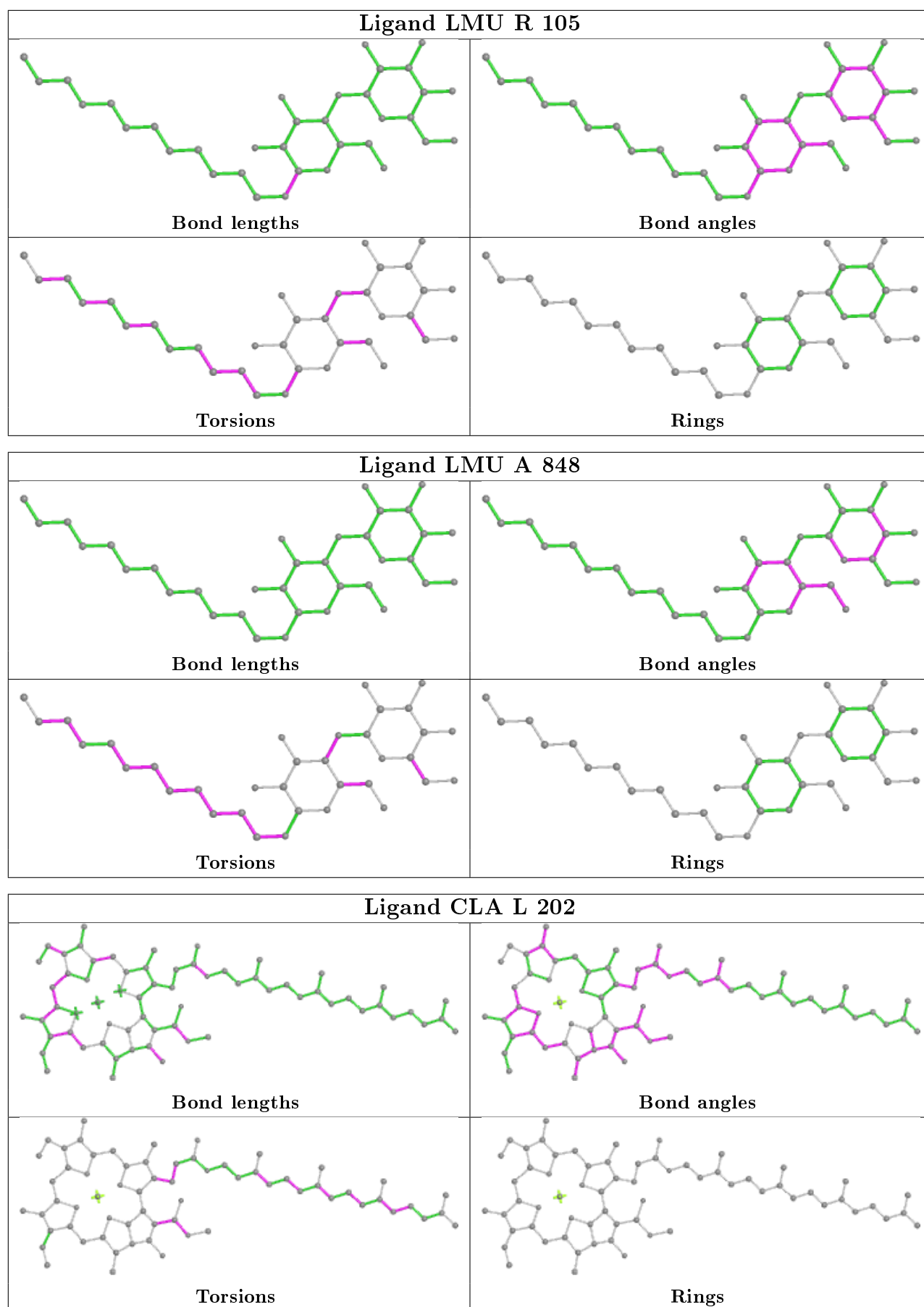


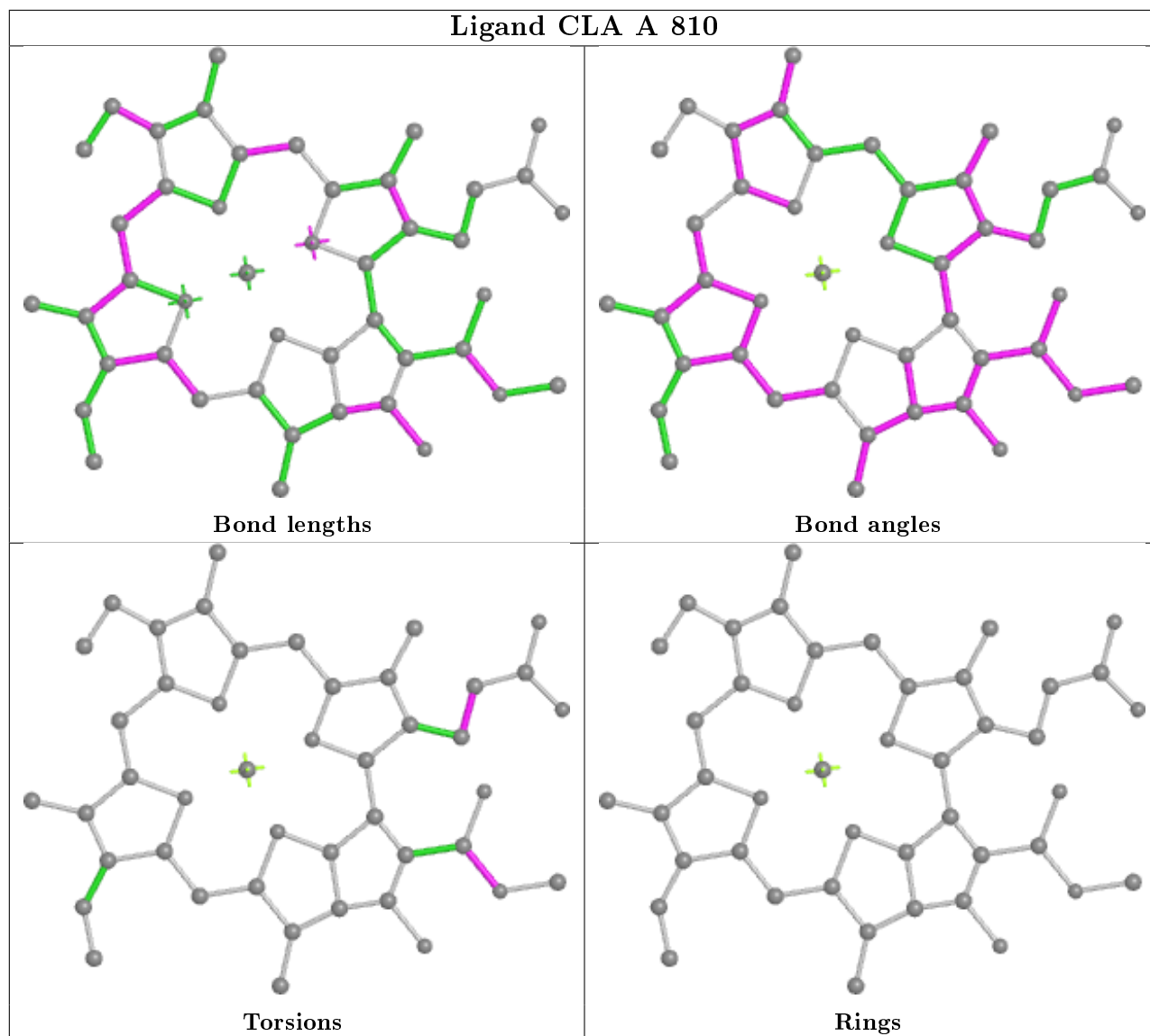
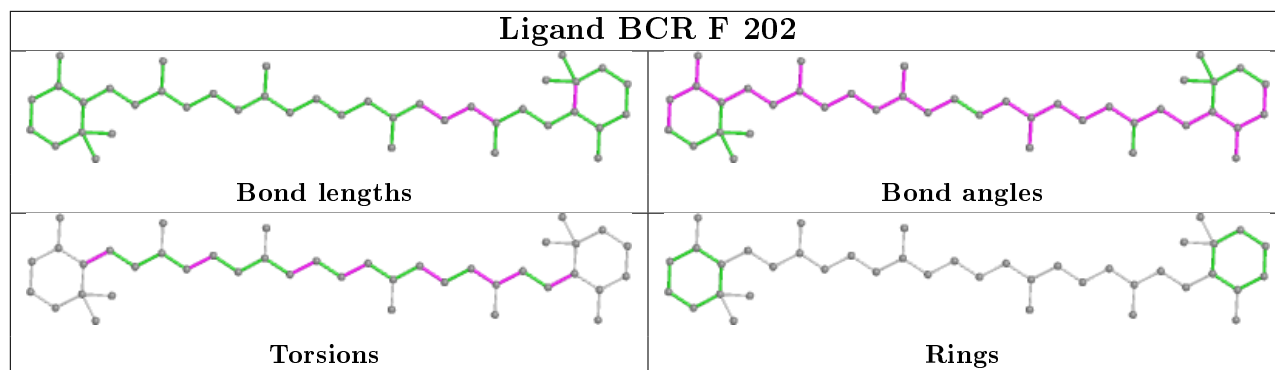


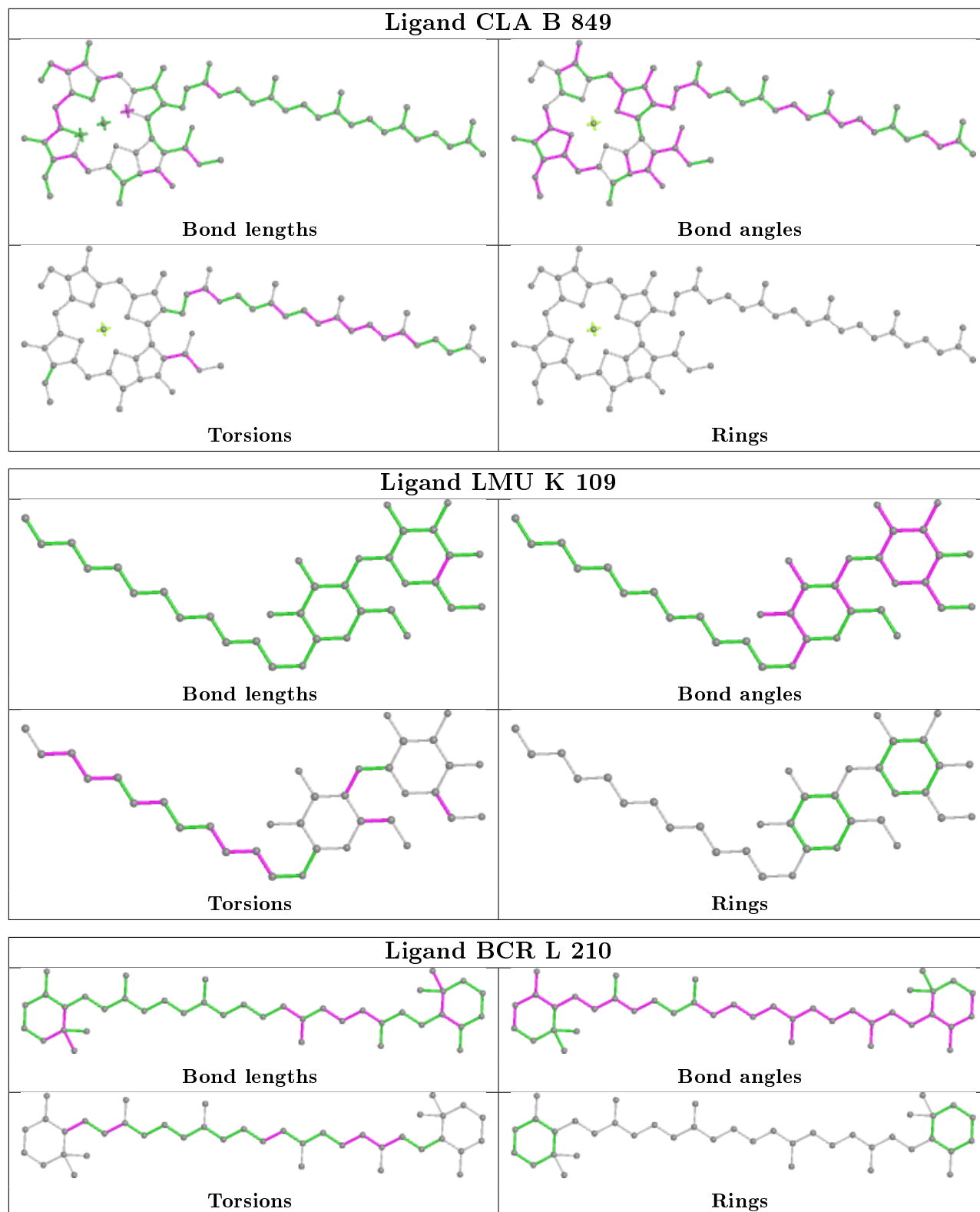


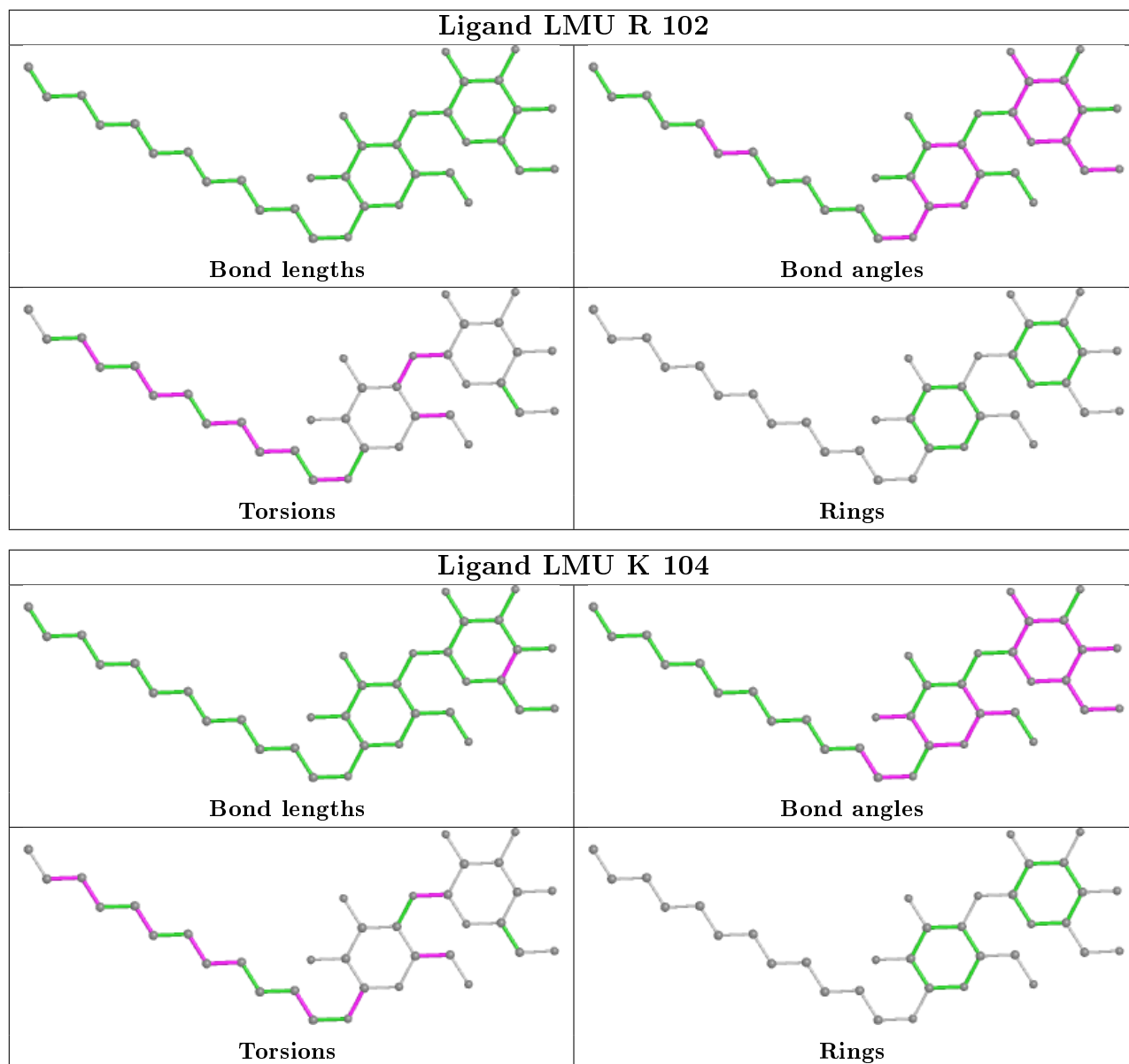


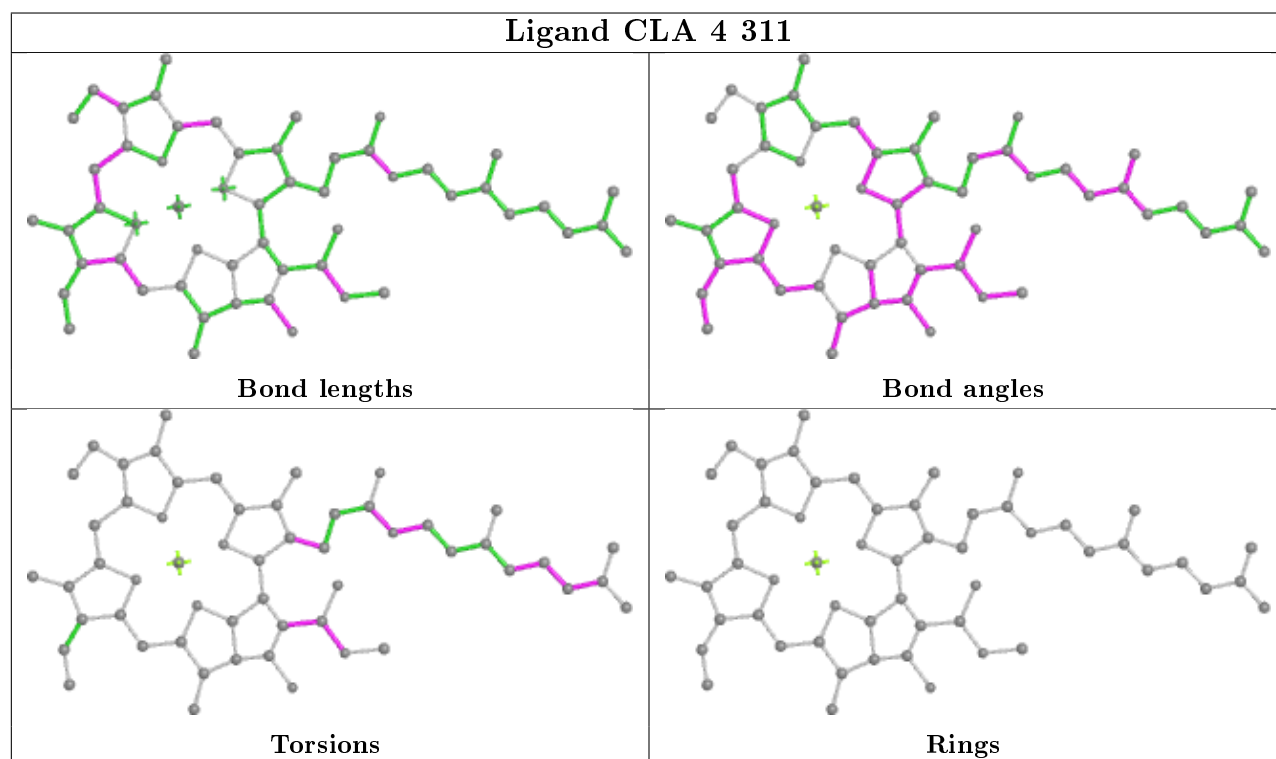
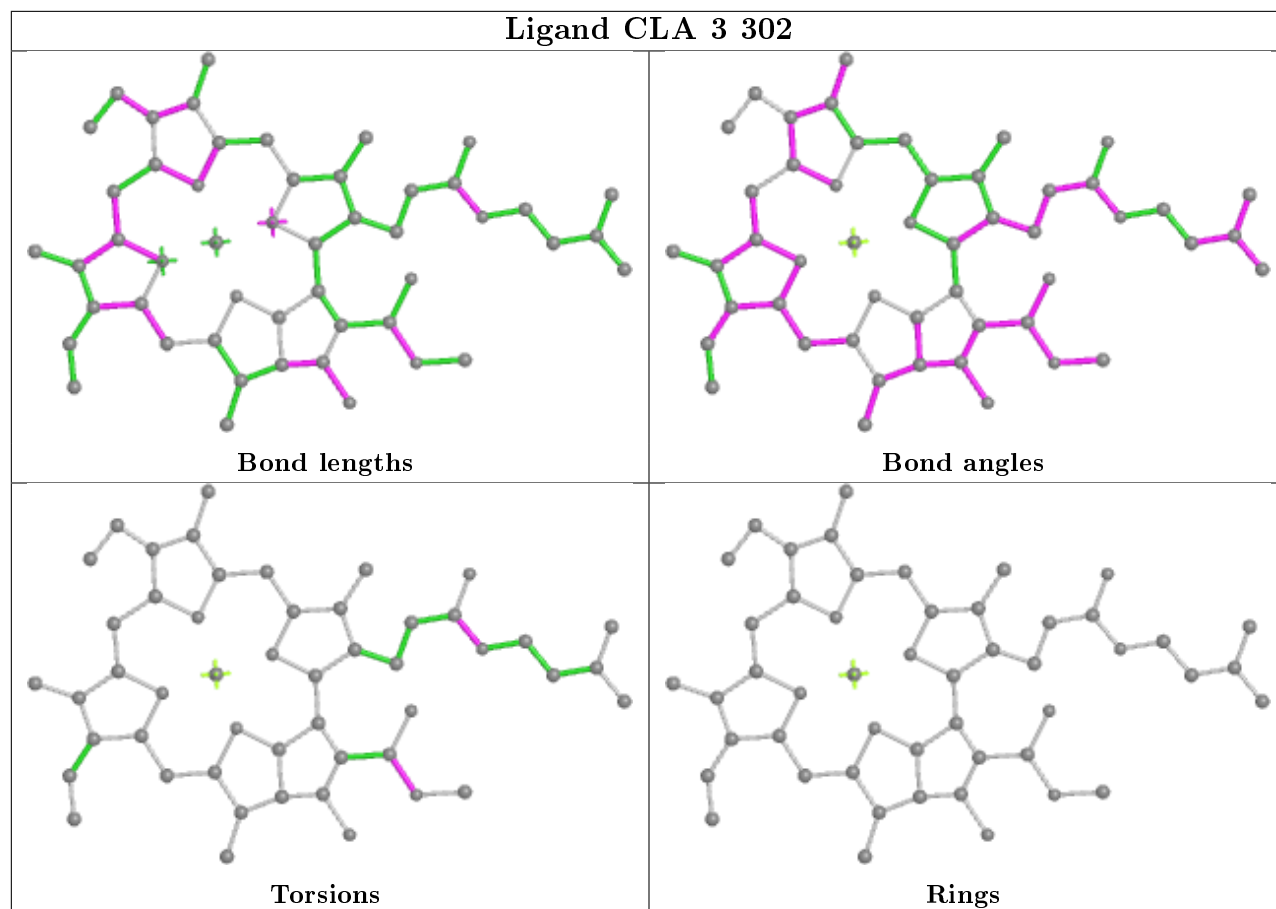


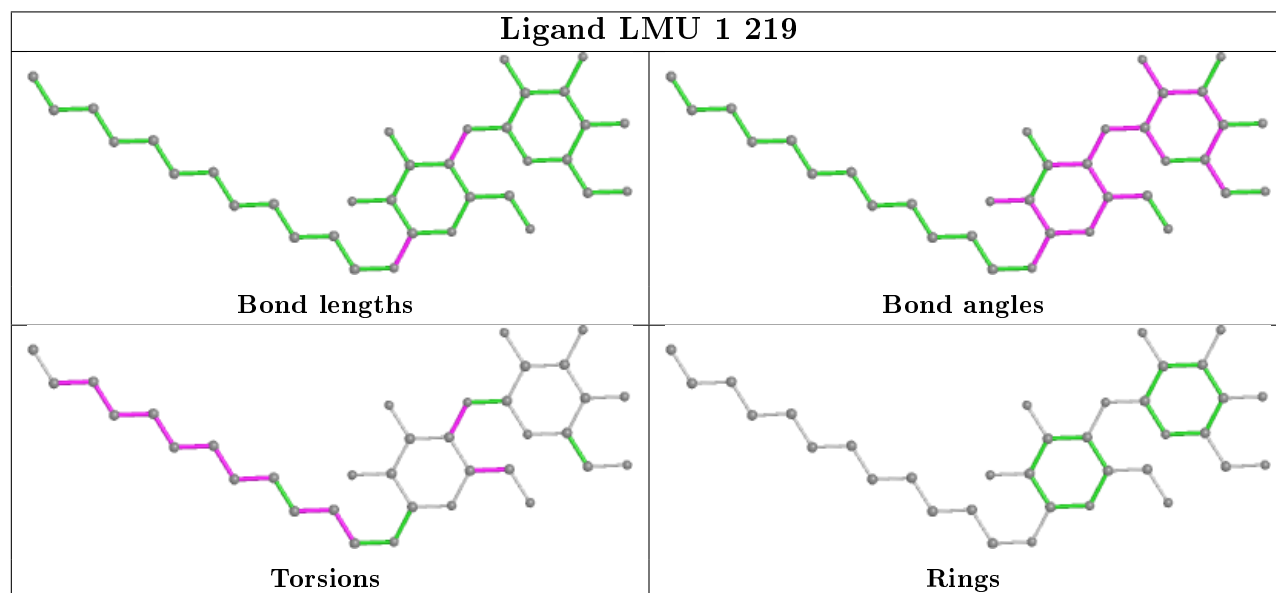
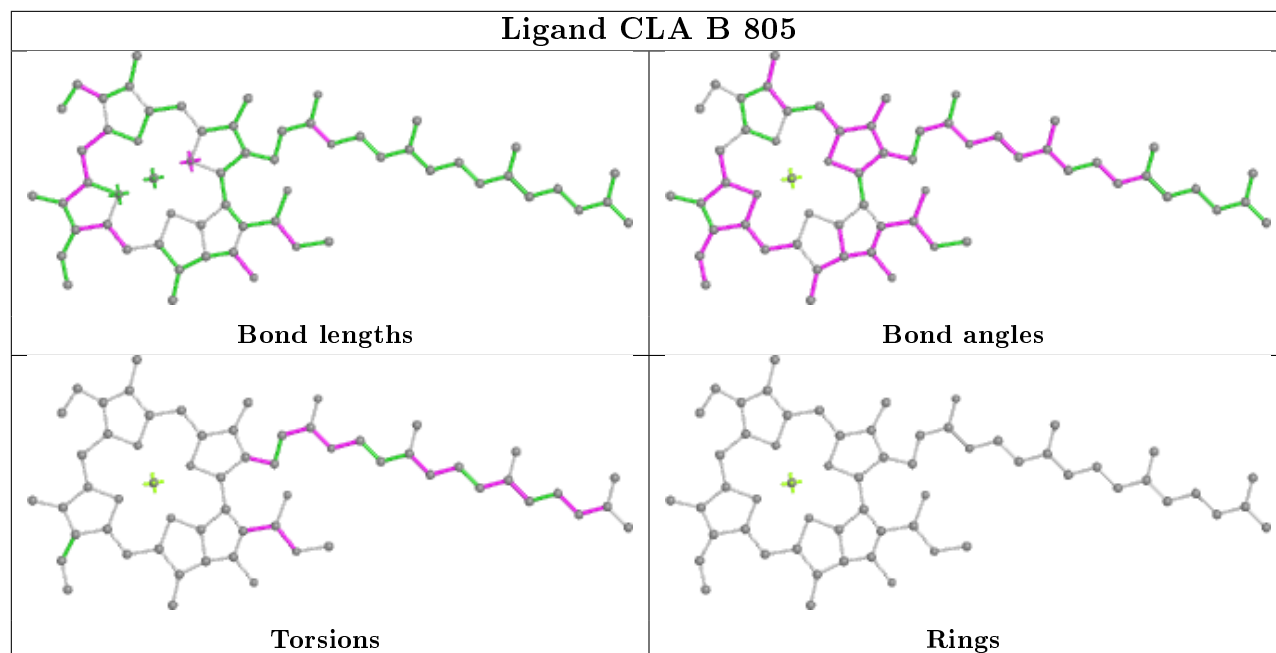


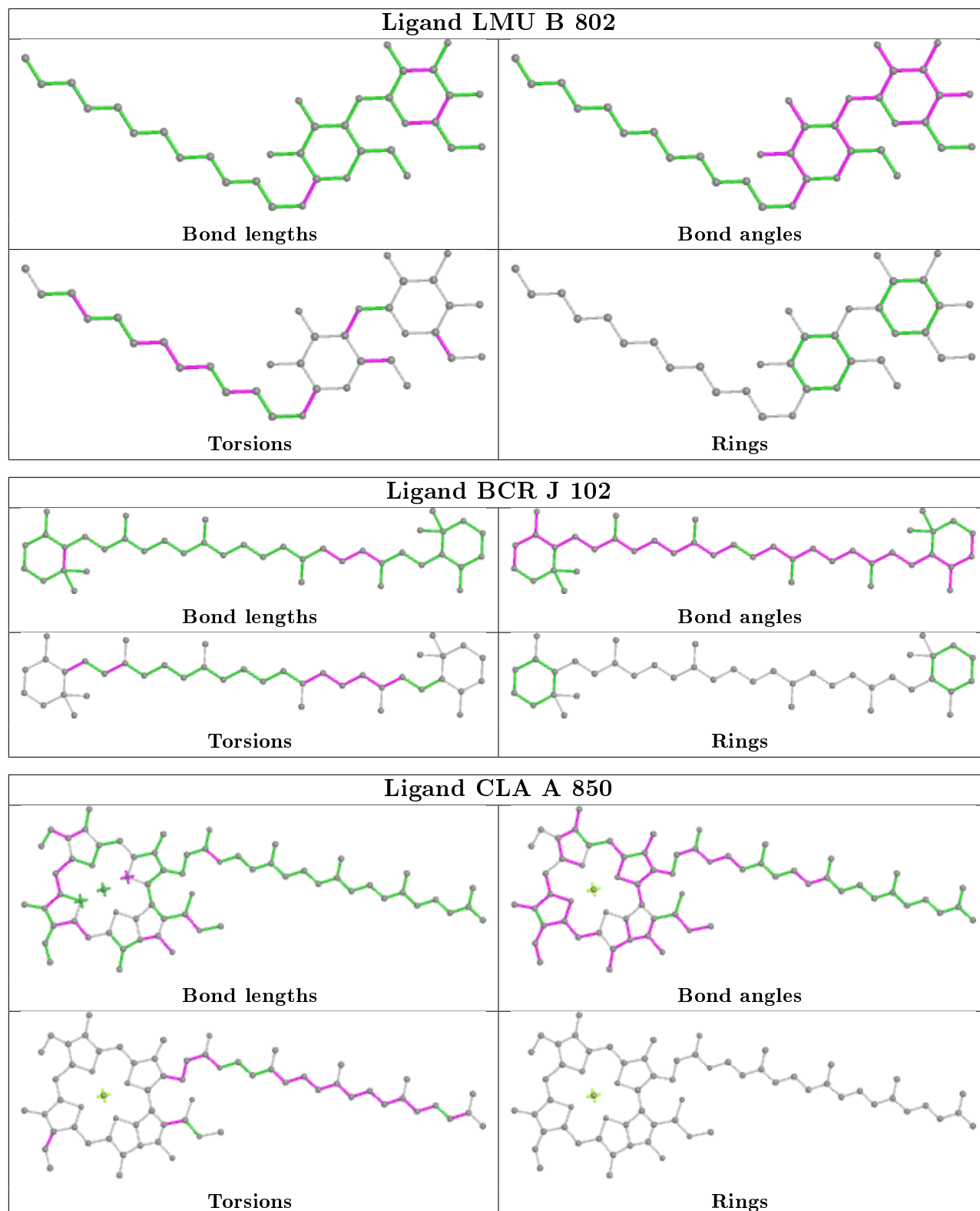


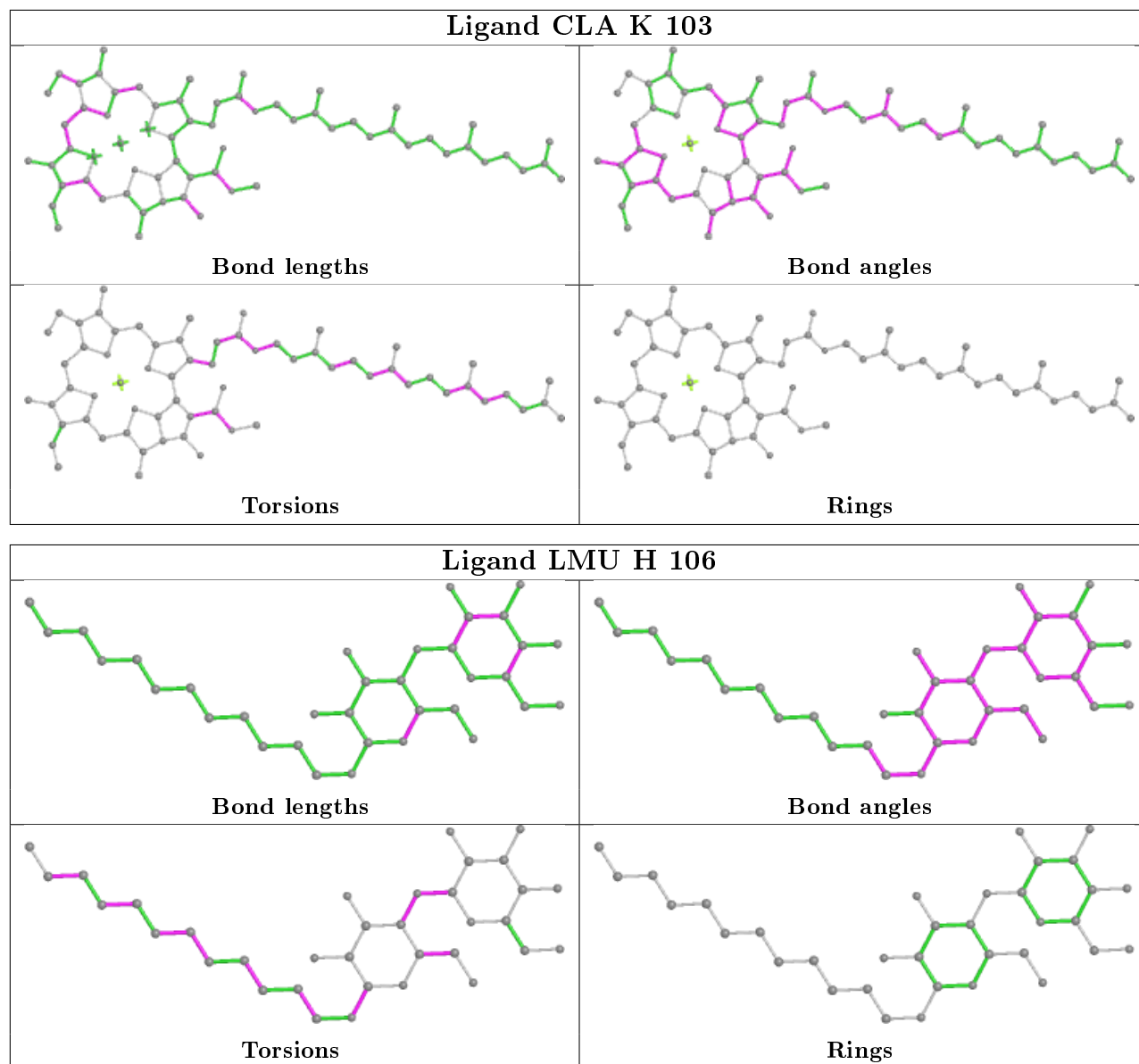


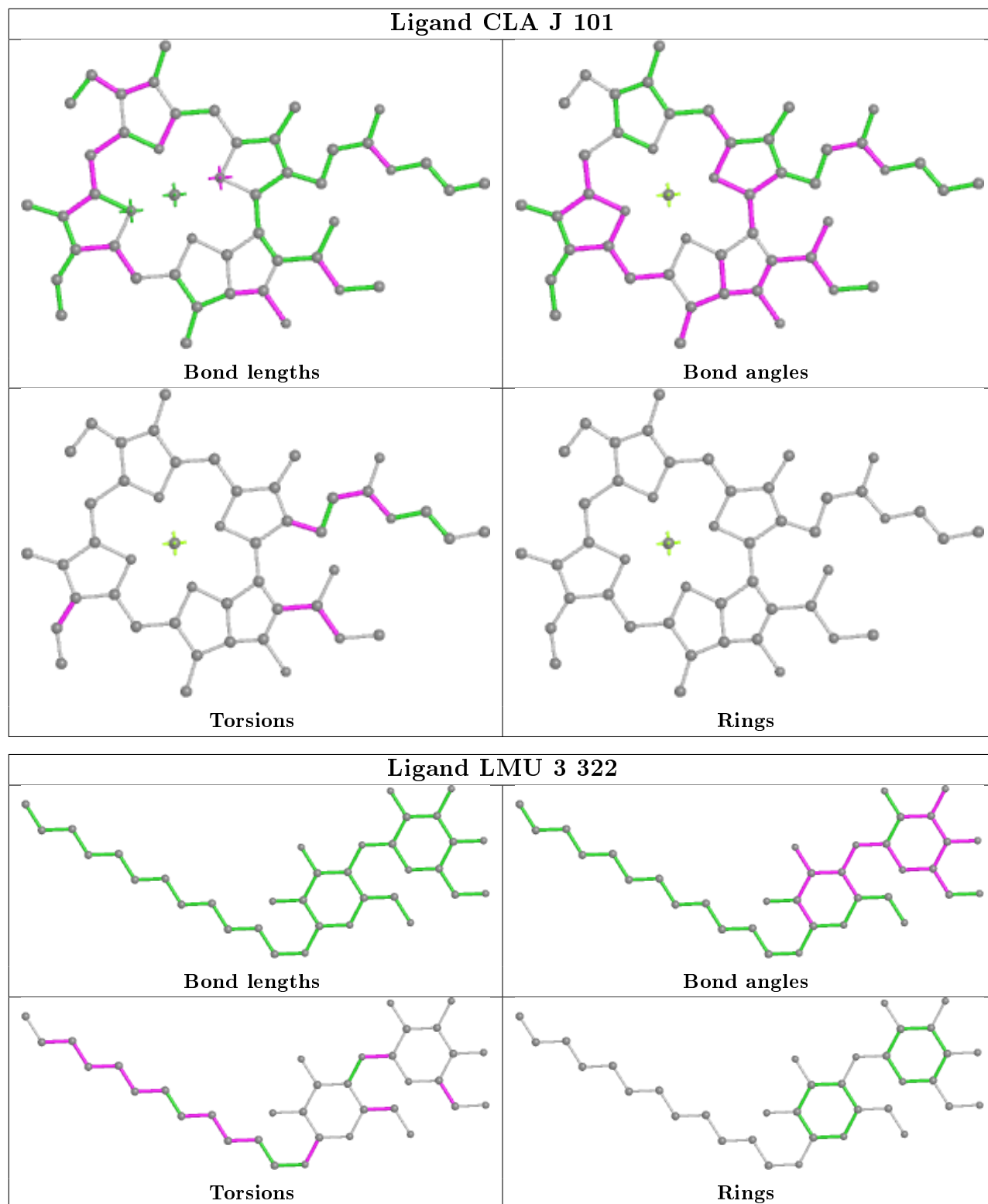


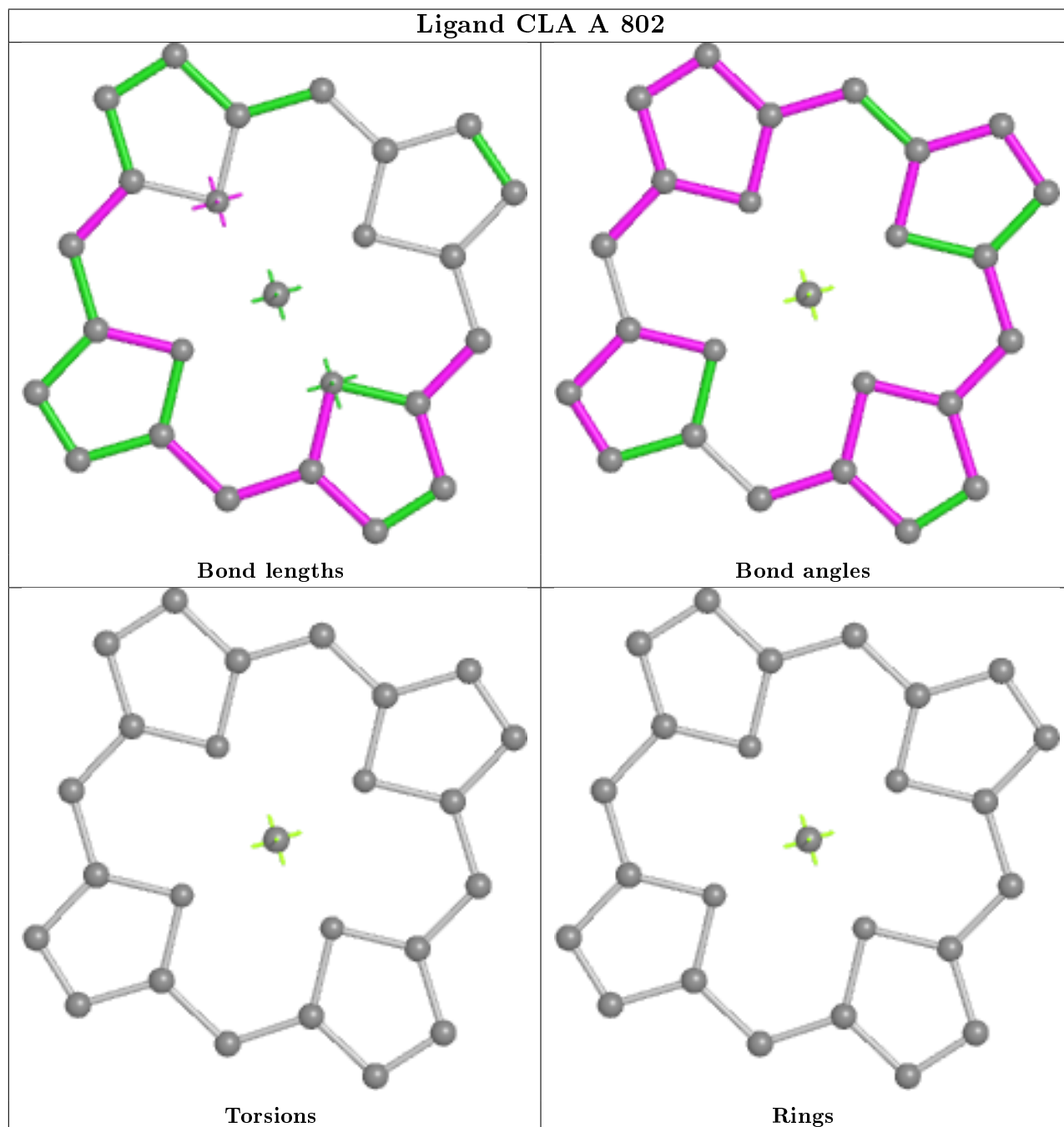
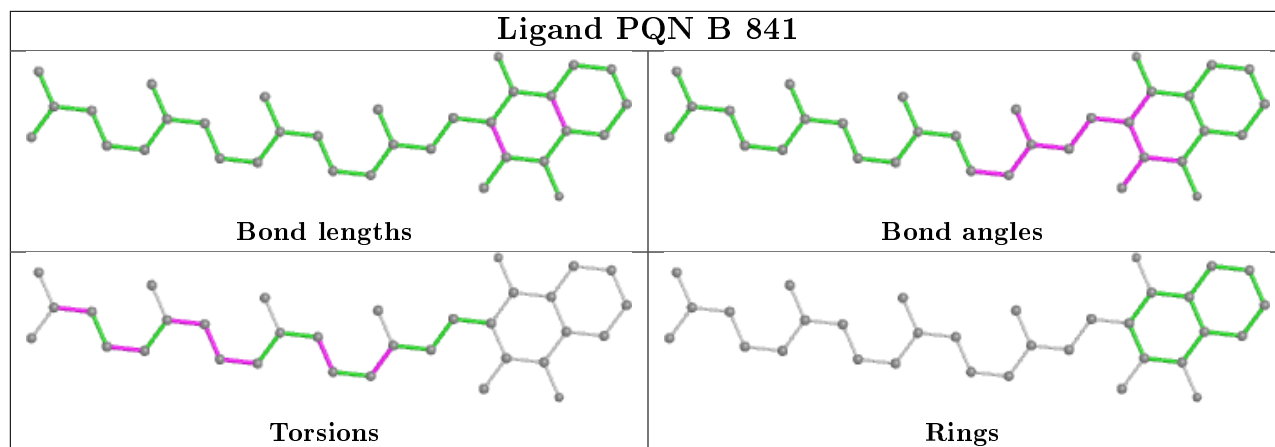


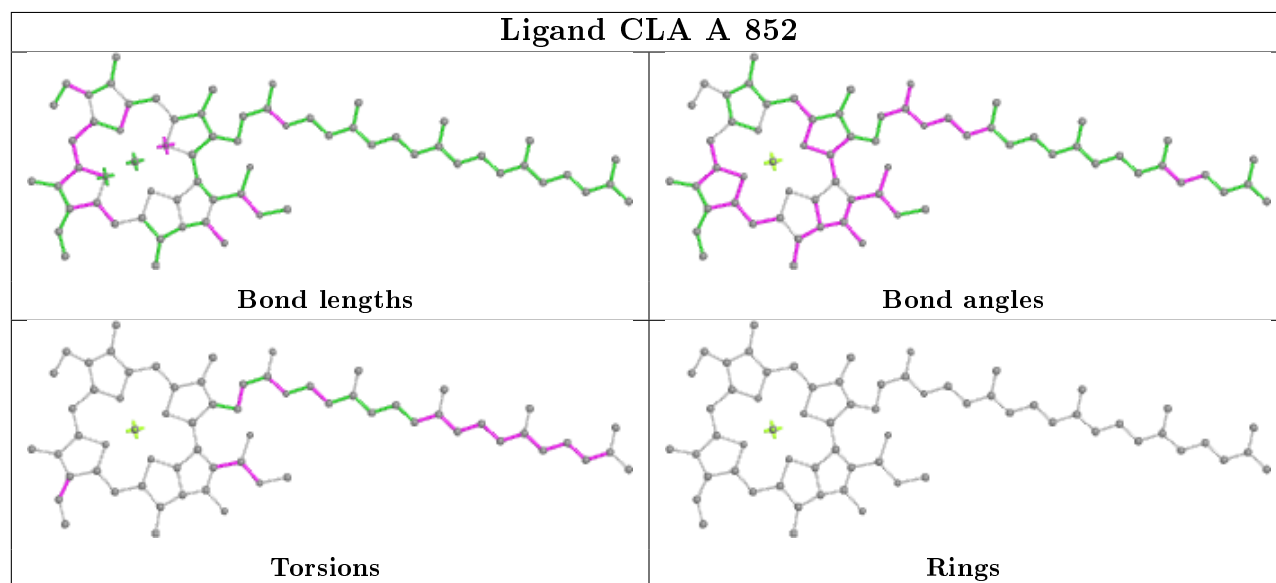
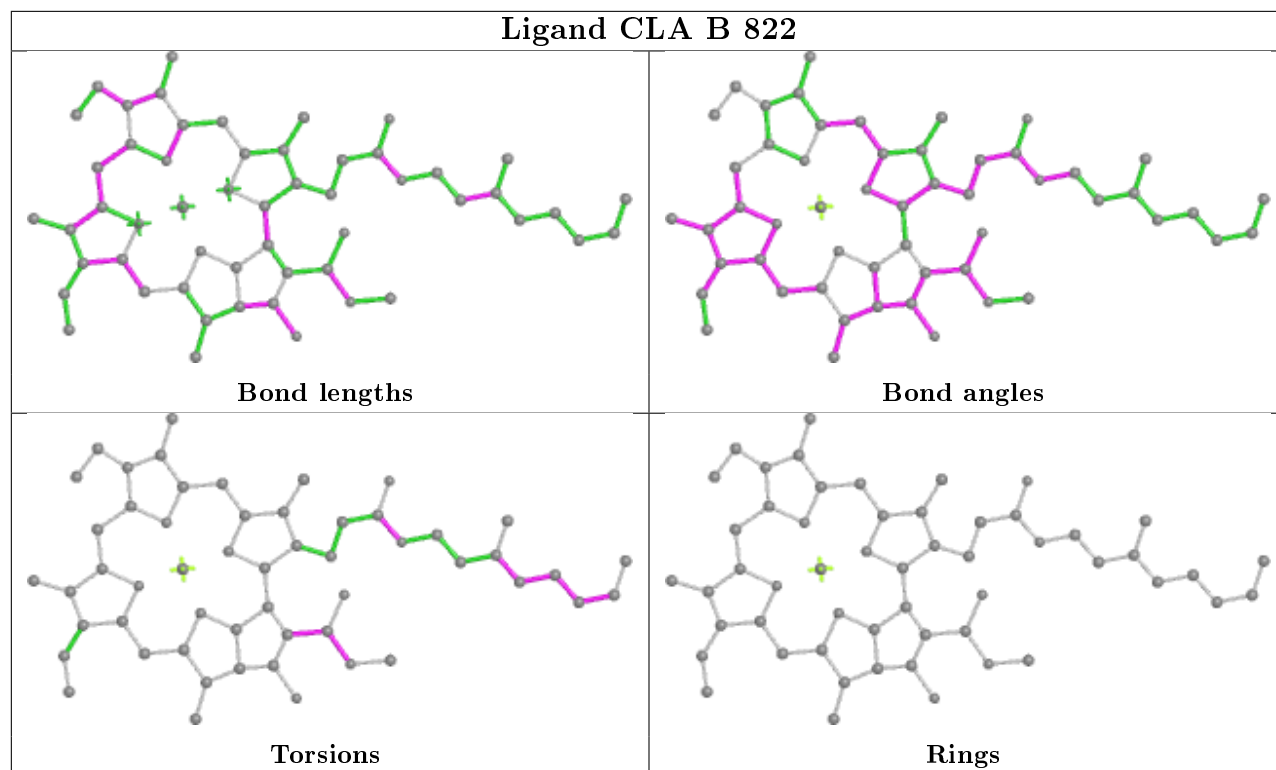


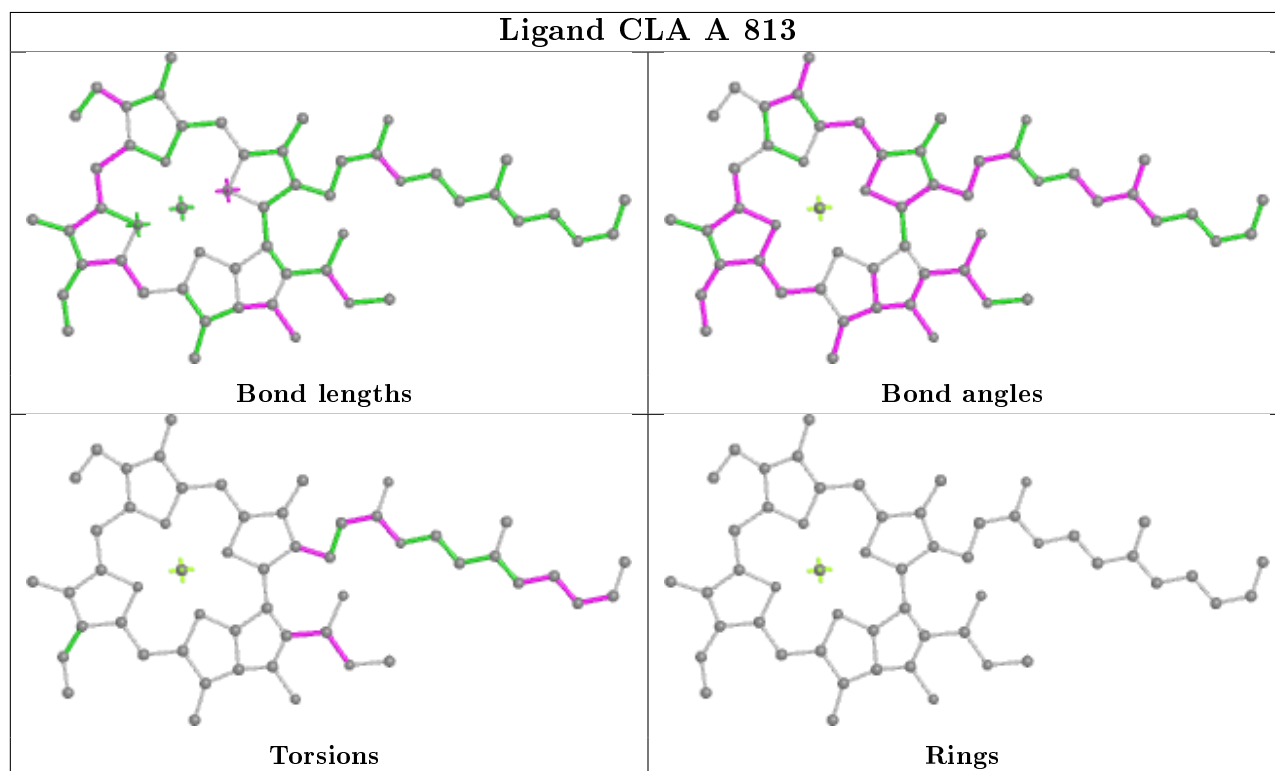
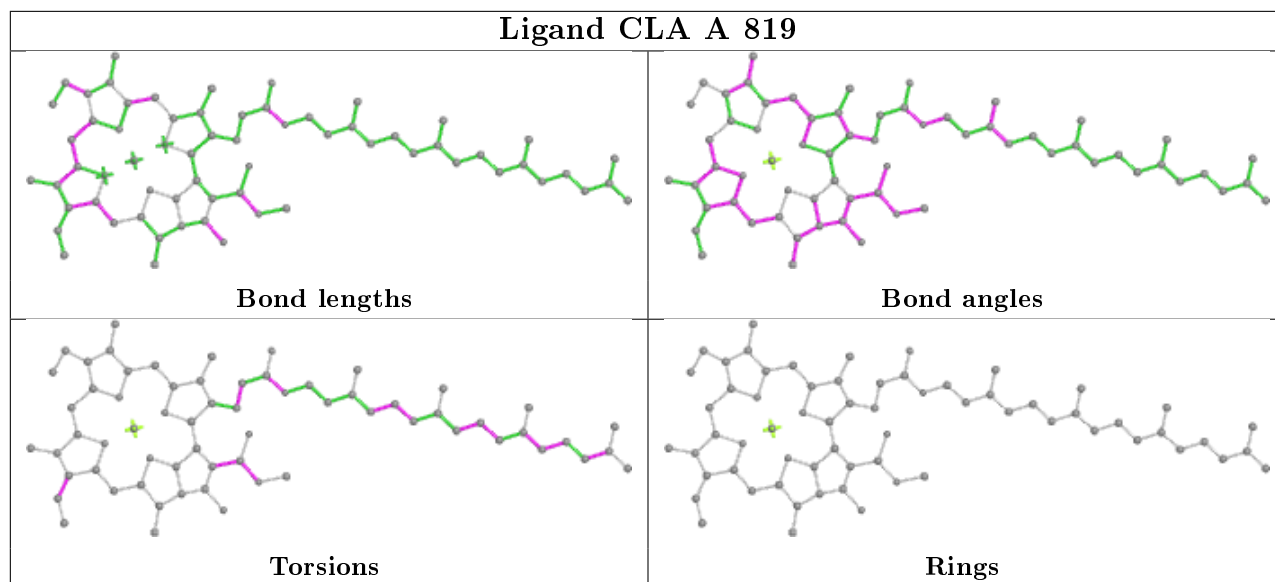


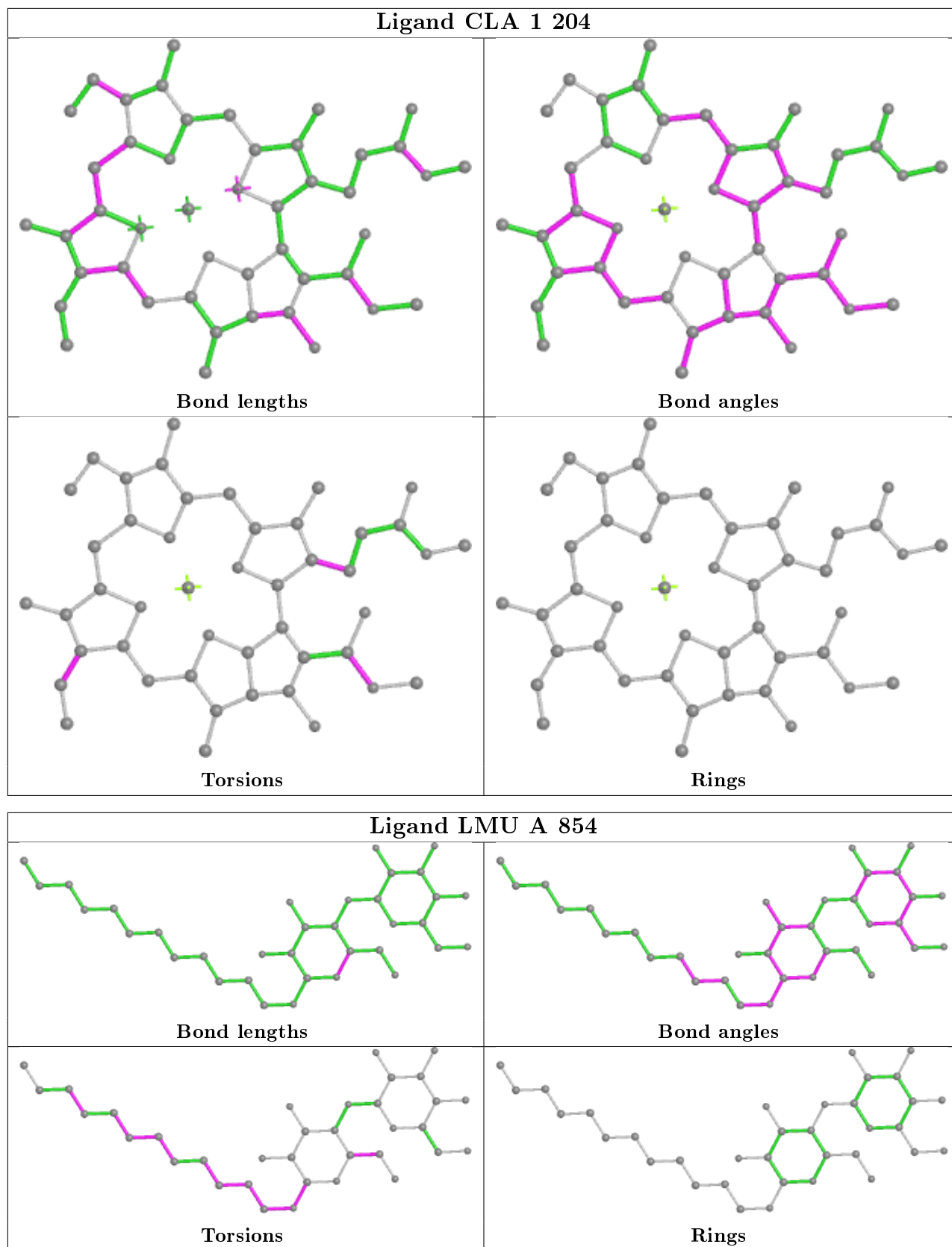


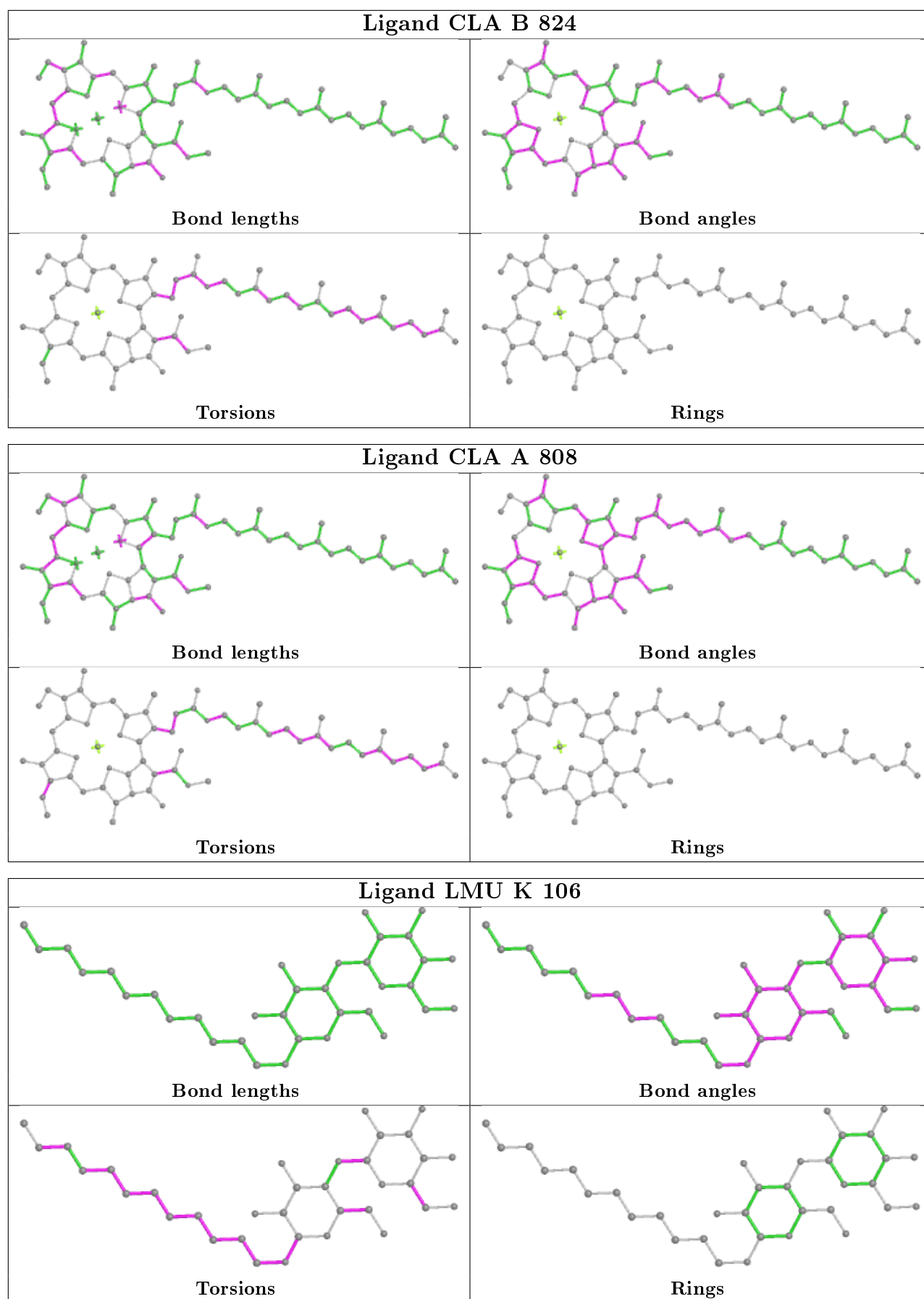


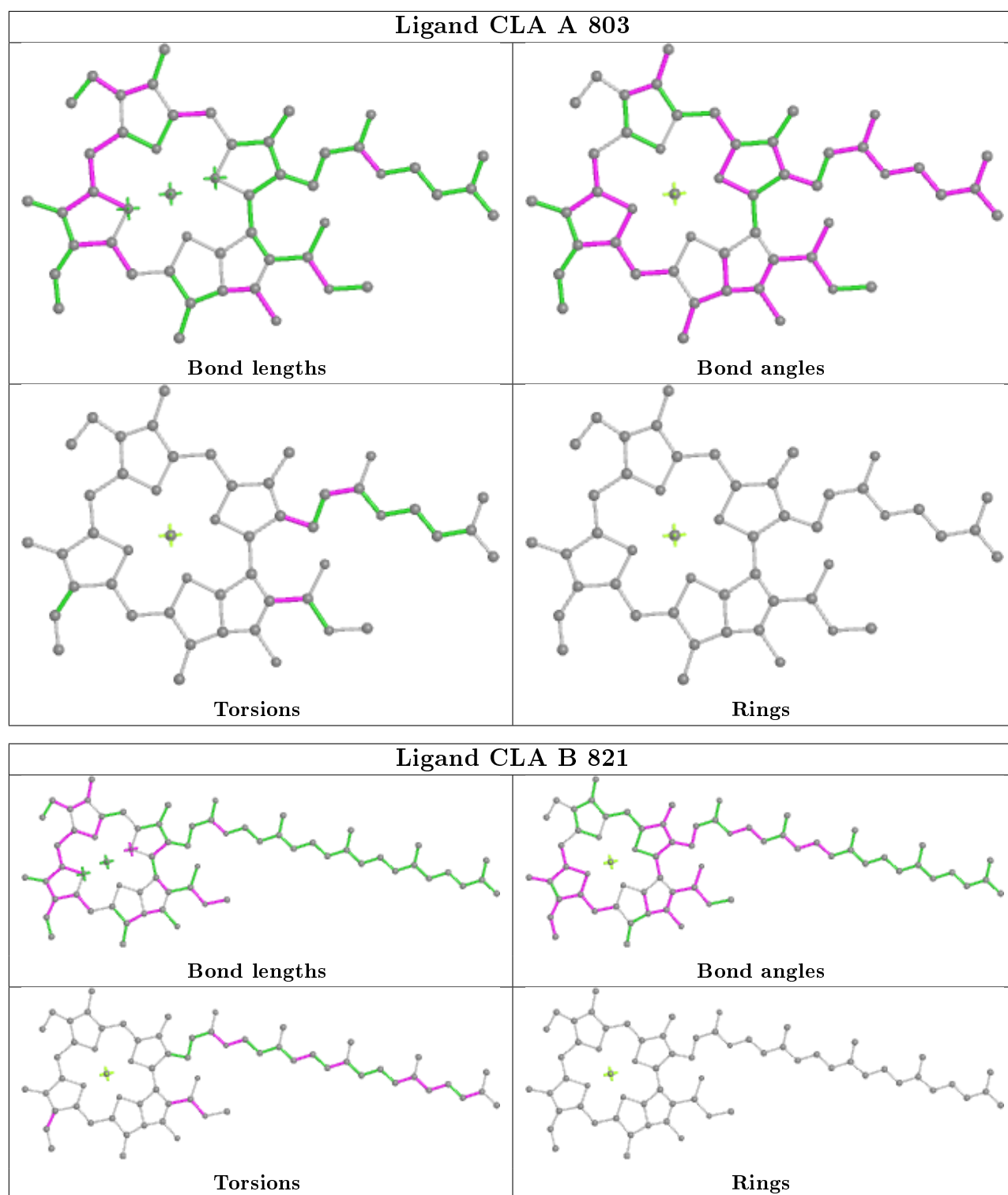


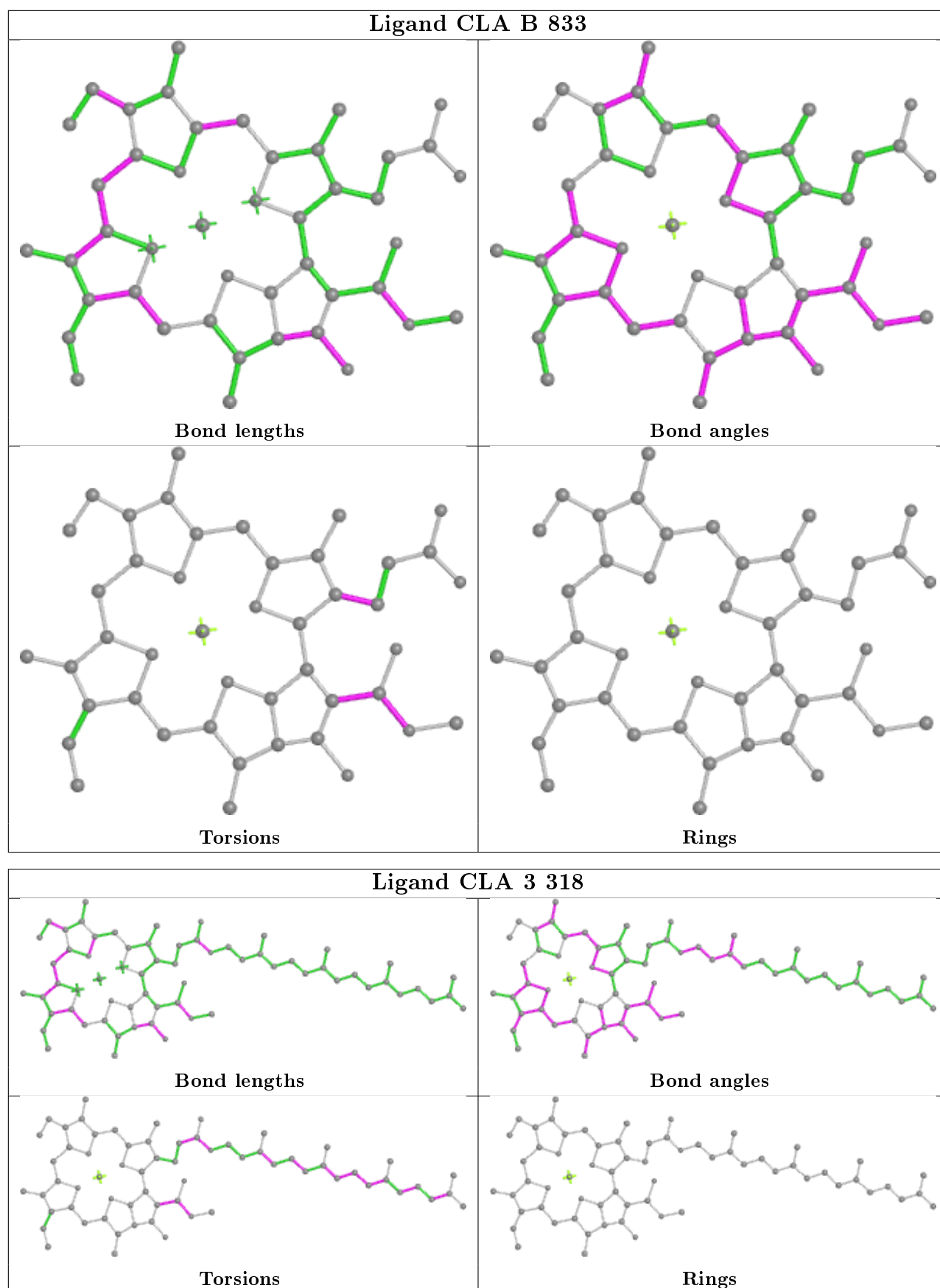


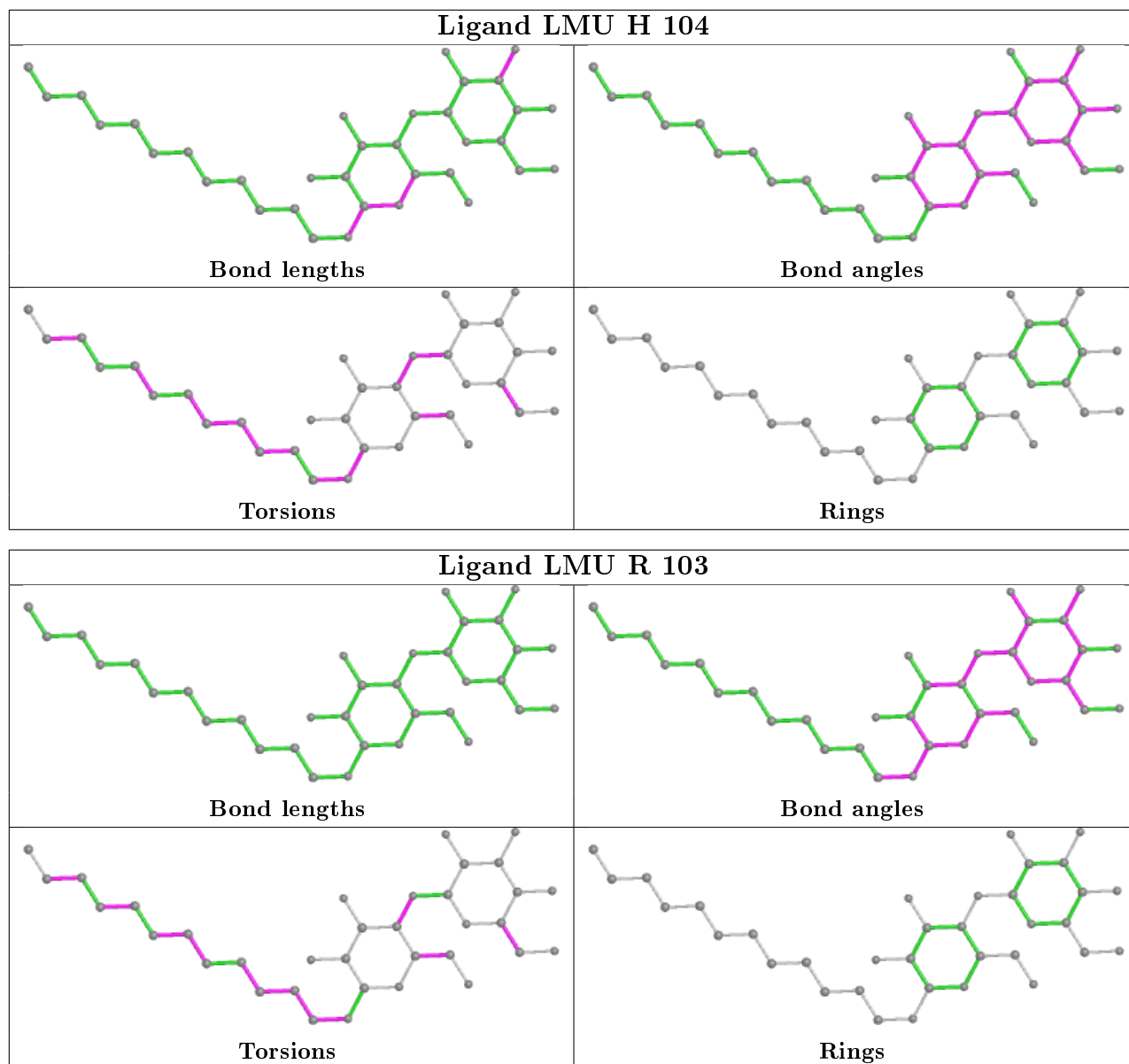


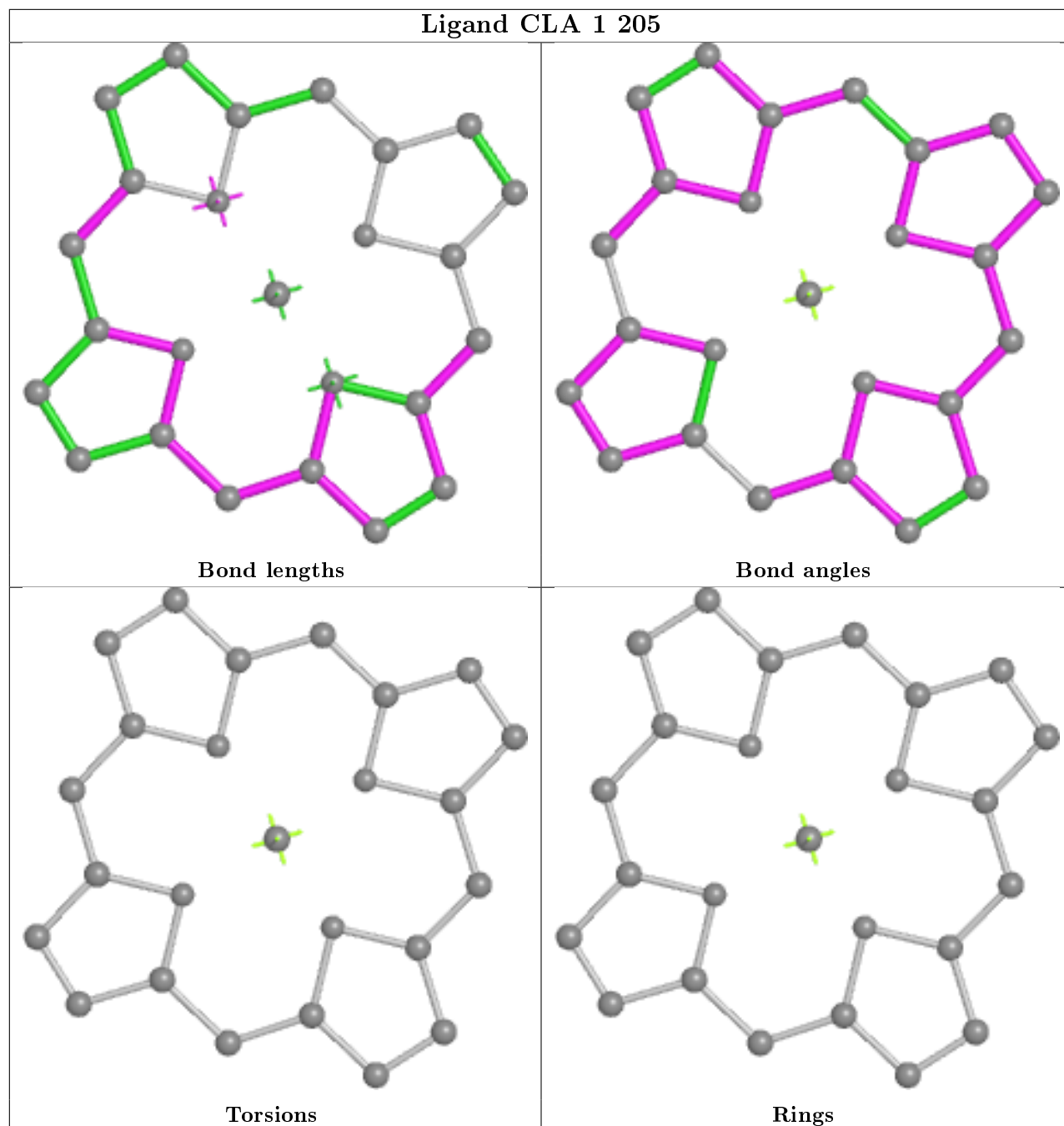


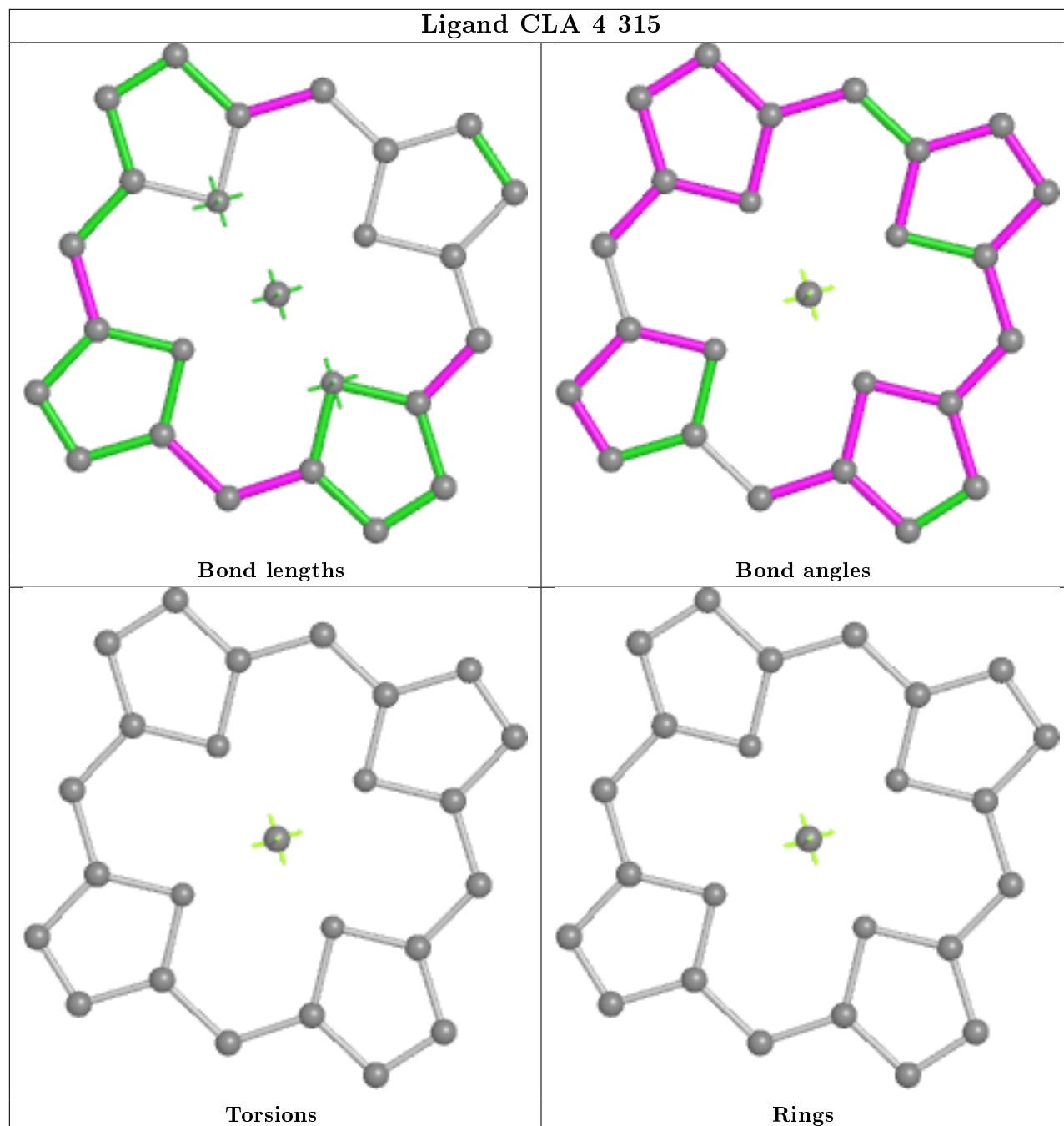


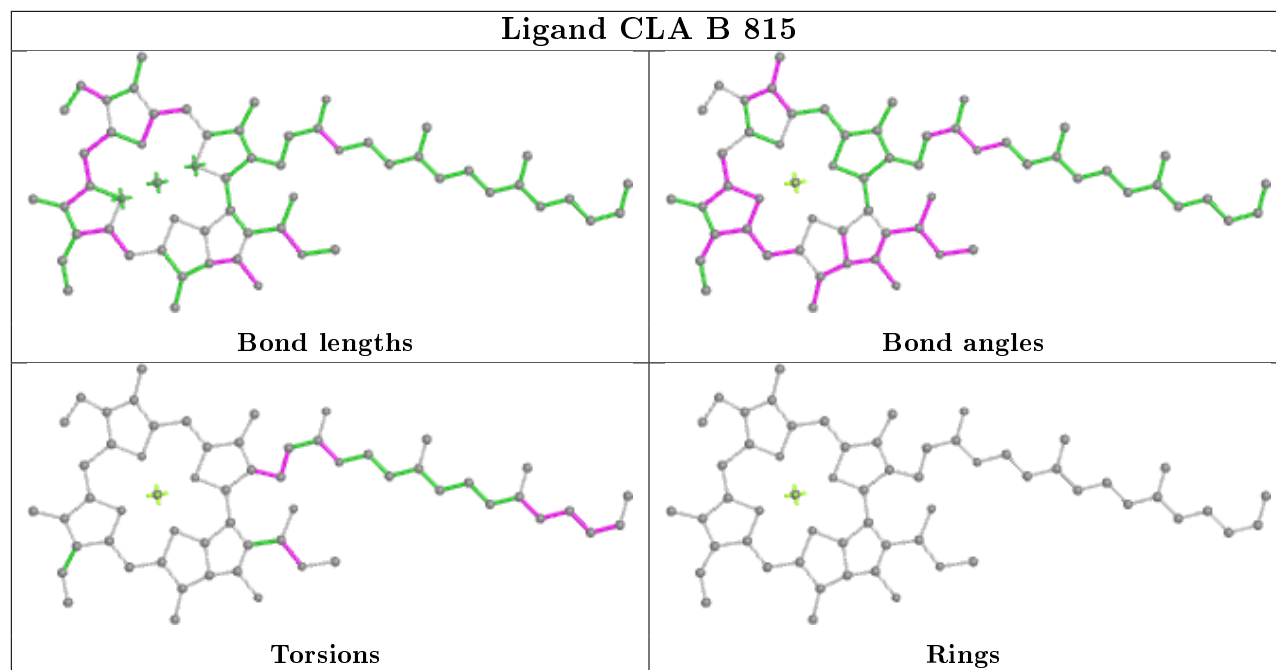


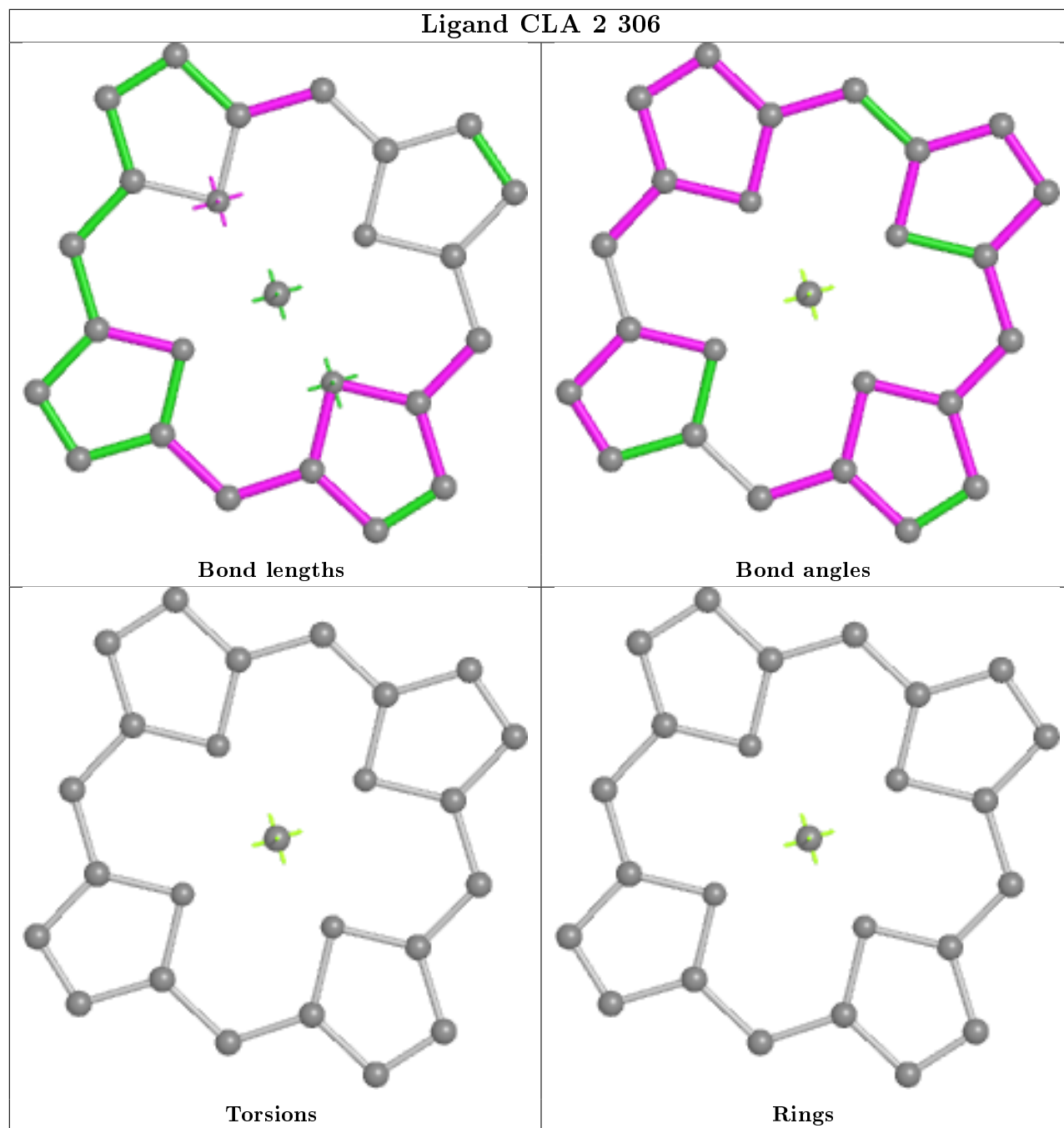


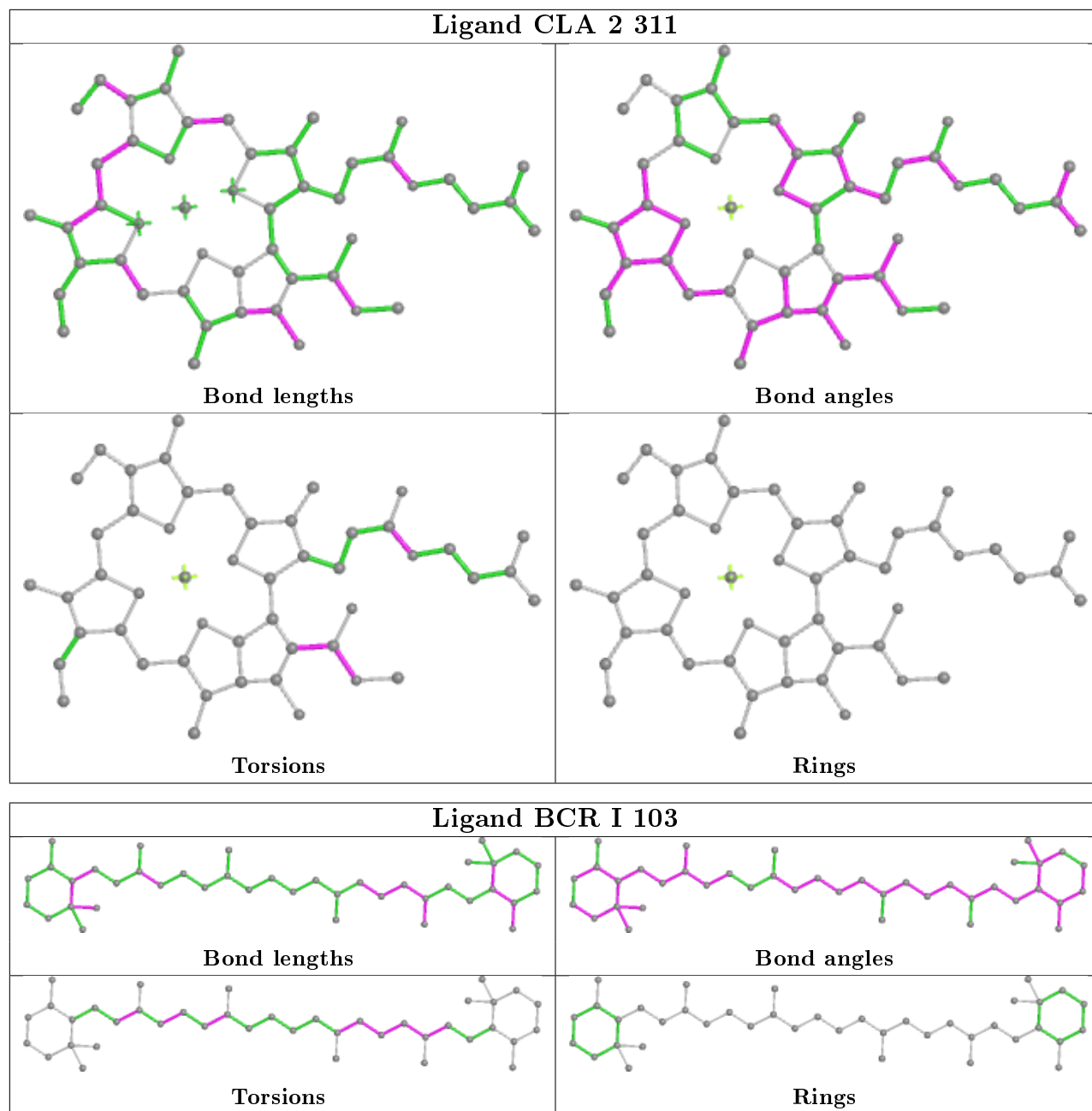


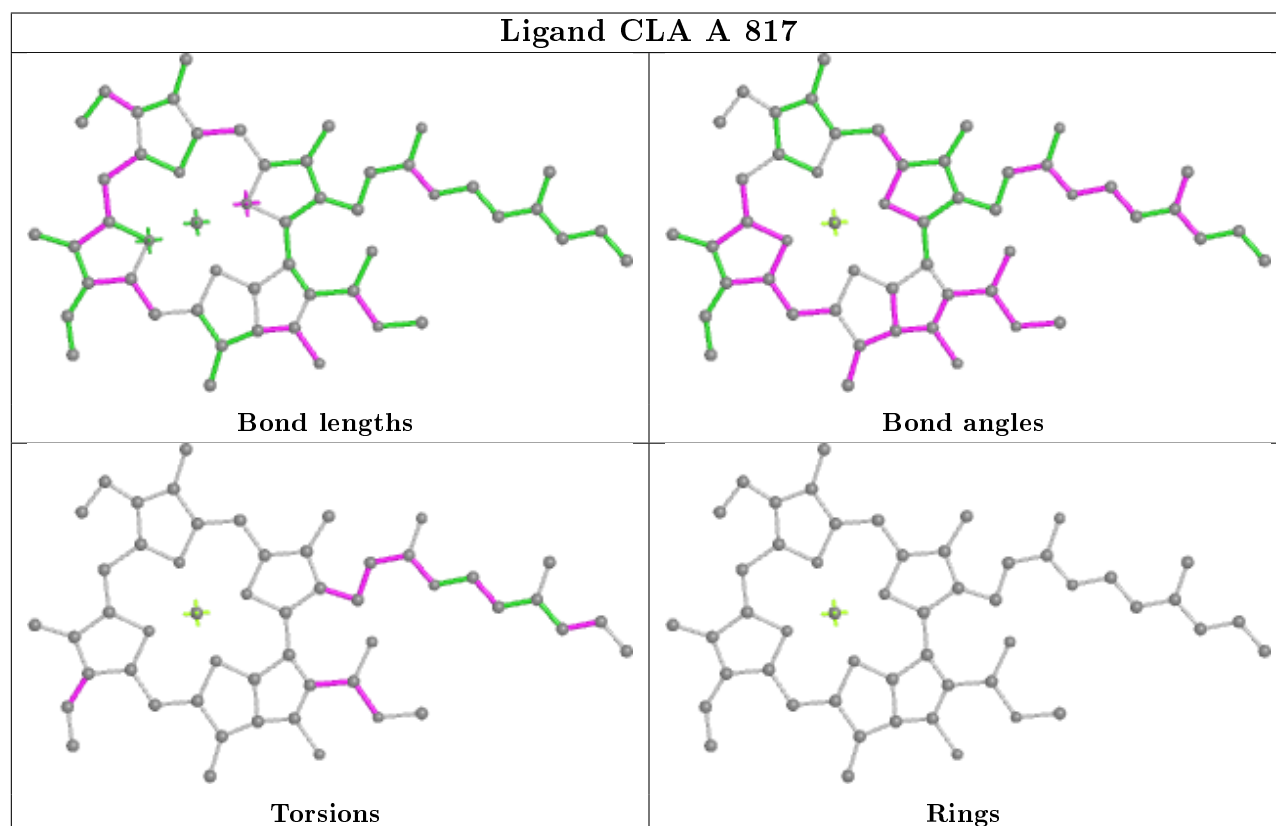
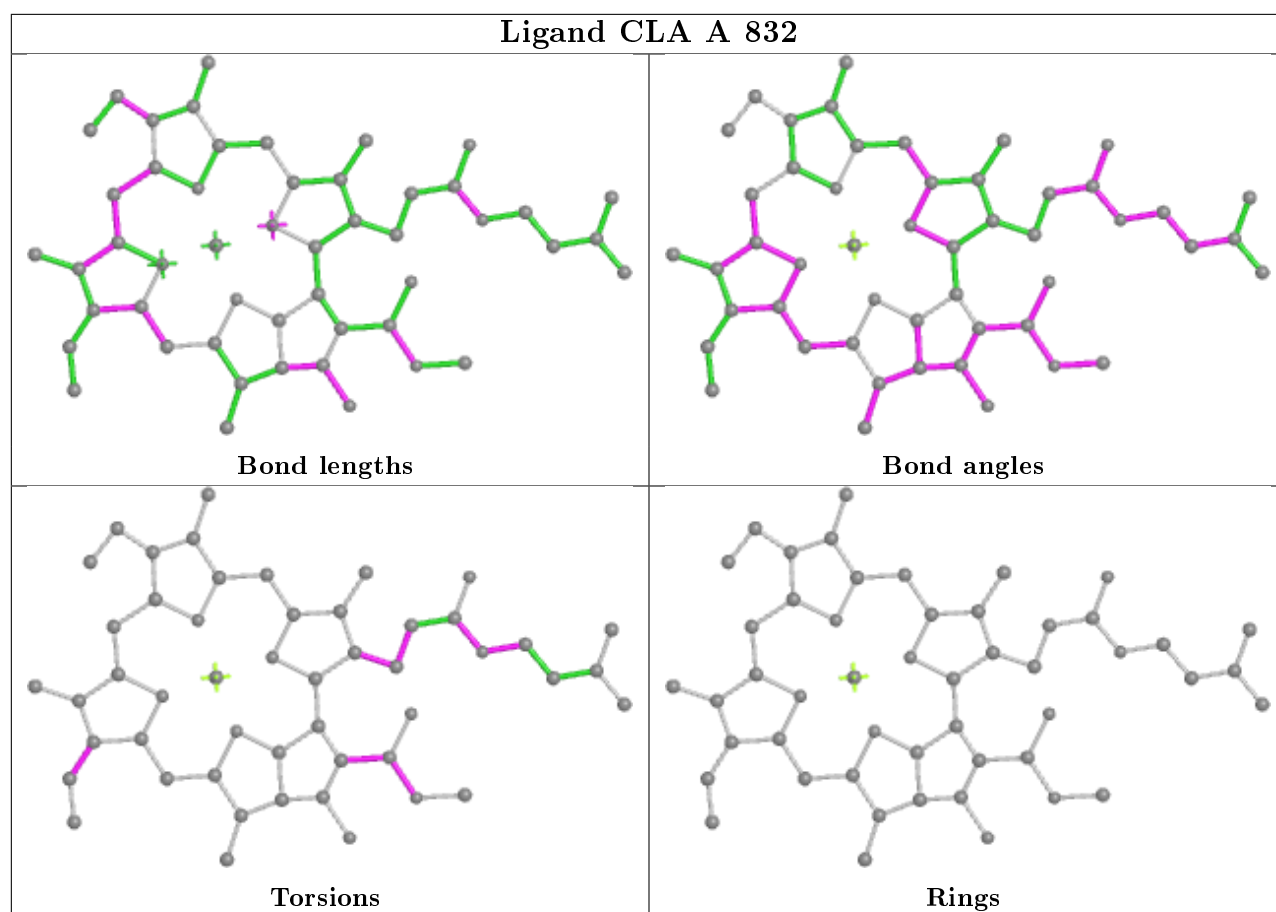


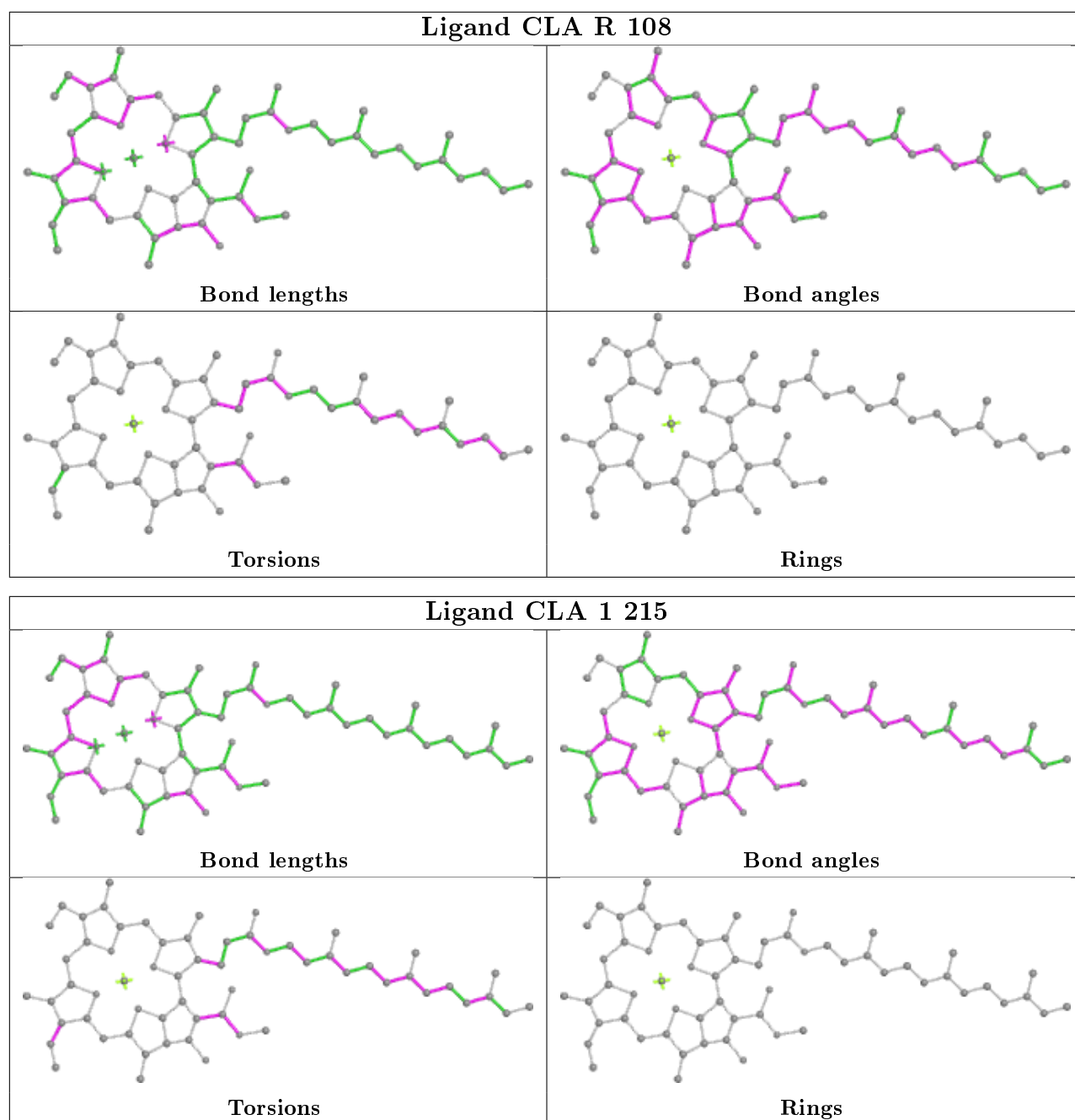


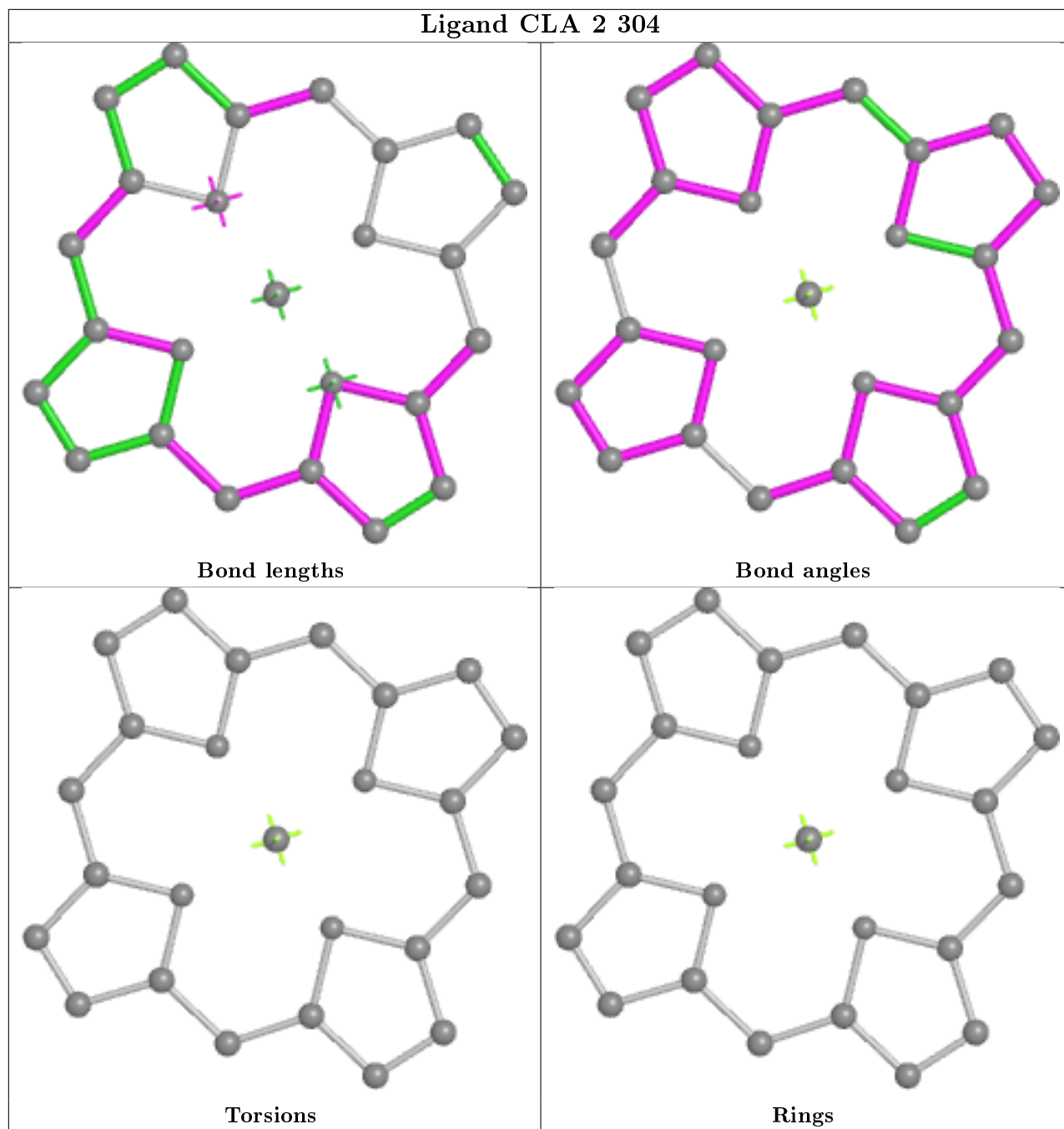


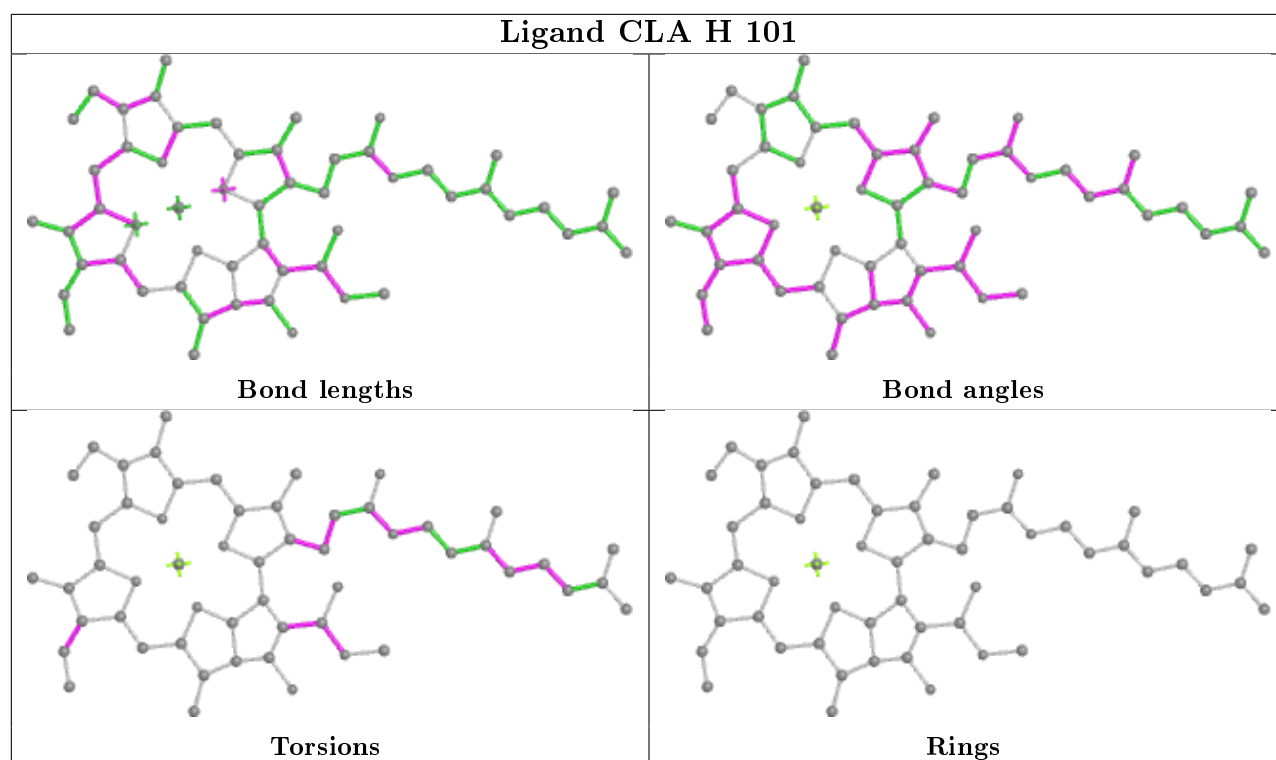


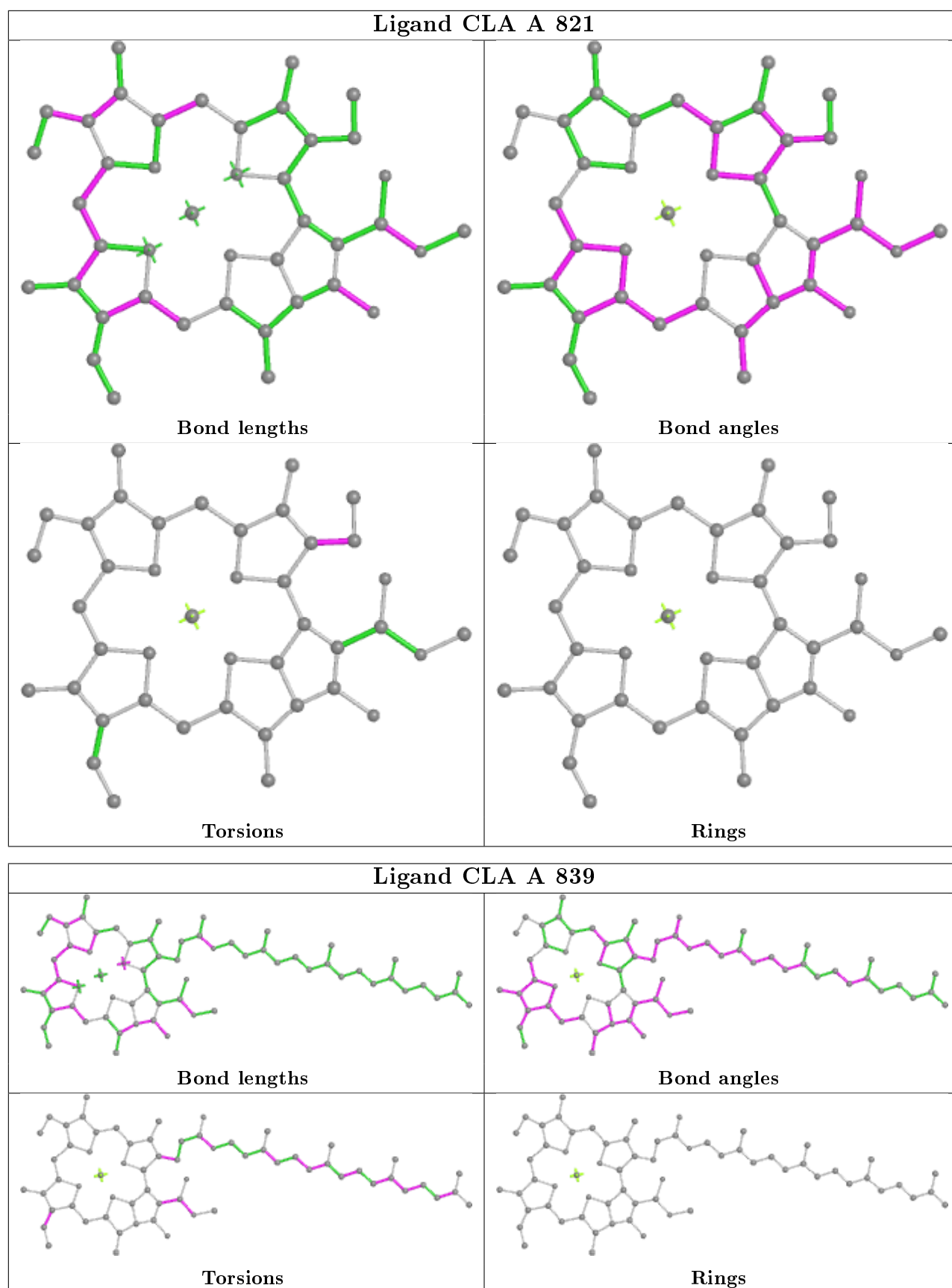


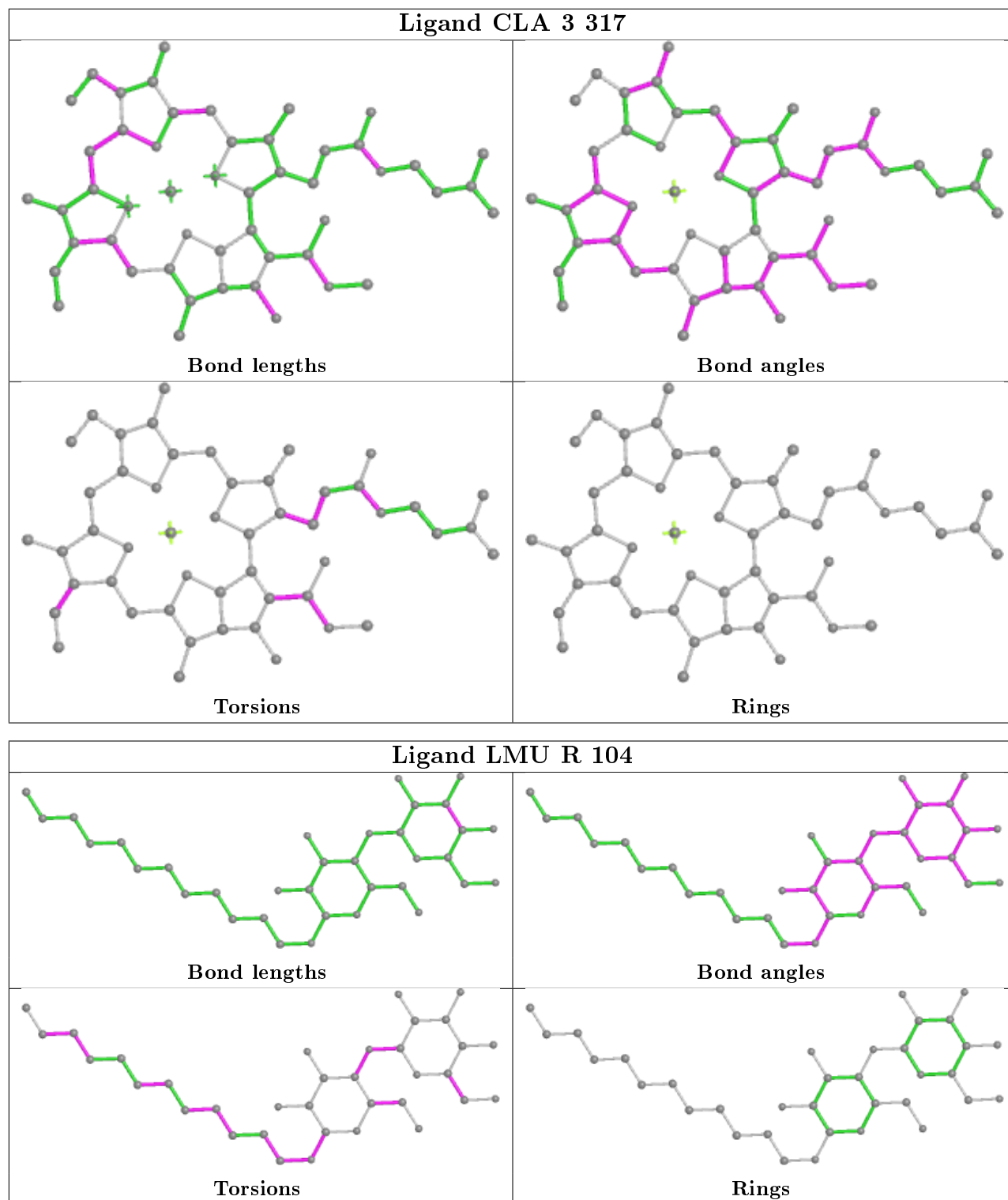


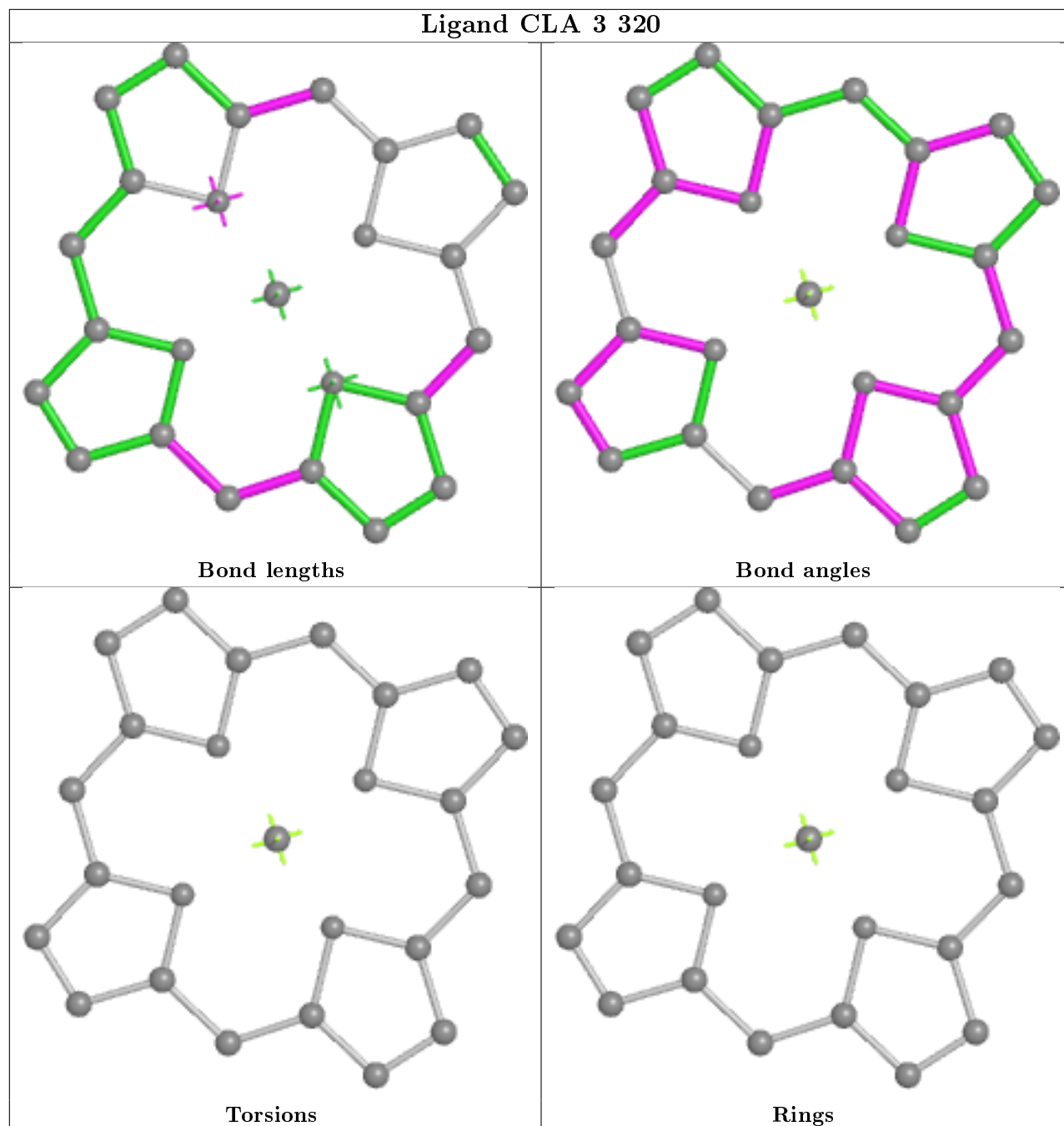


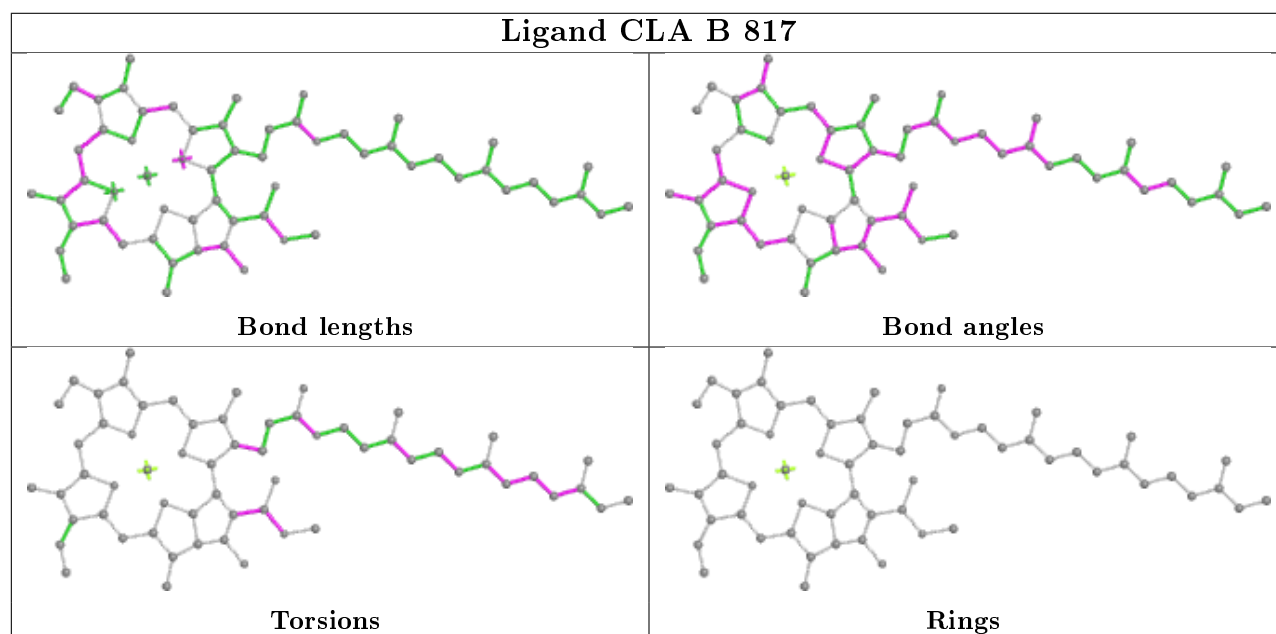
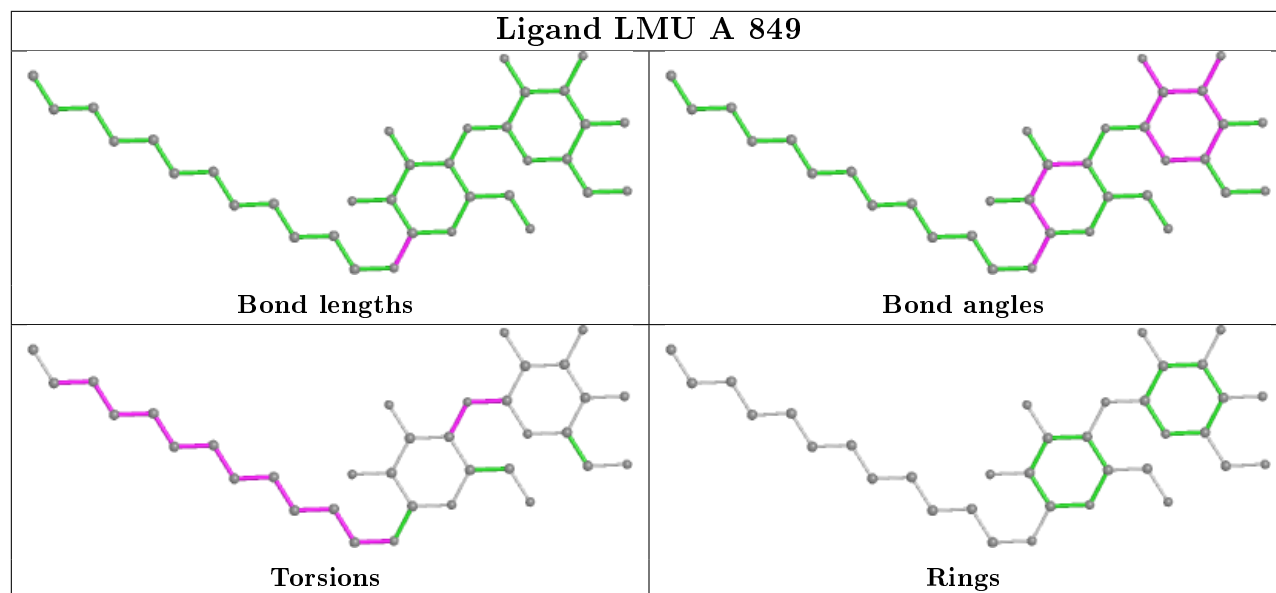


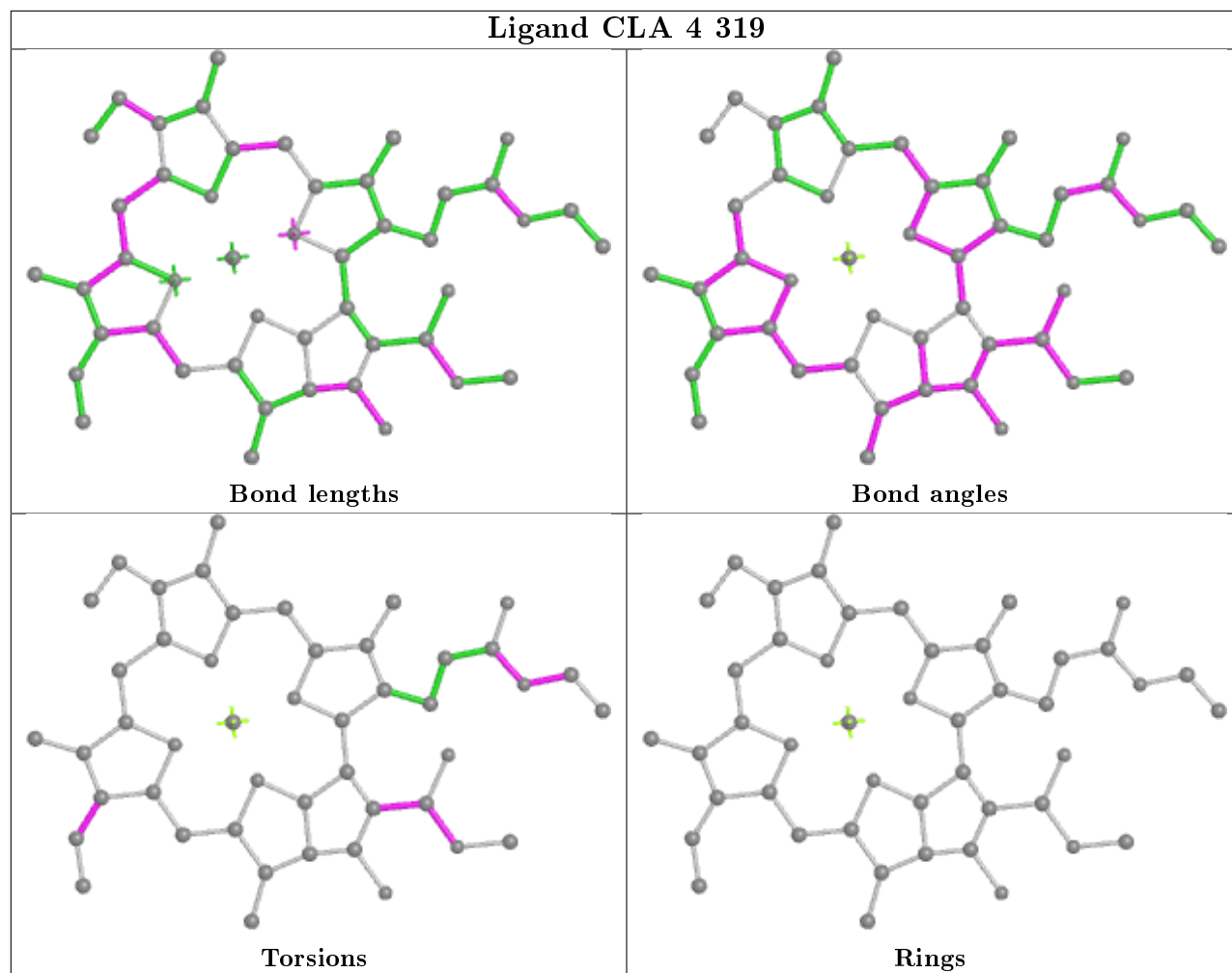


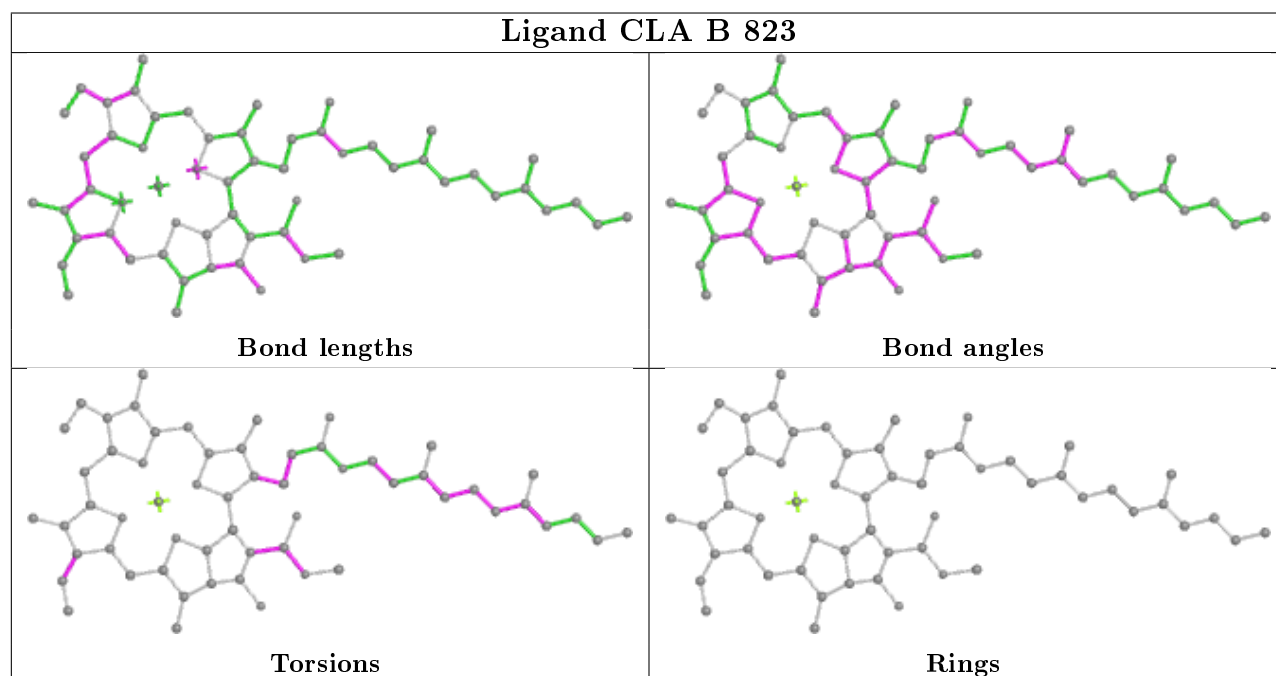
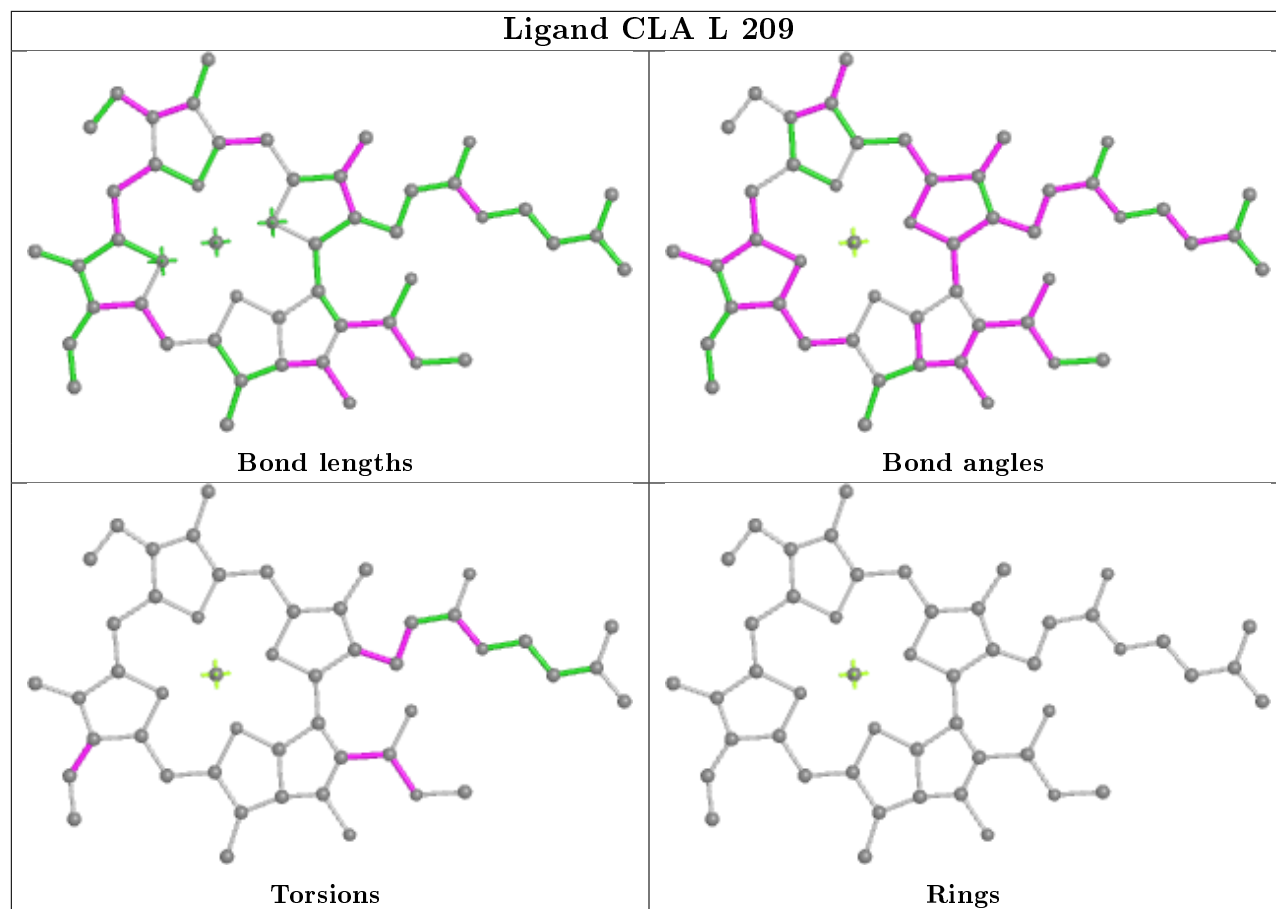


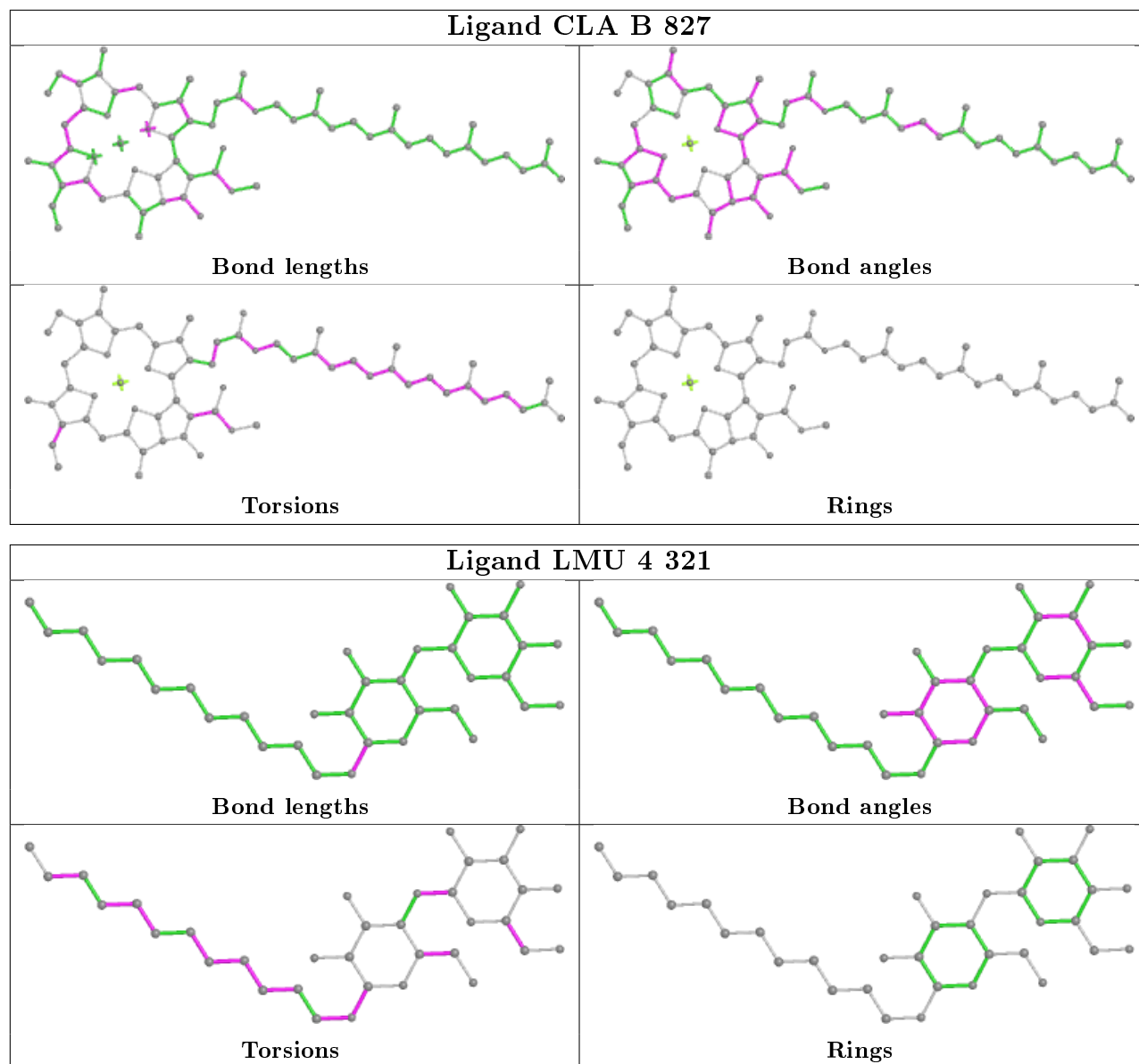


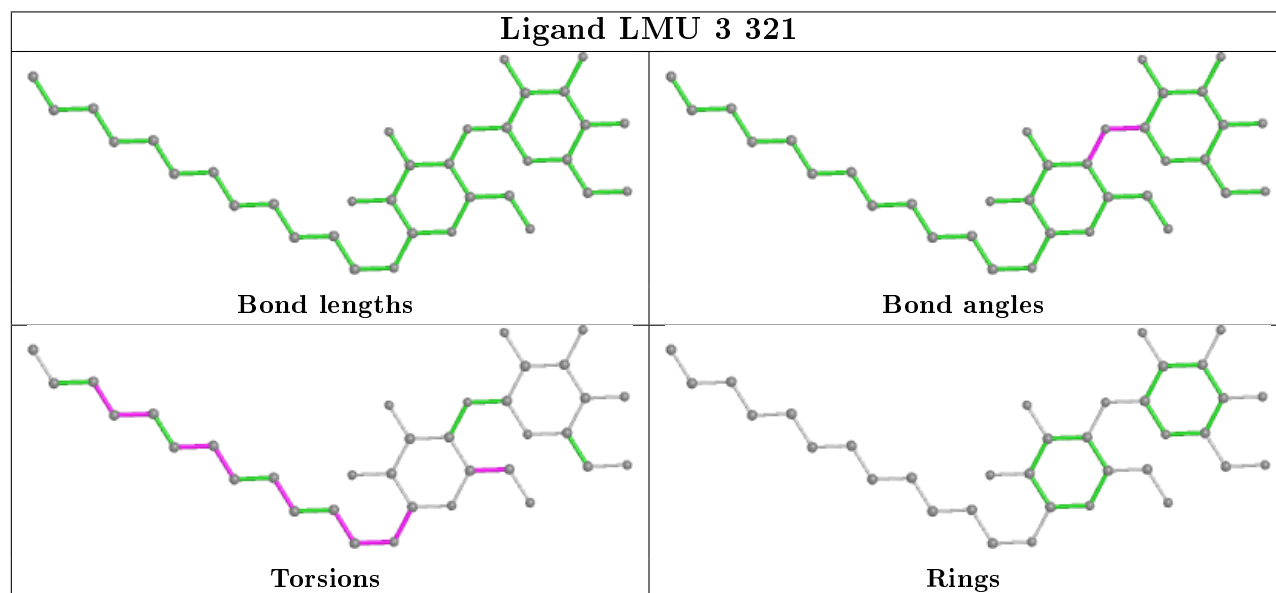
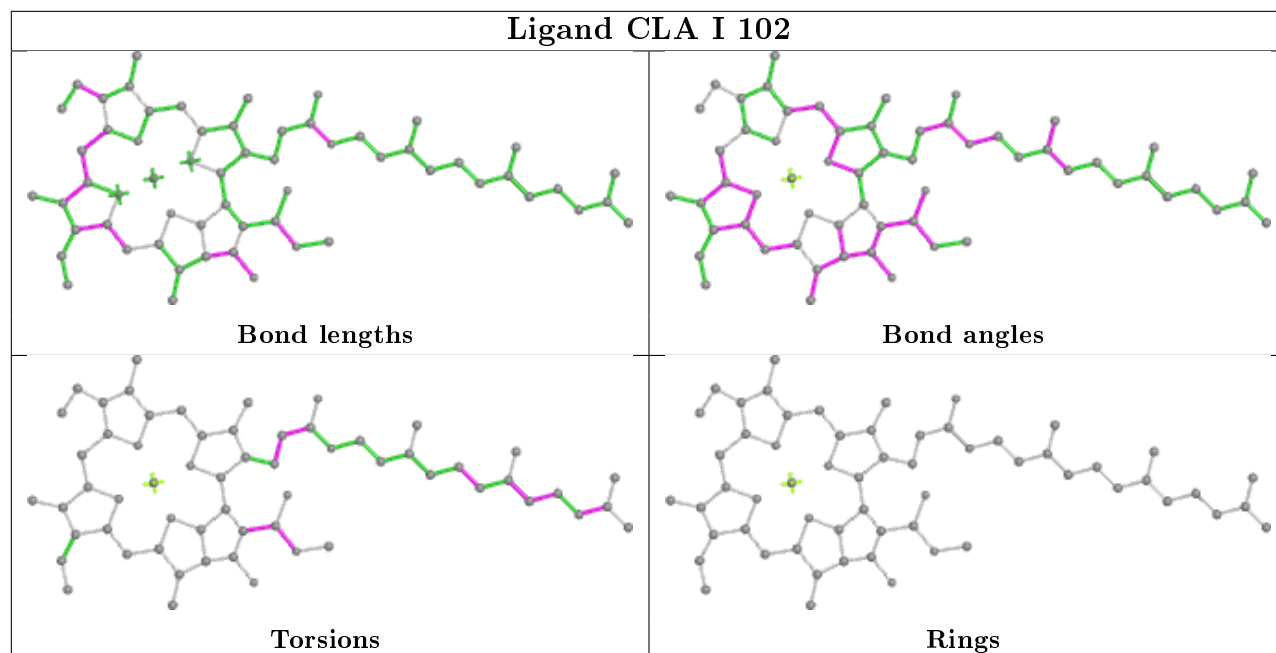


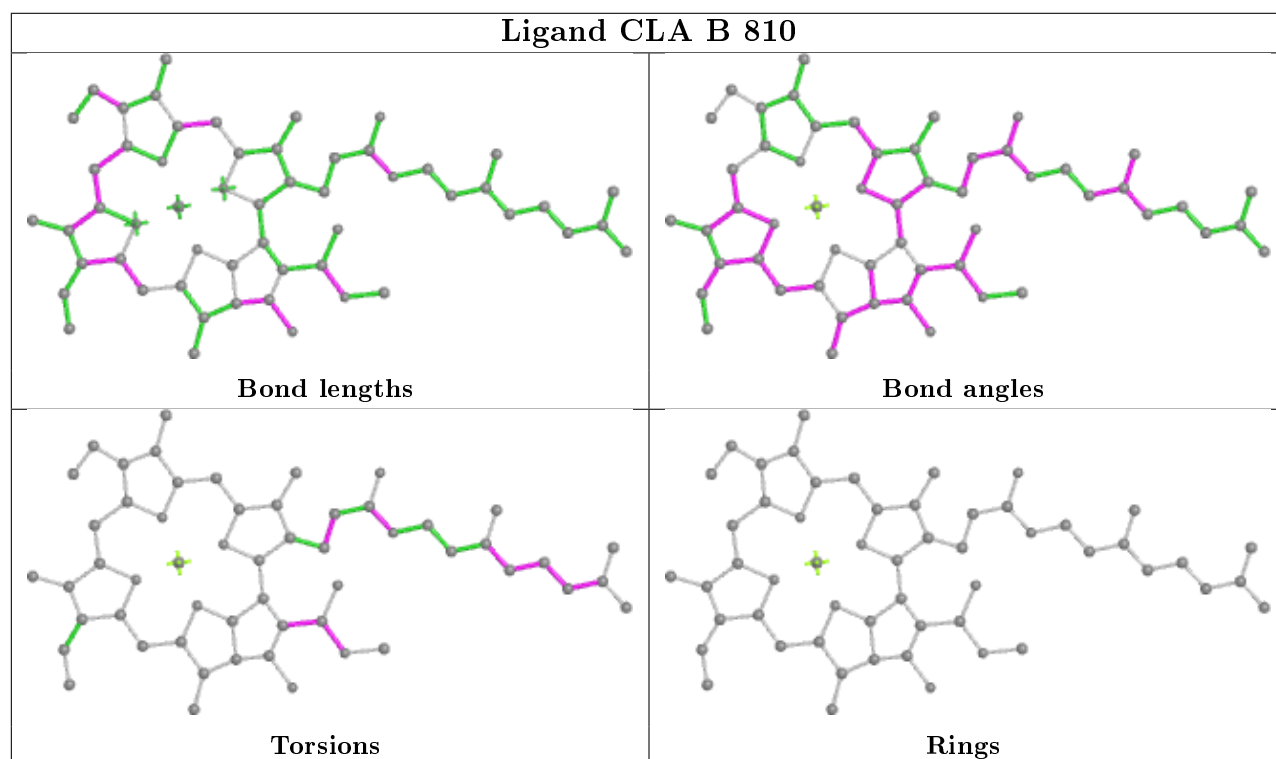
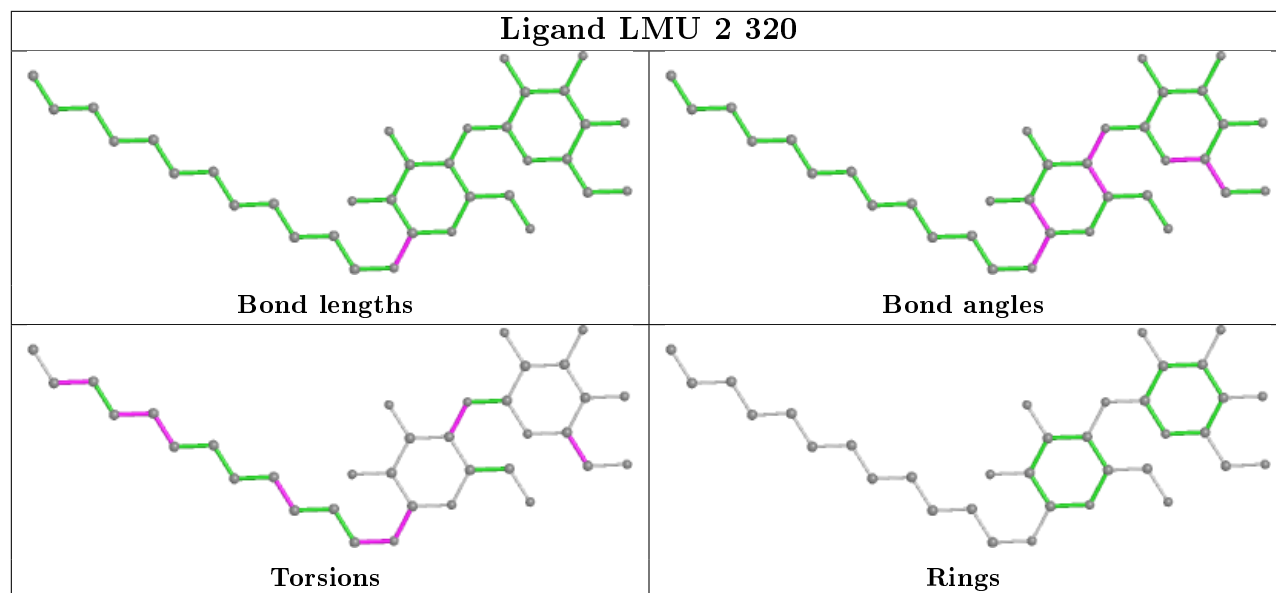


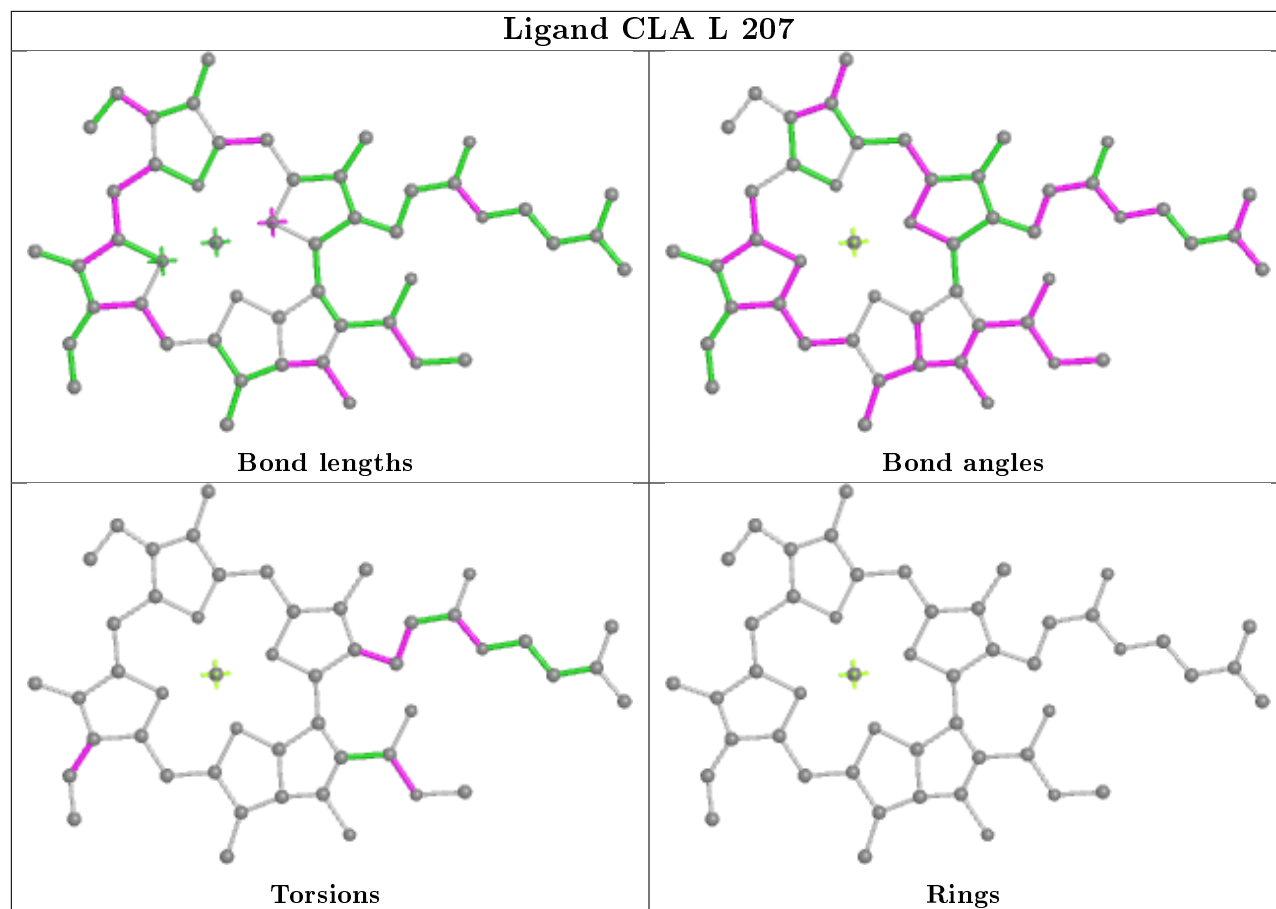


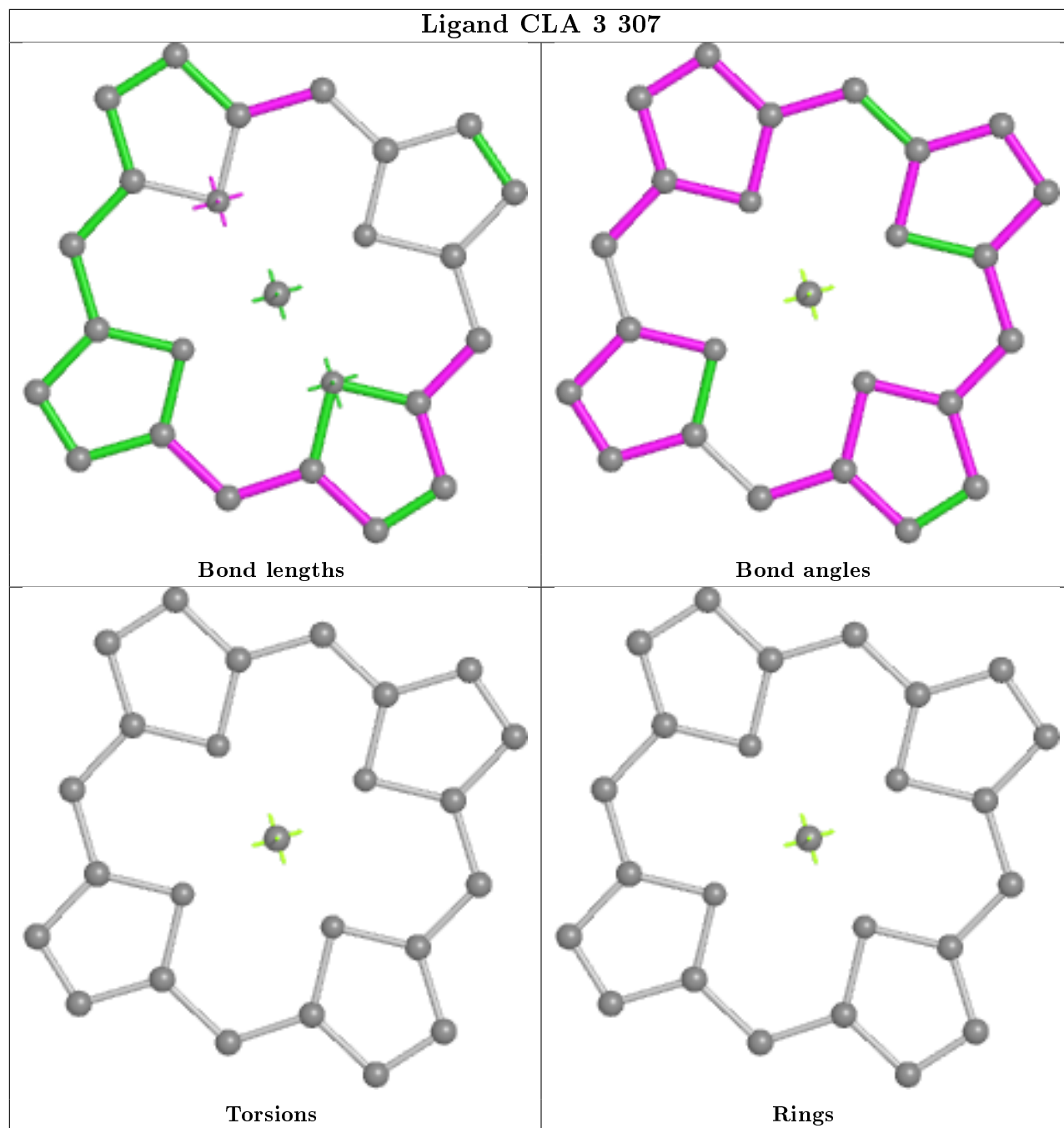


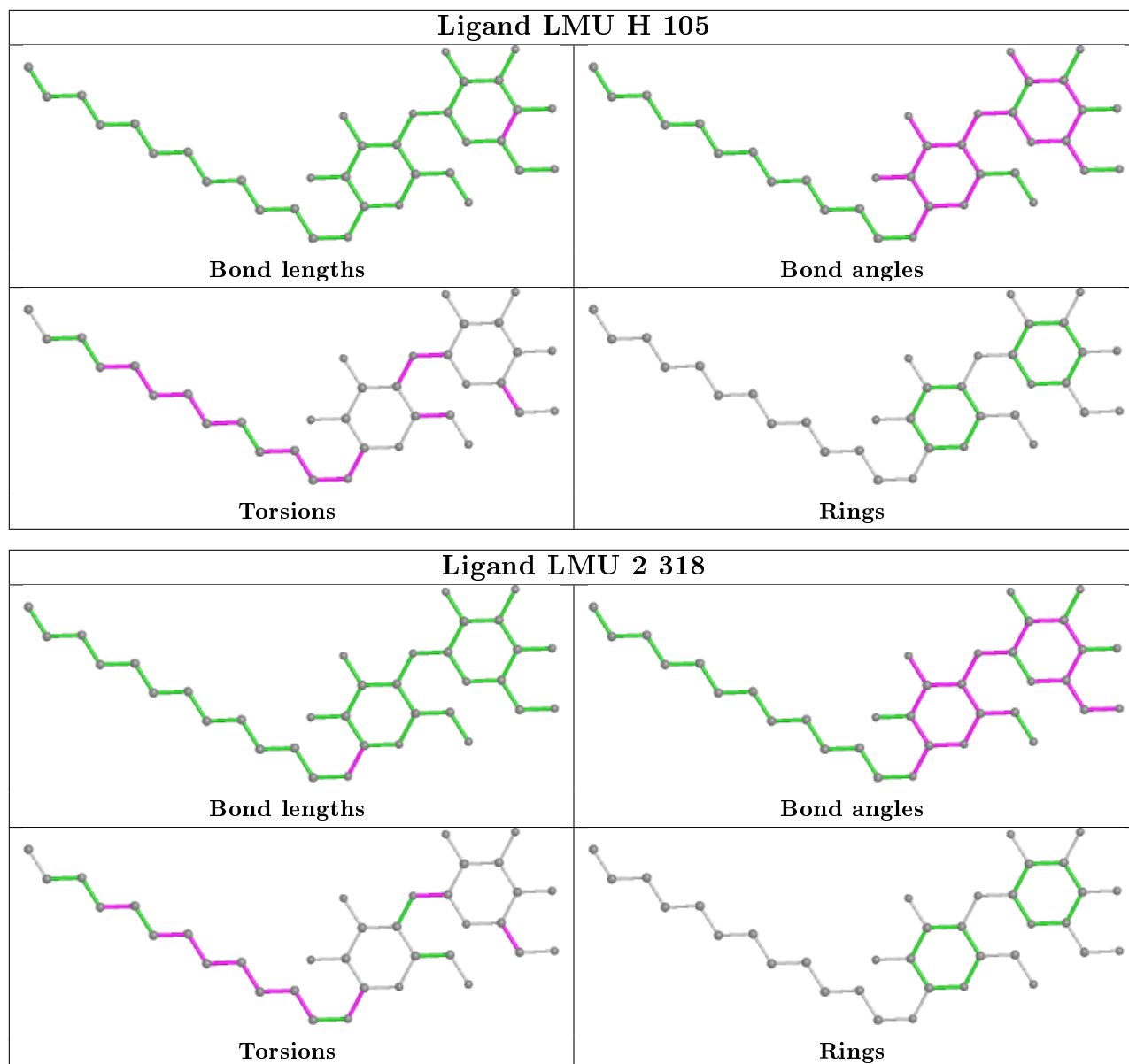


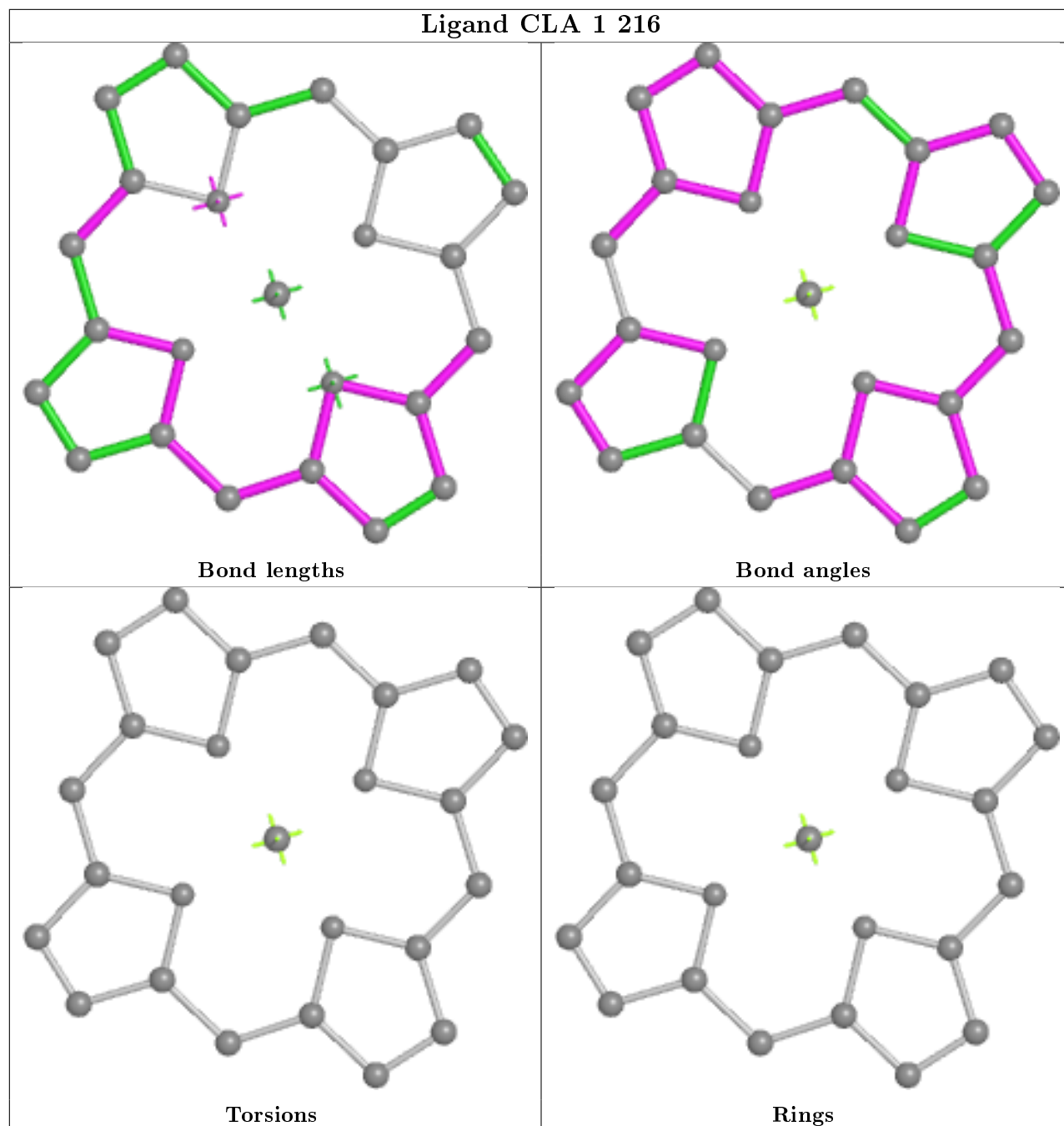


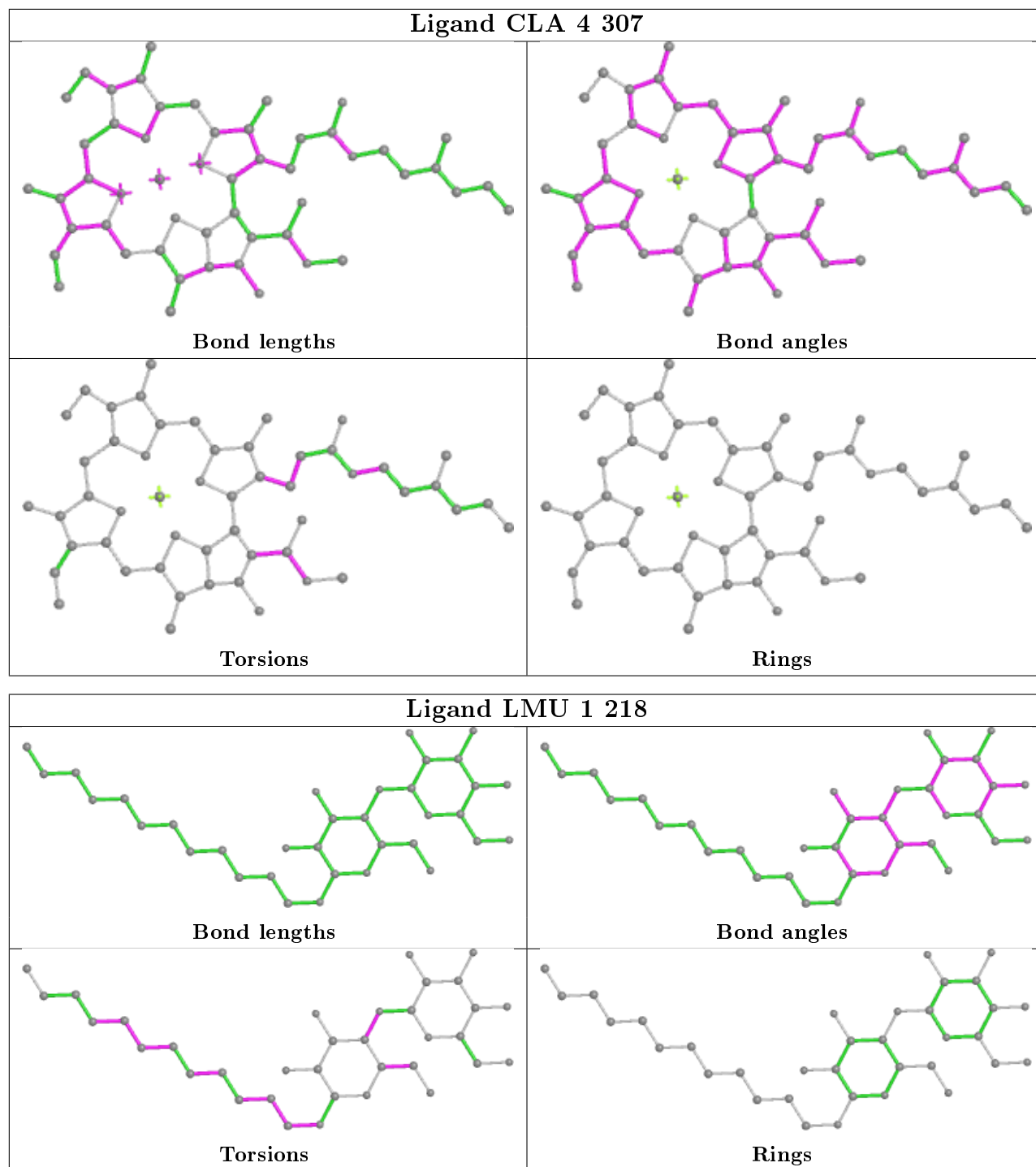


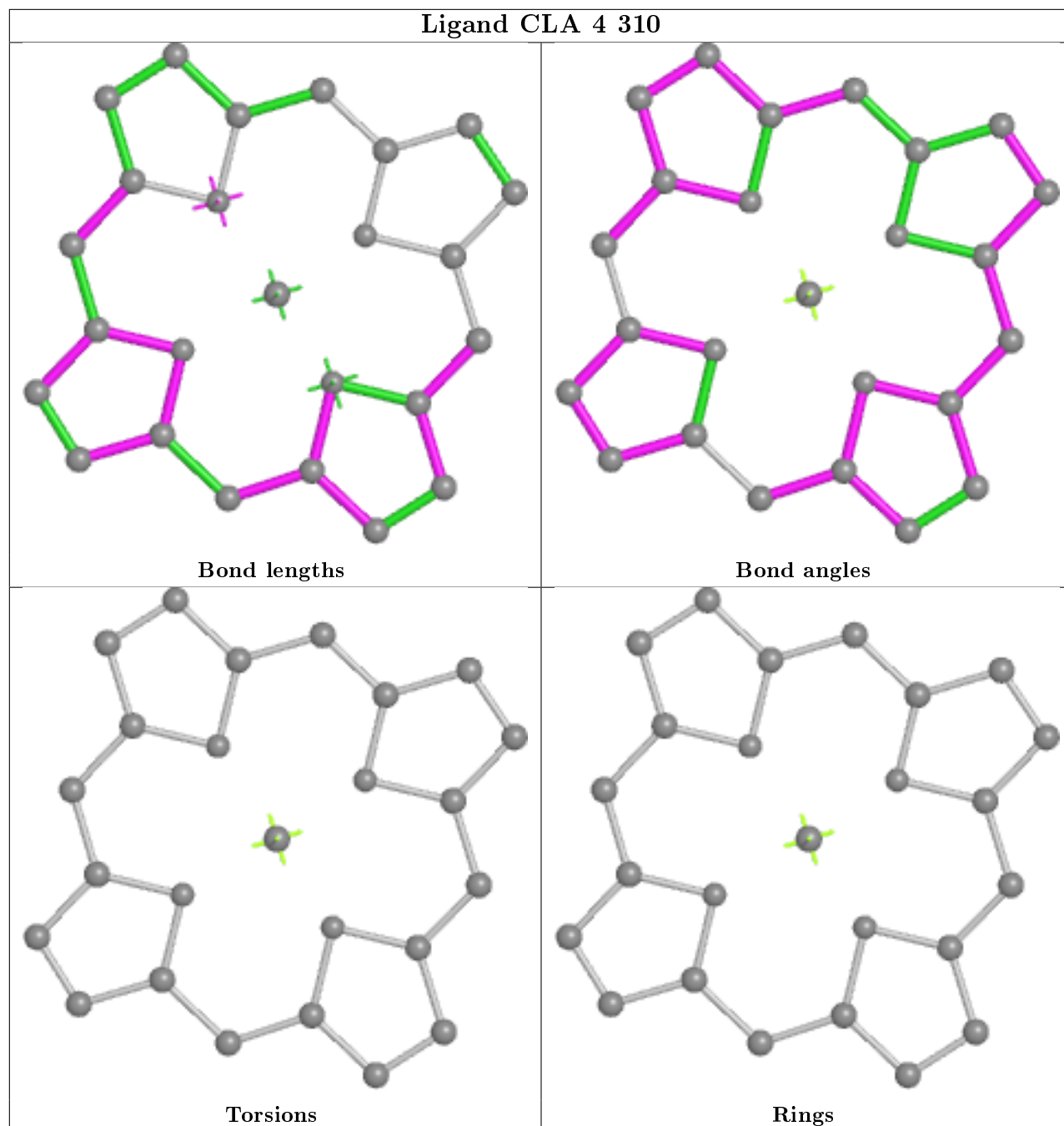


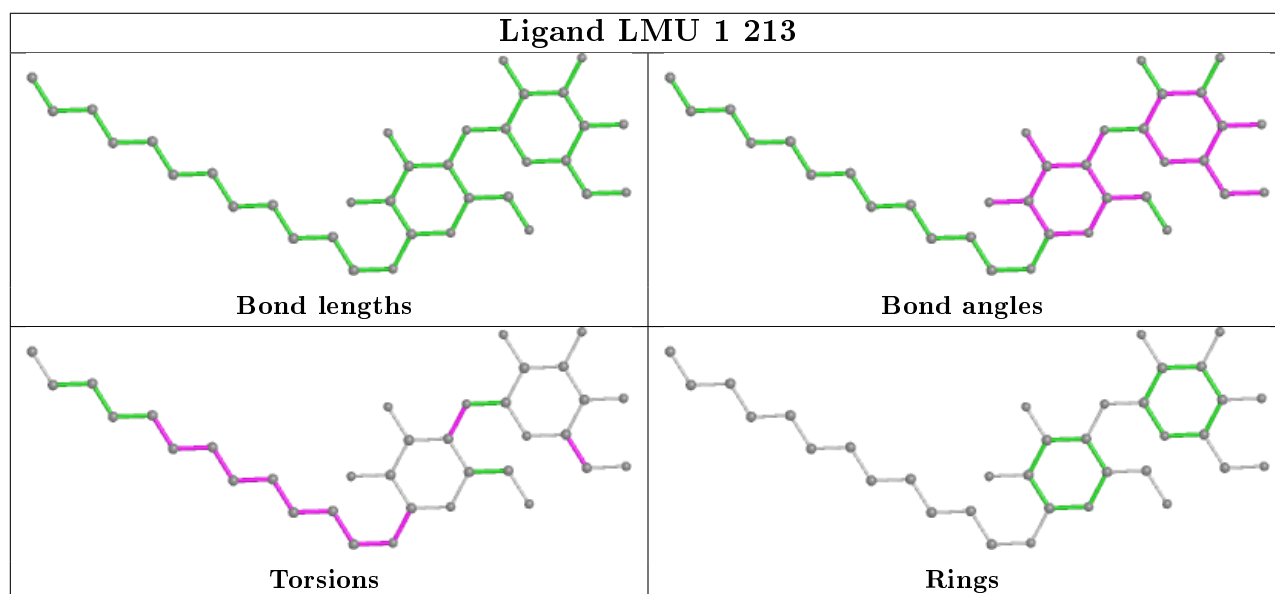
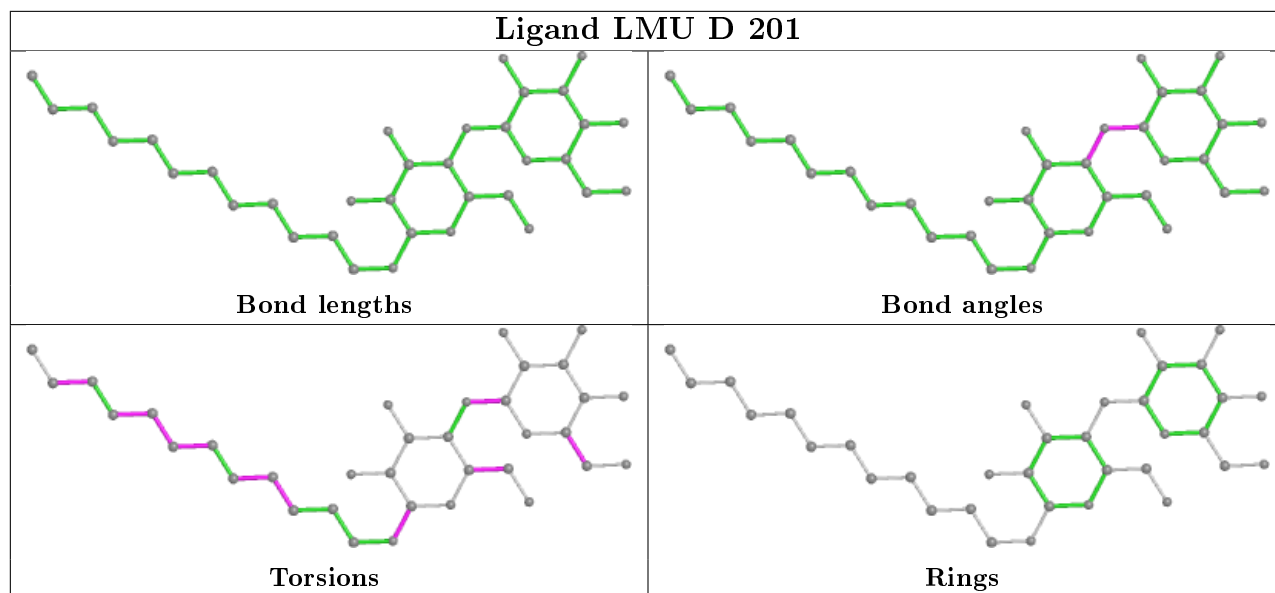


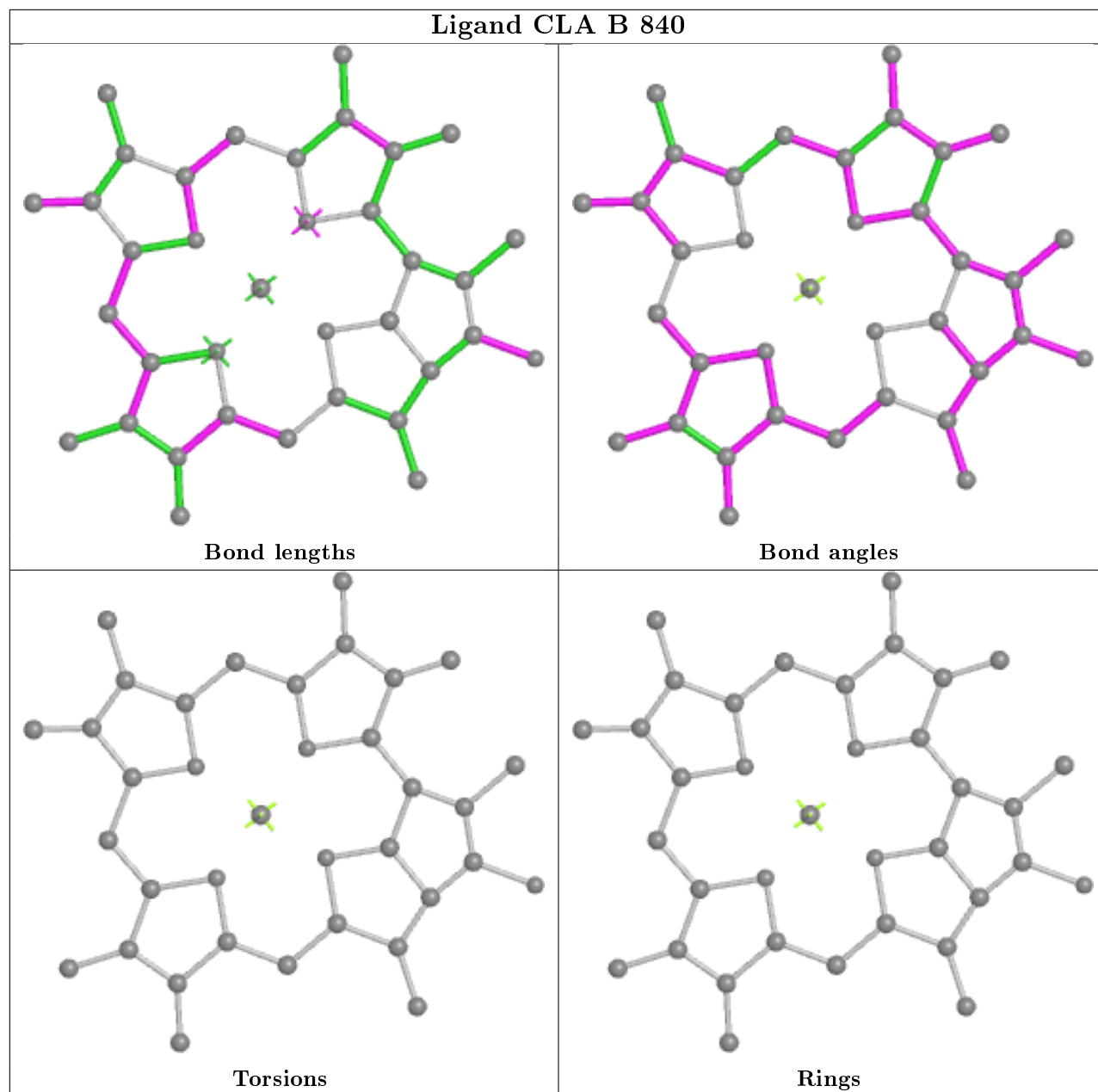


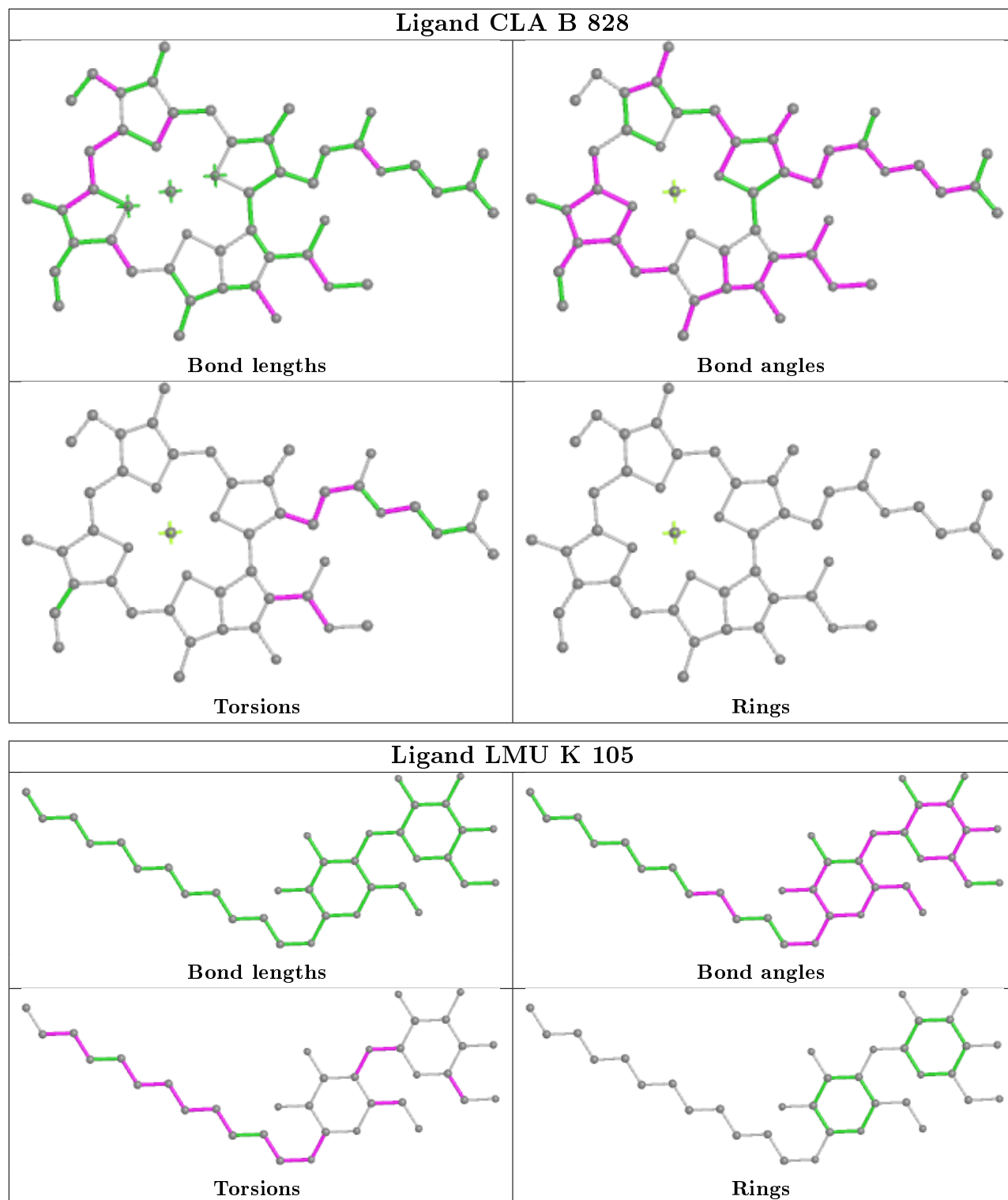


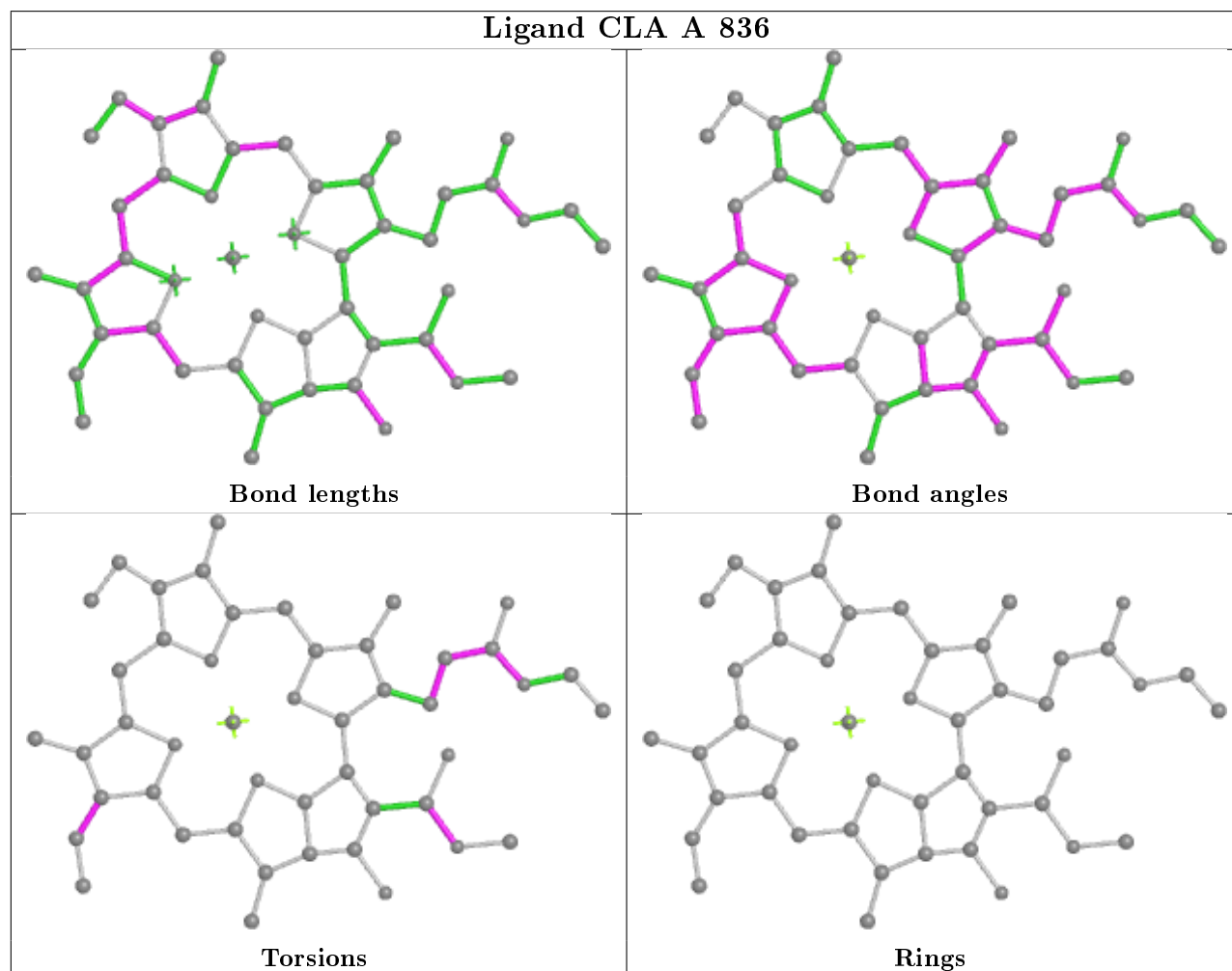
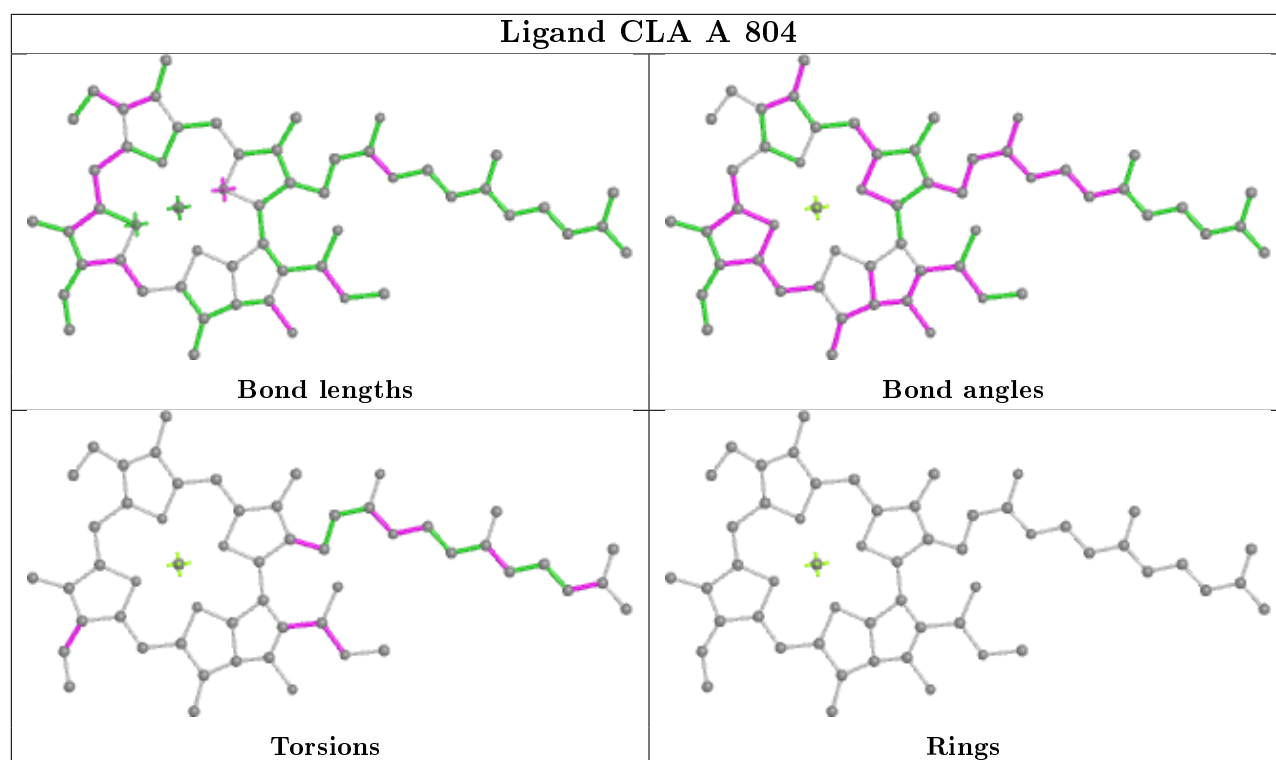


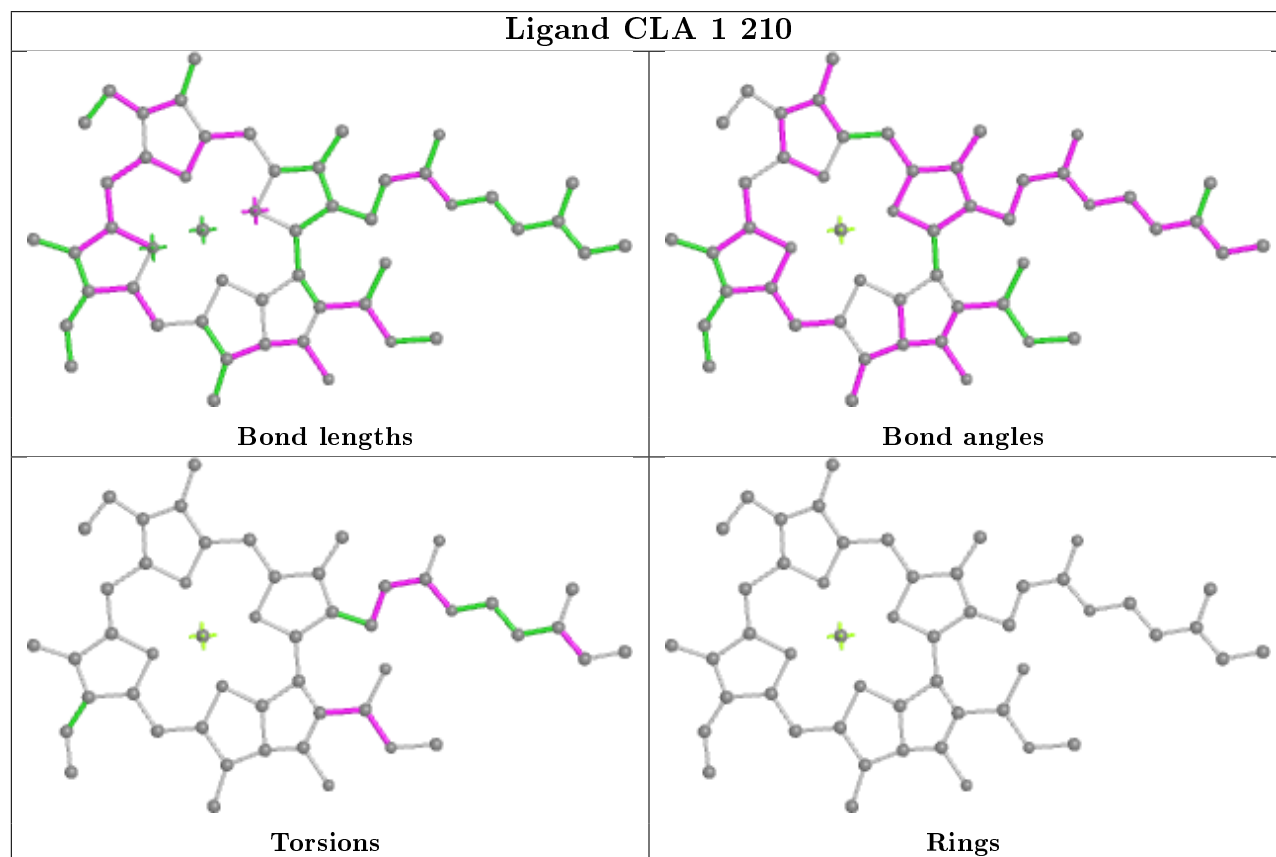
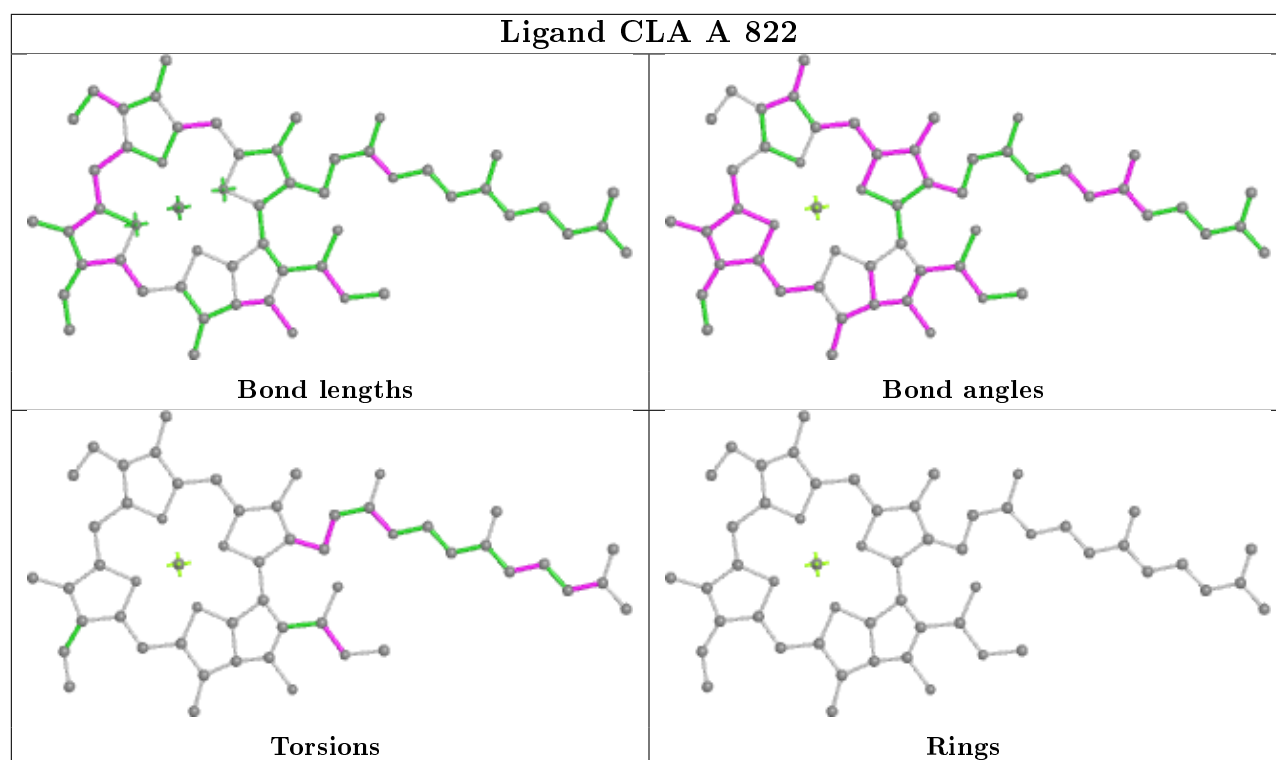


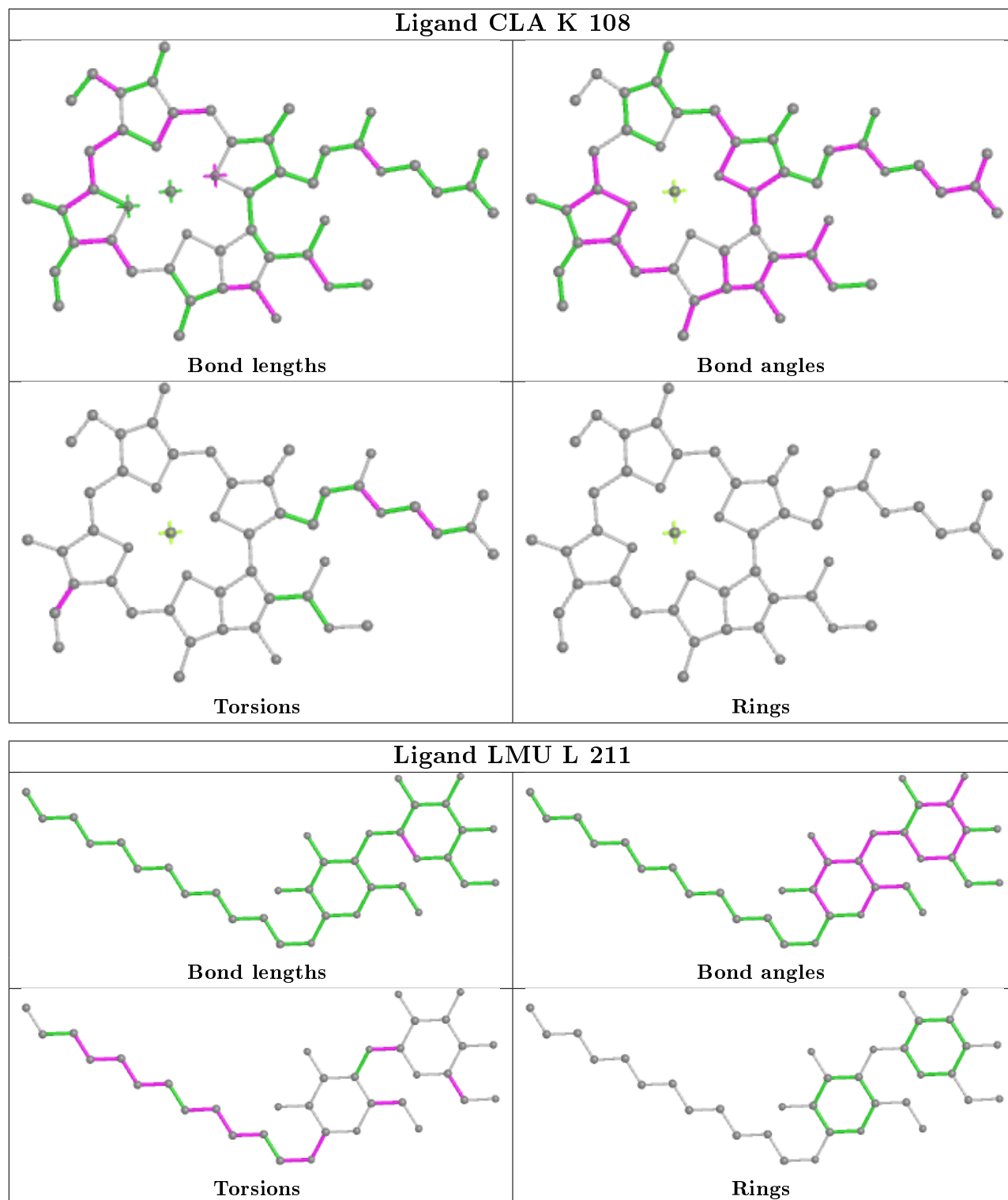


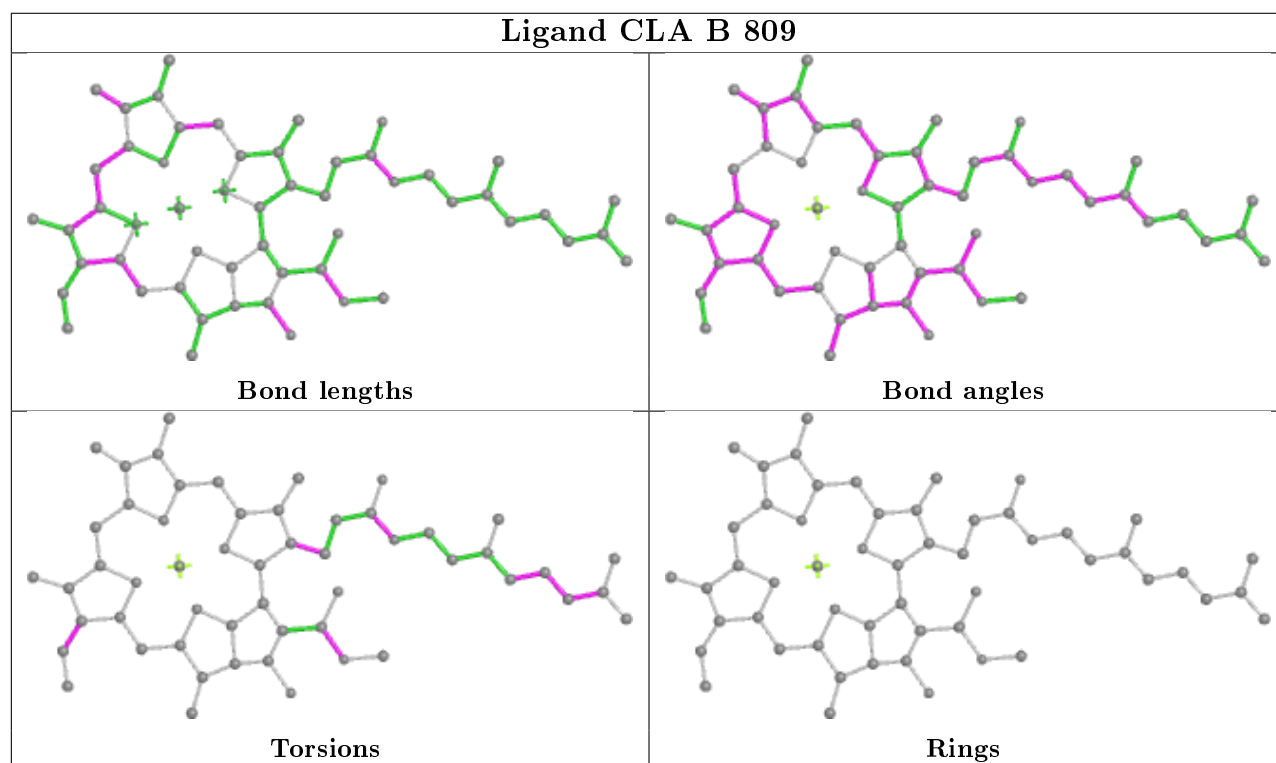
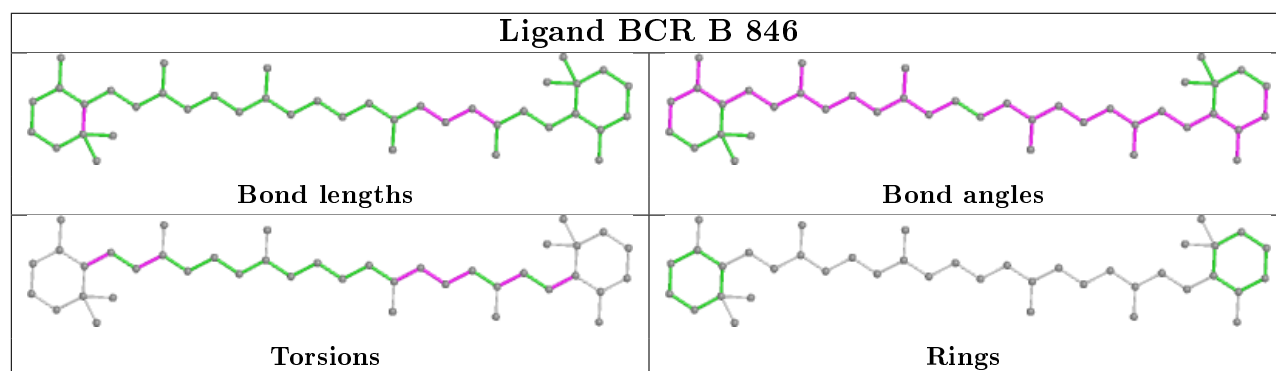
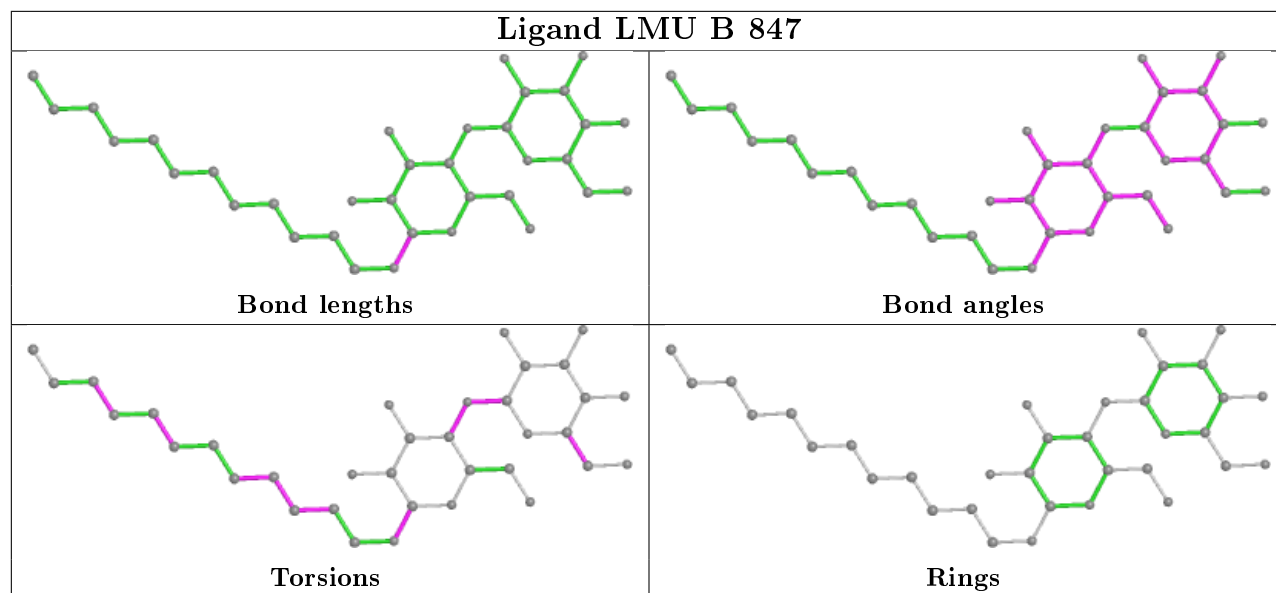


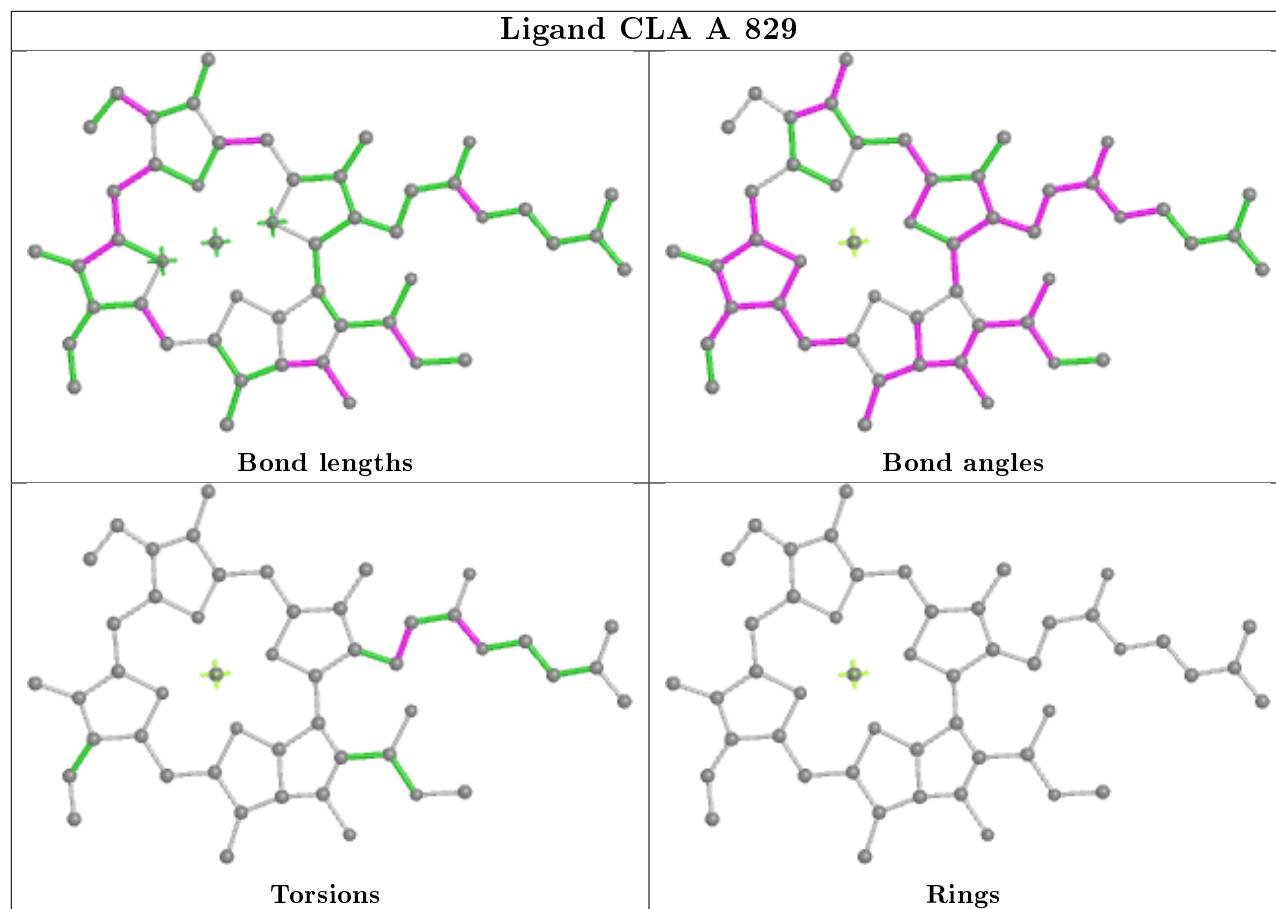


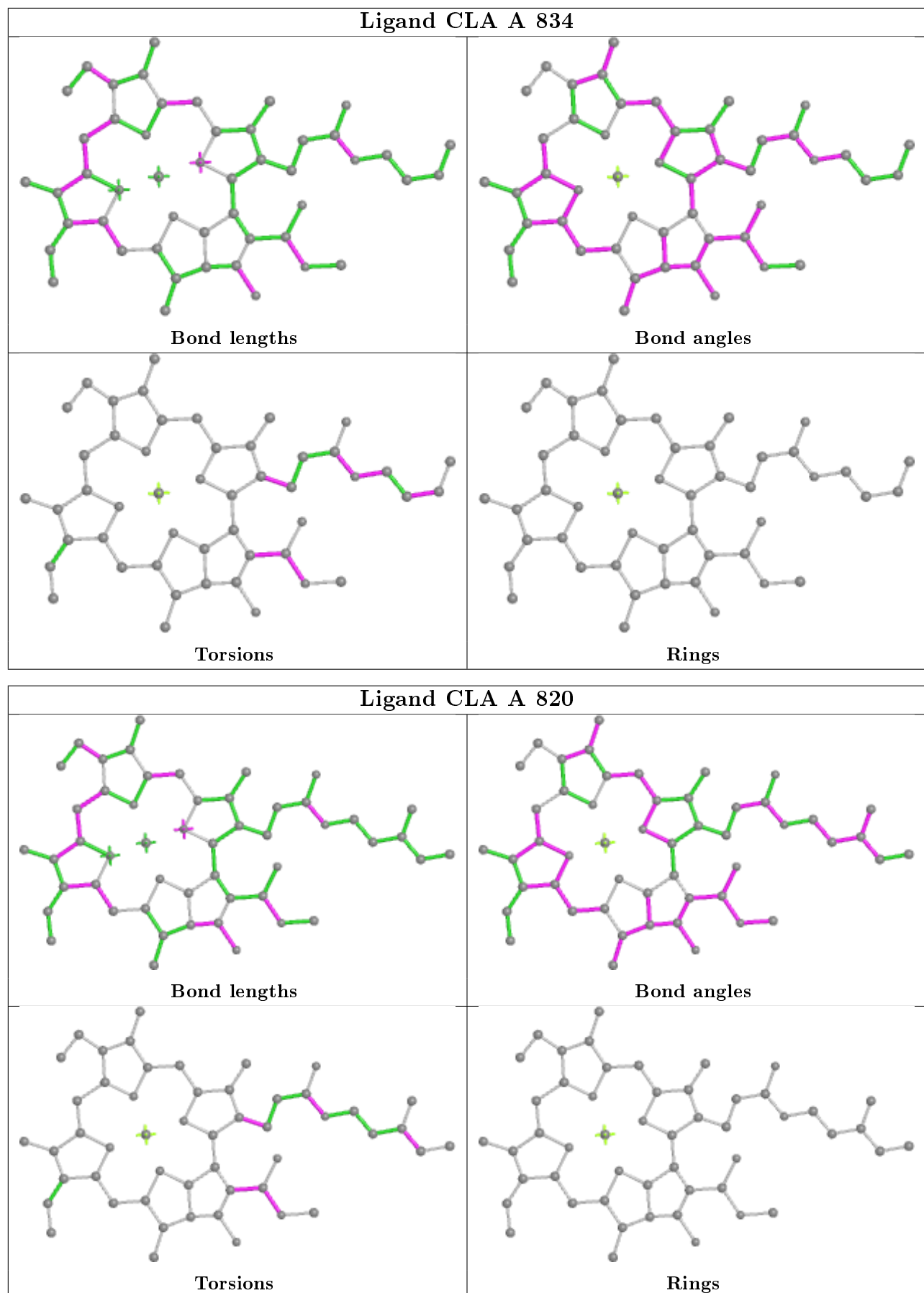


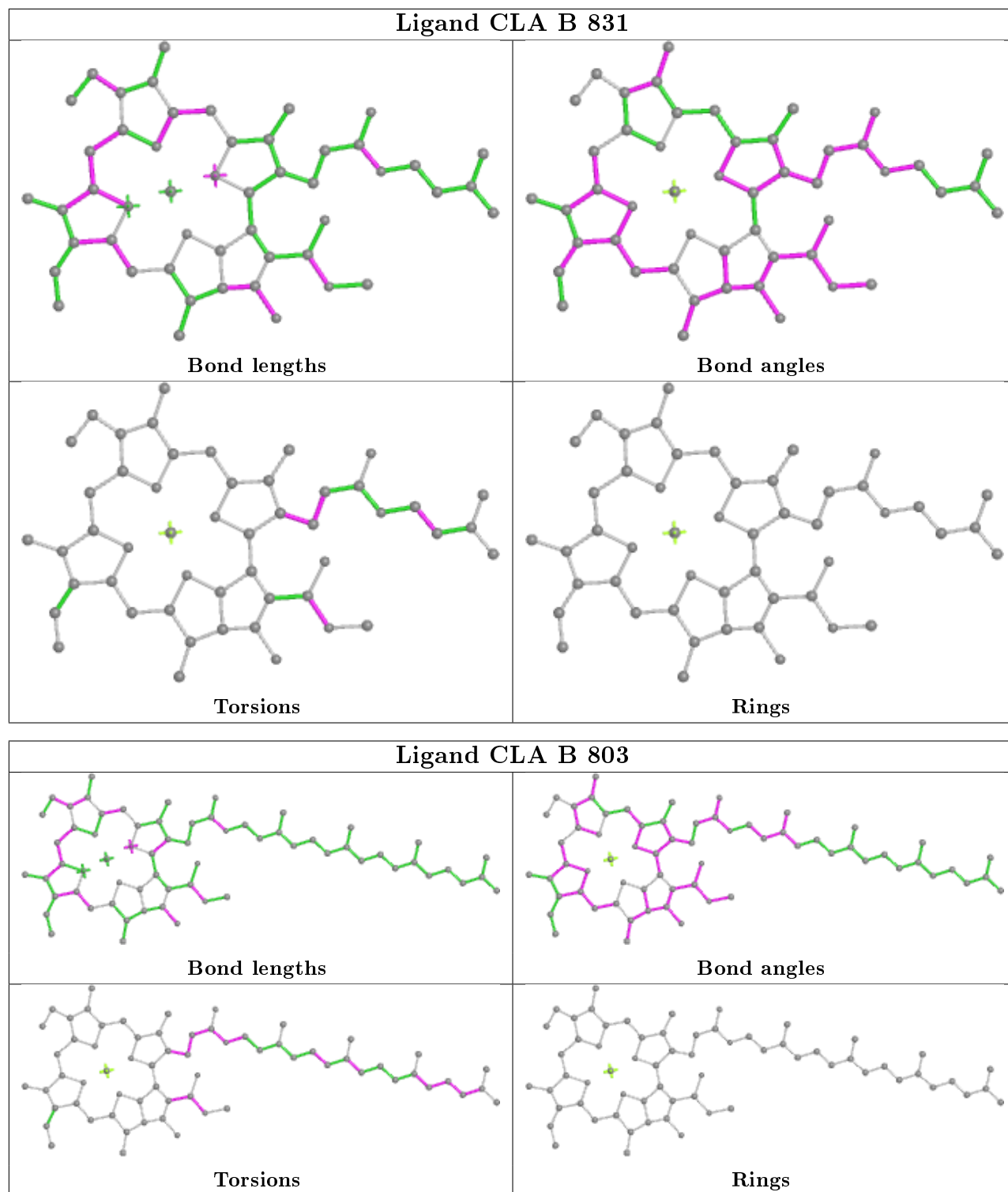


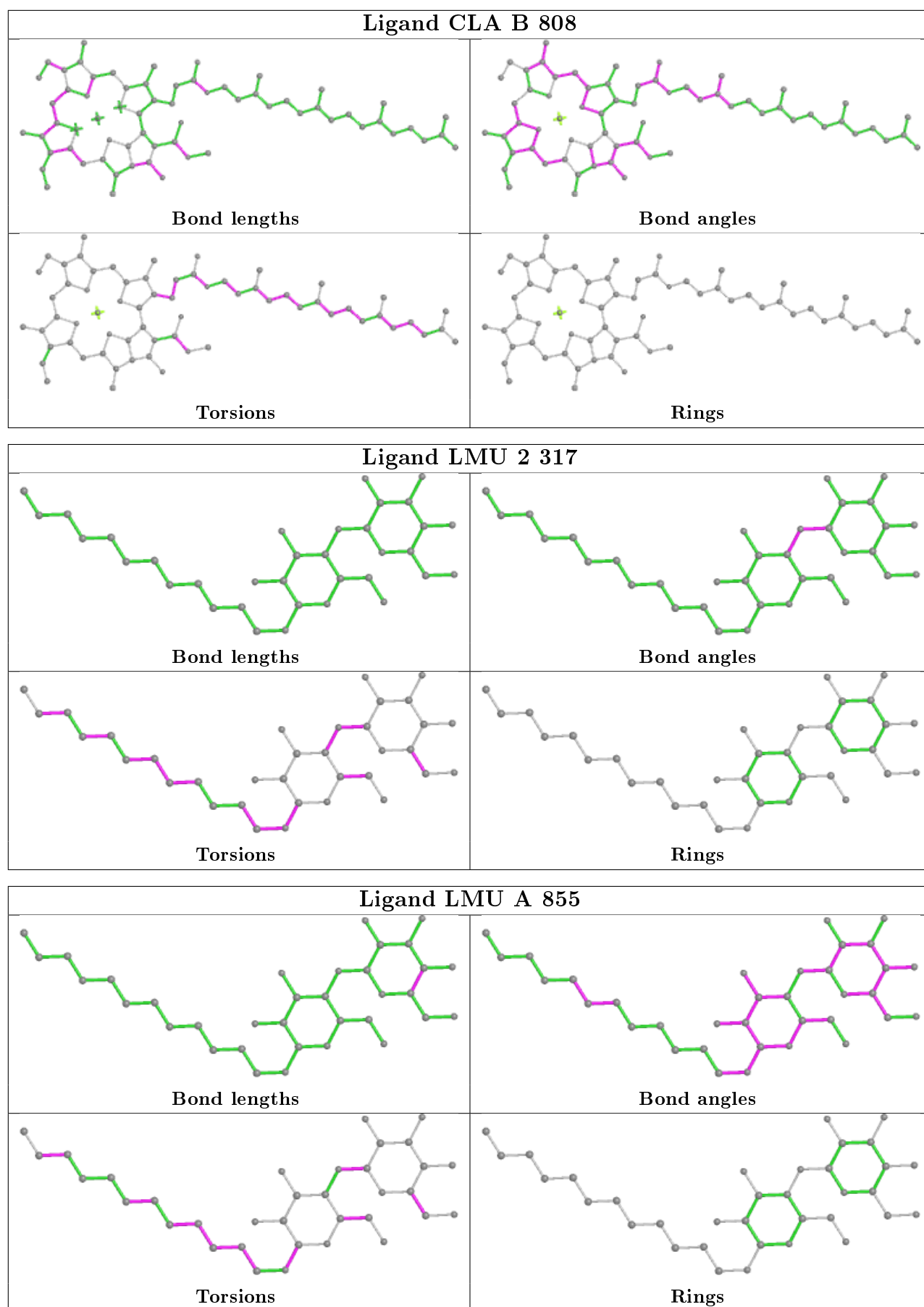


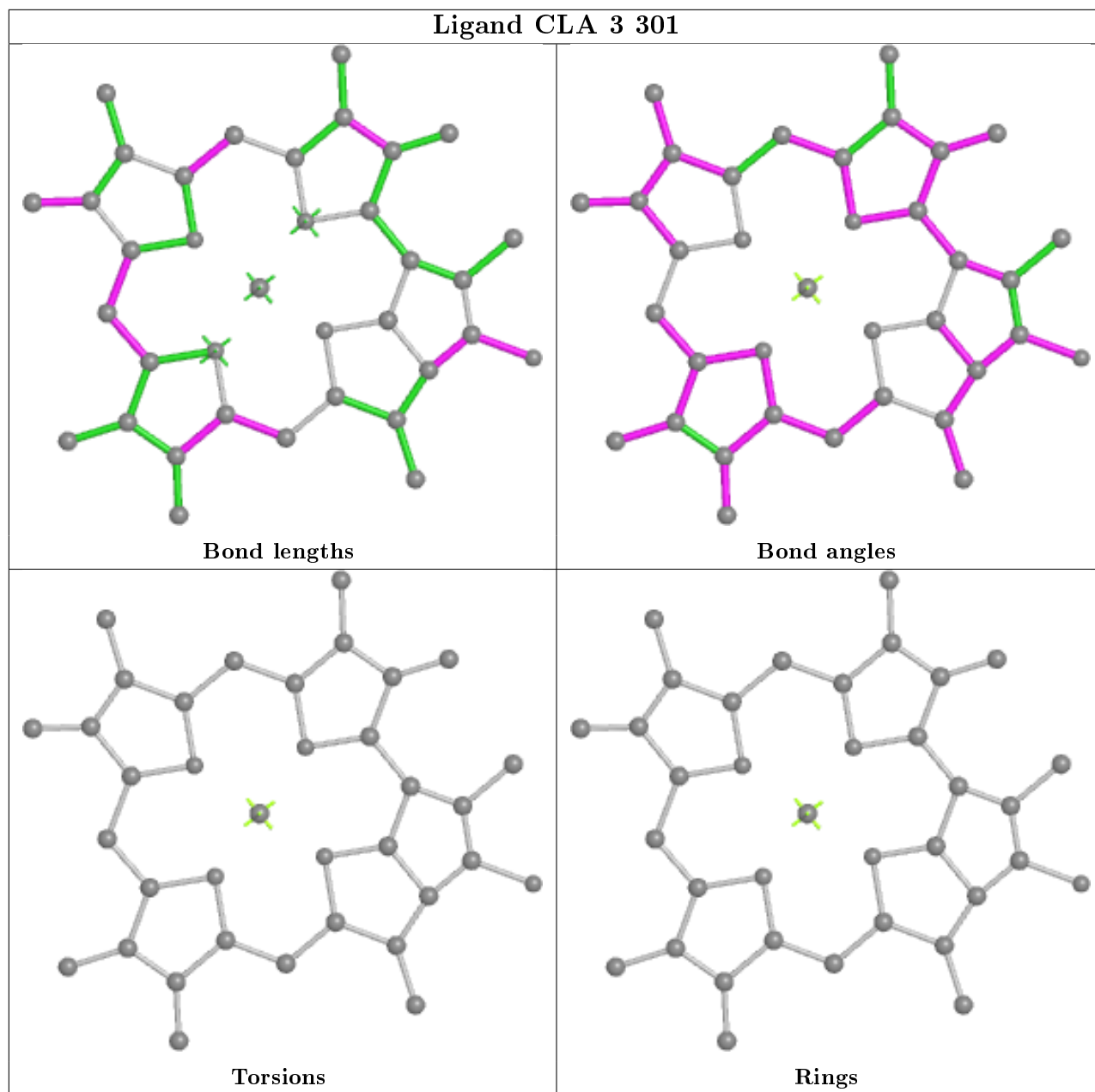


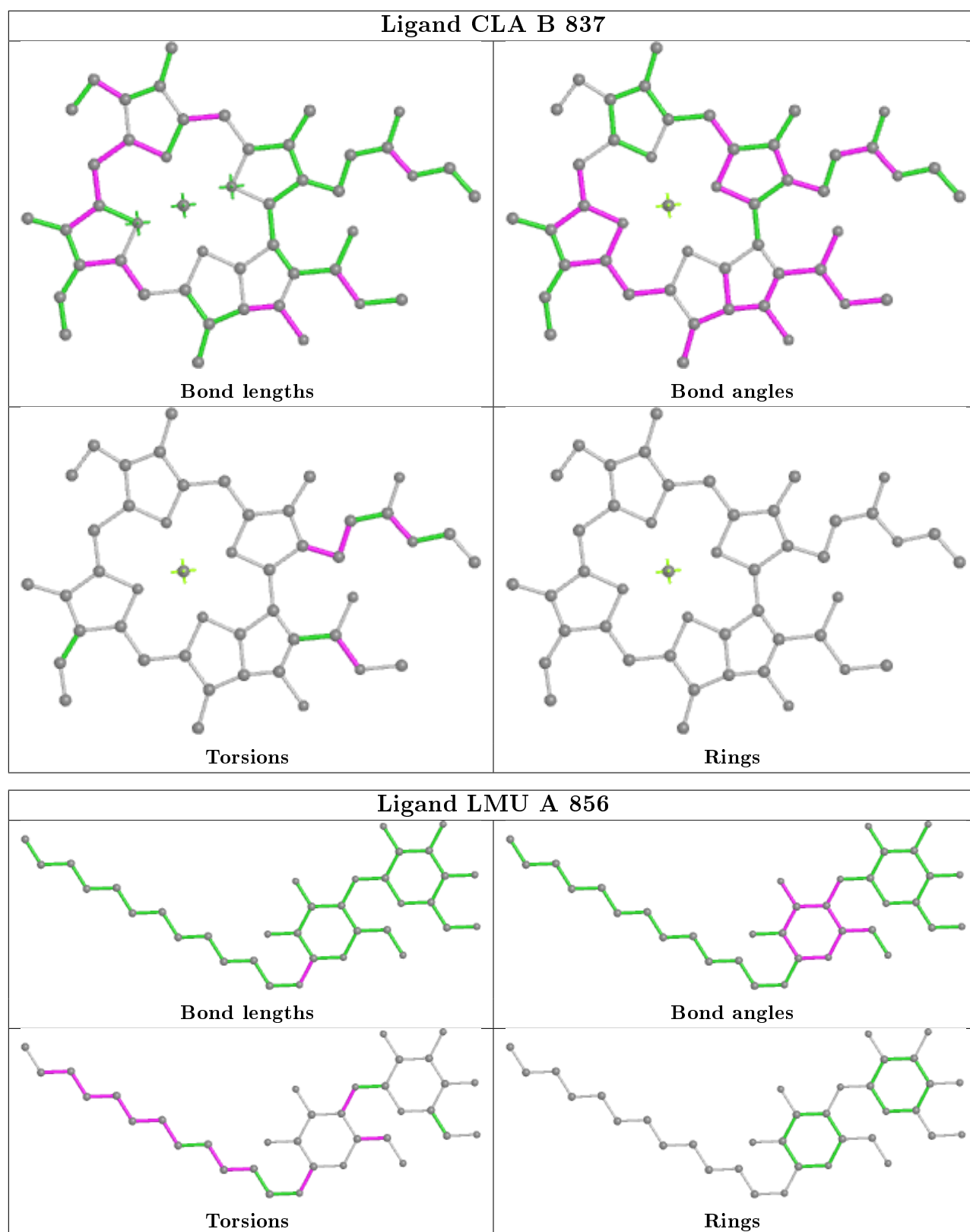


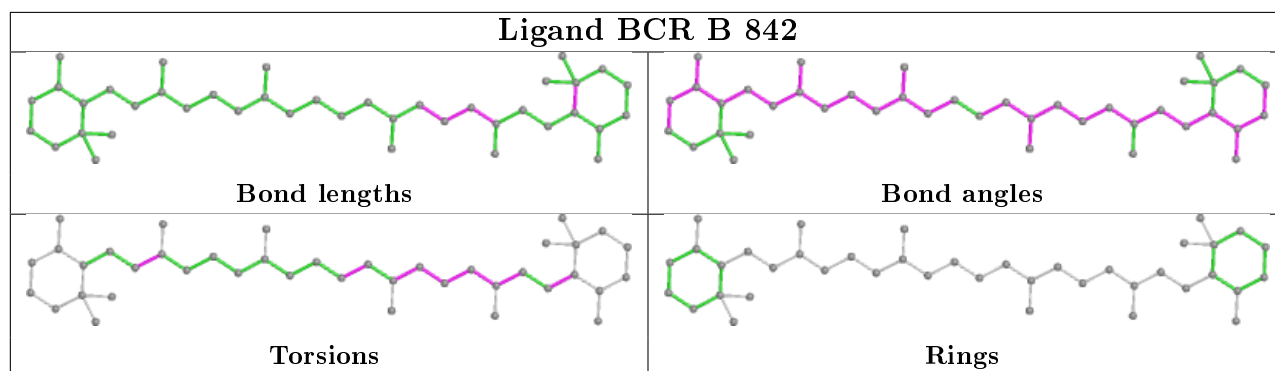
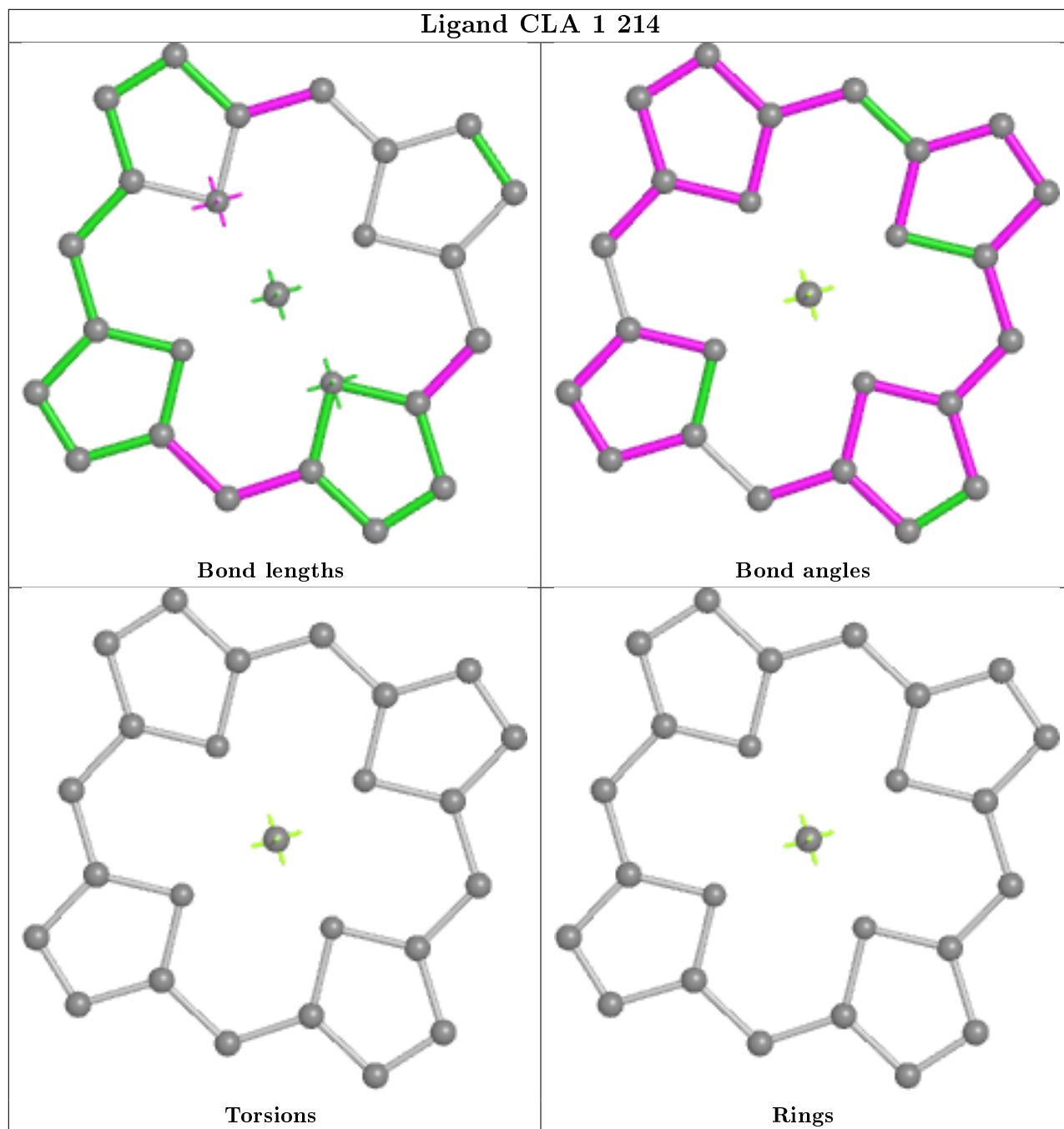




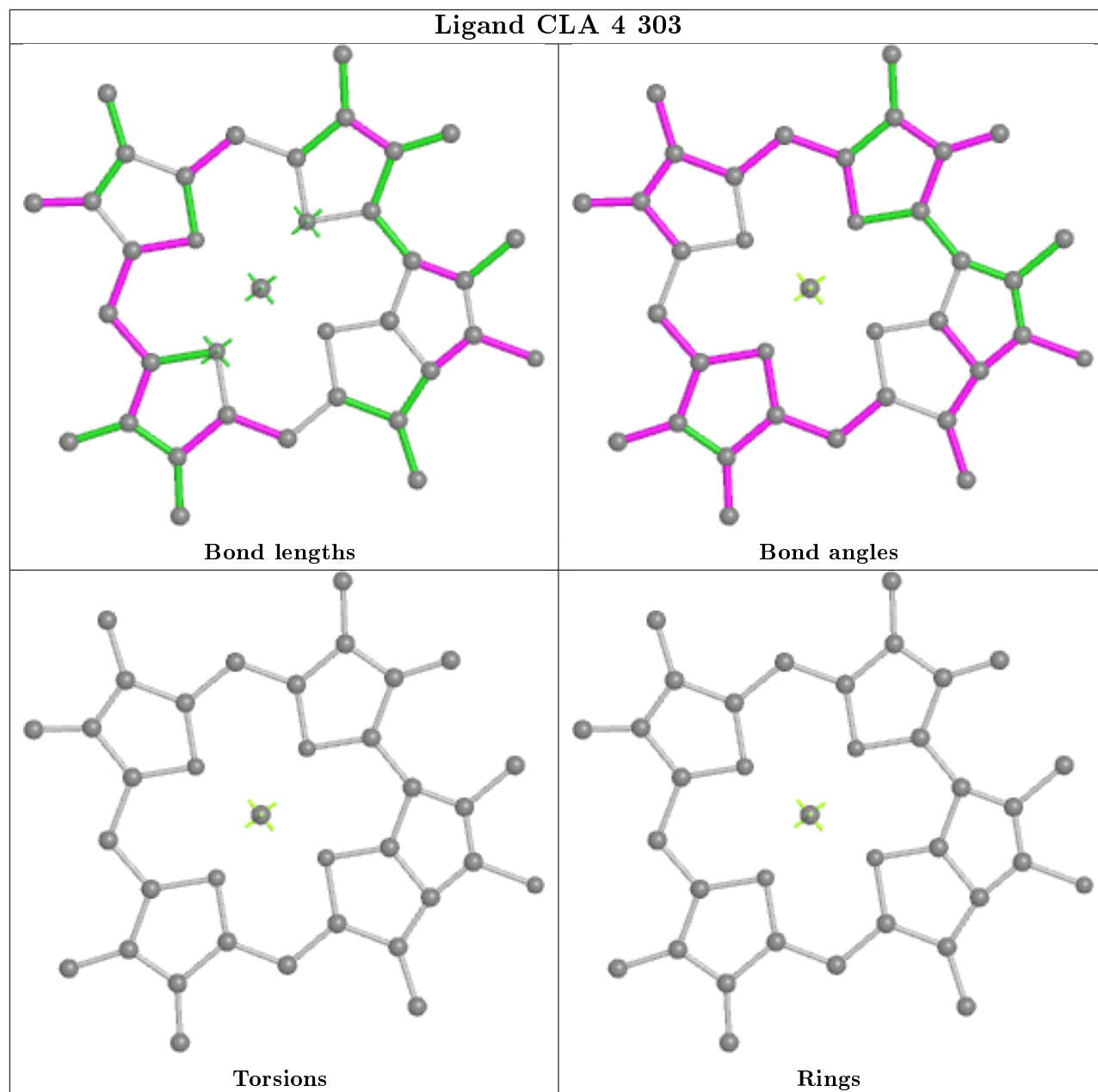


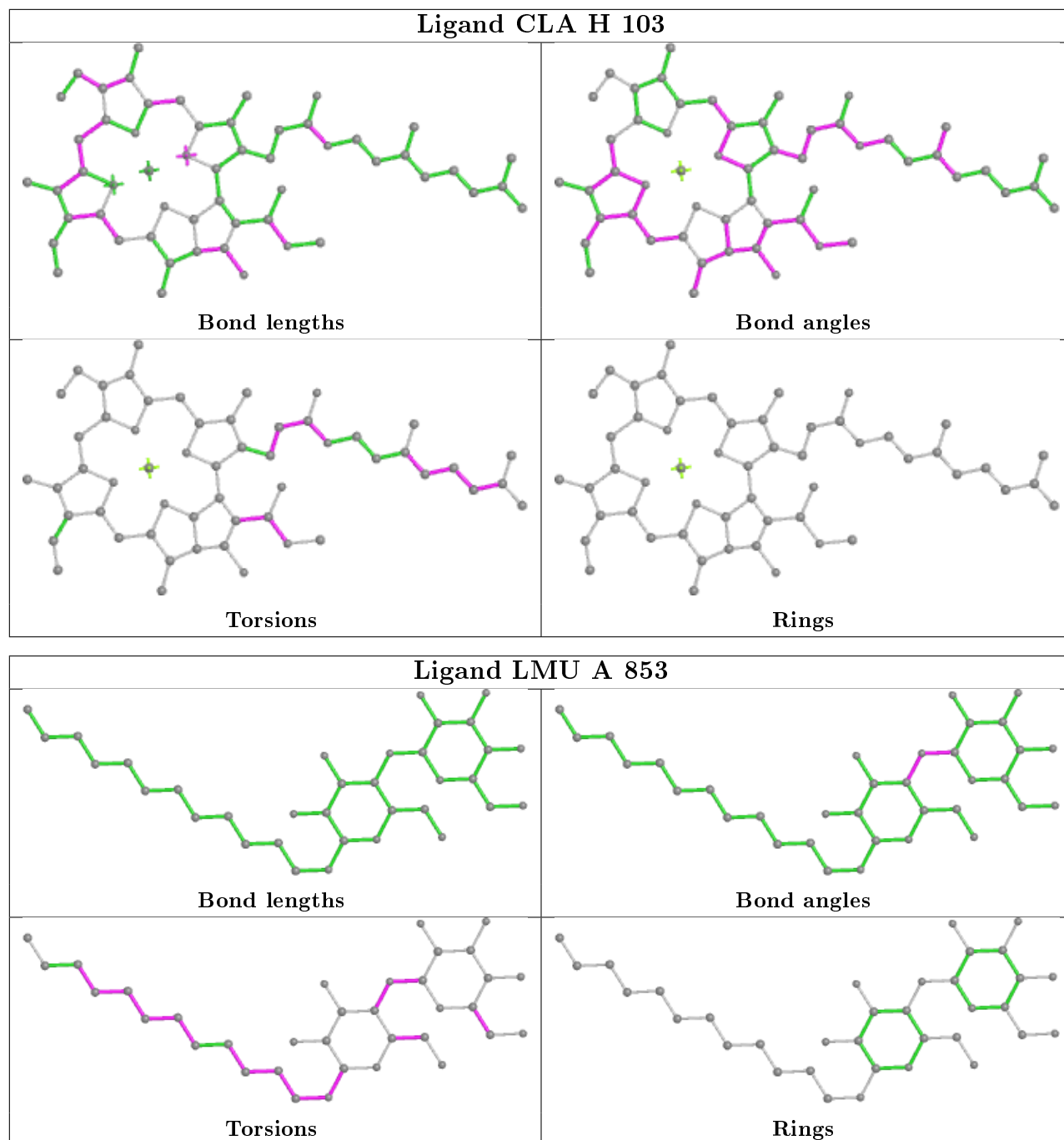


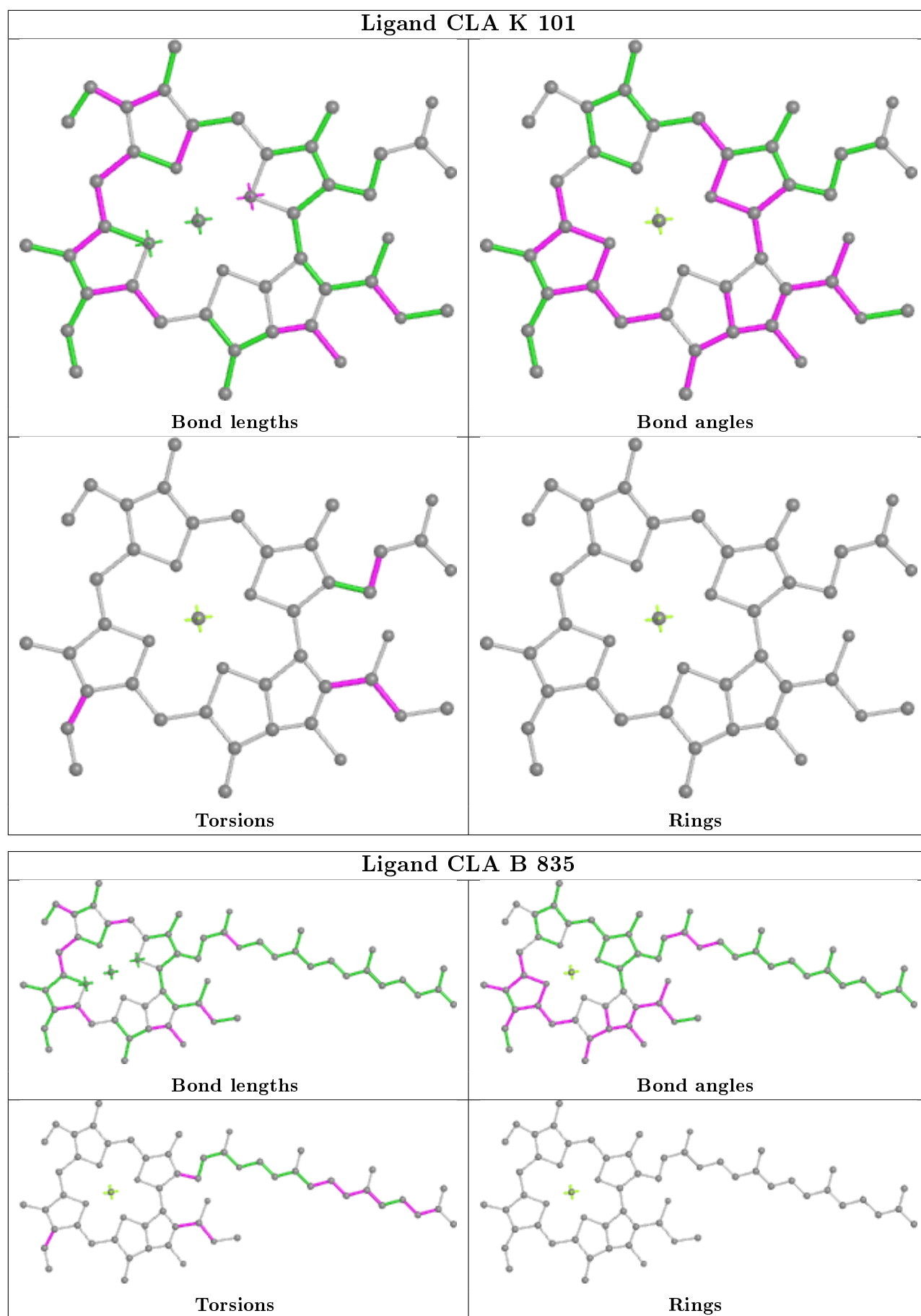


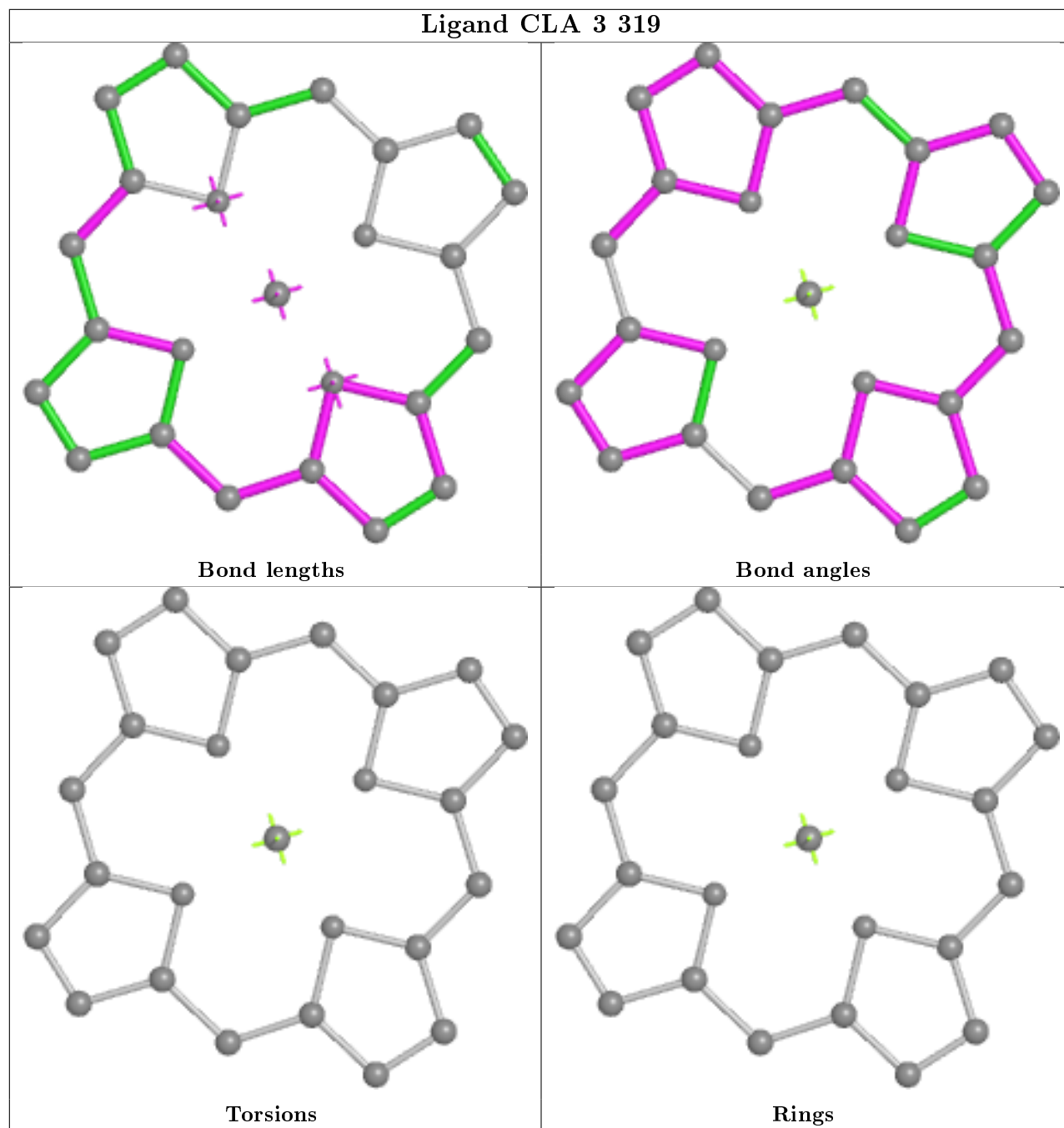


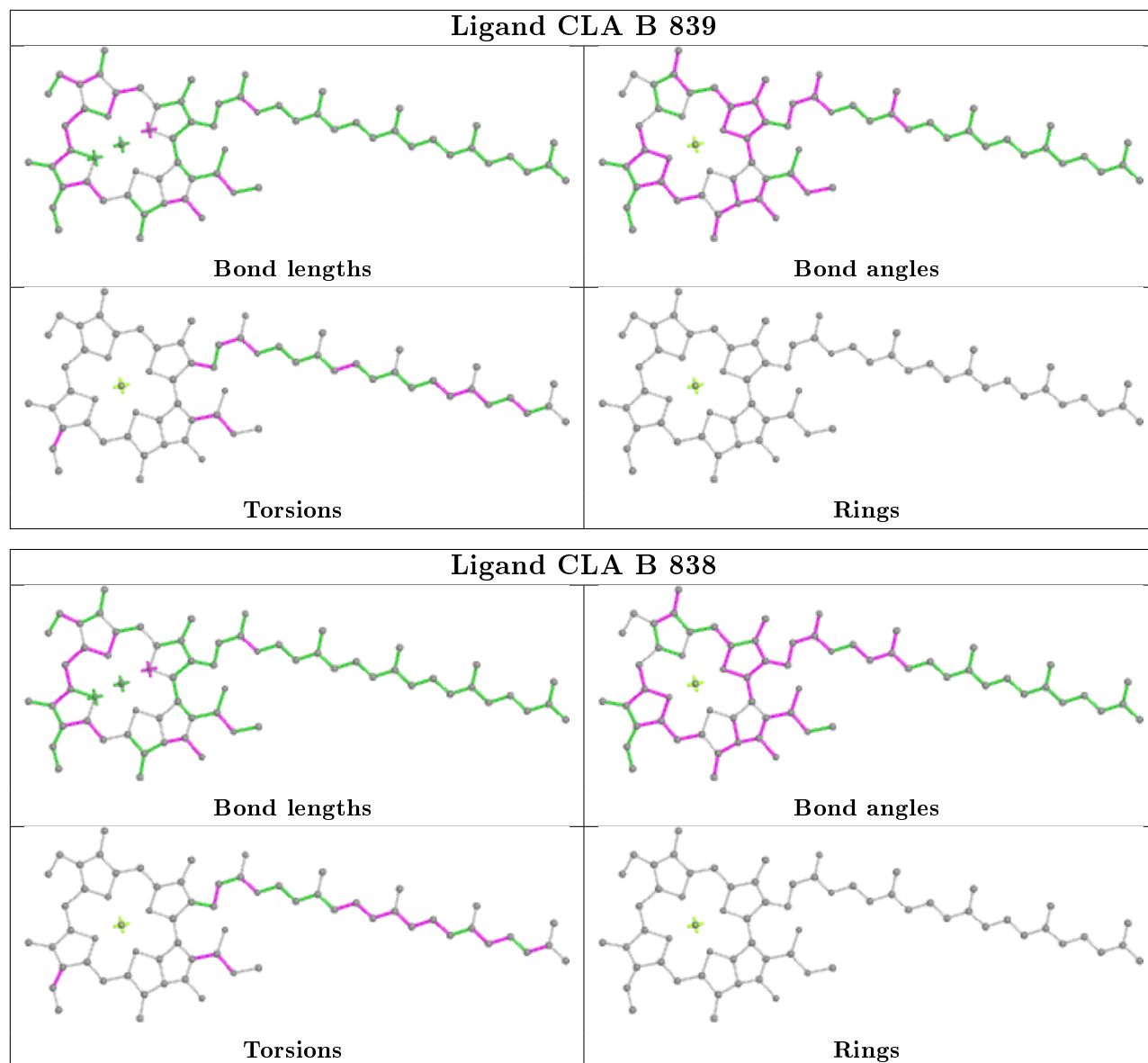
Ligand CLA 4 303

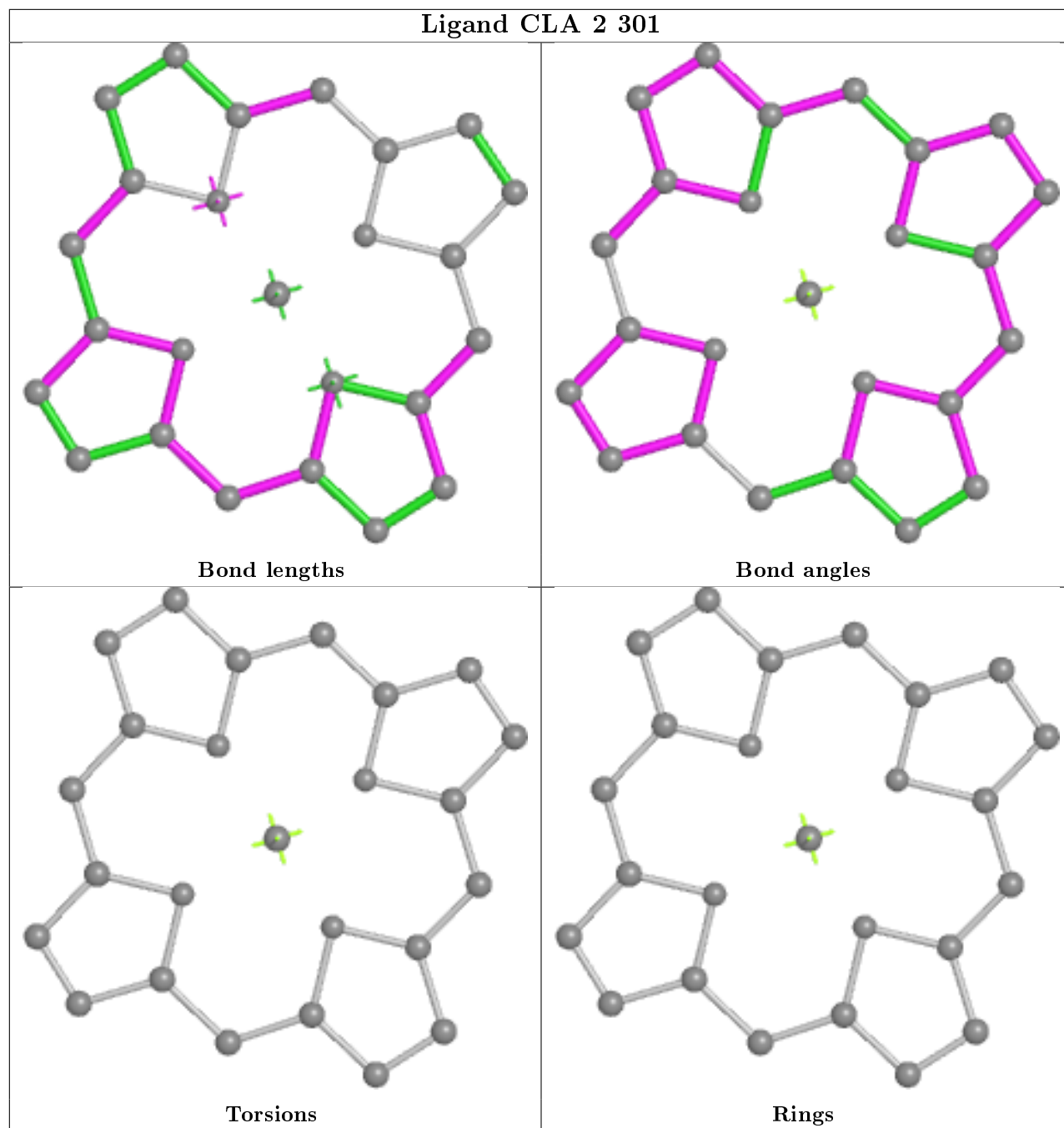


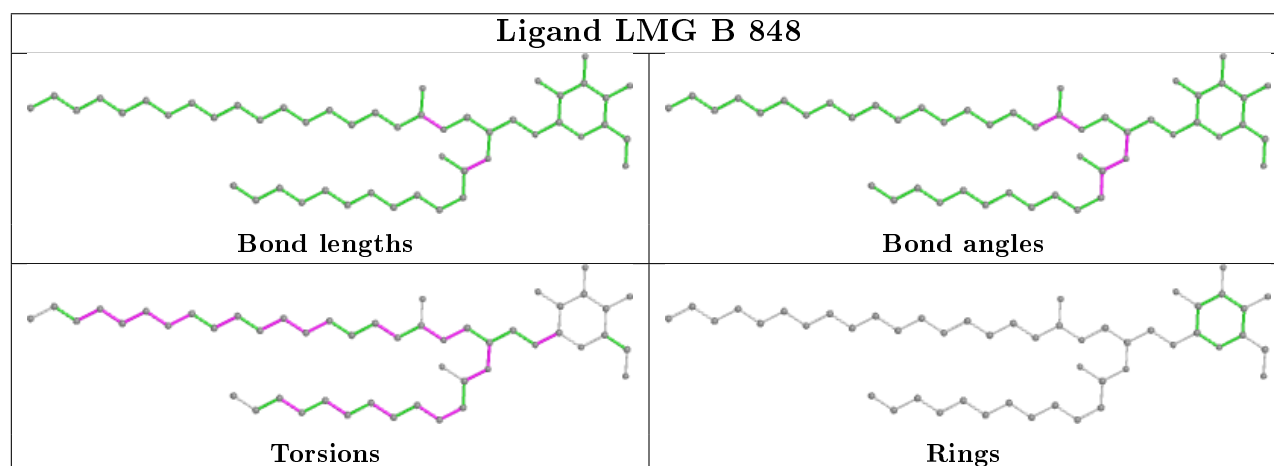
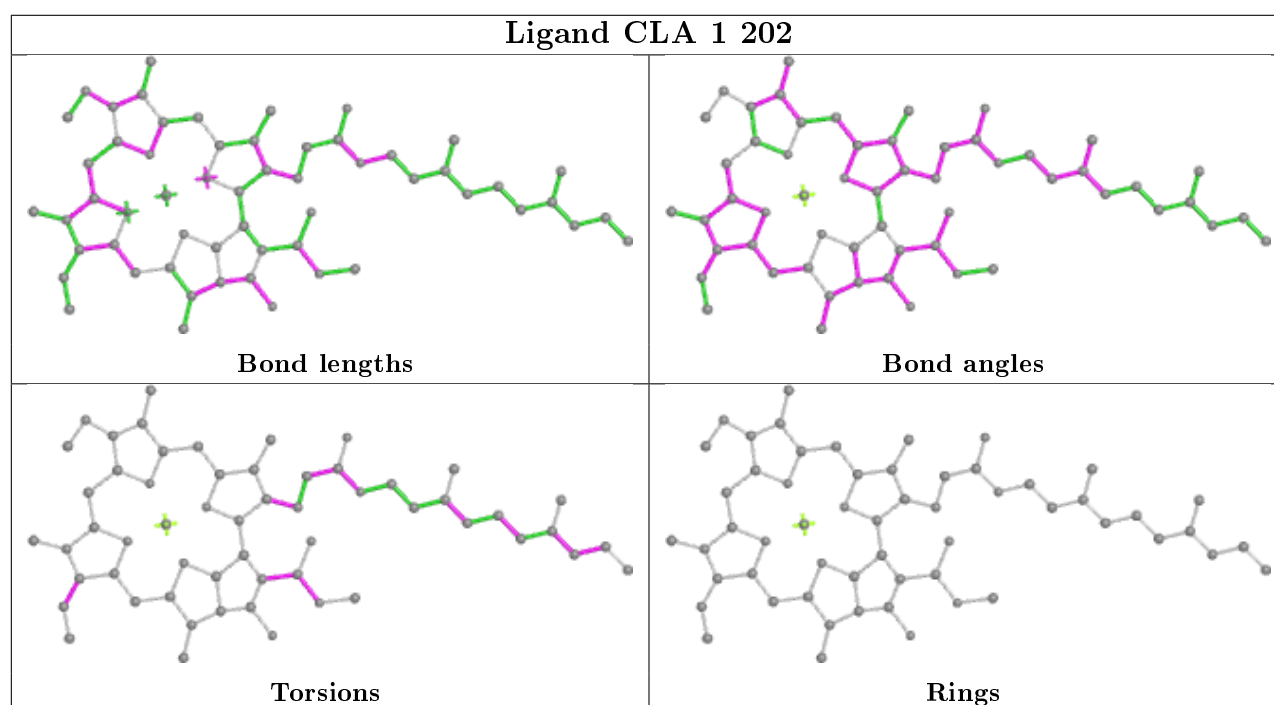
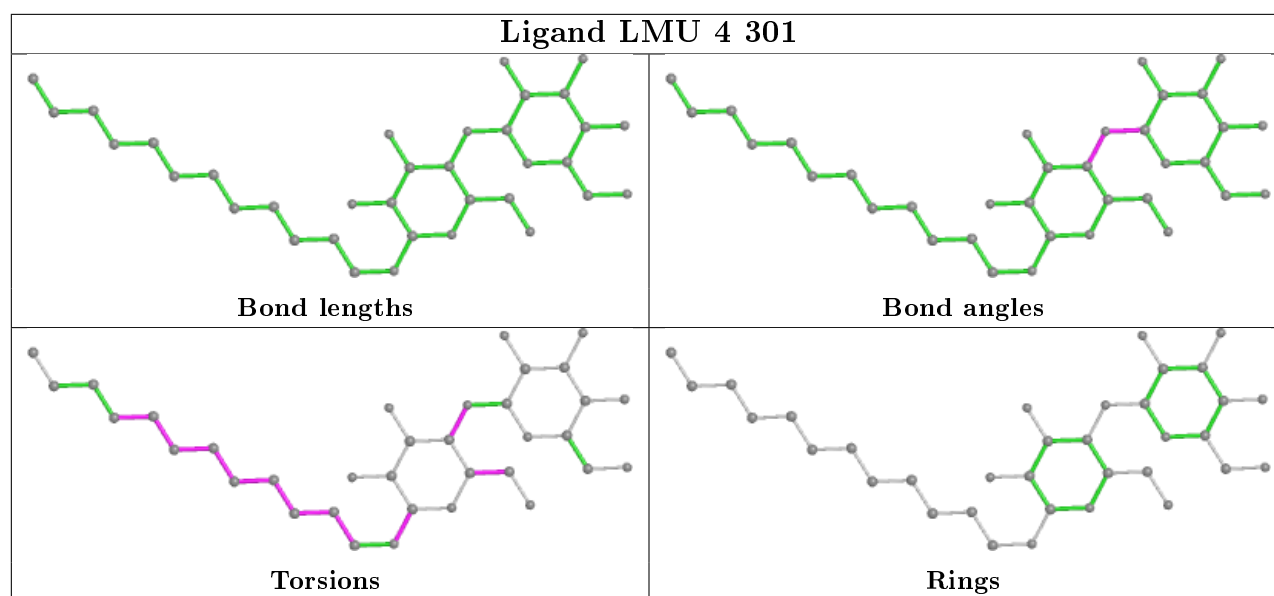


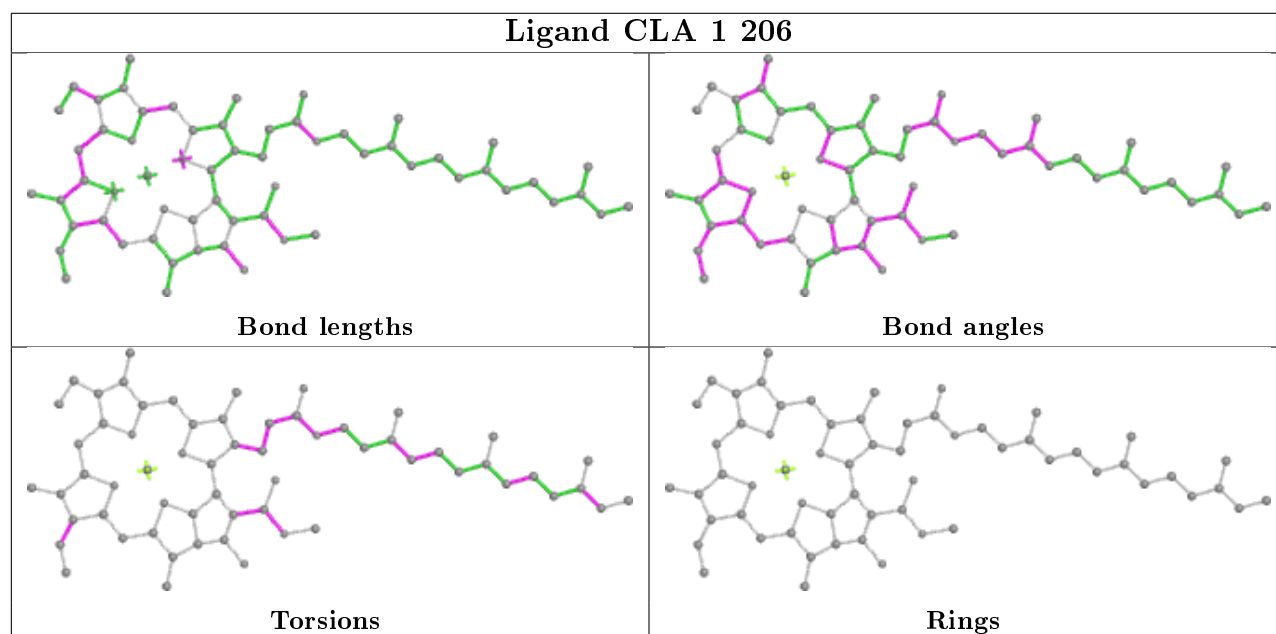
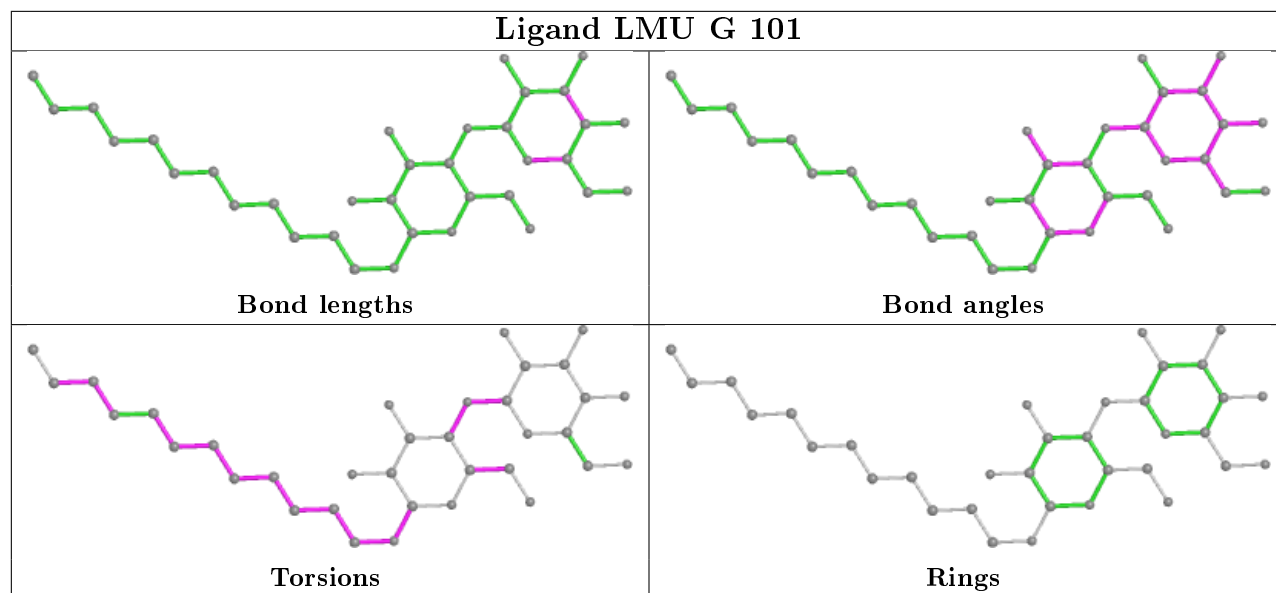


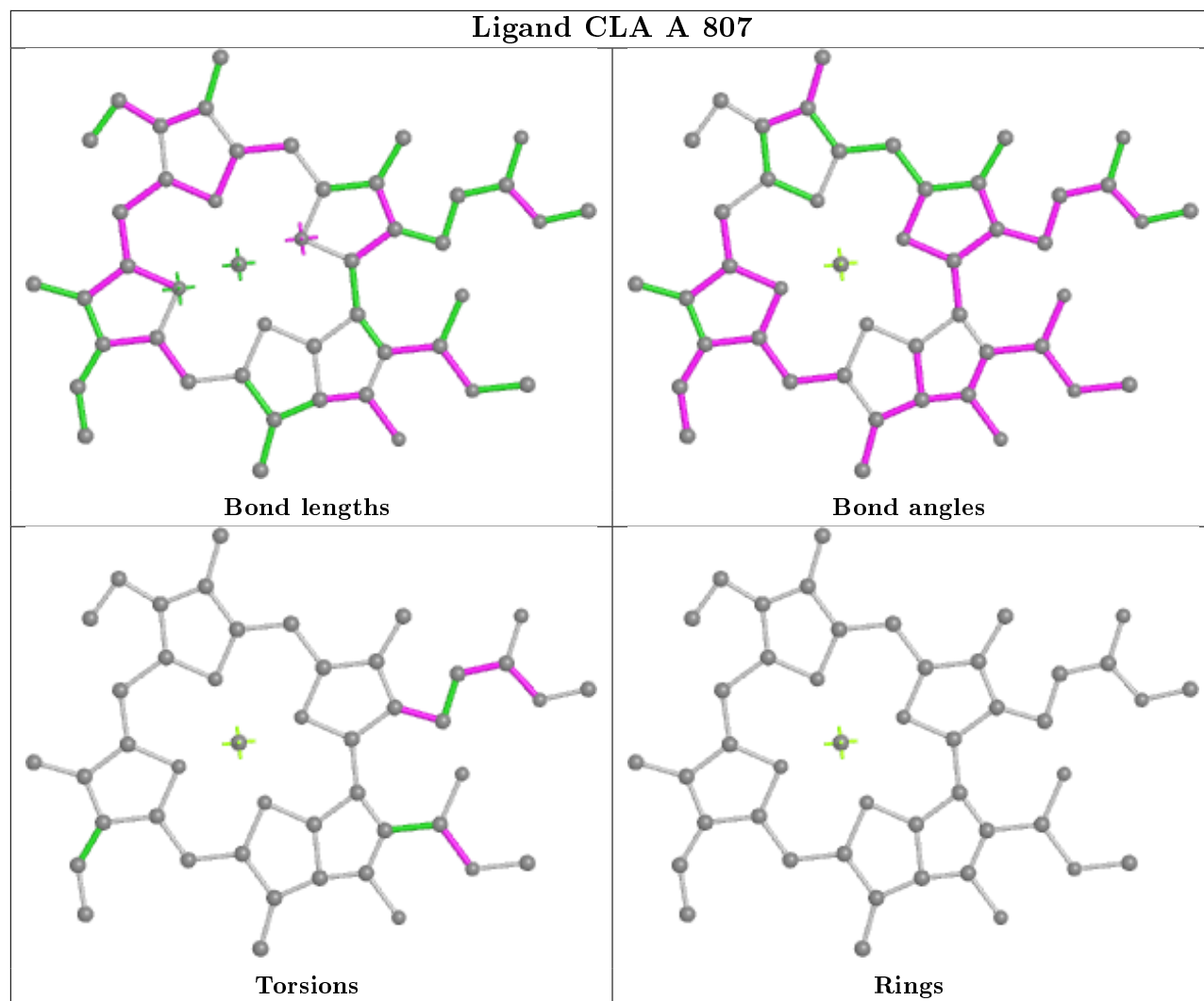


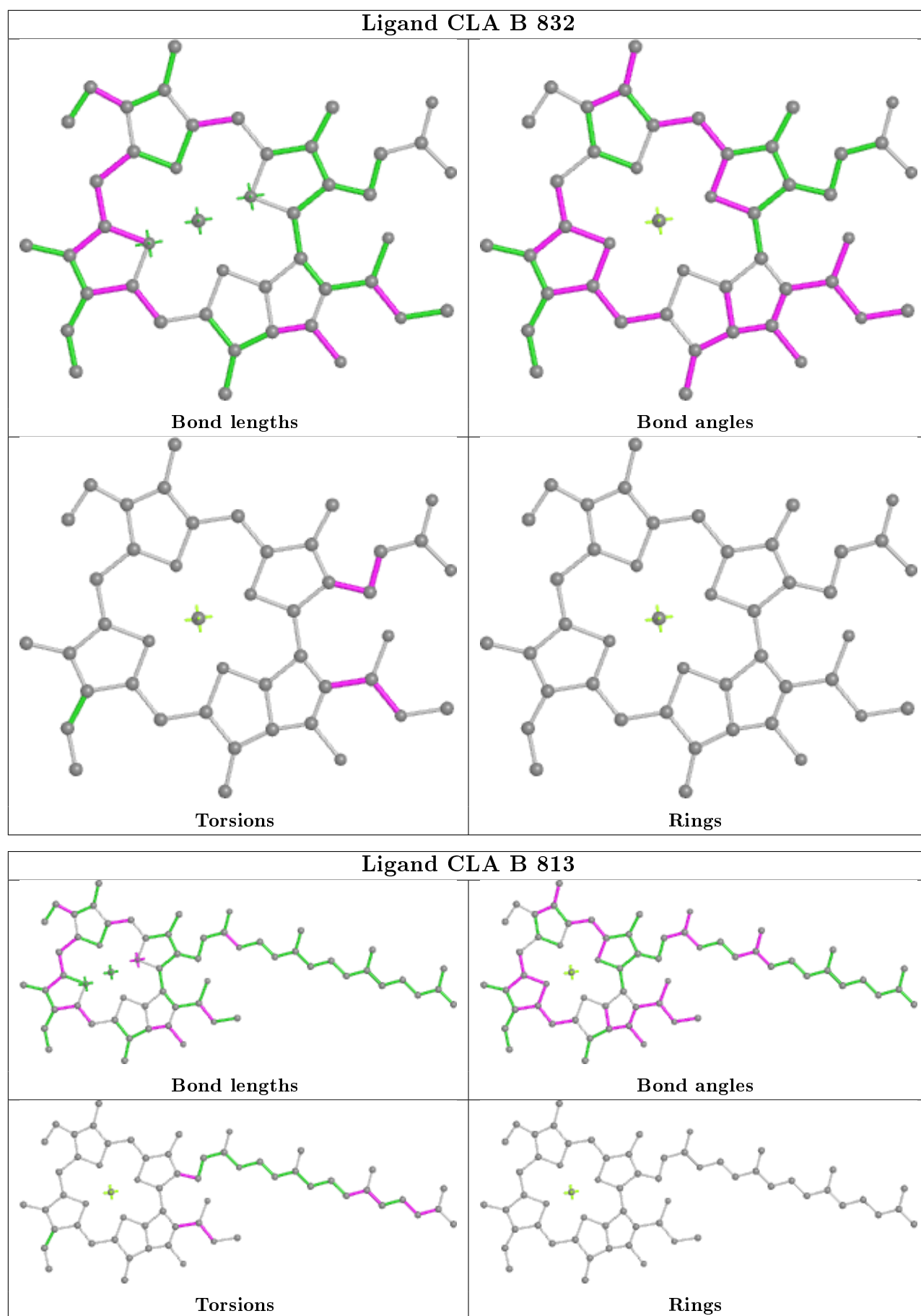


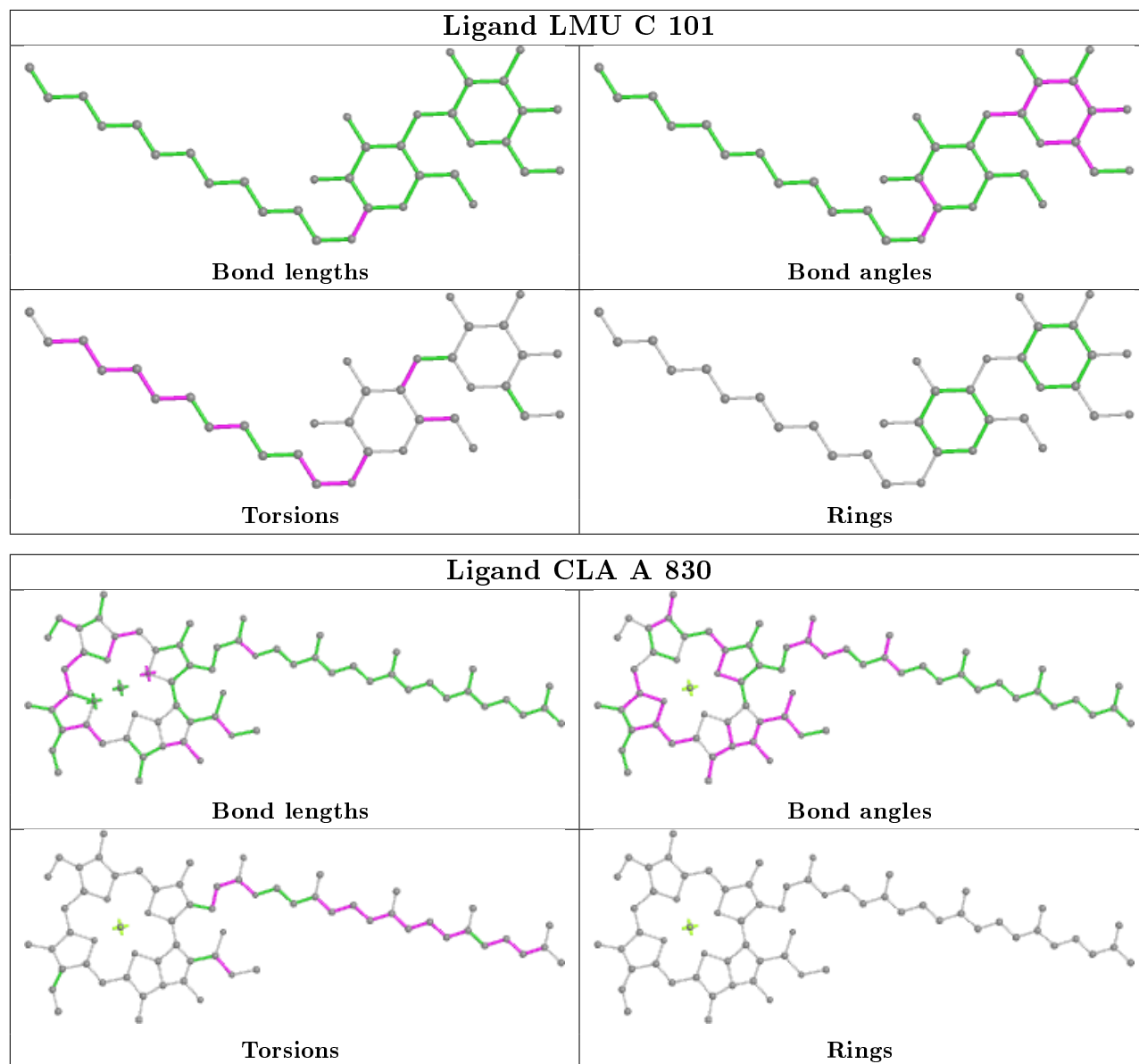


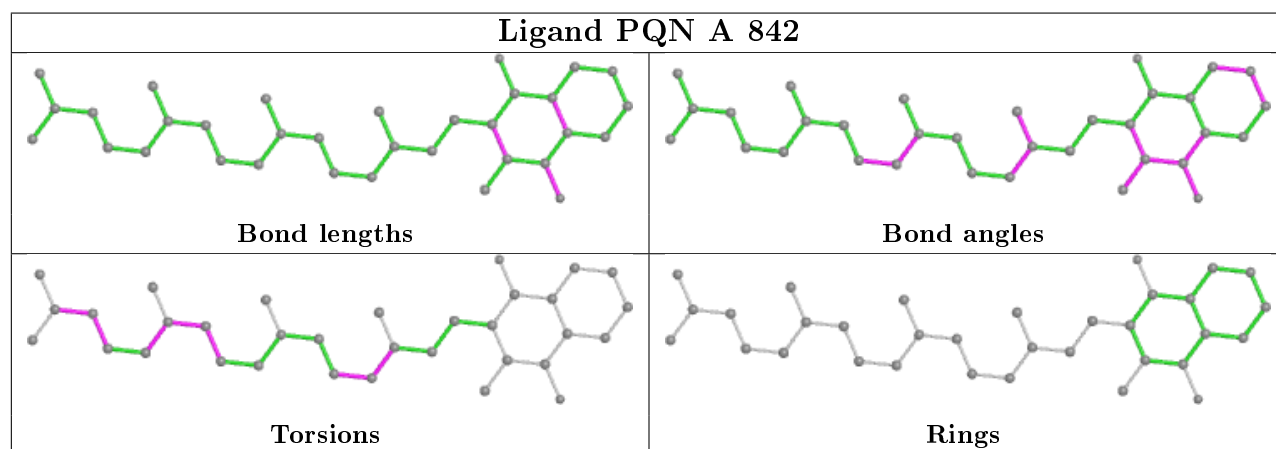
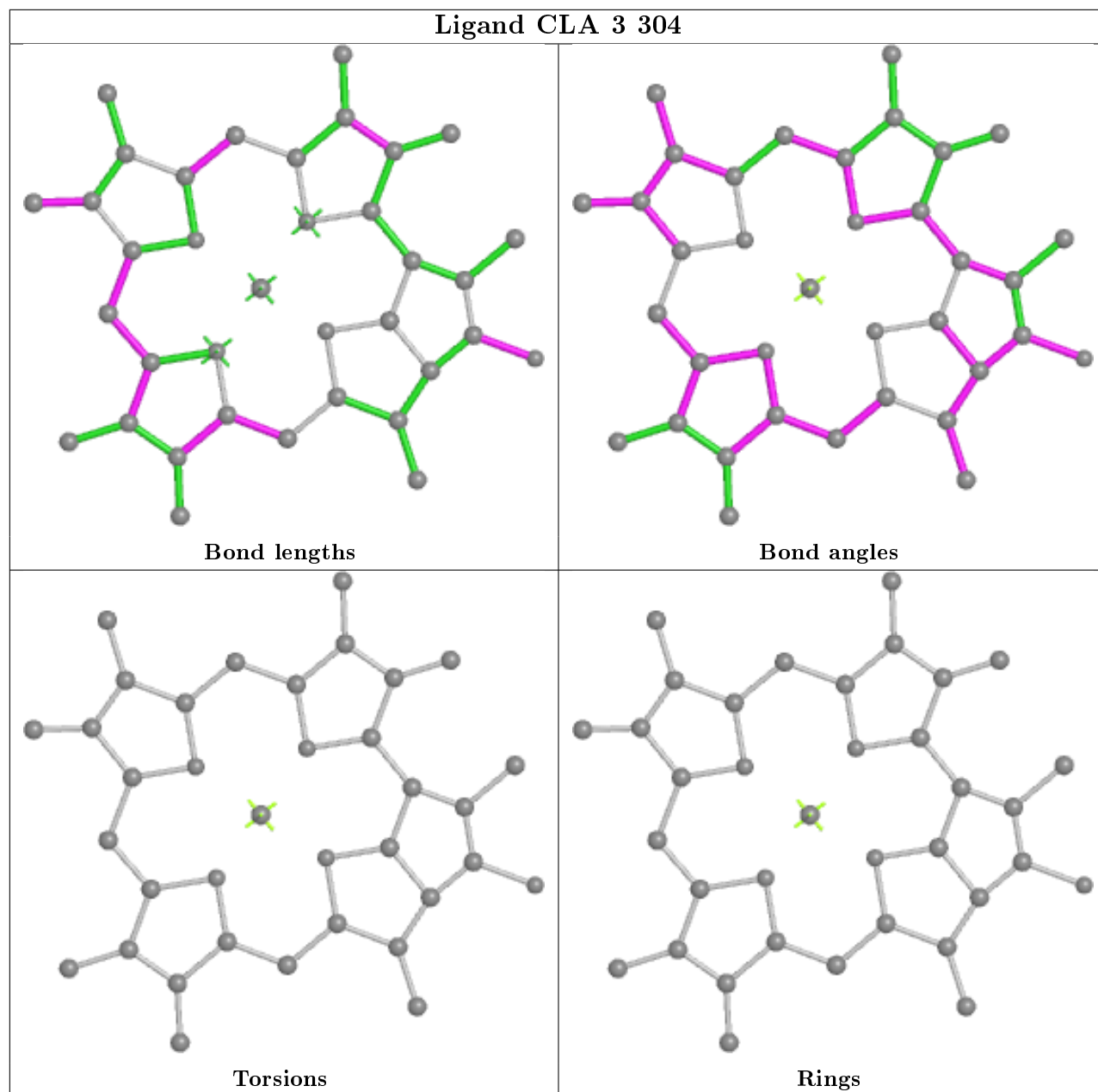


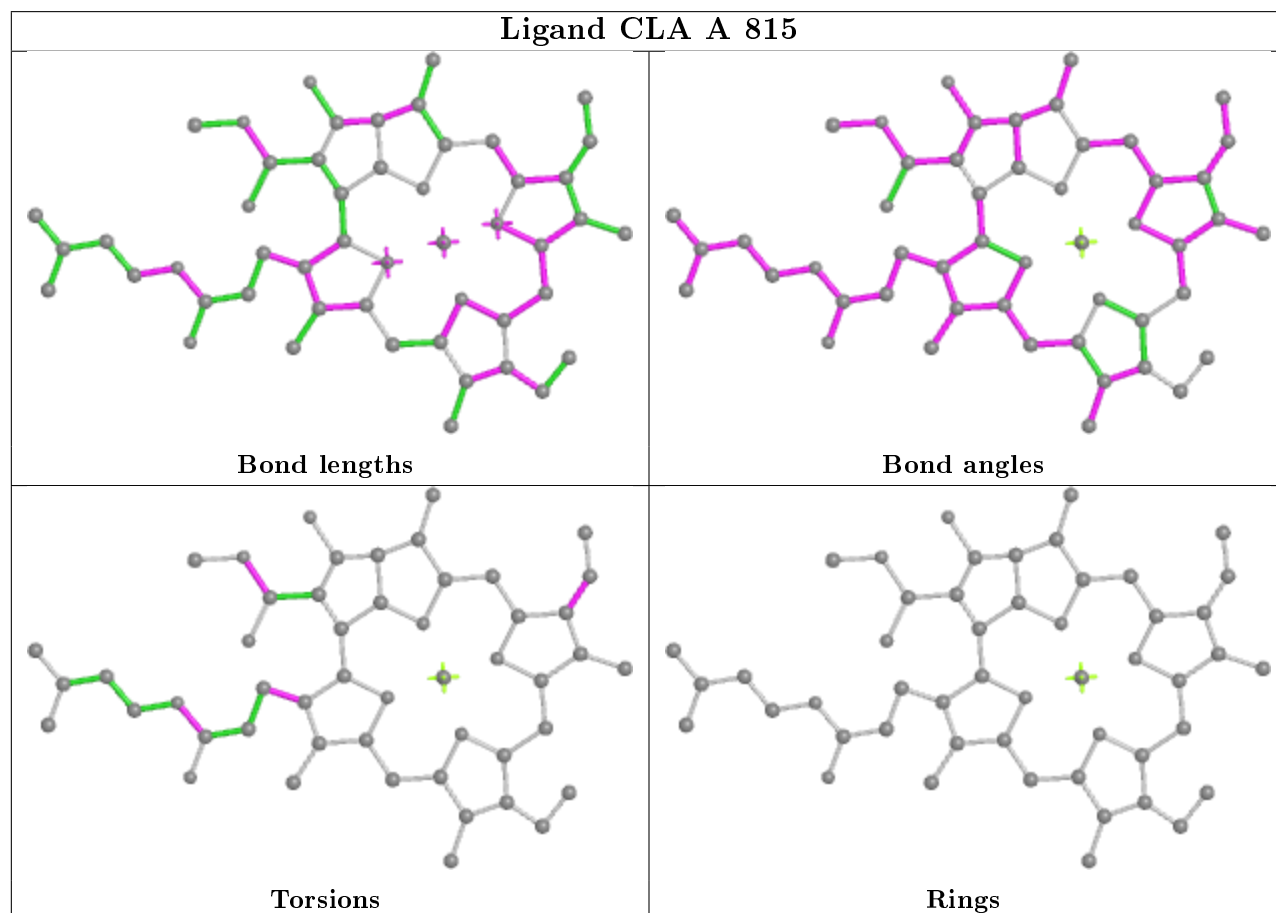
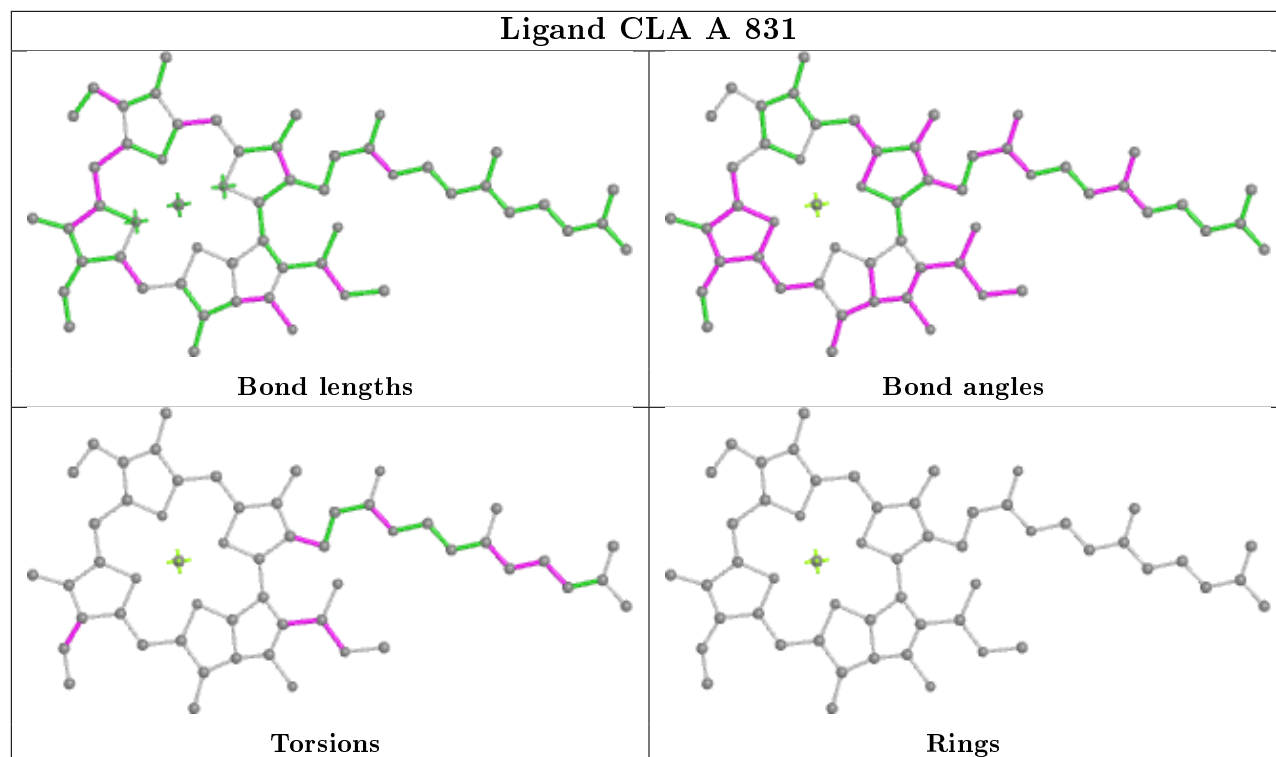


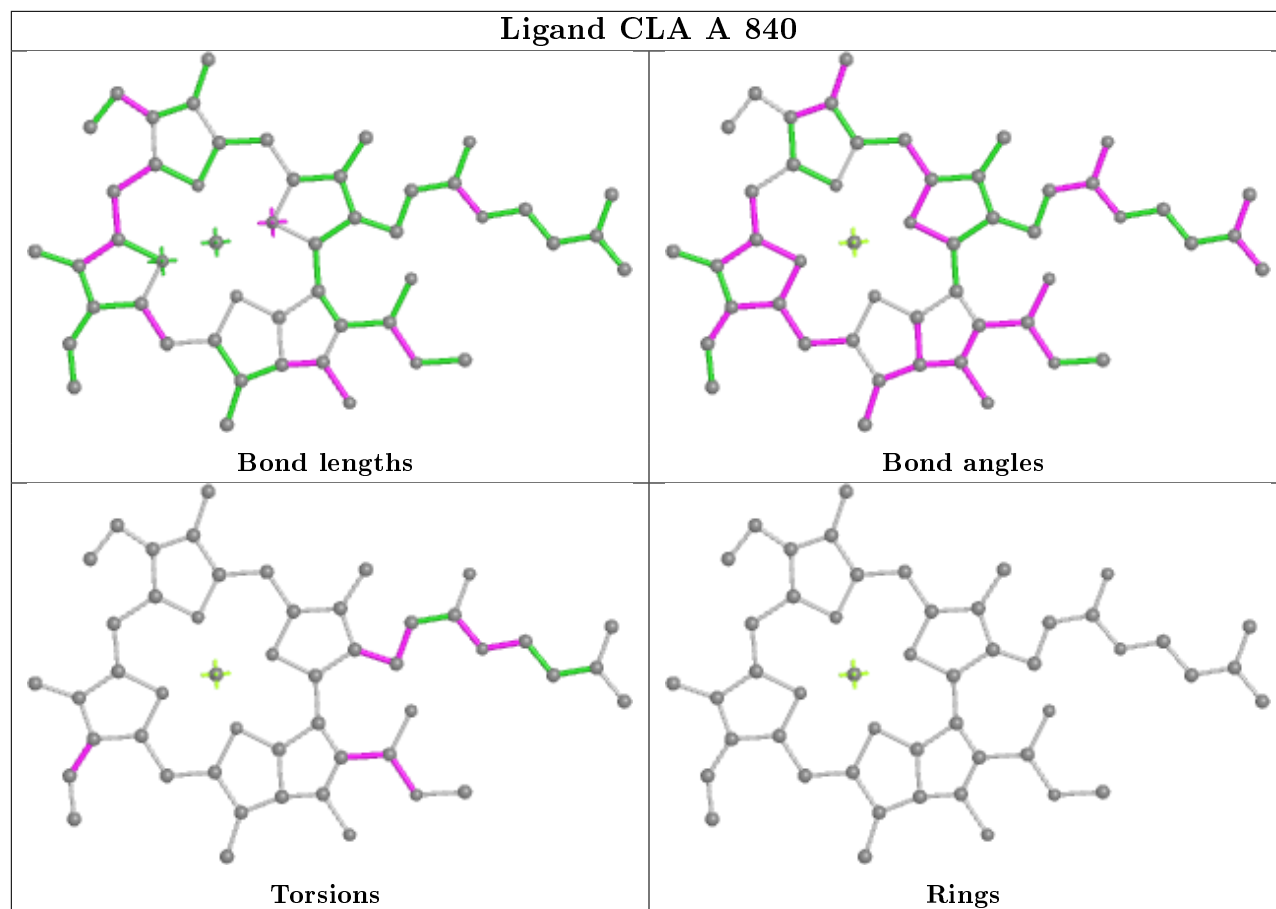


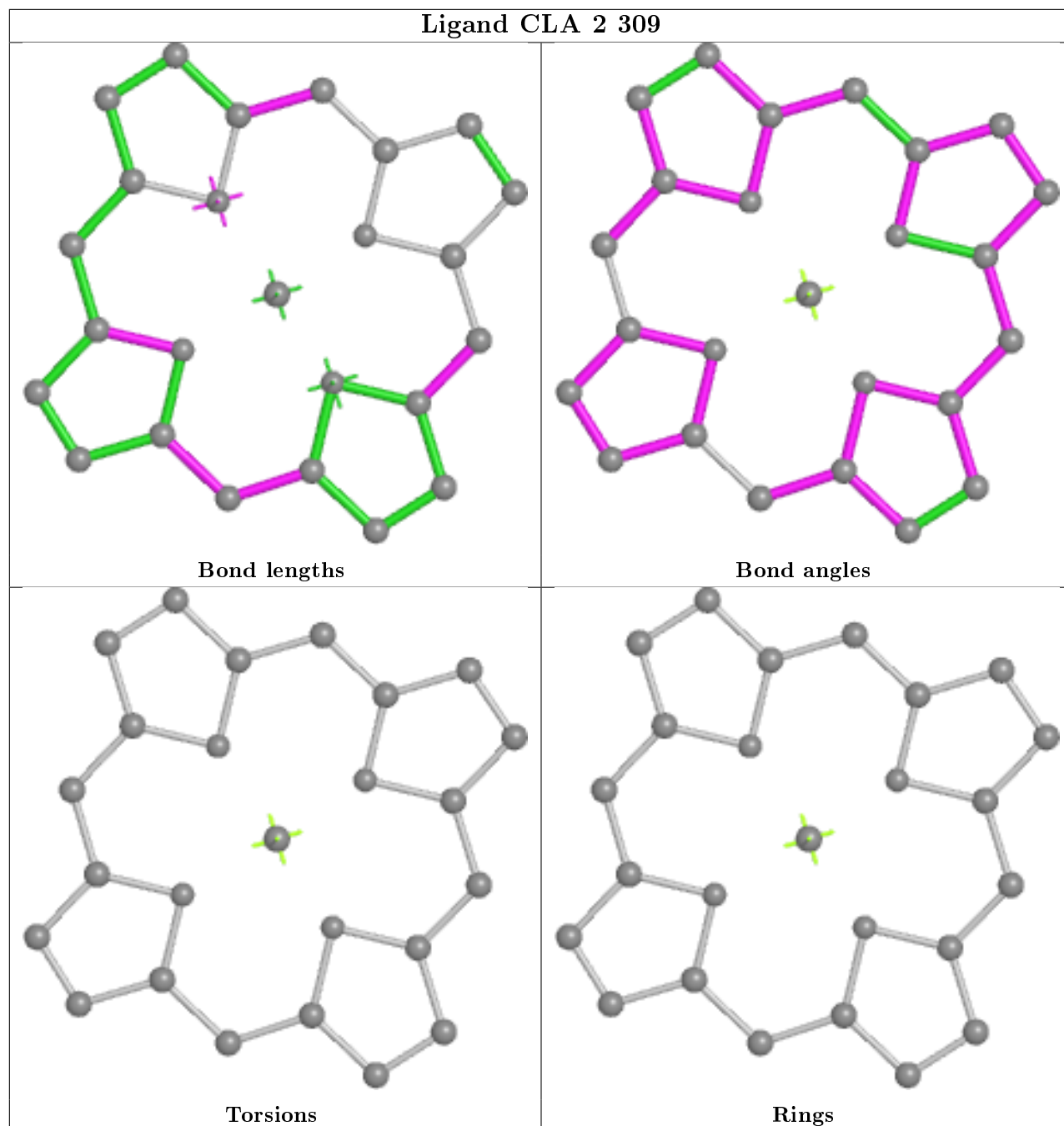


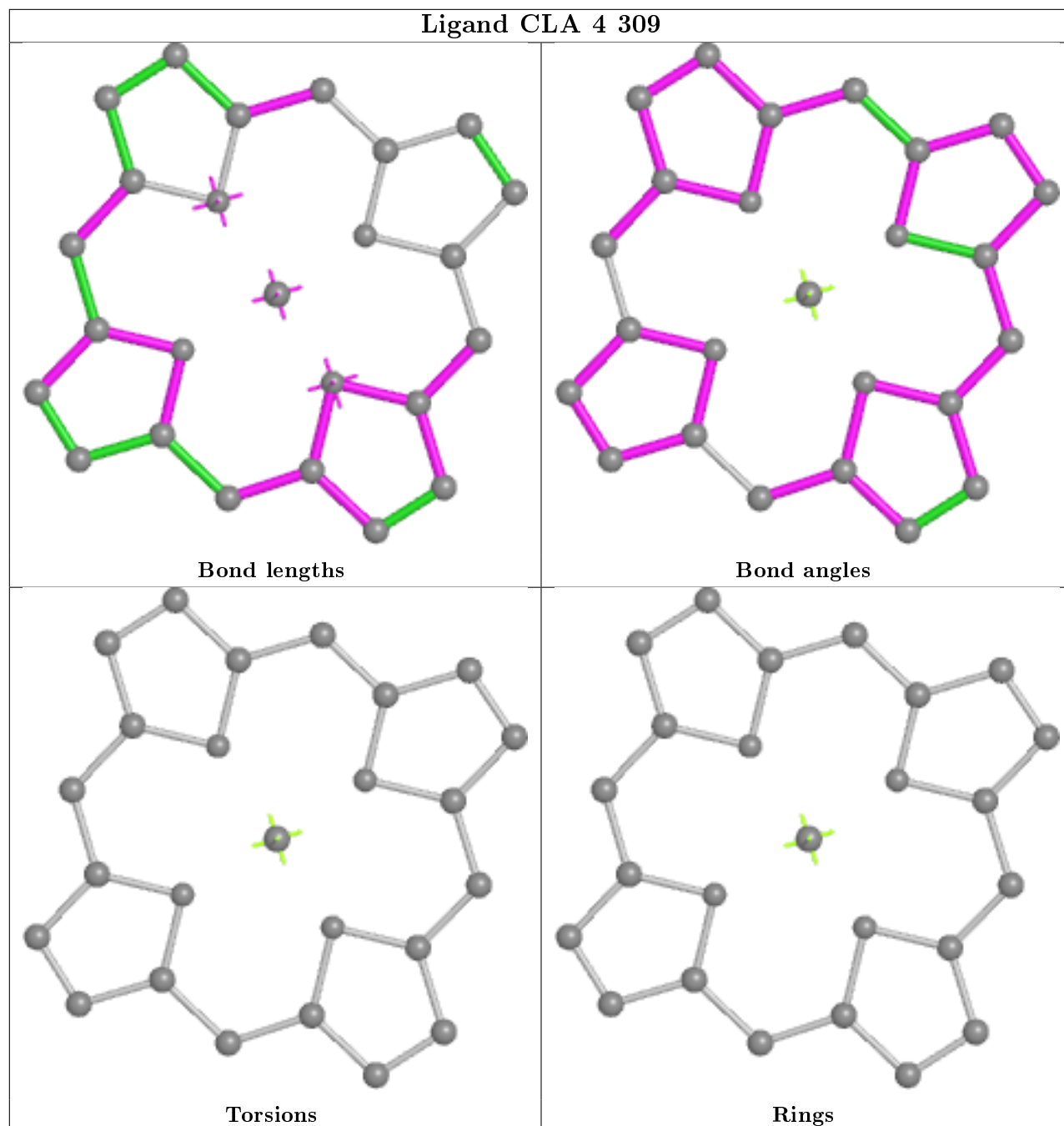


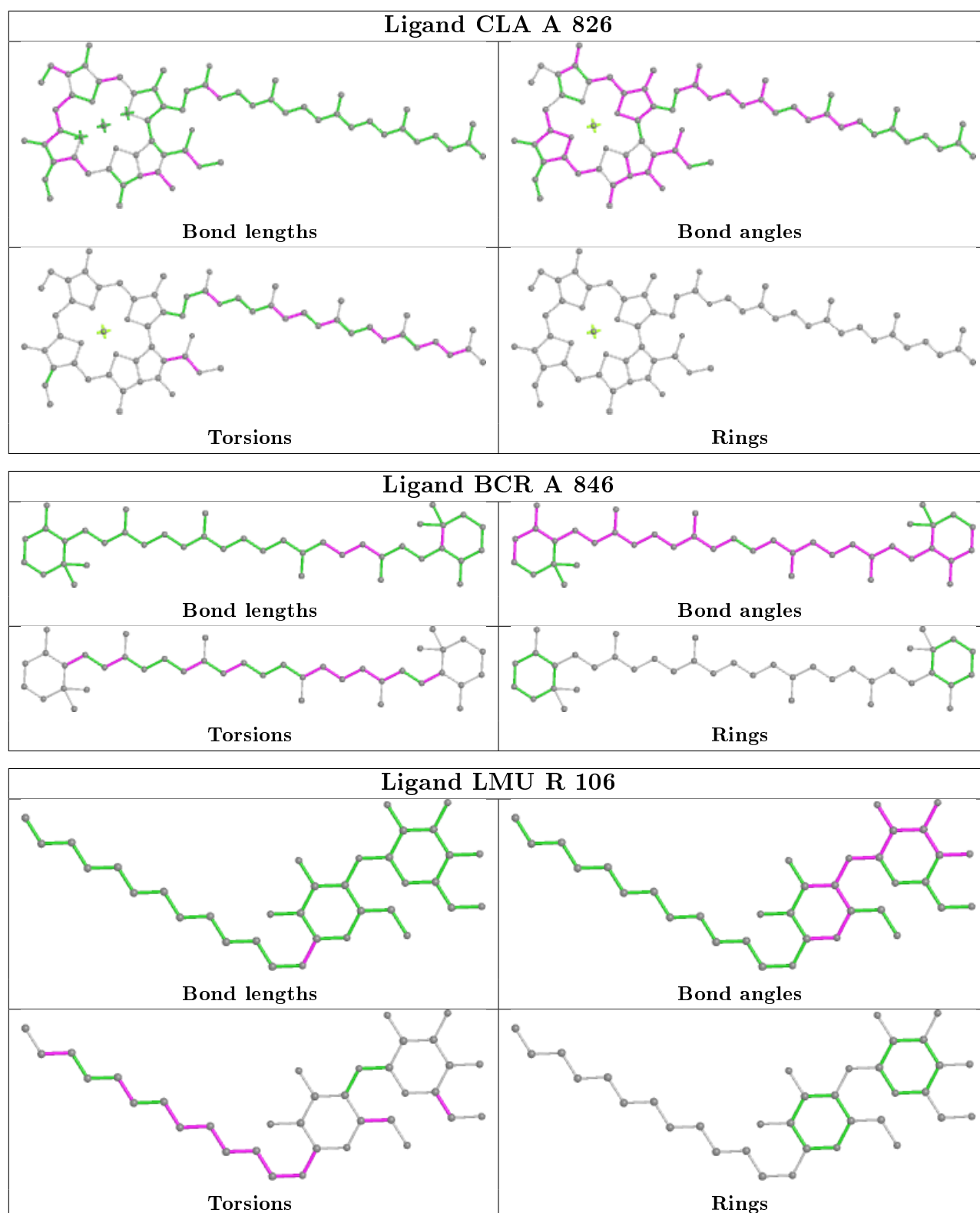


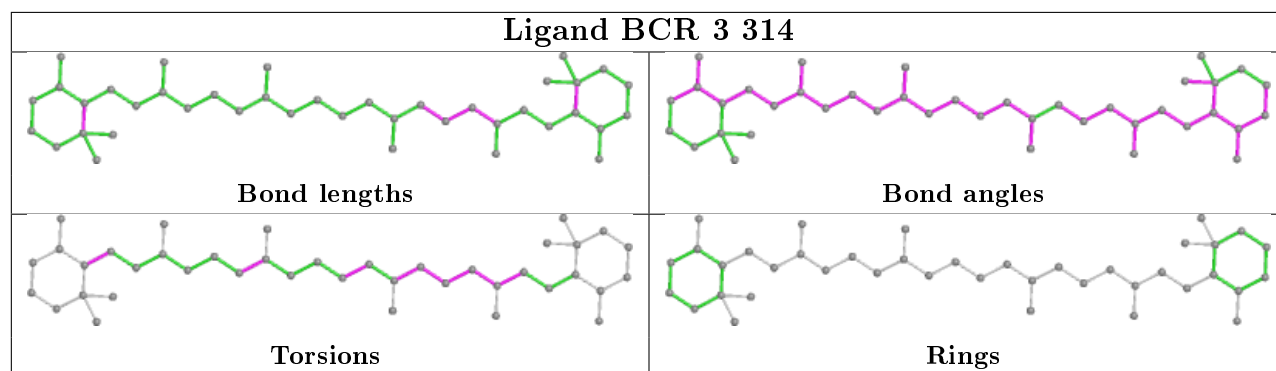
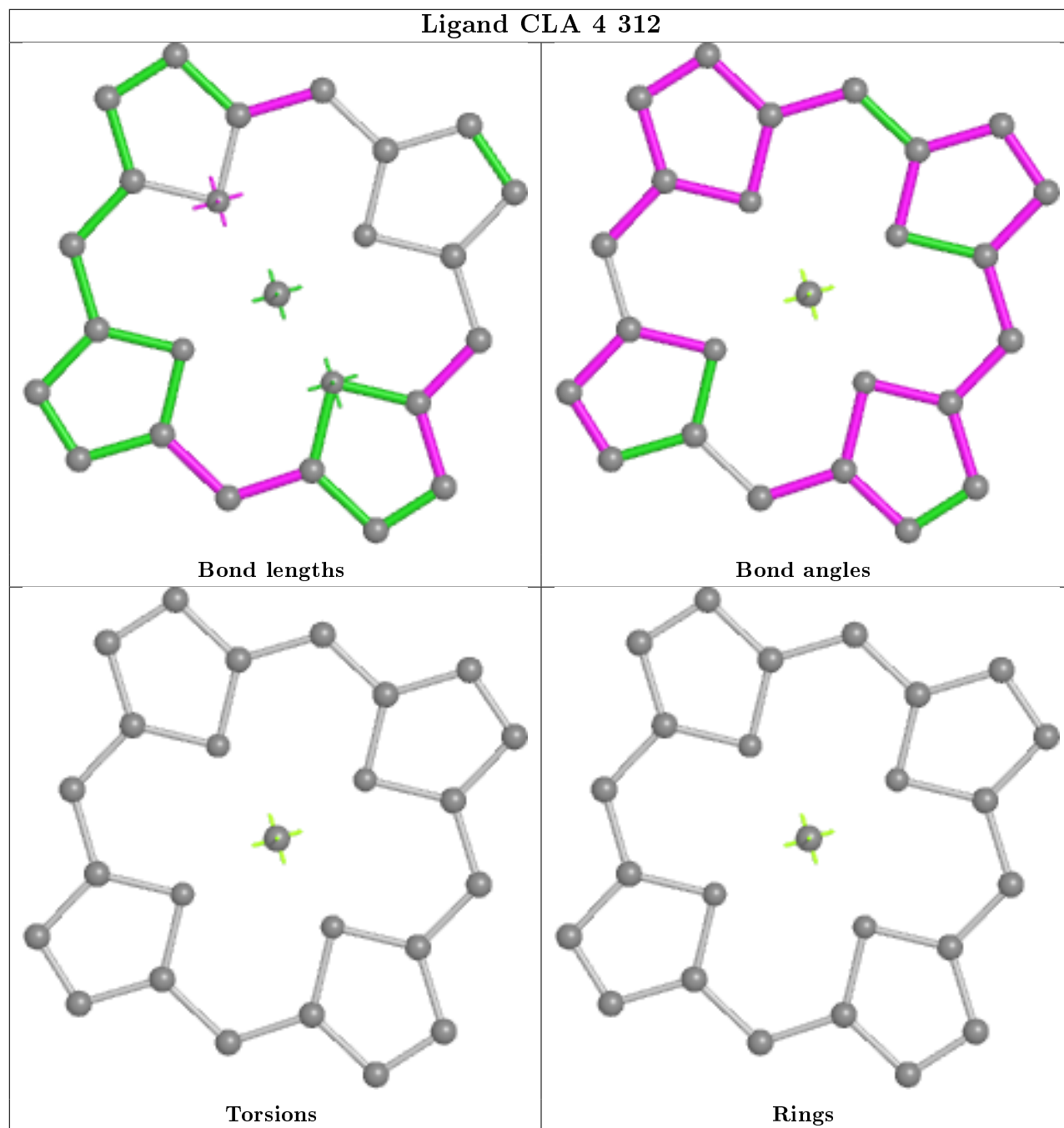


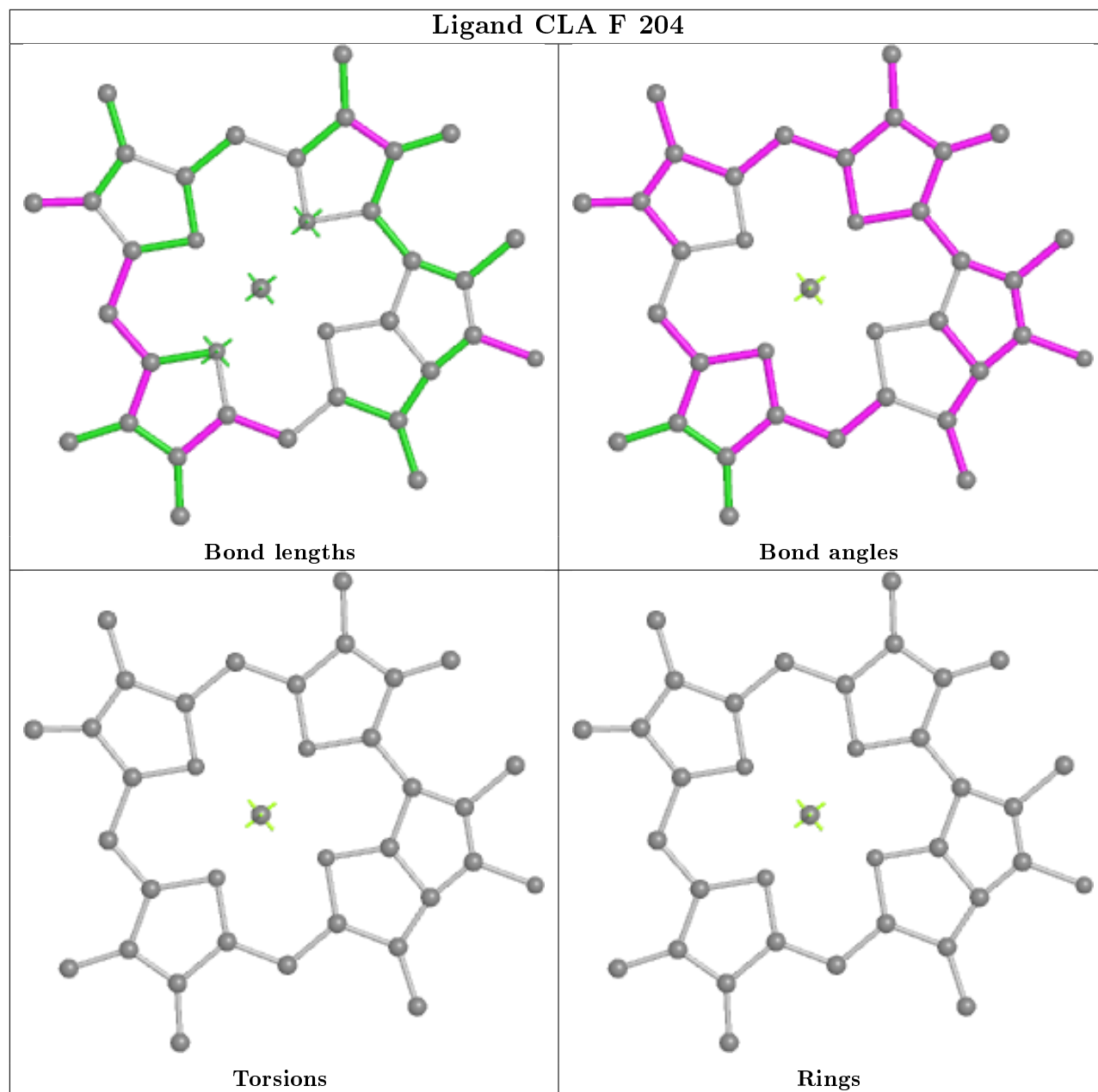


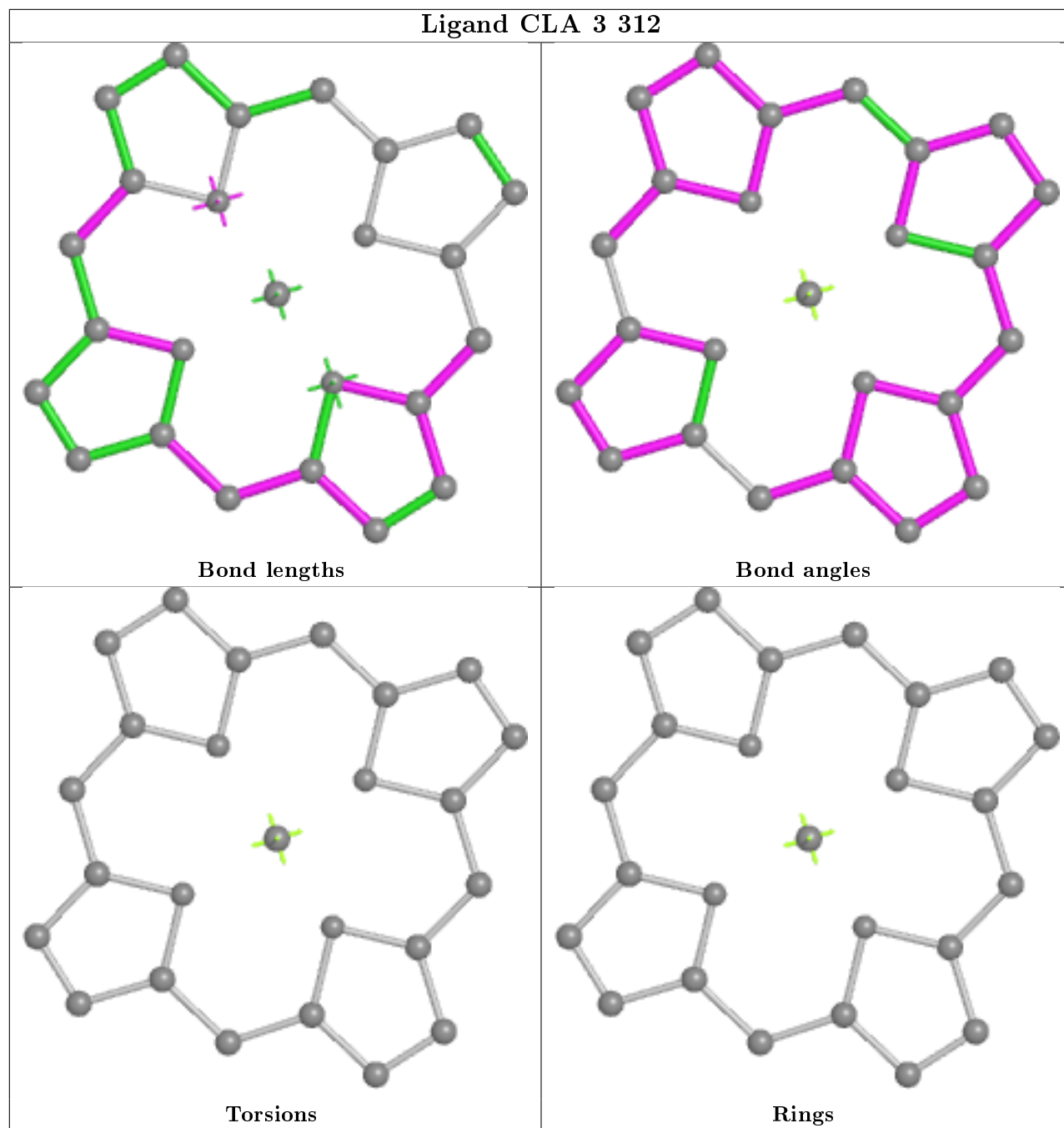


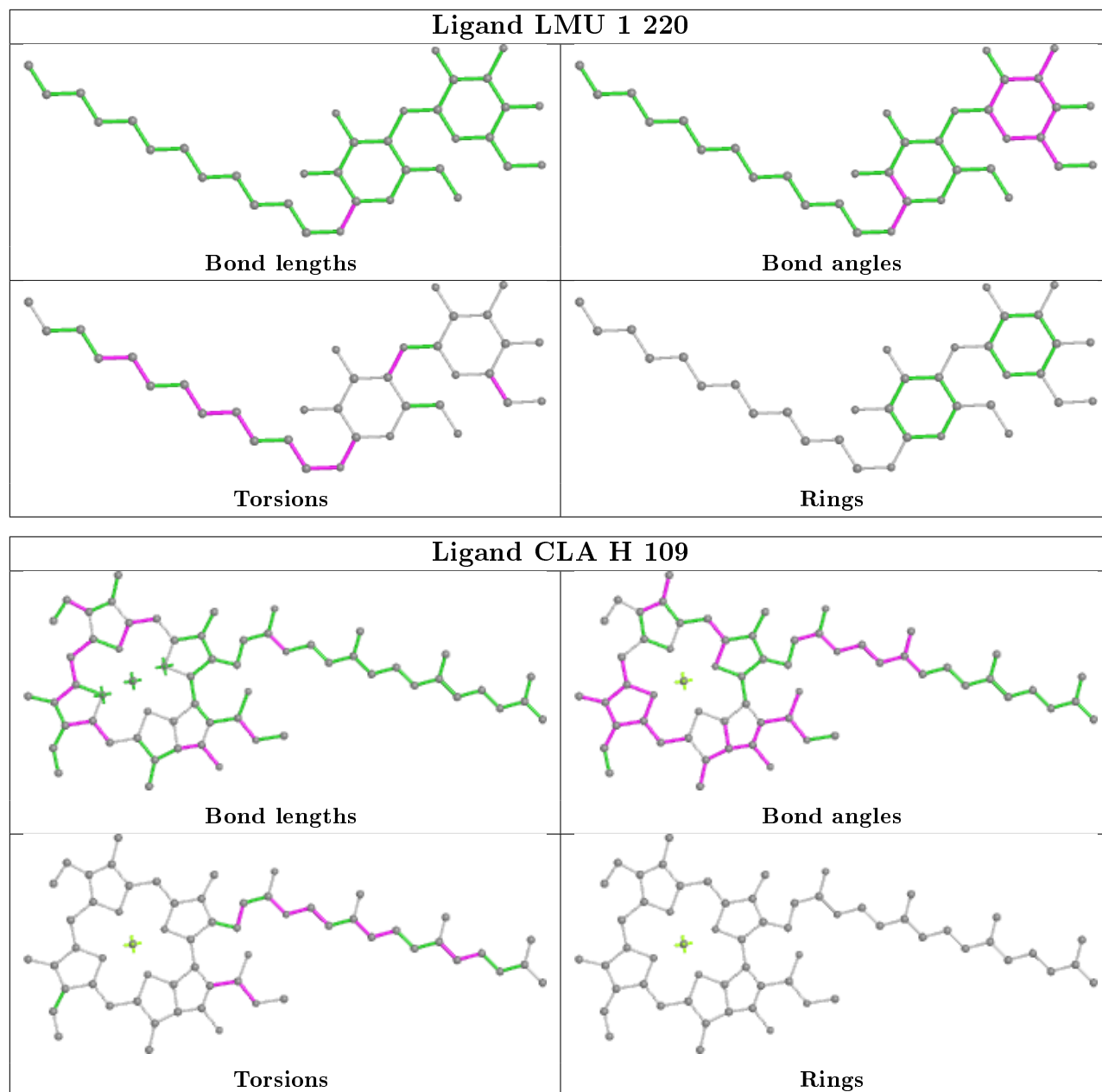


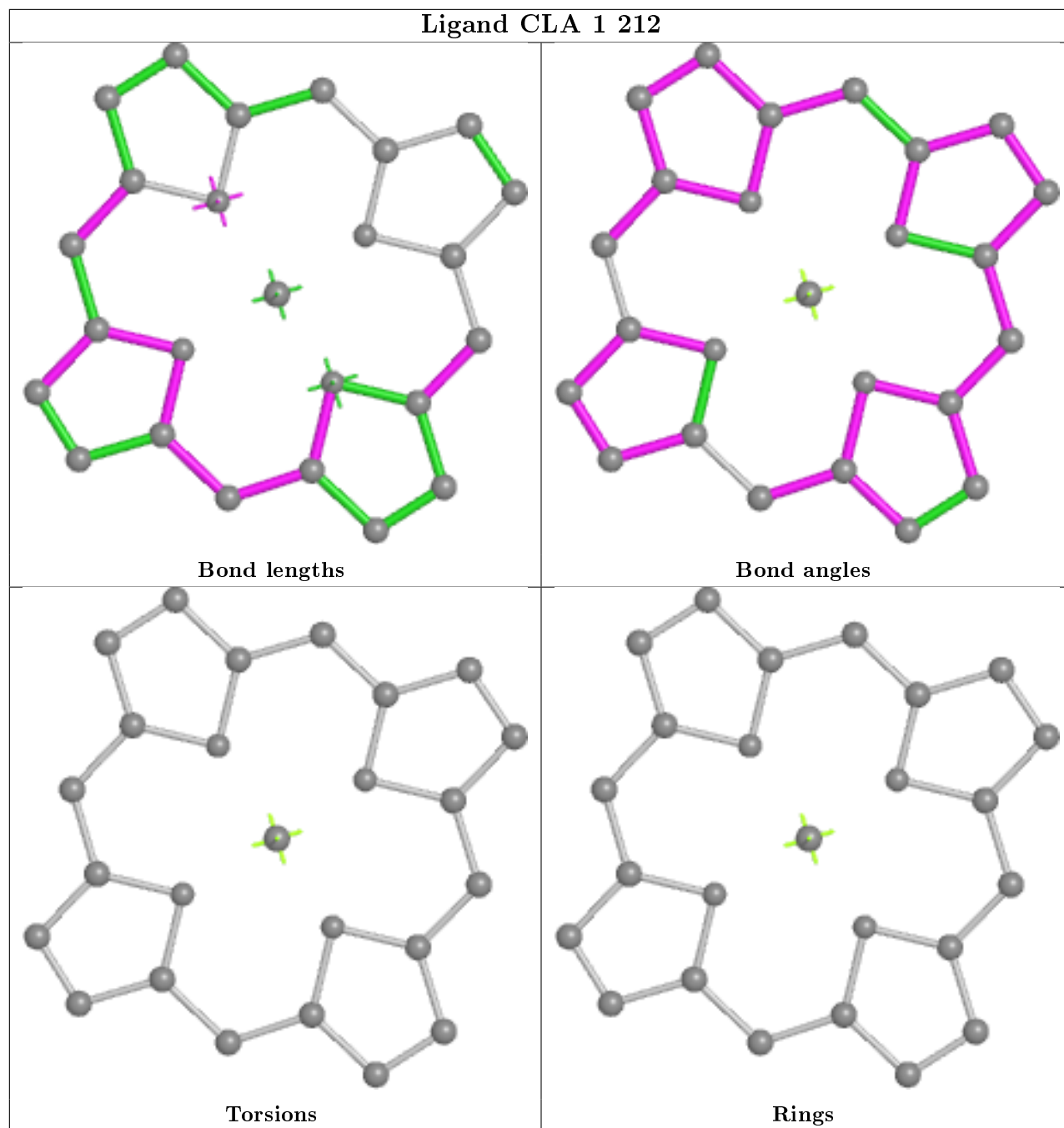


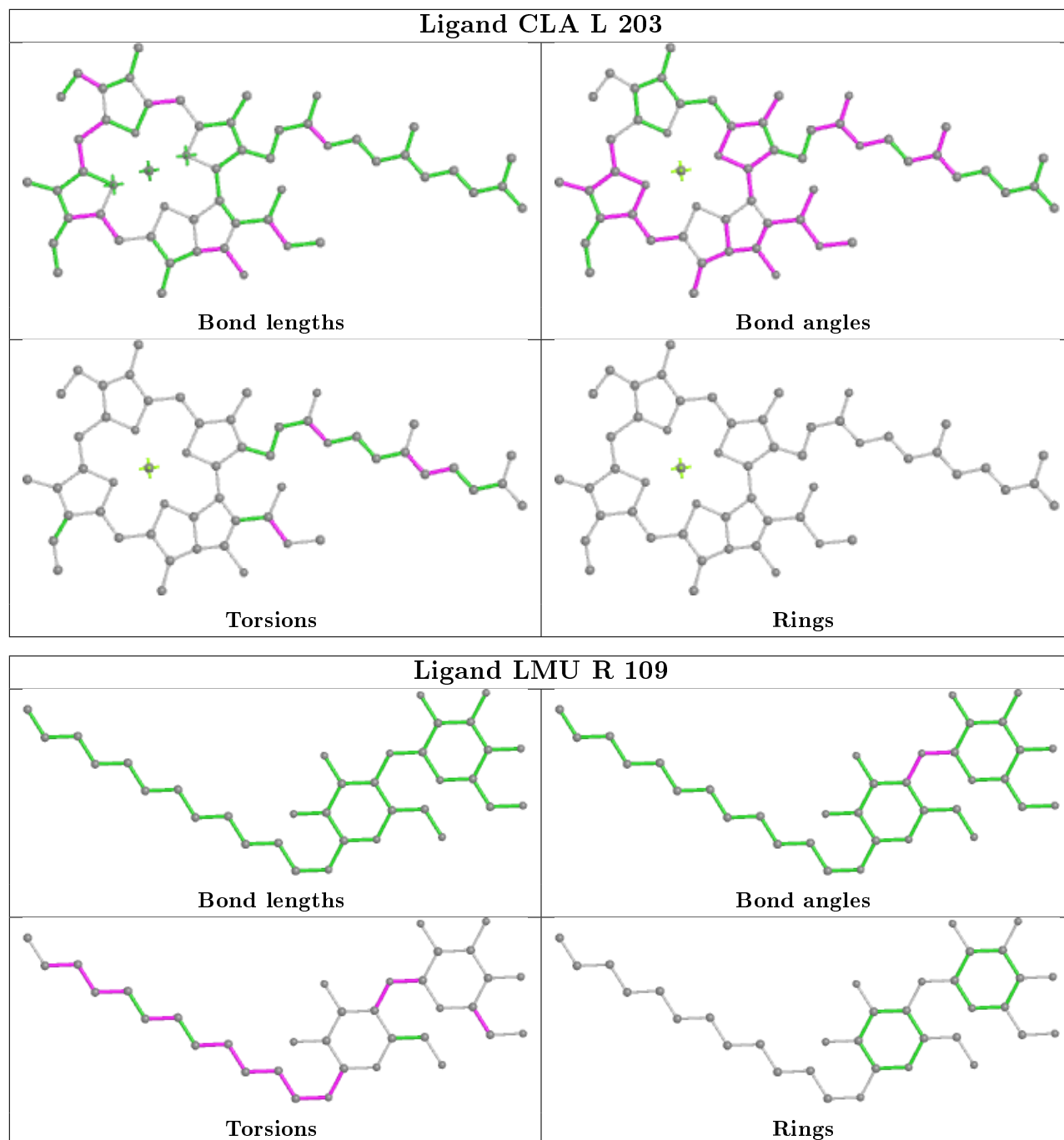


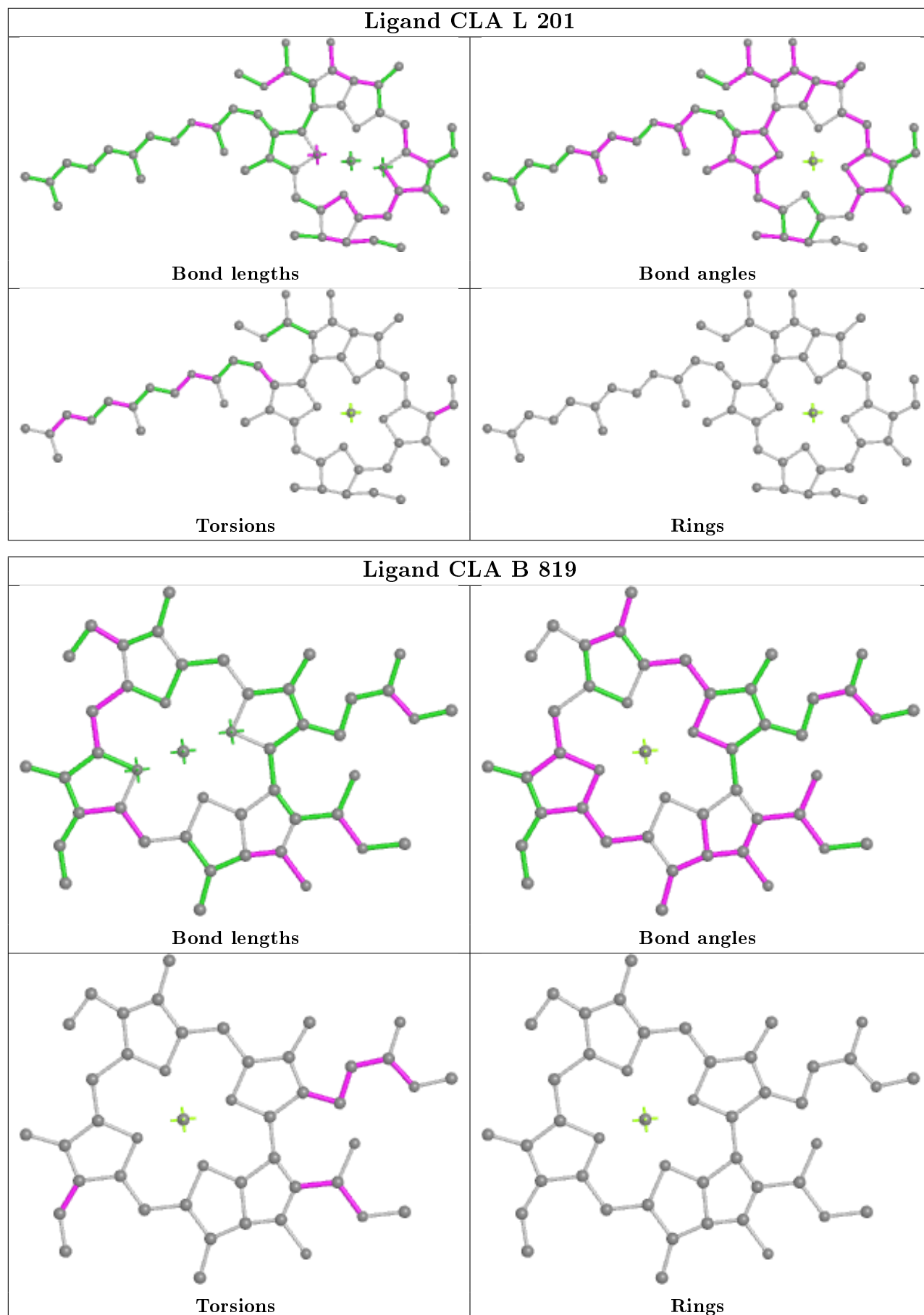


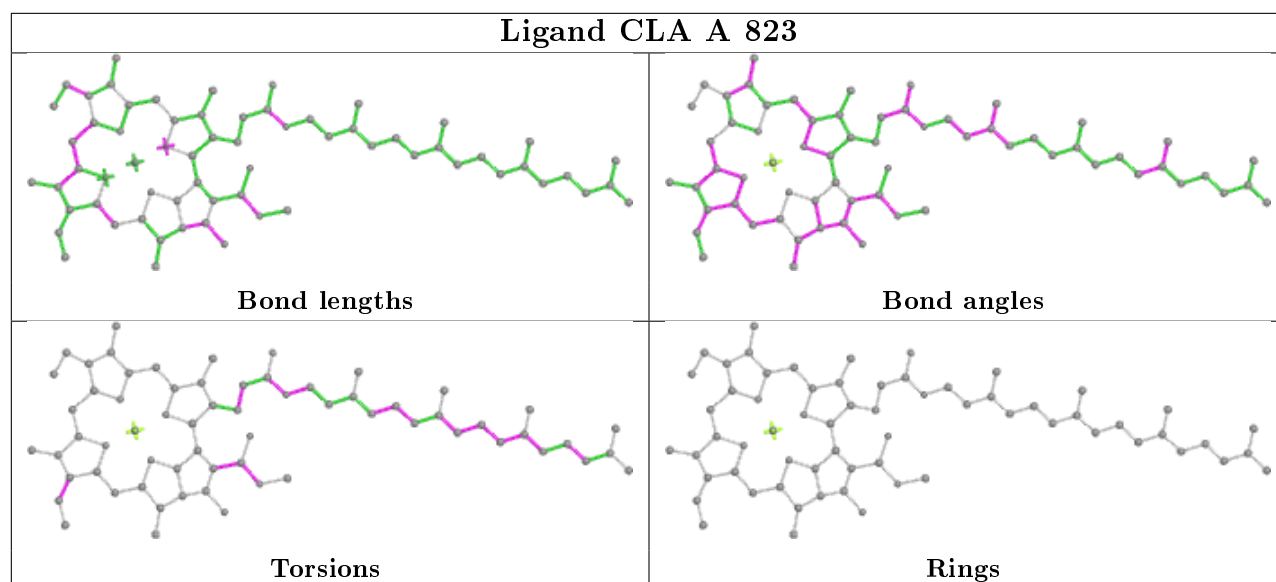
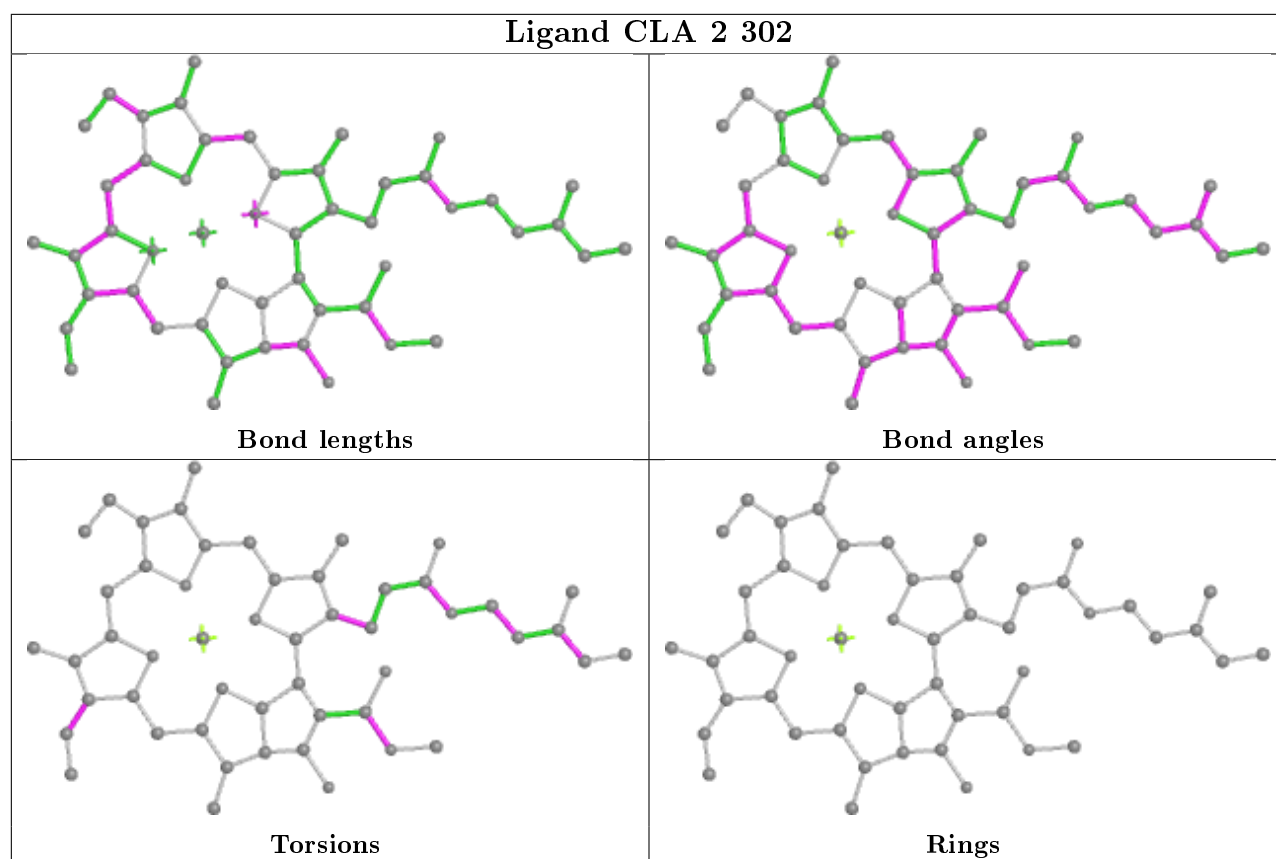


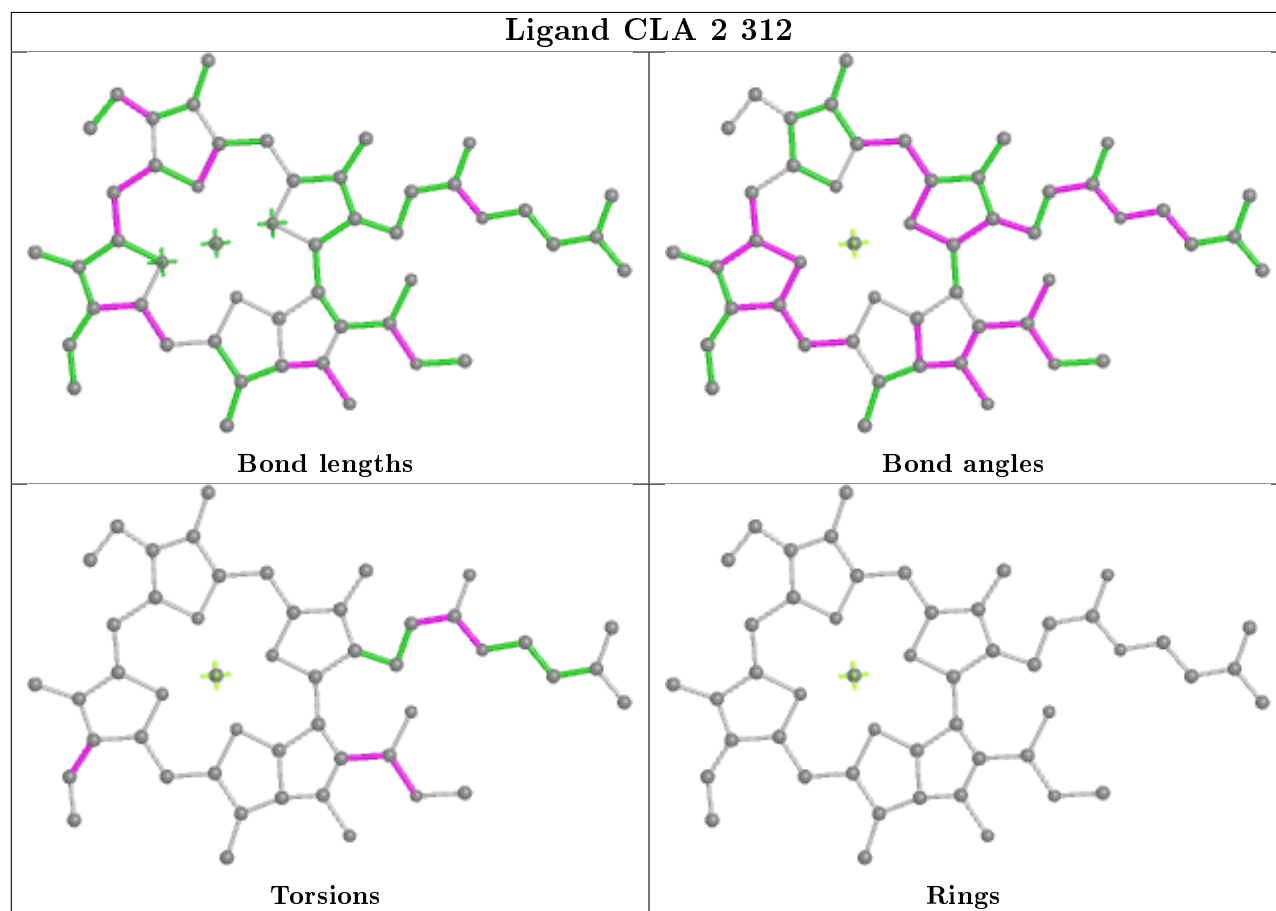
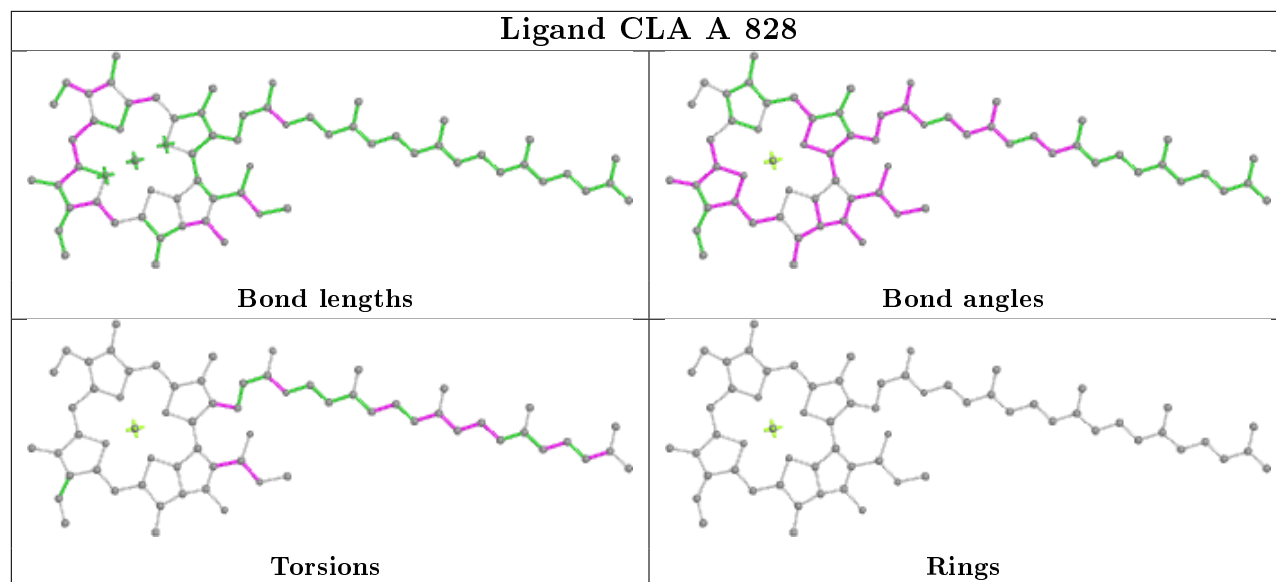


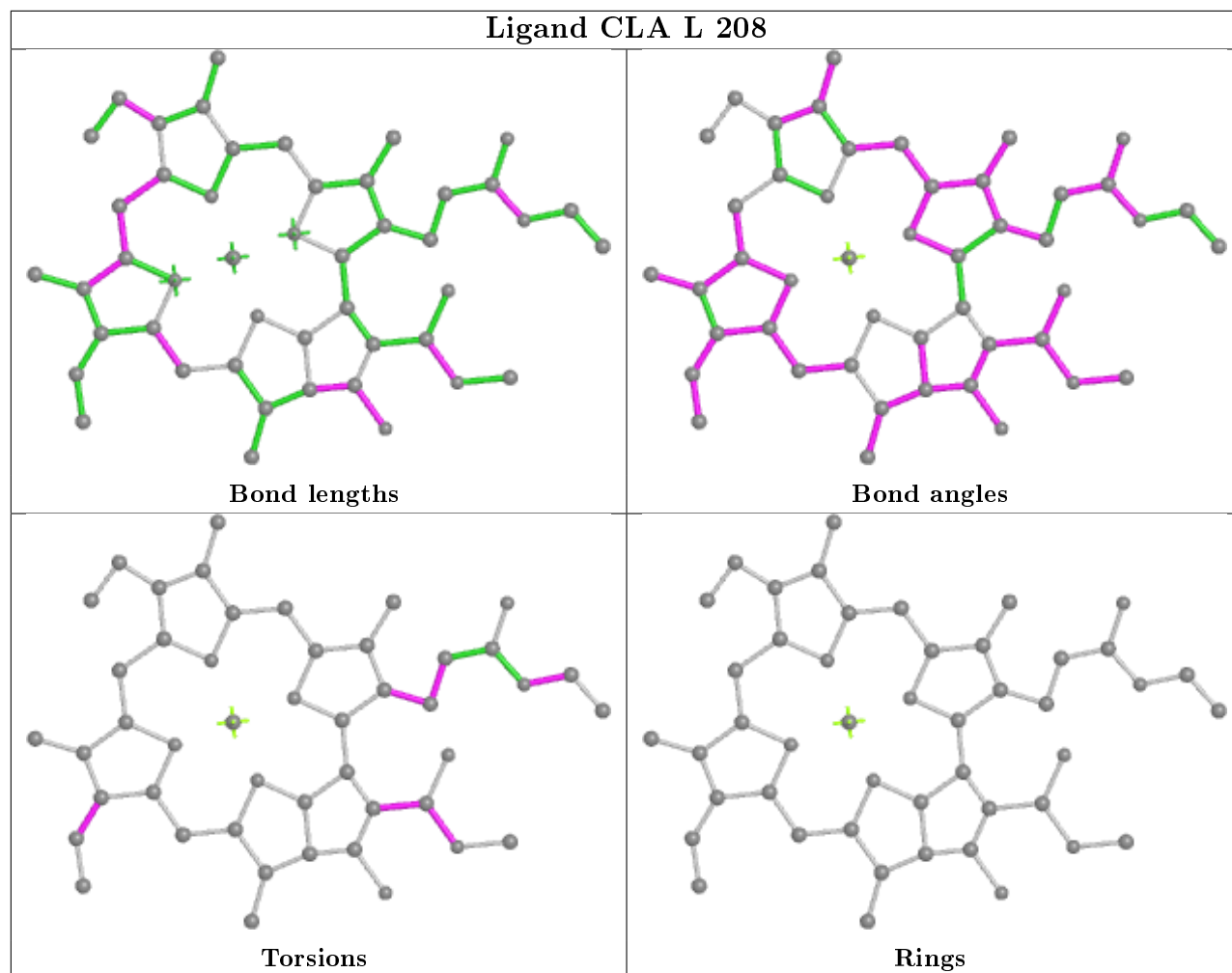


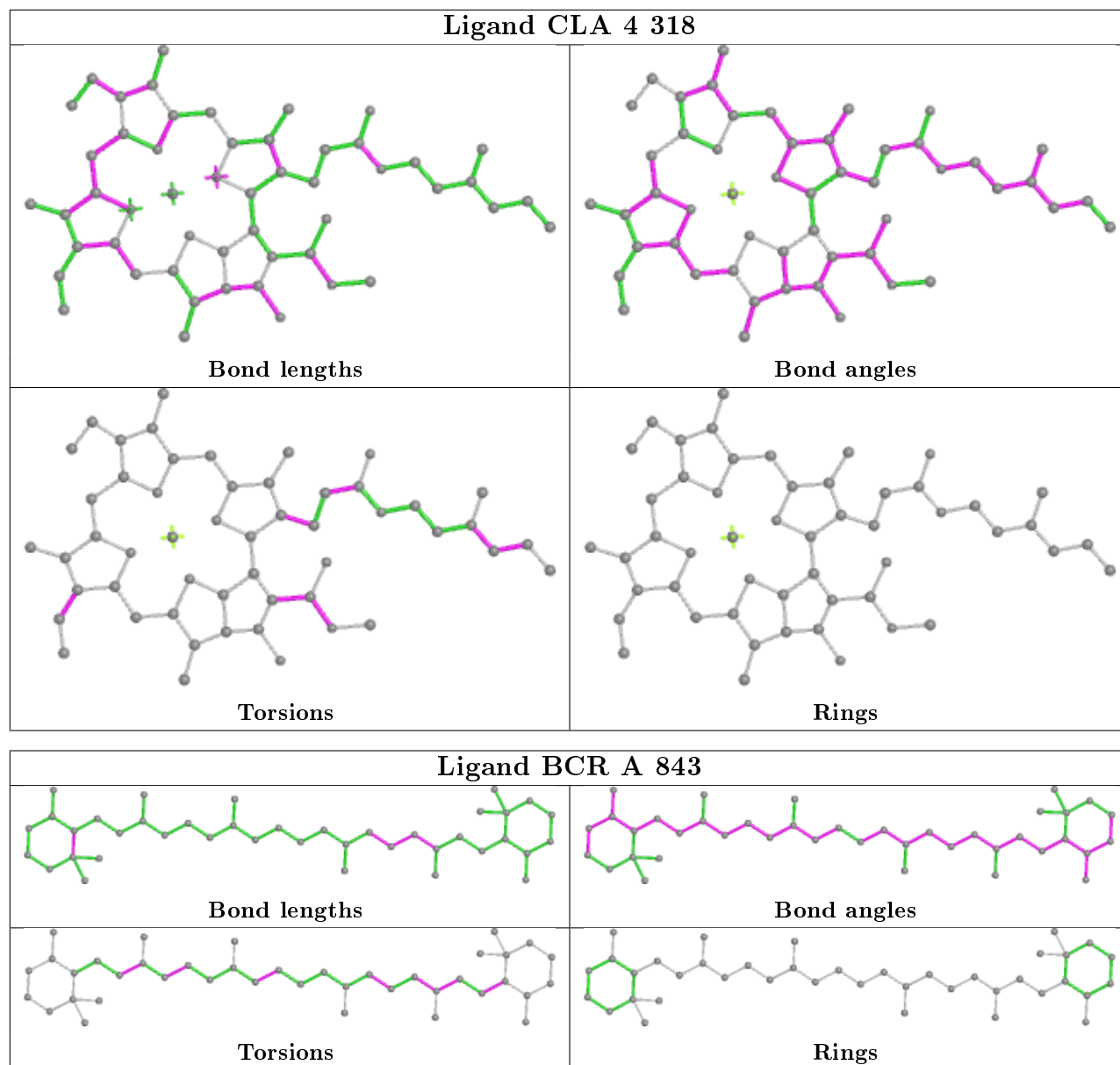


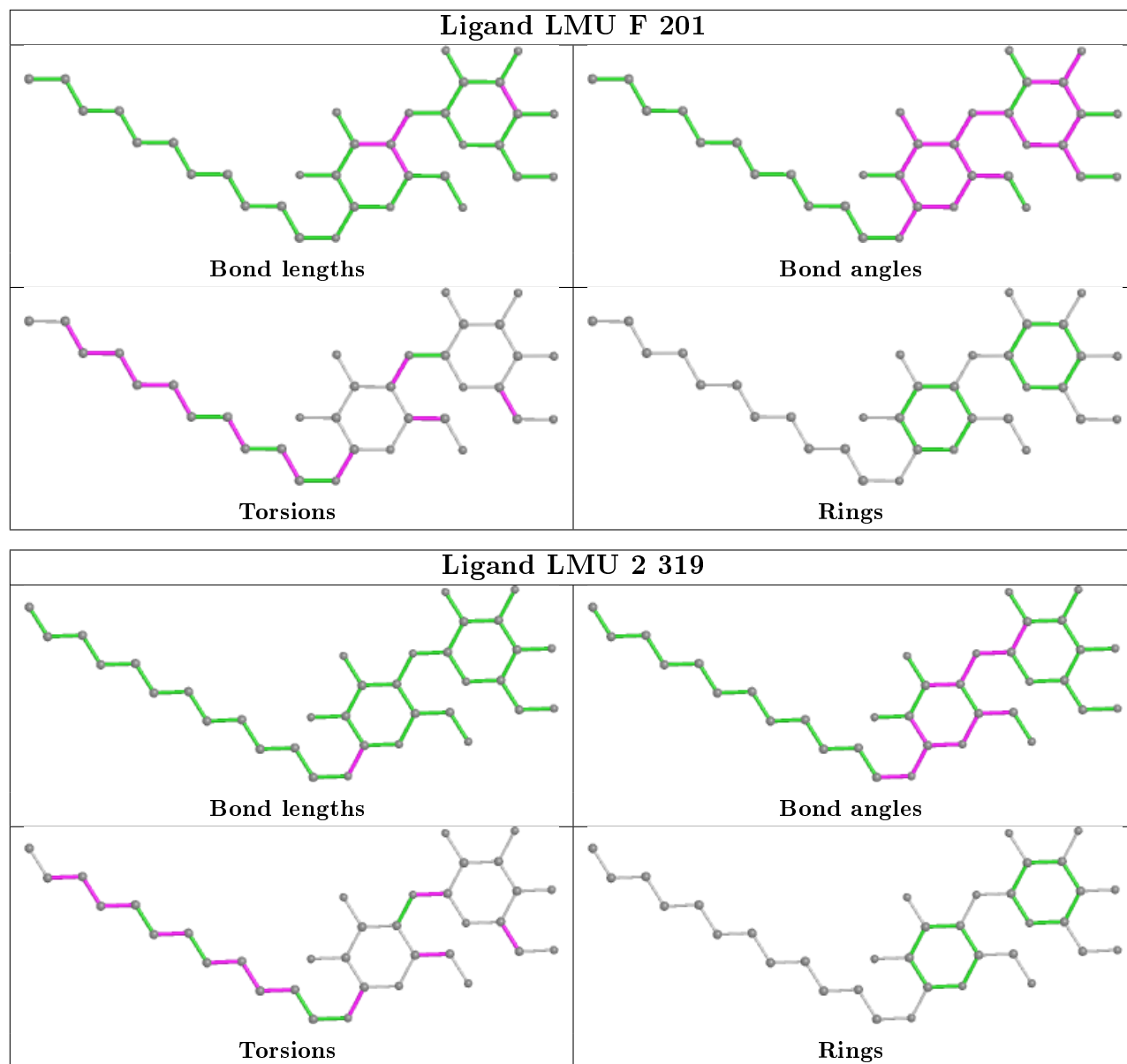


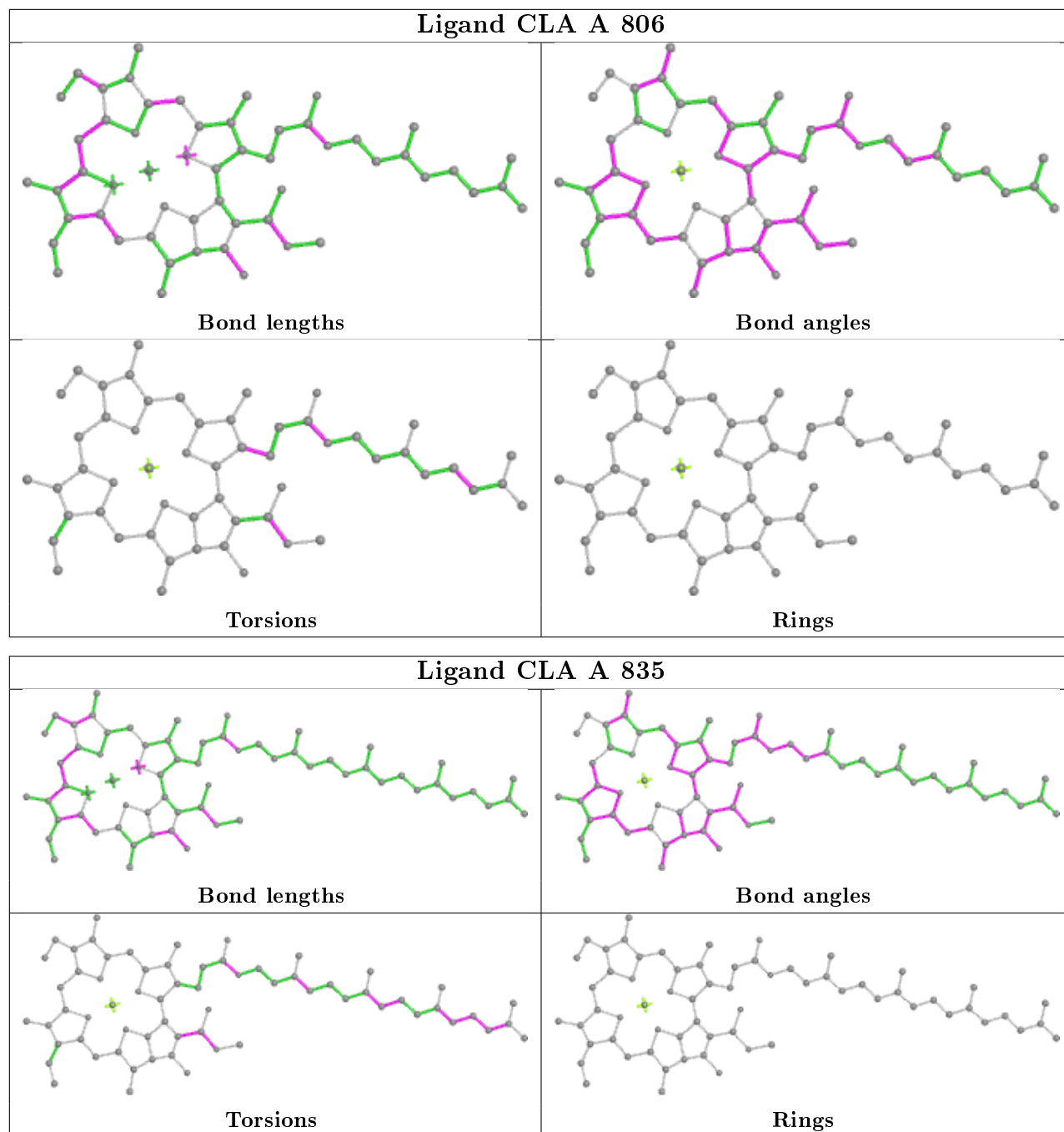


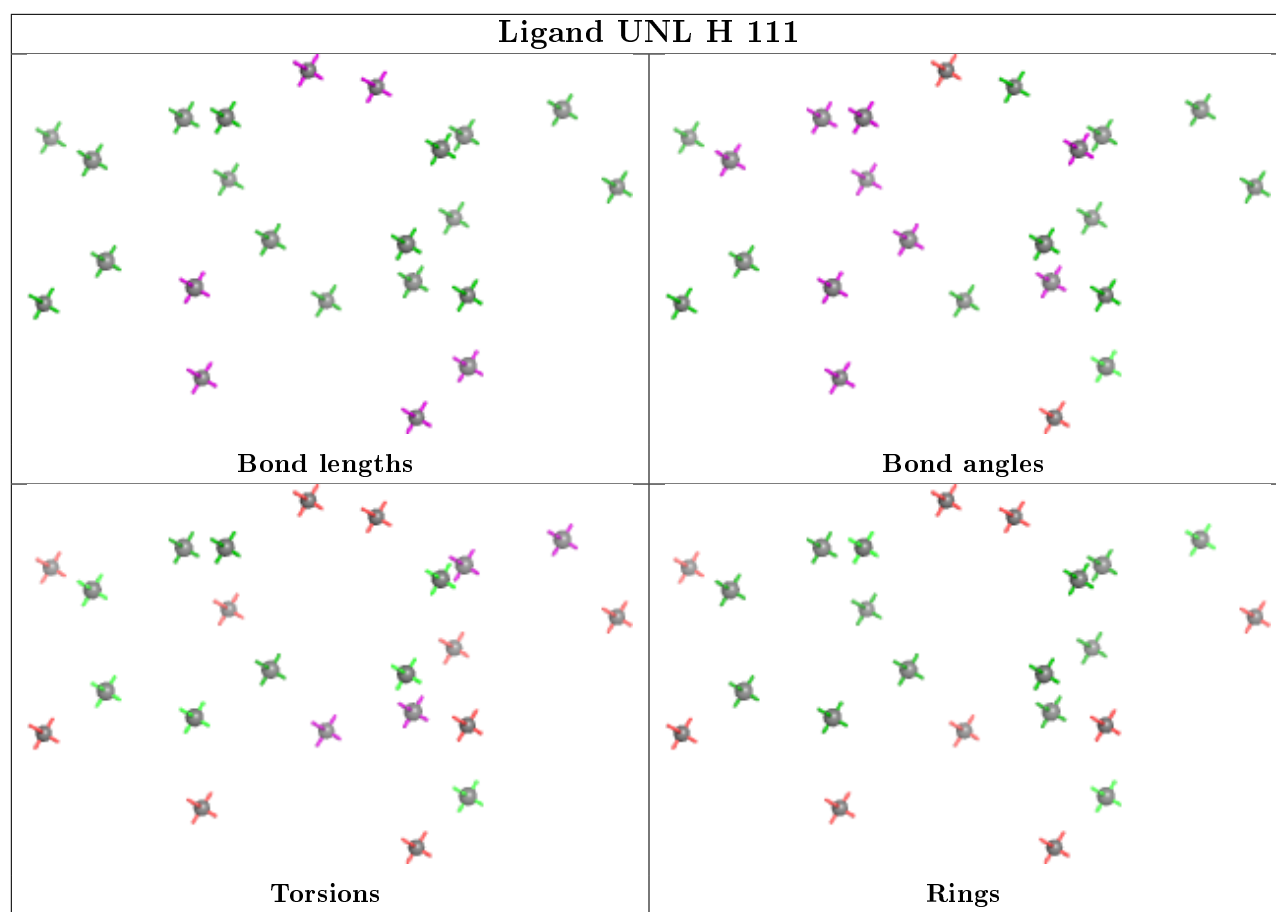












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	164/241 (68%)	1.40	44 (26%) 0 0	32, 62, 71, 73	0
2	2	176/269 (65%)	1.11	38 (21%) 0 1	20, 20, 20, 20	0
3	3	160/276 (57%)	1.92	64 (40%) 0 0	49, 79, 110, 112	0
4	4	166/251 (66%)	0.90	24 (14%) 2 3	20, 20, 20, 20	0
5	A	730/758 (96%)	0.90	87 (11%) 4 5	20, 20, 20, 20	0
6	B	733/734 (99%)	0.77	52 (7%) 16 15	20, 20, 20, 20	0
7	C	81/81 (100%)	1.17	11 (13%) 3 4	20, 20, 20, 20	0
8	D	138/212 (65%)	1.03	25 (18%) 1 1	20, 20, 20, 20	0
9	E	65/143 (45%)	1.17	16 (24%) 0 0	20, 20, 20, 20	0
10	F	154/231 (66%)	0.59	12 (7%) 13 13	20, 20, 20, 20	0
11	G	95/167 (56%)	0.62	10 (10%) 6 7	20, 20, 20, 20	0
12	H	69/144 (47%)	0.79	9 (13%) 3 4	20, 20, 20, 20	0
13	I	30/40 (75%)	0.33	1 (3%) 46 41	20, 20, 20, 20	0
14	J	42/44 (95%)	0.59	4 (9%) 8 8	20, 20, 20, 20	0
15	K	84/131 (64%)	1.95	32 (38%) 0 0	20, 20, 20, 20	0
16	L	161/216 (74%)	0.75	22 (13%) 3 4	20, 20, 20, 20	0
17	N	85/170 (50%)	0.99	15 (17%) 1 1	20, 20, 20, 20	0
18	R	0/53	-	-	-	-
All	All	3133/4161 (75%)	0.96	466 (14%) 2 3	20, 20, 65, 112	0

The worst 5 of 466 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	3	61	ASN	11.8
1	1	75	ALA	9.9
4	4	67	ILE	9.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	B	491	ASN	9.0
5	A	635	THR	8.2

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

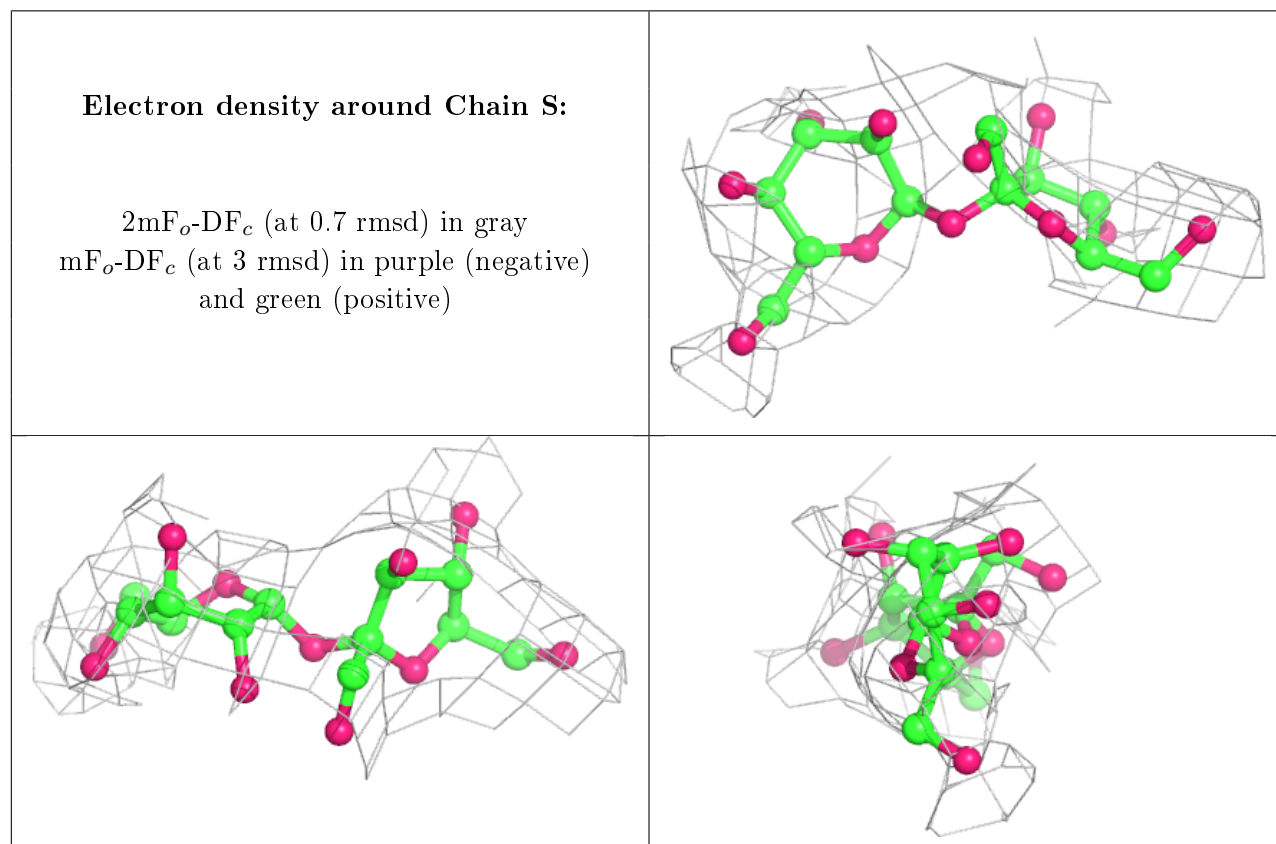
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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.

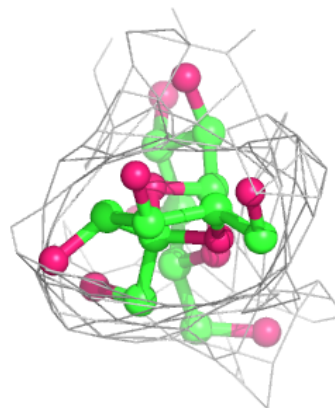
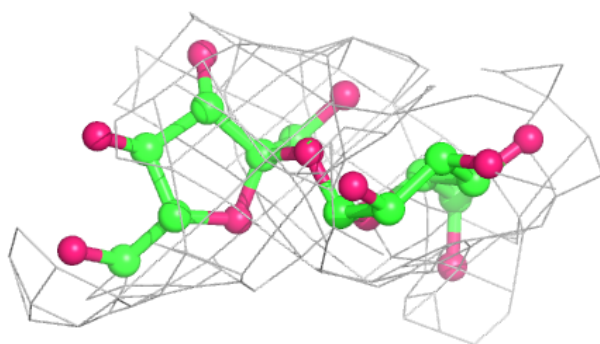
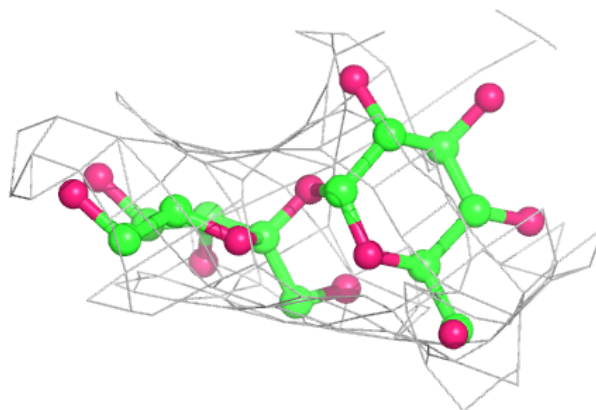
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
19	GLC	Q	1	11/12	0.43	0.79	20,20,20,20	0
19	FRU	a	2	12/12	0.62	0.35	20,20,20,20	0
19	FRU	M	2	12/12	0.64	0.49	20,20,20,20	0
19	FRU	O	2	12/12	0.64	0.49	20,20,20,20	0
19	FRU	Q	2	12/12	0.65	0.56	20,20,20,20	0
19	FRU	X	2	12/12	0.66	0.43	20,20,20,20	0
19	FRU	P	2	12/12	0.66	0.42	20,20,20,20	0
19	GLC	M	1	11/12	0.67	0.42	20,20,20,20	0
19	GLC	Y	1	11/12	0.67	0.32	20,20,20,20	0
19	GLC	W	1	11/12	0.69	0.32	20,20,20,20	0
19	GLC	a	1	11/12	0.69	0.40	20,20,20,20	0
19	FRU	S	2	12/12	0.70	0.25	20,20,20,20	0
19	GLC	S	1	11/12	0.71	0.34	20,20,20,20	0
19	GLC	O	1	10/12	0.72	0.23	20,20,20,20	0
19	FRU	V	2	12/12	0.73	0.21	20,20,20,20	0
19	FRU	U	2	12/12	0.74	0.31	2,36,60,60	0
19	FRU	Z	2	12/12	0.75	0.23	2,33,60,60	0
19	FRU	Y	2	12/12	0.76	0.29	20,20,20,20	0
19	GLC	P	1	11/12	0.77	0.32	20,20,20,20	0
19	GLC	T	1	11/12	0.77	0.23	20,20,20,20	0
19	GLC	V	1	11/12	0.78	0.38	20,20,20,20	0
19	FRU	W	2	12/12	0.80	0.20	20,20,20,20	0
19	GLC	X	1	11/12	0.82	0.53	20,20,20,20	0
19	GLC	Z	1	11/12	0.83	0.17	2,57,60,60	0
19	FRU	T	2	12/12	0.84	0.21	20,20,20,20	0
19	GLC	U	1	11/12	0.85	0.27	2,13,57,60	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



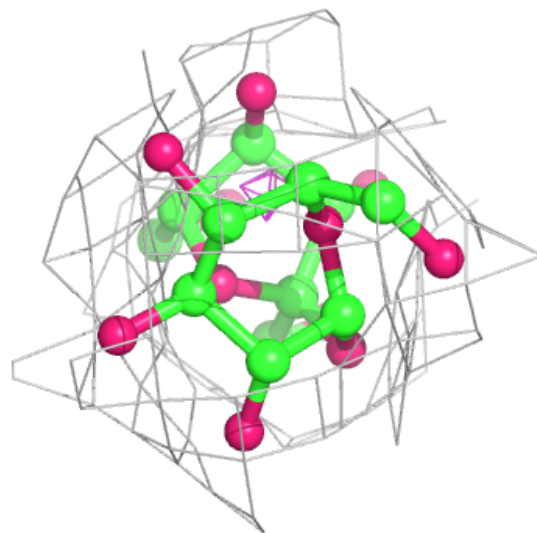
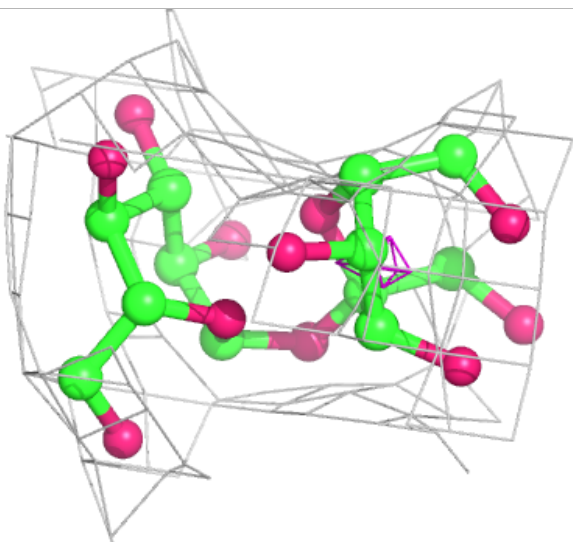
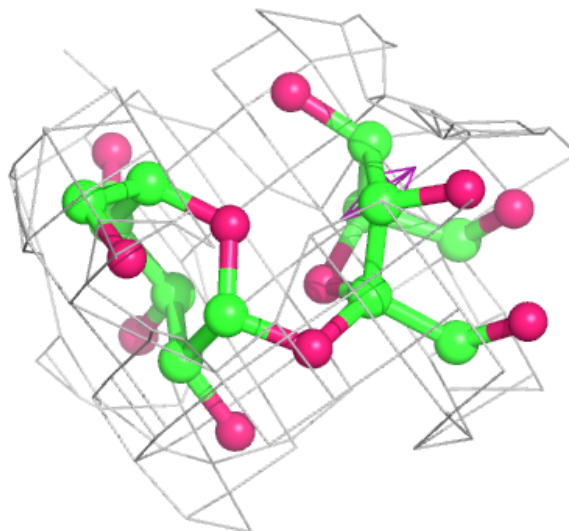
Electron density around Chain T:

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



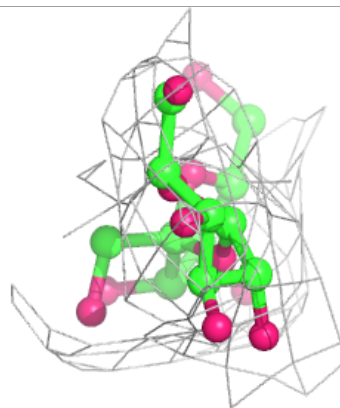
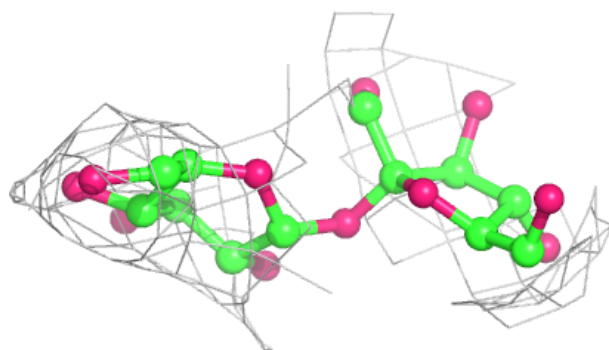
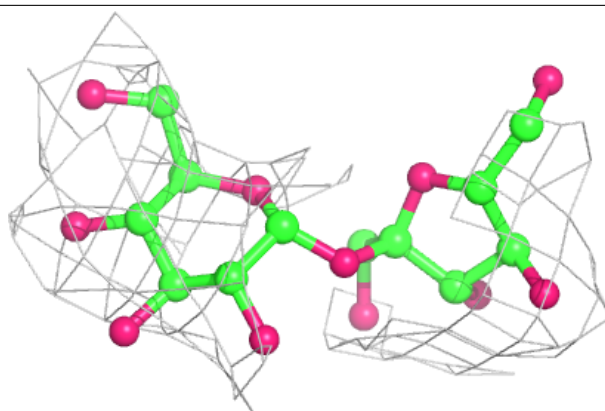
Electron density around Chain U:

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

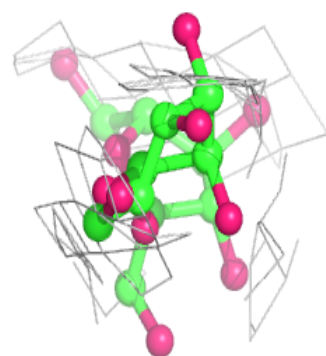
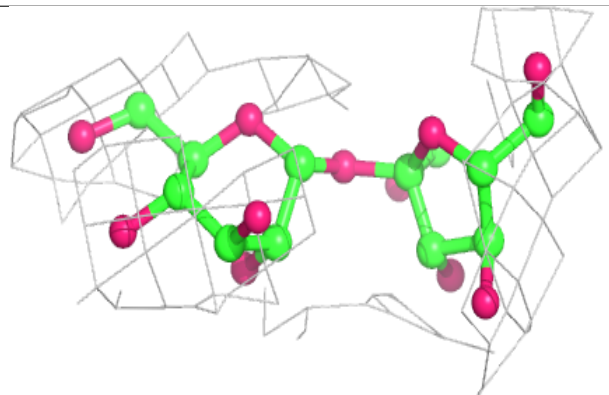
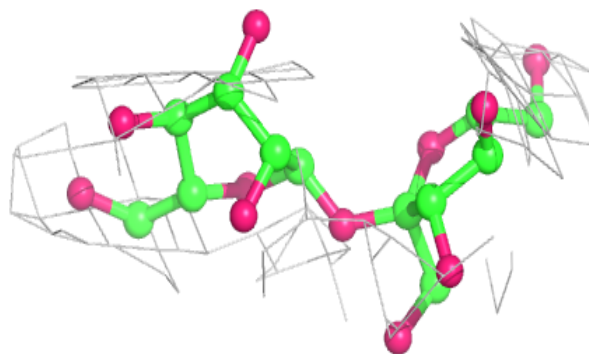


Electron density around Chain V:

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

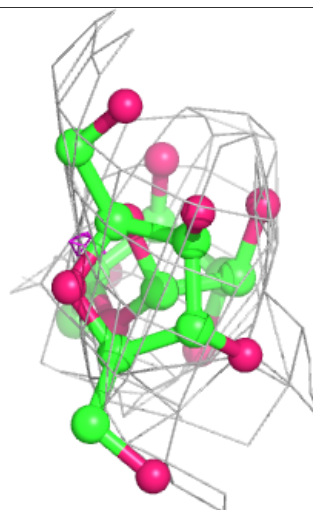
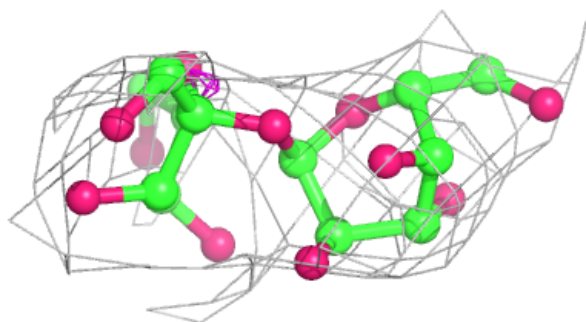
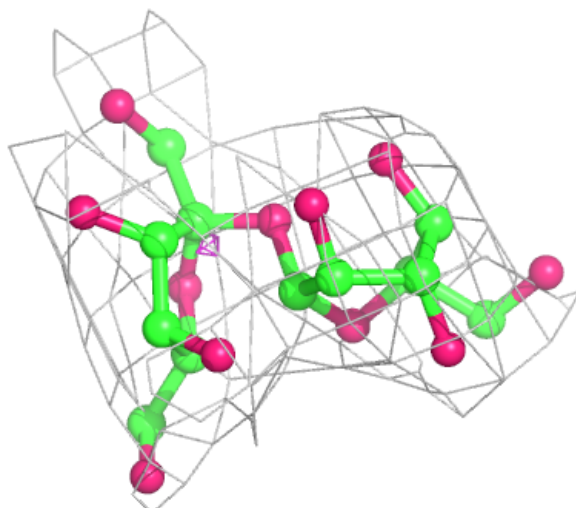
**Electron density around Chain W:**

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



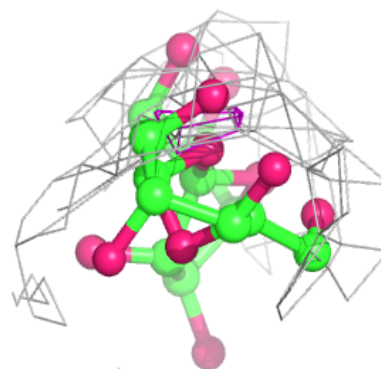
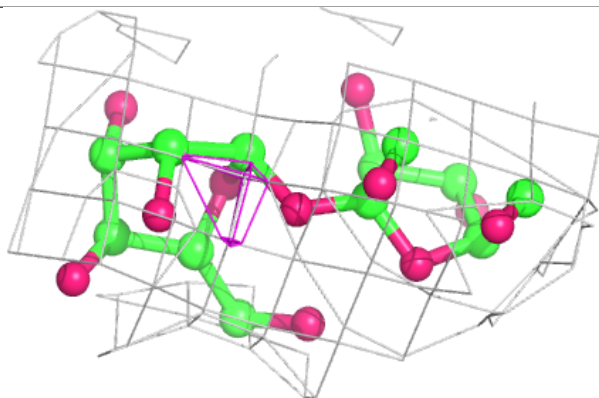
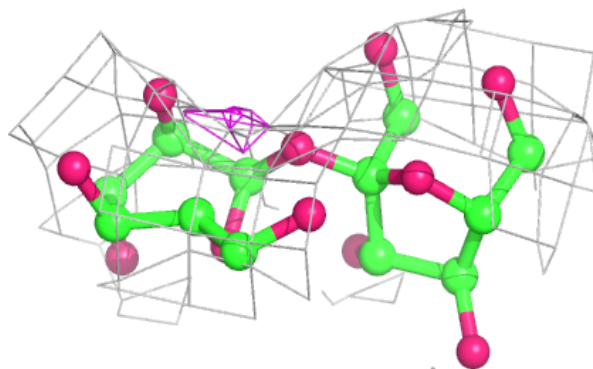
Electron density around Chain X:

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

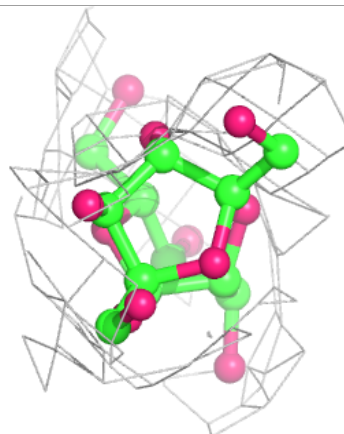
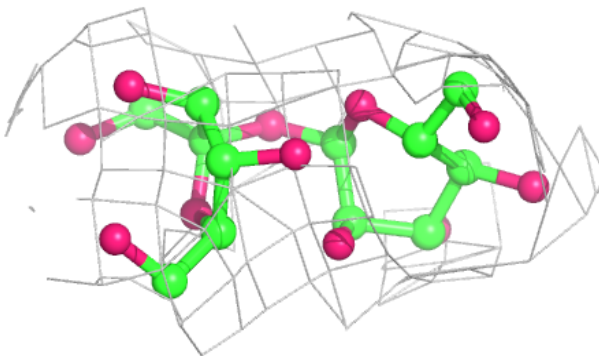
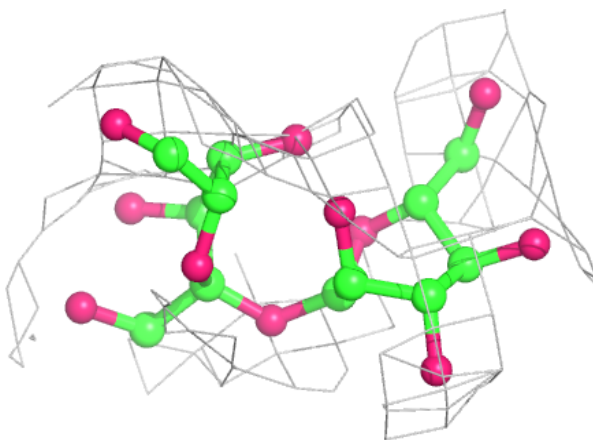


Electron density around Chain Y:

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

**Electron density around Chain Z:**

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



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	3	310	25/65	0.46	0.43	20,20,20,20	0
21	LMU	1	218	35/35	0.46	0.42	20,20,20,20	0
21	LMU	R	102	35/35	0.51	0.48	20,20,20,20	0
21	LMU	R	106	35/35	0.53	0.37	20,20,20,20	0
21	LMU	L	204	35/35	0.53	0.51	20,20,20,20	0
21	LMU	A	853	35/35	0.54	0.51	20,20,20,20	0
20	CLA	3	306	25/65	0.55	0.40	20,20,20,20	0
20	CLA	B	834	51/65	0.55	0.47	20,20,20,20	0
20	CLA	A	839	65/65	0.55	0.47	20,20,20,20	0
20	CLA	H	102	55/65	0.55	0.38	20,20,20,20	0
21	LMU	B	801	35/35	0.56	0.48	20,20,20,20	0
21	LMU	4	301	35/35	0.56	0.36	20,20,20,20	0
20	CLA	2	322	61/65	0.57	0.36	20,20,20,20	0
20	CLA	3	301	36/65	0.58	0.48	20,20,20,20	0
22	BCR	A	843	40/40	0.58	0.45	20,20,20,20	0
20	CLA	B	833	45/65	0.59	0.42	20,20,20,20	0
20	CLA	2	302	51/65	0.59	0.37	20,20,20,20	0
21	LMU	2	320	35/35	0.59	0.54	20,20,20,20	0
22	BCR	J	102	40/40	0.60	0.46	20,20,20,20	0
20	CLA	K	102	50/65	0.60	0.49	20,20,20,20	0
20	CLA	H	103	55/65	0.60	0.49	20,20,20,20	0
20	CLA	K	101	45/65	0.60	0.37	20,20,20,20	0
21	LMU	H	108	35/35	0.60	0.36	2,41,60,60	0
21	LMU	R	101	35/35	0.60	0.33	20,20,20,20	0
20	CLA	A	814	45/65	0.60	0.53	20,20,20,20	0
21	LMU	A	848	35/35	0.61	0.45	20,20,20,20	0
20	CLA	2	308	65/65	0.61	0.42	20,20,20,20	0
20	CLA	2	301	25/65	0.61	0.67	20,20,20,20	0
20	CLA	3	311	65/65	0.62	0.39	20,20,20,20	0
20	CLA	3	313	65/65	0.62	0.55	20,20,20,20	0
21	LMU	2	313	35/35	0.62	0.40	20,20,20,20	0
20	CLA	A	802	25/65	0.62	0.43	20,20,20,20	0
21	LMU	H	105	35/35	0.62	0.30	20,20,20,20	0
20	CLA	3	309	25/65	0.62	0.44	20,20,20,20	0
21	LMU	D	201	35/35	0.62	0.31	2,30,60,60	0
21	LMU	3	321	35/35	0.63	0.33	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	3	308	42/65	0.63	0.37	20,20,20,20	0
20	CLA	A	840	50/65	0.63	0.32	20,20,20,20	0
21	LMU	4	317	35/35	0.63	0.31	20,20,20,20	0
20	CLA	3	317	50/65	0.63	0.37	20,20,20,20	0
21	LMU	H	107	35/35	0.64	0.33	20,20,20,20	0
20	CLA	2	306	25/65	0.64	0.36	20,20,20,20	0
20	CLA	B	814	46/65	0.64	0.51	20,20,20,20	0
20	CLA	4	306	50/65	0.65	0.41	20,20,20,20	0
20	CLA	4	308	36/65	0.65	0.39	20,20,20,20	0
20	CLA	4	302	55/65	0.65	0.35	20,20,20,20	0
21	LMU	1	213	35/35	0.65	0.35	2,45,60,60	0
22	BCR	3	314	40/40	0.65	0.37	20,20,20,20	0
21	LMU	1	220	35/35	0.65	0.28	2,51,60,60	0
21	LMU	R	109	35/35	0.65	0.31	20,20,20,20	0
21	LMU	1	217	35/35	0.65	0.47	20,20,20,20	0
20	CLA	A	810	45/65	0.65	0.56	20,20,20,20	0
21	LMU	2	317	35/35	0.66	0.32	20,20,20,20	0
20	CLA	L	201	55/65	0.66	0.38	20,20,20,20	0
21	LMU	A	849	35/35	0.66	0.41	20,20,20,20	0
20	CLA	3	307	25/65	0.66	0.37	20,20,20,20	0
21	LMU	4	320	34/35	0.67	0.40	20,20,20,20	0
21	LMU	K	104	35/35	0.67	0.42	20,20,20,20	0
21	LMU	R	105	35/35	0.67	0.26	20,20,20,20	0
20	CLA	B	838	65/65	0.67	0.47	20,20,20,20	0
20	CLA	K	108	50/65	0.67	0.59	20,20,20,20	0
20	CLA	1	211	25/65	0.67	0.36	20,20,20,20	0
21	LMU	K	106	35/35	0.67	0.36	2,38,60,60	0
21	LMU	K	109	35/35	0.67	0.39	20,20,20,20	0
21	LMU	H	104	35/35	0.67	0.37	20,20,20,20	0
20	CLA	3	302	50/65	0.68	0.34	20,20,20,20	0
20	CLA	3	319	25/65	0.68	0.30	20,20,20,20	0
20	CLA	R	107	57/65	0.68	0.49	20,20,20,20	0
21	LMU	R	103	35/35	0.68	0.29	20,20,20,20	0
20	CLA	B	840	36/65	0.68	0.46	20,20,20,20	0
20	CLA	1	215	61/65	0.68	0.29	2,35,60,60	0
20	CLA	1	210	51/65	0.68	0.39	20,20,20,20	0
20	CLA	4	305	55/65	0.68	0.35	20,20,20,20	0
21	LMU	4	322	35/35	0.68	0.26	20,20,20,20	0
21	LMU	L	211	35/35	0.68	0.32	20,20,20,20	0
21	LMU	2	318	35/35	0.68	0.26	20,20,20,20	0
22	BCR	A	844	40/40	0.69	0.41	20,20,20,20	0
22	BCR	A	845	40/40	0.69	0.38	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	1	201	46/65	0.69	0.31	20,20,20,20	0
22	BCR	B	846	40/40	0.69	0.46	20,20,20,20	0
20	CLA	4	304	65/65	0.69	0.31	20,20,20,20	0
20	CLA	L	203	55/65	0.69	0.43	20,20,20,20	0
20	CLA	4	319	47/65	0.69	0.29	20,20,20,20	0
20	CLA	J	103	61/65	0.69	0.29	20,20,20,20	0
21	LMU	N	101	35/35	0.69	0.32	2,39,60,60	0
22	BCR	L	210	40/40	0.69	0.47	20,20,20,20	0
20	CLA	2	310	25/65	0.70	0.40	20,20,20,20	0
21	LMU	1	219	35/35	0.70	0.30	20,20,20,20	0
22	BCR	I	103	40/40	0.70	0.47	20,20,20,20	0
20	CLA	2	307	65/65	0.70	0.38	20,20,20,20	0
20	CLA	4	311	55/65	0.70	0.36	20,20,20,20	0
20	CLA	R	108	58/65	0.70	0.34	20,20,20,20	0
20	CLA	2	303	65/65	0.70	0.35	20,20,20,20	0
20	CLA	K	103	65/65	0.70	0.49	20,20,20,20	0
21	LMU	R	104	35/35	0.70	0.36	20,20,20,20	0
20	CLA	A	833	45/65	0.70	0.40	20,20,20,20	0
20	CLA	F	206	53/65	0.70	0.34	20,20,20,20	0
20	CLA	A	820	51/65	0.70	0.48	20,20,20,20	0
20	CLA	A	818	65/65	0.70	0.42	20,20,20,20	0
20	CLA	4	318	52/65	0.70	0.31	20,20,20,20	0
20	CLA	A	811	65/65	0.70	0.43	20,20,20,20	0
20	CLA	A	816	54/65	0.71	0.39	20,20,20,20	0
20	CLA	2	304	25/65	0.71	0.35	20,20,20,20	0
20	CLA	A	823	65/65	0.71	0.41	20,20,20,20	0
25	LMG	B	848	49/55	0.71	0.42	20,20,20,20	0
20	CLA	H	101	55/65	0.71	0.39	20,20,20,20	0
20	CLA	B	824	65/65	0.72	0.38	20,20,20,20	0
20	CLA	B	813	60/65	0.72	0.36	20,20,20,20	0
20	CLA	3	318	65/65	0.72	0.32	20,20,20,20	0
21	LMU	3	322	35/35	0.72	0.28	20,20,20,20	0
21	LMU	A	856	35/35	0.72	0.29	20,20,20,20	0
20	CLA	1	216	25/65	0.72	0.36	20,20,20,20	0
20	CLA	A	829	50/65	0.73	0.41	20,20,20,20	0
22	BCR	A	847	40/40	0.73	0.47	20,20,20,20	0
22	BCR	B	844	40/40	0.73	0.39	20,20,20,20	0
20	CLA	A	801	46/65	0.73	0.24	20,20,20,20	0
21	LMU	4	321	35/35	0.73	0.21	20,20,20,20	0
20	CLA	A	821	42/65	0.73	0.36	20,20,20,20	0
21	LMU	C	101	35/35	0.73	0.26	20,20,20,20	0
23	PQN	A	842	33/33	0.73	0.46	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	3	305	25/65	0.73	0.34	20,20,20,20	0
21	LMU	F	201	34/35	0.73	0.26	20,20,20,20	0
20	CLA	A	805	65/65	0.74	0.37	20,20,20,20	0
20	CLA	2	305	50/65	0.74	0.34	20,20,20,20	0
20	CLA	3	312	25/65	0.74	0.26	20,20,20,20	0
23	PQN	B	841	33/33	0.74	0.42	20,20,20,20	0
20	CLA	H	109	60/65	0.74	0.35	20,20,20,20	0
20	CLA	F	205	41/65	0.74	0.29	20,20,20,20	0
21	LMU	B	802	35/35	0.74	0.23	20,20,20,20	0
20	CLA	A	819	65/65	0.74	0.40	20,20,20,20	0
20	CLA	B	819	46/65	0.74	0.38	20,20,20,20	0
20	CLA	1	205	25/65	0.74	0.29	20,20,20,20	0
20	CLA	A	813	54/65	0.74	0.39	20,20,20,20	0
20	CLA	B	803	65/65	0.74	0.40	20,20,20,20	0
20	CLA	G	102	51/65	0.74	0.31	20,20,20,20	0
20	CLA	A	817	52/65	0.74	0.38	20,20,20,20	0
21	LMU	2	319	35/35	0.74	0.23	20,20,20,20	0
20	CLA	A	806	55/65	0.74	0.39	20,20,20,20	0
20	CLA	L	207	50/65	0.75	0.34	20,20,20,20	0
20	CLA	4	309	25/65	0.75	0.33	20,20,20,20	0
20	CLA	A	826	65/65	0.75	0.45	20,20,20,20	0
22	BCR	F	202	40/40	0.75	0.45	20,20,20,20	0
20	CLA	A	828	65/65	0.75	0.38	20,20,20,20	0
20	CLA	3	320	25/65	0.75	0.28	20,20,20,20	0
20	CLA	B	831	50/65	0.75	0.39	20,20,20,20	0
20	CLA	1	207	51/65	0.75	0.33	20,20,20,20	0
20	CLA	3	304	36/65	0.75	0.35	20,20,20,20	0
20	CLA	L	209	50/65	0.75	0.30	20,20,20,20	0
20	CLA	A	812	54/65	0.76	0.34	20,20,20,20	0
21	LMU	B	847	35/35	0.76	0.29	2,35,60,60	0
20	CLA	B	849	65/65	0.76	0.39	20,20,20,20	0
20	CLA	2	312	50/65	0.76	0.31	20,20,20,20	0
21	LMU	L	205	35/35	0.76	0.24	20,20,20,20	0
20	CLA	A	804	55/65	0.76	0.33	20,20,20,20	0
21	LMU	A	854	35/35	0.76	0.27	20,20,20,20	0
20	CLA	A	832	50/65	0.76	0.36	20,20,20,20	0
20	CLA	1	203	47/65	0.76	0.27	20,20,20,20	0
20	CLA	3	303	25/65	0.77	0.36	20,20,20,20	0
20	CLA	B	823	58/65	0.77	0.37	20,20,20,20	0
22	BCR	B	845	40/40	0.77	0.40	20,20,20,20	0
20	CLA	2	315	25/65	0.77	0.32	20,20,20,20	0
20	CLA	3	316	25/65	0.77	0.38	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	LMU	G	101	35/35	0.77	0.24	20,20,20,20	0
20	CLA	2	316	65/65	0.77	0.29	20,20,20,20	0
20	CLA	F	204	36/65	0.77	0.35	20,20,20,20	0
20	CLA	A	807	46/65	0.78	0.48	20,20,20,20	0
20	CLA	B	832	45/65	0.78	0.32	20,20,20,20	0
20	CLA	L	202	65/65	0.78	0.36	20,20,20,20	0
21	LMU	K	105	35/35	0.78	0.28	20,20,20,20	0
22	BCR	F	203	40/40	0.78	0.31	20,20,20,20	0
20	CLA	4	310	25/65	0.78	0.27	20,20,20,20	0
20	CLA	A	851	65/65	0.78	0.36	20,20,20,20	0
20	CLA	A	824	65/65	0.78	0.36	20,20,20,20	0
20	CLA	1	206	61/65	0.78	0.32	20,20,20,20	0
21	LMU	A	855	35/35	0.79	0.30	20,20,20,20	0
20	CLA	A	822	55/65	0.79	0.35	20,20,20,20	0
20	CLA	4	307	52/65	0.79	0.25	20,20,20,20	0
20	CLA	B	817	61/65	0.79	0.34	20,20,20,20	0
20	CLA	B	815	59/65	0.79	0.37	20,20,20,20	0
20	CLA	4	316	46/65	0.79	0.25	20,20,20,20	0
20	CLA	A	815	50/65	0.79	0.31	20,20,20,20	0
21	LMU	H	106	35/35	0.79	0.33	20,20,20,20	0
20	CLA	2	309	25/65	0.79	0.30	20,20,20,20	0
20	CLA	A	825	65/65	0.79	0.35	20,20,20,20	0
20	CLA	B	829	50/65	0.79	0.36	20,20,20,20	0
20	CLA	B	851	65/65	0.79	0.35	20,20,20,20	0
26	UNL	H	111	23/-	0.79	0.24	20,20,20,20	0
20	CLA	B	808	65/65	0.79	0.37	20,20,20,20	0
20	CLA	A	852	65/65	0.79	0.36	20,20,20,20	0
20	CLA	A	835	65/65	0.79	0.34	20,20,20,20	0
20	CLA	A	809	52/65	0.80	0.34	20,20,20,20	0
20	CLA	B	835	60/65	0.80	0.34	20,20,20,20	0
20	CLA	A	827	55/65	0.80	0.40	20,20,20,20	0
20	CLA	A	836	47/65	0.80	0.35	20,20,20,20	0
21	LMU	E	101	35/35	0.80	0.24	20,20,20,20	0
20	CLA	1	202	57/65	0.80	0.22	2,38,60,60	0
20	CLA	1	214	25/65	0.80	0.20	20,20,20,20	0
20	CLA	4	312	25/65	0.80	0.27	20,20,20,20	0
22	BCR	B	843	40/40	0.80	0.37	20,20,20,20	0
20	CLA	B	804	45/65	0.80	0.33	20,20,20,20	0
22	BCR	B	852	40/40	0.80	0.35	20,20,20,20	0
22	BCR	B	842	40/40	0.80	0.39	20,20,20,20	0
20	CLA	B	812	65/65	0.80	0.33	20,20,20,20	0
20	CLA	2	311	50/65	0.80	0.28	20,20,20,20	0

Continued on next page...

Continued from previous page...

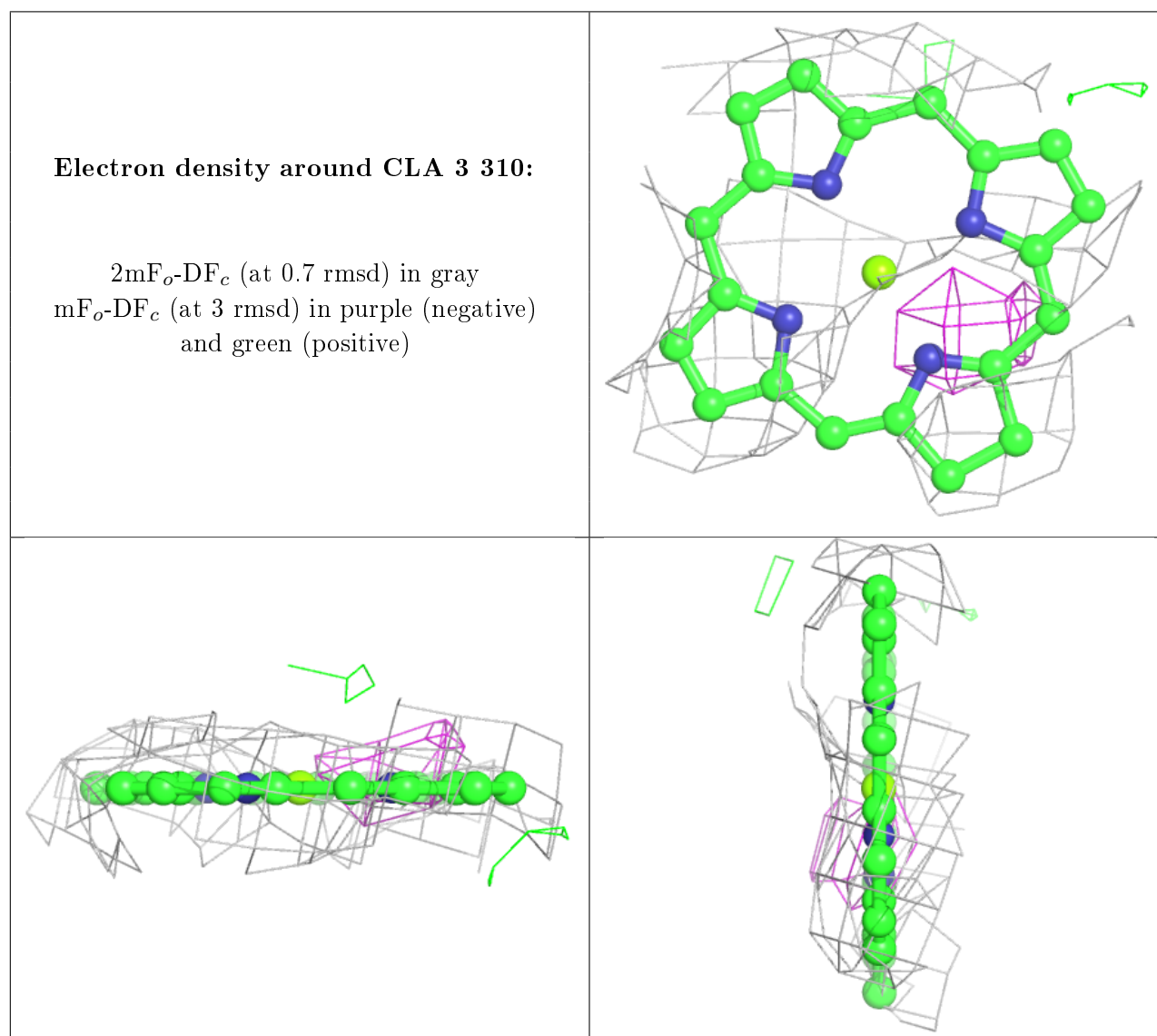
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	1	204	46/65	0.81	0.27	20,20,20,20	0
20	CLA	B	805	60/65	0.81	0.33	20,20,20,20	0
20	CLA	B	810	55/65	0.81	0.29	20,20,20,20	0
20	CLA	A	838	65/65	0.81	0.34	20,20,20,20	0
20	CLA	B	809	54/65	0.81	0.30	20,20,20,20	0
20	CLA	4	314	36/65	0.81	0.29	20,20,20,20	0
20	CLA	B	830	65/65	0.81	0.33	20,20,20,20	0
22	BCR	I	101	40/40	0.81	0.38	20,20,20,20	0
20	CLA	A	830	65/65	0.81	0.35	20,20,20,20	0
20	CLA	A	841	65/65	0.81	0.37	20,20,20,20	0
20	CLA	B	827	65/65	0.81	0.36	20,20,20,20	0
20	CLA	1	212	25/65	0.81	0.44	20,20,20,20	0
20	CLA	A	837	47/65	0.81	0.33	20,20,20,20	0
20	CLA	A	803	50/65	0.82	0.32	20,20,20,20	0
20	CLA	L	208	47/65	0.82	0.31	20,20,20,20	0
20	CLA	B	821	65/65	0.82	0.28	20,20,20,20	0
20	CLA	B	850	65/65	0.82	0.34	20,20,20,20	0
20	CLA	B	822	54/65	0.82	0.32	20,20,20,20	0
20	CLA	J	101	48/65	0.82	0.25	20,20,20,20	0
20	CLA	A	850	65/65	0.82	0.35	20,20,20,20	0
20	CLA	B	818	50/65	0.82	0.35	20,20,20,20	0
20	CLA	A	834	49/65	0.83	0.30	20,20,20,20	0
22	BCR	A	846	40/40	0.83	0.32	20,20,20,20	0
20	CLA	1	208	25/65	0.83	0.34	20,20,20,20	0
20	CLA	I	102	60/65	0.83	0.29	20,20,20,20	0
20	CLA	B	806	65/65	0.83	0.36	20,20,20,20	0
20	CLA	A	831	55/65	0.84	0.33	20,20,20,20	0
20	CLA	B	825	65/65	0.84	0.36	20,20,20,20	0
20	CLA	1	209	36/65	0.84	0.27	20,20,20,20	0
20	CLA	B	811	58/65	0.85	0.27	20,20,20,20	0
20	CLA	B	837	47/65	0.85	0.31	20,20,20,20	0
20	CLA	B	828	50/65	0.85	0.30	20,20,20,20	0
20	CLA	B	820	55/65	0.85	0.29	20,20,20,20	0
20	CLA	B	839	65/65	0.86	0.40	20,20,20,20	0
20	CLA	4	303	36/65	0.86	0.33	20,20,20,20	0
20	CLA	A	808	65/65	0.86	0.35	20,20,20,20	0
20	CLA	4	313	25/65	0.86	0.30	20,20,20,20	0
24	SF4	C	102	8/8	0.87	0.16	20,20,20,20	0
20	CLA	B	816	60/65	0.87	0.32	20,20,20,20	0
20	CLA	B	826	65/65	0.87	0.32	20,20,20,20	0
20	CLA	B	836	65/65	0.88	0.28	20,20,20,20	0
20	CLA	B	807	65/65	0.88	0.33	20,20,20,20	0

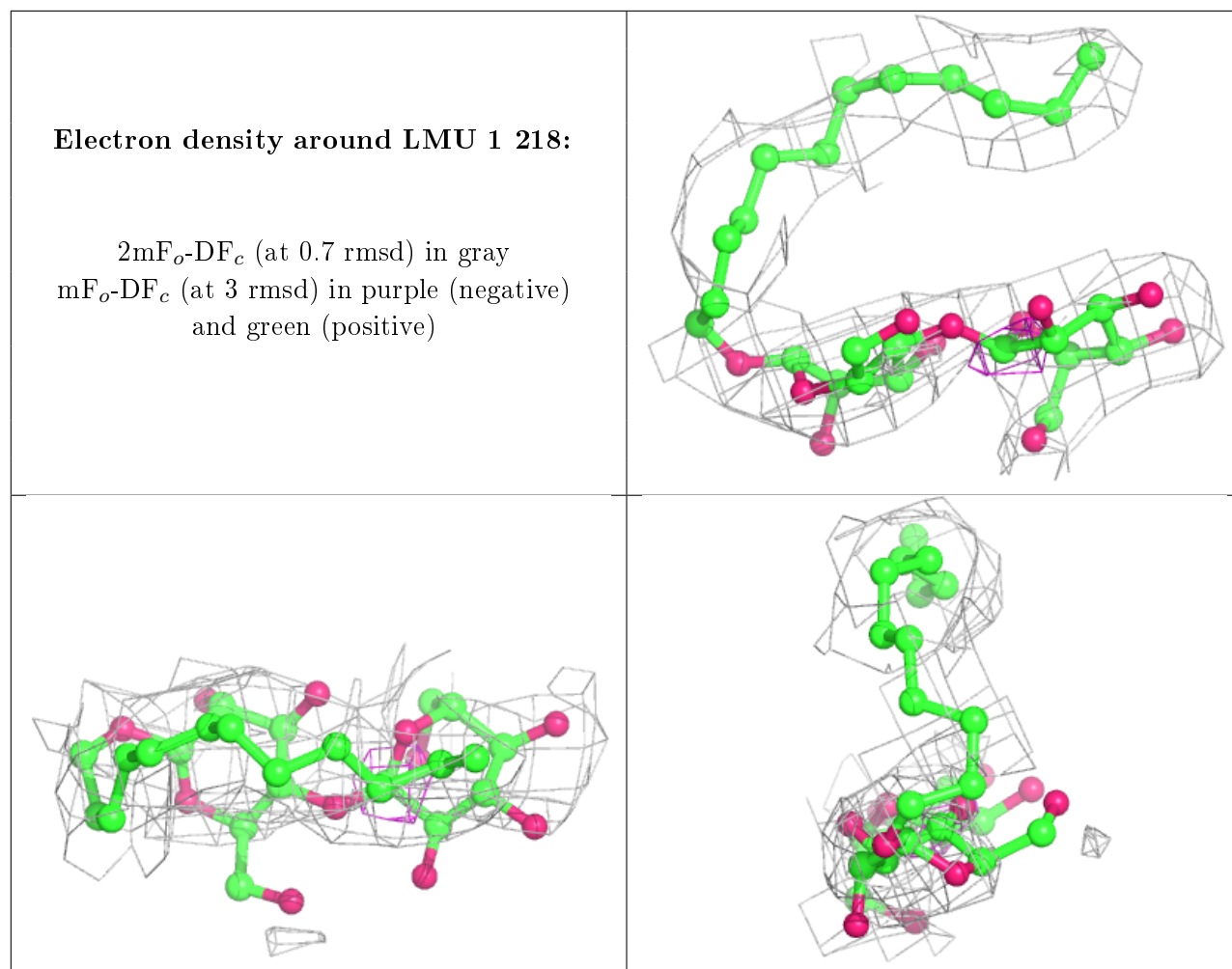
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	4	315	25/65	0.90	0.21	20,20,20,20	0
24	SF4	C	103	8/8	0.91	0.14	20,20,20,20	0
24	SF4	A	857	8/8	0.93	0.14	20,20,20,20	0

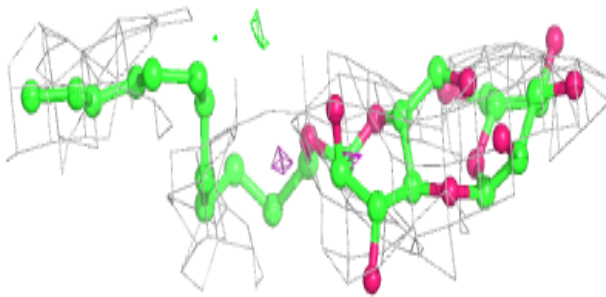
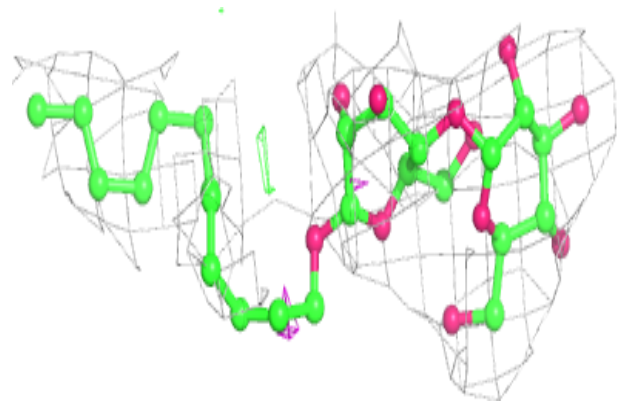
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



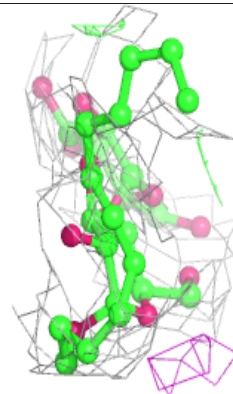
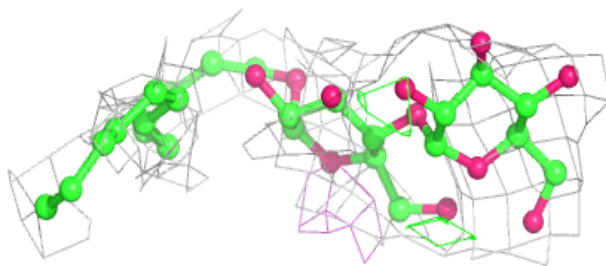
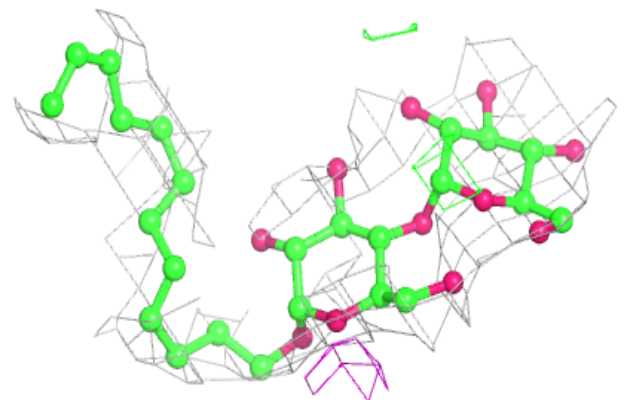


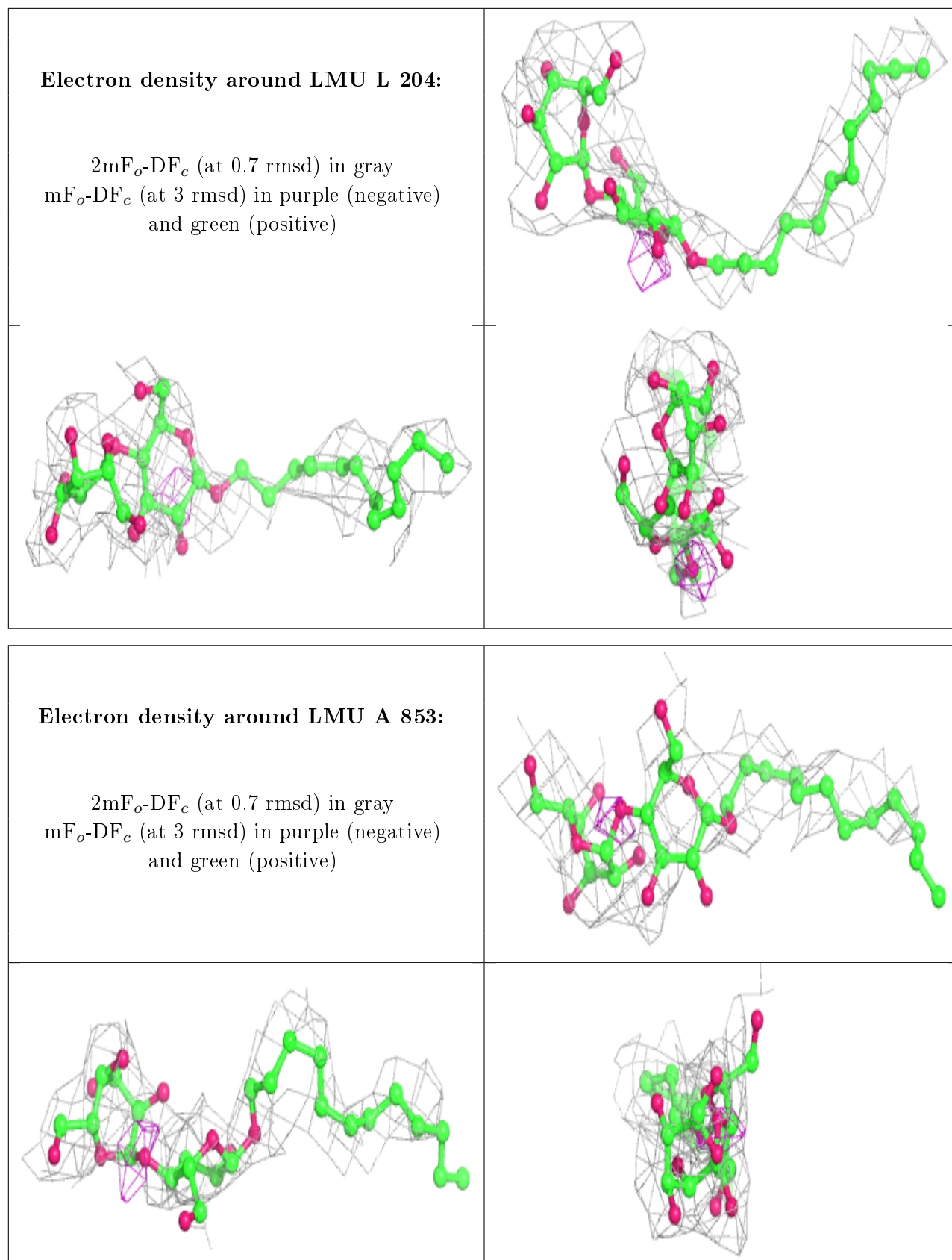
Electron density around LMU R 102:

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

**Electron density around LMU R 106:**

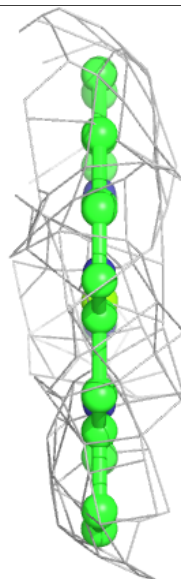
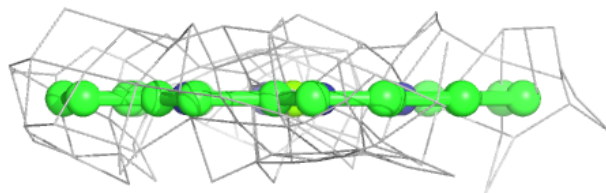
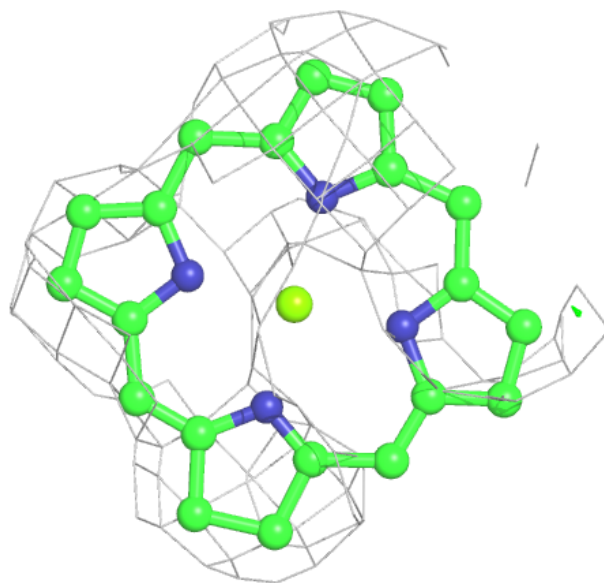
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





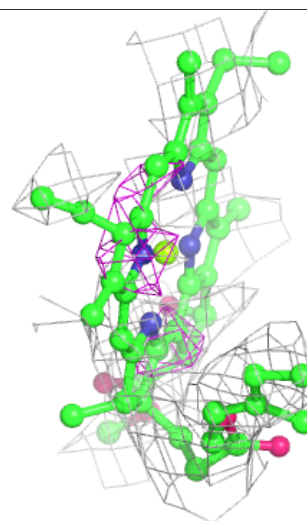
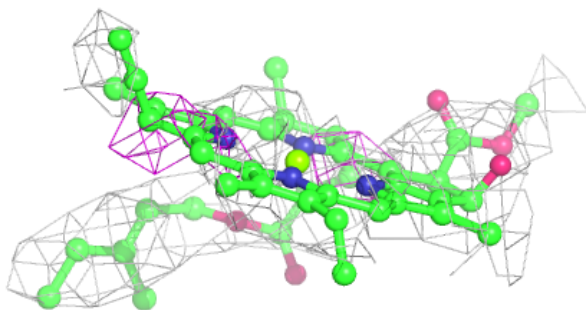
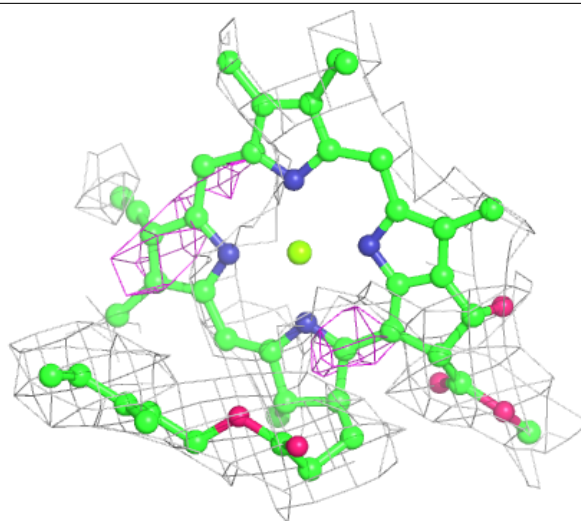
Electron density around CLA 3 306:

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



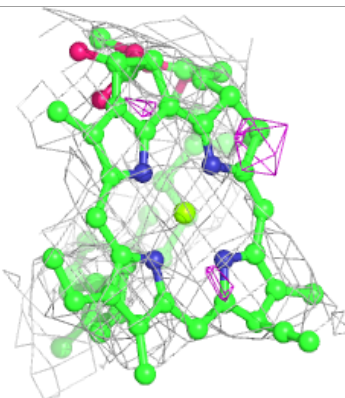
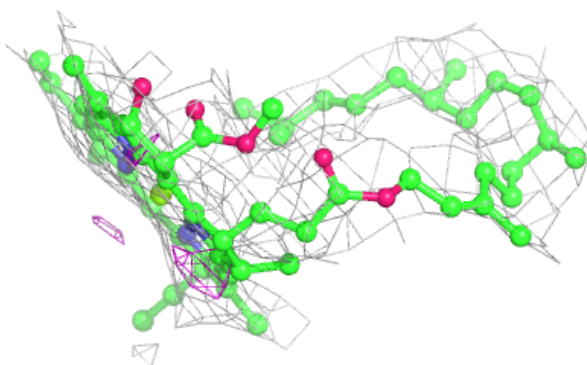
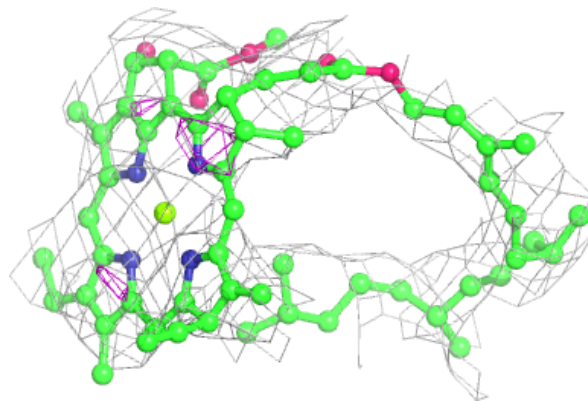
Electron density around CLA B 834:

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

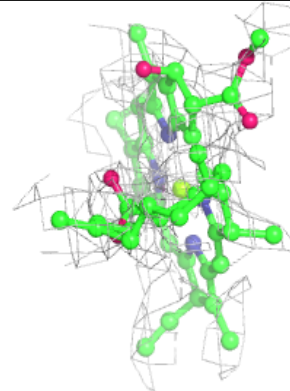
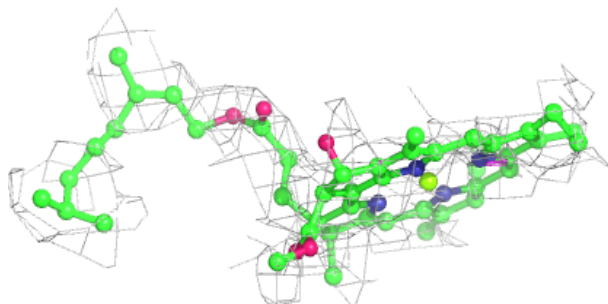
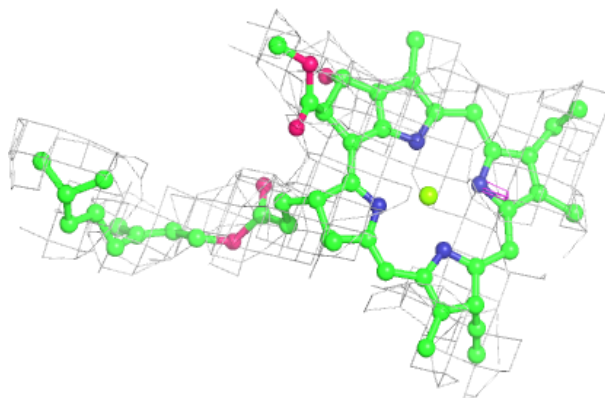


Electron density around CLA A 839:

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

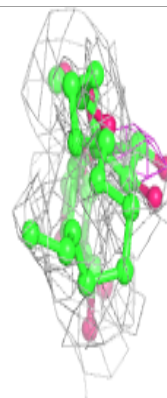
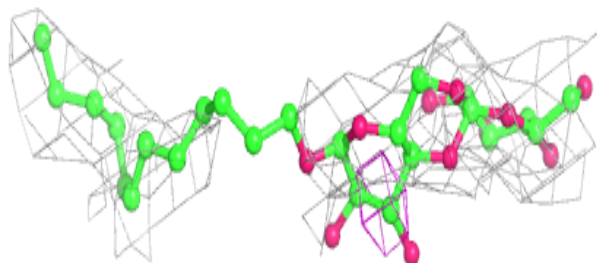
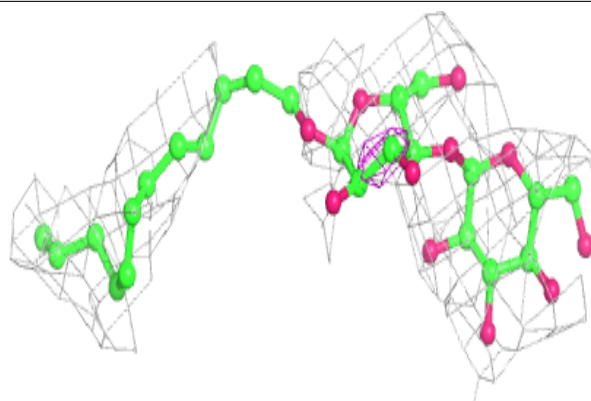
**Electron density around CLA H 102:**

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

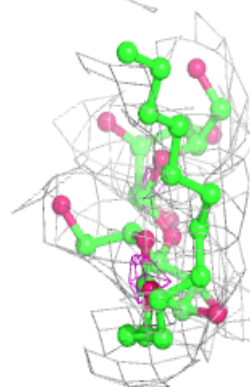
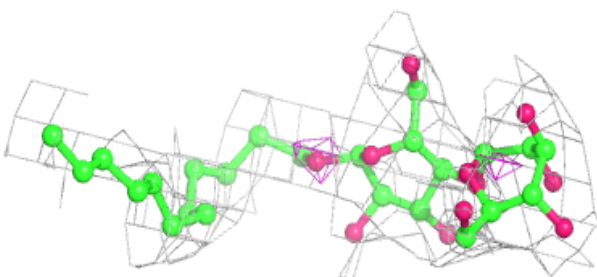
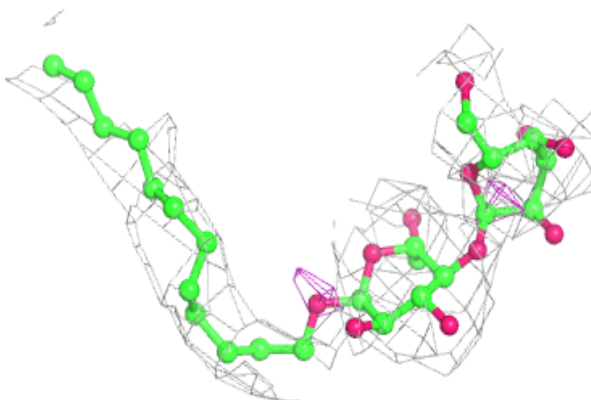


Electron density around LMU B 801:

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

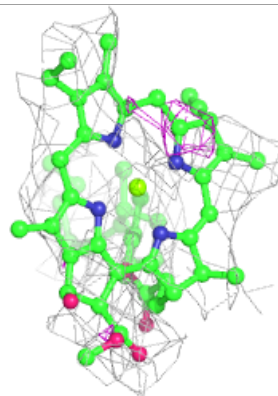
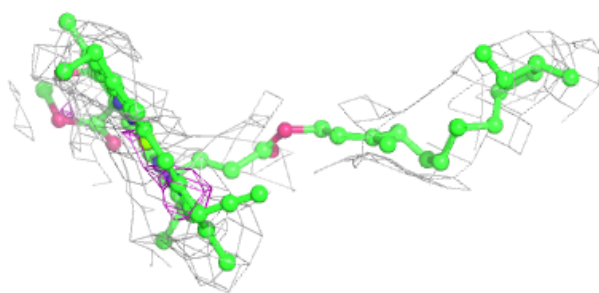
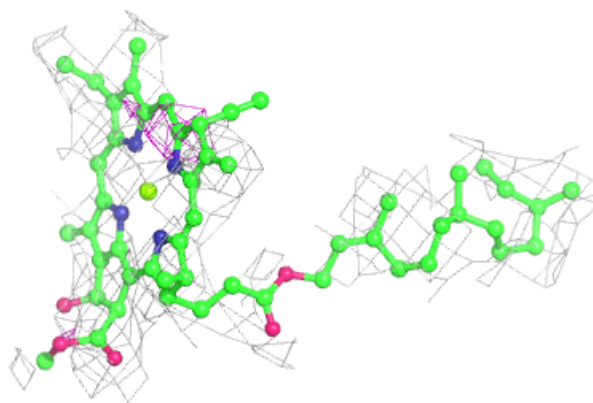
**Electron density around LMU 4 301:**

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



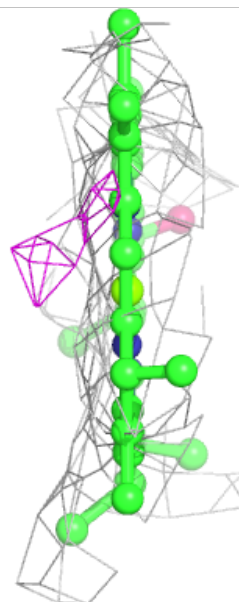
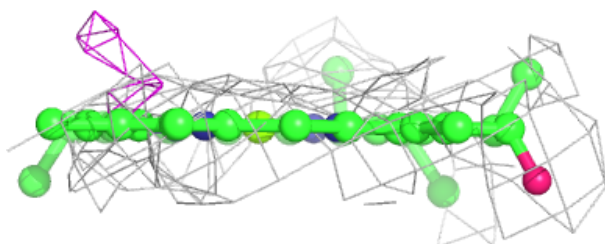
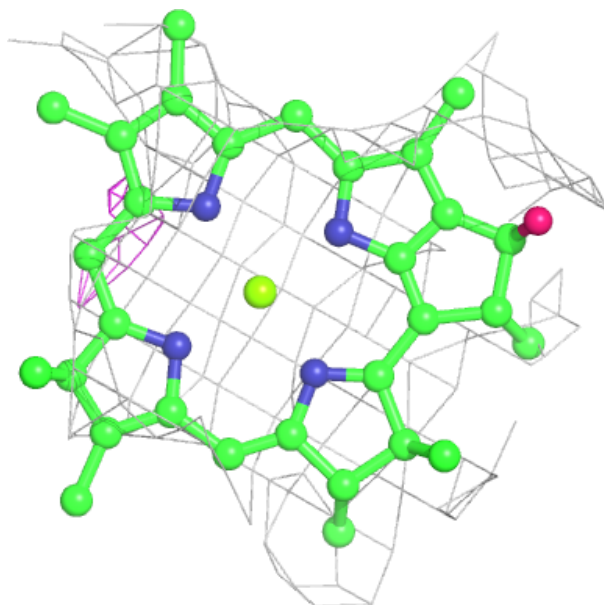
Electron density around CLA 2 322:

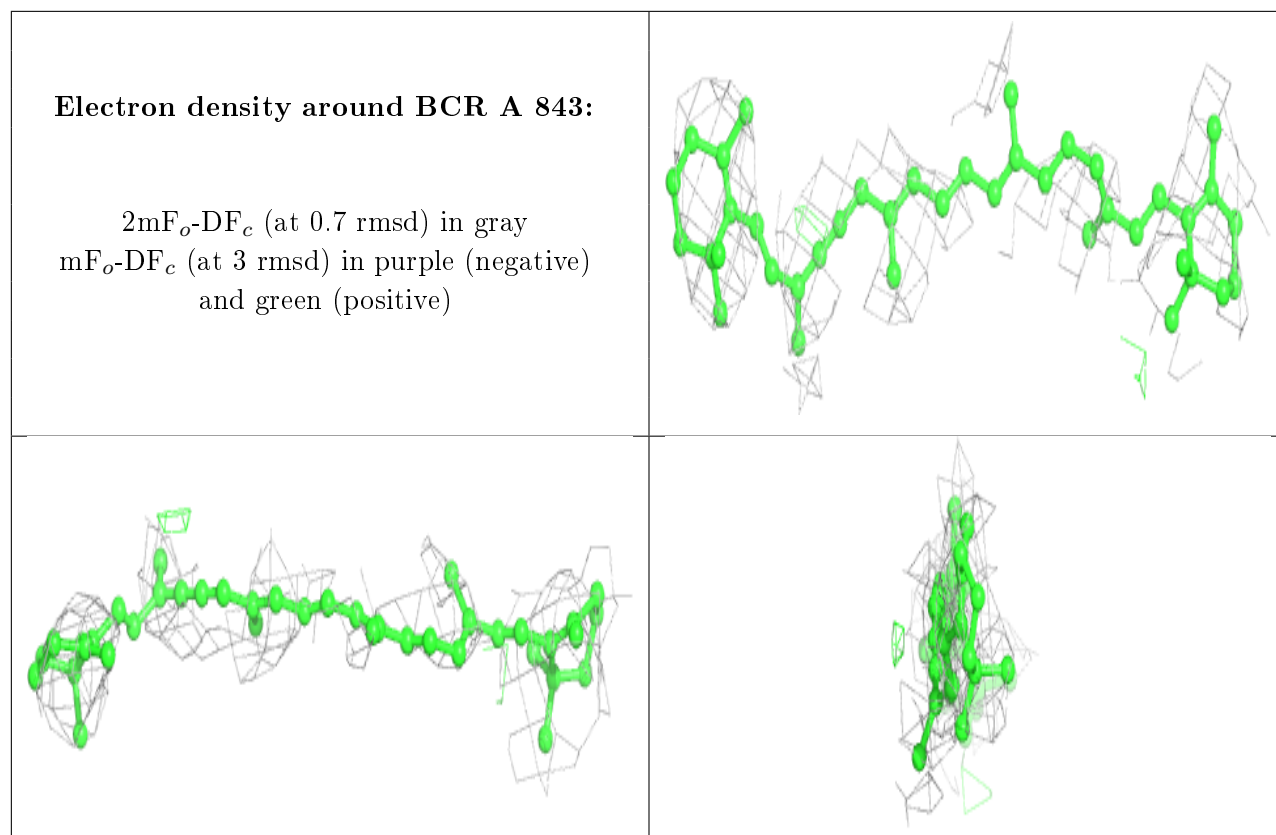
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 3 301:

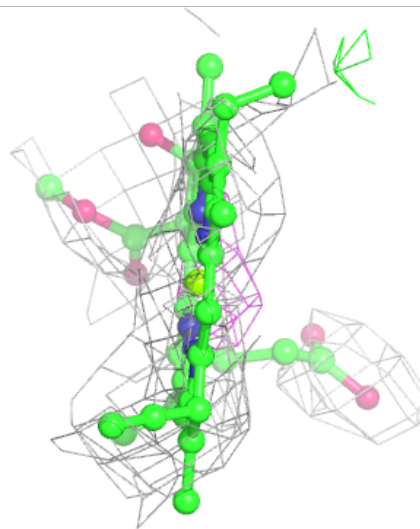
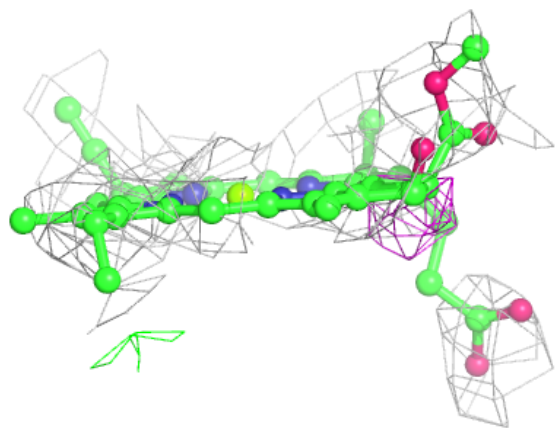
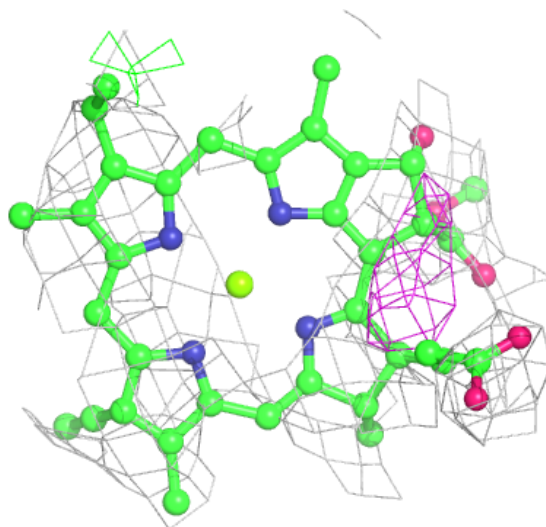
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





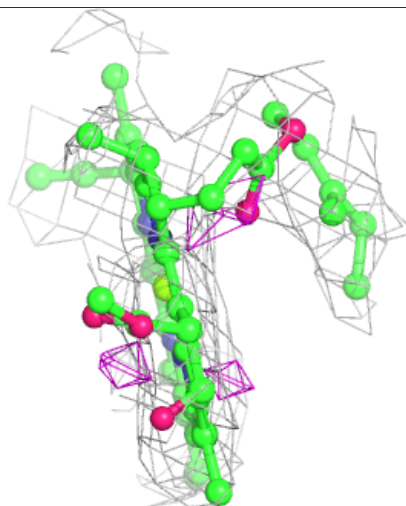
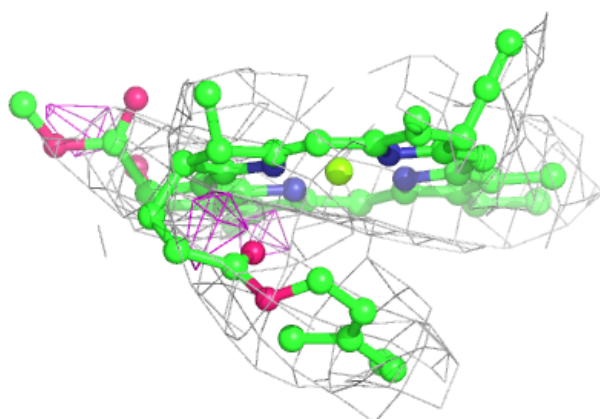
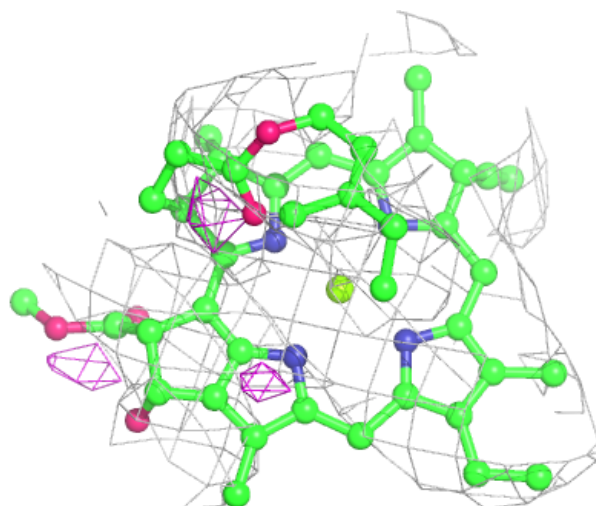
Electron density around CLA B 833:

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



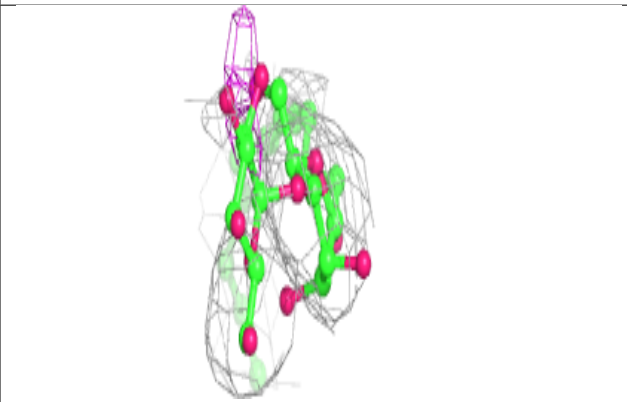
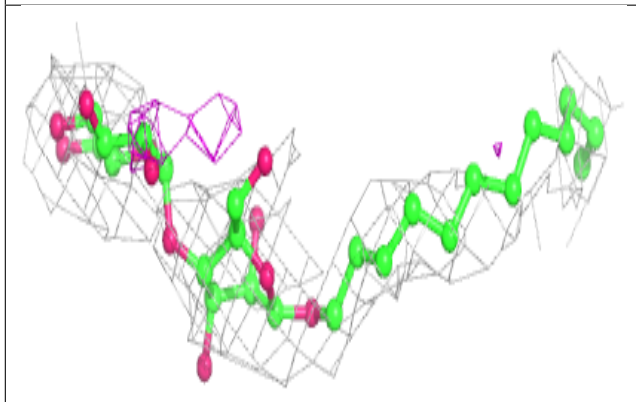
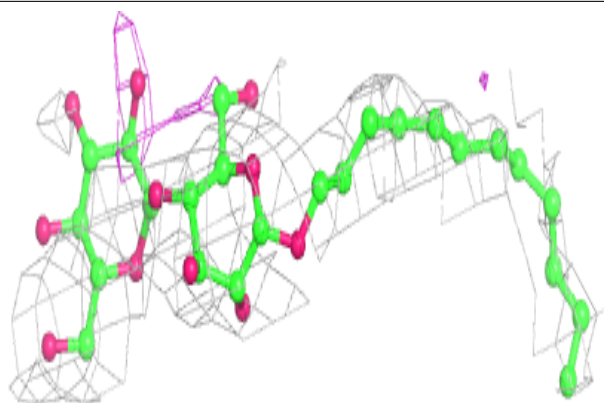
Electron density around CLA 2 302:

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

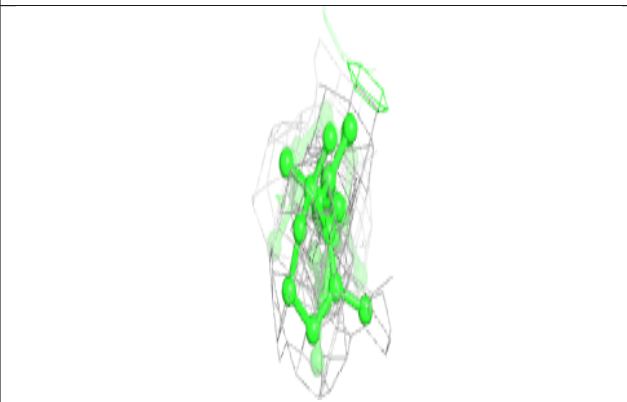
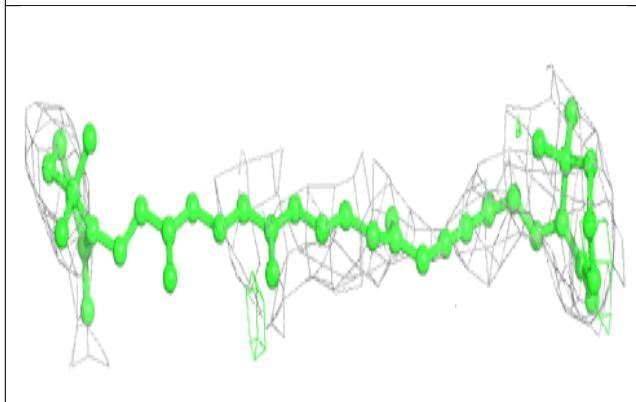
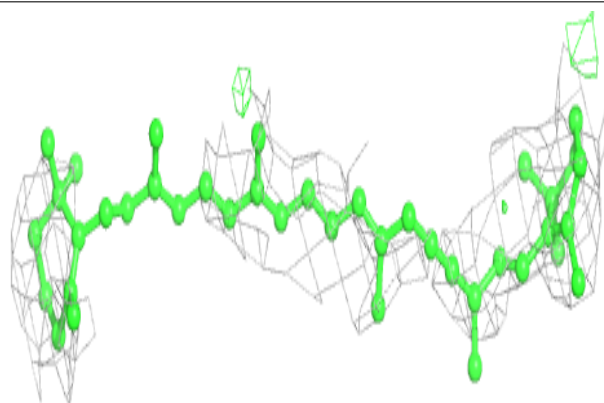


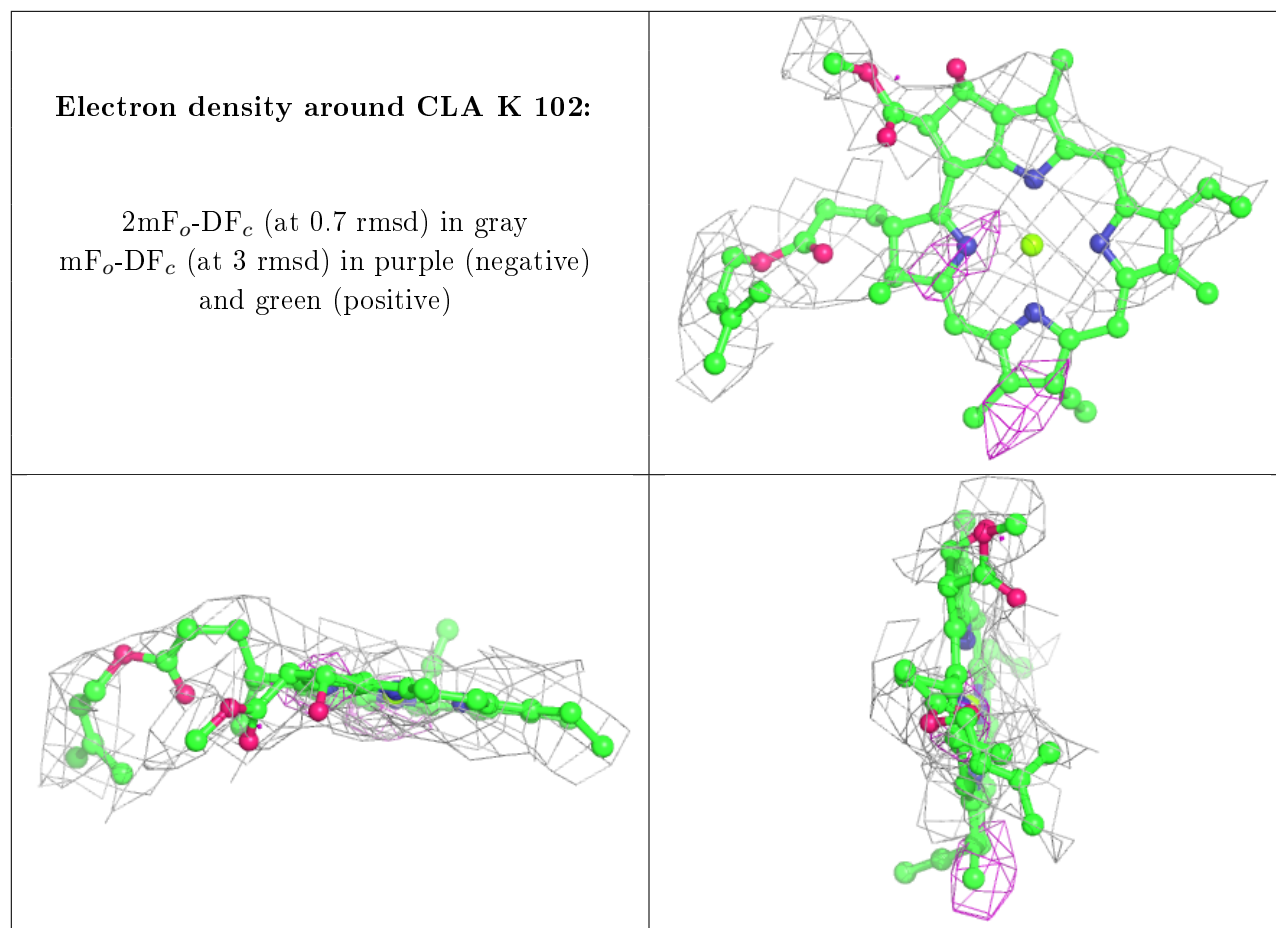
Electron density around LMU 2 320:

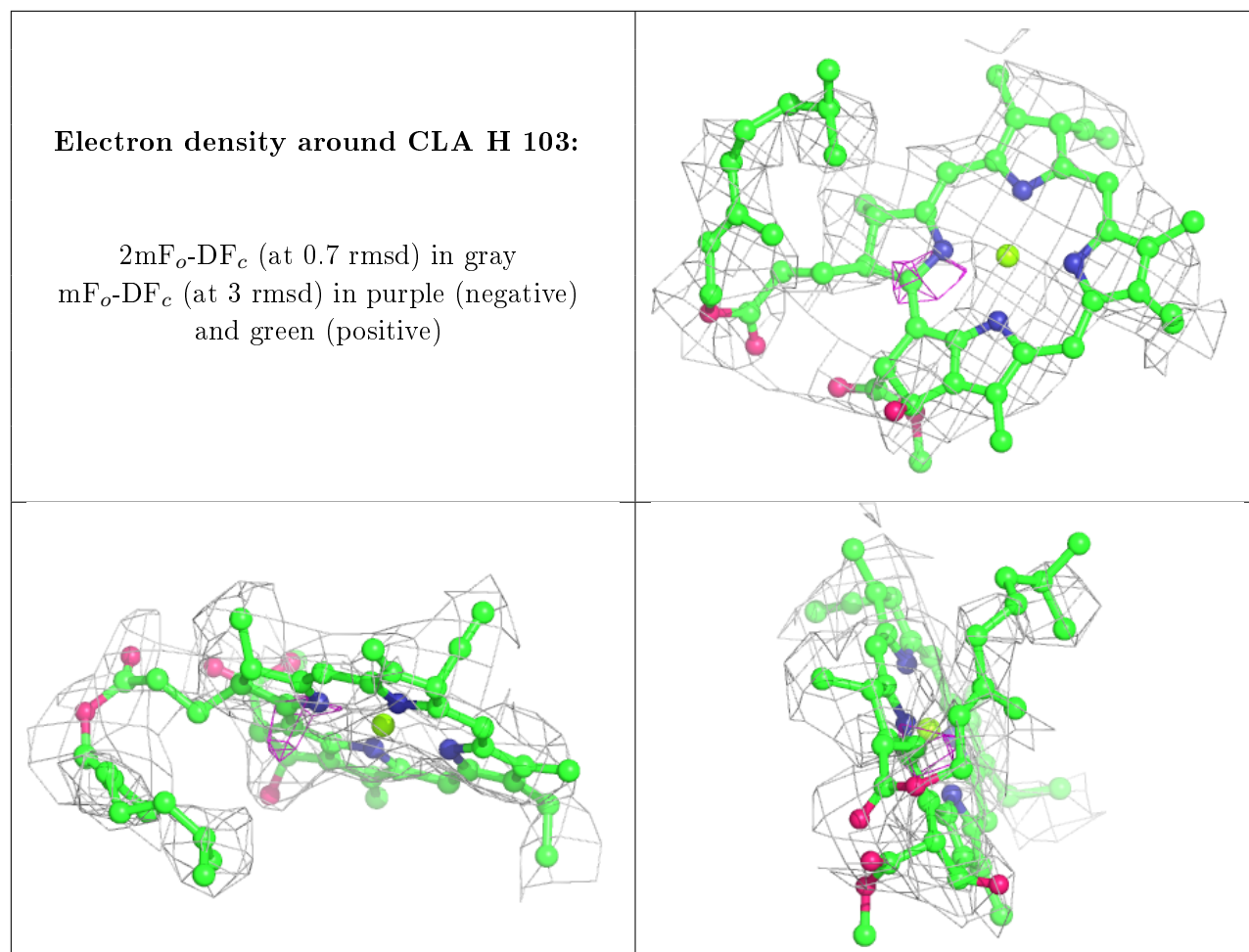
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

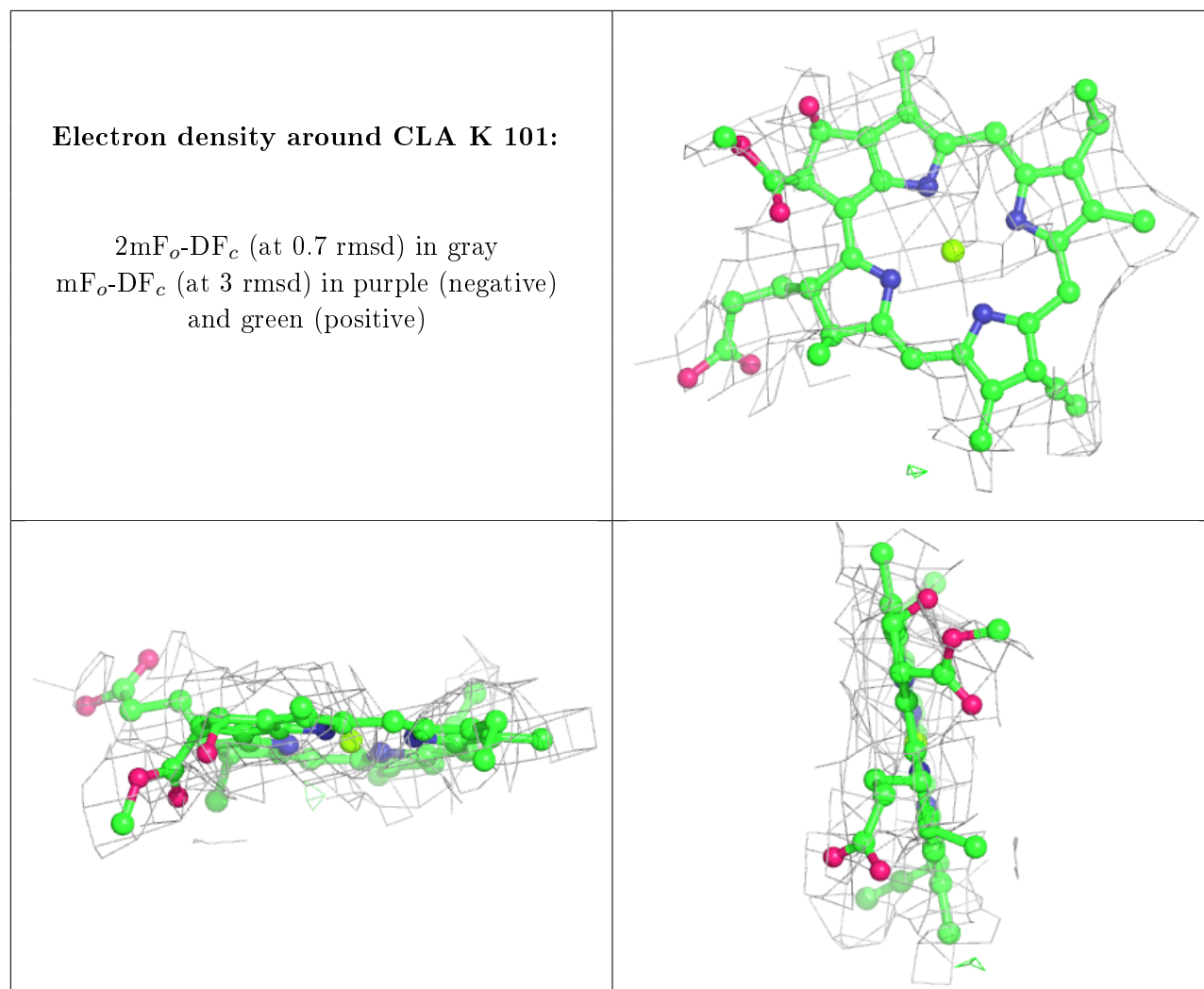
**Electron density around BCR J 102:**

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



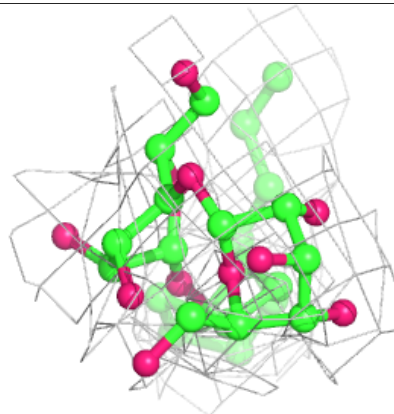
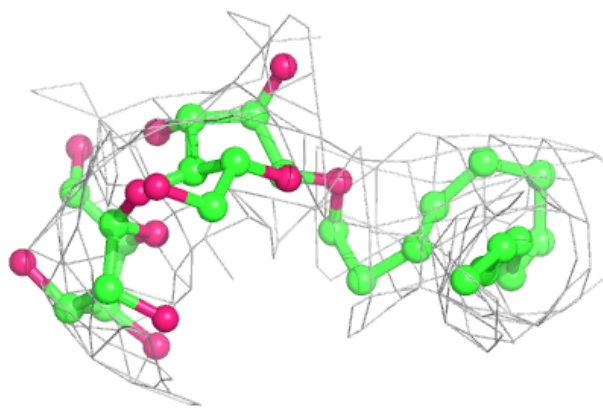
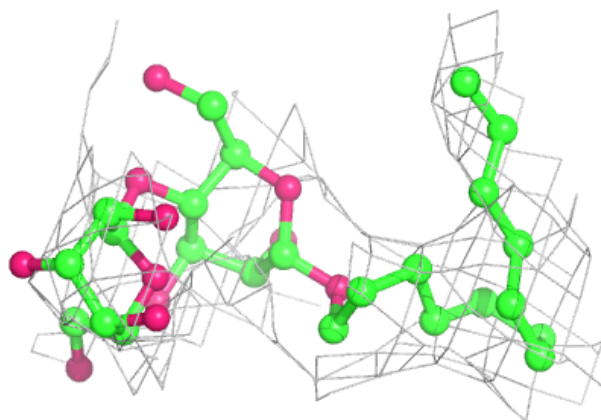






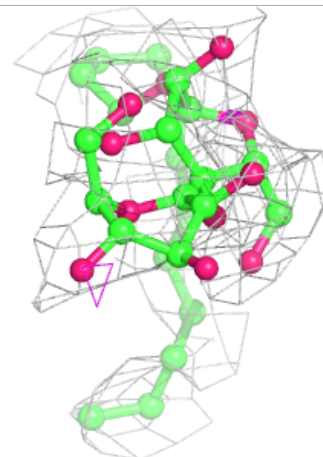
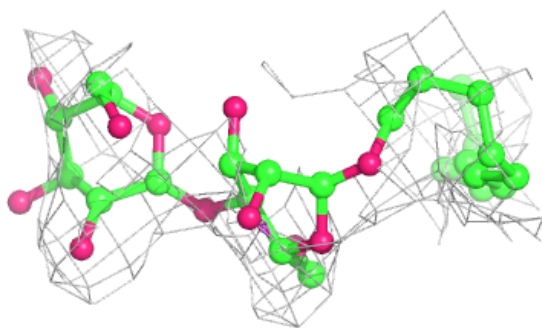
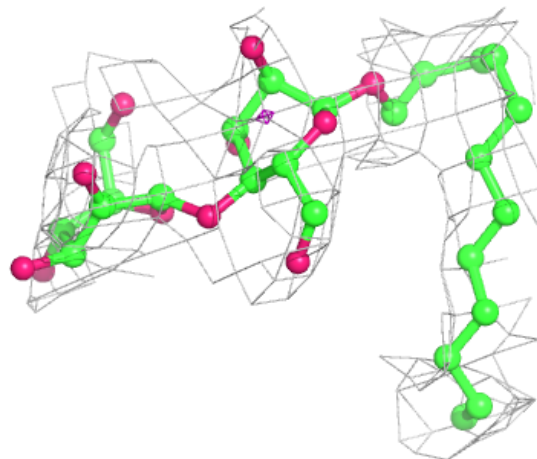
Electron density around LMU H 108:

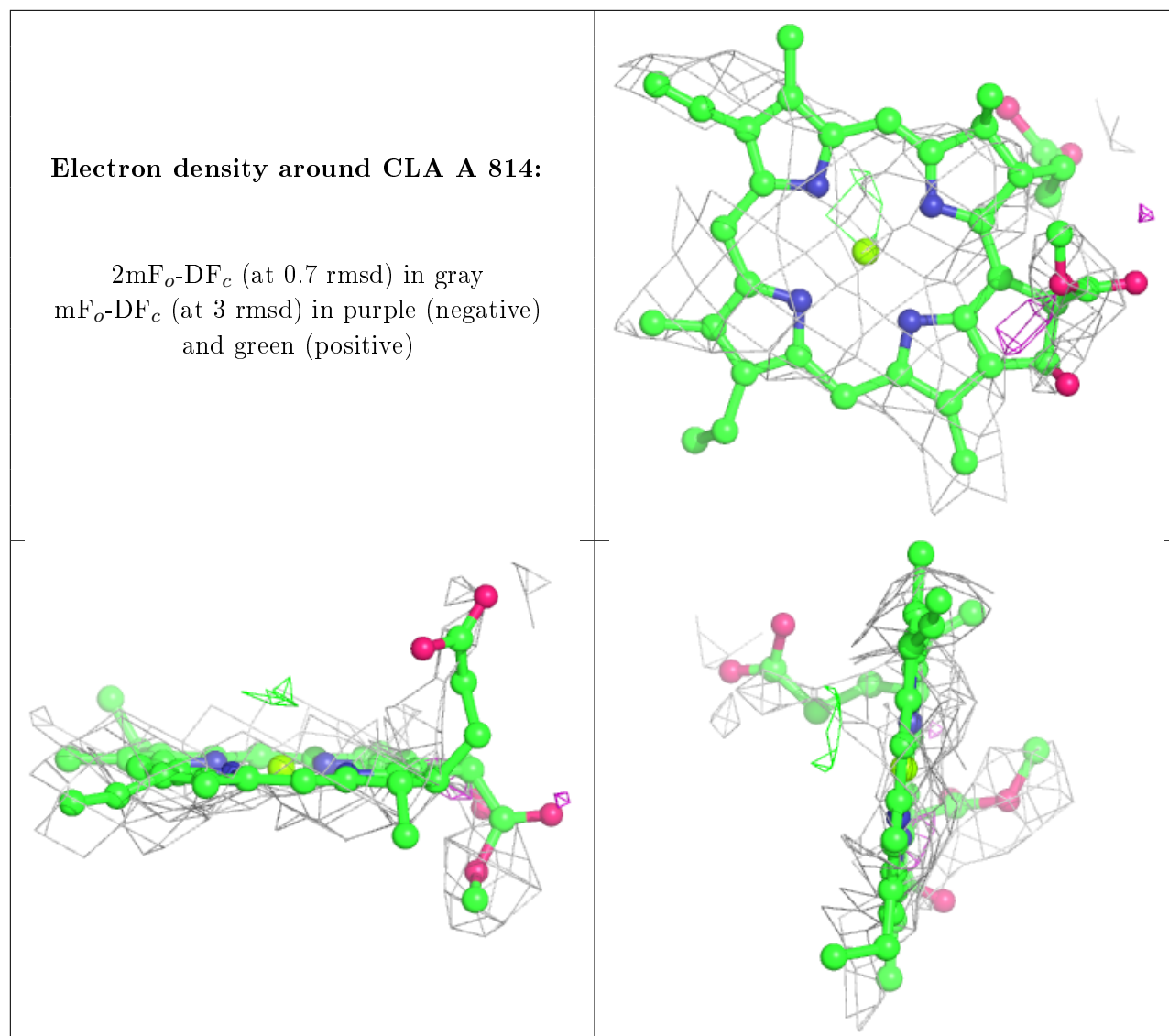
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMU R 101:

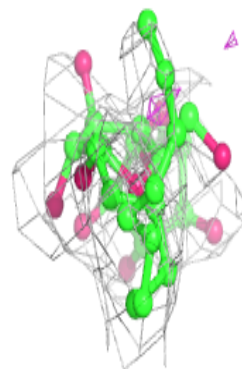
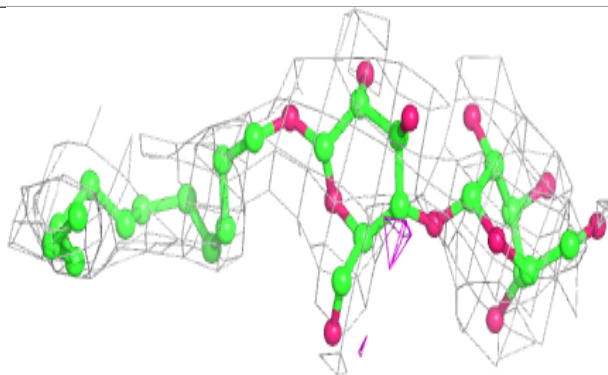
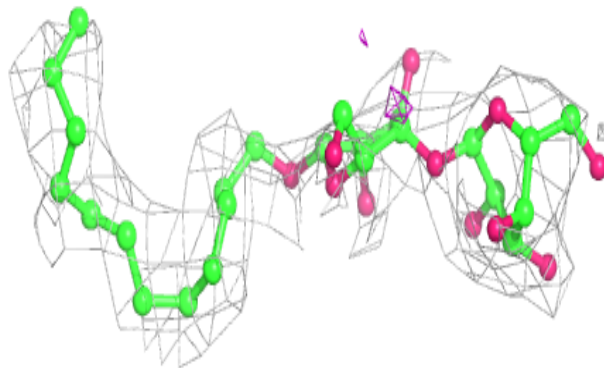
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



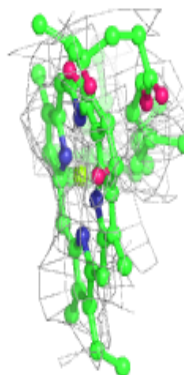
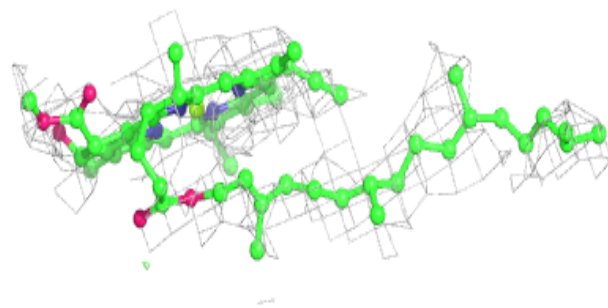
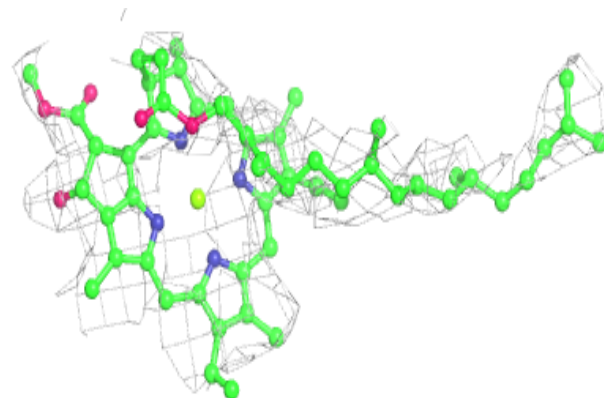


Electron density around LMU A 848:

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

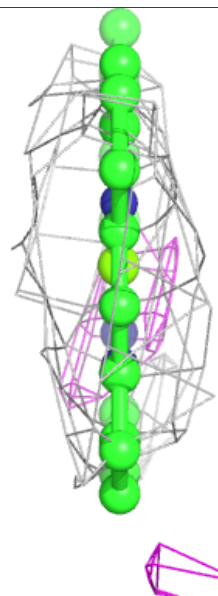
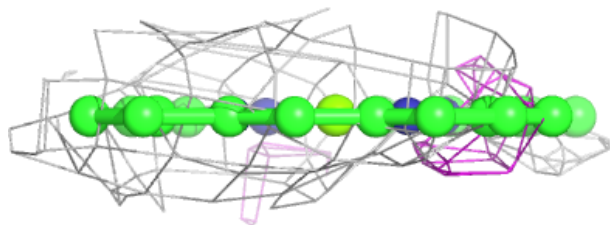
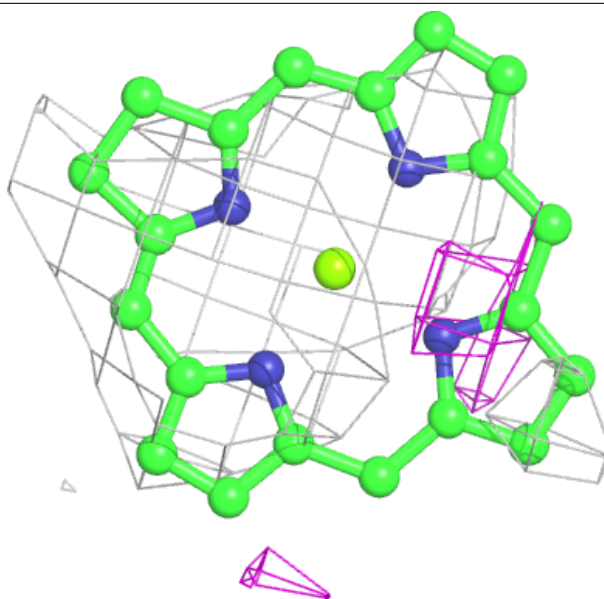
**Electron density around CLA 2 308:**

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



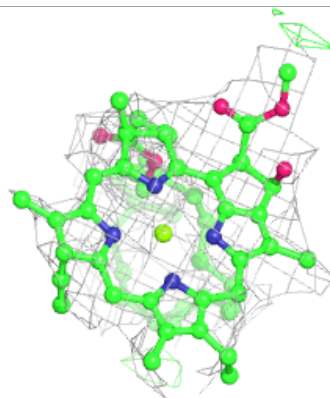
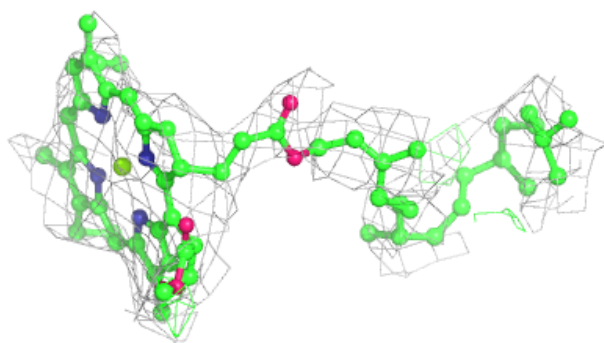
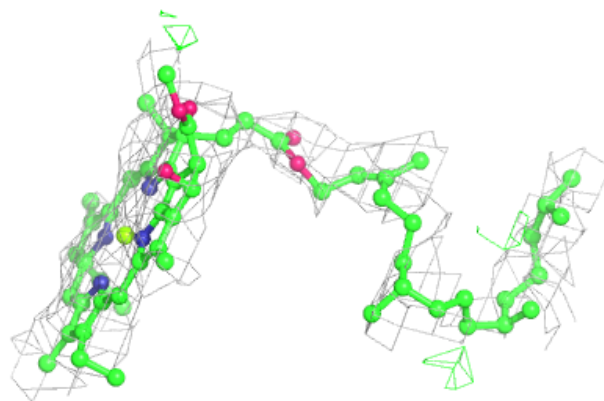
Electron density around CLA 2 301:

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



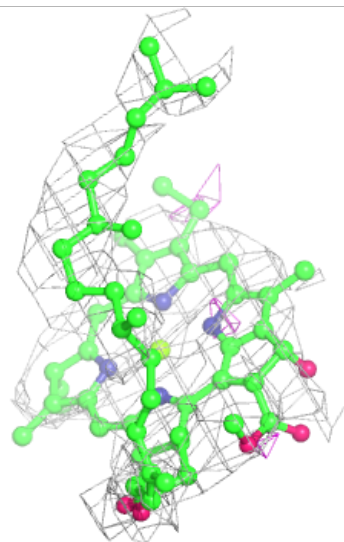
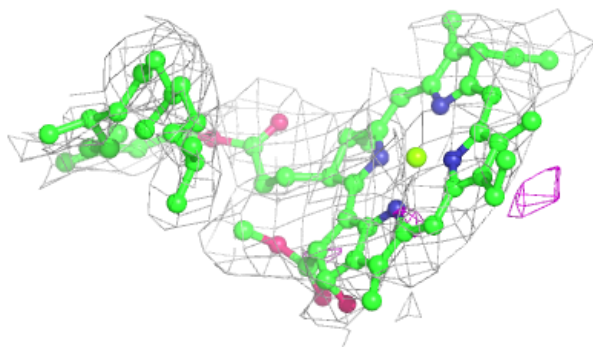
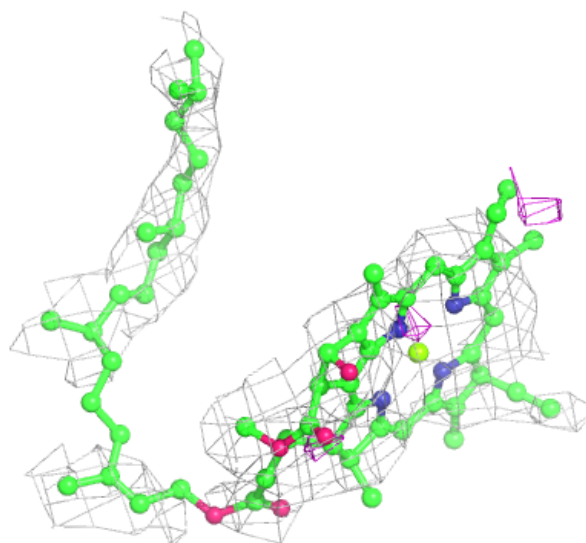
Electron density around CLA 3 311:

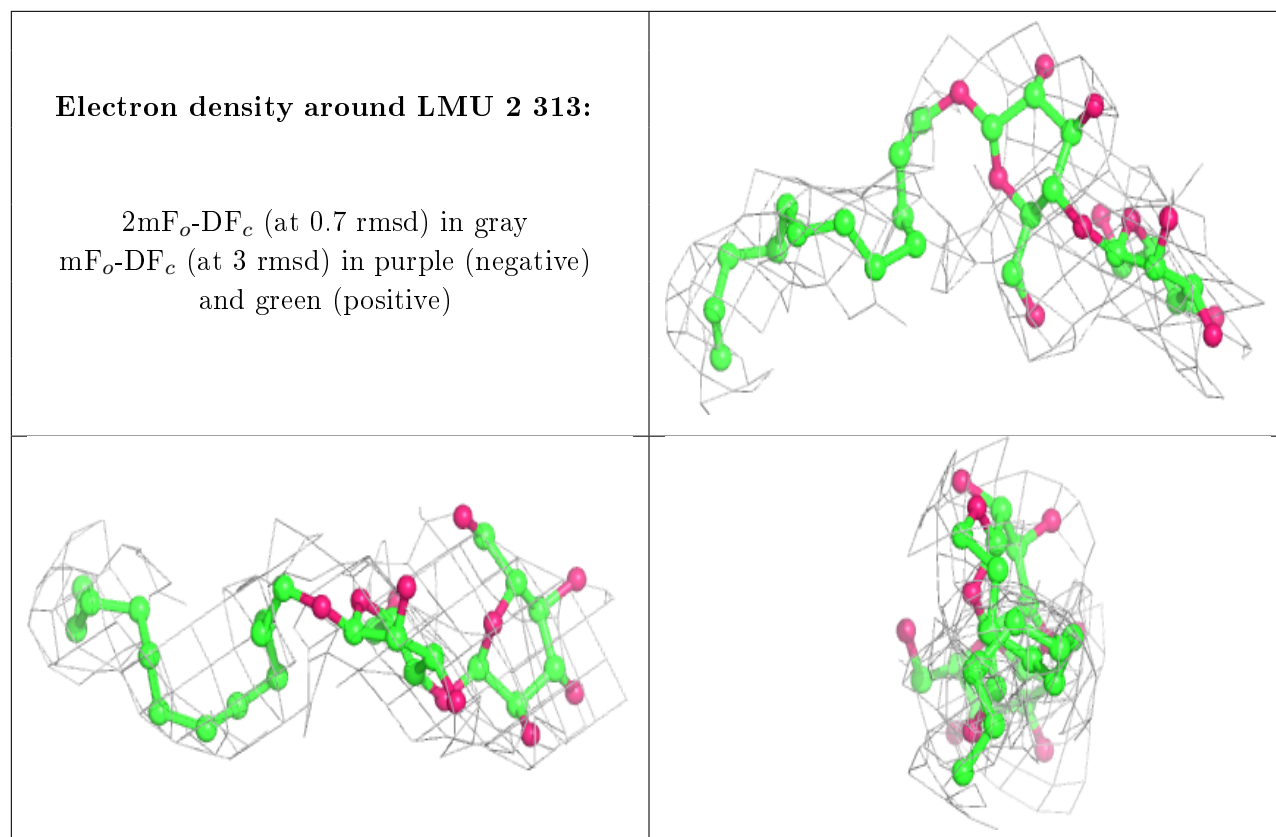
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

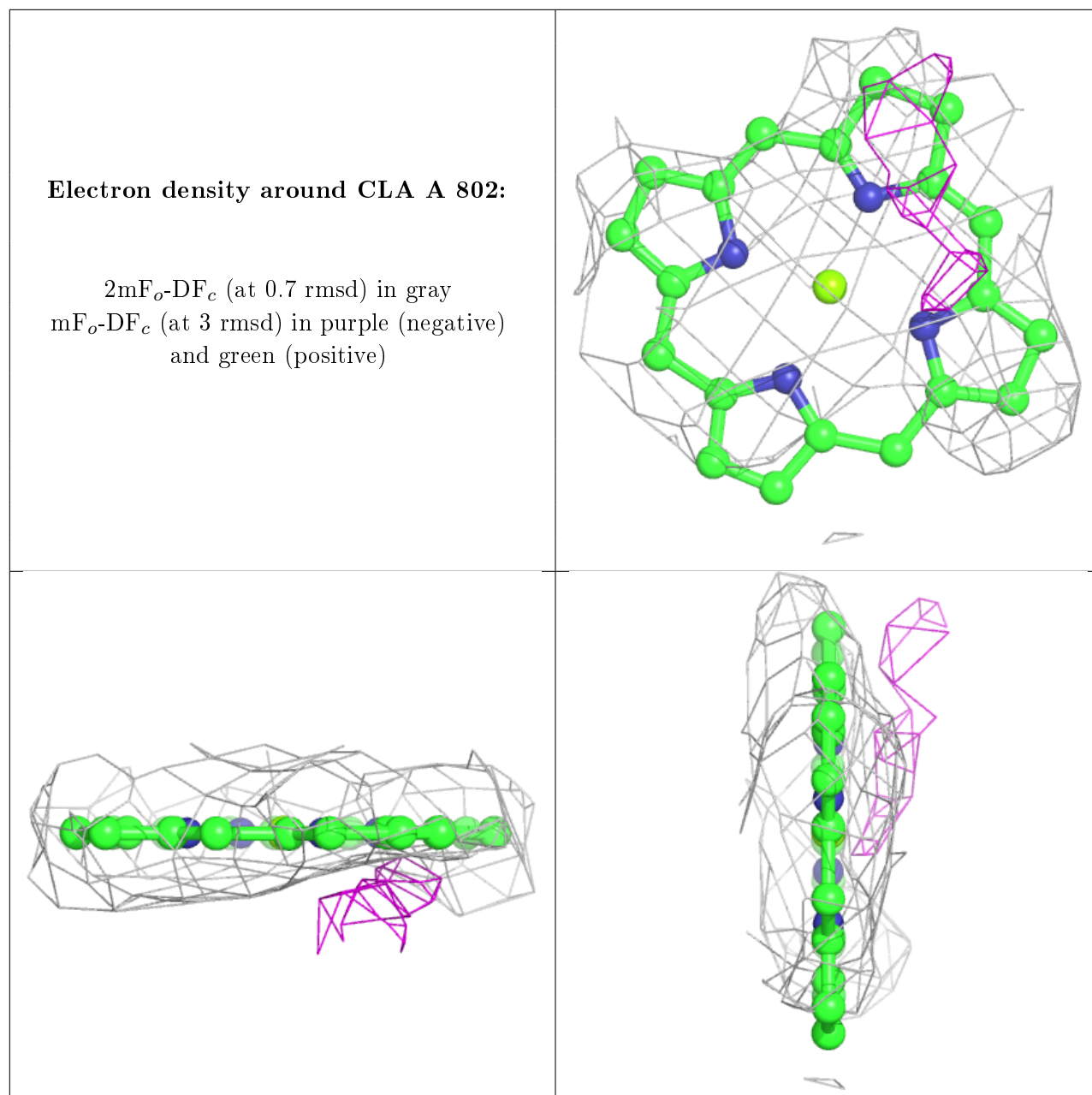


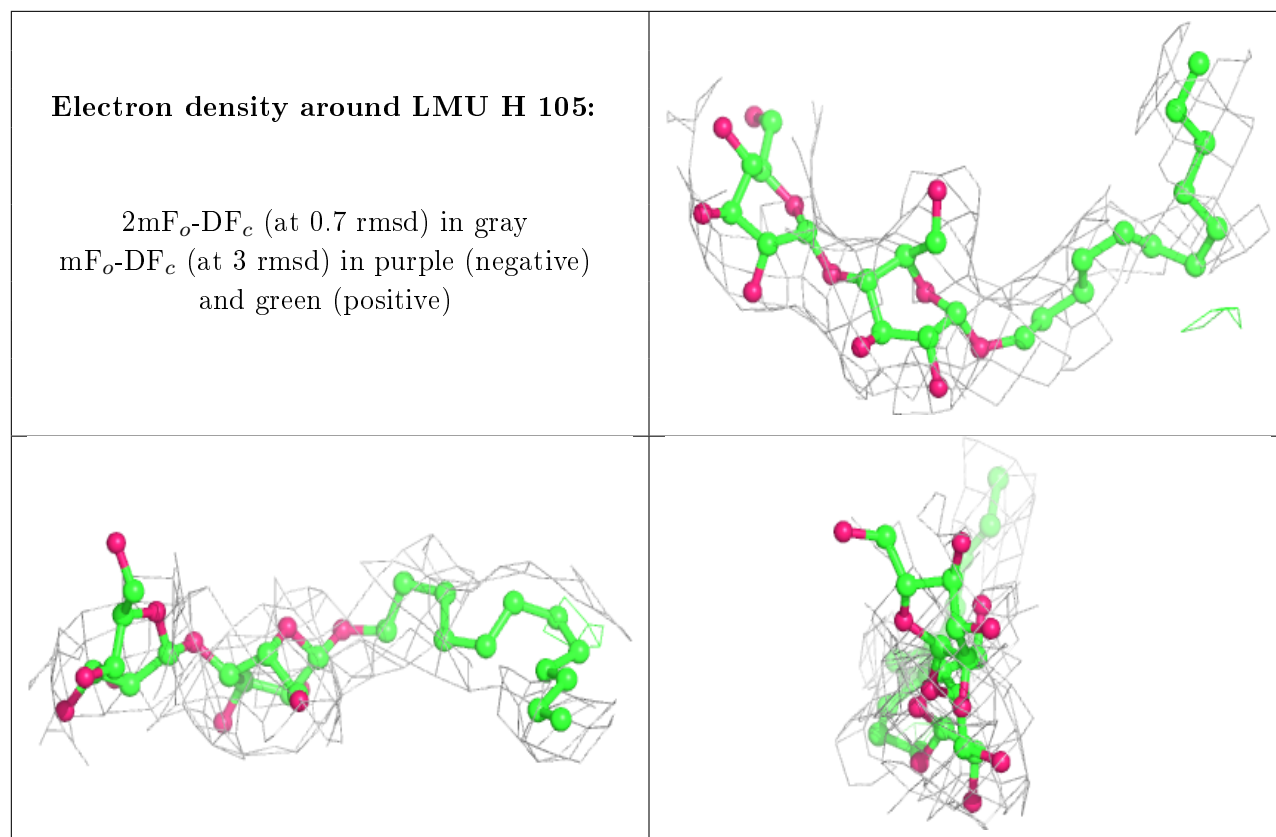
Electron density around CLA 3 313:

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



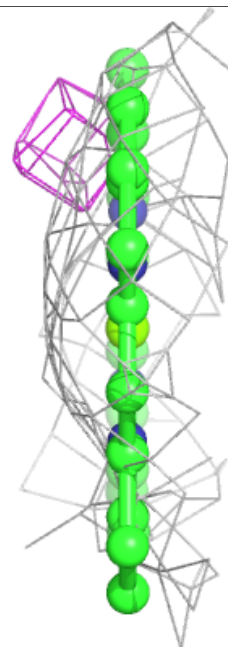
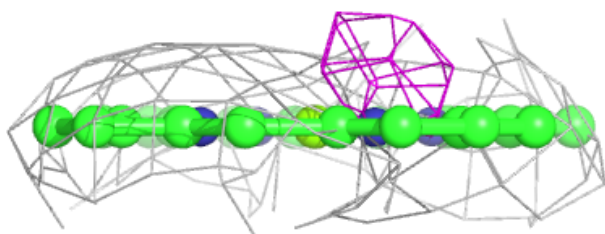
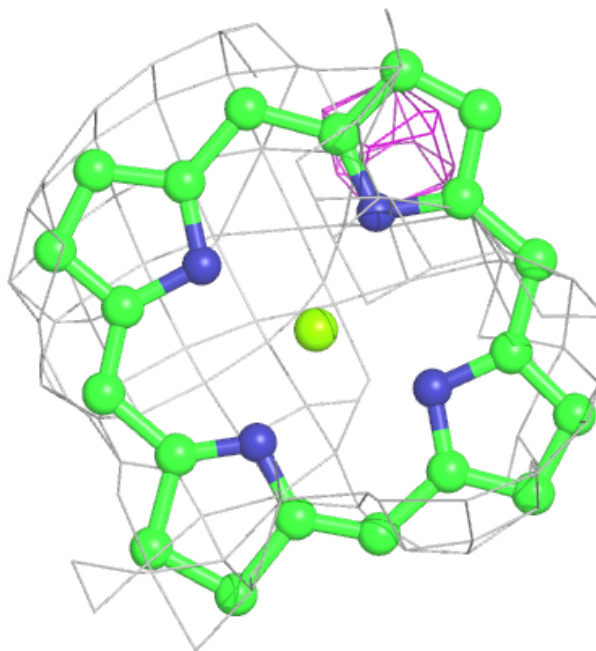


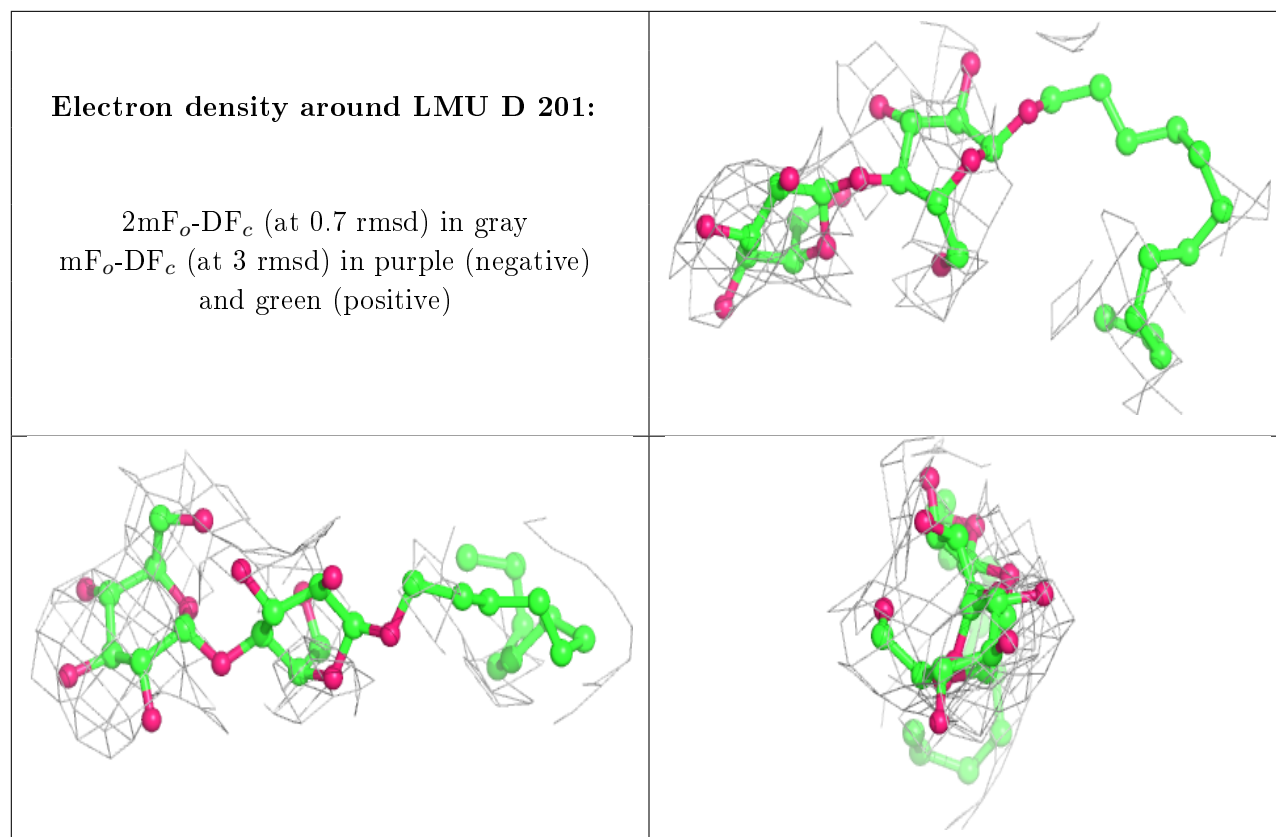


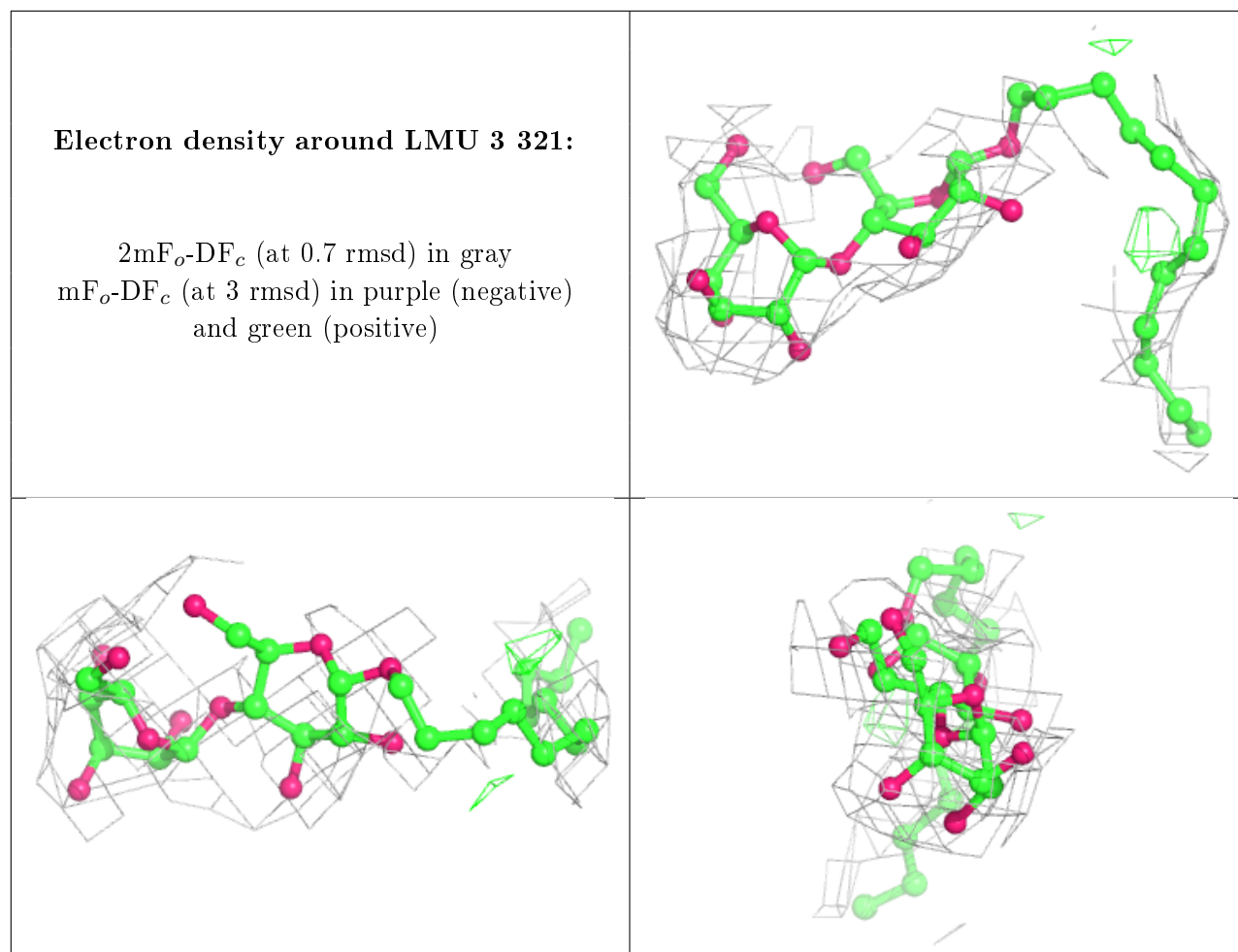


Electron density around CLA 3 309:

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

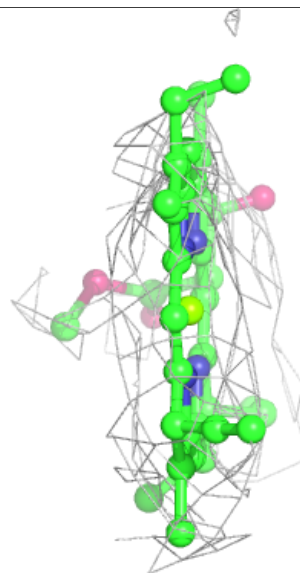
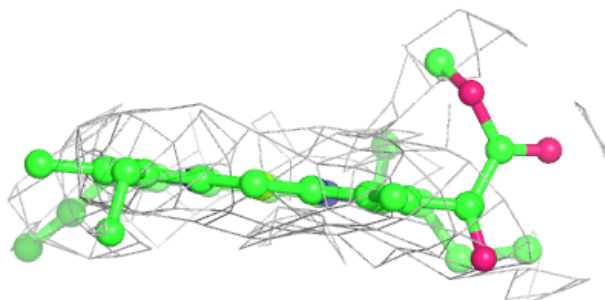
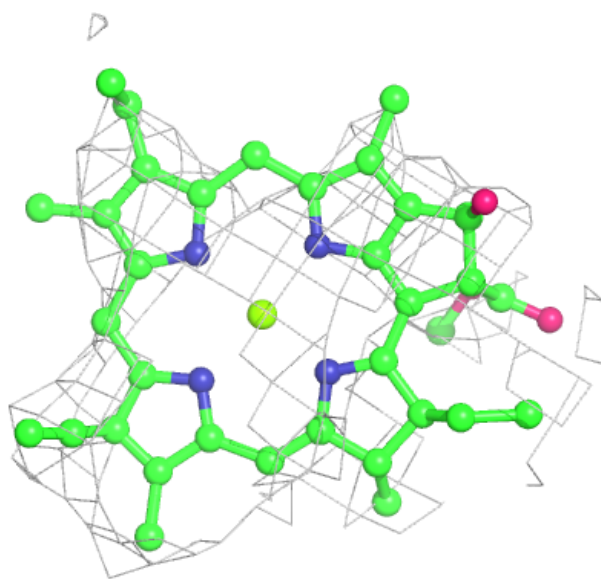






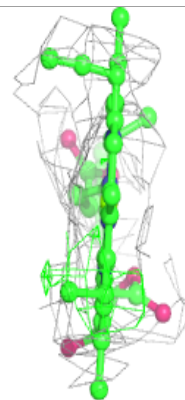
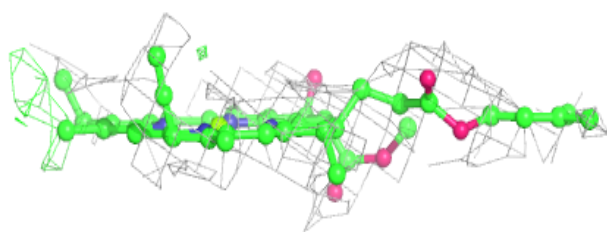
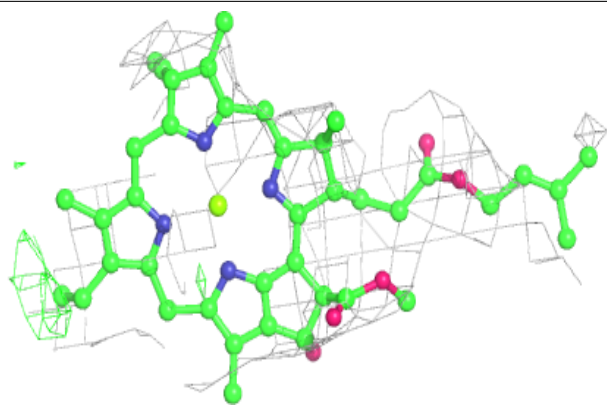
Electron density around CLA 3 308:

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

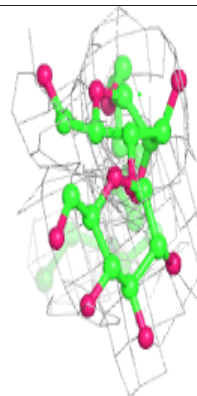
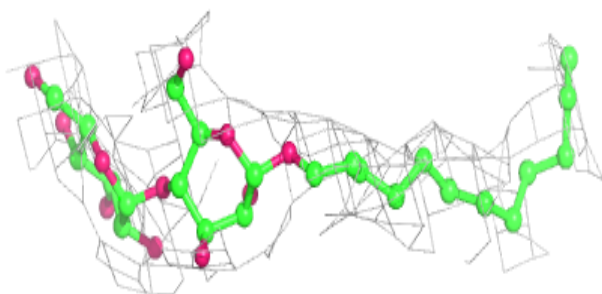
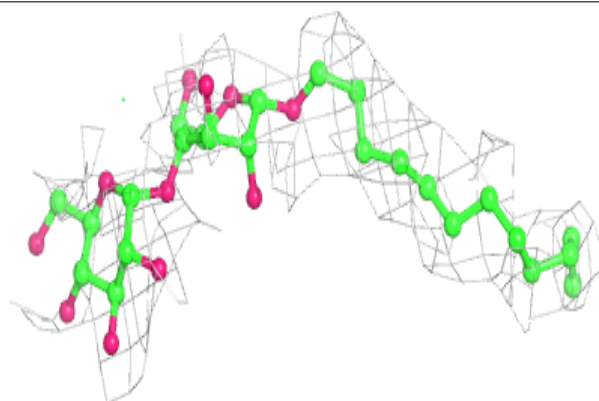


Electron density around CLA A 840:

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

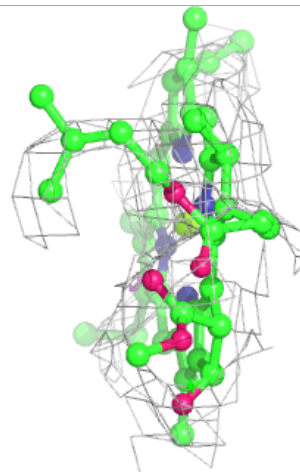
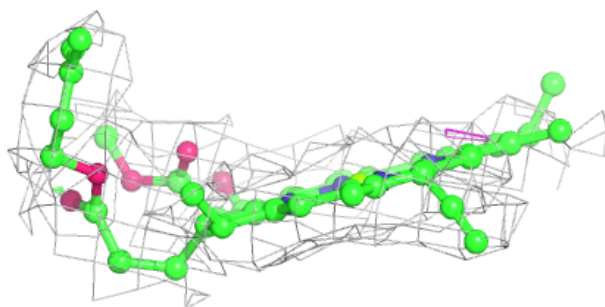
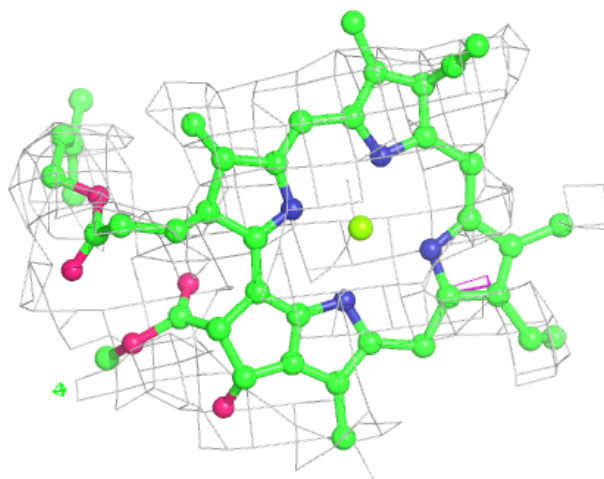
**Electron density around LMU 4 317:**

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



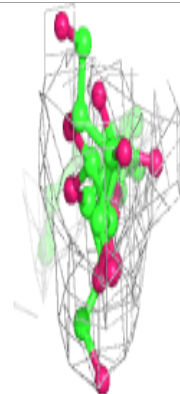
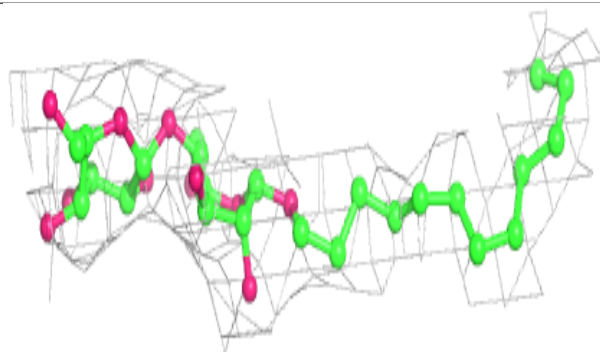
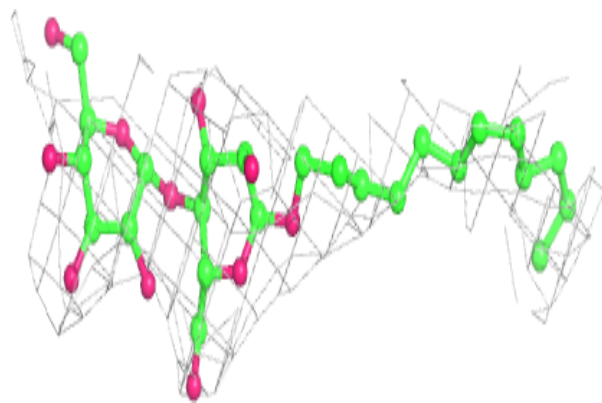
Electron density around CLA 3 317:

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



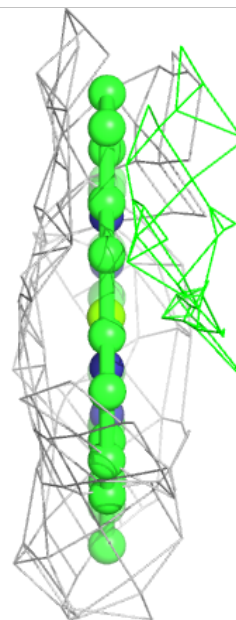
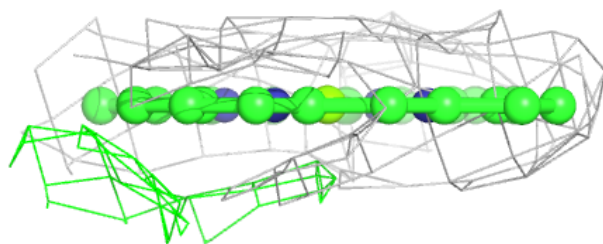
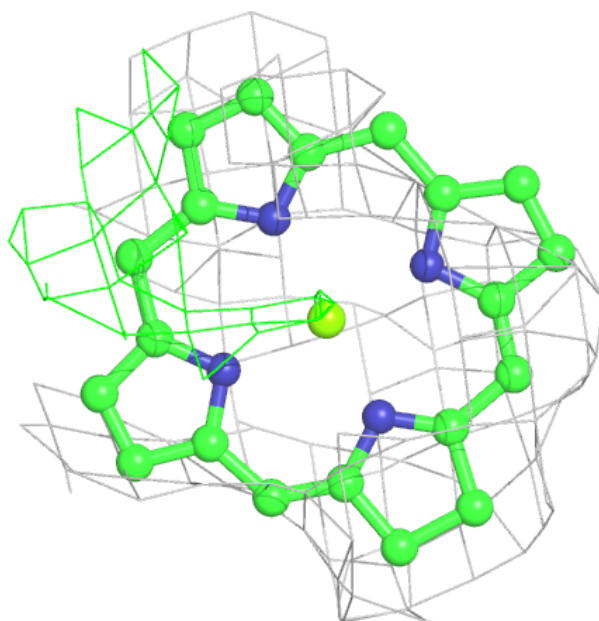
Electron density around LMU H 107:

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



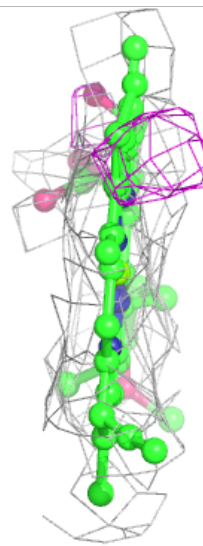
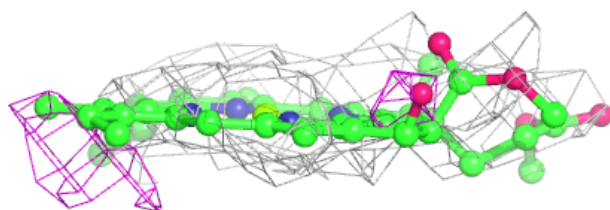
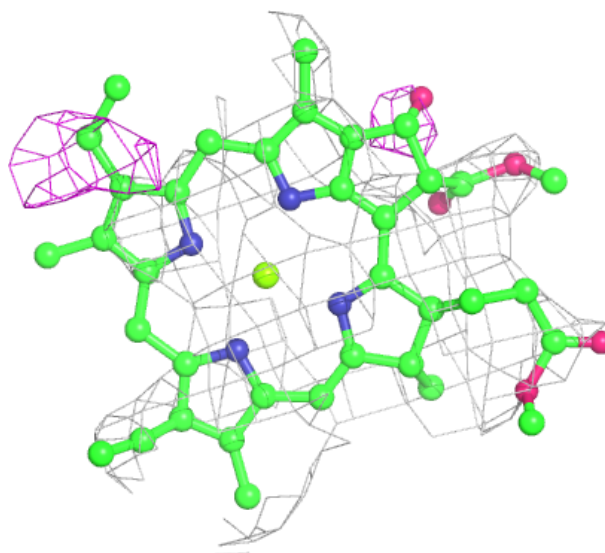
Electron density around CLA 2 306:

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



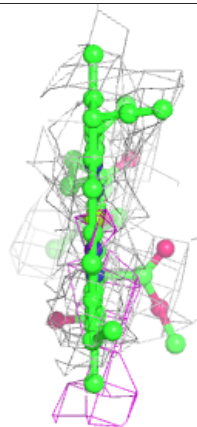
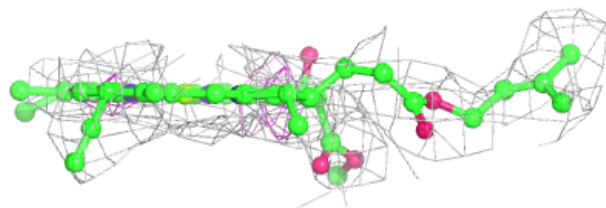
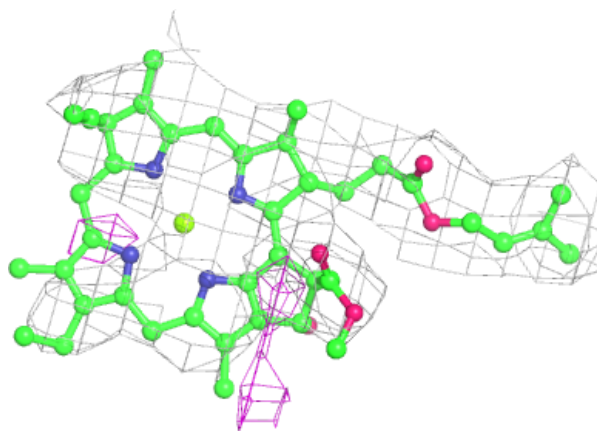
Electron density around CLA B 814:

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



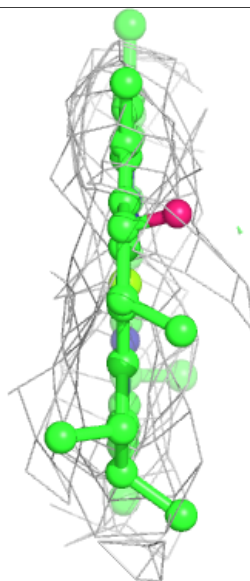
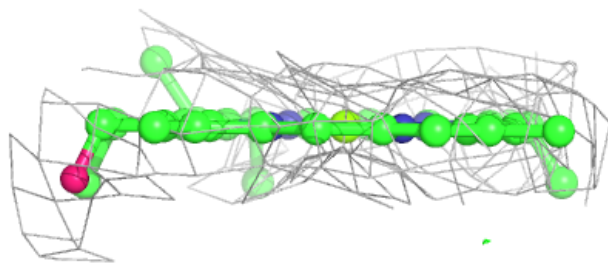
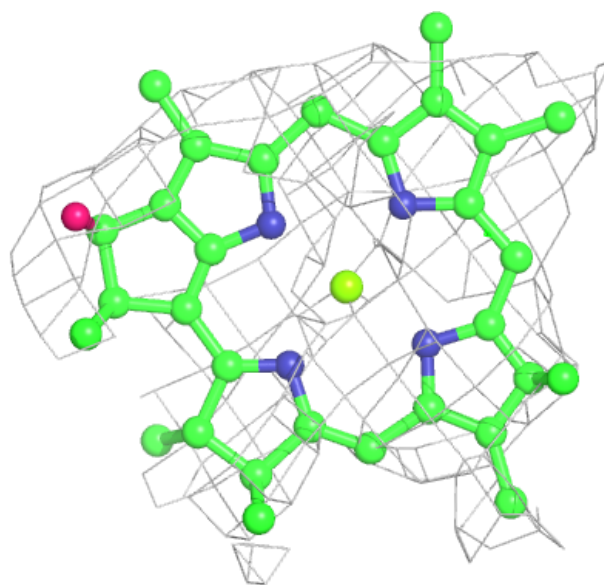
Electron density around CLA 4 306:

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



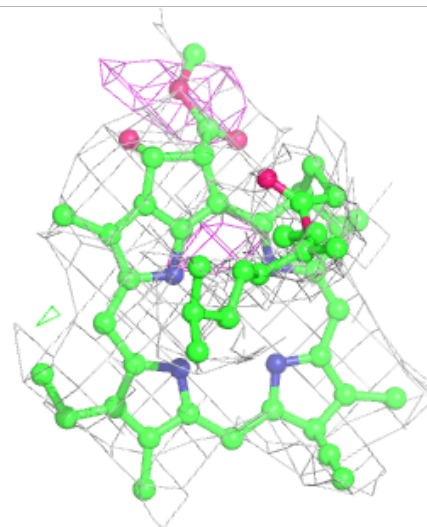
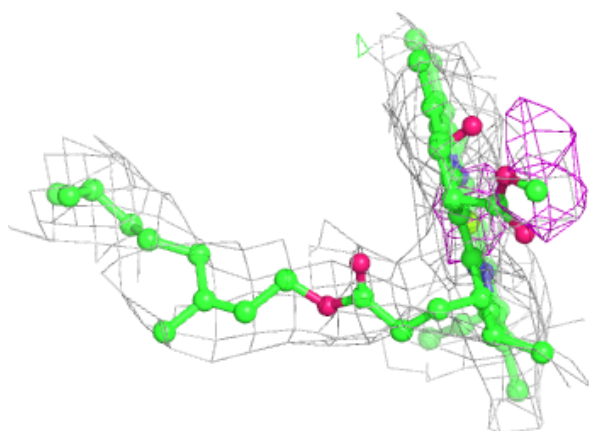
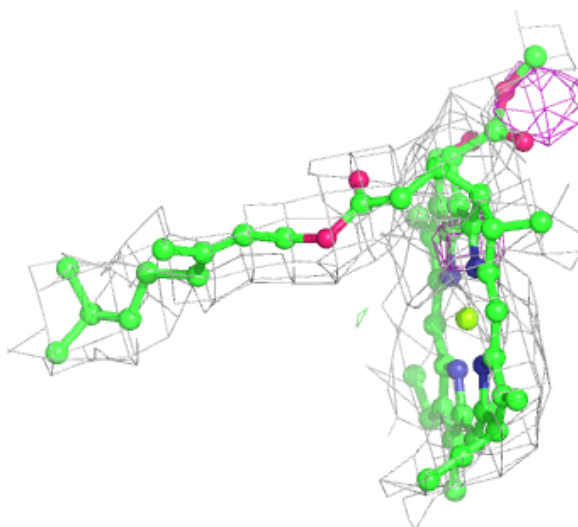
Electron density around CLA 4 308:

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



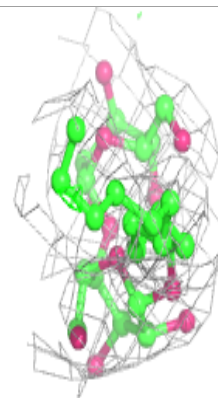
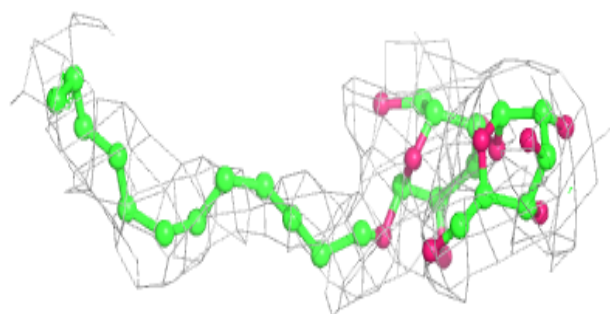
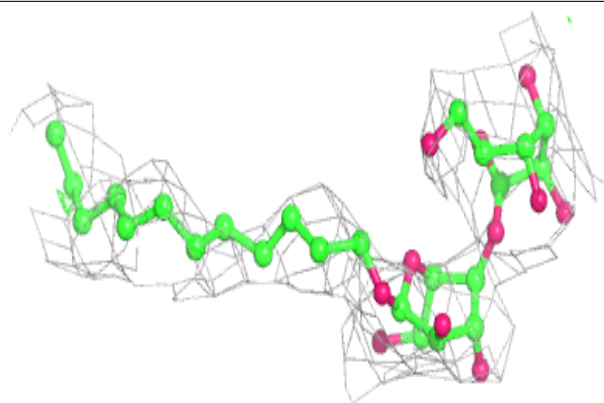
Electron density around CLA 4 302:

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

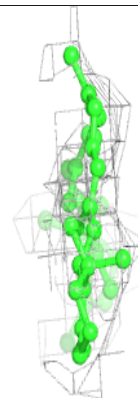
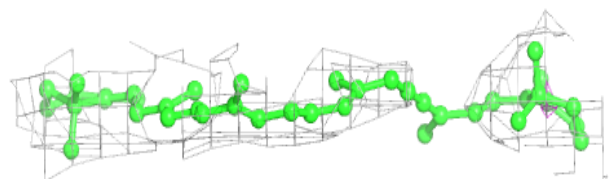
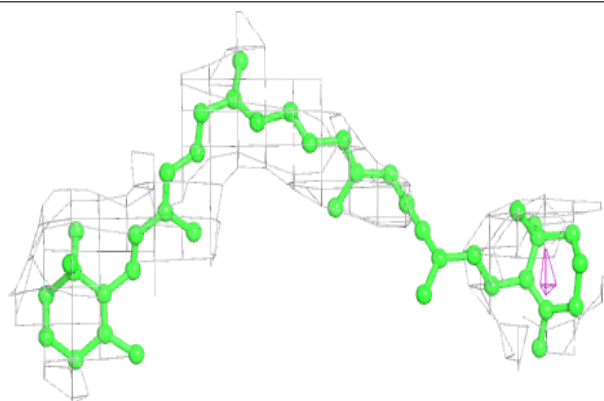


Electron density around LMU 1 213:

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

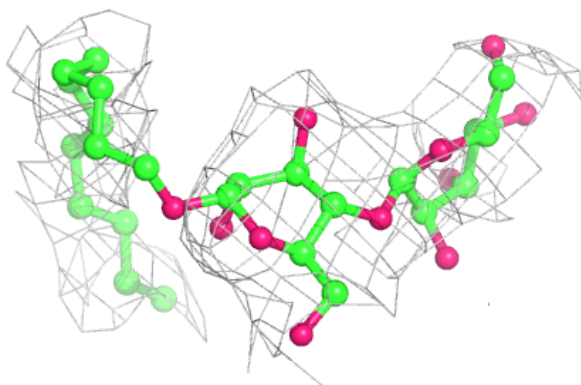
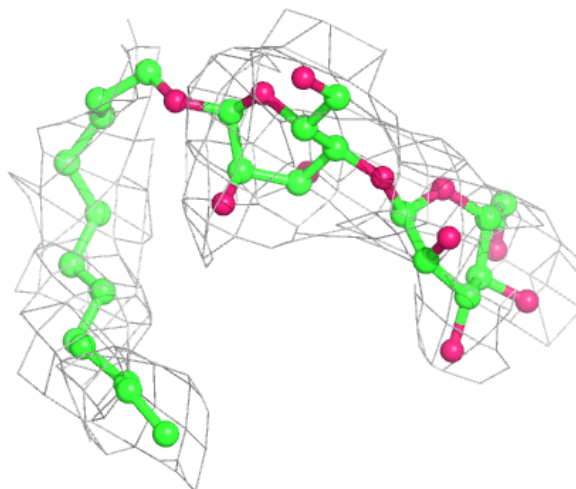
**Electron density around BCR 3 314:**

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



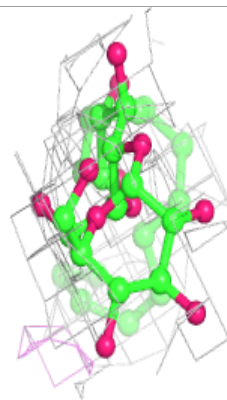
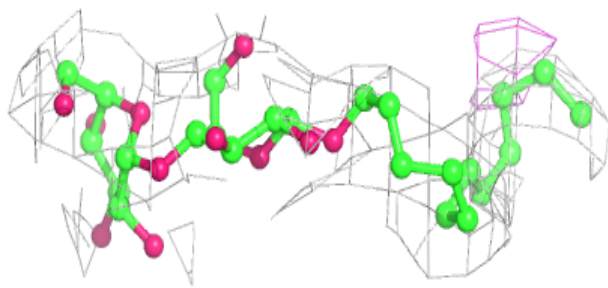
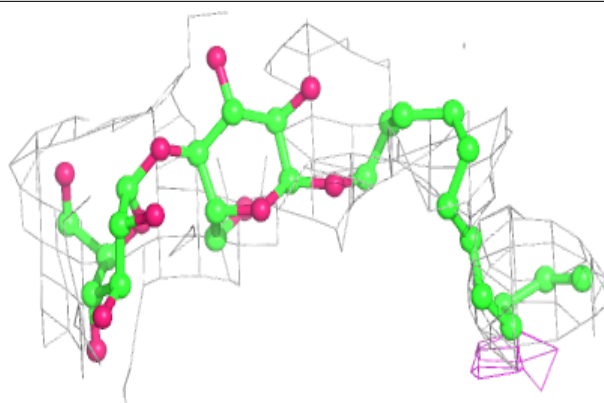
Electron density around LMU 1 220:

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

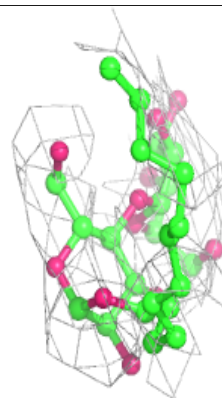
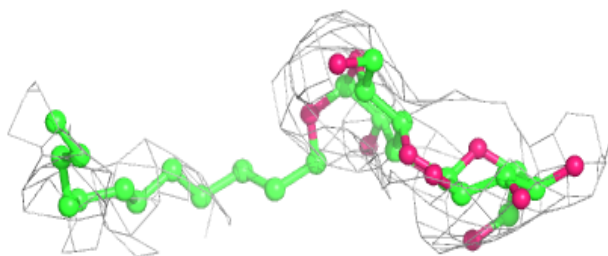
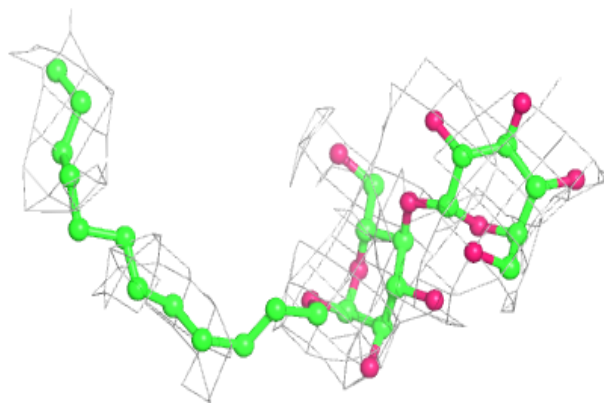


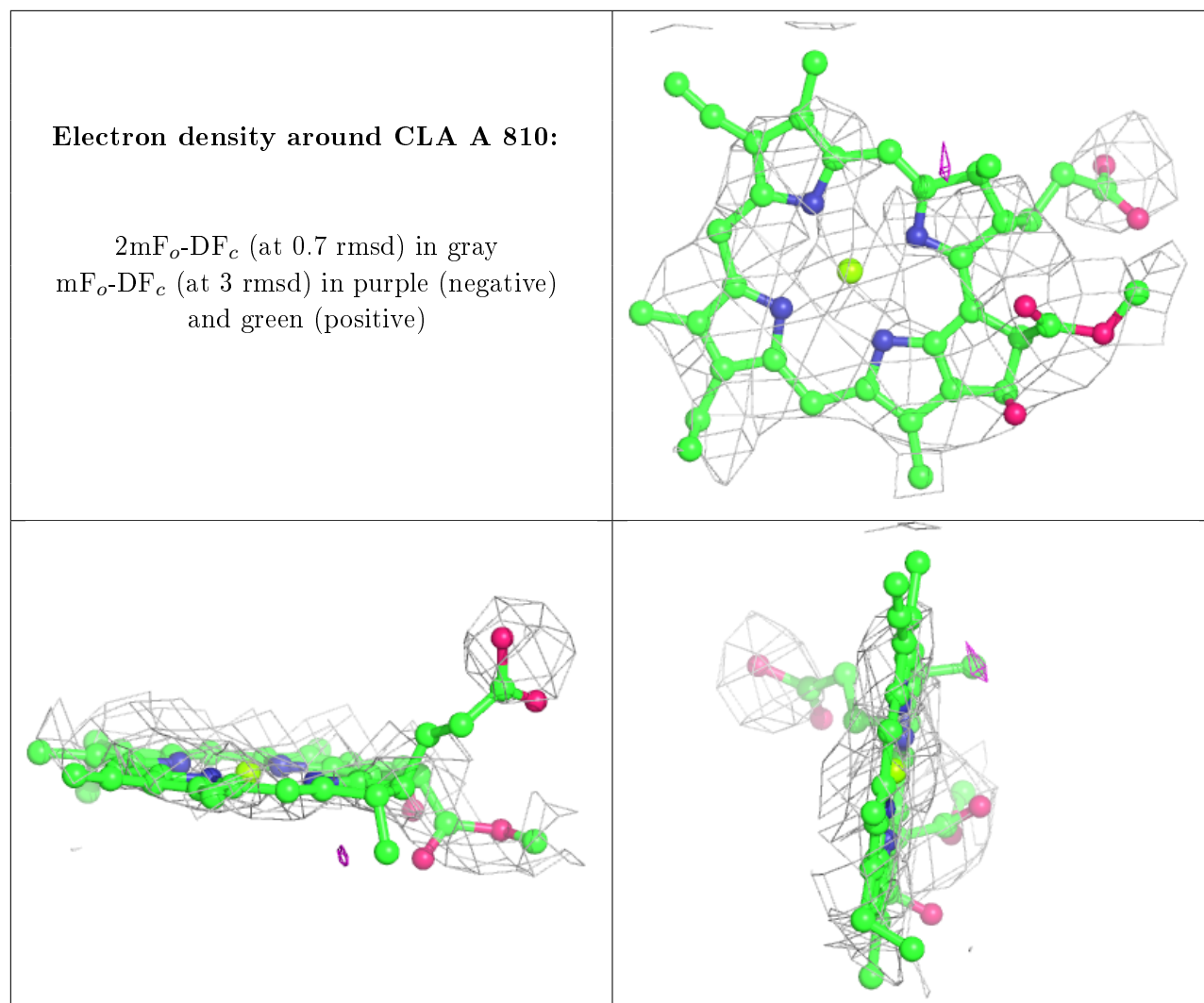
Electron density around LMU R 109:

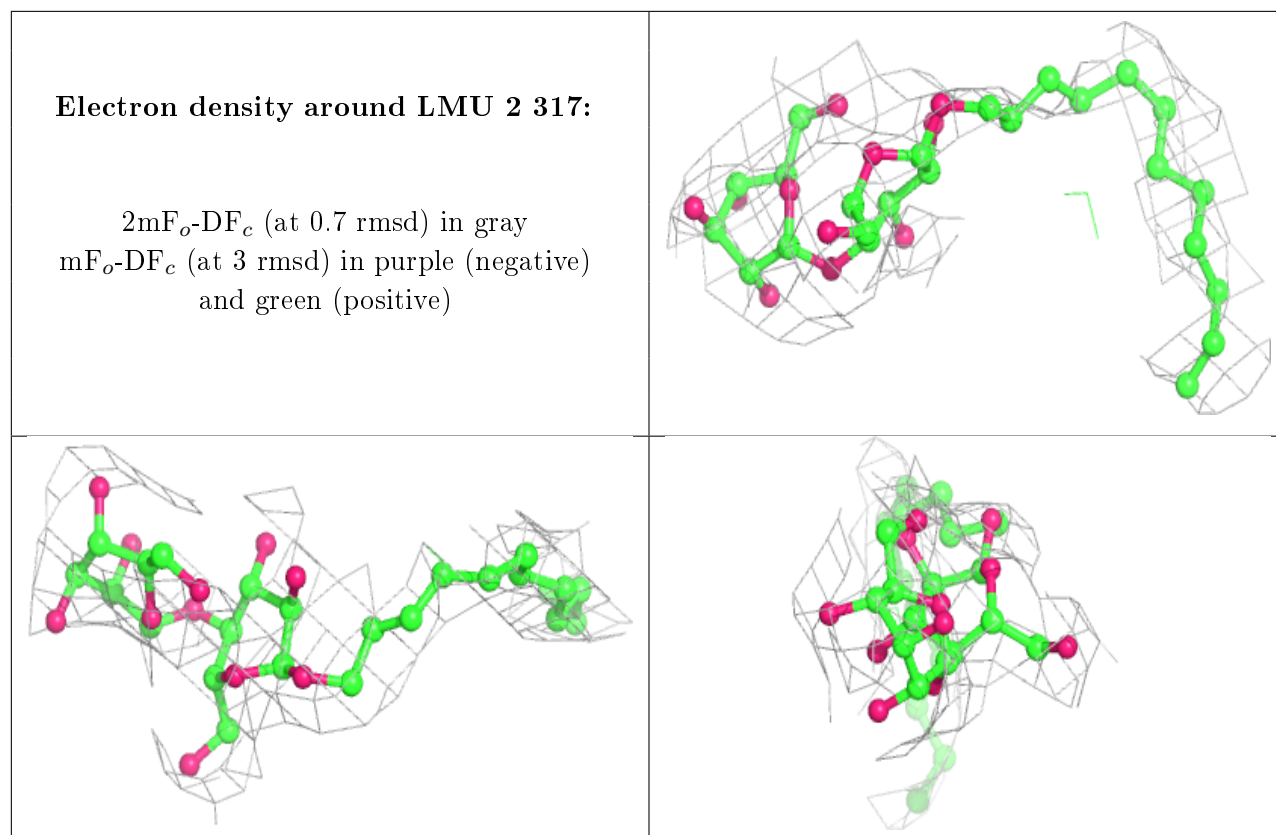
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around LMU 1 217:**

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

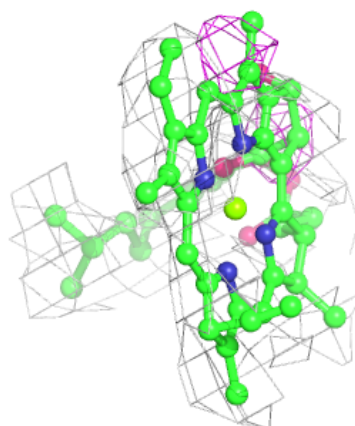
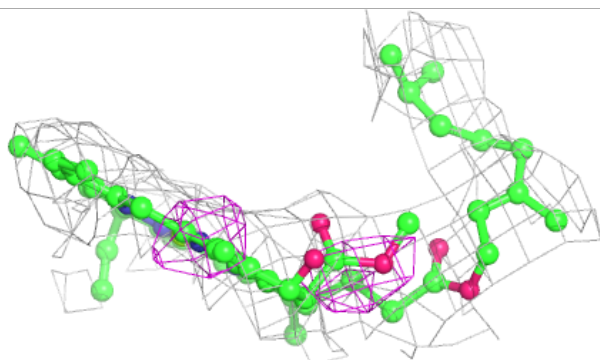
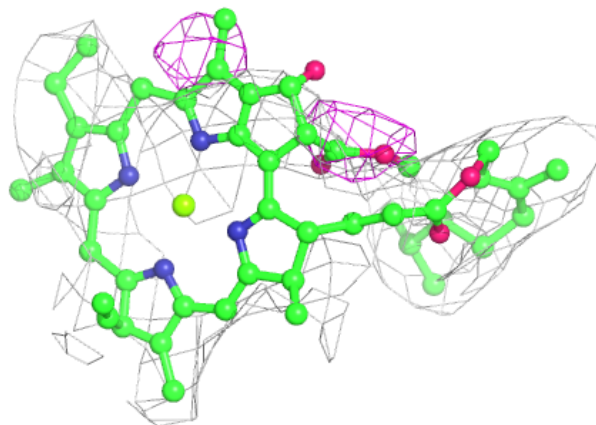


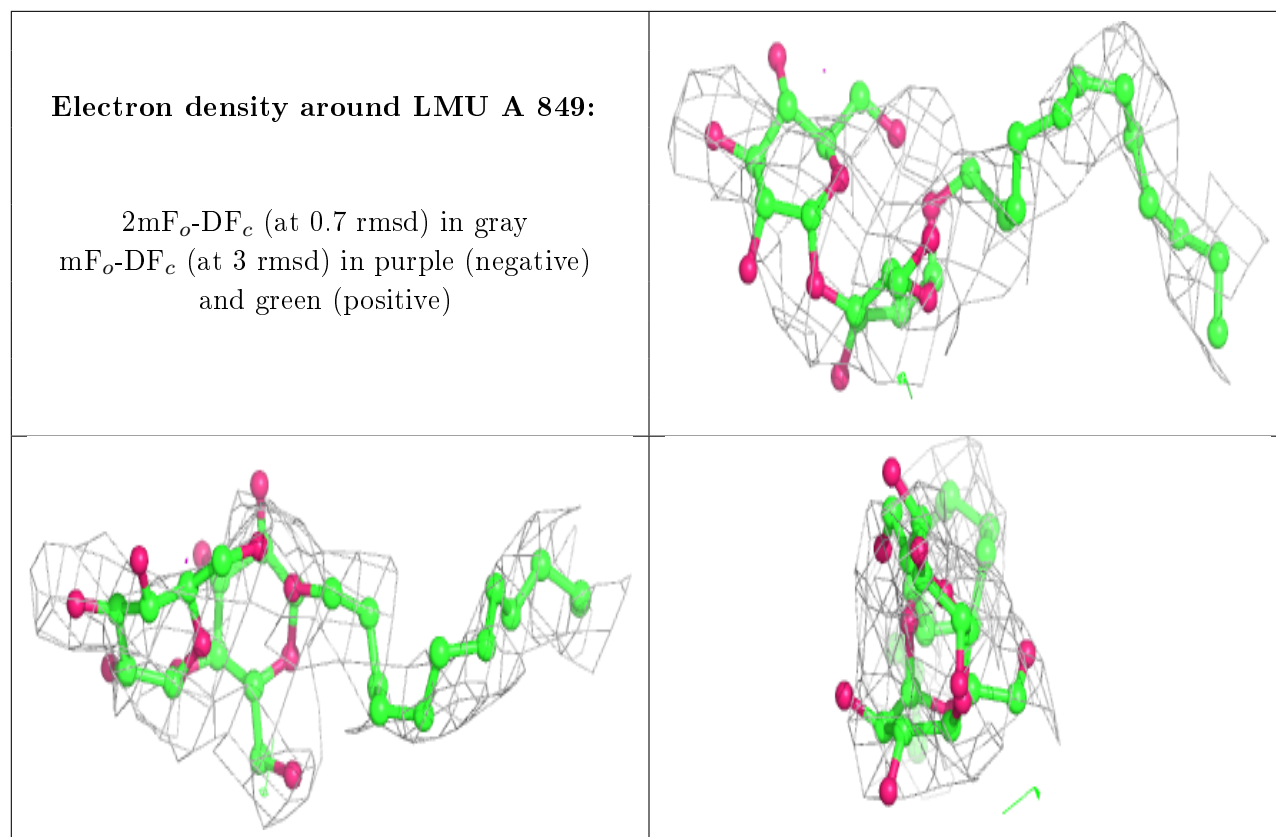




Electron density around CLA L 201:

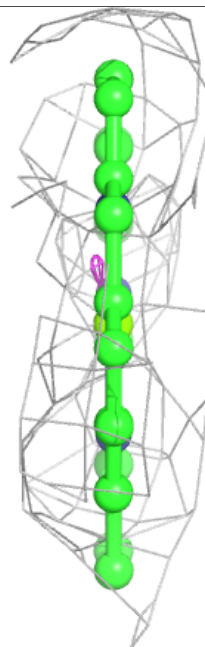
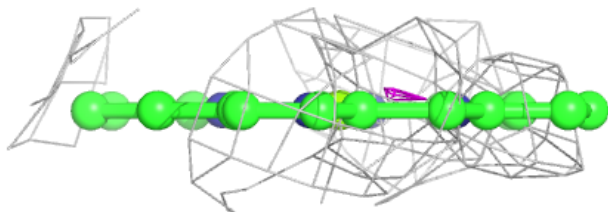
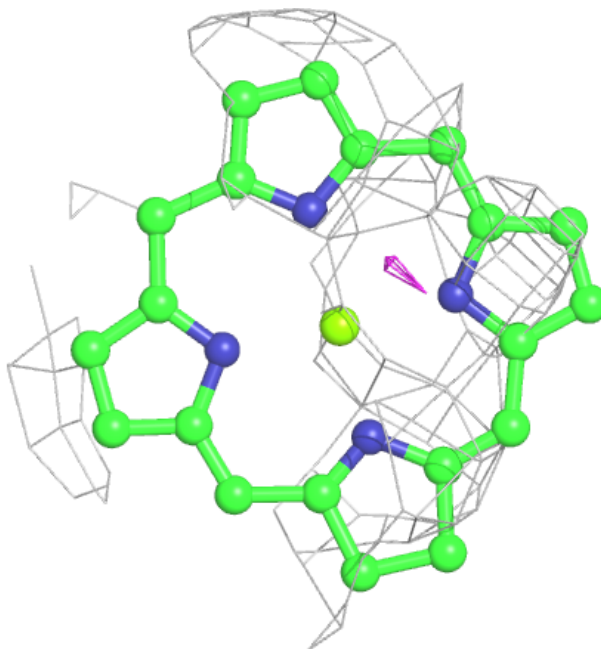
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

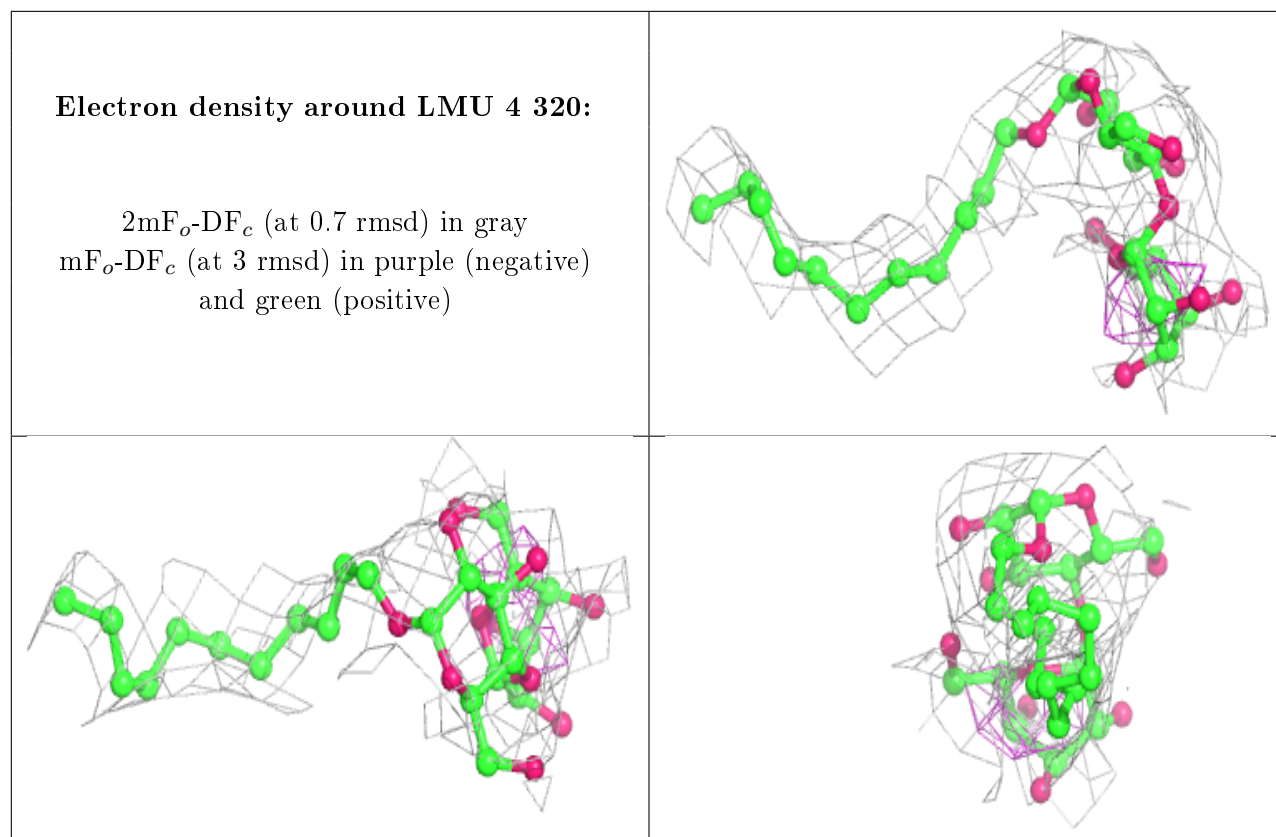




Electron density around CLA 3 307:

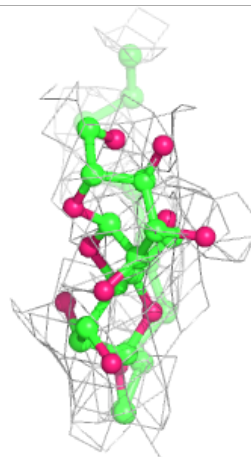
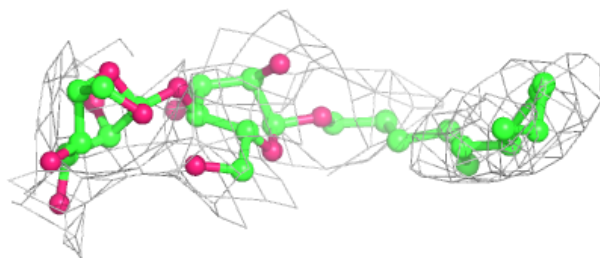
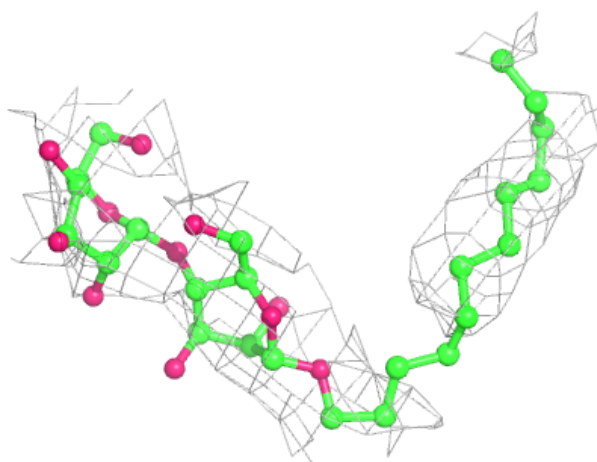
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





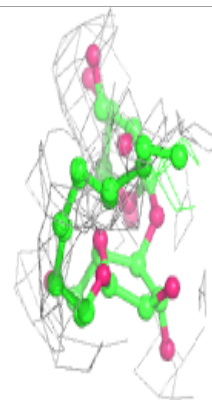
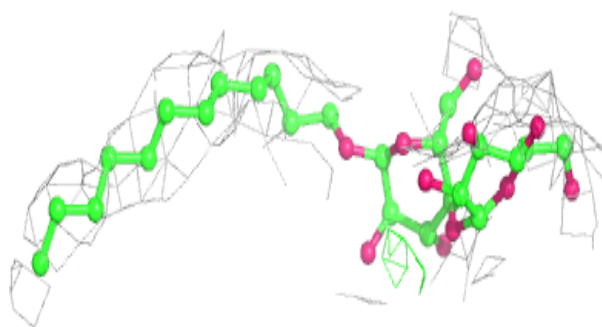
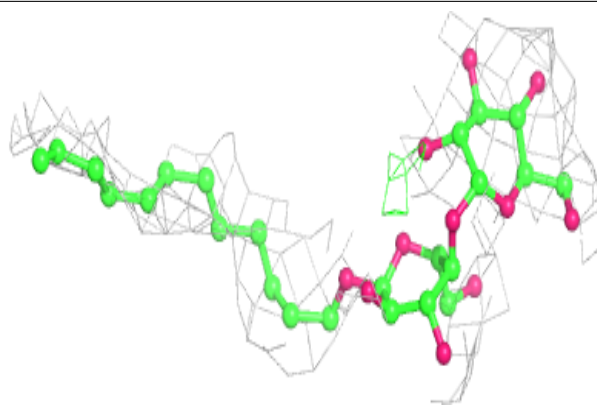
Electron density around LMU K 104:

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

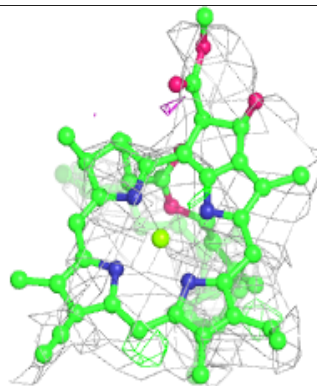
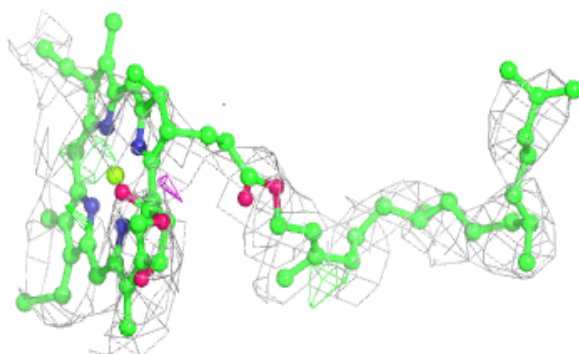
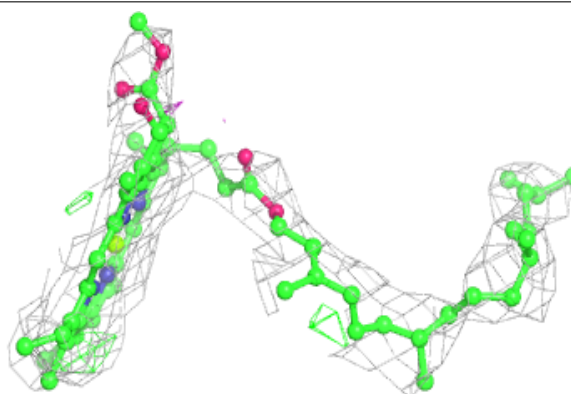


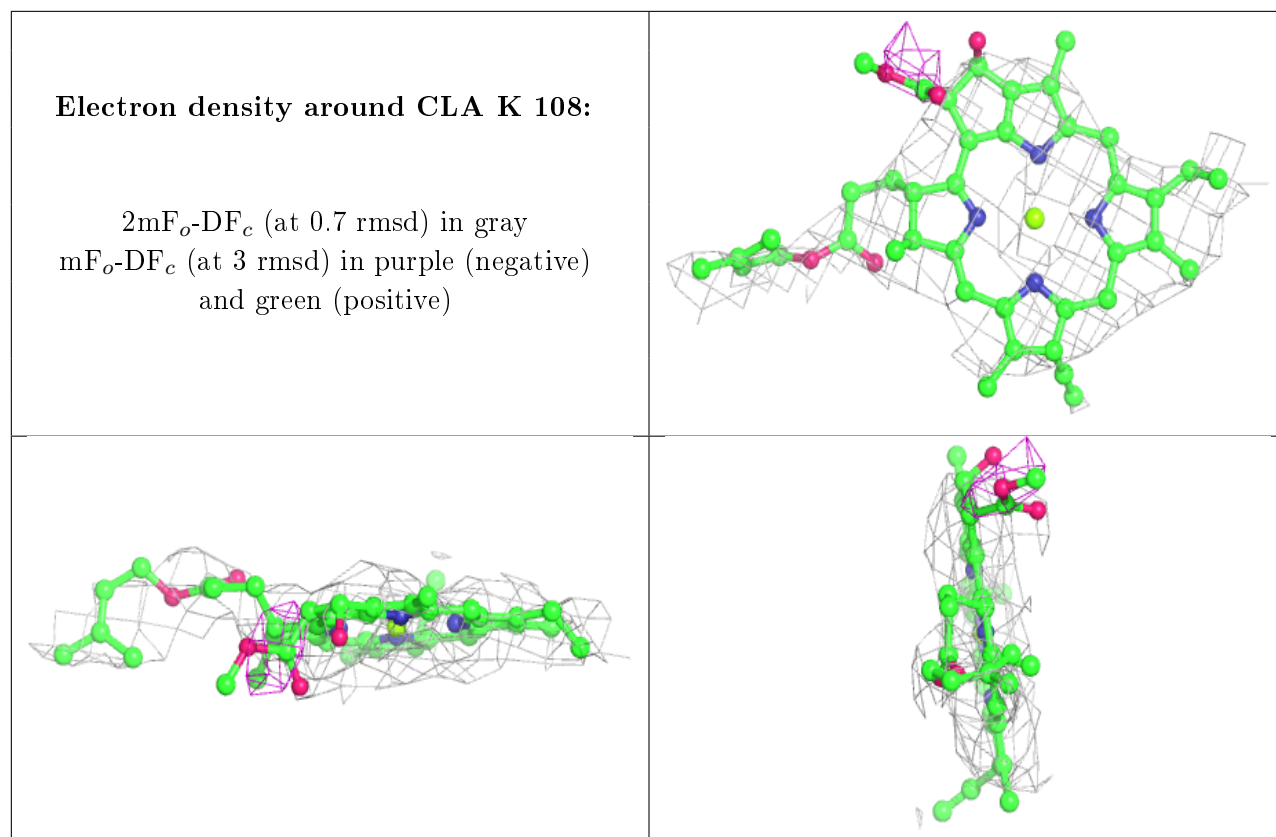
Electron density around LMU R 105:

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

**Electron density around CLA B 838:**

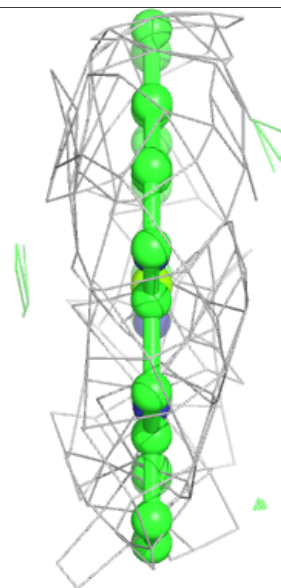
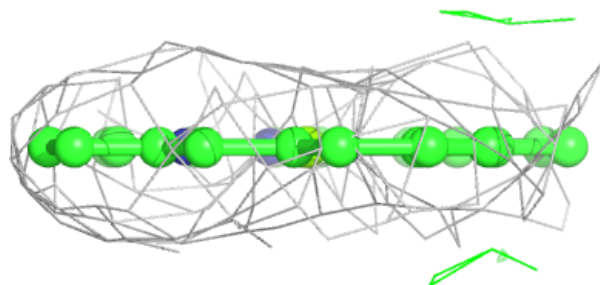
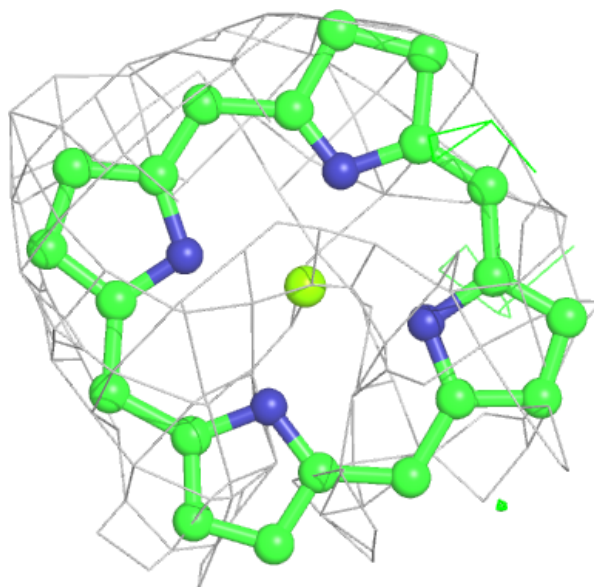
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





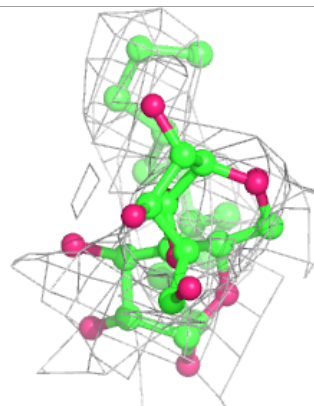
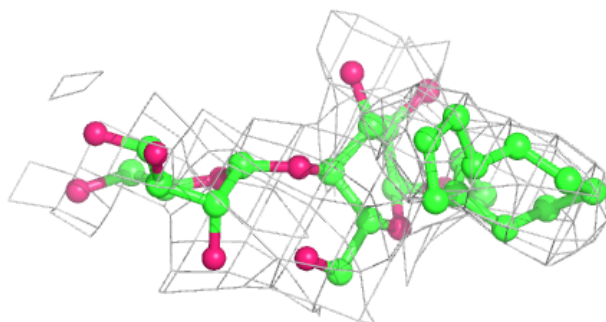
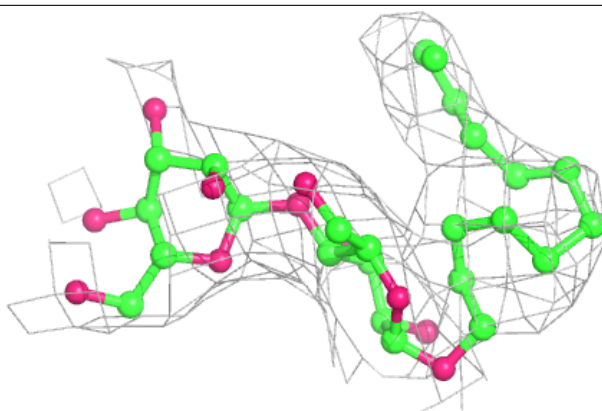
Electron density around CLA 1 211:

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

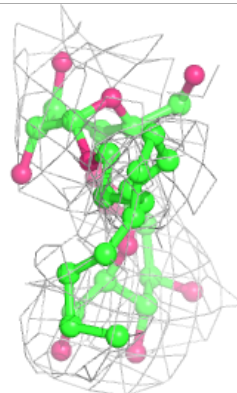
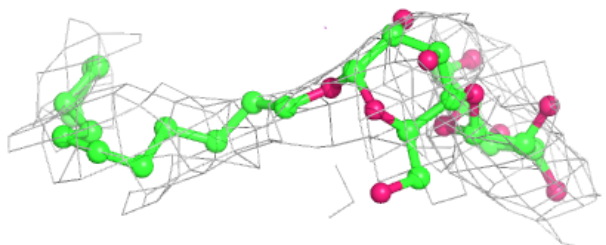
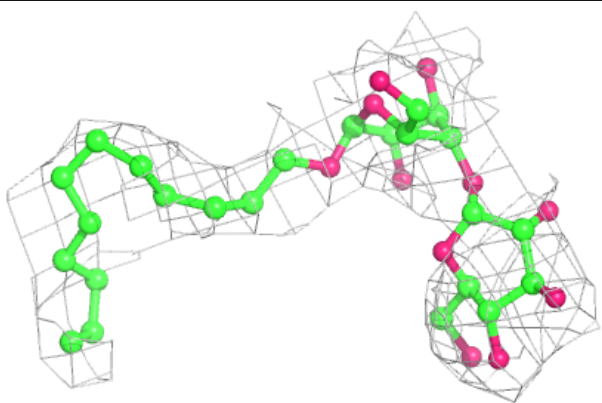


Electron density around LMU K 106:

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

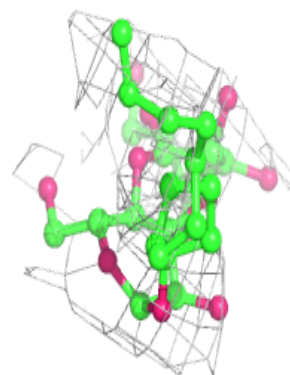
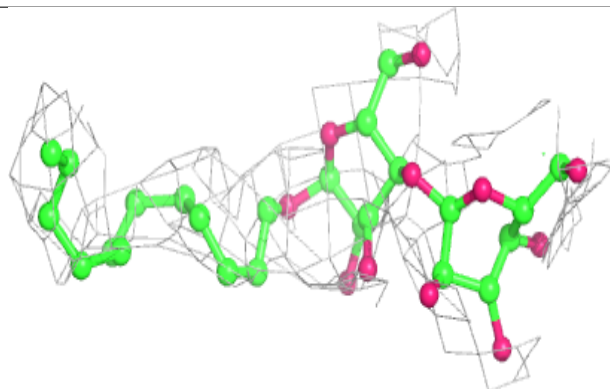
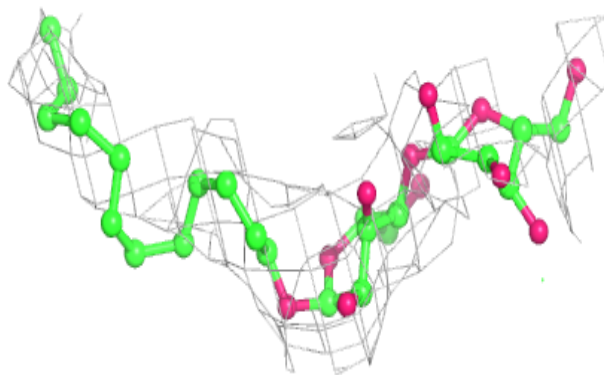
**Electron density around LMU K 109:**

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

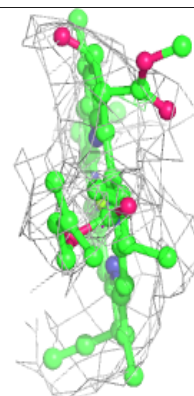
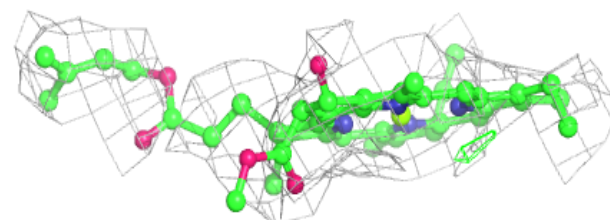
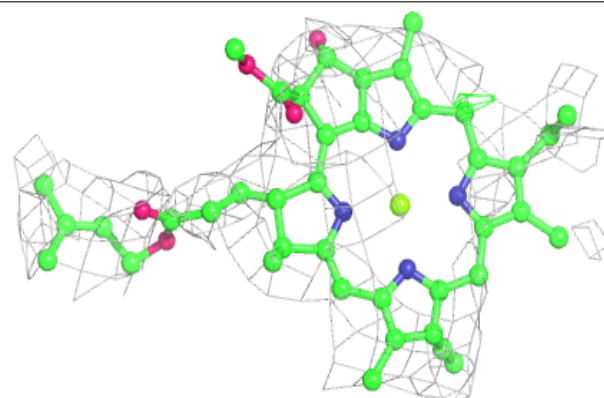


Electron density around LMU H 104:

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

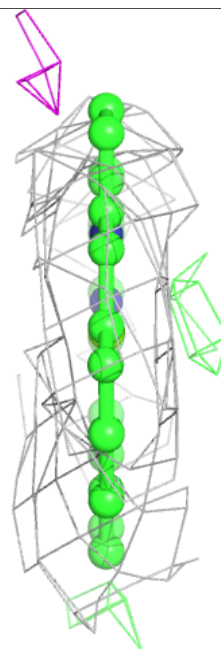
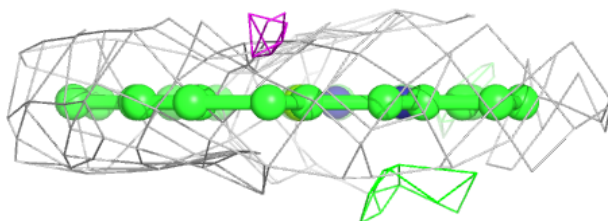
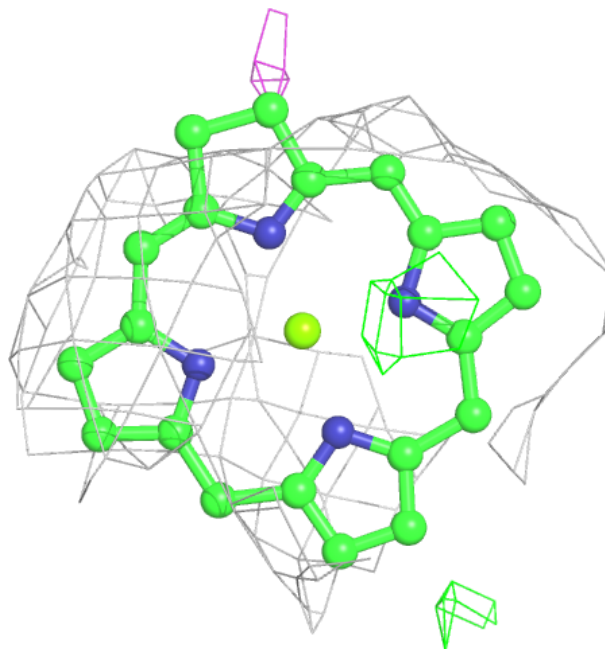
**Electron density around CLA 3 302:**

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



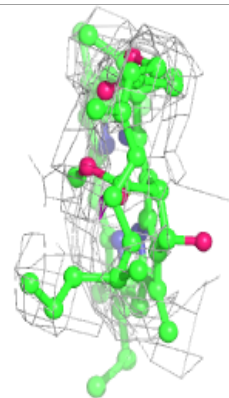
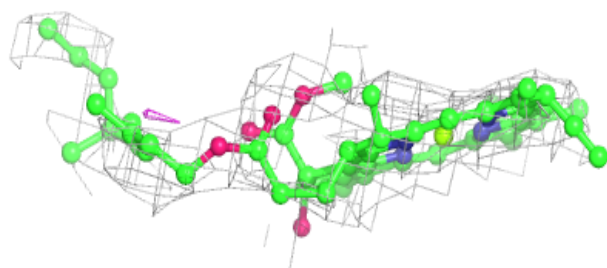
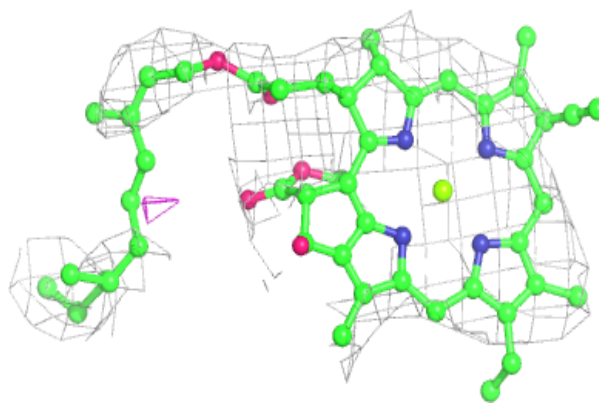
Electron density around CLA 3 319:

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

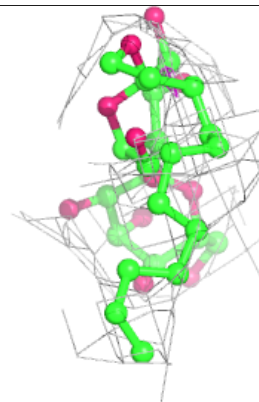
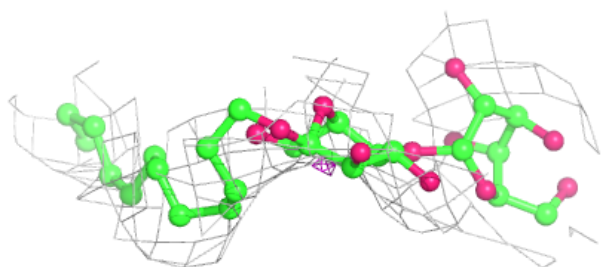
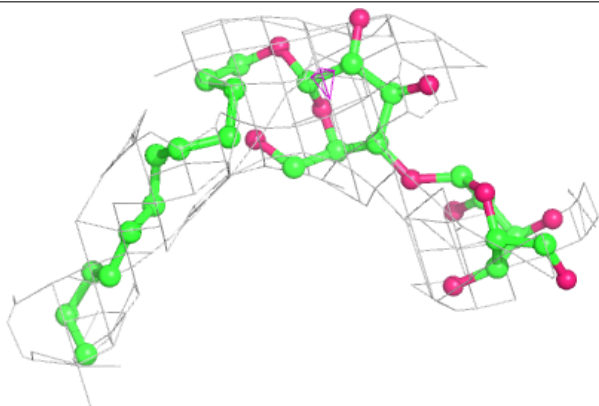


Electron density around CLA R 107:

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

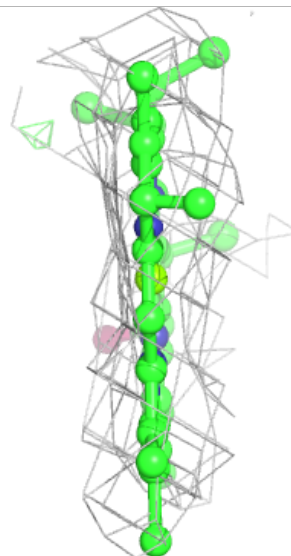
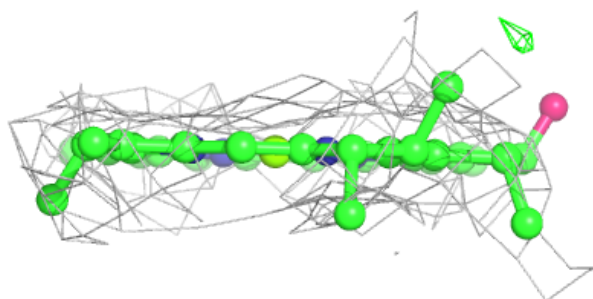
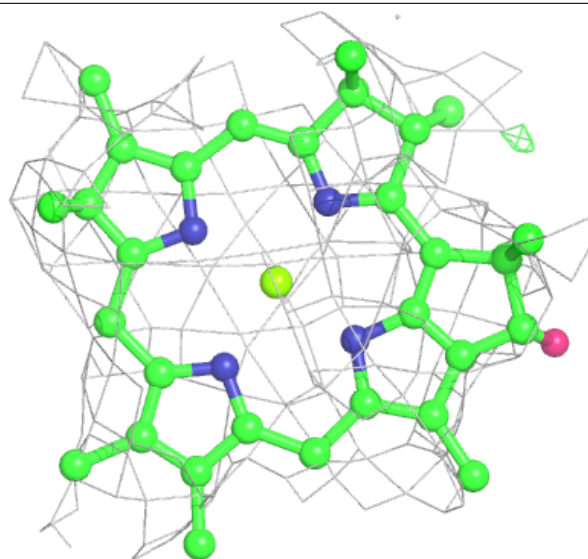
**Electron density around LMU R 103:**

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



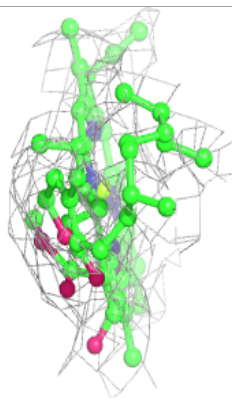
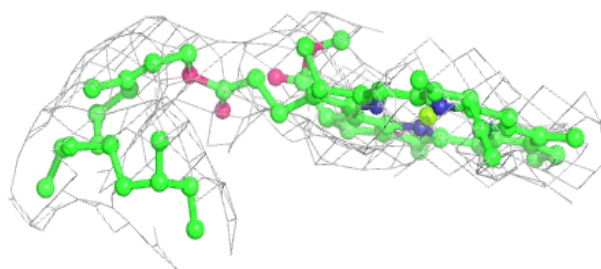
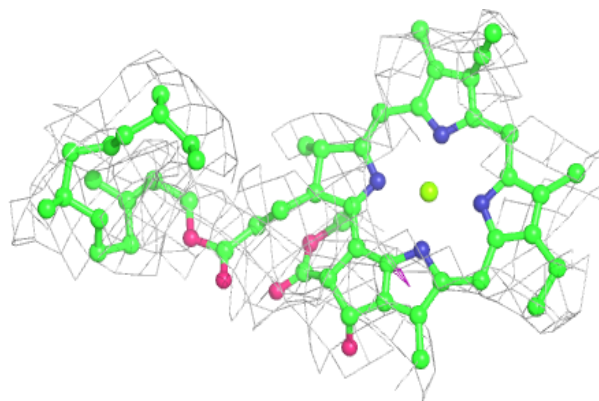
Electron density around CLA B 840:

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

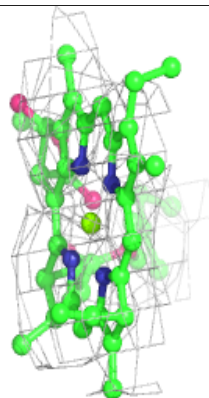
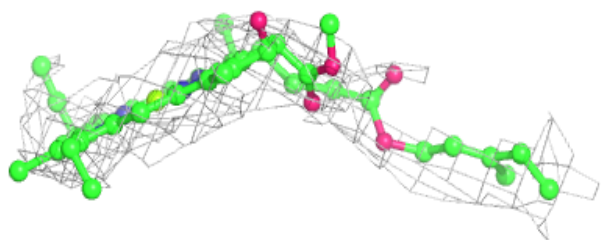
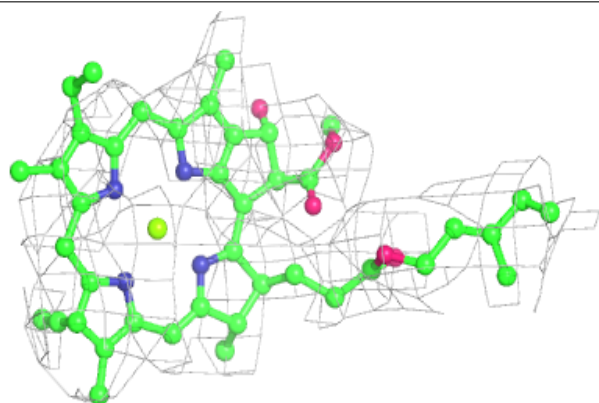


Electron density around CLA 1 215:

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

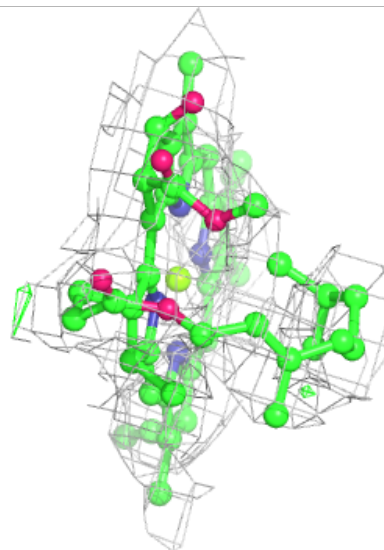
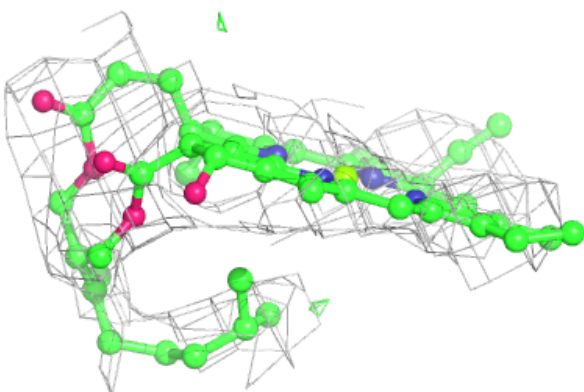
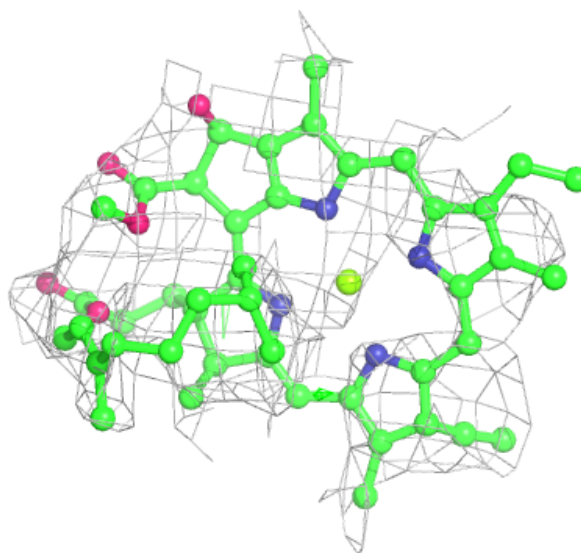
**Electron density around CLA 1 210:**

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



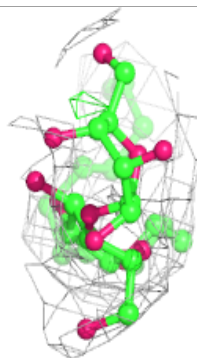
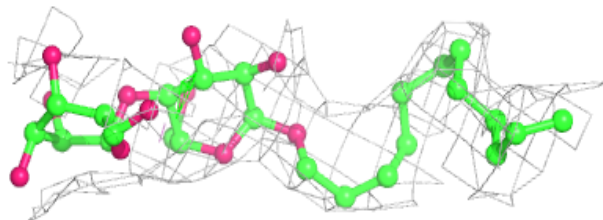
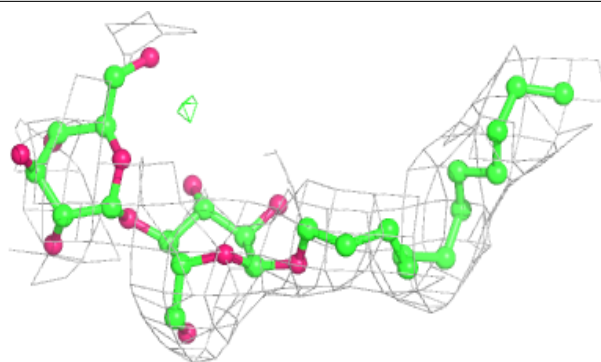
Electron density around CLA 4 305:

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

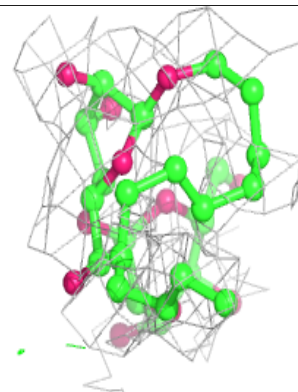
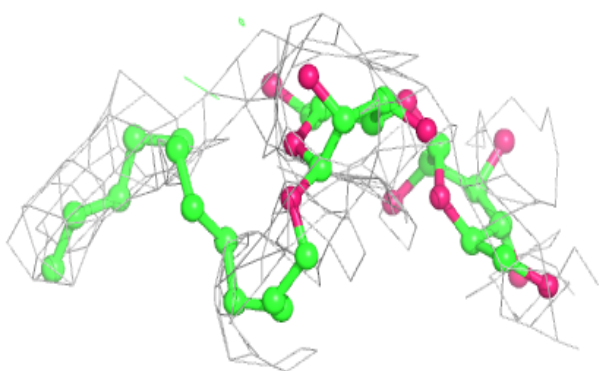
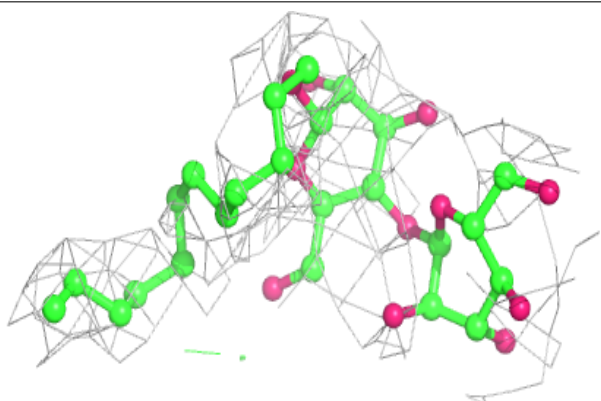


Electron density around LMU 4 322:

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

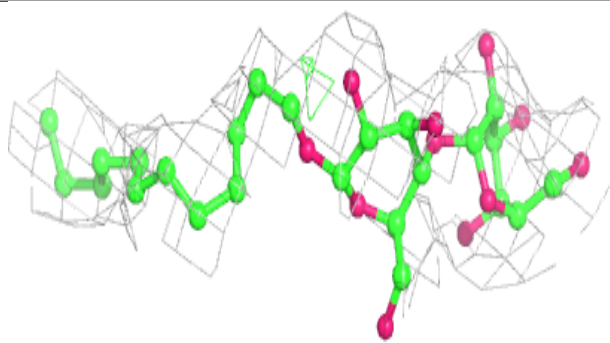
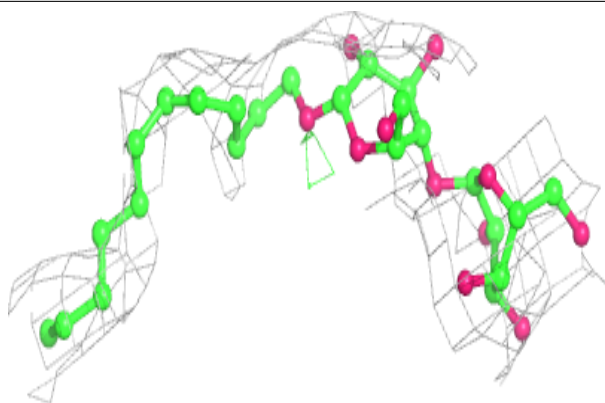
**Electron density around LMU L 211:**

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

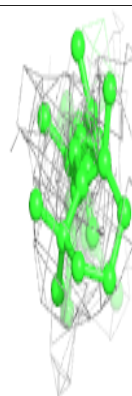
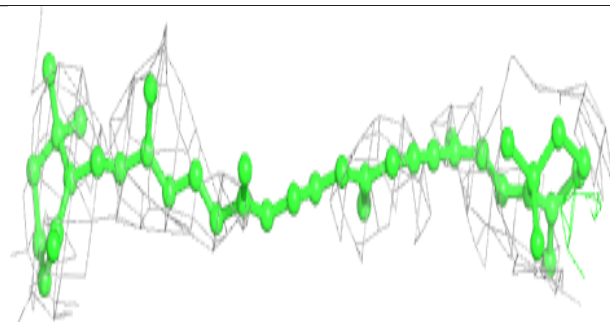
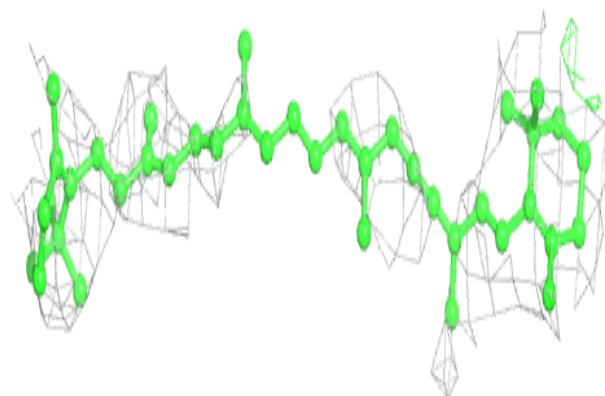


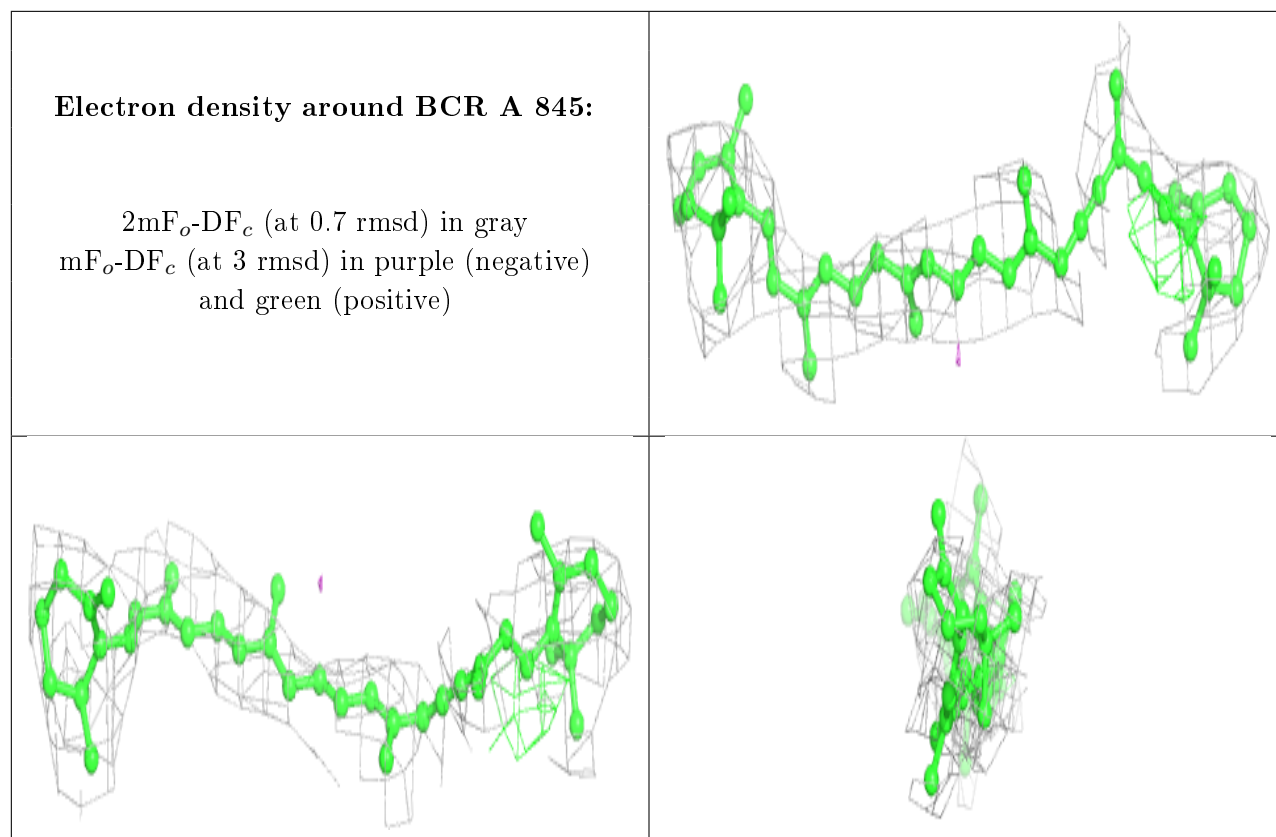
Electron density around LMU 2 318:

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

**Electron density around BCR A 844:**

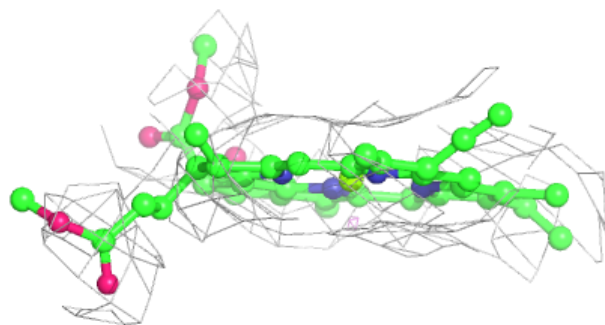
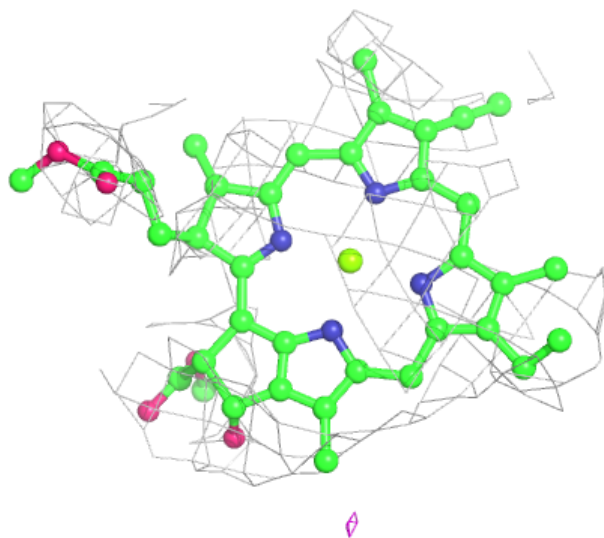
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

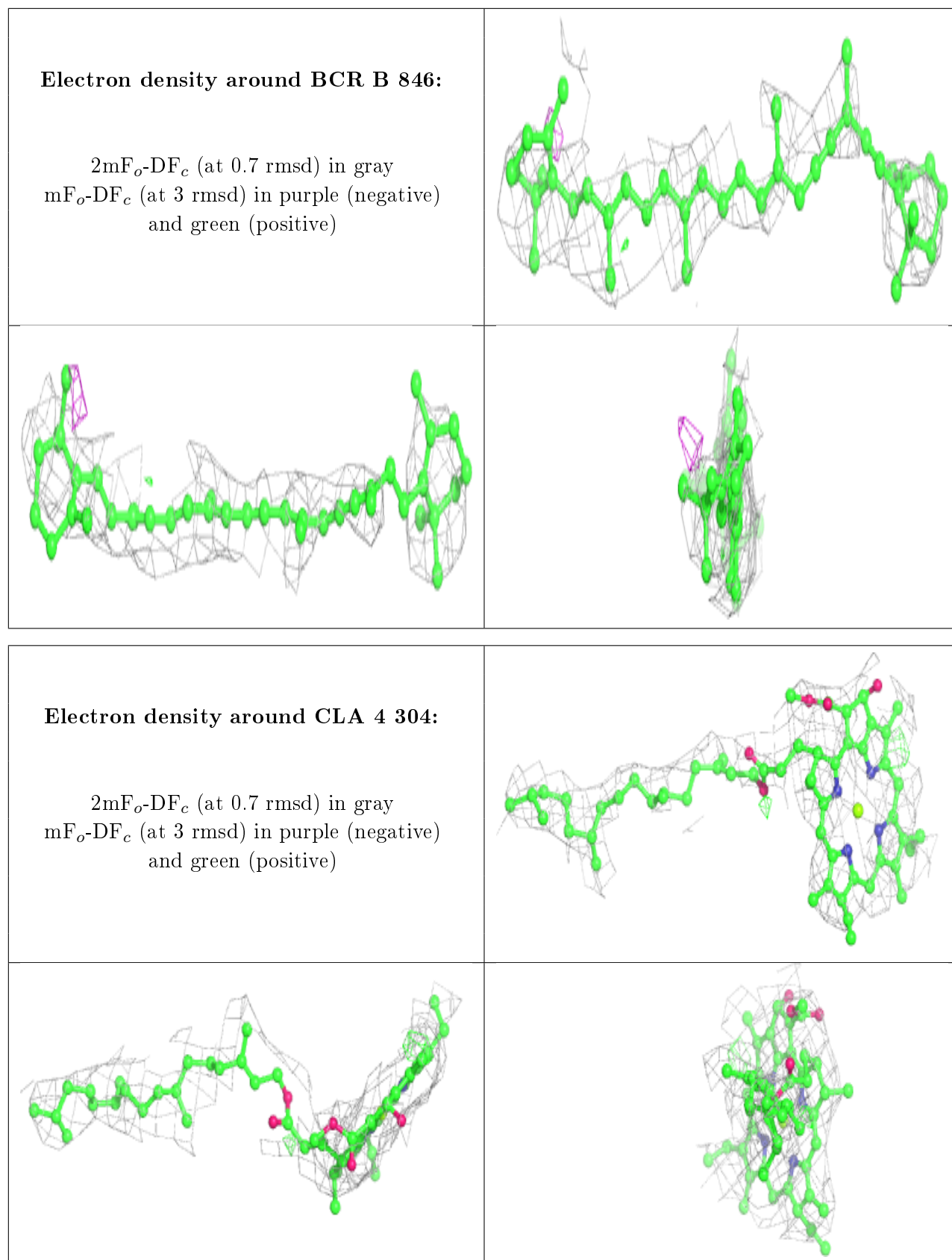




Electron density around CLA 1 201:

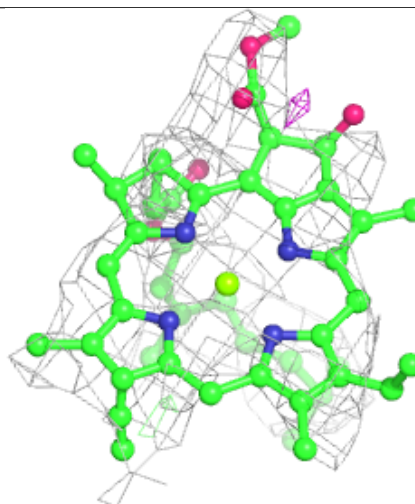
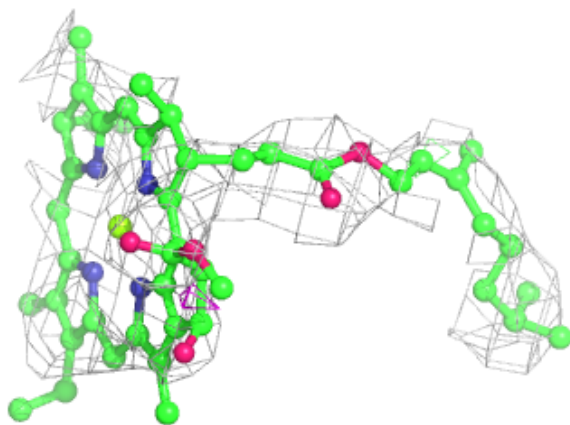
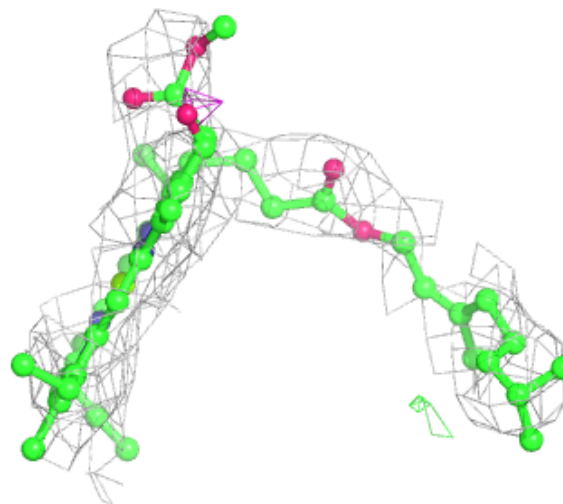
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





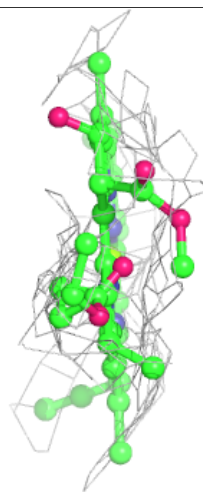
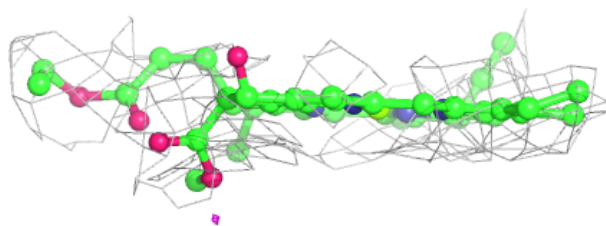
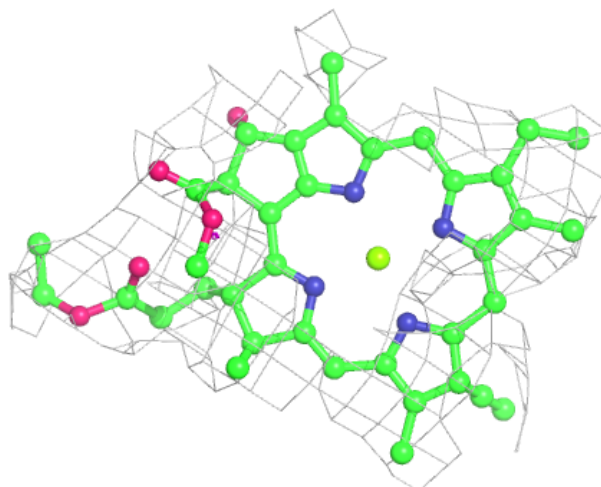
Electron density around CLA L 203:

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



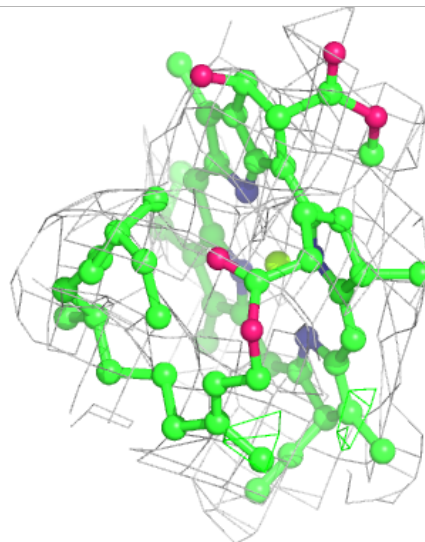
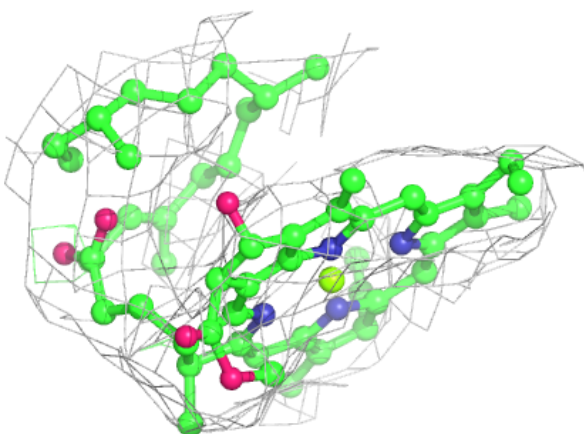
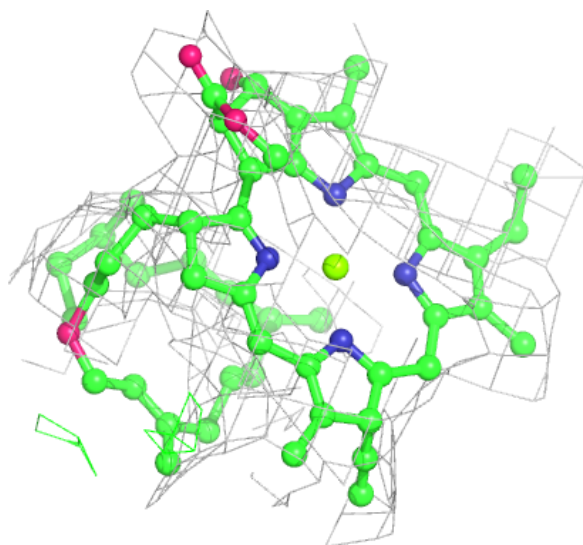
Electron density around CLA 4 319:

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



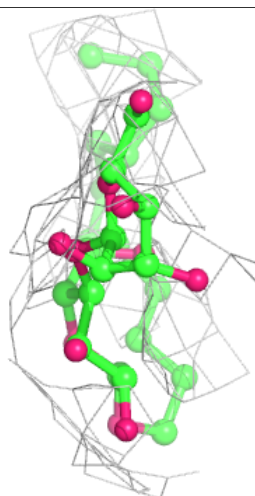
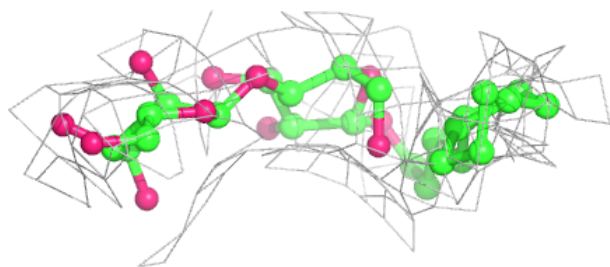
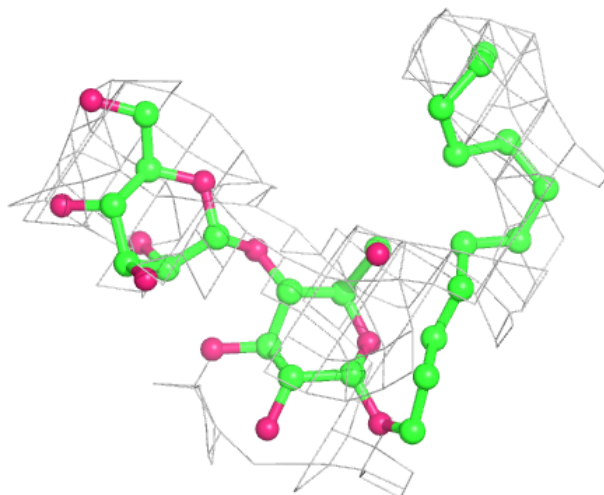
Electron density around CLA J 103:

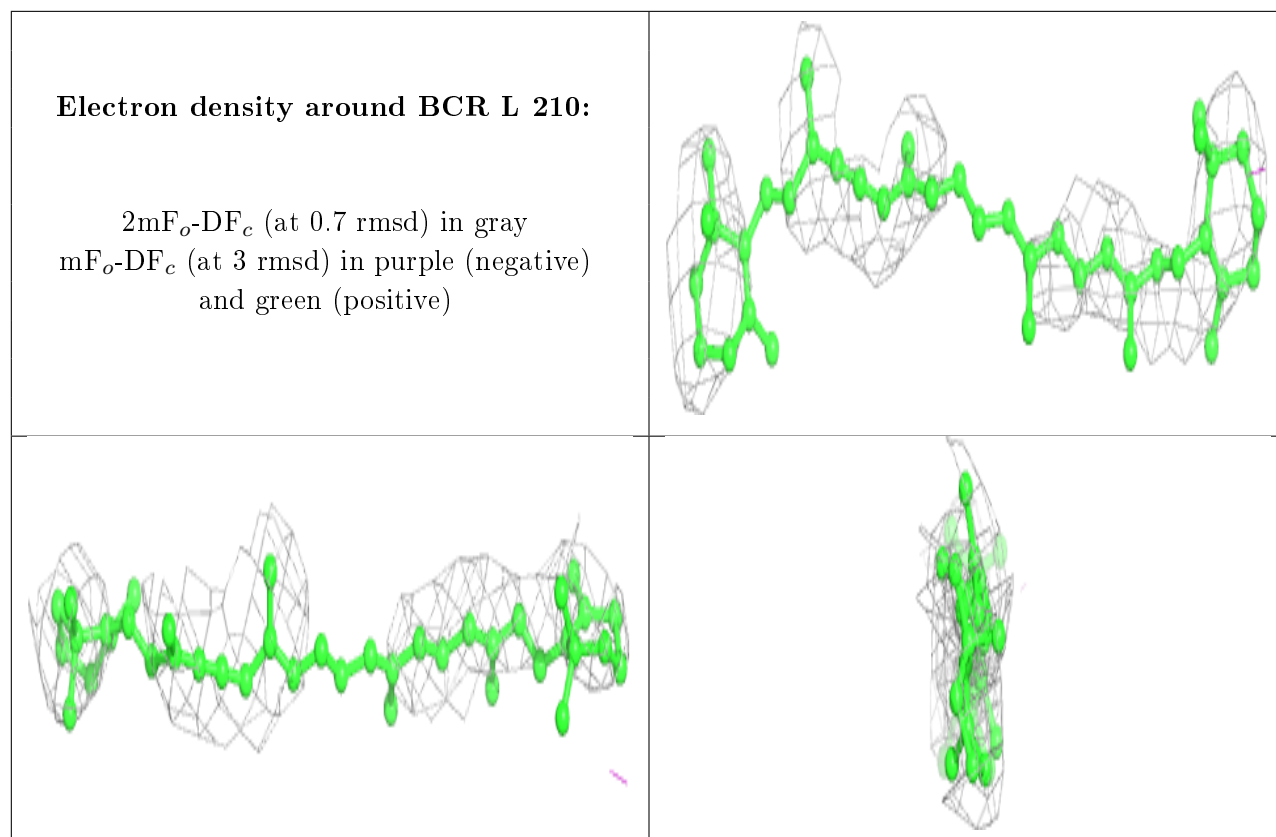
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMU N 101:

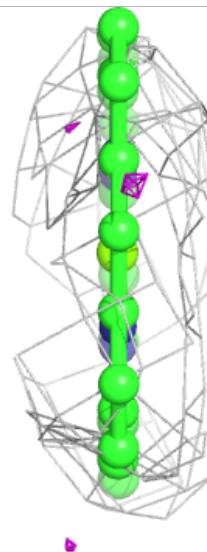
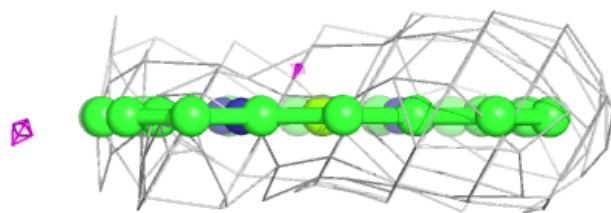
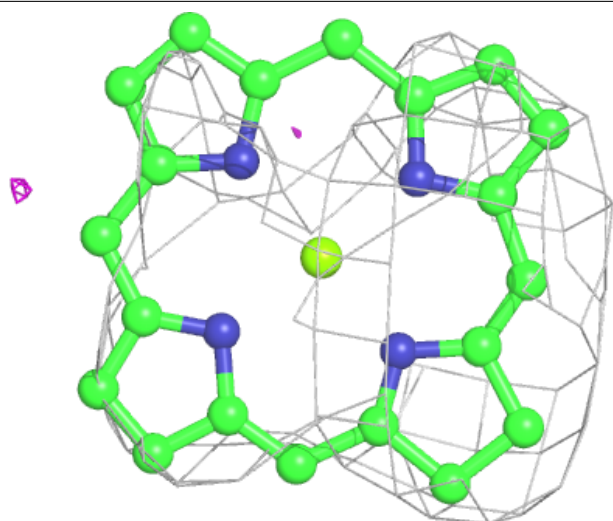
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





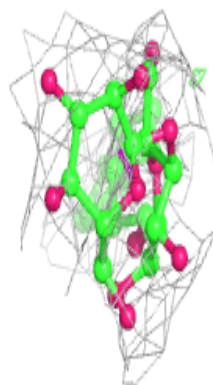
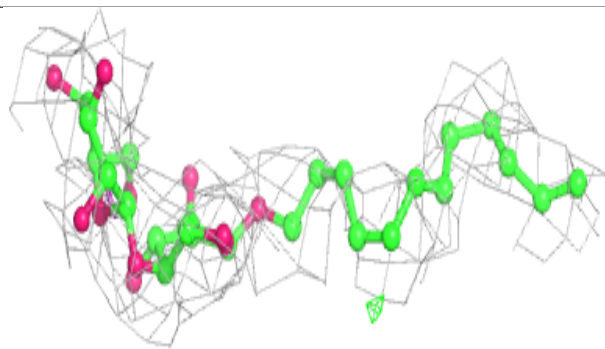
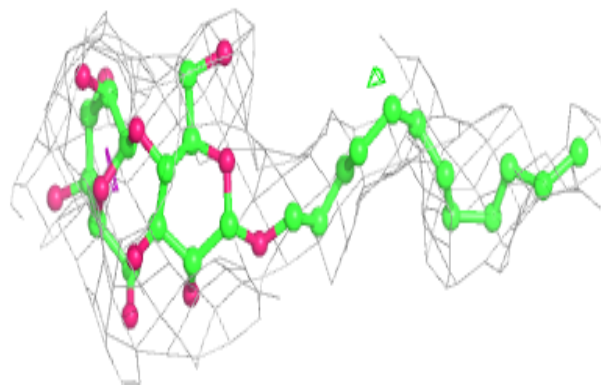
Electron density around CLA 2 310:

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

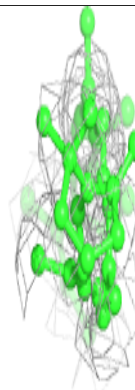
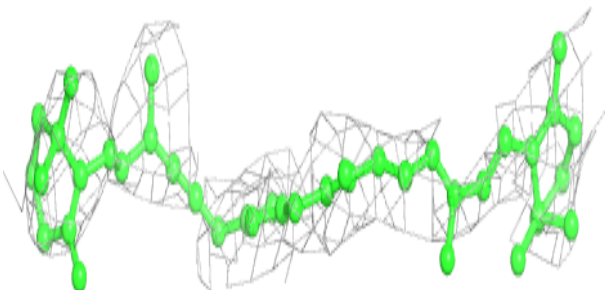
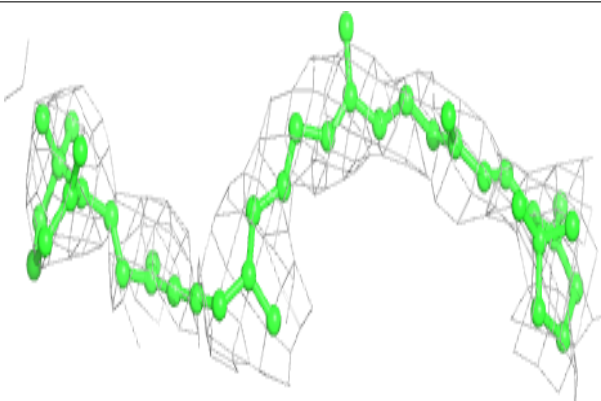


Electron density around LMU 1 219:

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

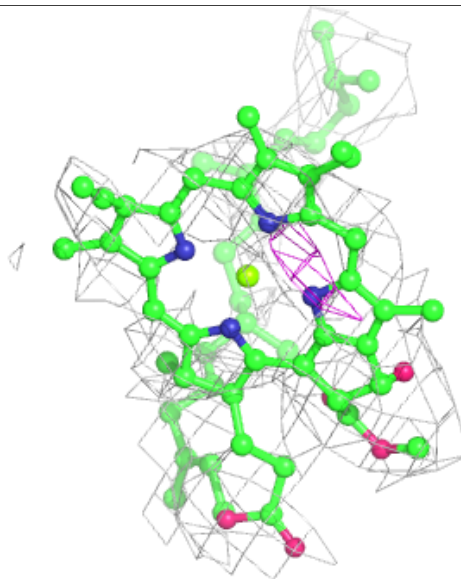
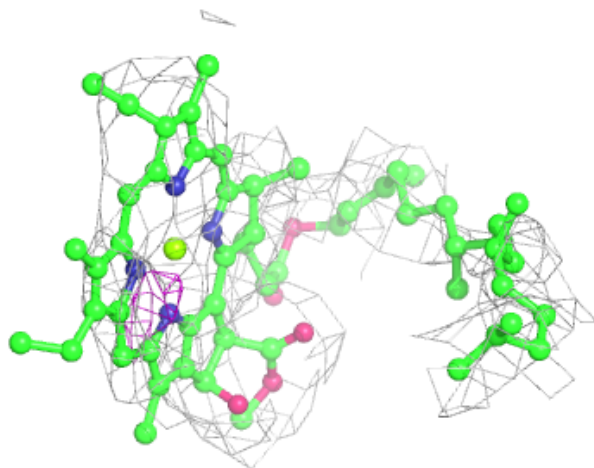
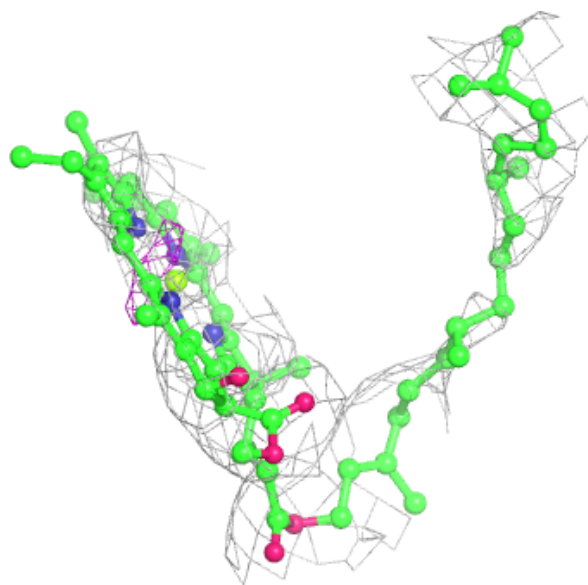
**Electron density around BCR I 103:**

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



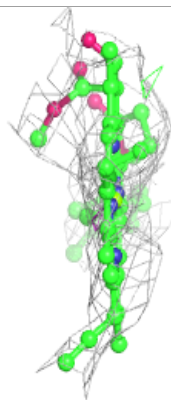
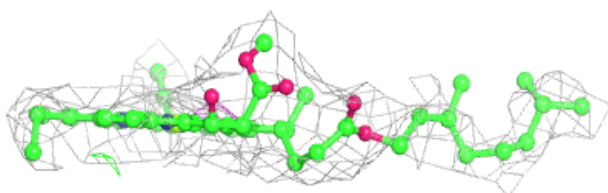
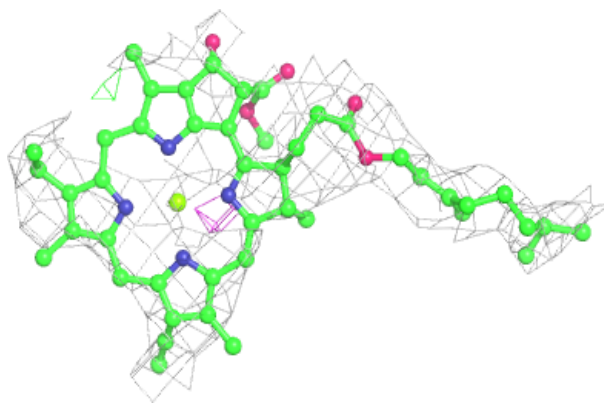
Electron density around CLA 2 307:

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

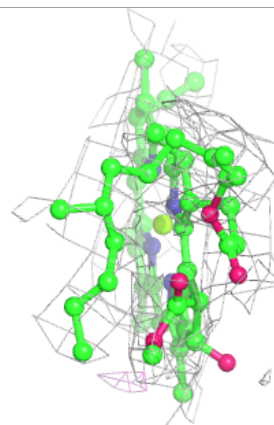
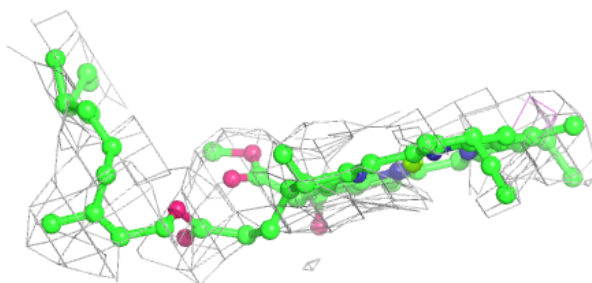
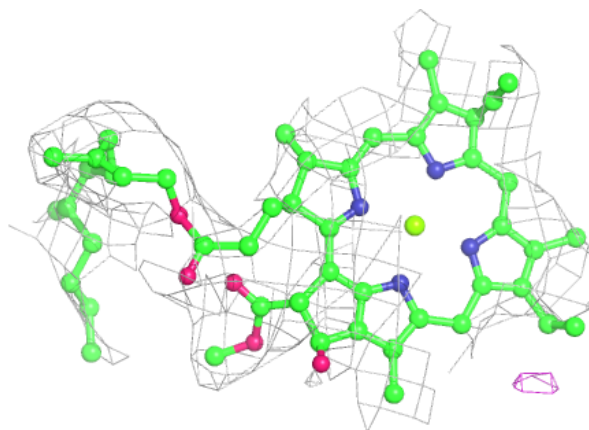


Electron density around CLA 4 311:

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

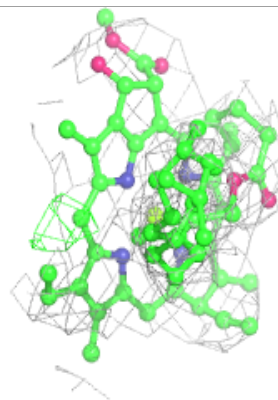
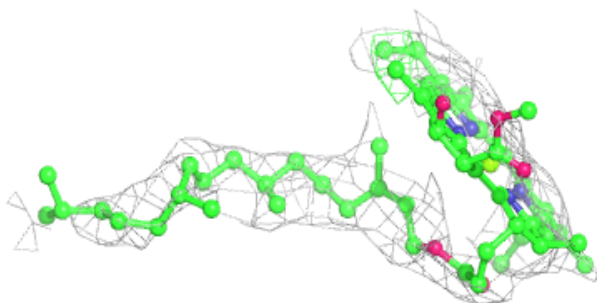
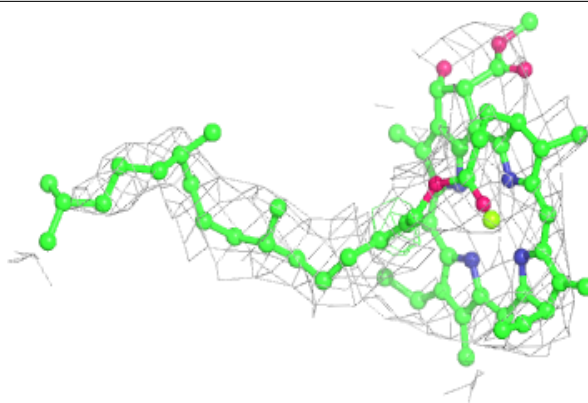
**Electron density around CLA R 108:**

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

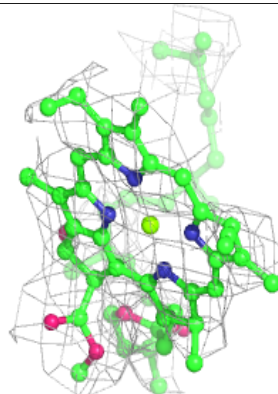
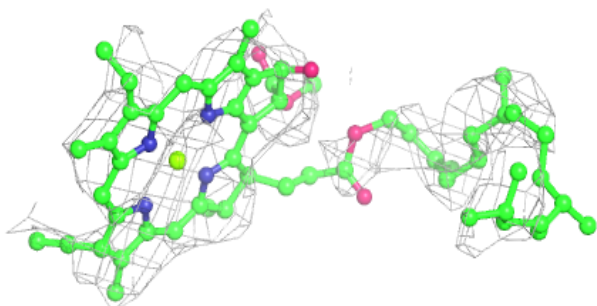
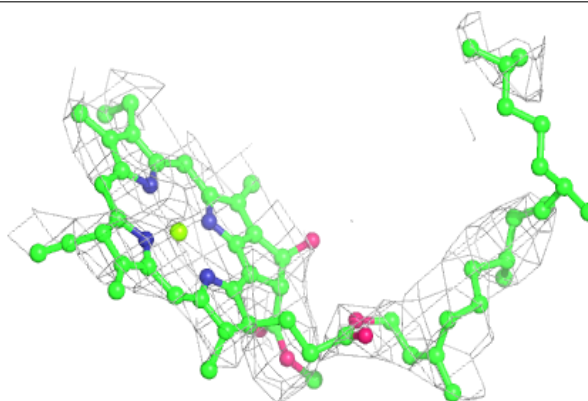


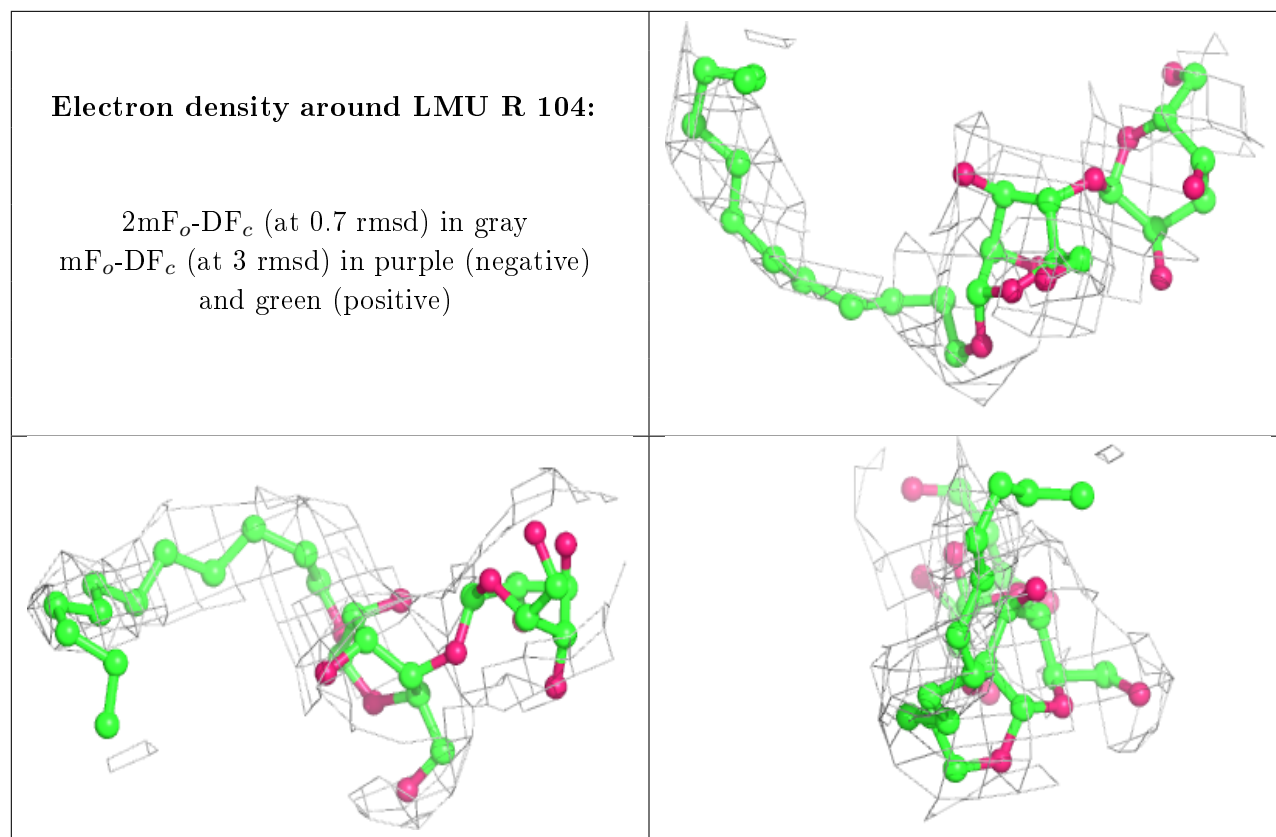
Electron density around CLA 2 303:

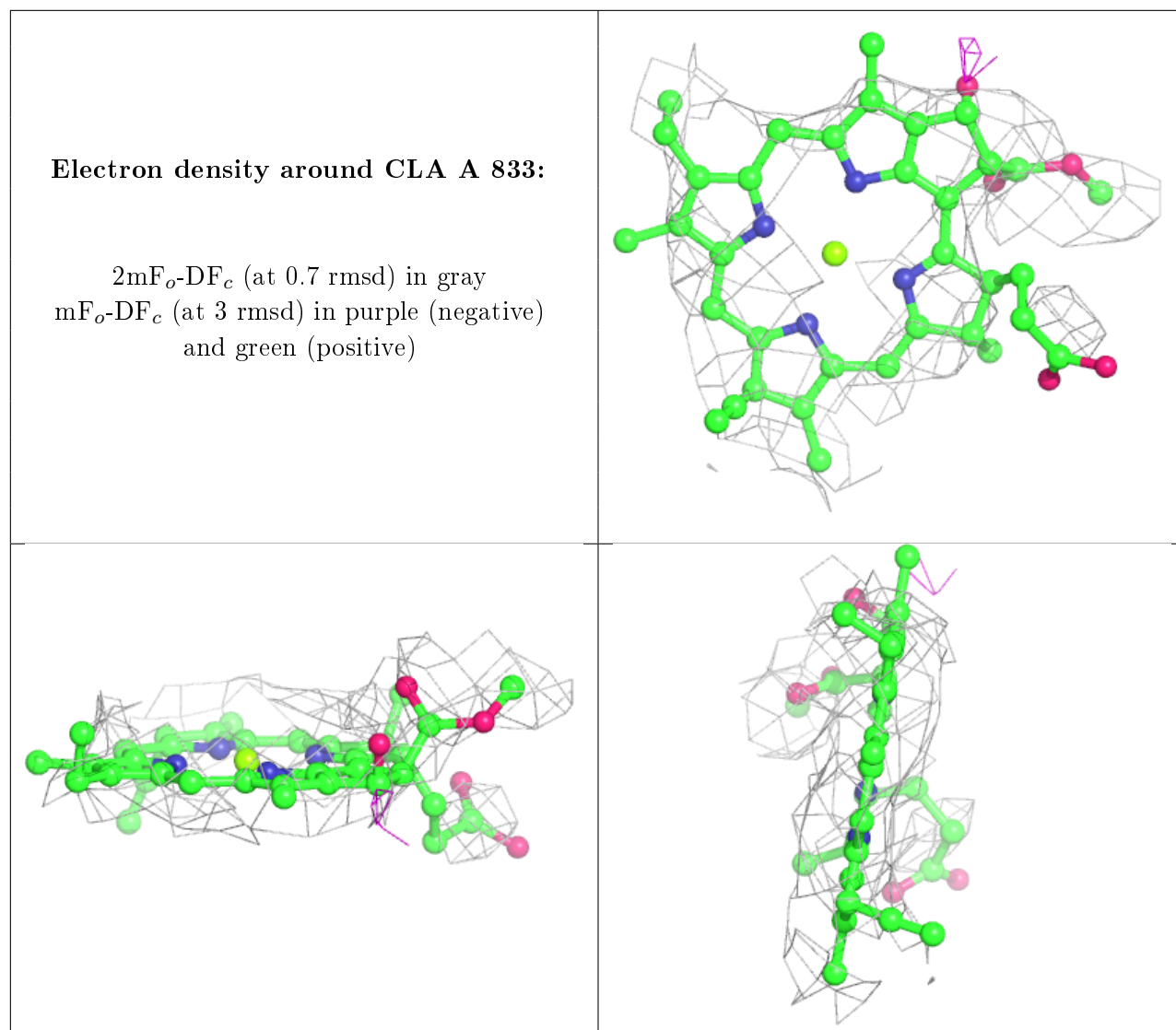
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CLA K 103:**

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

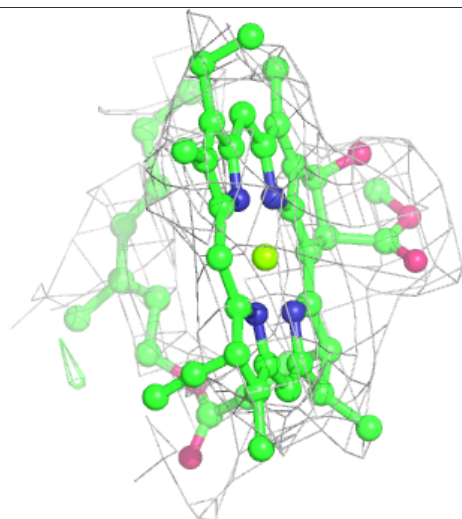
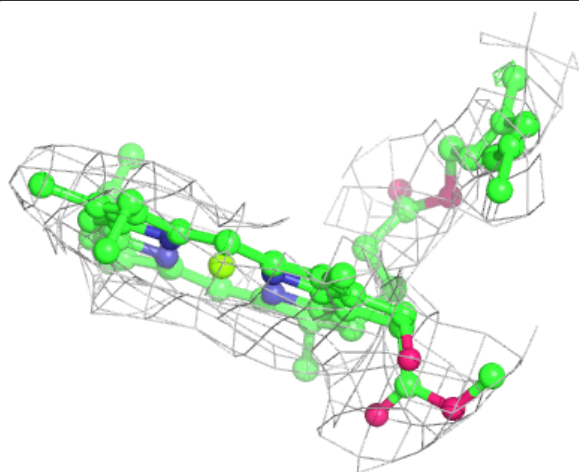
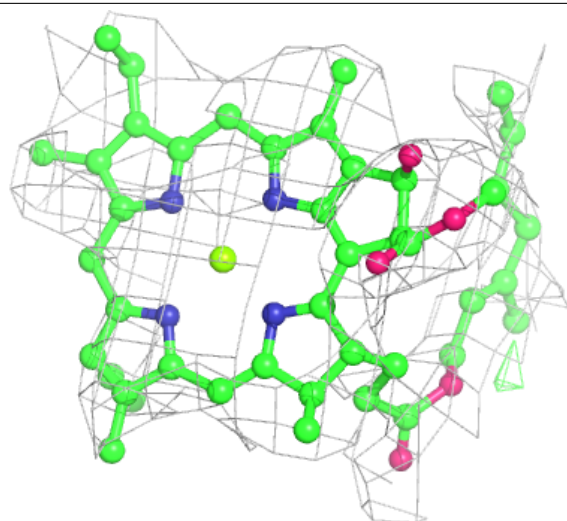


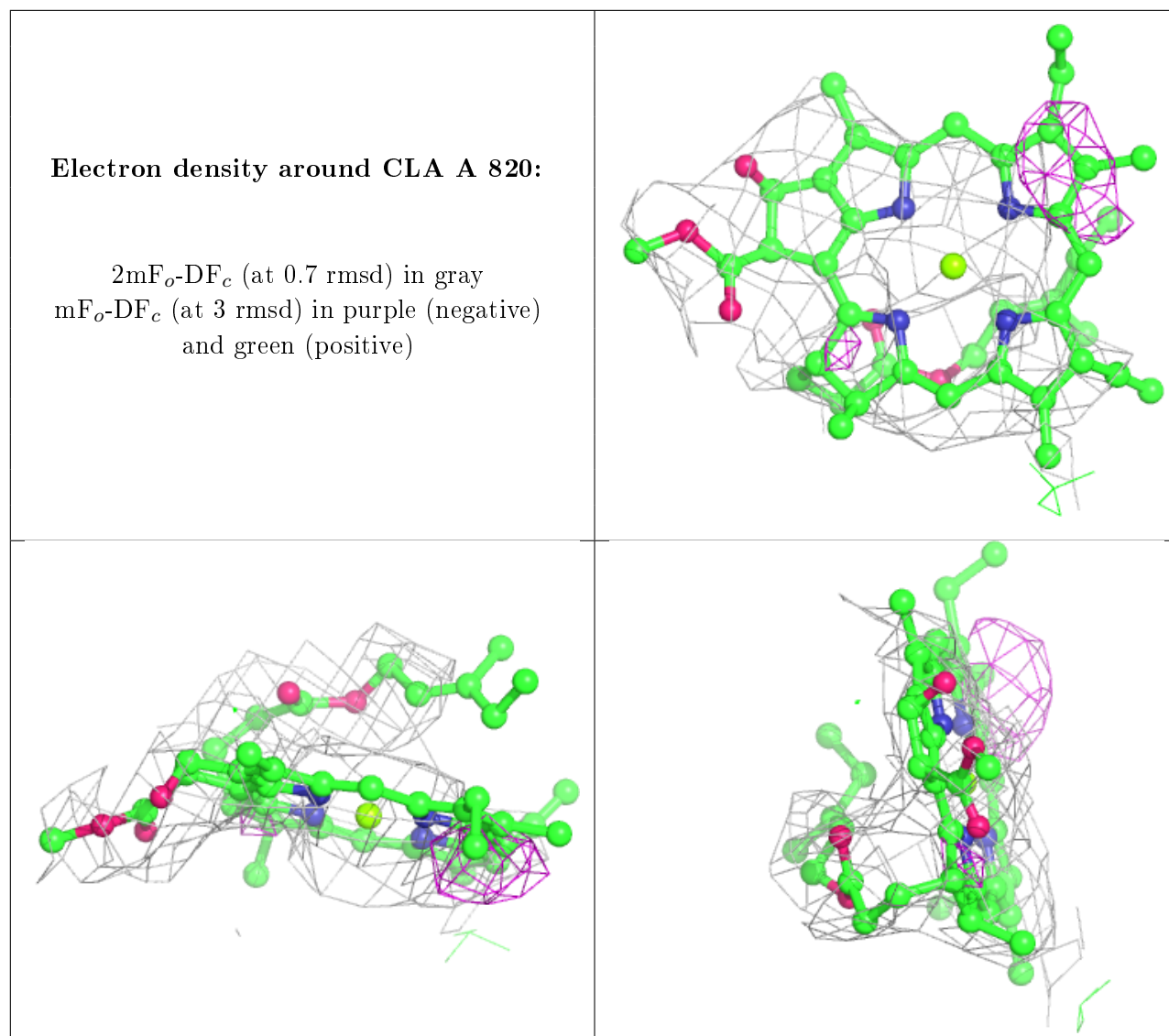




Electron density around CLA F 206:

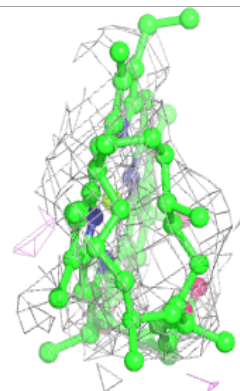
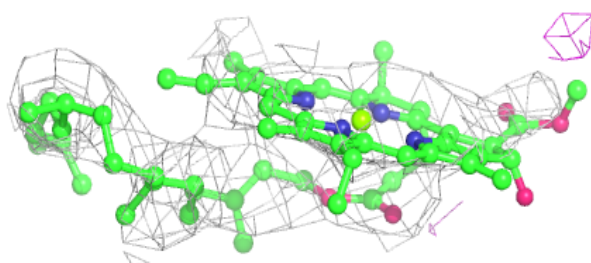
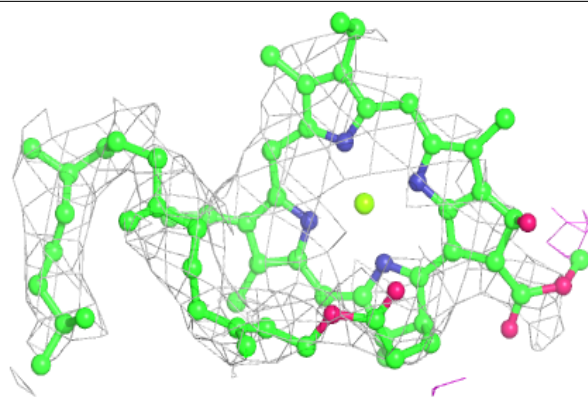
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



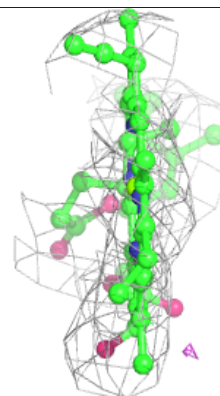
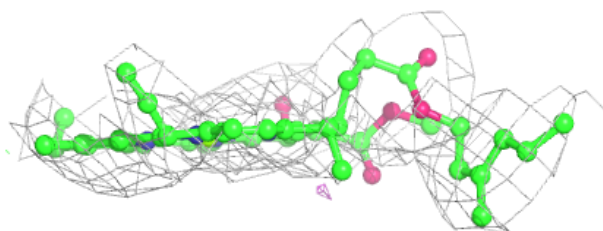
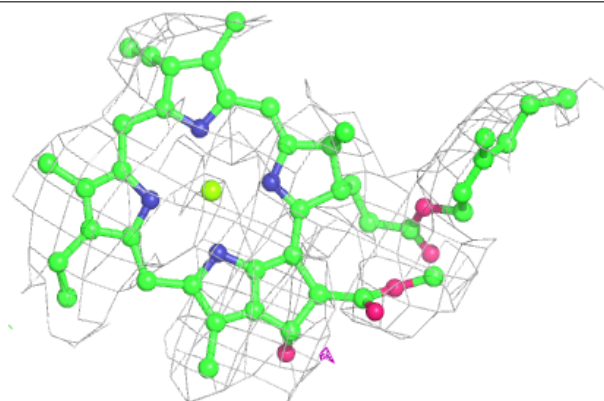


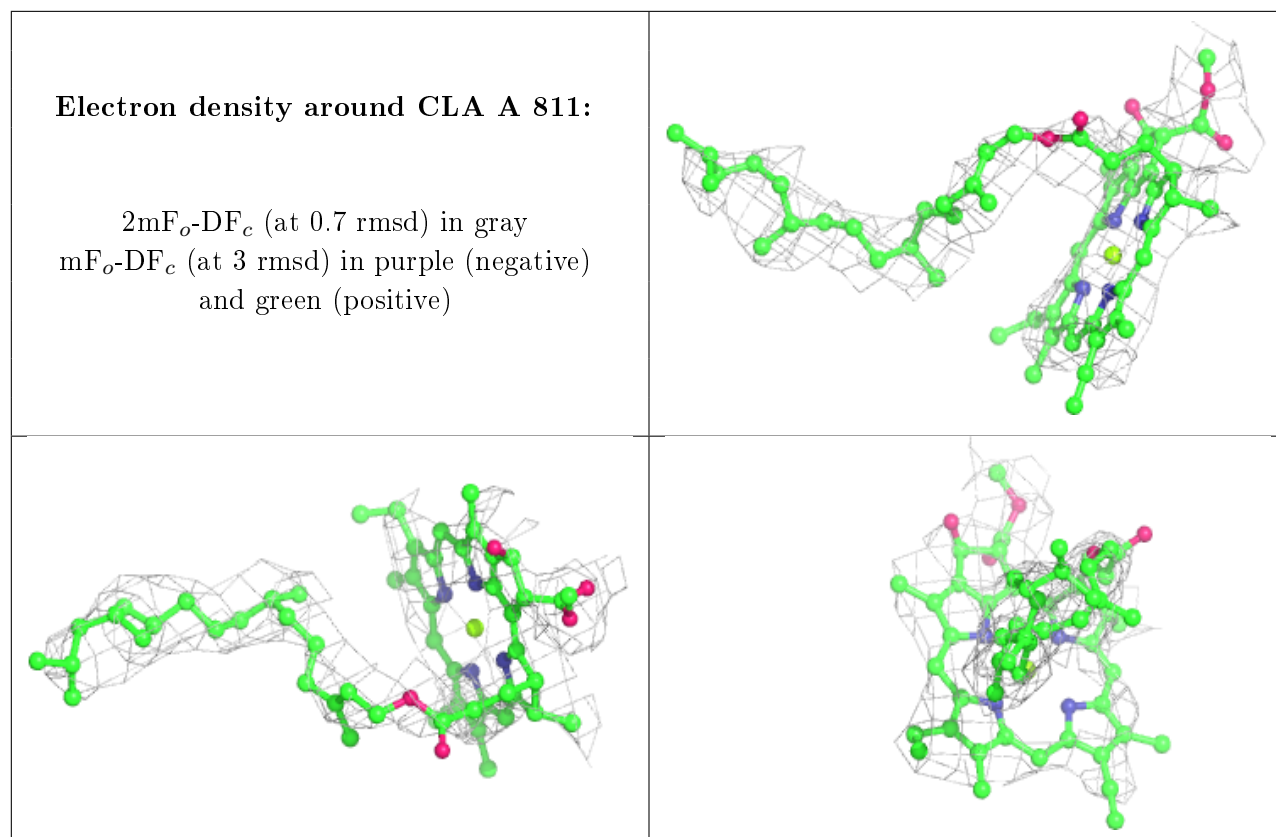
Electron density around CLA A 818:

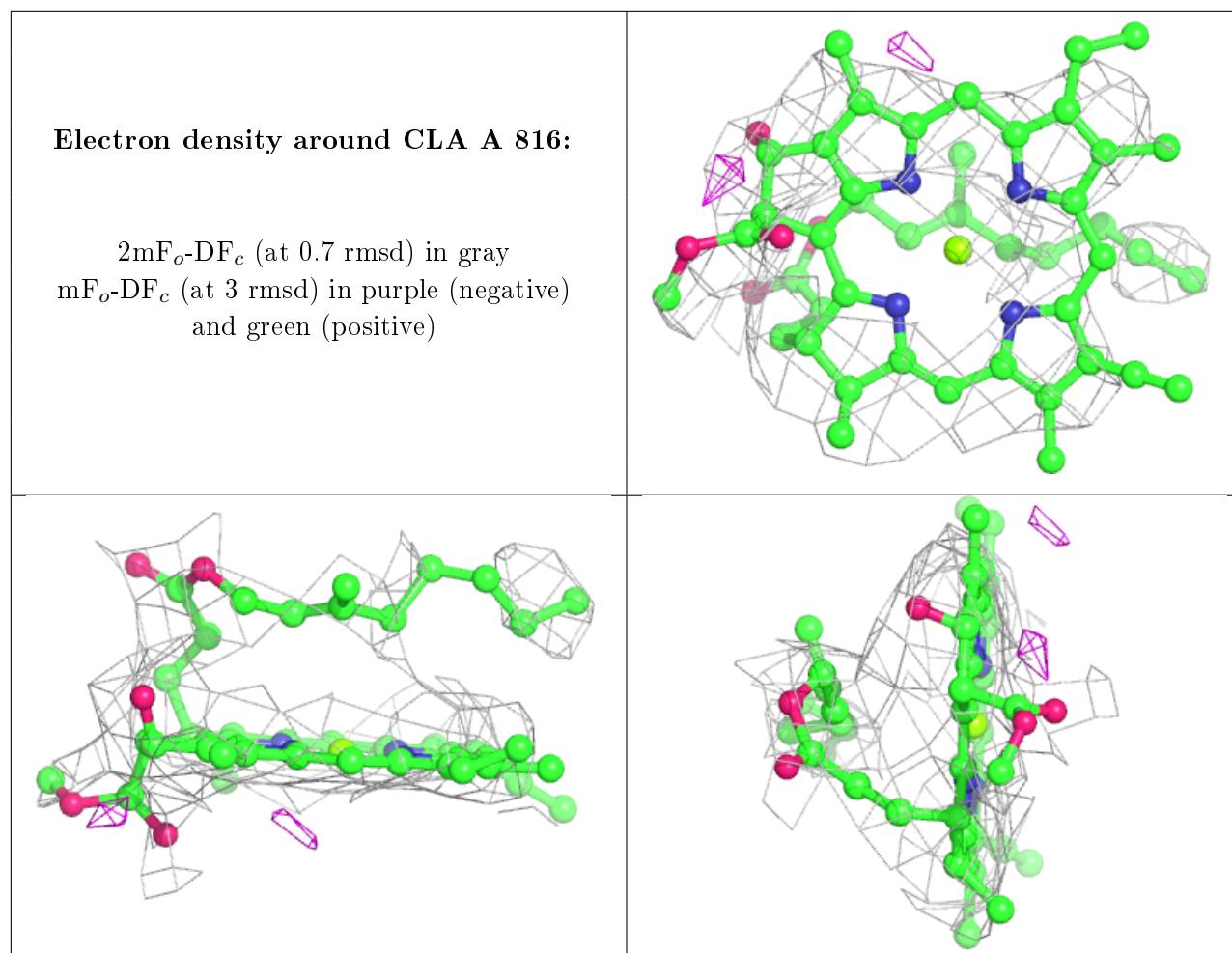
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CLA 4 318:**

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

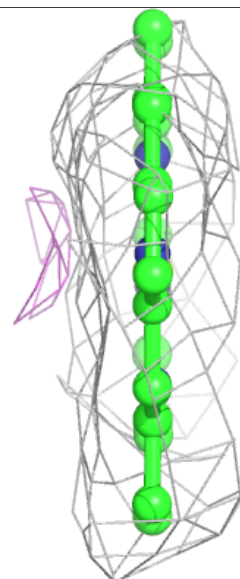
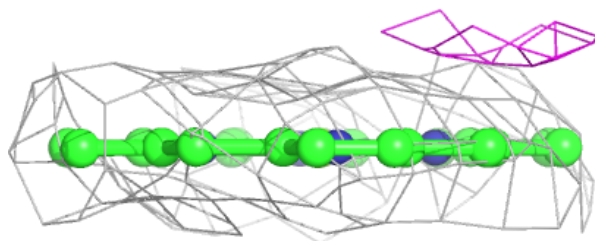
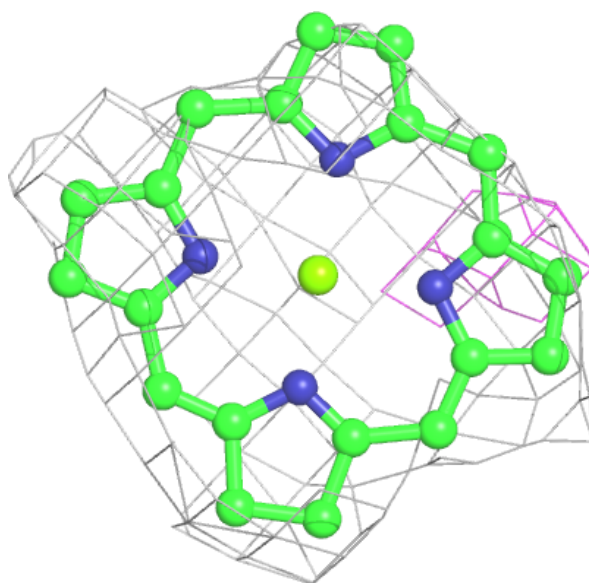






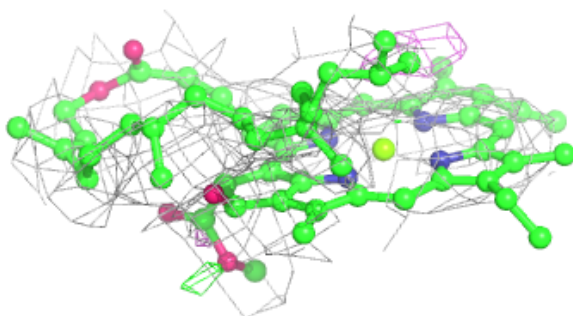
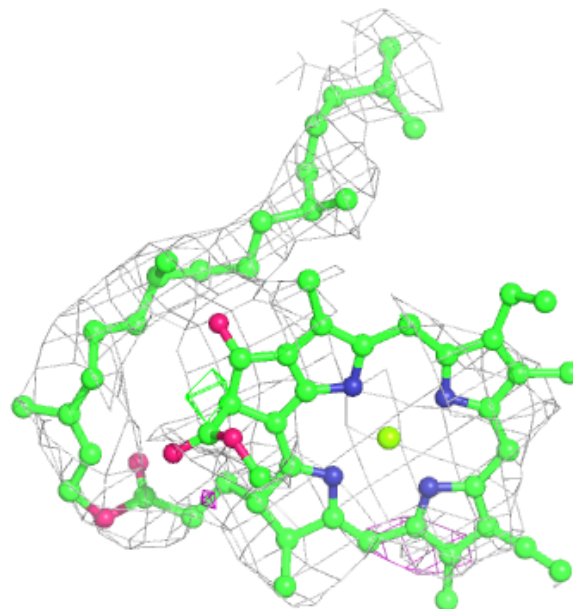
Electron density around CLA 2 304:

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



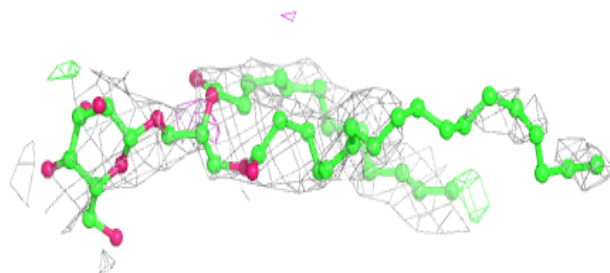
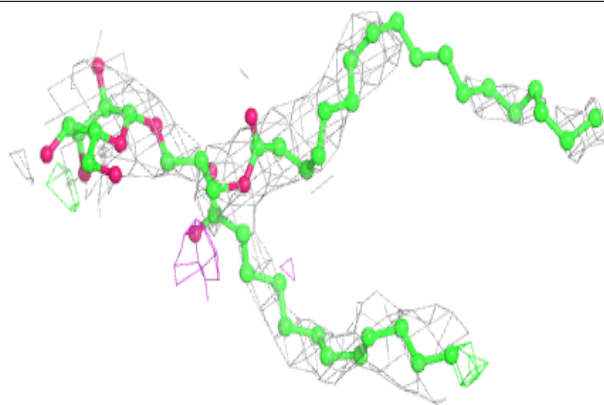
Electron density around CLA A 823:

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



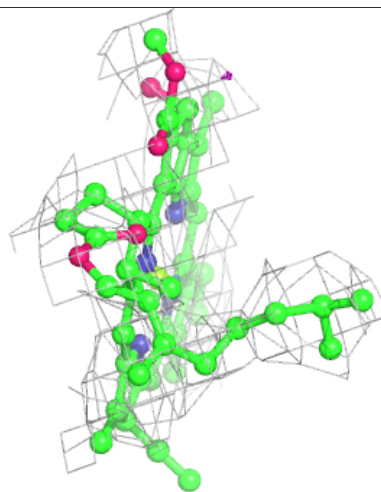
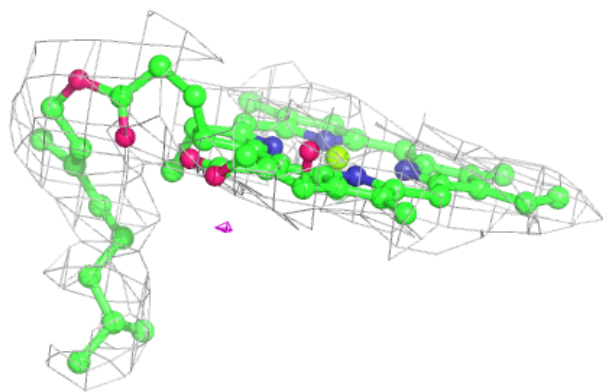
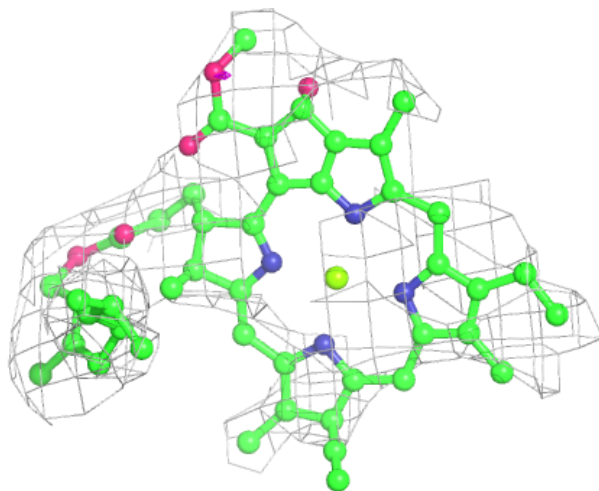
Electron density around LMG B 848:

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



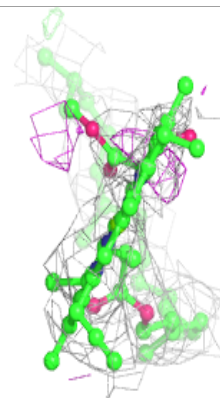
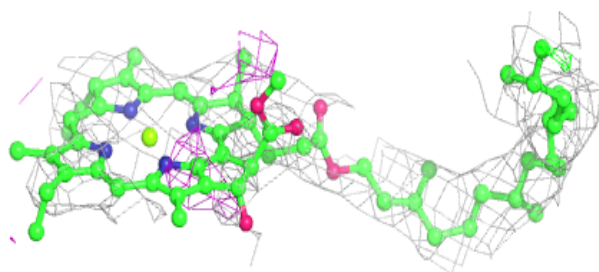
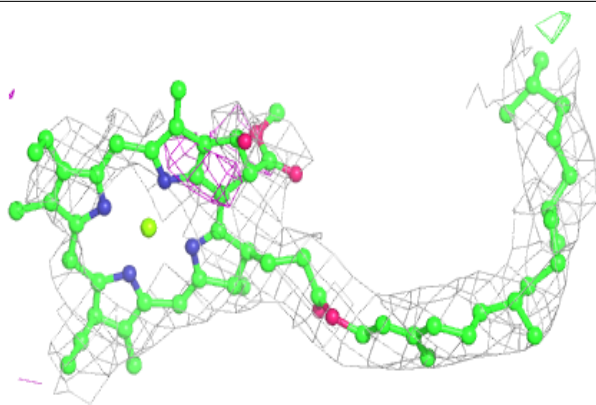
Electron density around CLA H 101:

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

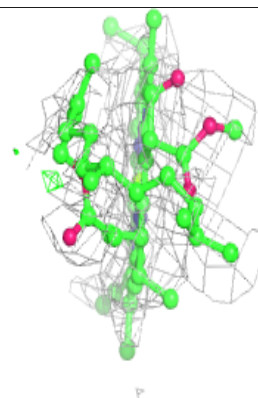
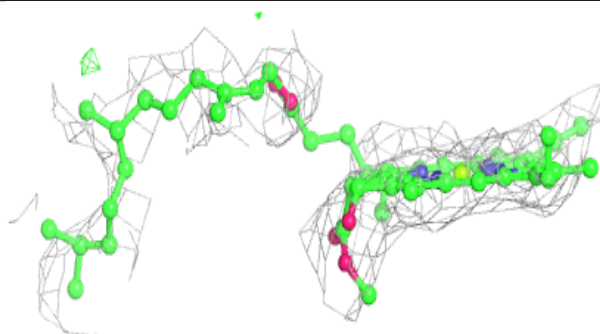
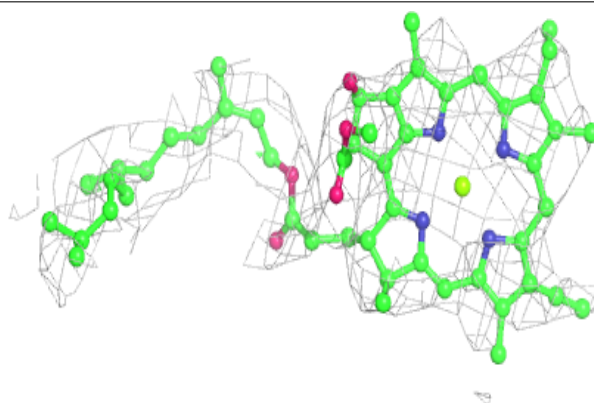


Electron density around CLA B 824:

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

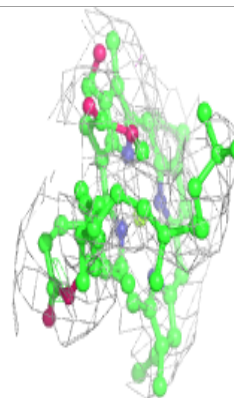
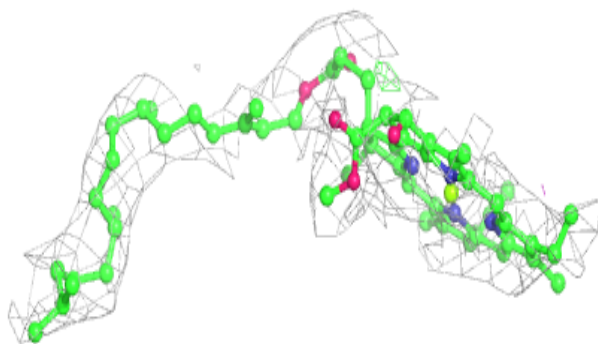
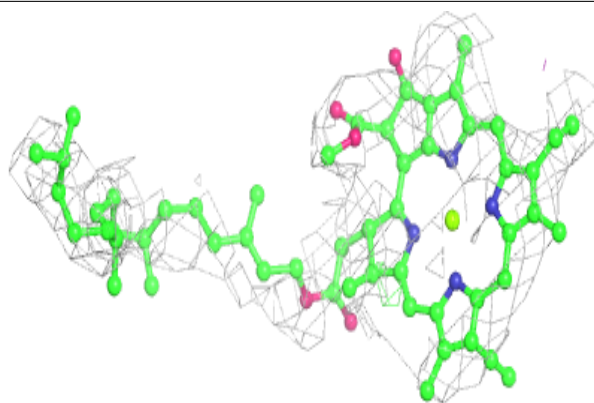
**Electron density around CLA B 813:**

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

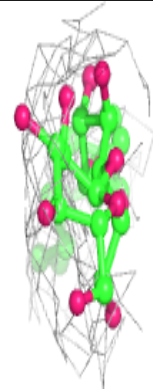
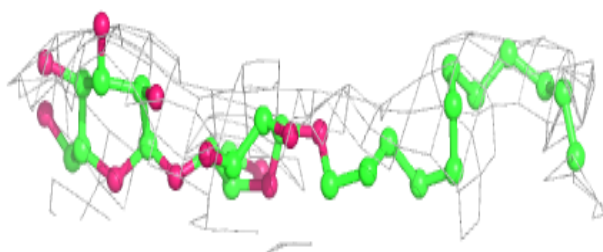
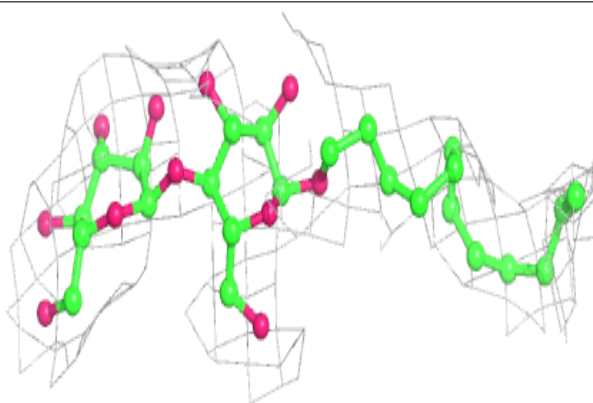


Electron density around CLA 3 318:

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

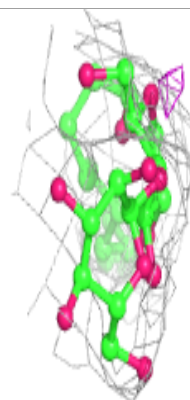
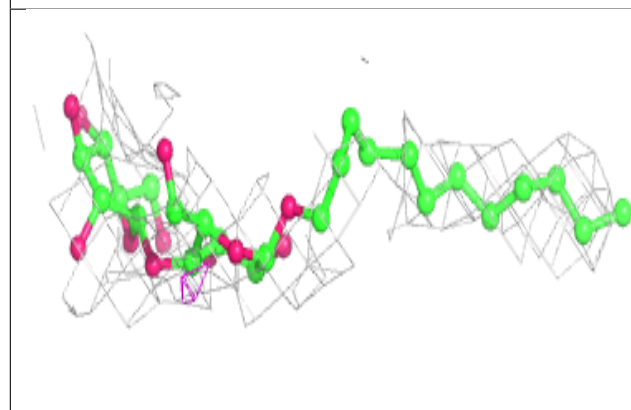
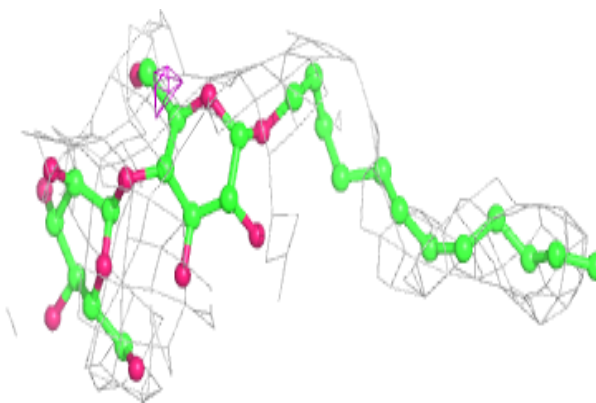
**Electron density around LMU 3 322:**

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



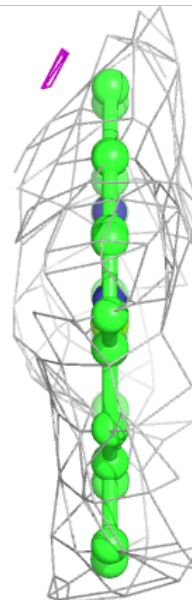
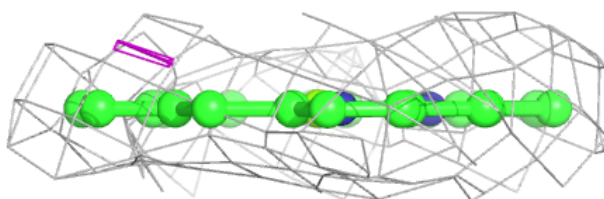
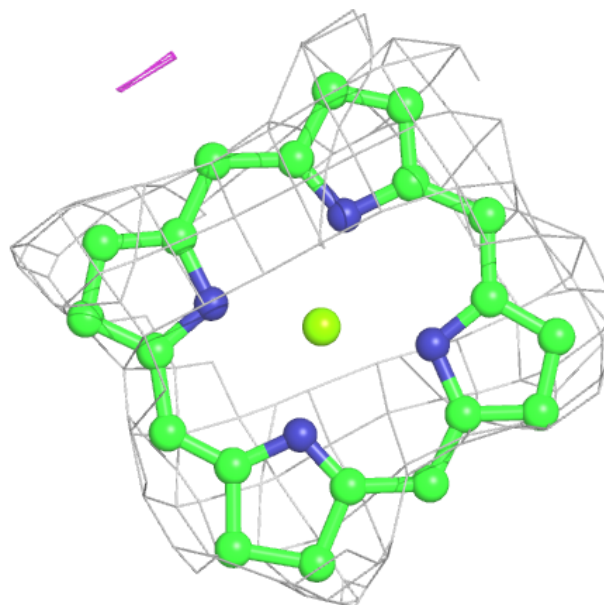
Electron density around LMU A 856:

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



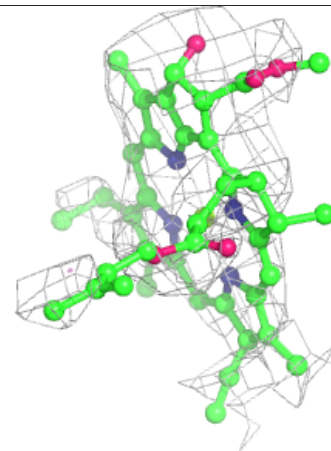
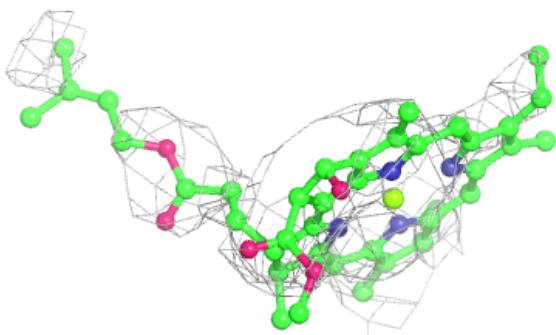
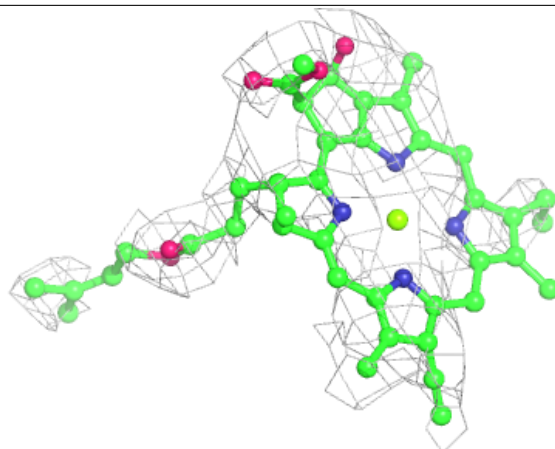
Electron density around CLA 1 216:

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

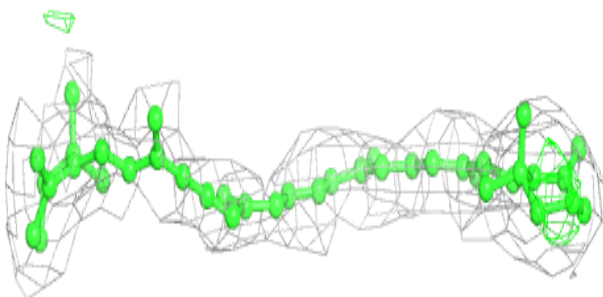
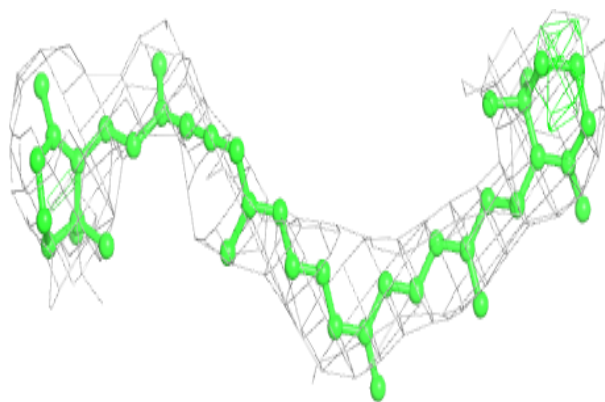


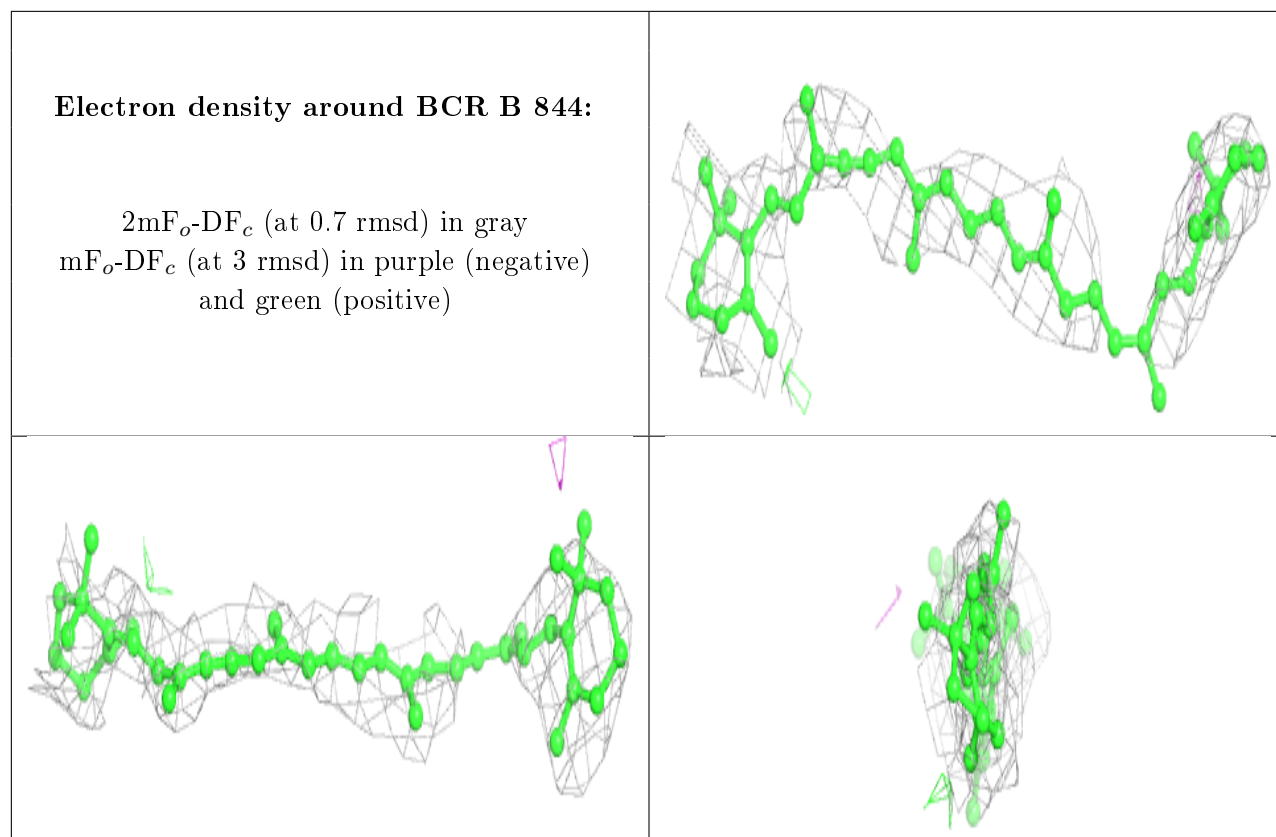
Electron density around CLA A 829:

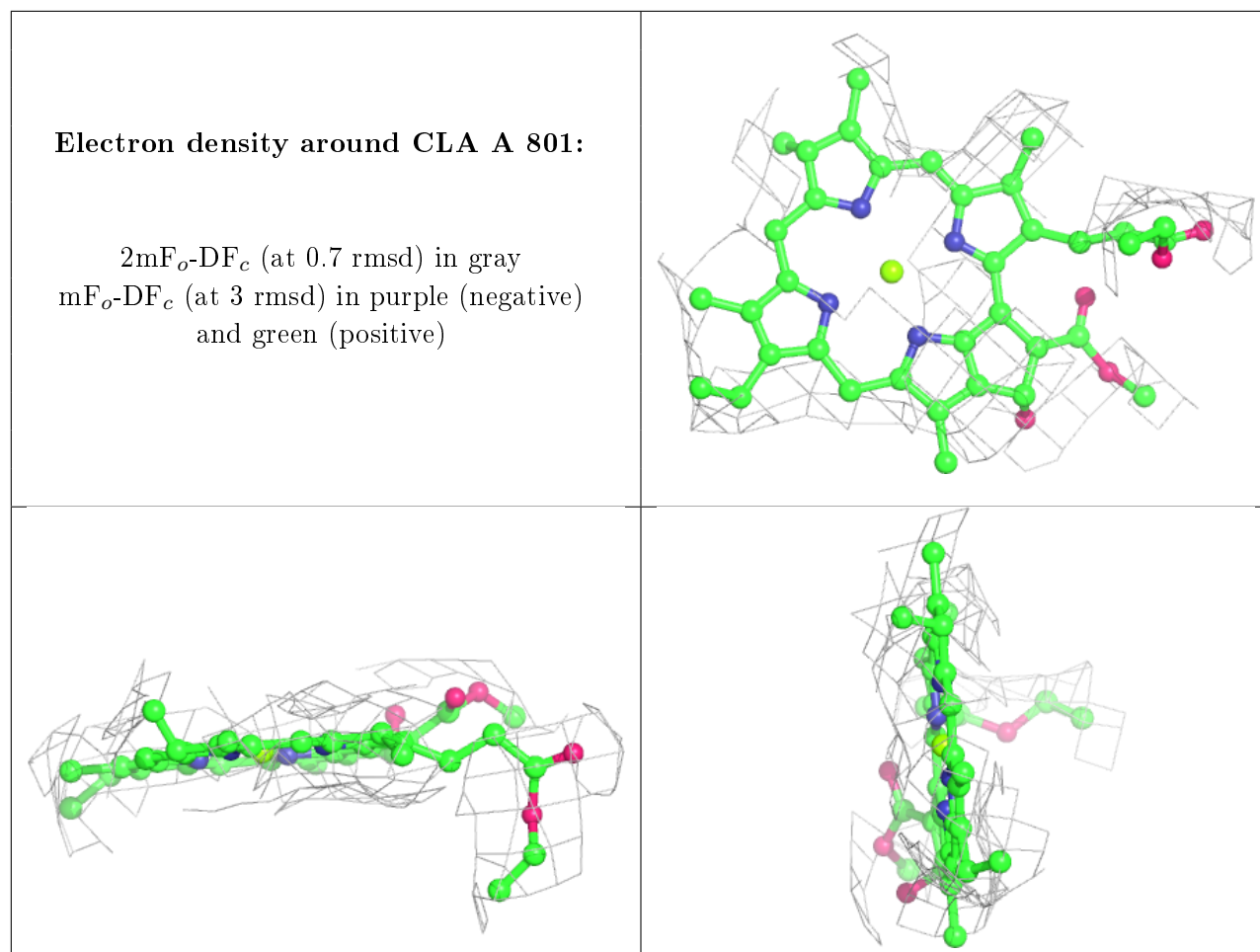
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

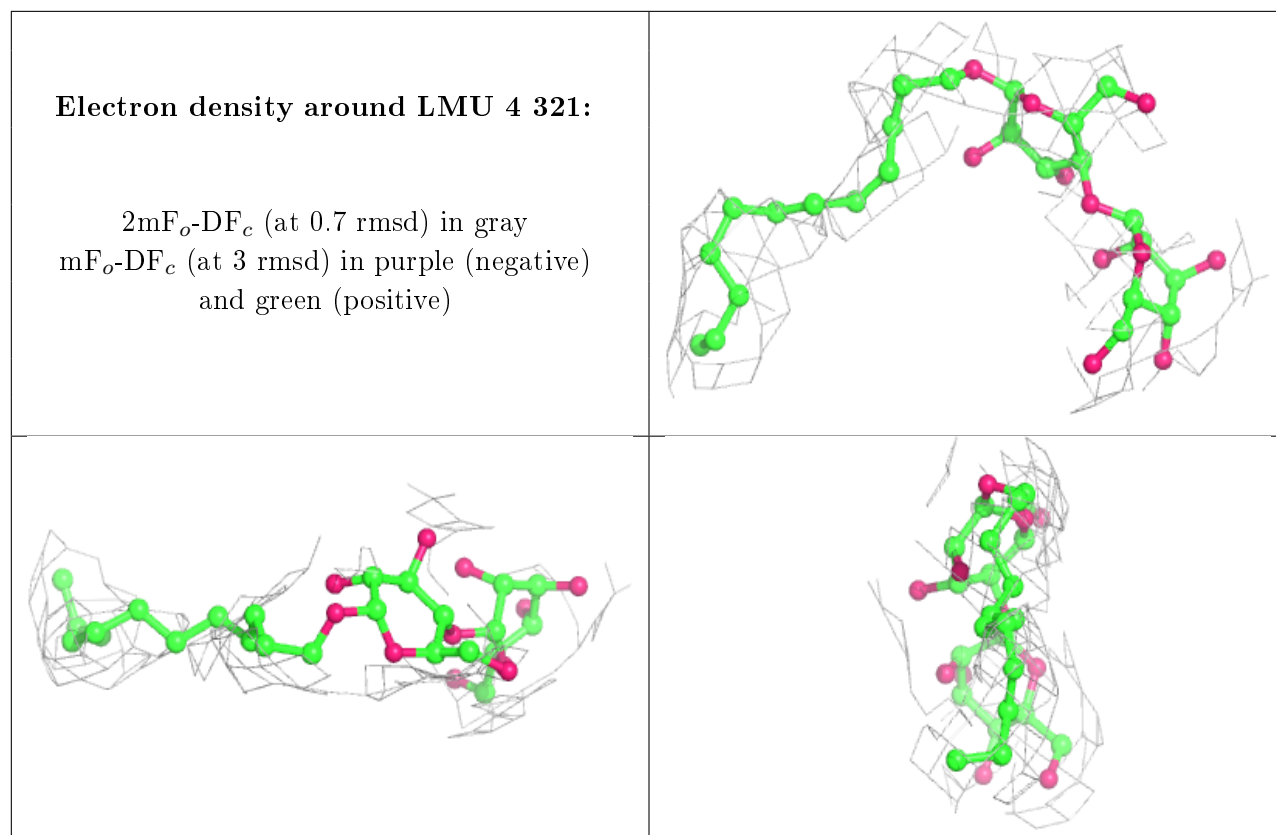
**Electron density around BCR A 847:**

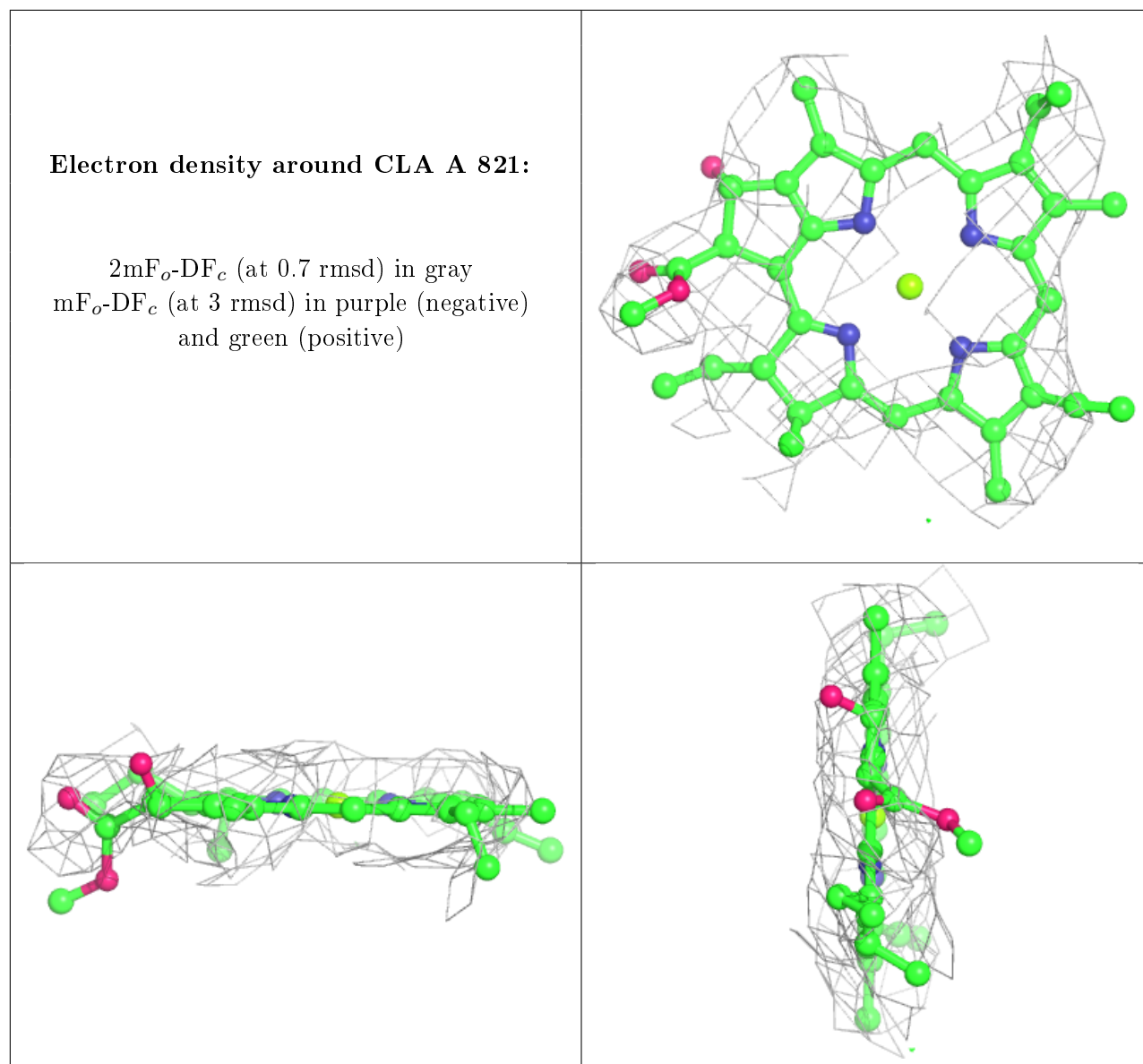
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





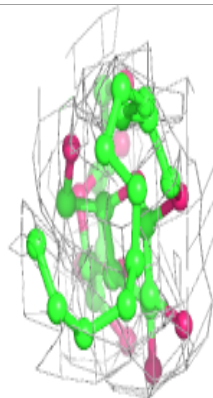
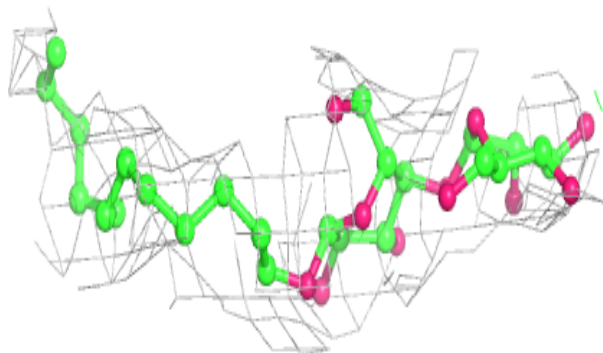
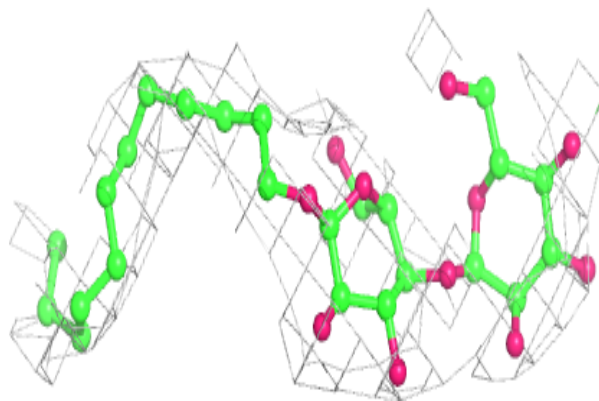




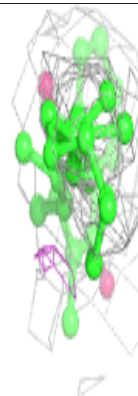
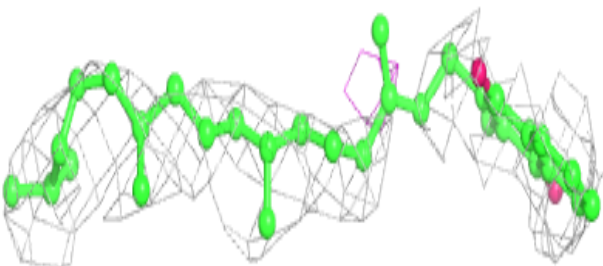
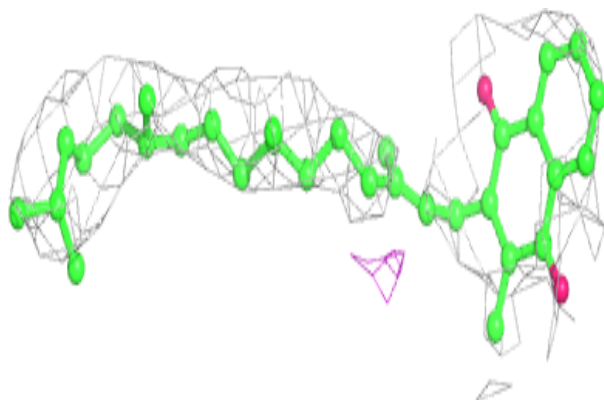


Electron density around LMU C 101:

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

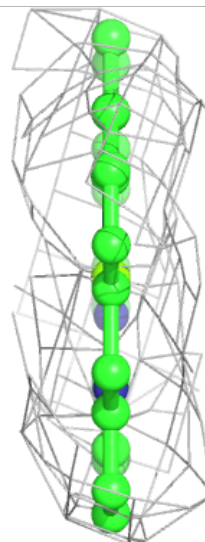
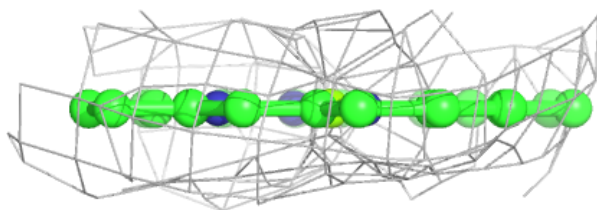
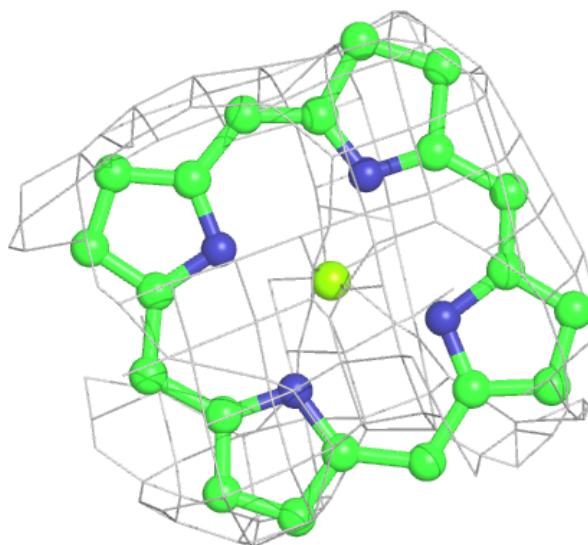
**Electron density around PQN A 842:**

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



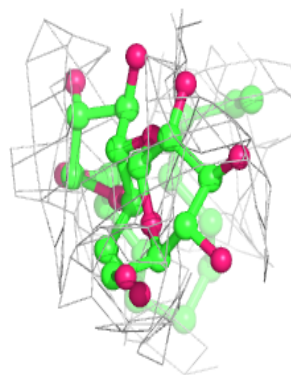
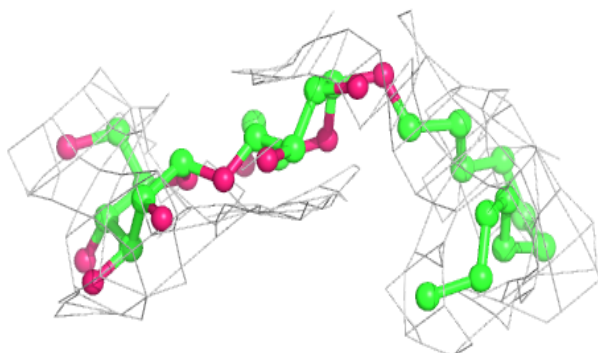
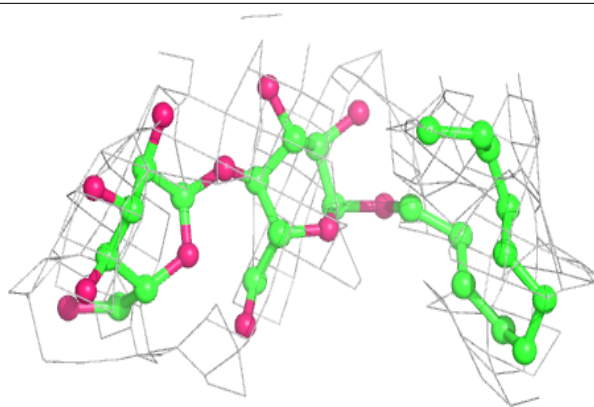
Electron density around CLA 3 305:

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

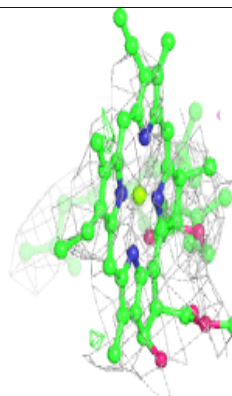
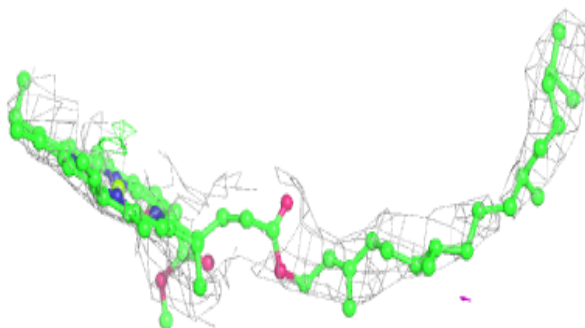
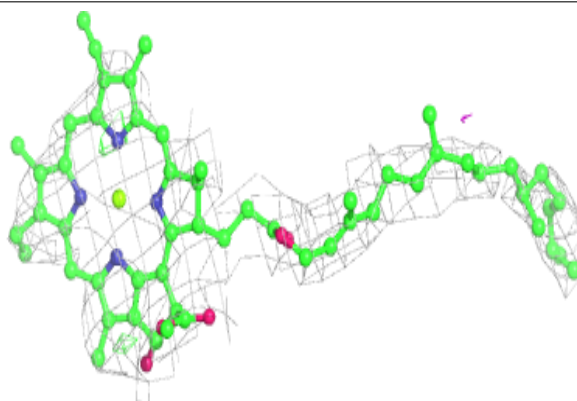


Electron density around LMU F 201:

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

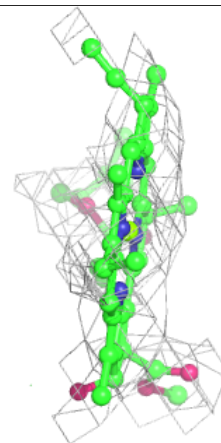
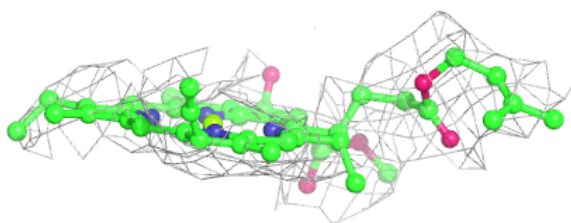
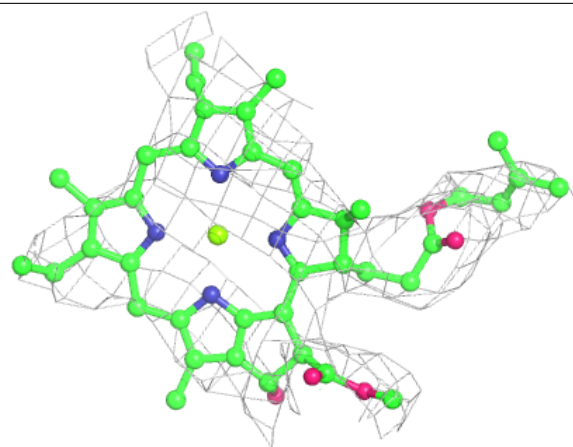
**Electron density around CLA A 805:**

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



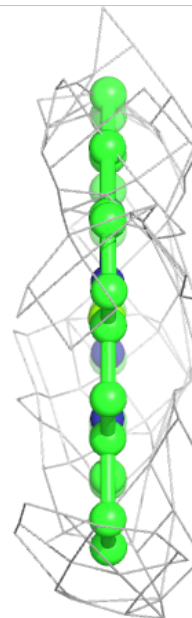
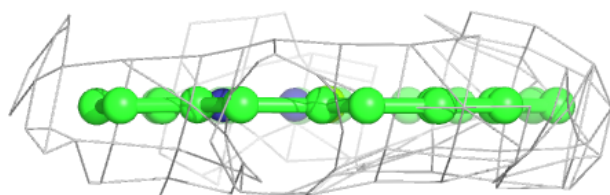
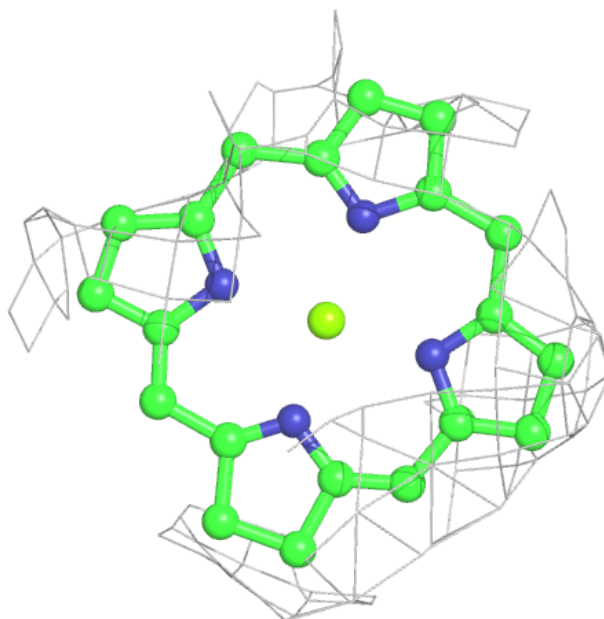
Electron density around CLA 2 305:

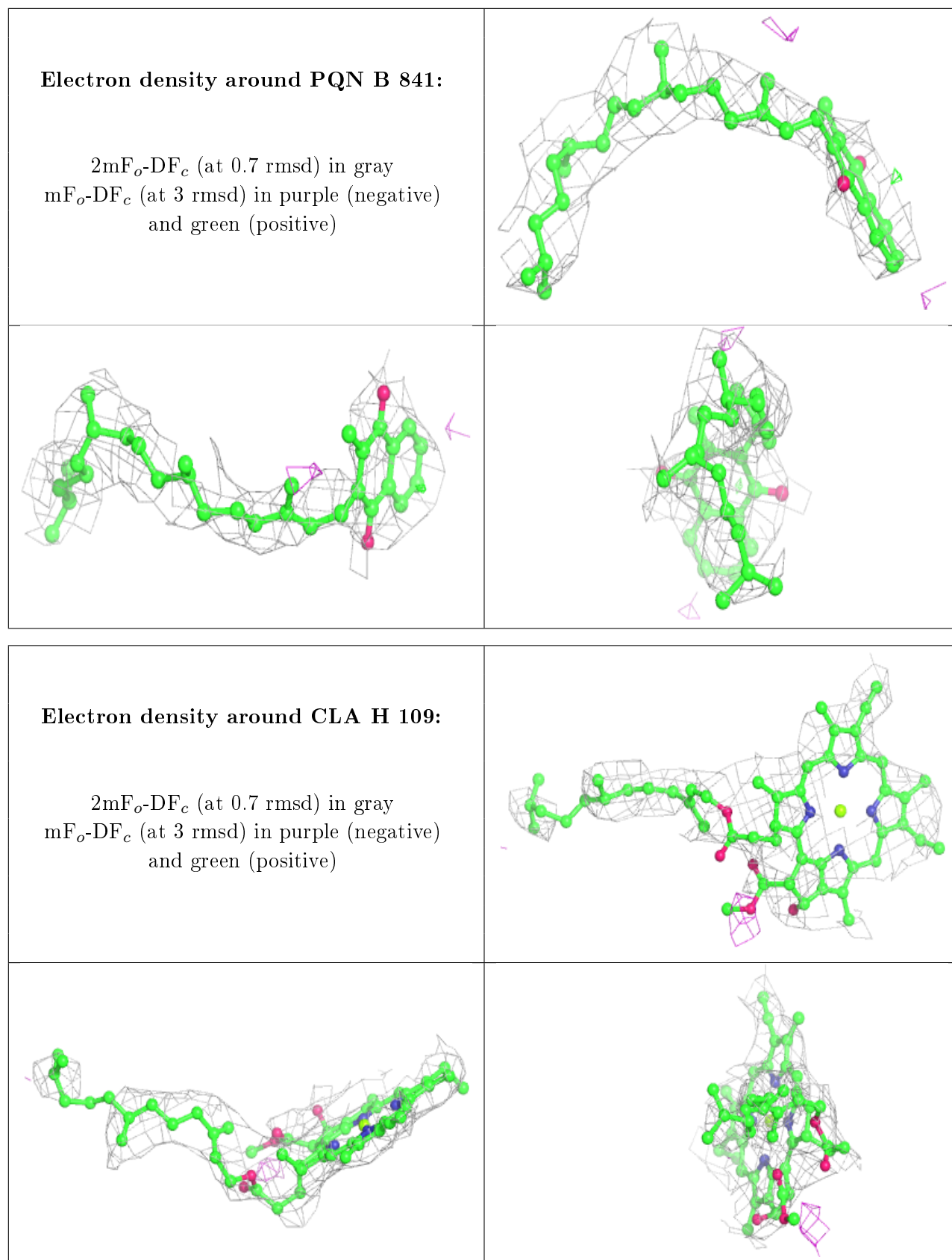
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 3 312:

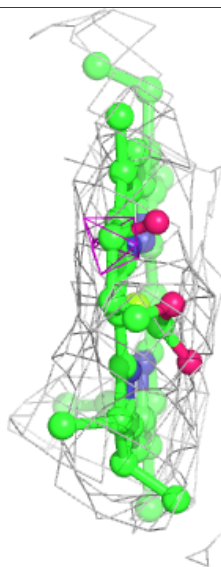
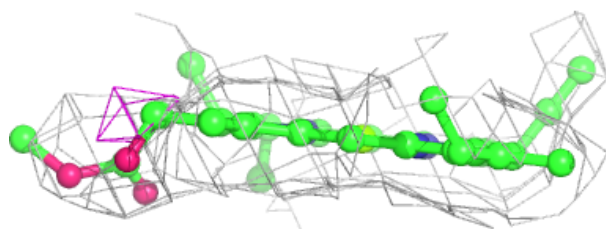
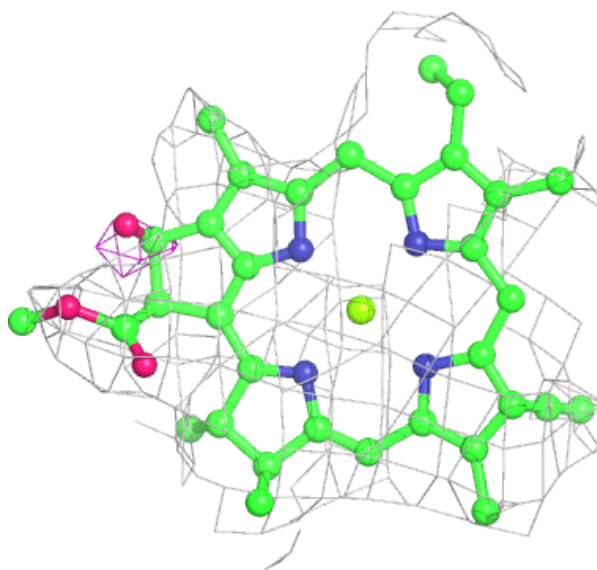
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





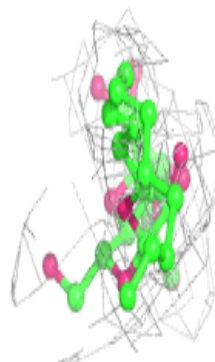
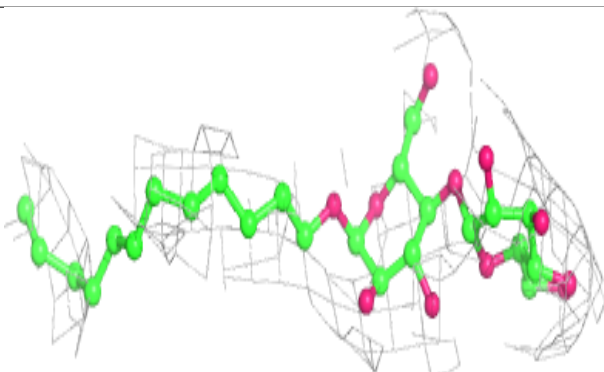
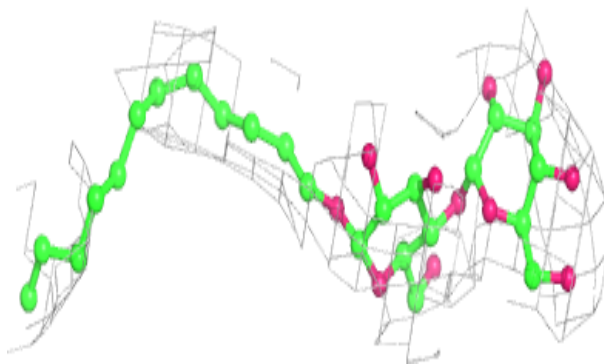
Electron density around CLA F 205:

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

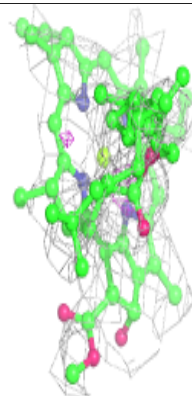
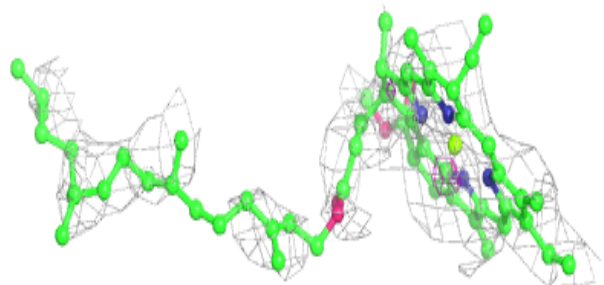
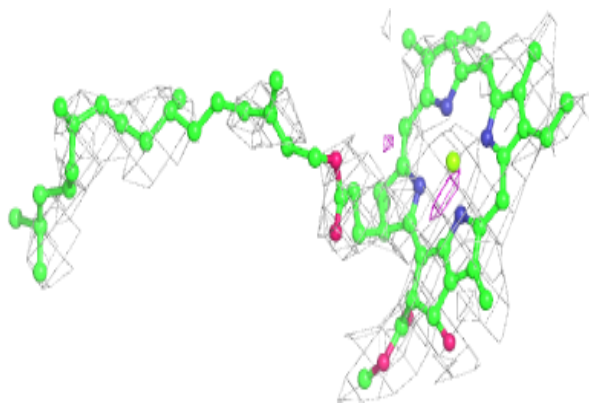


Electron density around LMU B 802:

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

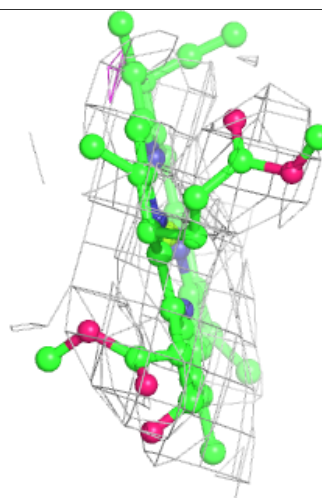
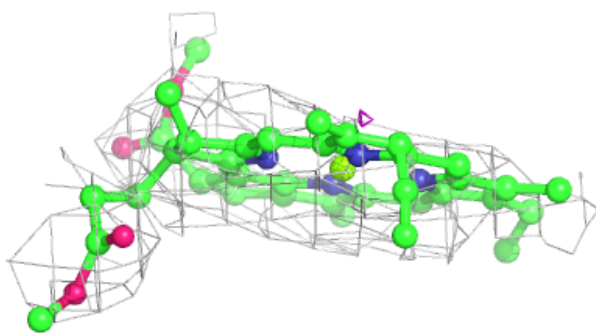
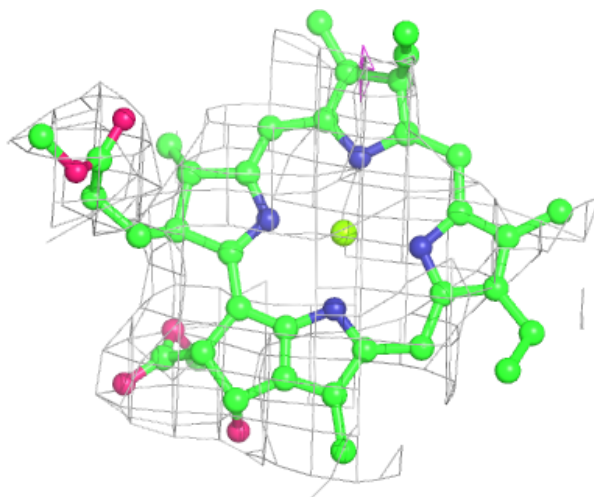
**Electron density around CLA A 819:**

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



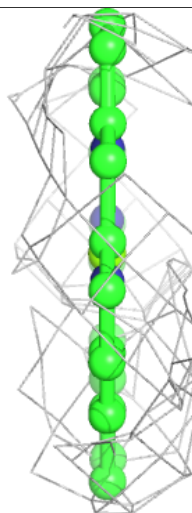
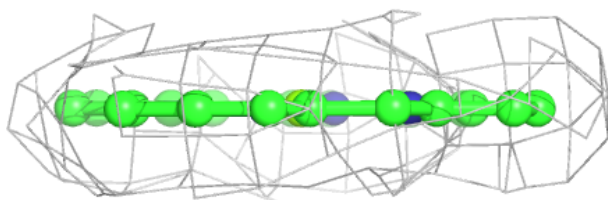
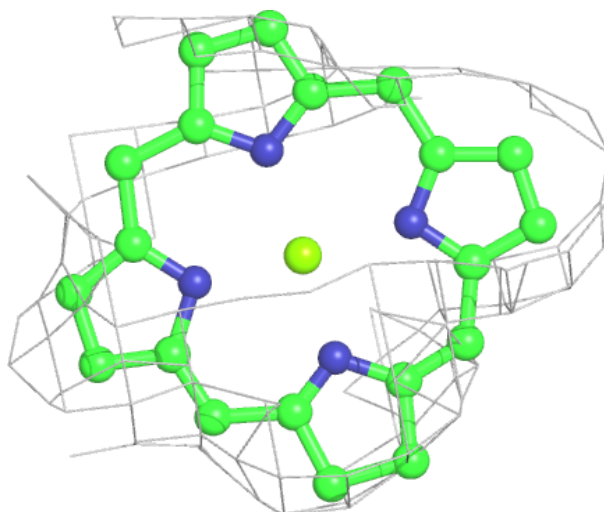
Electron density around CLA B 819:

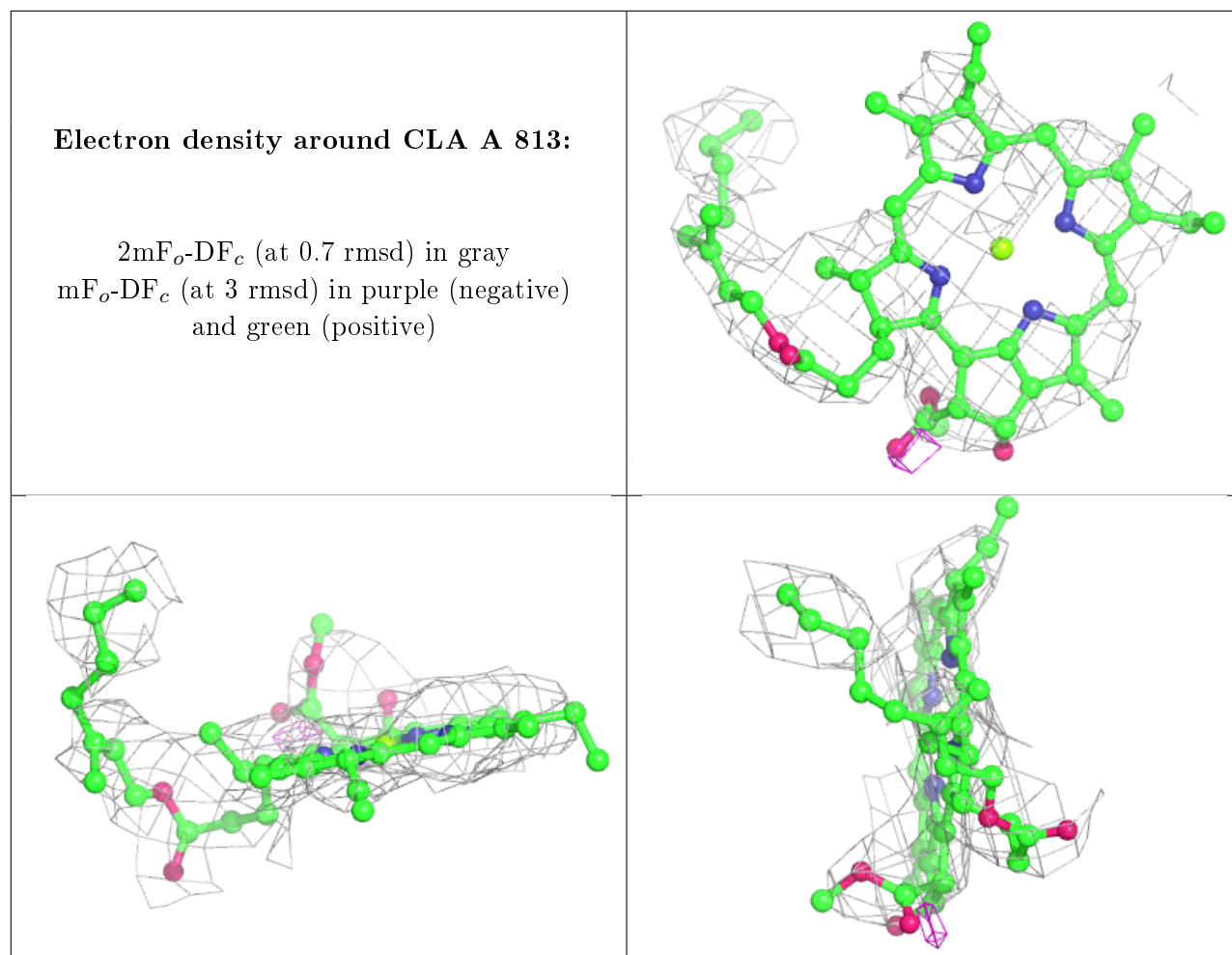
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

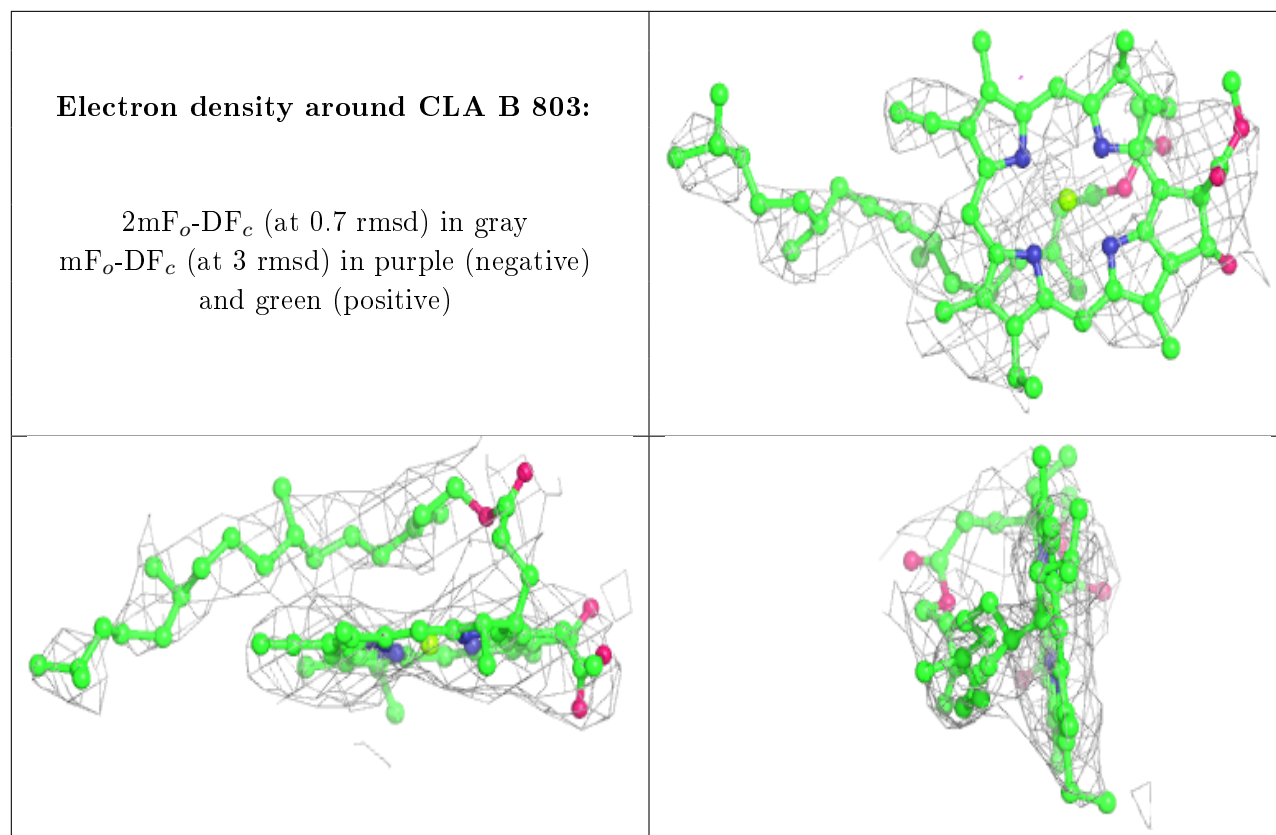


Electron density around CLA 1 205:

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

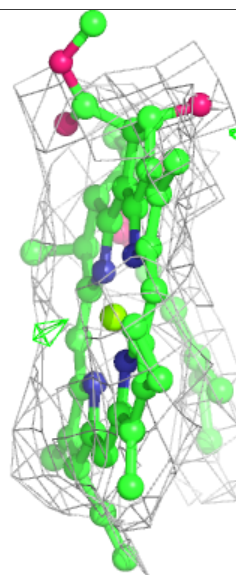
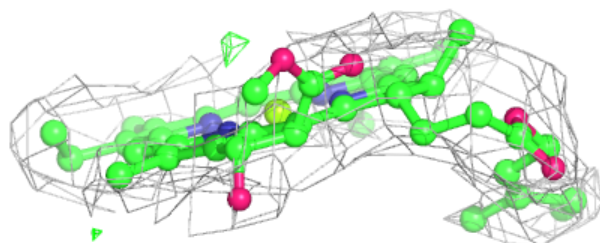
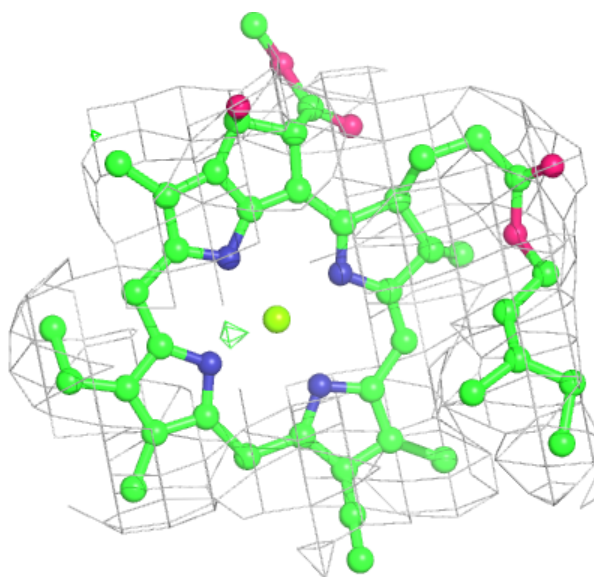






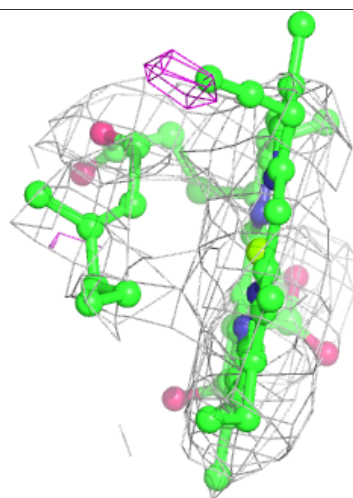
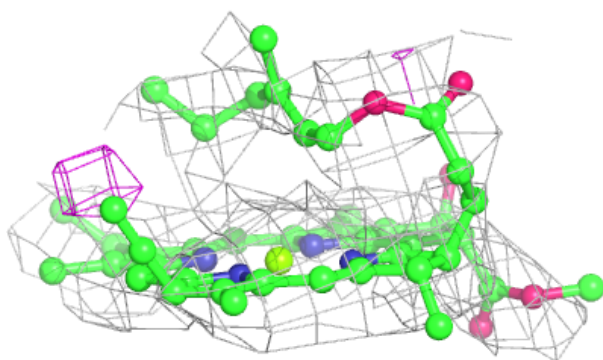
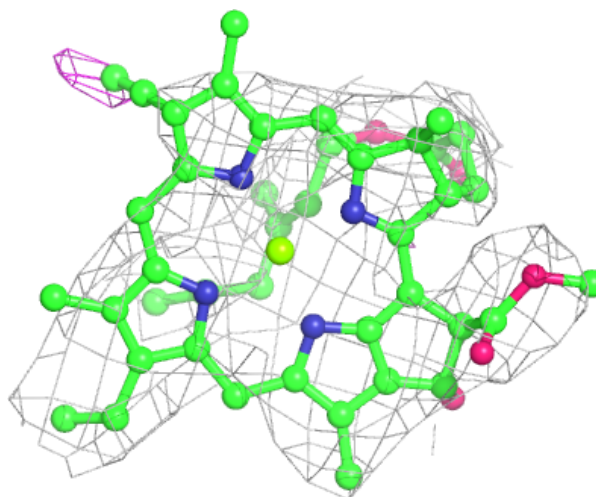
Electron density around CLA G 102:

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



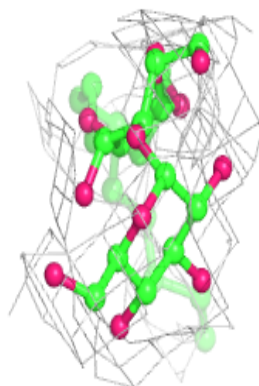
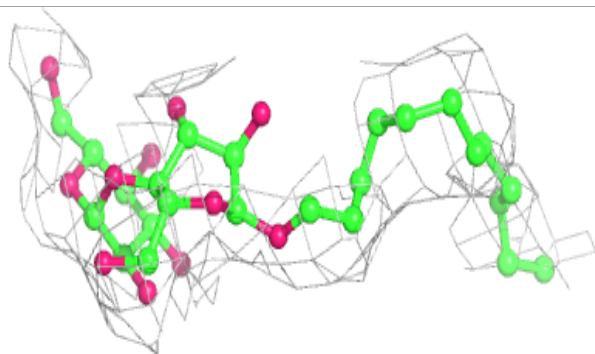
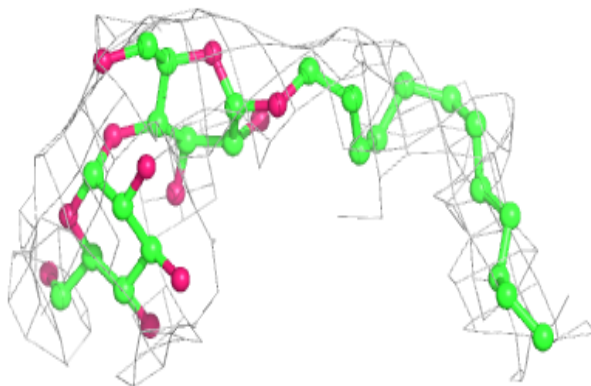
Electron density around CLA A 817:

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

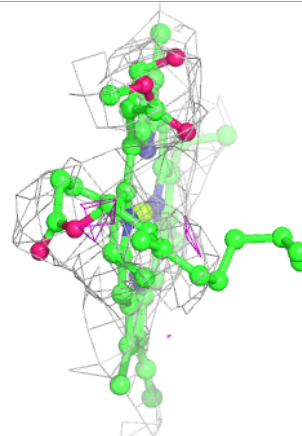
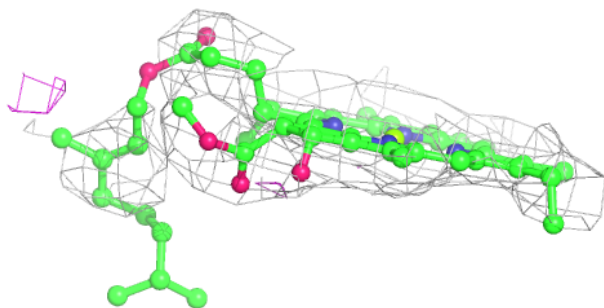
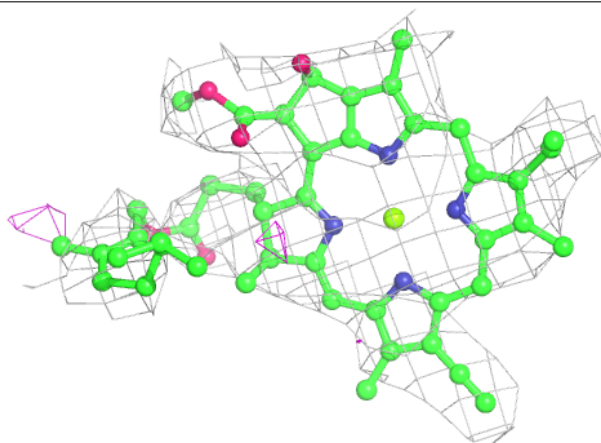


Electron density around LMU 2 319:

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

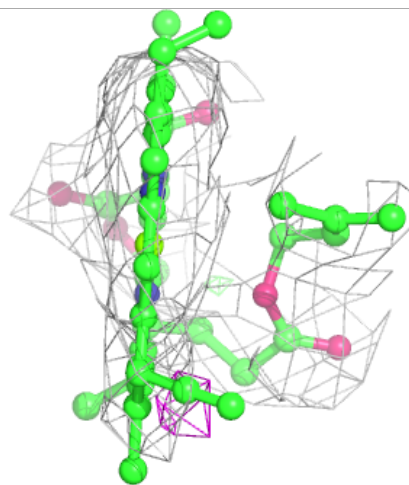
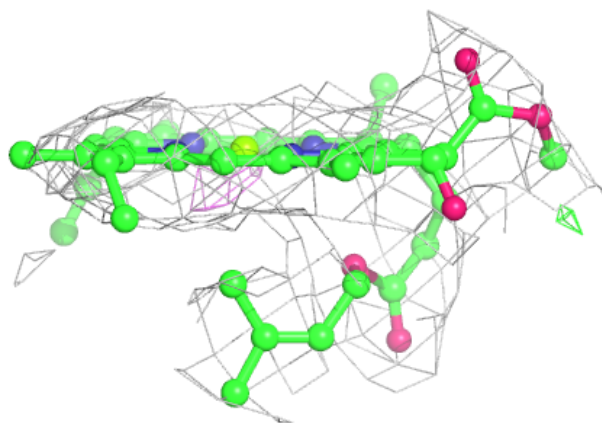
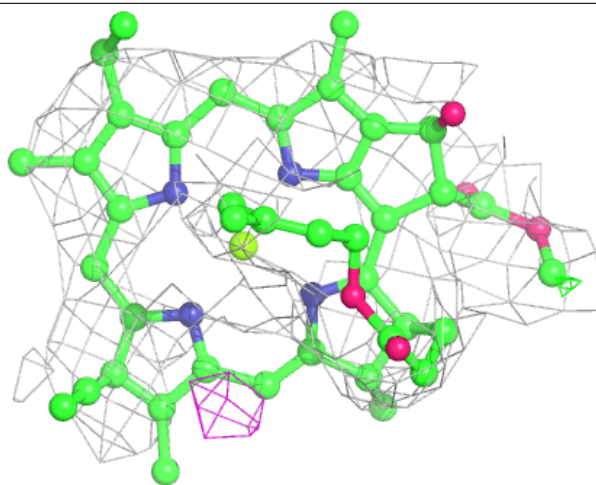
**Electron density around CLA A 806:**

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



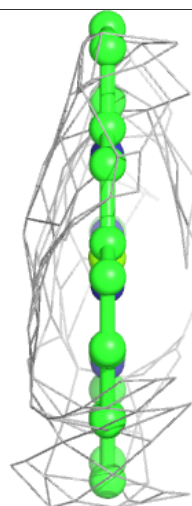
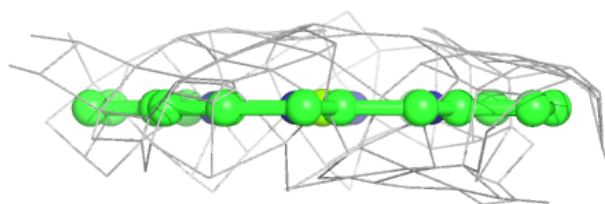
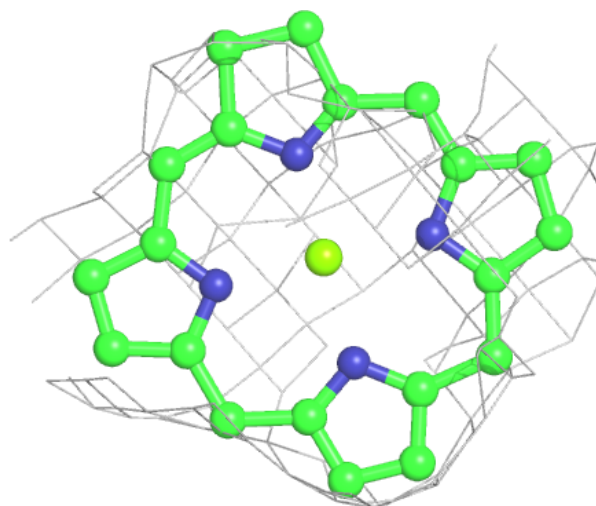
Electron density around CLA L 207:

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



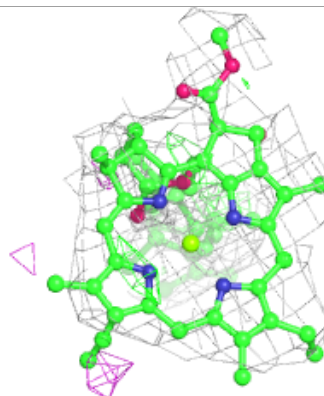
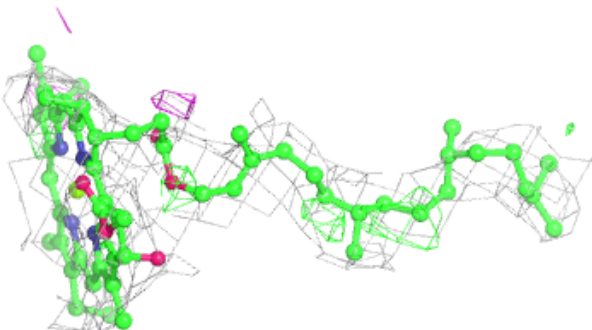
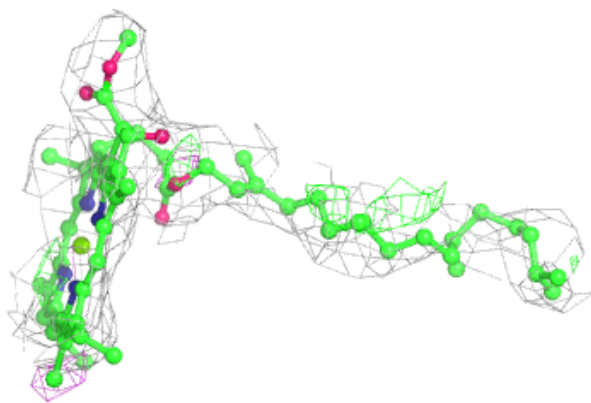
Electron density around CLA 4 309:

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

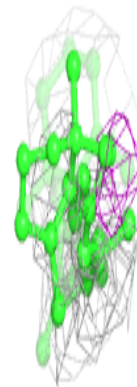
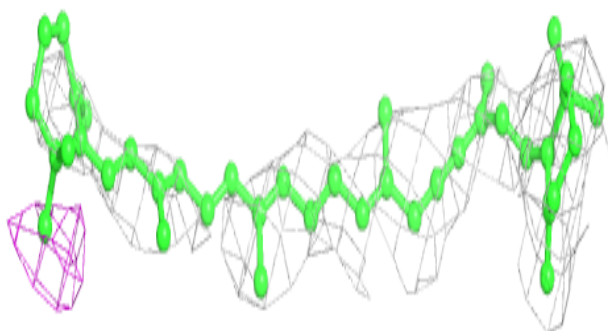
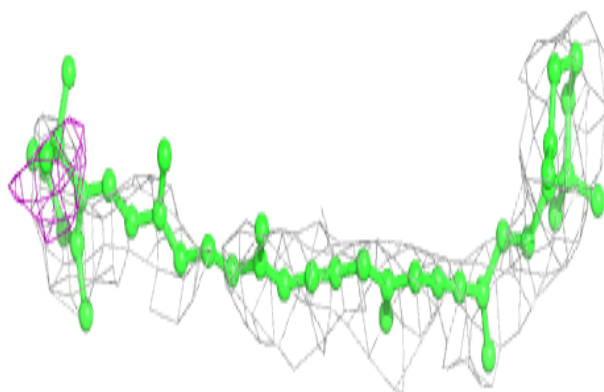


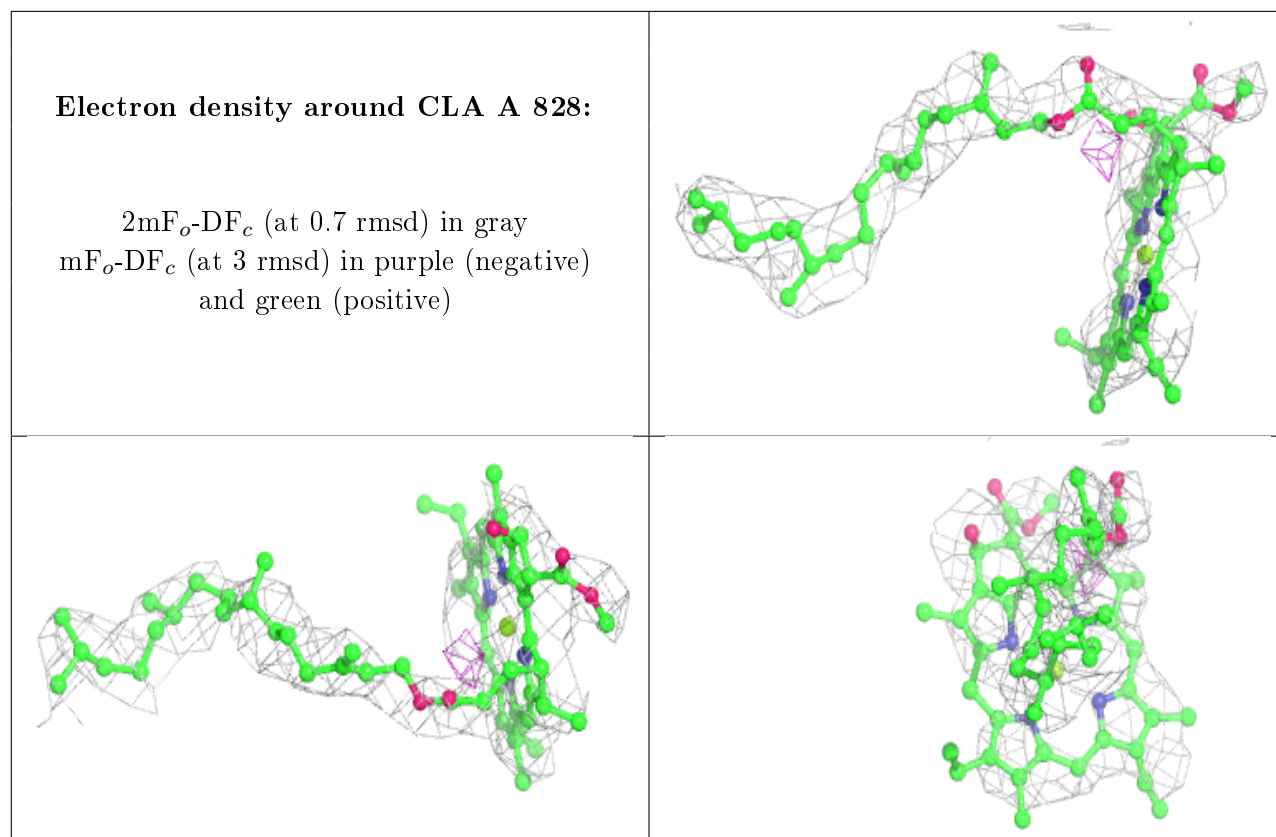
Electron density around CLA A 826:

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

**Electron density around BCR F 202:**

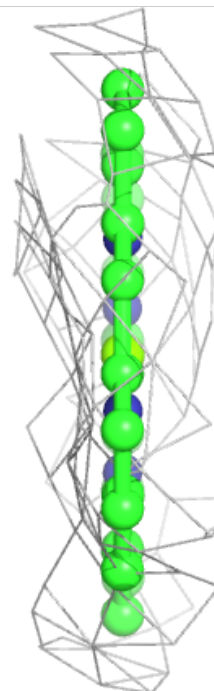
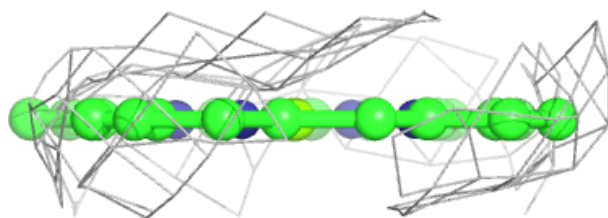
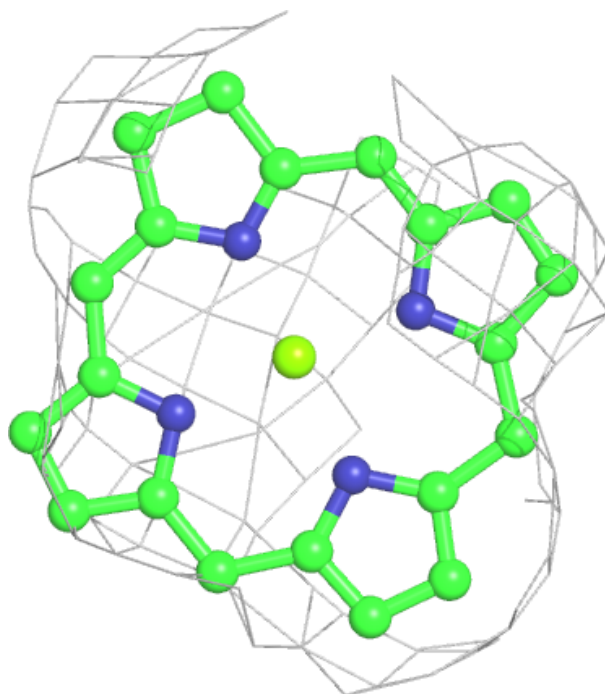
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





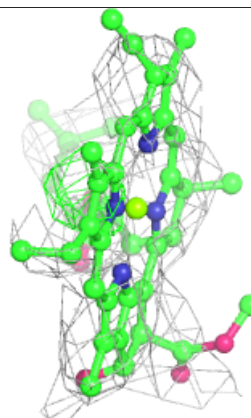
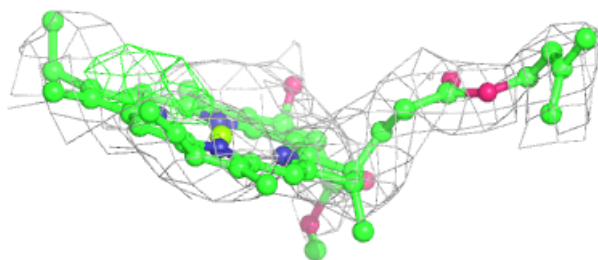
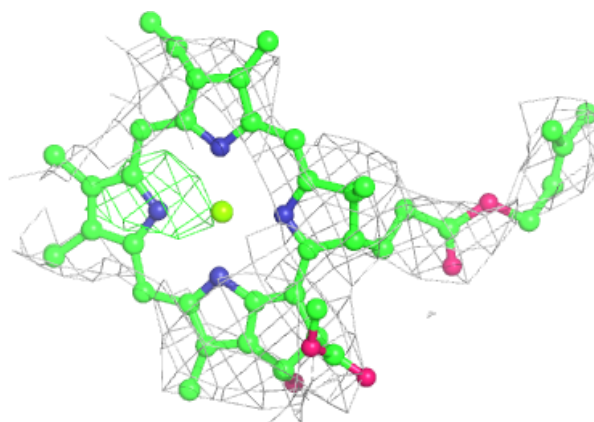
Electron density around CLA 3 320:

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



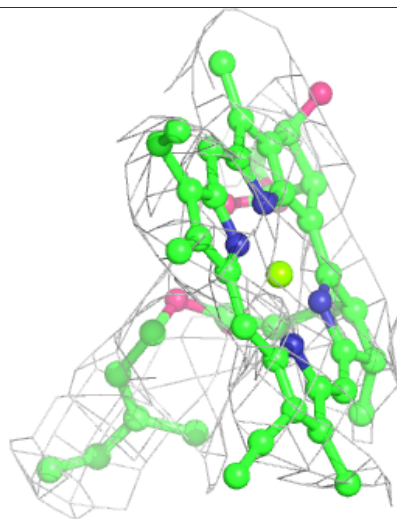
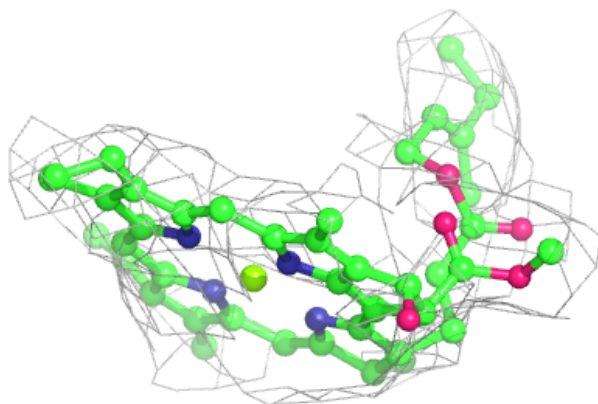
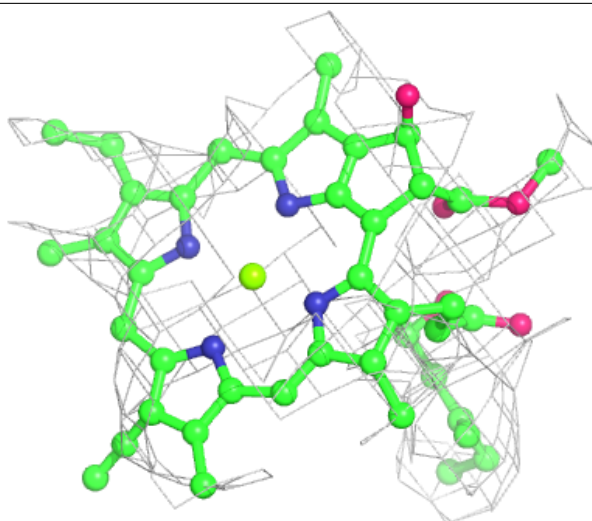
Electron density around CLA B 831:

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



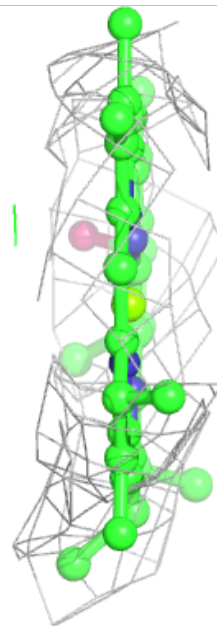
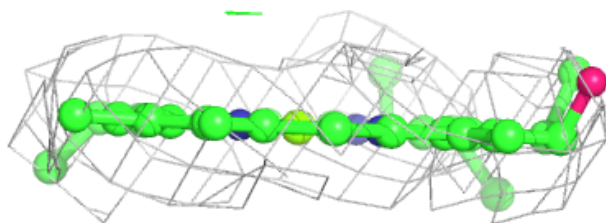
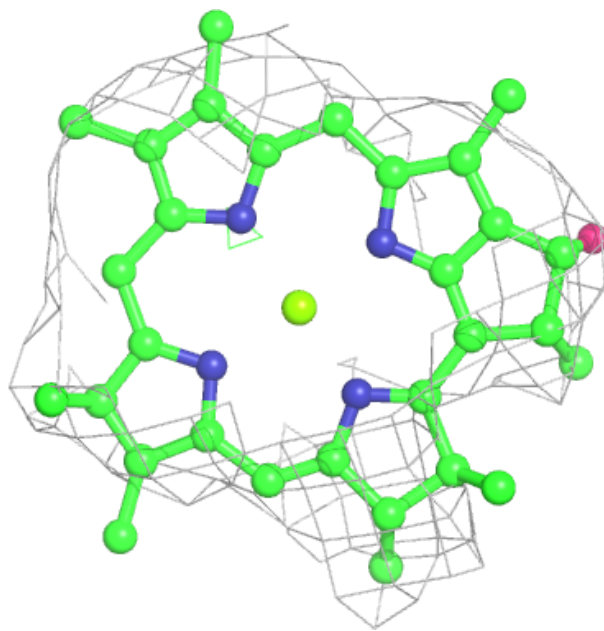
Electron density around CLA 1 207:

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



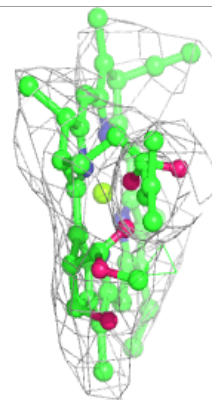
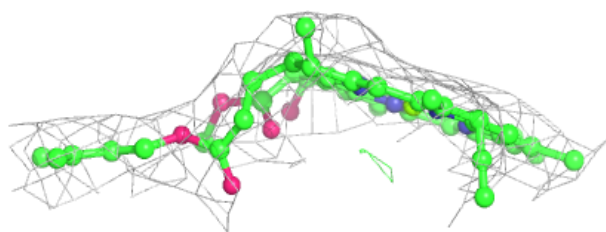
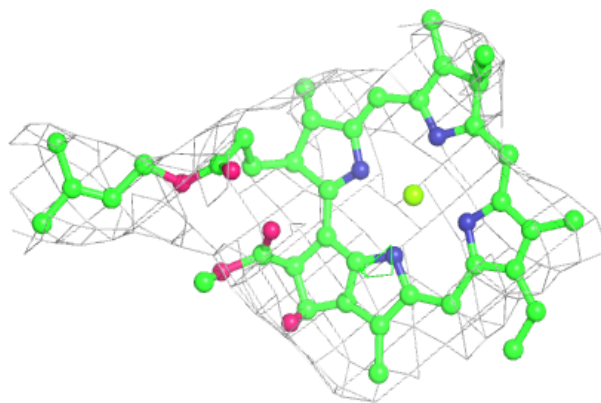
Electron density around CLA 3 304:

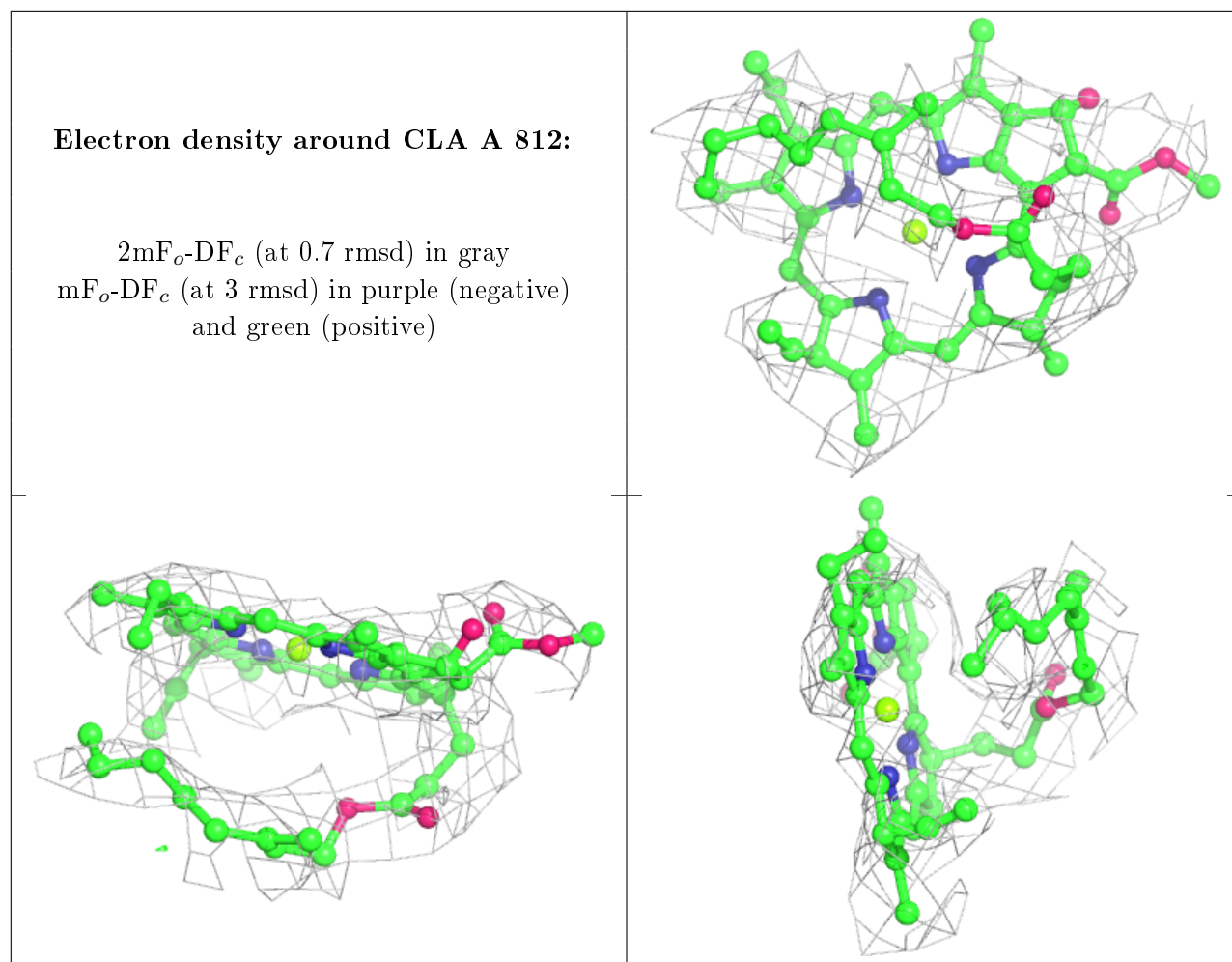
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA L 209:

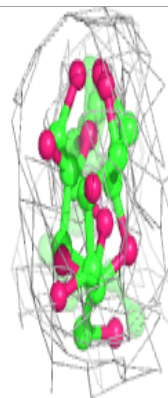
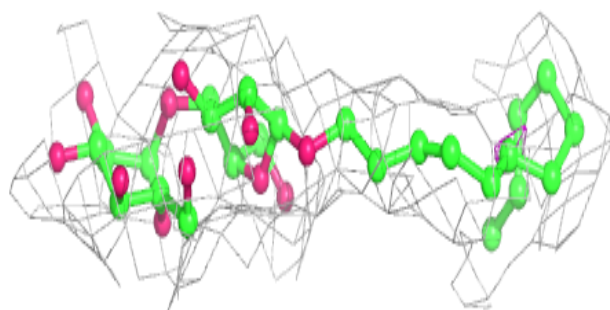
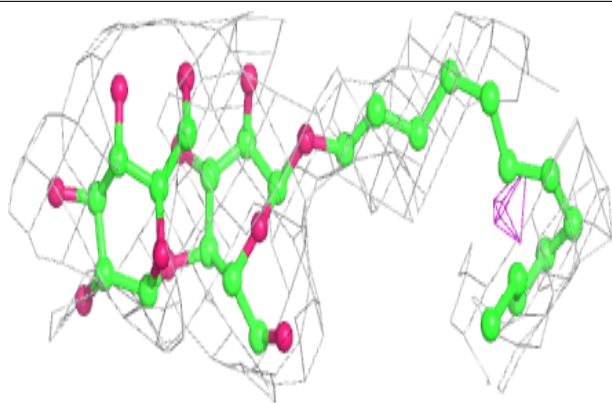
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



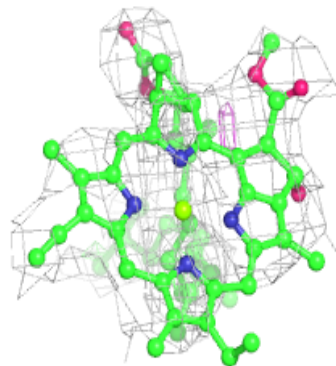
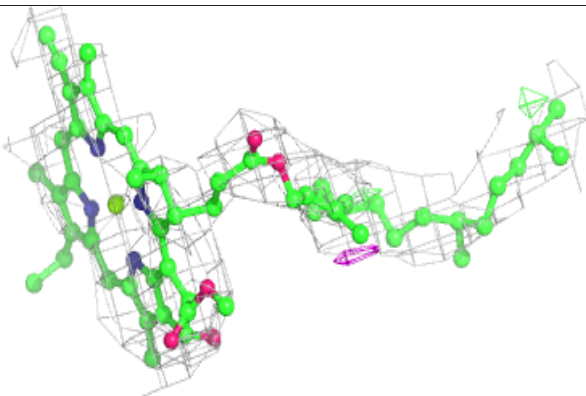
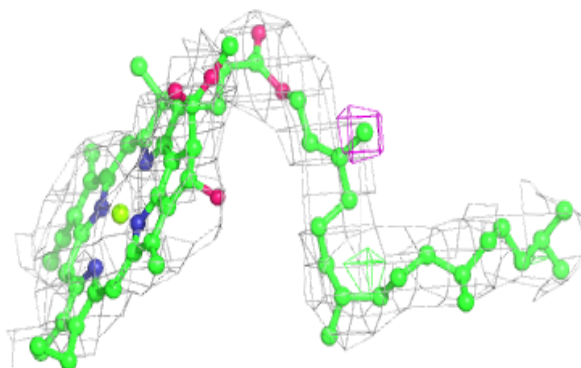


Electron density around LMU B 847:

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

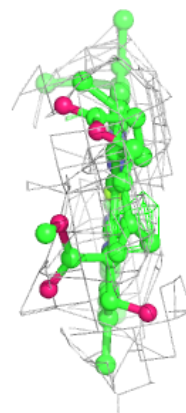
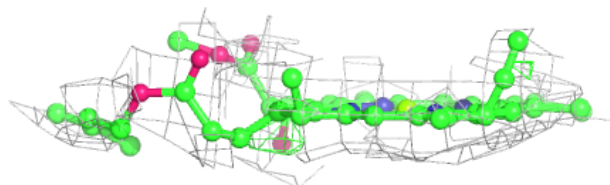
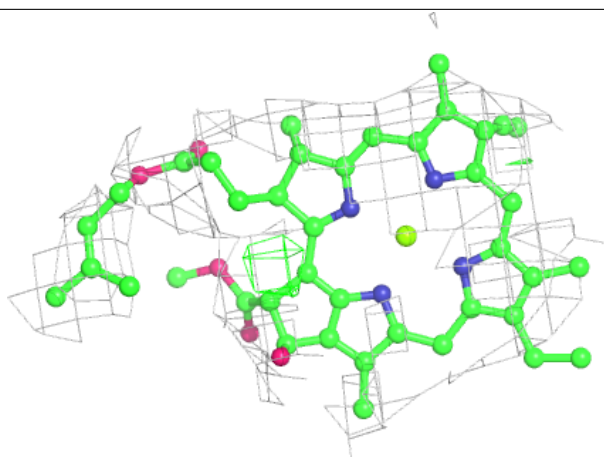
**Electron density around CLA B 849:**

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

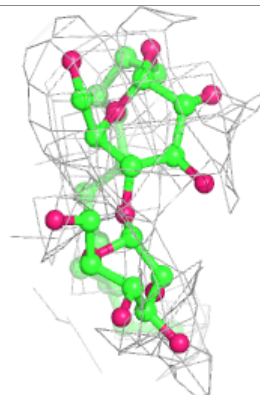
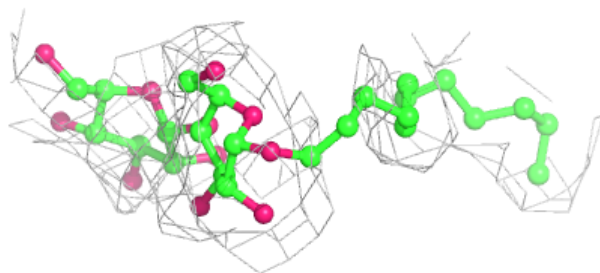
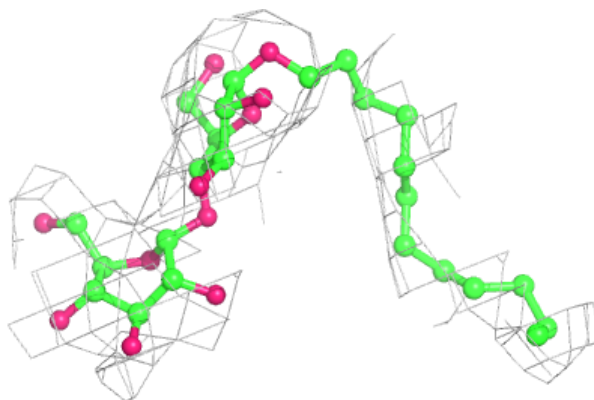


Electron density around CLA 2 312:

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

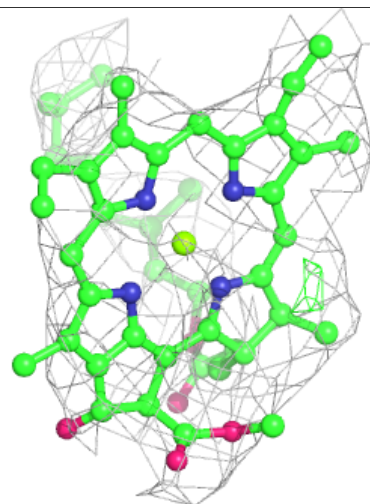
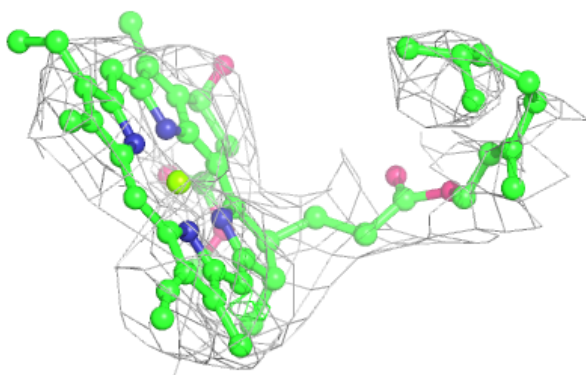
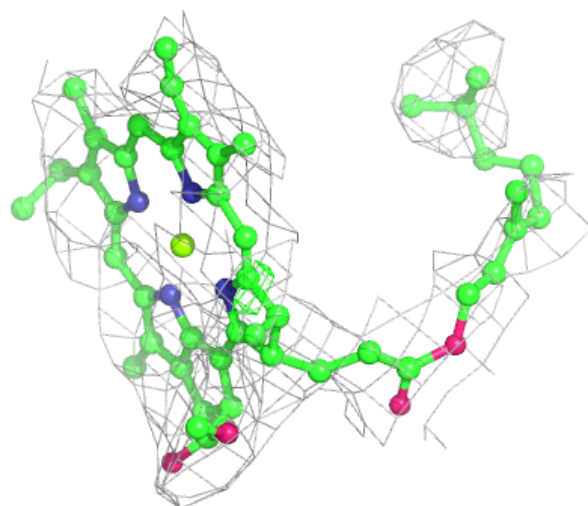
**Electron density around LMU L 205:**

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



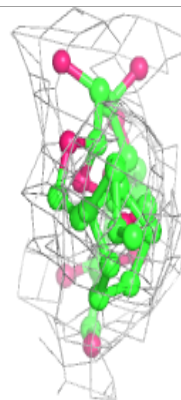
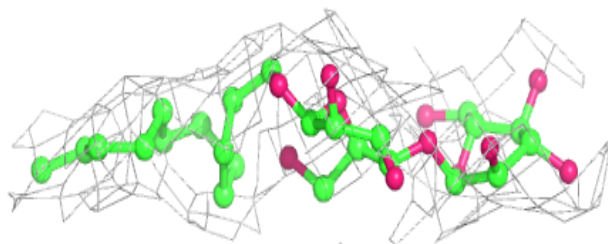
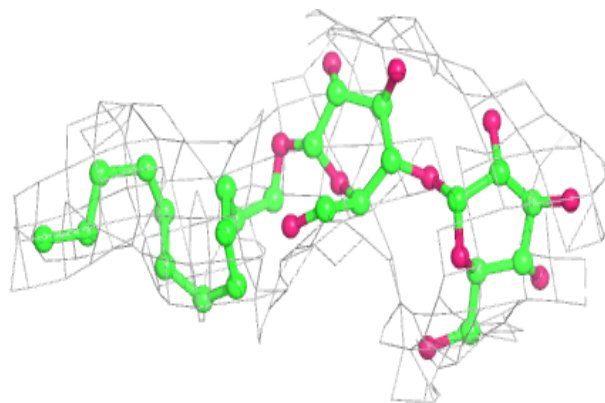
Electron density around CLA A 804:

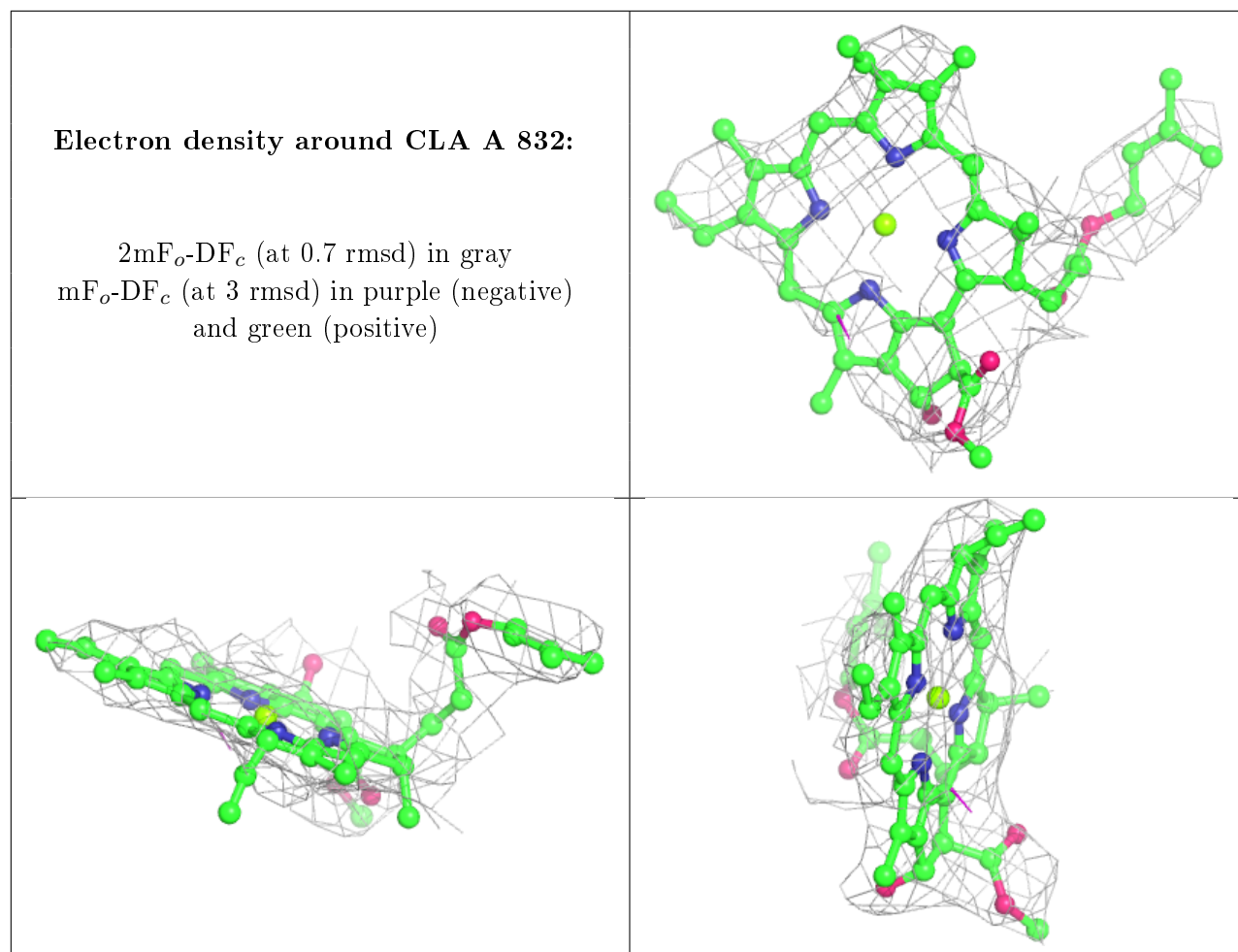
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMU A 854:

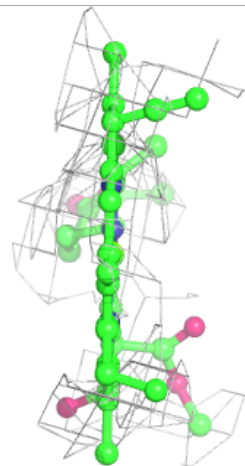
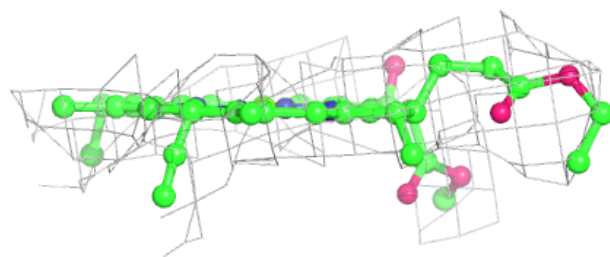
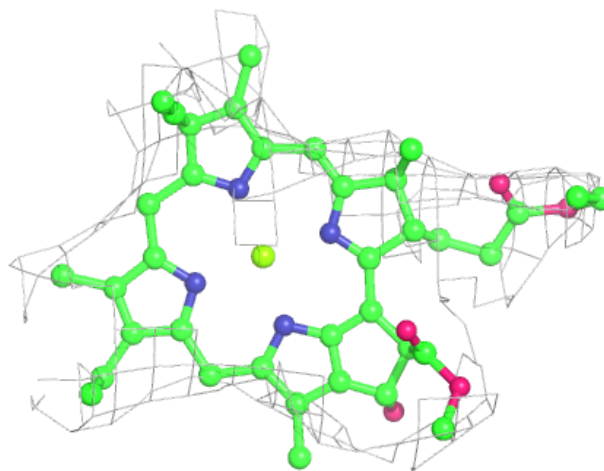
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





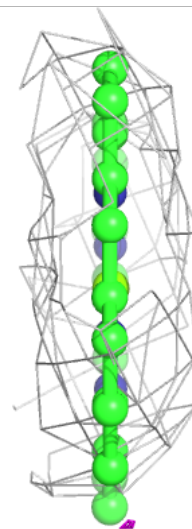
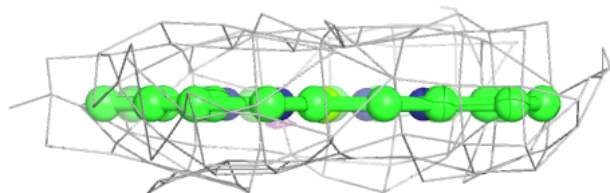
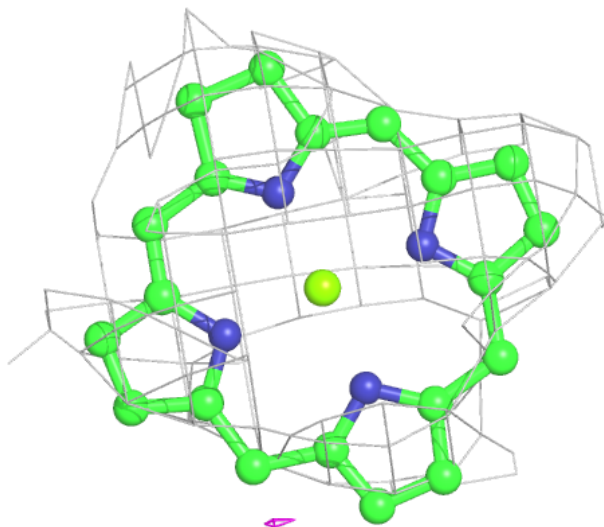
Electron density around CLA 1 203:

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



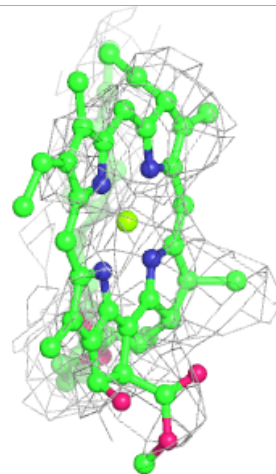
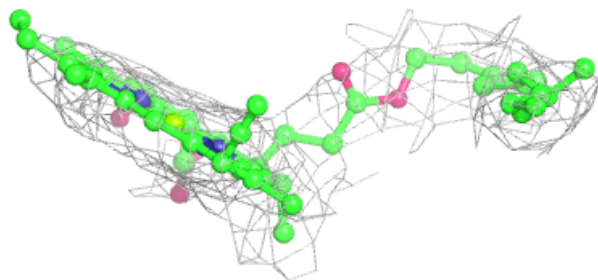
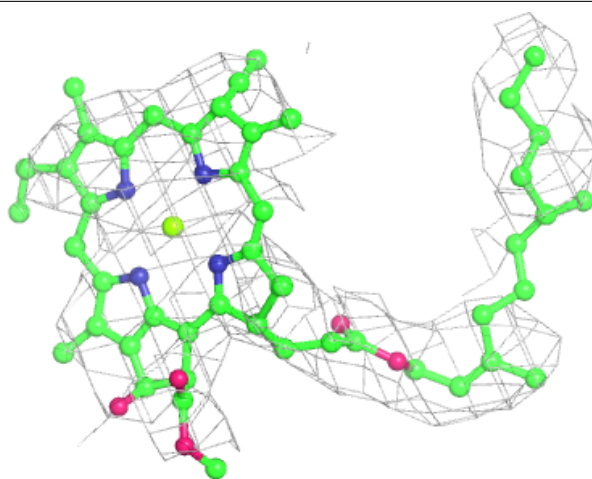
Electron density around CLA 3 303:

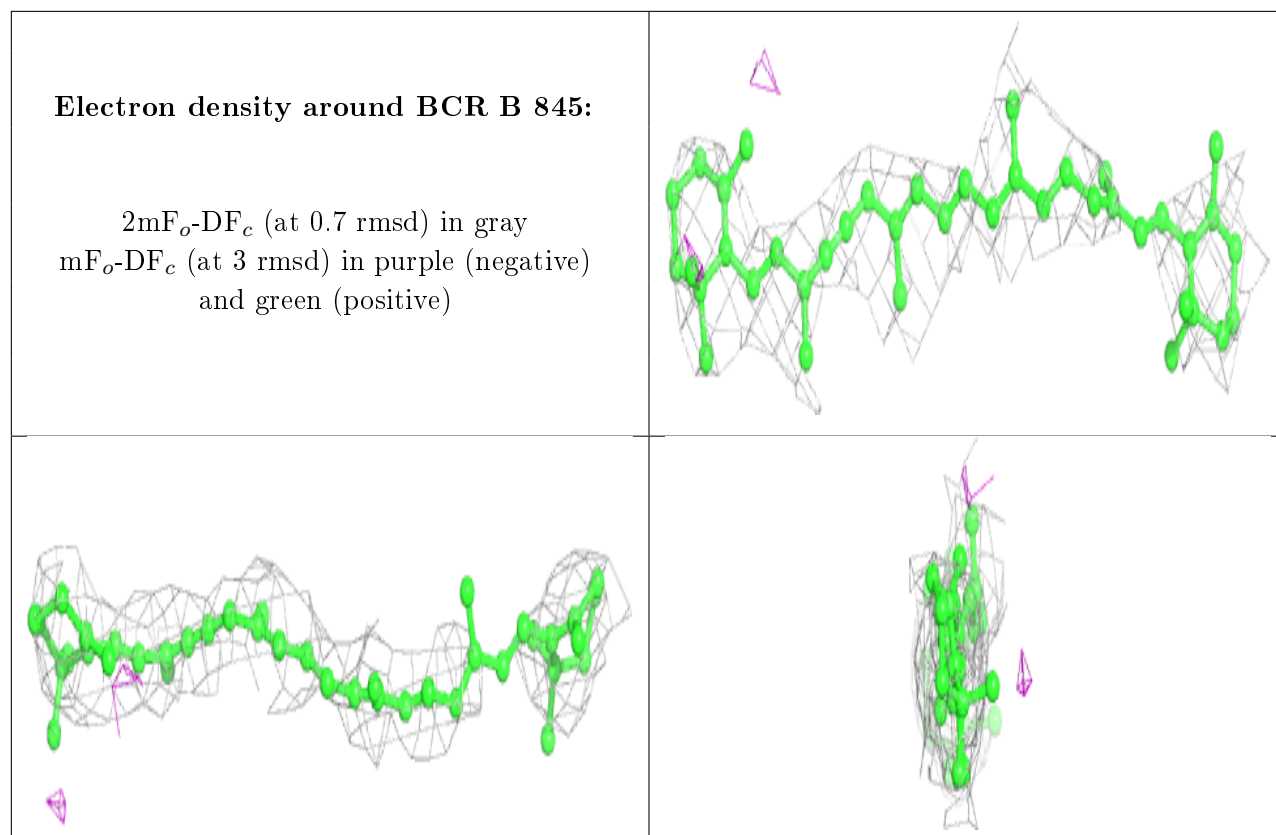
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 823:

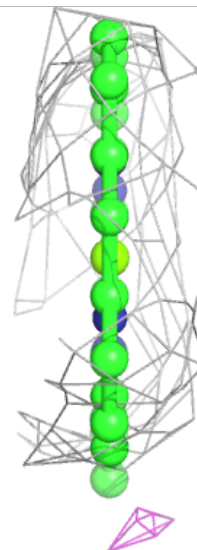
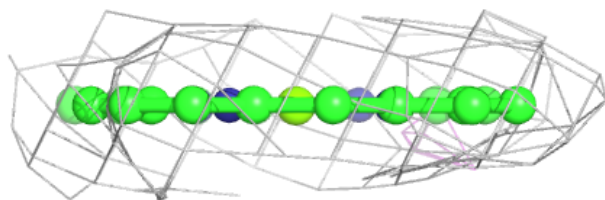
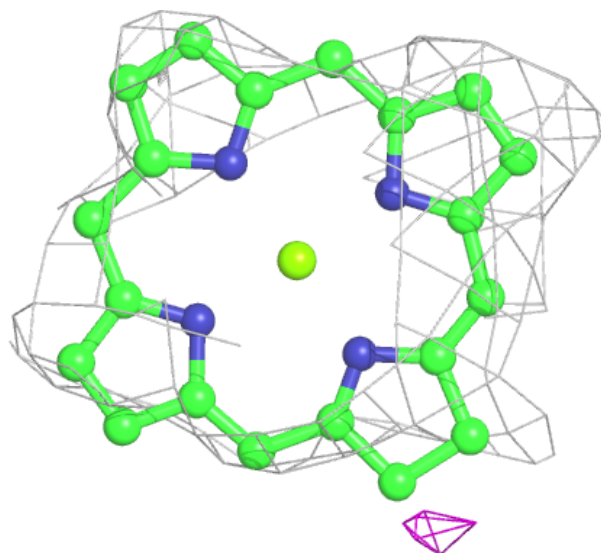
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





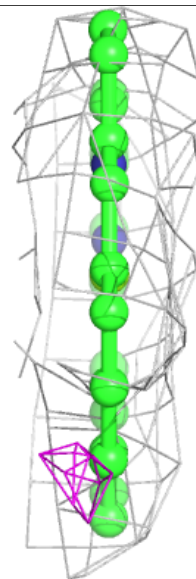
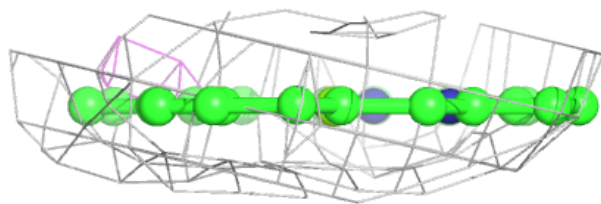
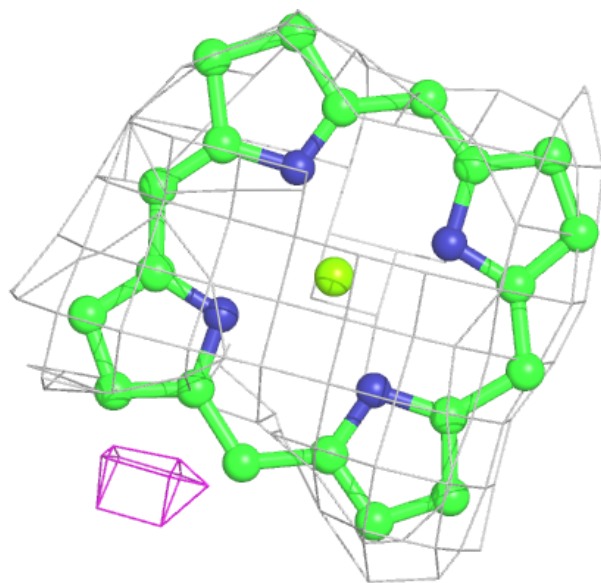
Electron density around CLA 2 315:

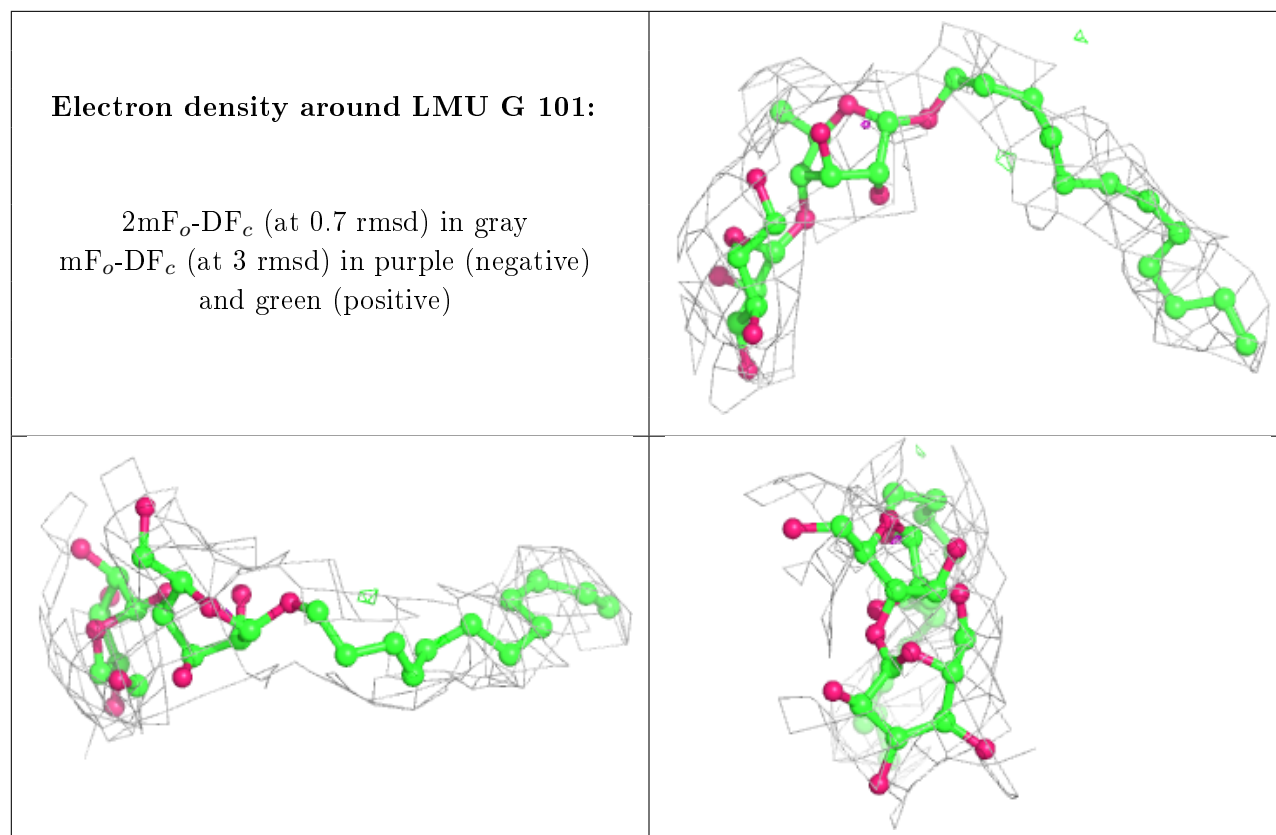
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 3 316:

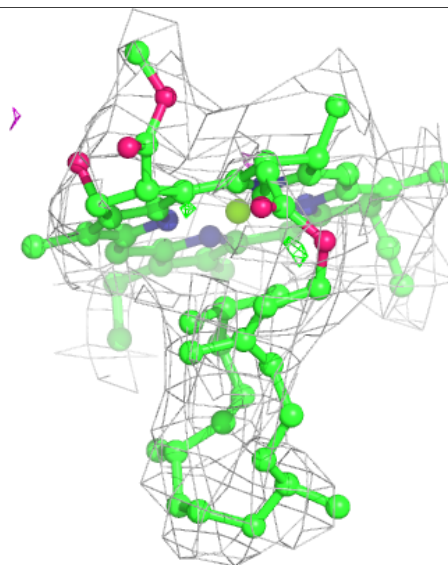
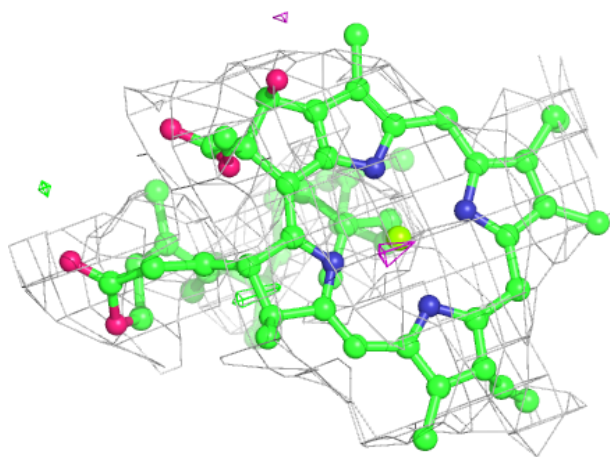
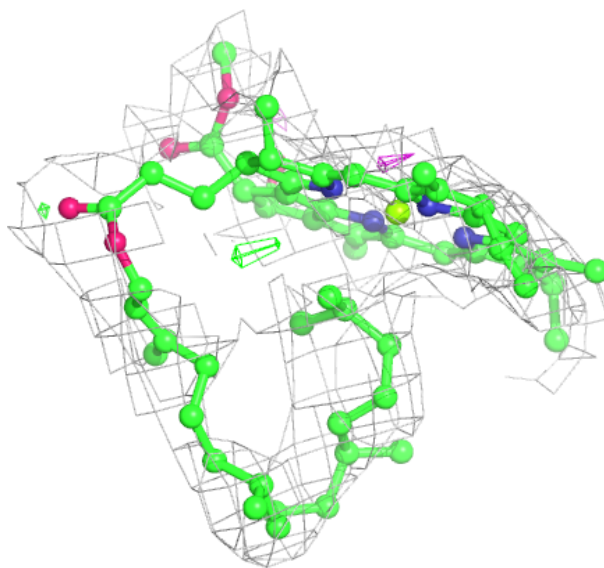
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





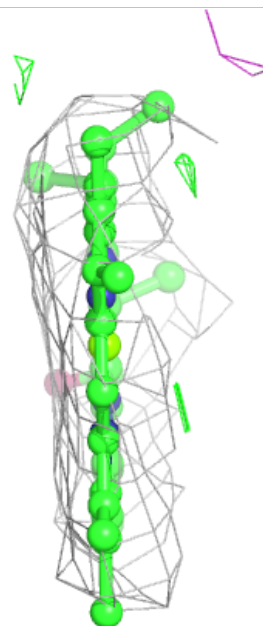
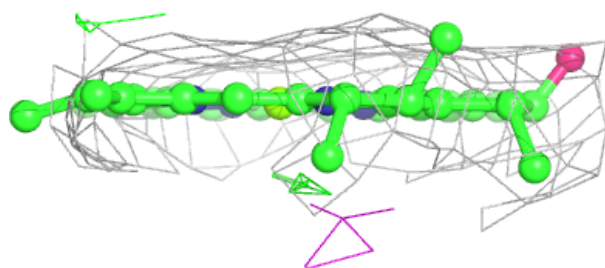
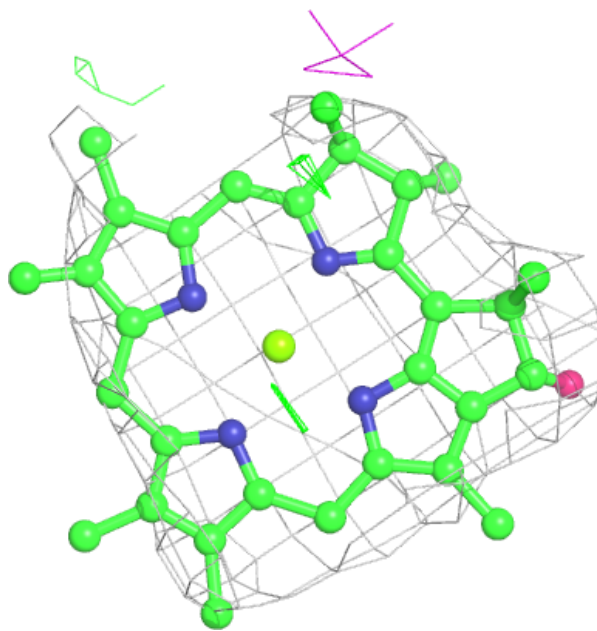
Electron density around CLA 2 316:

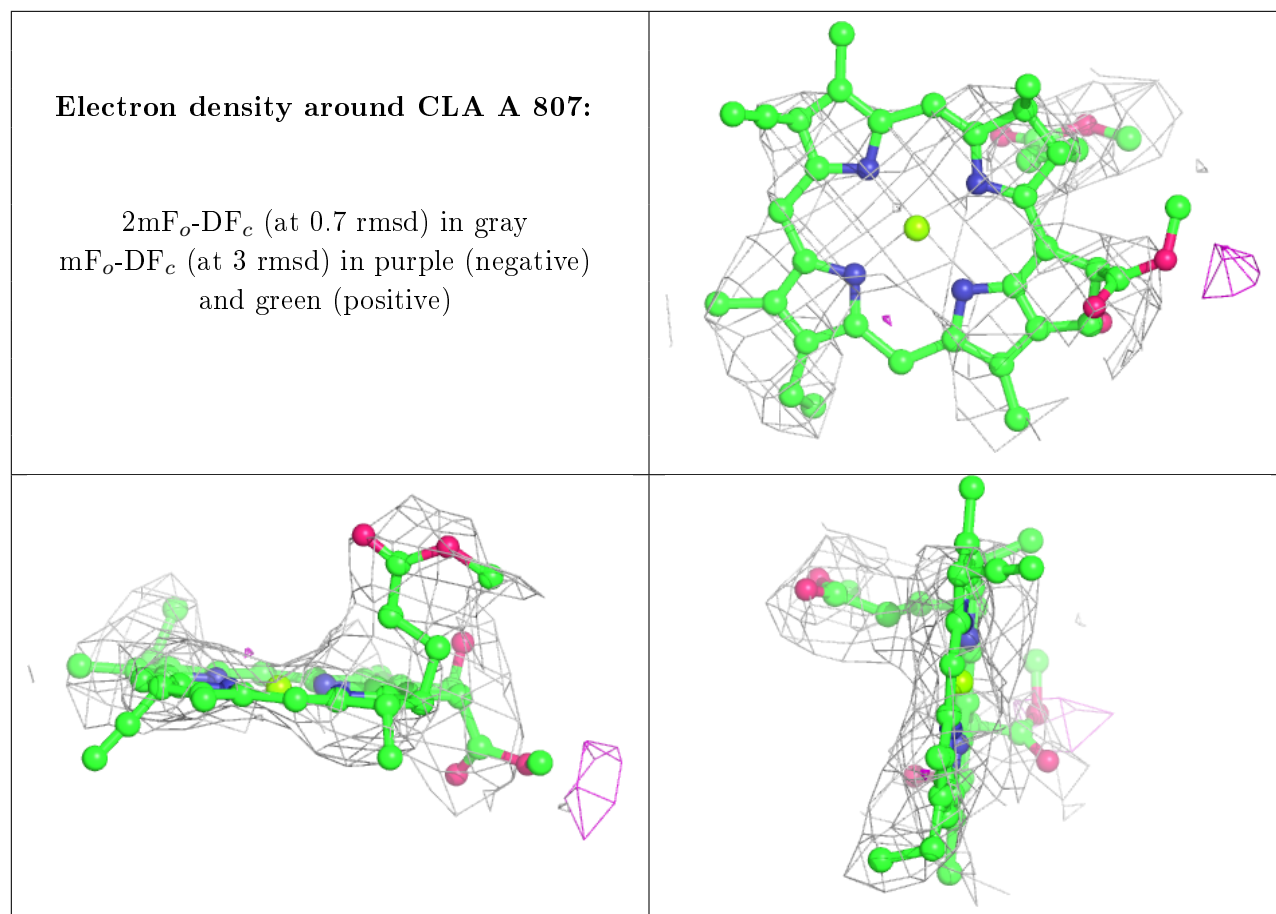
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA F 204:

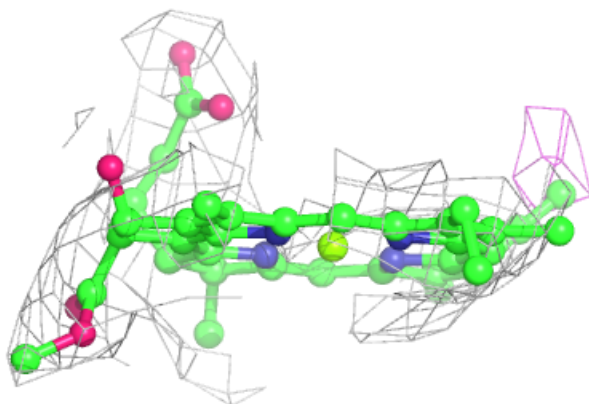
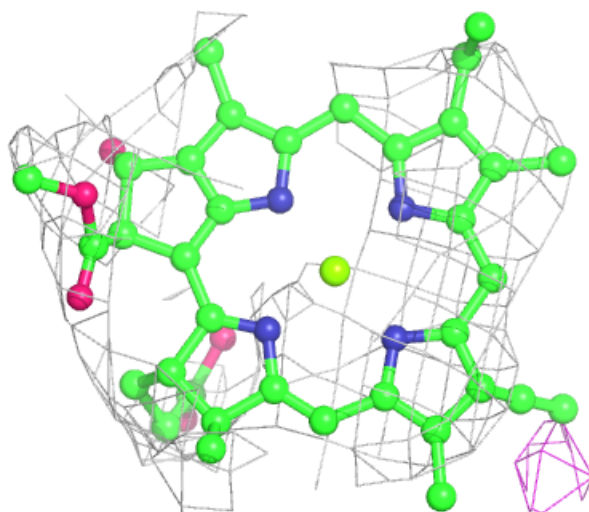
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





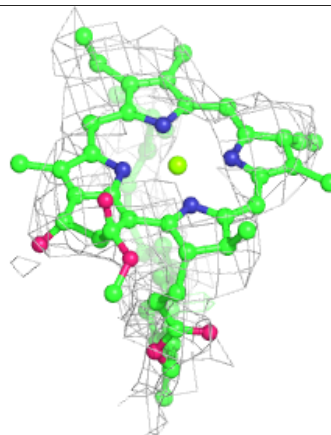
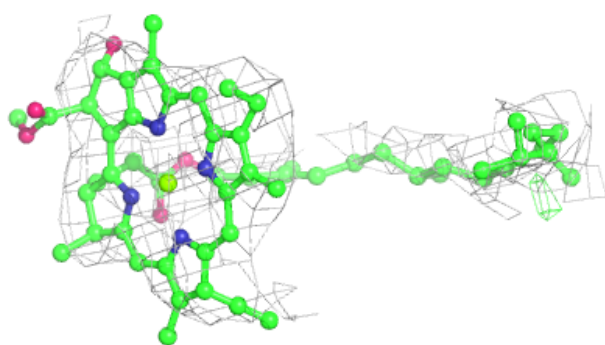
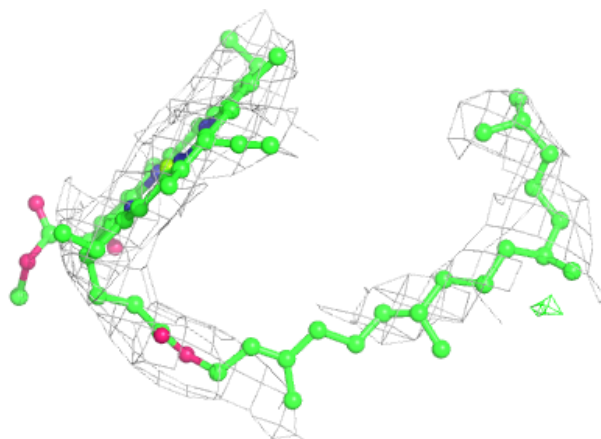
Electron density around CLA B 832:

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

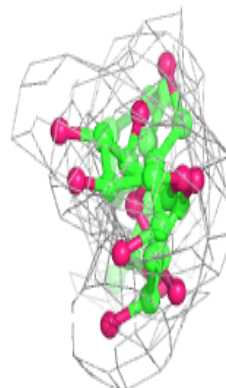
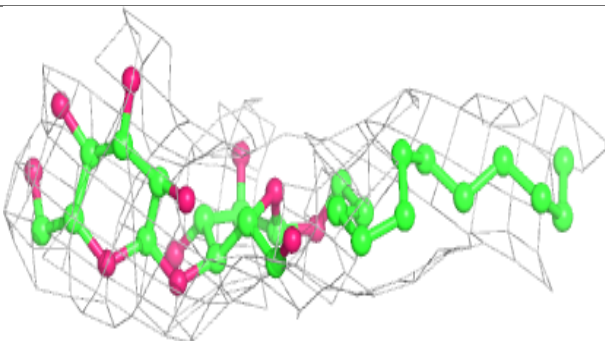
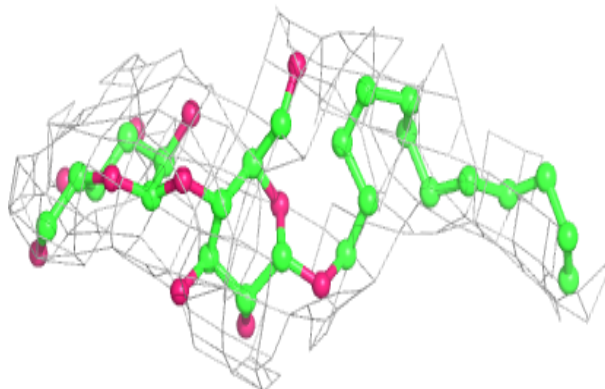


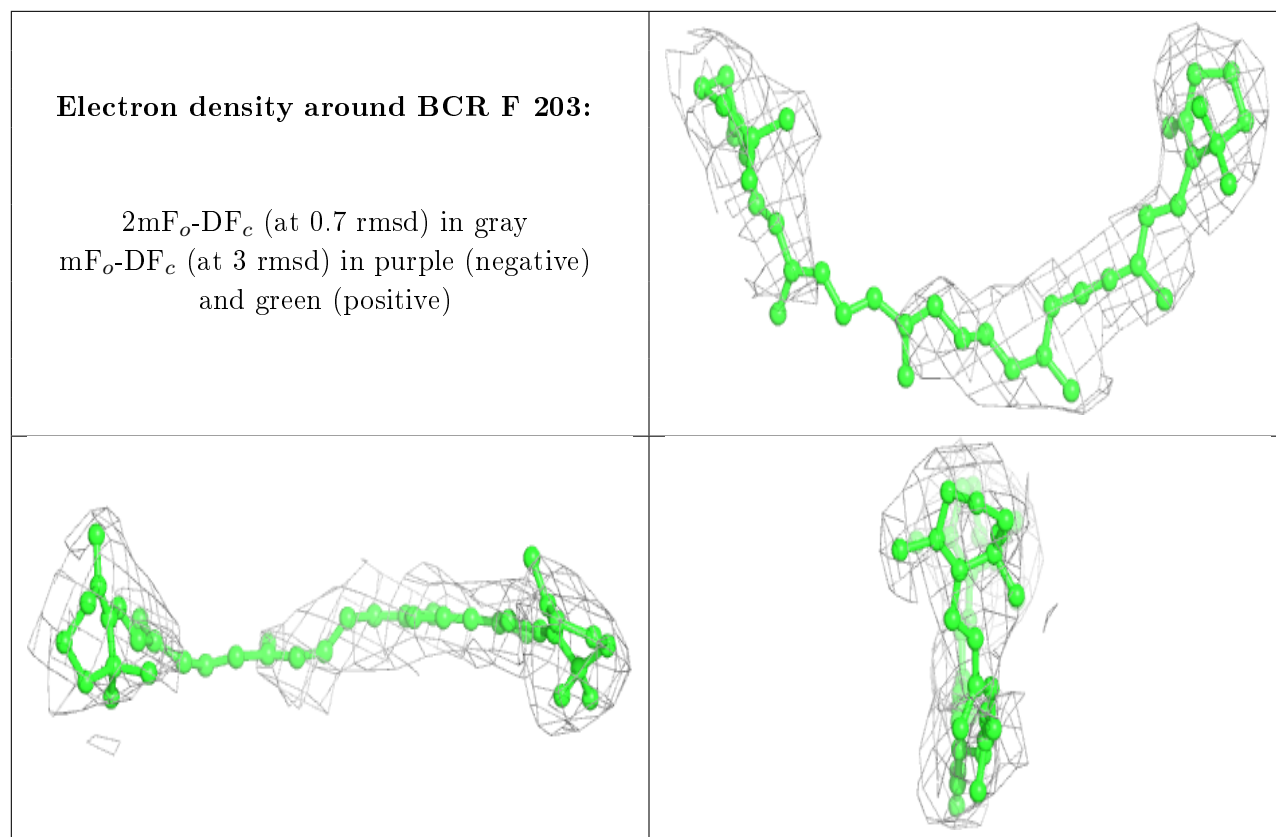
Electron density around CLA L 202:

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

**Electron density around LMU K 105:**

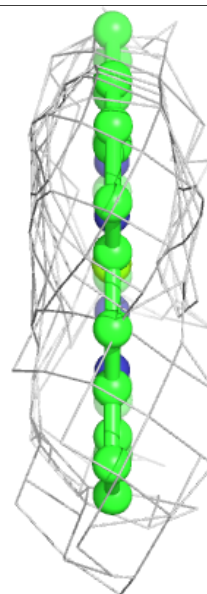
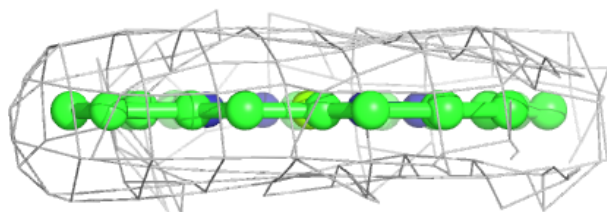
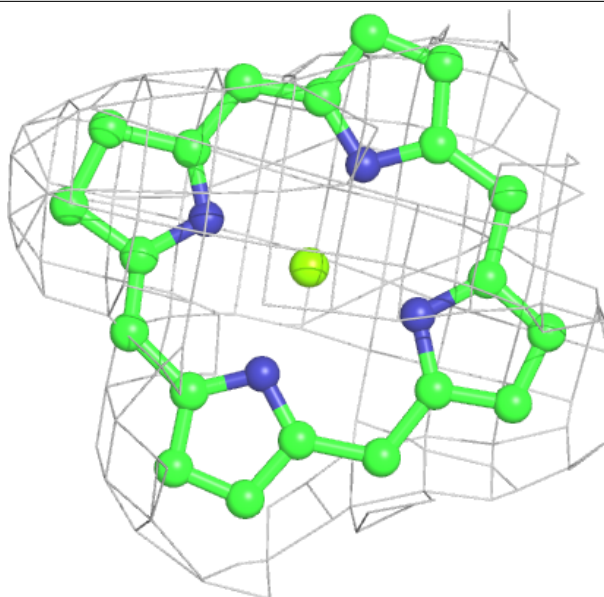
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





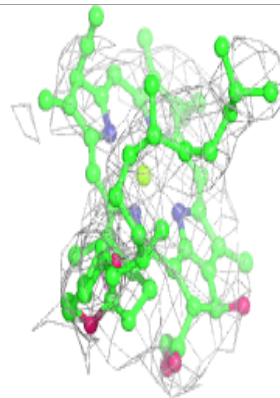
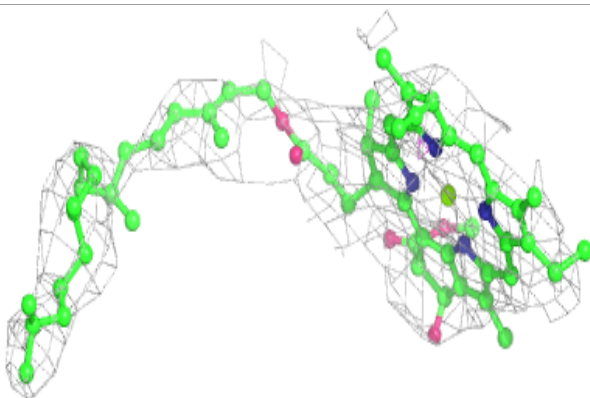
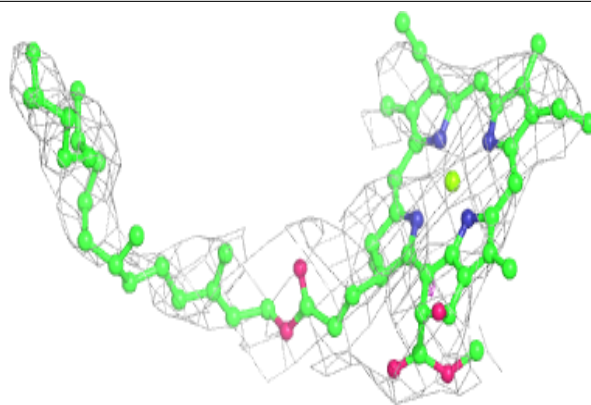
Electron density around CLA 4 310:

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

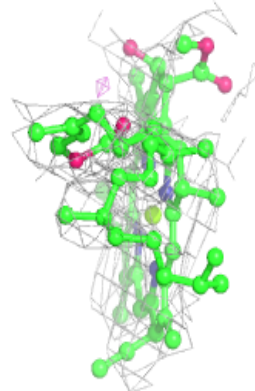
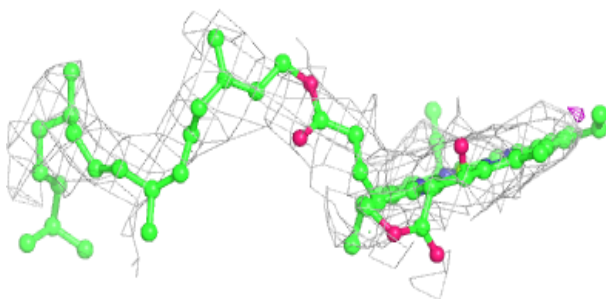
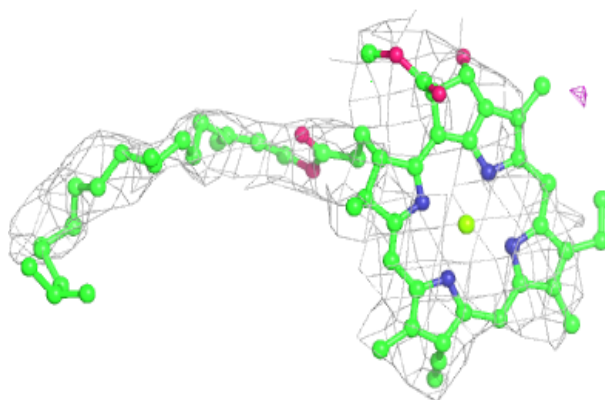


Electron density around CLA A 851:

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

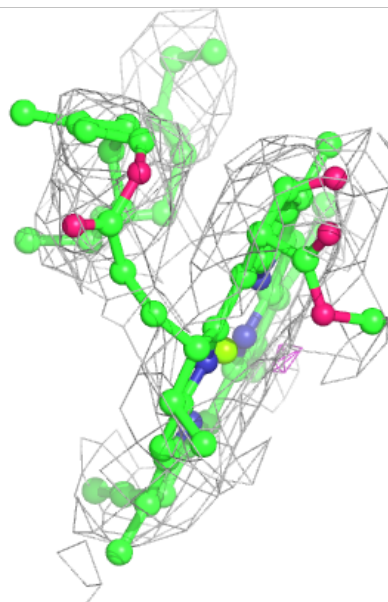
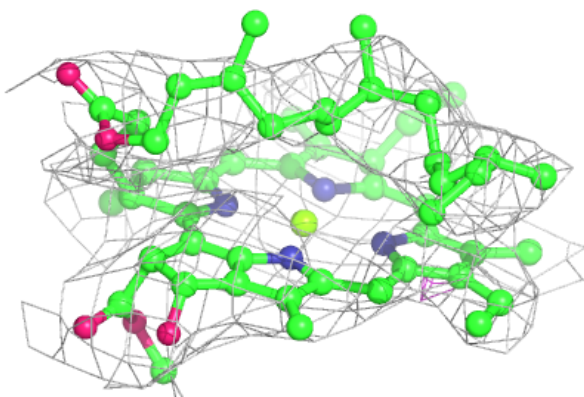
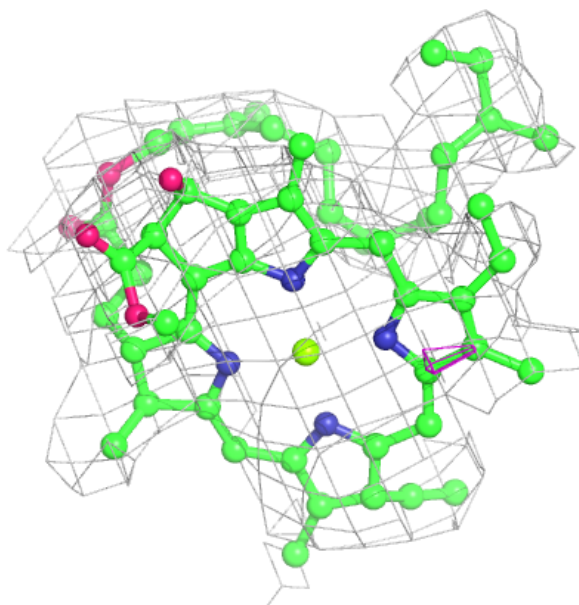
**Electron density around CLA A 824:**

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



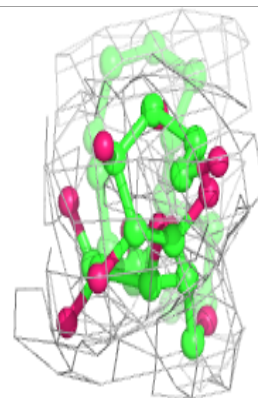
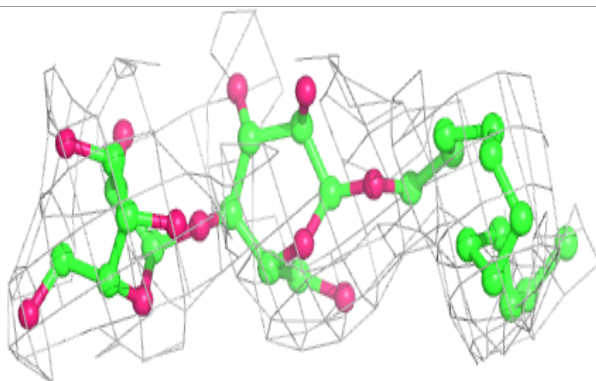
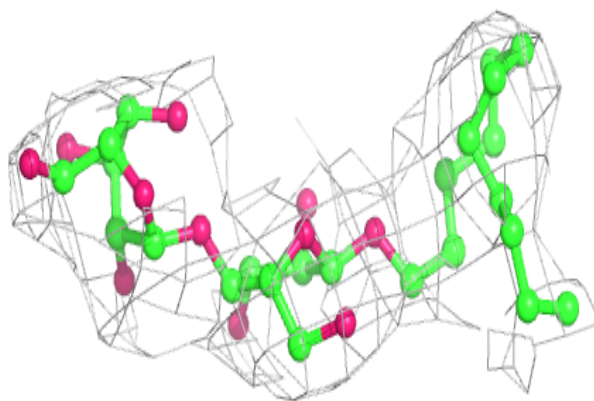
Electron density around CLA 1 206:

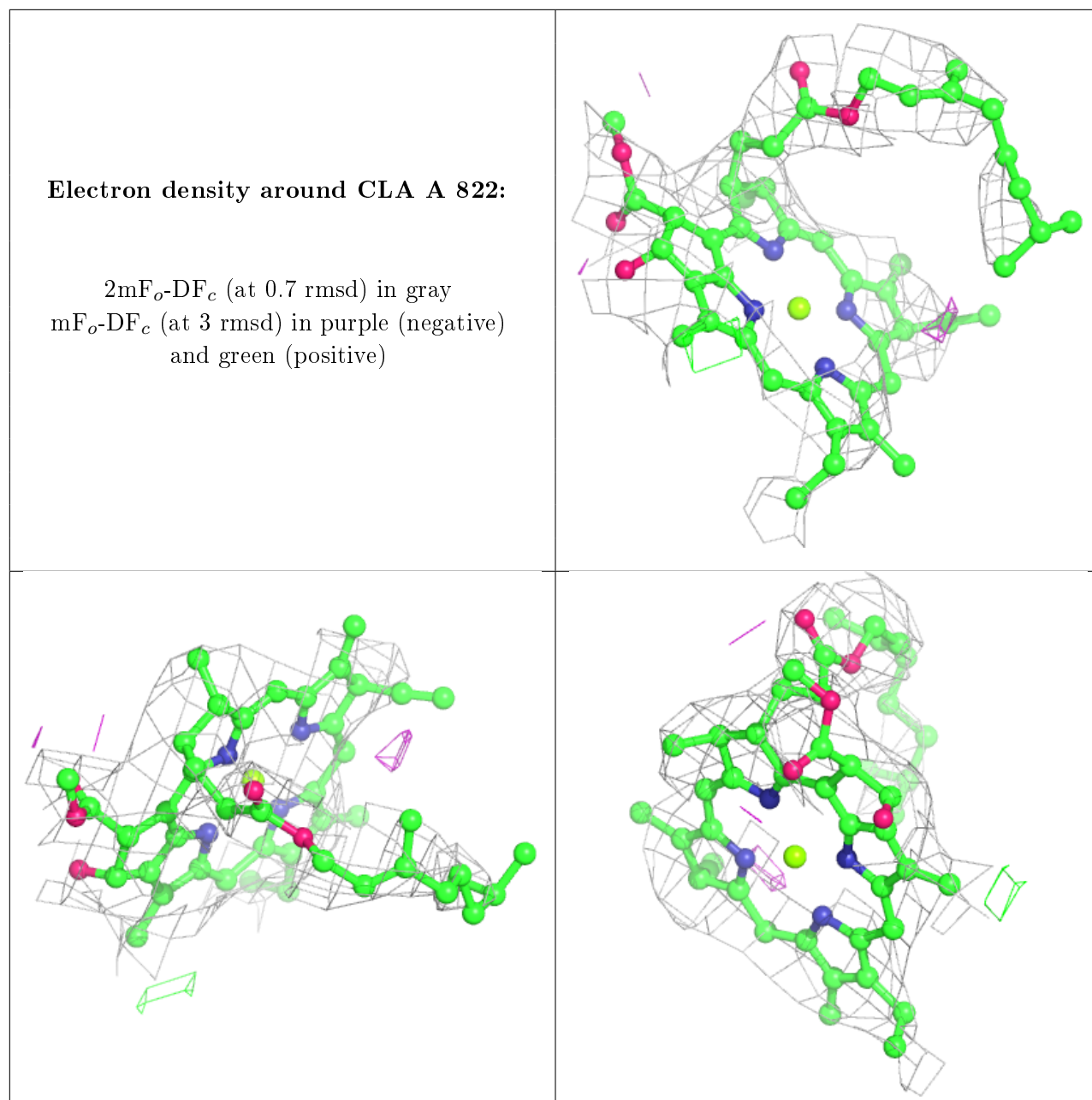
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMU A 855:

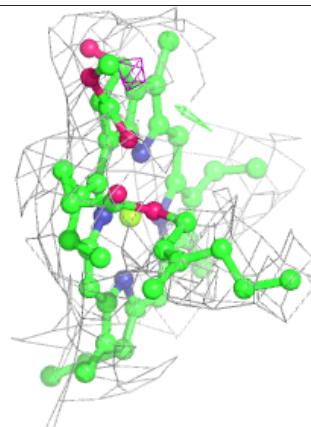
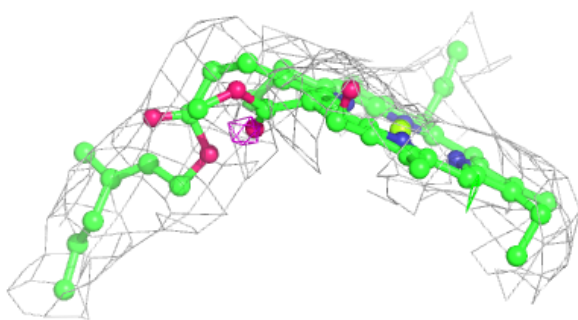
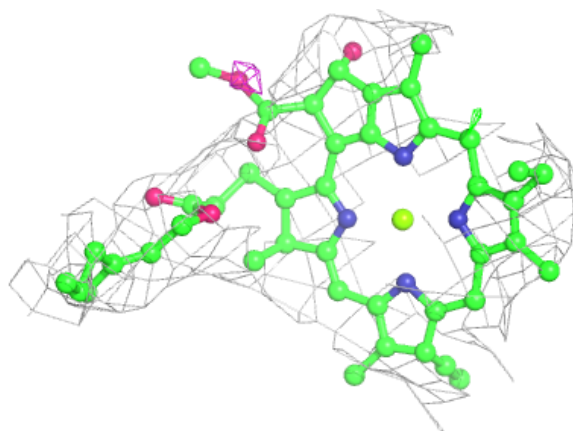
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





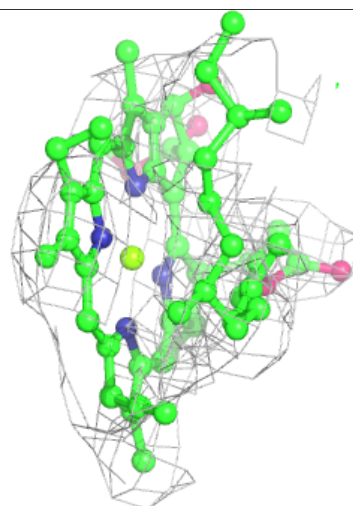
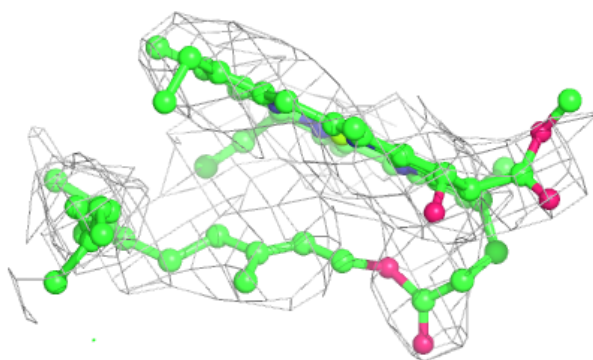
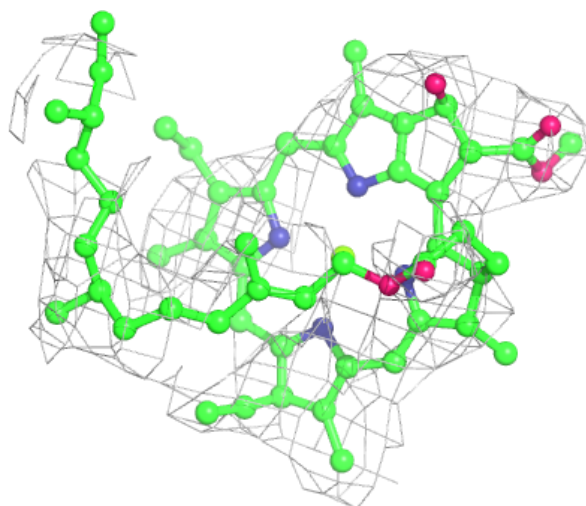
Electron density around CLA 4 307:

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



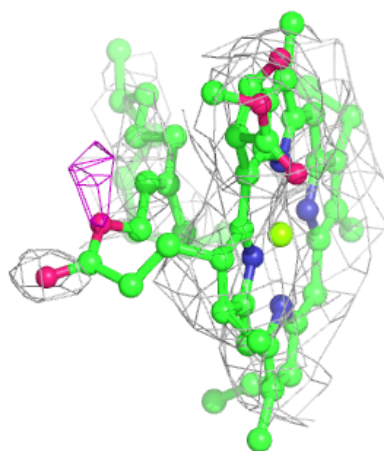
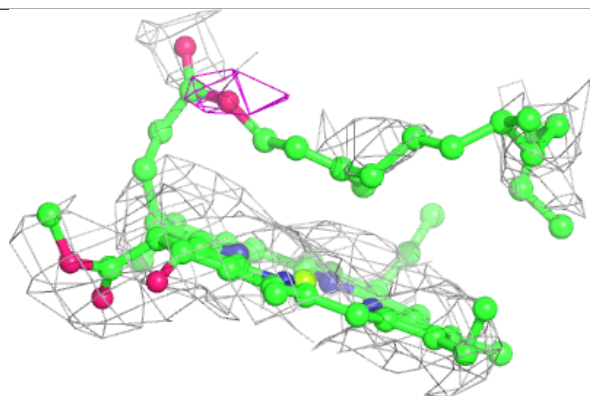
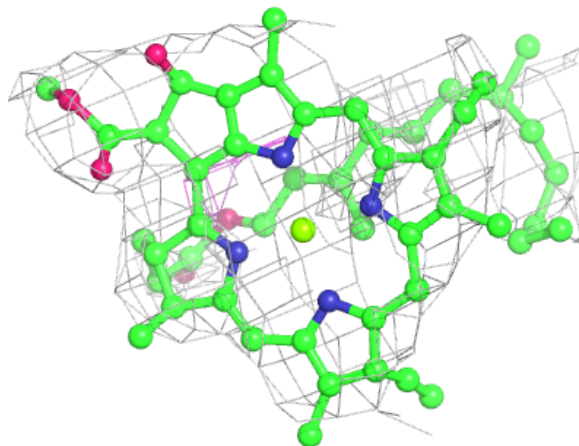
Electron density around CLA B 817:

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



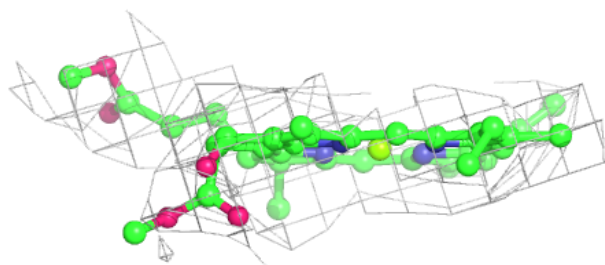
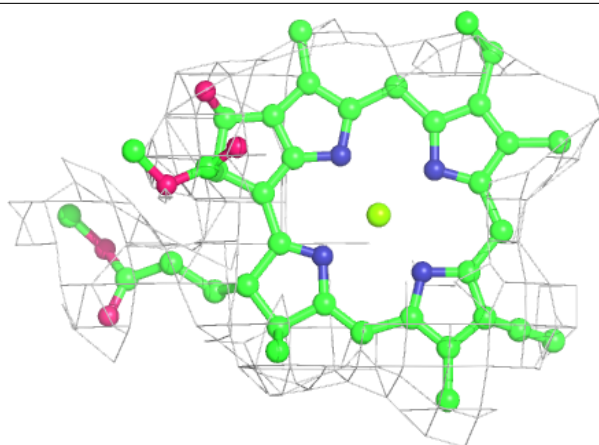
Electron density around CLA B 815:

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



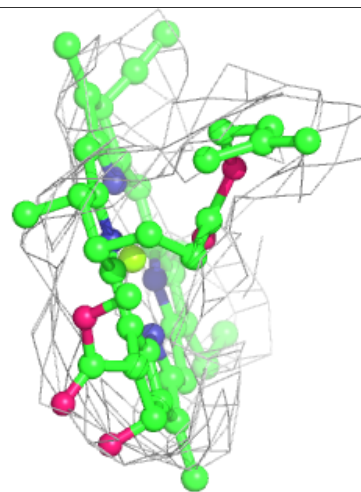
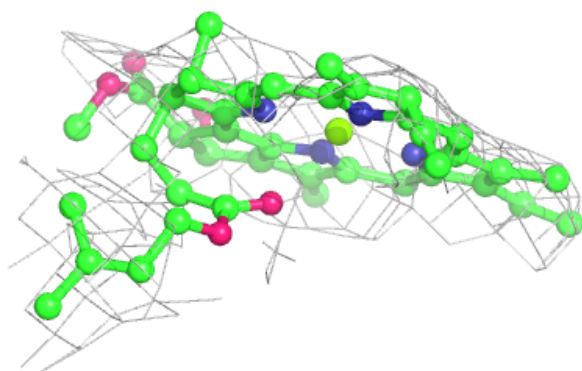
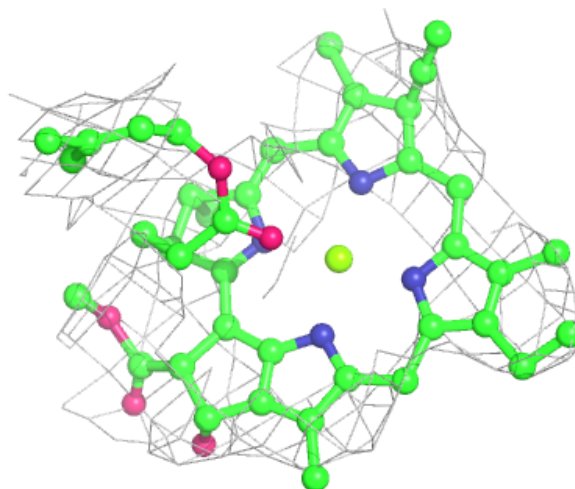
Electron density around CLA 4 316:

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



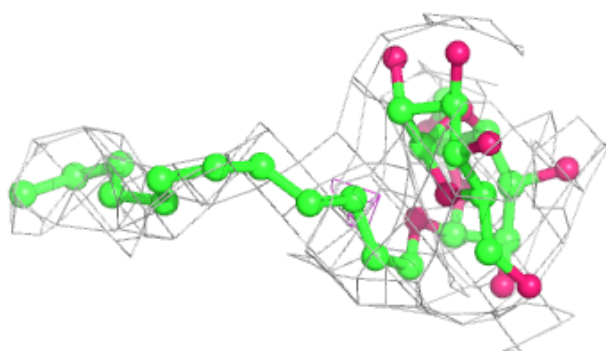
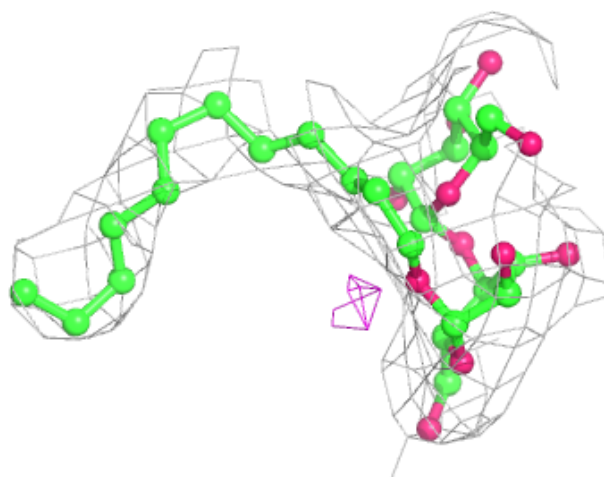
Electron density around CLA A 815:

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



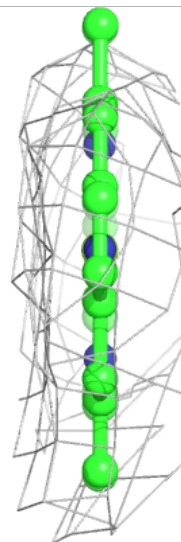
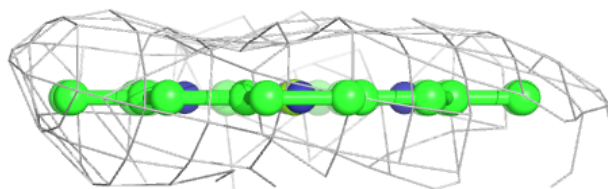
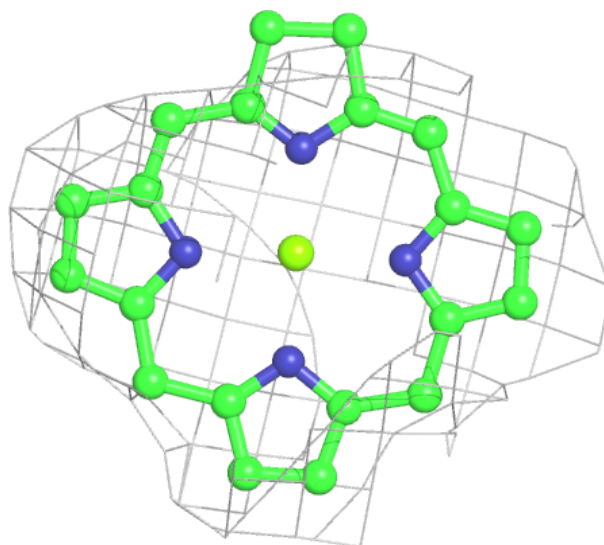
Electron density around LMU H 106:

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



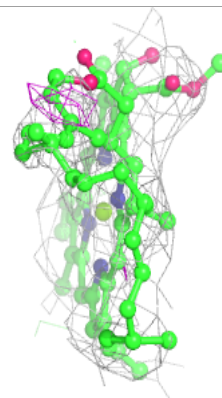
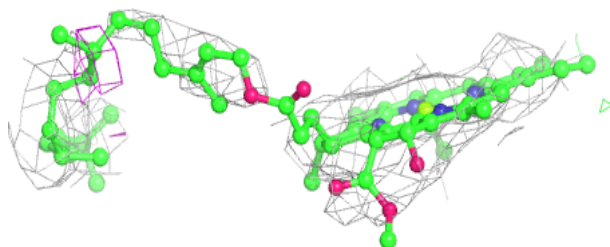
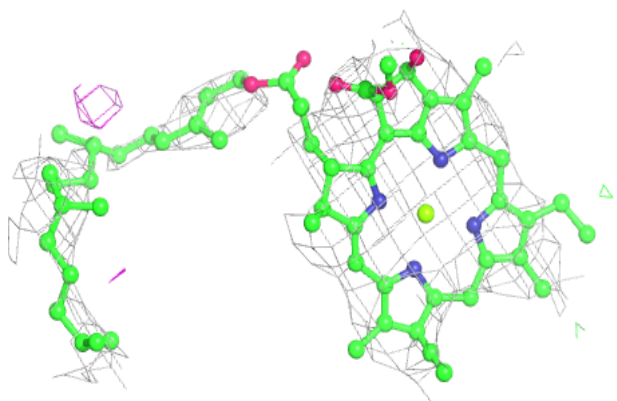
Electron density around CLA 2 309:

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

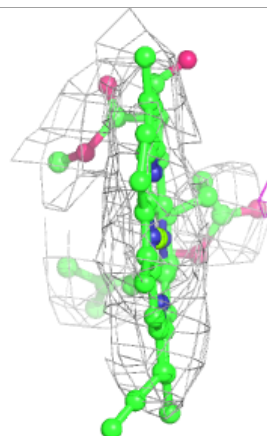
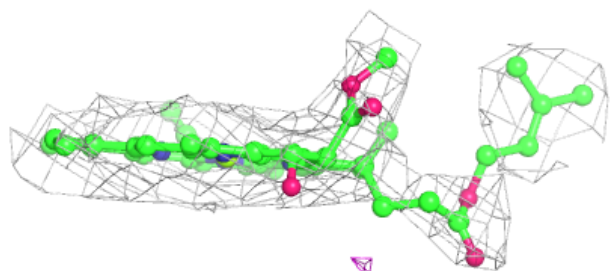
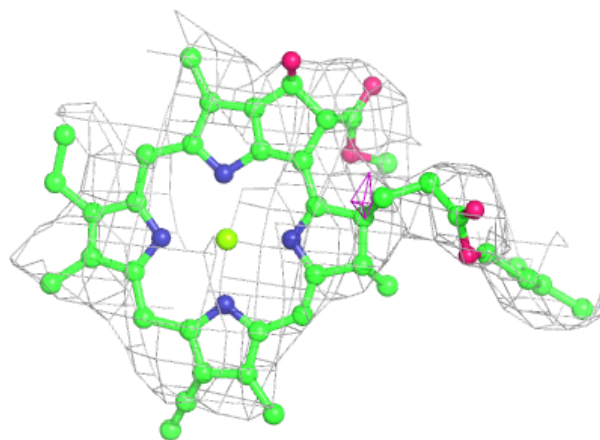


Electron density around CLA A 825:

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

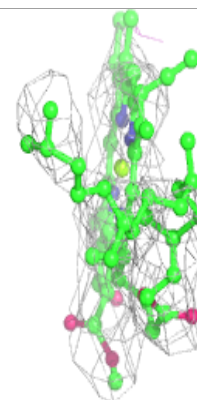
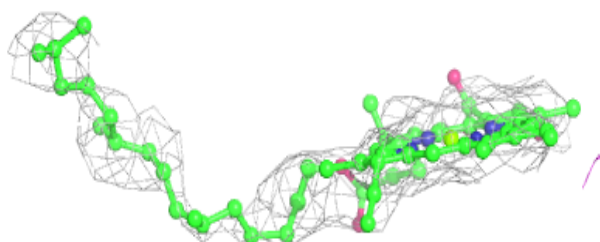
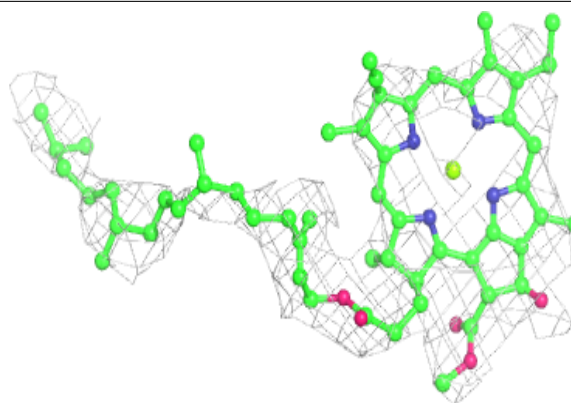
**Electron density around CLA B 829:**

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

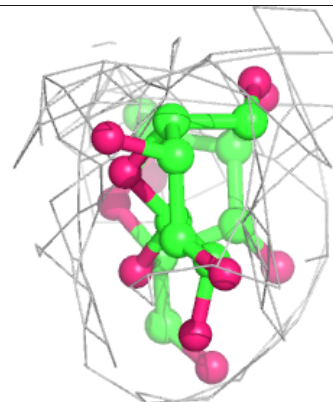
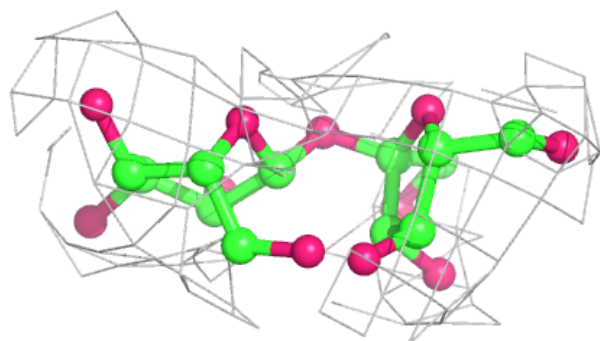
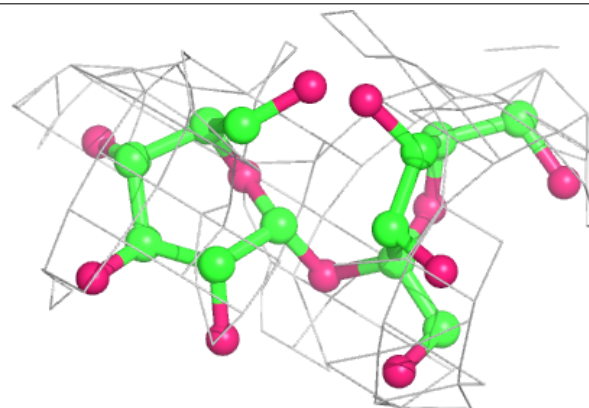


Electron density around CLA B 851:

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

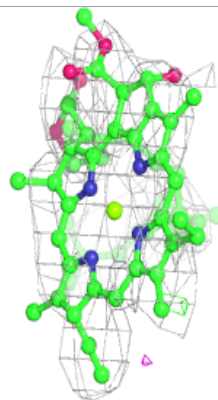
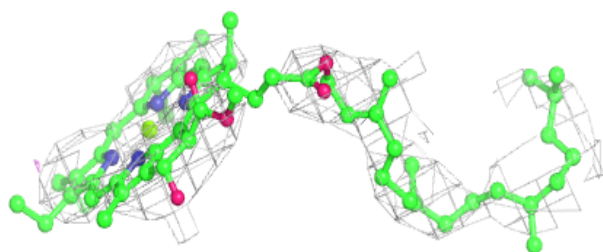
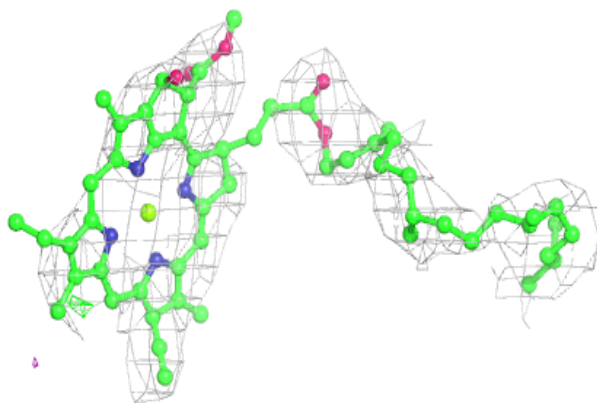
**Electron density around UNL H 111:**

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

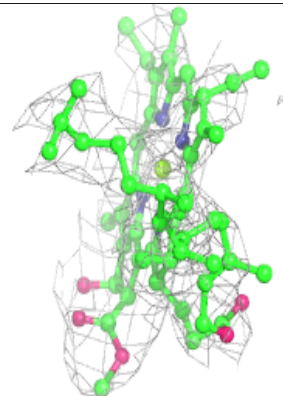
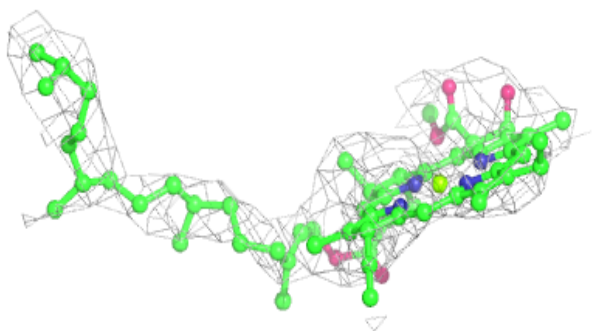
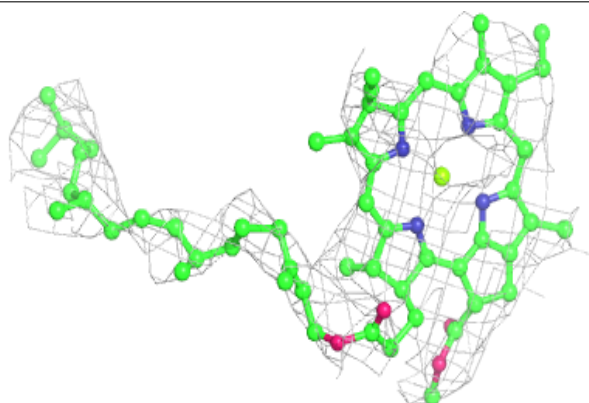


Electron density around CLA B 808:

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

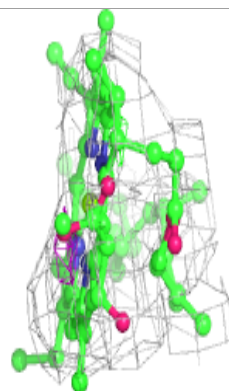
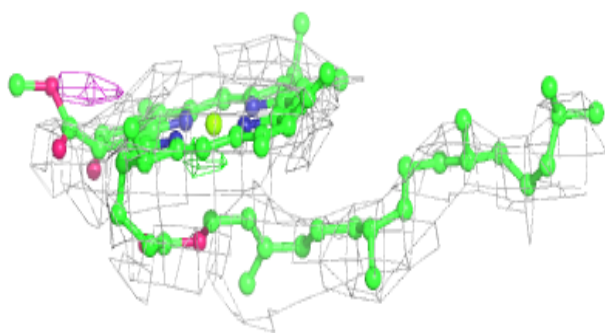
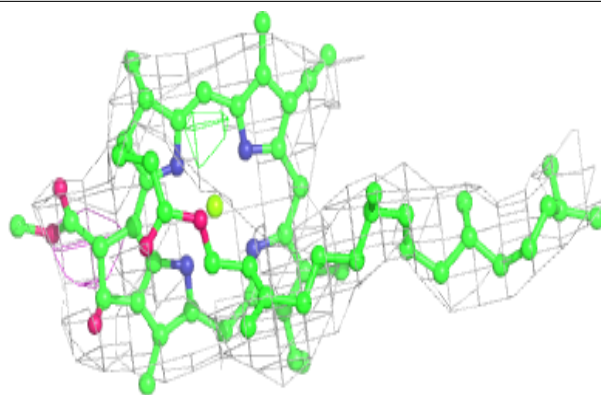
**Electron density around CLA A 852:**

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

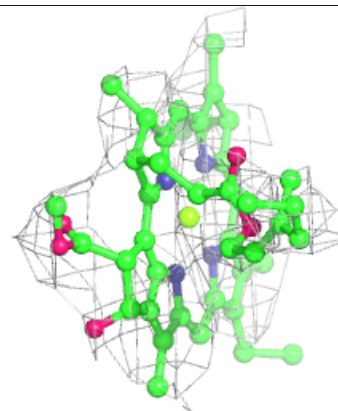
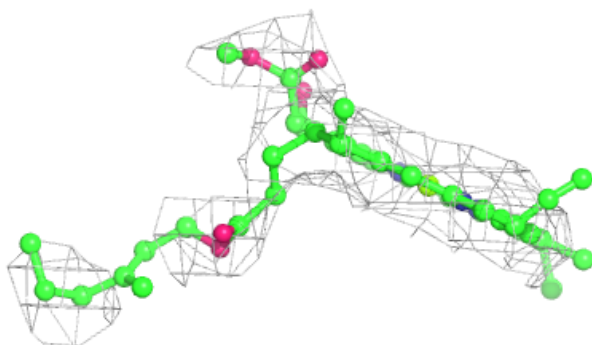
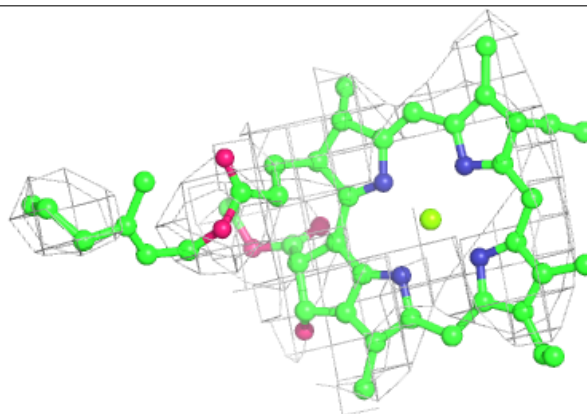


Electron density around CLA A 835:

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

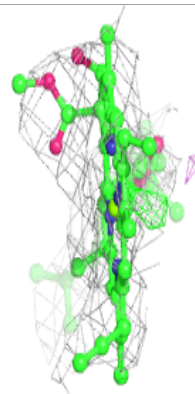
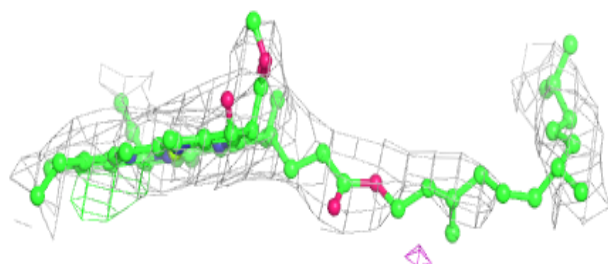
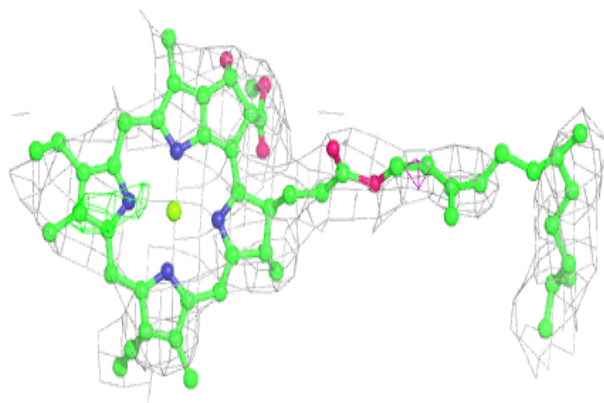
**Electron density around CLA A 809:**

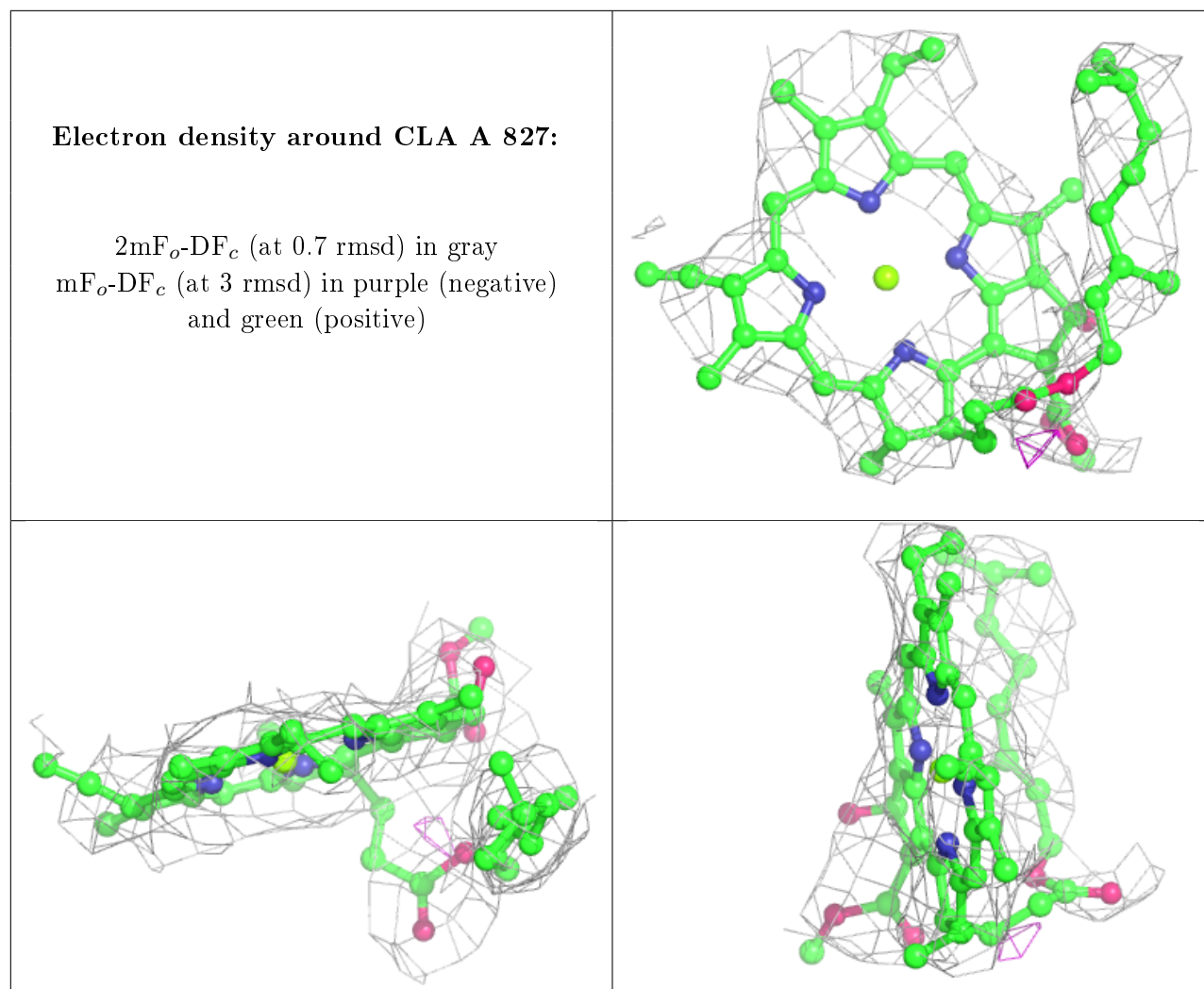
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 835:

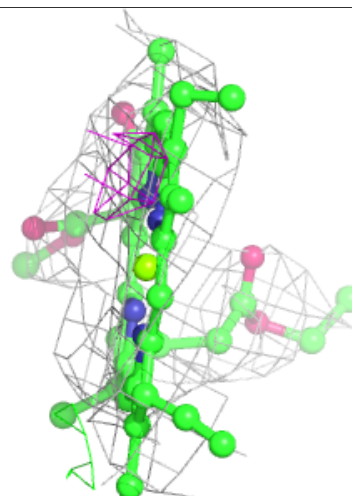
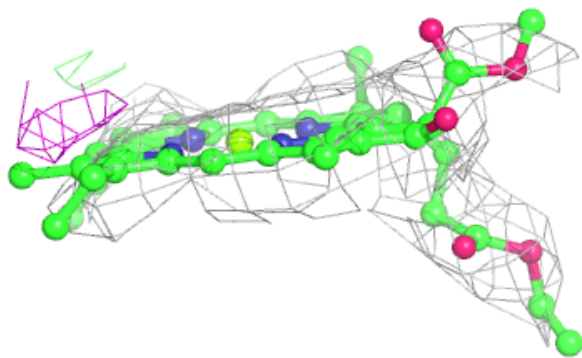
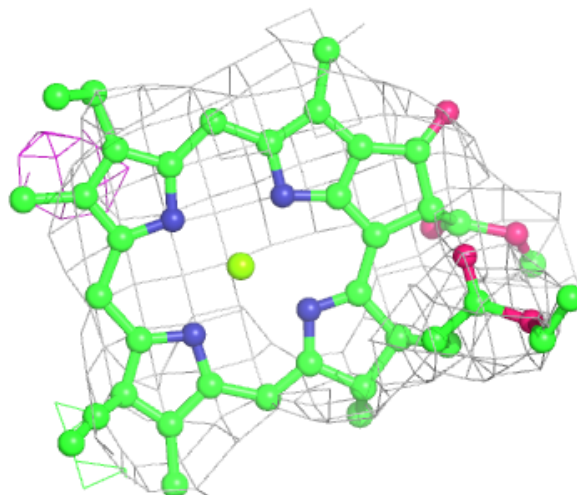
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





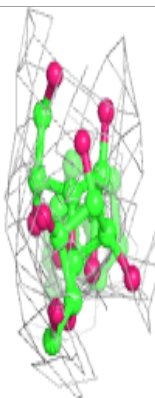
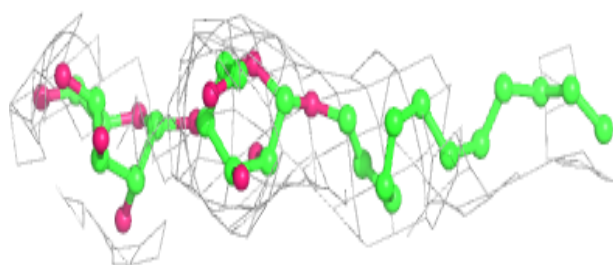
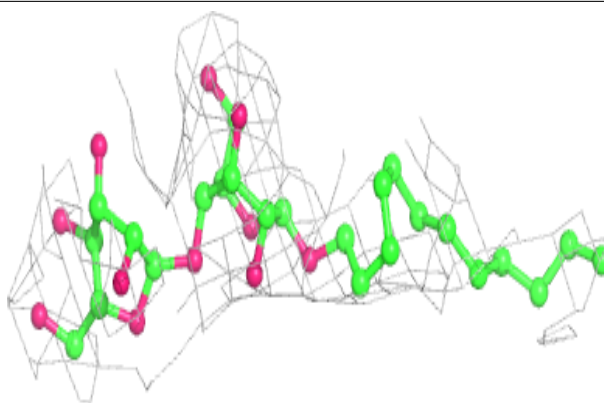
Electron density around CLA A 836:

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

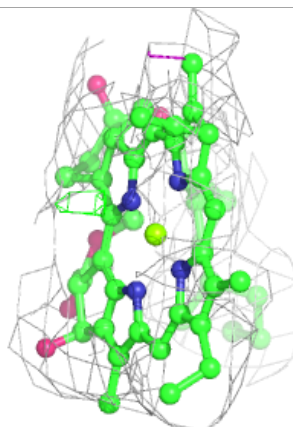
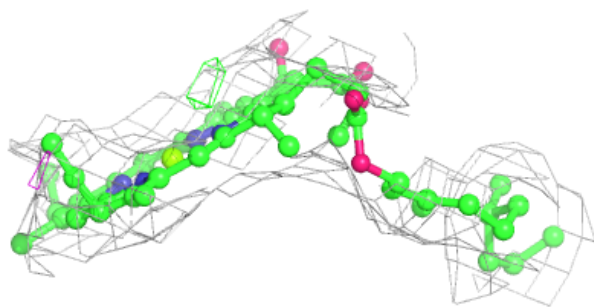
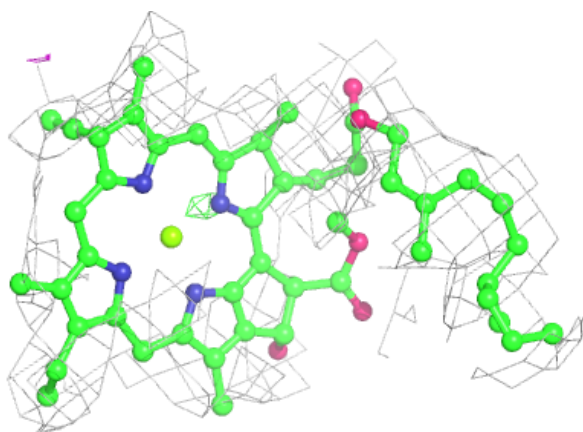


Electron density around LMU E 101:

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

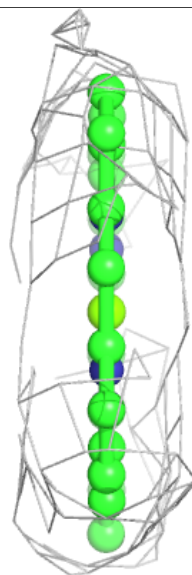
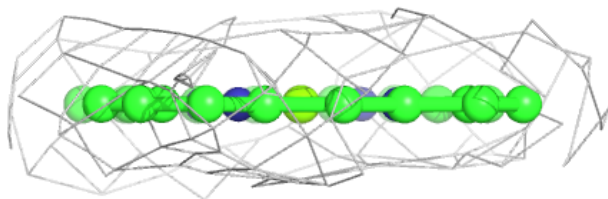
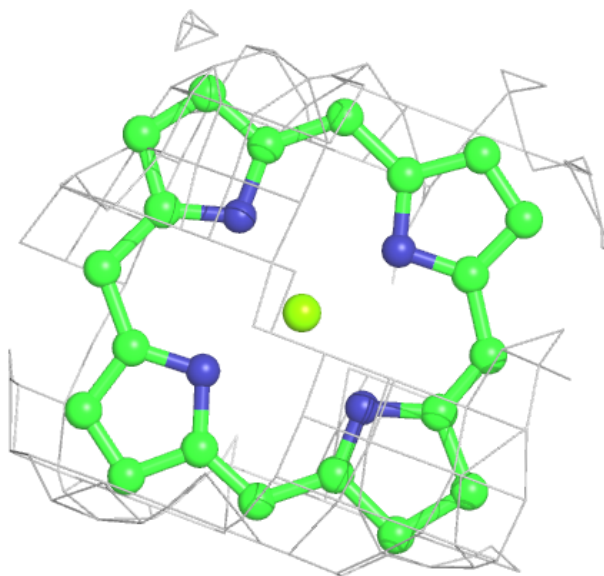
**Electron density around CLA 1 202:**

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



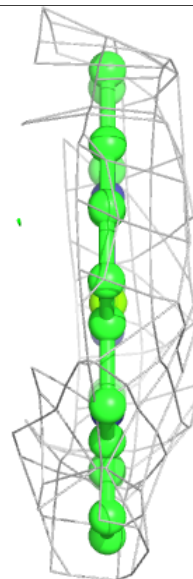
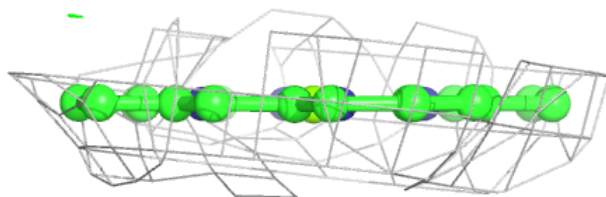
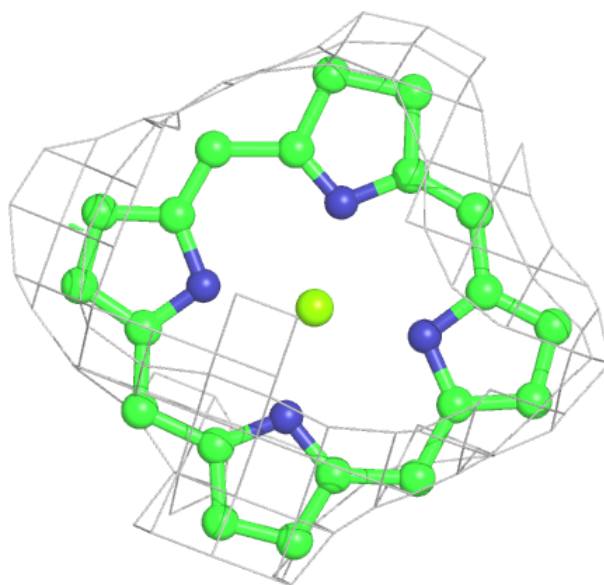
Electron density around CLA 1 214:

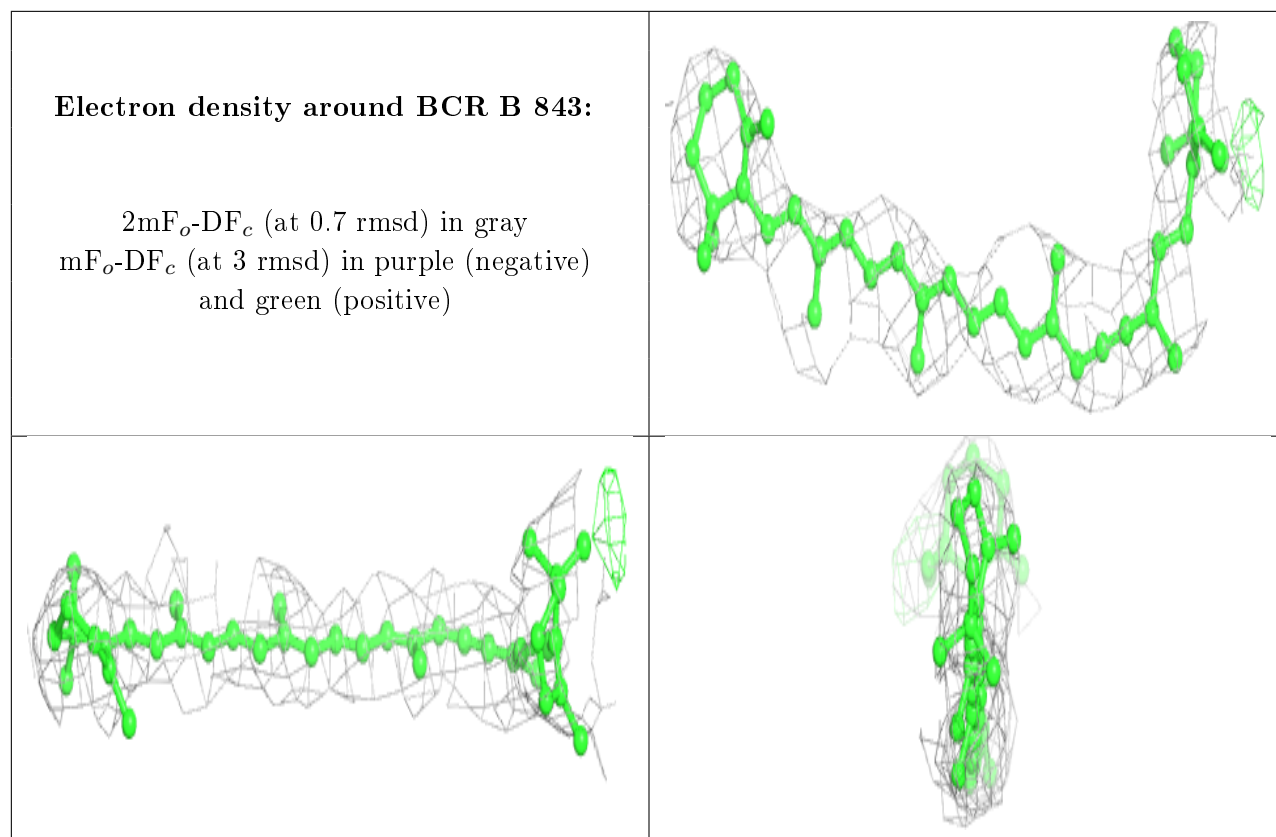
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 4 312:

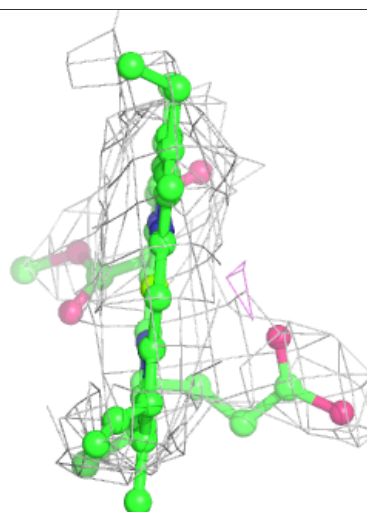
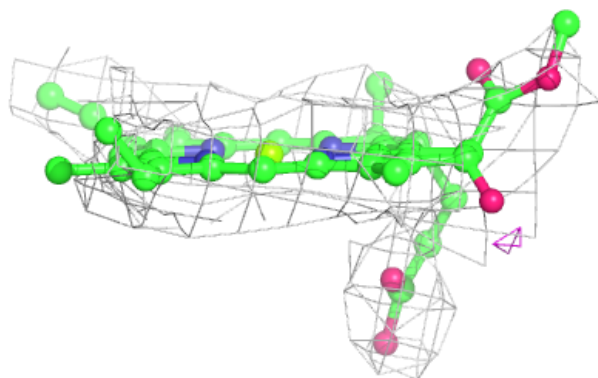
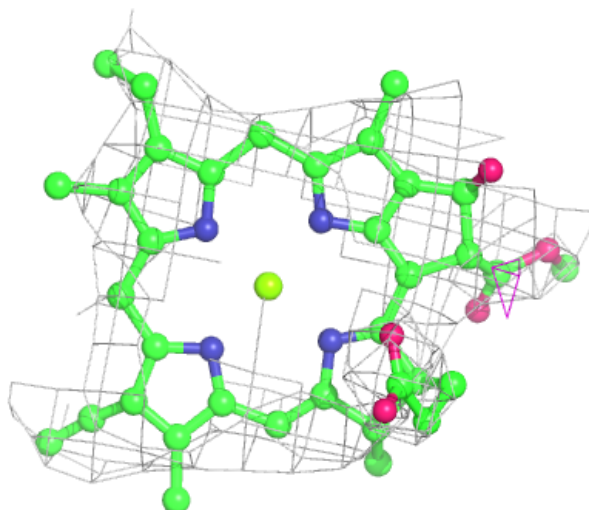
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

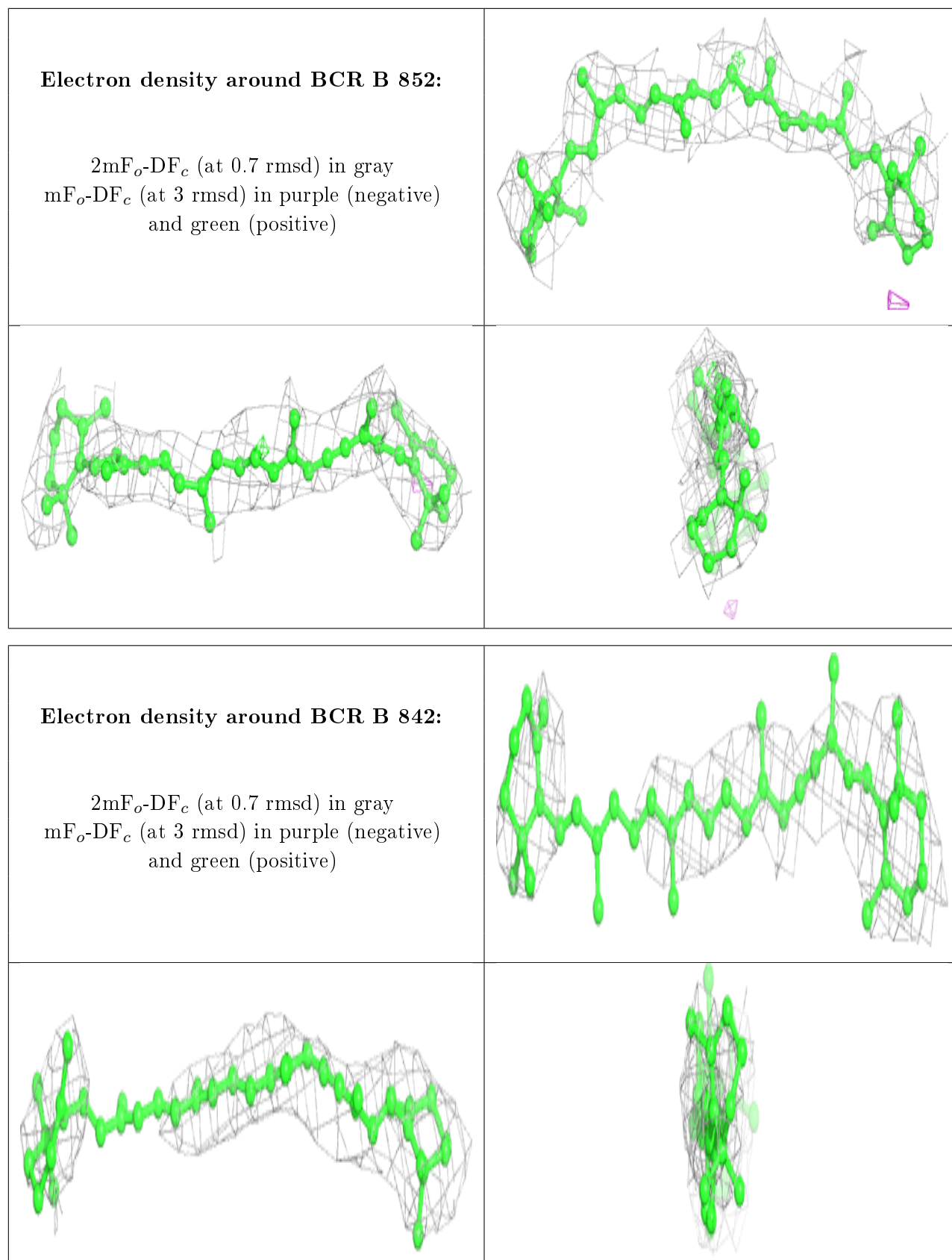




Electron density around CLA B 804:

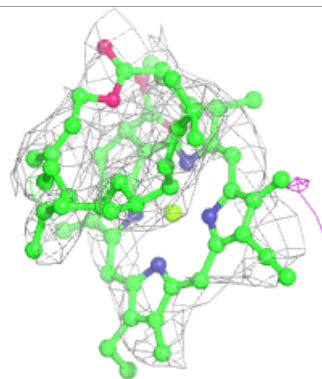
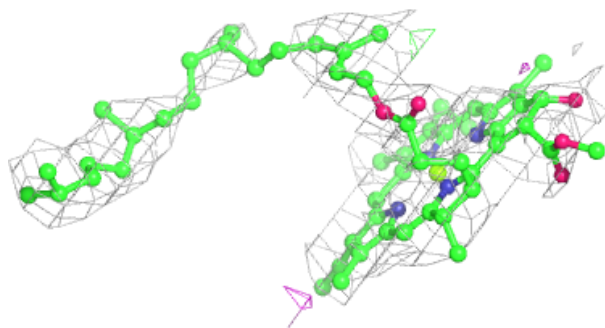
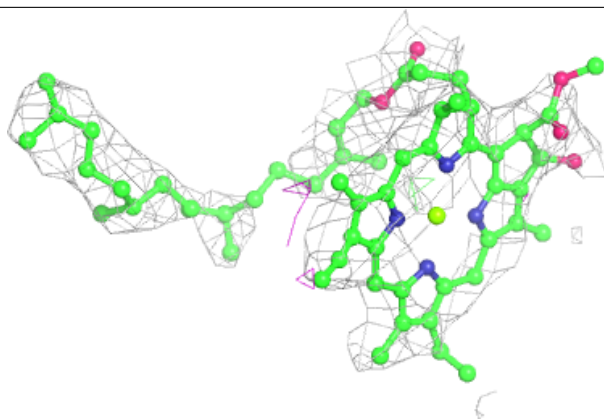
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



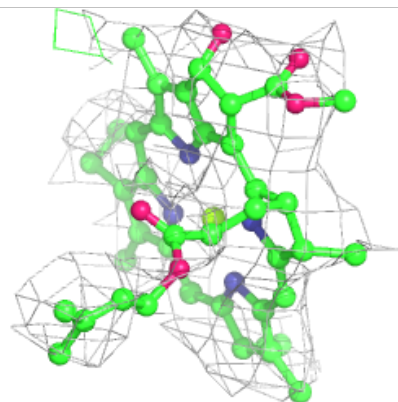
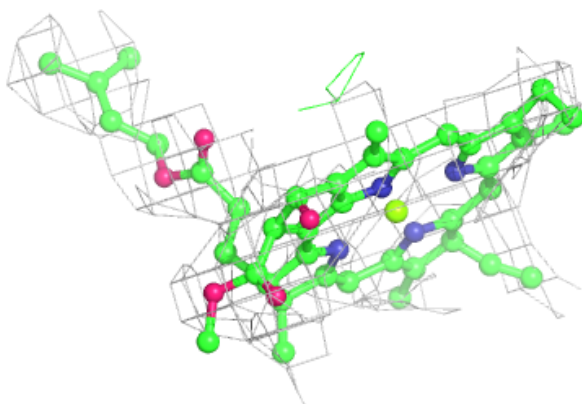
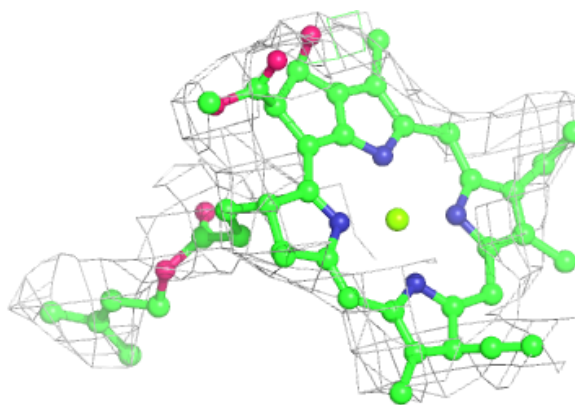


Electron density around CLA B 812:

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

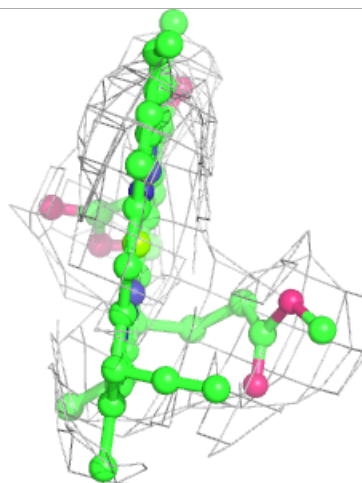
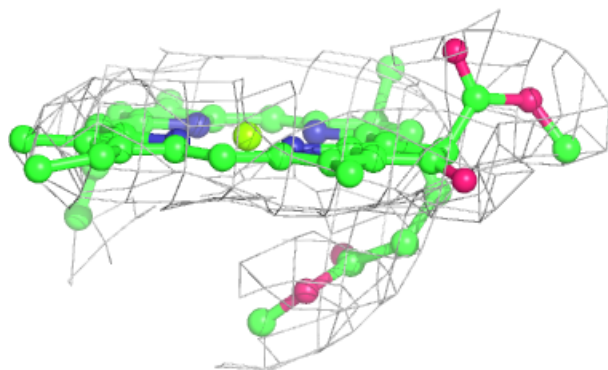
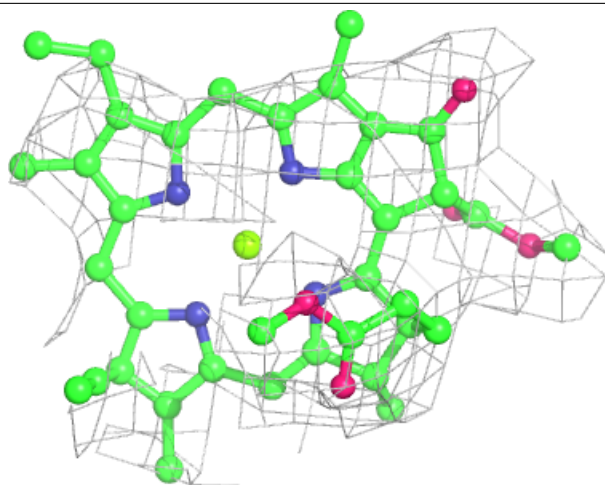
**Electron density around CLA 2 311:**

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



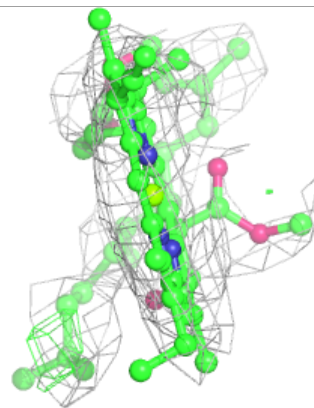
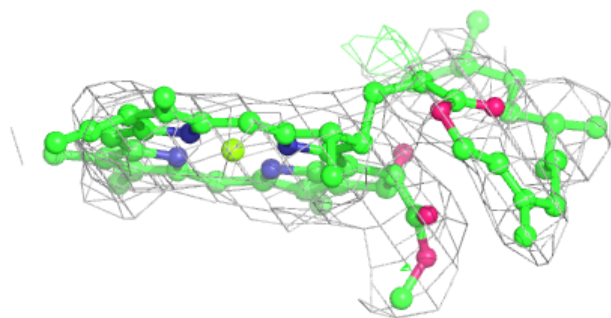
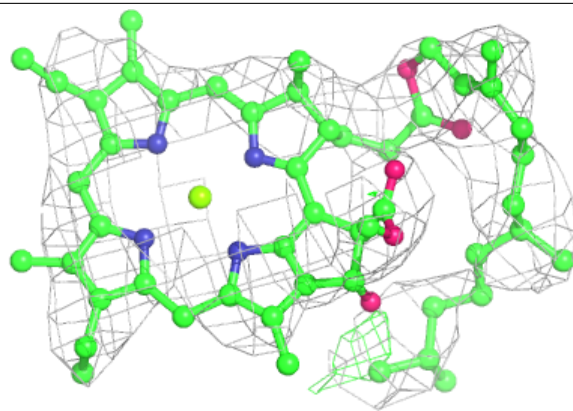
Electron density around CLA 1 204:

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



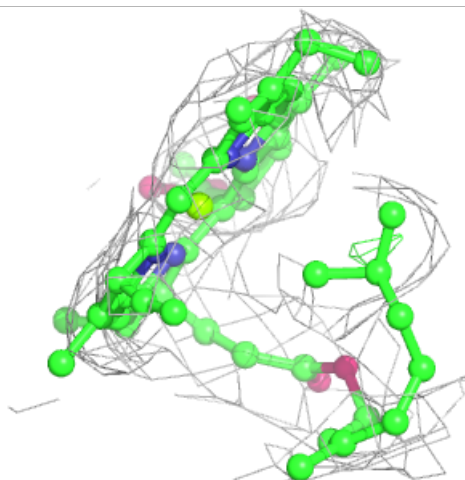
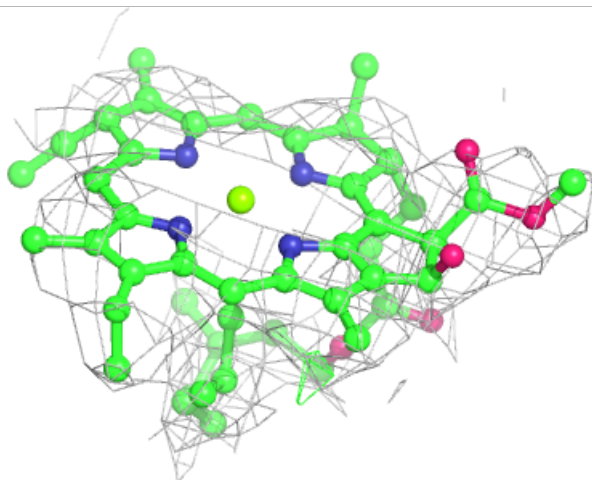
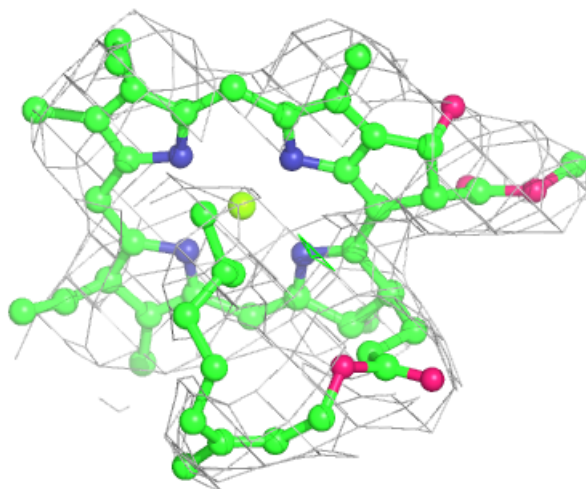
Electron density around CLA B 805:

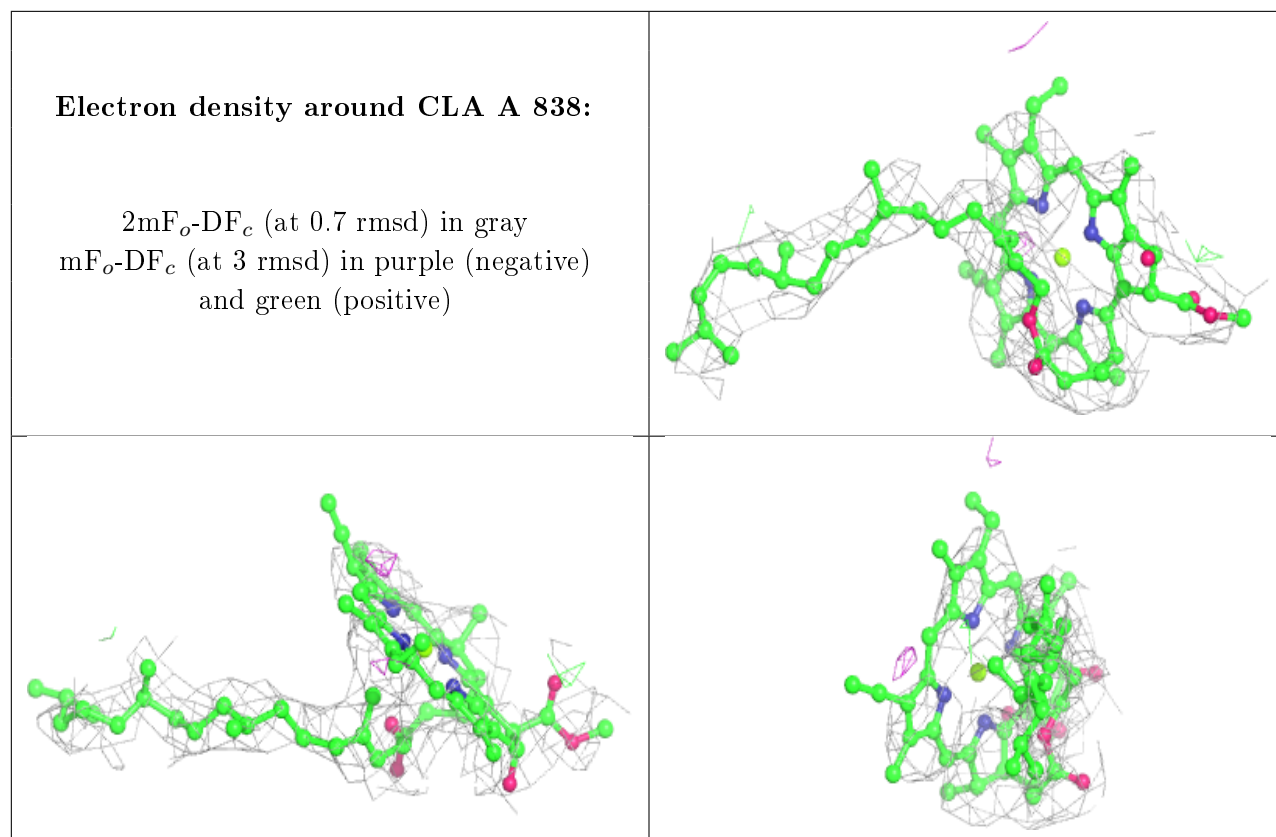
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 810:

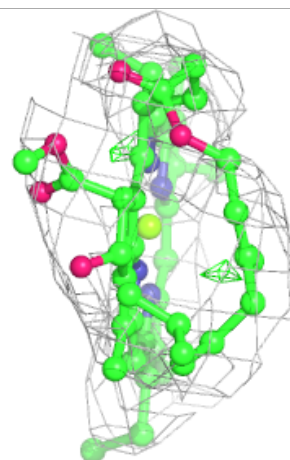
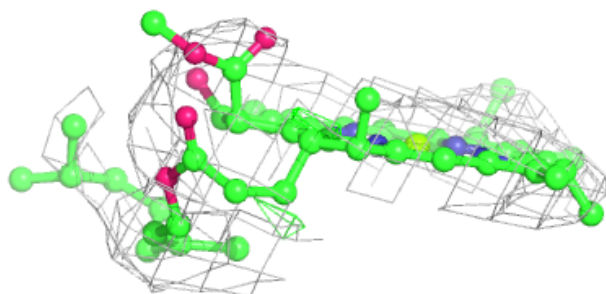
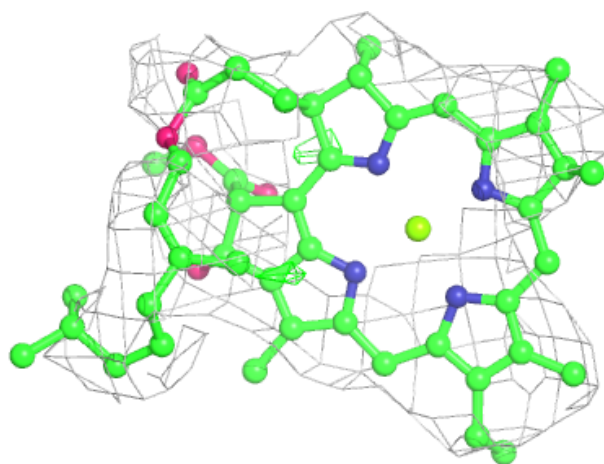
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





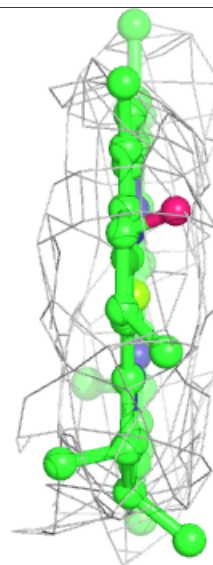
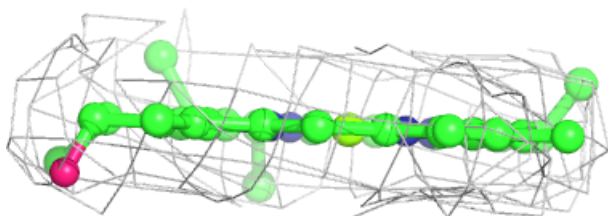
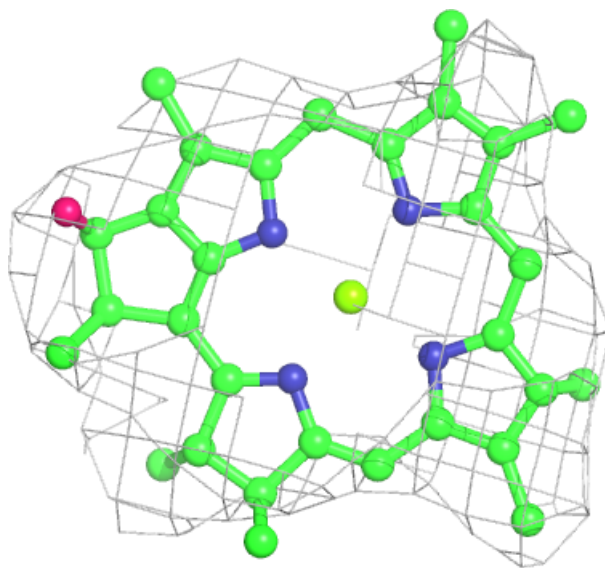
Electron density around CLA B 809:

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



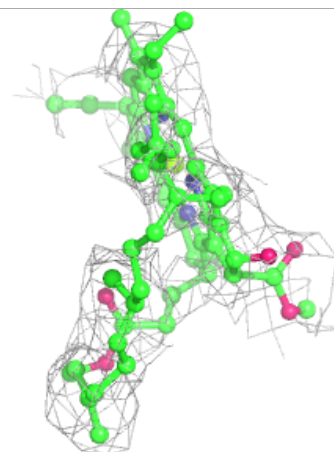
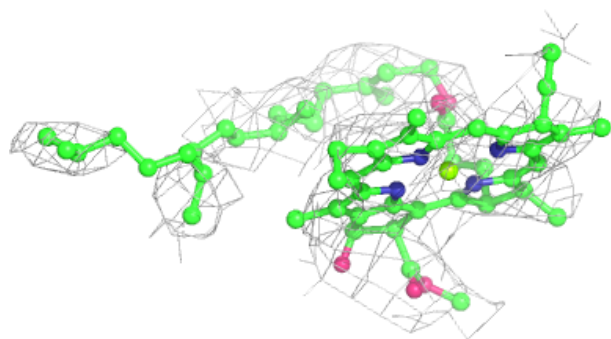
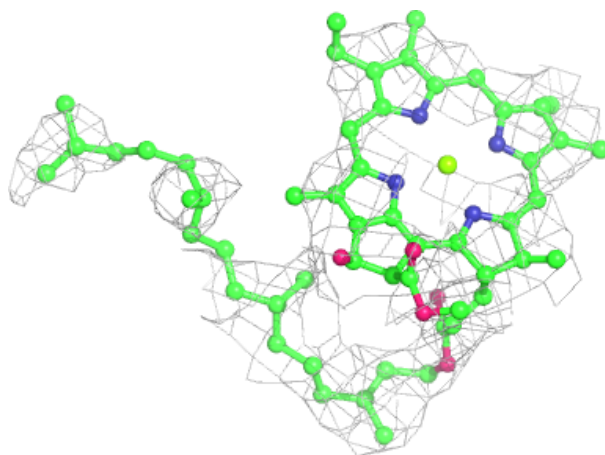
Electron density around CLA 4 314:

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



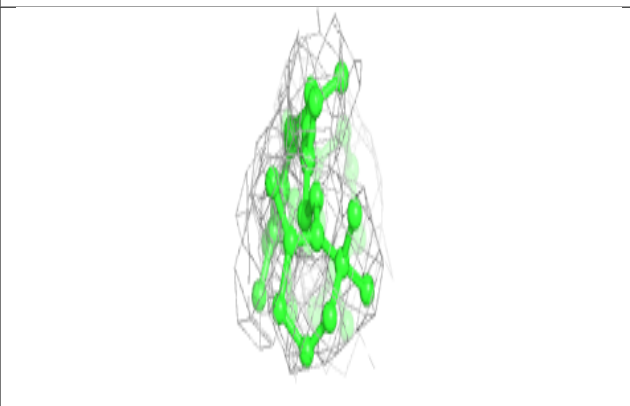
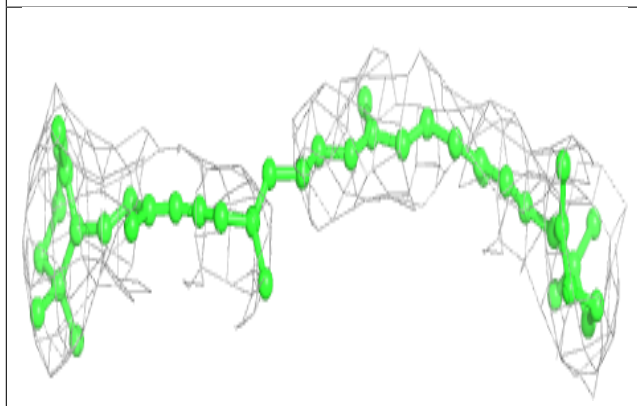
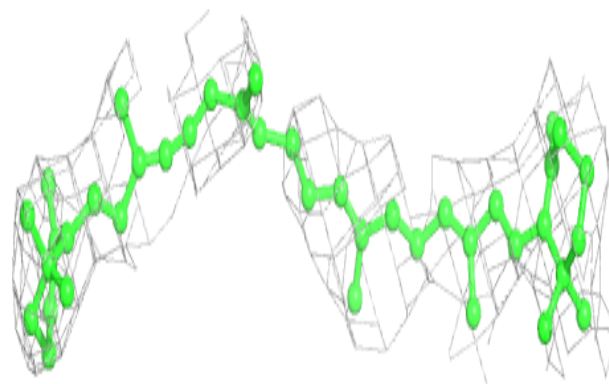
Electron density around CLA B 830:

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

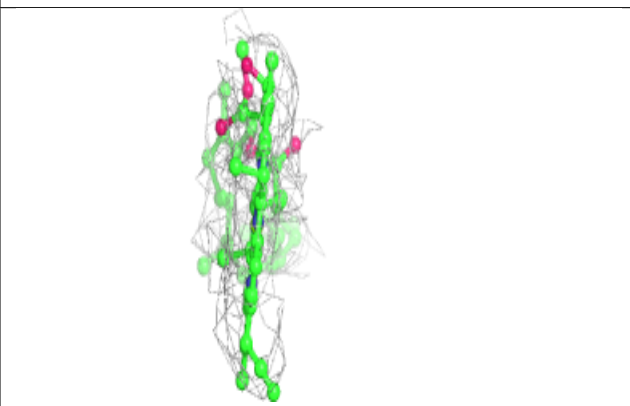
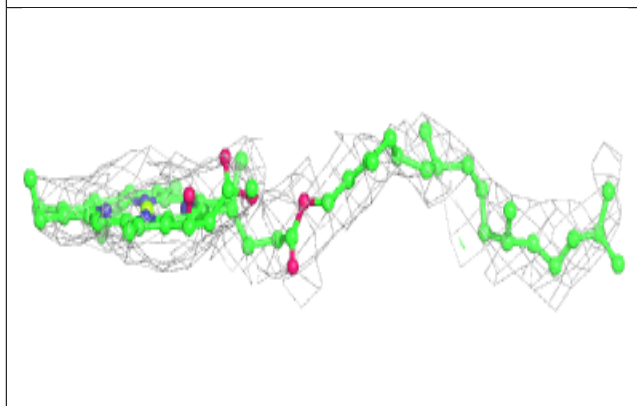
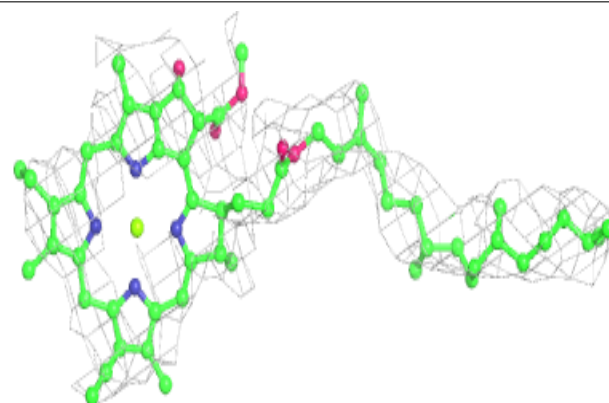


Electron density around BCR I 101:

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

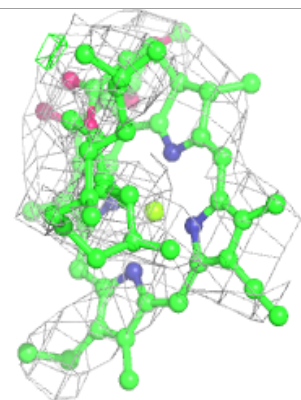
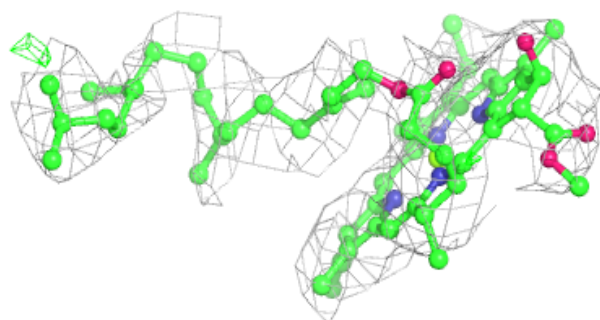
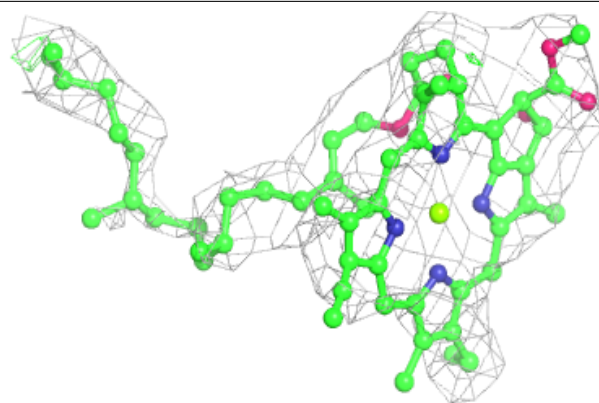
**Electron density around CLA A 830:**

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

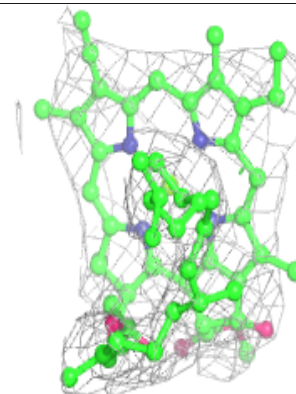
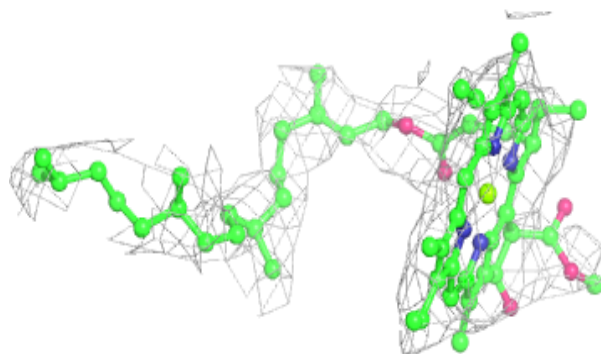
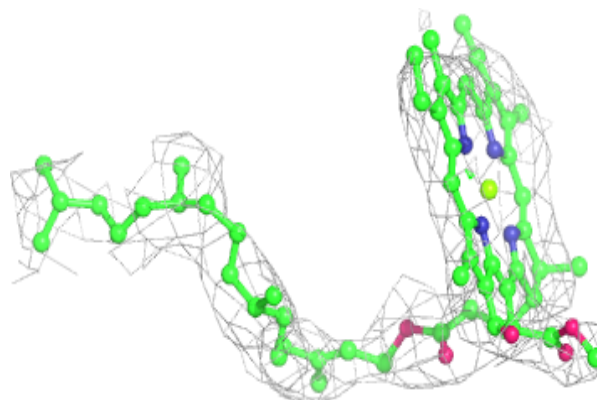


Electron density around CLA A 841:

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

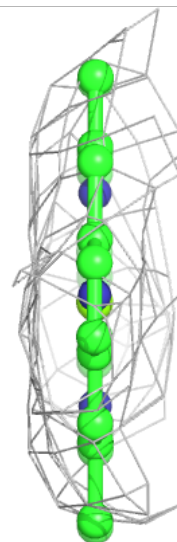
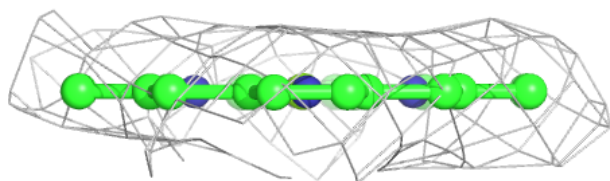
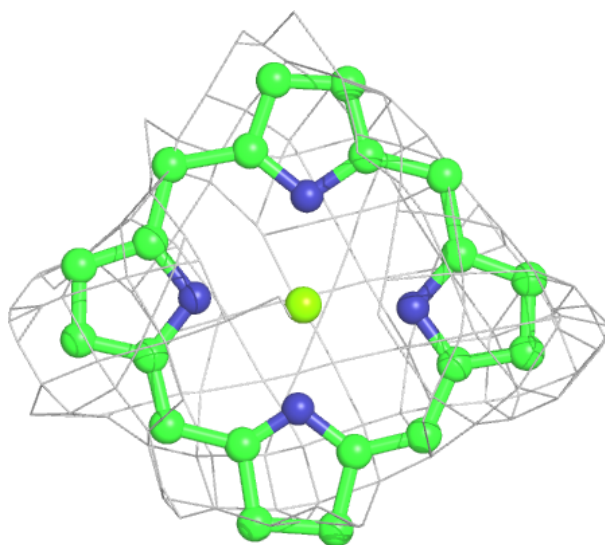
**Electron density around CLA B 827:**

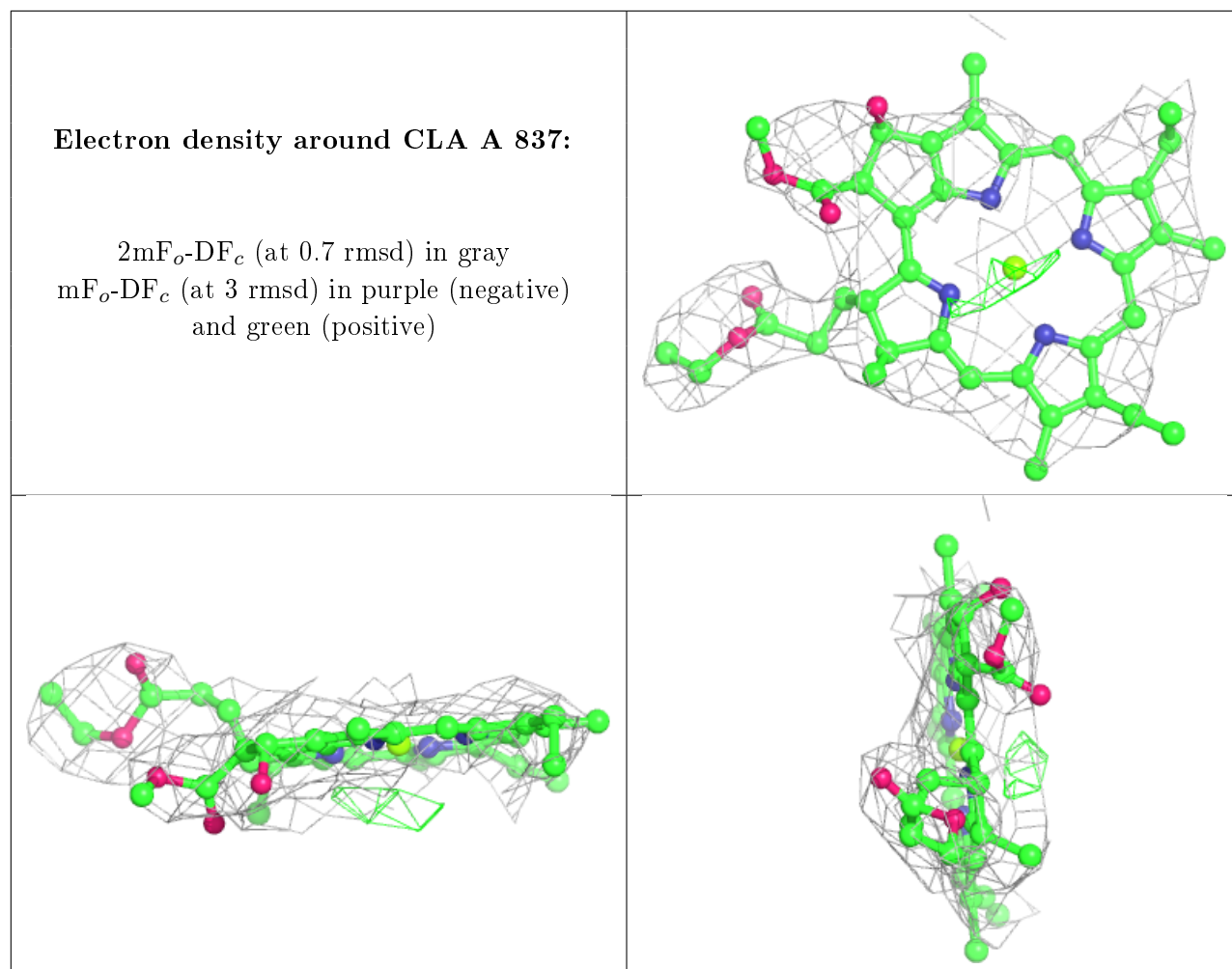
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

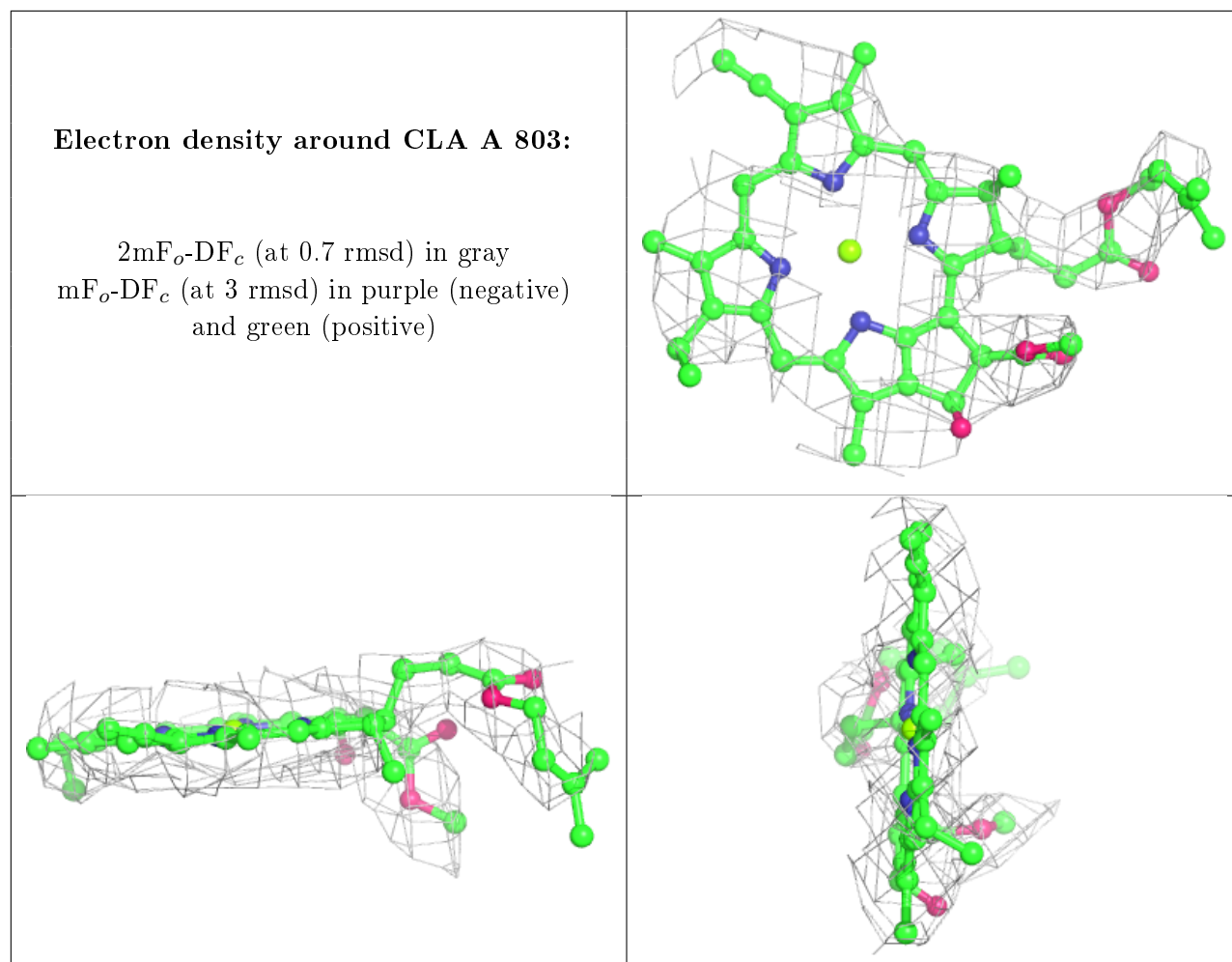


Electron density around CLA 1 212:

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

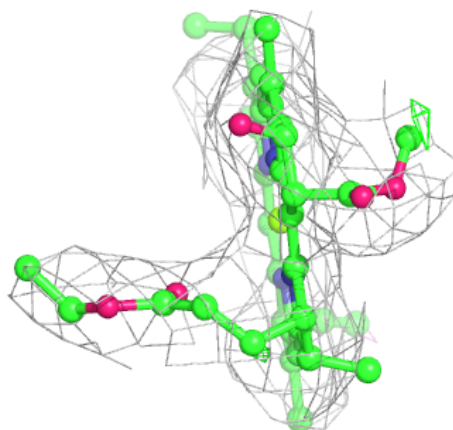
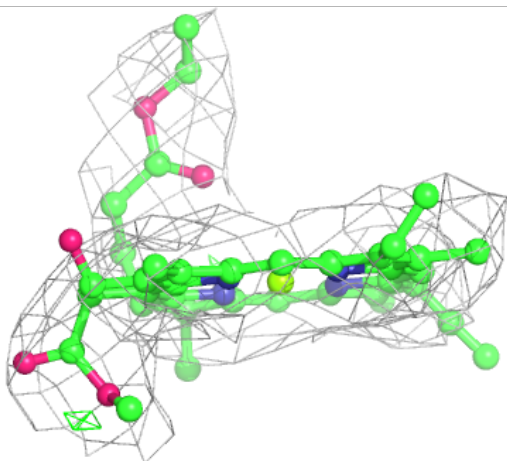
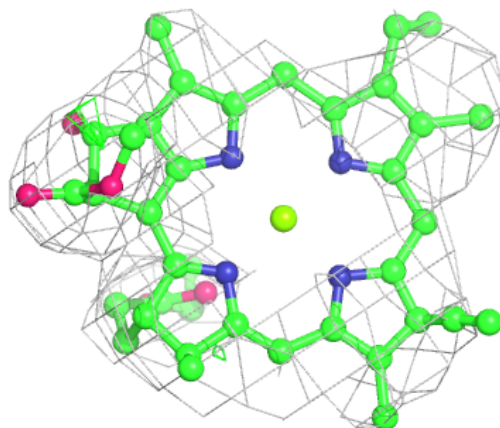






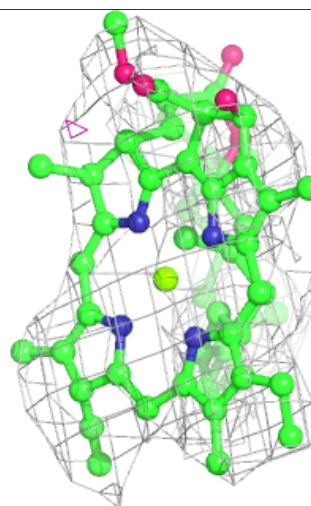
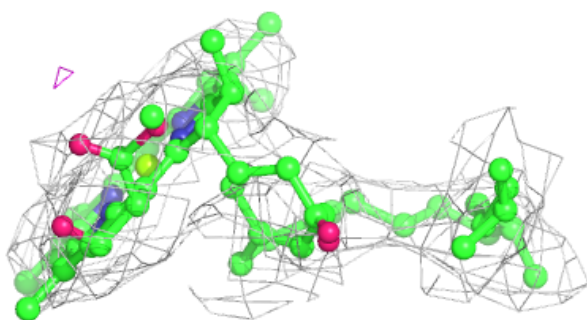
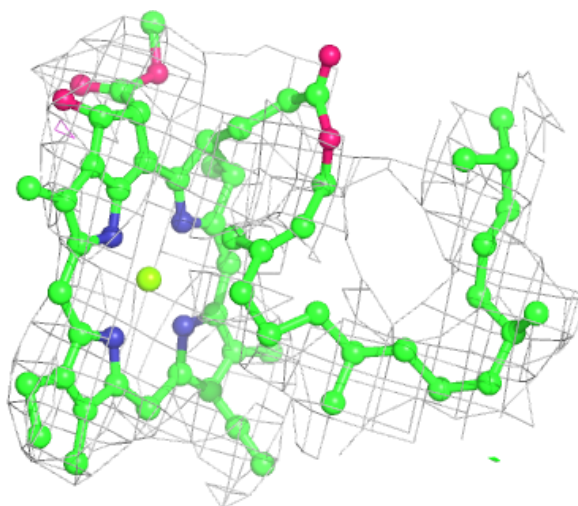
Electron density around CLA L 208:

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



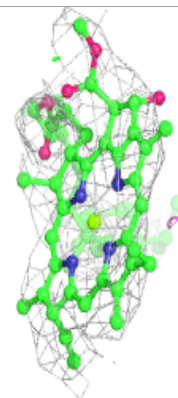
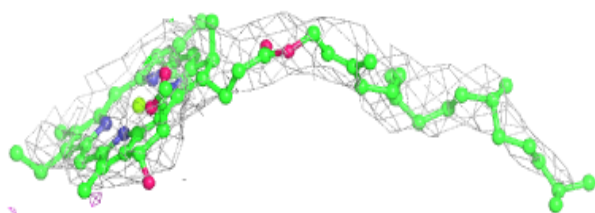
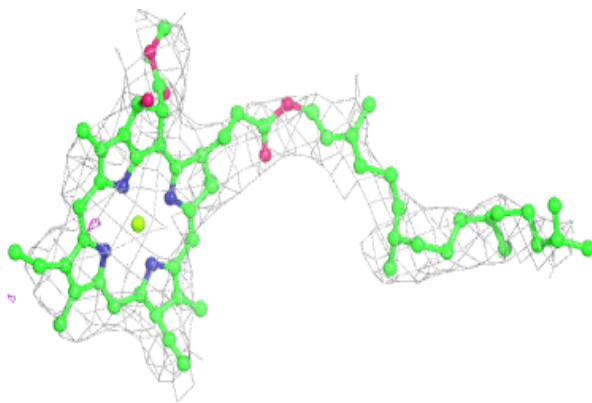
Electron density around CLA B 821:

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



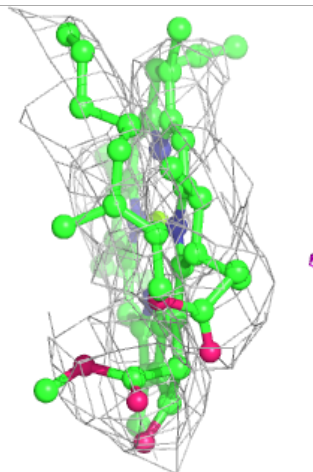
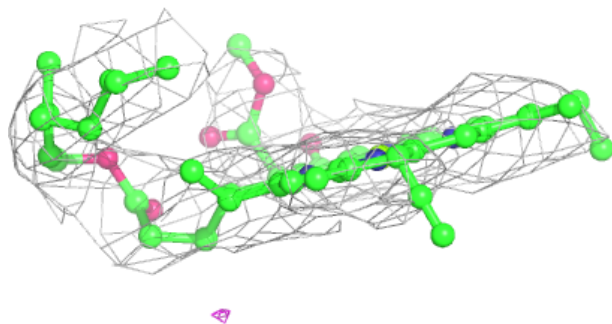
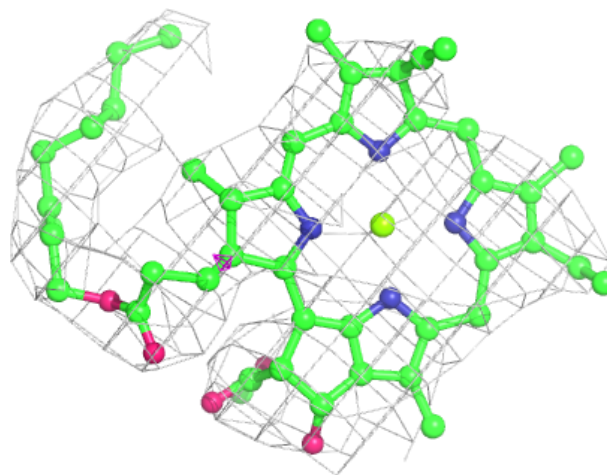
Electron density around CLA B 850:

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



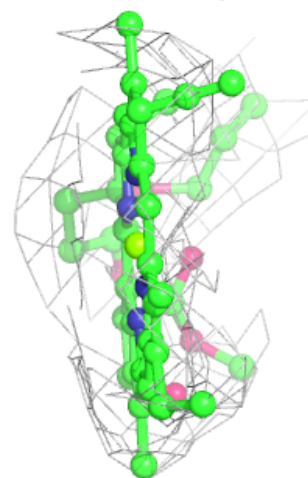
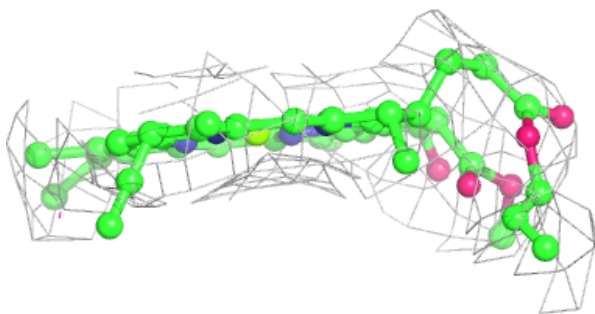
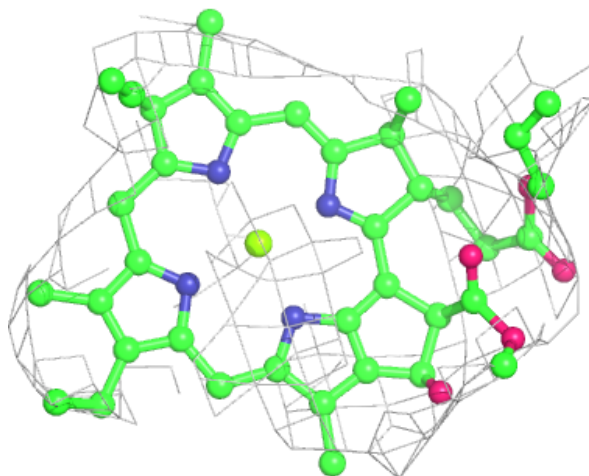
Electron density around CLA B 822:

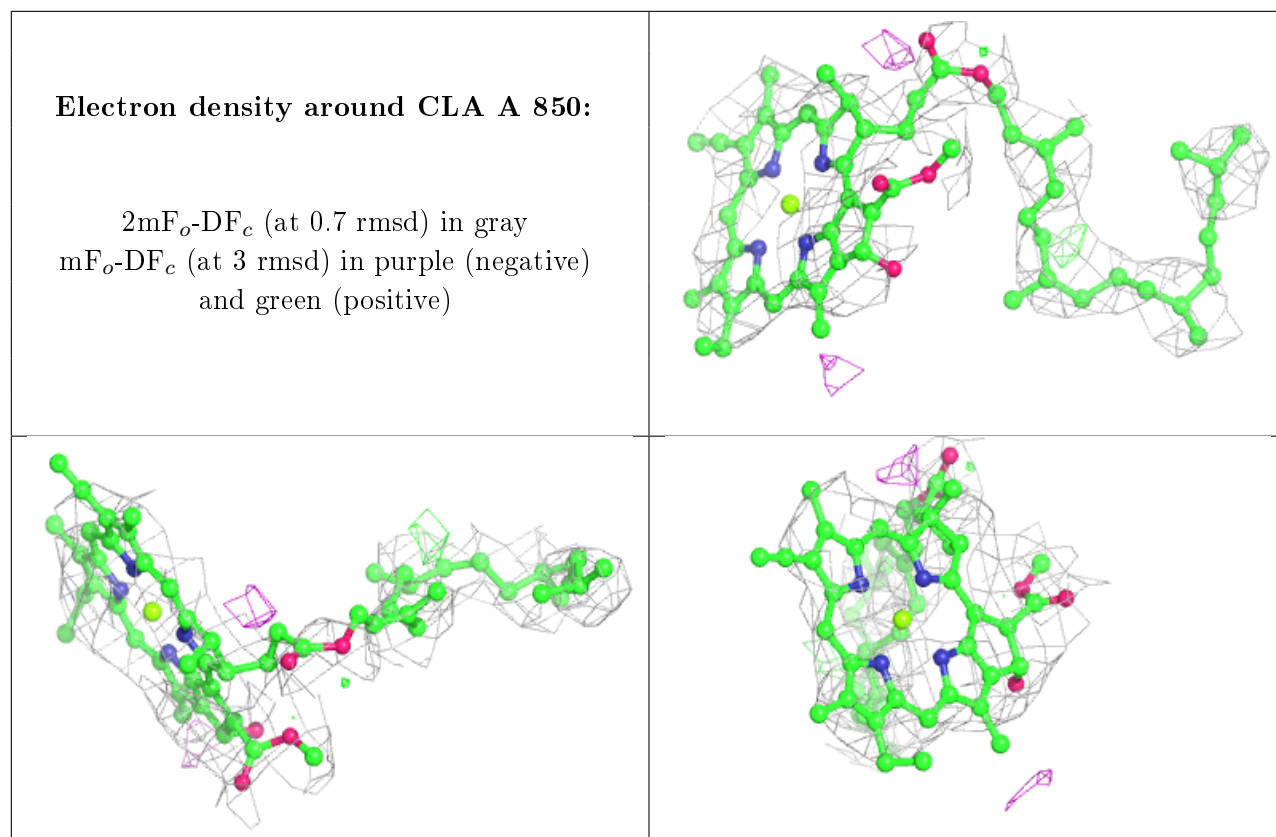
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA J 101:

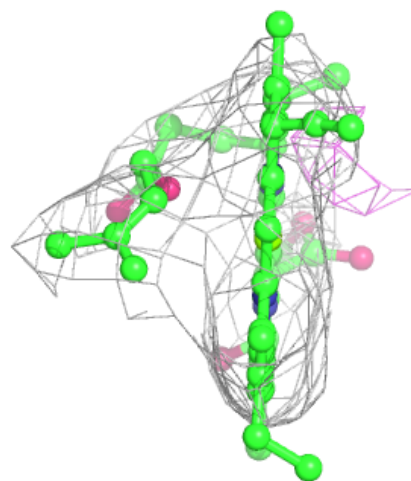
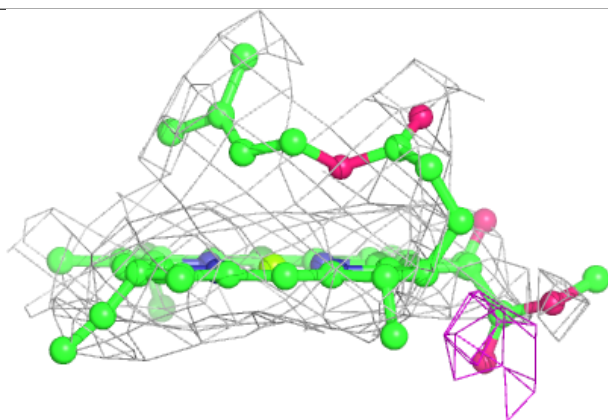
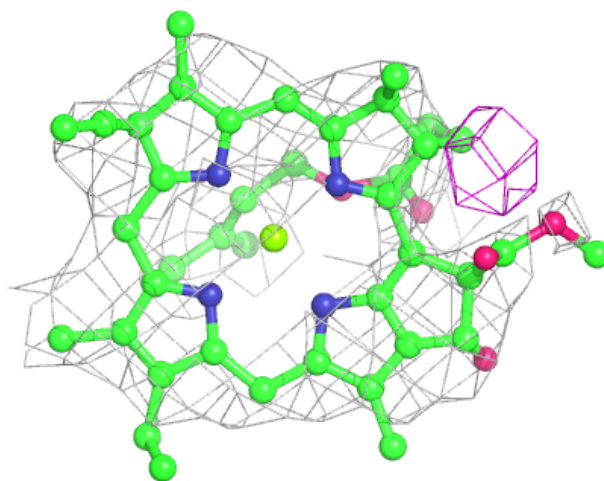
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





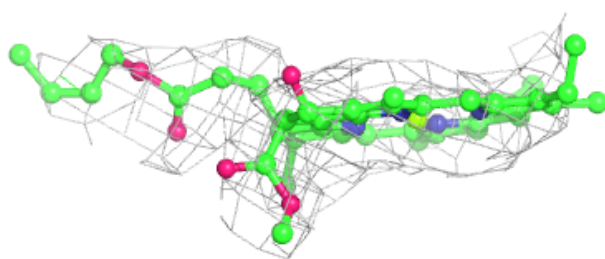
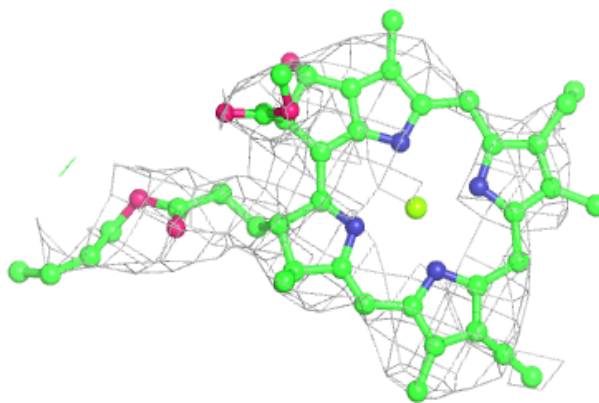
Electron density around CLA B 818:

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

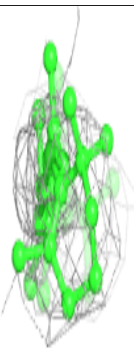
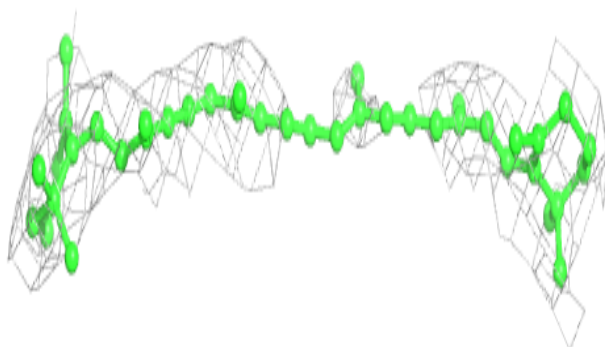
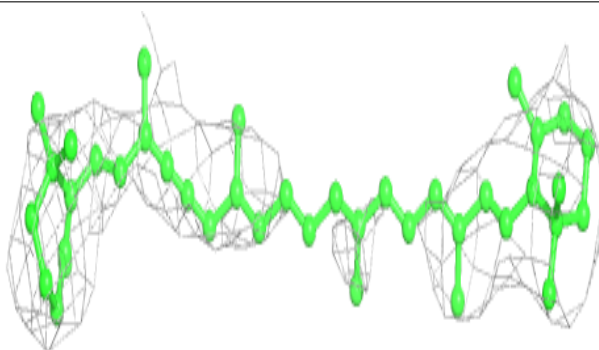


Electron density around CLA A 834:

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

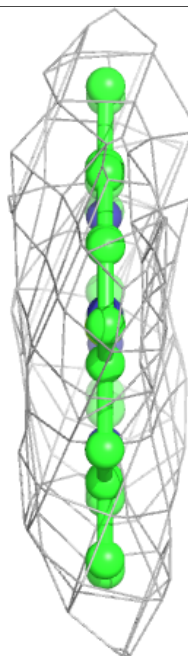
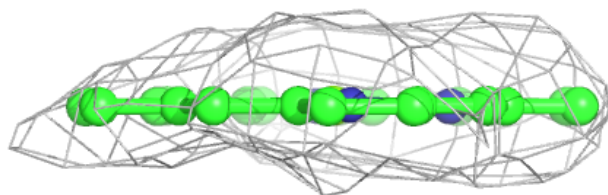
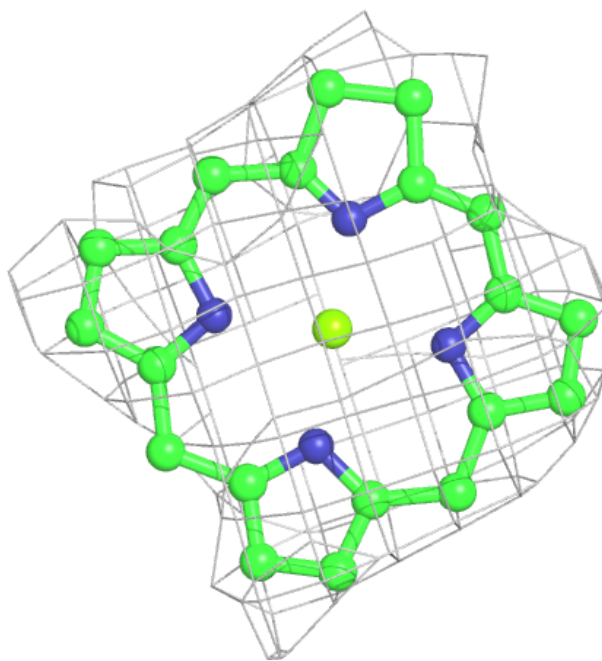
**Electron density around BCR A 846:**

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



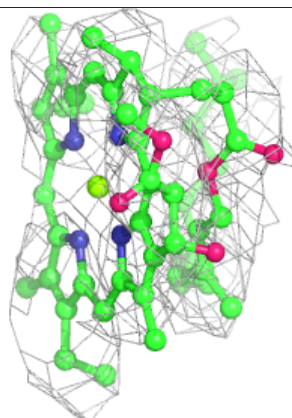
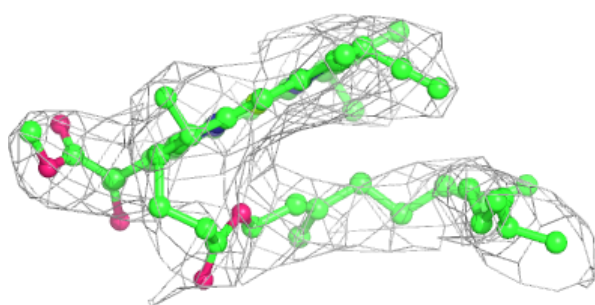
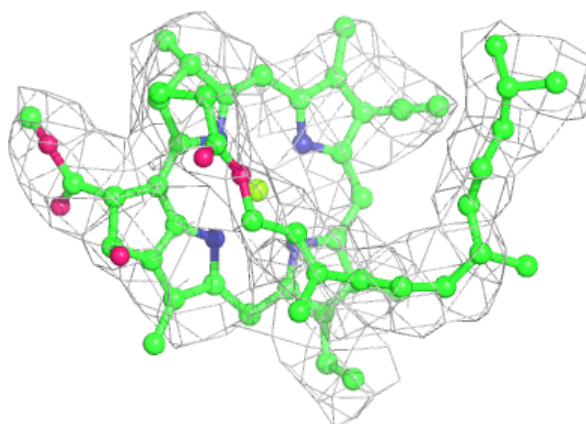
Electron density around CLA 1 208:

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



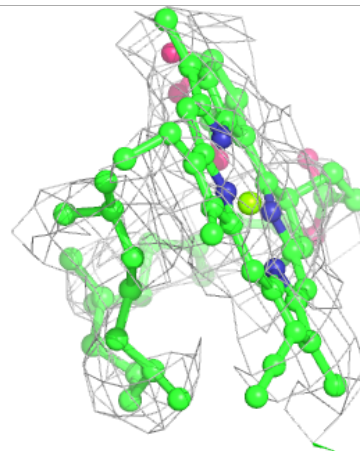
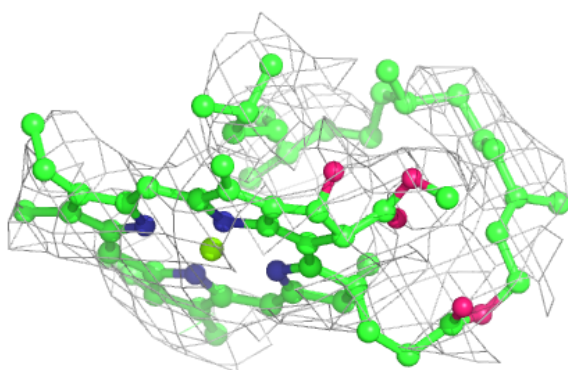
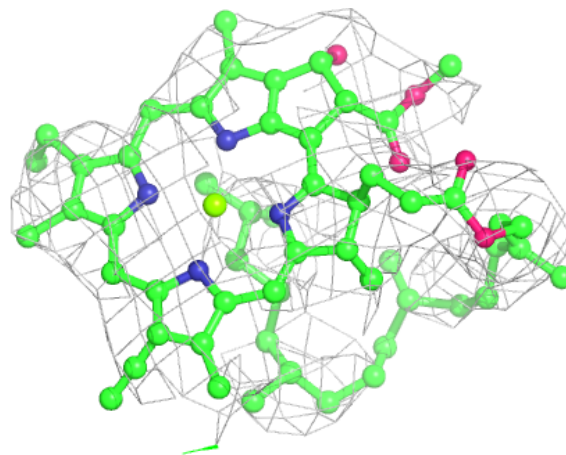
Electron density around CLA I 102:

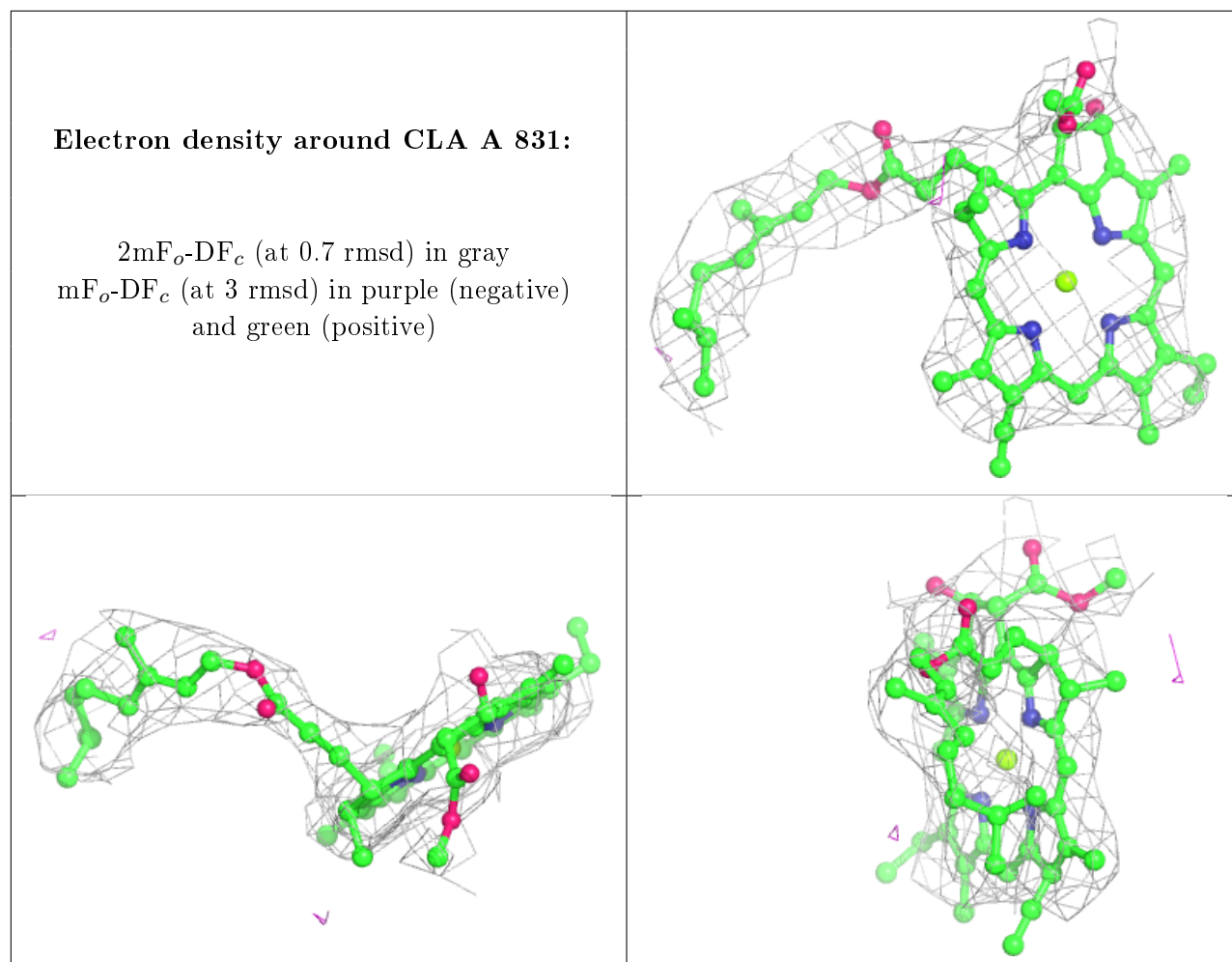
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 806:

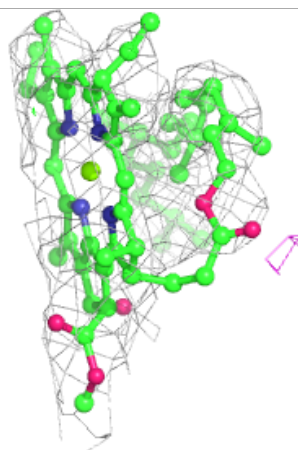
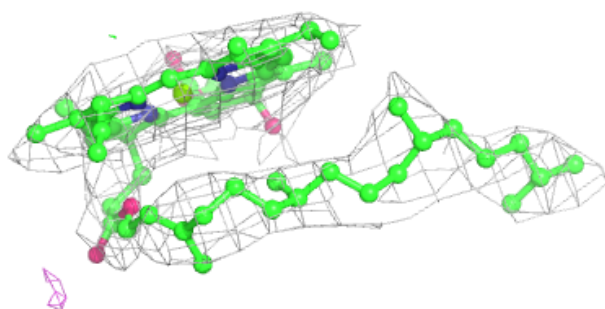
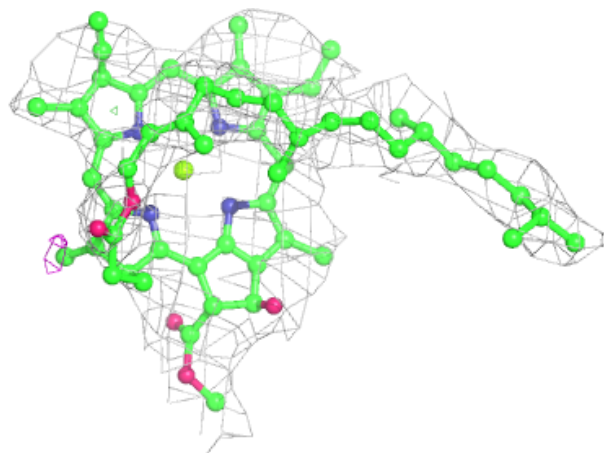
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





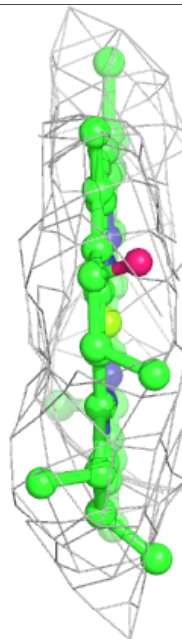
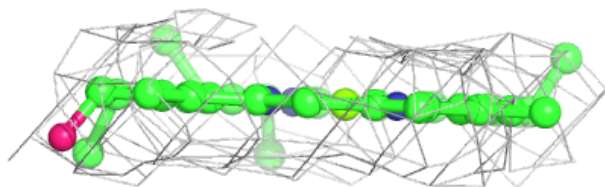
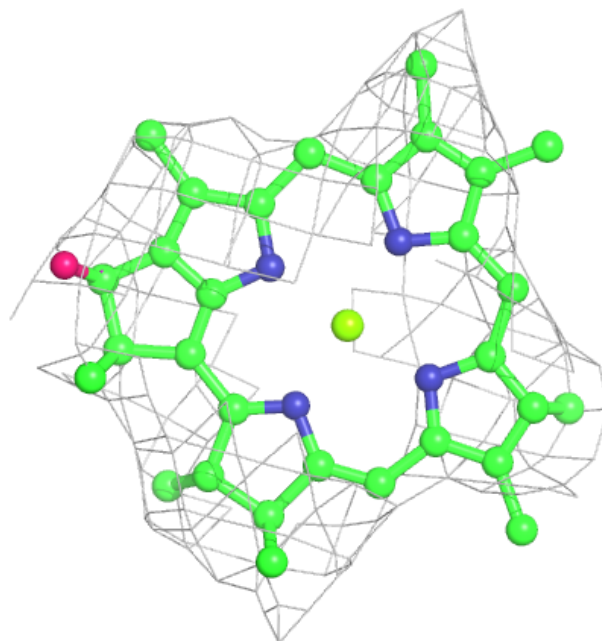
Electron density around CLA B 825:

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



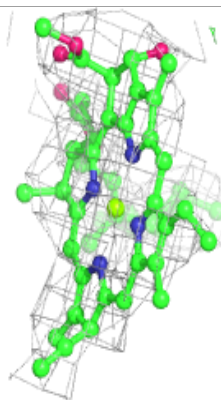
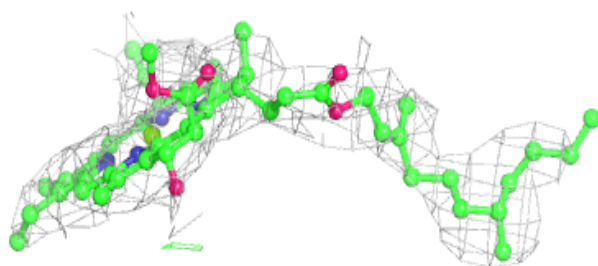
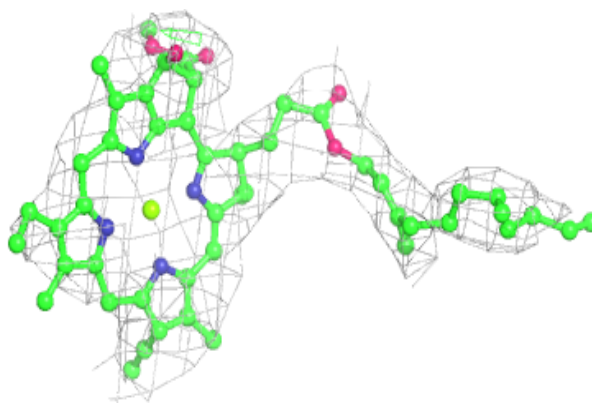
Electron density around CLA 1 209:

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



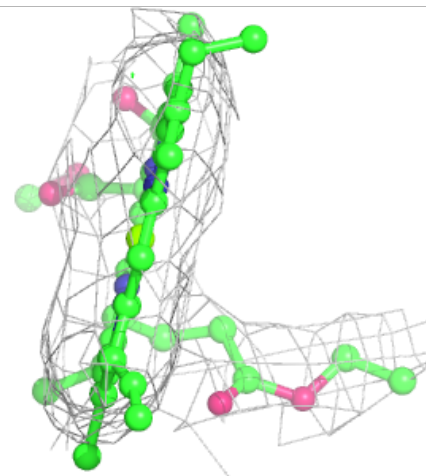
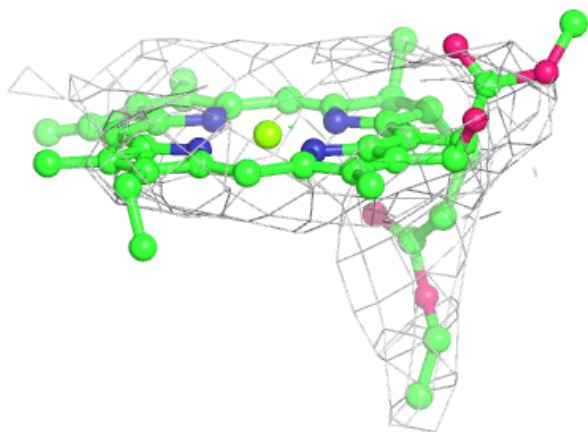
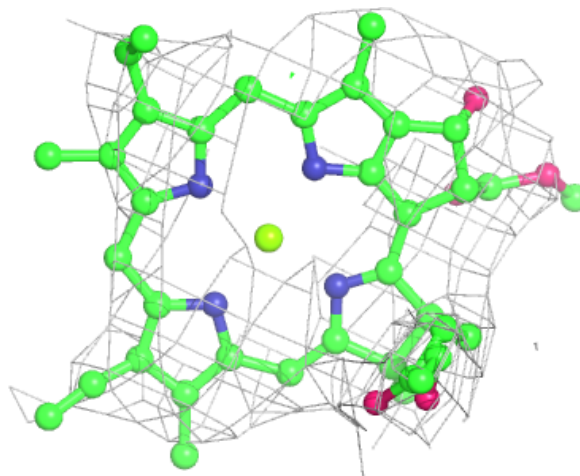
Electron density around CLA B 811:

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



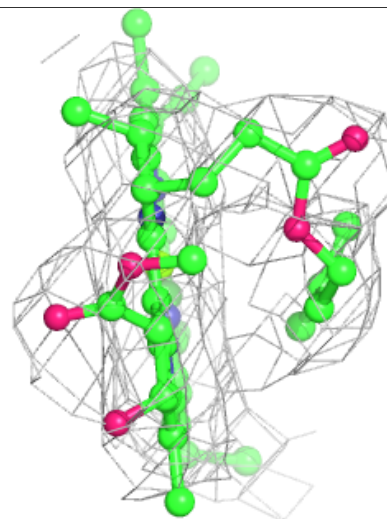
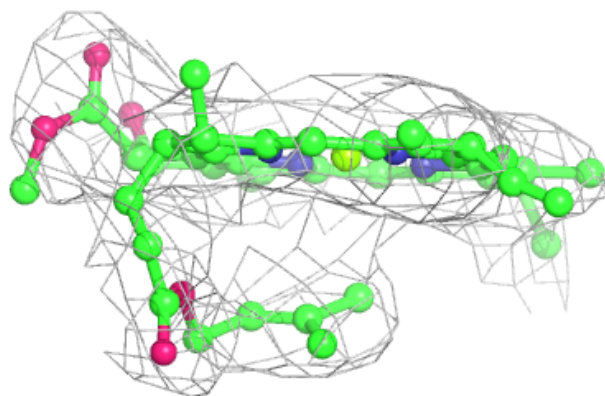
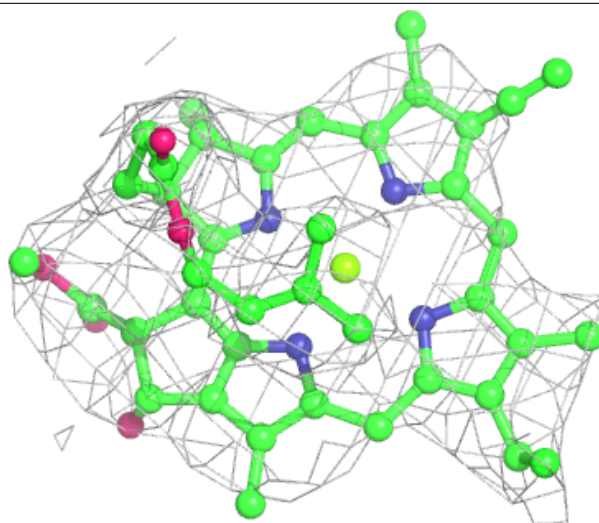
Electron density around CLA B 837:

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



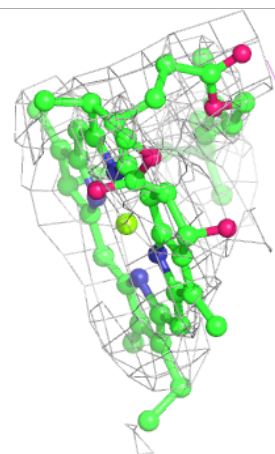
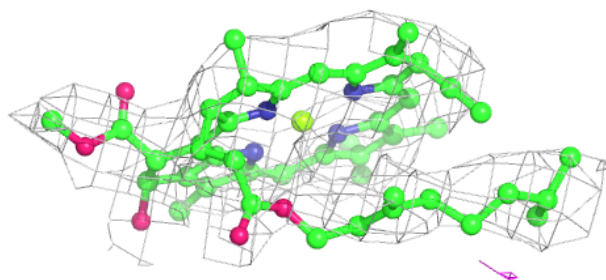
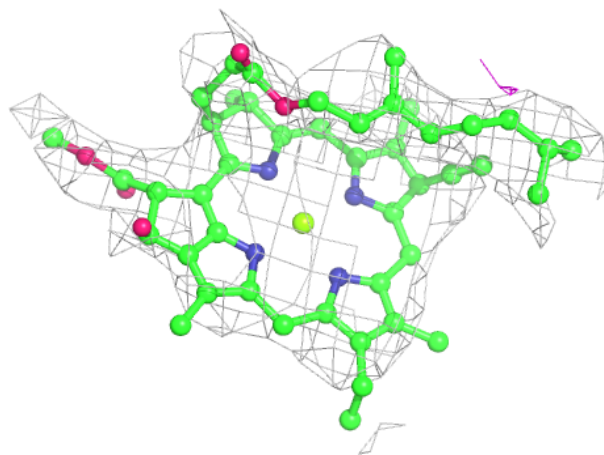
Electron density around CLA B 828:

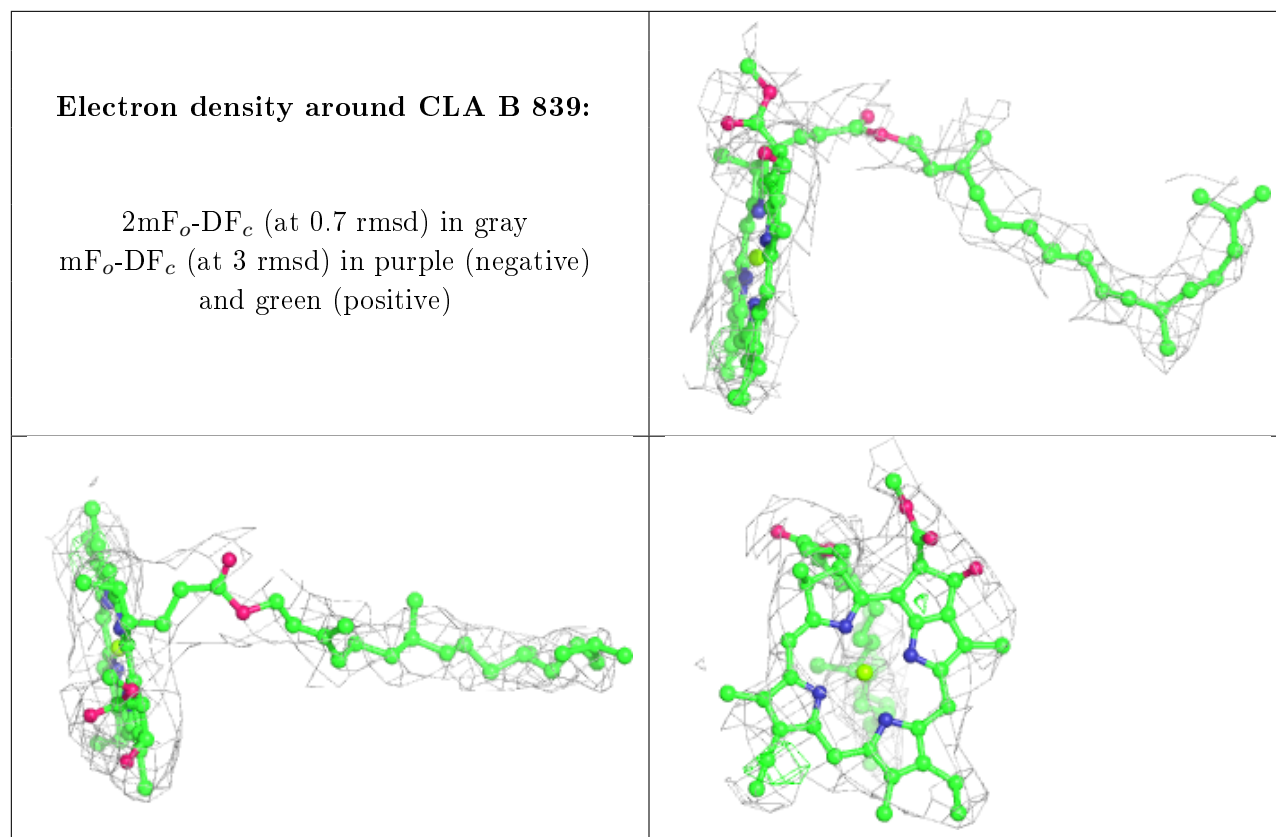
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 820:

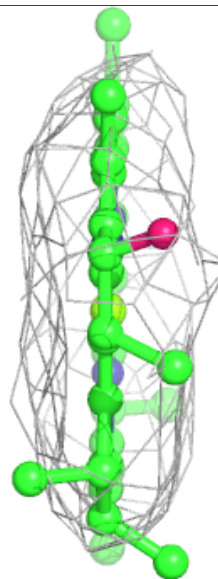
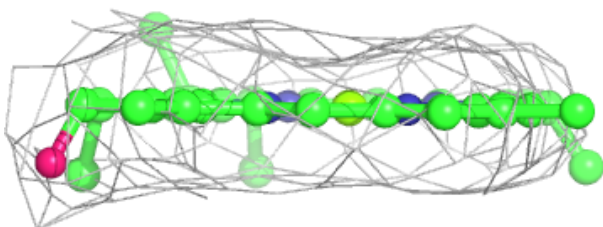
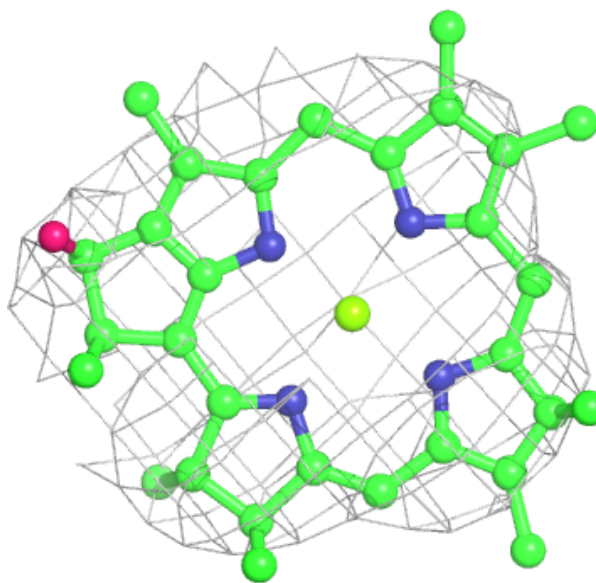
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

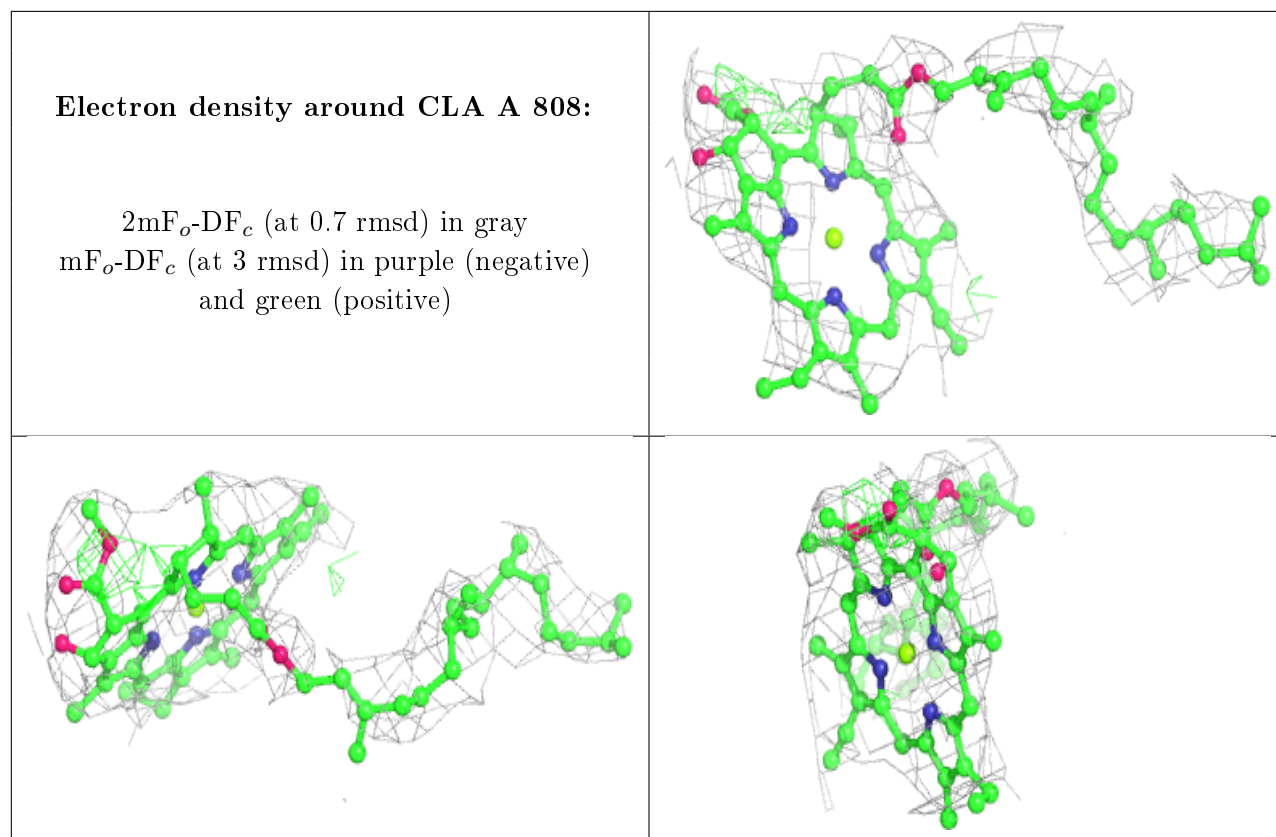




Electron density around CLA 4 303:

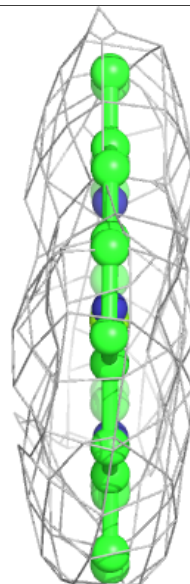
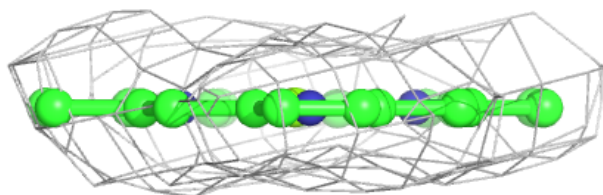
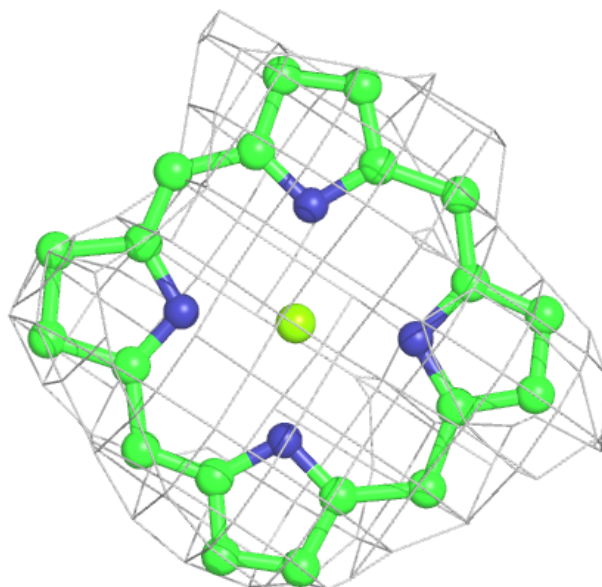
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





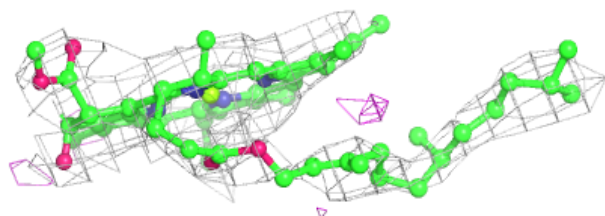
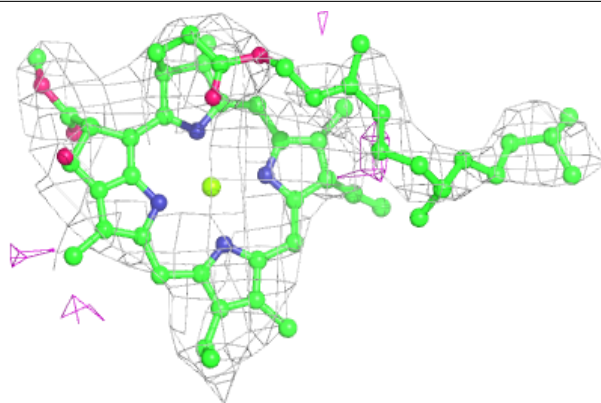
Electron density around CLA 4 313:

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

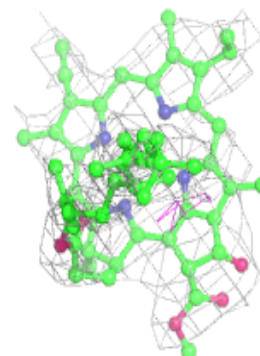
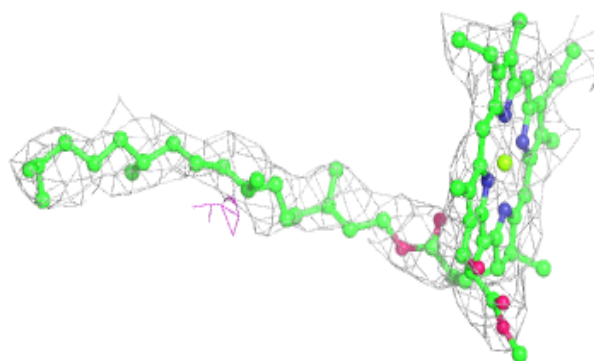


Electron density around CLA B 816:

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

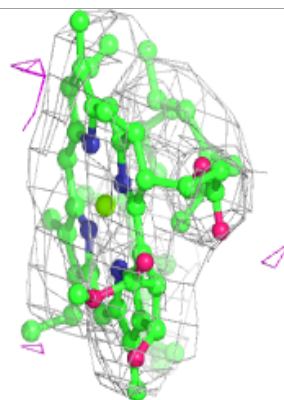
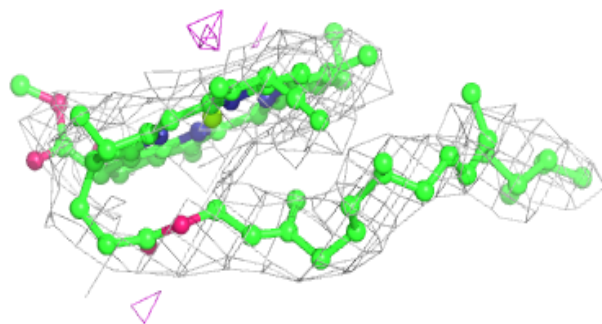
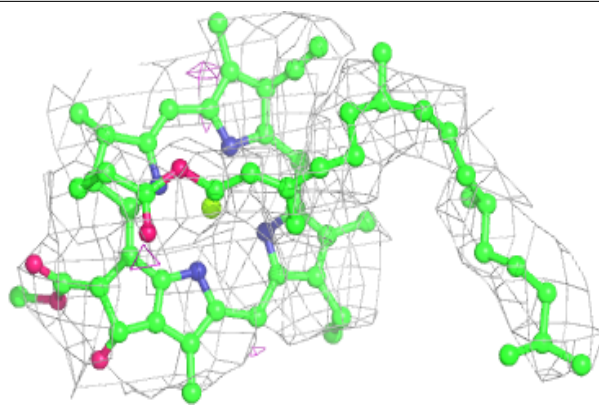
**Electron density around CLA B 826:**

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



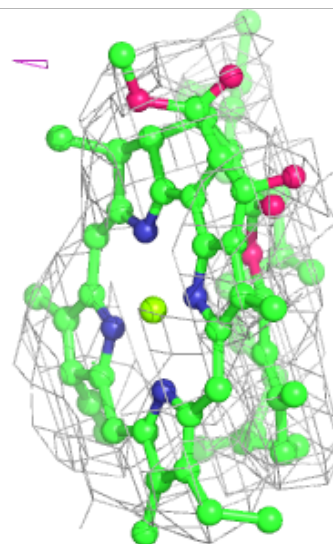
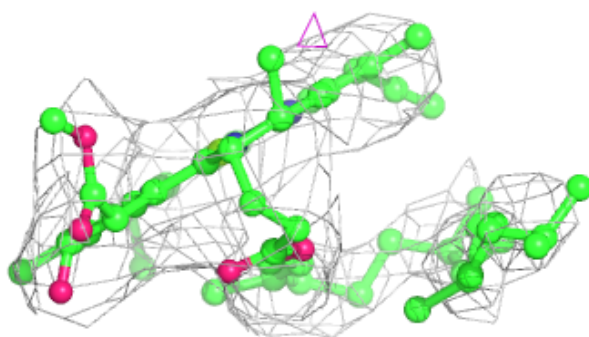
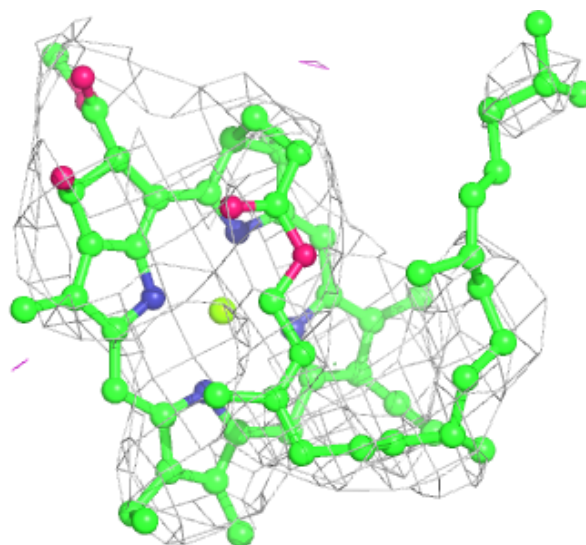
Electron density around CLA B 836:

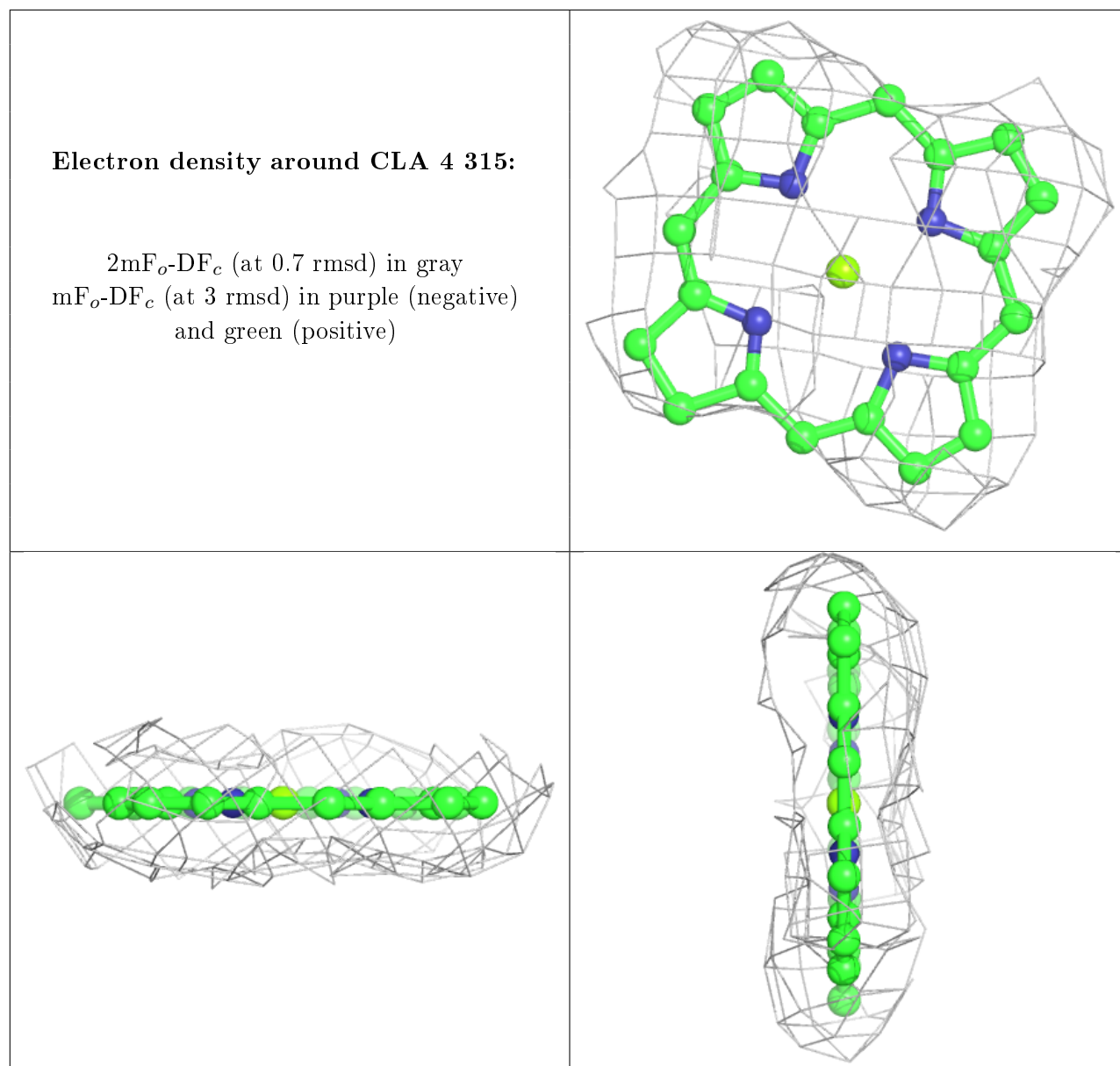
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 807:

$2mF_o-DF_c$ (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.