



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 10:04 AM BST

PDB ID : 2WSF
Title : Improved Model of Plant Photosystem I
Authors : Amunts, A.; Toporik, H.; Borovikov, A.; Nelson, N.
Deposited on : 2009-09-05
Resolution : 3.48 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

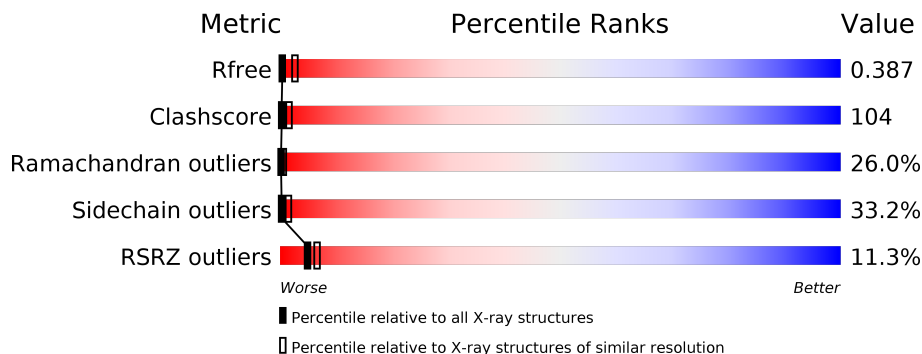
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 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	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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	

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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	FRU	M	2	X	-	-	-
19	GLC	O	1	-	-	X	-
19	FRU	O	2	X	-	-	X
19	GLC	P	1	-	-	X	-
19	FRU	P	2	X	-	X	-
19	FRU	Q	2	X	-	X	-
19	FRU	S	2	X	-	-	-
19	FRU	T	2	X	-	-	-
19	FRU	U	2	X	-	-	-
19	FRU	V	2	X	-	-	-
19	FRU	W	2	X	-	-	-
19	GLC	X	1	-	-	-	X
19	FRU	X	2	X	-	-	X
19	GLC	Y	1	-	-	X	-
19	FRU	Y	2	X	-	X	-
19	FRU	Z	2	X	-	X	-
19	FRU	a	2	X	-	-	-
20	CLA	1	201	X	-	-	-
20	CLA	1	202	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	-	-	X
20	CLA	1	212	X	-	-	-
20	CLA	1	213	X	-	-	-
20	CLA	1	214	X	-	-	-
20	CLA	1	215	X	-	-	-
20	CLA	2	301	X	-	-	X
20	CLA	2	302	X	-	-	-
20	CLA	2	303	X	-	X	-
20	CLA	2	304	X	-	-	X
20	CLA	2	305	X	-	-	-
20	CLA	2	306	X	-	-	-
20	CLA	2	307	X	-	X	-
20	CLA	2	308	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	317	X	-	-	-
20	CLA	3	301	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	-	-	-
20	CLA	3	307	X	-	-	-
20	CLA	3	308	X	-	-	-
20	CLA	3	309	X	-	-	-
20	CLA	3	310	X	-	-	-
20	CLA	3	311	X	-	-	X
20	CLA	3	313	X	-	-	X
20	CLA	3	314	X	-	-	X
20	CLA	3	315	X	-	-	-
20	CLA	3	316	X	-	-	X
20	CLA	3	317	X	-	-	-
20	CLA	3	318	X	-	-	-
20	CLA	4	301	X	-	X	-
20	CLA	4	302	X	-	-	-
20	CLA	4	303	X	-	-	-
20	CLA	4	304	X	-	X	-
20	CLA	4	305	X	-	-	X
20	CLA	4	306	X	-	-	-
20	CLA	4	307	X	-	-	-
20	CLA	4	308	X	-	-	-
20	CLA	4	309	X	-	-	-
20	CLA	4	310	X	-	X	-
20	CLA	4	311	X	-	-	-
20	CLA	4	312	X	-	-	-
20	CLA	4	313	X	-	-	-
20	CLA	4	314	X	-	-	-
20	CLA	4	315	X	-	-	-
20	CLA	4	317	X	-	-	X
20	CLA	4	318	X	-	-	-
20	CLA	A	801	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	802	X	-	-	X
20	CLA	A	803	X	-	-	-
20	CLA	A	804	X	-	X	-
20	CLA	A	805	X	-	-	-
20	CLA	A	806	X	-	-	-
20	CLA	A	807	X	-	X	-
20	CLA	A	808	X	-	X	-
20	CLA	A	809	X	-	X	-
20	CLA	A	810	X	-	-	-
20	CLA	A	811	X	-	X	X
20	CLA	A	812	X	-	-	-
20	CLA	A	813	X	-	X	-
20	CLA	A	814	X	-	-	-
20	CLA	A	815	X	-	-	-
20	CLA	A	816	X	-	X	-
20	CLA	A	817	X	-	-	-
20	CLA	A	818	X	-	X	-
20	CLA	A	819	X	-	X	-
20	CLA	A	820	X	-	-	-
20	CLA	A	821	X	-	-	-
20	CLA	A	822	X	-	-	-
20	CLA	A	823	X	-	-	-
20	CLA	A	824	X	-	X	-
20	CLA	A	825	X	-	X	-
20	CLA	A	826	X	-	X	-
20	CLA	A	827	X	-	-	-
20	CLA	A	828	X	-	-	-
20	CLA	A	829	X	-	-	-
20	CLA	A	830	X	-	X	-
20	CLA	A	831	X	-	X	-
20	CLA	A	832	X	-	-	-
20	CLA	A	833	X	-	-	-
20	CLA	A	834	X	-	-	-
20	CLA	A	835	X	-	-	-
20	CLA	A	836	X	-	-	-
20	CLA	A	837	X	-	-	-
20	CLA	A	838	X	-	X	-
20	CLA	A	839	X	-	X	-
20	CLA	A	840	X	-	-	-
20	CLA	A	841	X	-	-	-
20	CLA	A	849	X	-	X	-
20	CLA	A	850	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	851	X	-	X	-
20	CLA	B	802	X	-	-	-
20	CLA	B	803	X	-	X	-
20	CLA	B	806	X	-	X	-
20	CLA	B	807	X	-	-	-
20	CLA	B	808	X	-	X	-
20	CLA	B	809	X	-	X	-
20	CLA	B	810	X	-	-	-
20	CLA	B	811	X	-	-	-
20	CLA	B	812	X	-	-	-
20	CLA	B	813	X	-	-	-
20	CLA	B	814	X	-	X	-
20	CLA	B	815	X	-	-	-
20	CLA	B	816	X	-	-	-
20	CLA	B	817	X	-	-	X
20	CLA	B	818	X	-	-	-
20	CLA	B	819	X	-	-	-
20	CLA	B	820	X	-	-	-
20	CLA	B	821	X	-	-	-
20	CLA	B	822	X	-	-	-
20	CLA	B	823	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	-	X	-
20	CLA	B	830	X	-	X	-
20	CLA	B	831	X	-	-	-
20	CLA	B	832	X	-	X	-
20	CLA	B	833	X	-	-	-
20	CLA	B	834	X	-	X	-
20	CLA	B	835	X	-	X	-
20	CLA	B	836	X	-	-	-
20	CLA	B	837	X	-	-	-
20	CLA	B	838	X	-	X	-
20	CLA	B	839	X	-	X	-
20	CLA	B	840	X	-	-	-
20	CLA	B	841	X	-	-	-
20	CLA	B	842	X	-	-	-
20	CLA	B	850	X	-	-	-
20	CLA	F	201	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	F	205	X	-	-	-
20	CLA	F	206	X	-	-	-
20	CLA	F	207	X	-	-	-
20	CLA	G	105	X	-	-	X
20	CLA	H	101	X	-	-	X
20	CLA	H	102	X	-	-	-
20	CLA	H	111	X	-	X	-
20	CLA	H	112	X	-	-	-
20	CLA	I	102	X	-	-	-
20	CLA	J	101	X	-	-	-
20	CLA	J	103	X	-	-	-
20	CLA	K	101	X	-	-	-
20	CLA	K	102	X	-	X	-
20	CLA	K	103	X	-	-	-
20	CLA	K	104	X	-	-	-
20	CLA	L	201	X	-	X	-
20	CLA	L	202	X	-	-	X
20	CLA	L	203	X	-	X	-
20	CLA	L	204	X	-	-	X
20	CLA	L	208	X	-	-	-
20	CLA	L	209	X	-	X	-
20	CLA	L	210	X	-	-	-
20	CLA	R	107	X	-	-	-
20	CLA	R	108	X	-	-	-
21	LMU	2	313	-	-	X	-
21	LMU	A	852	-	-	-	X
21	LMU	A	853	-	-	X	-
21	LMU	G	101	-	-	X	-
21	LMU	K	107	-	-	X	-
22	BCR	2	318	-	-	-	X
22	BCR	A	843	-	-	X	X
22	BCR	A	844	-	-	X	-
22	BCR	A	845	-	-	X	-
22	BCR	B	801	-	-	X	-
22	BCR	B	846	-	-	X	-
22	BCR	B	847	-	-	X	-
22	BCR	F	203	-	-	X	-
22	BCR	F	204	-	-	X	-
22	BCR	G	104	-	-	-	X
22	BCR	I	103	-	-	X	X
22	BCR	J	102	-	-	X	-
22	BCR	L	211	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	PQN	A	842	X	-	-	-
23	PQN	B	843	X	-	X	-
24	SF4	A	856	-	-	X	-
24	SF4	C	102	-	-	X	-

2 Entry composition i

There are 26 unique types of molecules in this entry. The entry contains 36033 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	165	1264	822	208	230	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	1374	899	226	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	153	1186	781	193	207	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	1319	861	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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	L	162	Total	C	N	O	S	0	0	0
			1215	800	194	216	5			

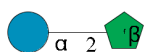
- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

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

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

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

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



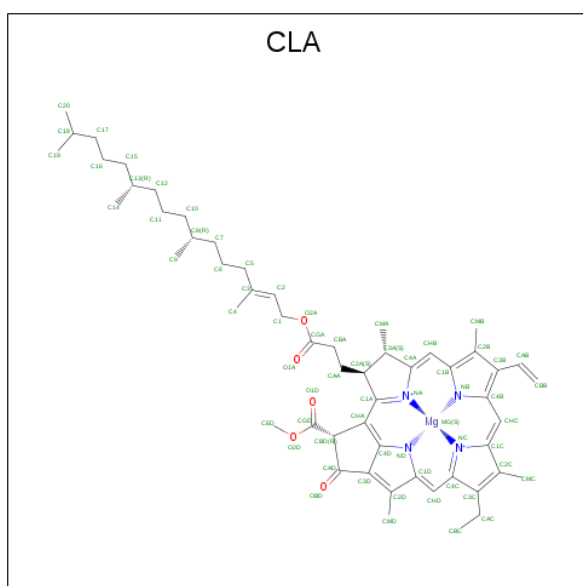
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
19	M	2	Total	C	O	0	0	0
			23	12	11			
19	O	2	Total	C	O	0	0	0
			22	12	10			
19	P	2	Total	C	O	0	0	0
			23	12	11			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
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
			22	12	10			
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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	1	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
20	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	1	1	Total	C	Mg	N		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	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
			51	41	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
			51	41	1	4	5		
20	2	1	Total	C	Mg	N	O	0	0
			58	48	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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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	O	0	0
			61	51	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	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	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	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
			50	40	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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	3	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
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		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		0	0
			25	20	1	4			
20	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
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
			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		
20	4	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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
			46	36	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
			54	44	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			56	46	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
			60	50	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
			50	40	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
			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
			60	50	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
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
			58	48	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			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
			47	37	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			59	49	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		0	0
			25	20	1	4			
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			54	44	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
			45	35	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
			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
			25	20	1	4			
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
			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
			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
			53	43	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			50	40	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
			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		

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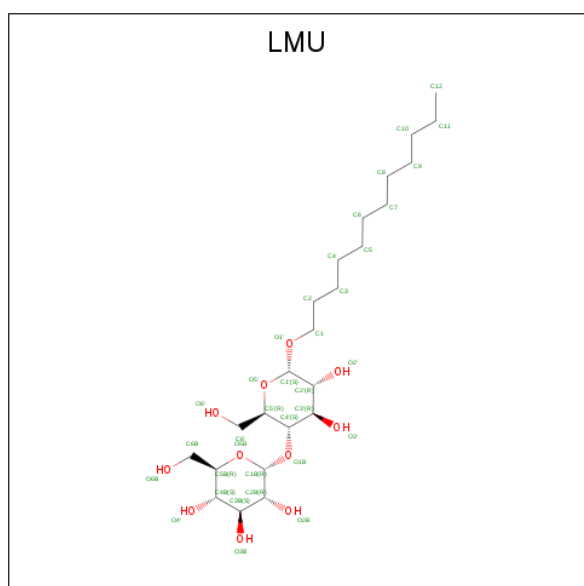
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
20	F	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	F	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	F	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
20	F	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
20	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
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
			58	48	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			55	45	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
			46	36	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
			50	40	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			60	50	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		

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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
			65	55	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	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		

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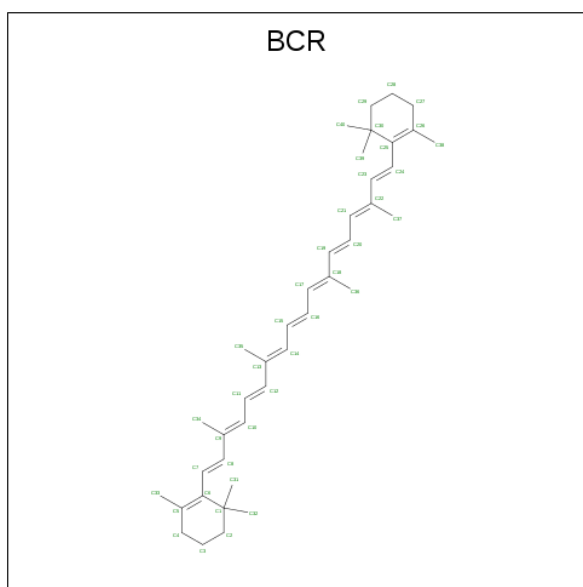
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	2	1	Total	C	O	0	0
			35	24	11		
21	3	1	Total	C	O	0	0
			35	24	11		
21	3	1	Total	C	O	0	0
			35	24	11		
21	4	1	Total	C	O	0	0
			35	24	11		
21	4	1	Total	C	O	0	0
			34	23	11		
21	4	1	Total	C	O	0	0
			35	24	11		
21	4	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	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	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
			25	14	11		
21	C	1	Total	C	O	0	0
			35	24	11		
21	D	1	Total	C	O	0	0
			35	24	11		
21	E	1	Total	C	O	0	0
			35	24	11		
21	F	1	Total	C	O	0	0
			34	23	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	G	1	Total	C	O	0	0
			35	24	11		
21	G	1	Total	C	O	0	0
			35	24	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	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	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		
21	R	1	Total	C	O	0	0
			35	24	11		

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



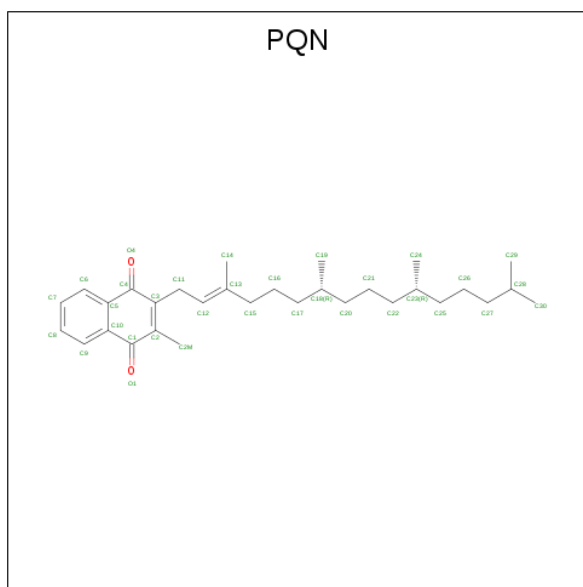
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	2	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	G	1	Total C 40 40	0	0
22	I	1	Total C 39 39	0	0
22	I	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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).



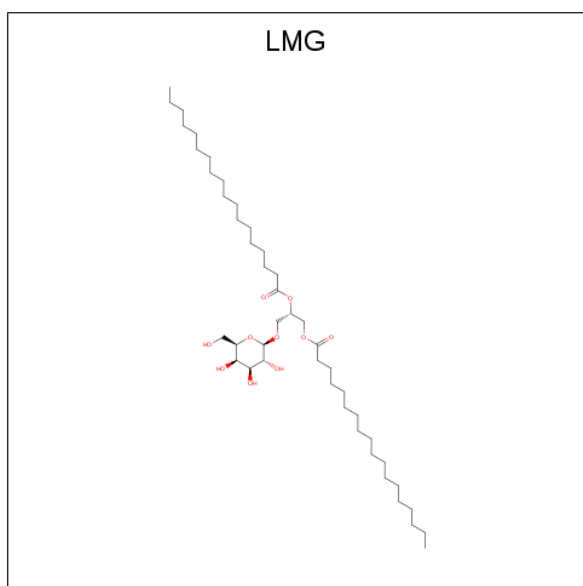
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 33 31 2	0	0
23	B	1	Total C O 33 31 2	0	0

- 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: $C_{45}H_{86}O_{10}$).



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

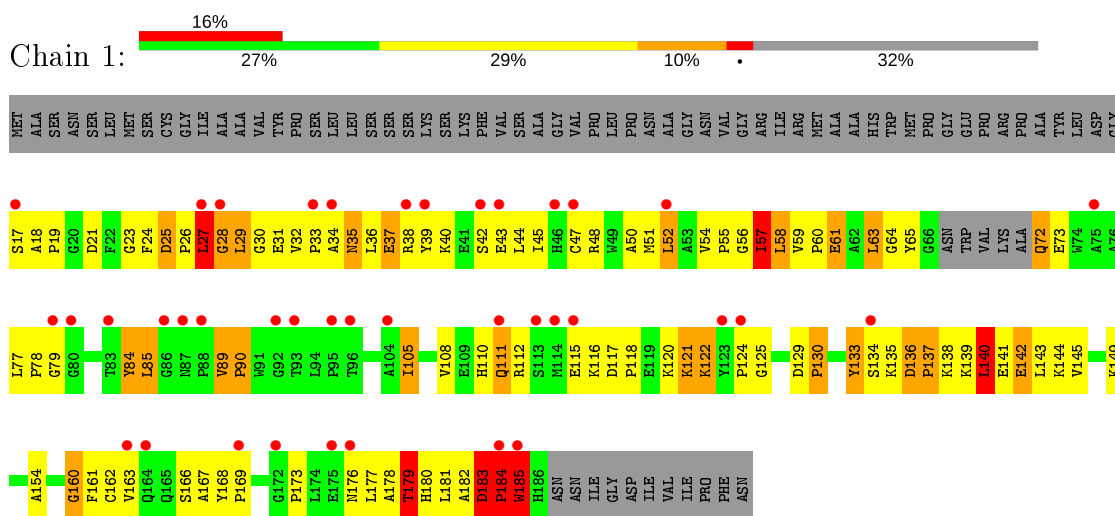
- Molecule 26 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

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

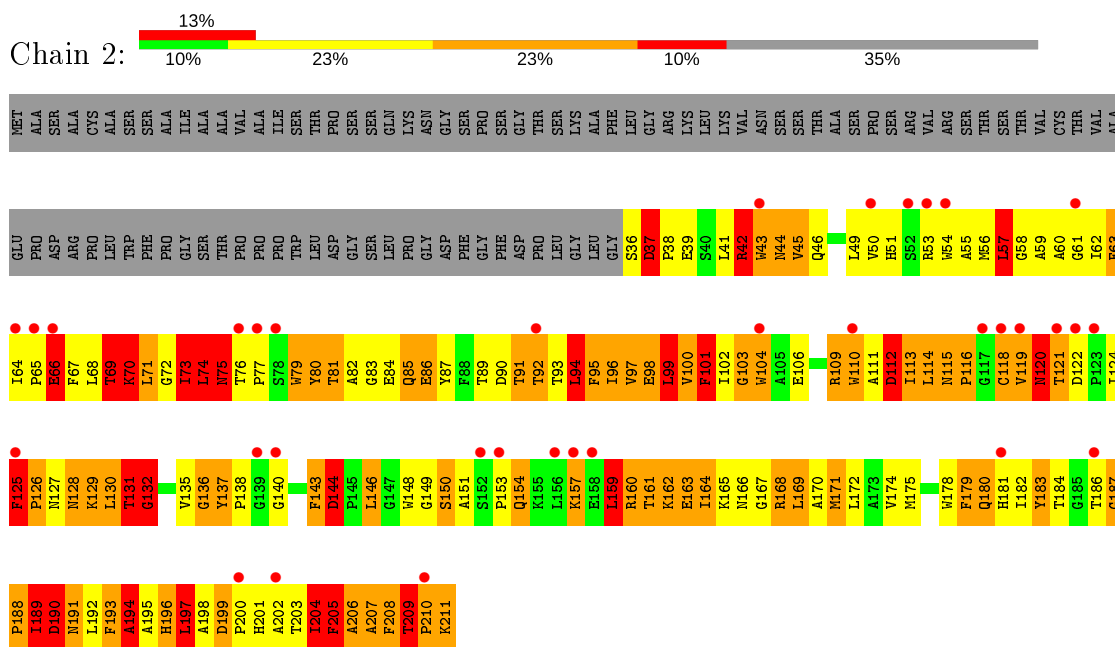
3 Residue-property plots

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

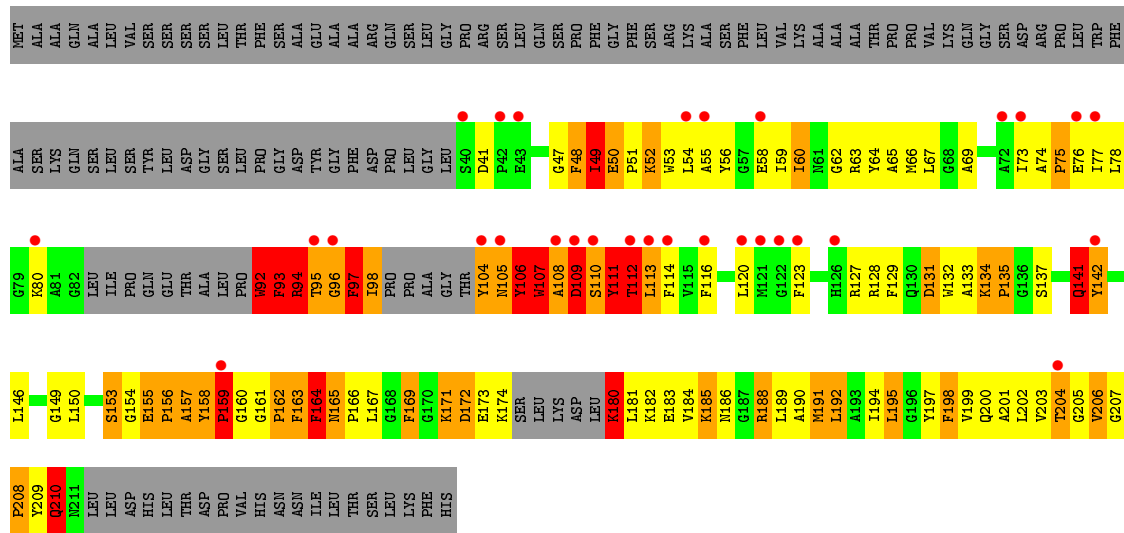
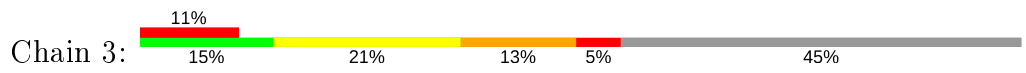
- Molecule 1: AT3G54890



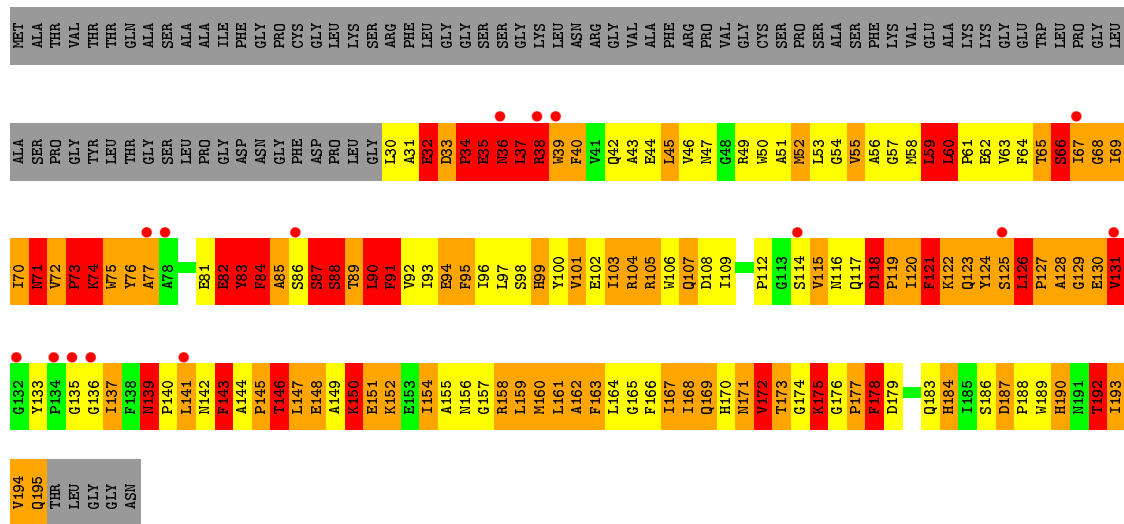
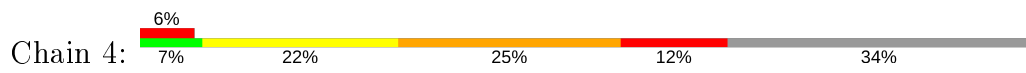
- Molecule 2: TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I



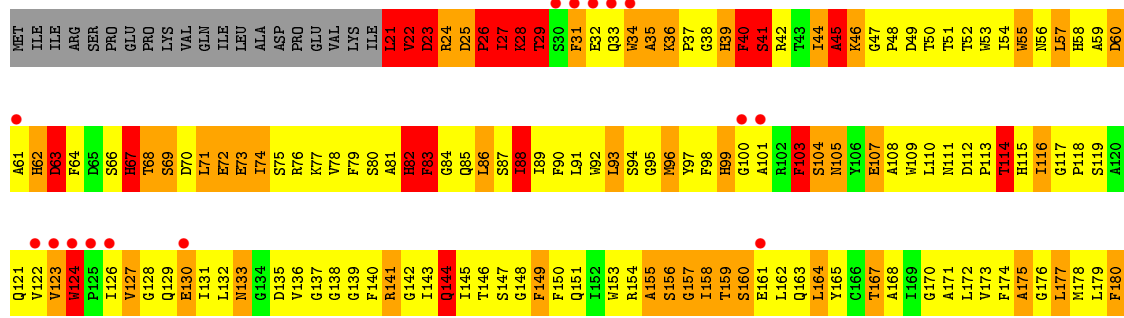
- Molecule 3: LHCA3

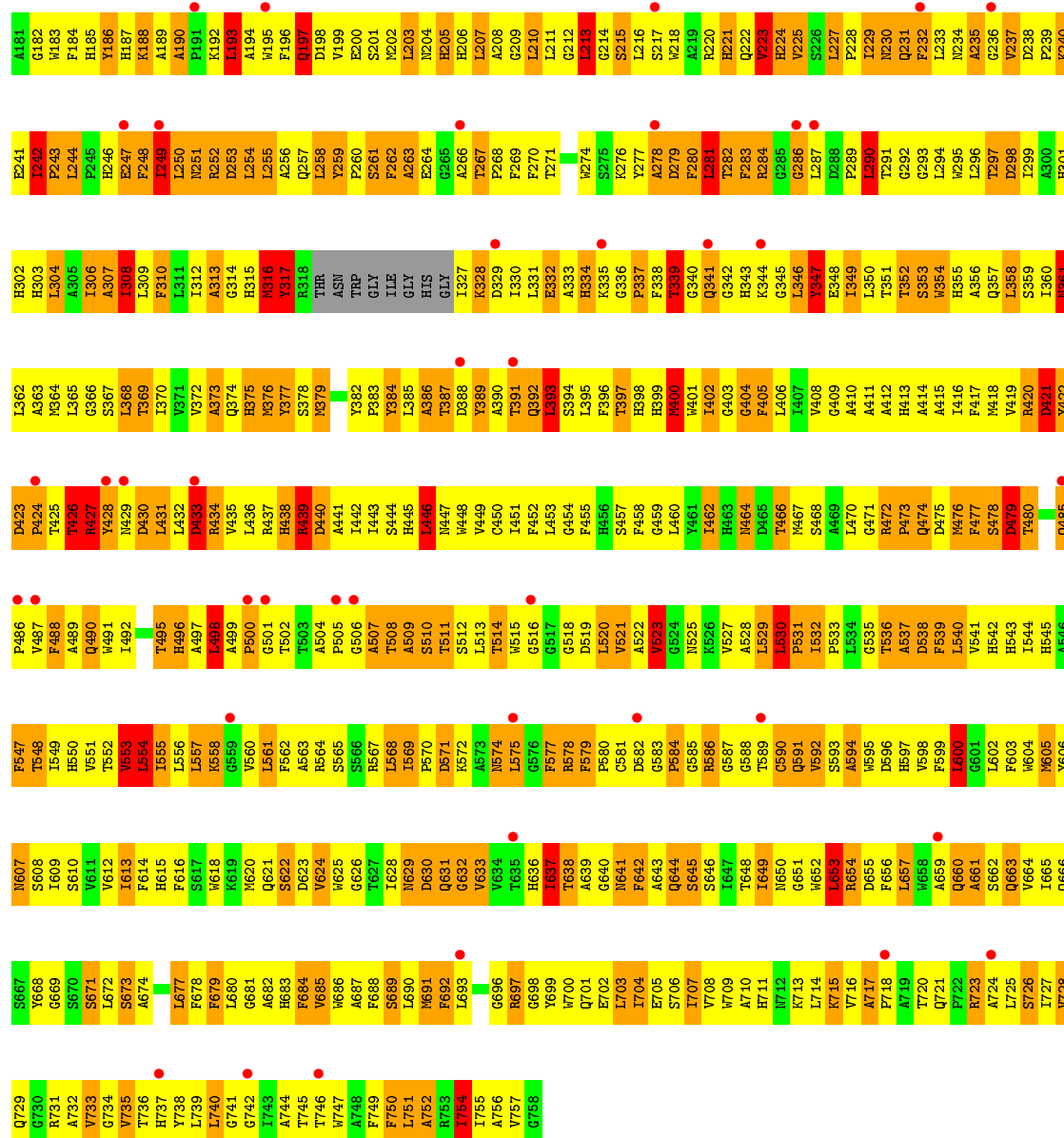


• Molecule 4: CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC

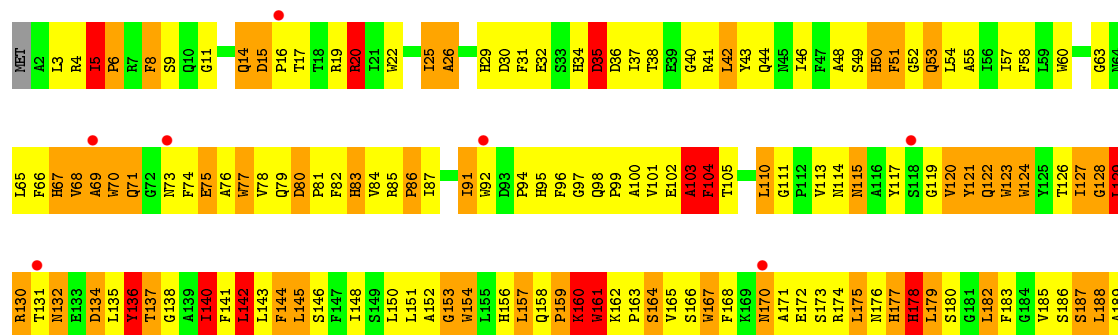
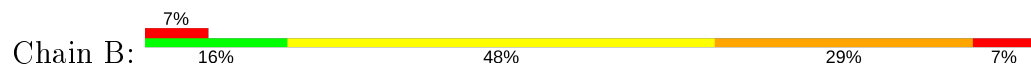


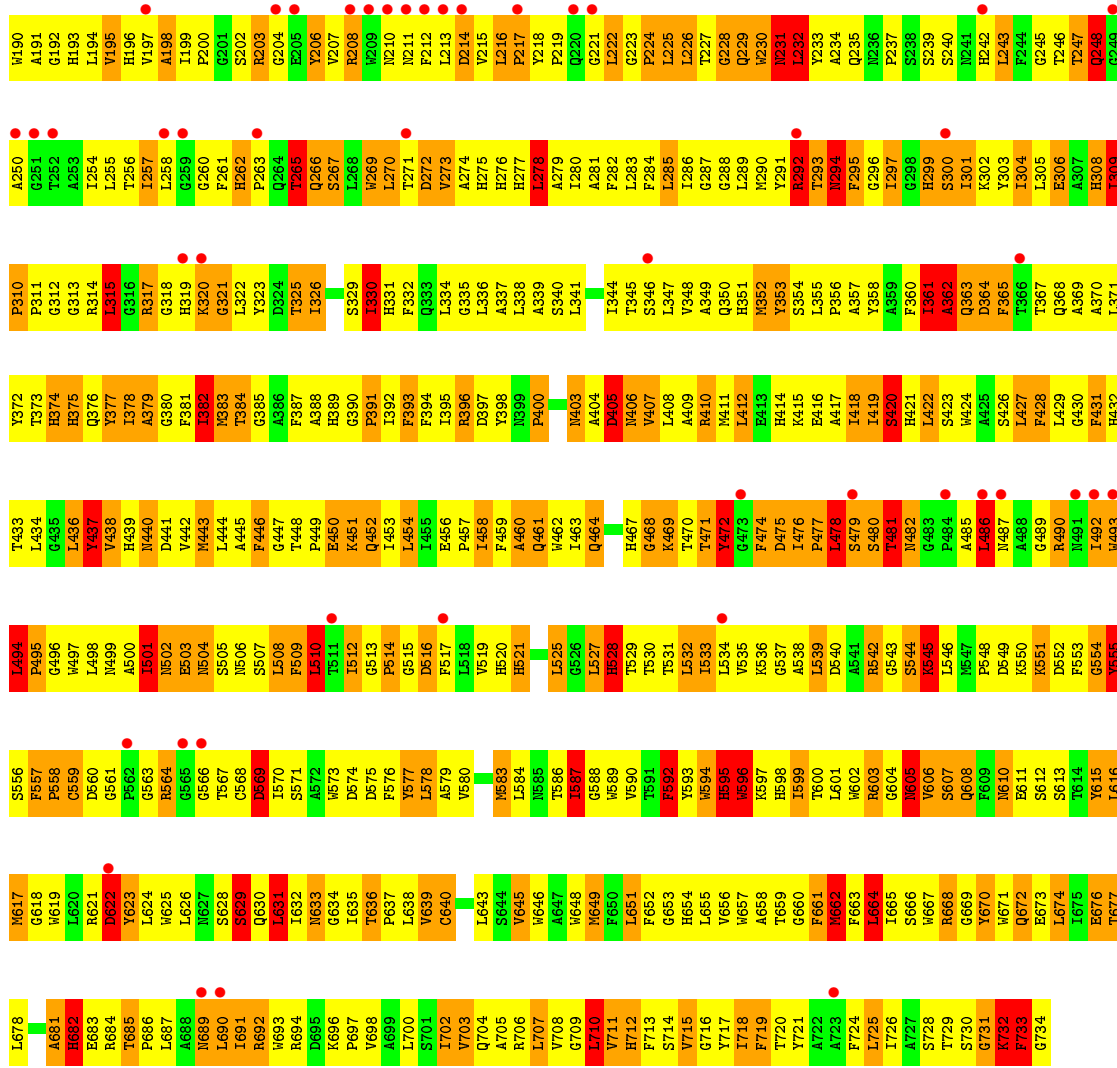
• Molecule 5: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1



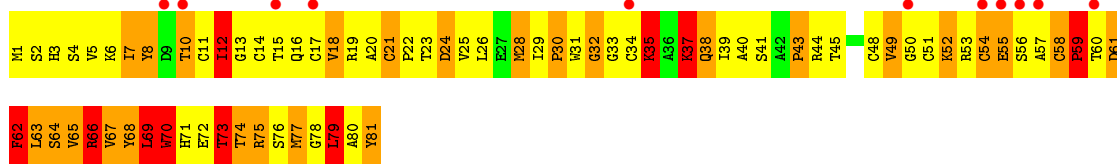


● Molecule 6: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2

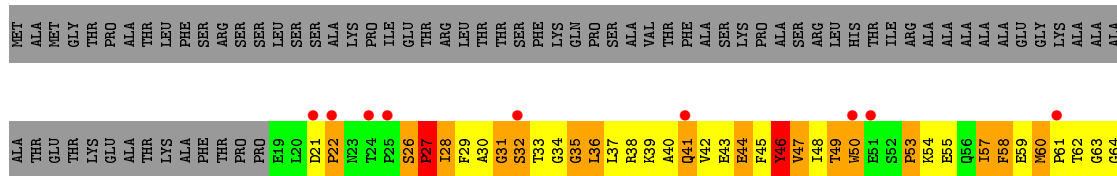




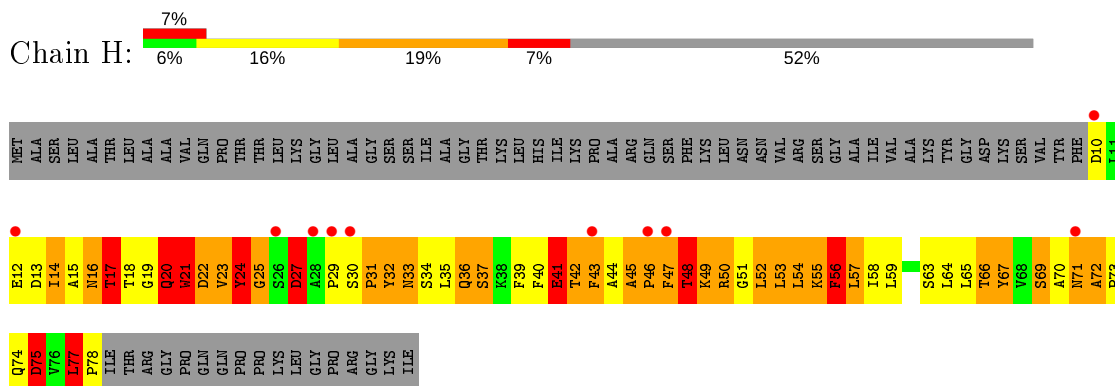
● Molecule 7: PHOTOSYSTEM I IRON-SULFUR CENTER



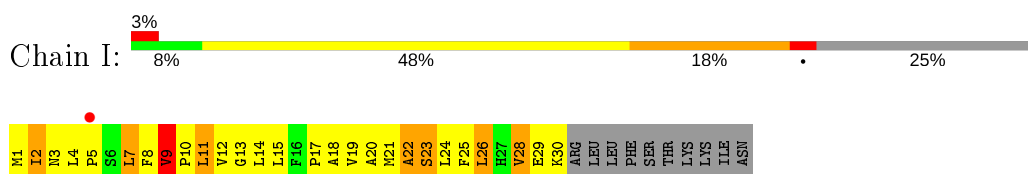
● Molecule 8: PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC



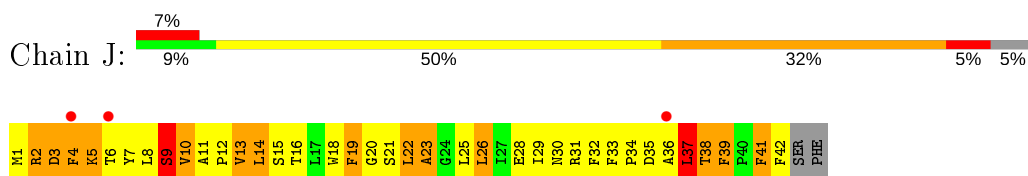
● Molecule 12: PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC



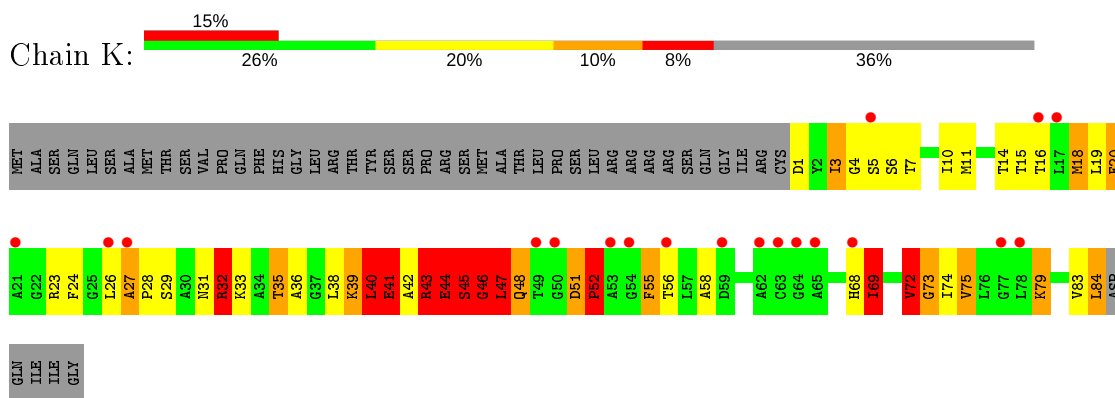
● Molecule 13: PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII



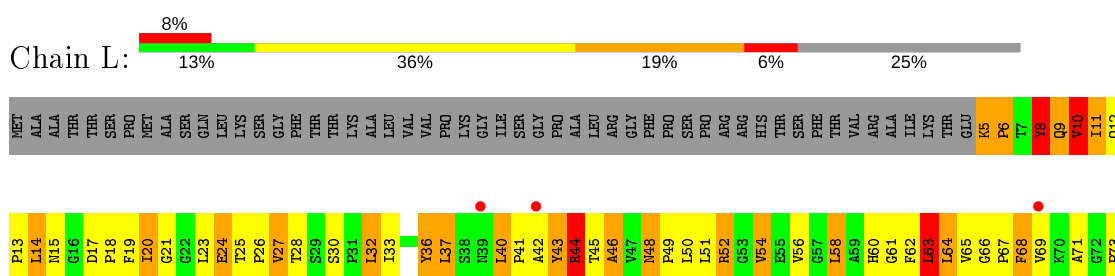
● Molecule 14: PHOTOSYSTEM I REACTION CENTER SUBUNIT IX

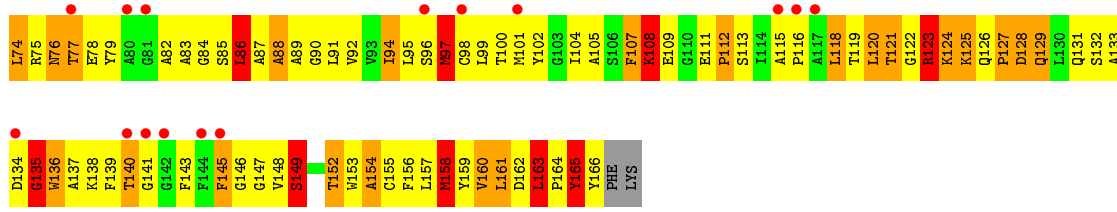


● Molecule 15: PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC

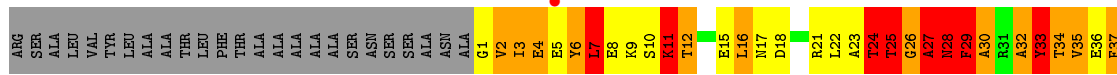
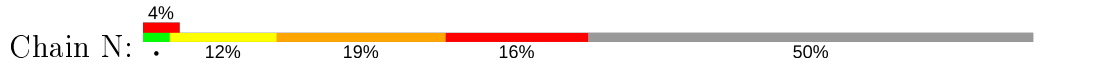


● Molecule 16: PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC





• 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




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



GLC1
FRU2

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

Chain S:  50% 50%GLC1
FRU2

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

Chain T:  100%GLC1
FRU2

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

Chain U:  100%GLC1
FRU2

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

Chain V:  100%GLC1
FRU2

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

Chain W:  50% 50%GLC1
FRU2


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

Chain X:  50% 50%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:  50% 50%

GLC1
FRU2

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

Chain a:  50% 50%

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	120.20Å 190.20Å 130.30Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	50.00 – 3.48 49.46 – 3.47	Depositor EDS
% Data completeness (in resolution range)	96.4 (50.00-3.48) 96.2 (49.46-3.47)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 3.48Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.391 , 0.425 0.383 , 0.387	Depositor DCC
R_{free} test set	1456 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	81.0	Xtrriage
Anisotropy	0.408	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.09 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.016 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	36033	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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	0.55	1/1303 (0.1%)	0.73	1/1774 (0.1%)
2	2	0.67	0/1420	1.10	7/1943 (0.4%)
3	3	0.60	0/1221	0.91	2/1642 (0.1%)
4	4	0.77	0/1359	1.12	10/1851 (0.5%)
5	A	0.61	1/5938 (0.0%)	0.88	9/8104 (0.1%)
6	B	0.58	0/6058	0.86	8/8278 (0.1%)
7	C	0.78	0/632	1.05	1/856 (0.1%)
8	D	0.71	0/1122	0.91	0/1514
9	E	0.70	0/530	0.95	1/718 (0.1%)
10	F	0.67	0/1250	0.88	0/1687
11	G	0.84	1/760 (0.1%)	1.20	7/1031 (0.7%)
12	H	0.70	0/543	1.02	0/741
13	I	0.62	0/235	0.80	0/320
14	J	0.65	0/349	0.91	0/475
15	K	0.65	1/599 (0.2%)	0.88	1/810 (0.1%)
16	L	0.69	1/1251 (0.1%)	0.94	2/1709 (0.1%)
17	N	0.89	0/699	1.22	5/936 (0.5%)
All	All	0.65	5/25269 (0.0%)	0.93	54/34389 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	3
2	2	0	17
3	3	0	17
4	4	0	20
5	A	0	20
6	B	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	C	0	1
8	D	0	1
9	E	0	3
10	F	0	7
11	G	1	13
12	H	0	9
15	K	0	6
16	L	0	2
17	N	0	22
18	R	0	16
All	All	1	169

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	165	TYR	CE2-CZ	-6.04	1.30	1.38
11	G	15	SER	CB-OG	5.83	1.49	1.42
1	1	185	TRP	CB-CG	-5.34	1.40	1.50
15	K	41	GLU	CG-CD	5.15	1.59	1.51
5	A	22	VAL	CA-CB	-5.05	1.44	1.54

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	180	LYS	C-N-CA	-10.34	95.85	121.70
11	G	46	ALA	N-CA-C	-10.20	83.47	111.00
6	B	731	GLY	N-CA-C	-7.75	93.73	113.10
11	G	16	LEU	CA-CB-CG	7.25	131.98	115.30
6	B	315	LEU	CA-CB-CG	7.00	131.41	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	G	21	PHE	CA

5 of 169 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	184	PRO	Peptide
1	1	185	TRP	Peptide
1	1	72	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	2	42	ARG	Peptide
2	2	73	ILE	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	1264	0	1229	137	3
2	2	1374	0	1331	301	2
3	3	1186	0	1147	293	16
4	4	1319	0	1282	610	5
5	A	5745	0	5597	1351	0
6	B	5848	0	5655	1211	15
7	C	619	0	608	204	0
8	D	1095	0	1112	189	0
9	E	520	0	528	129	0
10	F	1221	0	1249	201	0
11	G	740	0	708	191	1
12	H	529	0	514	106	0
13	I	229	0	252	55	0
14	J	338	0	340	64	0
15	K	593	0	619	110	0
16	L	1215	0	1222	311	5
17	N	685	0	668	321	1
18	R	265	0	68	78	0
19	M	23	0	21	0	0
19	O	22	0	18	10	0
19	P	23	0	21	10	0
19	Q	23	0	21	6	0
19	S	23	0	21	1	0
19	T	23	0	21	3	0
19	U	23	0	21	1	0
19	V	23	0	21	4	0
19	W	23	0	21	3	0
19	X	22	0	18	3	0
19	Y	23	0	21	1	41
19	Z	23	0	21	14	0
19	a	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	1	617	0	388	89	1
20	2	650	0	465	147	0
20	3	620	0	362	75	0
20	4	694	0	443	167	0
20	A	2346	0	2062	726	0
20	B	2226	0	2061	684	0
20	F	180	0	123	46	0
20	G	51	0	40	4	0
20	H	223	0	197	57	0
20	I	60	0	58	12	0
20	J	109	0	95	26	0
20	K	202	0	158	54	1
20	L	382	0	335	103	0
20	R	122	0	123	14	0
21	1	105	0	137	32	0
21	2	175	0	230	45	0
21	3	70	0	92	16	0
21	4	139	0	179	24	3
21	A	245	0	322	53	0
21	B	95	0	115	11	0
21	C	35	0	46	0	0
21	D	35	0	46	3	0
21	E	35	0	46	11	0
21	F	34	0	41	8	0
21	G	105	0	138	27	41
21	H	140	0	184	42	0
21	K	105	0	138	41	0
21	L	105	0	138	2	0
21	R	245	0	322	43	3
22	2	40	0	54	9	0
22	A	120	0	162	103	0
22	B	200	0	270	114	0
22	F	80	0	108	60	0
22	G	40	0	54	5	0
22	I	79	0	105	46	0
22	J	40	0	54	36	0
22	L	40	0	54	36	0
23	A	33	0	46	7	0
23	B	33	0	46	28	0
24	A	8	0	0	18	0
24	C	16	0	0	5	0
25	B	49	0	71	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	H	23	0	0	1	0
All	All	36033	0	34504	7353	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 104.

The worst 5 of 7353 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:160:MET:CE	20:4:306:CLA:HBB2	1.18	1.65
4:4:69:ILE:HD11	4:4:175:LYS:CB	1.26	1.65
3:3:97:PHE:CD2	3:3:98:ILE:HG23	1.33	1.62
1:1:185:TRP:CH2	20:1:213:CLA:H12	1.38	1.59
3:3:97:PHE:CE2	3:3:98:ILE:HD13	1.42	1.55

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)
19:Y:2:FRU:O2	21:G:101:LMU:C5B[1_456]	0.08	2.12
3:3:180:LYS:CD	6:B:490:ARG:CZ[1_556]	0.31	1.89
3:3:180:LYS:NZ	6:B:490:ARG:CD[1_556]	0.56	1.64
19:Y:1:GLC:O2	21:G:101:LMU:O4'[1_456]	1.01	1.19
3:3:180:LYS:CG	6:B:490:ARG:NE[1_556]	1.05	1.15

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	161/241 (67%)	84 (52%)	39 (24%)	38 (24%)	0 1
2	2	174/269 (65%)	67 (38%)	51 (29%)	56 (32%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	3	145/276 (52%)	76 (52%)	36 (25%)	33 (23%)	0	1
4	4	164/251 (65%)	57 (35%)	44 (27%)	63 (38%)	0	0
5	A	726/758 (96%)	366 (50%)	187 (26%)	173 (24%)	0	0
6	B	731/734 (100%)	379 (52%)	204 (28%)	148 (20%)	0	1
7	C	79/81 (98%)	23 (29%)	31 (39%)	25 (32%)	0	0
8	D	136/212 (64%)	47 (35%)	48 (35%)	41 (30%)	0	0
9	E	63/143 (44%)	30 (48%)	15 (24%)	18 (29%)	0	0
10	F	152/231 (66%)	71 (47%)	40 (26%)	41 (27%)	0	0
11	G	93/167 (56%)	38 (41%)	27 (29%)	28 (30%)	0	0
12	H	67/144 (46%)	30 (45%)	16 (24%)	21 (31%)	0	0
13	I	28/40 (70%)	11 (39%)	10 (36%)	7 (25%)	0	0
14	J	40/44 (91%)	19 (48%)	11 (28%)	10 (25%)	0	0
15	K	82/131 (63%)	50 (61%)	13 (16%)	19 (23%)	0	0
16	L	160/216 (74%)	72 (45%)	49 (31%)	39 (24%)	0	0
17	N	83/170 (49%)	21 (25%)	19 (23%)	43 (52%)	0	0
All	All	3084/4108 (75%)	1441 (47%)	840 (27%)	803 (26%)	0	0

5 of 803 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	25	ASP
1	1	30	GLY
1	1	35	ASN
1	1	58	LEU
1	1	73	GLU

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	127/190 (67%)	100 (79%)	27 (21%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2	140/216 (65%)	81 (58%)	59 (42%)	0	0
3	3	112/215 (52%)	76 (68%)	36 (32%)	0	1
4	4	138/201 (69%)	85 (62%)	53 (38%)	0	1
5	A	592/618 (96%)	410 (69%)	182 (31%)	0	2
6	B	598/600 (100%)	397 (66%)	201 (34%)	0	1
7	C	70/70 (100%)	41 (59%)	29 (41%)	0	0
8	D	118/173 (68%)	82 (70%)	36 (30%)	0	2
9	E	56/114 (49%)	38 (68%)	18 (32%)	0	1
10	F	127/190 (67%)	80 (63%)	47 (37%)	0	1
11	G	79/144 (55%)	53 (67%)	26 (33%)	0	1
12	H	57/115 (50%)	30 (53%)	27 (47%)	0	0
13	I	26/36 (72%)	22 (85%)	4 (15%)	2	14
14	J	36/39 (92%)	25 (69%)	11 (31%)	0	2
15	K	61/102 (60%)	43 (70%)	18 (30%)	0	2
16	L	125/169 (74%)	88 (70%)	37 (30%)	0	2
17	N	74/139 (53%)	43 (58%)	31 (42%)	0	0
All	All	2536/3331 (76%)	1694 (67%)	842 (33%)	0	1

5 of 842 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	121	TYR
6	B	438	VAL
16	L	14	LEU
6	B	142	LEU
6	B	278	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	67	HIS
6	B	333	GLN
15	K	80	ASN
6	B	71	GLN
6	B	193	HIS

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	0.54	0	15,15,17	2.23	2 (13%)
19	FRU	M	2	19	11,12,12	0.71	0	10,18,18	0.74	0
19	GLC	O	1	19	10,10,12	0.91	0	14,14,17	2.46	4 (28%)
19	FRU	O	2	19	11,12,12	0.62	0	10,18,18	1.15	1 (10%)
19	GLC	P	1	19	11,11,12	0.52	0	15,15,17	1.77	4 (26%)
19	FRU	P	2	19	11,12,12	0.70	0	10,18,18	1.23	2 (20%)
19	GLC	Q	1	19	11,11,12	0.60	0	15,15,17	2.44	5 (33%)
19	FRU	Q	2	19	11,12,12	0.78	0	10,18,18	1.18	1 (10%)
19	GLC	S	1	19	11,11,12	0.63	0	15,15,17	1.10	1 (6%)
19	FRU	S	2	19	11,12,12	0.79	0	10,18,18	1.56	2 (20%)
19	GLC	T	1	19	11,11,12	0.51	0	15,15,17	0.79	1 (6%)
19	FRU	T	2	19	11,12,12	0.64	0	10,18,18	1.26	1 (10%)
19	GLC	U	1	19	11,11,12	0.64	0	15,15,17	2.64	4 (26%)
19	FRU	U	2	19	11,12,12	0.65	0	10,18,18	1.39	3 (30%)
19	GLC	V	1	19	11,11,12	0.57	0	15,15,17	1.97	4 (26%)
19	FRU	V	2	19	11,12,12	0.76	0	10,18,18	1.22	1 (10%)
19	GLC	W	1	19	11,11,12	0.59	0	15,15,17	1.01	2 (13%)
19	FRU	W	2	19	11,12,12	0.55	0	10,18,18	1.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	GLC	X	1	19	10,10,12	0.91	0	14,14,17	2.11	5 (35%)
19	FRU	X	2	19	11,12,12	0.57	0	10,18,18	0.64	0
19	GLC	Y	1	19	11,11,12	1.69	3 (27%)	15,15,17	2.66	6 (40%)
19	FRU	Y	2	19	11,12,12	1.41	1 (9%)	10,18,18	1.43	2 (20%)
19	GLC	Z	1	19	11,11,12	0.43	0	15,15,17	1.12	2 (13%)
19	FRU	Z	2	19	11,12,12	0.68	0	10,18,18	1.12	0
19	GLC	a	1	19	11,11,12	0.78	0	15,15,17	1.58	2 (13%)
19	FRU	a	2	19	11,12,12	0.42	0	10,18,18	1.12	0

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	1/5/24/24	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	-	0/2/19/22	0/1/1/1
19	FRU	P	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	Q	1	19	-	2/2/19/22	0/1/1/1
19	FRU	Q	2	19	1/1/4/4	5/5/24/24	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	0/5/24/24	0/1/1/1
19	GLC	T	1	19	-	2/2/19/22	0/1/1/1
19	FRU	T	2	19	1/1/4/4	2/5/24/24	0/1/1/1
19	GLC	U	1	19	-	1/2/19/22	0/1/1/1
19	FRU	U	2	19	1/1/4/4	0/5/24/24	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	3/5/24/24	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	3/5/24/24	0/1/1/1
19	GLC	X	1	19	-	-	0/1/1/1
19	FRU	X	2	19	1/1/4/4	5/5/24/24	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
19	GLC	Z	1	19	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	FRU	Z	2	19	1/1/4/4	0/5/24/24	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	4/5/24/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Y	2	FRU	O2-C2	4.27	1.48	1.40
19	Y	1	GLC	C1-C2	3.36	1.59	1.52
19	Y	1	GLC	C2-C3	2.99	1.56	1.52
19	Y	1	GLC	O2-C2	2.25	1.48	1.43

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	1	GLC	C1-O5-C5	7.84	122.82	112.19
19	U	1	GLC	C1-O5-C5	7.72	122.65	112.19
19	O	1	GLC	C1-C2-C3	7.09	118.38	109.67
19	Y	1	GLC	C6-C5-C4	5.98	127.01	113.00
19	V	1	GLC	C1-O5-C5	4.74	118.61	112.19

5 of 13 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	P	2	FRU	C2
19	O	2	FRU	C2
19	T	2	FRU	C2
19	W	2	FRU	C2
19	X	2	FRU	C2

5 of 43 torsion outliers are listed below:

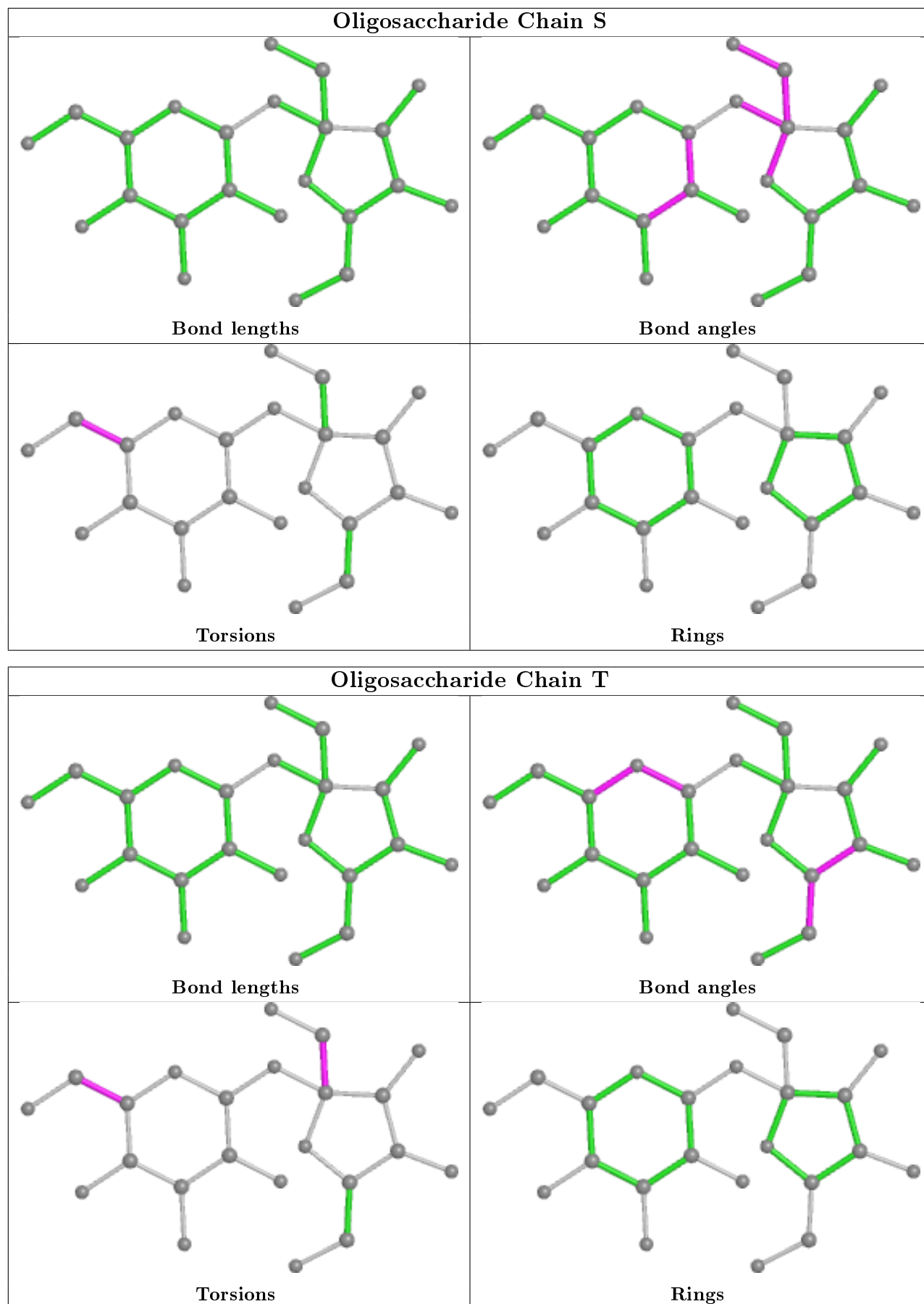
Mol	Chain	Res	Type	Atoms
19	P	2	FRU	C4-C5-C6-O6
19	P	2	FRU	O5-C5-C6-O6
19	W	2	FRU	O1-C1-C2-C3
19	W	2	FRU	O1-C1-C2-O2
19	W	2	FRU	O1-C1-C2-O5

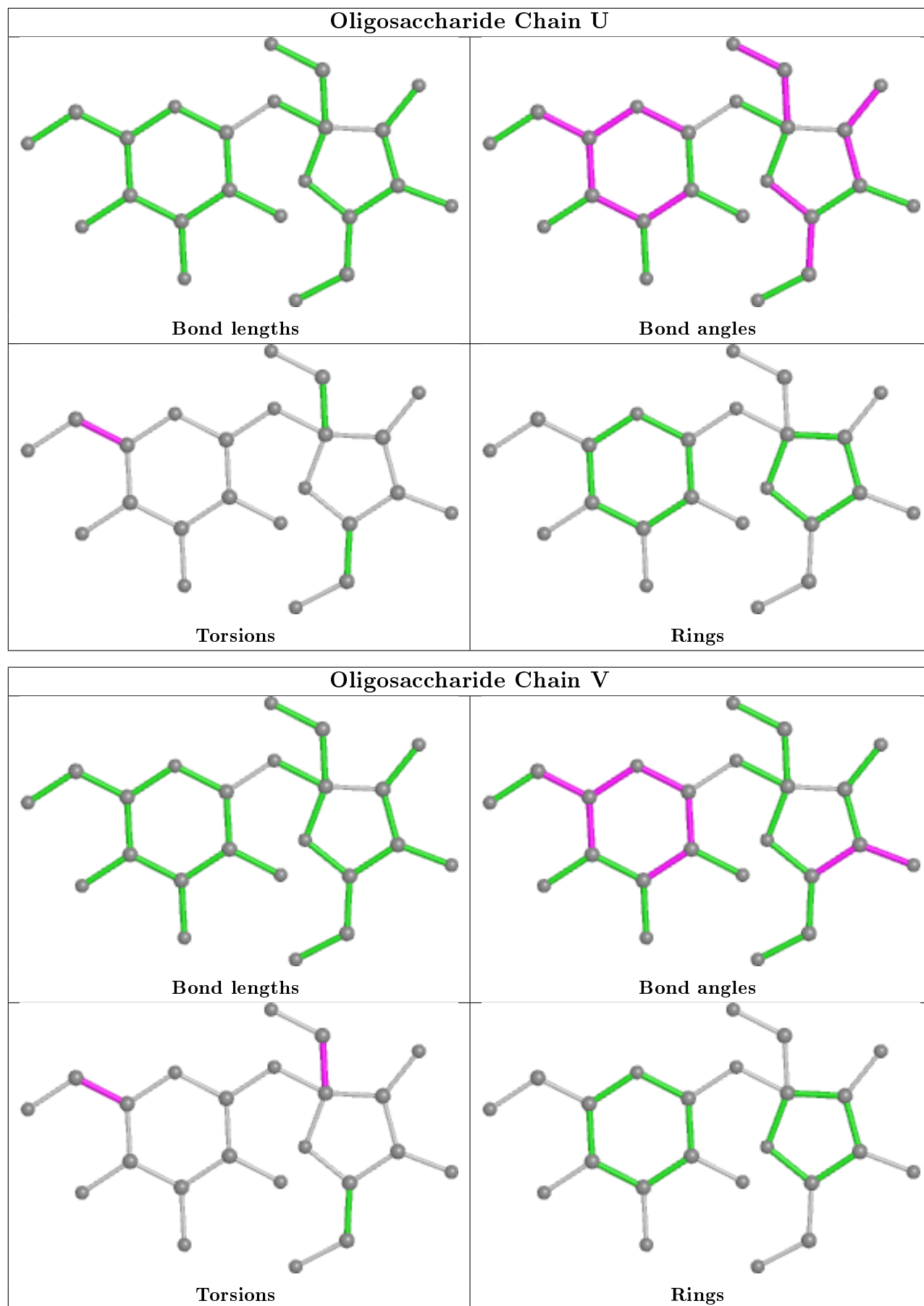
There are no ring outliers.

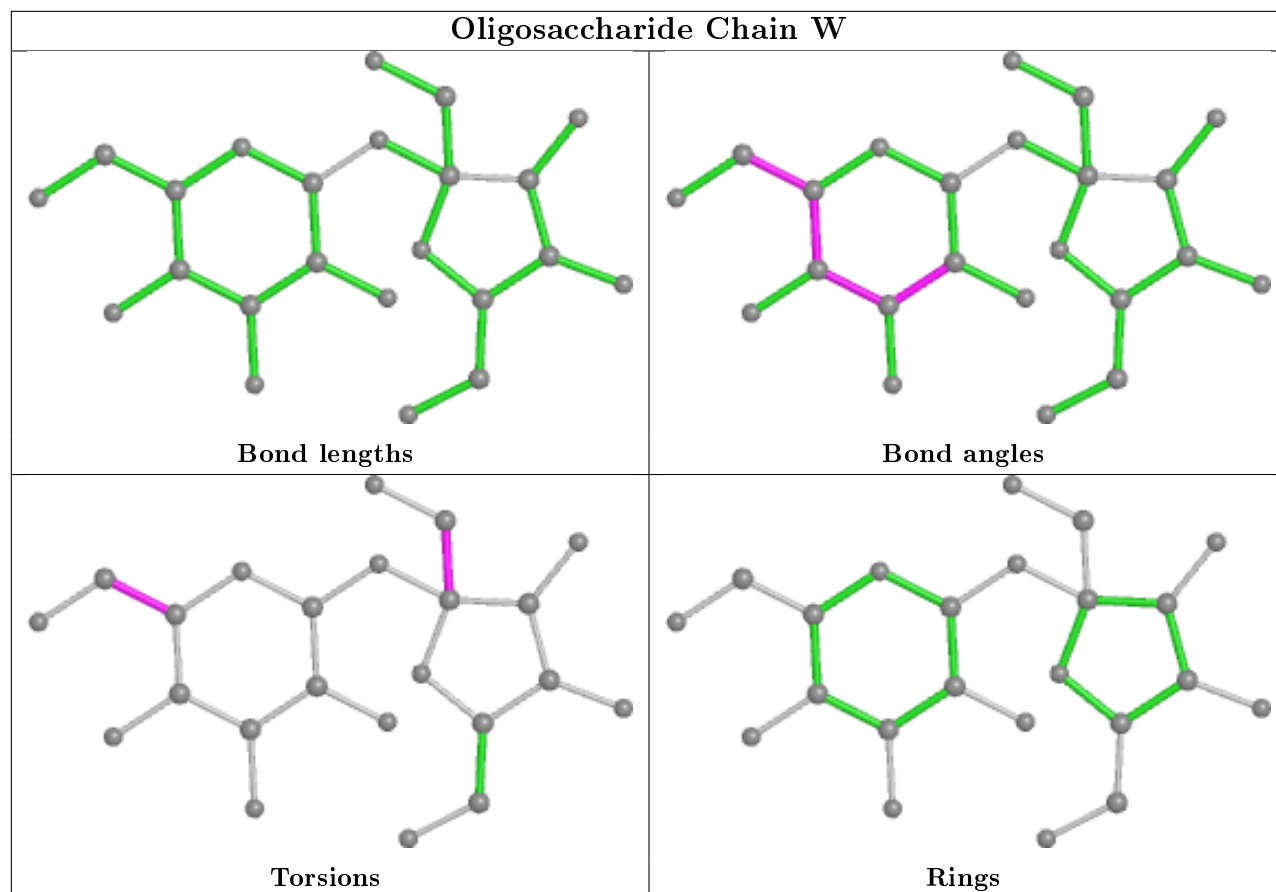
21 monomers are involved in 97 short contacts:

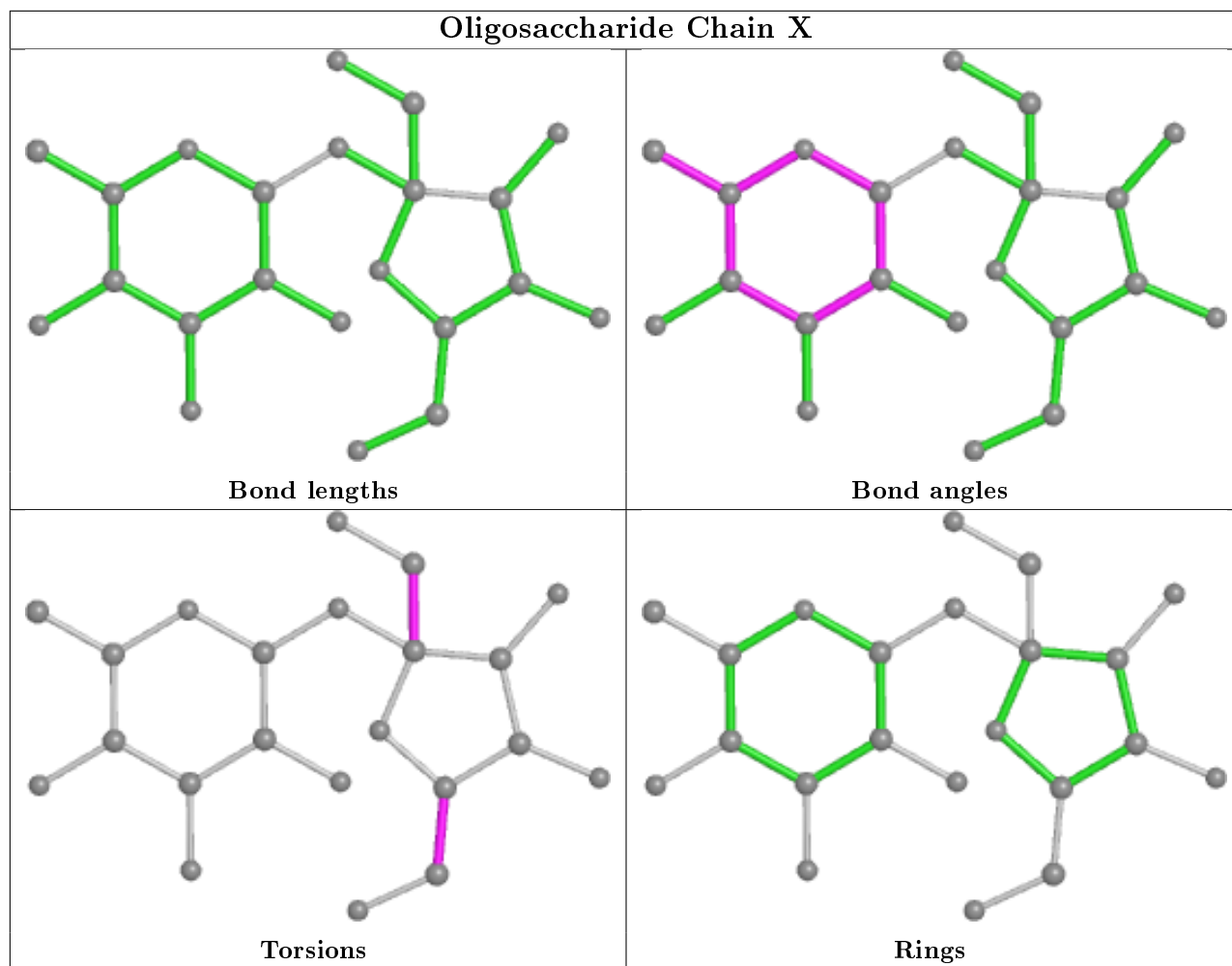
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	T	1	GLC	3	0
19	U	1	GLC	1	0
19	P	2	FRU	9	0
19	W	1	GLC	3	0
19	Q	1	GLC	3	0
19	O	2	FRU	3	0
19	V	1	GLC	3	0
19	T	2	FRU	3	0
19	W	2	FRU	3	0
19	Y	1	GLC	0	22
19	X	2	FRU	3	0
19	V	2	FRU	4	0
19	Y	2	FRU	1	19
19	Q	2	FRU	6	0
19	U	2	FRU	1	0
19	S	2	FRU	1	0
19	Z	2	FRU	13	0
19	X	1	GLC	3	0
19	Z	1	GLC	1	0
19	O	1	GLC	10	0
19	P	1	GLC	8	0

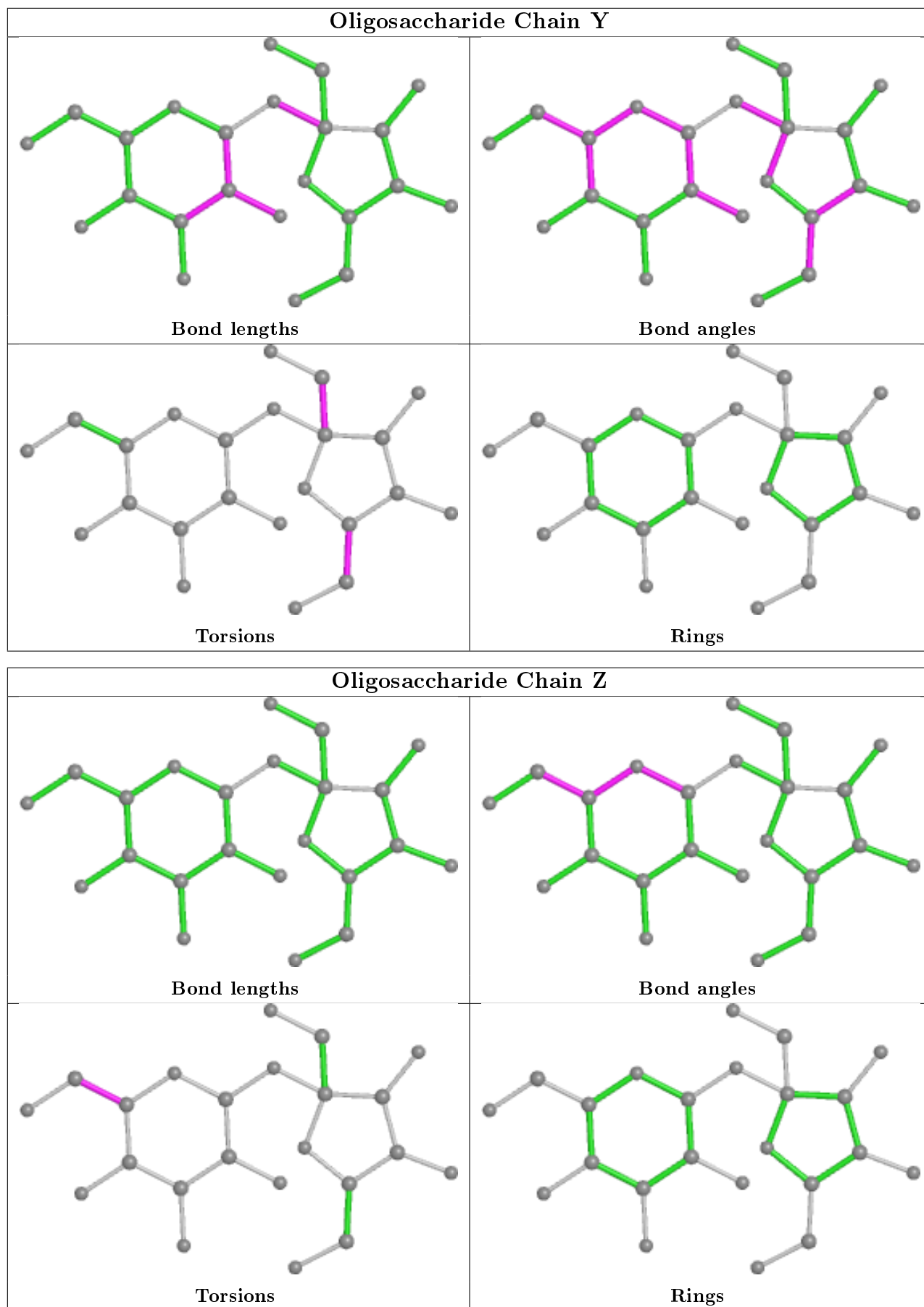
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry (i)

Of 244 ligands modelled in this entry, 1 is unknown - leaving 243 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
22	BCR	B	844	-	41,41,41	1.86	3 (7%)	56,56,56	5.19	24 (42%)
20	CLA	1	210	1	30,44,73	2.58	10 (33%)	35,78,113	4.23	14 (40%)
20	CLA	4	301	-	49,63,73	2.24	12 (24%)	55,101,113	3.44	18 (32%)
20	CLA	A	802	-	22,32,73	1.95	6 (27%)	26,54,113	3.29	16 (61%)
20	CLA	4	307	-	22,32,73	1.99	7 (31%)	26,54,113	3.04	15 (57%)
20	CLA	L	201	-	54,68,73	2.11	12 (22%)	61,107,113	2.89	20 (32%)
20	CLA	1	205	-	30,44,73	2.74	10 (33%)	35,78,113	4.18	15 (42%)
20	CLA	2	309	-	22,32,73	2.13	8 (36%)	26,54,113	2.94	16 (61%)
21	LMU	4	319	-	35,35,36	0.80	2 (5%)	46,46,47	1.81	11 (23%)
20	CLA	L	204	-	49,63,73	2.27	12 (24%)	55,101,113	3.14	21 (38%)
21	LMU	G	101	-	36,36,36	1.11	4 (11%)	47,47,47	2.03	11 (23%)
21	LMU	K	106	-	36,36,36	0.37	0	47,47,47	1.06	4 (8%)
21	LMU	2	322	-	36,36,36	0.82	1 (2%)	47,47,47	1.18	4 (8%)
21	LMU	2	321	-	36,36,36	0.46	0	47,47,47	1.27	3 (6%)
21	LMU	K	105	-	36,36,36	0.68	1 (2%)	47,47,47	1.54	8 (17%)
20	CLA	A	805	-	48,62,73	2.16	12 (25%)	53,99,113	3.40	19 (35%)
20	CLA	4	306	-	46,60,73	2.49	14 (30%)	51,97,113	4.29	31 (60%)
20	CLA	A	833	5	36,53,73	2.39	11 (30%)	39,89,113	4.25	21 (53%)
20	CLA	A	801	-	40,54,73	2.55	13 (32%)	48,90,113	5.20	26 (54%)
20	CLA	3	305	-	22,32,73	1.83	5 (22%)	26,54,113	2.95	13 (50%)
20	CLA	A	814	-	22,32,73	2.10	8 (36%)	26,54,113	3.20	14 (53%)
20	CLA	1	214	-	22,32,73	1.99	6 (27%)	26,54,113	3.30	15 (57%)
20	CLA	H	101	-	49,63,73	2.27	12 (24%)	55,101,113	3.89	22 (40%)
22	BCR	A	845	-	41,41,41	2.01	4 (9%)	56,56,56	5.71	26 (46%)
20	CLA	B	824	-	59,73,73	2.18	16 (27%)	67,113,113	3.18	20 (29%)
21	LMU	1	217	-	36,36,36	0.57	0	47,47,47	0.98	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	808	-	55,69,73	2.04	13 (23%)	62,108,113	3.25	23 (37%)
20	CLA	3	303	-	30,44,73	2.70	9 (30%)	35,78,113	4.20	16 (45%)
20	CLA	2	301	-	22,32,73	1.97	7 (31%)	26,54,113	3.11	17 (65%)
24	SF4	C	103	7	0,12,12	0.00	-	-		
20	CLA	B	826	-	52,66,73	2.13	12 (23%)	58,104,113	3.41	18 (31%)
21	LMU	H	104	-	36,36,36	0.60	0	47,47,47	1.63	7 (14%)
20	CLA	B	841	-	59,73,73	1.92	13 (22%)	67,113,113	2.86	19 (28%)
20	CLA	L	202	-	49,63,73	2.20	12 (24%)	55,101,113	3.45	19 (34%)
20	CLA	A	839	-	53,67,73	2.38	15 (28%)	59,105,113	3.40	23 (38%)
20	CLA	L	208	16	44,58,73	2.31	11 (25%)	49,95,113	3.62	20 (40%)
20	CLA	4	314	4	22,32,73	1.91	6 (27%)	26,54,113	2.82	17 (65%)
22	BCR	F	203	-	41,41,41	2.01	3 (7%)	56,56,56	5.47	19 (33%)
20	CLA	3	313	-	22,32,73	1.91	5 (22%)	26,54,113	3.11	16 (61%)
21	LMU	E	101	-	36,36,36	0.61	0	47,47,47	1.88	13 (27%)
20	CLA	B	819	-	35,49,73	2.78	14 (40%)	38,84,113	4.92	17 (44%)
20	CLA	A	841	-	22,32,73	2.05	8 (36%)	26,54,113	3.25	17 (65%)
20	CLA	4	315	-	40,54,73	2.43	13 (32%)	44,90,113	3.40	17 (38%)
20	CLA	A	850	-	59,73,73	2.04	12 (20%)	67,113,113	3.16	21 (31%)
20	CLA	3	318	-	30,44,73	2.63	11 (36%)	35,78,113	4.33	16 (45%)
20	CLA	B	829	-	59,73,73	2.00	13 (22%)	67,113,113	3.06	22 (32%)
20	CLA	2	310	2	44,58,73	2.46	13 (29%)	49,95,113	3.97	21 (42%)
20	CLA	A	807	-	40,54,73	2.35	11 (27%)	44,90,113	4.14	20 (45%)
20	CLA	R	108	-	59,73,73	2.04	11 (18%)	67,113,113	3.01	22 (32%)
22	BCR	I	101	-	39,40,41	1.67	3 (7%)	52,53,56	4.25	19 (36%)
20	CLA	1	209	-	22,32,73	2.13	7 (31%)	26,54,113	3.19	18 (69%)
21	LMU	R	104	-	36,36,36	0.57	0	47,47,47	1.29	5 (10%)
20	CLA	A	817	-	46,60,73	2.26	12 (26%)	51,97,113	3.65	18 (35%)
20	CLA	B	827	-	59,73,73	1.97	12 (20%)	67,113,113	3.29	20 (29%)
20	CLA	1	206	-	55,69,73	2.10	12 (21%)	62,108,113	3.16	22 (35%)
21	LMU	G	103	-	36,36,36	0.50	0	47,47,47	0.93	1 (2%)
20	CLA	B	834	-	36,53,73	2.48	11 (30%)	39,89,113	4.04	15 (38%)
22	BCR	B	801	-	41,41,41	2.52	6 (14%)	56,56,56	6.08	21 (37%)
20	CLA	A	809	-	46,60,73	2.17	11 (23%)	51,97,113	3.36	23 (45%)
20	CLA	A	840	-	49,63,73	2.17	13 (26%)	55,101,113	3.41	18 (32%)
20	CLA	A	825	-	59,73,73	1.94	12 (20%)	67,113,113	3.00	16 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PQN	B	843	-	34,34,34	1.66	2 (5%)	42,45,45	1.35	6 (14%)
20	CLA	A	831	-	59,73,73	2.08	16 (27%)	67,113,113	4.05	25 (37%)
21	LMU	D	201	-	36,36,36	0.47	0	47,47,47	1.44	6 (12%)
20	CLA	2	305	-	44,58,73	2.30	11 (25%)	49,95,113	3.40	19 (38%)
20	CLA	A	813	-	44,58,73	2.26	12 (27%)	49,95,113	3.51	19 (38%)
20	CLA	3	315	-	59,73,73	2.04	15 (25%)	67,113,113	3.41	21 (31%)
24	SF4	C	102	7	0,12,12	0.00	-	-		
21	LMU	1	218	-	36,36,36	0.70	0	47,47,47	1.65	8 (17%)
20	CLA	B	842	-	30,44,73	2.68	11 (36%)	35,78,113	4.37	18 (51%)
20	CLA	A	808	5	54,68,73	2.13	12 (22%)	61,107,113	3.23	23 (37%)
20	CLA	B	822	-	40,54,73	2.39	11 (27%)	44,90,113	4.01	17 (38%)
20	CLA	A	832	-	44,58,73	2.27	12 (27%)	49,95,113	3.39	19 (38%)
20	CLA	L	209	-	41,55,73	2.39	10 (24%)	45,91,113	3.98	21 (46%)
20	CLA	4	310	-	44,58,73	2.37	15 (34%)	49,95,113	4.02	17 (34%)
20	CLA	B	814	-	59,73,73	2.03	13 (22%)	67,113,113	3.19	21 (31%)
20	CLA	B	812	-	48,62,73	2.45	15 (31%)	58,100,113	4.27	24 (41%)
20	CLA	A	829	-	44,58,73	2.31	12 (27%)	49,95,113	3.67	18 (36%)
20	CLA	4	305	-	44,58,73	2.40	15 (34%)	49,95,113	3.94	21 (42%)
21	LMU	B	849	-	26,26,36	0.77	1 (3%)	37,37,47	1.28	6 (16%)
24	SF4	A	856	5,6	0,12,12	0.00	-	-		
21	LMU	B	805	-	36,36,36	0.67	1 (2%)	47,47,47	1.66	12 (25%)
20	CLA	1	215	-	45,59,73	2.40	14 (31%)	50,96,113	4.42	19 (38%)
20	CLA	3	301	-	30,44,73	2.57	11 (36%)	35,78,113	4.44	15 (42%)
20	CLA	A	811	20	59,73,73	2.02	12 (20%)	67,113,113	2.89	22 (32%)
20	CLA	A	835	-	59,73,73	2.08	12 (20%)	67,113,113	3.30	24 (35%)
20	CLA	B	831	-	44,58,73	2.31	9 (20%)	49,95,113	3.41	18 (36%)
21	LMU	4	321	-	36,36,36	0.46	0	47,47,47	1.46	7 (14%)
20	CLA	B	803	-	59,73,73	2.02	11 (18%)	67,113,113	3.12	20 (29%)
20	CLA	1	212	-	22,32,73	1.92	6 (27%)	26,54,113	3.07	16 (61%)
21	LMU	2	320	-	36,36,36	0.82	1 (2%)	47,47,47	1.56	11 (23%)
20	CLA	B	806	-	59,73,73	2.04	12 (20%)	67,113,113	2.79	19 (28%)
20	CLA	3	306	-	22,32,73	1.84	6 (27%)	26,54,113	3.11	17 (65%)
20	CLA	K	104	-	50,64,73	2.21	13 (26%)	56,102,113	3.77	20 (35%)
21	LMU	K	107	-	36,36,36	0.52	0	47,47,47	1.31	6 (12%)
20	CLA	2	306	-	22,32,73	1.93	7 (31%)	26,54,113	2.73	16 (61%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	837	-	54,68,73	2.05	11 (20%)	61,107,113	3.17	16 (26%)
20	CLA	A	836	-	41,55,73	2.41	12 (29%)	45,91,113	2.69	15 (33%)
20	CLA	2	311	-	44,58,73	2.31	12 (27%)	49,95,113	3.98	22 (44%)
20	CLA	A	812	-	48,62,73	2.14	12 (25%)	53,99,113	3.19	16 (30%)
20	CLA	B	840	-	59,73,73	1.99	12 (20%)	67,113,113	3.01	20 (29%)
20	CLA	H	112	-	49,63,73	2.18	10 (20%)	55,101,113	3.54	20 (36%)
21	LMU	A	846	-	36,36,36	0.70	0	47,47,47	1.27	7 (14%)
21	LMU	2	313	-	36,36,36	0.52	0	47,47,47	1.60	6 (12%)
20	CLA	B	838	-	59,73,73	1.92	11 (18%)	67,113,113	2.94	18 (26%)
20	CLA	A	818	-	54,68,73	2.29	14 (25%)	61,107,113	3.50	24 (39%)
22	BCR	I	103	-	41,41,41	2.13	5 (12%)	56,56,56	6.16	28 (50%)
20	CLA	3	310	-	59,73,73	2.05	15 (25%)	67,113,113	3.53	26 (38%)
20	CLA	1	202	-	35,49,73	2.57	11 (31%)	38,84,113	3.96	17 (44%)
21	LMU	R	106	-	36,36,36	0.52	0	47,47,47	1.23	4 (8%)
20	CLA	B	807	-	36,53,73	2.47	11 (30%)	39,89,113	3.90	15 (38%)
20	CLA	A	803	-	40,54,73	2.58	15 (37%)	44,90,113	4.30	18 (40%)
20	CLA	1	204	-	40,54,73	2.58	13 (32%)	44,90,113	4.32	22 (50%)
20	CLA	3	317	-	22,32,73	1.96	6 (27%)	26,54,113	3.16	15 (57%)
20	CLA	3	309	-	22,32,73	2.03	8 (36%)	26,54,113	3.45	15 (57%)
25	LMG	B	848	-	49,49,55	0.99	2 (4%)	57,57,63	1.08	3 (5%)
20	CLA	1	201	-	40,54,73	2.41	12 (30%)	44,90,113	4.05	21 (47%)
20	CLA	B	816	-	54,68,73	2.06	11 (20%)	61,107,113	2.96	20 (32%)
21	LMU	2	319	-	36,36,36	0.56	0	47,47,47	0.68	0
20	CLA	F	201	-	44,58,73	2.41	16 (36%)	49,95,113	3.85	18 (36%)
20	CLA	4	318	-	41,55,73	2.37	13 (31%)	45,91,113	4.42	22 (48%)
20	CLA	H	111	-	52,66,73	2.31	14 (26%)	58,104,113	3.09	24 (41%)
20	CLA	F	207	-	47,61,73	2.55	20 (42%)	52,98,113	3.81	25 (48%)
20	CLA	2	302	-	45,59,73	2.46	14 (31%)	50,96,113	3.78	21 (42%)
20	CLA	B	835	-	36,53,73	2.49	12 (33%)	39,89,113	3.80	17 (43%)
20	CLA	B	821	-	44,58,73	2.28	12 (27%)	49,95,113	3.78	20 (40%)
21	LMU	L	206	-	36,36,36	0.51	0	47,47,47	1.00	3 (6%)
20	CLA	J	101	-	42,56,73	2.34	12 (28%)	46,92,113	3.63	16 (34%)
20	CLA	A	828	-	59,73,73	2.00	12 (20%)	67,113,113	3.28	22 (32%)
21	LMU	H	105	-	36,36,36	0.72	1 (2%)	47,47,47	1.66	9 (19%)
20	CLA	F	206	-	35,49,73	2.58	12 (34%)	38,84,113	4.06	17 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	LMU	L	212	-	36,36,36	0.71	1 (2%)	47,47,47	1.29	4 (8%)
20	CLA	A	822	-	44,58,73	2.29	12 (27%)	49,95,113	3.59	20 (40%)
22	BCR	B	847	-	41,41,41	1.95	3 (7%)	56,56,56	5.45	17 (30%)
21	LMU	C	101	-	36,36,36	0.70	1 (2%)	47,47,47	1.26	4 (8%)
20	CLA	A	830	-	59,73,73	1.99	12 (20%)	67,113,113	3.13	16 (23%)
20	CLA	1	211	-	45,59,73	2.57	17 (37%)	50,96,113	4.19	22 (44%)
20	CLA	A	849	-	59,73,73	1.98	13 (22%)	67,113,113	3.52	22 (32%)
20	CLA	H	102	-	49,63,73	2.17	11 (22%)	55,101,113	3.49	20 (36%)
21	LMU	A	855	-	36,36,36	0.66	1 (2%)	47,47,47	1.38	7 (14%)
20	CLA	B	811	6	22,32,73	2.04	9 (40%)	26,54,113	2.86	14 (53%)
20	CLA	A	820	-	45,59,73	2.29	12 (26%)	50,96,113	3.64	18 (36%)
20	CLA	1	207	-	45,59,73	2.40	15 (33%)	50,96,113	4.10	21 (42%)
20	CLA	2	308	-	22,32,73	2.23	11 (50%)	26,54,113	3.36	16 (61%)
20	CLA	3	304	-	22,32,73	2.03	9 (40%)	26,54,113	3.22	15 (57%)
20	CLA	B	825	-	48,62,73	2.29	12 (25%)	53,99,113	3.07	20 (37%)
20	CLA	I	102	-	54,68,73	2.06	11 (20%)	61,107,113	3.33	17 (27%)
22	BCR	2	318	-	41,41,41	1.96	3 (7%)	56,56,56	5.70	19 (33%)
20	CLA	2	316	-	22,32,73	1.93	6 (27%)	26,54,113	2.71	13 (50%)
20	CLA	A	826	-	59,73,73	1.98	11 (18%)	67,113,113	3.45	22 (32%)
20	CLA	4	309	-	22,32,73	1.86	5 (22%)	26,54,113	3.06	14 (53%)
22	BCR	A	843	-	41,41,41	1.95	3 (7%)	56,56,56	5.48	21 (37%)
20	CLA	A	810	-	36,53,73	2.48	12 (33%)	39,89,113	4.12	18 (46%)
20	CLA	A	851	-	59,73,73	2.07	12 (20%)	67,113,113	3.17	21 (31%)
21	LMU	4	320	-	36,36,36	0.77	1 (2%)	47,47,47	1.28	7 (14%)
21	LMU	4	316	-	36,36,36	0.72	1 (2%)	47,47,47	1.08	3 (6%)
20	CLA	4	303	-	59,73,73	2.12	16 (27%)	67,113,113	3.61	25 (37%)
20	CLA	1	208	-	22,32,73	1.81	5 (22%)	26,54,113	3.02	17 (65%)
20	CLA	1	203	-	41,55,73	2.48	14 (34%)	45,91,113	4.72	20 (44%)
20	CLA	B	815	-	54,68,73	2.13	12 (22%)	61,107,113	2.85	17 (27%)
20	CLA	4	313	-	30,44,73	2.59	10 (33%)	35,78,113	4.47	18 (51%)
21	LMU	G	102	-	36,36,36	0.61	0	47,47,47	1.59	8 (17%)
20	CLA	K	103	-	44,58,73	2.36	12 (27%)	49,95,113	3.70	22 (44%)
21	LMU	R	105	-	36,36,36	0.75	1 (2%)	47,47,47	1.39	8 (17%)
21	LMU	L	205	-	36,36,36	0.65	0	47,47,47	1.92	13 (27%)
22	BCR	B	846	-	41,41,41	1.98	4 (9%)	56,56,56	5.56	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	836	-	45,59,73	2.28	11 (24%)	50,96,113	3.78	20 (40%)
21	LMU	3	320	-	36,36,36	0.44	0	47,47,47	1.12	4 (8%)
20	CLA	3	314	-	44,58,73	2.30	11 (25%)	49,95,113	3.02	20 (40%)
21	LMU	A	852	-	36,36,36	0.55	1 (2%)	47,47,47	0.85	1 (2%)
20	CLA	G	105	-	45,59,73	2.36	13 (28%)	50,96,113	3.72	18 (36%)
20	CLA	B	802	-	48,62,73	2.20	12 (25%)	53,99,113	3.65	21 (39%)
20	CLA	L	203	-	59,73,73	1.95	11 (18%)	67,113,113	3.44	23 (34%)
20	CLA	3	311	-	59,73,73	2.01	11 (18%)	67,113,113	3.11	20 (29%)
22	BCR	L	211	-	41,41,41	2.00	4 (9%)	56,56,56	5.64	17 (30%)
21	LMU	A	847	-	36,36,36	0.68	1 (2%)	47,47,47	1.42	7 (14%)
20	CLA	K	101	-	40,54,73	2.41	13 (32%)	44,90,113	3.87	15 (34%)
22	BCR	J	102	-	41,41,41	1.92	3 (7%)	56,56,56	5.54	18 (32%)
21	LMU	A	848	-	36,36,36	0.49	0	47,47,47	0.86	3 (6%)
20	CLA	K	102	-	44,58,73	2.30	13 (29%)	49,95,113	3.66	19 (38%)
20	CLA	A	815	-	44,58,73	2.31	10 (22%)	49,95,113	3.40	22 (44%)
20	CLA	4	308	-	22,32,73	2.10	10 (45%)	26,54,113	3.26	17 (65%)
22	BCR	B	845	-	41,41,41	1.76	3 (7%)	56,56,56	4.78	19 (33%)
20	CLA	A	824	-	53,67,73	2.09	12 (22%)	59,105,113	3.45	21 (35%)
20	CLA	2	317	-	59,73,73	2.12	15 (25%)	67,113,113	3.56	22 (32%)
20	CLA	R	107	-	51,65,73	2.16	11 (21%)	57,103,113	3.61	21 (36%)
20	CLA	B	828	-	59,73,73	2.02	12 (20%)	67,113,113	3.45	22 (32%)
20	CLA	B	810	-	54,68,73	2.14	12 (22%)	61,107,113	3.25	21 (34%)
20	CLA	B	818	-	47,61,73	2.24	12 (25%)	52,98,113	3.14	18 (34%)
20	CLA	A	834	-	40,54,73	2.41	12 (30%)	44,90,113	3.85	17 (38%)
20	CLA	B	832	-	53,67,73	2.17	12 (22%)	59,105,113	3.34	21 (35%)
21	LMU	F	202	-	35,35,36	0.57	0	46,46,47	1.36	5 (10%)
22	BCR	A	844	-	41,41,41	2.02	3 (7%)	56,56,56	5.57	21 (37%)
20	CLA	4	302	-	30,44,73	2.83	12 (40%)	35,78,113	4.57	17 (48%)
21	LMU	H	103	-	36,36,36	0.86	1 (2%)	47,47,47	2.09	12 (25%)
20	CLA	2	315	-	44,58,73	2.46	13 (29%)	49,95,113	3.85	17 (34%)
20	CLA	A	823	-	52,66,73	2.05	11 (21%)	58,104,113	2.94	20 (34%)
21	LMU	R	101	-	36,36,36	0.86	2 (5%)	47,47,47	2.08	11 (23%)
20	CLA	A	827	-	49,63,73	2.19	13 (26%)	55,101,113	3.43	20 (36%)
20	CLA	2	303	-	52,66,73	2.29	14 (26%)	58,104,113	3.85	21 (36%)
20	CLA	A	838	-	59,73,73	2.01	12 (20%)	67,113,113	3.21	22 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	4	304	-	49,63,73	2.17	12 (24%)	55,101,113	3.30	19 (34%)
20	CLA	A	804	20	49,63,73	2.28	12 (24%)	55,101,113	3.16	20 (36%)
21	LMU	1	216	-	36,36,36	0.45	0	47,47,47	1.38	6 (12%)
20	CLA	3	307	-	36,50,73	2.51	11 (30%)	39,85,113	4.34	20 (51%)
20	CLA	3	308	-	22,32,73	1.90	6 (27%)	26,54,113	3.26	16 (61%)
20	CLA	3	302	-	22,32,73	1.90	5 (22%)	26,54,113	2.95	14 (53%)
20	CLA	B	809	-	59,73,73	2.04	12 (20%)	67,113,113	3.23	23 (34%)
20	CLA	L	210	-	44,58,73	2.38	12 (27%)	49,95,113	3.99	18 (36%)
20	CLA	B	813	-	49,63,73	2.11	12 (24%)	55,101,113	3.46	19 (34%)
20	CLA	J	103	-	55,69,73	2.09	12 (21%)	62,108,113	2.94	19 (30%)
22	BCR	F	204	-	41,41,41	2.16	5 (12%)	56,56,56	5.75	24 (42%)
21	LMU	3	319	-	36,36,36	0.49	0	47,47,47	0.72	1 (2%)
20	CLA	A	806	-	50,64,73	2.13	11 (22%)	56,102,113	3.45	20 (35%)
20	CLA	B	830	-	59,73,73	2.01	13 (22%)	67,113,113	2.97	20 (29%)
20	CLA	2	304	-	22,32,73	2.04	9 (40%)	26,54,113	3.17	15 (57%)
21	LMU	R	109	-	36,36,36	0.49	0	47,47,47	0.82	1 (2%)
20	CLA	1	213	-	45,59,73	2.58	17 (37%)	50,96,113	4.36	25 (50%)
20	CLA	A	819	-	52,66,73	2.13	11 (21%)	58,104,113	3.46	22 (37%)
20	CLA	B	817	-	40,54,73	2.37	11 (27%)	44,90,113	3.66	19 (43%)
21	LMU	H	106	-	36,36,36	0.60	1 (2%)	47,47,47	1.58	11 (23%)
20	CLA	4	311	-	22,32,73	1.87	7 (31%)	26,54,113	3.12	15 (57%)
20	CLA	A	837	-	45,59,73	2.33	12 (26%)	50,96,113	3.79	20 (40%)
20	CLA	A	816	-	48,62,73	2.26	14 (29%)	53,99,113	3.79	23 (43%)
21	LMU	R	102	-	36,36,36	0.57	0	47,47,47	1.51	9 (19%)
20	CLA	2	307	-	59,73,73	1.99	12 (20%)	67,113,113	3.28	21 (31%)
20	CLA	B	823	-	49,63,73	2.22	12 (24%)	55,101,113	3.31	19 (34%)
20	CLA	B	833	-	44,58,73	2.31	13 (29%)	49,95,113	3.93	20 (40%)
20	CLA	3	316	-	22,32,73	2.12	9 (40%)	26,54,113	3.28	17 (65%)
22	BCR	G	104	-	41,41,41	1.87	3 (7%)	56,56,56	5.73	17 (30%)
20	CLA	A	821	5	36,50,73	2.41	11 (30%)	39,85,113	4.18	16 (41%)
23	PQN	A	842	-	34,34,34	1.69	2 (5%)	42,45,45	1.21	5 (11%)
21	LMU	A	853	-	36,36,36	0.50	0	47,47,47	1.42	6 (12%)
20	CLA	B	820	-	55,69,73	1.99	11 (20%)	62,108,113	3.43	21 (33%)
20	CLA	4	312	-	22,32,73	1.89	5 (22%)	26,54,113	3.09	16 (61%)
20	CLA	4	317	-	46,60,73	2.34	14 (30%)	51,97,113	4.00	22 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	F	205	-	30,44,73	2.51	10 (33%)	35,78,113	3.92	18 (51%)
20	CLA	B	850	-	59,73,73	1.97	13 (22%)	67,113,113	3.33	24 (35%)
20	CLA	B	839	-	41,55,73	2.60	15 (36%)	45,91,113	4.64	18 (40%)
20	CLA	2	312	-	55,69,73	2.10	11 (20%)	62,108,113	3.56	28 (45%)
21	LMU	R	103	-	36,36,36	0.70	1 (2%)	47,47,47	1.46	6 (12%)
21	LMU	B	804	-	36,36,36	0.70	0	47,47,47	1.75	12 (25%)
21	LMU	A	854	-	36,36,36	0.51	0	47,47,47	1.28	7 (14%)

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
22	BCR	B	844	-	-	7/29/63/63	0/2/2/2
20	CLA	1	210	1	3/3/14/25	-	-
20	CLA	A	829	-	3/3/17/25	5/19/117/135	-
20	CLA	A	802	-	3/3/7/25	-	-
20	CLA	4	307	-	3/3/7/25	-	-
20	CLA	L	201	-	4/4/19/25	14/31/129/135	-
20	CLA	1	205	-	3/3/14/25	-	-
20	CLA	2	309	-	3/3/7/25	-	-
21	LMU	4	319	-	-	13/20/60/61	0/2/2/2
20	CLA	L	204	-	4/4/18/25	7/25/123/135	-
21	LMU	G	101	-	-	13/21/61/61	0/2/2/2
21	LMU	K	106	-	-	13/21/61/61	0/2/2/2
20	CLA	B	823	-	4/4/18/25	10/25/123/135	-
21	LMU	2	321	-	-	18/21/61/61	0/2/2/2
21	LMU	K	105	-	-	12/21/61/61	0/2/2/2
20	CLA	A	805	-	3/3/17/25	13/24/122/135	-
20	CLA	4	306	-	4/4/17/25	7/22/120/135	-
20	CLA	A	833	5	3/3/16/25	5/11/111/135	-
20	CLA	A	801	-	5/5/16/25	11/16/112/135	-
20	CLA	3	305	-	3/3/7/25	-	-
20	CLA	A	814	-	3/3/7/25	-	-
20	CLA	1	214	-	3/3/7/25	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	A	845	-	-	10/29/63/63	0/2/2/2
21	LMU	1	217	-	-	9/21/61/61	0/2/2/2
20	CLA	B	808	-	4/4/19/25	19/33/131/135	-
20	CLA	3	303	-	3/3/14/25	-	-
20	CLA	2	301	-	3/3/7/25	-	-
24	SF4	C	103	7	-	-	0/6/5/5
20	CLA	B	826	-	4/4/18/25	19/29/127/135	-
21	LMU	H	104	-	-	12/21/61/61	0/2/2/2
20	CLA	B	841	-	4/4/20/25	18/37/135/135	-
20	CLA	L	202	-	4/4/18/25	14/25/123/135	-
20	CLA	A	839	-	4/4/18/25	14/29/127/135	-
20	CLA	L	208	16	3/3/17/25	8/19/117/135	-
20	CLA	4	314	4	3/3/7/25	-	-
22	BCR	F	203	-	-	13/29/63/63	0/2/2/2
20	CLA	3	313	-	3/3/7/25	-	-
21	LMU	E	101	-	-	14/21/61/61	0/2/2/2
20	CLA	B	819	-	3/3/15/25	2/8/106/135	-
20	CLA	A	841	-	3/3/7/25	-	-
20	CLA	4	315	-	3/3/16/25	9/15/113/135	-
20	CLA	A	850	-	4/4/20/25	18/37/135/135	-
20	CLA	3	318	-	3/3/14/25	-	-
20	CLA	B	829	-	4/4/20/25	18/37/135/135	-
20	CLA	2	310	2	3/3/17/25	5/19/117/135	-
20	CLA	A	807	-	3/3/16/25	7/15/113/135	-
20	CLA	R	108	-	4/4/20/25	20/37/135/135	-
22	BCR	I	101	-	-	10/29/60/63	0/2/2/2
20	CLA	1	209	-	3/3/7/25	-	-
20	CLA	H	101	-	5/5/18/25	11/25/123/135	-
21	LMU	2	322	-	-	8/21/61/61	0/2/2/2
20	CLA	A	817	-	3/3/17/25	14/22/120/135	-
21	LMU	R	104	-	-	14/21/61/61	0/2/2/2
25	LMG	B	848	-	-	27/44/64/70	0/1/1/1
20	CLA	1	206	-	4/4/19/25	20/33/131/135	-
21	LMU	G	102	-	-	14/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMU	3	319	-	-	12/21/61/61	0/2/2/2
21	LMU	G	103	-	-	14/21/61/61	0/2/2/2
20	CLA	B	834	-	3/3/16/25	8/11/111/135	-
22	BCR	B	801	-	-	13/29/63/63	0/2/2/2
20	CLA	A	809	-	3/3/17/25	10/22/120/135	-
20	CLA	A	840	-	4/4/18/25	8/25/123/135	-
20	CLA	A	825	-	4/4/20/25	24/37/135/135	-
23	PQN	B	843	-	1/1/8/9	10/23/43/43	0/2/2/2
20	CLA	A	831	-	4/4/20/25	19/37/135/135	-
24	SF4	C	102	7	-	-	0/6/5/5
21	LMU	D	201	-	-	9/21/61/61	0/2/2/2
20	CLA	2	305	-	3/3/17/25	7/19/117/135	-
20	CLA	A	813	-	3/3/17/25	9/19/117/135	-
20	CLA	3	315	-	4/4/20/25	17/37/135/135	-
20	CLA	K	102	-	3/3/17/25	4/19/117/135	-
21	LMU	1	218	-	-	13/21/61/61	0/2/2/2
20	CLA	B	842	-	3/3/14/25	-	-
20	CLA	A	808	5	4/4/19/25	15/31/129/135	-
20	CLA	B	822	-	3/3/16/25	12/15/113/135	-
20	CLA	A	832	-	3/3/17/25	11/19/117/135	-
20	CLA	L	209	-	3/3/16/25	9/16/114/135	-
20	CLA	4	310	-	3/3/17/25	10/19/117/135	-
20	CLA	B	814	-	4/4/20/25	22/37/135/135	-
20	CLA	B	812	-	4/4/18/25	8/25/121/135	-
20	CLA	4	301	-	4/4/18/25	13/25/123/135	-
20	CLA	4	305	-	3/3/17/25	9/19/117/135	-
21	LMU	B	849	-	-	5/11/51/61	0/2/2/2
24	SF4	A	856	5,6	-	-	0/6/5/5
21	LMU	B	805	-	-	13/21/61/61	0/2/2/2
20	CLA	1	215	-	4/4/17/25	8/21/119/135	-
20	CLA	3	301	-	3/3/14/25	-	-
20	CLA	A	811	20	4/4/20/25	23/37/135/135	-
20	CLA	A	835	-	4/4/20/25	15/37/135/135	-
20	CLA	B	831	-	3/3/17/25	10/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMU	4	321	-	-	15/21/61/61	0/2/2/2
20	CLA	B	803	-	4/4/20/25	19/37/135/135	-
20	CLA	1	212	-	3/3/7/25	-	-
21	LMU	2	320	-	-	11/21/61/61	0/2/2/2
20	CLA	B	806	-	4/4/20/25	20/37/135/135	-
20	CLA	3	306	-	3/3/7/25	-	-
21	LMU	K	107	-	-	17/21/61/61	0/2/2/2
20	CLA	2	306	-	3/3/7/25	-	-
20	CLA	B	837	-	4/4/19/25	14/31/129/135	-
20	CLA	A	836	-	3/3/16/25	7/16/114/135	-
20	CLA	2	311	-	3/3/17/25	11/19/117/135	-
20	CLA	A	812	-	3/3/17/25	13/24/122/135	-
20	CLA	B	840	-	4/4/20/25	17/37/135/135	-
21	LMU	R	109	-	-	14/21/61/61	0/2/2/2
20	CLA	H	112	-	4/4/18/25	8/25/123/135	-
21	LMU	A	846	-	-	17/21/61/61	0/2/2/2
21	LMU	2	313	-	-	16/21/61/61	0/2/2/2
20	CLA	B	838	-	4/4/20/25	13/37/135/135	-
20	CLA	A	818	-	4/4/19/25	14/31/129/135	-
22	BCR	I	103	-	-	15/29/63/63	0/2/2/2
20	CLA	3	310	-	4/4/20/25	18/37/135/135	-
21	LMU	H	105	-	-	17/21/61/61	0/2/2/2
20	CLA	1	202	-	3/3/15/25	4/8/106/135	-
21	LMU	R	106	-	-	12/21/61/61	0/2/2/2
20	CLA	B	807	-	3/3/16/25	5/11/111/135	-
20	CLA	A	803	-	3/3/16/25	3/15/113/135	-
20	CLA	1	204	-	3/3/16/25	10/15/113/135	-
20	CLA	3	317	-	3/3/7/25	-	-
20	CLA	3	309	-	3/3/7/25	-	-
20	CLA	A	838	-	4/4/20/25	18/37/135/135	-
20	CLA	1	201	-	3/3/16/25	10/15/113/135	-
20	CLA	B	816	-	4/4/19/25	14/31/129/135	-
21	LMU	2	319	-	-	13/21/61/61	0/2/2/2
20	CLA	F	201	-	3/3/17/25	9/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	318	-	3/3/16/25	12/16/114/135	-
20	CLA	H	111	-	4/4/18/25	18/29/127/135	-
20	CLA	F	207	-	6/6/17/25	11/23/121/135	-
20	CLA	2	302	-	3/3/17/25	12/21/119/135	-
20	CLA	B	835	-	3/3/16/25	5/11/111/135	-
20	CLA	B	821	-	3/3/17/25	6/19/117/135	-
21	LMU	L	206	-	-	14/21/61/61	0/2/2/2
20	CLA	J	101	-	3/3/16/25	10/17/115/135	-
20	CLA	A	828	-	4/4/20/25	20/37/135/135	-
20	CLA	B	827	-	4/4/20/25	21/37/135/135	-
20	CLA	F	206	-	3/3/15/25	3/8/106/135	-
21	LMU	L	212	-	-	16/21/61/61	0/2/2/2
20	CLA	A	822	-	3/3/17/25	6/19/117/135	-
22	BCR	B	847	-	-	12/29/63/63	0/2/2/2
21	LMU	C	101	-	-	14/21/61/61	0/2/2/2
20	CLA	A	830	-	4/4/20/25	18/37/135/135	-
20	CLA	1	211	-	4/4/17/25	8/21/119/135	-
20	CLA	A	849	-	4/4/20/25	26/37/135/135	-
20	CLA	H	102	-	4/4/18/25	14/25/123/135	-
21	LMU	A	855	-	-	13/21/61/61	0/2/2/2
20	CLA	B	811	6	3/3/7/25	-	-
20	CLA	A	820	-	3/3/17/25	8/21/119/135	-
20	CLA	1	207	-	4/4/17/25	9/21/119/135	-
20	CLA	2	308	-	3/3/7/25	-	-
20	CLA	3	304	-	3/3/7/25	-	-
20	CLA	B	825	-	3/3/17/25	9/24/122/135	-
20	CLA	I	102	-	4/4/19/25	13/31/129/135	-
22	BCR	2	318	-	-	15/29/63/63	0/2/2/2
20	CLA	2	316	-	3/3/7/25	-	-
20	CLA	A	826	-	4/4/20/25	15/37/135/135	-
20	CLA	4	309	-	3/3/7/25	-	-
22	BCR	A	843	-	-	14/29/63/63	0/2/2/2
20	CLA	A	851	-	4/4/20/25	25/37/135/135	-
21	LMU	4	320	-	-	16/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMU	4	316	-	-	13/21/61/61	0/2/2/2
20	CLA	4	303	-	5/5/20/25	22/37/135/135	-
20	CLA	1	208	-	3/3/7/25	-	-
20	CLA	1	203	-	3/3/16/25	8/16/114/135	-
20	CLA	B	815	-	4/4/19/25	17/31/129/135	-
20	CLA	4	313	-	3/3/14/25	-	-
20	CLA	K	104	-	4/4/18/25	11/27/125/135	-
20	CLA	K	103	-	3/3/17/25	10/19/117/135	-
21	LMU	R	105	-	-	14/21/61/61	0/2/2/2
21	LMU	L	205	-	-	13/21/61/61	0/2/2/2
22	BCR	B	846	-	-	14/29/63/63	0/2/2/2
20	CLA	B	836	-	3/3/17/25	10/21/119/135	-
21	LMU	3	320	-	-	11/21/61/61	0/2/2/2
20	CLA	3	314	-	3/3/17/25	8/19/117/135	-
21	LMU	A	852	-	-	20/21/61/61	0/2/2/2
20	CLA	G	105	-	3/3/17/25	10/21/119/135	-
20	CLA	B	802	-	3/3/17/25	10/24/122/135	-
20	CLA	L	203	-	4/4/20/25	16/37/135/135	-
20	CLA	3	311	-	4/4/20/25	21/37/135/135	-
22	BCR	L	211	-	-	10/29/63/63	0/2/2/2
21	LMU	A	847	-	-	13/21/61/61	0/2/2/2
20	CLA	K	101	-	3/3/16/25	6/15/113/135	-
22	BCR	J	102	-	-	11/29/63/63	0/2/2/2
21	LMU	A	848	-	-	12/21/61/61	0/2/2/2
20	CLA	A	815	-	3/3/17/25	10/19/117/135	-
20	CLA	4	308	-	3/3/7/25	-	-
22	BCR	B	845	-	-	9/29/63/63	0/2/2/2
20	CLA	A	824	-	4/4/18/25	14/30/128/135	-
20	CLA	2	317	-	4/4/20/25	15/37/135/135	-
20	CLA	R	107	-	4/4/18/25	14/28/126/135	-
20	CLA	B	828	-	4/4/20/25	16/37/135/135	-
20	CLA	B	810	-	4/4/19/25	10/31/129/135	-
20	CLA	B	818	-	3/3/17/25	8/23/121/135	-
20	CLA	A	834	-	3/3/16/25	7/15/113/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	832	-	4/4/18/25	16/30/128/135	-
21	LMU	F	202	-	-	13/20/60/61	0/2/2/2
22	BCR	A	844	-	-	14/29/63/63	0/2/2/2
20	CLA	4	302	-	3/3/14/25	-	-
21	LMU	H	103	-	-	14/21/61/61	0/2/2/2
20	CLA	2	315	-	3/3/17/25	8/19/117/135	-
20	CLA	A	823	-	4/4/18/25	12/29/127/135	-
21	LMU	R	101	-	-	13/21/61/61	0/2/2/2
20	CLA	A	827	-	4/4/18/25	10/25/123/135	-
20	CLA	2	303	-	4/4/18/25	15/29/127/135	-
20	CLA	4	304	-	4/4/18/25	12/25/123/135	-
20	CLA	A	804	20	4/4/18/25	12/25/123/135	-
21	LMU	1	216	-	-	11/21/61/61	0/2/2/2
20	CLA	3	307	-	3/3/15/25	7/10/108/135	-
20	CLA	3	308	-	3/3/7/25	-	-
20	CLA	3	302	-	3/3/7/25	-	-
20	CLA	B	809	-	4/4/20/25	16/37/135/135	-
20	CLA	L	210	-	4/4/17/25	10/19/117/135	-
20	CLA	B	813	-	4/4/18/25	12/25/123/135	-
20	CLA	J	103	-	4/4/19/25	20/33/131/135	-
22	BCR	F	204	-	-	9/29/63/63	0/2/2/2
20	CLA	B	824	-	4/4/20/25	19/37/135/135	-
20	CLA	A	806	-	4/4/18/25	7/27/125/135	-
20	CLA	B	830	-	4/4/20/25	25/37/135/135	-
20	CLA	2	304	-	3/3/7/25	-	-
20	CLA	A	810	-	3/3/16/25	2/11/111/135	-
20	CLA	1	213	-	5/5/17/25	10/21/119/135	-
20	CLA	A	819	-	4/4/18/25	11/29/127/135	-
20	CLA	B	817	-	3/3/16/25	11/15/113/135	-
21	LMU	H	106	-	-	9/21/61/61	0/2/2/2
20	CLA	4	311	-	3/3/7/25	-	-
20	CLA	A	837	-	3/3/17/25	14/21/119/135	-
20	CLA	A	816	-	3/3/17/25	10/24/122/135	-
21	LMU	R	102	-	-	11/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	2	307	-	4/4/20/25	21/37/135/135	-
20	CLA	B	833	-	3/3/17/25	6/19/117/135	-
20	CLA	3	316	-	3/3/7/25	-	-
22	BCR	G	104	-	-	14/29/63/63	0/2/2/2
20	CLA	A	821	5	3/3/15/25	2/10/108/135	-
23	PQN	A	842	-	1/1/8/9	11/23/43/43	0/2/2/2
21	LMU	A	853	-	-	11/21/61/61	0/2/2/2
20	CLA	B	820	-	4/4/19/25	15/33/131/135	-
20	CLA	4	312	-	3/3/7/25	-	-
20	CLA	4	317	-	3/3/17/25	11/22/120/135	-
20	CLA	F	205	-	3/3/14/25	-	-
20	CLA	B	850	-	4/4/20/25	21/37/135/135	-
20	CLA	B	839	-	3/3/16/25	11/16/114/135	-
20	CLA	2	312	-	4/4/19/25	22/33/131/135	-
21	LMU	R	103	-	-	11/21/61/61	0/2/2/2
21	LMU	B	804	-	-	16/21/61/61	0/2/2/2
21	LMU	A	854	-	-	16/21/61/61	0/2/2/2

The worst 5 of 2070 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	801	BCR	C21-C22	-9.91	1.22	1.35
22	B	801	BCR	C20-C21	-9.21	1.14	1.43
20	1	205	CLA	CAB-C3B	-8.82	1.33	1.51
20	B	812	CLA	CAB-C3B	-8.73	1.33	1.51
20	4	302	CLA	CAB-C3B	-8.49	1.34	1.51

The worst 5 of 3982 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	104	BCR	C20-C21-C22	36.27	179.07	127.31
22	L	211	BCR	C20-C21-C22	35.78	178.38	127.31
22	A	845	BCR	C20-C21-C22	35.54	178.03	127.31
22	J	102	BCR	C20-C21-C22	35.47	177.93	127.31
22	B	846	BCR	C20-C21-C22	35.39	177.82	127.31

5 of 604 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	1	210	CLA	NC
20	1	210	CLA	ND
20	1	210	CLA	NA
20	A	829	CLA	NC
20	A	829	CLA	ND

5 of 2536 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	L	201	CLA	C1A-C2A-CAA-CBA
20	L	201	CLA	C2A-CAA-CBA-CGA
20	L	201	CLA	CHA-CBD-CGD-O1D
20	L	201	CLA	CHA-CBD-CGD-O2D
20	L	201	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

224 monomers are involved in 2729 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	844	BCR	8	0
20	1	210	CLA	8	0
20	4	301	CLA	34	0
20	L	201	CLA	23	0
20	1	205	CLA	6	0
21	4	319	LMU	8	3
20	L	204	CLA	13	0
21	G	101	LMU	4	41
21	K	106	LMU	8	0
21	2	321	LMU	5	0
21	K	105	LMU	13	0
20	A	805	CLA	16	0
20	4	306	CLA	18	0
20	A	833	CLA	13	0
20	A	801	CLA	9	0
20	3	305	CLA	3	0
20	A	814	CLA	14	0
20	H	101	CLA	15	0
22	A	845	BCR	48	0
20	B	824	CLA	30	0
21	1	217	LMU	20	0
20	B	808	CLA	31	0
20	3	303	CLA	4	0
24	C	103	SF4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	826	CLA	39	0
21	H	104	LMU	9	0
20	B	841	CLA	17	0
20	L	202	CLA	10	0
20	A	839	CLA	27	0
20	L	208	CLA	3	0
20	4	314	CLA	10	0
22	F	203	BCR	26	0
21	E	101	LMU	11	0
20	B	819	CLA	7	0
20	A	841	CLA	1	0
20	4	315	CLA	5	0
20	A	850	CLA	30	0
20	B	829	CLA	25	0
20	2	310	CLA	21	0
20	A	807	CLA	33	0
20	R	108	CLA	4	0
22	I	101	BCR	9	0
20	1	209	CLA	1	0
21	R	104	LMU	5	0
20	A	817	CLA	8	0
20	B	827	CLA	36	0
20	1	206	CLA	9	0
21	G	103	LMU	16	0
20	B	834	CLA	23	0
22	B	801	BCR	24	0
20	A	809	CLA	32	0
20	A	840	CLA	6	0
20	A	825	CLA	51	0
23	B	843	PQN	28	0
20	A	831	CLA	37	0
21	D	201	LMU	3	0
20	2	305	CLA	16	0
20	A	813	CLA	21	0
20	3	315	CLA	13	0
24	C	102	SF4	4	0
21	1	218	LMU	9	0
20	B	842	CLA	2	0
20	A	808	CLA	21	0
20	B	822	CLA	16	0
20	A	832	CLA	19	0
20	L	209	CLA	27	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	4	310	CLA	25	0
20	B	814	CLA	30	0
20	B	812	CLA	9	0
20	A	829	CLA	7	0
20	4	305	CLA	5	0
21	B	849	LMU	1	0
24	A	856	SF4	18	0
21	B	805	LMU	3	0
20	1	215	CLA	1	0
20	3	301	CLA	1	0
20	A	811	CLA	22	0
20	A	835	CLA	15	0
20	B	831	CLA	11	0
21	4	321	LMU	13	0
20	B	803	CLA	44	0
20	1	212	CLA	2	0
21	2	320	LMU	5	0
20	B	806	CLA	25	0
20	3	306	CLA	7	0
20	K	104	CLA	17	0
21	K	107	LMU	21	0
20	B	837	CLA	12	0
20	A	836	CLA	6	0
20	2	311	CLA	6	0
20	A	812	CLA	4	0
20	B	840	CLA	18	0
20	H	112	CLA	13	0
21	A	846	LMU	5	0
21	2	313	LMU	29	0
20	B	838	CLA	42	0
20	A	818	CLA	46	0
22	I	103	BCR	38	0
20	3	310	CLA	17	0
20	1	202	CLA	1	0
21	R	106	LMU	9	0
20	B	807	CLA	9	0
20	A	803	CLA	20	0
20	1	204	CLA	15	0
20	3	309	CLA	1	0
25	B	848	LMG	17	0
20	1	201	CLA	13	0
20	B	816	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	2	319	LMU	6	0
20	F	201	CLA	29	0
20	4	318	CLA	14	0
20	H	111	CLA	27	0
20	F	207	CLA	13	0
20	2	302	CLA	13	0
20	B	835	CLA	30	0
20	B	821	CLA	7	0
20	J	101	CLA	12	0
20	A	828	CLA	18	0
21	H	105	LMU	18	0
20	F	206	CLA	5	0
21	L	212	LMU	1	0
20	A	822	CLA	20	0
22	B	847	BCR	32	0
20	A	830	CLA	31	0
20	1	211	CLA	7	0
20	A	849	CLA	21	0
20	H	102	CLA	2	0
20	B	811	CLA	4	0
20	A	820	CLA	8	0
20	1	207	CLA	6	1
20	2	308	CLA	1	0
20	3	304	CLA	2	0
20	B	825	CLA	24	0
20	I	102	CLA	12	0
22	2	318	BCR	9	0
20	A	826	CLA	49	0
22	A	843	BCR	32	0
20	A	810	CLA	4	0
20	A	851	CLA	26	0
21	4	320	LMU	2	0
21	4	316	LMU	1	0
20	4	303	CLA	18	0
20	1	208	CLA	3	0
20	1	203	CLA	8	0
20	B	815	CLA	17	0
20	4	313	CLA	5	0
21	G	102	LMU	7	0
20	K	103	CLA	9	0
21	L	205	LMU	1	0
22	B	846	BCR	32	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	836	CLA	9	0
21	3	320	LMU	14	0
20	3	314	CLA	1	0
21	A	852	LMU	5	0
20	G	105	CLA	4	0
20	B	802	CLA	17	0
20	L	203	CLA	29	0
20	3	311	CLA	10	0
22	L	211	BCR	36	0
21	A	847	LMU	4	0
20	K	101	CLA	16	1
22	J	102	BCR	36	0
21	A	848	LMU	4	0
20	K	102	CLA	27	0
20	A	815	CLA	4	0
22	B	845	BCR	18	0
20	A	824	CLA	43	0
20	2	317	CLA	11	0
20	R	107	CLA	10	0
20	B	828	CLA	13	0
20	B	810	CLA	18	0
20	B	818	CLA	17	0
20	A	834	CLA	7	0
20	B	832	CLA	24	0
21	F	202	LMU	8	0
22	A	844	BCR	23	0
20	4	302	CLA	3	0
21	H	103	LMU	6	0
20	2	315	CLA	17	0
20	A	823	CLA	10	0
21	R	101	LMU	3	0
20	A	827	CLA	19	0
20	2	303	CLA	25	0
20	A	838	CLA	33	0
20	4	304	CLA	21	0
20	A	804	CLA	36	0
21	1	216	LMU	3	0
20	3	307	CLA	14	0
20	3	308	CLA	2	0
20	B	809	CLA	22	0
20	L	210	CLA	9	0
20	B	813	CLA	8	0

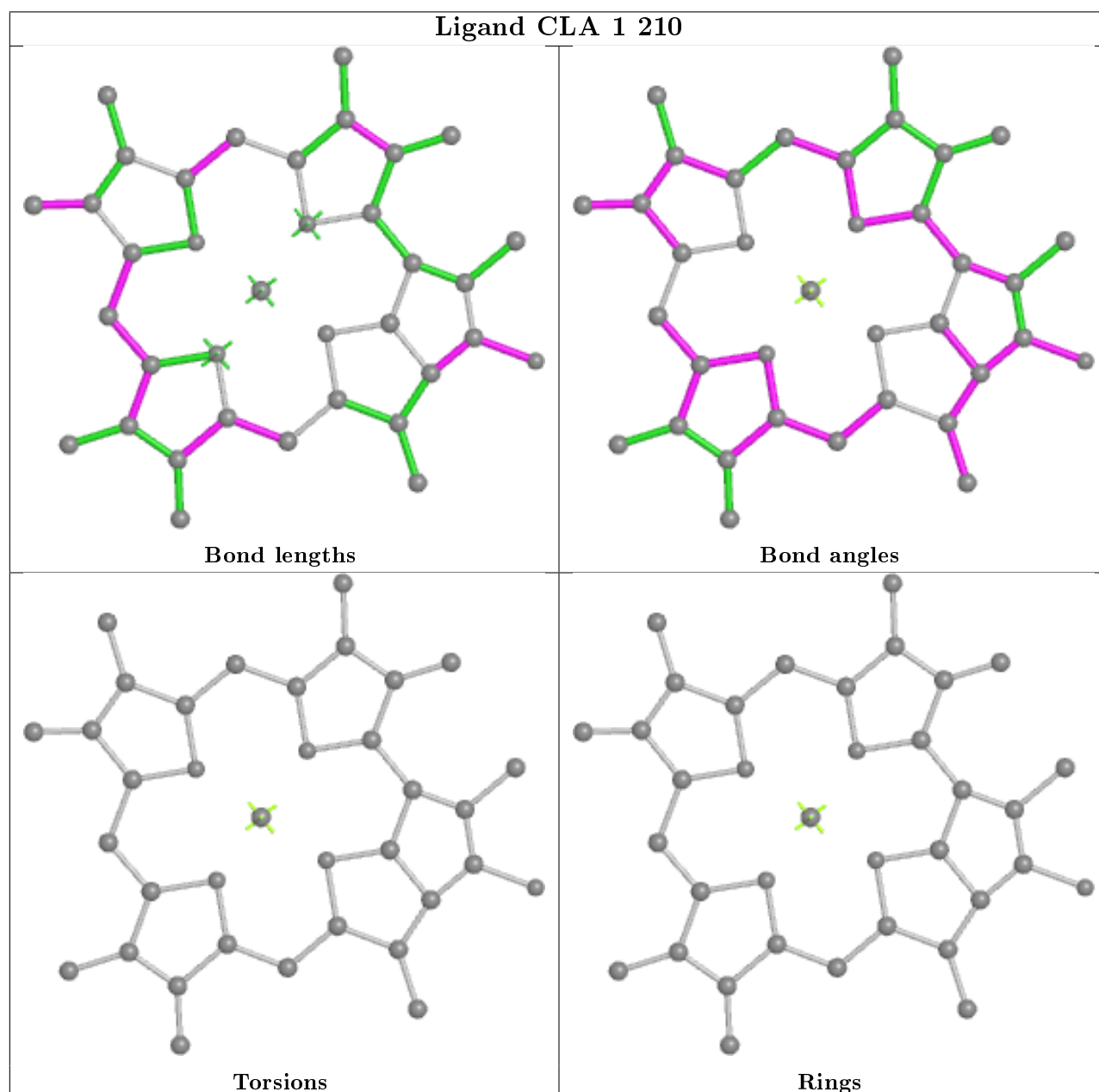
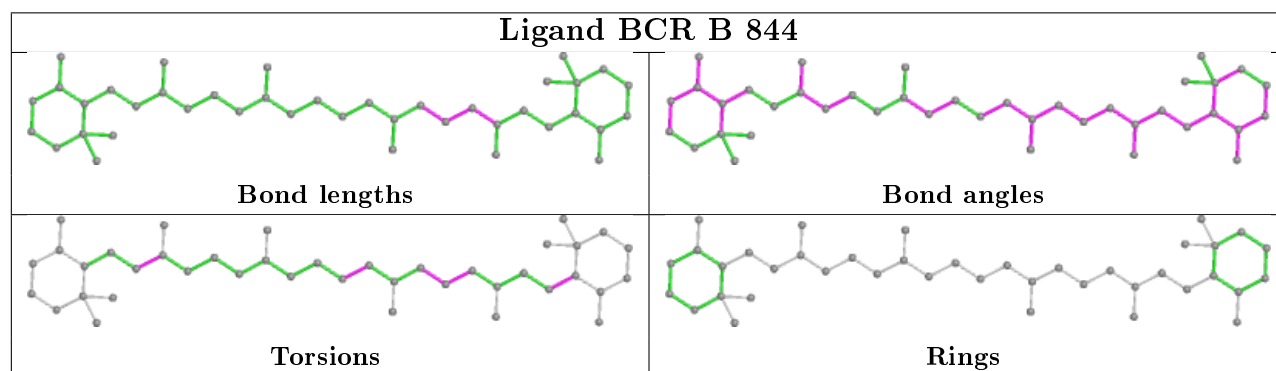
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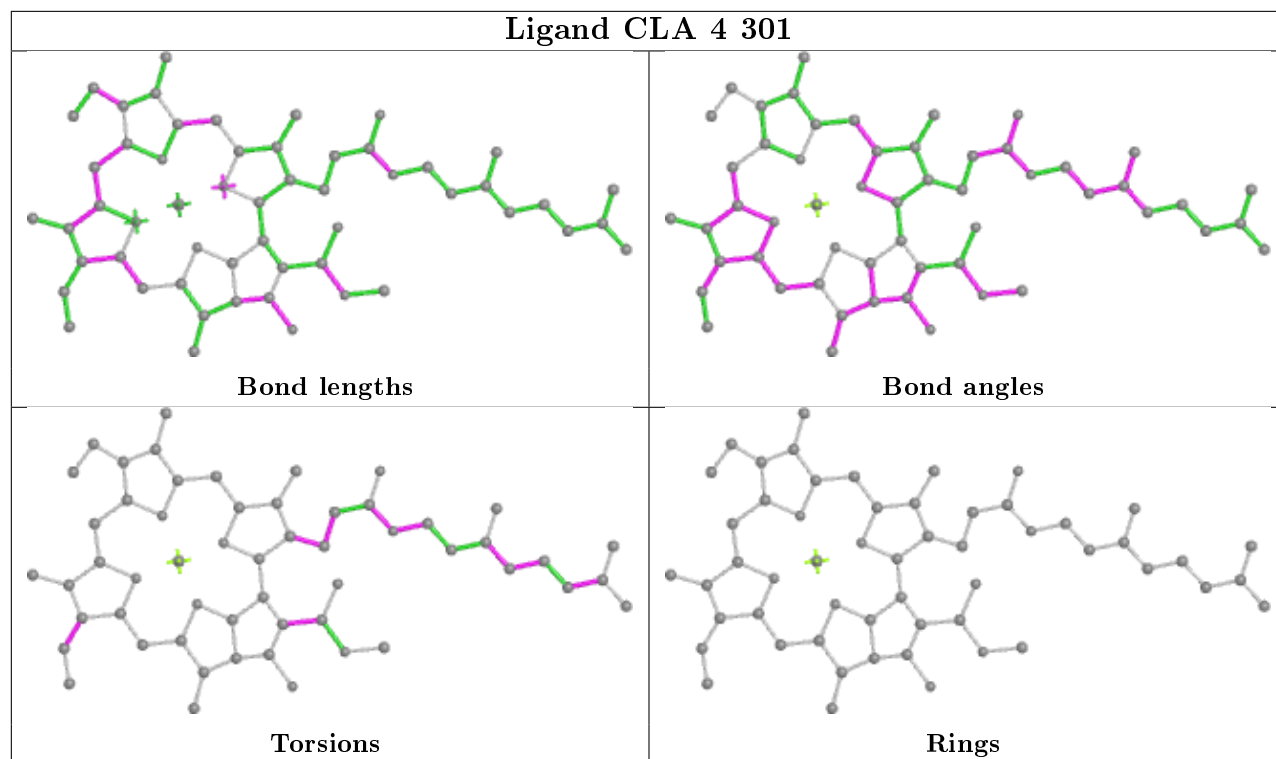
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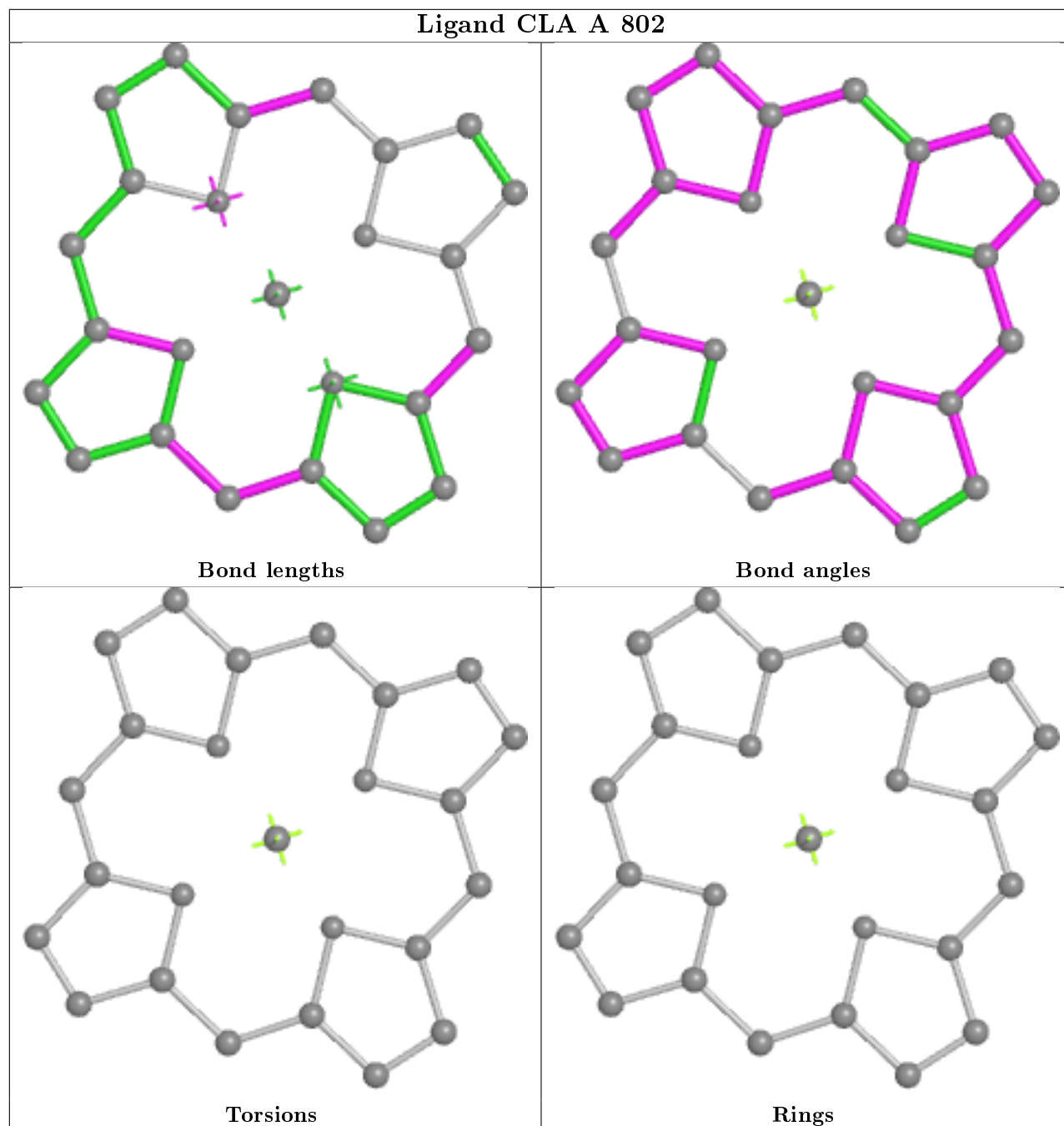
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	J	103	CLA	14	0
22	F	204	BCR	34	0
21	3	319	LMU	2	0
20	A	806	CLA	13	0
20	B	830	CLA	24	0
20	2	304	CLA	2	0
21	R	109	LMU	9	3
20	1	213	CLA	16	0
20	A	819	CLA	33	0
20	B	817	CLA	19	0
21	H	106	LMU	9	0
20	4	311	CLA	3	0
20	A	837	CLA	17	0
20	A	816	CLA	21	0
21	R	102	LMU	8	0
20	2	307	CLA	22	0
20	B	823	CLA	15	0
20	B	833	CLA	18	0
22	G	104	BCR	5	0
20	A	821	CLA	8	0
23	A	842	PQN	7	0
21	A	853	LMU	21	0
20	B	820	CLA	17	0
20	4	312	CLA	4	0
20	4	317	CLA	3	0
20	F	205	CLA	1	0
20	B	850	CLA	18	0
20	B	839	CLA	47	0
20	2	312	CLA	19	0
21	R	103	LMU	9	0
21	B	804	LMU	7	0
21	A	854	LMU	15	0

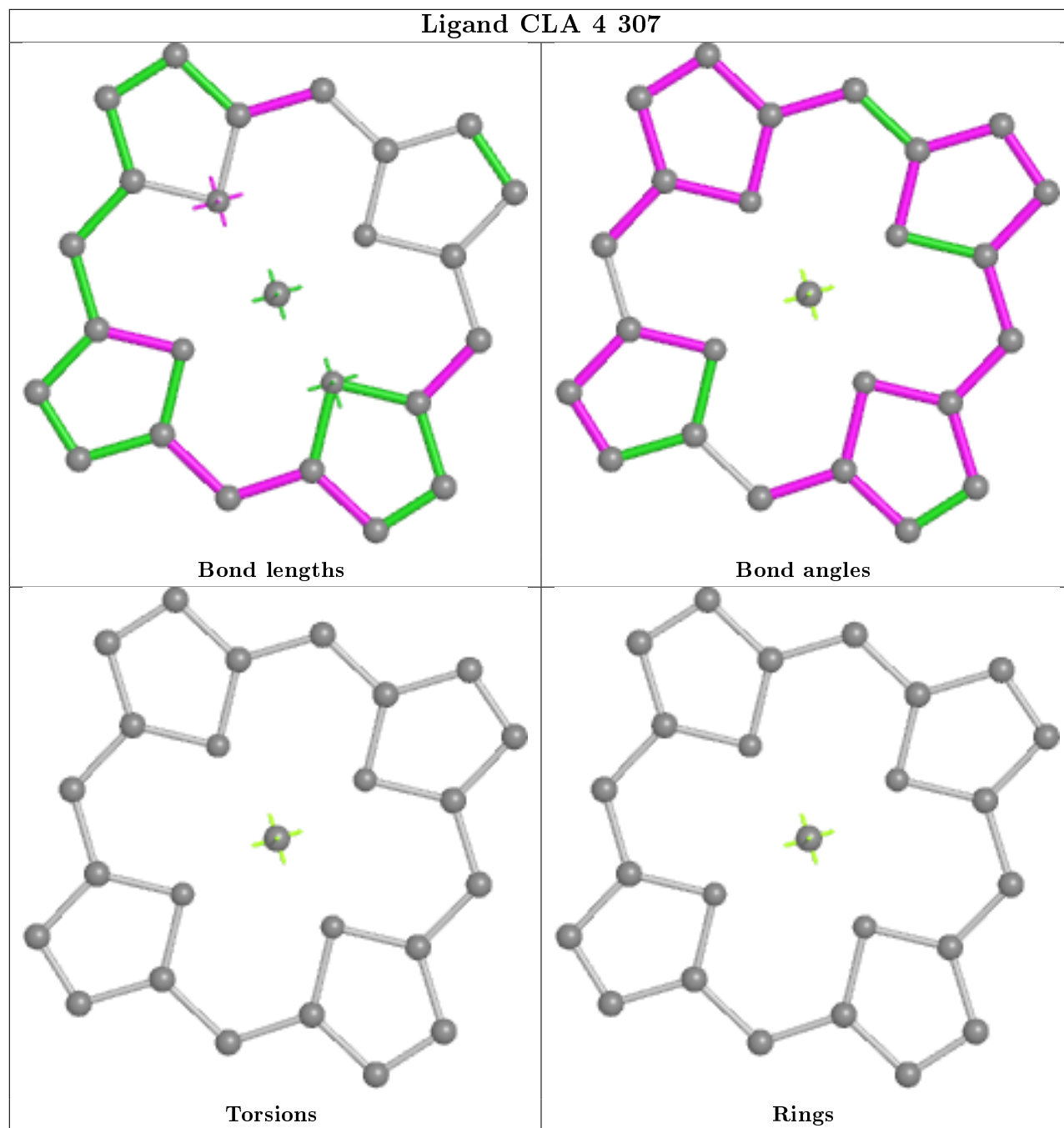
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

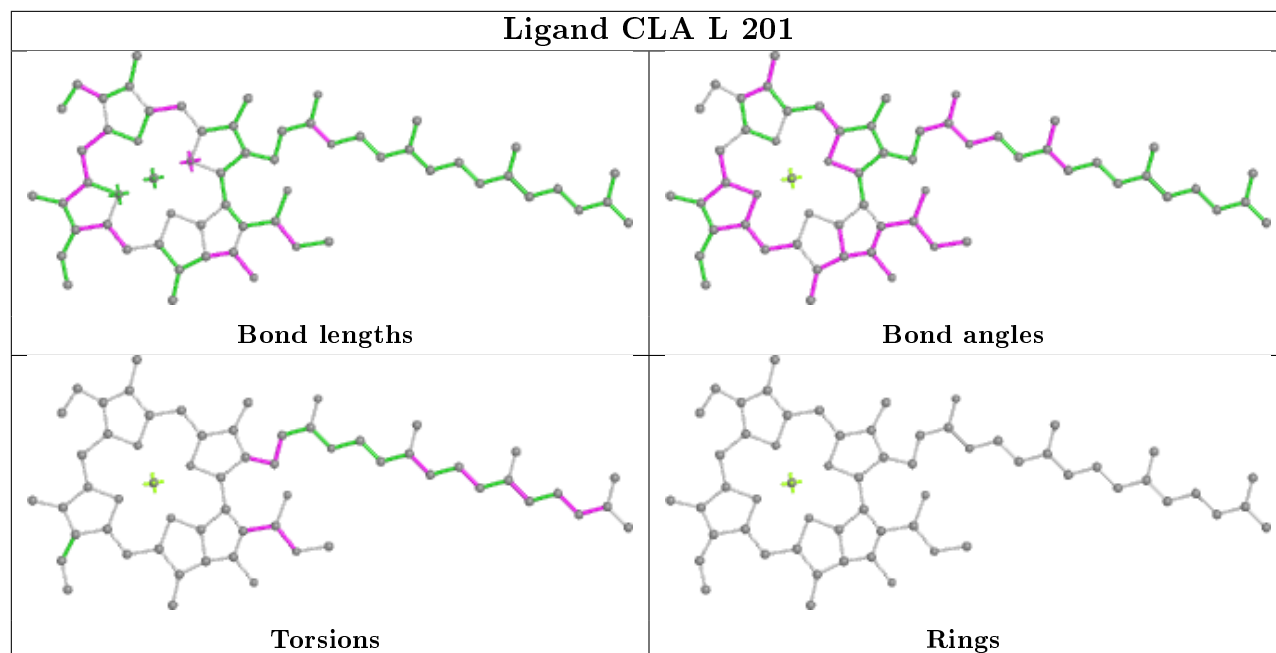
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

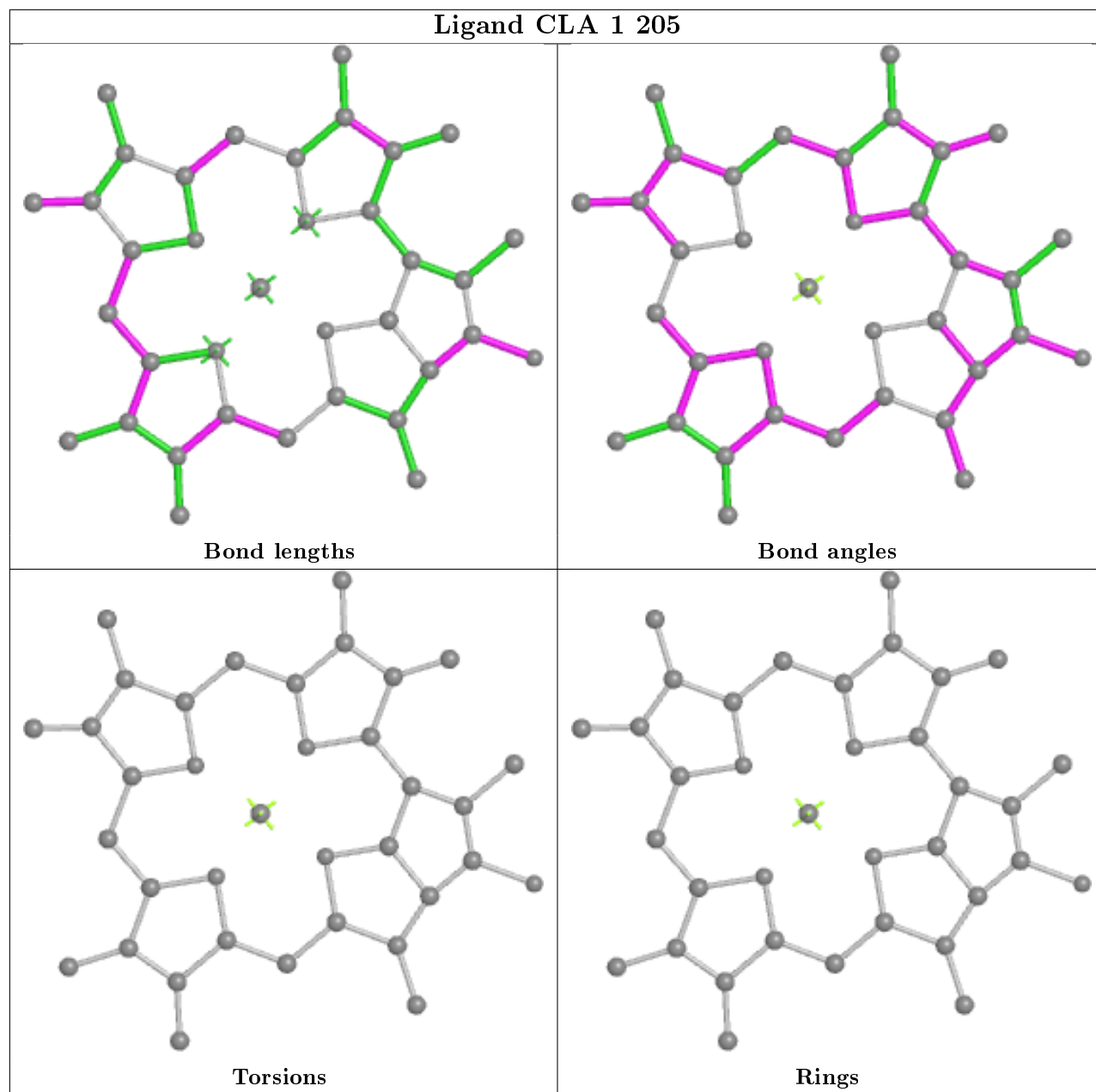


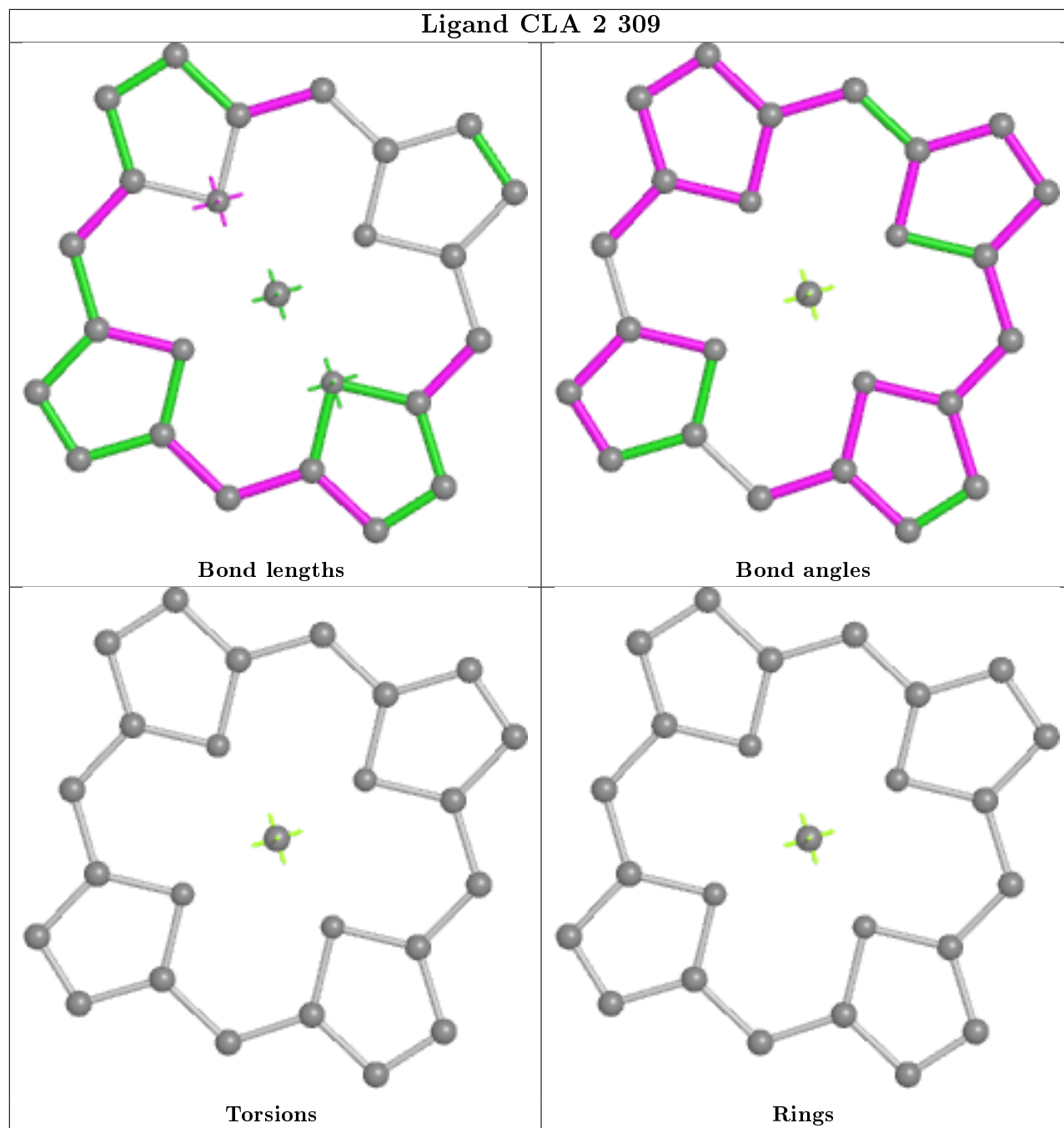


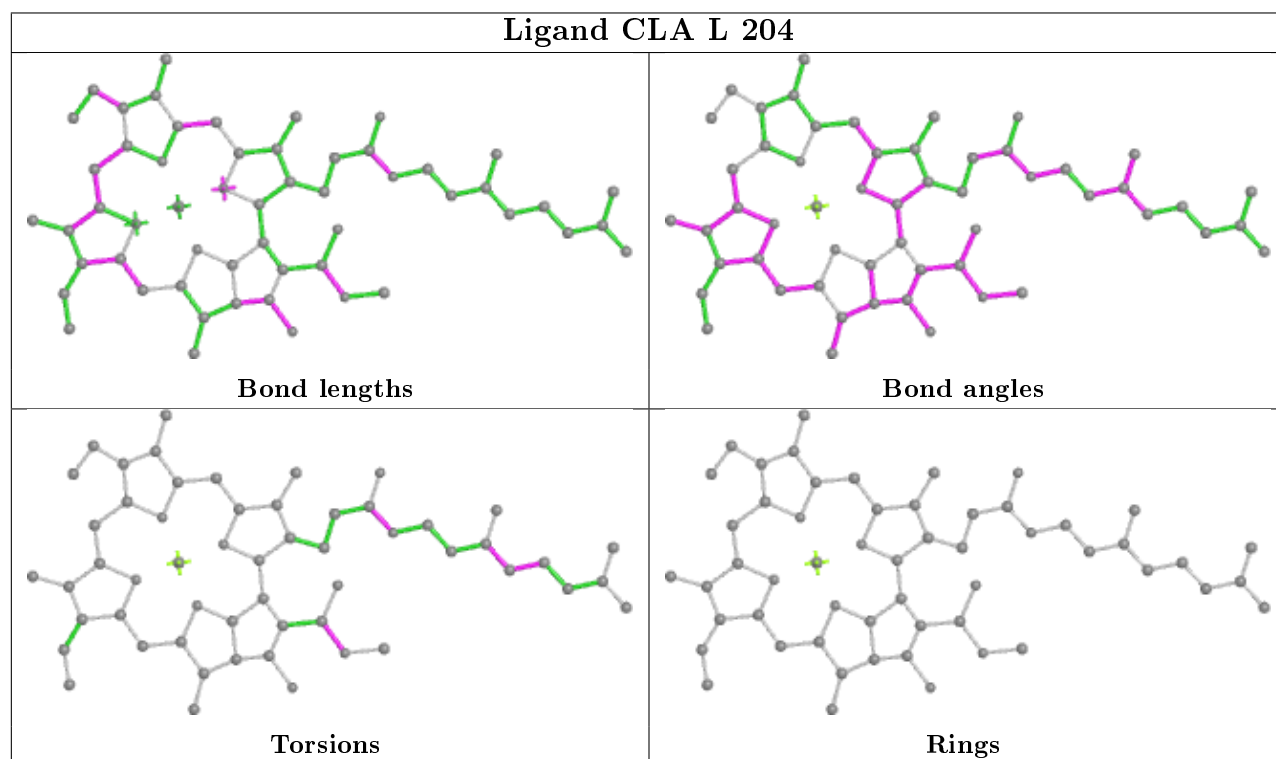
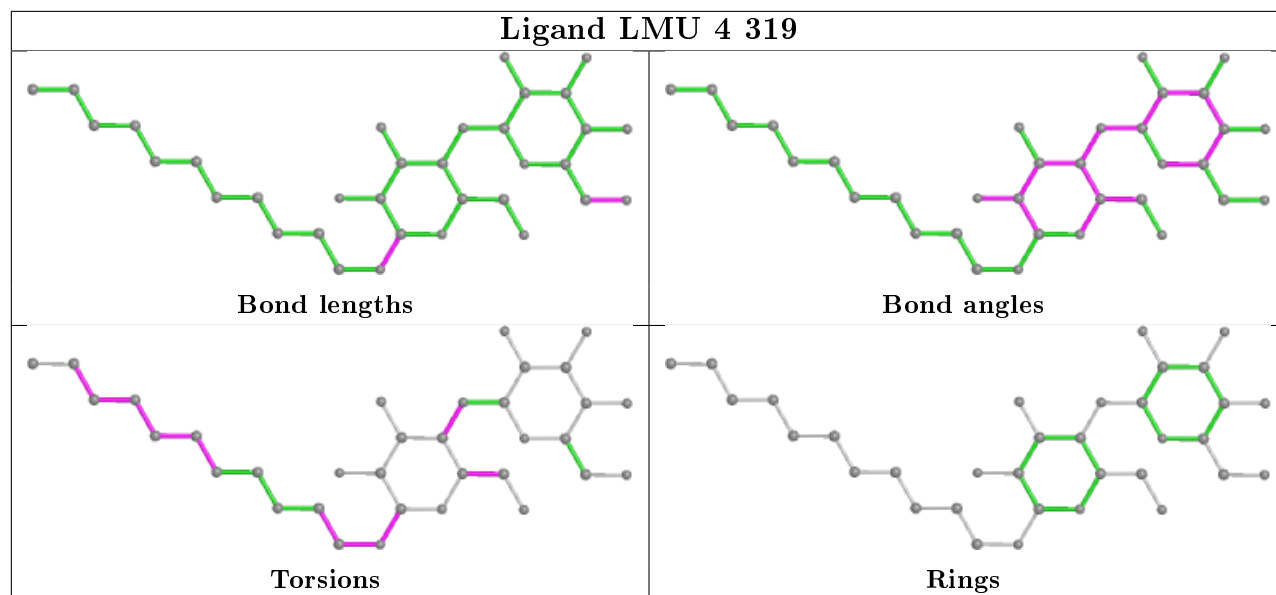


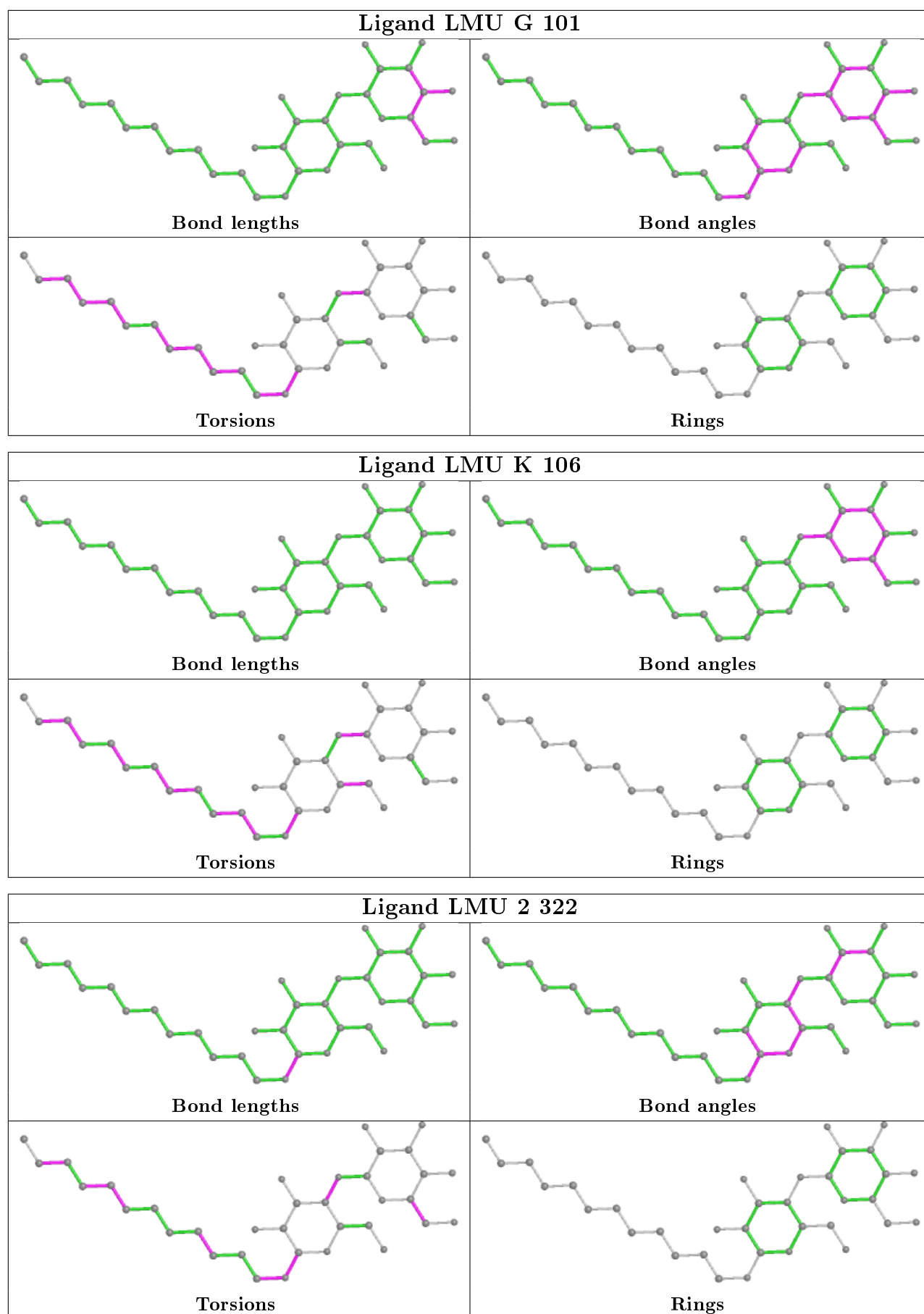


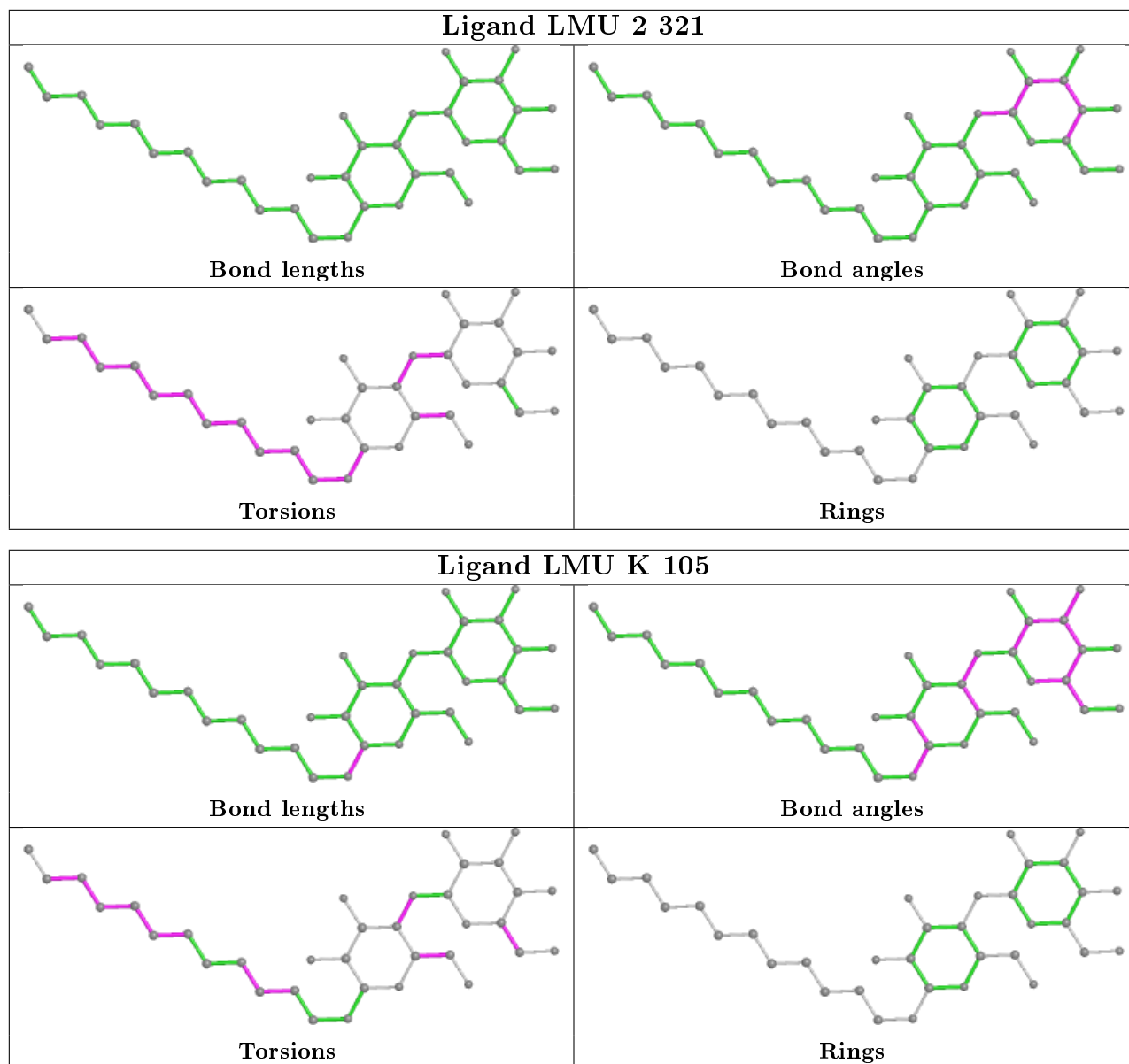


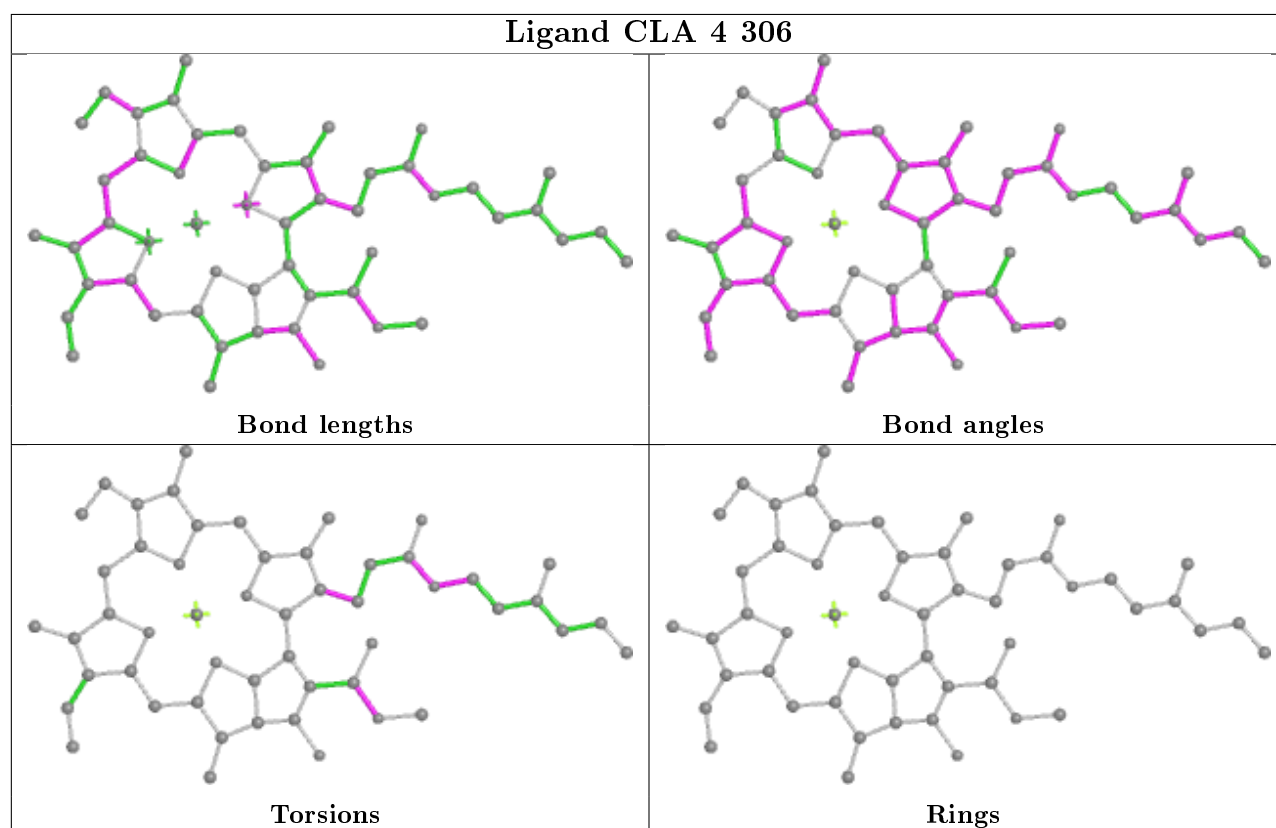
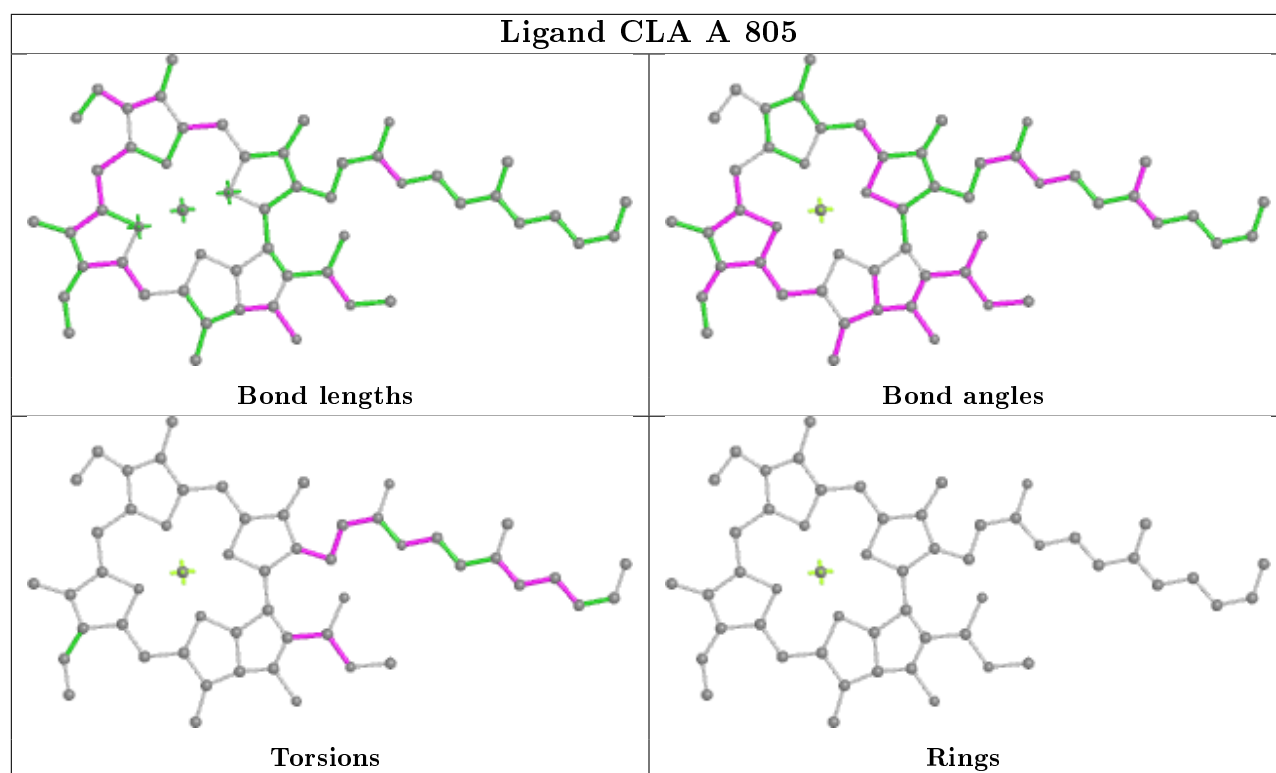


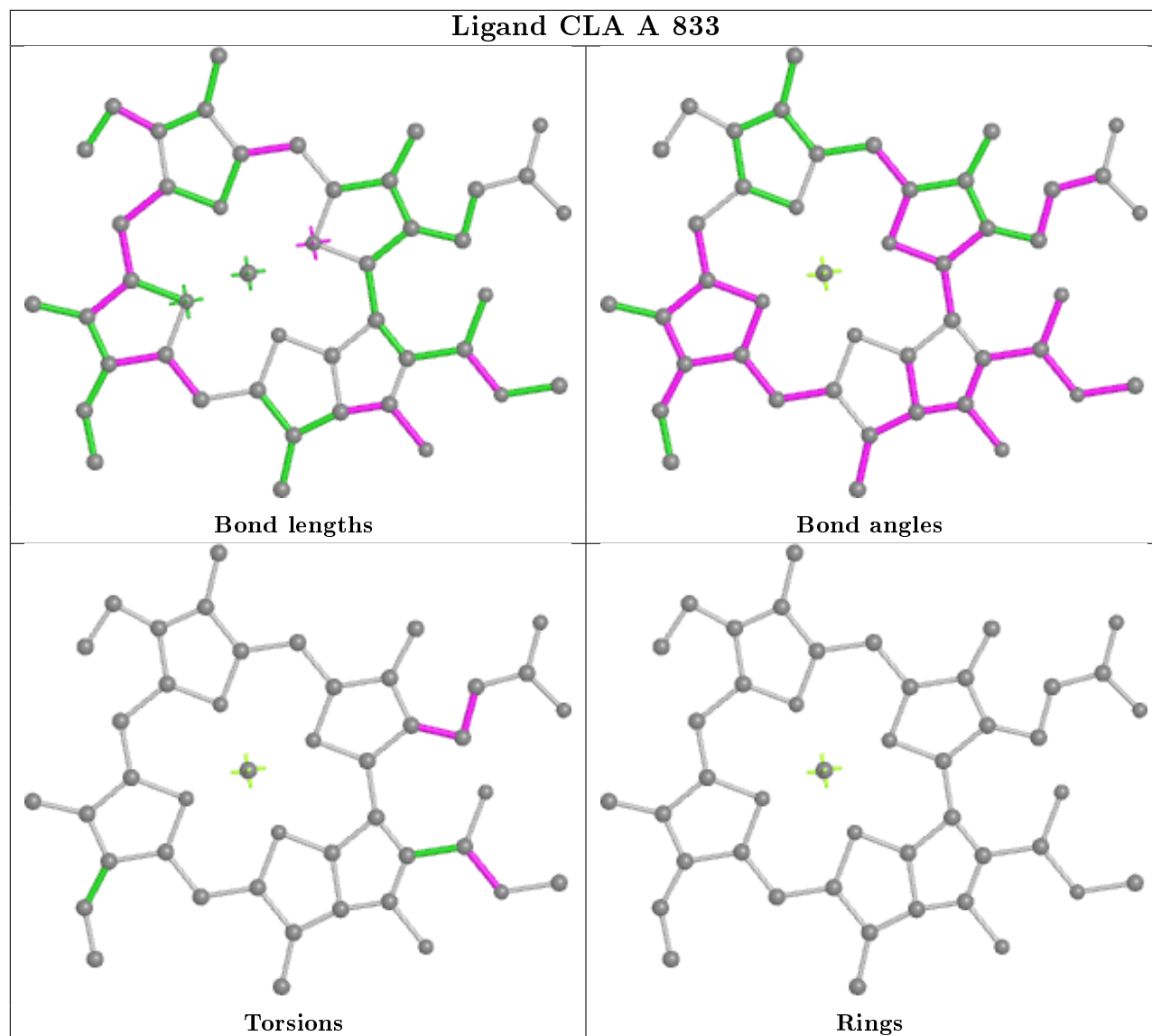


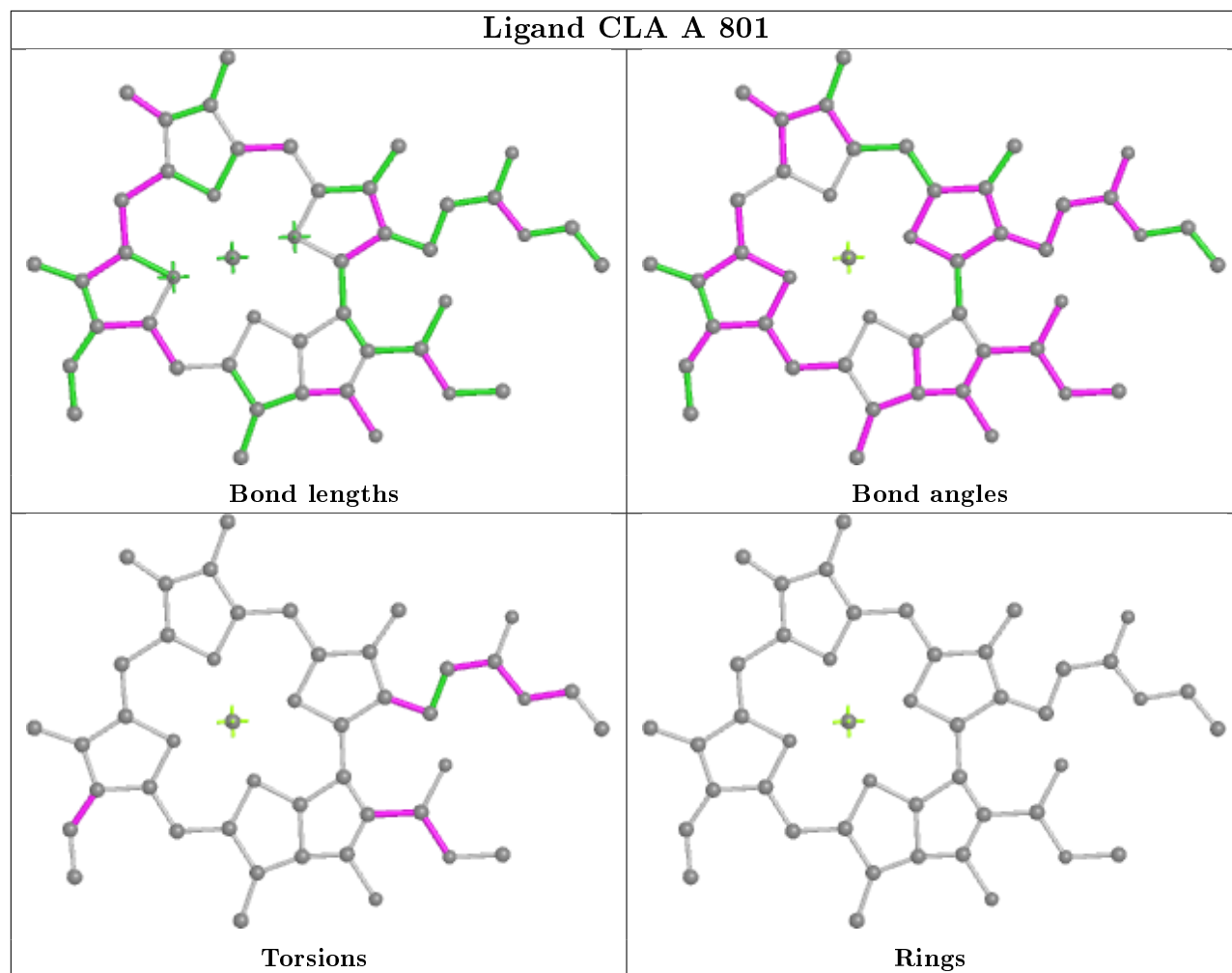


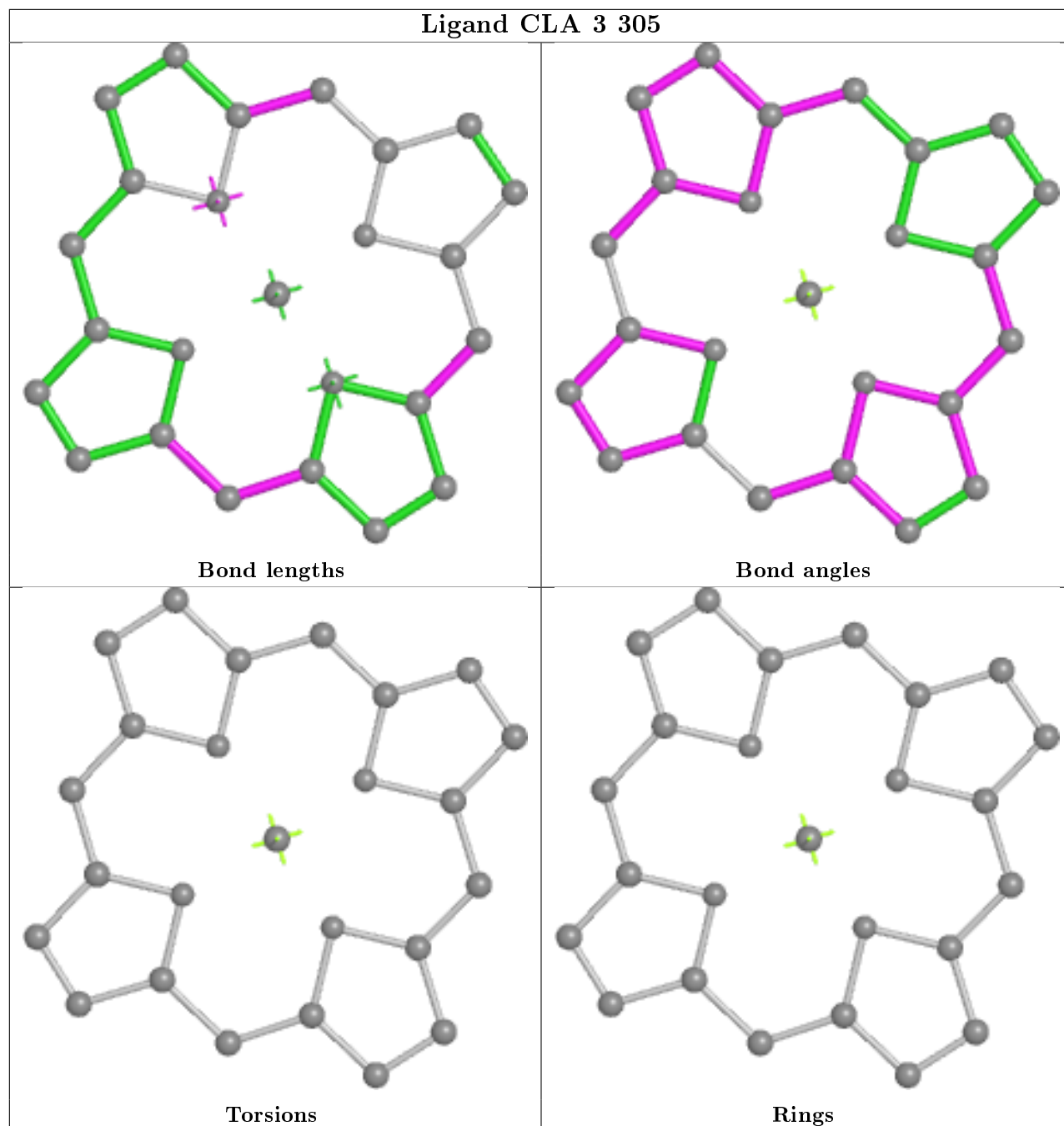


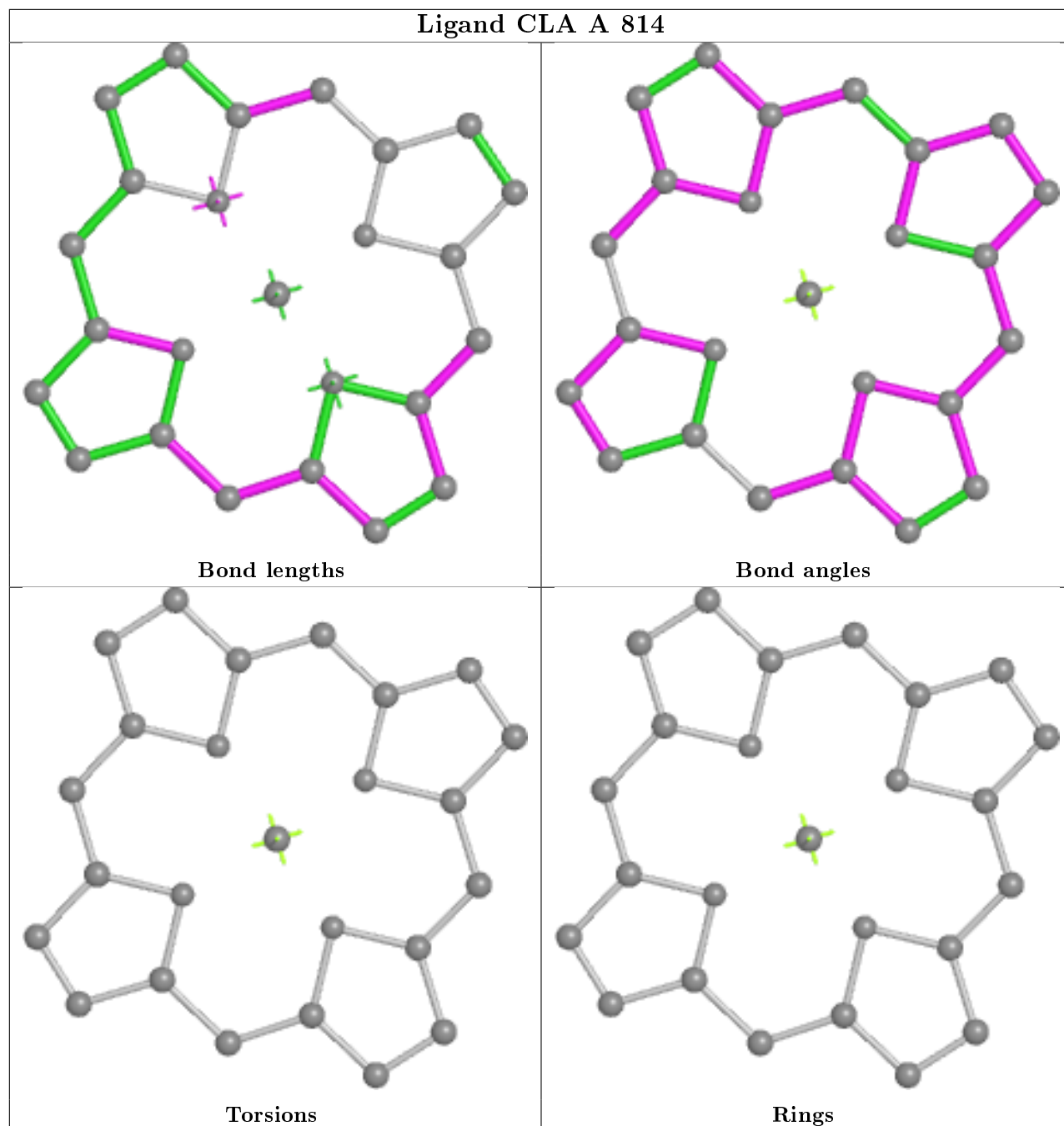


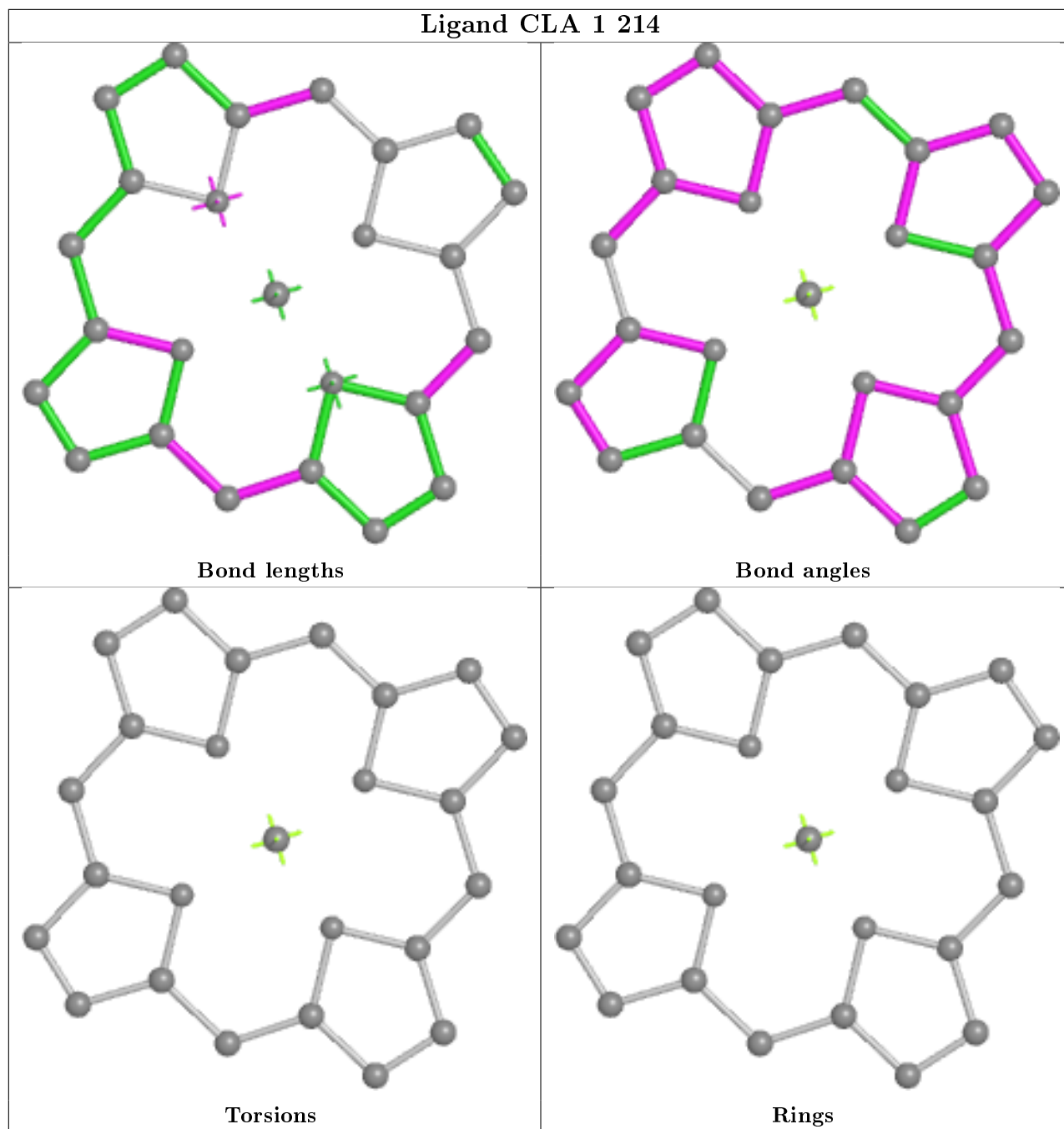


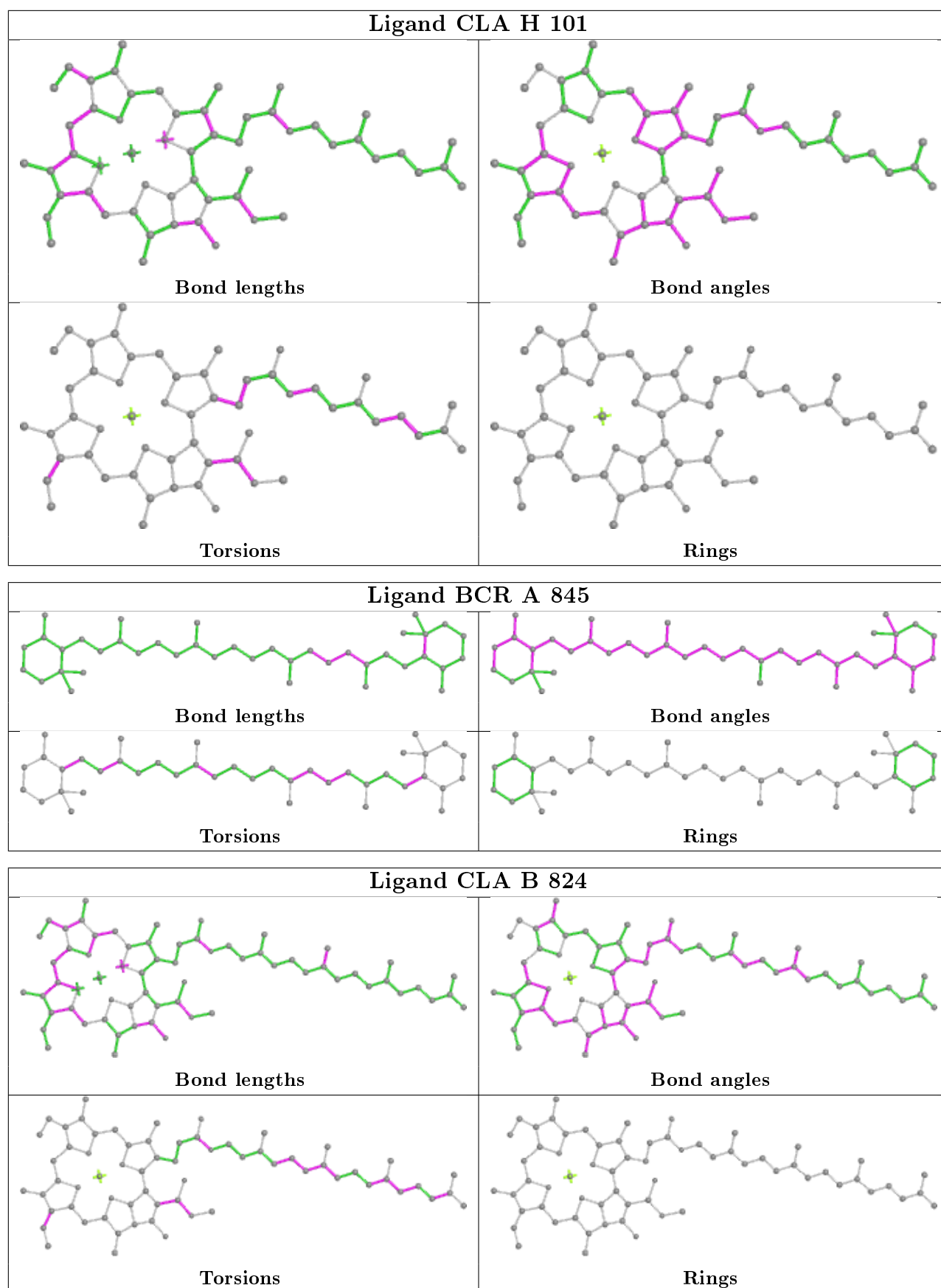


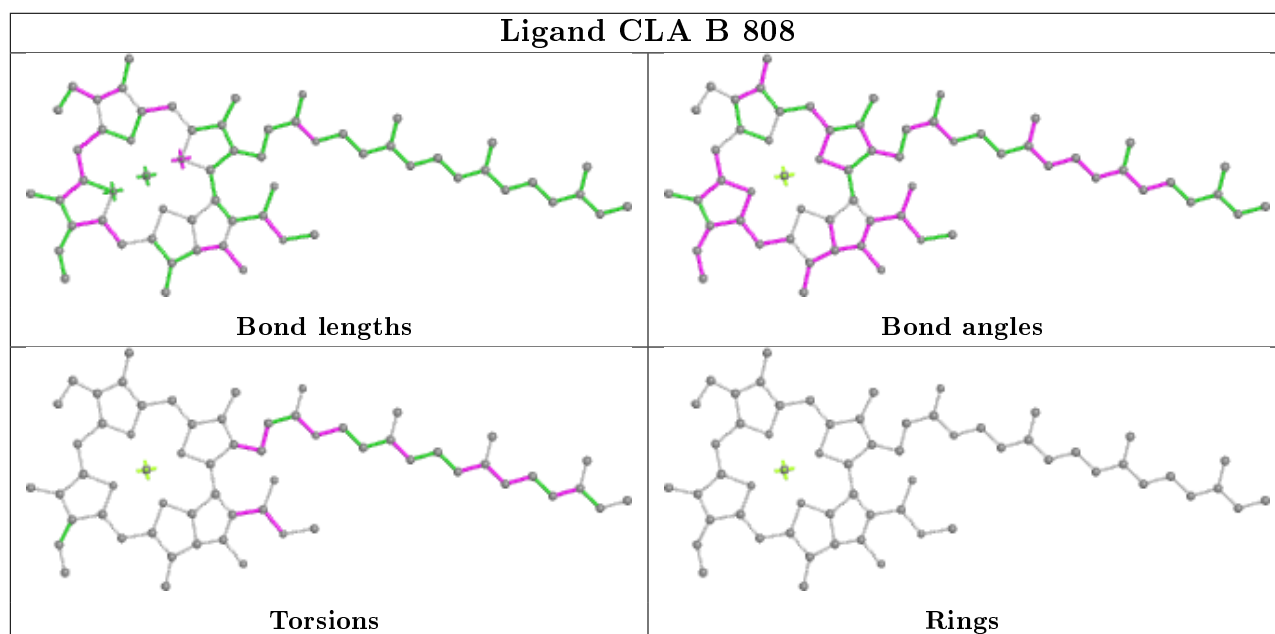
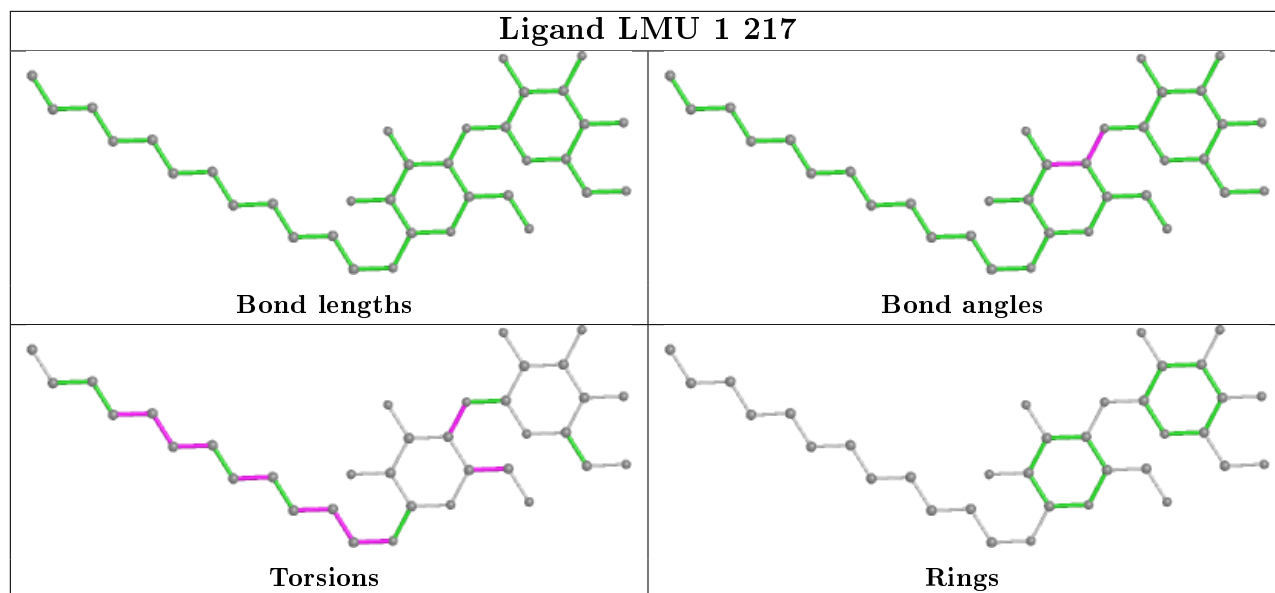


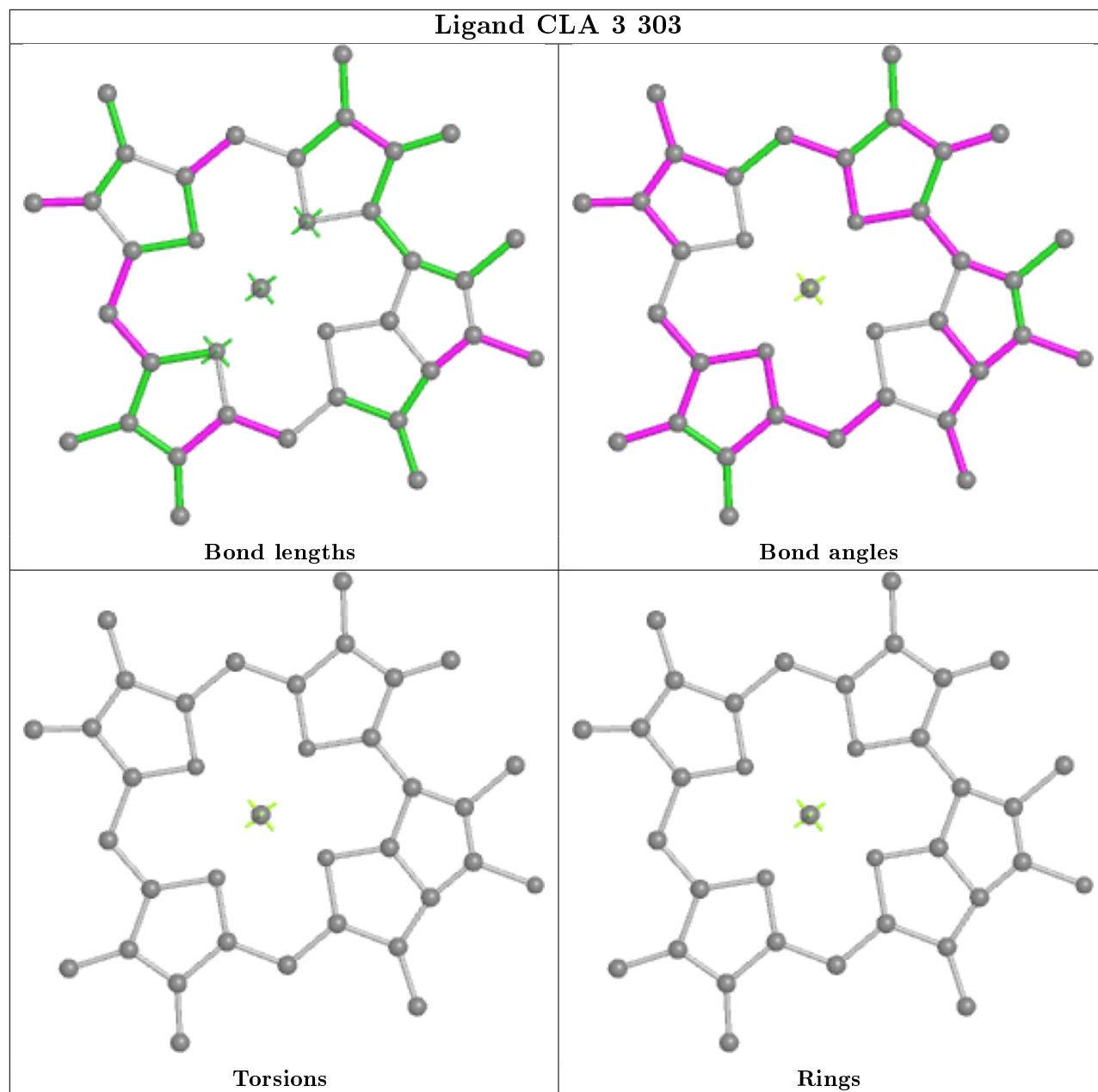


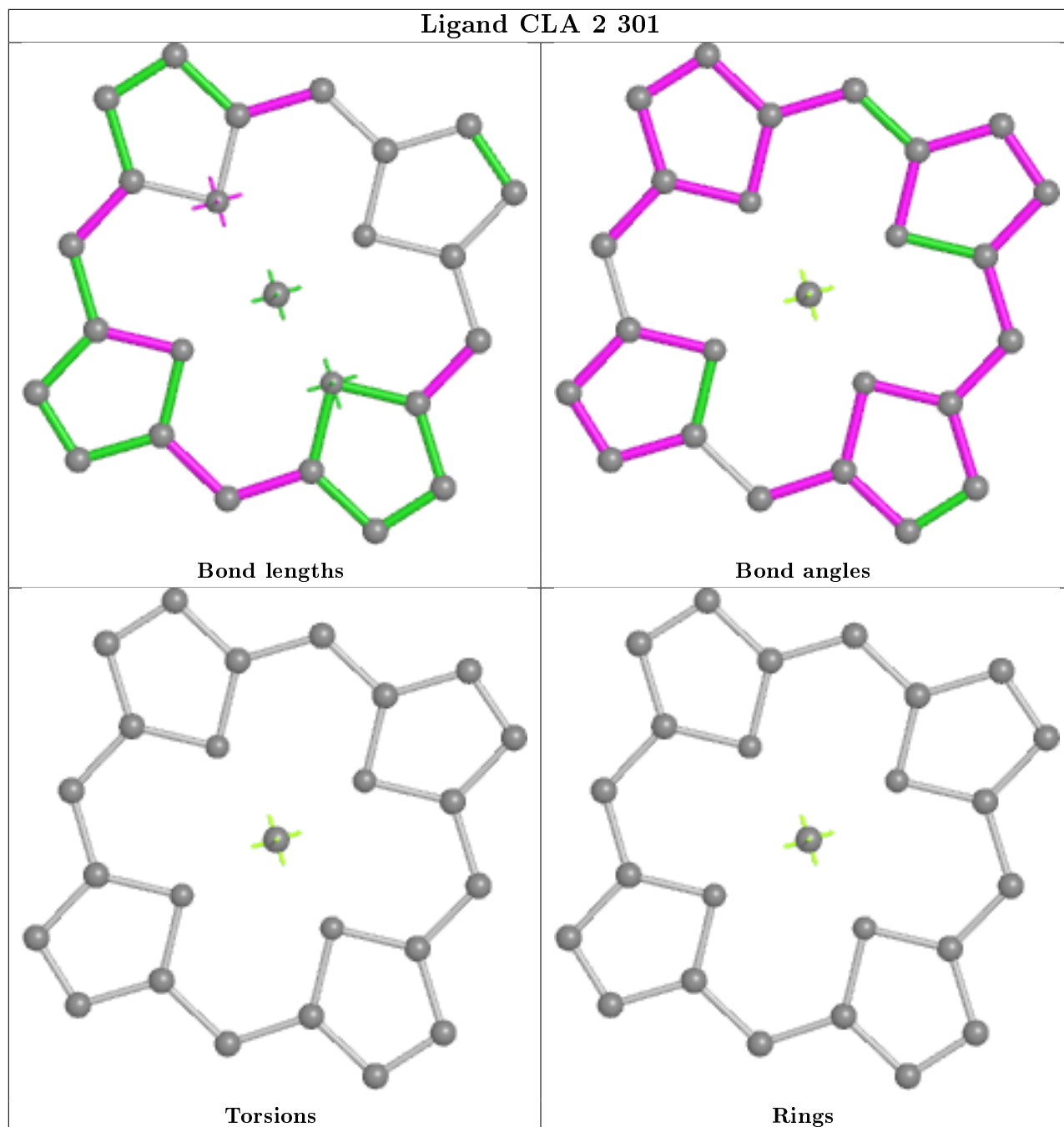


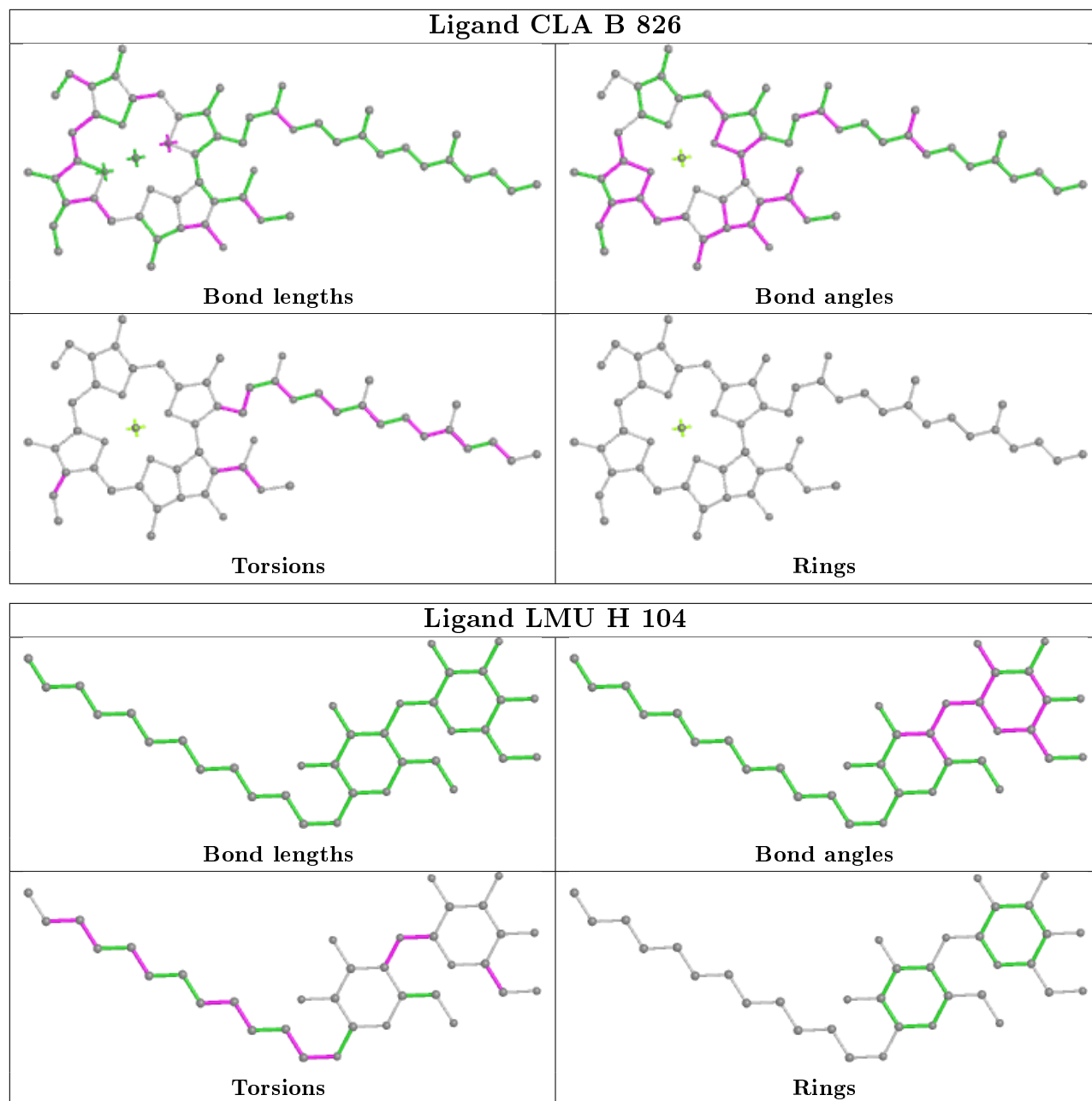


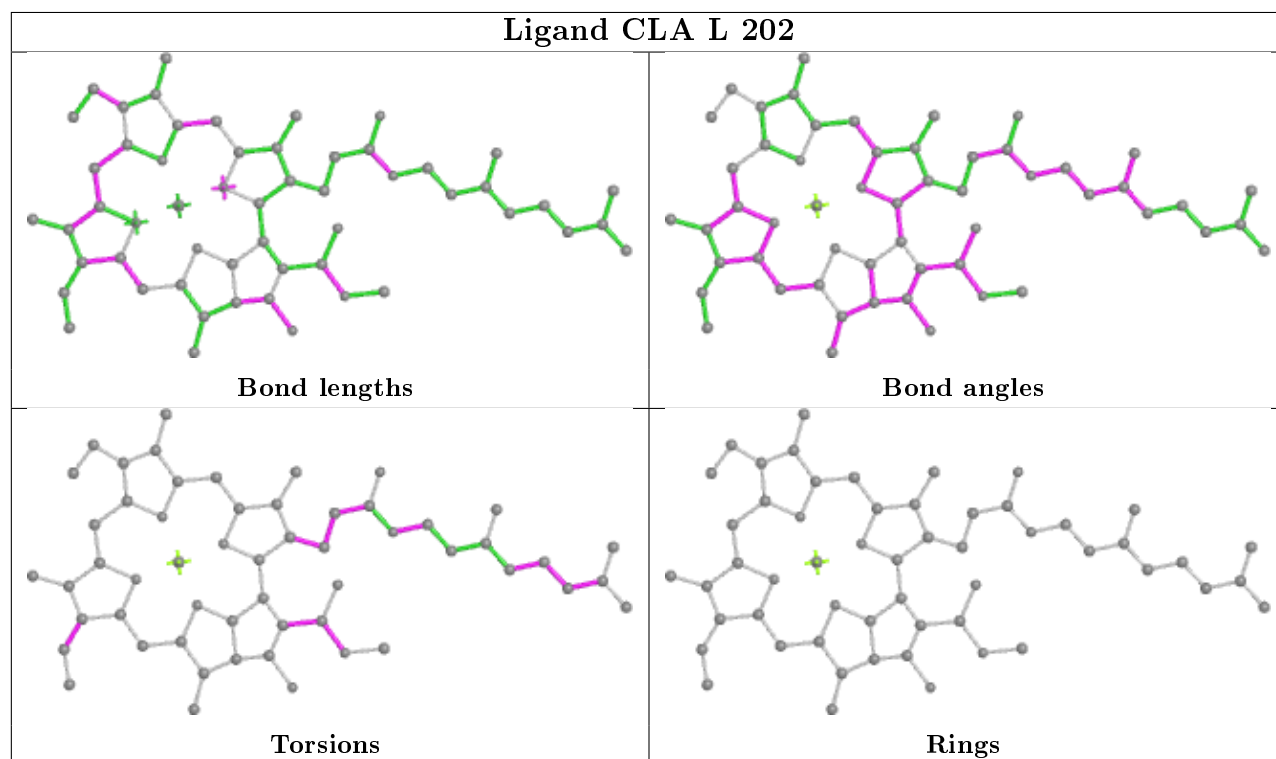
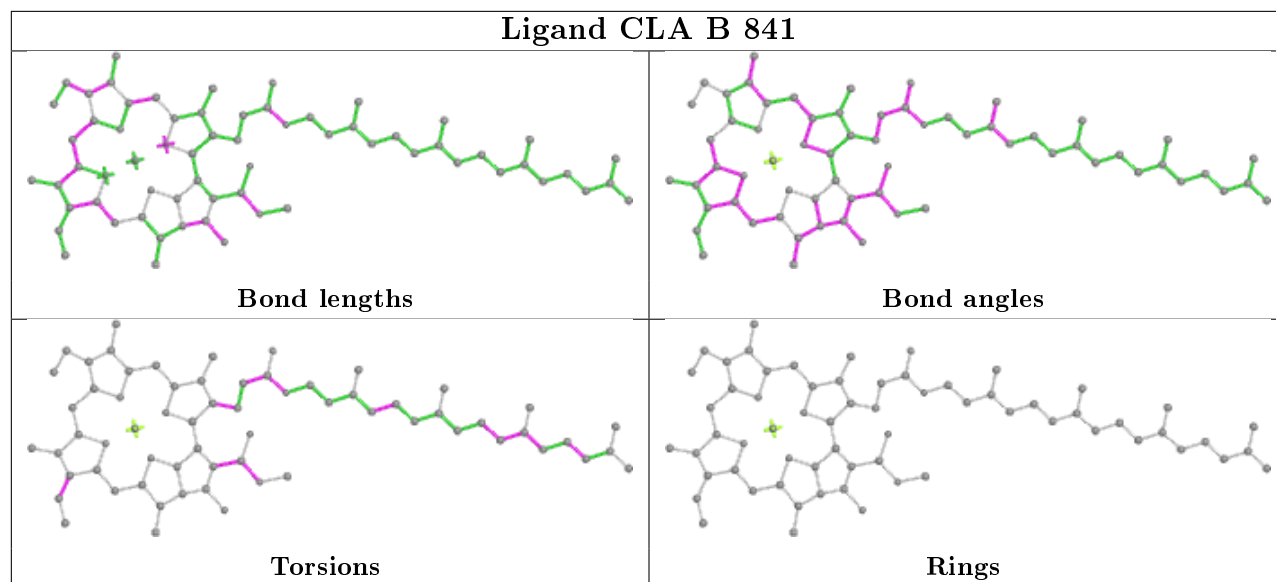


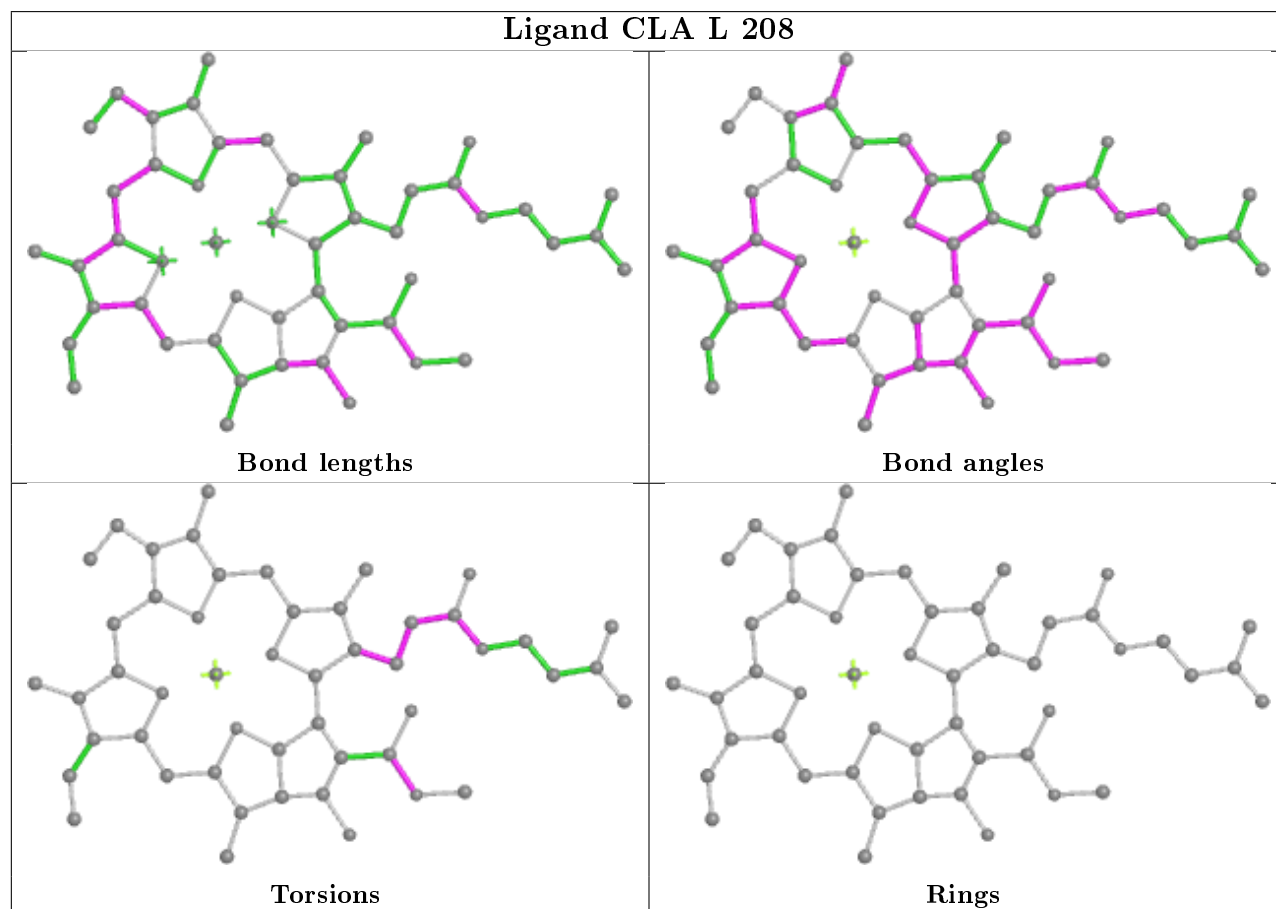
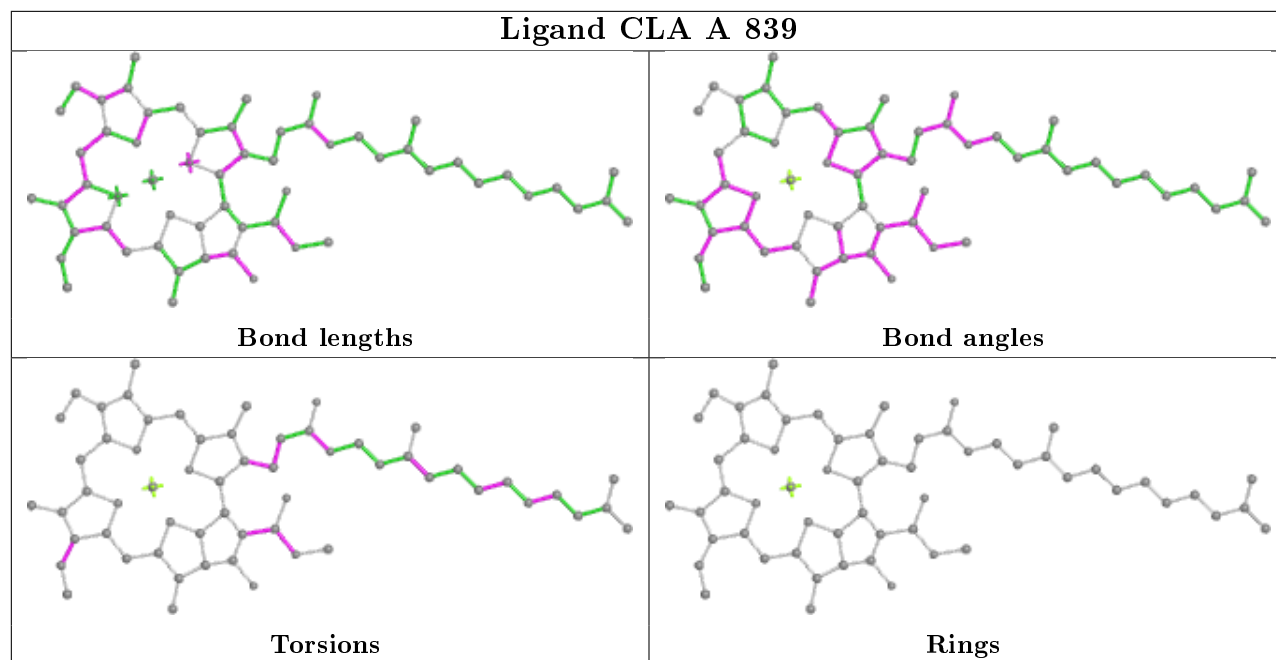


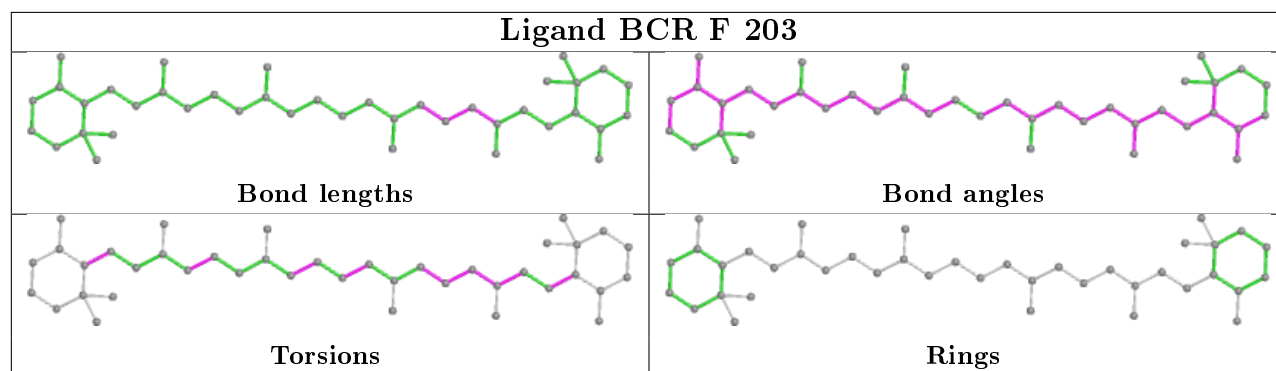
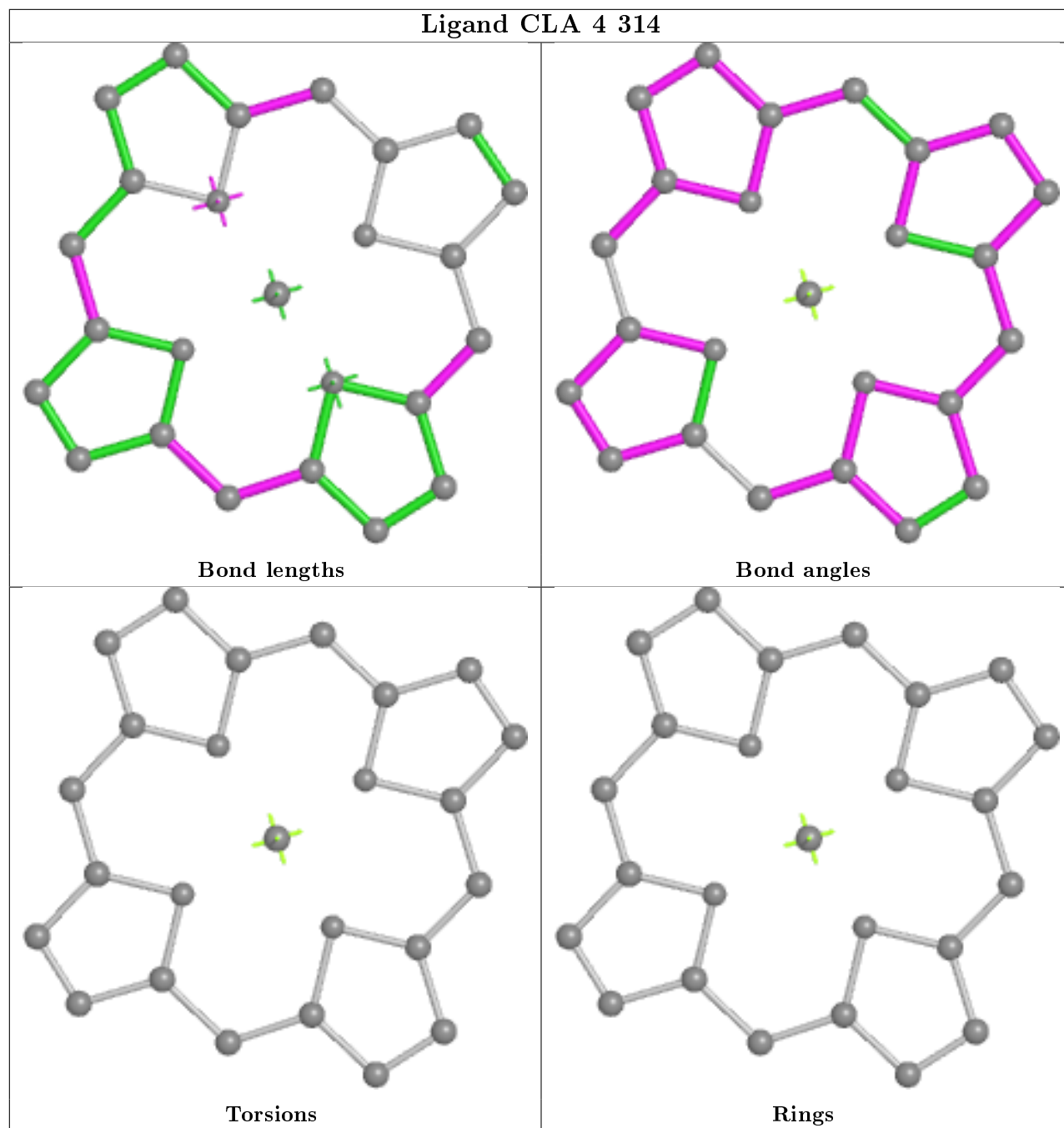


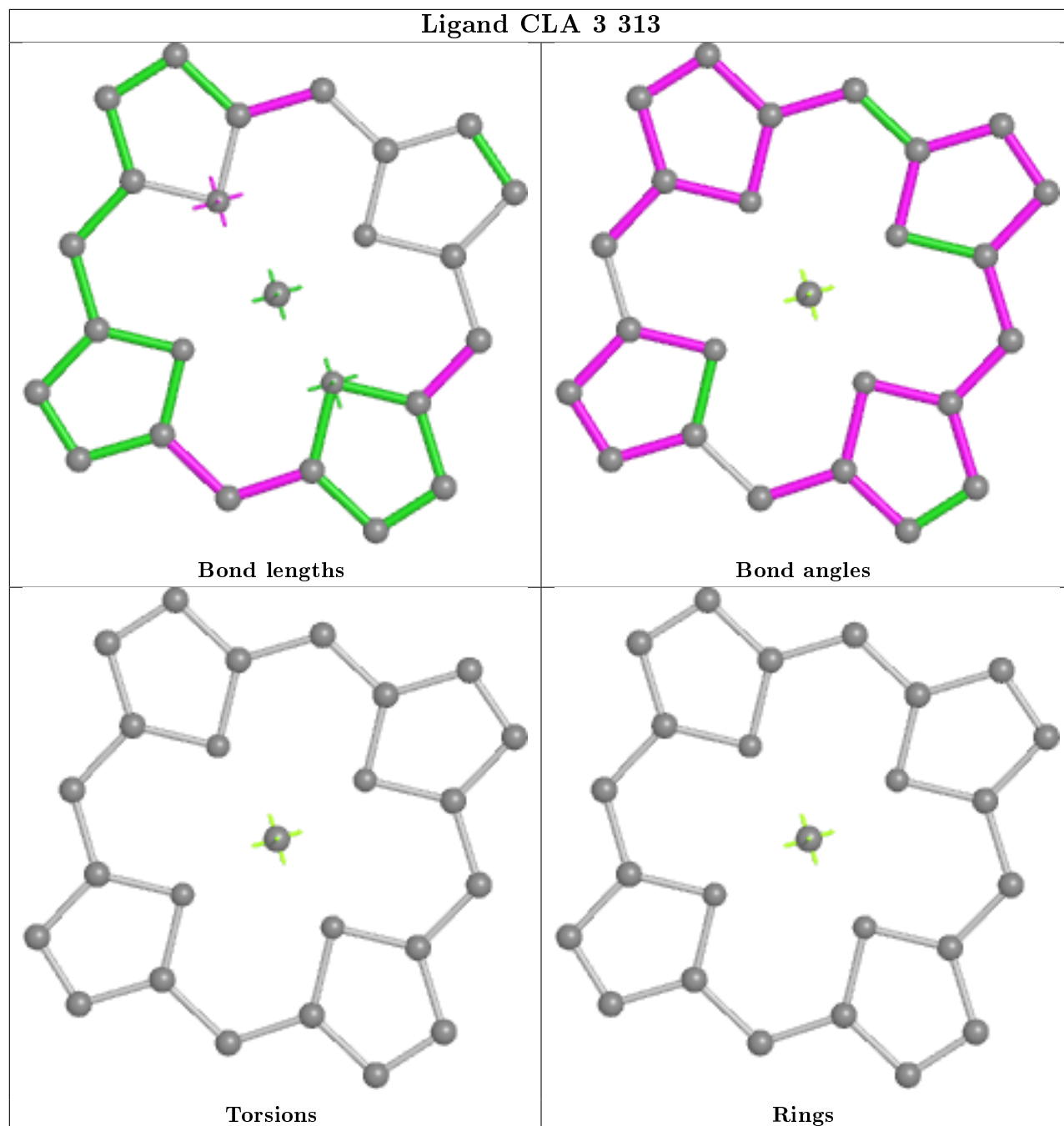


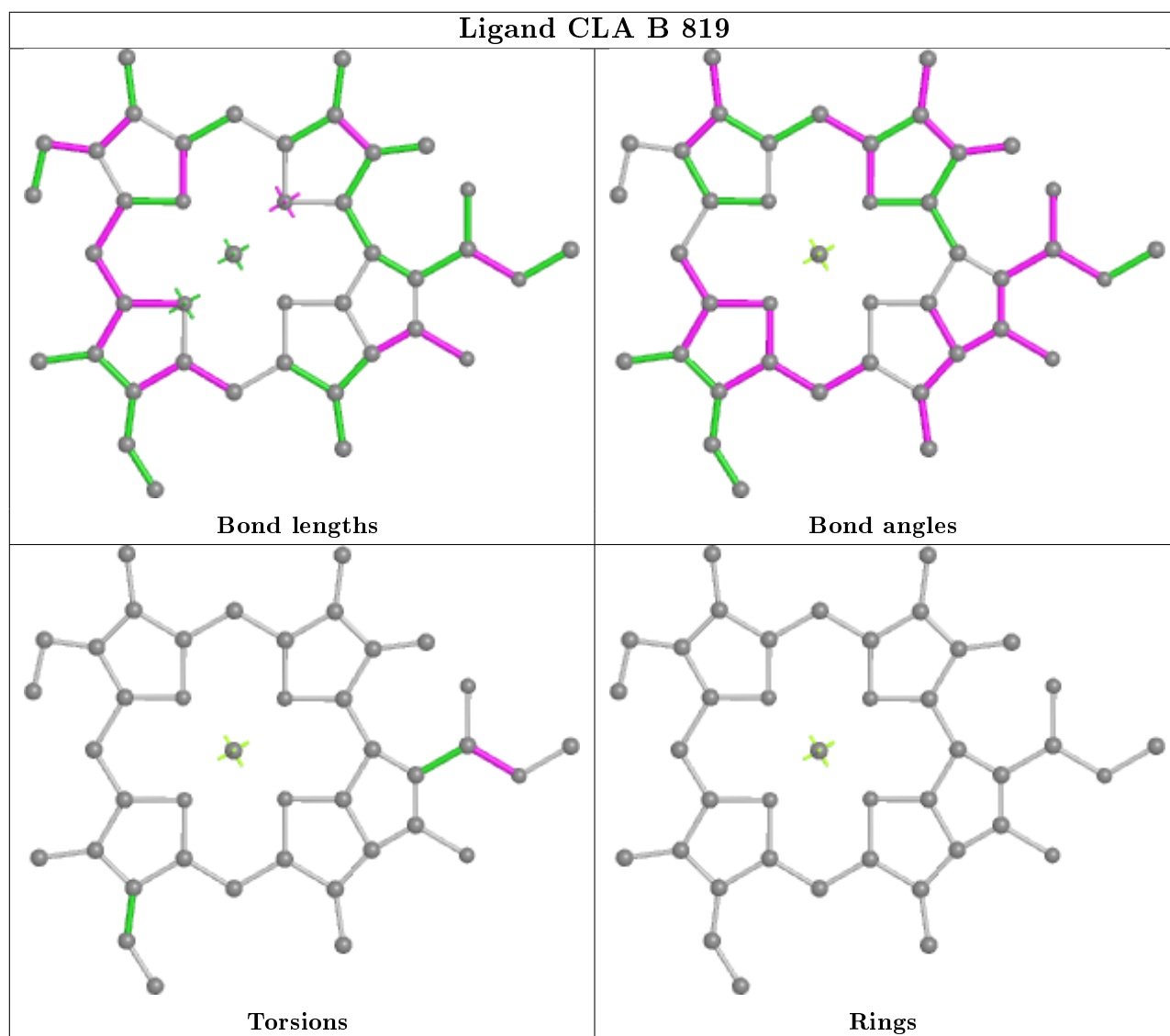
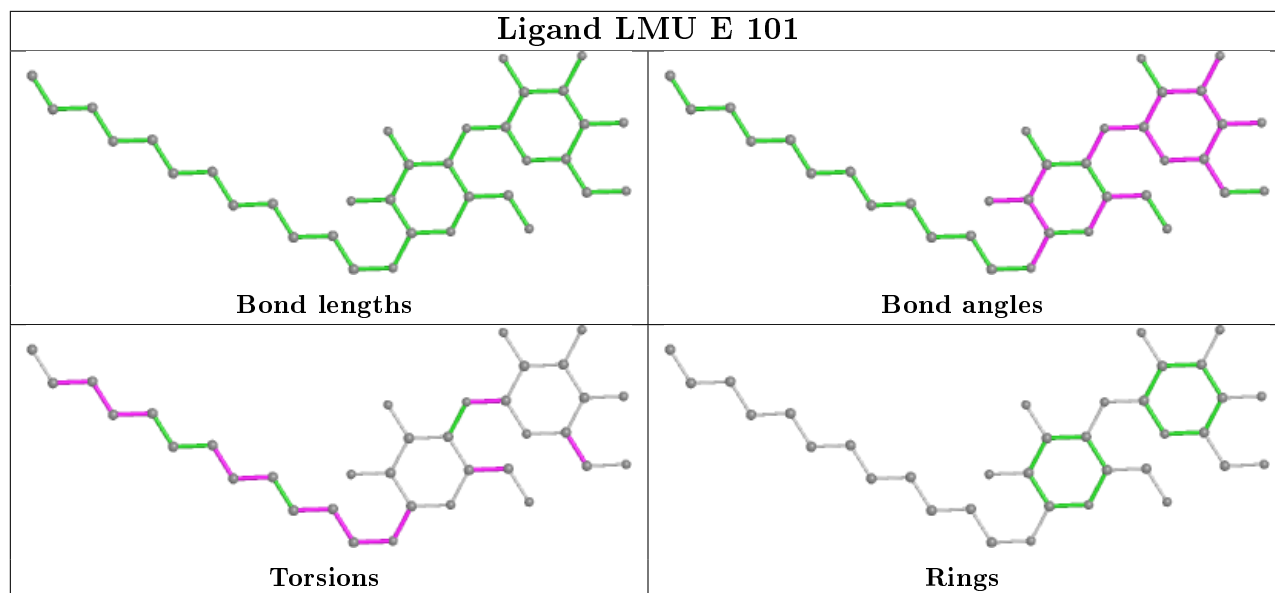


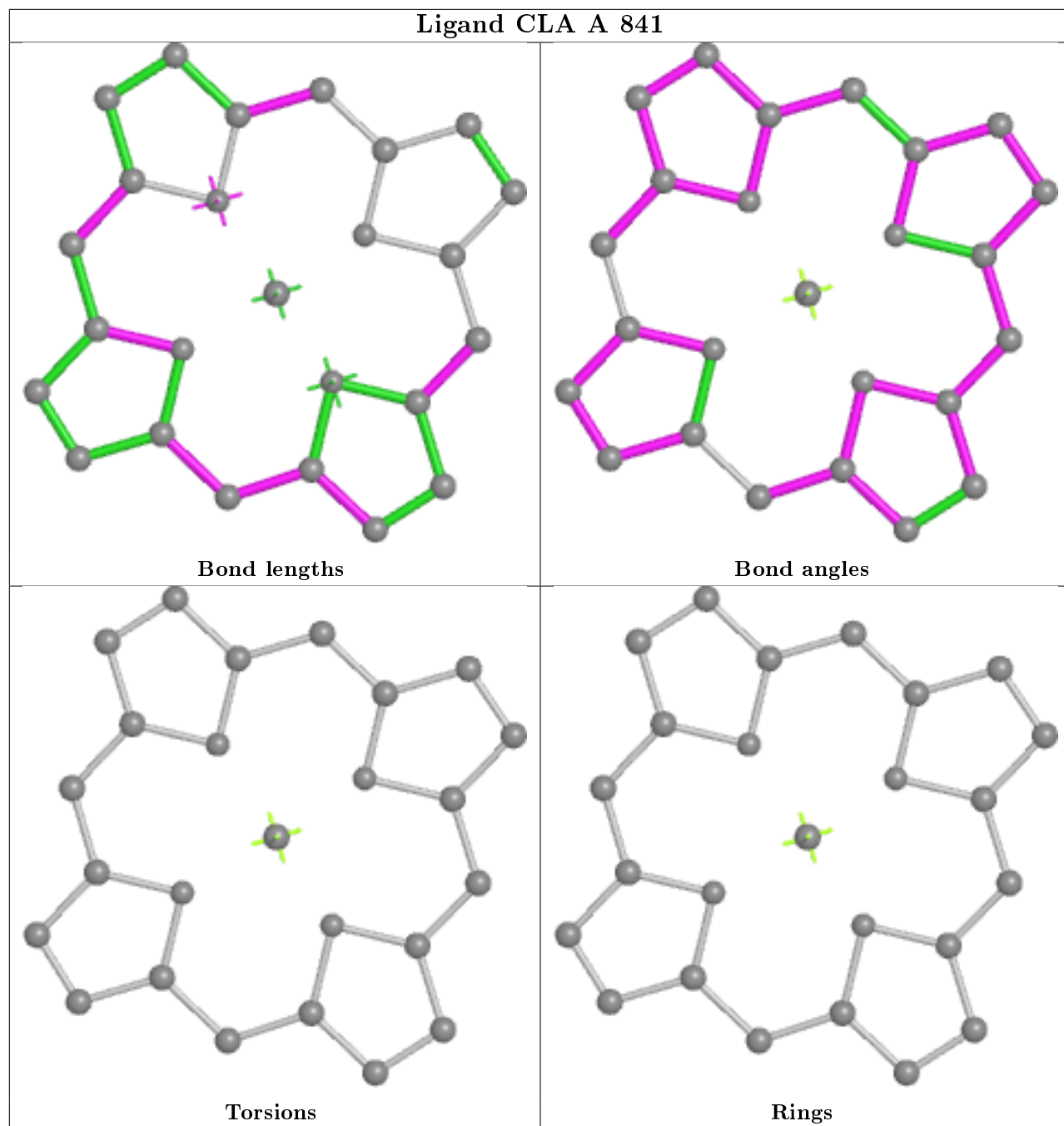


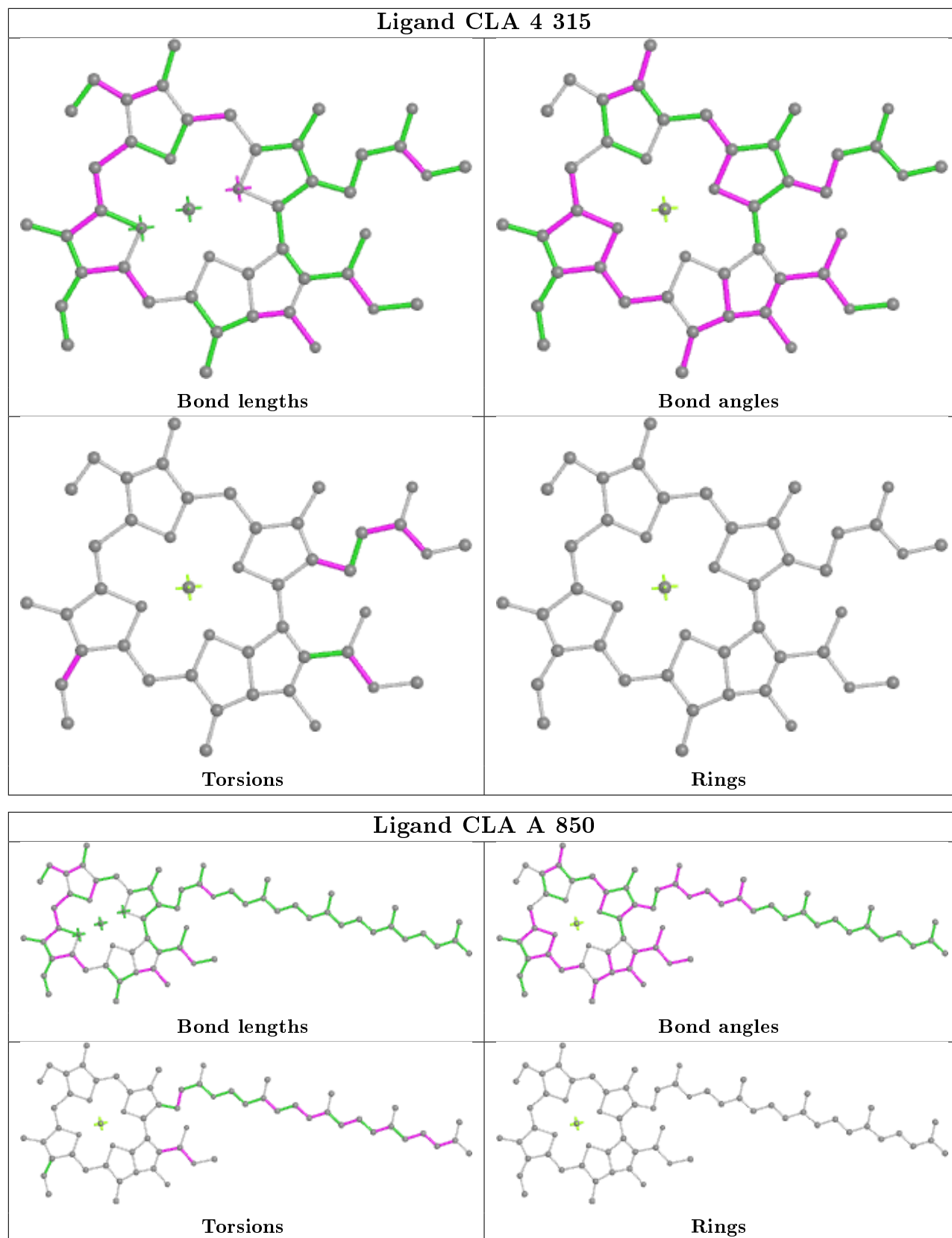


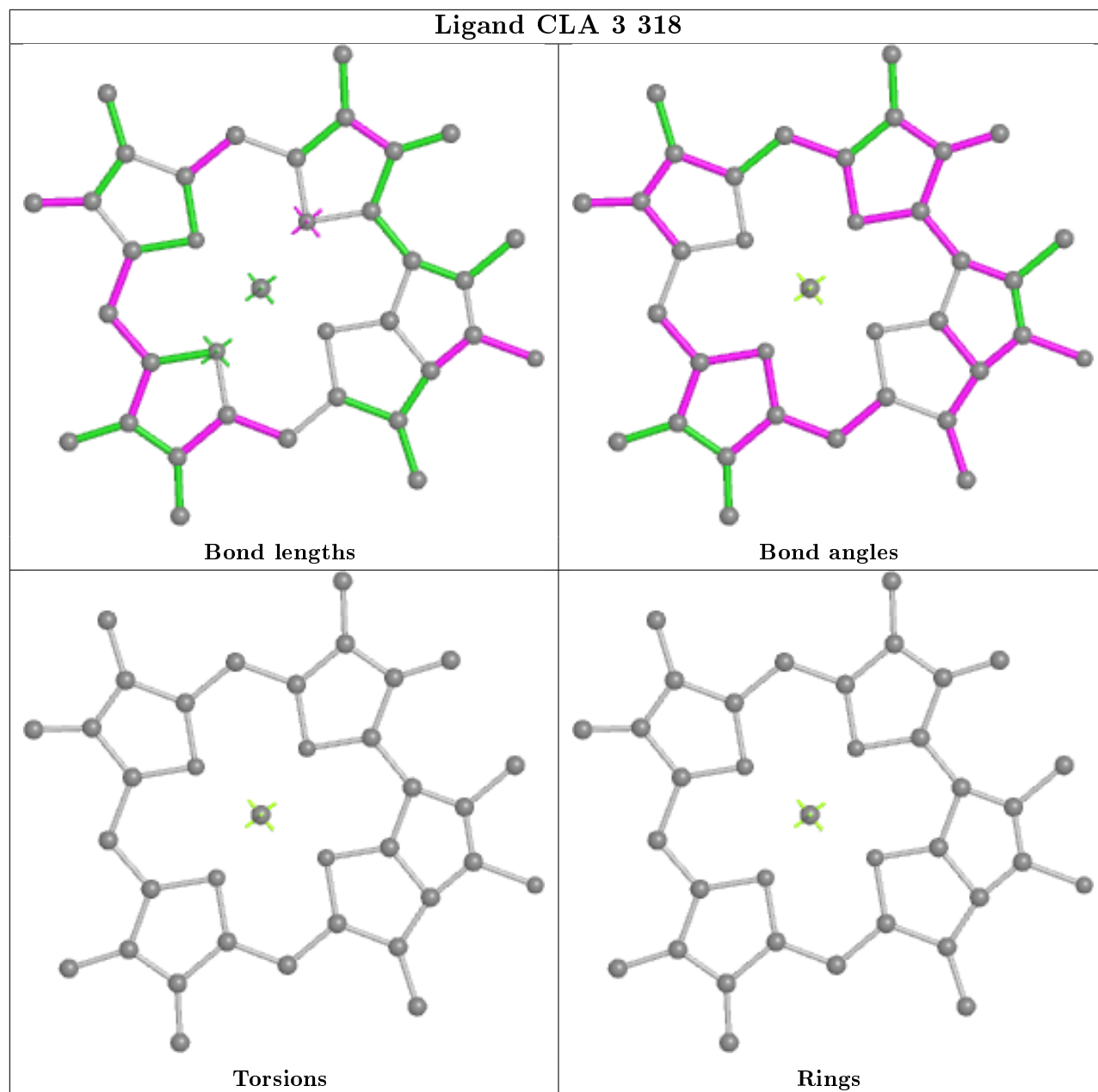


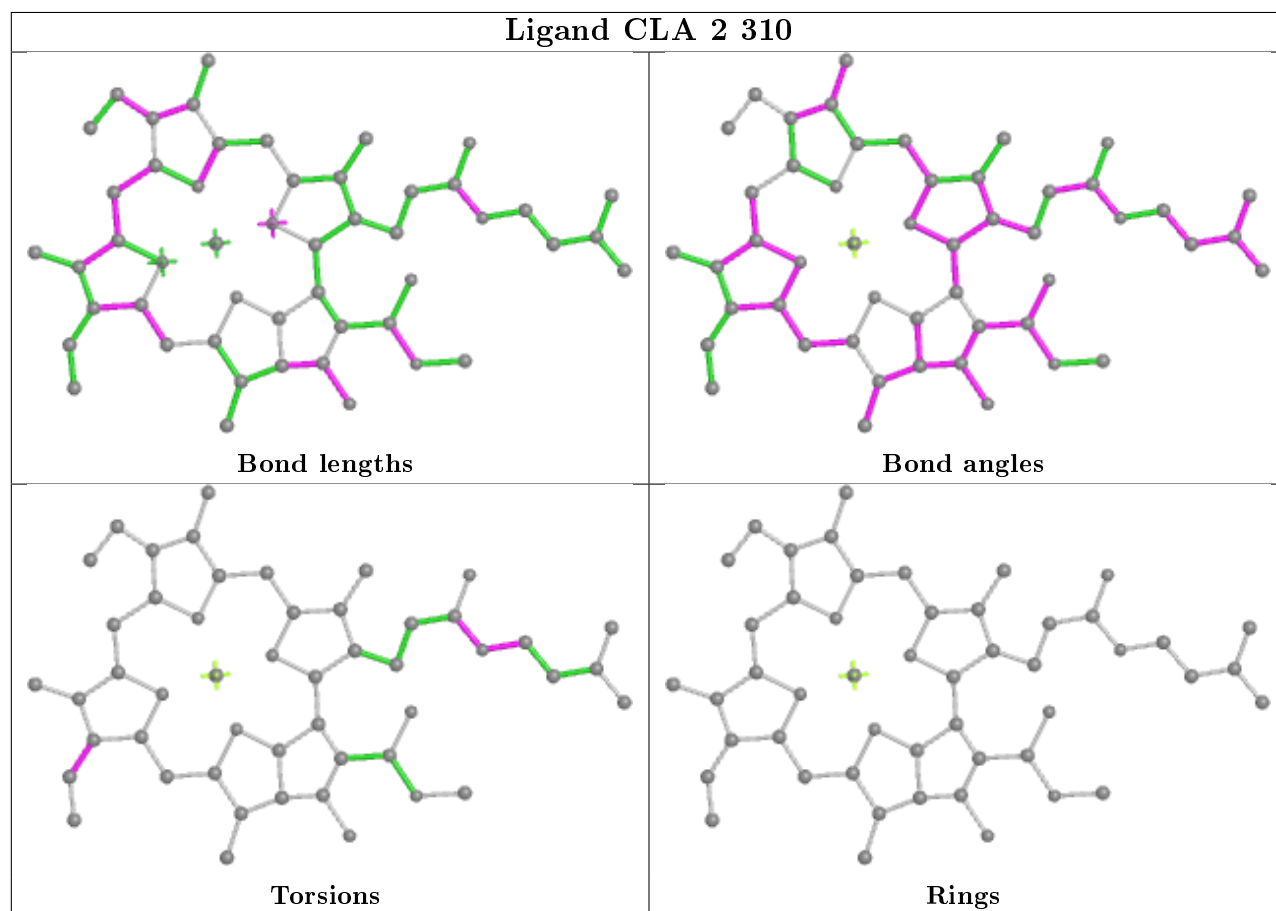
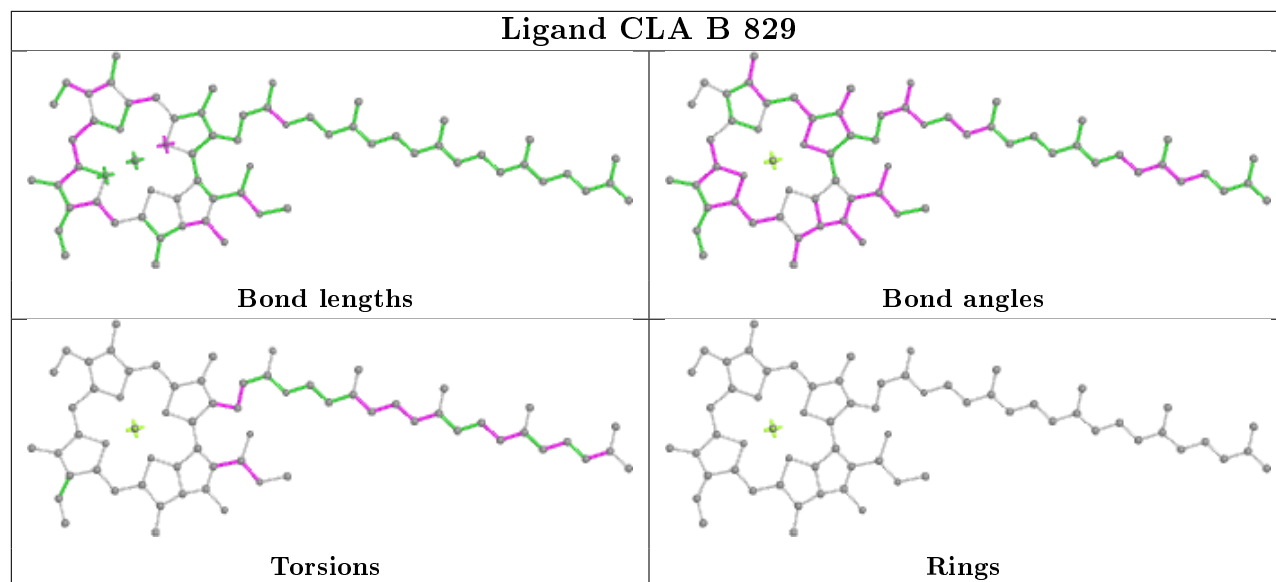


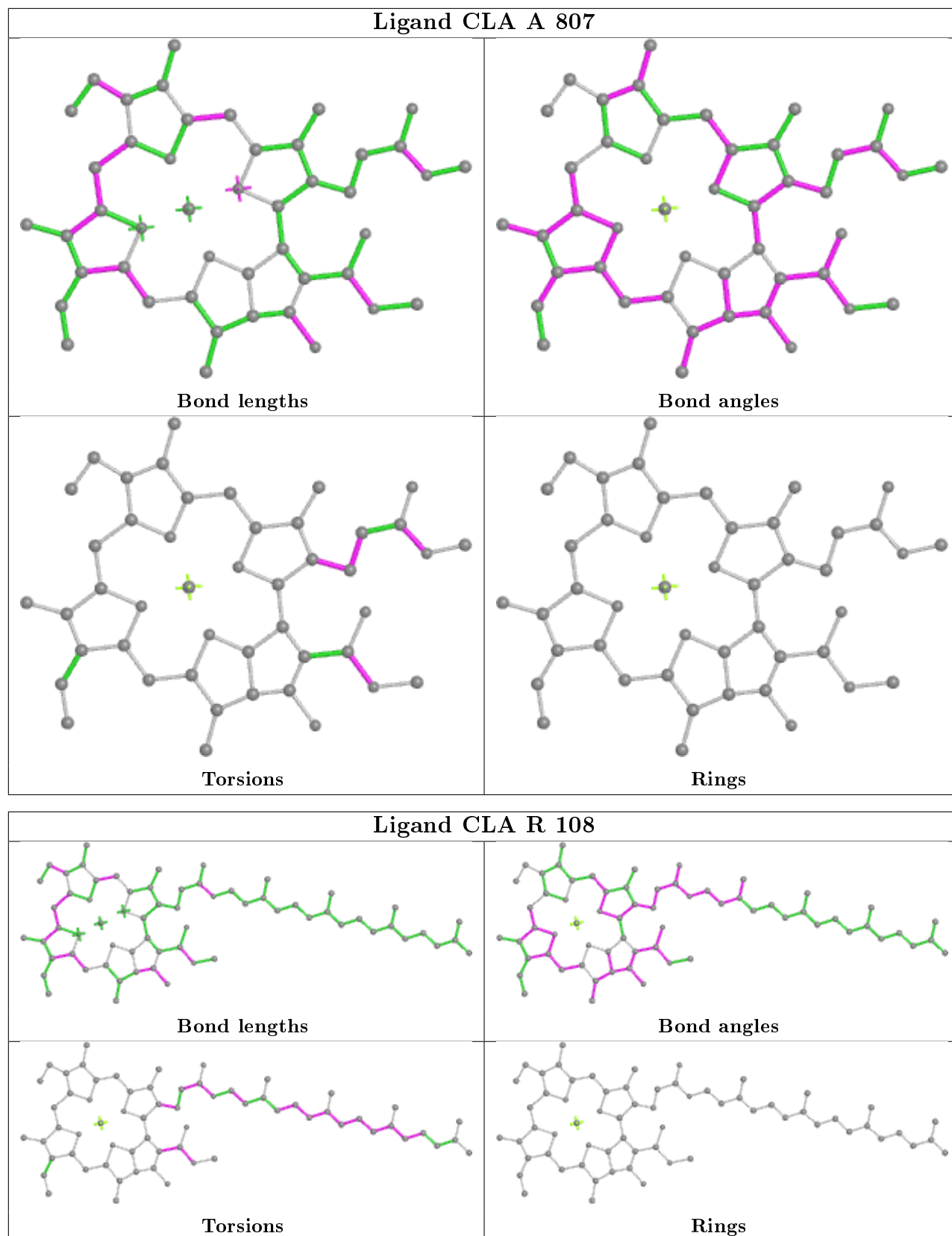


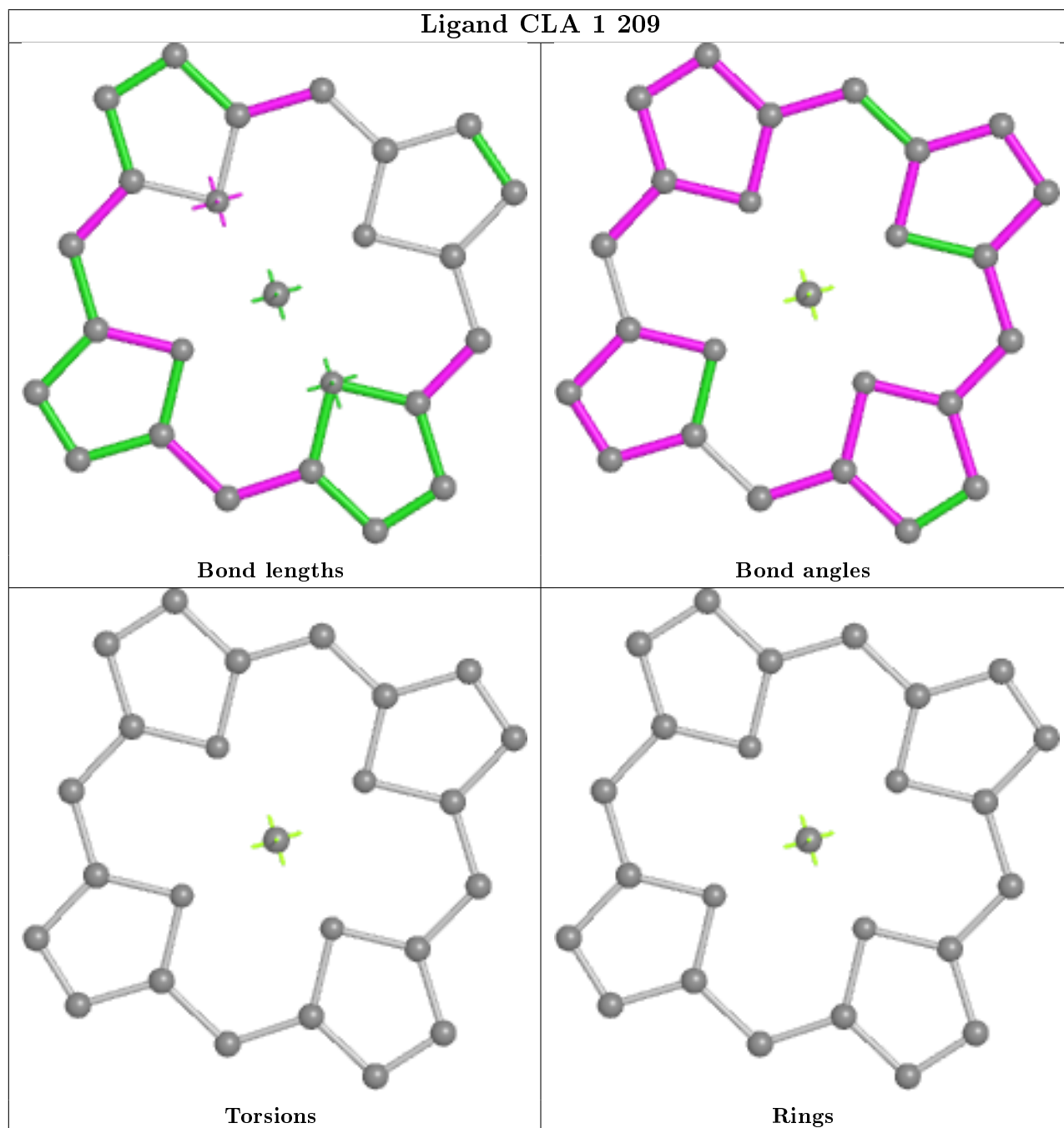
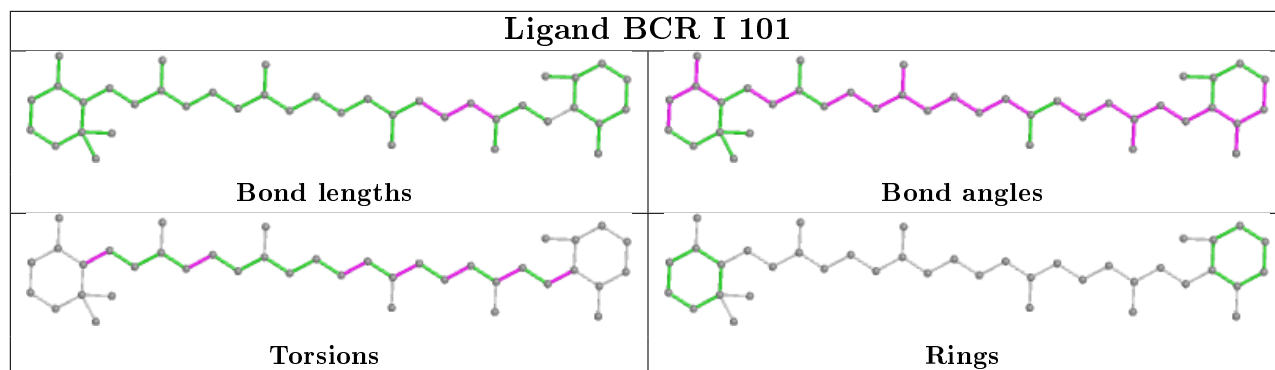


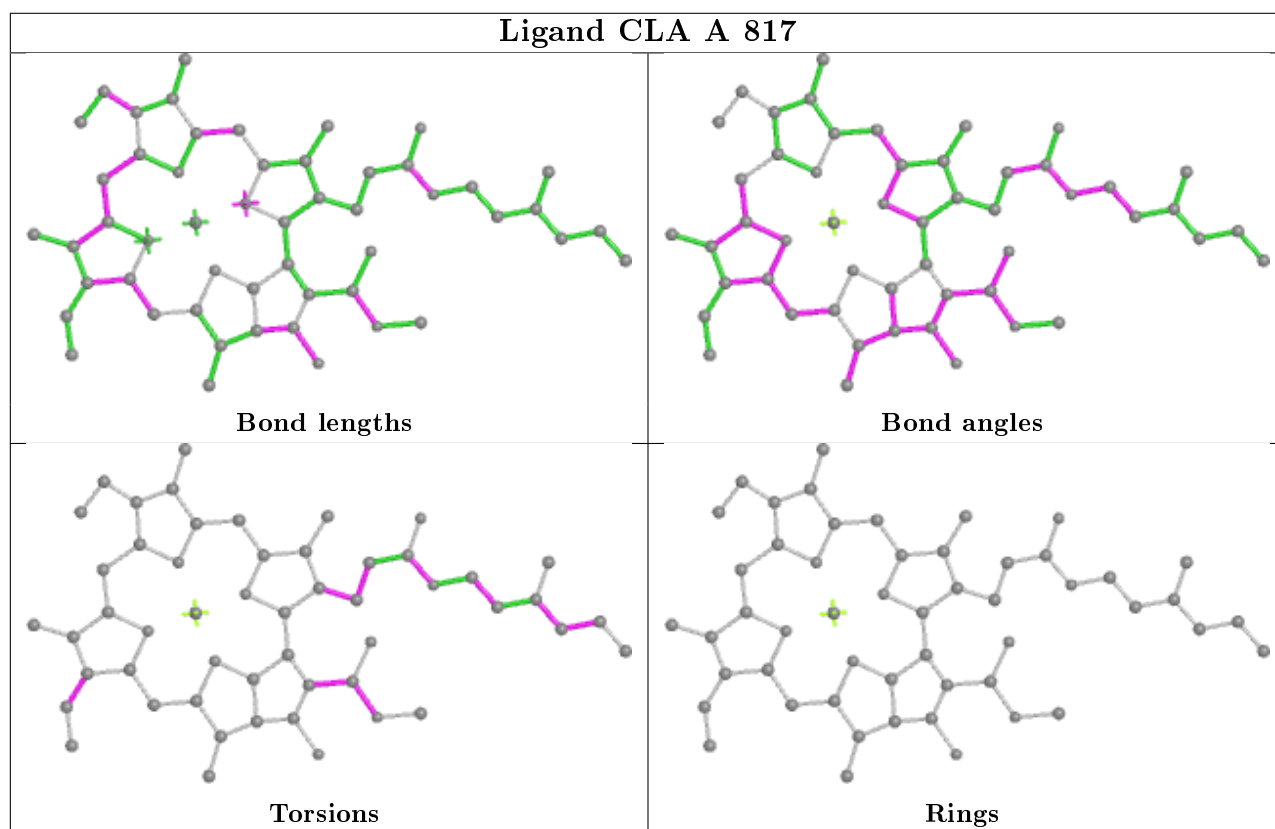
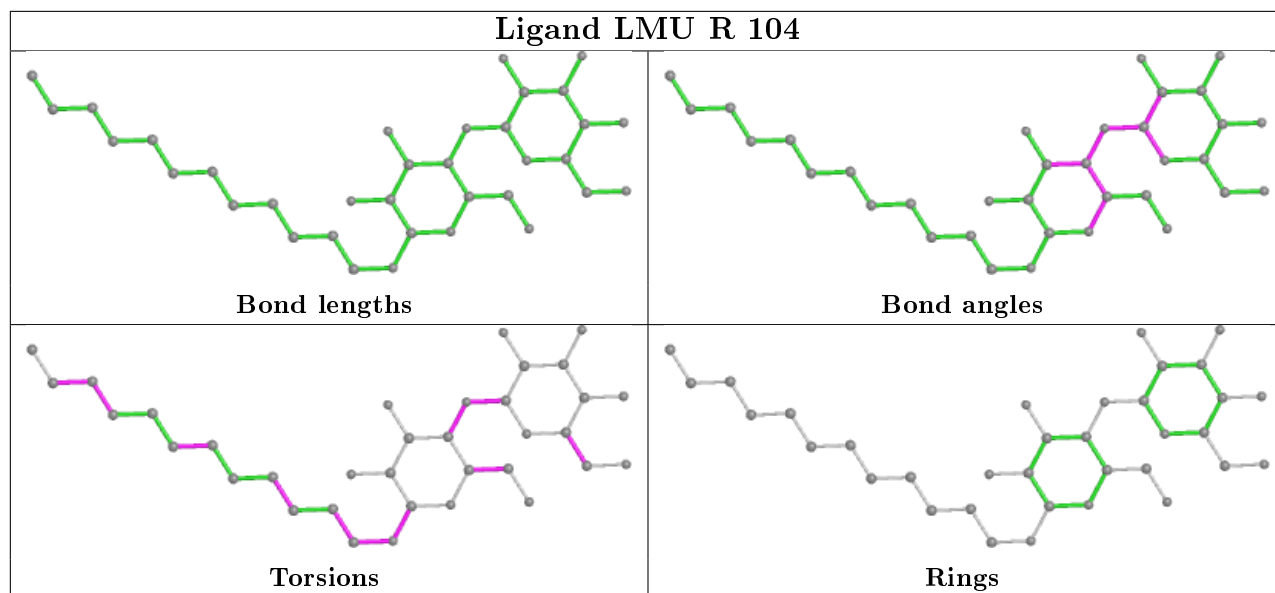


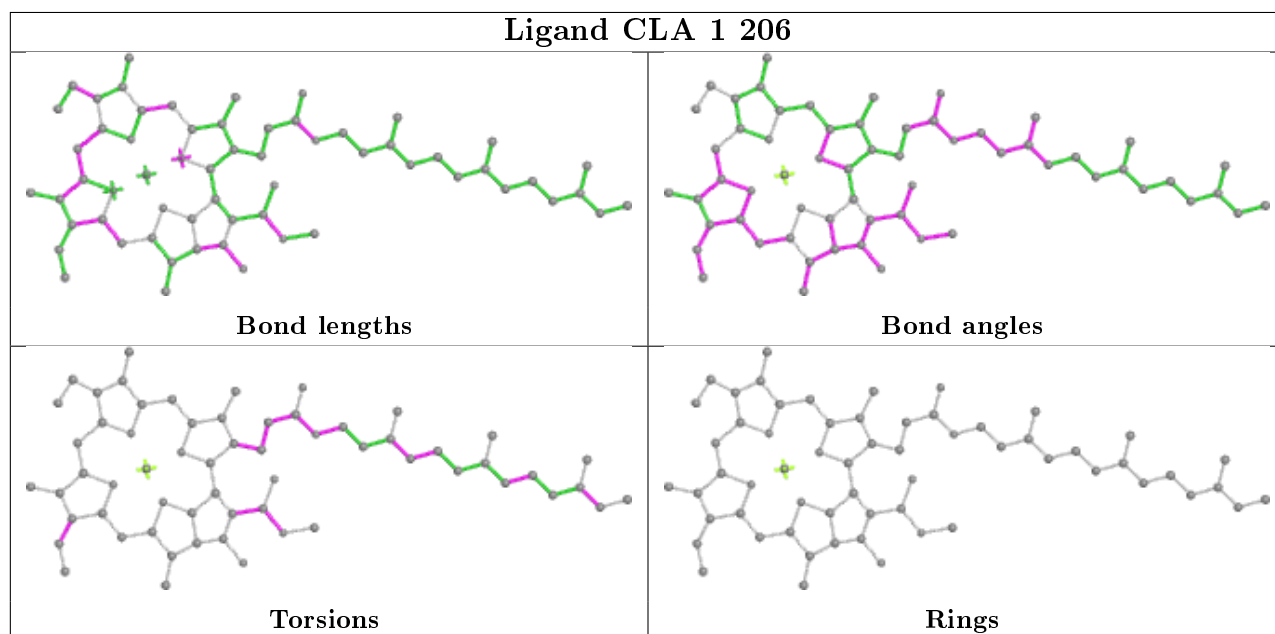
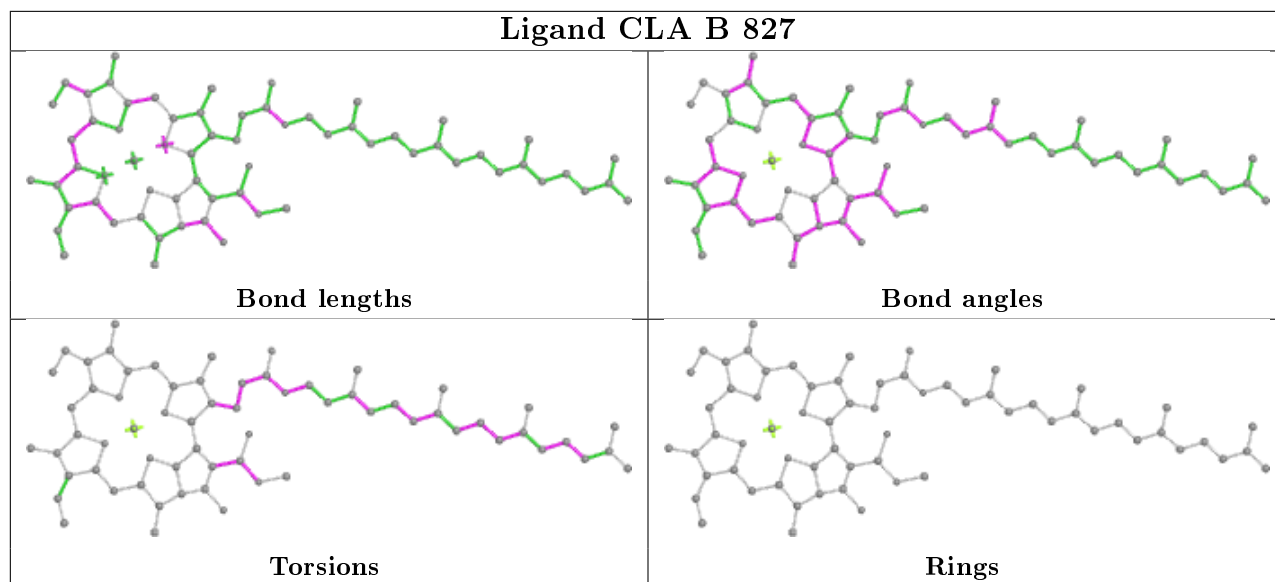


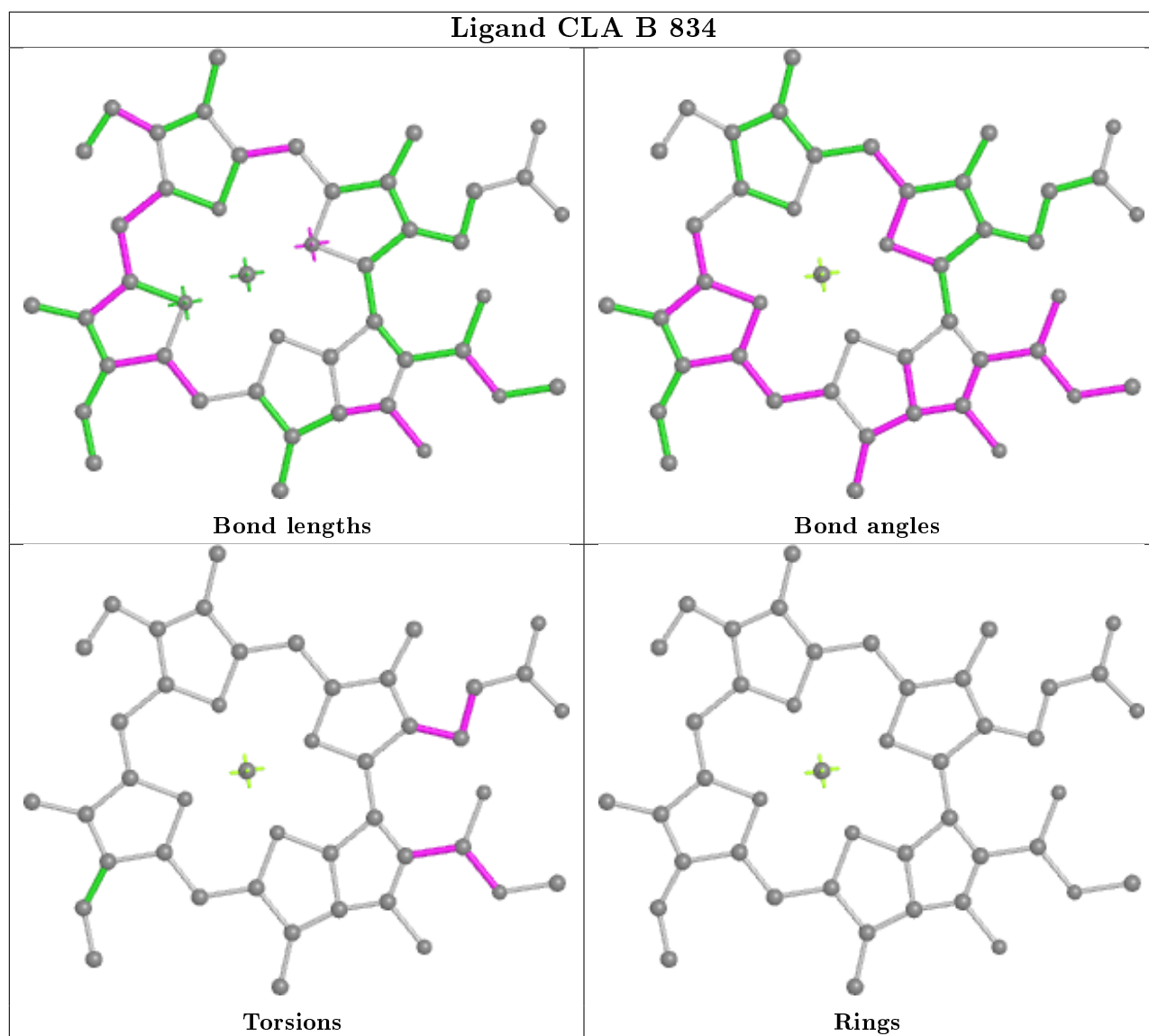
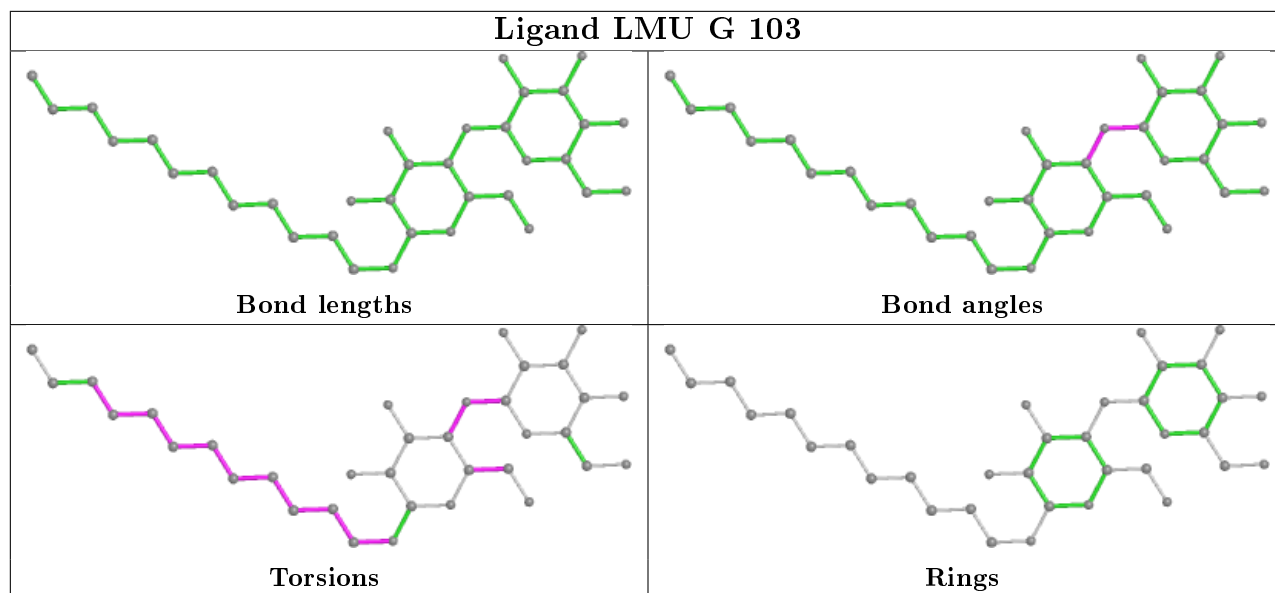


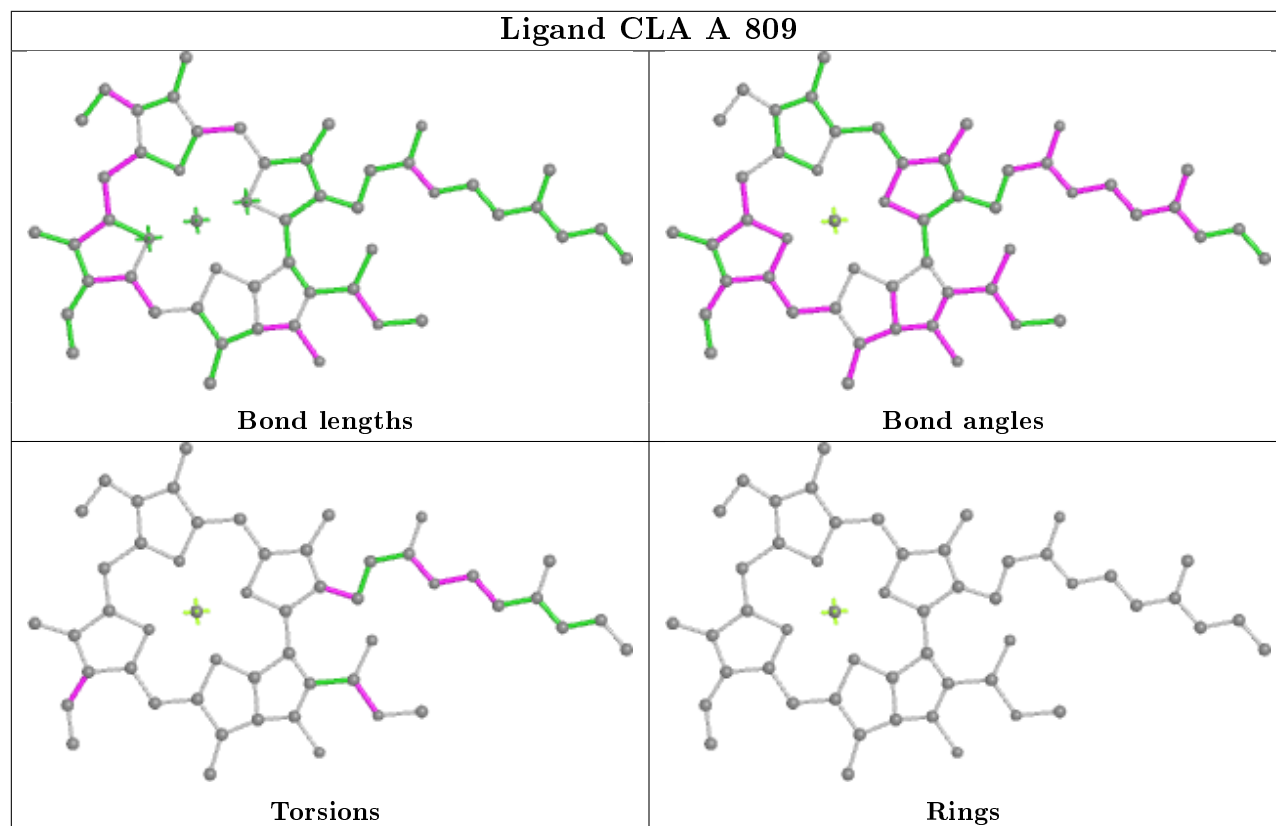
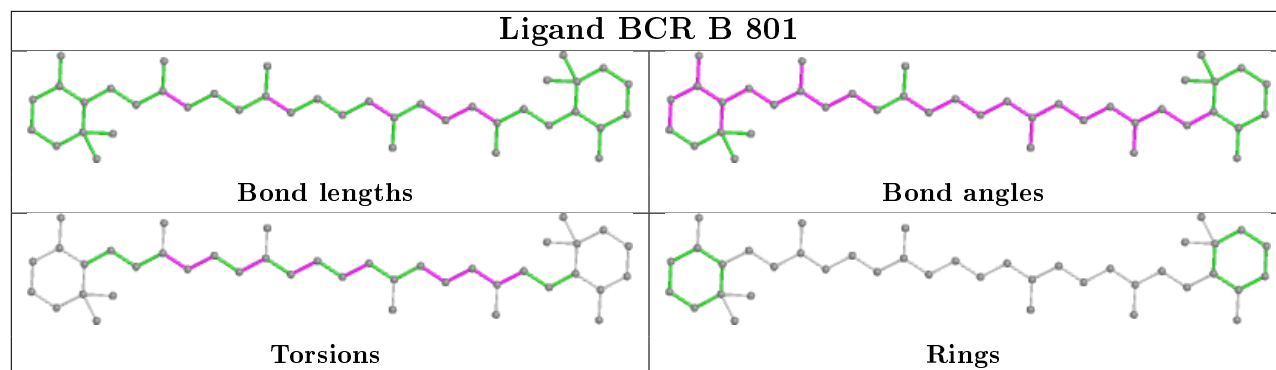


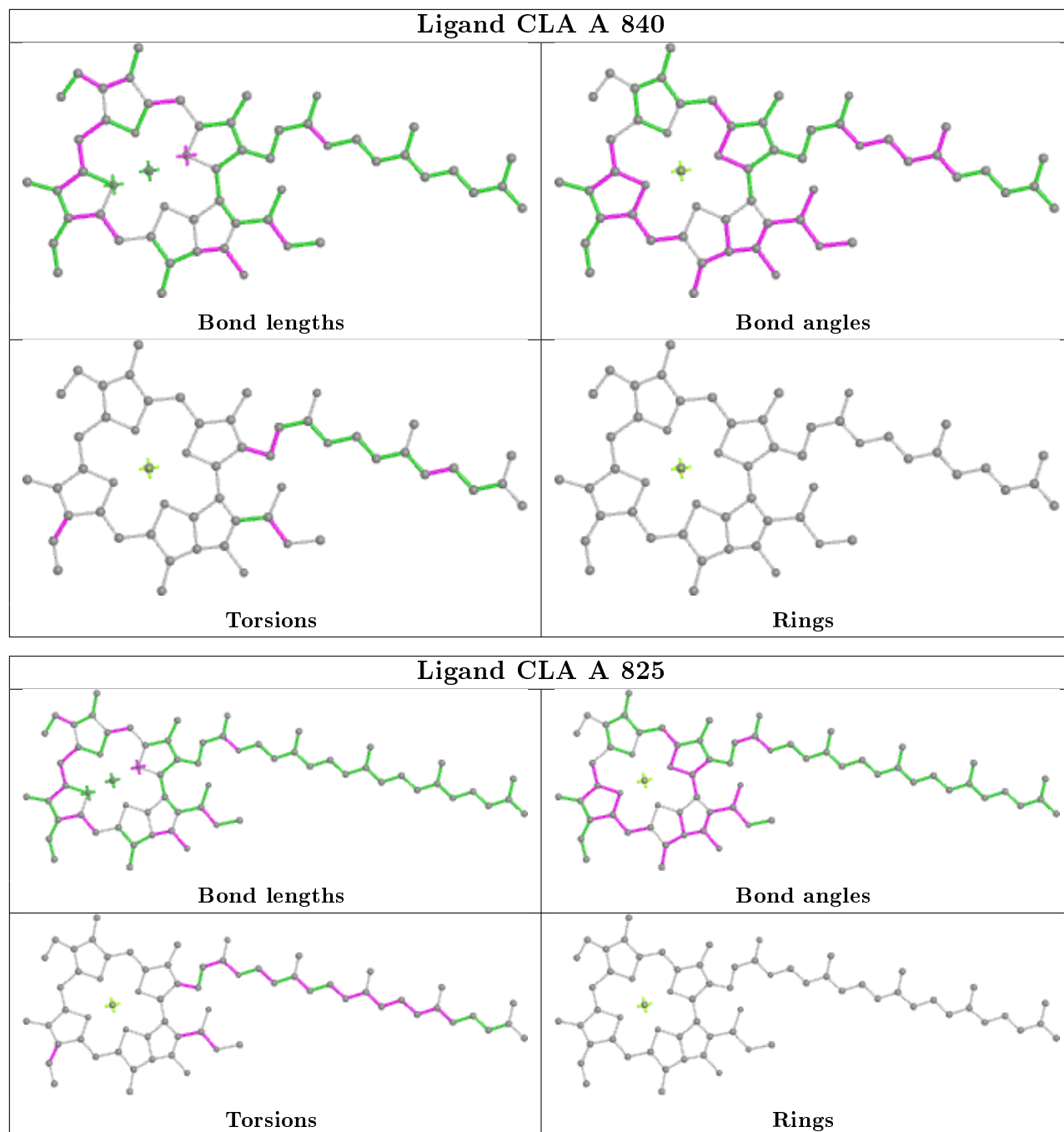


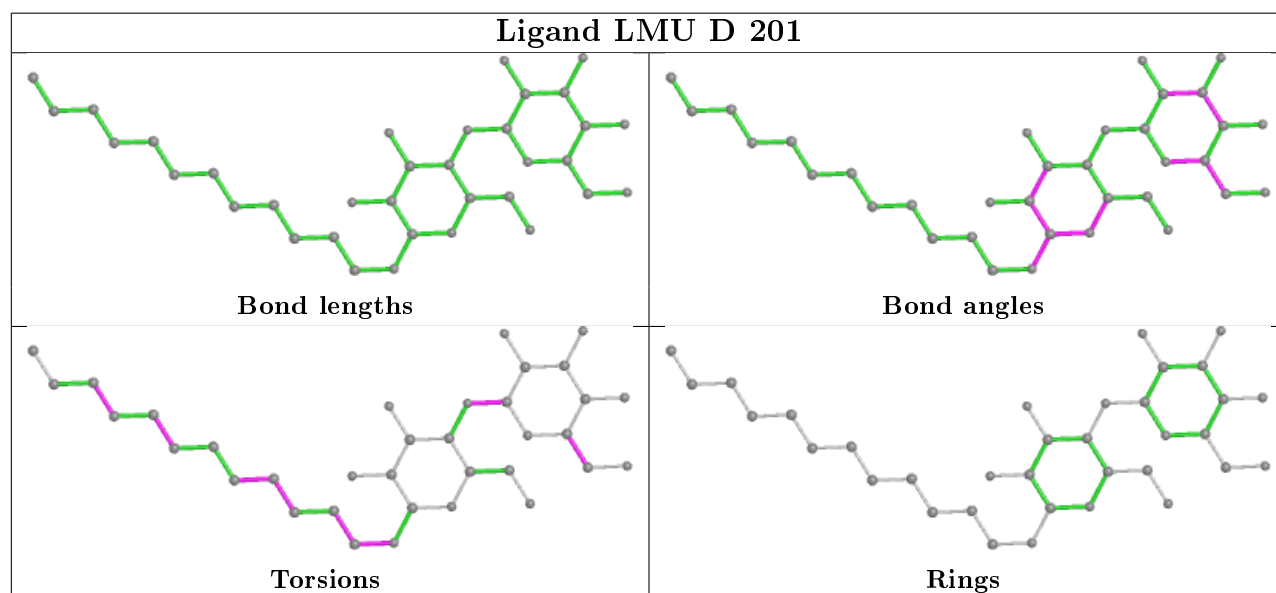
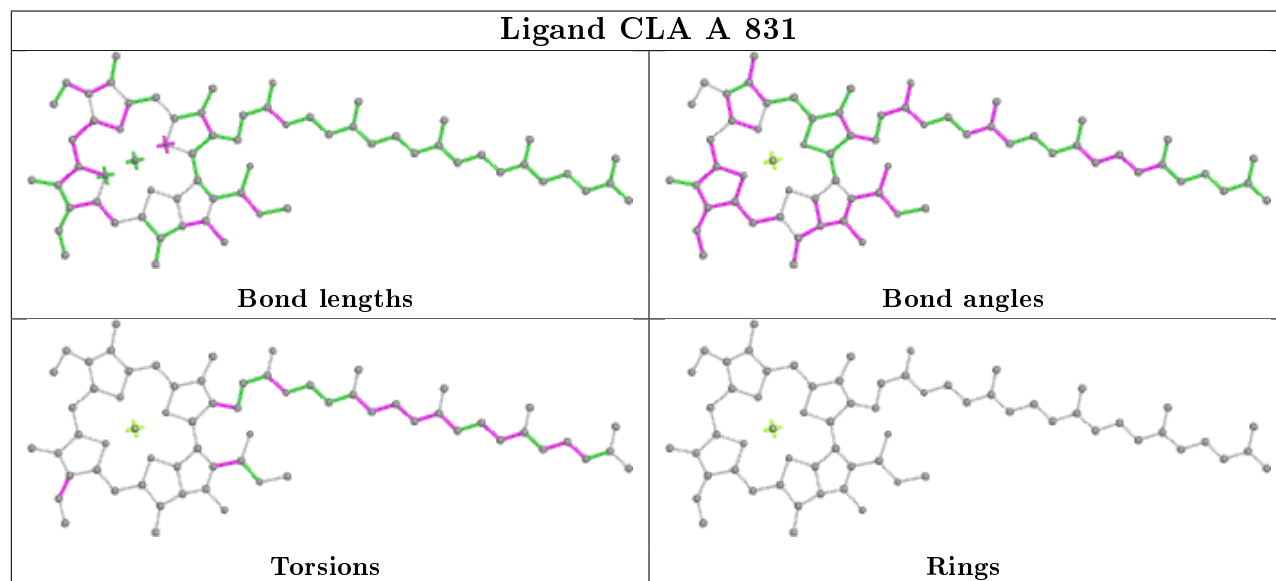
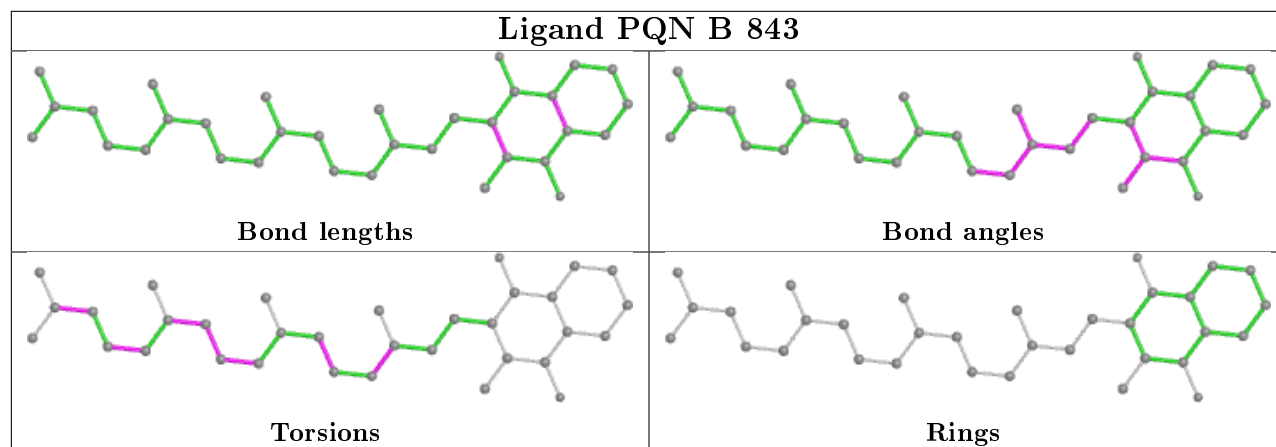


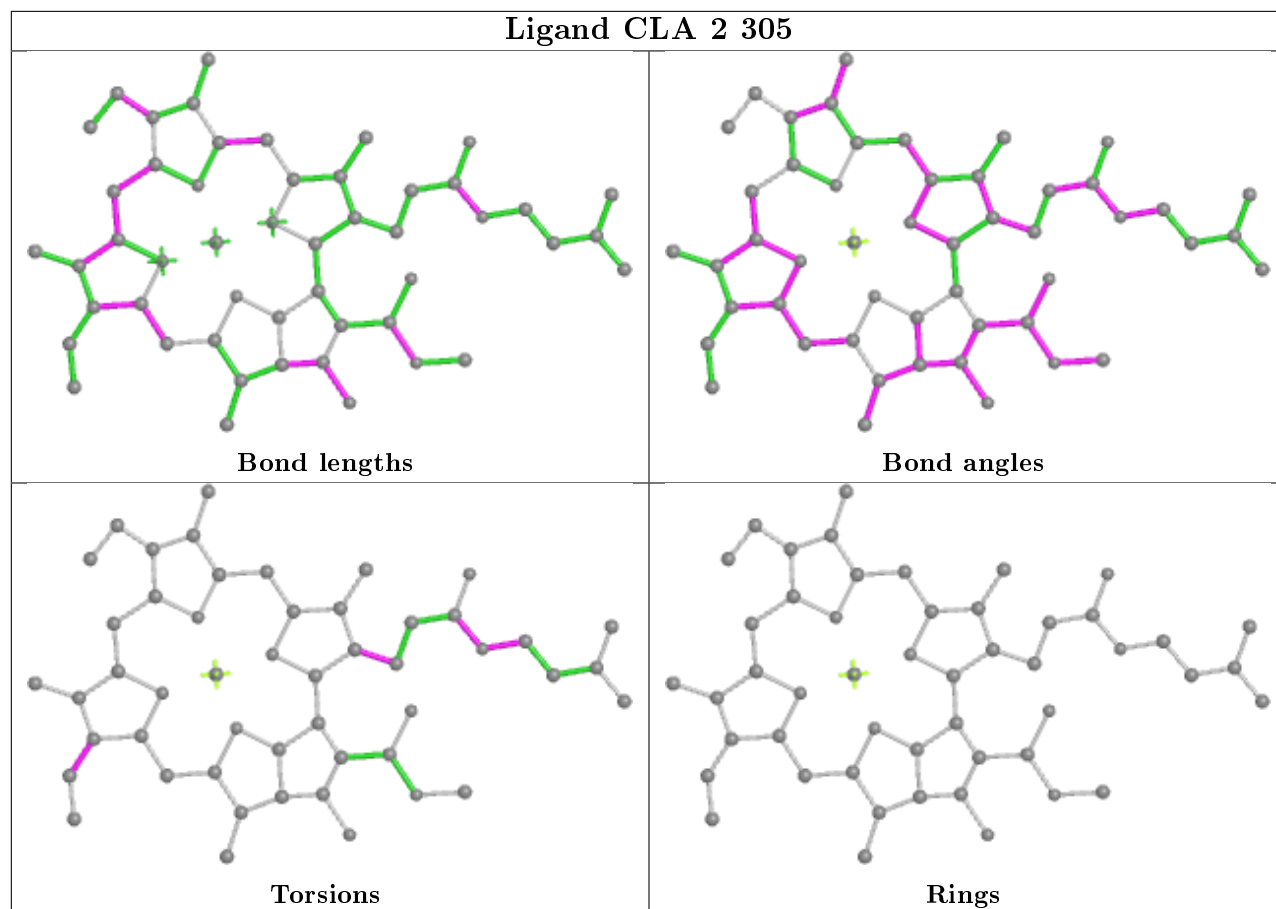


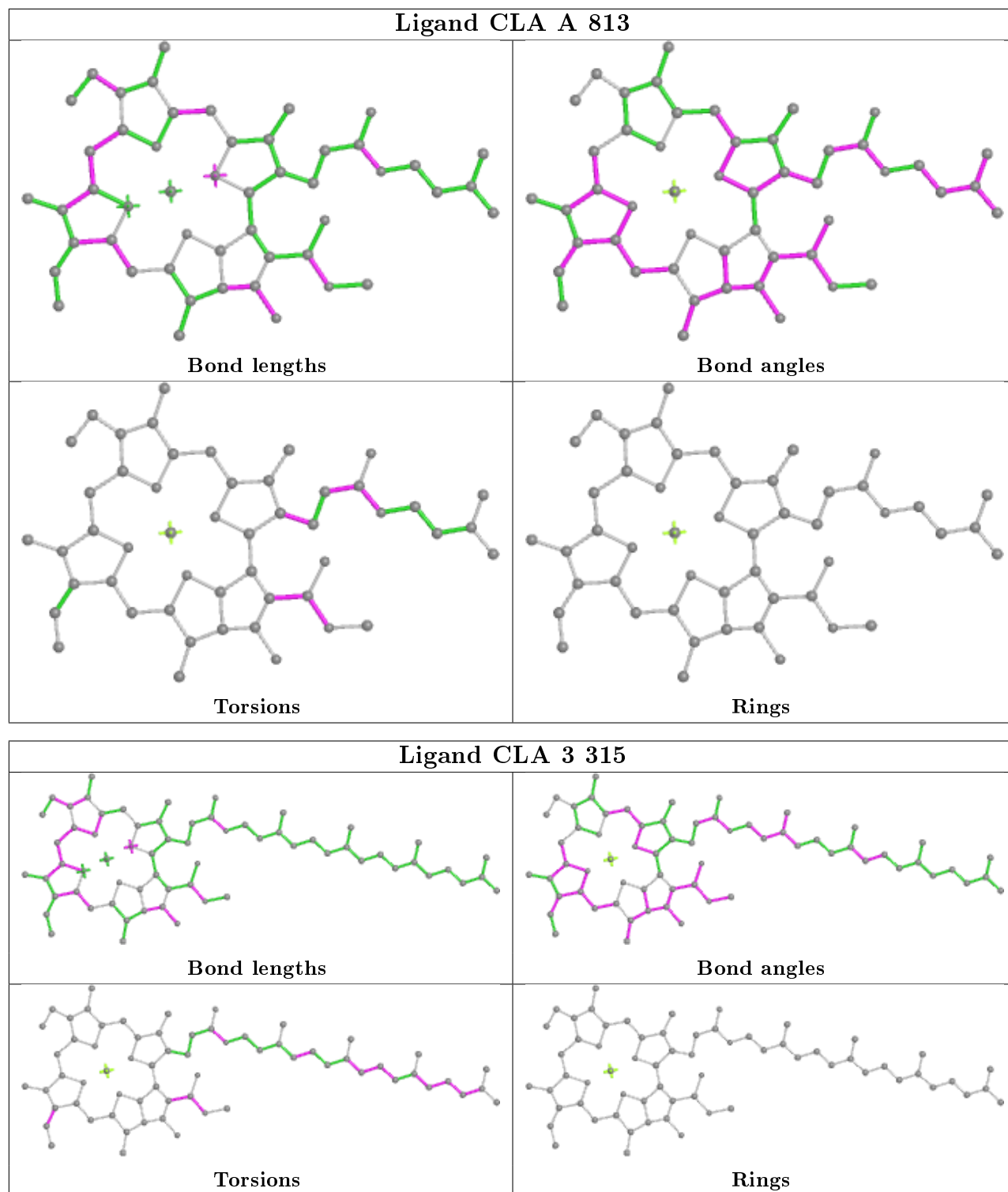


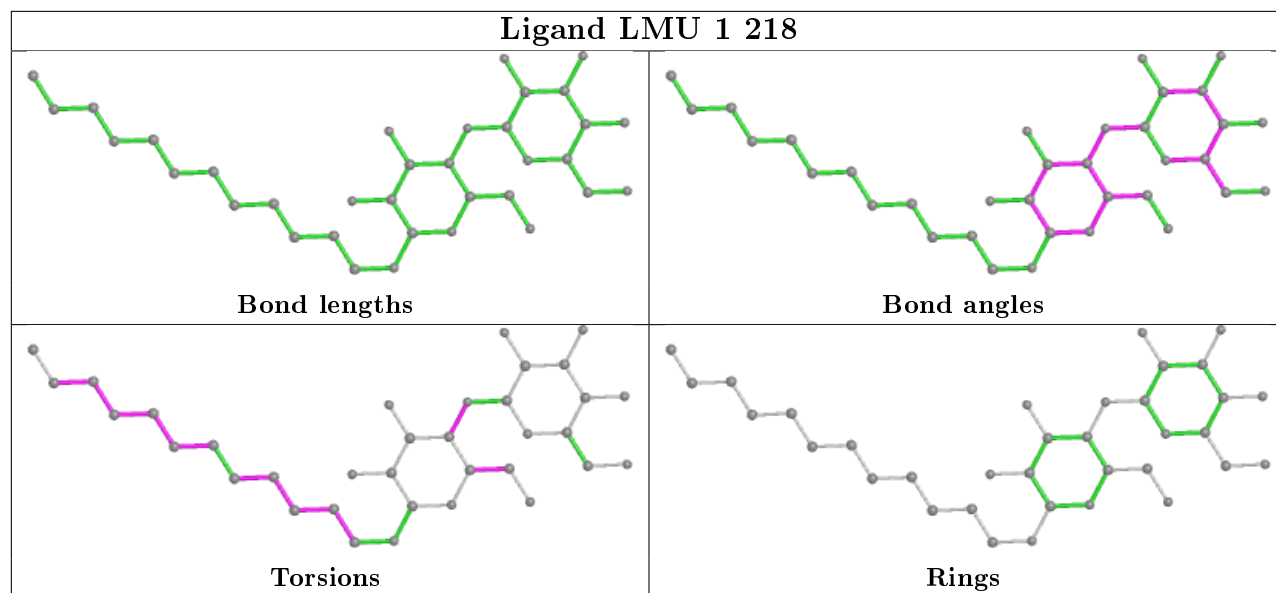


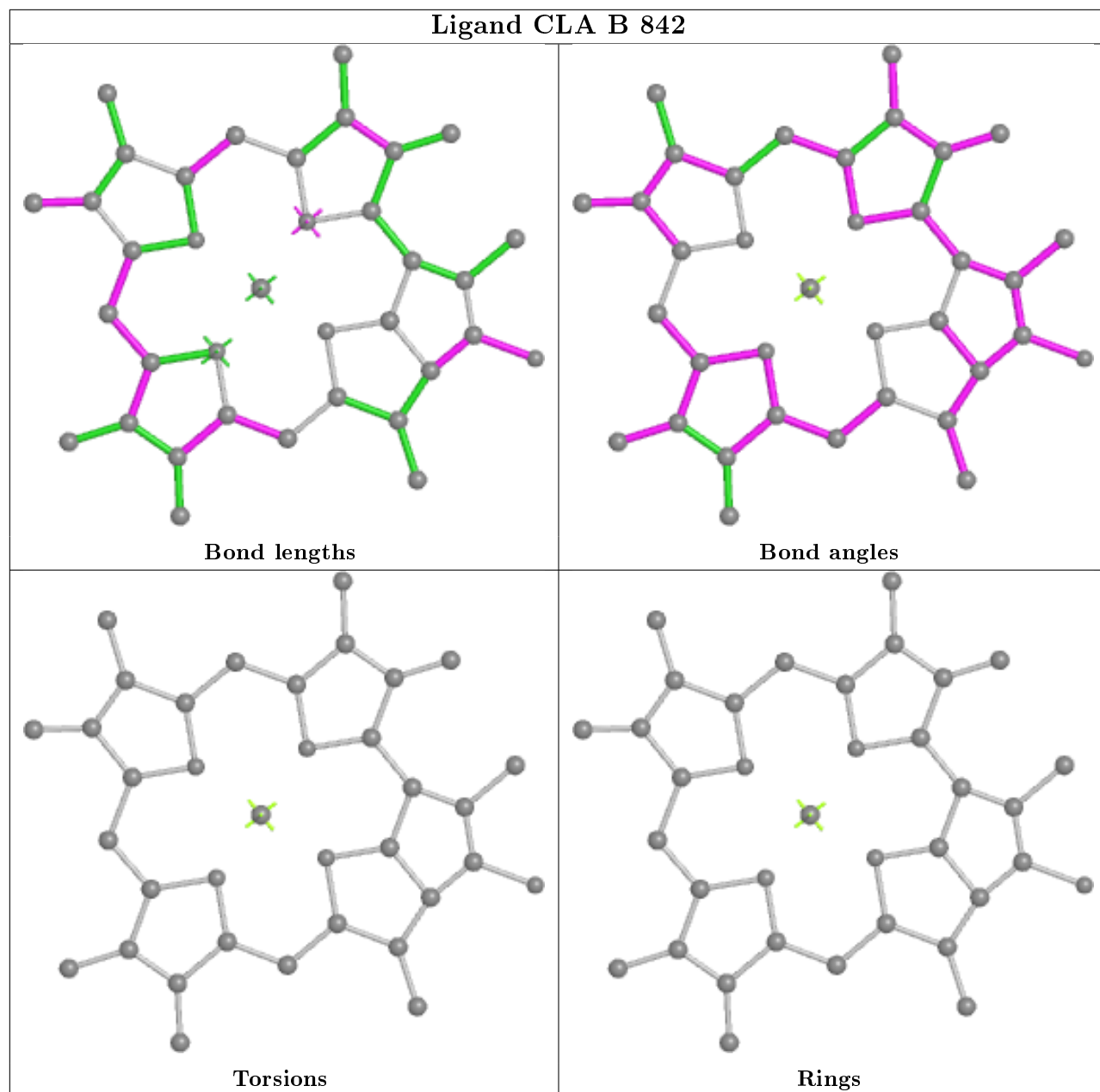


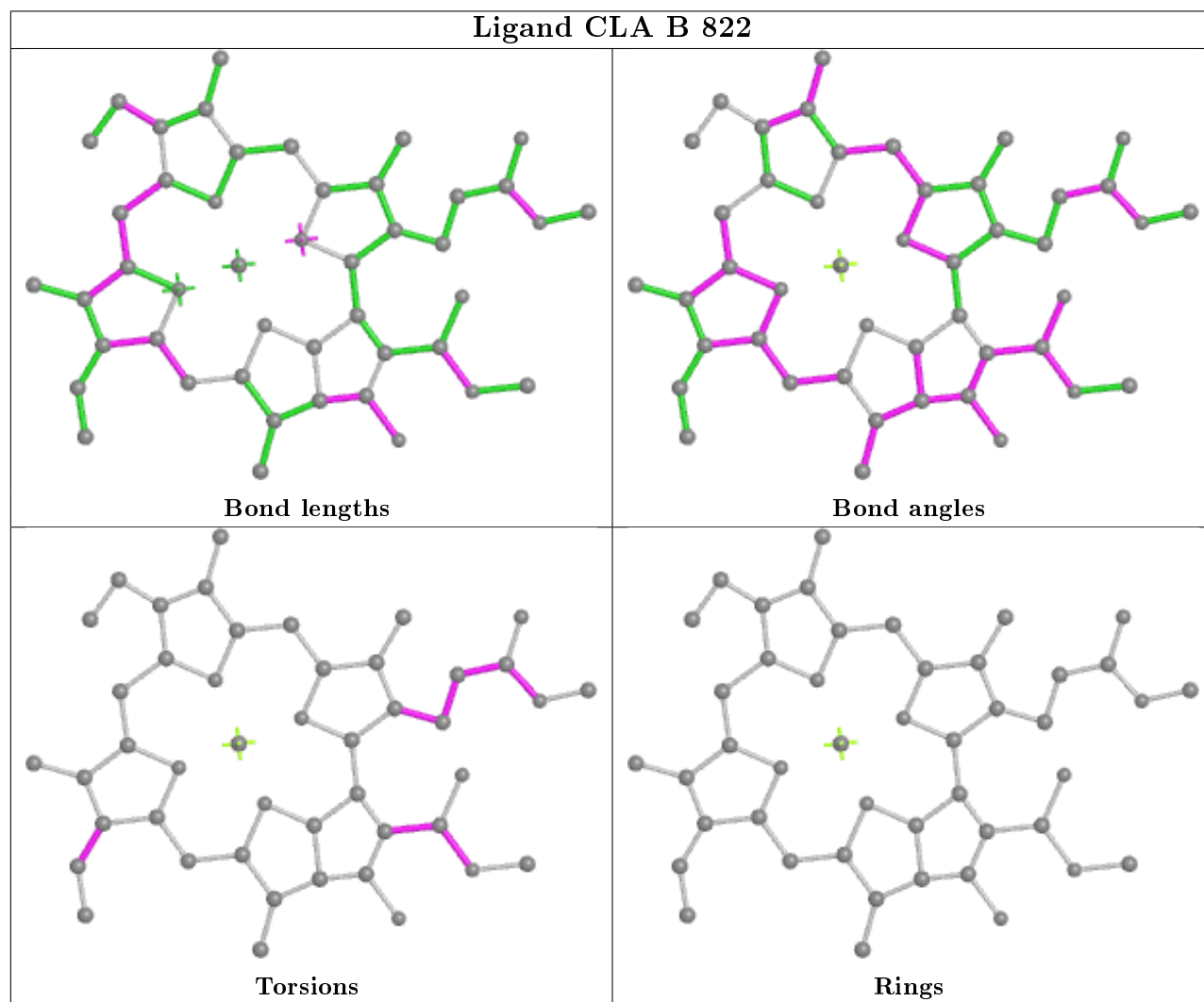
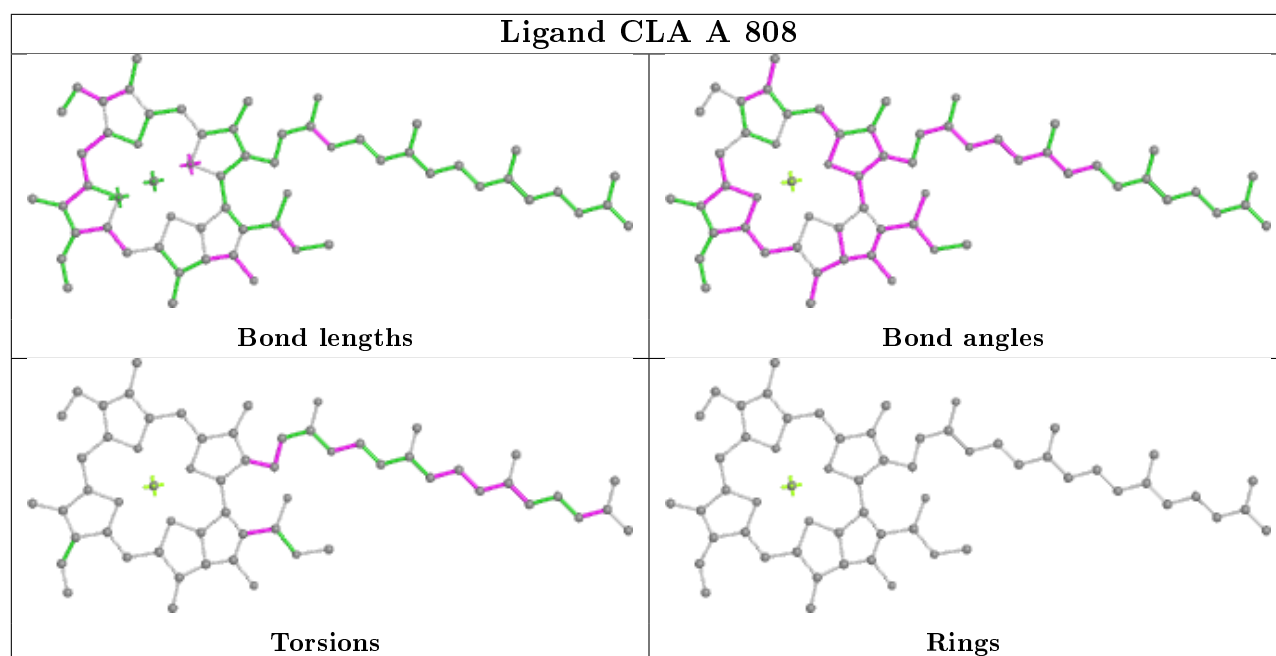


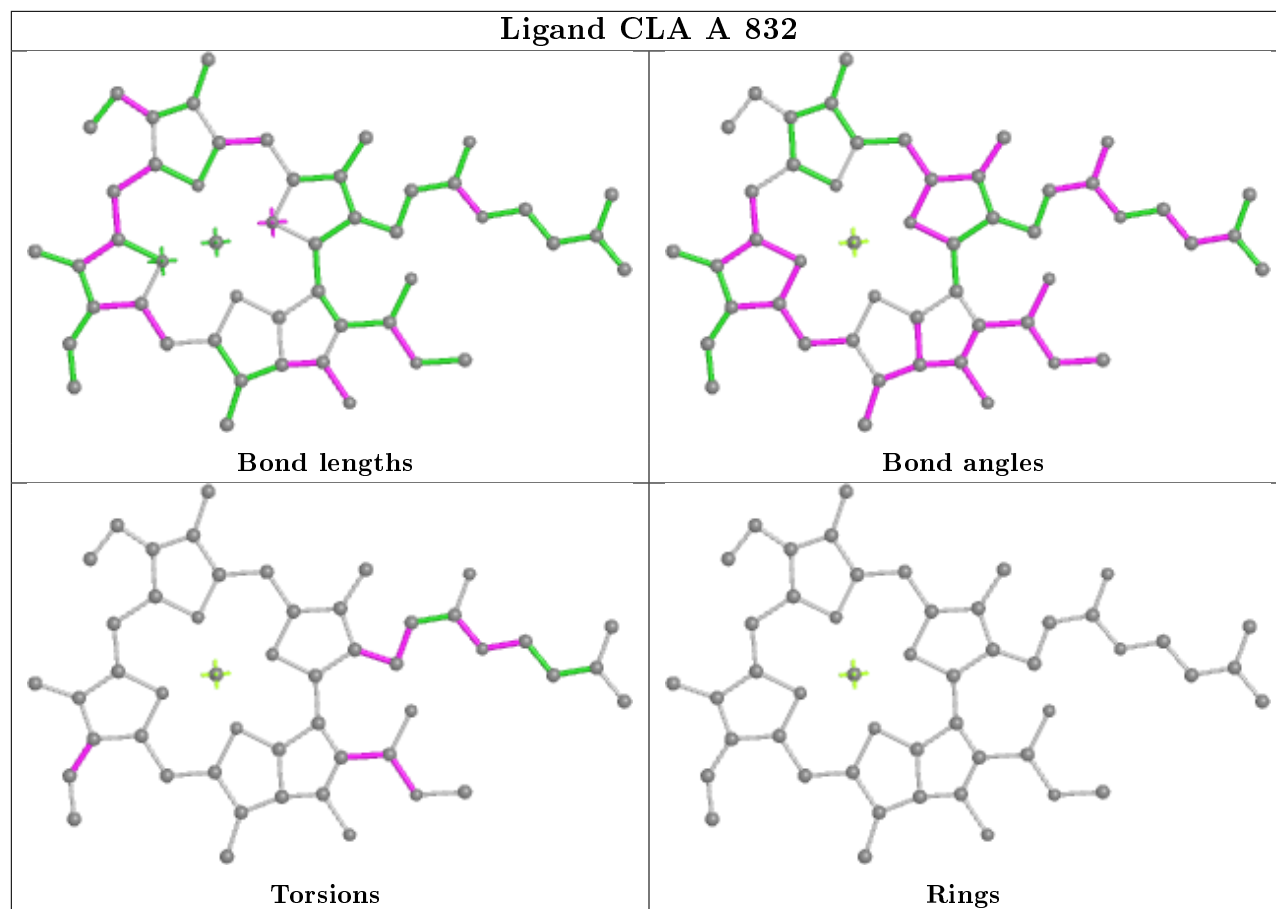


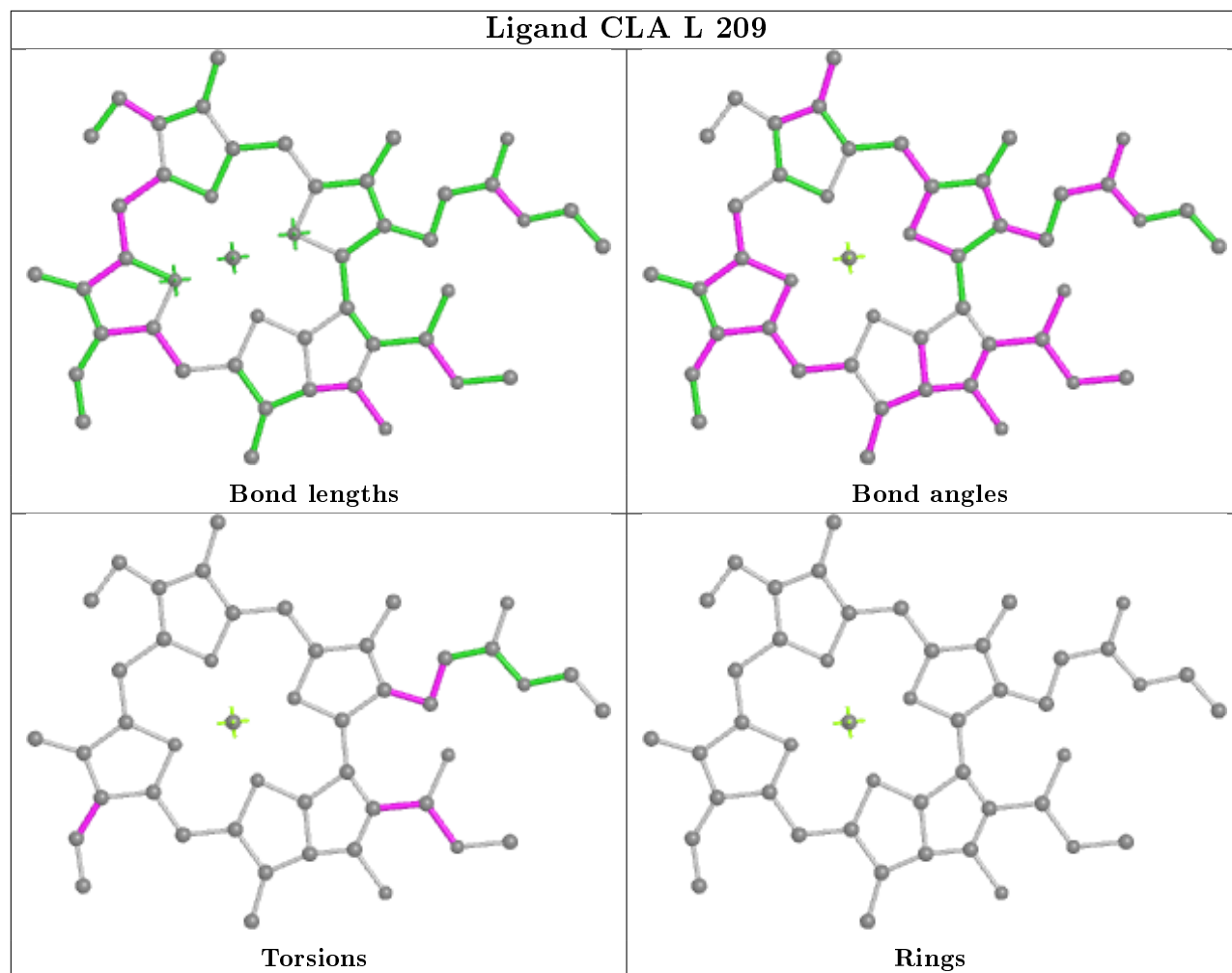


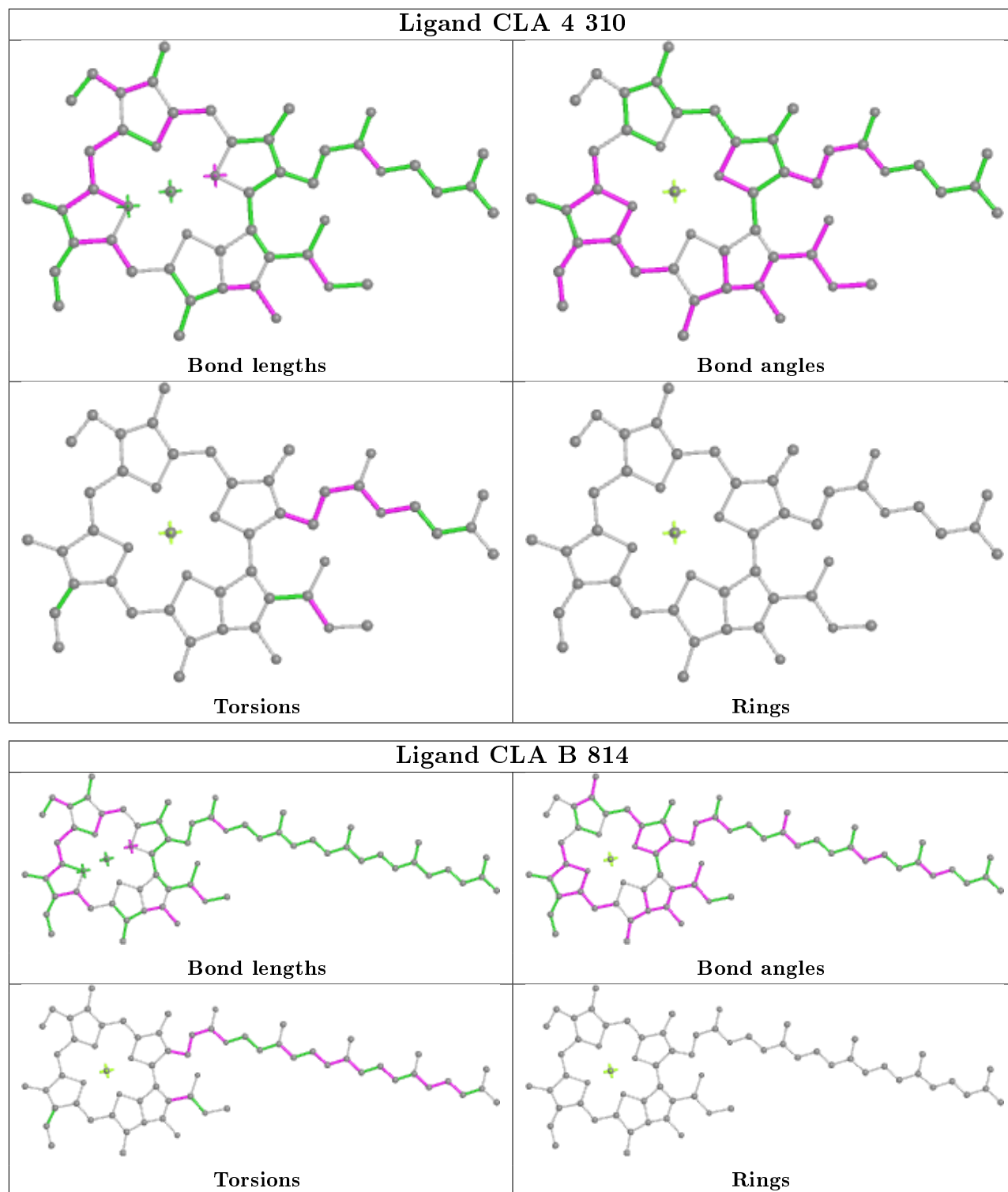


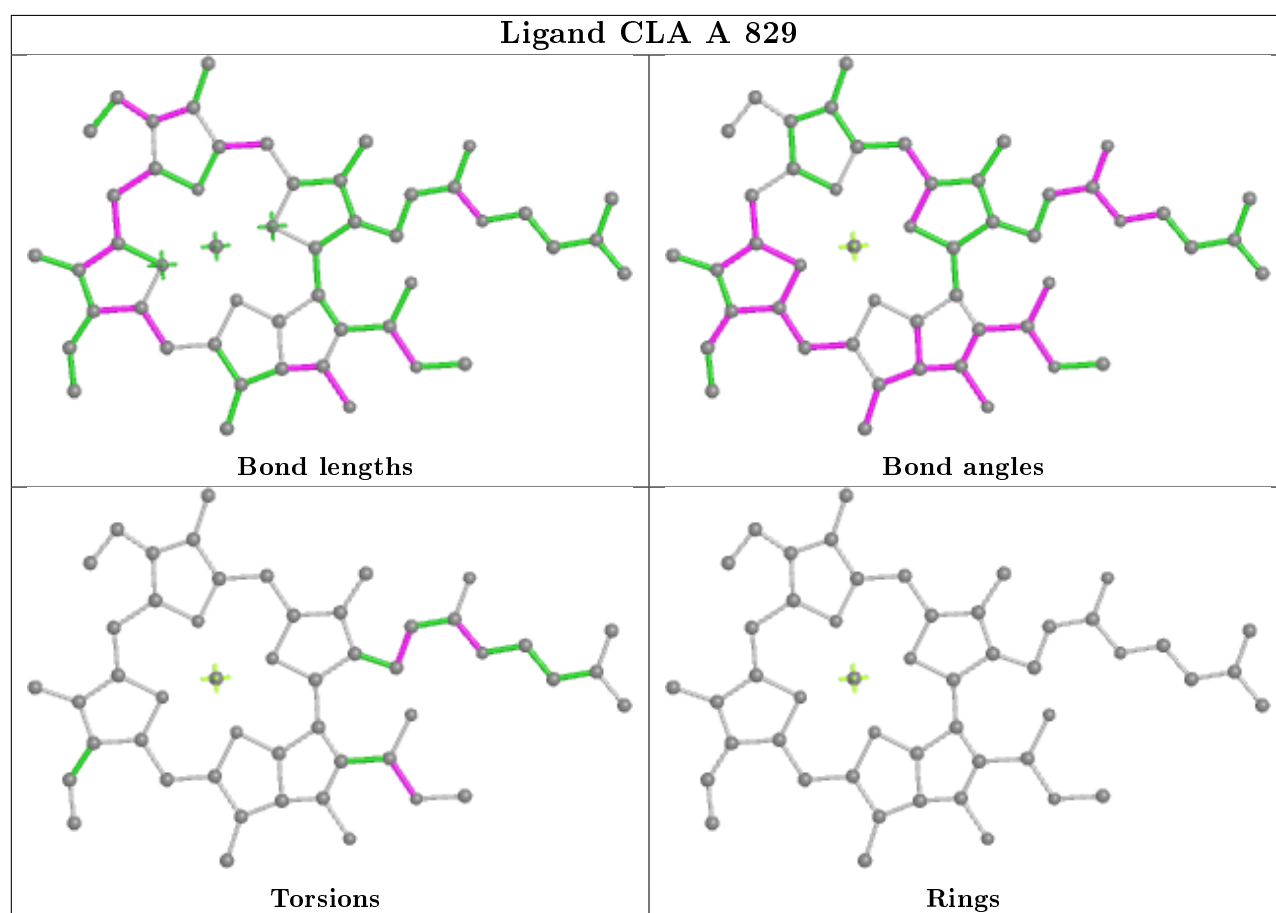
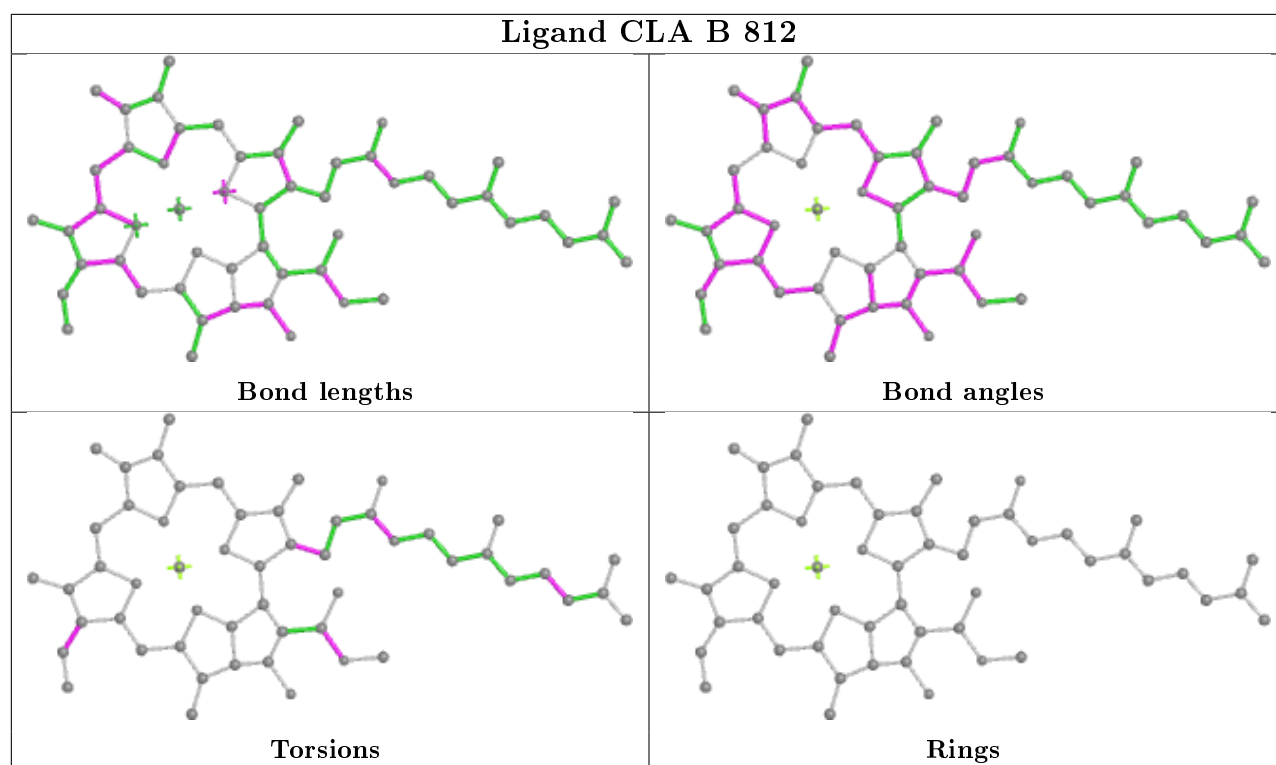


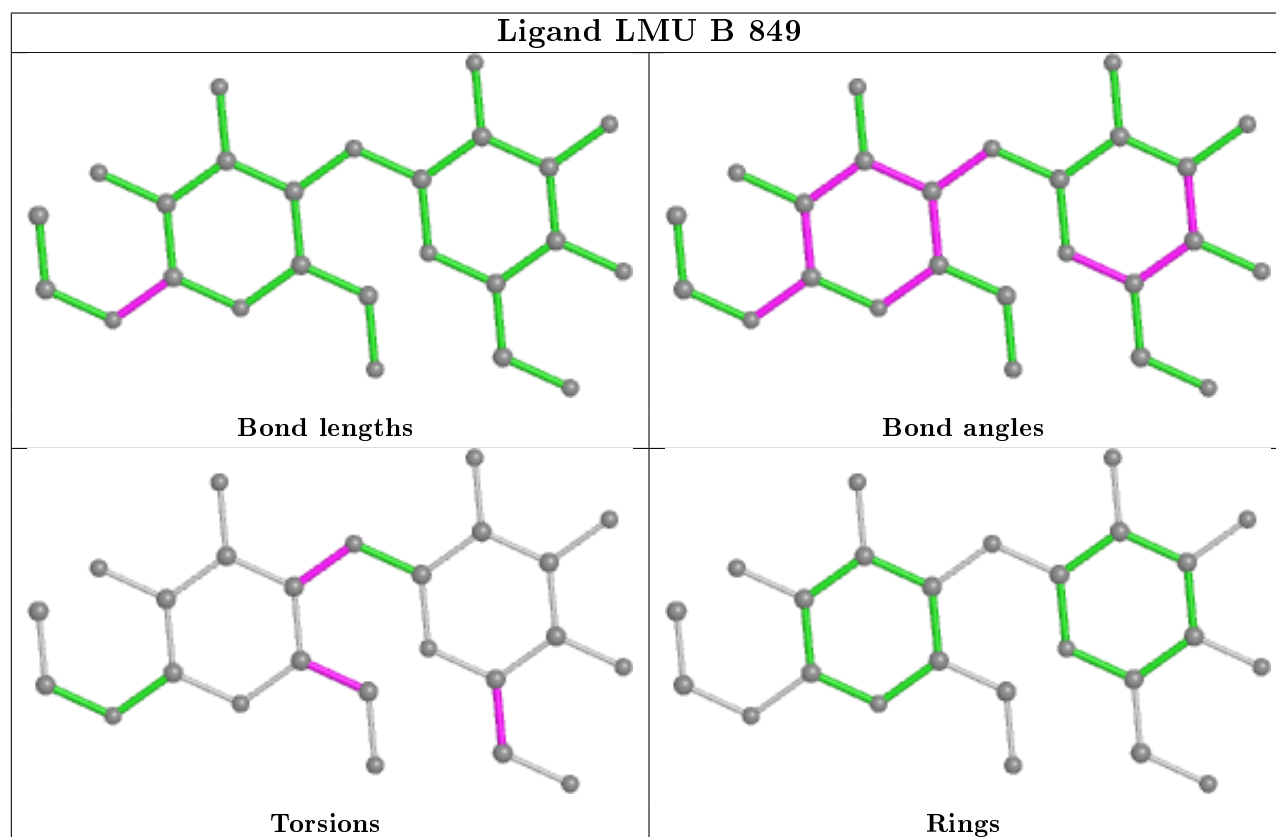
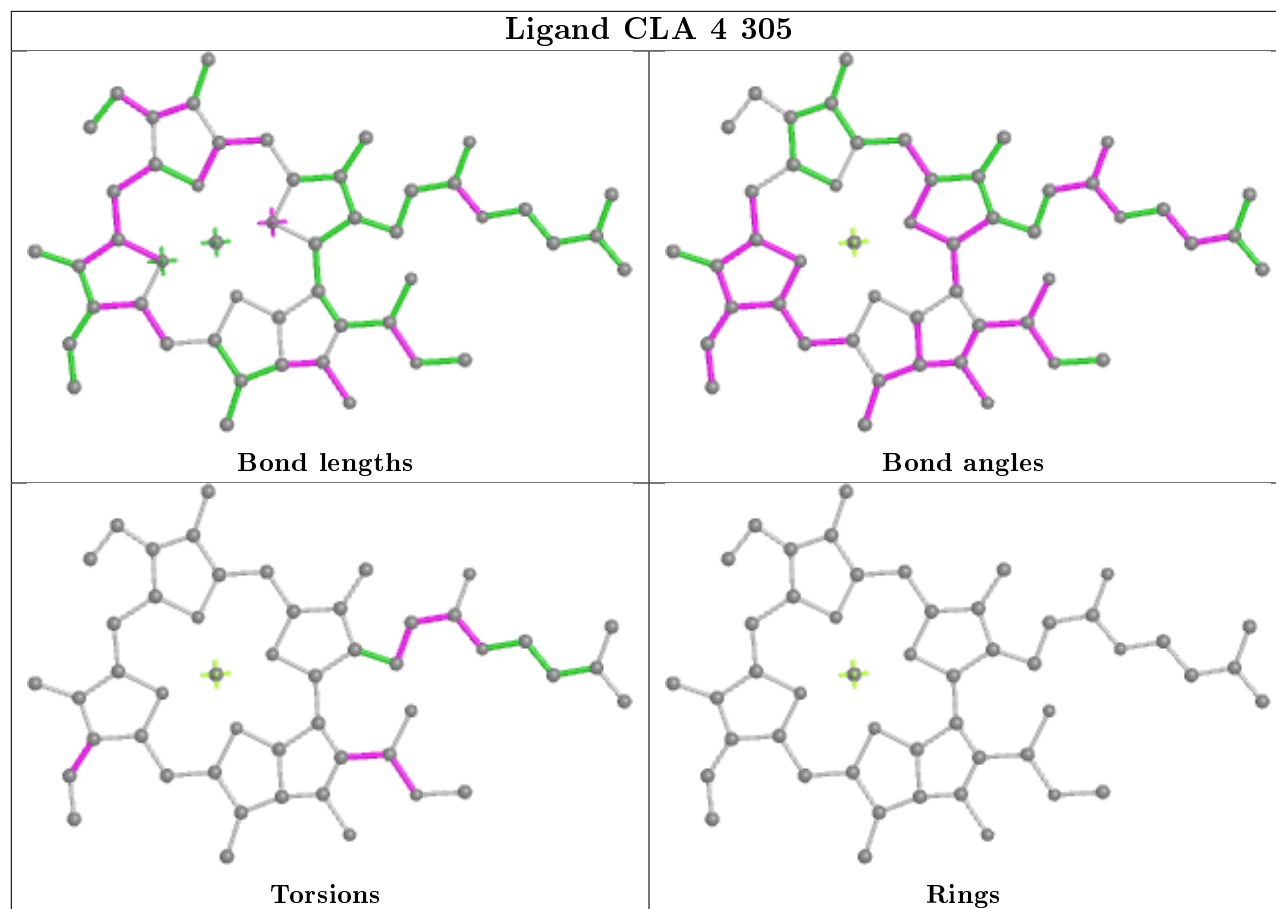


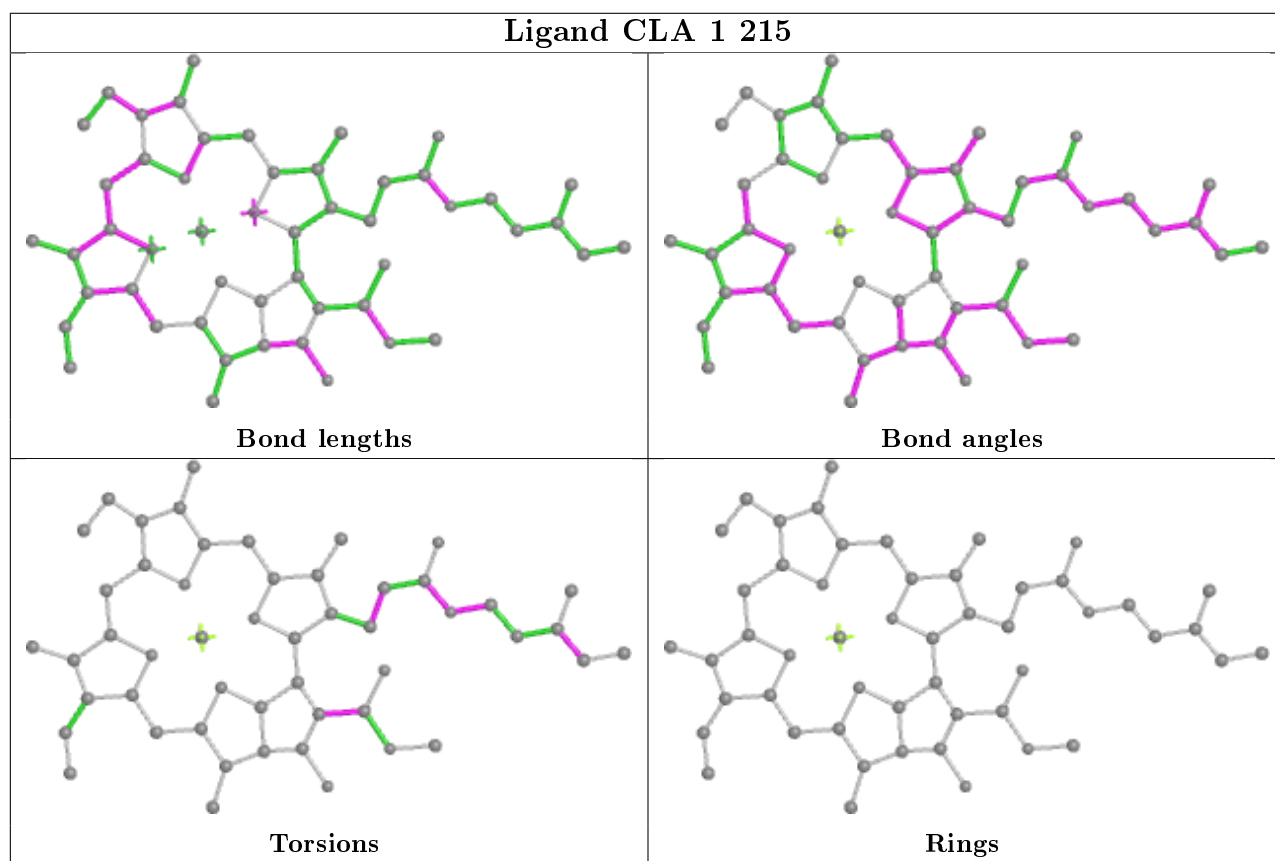
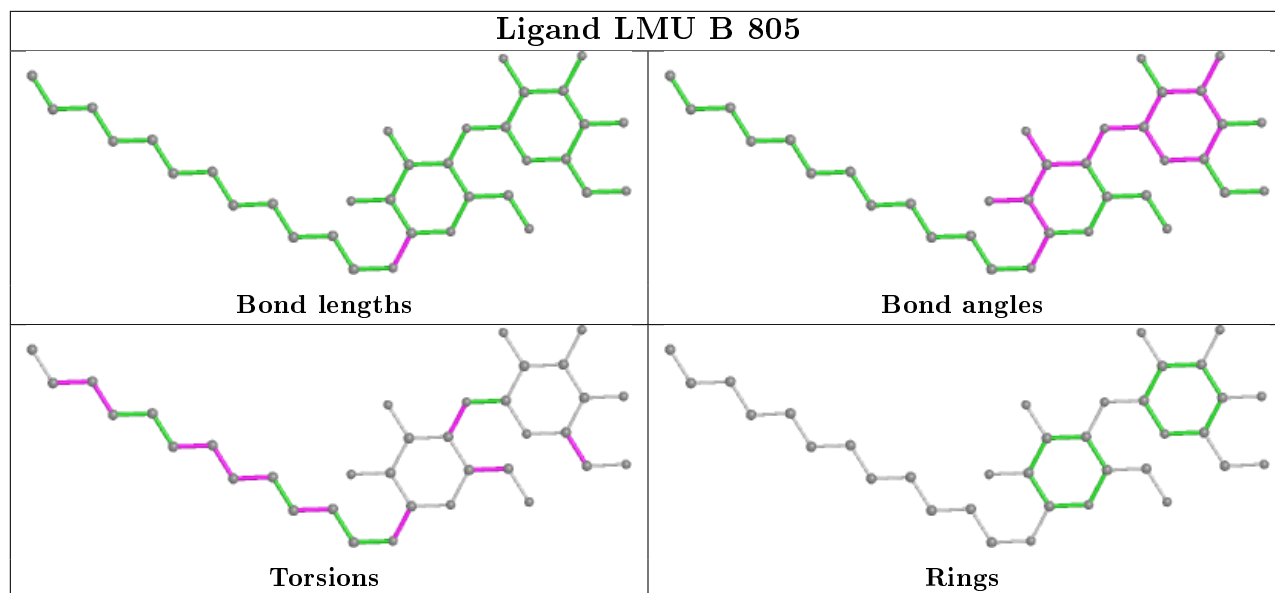




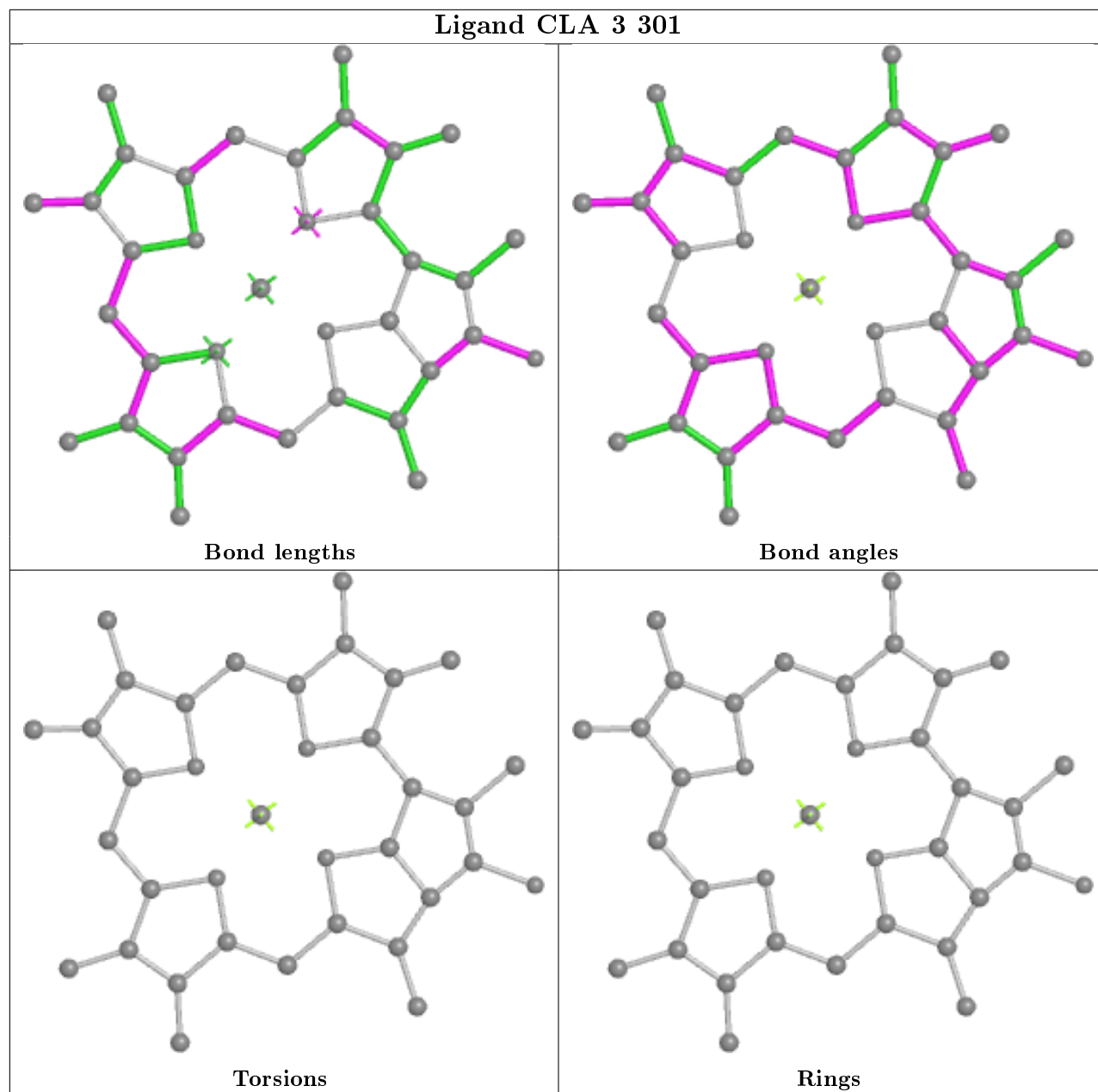


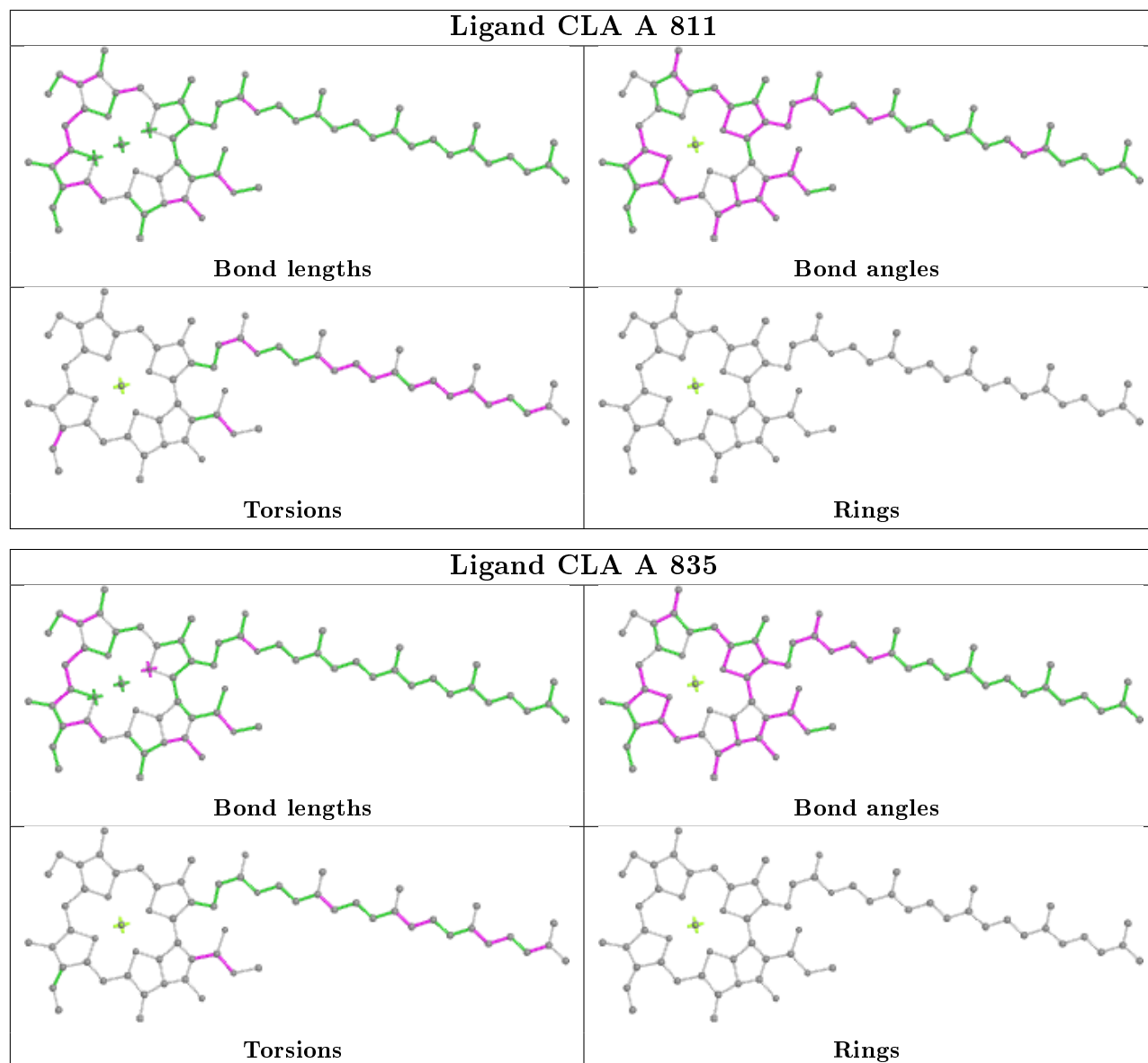


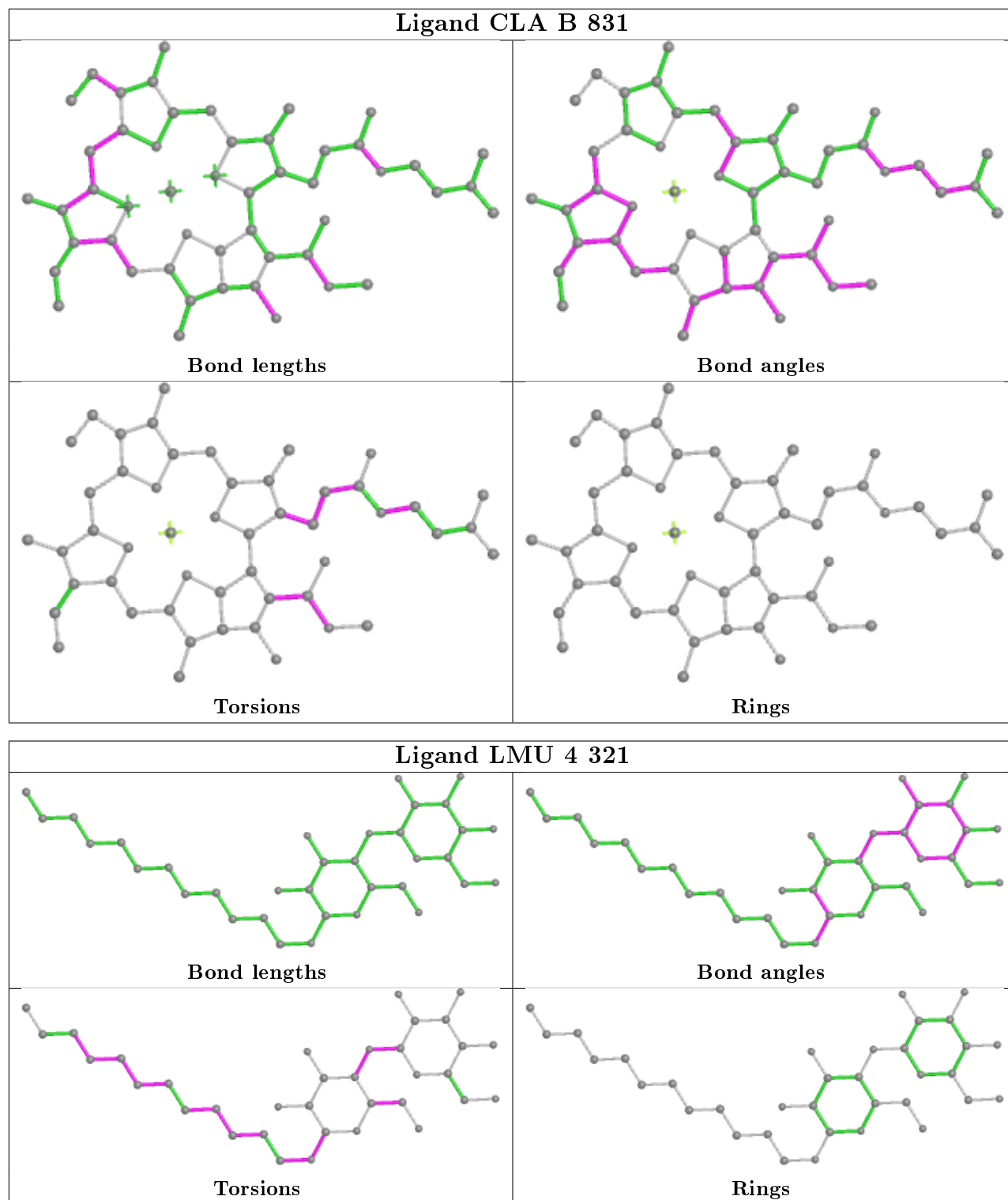


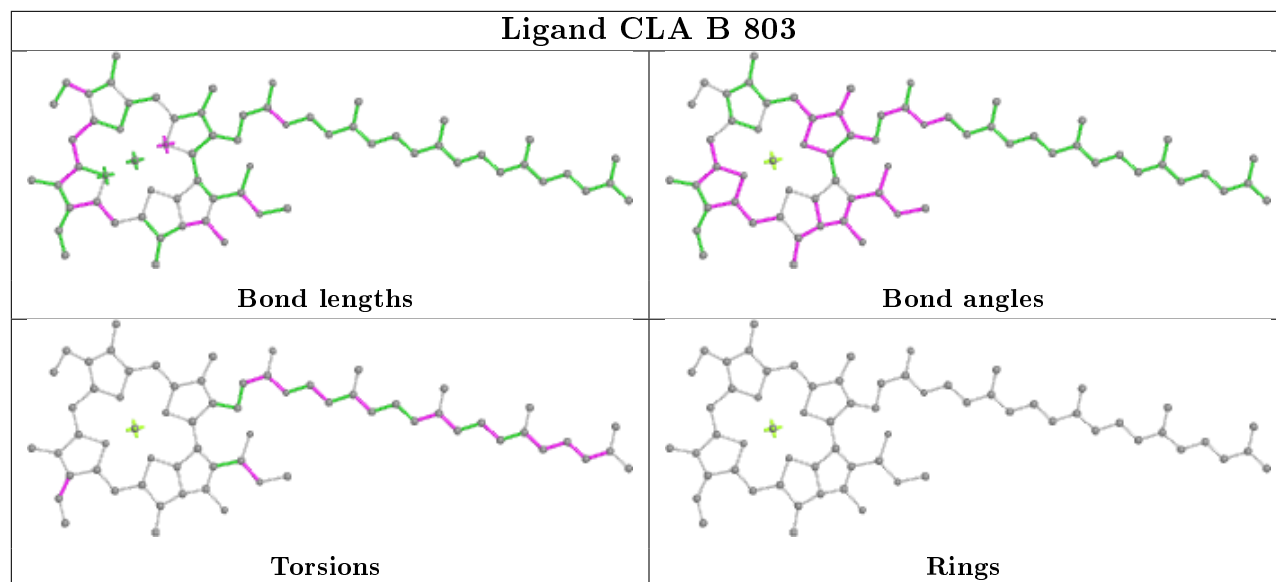


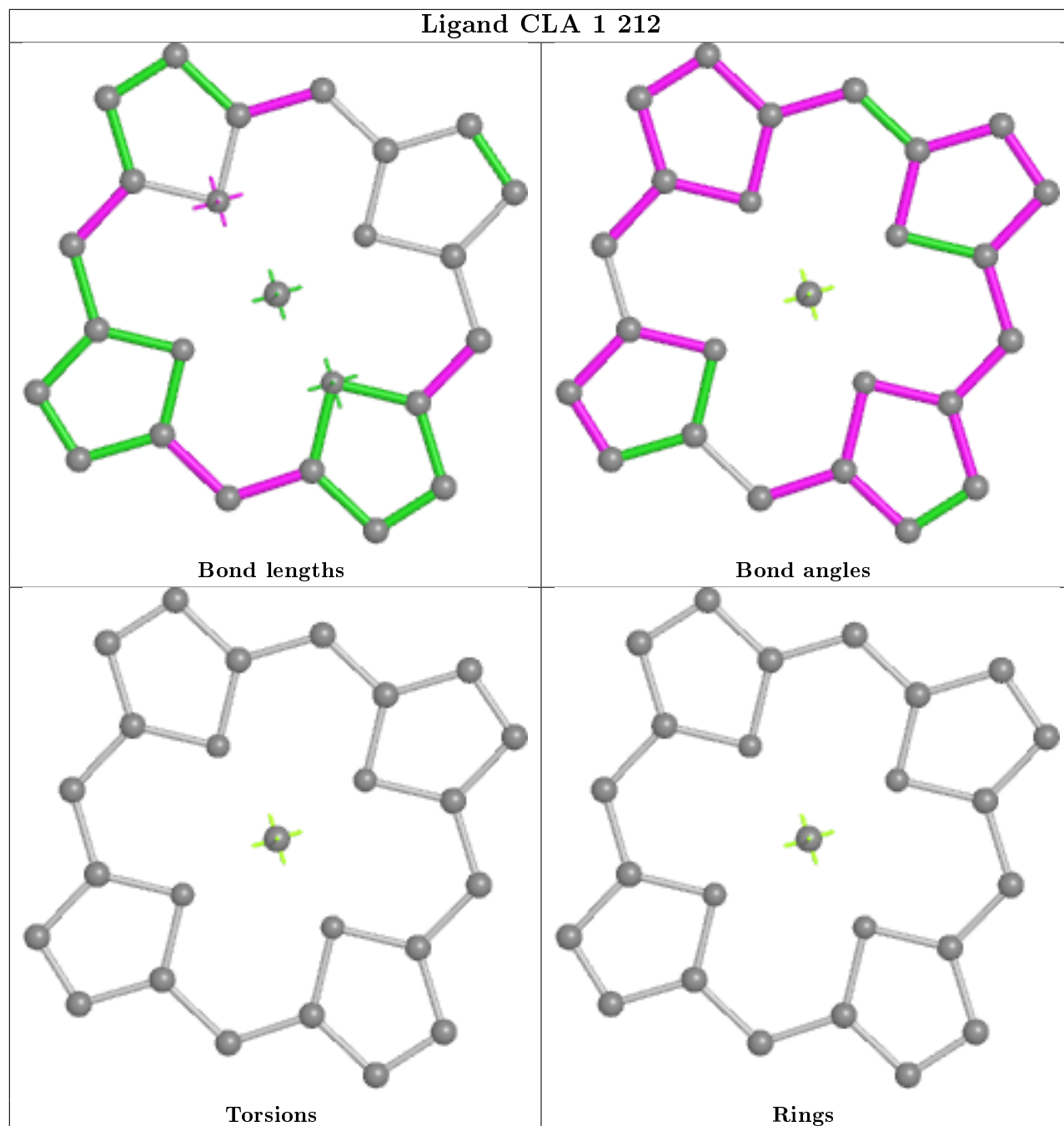
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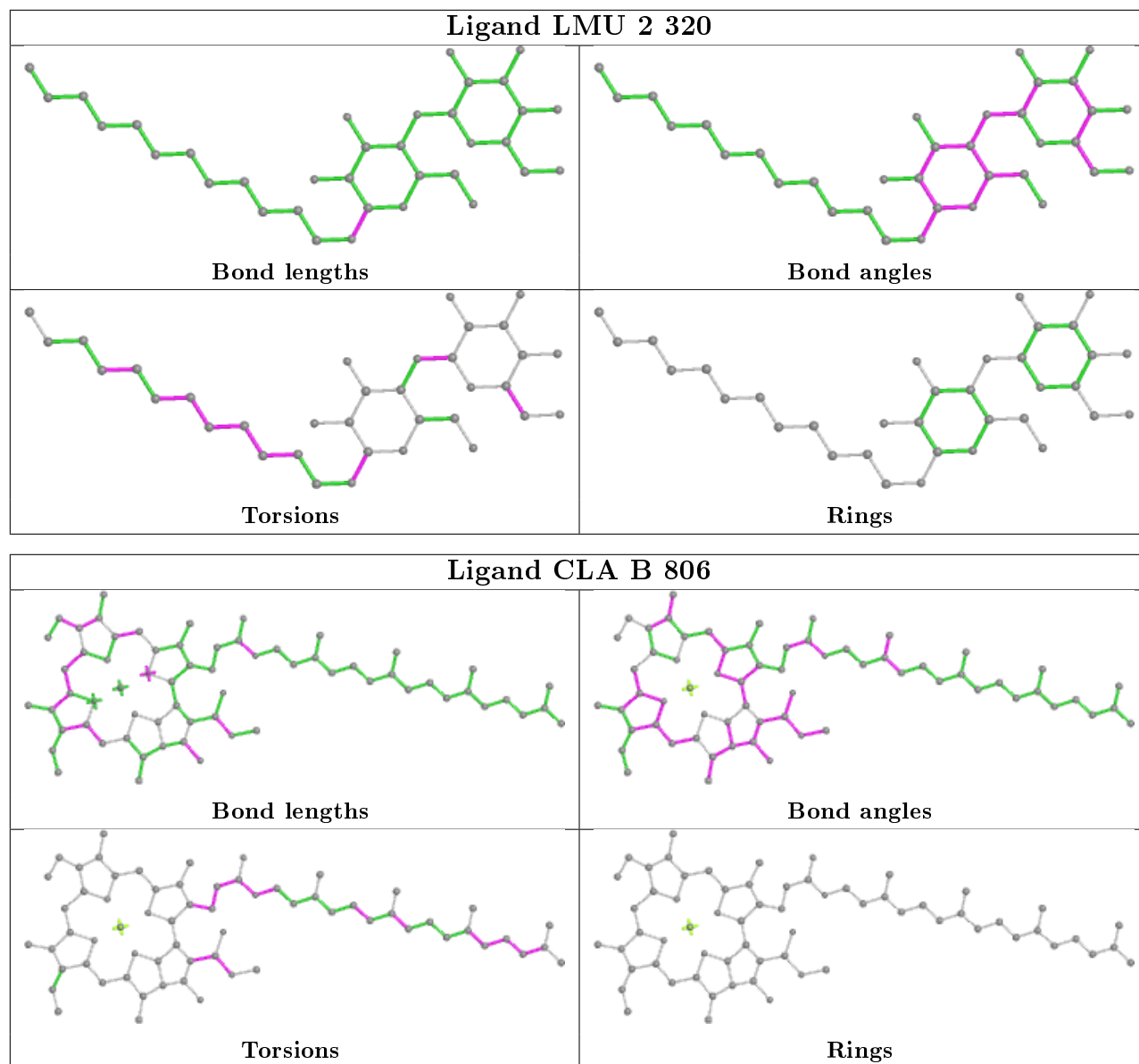


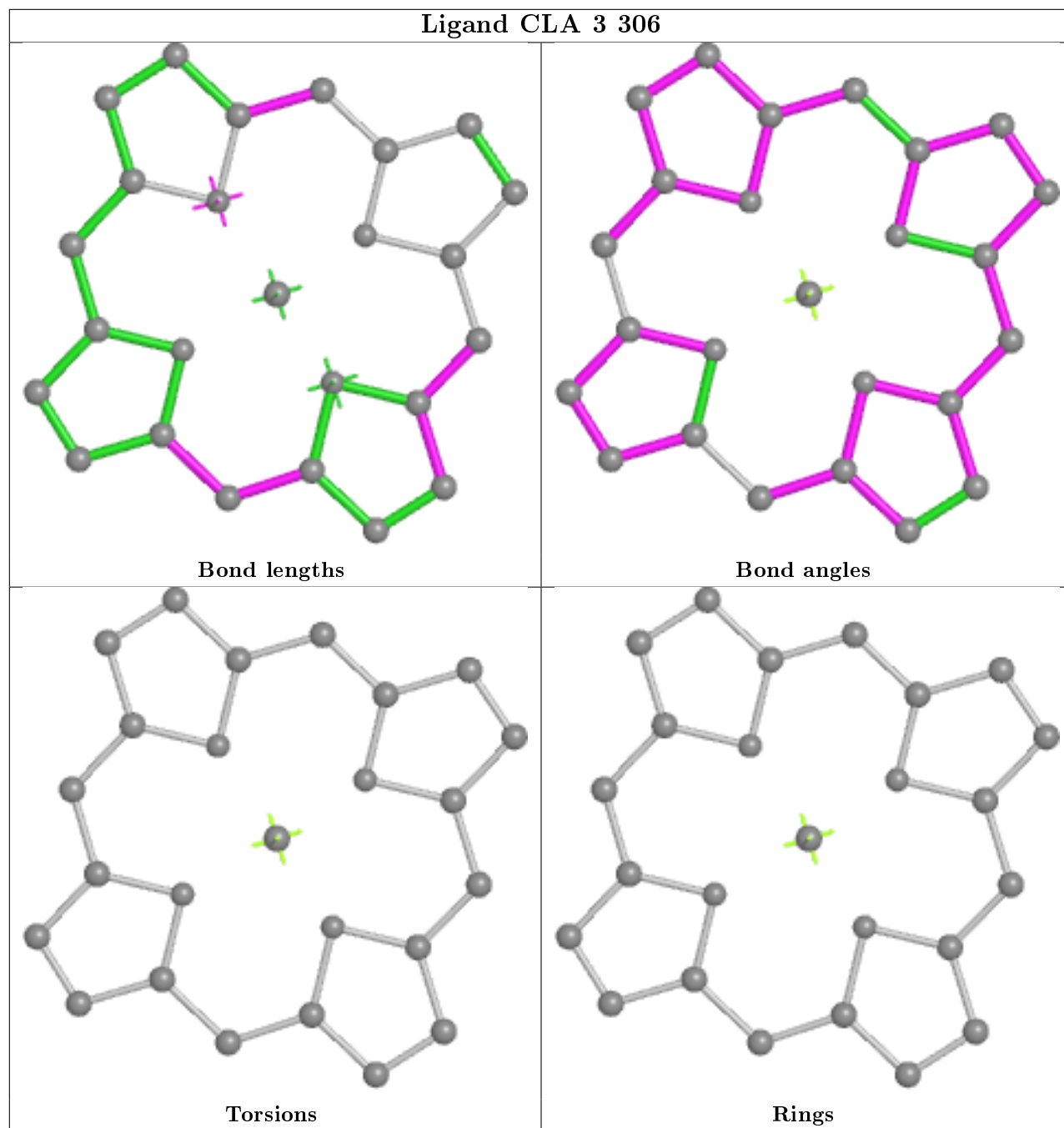


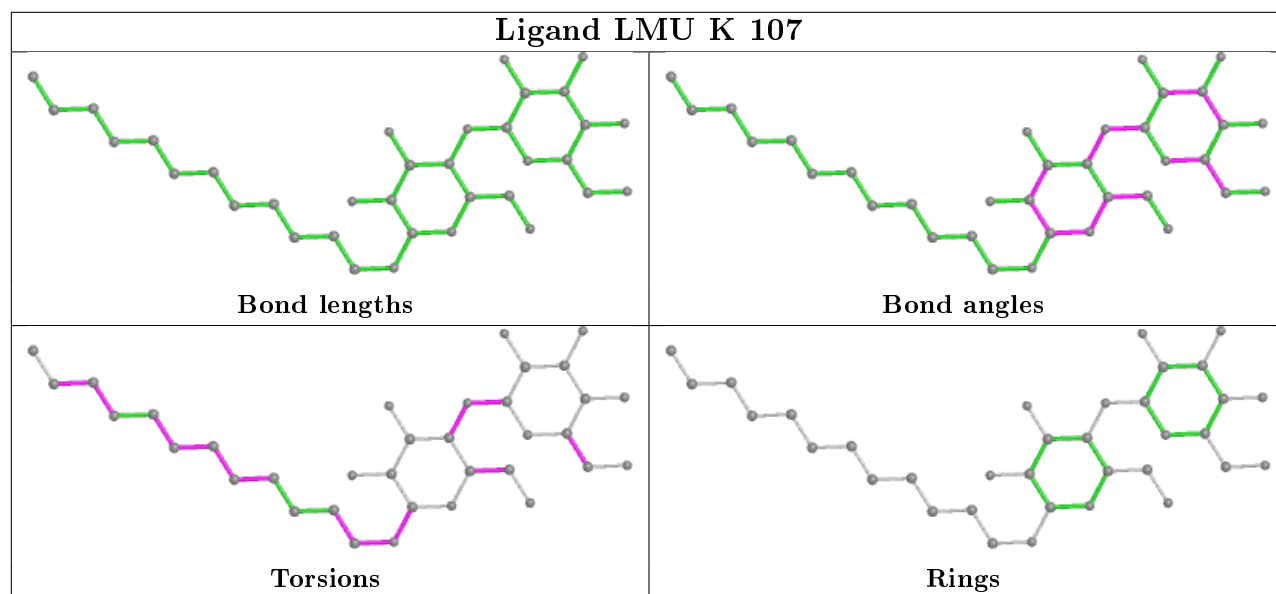
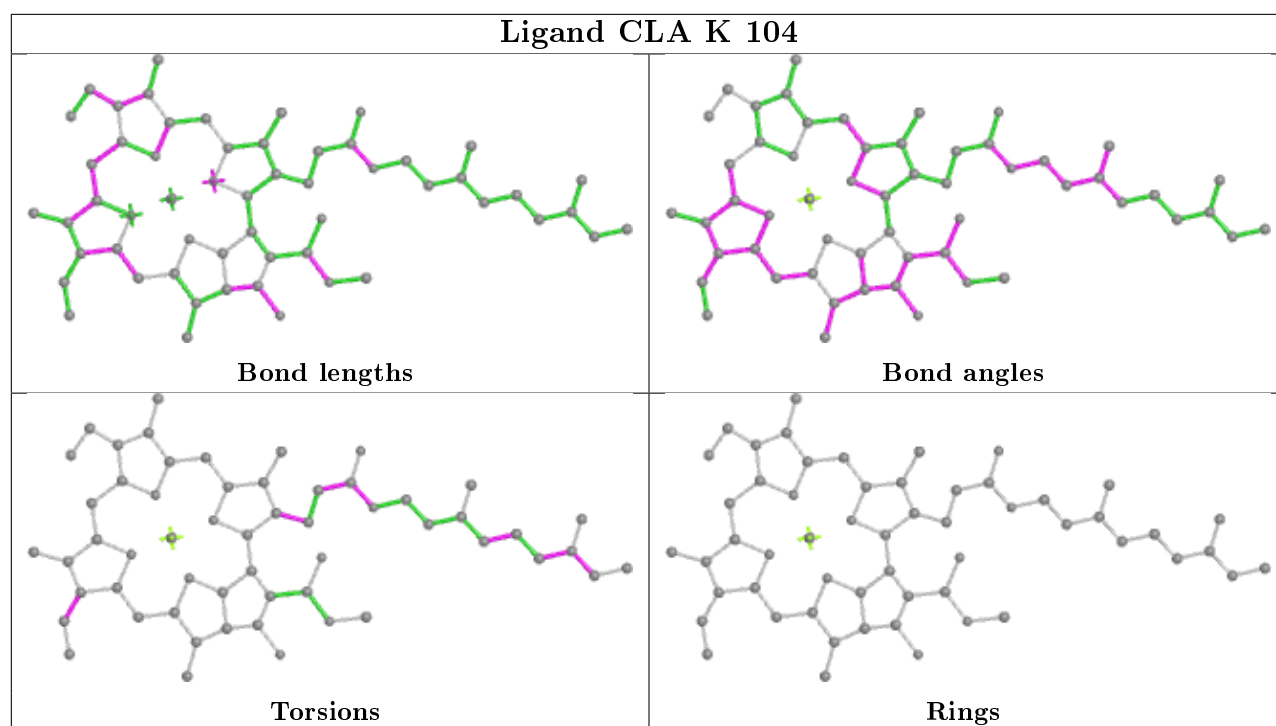


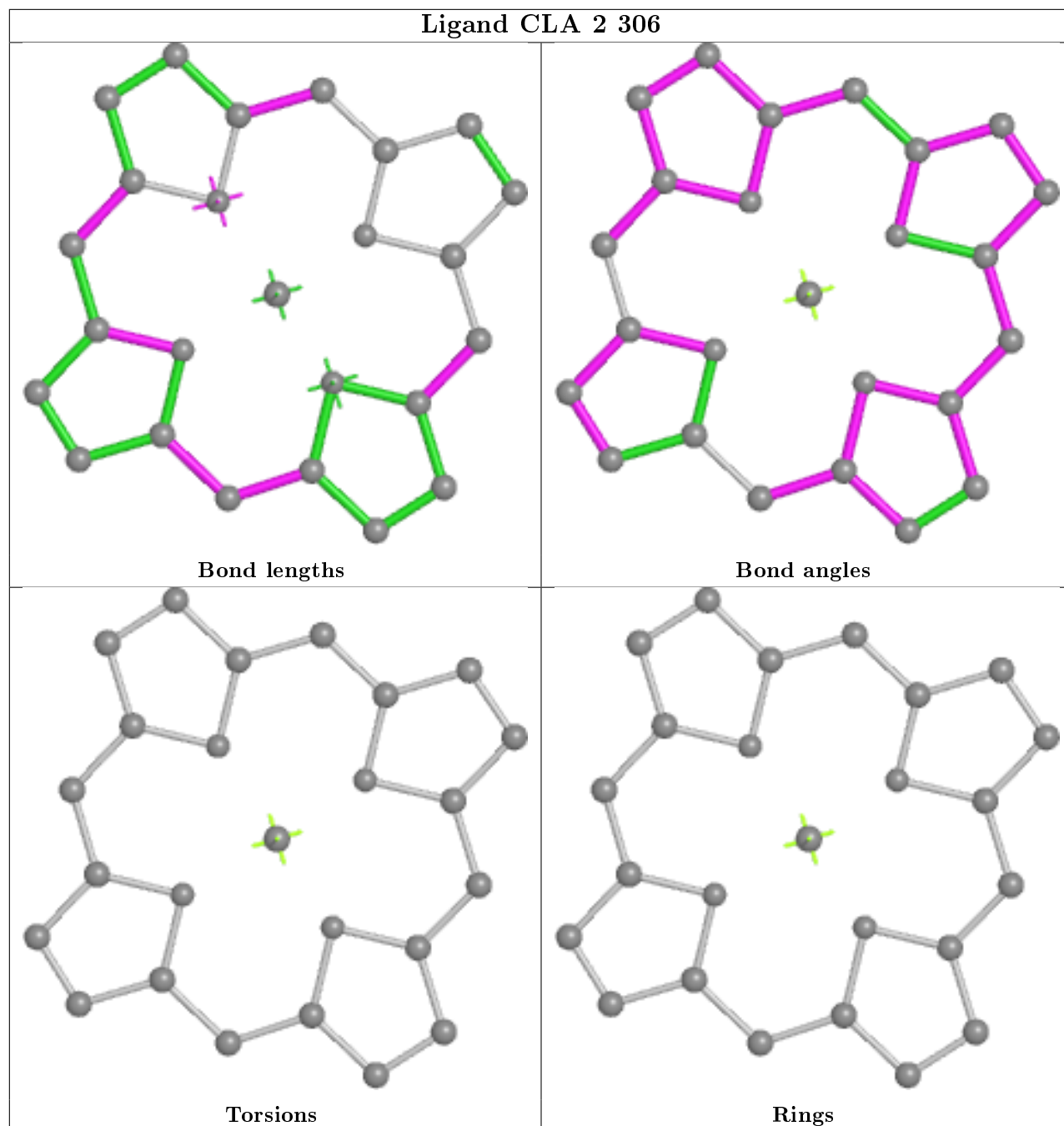


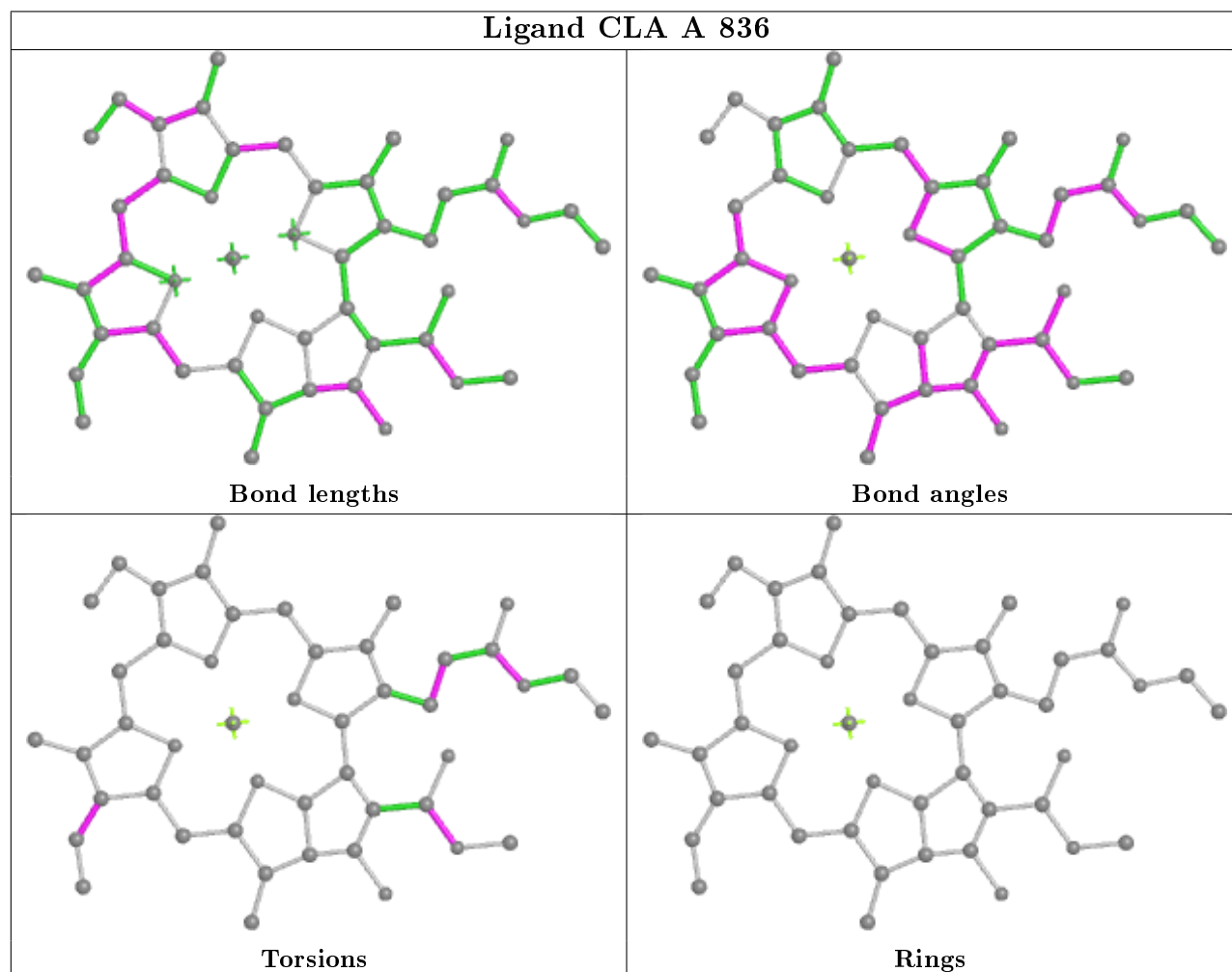
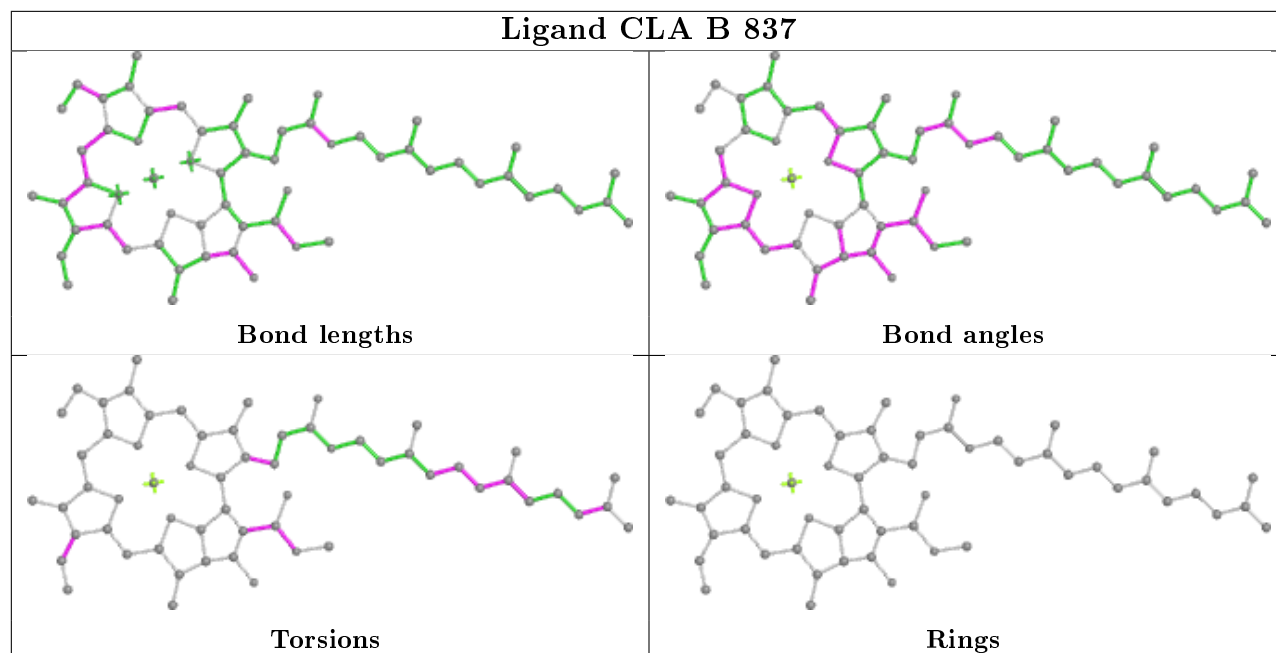


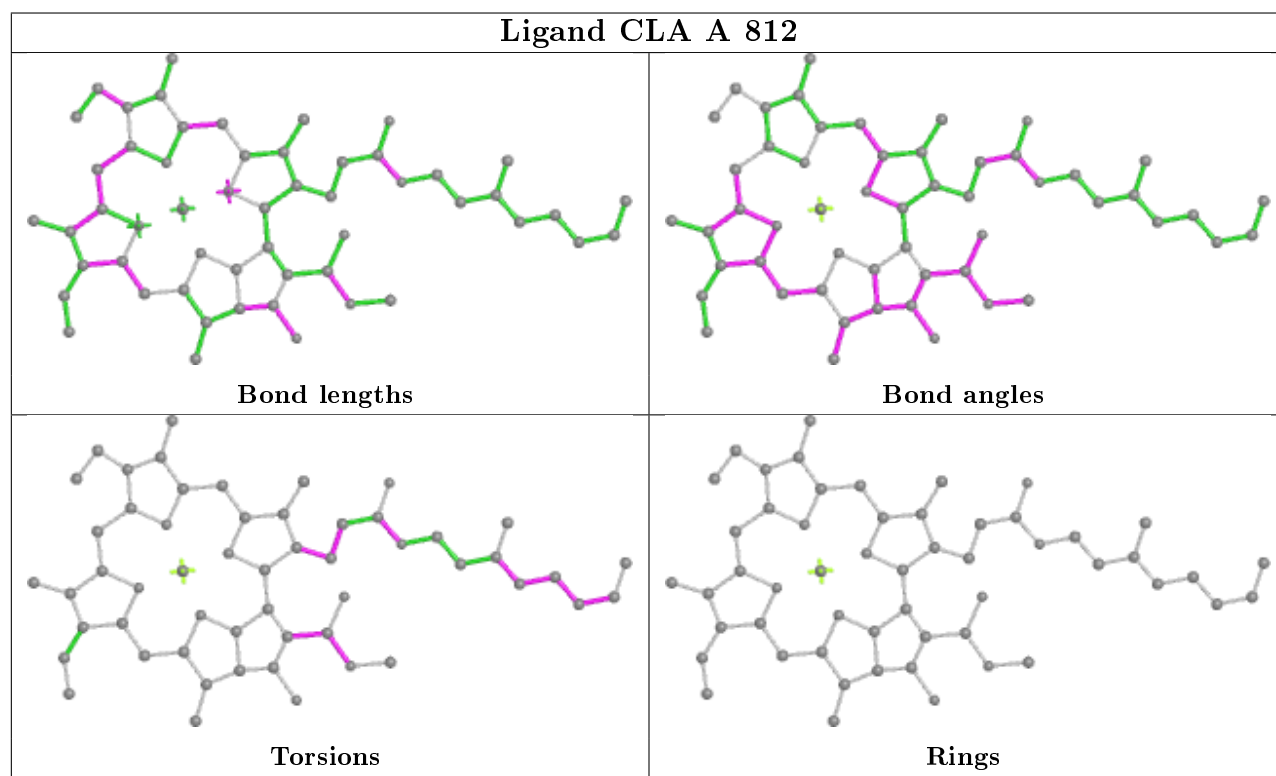
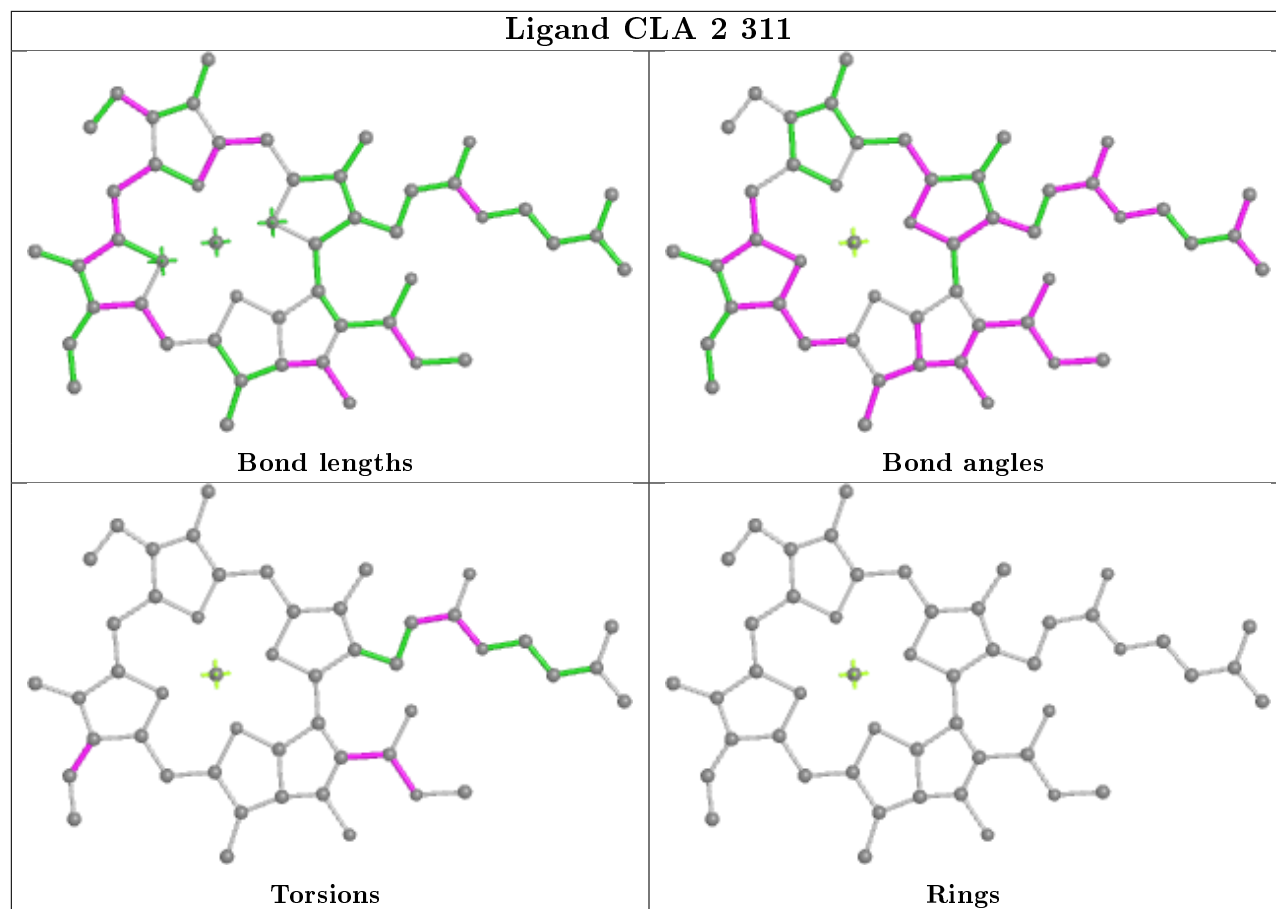


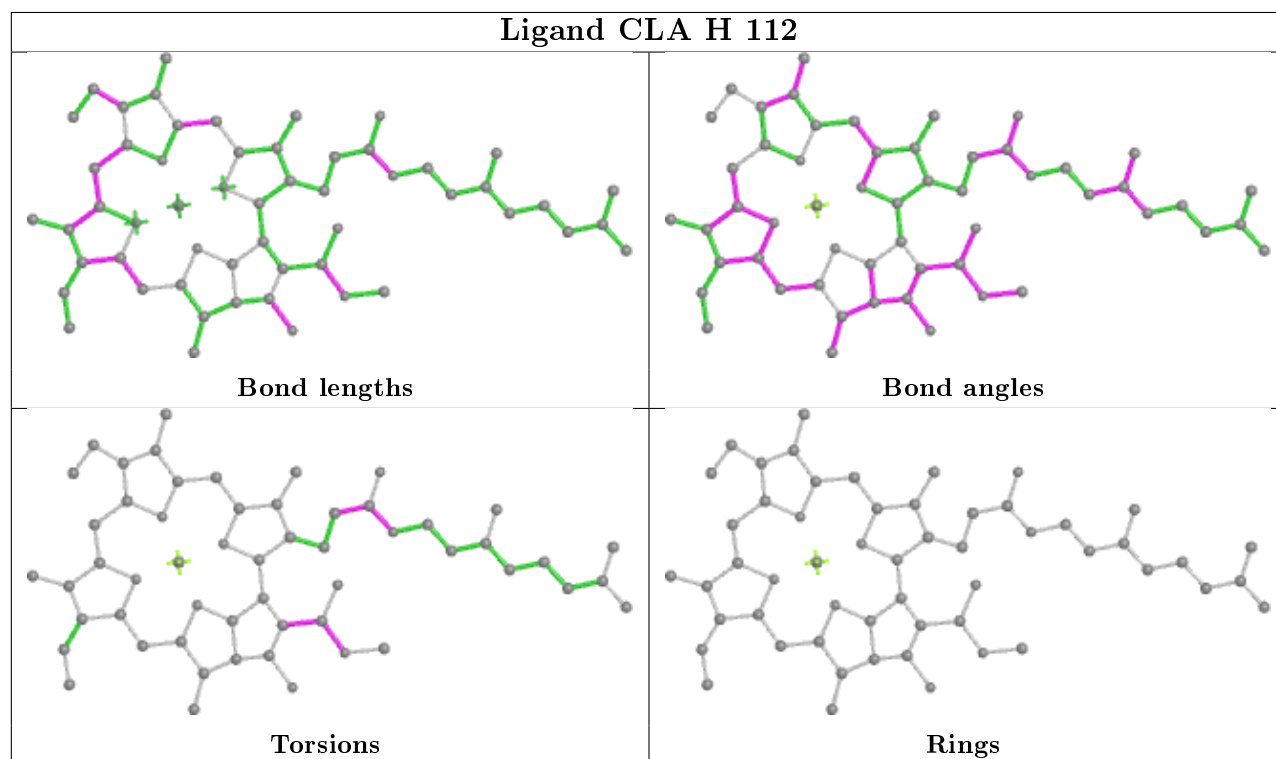
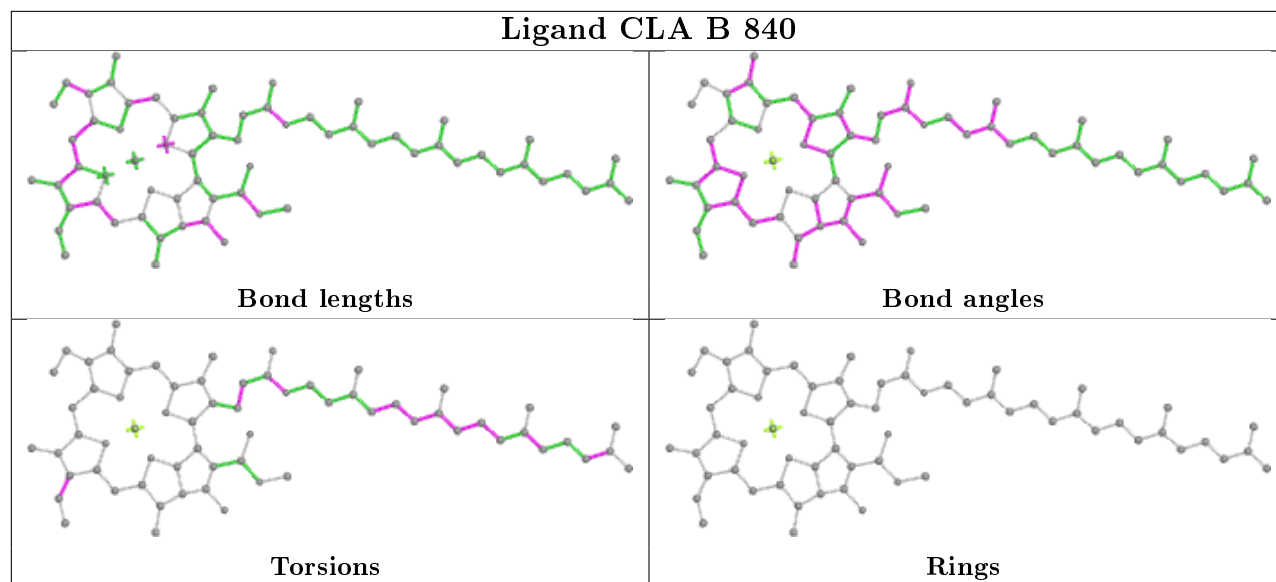


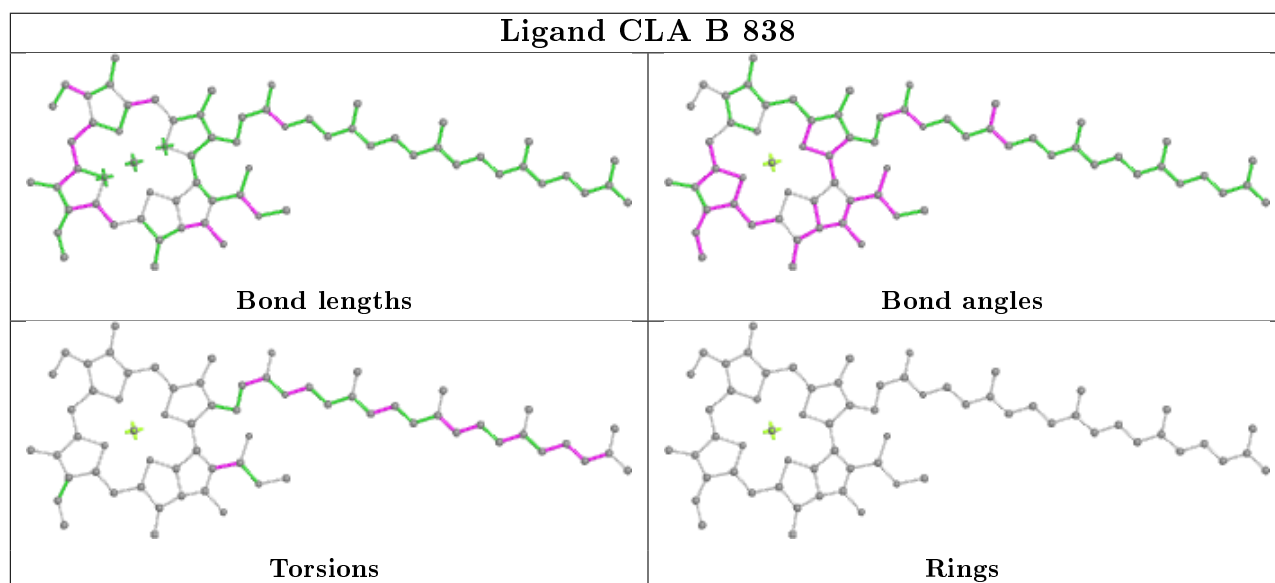
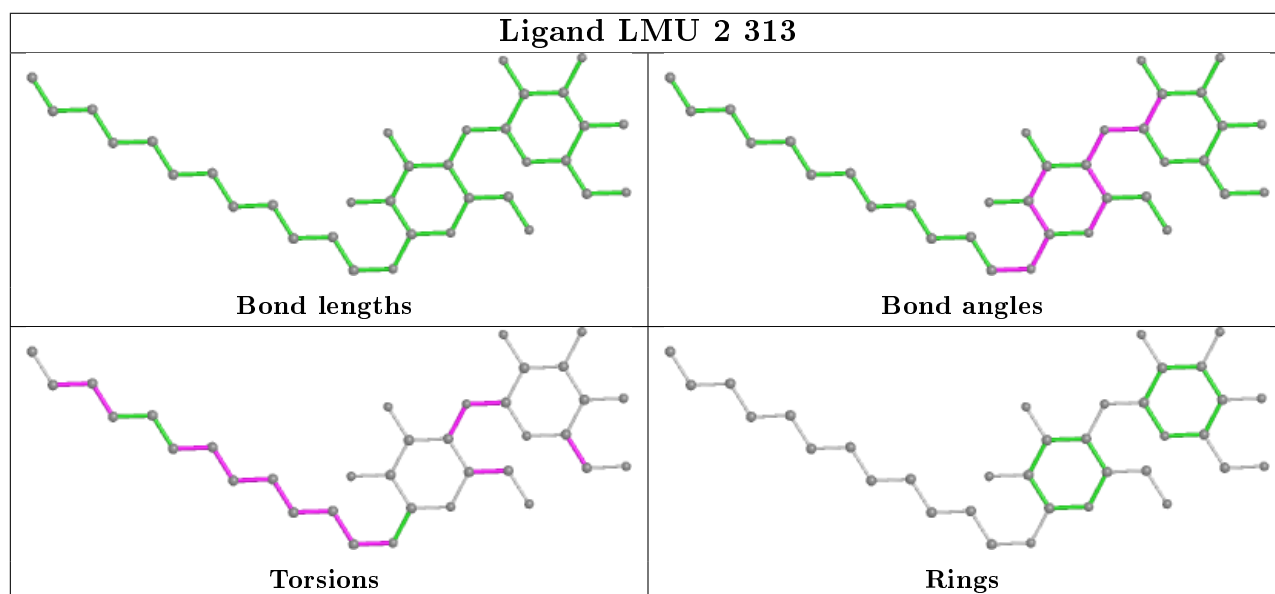
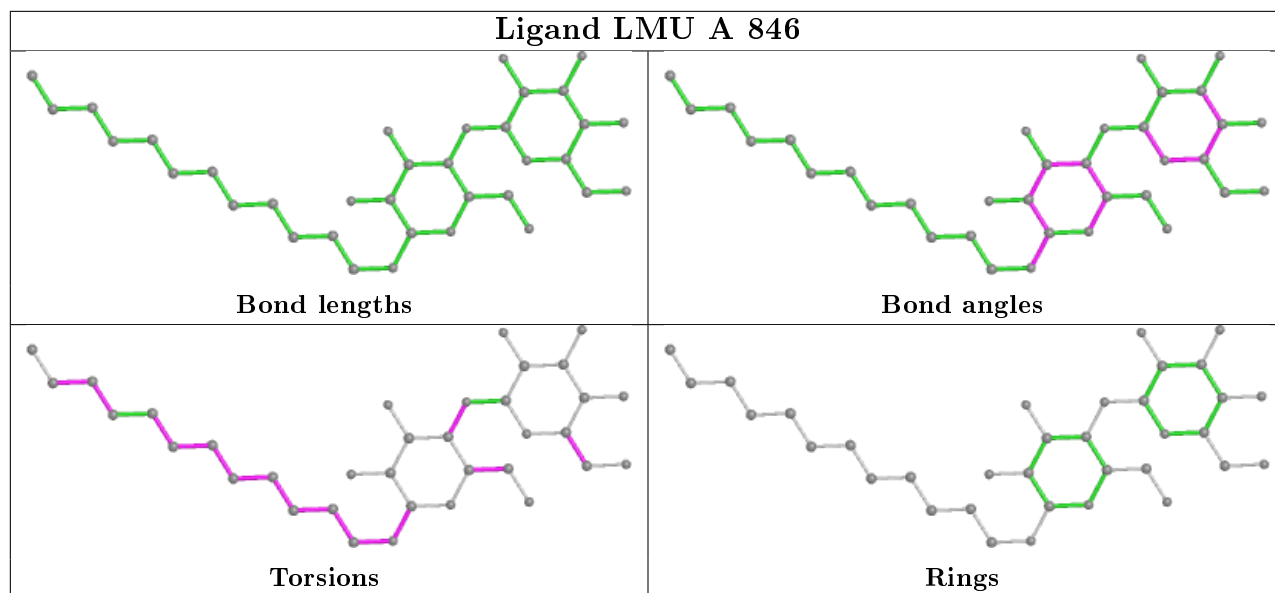


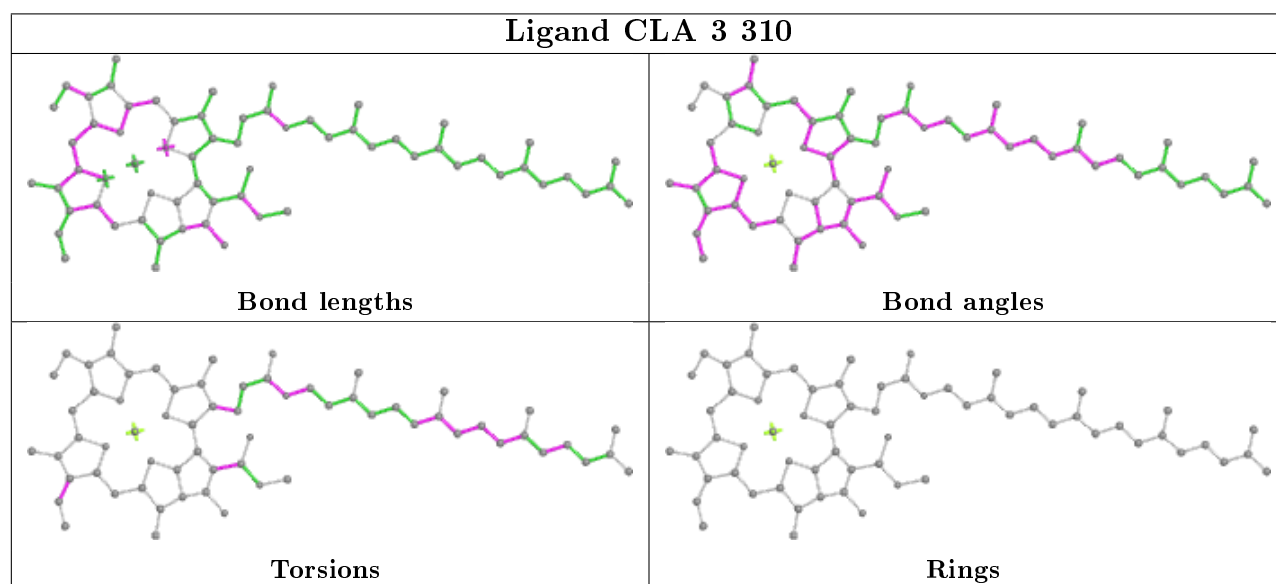
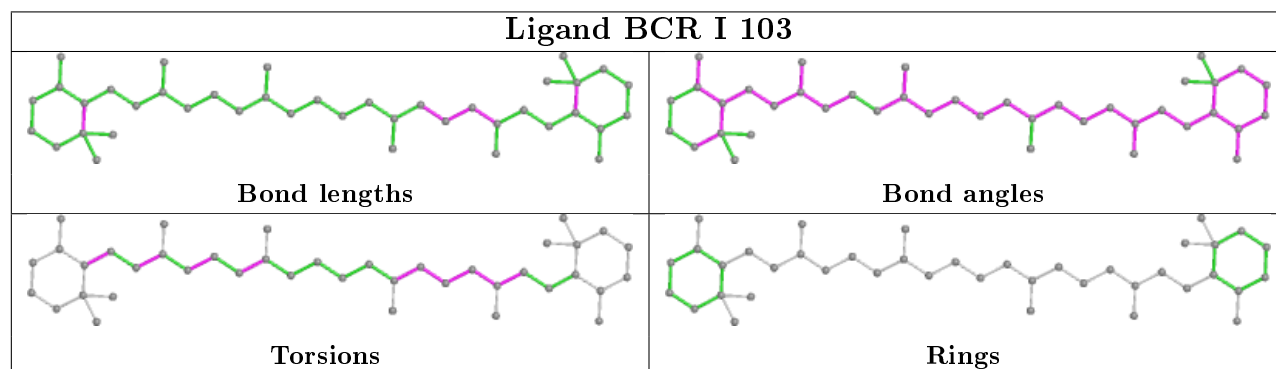
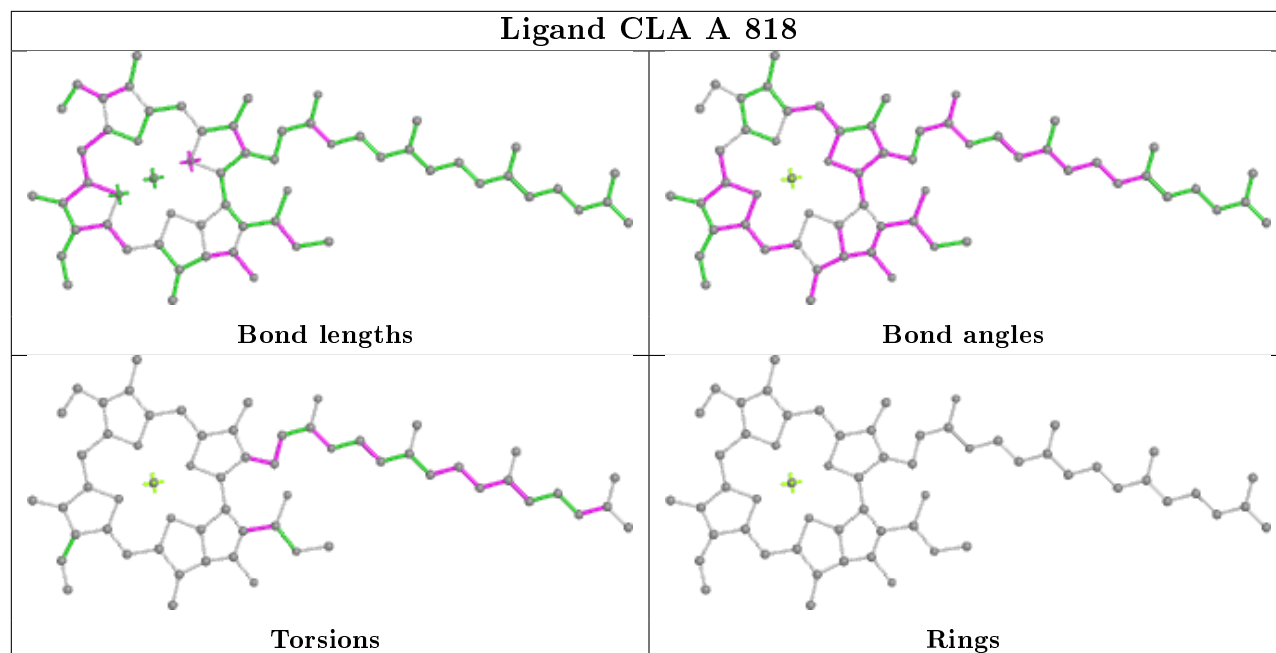


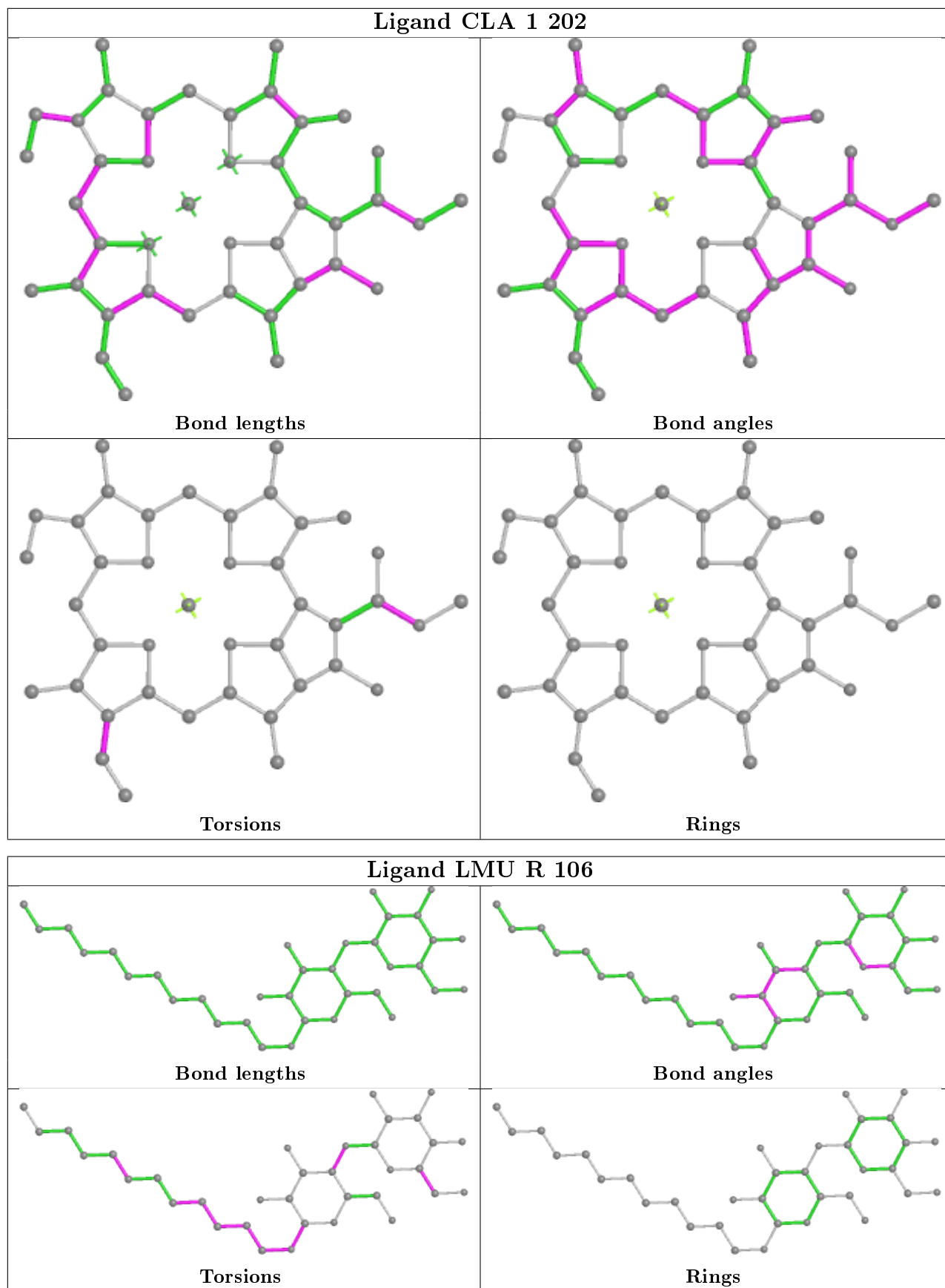


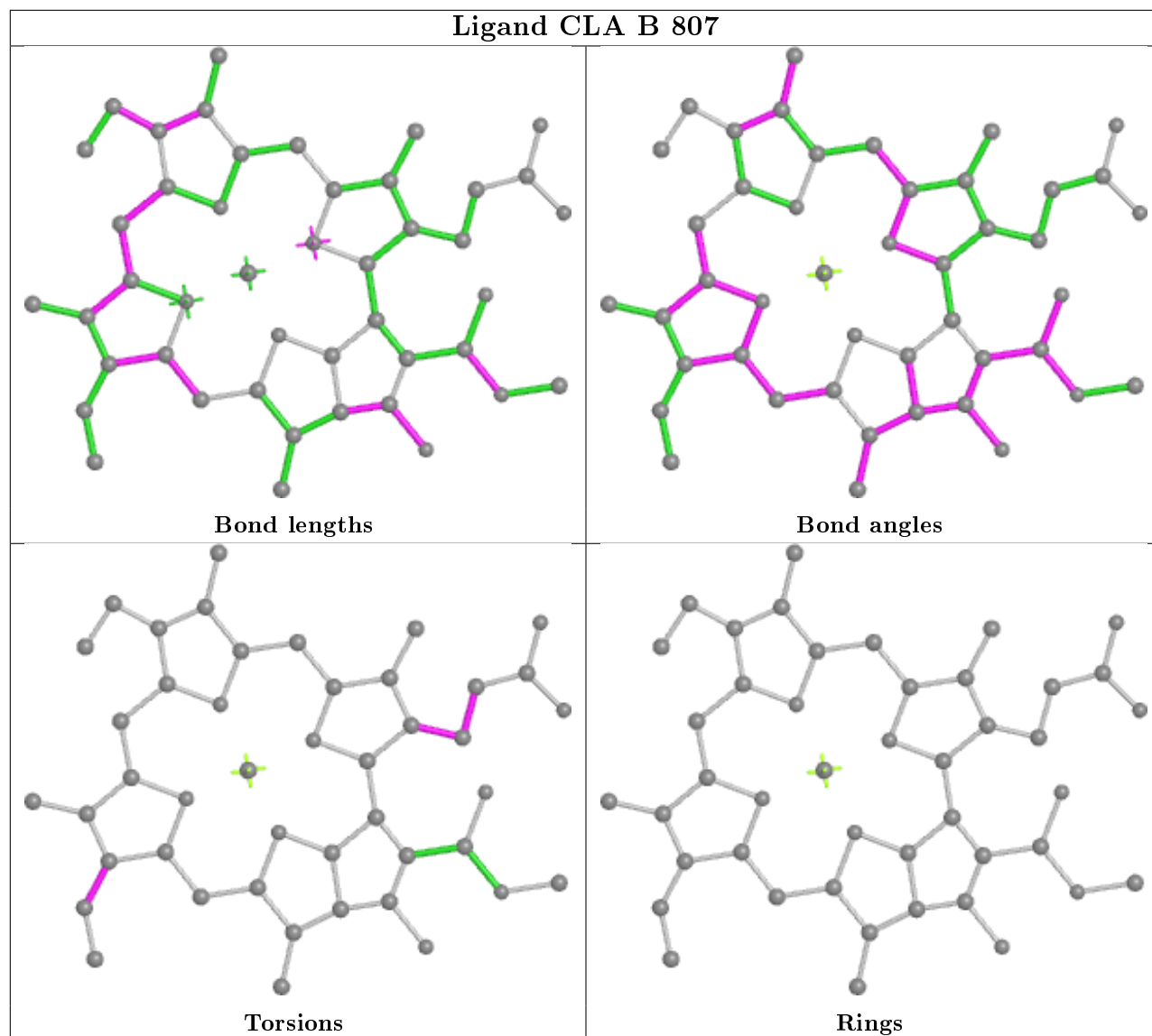


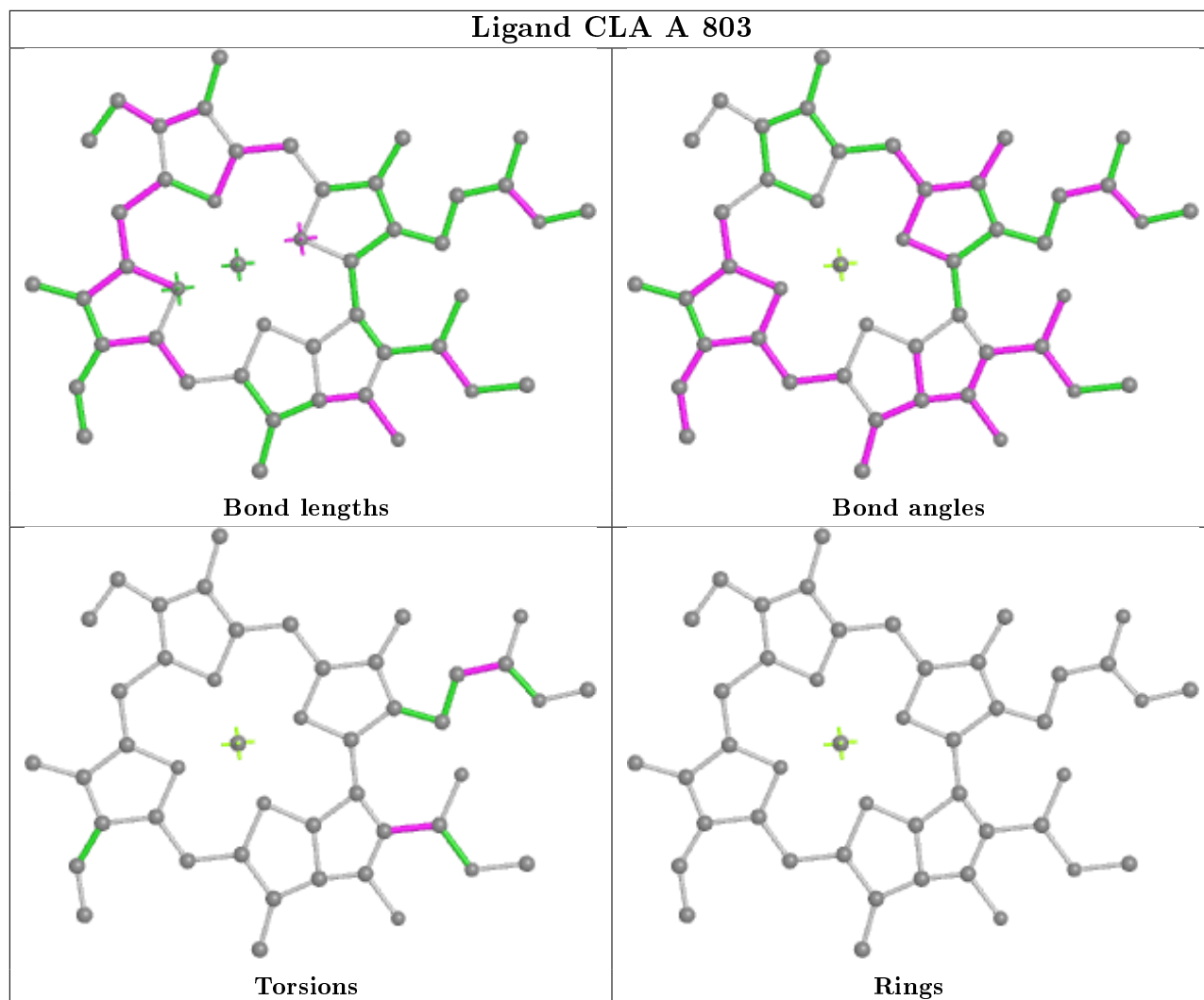


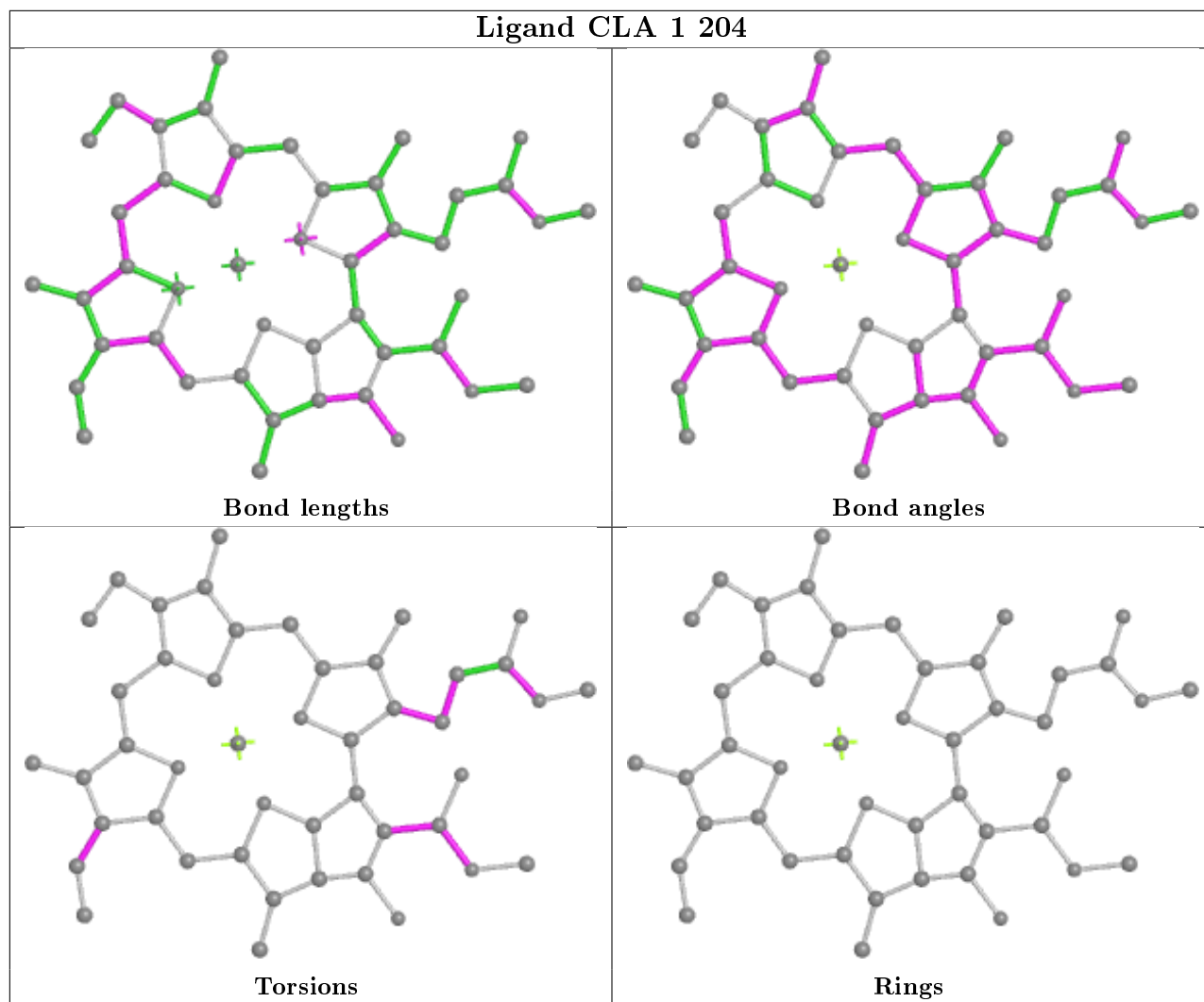


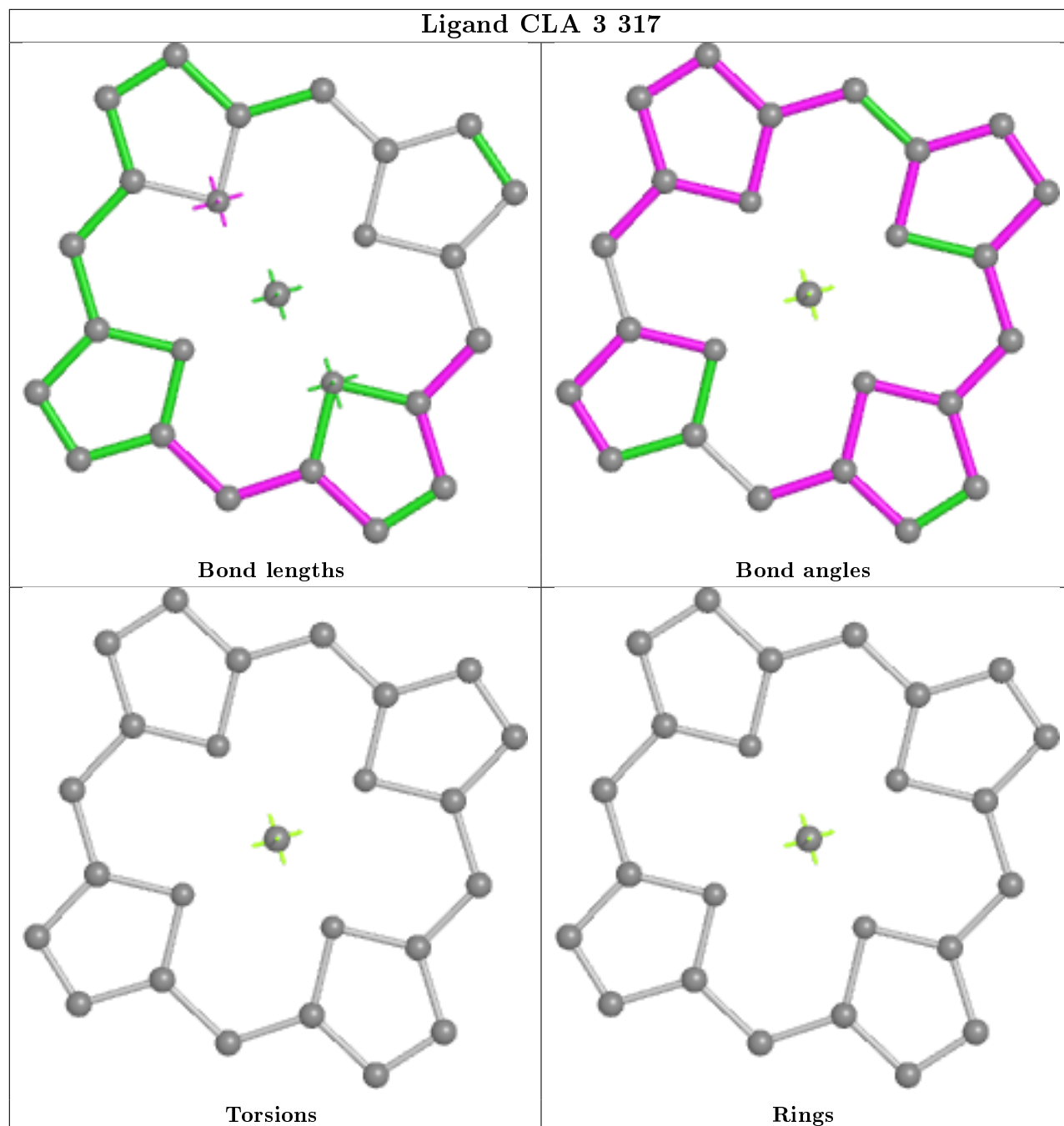


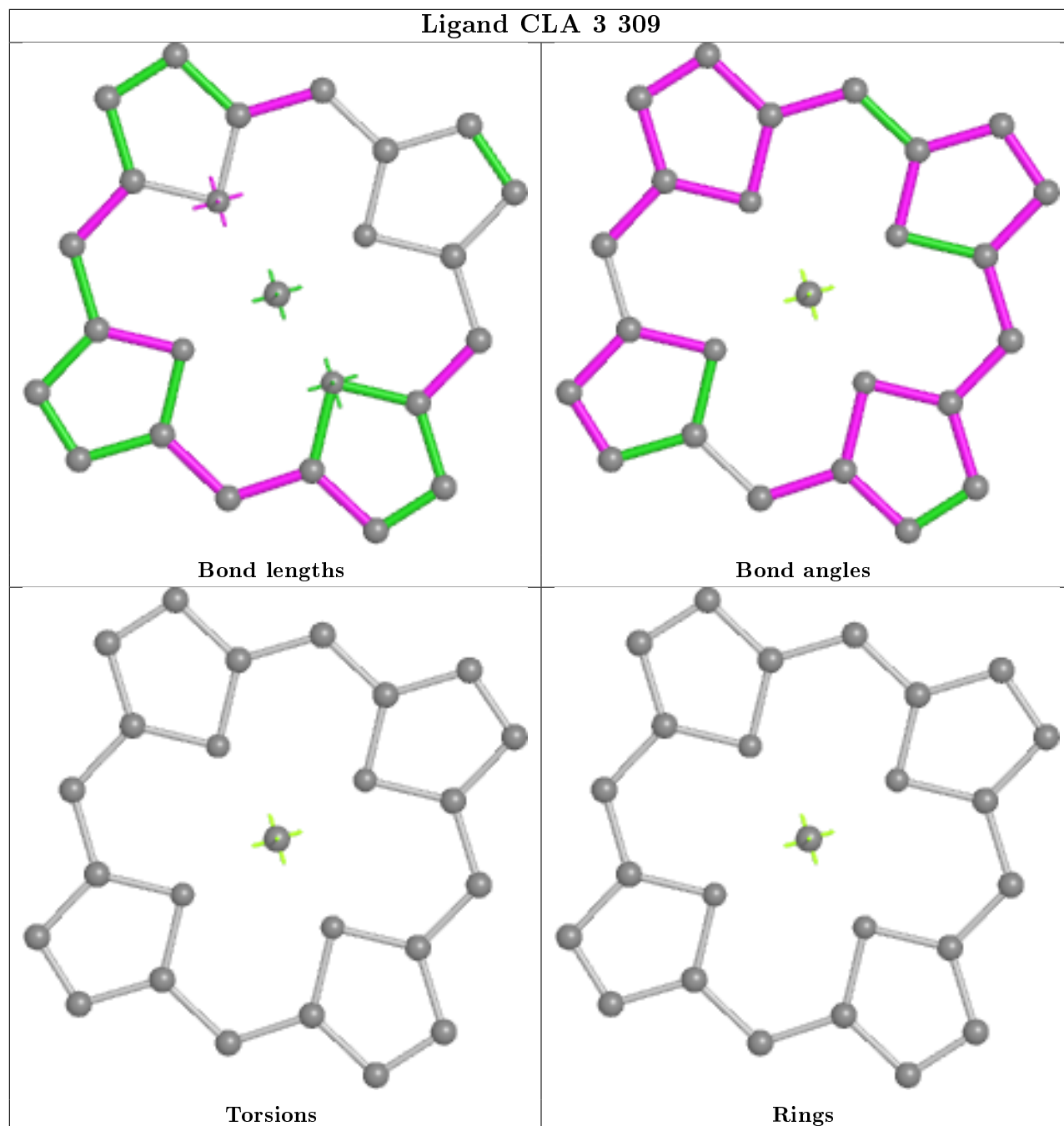


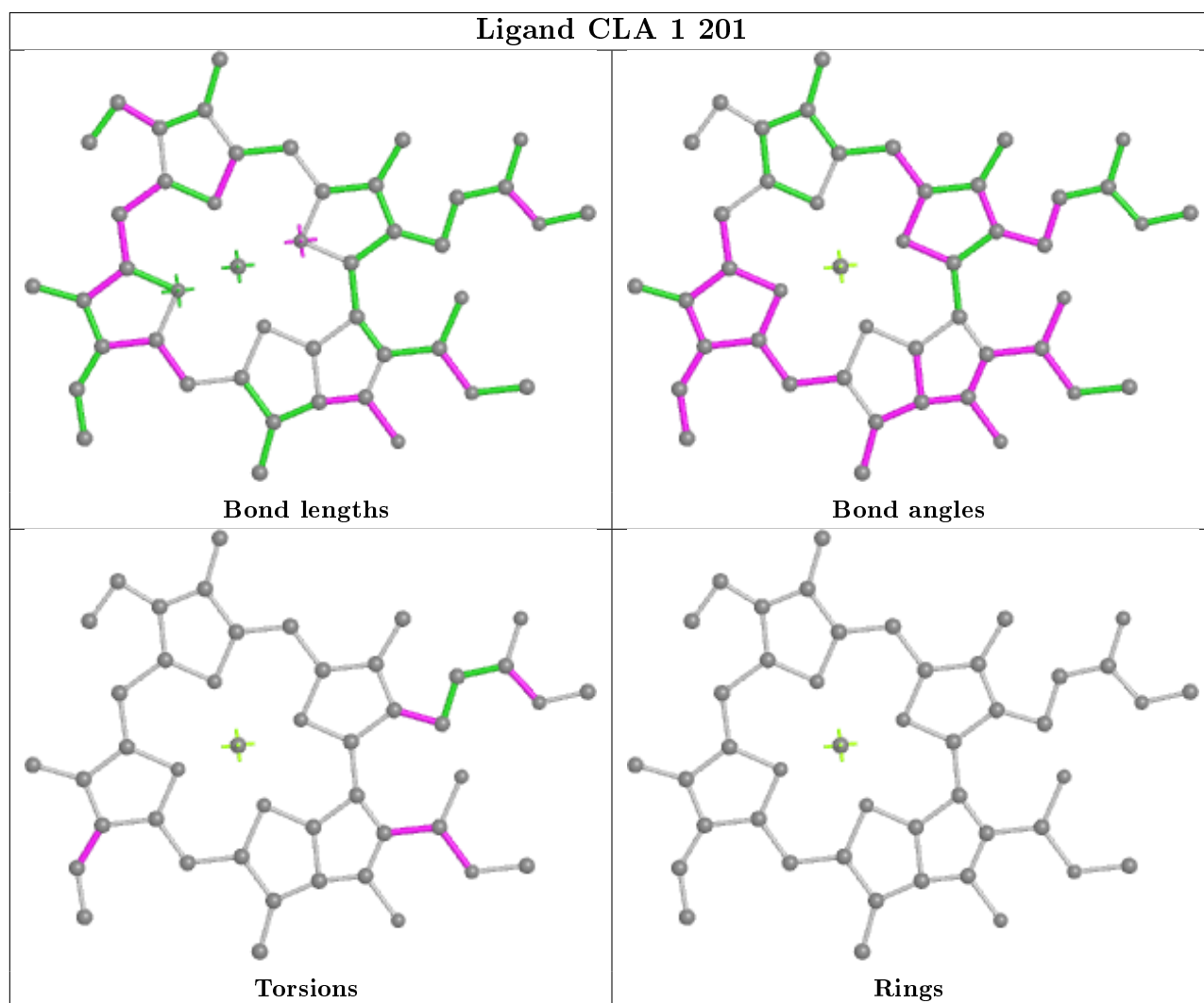
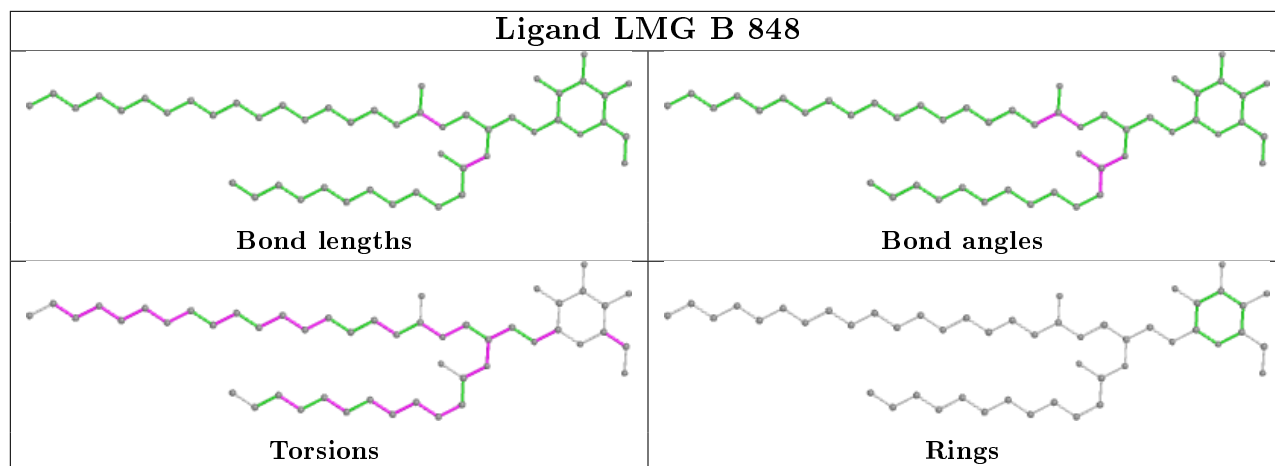


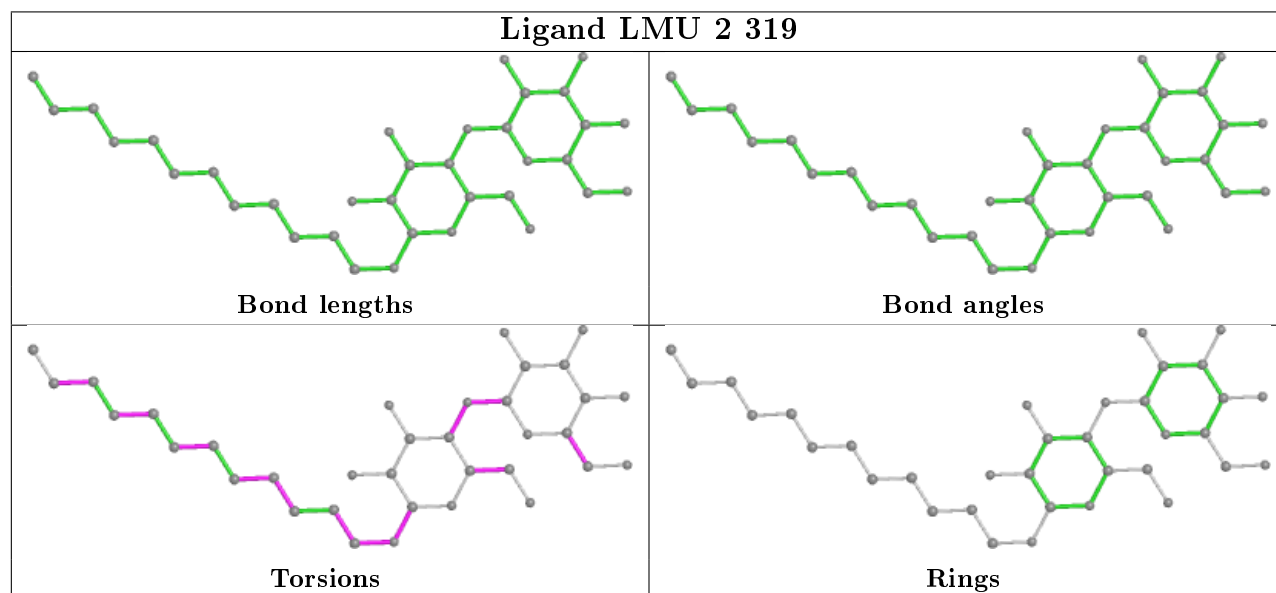
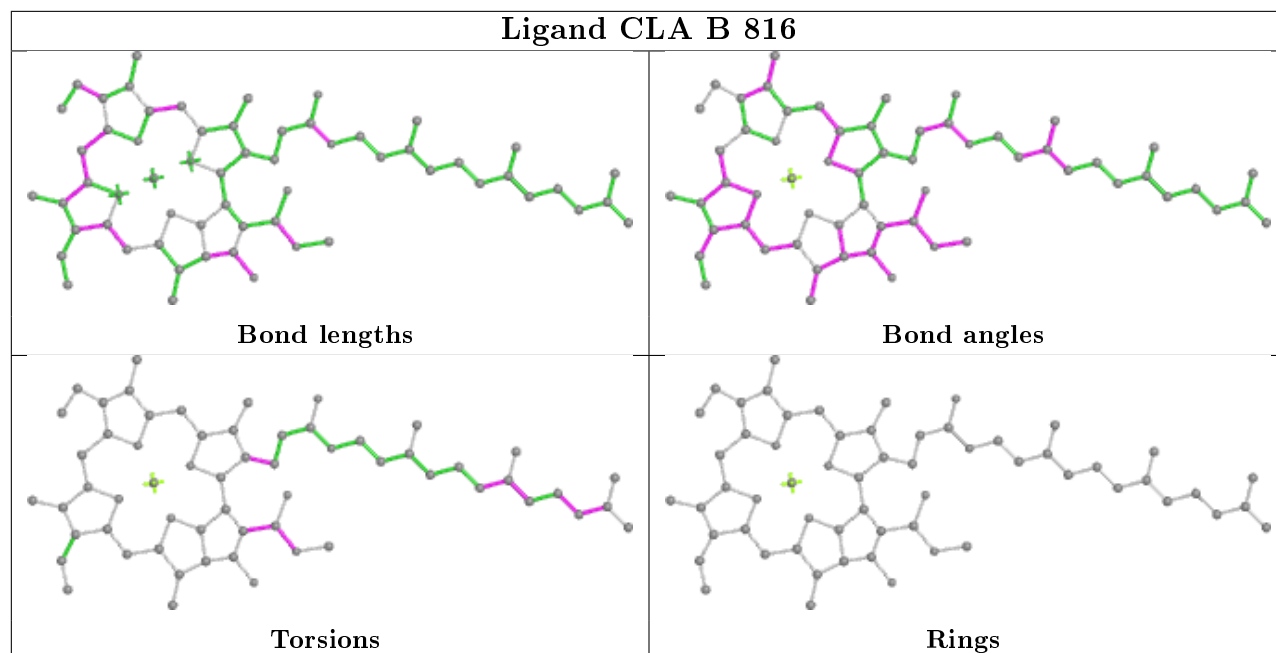


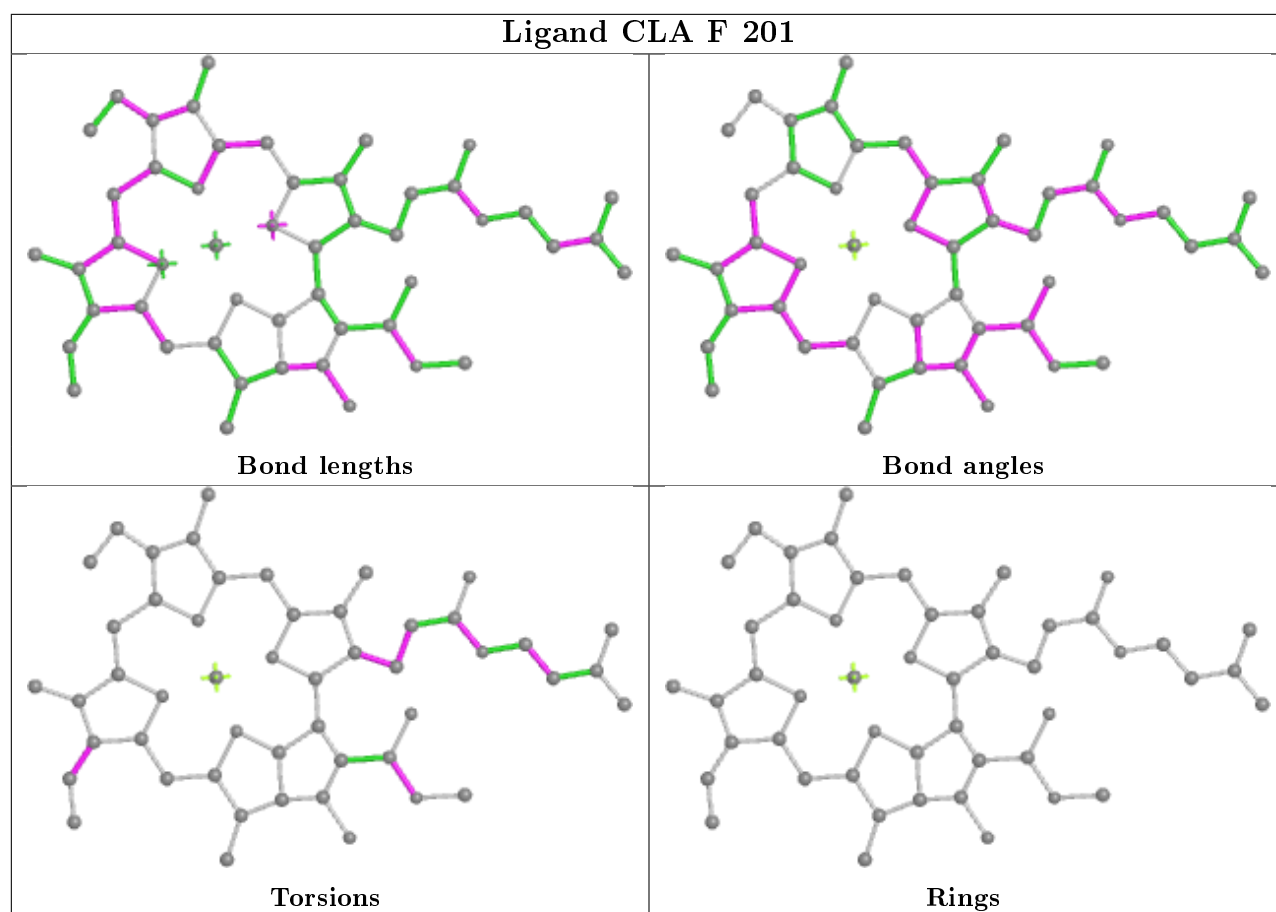


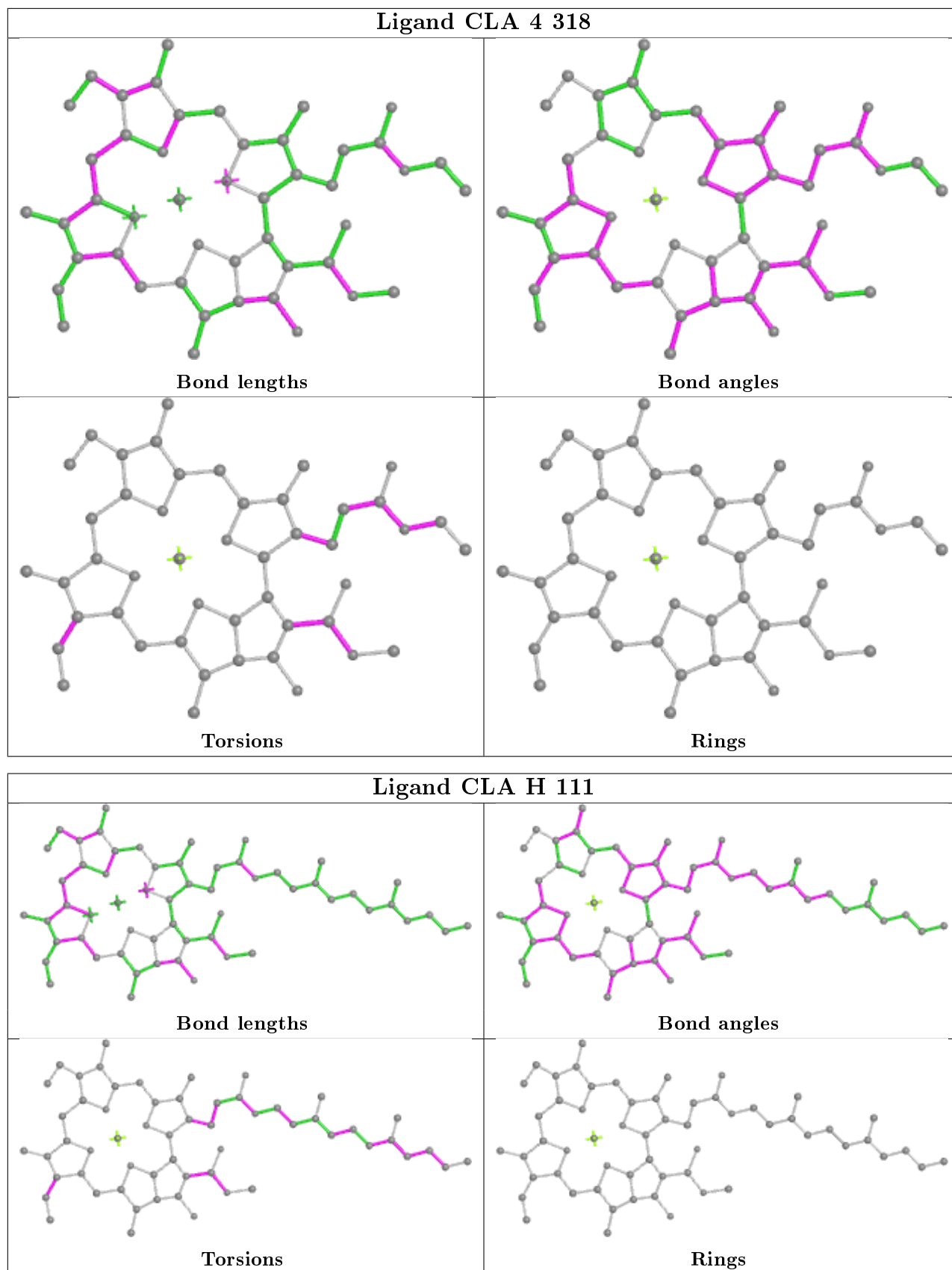




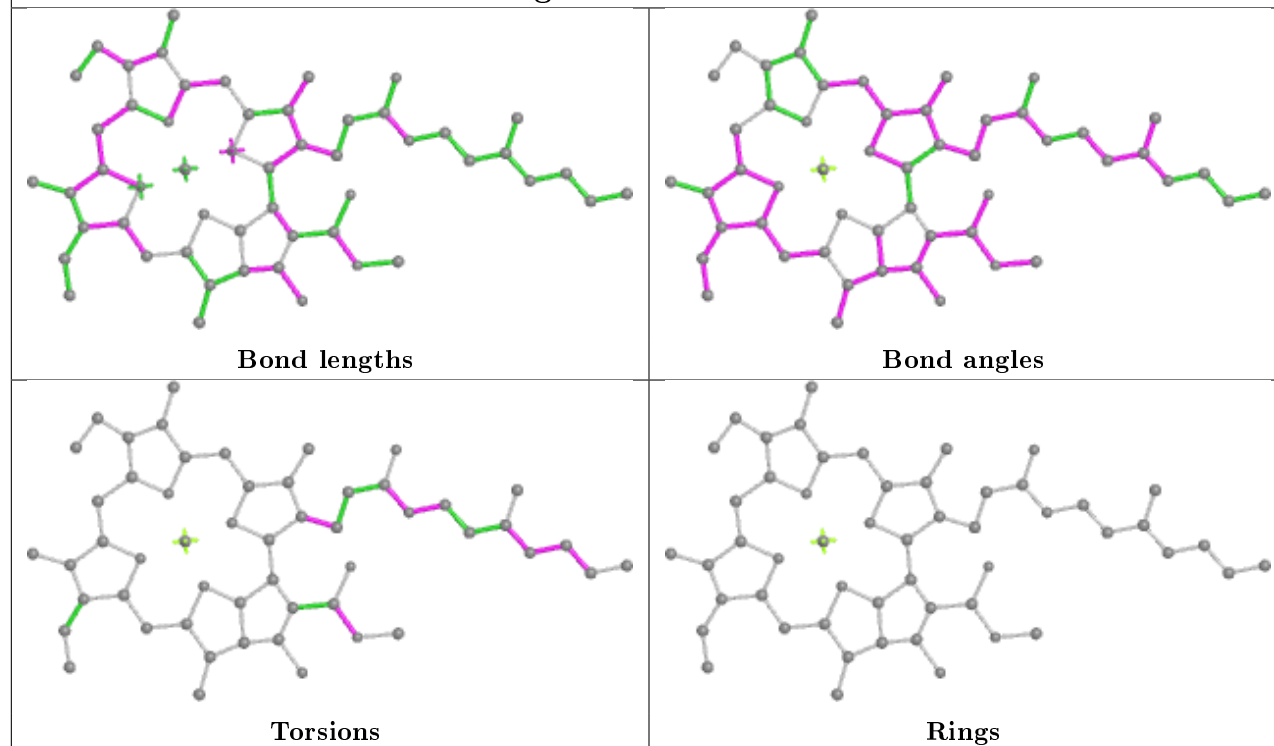




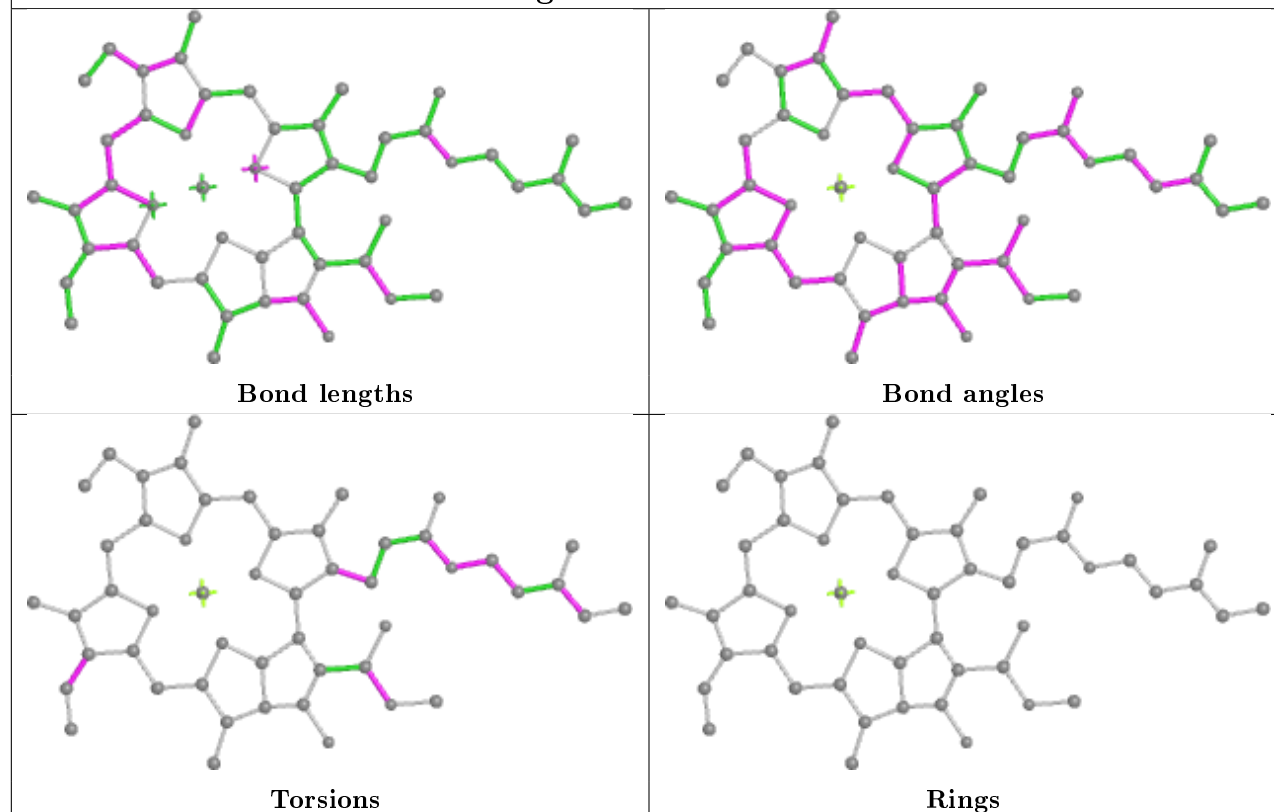


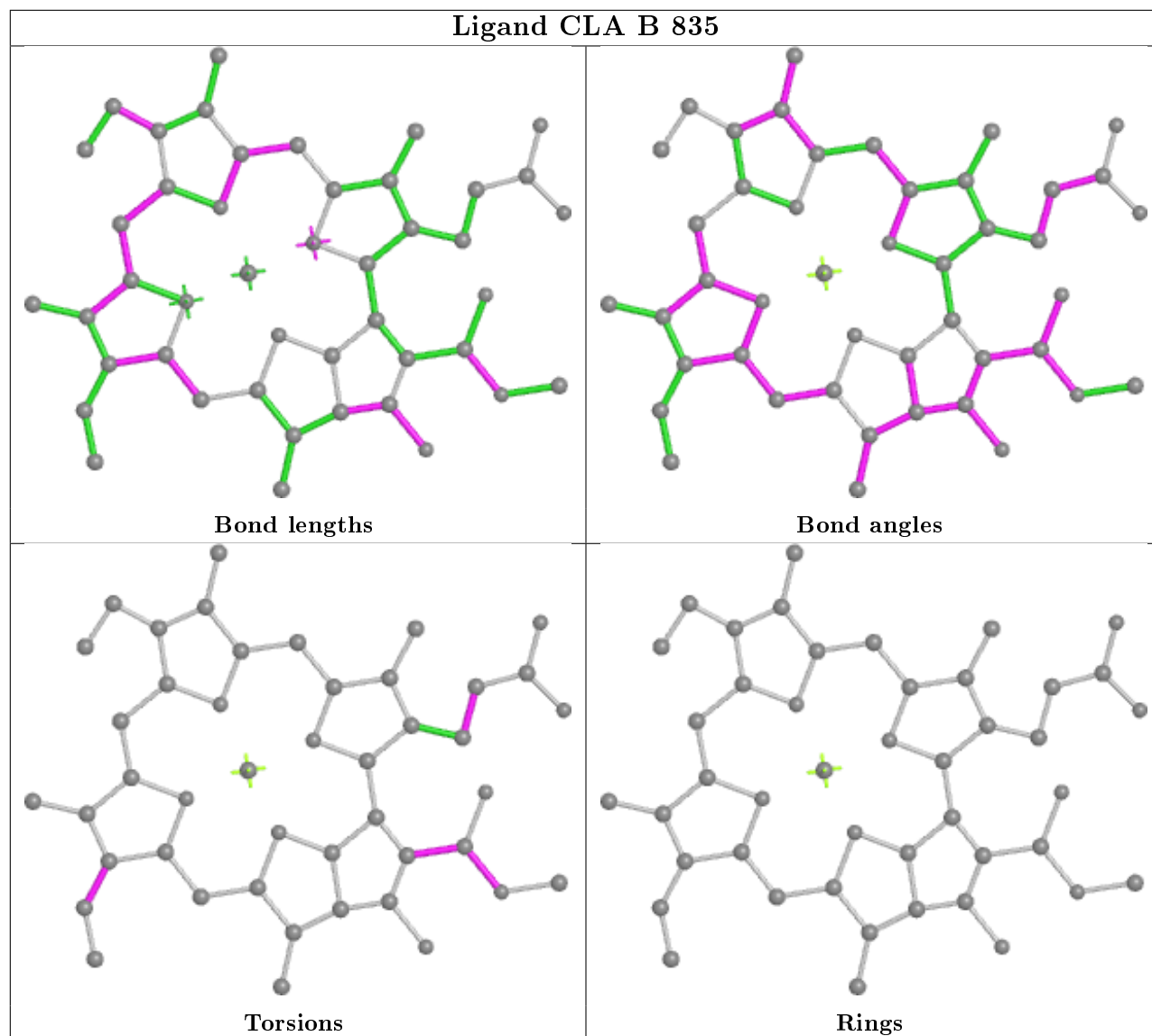


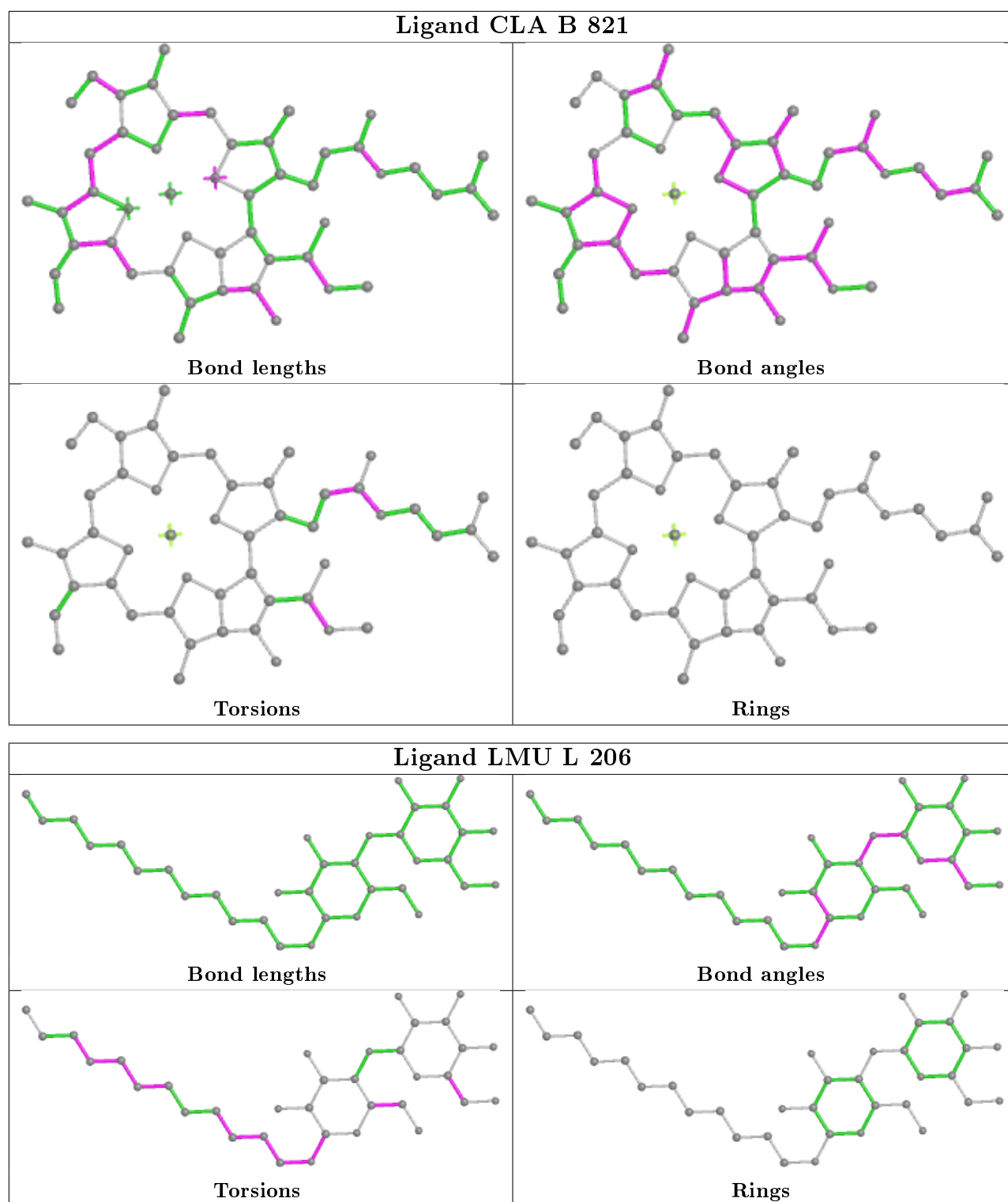
Ligand CLA F 207

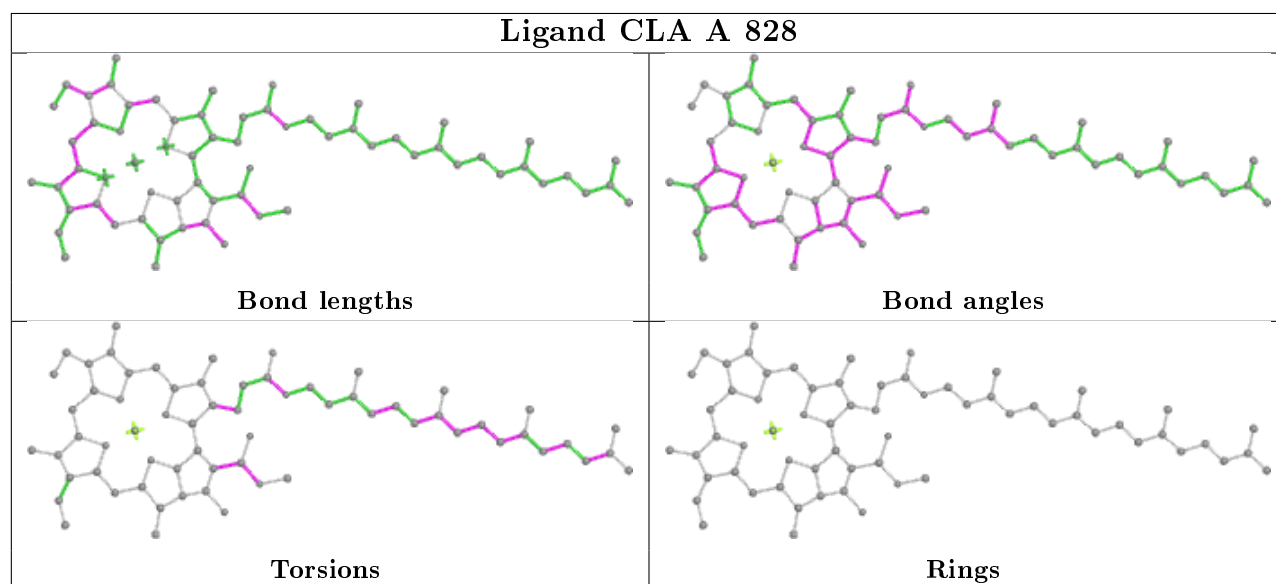
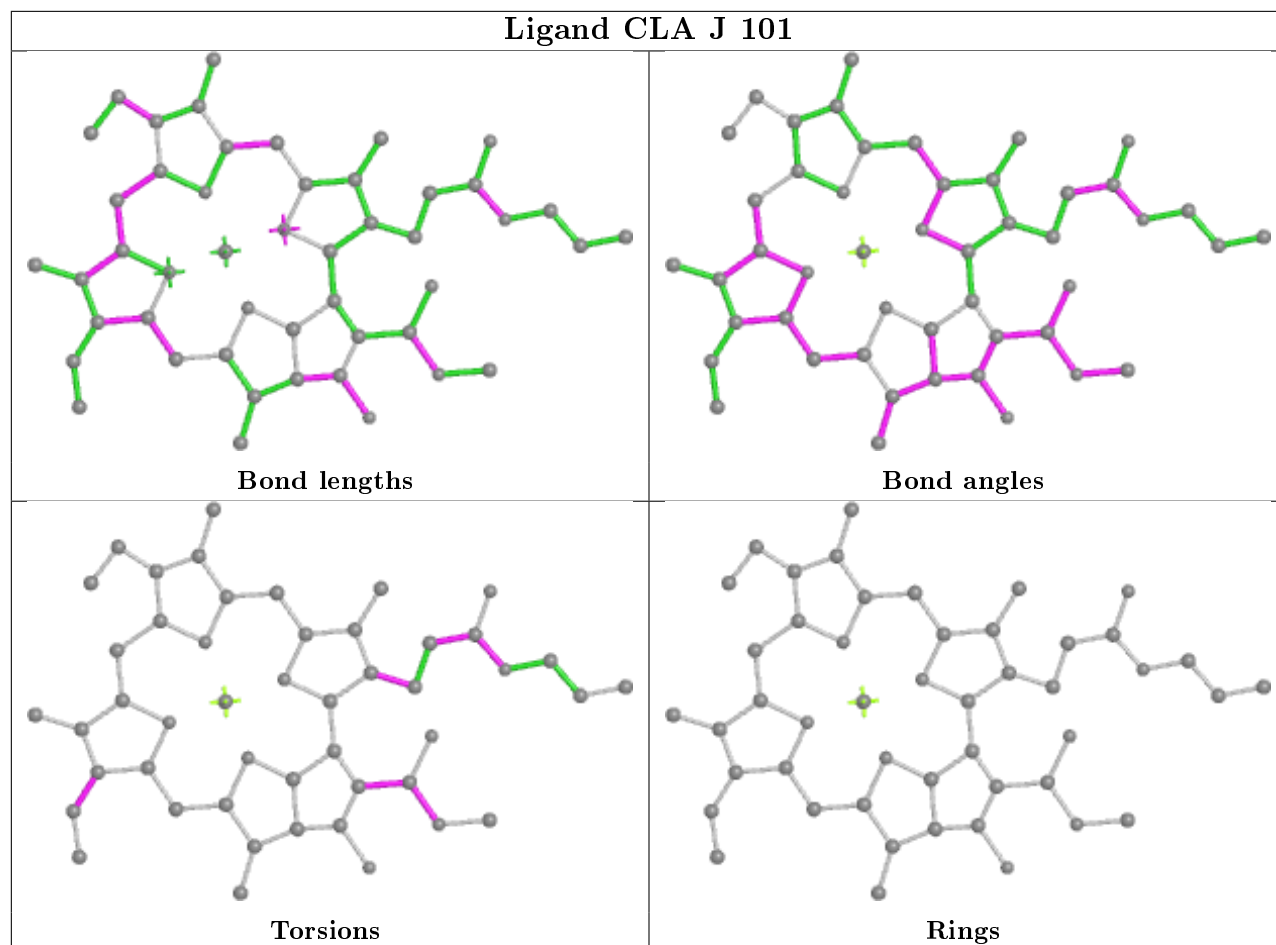


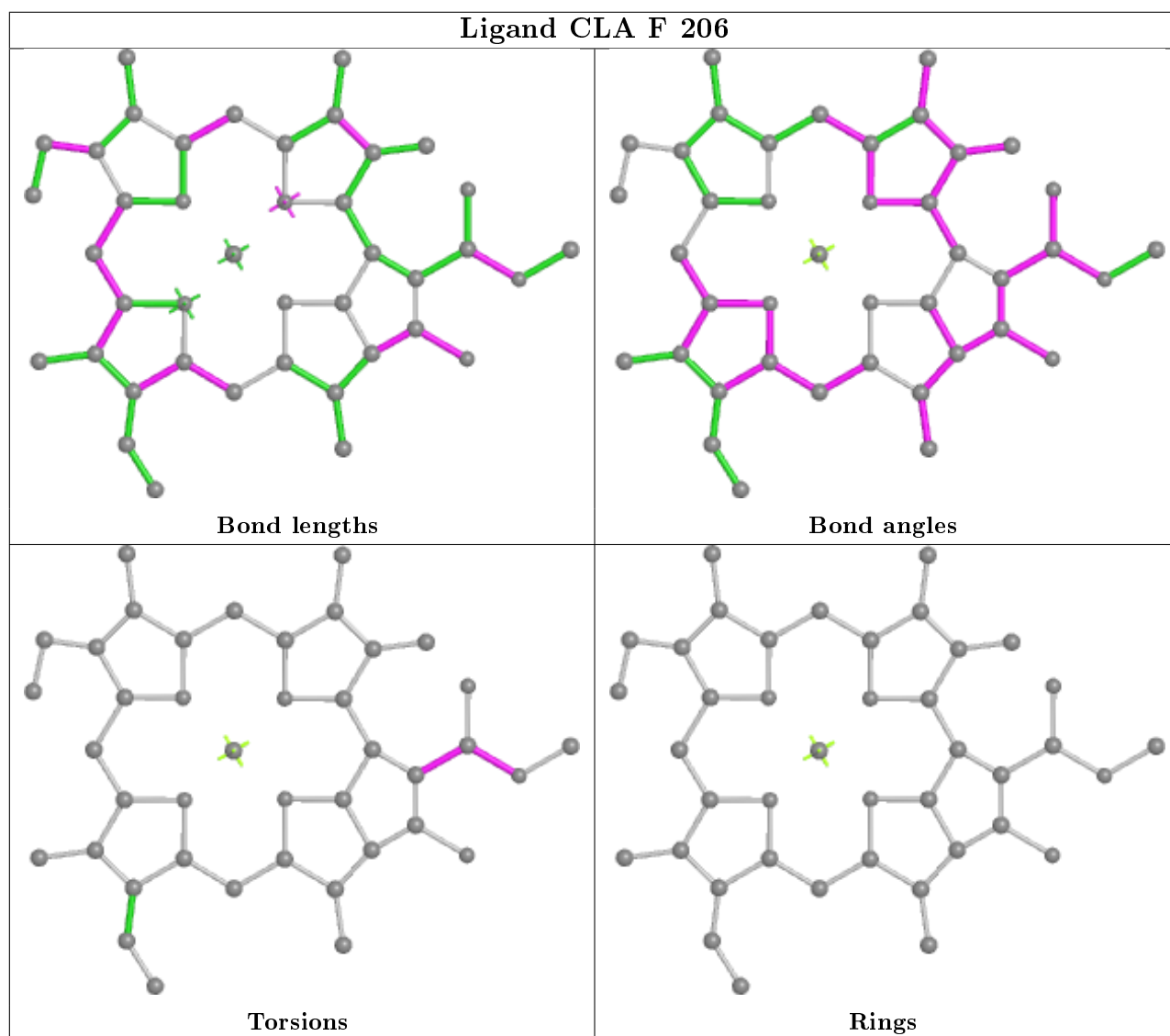
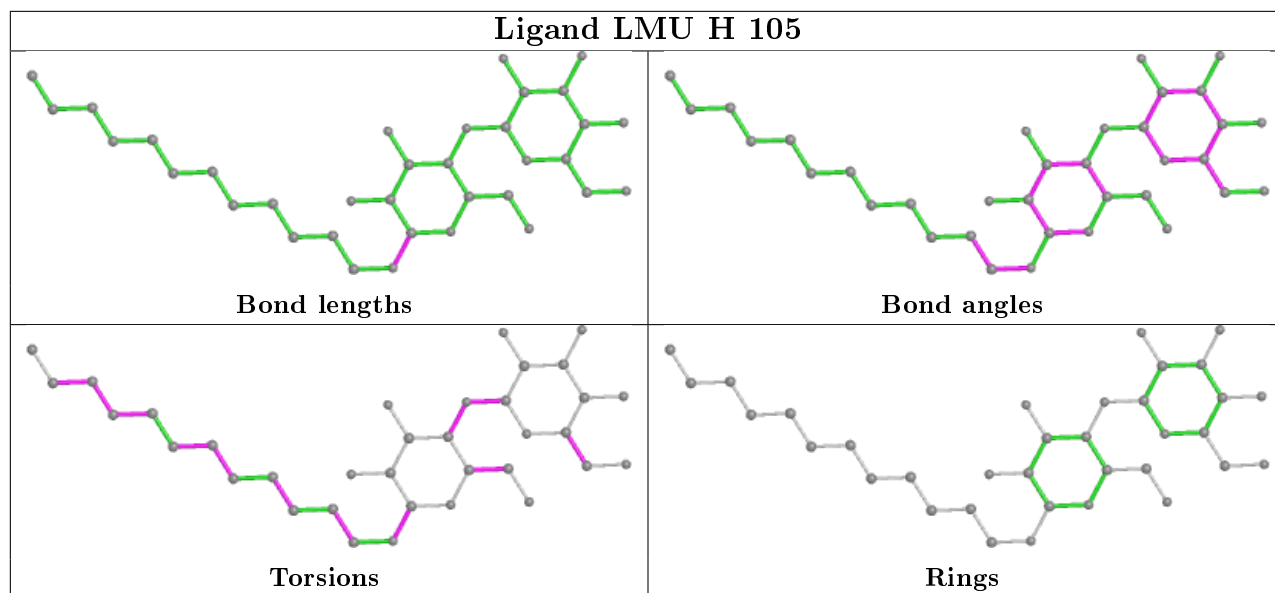
Ligand CLA 2 302

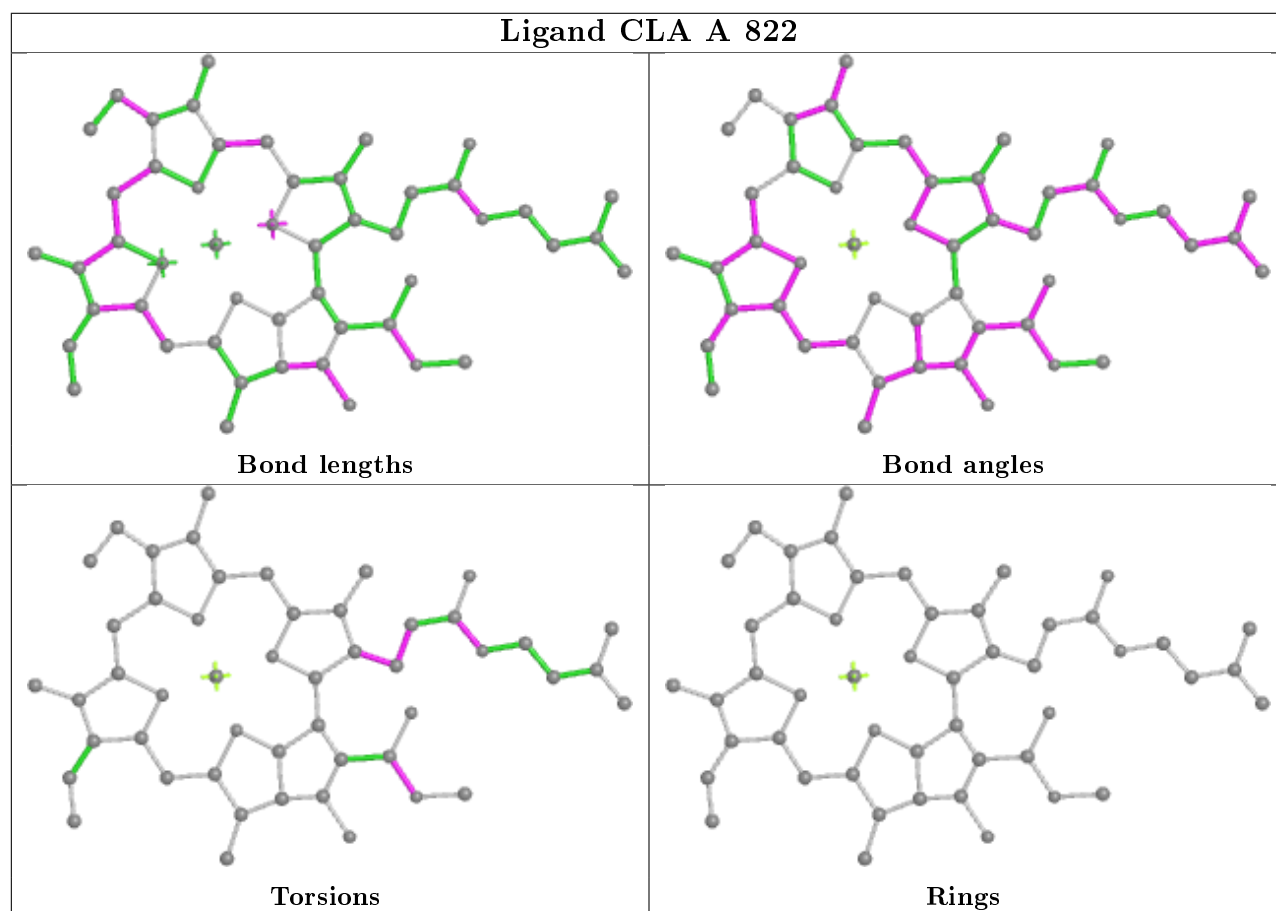
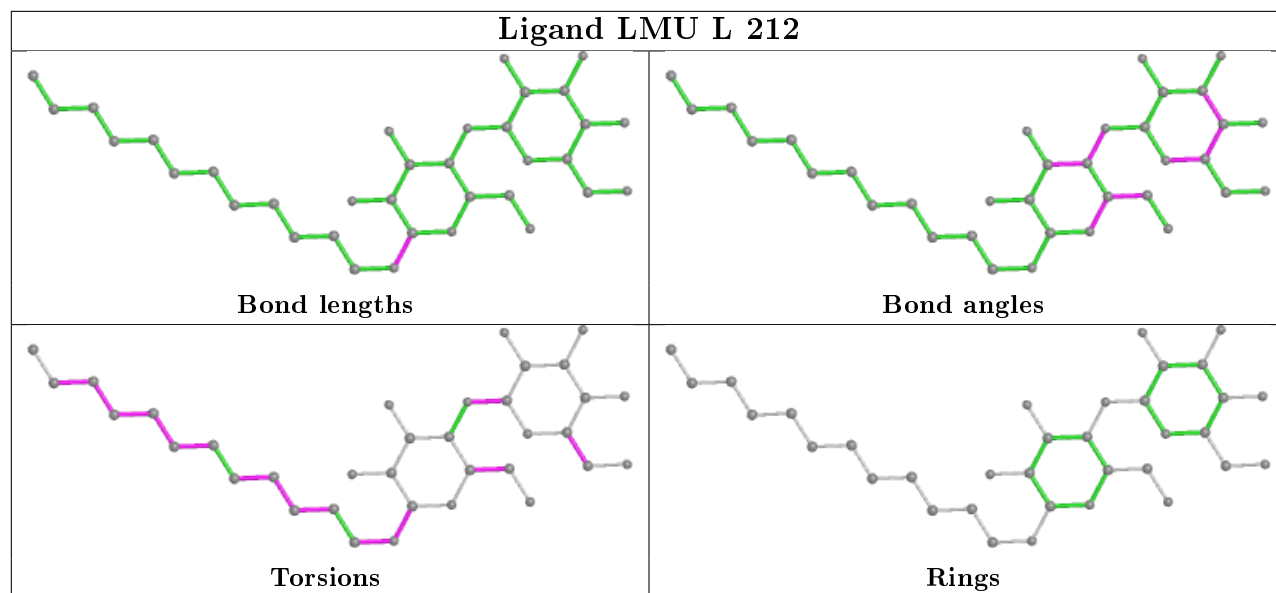


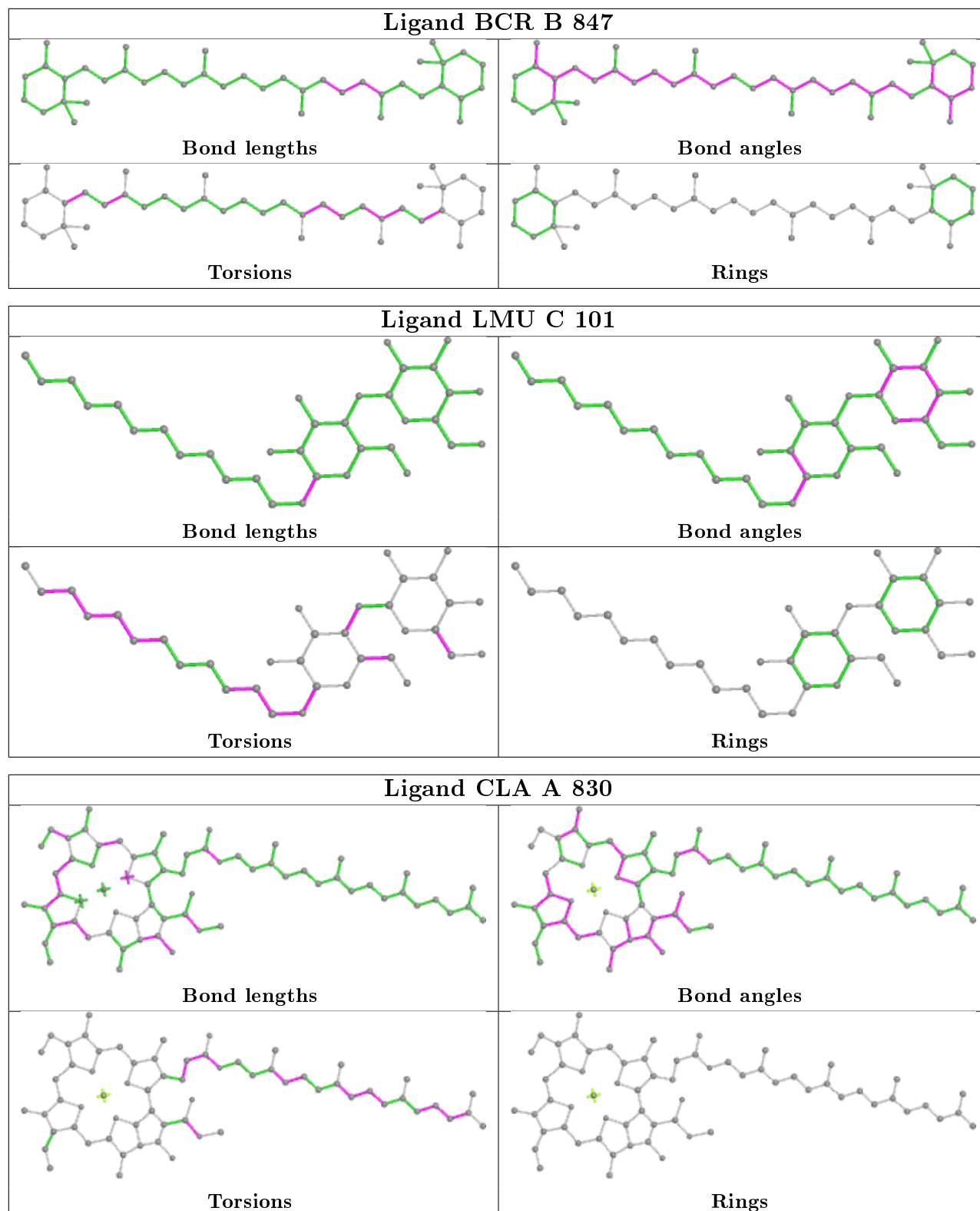


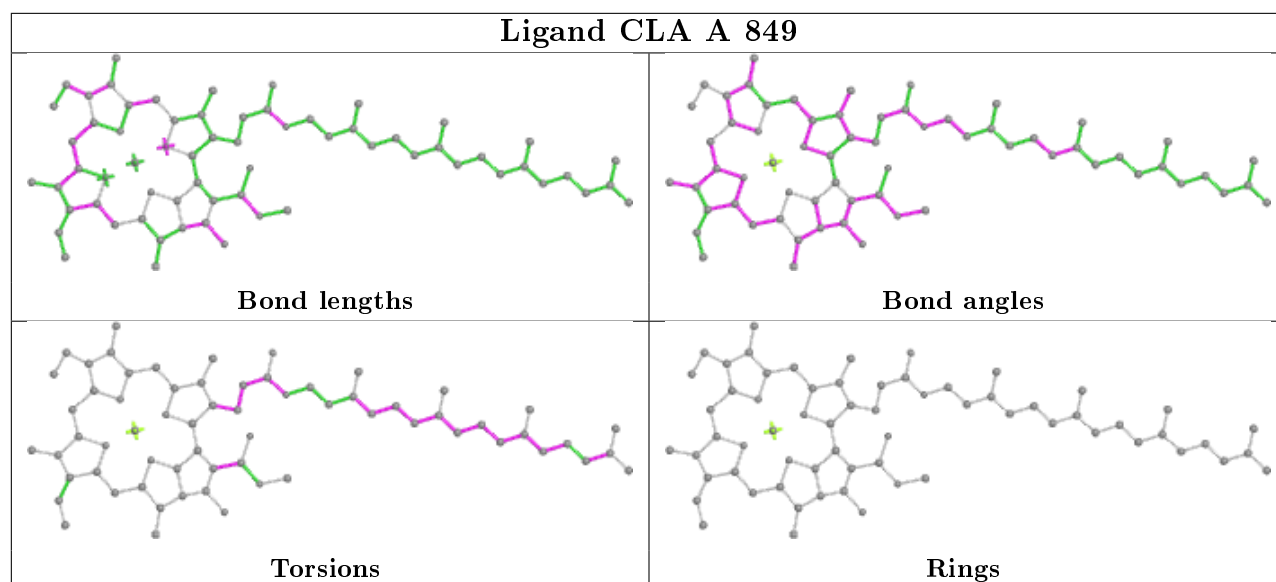
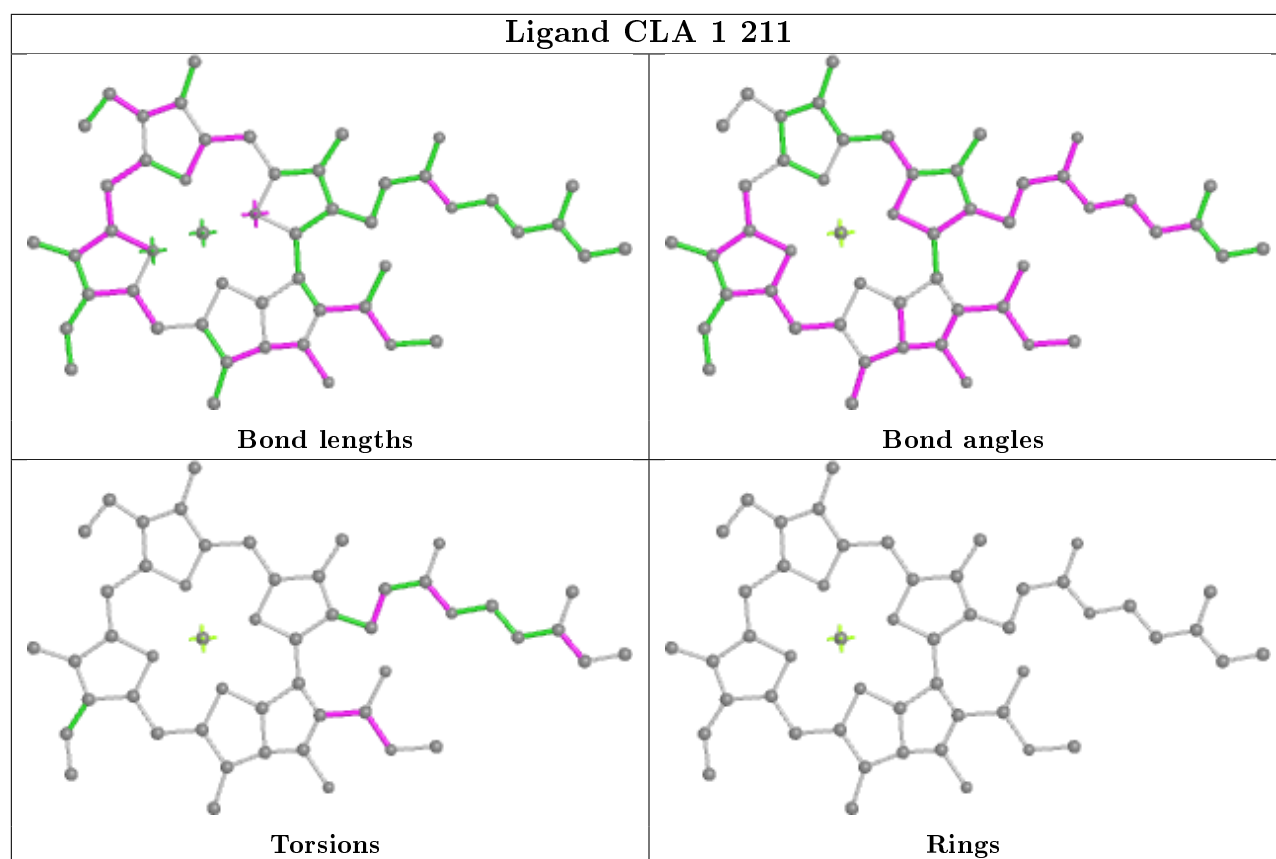


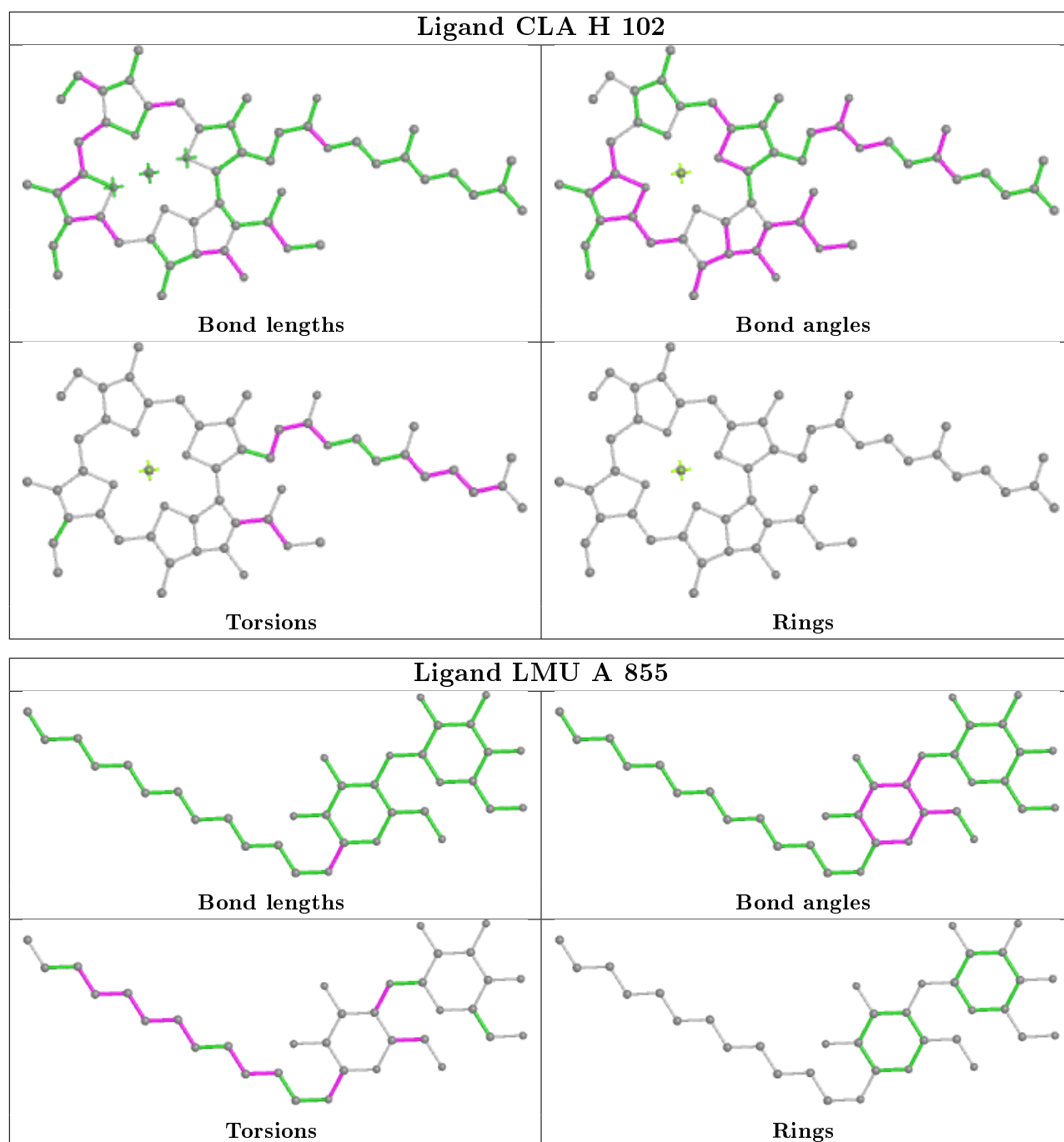


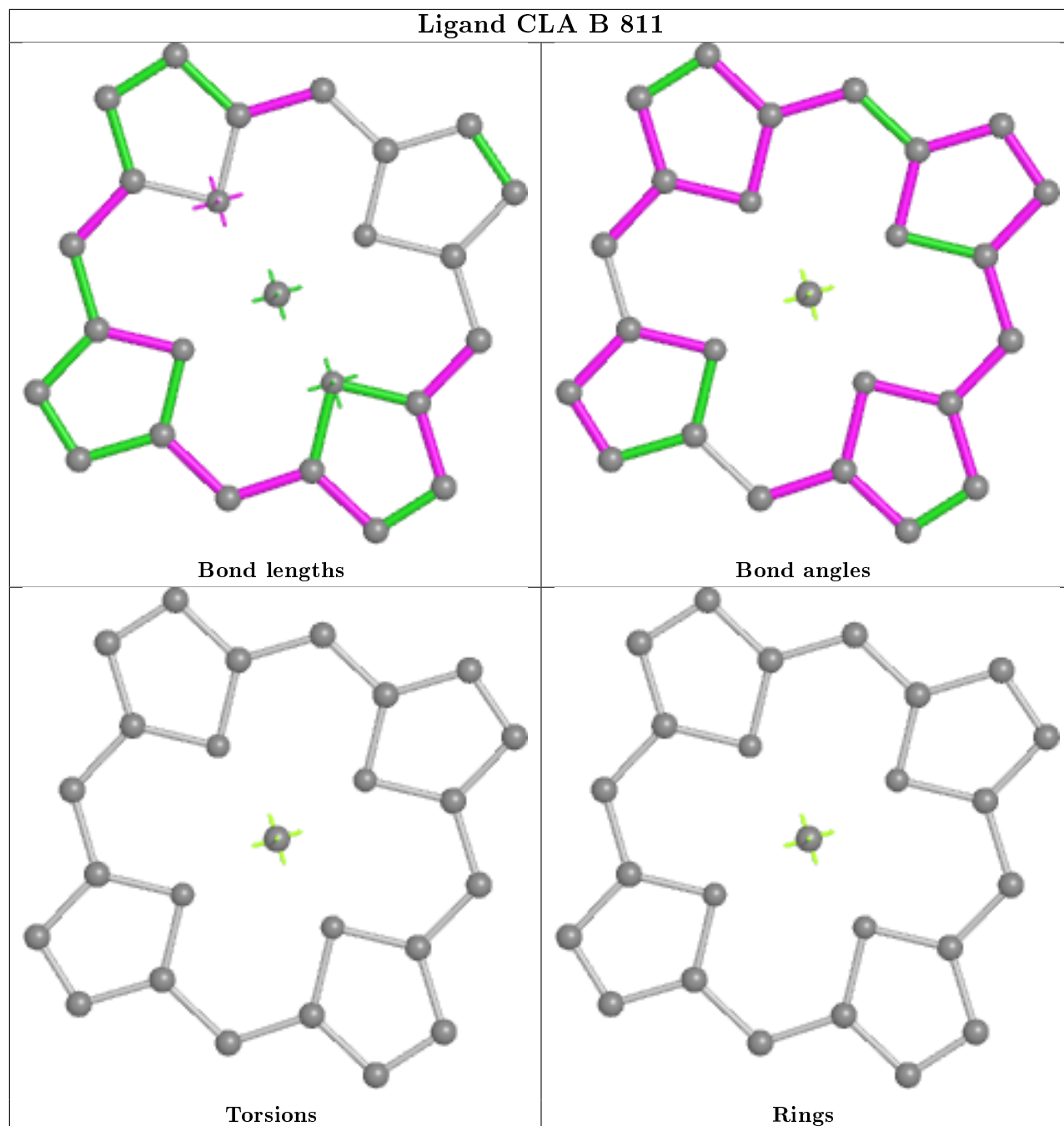


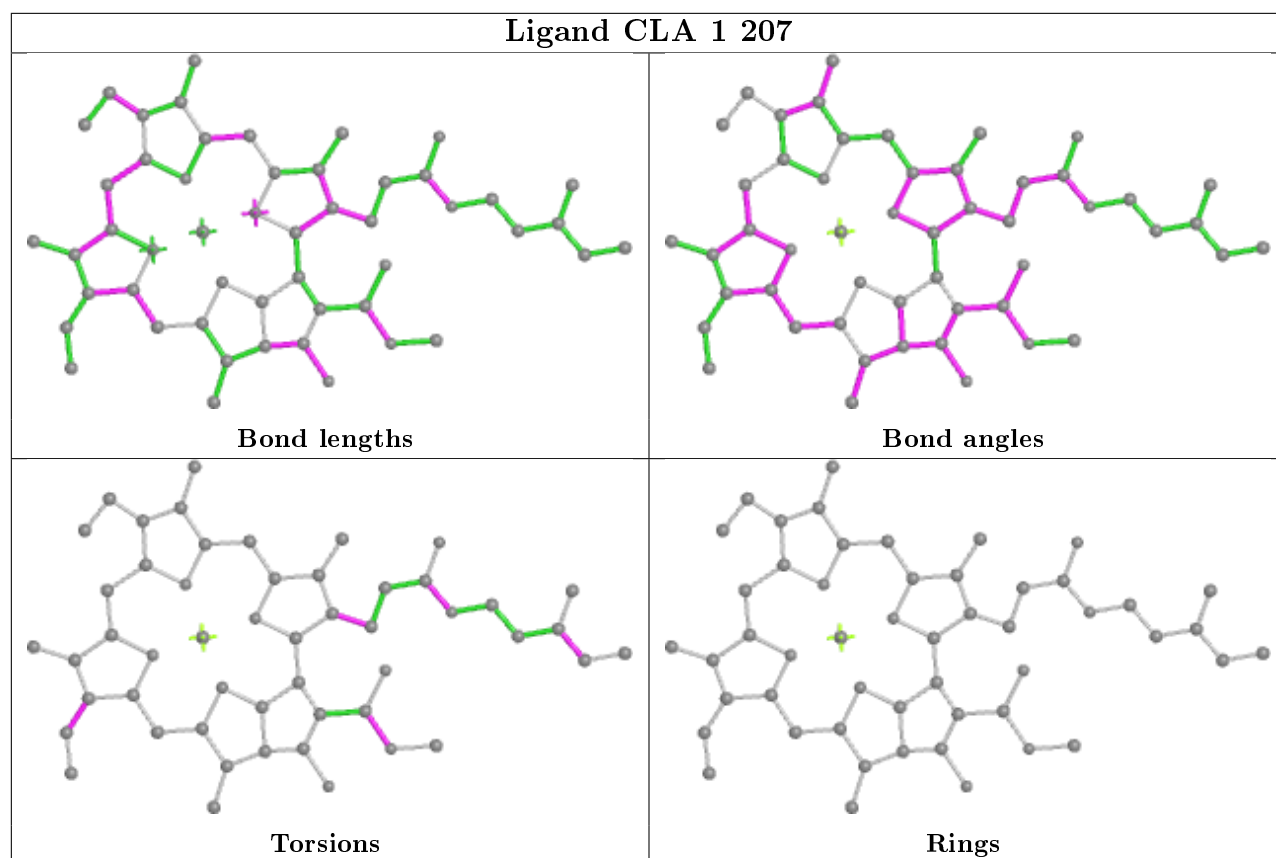
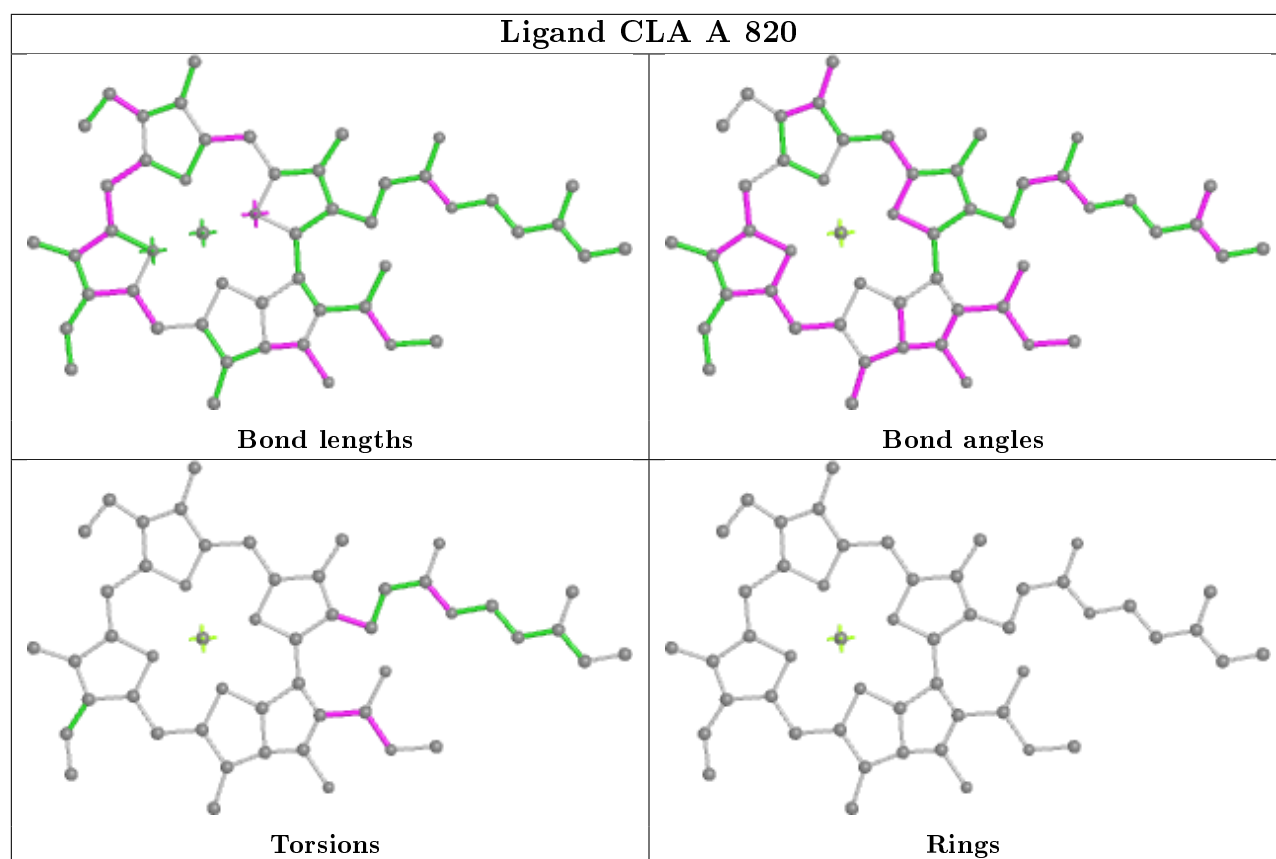


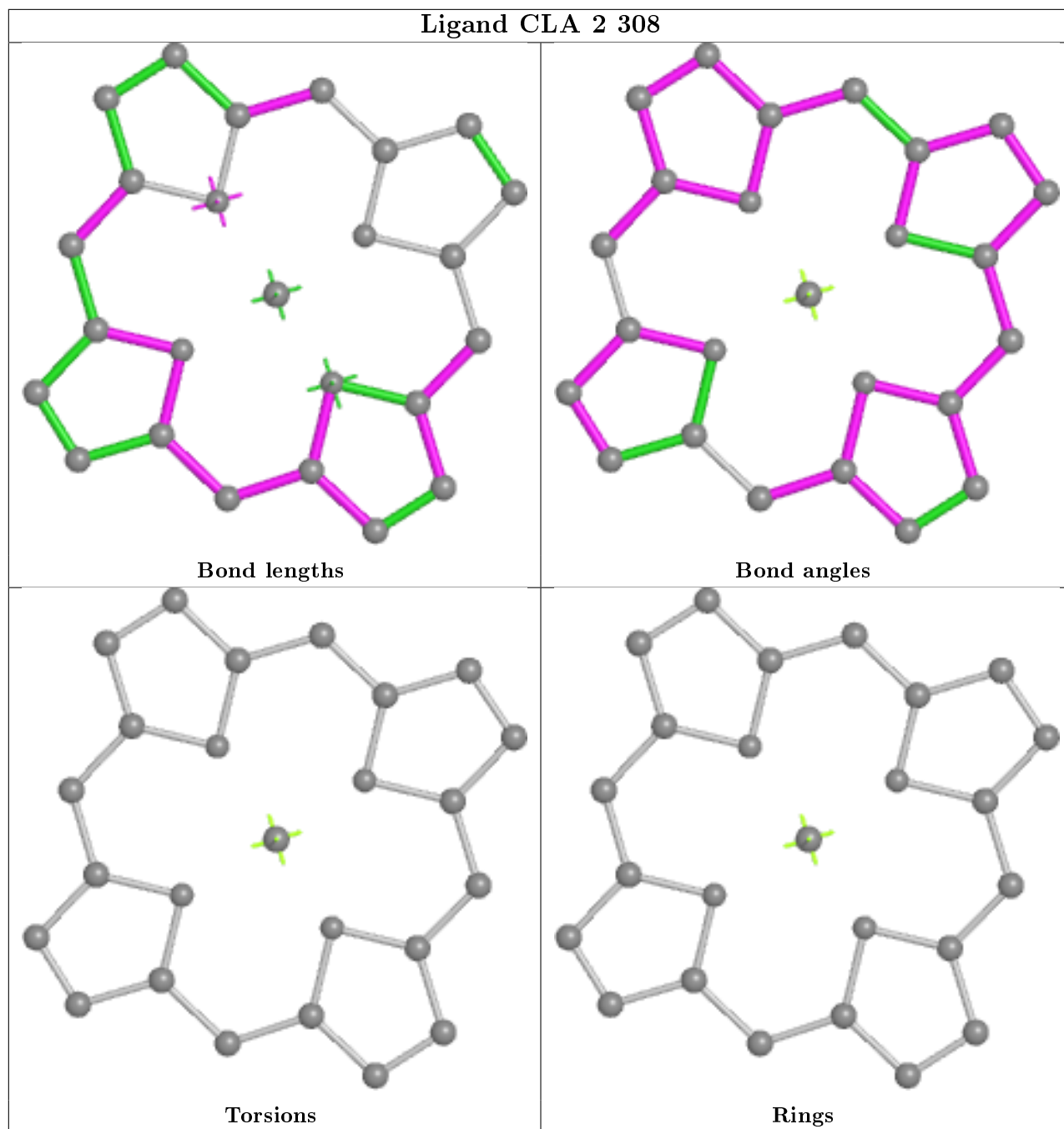


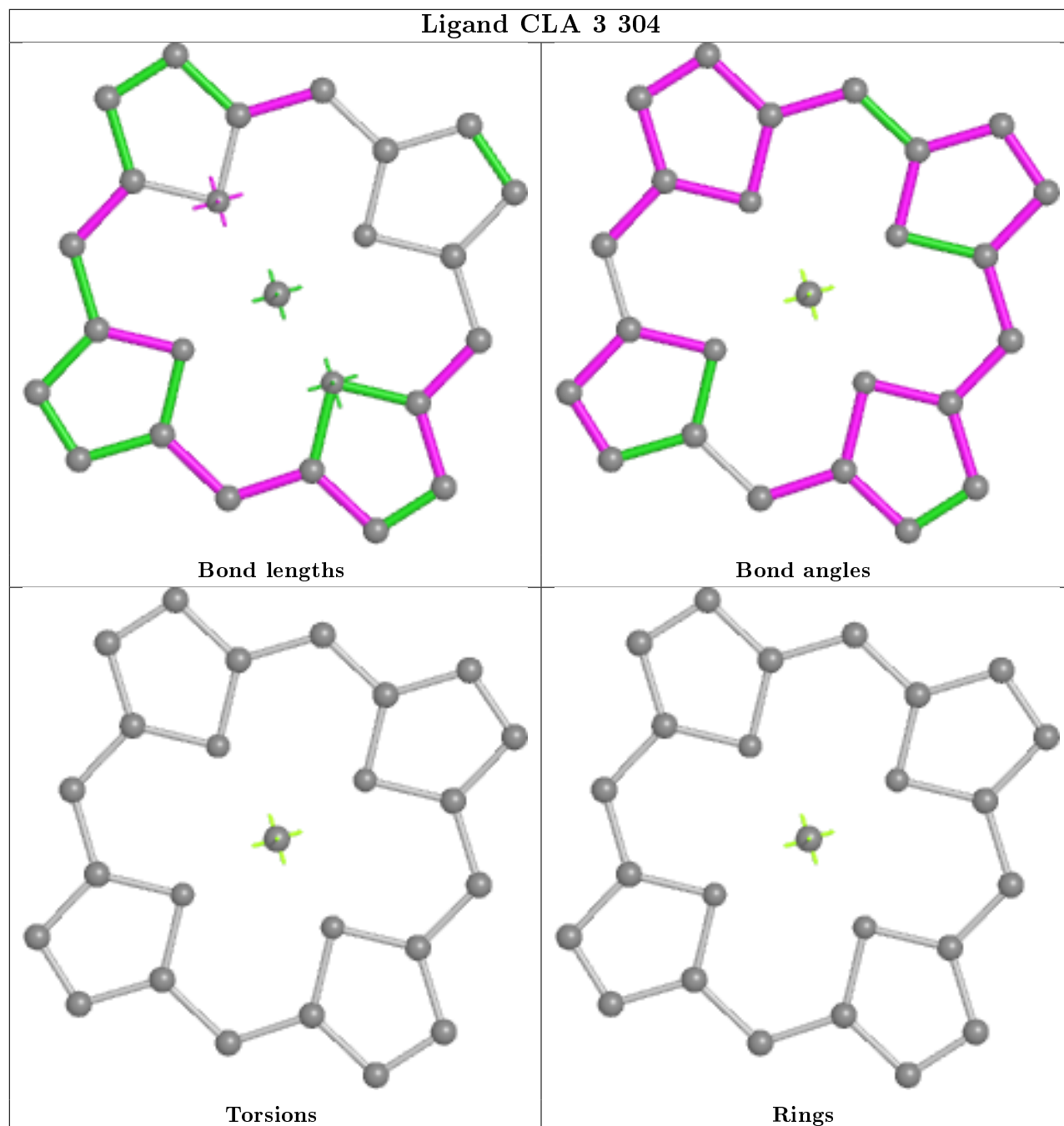


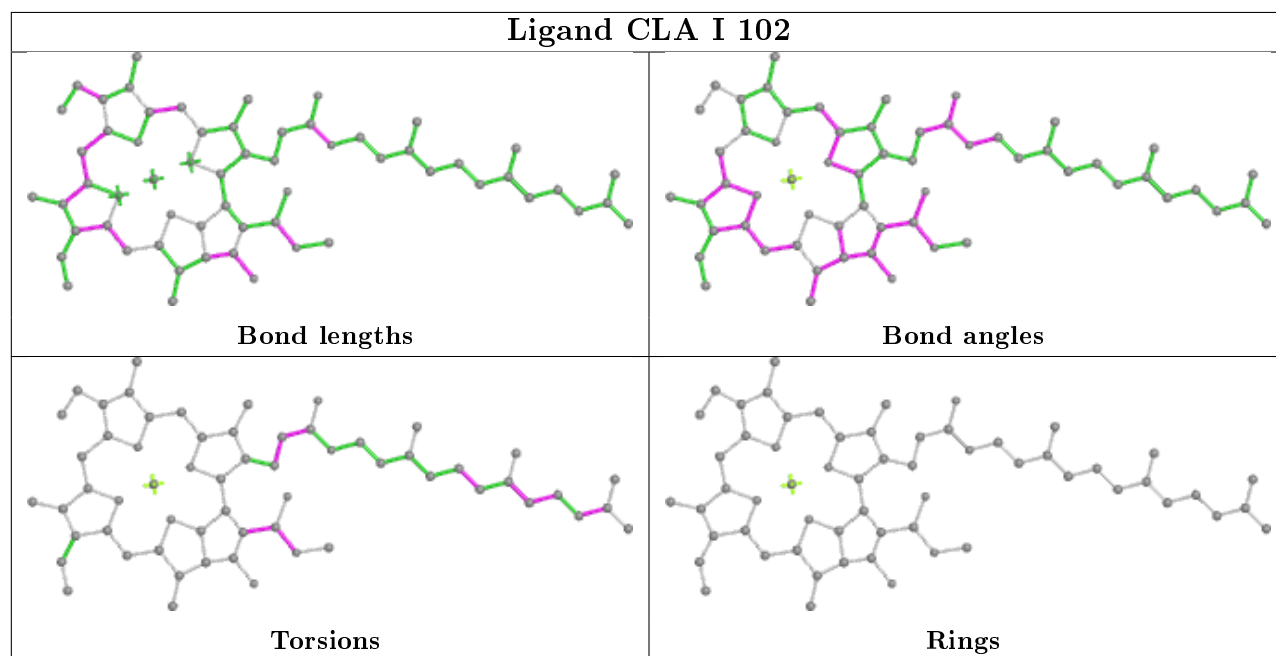
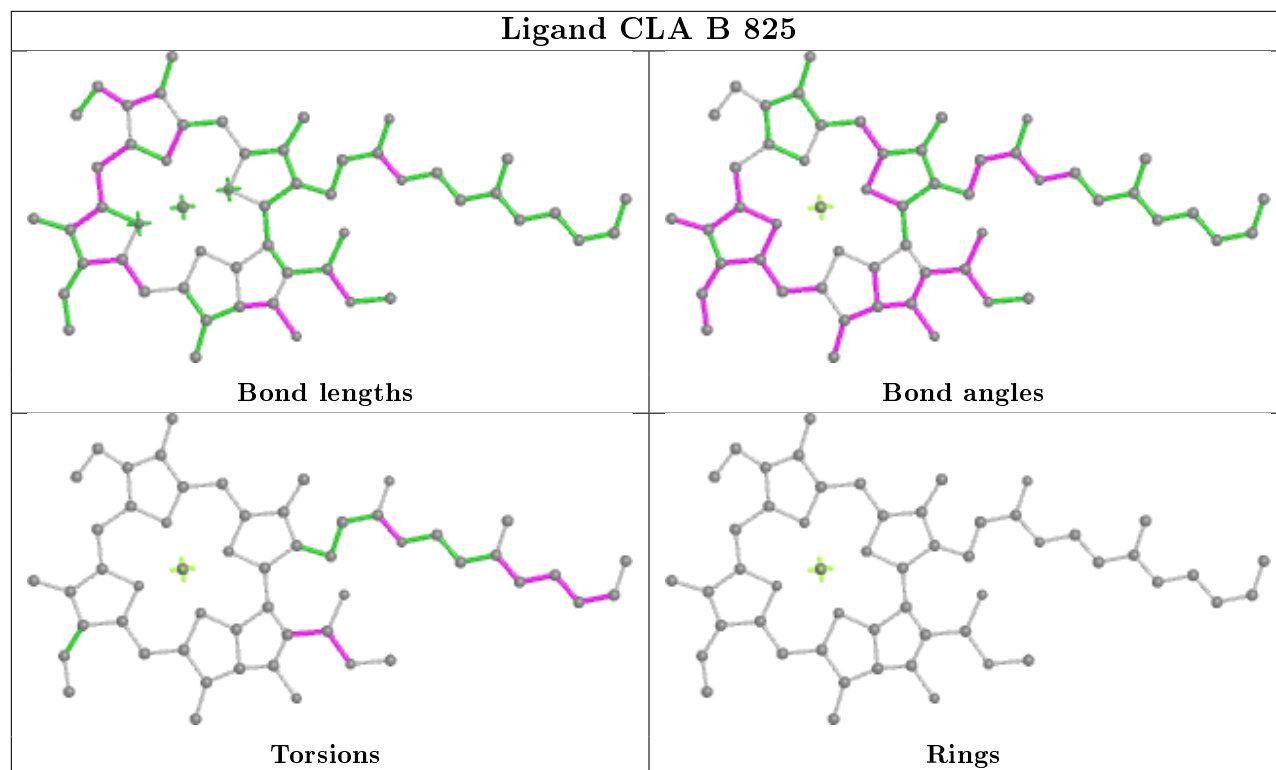


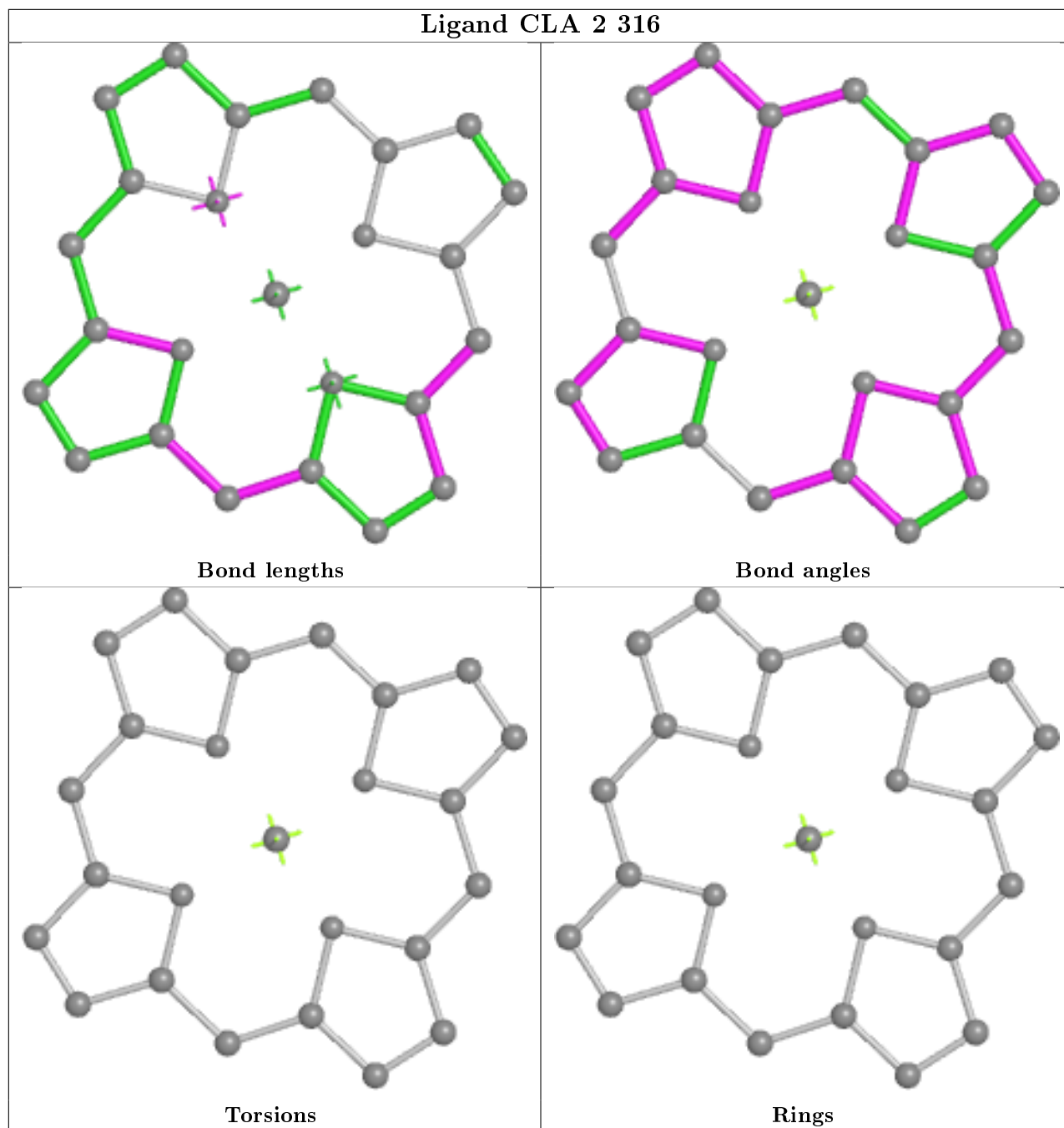
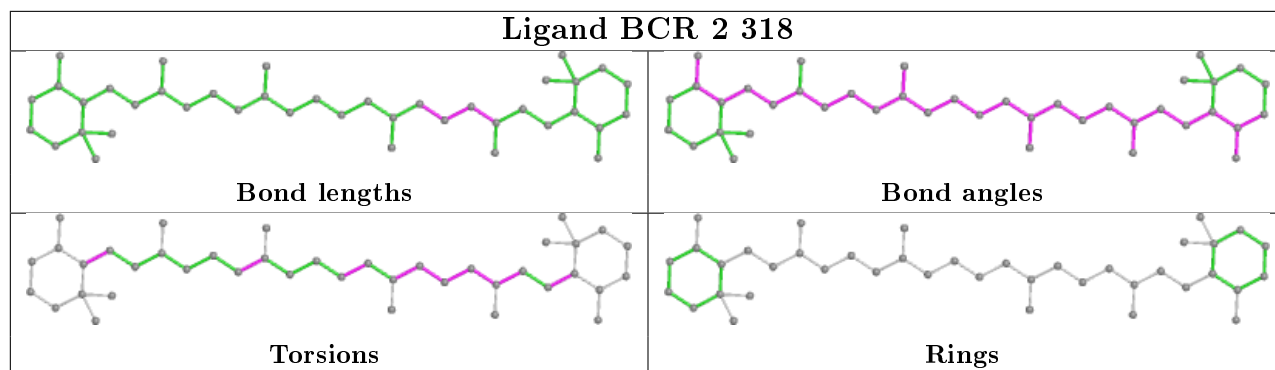


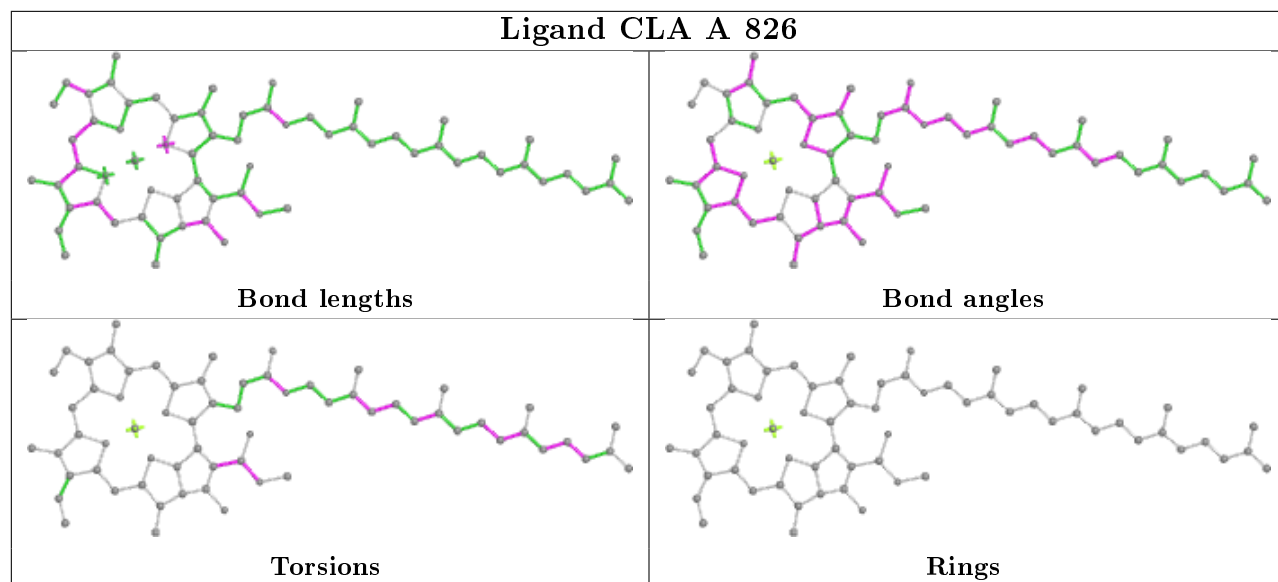


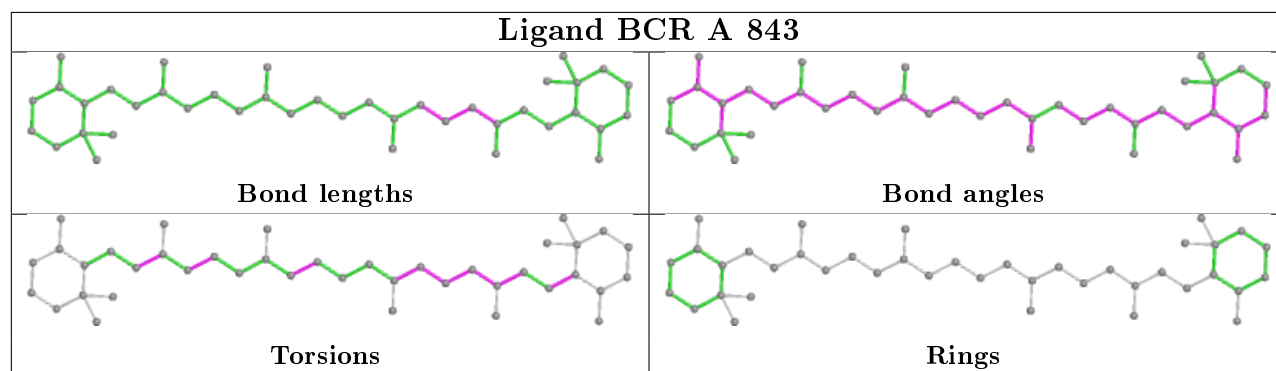
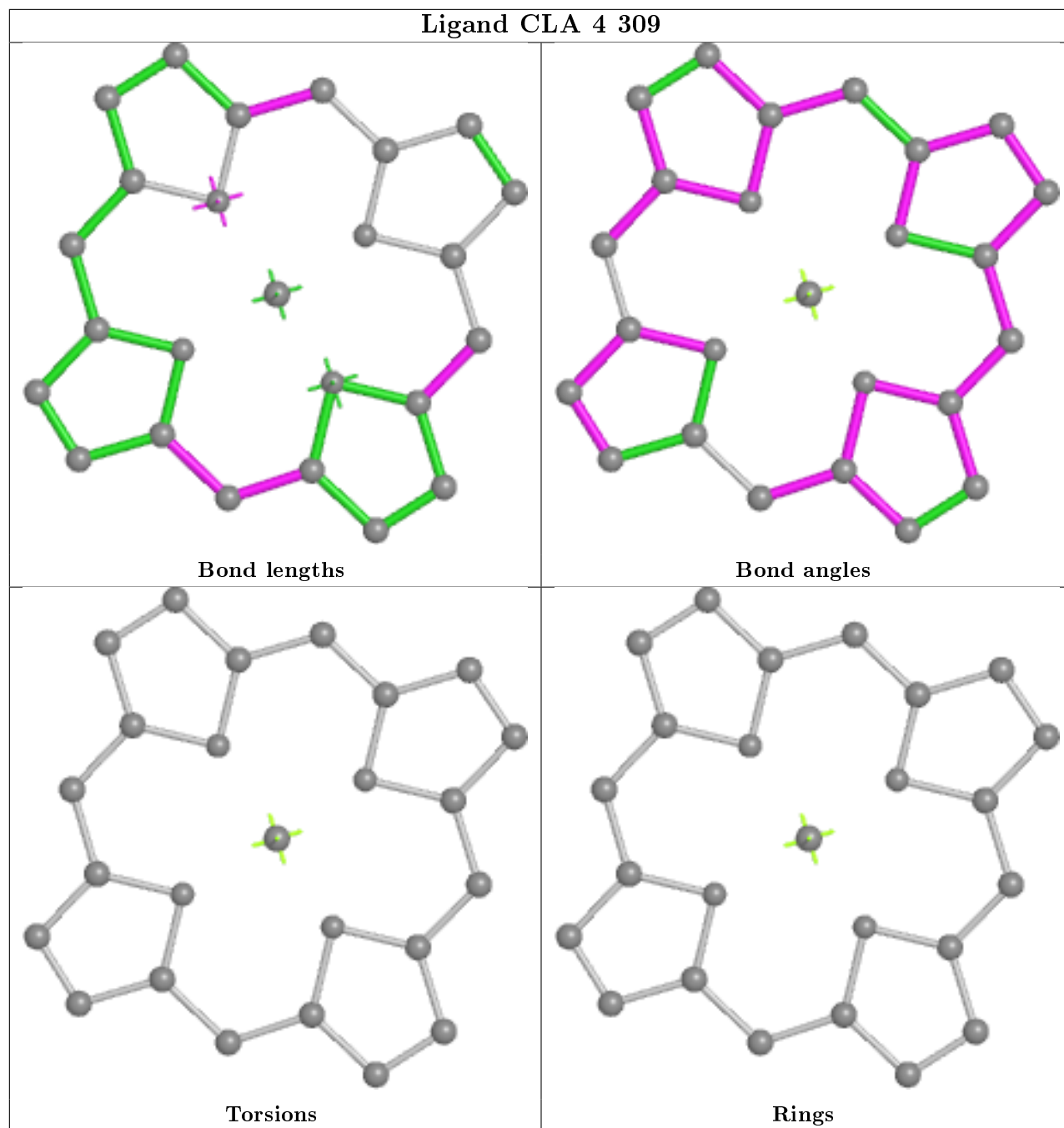


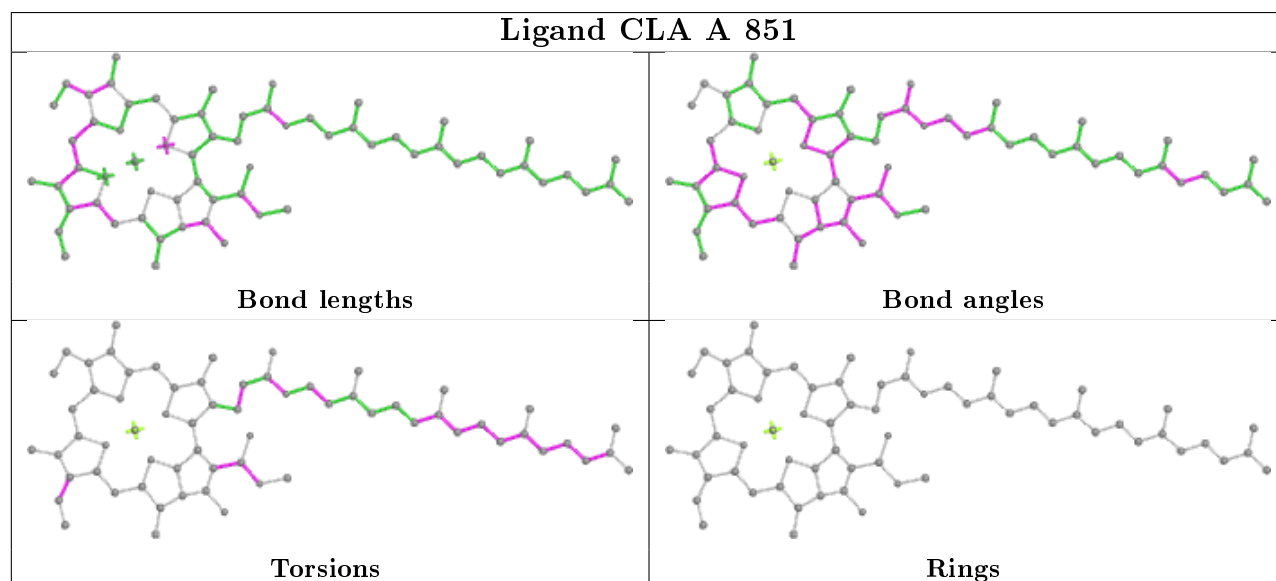
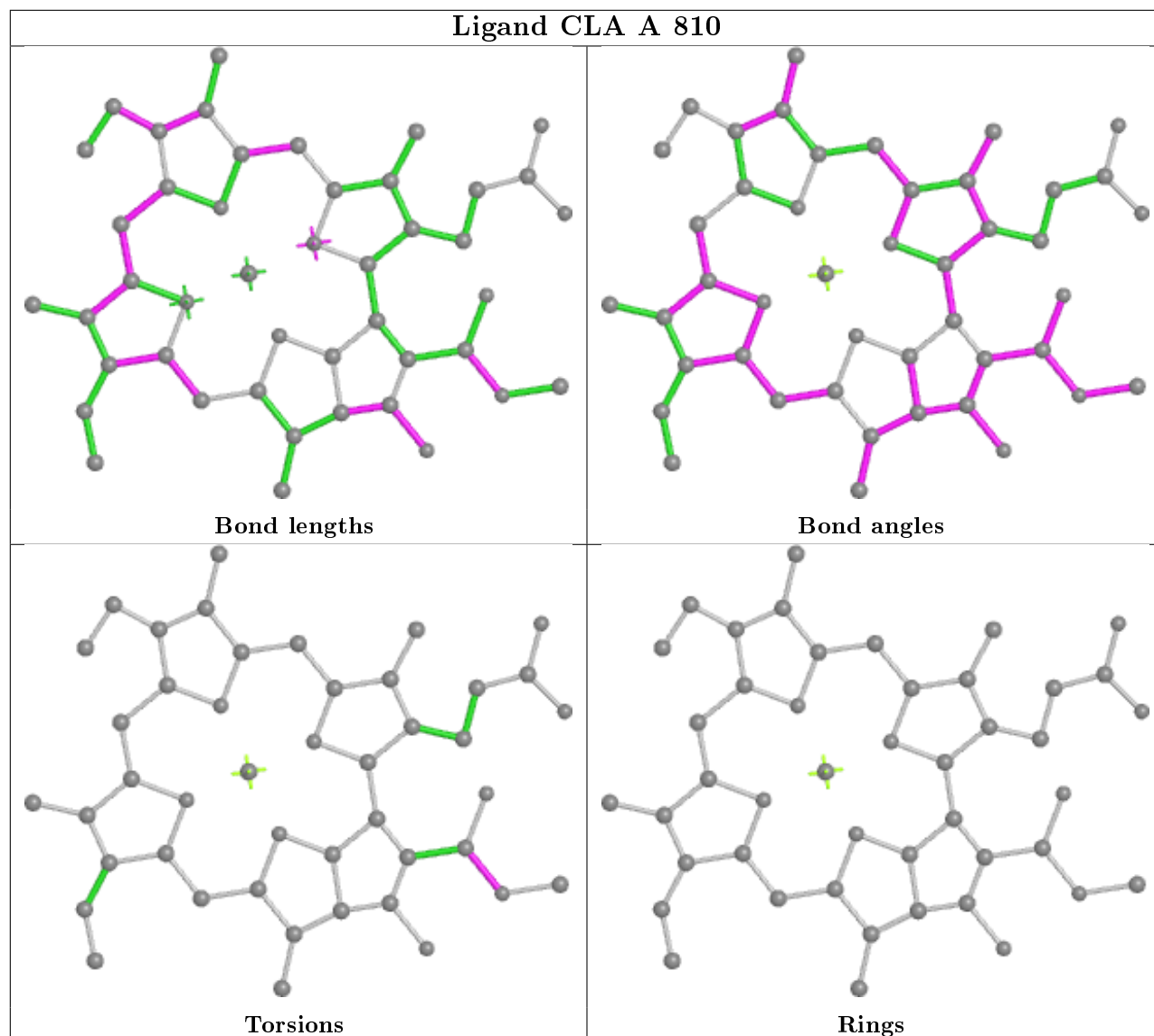


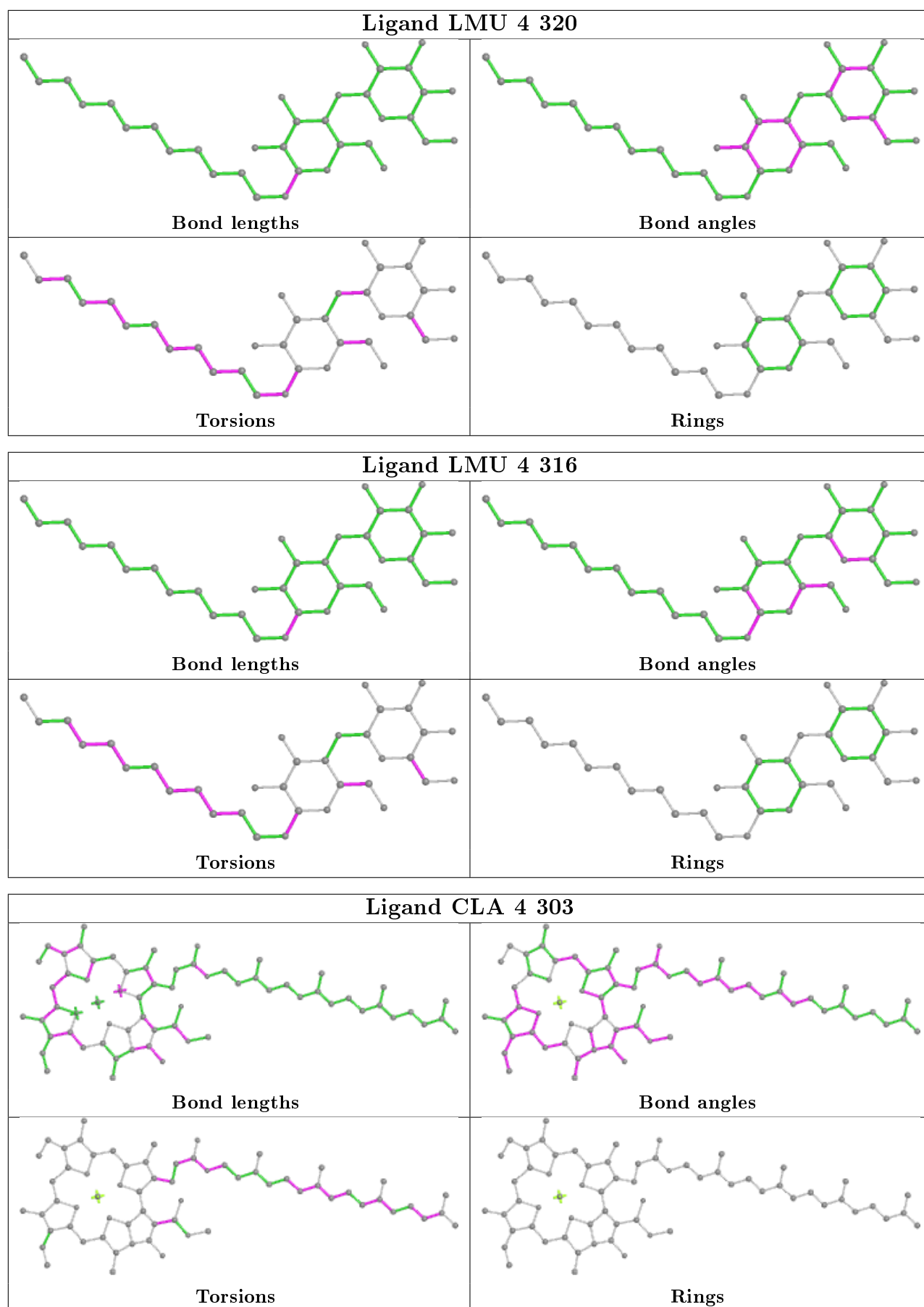


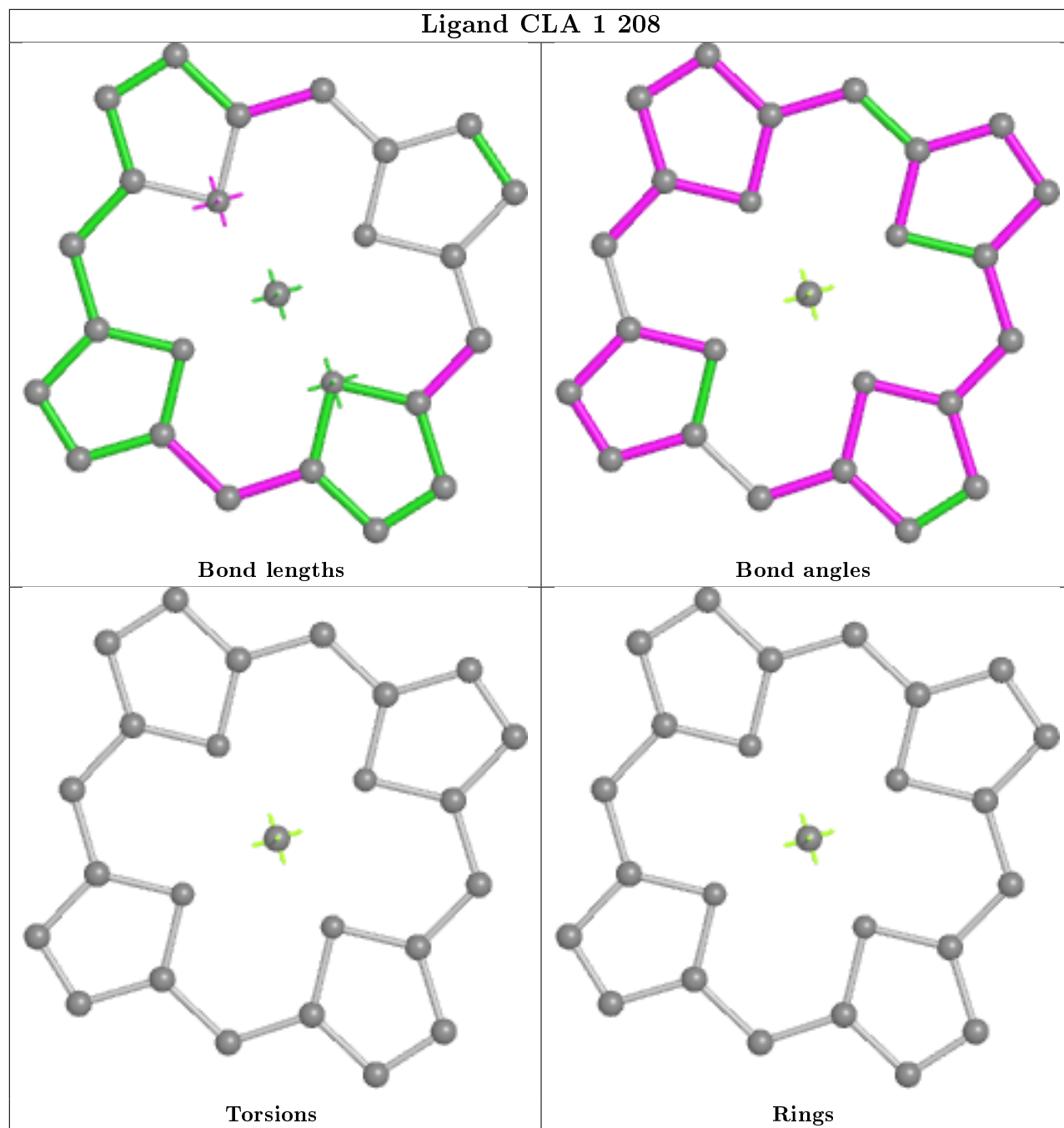


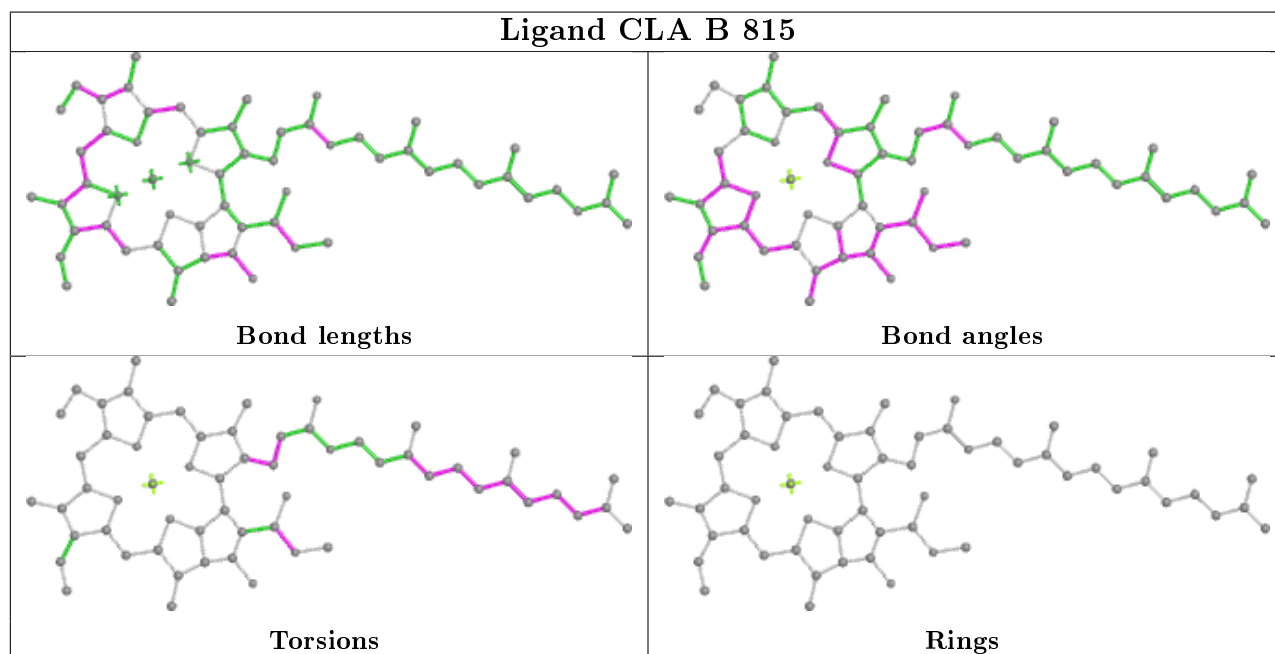
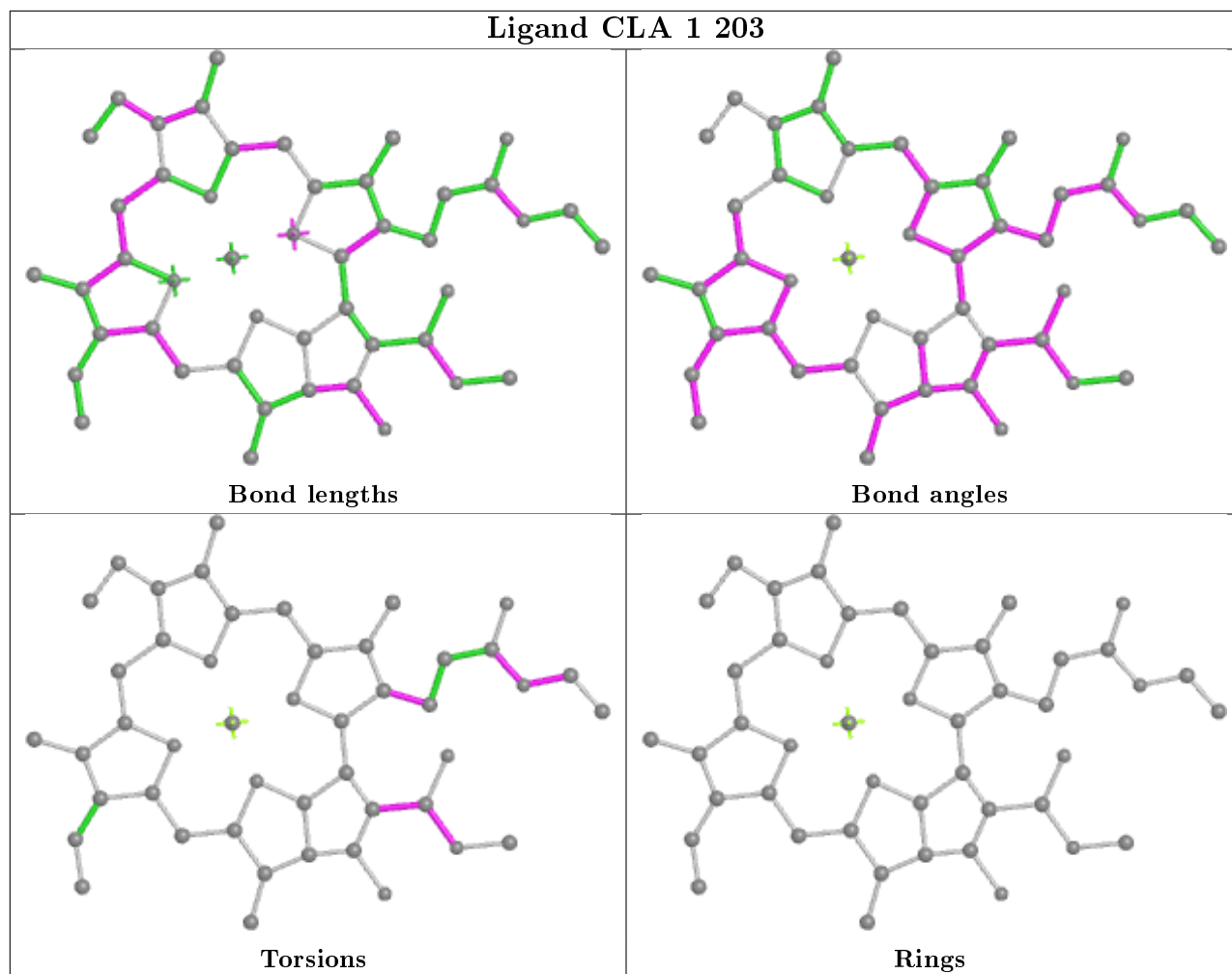


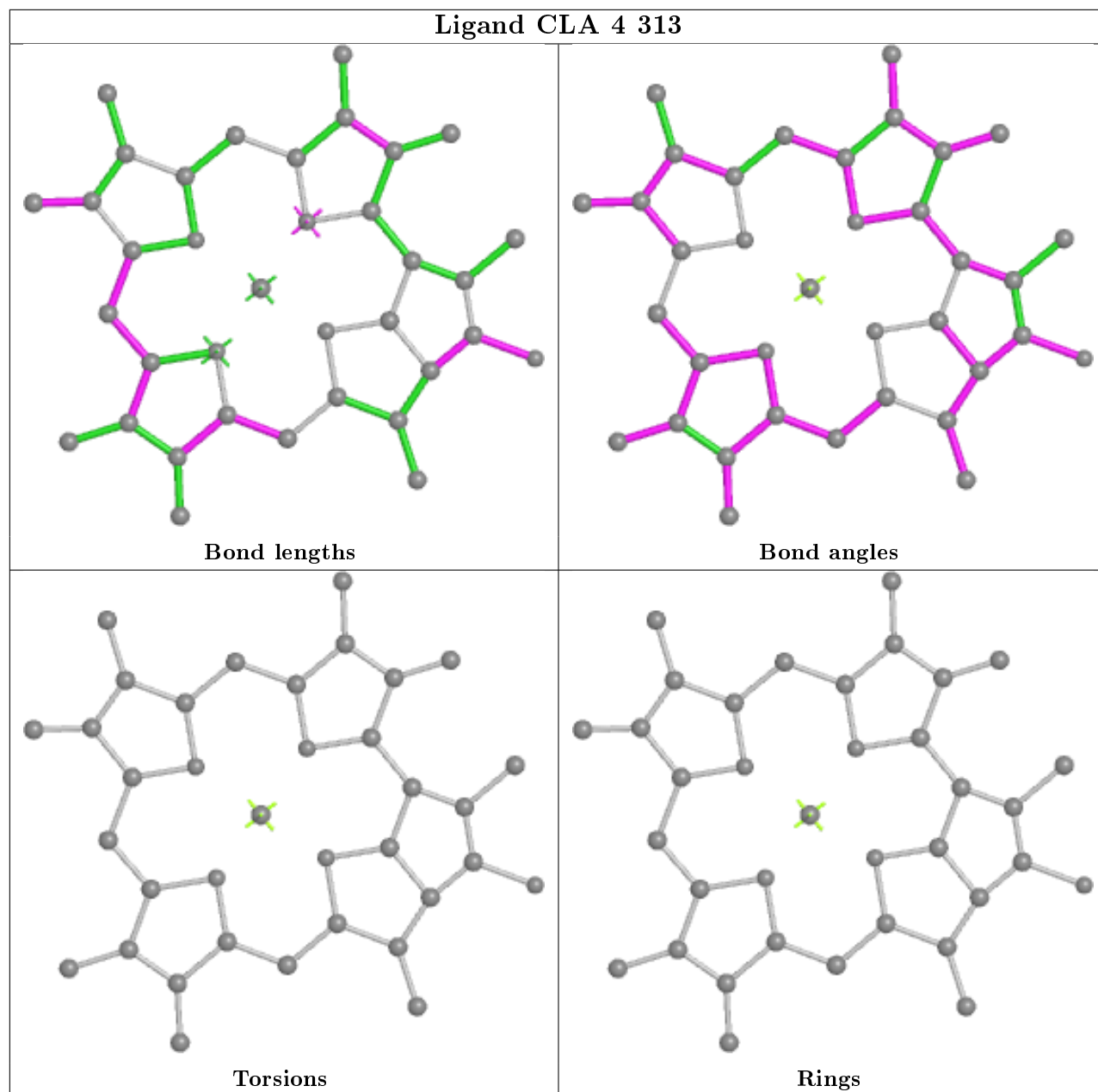


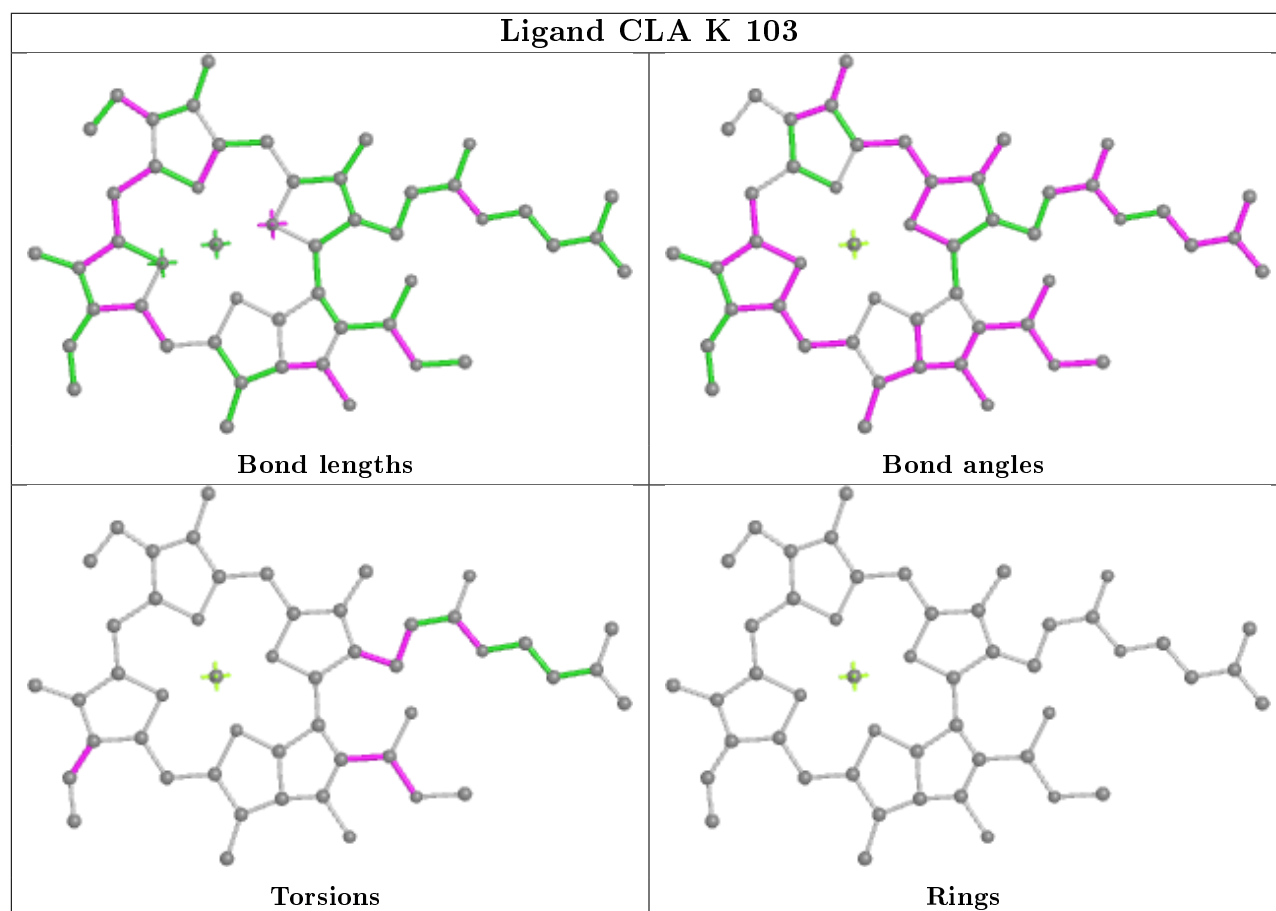
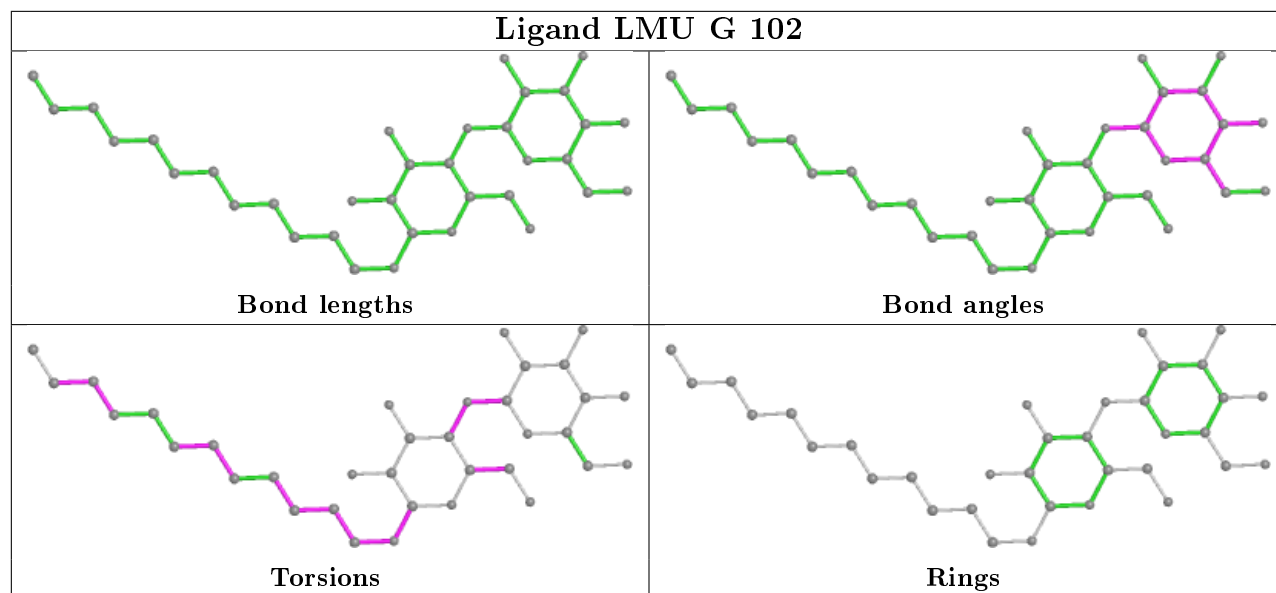


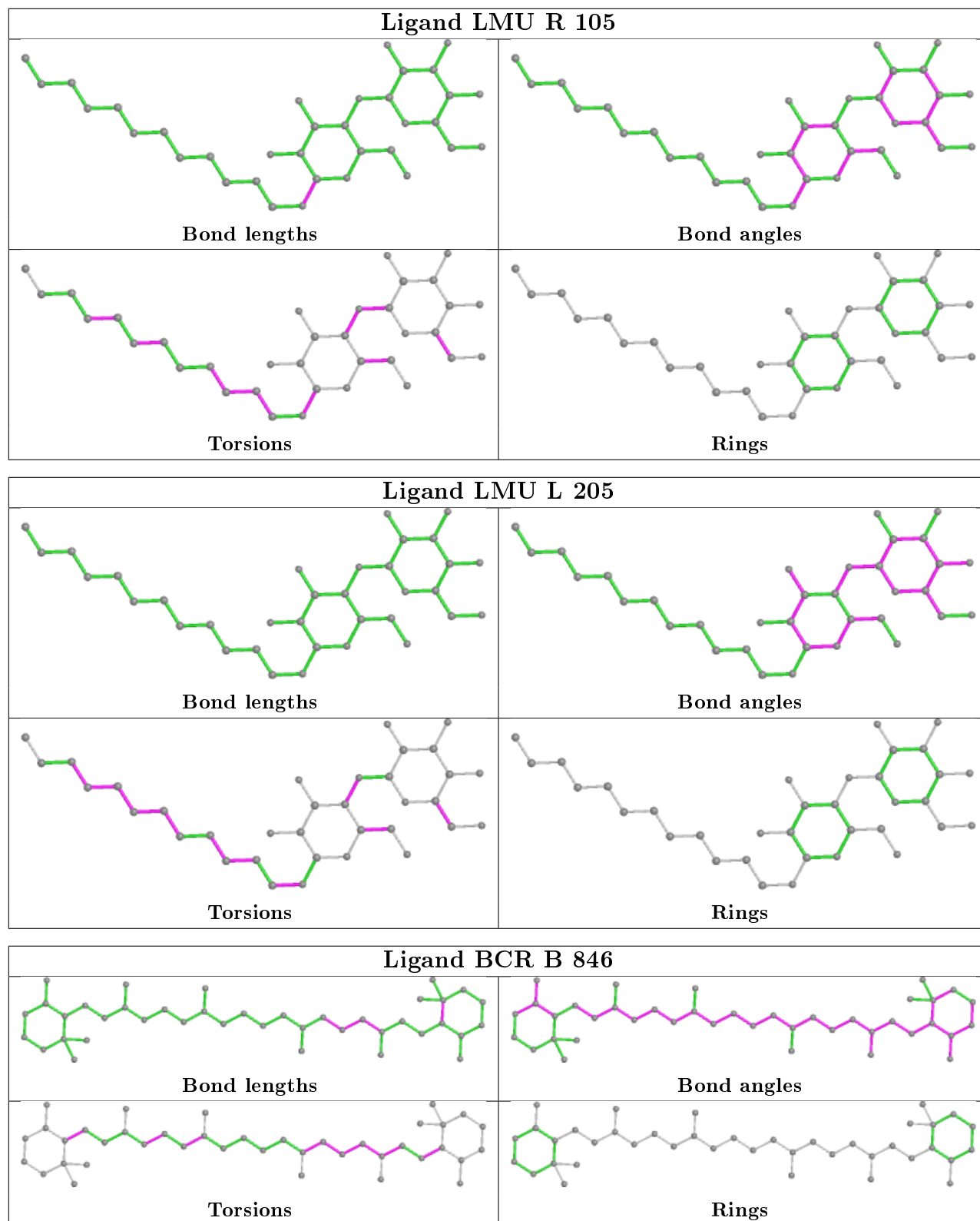


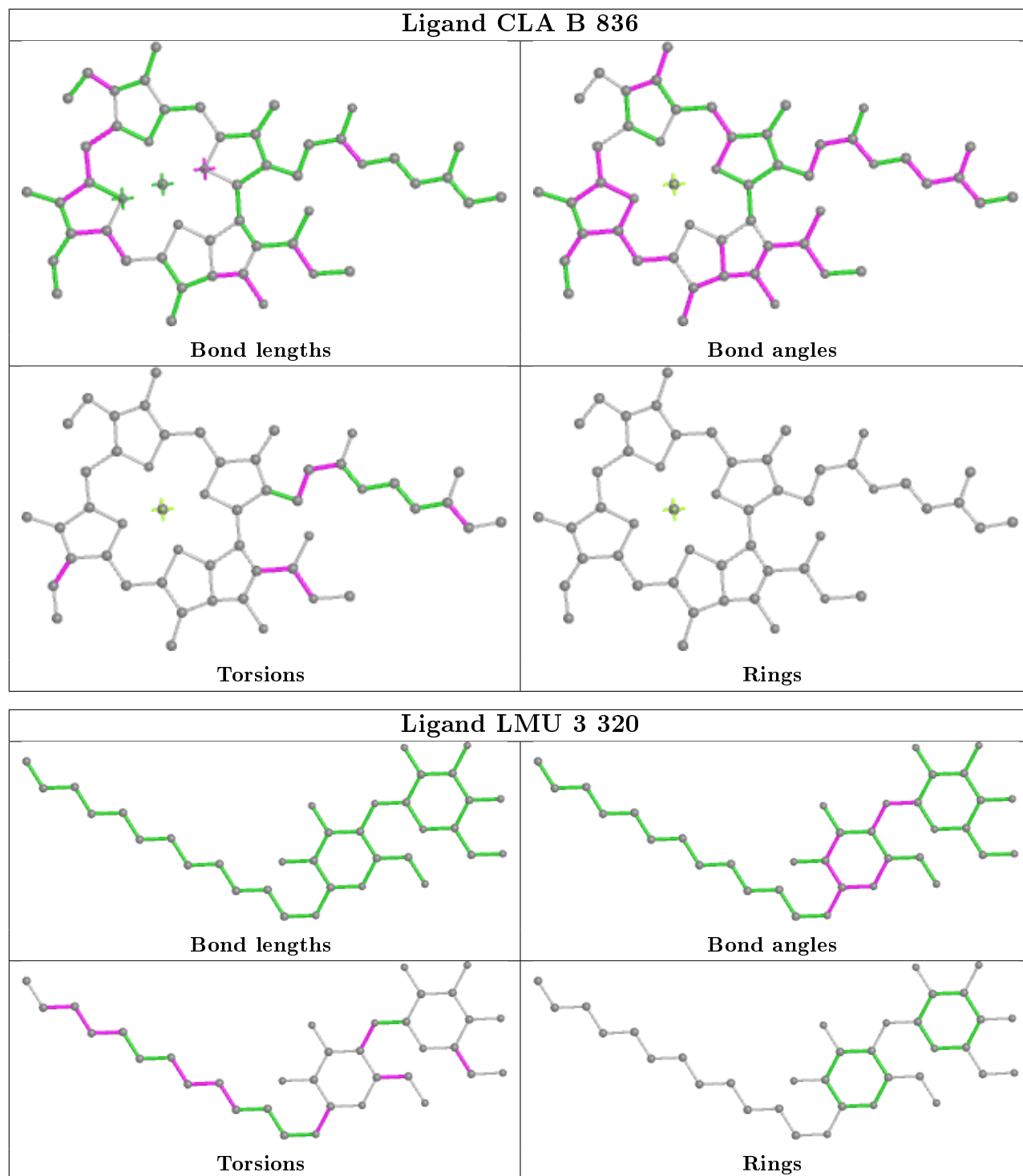


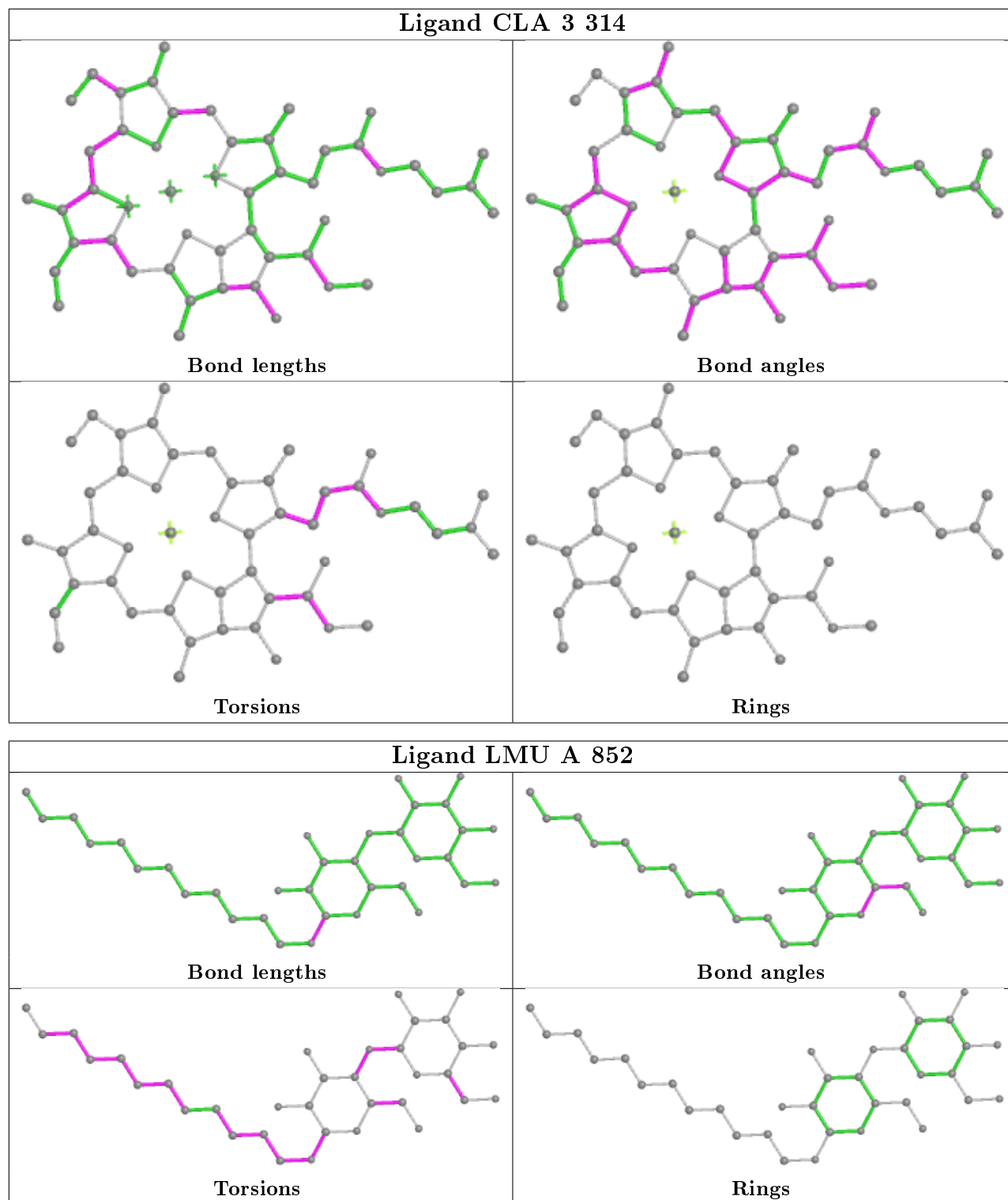


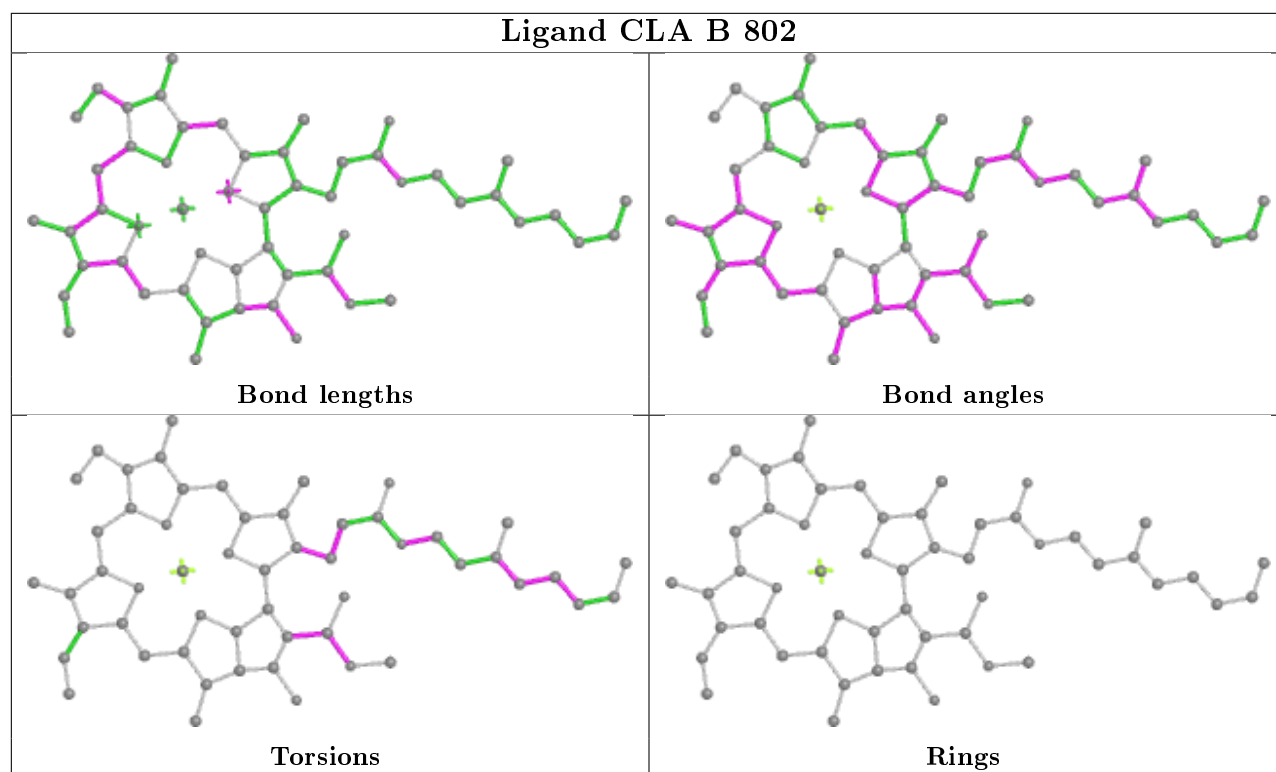
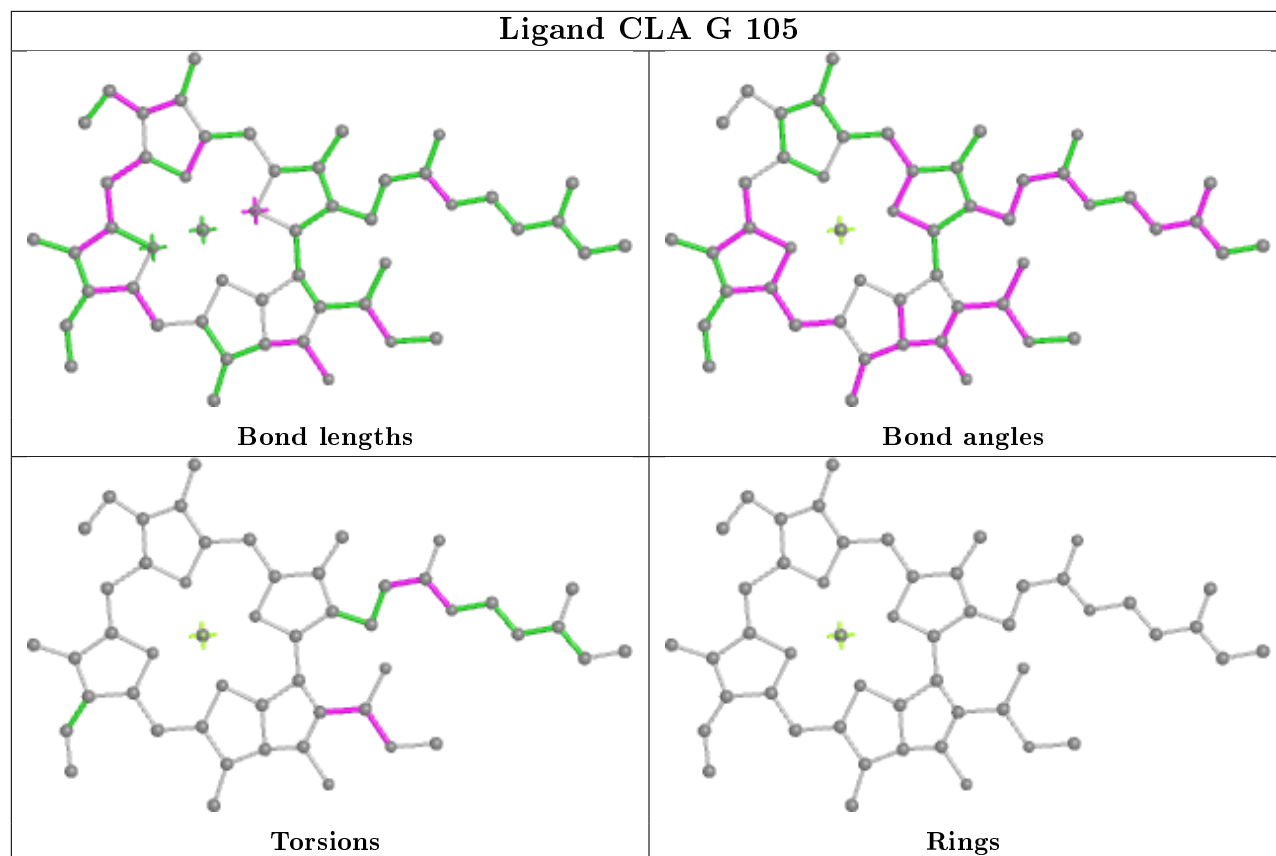


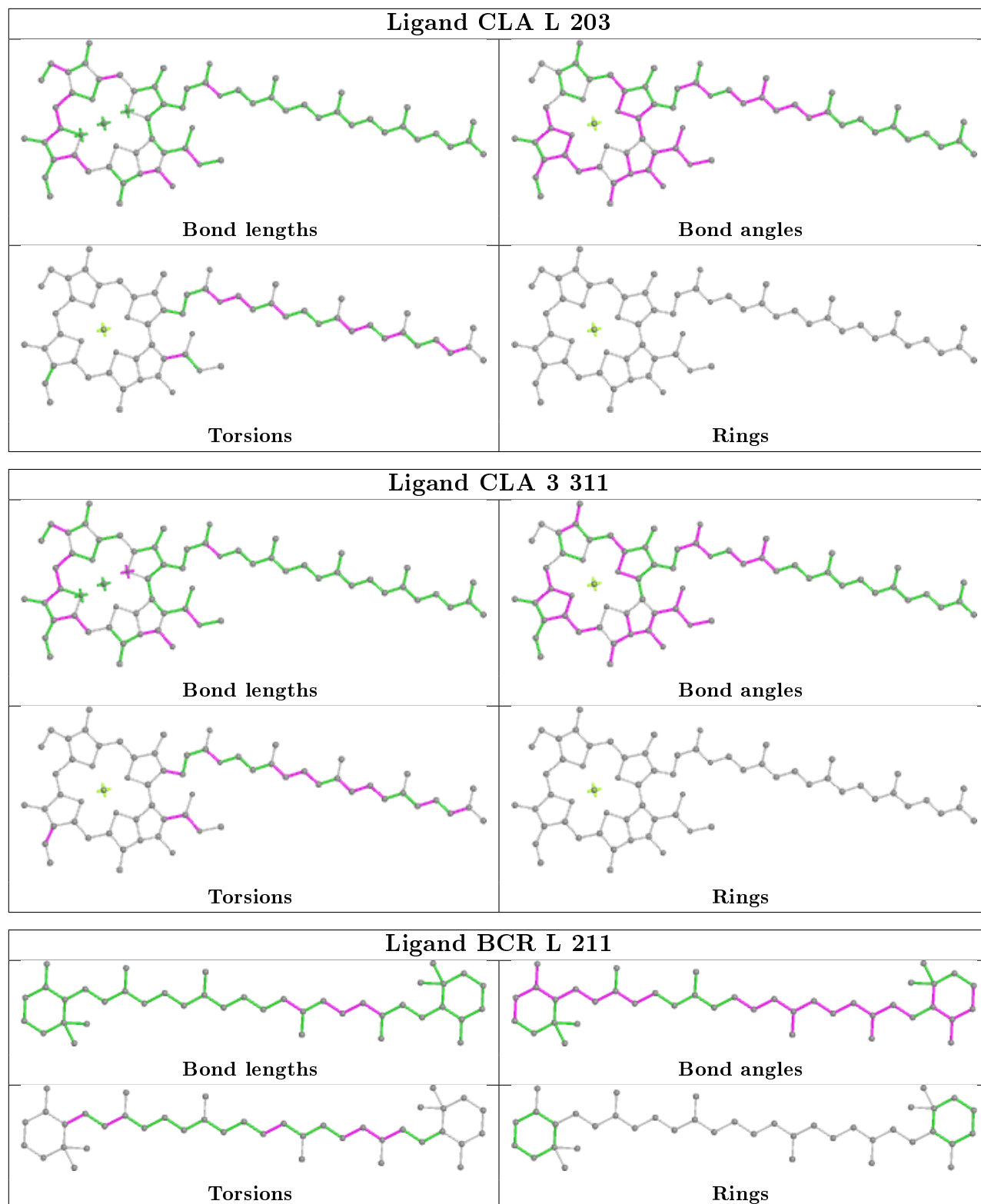


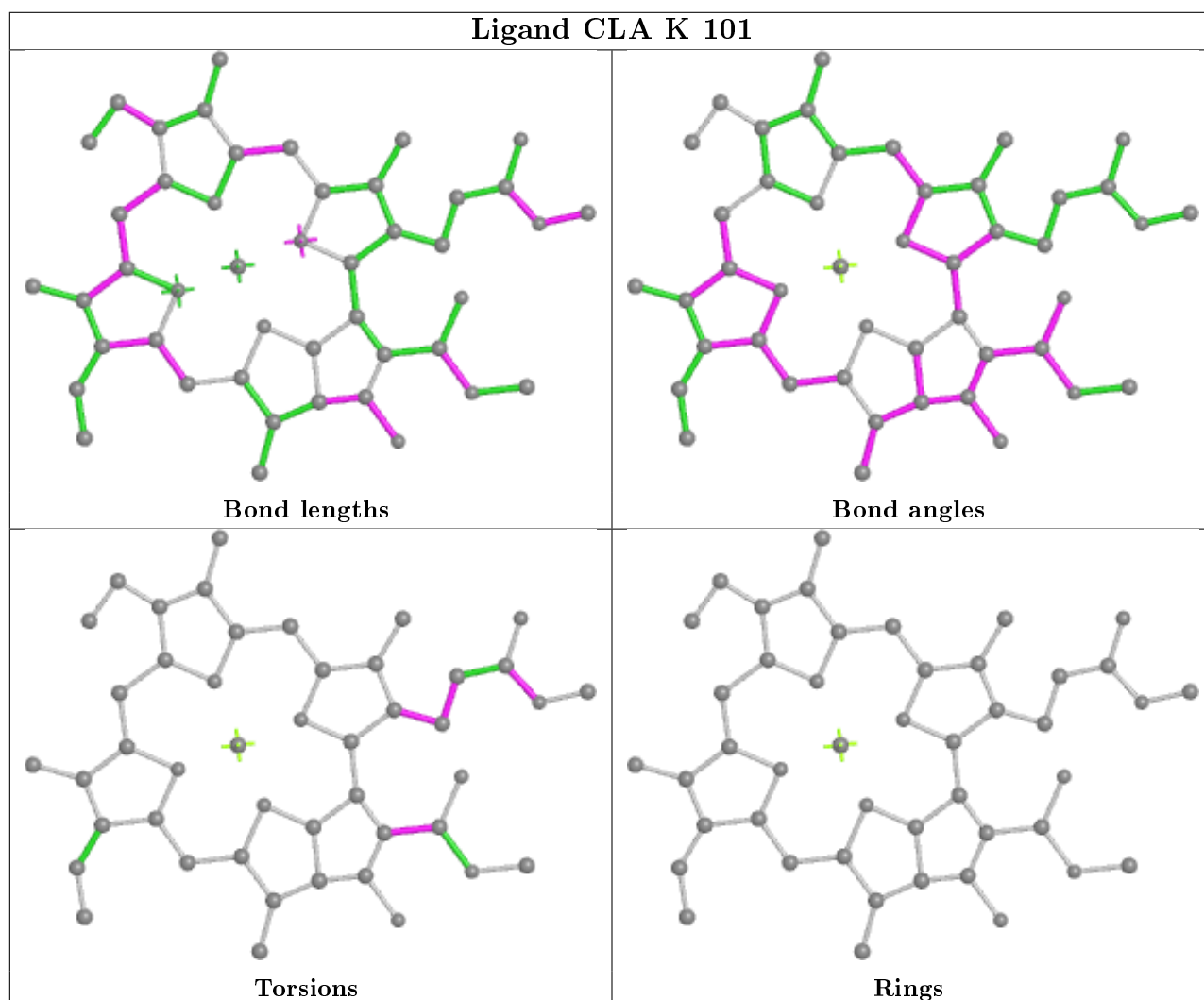
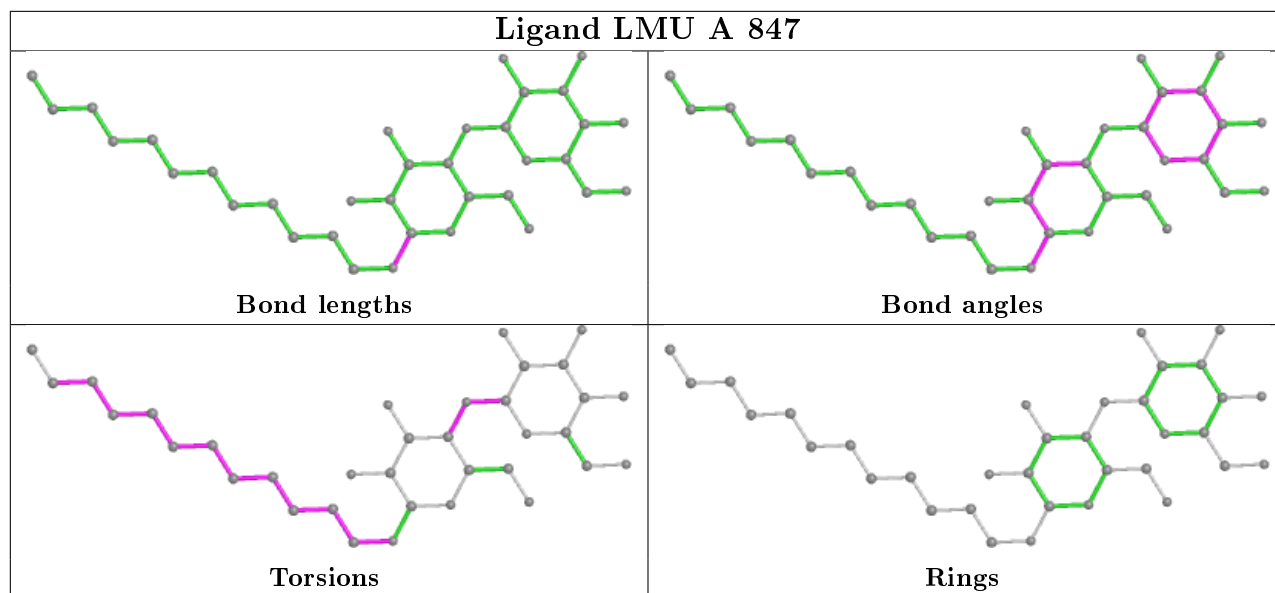


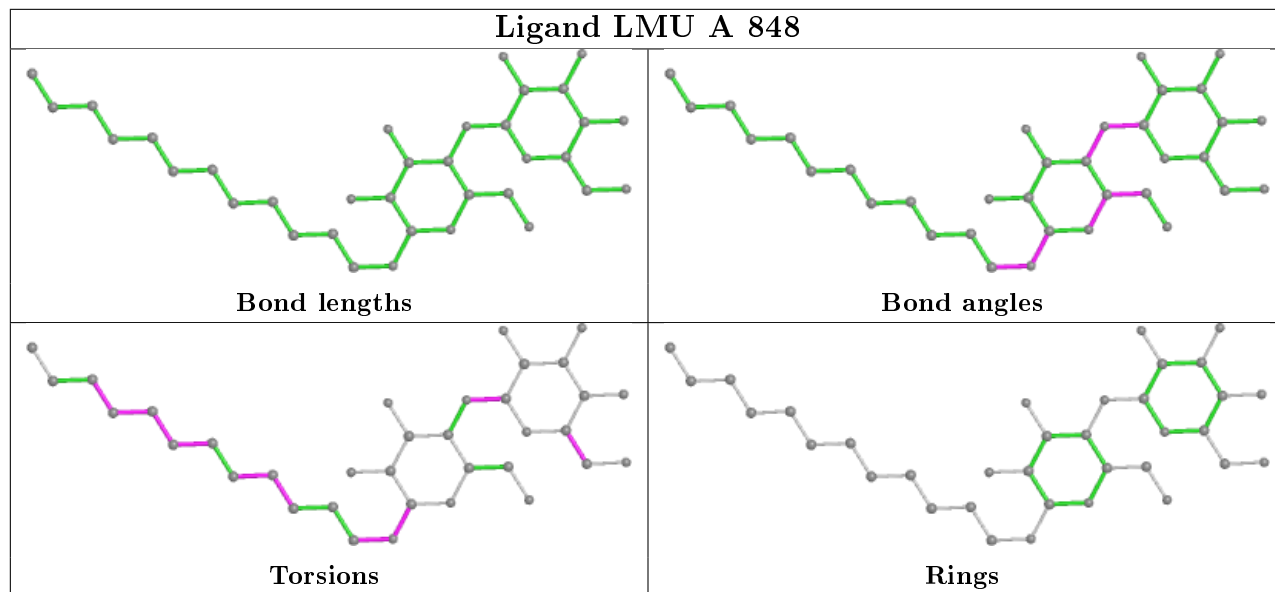
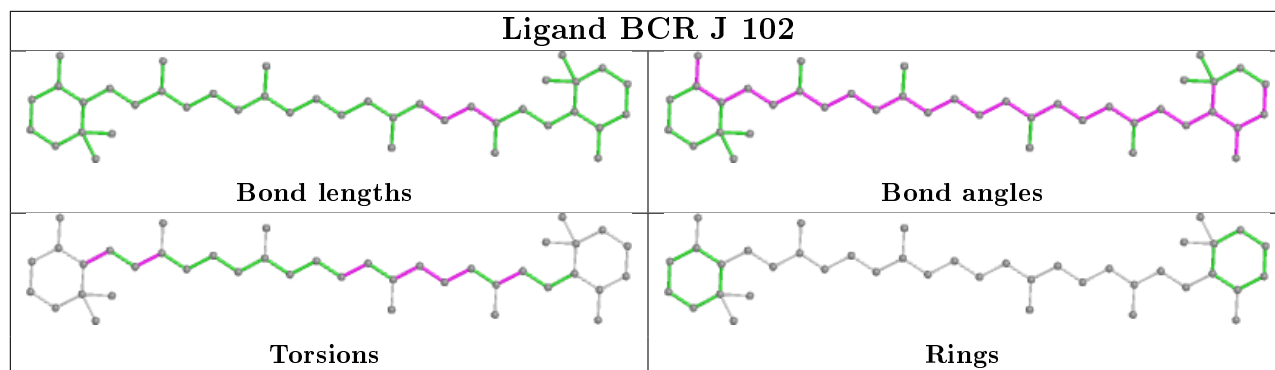


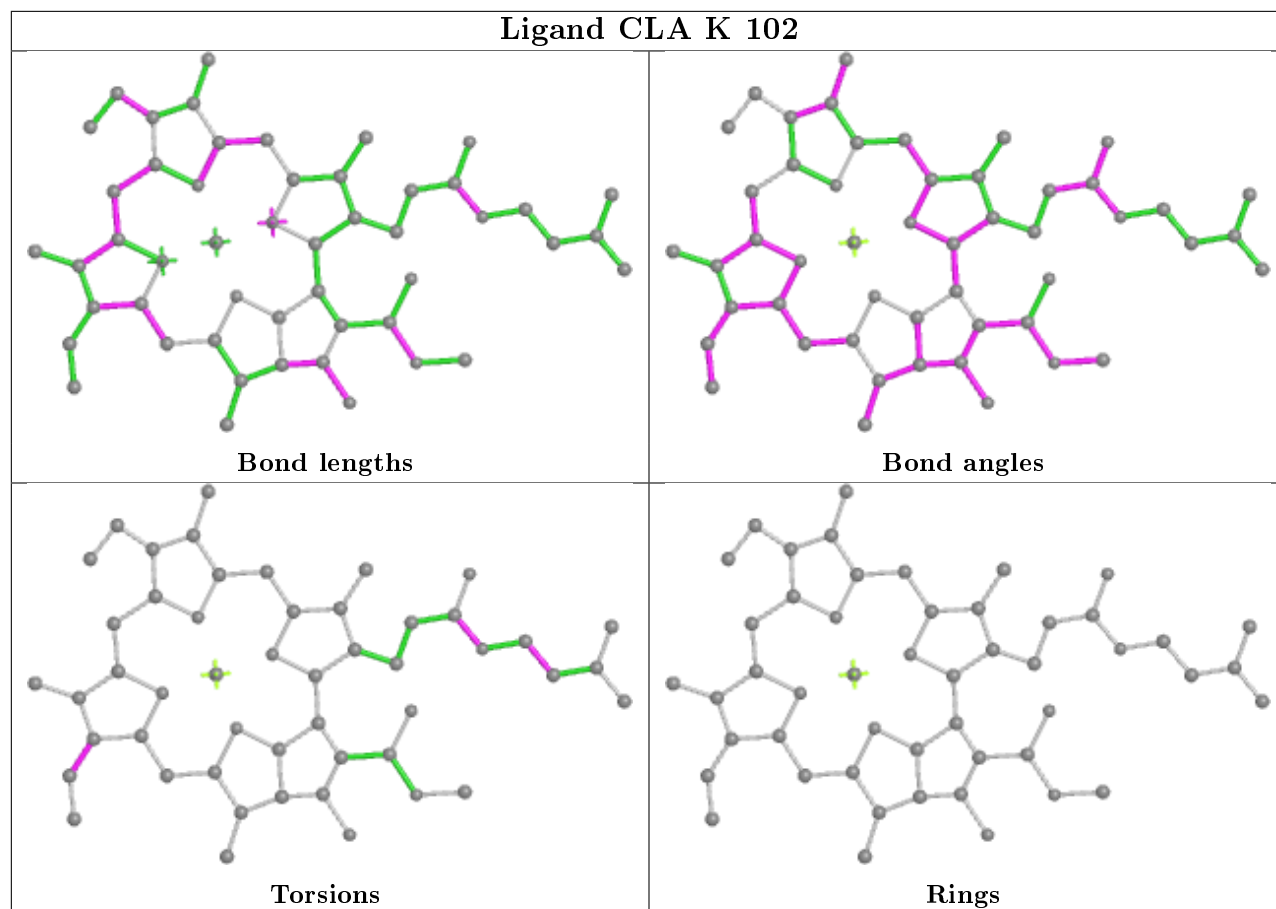


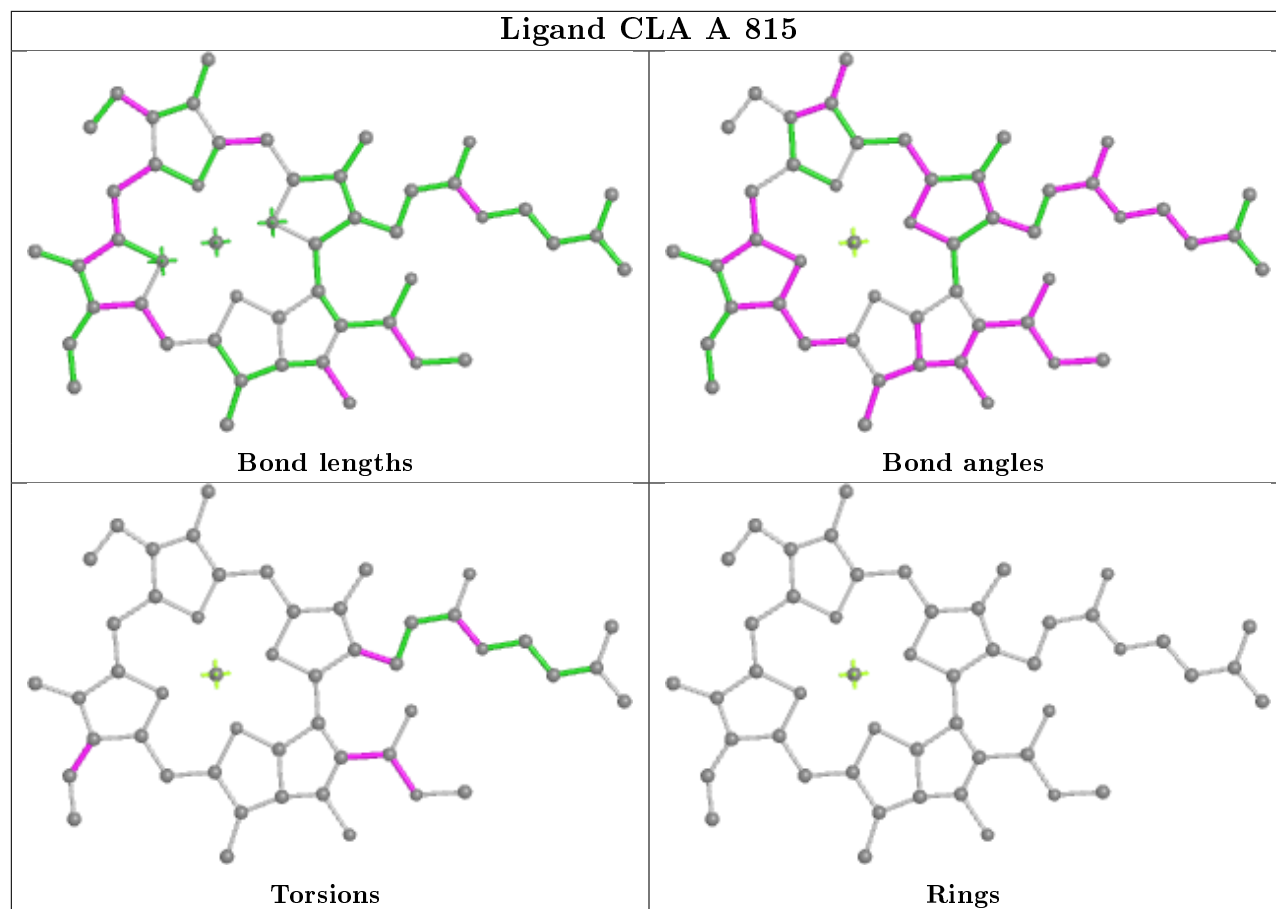


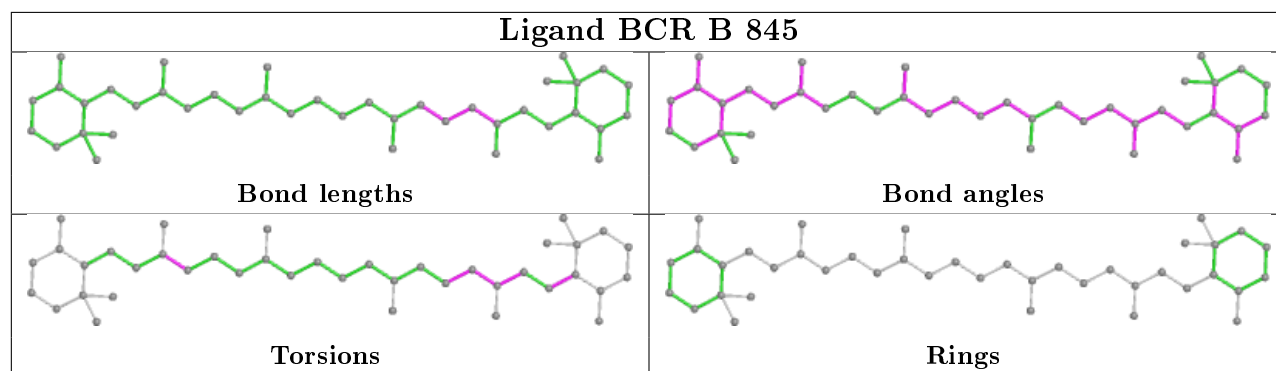
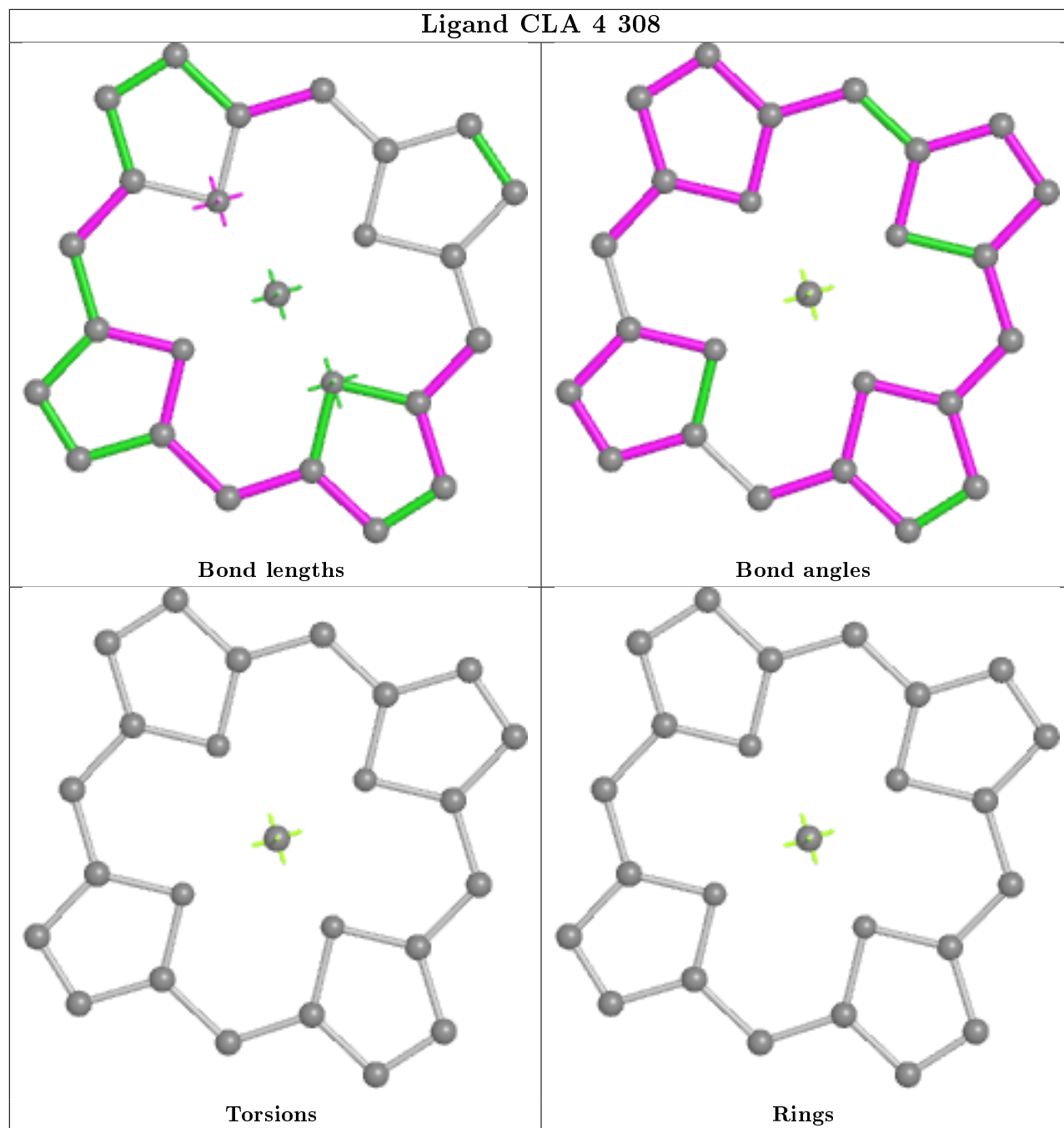


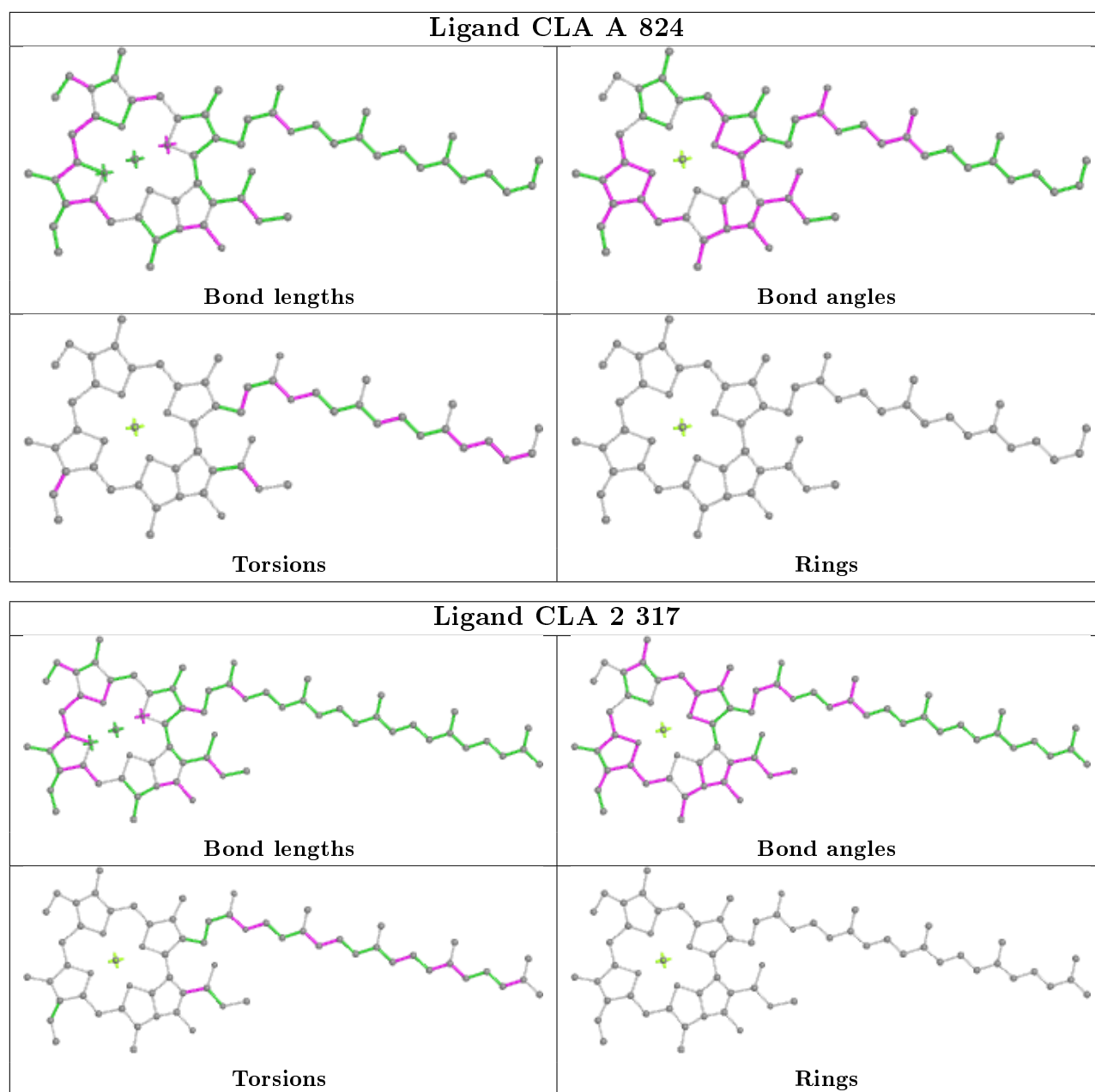


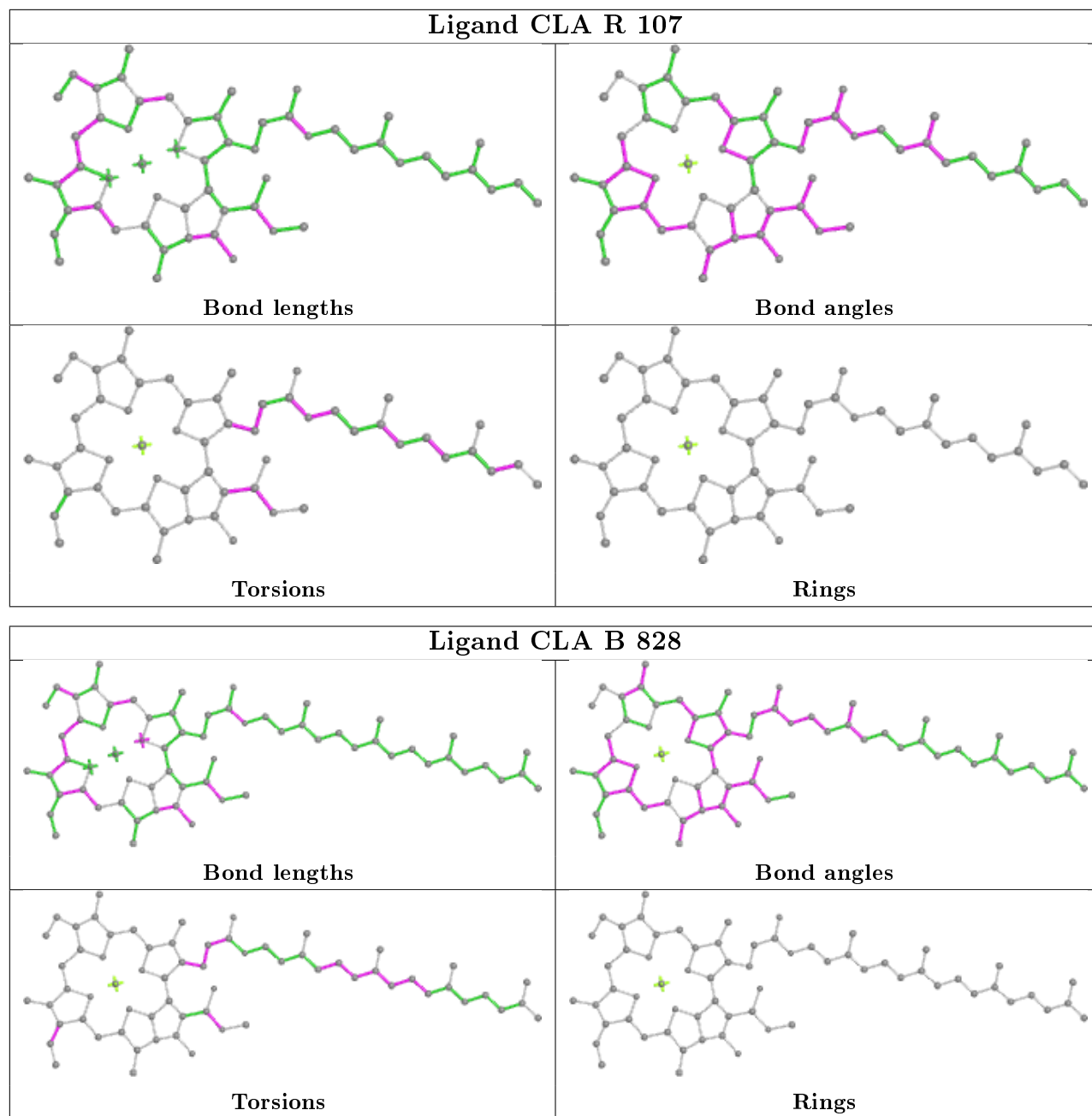


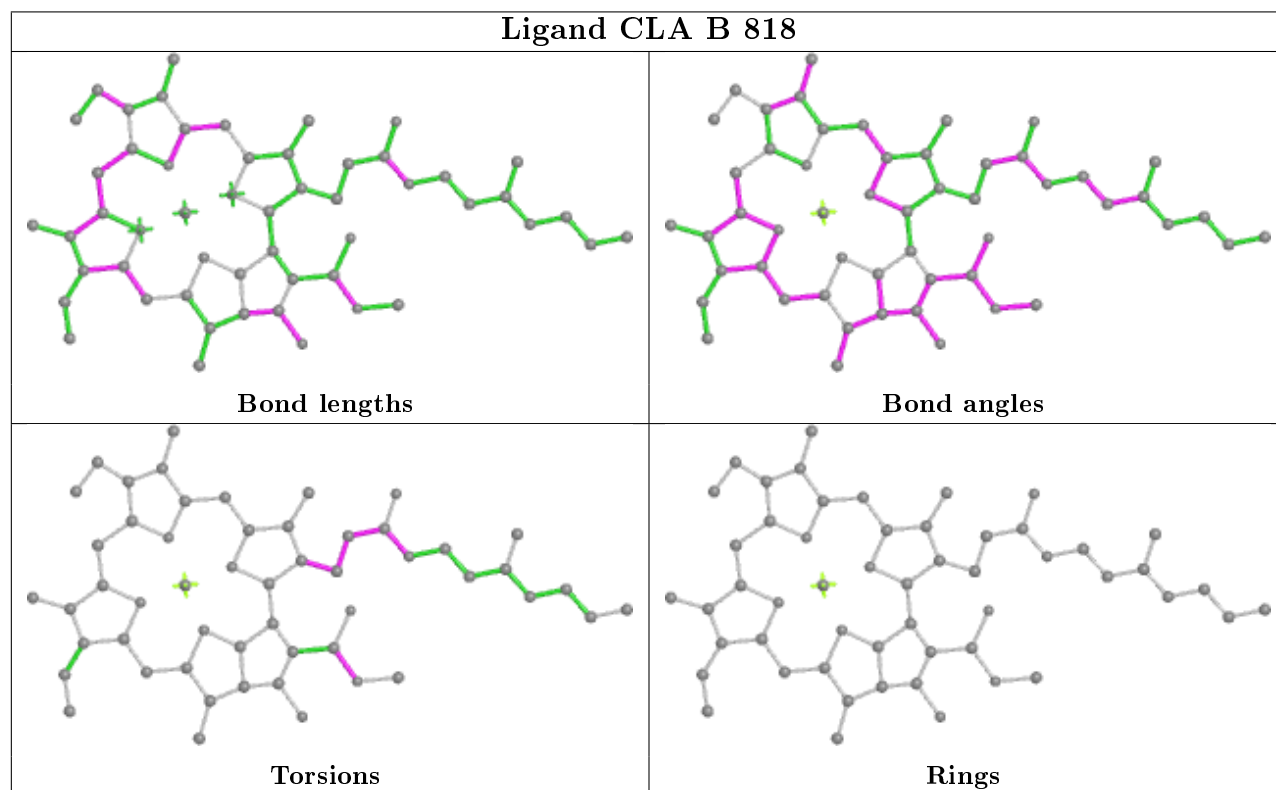
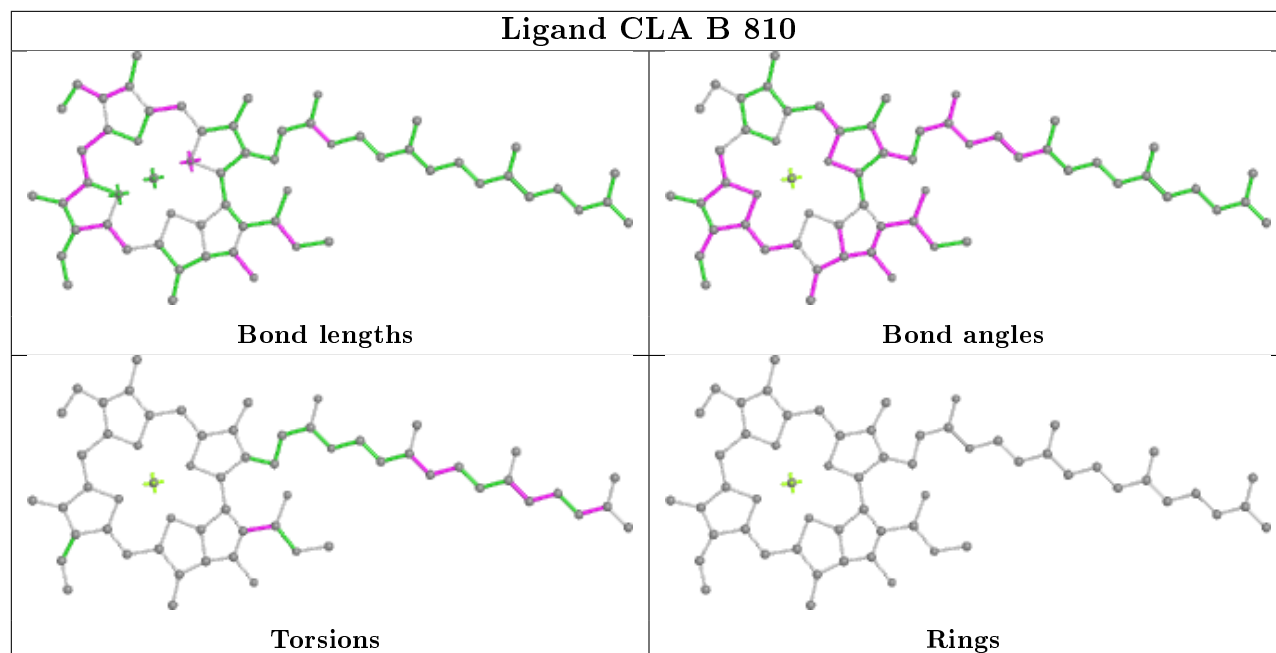


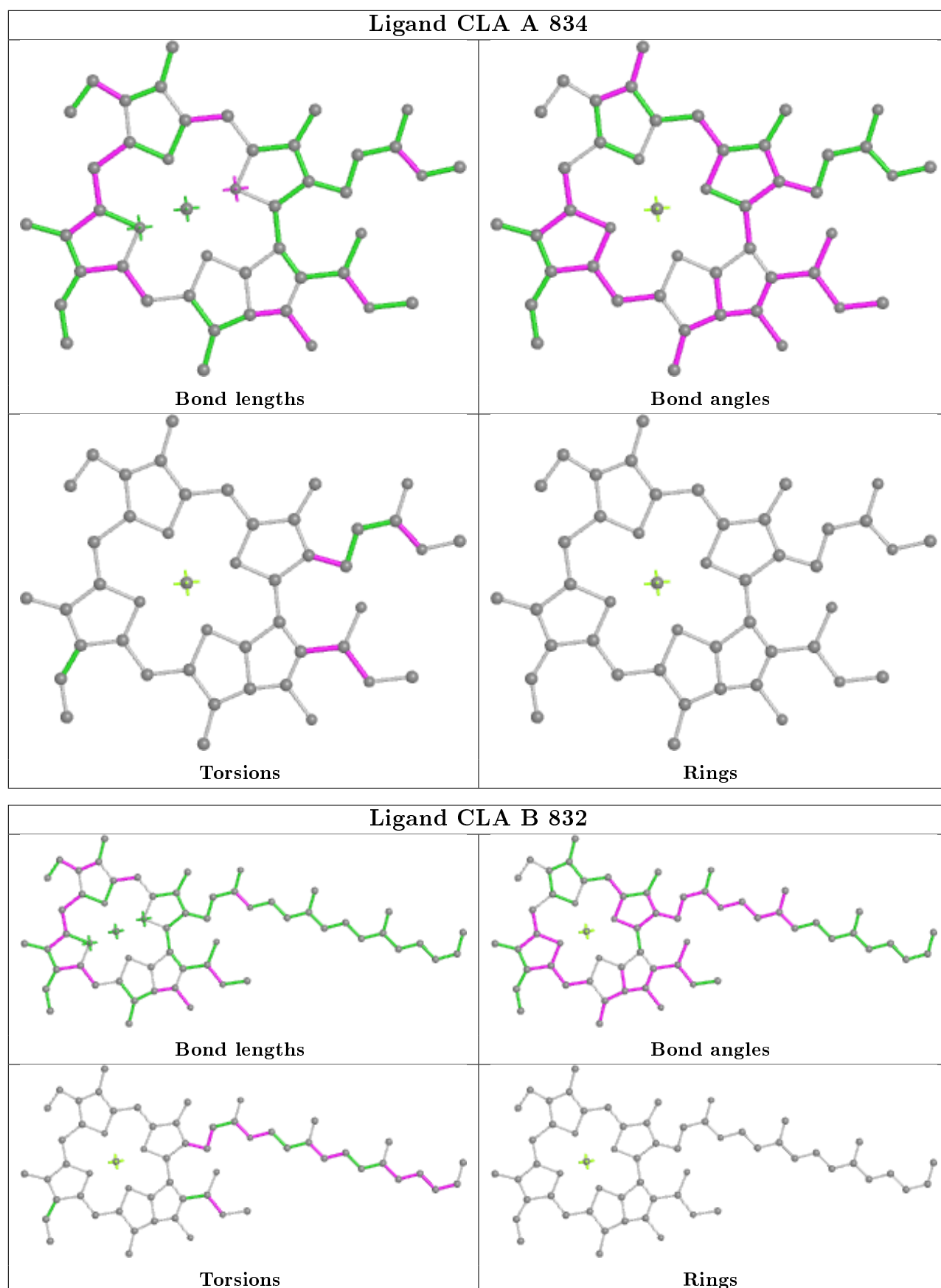


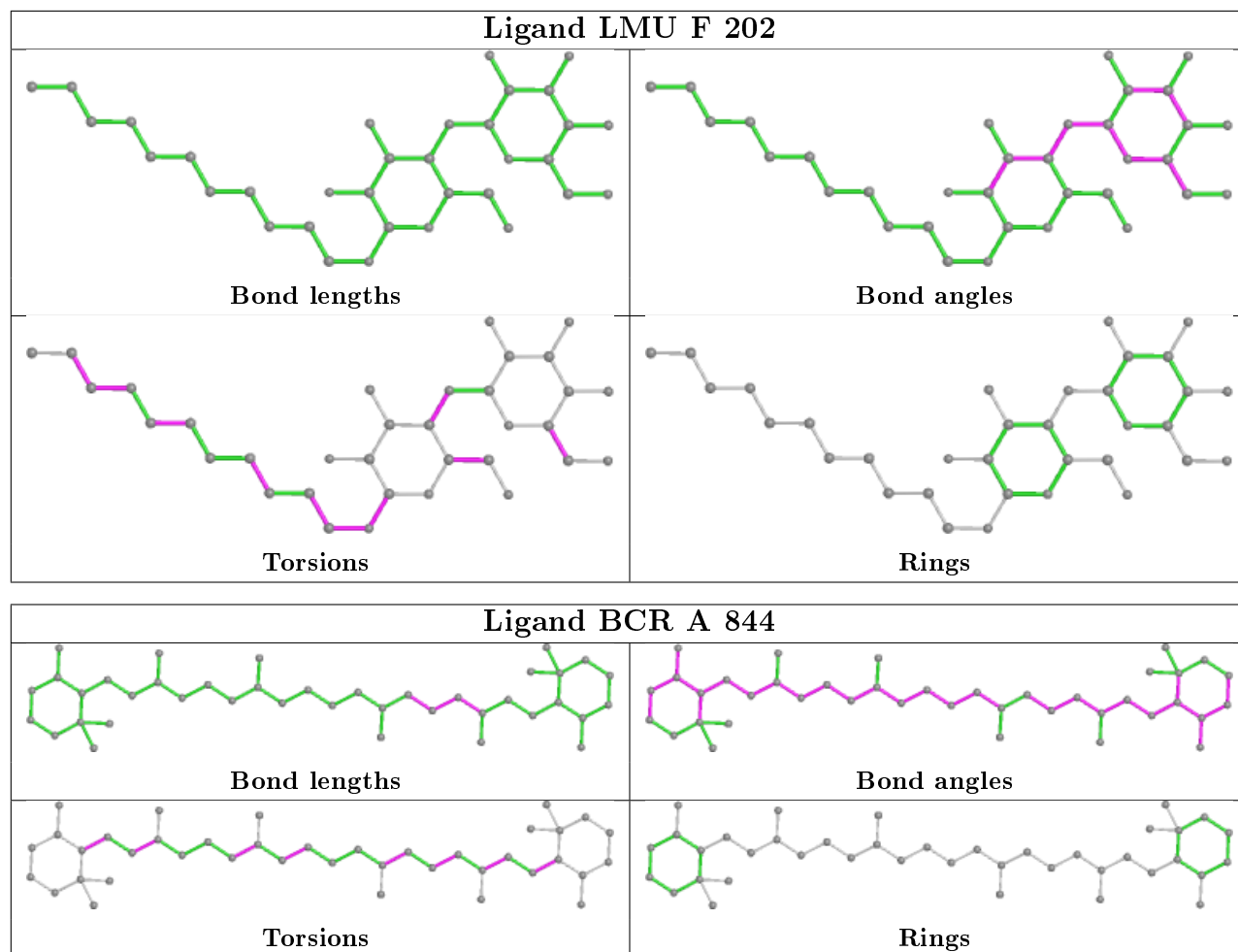




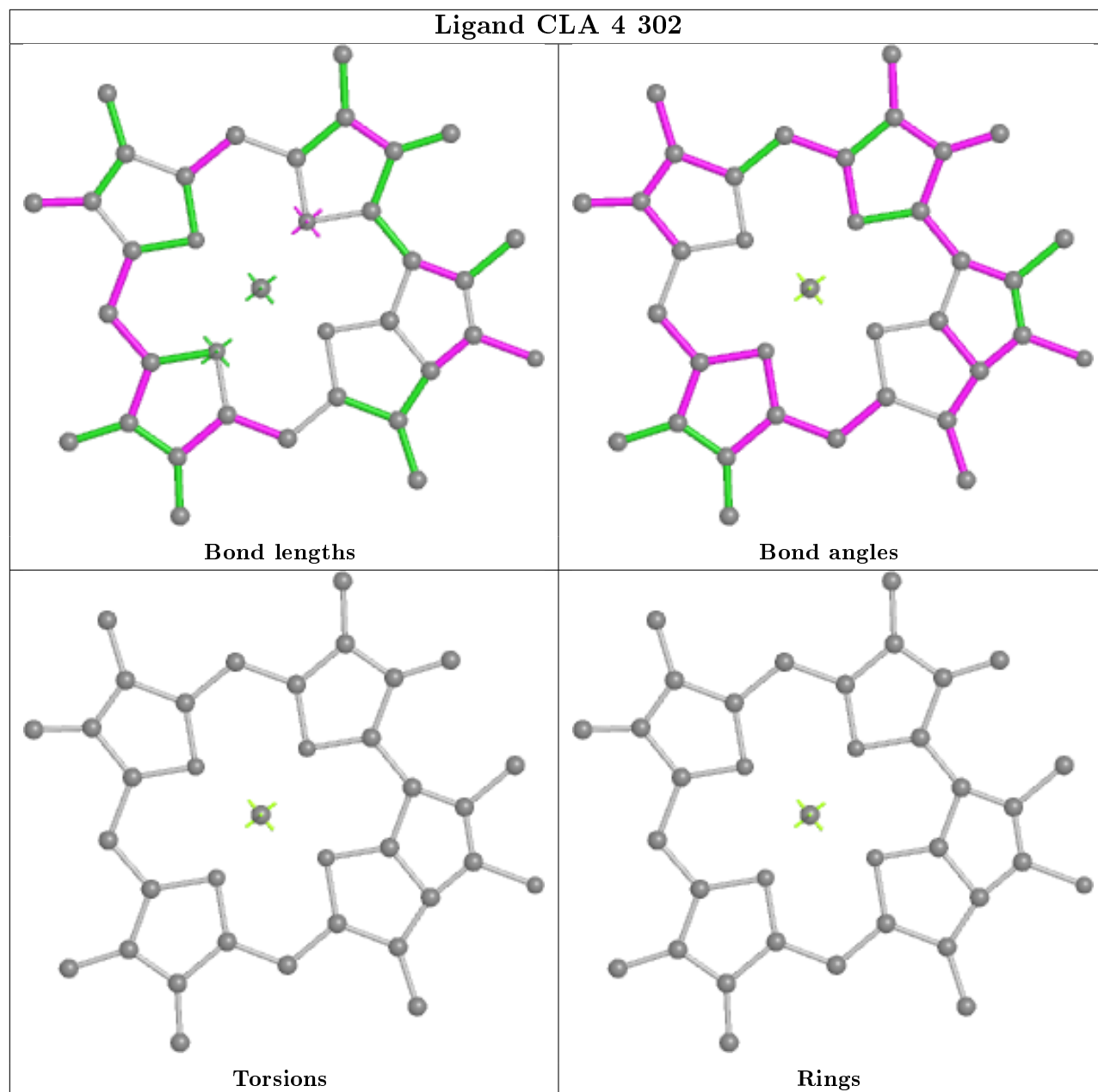


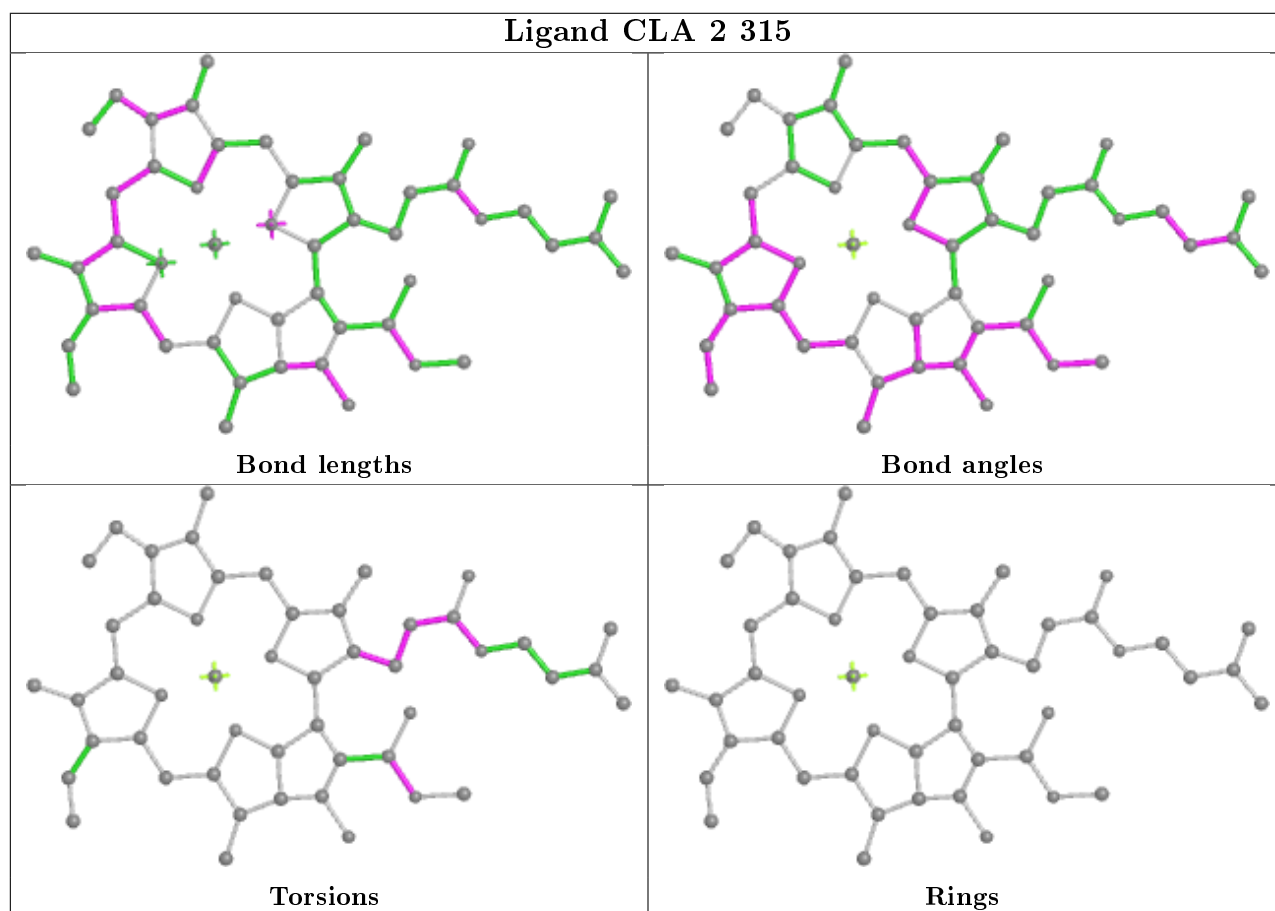
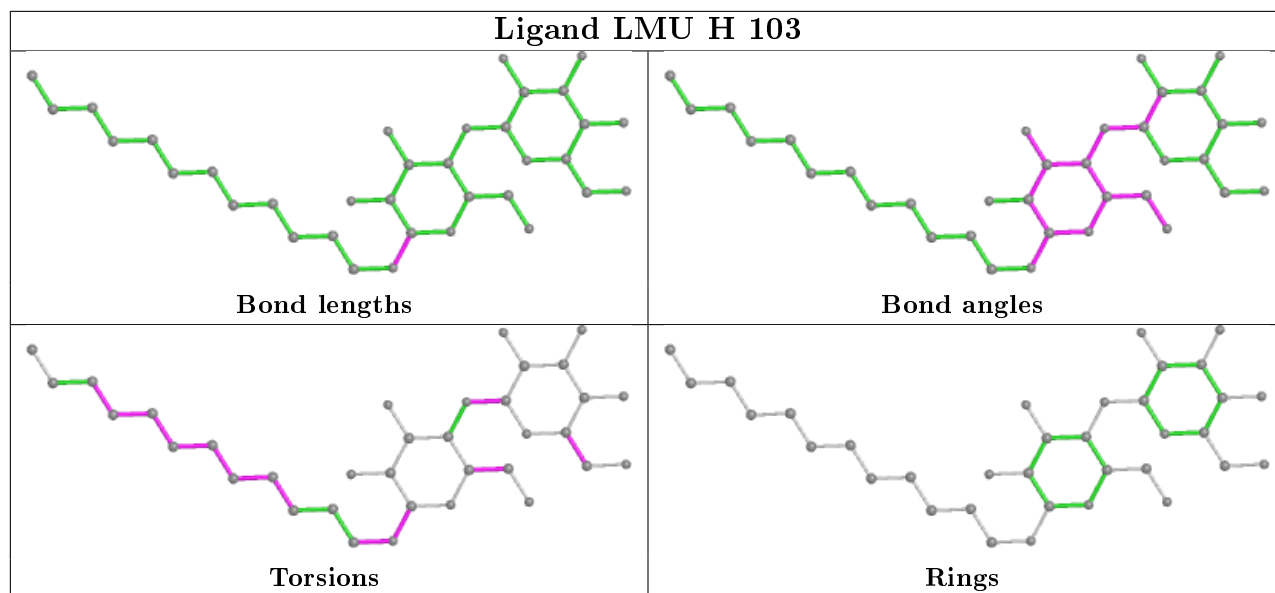


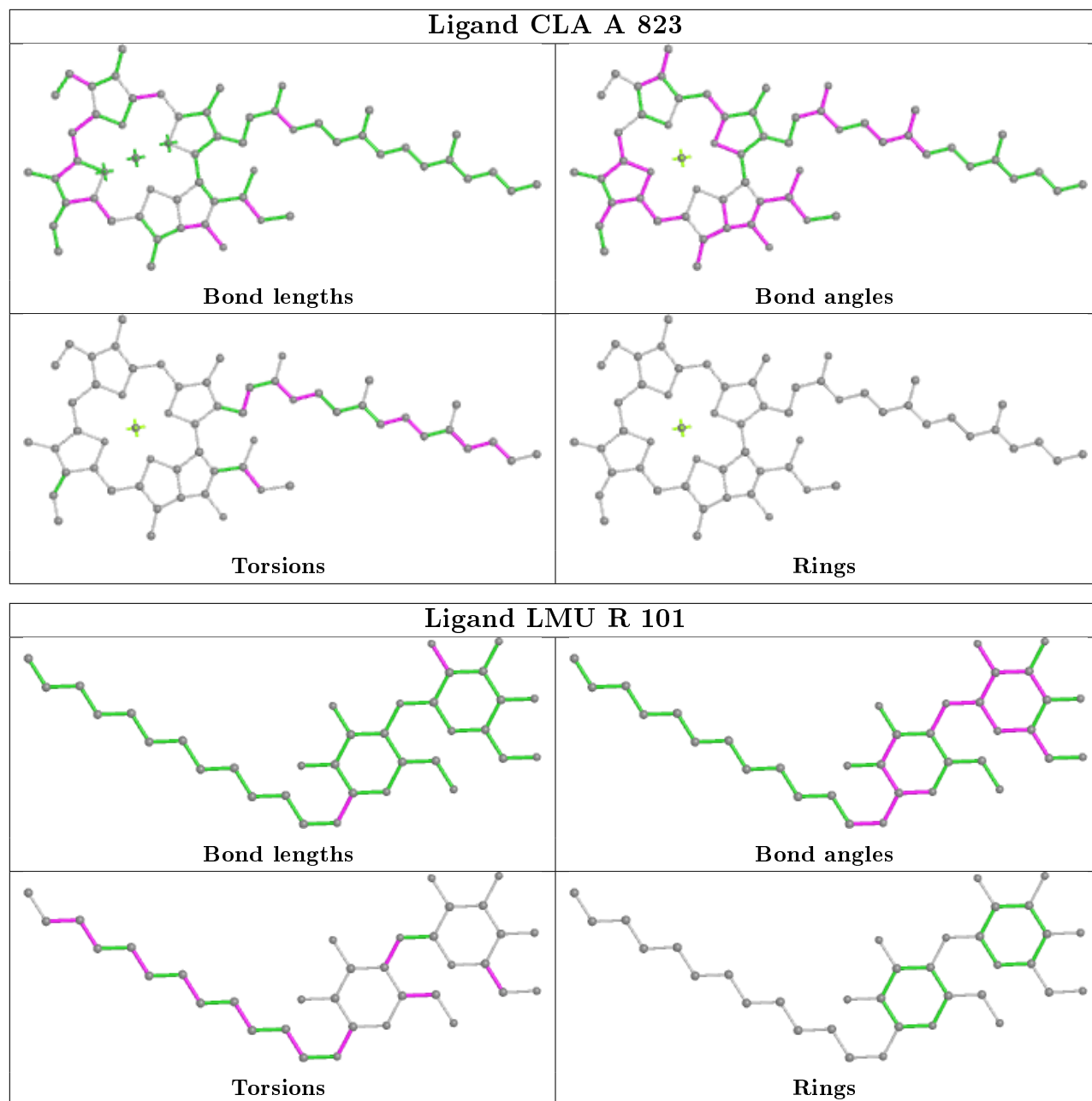


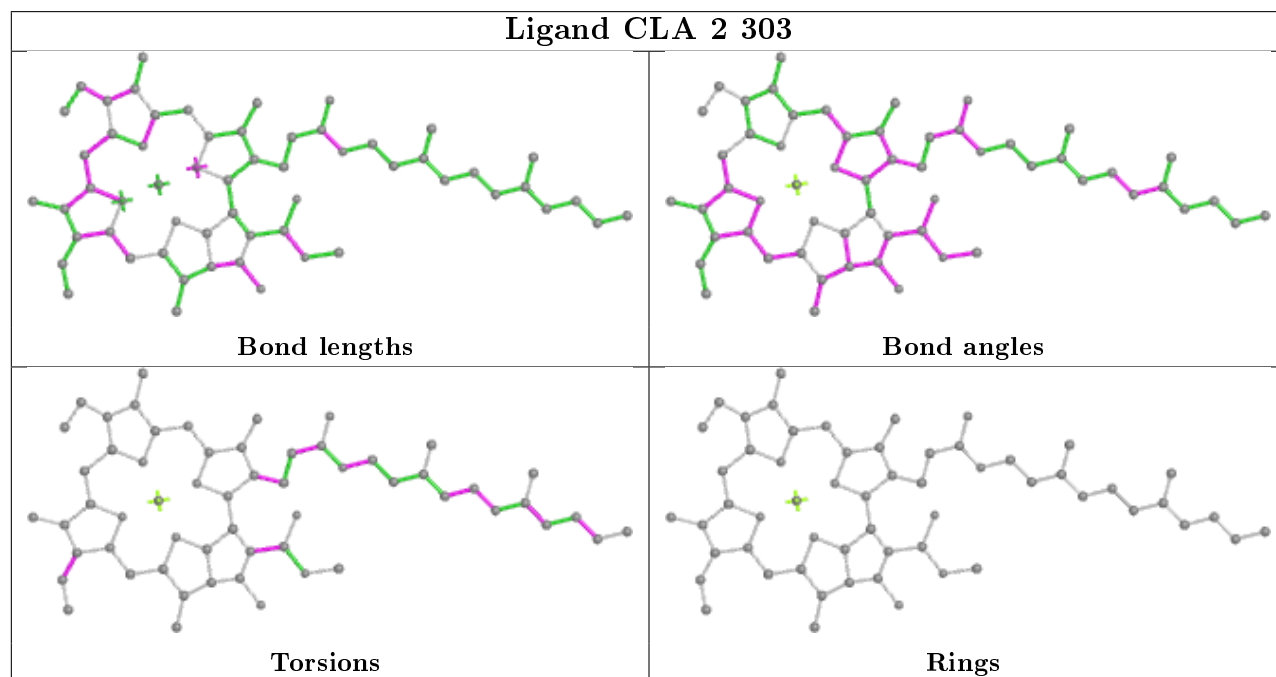
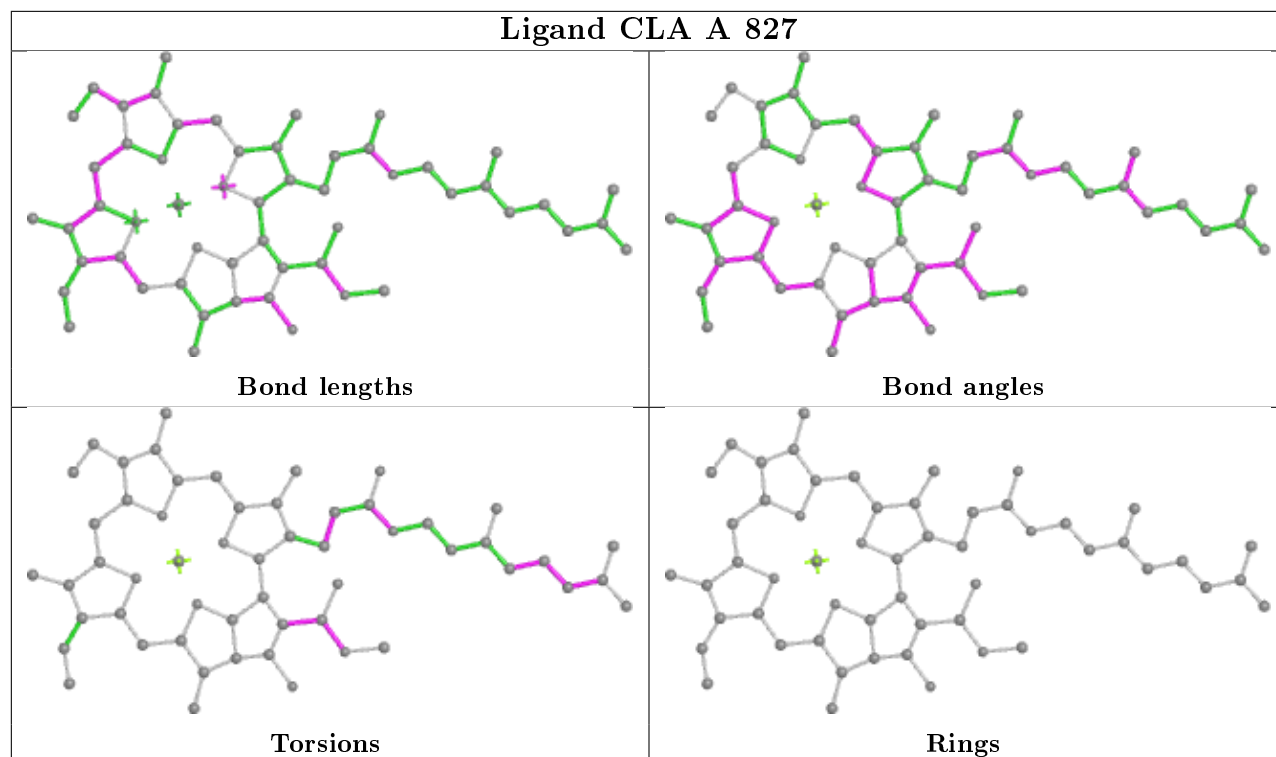


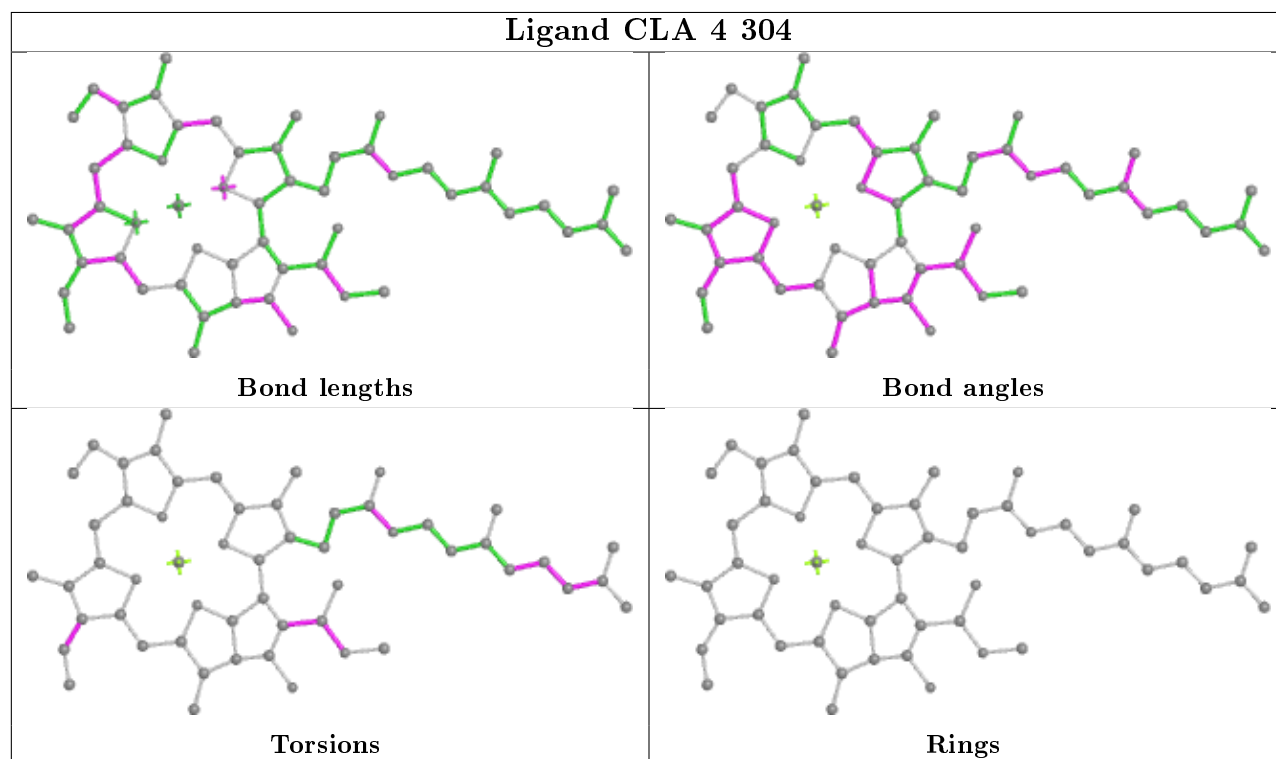
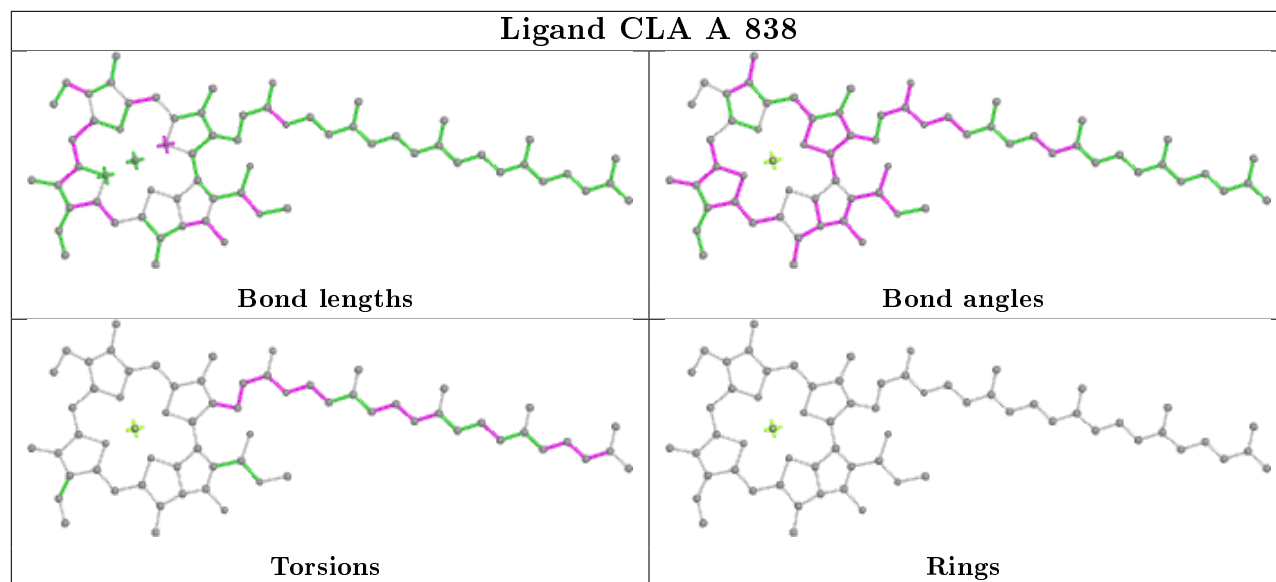
Ligand CLA 4 302

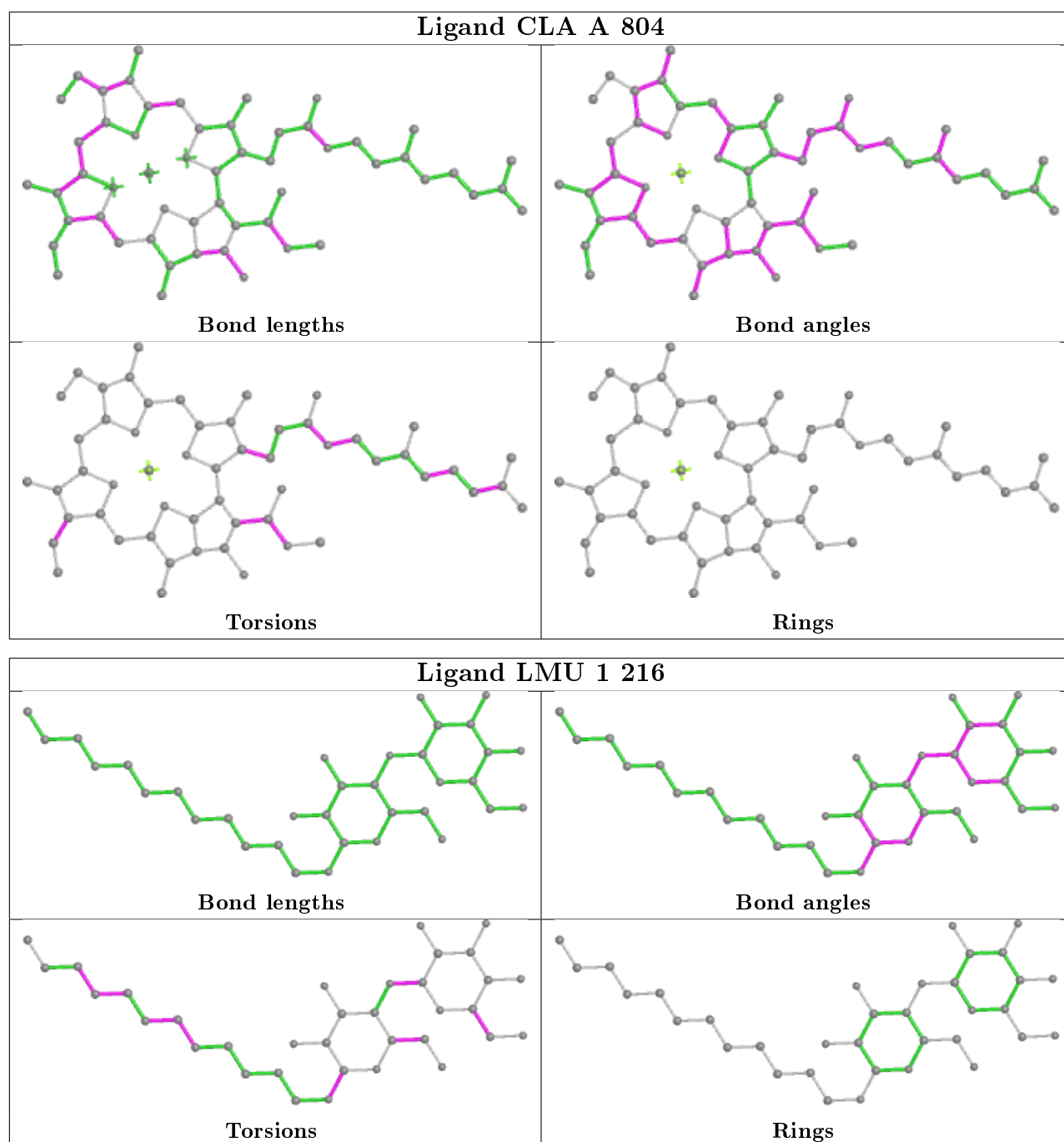




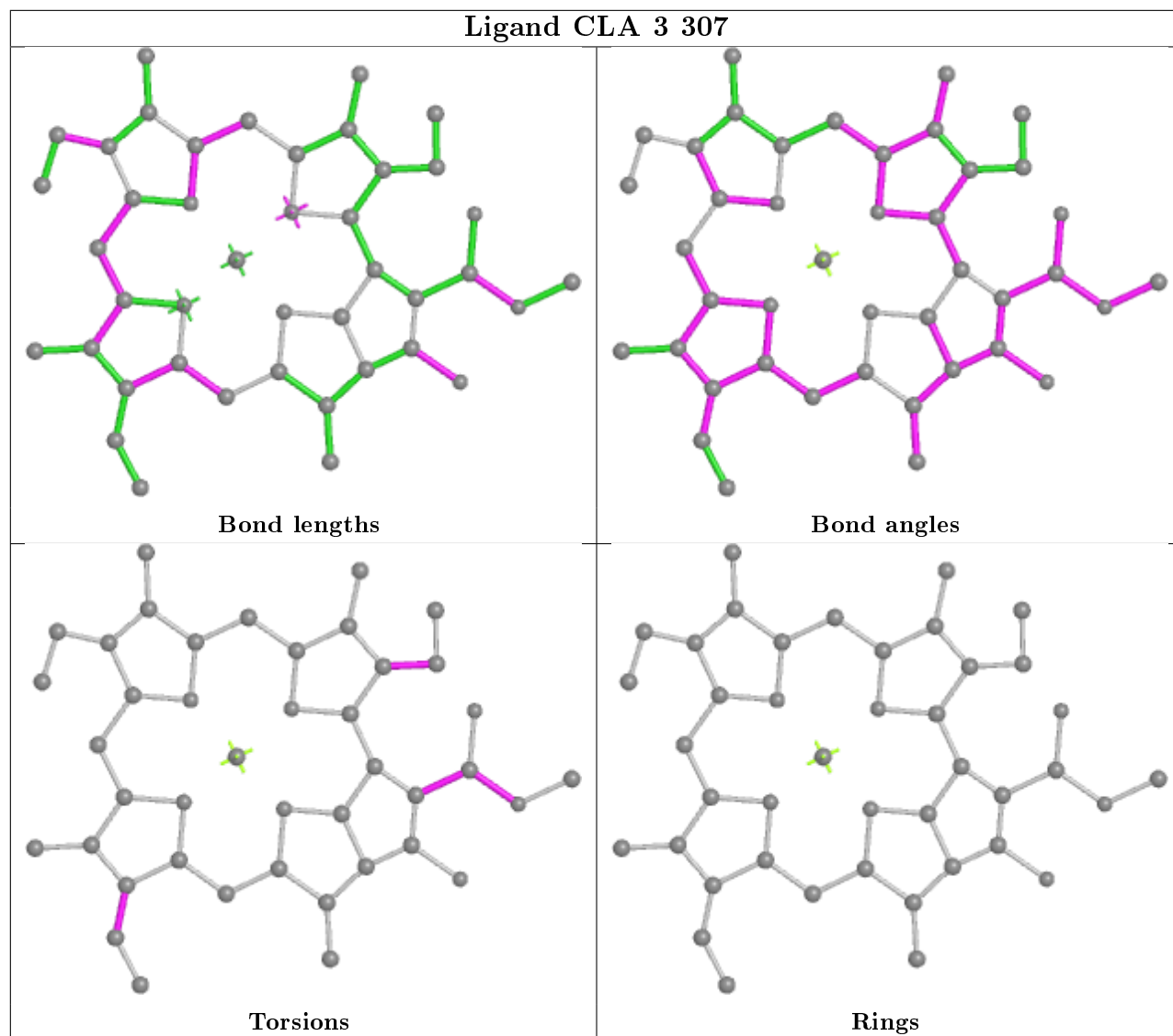


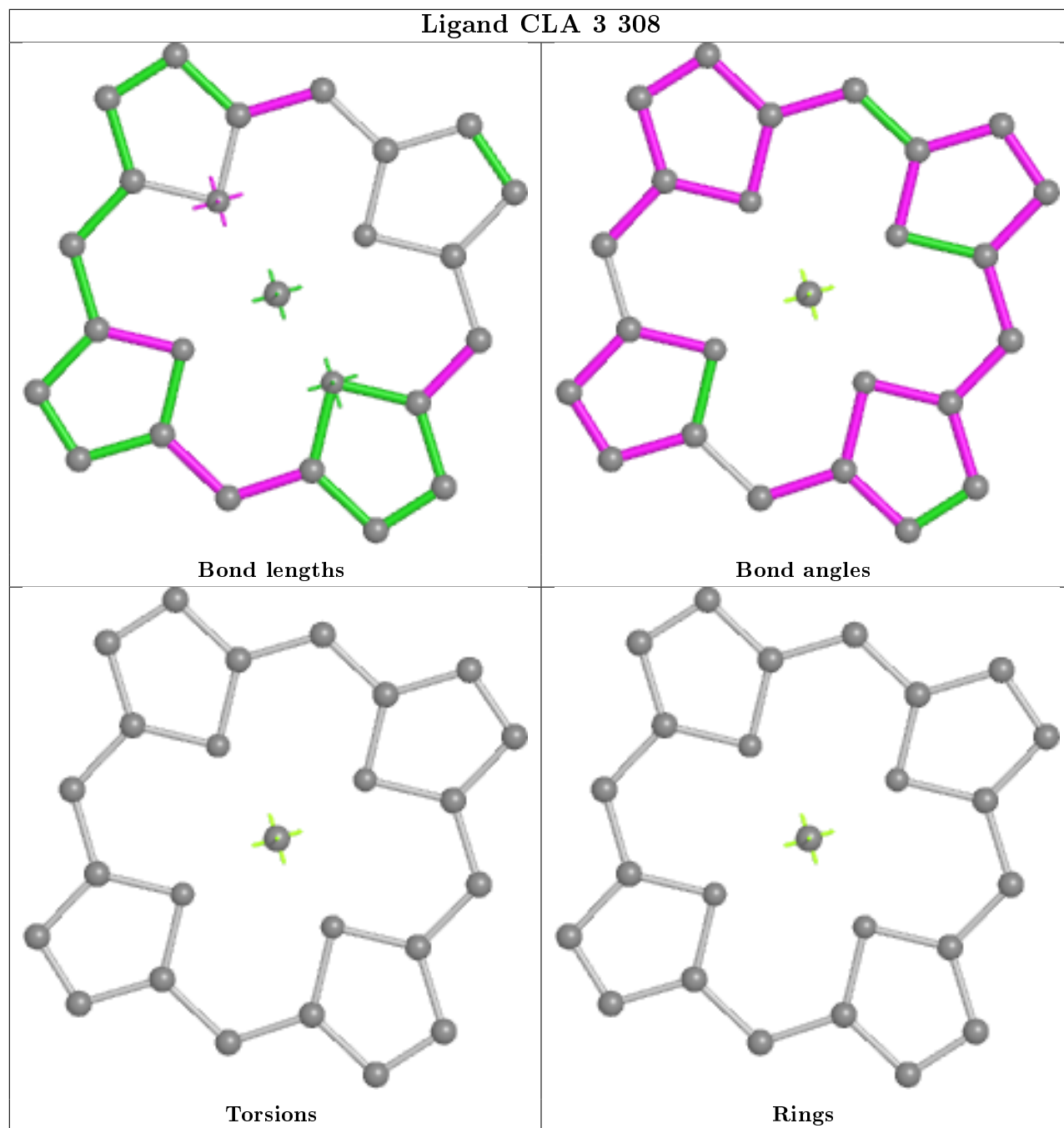


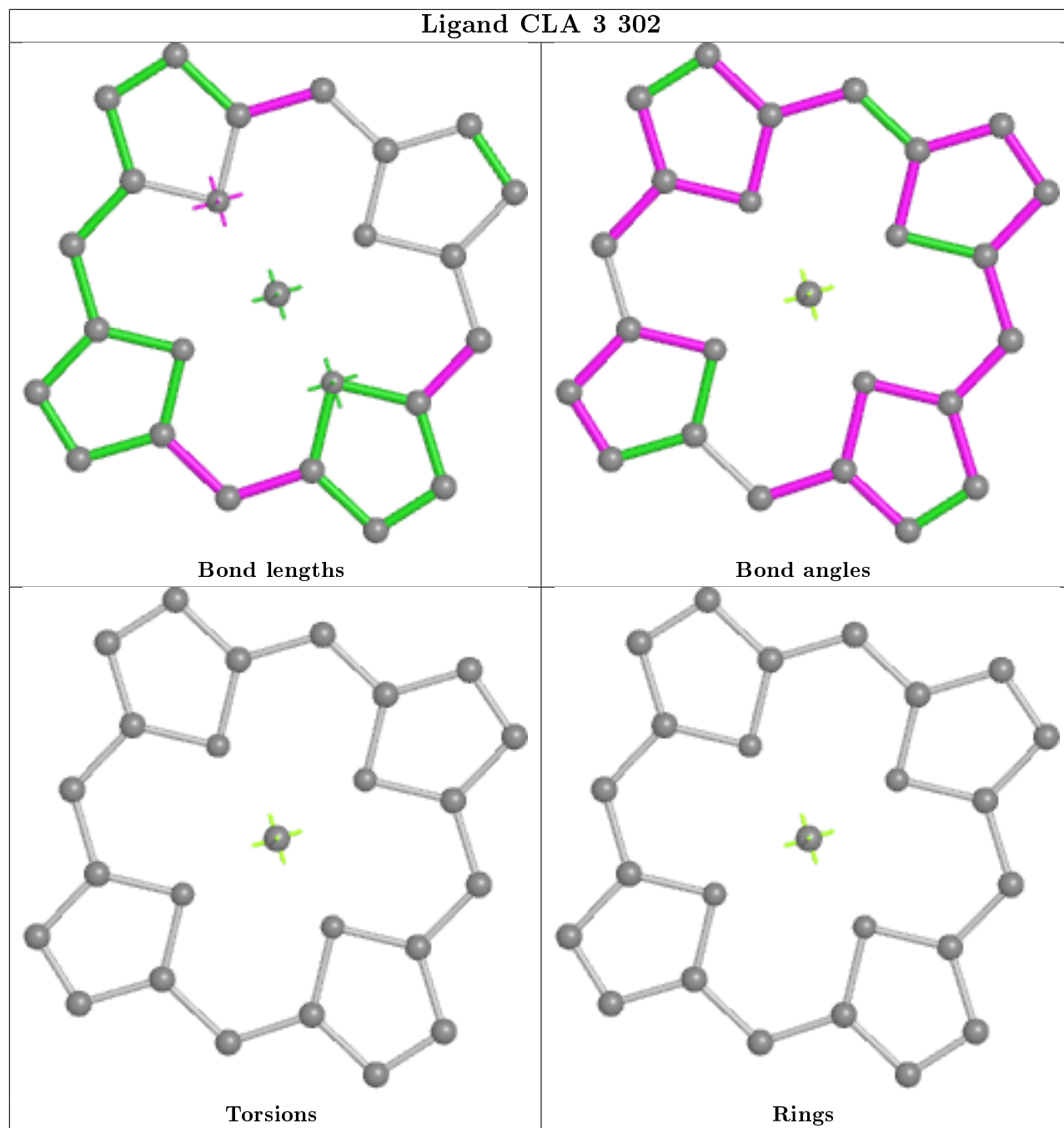


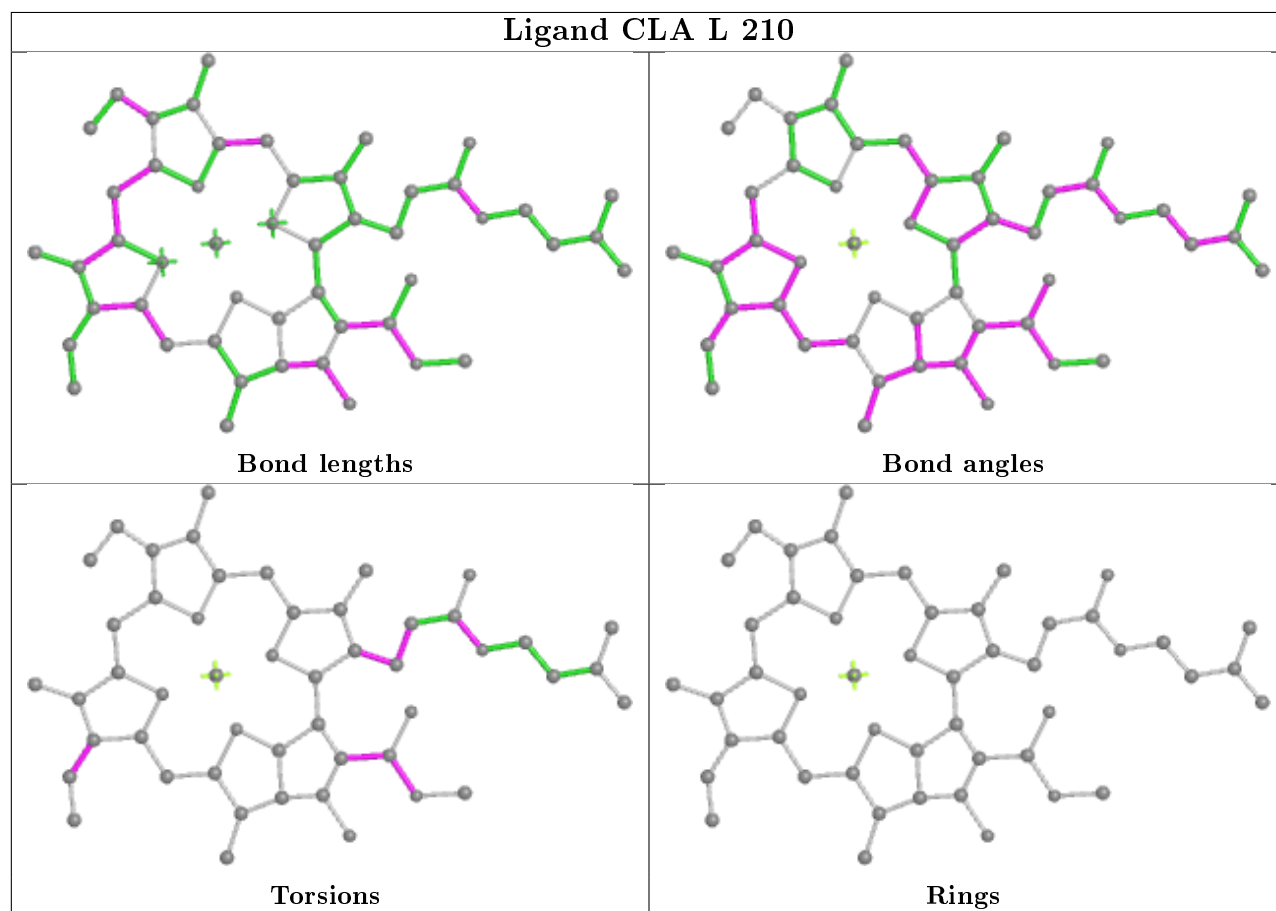
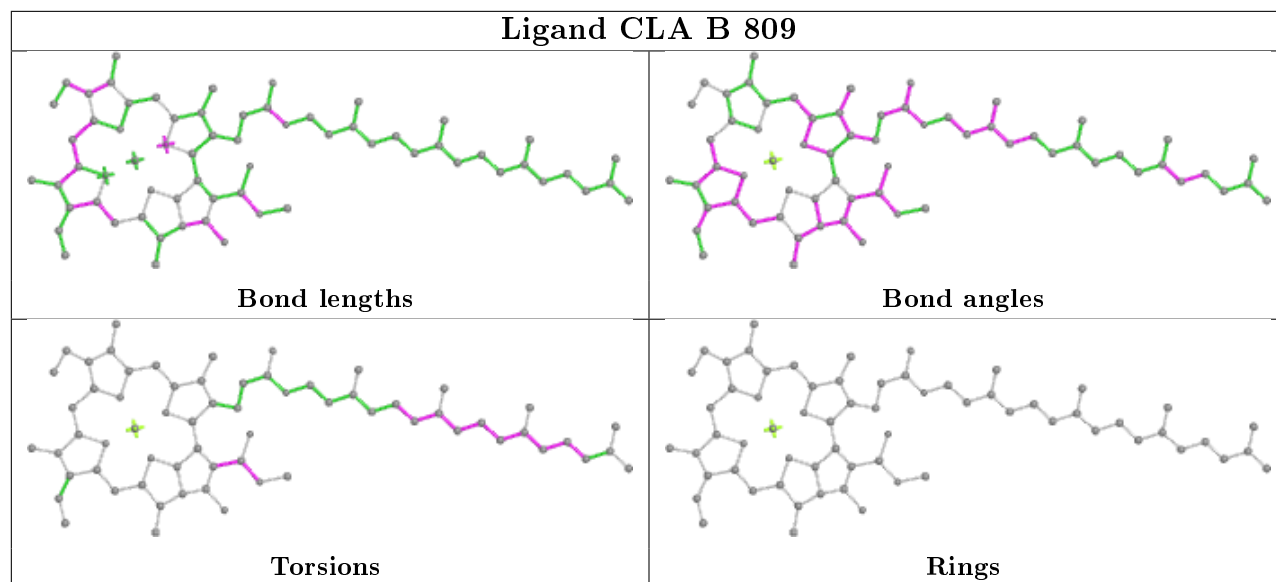


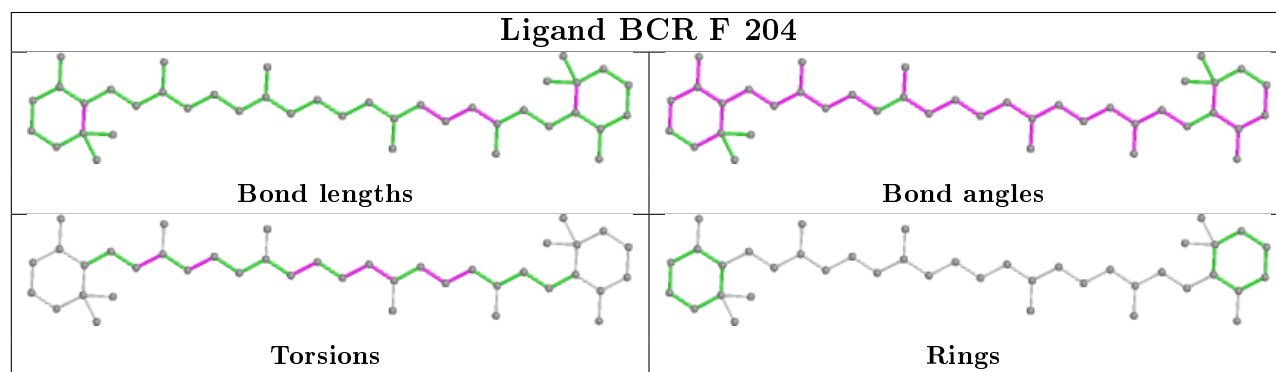
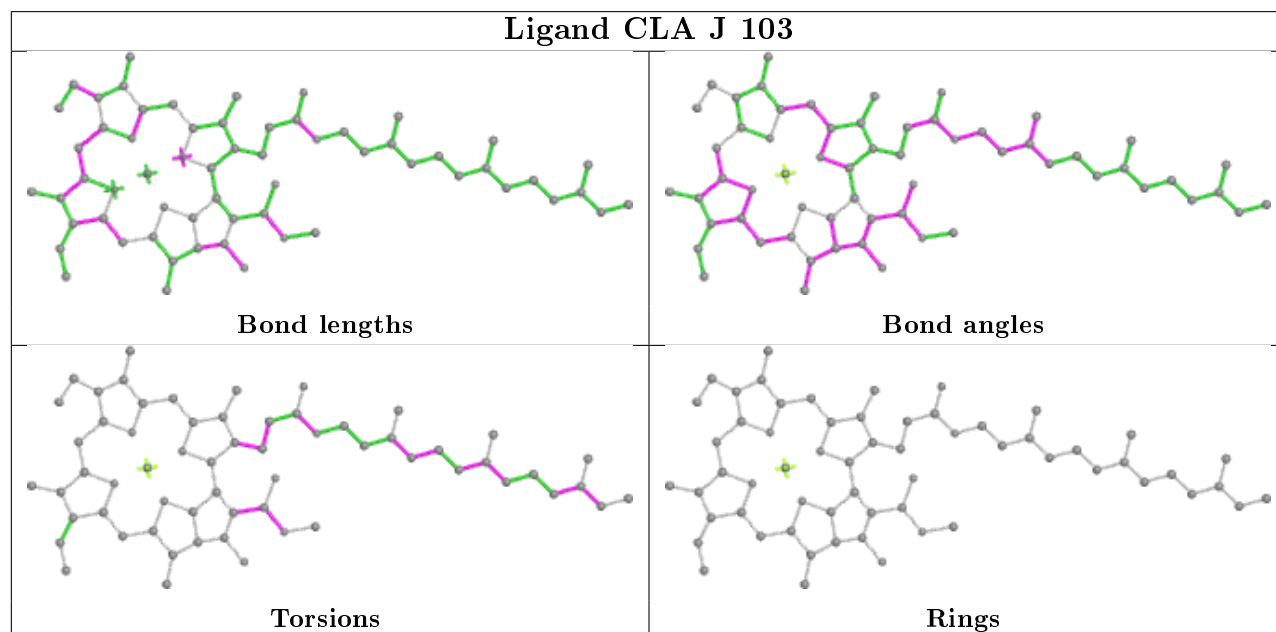
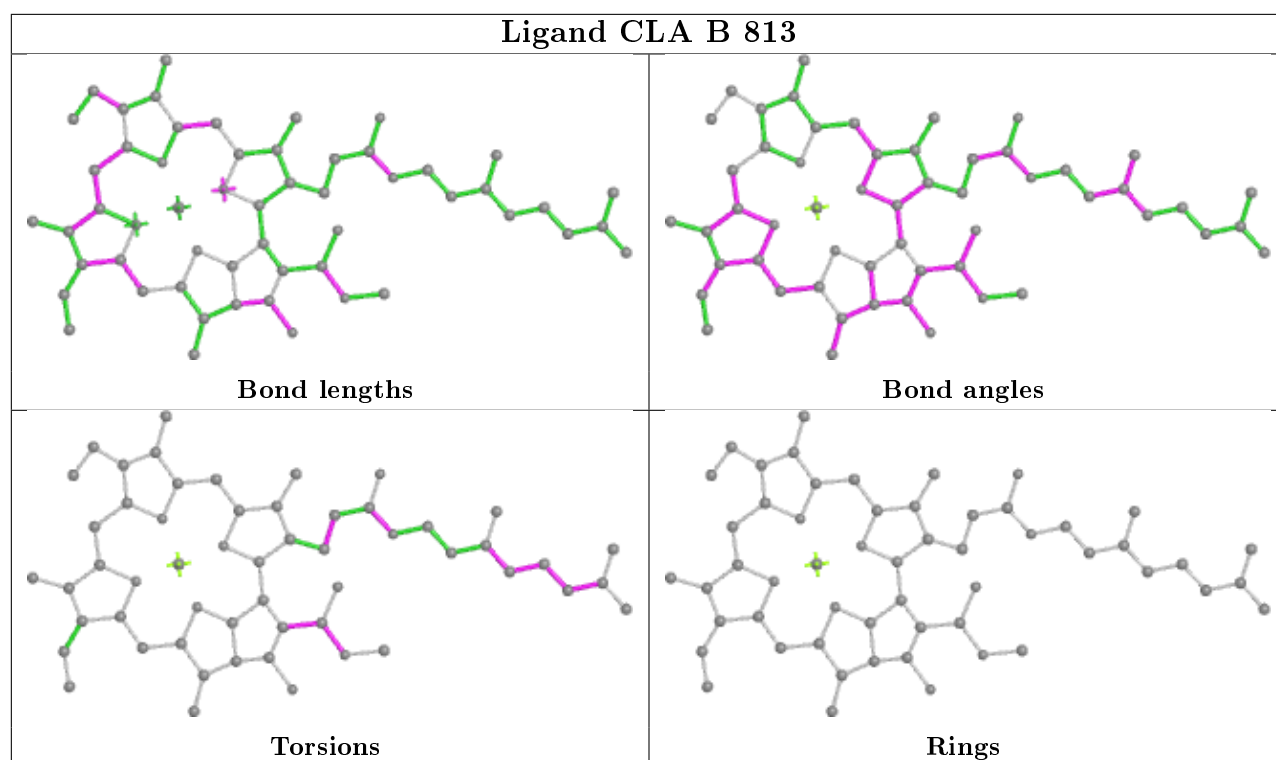
Ligand CLA 3 307

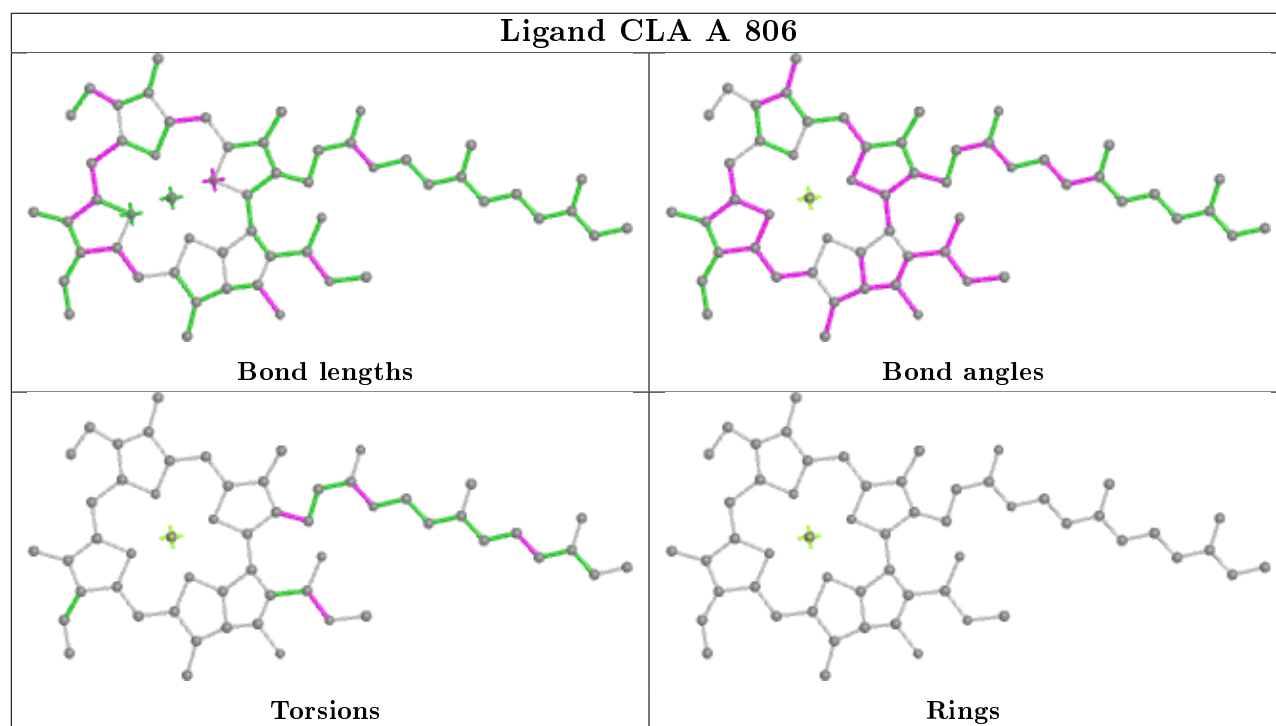
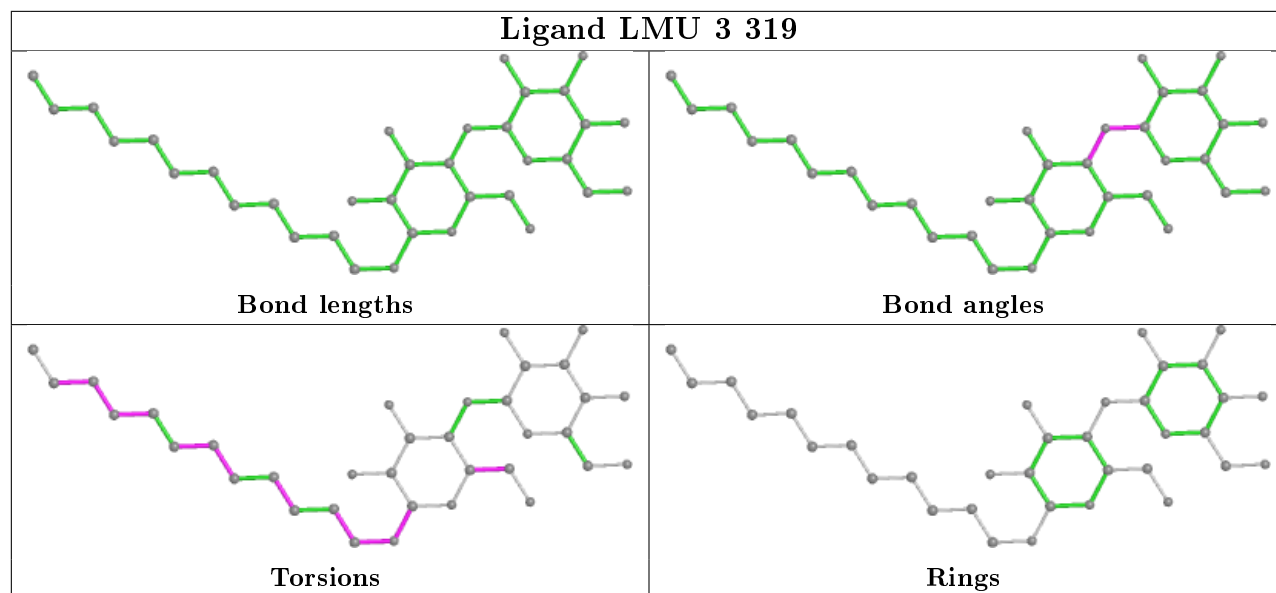


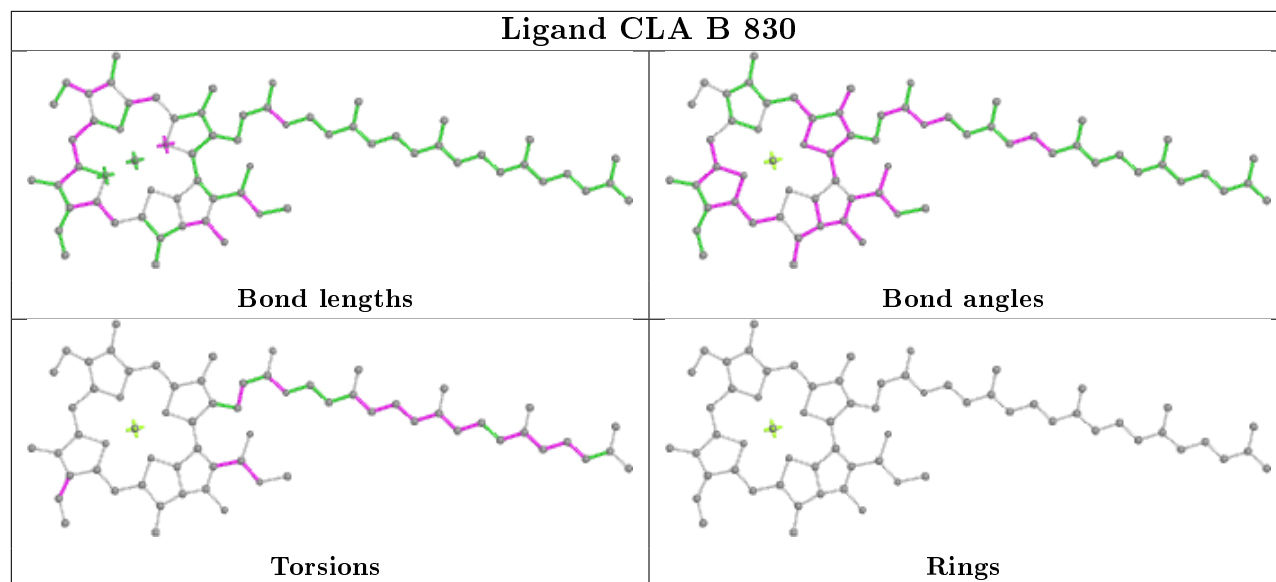


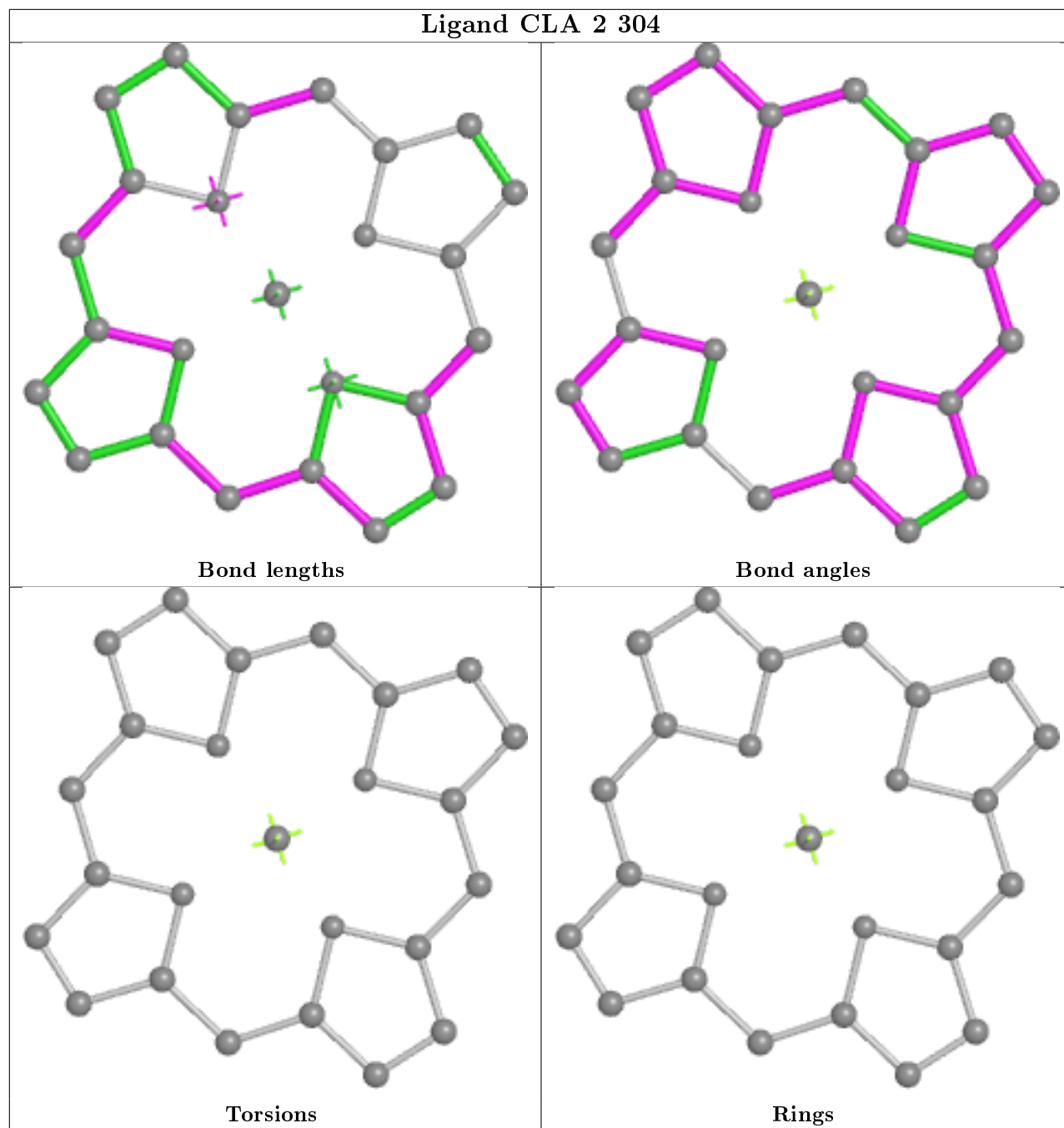


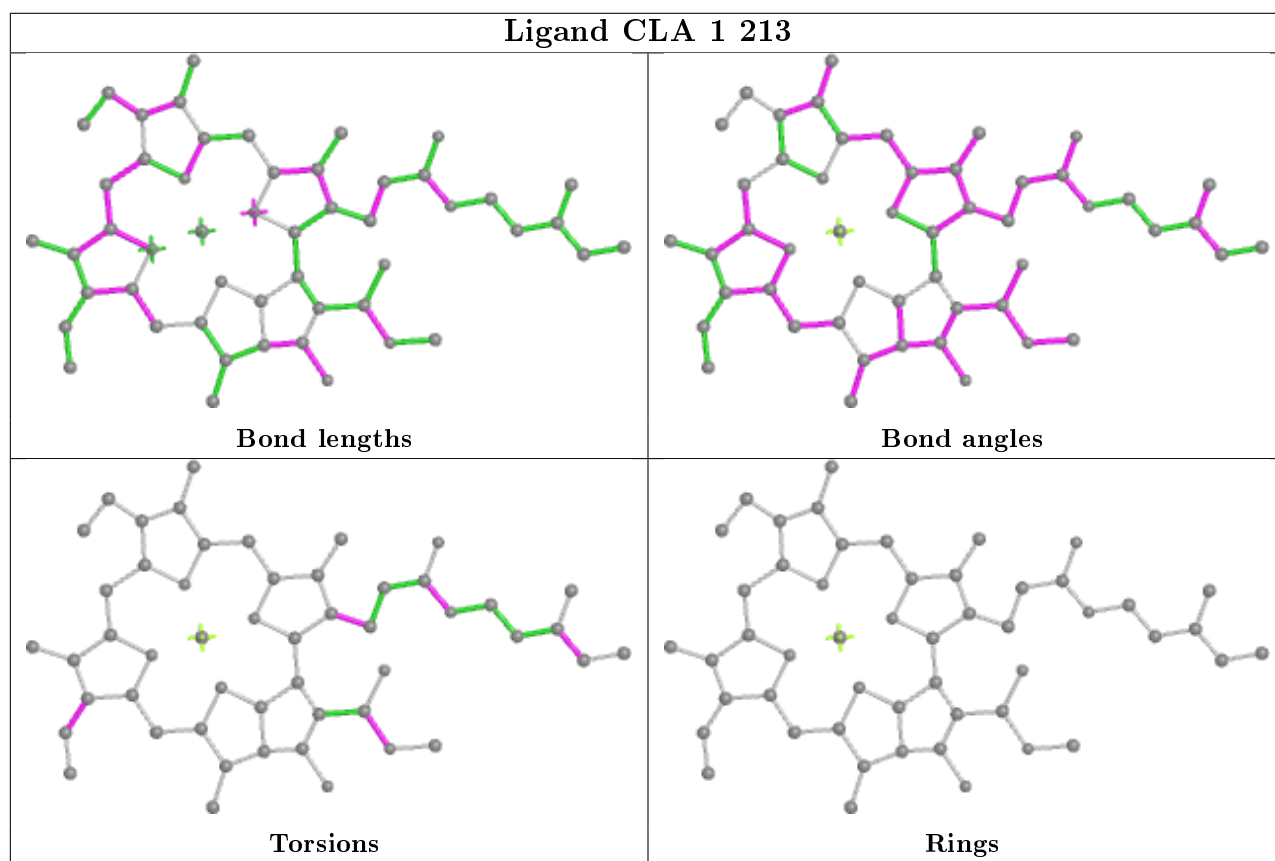
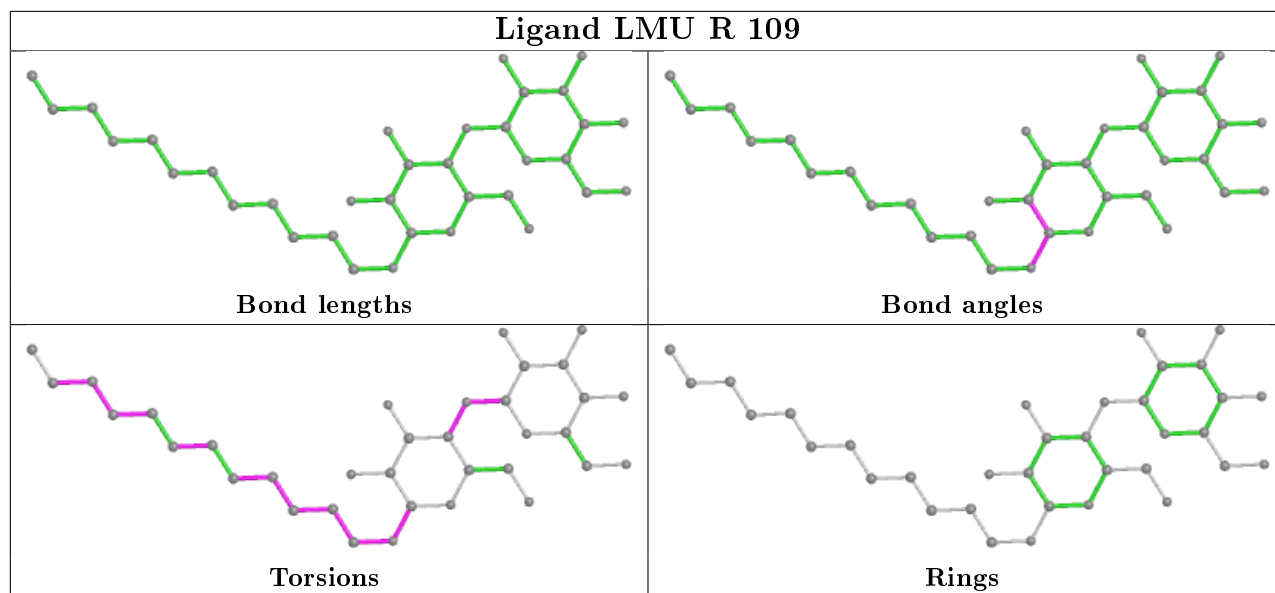


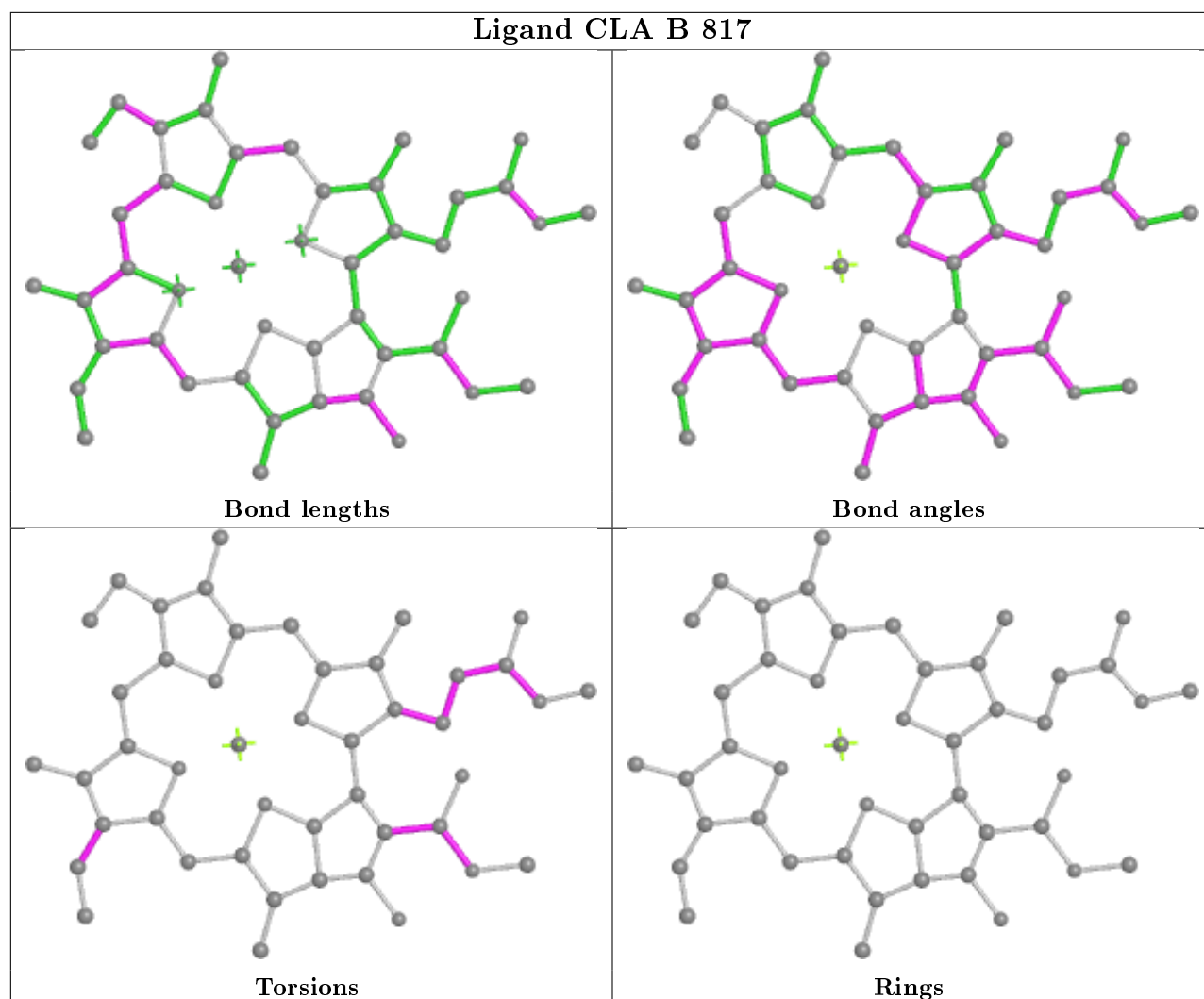
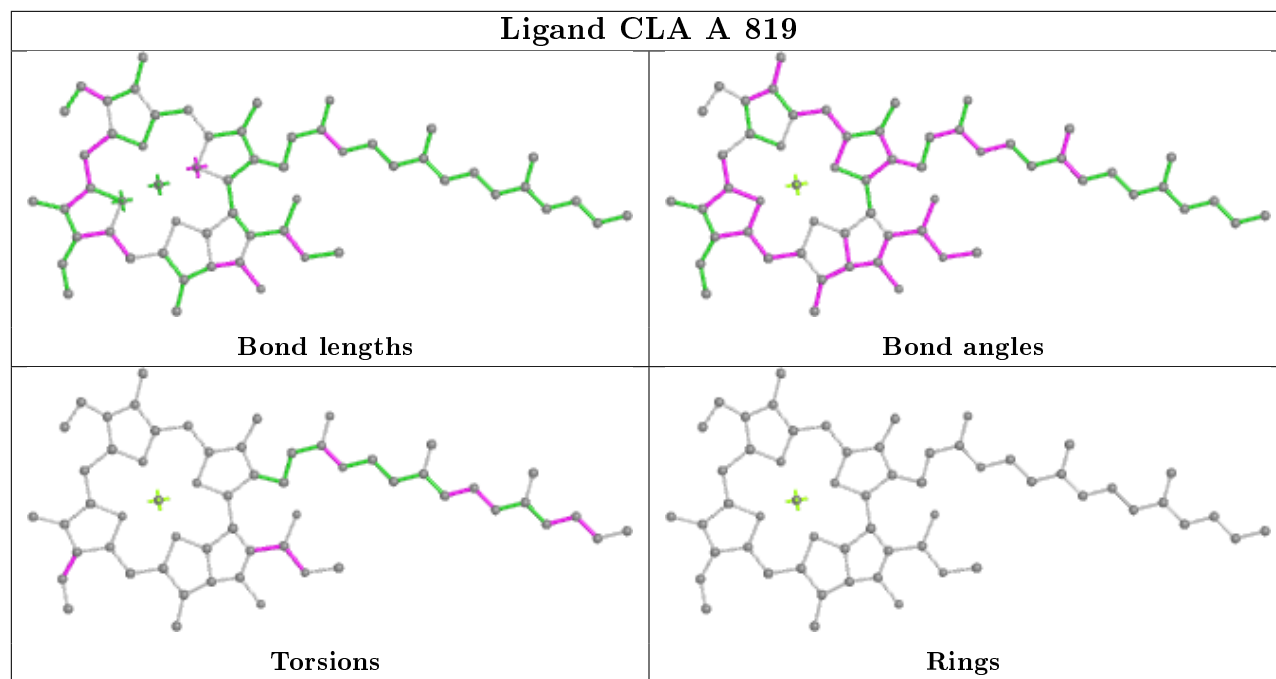


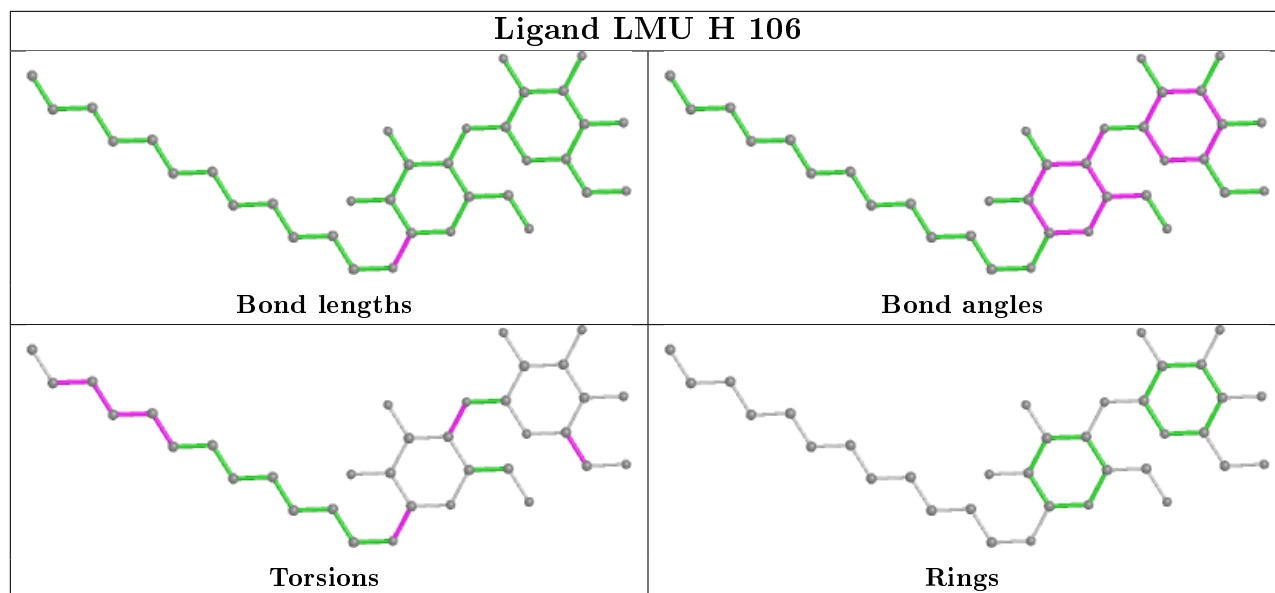


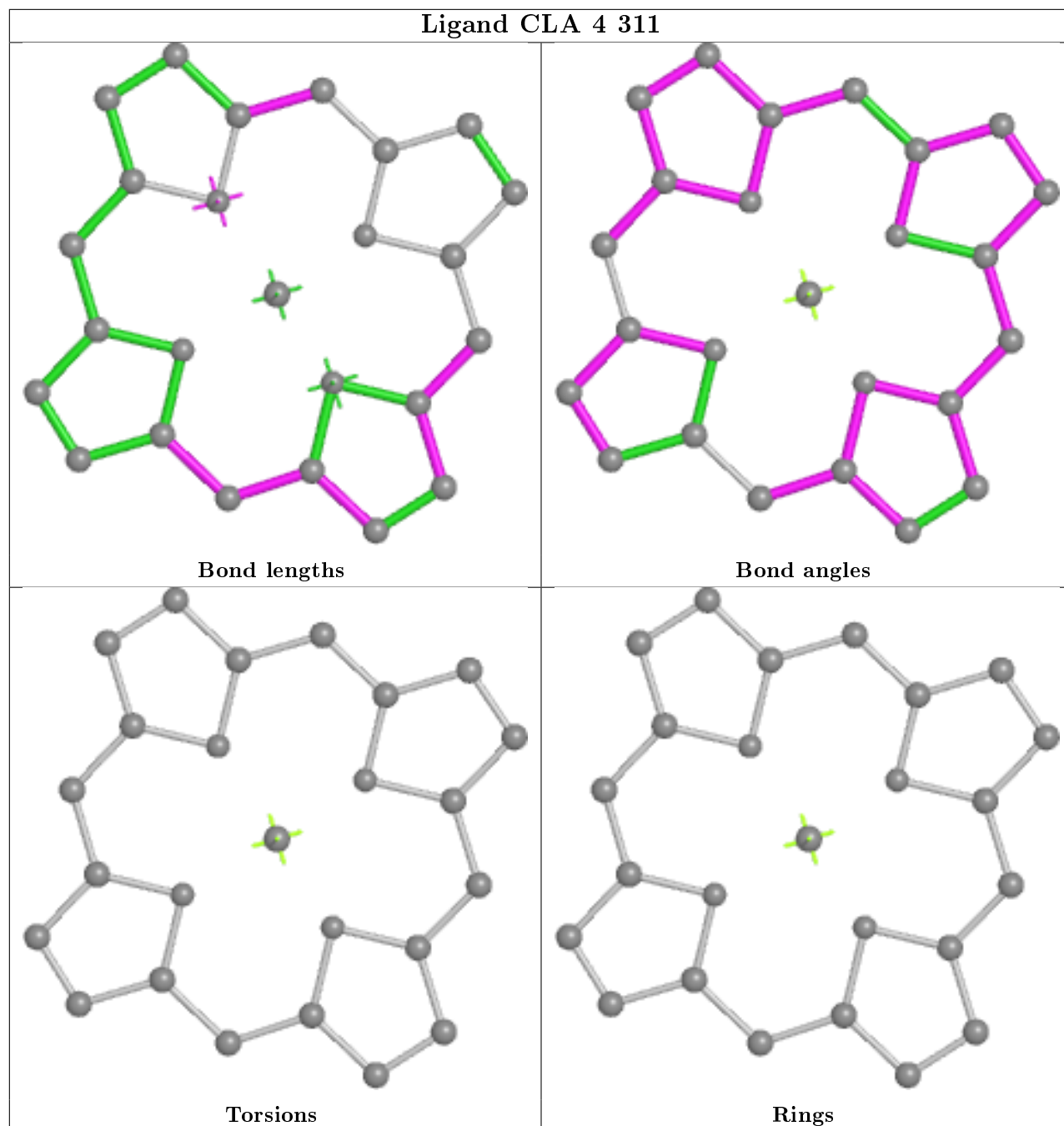


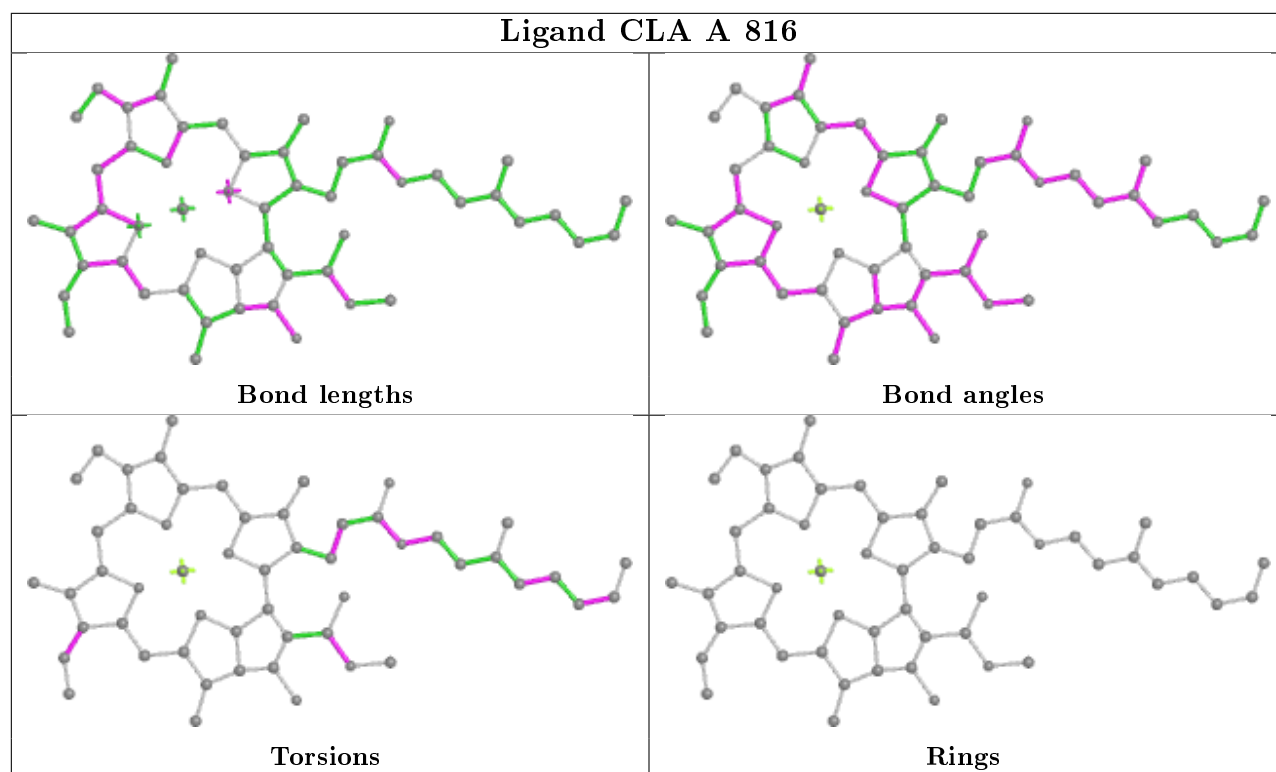
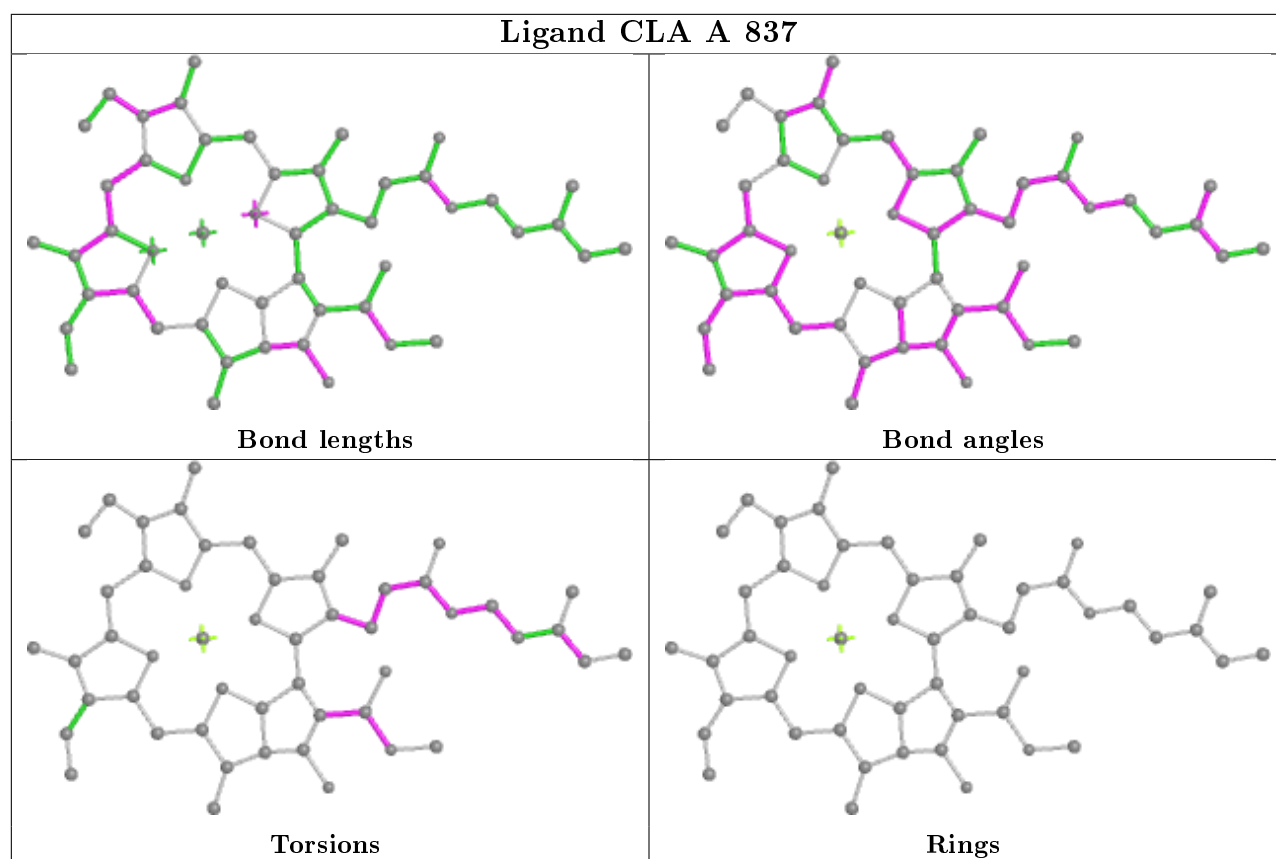


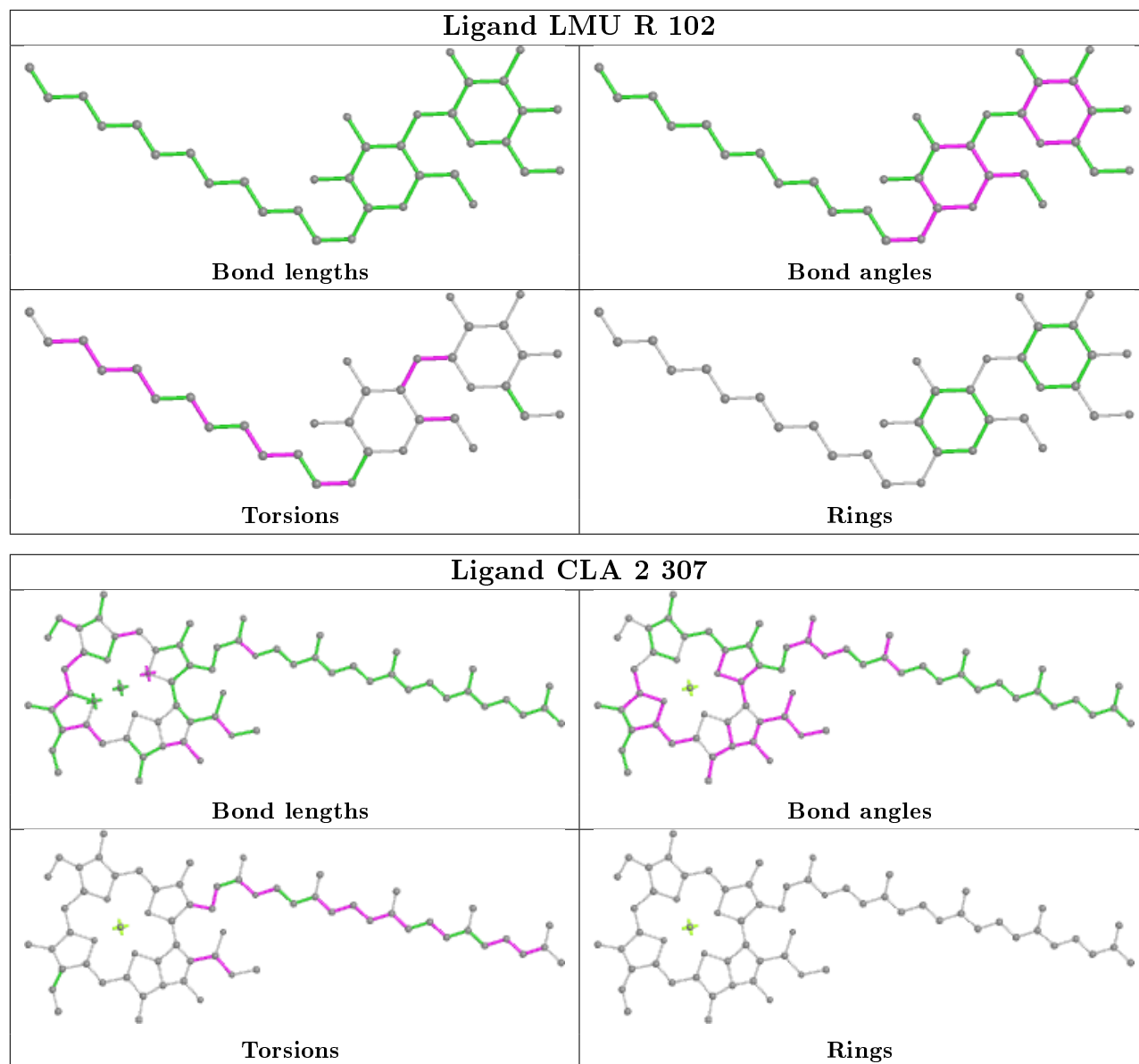


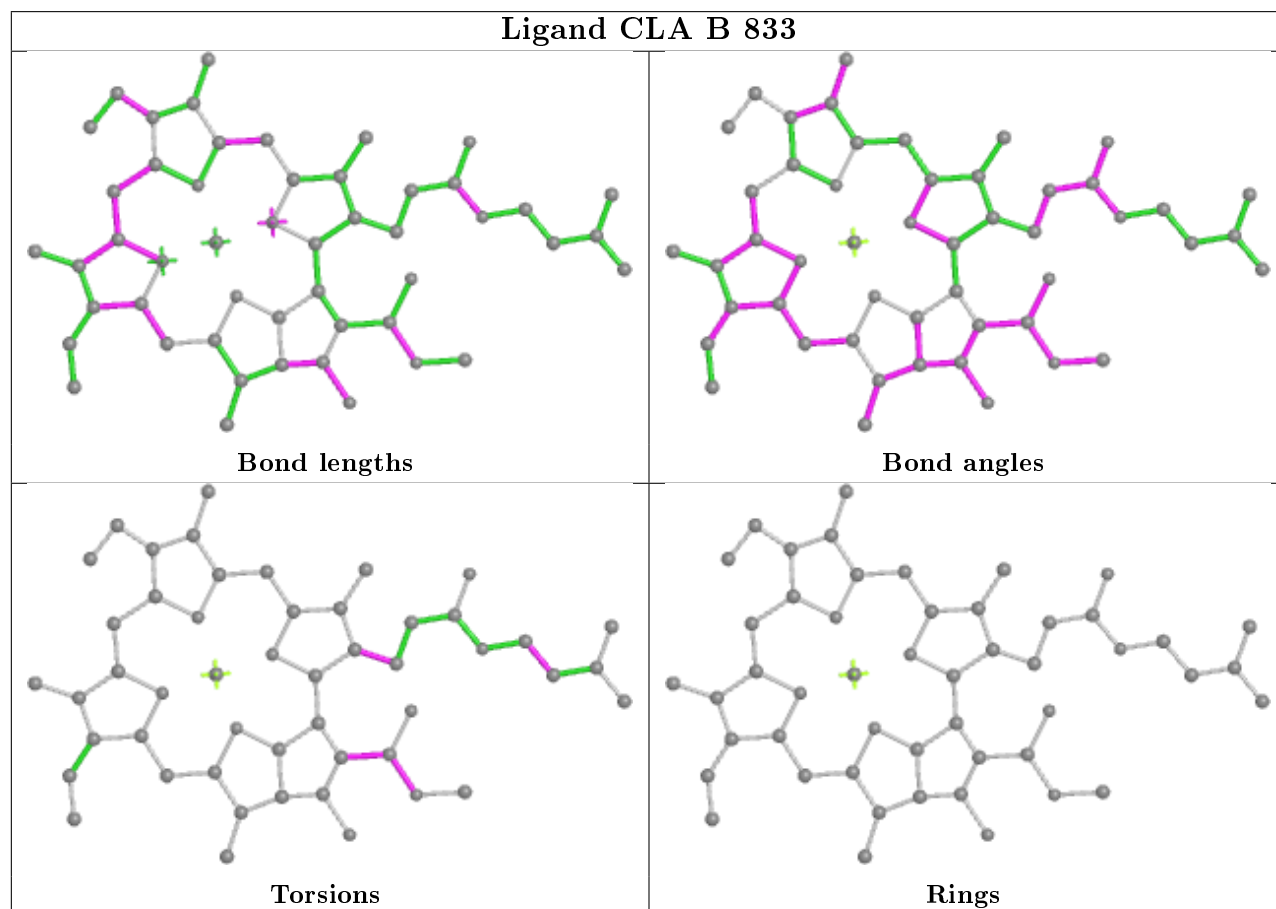
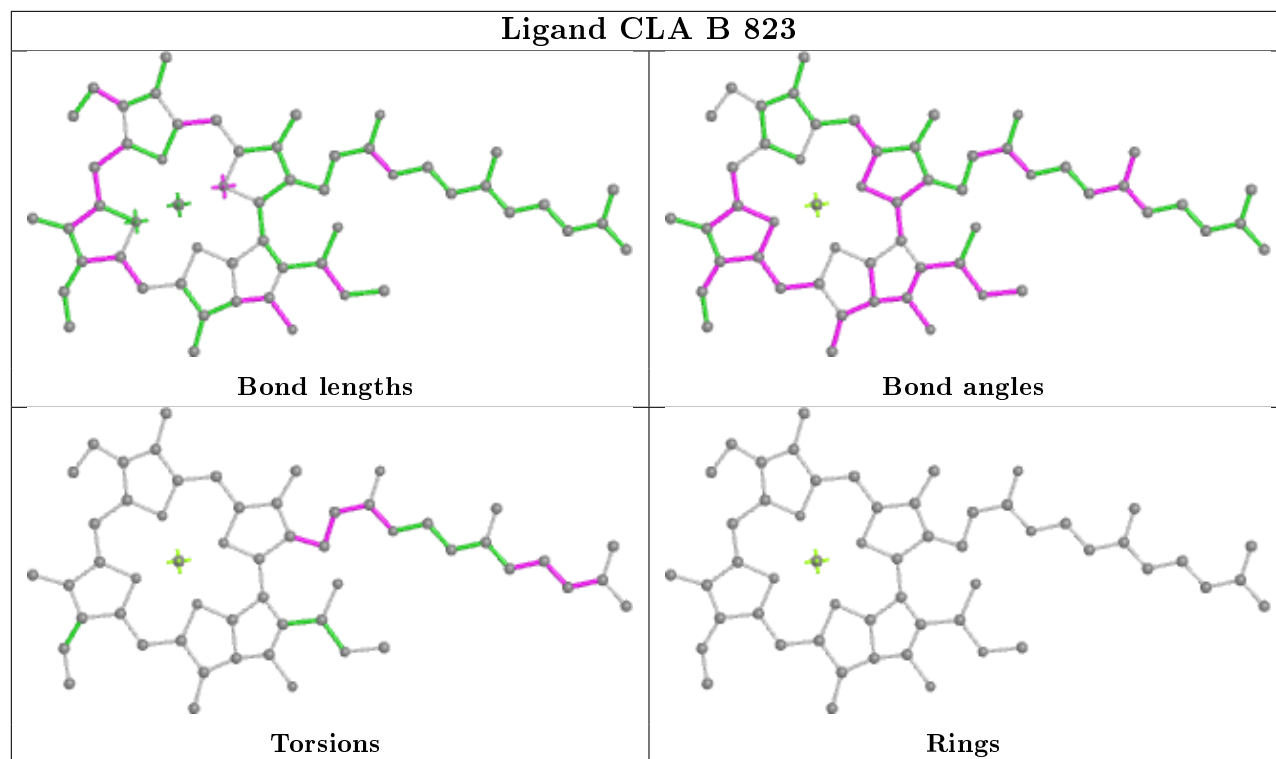


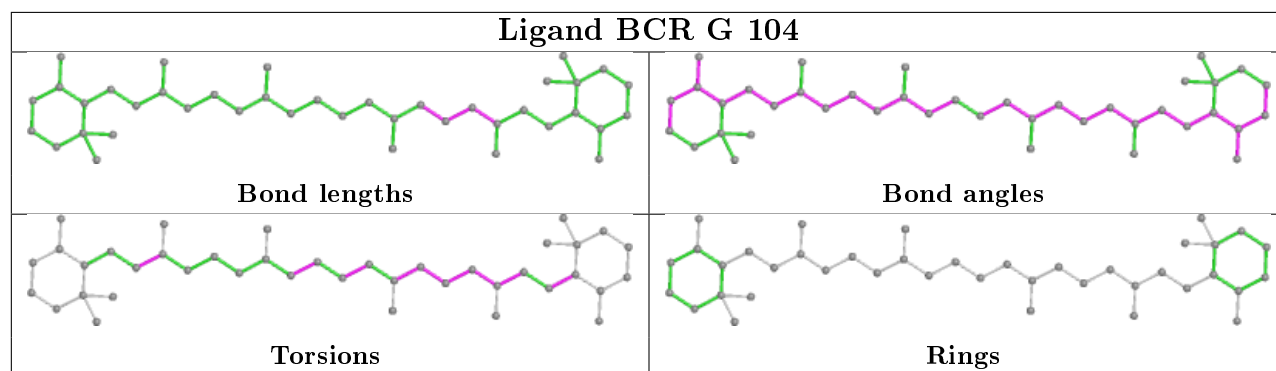
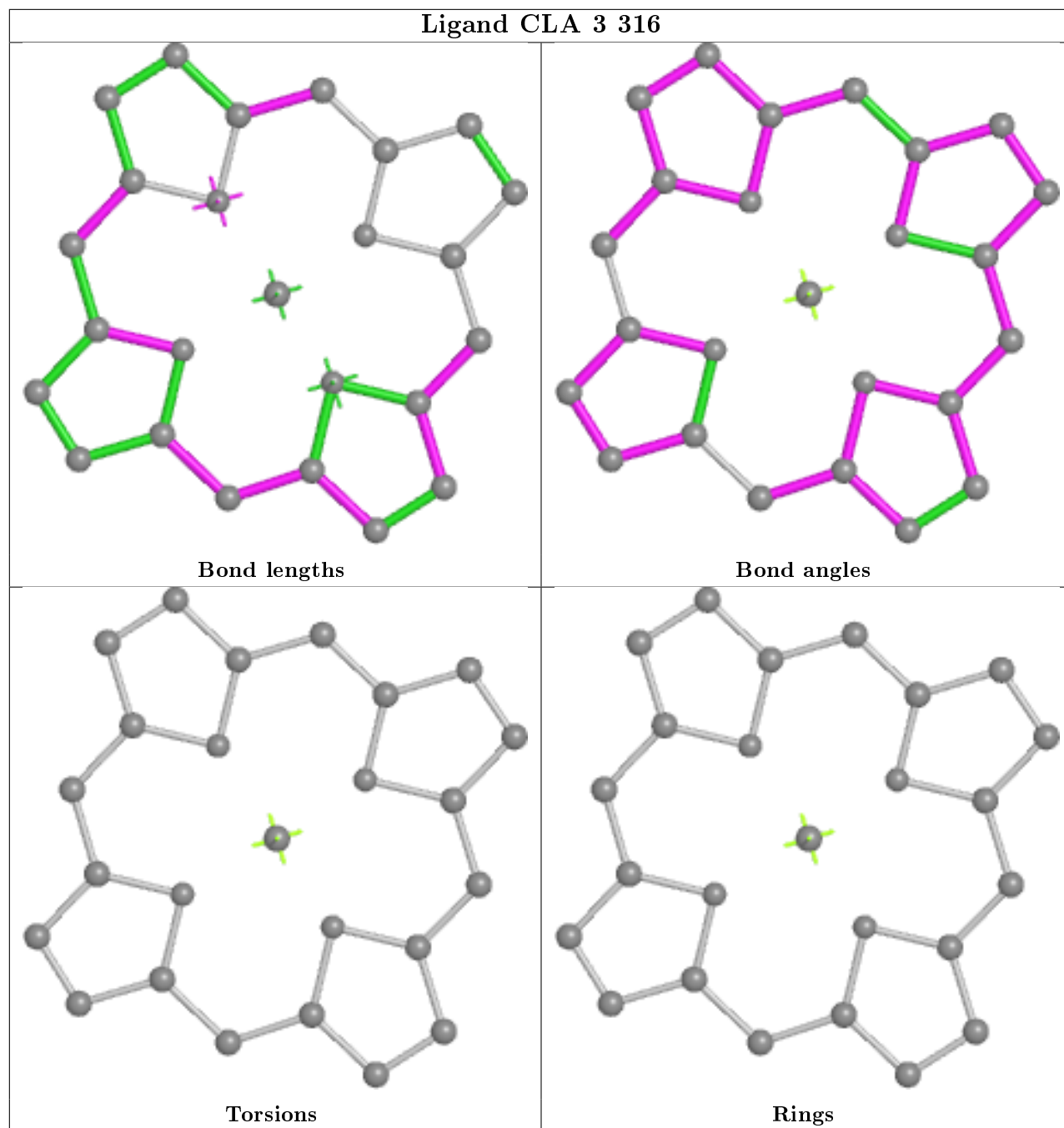


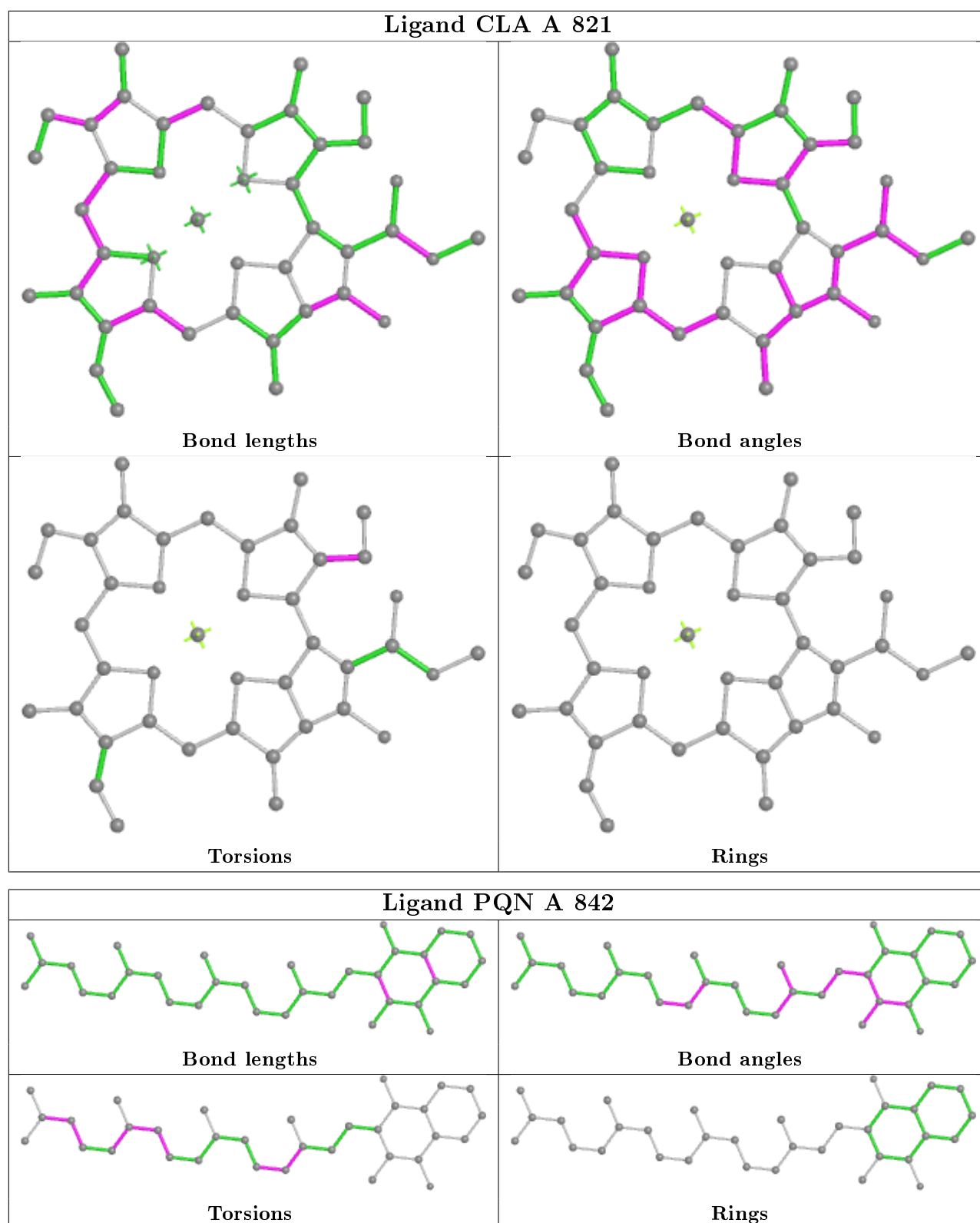


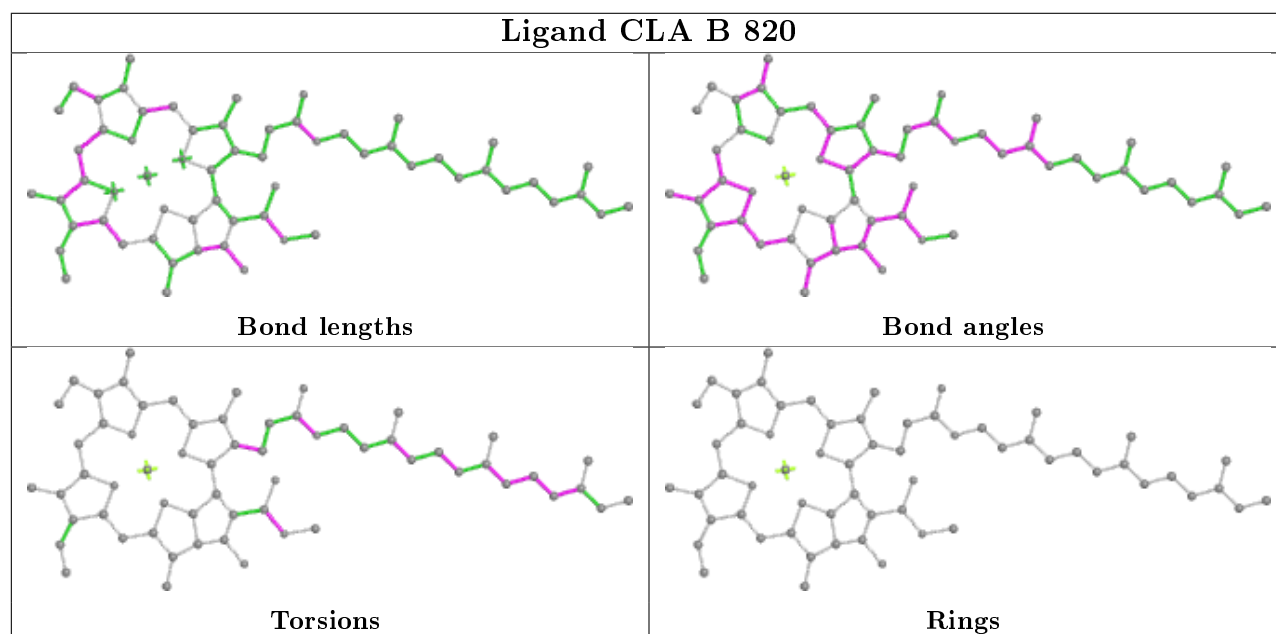
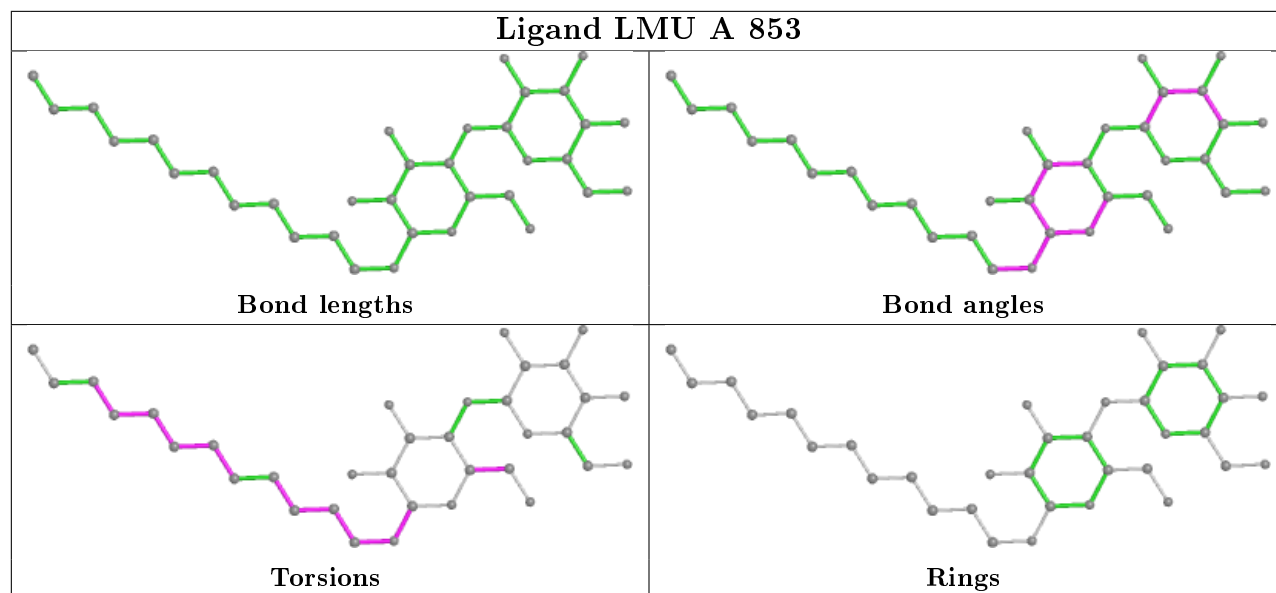


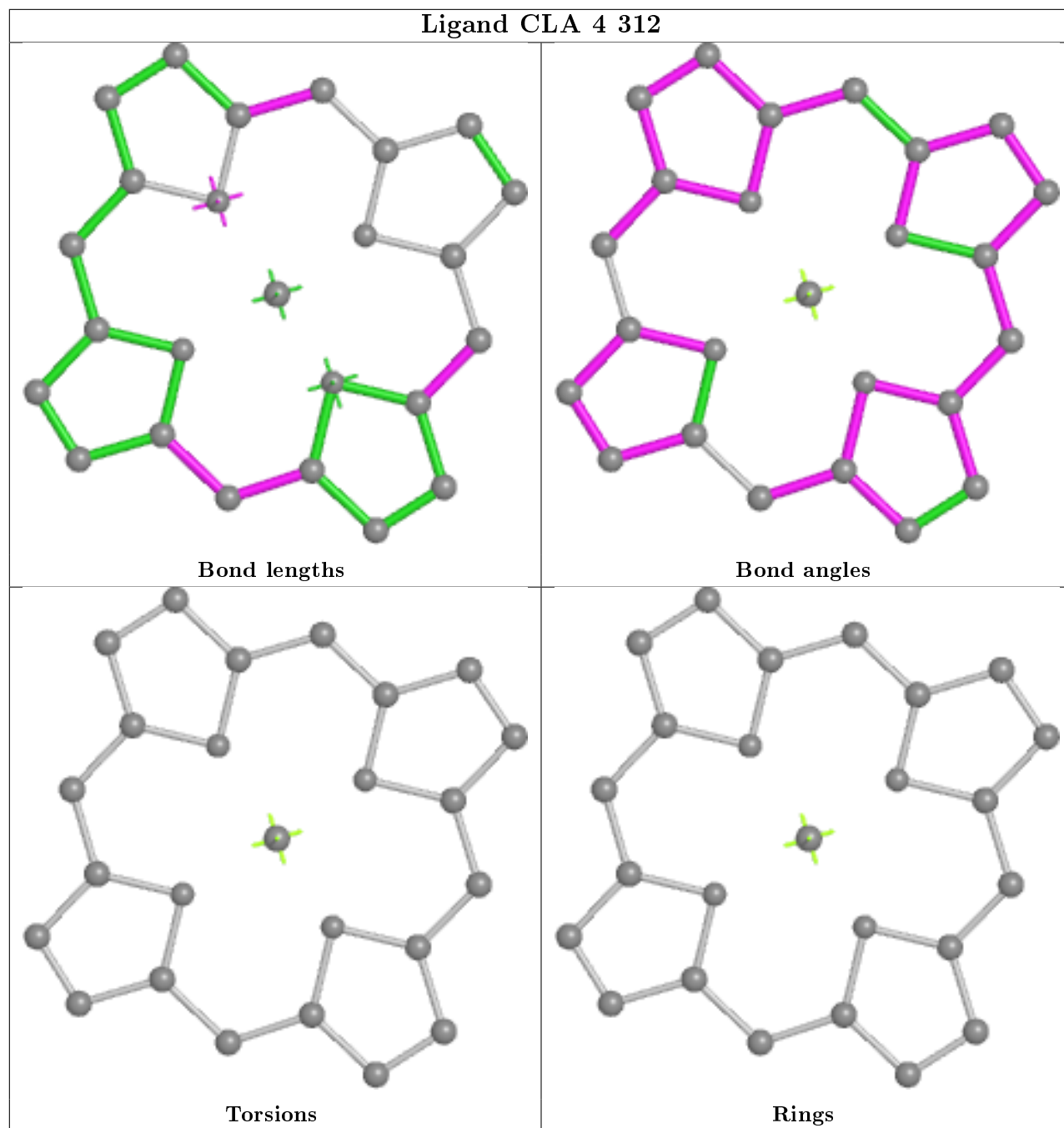


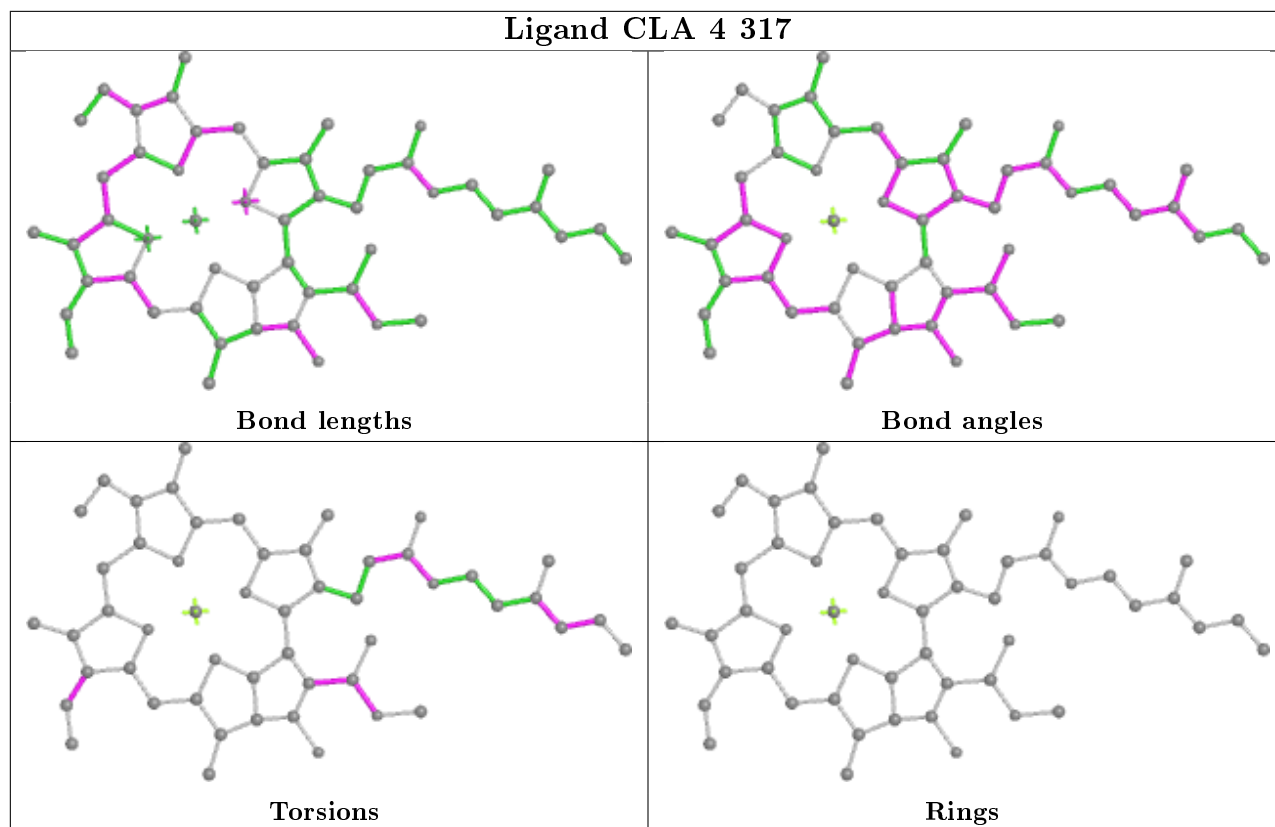


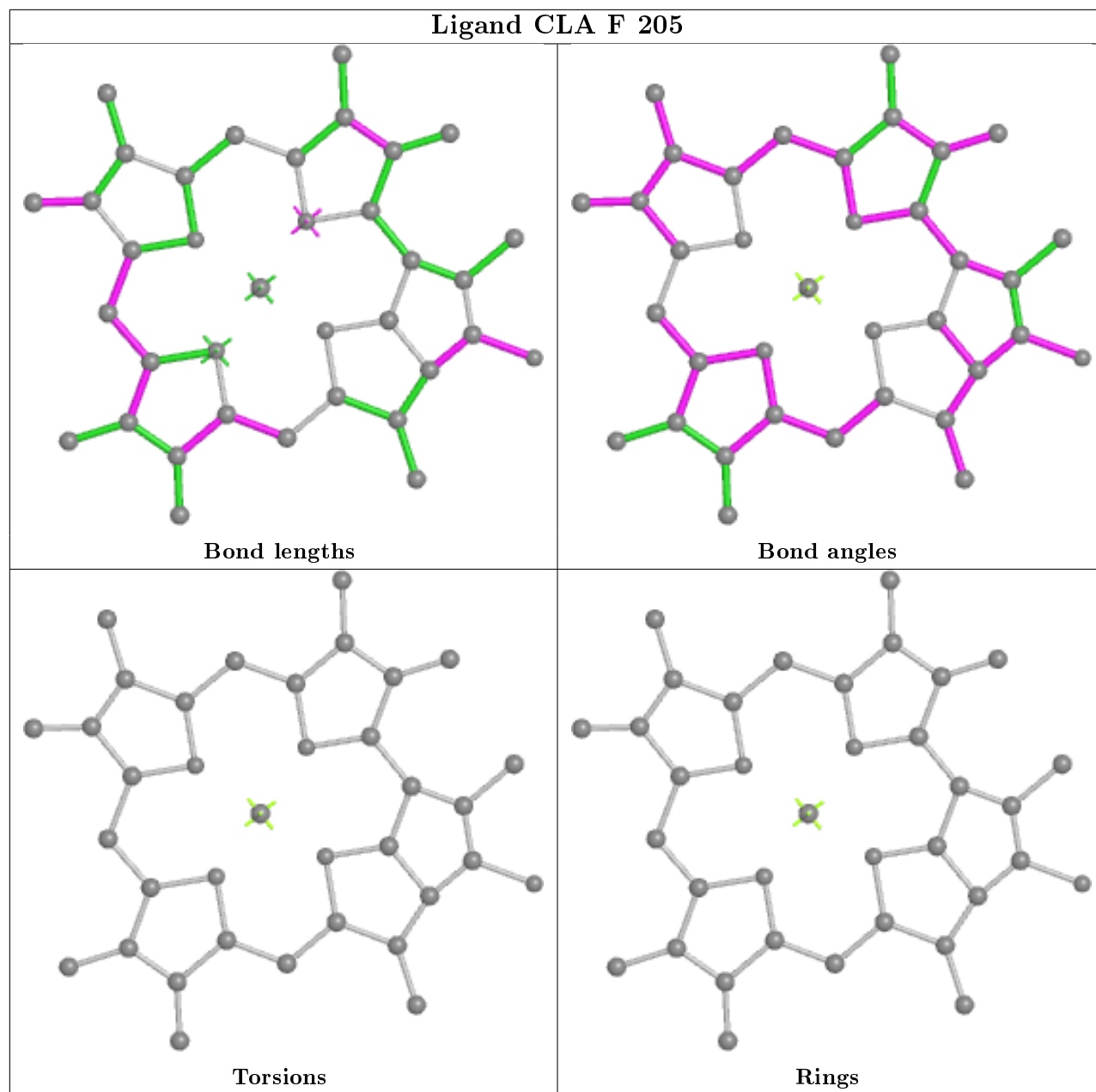


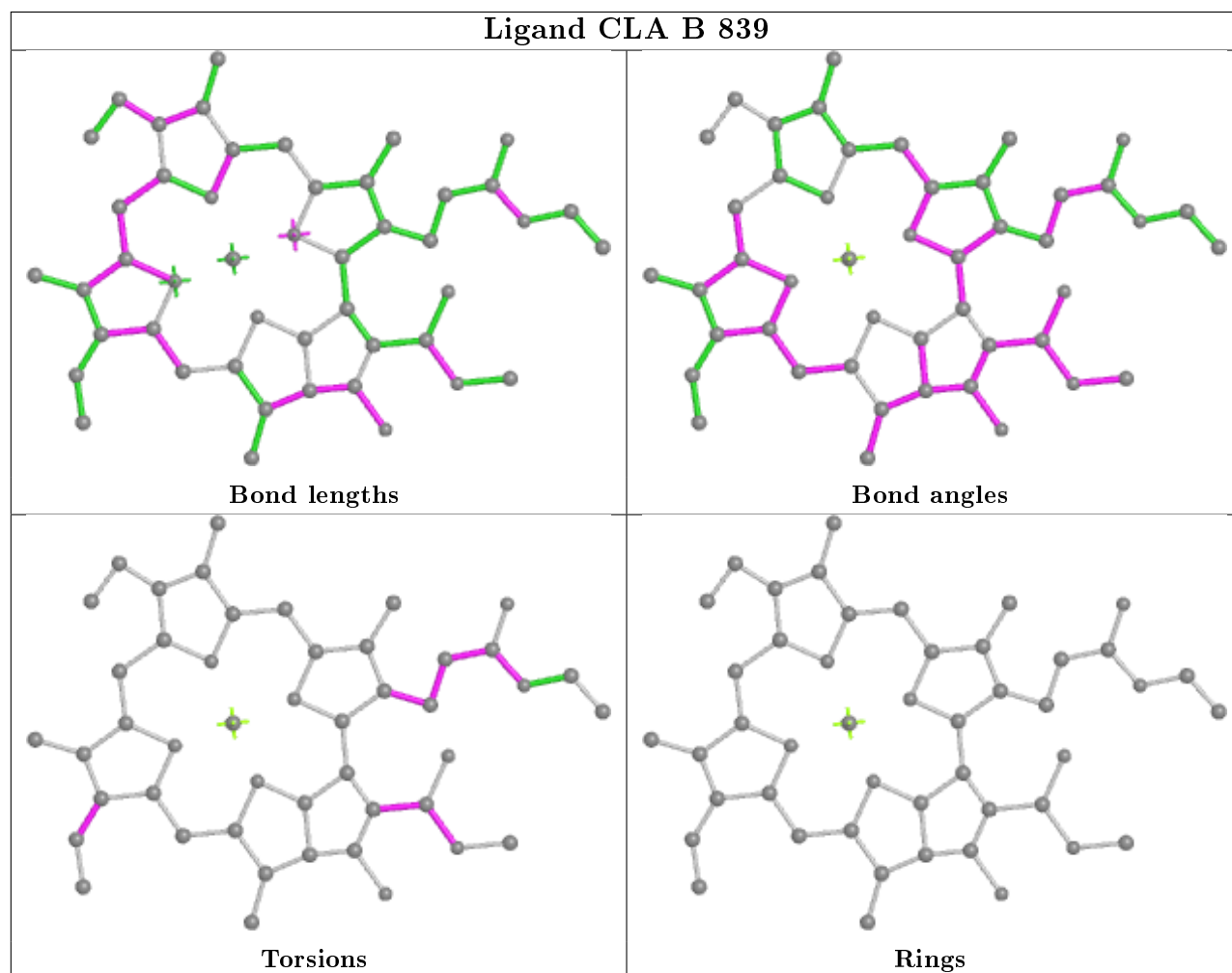
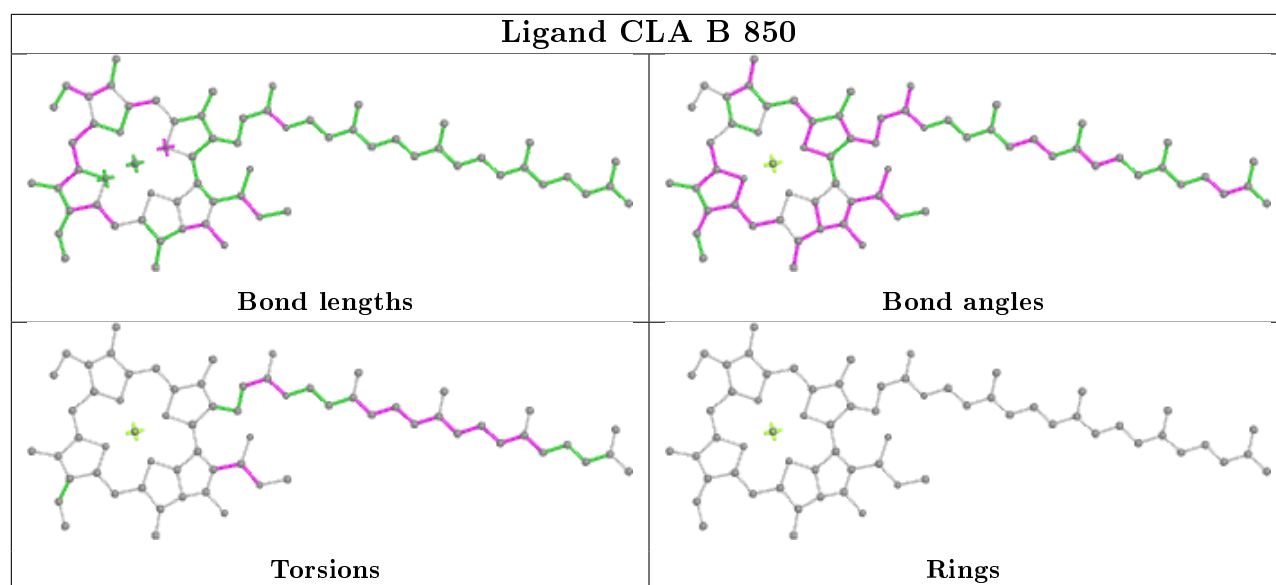


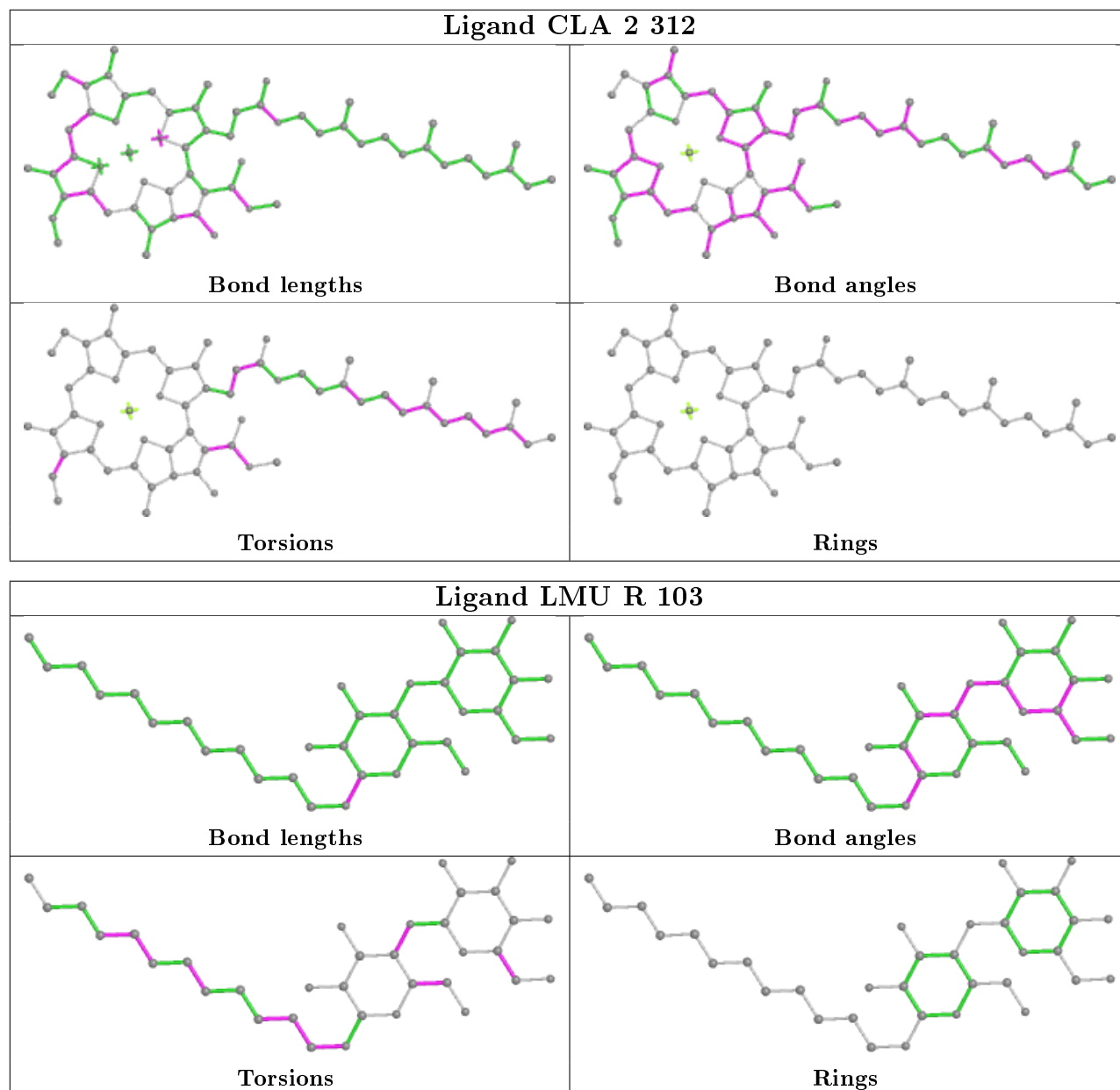


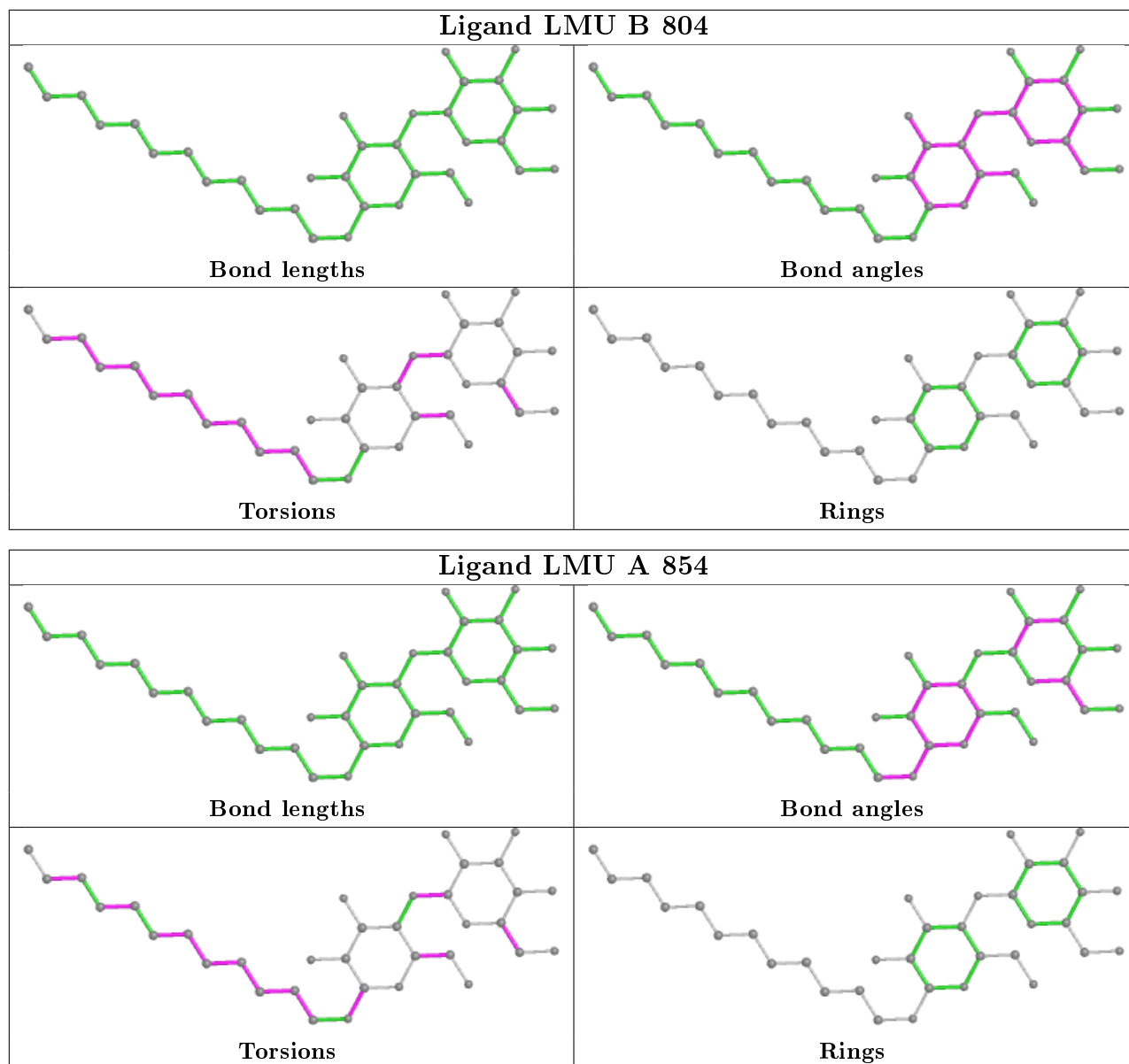


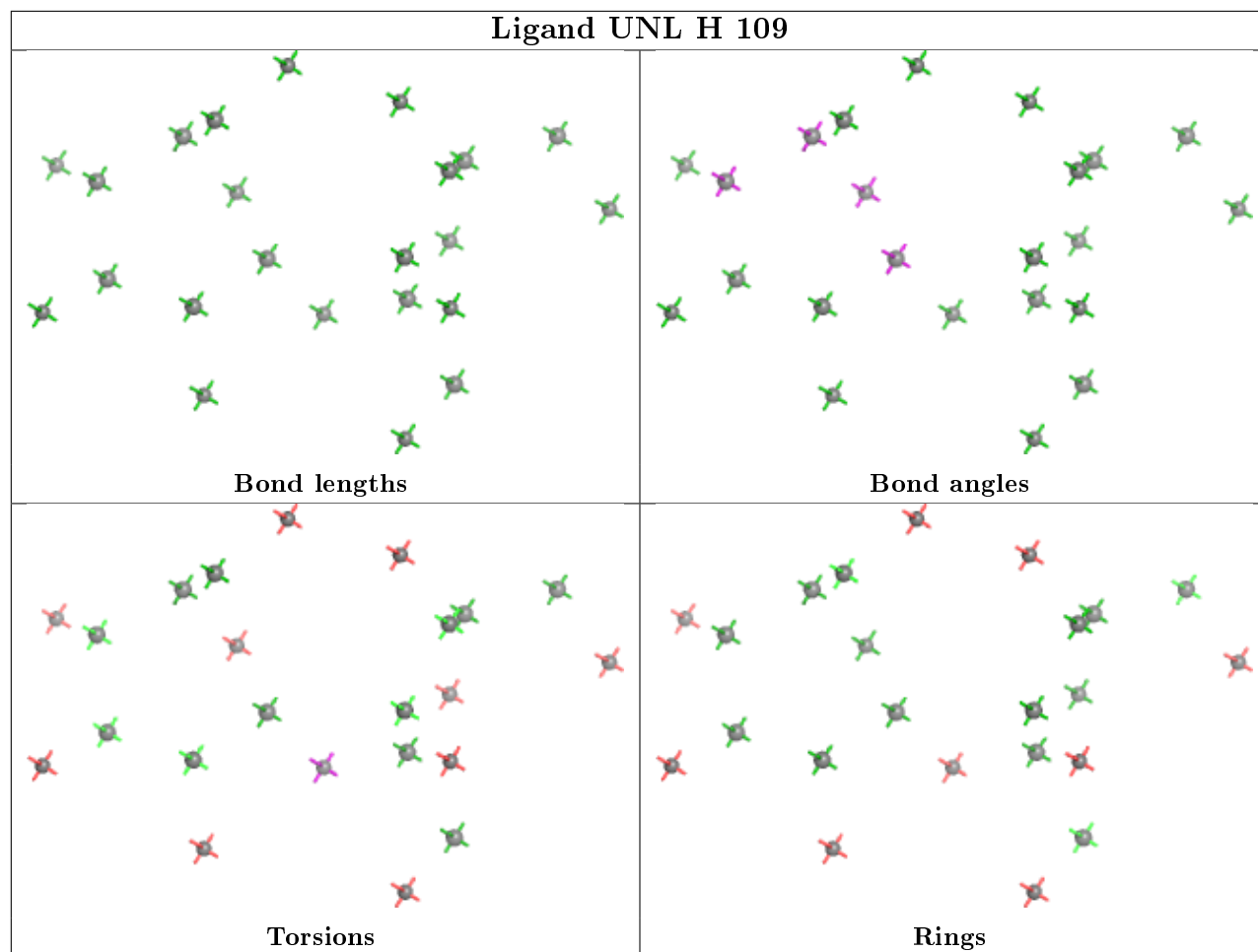












5.7 Other polymers [i](#)

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	165/241 (68%)	1.34	39 (23%) 0 0	21, 24, 25, 25	0
2	2	176/269 (65%)	0.89	34 (19%) 1 1	21, 23, 24, 25	0
3	3	153/276 (55%)	1.12	30 (19%) 1 1	49, 78, 110, 112	0
4	4	166/251 (66%)	0.57	15 (9%) 9 11	21, 23, 24, 25	0
5	A	730/758 (96%)	0.62	56 (7%) 13 15	20, 22, 23, 25	0
6	B	733/734 (99%)	0.67	53 (7%) 15 17	20, 22, 24, 25	0
7	C	81/81 (100%)	0.83	11 (13%) 3 4	21, 22, 23, 23	0
8	D	138/212 (65%)	0.90	25 (18%) 1 2	21, 23, 24, 25	0
9	E	65/143 (45%)	0.71	10 (15%) 2 3	21, 22, 24, 24	0
10	F	154/231 (66%)	0.60	12 (7%) 13 15	21, 22, 23, 24	0
11	G	95/167 (56%)	0.95	12 (12%) 3 5	21, 23, 24, 25	0
12	H	69/144 (47%)	0.83	10 (14%) 2 3	21, 23, 24, 25	0
13	I	30/40 (75%)	0.32	1 (3%) 46 43	21, 22, 23, 23	0
14	J	42/44 (95%)	0.51	3 (7%) 16 17	21, 23, 23, 24	0
15	K	84/131 (64%)	1.48	19 (22%) 0 0	21, 24, 24, 26	0
16	L	162/216 (75%)	0.60	18 (11%) 5 7	20, 23, 24, 25	0
17	N	85/170 (50%)	0.61	7 (8%) 11 13	22, 23, 24, 25	0
18	R	0/53	-	-	-	-
All	All	3128/4161 (75%)	0.76	355 (11%) 5 6	20, 23, 25, 112	0

The worst 5 of 355 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	K	16	THR	10.2
3	3	40	SER	8.6
1	1	92	GLY	7.8

Continued on next page...

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Mol	Chain	Res	Type	RSRZ
1	1	87	ASN	7.4
15	K	64	GLY	7.0

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

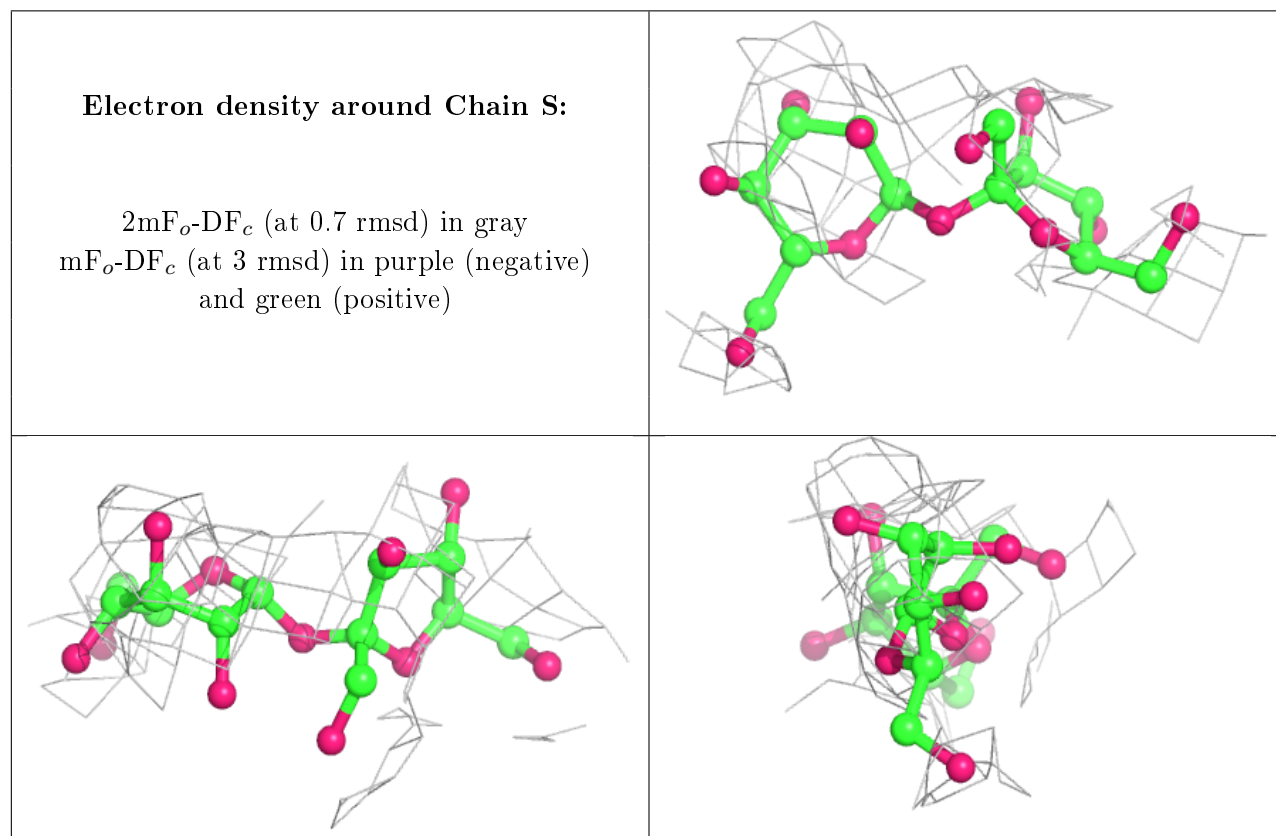
There are no non-standard protein/DNA/RNA residues in this entry.

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.

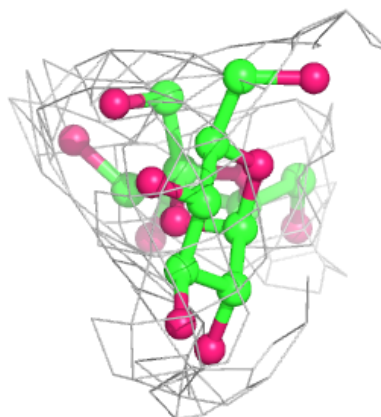
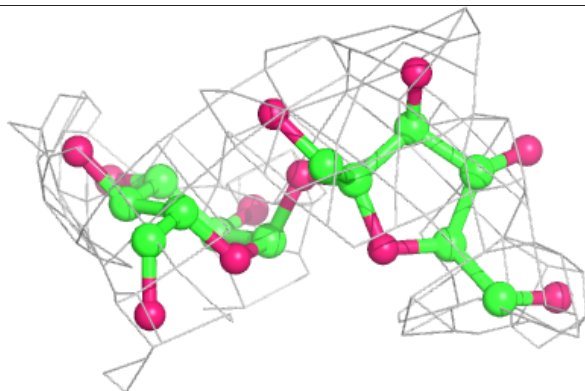
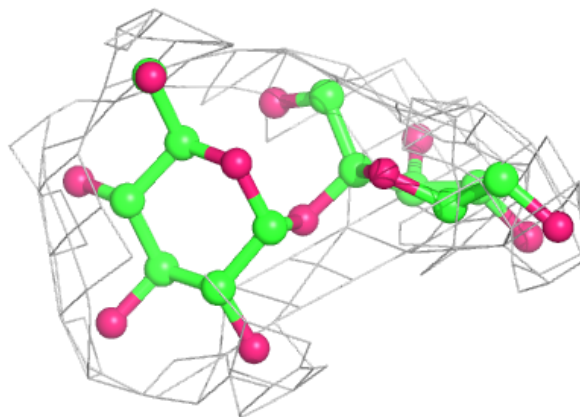
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
19	GLC	X	1	10/12	0.65	0.43	6,52,60,60	0
19	GLC	M	1	11/12	0.66	0.33	2,44,60,60	0
19	FRU	X	2	12/12	0.67	0.49	11,32,60,60	0
19	FRU	U	2	12/12	0.68	0.29	2,34,60,60	0
19	GLC	W	1	11/12	0.69	0.35	9,40,60,60	0
19	FRU	W	2	12/12	0.69	0.33	17,37,60,60	0
19	GLC	S	1	11/12	0.71	0.39	2,19,60,60	0
19	GLC	U	1	11/12	0.74	0.31	2,60,60,60	0
19	GLC	Z	1	11/12	0.74	0.28	4,31,60,60	0
19	GLC	V	1	11/12	0.76	0.22	2,57,60,60	0
19	FRU	Z	2	12/12	0.76	0.25	3,43,60,60	0
19	GLC	a	1	11/12	0.76	0.21	2,23,50,54	0
19	FRU	O	2	12/12	0.76	0.43	2,28,60,60	0
19	GLC	T	1	11/12	0.79	0.22	13,47,60,60	0
19	FRU	S	2	12/12	0.79	0.21	2,32,60,60	0
19	FRU	a	2	12/12	0.80	0.21	6,32,60,60	0
19	GLC	Y	1	11/12	0.81	0.28	2,34,60,60	0
19	FRU	Q	2	12/12	0.82	0.32	2,28,60,60	0
19	FRU	Y	2	12/12	0.83	0.28	2,30,60,60	0
19	GLC	Q	1	11/12	0.83	0.23	2,27,60,60	0
19	FRU	V	2	12/12	0.83	0.25	2,33,60,60	0
19	FRU	M	2	12/12	0.84	0.39	9,35,60,60	0
19	FRU	T	2	12/12	0.85	0.24	6,39,60,60	0
19	FRU	P	2	12/12	0.85	0.20	2,36,60,60	0
19	GLC	O	1	10/12	0.85	0.16	4,38,60,60	0
19	GLC	P	1	11/12	0.85	0.24	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.

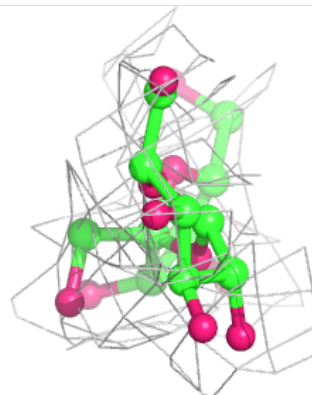
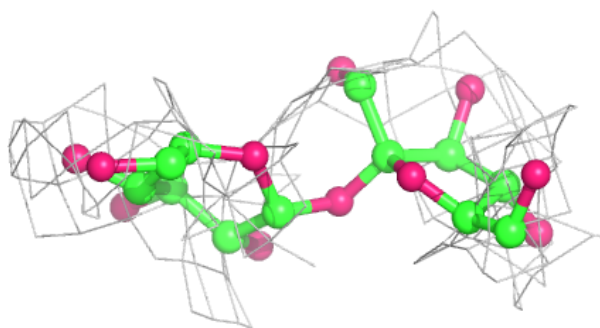
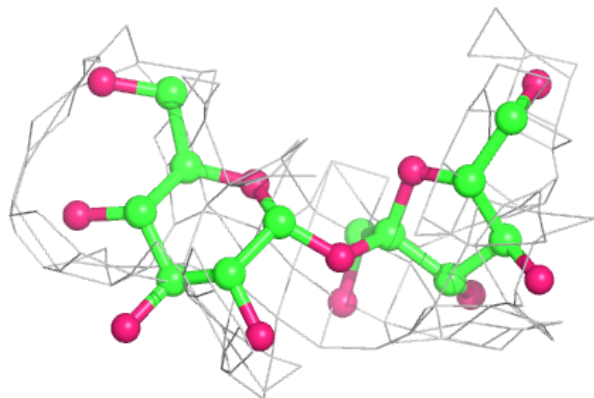


Electron density around Chain T:

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

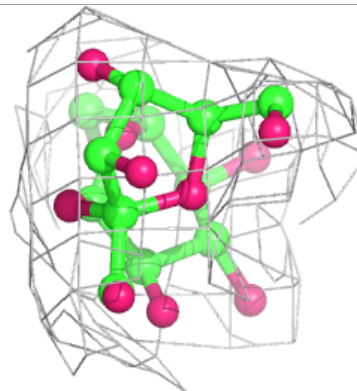
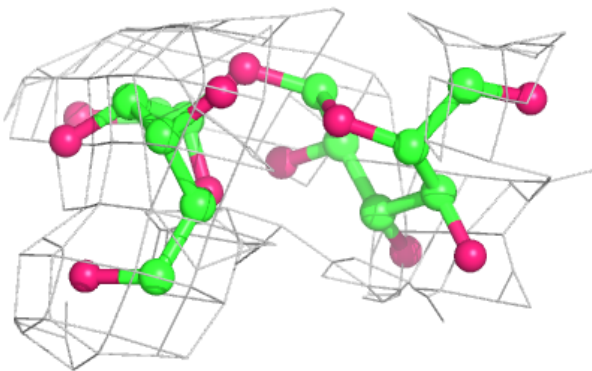
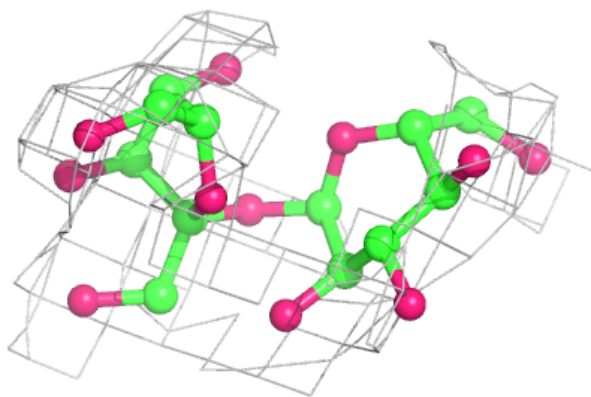
**Electron density around Chain U:**

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



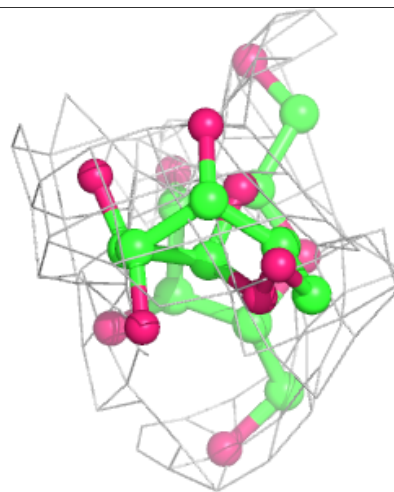
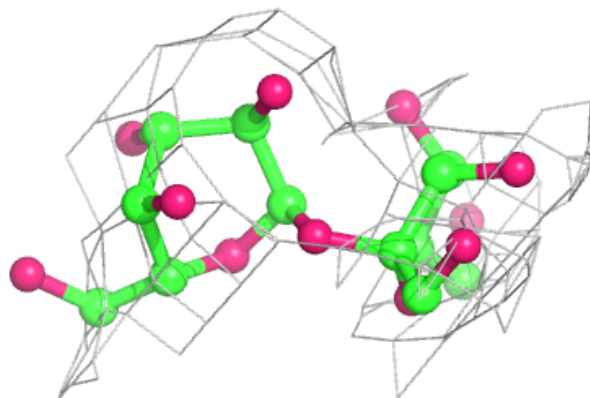
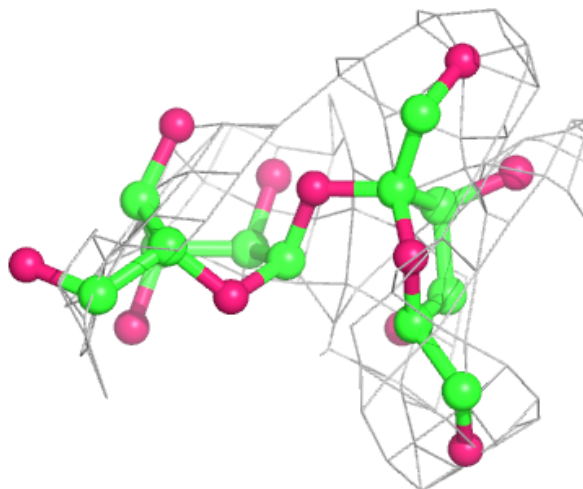
Electron density around Chain V:

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



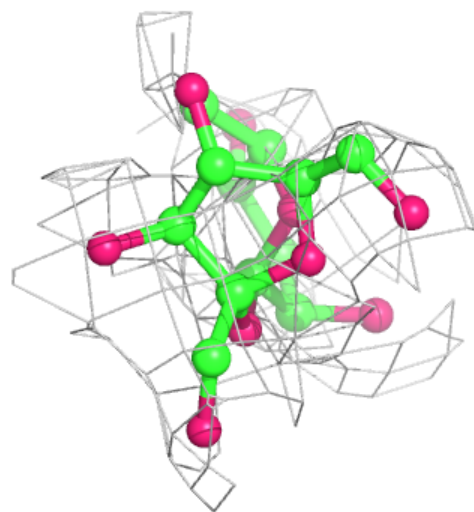
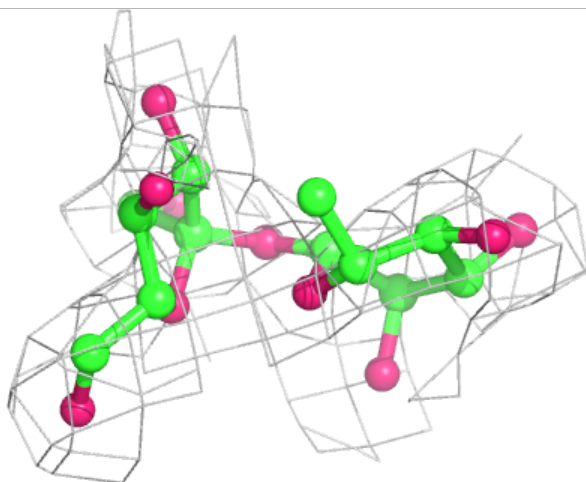
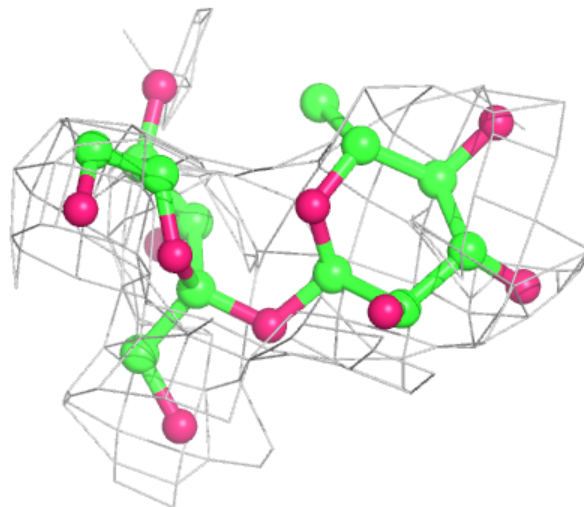
Electron density around Chain W:

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



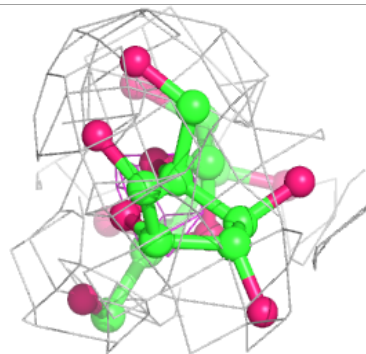
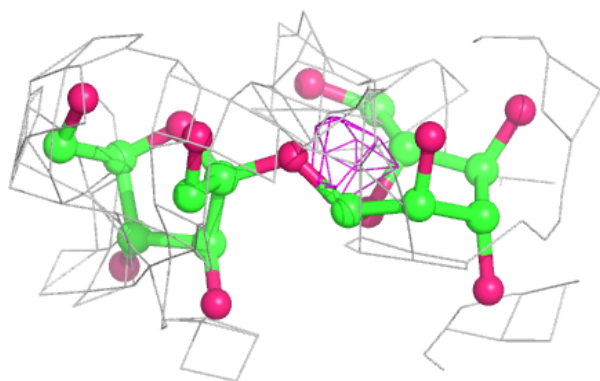
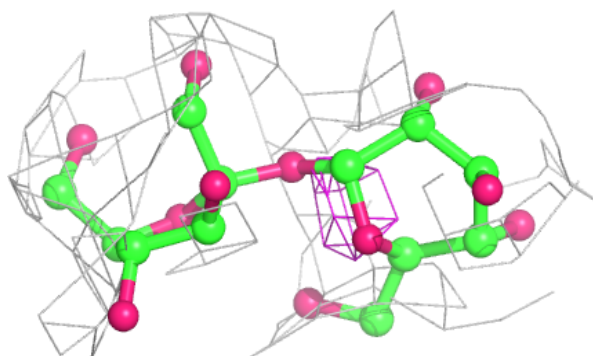
Electron density around Chain X:

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

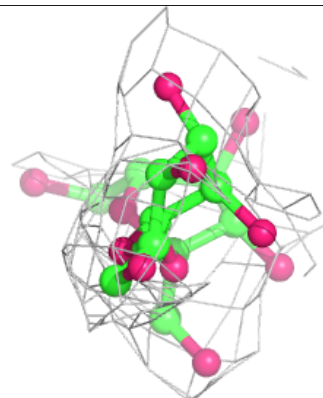
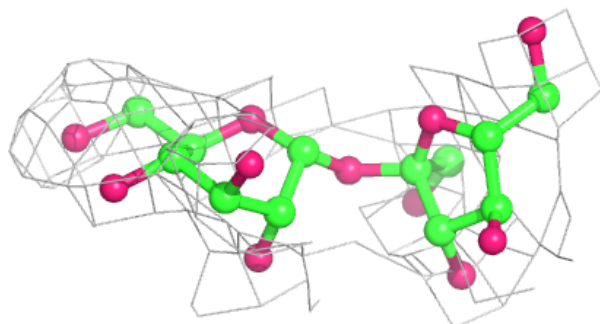
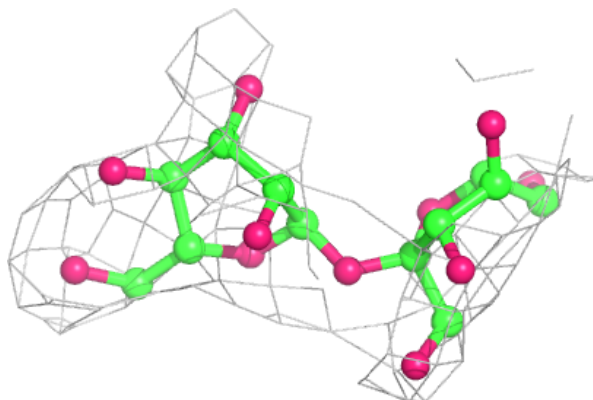


Electron density around Chain Y:

$2mF_o-DF_c$ (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
21	LMU	A	852	35/35	0.54	0.49	2,39,60,60	0
20	CLA	H	102	55/65	0.56	0.39	2,49,60,60	0
21	LMU	A	853	35/35	0.57	0.37	2,45,60,60	0
21	LMU	G	103	35/35	0.58	0.30	2,51,60,60	0
21	LMU	4	320	35/35	0.58	0.27	2,43,60,60	0
21	LMU	B	804	35/35	0.58	0.32	2,34,60,60	0
20	CLA	1	211	51/65	0.59	0.52	2,42,60,60	0
21	LMU	2	321	35/35	0.60	0.39	2,40,60,60	0
22	BCR	2	318	40/40	0.60	0.40	2,32,60,60	0
20	CLA	4	317	52/65	0.61	0.42	2,34,60,60	0
21	LMU	L	205	35/35	0.62	0.22	2,31,60,60	0
20	CLA	3	314	50/65	0.62	0.41	2,56,60,60	0
20	CLA	B	835	45/65	0.62	0.36	12,37,60,60	0
22	BCR	A	843	40/40	0.63	0.45	2,45,60,60	0
21	LMU	H	103	35/35	0.63	0.33	2,15,60,60	0
20	CLA	A	802	25/65	0.63	0.53	2,42,60,60	0
21	LMU	2	322	35/35	0.63	0.33	2,40,60,60	0
20	CLA	1	215	51/65	0.63	0.40	2,51,60,60	0
20	CLA	B	817	46/65	0.64	0.43	2,28,60,60	0
20	CLA	L	204	55/65	0.64	0.45	2,44,60,60	0
20	CLA	4	303	65/65	0.64	0.36	2,32,60,60	0
20	CLA	3	305	25/65	0.64	0.34	17,42,60,60	0
21	LMU	A	848	35/35	0.65	0.29	2,45,60,60	0
20	CLA	K	103	50/65	0.65	0.32	2,60,60,60	0
20	CLA	3	318	36/65	0.66	0.40	2,51,60,60	0
20	CLA	3	311	65/65	0.66	0.41	2,46,60,60	0
20	CLA	A	840	55/65	0.67	0.36	2,44,60,60	0
20	CLA	H	112	55/65	0.67	0.34	2,33,60,60	0
20	CLA	B	836	51/65	0.67	0.37	2,45,60,60	0
20	CLA	H	101	55/65	0.68	0.47	2,47,60,60	0
20	CLA	F	206	41/65	0.68	0.33	2,41,60,60	0
21	LMU	H	106	35/35	0.68	0.29	2,41,60,60	0
21	LMU	R	104	35/35	0.68	0.23	2,36,60,60	0
22	BCR	I	103	40/40	0.68	0.40	2,38,60,60	0
20	CLA	4	308	25/65	0.68	0.30	2,29,60,60	0
20	CLA	3	309	25/65	0.69	0.27	2,47,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	1	201	46/65	0.69	0.25	2,56,60,60	0
21	LMU	K	106	35/35	0.69	0.24	2,38,60,60	0
20	CLA	4	304	55/65	0.69	0.36	4,39,60,60	0
21	LMU	1	217	35/35	0.69	0.23	2,44,60,60	0
21	LMU	E	101	35/35	0.69	0.28	2,30,60,60	0
22	BCR	G	104	40/40	0.69	0.48	2,33,60,60	0
21	LMU	A	846	35/35	0.69	0.25	2,26,60,60	0
21	LMU	2	313	35/35	0.69	0.27	2,21,60,60	0
20	CLA	4	307	25/65	0.69	0.35	2,39,60,60	0
20	CLA	3	310	65/65	0.70	0.33	2,26,60,60	0
20	CLA	3	303	36/65	0.70	0.26	2,53,60,60	0
21	LMU	B	805	35/35	0.70	0.29	2,37,60,60	0
21	LMU	R	105	35/35	0.70	0.27	2,35,60,60	0
20	CLA	G	105	51/65	0.70	0.42	2,44,60,60	0
20	CLA	3	302	25/65	0.70	0.41	15,54,60,60	0
21	LMU	A	854	35/35	0.70	0.27	2,32,60,60	0
20	CLA	R	108	65/65	0.71	0.34	2,35,60,60	0
20	CLA	A	841	25/65	0.71	0.30	2,43,60,60	0
20	CLA	K	101	46/65	0.71	0.25	2,51,60,60	0
20	CLA	2	312	61/65	0.71	0.25	2,34,60,60	0
21	LMU	R	103	35/35	0.71	0.38	2,35,60,60	0
21	LMU	K	107	35/35	0.71	0.26	2,38,60,60	0
20	CLA	3	313	25/65	0.71	0.43	2,30,60,60	0
20	CLA	L	202	55/65	0.72	0.44	2,46,60,60	0
22	BCR	B	845	40/40	0.72	0.38	2,21,60,60	0
20	CLA	R	107	57/65	0.72	0.30	2,38,60,60	0
20	CLA	B	816	60/65	0.72	0.34	2,40,60,60	0
21	LMU	R	101	35/35	0.72	0.32	2,45,60,60	0
22	BCR	L	211	40/40	0.72	0.47	2,18,60,60	0
21	LMU	R	106	35/35	0.72	0.23	2,27,60,60	0
21	LMU	3	319	35/35	0.72	0.31	2,44,60,60	0
20	CLA	2	304	25/65	0.73	0.45	2,27,60,60	0
20	CLA	A	833	45/65	0.73	0.27	2,37,60,60	0
20	CLA	A	801	46/65	0.73	0.35	2,43,60,60	0
20	CLA	2	301	25/65	0.73	0.47	2,48,60,60	0
20	CLA	1	206	61/65	0.73	0.29	2,35,60,60	0
22	BCR	A	844	40/40	0.73	0.39	2,34,60,60	0
21	LMU	G	102	35/35	0.73	0.26	2,33,60,60	0
20	CLA	1	208	25/65	0.73	0.27	2,31,60,60	0
20	CLA	1	205	36/65	0.73	0.29	2,52,60,60	0
20	CLA	1	207	51/65	0.73	0.31	2,36,60,60	0
21	LMU	C	101	35/35	0.74	0.38	2,35,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	2	305	50/65	0.74	0.30	2,48,60,60	0
20	CLA	4	301	55/65	0.74	0.35	2,33,60,60	0
20	CLA	A	820	51/65	0.74	0.30	2,44,60,60	0
20	CLA	K	102	50/65	0.75	0.32	2,28,60,60	0
21	LMU	L	206	35/35	0.75	0.24	2,23,60,60	0
20	CLA	2	311	50/65	0.75	0.31	2,25,60,60	0
21	LMU	L	212	35/35	0.75	0.30	2,22,60,60	0
21	LMU	2	320	35/35	0.75	0.25	2,29,60,60	0
21	LMU	K	105	35/35	0.75	0.26	2,37,60,60	0
20	CLA	3	317	25/65	0.75	0.27	2,42,60,60	0
20	CLA	4	305	50/65	0.75	0.41	2,21,60,60	0
20	CLA	1	203	47/65	0.75	0.27	2,17,60,60	0
20	CLA	3	307	42/65	0.75	0.26	2,53,60,60	0
20	CLA	A	811	65/65	0.75	0.40	2,15,60,60	0
20	CLA	2	307	65/65	0.76	0.25	2,24,60,60	0
20	CLA	3	316	25/65	0.76	0.48	2,47,60,60	0
20	CLA	3	306	25/65	0.76	0.28	2,56,60,60	0
20	CLA	4	318	47/65	0.76	0.28	2,37,60,60	0
20	CLA	2	302	51/65	0.76	0.23	2,33,60,60	0
20	CLA	4	315	46/65	0.76	0.31	2,45,60,60	0
20	CLA	4	314	25/65	0.76	0.30	2,35,60,60	0
20	CLA	1	213	51/65	0.76	0.40	2,39,60,60	0
21	LMU	4	316	35/35	0.76	0.38	2,37,60,60	0
21	LMU	A	847	35/35	0.76	0.26	2,27,60,60	0
20	CLA	2	315	50/65	0.77	0.40	2,33,60,60	0
20	CLA	1	210	36/65	0.77	0.31	2,35,60,60	0
20	CLA	2	310	50/65	0.77	0.32	2,18,60,60	0
25	LMG	B	848	49/55	0.77	0.35	2,20,60,60	0
20	CLA	3	301	36/65	0.77	0.28	2,34,60,60	0
20	CLA	J	101	48/65	0.77	0.28	2,34,60,60	0
21	LMU	H	104	35/35	0.77	0.23	2,16,60,60	0
20	CLA	K	104	56/65	0.77	0.31	2,36,60,60	0
21	LMU	4	321	35/35	0.77	0.27	2,21,55,60	0
21	LMU	R	102	35/35	0.77	0.22	2,38,60,60	0
20	CLA	2	306	25/65	0.78	0.22	2,57,60,60	0
20	CLA	4	309	25/65	0.78	0.39	2,40,60,60	0
20	CLA	A	821	42/65	0.78	0.29	2,46,60,60	0
20	CLA	J	103	61/65	0.78	0.24	2,19,60,60	0
20	CLA	4	302	36/65	0.78	0.35	2,26,60,60	0
22	BCR	J	102	40/40	0.78	0.35	2,31,60,60	0
20	CLA	L	208	50/65	0.78	0.31	2,27,60,60	0
20	CLA	A	823	58/65	0.78	0.36	2,18,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	B	822	46/65	0.78	0.34	2,34,60,60	0
20	CLA	B	815	60/65	0.78	0.35	2,19,60,60	0
20	CLA	3	315	65/65	0.79	0.29	2,33,60,60	0
20	CLA	A	817	52/65	0.79	0.36	2,33,60,60	0
20	CLA	A	810	45/65	0.79	0.33	2,38,60,60	0
21	LMU	F	202	34/35	0.79	0.22	2,23,60,60	0
20	CLA	2	316	25/65	0.79	0.28	2,36,60,60	0
20	CLA	A	814	25/65	0.79	0.29	2,31,60,60	0
20	CLA	3	308	25/65	0.79	0.26	2,37,60,60	0
21	LMU	3	320	35/35	0.79	0.20	2,28,59,60	0
20	CLA	B	813	55/65	0.79	0.29	2,28,60,60	0
21	LMU	4	319	34/35	0.80	0.24	2,22,60,60	0
20	CLA	A	839	59/65	0.80	0.29	2,30,60,60	0
20	CLA	A	805	54/65	0.80	0.29	2,10,60,60	0
20	CLA	4	310	50/65	0.80	0.24	2,20,60,60	0
21	LMU	2	319	35/35	0.80	0.20	2,25,60,60	0
20	CLA	A	834	46/65	0.80	0.39	2,20,60,60	0
26	UNL	H	109	23/-	0.80	0.22	2,31,60,60	0
20	CLA	1	212	25/65	0.80	0.26	2,42,60,60	0
20	CLA	1	204	46/65	0.80	0.28	2,35,60,60	0
21	LMU	D	201	35/35	0.81	0.22	2,12,50,57	0
20	CLA	L	201	60/65	0.81	0.29	2,18,60,60	0
20	CLA	2	309	25/65	0.81	0.42	2,34,60,60	0
21	LMU	B	849	25/35	0.81	0.21	2,36,60,60	0
20	CLA	A	819	58/65	0.81	0.35	2,20,60,60	0
20	CLA	1	214	25/65	0.81	0.29	5,42,60,60	0
21	LMU	1	218	35/35	0.81	0.20	2,46,60,60	0
20	CLA	B	842	36/65	0.81	0.30	2,52,60,60	0
20	CLA	A	825	65/65	0.81	0.32	2,16,60,60	0
20	CLA	H	111	58/65	0.82	0.32	2,15,60,60	0
21	LMU	R	109	35/35	0.82	0.24	2,21,60,60	0
22	BCR	B	846	40/40	0.82	0.33	2,11,60,60	0
20	CLA	A	815	50/65	0.82	0.27	2,21,60,60	0
20	CLA	B	812	54/65	0.82	0.25	2,17,60,60	0
21	LMU	A	855	35/35	0.82	0.22	2,29,60,60	0
20	CLA	A	824	59/65	0.82	0.29	2,25,60,60	0
20	CLA	A	807	46/65	0.82	0.29	2,20,60,60	0
20	CLA	L	210	50/65	0.82	0.26	2,18,60,60	0
20	CLA	B	820	61/65	0.82	0.30	2,16,60,60	0
20	CLA	B	827	65/65	0.82	0.32	2,15,60,60	0
20	CLA	3	304	25/65	0.82	0.19	2,28,60,60	0
22	BCR	A	845	40/40	0.82	0.34	2,5,44,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	A	812	54/65	0.82	0.25	2,28,60,60	0
22	BCR	B	847	40/40	0.82	0.33	2,10,60,60	0
21	LMU	1	216	35/35	0.83	0.25	2,11,50,60	0
21	LMU	G	101	35/35	0.83	0.25	2,34,60,60	0
20	CLA	B	806	65/65	0.83	0.28	2,11,60,60	0
20	CLA	4	306	52/65	0.83	0.25	2,26,60,60	0
20	CLA	L	203	65/65	0.83	0.31	2,22,60,60	0
20	CLA	A	829	50/65	0.83	0.30	2,32,60,60	0
22	BCR	I	101	39/40	0.83	0.31	2,8,60,60	0
20	CLA	2	317	65/65	0.83	0.26	2,15,60,60	0
20	CLA	B	837	60/65	0.83	0.32	2,2,60,60	0
20	CLA	2	303	58/65	0.83	0.23	2,22,60,60	0
20	CLA	B	834	45/65	0.83	0.28	2,16,60,60	0
20	CLA	A	804	55/65	0.83	0.32	2,11,60,60	0
20	CLA	A	816	54/65	0.83	0.28	2,31,60,60	0
20	CLA	4	311	25/65	0.84	0.26	2,15,60,60	0
20	CLA	B	823	55/65	0.84	0.28	2,30,60,60	0
20	CLA	A	813	50/65	0.84	0.27	2,29,60,60	0
20	CLA	A	835	65/65	0.84	0.29	2,6,60,60	0
20	CLA	F	207	53/65	0.84	0.28	2,22,60,60	0
23	PQN	A	842	33/33	0.84	0.32	2,4,59,60	0
22	BCR	B	844	40/40	0.84	0.30	2,5,60,60	0
20	CLA	B	821	50/65	0.84	0.30	2,37,60,60	0
20	CLA	B	807	45/65	0.84	0.27	2,14,56,60	0
20	CLA	A	806	56/65	0.84	0.30	2,2,54,60	0
20	CLA	A	832	50/65	0.84	0.26	2,18,56,60	0
20	CLA	L	209	47/65	0.84	0.26	2,13,45,60	0
20	CLA	1	209	25/65	0.84	0.31	11,37,60,60	0
20	CLA	I	102	60/65	0.84	0.29	2,18,60,60	0
20	CLA	A	818	60/65	0.84	0.33	2,11,52,60	0
20	CLA	B	832	59/65	0.85	0.28	2,6,60,60	0
21	LMU	H	105	35/35	0.85	0.20	2,31,60,60	0
20	CLA	B	803	65/65	0.85	0.31	2,14,56,60	0
20	CLA	B	840	65/65	0.85	0.30	2,11,60,60	0
20	CLA	A	838	65/65	0.85	0.31	2,8,60,60	0
20	CLA	B	826	58/65	0.85	0.31	2,13,60,60	0
20	CLA	B	825	54/65	0.85	0.31	2,15,60,60	0
20	CLA	B	818	53/65	0.85	0.28	2,14,60,60	0
20	CLA	A	828	65/65	0.85	0.29	2,12,60,60	0
20	CLA	B	824	65/65	0.85	0.26	2,17,60,60	0
20	CLA	B	833	50/65	0.85	0.29	2,11,53,60	0
20	CLA	4	313	36/65	0.86	0.24	2,21,60,60	0

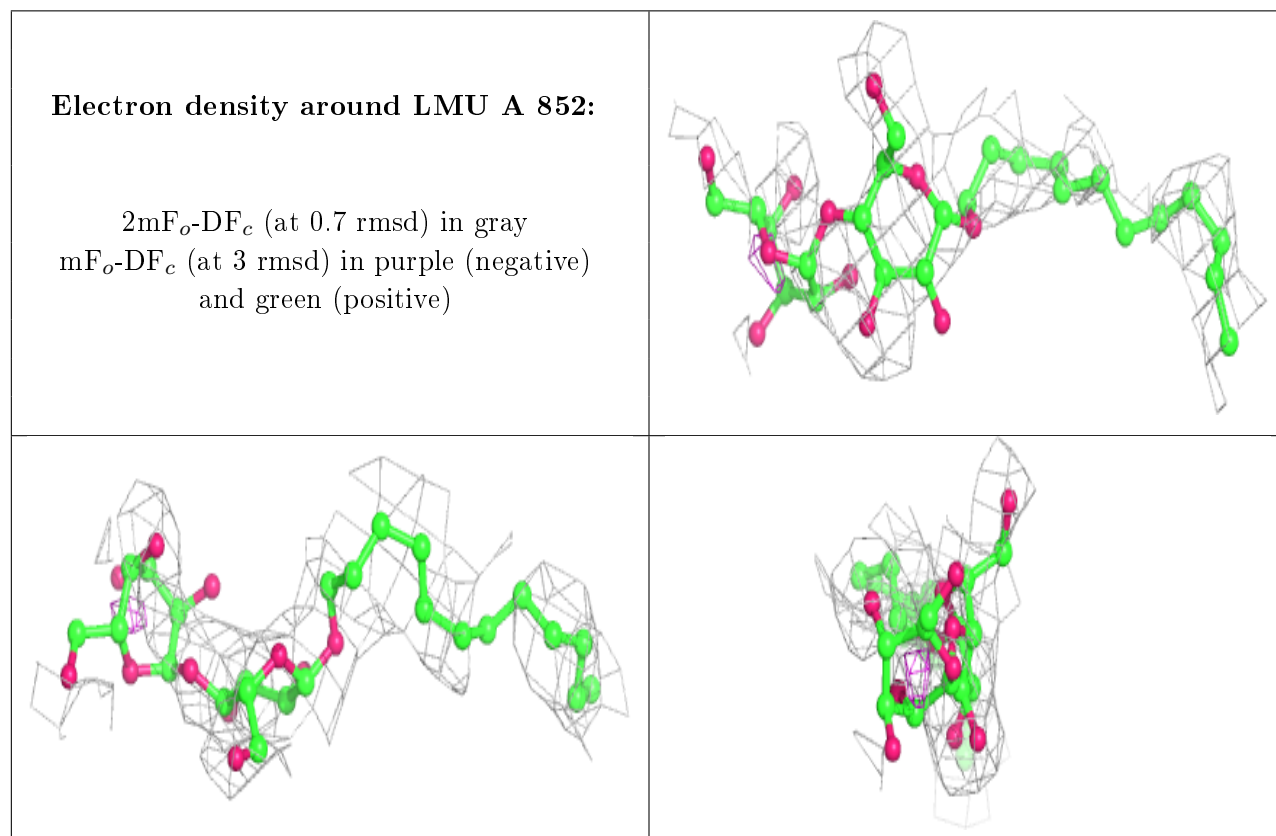
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
20	CLA	A	851	65/65	0.86	0.28	2,2,60,60	0
20	CLA	A	803	46/65	0.86	0.30	2,14,49,60	0
20	CLA	A	827	55/65	0.86	0.30	2,12,60,60	0
20	CLA	A	837	51/65	0.86	0.28	2,12,60,60	0
23	PQN	B	843	33/33	0.86	0.28	2,2,46,51	0
20	CLA	B	811	25/65	0.86	0.28	2,2,60,60	0
20	CLA	B	841	65/65	0.86	0.32	2,2,55,60	0
20	CLA	1	202	41/65	0.86	0.22	2,41,60,60	0
20	CLA	F	201	50/65	0.86	0.23	2,7,51,60	0
20	CLA	B	829	65/65	0.87	0.26	2,11,46,60	0
20	CLA	2	308	25/65	0.87	0.19	2,12,60,60	0
22	BCR	F	203	40/40	0.88	0.28	2,2,60,60	0
20	CLA	4	312	25/65	0.88	0.19	2,2,26,32	0
20	CLA	A	830	65/65	0.88	0.25	2,9,59,60	0
20	CLA	F	205	36/65	0.88	0.24	2,17,60,60	0
20	CLA	B	850	65/65	0.88	0.28	2,2,55,60	0
20	CLA	B	838	65/65	0.88	0.24	2,7,60,60	0
20	CLA	A	850	65/65	0.88	0.27	2,4,48,60	0
20	CLA	A	826	65/65	0.88	0.29	2,2,50,60	0
20	CLA	A	831	65/65	0.88	0.25	2,14,60,60	0
20	CLA	B	810	60/65	0.89	0.27	2,2,60,60	0
20	CLA	B	831	50/65	0.89	0.26	2,12,60,60	0
20	CLA	B	839	47/65	0.89	0.25	2,5,55,60	0
22	BCR	F	204	40/40	0.89	0.22	2,6,60,60	0
20	CLA	A	822	50/65	0.89	0.23	2,7,60,60	0
20	CLA	A	836	47/65	0.89	0.23	2,8,50,60	0
20	CLA	B	808	61/65	0.89	0.27	2,9,48,60	0
20	CLA	A	849	65/65	0.90	0.27	2,2,48,60	0
20	CLA	B	809	65/65	0.90	0.26	2,2,53,60	0
20	CLA	B	819	41/65	0.90	0.27	2,5,40,60	0
20	CLA	B	830	65/65	0.90	0.24	2,6,53,60	0
20	CLA	B	814	65/65	0.90	0.26	2,13,60,60	0
20	CLA	B	828	65/65	0.90	0.26	2,10,56,60	0
22	BCR	B	801	40/40	0.91	0.23	2,4,50,60	0
20	CLA	A	808	60/65	0.91	0.29	2,10,60,60	0
20	CLA	A	809	52/65	0.91	0.24	2,10,60,60	0
20	CLA	B	802	54/65	0.92	0.27	2,6,45,60	0
24	SF4	C	103	8/8	0.96	0.08	12,19,20,24	0
24	SF4	C	102	8/8	0.97	0.08	18,22,26,32	0
24	SF4	A	856	8/8	0.98	0.05	23,24,24,25	0

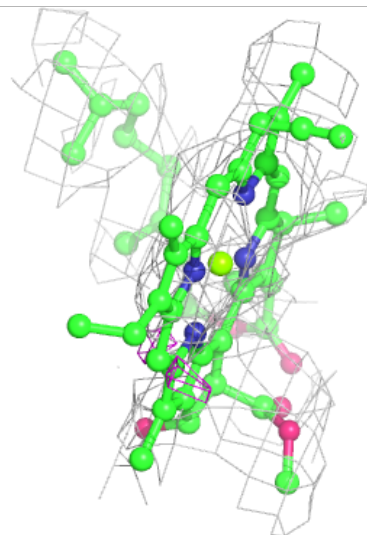
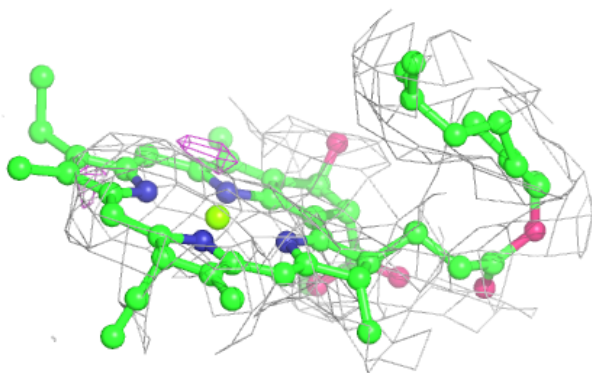
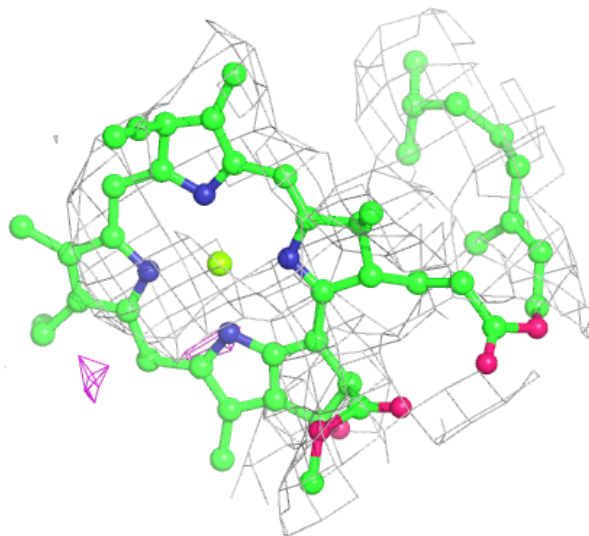
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



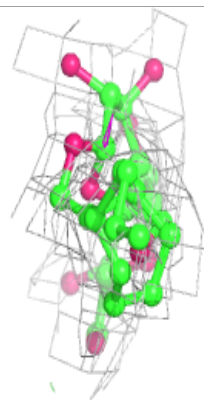
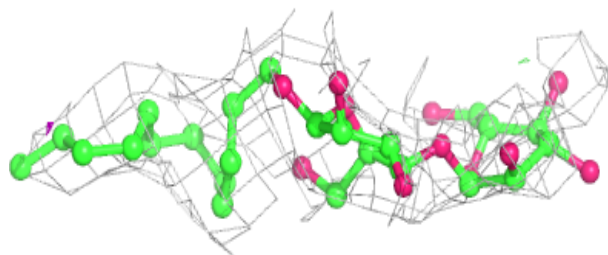
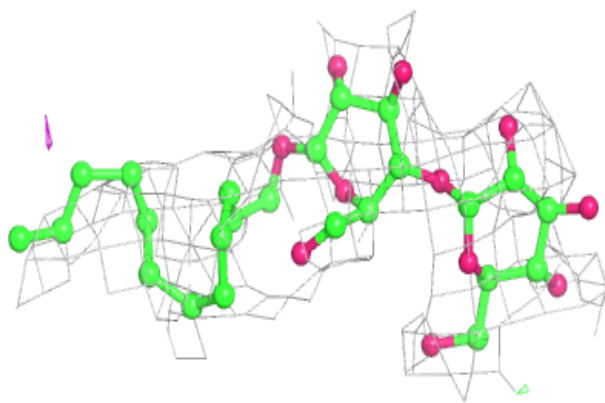
Electron density around CLA H 102:

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

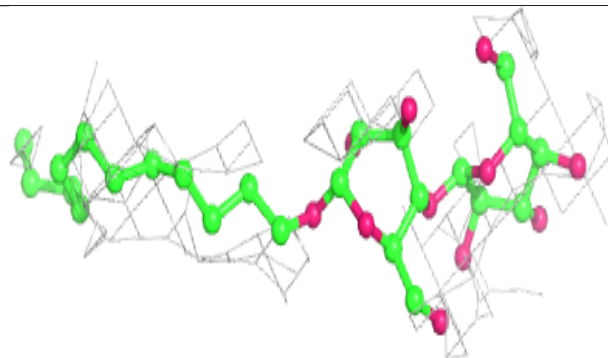
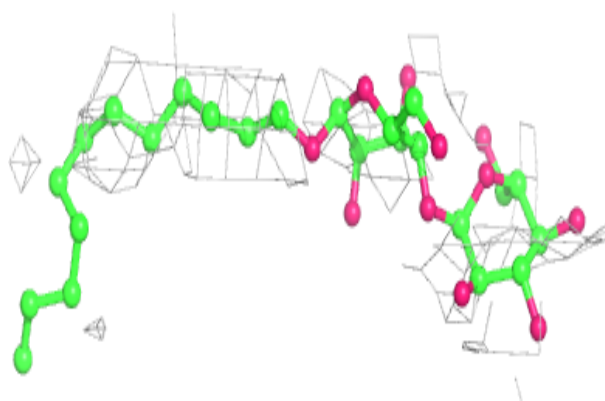


Electron density around LMU A 853:

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

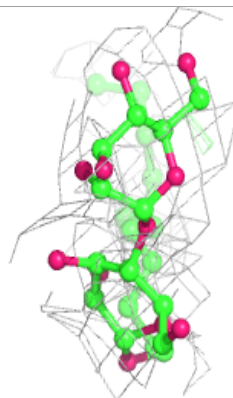
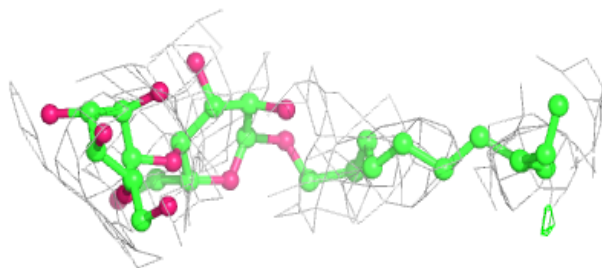
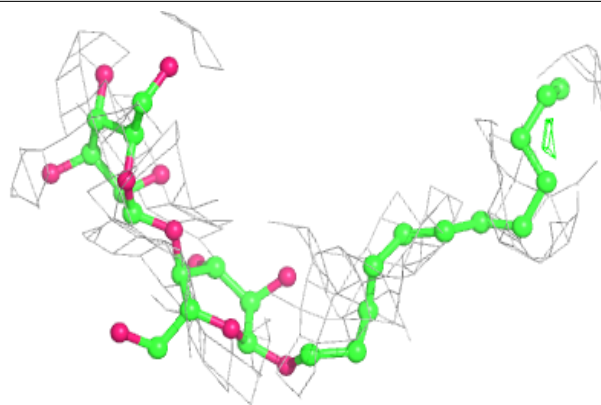
**Electron density around LMU G 103:**

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

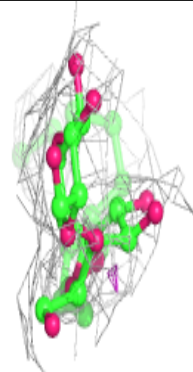
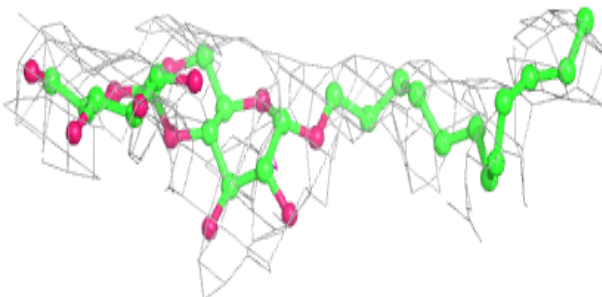
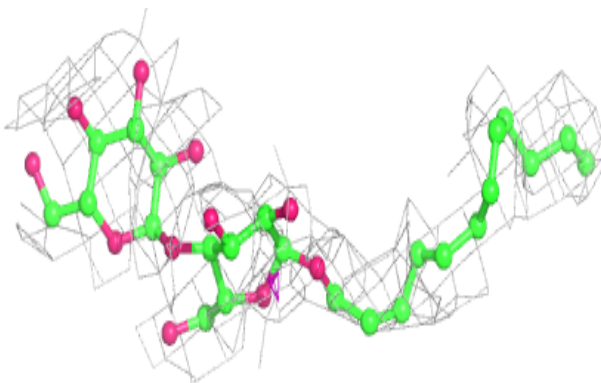


Electron density around LMU 4 320:

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

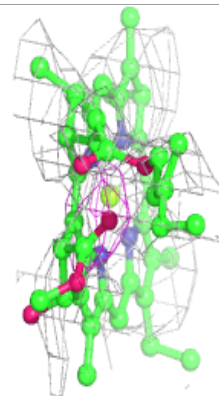
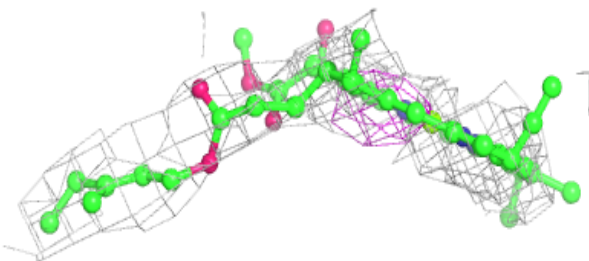
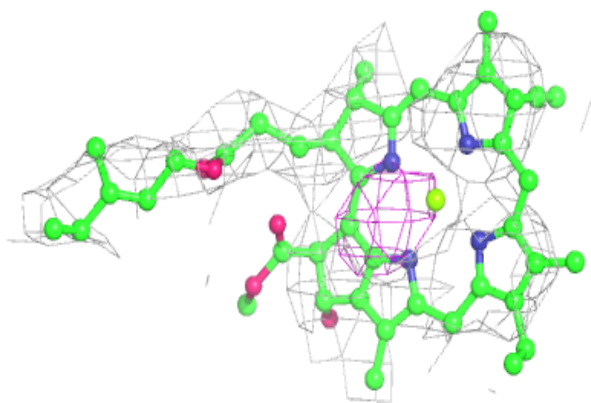
**Electron density around LMU B 804:**

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

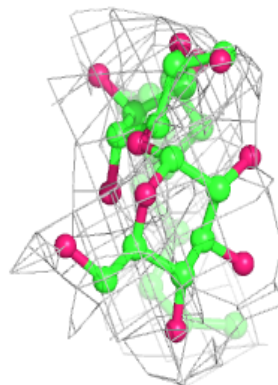
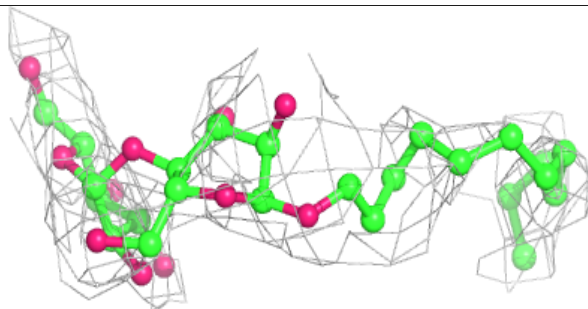
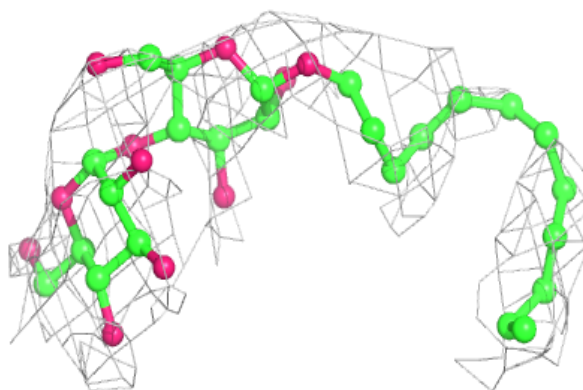


Electron density around CLA 1 211:

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

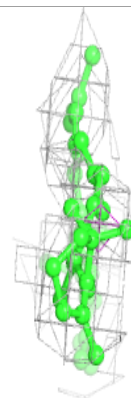
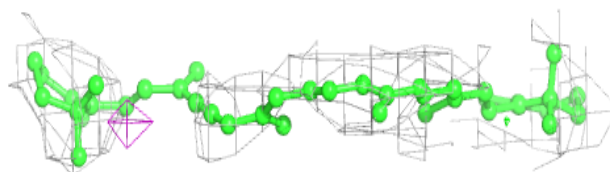
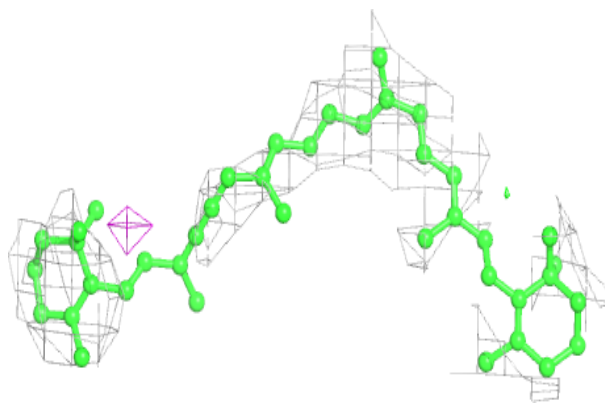
**Electron density around LMU 2 321:**

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



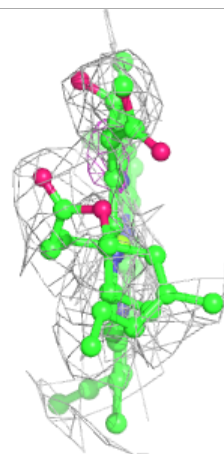
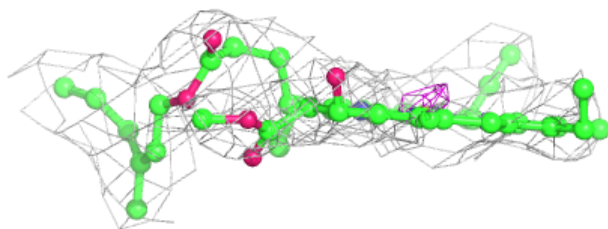
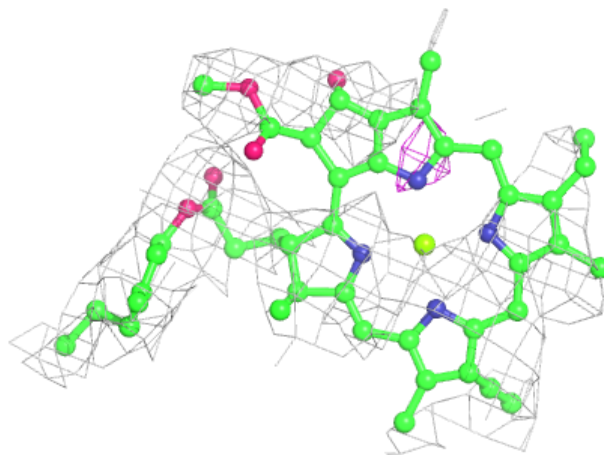
Electron density around BCR 2 318:

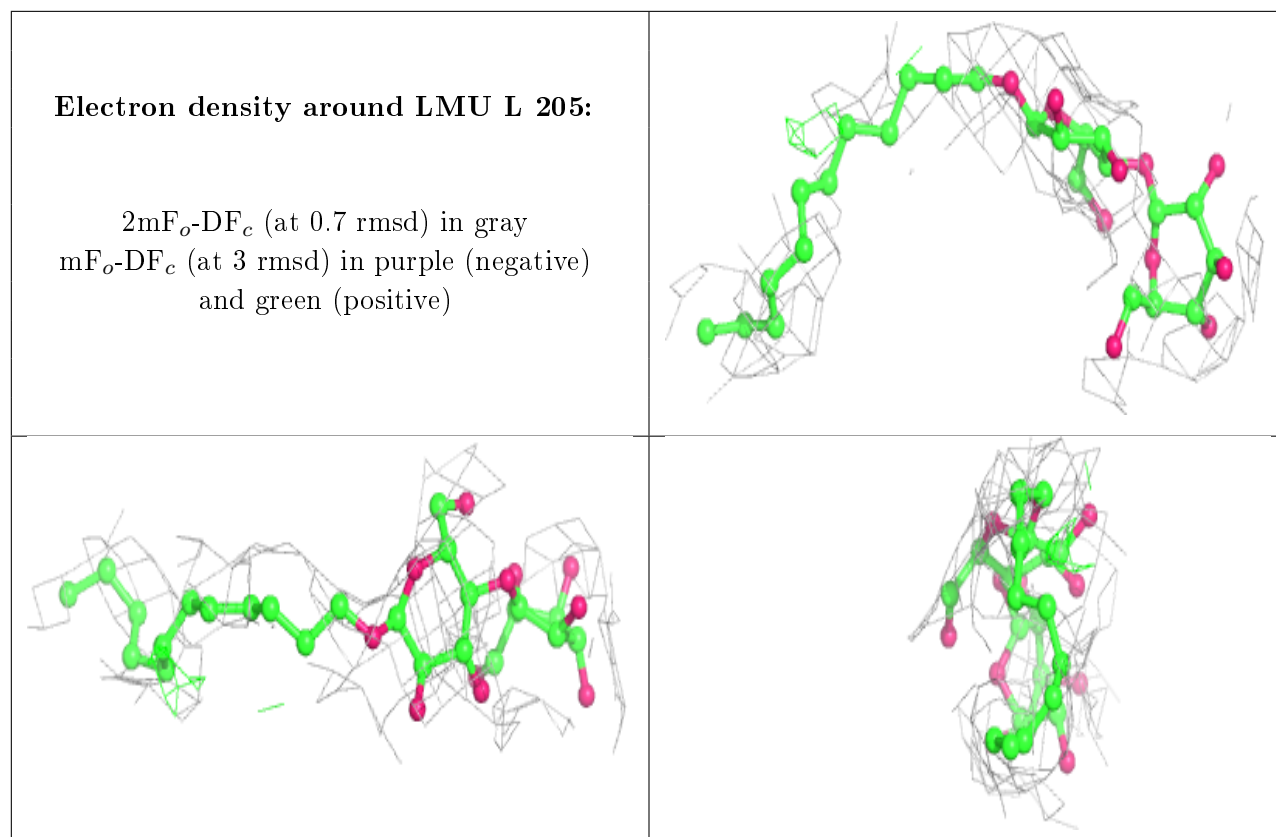
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 4 317:

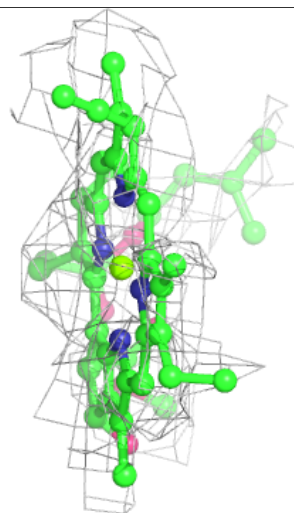
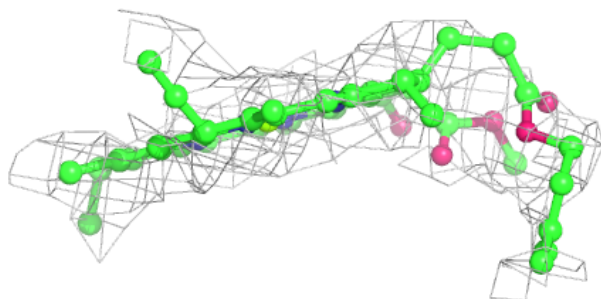
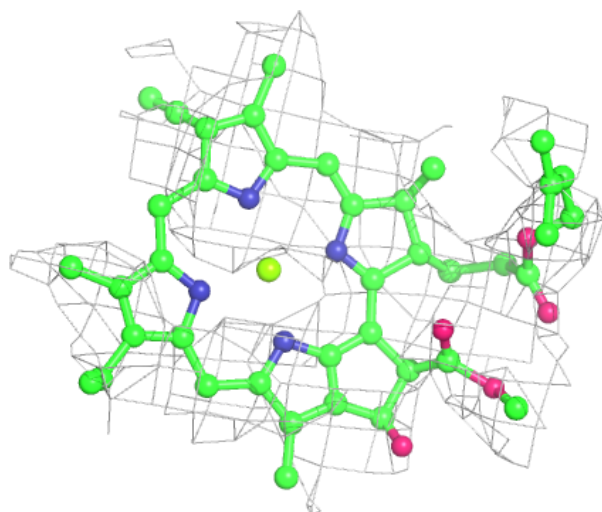
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





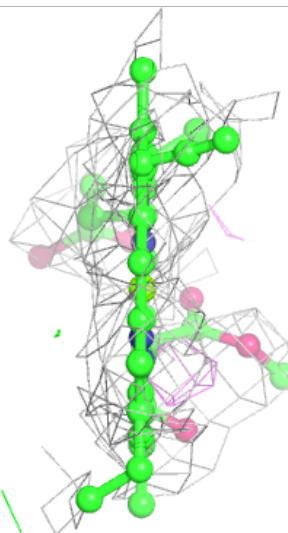
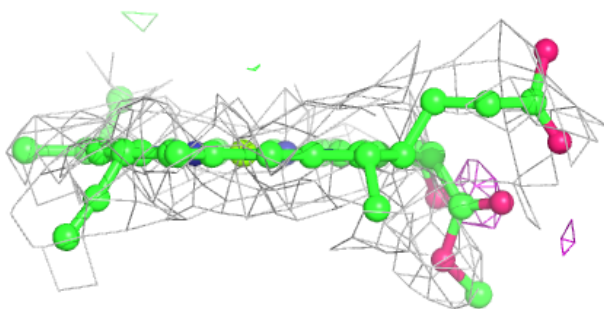
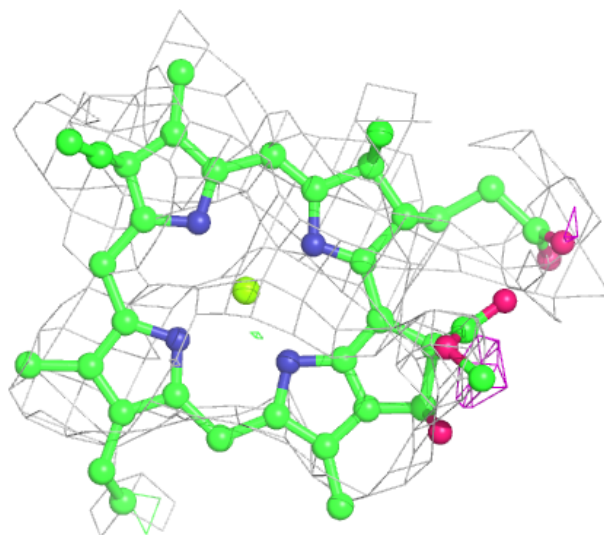
Electron density around CLA 3 314:

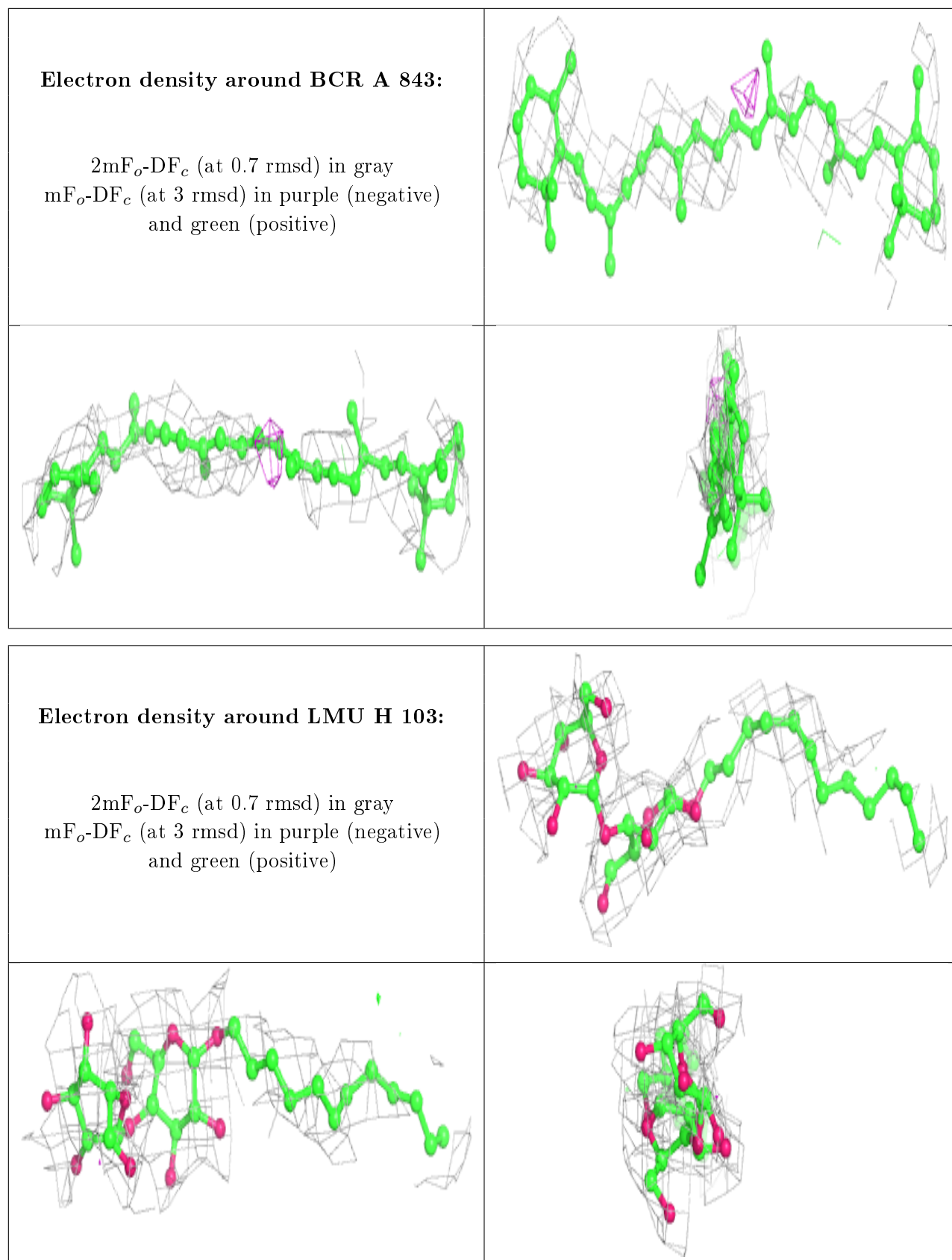
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 835:

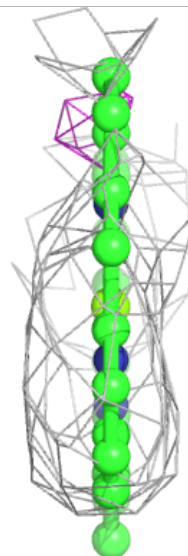
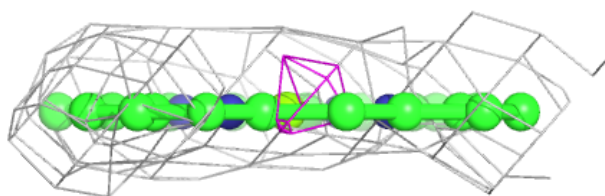
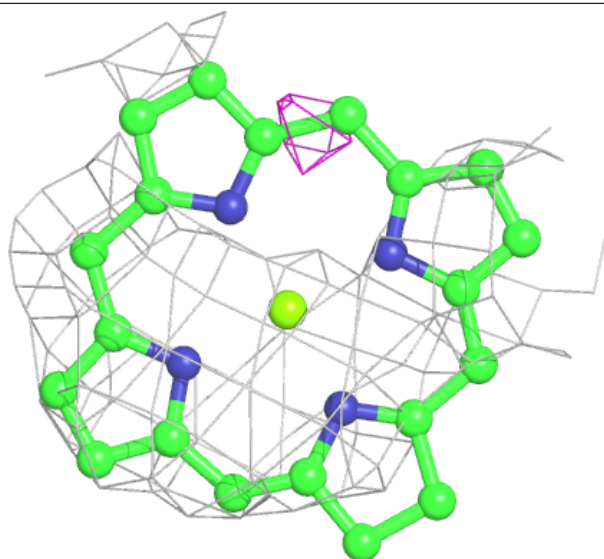
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





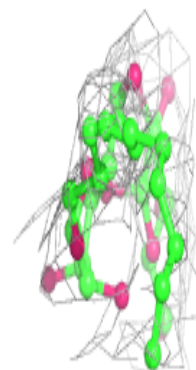
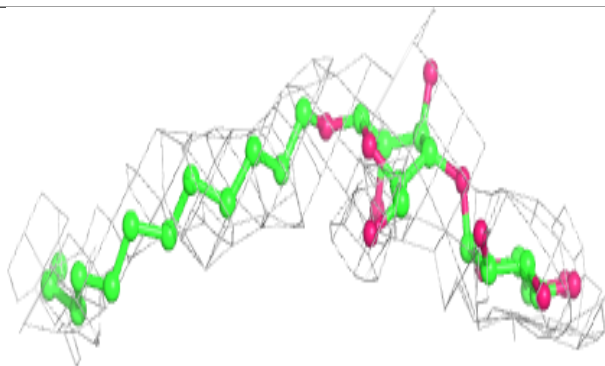
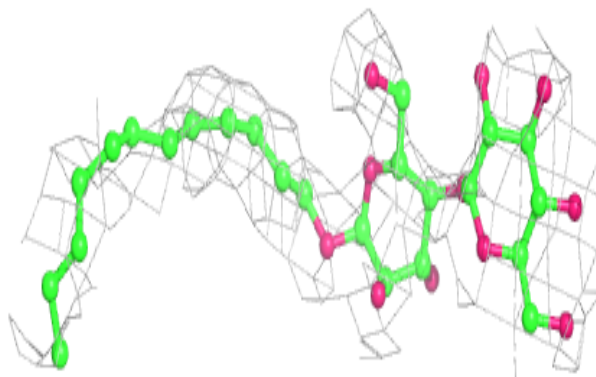
Electron density around CLA A 802:

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

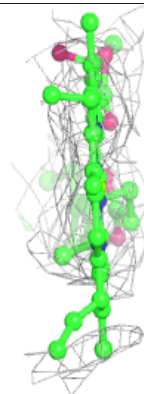
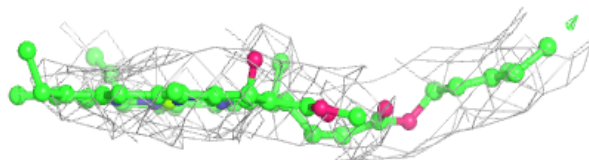
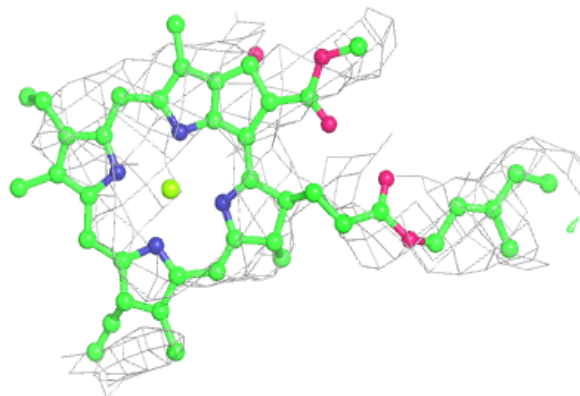


Electron density around LMU 2 322:

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

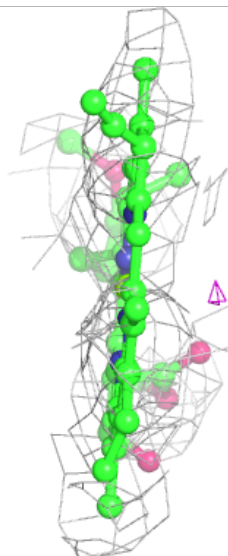
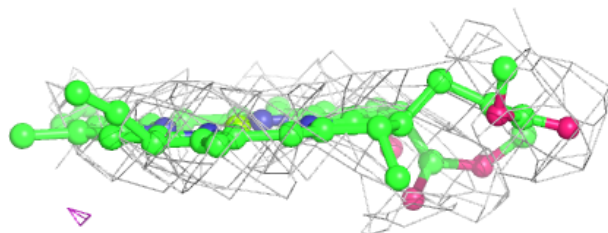
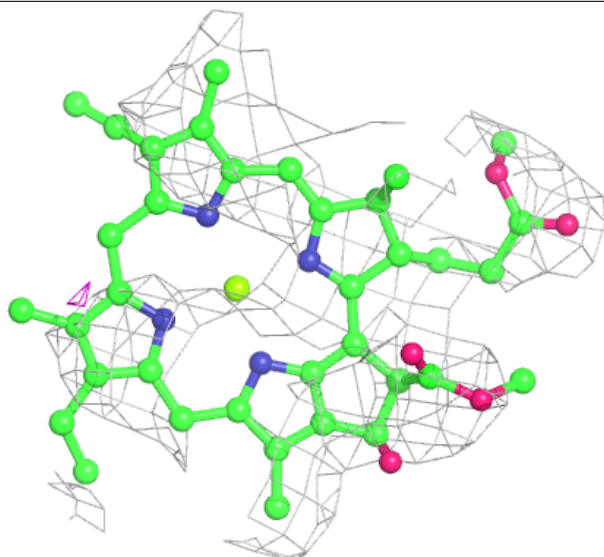
**Electron density around CLA 1 215:**

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



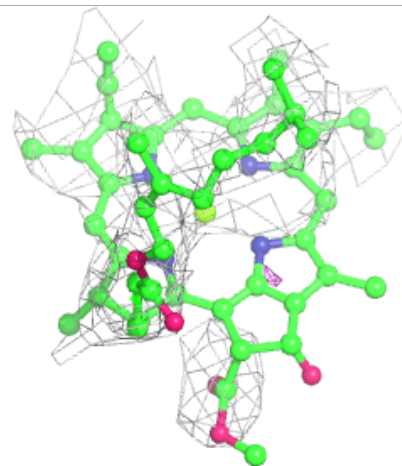
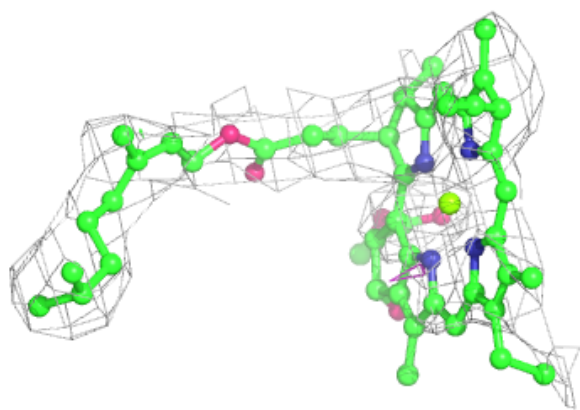
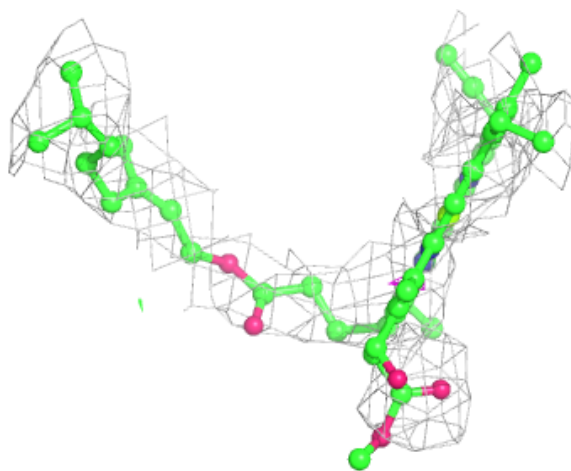
Electron density around CLA B 817:

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



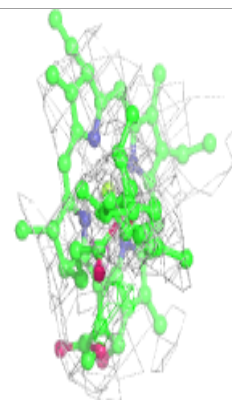
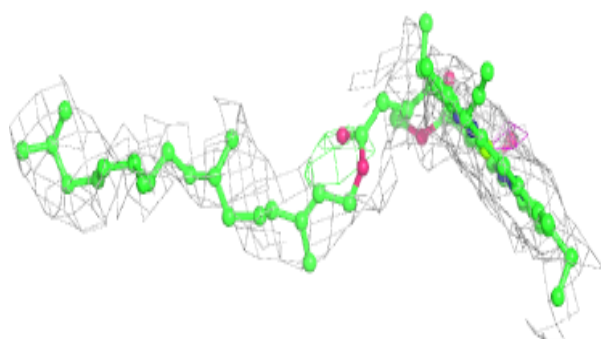
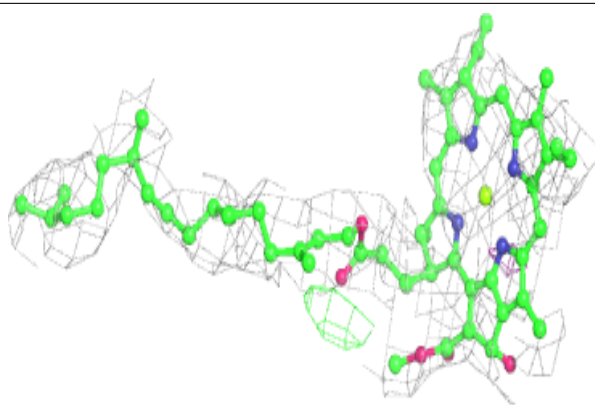
Electron density around CLA L 204:

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



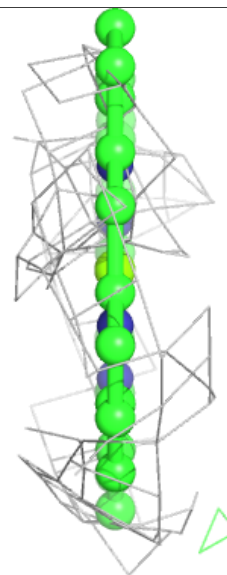
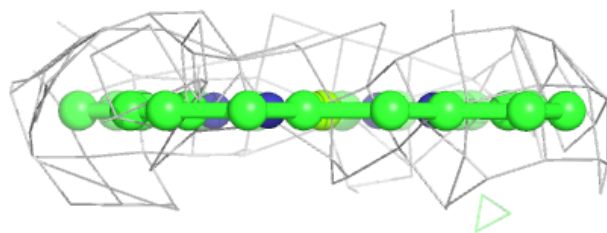
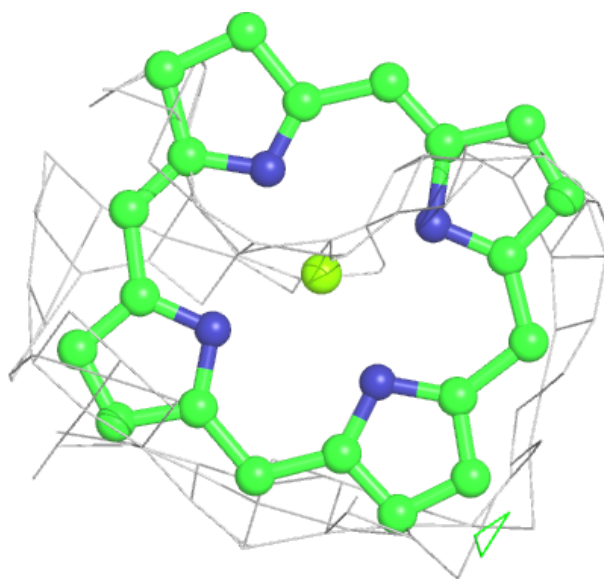
Electron density around CLA 4 303:

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



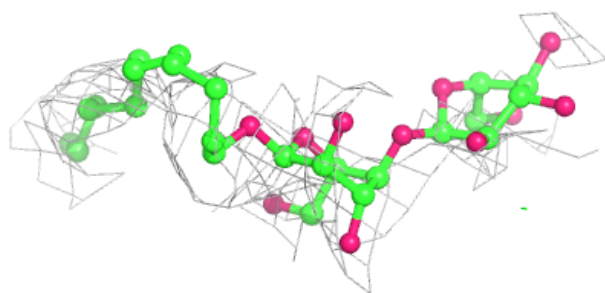
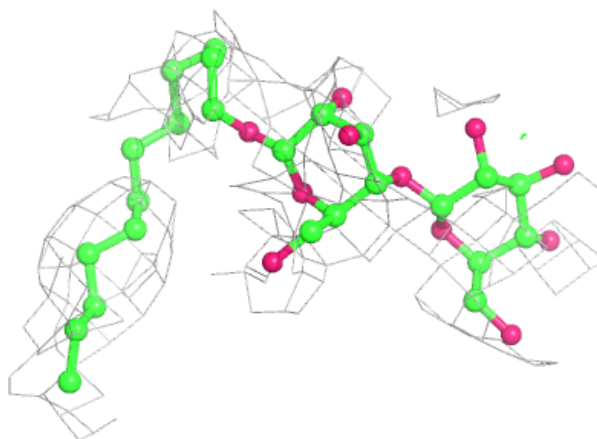
Electron density around CLA 3 305:

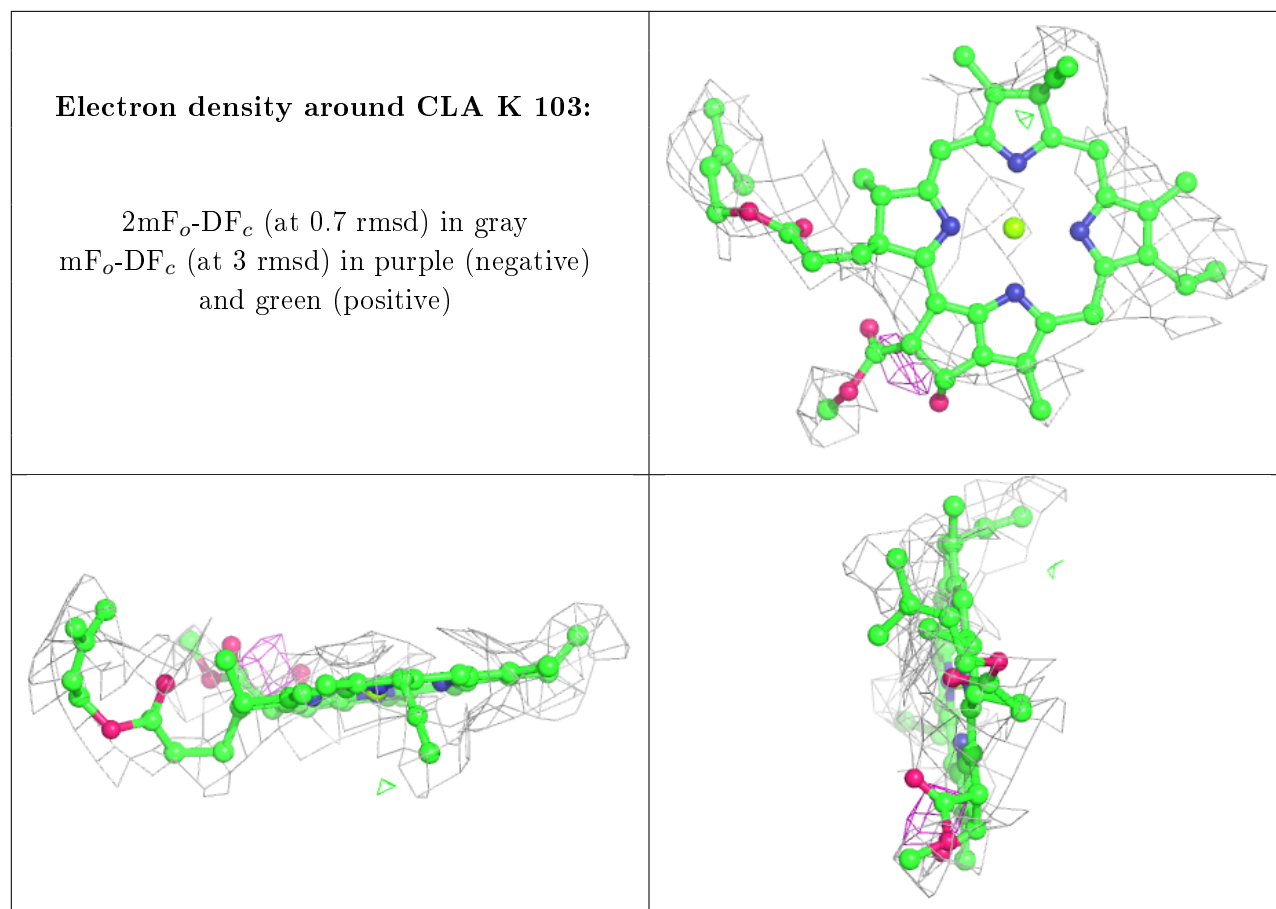
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMU A 848:

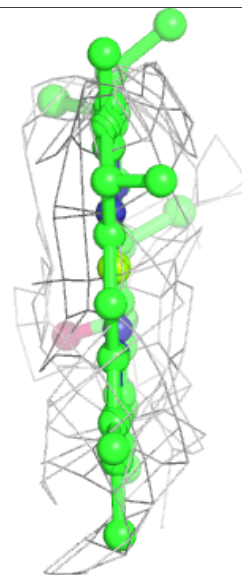
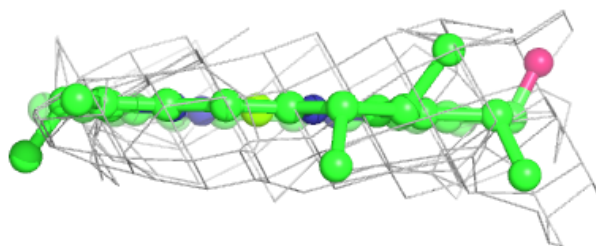
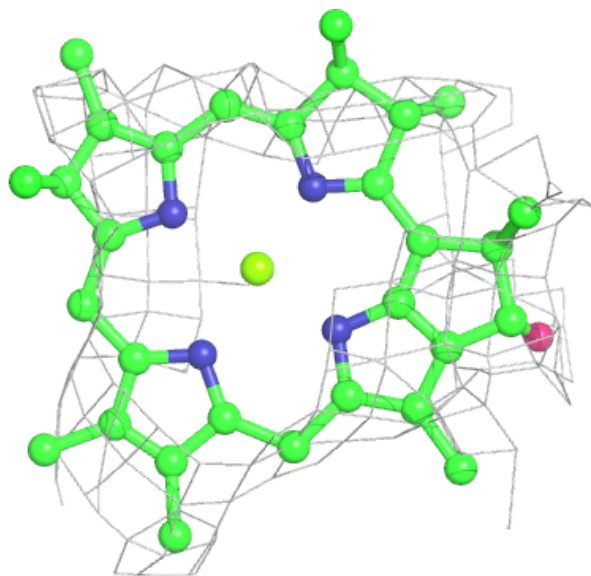
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





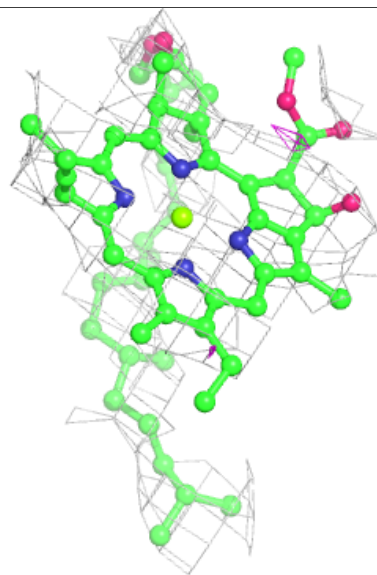
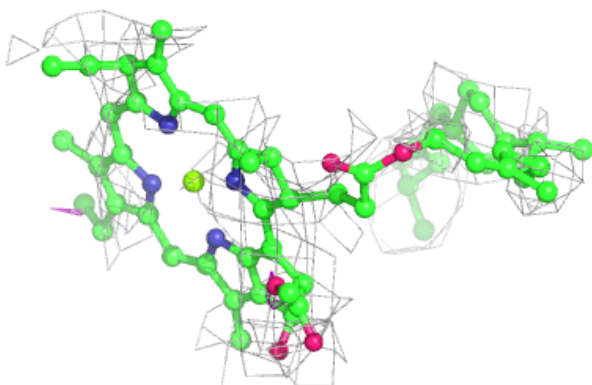
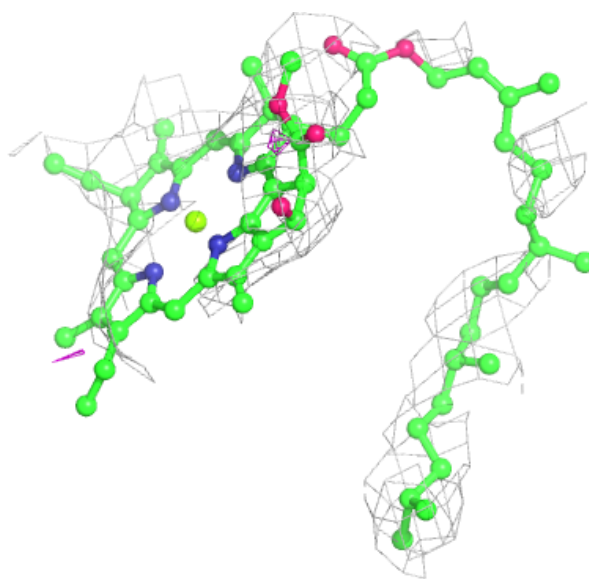
Electron density around CLA 3 318:

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



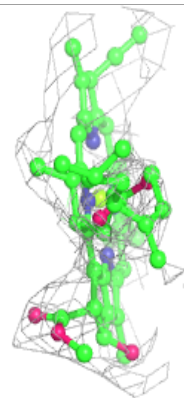
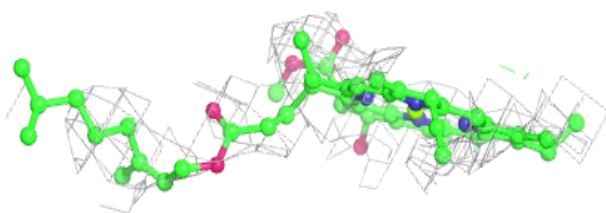
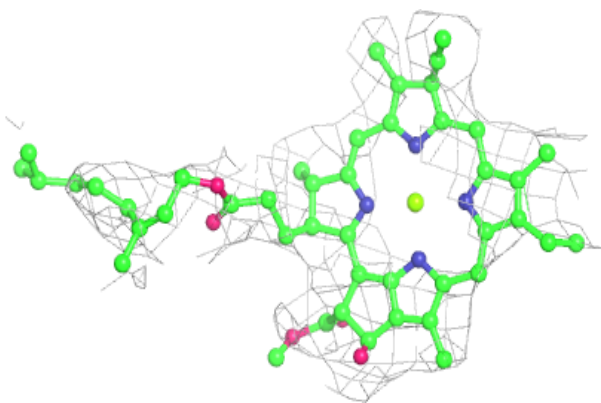
Electron density around CLA 3 311:

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

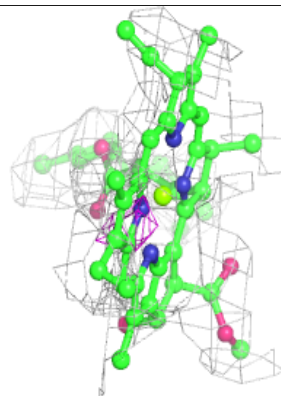
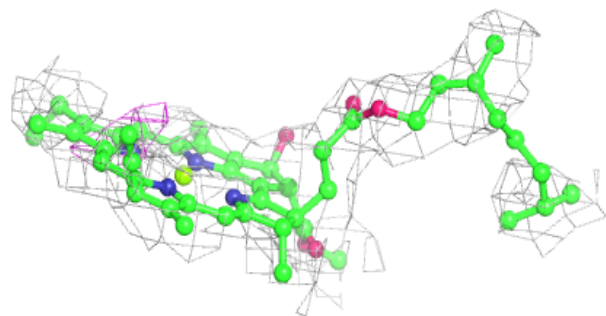
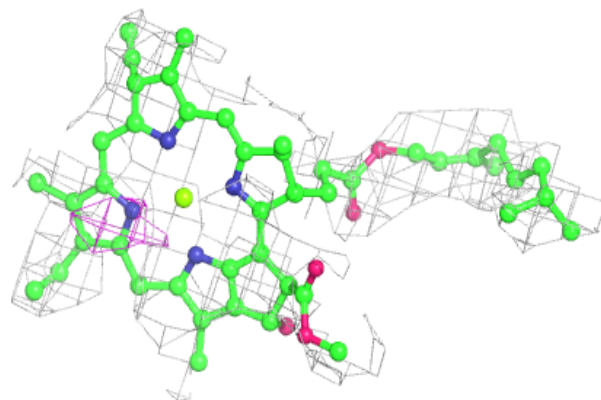


Electron density around CLA A 840:

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

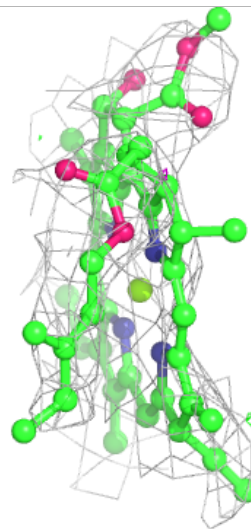
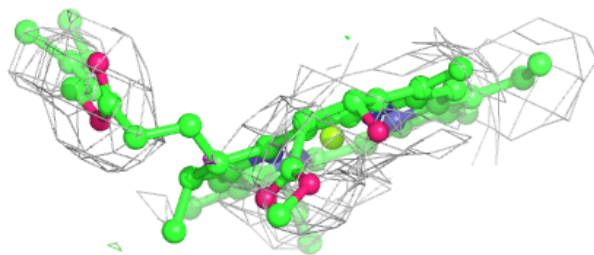
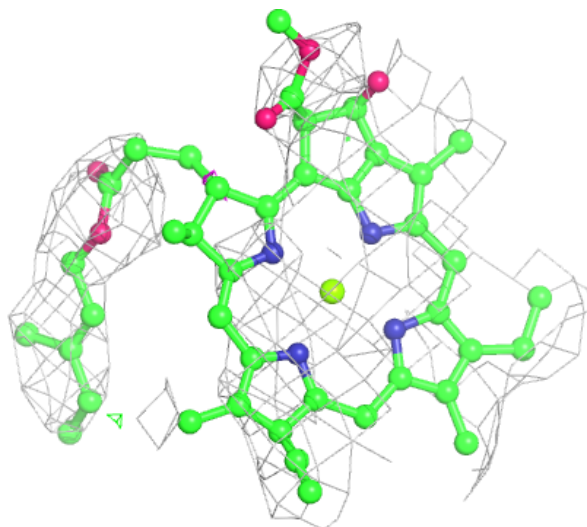
**Electron density around CLA H 112:**

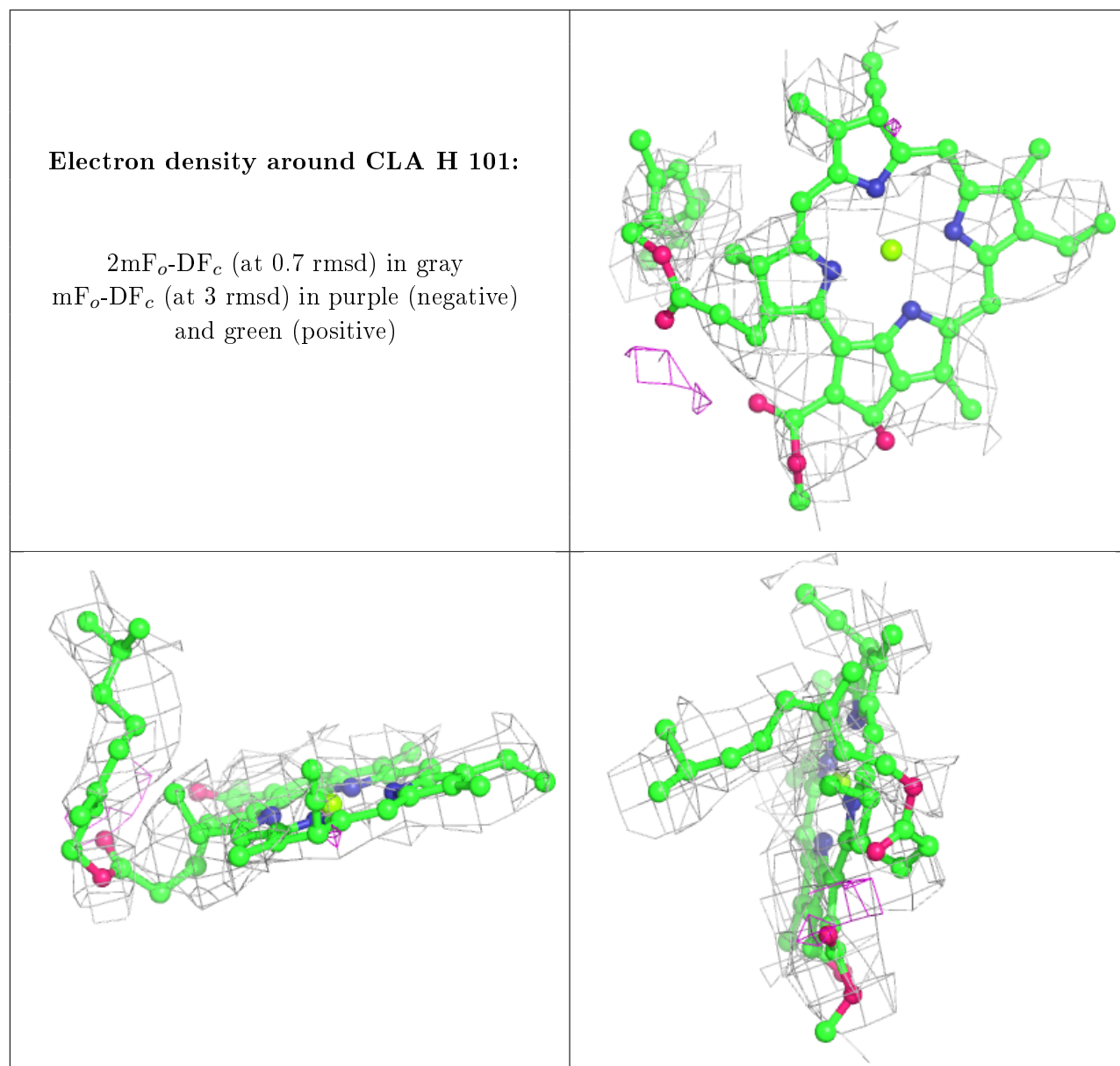
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 836:

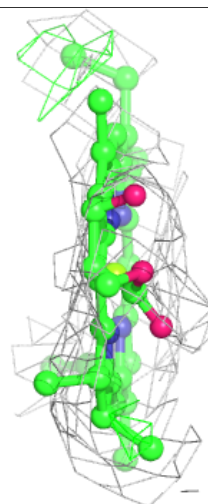
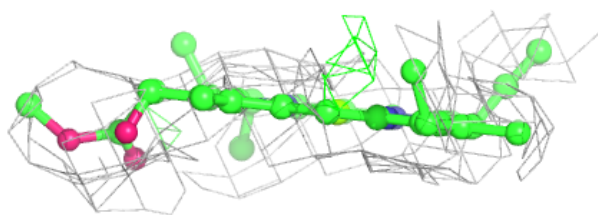
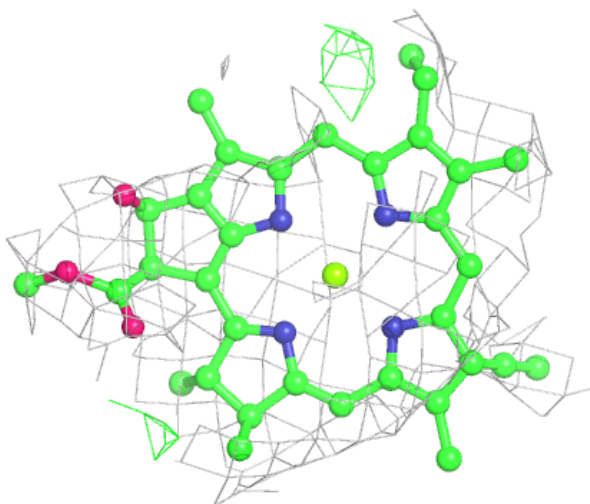
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





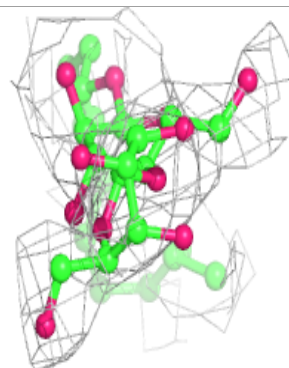
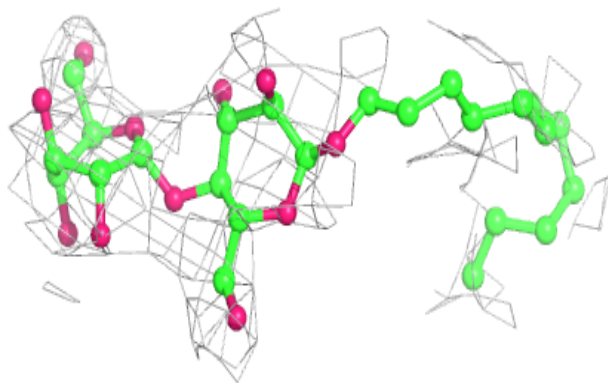
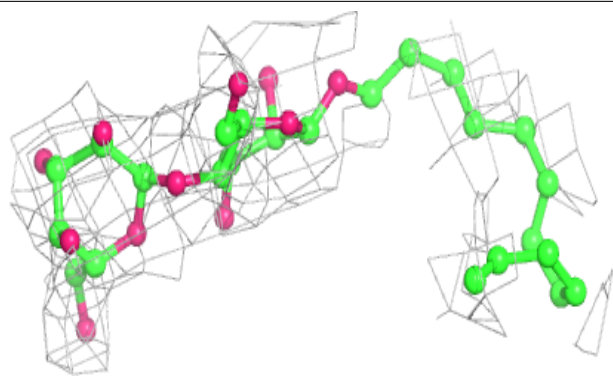
Electron density around CLA F 206:

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

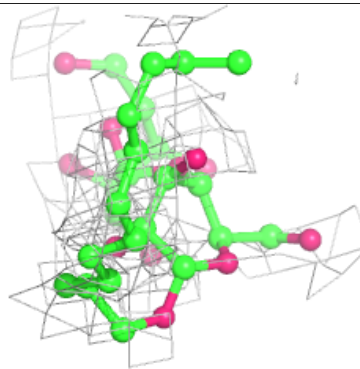
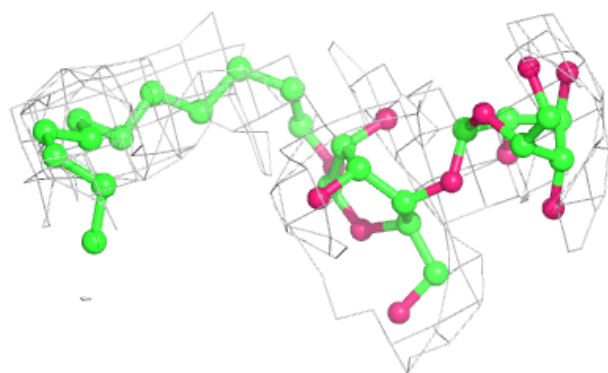
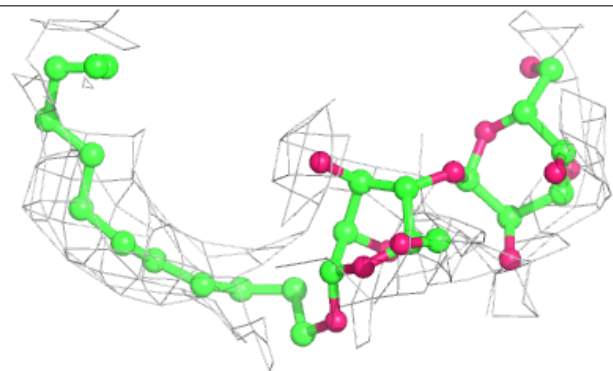


Electron density around LMU H 106:

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

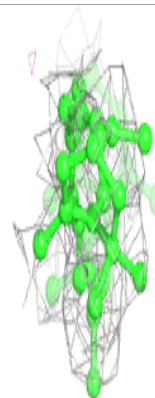
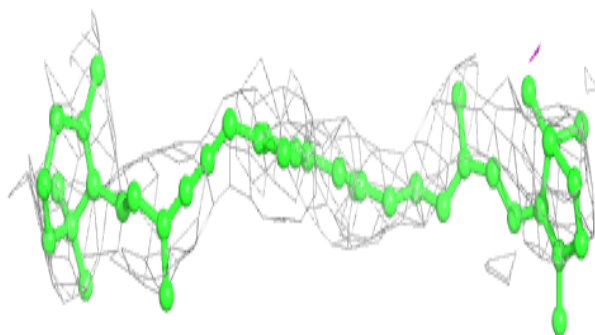
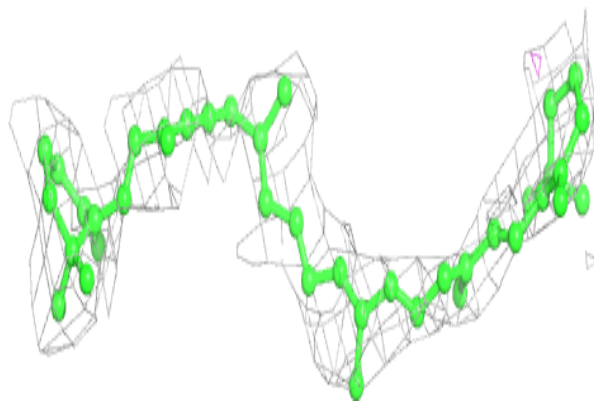
**Electron density around LMU R 104:**

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



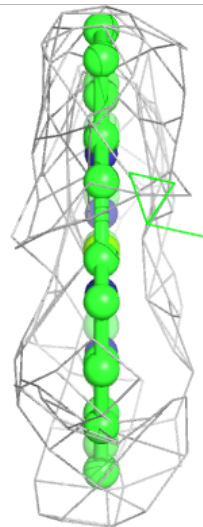
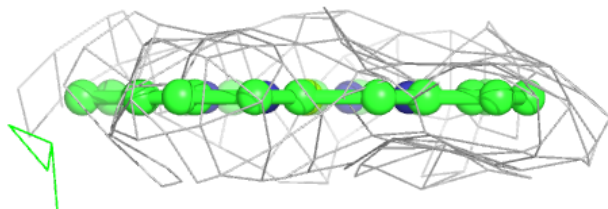
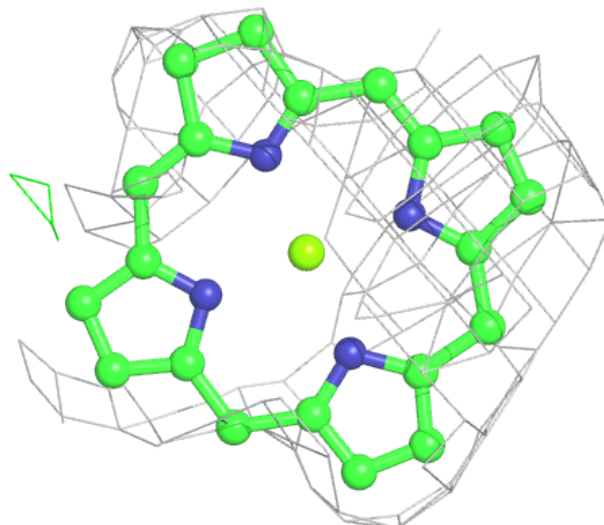
Electron density around BCR I 103:

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



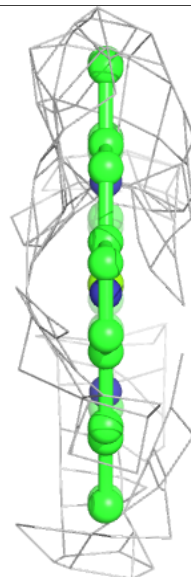
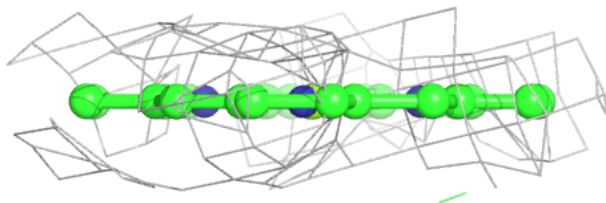
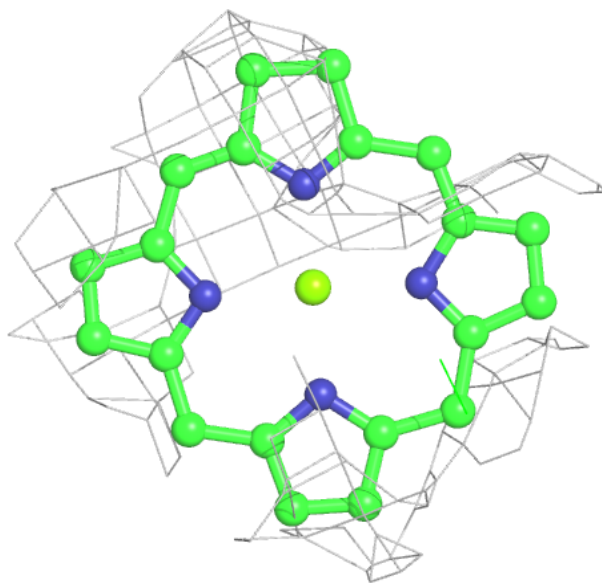
Electron density around CLA 4 308:

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



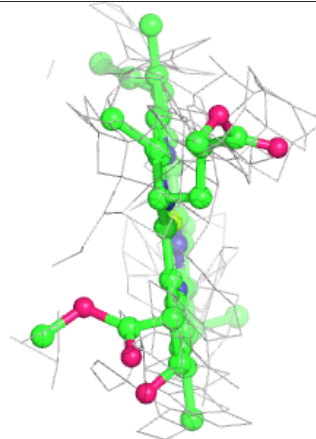
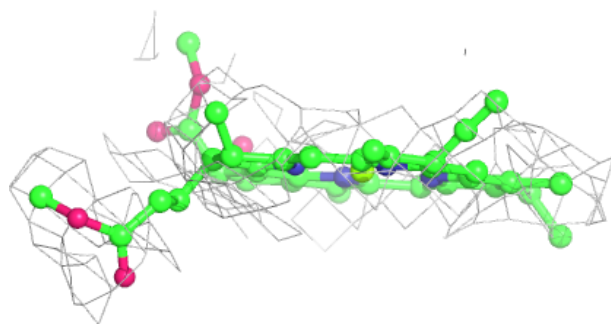
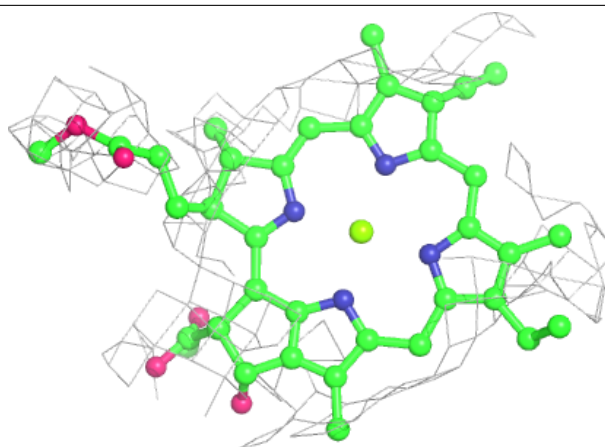
Electron density around CLA 3 309:

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



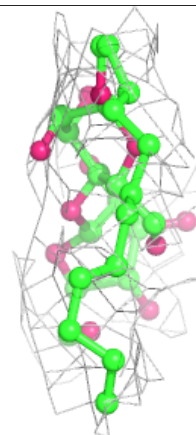
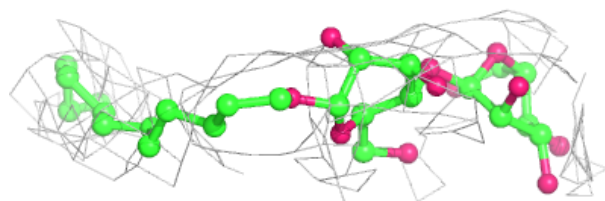
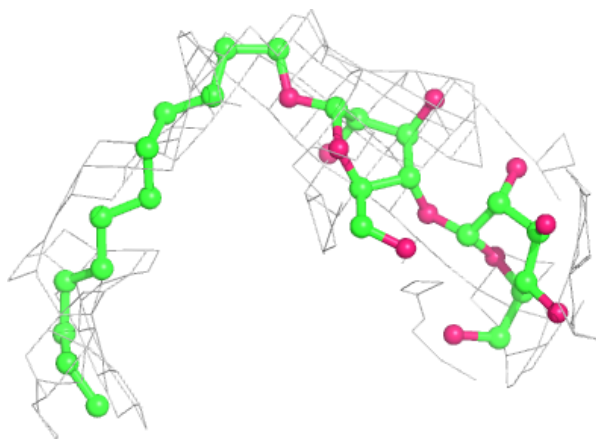
Electron density around CLA 1 201:

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



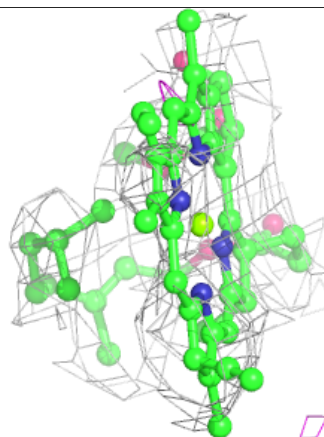
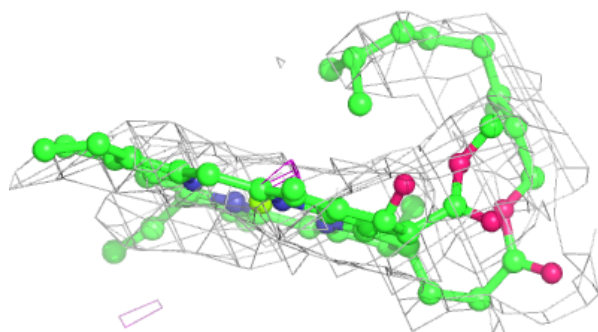
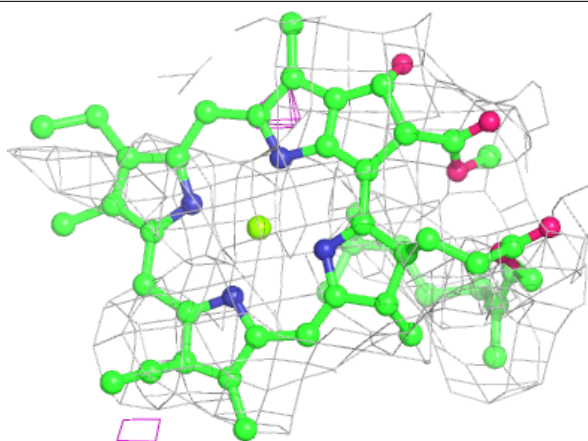
Electron density around LMU K 106:

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



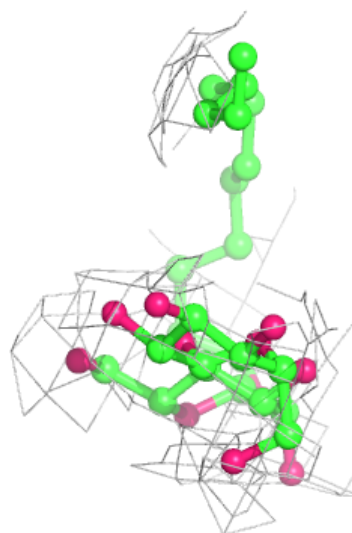
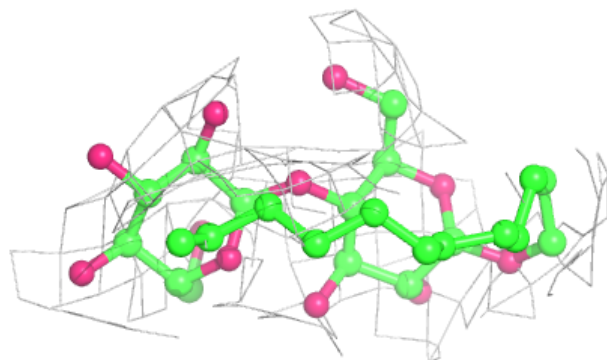
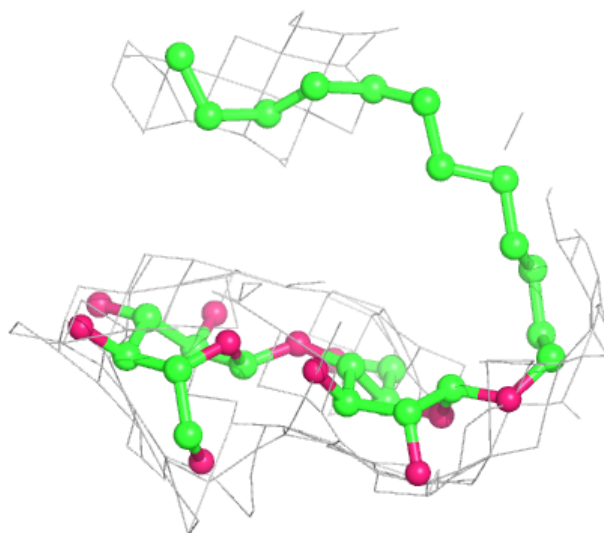
Electron density around CLA 4 304:

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



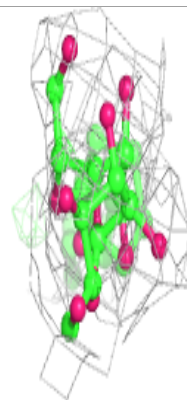
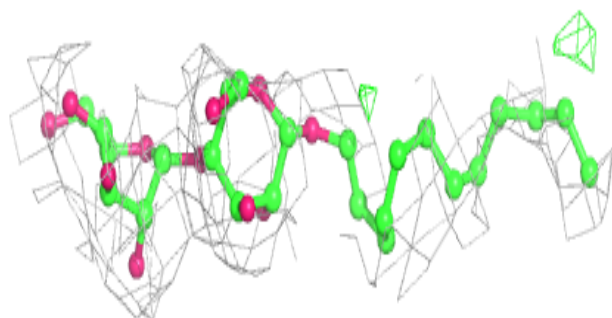
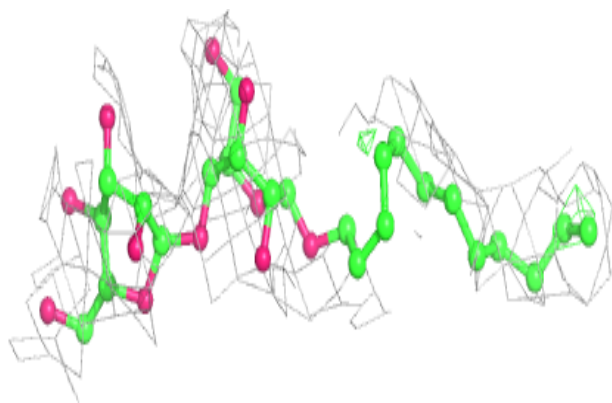
Electron density around LMU 1 217:

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

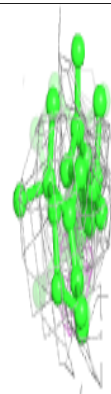
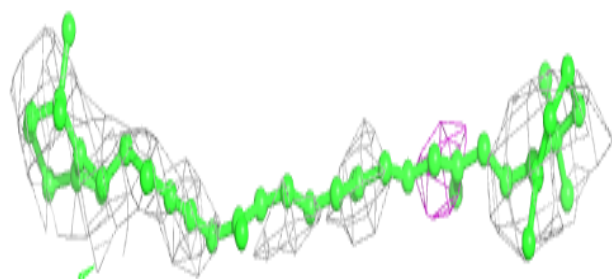
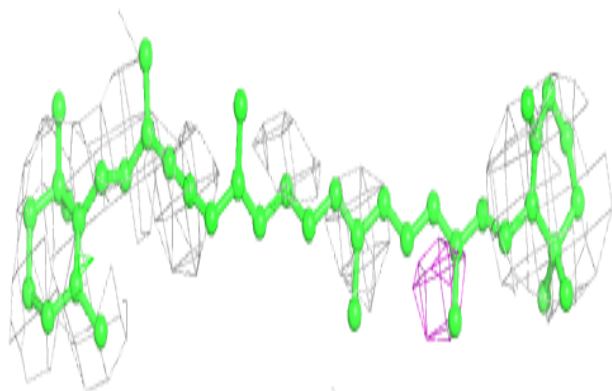


Electron density around LMU E 101:

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

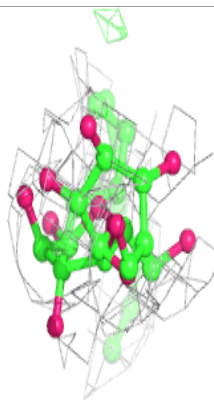
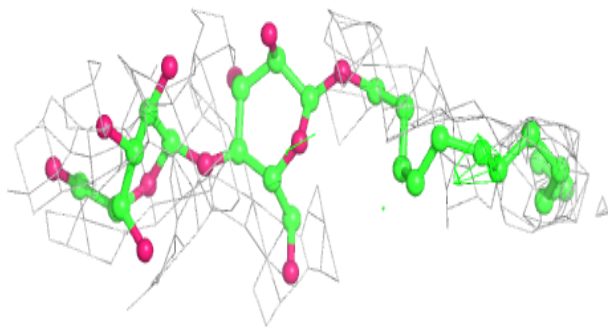
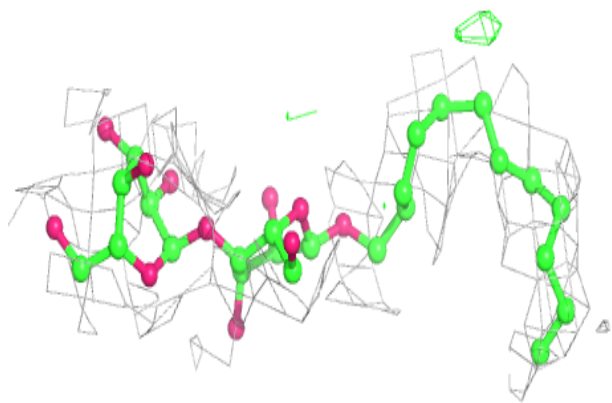
**Electron density around BCR G 104:**

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

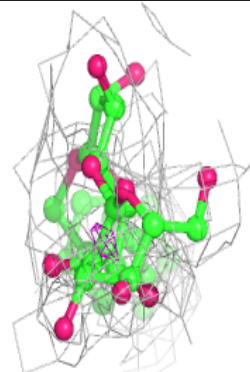
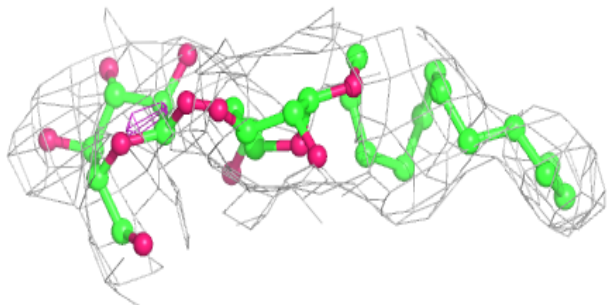
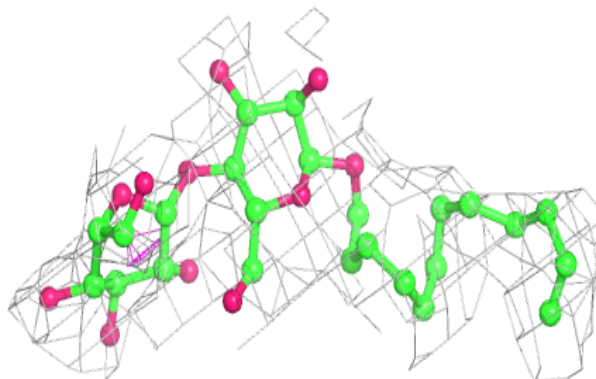


Electron density around LMU A 846:

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

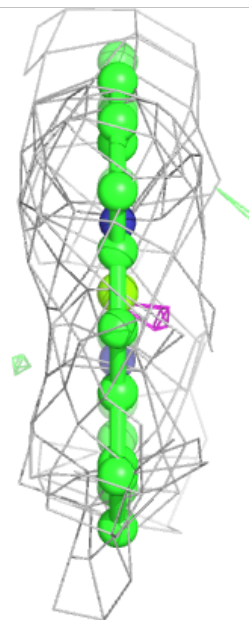
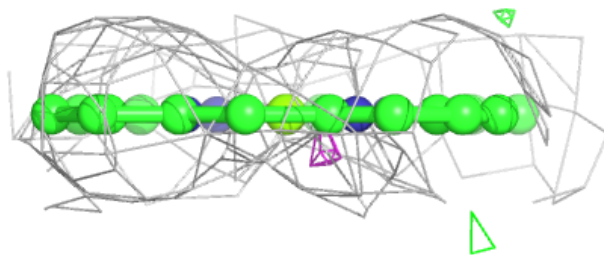
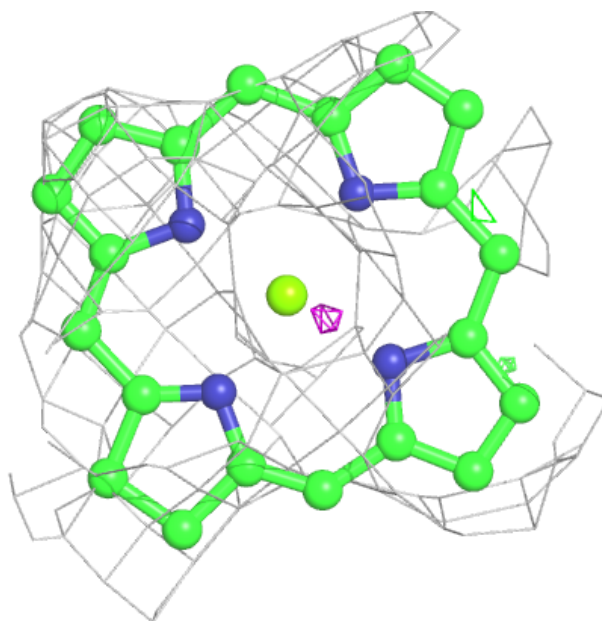
**Electron density around LMU 2 313:**

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



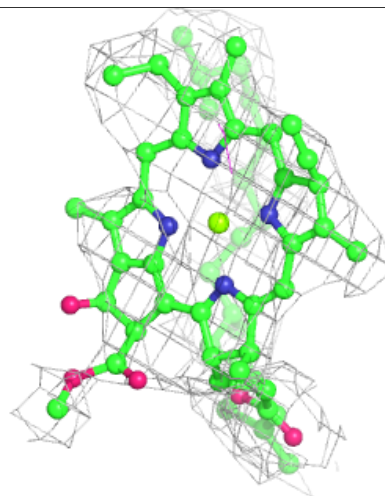
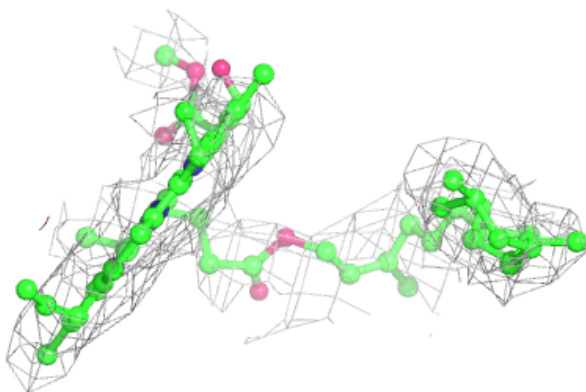
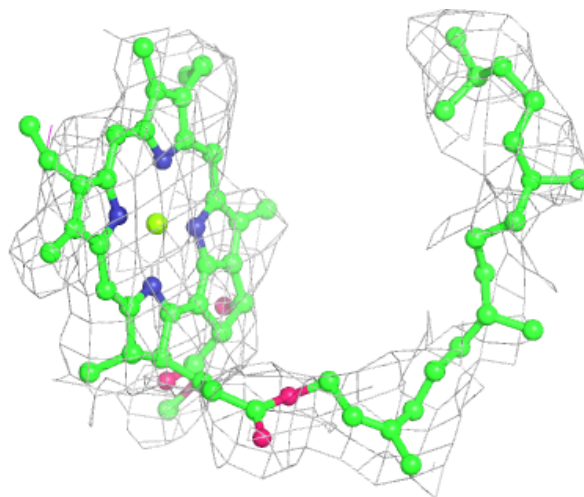
Electron density around CLA 4 307:

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



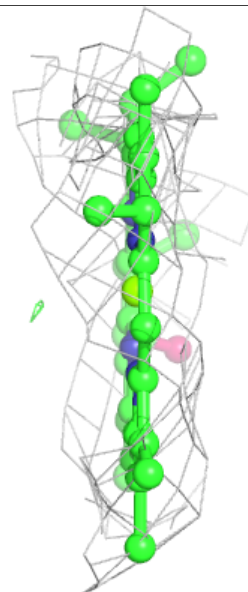
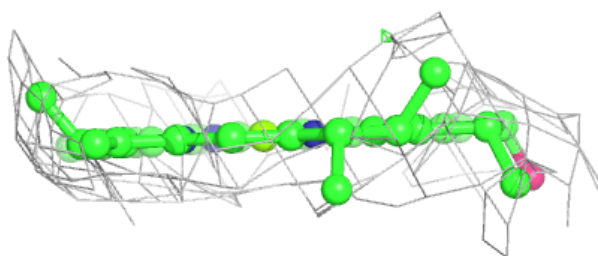
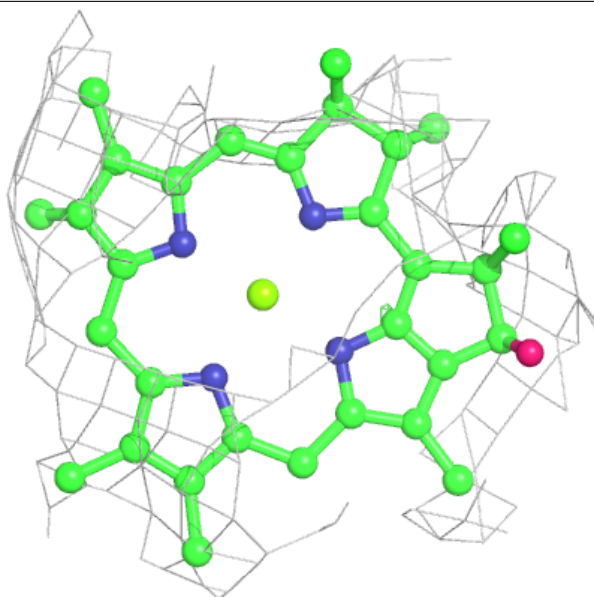
Electron density around CLA 3 310:

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



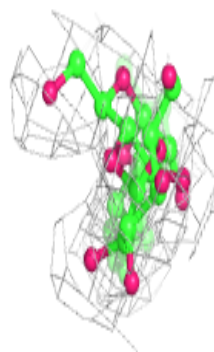
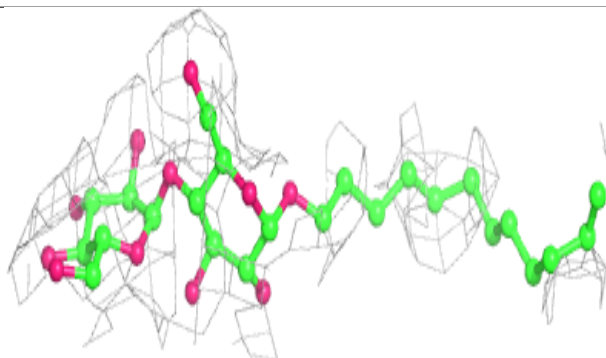
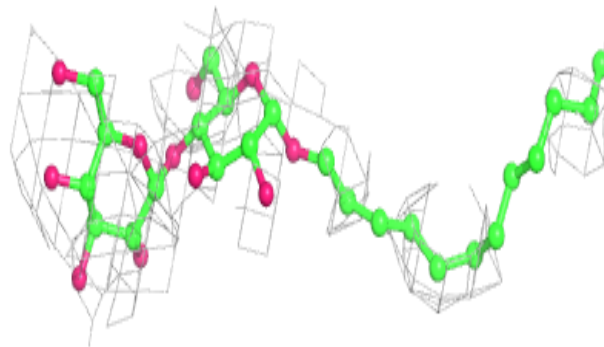
Electron density around CLA 3 303:

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

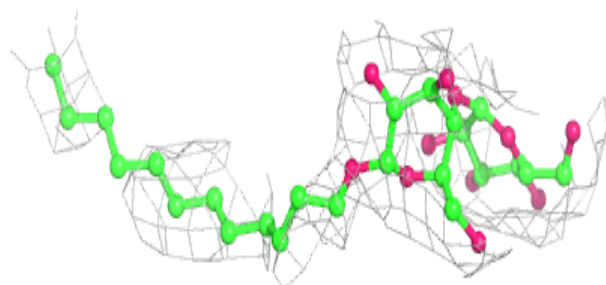
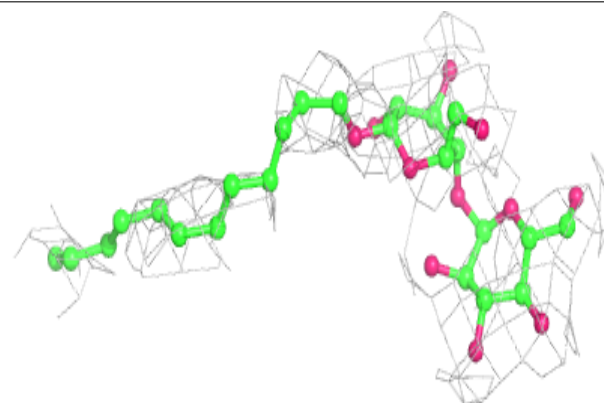


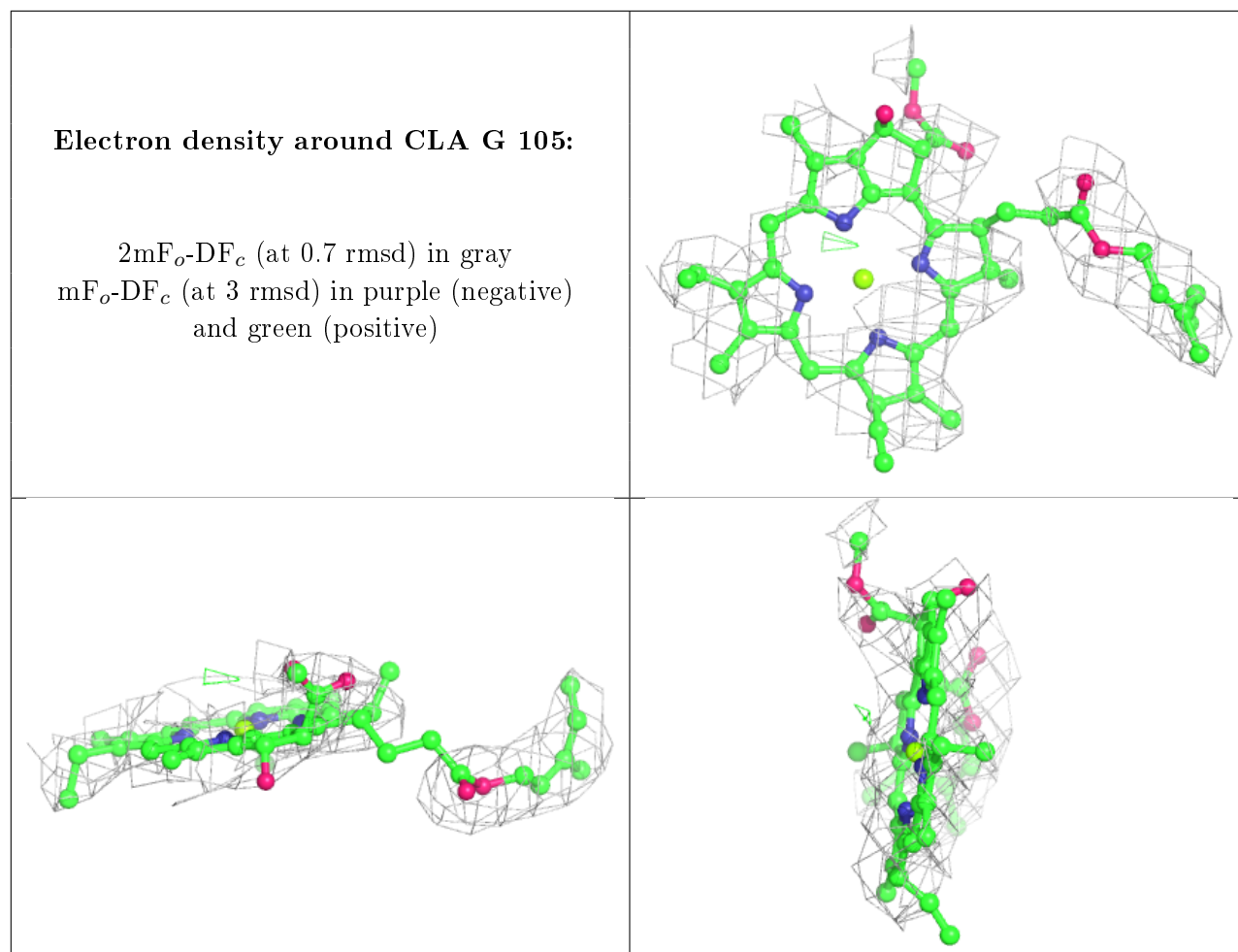
Electron density around LMU B 805:

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

**Electron density around LMU R 105:**

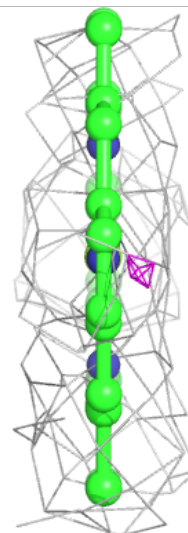
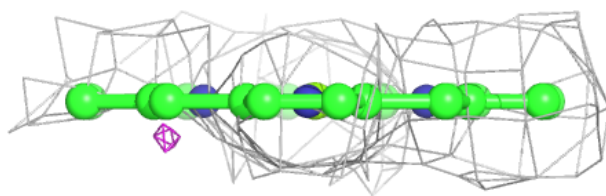
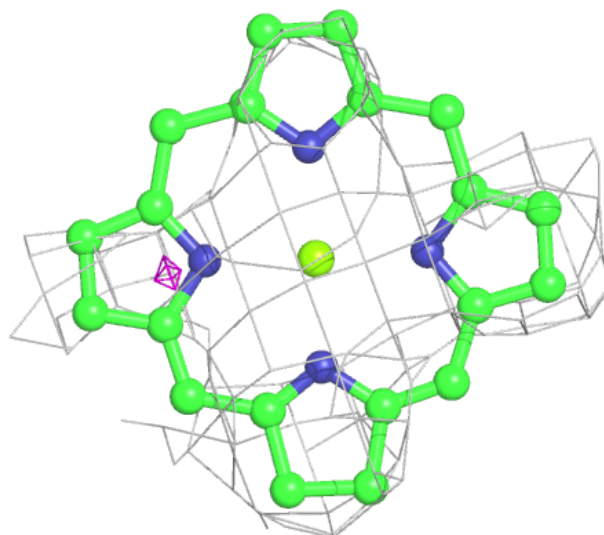
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





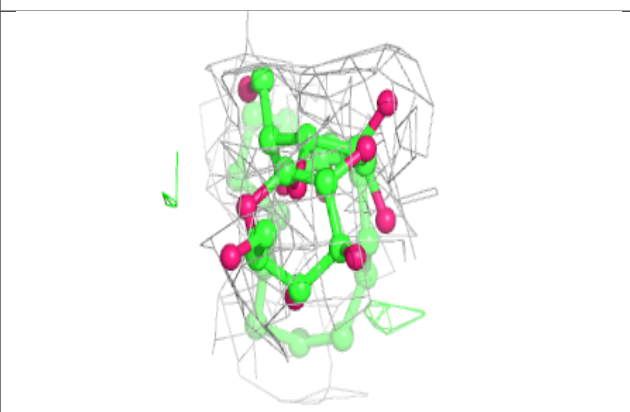
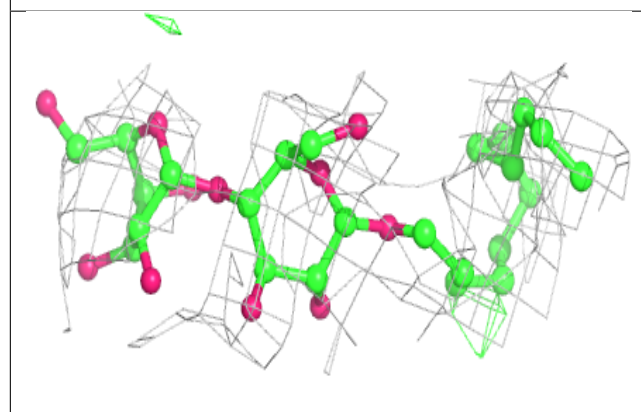
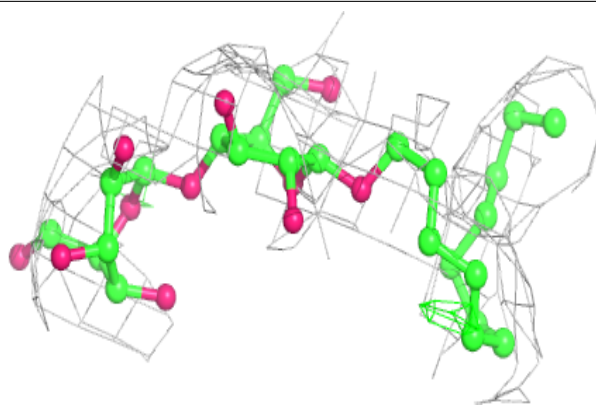
Electron density around CLA 3 302:

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

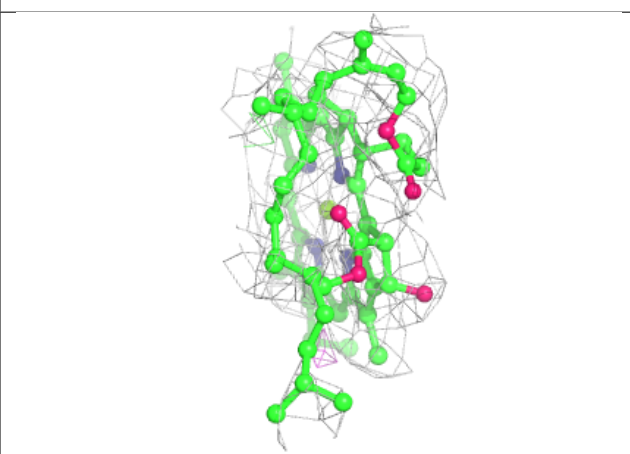
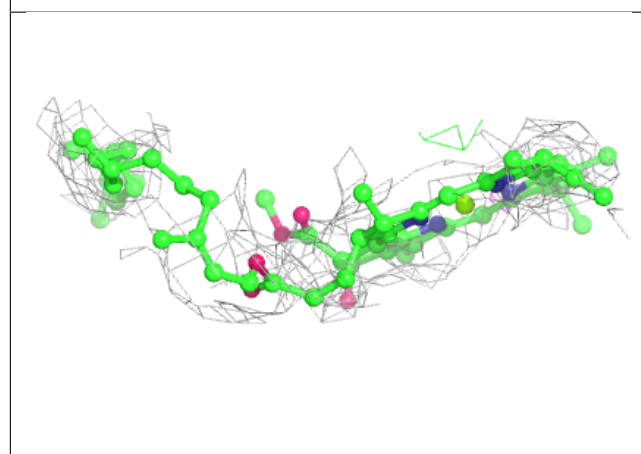
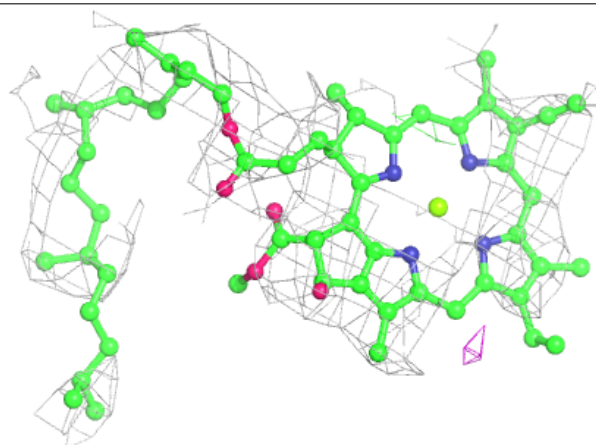


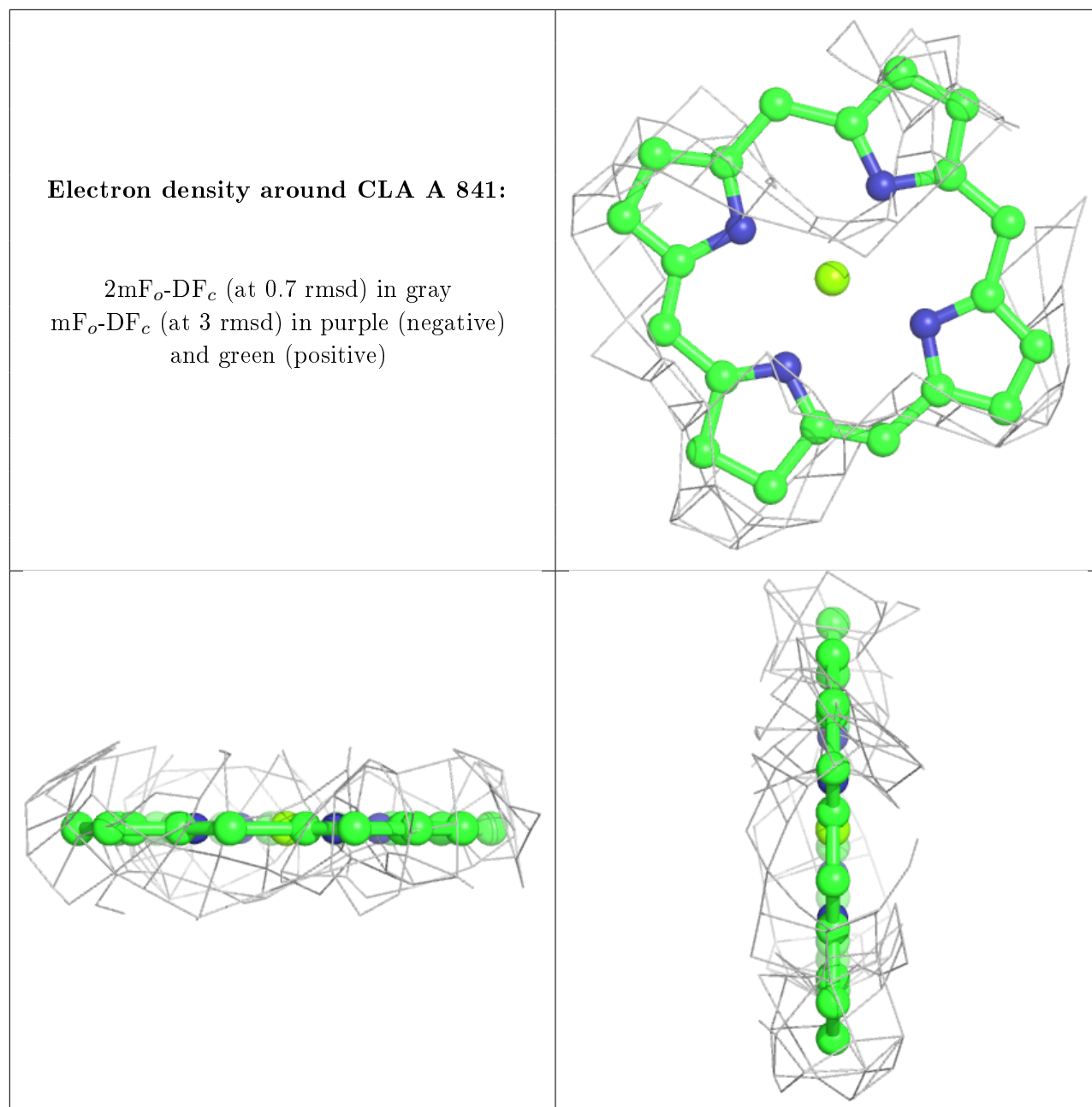
Electron density around LMU A 854:

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

**Electron density around CLA R 108:**

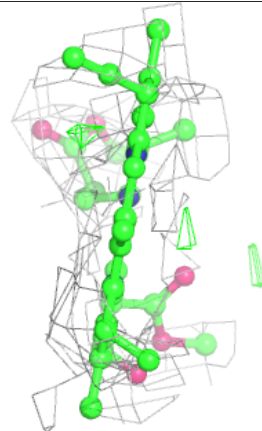
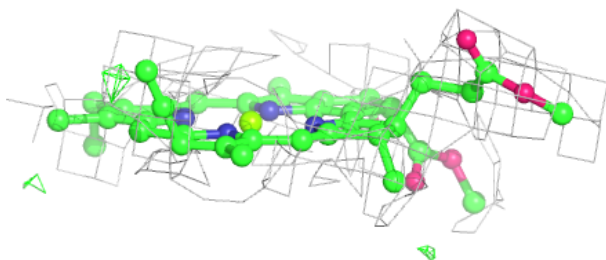
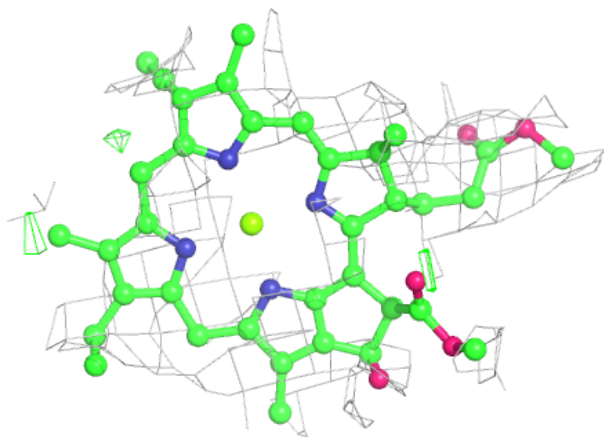
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



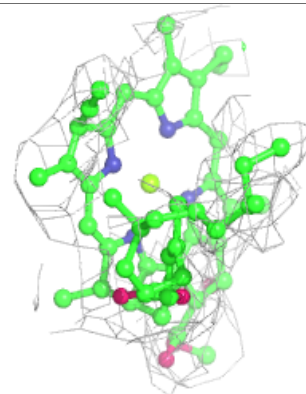
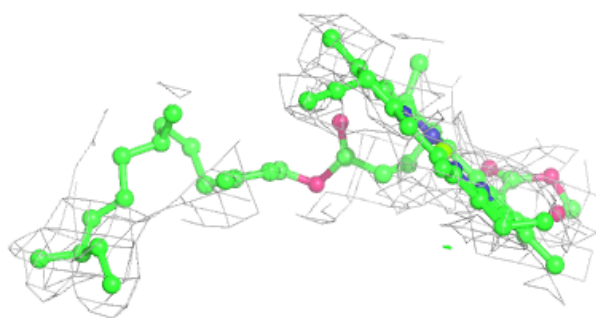
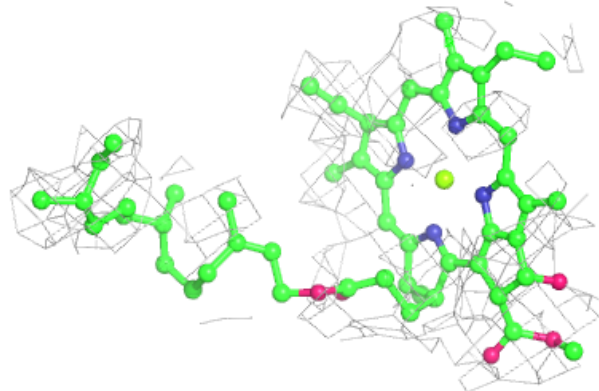


Electron density around CLA K 101:

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

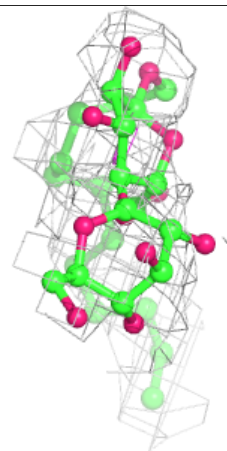
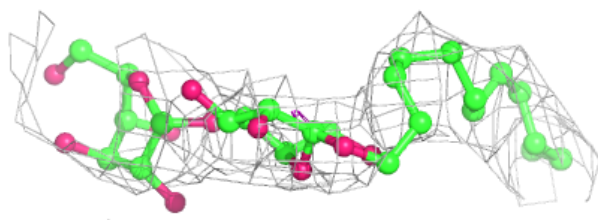
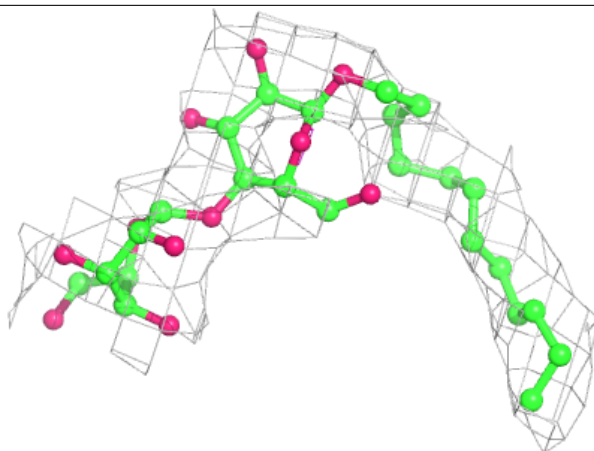
**Electron density around CLA 2 312:**

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

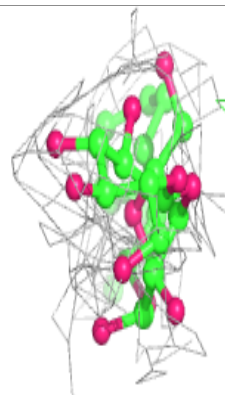
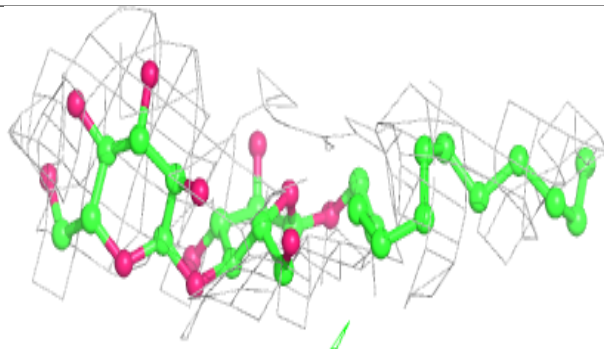
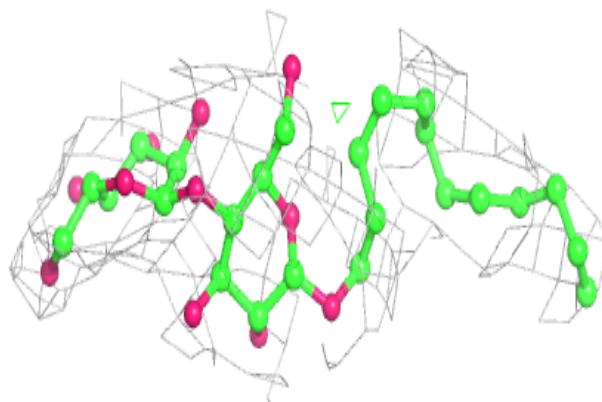


Electron density around LMU R 103:

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

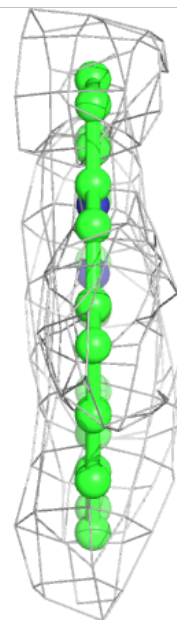
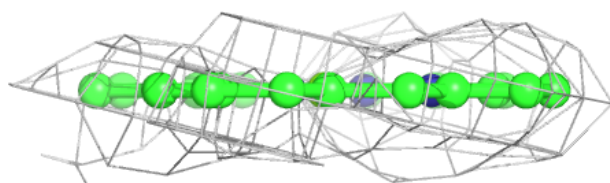
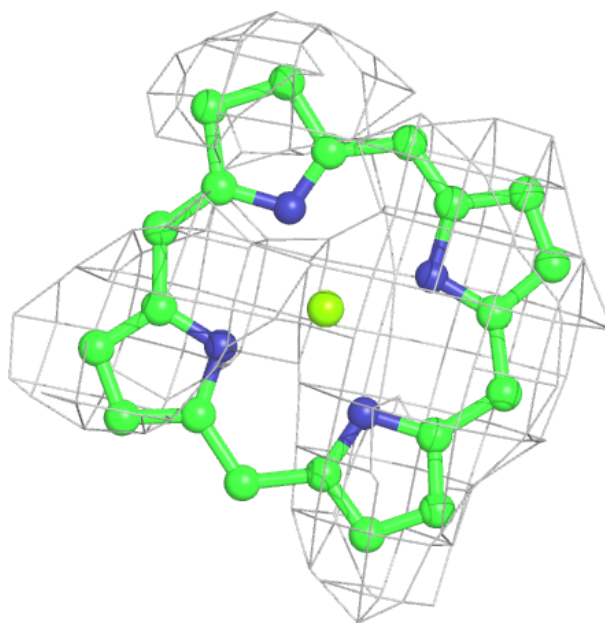
**Electron density around LMU K 107:**

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



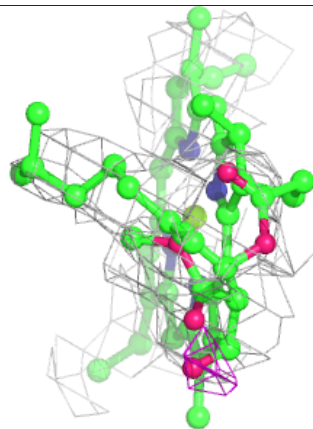
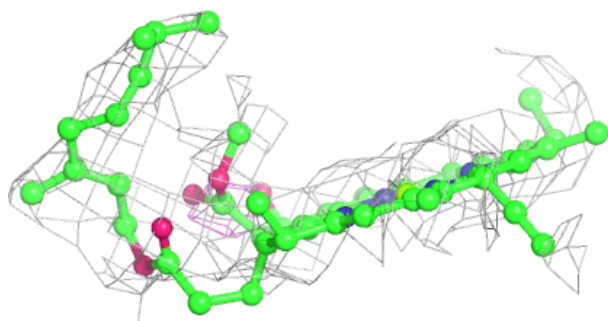
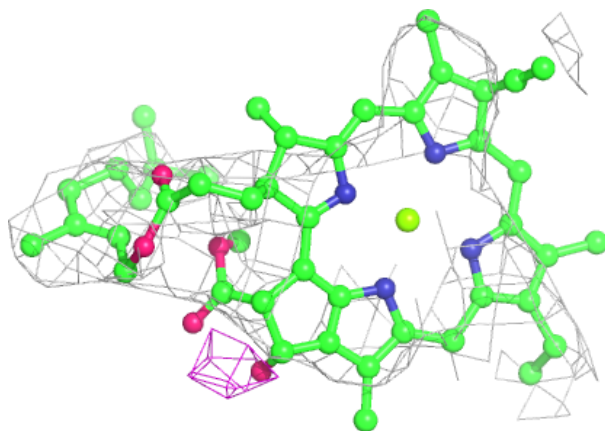
Electron density around CLA 3 313:

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

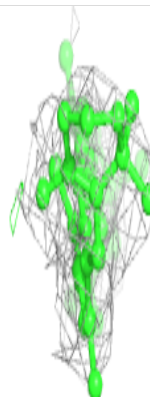
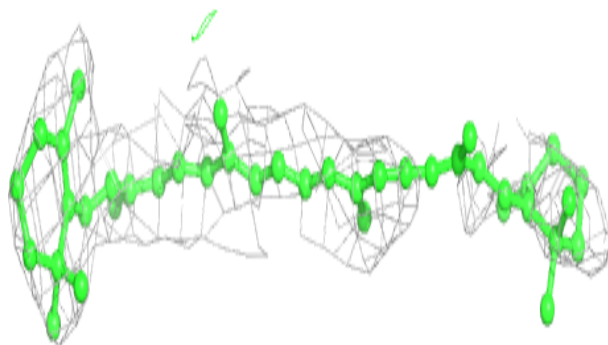
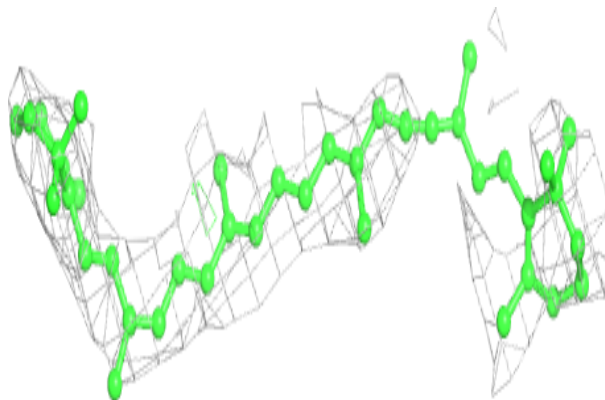


Electron density around CLA L 202:

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

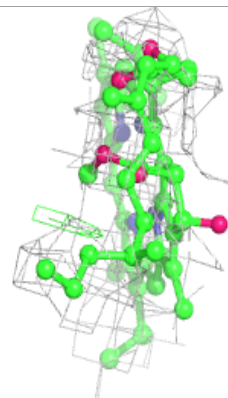
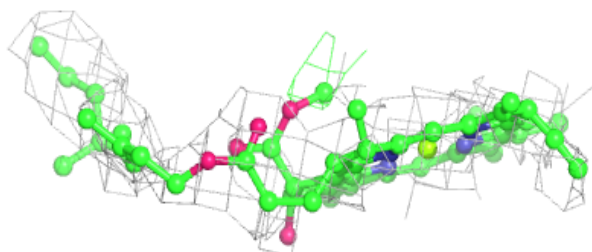
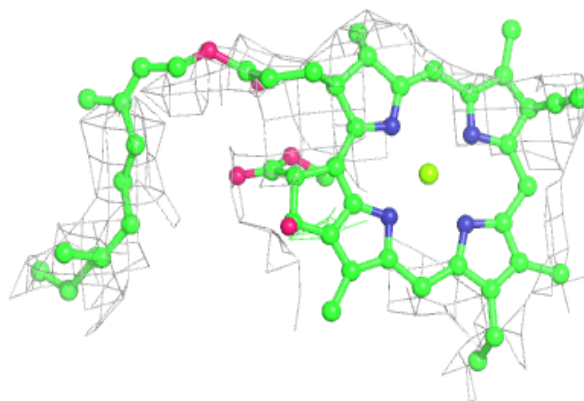
**Electron density around BCR B 845:**

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

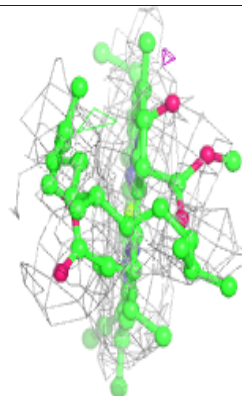
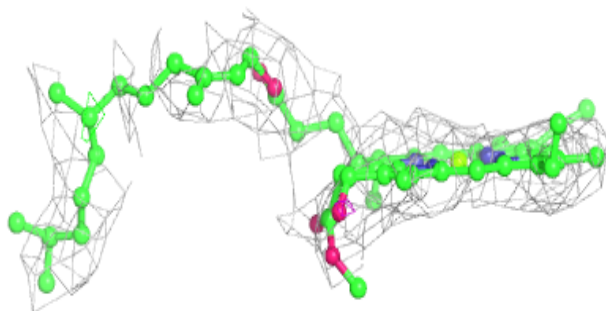
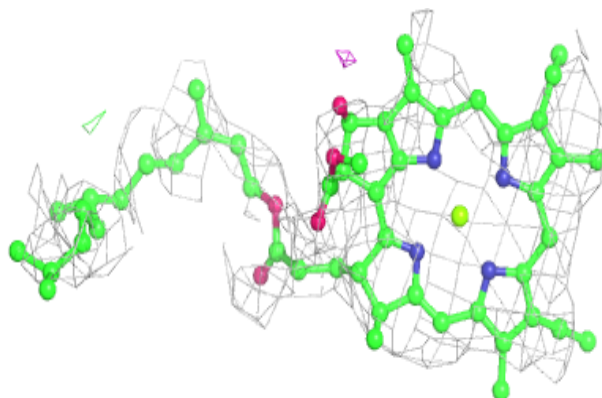


Electron density around CLA R 107:

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

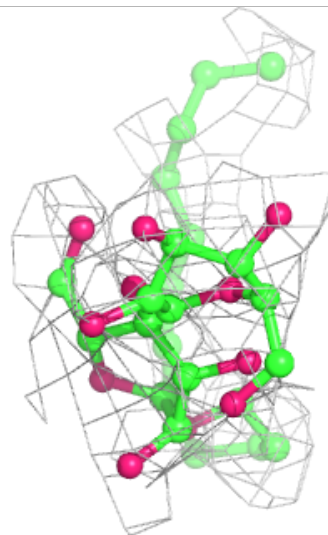
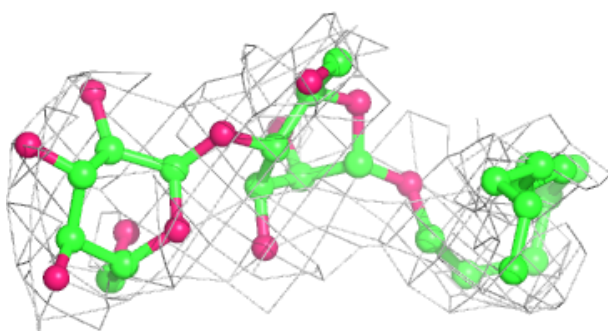
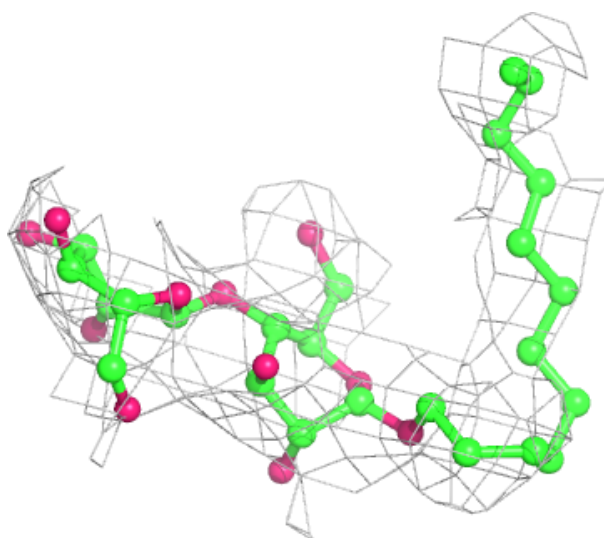
**Electron density around CLA B 816:**

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



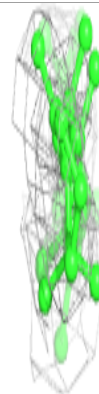
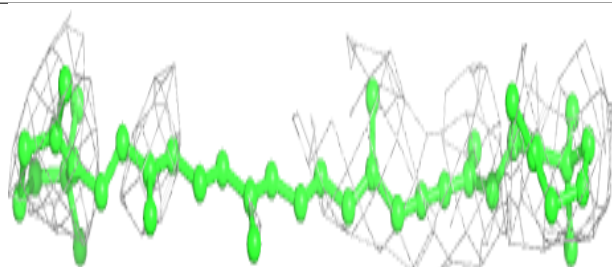
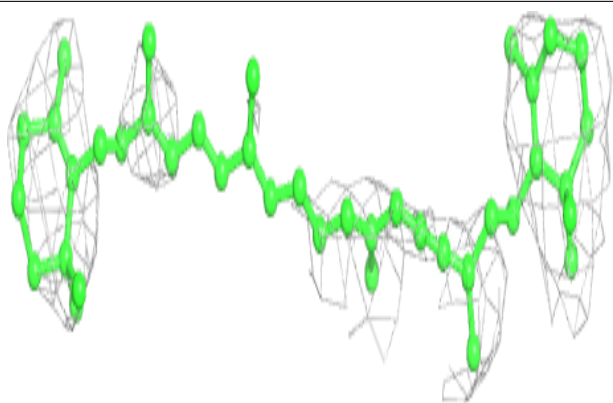
Electron density around LMU R 101:

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

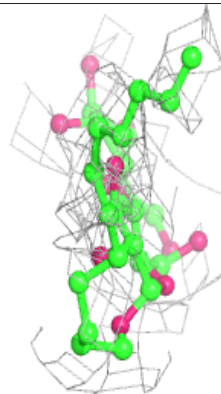
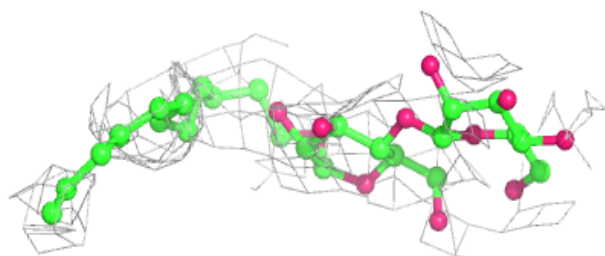
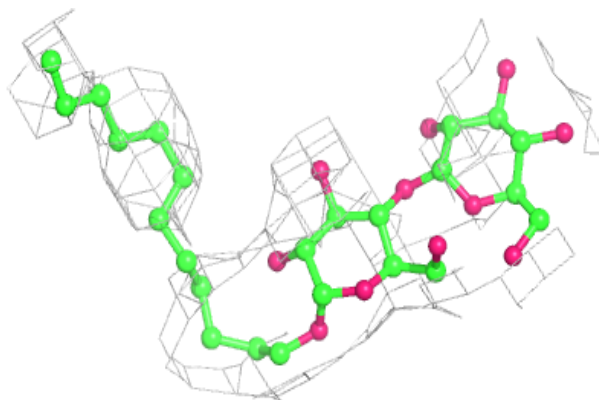


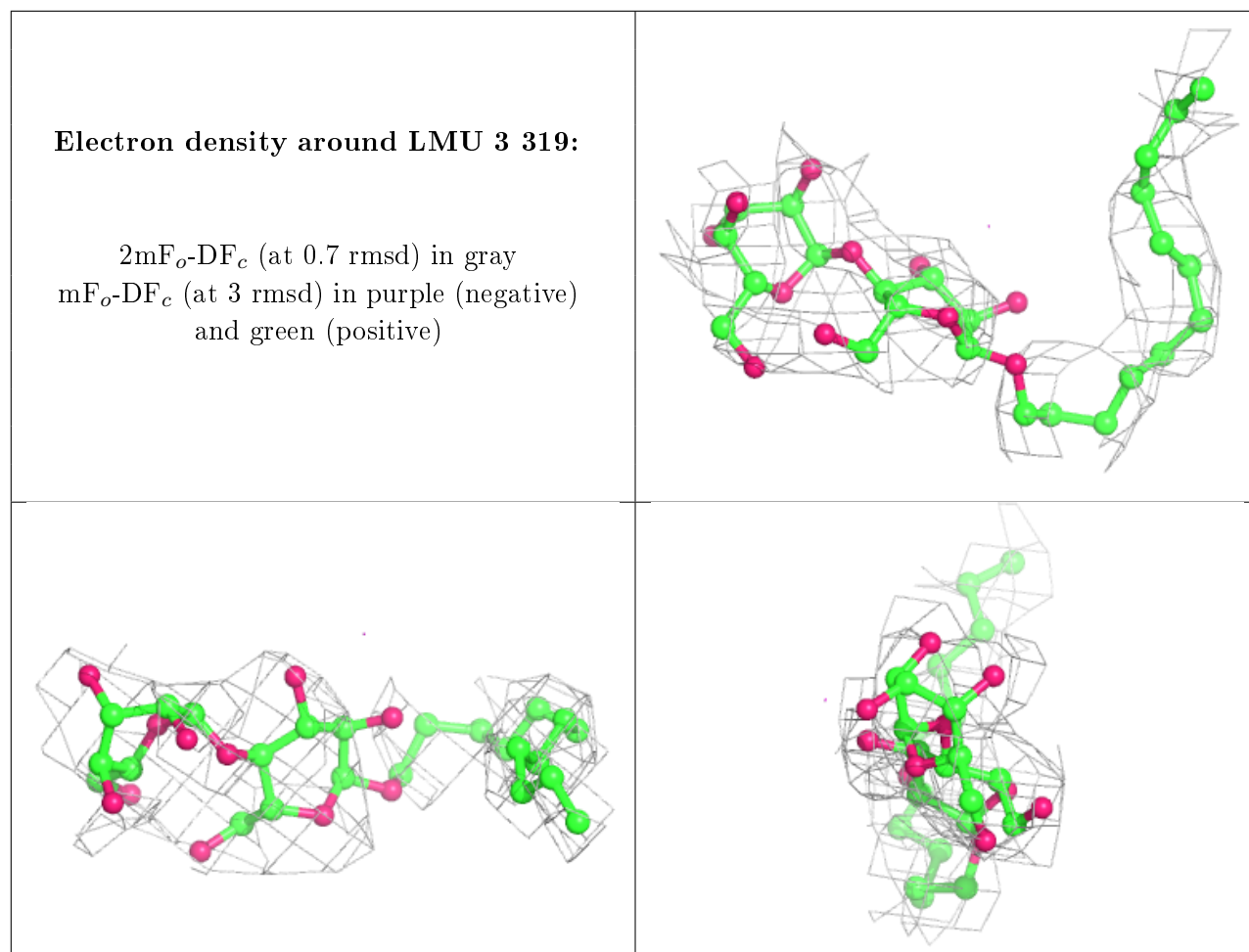
Electron density around BCR L 211:

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

**Electron density around LMU R 106:**

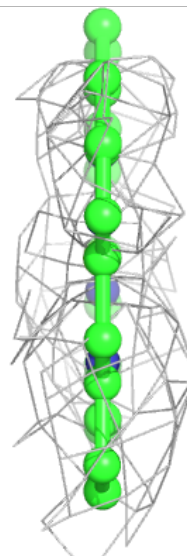
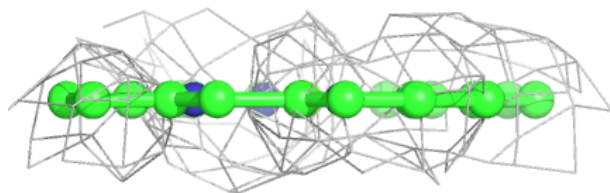
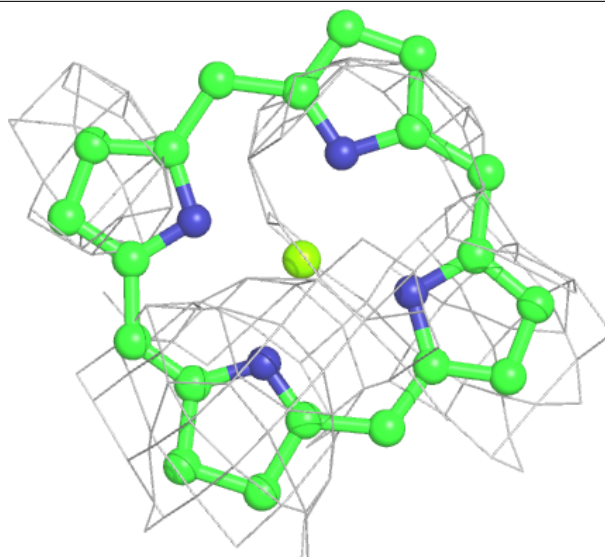
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

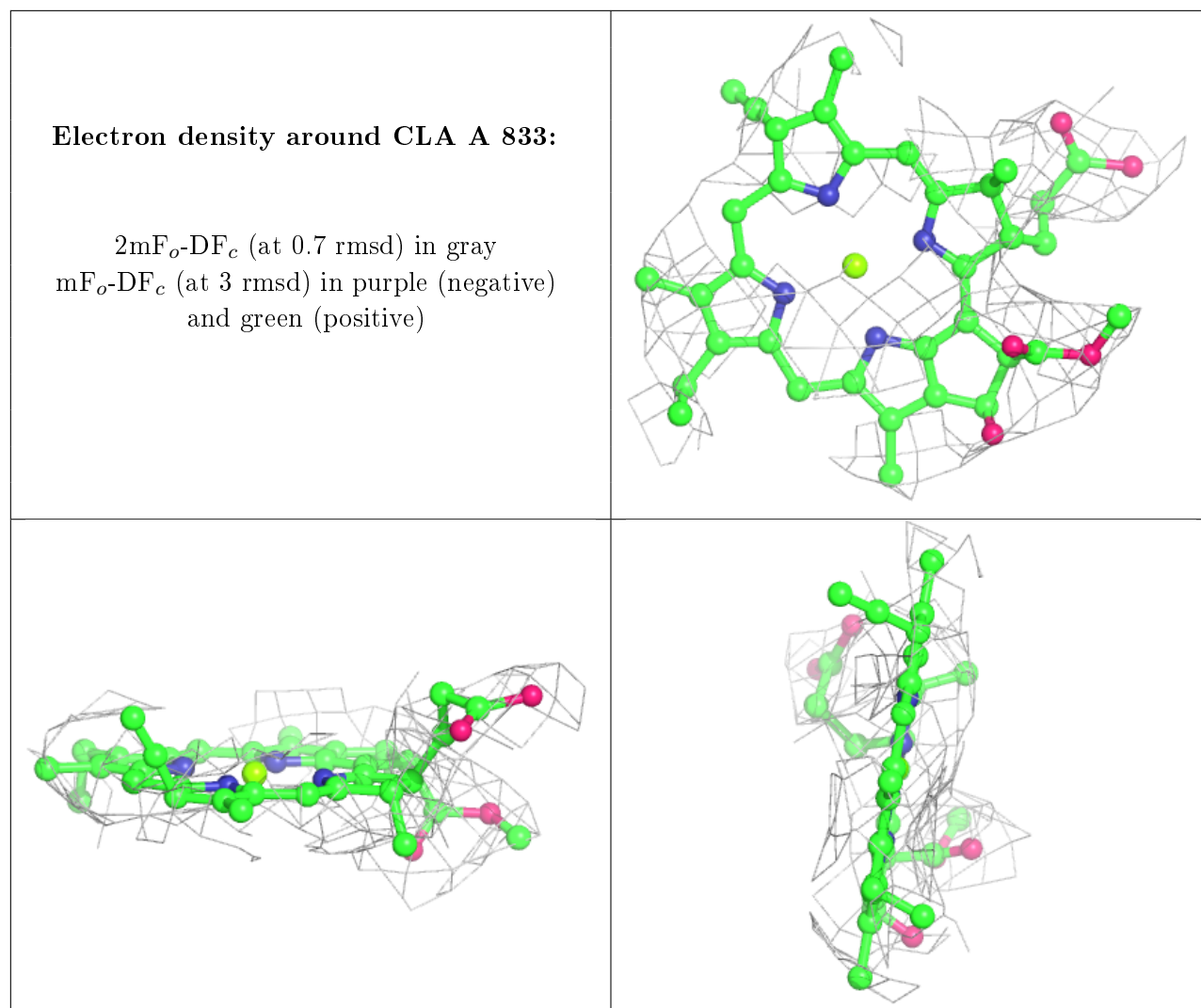


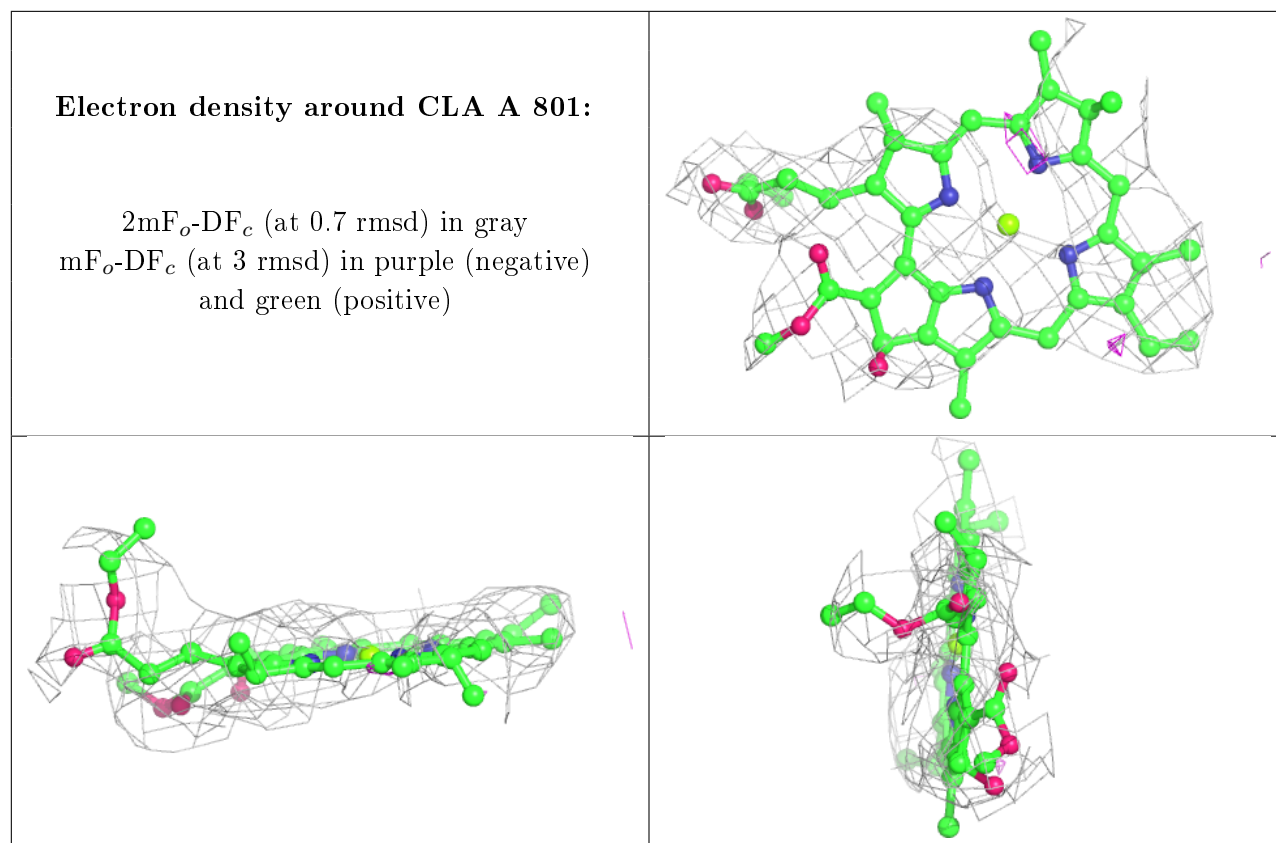


Electron density around CLA 2 304:

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

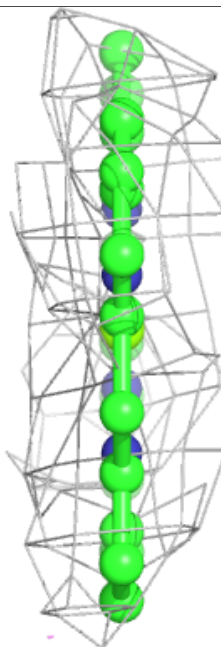
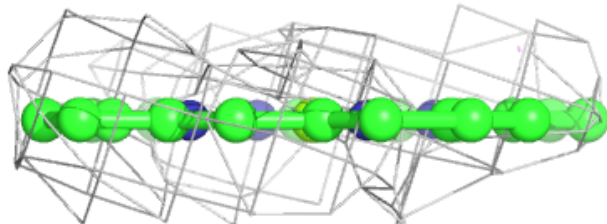
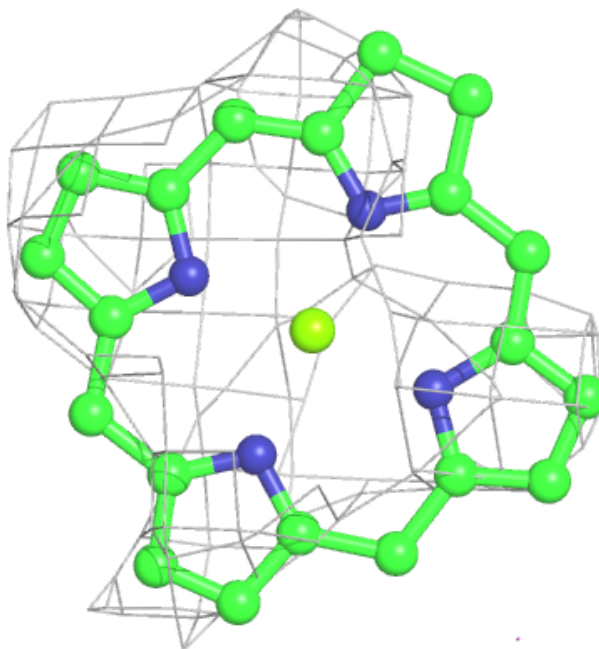






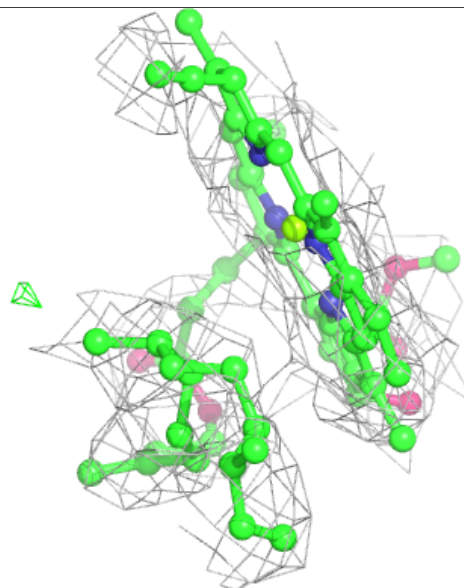
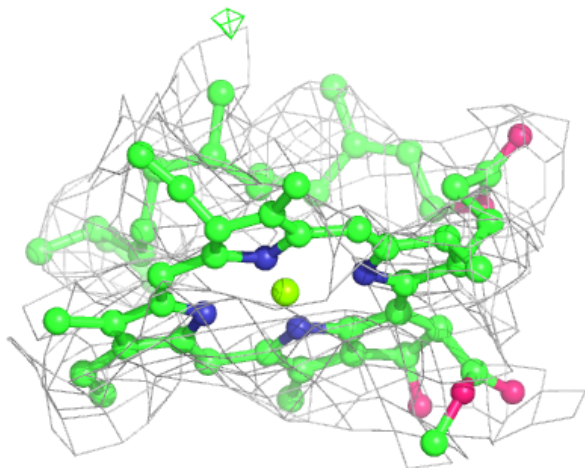
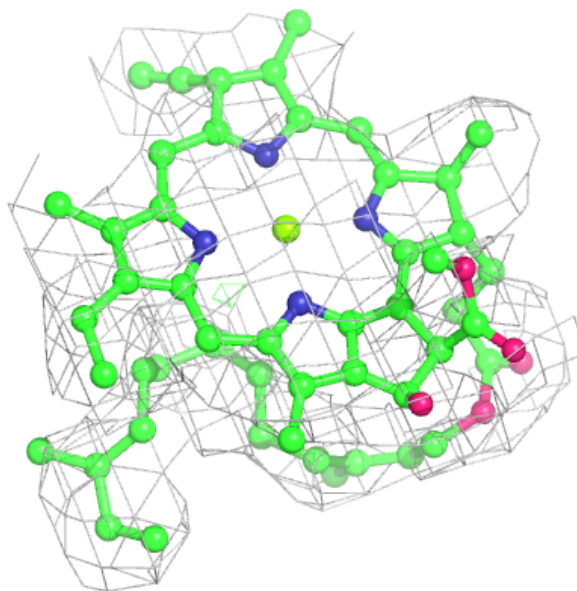
Electron density around CLA 2 301:

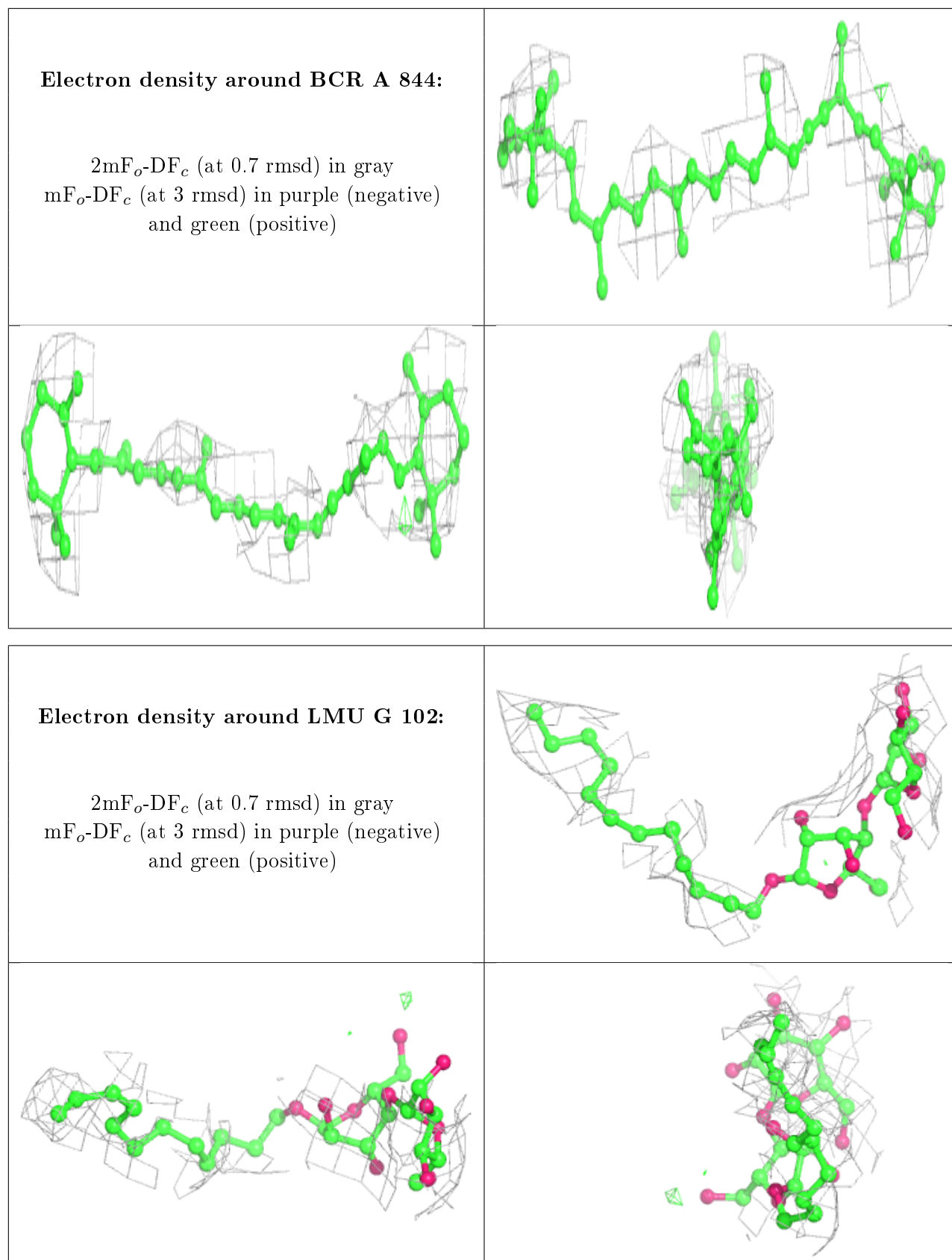
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 1 206:

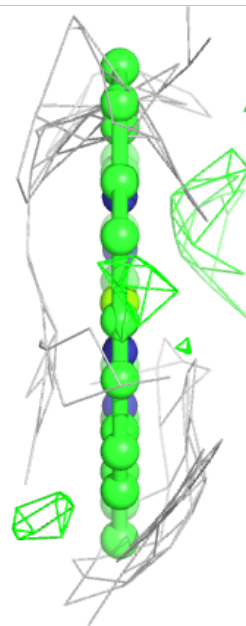
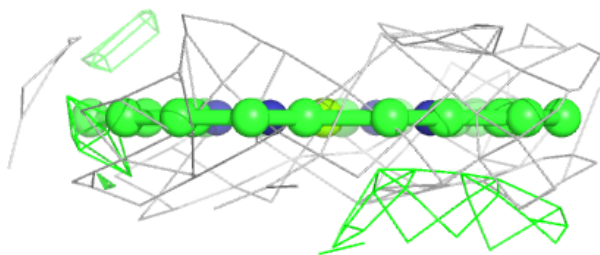
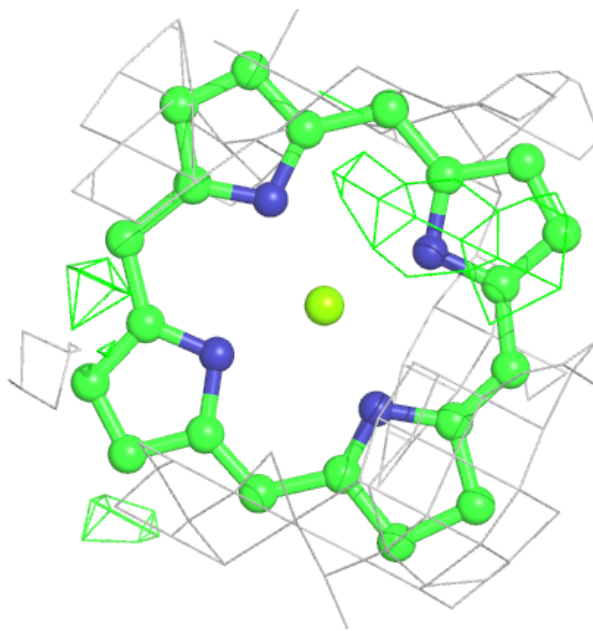
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





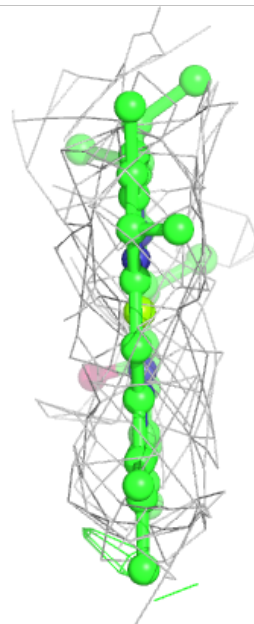
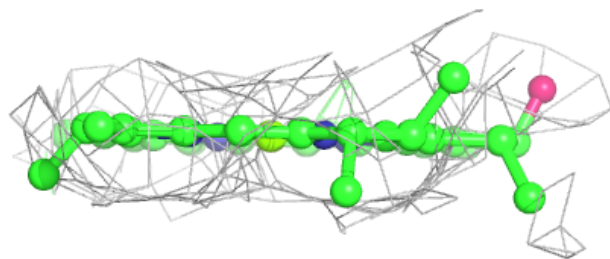
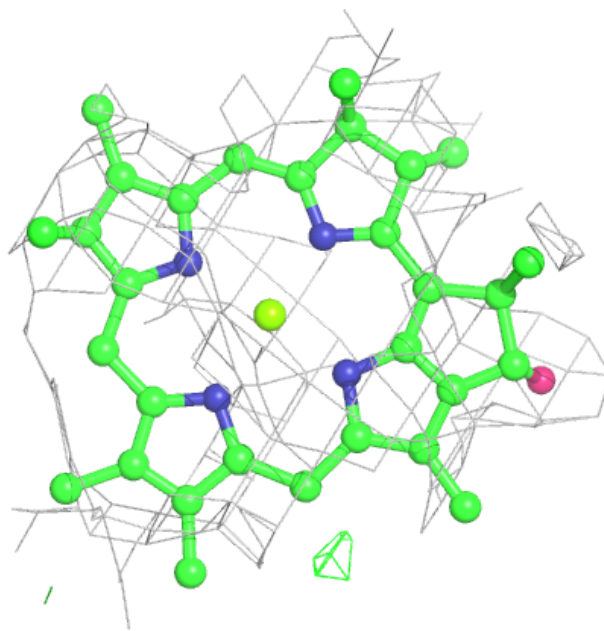
Electron density around CLA 1 208:

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



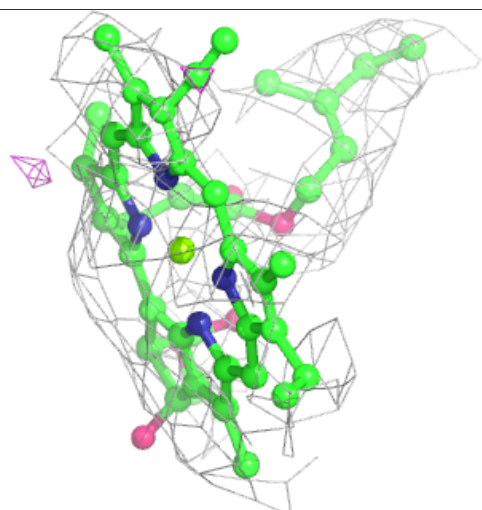
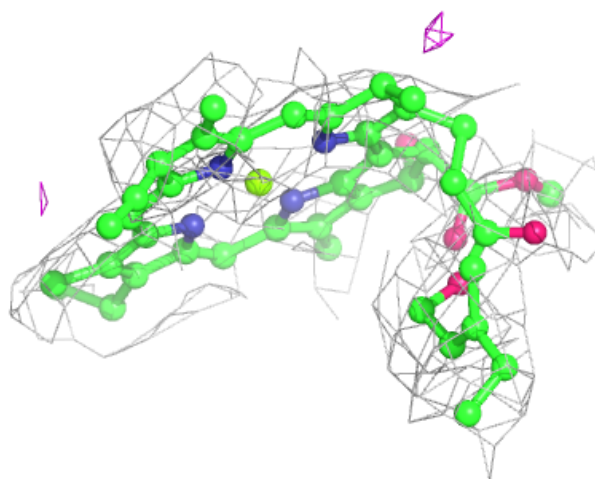
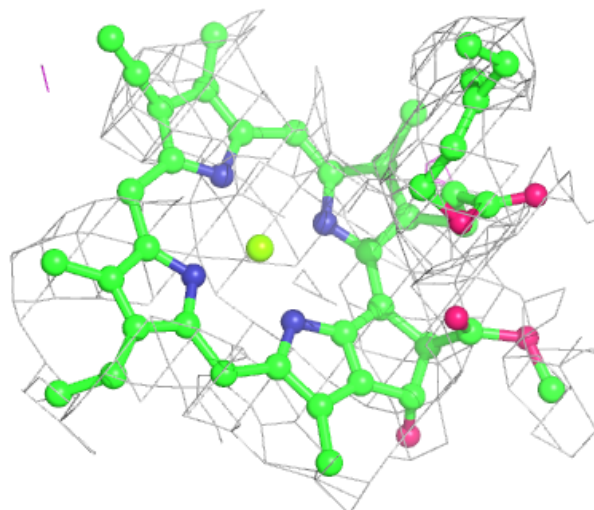
Electron density around CLA 1 205:

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



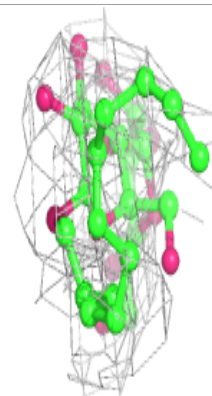
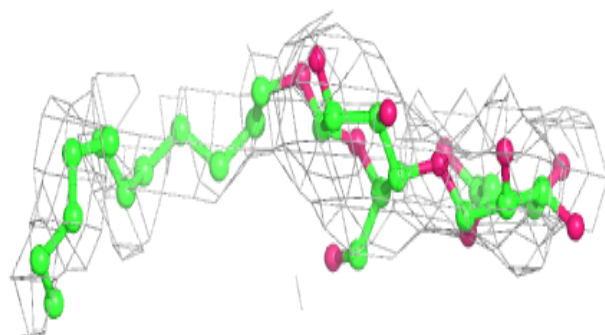
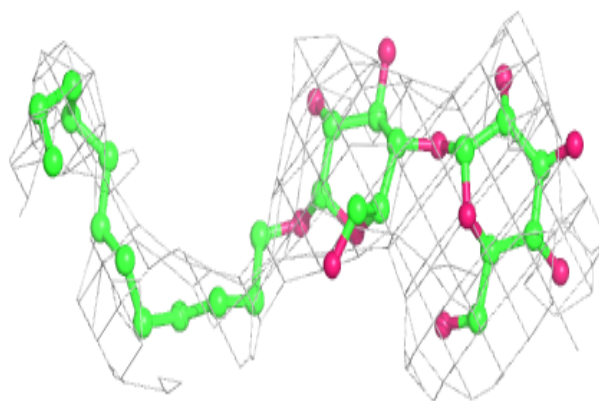
Electron density around CLA 1 207:

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

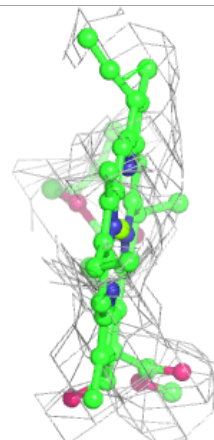
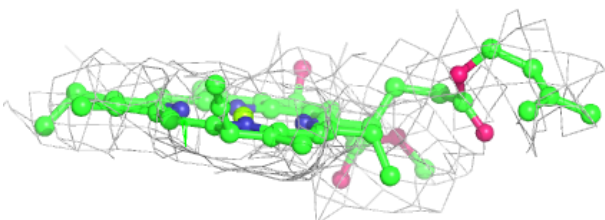
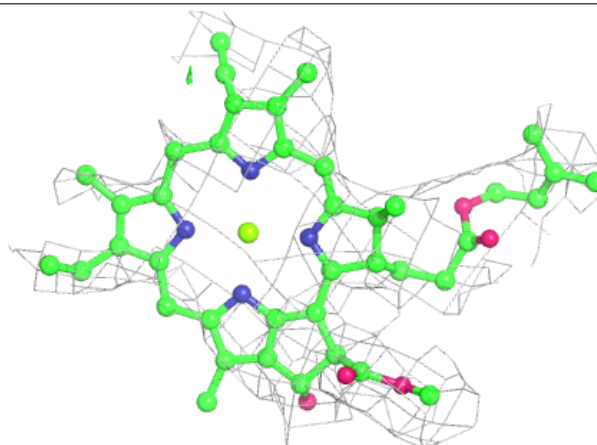


Electron density around LMU C 101:

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

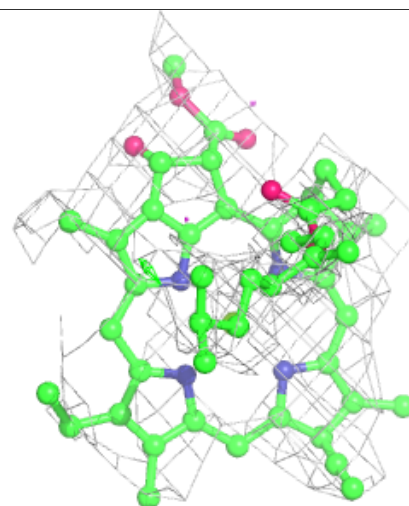
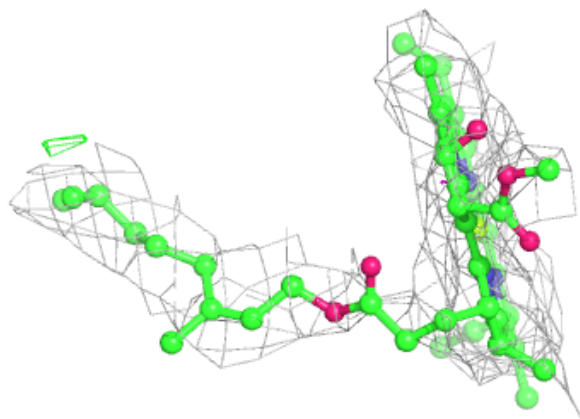
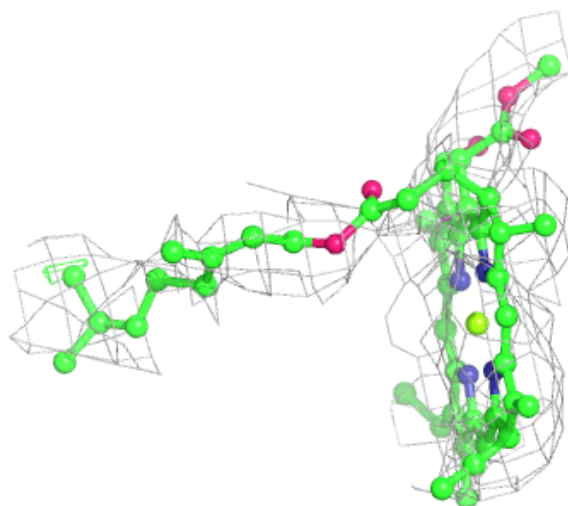
**Electron density around CLA 2 305:**

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



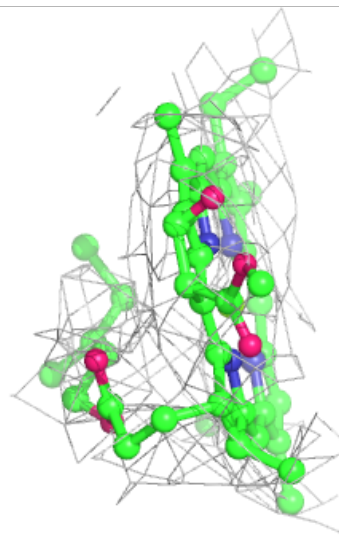
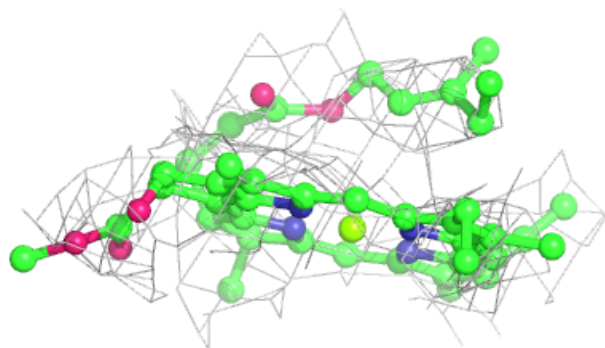
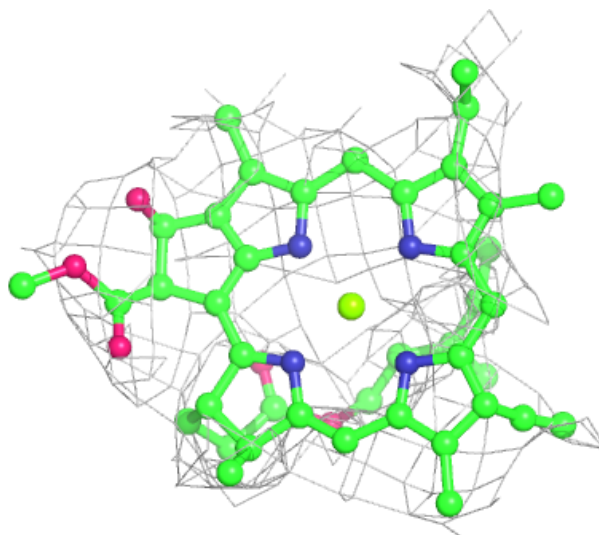
Electron density around CLA 4 301:

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



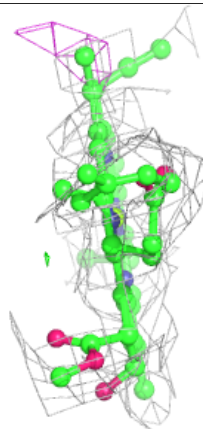
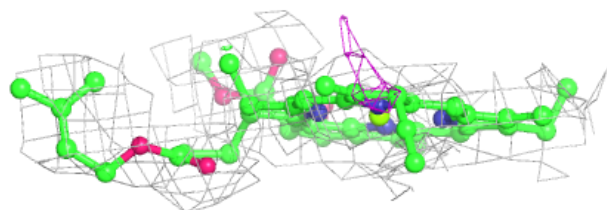
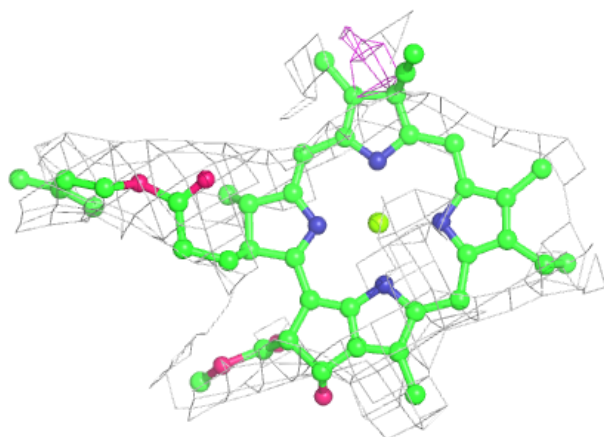
Electron density around CLA A 820:

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

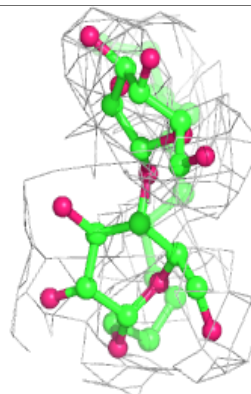
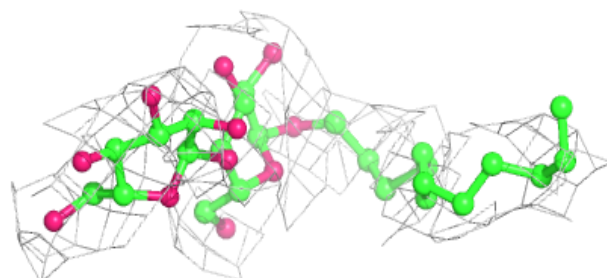
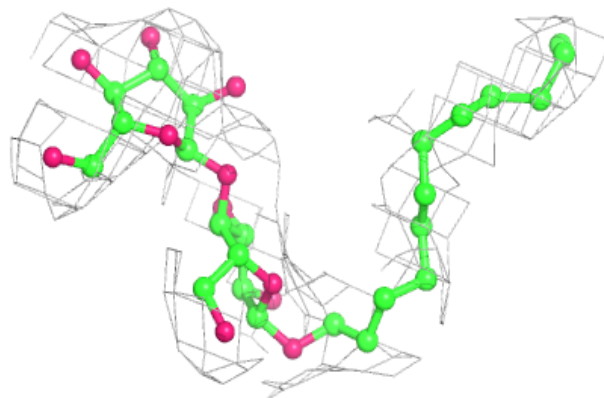


Electron density around CLA K 102:

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

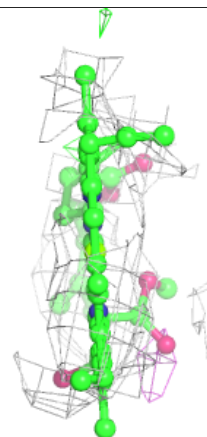
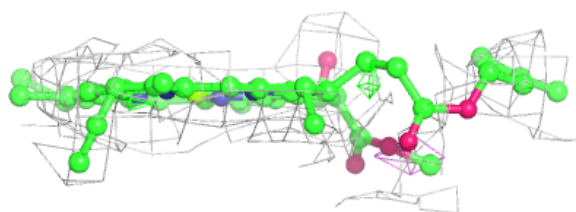
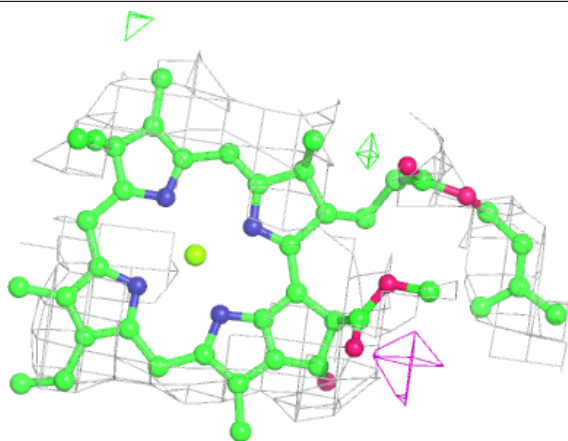
**Electron density around LMU L 206:**

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

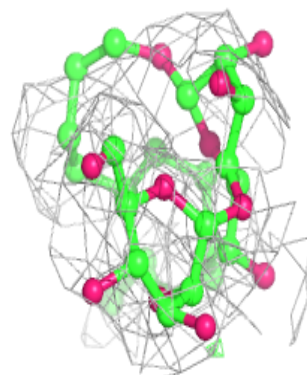
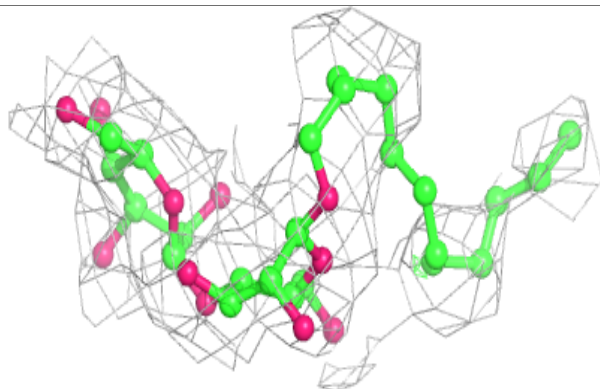
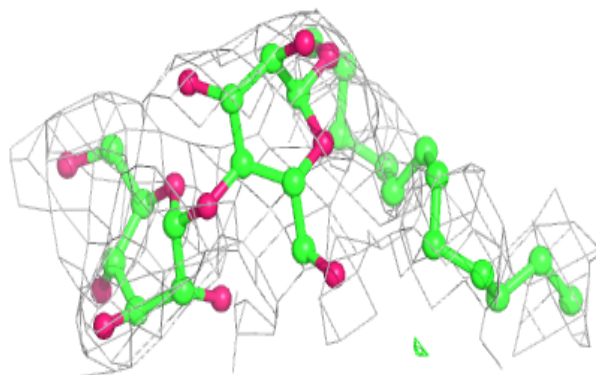


Electron density around CLA 2 311:

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

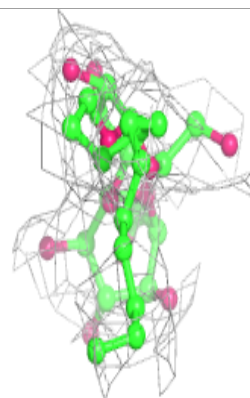
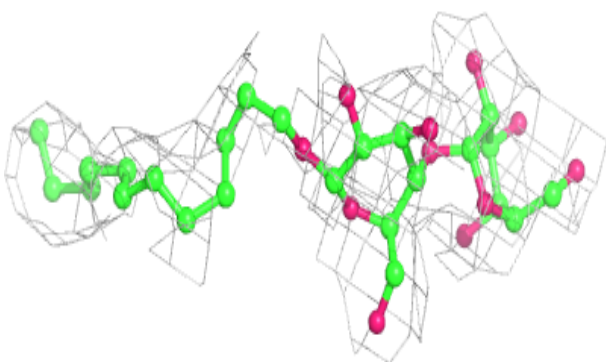
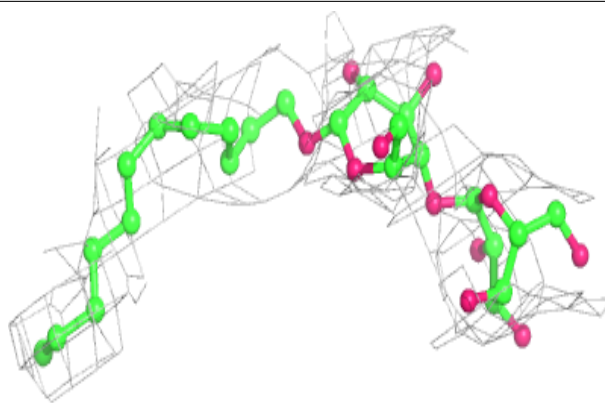
**Electron density around LMU L 212:**

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

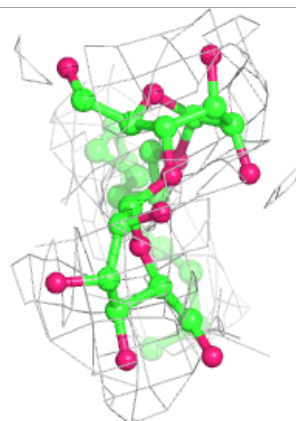
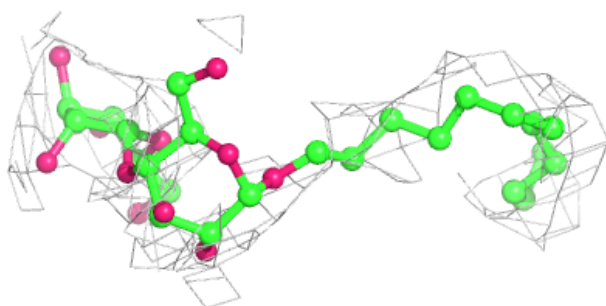
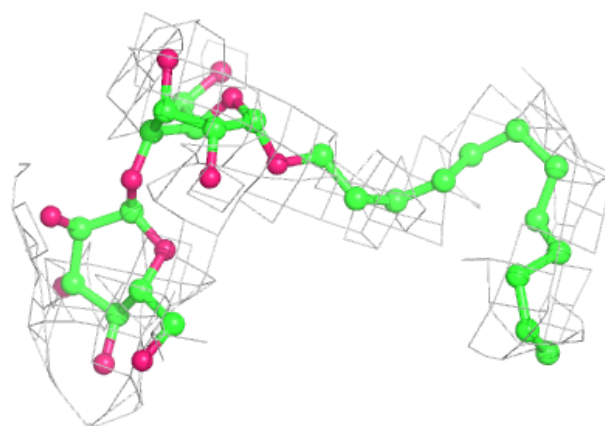


Electron density around LMU 2 320:

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

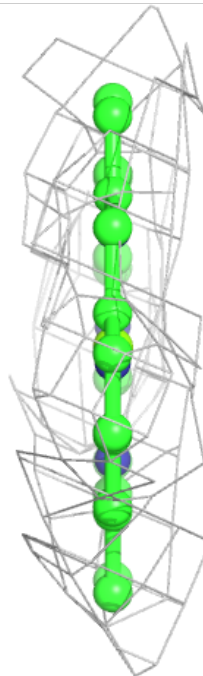
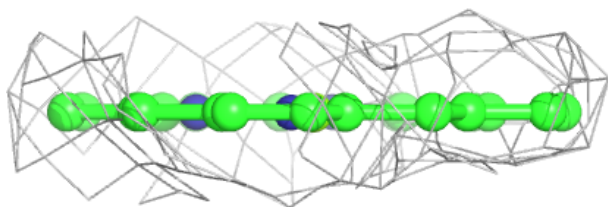
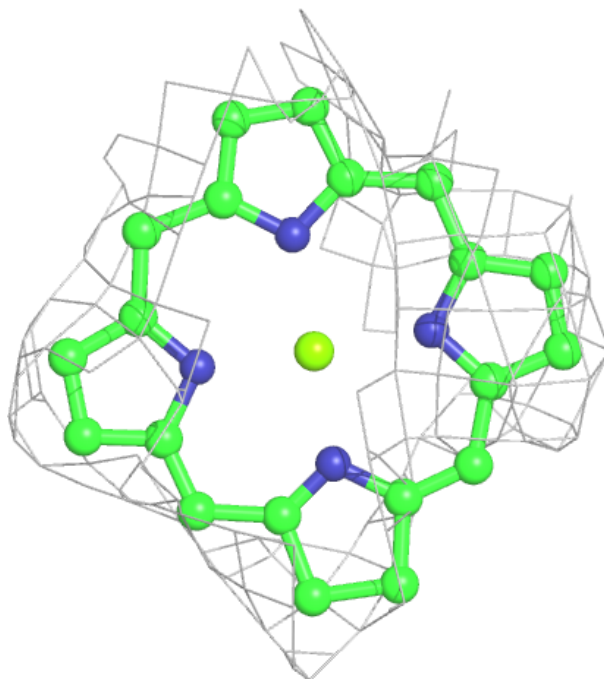
**Electron density around LMU K 105:**

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



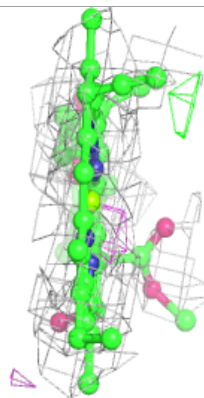
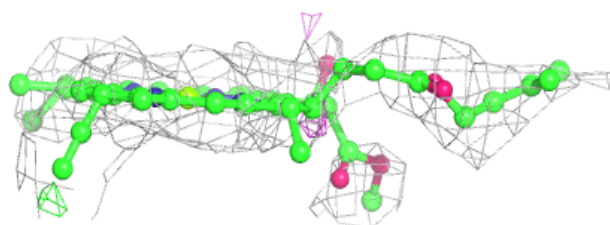
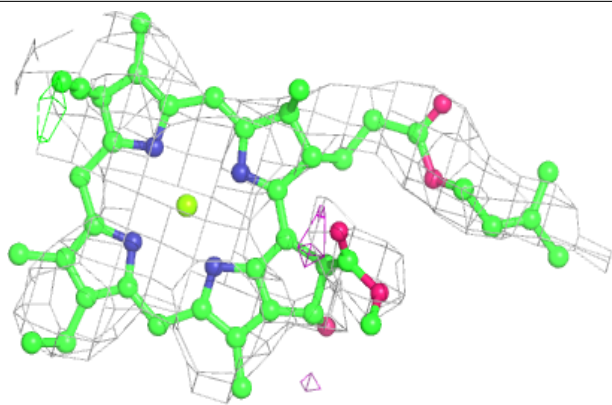
Electron density around CLA 3 317:

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



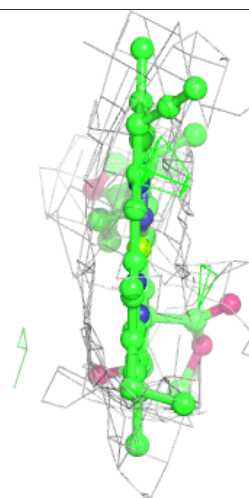
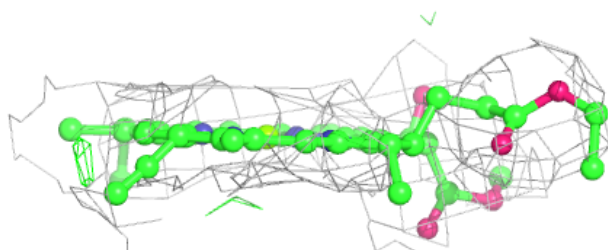
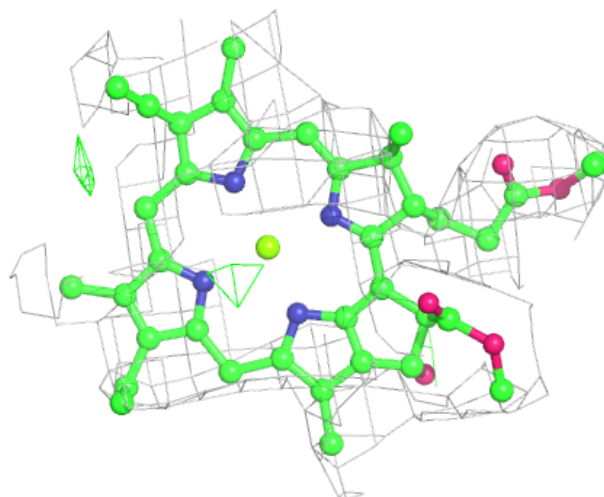
Electron density around CLA 4 305:

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



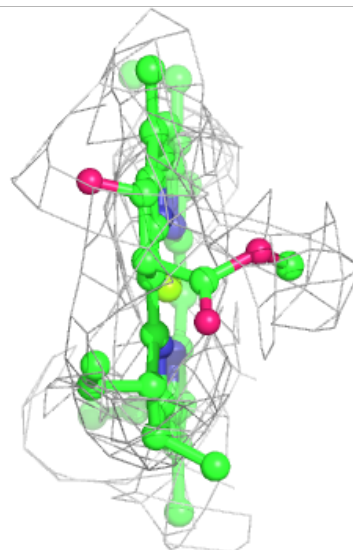
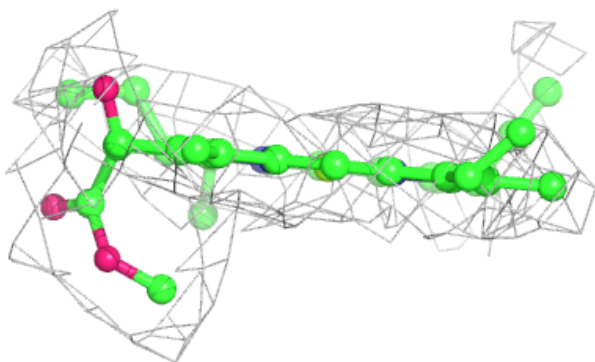
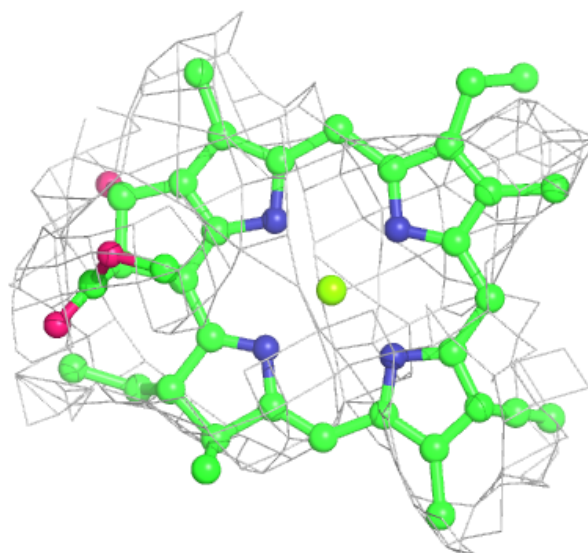
Electron density around CLA 1 203:

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



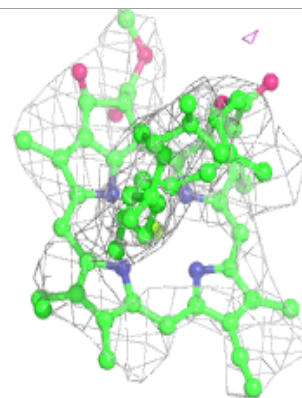
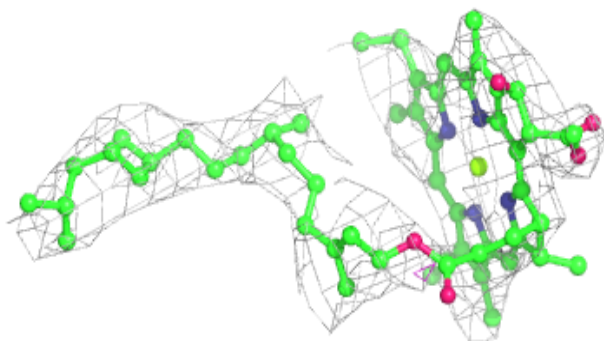
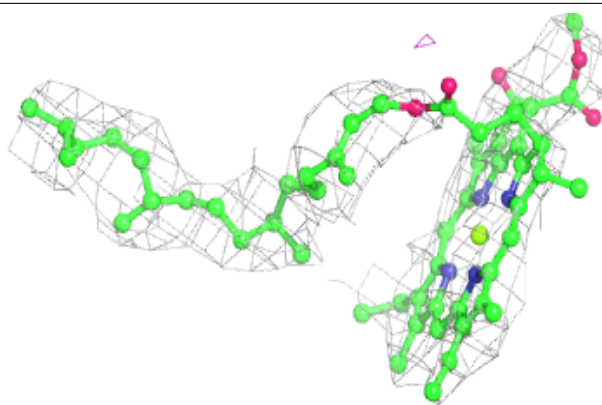
Electron density around CLA 3 307:

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

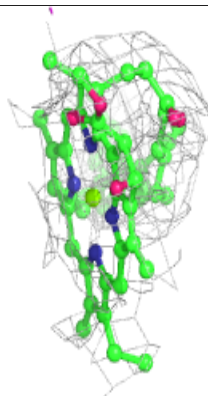
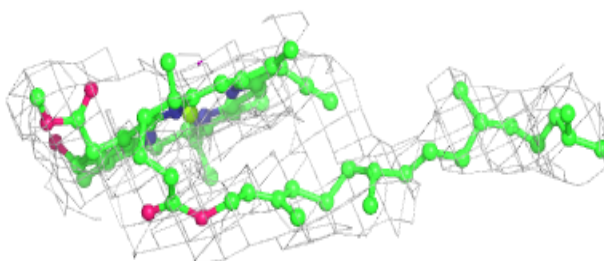
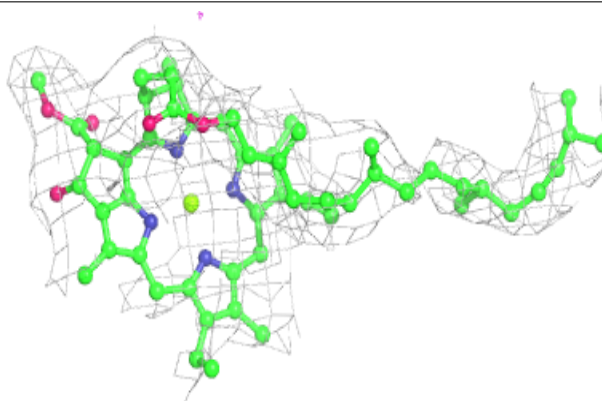


Electron density around CLA A 811:

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

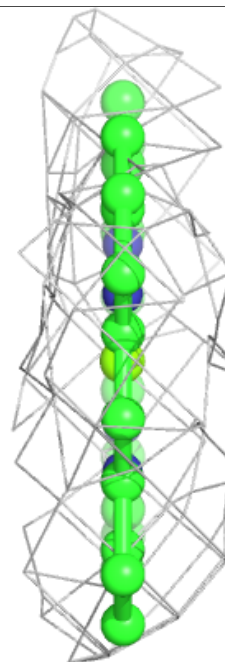
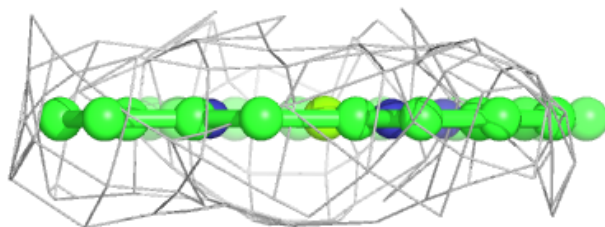
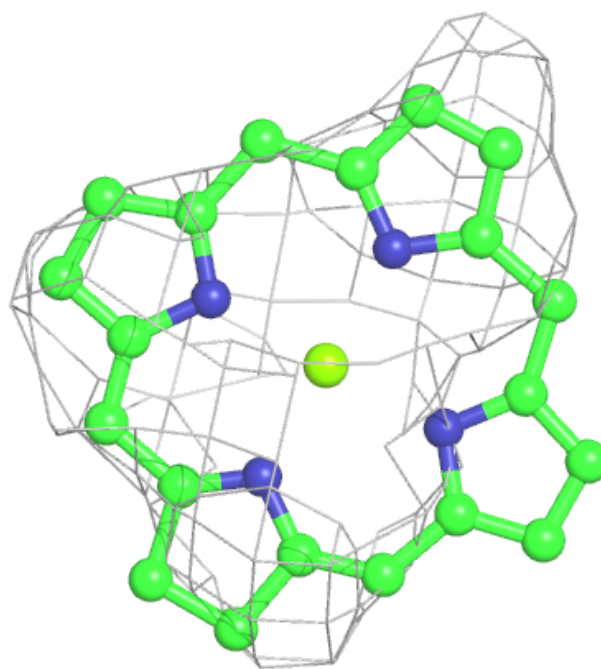
**Electron density around CLA 2 307:**

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



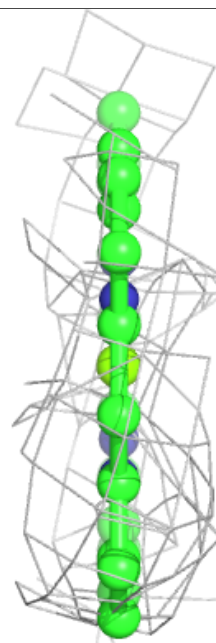
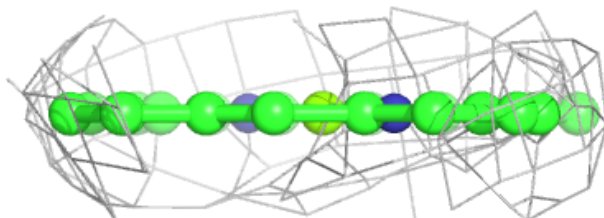
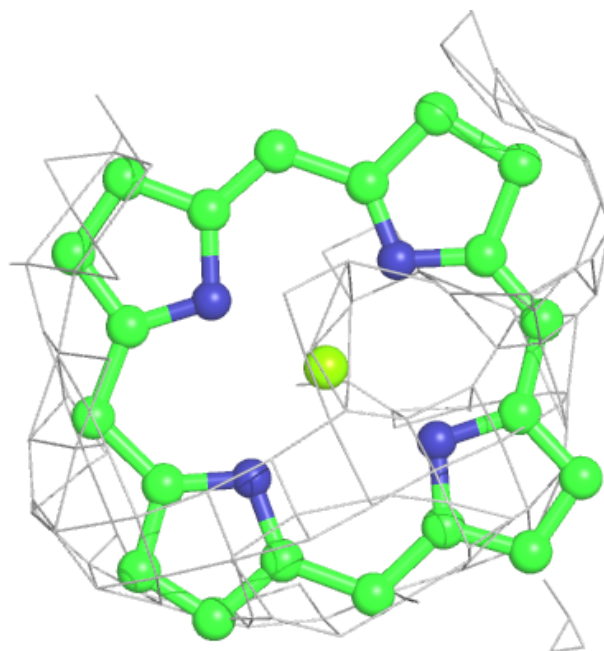
Electron density around CLA 3 316:

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



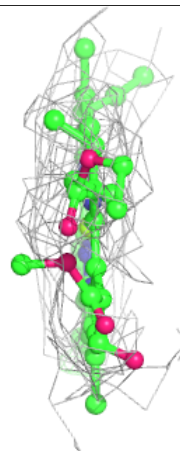
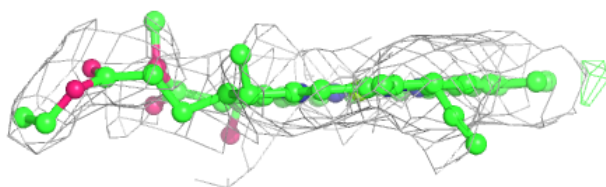
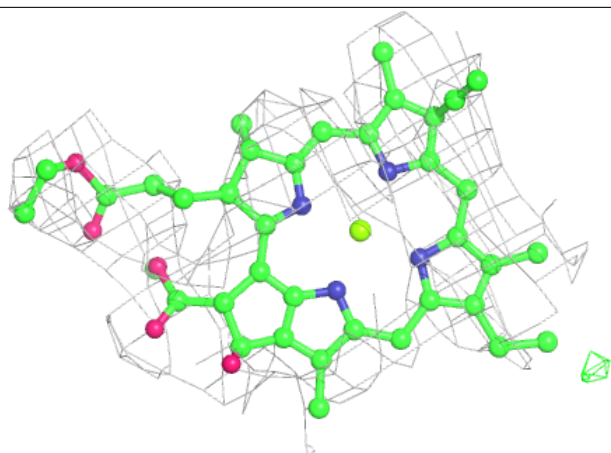
Electron density around CLA 3 306:

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



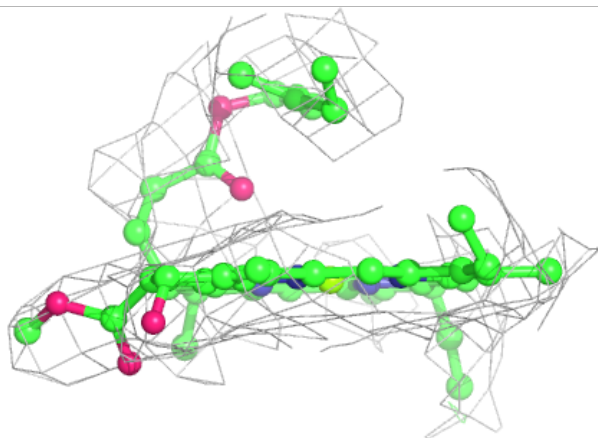
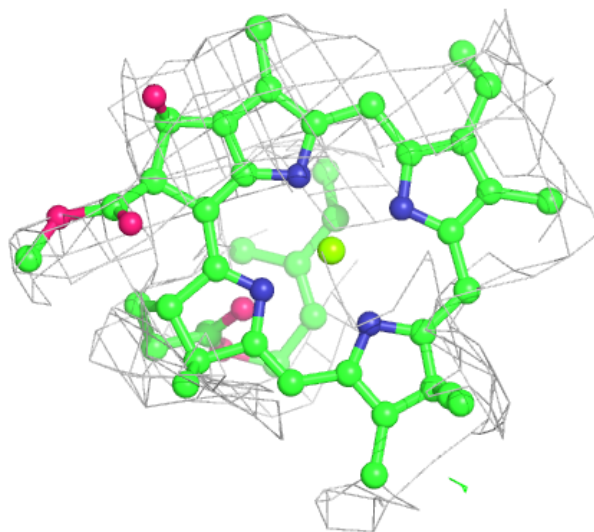
Electron density around CLA 4 318:

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



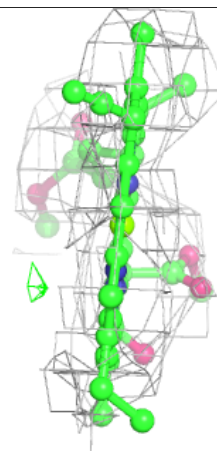
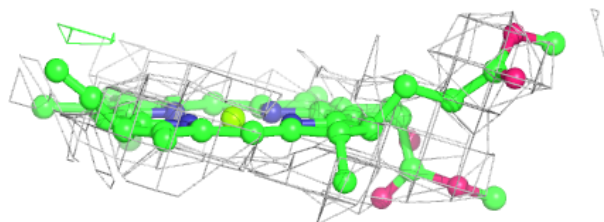
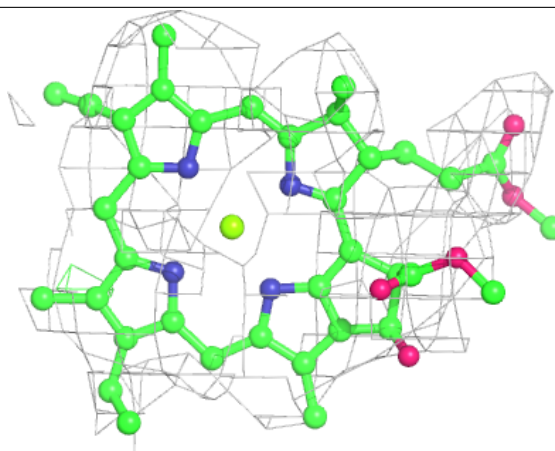
Electron density around CLA 2 302:

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



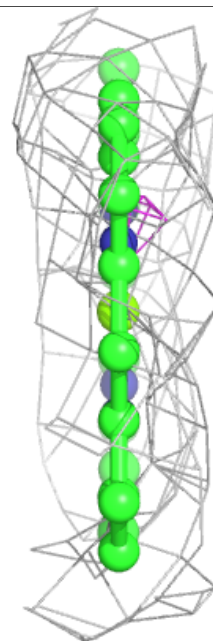
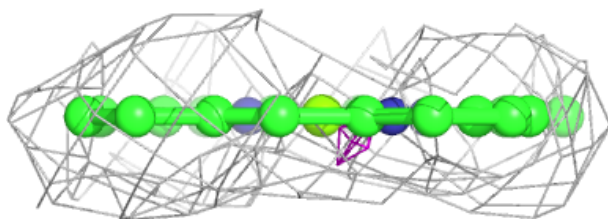
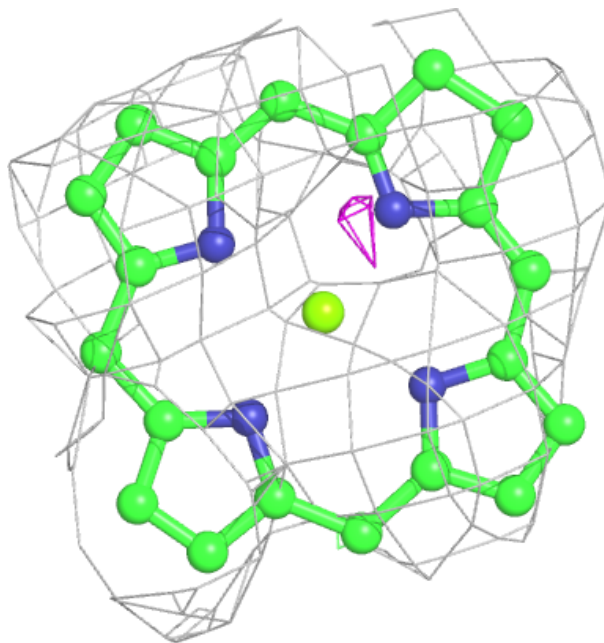
Electron density around CLA 4 315:

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



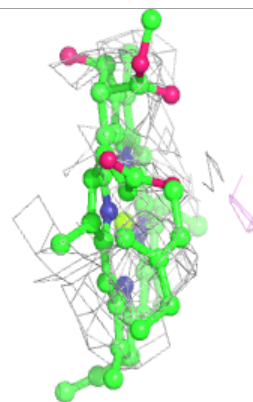
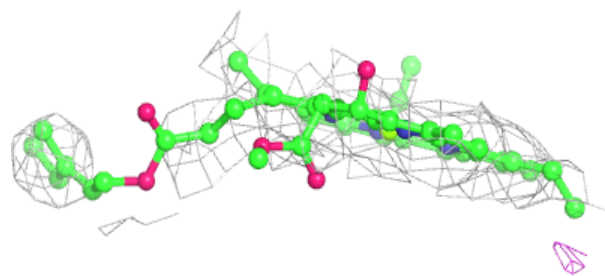
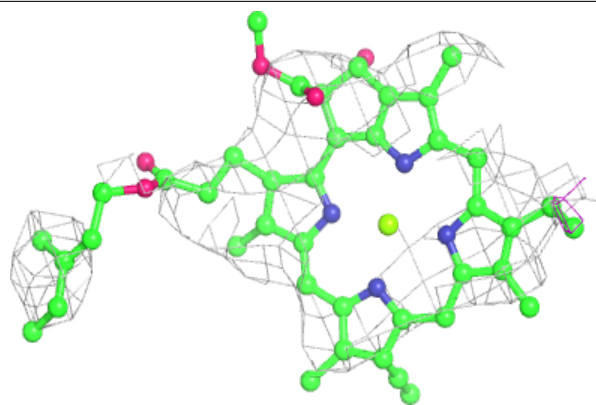
Electron density around CLA 4 314:

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

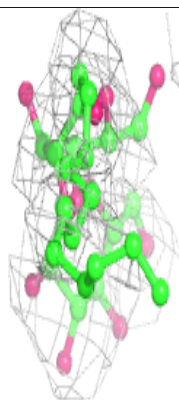
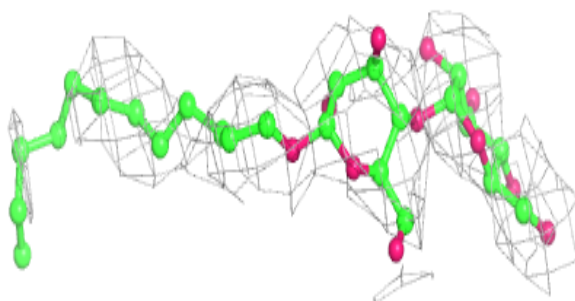
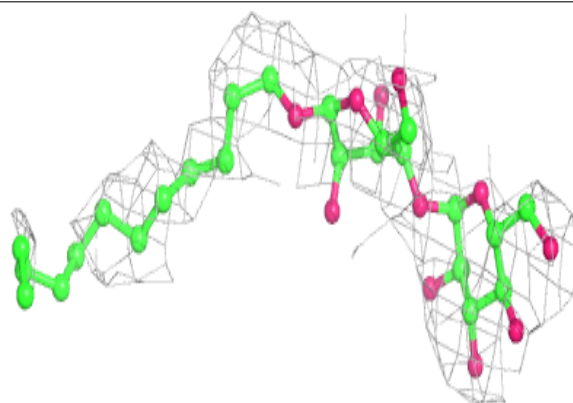


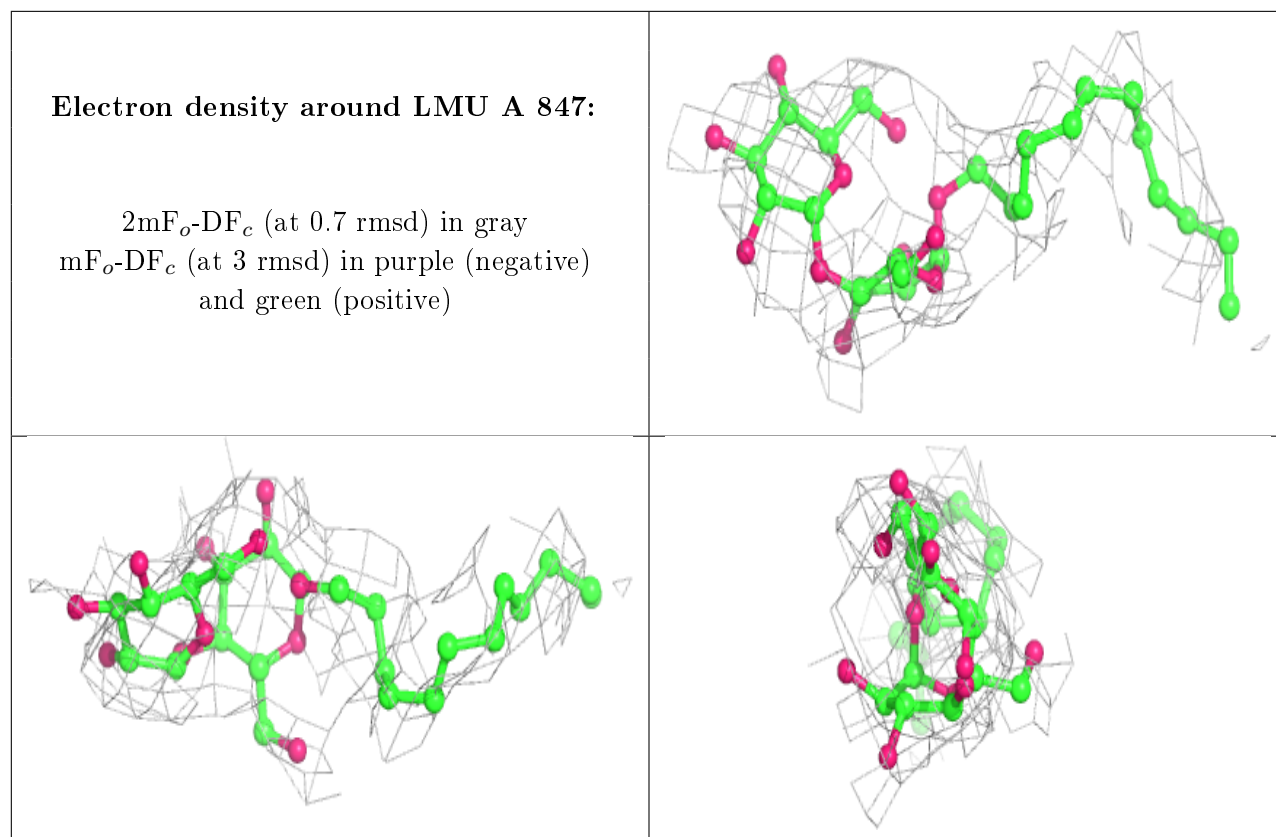
Electron density around CLA 1 213:

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

**Electron density around LMU 4 316:**

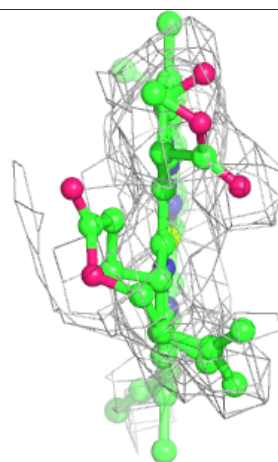
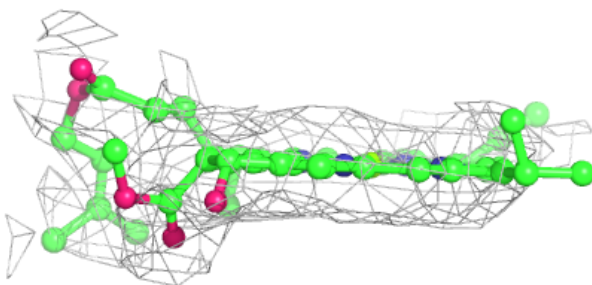
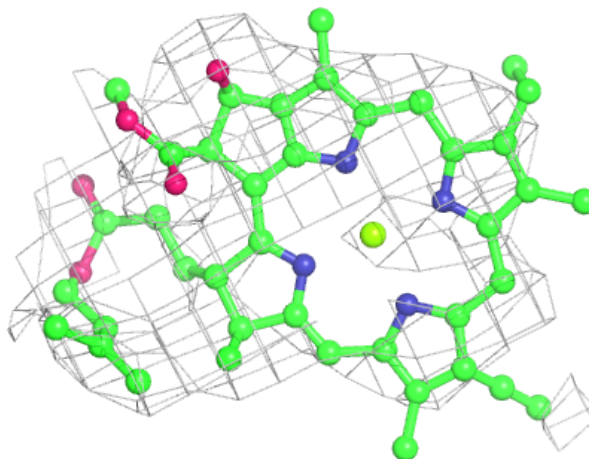
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





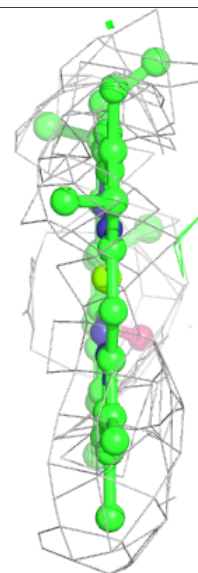
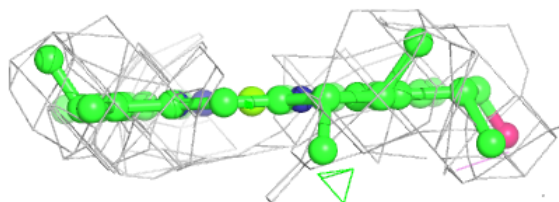
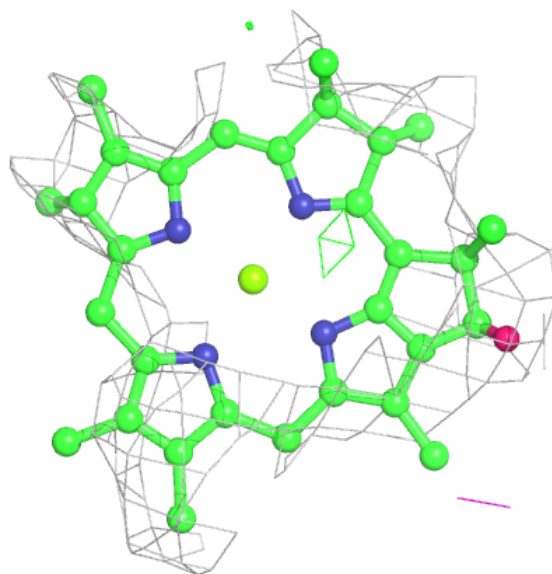
Electron density around CLA 2 315:

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



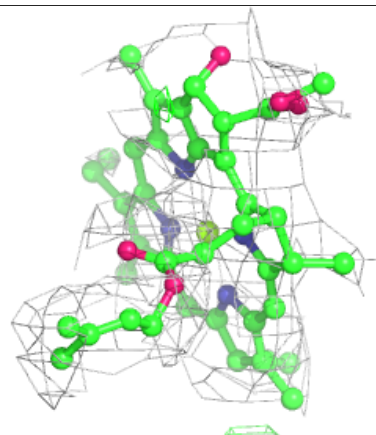
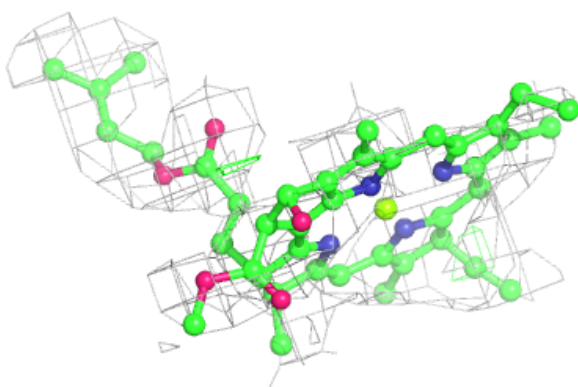
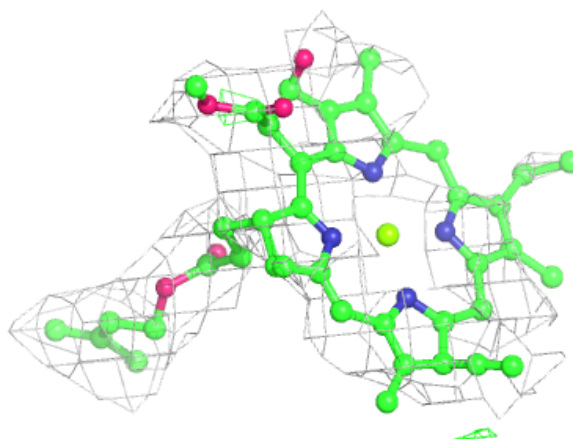
Electron density around CLA 1 210:

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

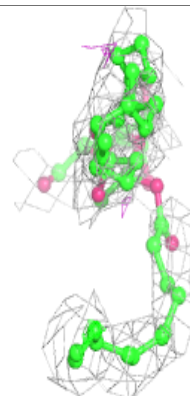
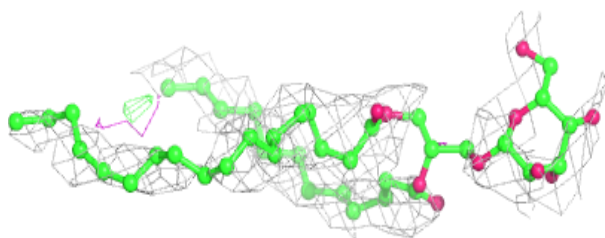
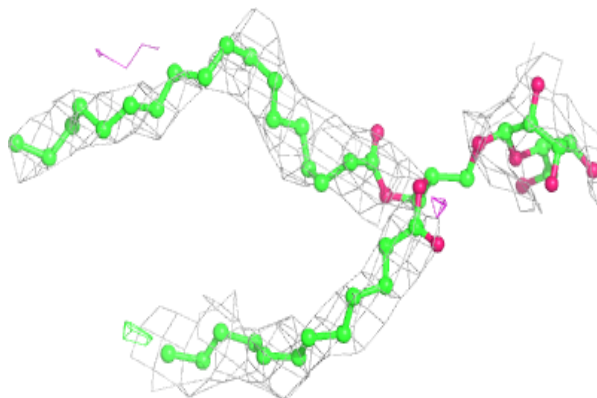


Electron density around CLA 2 310:

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

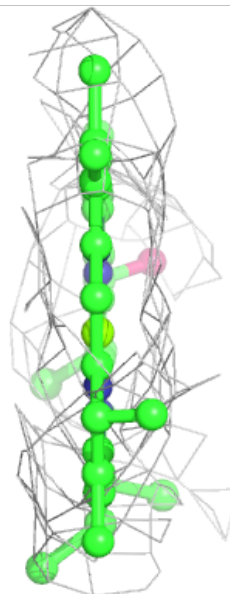
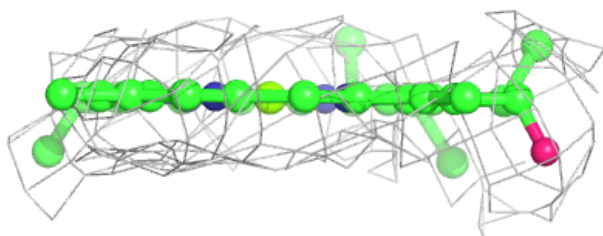
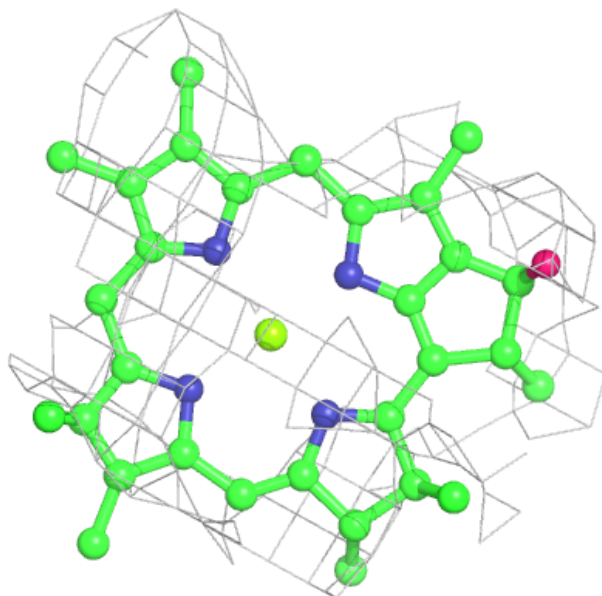
**Electron density around LMG B 848:**

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



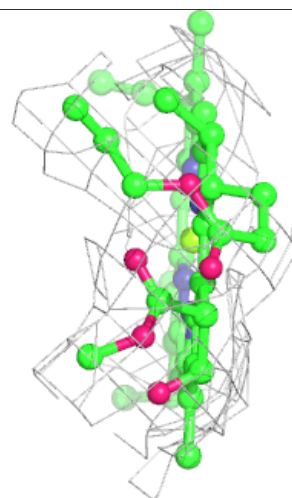
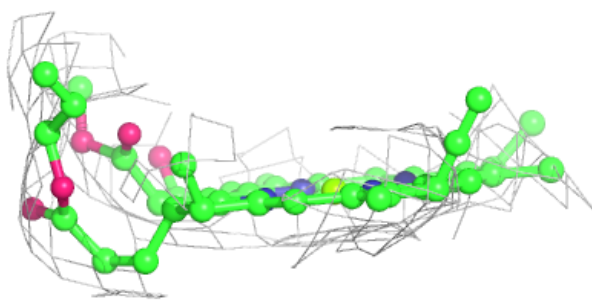
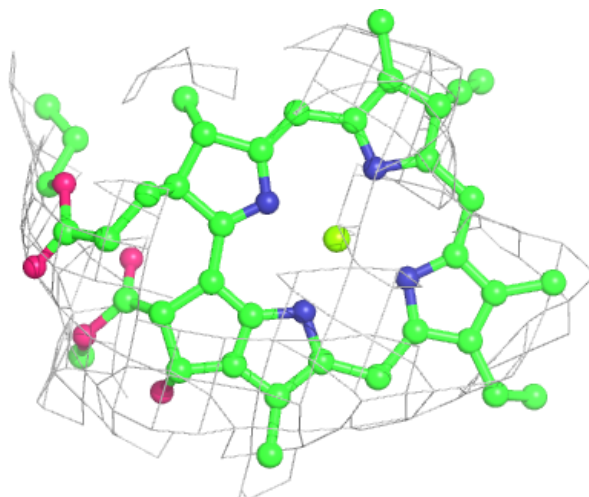
Electron density around CLA 3 301:

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



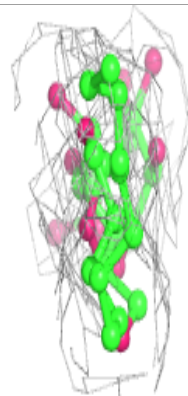
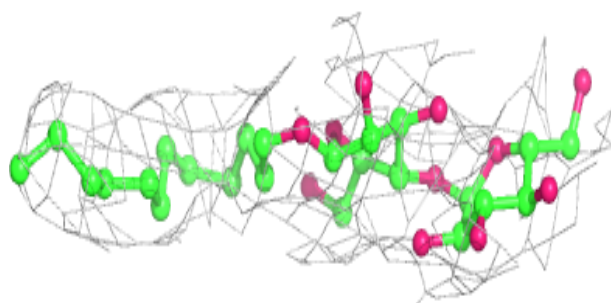
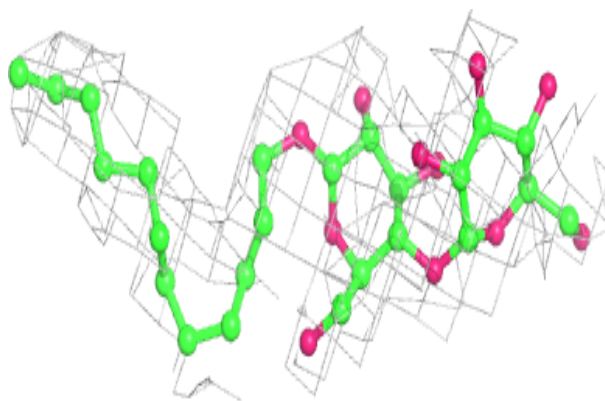
Electron density around CLA J 101:

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

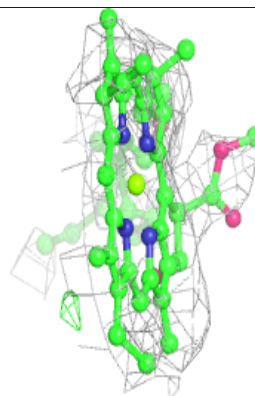
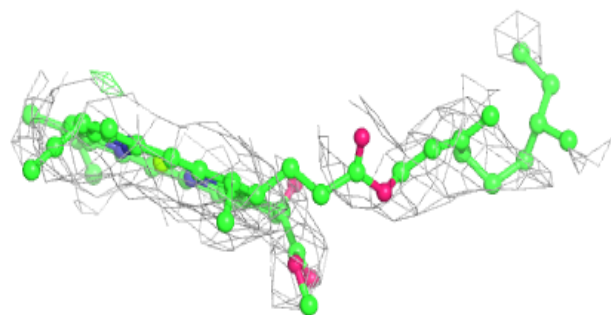
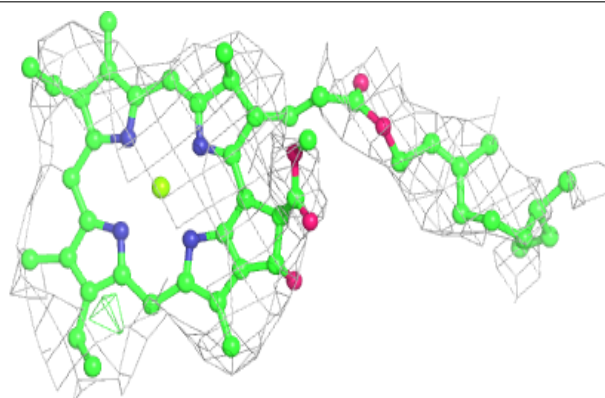


Electron density around LMU H 104:

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

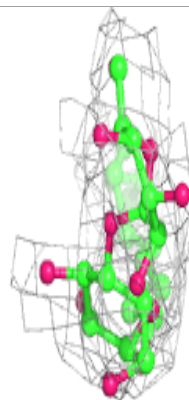
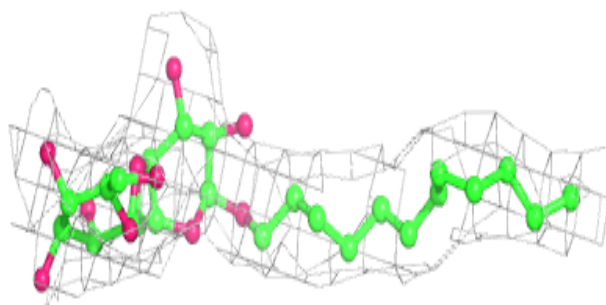
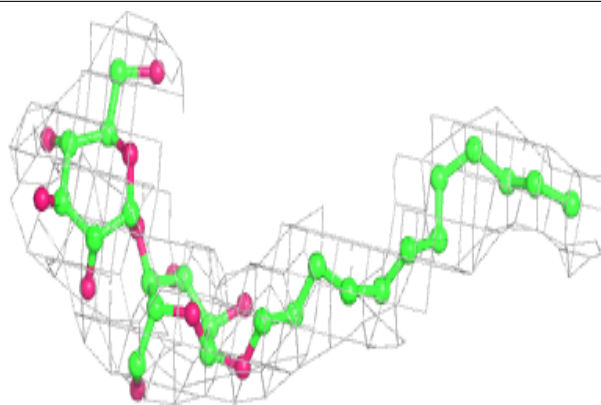
**Electron density around CLA K 104:**

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

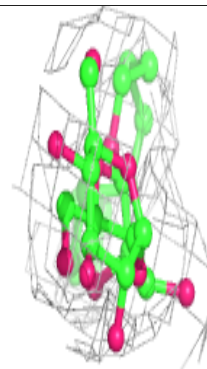
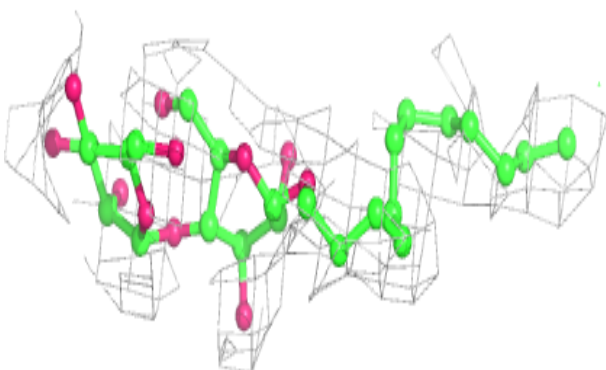
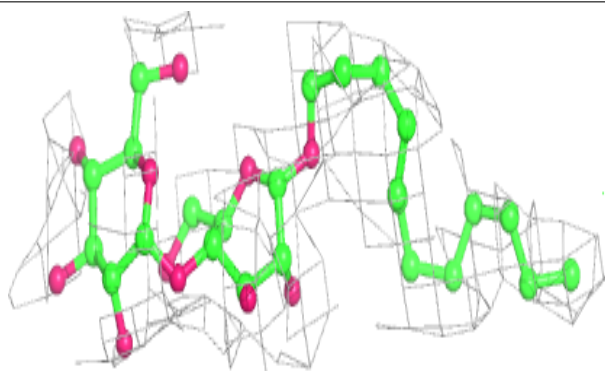


Electron density around LMU 4 321:

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

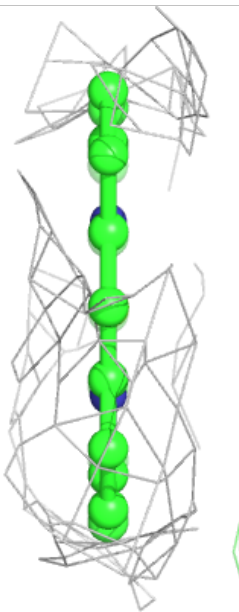
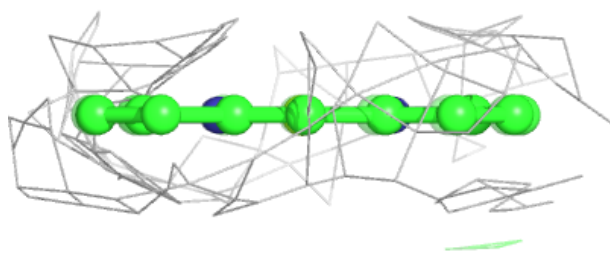
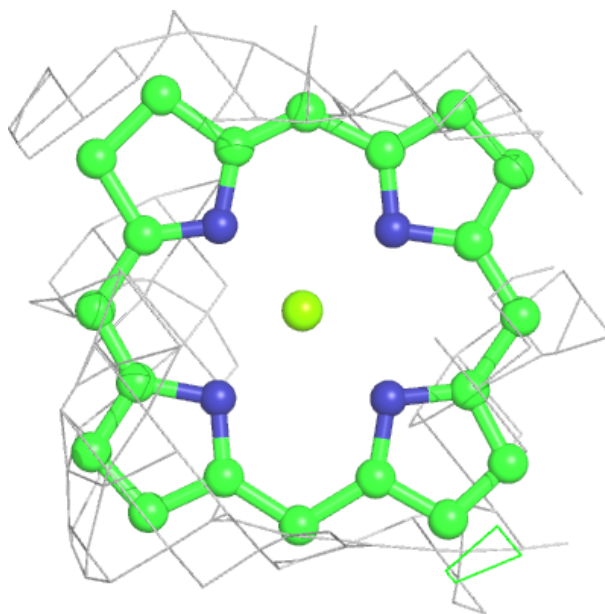
**Electron density around LMU R 102:**

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



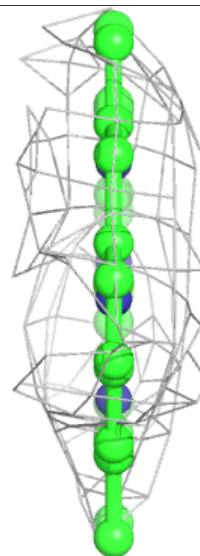
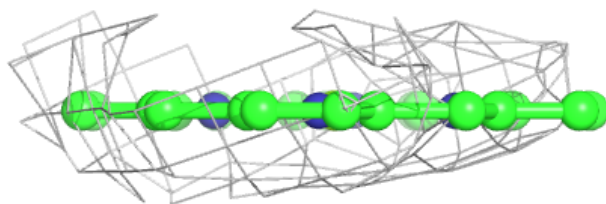
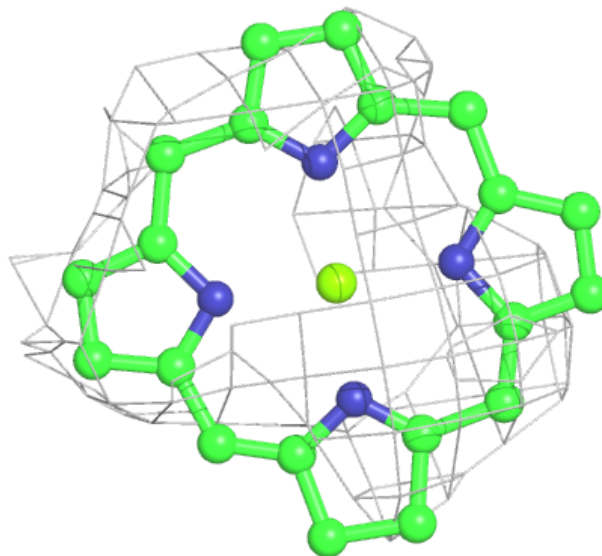
Electron density around CLA 2 306:

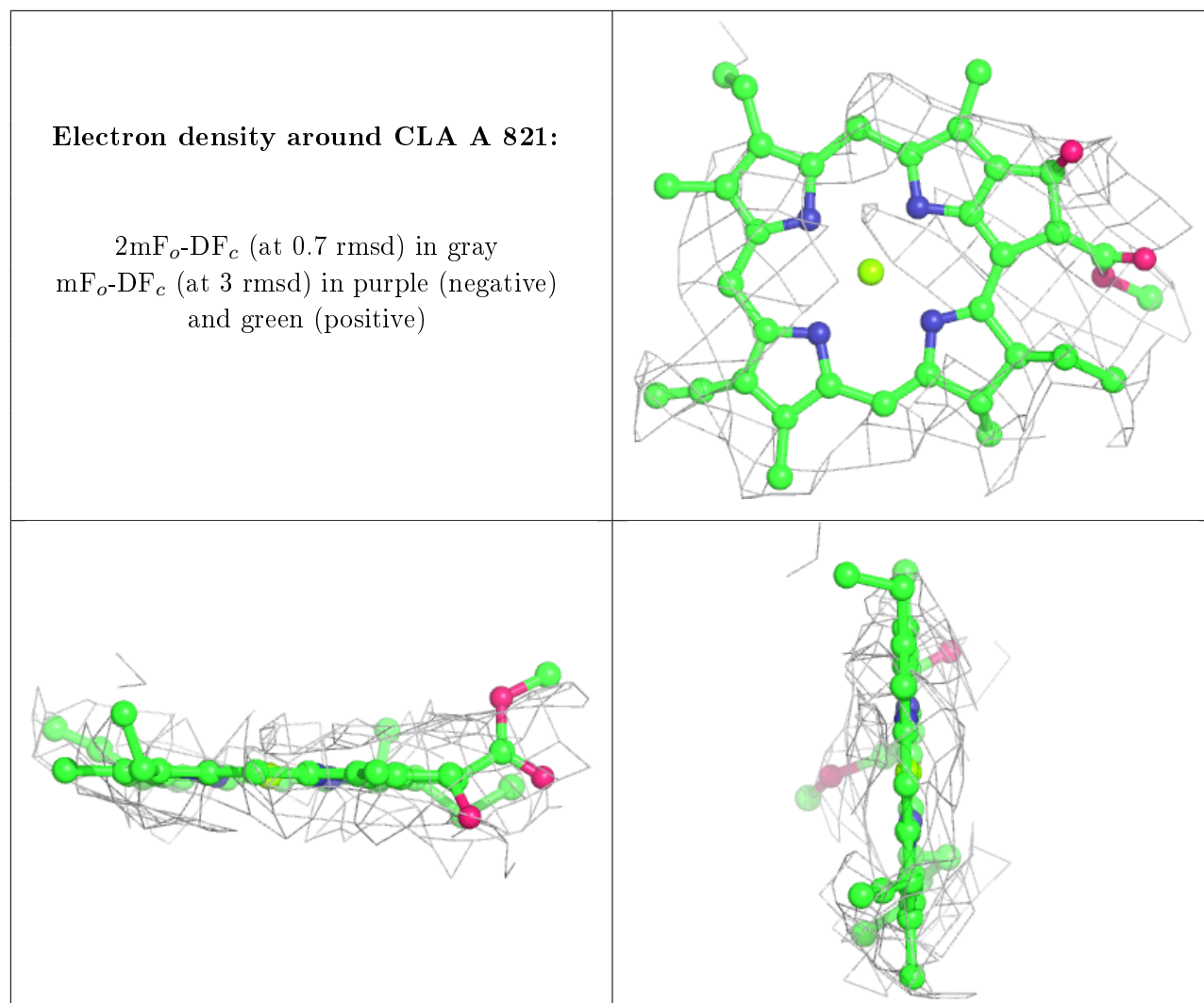
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 4 309:

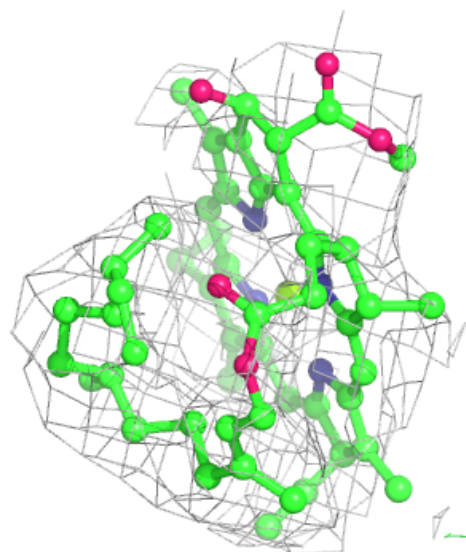
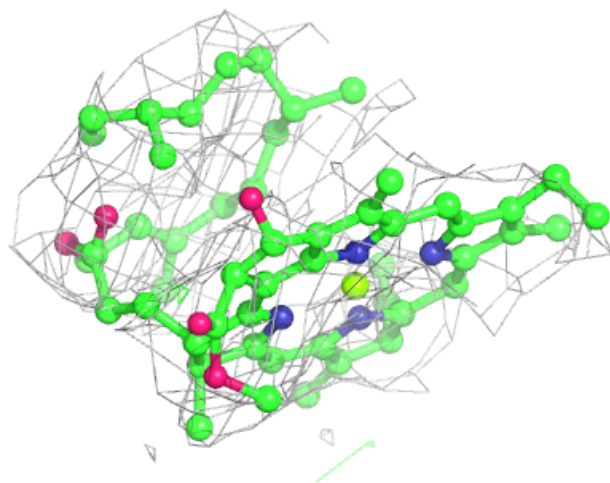
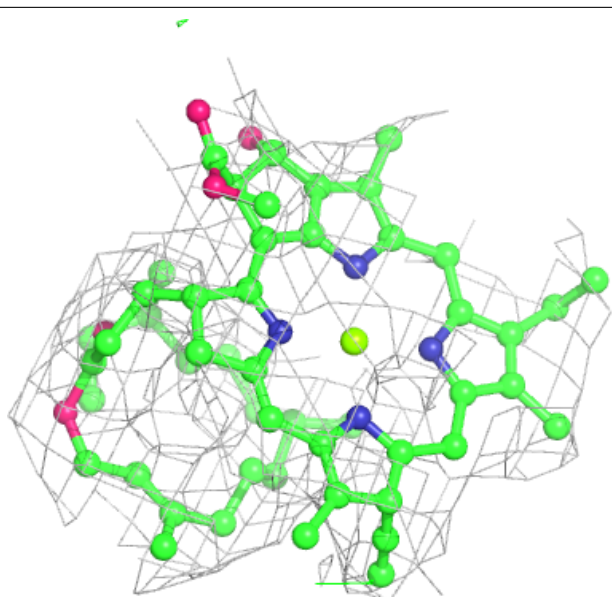
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





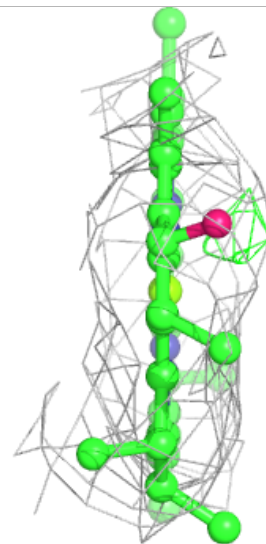
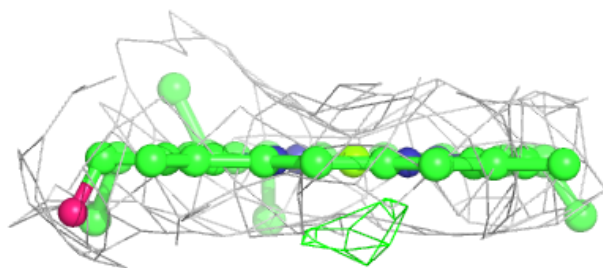
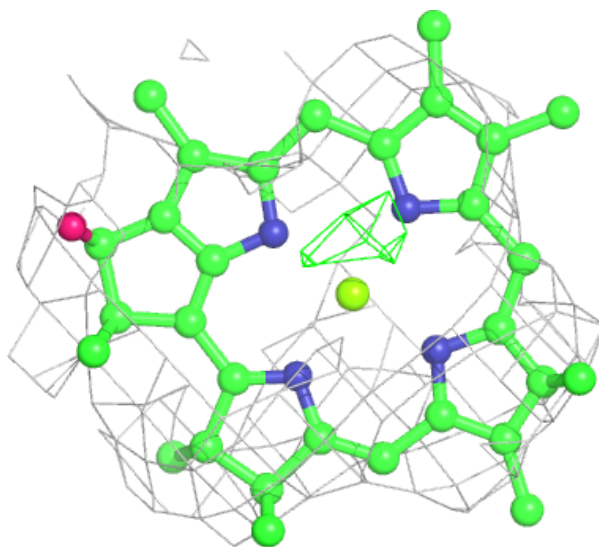
Electron density around CLA J 103:

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



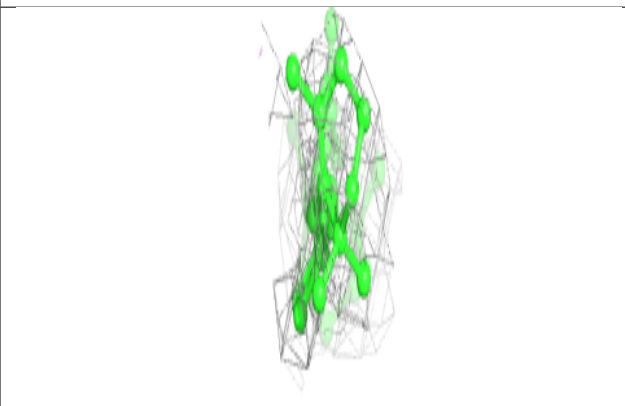
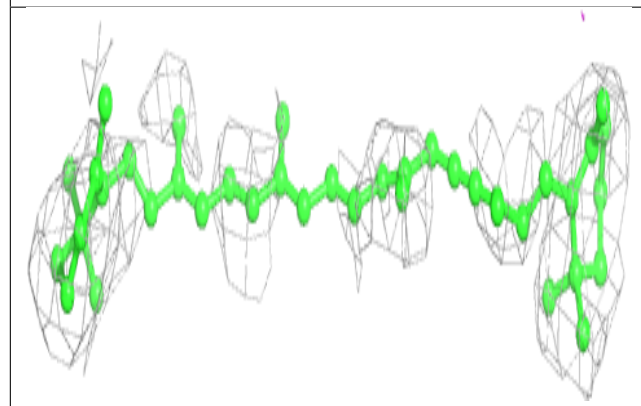
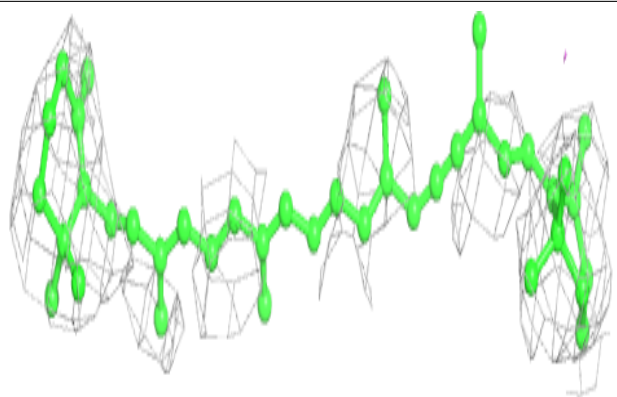
Electron density around CLA 4 302:

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



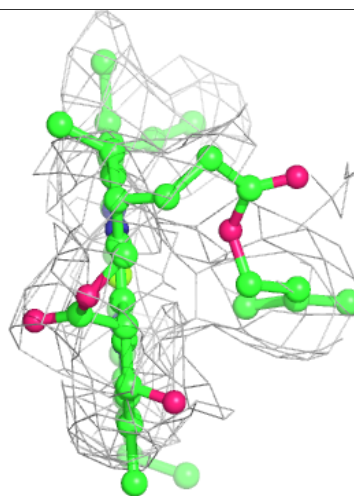
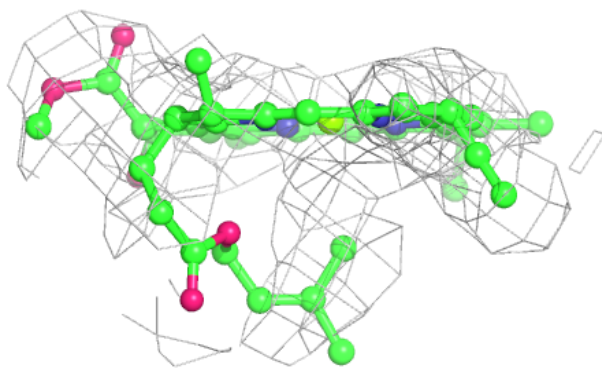
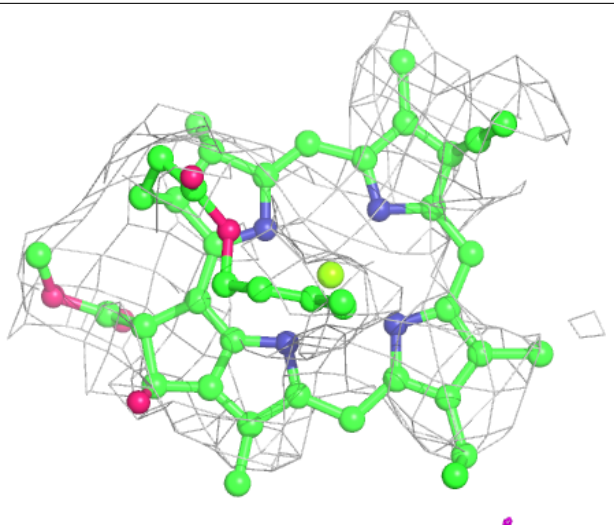
Electron density around BCR J 102:

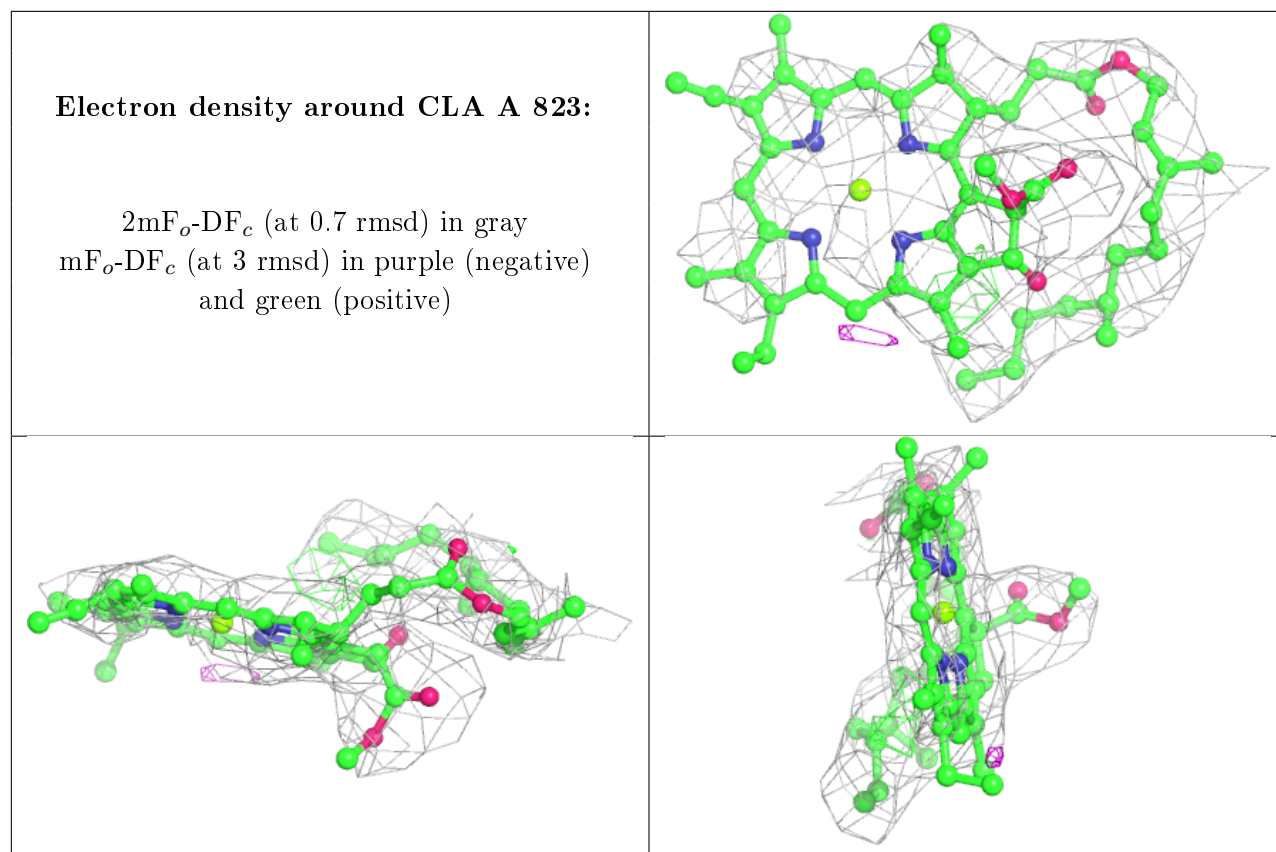
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA L 208:

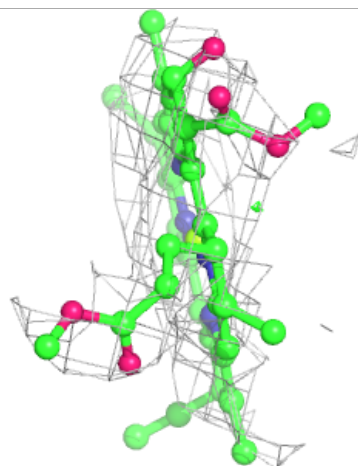
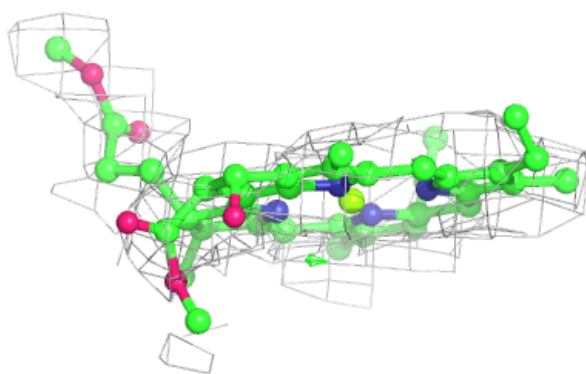
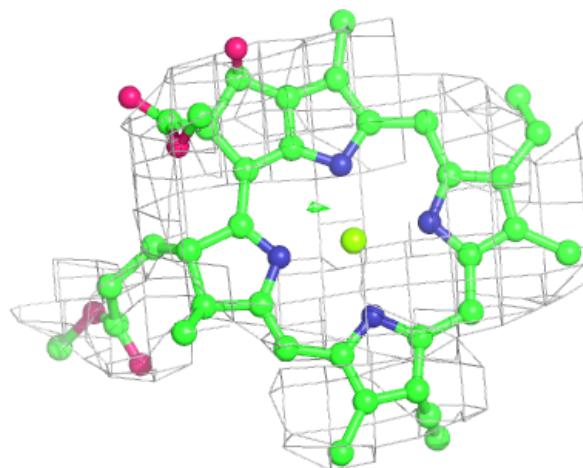
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





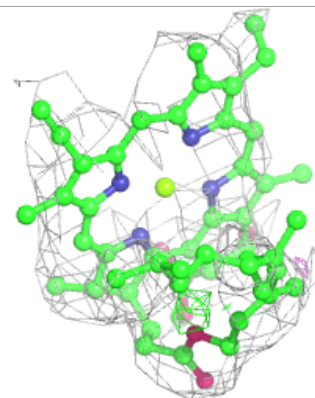
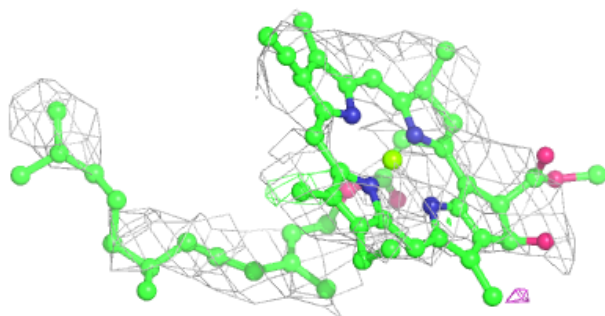
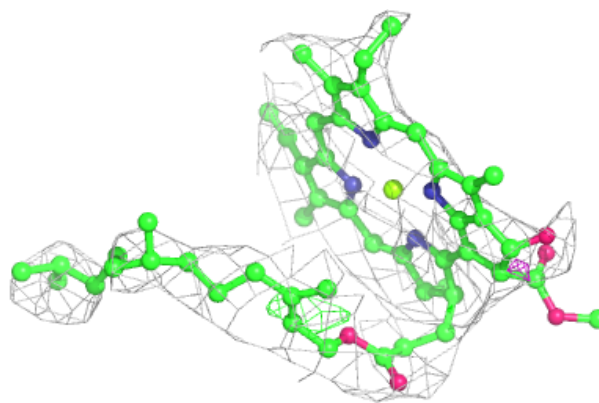
Electron density around CLA B 822:

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

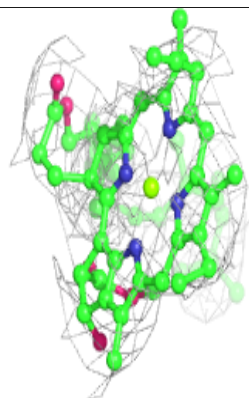
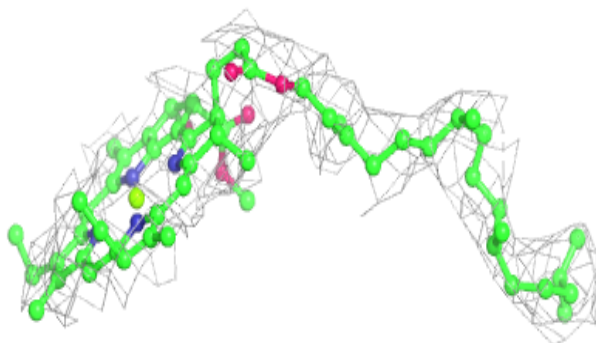
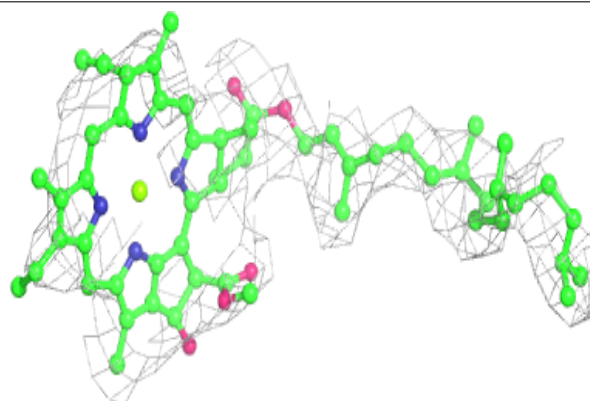


Electron density around CLA B 815:

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

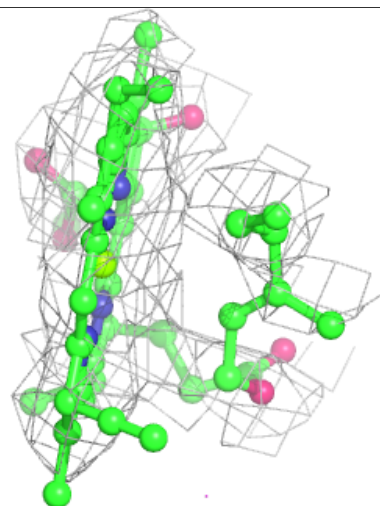
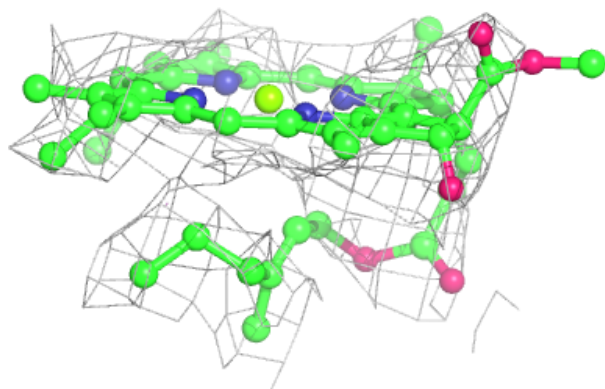
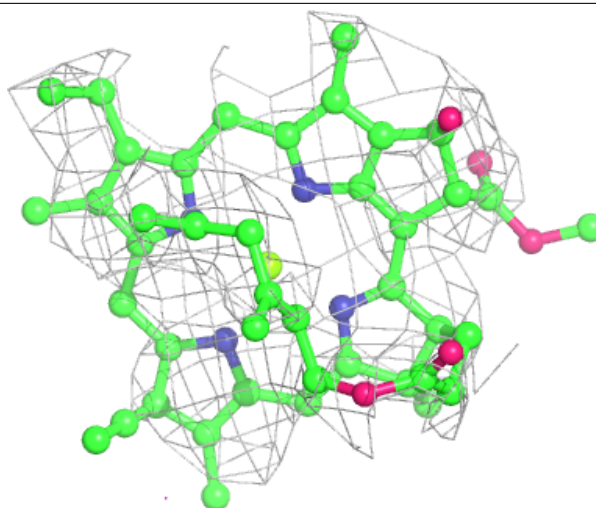
**Electron density around CLA 3 315:**

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



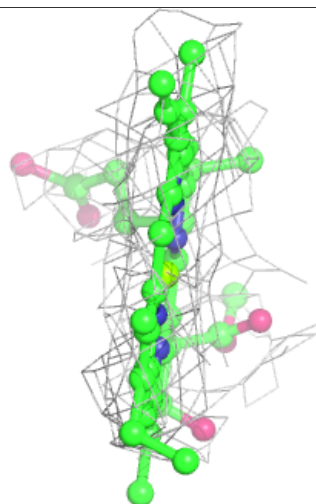
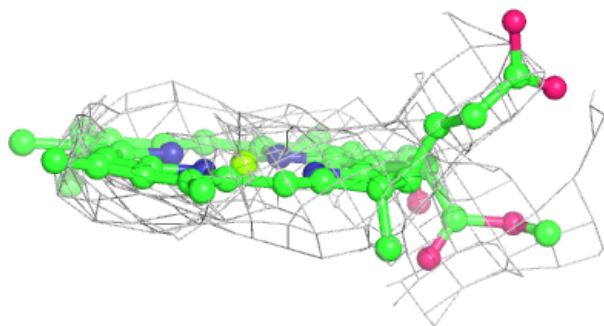
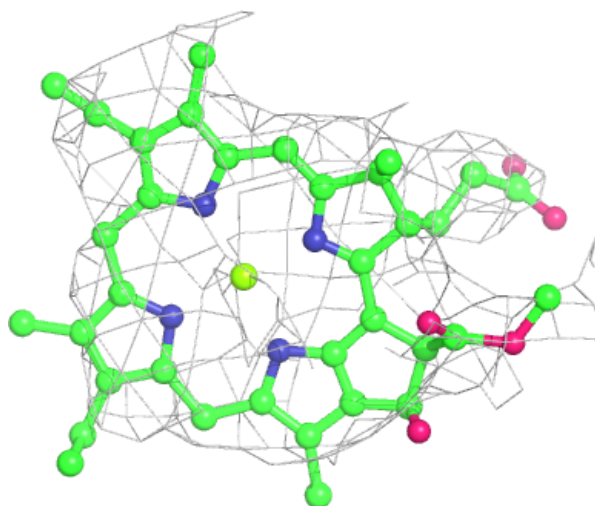
Electron density around CLA A 817:

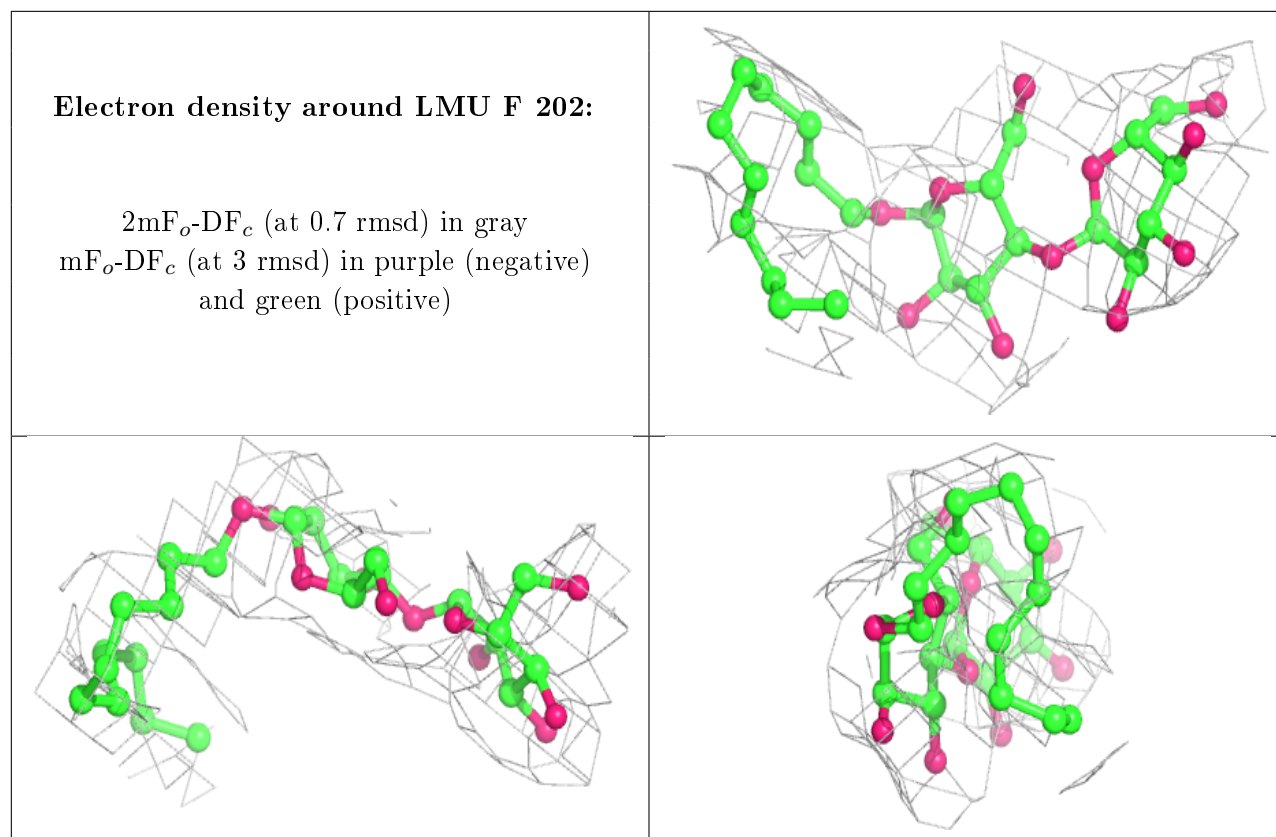
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA A 810:

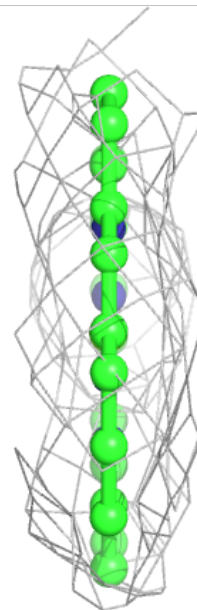
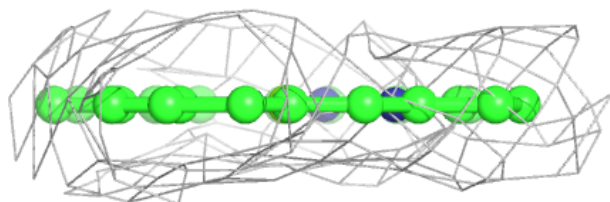
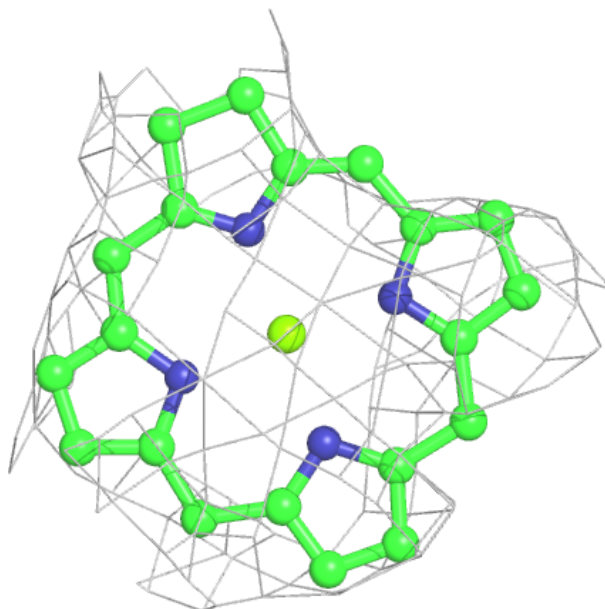
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

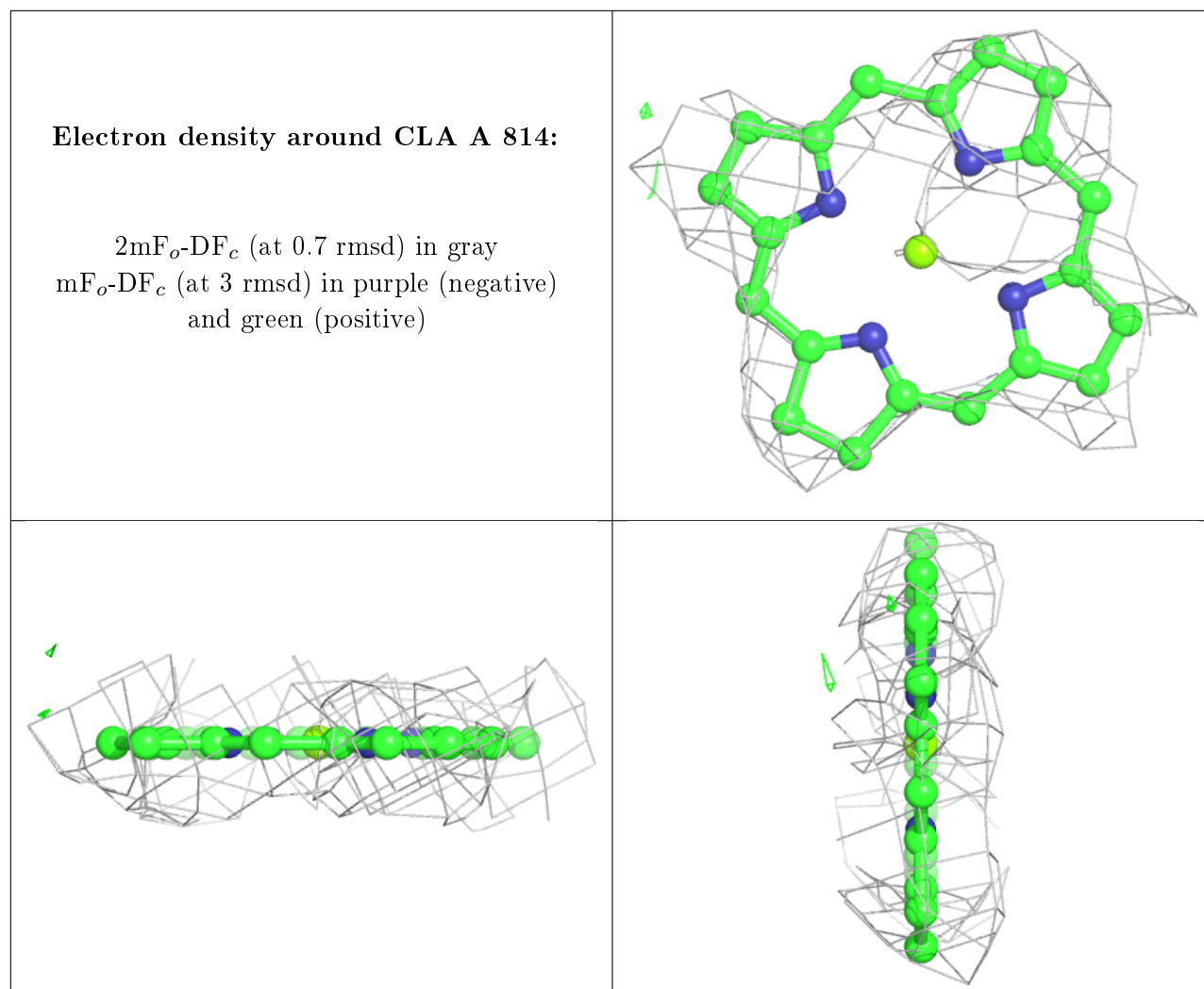




Electron density around CLA 2 316:

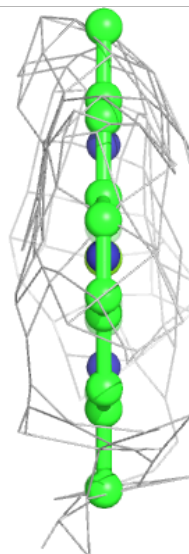
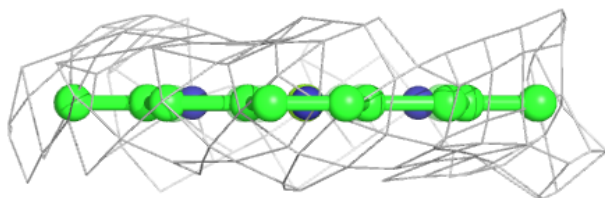
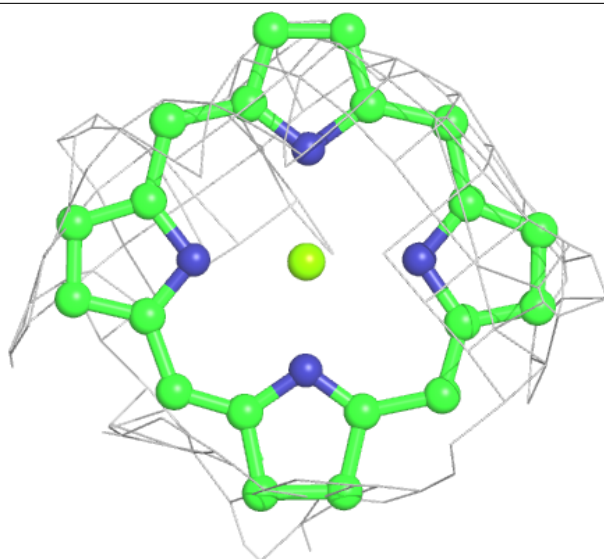
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

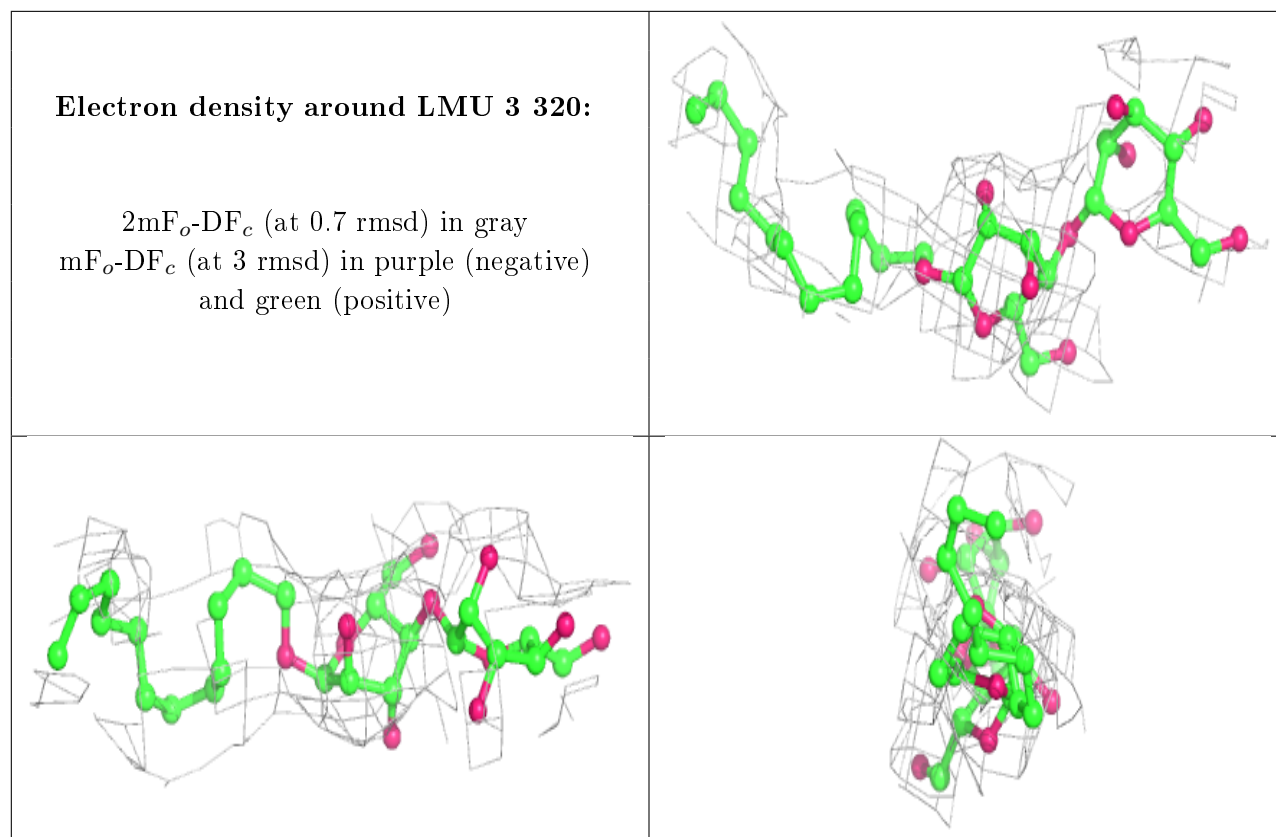




Electron density around CLA 3 308:

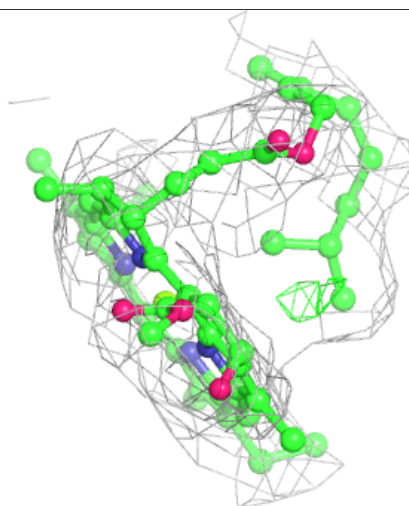
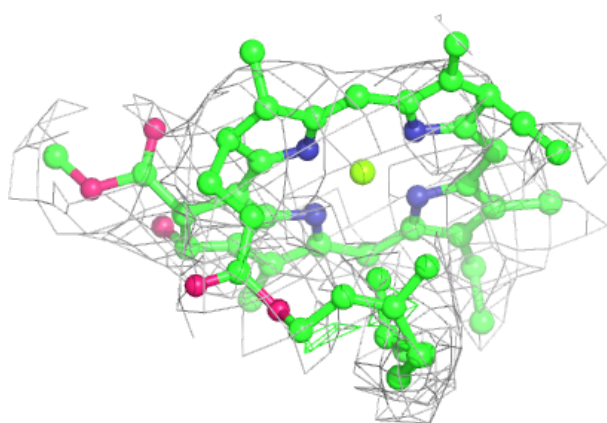
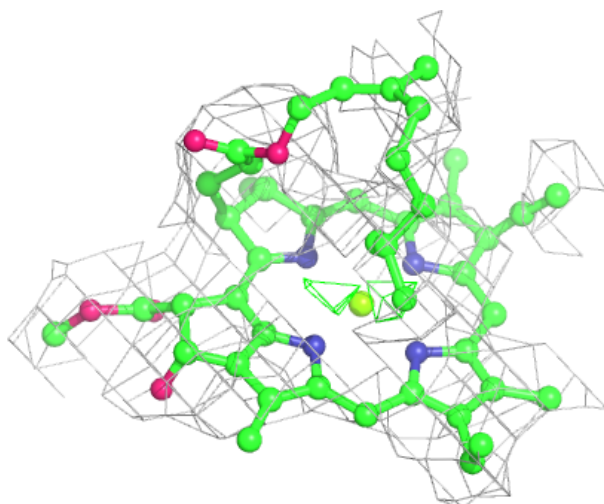
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





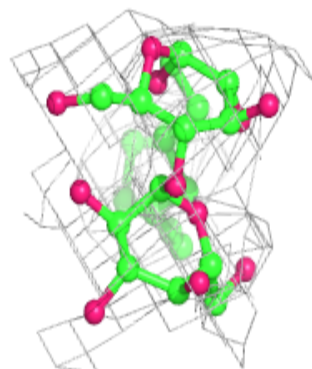
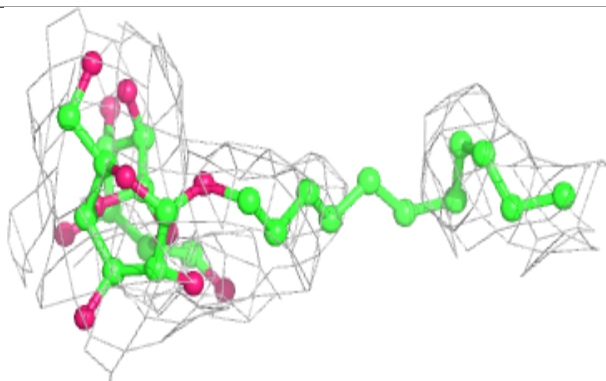
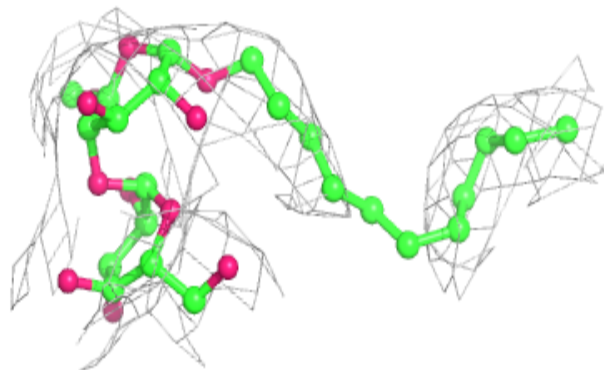
Electron density around CLA B 813:

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

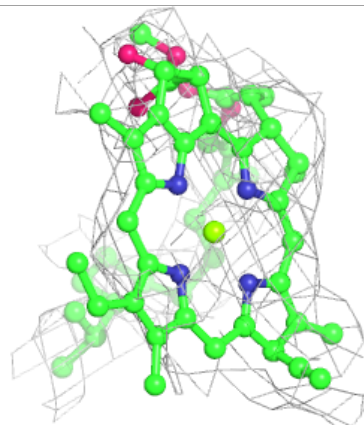
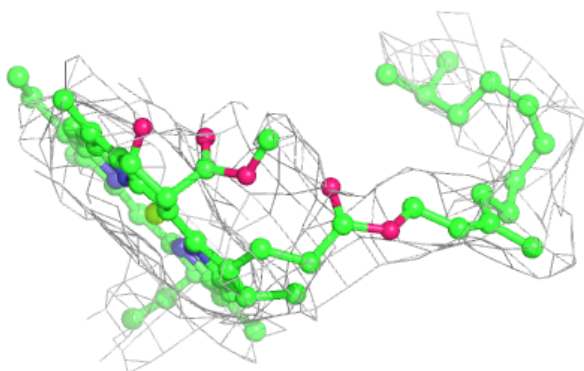
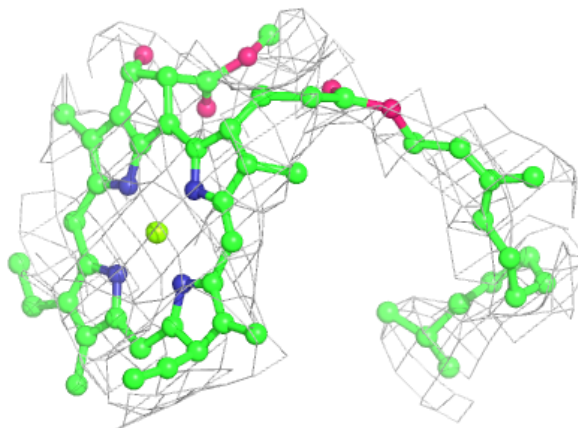


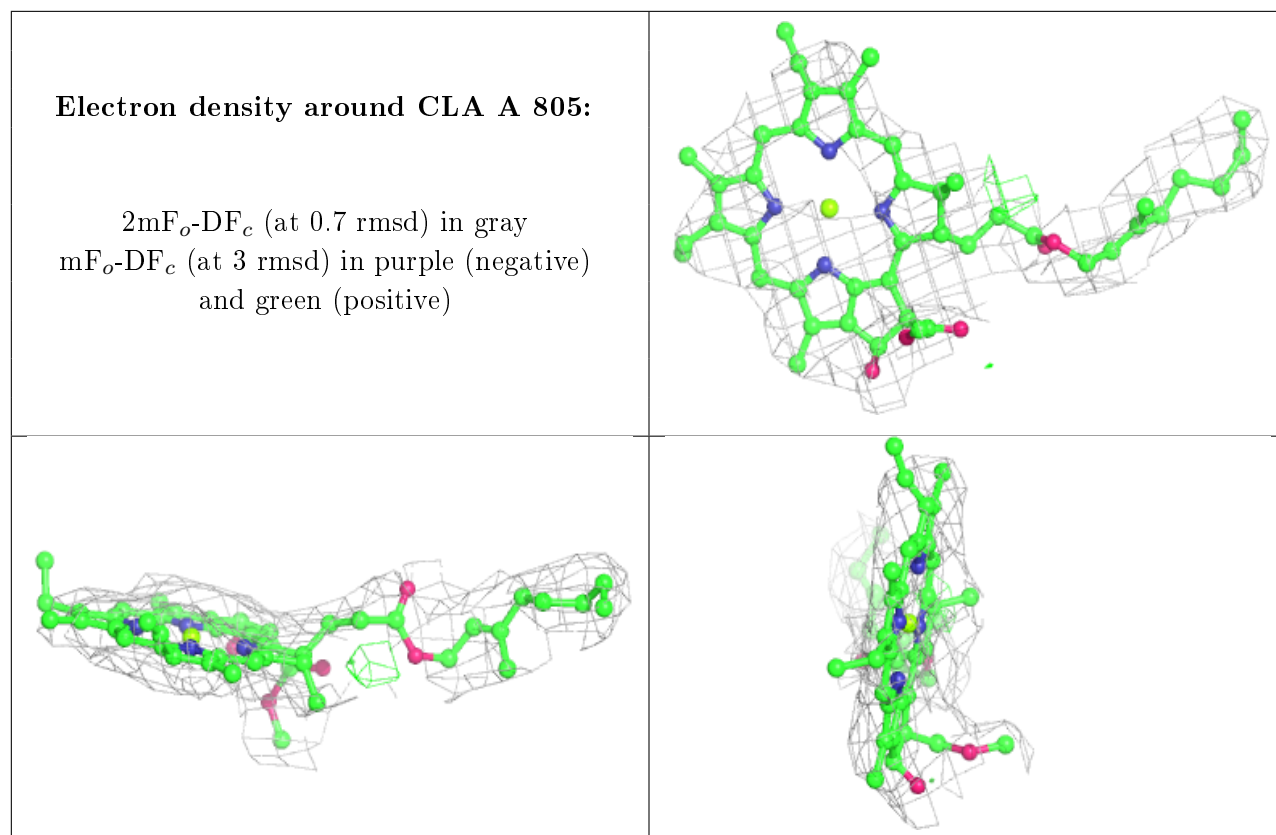
Electron density around LMU 4 319:

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

**Electron density around CLA A 839:**

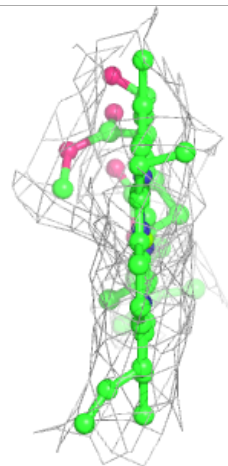
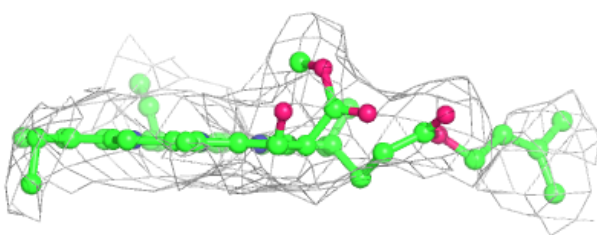
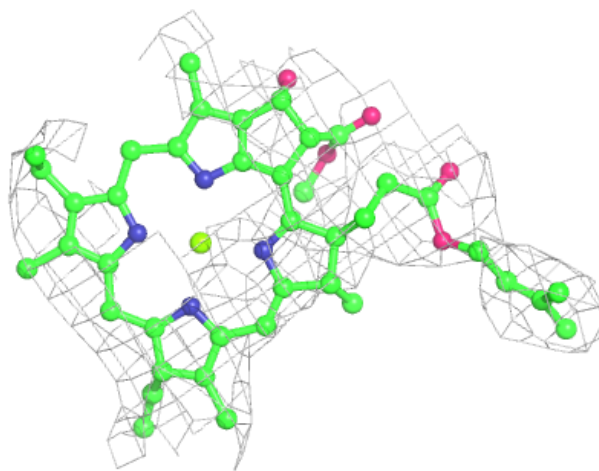
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





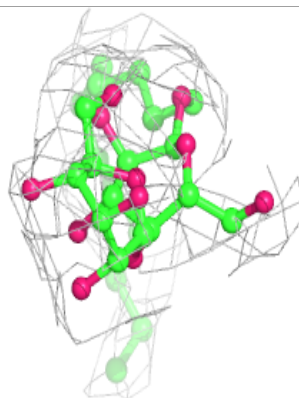
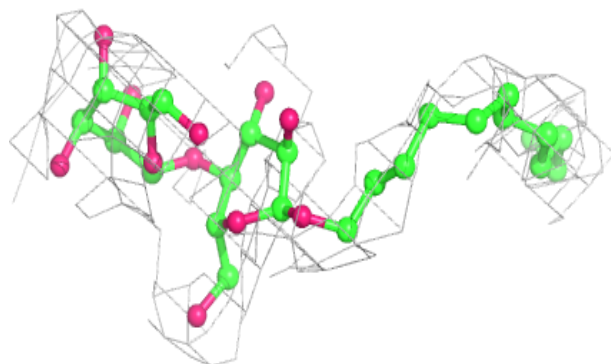
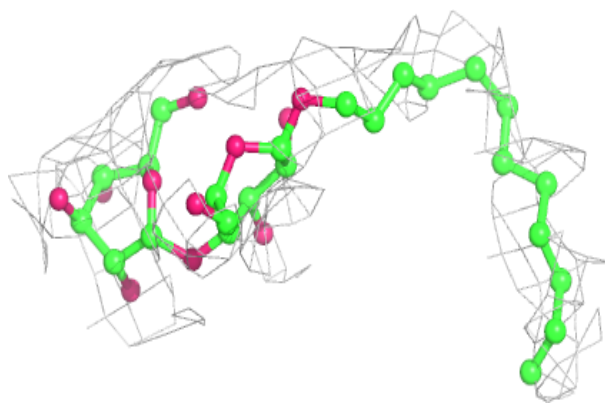
Electron density around CLA 4 310:

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

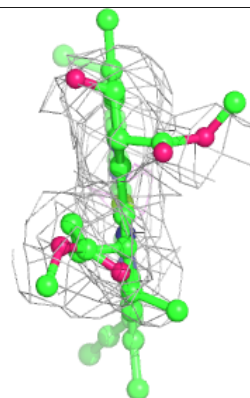
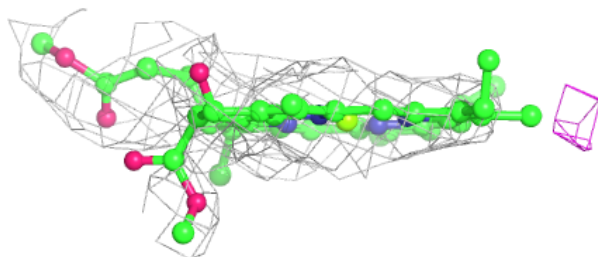
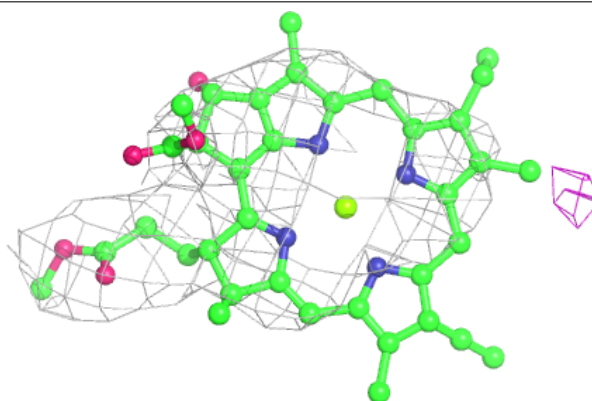


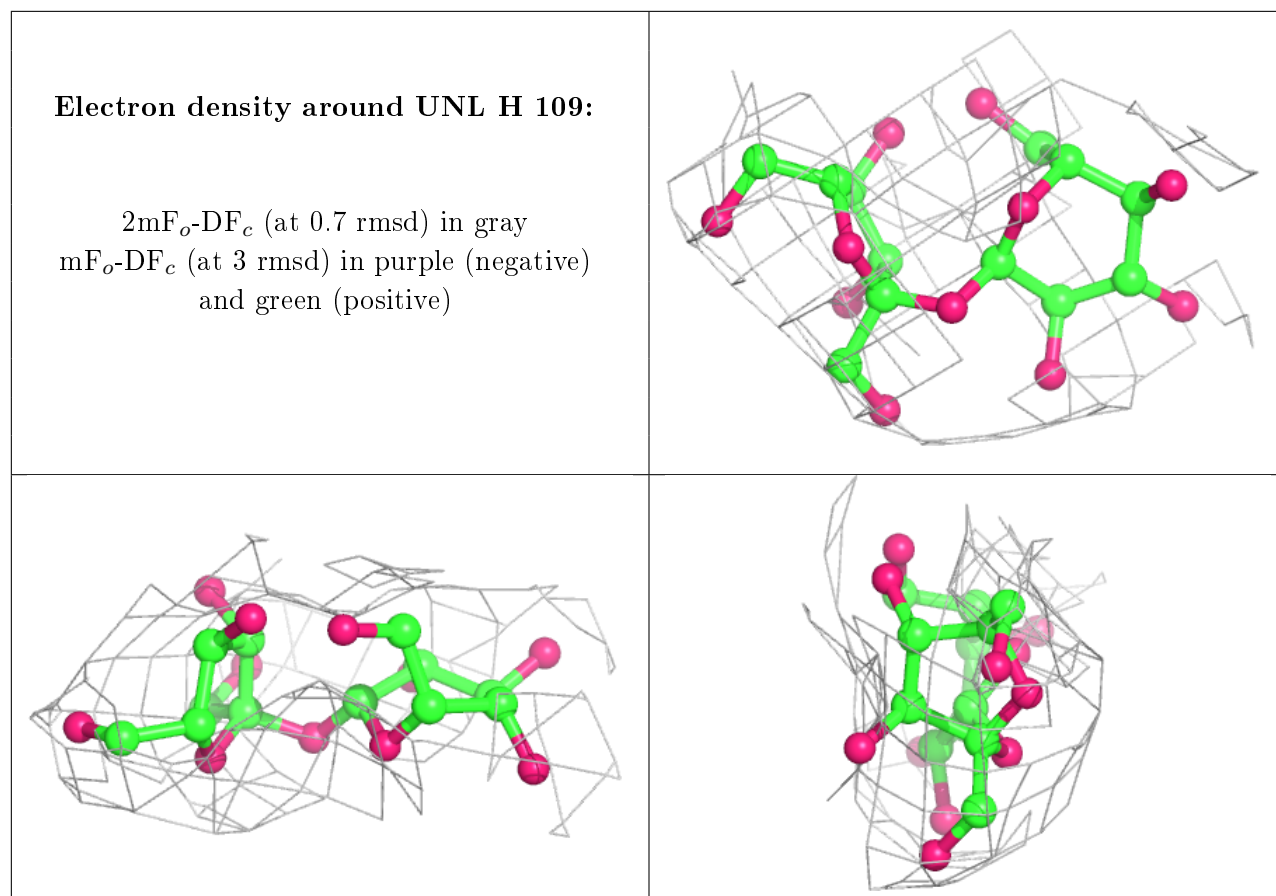
Electron density around LMU 2 319:

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

**Electron density around CLA A 834:**

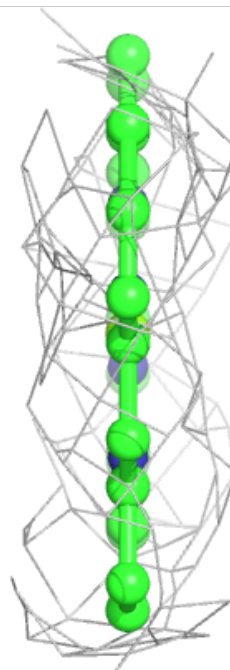
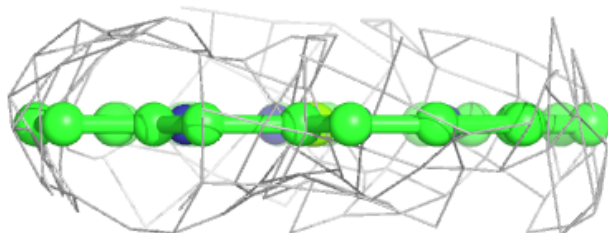
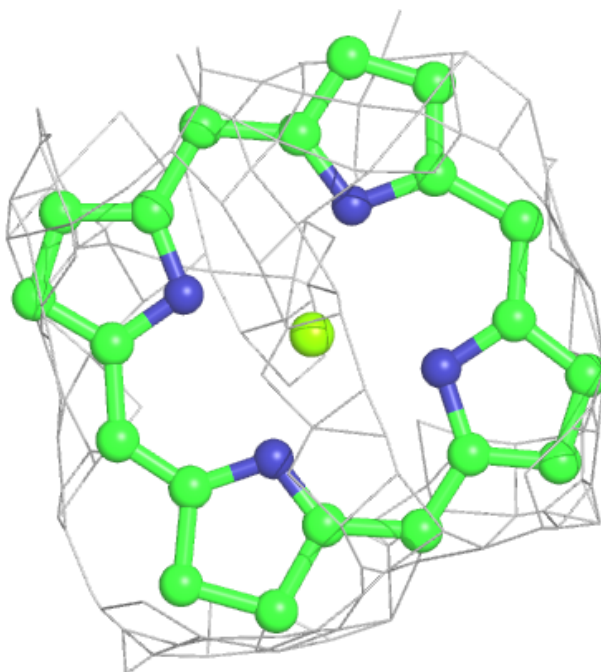
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





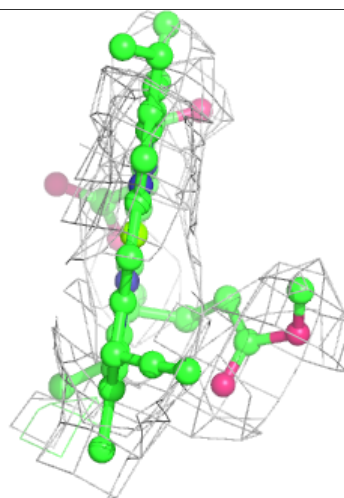
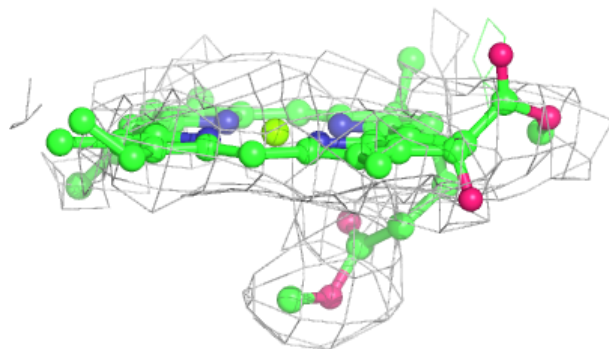
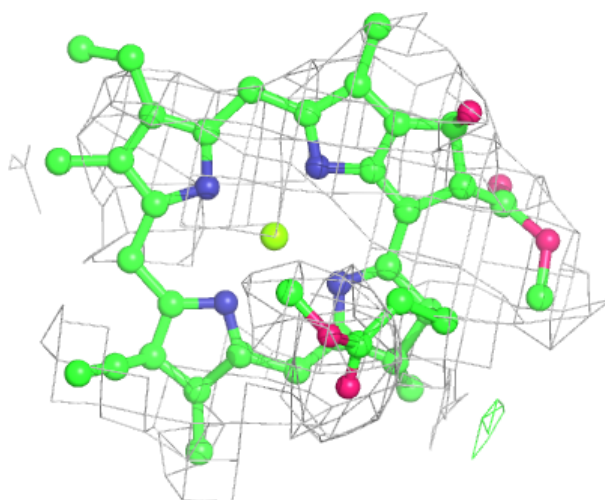
Electron density around CLA 1 212:

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



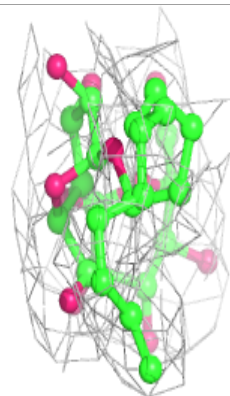
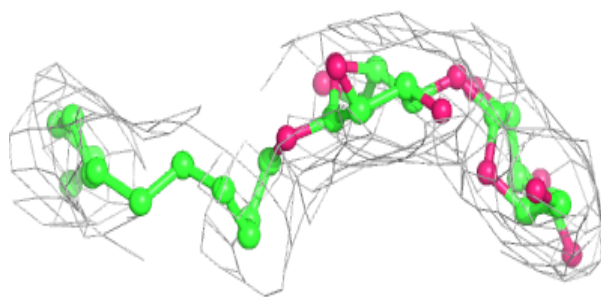
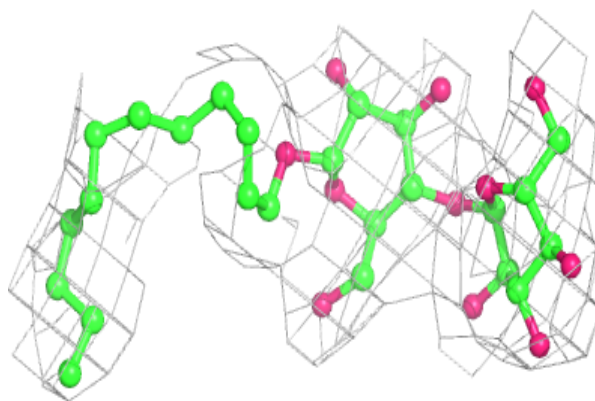
Electron density around CLA 1 204:

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

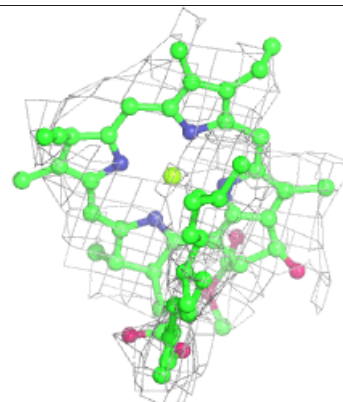
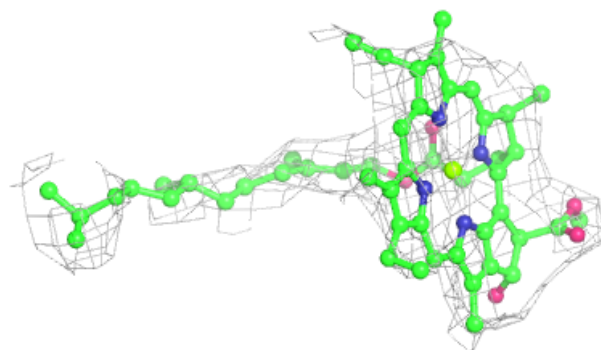
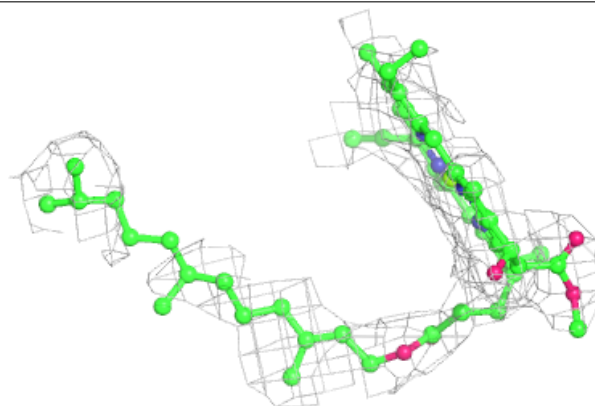


Electron density around LMU D 201:

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

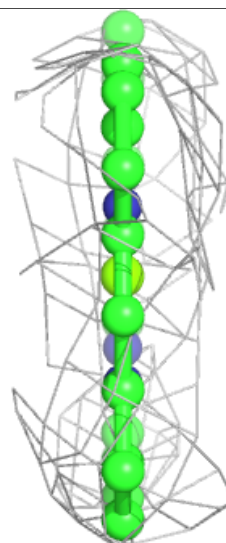
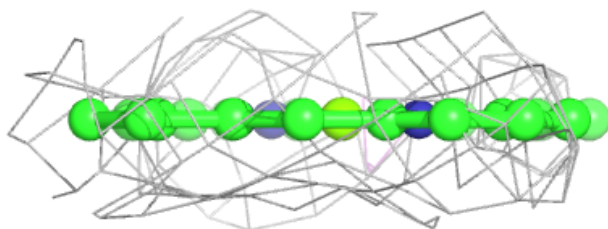
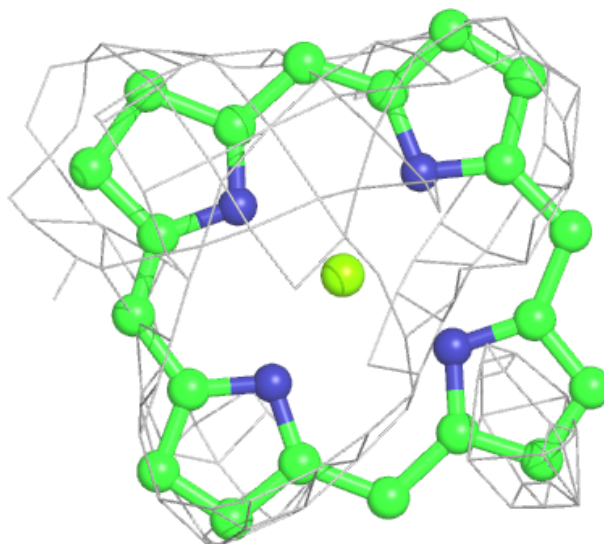
**Electron density around CLA L 201:**

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



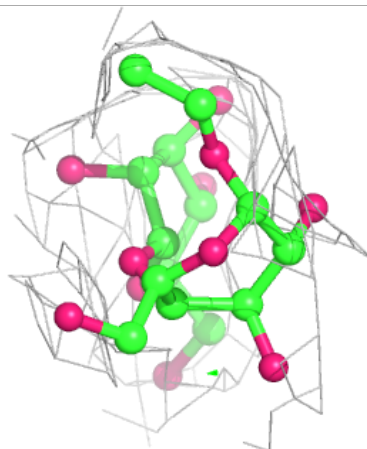
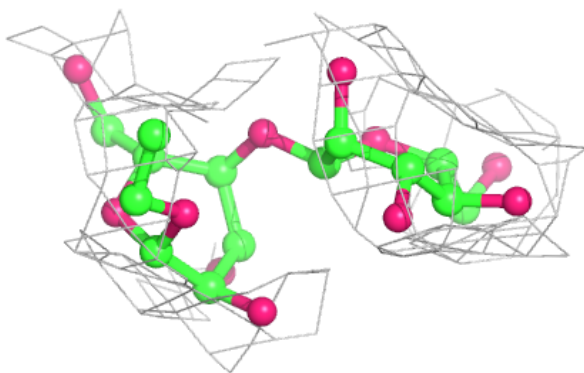
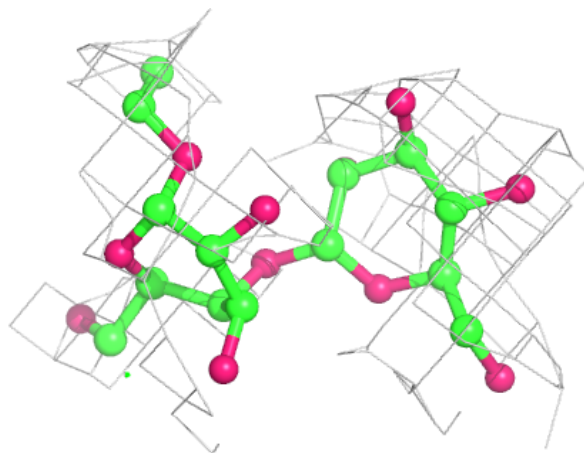
Electron density around CLA 2 309:

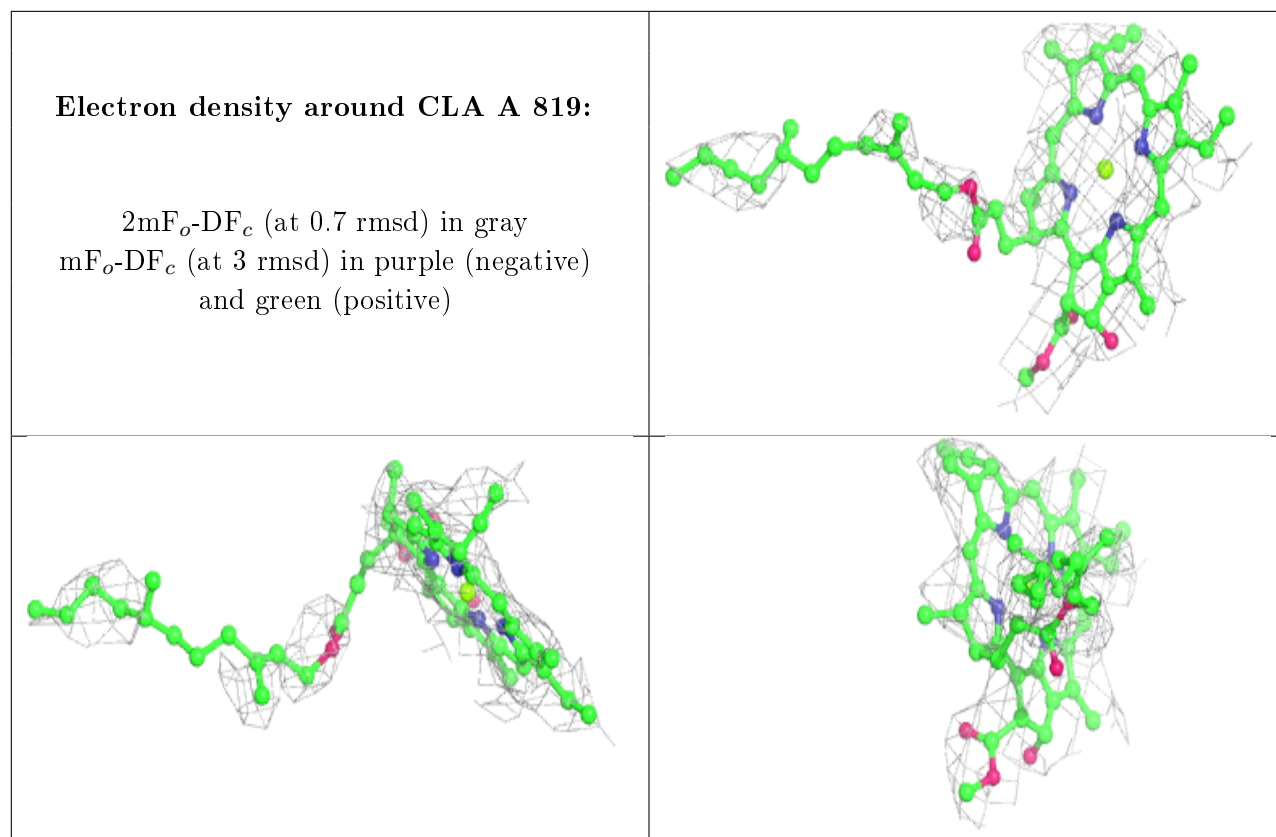
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMU B 849:

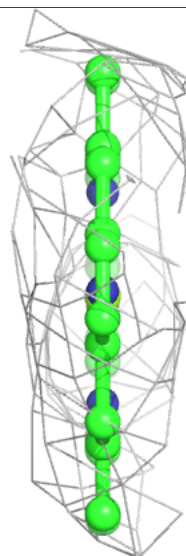
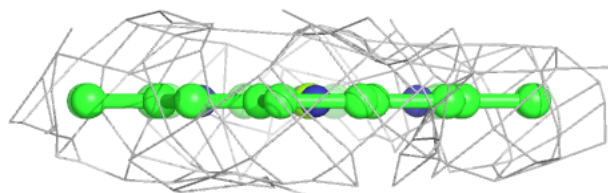
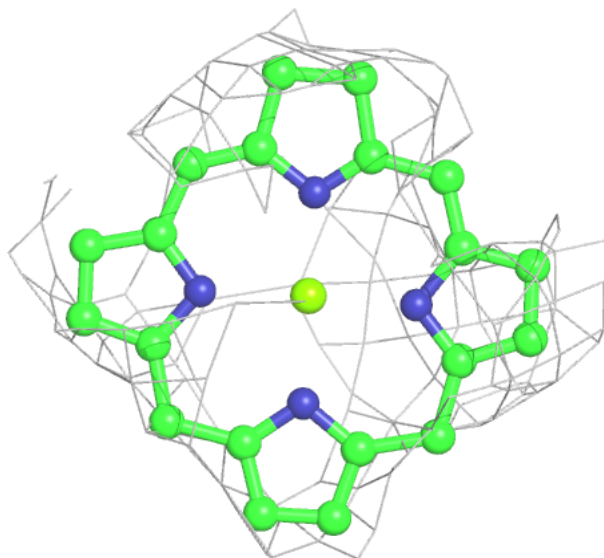
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

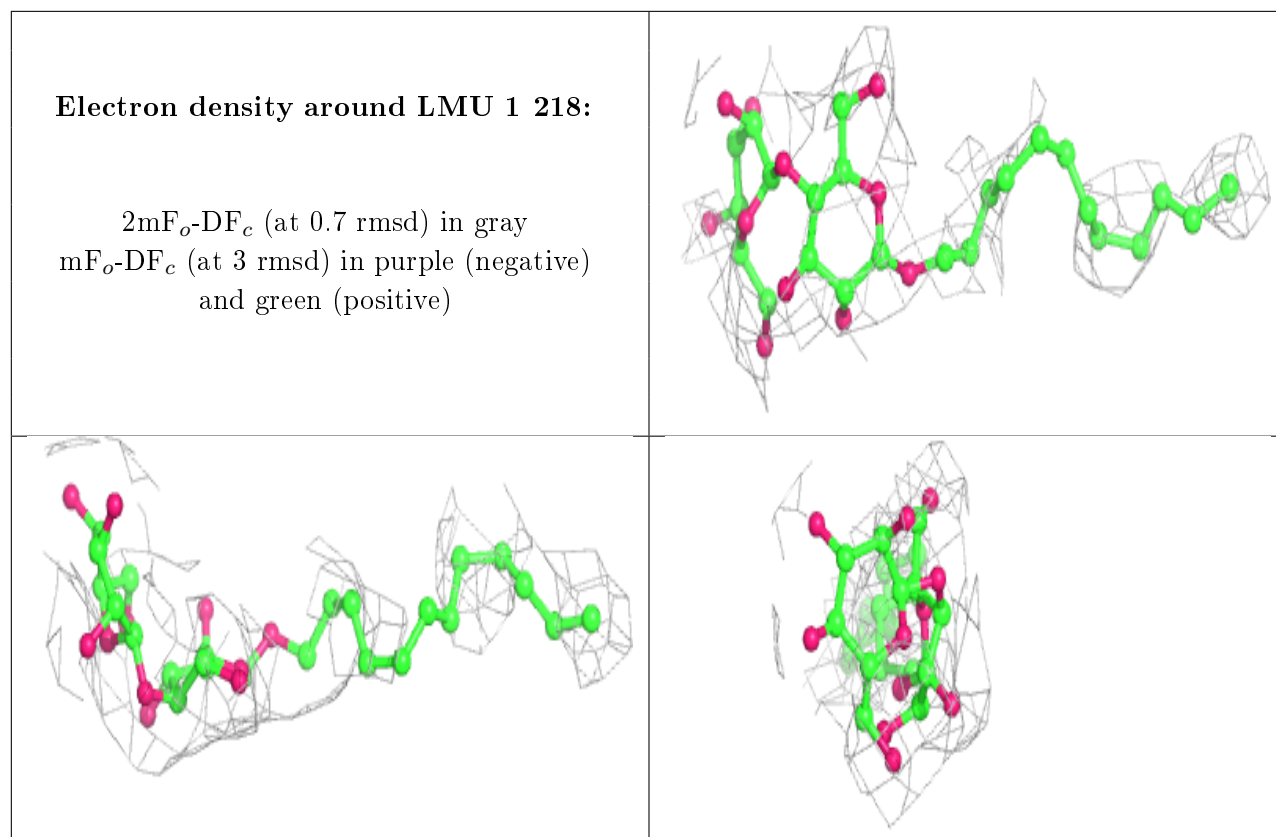




Electron density around CLA 1 214:

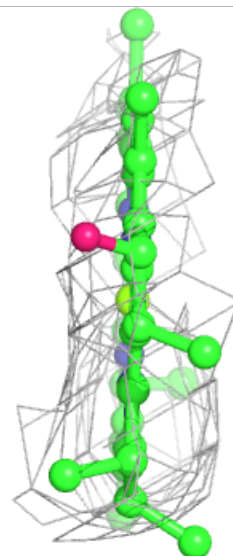
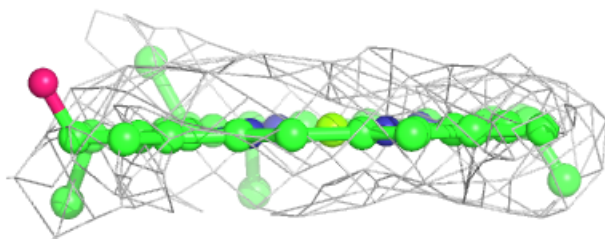
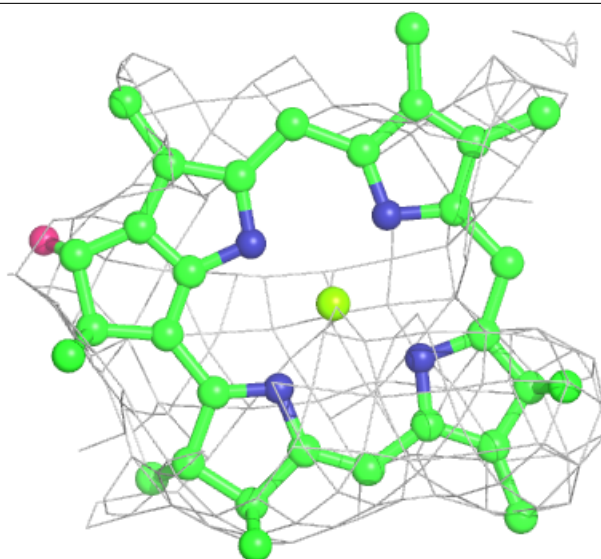
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





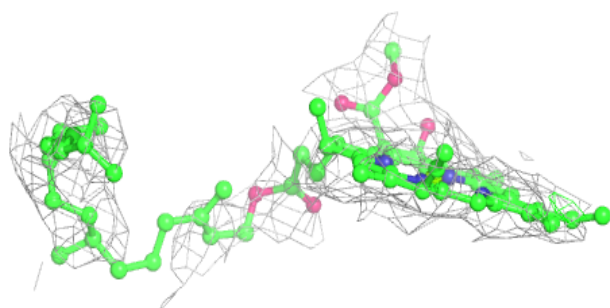
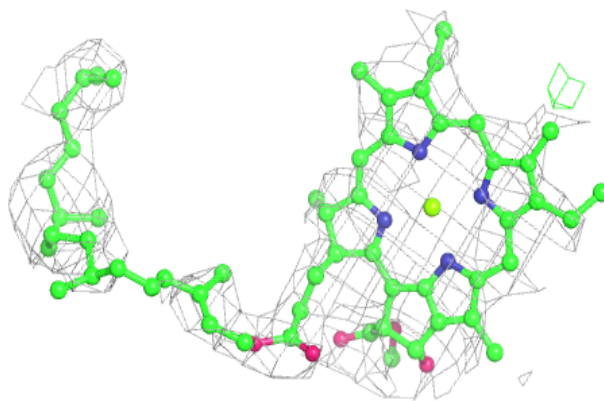
Electron density around CLA B 842:

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

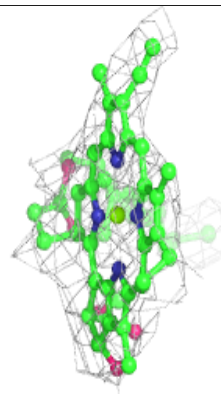
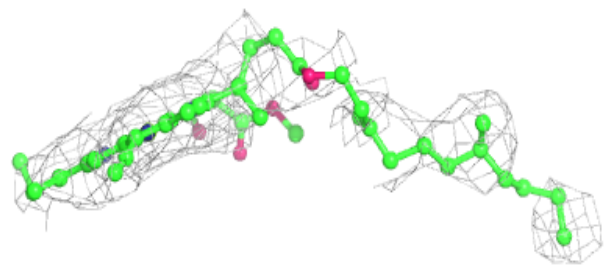
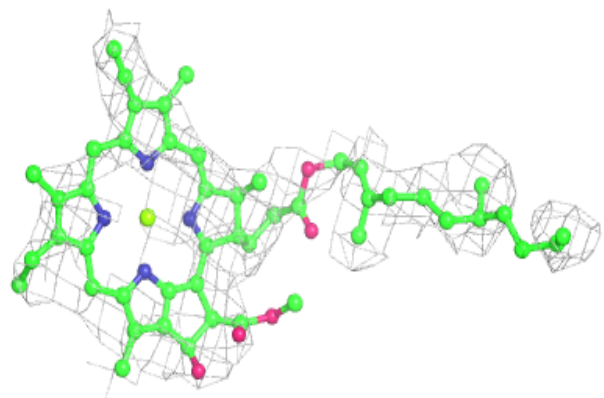


Electron density around CLA A 825:

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

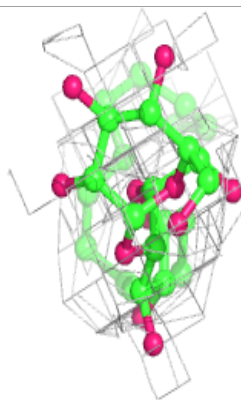
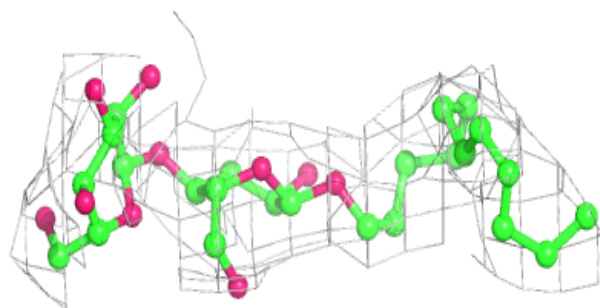
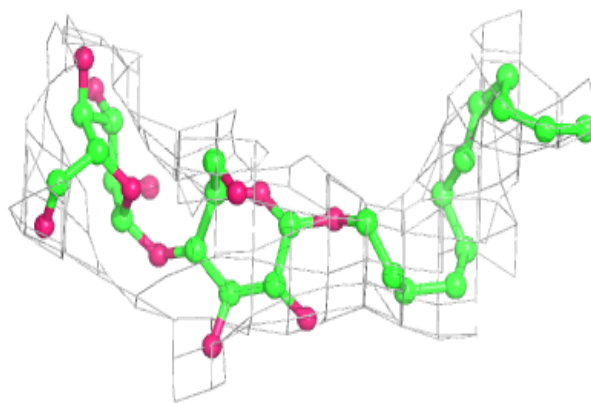
**Electron density around CLA H 111:**

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

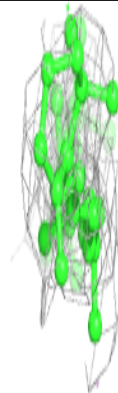
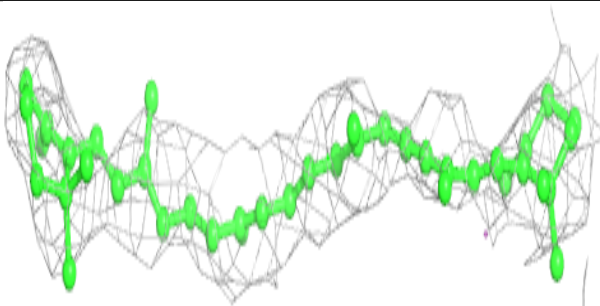
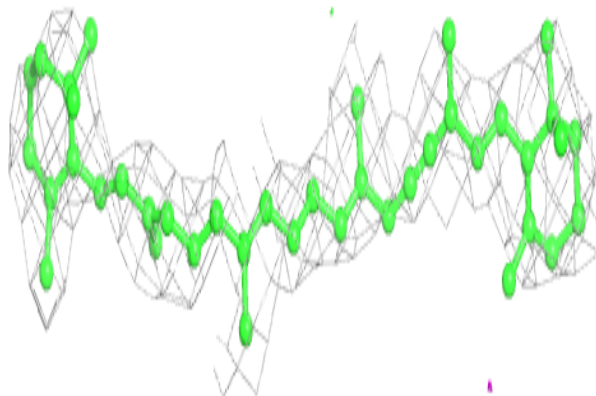


Electron density around LMU R 109:

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

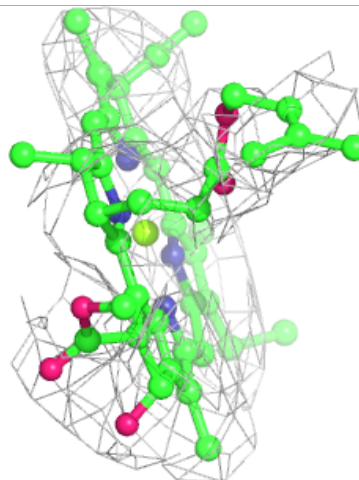
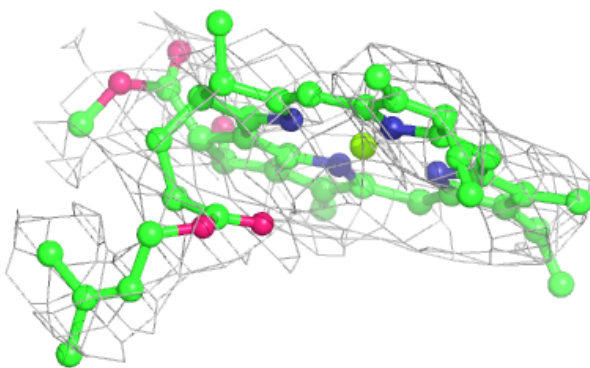
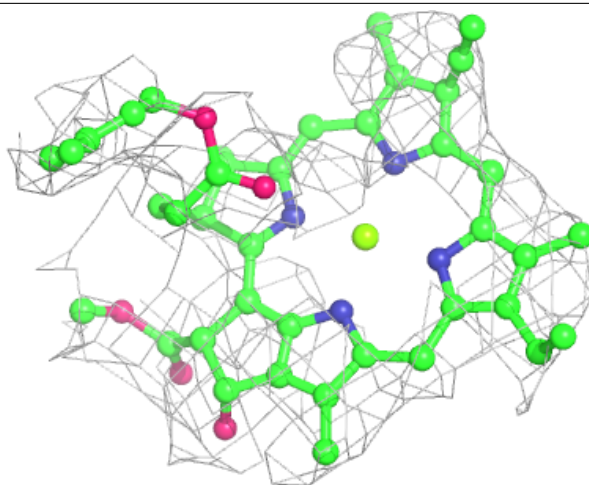
**Electron density around BCR B 846:**

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



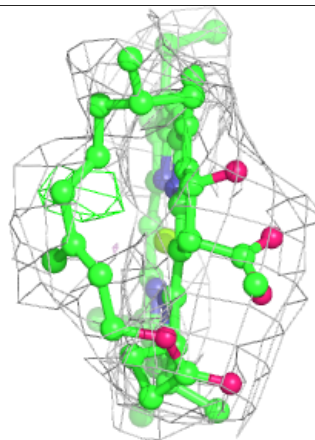
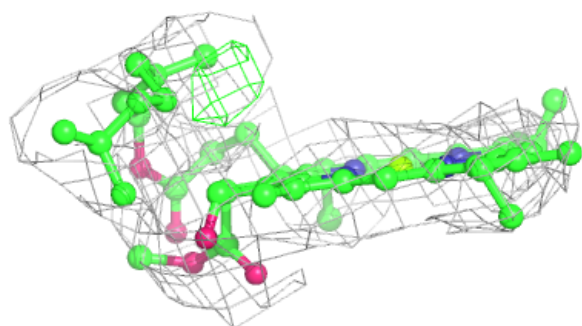
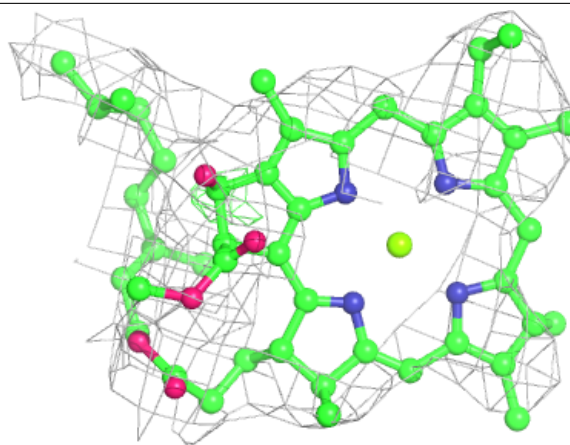
Electron density around CLA A 815:

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

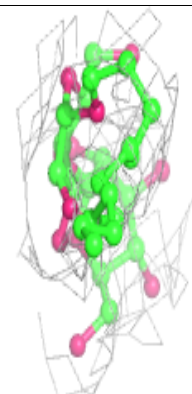
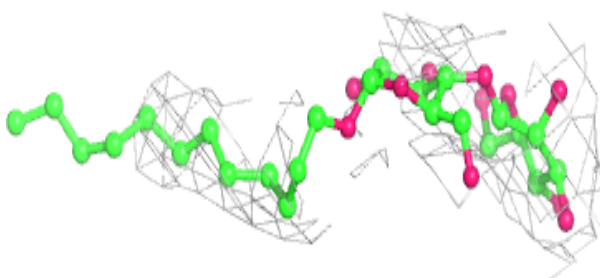
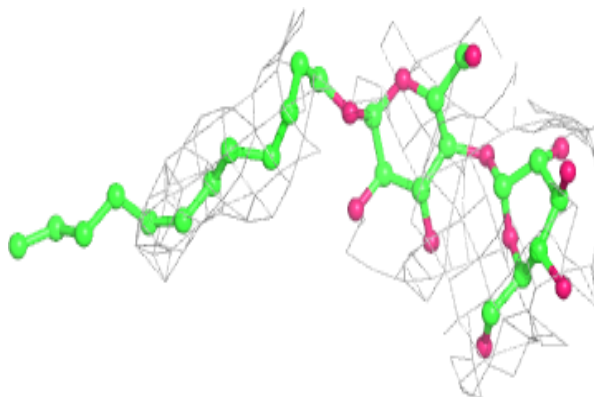


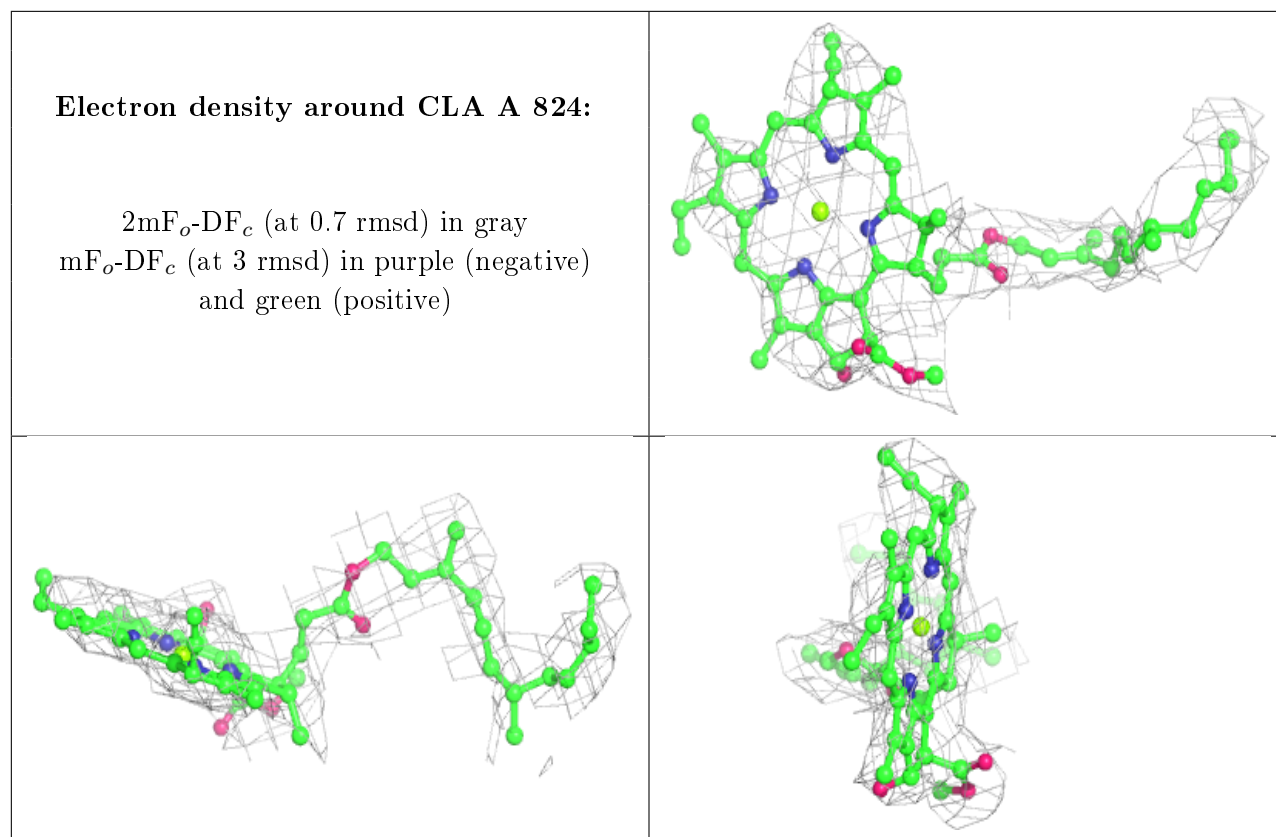
Electron density around CLA B 812:

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

**Electron density around LMU A 855:**

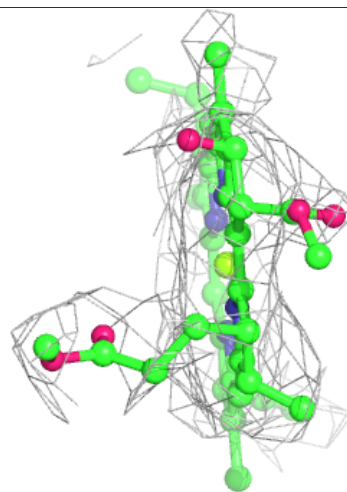
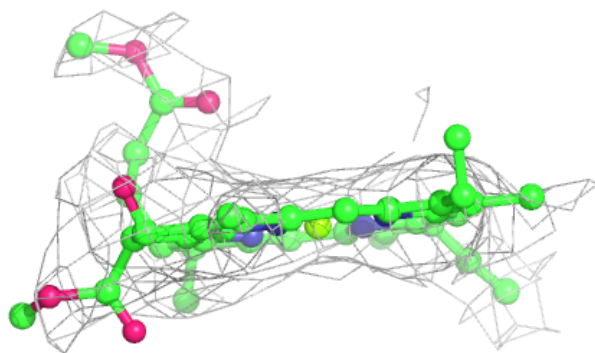
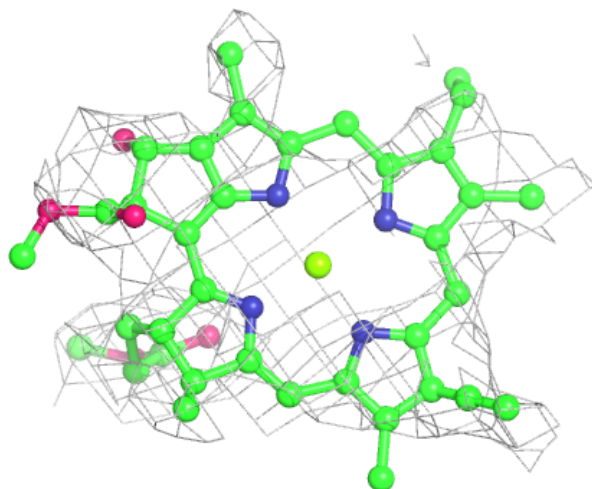
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





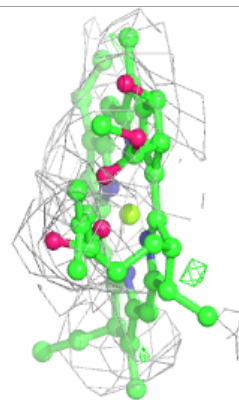
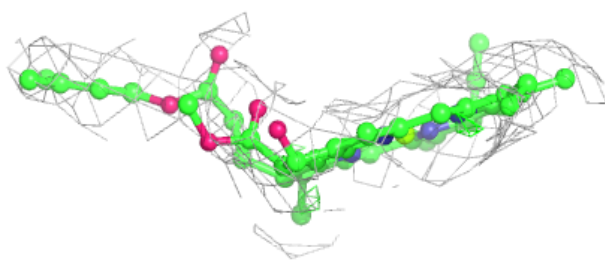
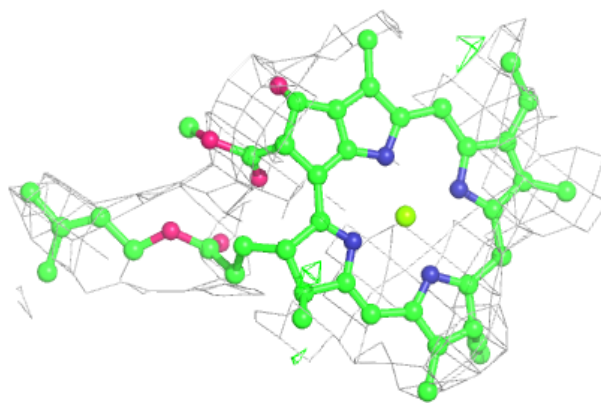
Electron density around CLA A 807:

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



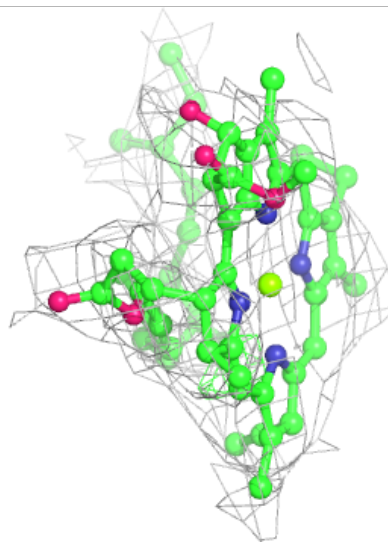
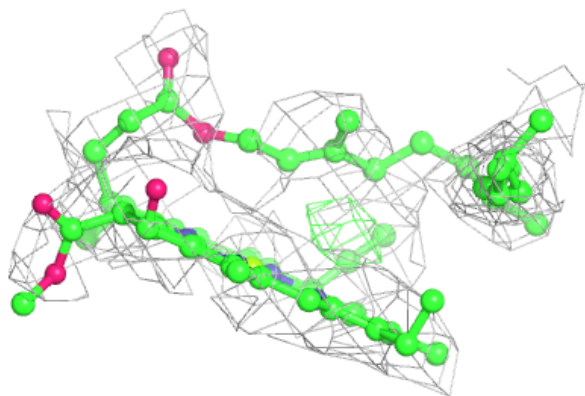
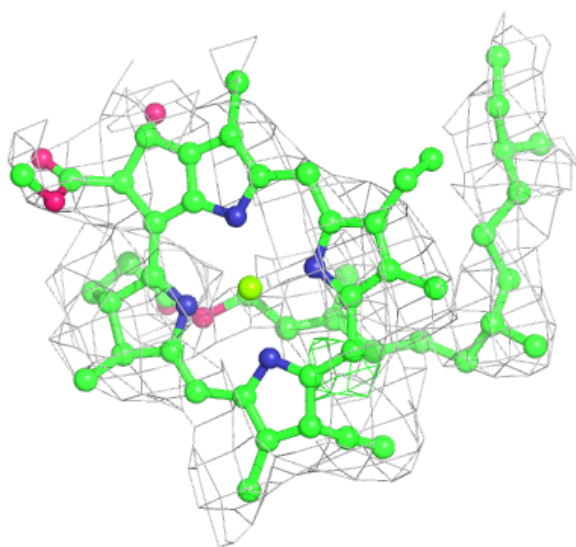
Electron density around CLA L 210:

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



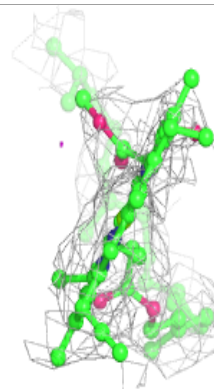
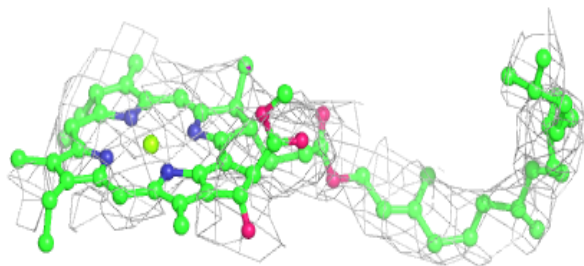
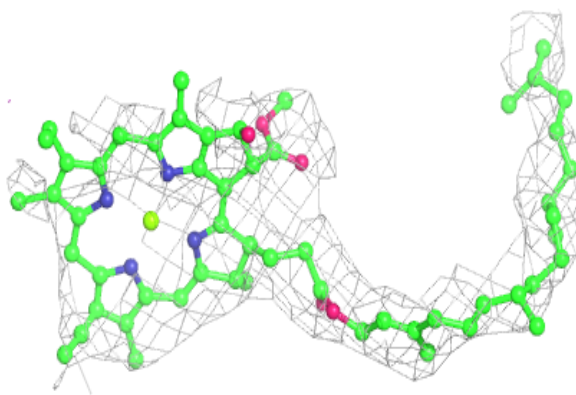
Electron density around CLA B 820:

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



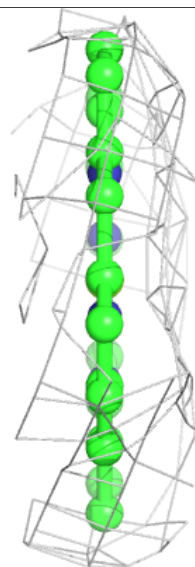
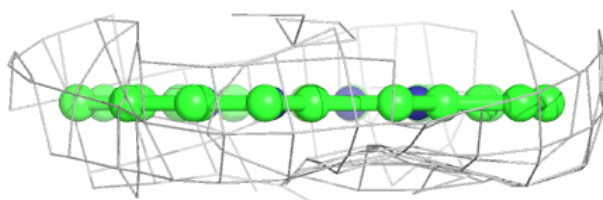
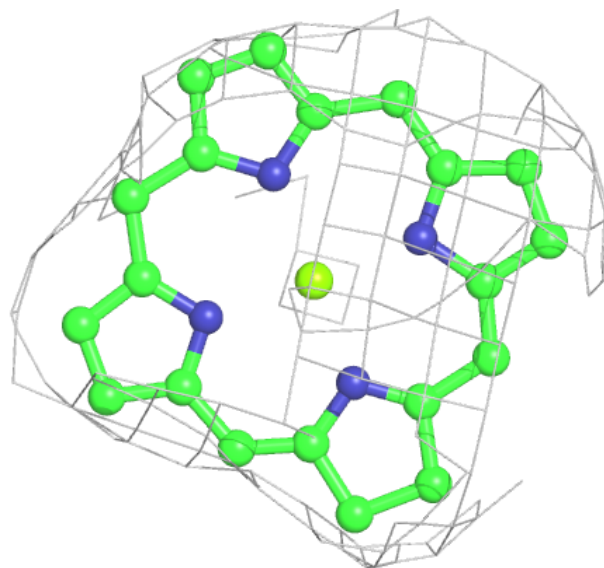
Electron density around CLA B 827:

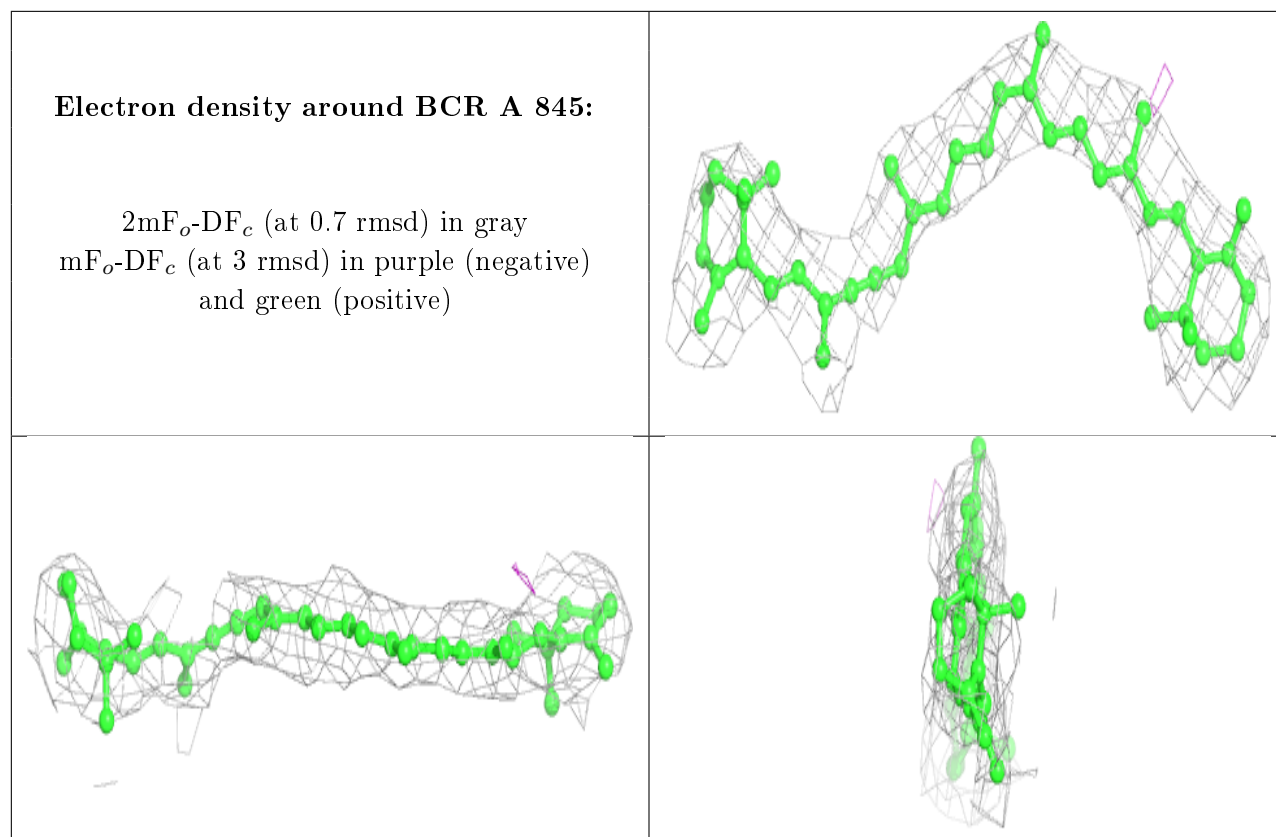
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 3 304:

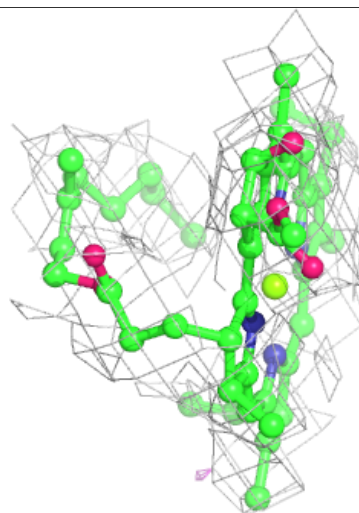
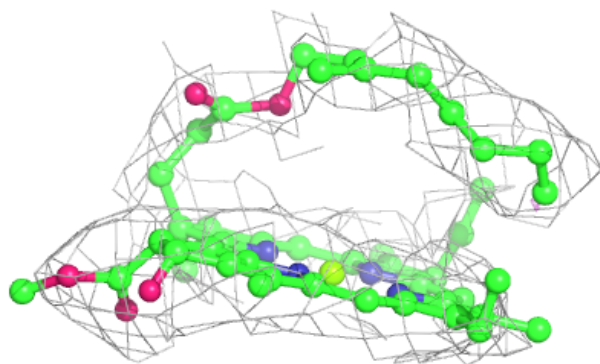
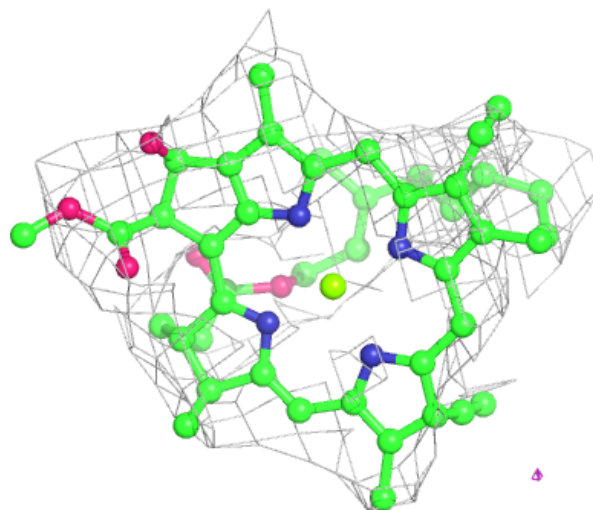
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

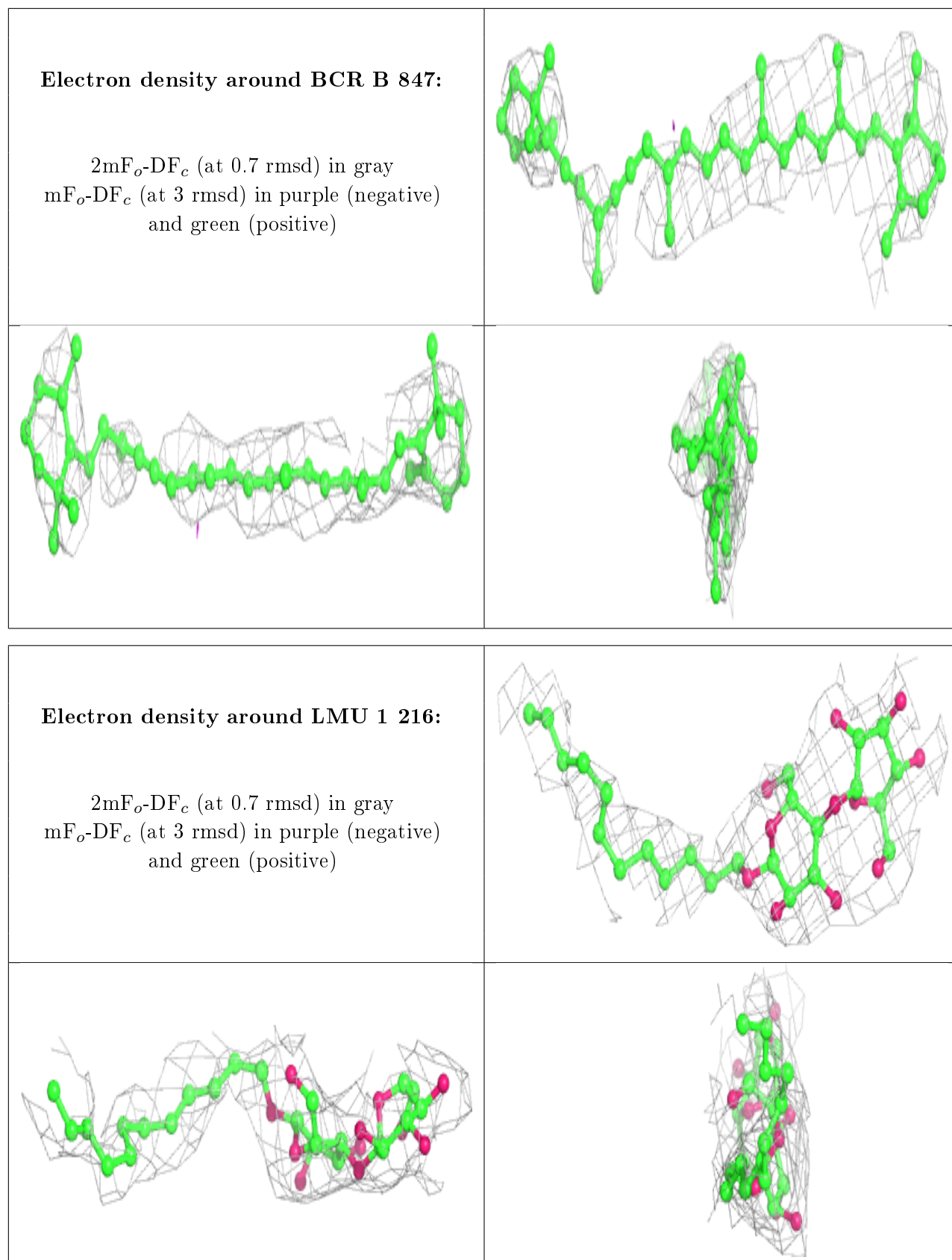




Electron density around CLA A 812:

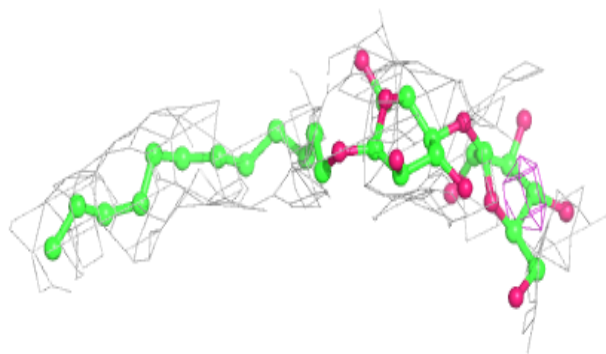
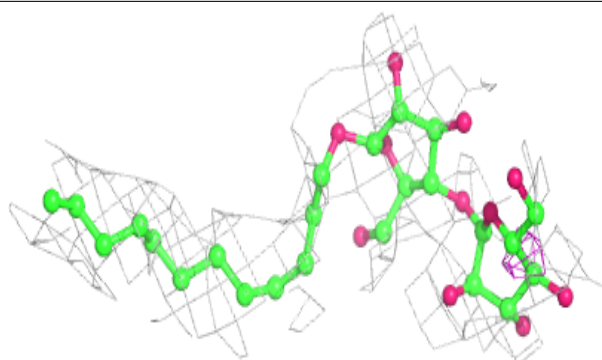
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



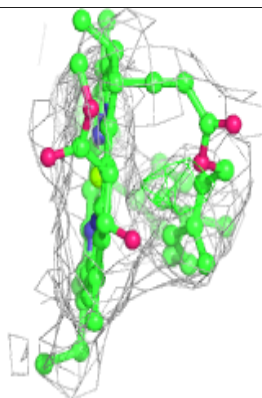
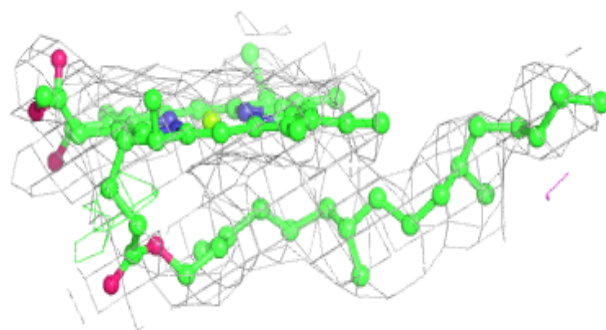
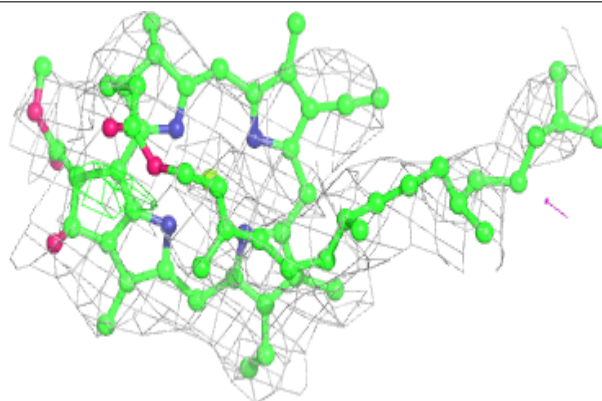


Electron density around LMU G 101:

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

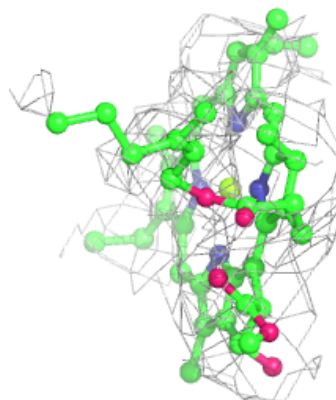
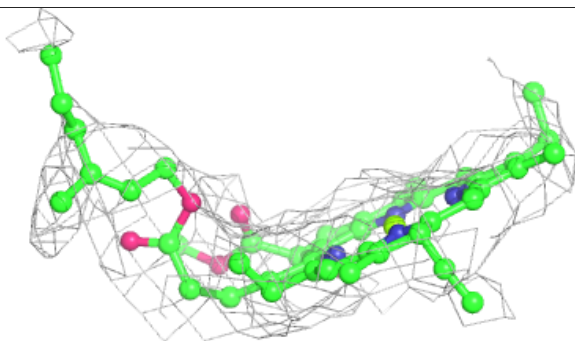
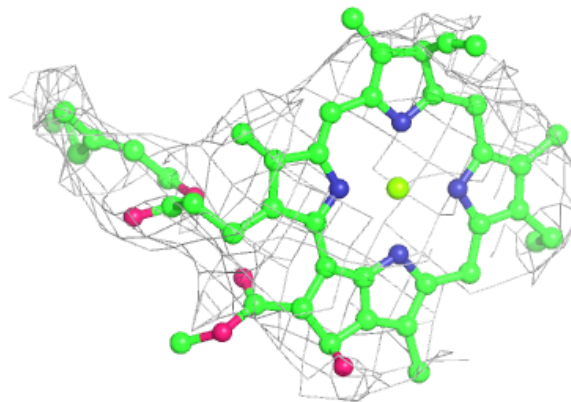
**Electron density around CLA B 806:**

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

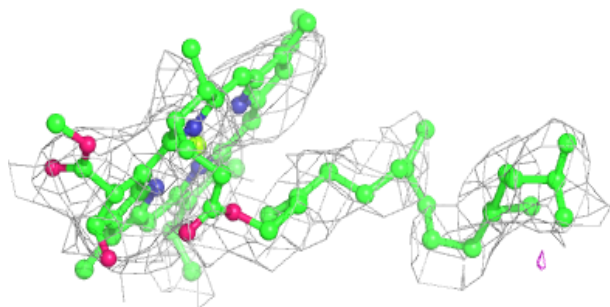
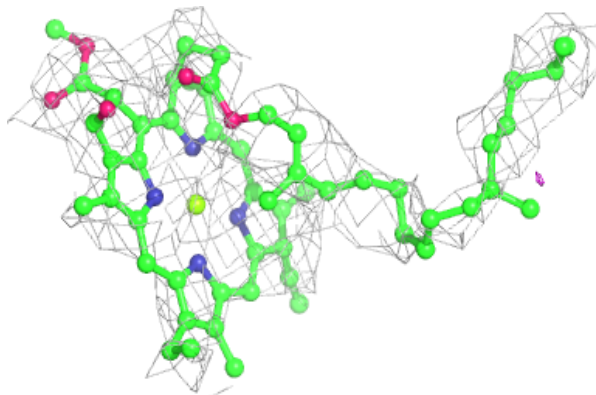


Electron density around CLA 4 306:

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

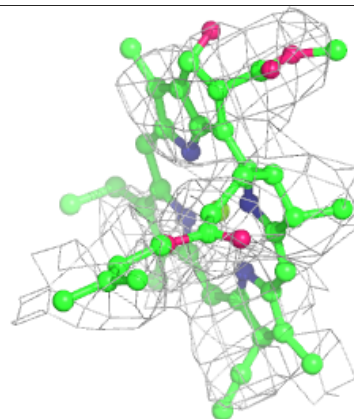
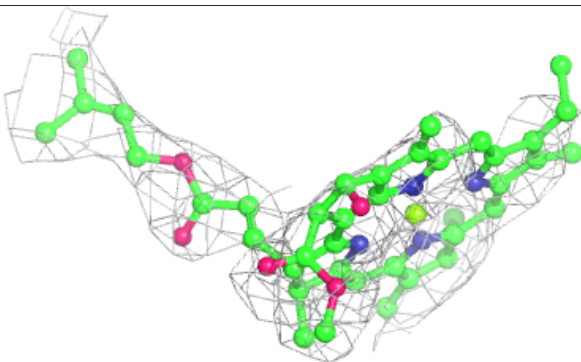
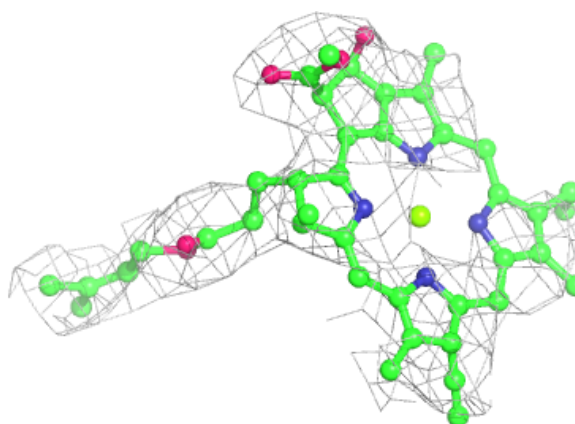
**Electron density around CLA L 203:**

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

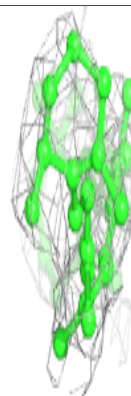
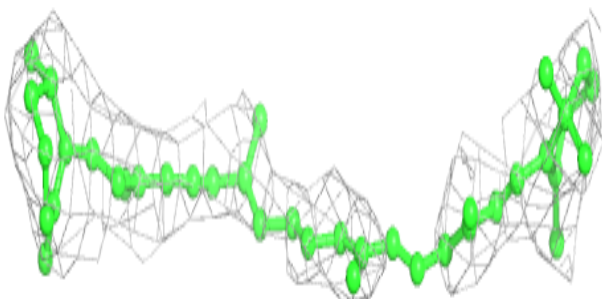
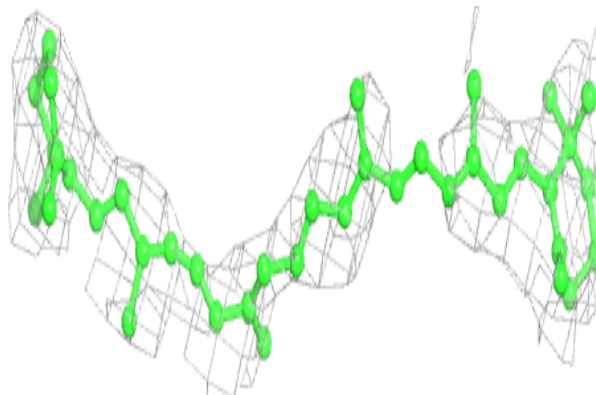


Electron density around CLA A 829:

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

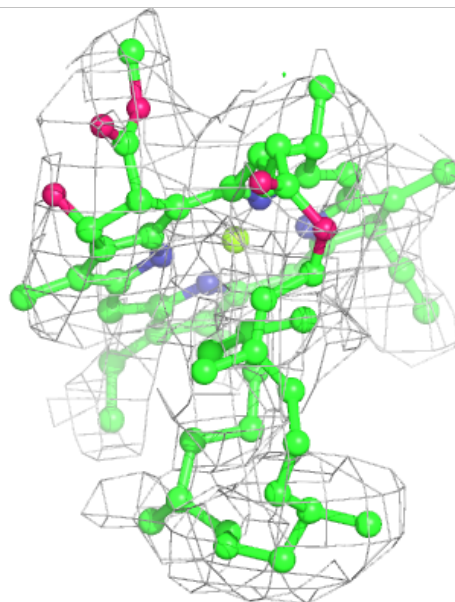
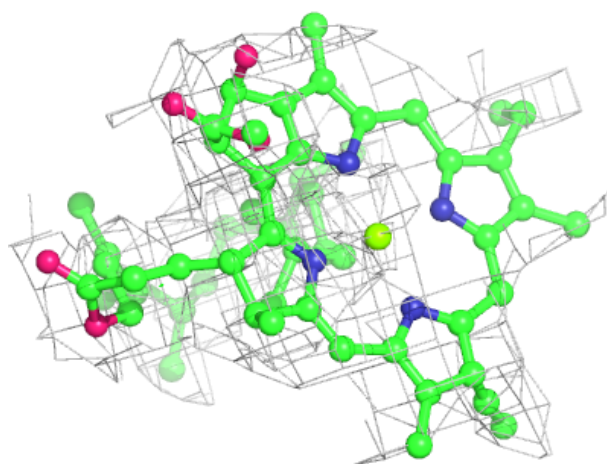
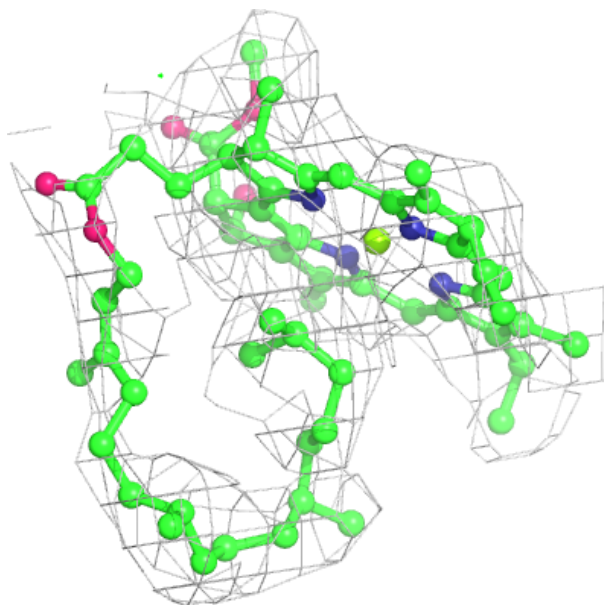
**Electron density around BCR I 101:**

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



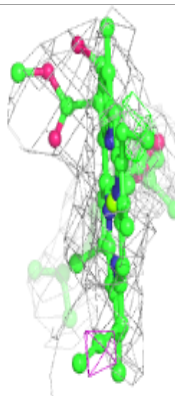
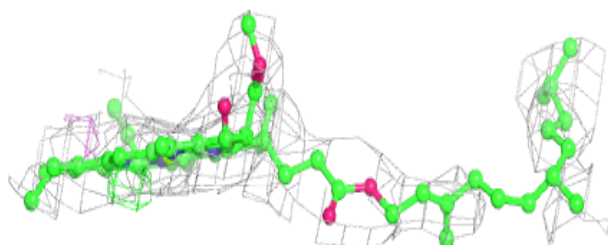
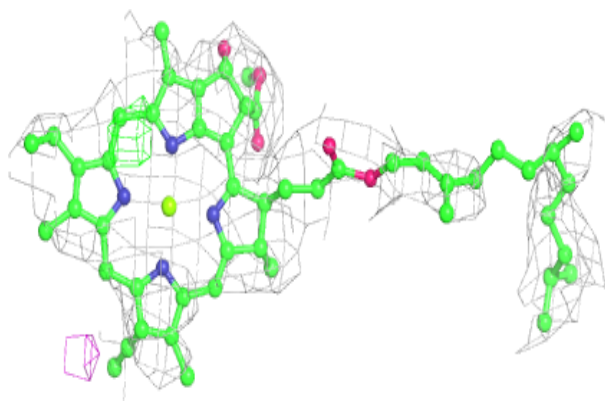
Electron density around CLA 2 317:

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

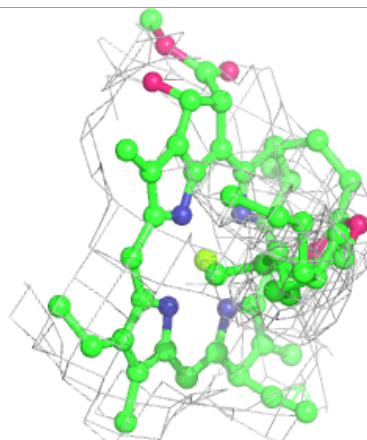
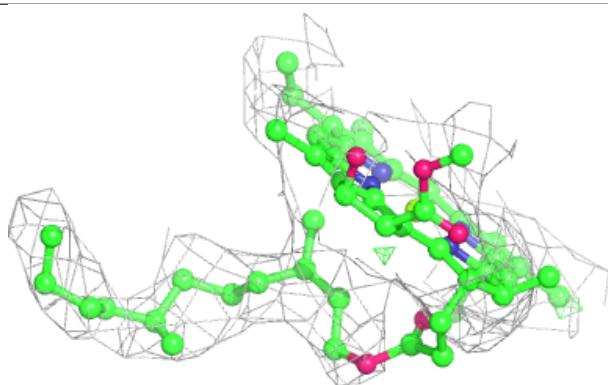
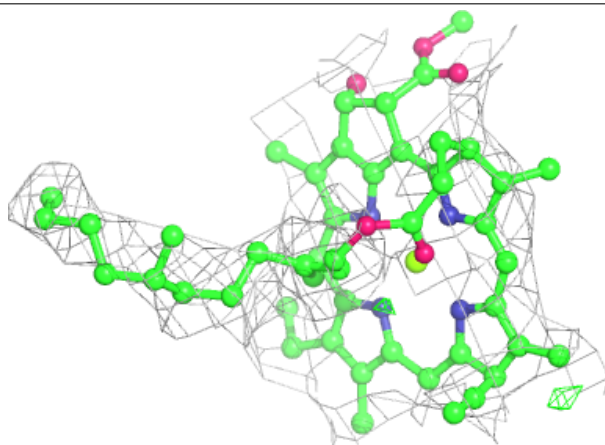


Electron density around CLA B 837:

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

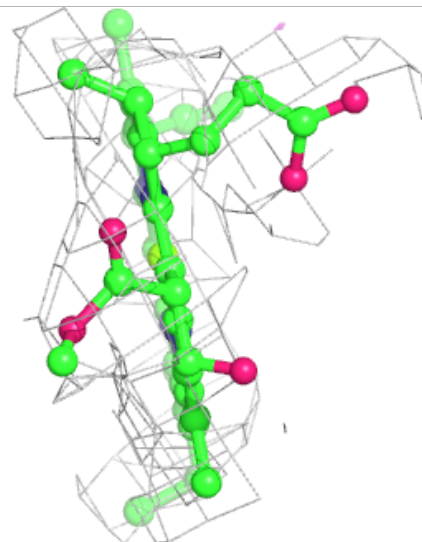
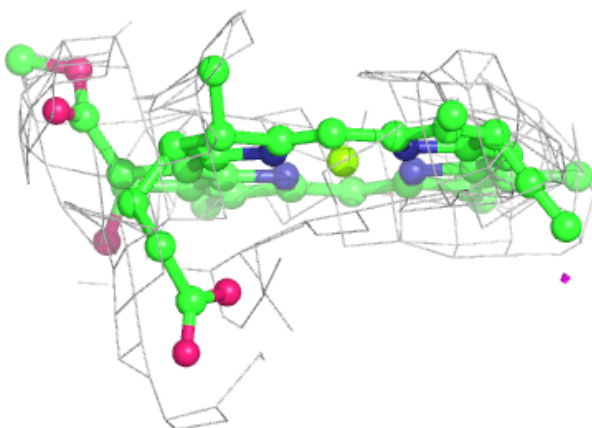
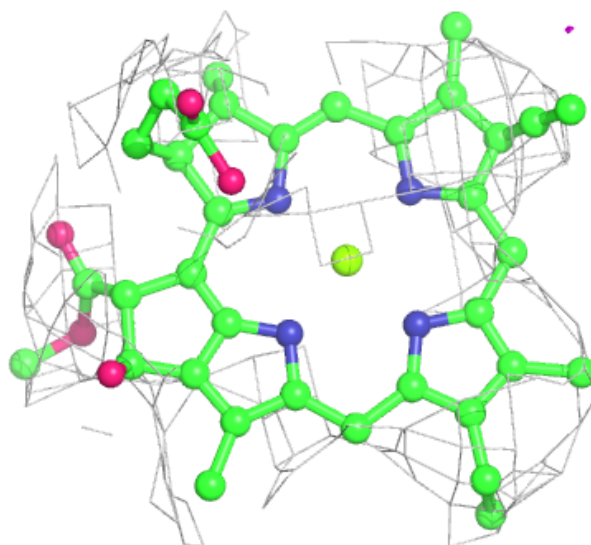
**Electron density around CLA 2 303:**

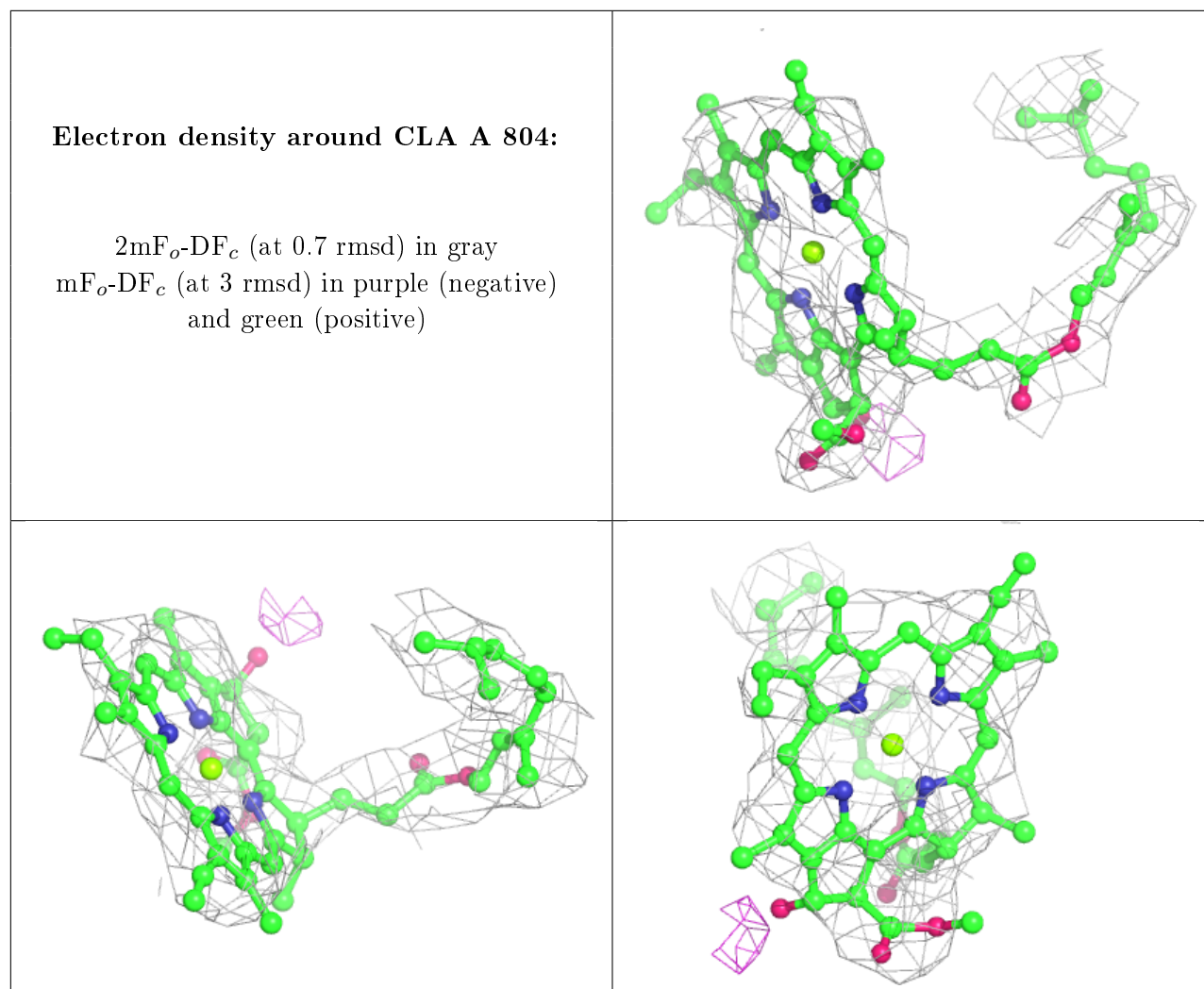
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

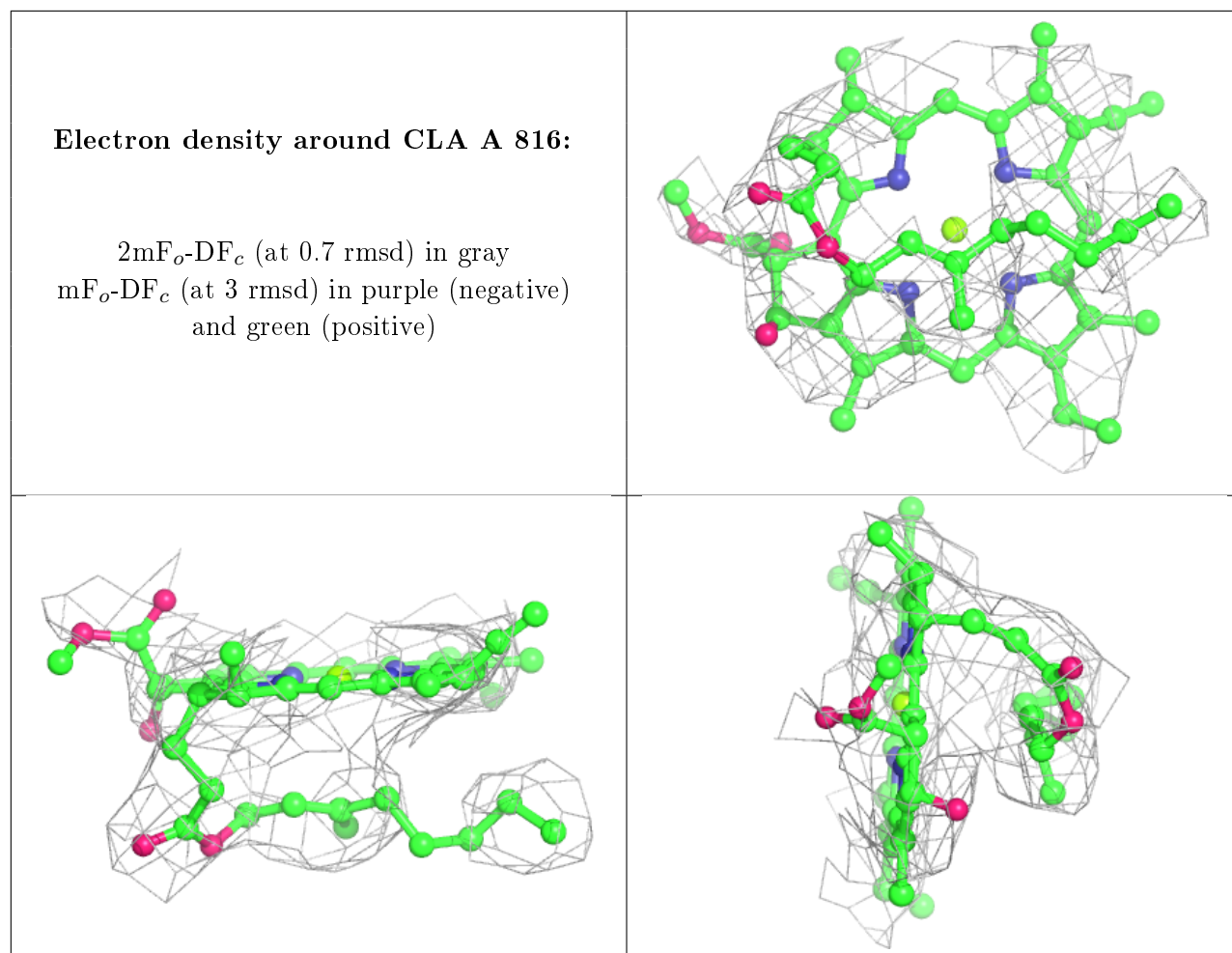


Electron density around CLA B 834:

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

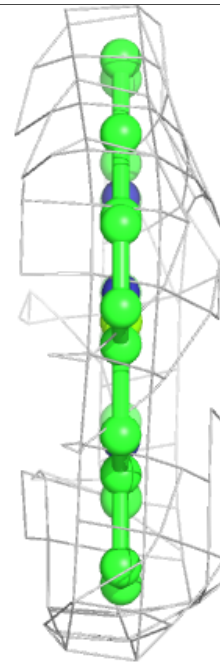
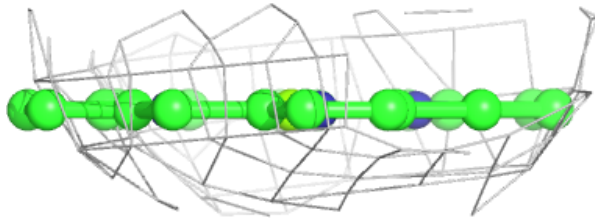
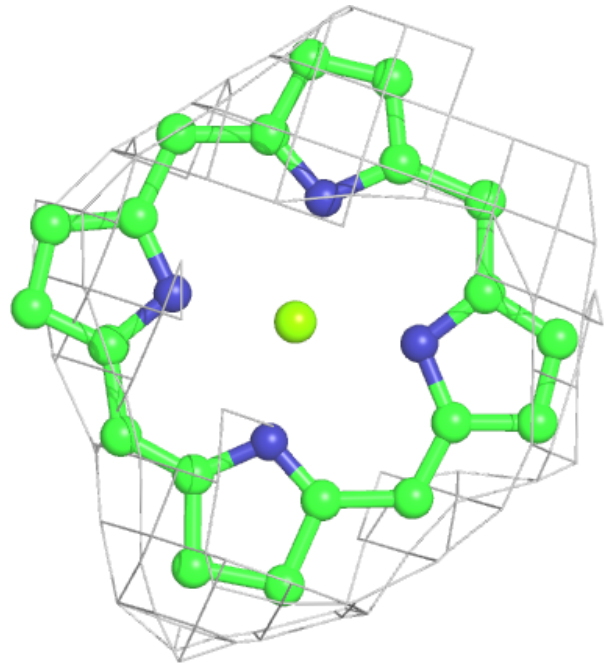






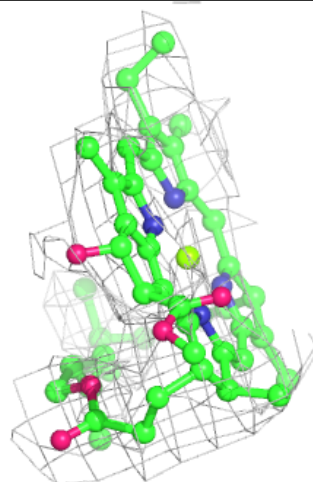
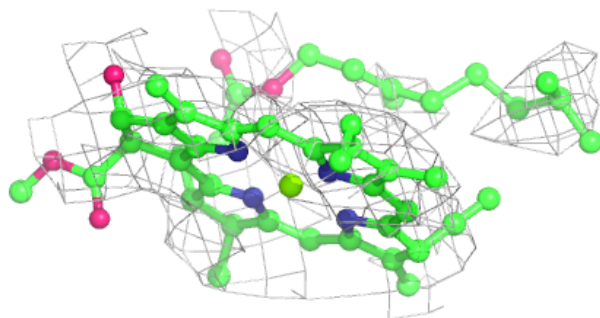
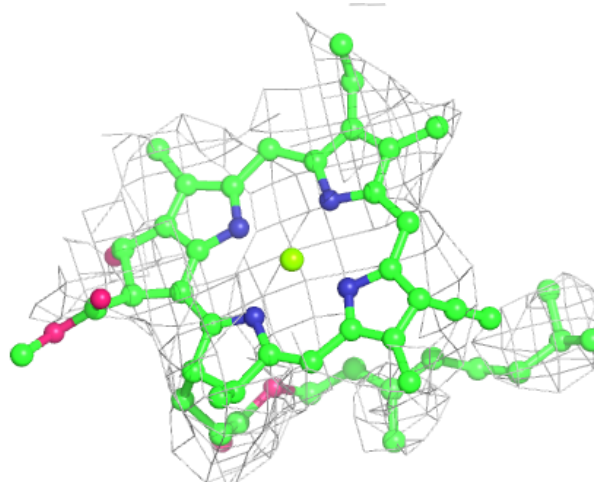
Electron density around CLA 4 311:

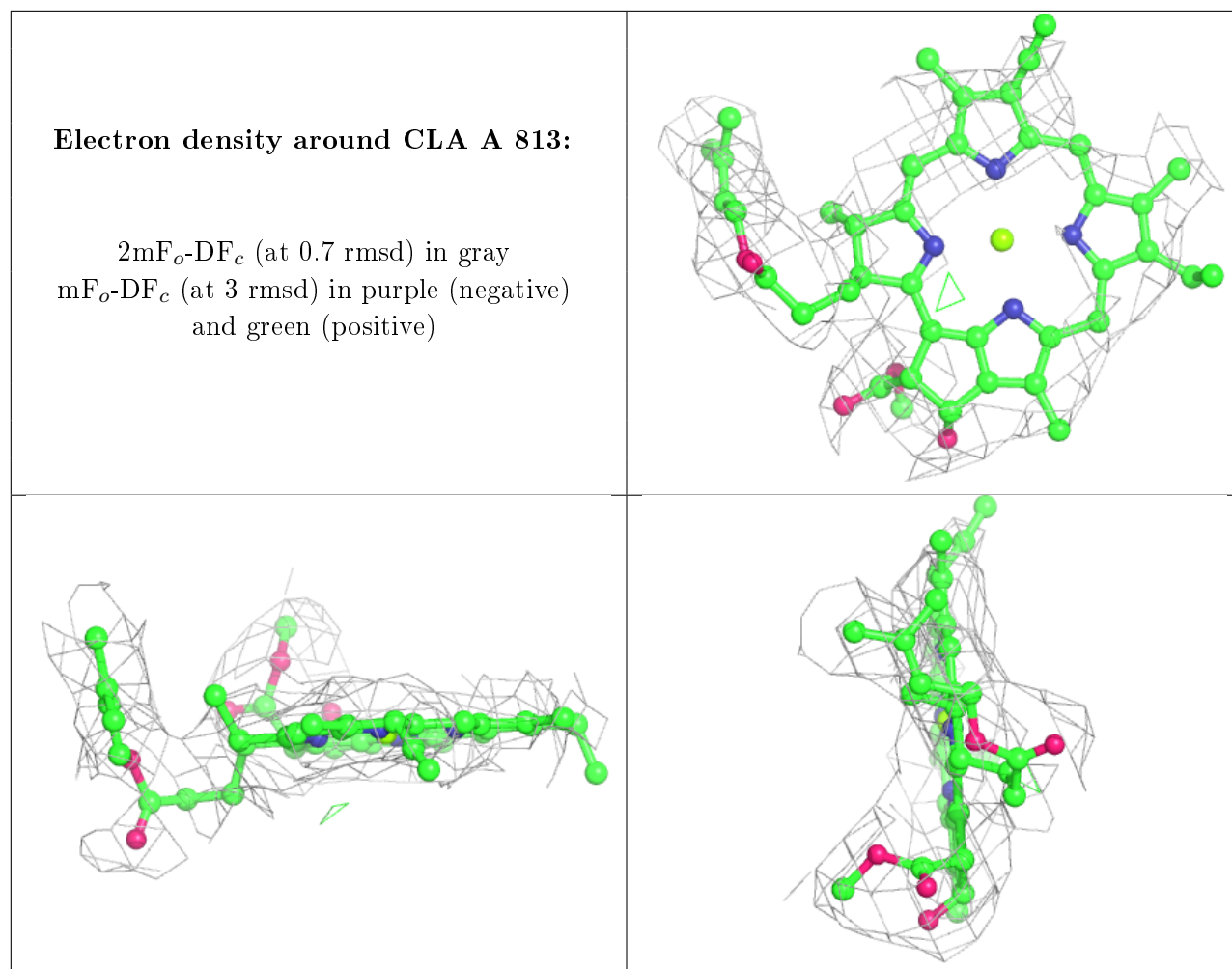
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

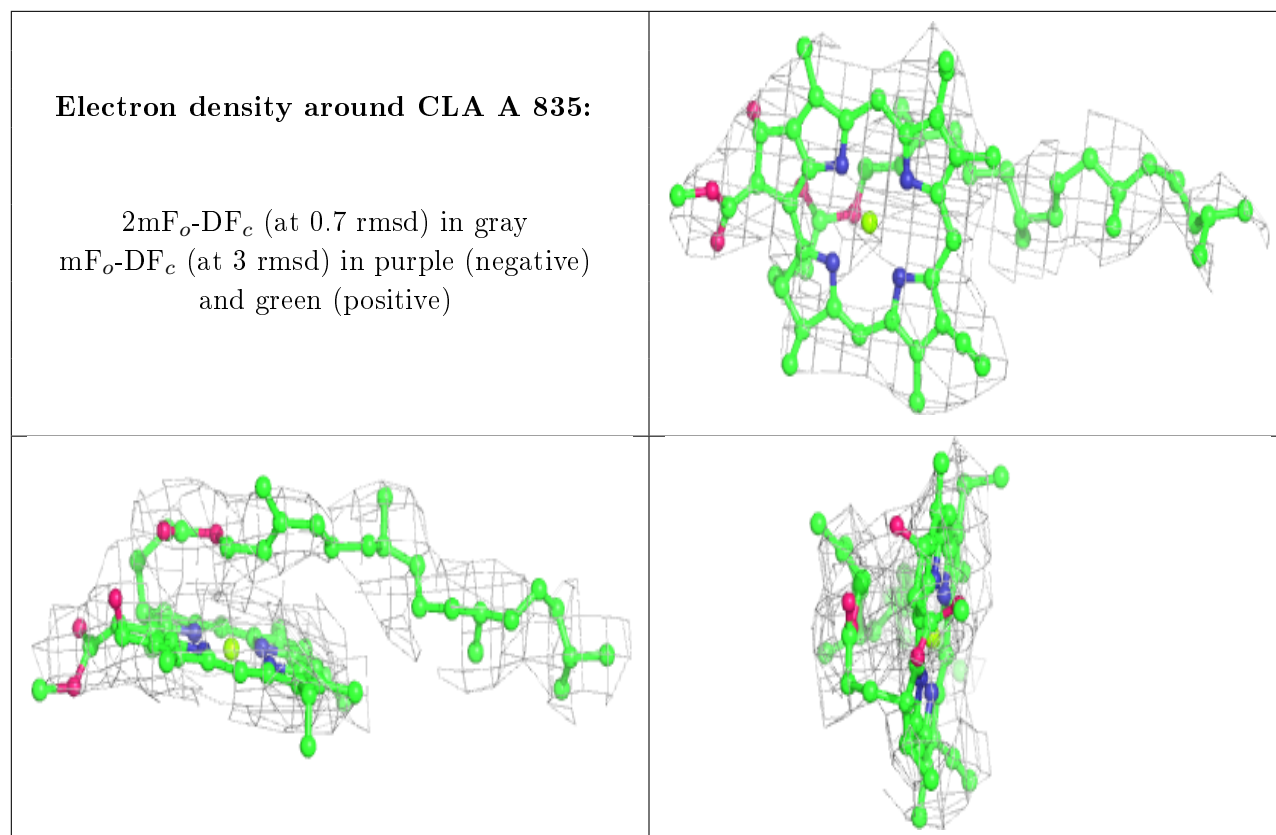


Electron density around CLA B 823:

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

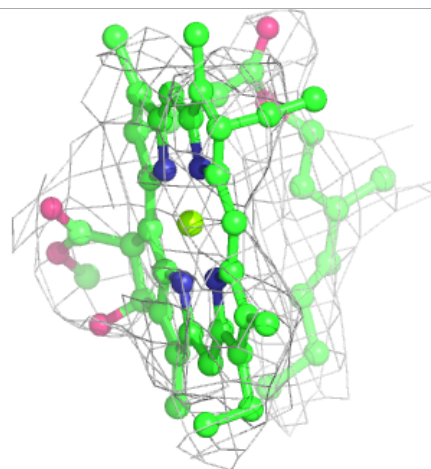
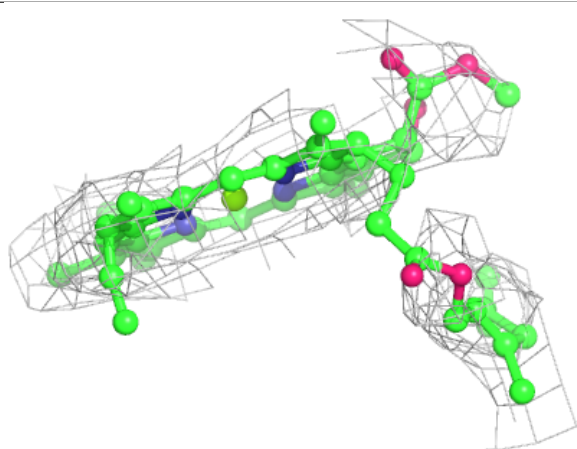
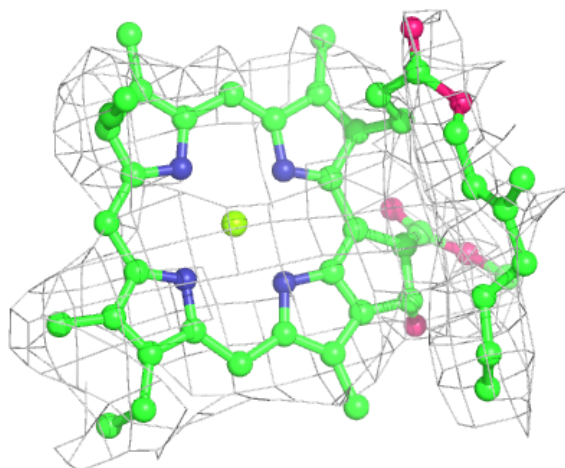






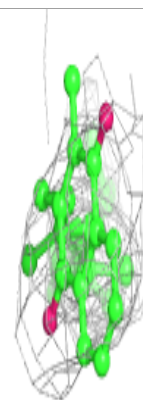
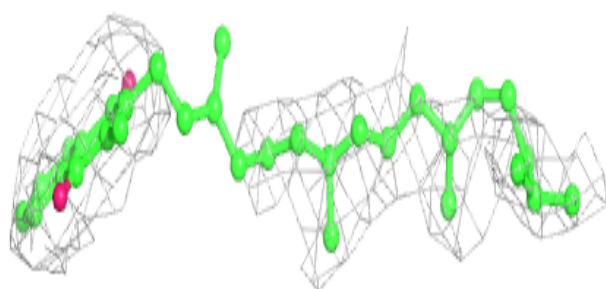
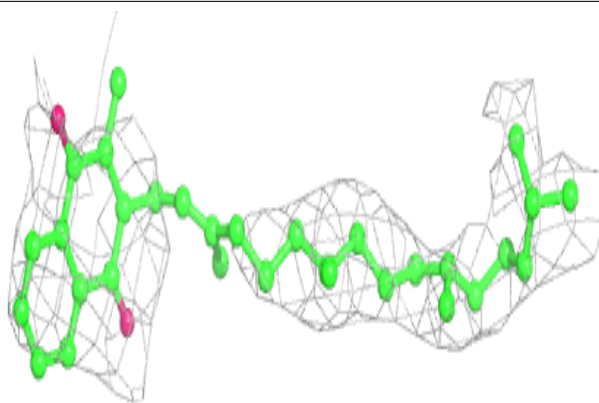
Electron density around CLA F 207:

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

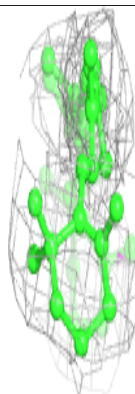
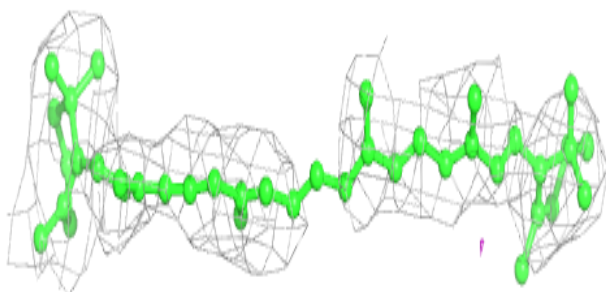
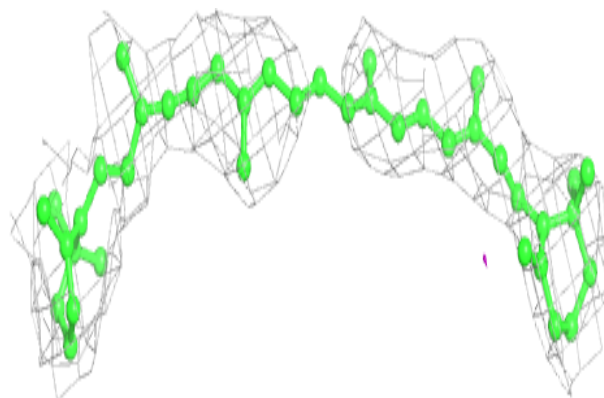


Electron density around PQN A 842:

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

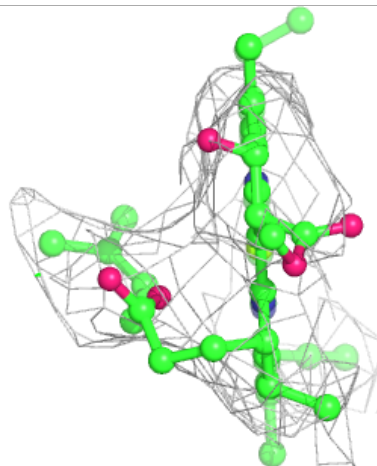
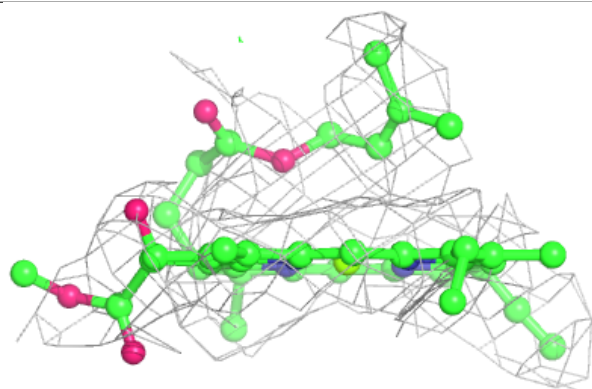
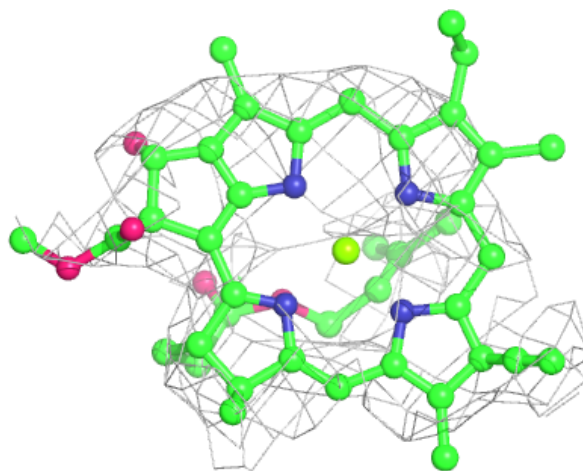
**Electron density around BCR B 844:**

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



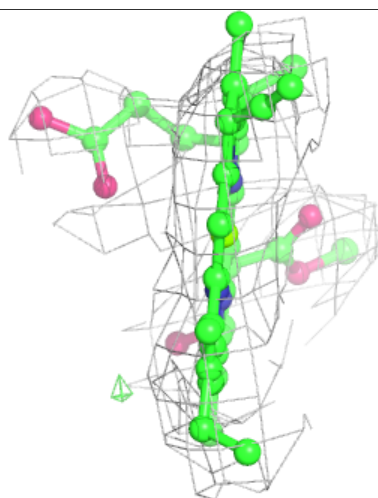
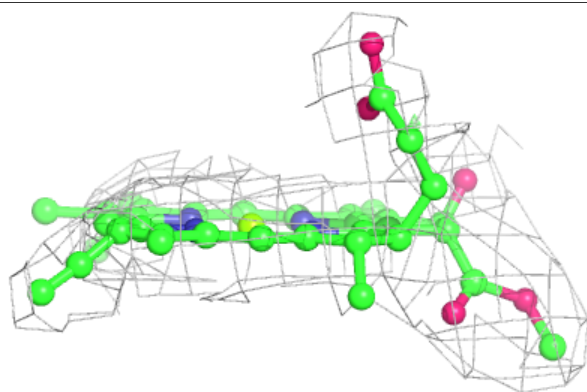
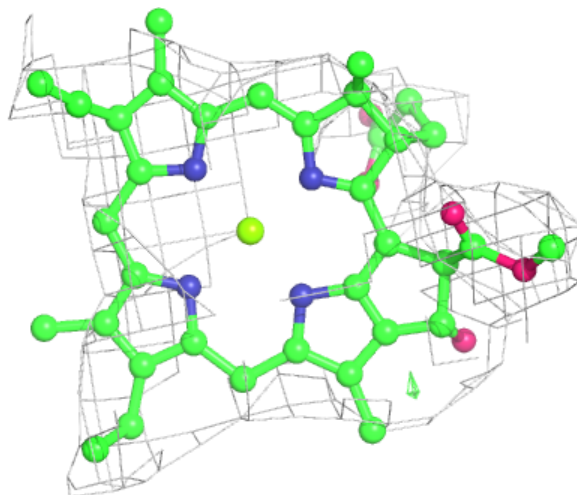
Electron density around CLA B 821:

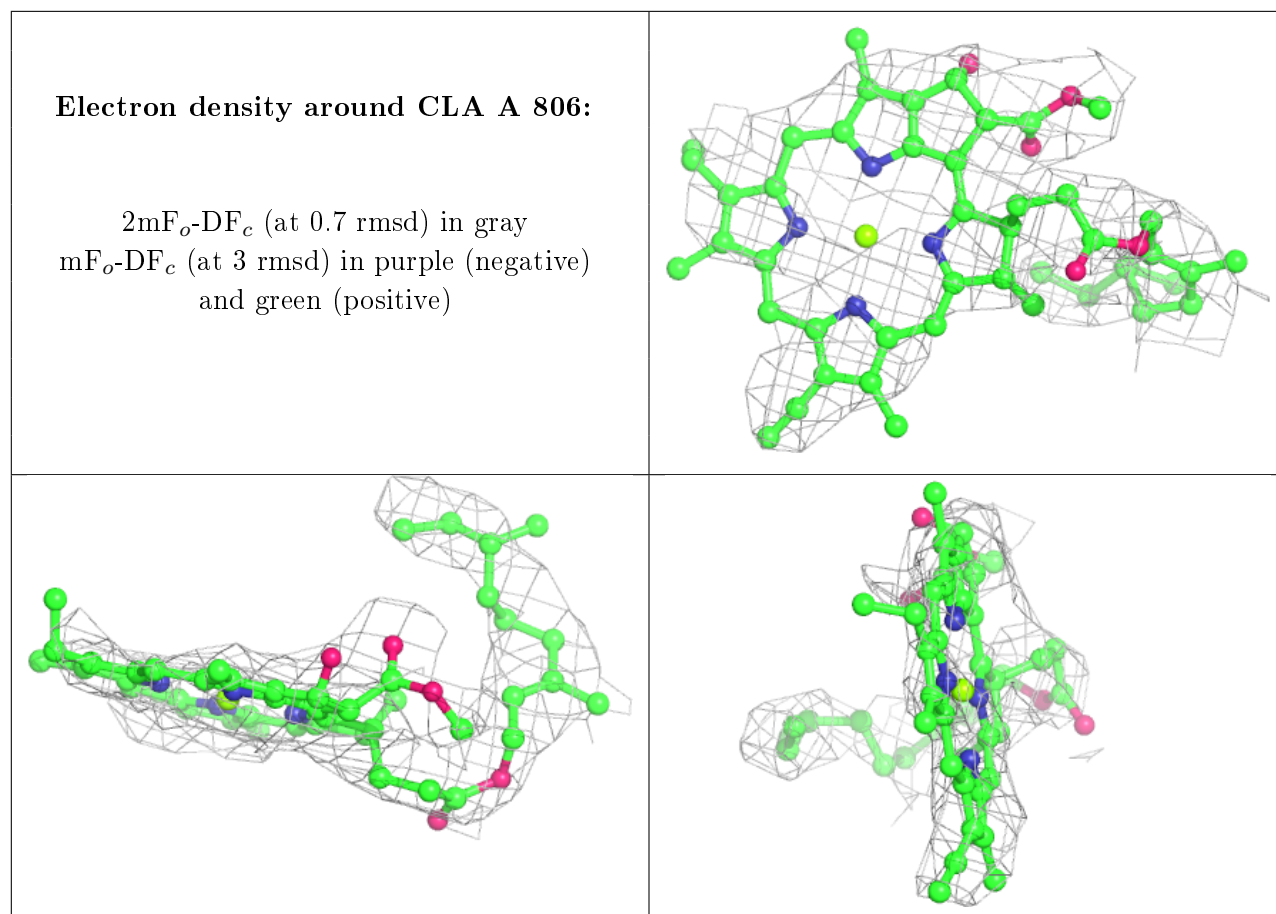
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 807:

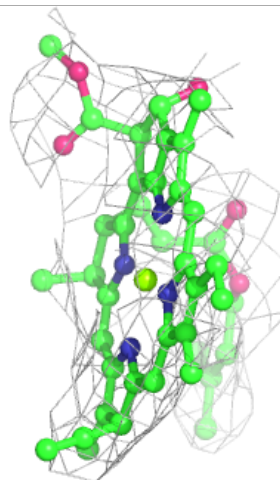
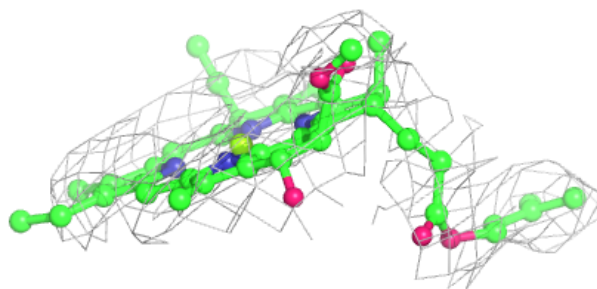
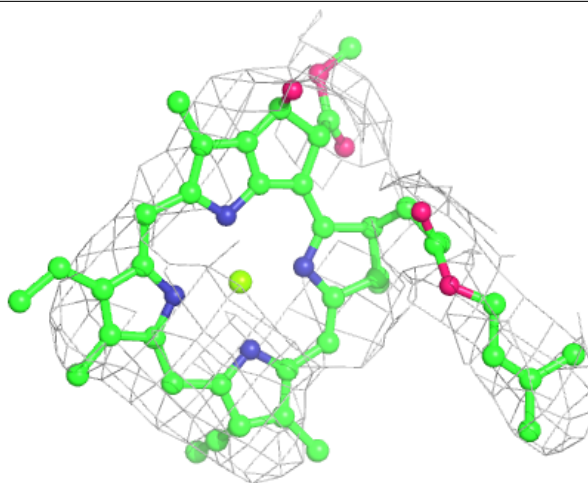
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





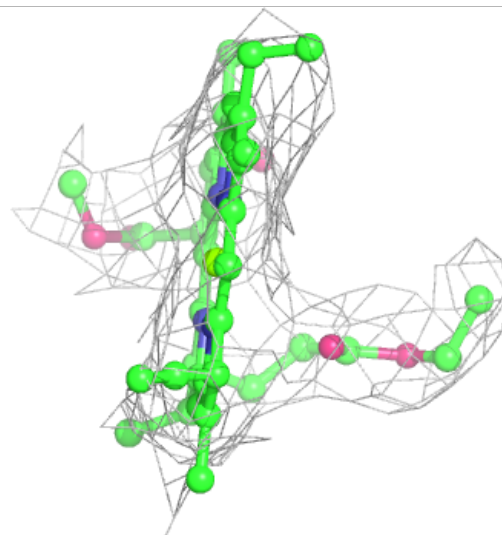
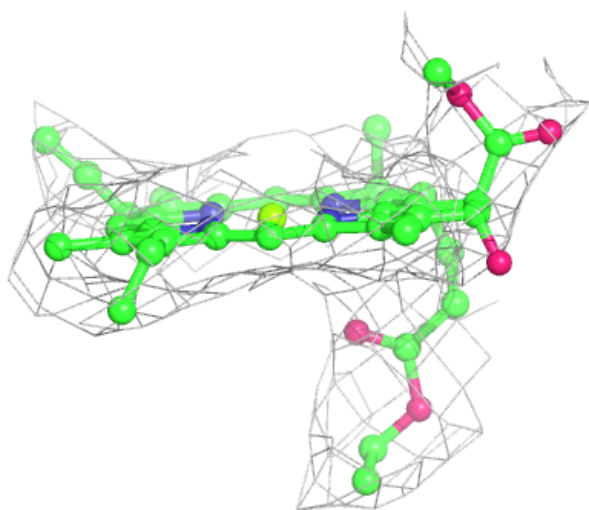
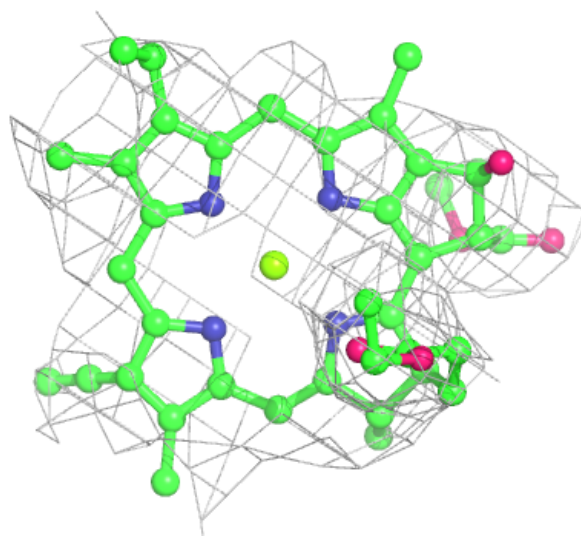
Electron density around CLA A 832:

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



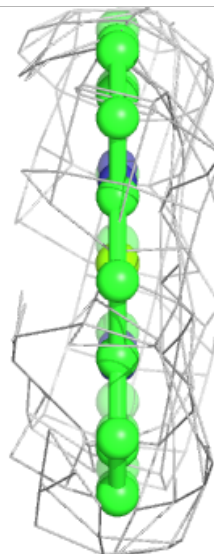
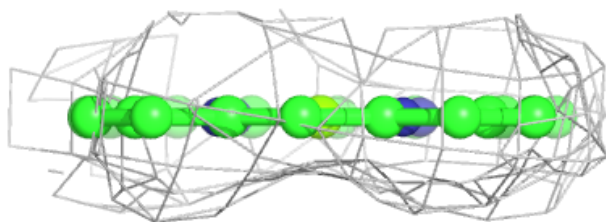
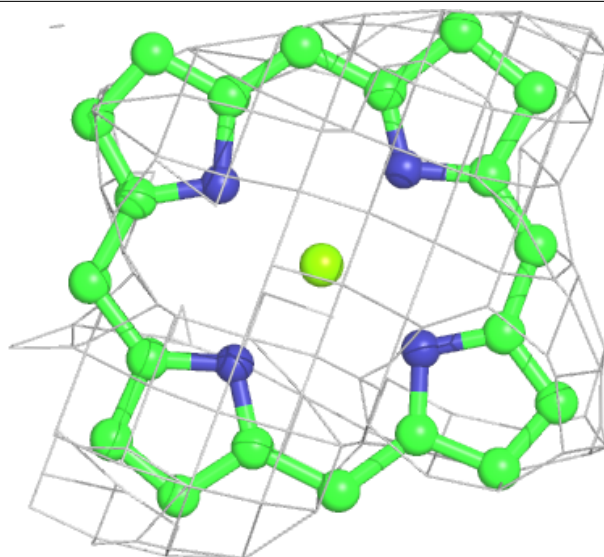
Electron density around CLA L 209:

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



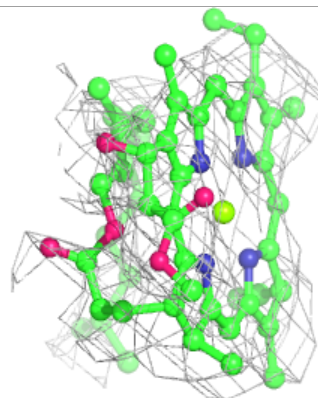
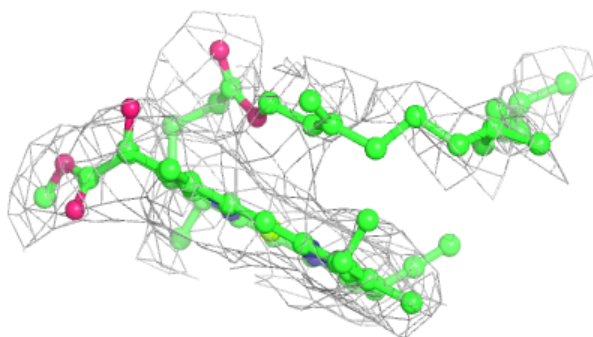
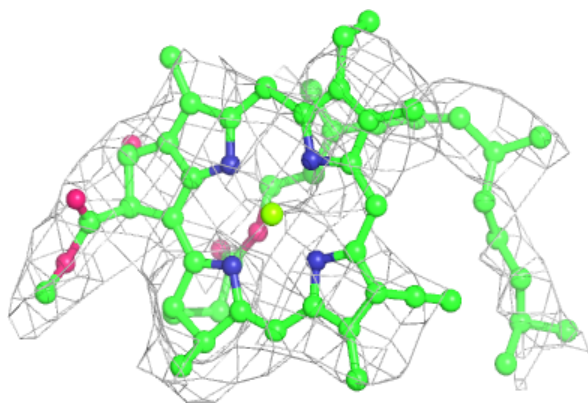
Electron density around CLA 1 209:

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

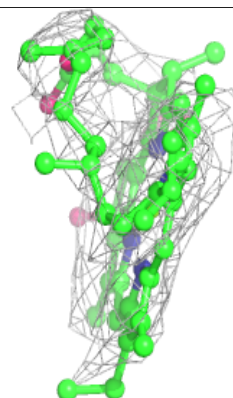
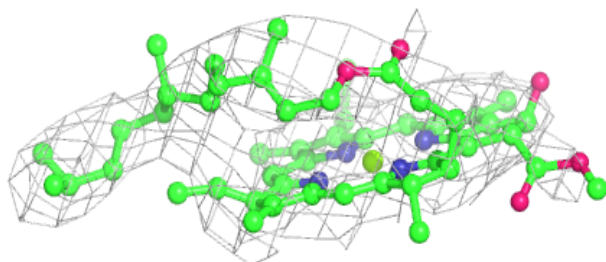
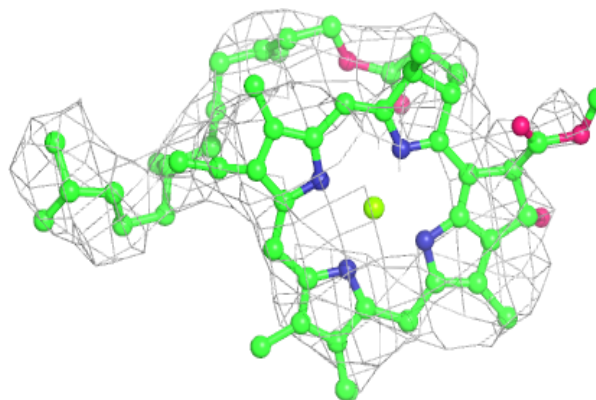


Electron density around CLA I 102:

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

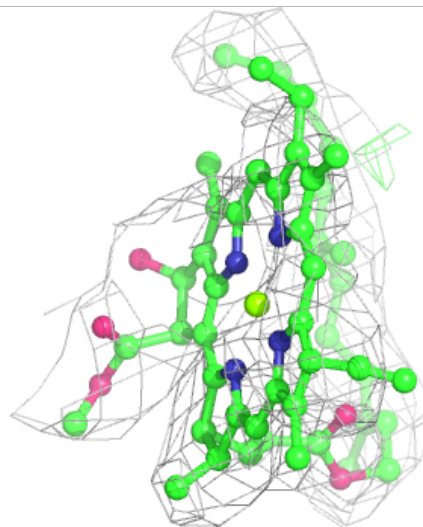
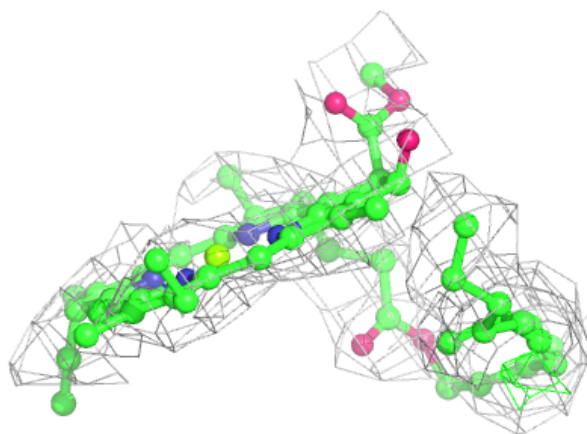
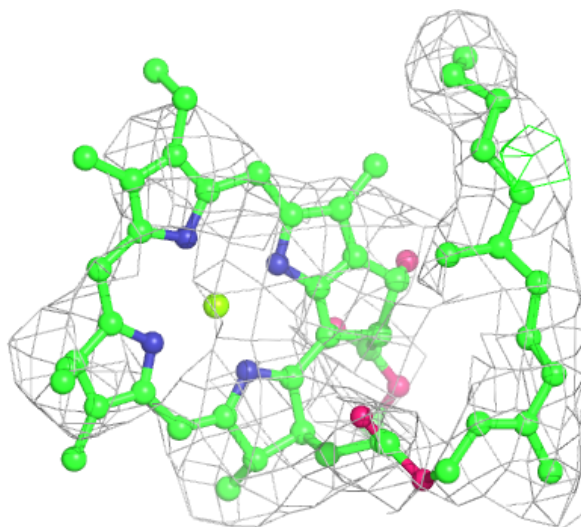
**Electron density around CLA A 818:**

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



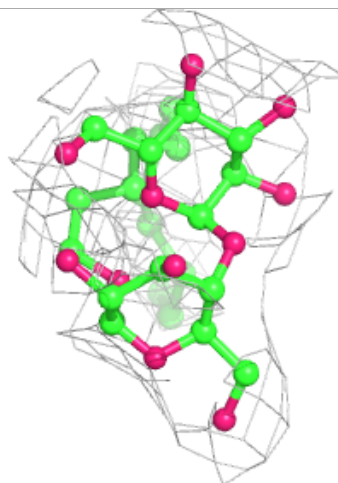
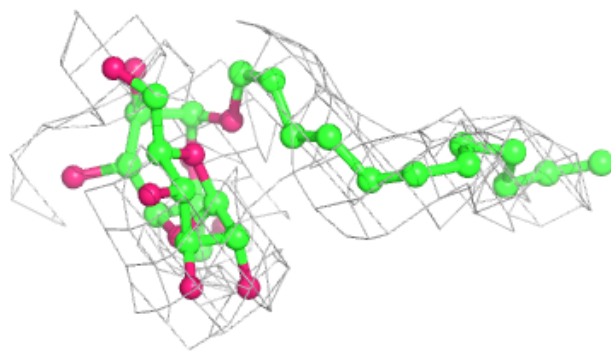
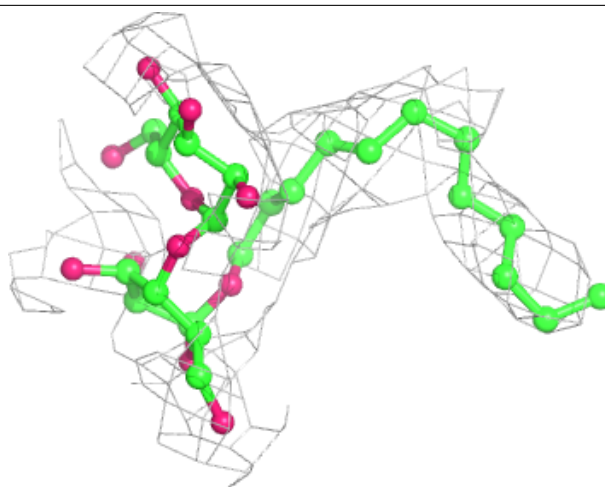
Electron density around CLA B 832:

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



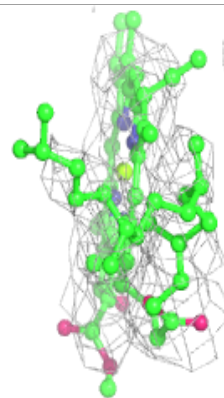
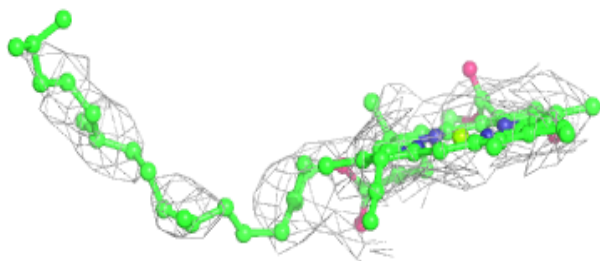
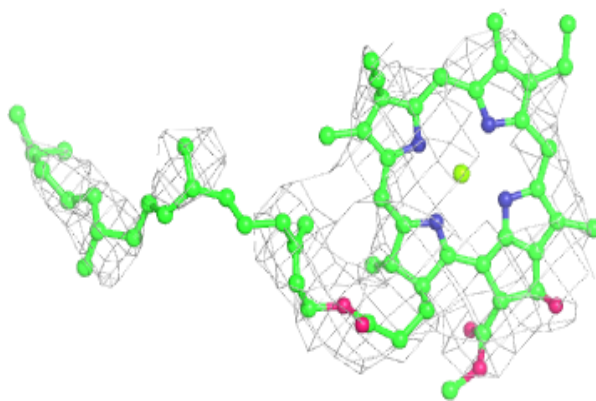
Electron density around LMU H 105:

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

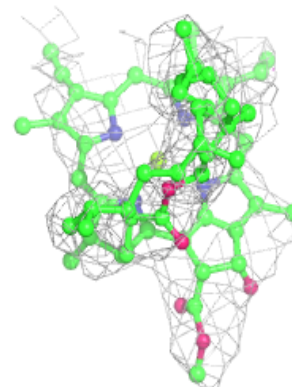
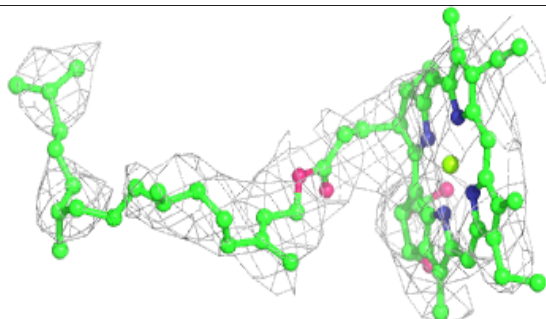
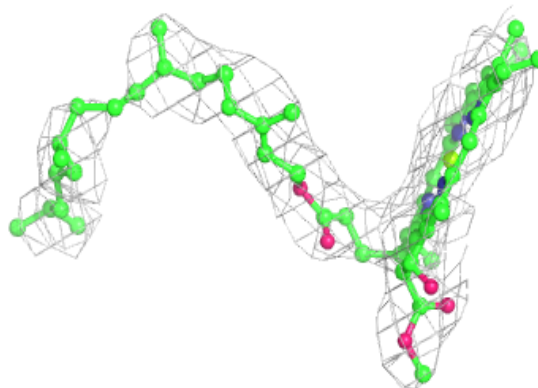


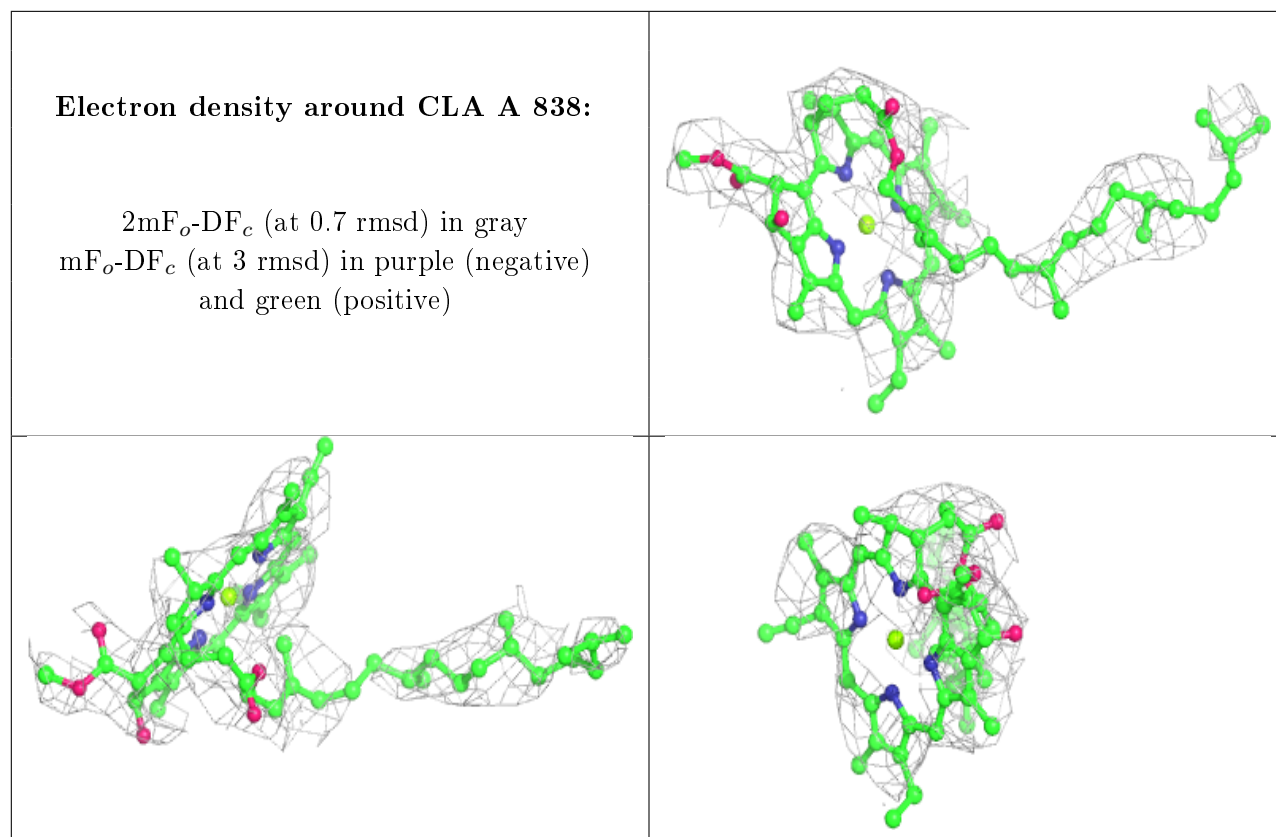
Electron density around CLA B 803:

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

**Electron density around CLA B 840:**

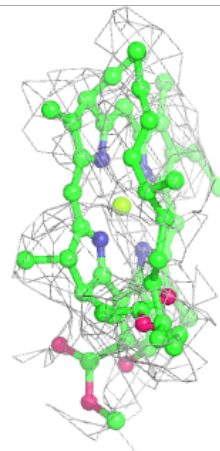
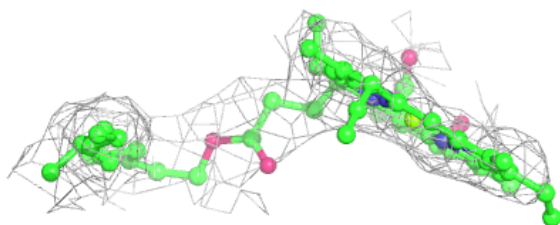
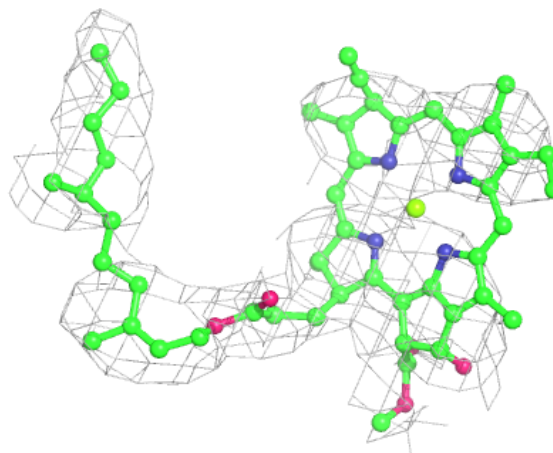
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





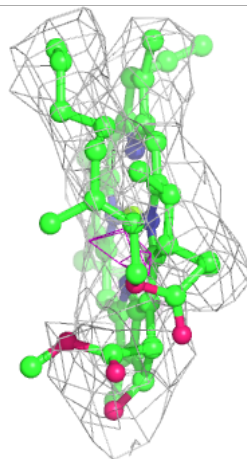
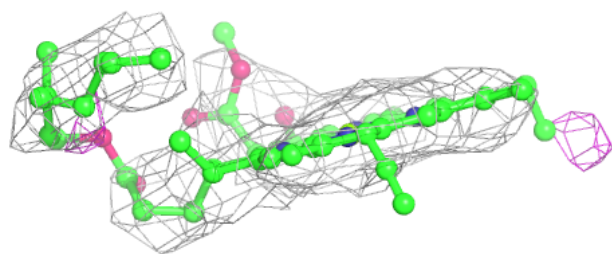
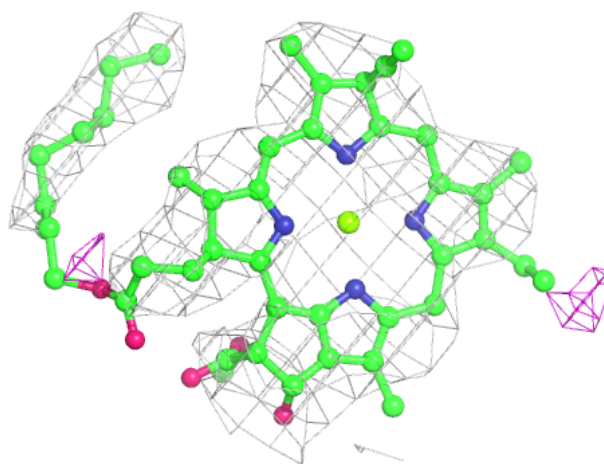
Electron density around CLA B 826:

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



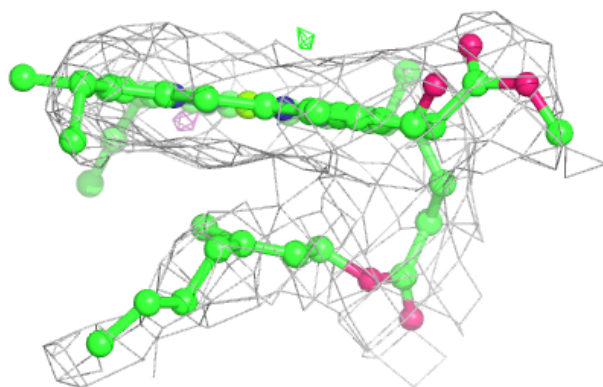
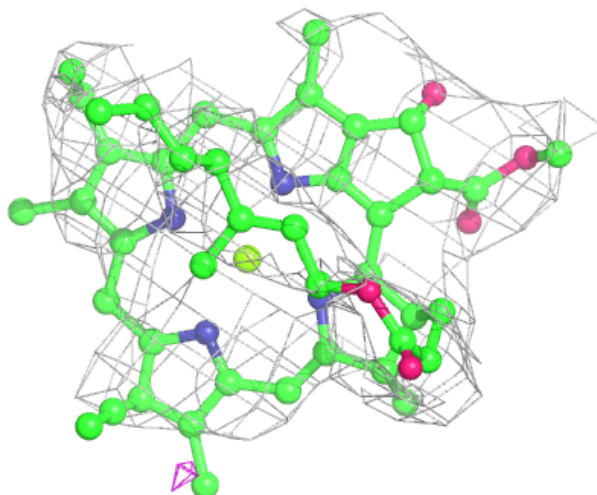
Electron density around CLA B 825:

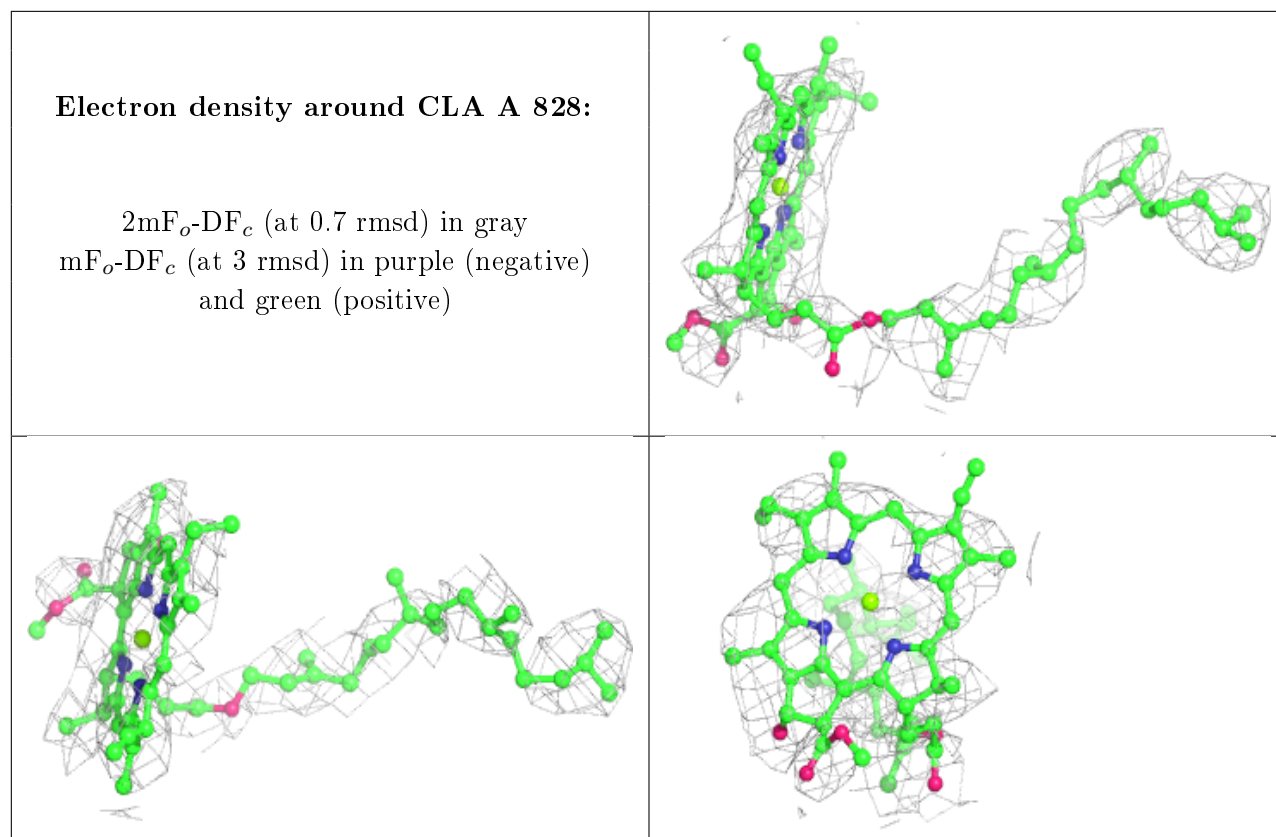
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 818:

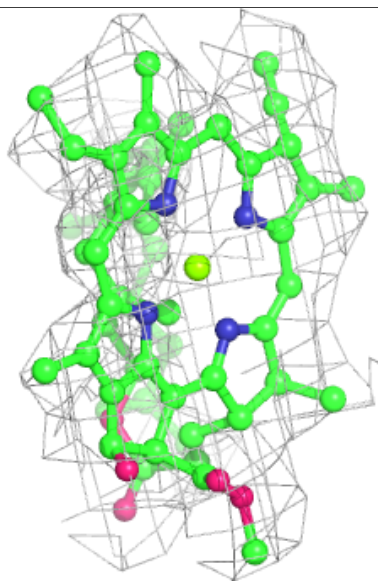
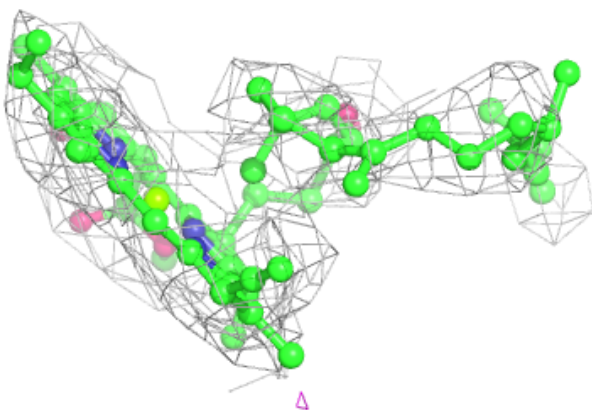
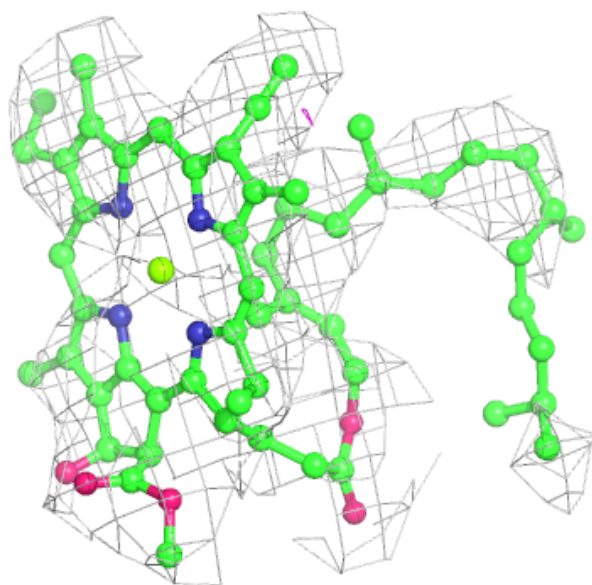
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





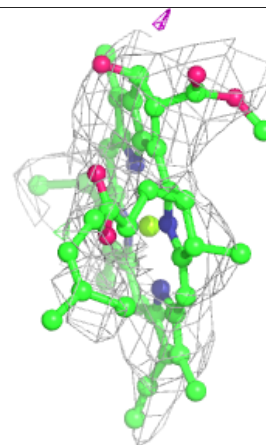
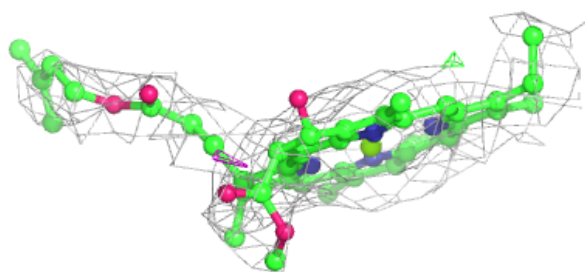
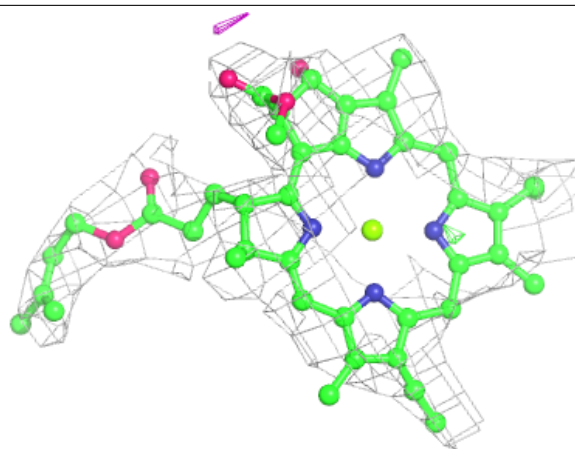
Electron density around CLA B 824:

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



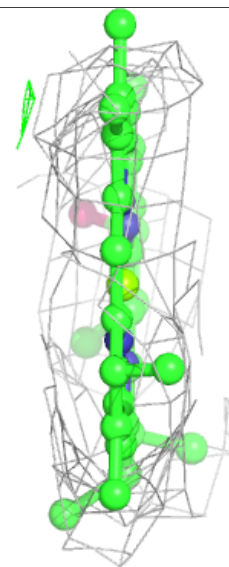
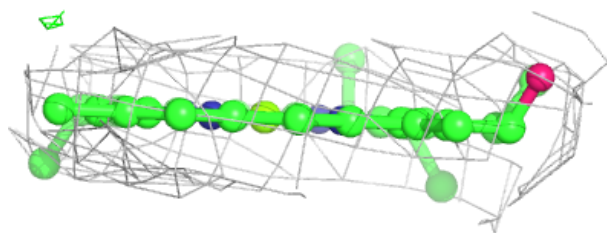
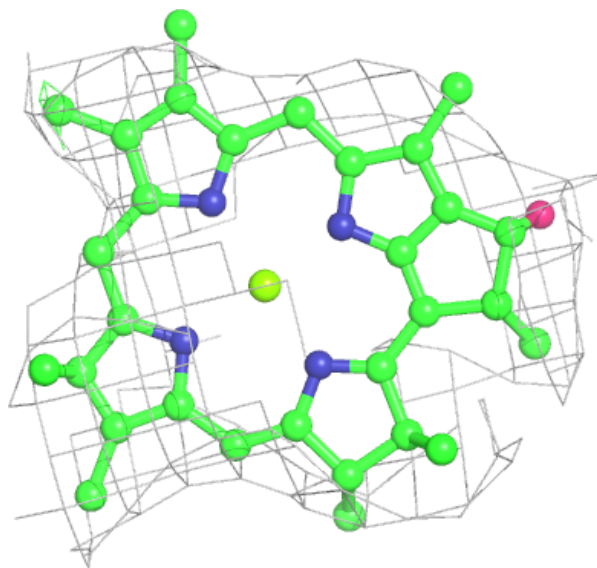
Electron density around CLA B 833:

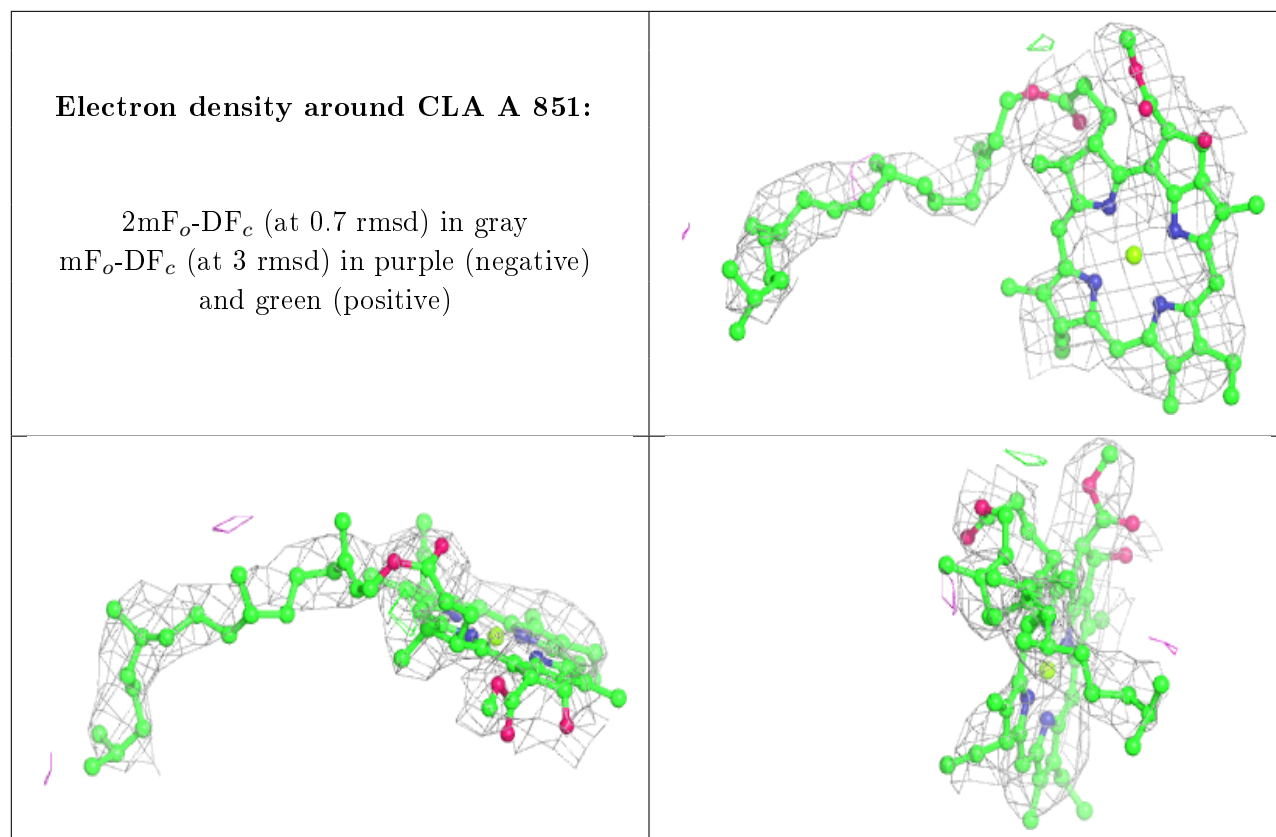
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

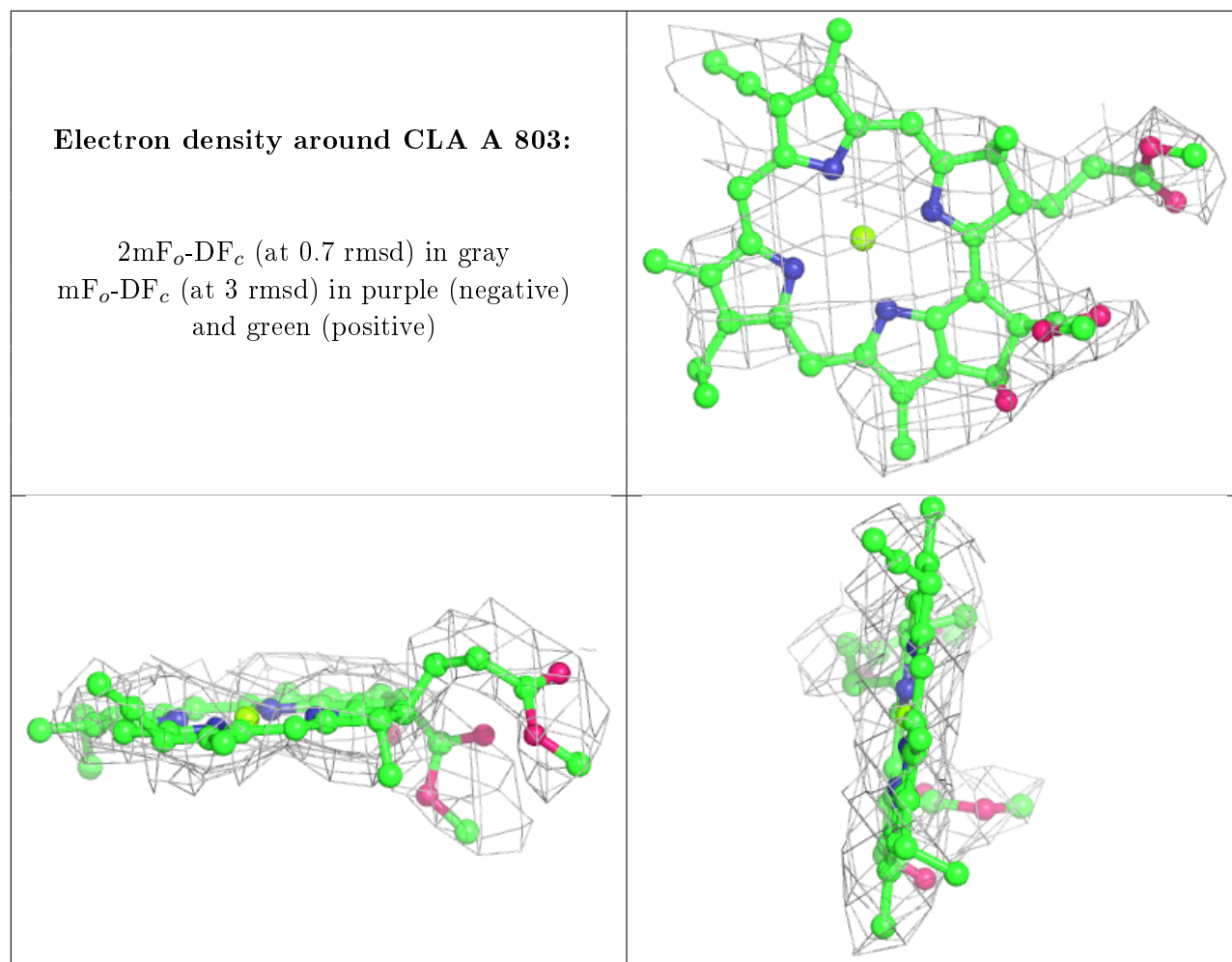


Electron density around CLA 4 313:

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

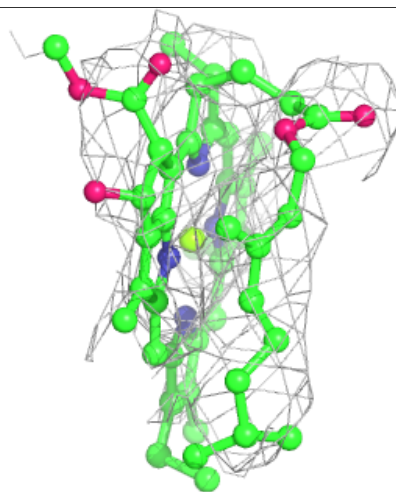
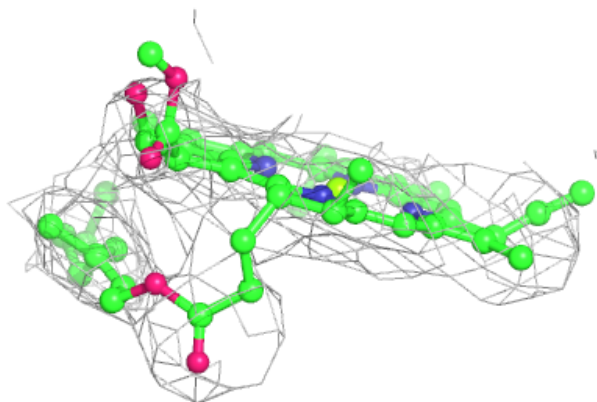
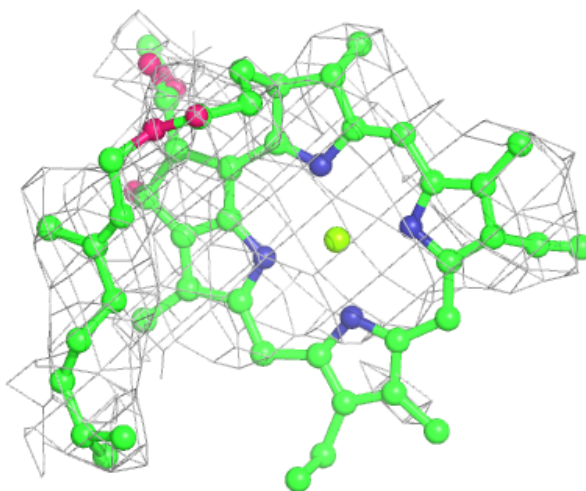






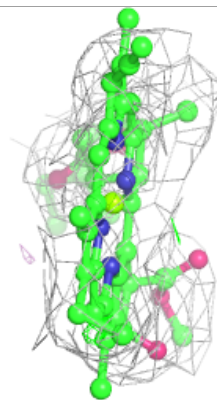
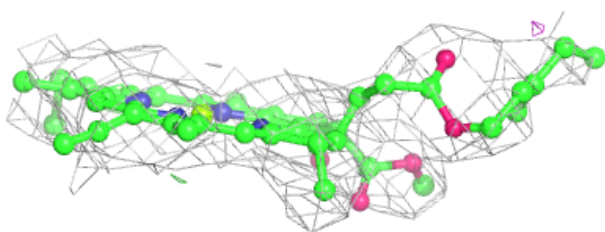
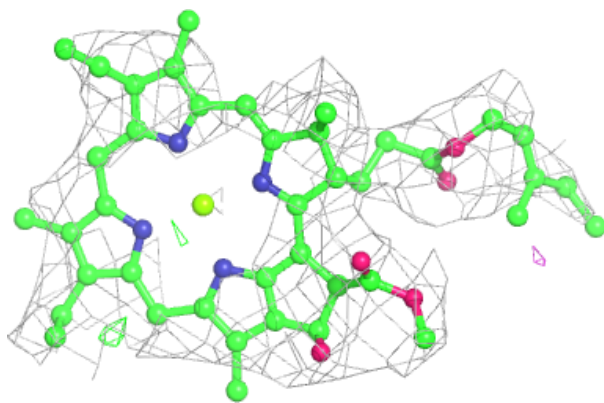
Electron density around CLA A 827:

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

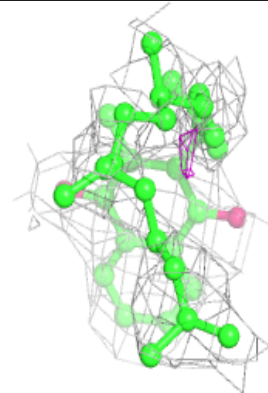
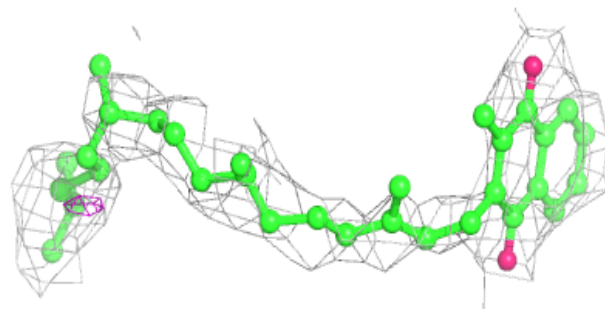
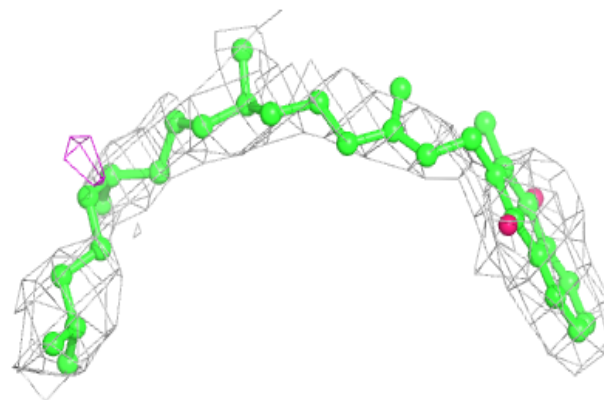


Electron density around CLA A 837:

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

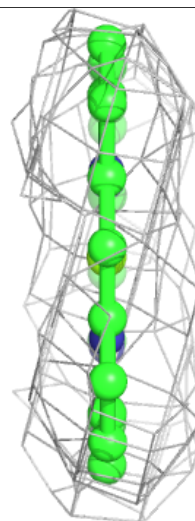
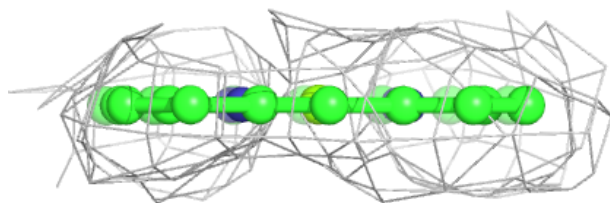
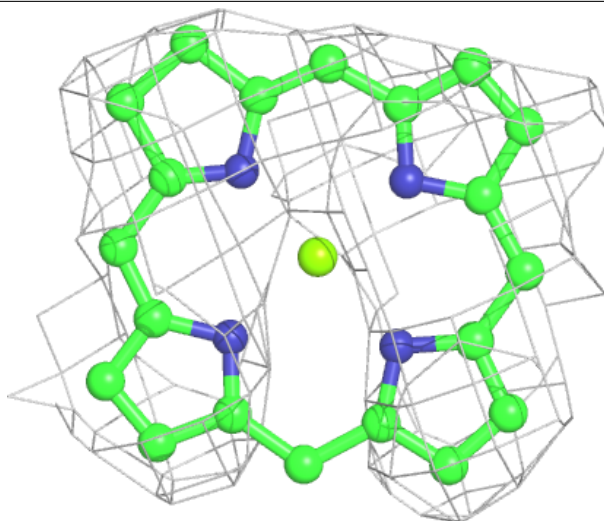
**Electron density around PQN B 843:**

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



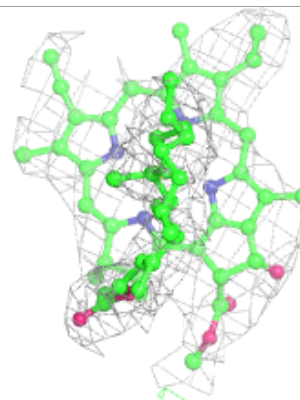
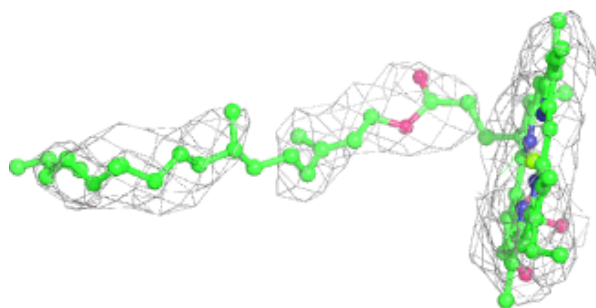
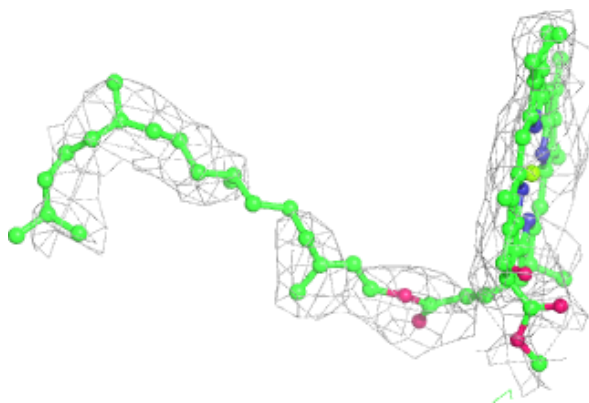
Electron density around CLA B 811:

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

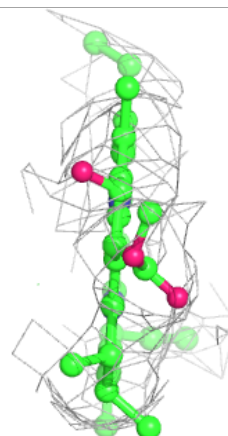
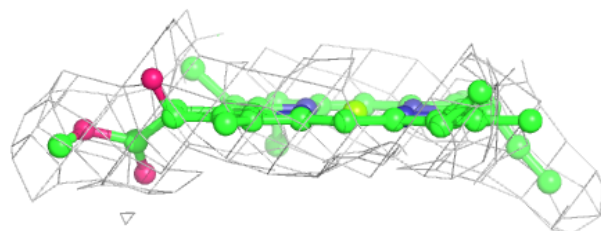
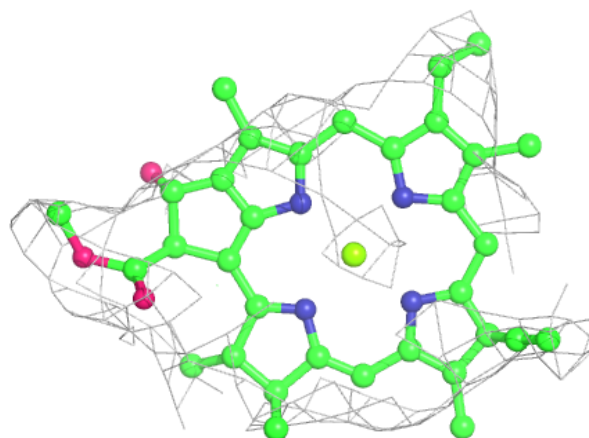


Electron density around CLA B 841:

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

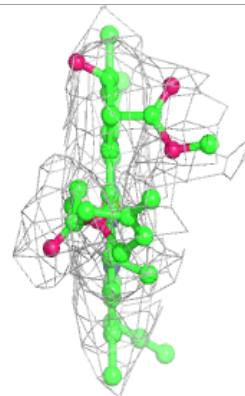
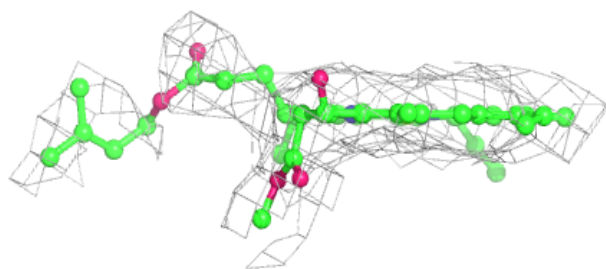
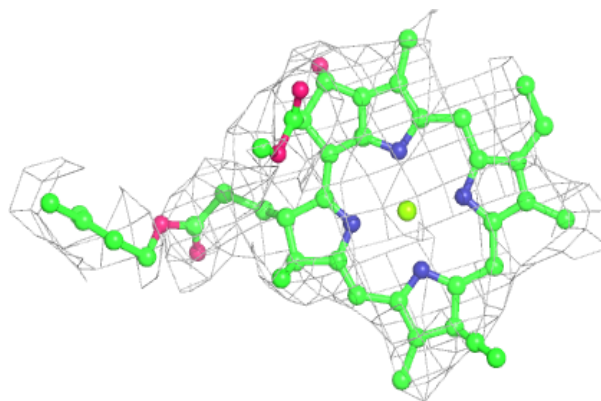
**Electron density around CLA 1 202:**

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

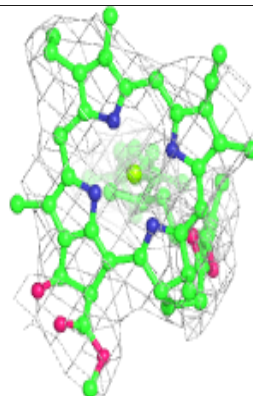
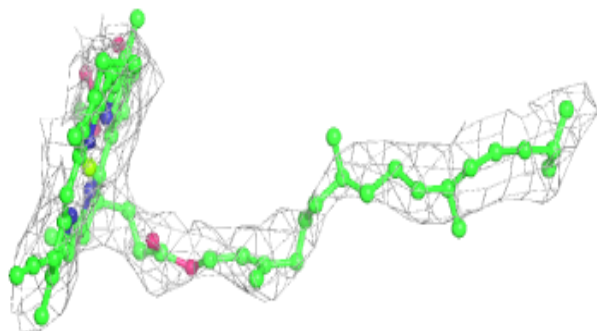
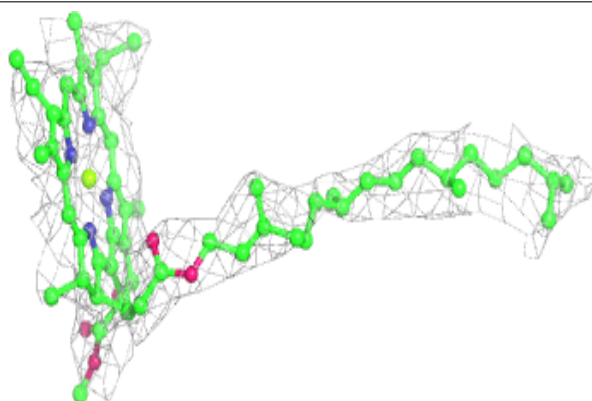


Electron density around CLA F 201:

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

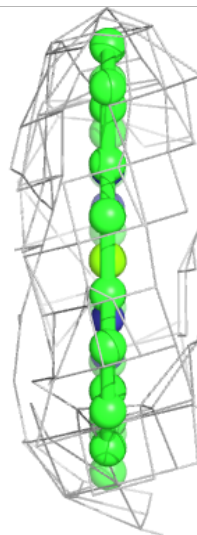
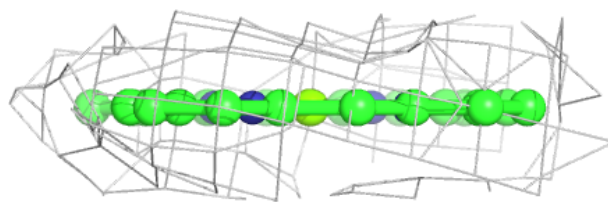
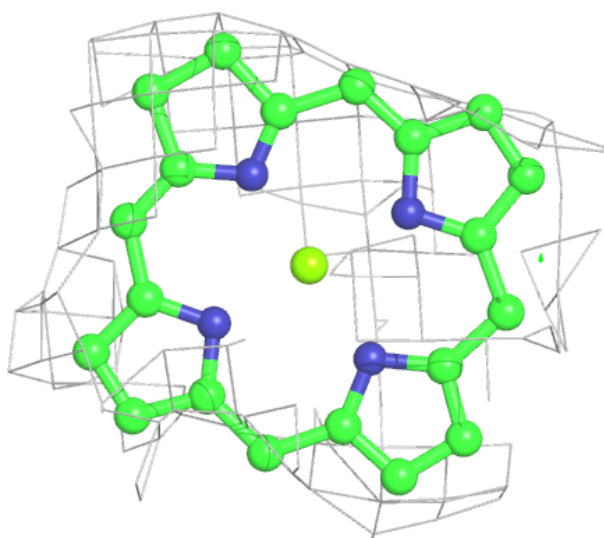
**Electron density around CLA B 829:**

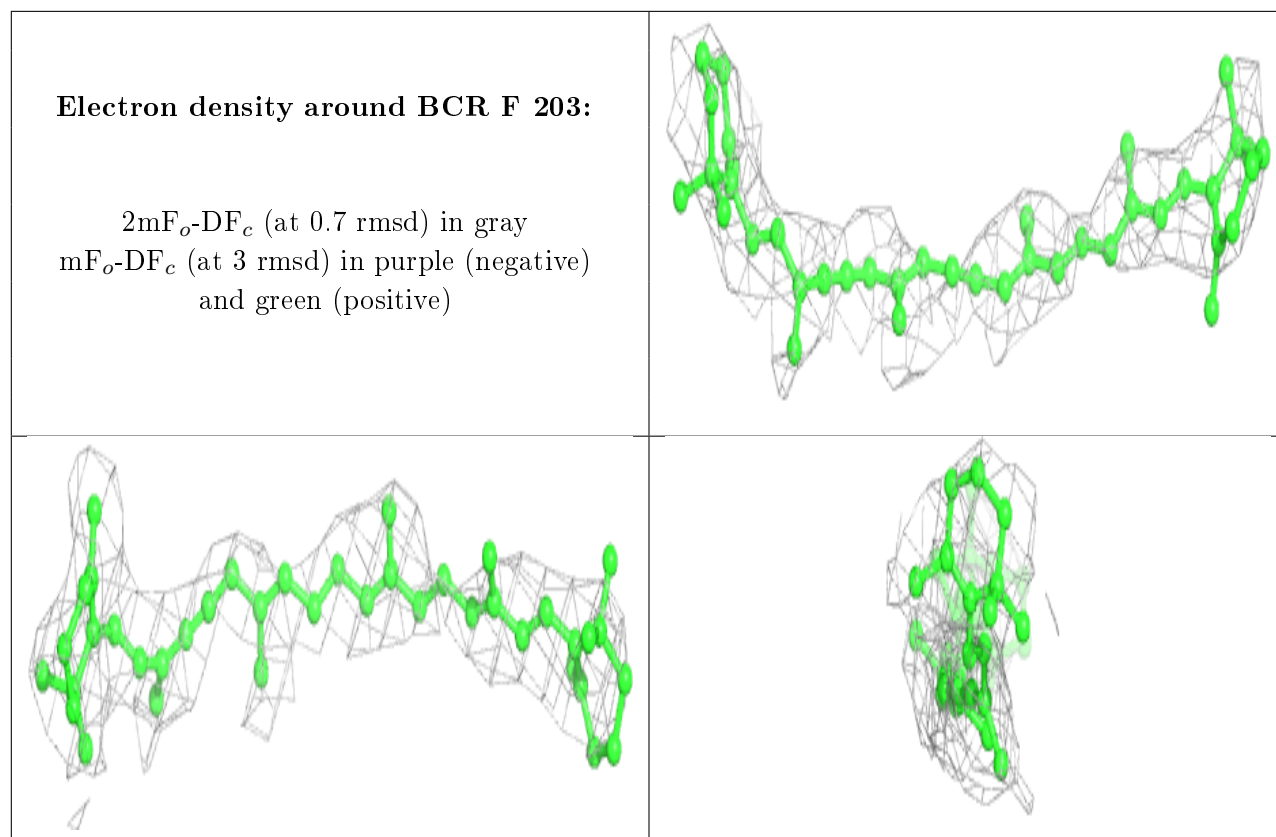
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 2 308:

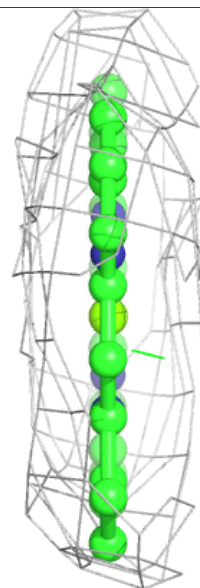
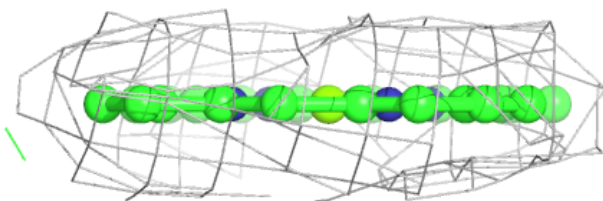
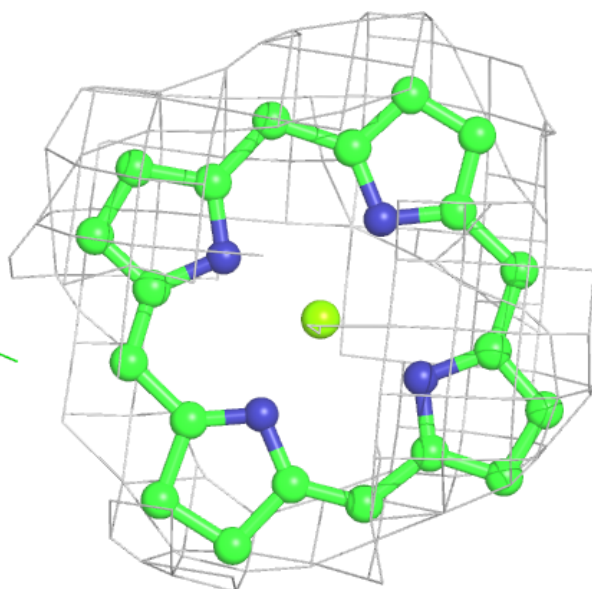
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

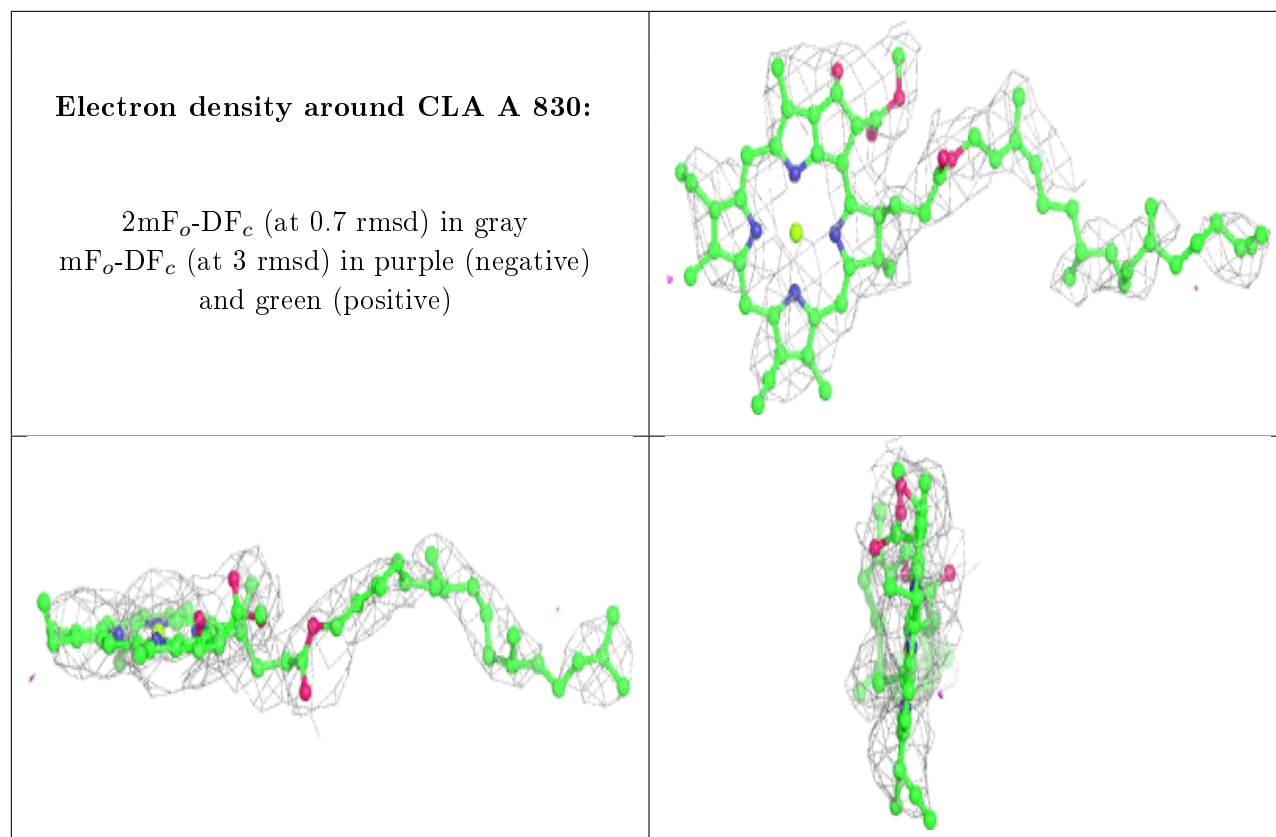




Electron density around CLA 4 312:

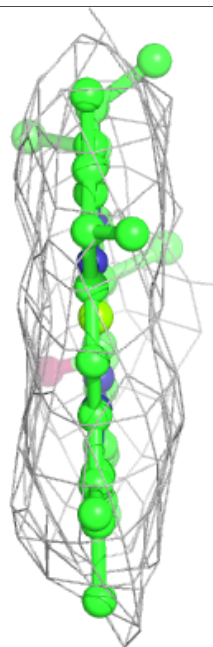
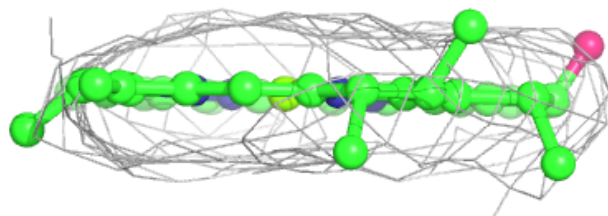
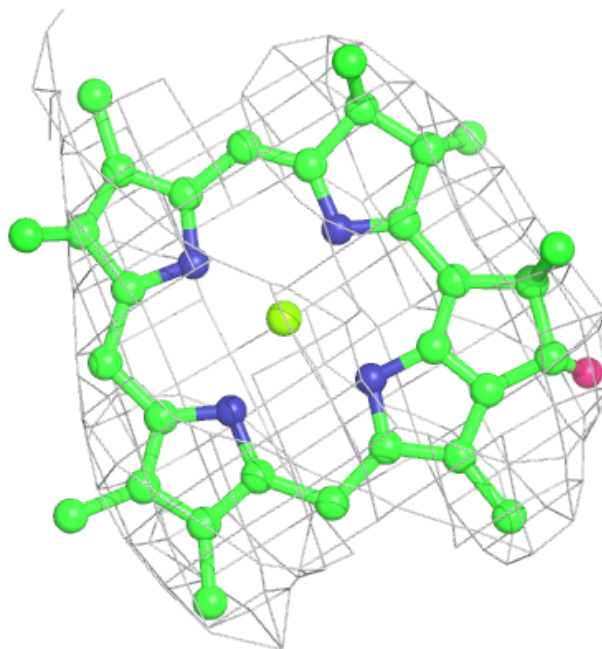
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





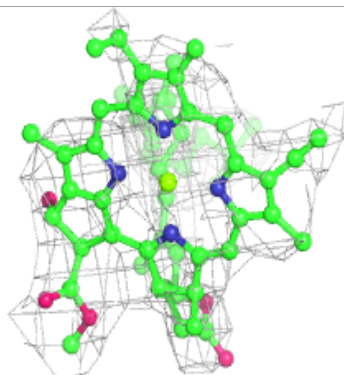
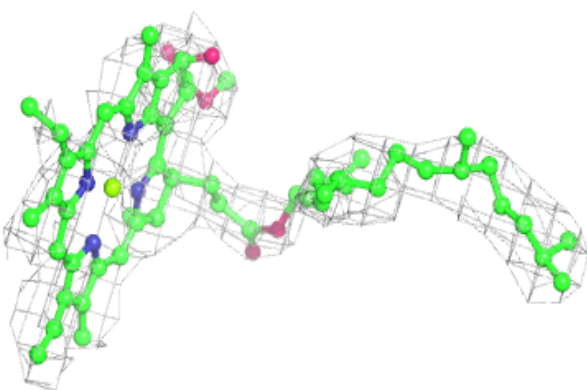
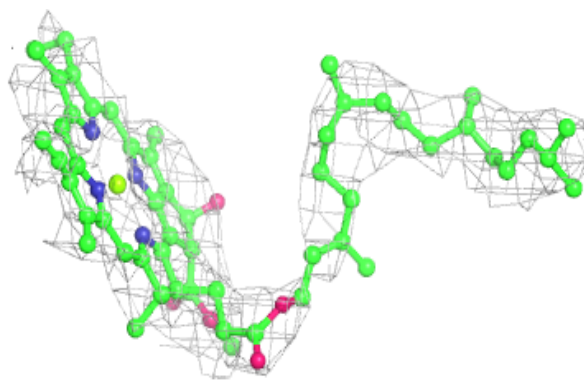
Electron density around CLA F 205:

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

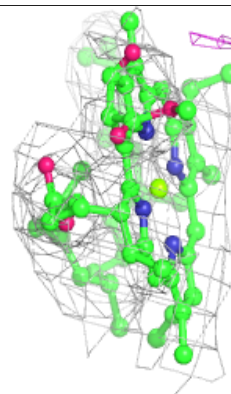
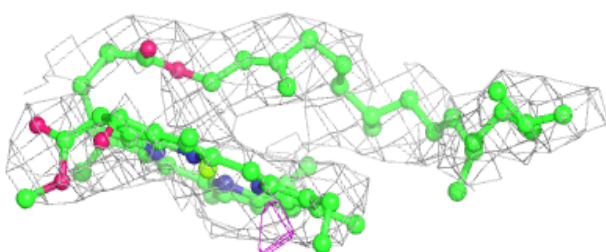
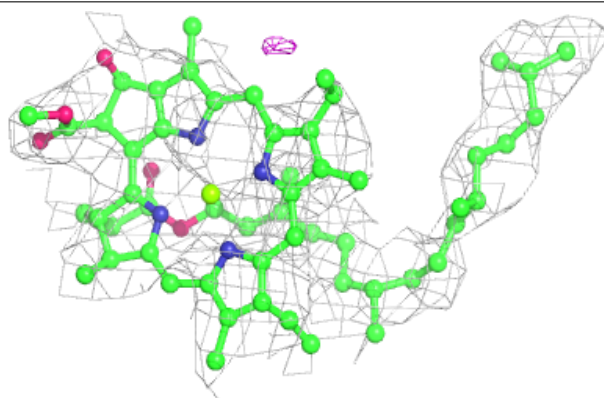


Electron density around CLA B 850:

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

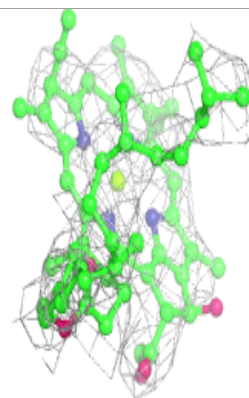
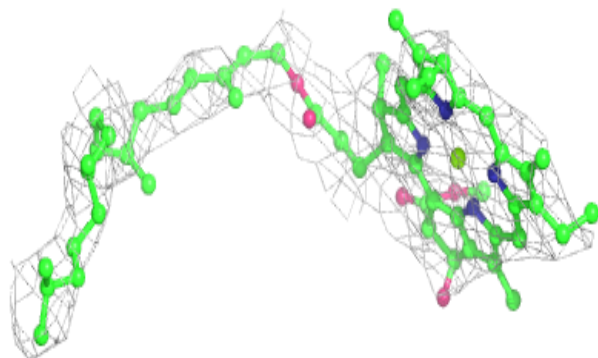
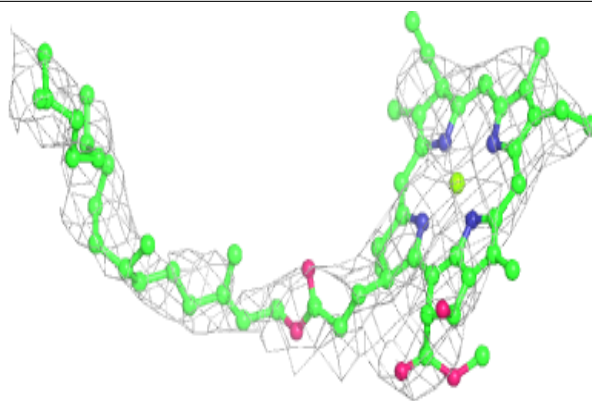
**Electron density around CLA B 838:**

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

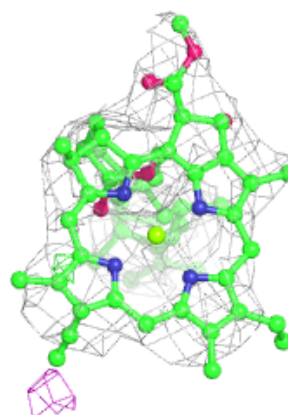
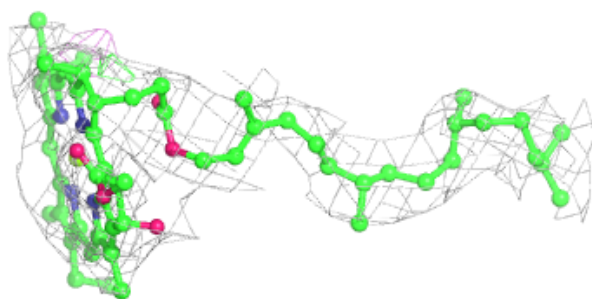
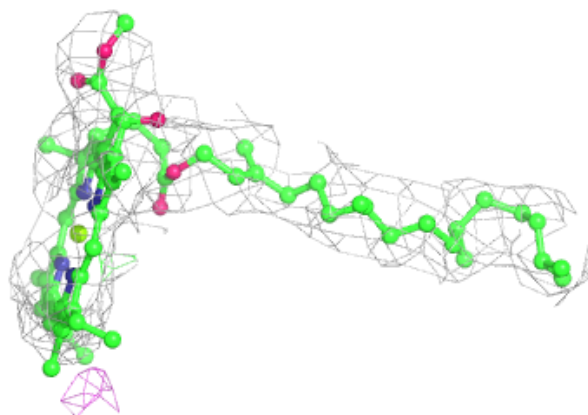


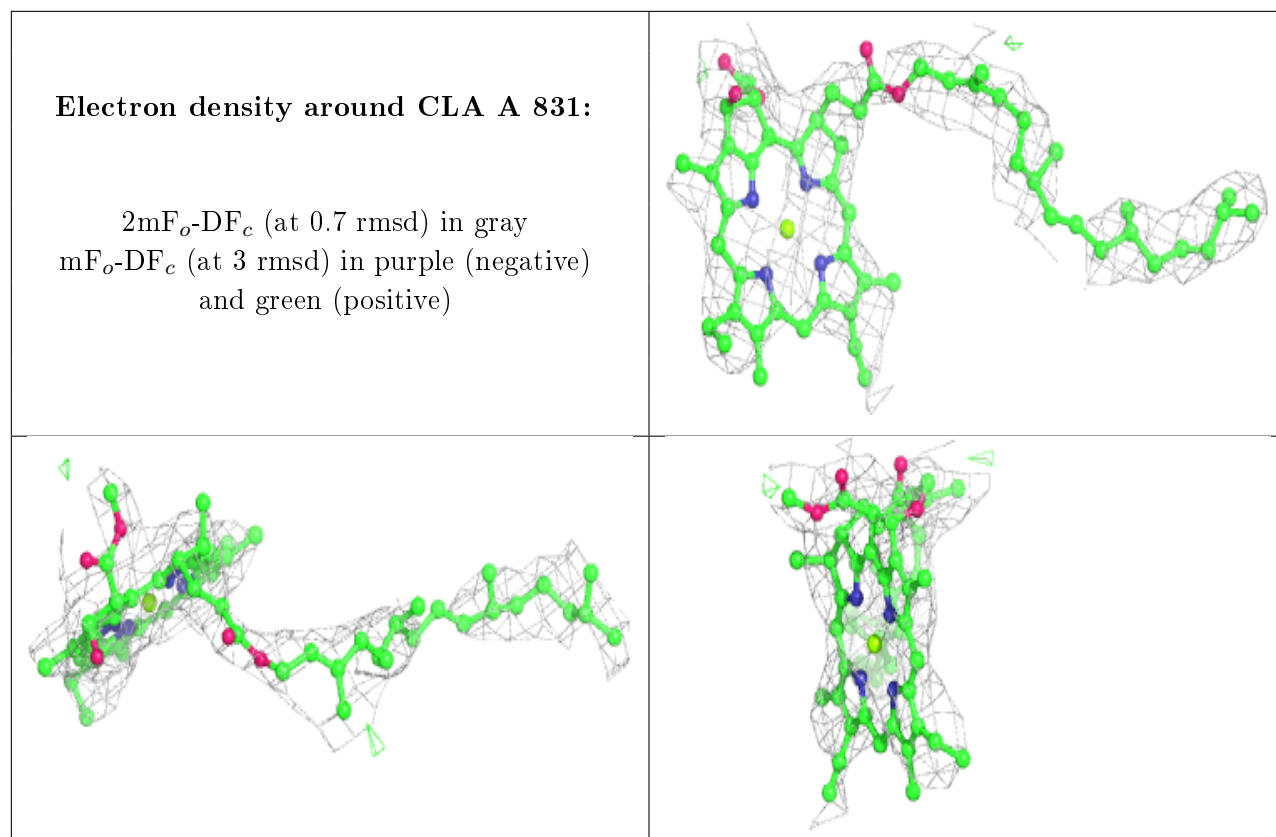
Electron density around CLA A 850:

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

**Electron density around CLA A 826:**

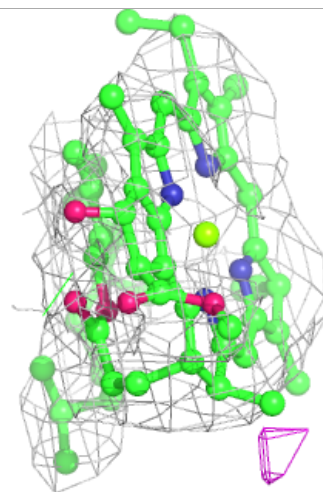
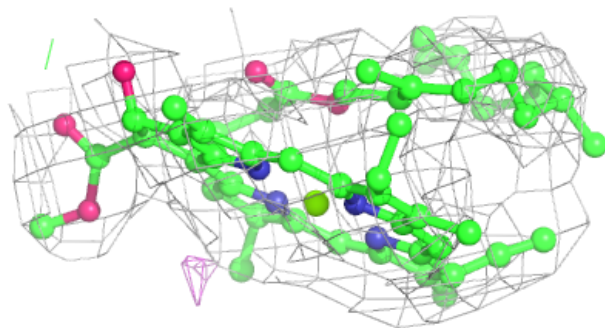
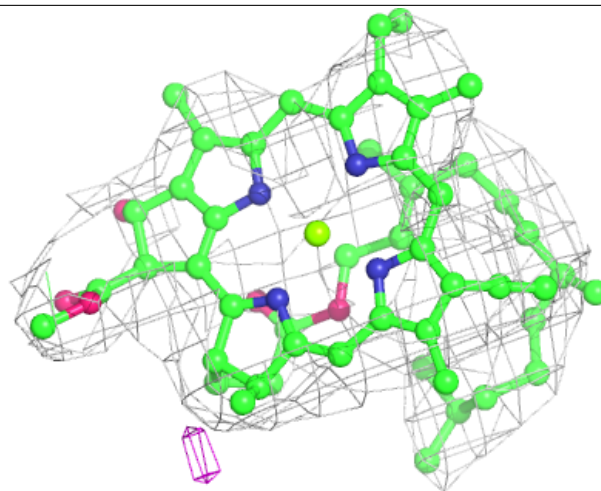
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





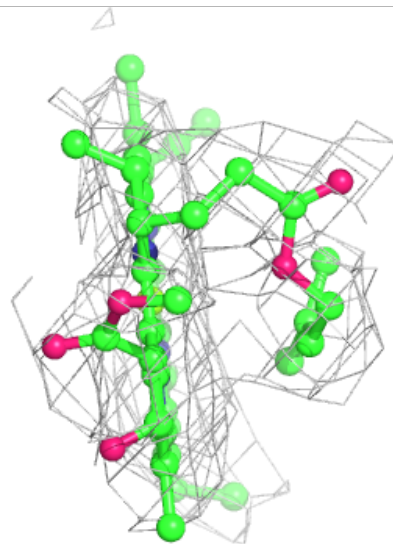
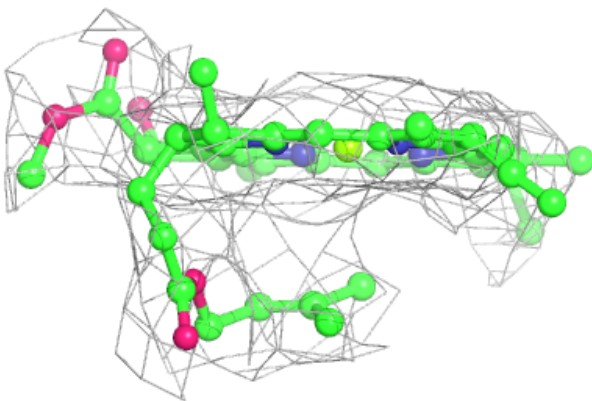
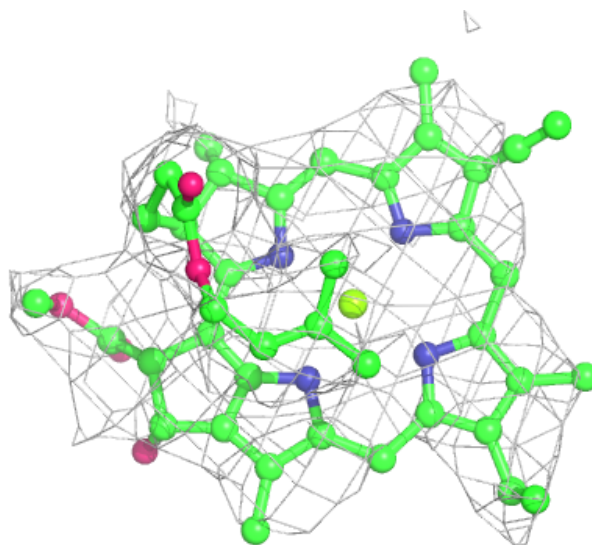
Electron density around CLA B 810:

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



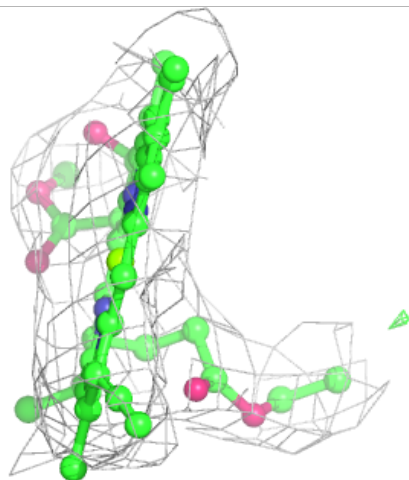
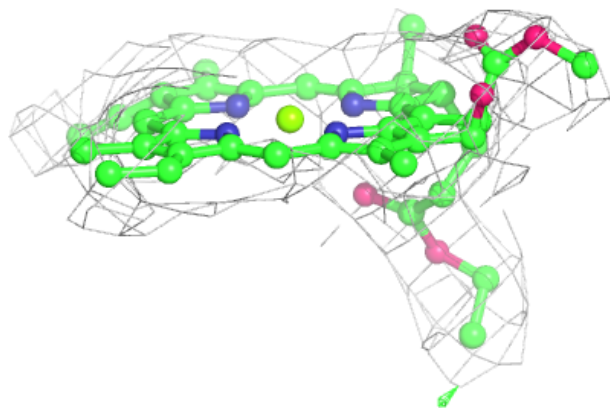
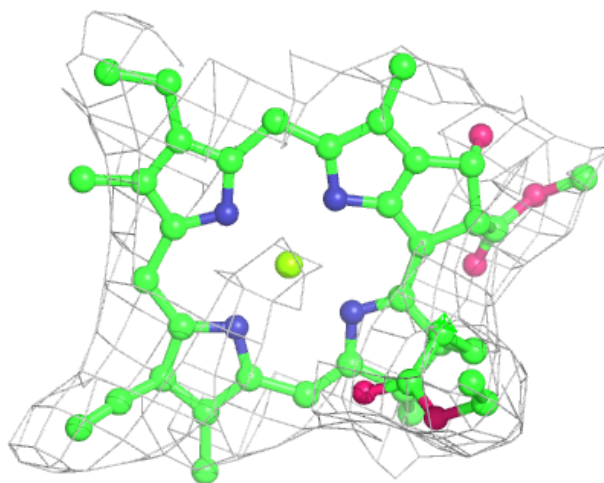
Electron density around CLA B 831:

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



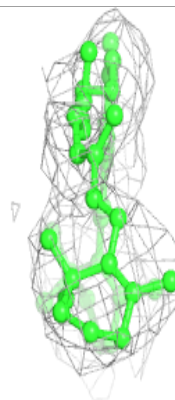
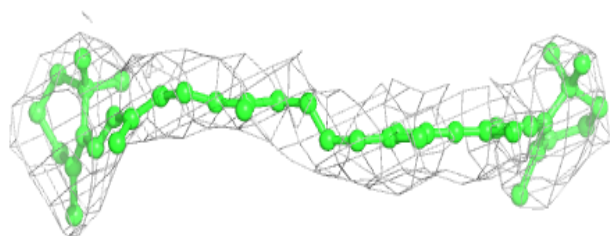
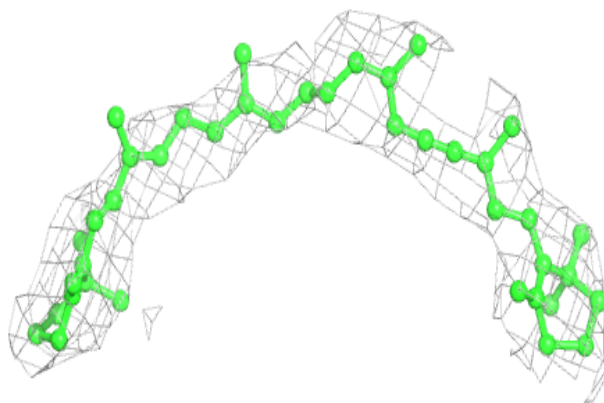
Electron density around CLA B 839:

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



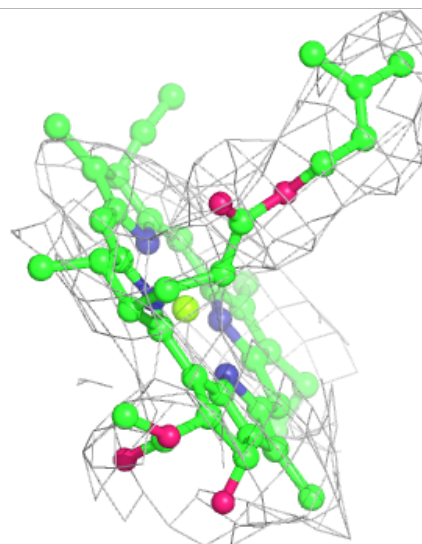
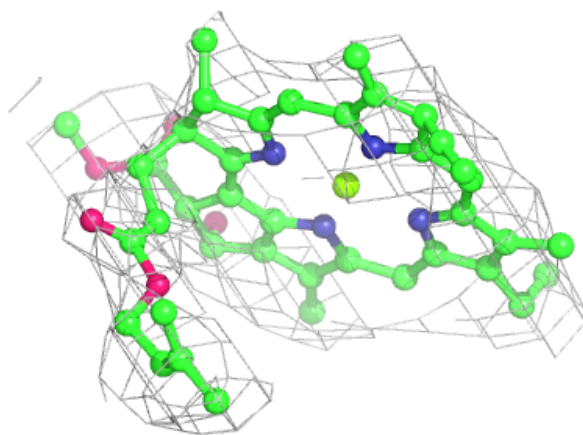
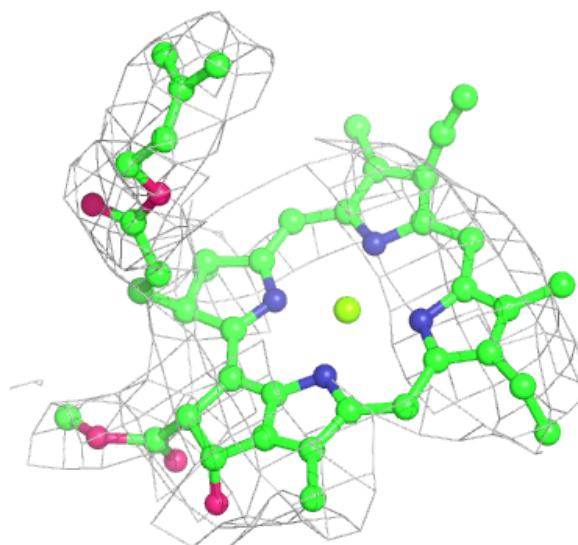
Electron density around BCR F 204:

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



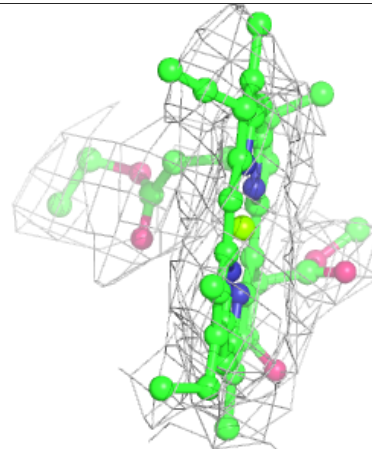
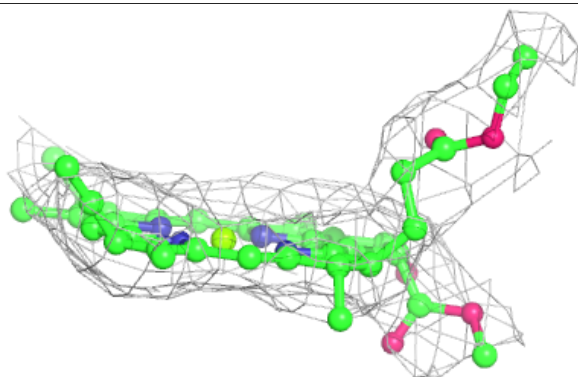
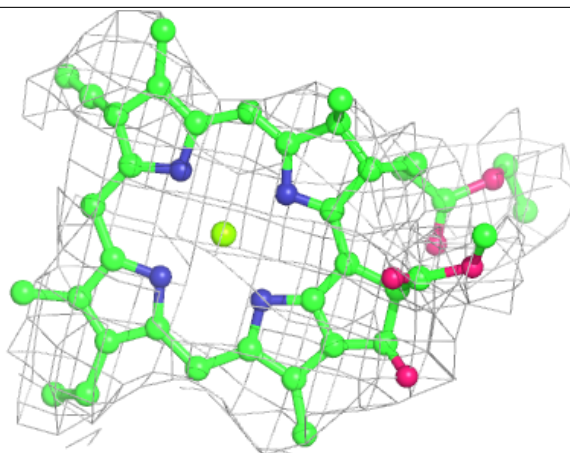
Electron density around CLA A 822:

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

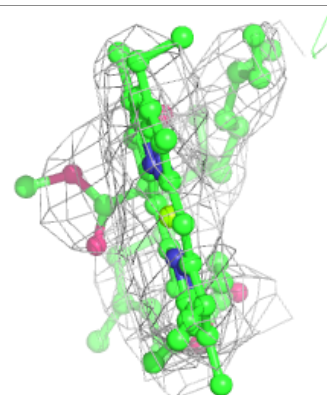
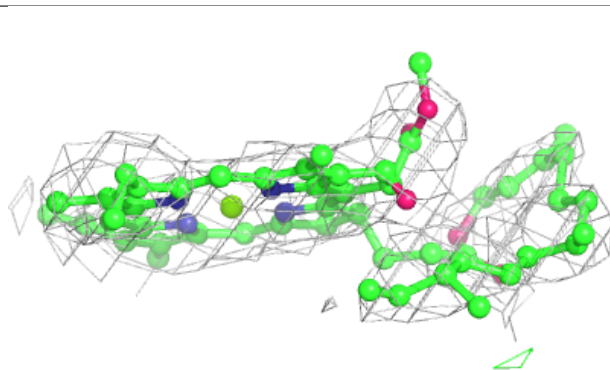
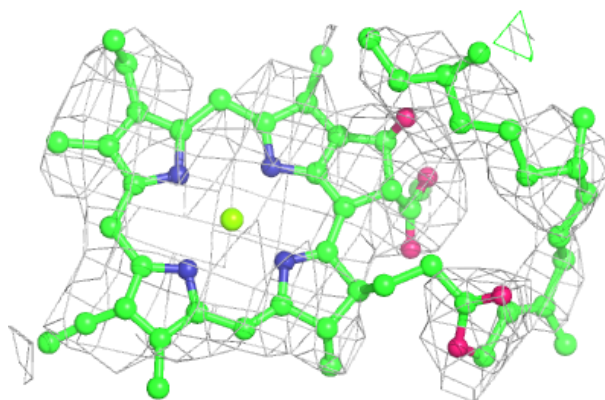


Electron density around CLA A 836:

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

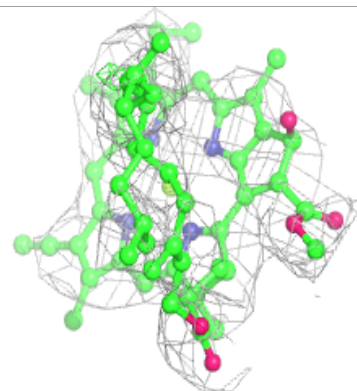
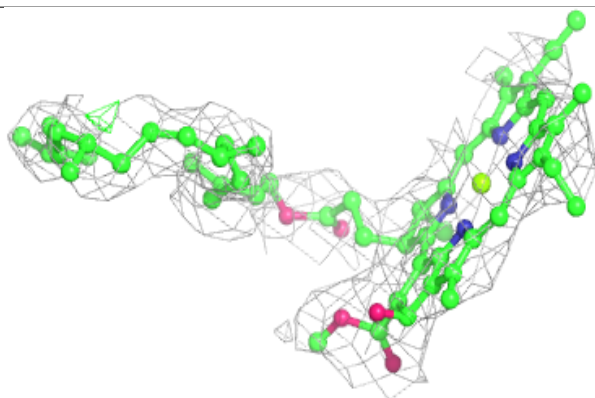
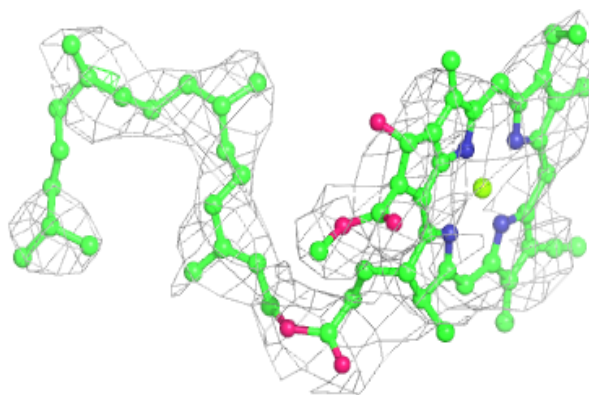
**Electron density around CLA B 808:**

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

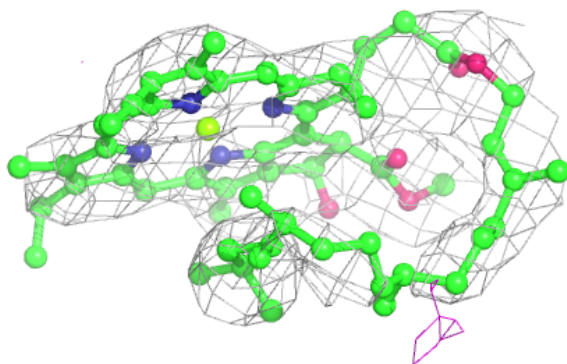
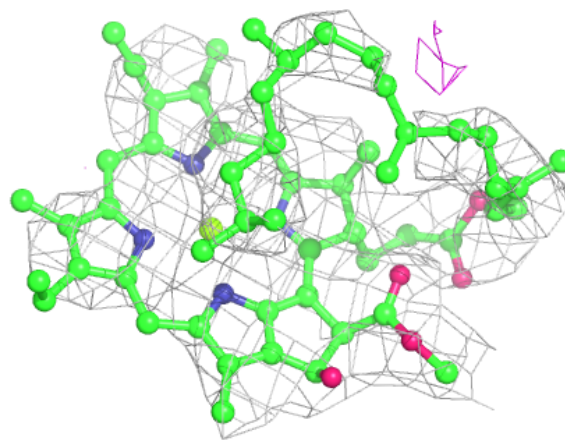


Electron density around CLA A 849:

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

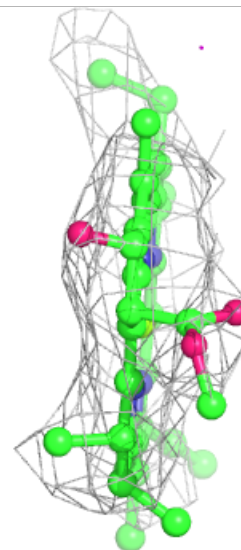
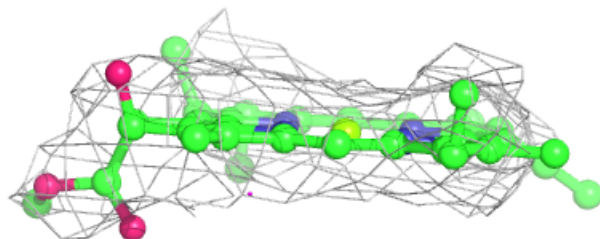
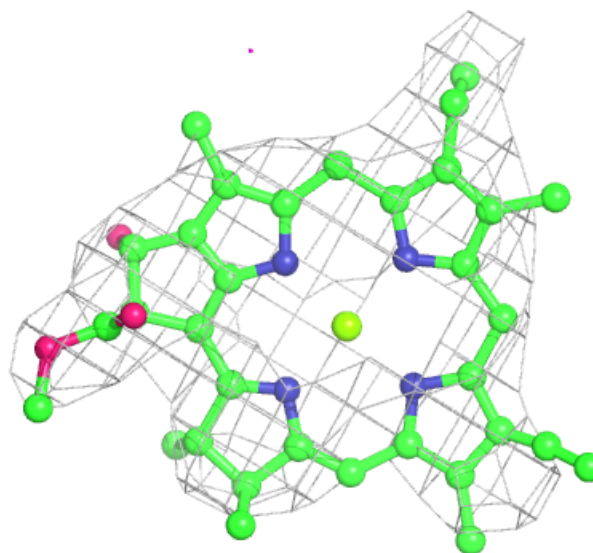
**Electron density around CLA B 809:**

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



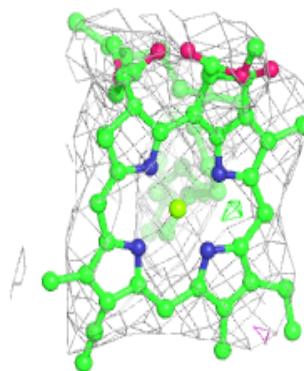
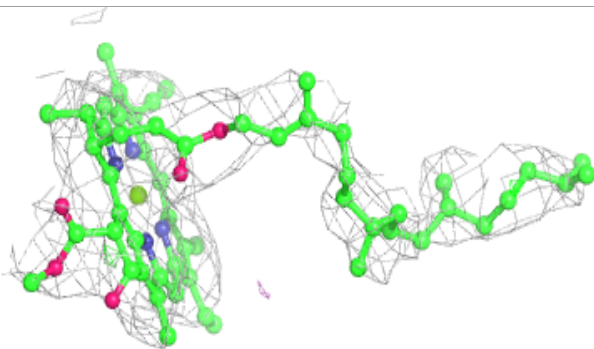
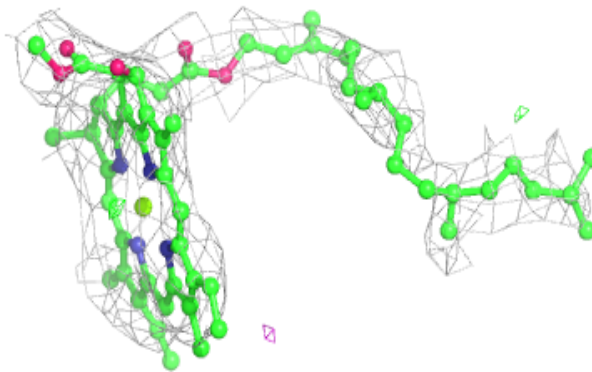
Electron density around CLA B 819:

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

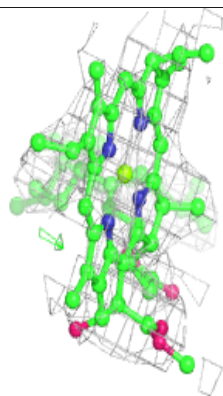
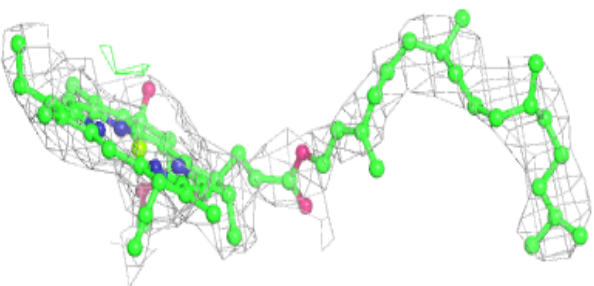
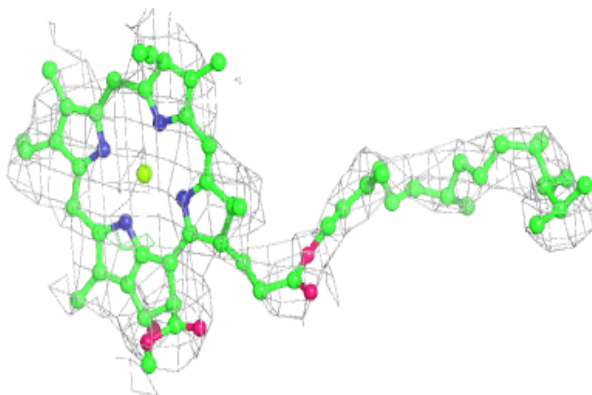


Electron density around CLA B 830:

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

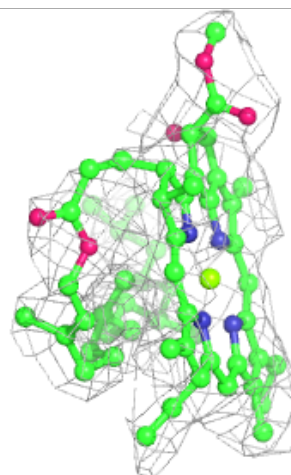
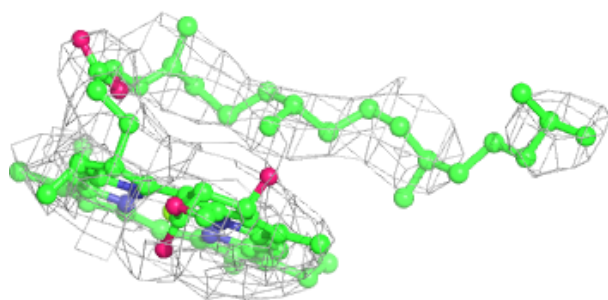
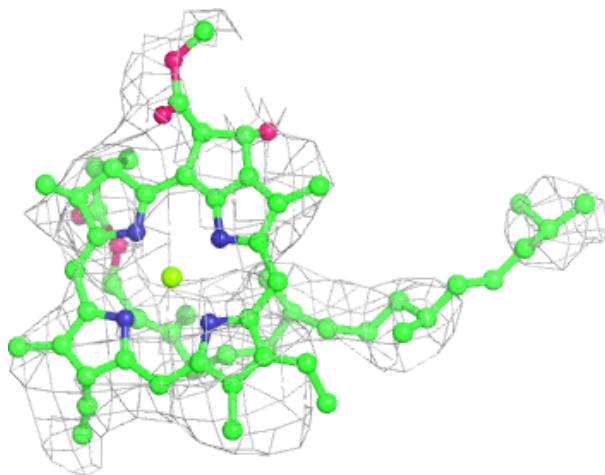
**Electron density around CLA B 814:**

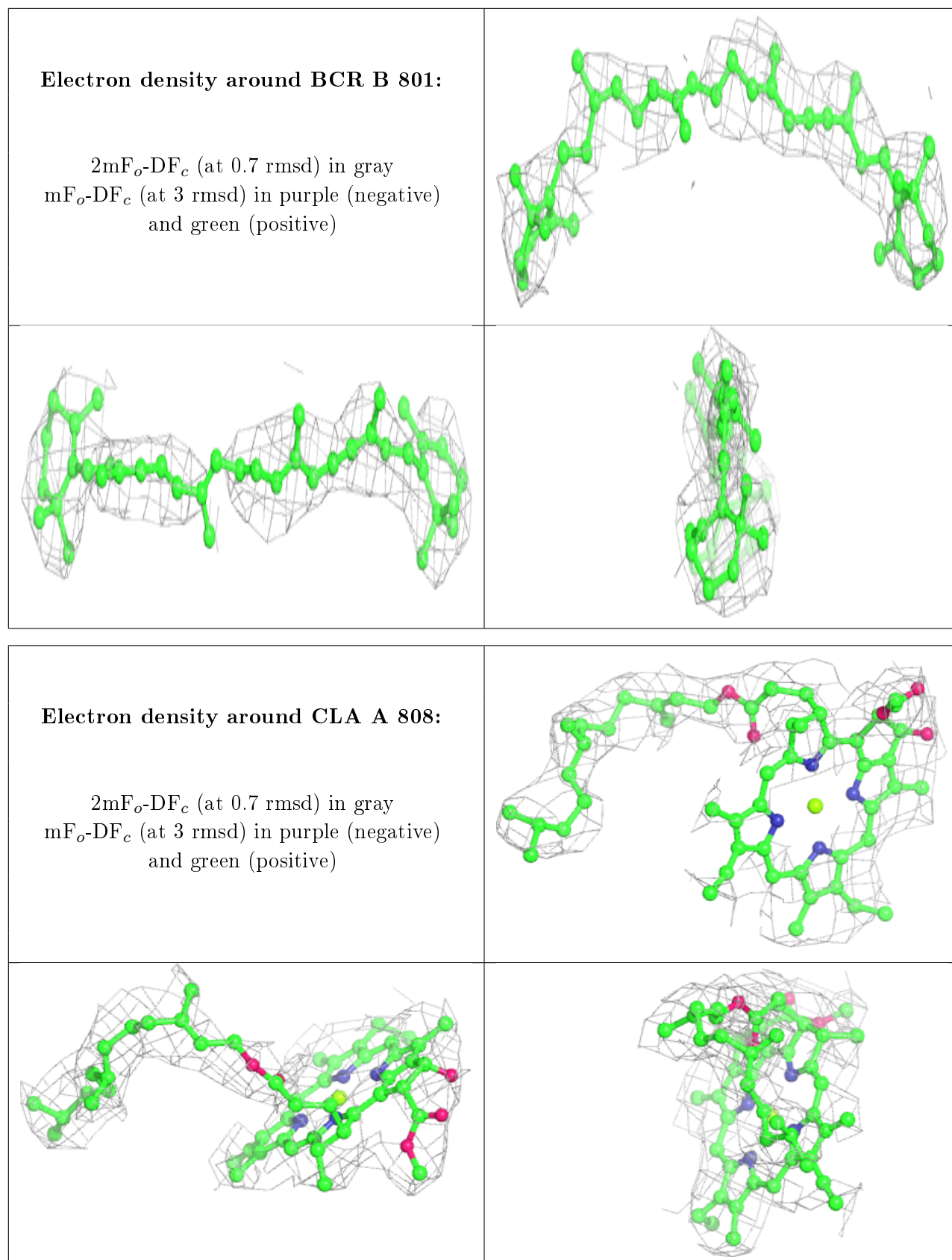
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 828:

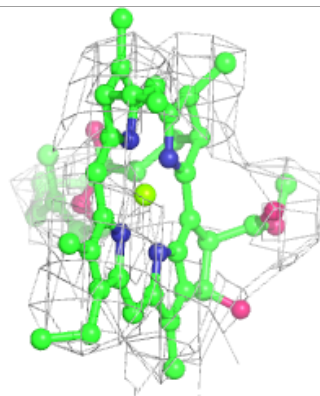
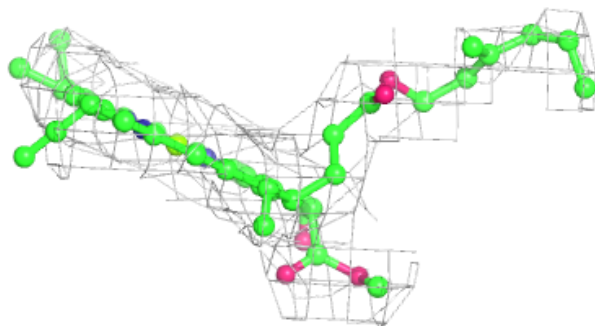
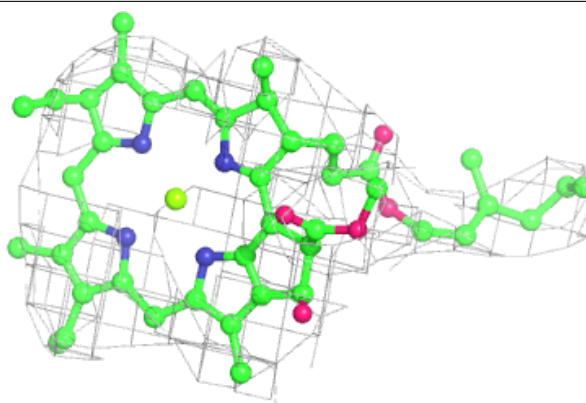
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



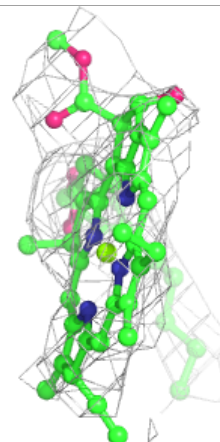
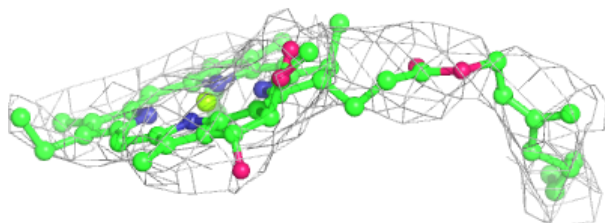
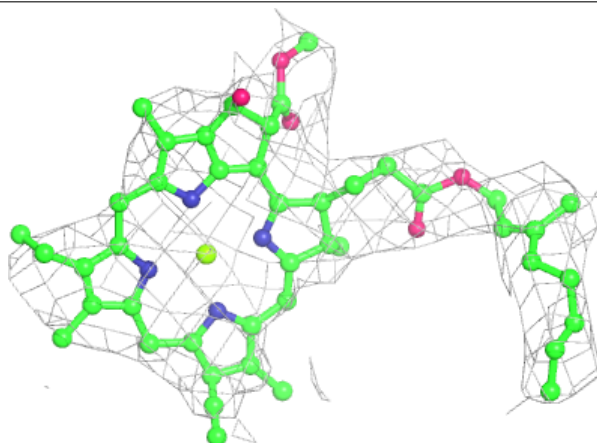


Electron density around CLA A 809:

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

**Electron density around CLA B 802:**

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



6.5 Other polymers

There are no such residues in this entry.