



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2023 – 04:07 PM EDT

PDB ID : 6PGK  
Title : Membrane Protein Megahertz Crystallography at the European XFEL, Photosystem I XFEL at 2.9 Å  
Authors : Fromme, R.; Gisriel, C.; Fromme, P.  
Deposited on : 2019-06-24  
Resolution : 2.90 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

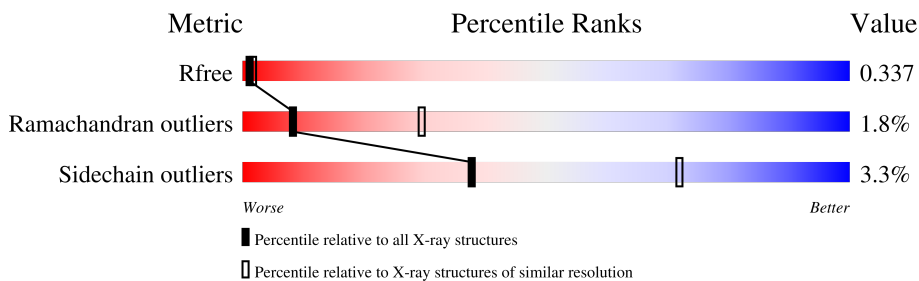
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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.



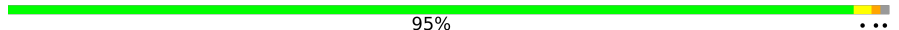

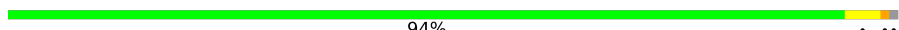
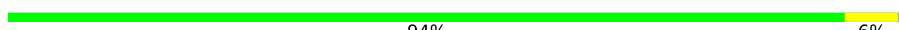






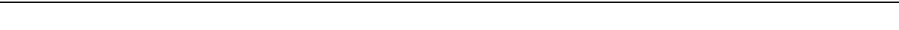

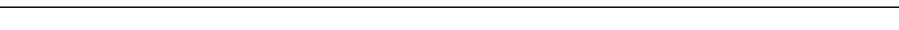
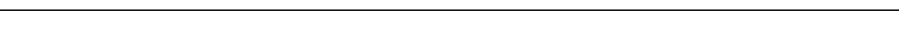
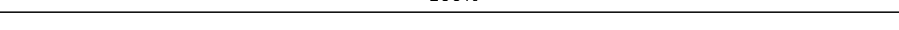
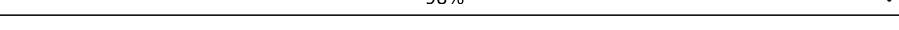
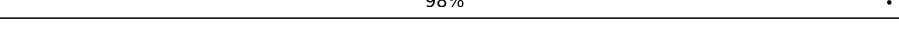

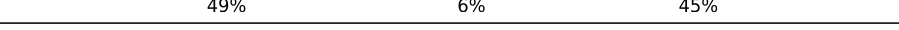
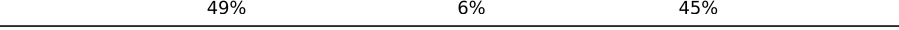
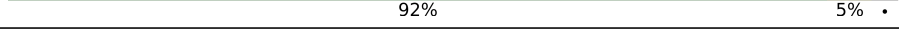
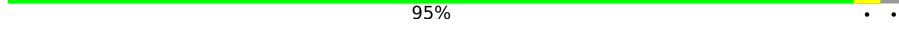

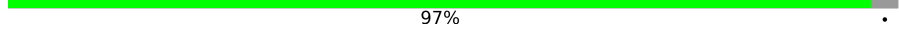
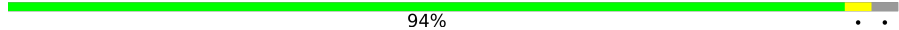
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	755	94% . .
1	G	755	94% . .
1	Y	755	94% . .
2	B	741	95% 5%
2	H	741	96% .
2	Z	741	95% .
3	C	81	94% . . .
3	N	81	95% . .




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Mol	Chain	Length	Quality of chain
3	a	81	95% 
4	D	139	94%  6%
4	O	139	94%  ..
4	b	139	94%  6%
5	E	76	83%  8% 9%
5	P	76	83%  7% 9%
5	c	76	84%  7% 9%
6	F	164	84%  14%
6	Q	164	84%  14%
6	d	164	83%  14%
7	I	38	100% 
7	R	38	100% 
7	e	38	95%  5%
8	J	41	100% 
8	S	41	98%  .
8	f	41	98%  .
9	K	83	52%  .. 45%
9	T	83	49%  45%
9	g	83	49%  45%
10	L	155	92%  5%
10	U	155	95%  ..
10	h	155	90%  7%
11	M	31	97%  .
11	V	31	94%  ..
11	i	31	97%  .

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Mol	Chain	Length	Quality of chain
12	W	39	
12	X	39	
12	j	39	

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
13	CL0	A	801	X	-	-	-
13	CL0	G	801	X	-	-	-
13	CL0	Y	801	X	-	-	-
14	CLA	A	802	X	-	-	-
14	CLA	A	803	X	-	-	-
14	CLA	A	804	X	-	-	-
14	CLA	A	805	X	-	-	-
14	CLA	A	806	X	-	-	-
14	CLA	A	807	X	-	-	-
14	CLA	A	808	X	-	-	-
14	CLA	A	809	X	-	-	-
14	CLA	A	810	X	-	-	-
14	CLA	A	811	X	-	-	-
14	CLA	A	812	X	-	-	-
14	CLA	A	813	X	-	-	-
14	CLA	A	814	X	-	-	-
14	CLA	A	815	X	-	-	-
14	CLA	A	816	X	-	-	-
14	CLA	A	817	X	-	-	-
14	CLA	A	818	X	-	-	-
14	CLA	A	819	X	-	-	-
14	CLA	A	820	X	-	-	-
14	CLA	A	821	X	-	-	-
14	CLA	A	822	X	-	-	-
14	CLA	A	823	X	-	-	-
14	CLA	A	824	X	-	-	-
14	CLA	A	825	X	-	-	-
14	CLA	A	826	X	-	-	-
14	CLA	A	827	X	-	-	-
14	CLA	A	828	X	-	-	-
14	CLA	A	829	X	-	-	-
14	CLA	A	830	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	831	X	-	-	-
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	839	X	-	-	-
14	CLA	A	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	842	X	-	-	-
14	CLA	A	852	X	-	-	-
14	CLA	B	801	X	-	-	-
14	CLA	B	802	X	-	-	-
14	CLA	B	803	X	-	-	-
14	CLA	B	804	X	-	-	-
14	CLA	B	805	X	-	-	-
14	CLA	B	806	X	-	-	-
14	CLA	B	807	X	-	-	-
14	CLA	B	808	X	-	-	-
14	CLA	B	809	X	-	-	-
14	CLA	B	810	X	-	-	-
14	CLA	B	811	X	-	-	-
14	CLA	B	812	X	-	-	-
14	CLA	B	813	X	-	-	-
14	CLA	B	814	X	-	-	-
14	CLA	B	815	X	-	-	-
14	CLA	B	816	X	-	-	-
14	CLA	B	817	X	-	-	-
14	CLA	B	818	X	-	-	-
14	CLA	B	819	X	-	-	-
14	CLA	B	820	X	-	-	-
14	CLA	B	821	X	-	-	-
14	CLA	B	822	X	-	-	-
14	CLA	B	823	X	-	-	-
14	CLA	B	824	X	-	-	-
14	CLA	B	825	X	-	-	-
14	CLA	B	826	X	-	-	-
14	CLA	B	827	X	-	-	-
14	CLA	B	828	X	-	-	-
14	CLA	B	829	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	830	X	-	-	-
14	CLA	B	831	X	-	-	-
14	CLA	B	832	X	-	-	-
14	CLA	B	833	X	-	-	-
14	CLA	B	834	X	-	-	-
14	CLA	B	835	X	-	-	-
14	CLA	B	836	X	-	-	-
14	CLA	B	837	X	-	-	-
14	CLA	B	838	X	-	-	-
14	CLA	B	839	X	-	-	-
14	CLA	B	840	X	-	-	-
14	CLA	B	841	X	-	-	-
14	CLA	F	202	X	-	-	-
14	CLA	G	802	X	-	-	-
14	CLA	G	803	X	-	-	-
14	CLA	G	804	X	-	-	-
14	CLA	G	805	X	-	-	-
14	CLA	G	806	X	-	-	-
14	CLA	G	807	X	-	-	-
14	CLA	G	808	X	-	-	-
14	CLA	G	809	X	-	-	-
14	CLA	G	810	X	-	-	-
14	CLA	G	811	X	-	-	-
14	CLA	G	812	X	-	-	-
14	CLA	G	813	X	-	-	-
14	CLA	G	814	X	-	-	-
14	CLA	G	815	X	-	-	-
14	CLA	G	816	X	-	-	-
14	CLA	G	817	X	-	-	-
14	CLA	G	818	X	-	-	-
14	CLA	G	819	X	-	-	-
14	CLA	G	820	X	-	-	-
14	CLA	G	821	X	-	-	-
14	CLA	G	822	X	-	-	-
14	CLA	G	823	X	-	-	-
14	CLA	G	824	X	-	-	-
14	CLA	G	825	X	-	-	-
14	CLA	G	826	X	-	-	-
14	CLA	G	827	X	-	-	-
14	CLA	G	828	X	-	-	-
14	CLA	G	829	X	-	-	-
14	CLA	G	830	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	G	831	X	-	-	-
14	CLA	G	832	X	-	-	-
14	CLA	G	833	X	-	-	-
14	CLA	G	834	X	-	-	-
14	CLA	G	835	X	-	-	-
14	CLA	G	836	X	-	-	-
14	CLA	G	837	X	-	-	-
14	CLA	G	838	X	-	-	-
14	CLA	G	839	X	-	-	-
14	CLA	G	840	X	-	-	-
14	CLA	G	841	X	-	-	-
14	CLA	G	842	X	-	-	-
14	CLA	G	843	X	-	-	-
14	CLA	G	853	X	-	-	-
14	CLA	H	801	X	-	-	-
14	CLA	H	802	X	-	-	-
14	CLA	H	803	X	-	-	-
14	CLA	H	804	X	-	-	-
14	CLA	H	805	X	-	-	-
14	CLA	H	806	X	-	-	-
14	CLA	H	807	X	-	-	-
14	CLA	H	808	X	-	-	-
14	CLA	H	809	X	-	-	-
14	CLA	H	810	X	-	-	-
14	CLA	H	811	X	-	-	-
14	CLA	H	812	X	-	-	-
14	CLA	H	813	X	-	-	-
14	CLA	H	814	X	-	-	-
14	CLA	H	815	X	-	-	-
14	CLA	H	816	X	-	-	-
14	CLA	H	817	X	-	-	-
14	CLA	H	818	X	-	-	-
14	CLA	H	819	X	-	-	-
14	CLA	H	820	X	-	-	-
14	CLA	H	821	X	-	-	-
14	CLA	H	822	X	-	-	-
14	CLA	H	823	X	-	-	-
14	CLA	H	824	X	-	-	-
14	CLA	H	825	X	-	-	-
14	CLA	H	826	X	-	-	-
14	CLA	H	827	X	-	-	-
14	CLA	H	828	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	H	829	X	-	-	-
14	CLA	H	830	X	-	-	-
14	CLA	H	831	X	-	-	-
14	CLA	H	832	X	-	-	-
14	CLA	H	833	X	-	-	-
14	CLA	H	834	X	-	-	-
14	CLA	H	835	X	-	-	-
14	CLA	H	836	X	-	-	-
14	CLA	H	837	X	-	-	-
14	CLA	H	838	X	-	-	-
14	CLA	J	101	X	-	-	-
14	CLA	J	102	X	-	-	-
14	CLA	K	101	X	-	-	-
14	CLA	K	103	X	-	-	-
14	CLA	L	201	X	-	-	-
14	CLA	L	202	X	-	-	-
14	CLA	L	205	X	-	-	-
14	CLA	L	206	X	-	-	-
14	CLA	L	207	X	-	-	-
14	CLA	Q	201	X	-	-	-
14	CLA	Q	203	X	-	-	-
14	CLA	S	1101	X	-	-	-
14	CLA	S	1102	X	-	-	-
14	CLA	S	1103	X	-	-	-
14	CLA	T	101	X	-	-	-
14	CLA	T	103	X	-	-	-
14	CLA	U	1002	X	-	-	-
14	CLA	U	1003	X	-	-	-
14	CLA	U	1004	X	-	-	-
14	CLA	U	1006	X	-	-	-
14	CLA	V	1201	X	-	-	-
14	CLA	W	1701	X	-	-	-
14	CLA	X	1701	X	-	-	-
14	CLA	Y	802	X	-	-	-
14	CLA	Y	803	X	-	-	-
14	CLA	Y	804	X	-	-	-
14	CLA	Y	805	X	-	-	-
14	CLA	Y	806	X	-	-	-
14	CLA	Y	807	X	-	-	-
14	CLA	Y	808	X	-	-	-
14	CLA	Y	809	X	-	-	-
14	CLA	Y	810	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	Y	811	X	-	-	-
14	CLA	Y	812	X	-	-	-
14	CLA	Y	813	X	-	-	-
14	CLA	Y	814	X	-	-	-
14	CLA	Y	815	X	-	-	-
14	CLA	Y	816	X	-	-	-
14	CLA	Y	817	X	-	-	-
14	CLA	Y	818	X	-	-	-
14	CLA	Y	819	X	-	-	-
14	CLA	Y	820	X	-	-	-
14	CLA	Y	821	X	-	-	-
14	CLA	Y	822	X	-	-	-
14	CLA	Y	823	X	-	-	-
14	CLA	Y	824	X	-	-	-
14	CLA	Y	825	X	-	-	-
14	CLA	Y	826	X	-	-	-
14	CLA	Y	827	X	-	-	-
14	CLA	Y	828	X	-	-	-
14	CLA	Y	829	X	-	-	-
14	CLA	Y	830	X	-	-	-
14	CLA	Y	831	X	-	-	-
14	CLA	Y	832	X	-	-	-
14	CLA	Y	833	X	-	-	-
14	CLA	Y	834	X	-	-	-
14	CLA	Y	835	X	-	-	-
14	CLA	Y	836	X	-	-	-
14	CLA	Y	837	X	-	-	-
14	CLA	Y	838	X	-	-	-
14	CLA	Y	839	X	-	-	-
14	CLA	Y	840	X	-	-	-
14	CLA	Y	841	X	-	-	-
14	CLA	Y	842	X	-	-	-
14	CLA	Y	843	X	-	-	-
14	CLA	Y	854	X	-	-	-
14	CLA	Y	855	X	-	-	-
14	CLA	Z	801	X	-	-	-
14	CLA	Z	802	X	-	-	-
14	CLA	Z	803	X	-	-	-
14	CLA	Z	804	X	-	-	-
14	CLA	Z	805	X	-	-	-
14	CLA	Z	806	X	-	-	-
14	CLA	Z	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	Z	808	X	-	-	-
14	CLA	Z	809	X	-	-	-
14	CLA	Z	810	X	-	-	-
14	CLA	Z	811	X	-	-	-
14	CLA	Z	812	X	-	-	-
14	CLA	Z	813	X	-	-	-
14	CLA	Z	814	X	-	-	-
14	CLA	Z	815	X	-	-	-
14	CLA	Z	816	X	-	-	-
14	CLA	Z	817	X	-	-	-
14	CLA	Z	818	X	-	-	-
14	CLA	Z	819	X	-	-	-
14	CLA	Z	820	X	-	-	-
14	CLA	Z	821	X	-	-	-
14	CLA	Z	822	X	-	-	-
14	CLA	Z	823	X	-	-	-
14	CLA	Z	824	X	-	-	-
14	CLA	Z	825	X	-	-	-
14	CLA	Z	826	X	-	-	-
14	CLA	Z	827	X	-	-	-
14	CLA	Z	828	X	-	-	-
14	CLA	Z	829	X	-	-	-
14	CLA	Z	830	X	-	-	-
14	CLA	Z	831	X	-	-	-
14	CLA	Z	832	X	-	-	-
14	CLA	Z	833	X	-	-	-
14	CLA	Z	834	X	-	-	-
14	CLA	Z	835	X	-	-	-
14	CLA	Z	836	X	-	-	-
14	CLA	Z	837	X	-	-	-
14	CLA	Z	838	X	-	-	-
14	CLA	Z	839	X	-	-	-
14	CLA	d	201	X	-	-	-
14	CLA	d	202	X	-	-	-
14	CLA	f	101	X	-	-	-
14	CLA	f	102	X	-	-	-
14	CLA	g	101	X	-	-	-
14	CLA	g	102	X	-	-	-
14	CLA	h	201	X	-	-	-
14	CLA	h	205	X	-	-	-
14	CLA	h	206	X	-	-	-
14	CLA	h	207	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	j	102	X	-	-	-

## 2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 72532 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	741	5791	3799	989	977	26	0	0	0
1	G	741	5791	3799	989	977	26	0	0	0
1	Y	741	5791	3799	989	977	26	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	739	5889	3876	987	1005	21	0	0	0
2	H	739	5889	3876	987	1005	21	0	0	0
2	Z	739	5889	3876	987	1005	21	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	80	598	367	103	117	11	0	0	0
3	N	80	598	367	103	117	11	0	0	0
3	a	80	598	367	103	117	11	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	138	1075	682	186	204	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	O	138	Total	C	N	O	S	0	0	0
			1075	682	186	204	3			
4	b	138	Total	C	N	O	S	0	0	0
			1075	682	186	204	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	69	Total	C	N	O		0	0	0
			539	342	93	104				
5	P	69	Total	C	N	O		0	0	0
			539	342	93	104				
5	c	69	Total	C	N	O		0	0	0
			539	342	93	104				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	141	Total	C	N	O	S	0	0	0
			1065	680	184	197	4			
6	Q	141	Total	C	N	O	S	0	0	0
			1065	680	184	197	4			
6	d	141	Total	C	N	O	S	0	0	0
			1065	680	184	197	4			

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	38	Total	C	N	O	S	0	0	0
			301	208	40	48	5			
7	R	38	Total	C	N	O	S	0	0	0
			301	208	40	48	5			
7	e	38	Total	C	N	O	S	0	0	0
			301	208	40	48	5			

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	41	Total	C	N	O	S	0	0	0
			338	231	51	54	2			
8	S	41	Total	C	N	O	S	0	0	0
			338	231	51	54	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	f	41	Total	C	N	O	S	0	0	0
			338	231	51	54	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	46	Total	C	N	O	S	0	0	0
			328	214	57	56	1			
9	T	46	Total	C	N	O	S	0	0	0
			328	214	57	56	1			
9	g	46	Total	C	N	O	S	0	0	0
			328	214	57	56	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	151	Total	C	N	O	S	0	0	0
			1119	735	179	201	4			
10	U	151	Total	C	N	O	S	0	0	0
			1119	735	179	201	4			
10	h	151	Total	C	N	O	S	0	0	0
			1119	735	179	201	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	143	LEU	SER	conflict	UNP Q8DGB4
U	143	LEU	SER	conflict	UNP Q8DGB4
h	143	LEU	SER	conflict	UNP Q8DGB4

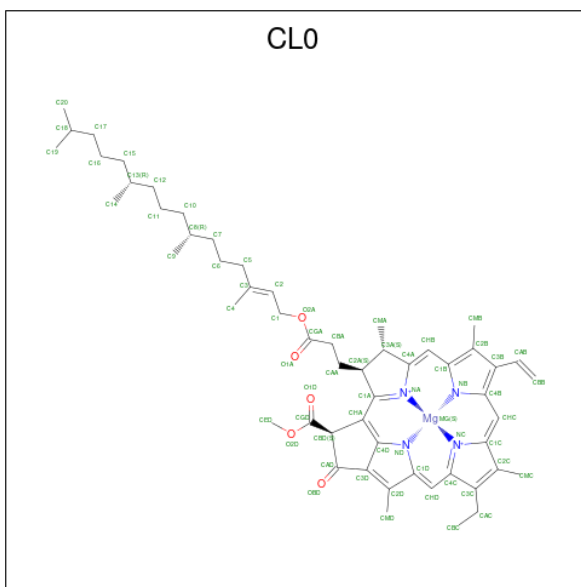
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	M	30	Total	C	N	O	0	0	0
			233	156	35	42			
11	V	30	Total	C	N	O	0	0	0
			233	156	35	42			
11	i	30	Total	C	N	O	0	0	0
			233	156	35	42			

- Molecule 12 is a protein called Photosystem I 4.8K protein.

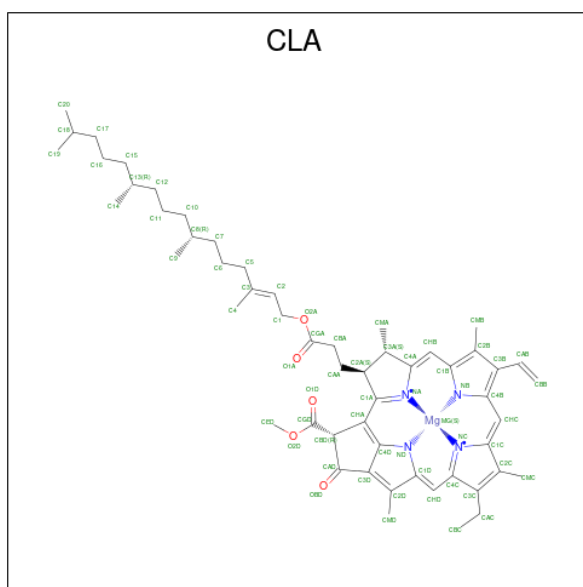
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	W	26	Total	C	N	O	0	0	0
			219	157	31	31			
12	X	26	Total	C	N	O	0	0	0
			219	157	31	31			
12	j	26	Total	C	N	O	0	0	0
			219	157	31	31			

- Molecule 13 is CHLOROPHYLL A ISOMER (three-letter code: CLO) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
14	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	G	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	G	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	H	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	J	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	J	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	K	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
14	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Q	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Q	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	S	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	S	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	S	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	T	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
14	T	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	U	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	U	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	U	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	U	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	V	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	W	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	X	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	Y	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Y	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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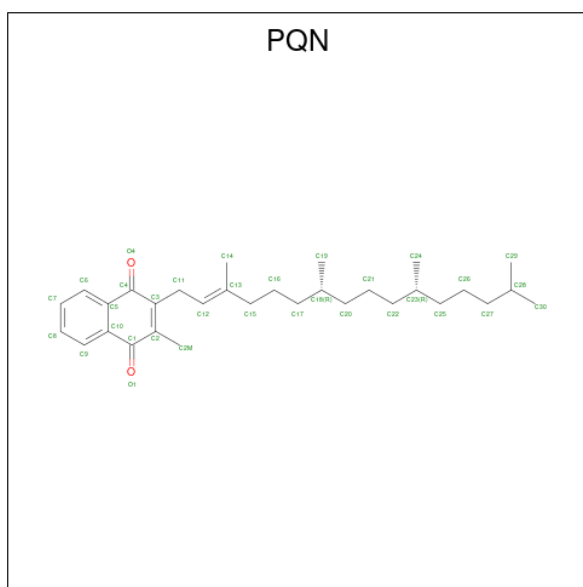
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	Z	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	Z	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	d	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
14	d	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	f	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	f	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	g	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
14	g	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	h	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	h	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	h	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	h	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	j	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

- Molecule 15 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



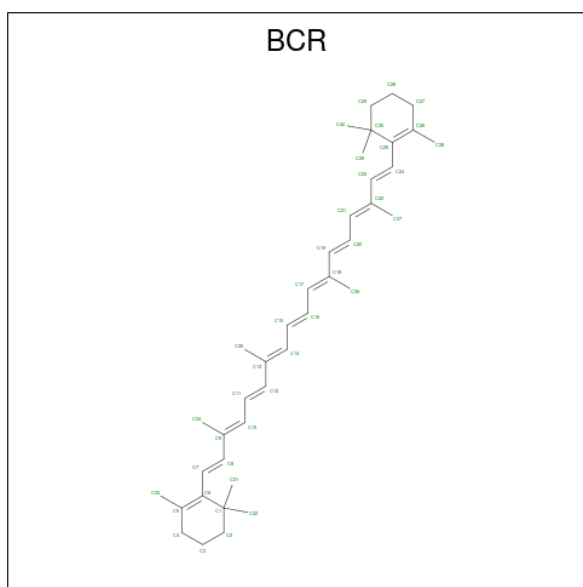
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	A	1	Total	C	O	0	0
			33	31	2		
15	B	1	Total	C	O	0	0
			33	31	2		
15	G	1	Total	C	O	0	0
			33	31	2		
15	H	1	Total	C	O	0	0
			33	31	2		
15	Y	1	Total	C	O	0	0
			33	31	2		
15	Z	1	Total	C	O	0	0
			33	31	2		

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	A	1	Total	Fe	S	0	0
			8	4	4		
16	C	1	Total	Fe	S	0	0
			8	4	4		
16	C	1	Total	Fe	S	0	0
			8	4	4		
16	G	1	Total	Fe	S	0	0
			8	4	4		
16	N	1	Total	Fe	S	0	0
			8	4	4		
16	N	1	Total	Fe	S	0	0
			8	4	4		
16	Y	1	Total	Fe	S	0	0
			8	4	4		
16	a	1	Total	Fe	S	0	0
			8	4	4		
16	a	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total C 40 40	0	0
17	A	1	Total C 40 40	0	0
17	A	1	Total C 40 40	0	0
17	A	1	Total C 40 40	0	0
17	A	1	Total C 40 40	0	0
17	B	1	Total C 30 30	0	0
17	B	1	Total C 40 40	0	0
17	B	1	Total C 40 40	0	0
17	B	1	Total C 25 25	0	0
17	B	1	Total C 40 40	0	0
17	B	1	Total C 40 40	0	0
17	B	1	Total C 40 40	0	0
17	B	1	Total C 40 40	0	0
17	F	1	Total C 40 40	0	0
17	F	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	G	1	Total C 40 40	0	0
17	G	1	Total C 40 40	0	0
17	G	1	Total C 40 40	0	0
17	G	1	Total C 40 40	0	0
17	G	1	Total C 40 40	0	0
17	G	1	Total C 40 40	0	0
17	H	1	Total C 40 40	0	0
17	H	1	Total C 40 40	0	0
17	H	1	Total C 40 40	0	0
17	H	1	Total C 25 25	0	0
17	H	1	Total C 40 40	0	0
17	H	1	Total C 40 40	0	0
17	H	1	Total C 40 40	0	0
17	I	1	Total C 40 40	0	0
17	J	1	Total C 40 40	0	0
17	J	1	Total C 40 40	0	0
17	K	1	Total C 40 40	0	0
17	L	1	Total C 40 40	0	0
17	L	1	Total C 40 40	0	0
17	L	1	Total C 40 40	0	0
17	M	1	Total C 40 40	0	0

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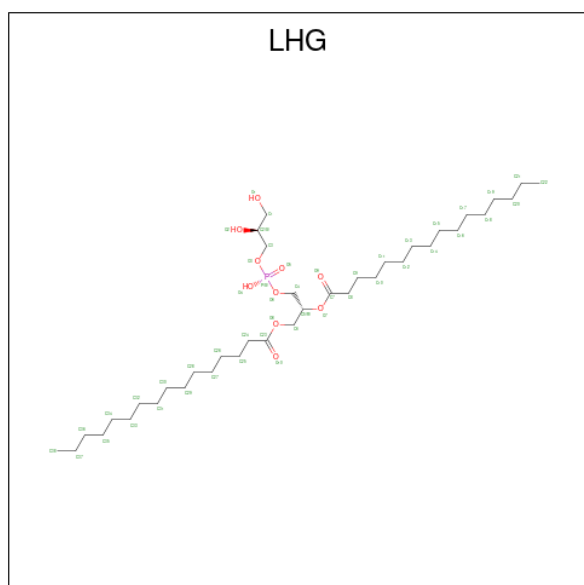
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	Q	1	Total C 40 40	0	0
17	Q	1	Total C 40 40	0	0
17	R	1	Total C 40 40	0	0
17	R	1	Total C 40 40	0	0
17	S	1	Total C 40 40	0	0
17	T	1	Total C 40 40	0	0
17	U	1	Total C 40 40	0	0
17	U	1	Total C 40 40	0	0
17	U	1	Total C 40 40	0	0
17	V	1	Total C 40 40	0	0
17	Y	1	Total C 40 40	0	0
17	Y	1	Total C 40 40	0	0
17	Y	1	Total C 40 40	0	0
17	Y	1	Total C 40 40	0	0
17	Y	1	Total C 40 40	0	0
17	Y	1	Total C 40 40	0	0
17	Y	1	Total C 40 40	0	0
17	Z	1	Total C 40 40	0	0
17	Z	1	Total C 40 40	0	0
17	Z	1	Total C 40 40	0	0
17	Z	1	Total C 25 25	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	Z	1	Total C 40 40	0	0
17	Z	1	Total C 40 40	0	0
17	d	1	Total C 40 40	0	0
17	e	1	Total C 40 40	0	0
17	f	1	Total C 40 40	0	0
17	f	1	Total C 40 40	0	0
17	f	1	Total C 40 40	0	0
17	h	1	Total C 40 40	0	0
17	h	1	Total C 40 40	0	0
17	i	1	Total C 40 40	0	0

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



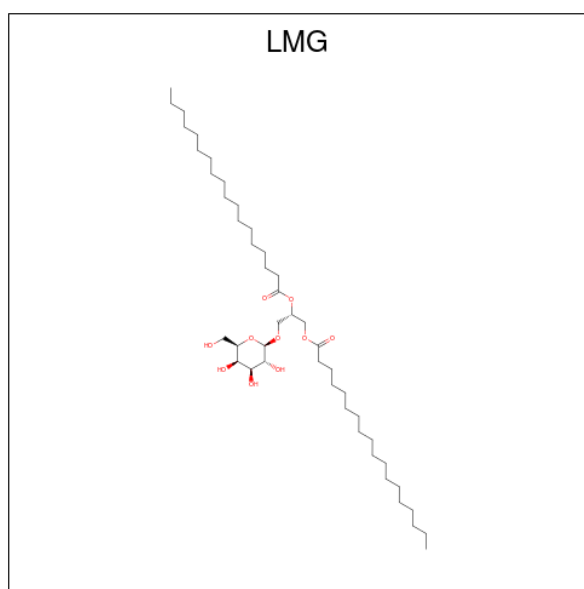
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O P 49 38 10 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
18	A	1	Total 32	C 21	O 10	P 1	0	0
18	B	1	Total 39	C 28	O 10	P 1	0	0
18	G	1	Total 49	C 38	O 10	P 1	0	0
18	G	1	Total 32	C 21	O 10	P 1	0	0
18	H	1	Total 37	C 26	O 10	P 1	0	0
18	Y	1	Total 49	C 38	O 10	P 1	0	0
18	Y	1	Total 25	C 14	O 10	P 1	0	0
18	j	1	Total 28	C 17	O 10	P 1	0	0

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
19	B	1	Total 52	C 42	O 10	0	0
19	H	1	Total 49	C 39	O 10	0	0
19	Z	1	Total 49	C 39	O 10	0	0

- Molecule 20 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	L	1	Total Ca 1 1	0	0
20	U	1	Total Ca 1 1	0	0
20	h	1	Total Ca 1 1	0	0

- Molecule 21 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	9	Total O 9 9	0	0
21	B	9	Total O 9 9	0	0
21	C	1	Total O 1 1	0	0
21	D	2	Total O 2 2	0	0
21	E	1	Total O 1 1	0	0
21	G	8	Total O 8 8	0	0
21	H	3	Total O 3 3	0	0
21	J	1	Total O 1 1	0	0
21	K	1	Total O 1 1	0	0
21	L	5	Total O 5 5	0	0
21	N	1	Total O 1 1	0	0
21	O	2	Total O 2 2	0	0
21	Q	2	Total O 2 2	0	0
21	T	1	Total O 1 1	0	0
21	U	4	Total O 4 4	0	0
21	W	1	Total O 1 1	0	0

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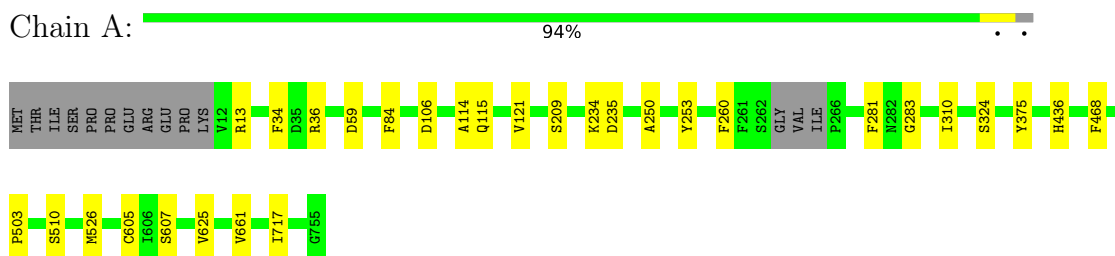
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
21	Y	8	Total O 8 8	0	0
21	Z	2	Total O 2 2	0	0
21	b	4	Total O 4 4	0	0
21	c	1	Total O 1 1	0	0
21	d	2	Total O 2 2	0	0
21	f	1	Total O 1 1	0	0
21	h	1	Total O 1 1	0	0
21	j	1	Total O 1 1	0	0

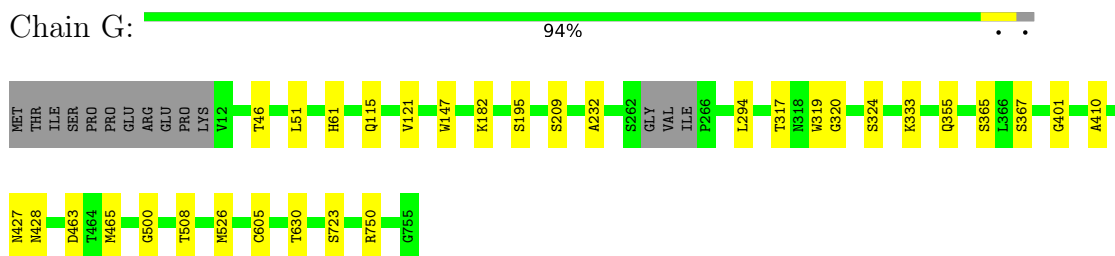
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

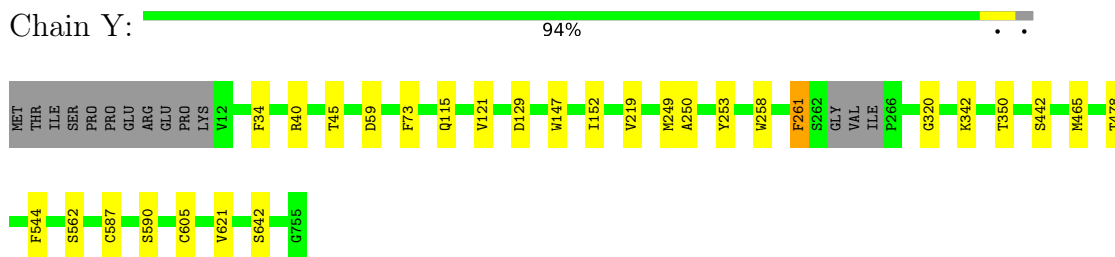
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



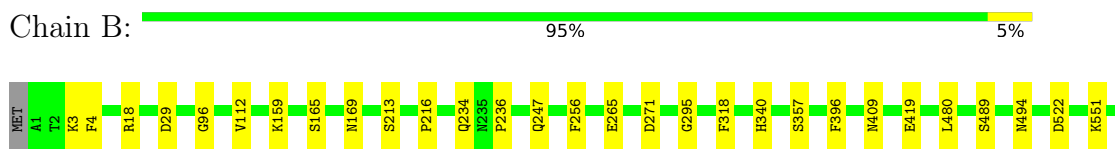
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



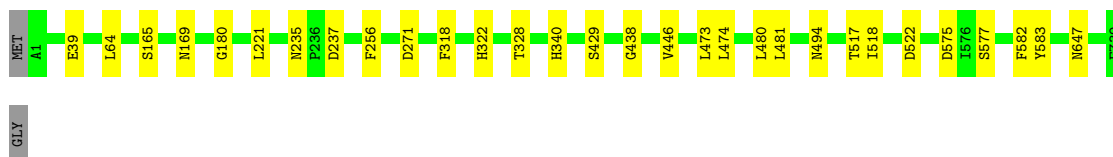
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





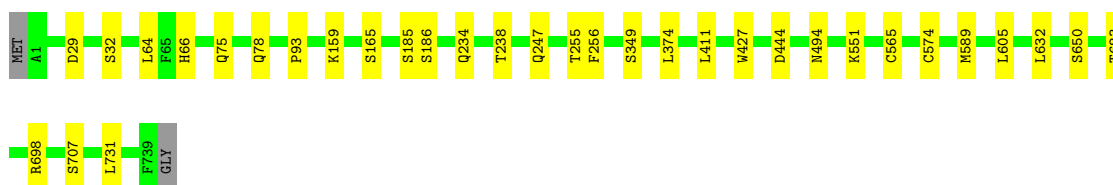
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain H: 96%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain Z: 95%



- Molecule 3: Photosystem I iron-sulfur center

Chain C: 94%



- Molecule 3: Photosystem I iron-sulfur center

Chain N: 95%



- Molecule 3: Photosystem I iron-sulfur center

Chain a: 95%



- Molecule 4: Photosystem I reaction center subunit II

Chain D: 94%





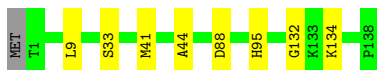
- Molecule 4: Photosystem I reaction center subunit II

Chain O:  94% • •




- Molecule 4: Photosystem I reaction center subunit II

Chain b:  94% 6% •




- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  83% 8% 9%




- Molecule 5: Photosystem I reaction center subunit IV

Chain P:  83% 7% • 9%




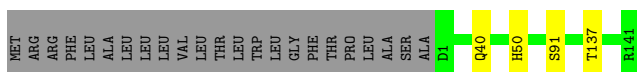
- Molecule 5: Photosystem I reaction center subunit IV

Chain c:  84% 7% 9%




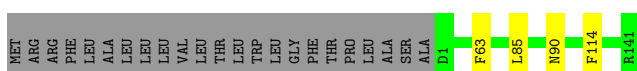
- Molecule 6: Photosystem I reaction center subunit III

Chain F:  84% • 14%




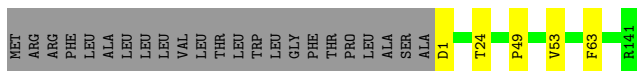
- Molecule 6: Photosystem I reaction center subunit III

Chain Q:  84% • 14%



- Molecule 6: Photosystem I reaction center subunit III

Chain d:  83% 14%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Photosystem I reaction center subunit VIII

Chain R:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Photosystem I reaction center subunit VIII

Chain e:  95% 5%



- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: Photosystem I reaction center subunit IX

Chain S:  98%



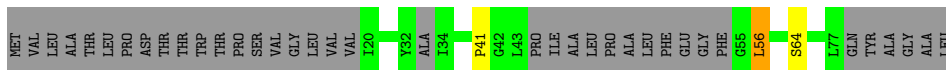
- Molecule 8: Photosystem I reaction center subunit IX

Chain f:  98%



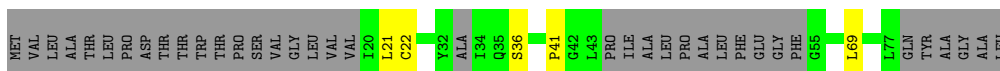
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain K:  52% 45%



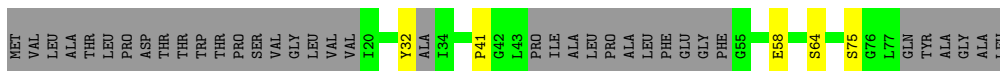
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain T:  49% 6% 45%



- Molecule 9: Photosystem I reaction center subunit PsaK

Chain g:  49% 6% 45%



- Molecule 10: Photosystem I reaction center subunit XI

Chain L:  92% 5% .



- Molecule 10: Photosystem I reaction center subunit XI

Chain U:  95% . .



- Molecule 10: Photosystem I reaction center subunit XI

Chain h:  90% 7% .



- Molecule 11: Photosystem I reaction center subunit XII

Chain M:  97% .



- Molecule 11: Photosystem I reaction center subunit XII

Chain V:  94% . .



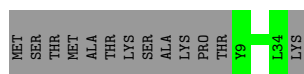
- Molecule 11: Photosystem I reaction center subunit XII

Chain i:  97%



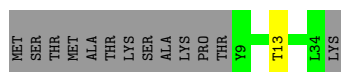
- Molecule 12: Photosystem I 4.8K protein

Chain W:  67% 33%



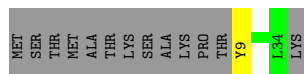
- Molecule 12: Photosystem I 4.8K protein

Chain X:  64% 33%



- Molecule 12: Photosystem I 4.8K protein

Chain j:  64% 33%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	279.10Å 164.60Å 284.10Å 90.00° 119.25° 90.00°	Depositor
Resolution (Å)	39.88 – 2.90 64.24 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.88-2.90) 92.7 (64.24-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.298 , 0.336 0.300 , 0.337	Depositor DCC
$R_{free}$ test set	24635 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.2	Xtrriage
Anisotropy	0.073	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 65.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.27$ , $\langle L^2 \rangle = 0.11$	Xtrriage
Estimated twinning fraction	0.268 for -h-l,k,h 0.268 for l,k,-h-l 0.347 for h,-k,-h-l 0.260 for -h-l,-k,l 0.259 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	72532	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.66	0/5990	0.74	0/8168
1	G	0.66	0/5990	0.75	0/8168
1	Y	0.66	0/5990	0.75	0/8168
2	B	0.64	0/6107	0.74	0/8345
2	H	0.66	0/6107	0.75	0/8345
2	Z	0.65	0/6107	0.73	0/8345
3	C	0.69	0/608	0.84	0/824
3	N	0.68	0/608	0.85	0/824
3	a	0.69	0/608	0.82	0/824
4	D	0.64	0/1101	0.78	0/1492
4	O	0.63	0/1101	0.77	0/1492
4	b	0.64	0/1101	0.79	0/1492
5	E	0.68	0/551	0.78	0/750
5	P	0.68	0/551	0.76	0/750
5	c	0.67	0/551	0.77	0/750
6	F	0.69	0/1087	0.78	0/1476
6	Q	0.68	0/1087	0.76	0/1476
6	d	0.68	0/1087	0.77	0/1476
7	I	0.66	0/312	0.71	0/425
7	R	0.66	0/312	0.69	0/425
7	e	0.64	0/312	0.76	0/425
8	J	0.64	0/350	0.72	0/477
8	S	0.65	0/350	0.71	0/477
8	f	0.64	0/350	0.71	0/477
9	K	0.72	0/331	0.80	0/444
9	T	0.72	0/331	0.86	0/444
9	g	0.73	0/331	0.82	0/444
10	L	0.68	0/1148	0.78	0/1558
10	U	0.68	0/1148	0.75	0/1558
10	h	0.68	0/1148	0.77	0/1558
11	M	0.68	0/236	0.76	0/322
11	V	0.69	0/236	0.75	0/322

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
11	i	0.70	0/236	0.74	0/322
12	W	0.65	0/227	0.69	0/310
12	X	0.66	0/227	0.70	0/310
12	j	0.66	0/227	0.65	0/310
All	All	0.66	0/54144	0.75	0/73773

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
9	K	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	K	56	LEU	Peptide

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	737/755 (98%)	634 (86%)	89 (12%)	14 (2%)	8	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	737/755 (98%)	634 (86%)	86 (12%)	17 (2%)	6	23
1	Y	737/755 (98%)	627 (85%)	98 (13%)	12 (2%)	9	32
2	B	737/741 (100%)	639 (87%)	84 (11%)	14 (2%)	8	28
2	H	737/741 (100%)	658 (89%)	69 (9%)	10 (1%)	11	36
2	Z	737/741 (100%)	642 (87%)	86 (12%)	9 (1%)	13	40
3	C	78/81 (96%)	72 (92%)	4 (5%)	2 (3%)	5	20
3	N	78/81 (96%)	69 (88%)	8 (10%)	1 (1%)	12	37
3	a	78/81 (96%)	64 (82%)	12 (15%)	2 (3%)	5	20
4	D	136/139 (98%)	119 (88%)	14 (10%)	3 (2%)	6	24
4	O	136/139 (98%)	122 (90%)	11 (8%)	3 (2%)	6	24
4	b	136/139 (98%)	117 (86%)	15 (11%)	4 (3%)	4	18
5	E	67/76 (88%)	58 (87%)	6 (9%)	3 (4%)	2	9
5	P	67/76 (88%)	56 (84%)	6 (9%)	5 (8%)	1	2
5	c	67/76 (88%)	56 (84%)	8 (12%)	3 (4%)	2	9
6	F	139/164 (85%)	126 (91%)	12 (9%)	1 (1%)	22	54
6	Q	139/164 (85%)	124 (89%)	14 (10%)	1 (1%)	22	54
6	d	139/164 (85%)	118 (85%)	18 (13%)	3 (2%)	6	24
7	I	36/38 (95%)	30 (83%)	6 (17%)	0	100	100
7	R	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
7	e	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	5	19
8	J	39/41 (95%)	34 (87%)	5 (13%)	0	100	100
8	S	39/41 (95%)	34 (87%)	5 (13%)	0	100	100
8	f	39/41 (95%)	38 (97%)	0	1 (3%)	5	20
9	K	40/83 (48%)	31 (78%)	7 (18%)	2 (5%)	2	7
9	T	40/83 (48%)	33 (82%)	4 (10%)	3 (8%)	1	2
9	g	40/83 (48%)	30 (75%)	8 (20%)	2 (5%)	2	7
10	L	149/155 (96%)	124 (83%)	22 (15%)	3 (2%)	7	27
10	U	149/155 (96%)	138 (93%)	11 (7%)	0	100	100
10	h	149/155 (96%)	129 (87%)	17 (11%)	3 (2%)	7	27
11	M	28/31 (90%)	26 (93%)	2 (7%)	0	100	100
11	V	28/31 (90%)	26 (93%)	2 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	i	28/31 (90%)	28 (100%)	0	0	100	100
12	W	24/39 (62%)	23 (96%)	1 (4%)	0	100	100
12	X	24/39 (62%)	24 (100%)	0	0	100	100
12	j	24/39 (62%)	23 (96%)	1 (4%)	0	100	100
All	All	6630/7029 (94%)	5768 (87%)	740 (11%)	122 (2%)	8	29

5 of 122 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	VAL
4	D	95	HIS
5	E	55	VAL
1	G	320	GLY
1	G	508	THR

### 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	A	590/603 (98%)	574 (97%)	16 (3%)	44	77
1	G	590/603 (98%)	575 (98%)	15 (2%)	47	78
1	Y	590/603 (98%)	572 (97%)	18 (3%)	40	74
2	B	597/598 (100%)	575 (96%)	22 (4%)	34	68
2	H	597/598 (100%)	577 (97%)	20 (3%)	37	71
2	Z	597/598 (100%)	573 (96%)	24 (4%)	31	65
3	C	67/68 (98%)	64 (96%)	3 (4%)	27	61
3	N	67/68 (98%)	65 (97%)	2 (3%)	41	75
3	a	67/68 (98%)	65 (97%)	2 (3%)	41	75
4	D	115/116 (99%)	110 (96%)	5 (4%)	29	62
4	O	115/116 (99%)	110 (96%)	5 (4%)	29	62
4	b	115/116 (99%)	111 (96%)	4 (4%)	36	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	59/65 (91%)	56 (95%)	3 (5%)	24	56
5	P	59/65 (91%)	57 (97%)	2 (3%)	37	71
5	c	59/65 (91%)	58 (98%)	1 (2%)	60	86
6	F	109/128 (85%)	106 (97%)	3 (3%)	43	76
6	Q	109/128 (85%)	106 (97%)	3 (3%)	43	76
6	d	109/128 (85%)	108 (99%)	1 (1%)	78	93
7	I	32/32 (100%)	32 (100%)	0	100	100
7	R	32/32 (100%)	32 (100%)	0	100	100
7	e	32/32 (100%)	31 (97%)	1 (3%)	40	74
8	J	36/36 (100%)	36 (100%)	0	100	100
8	S	36/36 (100%)	35 (97%)	1 (3%)	43	76
8	f	36/36 (100%)	36 (100%)	0	100	100
9	K	33/61 (54%)	32 (97%)	1 (3%)	41	75
9	T	33/61 (54%)	31 (94%)	2 (6%)	18	48
9	g	33/61 (54%)	30 (91%)	3 (9%)	9	28
10	L	117/120 (98%)	112 (96%)	5 (4%)	29	62
10	U	117/120 (98%)	113 (97%)	4 (3%)	37	71
10	h	117/120 (98%)	109 (93%)	8 (7%)	16	42
11	M	25/26 (96%)	25 (100%)	0	100	100
11	V	25/26 (96%)	24 (96%)	1 (4%)	31	65
11	i	25/26 (96%)	25 (100%)	0	100	100
12	W	20/31 (64%)	20 (100%)	0	100	100
12	X	20/31 (64%)	19 (95%)	1 (5%)	24	57
12	j	20/31 (64%)	19 (95%)	1 (5%)	24	57
All	All	5400/5652 (96%)	5223 (97%)	177 (3%)	38	72

5 of 177 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	40	ARG
2	Z	411	LEU
1	Y	147	TRP
1	Y	605	CYS
2	Z	632	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	331	ASN
4	O	63	GLN
2	Z	494	ASN
2	H	378	HIS
2	H	647	ASN

### 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](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 381 ligands modelled in this entry, 3 are monoatomic - leaving 378 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
14	CLA	Z	835	-	60,68,73	2.31	22 (36%)	70,107,113	2.52	22 (31%)
14	CLA	B	827	-	65,73,73	2.22	20 (30%)	76,113,113	2.52	25 (32%)
14	CLA	H	815	-	55,63,73	2.43	18 (32%)	64,101,113	2.86	25 (39%)
14	CLA	A	822	-	65,73,73	2.29	21 (32%)	76,113,113	2.77	25 (32%)
14	CLA	F	202	-	45,53,73	2.57	17 (37%)	52,89,113	2.89	22 (42%)
14	CLA	Y	855	-	65,73,73	2.18	17 (26%)	76,113,113	2.41	22 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	B	809	-	65,73,73	2.24	18 (27%)	76,113,113	2.64	24 (31%)
14	CLA	H	804	-	65,73,73	2.28	19 (29%)	76,113,113	2.48	24 (31%)
17	BCR	G	846	-	41,41,41	2.81	7 (17%)	56,56,56	7.22	30 (53%)
14	CLA	G	803	-	65,73,73	2.20	18 (27%)	76,113,113	2.42	27 (35%)
14	CLA	G	802	-	65,73,73	2.24	19 (29%)	76,113,113	2.52	22 (28%)
14	CLA	G	809	-	65,73,73	2.20	19 (29%)	76,113,113	2.54	26 (34%)
14	CLA	H	806	-	65,73,73	2.23	19 (29%)	76,113,113	2.40	19 (25%)
14	CLA	B	810	2	65,73,73	2.26	21 (32%)	76,113,113	2.85	27 (35%)
16	SF4	a	101	3	0,12,12	-	-	-	-	-
14	CLA	B	836	-	45,53,73	2.55	20 (44%)	52,89,113	3.08	22 (42%)
14	CLA	G	822	-	65,73,73	2.23	19 (29%)	76,113,113	2.83	26 (34%)
14	CLA	A	834	-	55,63,73	2.46	20 (36%)	64,101,113	2.63	24 (37%)
14	CLA	A	819	-	65,73,73	2.20	20 (30%)	76,113,113	2.50	22 (28%)
14	CLA	A	803	-	65,73,73	2.27	22 (33%)	76,113,113	2.67	25 (32%)
14	CLA	A	815	-	50,58,73	2.55	19 (38%)	58,95,113	3.25	25 (43%)
14	CLA	G	808	1	65,73,73	2.24	18 (27%)	76,113,113	2.64	25 (32%)
14	CLA	G	814	-	50,58,73	2.58	19 (38%)	58,95,113	3.20	30 (51%)
14	CLA	Z	817	-	60,68,73	2.40	19 (31%)	70,107,113	2.47	25 (35%)
14	CLA	A	812	-	54,62,73	2.50	20 (37%)	62,99,113	2.69	24 (38%)
14	CLA	G	813	-	60,68,73	2.29	21 (35%)	70,107,113	2.71	25 (35%)
14	CLA	J	102	-	55,63,73	2.52	21 (38%)	64,101,113	2.77	25 (39%)
14	CLA	B	813	-	65,73,73	2.24	20 (30%)	76,113,113	2.72	26 (34%)
14	CLA	H	807	-	65,73,73	2.31	21 (32%)	76,113,113	2.66	27 (35%)
14	CLA	H	819	-	45,53,73	2.55	18 (40%)	52,89,113	3.12	22 (42%)
19	LMG	Z	847	-	49,49,55	1.26	6 (12%)	57,57,63	1.24	5 (8%)
14	CLA	A	817	-	60,68,73	2.32	20 (33%)	70,107,113	2.61	27 (38%)
17	BCR	B	843	-	30,30,41	3.42	6 (20%)	39,39,56	8.21	19 (48%)
17	BCR	Y	850	-	41,41,41	2.70	6 (14%)	56,56,56	7.10	24 (42%)
17	BCR	L	203	-	41,41,41	2.92	6 (14%)	56,56,56	6.97	29 (51%)
14	CLA	Z	839	-	65,73,73	2.32	21 (32%)	76,113,113	2.71	25 (32%)
13	CL0	G	801	-	65,73,73	2.44	20 (30%)	76,113,113	2.73	27 (35%)
14	CLA	H	837	-	65,73,73	2.26	20 (30%)	76,113,113	2.32	24 (31%)
14	CLA	f	102	-	55,63,73	2.49	20 (36%)	64,101,113	2.69	25 (39%)
14	CLA	Z	822	2	55,63,73	2.46	19 (34%)	64,101,113	2.83	27 (42%)
14	CLA	U	1006	2	65,73,73	2.25	19 (29%)	76,113,113	2.68	30 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	H	816	-	65,73,73	2.19	20 (30%)	76,113,113	2.76	29 (38%)
15	PQN	Z	840	-	34,34,34	1.66	2 (5%)	42,45,45	1.10	4 (9%)
17	BCR	h	202	-	41,41,41	2.53	8 (19%)	56,56,56	7.31	28 (50%)
14	CLA	H	833	-	45,53,73	2.57	18 (40%)	52,89,113	2.84	23 (44%)
14	CLA	H	808	2	65,73,73	2.20	19 (29%)	76,113,113	2.65	27 (35%)
14	CLA	B	821	-	45,53,73	2.58	19 (42%)	52,89,113	3.01	23 (44%)
14	CLA	B	817	-	65,73,73	2.17	20 (30%)	76,113,113	2.45	24 (31%)
14	CLA	G	811	-	65,73,73	2.32	20 (30%)	76,113,113	2.44	21 (27%)
14	CLA	Y	842	-	65,73,73	2.24	20 (30%)	76,113,113	2.62	23 (30%)
14	CLA	Z	809	-	55,63,73	2.47	20 (36%)	64,101,113	2.73	24 (37%)
14	CLA	B	825	-	65,73,73	2.31	20 (30%)	76,113,113	2.65	25 (32%)
14	CLA	Z	805	-	65,73,73	2.27	21 (32%)	76,113,113	2.56	26 (34%)
14	CLA	A	806	-	65,73,73	2.27	21 (32%)	76,113,113	2.50	23 (30%)
17	BCR	G	849	-	41,41,41	2.83	7 (17%)	56,56,56	6.96	25 (44%)
14	CLA	H	812	-	65,73,73	2.28	20 (30%)	76,113,113	2.49	22 (28%)
14	CLA	g	102	-	45,53,73	2.64	18 (40%)	52,89,113	2.90	21 (40%)
14	CLA	B	818	-	60,68,73	2.34	20 (33%)	70,107,113	2.67	24 (34%)
14	CLA	B	801	-	65,73,73	2.15	16 (24%)	76,113,113	2.52	22 (28%)
14	CLA	Z	831	-	55,63,73	2.40	19 (34%)	64,101,113	2.66	27 (42%)
18	LHG	H	847	-	36,36,48	1.10	2 (5%)	39,42,54	0.92	3 (7%)
14	CLA	Y	806	-	65,73,73	2.25	17 (26%)	76,113,113	2.58	25 (32%)
17	BCR	A	847	-	41,41,41	2.70	6 (14%)	56,56,56	7.09	26 (46%)
14	CLA	Z	838	-	65,73,73	2.25	20 (30%)	76,113,113	2.53	23 (30%)
17	BCR	e	101	-	41,41,41	2.73	6 (14%)	56,56,56	7.45	26 (46%)
14	CLA	L	201	-	65,73,73	2.23	19 (29%)	76,113,113	2.64	26 (34%)
14	CLA	Z	819	-	45,53,73	2.67	17 (37%)	52,89,113	3.11	23 (44%)
14	CLA	G	830	-	65,73,73	2.23	19 (29%)	76,113,113	2.53	22 (28%)
14	CLA	B	828	-	65,73,73	2.22	20 (30%)	76,113,113	2.55	25 (32%)
14	CLA	Z	826	-	65,73,73	2.20	19 (29%)	76,113,113	2.47	22 (28%)
19	LMG	B	849	-	52,52,55	1.29	7 (13%)	60,60,63	0.99	3 (5%)
17	BCR	L	208	-	41,41,41	3.06	7 (17%)	56,56,56	6.91	24 (42%)
14	CLA	B	831	-	45,53,73	2.59	19 (42%)	52,89,113	2.87	24 (46%)
16	SF4	N	102	3,21	0,12,12	-	-	-	-	-
14	CLA	K	103	-	45,53,73	2.55	18 (40%)	52,89,113	2.95	20 (38%)
14	CLA	B	815	-	45,53,73	2.52	16 (35%)	52,89,113	2.94	24 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	A	811	14	65,73,73	2.25	20 (30%)	76,113,113	2.43	22 (28%)
14	CLA	B	802	-	65,73,73	2.21	19 (29%)	76,113,113	2.53	26 (34%)
14	CLA	B	840	-	65,73,73	2.24	20 (30%)	76,113,113	2.41	25 (32%)
14	CLA	Y	822	-	65,73,73	2.31	20 (30%)	76,113,113	2.60	22 (28%)
17	BCR	T	102	-	41,41,41	2.46	6 (14%)	56,56,56	7.40	24 (42%)
14	CLA	Y	814	-	55,63,73	2.49	20 (36%)	64,101,113	2.73	22 (34%)
14	CLA	B	808	-	65,73,73	2.20	20 (30%)	76,113,113	2.48	25 (32%)
14	CLA	A	809	1	65,73,73	2.22	20 (30%)	76,113,113	2.69	25 (32%)
14	CLA	Y	840	-	65,73,73	2.31	20 (30%)	76,113,113	2.64	24 (31%)
14	CLA	H	820	-	45,53,73	2.65	19 (42%)	52,89,113	3.11	25 (48%)
14	CLA	G	837	-	65,73,73	2.23	20 (30%)	76,113,113	2.59	26 (34%)
14	CLA	h	206	-	65,73,73	2.28	17 (26%)	76,113,113	2.83	27 (35%)
14	CLA	G	818	-	65,73,73	2.27	19 (29%)	76,113,113	2.65	26 (34%)
14	CLA	G	823	-	50,58,73	2.54	20 (40%)	58,95,113	2.97	24 (41%)
14	CLA	A	852	-	65,73,73	2.24	19 (29%)	76,113,113	2.64	26 (34%)
17	BCR	f	103	-	41,41,41	2.56	6 (14%)	56,56,56	7.19	28 (50%)
14	CLA	G	833	-	65,73,73	2.26	19 (29%)	76,113,113	2.53	23 (30%)
17	BCR	R	102	-	41,41,41	3.00	8 (19%)	56,56,56	6.94	23 (41%)
14	CLA	Y	829	-	65,73,73	2.32	21 (32%)	76,113,113	2.44	22 (28%)
14	CLA	H	830	-	55,63,73	2.43	19 (34%)	64,101,113	2.53	22 (34%)
14	CLA	h	201	-	65,73,73	2.26	21 (32%)	76,113,113	2.40	23 (30%)
14	CLA	J	101	8	45,53,73	2.59	17 (37%)	52,89,113	2.88	20 (38%)
17	BCR	B	851	-	41,41,41	2.77	6 (14%)	56,56,56	7.08	27 (48%)
15	PQN	Y	844	-	34,34,34	1.82	2 (5%)	42,45,45	0.83	1 (2%)
14	CLA	Y	815	-	50,58,73	2.61	20 (40%)	58,95,113	3.05	24 (41%)
14	CLA	Z	806	-	65,73,73	2.23	19 (29%)	76,113,113	2.58	23 (30%)
14	CLA	G	853	-	45,53,73	2.63	19 (42%)	52,89,113	2.74	18 (34%)
14	CLA	Y	811	14	65,73,73	2.32	17 (26%)	76,113,113	2.51	24 (31%)
14	CLA	Y	843	18	50,58,73	2.64	20 (40%)	58,95,113	3.02	25 (43%)
18	LHG	B	850	-	38,38,48	1.09	2 (5%)	41,44,54	1.28	4 (9%)
14	CLA	A	836	-	50,58,73	2.64	20 (40%)	58,95,113	2.84	22 (37%)
14	CLA	Z	836	-	65,73,73	2.19	19 (29%)	76,113,113	2.53	21 (27%)
14	CLA	V	1201	-	54,62,73	2.52	18 (33%)	62,99,113	2.76	22 (35%)
14	CLA	A	830	-	65,73,73	2.21	21 (32%)	76,113,113	2.59	20 (26%)
14	CLA	B	823	-	60,68,73	2.40	20 (33%)	70,107,113	2.48	22 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	B	820	-	45,53,73	2.61	19 (42%)	52,89,113	2.87	22 (42%)
14	CLA	G	807	-	51,59,73	2.59	21 (41%)	59,96,113	2.95	23 (38%)
14	CLA	f	101	8	45,53,73	2.65	20 (44%)	52,89,113	2.89	21 (40%)
14	CLA	Z	815	-	65,73,73	2.20	20 (30%)	76,113,113	2.54	23 (30%)
14	CLA	Y	841	-	65,73,73	2.21	20 (30%)	76,113,113	2.42	20 (26%)
14	CLA	Y	836	1	45,53,73	2.57	18 (40%)	52,89,113	2.94	20 (38%)
14	CLA	Y	854	-	65,73,73	2.18	18 (27%)	76,113,113	2.53	24 (31%)
17	BCR	Y	847	-	41,41,41	2.71	6 (14%)	56,56,56	7.10	29 (51%)
14	CLA	Z	828	-	45,53,73	2.52	19 (42%)	52,89,113	2.91	23 (44%)
14	CLA	Y	839	-	50,58,73	2.58	21 (42%)	58,95,113	3.07	25 (43%)
17	BCR	Z	844	-	25,25,41	2.29	2 (8%)	33,33,56	7.89	20 (60%)
17	BCR	A	849	-	41,41,41	2.67	6 (14%)	56,56,56	7.34	26 (46%)
14	CLA	Z	818	-	45,53,73	2.64	18 (40%)	52,89,113	2.96	26 (50%)
17	BCR	G	850	-	41,41,41	2.70	6 (14%)	56,56,56	7.31	27 (48%)
14	CLA	H	826	-	65,73,73	2.22	19 (29%)	76,113,113	2.58	25 (32%)
14	CLA	G	816	-	50,58,73	2.61	21 (42%)	58,95,113	2.89	22 (37%)
14	CLA	Z	833	-	45,53,73	2.65	16 (35%)	52,89,113	2.76	19 (36%)
17	BCR	B	844	-	41,41,41	2.78	6 (14%)	56,56,56	7.31	25 (44%)
14	CLA	A	813	-	60,68,73	2.33	20 (33%)	70,107,113	2.58	24 (34%)
14	CLA	B	806	-	65,73,73	2.15	19 (29%)	76,113,113	2.78	24 (31%)
14	CLA	h	205	10	65,73,73	2.29	19 (29%)	76,113,113	2.61	24 (31%)
14	CLA	Z	801	-	65,73,73	2.21	18 (27%)	76,113,113	2.48	23 (30%)
14	CLA	G	805	-	65,73,73	2.15	18 (27%)	76,113,113	2.68	24 (31%)
14	CLA	Z	823	-	65,73,73	2.33	20 (30%)	76,113,113	2.67	27 (35%)
16	SF4	C	101	3,21	0,12,12	-	-	-	-	-
14	CLA	A	833	-	65,73,73	2.25	18 (27%)	76,113,113	2.50	28 (36%)
14	CLA	Z	825	-	65,73,73	2.23	19 (29%)	76,113,113	2.38	21 (27%)
17	BCR	H	845	-	41,41,41	2.78	8 (19%)	56,56,56	7.11	28 (50%)
14	CLA	H	832	-	45,53,73	2.62	20 (44%)	52,89,113	2.86	22 (42%)
18	LHG	G	852	14	31,31,48	1.26	2 (6%)	34,37,54	1.31	4 (11%)
14	CLA	G	834	-	55,63,73	2.47	20 (36%)	64,101,113	2.60	23 (35%)
14	CLA	Z	812	-	65,73,73	2.42	20 (30%)	76,113,113	2.40	21 (27%)
17	BCR	B	848	-	41,41,41	2.76	7 (17%)	56,56,56	6.90	27 (48%)
14	CLA	G	815	-	50,58,73	2.54	19 (38%)	58,95,113	3.16	26 (44%)
14	CLA	Y	837	-	50,58,73	2.56	20 (40%)	58,95,113	2.91	23 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	G	840	-	50,58,73	2.63	17 (34%)	58,95,113	2.66	22 (37%)
14	CLA	Y	823	-	50,58,73	2.63	20 (40%)	58,95,113	2.74	25 (43%)
16	SF4	C	102	3	0,12,12	-	-	-	-	-
14	CLA	G	824	-	60,68,73	2.34	19 (31%)	70,107,113	2.55	22 (31%)
14	CLA	G	838	-	50,58,73	2.60	20 (40%)	58,95,113	2.98	24 (41%)
14	CLA	A	825	-	65,73,73	2.29	21 (32%)	76,113,113	2.69	24 (31%)
14	CLA	B	838	-	65,73,73	2.17	19 (29%)	76,113,113	2.67	25 (32%)
14	CLA	Y	805	-	65,73,73	2.13	19 (29%)	76,113,113	2.65	28 (36%)
14	CLA	A	824	-	60,68,73	2.37	20 (33%)	70,107,113	2.51	24 (34%)
17	BCR	F	203	-	41,41,41	2.71	7 (17%)	56,56,56	7.14	29 (51%)
15	PQN	H	839	-	34,34,34	1.61	2 (5%)	42,45,45	1.28	6 (14%)
14	CLA	Y	803	-	65,73,73	2.35	20 (30%)	76,113,113	2.55	25 (32%)
14	CLA	H	825	-	65,73,73	2.27	20 (30%)	76,113,113	2.48	26 (34%)
14	CLA	Y	809	-	65,73,73	2.26	20 (30%)	76,113,113	2.45	23 (30%)
14	CLA	Z	821	-	60,68,73	2.40	20 (33%)	70,107,113	2.46	25 (35%)
14	CLA	L	207	-	65,73,73	2.28	19 (29%)	76,113,113	2.45	21 (27%)
14	CLA	A	838	-	50,58,73	2.45	19 (38%)	58,95,113	2.91	21 (36%)
14	CLA	H	802	-	65,73,73	2.25	20 (30%)	76,113,113	2.42	26 (34%)
14	CLA	B	814	-	65,73,73	2.37	20 (30%)	76,113,113	2.46	25 (32%)
17	BCR	K	102	-	41,41,41	2.78	6 (14%)	56,56,56	7.21	24 (42%)
18	LHG	A	851	14	31,31,48	1.19	2 (6%)	34,37,54	1.20	3 (8%)
17	BCR	Z	845	-	41,41,41	2.59	8 (19%)	56,56,56	7.27	30 (53%)
14	CLA	Y	812	-	55,63,73	2.42	18 (32%)	64,101,113	2.76	27 (42%)
14	CLA	A	835	1	45,53,73	2.59	19 (42%)	52,89,113	2.89	22 (42%)
17	BCR	G	847	-	41,41,41	2.78	6 (14%)	56,56,56	6.97	26 (46%)
14	CLA	X	1701	-	45,53,73	2.61	20 (44%)	52,89,113	2.93	21 (40%)
18	LHG	A	850	-	48,48,48	0.99	2 (4%)	51,54,54	1.05	3 (5%)
14	CLA	B	829	-	65,73,73	2.21	18 (27%)	76,113,113	2.57	21 (27%)
18	LHG	Y	853	14	24,24,48	1.51	2 (8%)	27,30,54	1.60	4 (14%)
14	CLA	Q	201	-	65,73,73	2.16	19 (29%)	76,113,113	2.64	23 (30%)
17	BCR	A	845	-	41,41,41	2.55	6 (14%)	56,56,56	7.14	28 (50%)
14	CLA	Z	807	-	65,73,73	2.25	20 (30%)	76,113,113	2.66	26 (34%)
17	BCR	I	101	-	41,41,41	2.59	7 (17%)	56,56,56	7.30	26 (46%)
14	CLA	U	1002	10	65,73,73	2.21	20 (30%)	76,113,113	2.75	28 (36%)
17	BCR	H	842	-	41,41,41	2.74	6 (14%)	56,56,56	7.14	24 (42%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	G	826	-	60,68,73	2.30	19 (31%)	70,107,113	2.72	24 (34%)
18	LHG	G	851	-	48,48,48	0.93	2 (4%)	51,54,54	1.10	3 (5%)
14	CLA	j	102	-	45,53,73	2.58	17 (37%)	52,89,113	2.91	21 (40%)
14	CLA	G	806	-	65,73,73	2.19	19 (29%)	76,113,113	2.53	22 (28%)
14	CLA	H	824	-	65,73,73	2.23	21 (32%)	76,113,113	2.85	31 (40%)
14	CLA	Y	828	-	65,73,73	2.17	20 (30%)	76,113,113	2.35	24 (31%)
14	CLA	B	835	-	45,53,73	2.63	21 (46%)	52,89,113	2.90	22 (42%)
17	BCR	U	1008	-	41,41,41	2.56	6 (14%)	56,56,56	7.17	25 (44%)
14	CLA	H	814	-	45,53,73	2.61	19 (42%)	52,89,113	3.00	27 (51%)
14	CLA	Z	816	-	60,68,73	2.33	20 (33%)	70,107,113	2.61	25 (35%)
14	CLA	H	811	-	45,53,73	2.55	18 (40%)	52,89,113	2.80	22 (42%)
14	CLA	G	832	-	65,73,73	2.20	18 (27%)	76,113,113	2.48	25 (32%)
14	CLA	G	827	-	65,73,73	2.26	19 (29%)	76,113,113	2.35	24 (31%)
17	BCR	d	203	-	41,41,41	2.62	6 (14%)	56,56,56	7.01	27 (48%)
14	CLA	A	837	-	65,73,73	2.20	19 (29%)	76,113,113	2.62	25 (32%)
14	CLA	H	827	-	65,73,73	2.21	20 (30%)	76,113,113	2.65	24 (31%)
17	BCR	B	846	-	25,25,41	2.18	2 (8%)	33,33,56	8.00	15 (45%)
14	CLA	h	207	-	65,73,73	2.29	19 (29%)	76,113,113	2.52	24 (31%)
14	CLA	B	841	-	65,73,73	2.17	19 (29%)	76,113,113	2.85	30 (39%)
14	CLA	H	821	-	55,63,73	2.55	20 (36%)	64,101,113	2.83	22 (34%)
14	CLA	Z	808	2	65,73,73	2.18	20 (30%)	76,113,113	2.49	21 (27%)
14	CLA	Z	837	-	45,53,73	2.57	18 (40%)	52,89,113	3.12	20 (38%)
14	CLA	B	805	-	54,62,73	2.50	20 (37%)	62,99,113	2.96	24 (38%)
14	CLA	Y	810	-	45,53,73	2.56	19 (42%)	52,89,113	3.01	19 (36%)
14	CLA	H	809	2	65,73,73	2.22	18 (27%)	76,113,113	2.63	27 (35%)
14	CLA	B	839	-	45,53,73	2.60	18 (40%)	52,89,113	2.83	18 (34%)
14	CLA	Y	820	-	60,68,73	2.30	20 (33%)	70,107,113	2.53	24 (34%)
14	CLA	A	831	-	50,58,73	2.51	19 (38%)	58,95,113	2.77	23 (39%)
14	CLA	T	101	-	42,49,73	2.55	17 (40%)	48,83,113	2.93	20 (41%)
14	CLA	B	804	-	65,73,73	2.19	20 (30%)	76,113,113	2.51	22 (28%)
16	SF4	a	102	3	0,12,12	-	-	-	-	-
14	CLA	A	802	-	65,73,73	2.19	21 (32%)	76,113,113	2.57	29 (38%)
18	LHG	Y	852	-	48,48,48	1.01	2 (4%)	51,54,54	1.00	2 (3%)
14	CLA	Y	831	-	50,58,73	2.55	20 (40%)	58,95,113	2.95	27 (46%)
14	CLA	Z	813	-	45,53,73	2.65	20 (44%)	52,89,113	3.08	25 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	B	834	-	45,53,73	2.71	20 (44%)	52,89,113	3.29	25 (48%)
17	BCR	Y	851	-	41,41,41	2.94	6 (14%)	56,56,56	7.30	29 (51%)
14	CLA	B	807	-	65,73,73	2.22	19 (29%)	76,113,113	2.47	26 (34%)
14	CLA	B	819	-	60,68,73	2.35	21 (35%)	70,107,113	2.60	27 (38%)
17	BCR	M	101	-	41,41,41	2.80	6 (14%)	56,56,56	7.13	27 (48%)
14	CLA	Y	813	-	60,68,73	2.31	20 (33%)	70,107,113	2.54	23 (32%)
18	LHG	j	101	-	27,27,48	1.28	2 (7%)	30,33,54	1.36	4 (13%)
17	BCR	Z	843	-	41,41,41	2.56	6 (14%)	56,56,56	7.31	29 (51%)
14	CLA	A	829	-	65,73,73	2.24	21 (32%)	76,113,113	2.29	23 (30%)
14	CLA	Z	829	-	45,53,73	2.66	20 (44%)	52,89,113	3.14	25 (48%)
17	BCR	G	848	-	41,41,41	2.71	6 (14%)	56,56,56	7.23	31 (55%)
17	BCR	H	840	-	41,41,41	2.81	6 (14%)	56,56,56	7.12	21 (37%)
14	CLA	A	842	18	50,58,73	2.60	19 (38%)	58,95,113	3.12	21 (36%)
14	CLA	B	816	-	55,63,73	2.49	18 (32%)	64,101,113	2.65	23 (35%)
14	CLA	A	823	-	50,58,73	2.60	20 (40%)	58,95,113	2.92	23 (39%)
14	CLA	S	1102	8	45,53,73	2.57	18 (40%)	52,89,113	2.78	20 (38%)
14	CLA	A	808	1	65,73,73	2.25	19 (29%)	76,113,113	2.59	22 (28%)
14	CLA	G	825	-	65,73,73	2.21	19 (29%)	76,113,113	2.54	27 (35%)
14	CLA	L	205	10	65,73,73	2.32	19 (29%)	76,113,113	2.38	24 (31%)
14	CLA	H	823	2	55,63,73	2.58	20 (36%)	64,101,113	2.77	26 (40%)
14	CLA	A	826	-	60,68,73	2.33	20 (33%)	70,107,113	2.66	22 (31%)
14	CLA	H	836	-	45,53,73	2.56	21 (46%)	52,89,113	3.23	23 (44%)
14	CLA	B	803	-	65,73,73	2.15	18 (27%)	76,113,113	2.55	25 (32%)
14	CLA	H	834	-	60,68,73	2.24	19 (31%)	70,107,113	2.65	26 (37%)
14	CLA	Z	814	-	55,63,73	2.47	20 (36%)	64,101,113	2.90	26 (40%)
14	CLA	Z	827	-	65,73,73	2.15	20 (30%)	76,113,113	2.66	24 (31%)
14	CLA	U	1003	-	65,73,73	2.29	20 (30%)	76,113,113	2.50	24 (31%)
14	CLA	A	832	-	65,73,73	2.28	19 (29%)	76,113,113	2.53	24 (31%)
14	CLA	Y	826	-	60,68,73	2.34	20 (33%)	70,107,113	2.67	24 (34%)
14	CLA	A	827	-	65,73,73	2.25	20 (30%)	76,113,113	2.40	23 (30%)
14	CLA	H	813	-	65,73,73	2.26	19 (29%)	76,113,113	2.46	24 (31%)
14	CLA	G	821	-	65,73,73	2.27	19 (29%)	76,113,113	2.38	22 (28%)
14	CLA	H	828	-	65,73,73	2.28	20 (30%)	76,113,113	2.71	24 (31%)
14	CLA	A	820	-	60,68,73	2.35	21 (35%)	70,107,113	2.63	24 (34%)
13	CL0	A	801	-	65,73,73	2.40	19 (29%)	76,113,113	2.48	20 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	H	810	-	55,63,73	2.34	19 (34%)	64,101,113	2.75	20 (31%)
14	CLA	L	206	-	65,73,73	2.31	20 (30%)	76,113,113	2.46	23 (30%)
17	BCR	i	101	-	41,41,41	2.84	7 (17%)	56,56,56	7.60	32 (57%)
17	BCR	J	104	-	41,41,41	2.91	7 (17%)	56,56,56	7.08	27 (48%)
17	BCR	Z	842	-	41,41,41	2.69	8 (19%)	56,56,56	7.04	26 (46%)
17	BCR	Y	846	-	41,41,41	2.50	6 (14%)	56,56,56	7.20	24 (42%)
14	CLA	A	840	-	65,73,73	2.28	20 (30%)	76,113,113	2.50	22 (28%)
17	BCR	B	847	-	41,41,41	2.87	6 (14%)	56,56,56	7.00	24 (42%)
14	CLA	Y	802	-	65,73,73	2.13	17 (26%)	76,113,113	2.44	23 (30%)
14	CLA	Z	802	-	65,73,73	2.23	19 (29%)	76,113,113	2.48	25 (32%)
14	CLA	A	828	-	65,73,73	2.24	20 (30%)	76,113,113	2.48	22 (28%)
14	CLA	K	101	-	42,49,73	2.62	17 (40%)	48,83,113	2.95	24 (50%)
14	CLA	G	835	1	45,53,73	2.57	19 (42%)	52,89,113	2.95	23 (44%)
14	CLA	A	818	-	65,73,73	2.28	20 (30%)	76,113,113	2.58	26 (34%)
17	BCR	f	104	-	41,41,41	2.95	6 (14%)	56,56,56	6.95	28 (50%)
17	BCR	J	103	-	41,41,41	2.61	6 (14%)	56,56,56	6.88	28 (50%)
19	LMG	H	846	-	49,49,55	1.36	6 (12%)	57,57,63	1.18	4 (7%)
16	SF4	A	844	1,2	0,12,12	-	-	-	-	-
14	CLA	A	810	-	45,53,73	2.61	19 (42%)	52,89,113	2.85	20 (38%)
14	CLA	Y	827	-	65,73,73	2.31	20 (30%)	76,113,113	2.54	27 (35%)
14	CLA	B	833	-	55,63,73	2.41	20 (36%)	64,101,113	2.86	27 (42%)
14	CLA	L	202	-	65,73,73	2.18	19 (29%)	76,113,113	2.78	28 (36%)
17	BCR	H	844	-	41,41,41	2.75	6 (14%)	56,56,56	7.04	29 (51%)
14	CLA	G	839	-	65,73,73	2.23	20 (30%)	76,113,113	2.64	27 (35%)
17	BCR	H	843	-	25,25,41	2.03	2 (8%)	33,33,56	8.12	17 (51%)
16	SF4	Y	845	1,2	0,12,12	-	-	-	-	-
14	CLA	Y	833	-	65,73,73	2.27	19 (29%)	76,113,113	2.55	24 (31%)
17	BCR	Z	841	-	41,41,41	2.90	6 (14%)	56,56,56	7.13	25 (44%)
14	CLA	G	831	-	50,58,73	2.50	19 (38%)	58,95,113	2.90	24 (41%)
17	BCR	Y	848	-	41,41,41	2.60	6 (14%)	56,56,56	7.21	29 (51%)
17	BCR	Q	202	-	41,41,41	2.79	6 (14%)	56,56,56	6.74	27 (48%)
14	CLA	G	819	-	65,73,73	2.32	20 (30%)	76,113,113	2.68	25 (32%)
17	BCR	G	854	-	41,41,41	2.96	6 (14%)	56,56,56	7.14	27 (48%)
17	BCR	V	1202	-	41,41,41	2.74	7 (17%)	56,56,56	7.27	30 (53%)
14	CLA	Y	808	1	65,73,73	2.24	18 (27%)	76,113,113	2.61	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	S	1101	-	65,73,73	2.23	20 (30%)	76,113,113	2.59	23 (30%)
14	CLA	G	804	-	59,67,73	2.33	20 (33%)	68,105,113	2.67	21 (30%)
17	BCR	U	1007	-	41,41,41	2.80	6 (14%)	56,56,56	7.10	21 (37%)
14	CLA	A	821	-	65,73,73	2.29	19 (29%)	76,113,113	2.50	22 (28%)
14	CLA	G	829	-	65,73,73	2.26	19 (29%)	76,113,113	2.37	26 (34%)
17	BCR	h	203	-	41,41,41	3.00	7 (17%)	56,56,56	7.05	27 (48%)
14	CLA	Z	834	-	45,53,73	2.60	21 (46%)	52,89,113	3.05	23 (44%)
14	CLA	Z	820	-	55,63,73	2.50	19 (34%)	64,101,113	2.48	23 (35%)
17	BCR	R	101	-	41,41,41	2.76	6 (14%)	56,56,56	7.47	24 (42%)
14	CLA	G	842	-	65,73,73	2.20	21 (32%)	76,113,113	2.32	23 (30%)
14	CLA	Y	818	-	65,73,73	2.29	19 (29%)	76,113,113	2.68	25 (32%)
14	CLA	H	801	-	65,73,73	2.30	18 (27%)	76,113,113	2.57	25 (32%)
14	CLA	A	816	-	50,58,73	2.64	20 (40%)	58,95,113	2.91	21 (36%)
17	BCR	S	1104	-	41,41,41	2.89	7 (17%)	56,56,56	7.21	27 (48%)
14	CLA	A	807	-	51,59,73	2.52	19 (37%)	59,96,113	2.98	22 (37%)
14	CLA	Z	830	-	65,73,73	2.18	18 (27%)	76,113,113	2.47	22 (28%)
14	CLA	A	804	14	59,67,73	2.32	20 (33%)	68,105,113	2.86	22 (32%)
14	CLA	G	817	-	60,68,73	2.44	19 (31%)	70,107,113	2.52	27 (38%)
14	CLA	H	831	-	45,53,73	2.63	19 (42%)	52,89,113	2.92	20 (38%)
14	CLA	Z	804	-	65,73,73	2.23	21 (32%)	76,113,113	2.63	26 (34%)
14	CLA	Y	830	-	65,73,73	2.25	19 (29%)	76,113,113	2.69	23 (30%)
15	PQN	G	844	-	34,34,34	1.53	2 (5%)	42,45,45	1.24	6 (14%)
14	CLA	G	812	-	54,62,73	2.50	19 (35%)	62,99,113	2.64	20 (32%)
14	CLA	Y	825	-	65,73,73	2.31	20 (30%)	76,113,113	2.53	24 (31%)
14	CLA	g	101	-	42,49,73	2.60	15 (35%)	48,83,113	2.82	21 (43%)
14	CLA	S	1103	-	55,63,73	2.45	20 (36%)	64,101,113	2.85	24 (37%)
14	CLA	Y	832	-	65,73,73	2.27	19 (29%)	76,113,113	2.64	25 (32%)
17	BCR	L	209	-	41,41,41	2.75	6 (14%)	56,56,56	7.10	26 (46%)
14	CLA	Z	803	-	54,62,73	2.49	19 (35%)	62,99,113	2.95	25 (40%)
14	CLA	G	810	-	45,53,73	2.59	19 (42%)	52,89,113	2.99	22 (42%)
14	CLA	G	843	18	50,58,73	2.60	21 (42%)	58,95,113	2.89	25 (43%)
14	CLA	H	817	-	60,68,73	2.32	20 (33%)	70,107,113	2.65	22 (31%)
14	CLA	Z	810	-	45,53,73	2.54	16 (35%)	52,89,113	2.87	22 (42%)
17	BCR	B	845	-	41,41,41	2.72	7 (17%)	56,56,56	7.05	27 (48%)
17	BCR	A	846	-	41,41,41	2.62	6 (14%)	56,56,56	7.05	26 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	Z	824	-	65,73,73	2.21	17 (26%)	76,113,113	2.40	23 (30%)
17	BCR	A	848	-	41,41,41	2.57	6 (14%)	56,56,56	7.07	22 (39%)
16	SF4	G	845	1,2	0,12,12	-	-	-	-	-
14	CLA	Y	834	-	65,73,73	2.20	18 (27%)	76,113,113	2.48	26 (34%)
14	CLA	Q	203	-	45,53,73	2.55	18 (40%)	52,89,113	2.95	21 (40%)
14	CLA	B	826	-	65,73,73	2.25	20 (30%)	76,113,113	2.52	31 (40%)
14	CLA	G	836	-	50,58,73	2.60	20 (40%)	58,95,113	2.86	24 (41%)
16	SF4	N	101	3	0,12,12	-	-	-	-	-
14	CLA	Z	811	-	65,73,73	2.21	18 (27%)	76,113,113	2.51	25 (32%)
14	CLA	G	828	-	65,73,73	2.20	18 (27%)	76,113,113	2.55	28 (36%)
13	CL0	Y	801	-	65,73,73	2.31	18 (27%)	76,113,113	2.61	22 (28%)
14	CLA	Y	824	-	60,68,73	2.38	20 (33%)	70,107,113	2.62	22 (31%)
14	CLA	Y	838	-	65,73,73	2.24	20 (30%)	76,113,113	2.54	24 (31%)
17	BCR	H	841	-	41,41,41	3.03	7 (17%)	56,56,56	6.95	26 (46%)
14	CLA	B	822	-	55,63,73	2.49	19 (34%)	64,101,113	2.69	25 (39%)
14	CLA	T	103	-	45,53,73	2.64	20 (44%)	52,89,113	2.92	18 (34%)
17	BCR	U	1005	-	41,41,41	2.72	6 (14%)	56,56,56	6.90	21 (37%)
14	CLA	Y	835	-	55,63,73	2.56	21 (38%)	64,101,113	2.66	22 (34%)
14	CLA	B	832	-	65,73,73	2.19	19 (29%)	76,113,113	2.68	23 (30%)
14	CLA	Y	807	-	51,59,73	2.59	21 (41%)	59,96,113	2.94	23 (38%)
14	CLA	B	837	-	60,68,73	2.34	18 (30%)	70,107,113	2.72	22 (31%)
14	CLA	W	1701	-	45,53,73	2.55	19 (42%)	52,89,113	2.91	20 (38%)
17	BCR	Y	849	-	41,41,41	2.74	6 (14%)	56,56,56	7.20	24 (42%)
15	PQN	B	842	-	34,34,34	1.53	3 (8%)	42,45,45	1.22	6 (14%)
14	CLA	U	1004	-	65,73,73	2.20	19 (29%)	76,113,113	2.63	19 (25%)
14	CLA	d	202	-	45,53,73	2.64	18 (40%)	52,89,113	2.79	20 (38%)
14	CLA	Y	816	-	50,58,73	2.49	19 (38%)	58,95,113	2.93	23 (39%)
17	BCR	Y	856	-	41,41,41	2.71	7 (17%)	56,56,56	7.00	30 (53%)
14	CLA	B	812	-	50,58,73	2.58	19 (38%)	58,95,113	2.89	24 (41%)
14	CLA	B	824	2	55,63,73	2.48	18 (32%)	64,101,113	2.74	26 (40%)
14	CLA	H	822	-	60,68,73	2.26	17 (28%)	70,107,113	2.75	26 (37%)
14	CLA	A	814	-	50,58,73	2.57	20 (40%)	58,95,113	3.00	27 (46%)
14	CLA	H	838	-	65,73,73	2.22	19 (29%)	76,113,113	2.72	27 (35%)
14	CLA	Y	819	-	65,73,73	2.24	19 (29%)	76,113,113	2.59	22 (28%)
17	BCR	Q	204	-	41,41,41	2.72	7 (17%)	56,56,56	7.13	28 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	Z	832	-	45,53,73	2.70	19 (42%)	52,89,113	2.96	24 (46%)
14	CLA	Y	804	14	59,67,73	2.36	20 (33%)	68,105,113	2.93	26 (38%)
14	CLA	G	841	-	65,73,73	2.29	19 (29%)	76,113,113	2.50	24 (31%)
14	CLA	Y	821	-	65,73,73	2.36	20 (30%)	76,113,113	2.32	22 (28%)
17	BCR	F	201	-	41,41,41	2.76	6 (14%)	56,56,56	6.88	24 (42%)
14	CLA	Y	817	-	60,68,73	2.41	20 (33%)	70,107,113	2.45	23 (32%)
14	CLA	B	811	-	55,63,73	2.41	19 (34%)	64,101,113	2.65	27 (42%)
14	CLA	H	803	-	65,73,73	2.20	19 (29%)	76,113,113	2.50	24 (31%)
15	PQN	A	843	-	34,34,34	1.61	2 (5%)	42,45,45	1.09	3 (7%)
17	BCR	f	105	-	41,41,41	2.74	6 (14%)	56,56,56	7.07	26 (46%)
14	CLA	G	820	-	60,68,73	2.38	21 (35%)	70,107,113	2.63	25 (35%)
14	CLA	A	841	-	65,73,73	2.26	20 (30%)	76,113,113	2.51	24 (31%)
14	CLA	A	805	-	65,73,73	2.18	20 (30%)	76,113,113	2.47	22 (28%)
17	BCR	Z	846	-	41,41,41	2.70	7 (17%)	56,56,56	7.02	20 (35%)
14	CLA	H	818	-	60,68,73	2.41	21 (35%)	70,107,113	2.62	23 (32%)
14	CLA	H	835	-	65,73,73	2.18	20 (30%)	76,113,113	2.60	22 (28%)
14	CLA	A	839	-	50,58,73	2.60	20 (40%)	58,95,113	2.68	22 (37%)
14	CLA	H	829	-	45,53,73	2.54	18 (40%)	52,89,113	2.94	21 (40%)
14	CLA	H	805	-	65,73,73	2.24	19 (29%)	76,113,113	2.39	23 (30%)
14	CLA	B	830	-	45,53,73	2.49	19 (42%)	52,89,113	3.14	24 (46%)
17	BCR	H	848	-	41,41,41	2.77	6 (14%)	56,56,56	7.05	28 (50%)
14	CLA	d	201	-	50,58,73	2.61	20 (40%)	58,95,113	2.91	25 (43%)

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
14	CLA	Z	835	-	1/1/14/20	11/31/109/115	-
14	CLA	B	827	-	1/1/15/20	14/37/115/115	-
14	CLA	H	815	-	1/1/13/20	11/25/103/115	-
14	CLA	A	822	-	1/1/15/20	15/37/115/115	-
14	CLA	F	202	-	1/1/11/20	4/13/91/115	-
14	CLA	Y	855	-	1/1/15/20	12/37/115/115	-
14	CLA	B	809	-	1/1/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	804	-	1/1/15/20	12/37/115/115	-
17	BCR	G	846	-	-	7/29/63/63	0/2/2/2
14	CLA	G	803	-	1/1/15/20	12/37/115/115	-
14	CLA	G	802	-	1/1/15/20	19/37/115/115	-
14	CLA	G	809	-	1/1/15/20	15/37/115/115	-
14	CLA	H	806	-	1/1/15/20	10/37/115/115	-
14	CLA	B	810	2	1/1/15/20	15/37/115/115	-
16	SF4	a	101	3	-	-	0/6/5/5
14	CLA	B	836	-	1/1/11/20	4/13/91/115	-
14	CLA	G	822	-	1/1/15/20	12/37/115/115	-
14	CLA	A	834	-	1/1/13/20	9/25/103/115	-
14	CLA	A	819	-	1/1/15/20	15/37/115/115	-
14	CLA	A	803	-	1/1/15/20	19/37/115/115	-
14	CLA	A	815	-	1/1/12/20	9/19/97/115	-
14	CLA	G	808	1	1/1/15/20	19/37/115/115	-
14	CLA	G	814	-	1/1/12/20	3/19/97/115	-
14	CLA	Z	817	-	1/1/14/20	15/31/109/115	-
14	CLA	A	812	-	1/1/12/20	11/24/102/115	-
14	CLA	G	813	-	1/1/14/20	10/31/109/115	-
14	CLA	J	102	-	1/1/13/20	14/25/103/115	-
14	CLA	B	813	-	1/1/15/20	19/37/115/115	-
14	CLA	H	807	-	1/1/15/20	9/37/115/115	-
14	CLA	H	819	-	1/1/11/20	9/13/91/115	-
19	LMG	Z	847	-	-	16/44/64/70	0/1/1/1
14	CLA	A	817	-	1/1/14/20	15/31/109/115	-
17	BCR	B	843	-	-	3/24/41/63	0/1/1/2
17	BCR	Y	850	-	-	7/29/63/63	0/2/2/2
17	BCR	L	203	-	-	13/29/63/63	0/2/2/2
14	CLA	Z	839	-	1/1/15/20	19/37/115/115	-
13	CL0	G	801	-	3/3/20/25	13/37/135/135	-
14	CLA	H	837	-	1/1/15/20	12/37/115/115	-
14	CLA	f	102	-	1/1/13/20	15/25/103/115	-
14	CLA	Z	822	2	1/1/13/20	10/25/103/115	-
14	CLA	U	1006	2	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	816	-	1/1/15/20	12/37/115/115	-
15	PQN	Z	840	-	-	10/23/43/43	0/2/2/2
17	BCR	h	202	-	-	8/29/63/63	0/2/2/2
14	CLA	H	833	-	1/1/11/20	6/13/91/115	-
14	CLA	H	808	2	1/1/15/20	10/37/115/115	-
14	CLA	B	821	-	1/1/11/20	8/13/91/115	-
14	CLA	B	817	-	1/1/15/20	9/37/115/115	-
14	CLA	G	811	-	1/1/15/20	18/37/115/115	-
14	CLA	Y	842	-	1/1/15/20	15/37/115/115	-
14	CLA	Z	809	-	1/1/13/20	10/25/103/115	-
14	CLA	B	825	-	1/1/15/20	14/37/115/115	-
14	CLA	Z	805	-	1/1/15/20	19/37/115/115	-
14	CLA	A	806	-	1/1/15/20	21/37/115/115	-
17	BCR	G	849	-	-	8/29/63/63	0/2/2/2
14	CLA	H	812	-	1/1/15/20	18/37/115/115	-
14	CLA	g	102	-	1/1/11/20	5/13/91/115	-
14	CLA	B	818	-	1/1/14/20	10/31/109/115	-
14	CLA	B	801	-	1/1/15/20	21/37/115/115	-
14	CLA	Z	831	-	1/1/13/20	12/25/103/115	-
18	LHG	H	847	-	-	18/41/41/53	-
14	CLA	Y	806	-	1/1/15/20	14/37/115/115	-
17	BCR	A	847	-	-	4/29/63/63	0/2/2/2
14	CLA	Z	838	-	1/1/15/20	12/37/115/115	-
17	BCR	e	101	-	-	10/29/63/63	0/2/2/2
14	CLA	L	201	-	1/1/15/20	13/37/115/115	-
14	CLA	Z	819	-	1/1/11/20	7/13/91/115	-
14	CLA	G	830	-	1/1/15/20	15/37/115/115	-
14	CLA	B	828	-	1/1/15/20	15/37/115/115	-
14	CLA	Z	826	-	1/1/15/20	14/37/115/115	-
19	LMG	B	849	-	-	14/47/67/70	0/1/1/1
17	BCR	L	208	-	-	12/29/63/63	0/2/2/2
14	CLA	B	831	-	1/1/11/20	8/13/91/115	-
16	SF4	N	102	3,21	-	-	0/6/5/5
14	CLA	K	103	-	1/1/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	815	-	1/1/11/20	4/13/91/115	-
14	CLA	A	811	14	1/1/15/20	17/37/115/115	-
14	CLA	B	802	-	1/1/15/20	19/37/115/115	-
14	CLA	B	840	-	1/1/15/20	12/37/115/115	-
14	CLA	Y	822	-	1/1/15/20	18/37/115/115	-
17	BCR	T	102	-	-	9/29/63/63	0/2/2/2
14	CLA	Y	814	-	1/1/13/20	11/25/103/115	-
14	CLA	B	808	-	1/1/15/20	13/37/115/115	-
14	CLA	A	809	1	1/1/15/20	17/37/115/115	-
14	CLA	Y	840	-	1/1/15/20	13/37/115/115	-
14	CLA	H	820	-	1/1/11/20	4/13/91/115	-
14	CLA	G	837	-	1/1/15/20	19/37/115/115	-
14	CLA	h	206	-	1/1/15/20	13/37/115/115	-
14	CLA	G	818	-	1/1/15/20	17/37/115/115	-
14	CLA	G	823	-	1/1/12/20	6/19/97/115	-
14	CLA	A	852	-	1/1/15/20	11/37/115/115	-
17	BCR	f	103	-	-	9/29/63/63	0/2/2/2
14	CLA	G	833	-	1/1/15/20	15/37/115/115	-
17	BCR	R	102	-	-	11/29/63/63	0/2/2/2
14	CLA	Y	829	-	1/1/15/20	17/37/115/115	-
14	CLA	H	830	-	1/1/13/20	12/25/103/115	-
14	CLA	h	201	-	1/1/15/20	12/37/115/115	-
14	CLA	J	101	8	1/1/11/20	5/13/91/115	-
17	BCR	B	851	-	-	7/29/63/63	0/2/2/2
15	PQN	Y	844	-	-	6/23/43/43	0/2/2/2
14	CLA	Y	815	-	1/1/12/20	10/19/97/115	-
14	CLA	Z	806	-	1/1/15/20	19/37/115/115	-
14	CLA	G	853	-	1/1/11/20	5/13/91/115	-
14	CLA	Y	811	14	1/1/15/20	21/37/115/115	-
14	CLA	Y	843	18	1/1/12/20	11/19/97/115	-
18	LHG	B	850	-	-	24/43/43/53	-
14	CLA	A	836	-	1/1/12/20	7/19/97/115	-
14	CLA	Z	836	-	1/1/15/20	10/37/115/115	-
14	CLA	V	1201	-	1/1/12/20	9/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	830	-	1/1/15/20	12/37/115/115	-
14	CLA	B	823	-	1/1/14/20	15/31/109/115	-
14	CLA	B	820	-	1/1/11/20	4/13/91/115	-
14	CLA	G	807	-	1/1/12/20	10/21/99/115	-
14	CLA	f	101	8	1/1/11/20	5/13/91/115	-
14	CLA	Z	815	-	1/1/15/20	17/37/115/115	-
14	CLA	Y	841	-	1/1/15/20	14/37/115/115	-
14	CLA	Y	836	1	1/1/11/20	4/13/91/115	-
14	CLA	Y	854	-	1/1/15/20	15/37/115/115	-
17	BCR	Y	847	-	-	6/29/63/63	0/2/2/2
14	CLA	Z	828	-	1/1/11/20	5/13/91/115	-
14	CLA	Y	839	-	1/1/12/20	11/19/97/115	-
17	BCR	Z	844	-	-	8/18/35/63	0/1/1/2
17	BCR	A	849	-	-	10/29/63/63	0/2/2/2
14	CLA	Z	818	-	1/1/11/20	5/13/91/115	-
17	BCR	G	850	-	-	9/29/63/63	0/2/2/2
14	CLA	H	826	-	1/1/15/20	12/37/115/115	-
14	CLA	G	816	-	1/1/12/20	9/19/97/115	-
14	CLA	Z	833	-	1/1/11/20	8/13/91/115	-
17	BCR	B	844	-	-	8/29/63/63	0/2/2/2
14	CLA	A	813	-	1/1/14/20	10/31/109/115	-
14	CLA	B	806	-	1/1/15/20	14/37/115/115	-
14	CLA	h	205	10	1/1/15/20	23/37/115/115	-
14	CLA	Z	801	-	1/1/15/20	20/37/115/115	-
14	CLA	G	805	-	1/1/15/20	20/37/115/115	-
14	CLA	Z	823	-	1/1/15/20	17/37/115/115	-
16	SF4	C	101	3,21	-	-	0/6/5/5
14	CLA	A	833	-	1/1/15/20	12/37/115/115	-
14	CLA	Z	825	-	1/1/15/20	15/37/115/115	-
17	BCR	H	845	-	-	8/29/63/63	0/2/2/2
14	CLA	H	832	-	1/1/11/20	8/13/91/115	-
18	LHG	G	852	14	-	15/36/36/53	-
14	CLA	G	834	-	1/1/13/20	8/25/103/115	-
14	CLA	Z	812	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	B	848	-	-	3/29/63/63	0/2/2/2
14	CLA	G	815	-	1/1/12/20	6/19/97/115	-
14	CLA	Y	837	-	1/1/12/20	7/19/97/115	-
14	CLA	G	840	-	1/1/12/20	4/19/97/115	-
14	CLA	Y	823	-	1/1/12/20	6/19/97/115	-
16	SF4	C	102	3	-	-	0/6/5/5
14	CLA	G	824	-	1/1/14/20	16/31/109/115	-
14	CLA	G	838	-	1/1/12/20	3/19/97/115	-
14	CLA	A	825	-	1/1/15/20	15/37/115/115	-
14	CLA	B	838	-	1/1/15/20	13/37/115/115	-
14	CLA	Y	805	-	1/1/15/20	13/37/115/115	-
14	CLA	A	824	-	1/1/14/20	17/31/109/115	-
17	BCR	F	203	-	-	6/29/63/63	0/2/2/2
15	PQN	H	839	-	-	8/23/43/43	0/2/2/2
14	CLA	Y	803	-	1/1/15/20	18/37/115/115	-
14	CLA	H	825	-	1/1/15/20	11/37/115/115	-
14	CLA	Y	809	-	1/1/15/20	18/37/115/115	-
14	CLA	Z	821	-	1/1/14/20	14/31/109/115	-
14	CLA	L	207	-	1/1/15/20	19/37/115/115	-
14	CLA	A	838	-	1/1/12/20	9/19/97/115	-
14	CLA	H	802	-	1/1/15/20	19/37/115/115	-
14	CLA	B	814	-	1/1/15/20	22/37/115/115	-
17	BCR	K	102	-	-	8/29/63/63	0/2/2/2
18	LHG	A	851	14	-	17/36/36/53	-
17	BCR	Z	845	-	-	8/29/63/63	0/2/2/2
14	CLA	Y	812	-	1/1/13/20	12/25/103/115	-
14	CLA	A	835	1	1/1/11/20	3/13/91/115	-
17	BCR	G	847	-	-	9/29/63/63	0/2/2/2
14	CLA	X	1701	-	1/1/11/20	5/13/91/115	-
18	LHG	A	850	-	-	28/53/53/53	-
14	CLA	B	829	-	1/1/15/20	11/37/115/115	-
18	LHG	Y	853	14	-	20/28/28/53	-
14	CLA	Q	201	-	1/1/15/20	18/37/115/115	-
17	BCR	A	845	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	Z	807	-	1/1/15/20	12/37/115/115	-
17	BCR	I	101	-	-	8/29/63/63	0/2/2/2
14	CLA	U	1002	10	1/1/15/20	25/37/115/115	-
17	BCR	H	842	-	-	8/29/63/63	0/2/2/2
14	CLA	G	826	-	1/1/14/20	16/31/109/115	-
18	LHG	G	851	-	-	28/53/53/53	-
14	CLA	j	102	-	1/1/11/20	7/13/91/115	-
14	CLA	G	806	-	1/1/15/20	20/37/115/115	-
14	CLA	H	824	-	1/1/15/20	18/37/115/115	-
14	CLA	Y	828	-	1/1/15/20	16/37/115/115	-
14	CLA	B	835	-	1/1/11/20	2/13/91/115	-
17	BCR	U	1008	-	-	5/29/63/63	0/2/2/2
14	CLA	H	814	-	1/1/11/20	6/13/91/115	-
14	CLA	Z	816	-	1/1/14/20	13/31/109/115	-
14	CLA	H	811	-	1/1/11/20	5/13/91/115	-
14	CLA	G	832	-	1/1/15/20	14/37/115/115	-
14	CLA	G	827	-	1/1/15/20	18/37/115/115	-
17	BCR	d	203	-	-	10/29/63/63	0/2/2/2
14	CLA	A	837	-	1/1/15/20	15/37/115/115	-
14	CLA	H	827	-	1/1/15/20	16/37/115/115	-
17	BCR	B	846	-	-	3/18/35/63	0/1/1/2
14	CLA	h	207	-	1/1/15/20	15/37/115/115	-
14	CLA	B	841	-	1/1/15/20	20/37/115/115	-
14	CLA	H	821	-	1/1/13/20	9/25/103/115	-
14	CLA	Z	808	2	1/1/15/20	13/37/115/115	-
14	CLA	Z	837	-	1/1/11/20	4/13/91/115	-
14	CLA	B	805	-	1/1/12/20	10/24/102/115	-
14	CLA	Y	810	-	1/1/11/20	7/13/91/115	-
14	CLA	H	809	2	1/1/15/20	17/37/115/115	-
14	CLA	B	839	-	1/1/11/20	3/13/91/115	-
14	CLA	Y	820	-	1/1/14/20	14/31/109/115	-
14	CLA	A	831	-	1/1/12/20	5/19/97/115	-
14	CLA	T	101	-	1/1/9/20	7/7/81/115	-
14	CLA	B	804	-	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	SF4	a	102	3	-	-	0/6/5/5
14	CLA	A	802	-	1/1/15/20	11/37/115/115	-
18	LHG	Y	852	-	-	27/53/53/53	-
14	CLA	Y	831	-	1/1/12/20	3/19/97/115	-
14	CLA	Z	813	-	1/1/11/20	3/13/91/115	-
14	CLA	B	834	-	1/1/11/20	3/13/91/115	-
17	BCR	Y	851	-	-	10/29/63/63	0/2/2/2
14	CLA	B	807	-	1/1/15/20	18/37/115/115	-
14	CLA	B	819	-	1/1/14/20	19/31/109/115	-
17	BCR	M	101	-	-	9/29/63/63	0/2/2/2
14	CLA	Y	813	-	1/1/14/20	10/31/109/115	-
18	LHG	j	101	-	-	16/32/32/53	-
17	BCR	Z	843	-	-	7/29/63/63	0/2/2/2
14	CLA	A	829	-	1/1/15/20	17/37/115/115	-
14	CLA	Z	829	-	1/1/11/20	9/13/91/115	-
17	BCR	G	848	-	-	8/29/63/63	0/2/2/2
17	BCR	H	840	-	-	8/29/63/63	0/2/2/2
14	CLA	A	842	18	1/1/12/20	10/19/97/115	-
14	CLA	B	816	-	1/1/13/20	9/25/103/115	-
14	CLA	A	823	-	1/1/12/20	8/19/97/115	-
14	CLA	S	1102	8	1/1/11/20	8/13/91/115	-
14	CLA	A	808	1	1/1/15/20	23/37/115/115	-
14	CLA	G	825	-	1/1/15/20	19/37/115/115	-
14	CLA	L	205	10	1/1/15/20	24/37/115/115	-
14	CLA	H	823	2	1/1/13/20	10/25/103/115	-
14	CLA	A	826	-	1/1/14/20	11/31/109/115	-
14	CLA	H	836	-	1/1/11/20	1/13/91/115	-
14	CLA	B	803	-	1/1/15/20	16/37/115/115	-
14	CLA	H	834	-	1/1/14/20	11/31/109/115	-
14	CLA	Z	814	-	1/1/13/20	12/25/103/115	-
14	CLA	Z	827	-	1/1/15/20	13/37/115/115	-
14	CLA	U	1003	-	1/1/15/20	13/37/115/115	-
14	CLA	A	832	-	1/1/15/20	15/37/115/115	-
14	CLA	Y	826	-	1/1/14/20	7/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	827	-	1/1/15/20	13/37/115/115	-
14	CLA	H	813	-	1/1/15/20	17/37/115/115	-
14	CLA	G	821	-	1/1/15/20	16/37/115/115	-
14	CLA	H	828	-	1/1/15/20	13/37/115/115	-
14	CLA	A	820	-	1/1/14/20	15/31/109/115	-
13	CL0	A	801	-	3/3/20/25	14/37/135/135	-
14	CLA	H	810	-	1/1/13/20	13/25/103/115	-
14	CLA	L	206	-	1/1/15/20	14/37/115/115	-
17	BCR	i	101	-	-	9/29/63/63	0/2/2/2
17	BCR	J	104	-	-	13/29/63/63	0/2/2/2
17	BCR	Z	842	-	-	6/29/63/63	0/2/2/2
17	BCR	Y	846	-	-	9/29/63/63	0/2/2/2
14	CLA	A	840	-	1/1/15/20	14/37/115/115	-
17	BCR	B	847	-	-	11/29/63/63	0/2/2/2
14	CLA	Y	802	-	1/1/15/20	9/37/115/115	-
14	CLA	Z	802	-	1/1/15/20	22/37/115/115	-
14	CLA	A	828	-	1/1/15/20	15/37/115/115	-
14	CLA	K	101	-	1/1/9/20	5/7/81/115	-
14	CLA	G	835	1	1/1/11/20	6/13/91/115	-
14	CLA	A	818	-	1/1/15/20	23/37/115/115	-
17	BCR	f	104	-	-	6/29/63/63	0/2/2/2
17	BCR	J	103	-	-	6/29/63/63	0/2/2/2
19	LMG	H	846	-	-	11/44/64/70	0/1/1/1
16	SF4	A	844	1,2	-	-	0/6/5/5
14	CLA	A	810	-	1/1/11/20	7/13/91/115	-
14	CLA	Y	827	-	1/1/15/20	19/37/115/115	-
14	CLA	B	833	-	1/1/13/20	10/25/103/115	-
14	CLA	L	202	-	1/1/15/20	16/37/115/115	-
17	BCR	H	844	-	-	8/29/63/63	0/2/2/2
14	CLA	G	839	-	1/1/15/20	17/37/115/115	-
17	BCR	H	843	-	-	7/18/35/63	0/1/1/2
16	SF4	Y	845	1,2	-	-	0/6/5/5
14	CLA	Y	833	-	1/1/15/20	13/37/115/115	-
17	BCR	Z	841	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	831	-	1/1/12/20	8/19/97/115	-
17	BCR	Y	848	-	-	10/29/63/63	0/2/2/2
17	BCR	Q	202	-	-	11/29/63/63	0/2/2/2
14	CLA	G	819	-	1/1/15/20	15/37/115/115	-
17	BCR	G	854	-	-	8/29/63/63	0/2/2/2
17	BCR	V	1202	-	-	8/29/63/63	0/2/2/2
14	CLA	Y	808	1	1/1/15/20	21/37/115/115	-
14	CLA	S	1101	-	1/1/15/20	23/37/115/115	-
14	CLA	G	804	-	1/1/13/20	12/30/108/115	-
17	BCR	U	1007	-	-	16/29/63/63	0/2/2/2
14	CLA	A	821	-	1/1/15/20	16/37/115/115	-
14	CLA	G	829	-	1/1/15/20	19/37/115/115	-
17	BCR	h	203	-	-	10/29/63/63	0/2/2/2
14	CLA	Z	834	-	1/1/11/20	8/13/91/115	-
14	CLA	Z	820	-	1/1/13/20	8/25/103/115	-
17	BCR	R	101	-	-	12/29/63/63	0/2/2/2
14	CLA	G	842	-	1/1/15/20	17/37/115/115	-
14	CLA	Y	818	-	1/1/15/20	16/37/115/115	-
14	CLA	H	801	-	1/1/15/20	14/37/115/115	-
14	CLA	A	816	-	1/1/12/20	10/19/97/115	-
17	BCR	S	1104	-	-	11/29/63/63	0/2/2/2
14	CLA	A	807	-	1/1/12/20	9/21/99/115	-
14	CLA	Z	830	-	1/1/15/20	16/37/115/115	-
14	CLA	A	804	14	1/1/13/20	14/30/108/115	-
14	CLA	G	817	-	1/1/14/20	9/31/109/115	-
14	CLA	H	831	-	1/1/11/20	8/13/91/115	-
14	CLA	Z	804	-	1/1/15/20	14/37/115/115	-
14	CLA	Y	830	-	1/1/15/20	10/37/115/115	-
15	PQN	G	844	-	-	10/23/43/43	0/2/2/2
14	CLA	G	812	-	1/1/12/20	12/24/102/115	-
14	CLA	Y	825	-	1/1/15/20	15/37/115/115	-
14	CLA	g	101	-	1/1/9/20	3/7/81/115	-
14	CLA	S	1103	-	1/1/13/20	14/25/103/115	-
14	CLA	Y	832	-	1/1/15/20	22/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	L	209	-	-	9/29/63/63	0/2/2/2
14	CLA	Z	803	-	1/1/12/20	9/24/102/115	-
14	CLA	G	810	-	1/1/11/20	8/13/91/115	-
14	CLA	G	843	18	1/1/12/20	8/19/97/115	-
14	CLA	H	817	-	1/1/14/20	13/31/109/115	-
14	CLA	Z	810	-	1/1/11/20	4/13/91/115	-
17	BCR	B	845	-	-	9/29/63/63	0/2/2/2
17	BCR	A	846	-	-	12/29/63/63	0/2/2/2
14	CLA	Z	824	-	1/1/15/20	15/37/115/115	-
17	BCR	A	848	-	-	7/29/63/63	0/2/2/2
16	SF4	G	845	1,2	-	-	0/6/5/5
14	CLA	Y	834	-	1/1/15/20	12/37/115/115	-
14	CLA	Q	203	-	1/1/11/20	4/13/91/115	-
14	CLA	B	826	-	1/1/15/20	16/37/115/115	-
14	CLA	G	836	-	1/1/12/20	9/19/97/115	-
16	SF4	N	101	3	-	-	0/6/5/5
14	CLA	Z	811	-	1/1/15/20	19/37/115/115	-
14	CLA	G	828	-	1/1/15/20	11/37/115/115	-
13	CL0	Y	801	-	3/3/20/25	14/37/135/135	-
14	CLA	Y	824	-	1/1/14/20	20/31/109/115	-
14	CLA	Y	838	-	1/1/15/20	22/37/115/115	-
17	BCR	H	841	-	-	13/29/63/63	0/2/2/2
14	CLA	B	822	-	1/1/13/20	9/25/103/115	-
14	CLA	T	103	-	1/1/11/20	4/13/91/115	-
17	BCR	U	1005	-	-	13/29/63/63	0/2/2/2
14	CLA	Y	835	-	1/1/13/20	9/25/103/115	-
14	CLA	B	832	-	1/1/15/20	20/37/115/115	-
14	CLA	Y	807	-	1/1/12/20	11/21/99/115	-
14	CLA	B	837	-	1/1/14/20	8/31/109/115	-
14	CLA	W	1701	-	1/1/11/20	4/13/91/115	-
17	BCR	Y	849	-	-	11/29/63/63	0/2/2/2
15	PQN	B	842	-	-	12/23/43/43	0/2/2/2
14	CLA	U	1004	-	1/1/15/20	19/37/115/115	-
14	CLA	d	202	-	1/1/11/20	2/13/91/115	-

*Continued on next page...*



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	Y	816	-	1/1/12/20	5/19/97/115	-
17	BCR	Y	856	-	-	11/29/63/63	0/2/2/2
14	CLA	B	812	-	1/1/12/20	9/19/97/115	-
14	CLA	B	824	2	1/1/13/20	10/25/103/115	-
14	CLA	H	822	-	1/1/14/20	13/31/109/115	-
14	CLA	A	814	-	1/1/12/20	9/19/97/115	-
14	CLA	H	838	-	1/1/15/20	13/37/115/115	-
14	CLA	Y	819	-	1/1/15/20	20/37/115/115	-
17	BCR	Q	204	-	-	7/29/63/63	0/2/2/2
14	CLA	Z	832	-	1/1/11/20	7/13/91/115	-
14	CLA	Y	804	14	1/1/13/20	15/30/108/115	-
14	CLA	G	841	-	1/1/15/20	17/37/115/115	-
14	CLA	Y	821	-	1/1/15/20	18/37/115/115	-
17	BCR	F	201	-	-	13/29/63/63	0/2/2/2
14	CLA	Y	817	-	1/1/14/20	9/31/109/115	-
14	CLA	B	811	-	1/1/13/20	15/25/103/115	-
14	CLA	H	803	-	1/1/15/20	12/37/115/115	-
15	PQN	A	843	-	-	5/23/43/43	0/2/2/2
17	BCR	f	105	-	-	6/29/63/63	0/2/2/2
14	CLA	G	820	-	1/1/14/20	15/31/109/115	-
14	CLA	A	841	-	1/1/15/20	13/37/115/115	-
14	CLA	A	805	-	1/1/15/20	22/37/115/115	-
17	BCR	Z	846	-	-	10/29/63/63	0/2/2/2
14	CLA	H	818	-	1/1/14/20	16/31/109/115	-
14	CLA	H	835	-	1/1/15/20	16/37/115/115	-
14	CLA	A	839	-	1/1/12/20	4/19/97/115	-
14	CLA	H	829	-	1/1/11/20	6/13/91/115	-
14	CLA	H	805	-	1/1/15/20	19/37/115/115	-
14	CLA	B	830	-	1/1/11/20	6/13/91/115	-
17	BCR	H	848	-	-	8/29/63/63	0/2/2/2
14	CLA	d	201	-	1/1/12/20	4/19/97/115	-

The worst 5 of 5965 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	801	CL0	MG-NA	9.56	2.29	2.06
13	G	801	CL0	MG-NA	9.35	2.28	2.06
17	G	854	BCR	C10-C9	-8.86	1.24	1.35
15	Y	844	PQN	C3-C2	8.79	1.51	1.35
17	L	208	BCR	C10-C9	-8.72	1.24	1.35

The worst 5 of 8548 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	i	101	BCR	C16-C17-C18	30.09	170.25	127.31
17	A	845	BCR	C16-C17-C18	29.27	169.09	127.31
17	G	846	BCR	C16-C17-C18	28.74	168.33	127.31
17	R	101	BCR	C16-C17-C18	28.38	167.81	127.31
17	A	849	BCR	C16-C17-C18	28.06	167.35	127.31

5 of 291 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	801	CL0	NC
13	A	801	CL0	NA
13	A	801	CL0	ND
13	G	801	CL0	NC
13	G	801	CL0	NA

5 of 4379 torsion outliers are listed below:

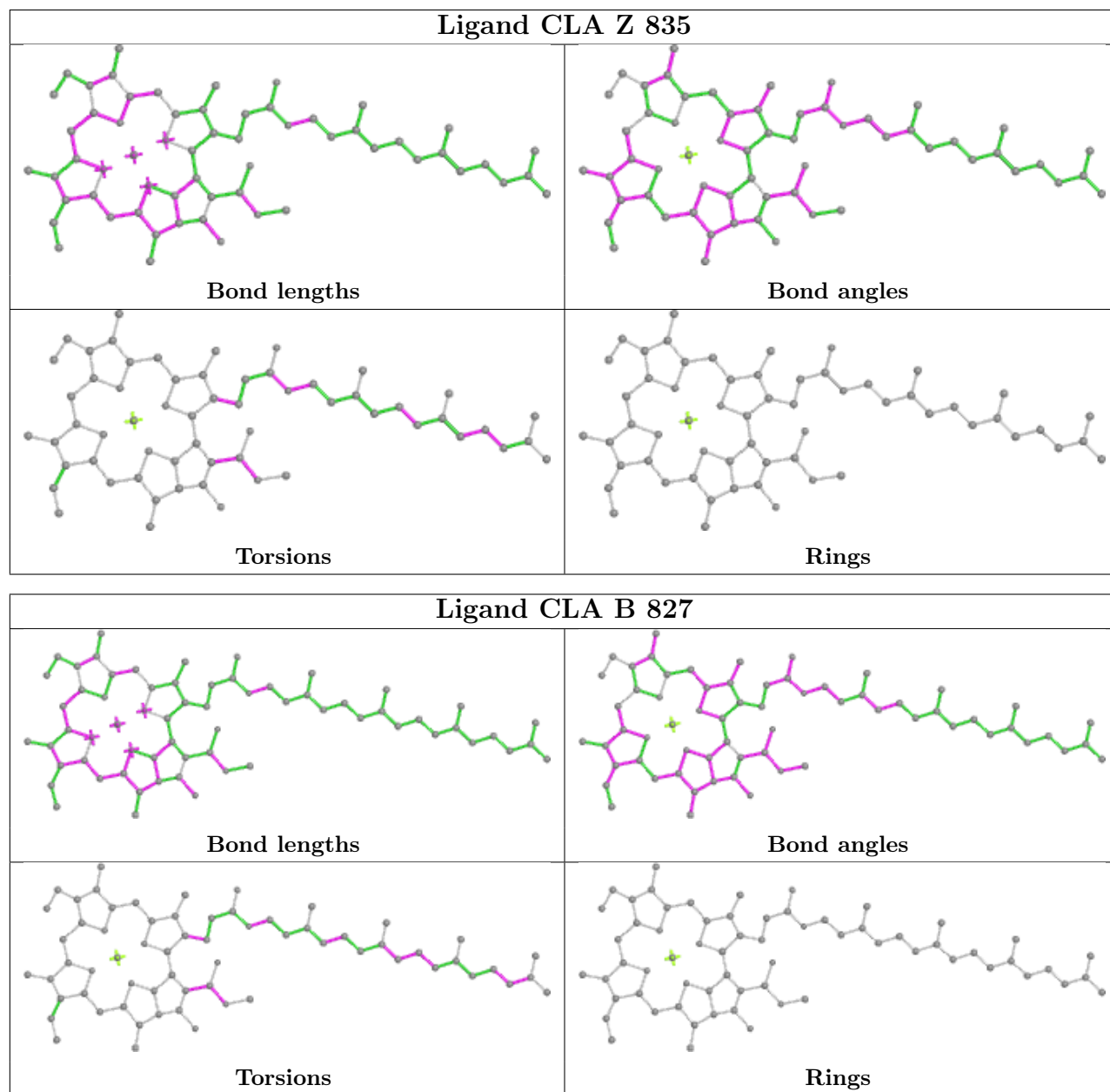
Mol	Chain	Res	Type	Atoms
13	G	801	CL0	CBD-CGD-O2D-CED
13	G	801	CL0	C2-C3-C5-C6
13	G	801	CL0	C4-C3-C5-C6
13	Y	801	CL0	C1A-C2A-CAA-CBA
13	Y	801	CL0	C3A-C2A-CAA-CBA

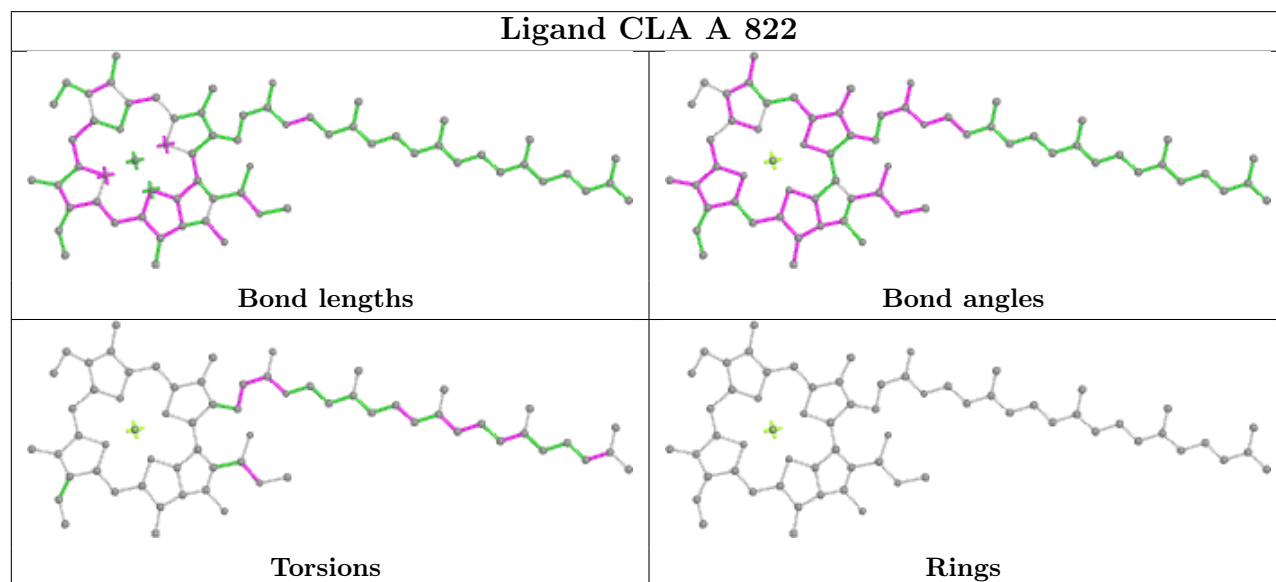
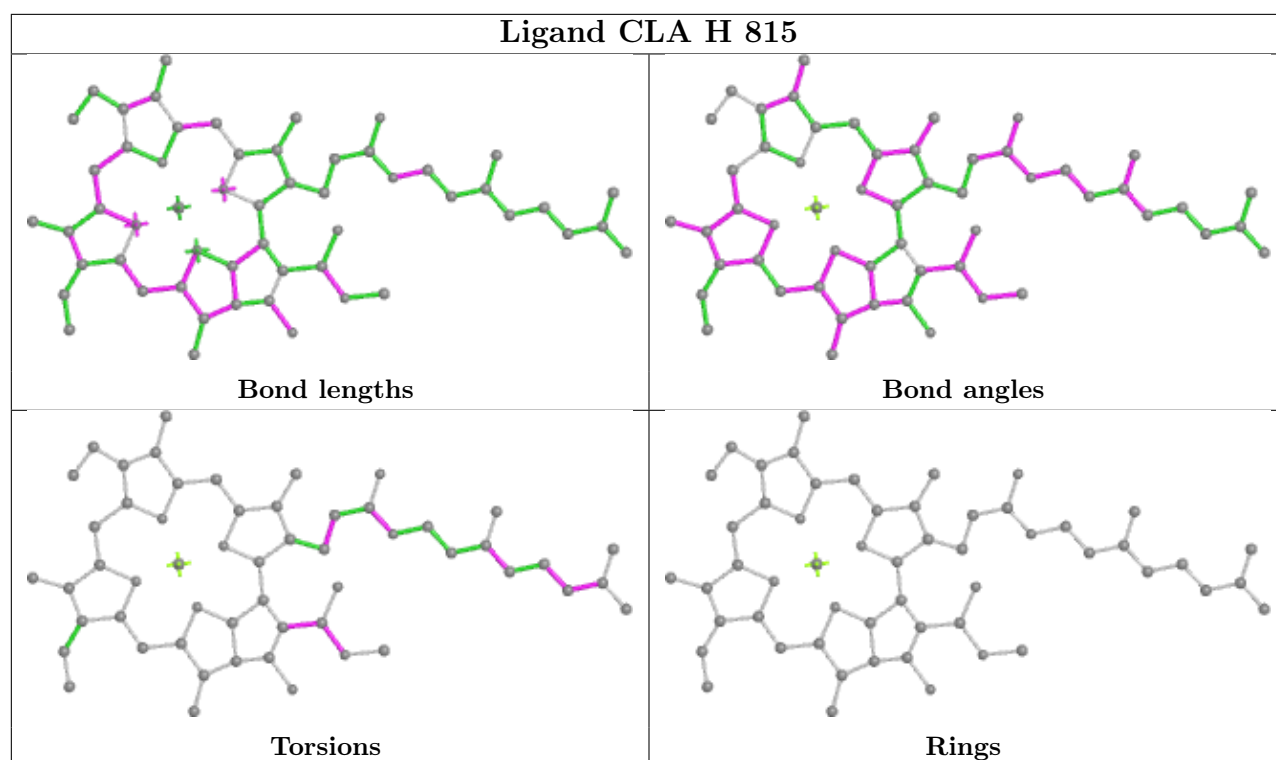
There are no ring outliers.

No monomer is involved in short contacts.

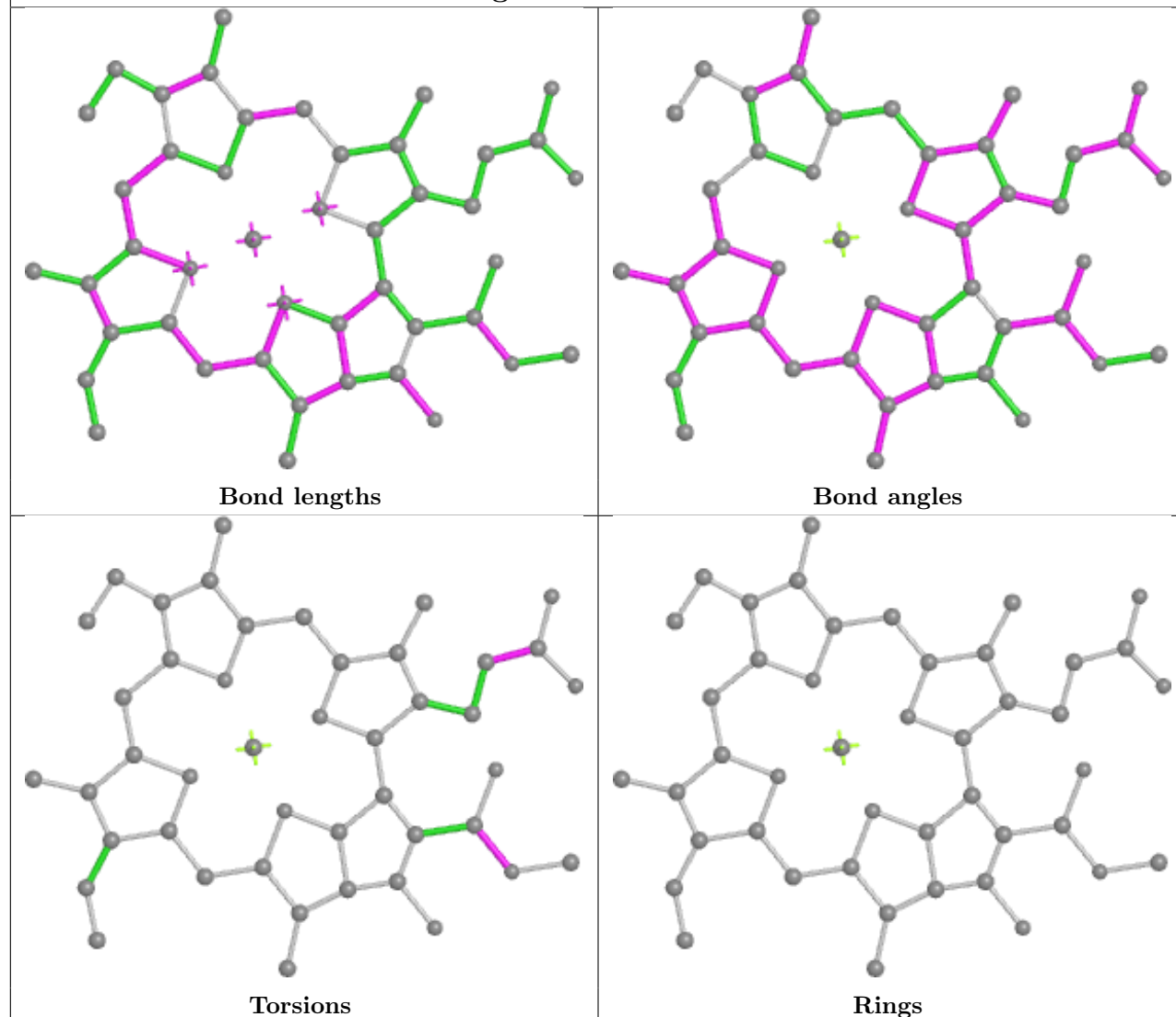
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

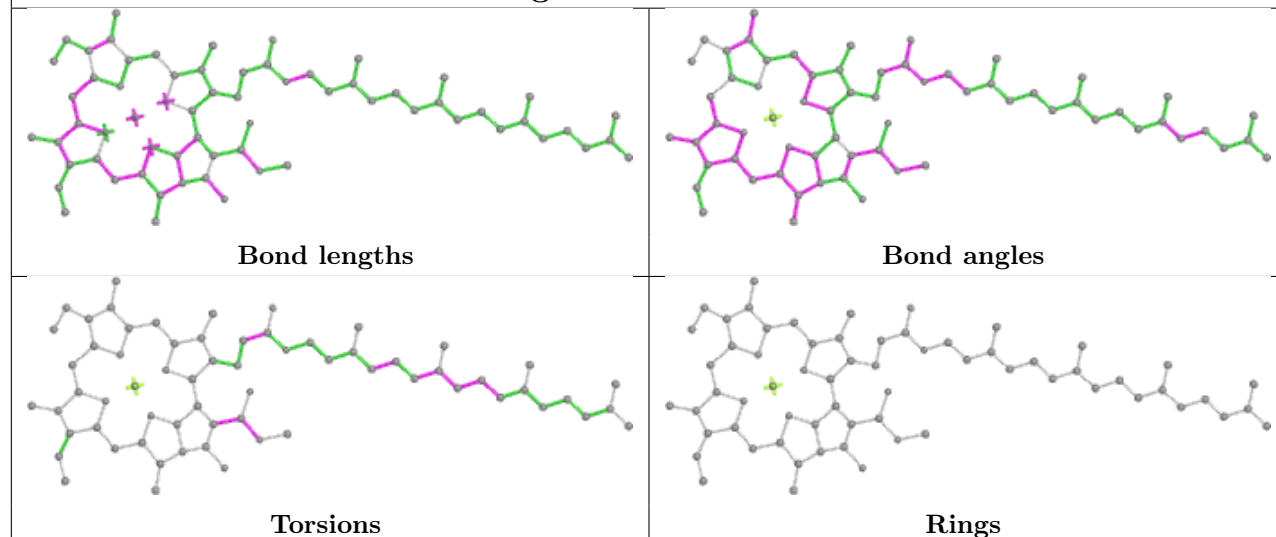


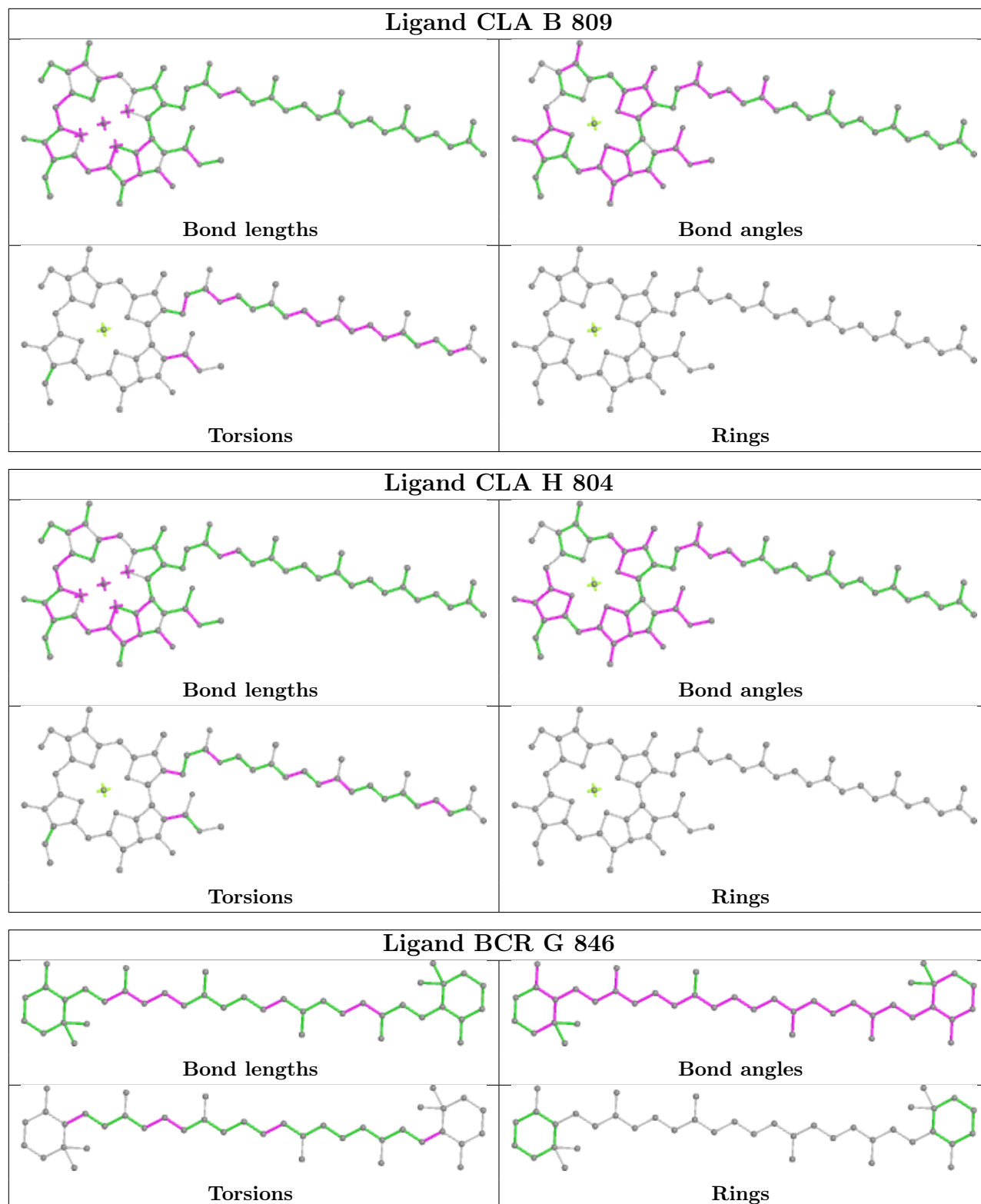


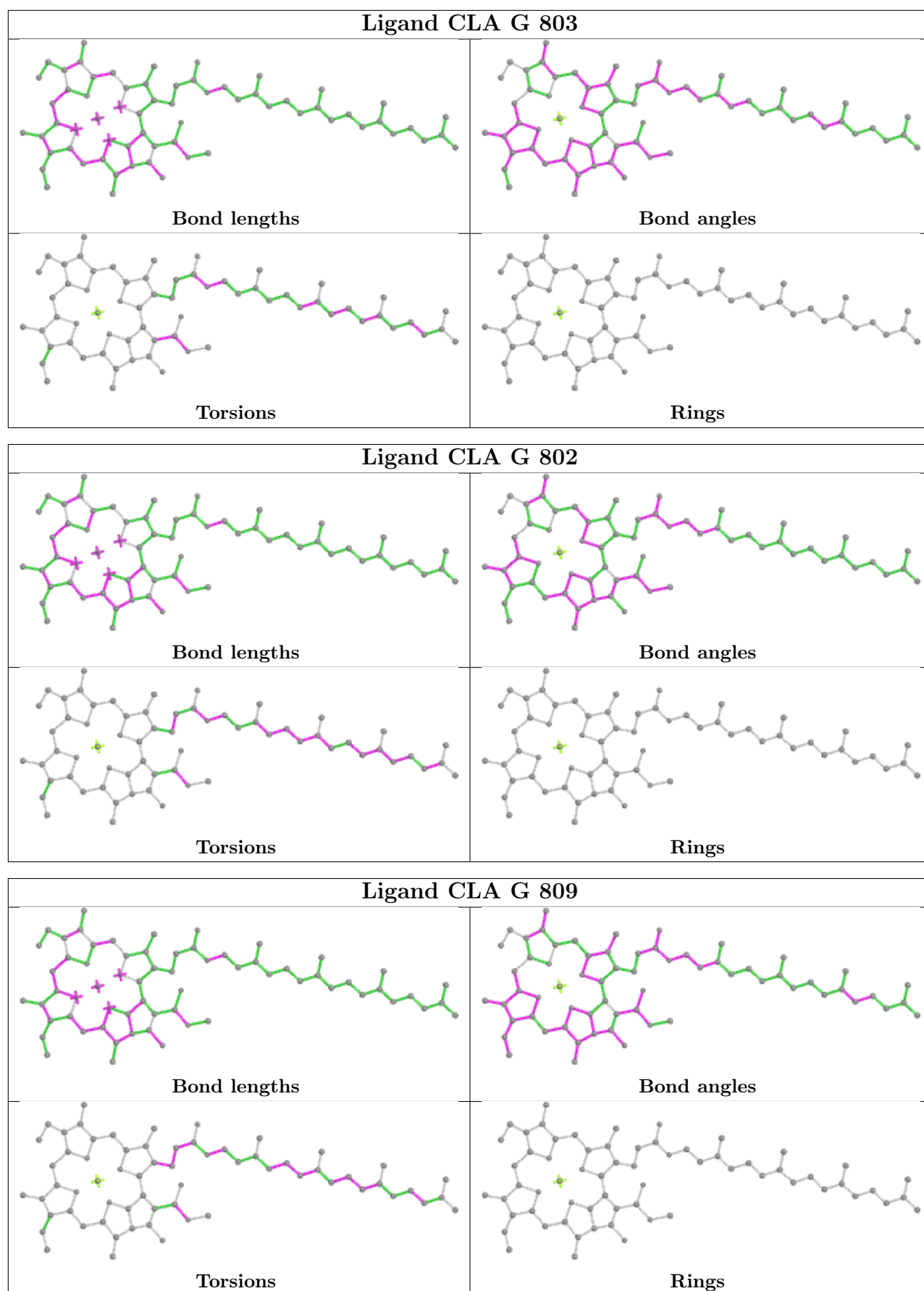
## Ligand CLA F 202

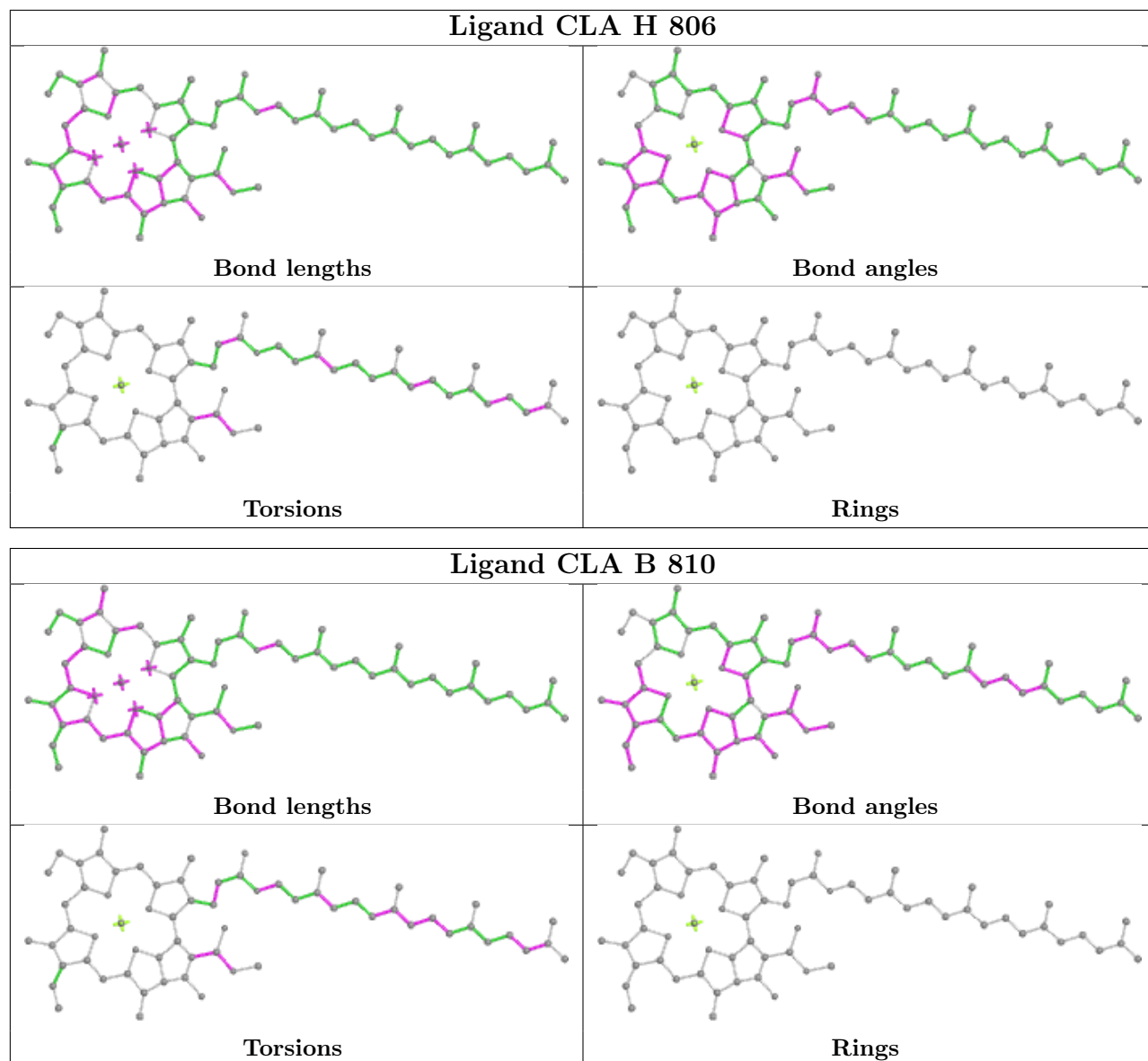


## Ligand CLA Y 855

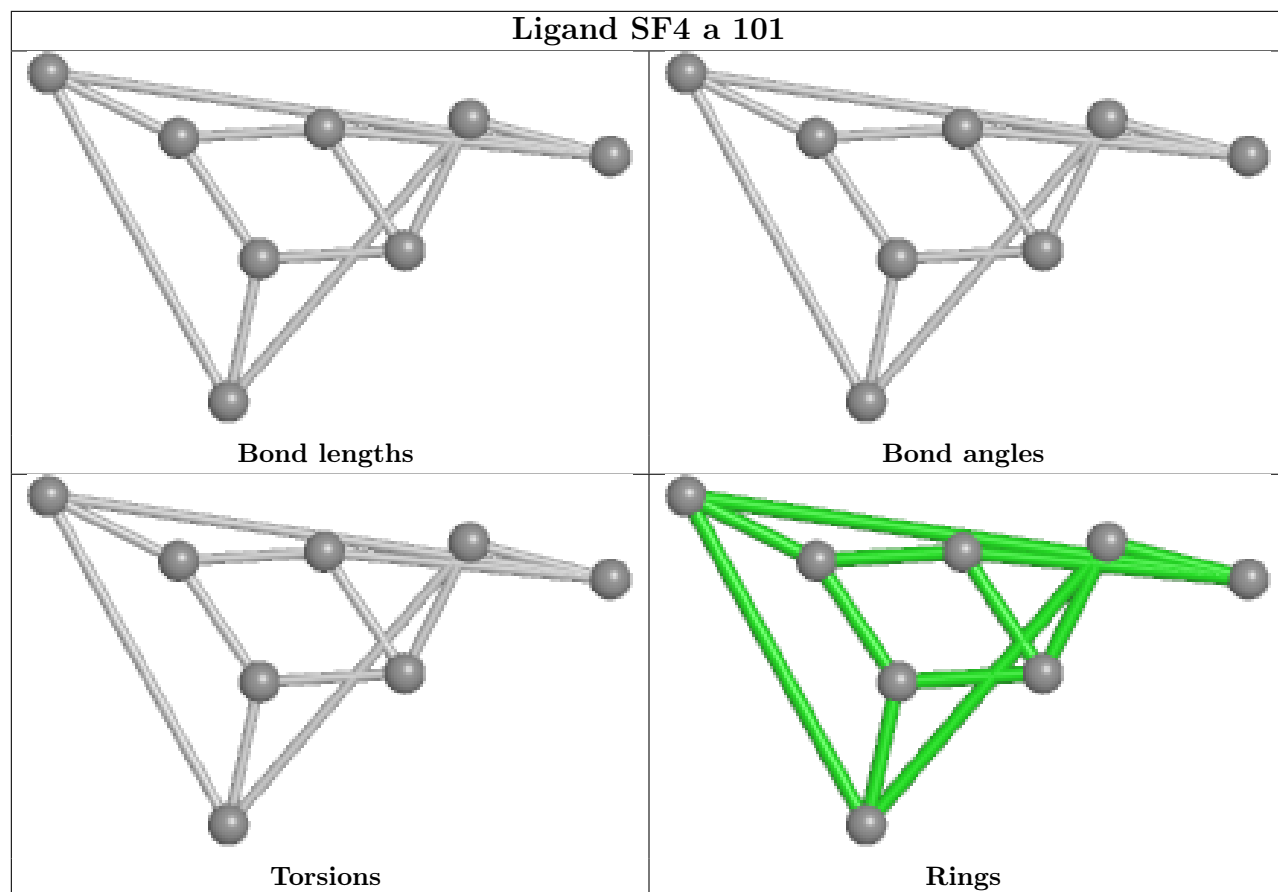




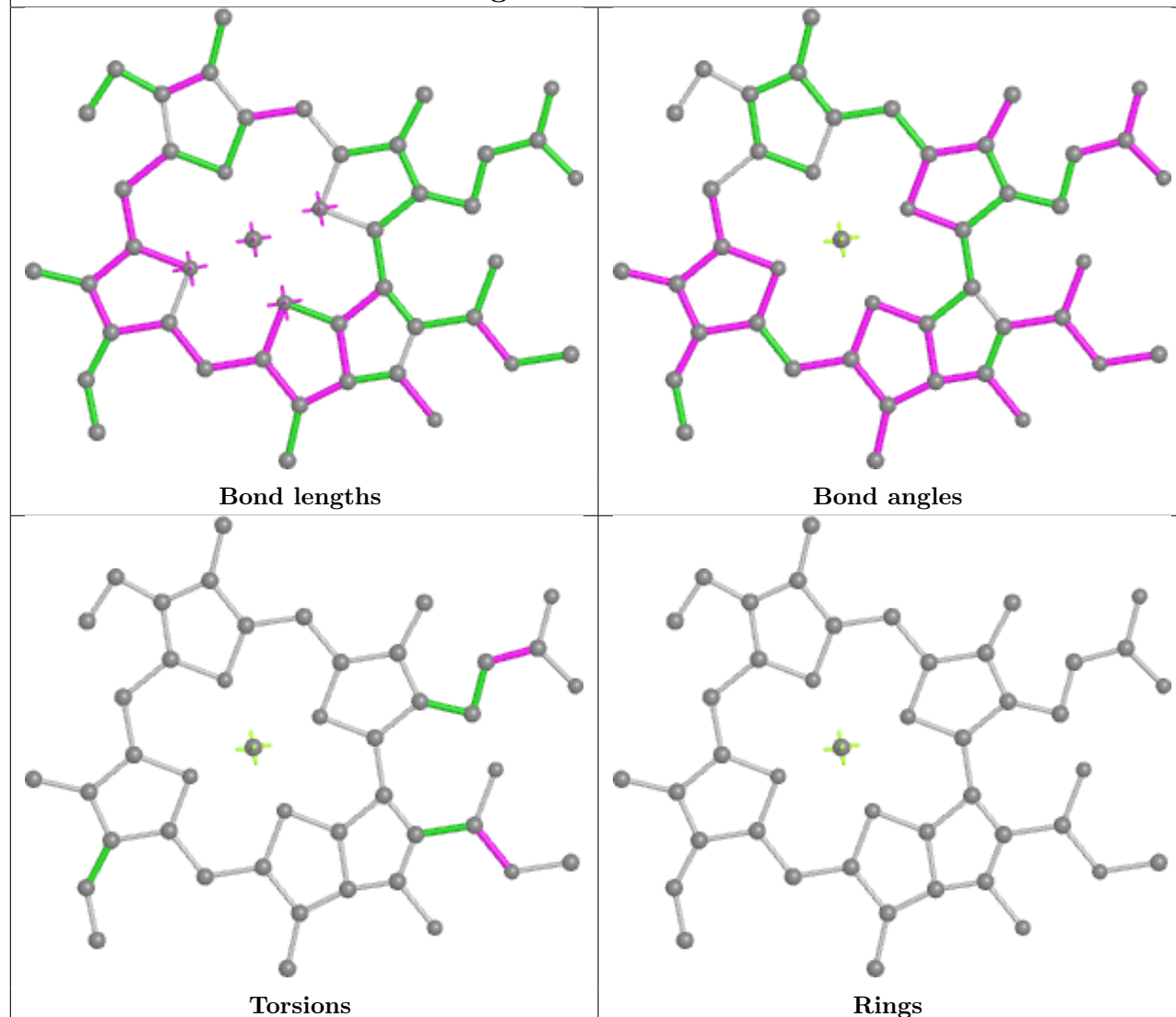




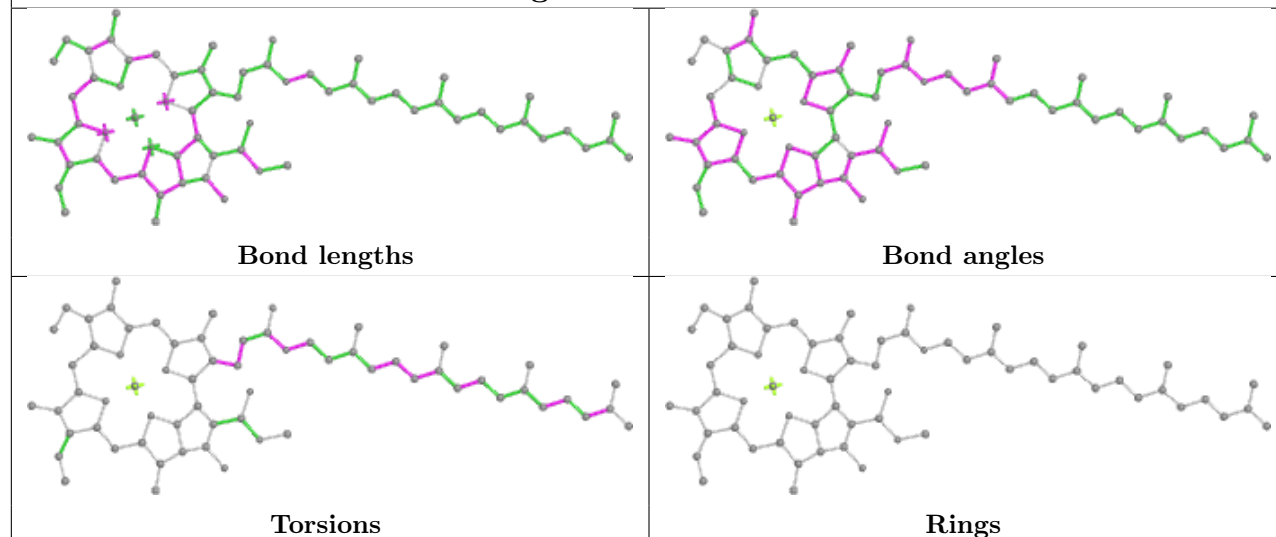


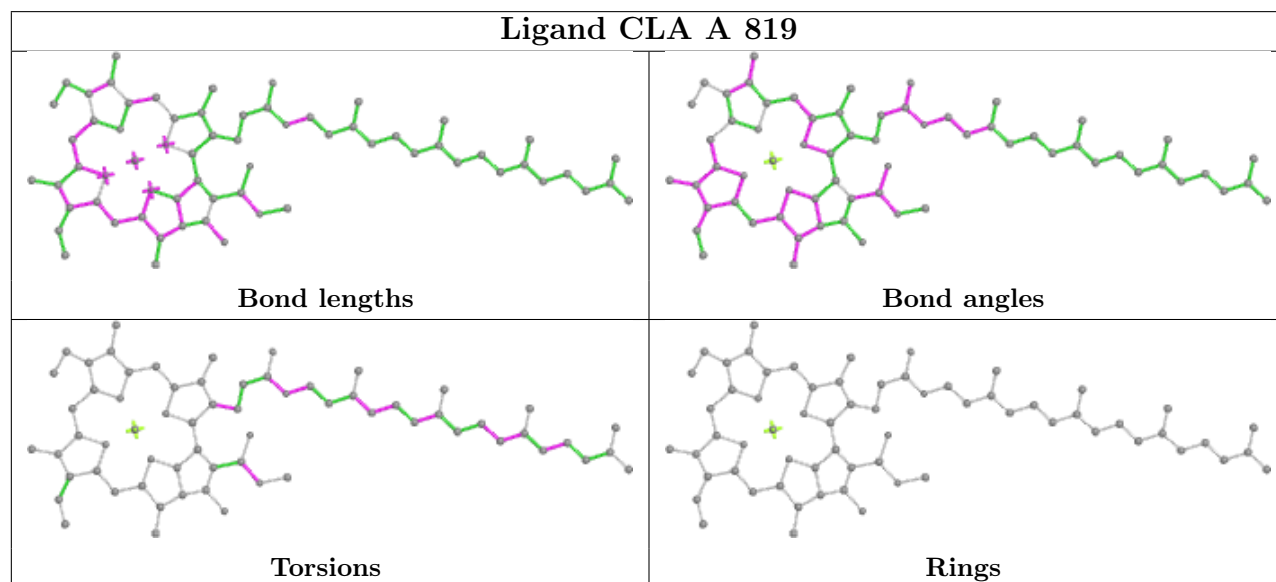
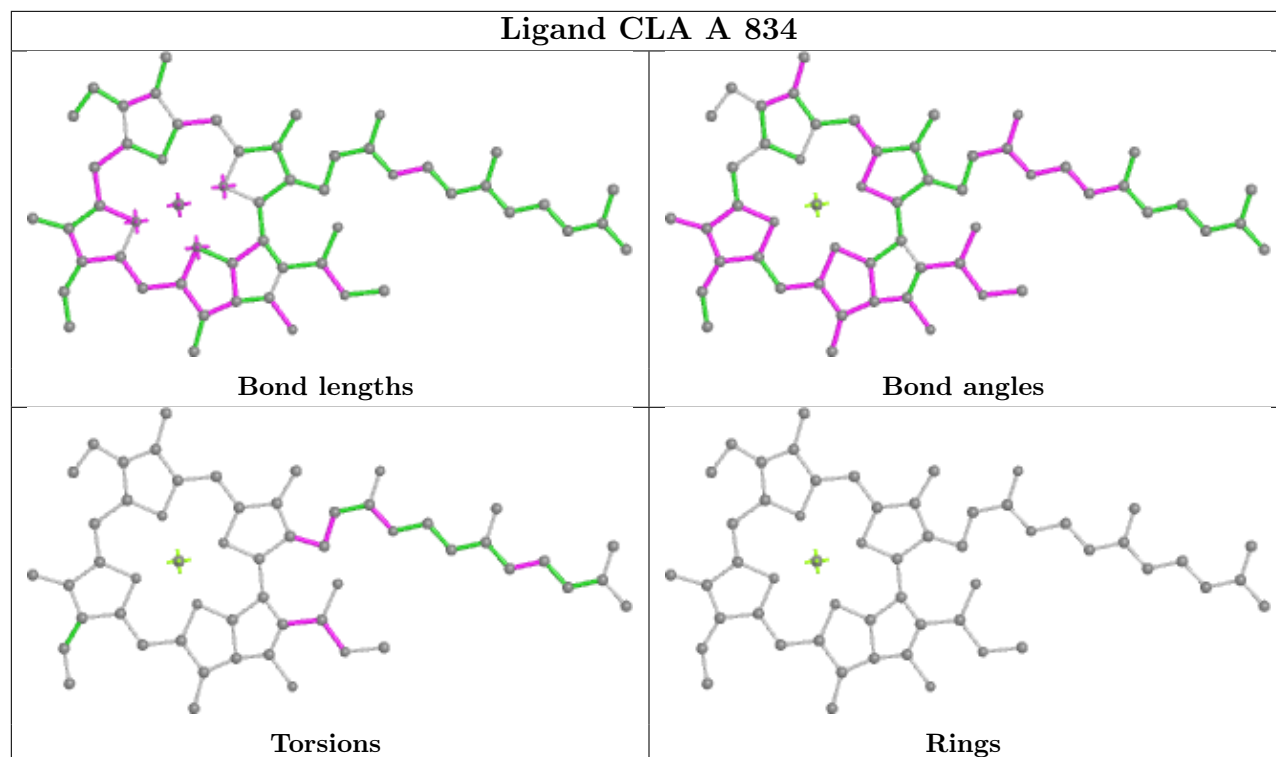


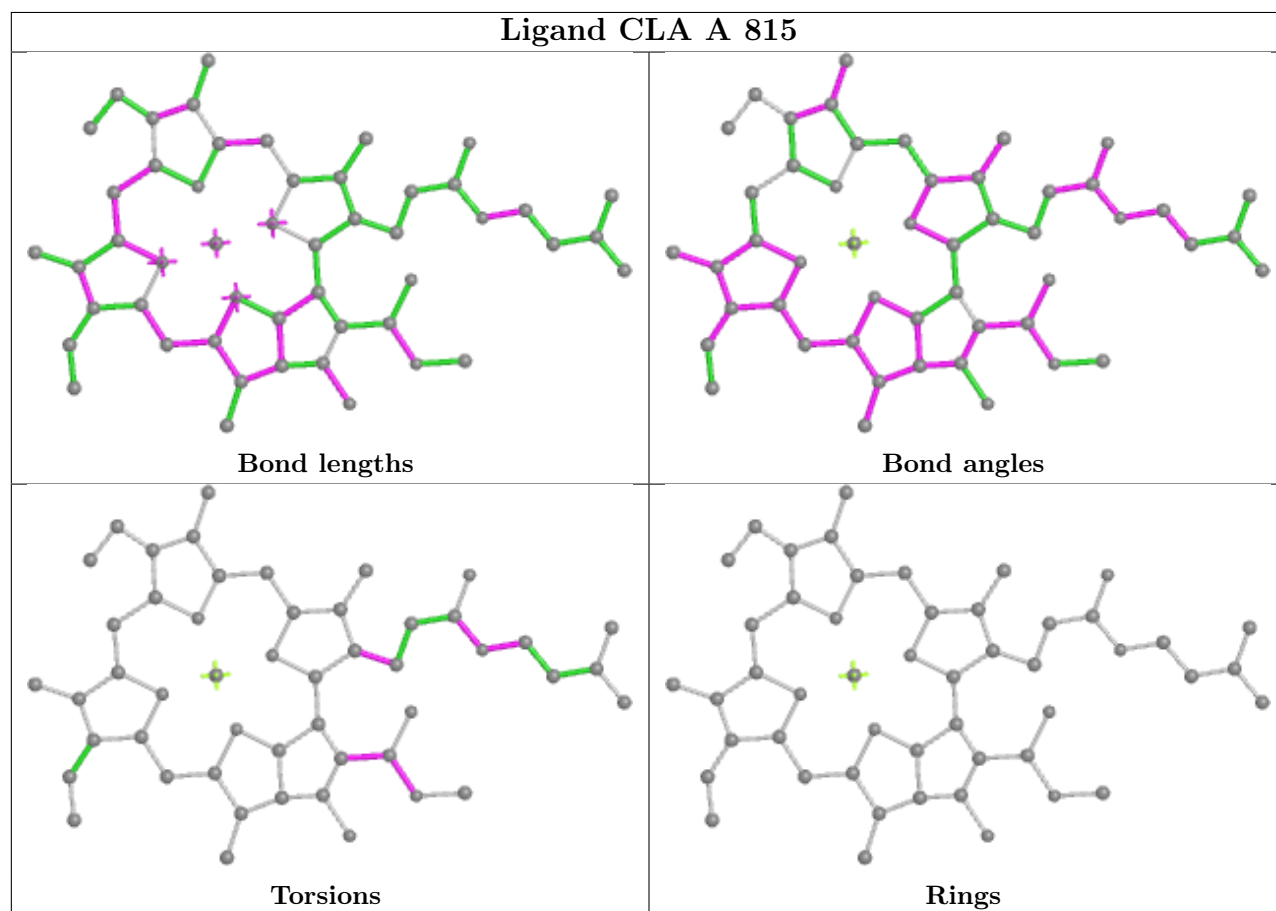
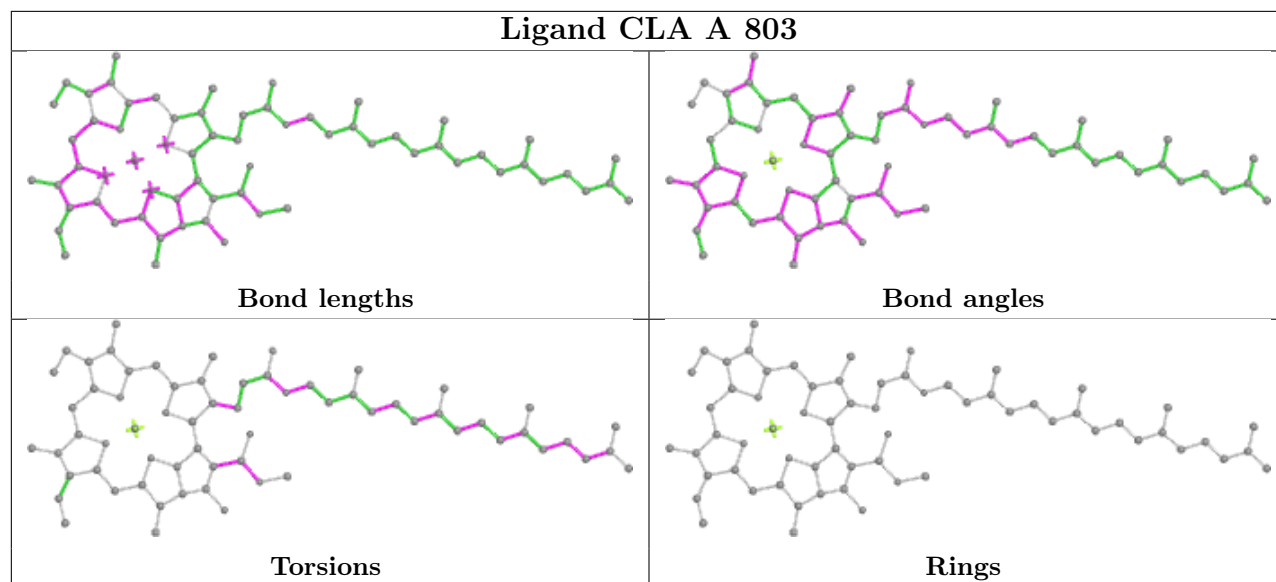
## Ligand CLA B 836

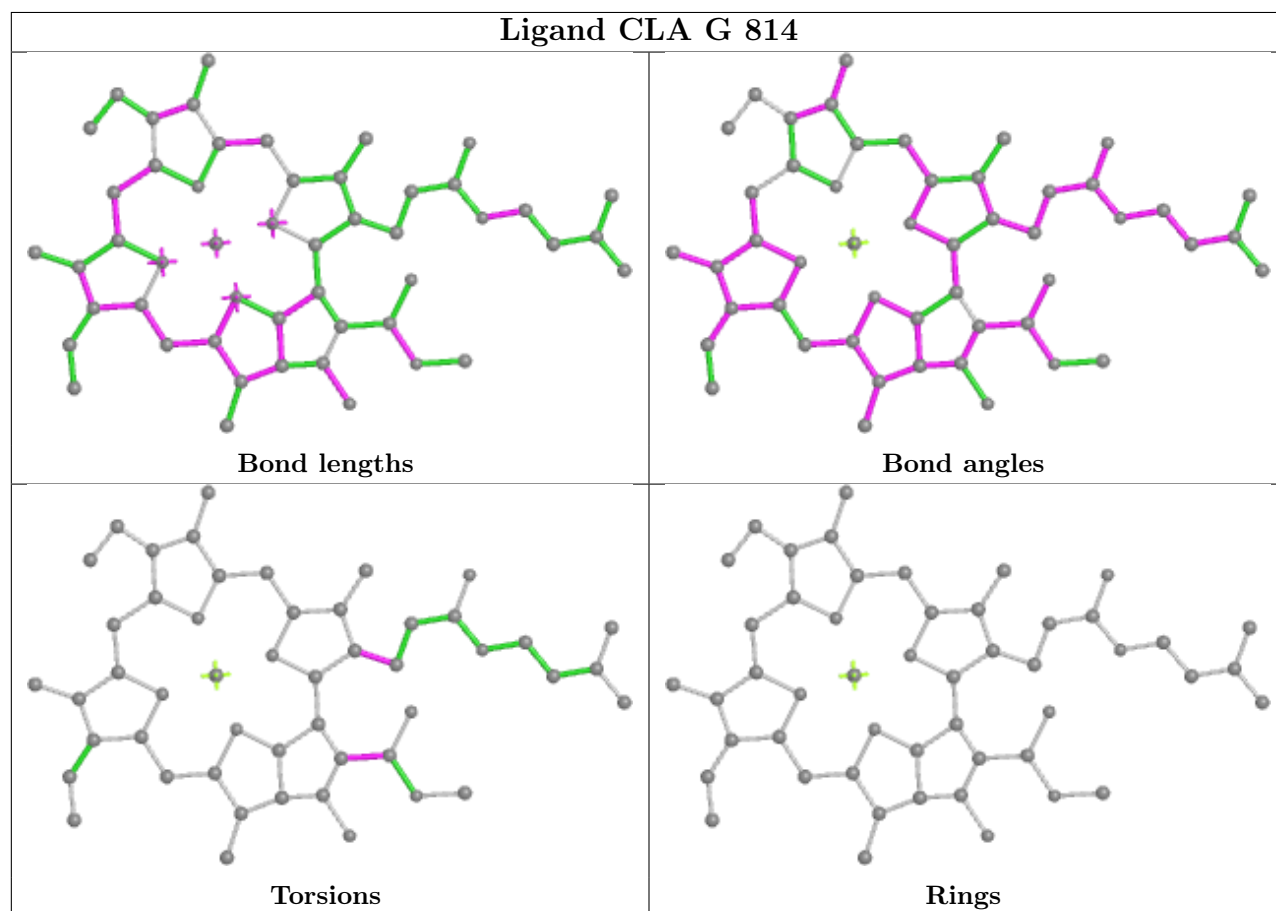
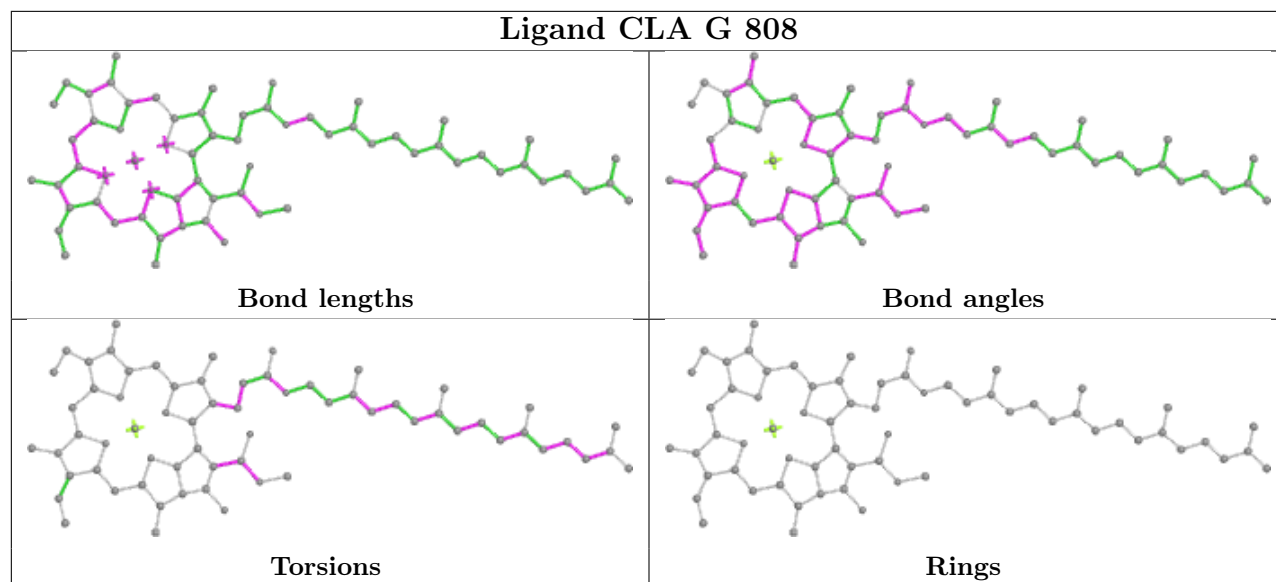


## Ligand CLA G 822

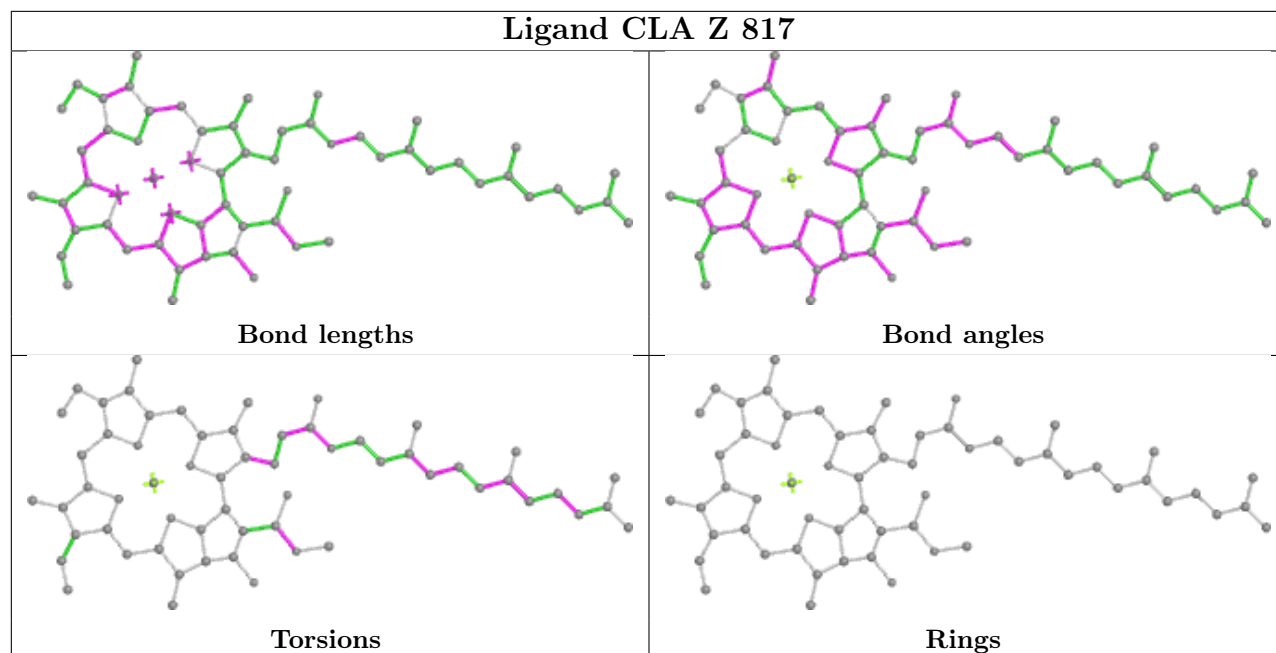




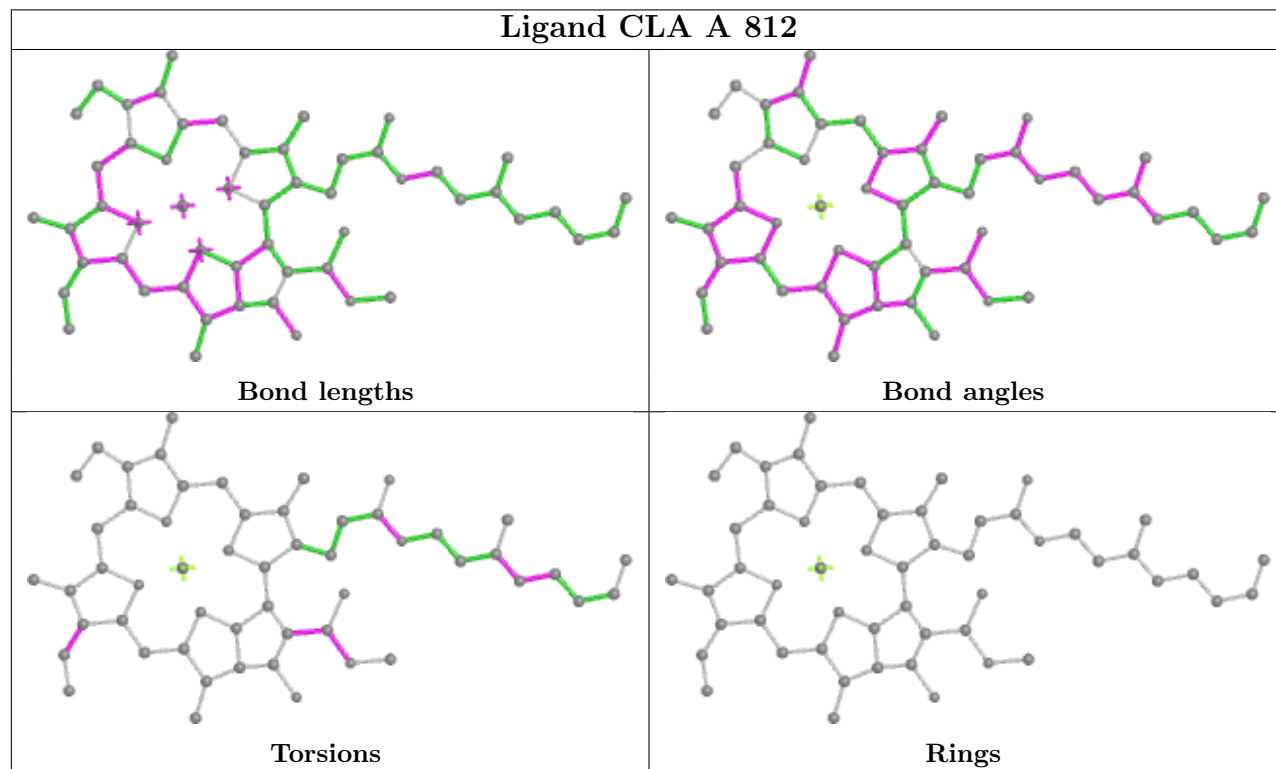


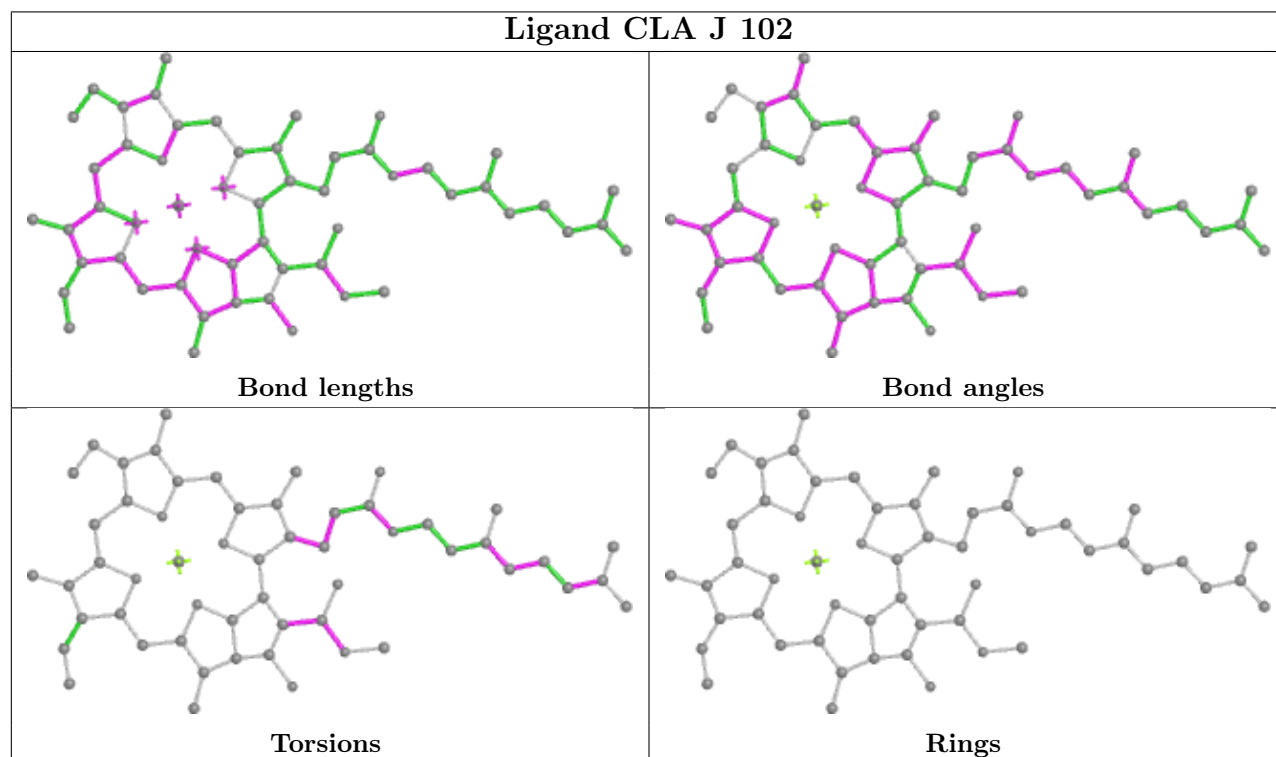
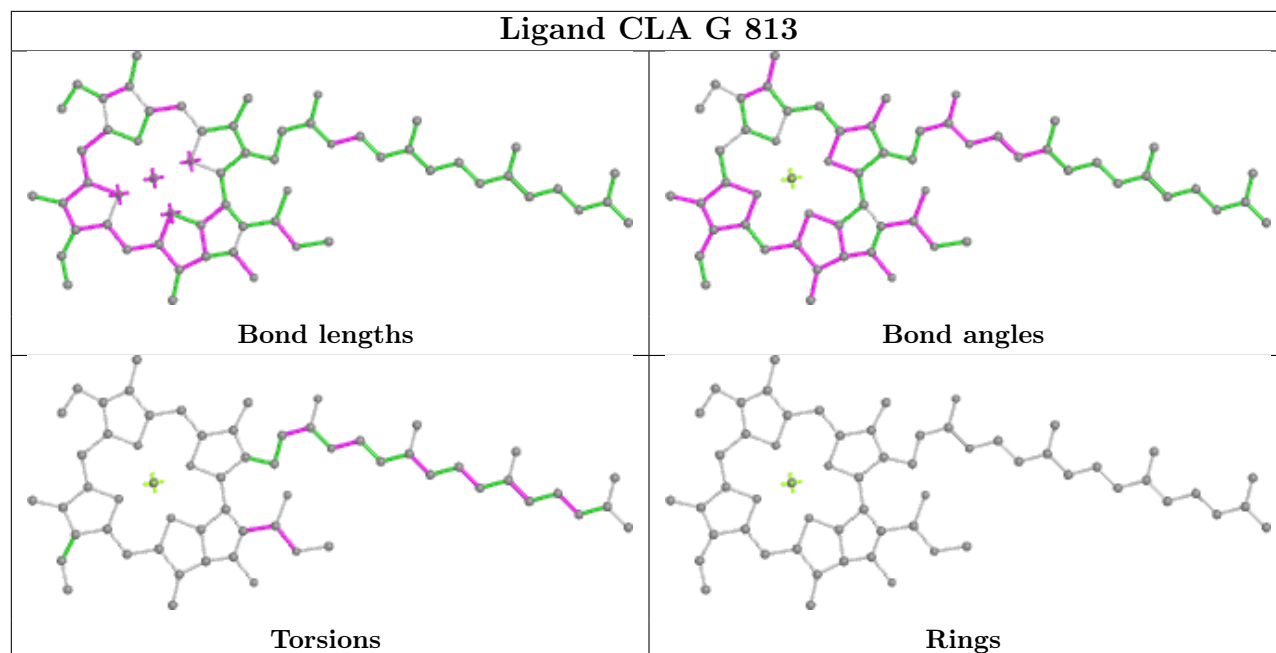


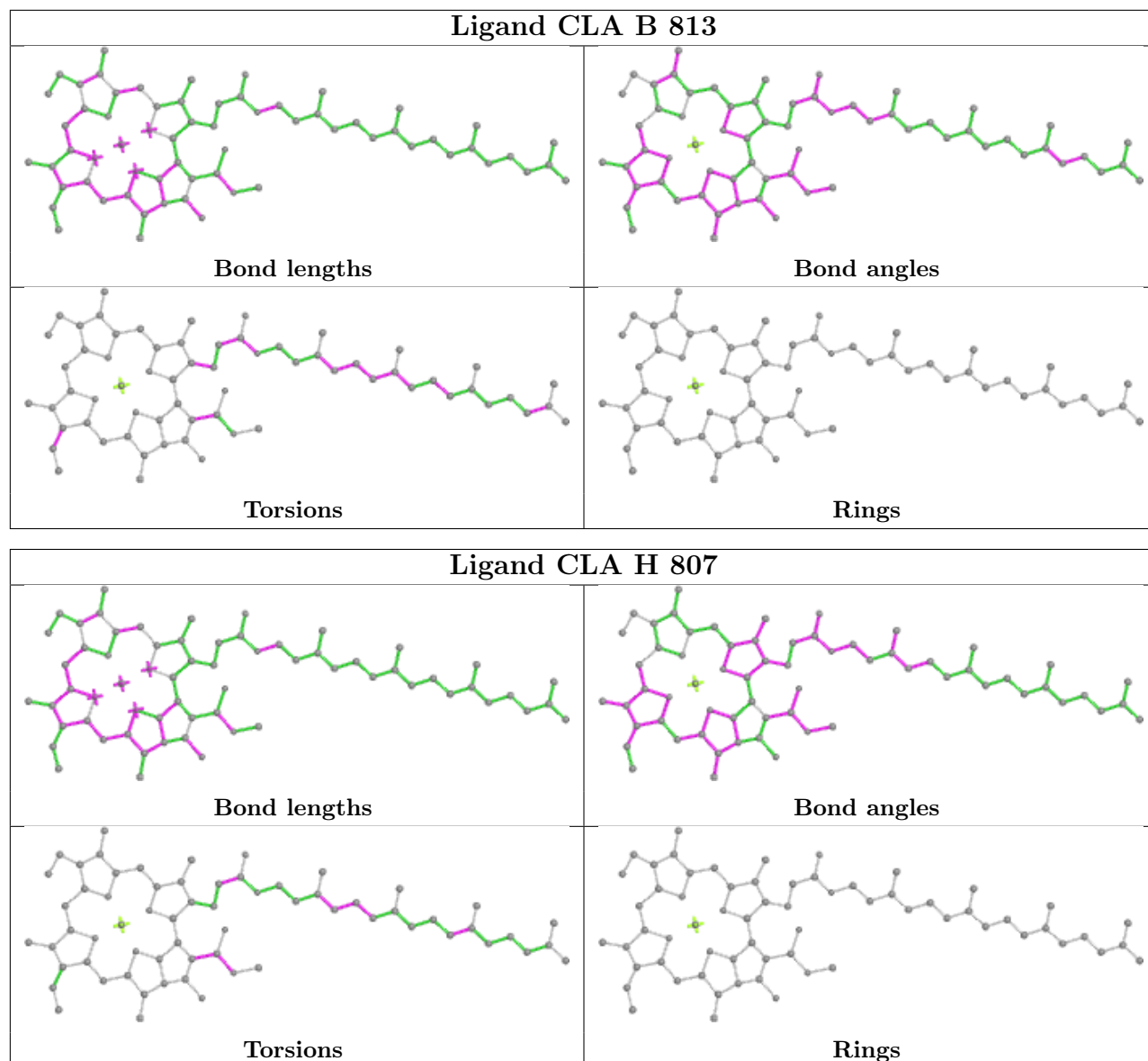
## Ligand CLA Z 817



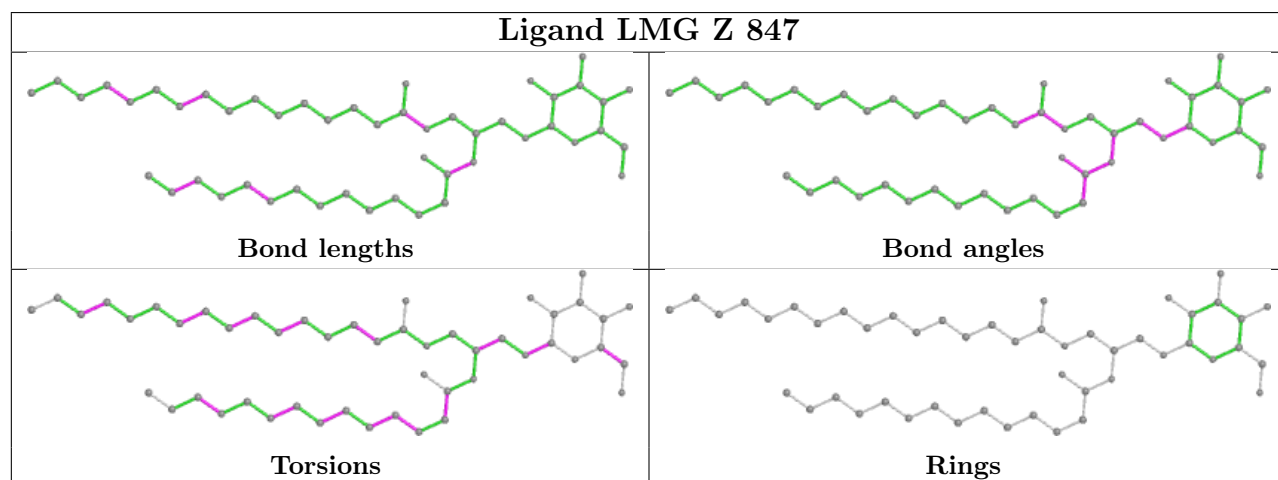
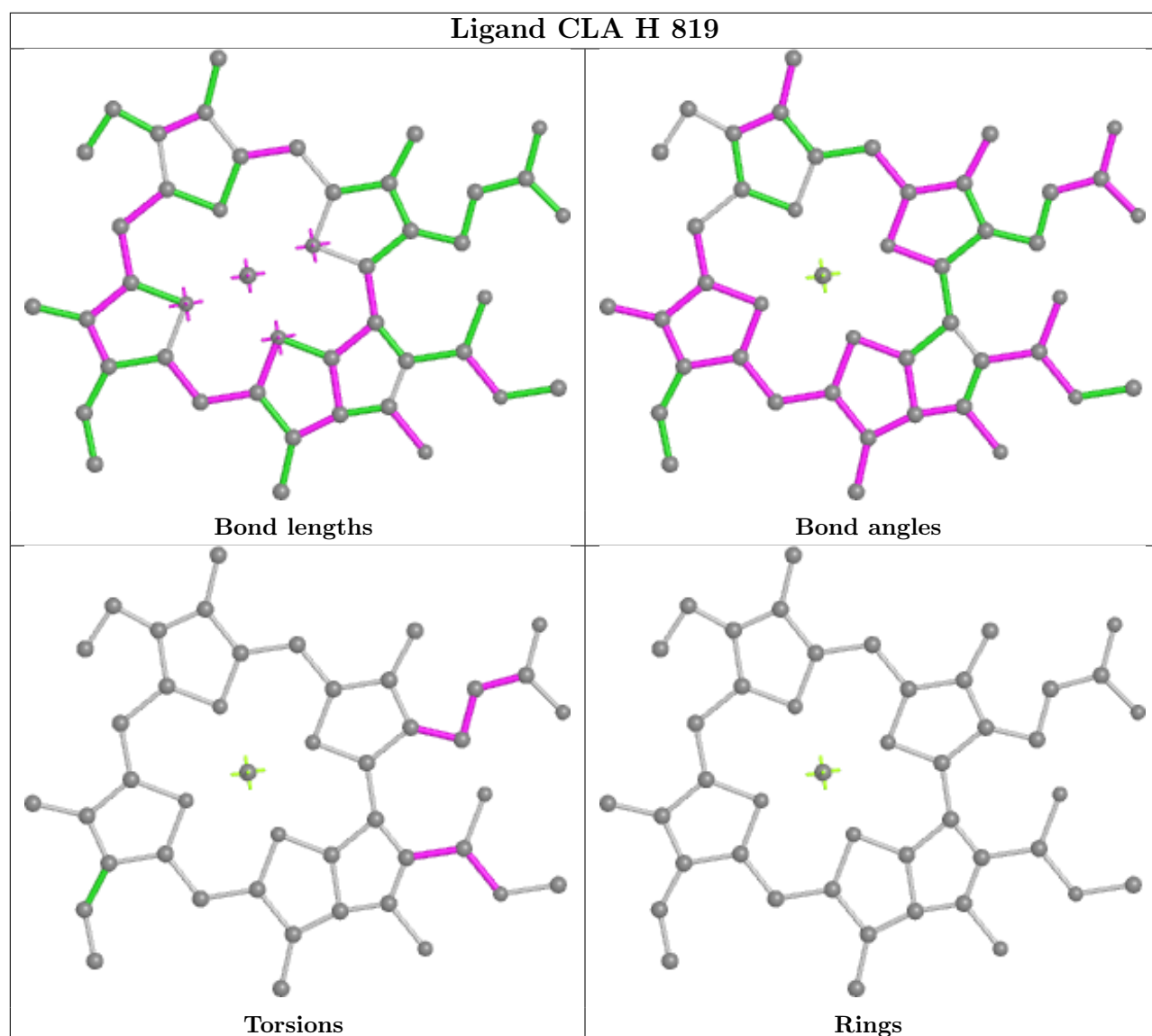
## Ligand CLA A 812

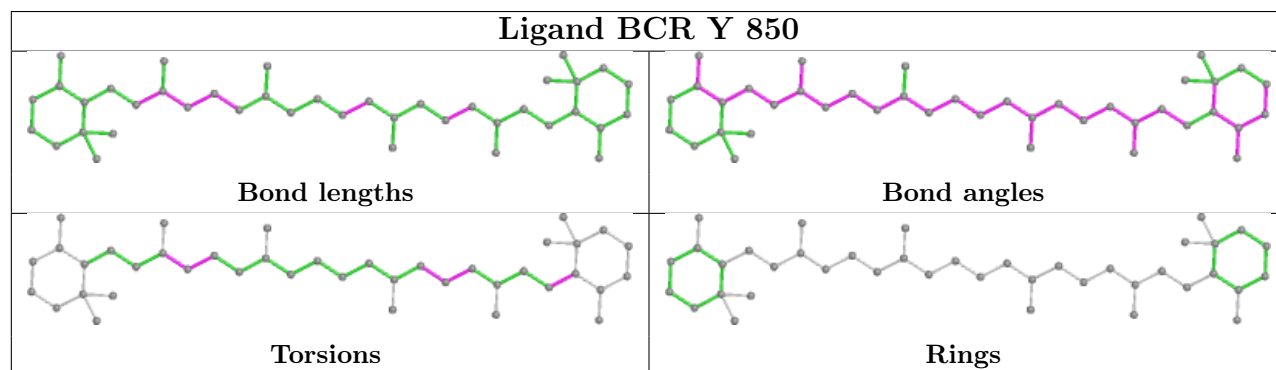
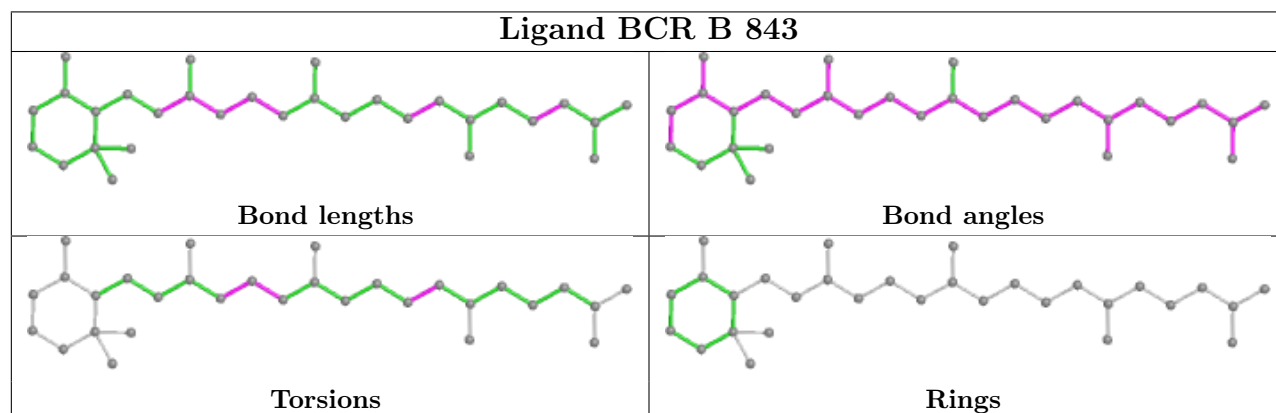
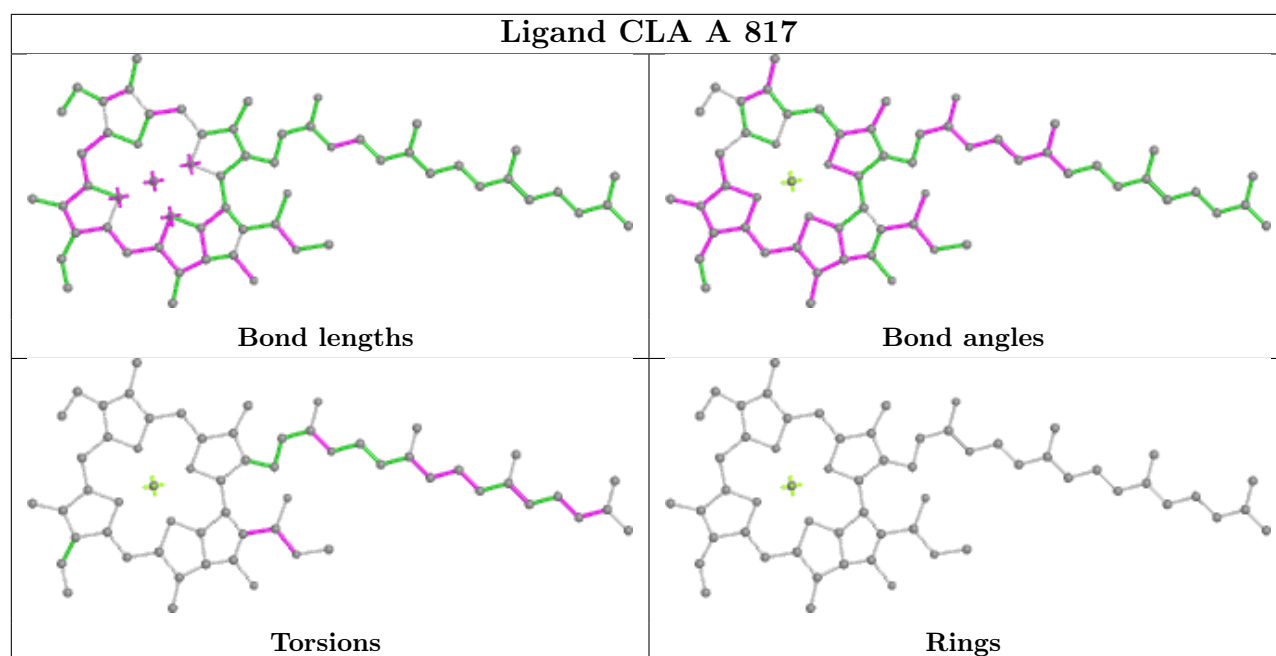


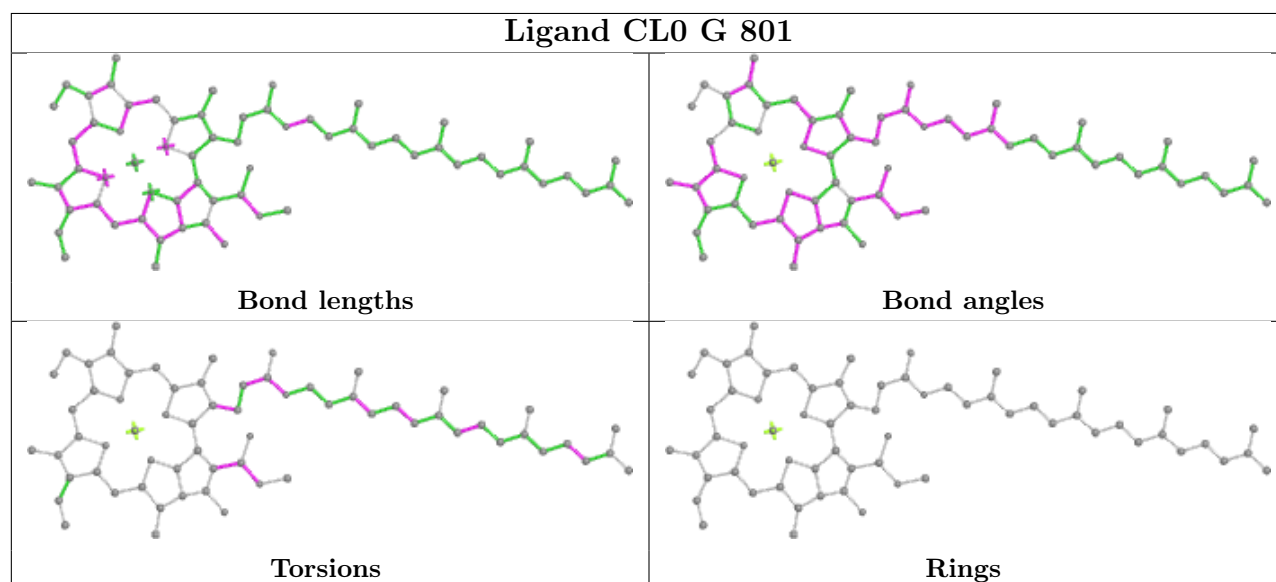
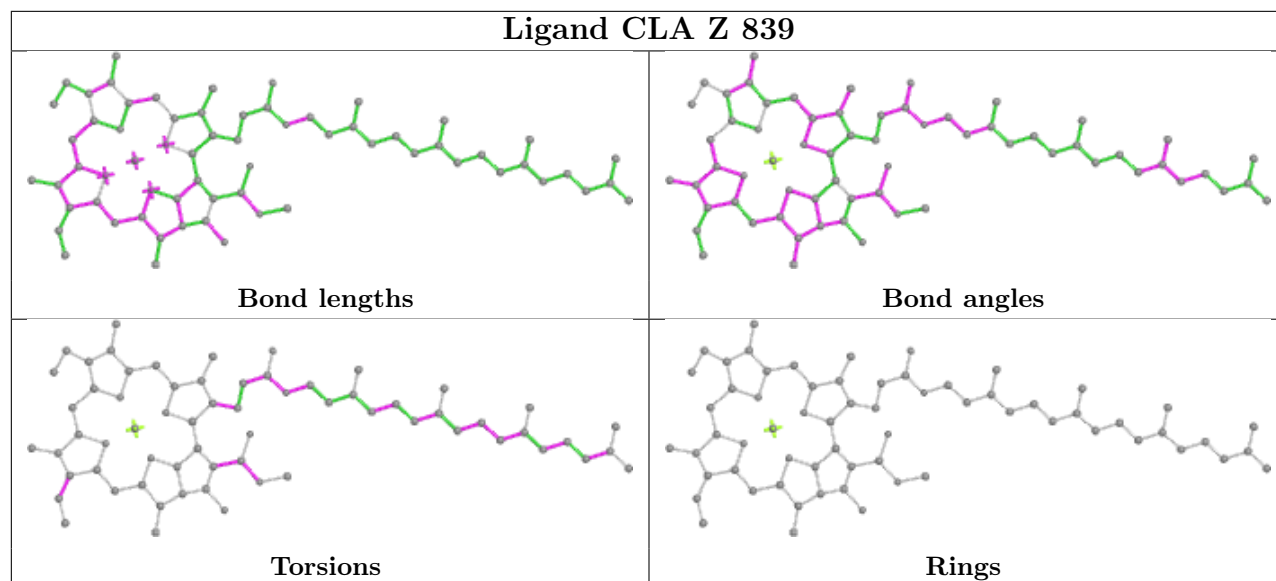
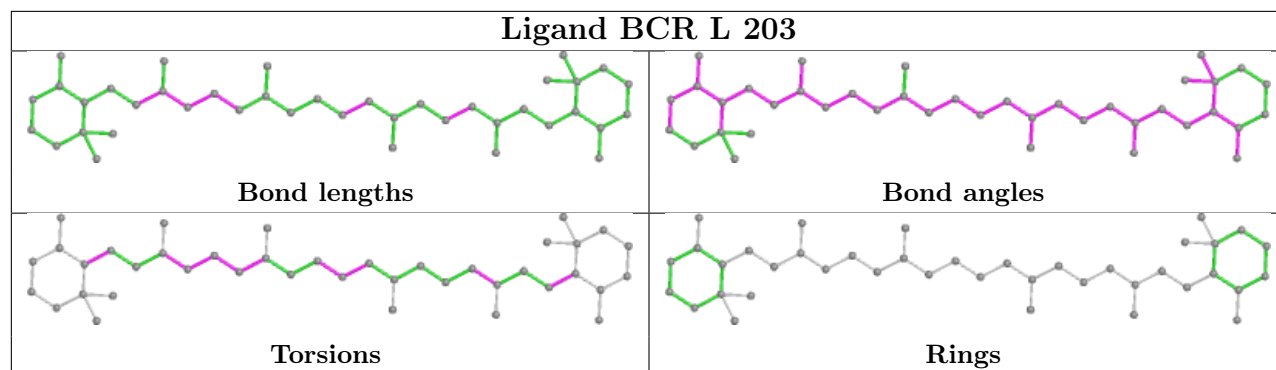


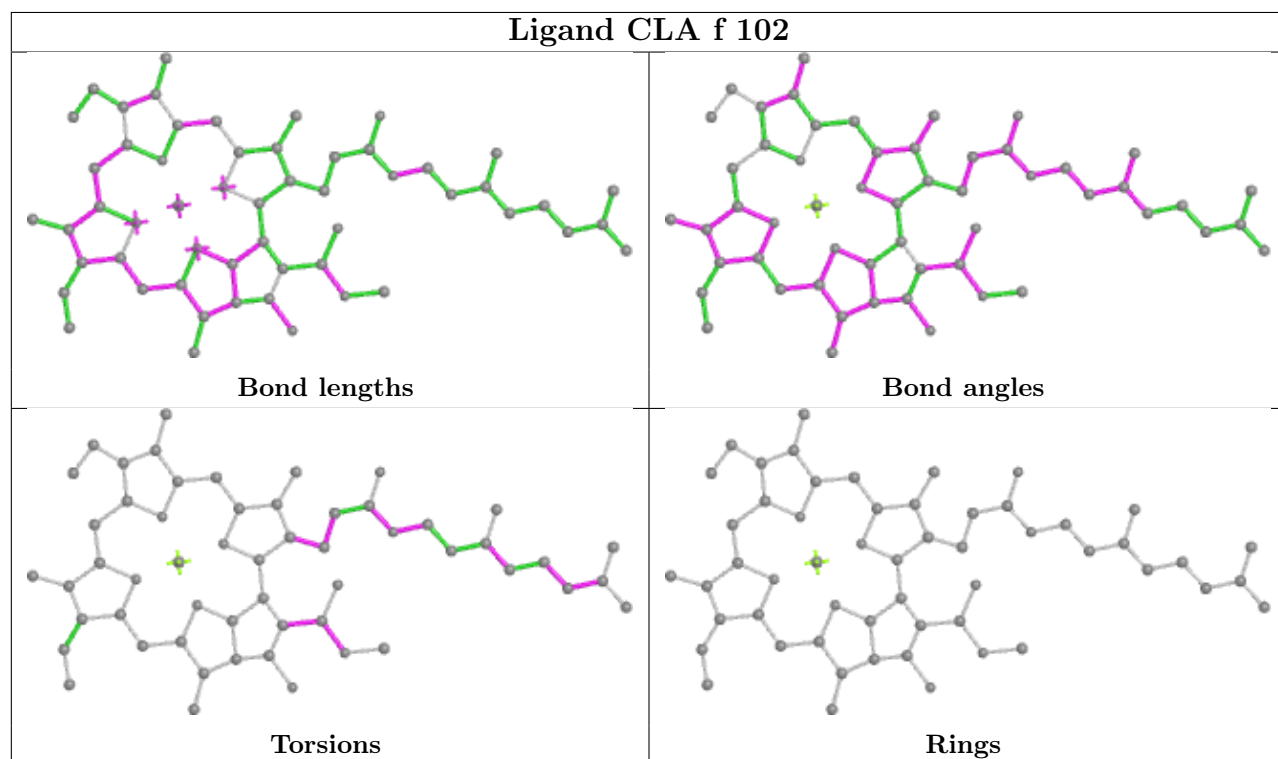
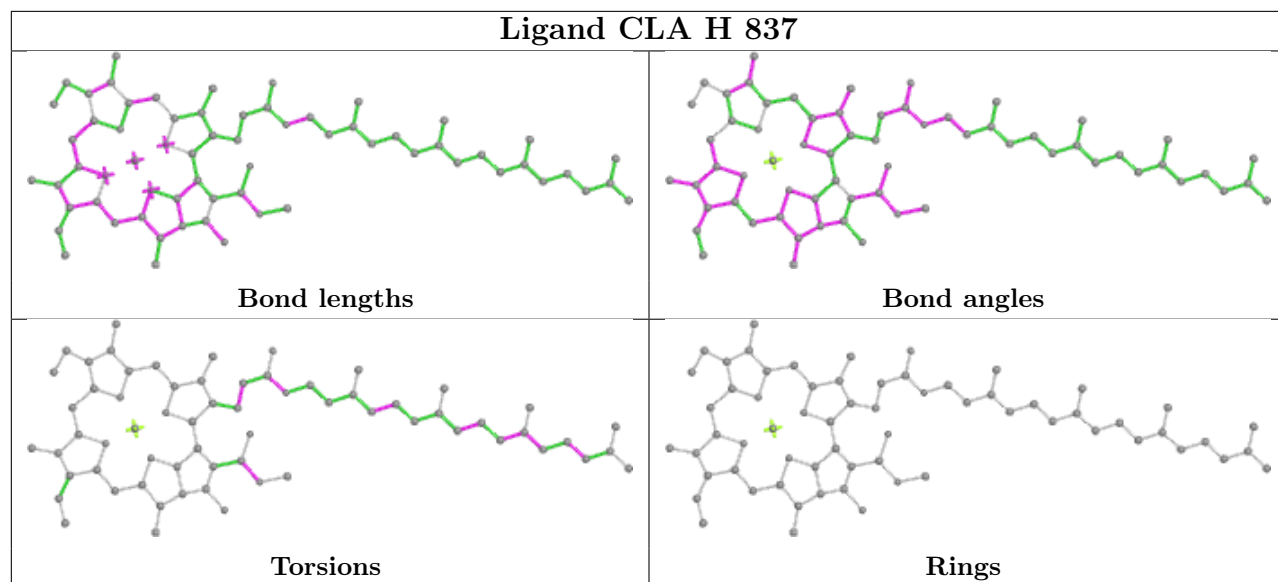


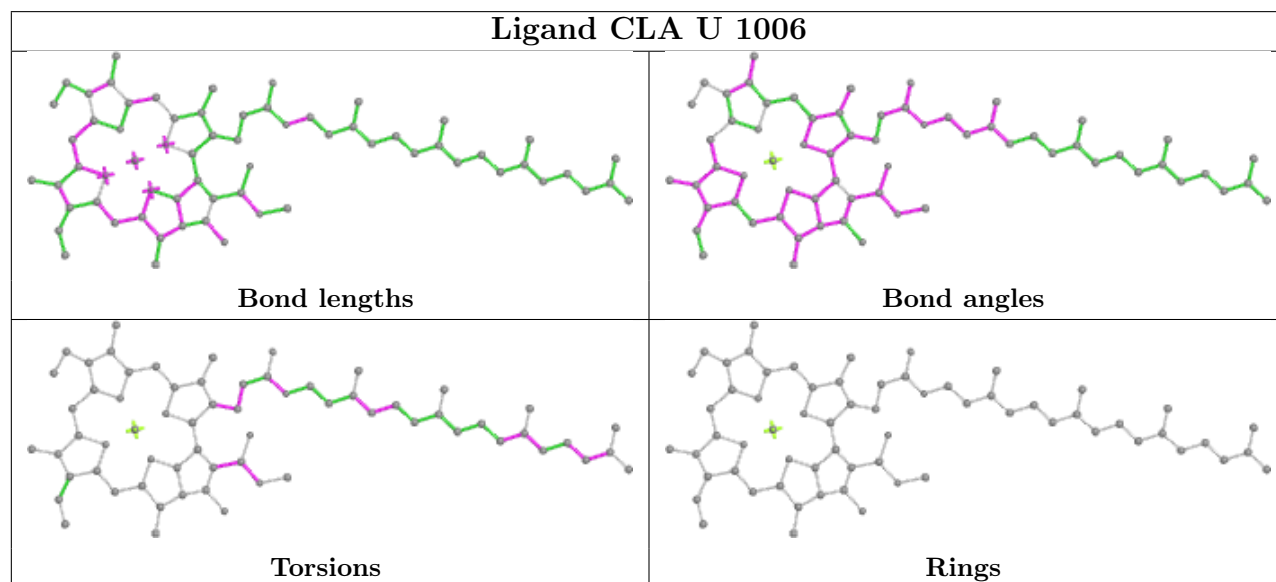
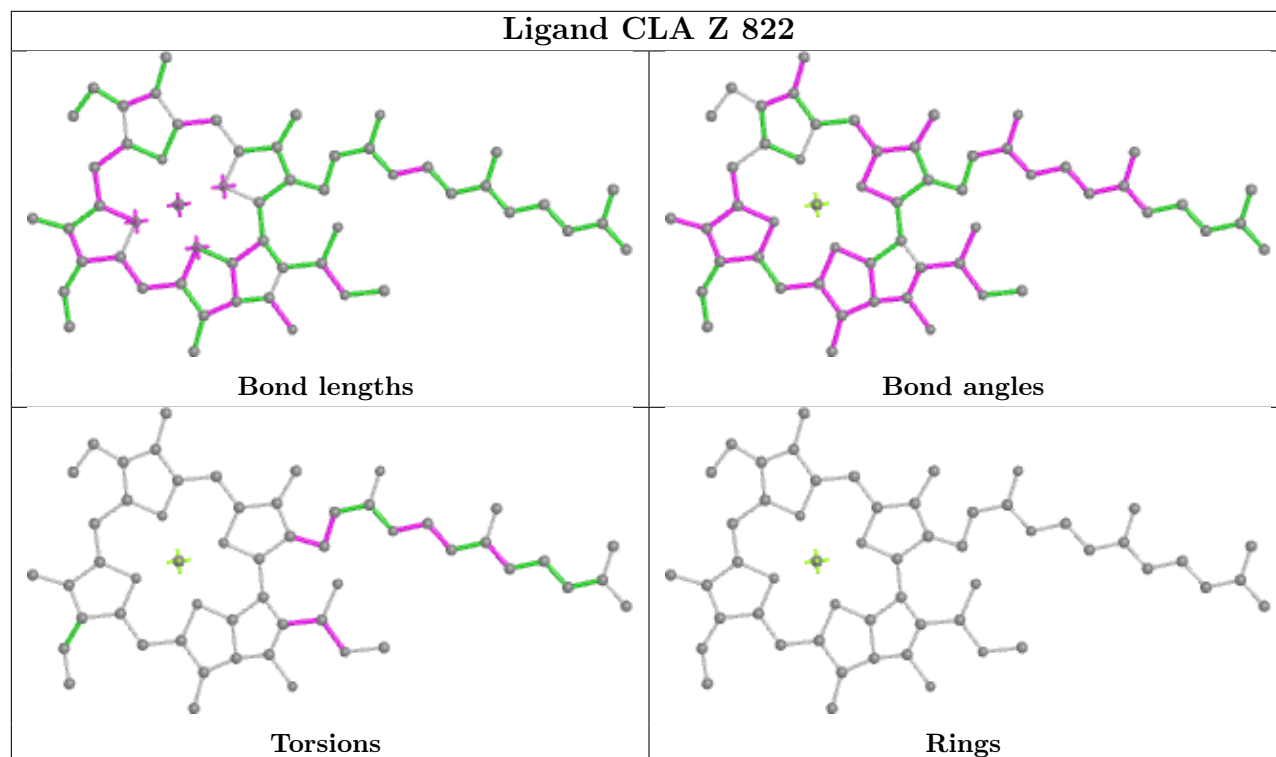


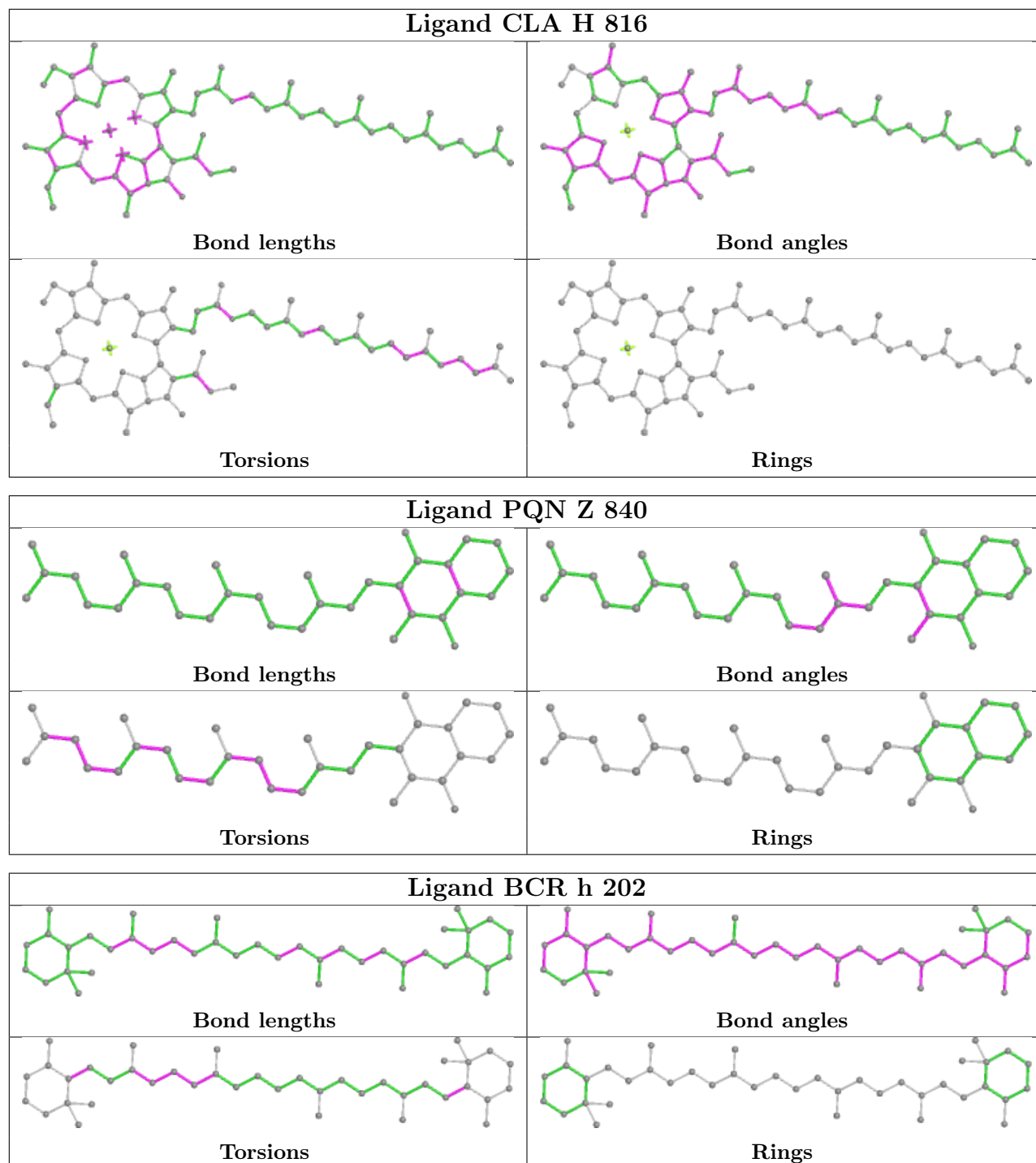




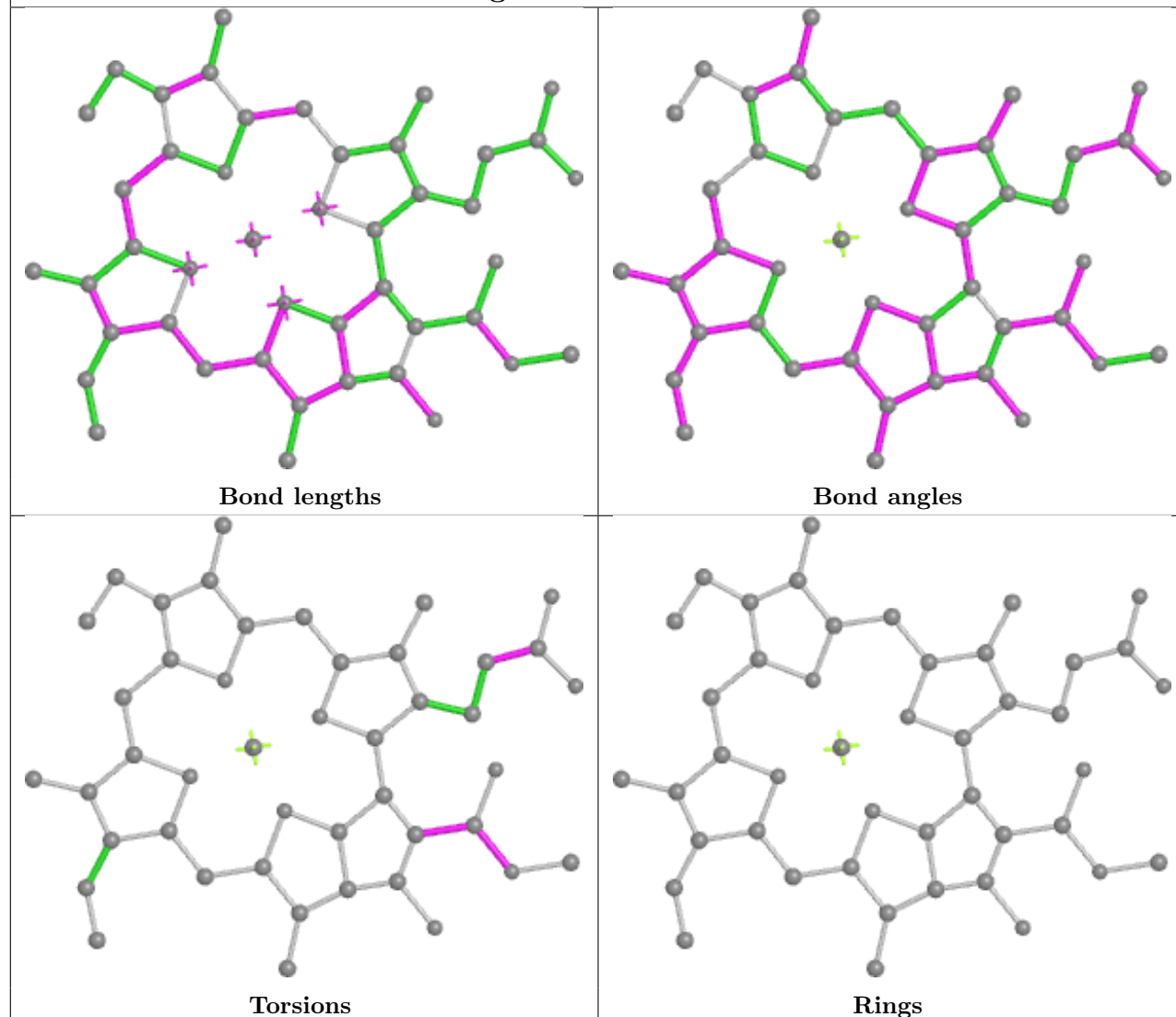




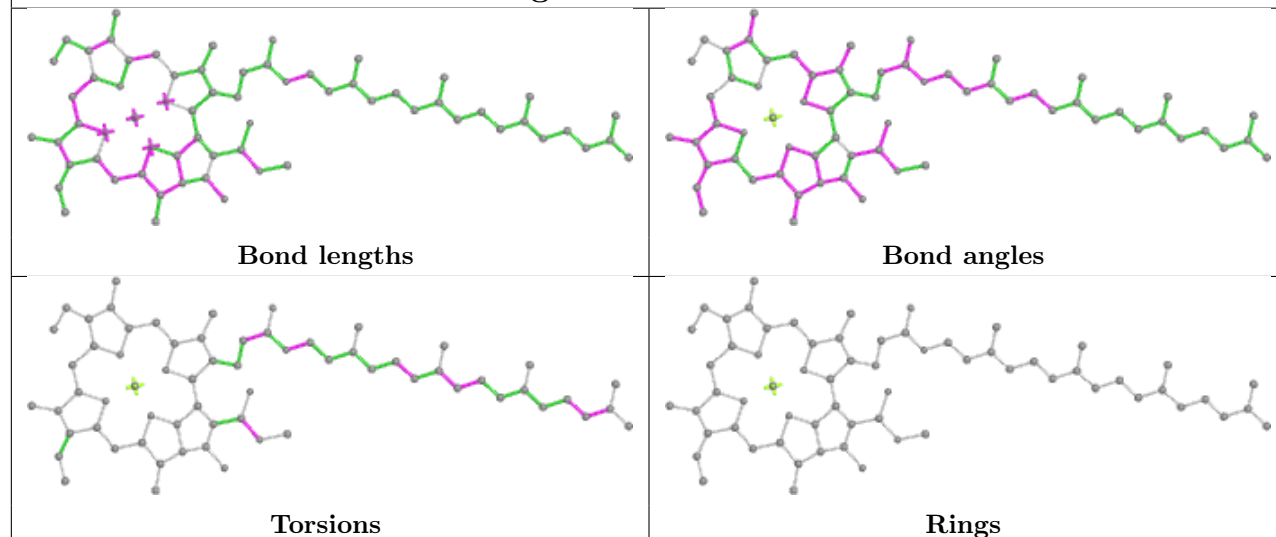




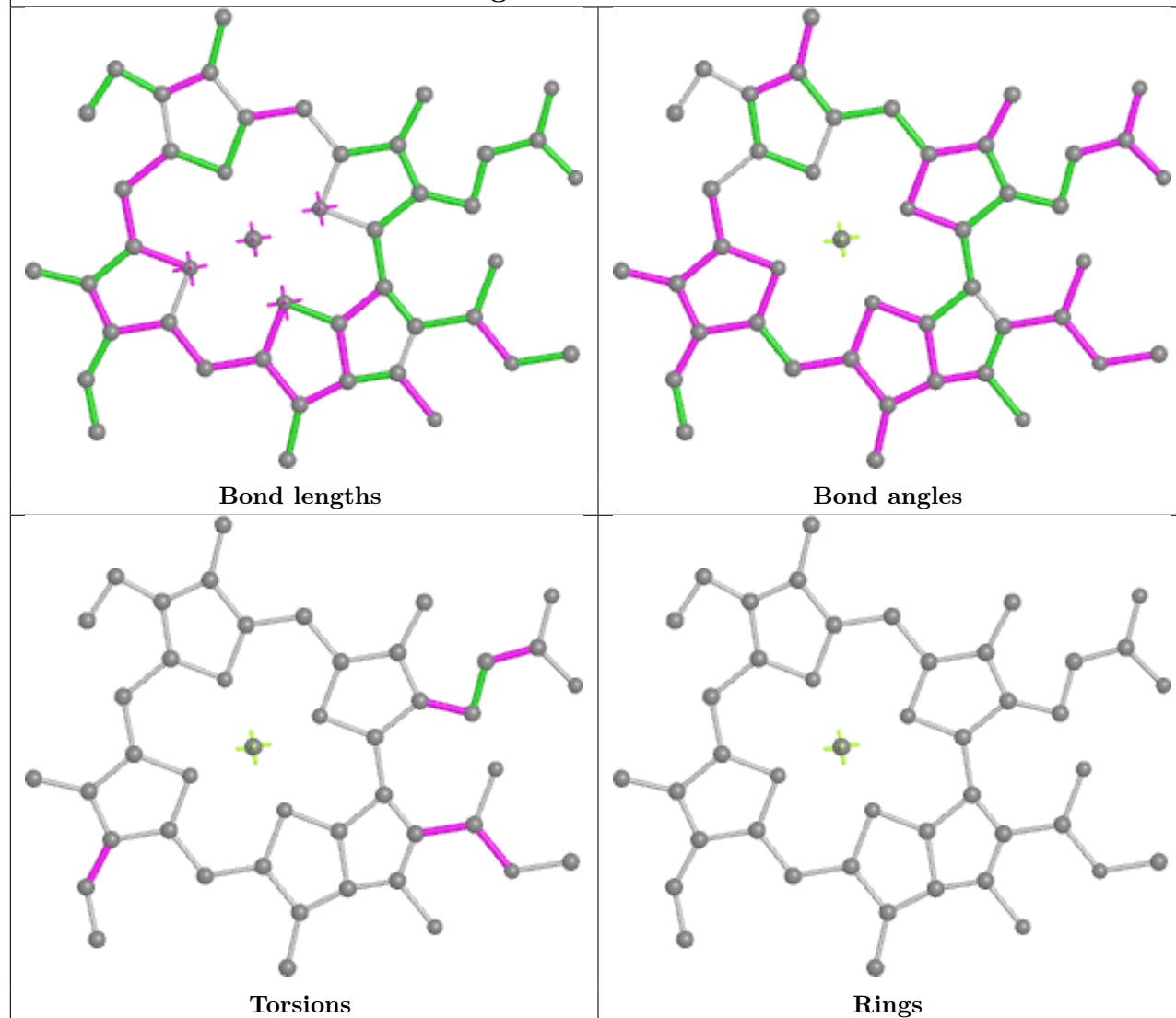
## Ligand CLA H 833



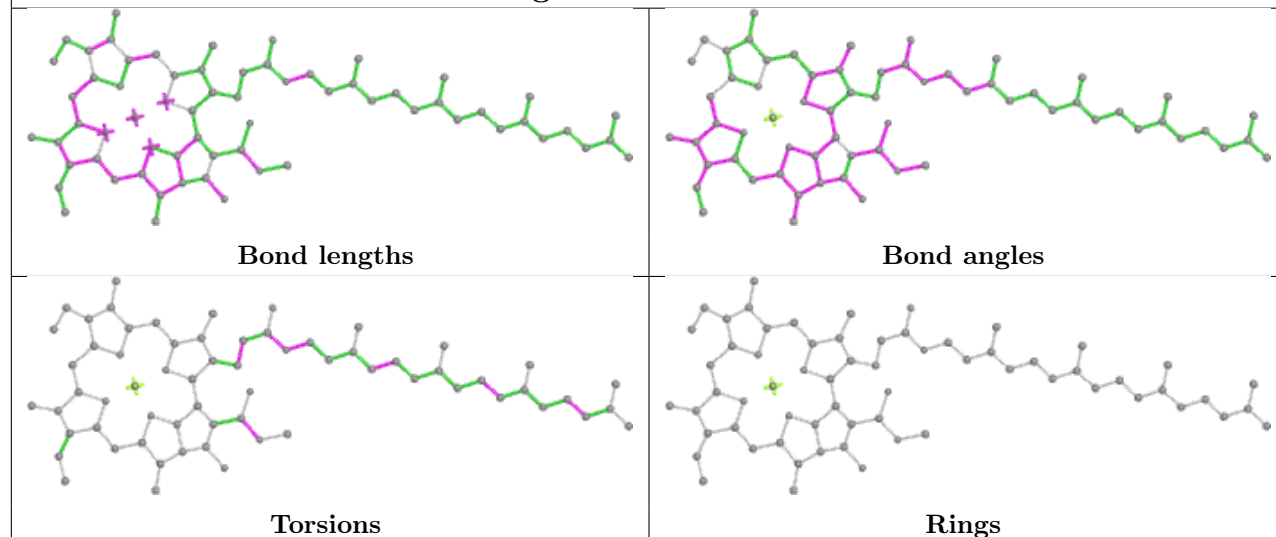
## Ligand CLA H 808



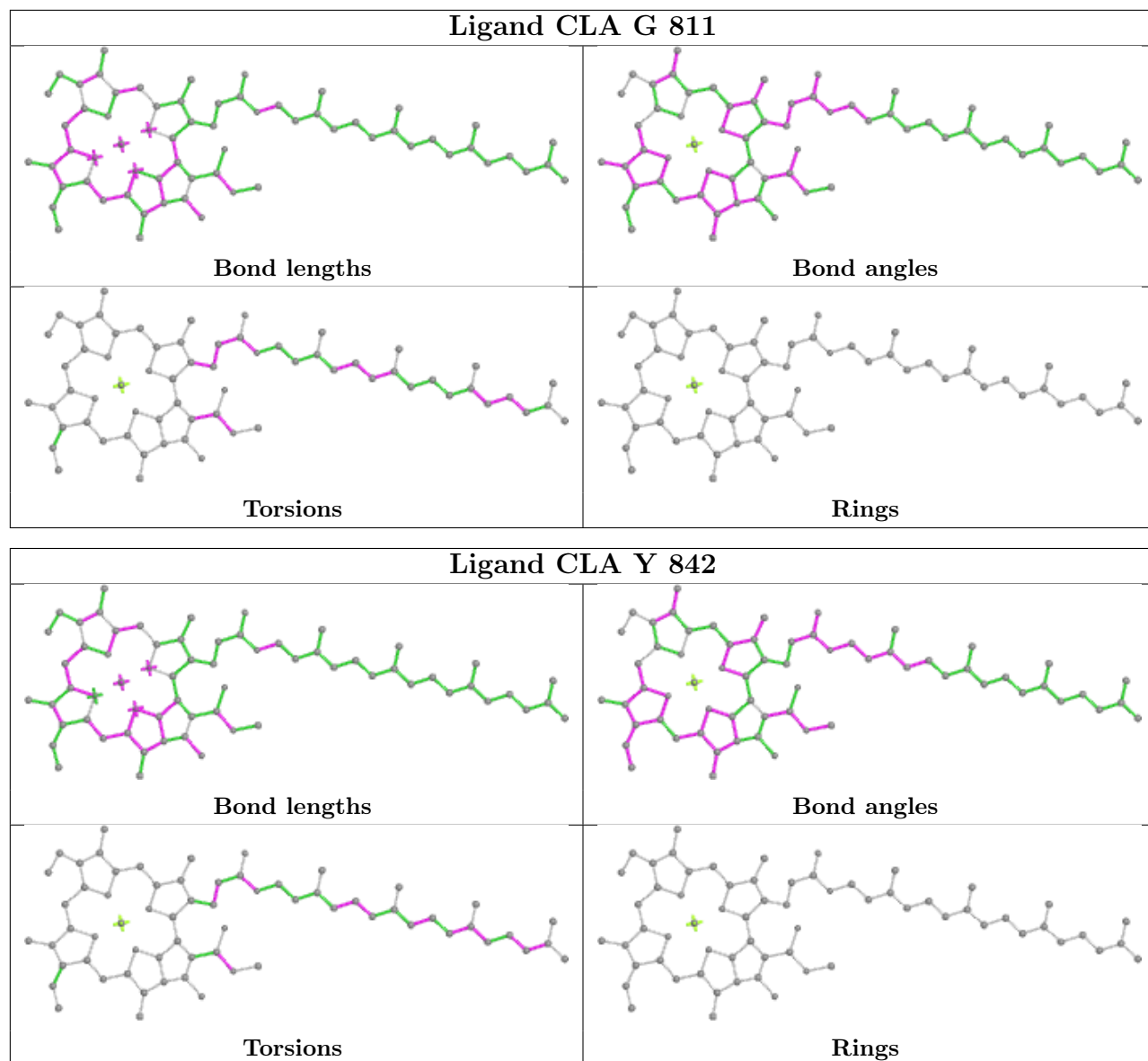
## Ligand CLA B 821



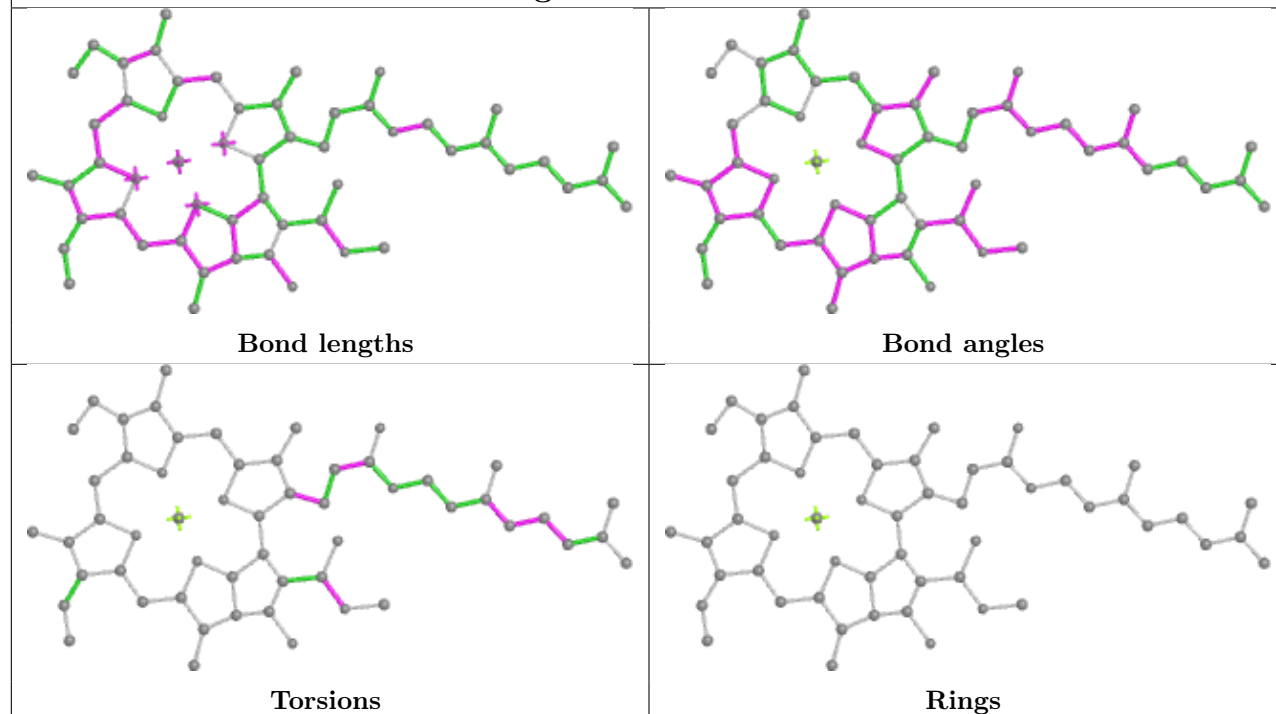
## Ligand CLA B 817



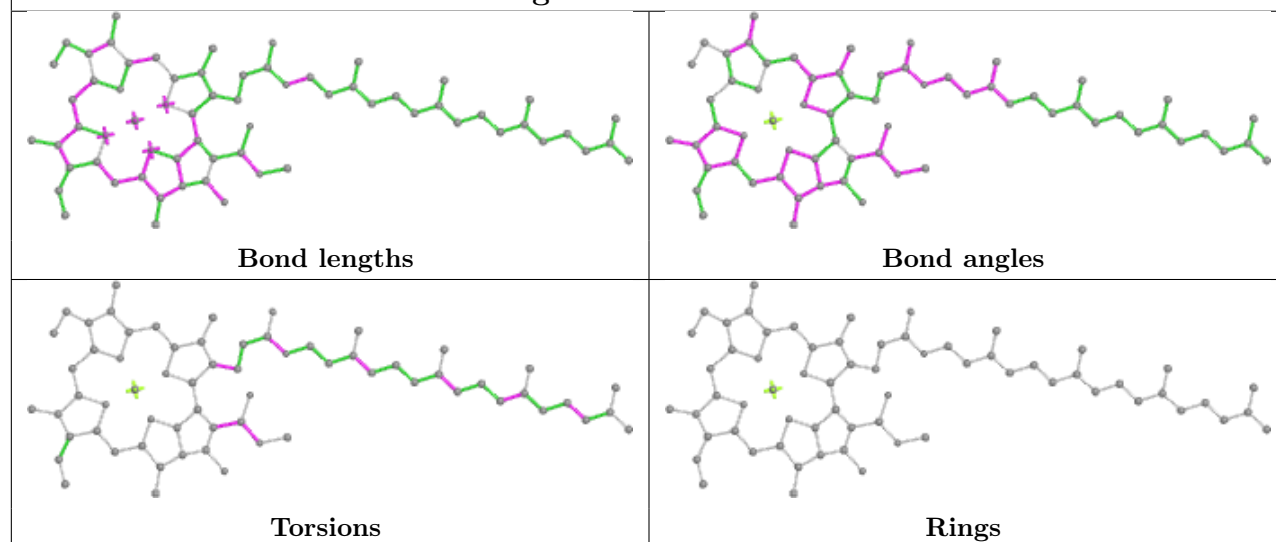


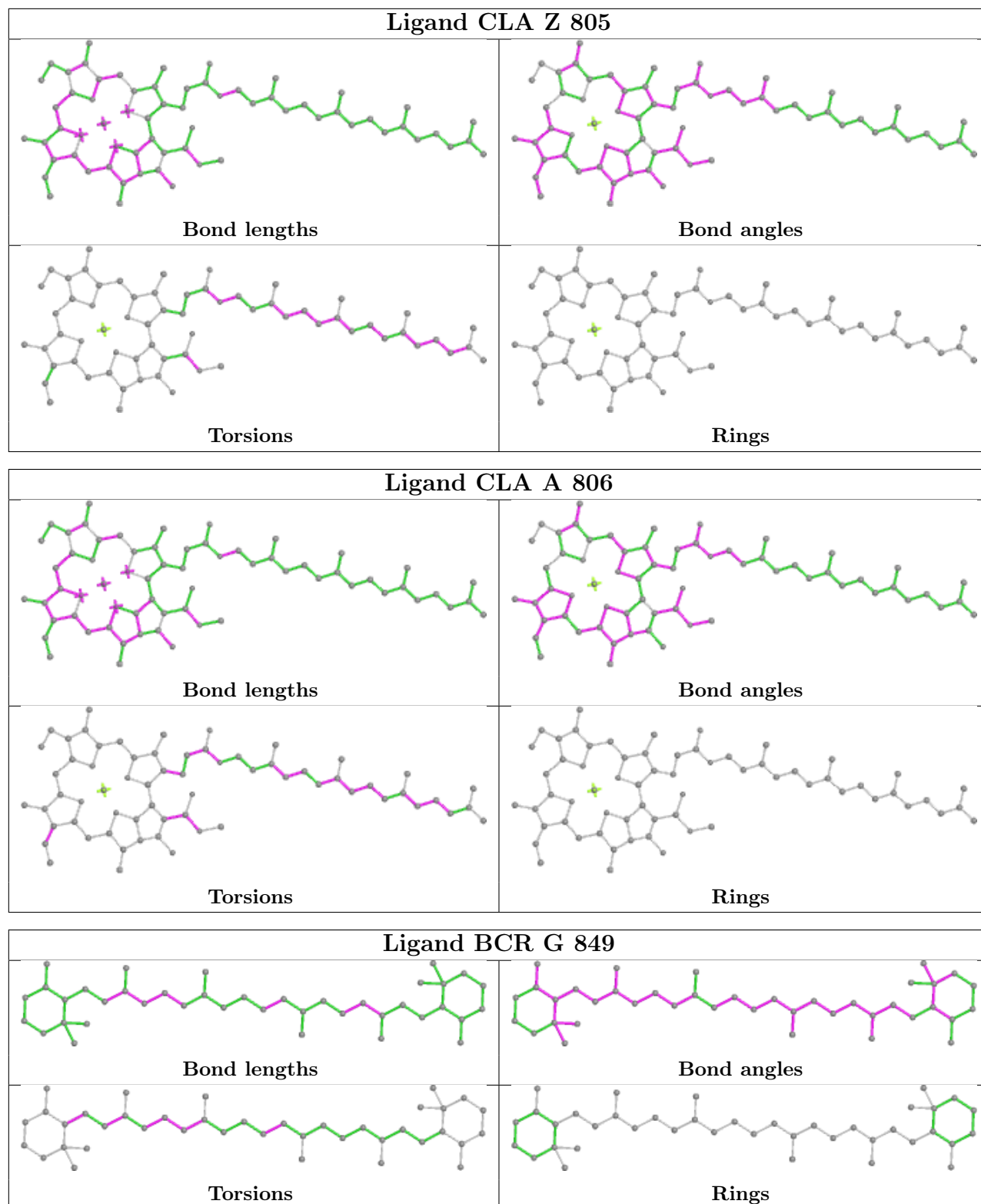


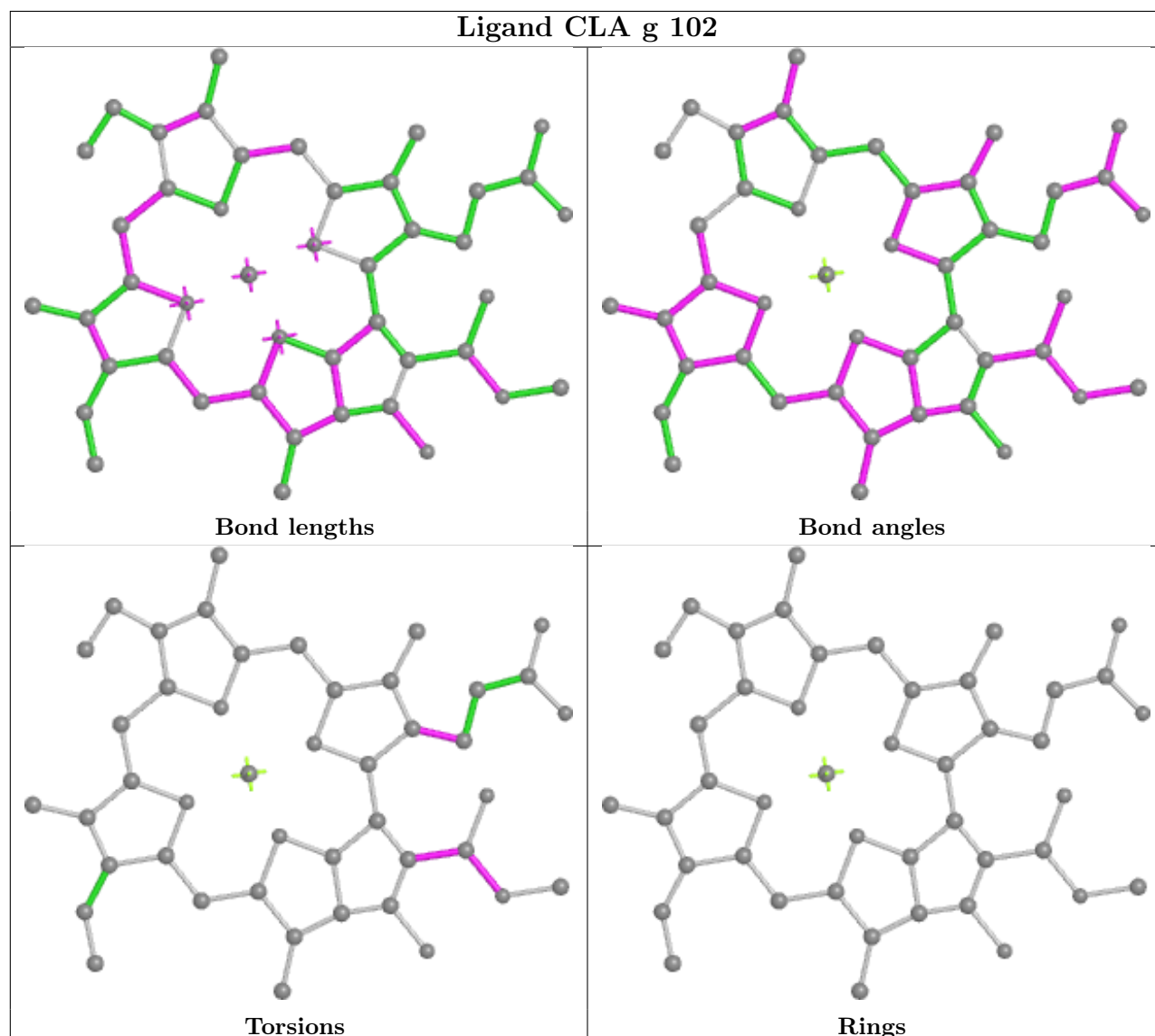
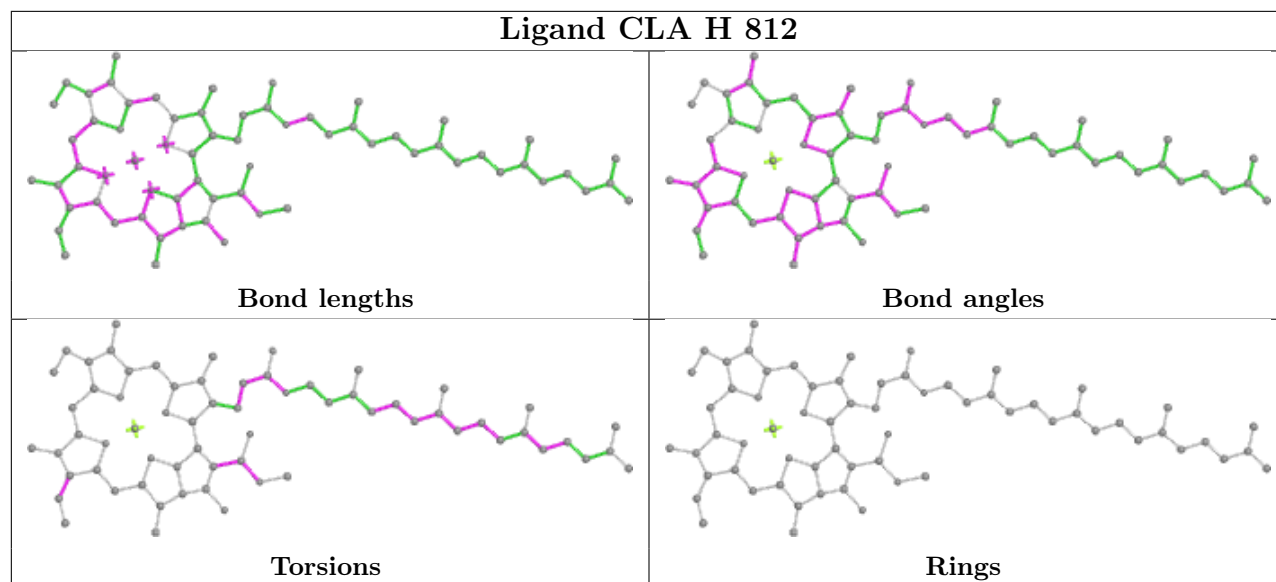
## Ligand CLA Z 809

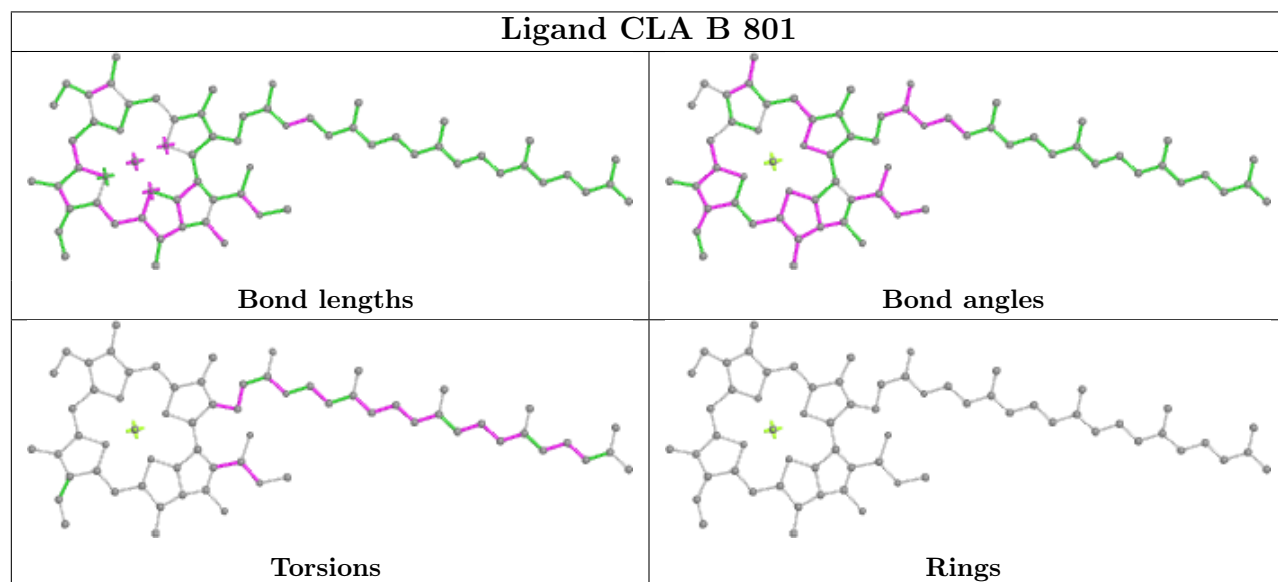
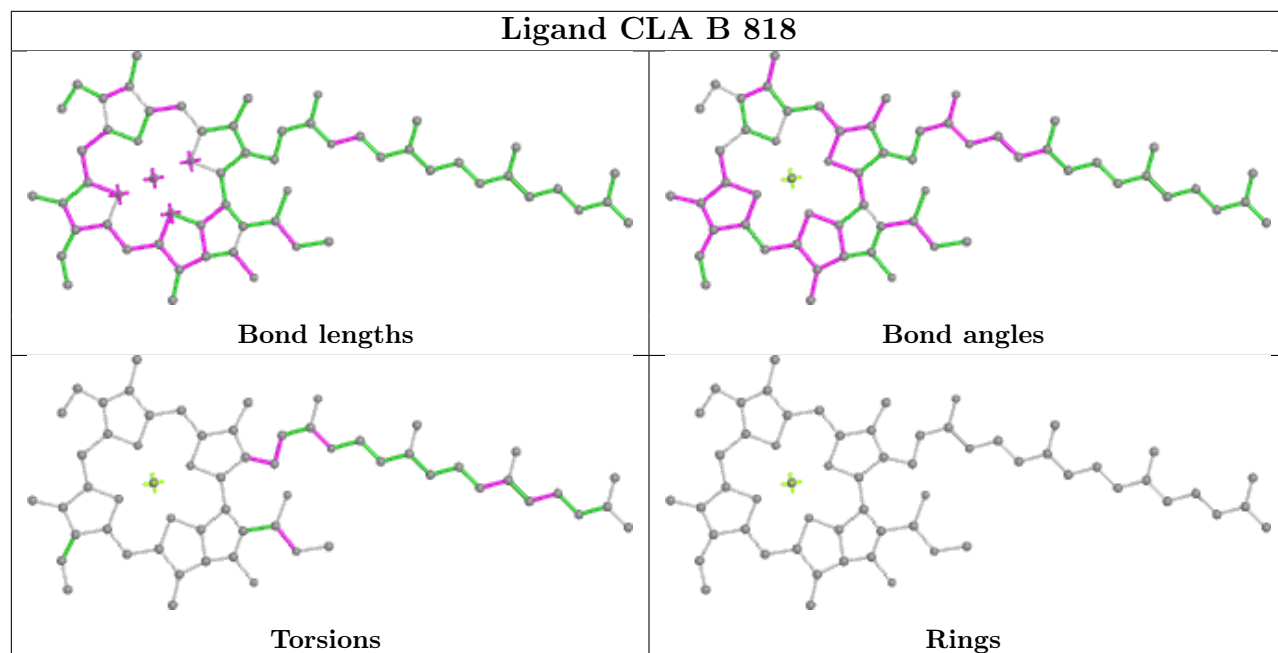


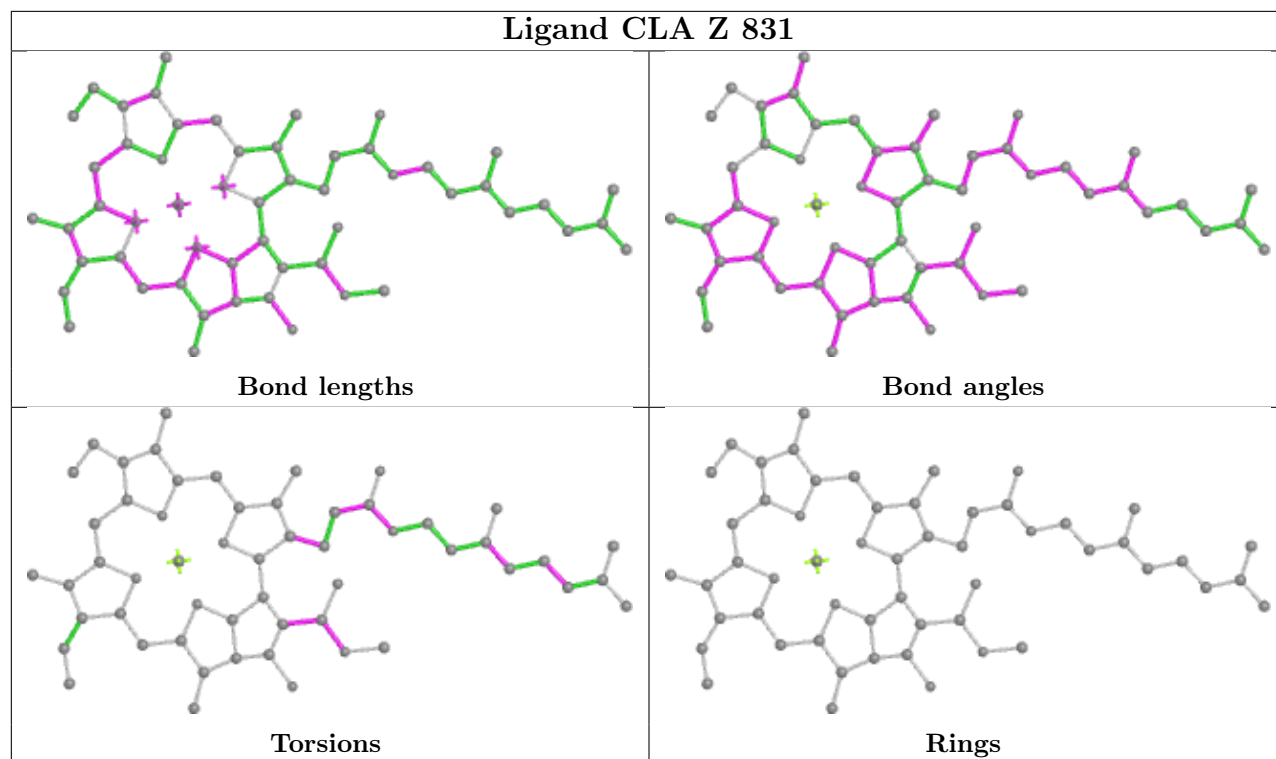
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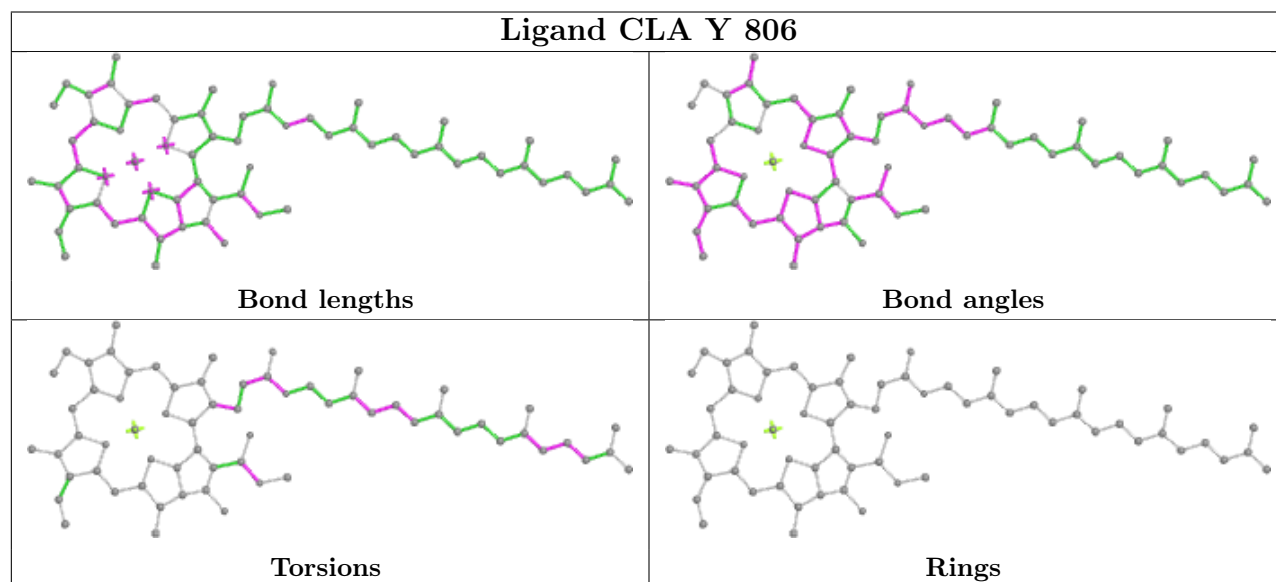
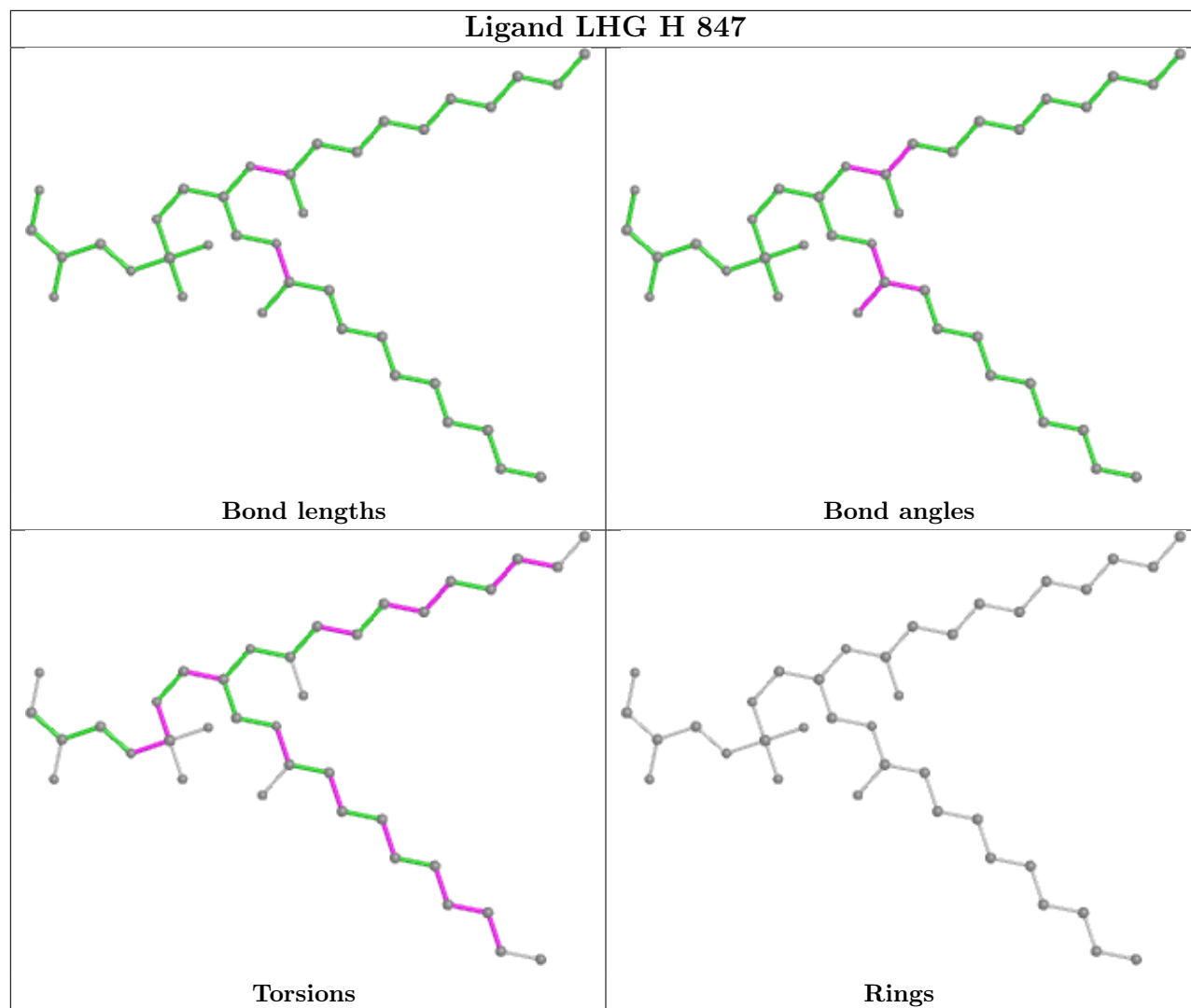


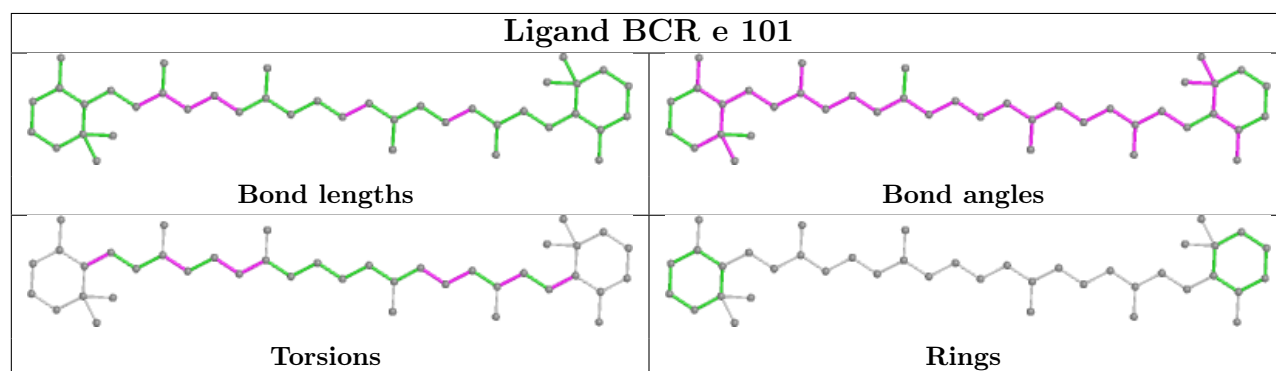
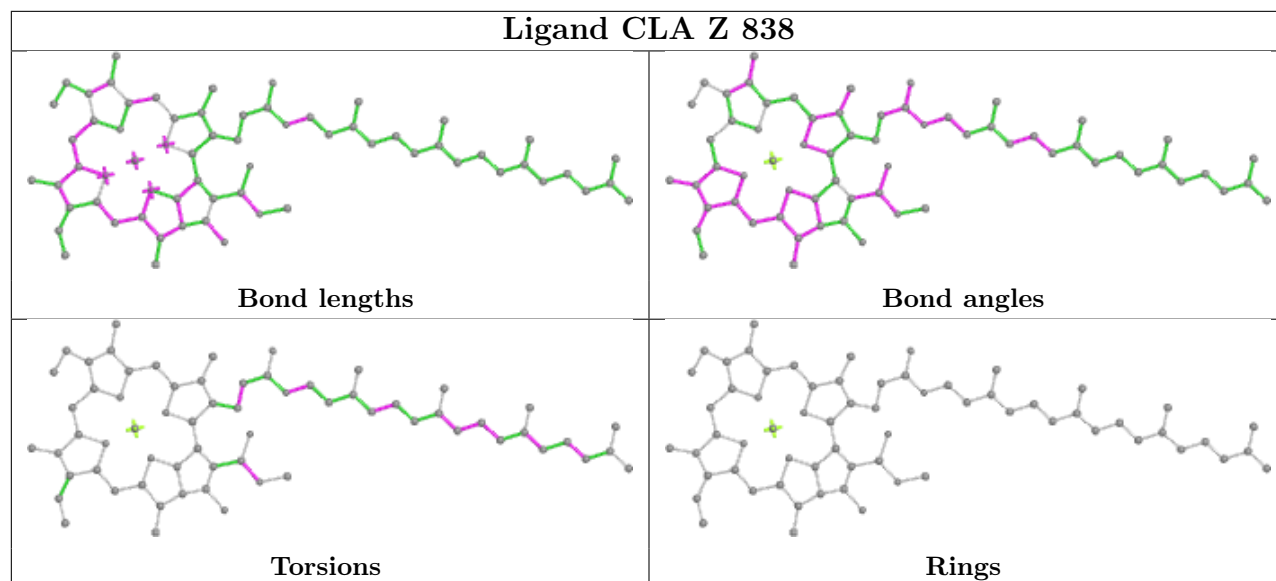
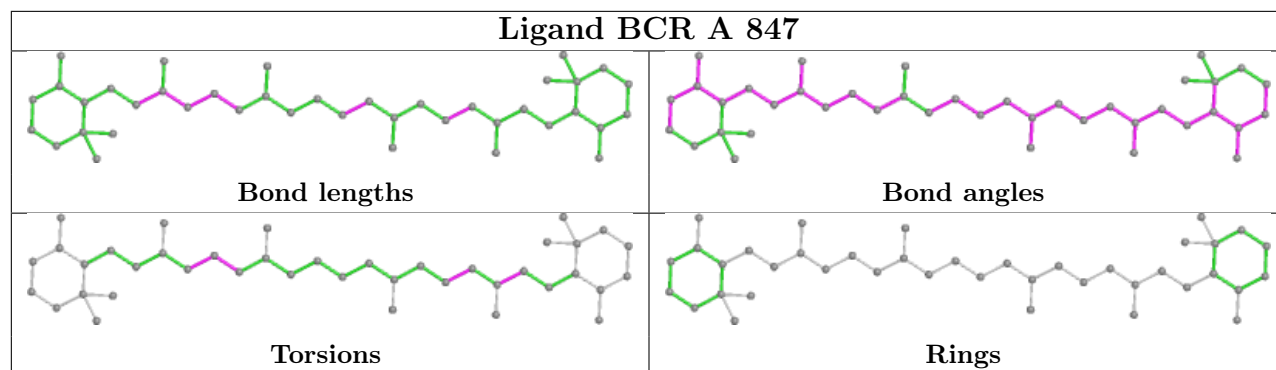




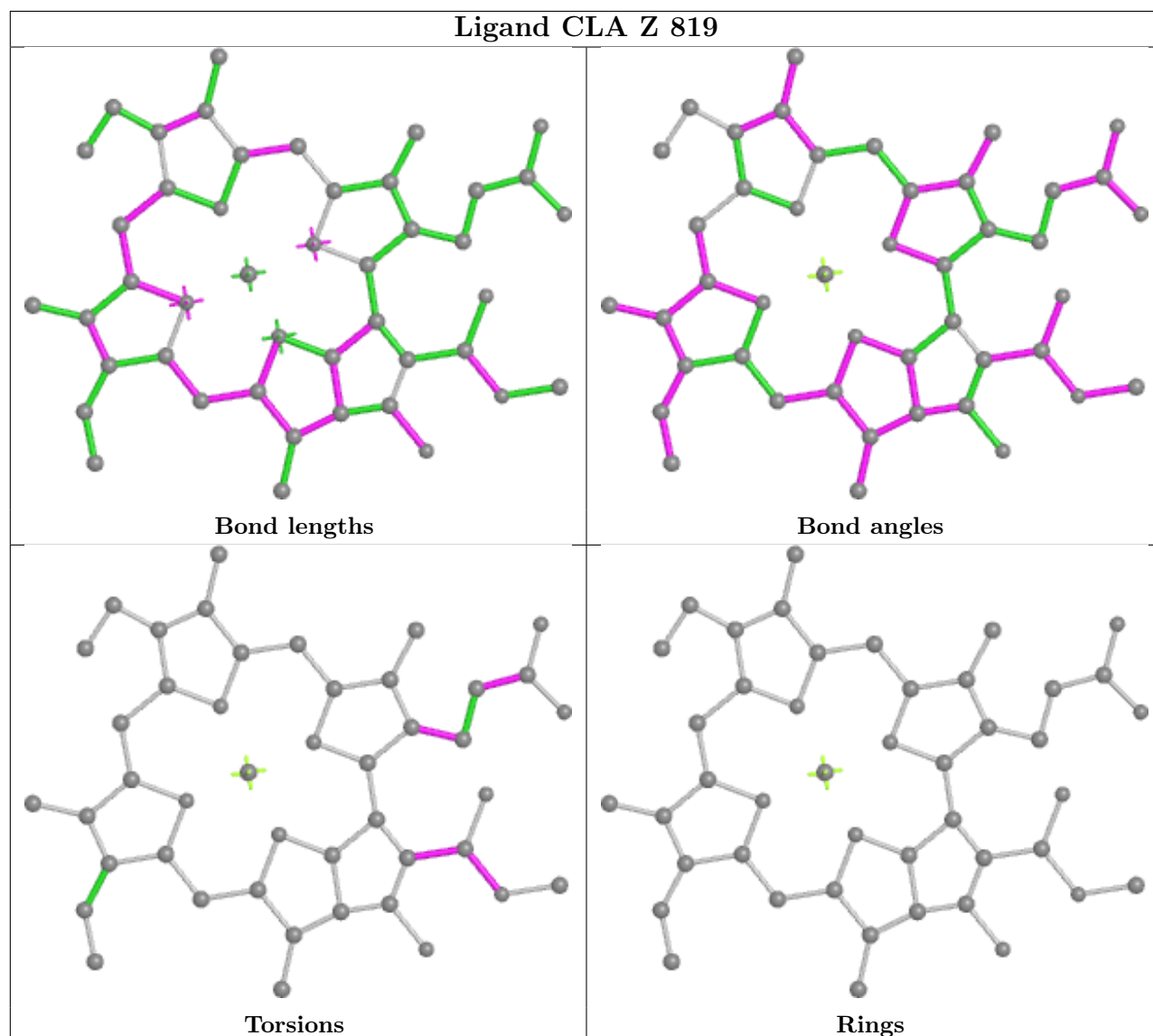
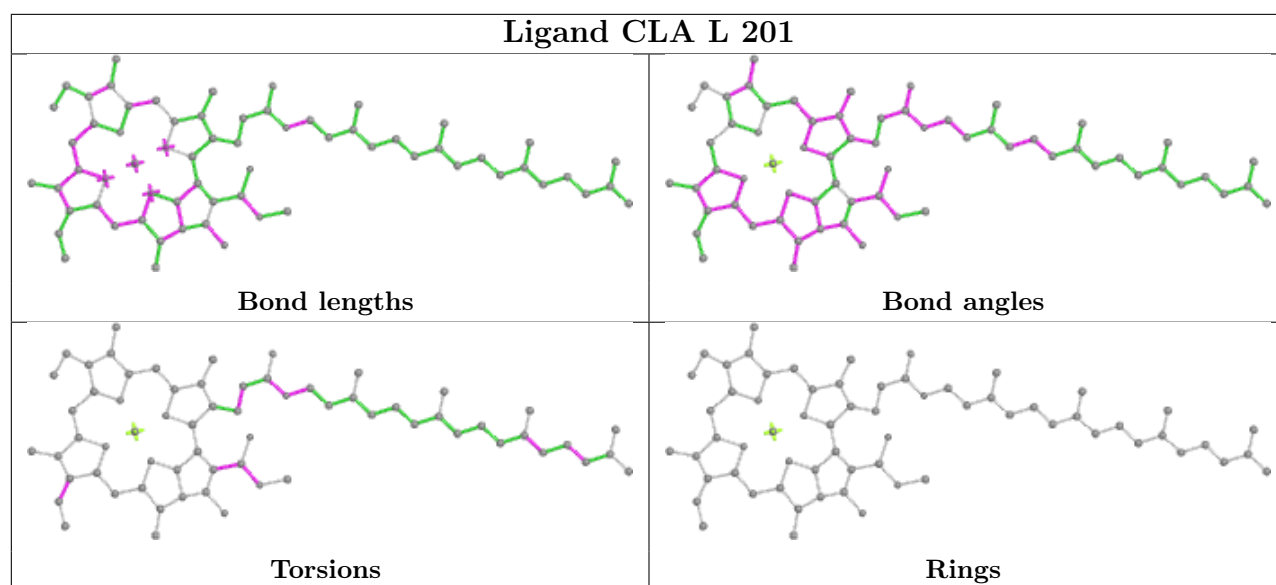


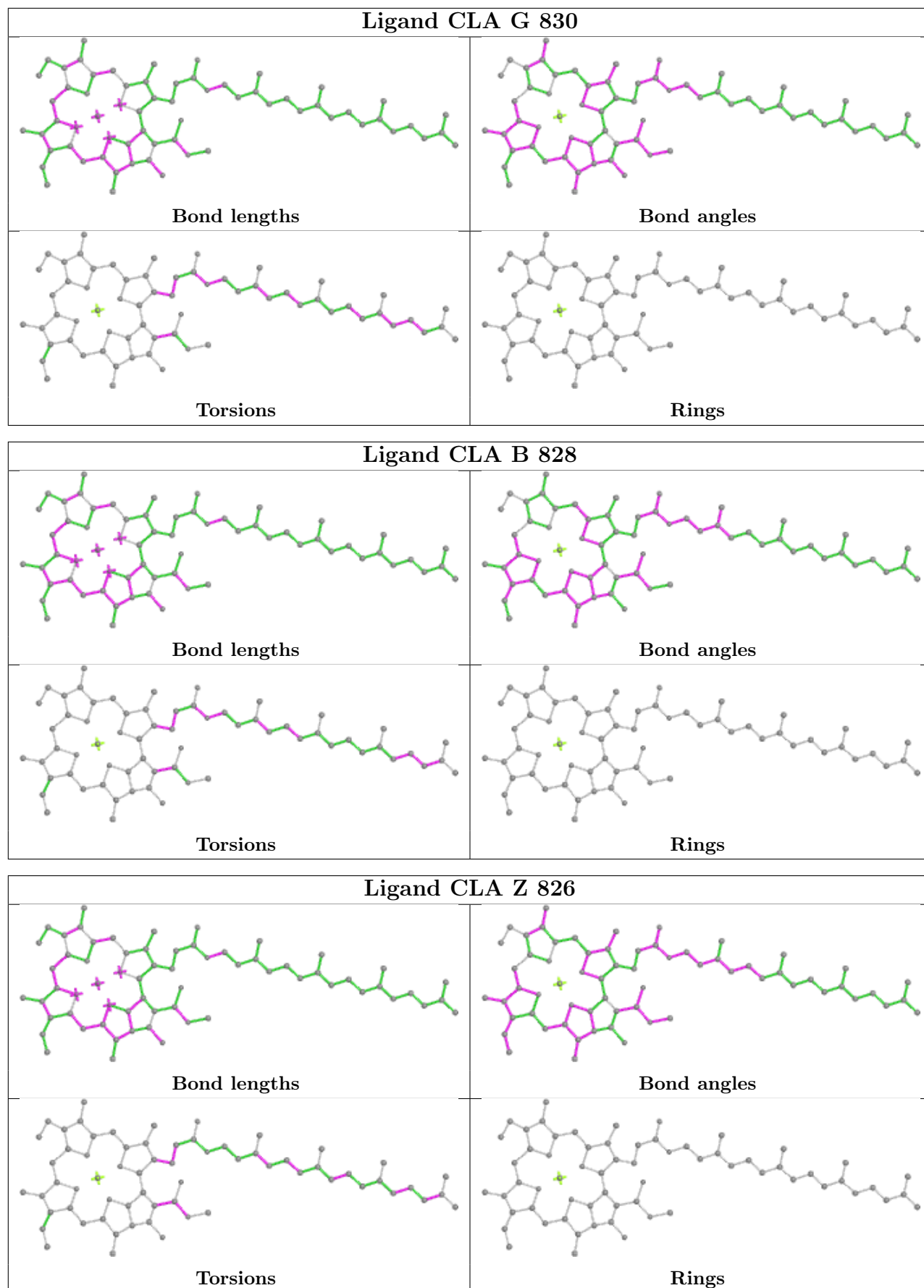


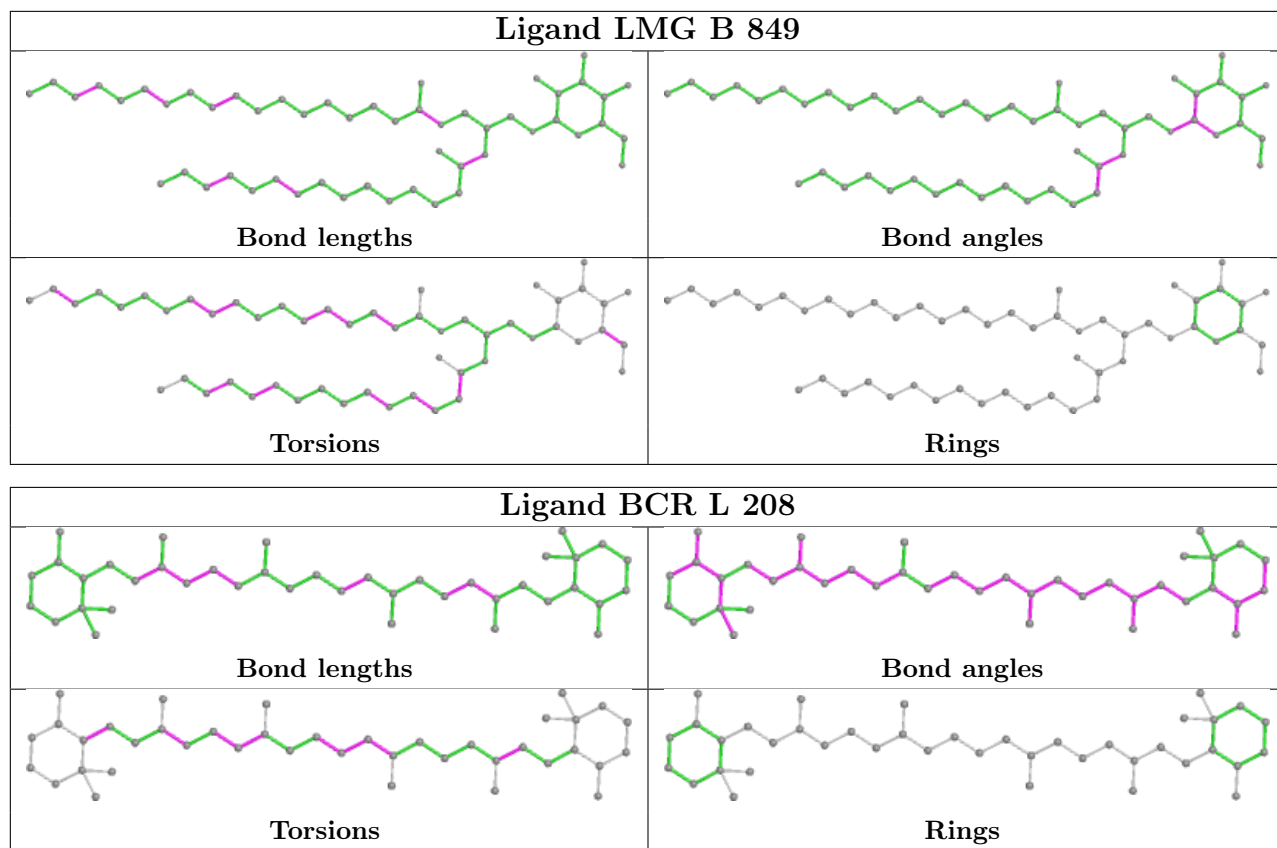


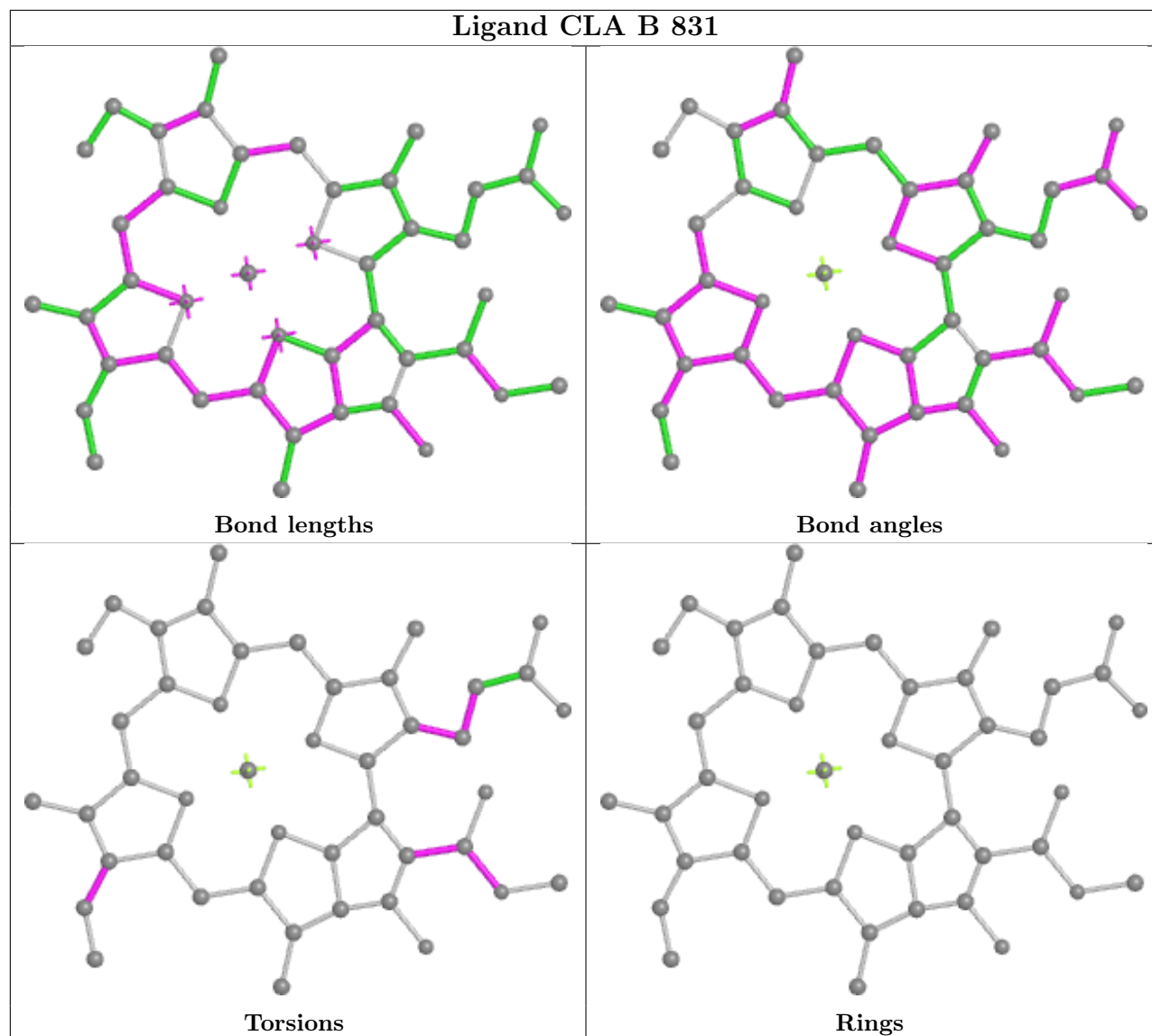


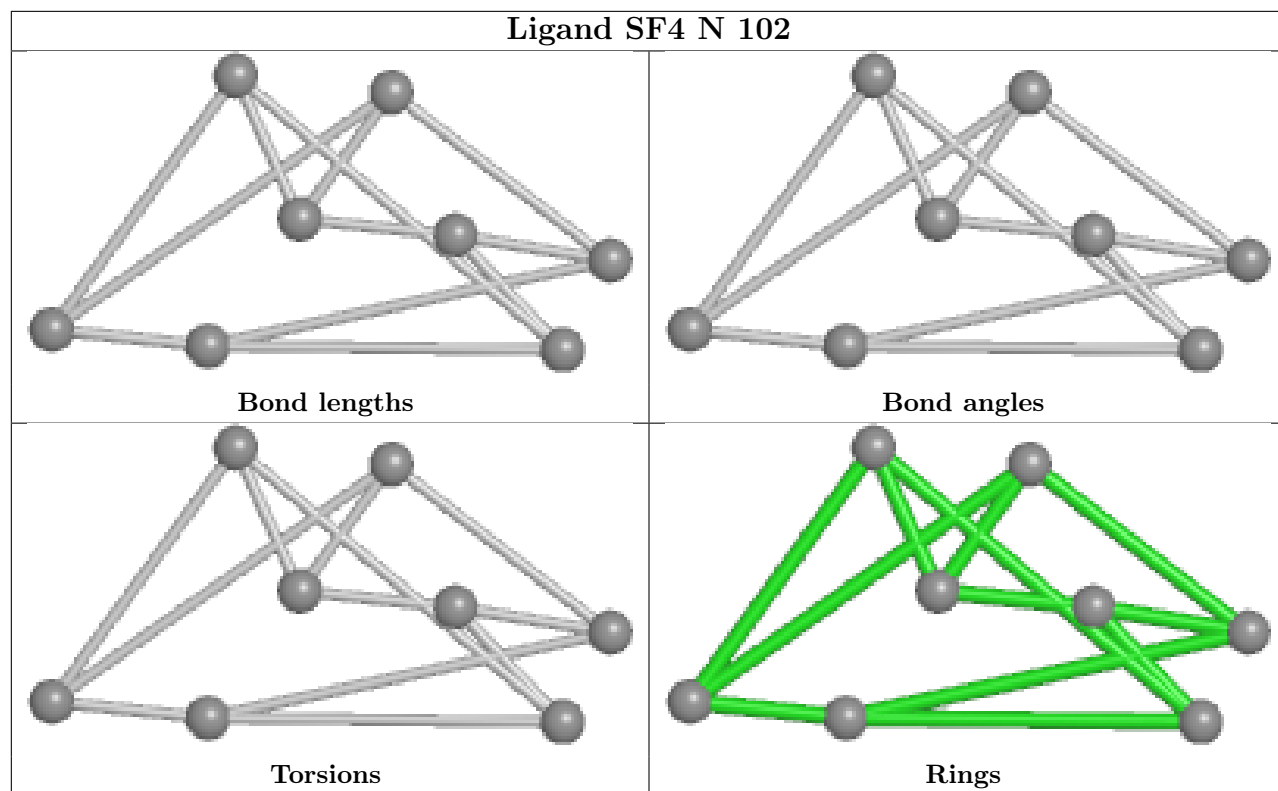


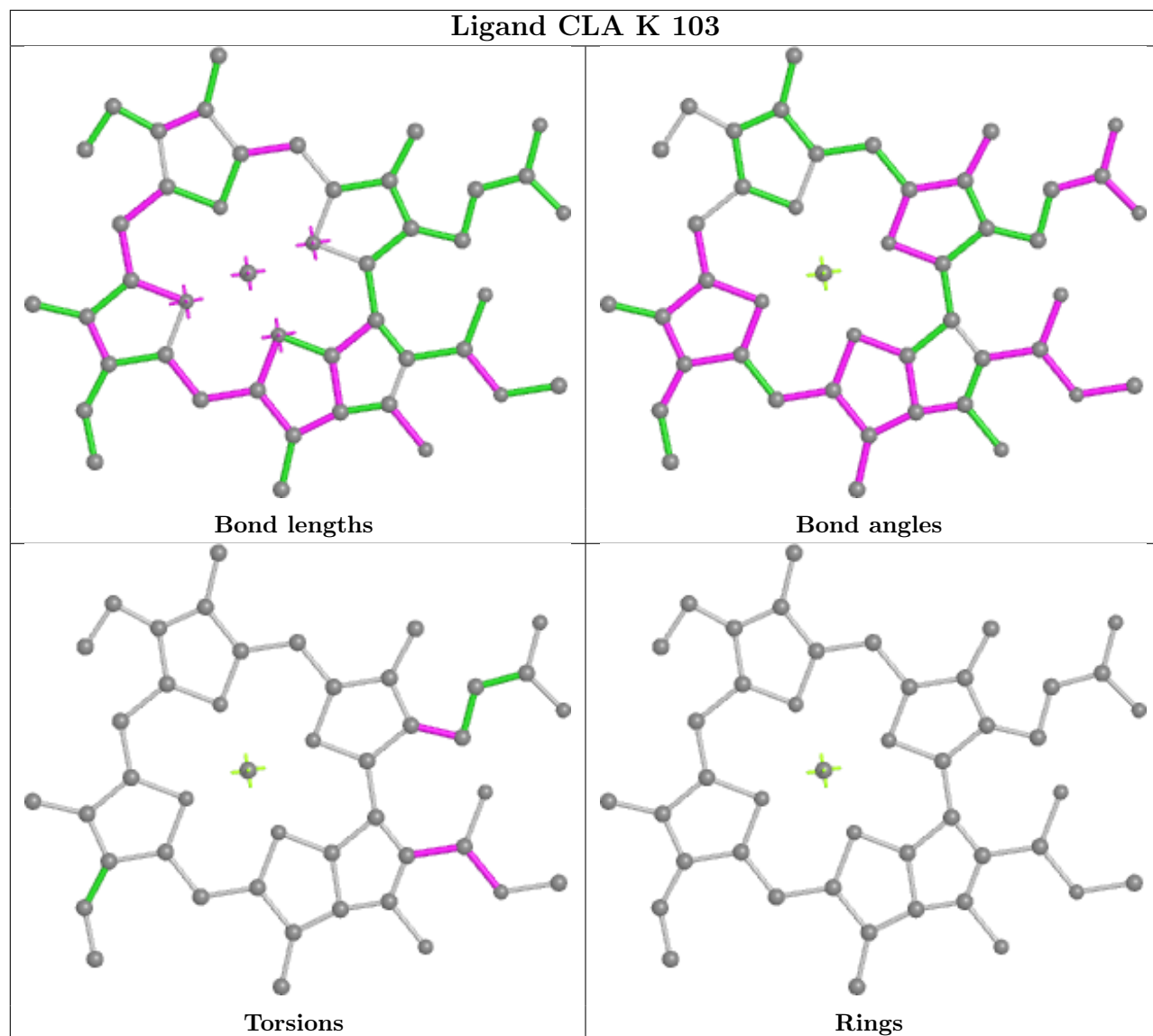




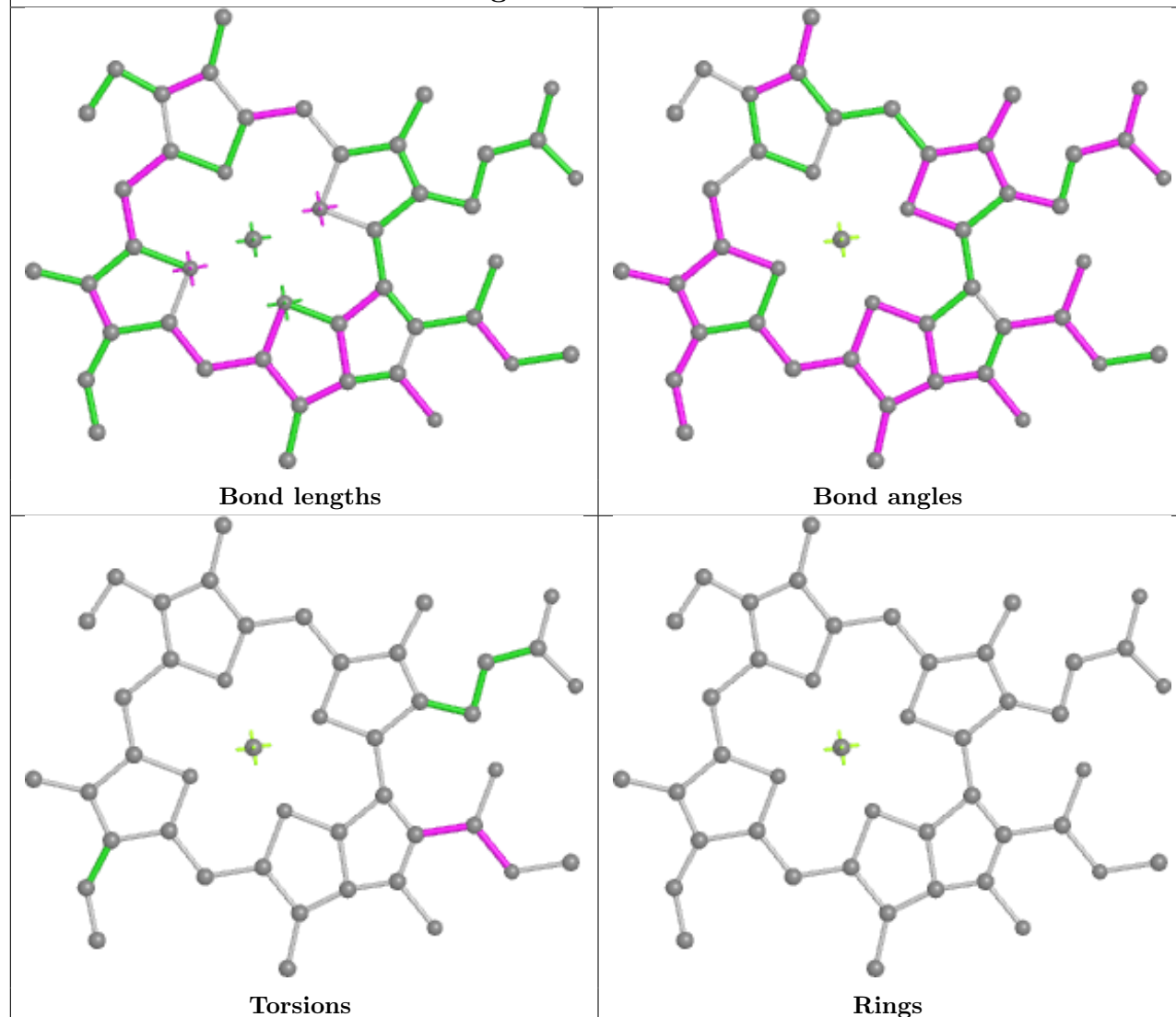




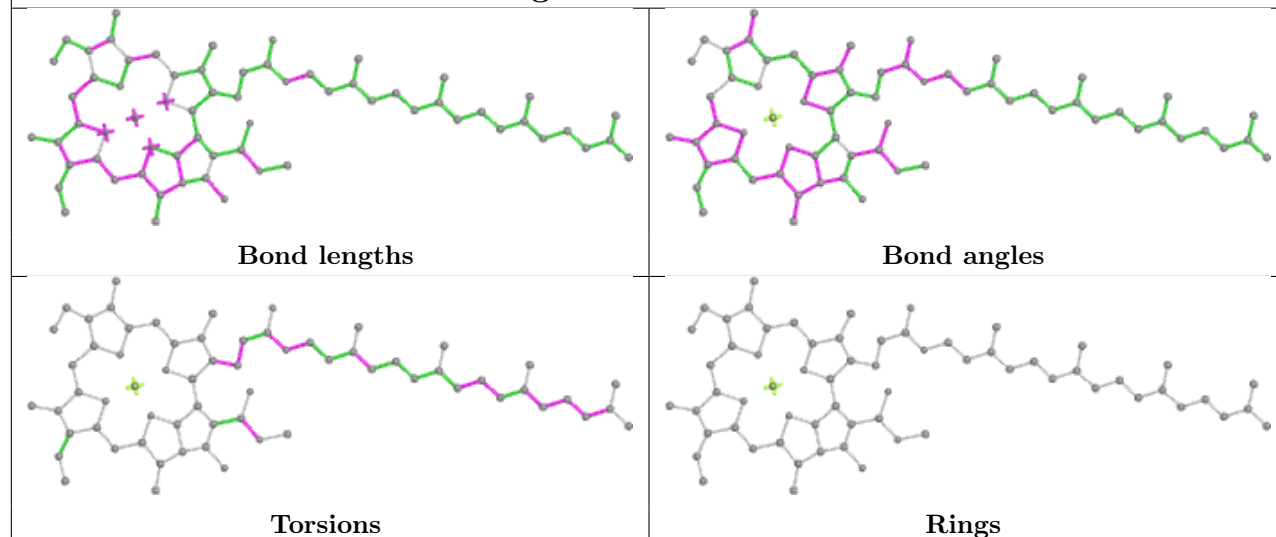


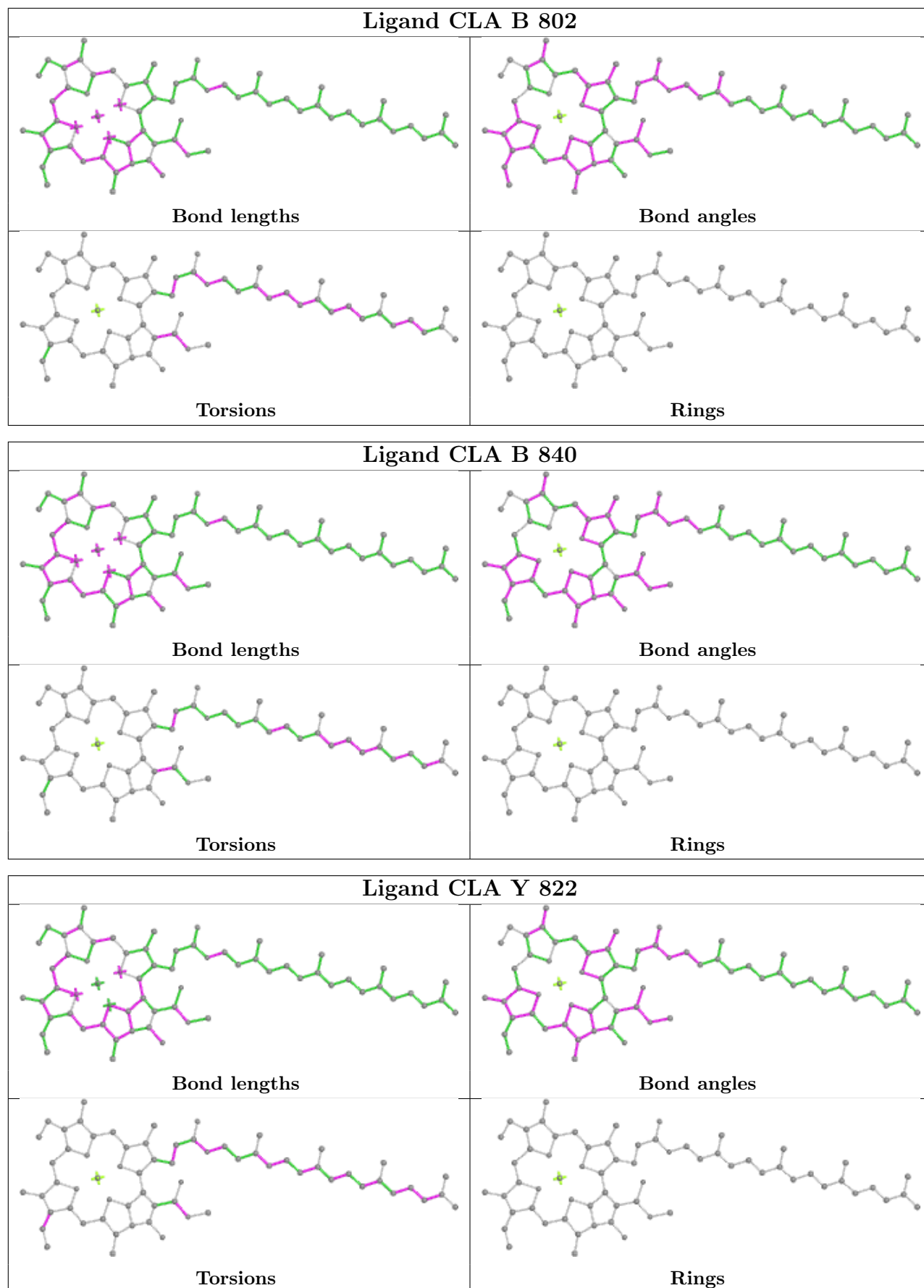


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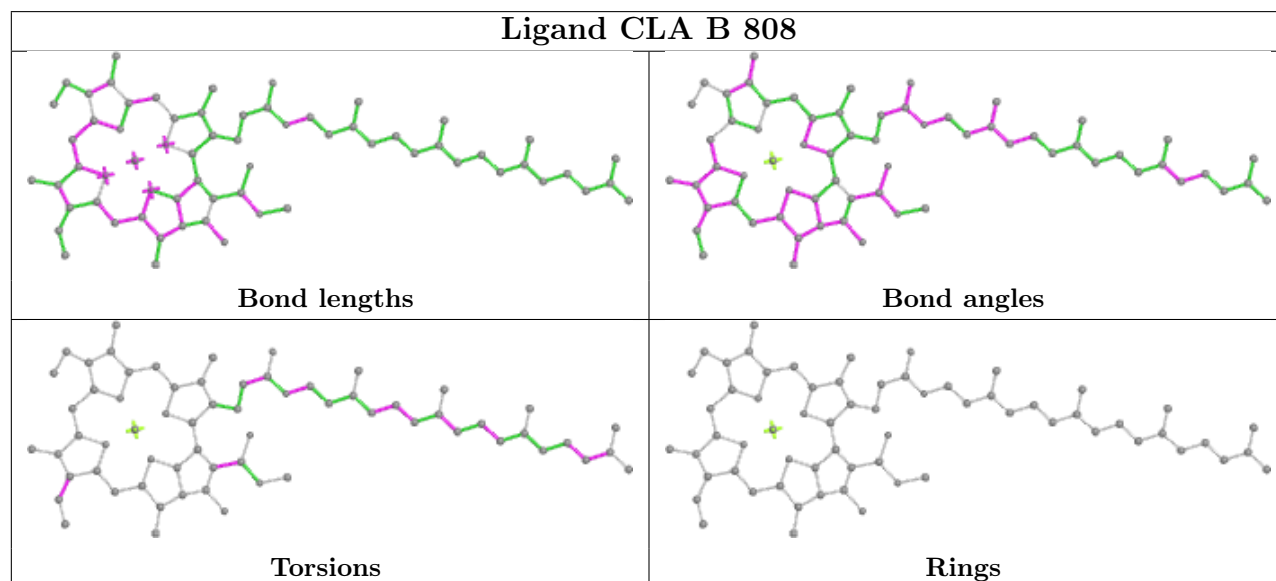
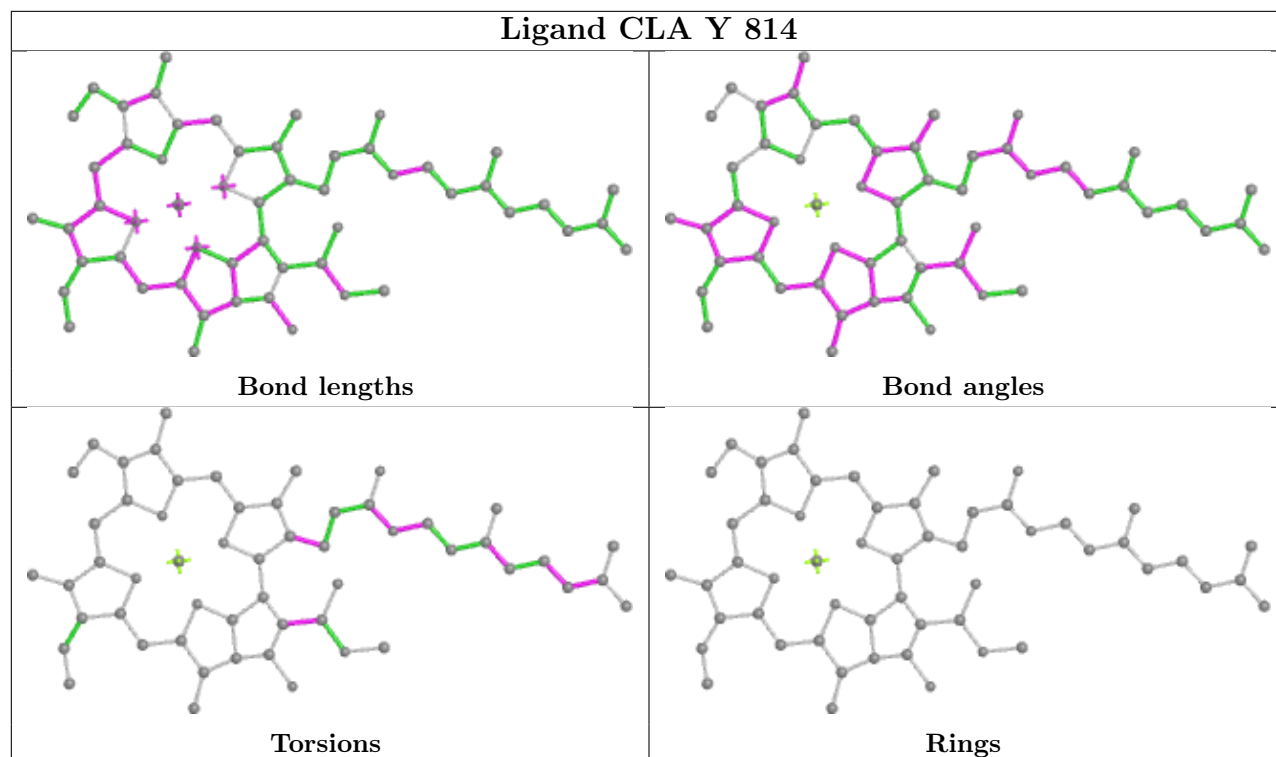
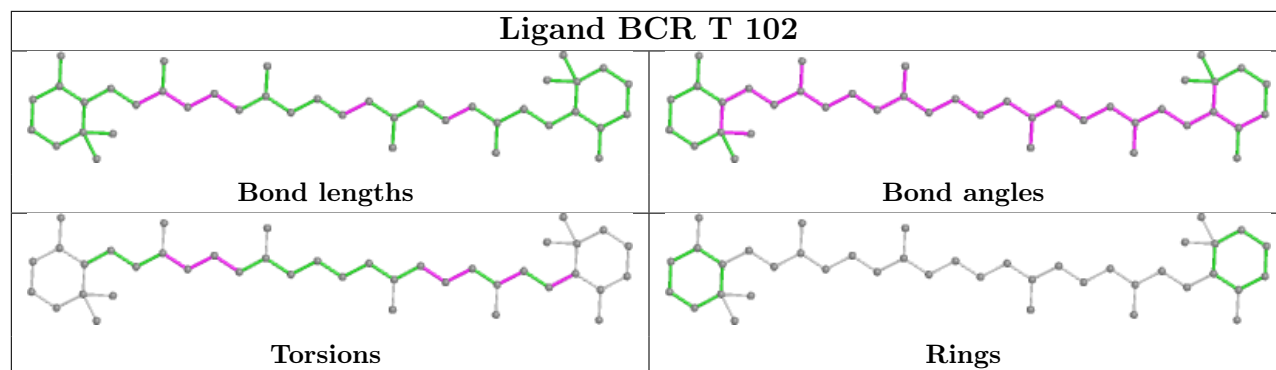


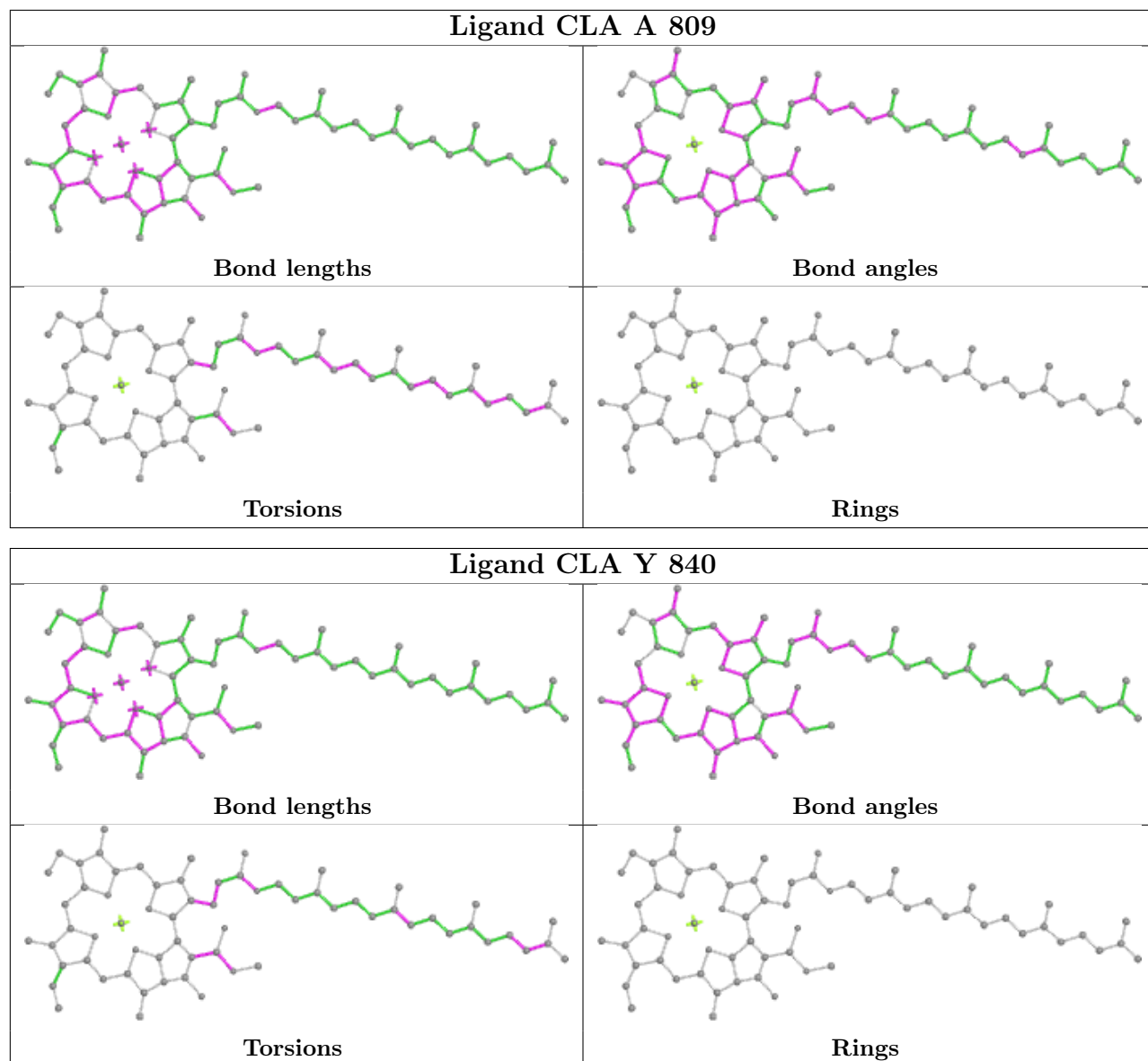
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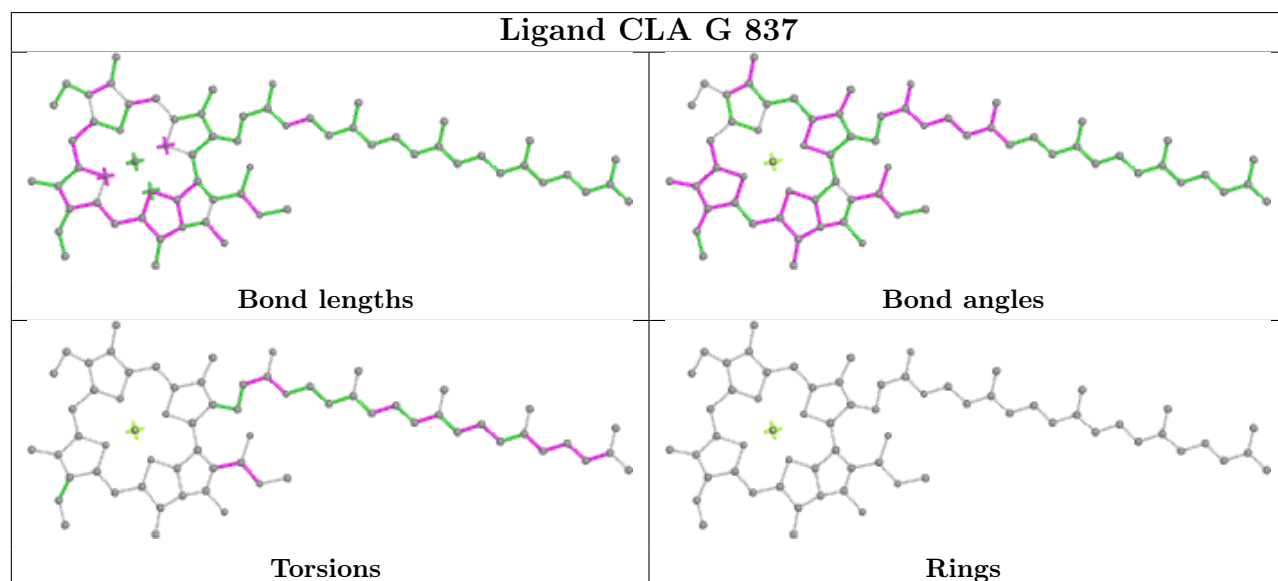
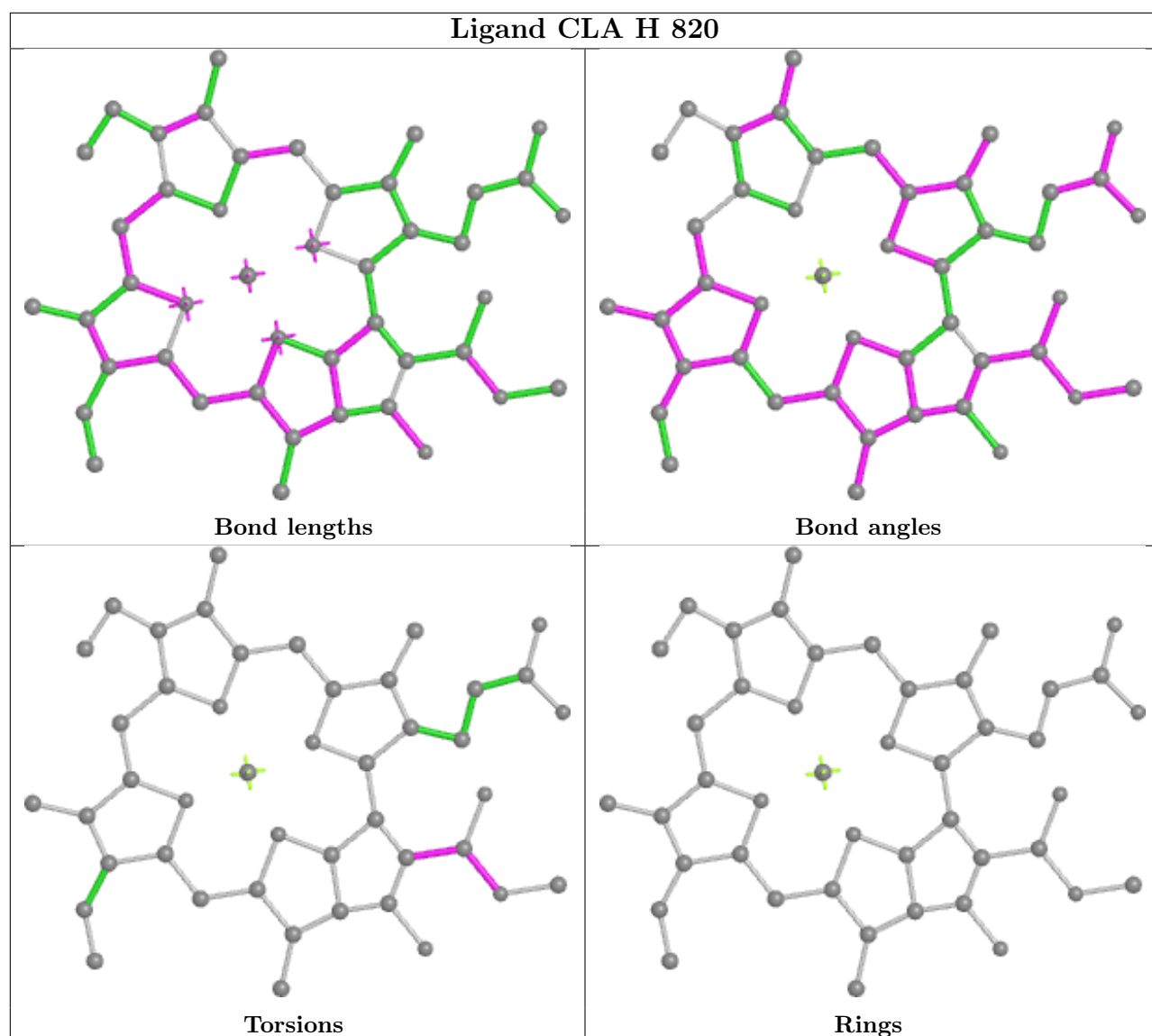


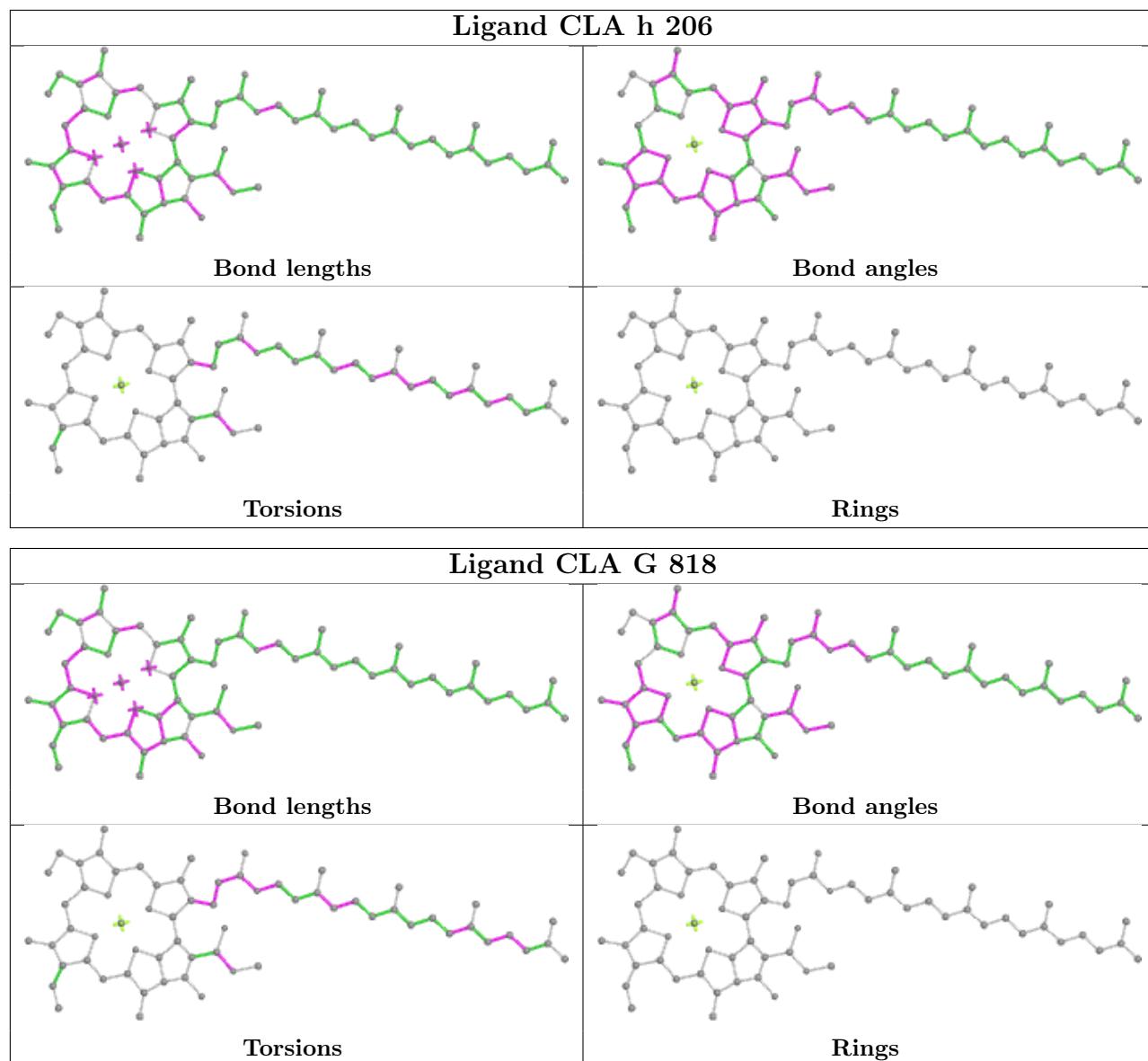


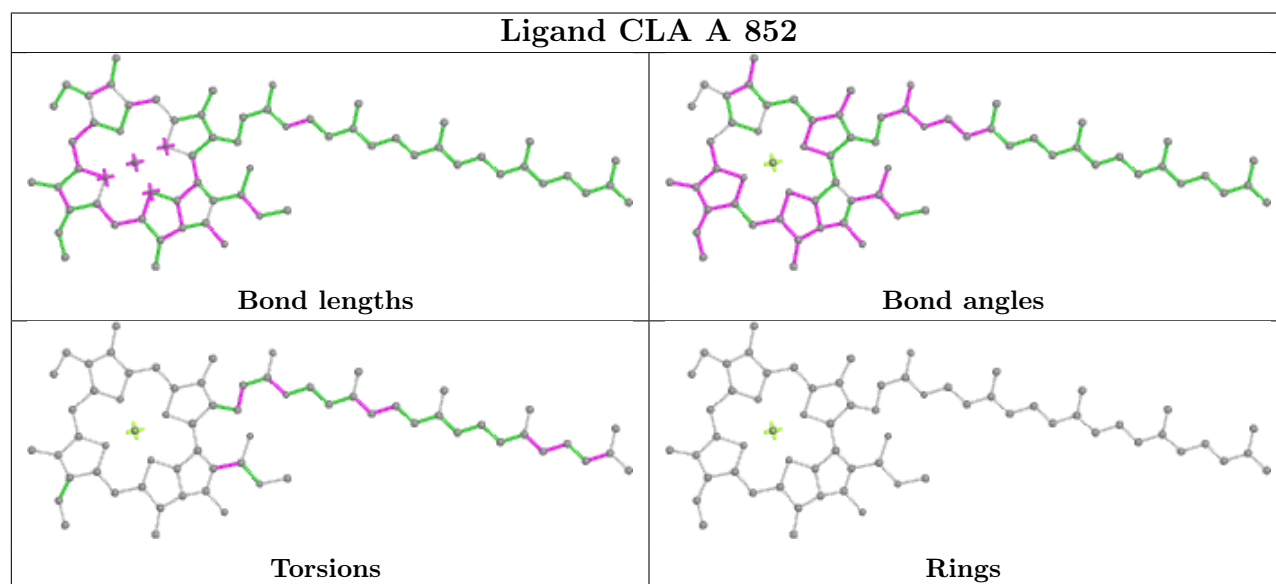
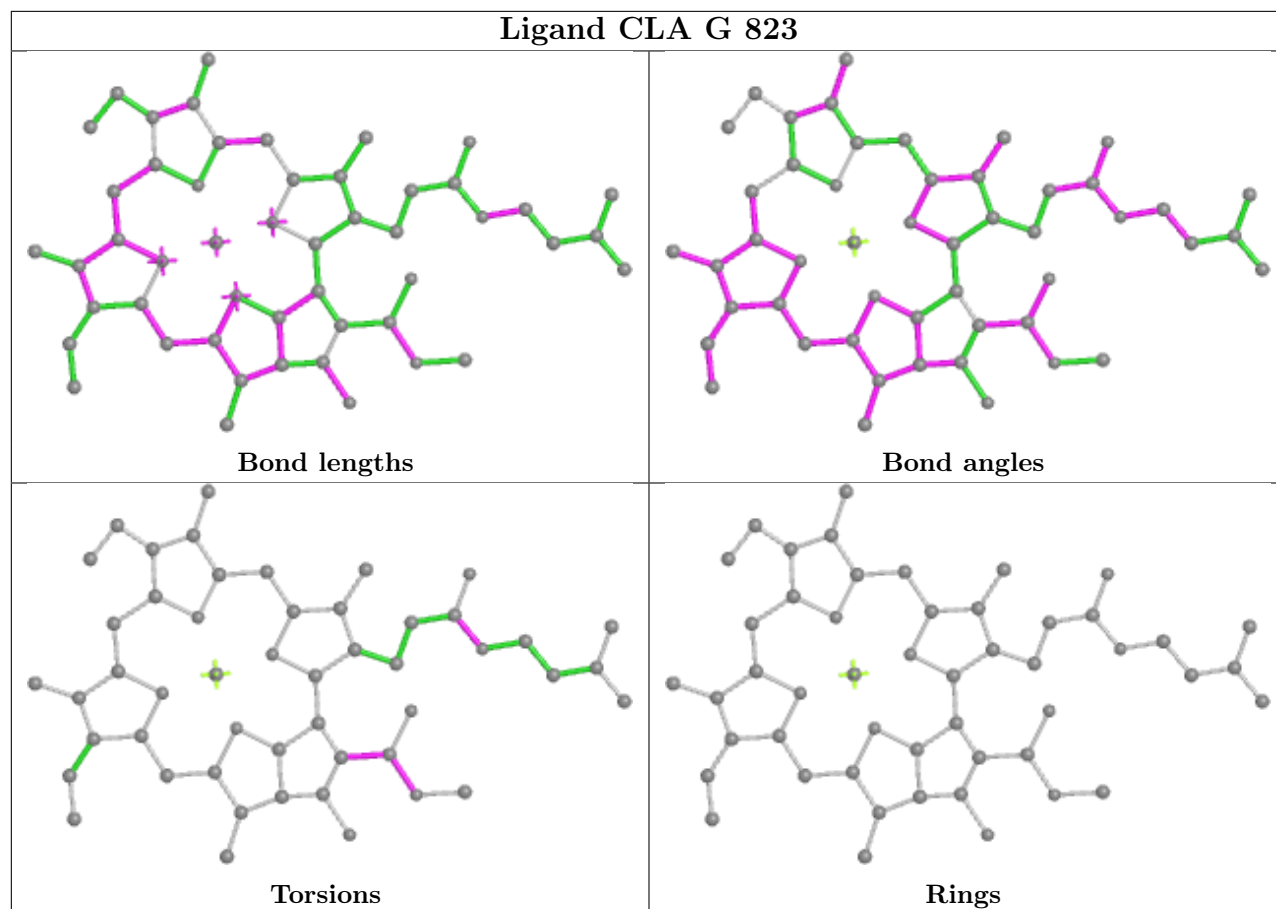


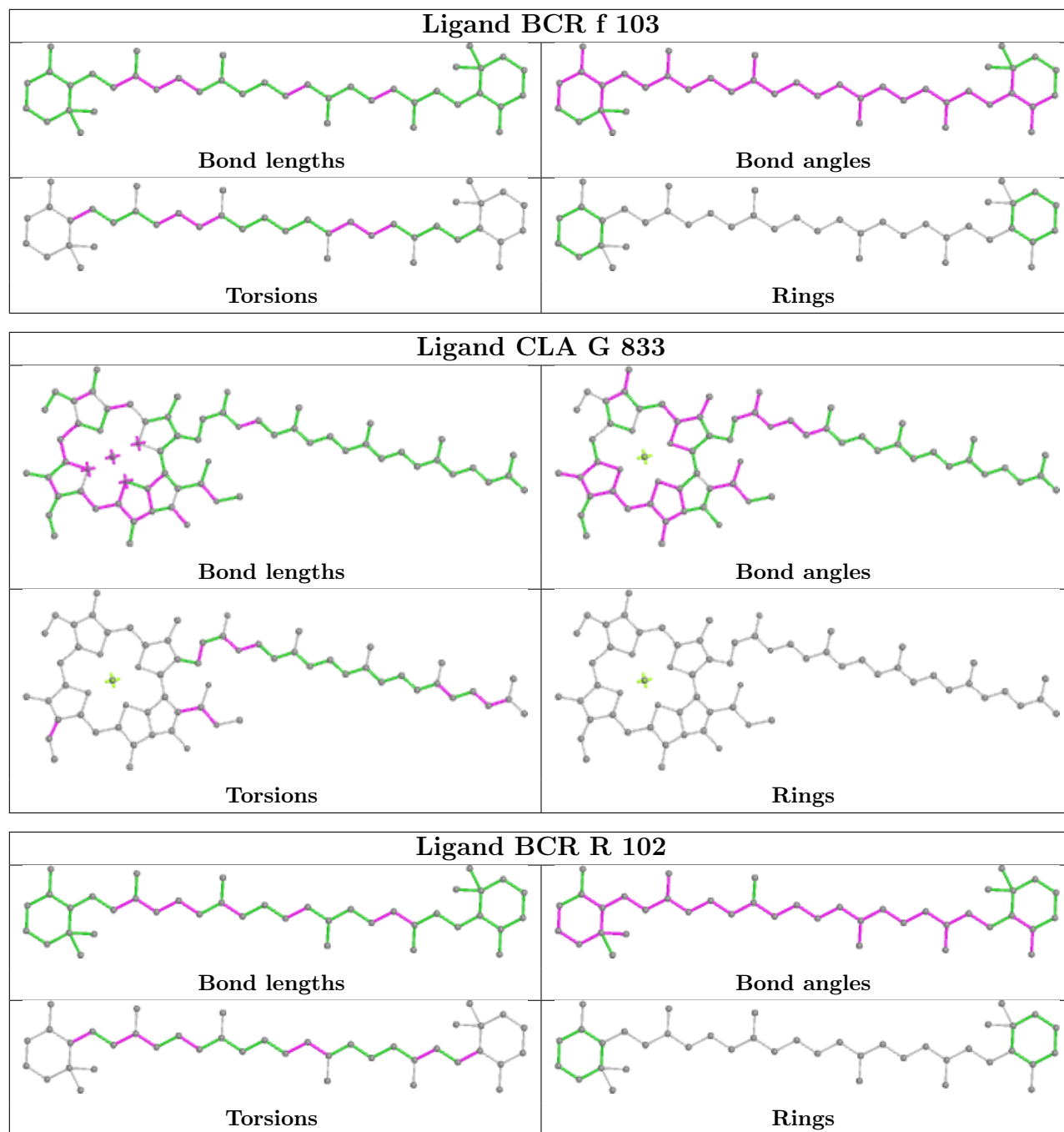


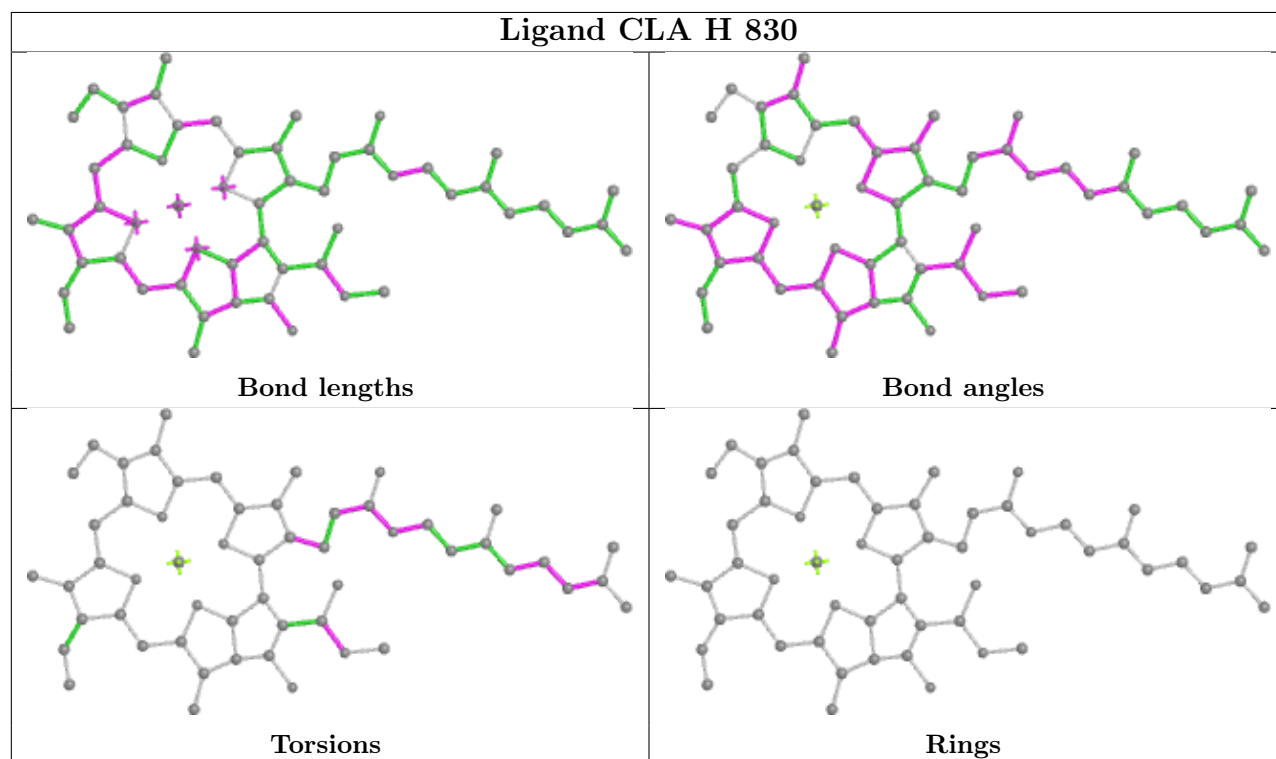
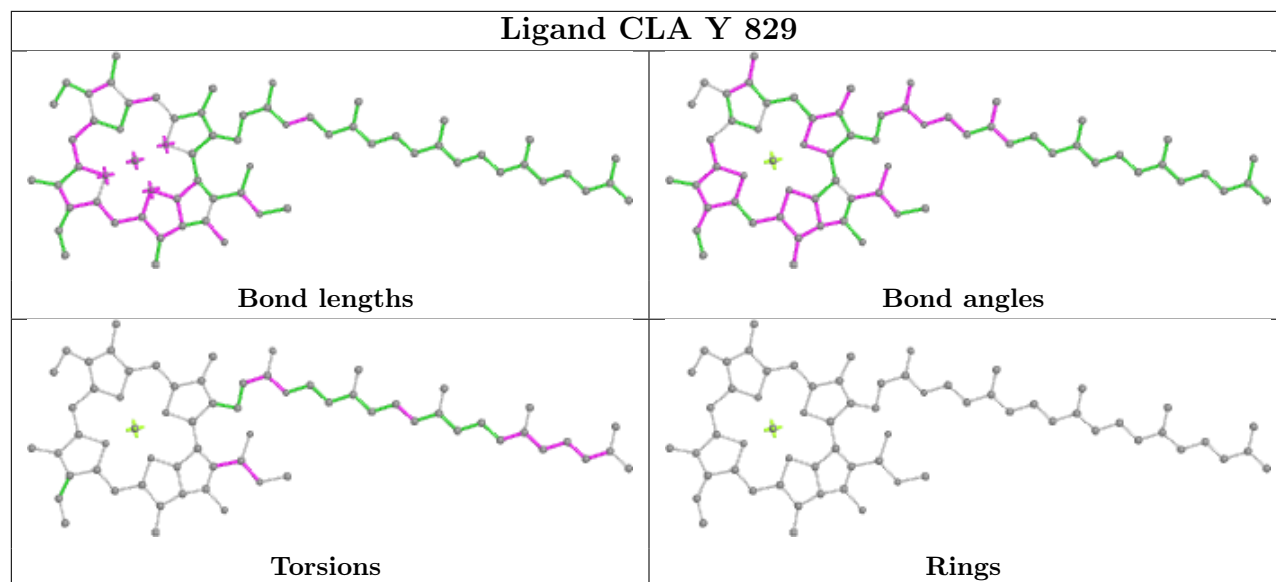


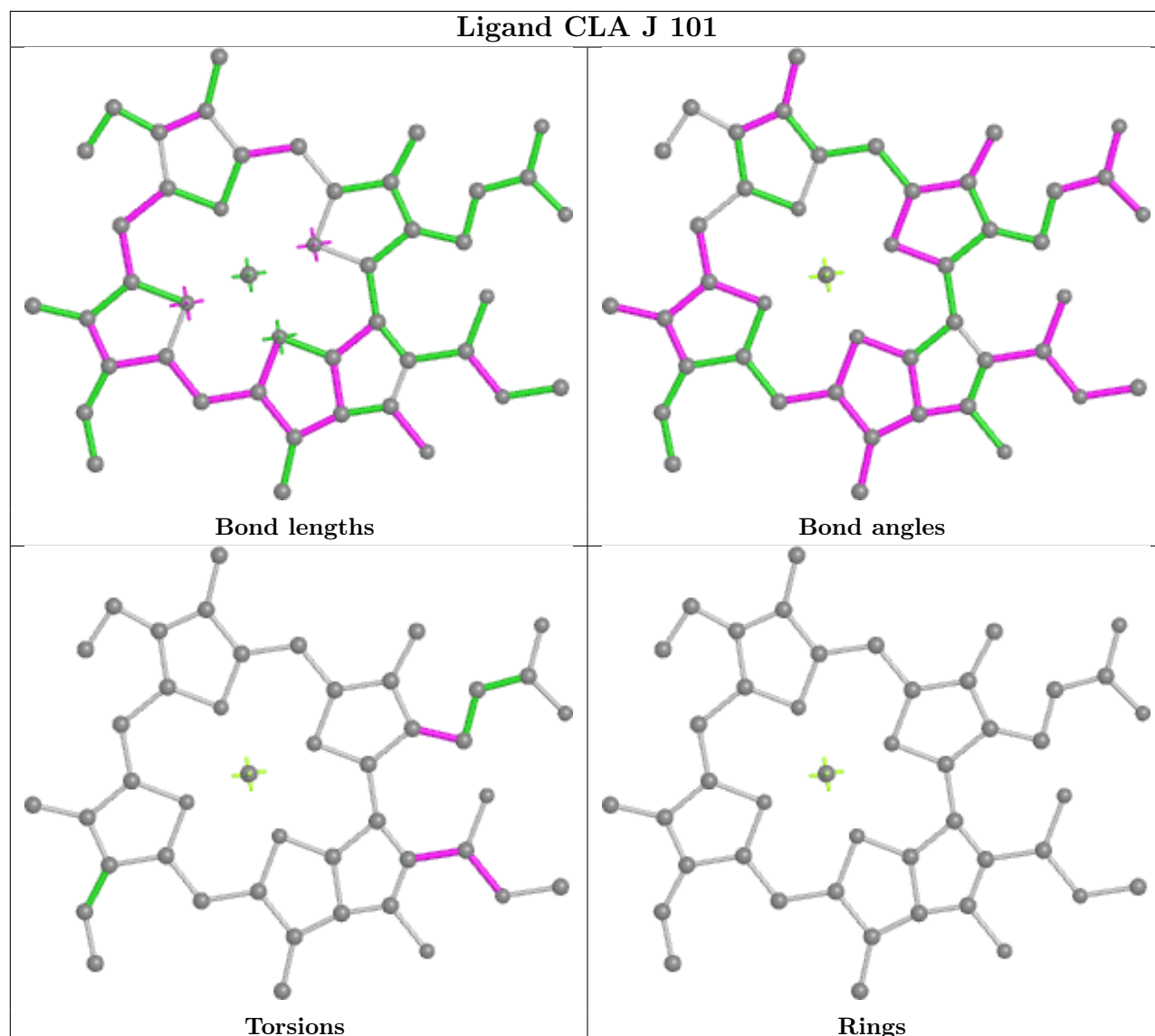
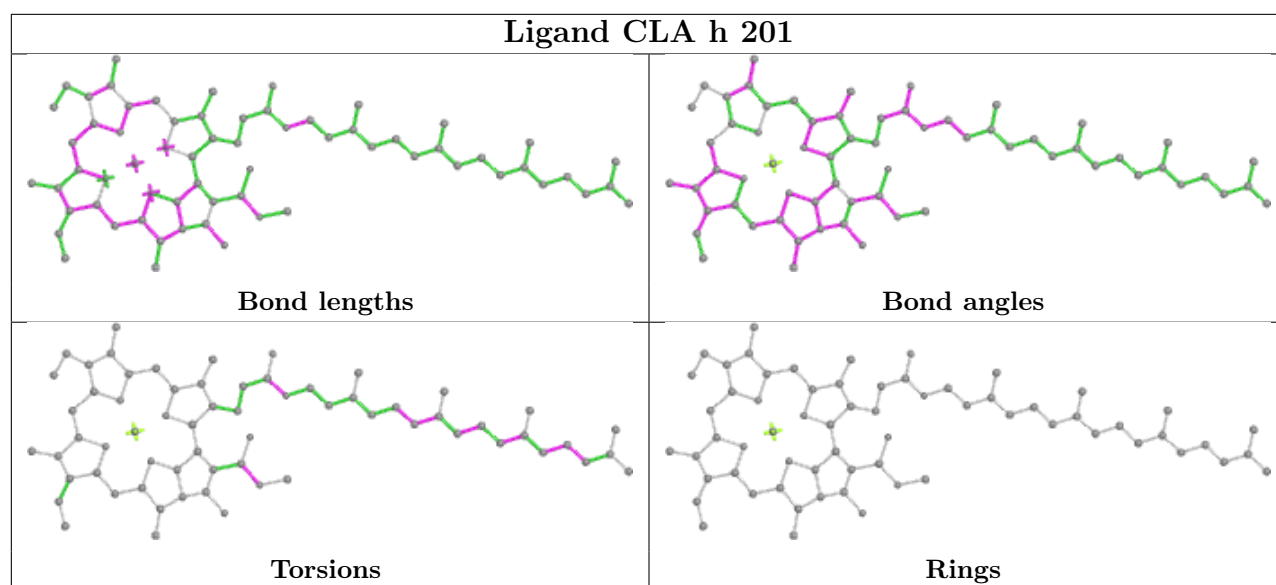




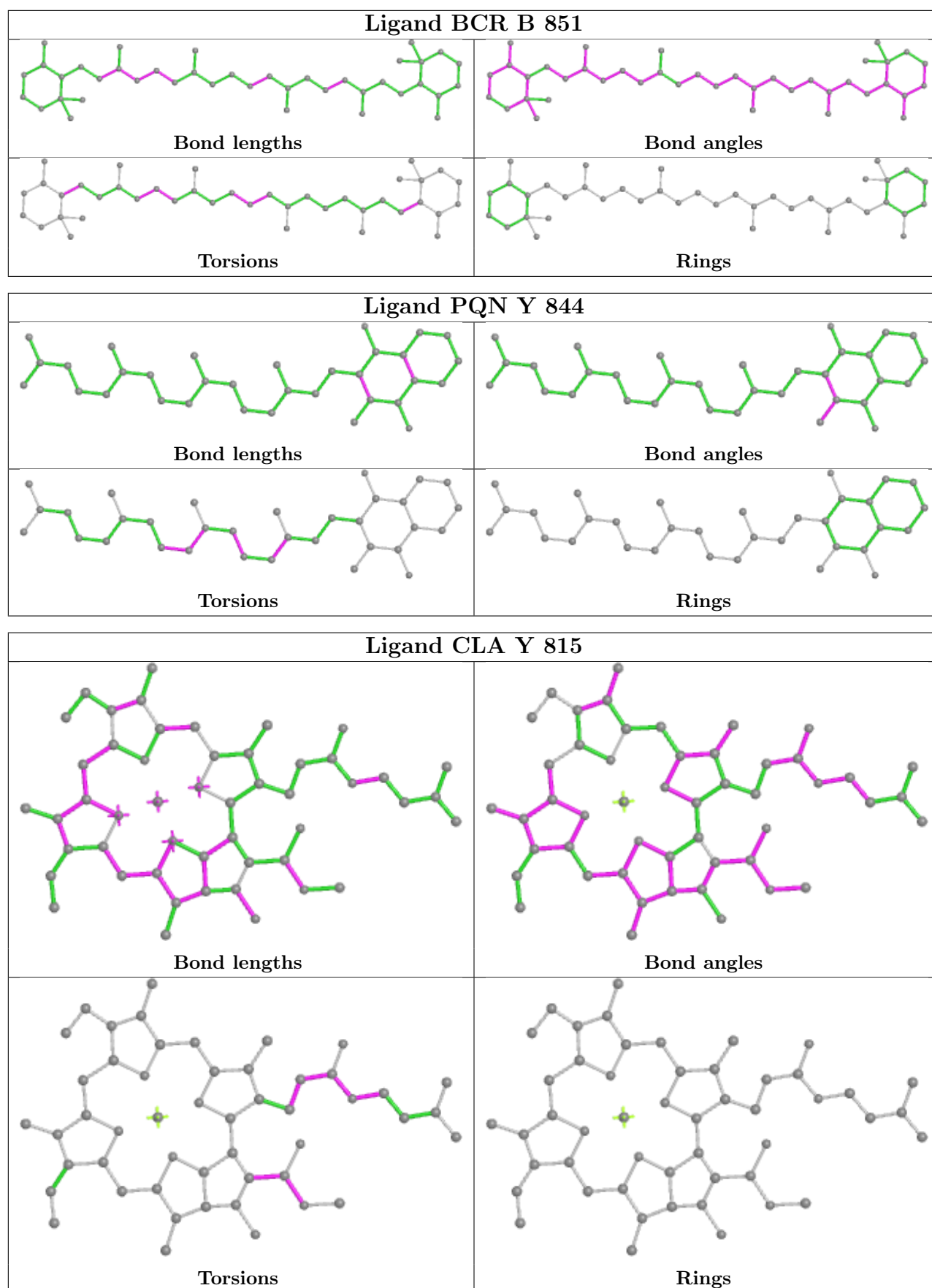


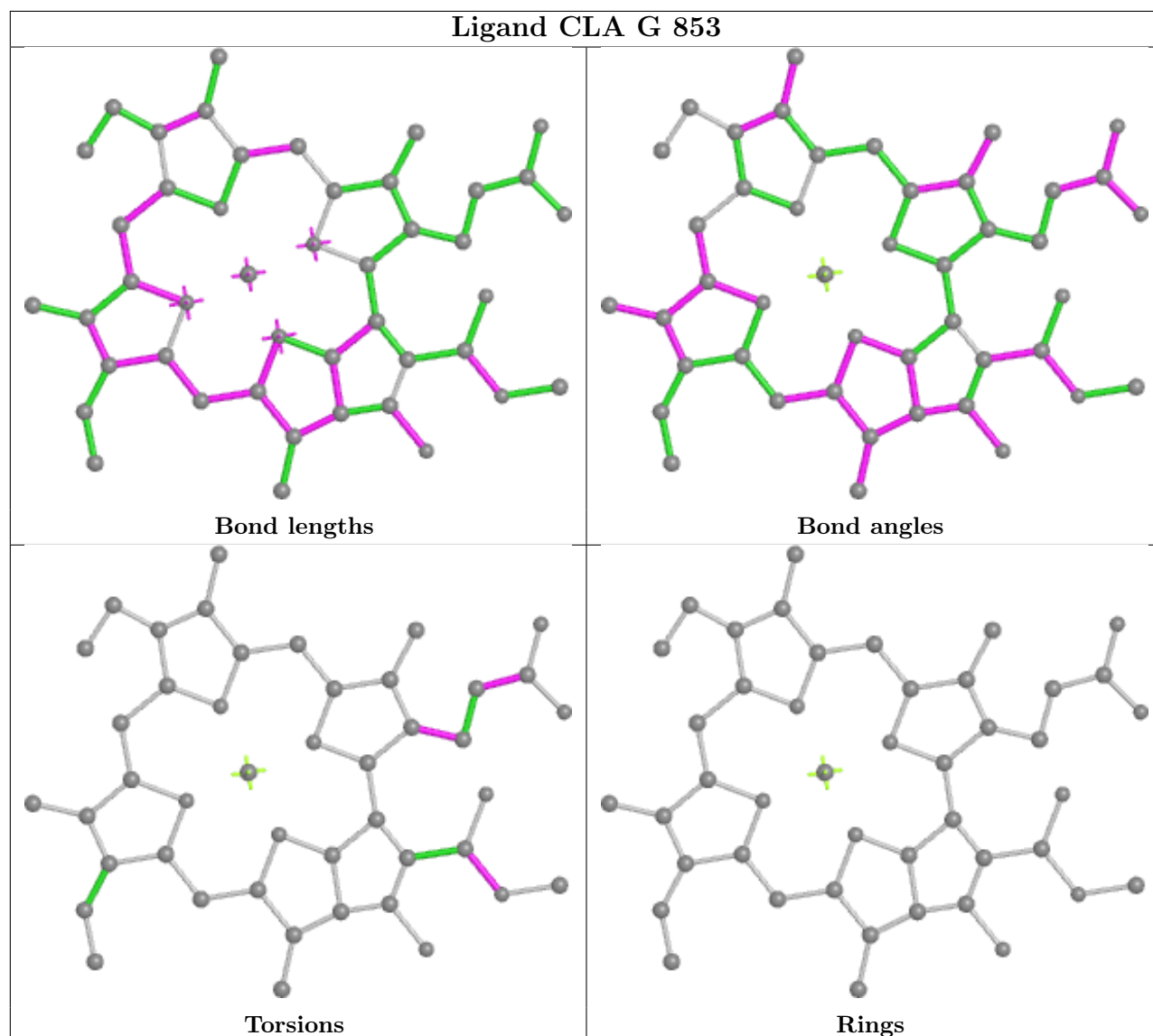
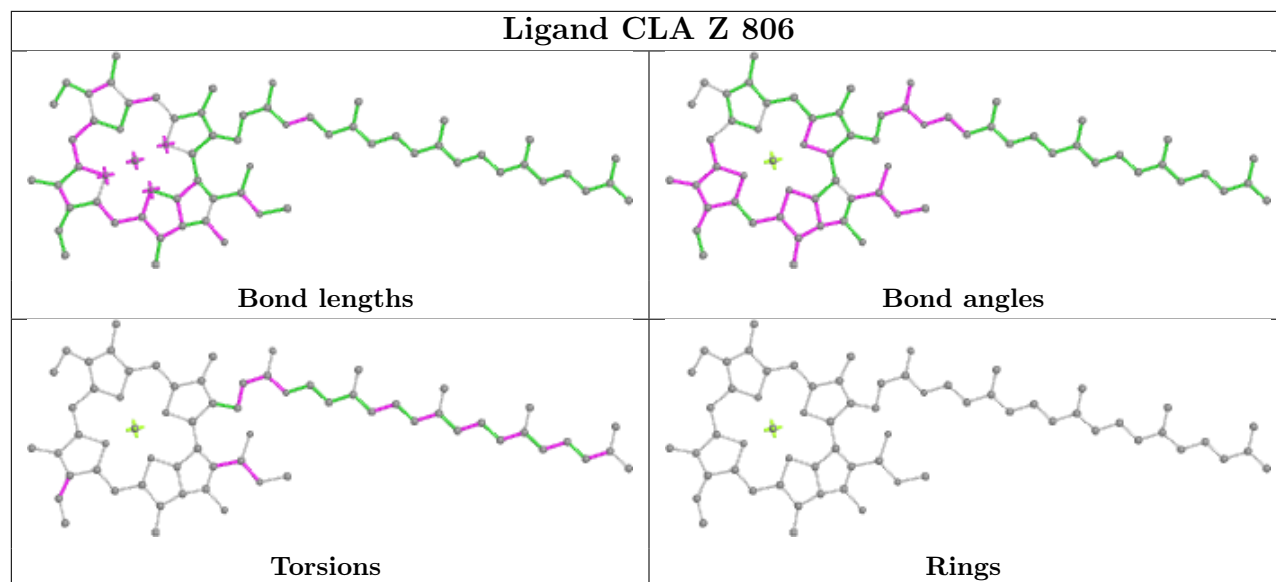


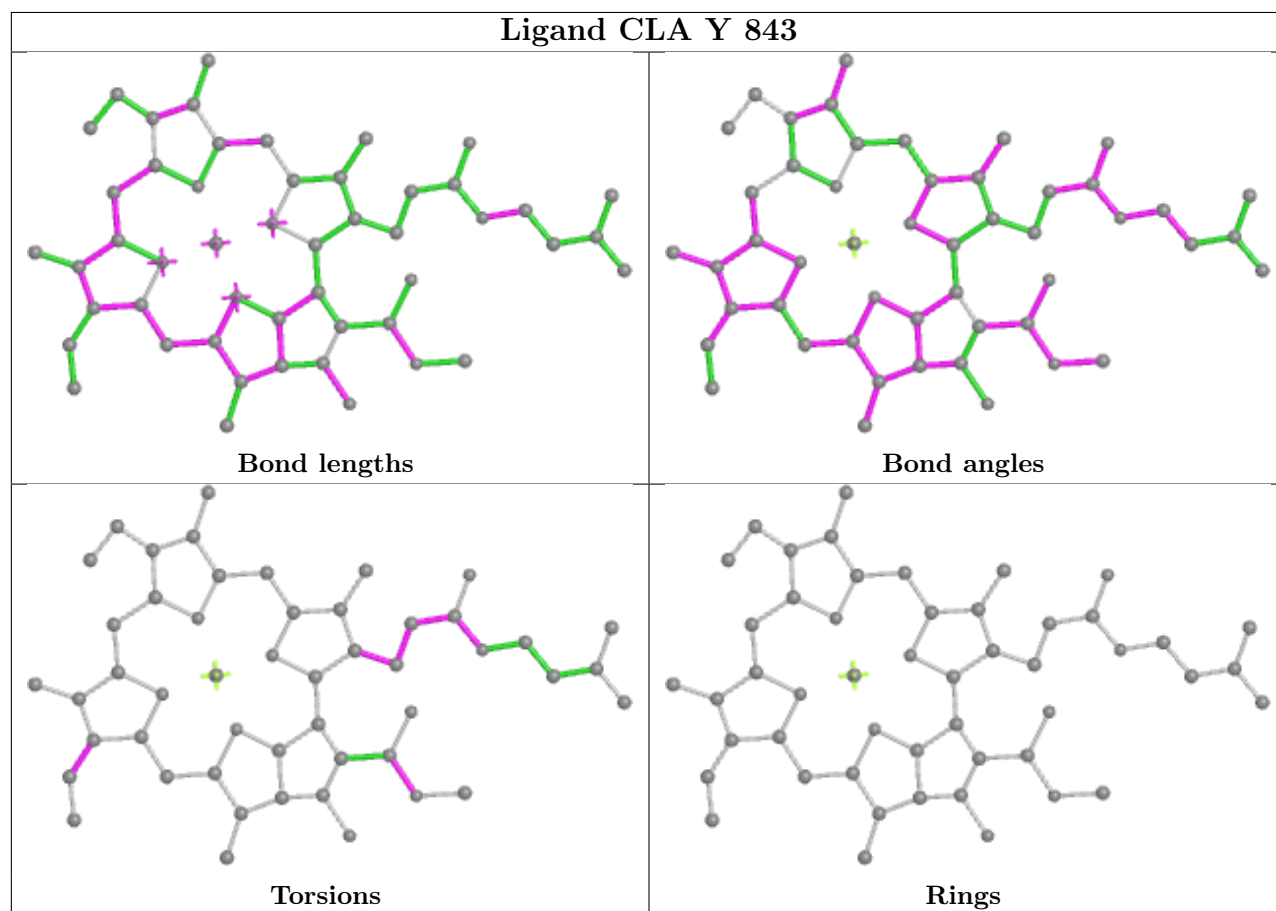
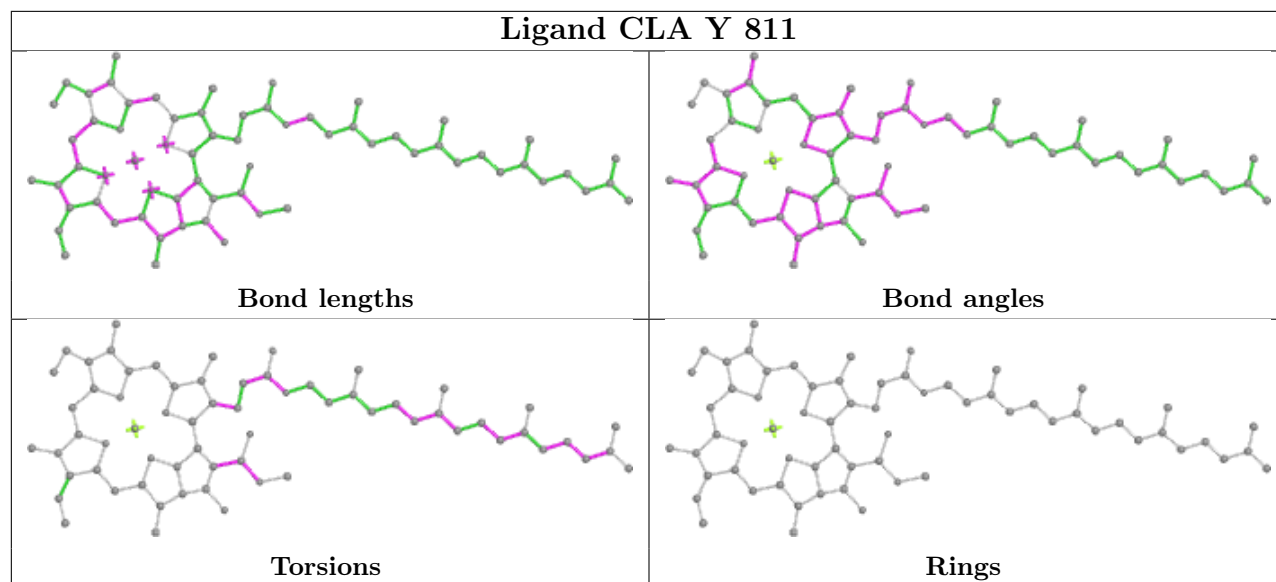


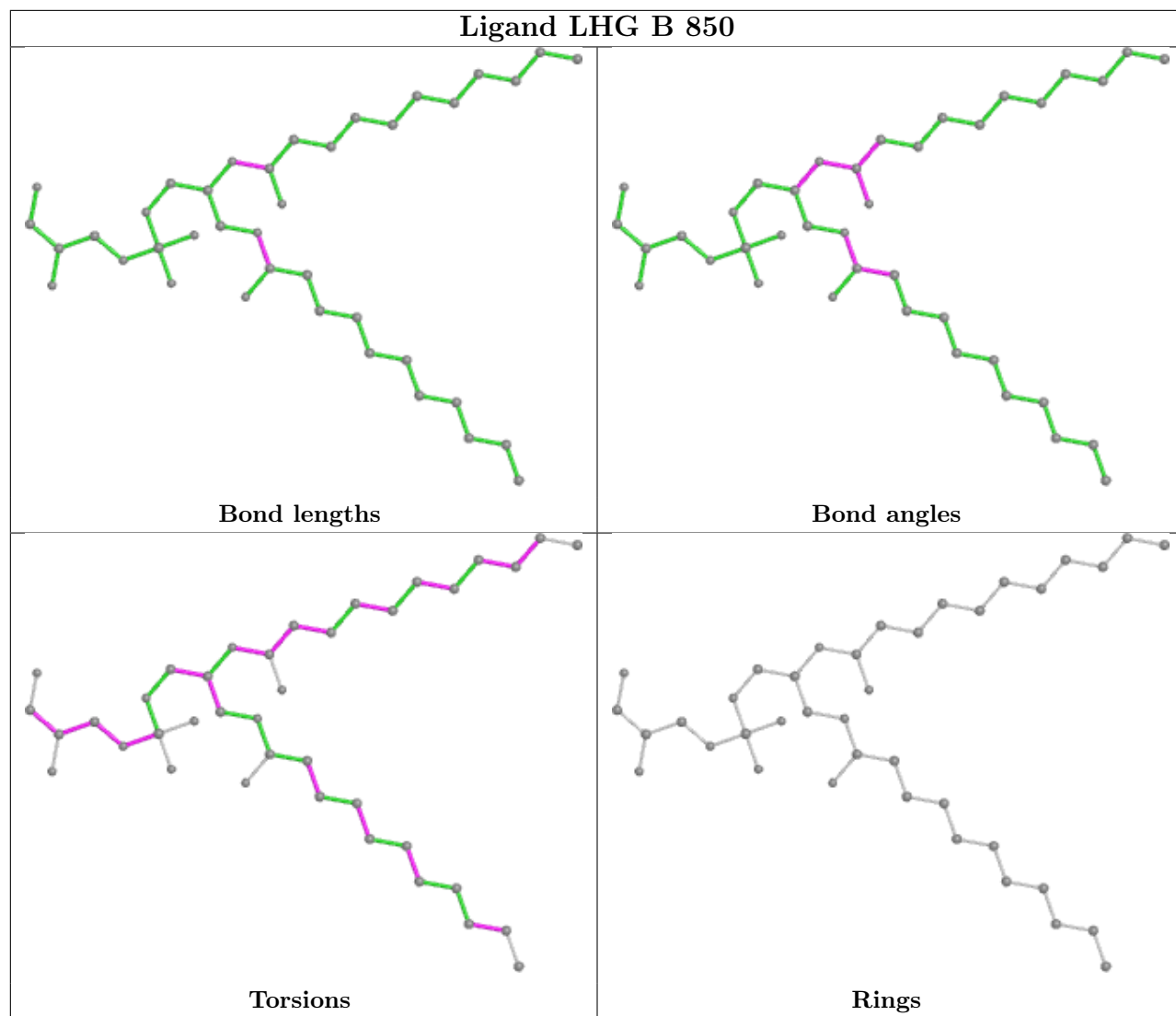


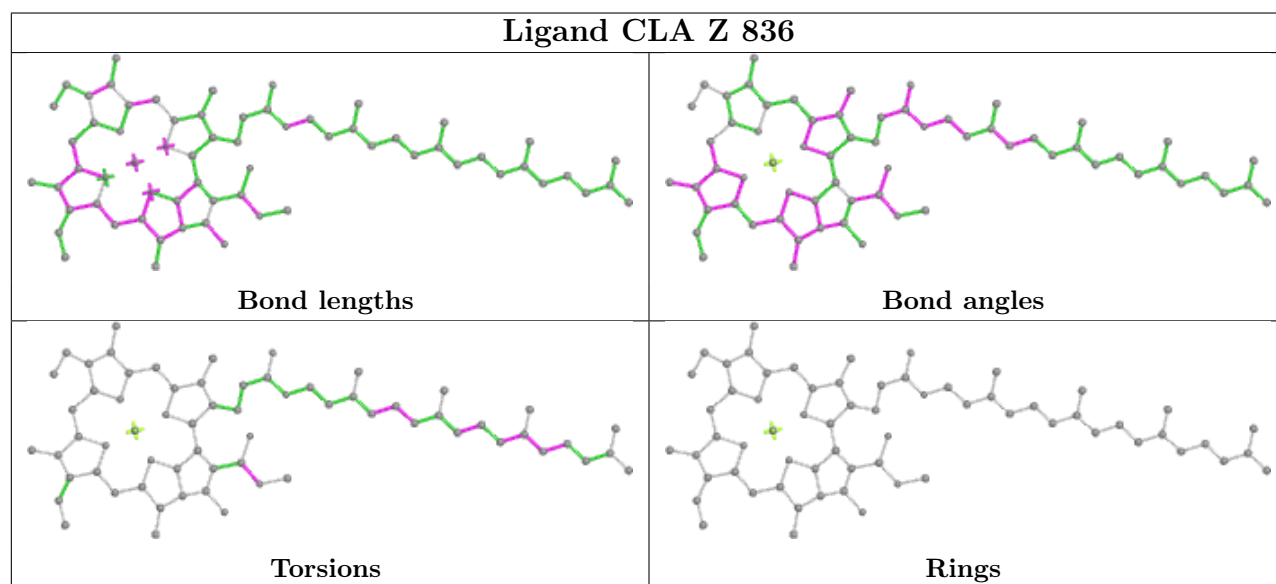
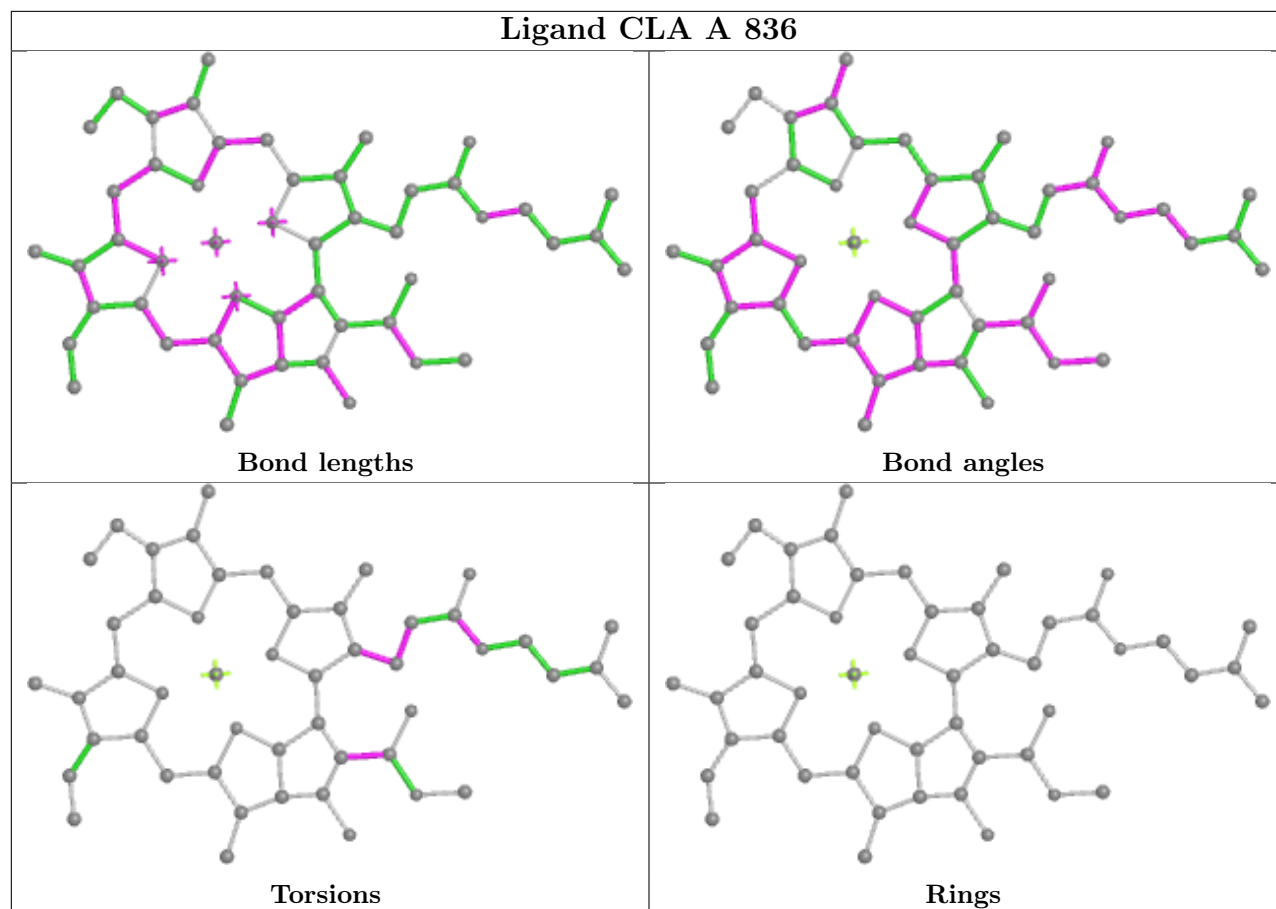


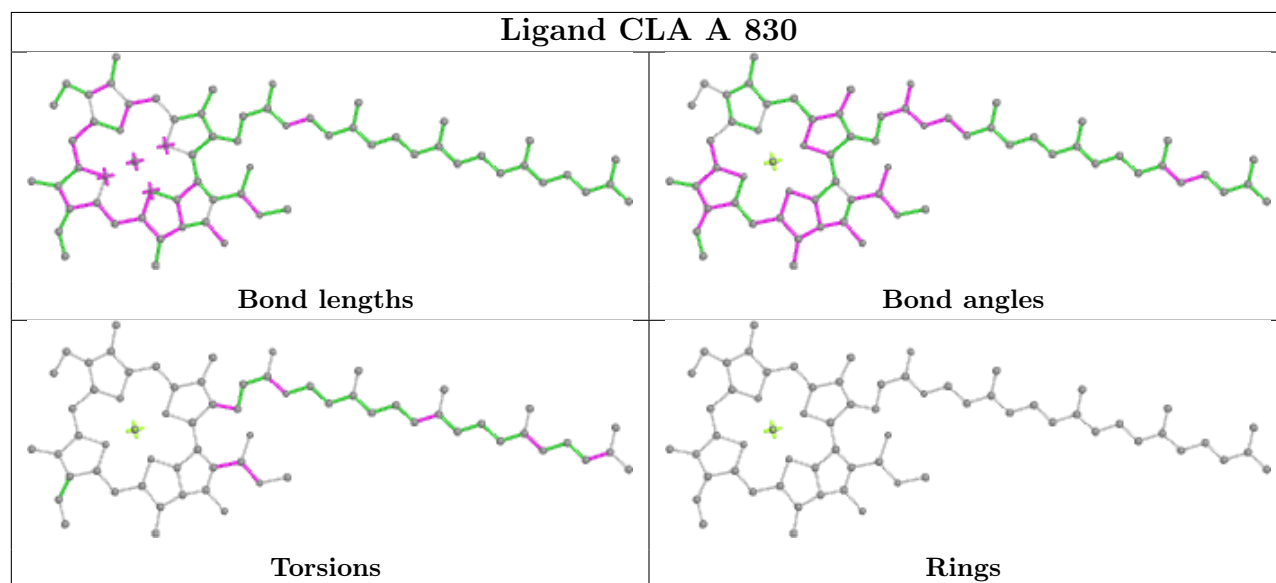
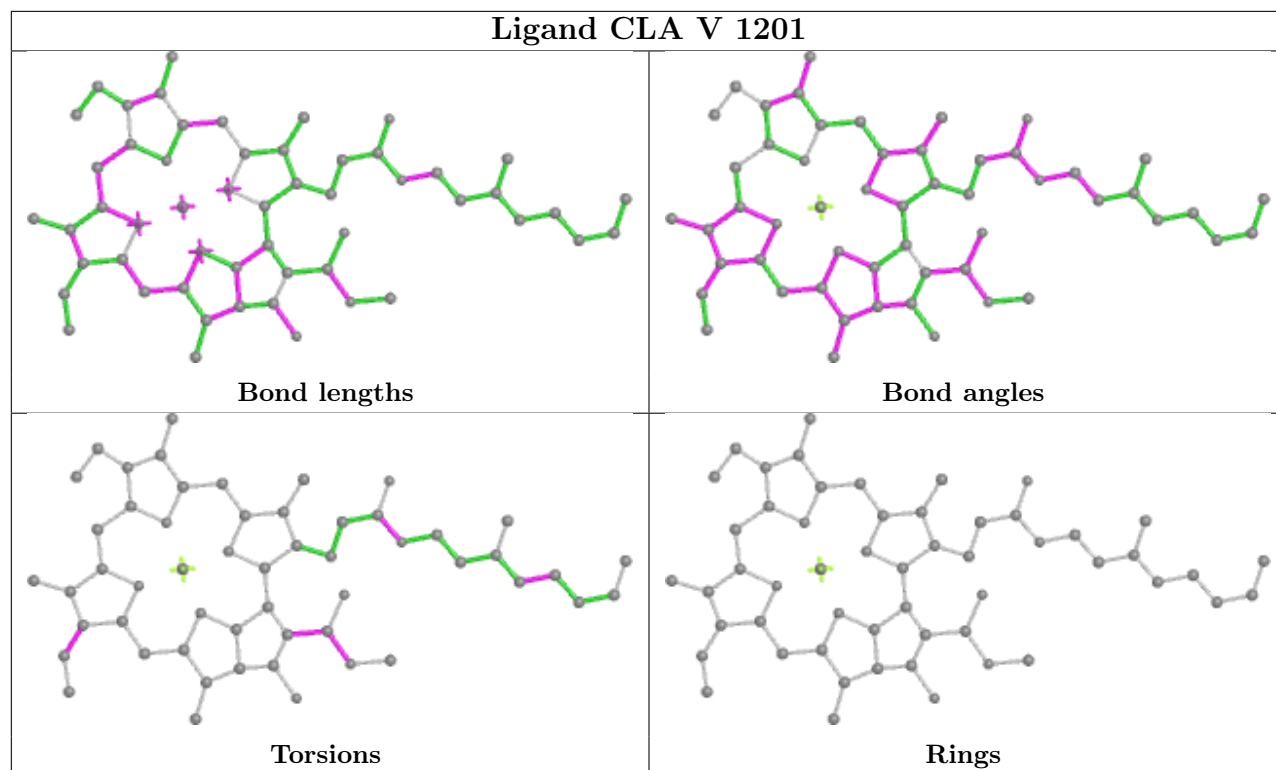


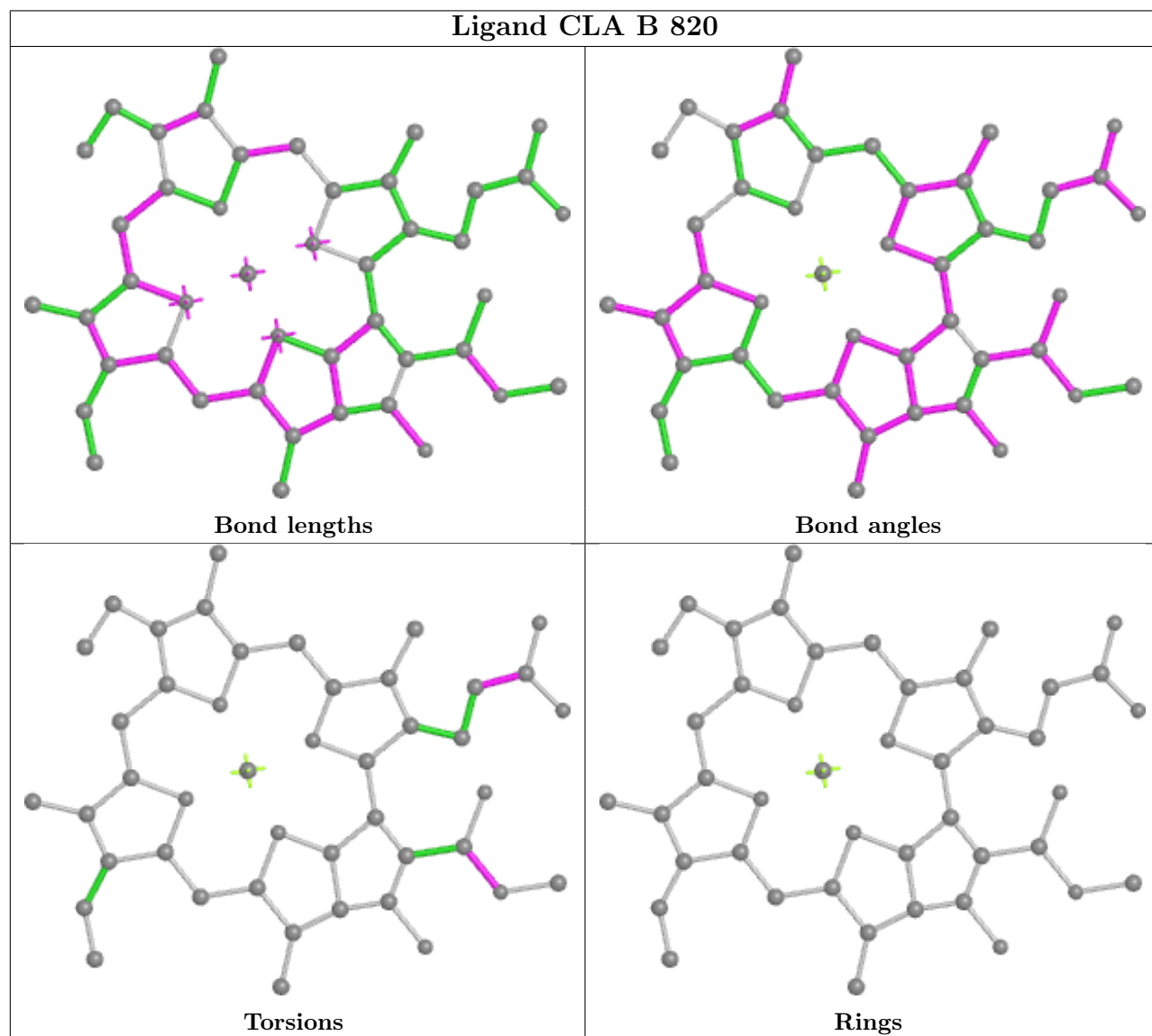
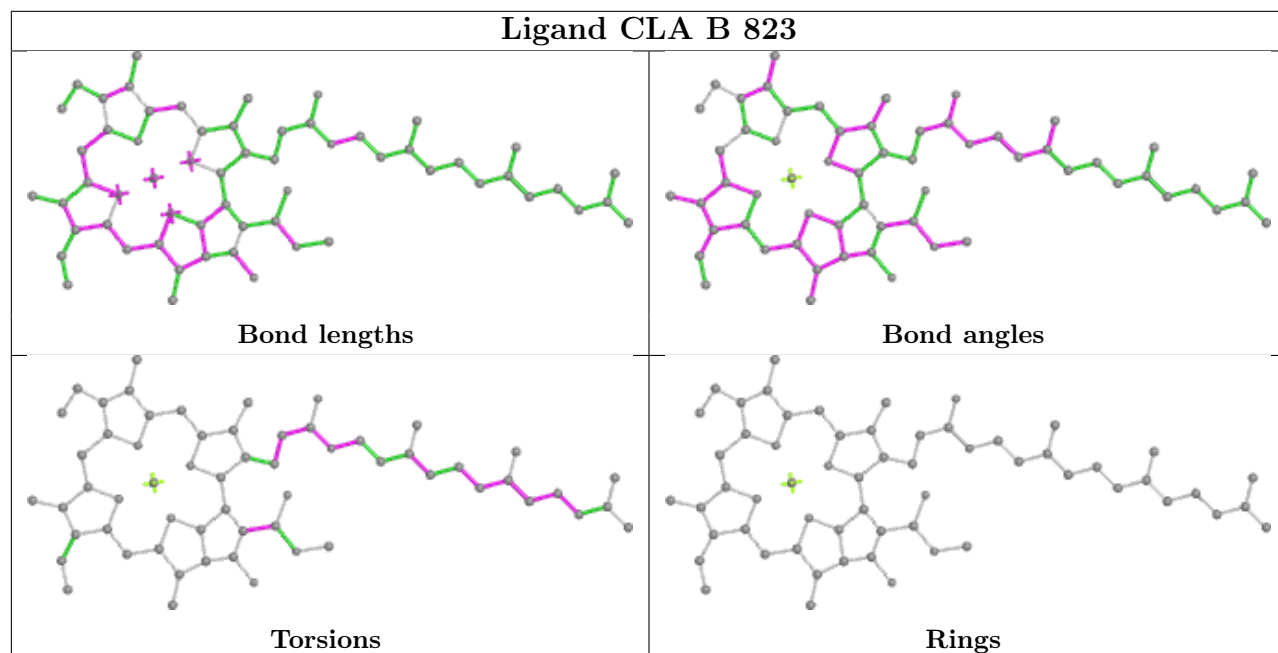


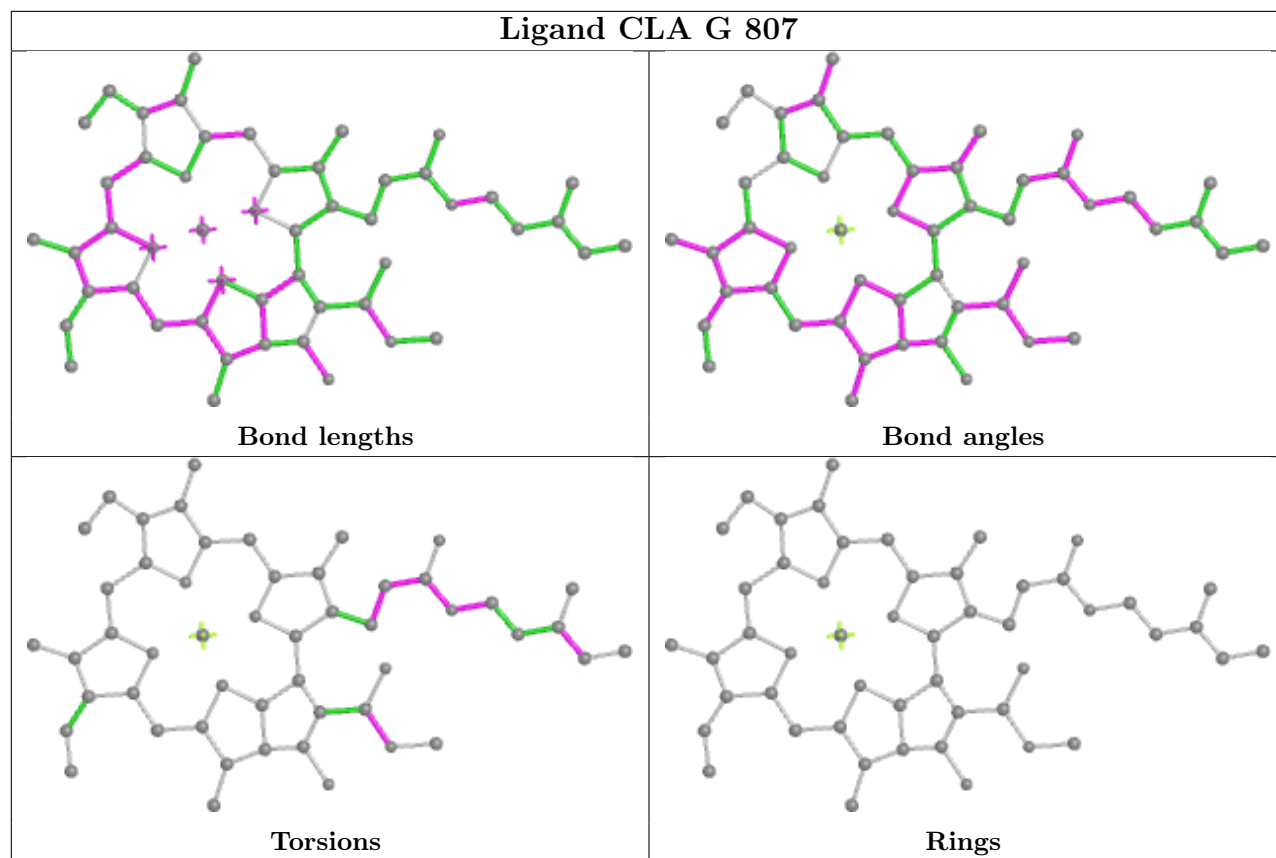




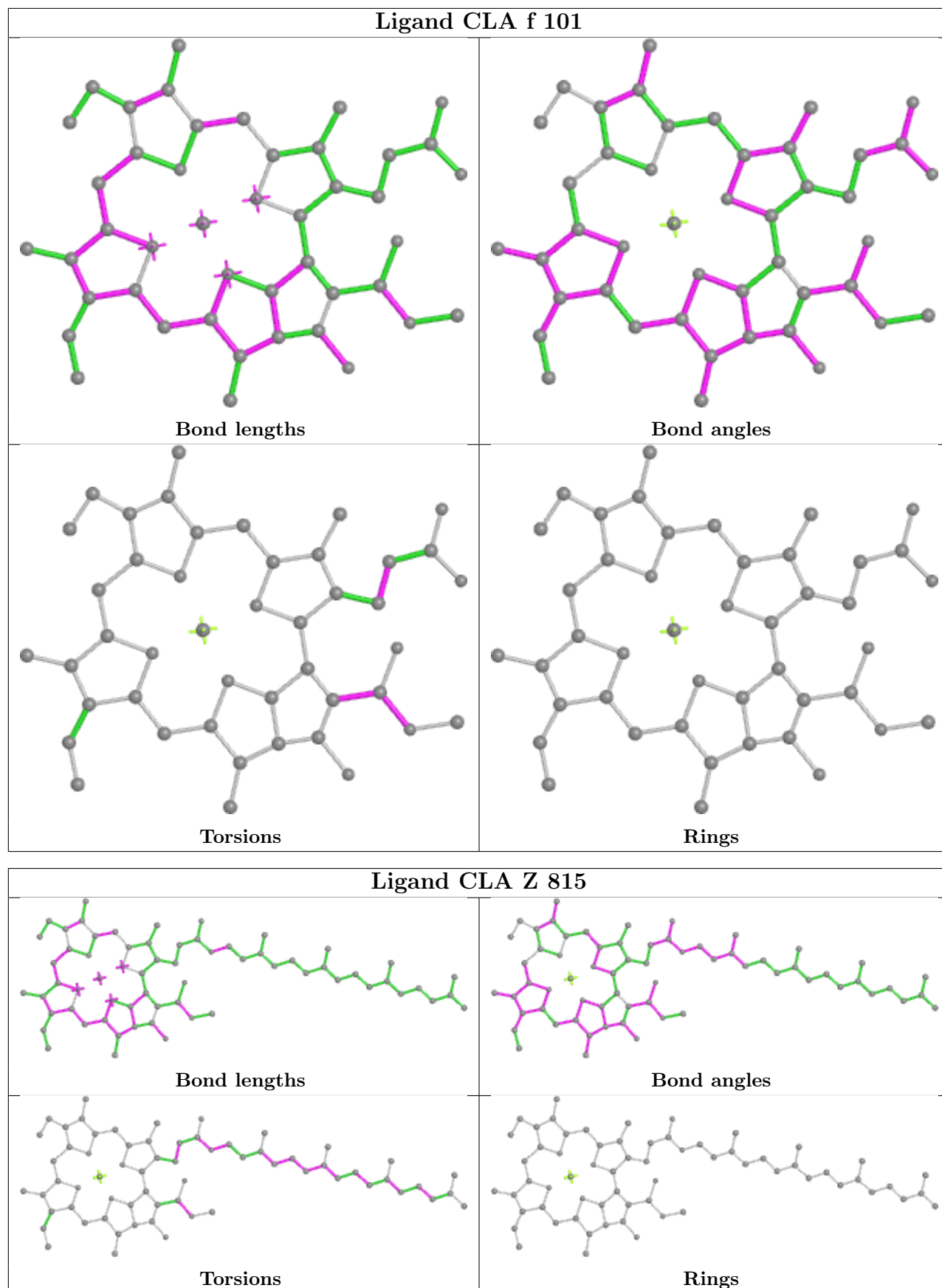


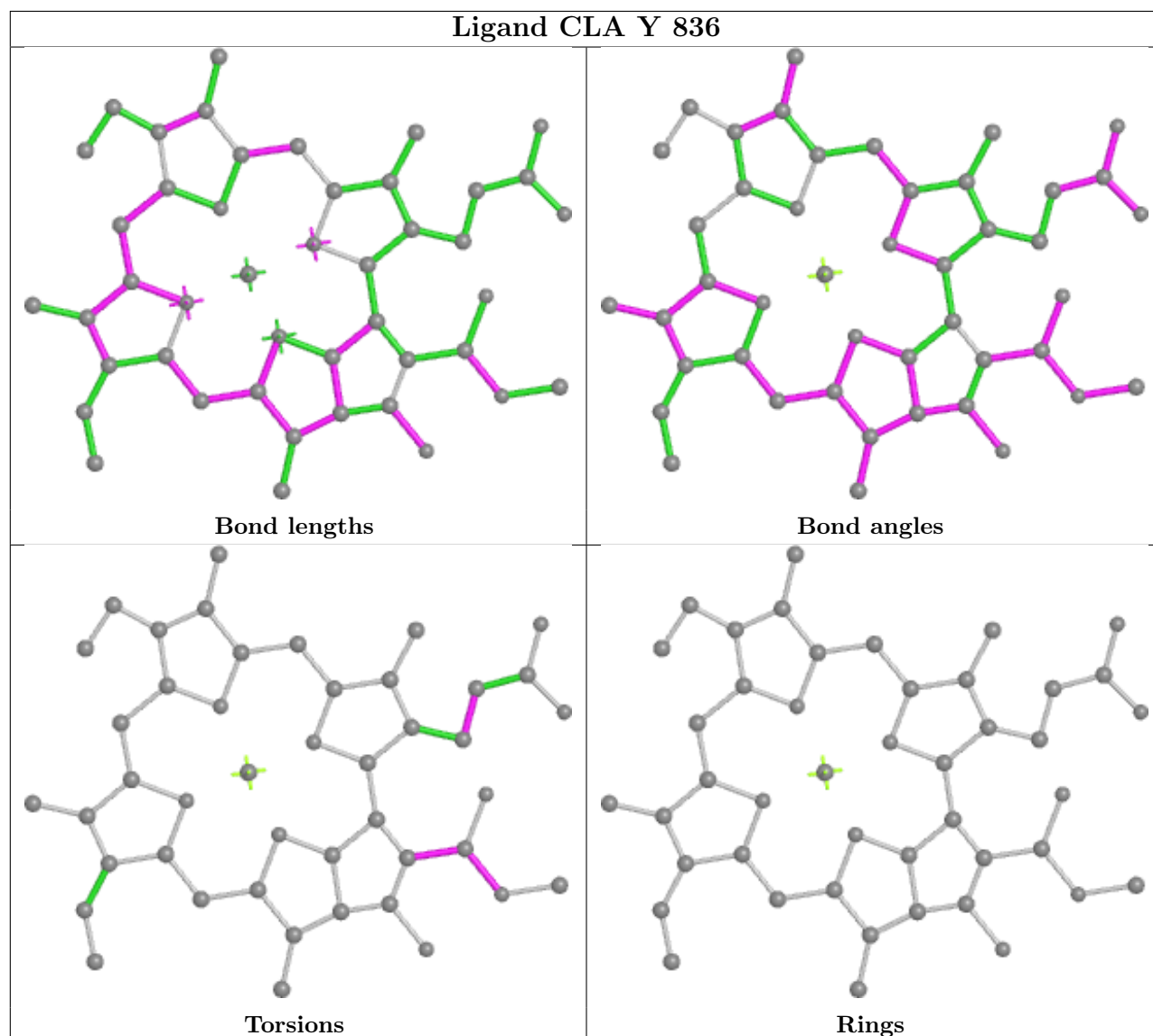
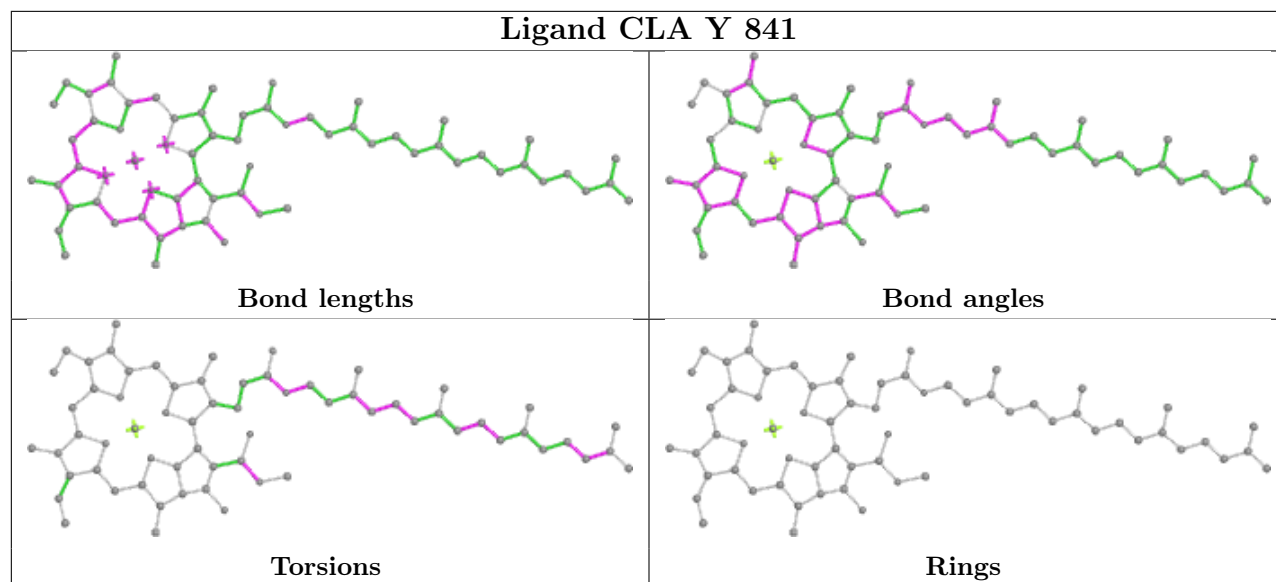


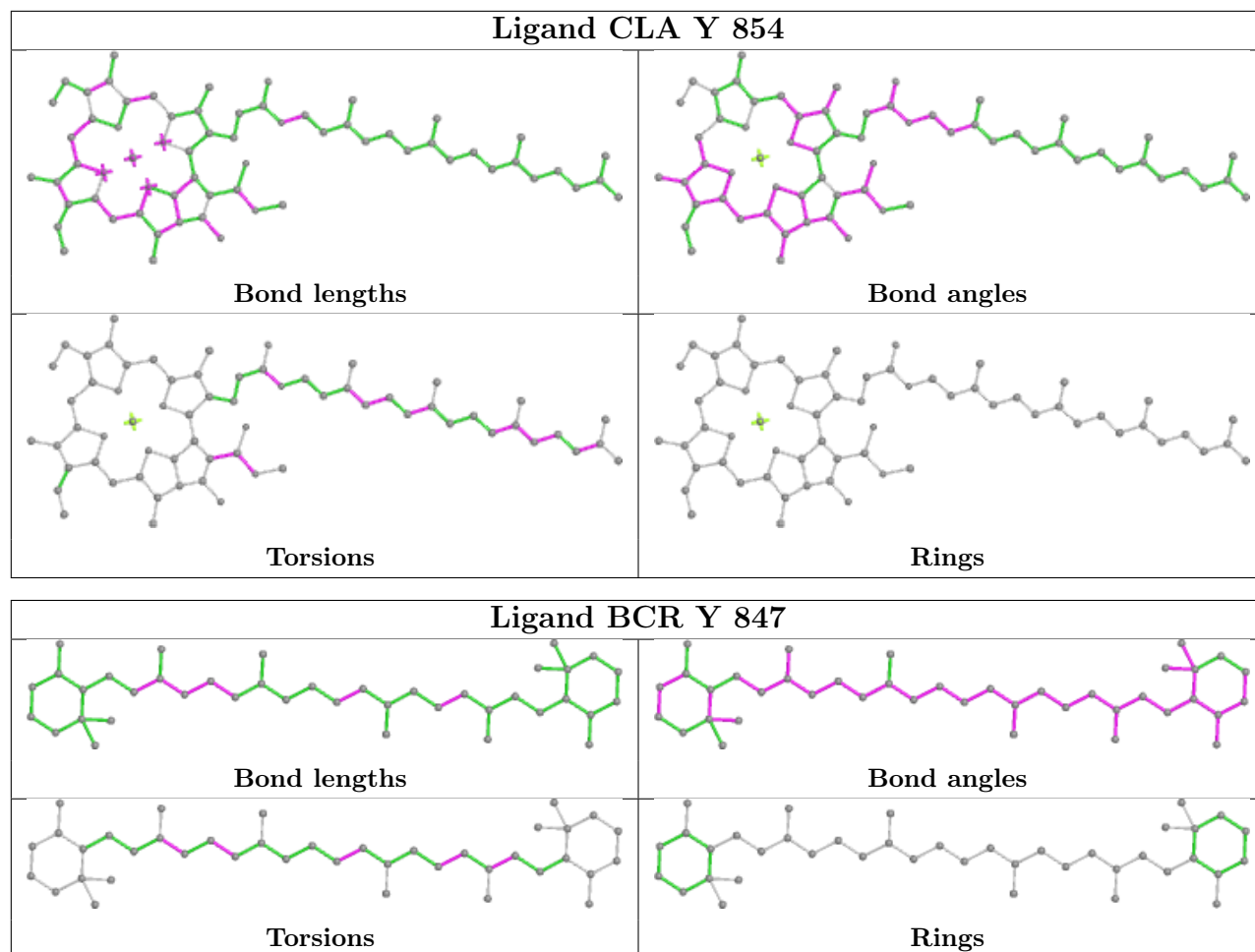




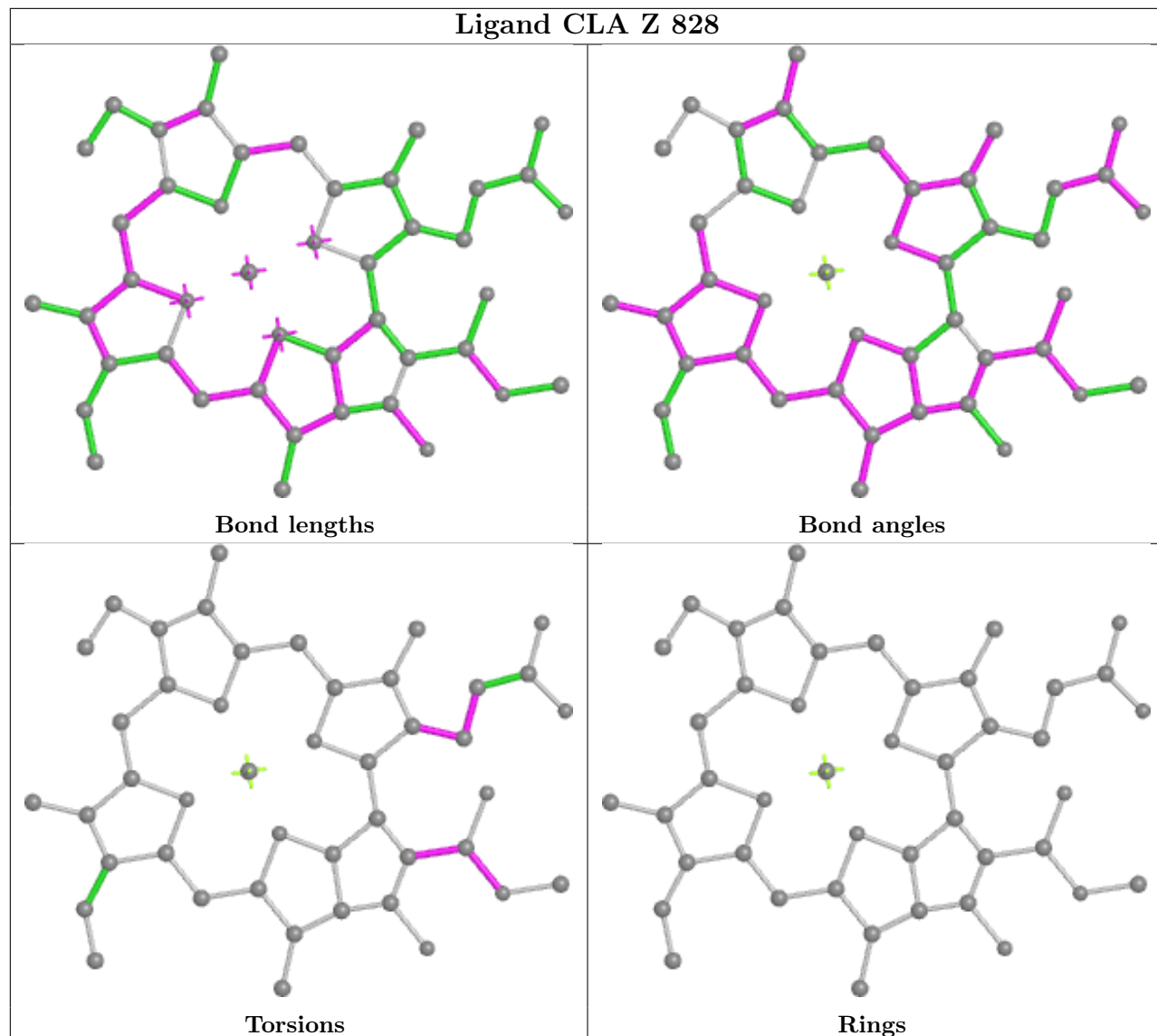


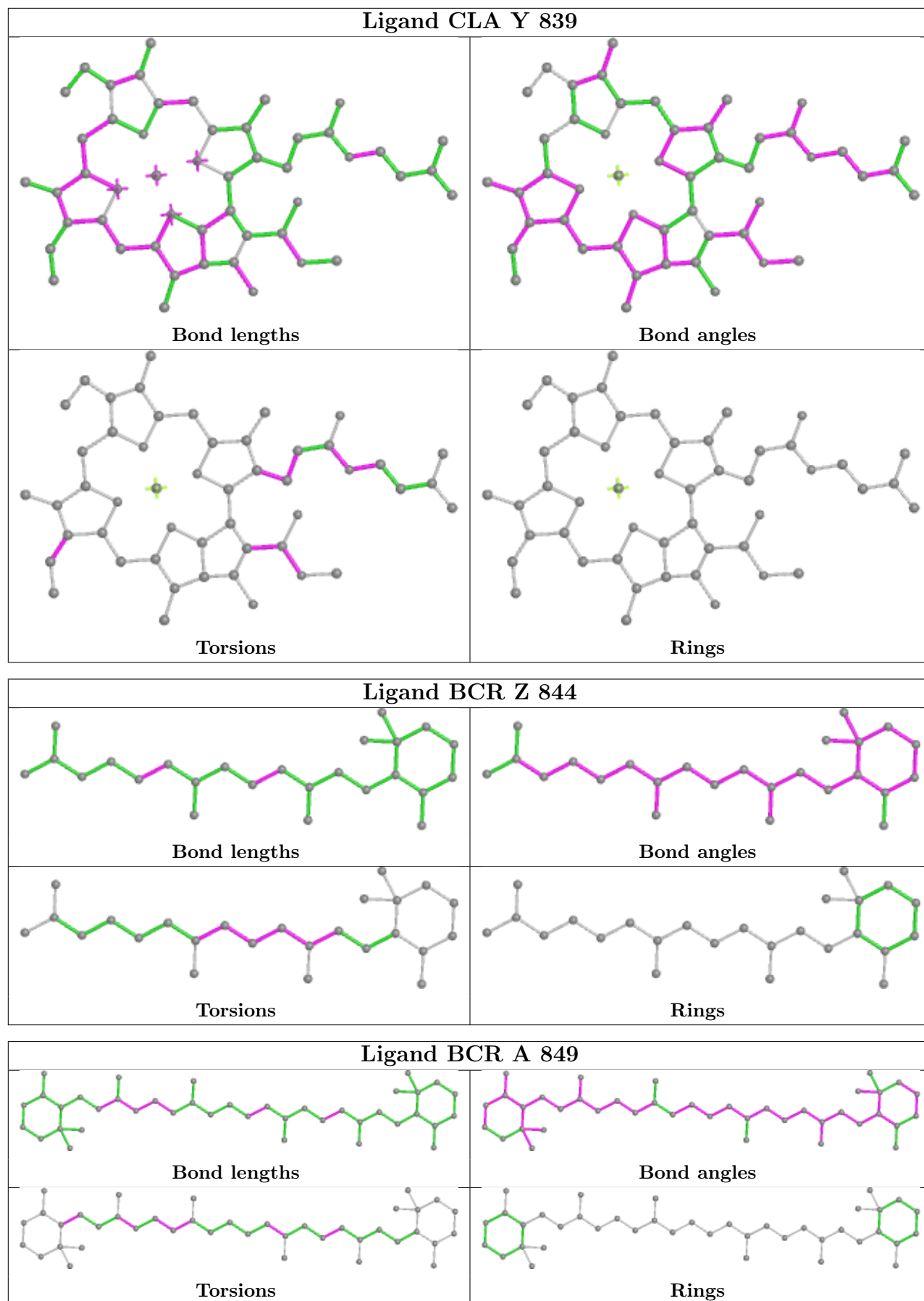


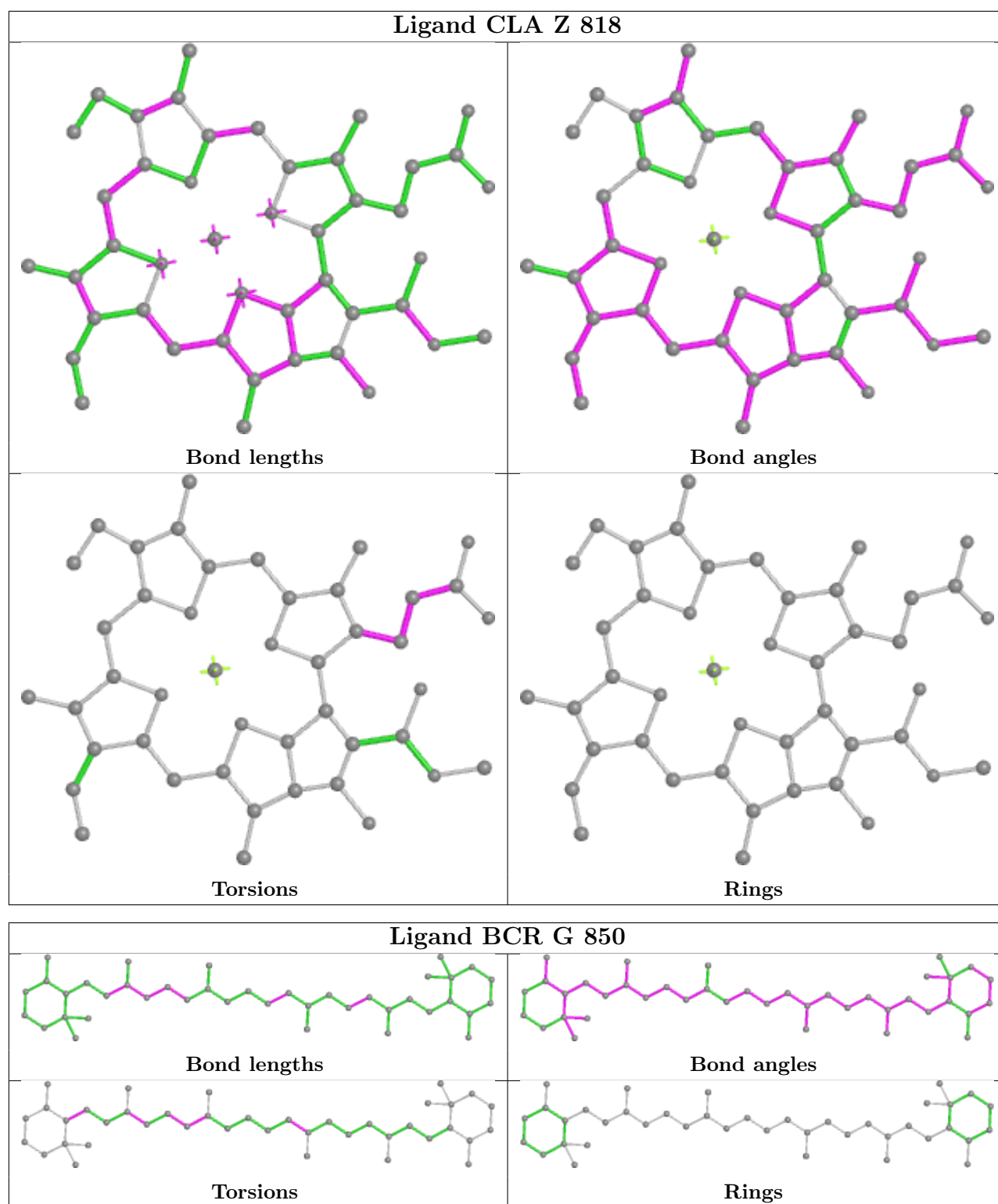


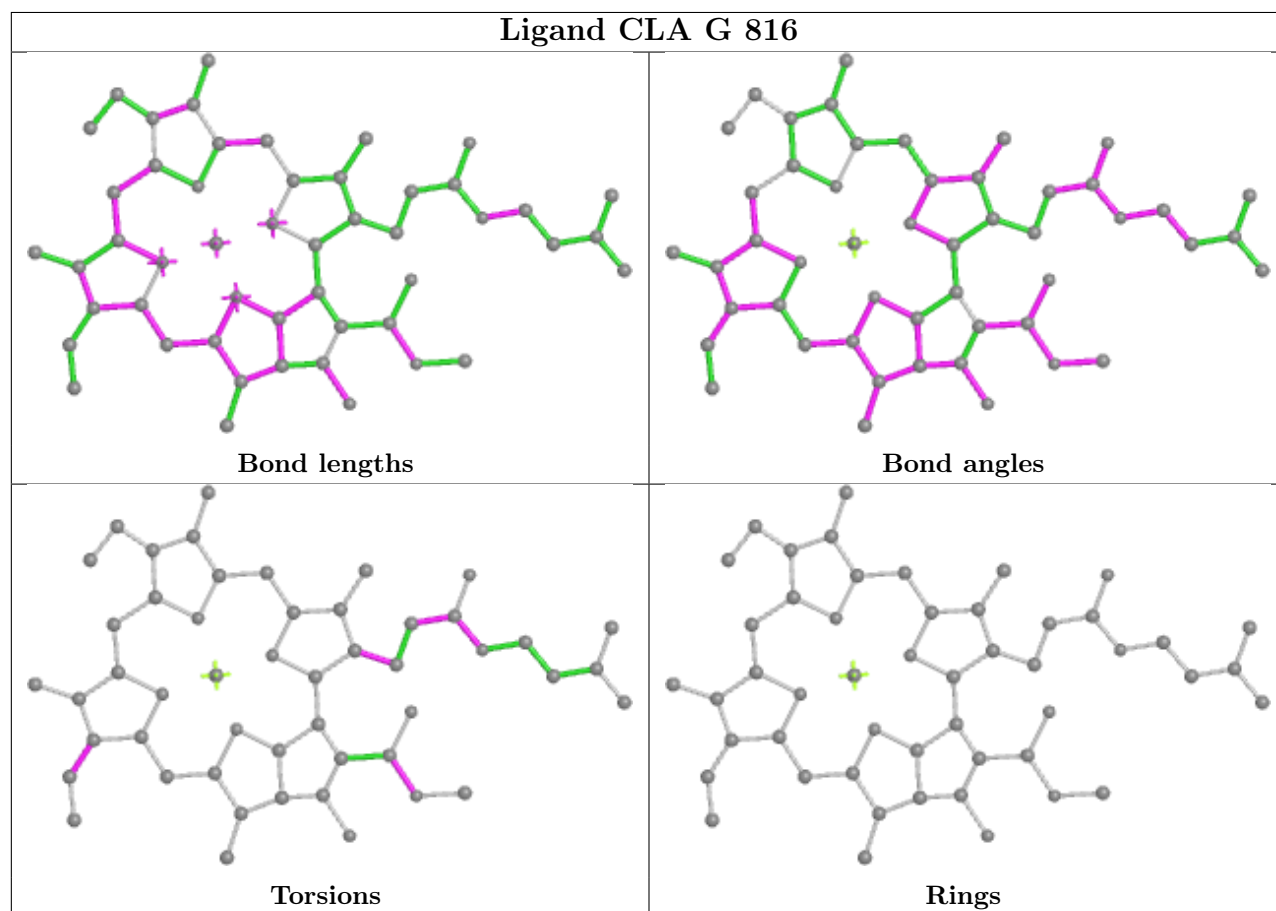
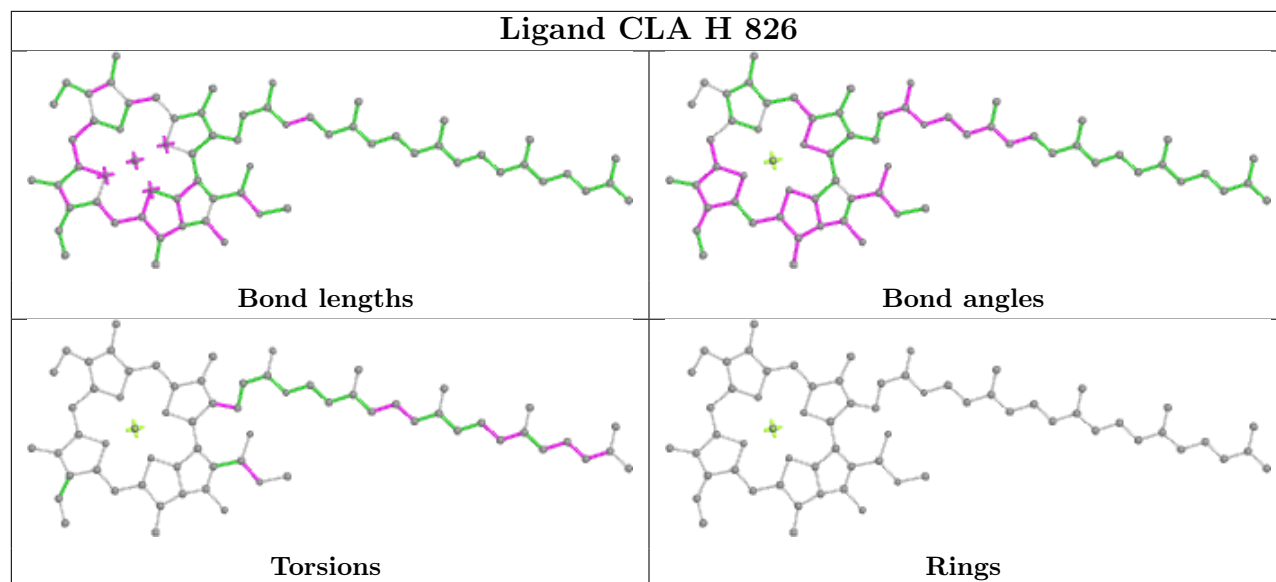


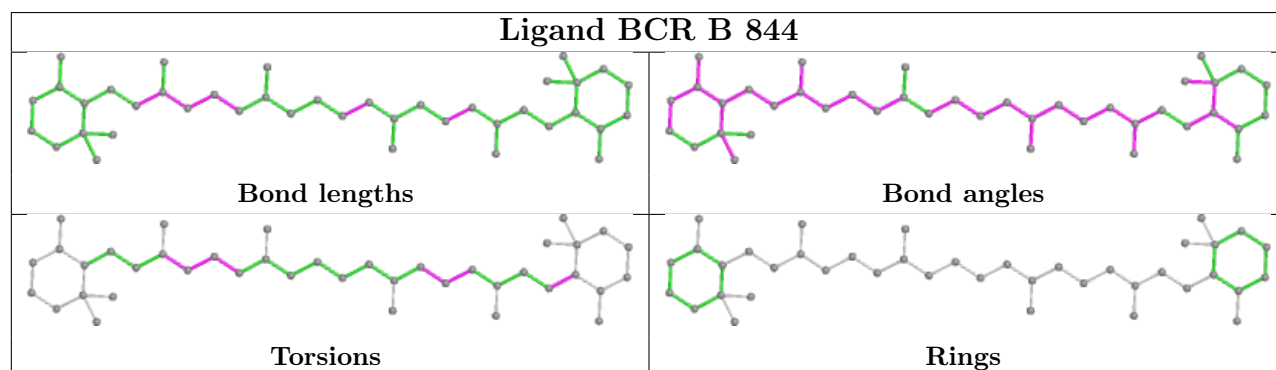
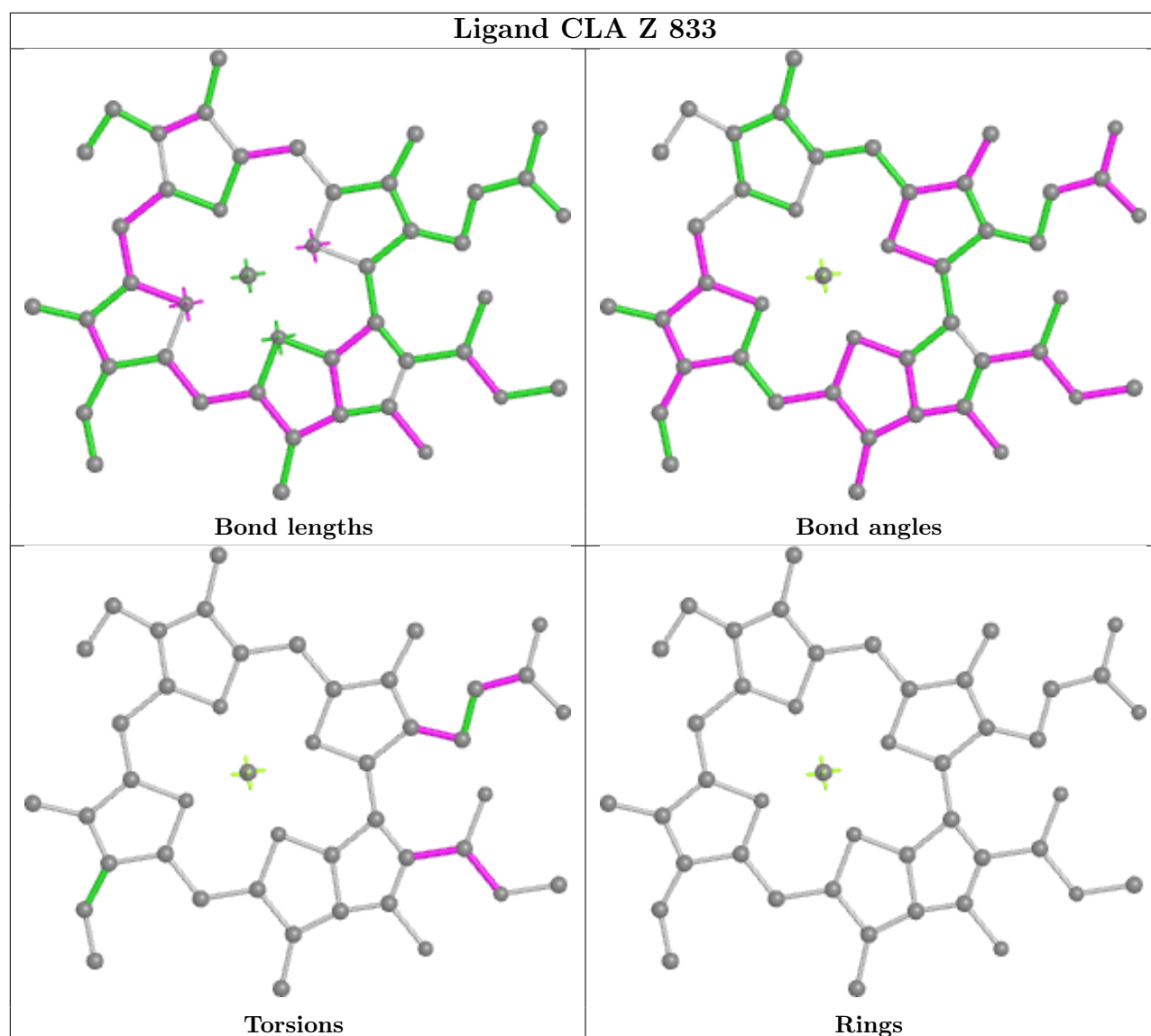
## Ligand CLA Z 828



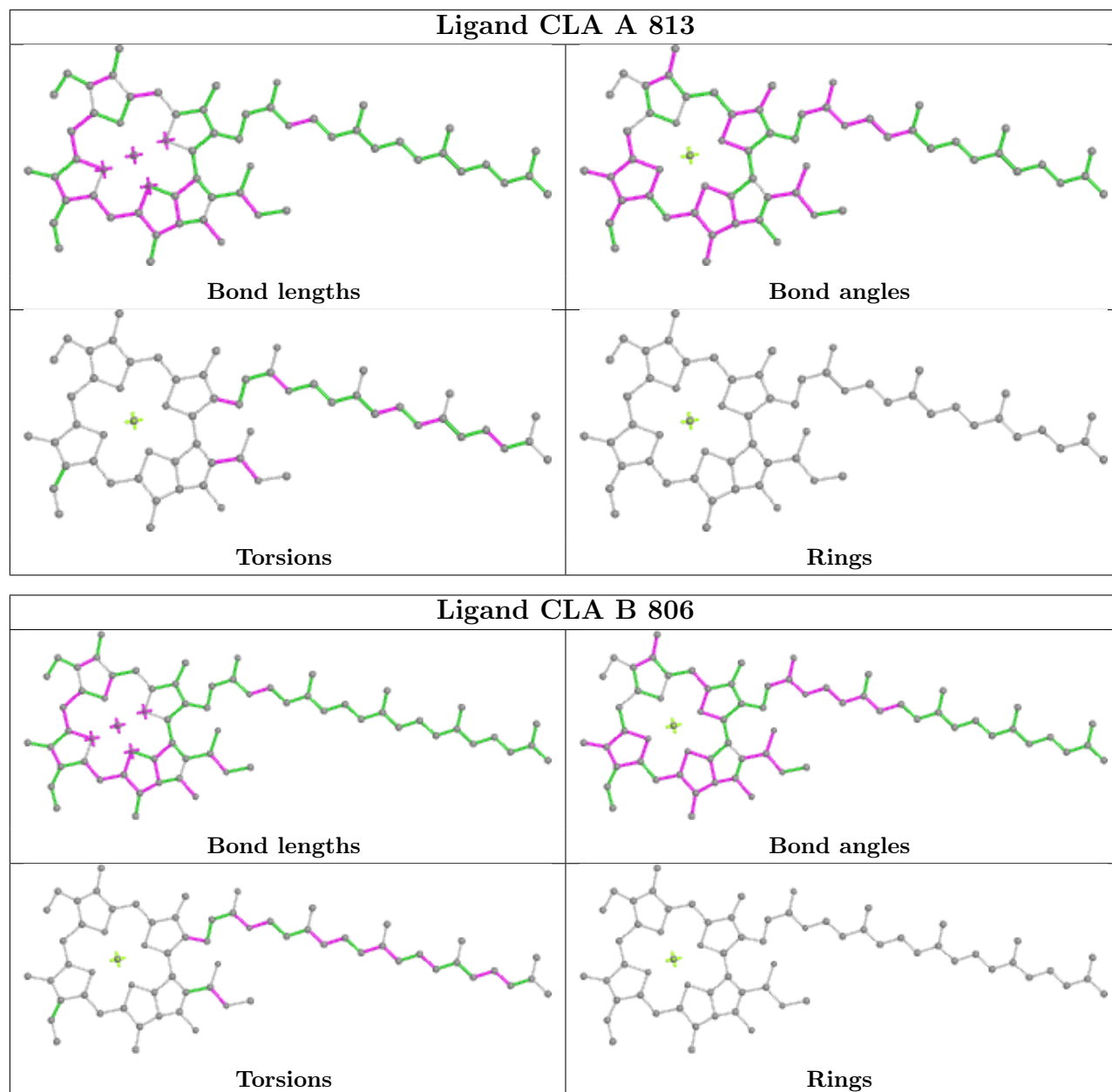


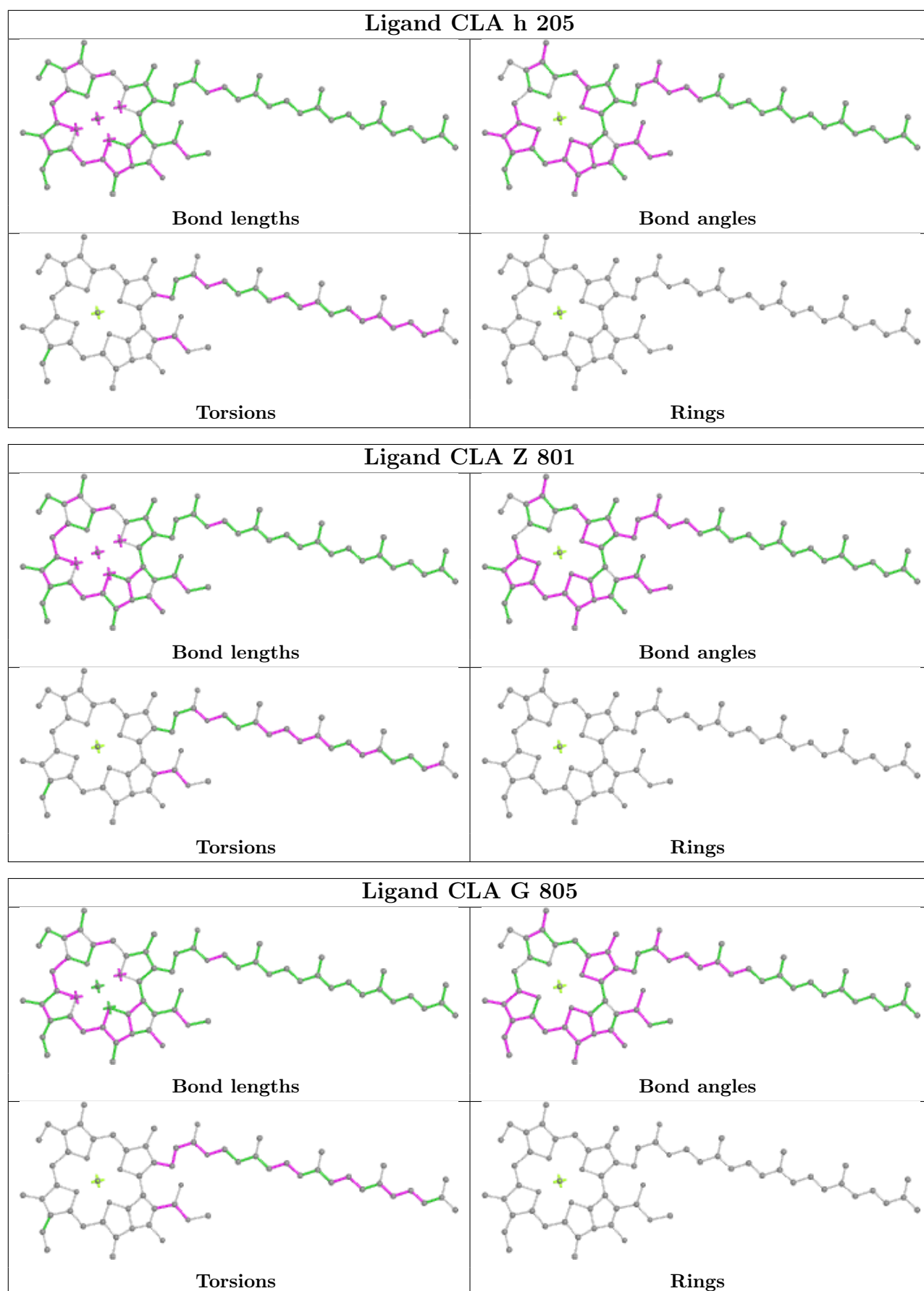


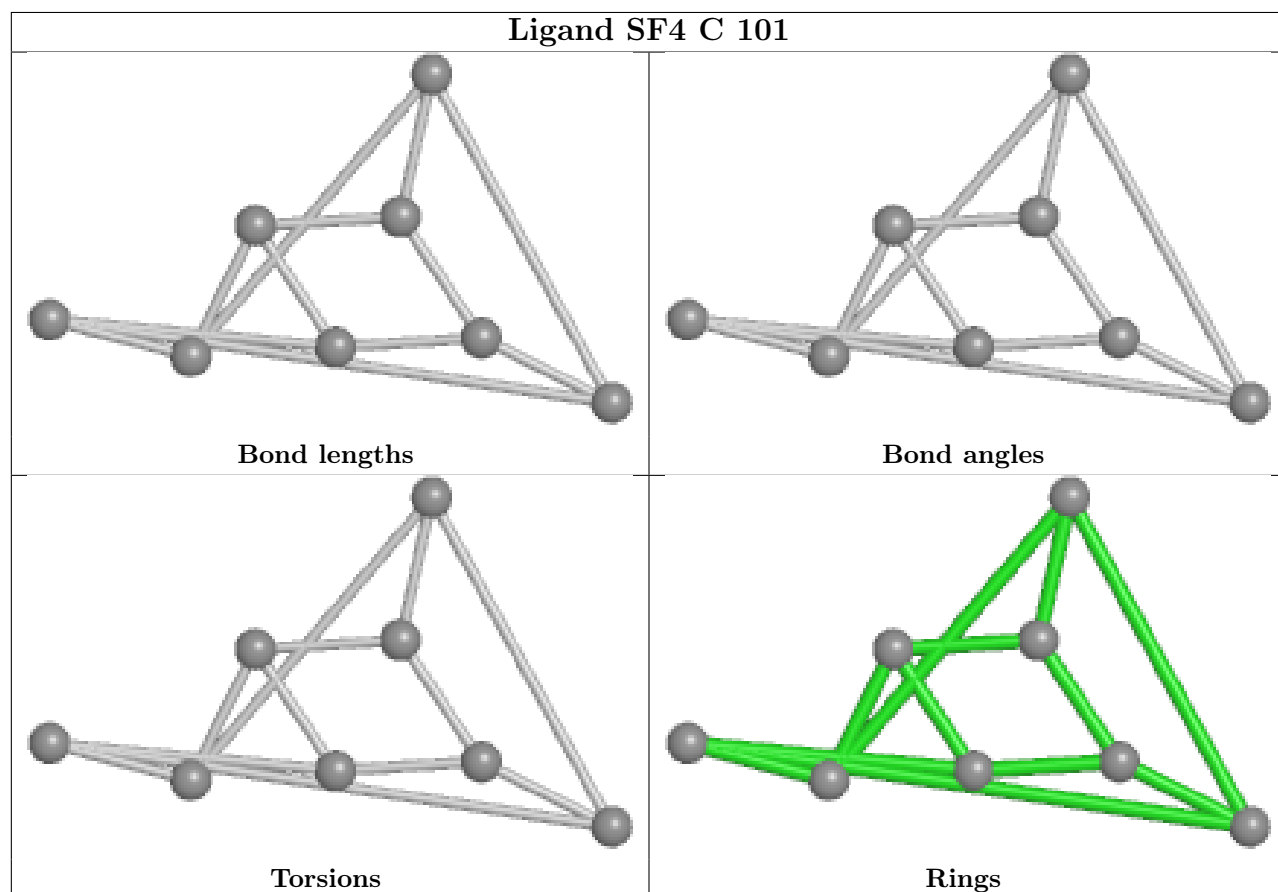
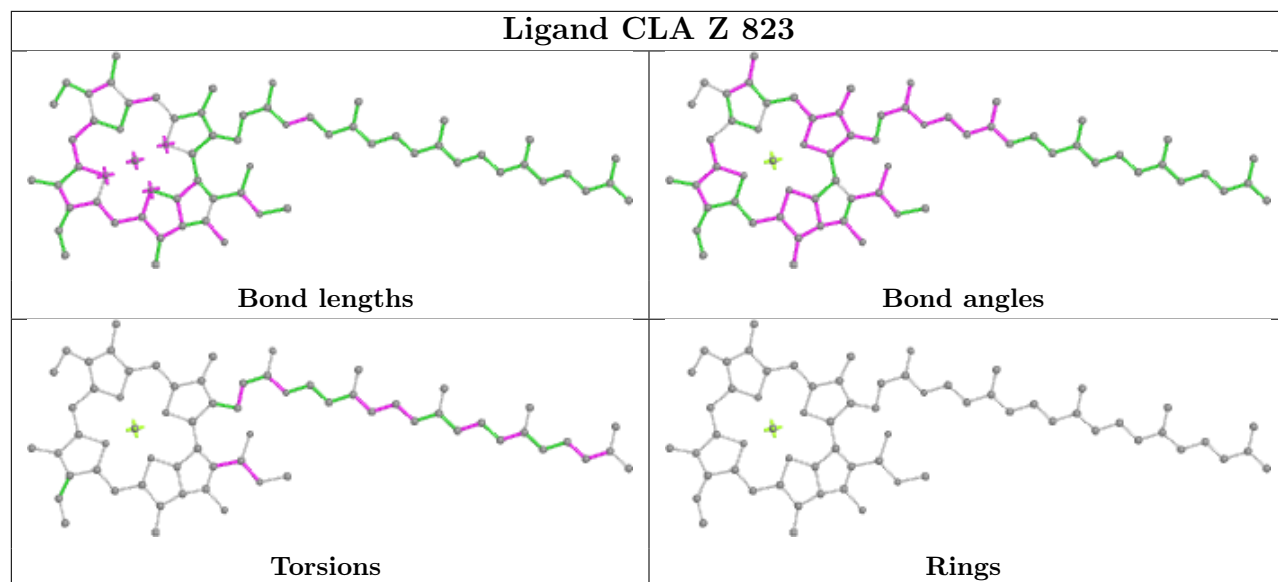


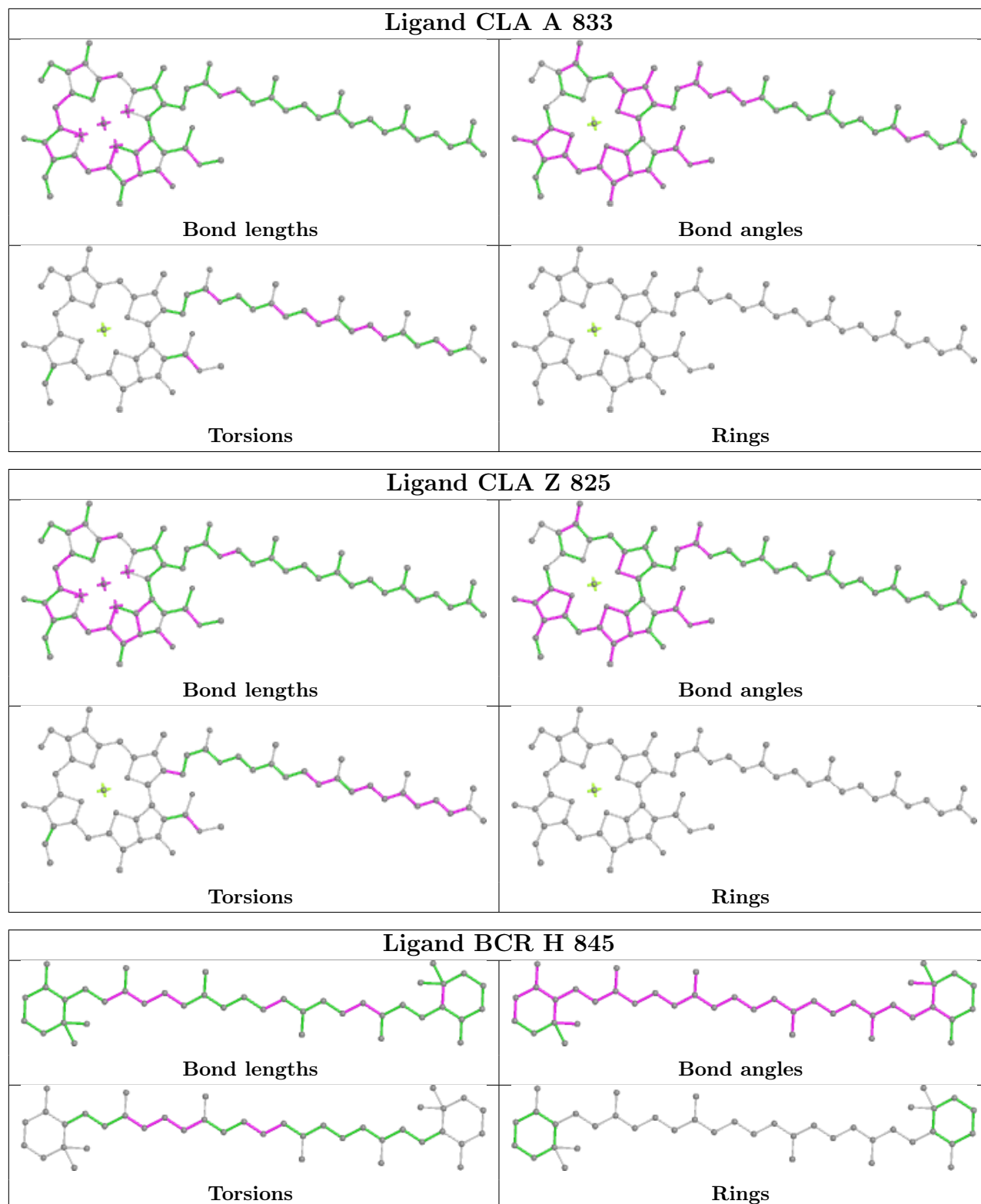


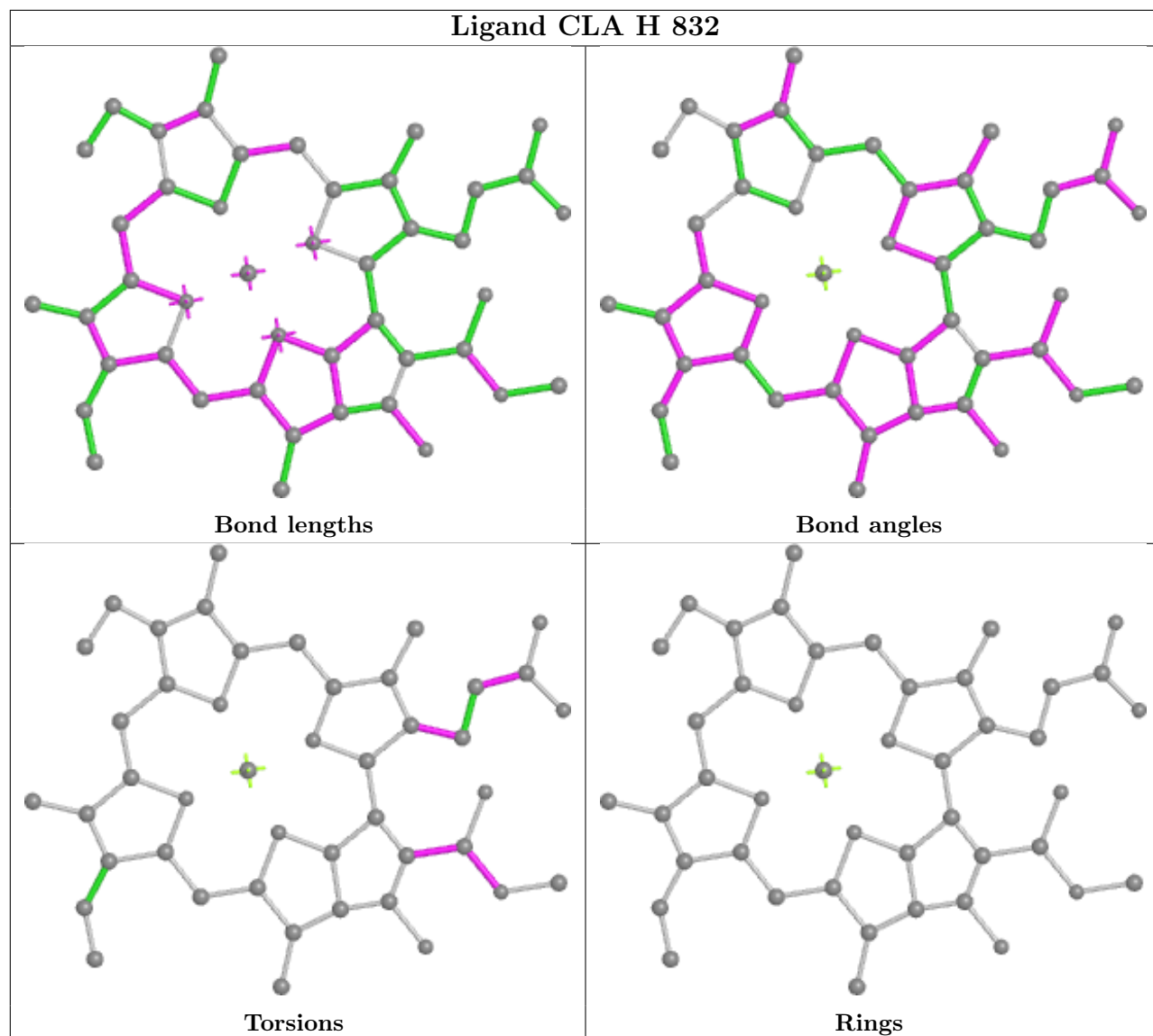


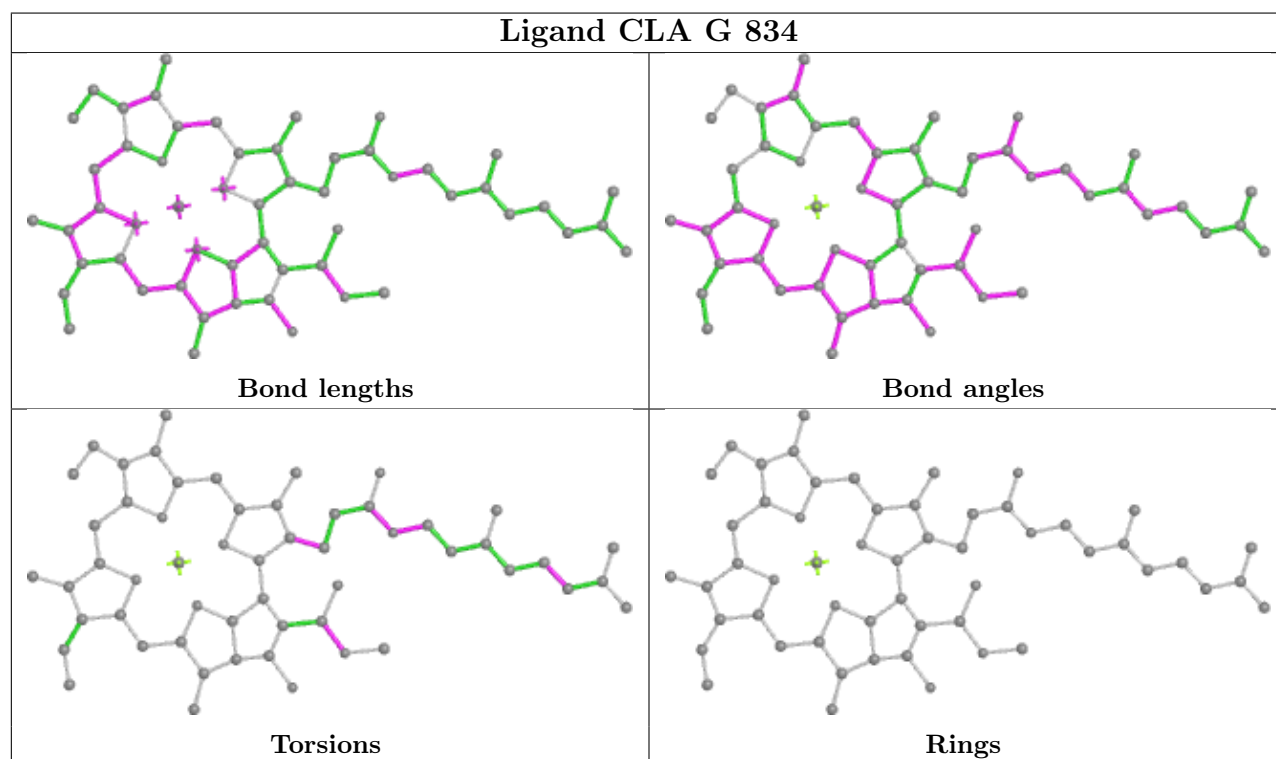
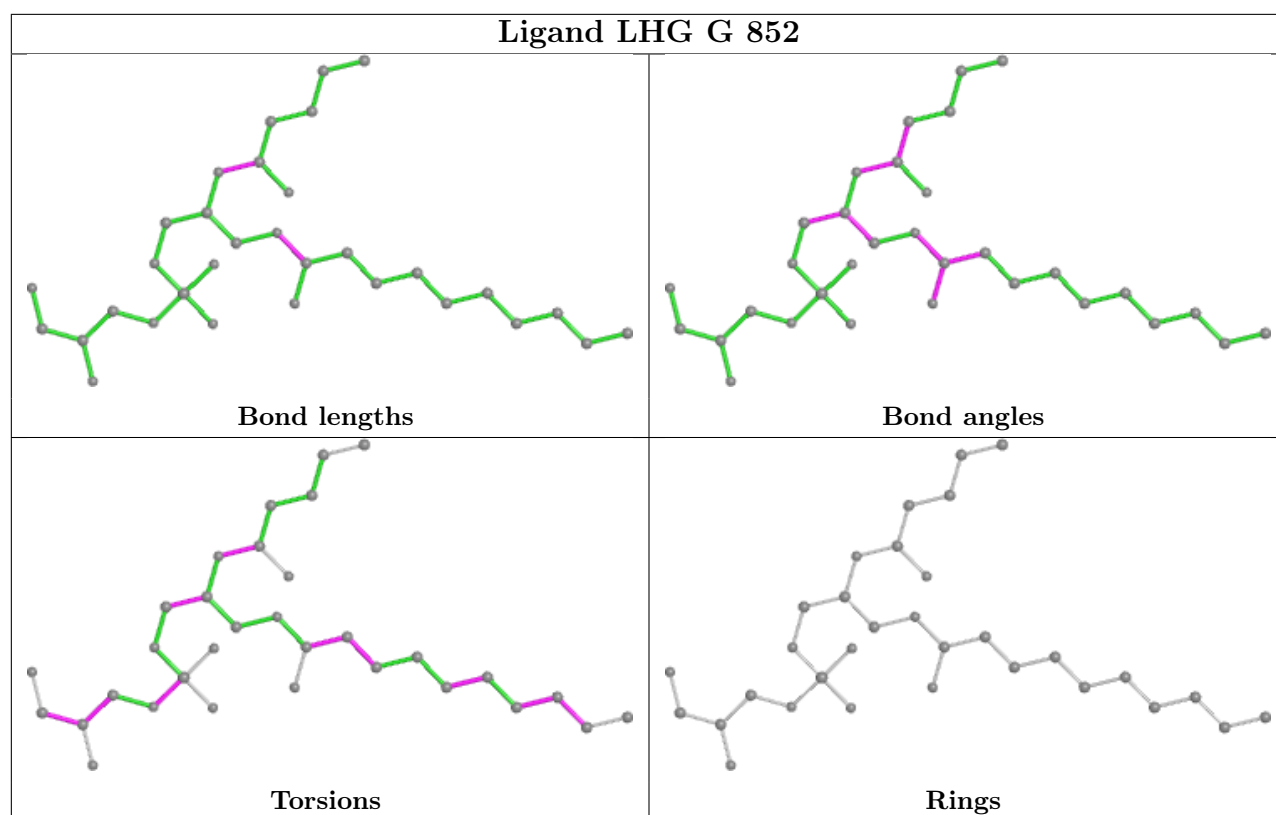


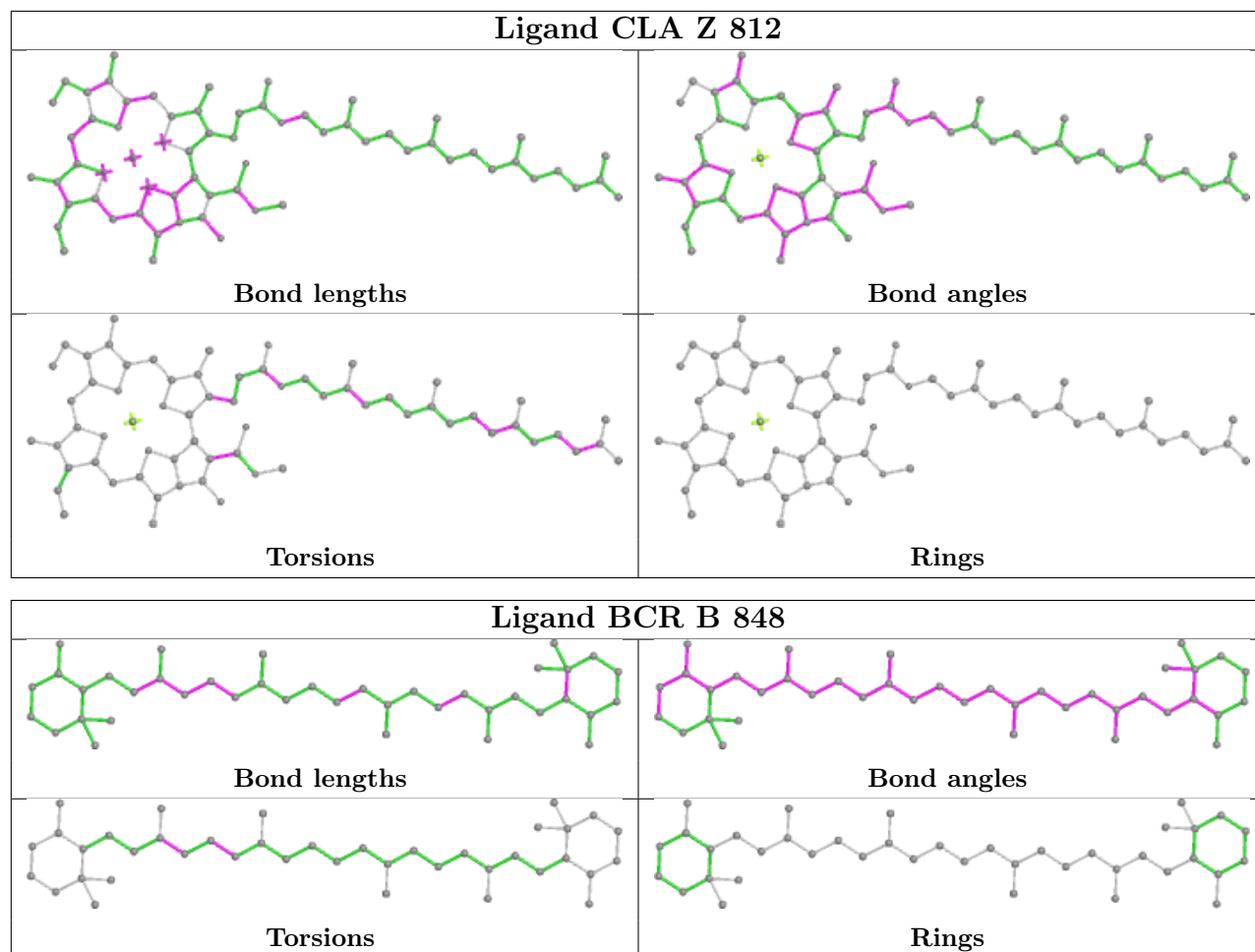


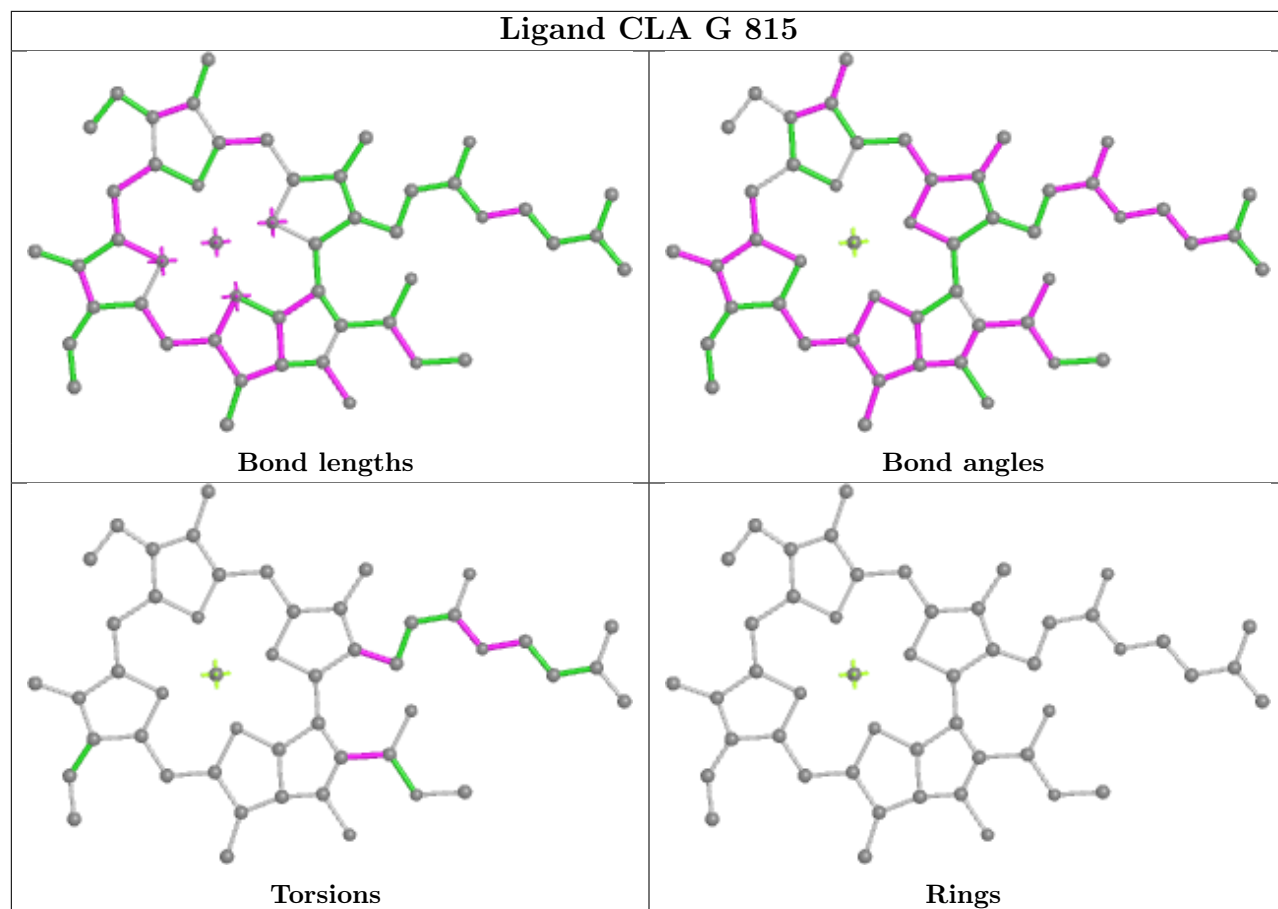




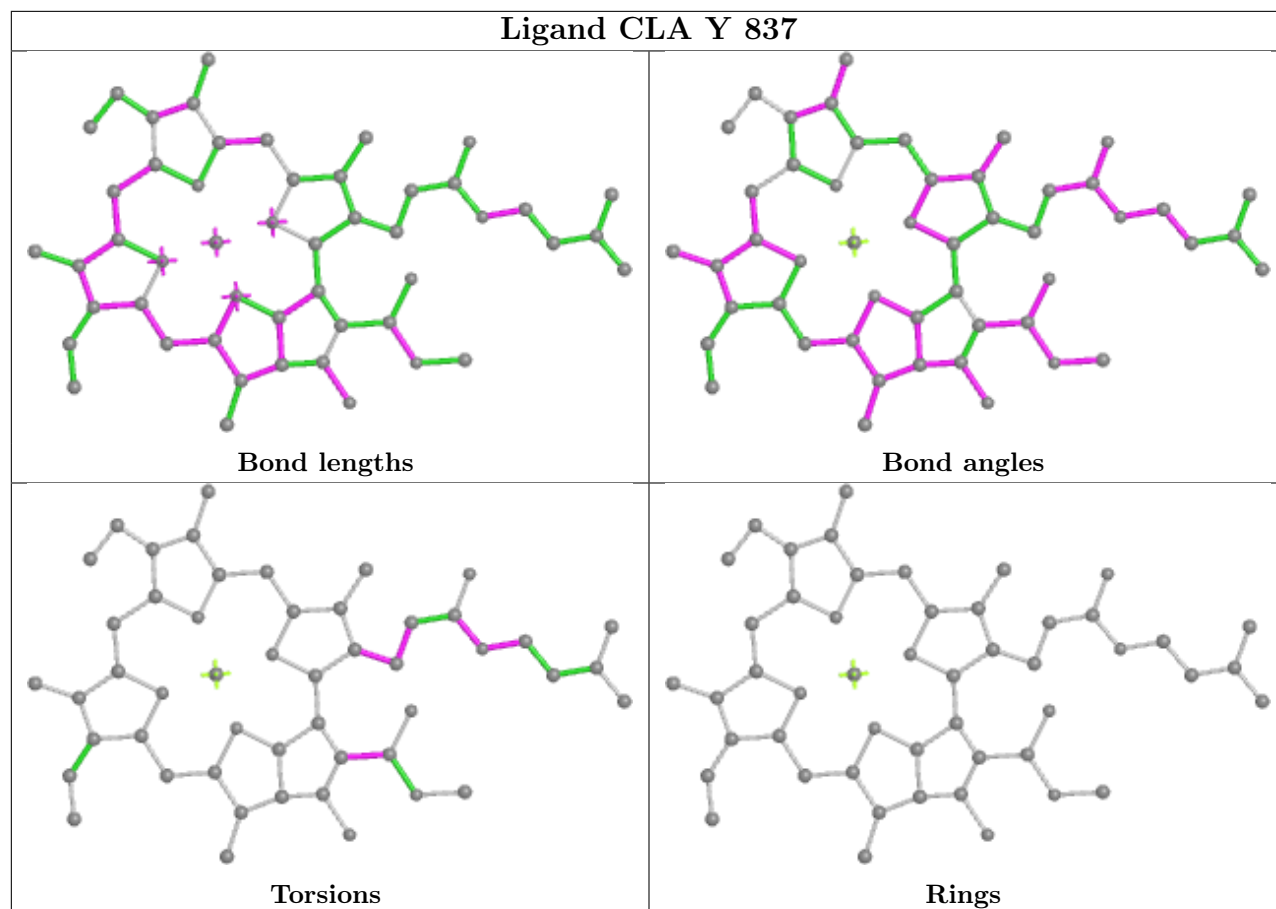


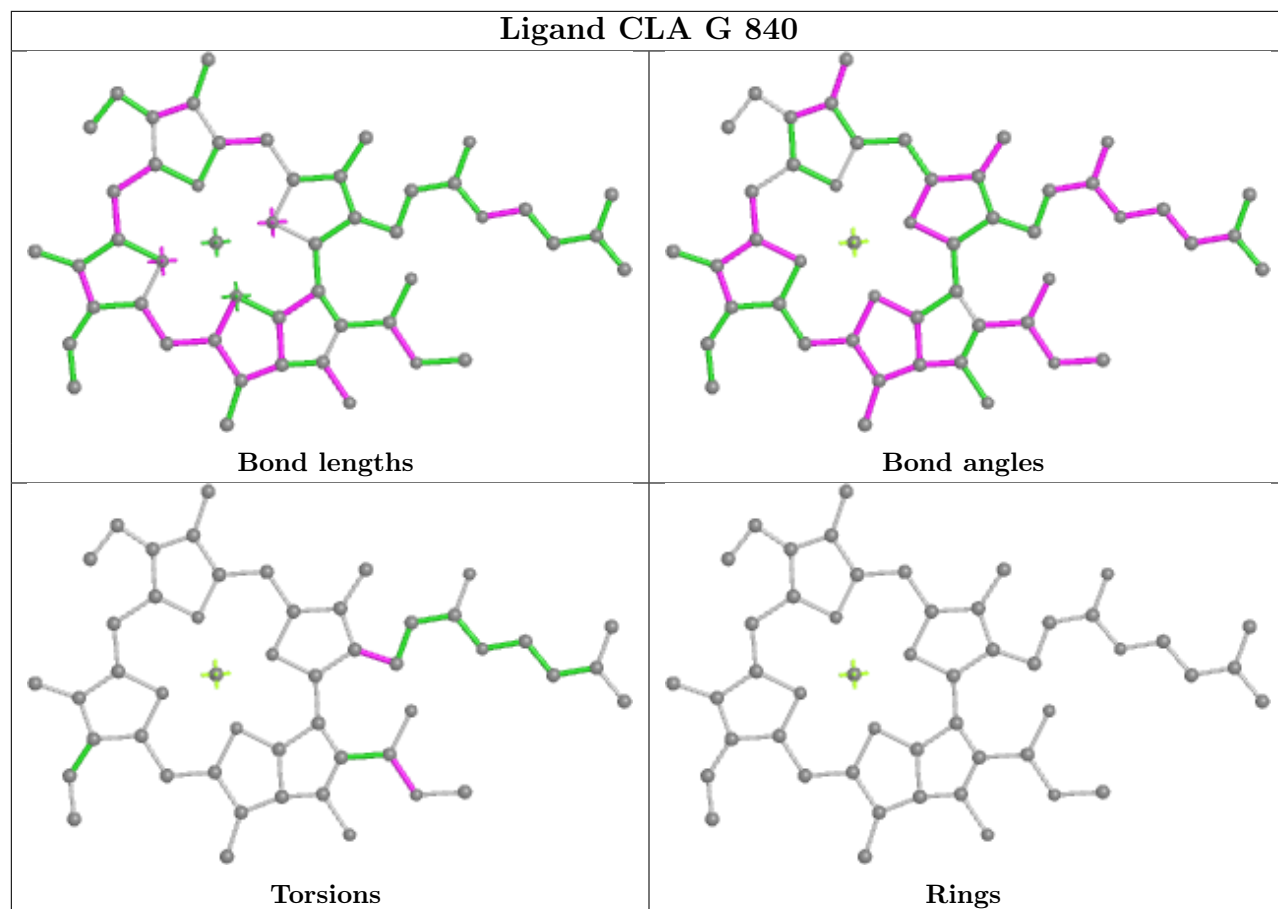


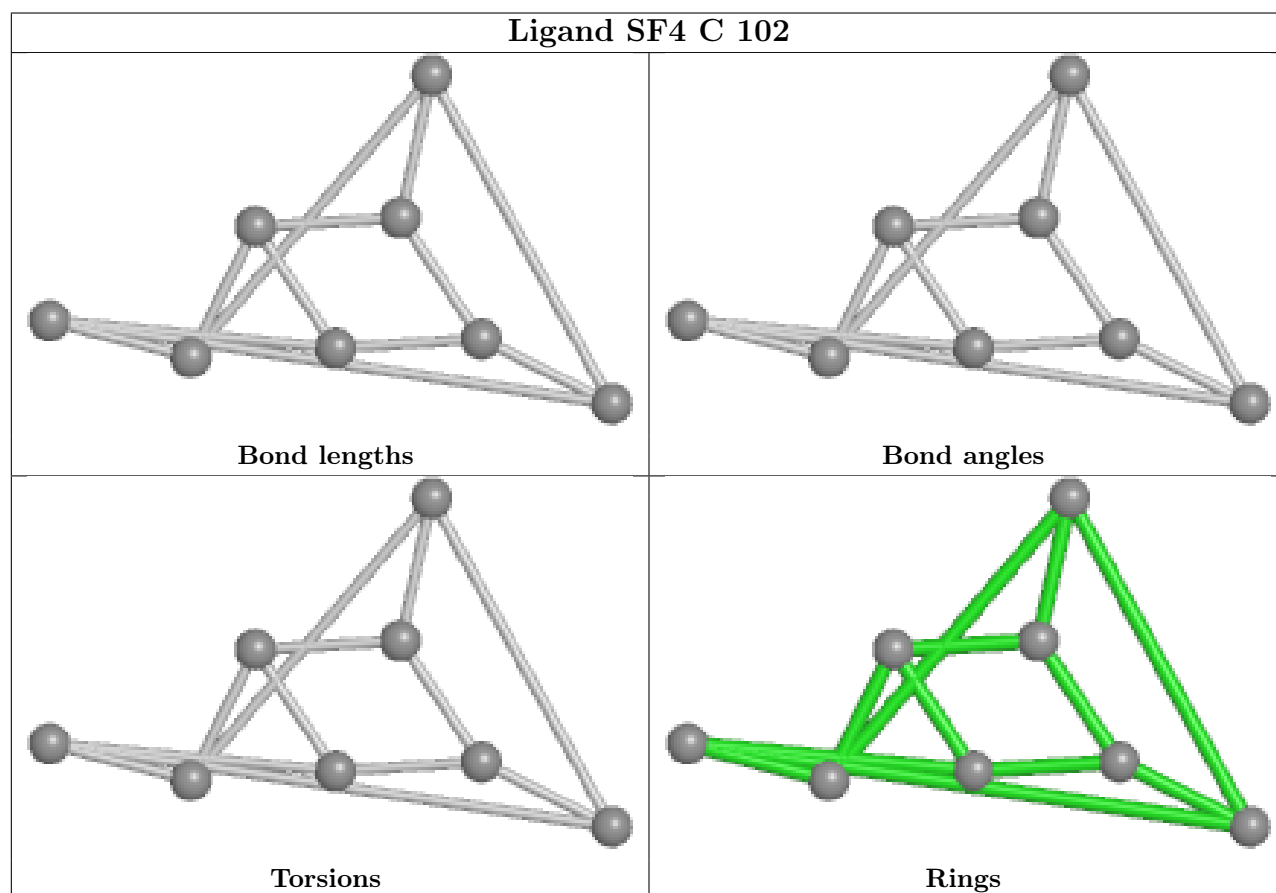
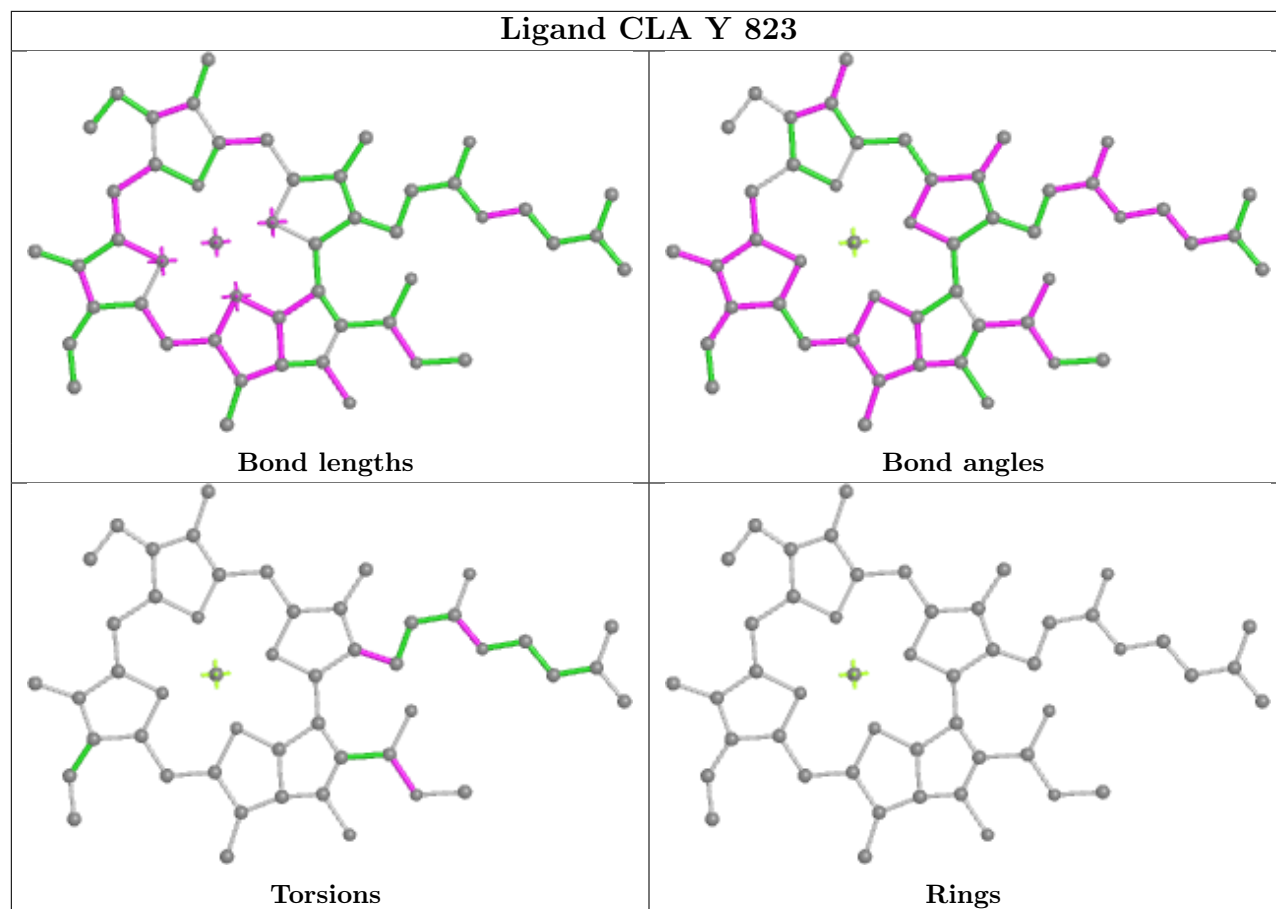


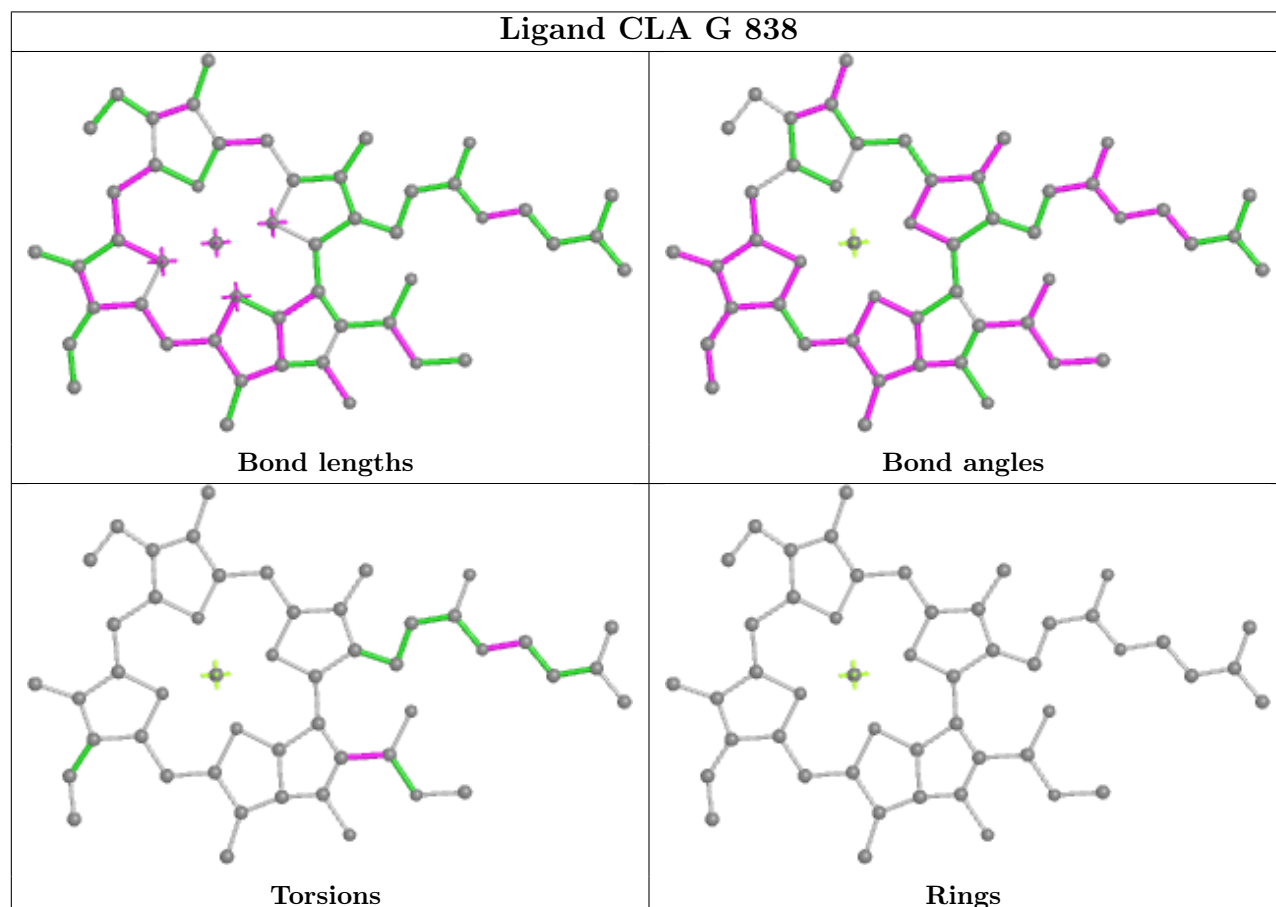
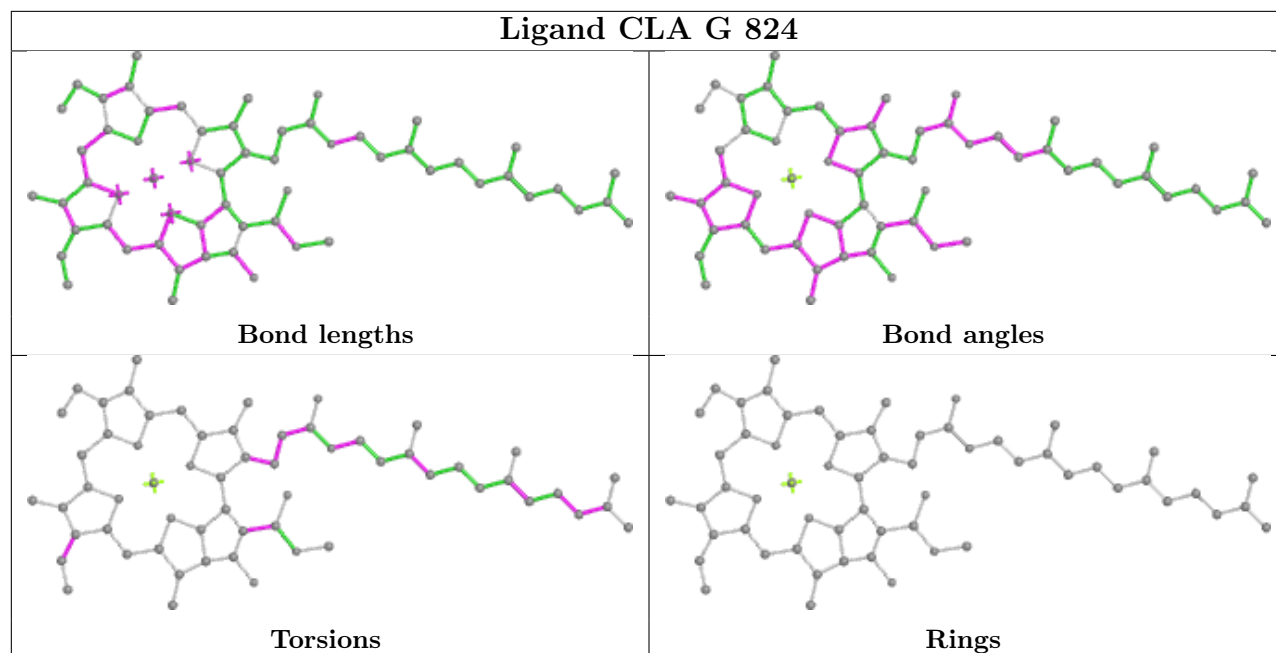


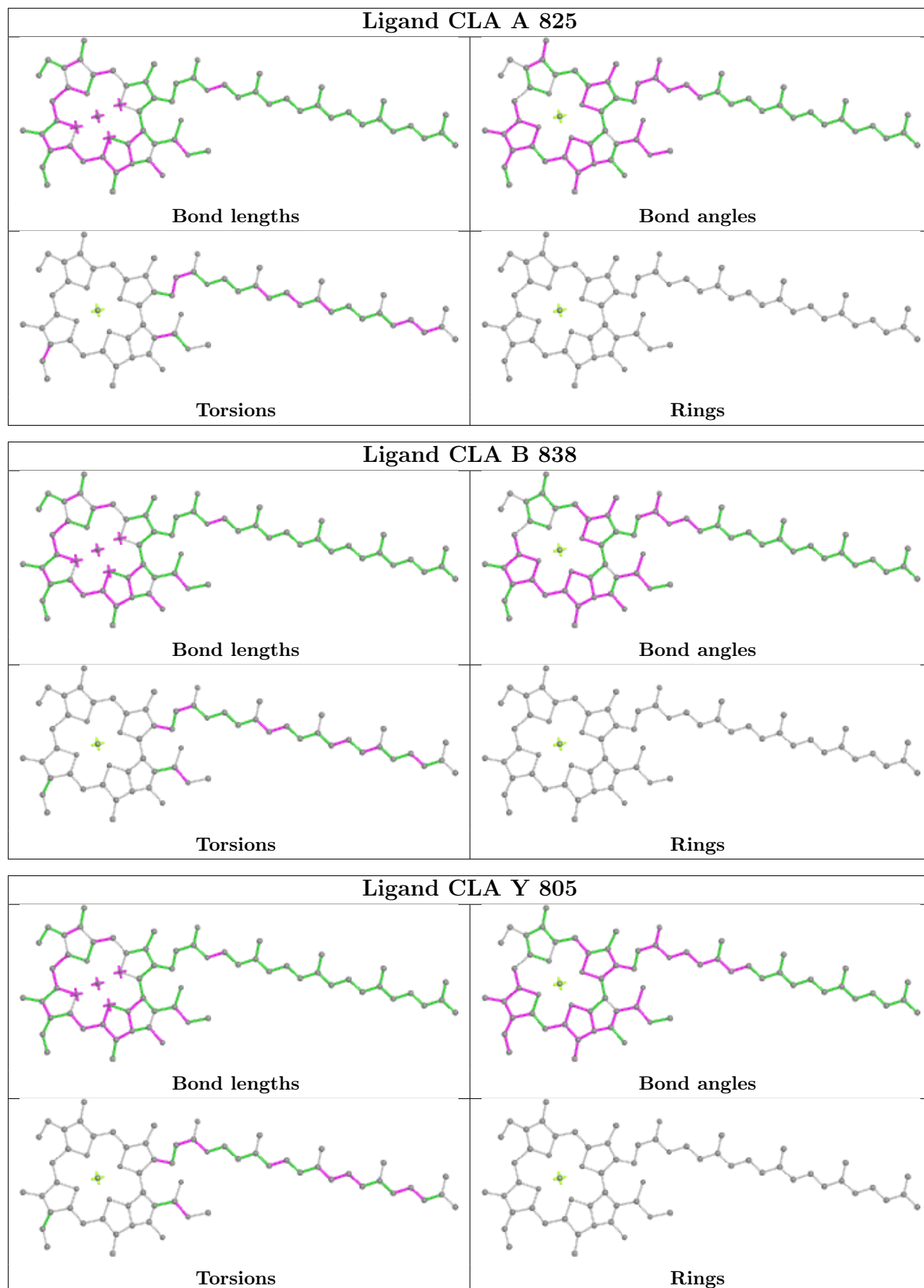


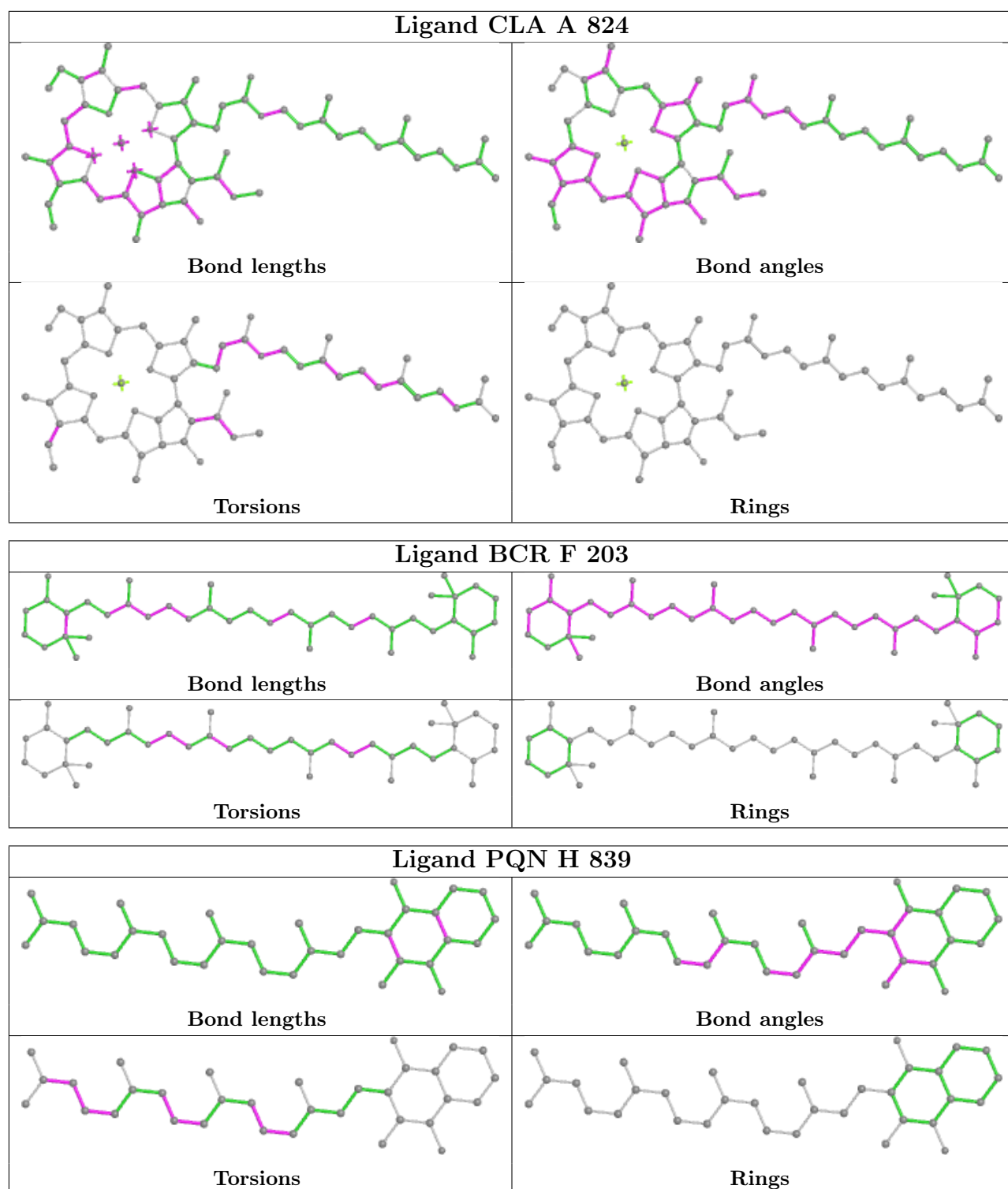


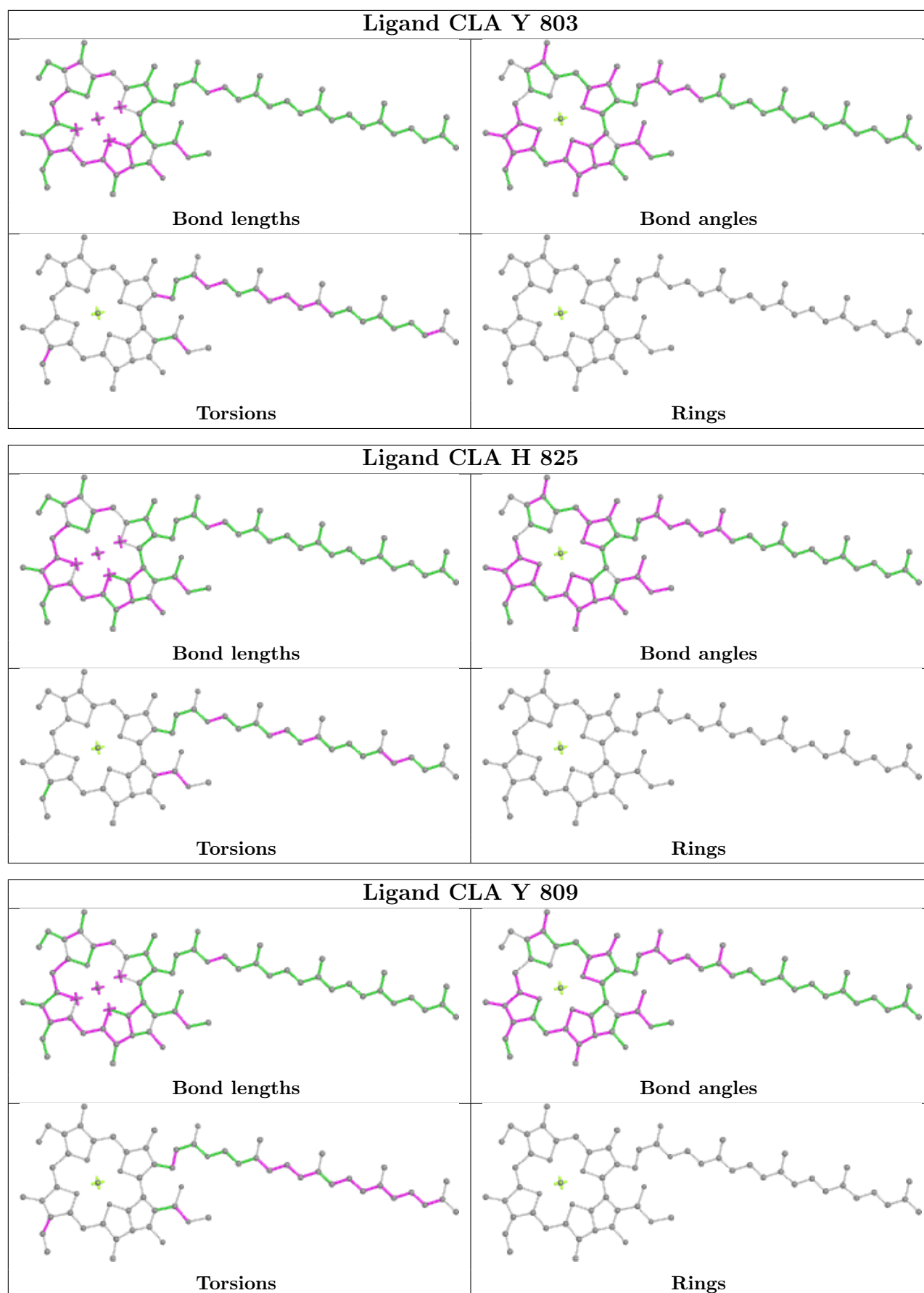


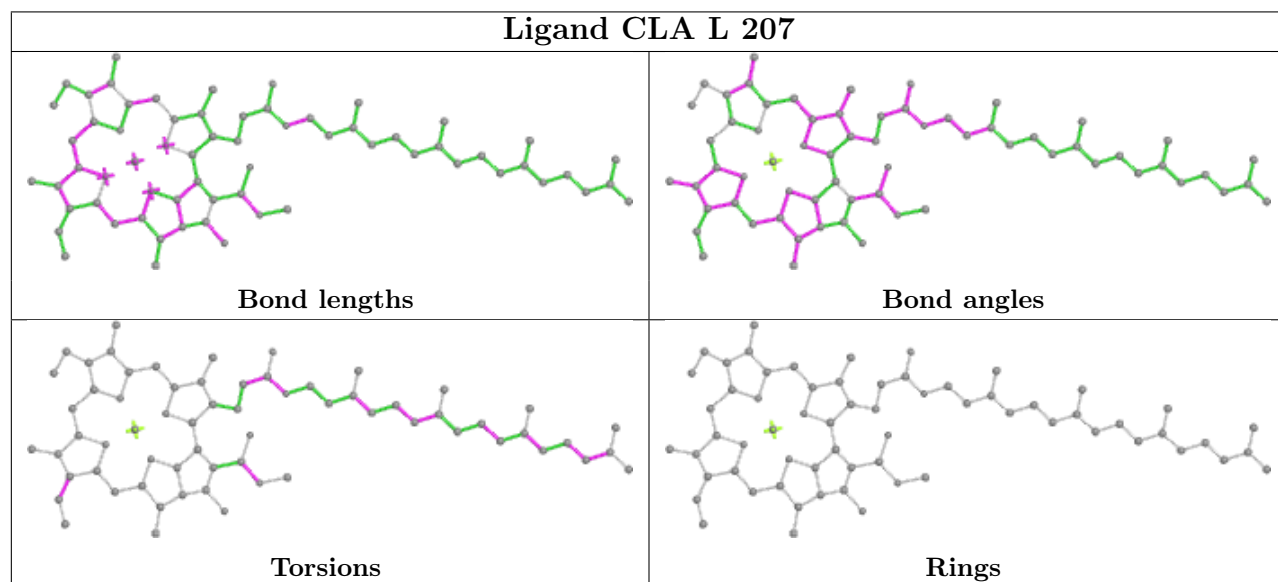
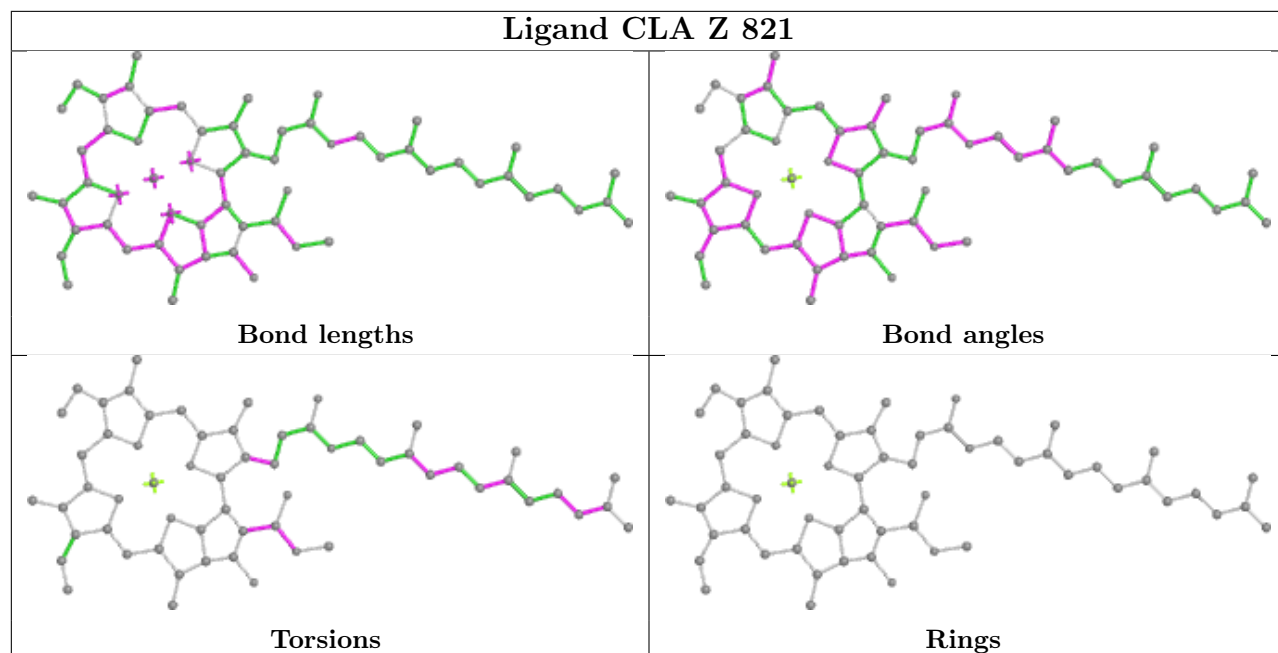




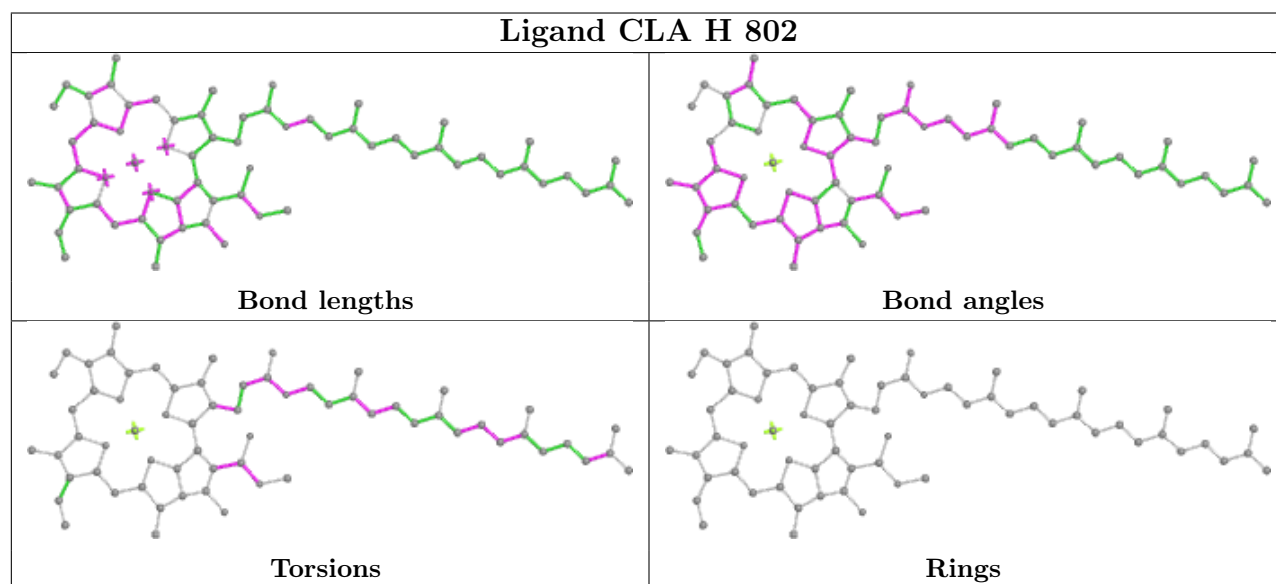
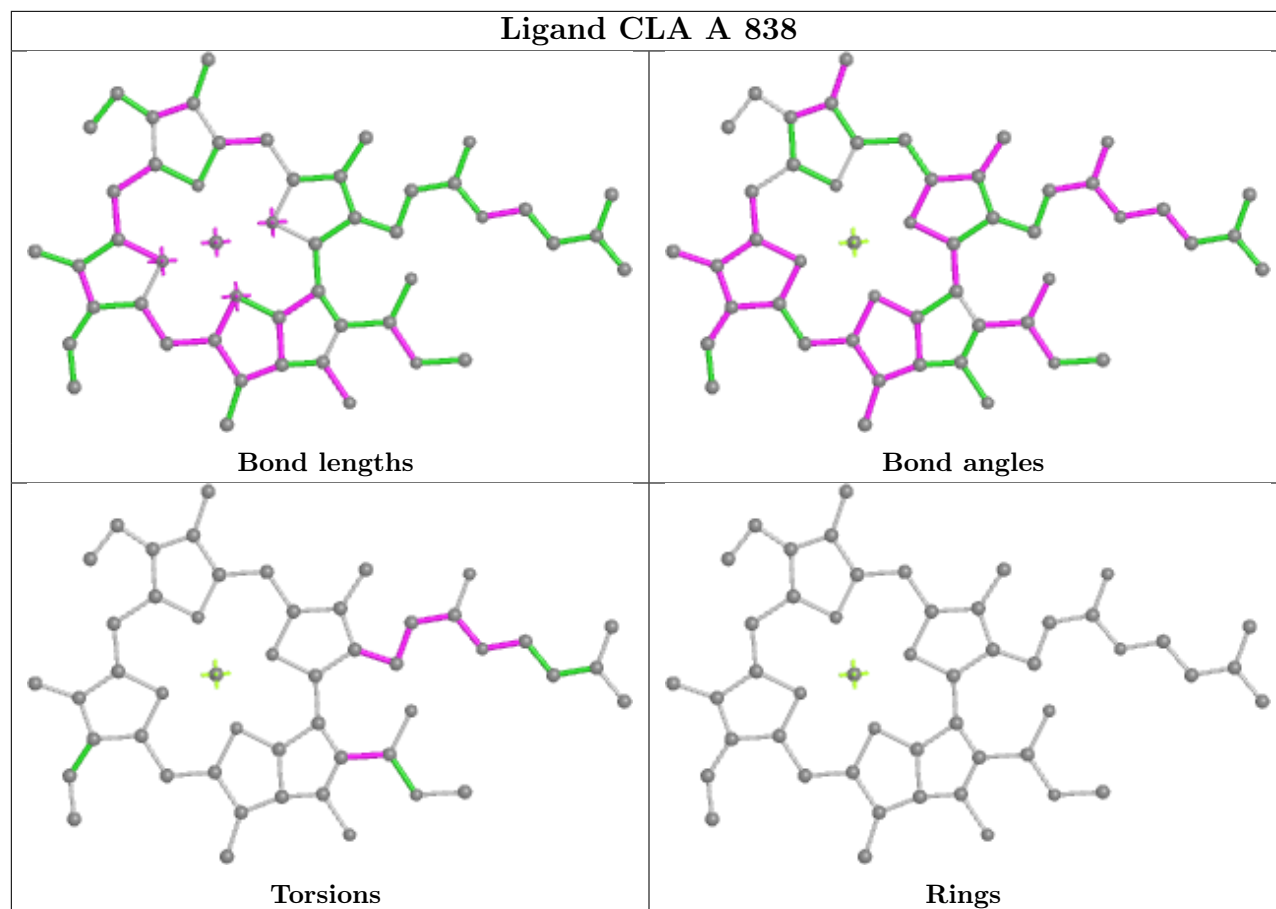


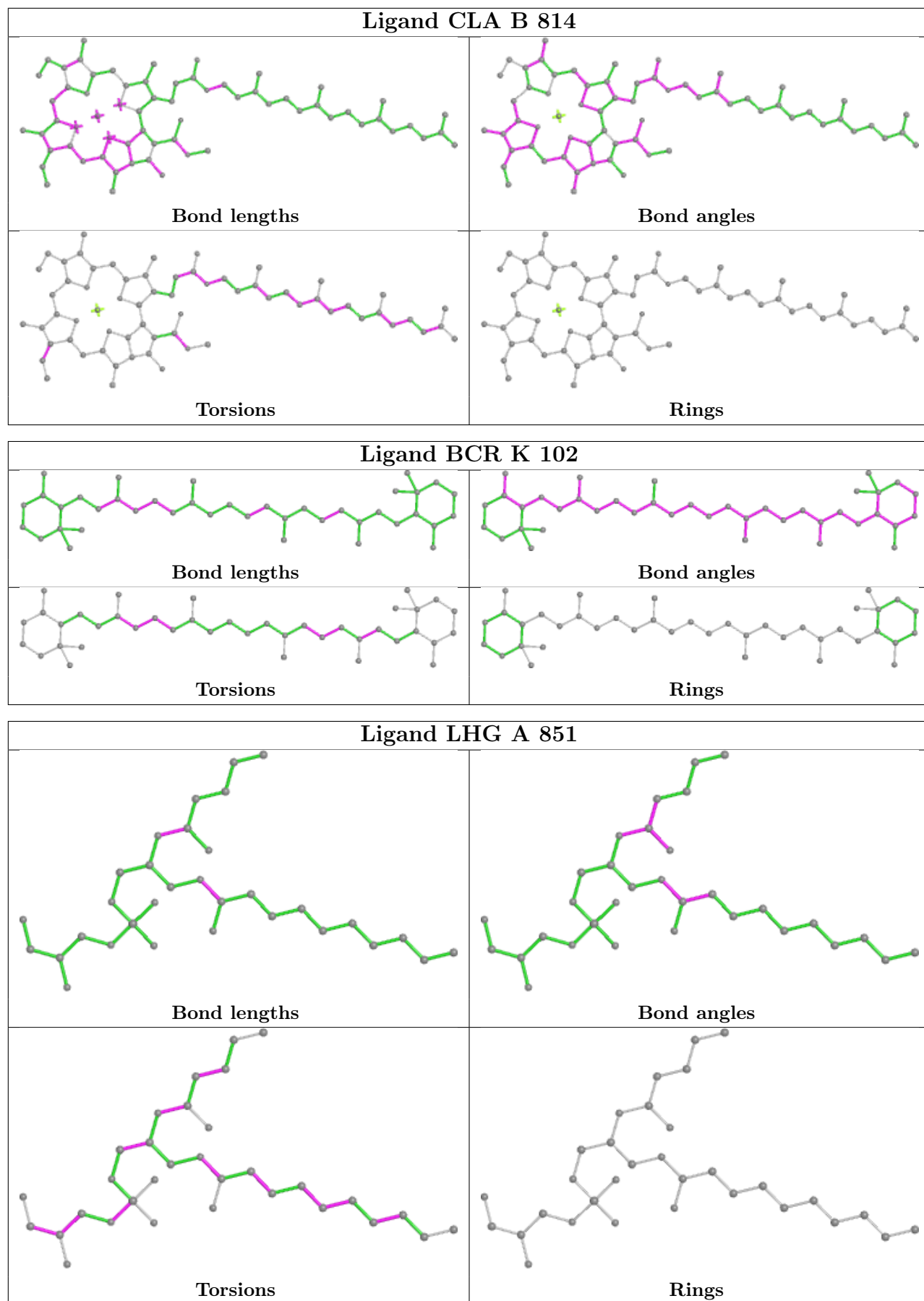


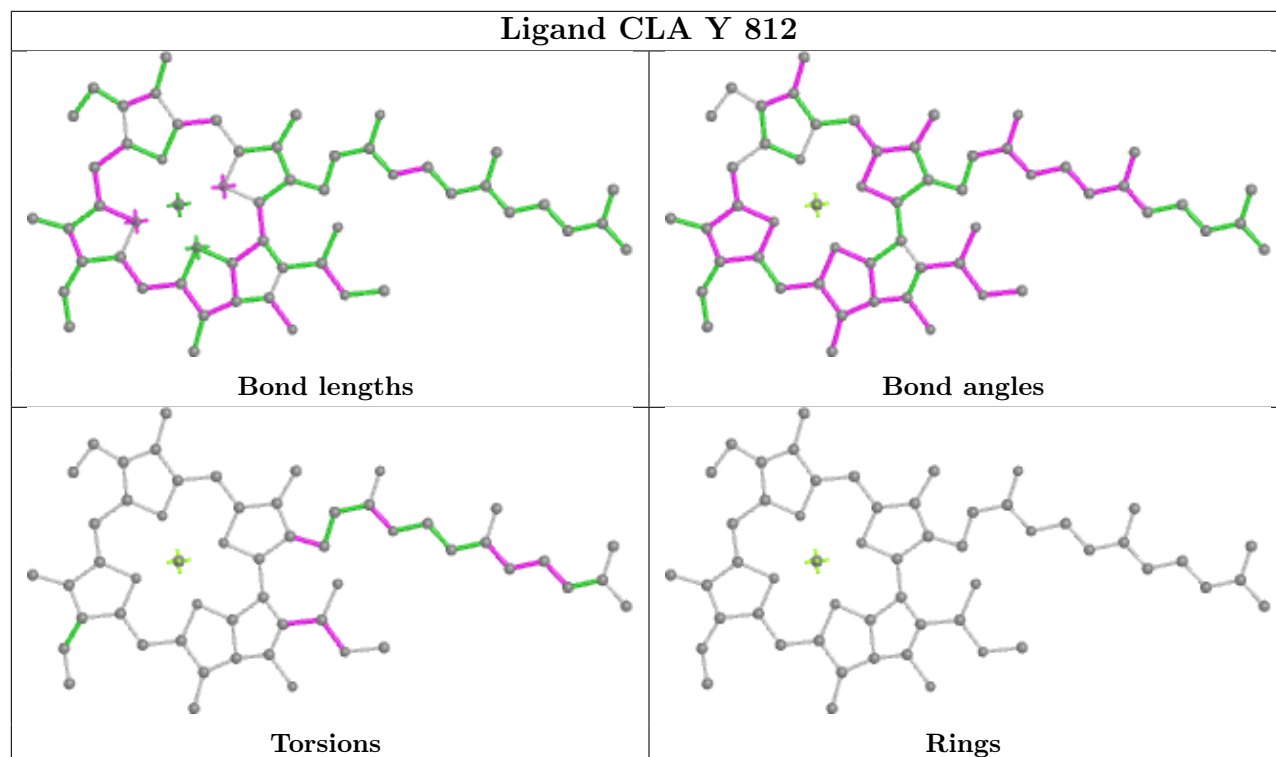
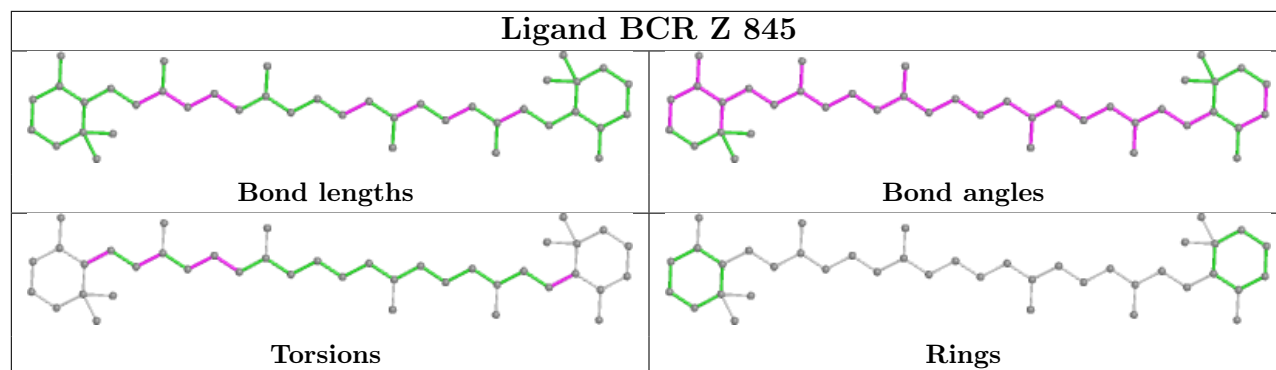


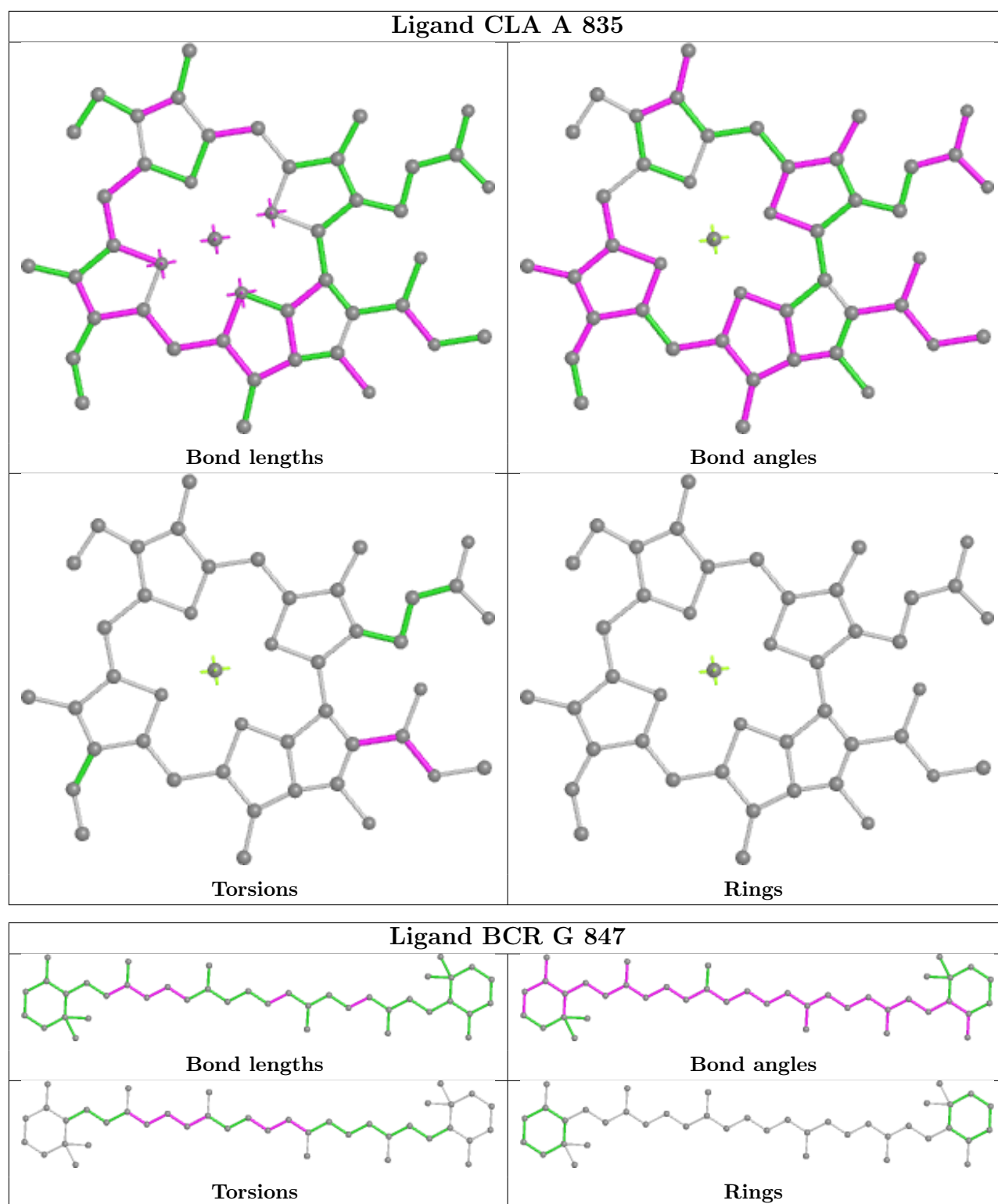


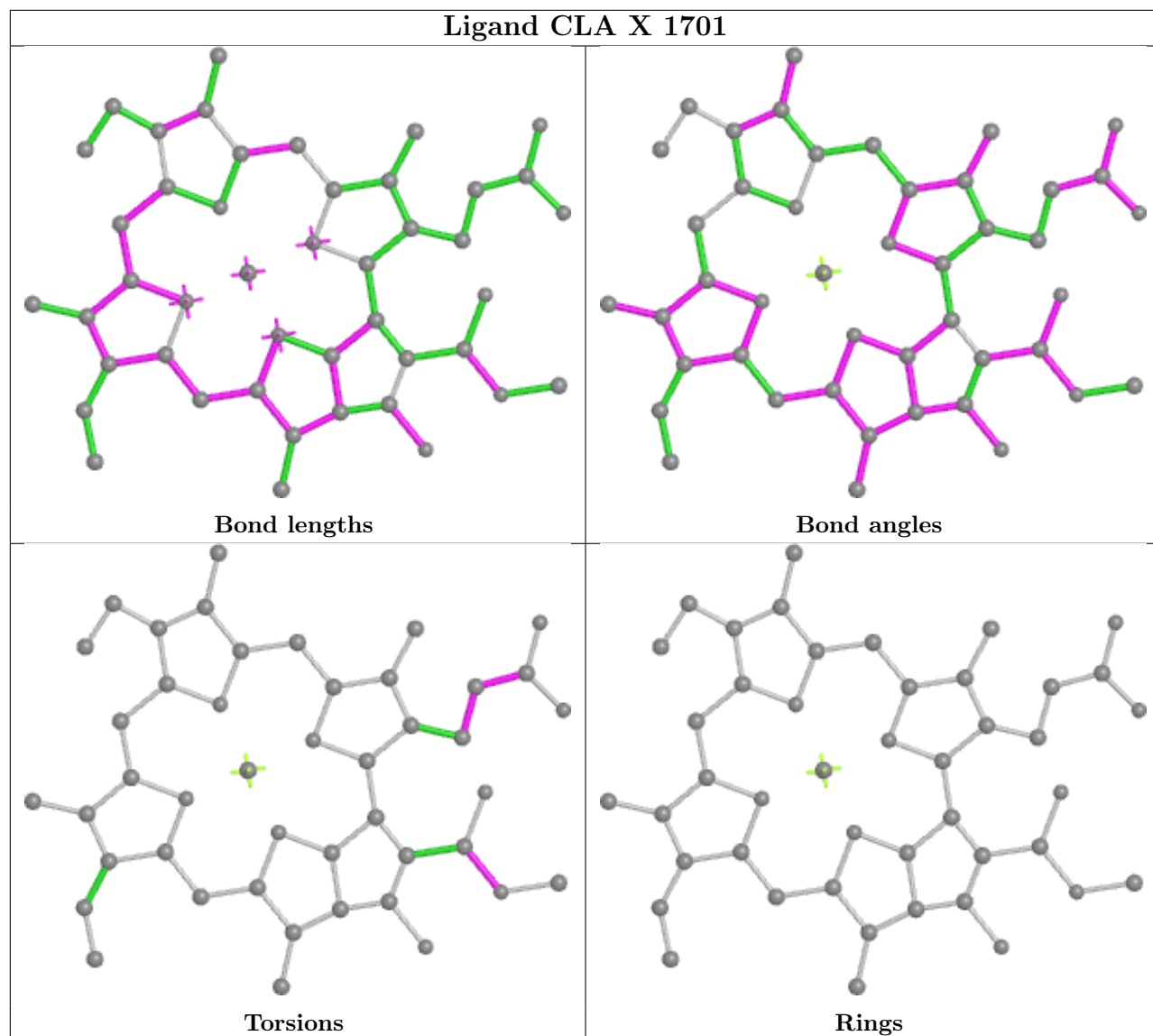


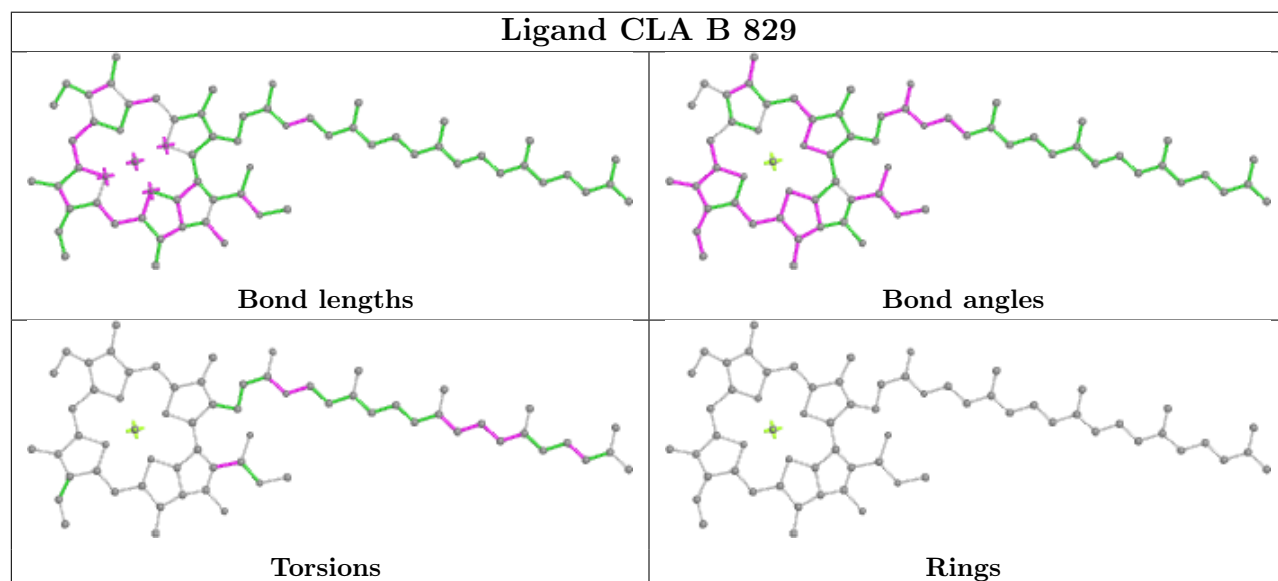
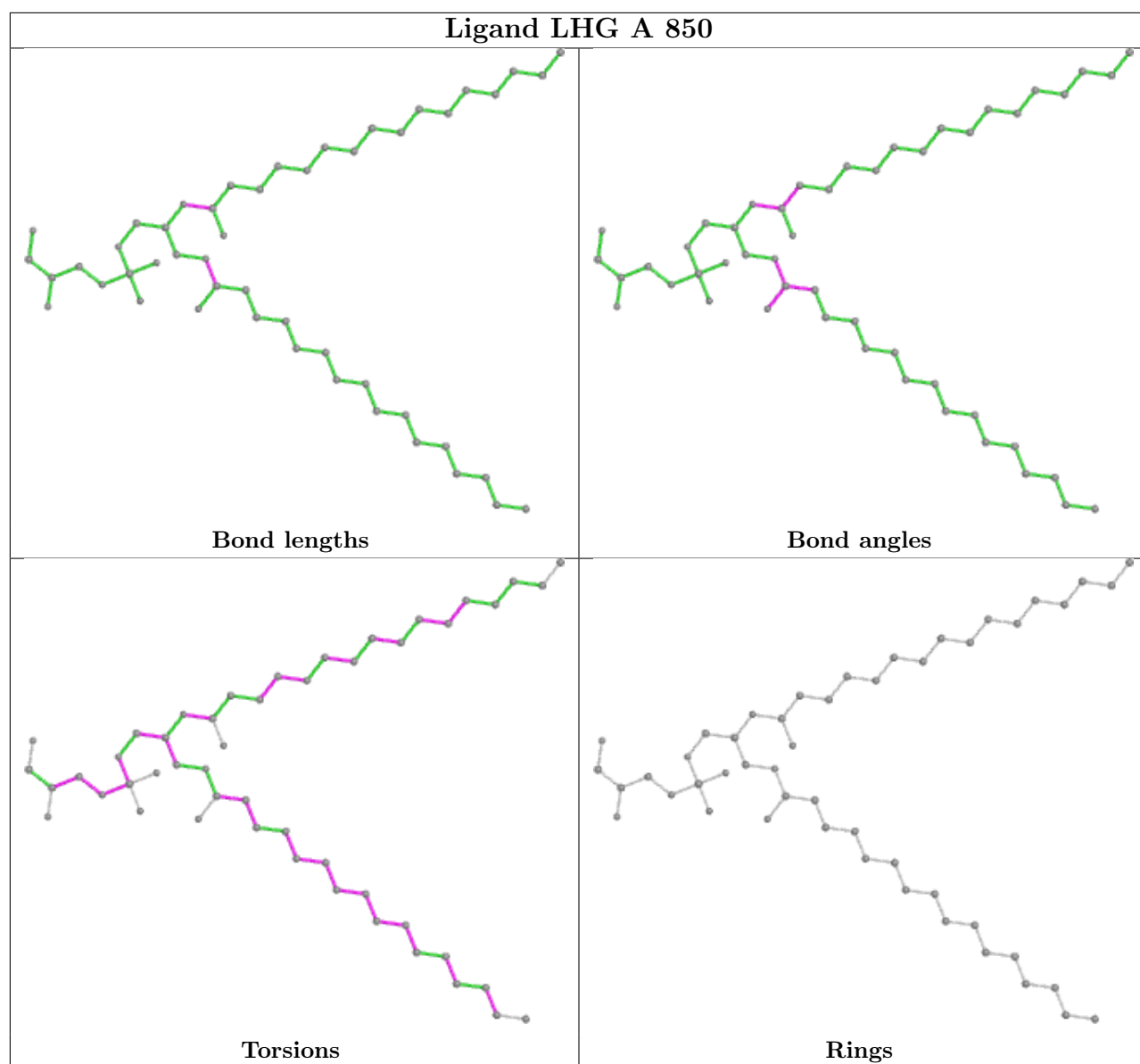


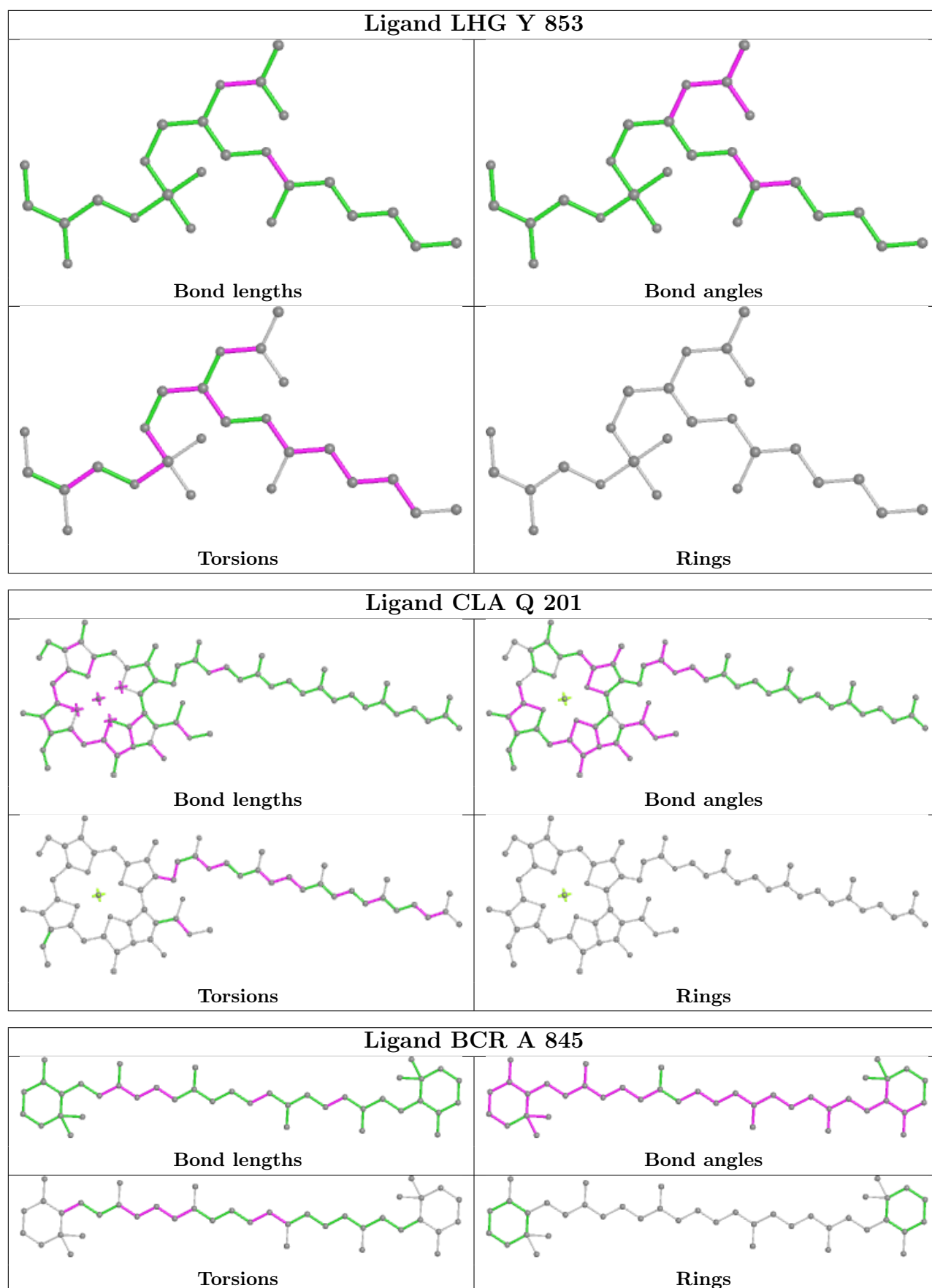


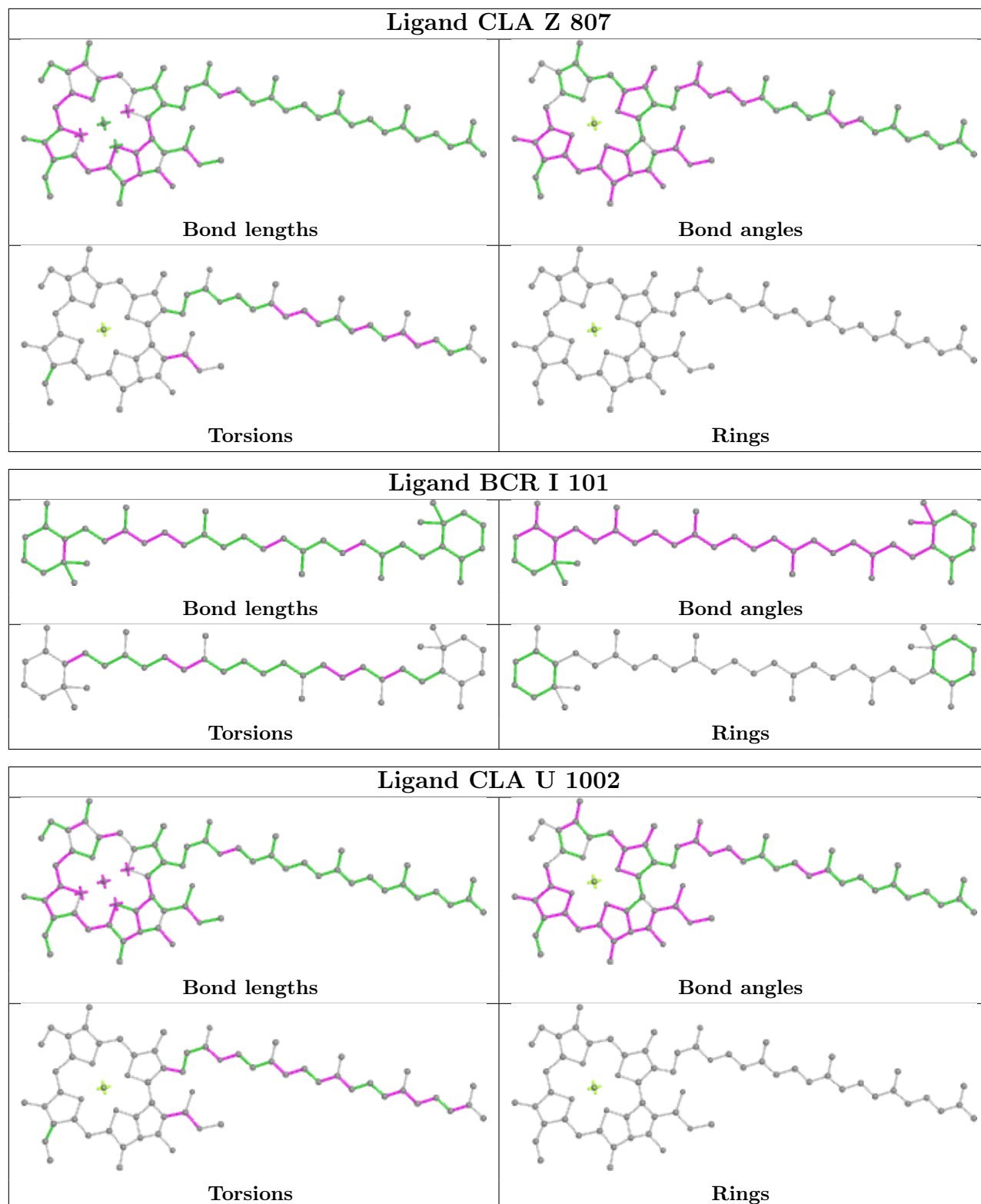




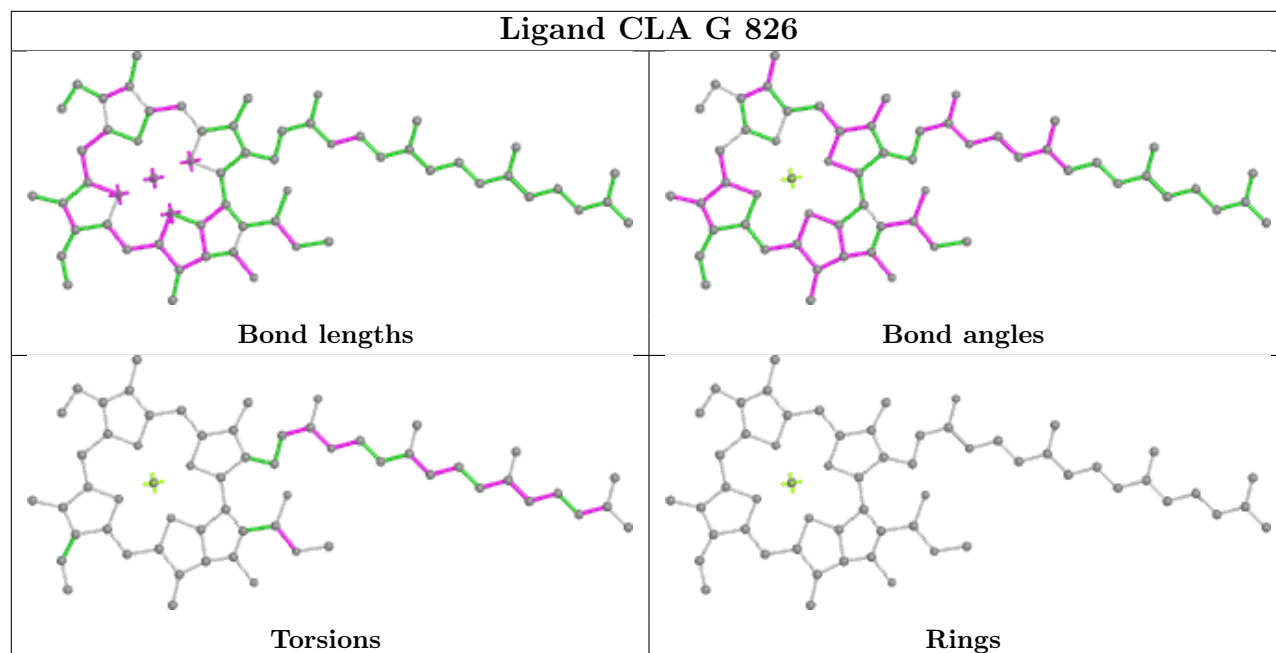
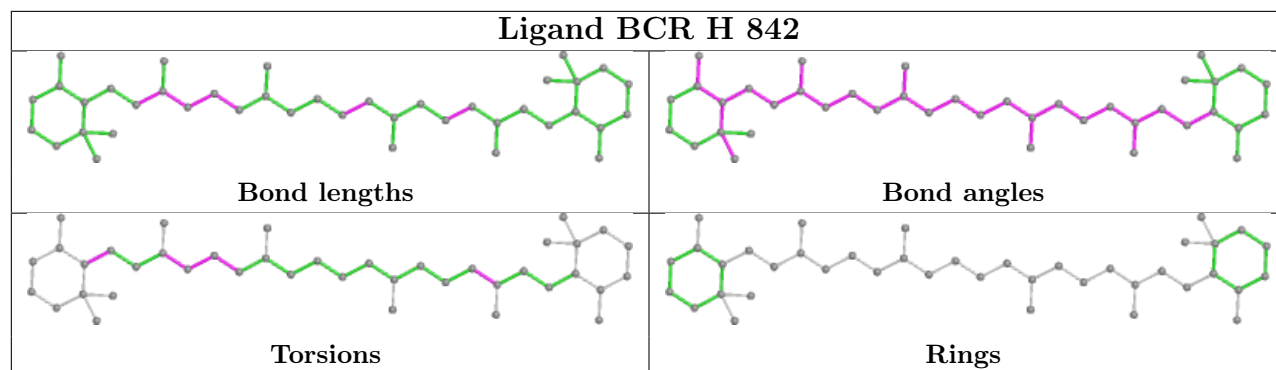


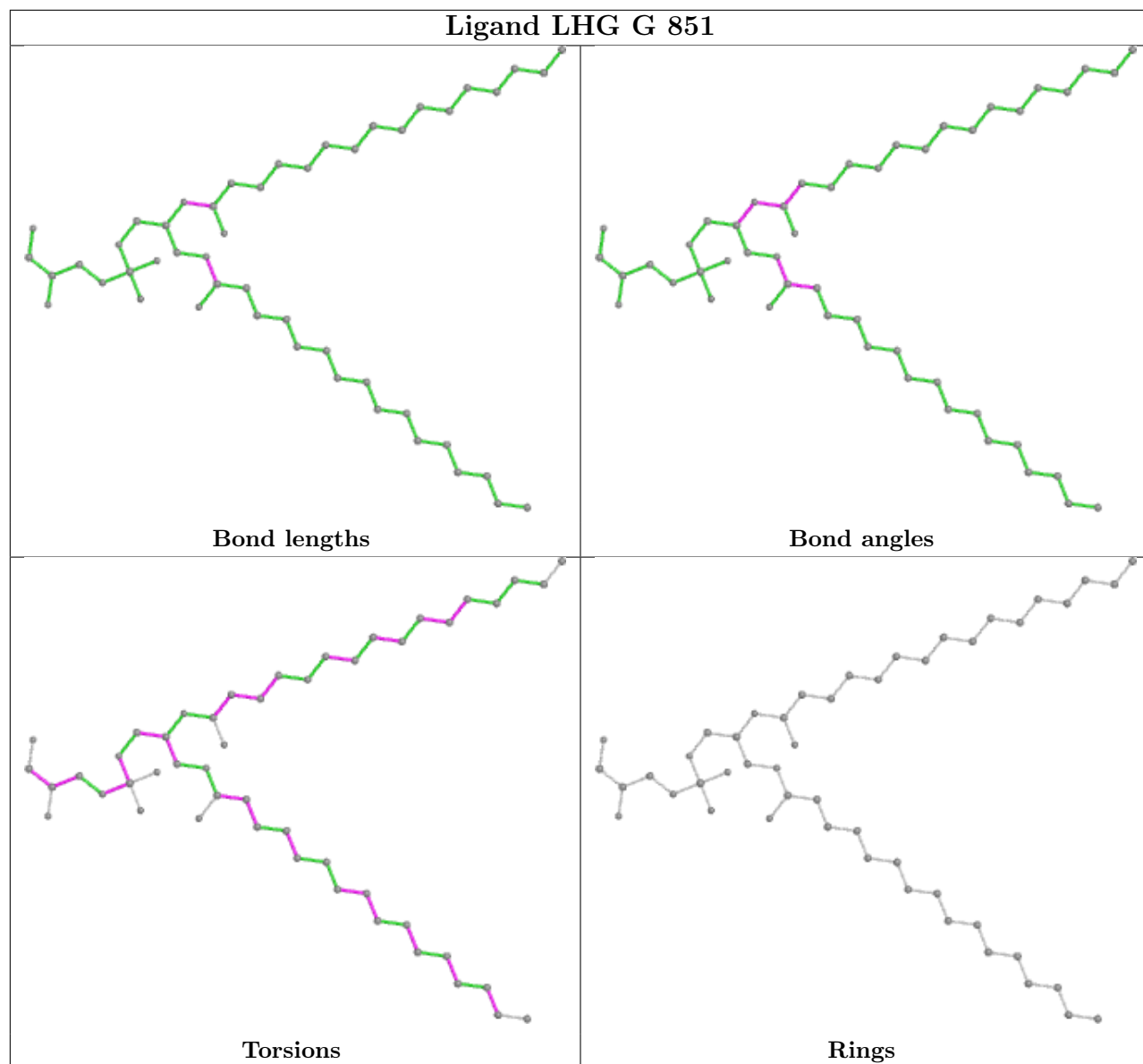




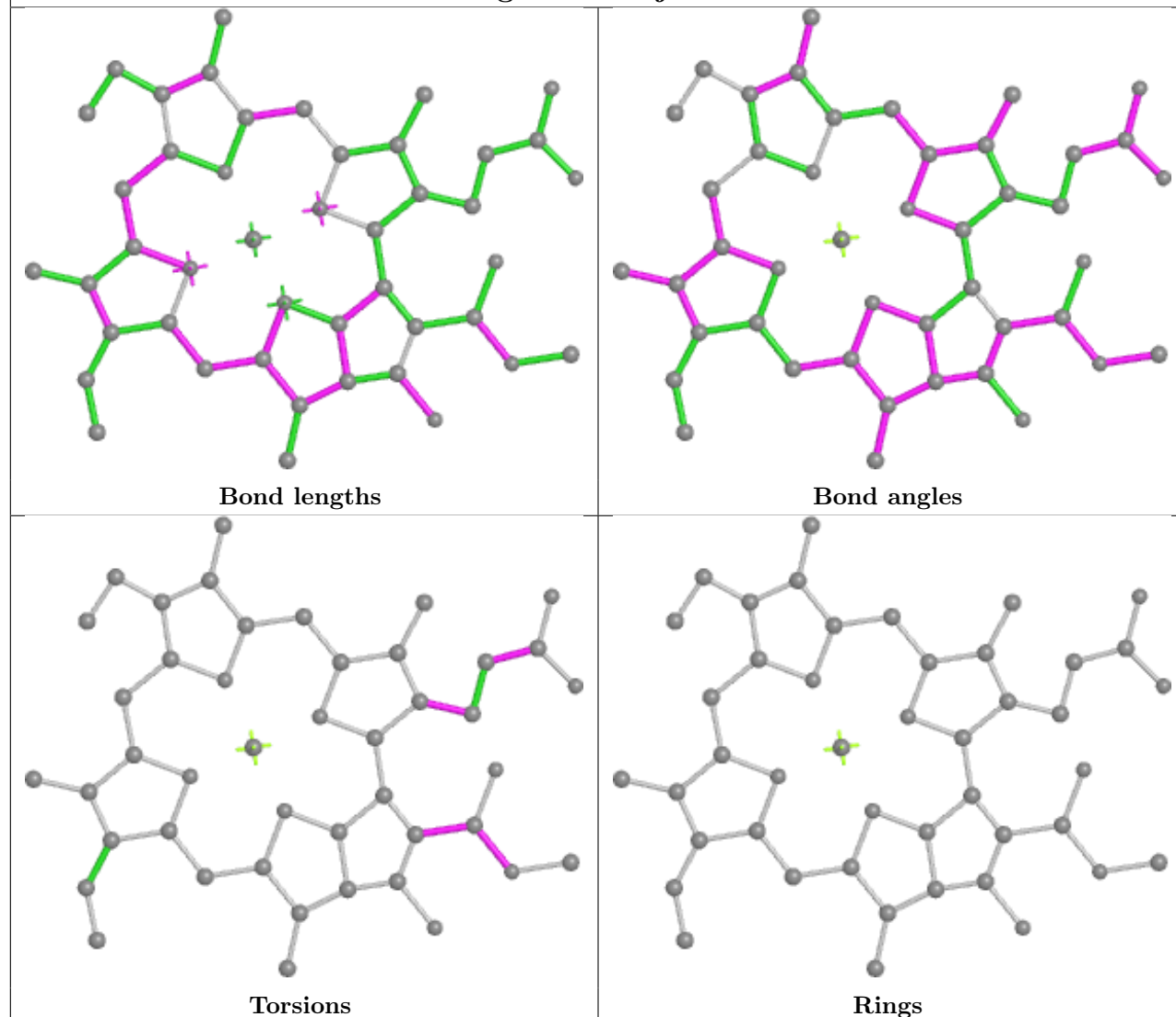




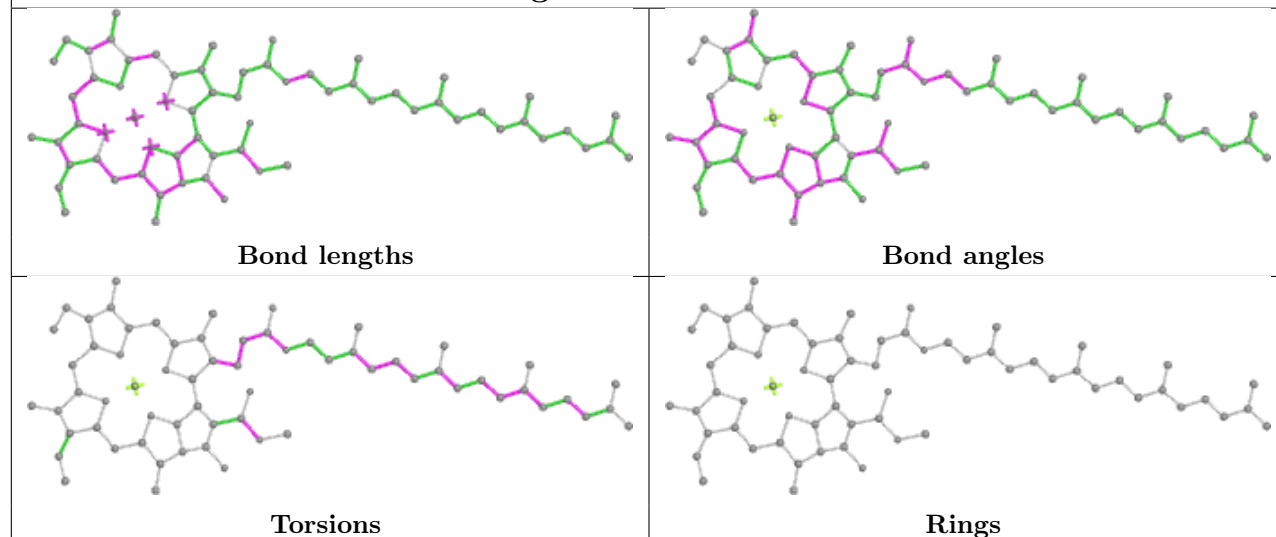


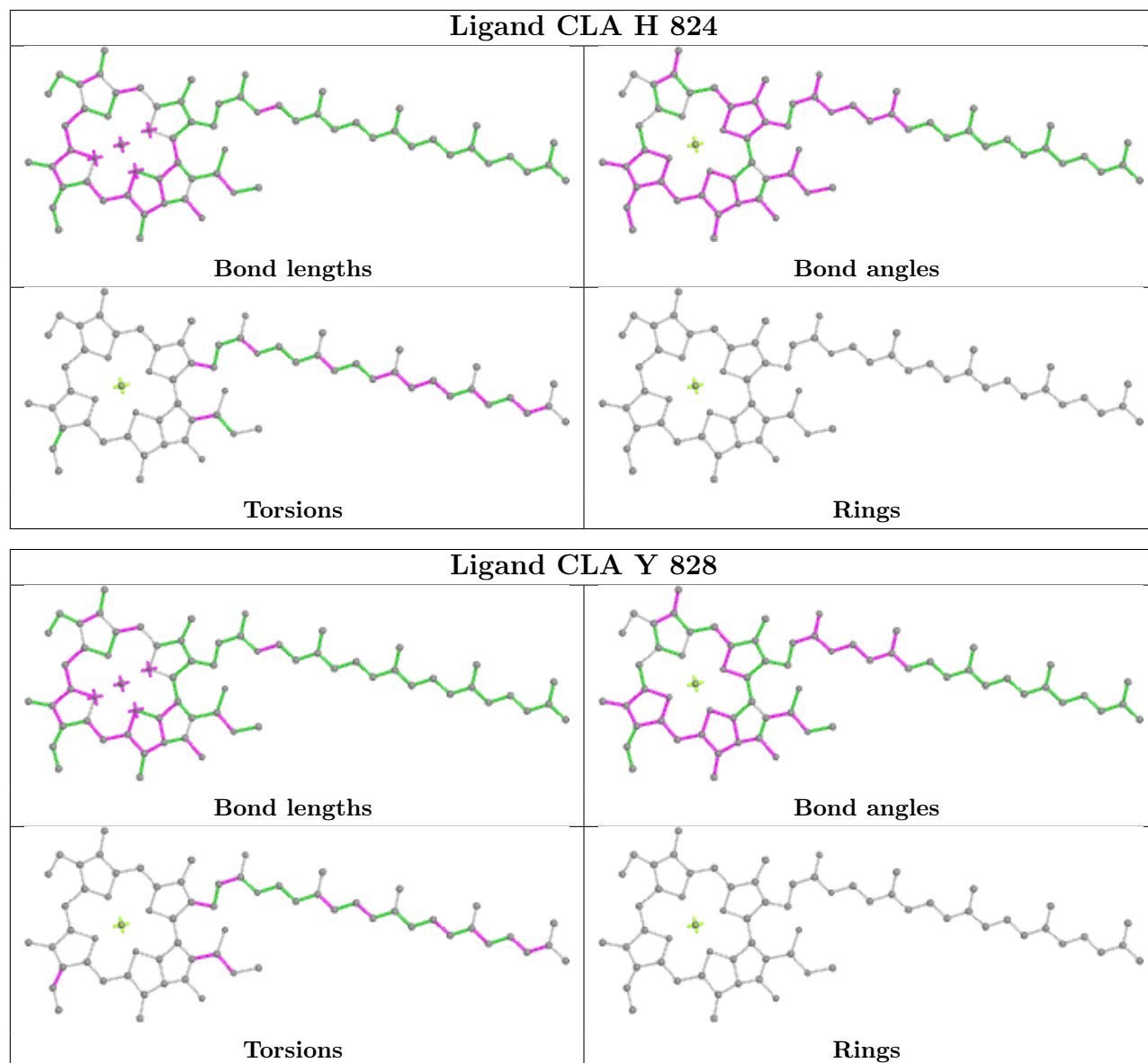


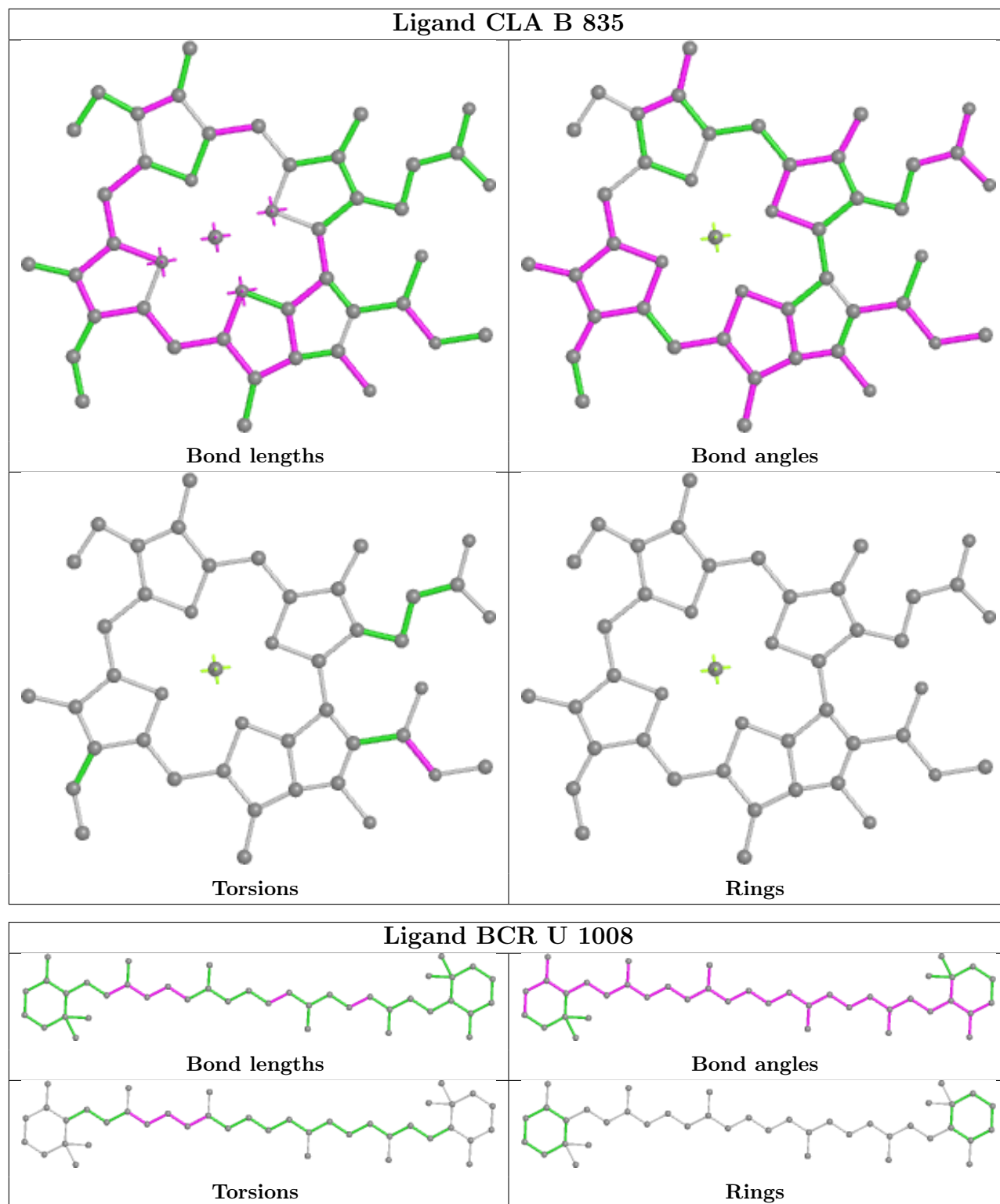
## Ligand CLA j 102

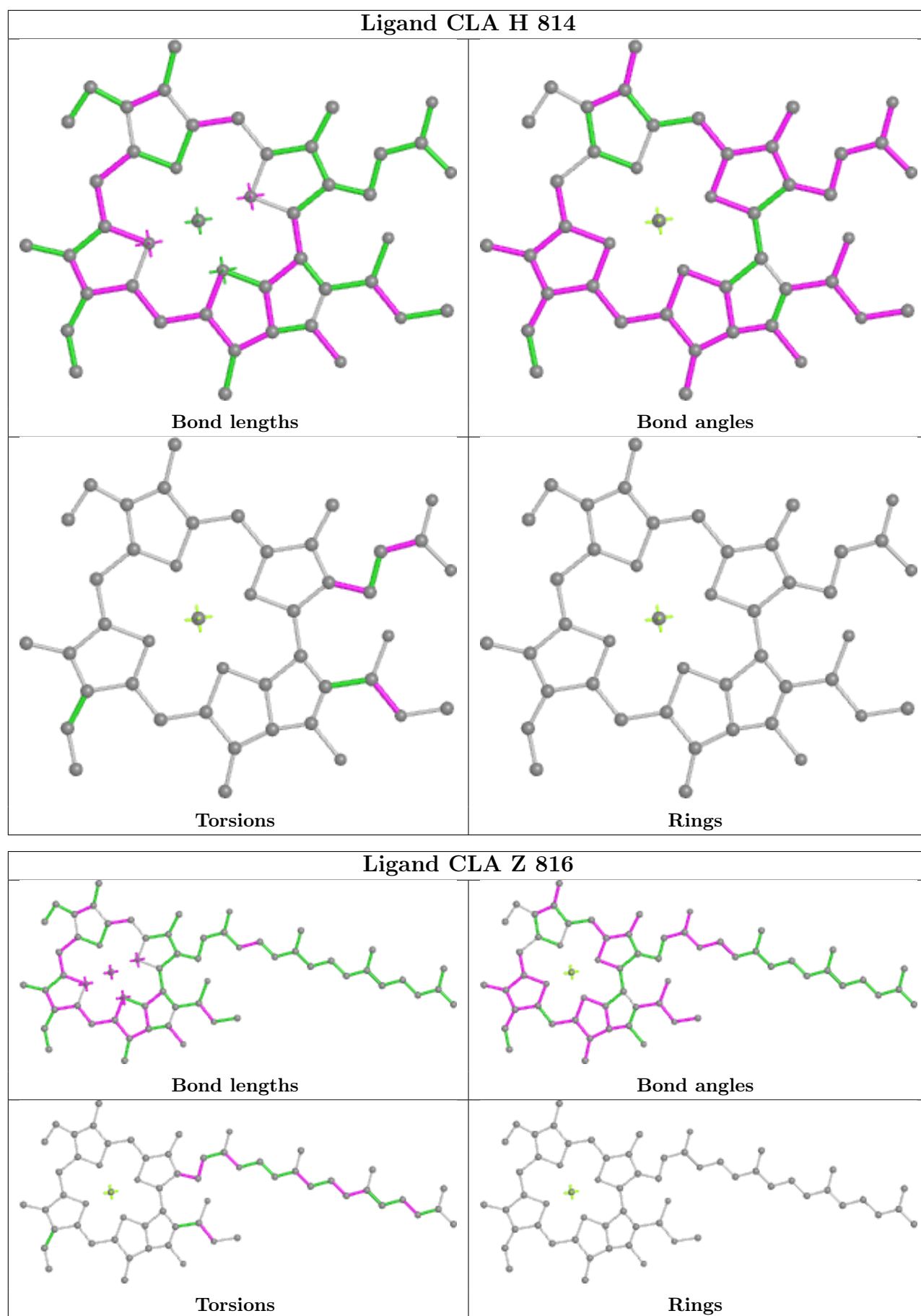


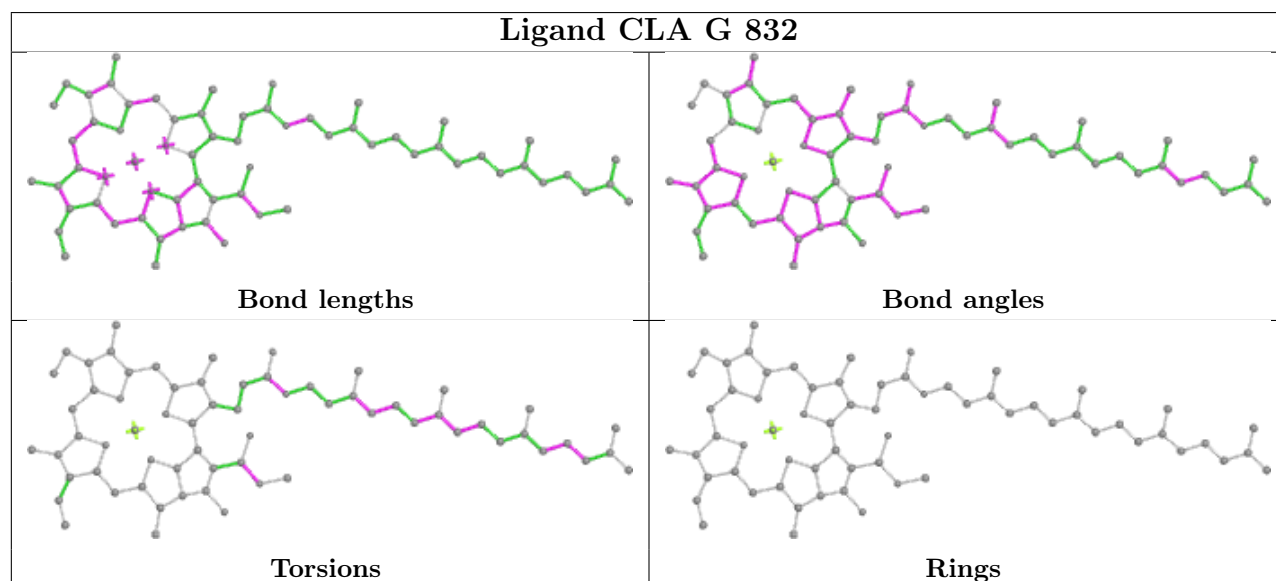
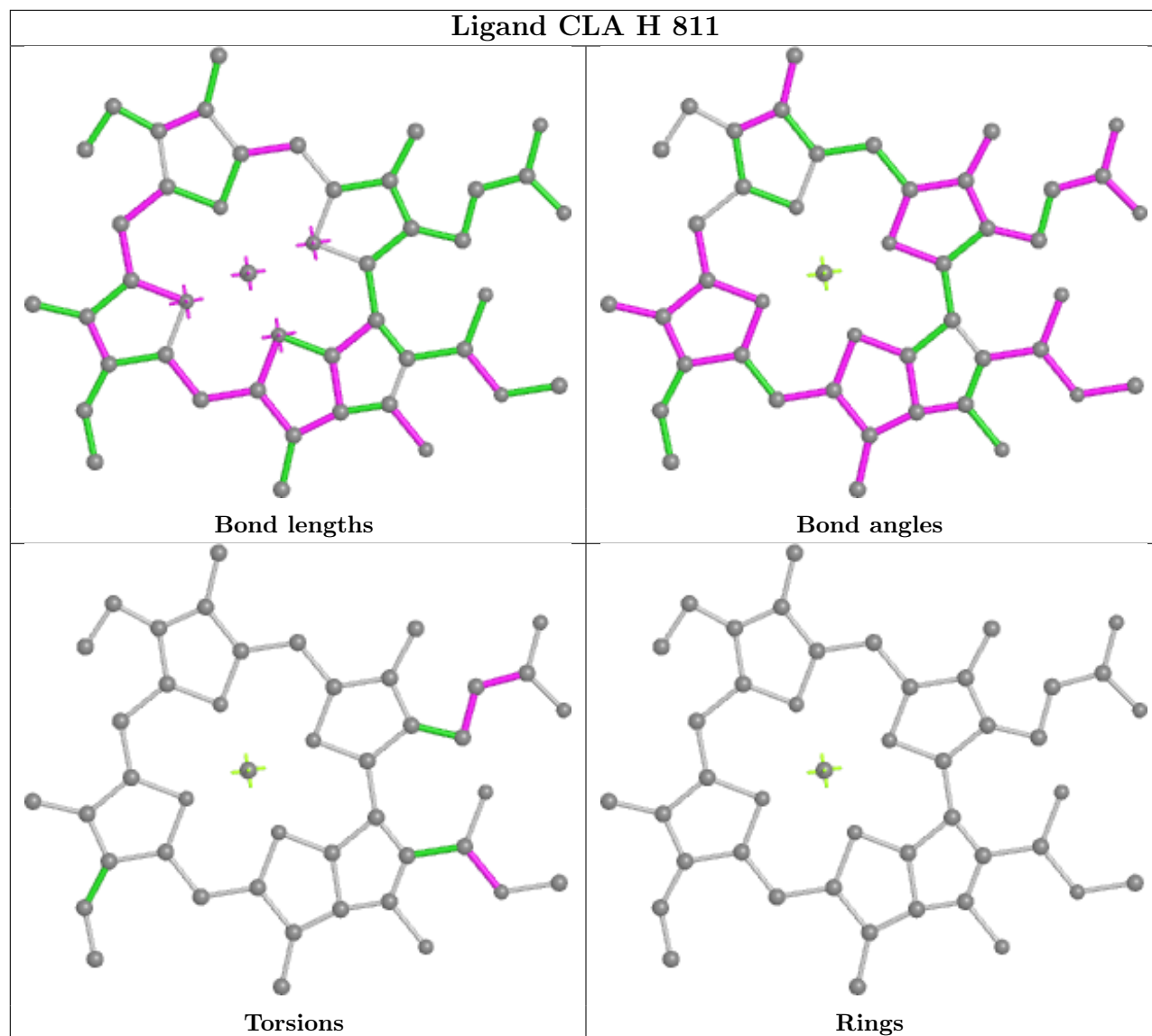
## Ligand CLA G 806

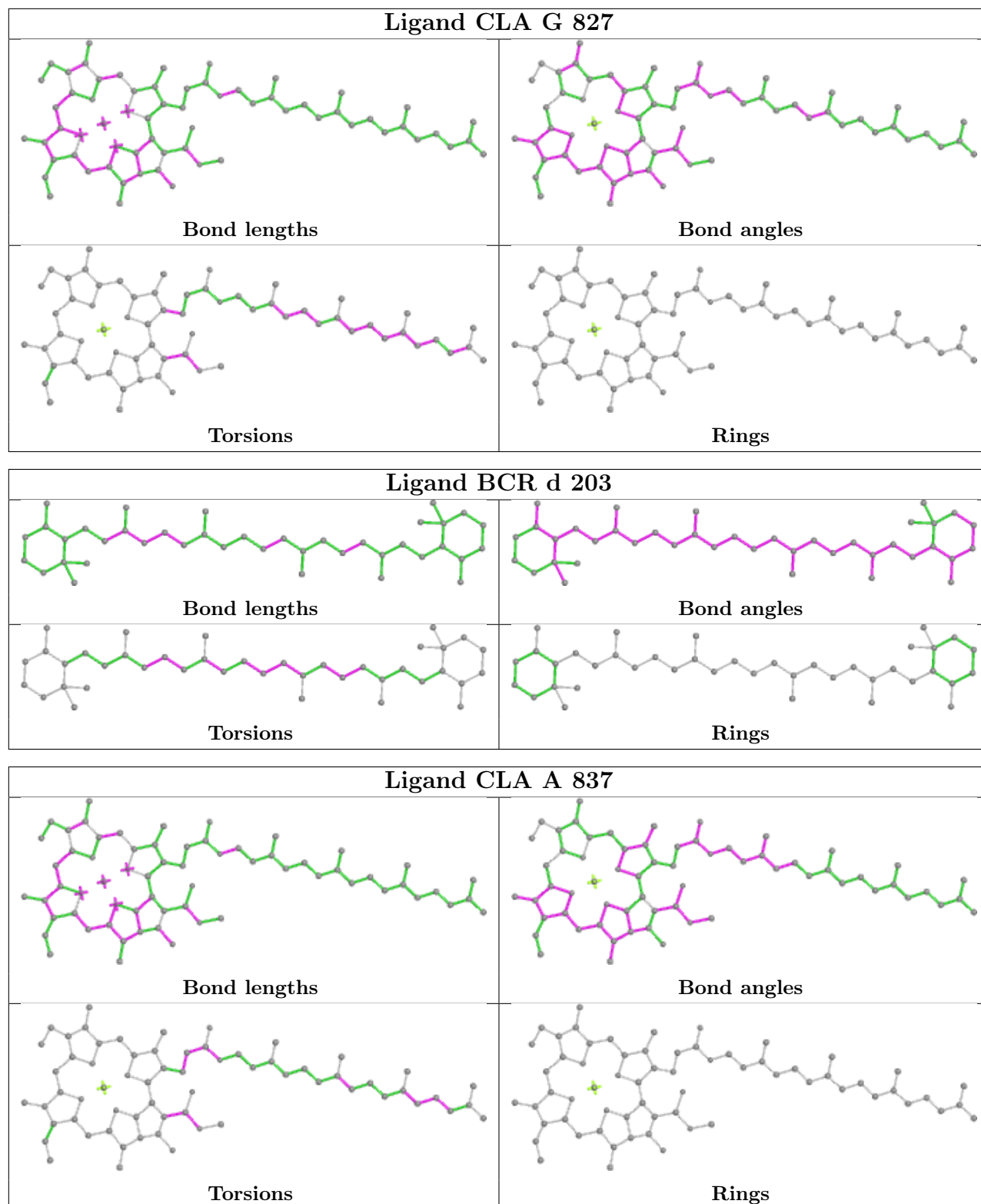




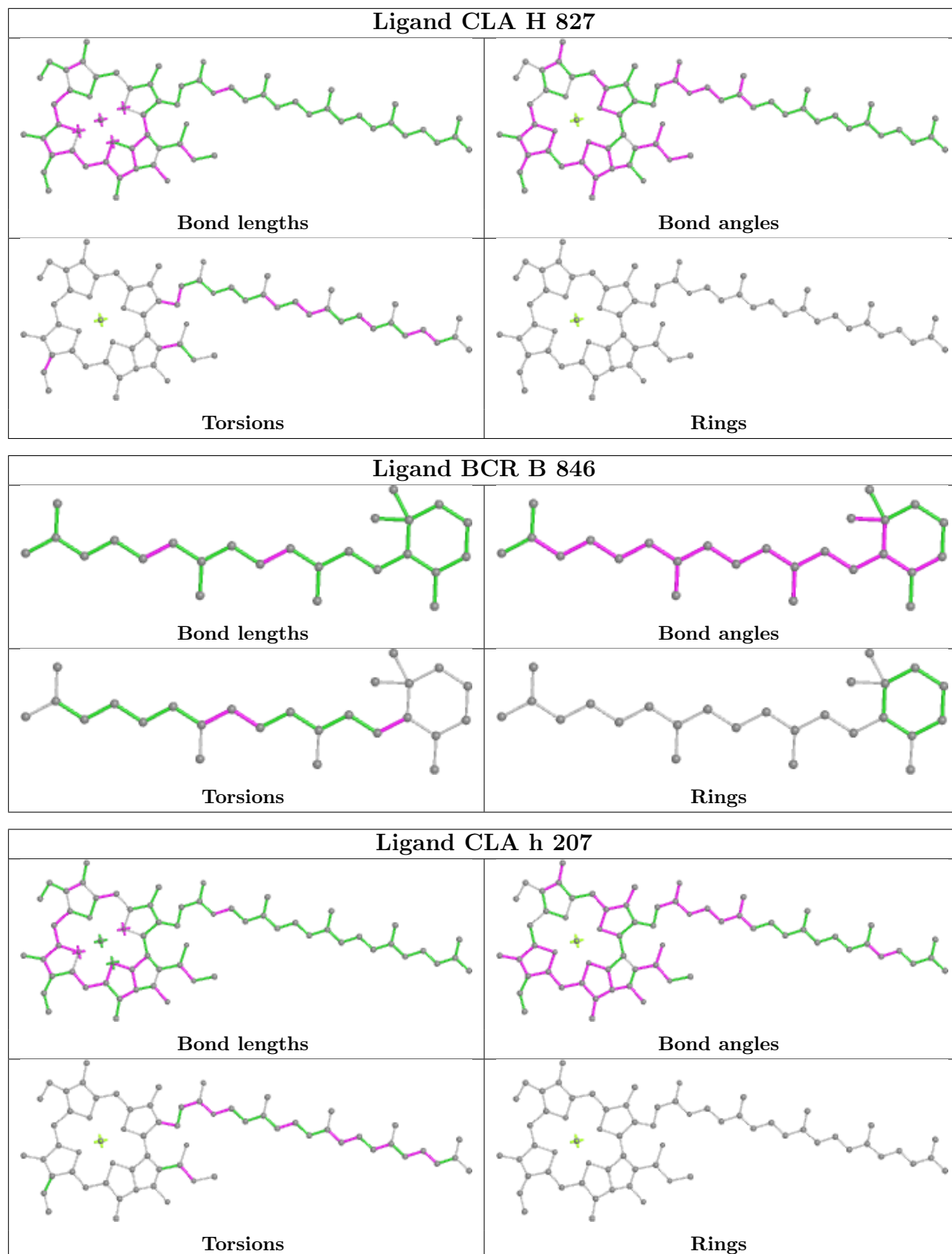


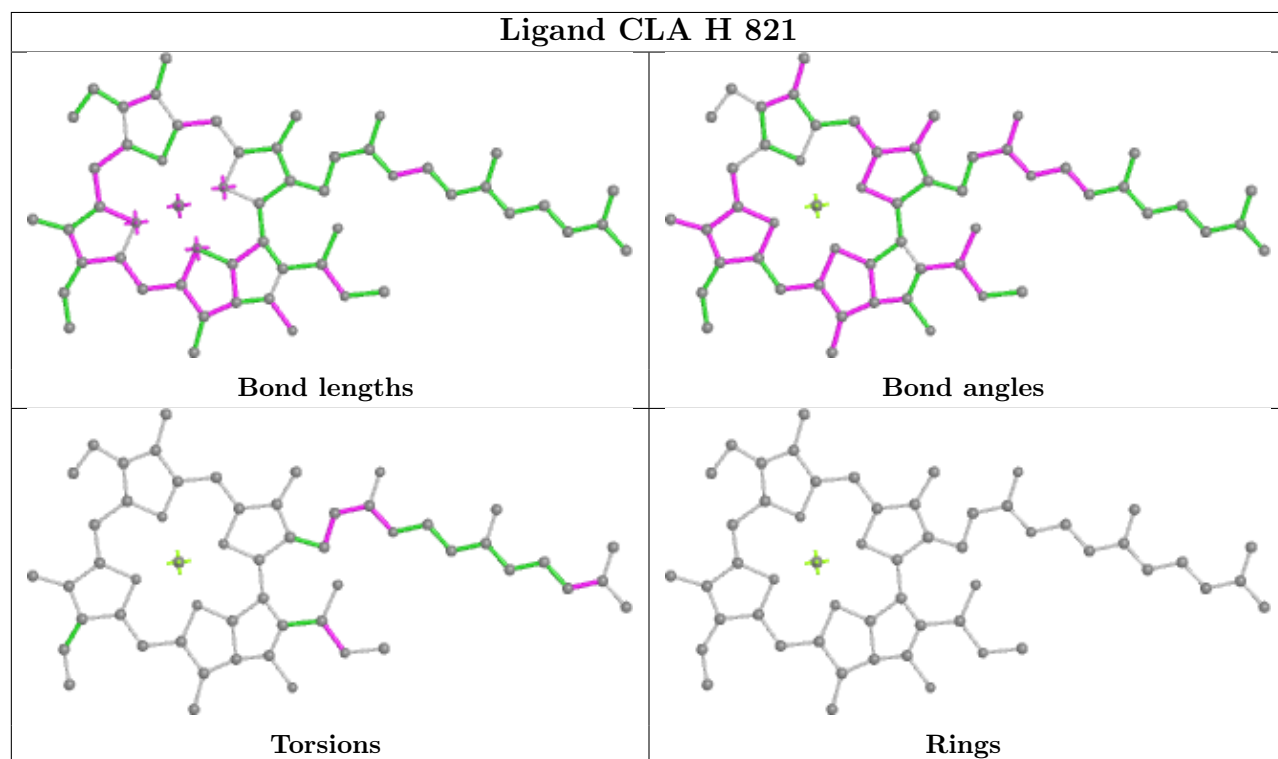
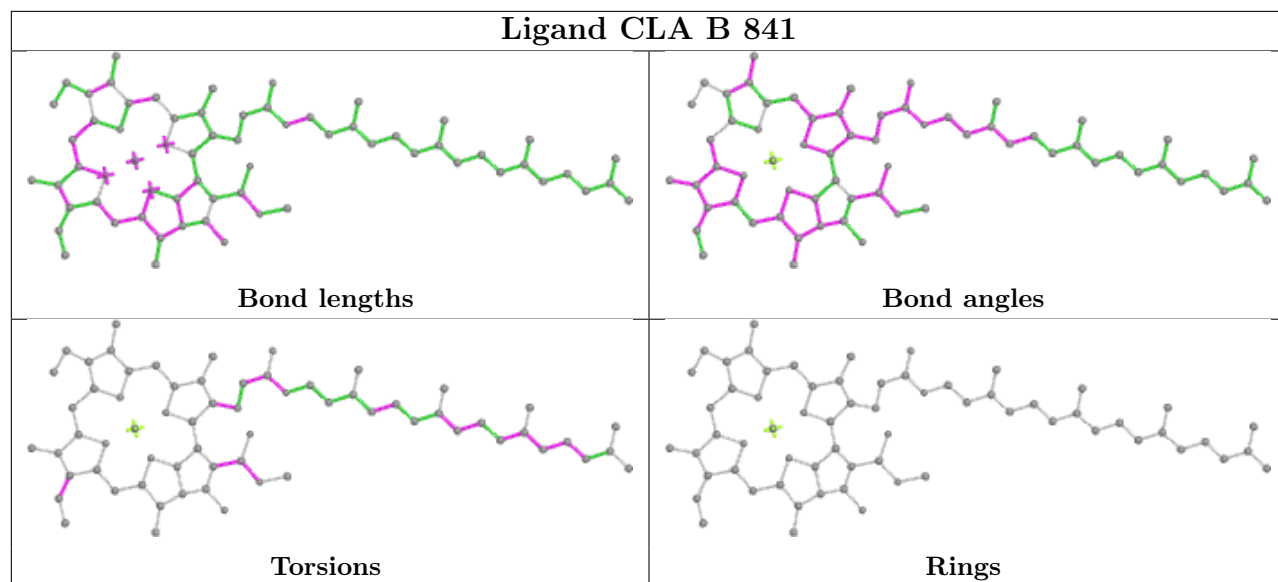


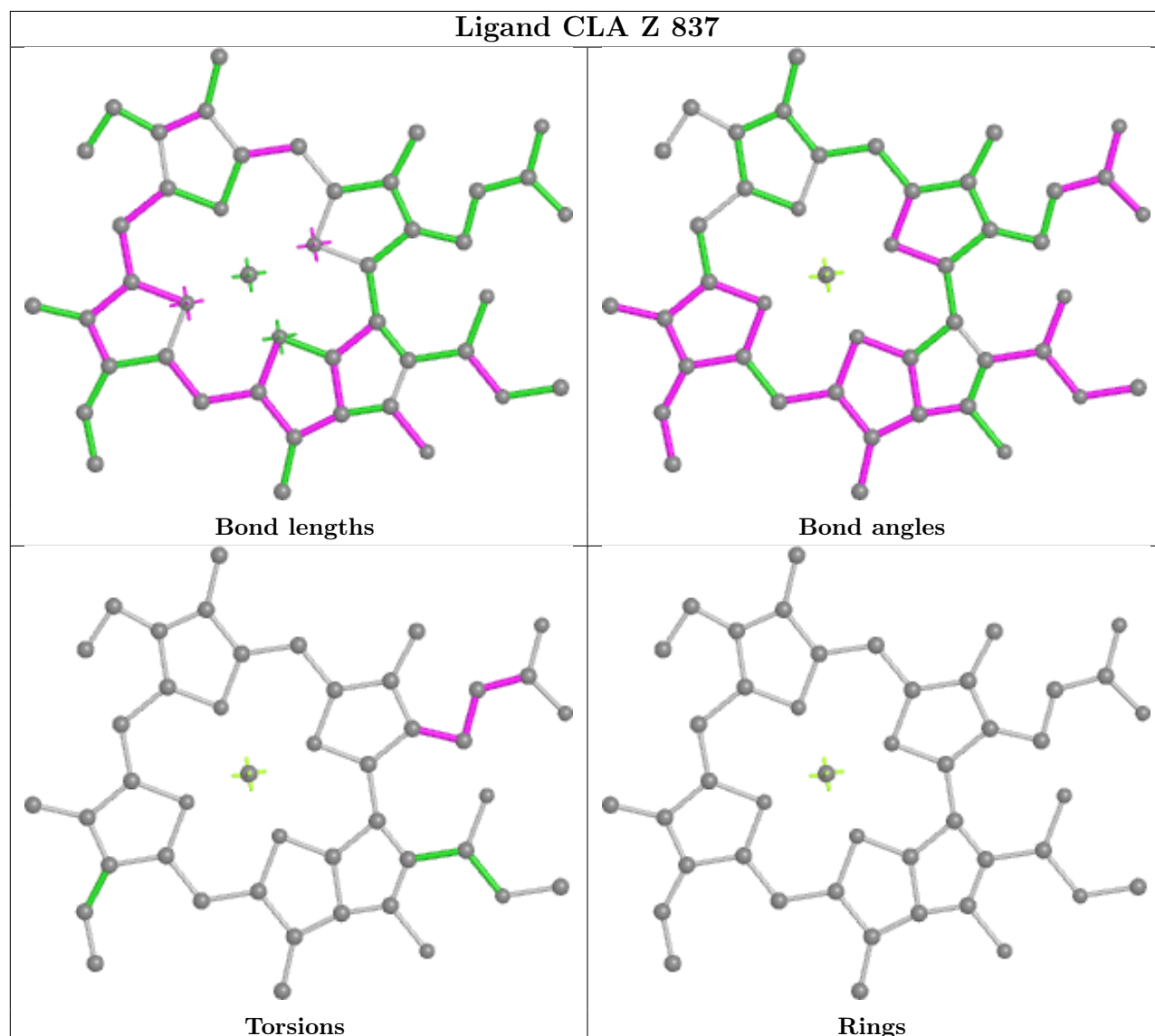
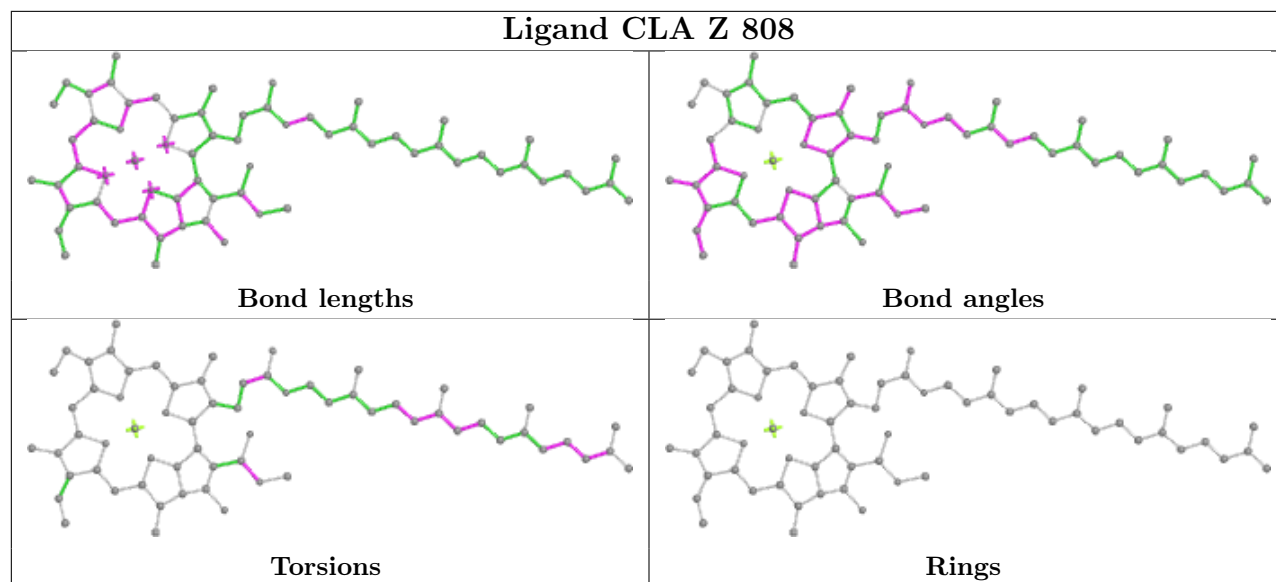


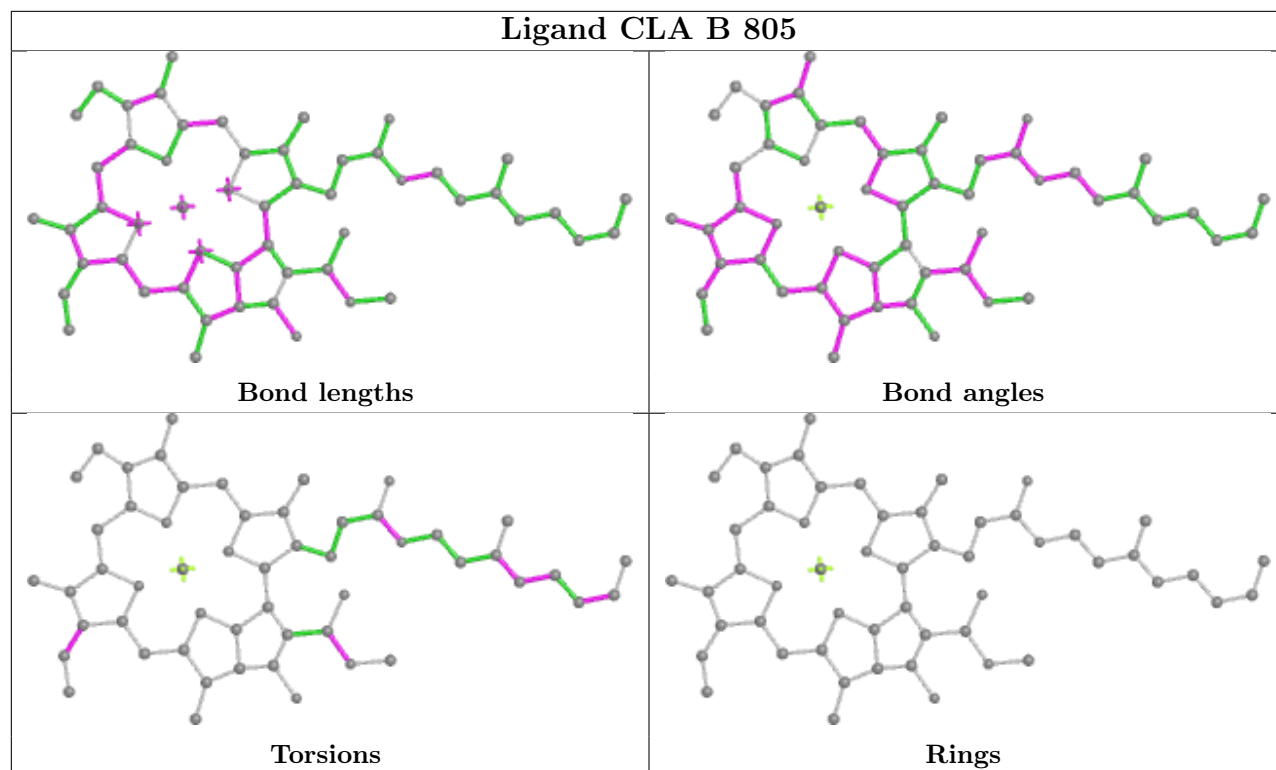




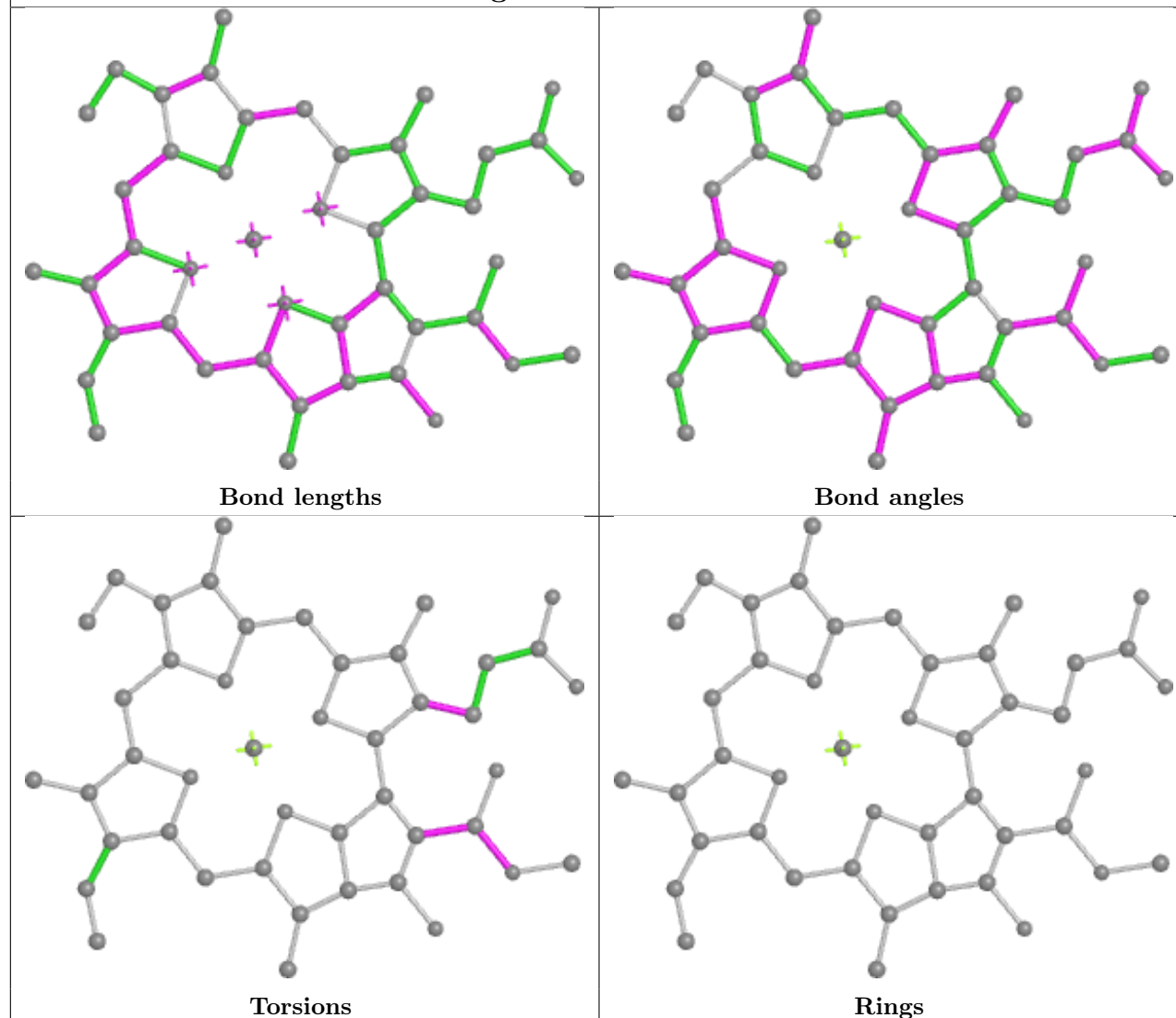




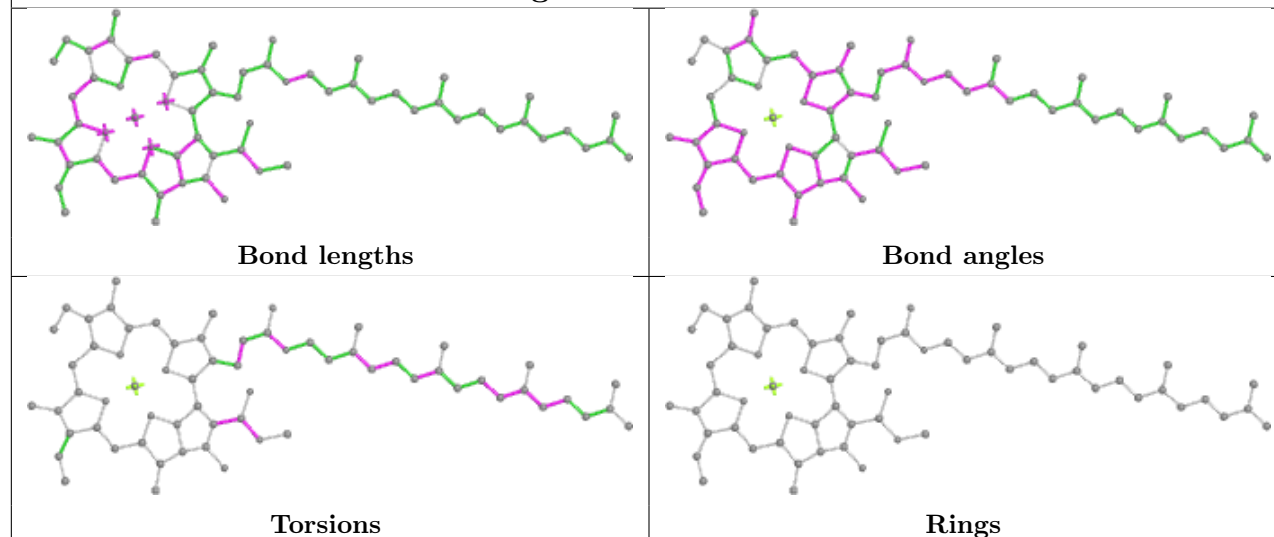




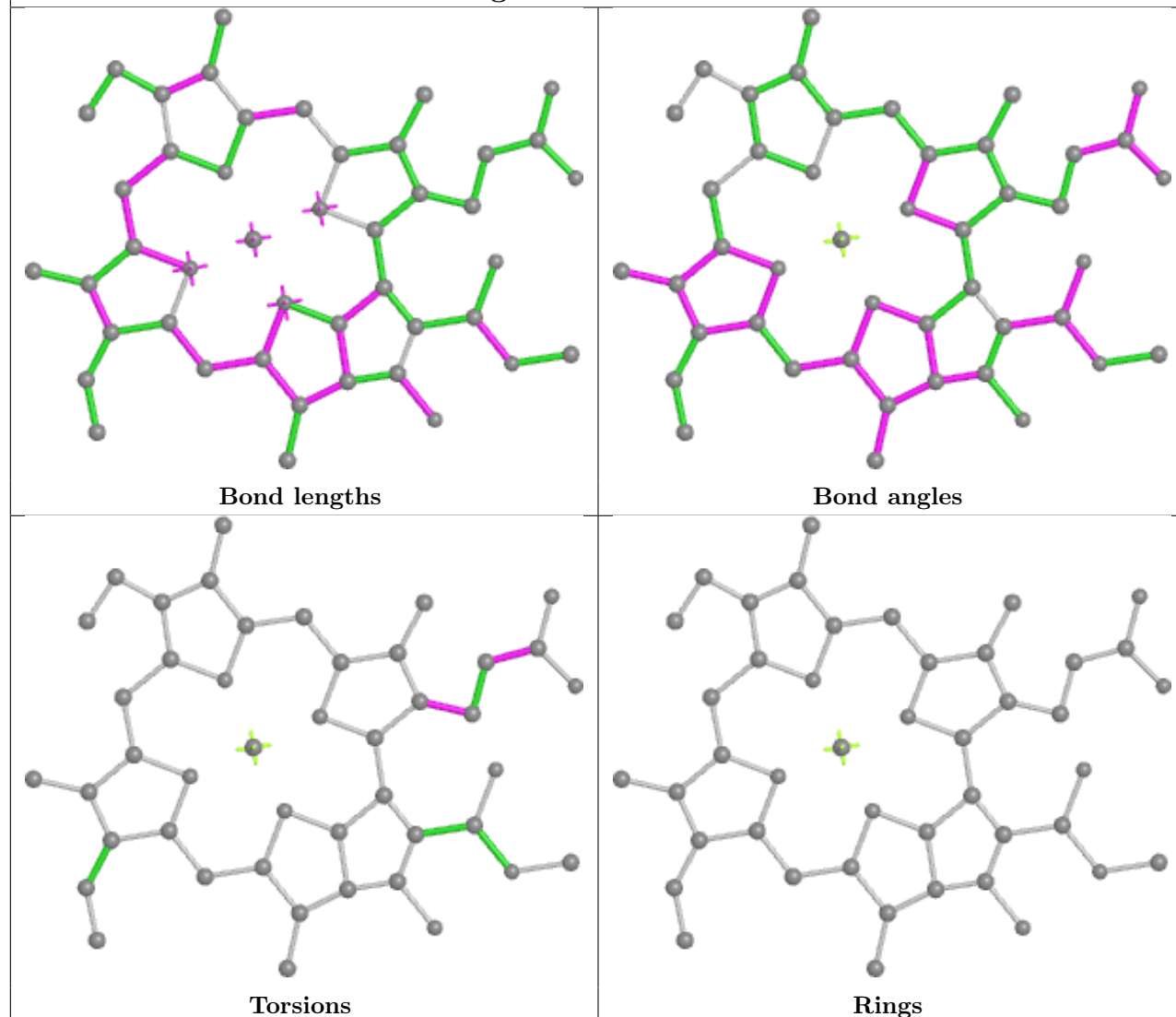
## Ligand CLA Y 810



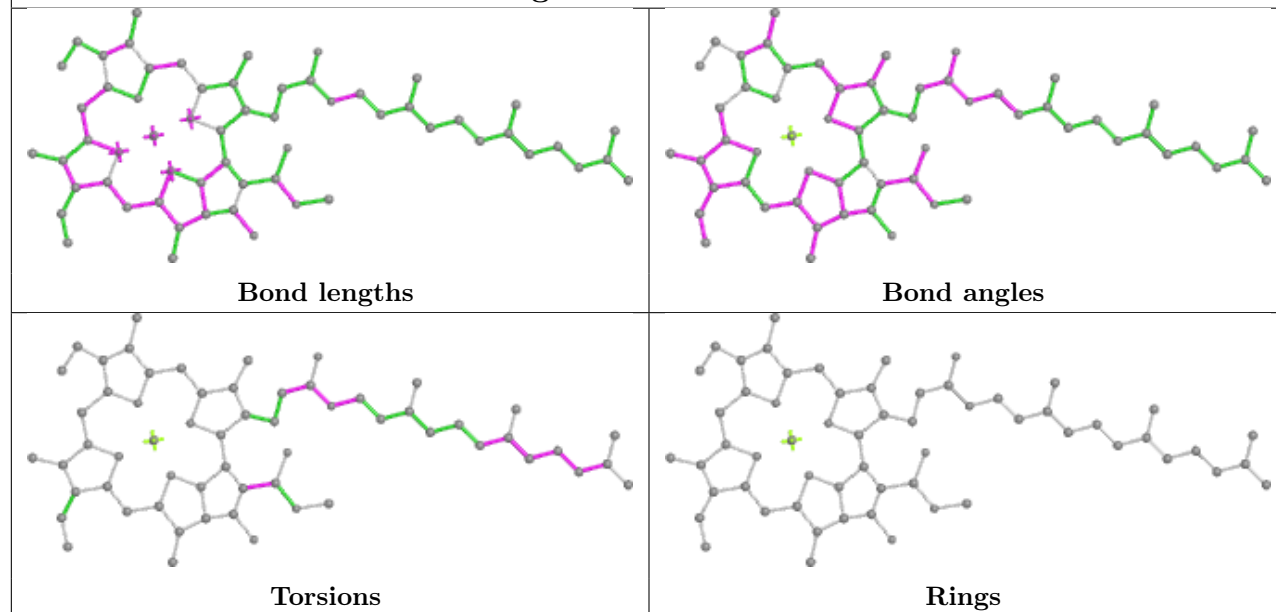
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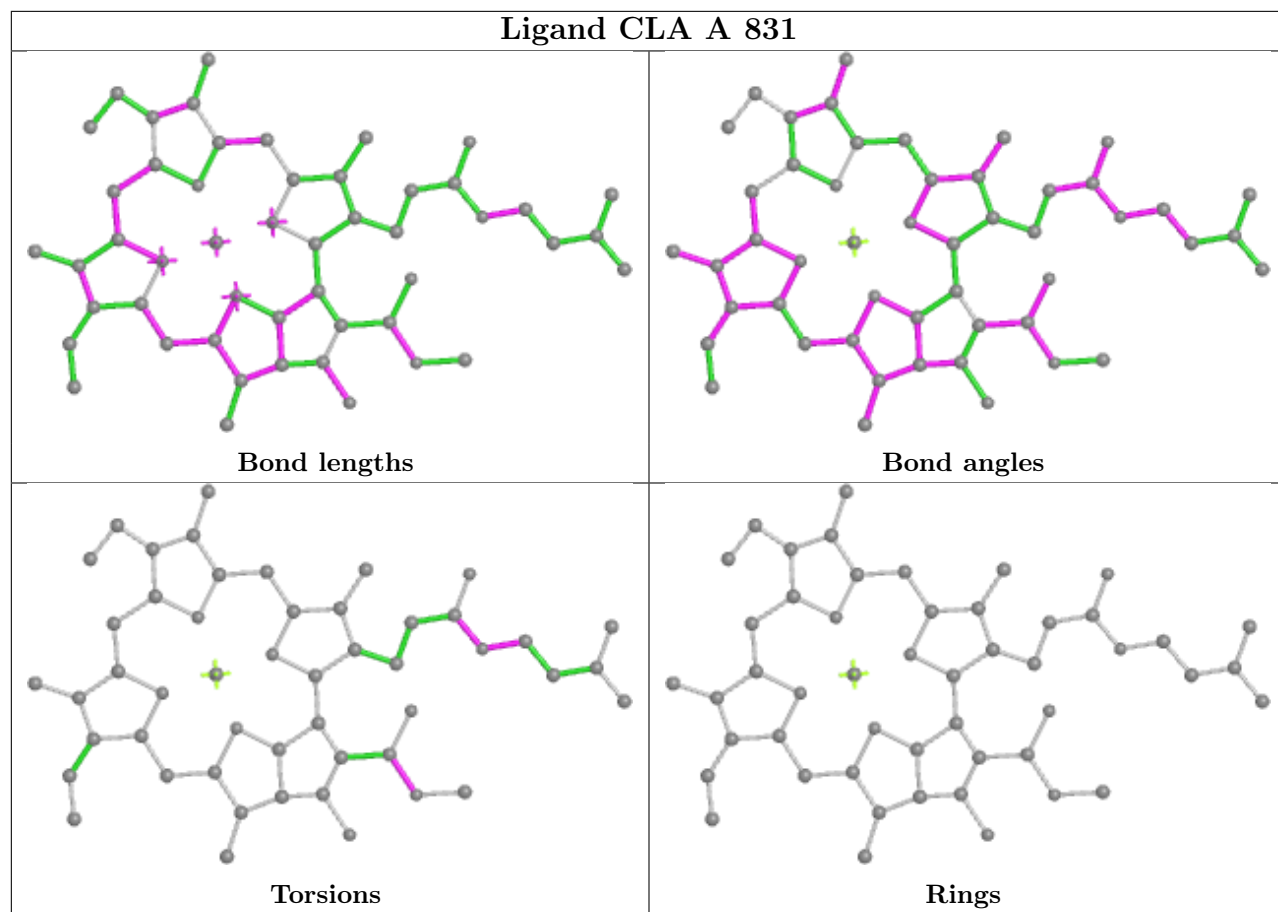


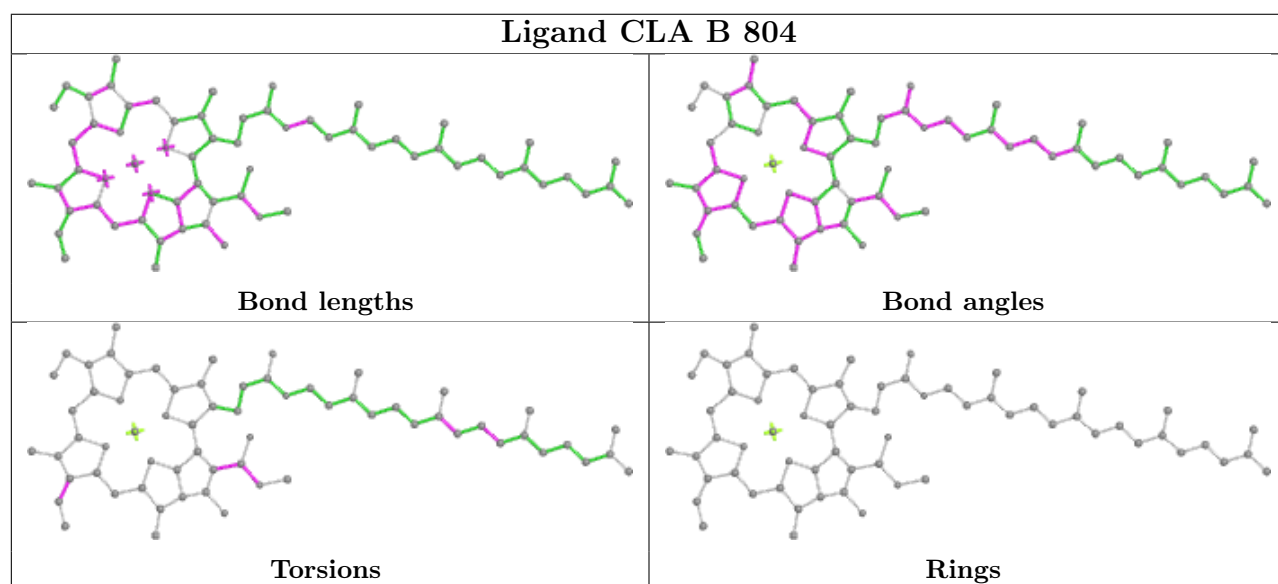
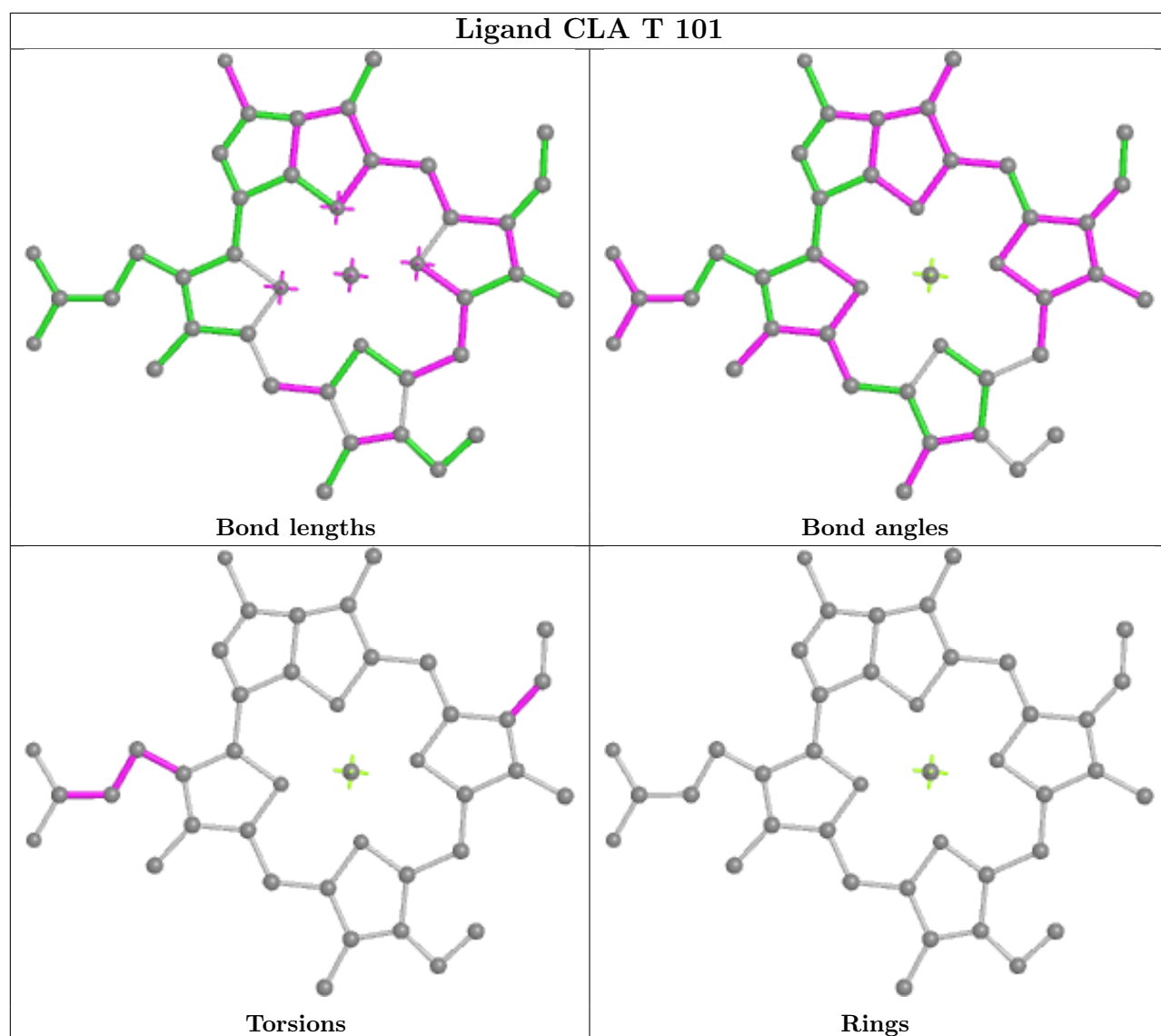
## Ligand CLA B 839



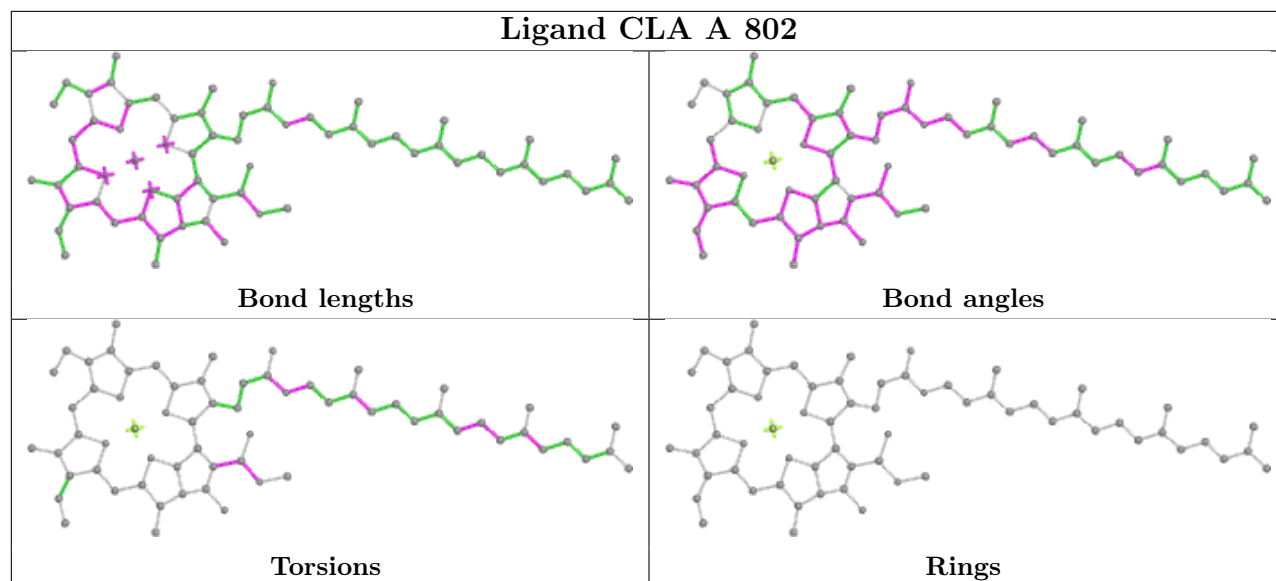
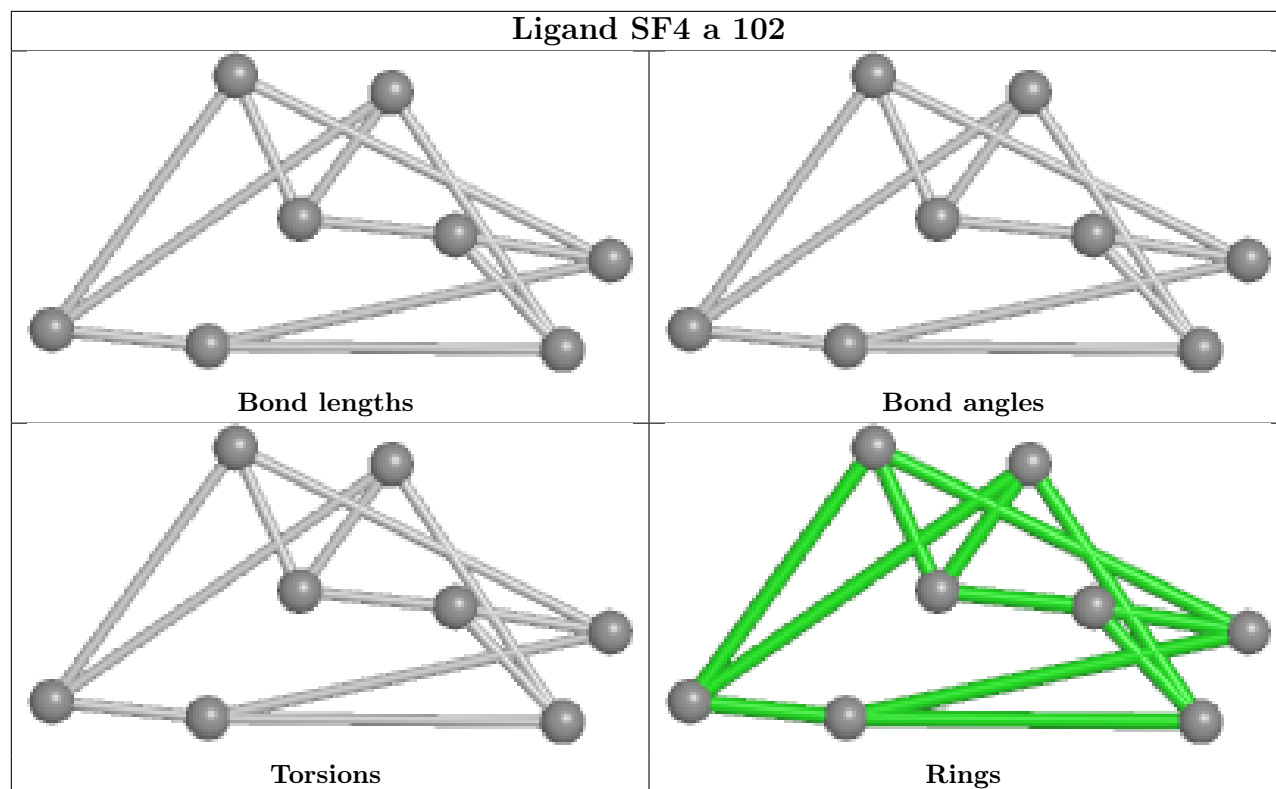
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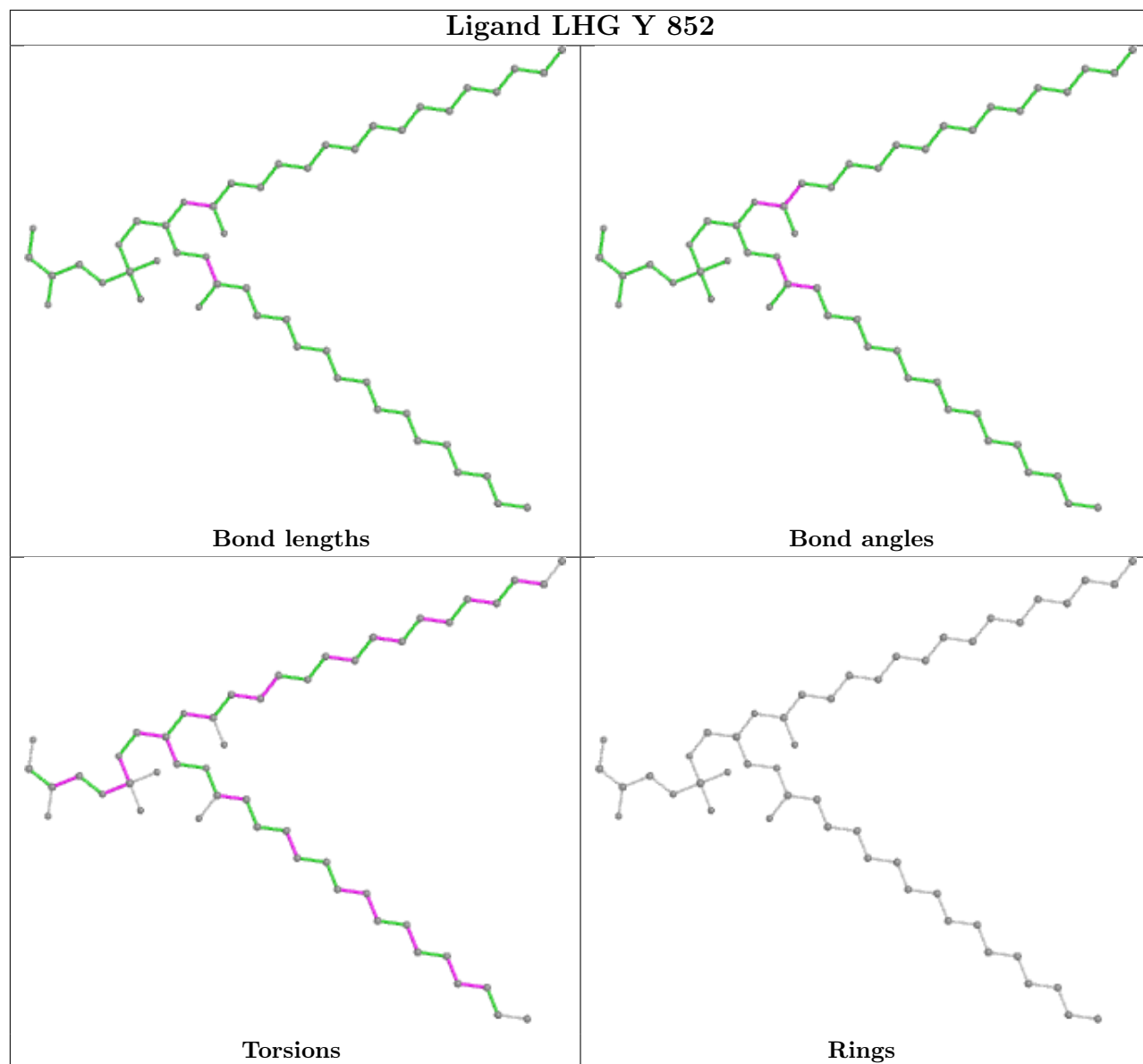


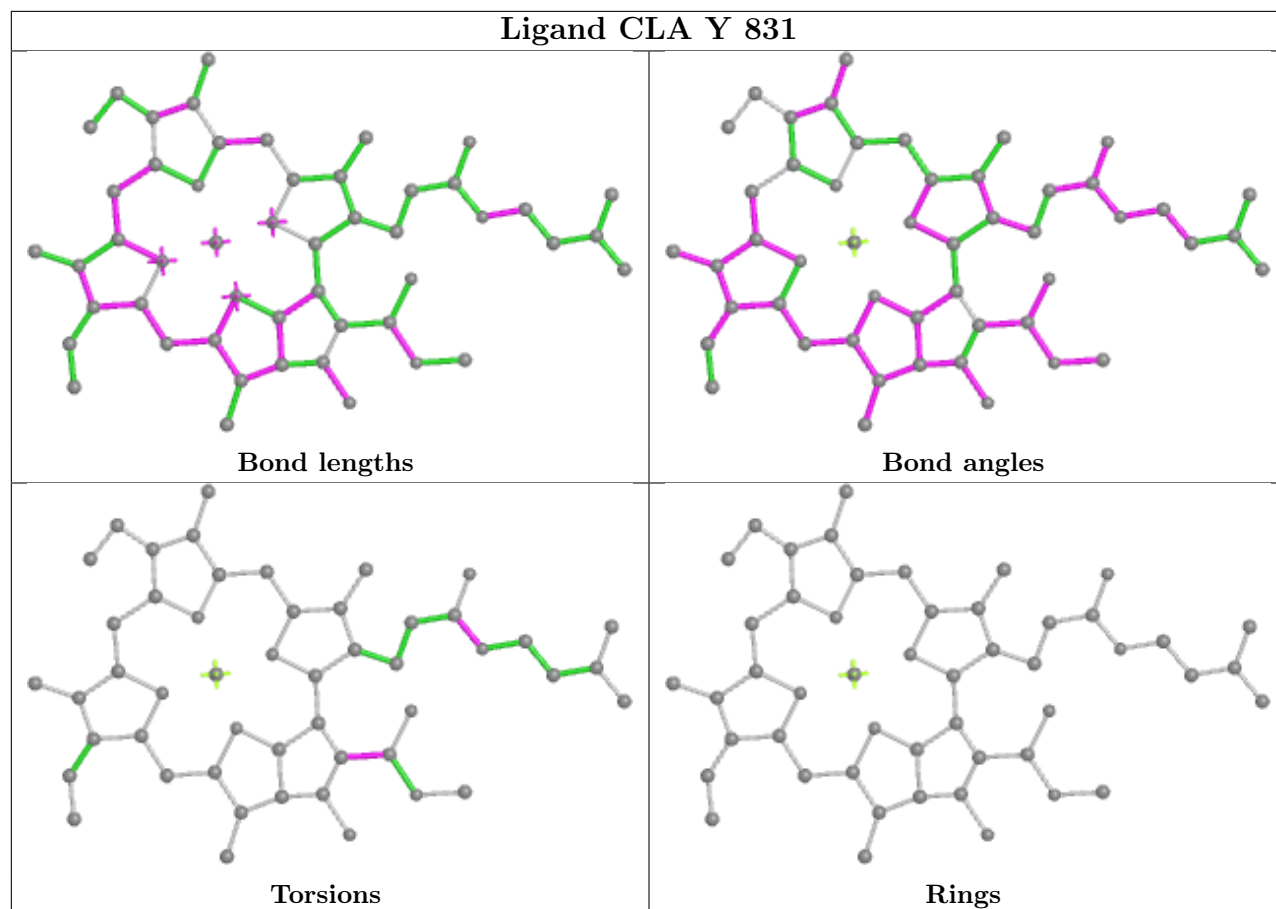


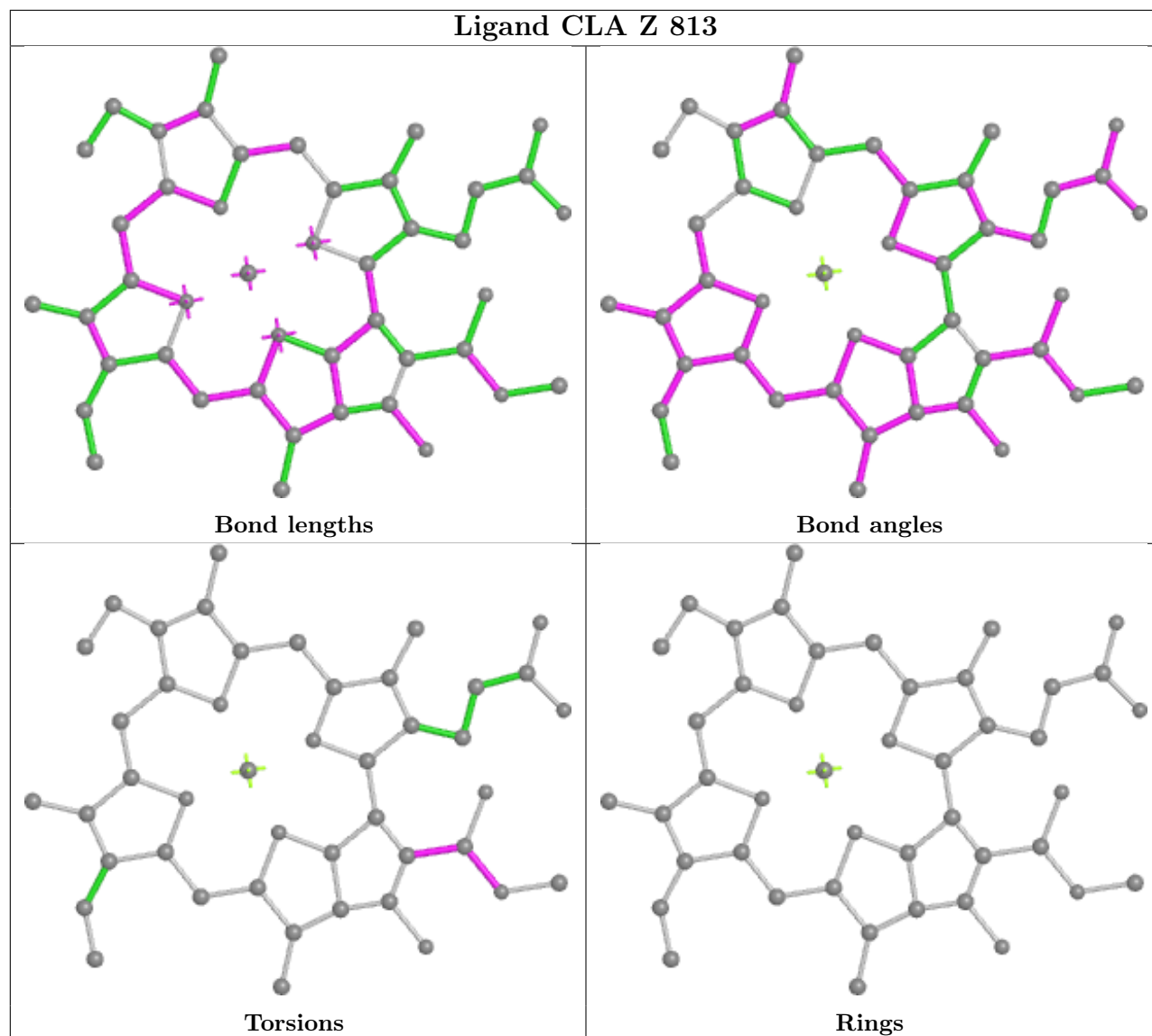


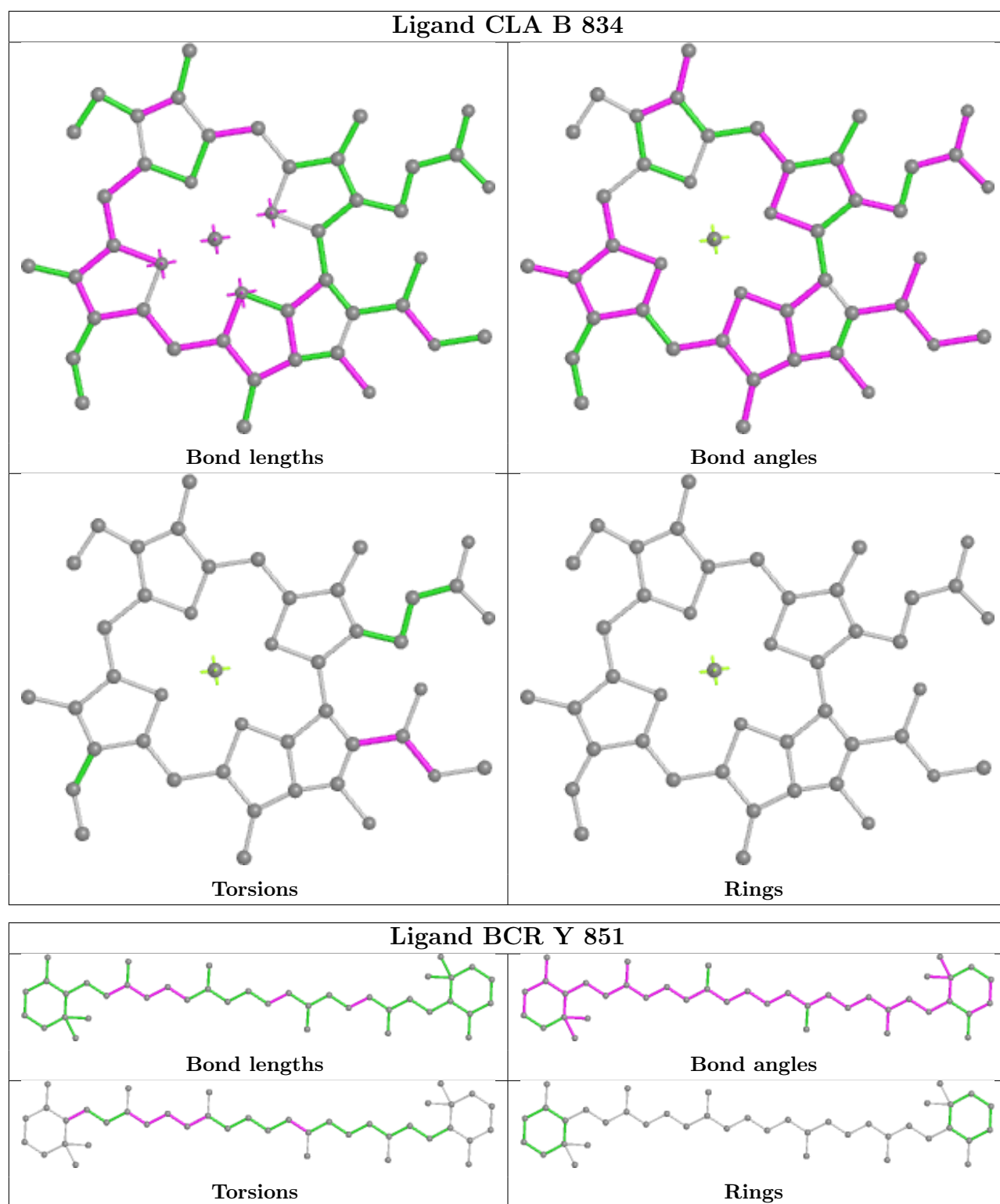


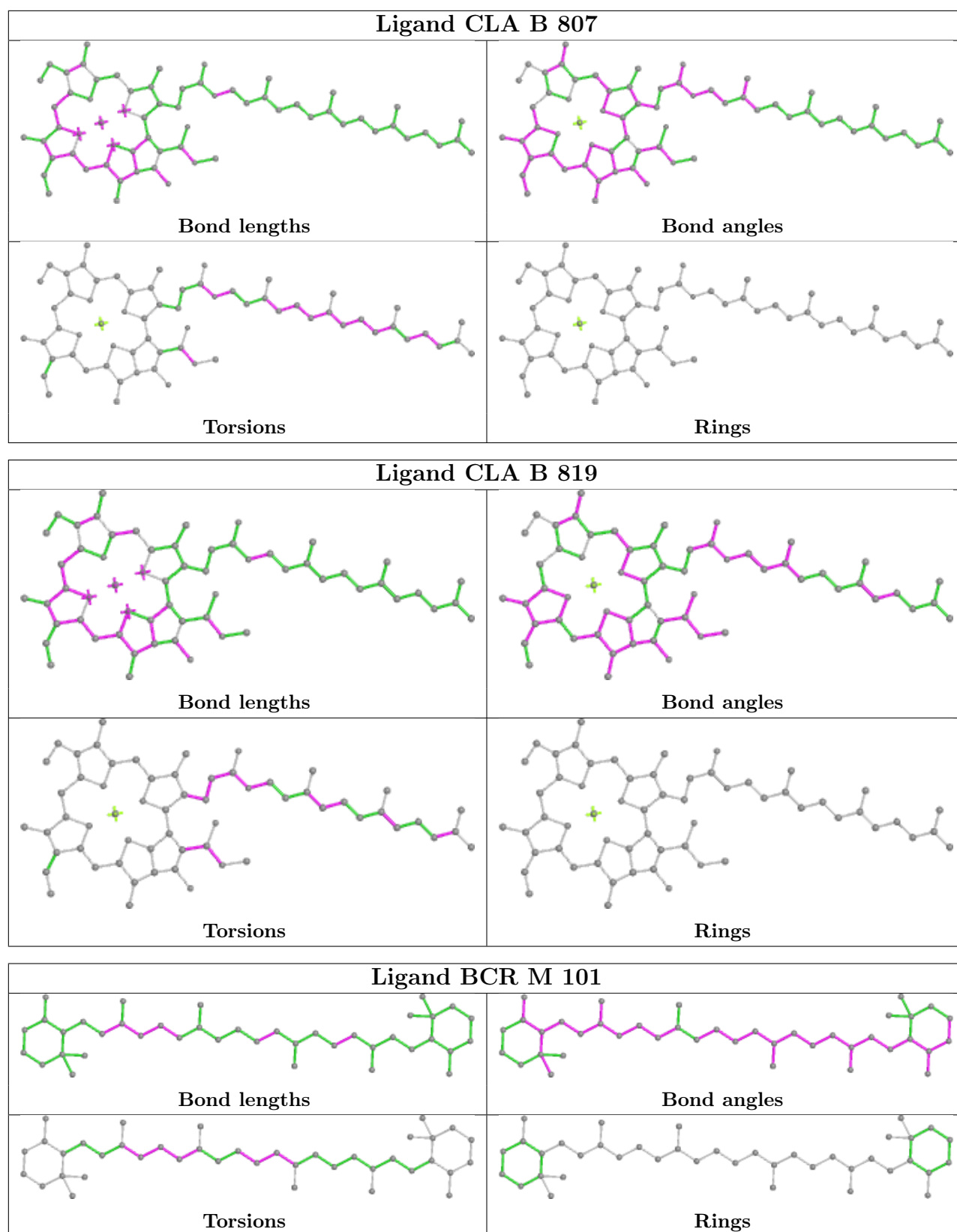


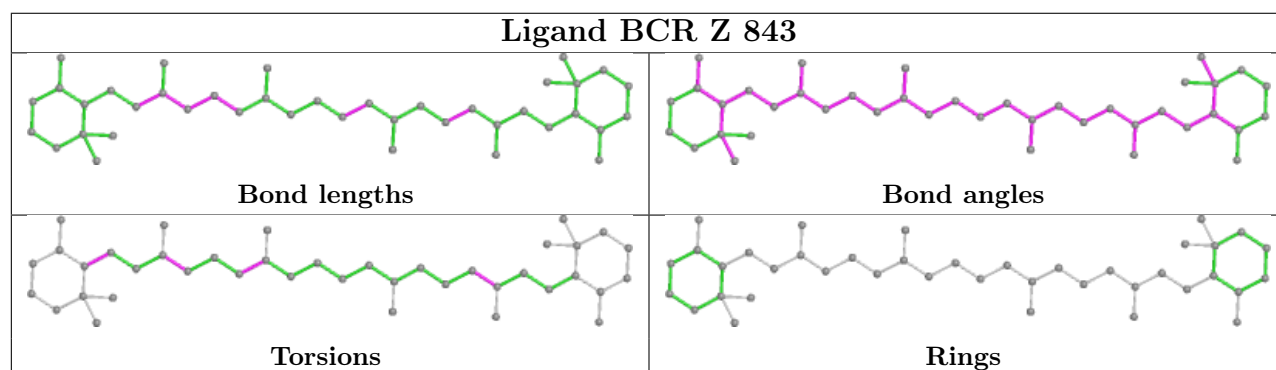
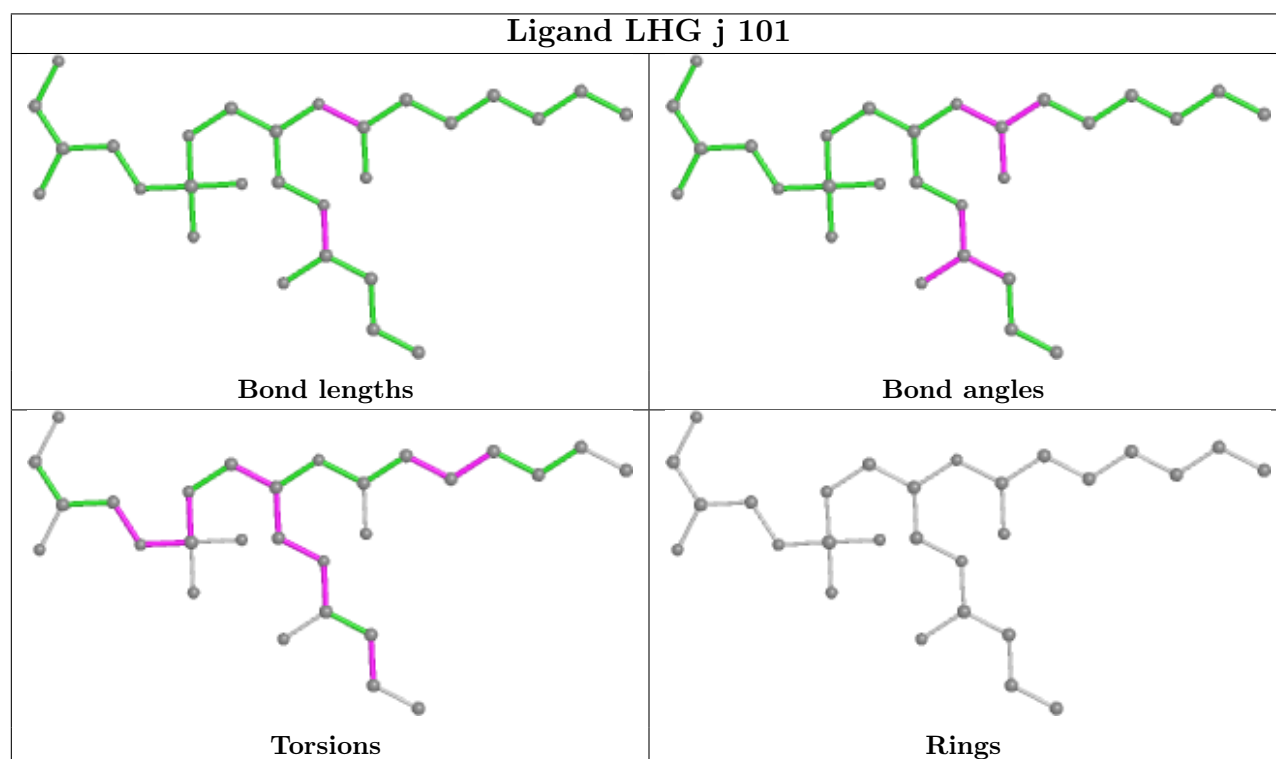
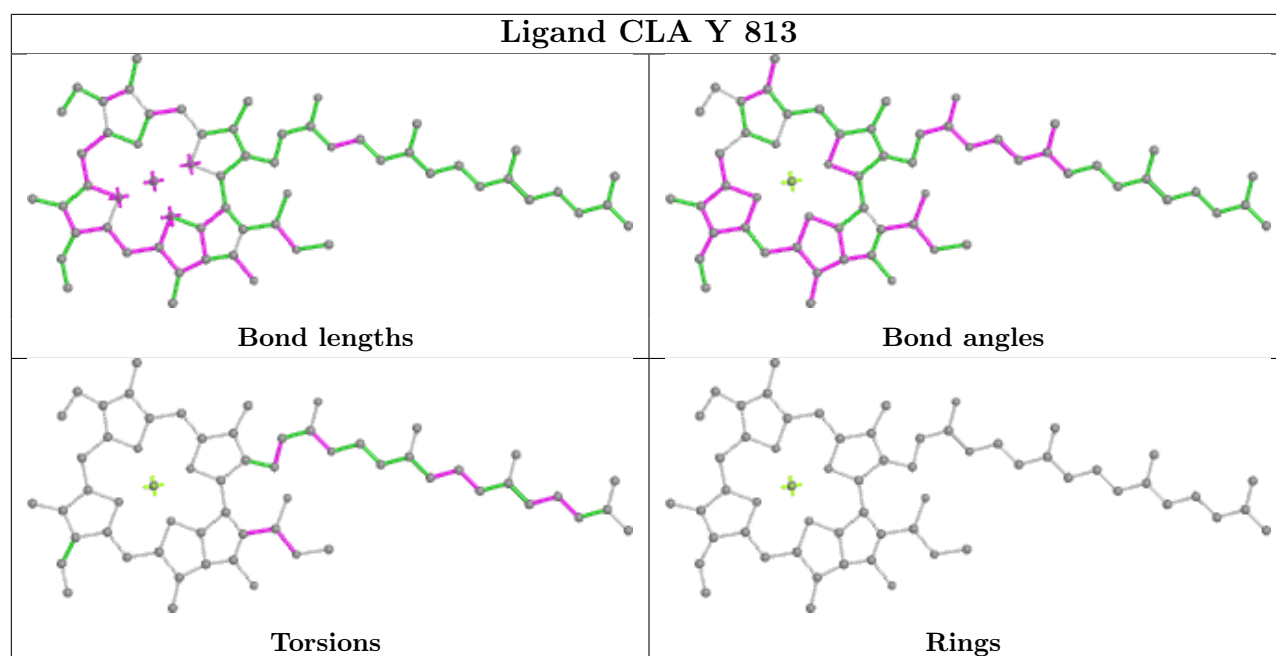


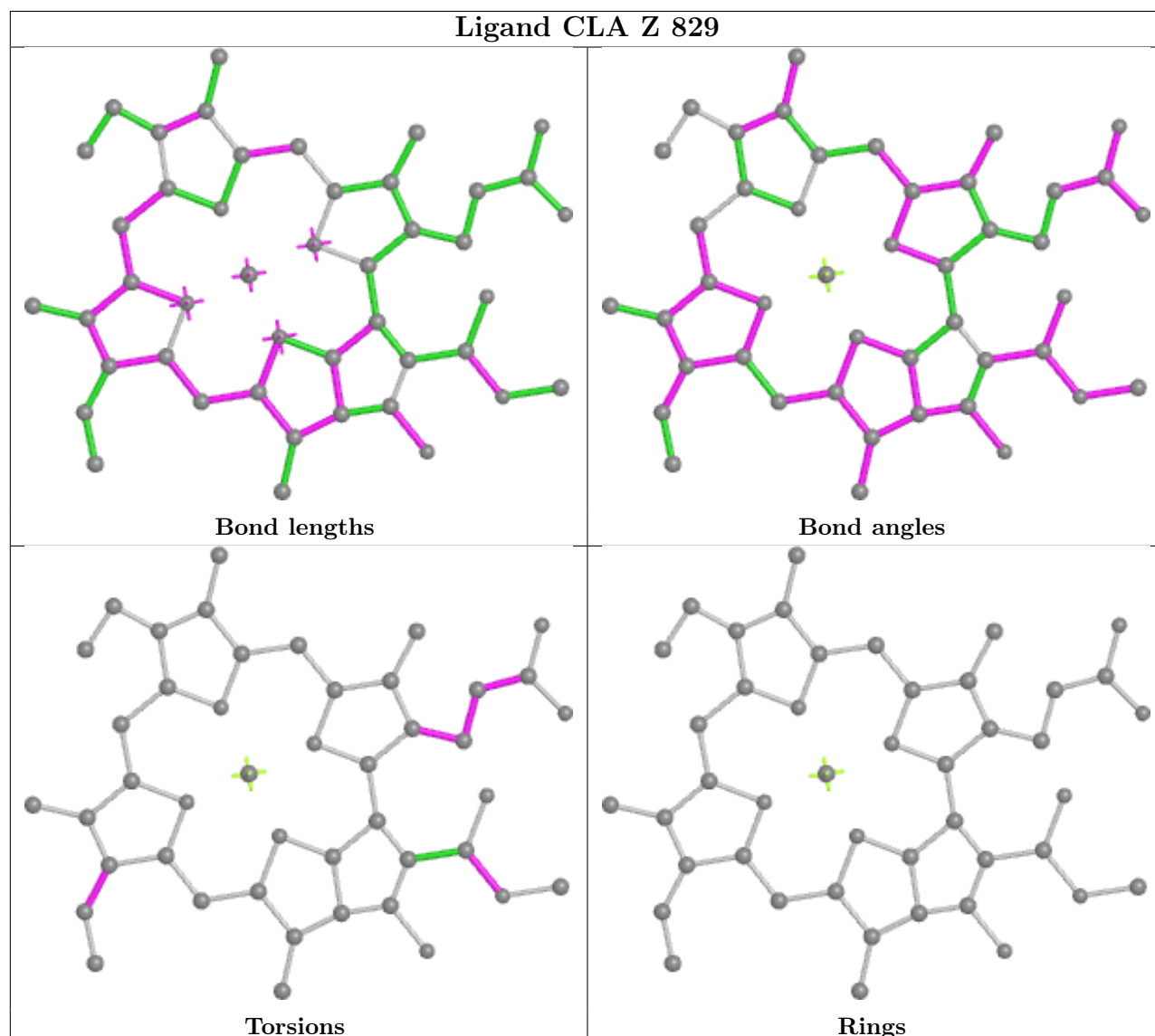
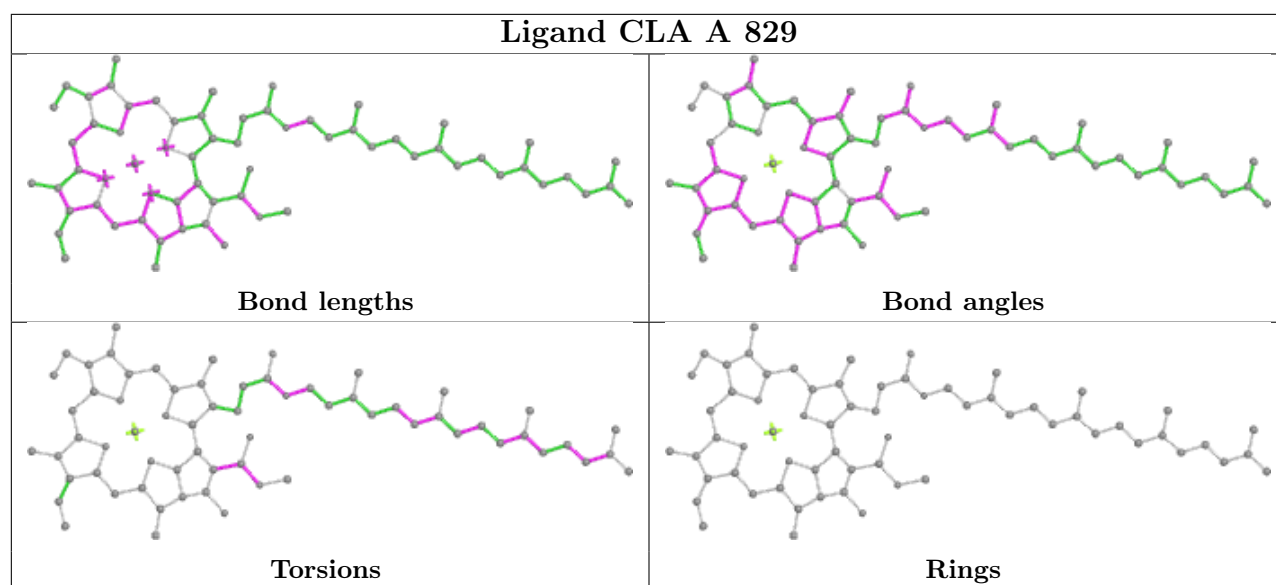




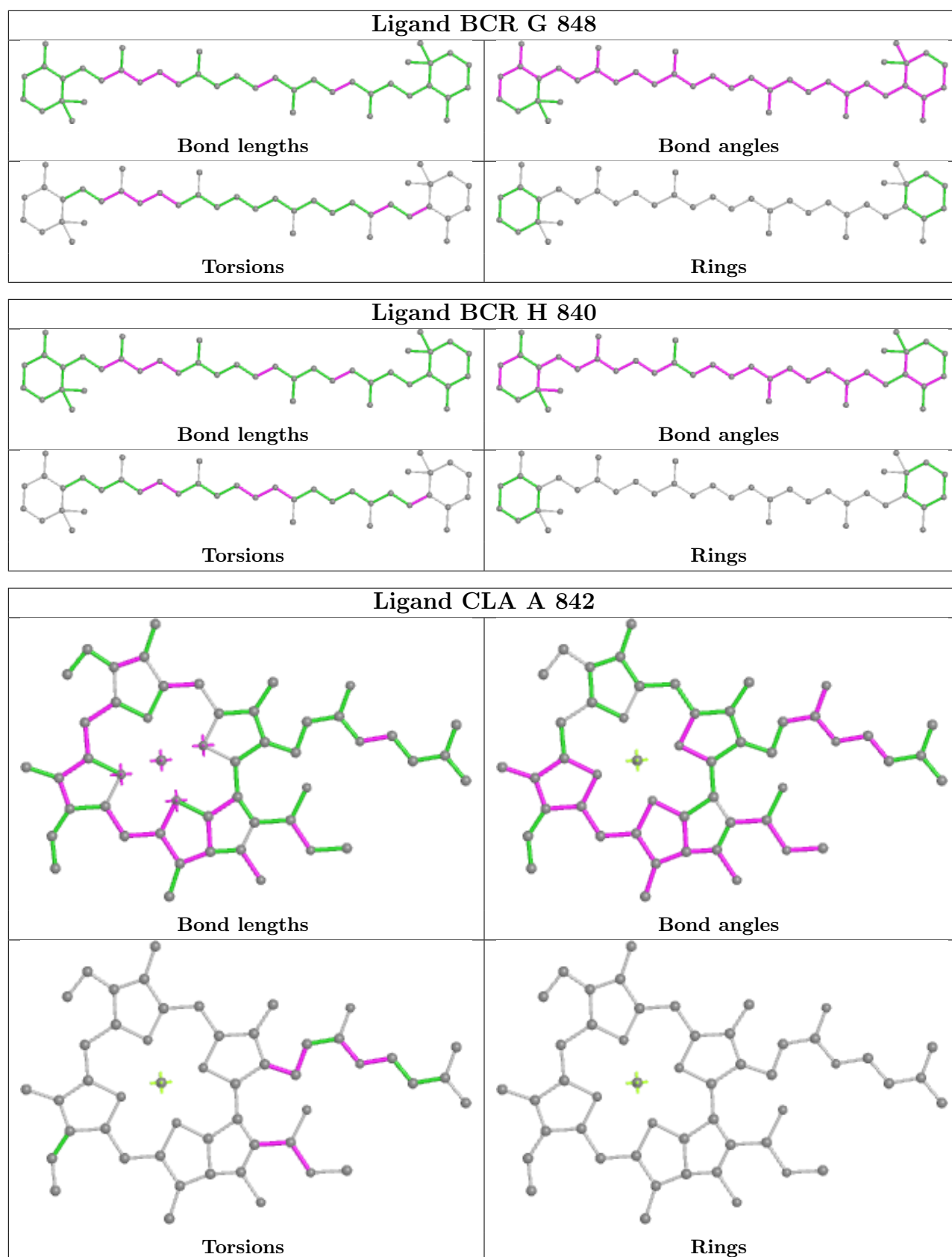




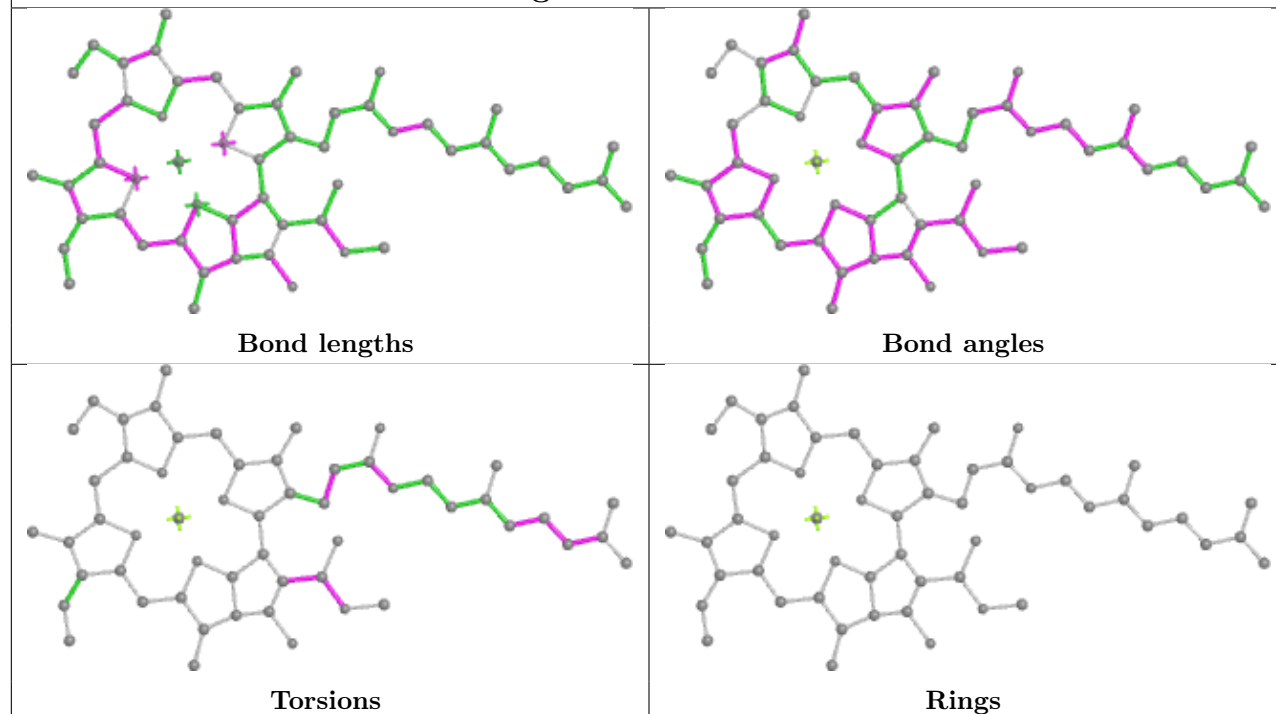




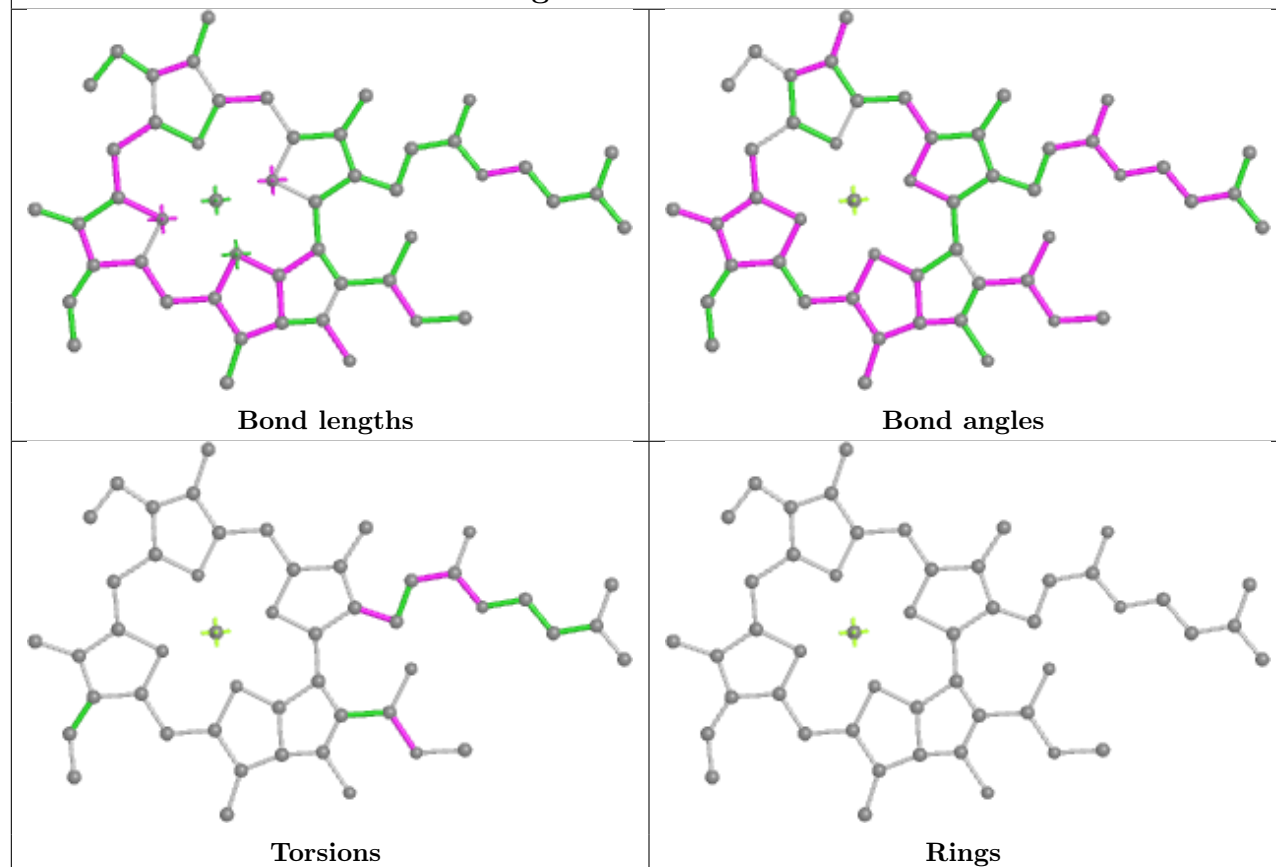


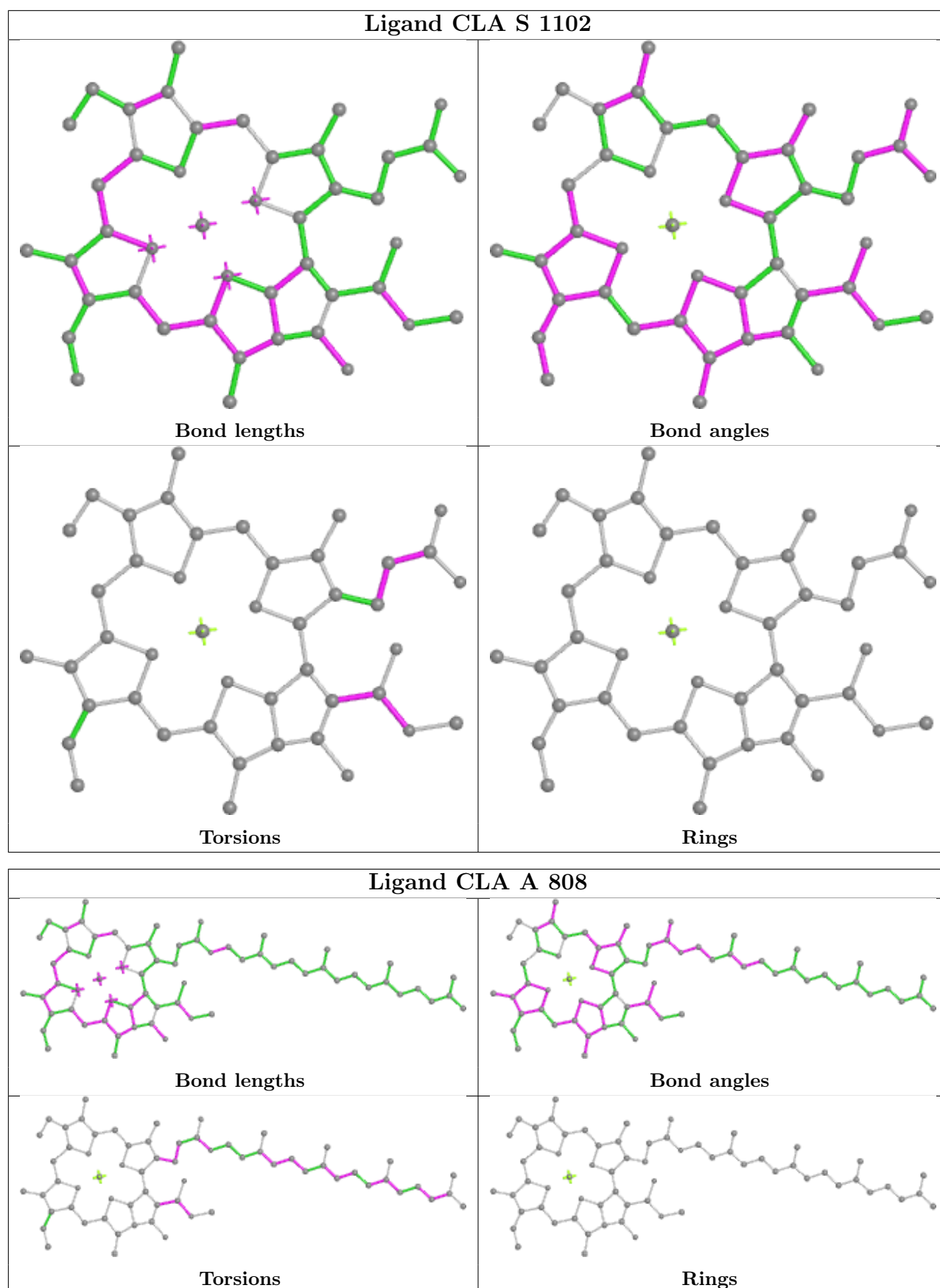


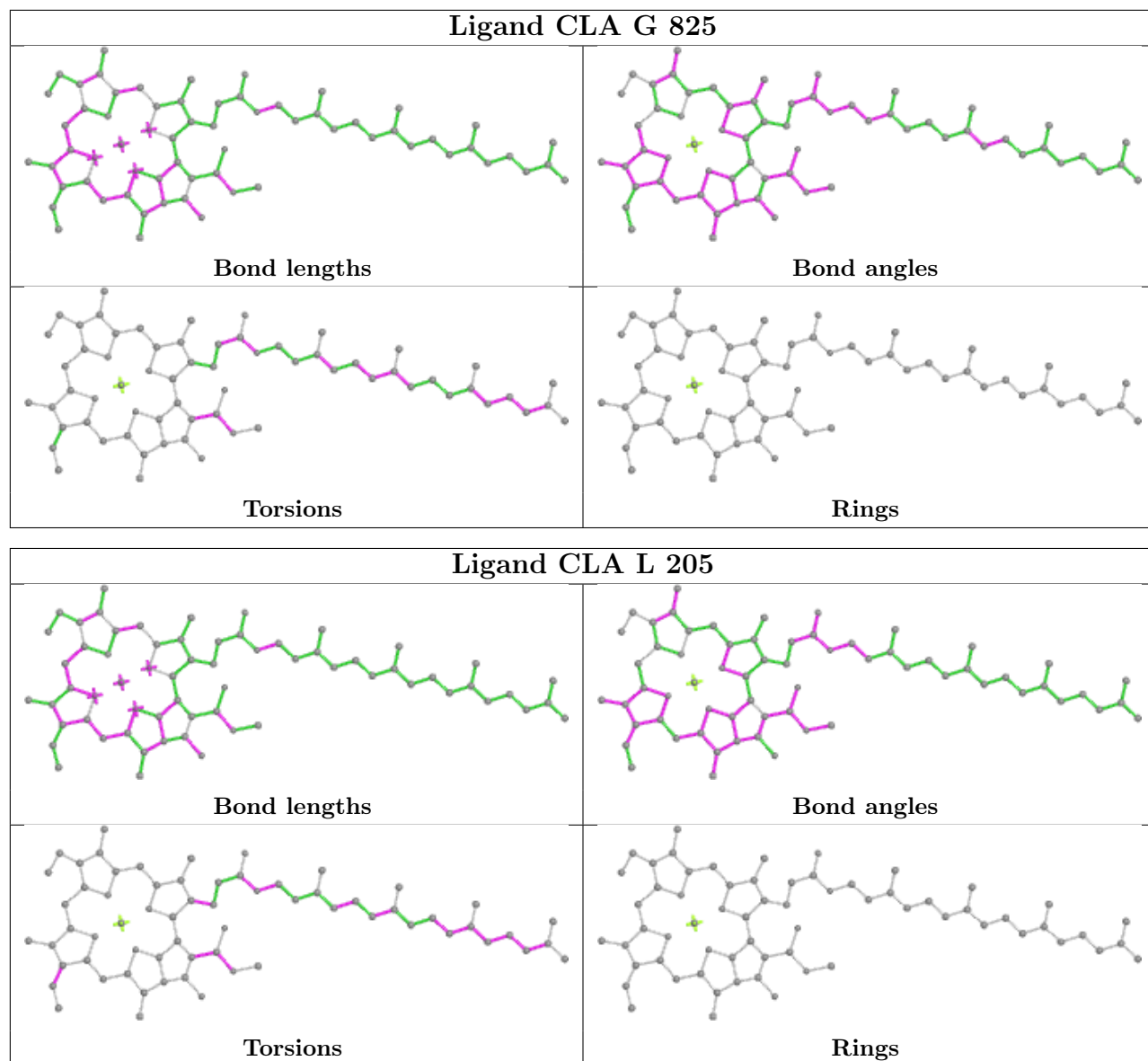
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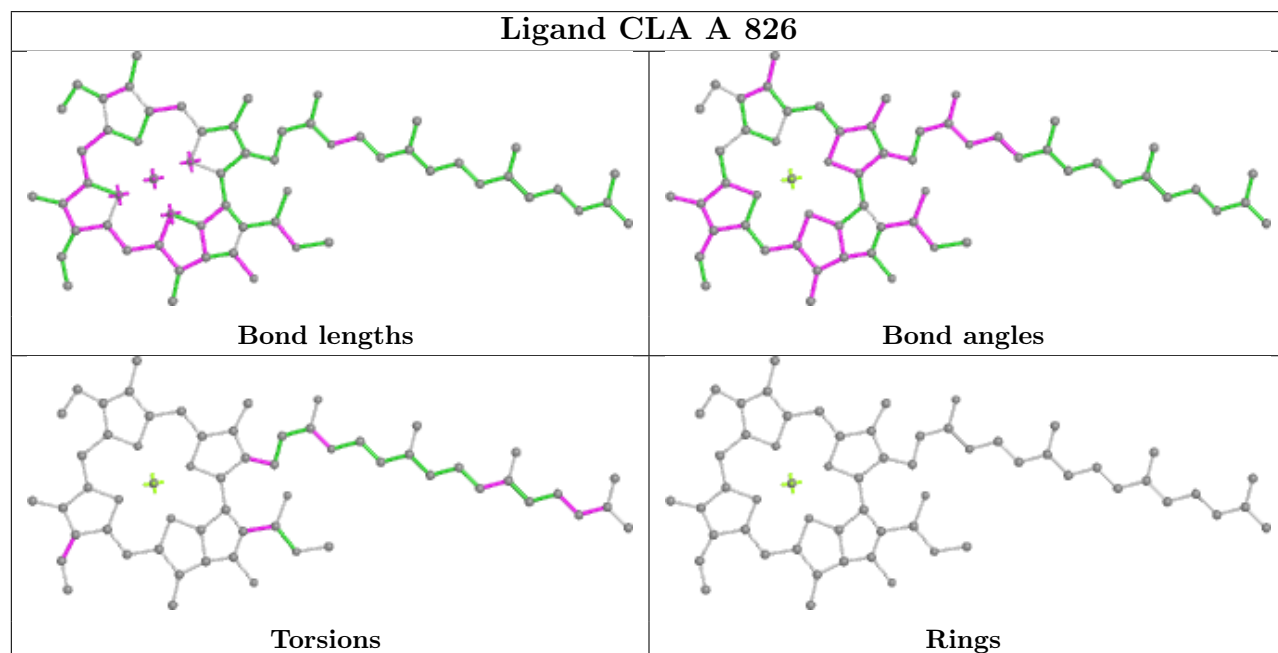
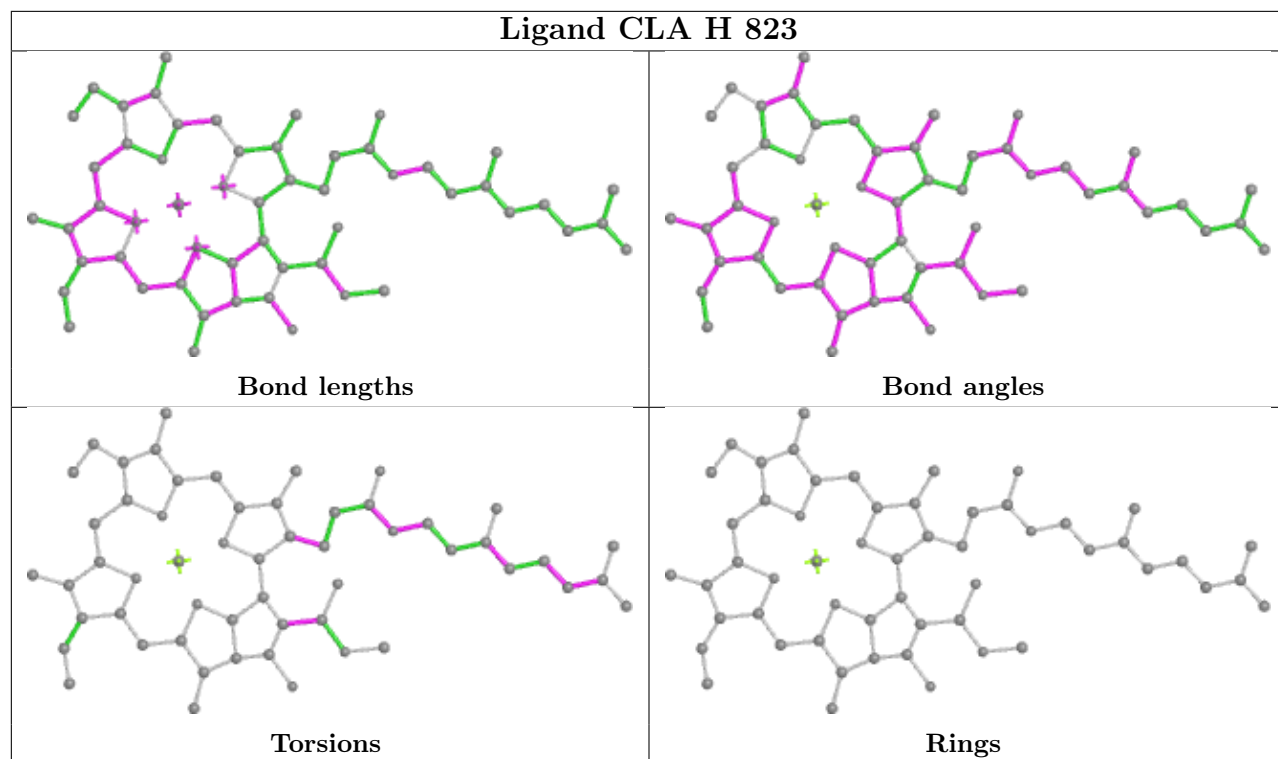


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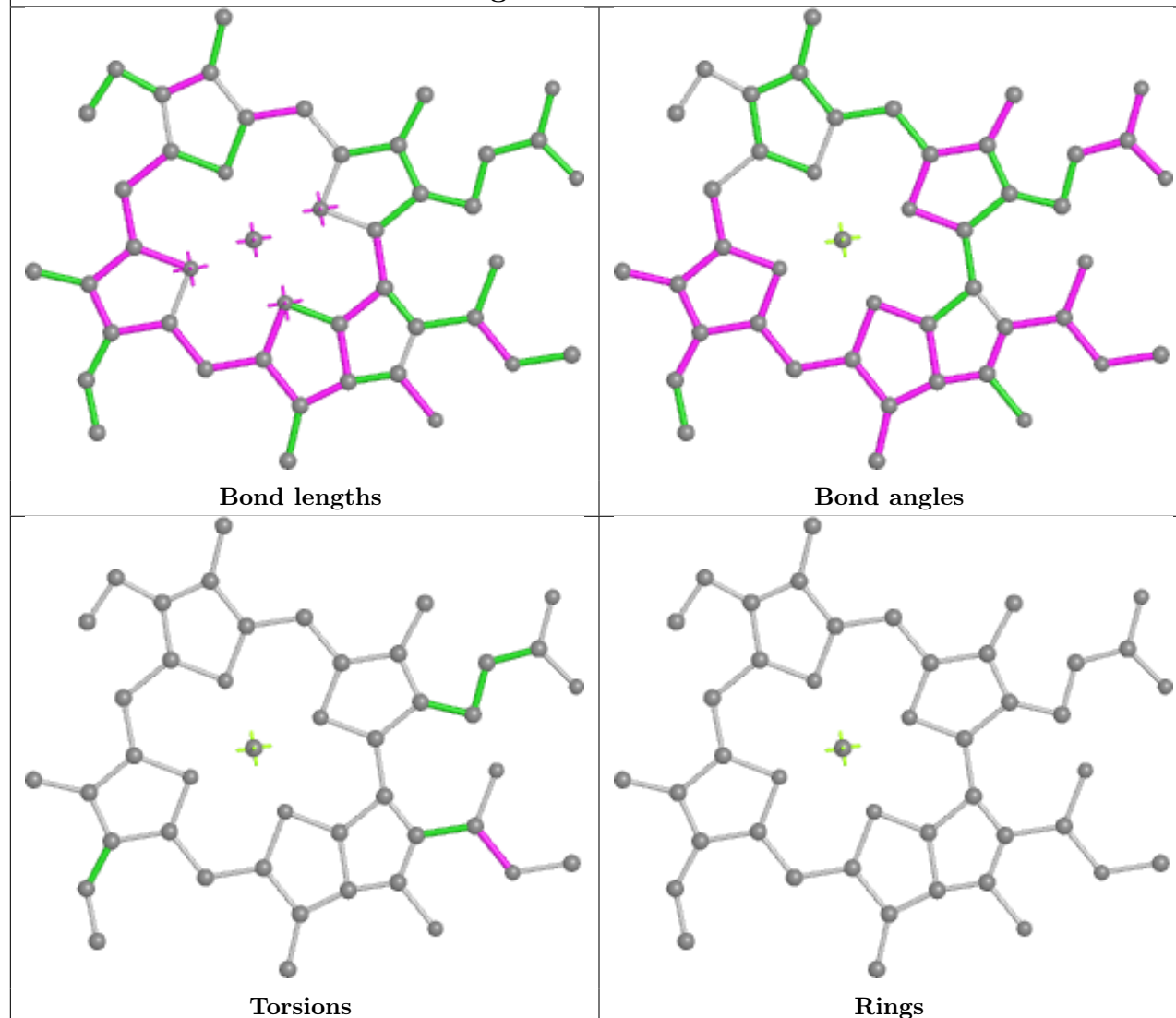




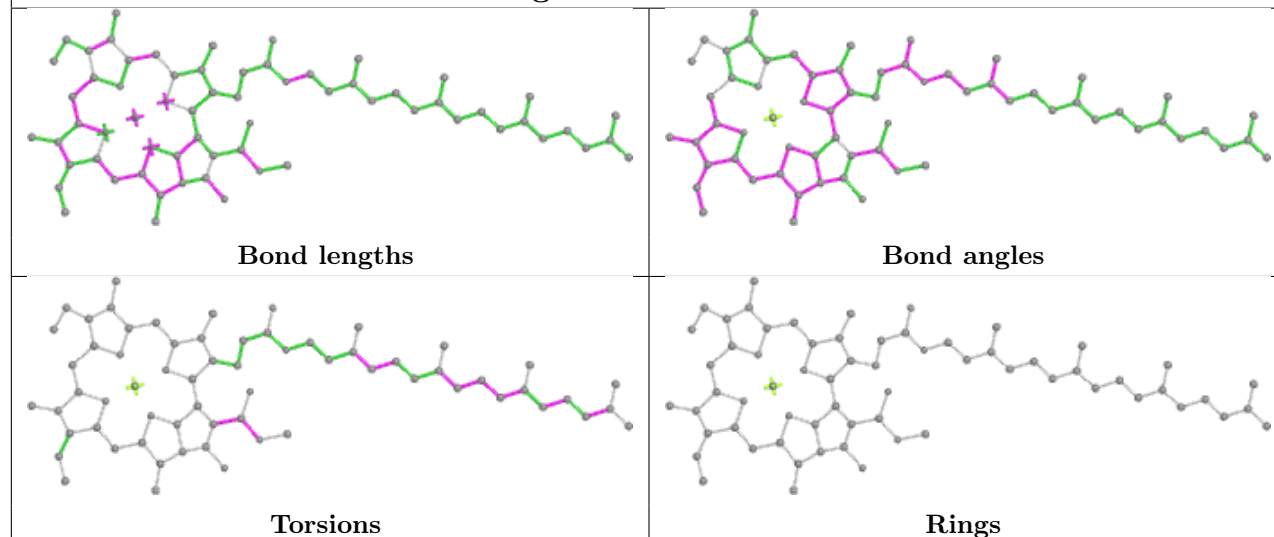


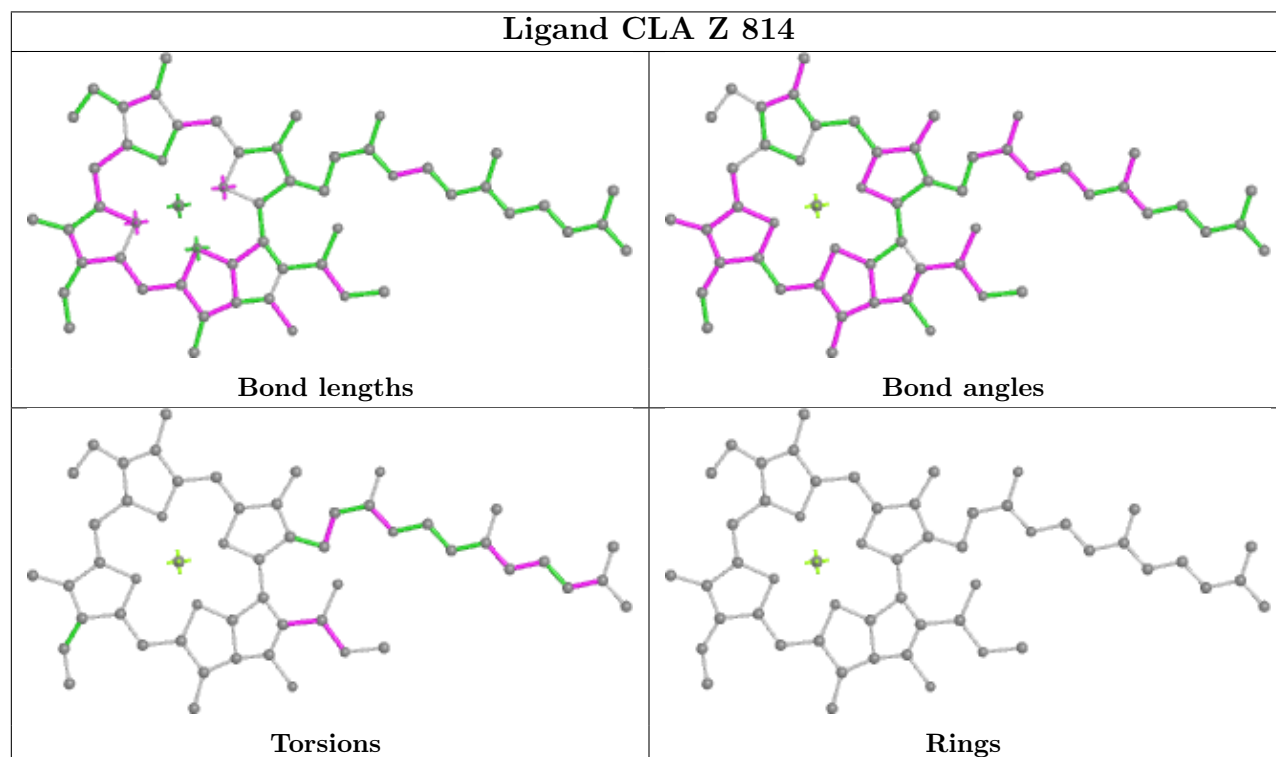
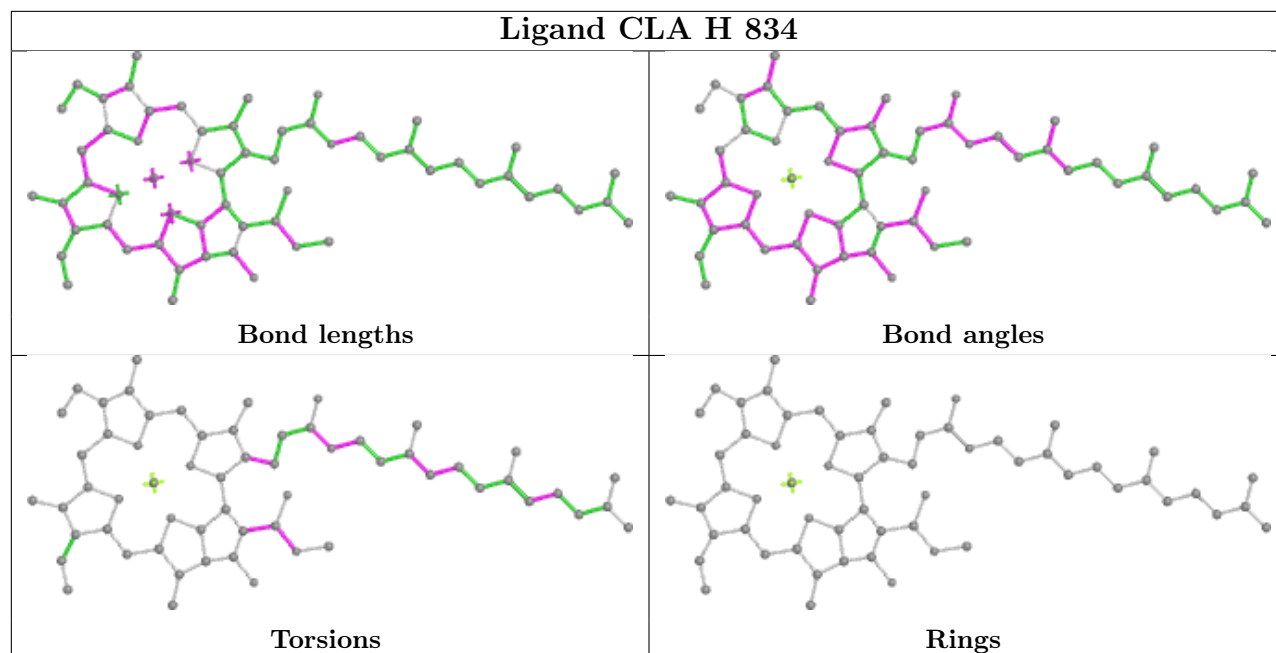


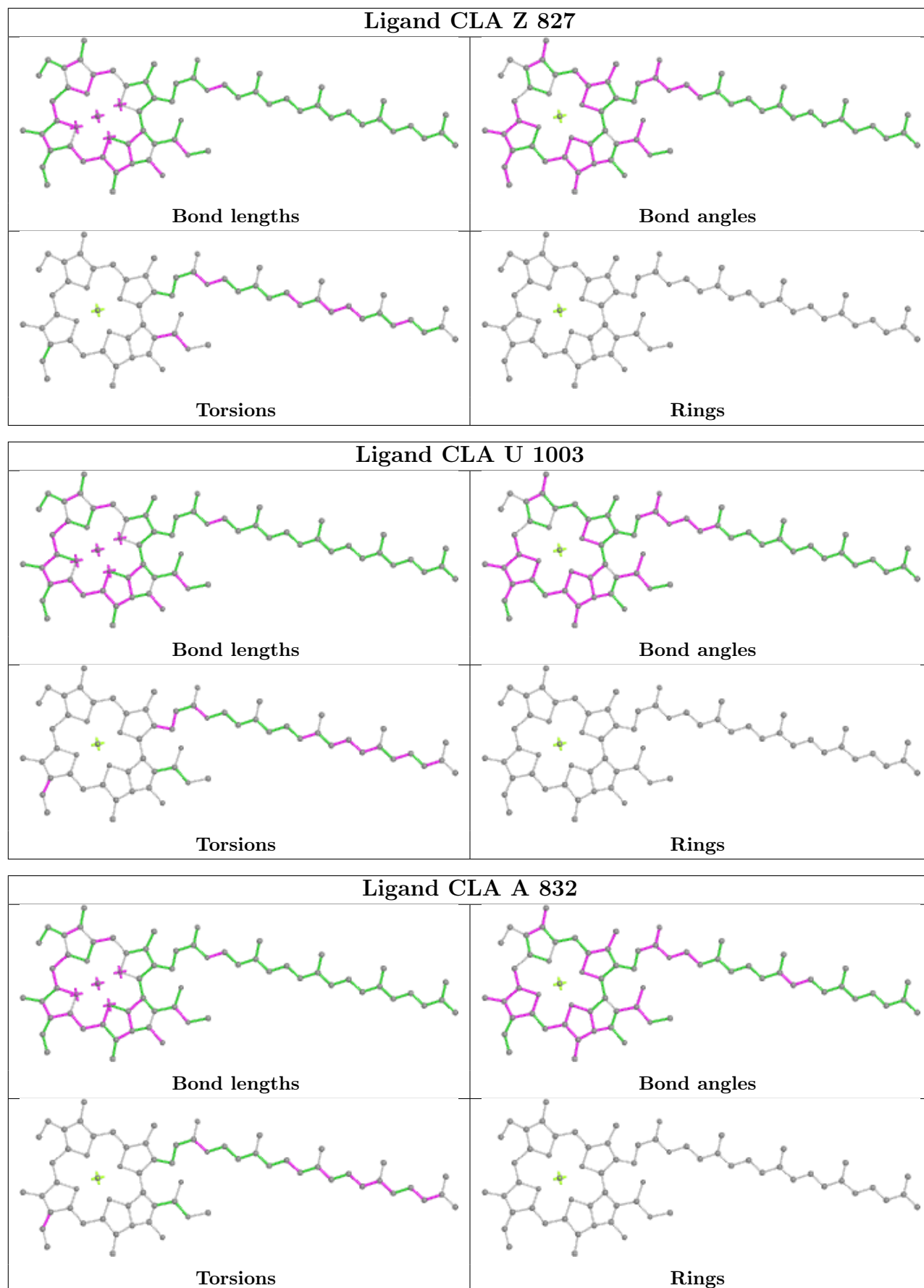
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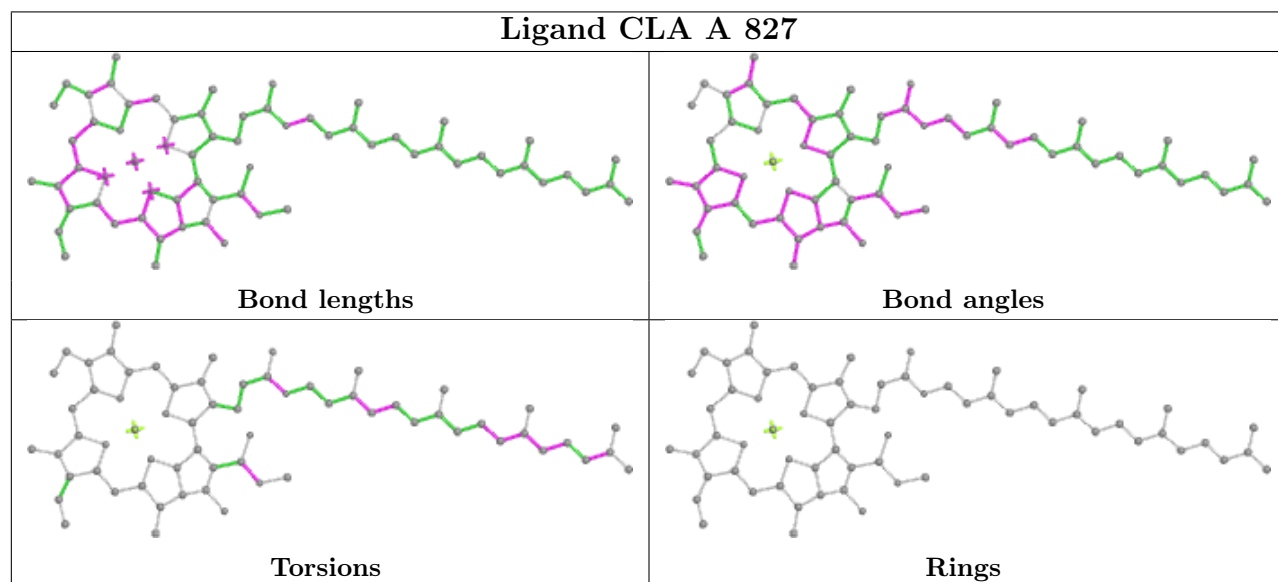
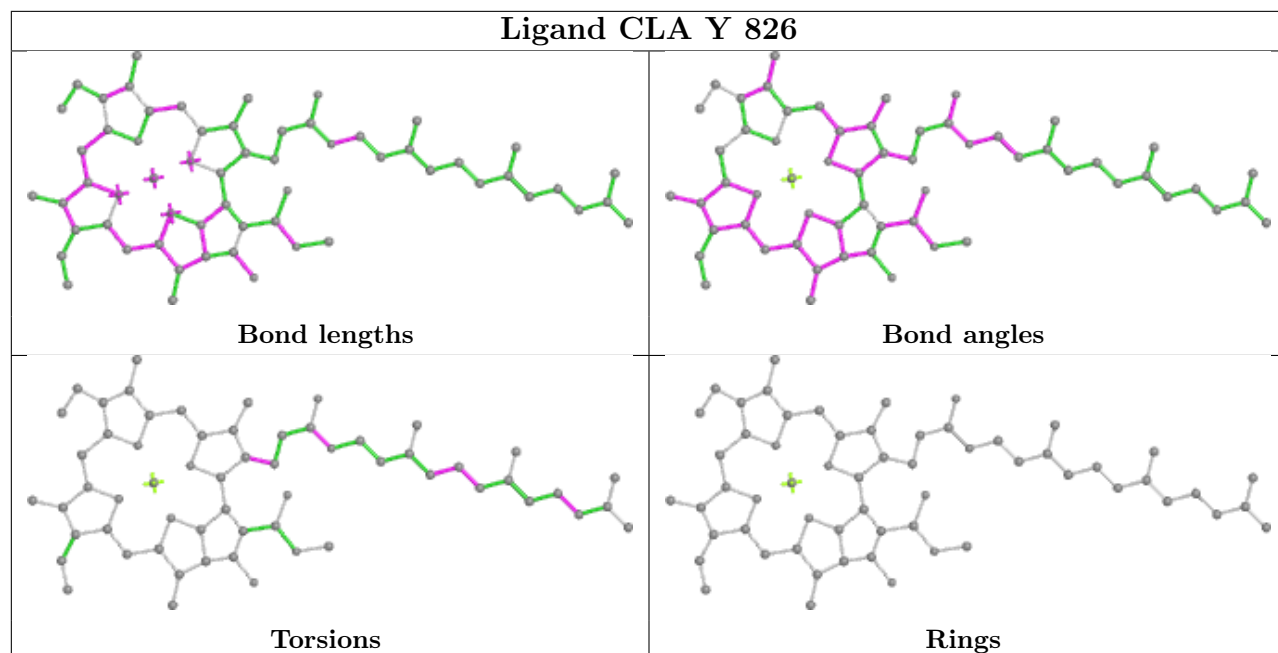
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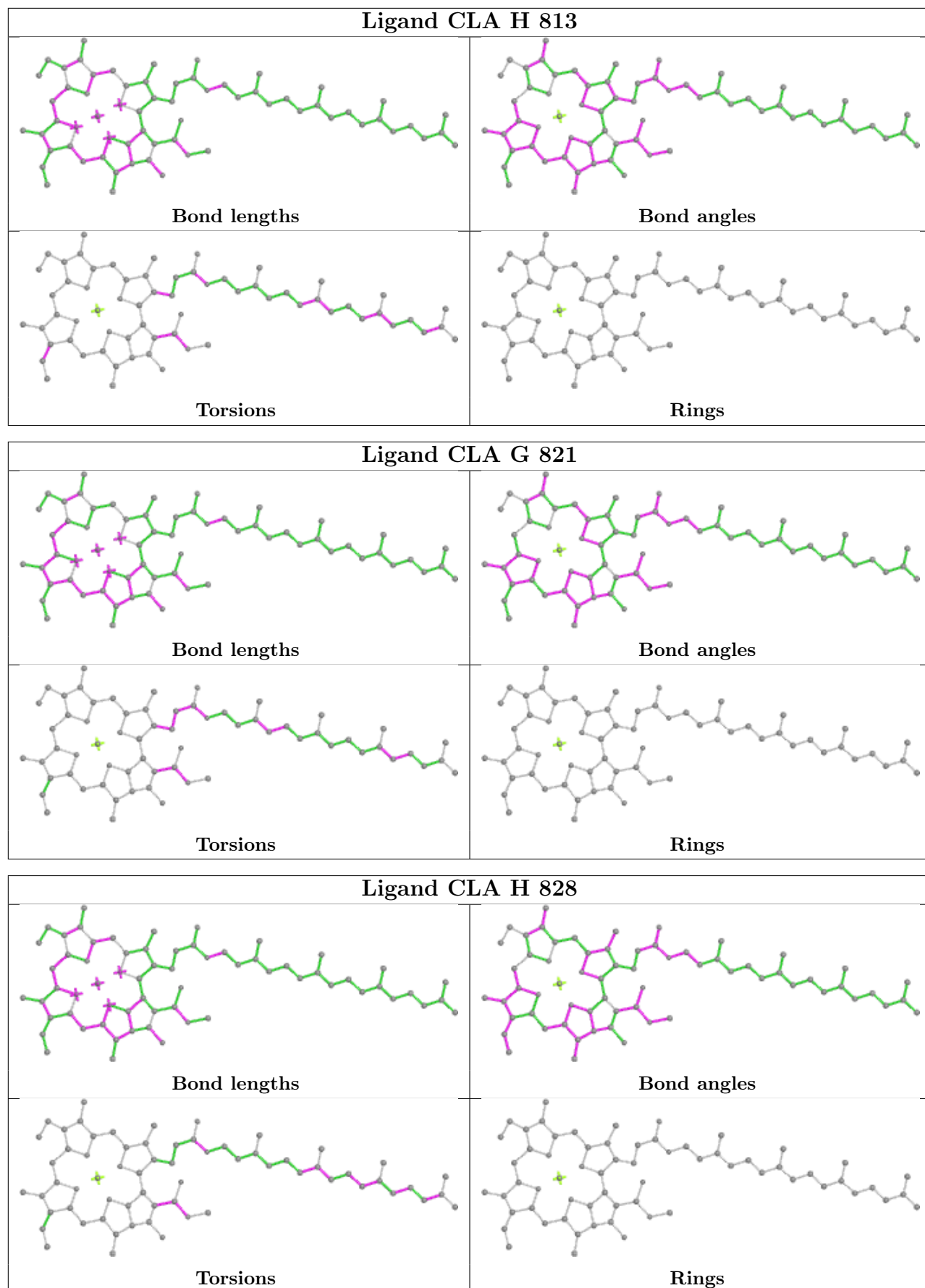


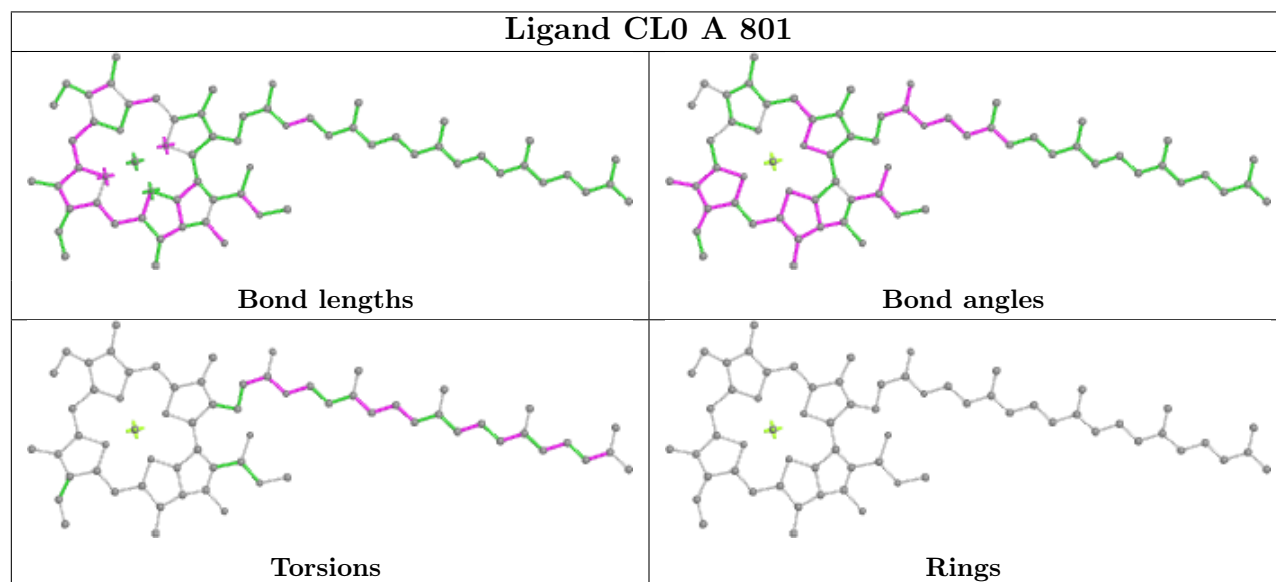
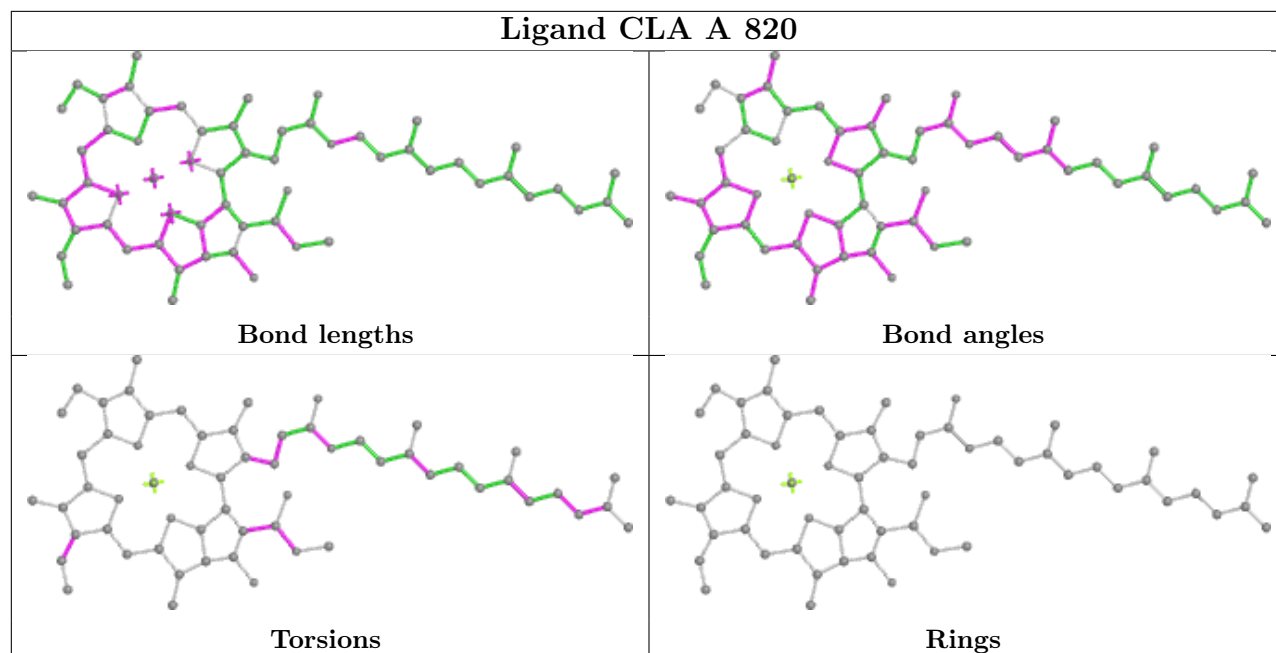


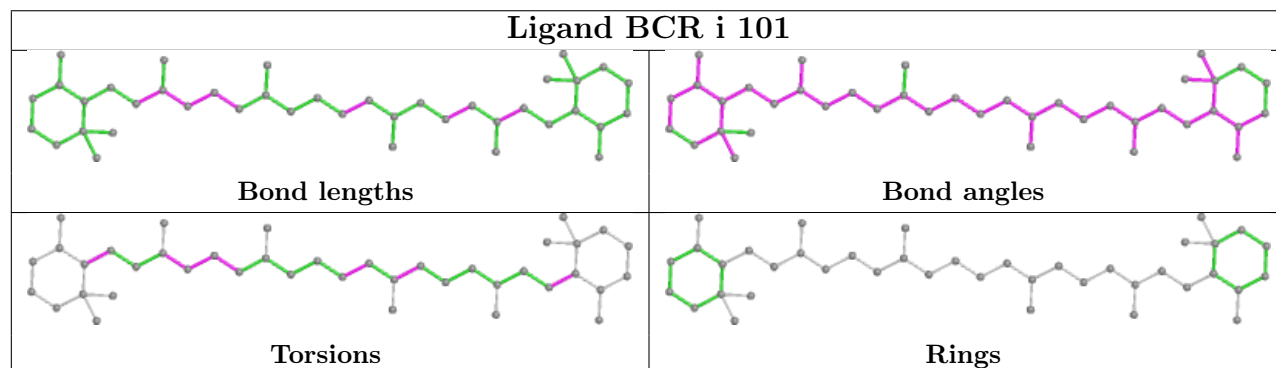
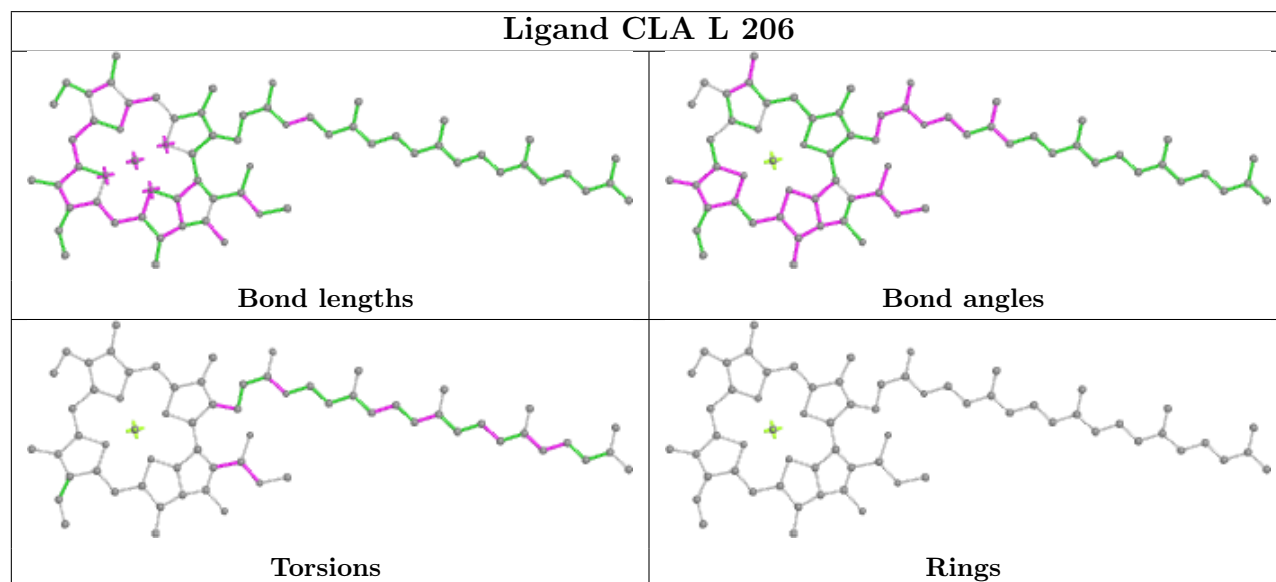
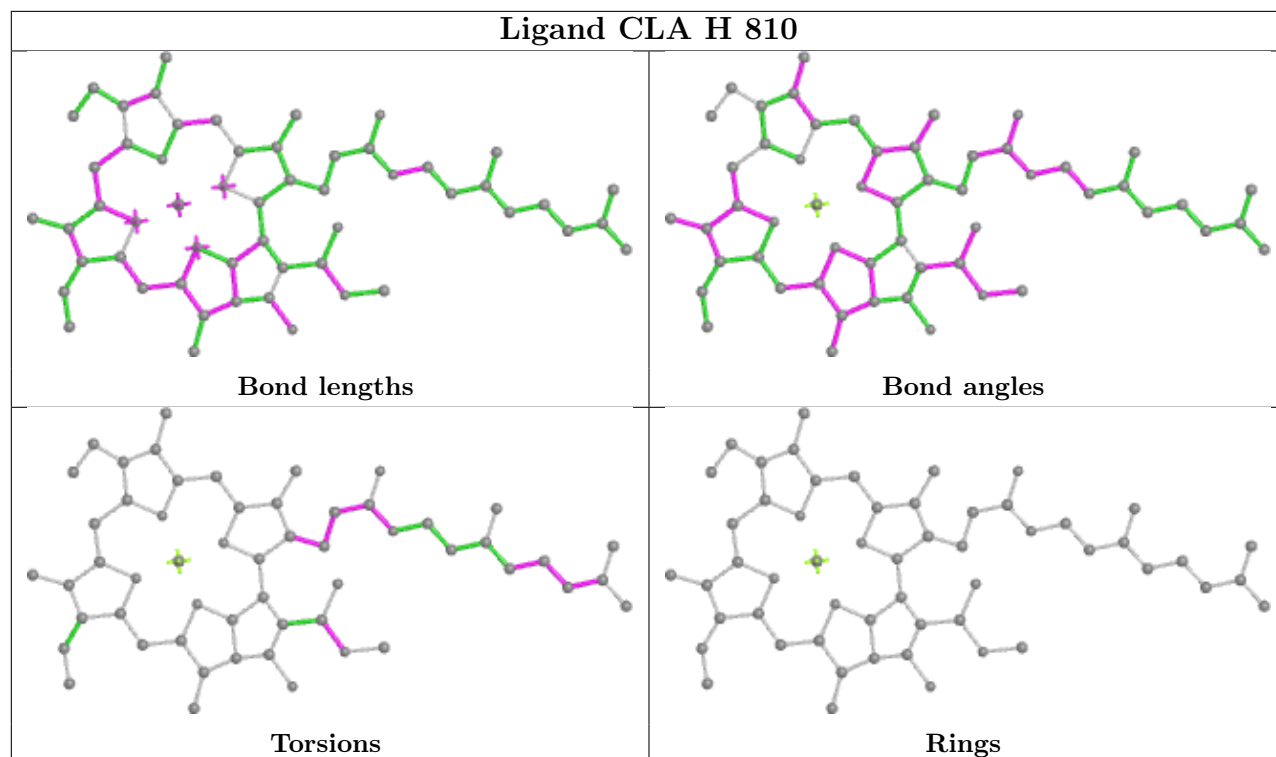


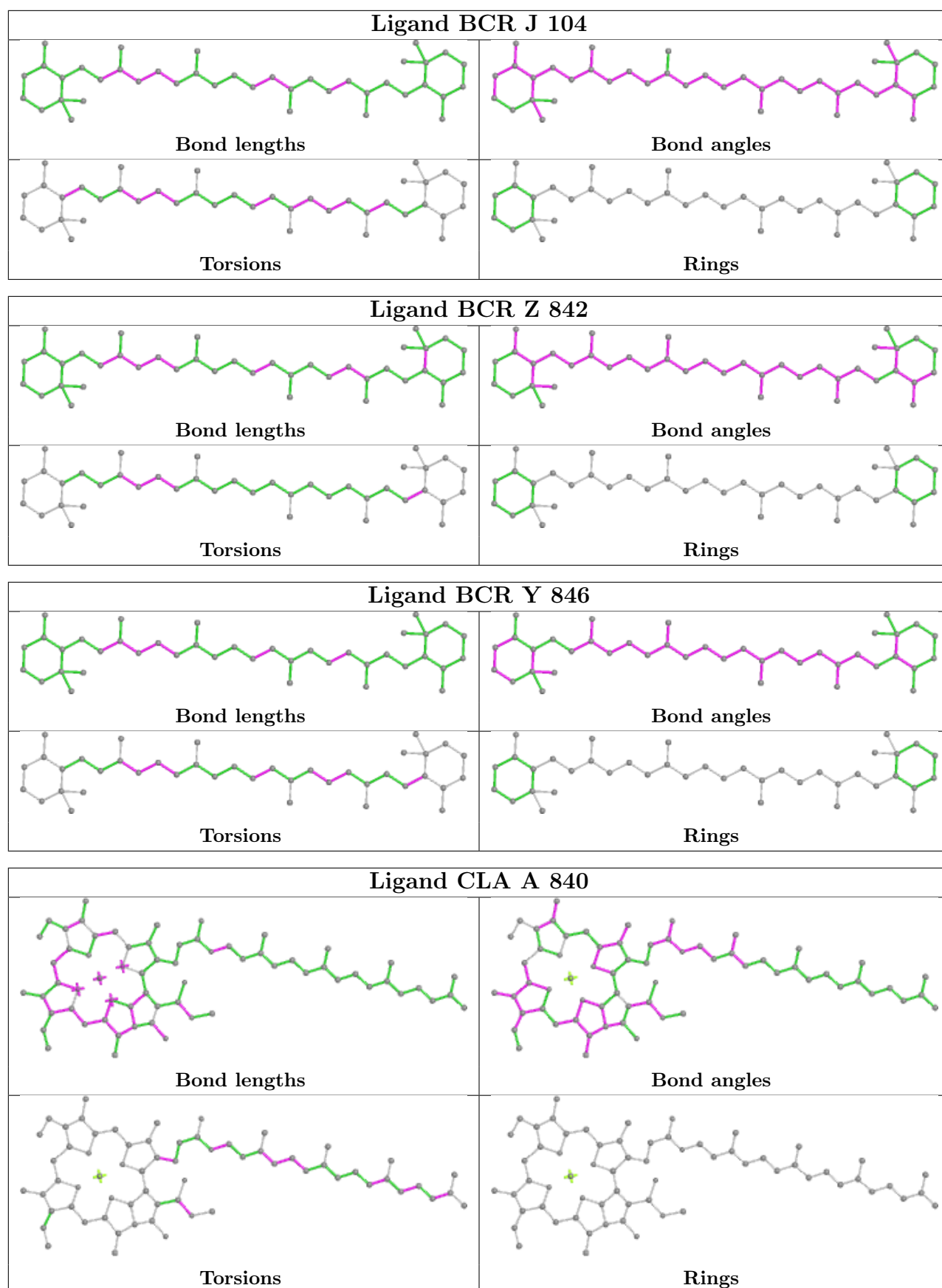


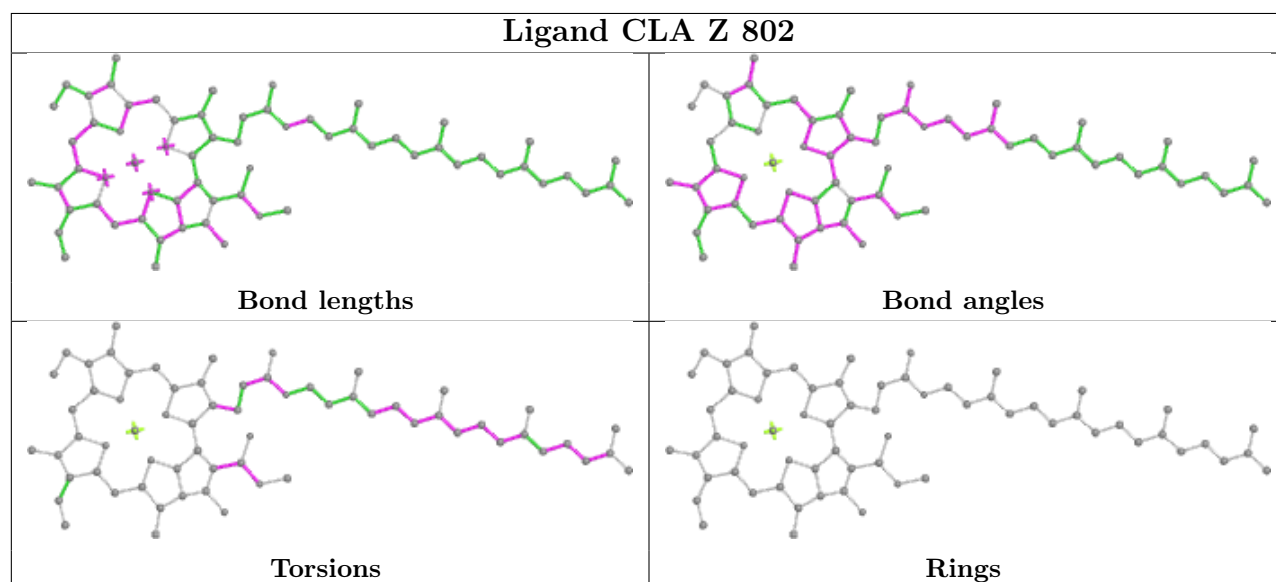
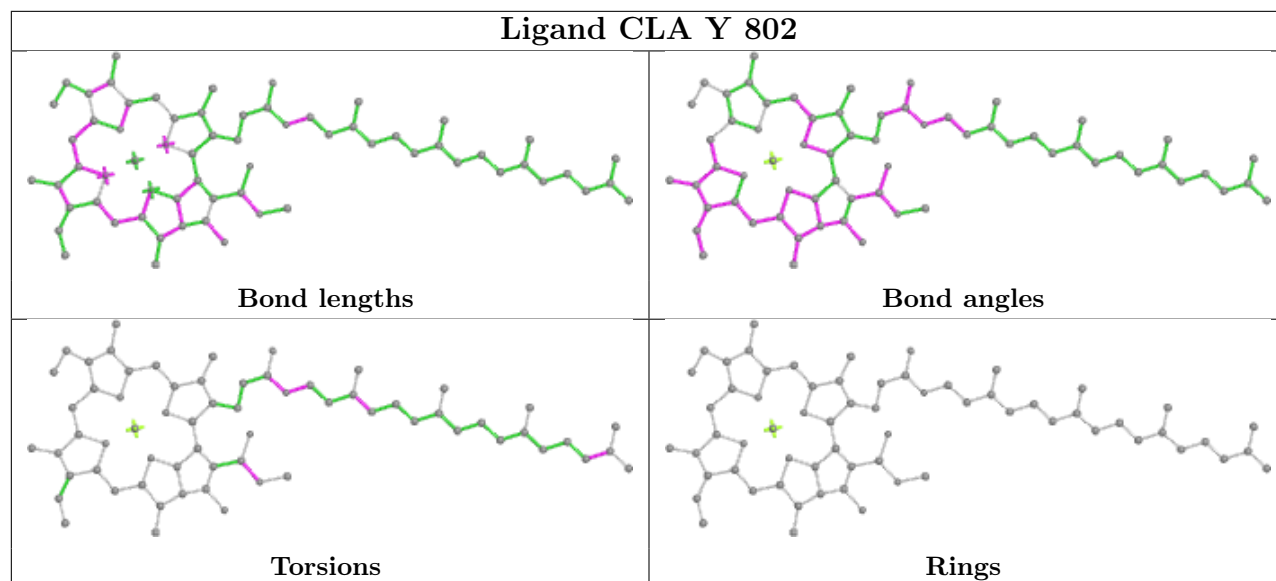
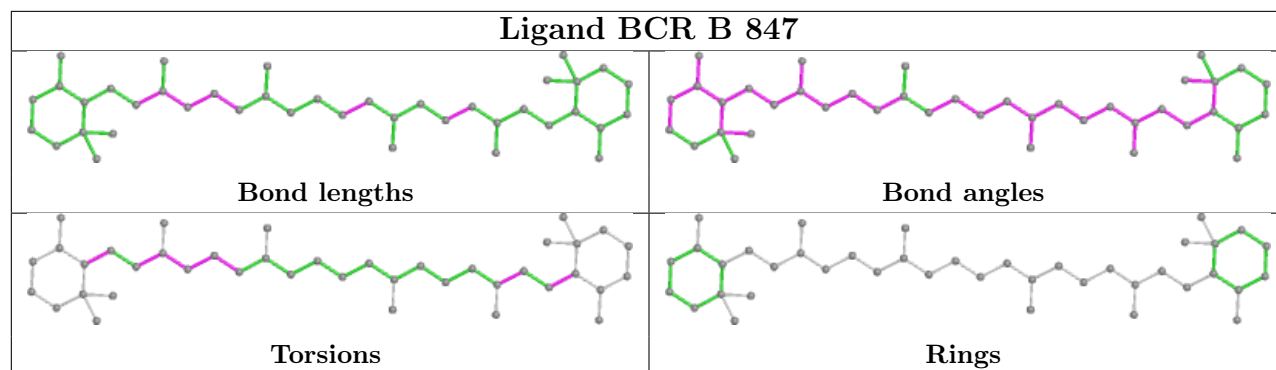


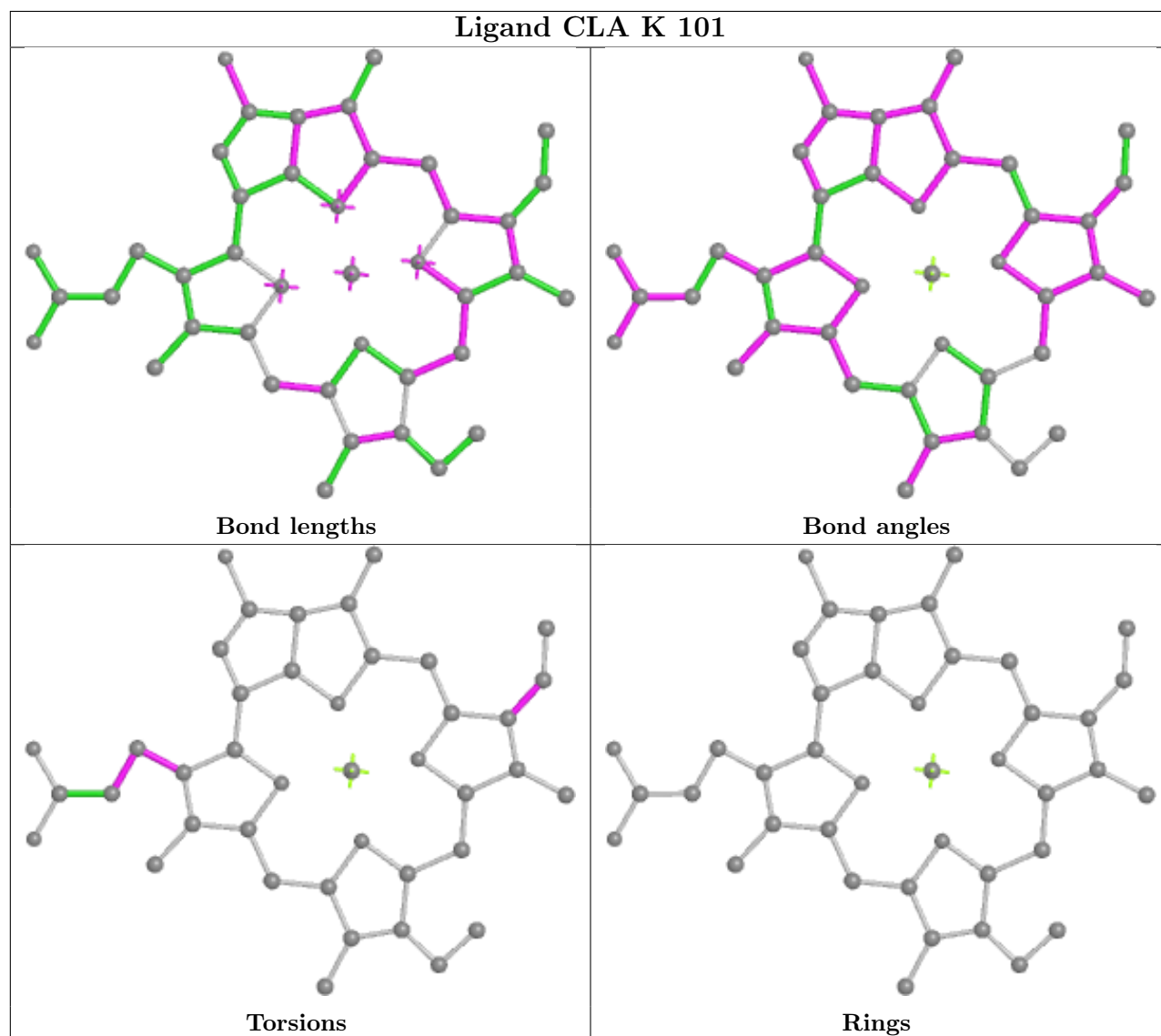
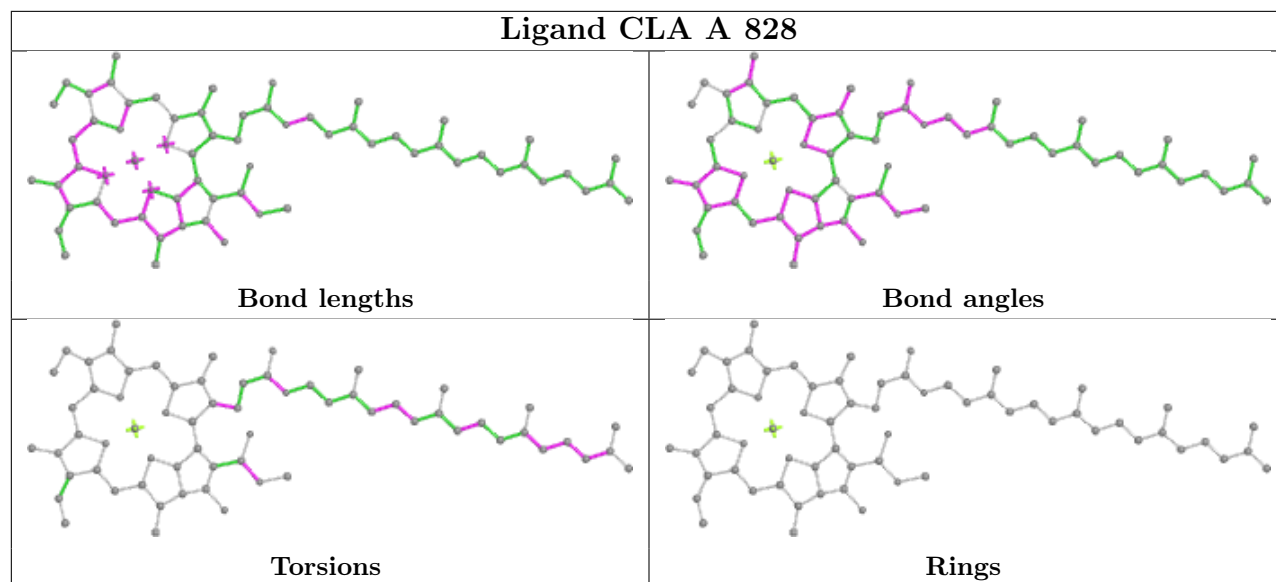




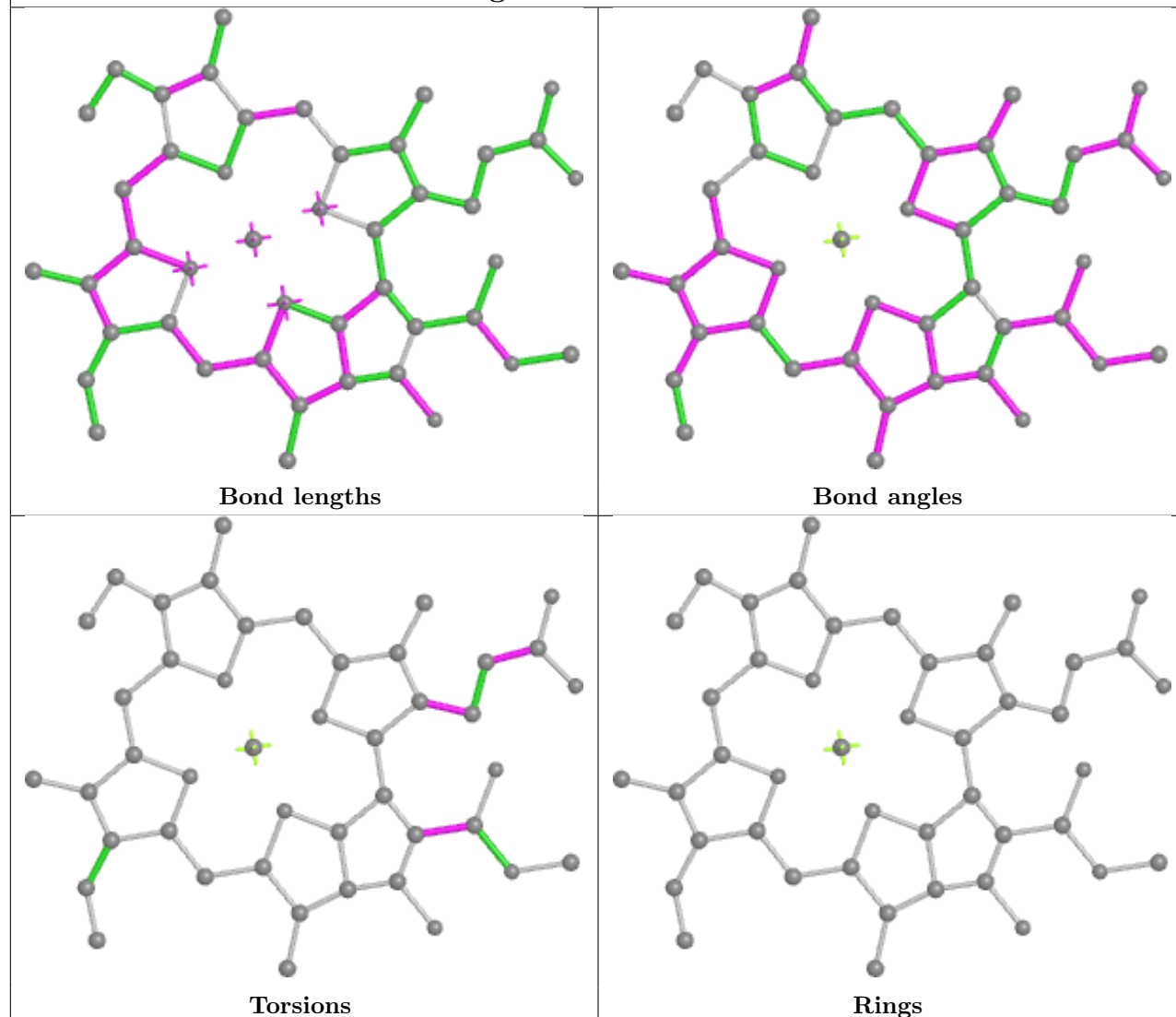




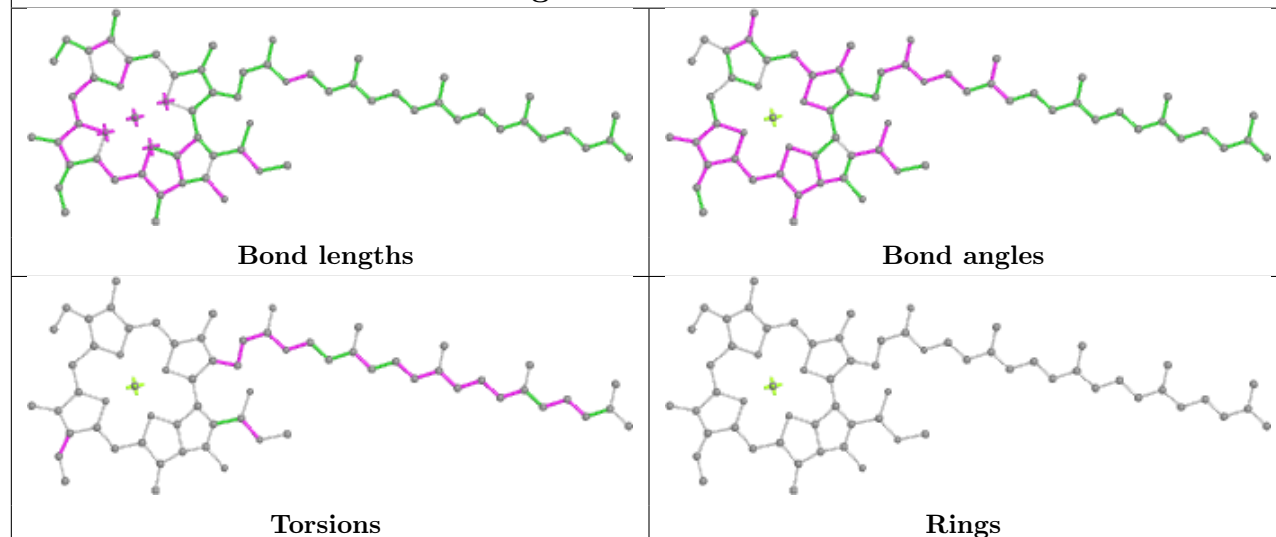




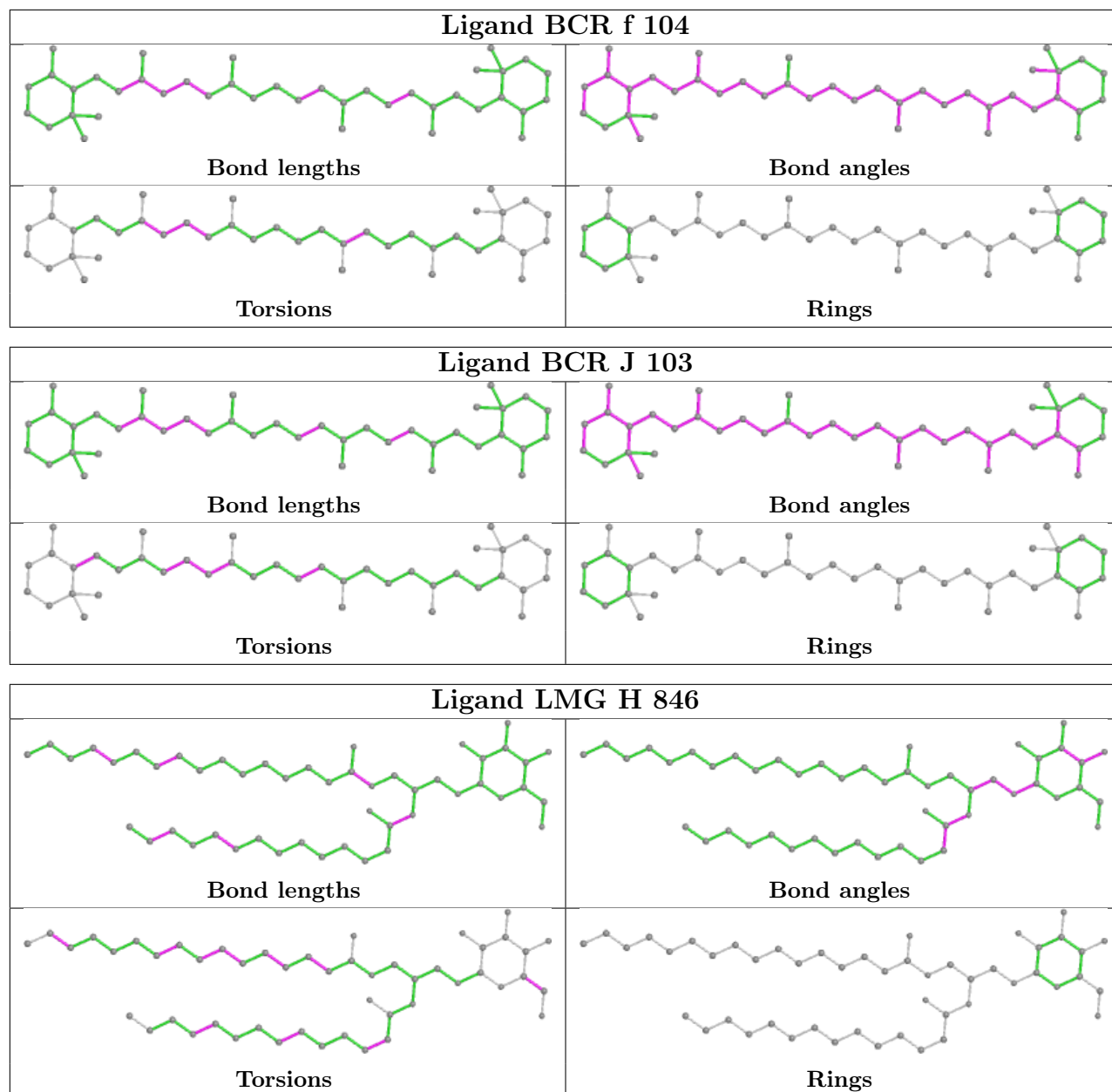
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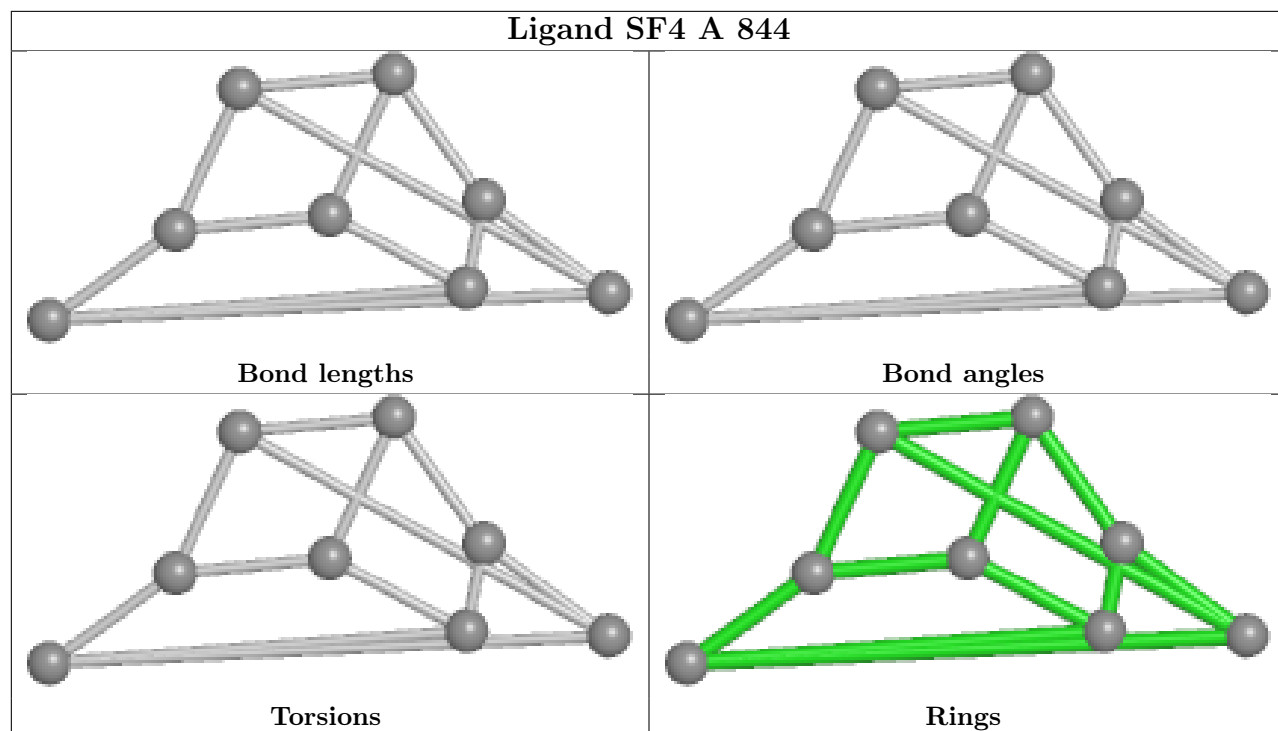


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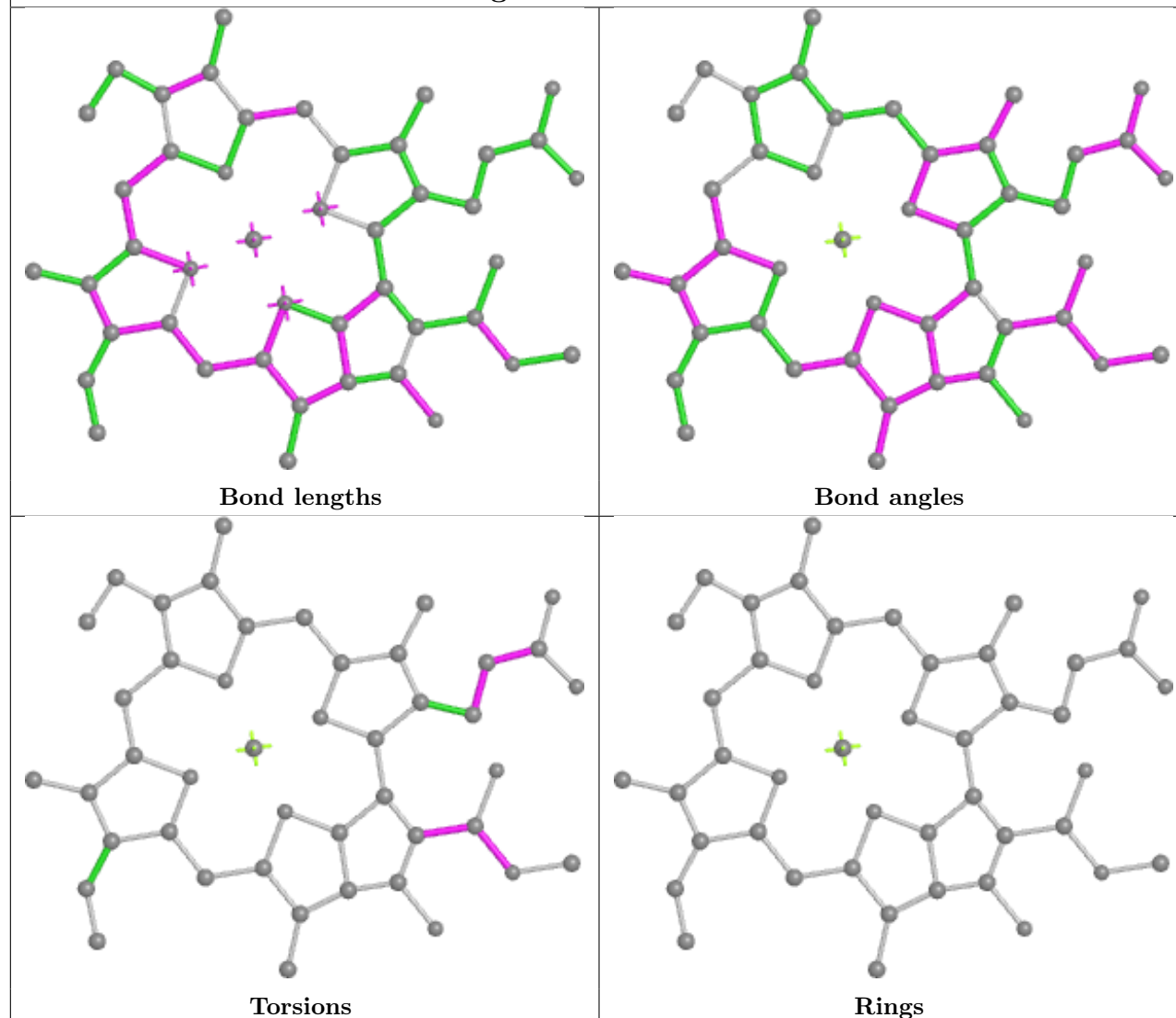




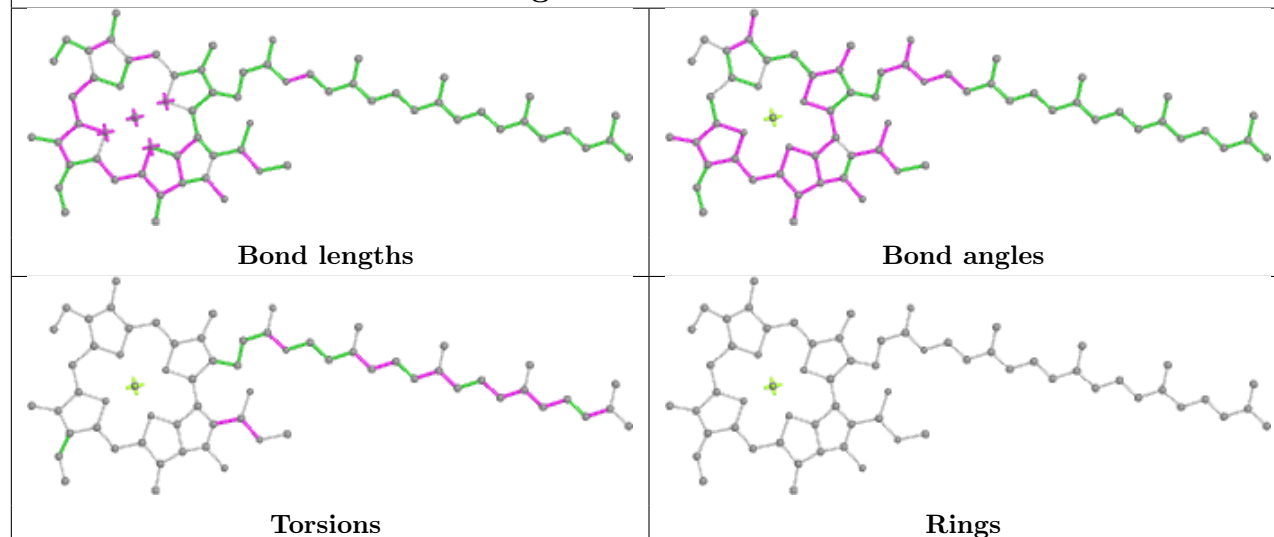


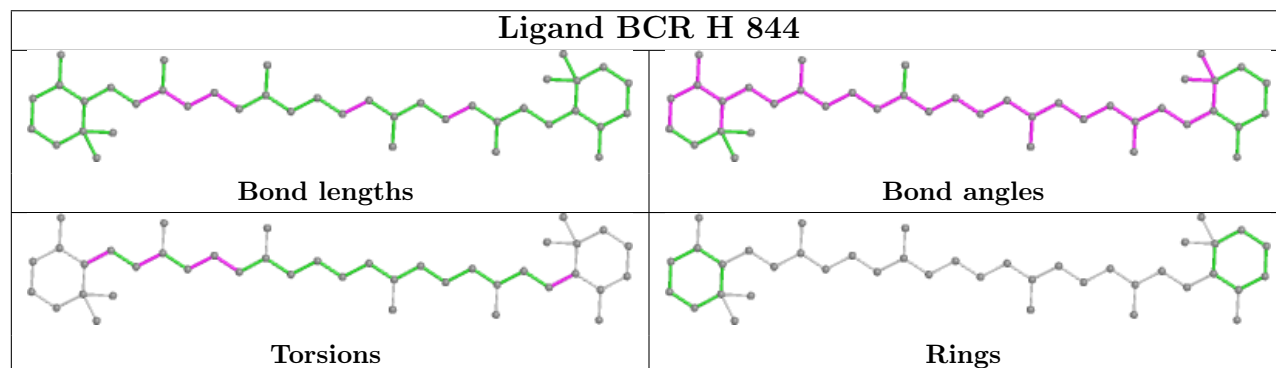
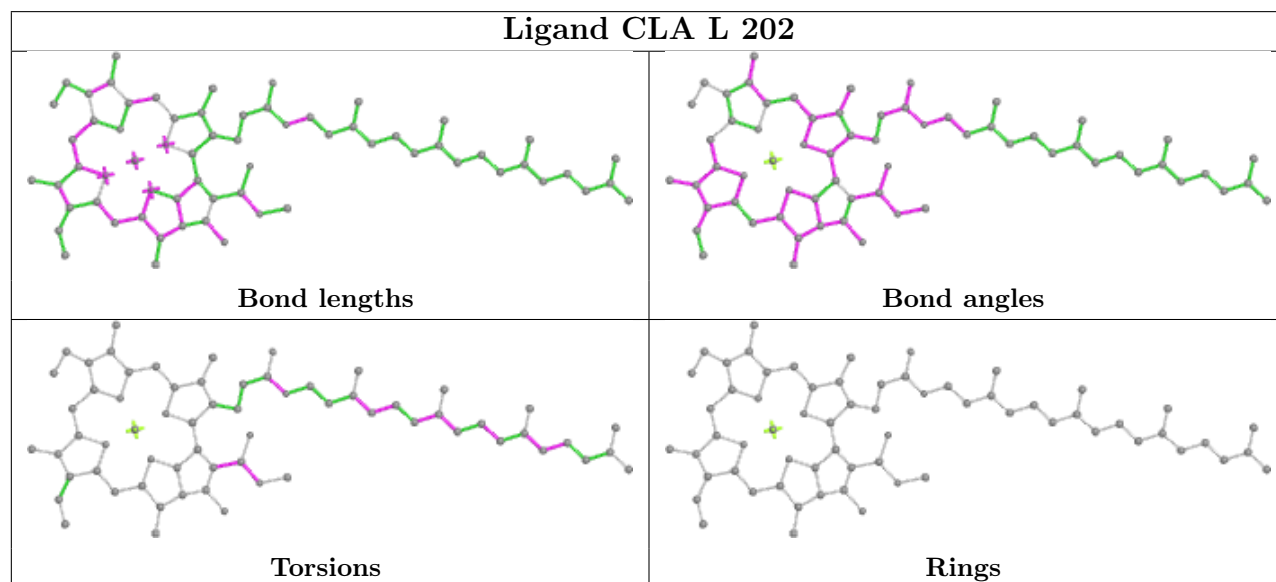
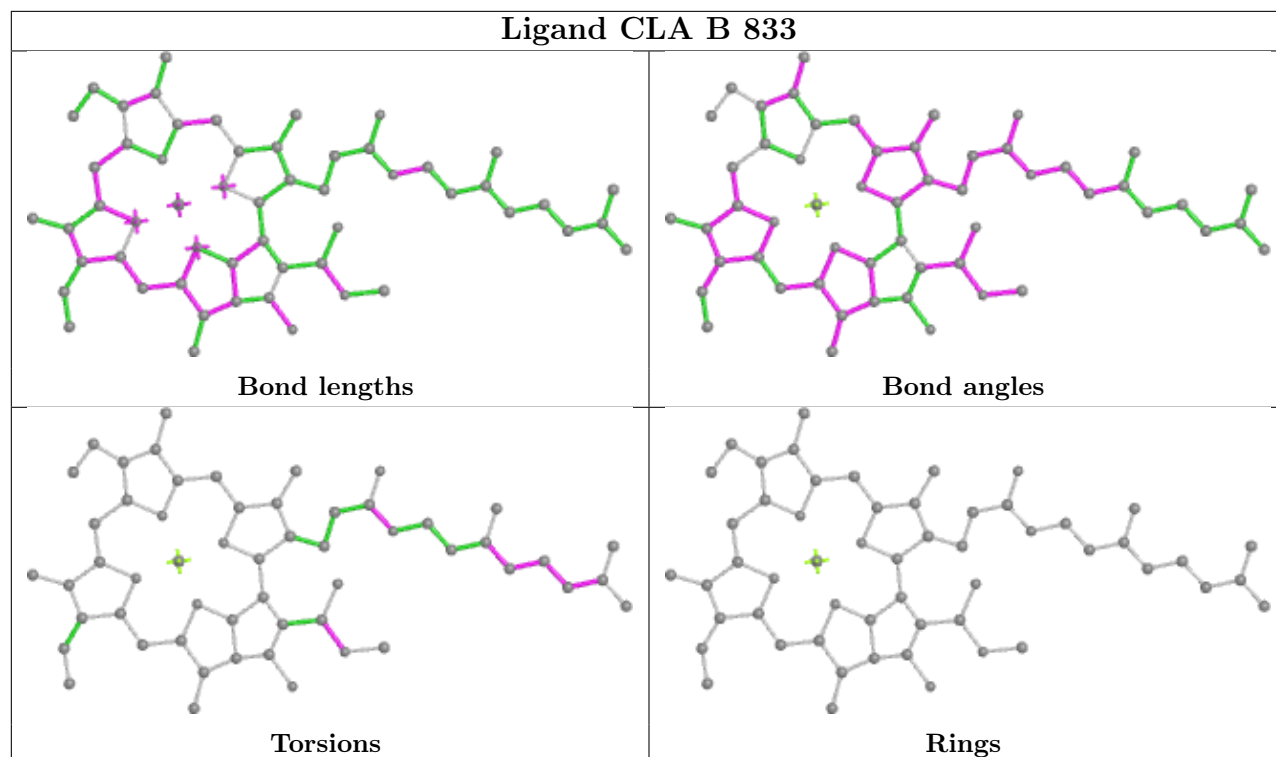


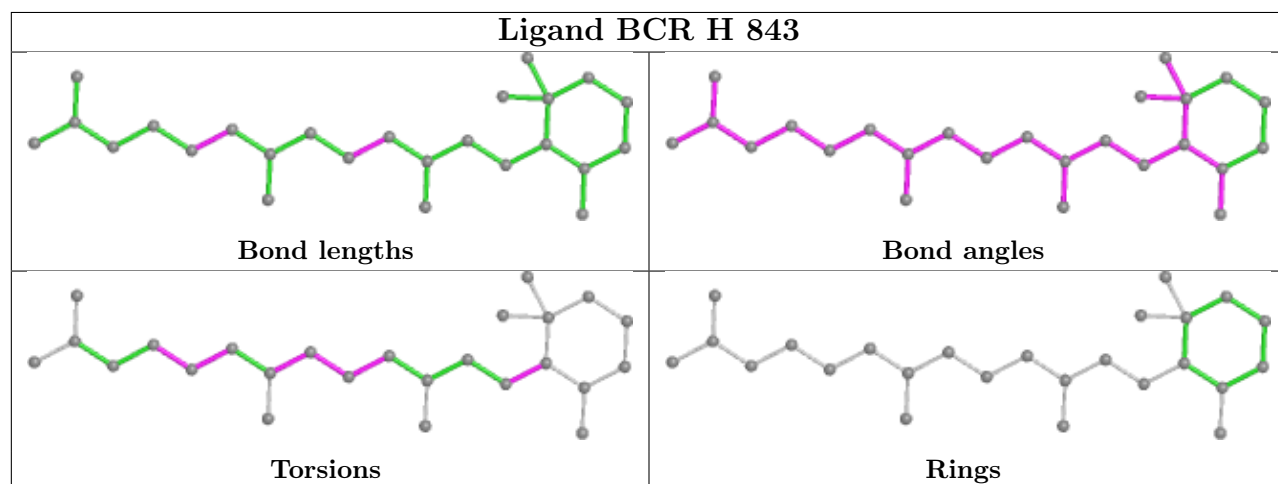
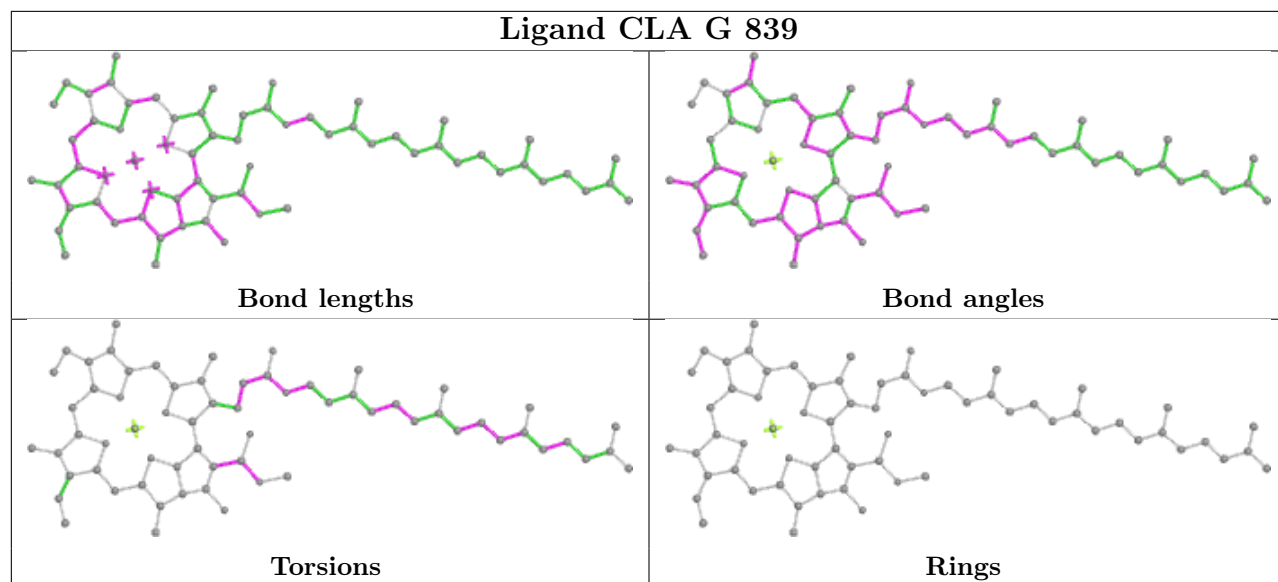
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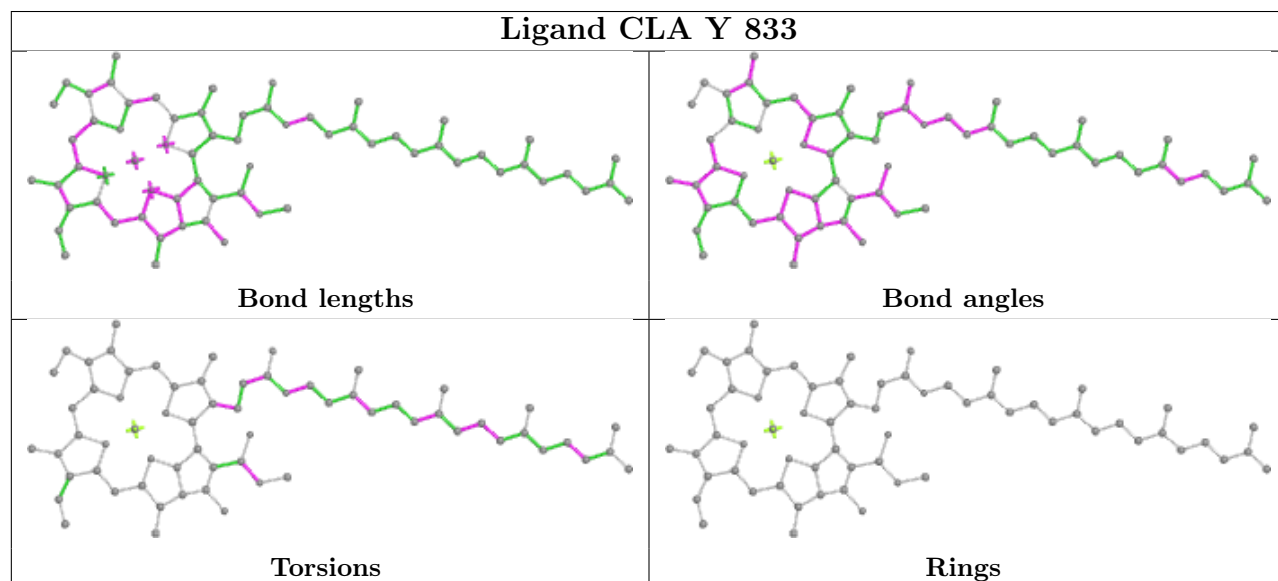
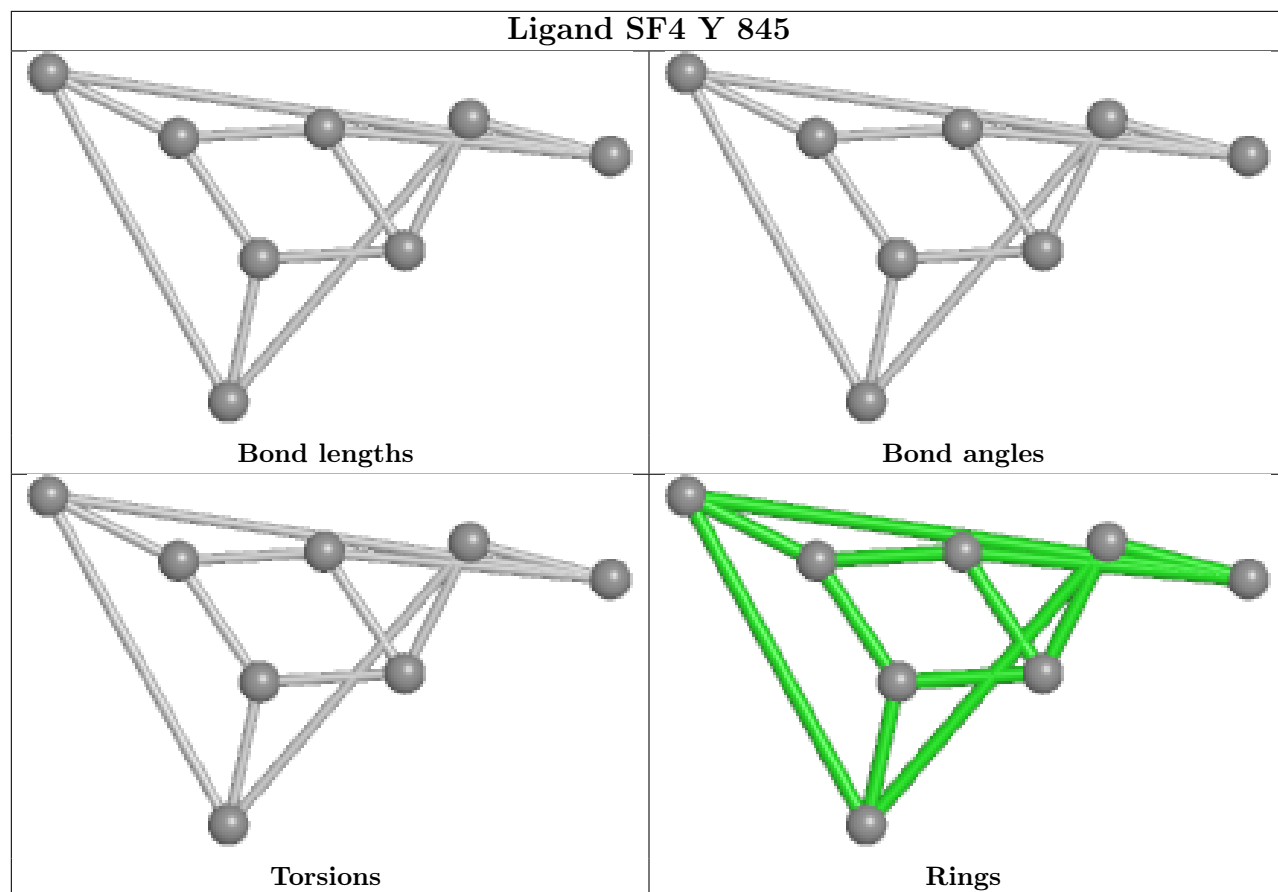


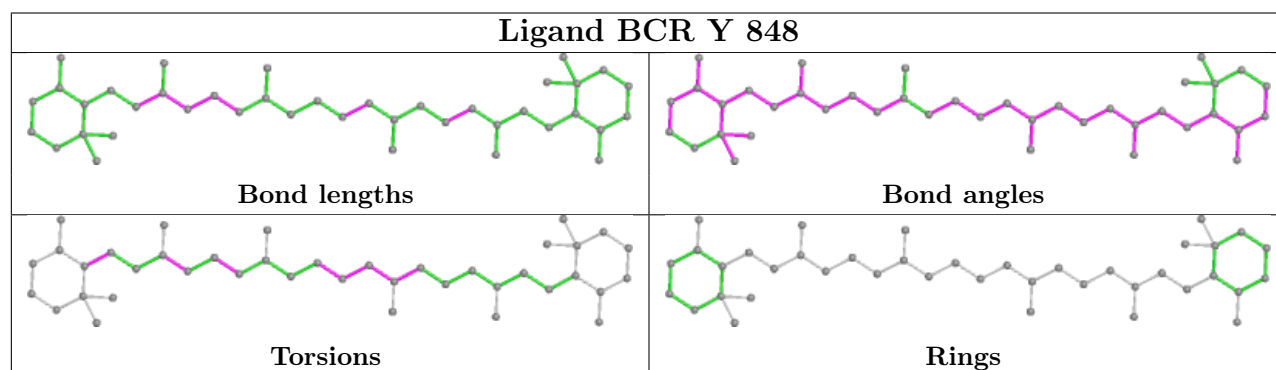
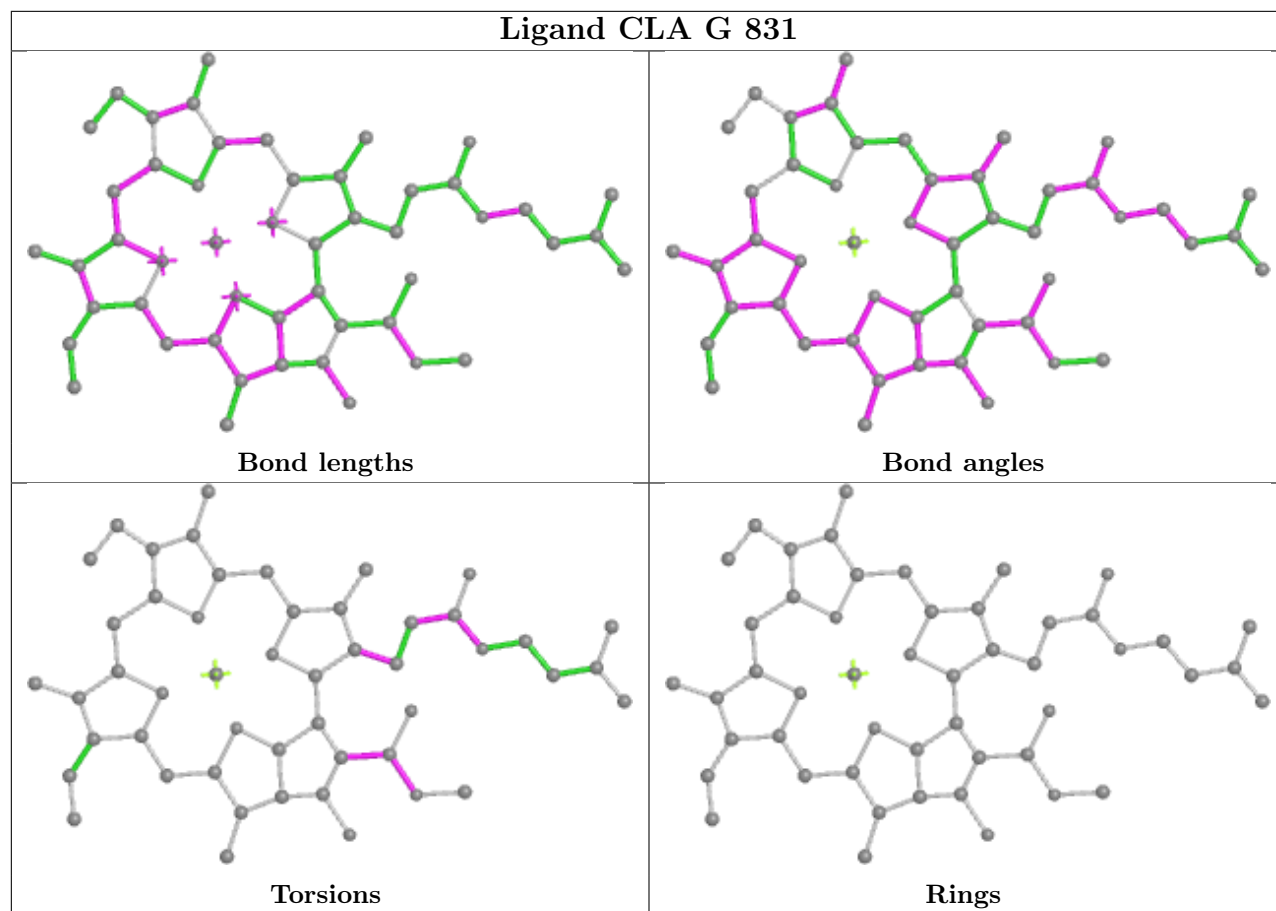
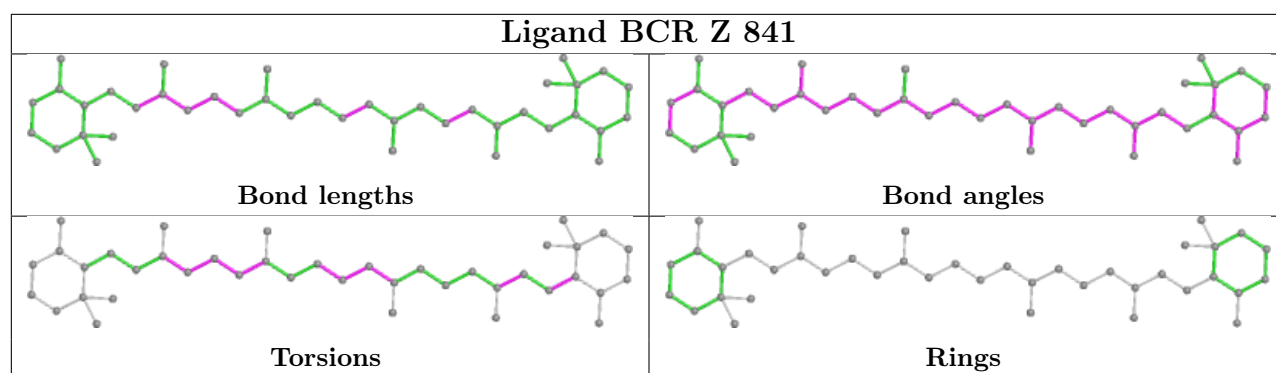
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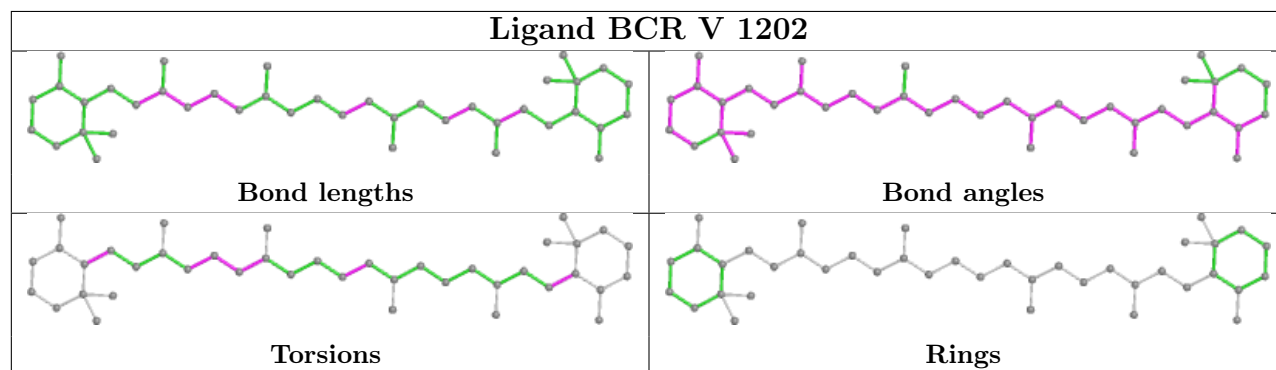
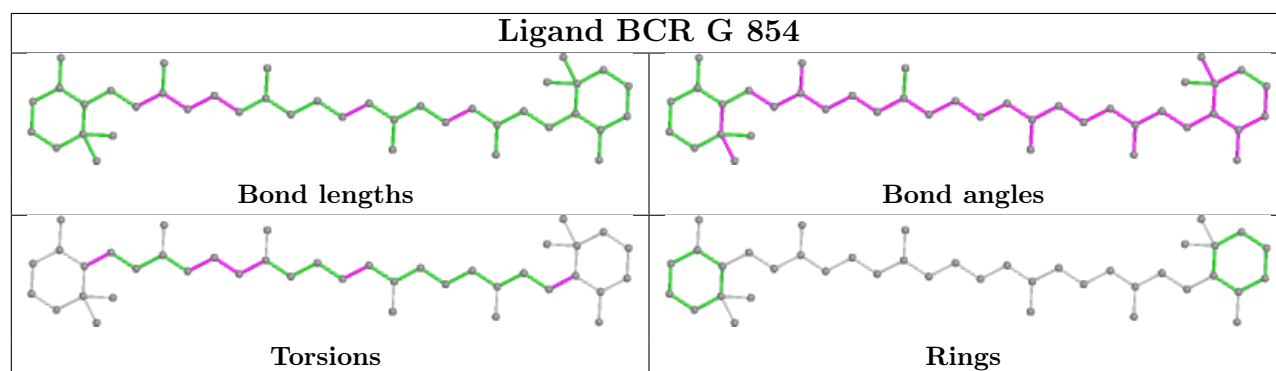
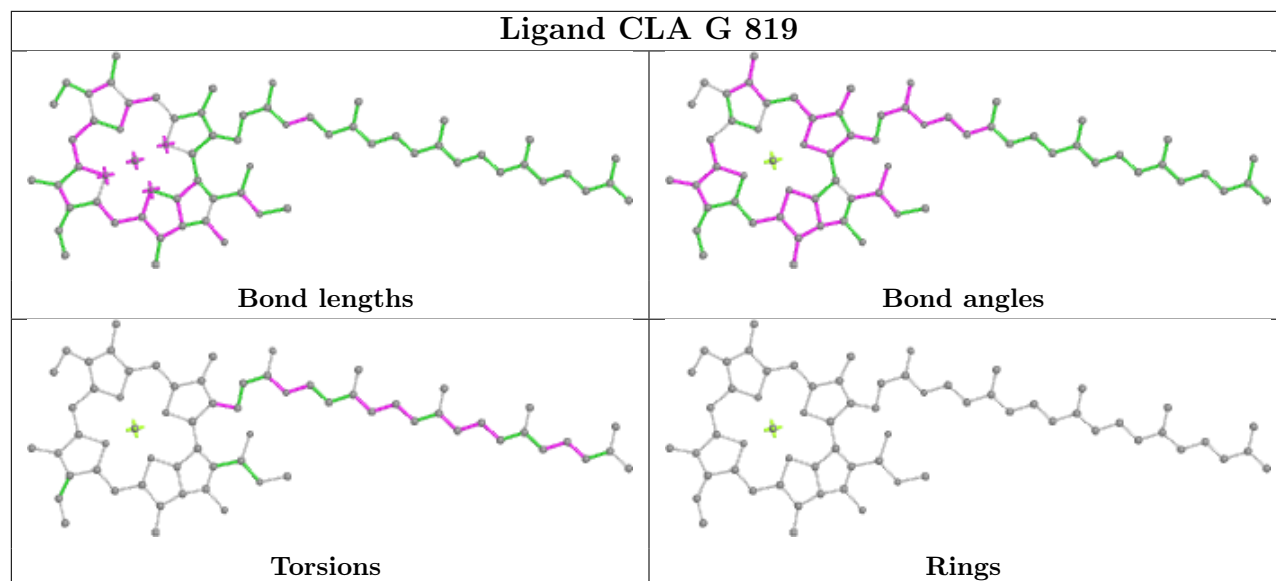
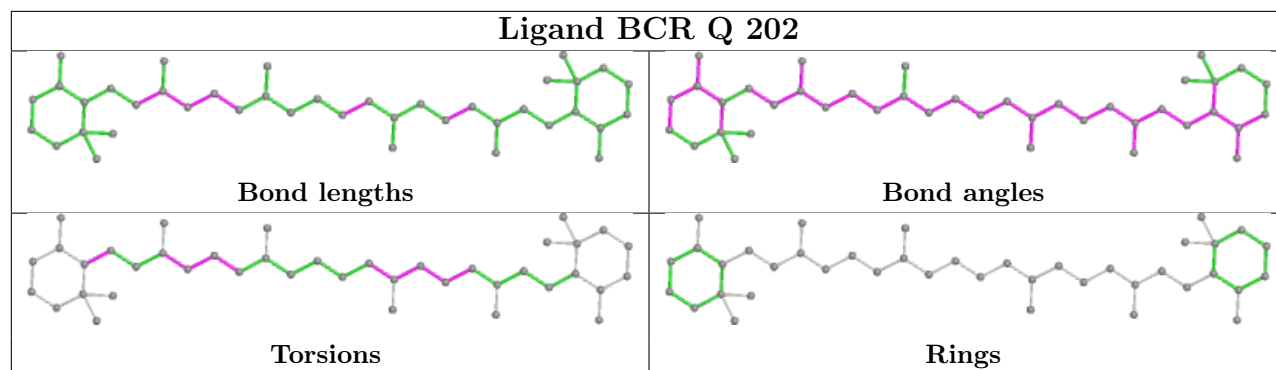




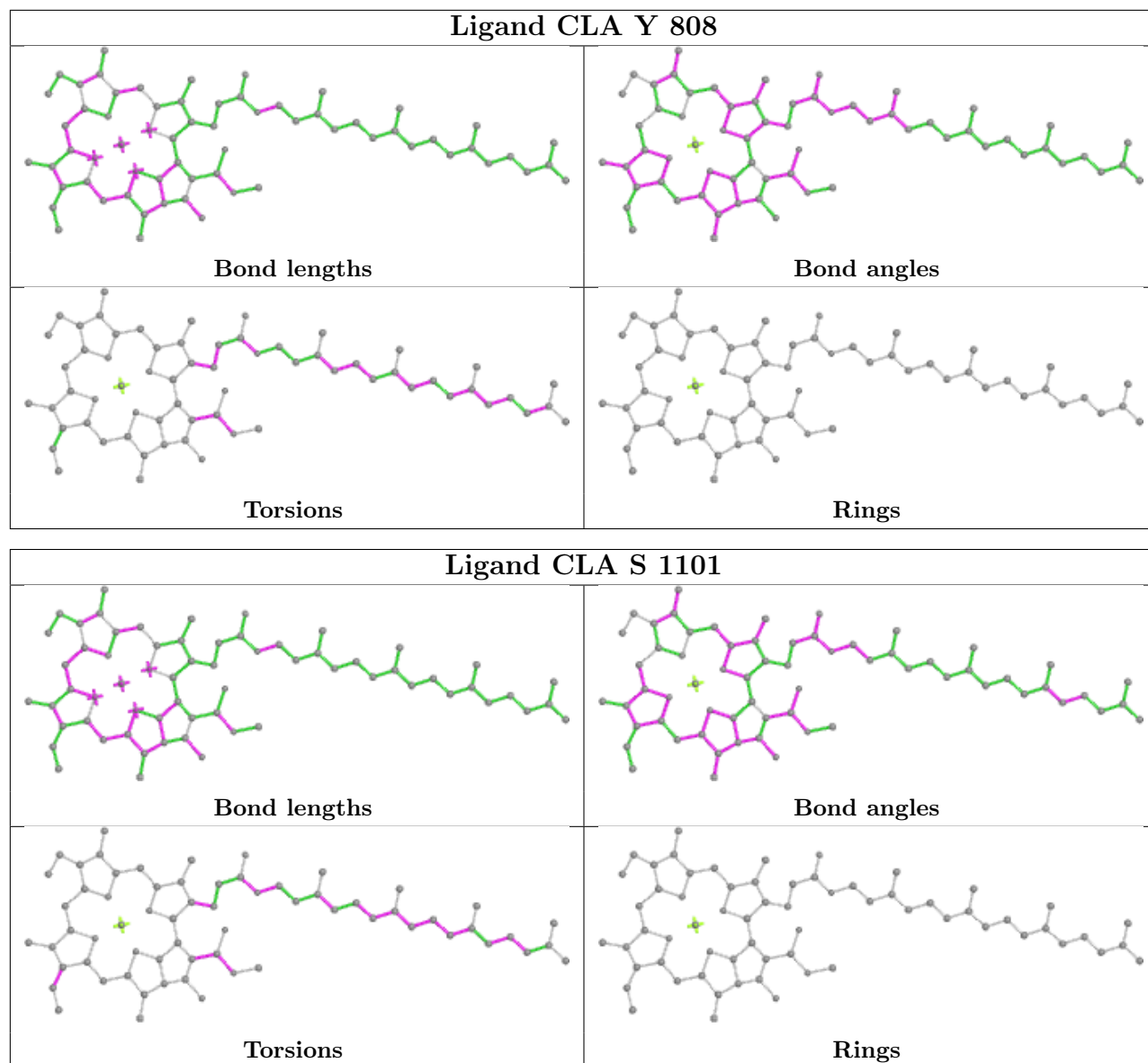


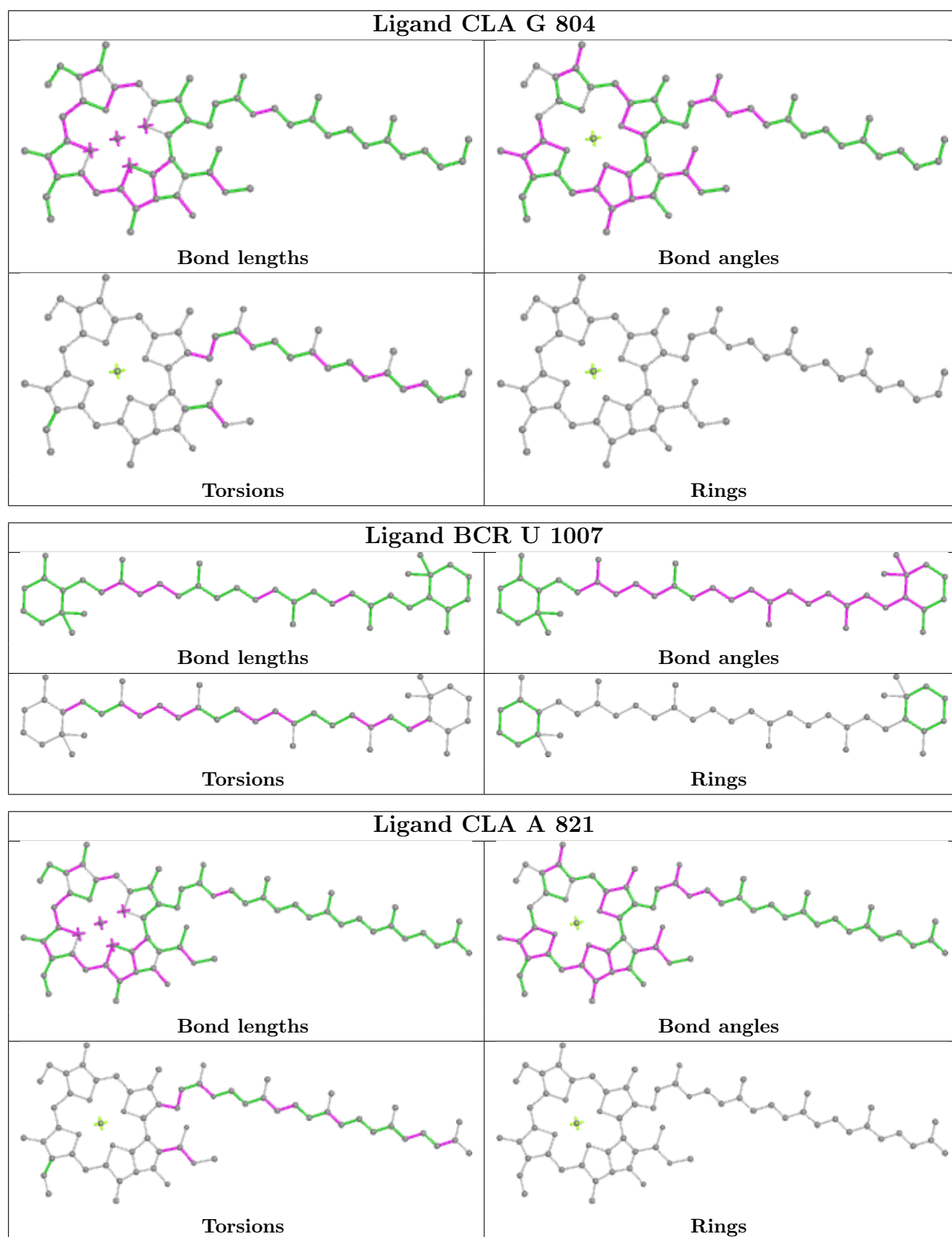


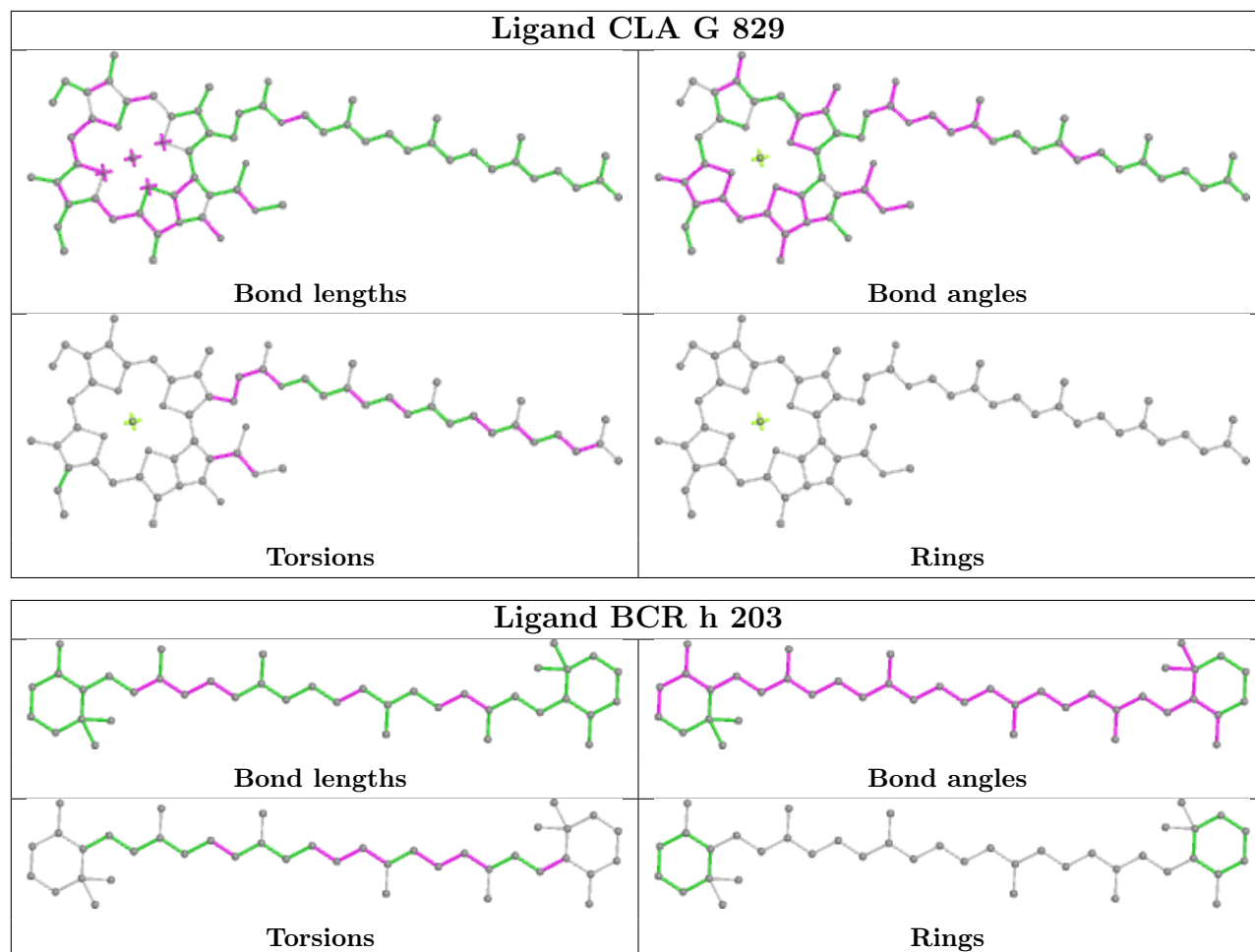


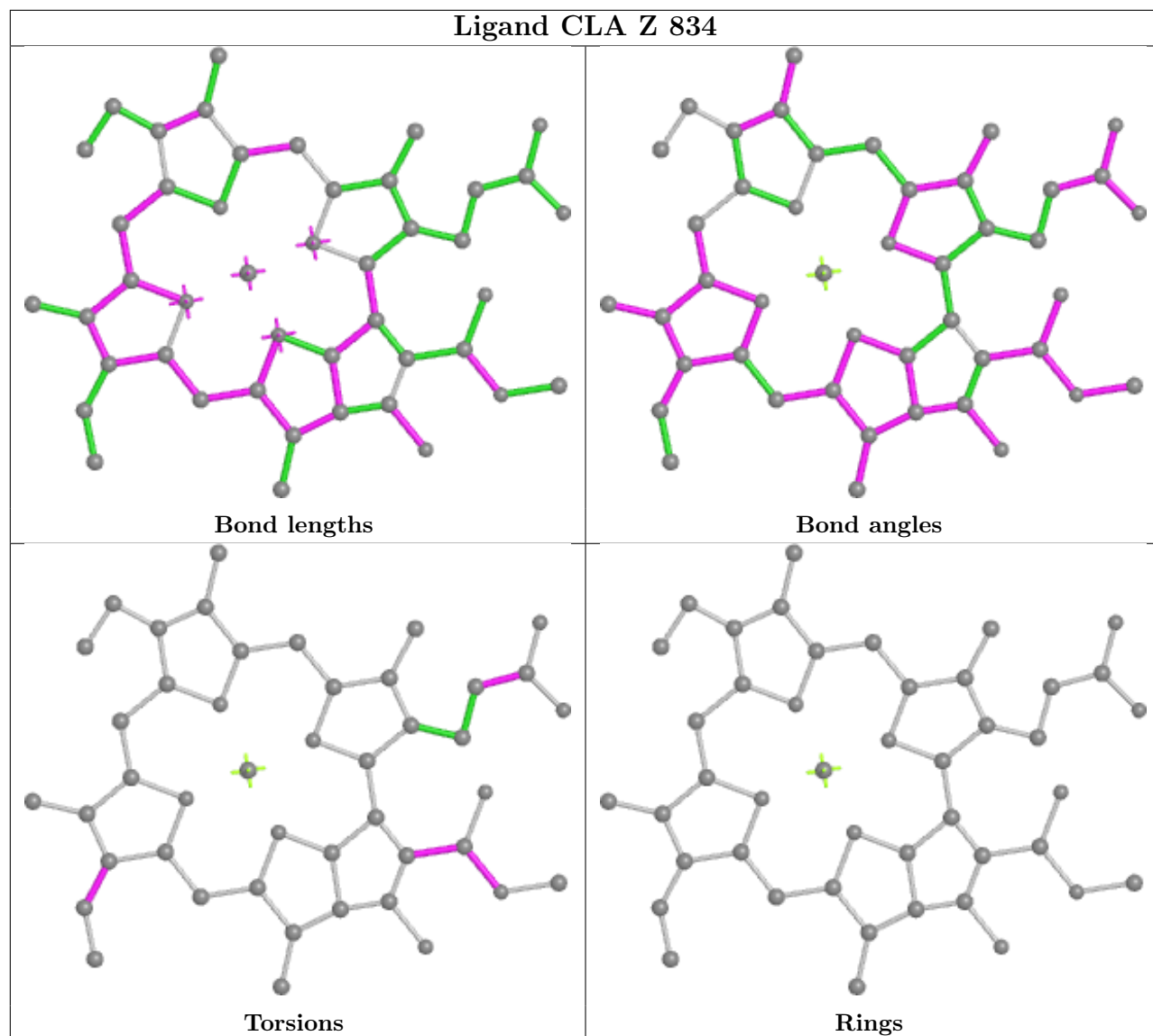


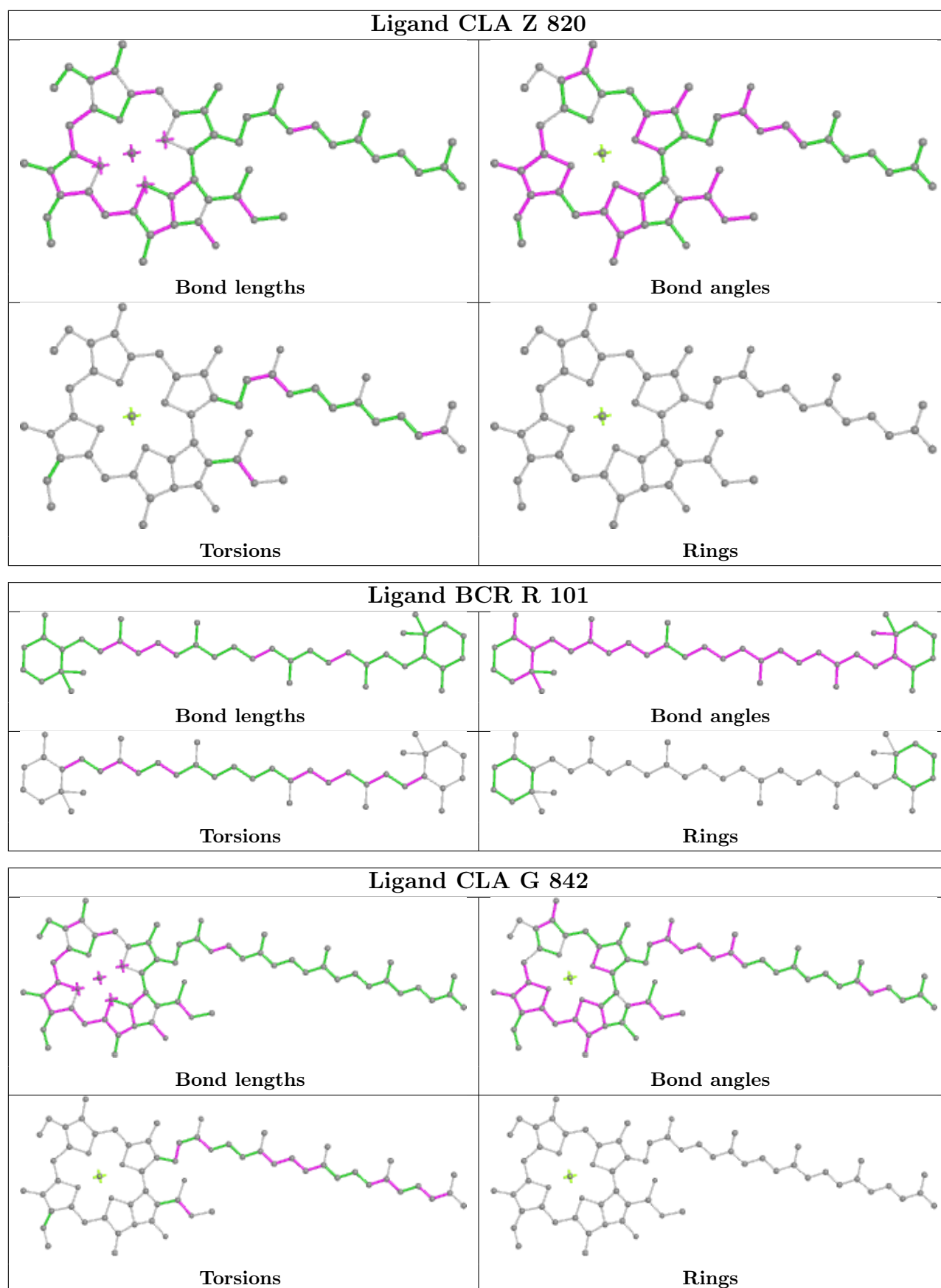


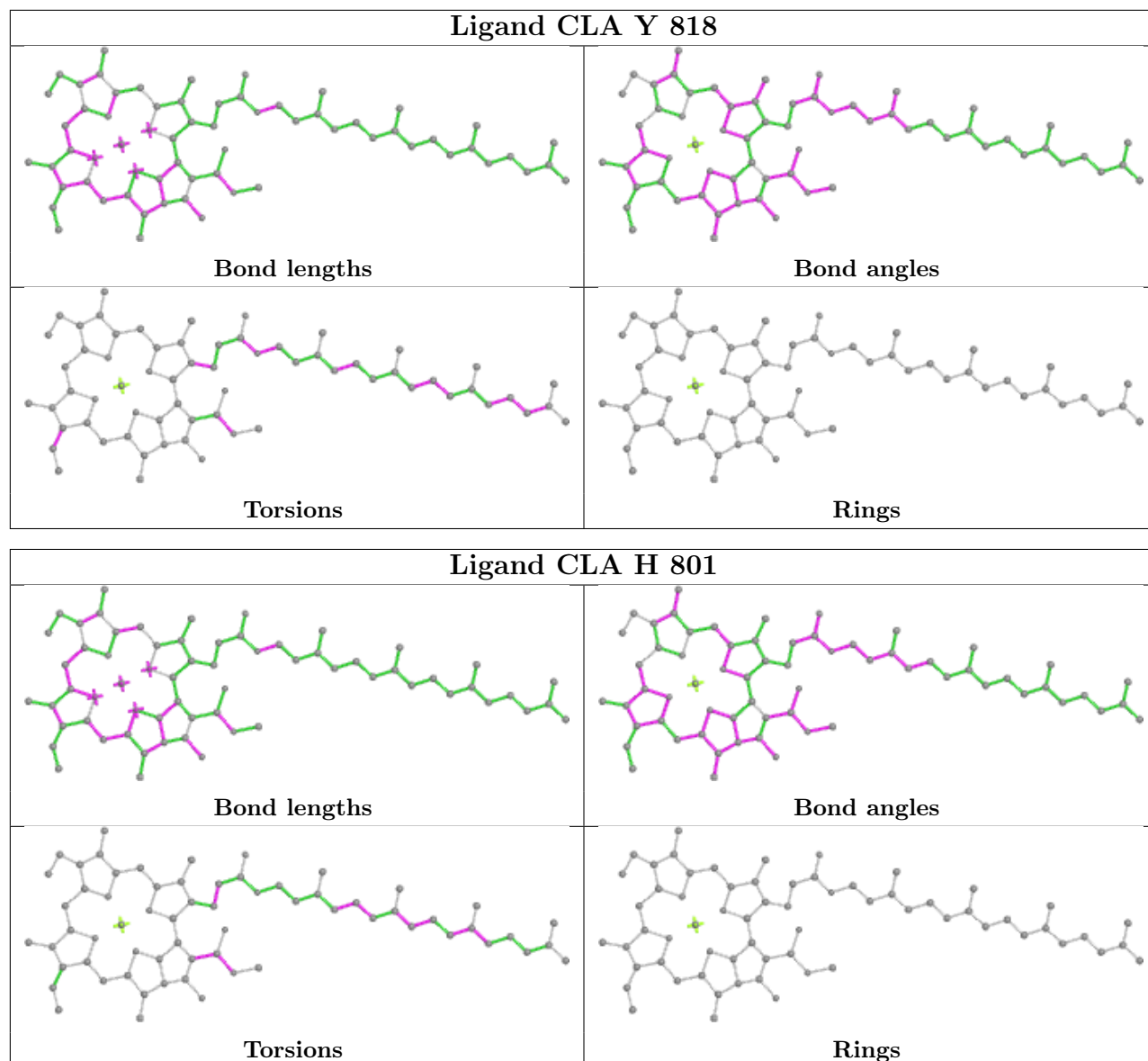


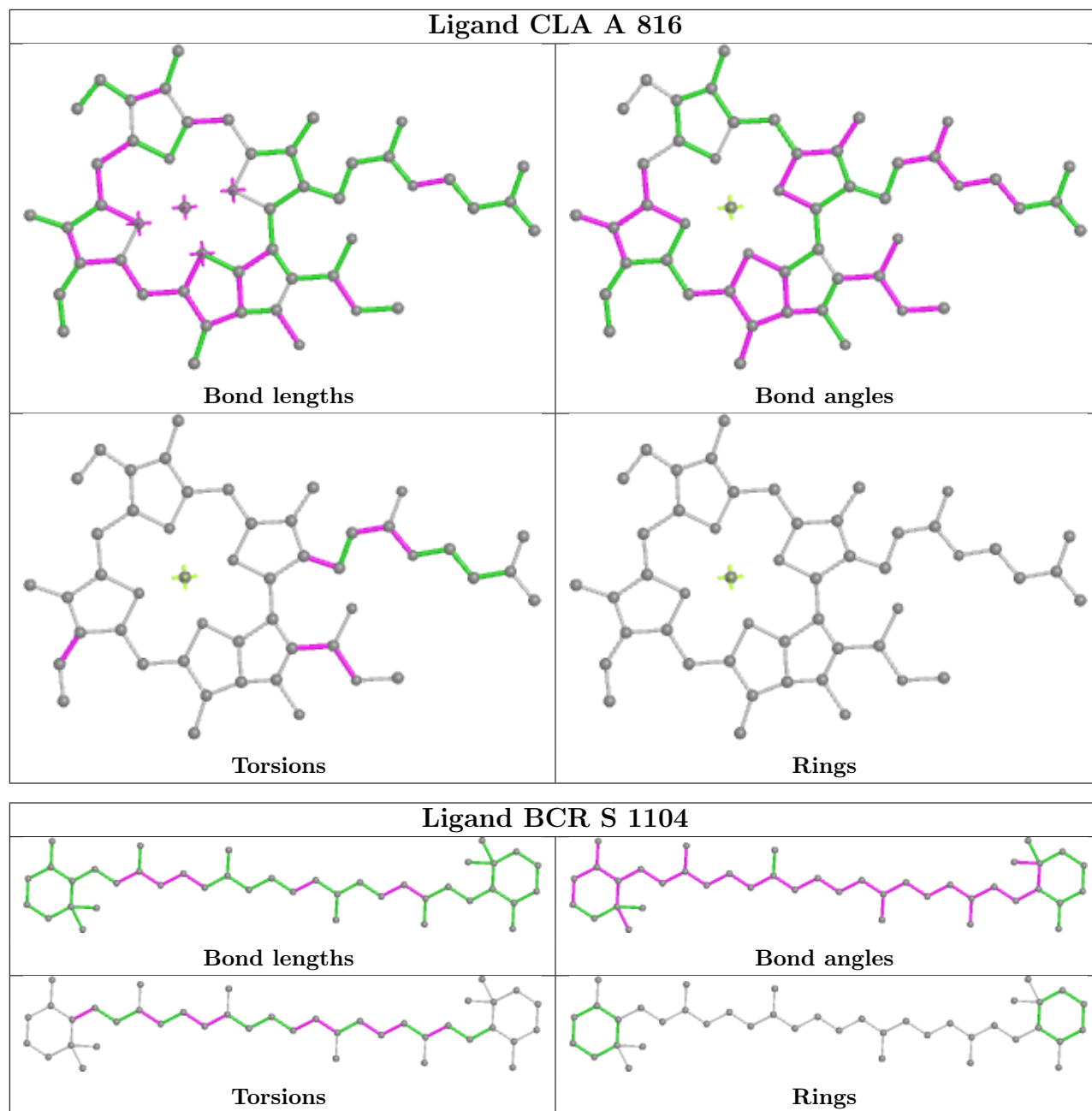


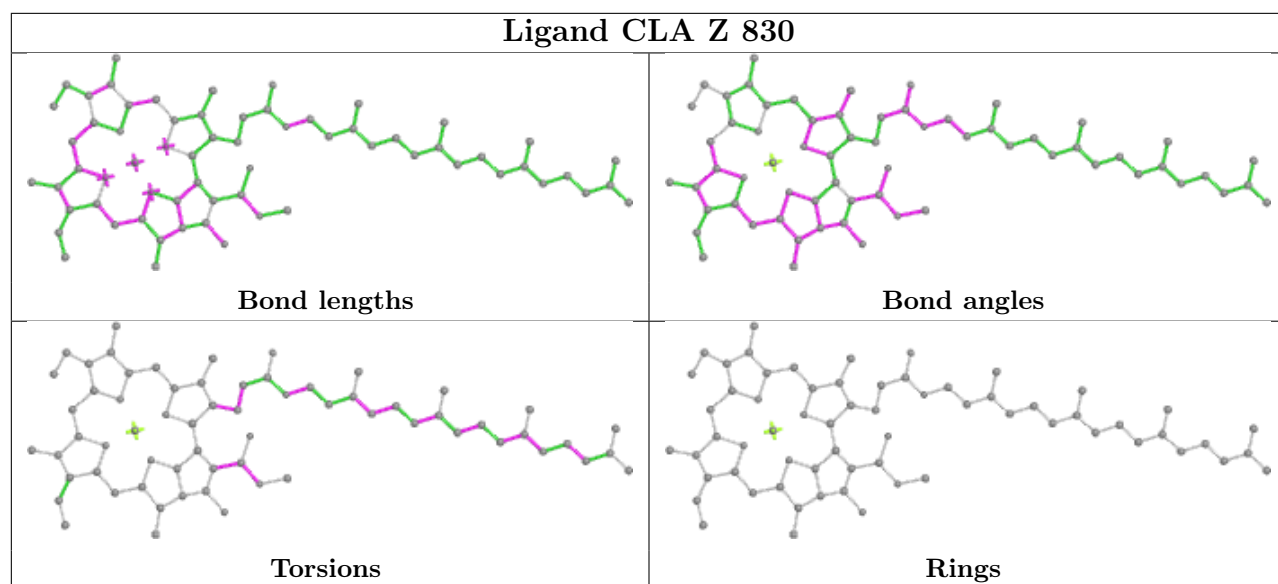
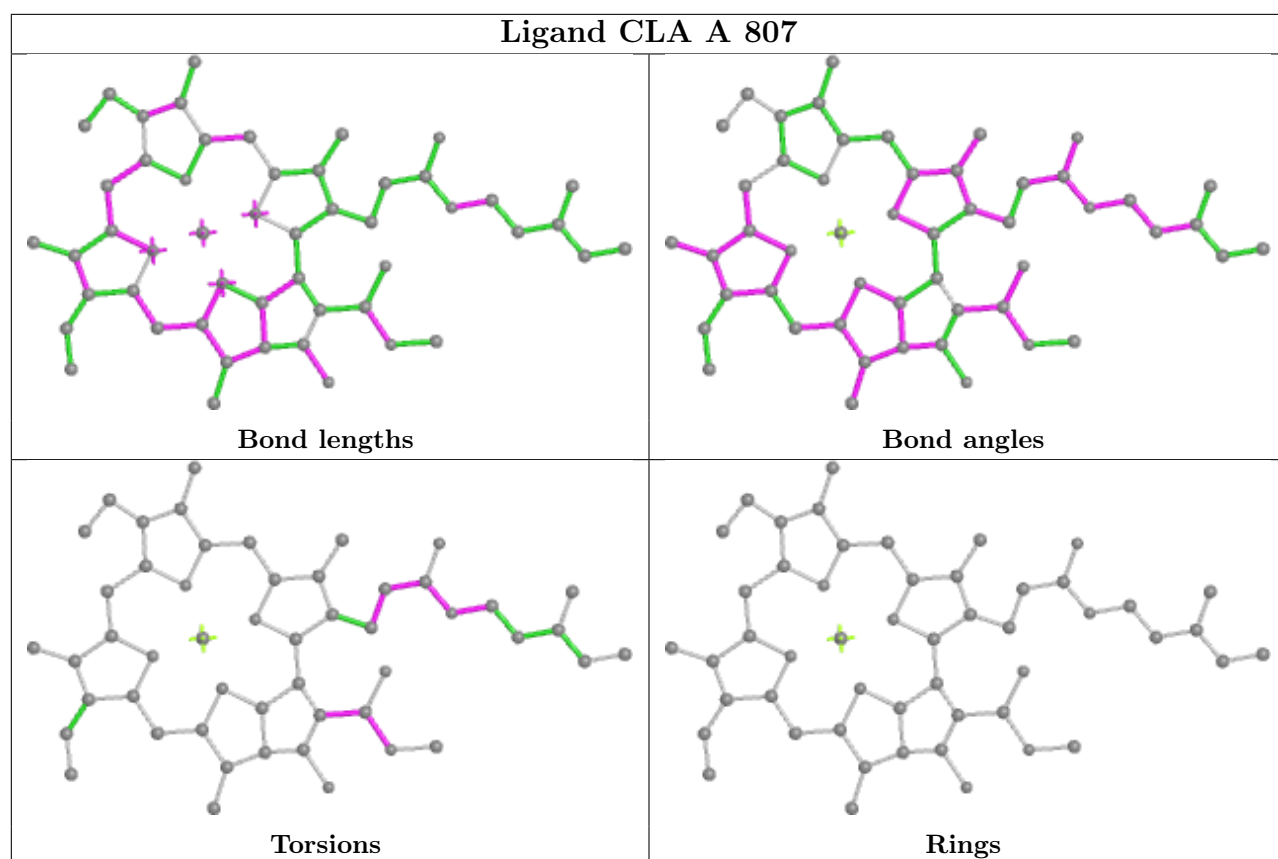




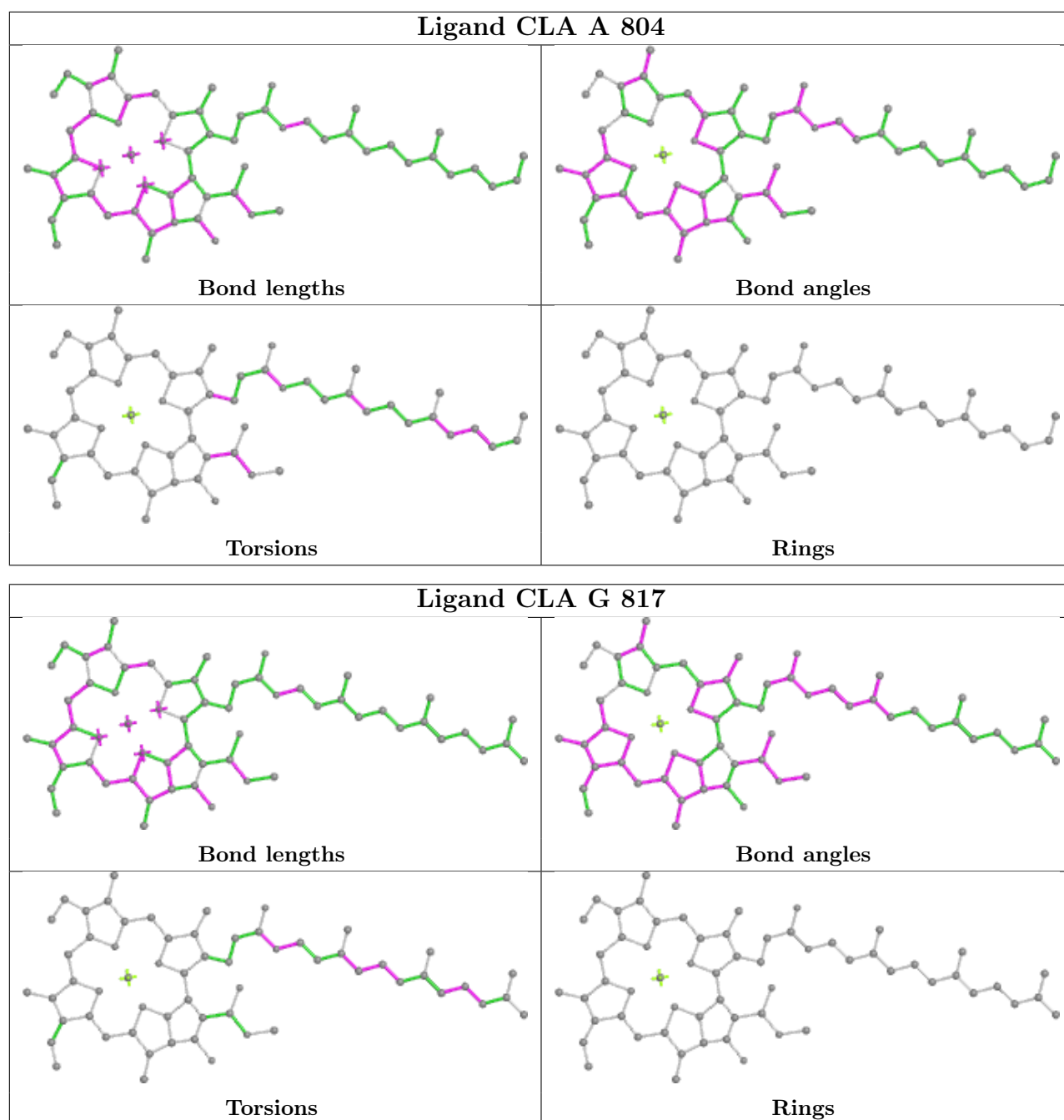


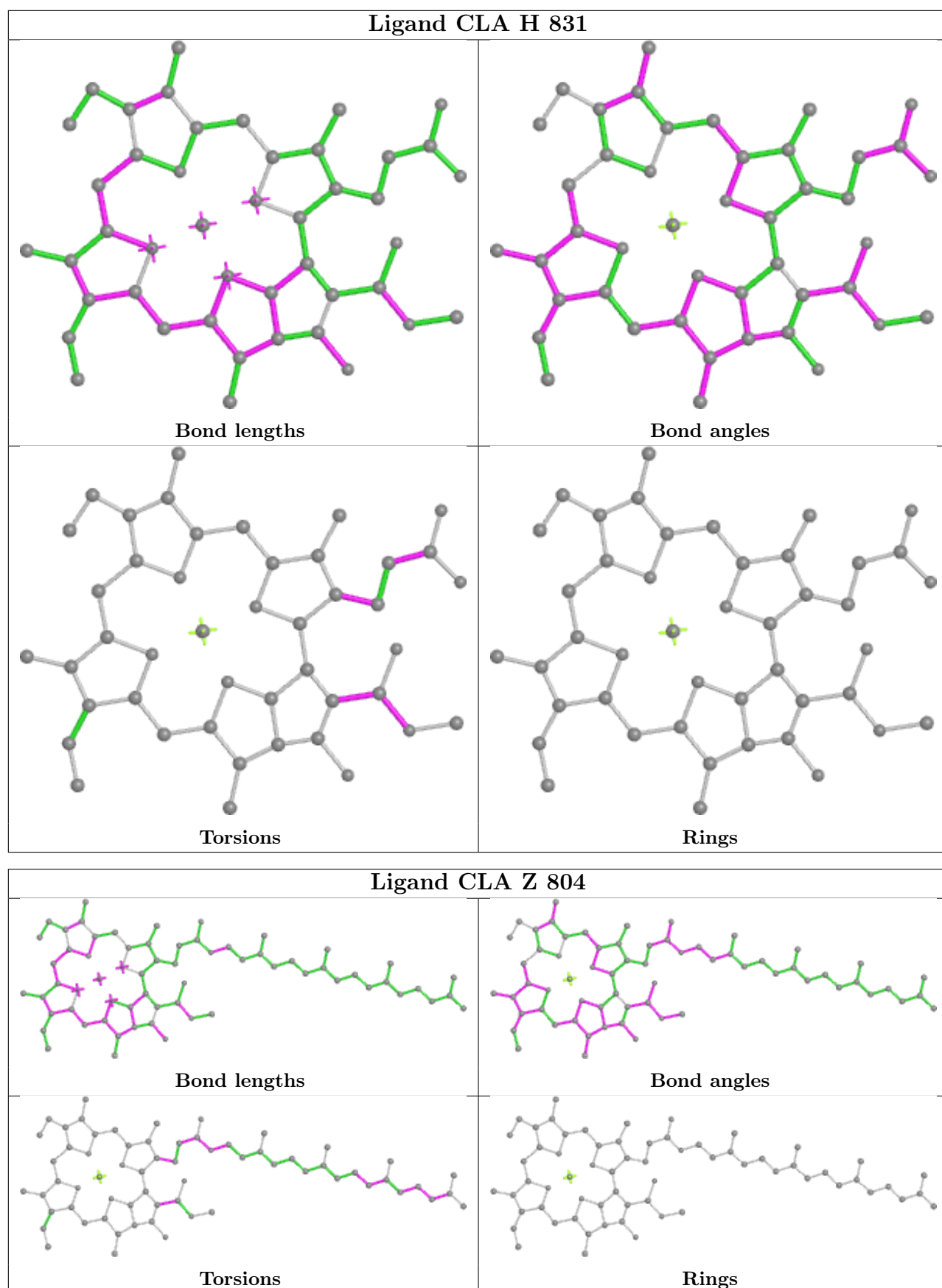


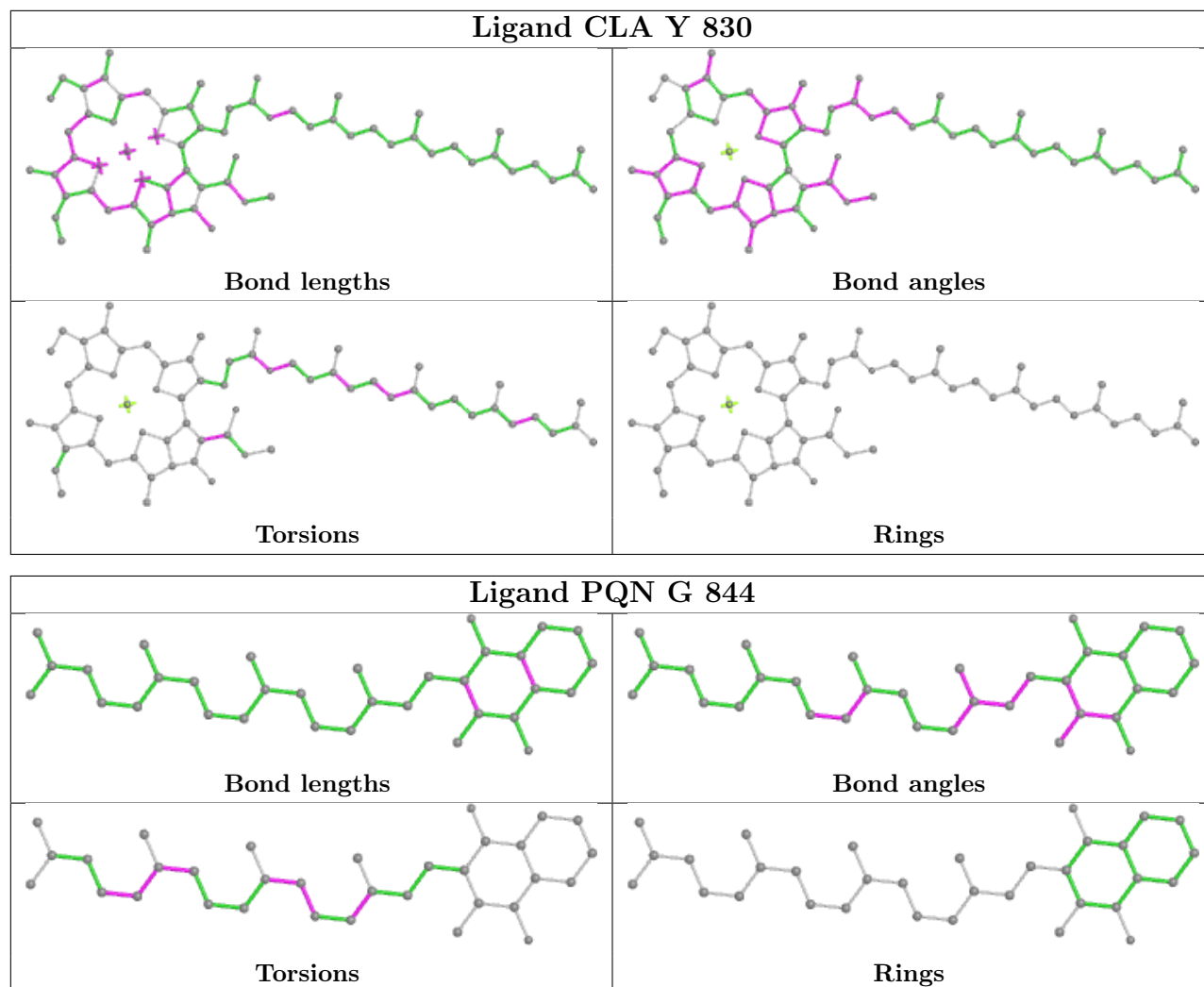


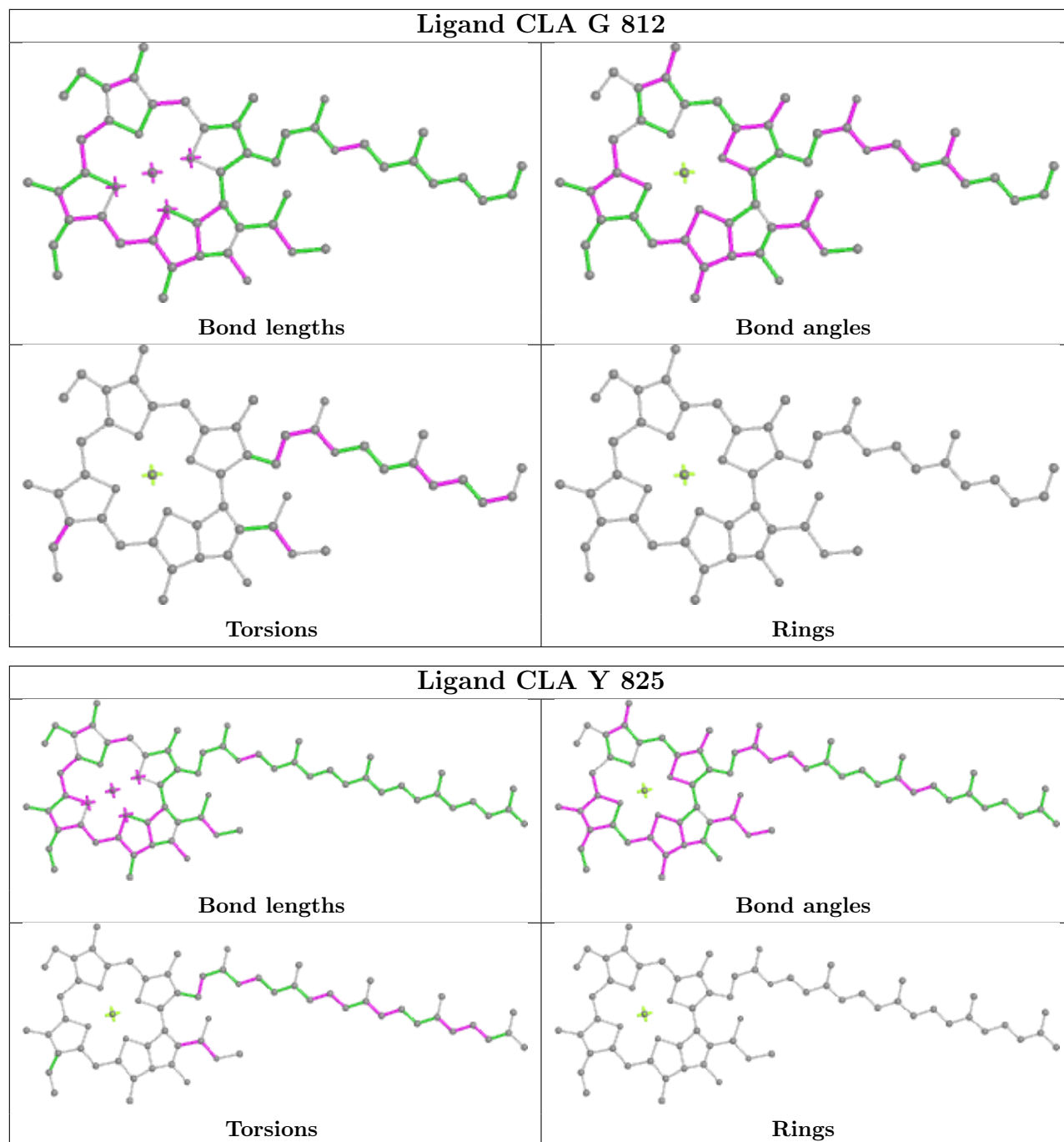


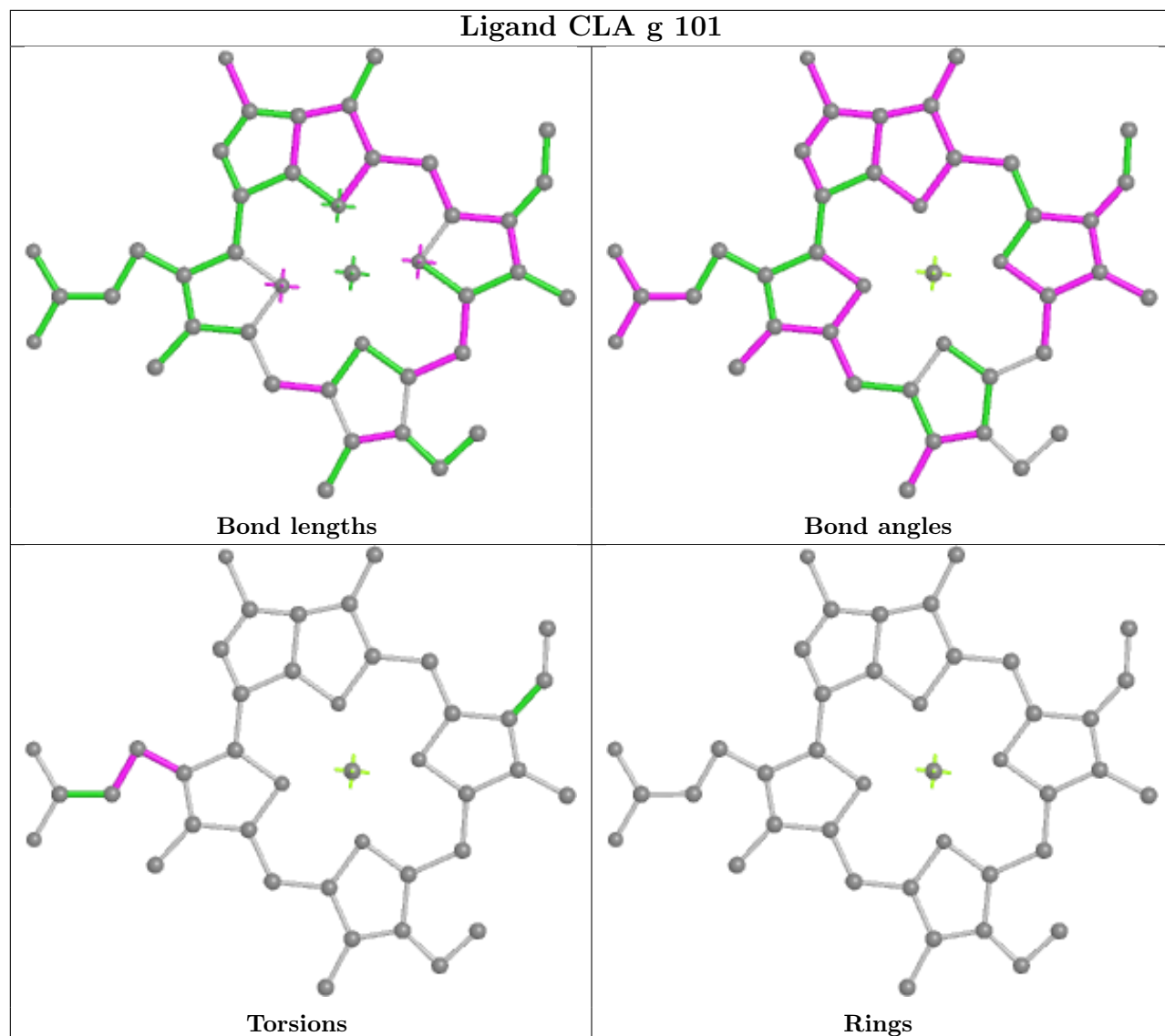


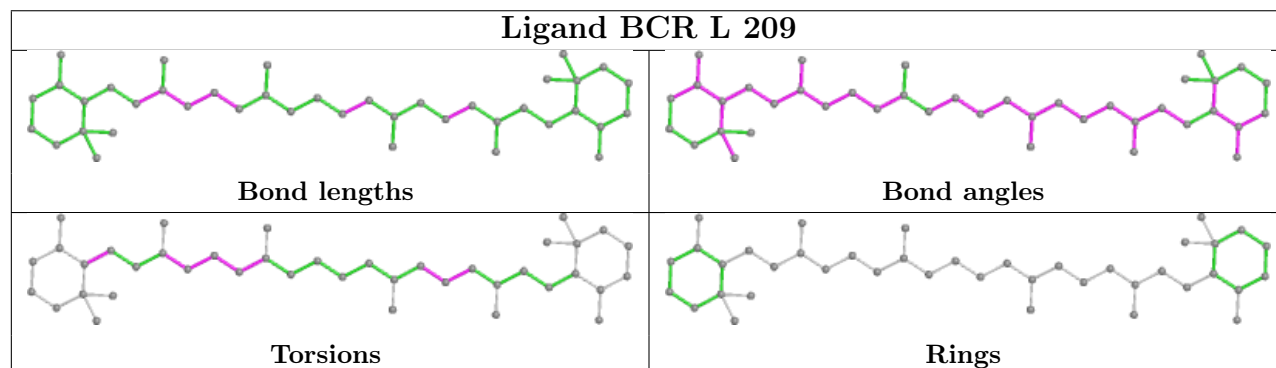
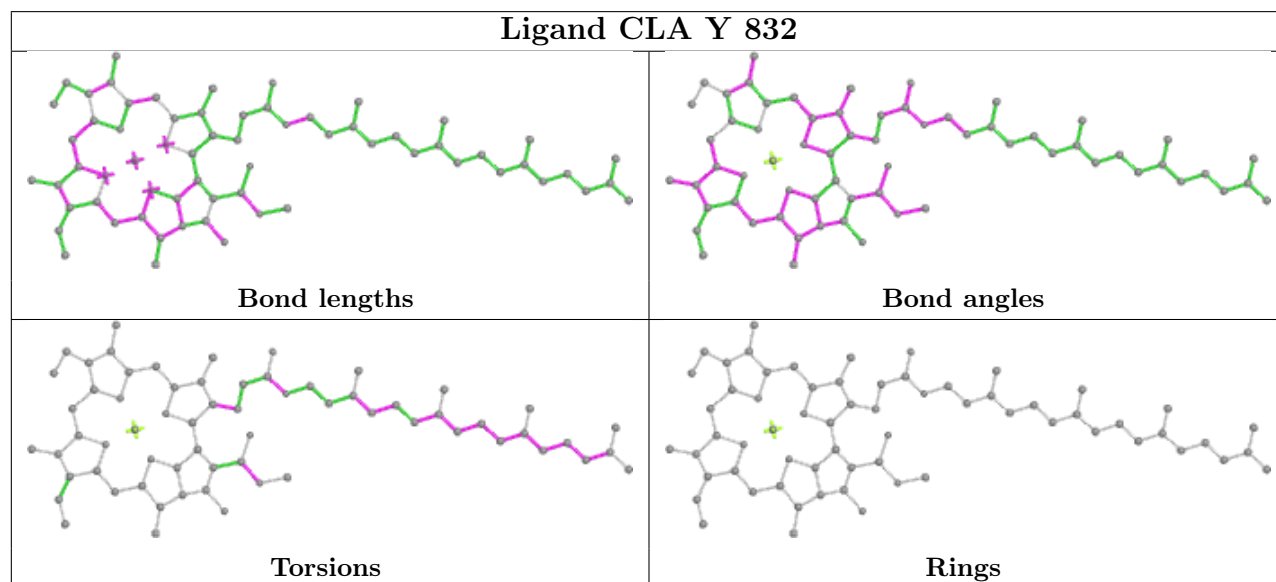
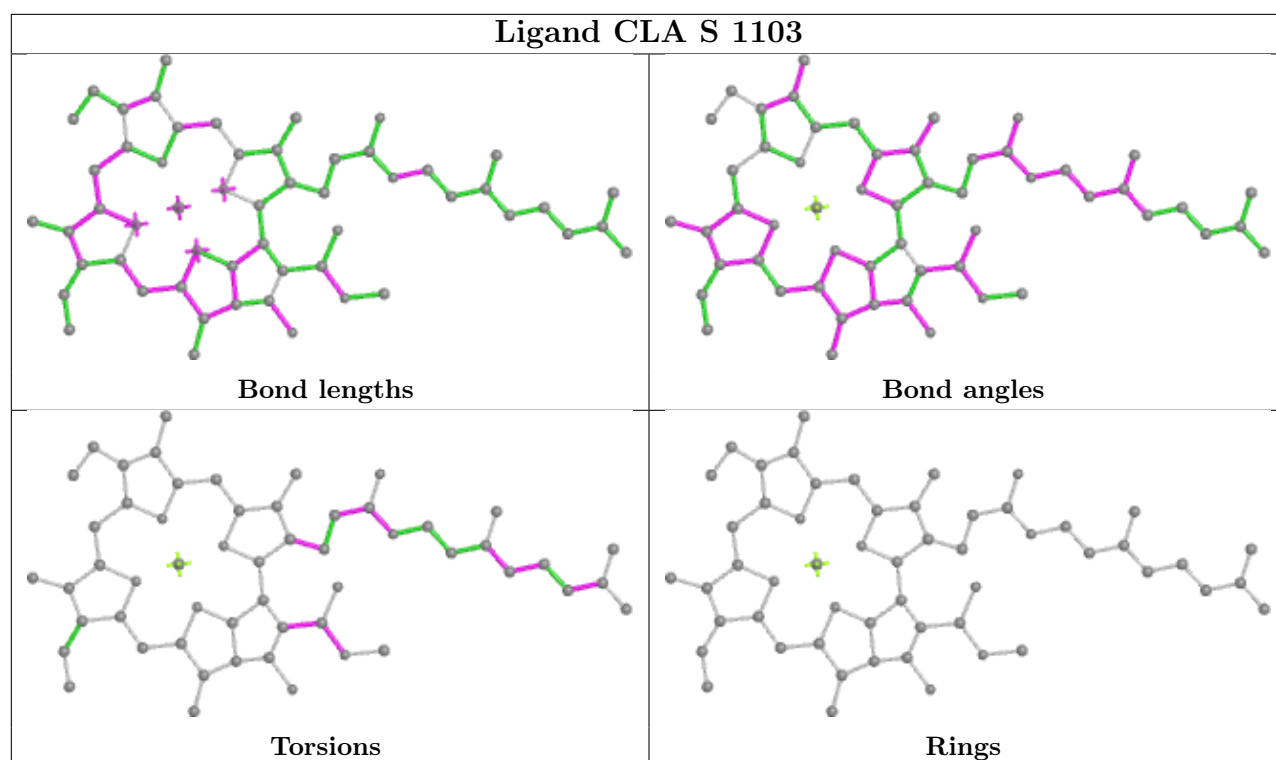


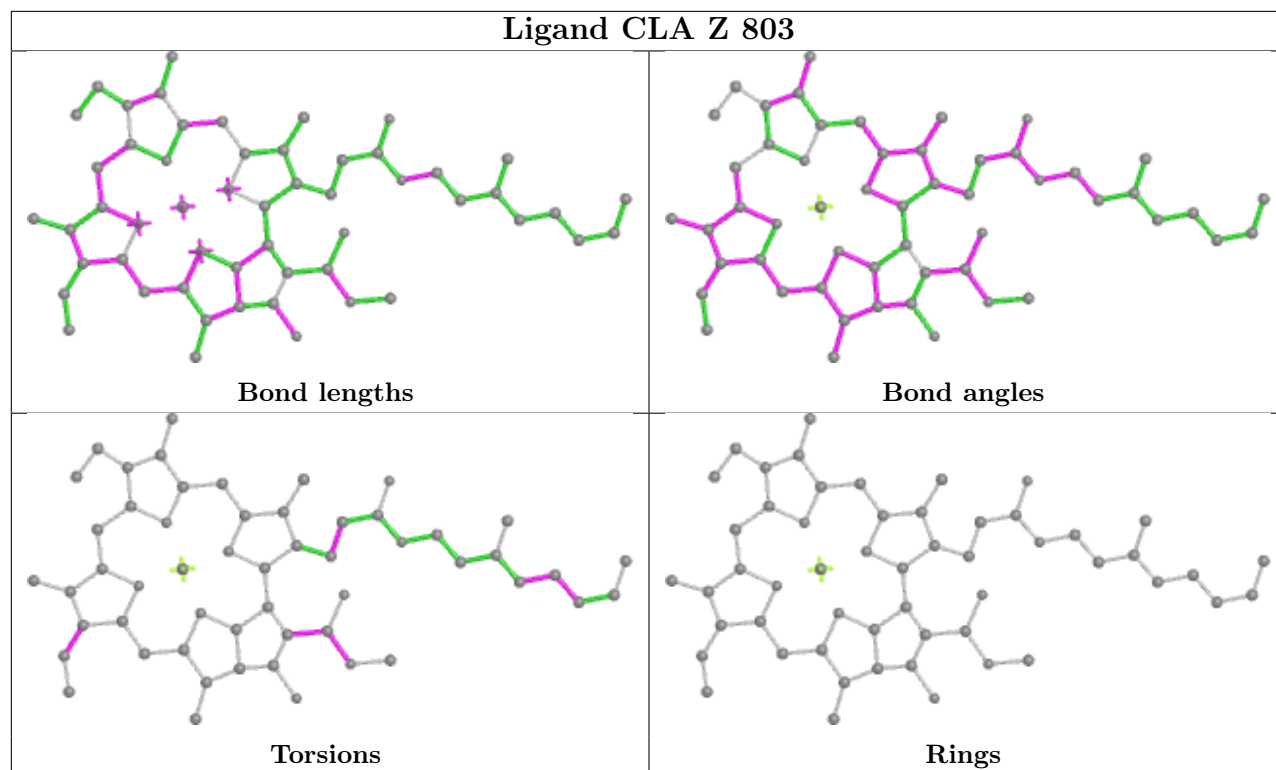


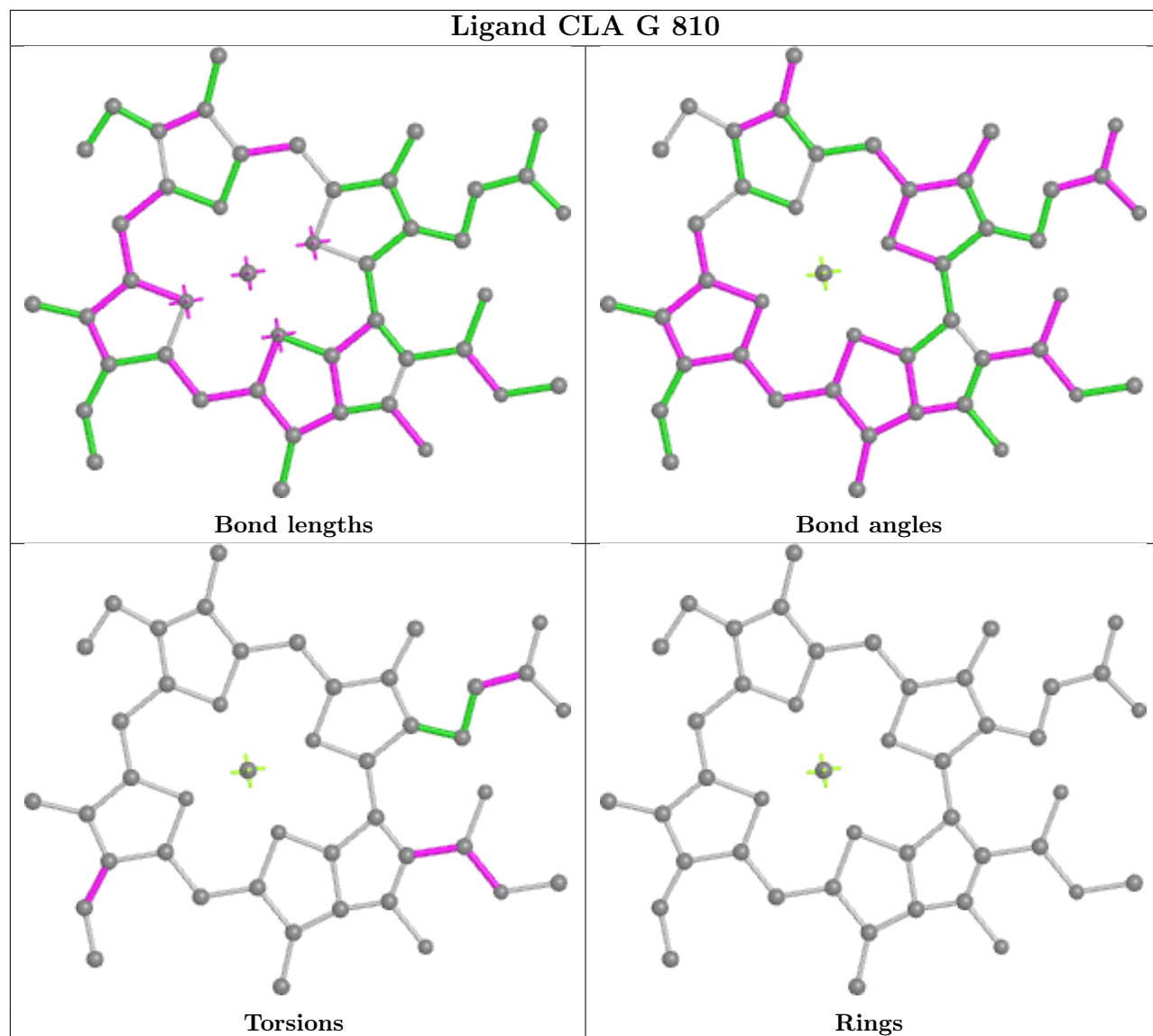




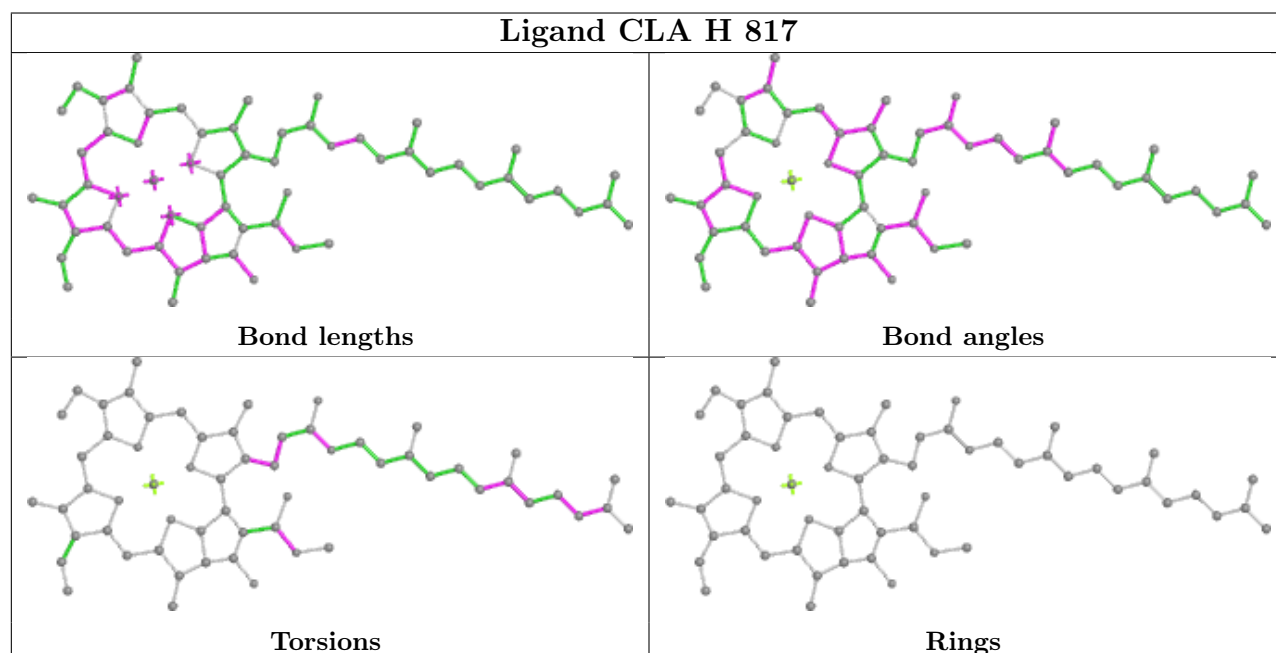
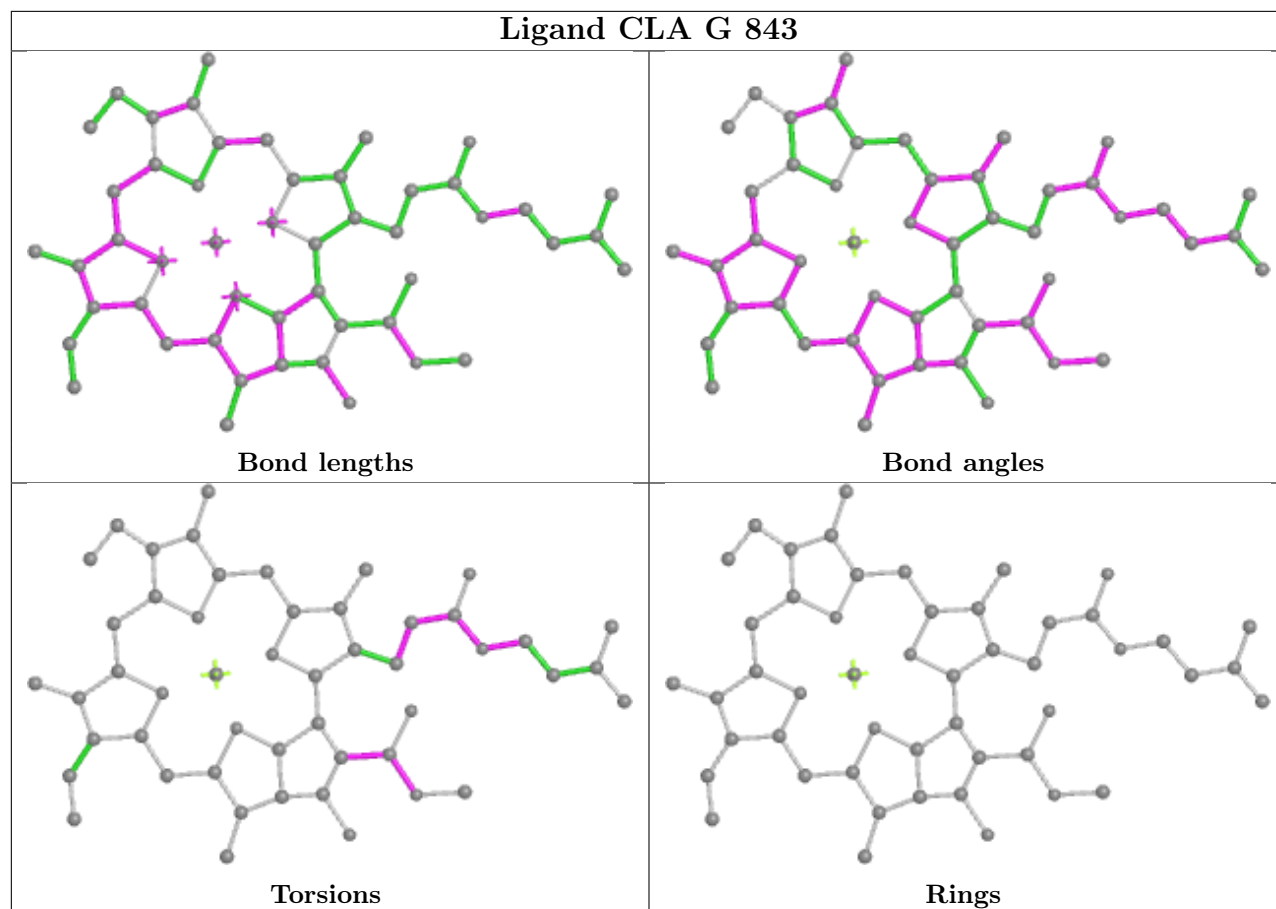


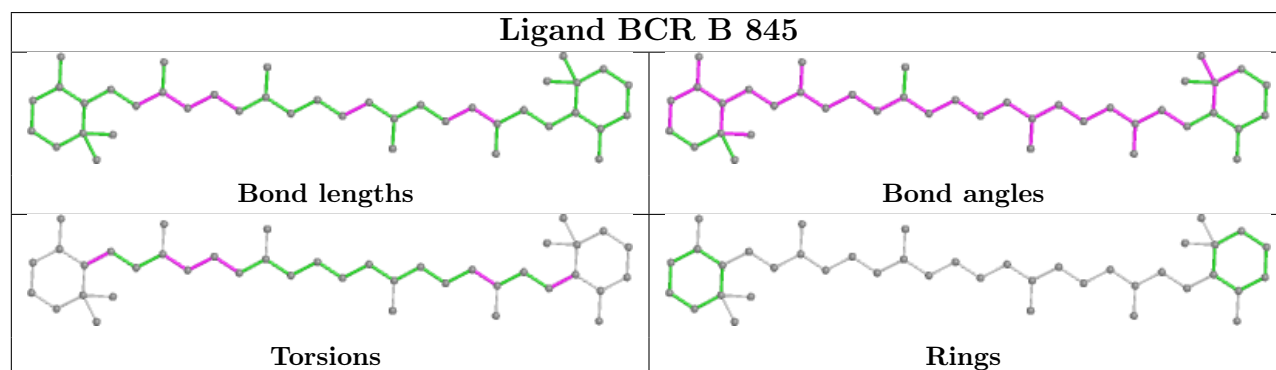
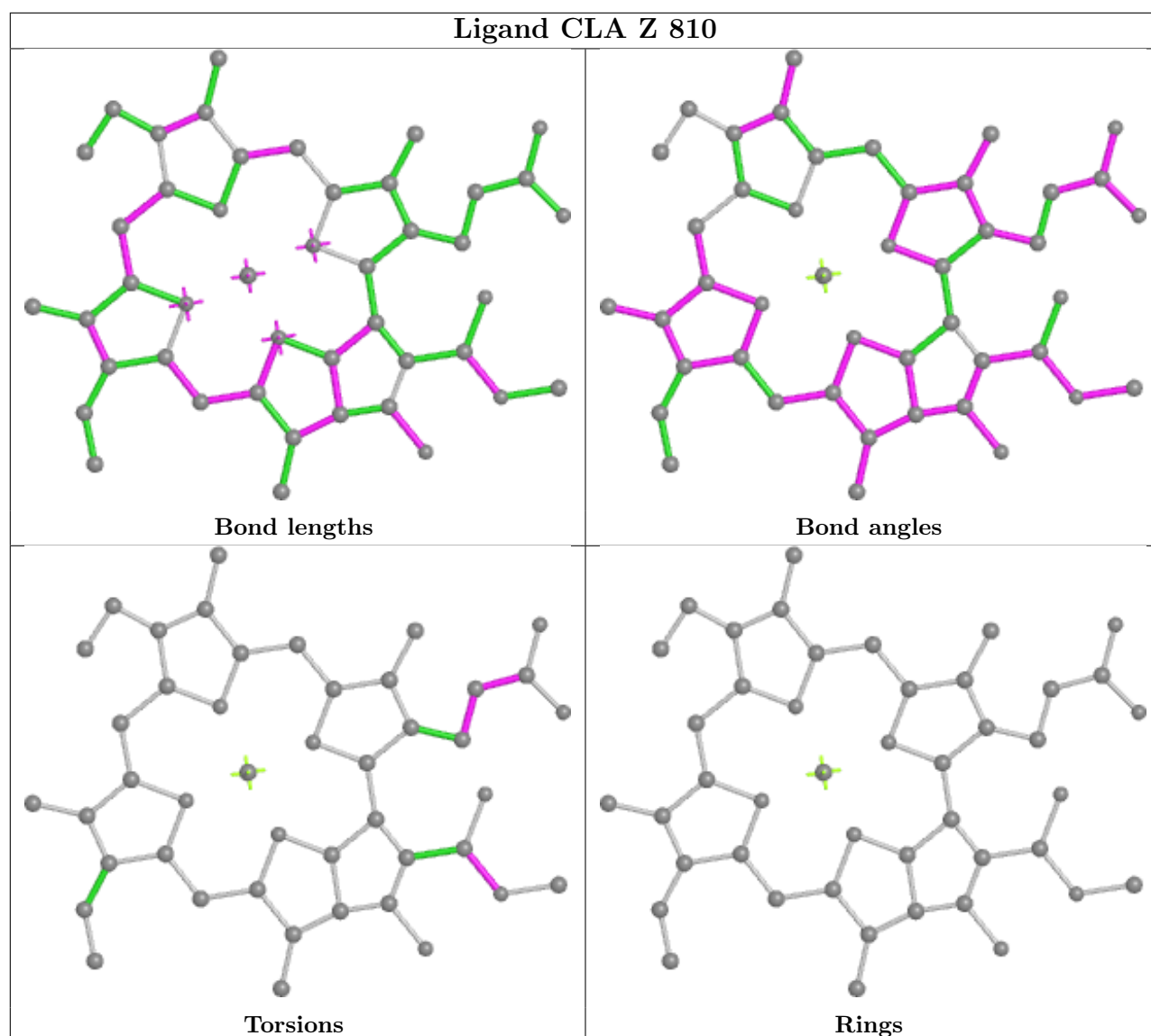


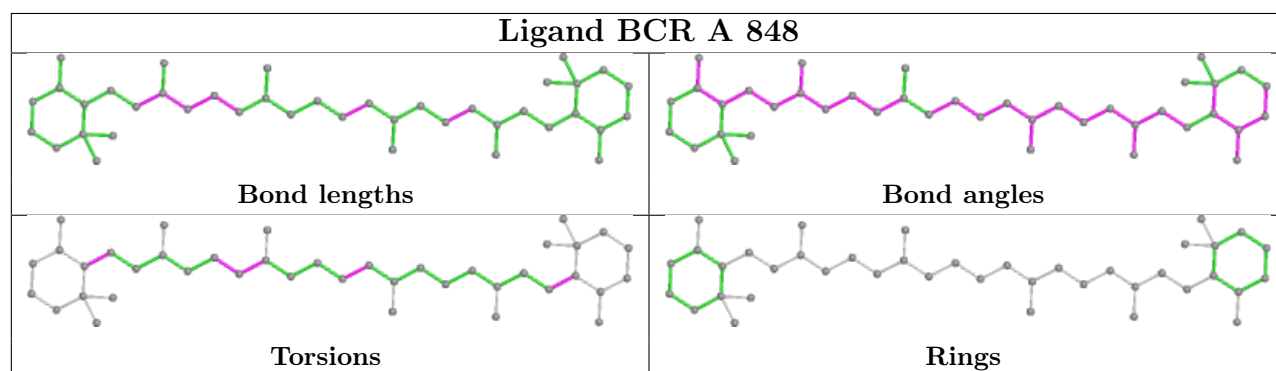
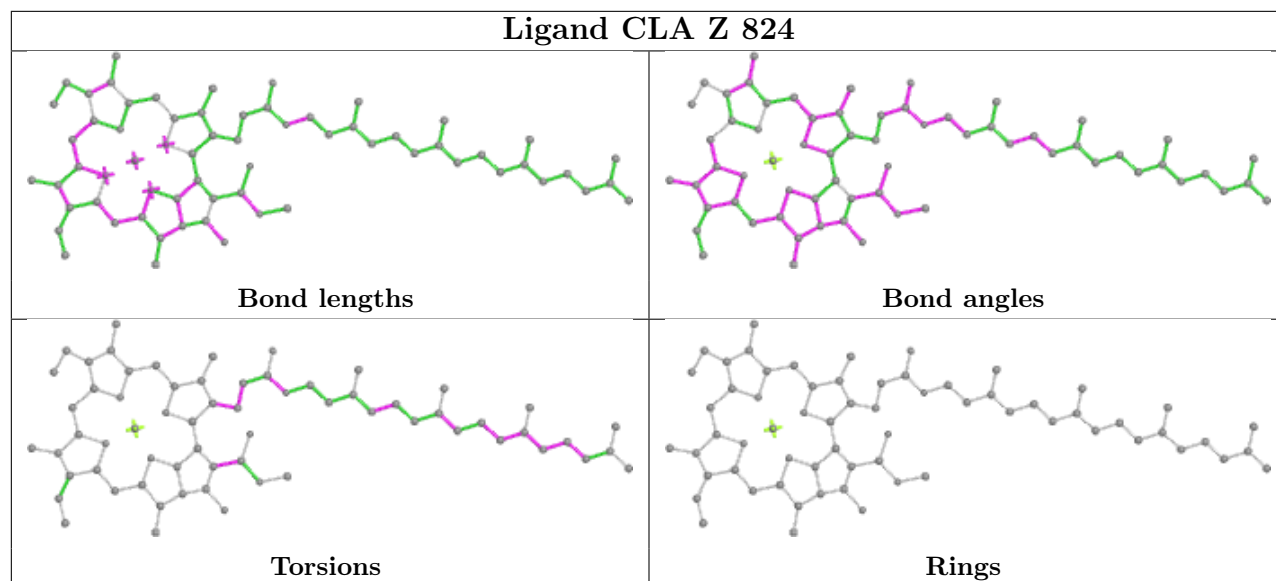
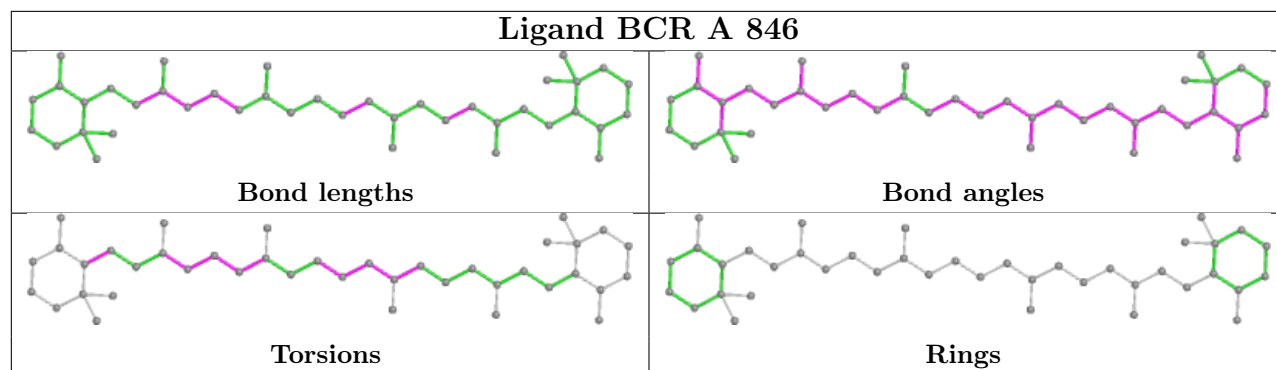


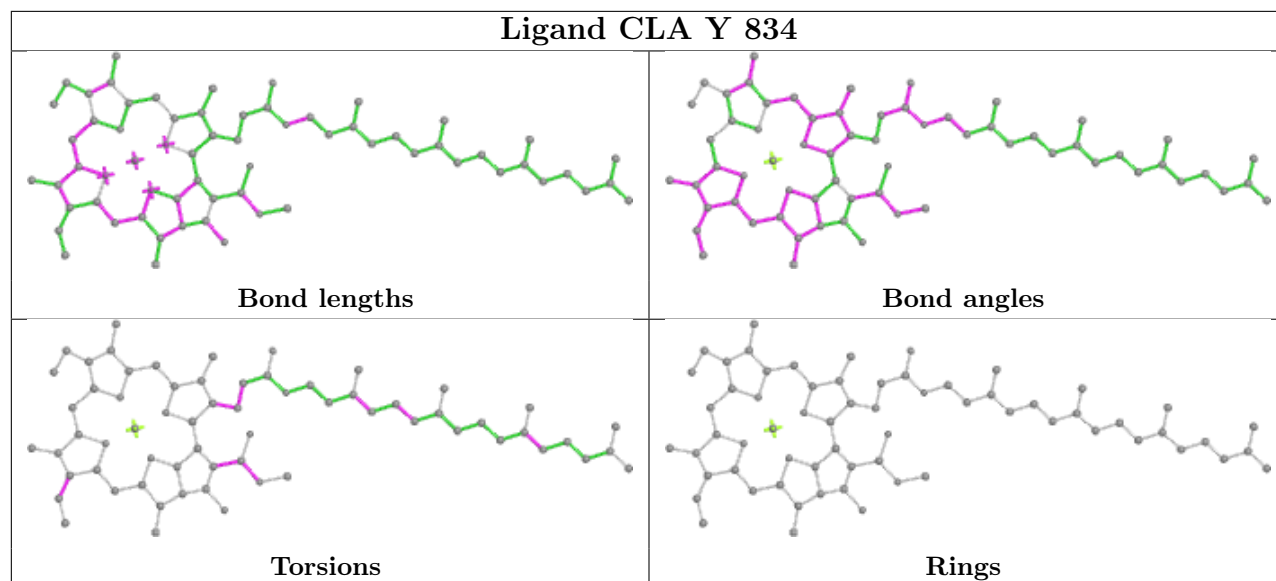
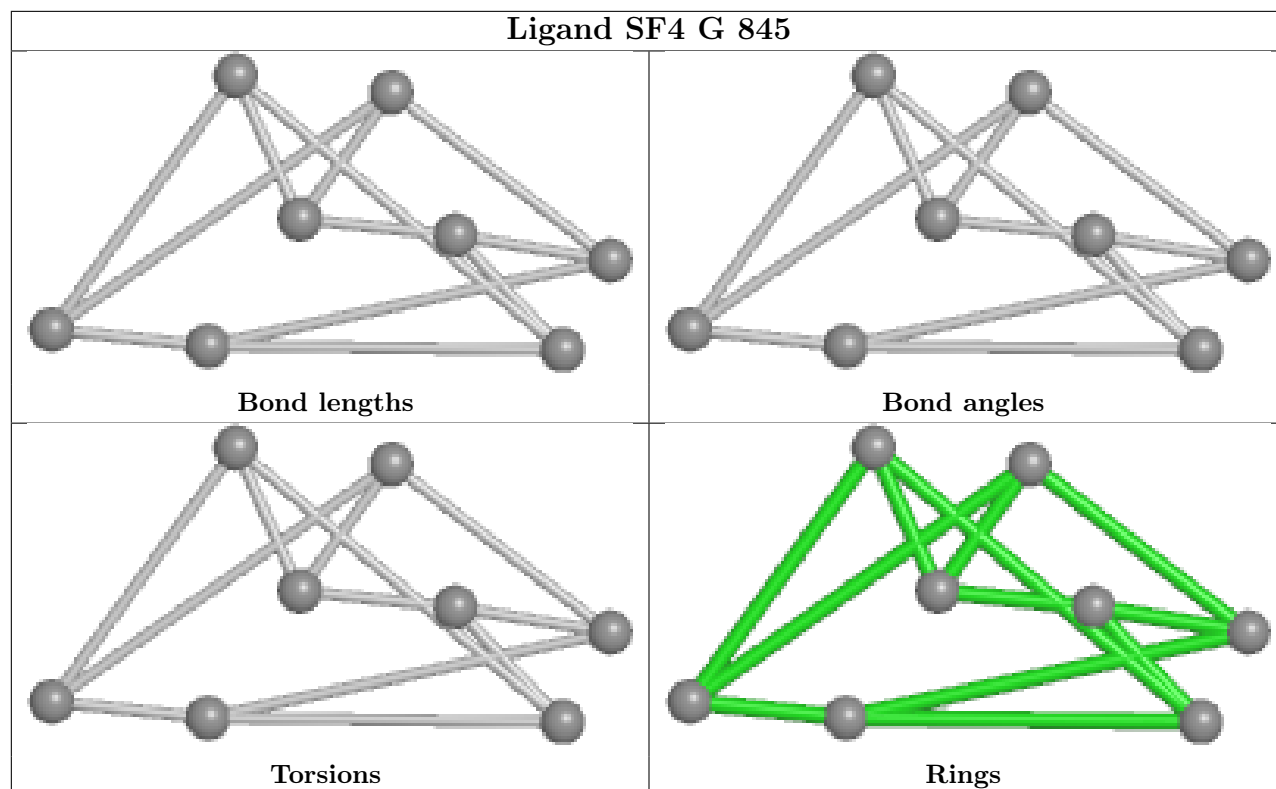


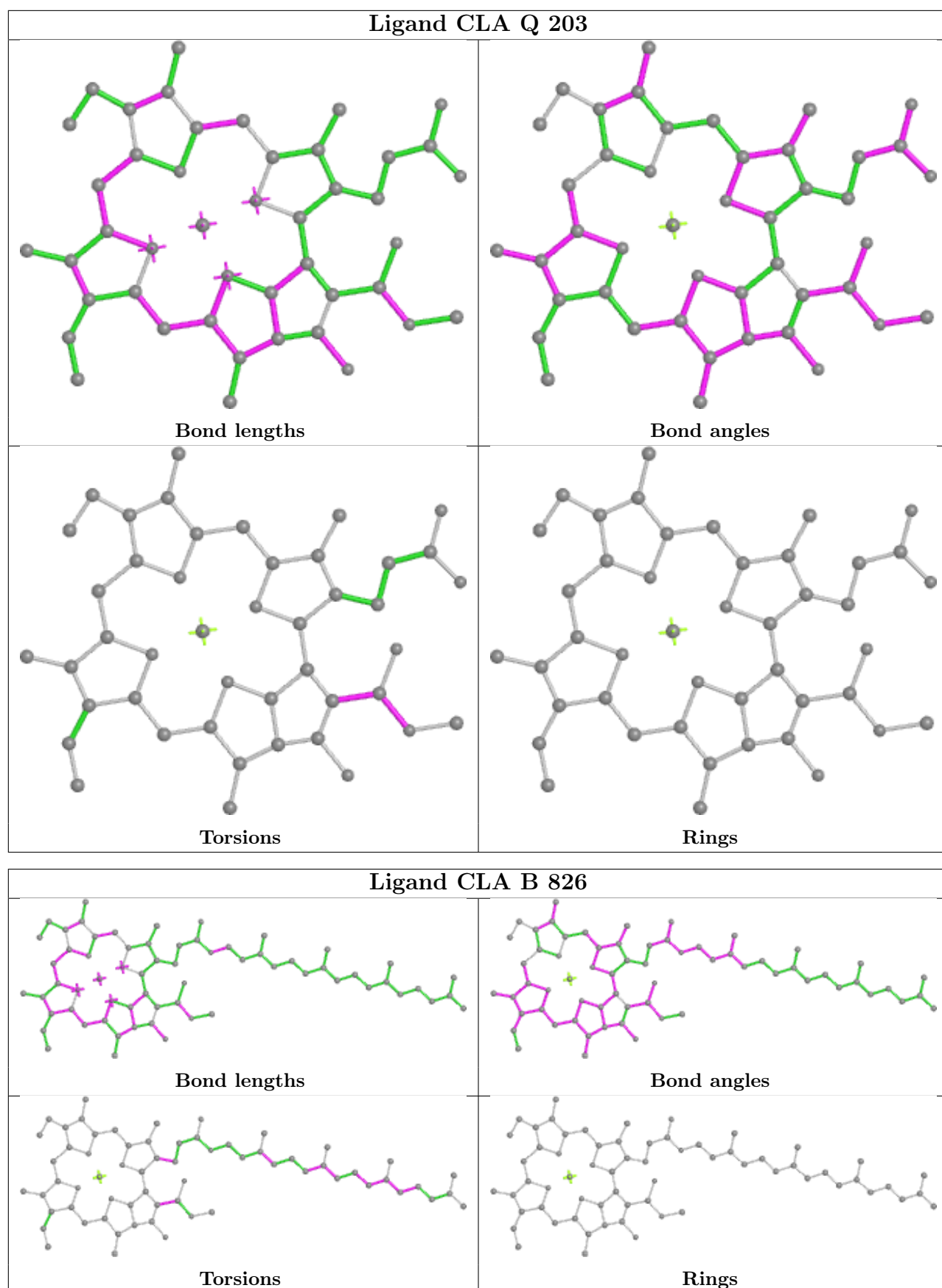


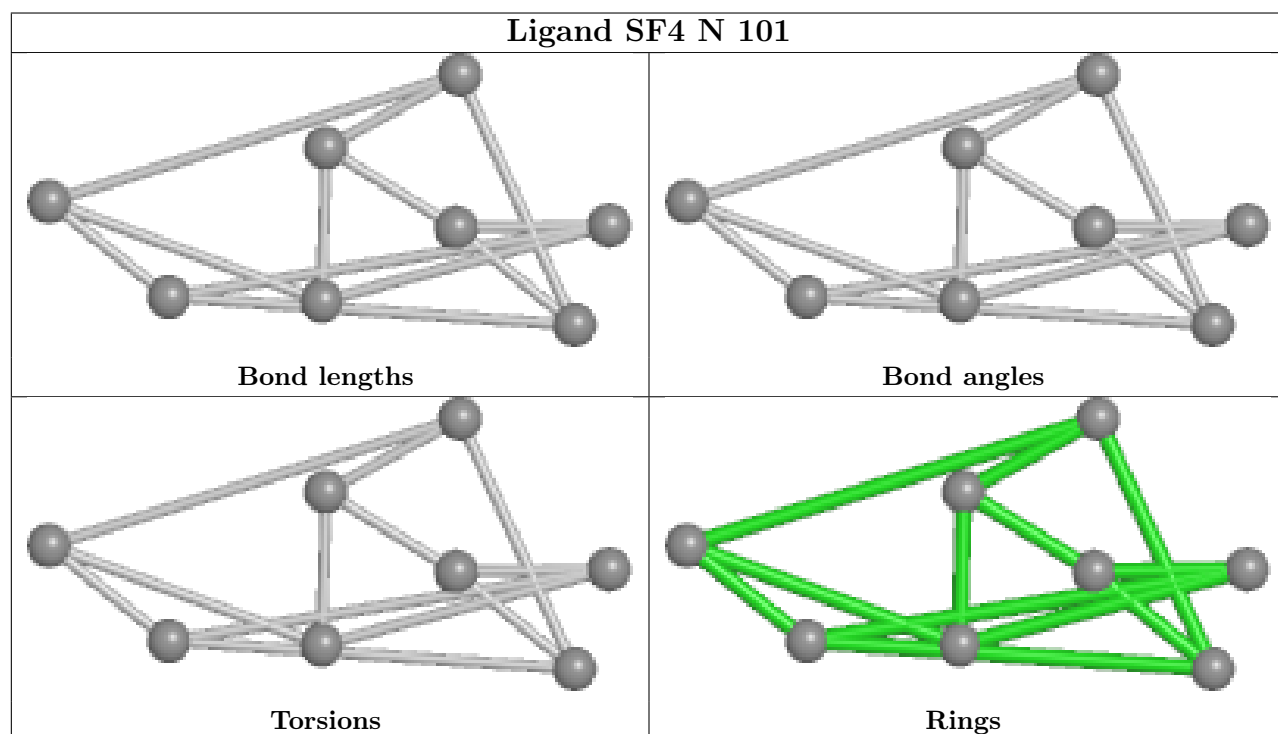
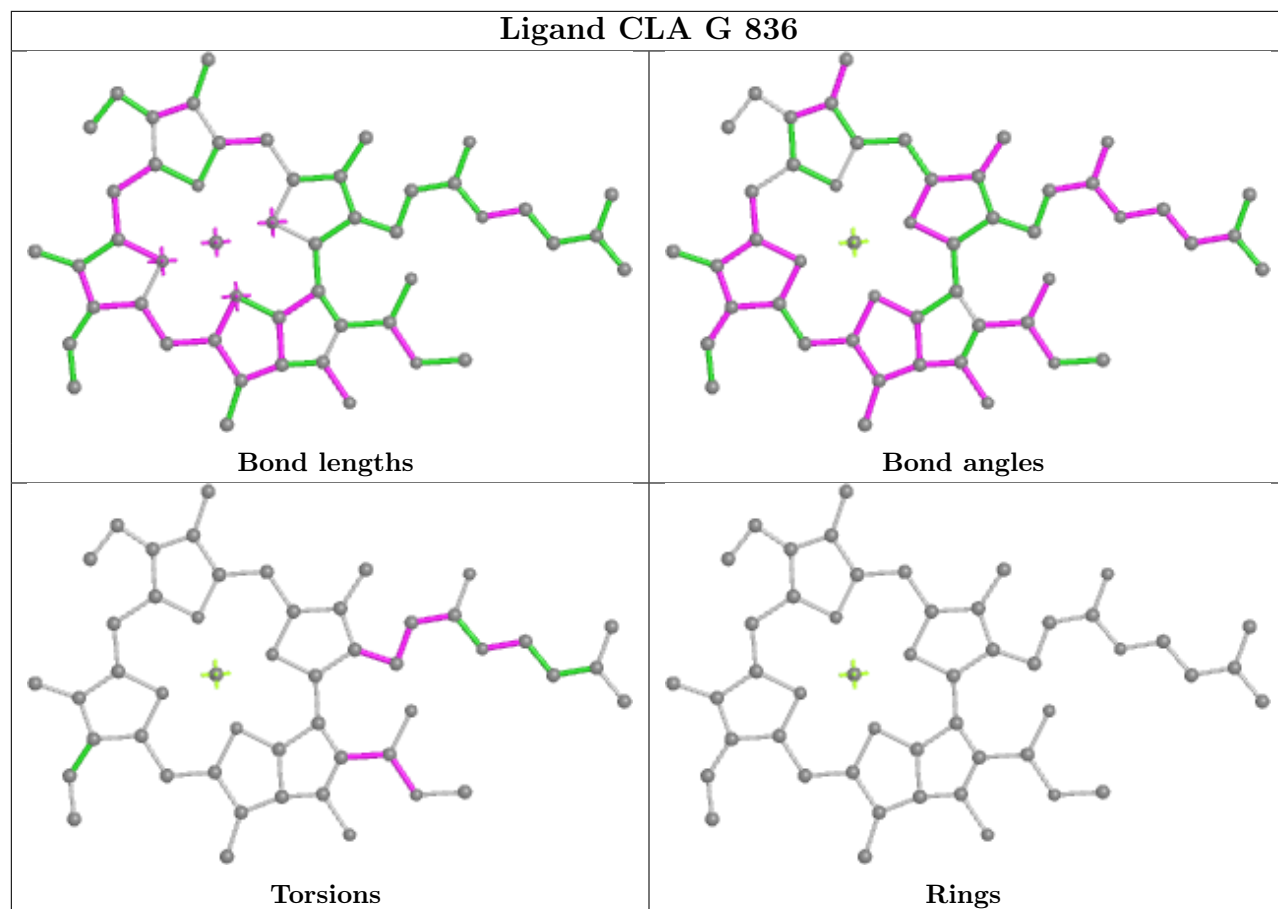


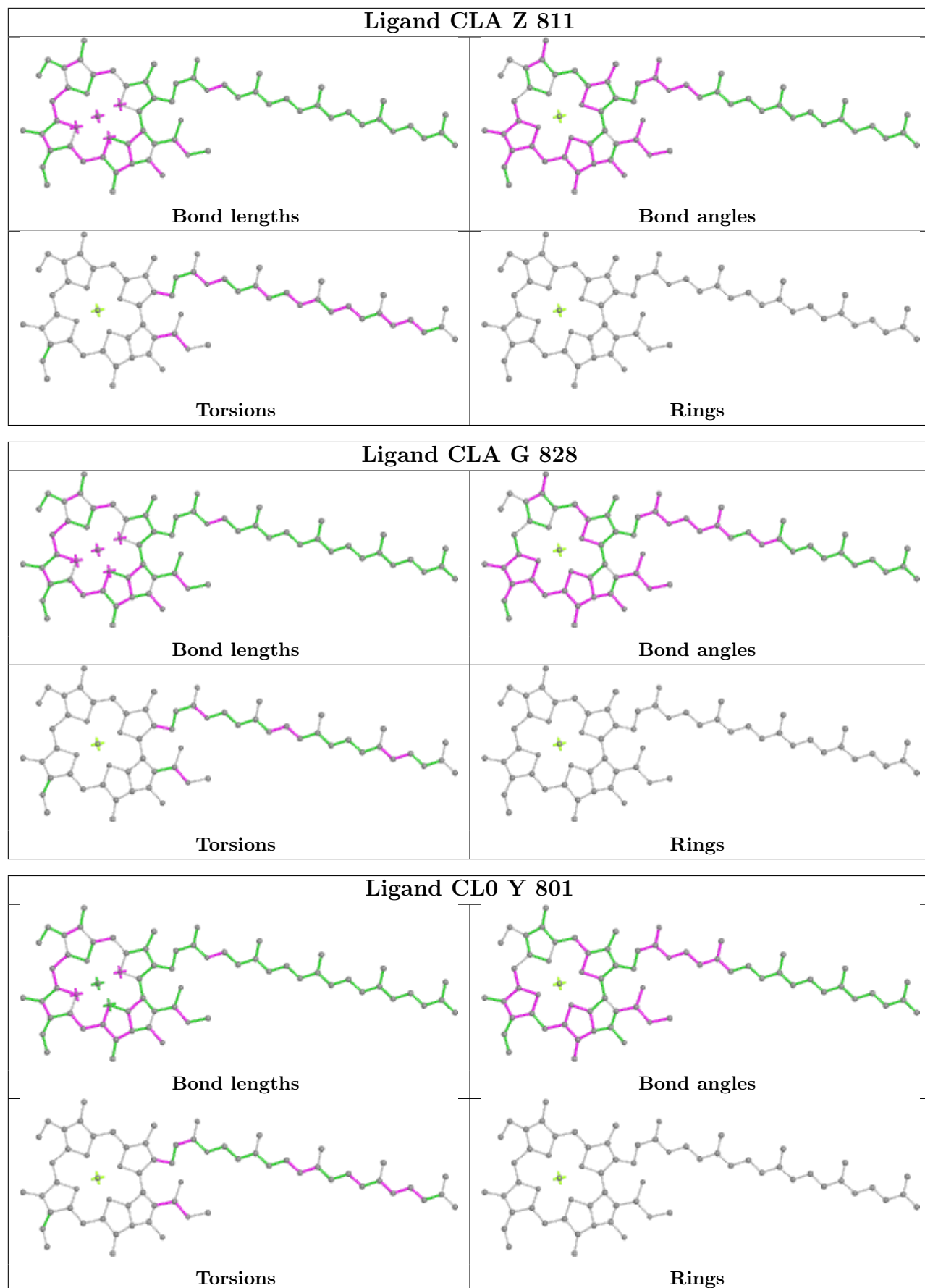


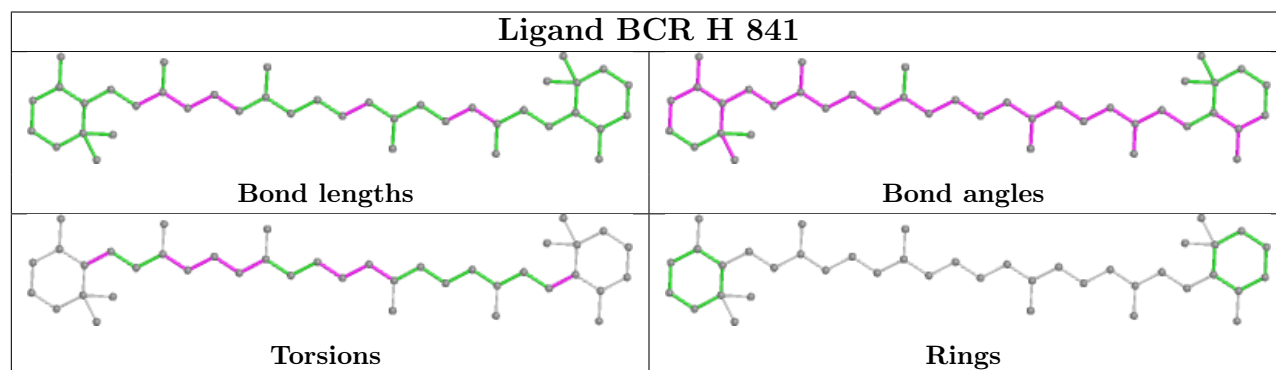
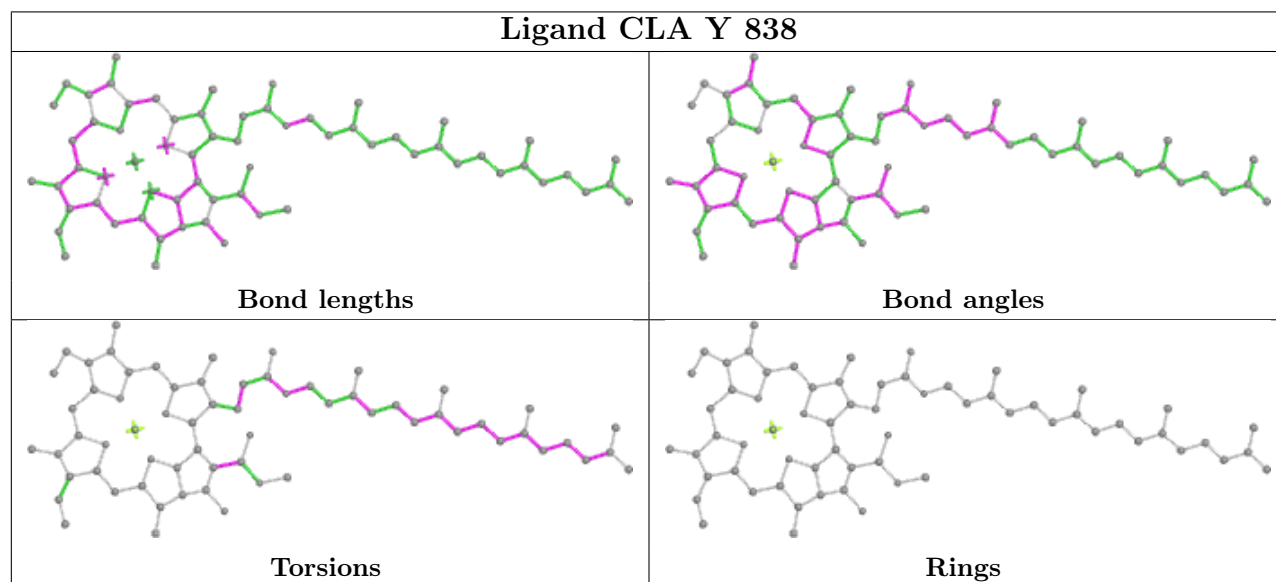
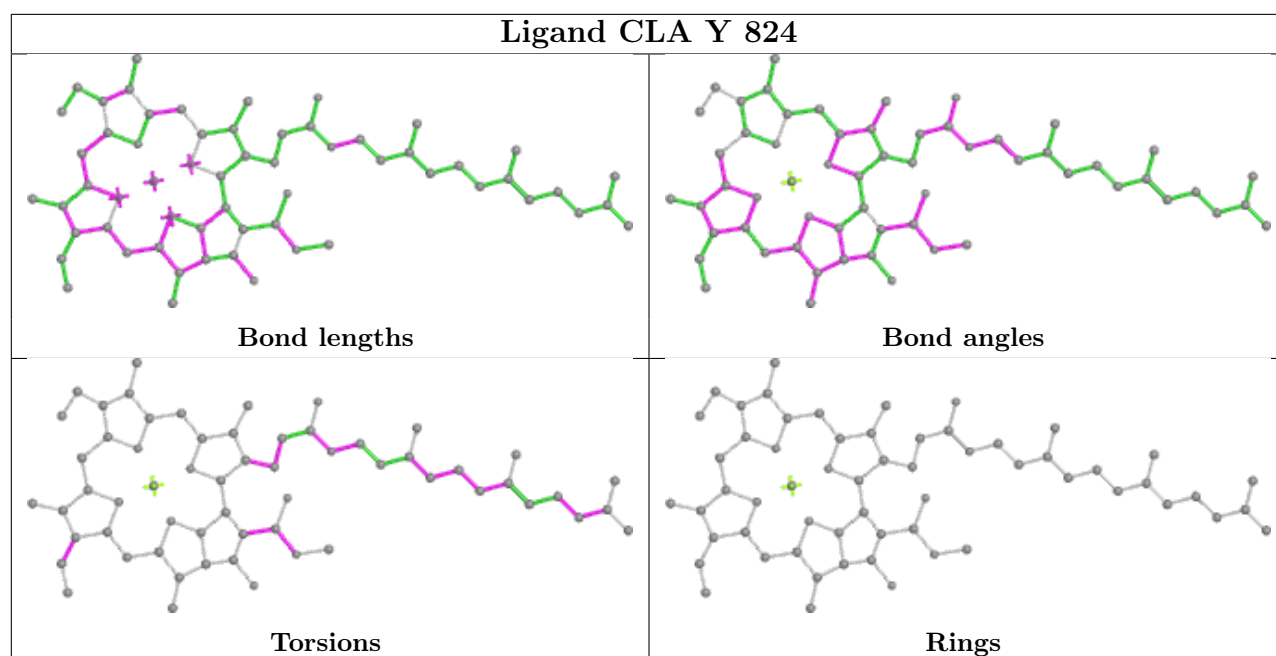




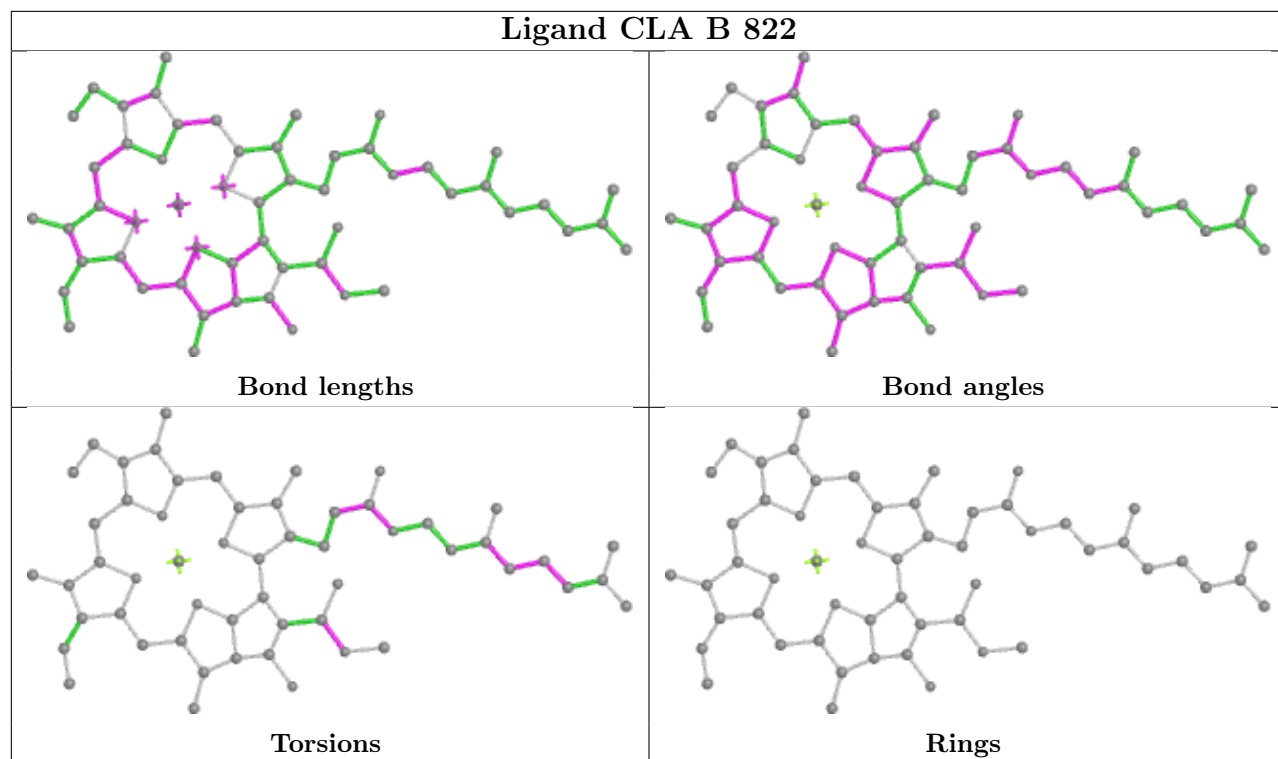


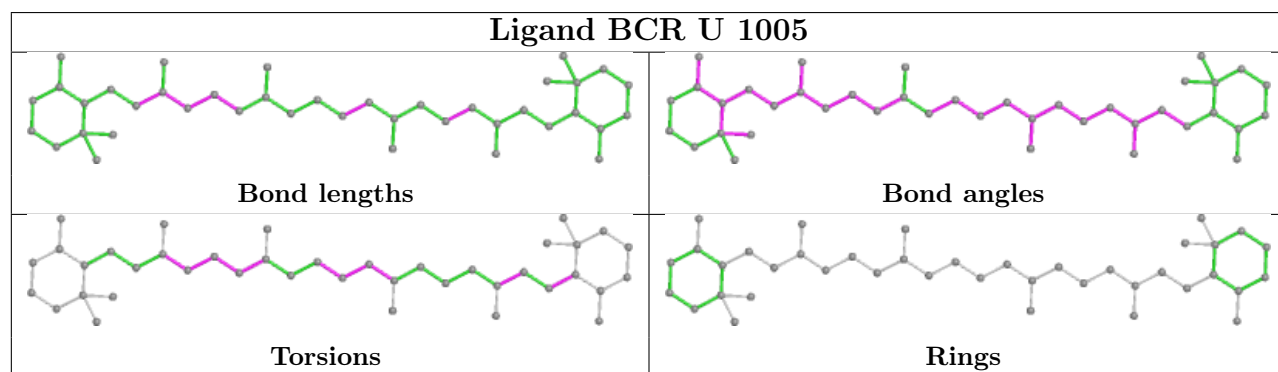
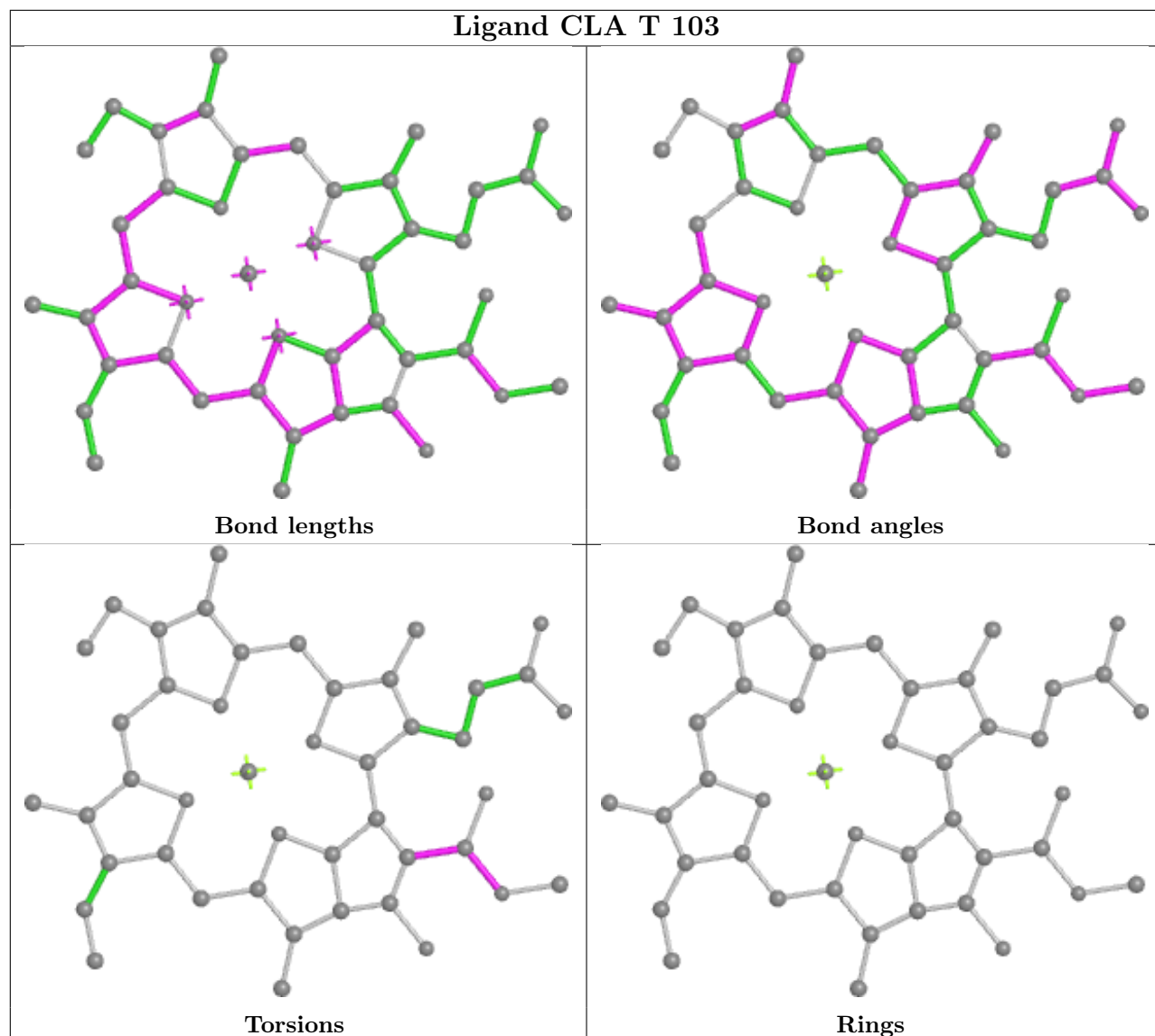


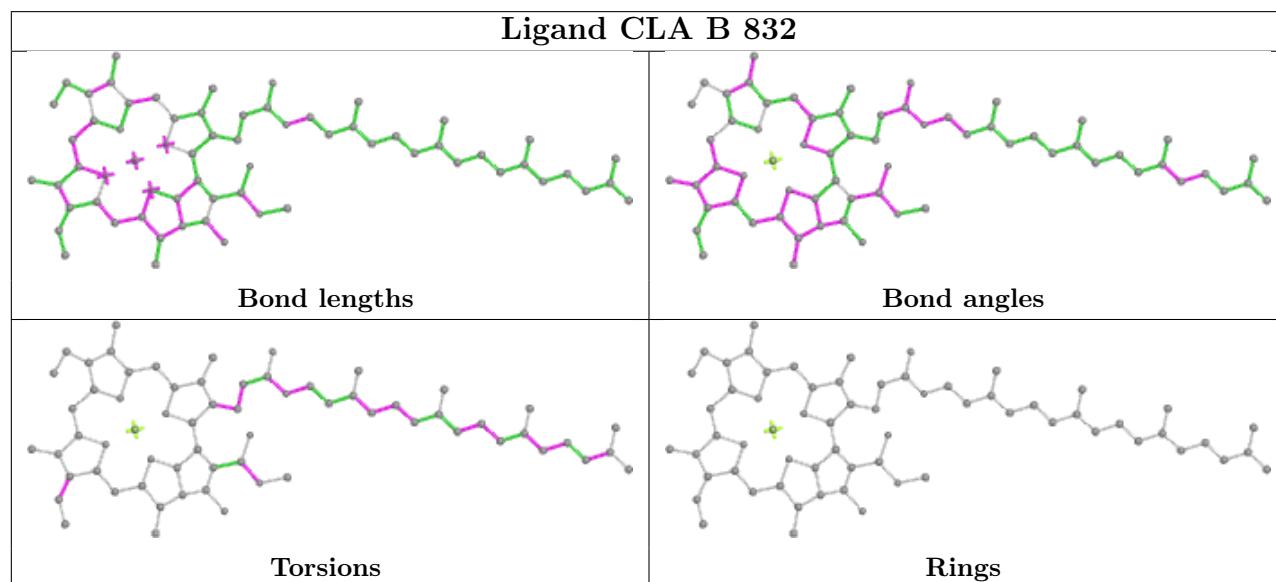
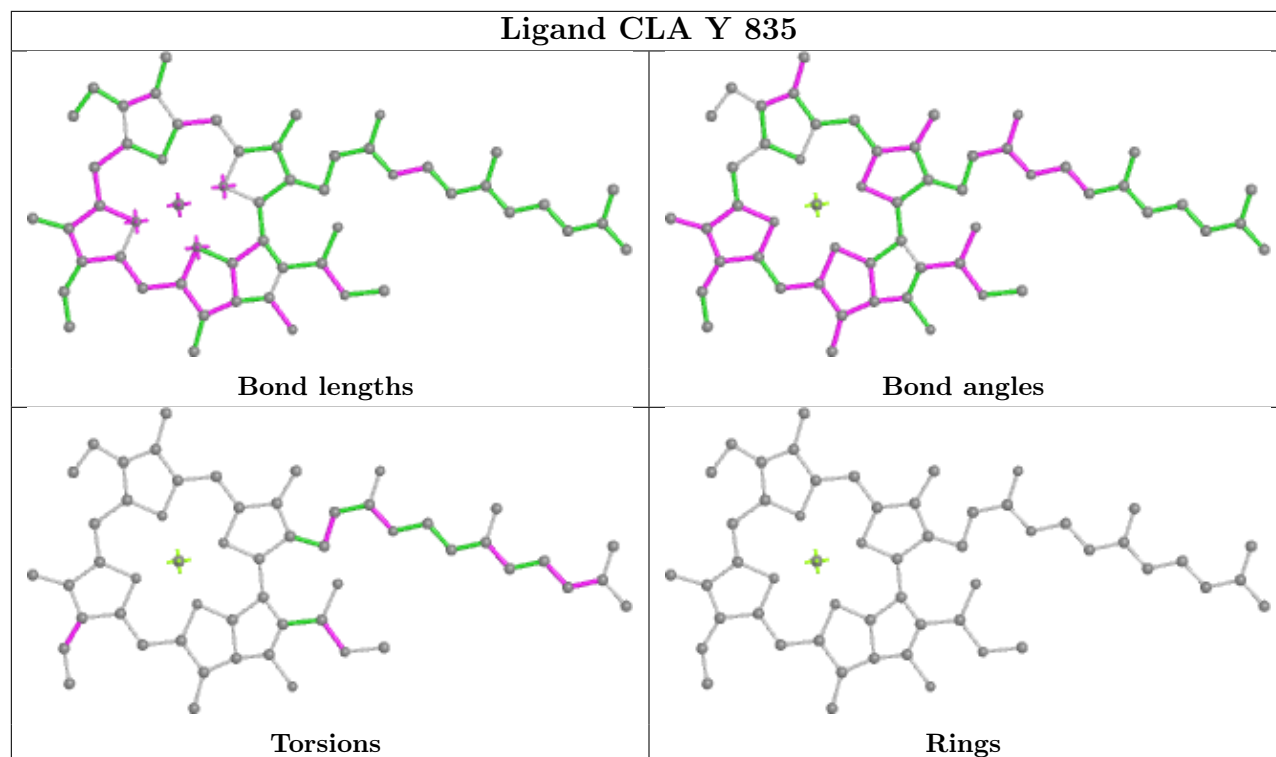


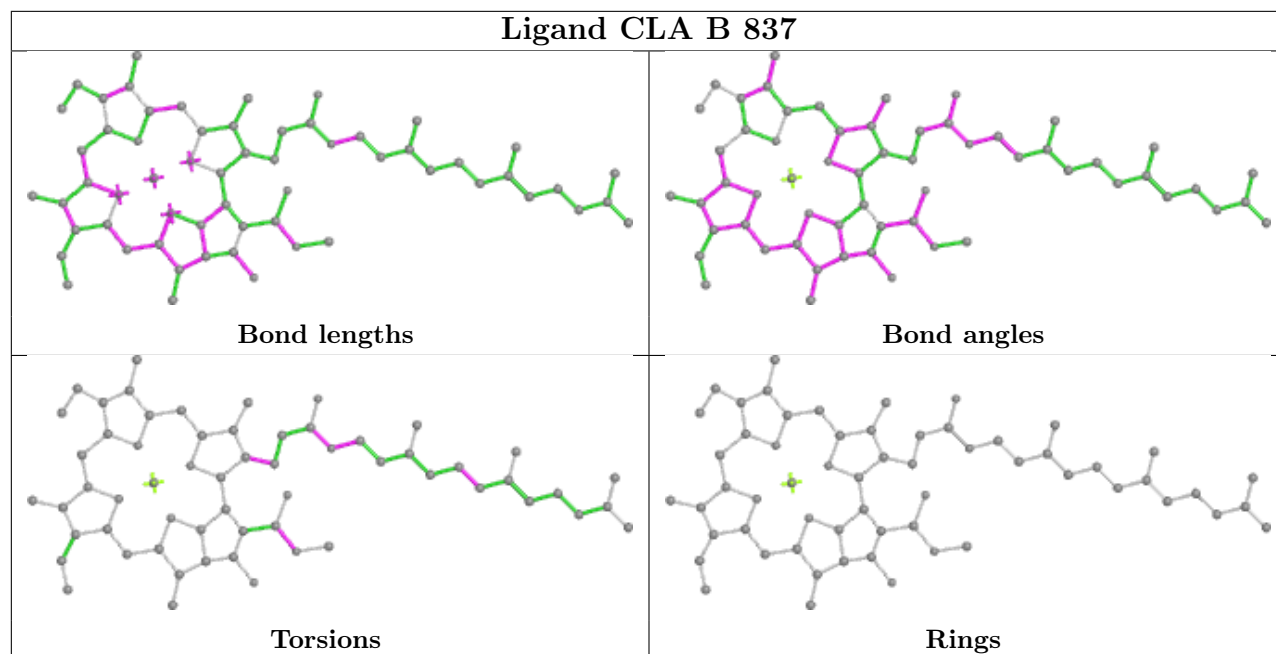
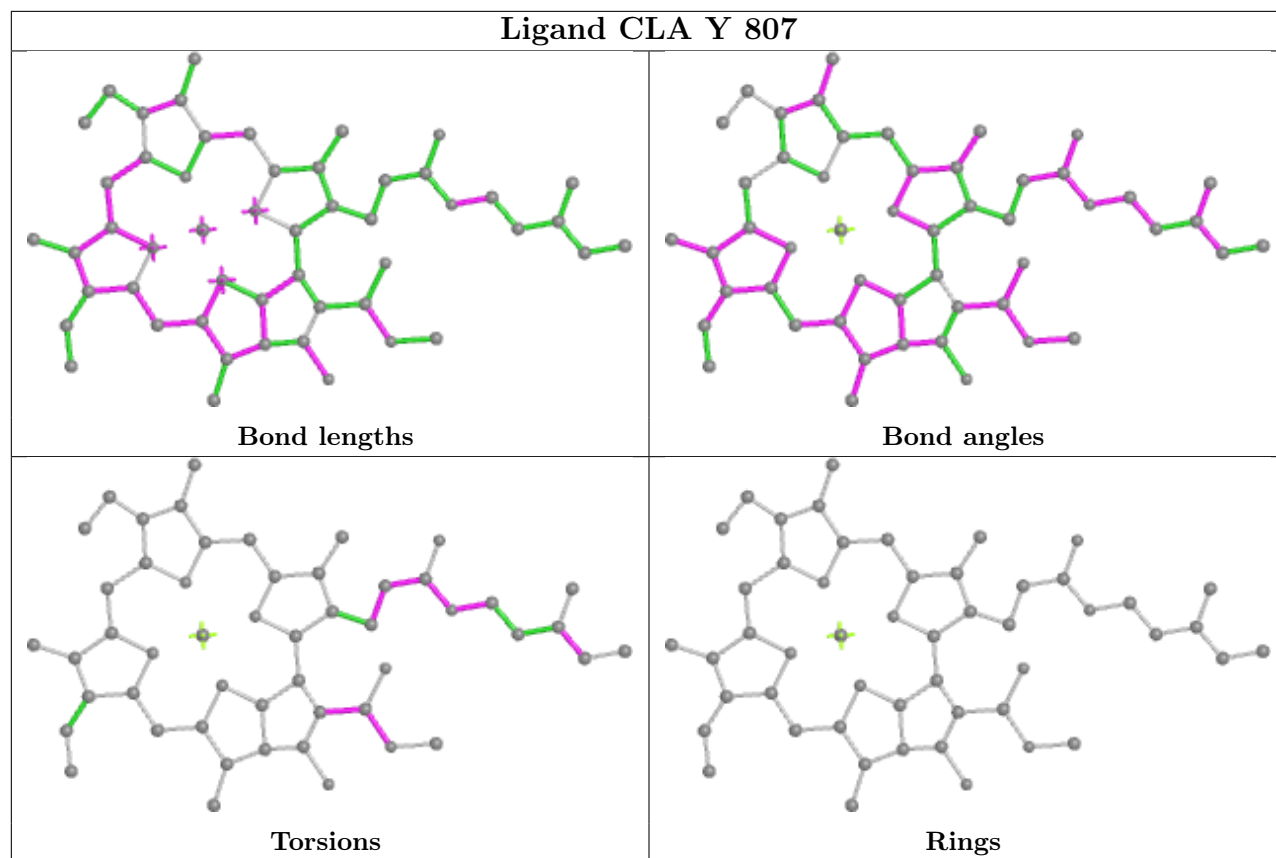


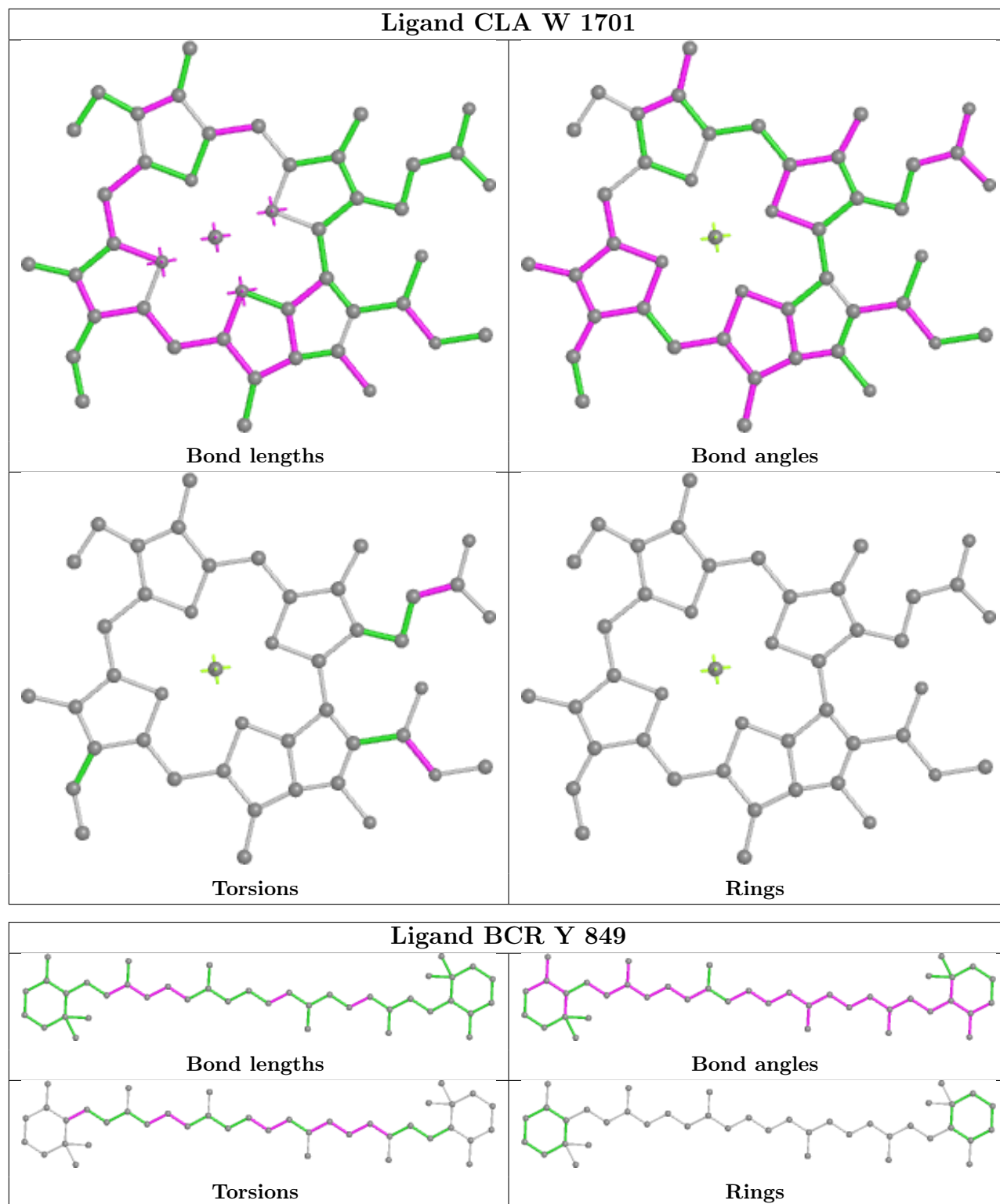


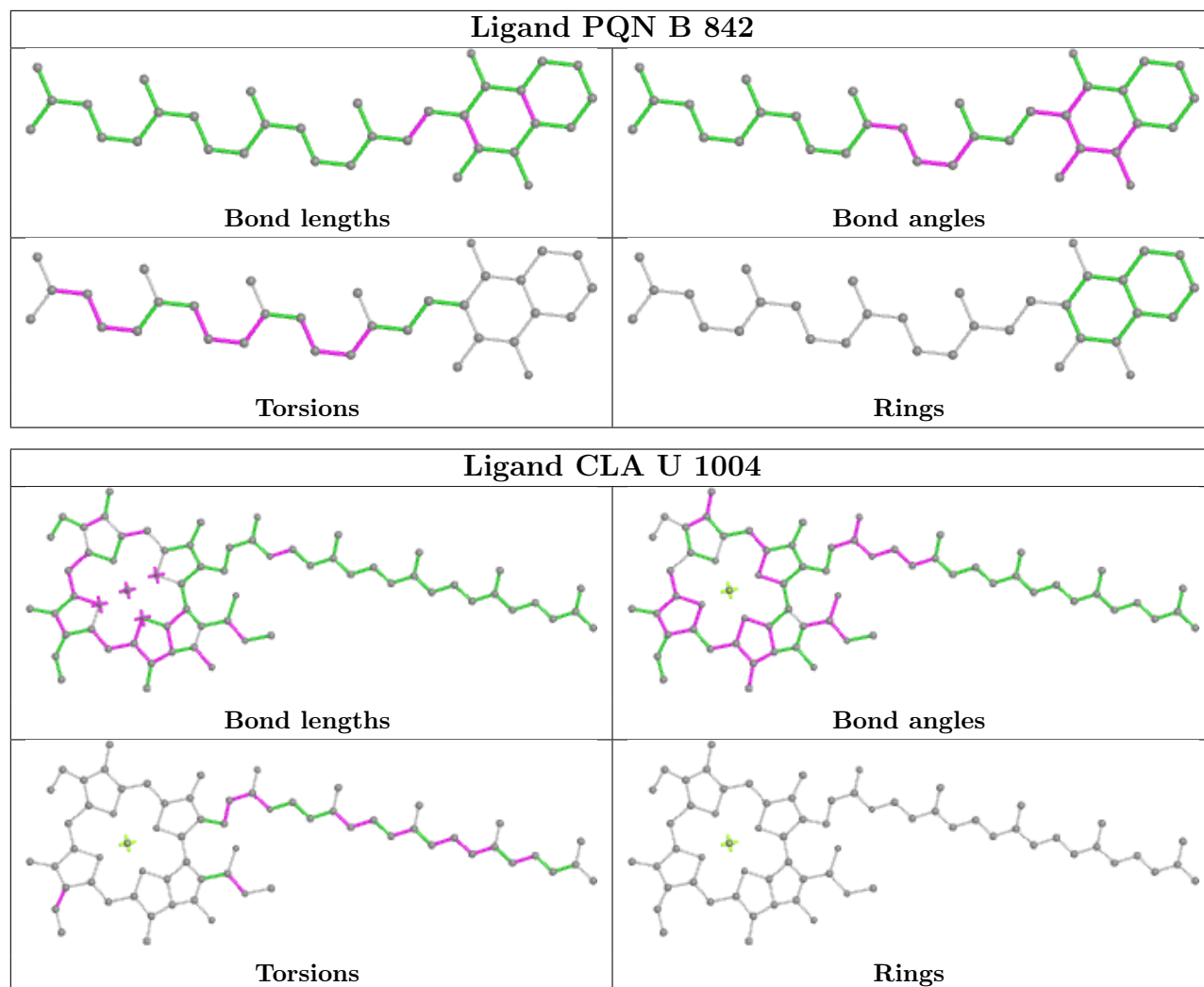


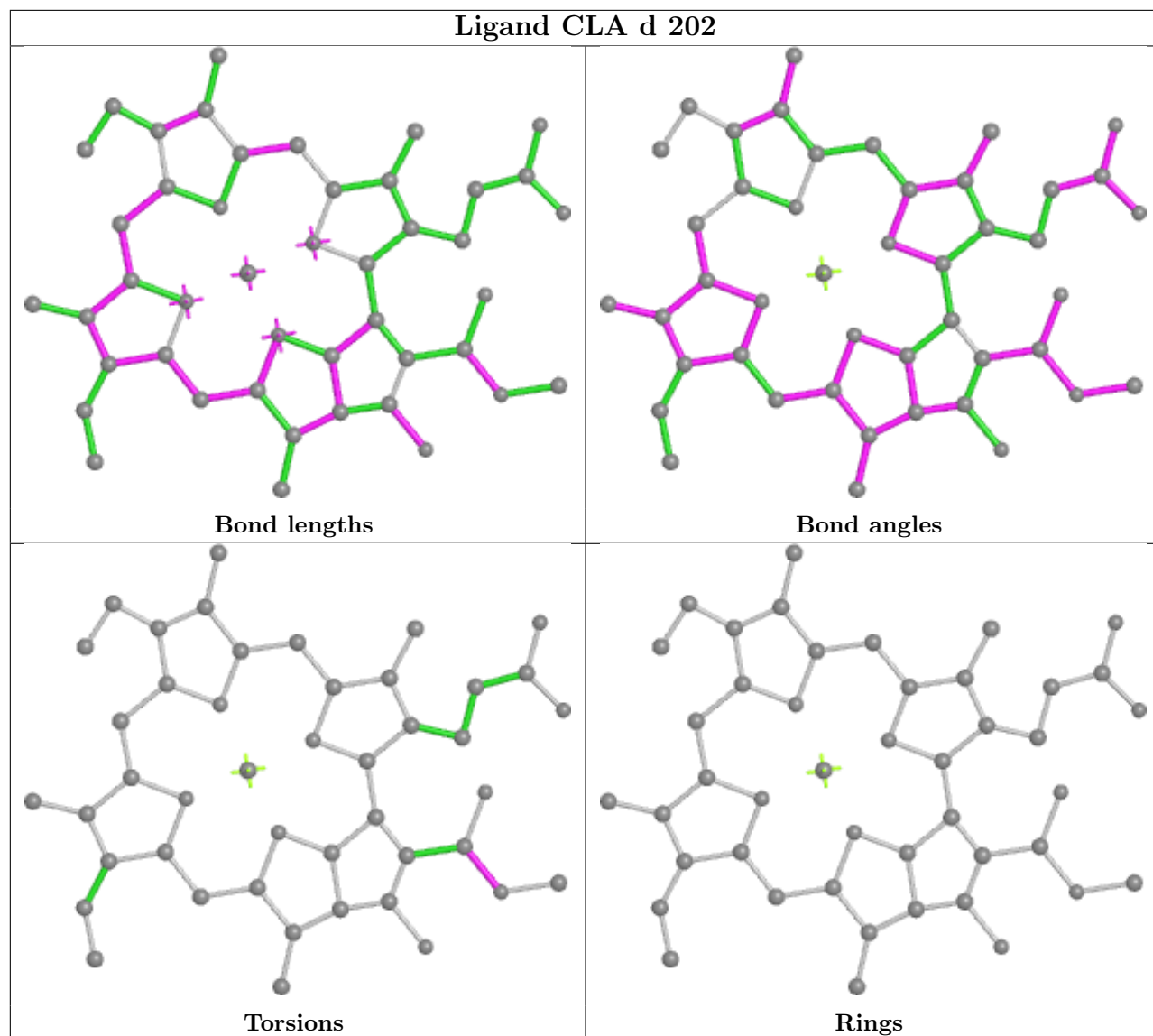


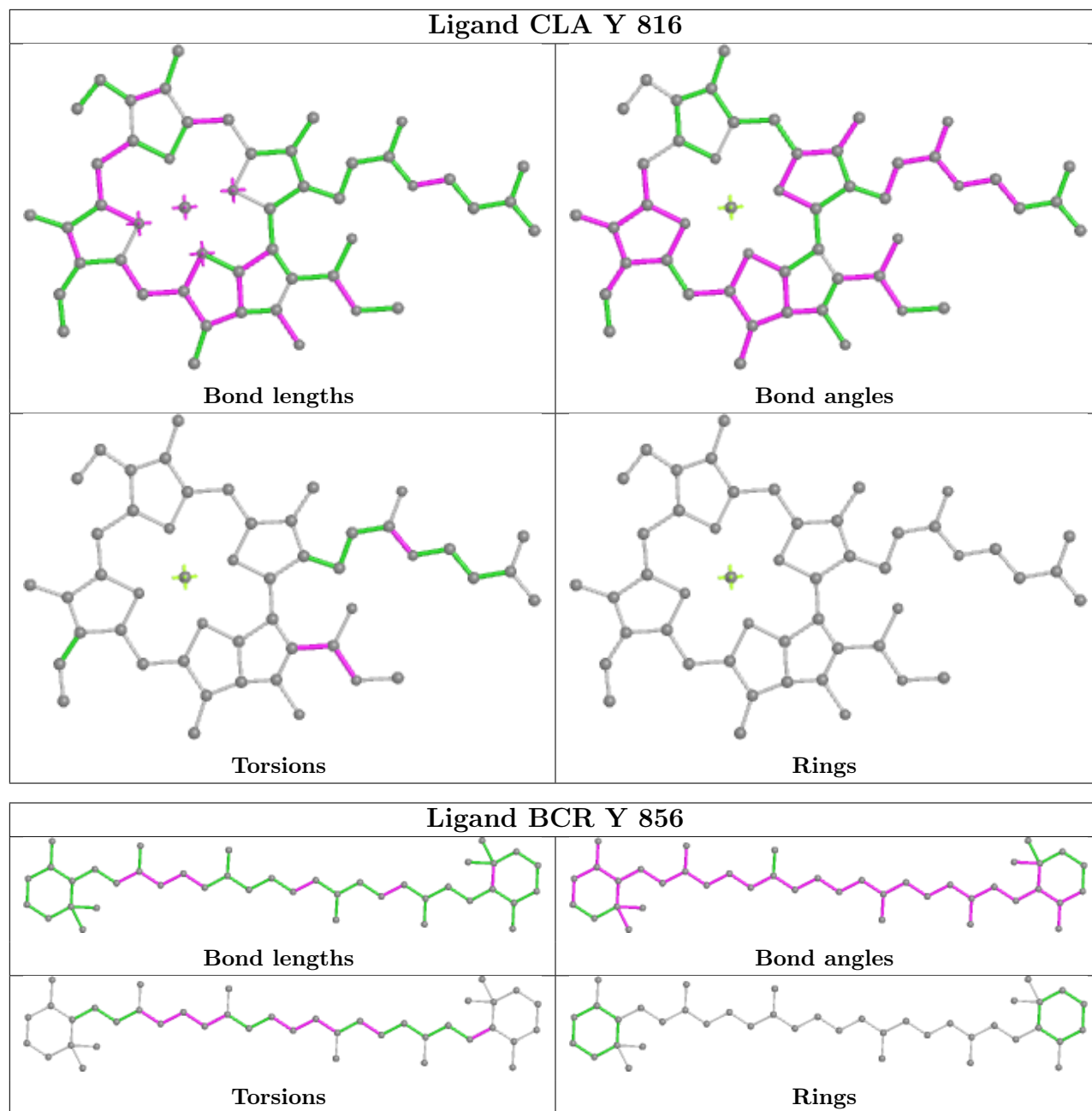




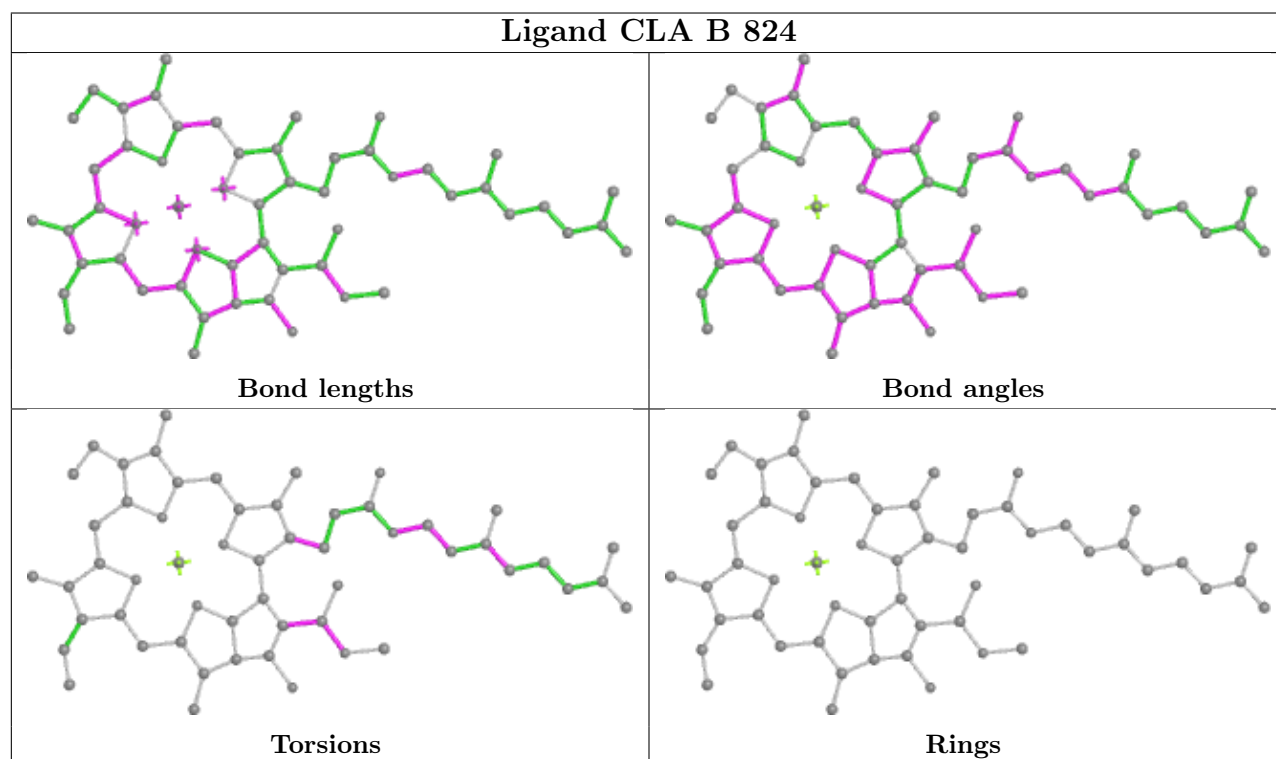
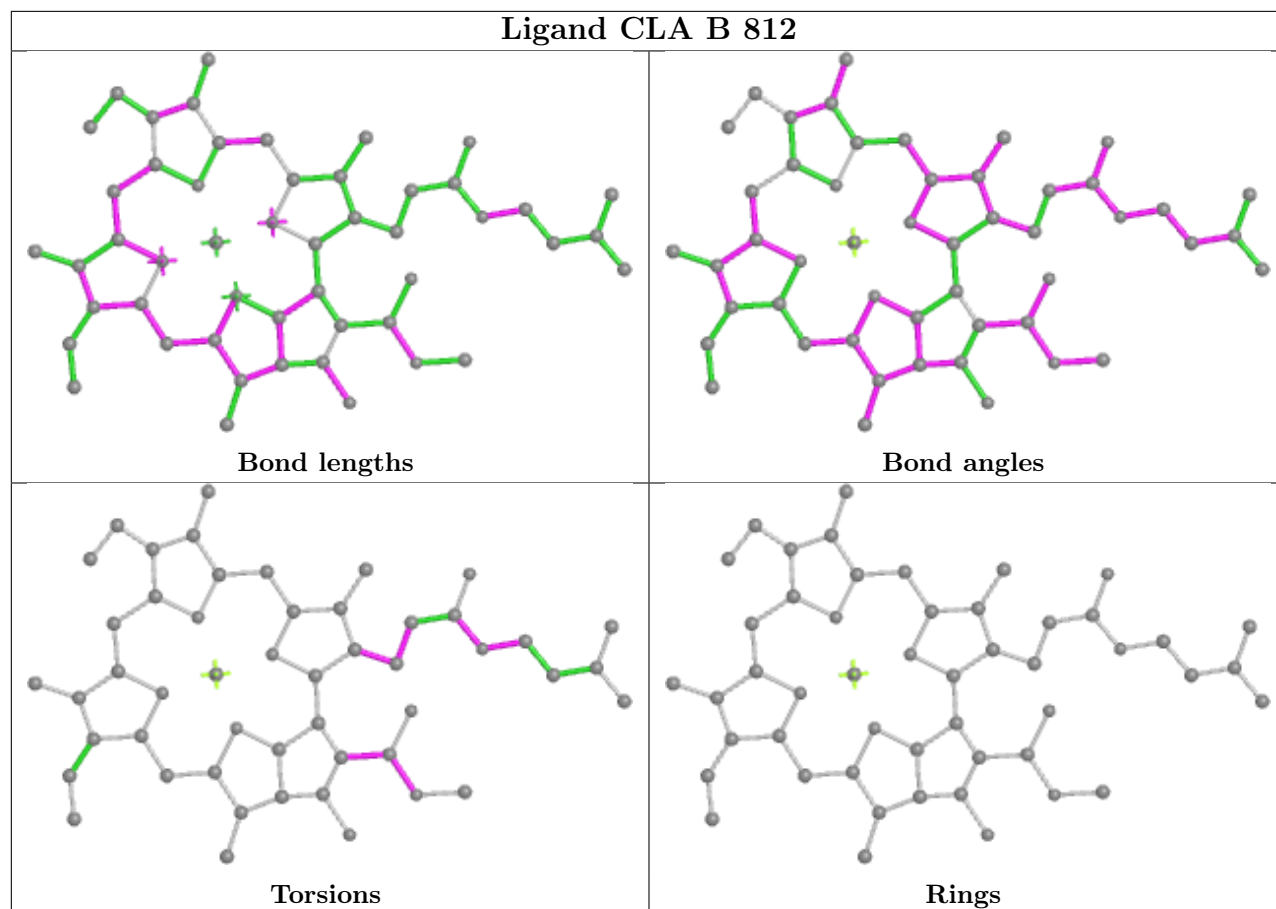


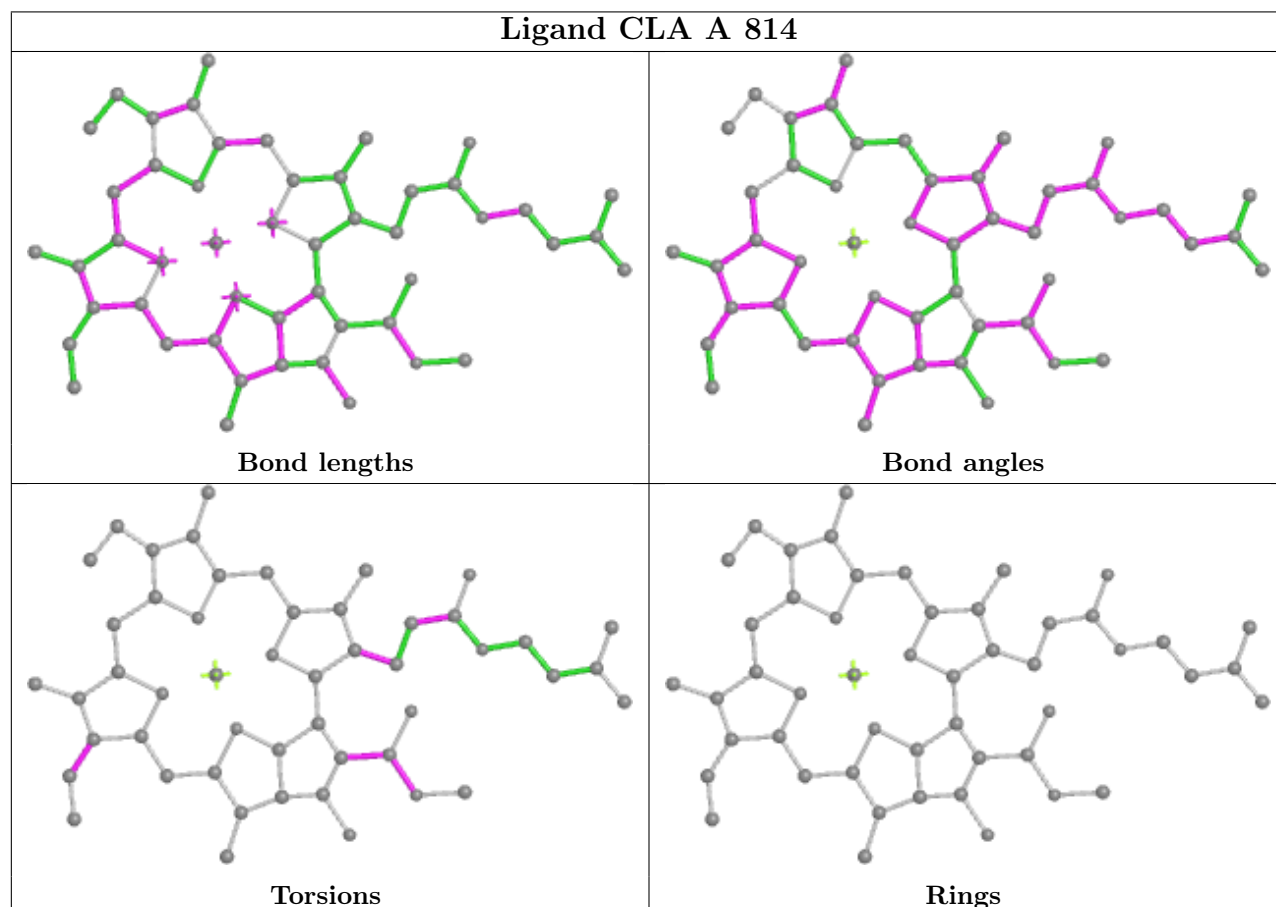
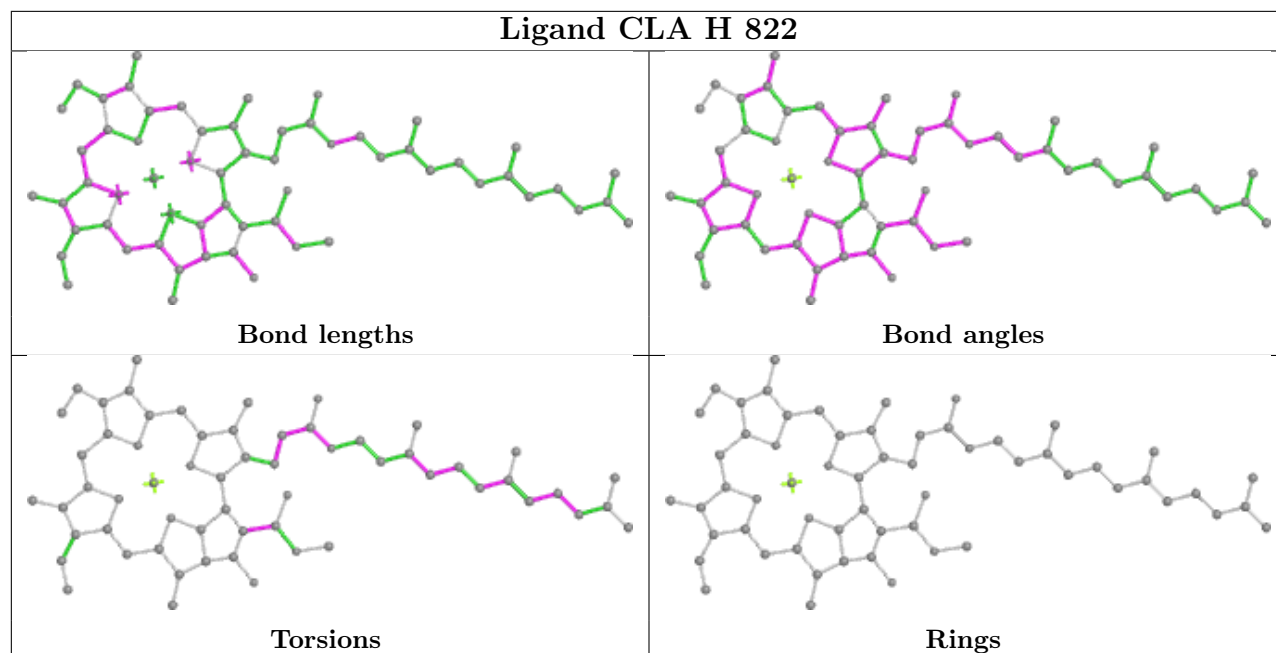


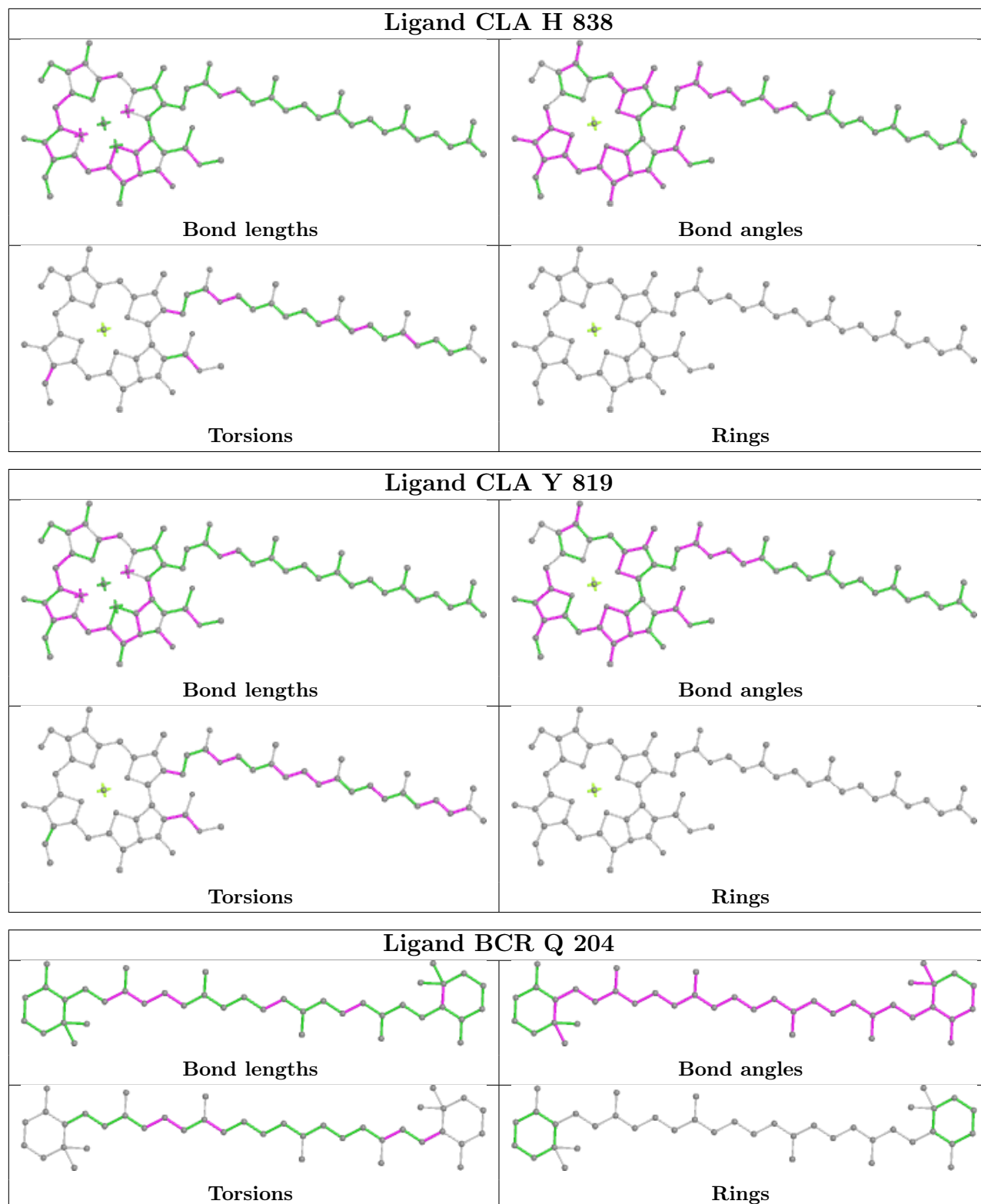


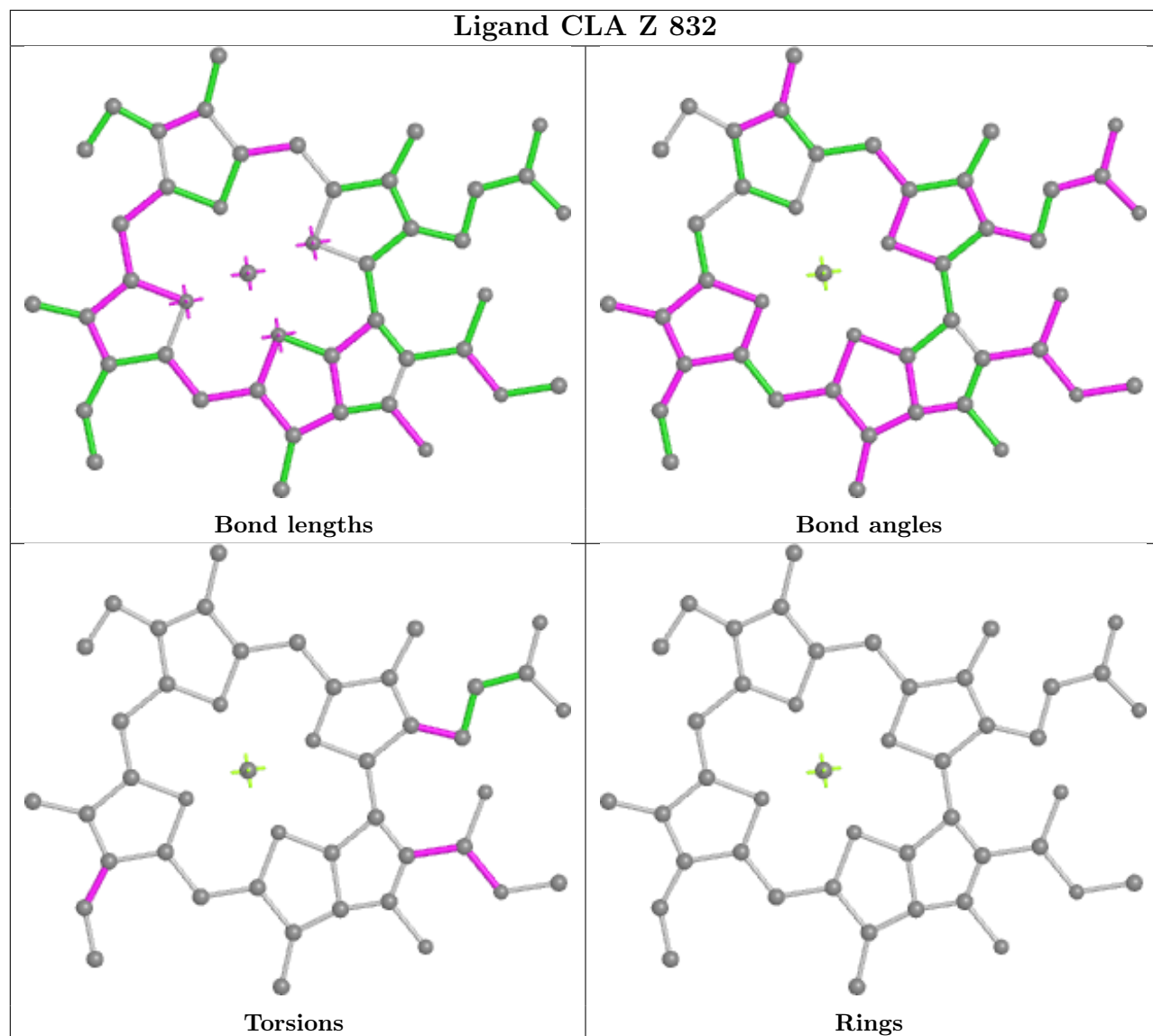


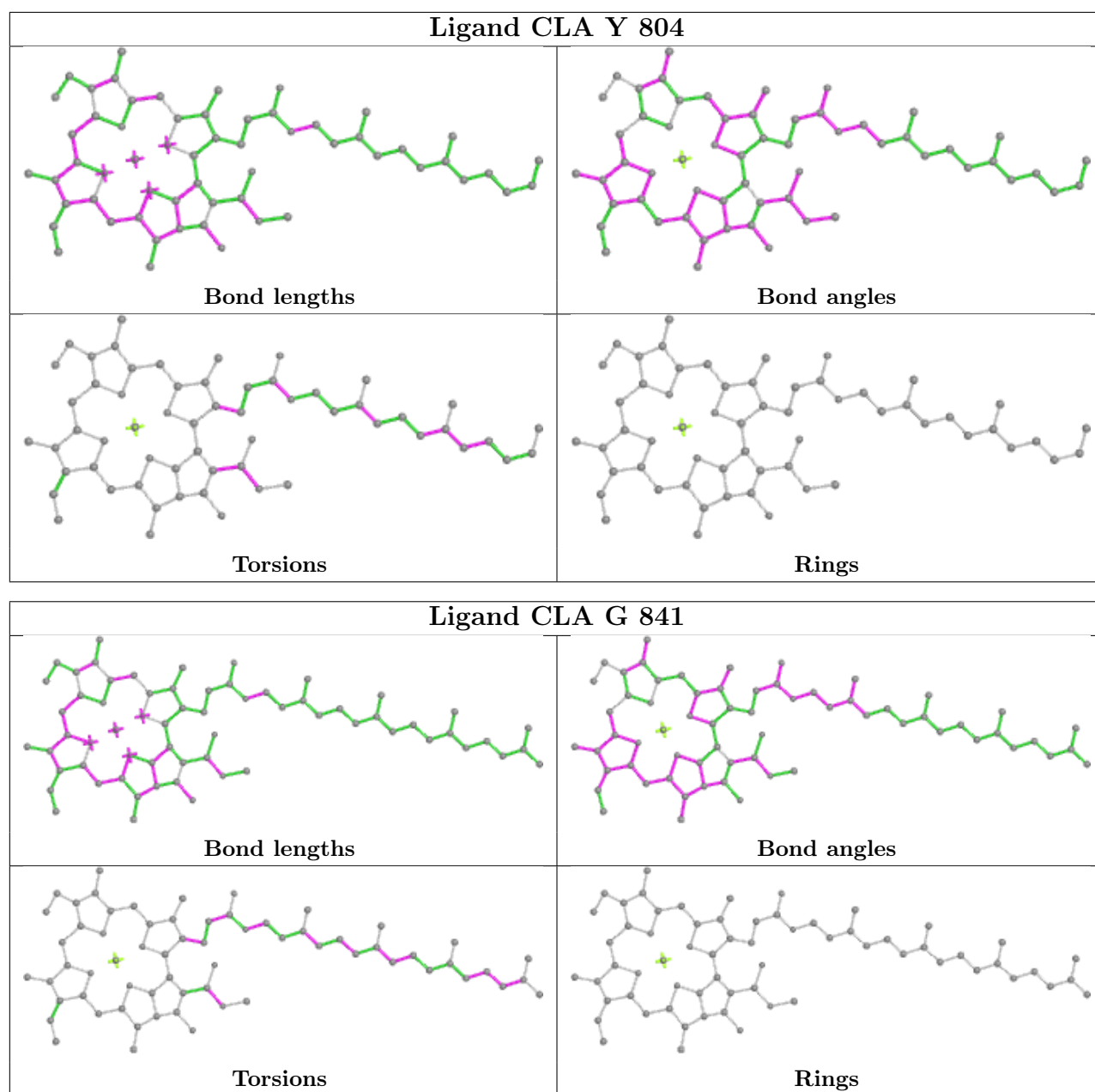


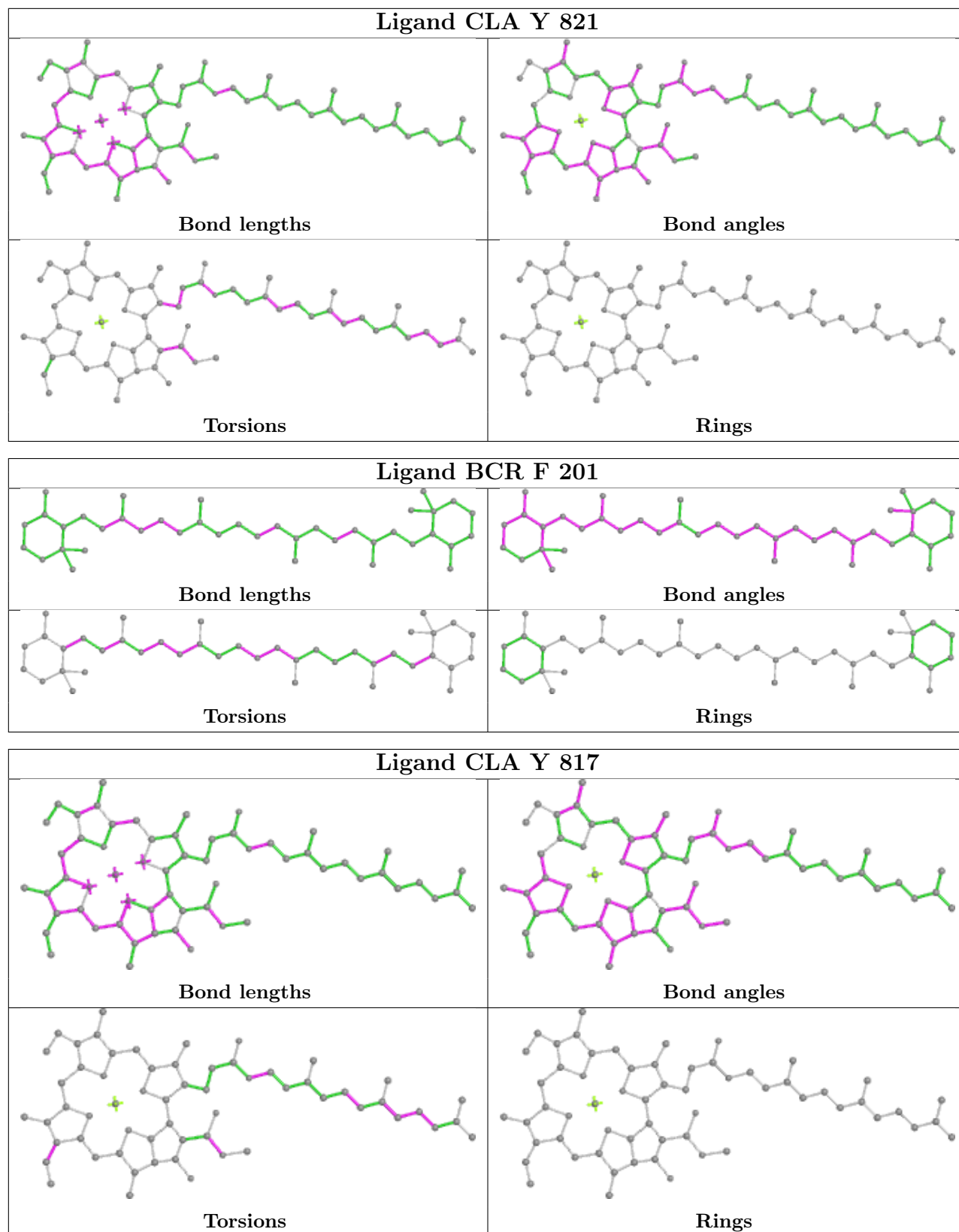


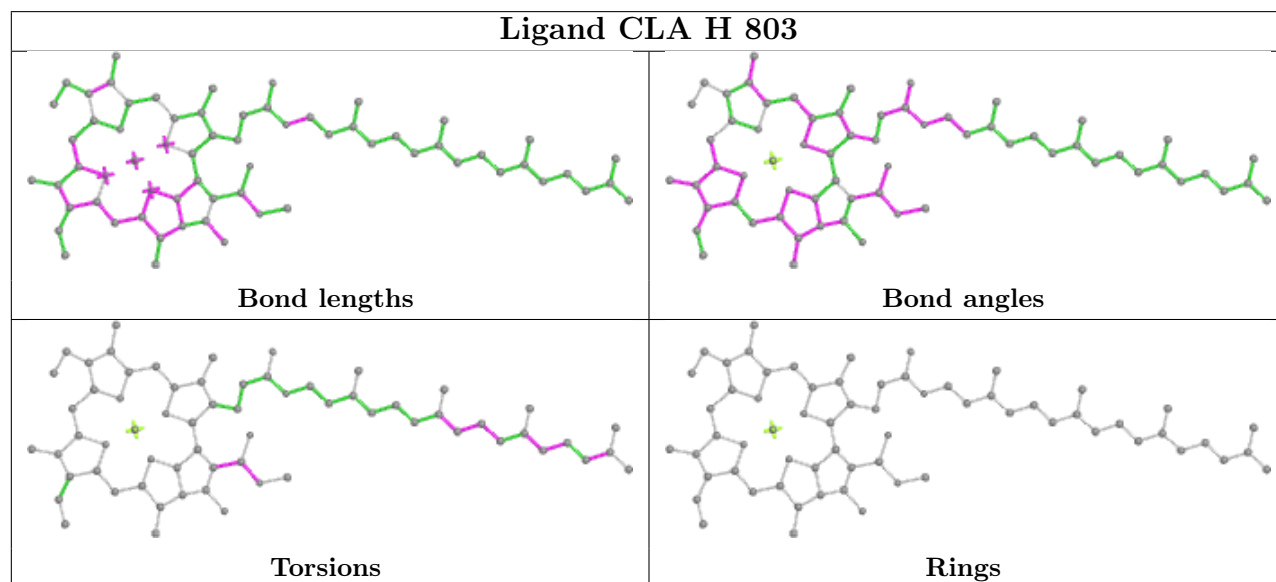
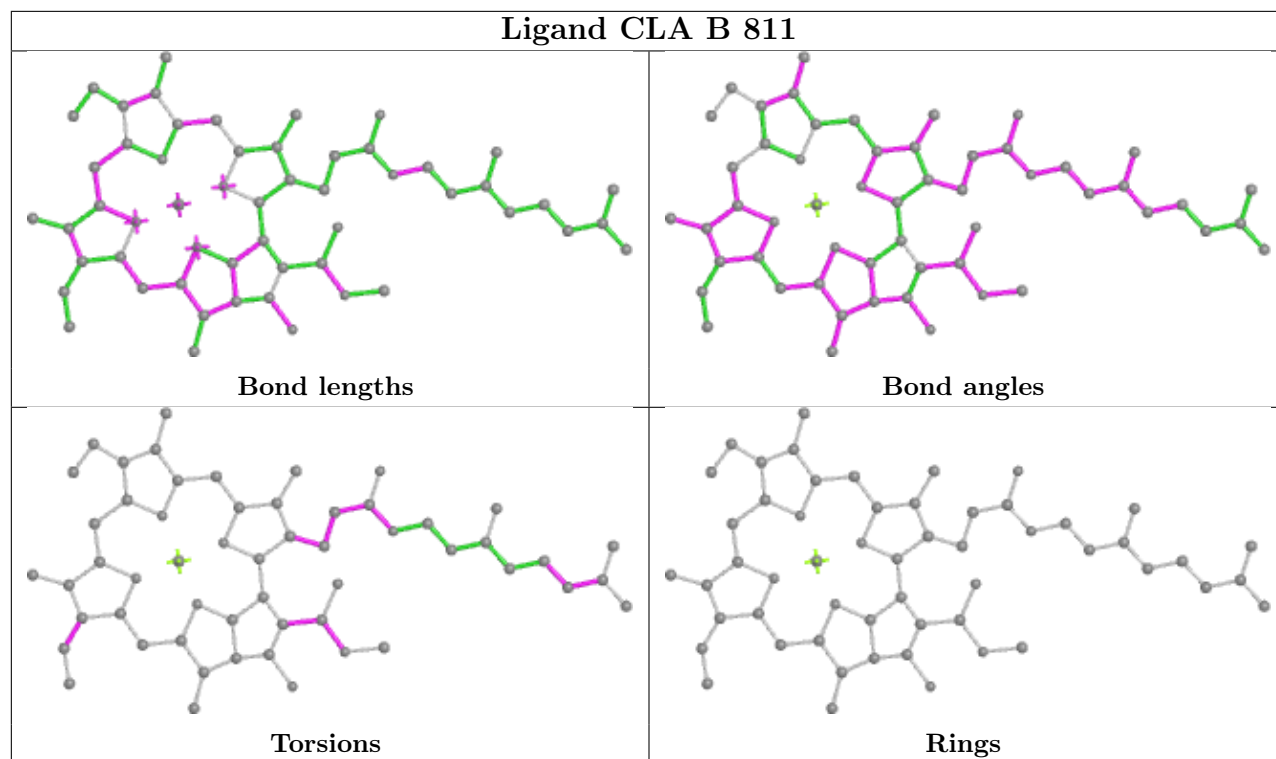


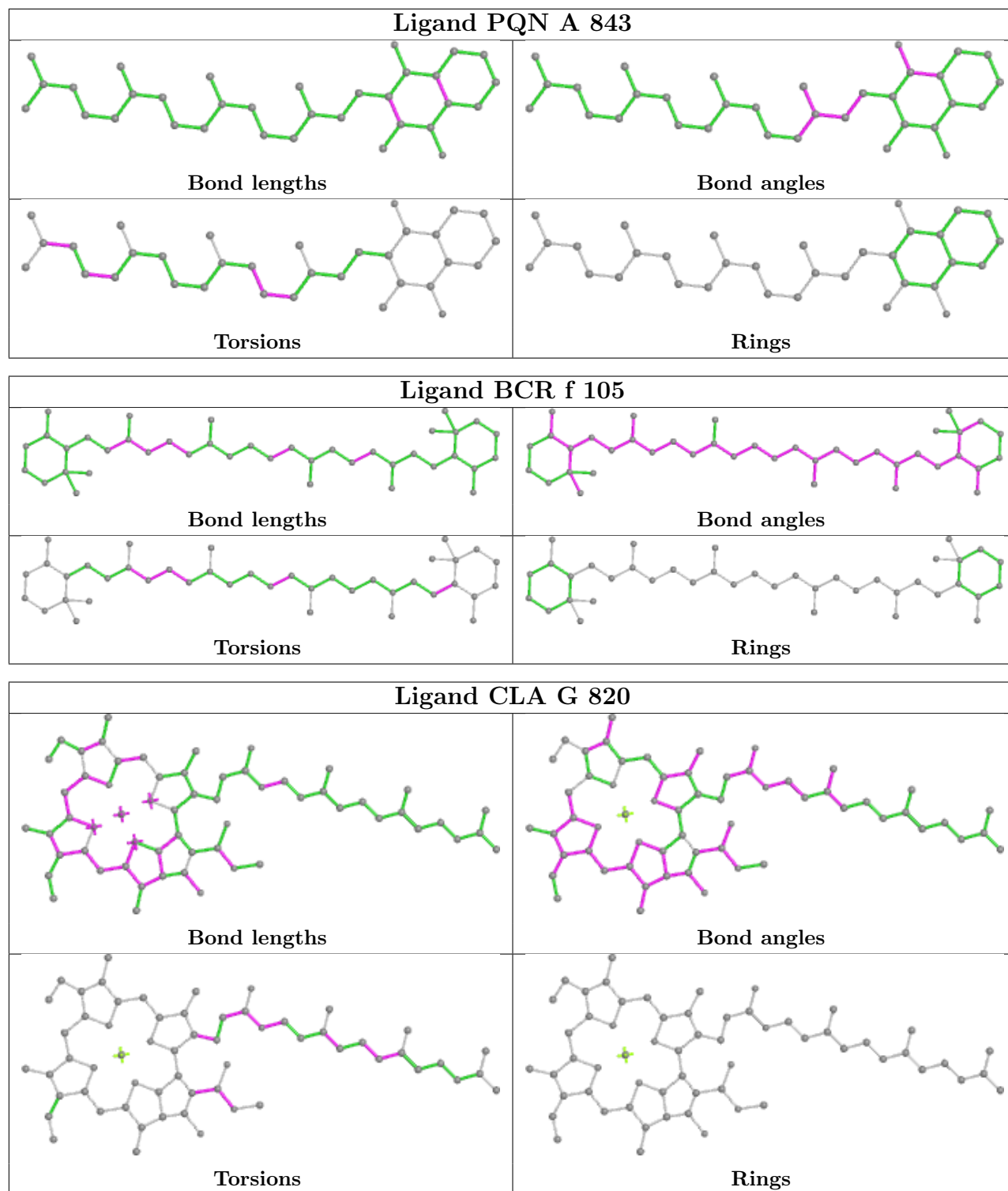




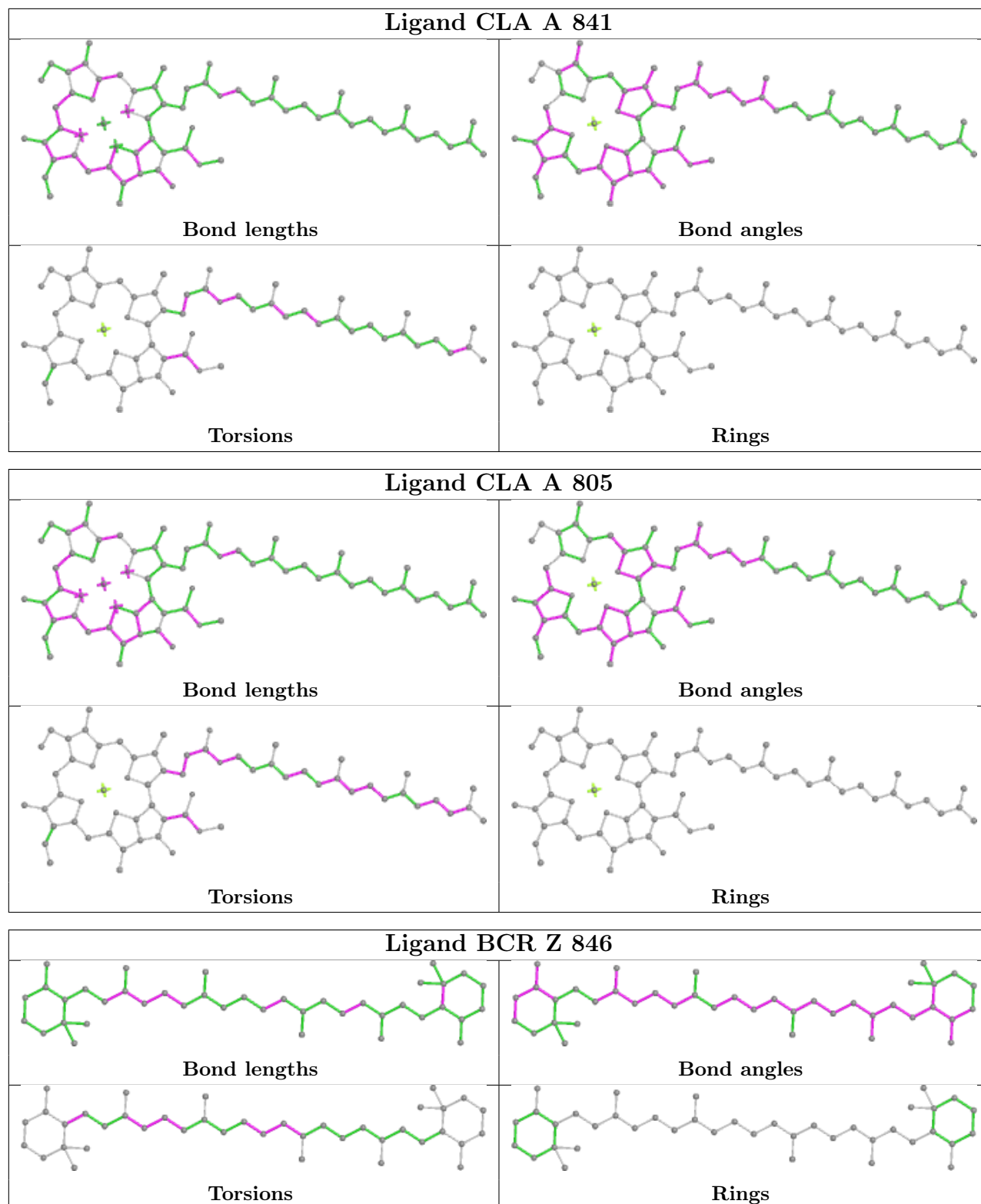


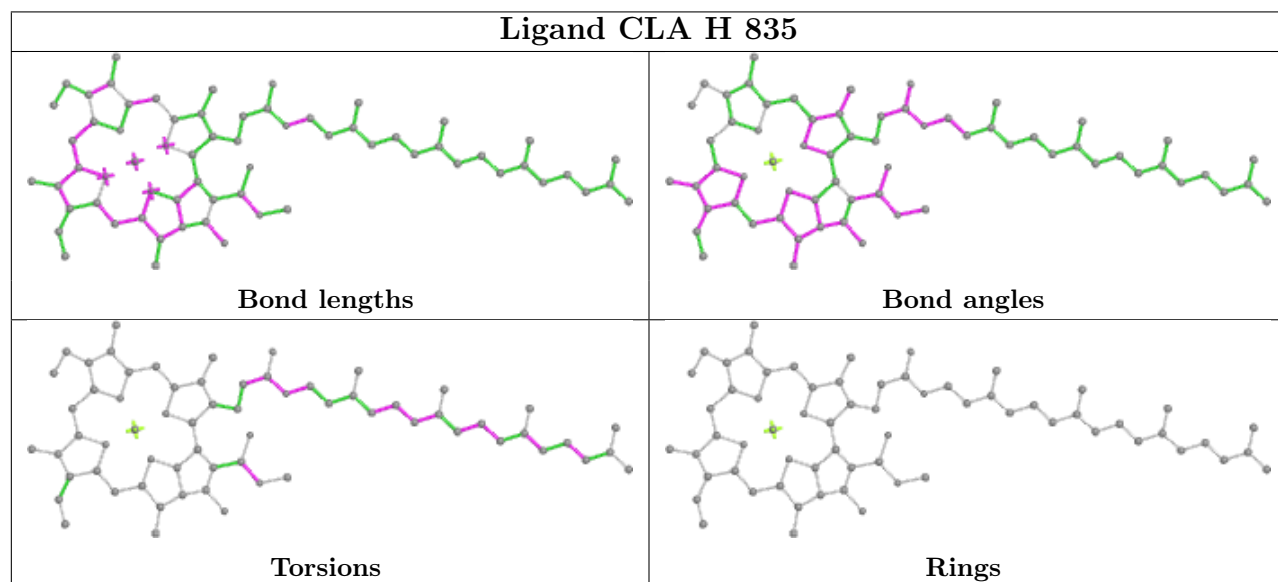
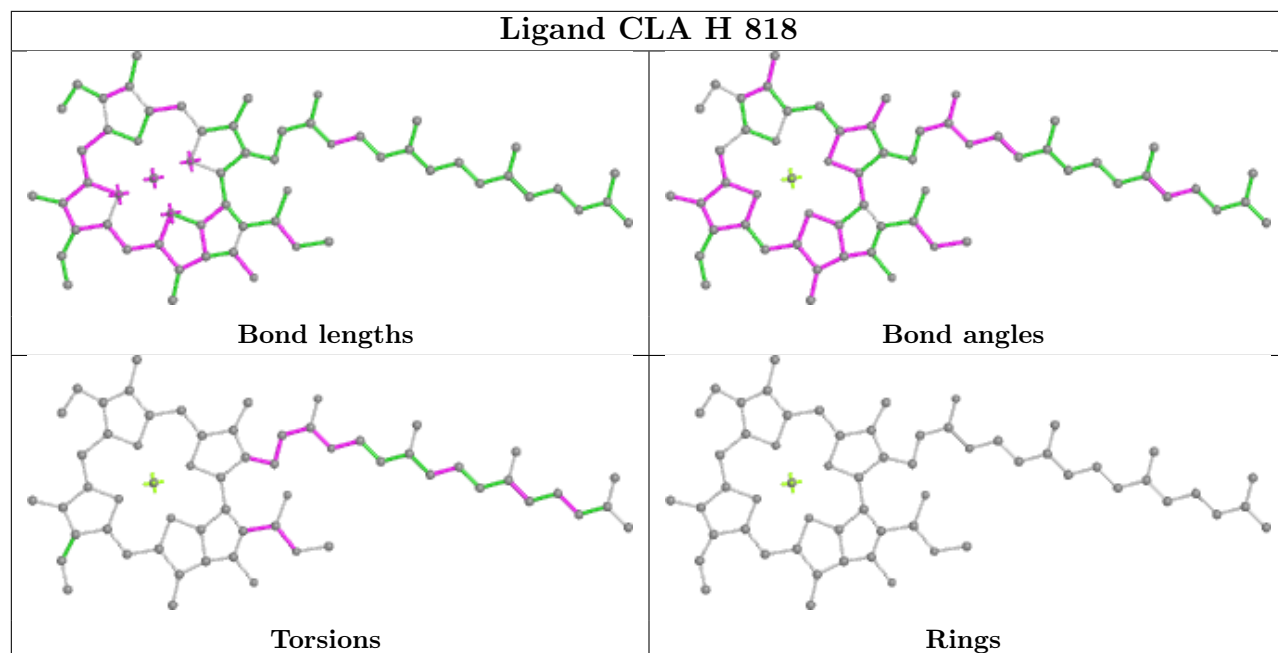


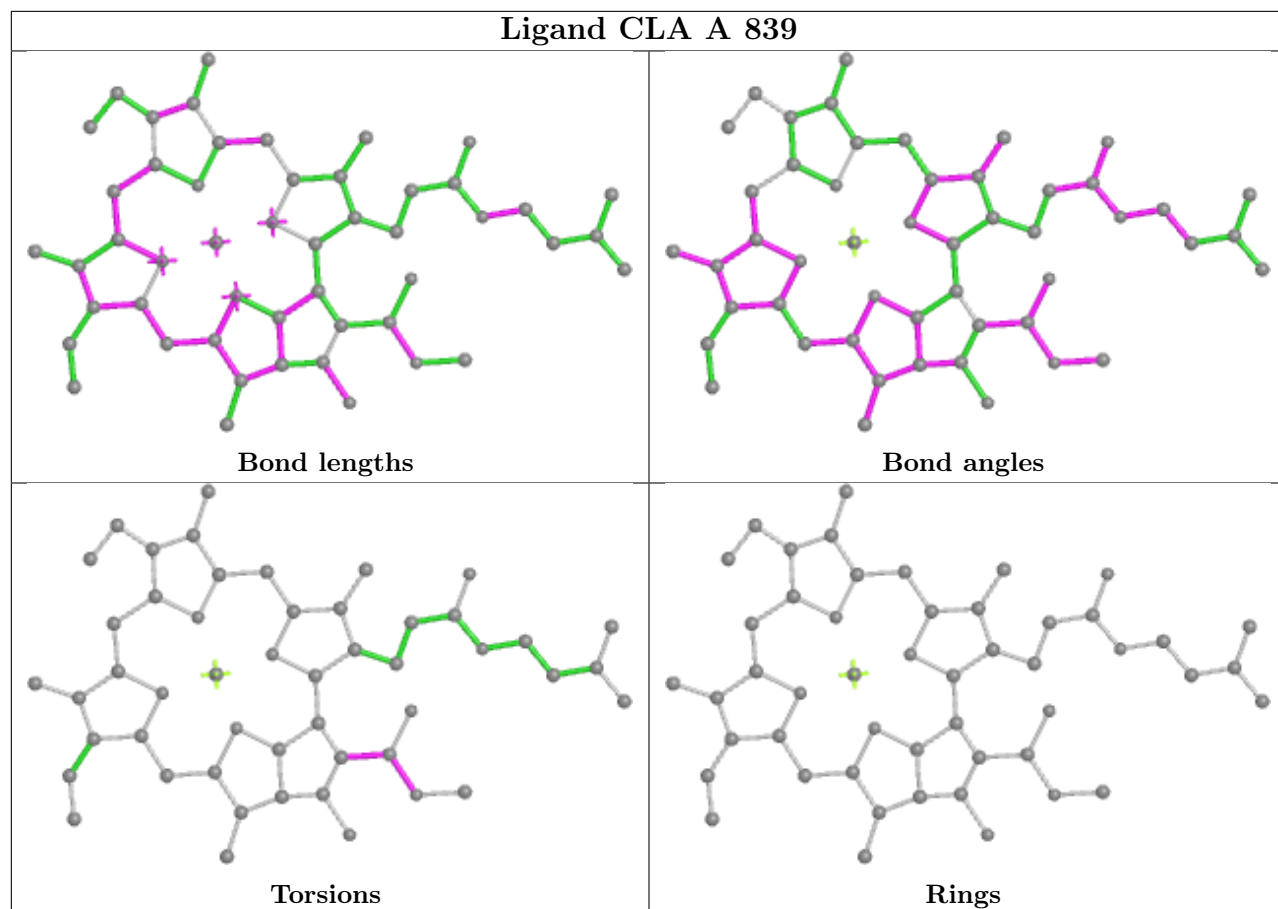


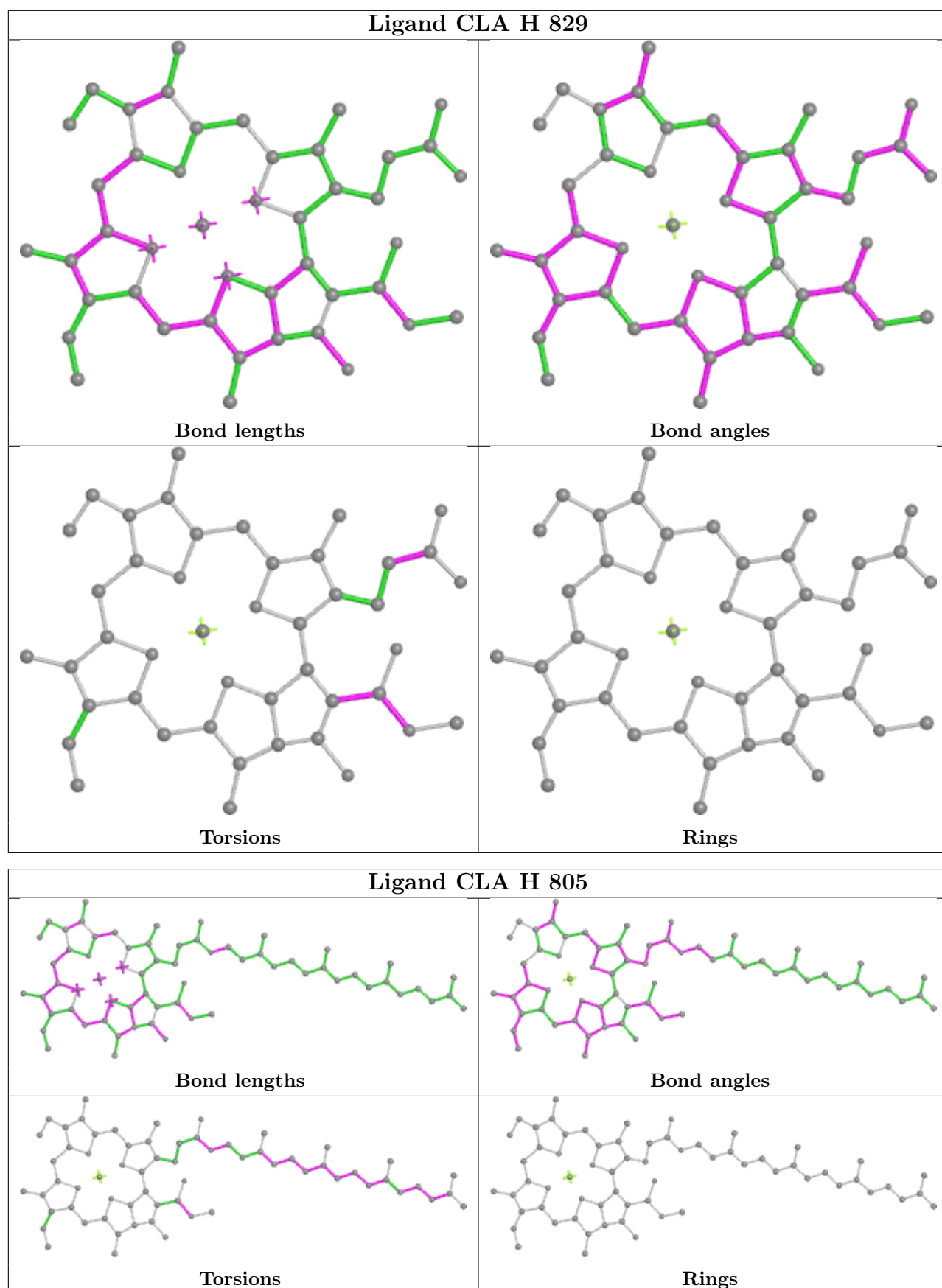


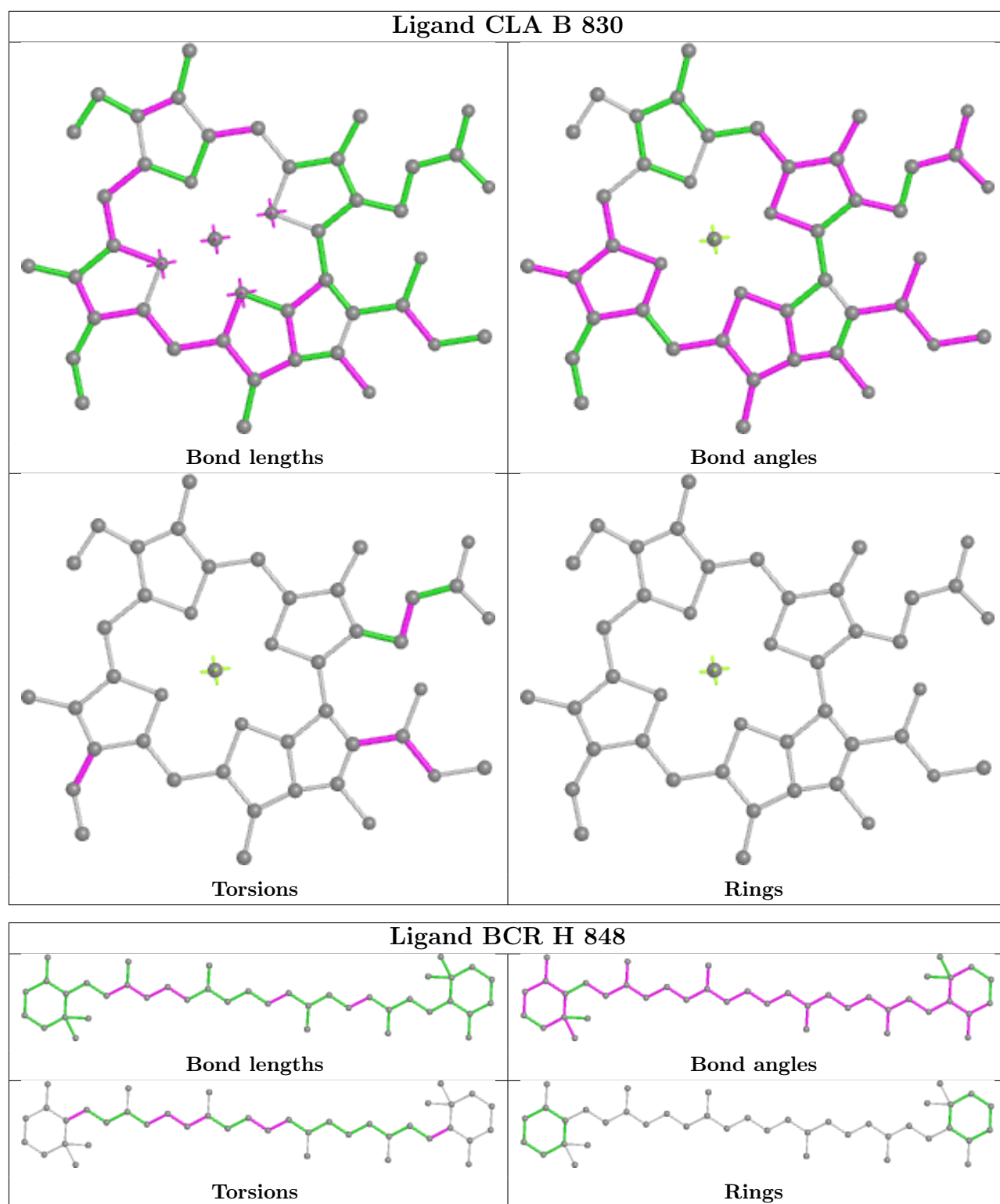


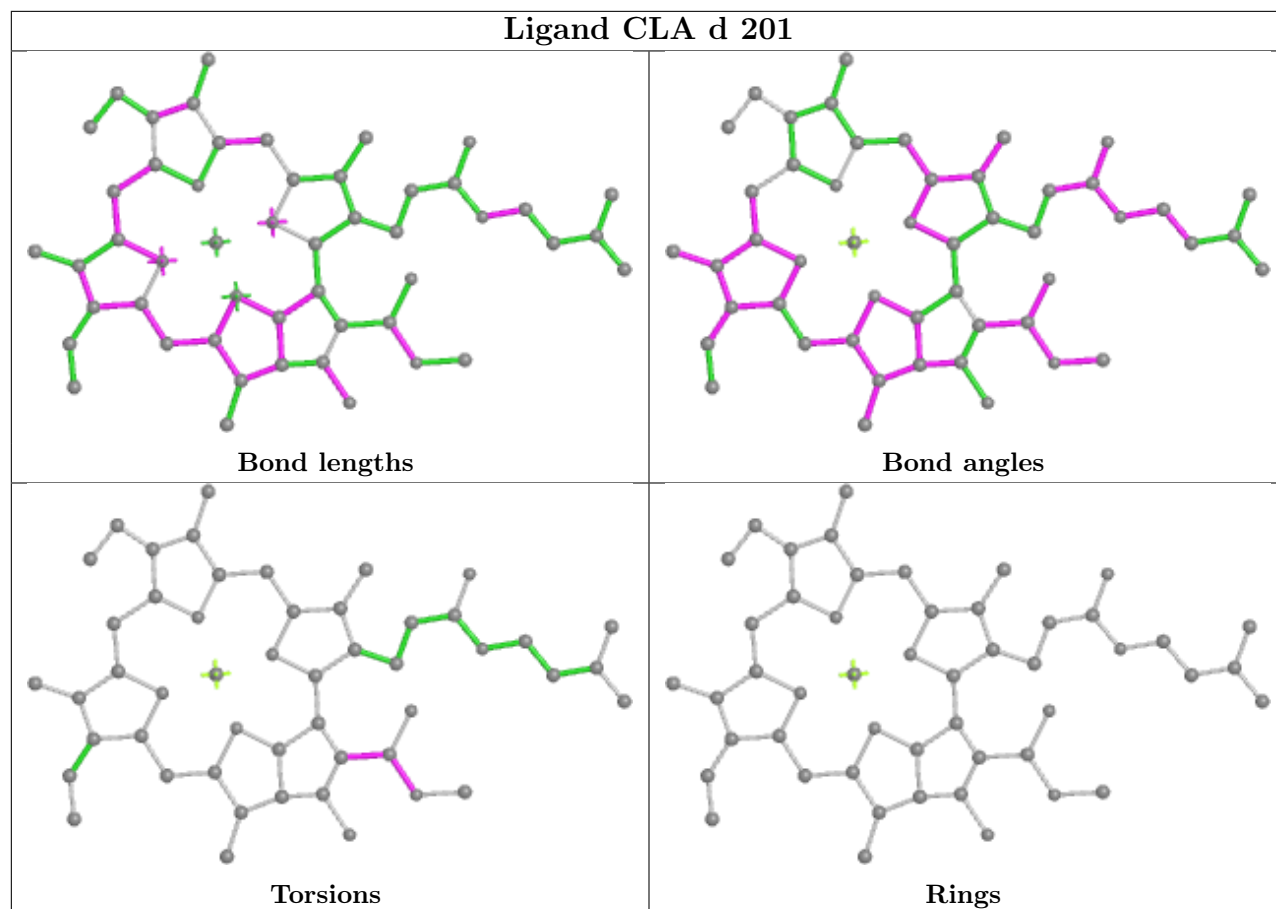












## 5.7 Other polymers [\(i\)](#)

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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

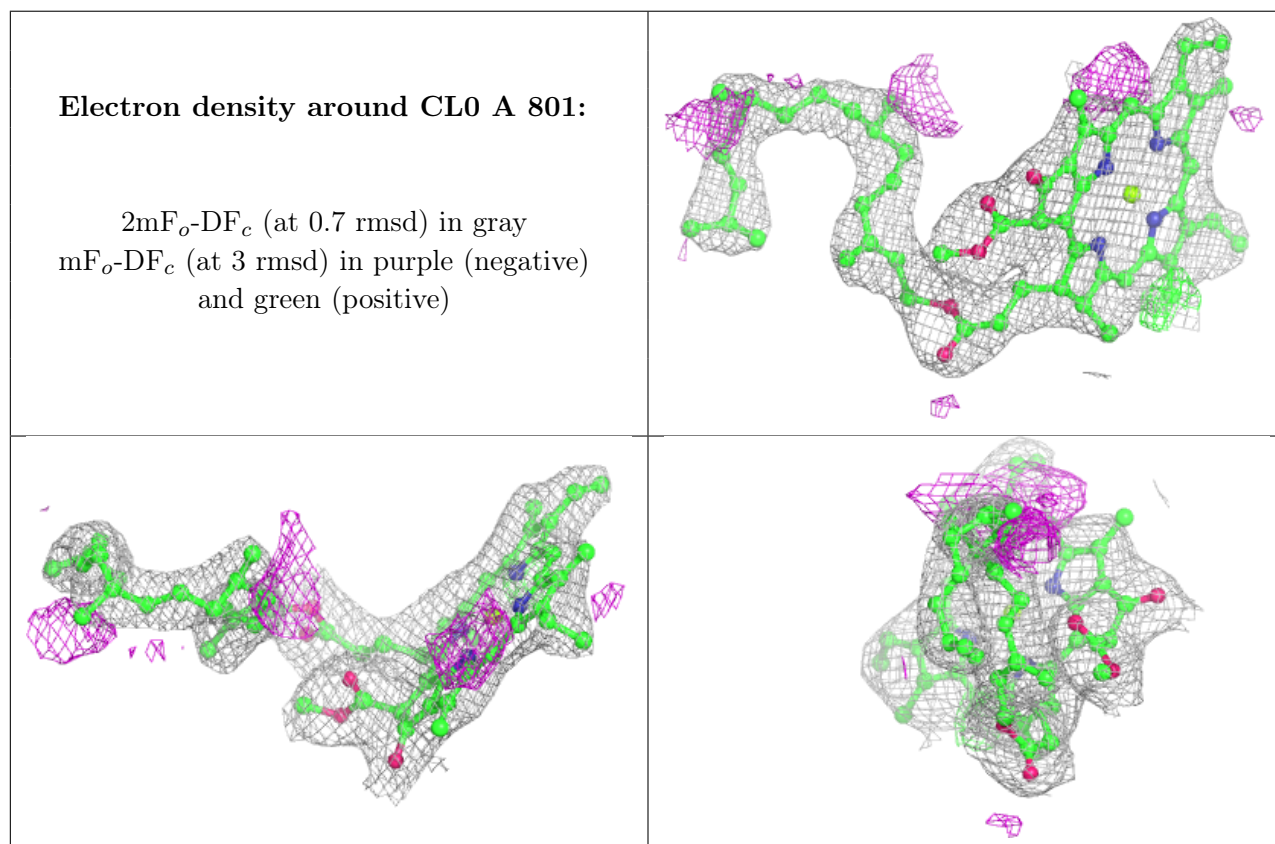
### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

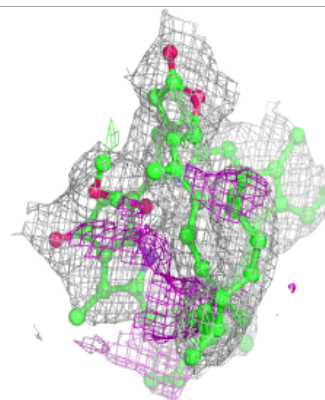
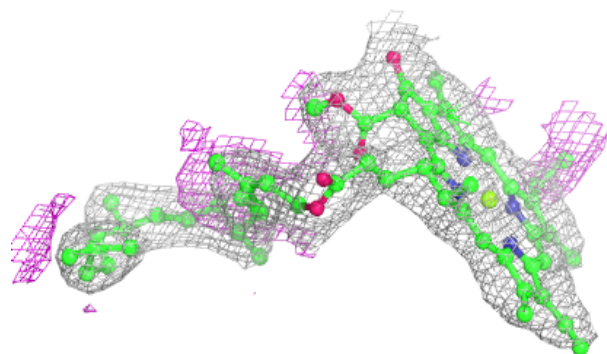
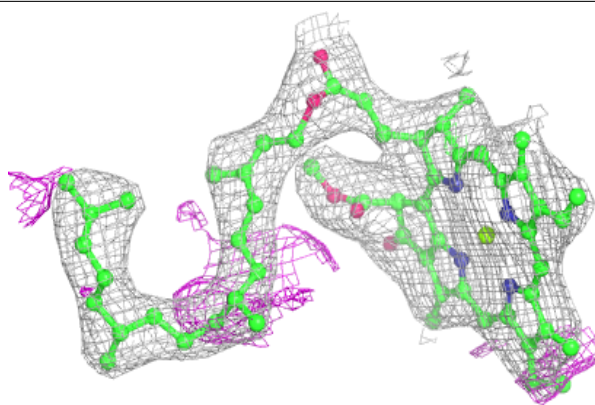
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

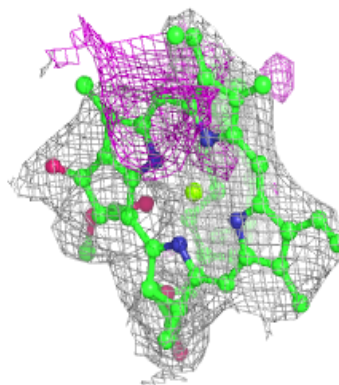
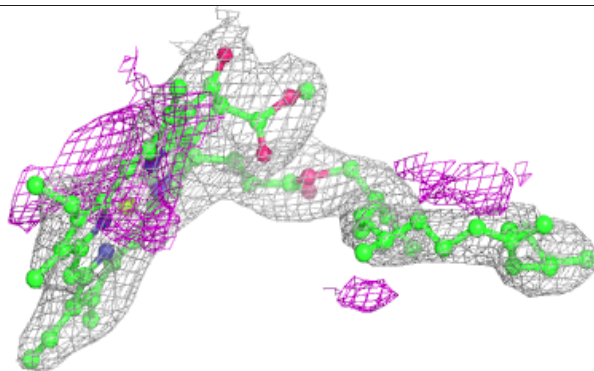
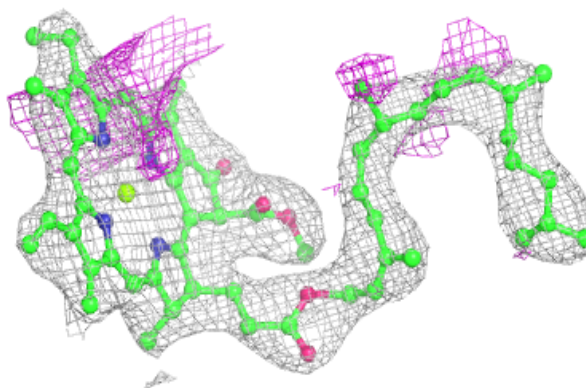


**Electron density around CL0 G 801:**

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

**Electron density around CL0 Y 801:**

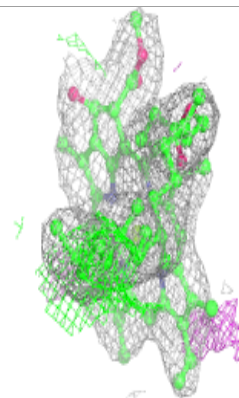
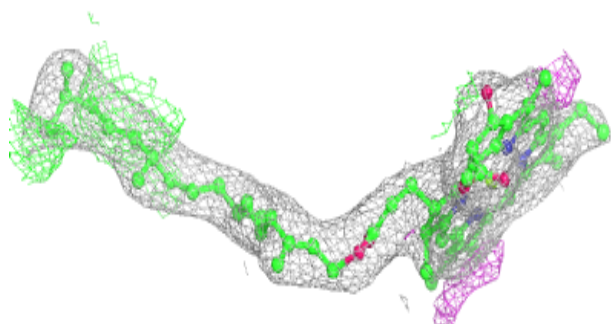
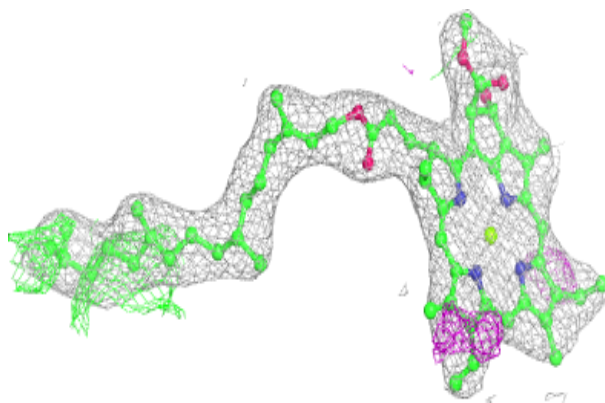
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



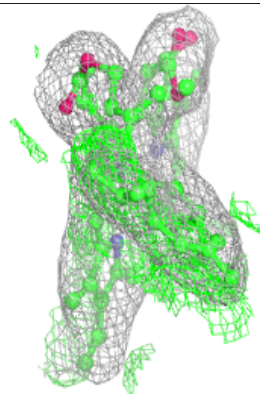
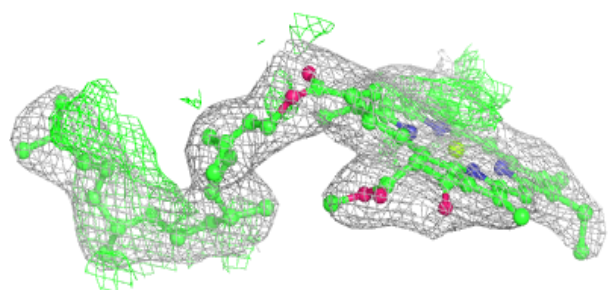
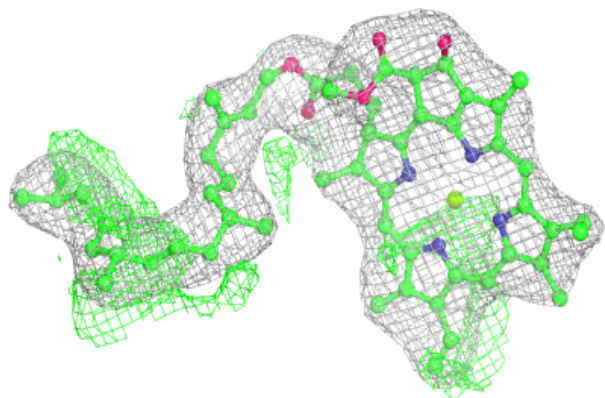


**Electron density around CLA A 802:**

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

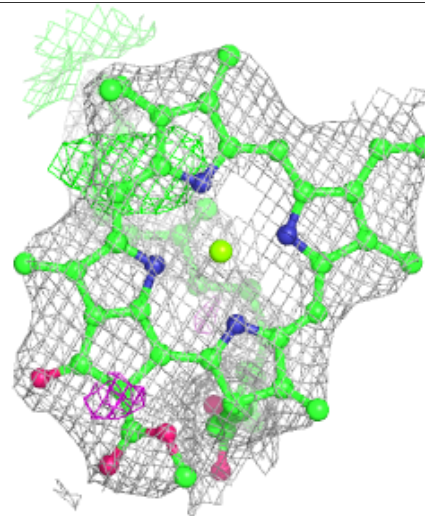
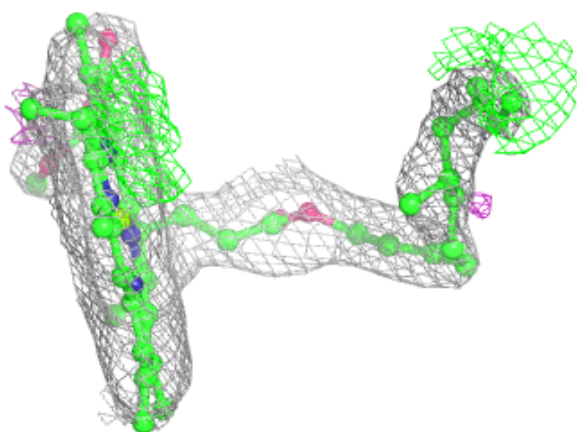
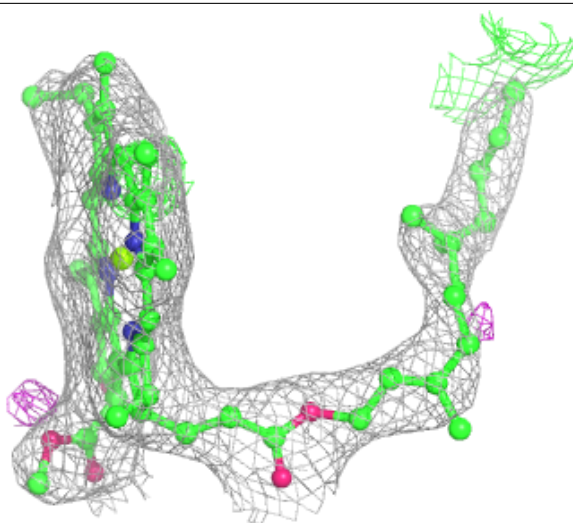
**Electron density around CLA A 803:**

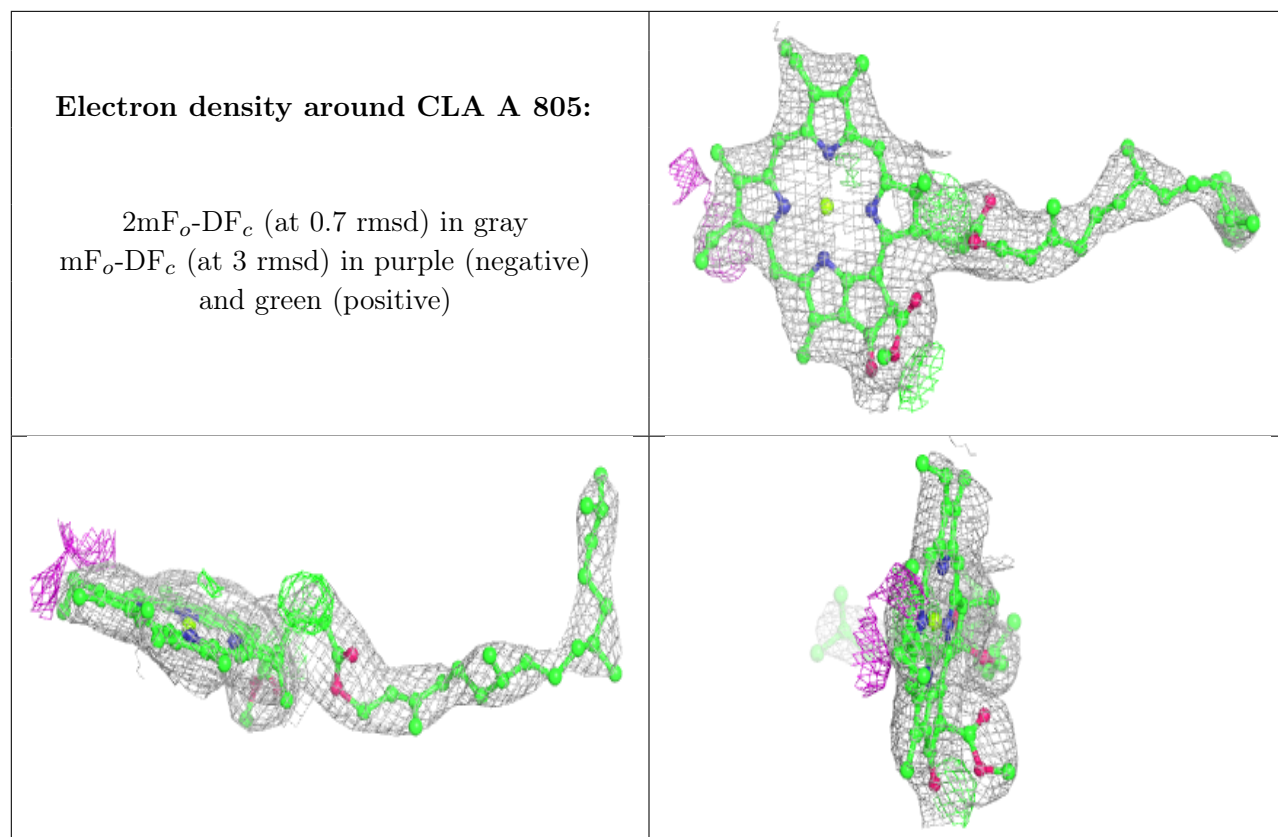
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA A 804:**

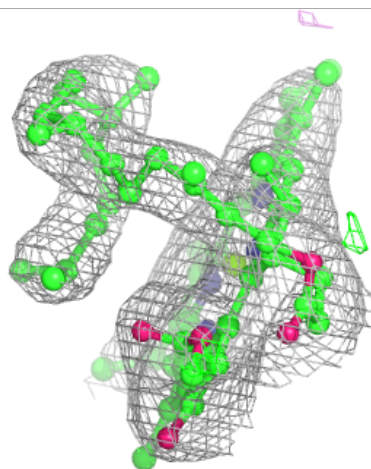
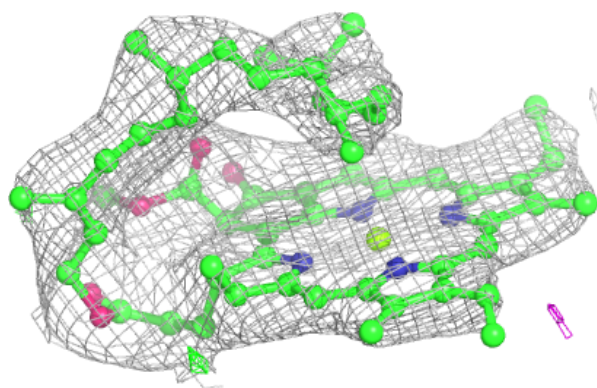
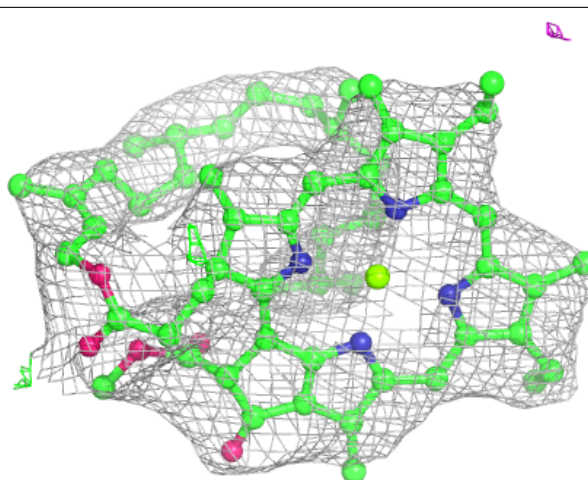
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





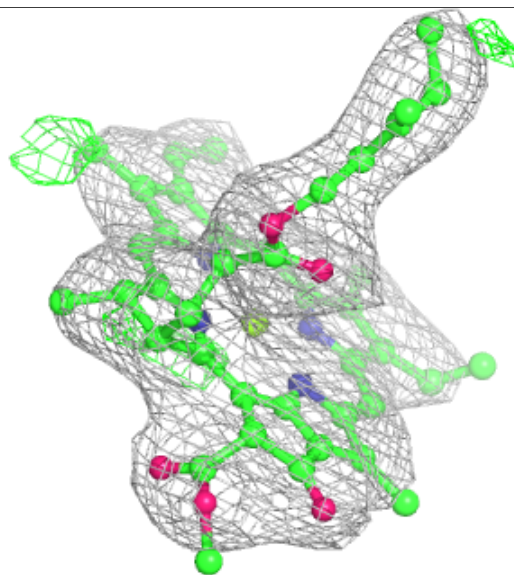
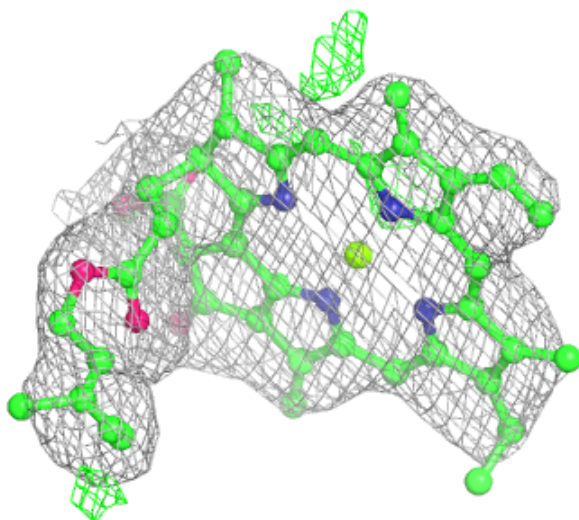
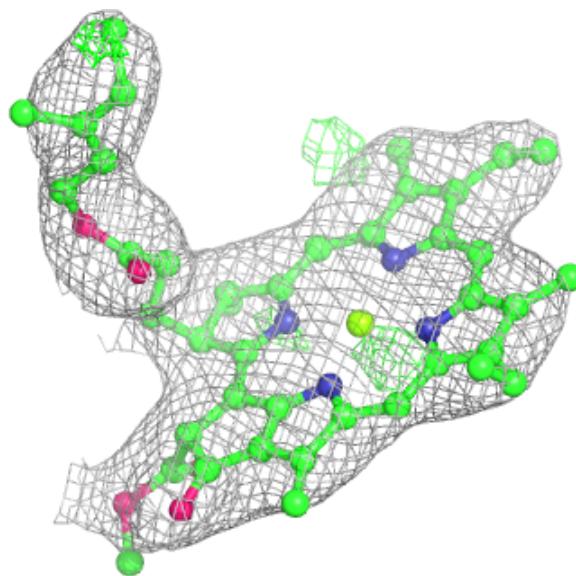
**Electron density around CLA A 806:**

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



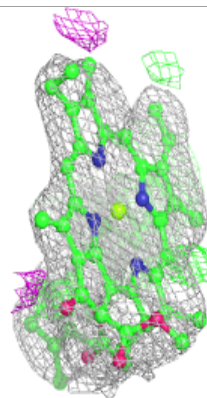
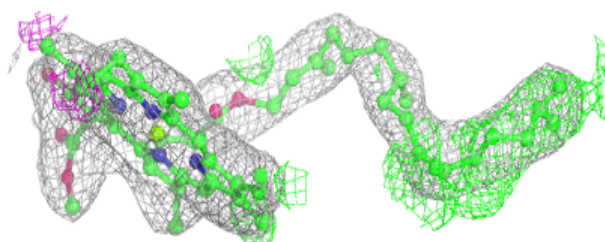
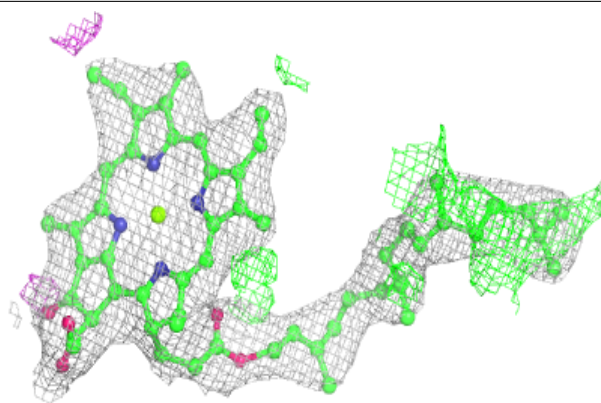
**Electron density around CLA A 807:**

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

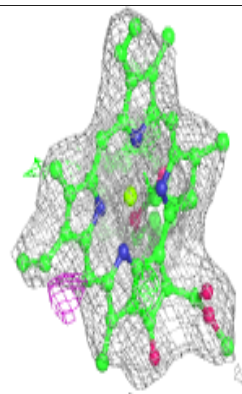
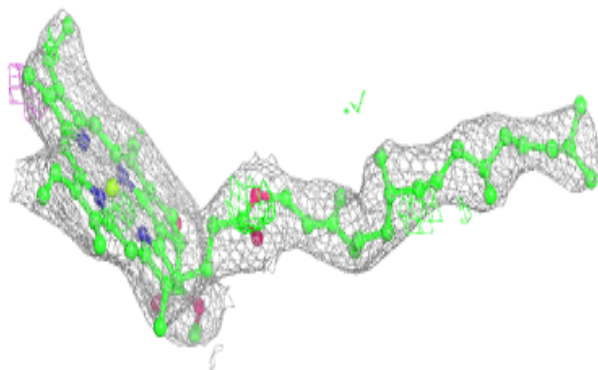
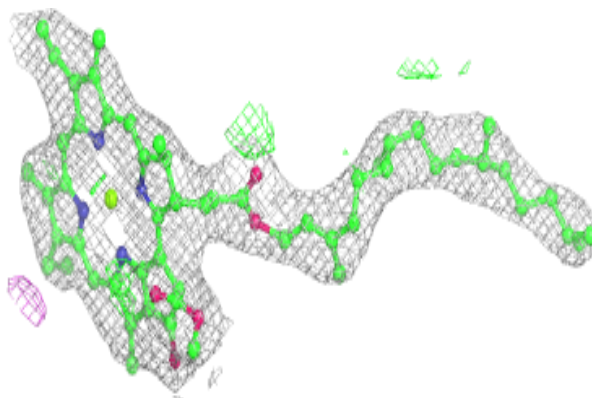


**Electron density around CLA A 808:**

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

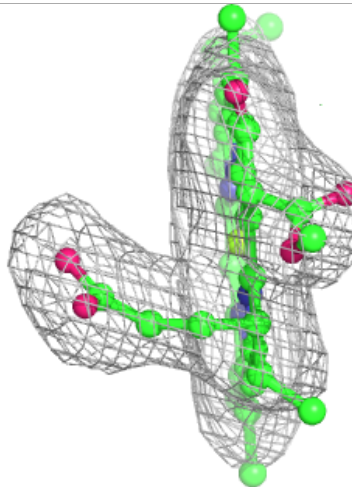
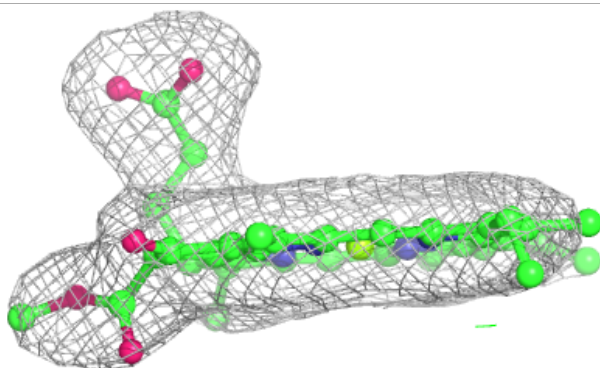
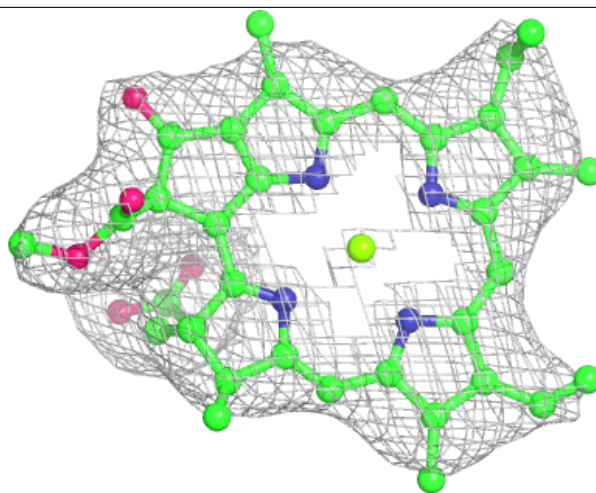
**Electron density around CLA A 809:**

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



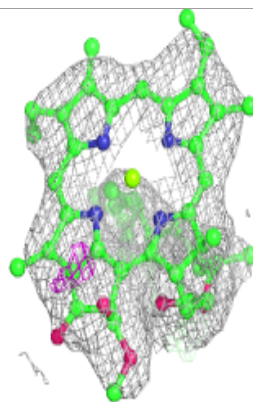
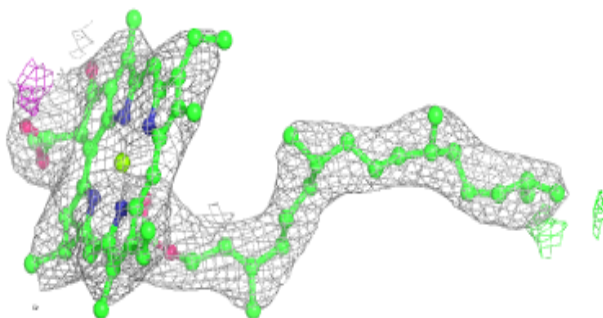
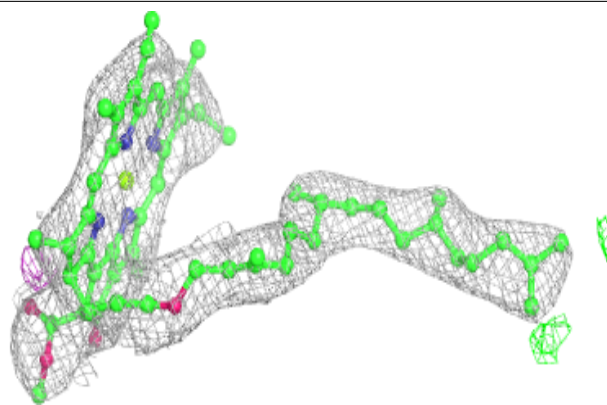
**Electron density around CLA A 810:**

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

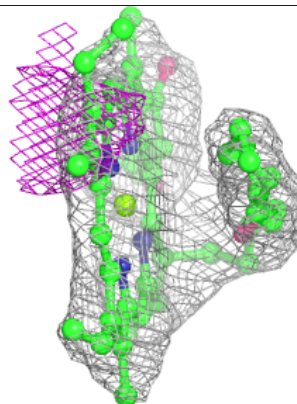
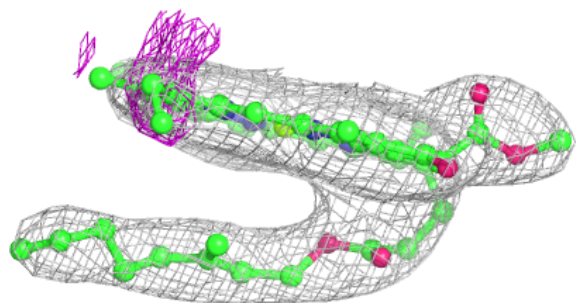
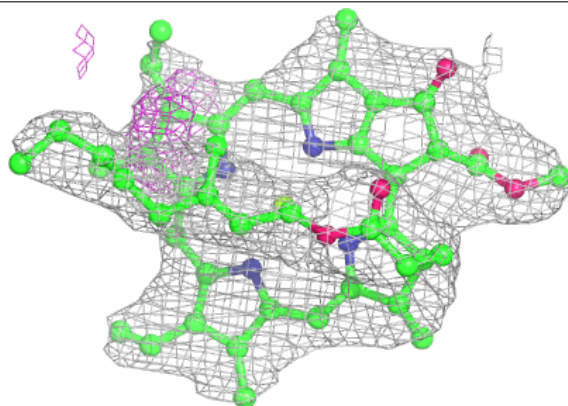


**Electron density around CLA A 811:**

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

**Electron density around CLA A 812:**

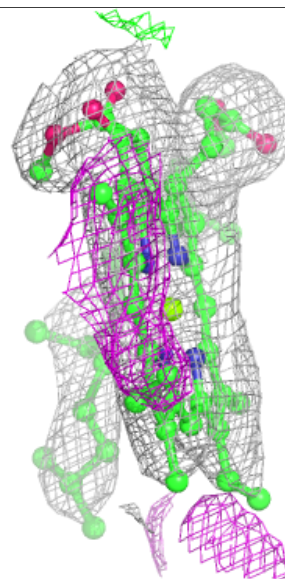
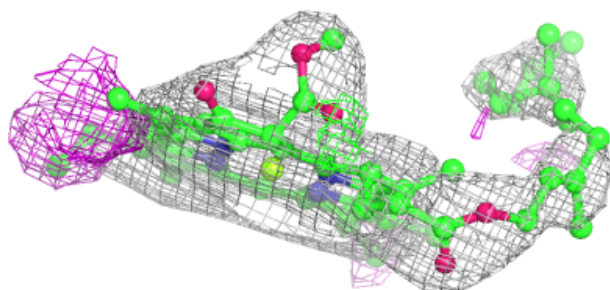
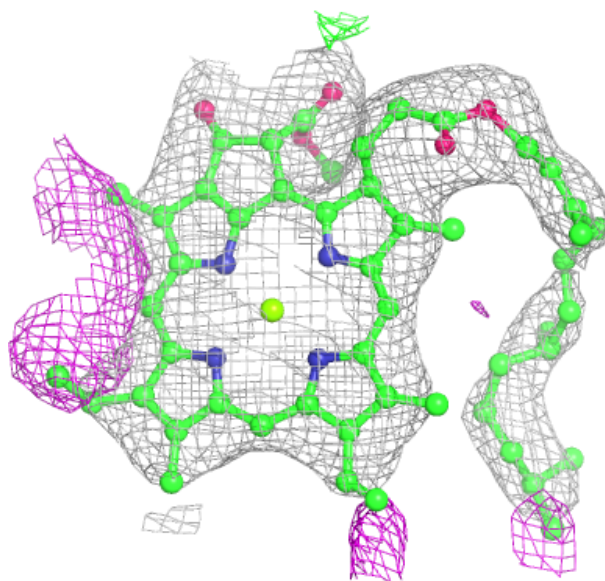
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

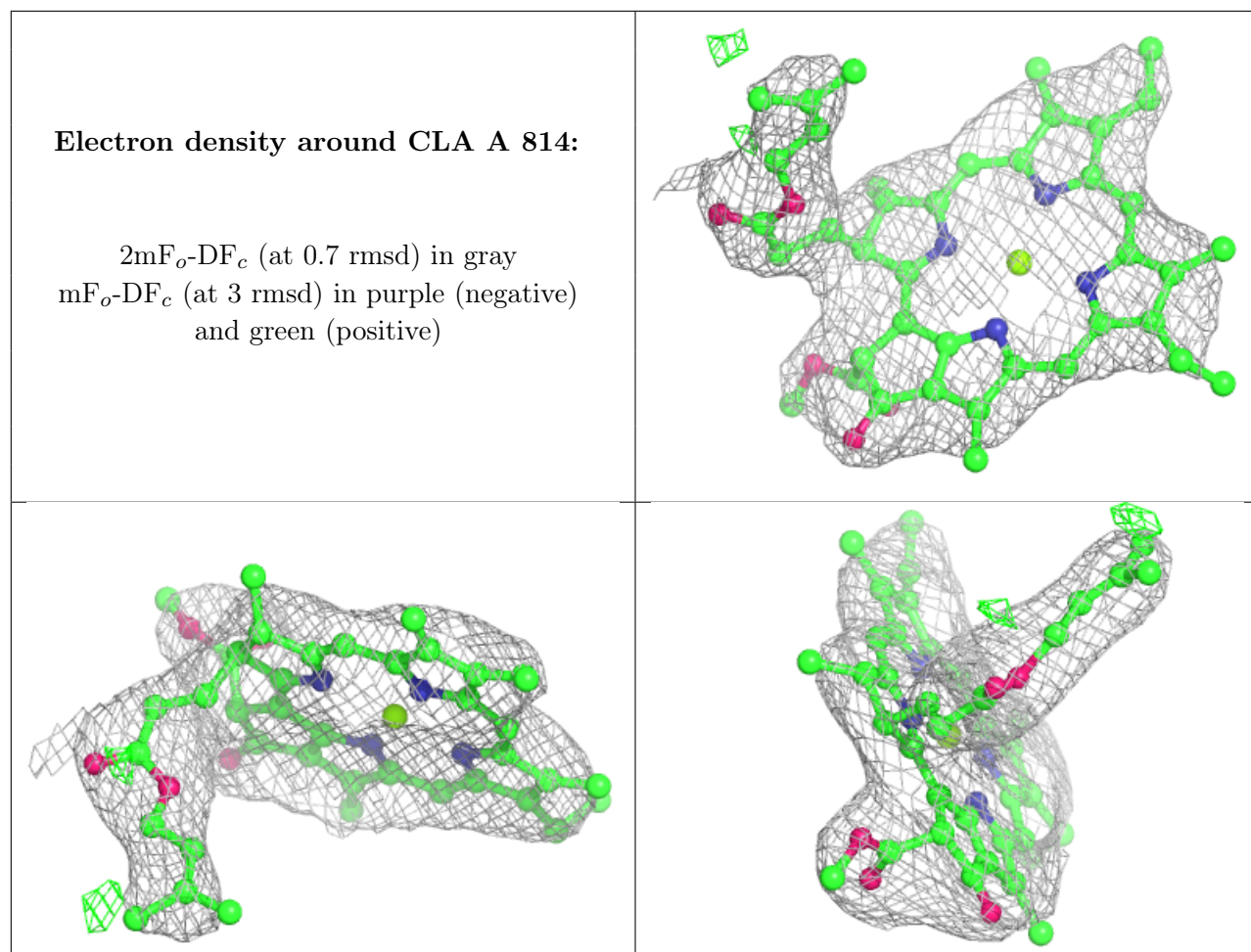




**Electron density around CLA A 813:**

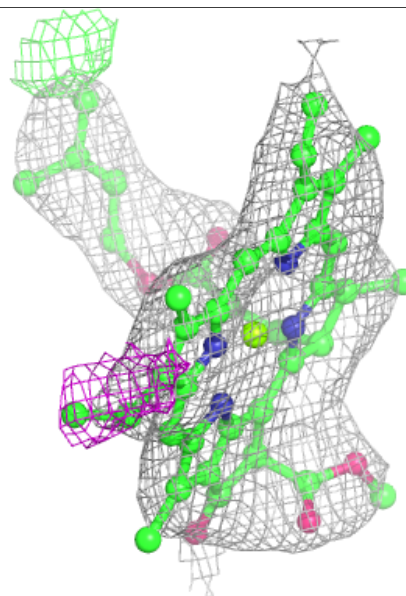
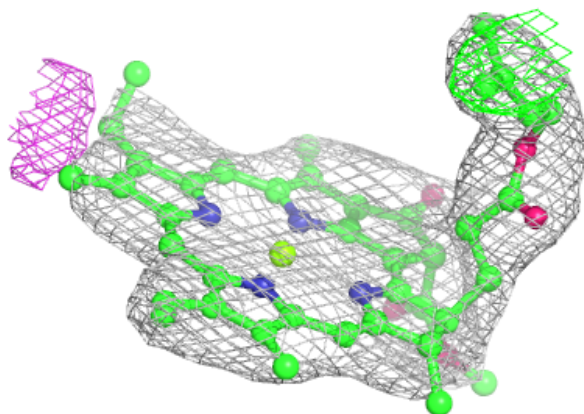
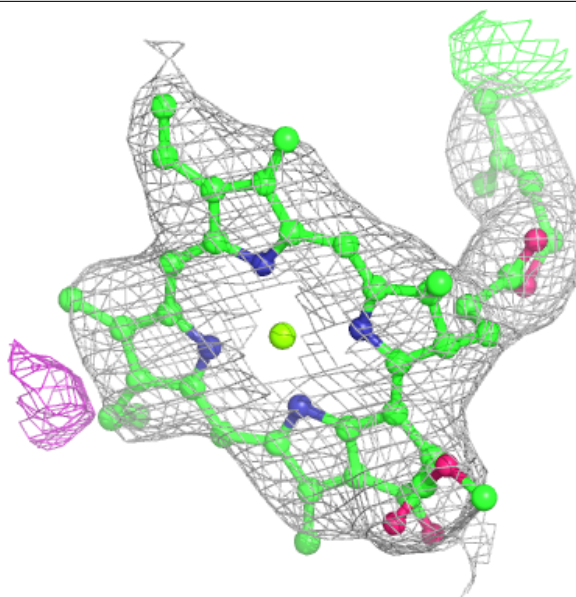
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





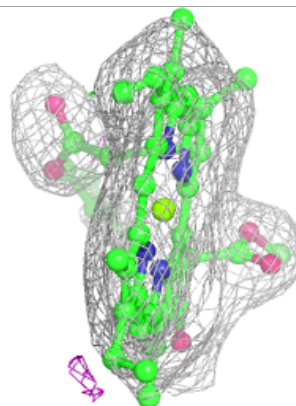
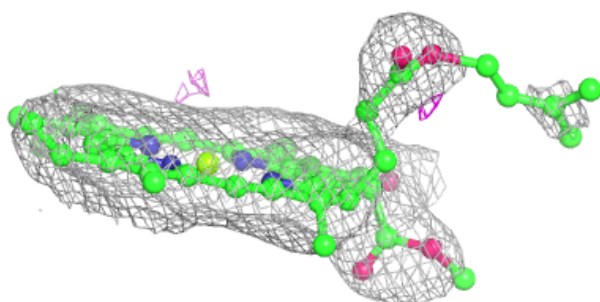
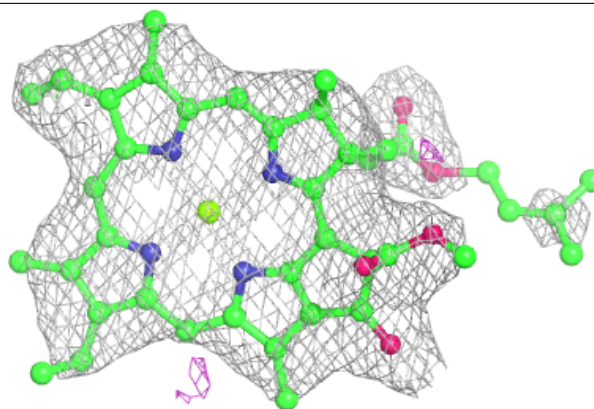
**Electron density around CLA A 815:**

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

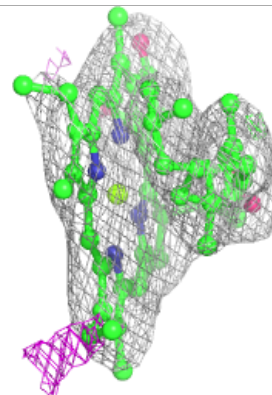
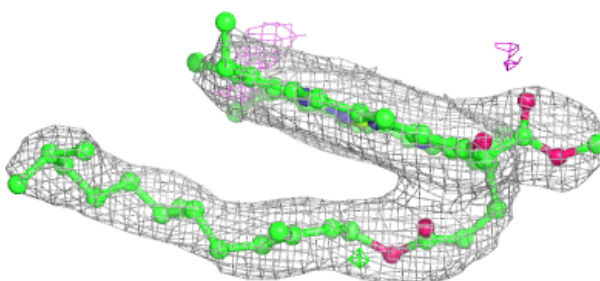
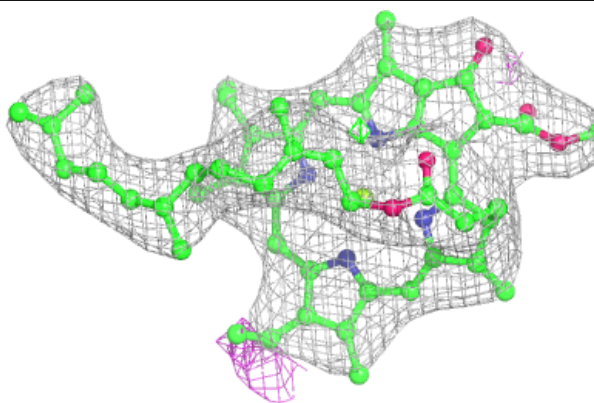


**Electron density around CLA A 816:**

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

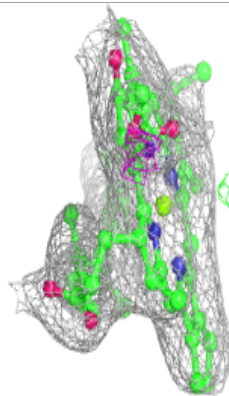
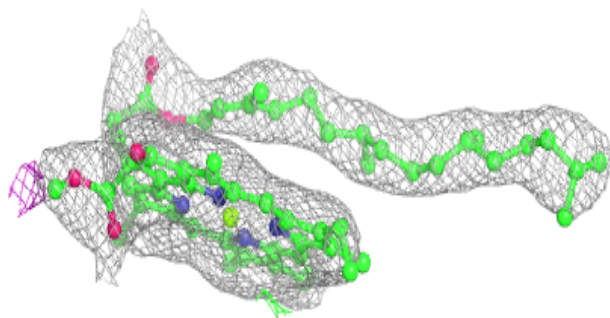
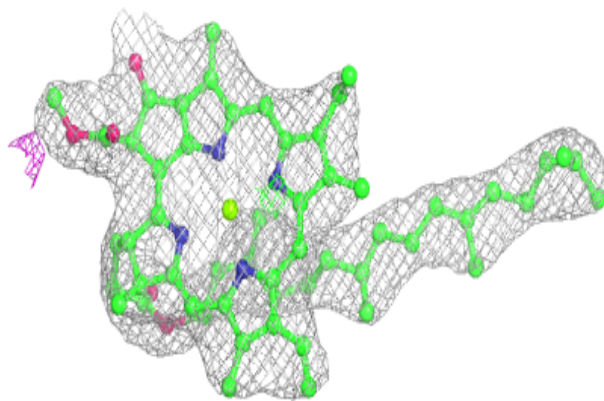
**Electron density around CLA A 817:**

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

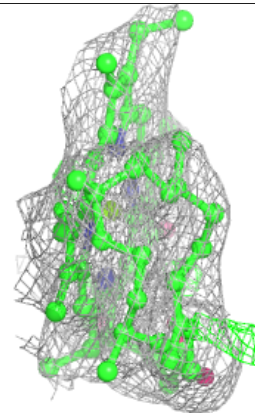
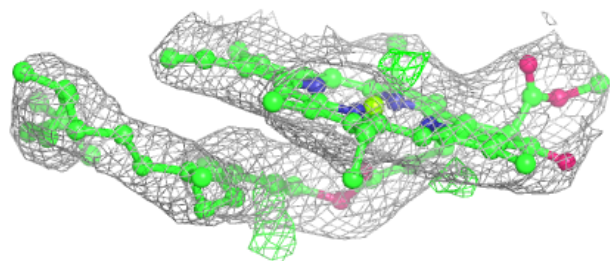
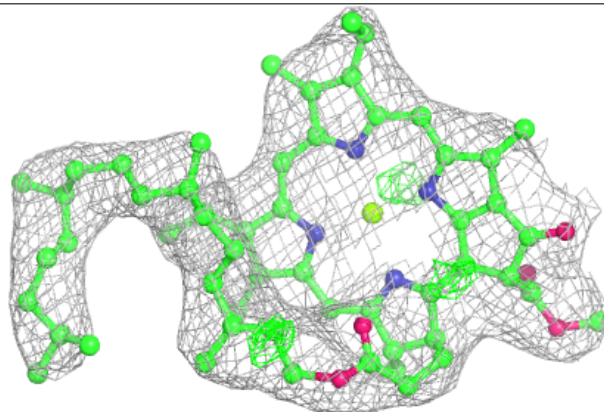


**Electron density around CLA A 818:**

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

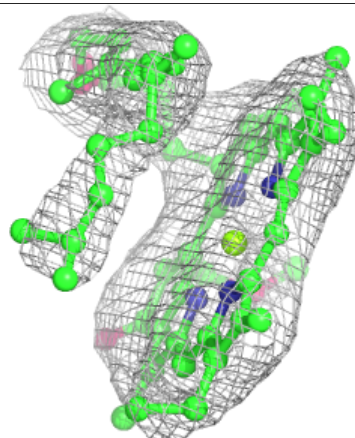
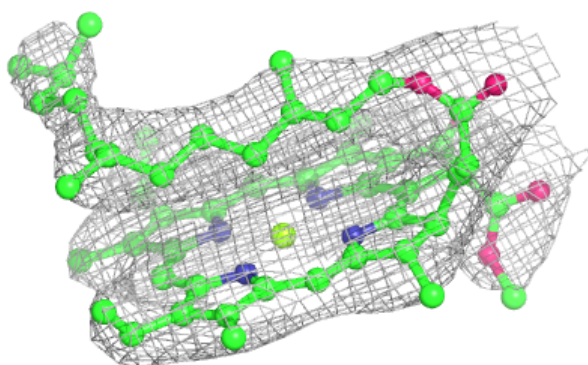
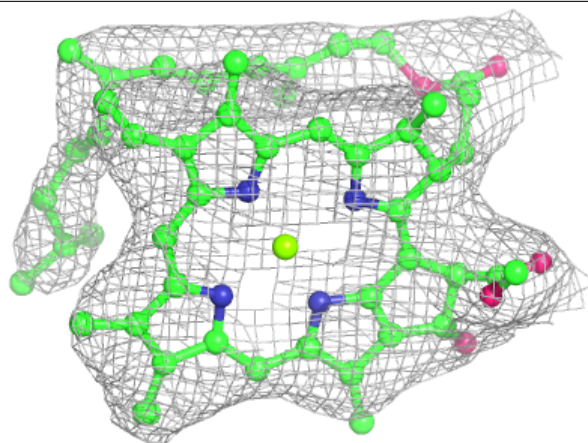
**Electron density around CLA A 819:**

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

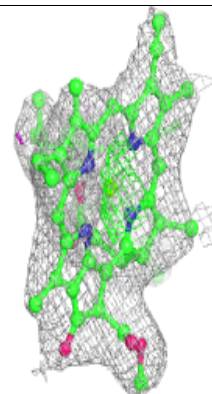
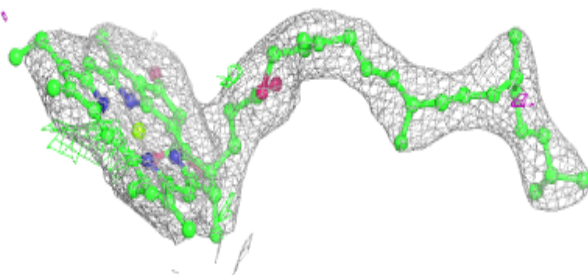
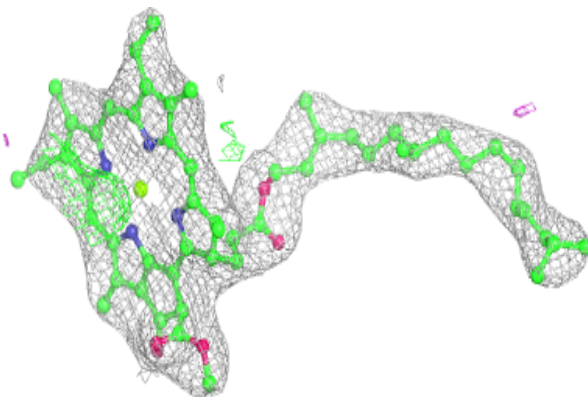


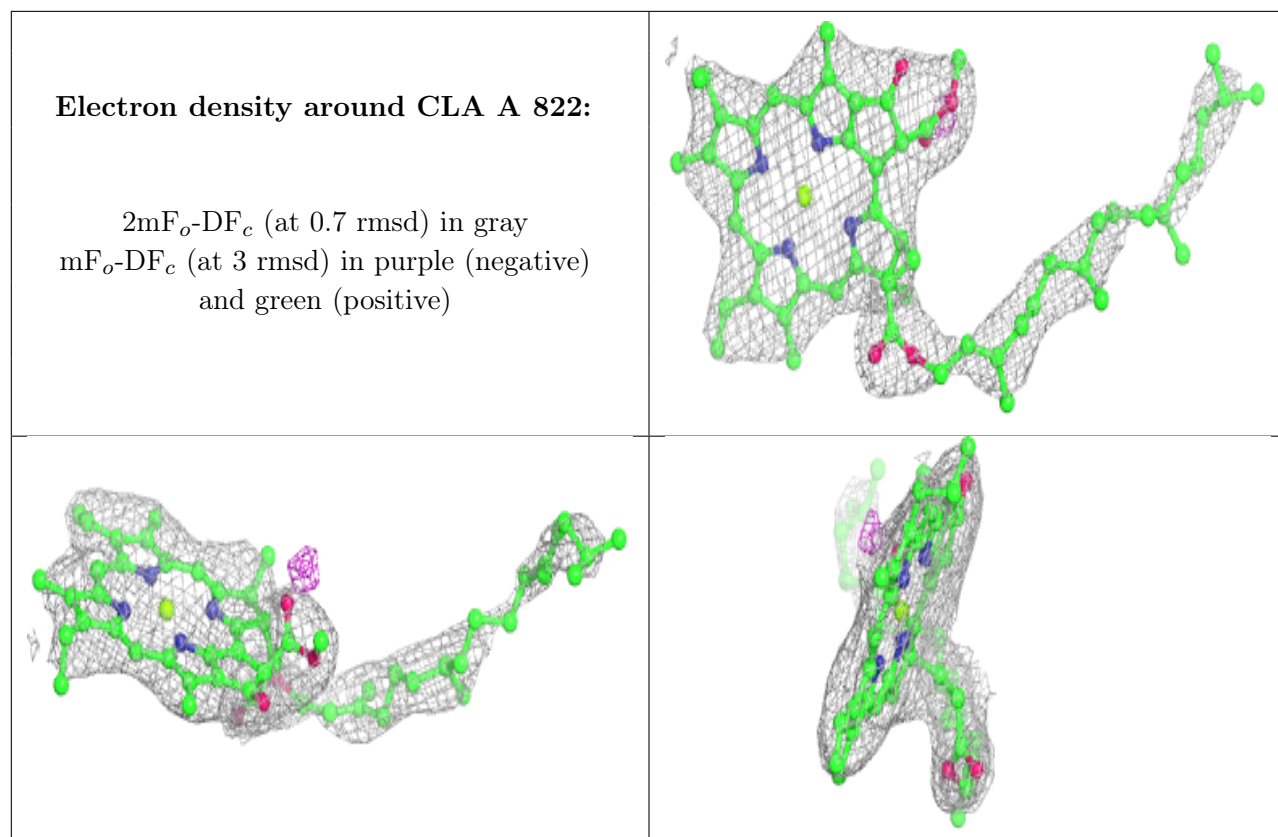
**Electron density around CLA A 820:**

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

**Electron density around CLA A 821:**

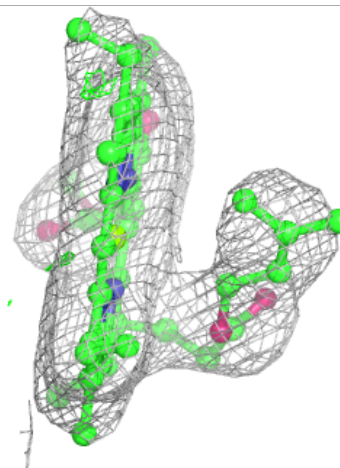
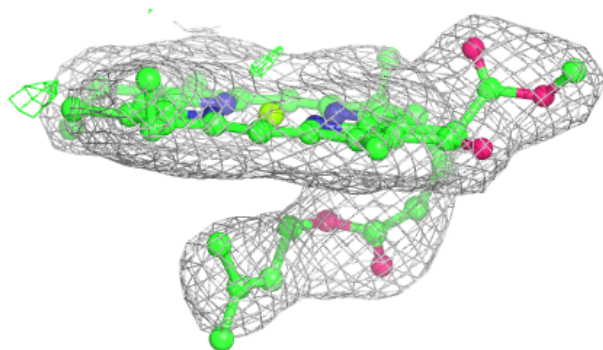
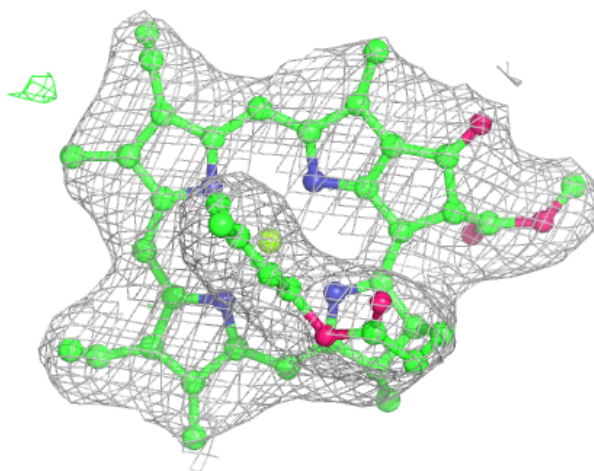
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA A 823:**

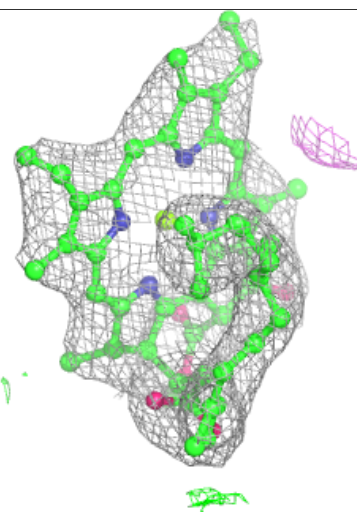
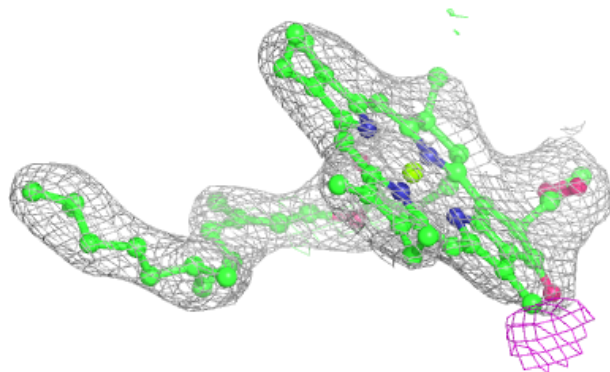
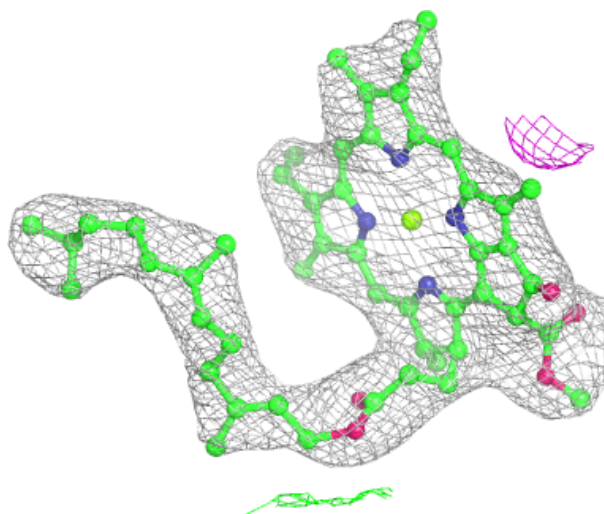
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





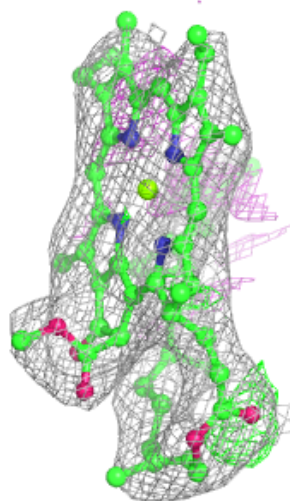
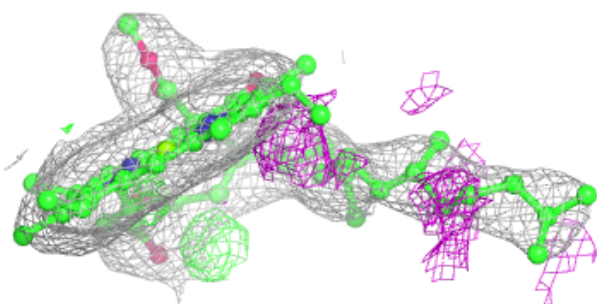
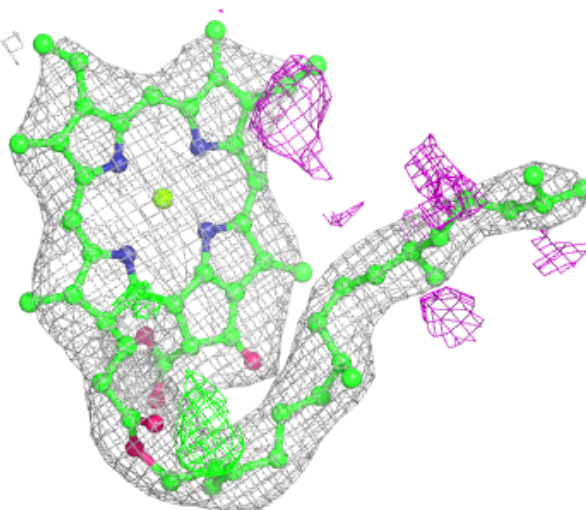
**Electron density around CLA A 824:**

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



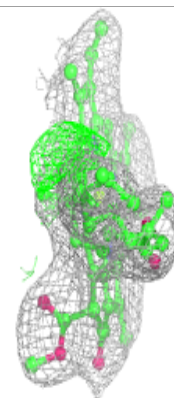
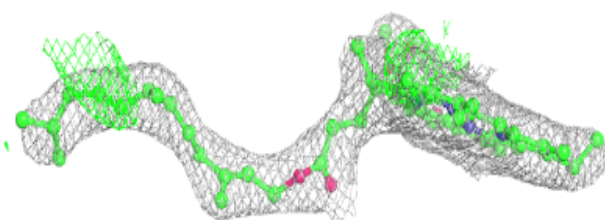
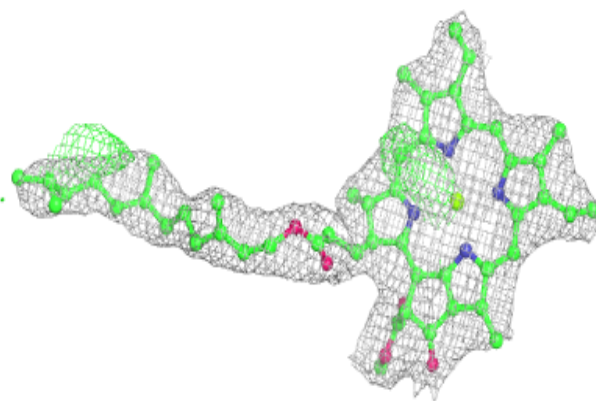
**Electron density around CLA A 825:**

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

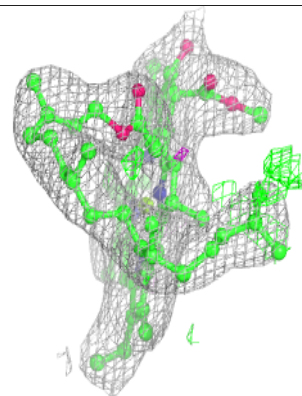
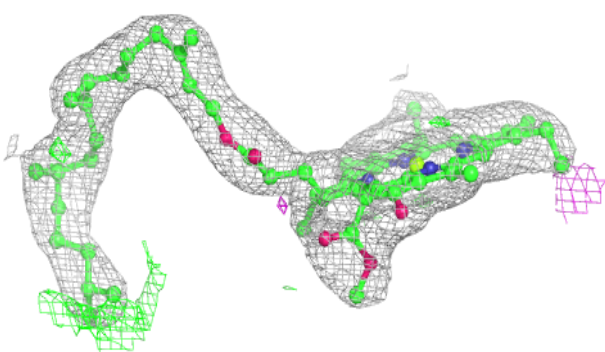
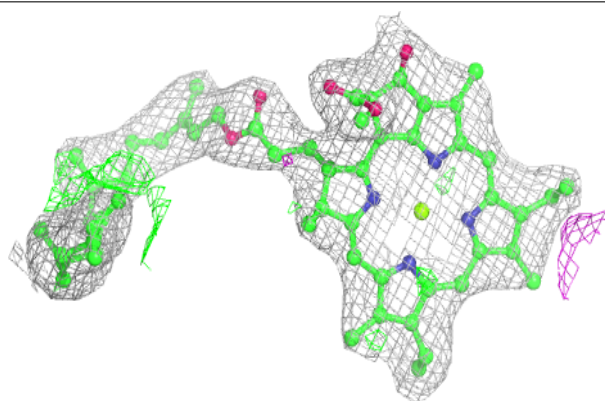


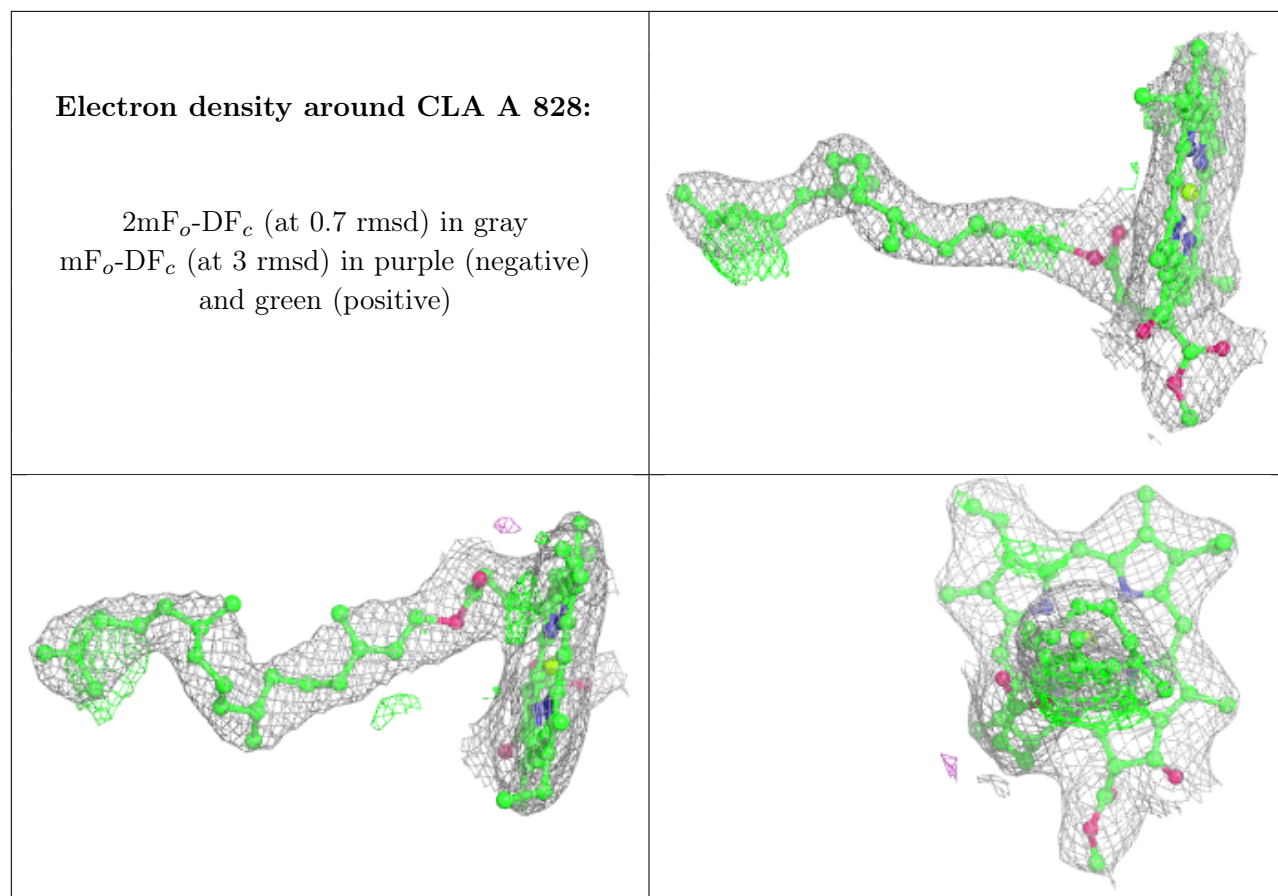
**Electron density around CLA A 826:**

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

**Electron density around CLA A 827:**

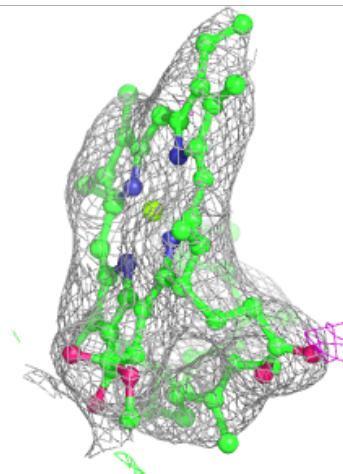
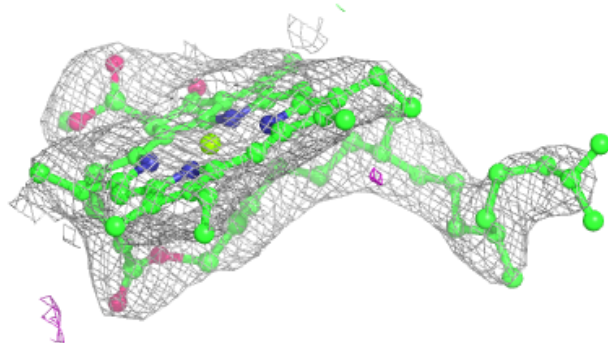
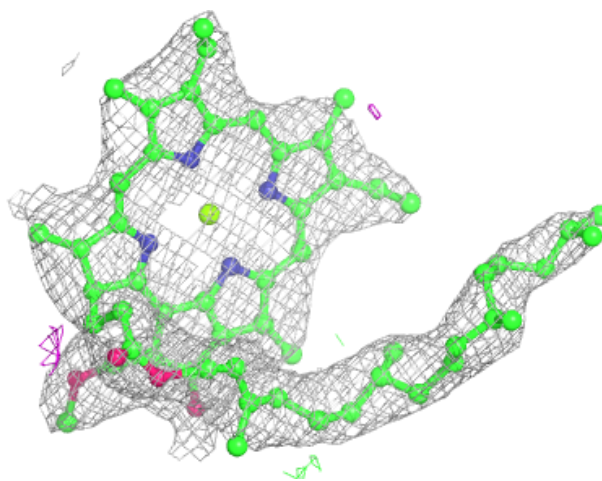
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

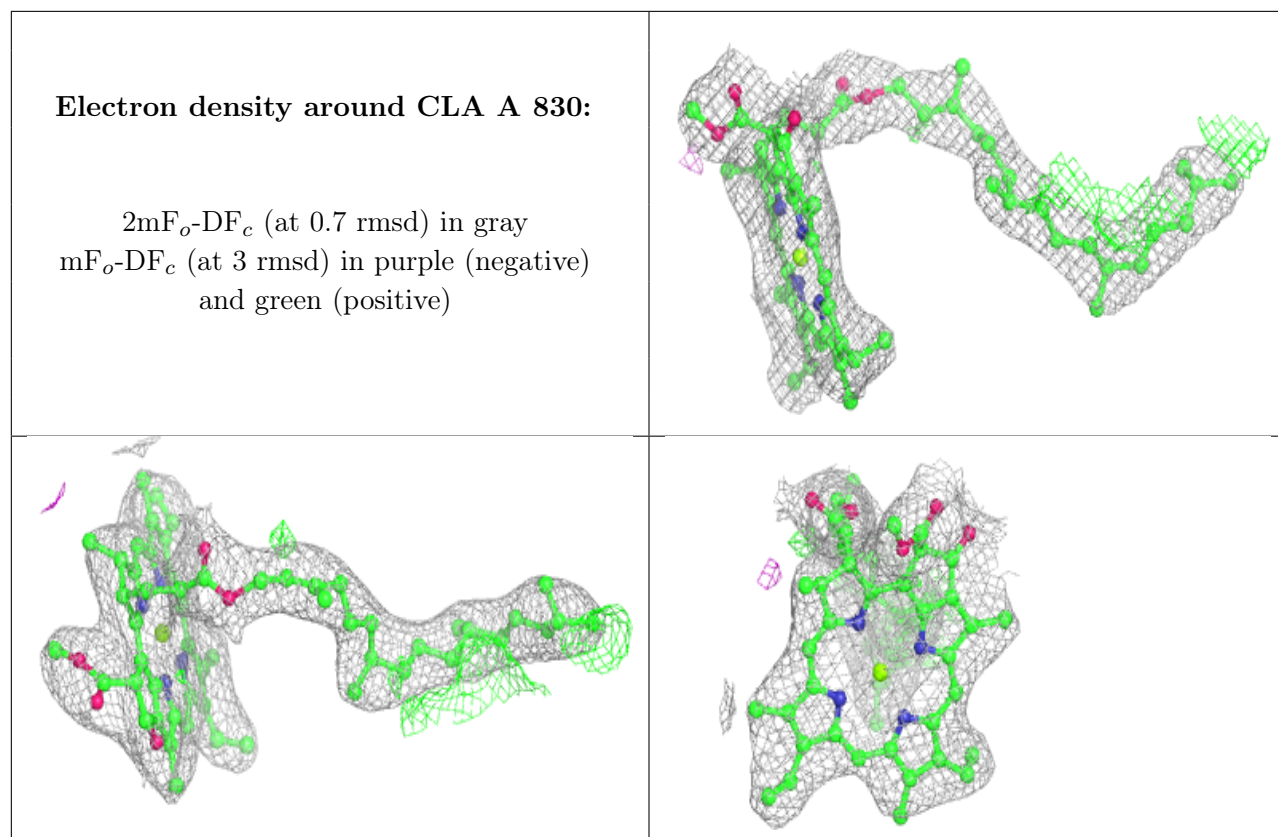




**Electron density around CLA A 829:**

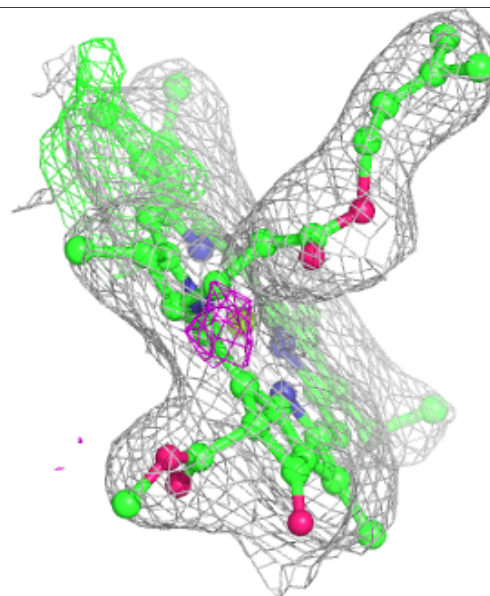
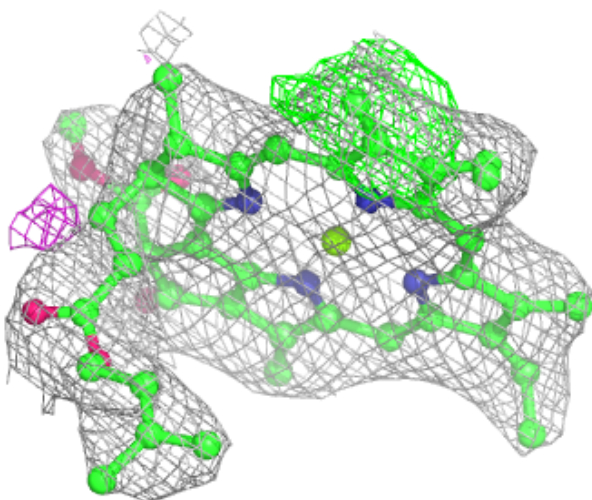
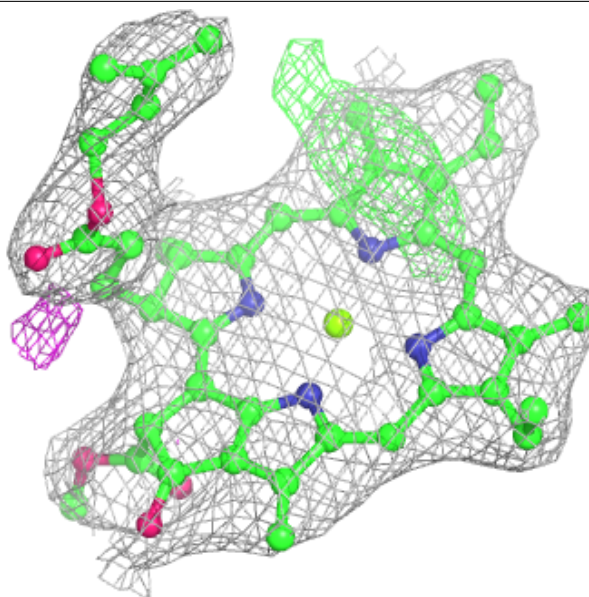
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





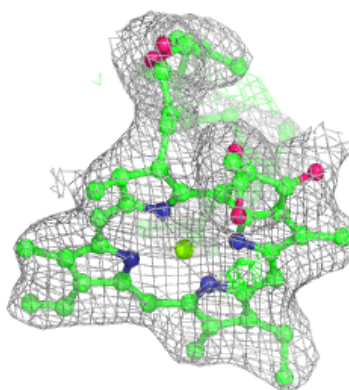
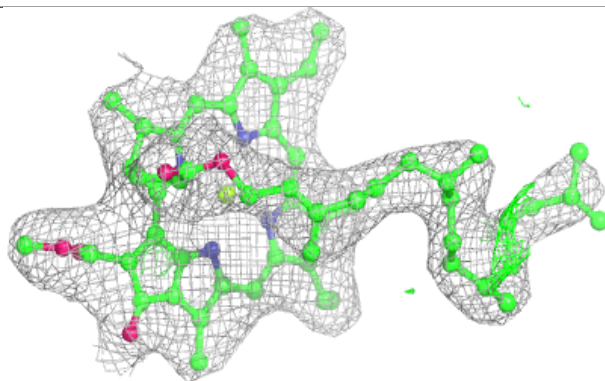
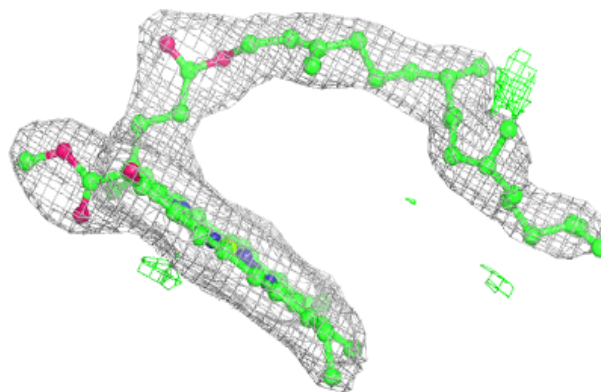
**Electron density around CLA A 831:**

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

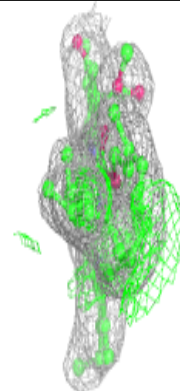
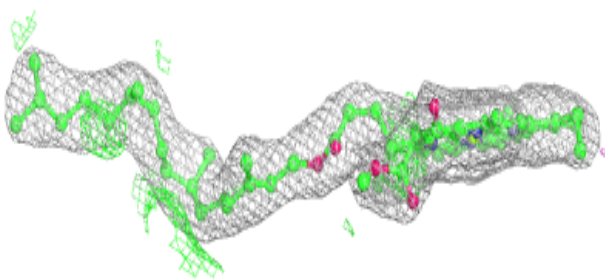
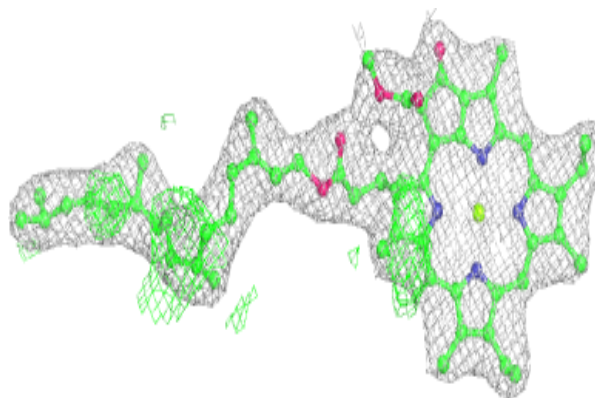


**Electron density around CLA A 832:**

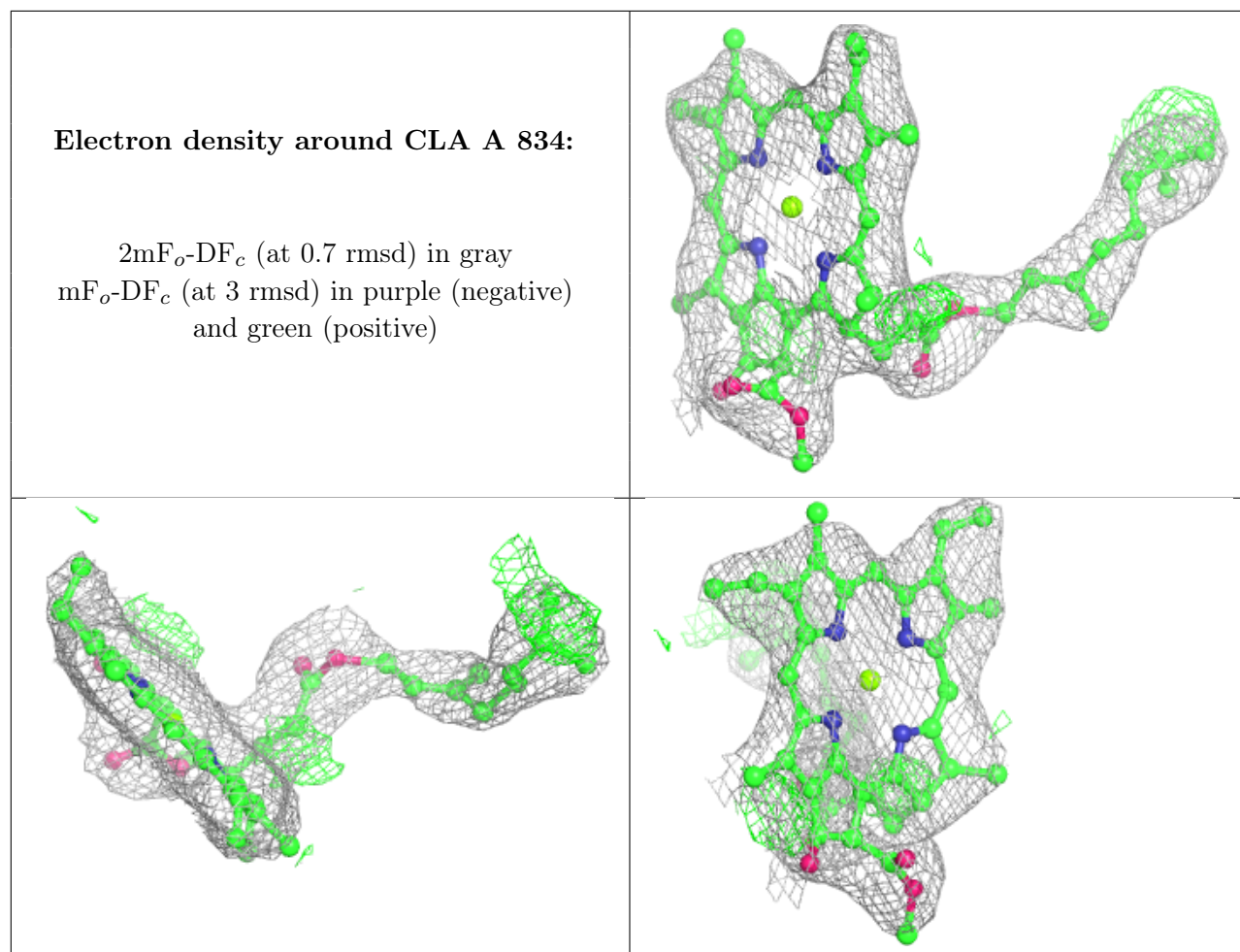
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA A 833:**

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

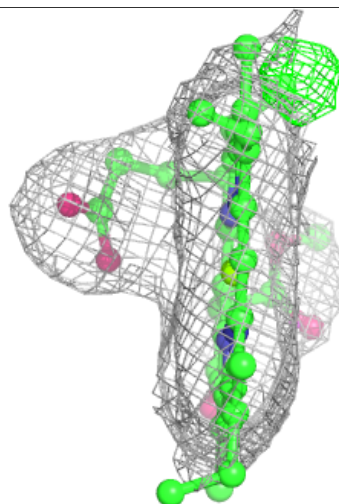
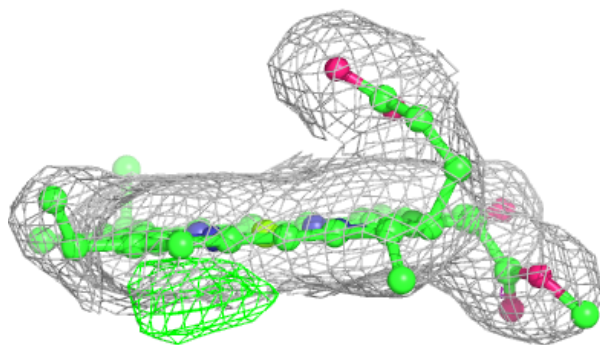
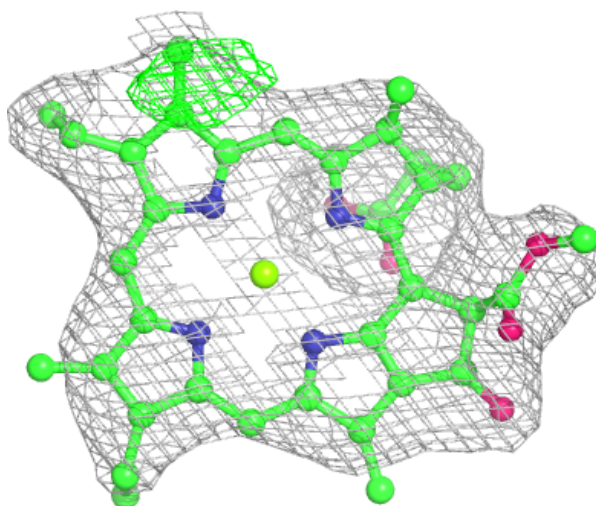






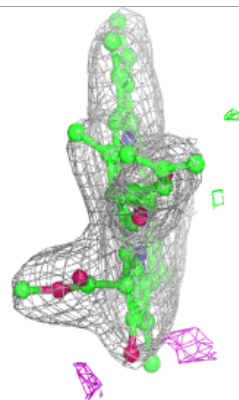
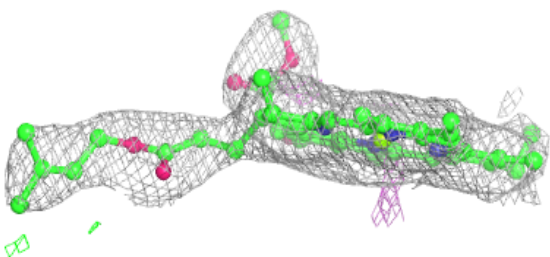
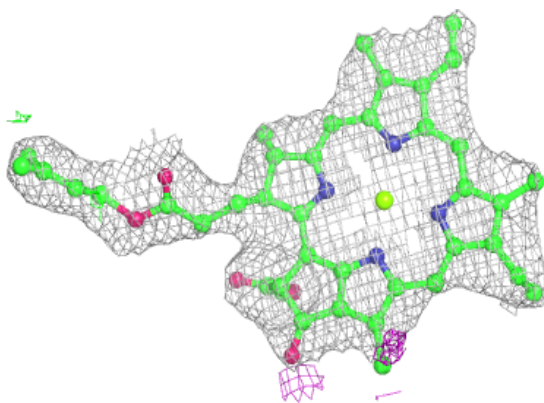
**Electron density around CLA A 835:**

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

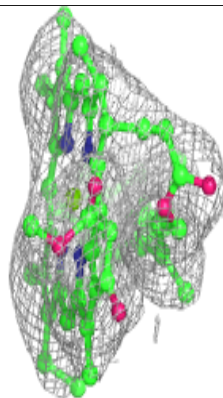
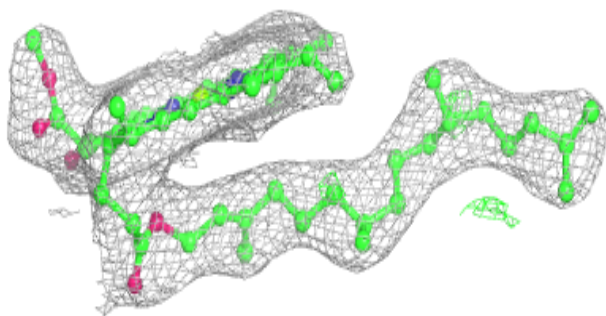
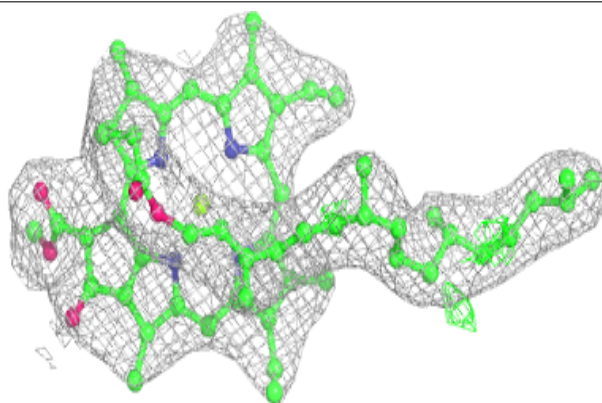


**Electron density around CLA A 836:**

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

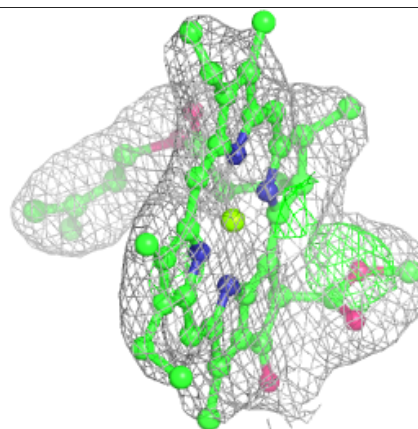
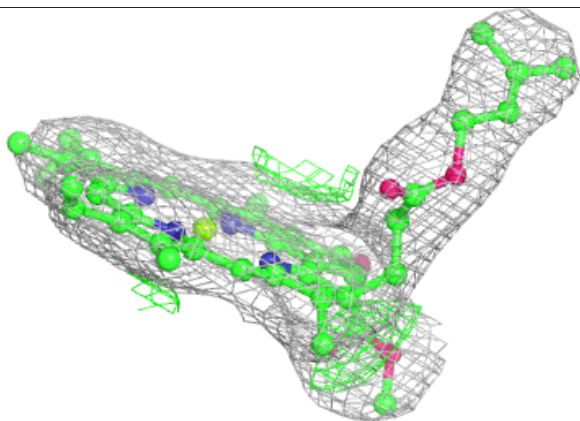
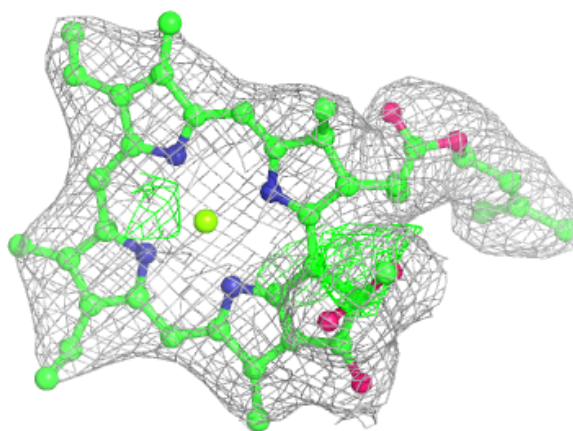
**Electron density around CLA A 837:**

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

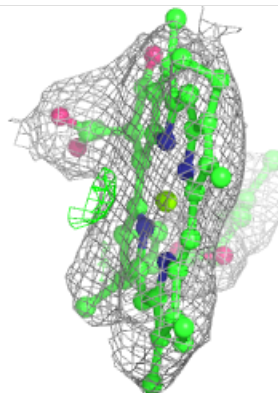
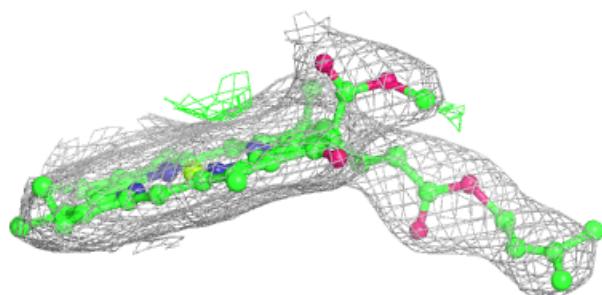
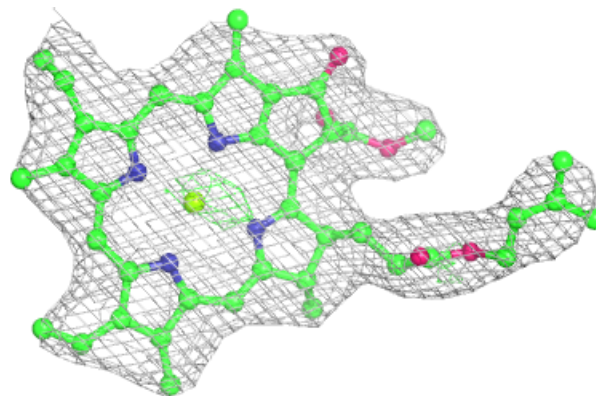


**Electron density around CLA A 838:**

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

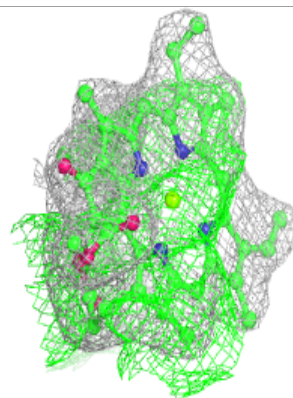
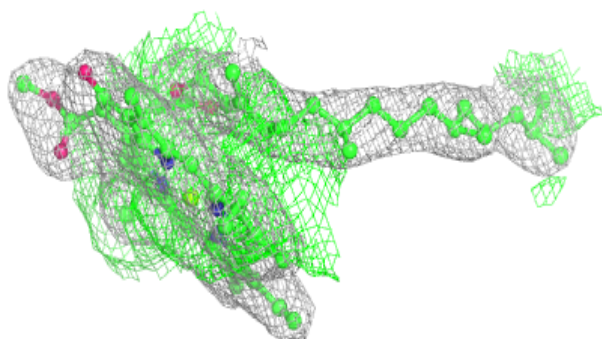
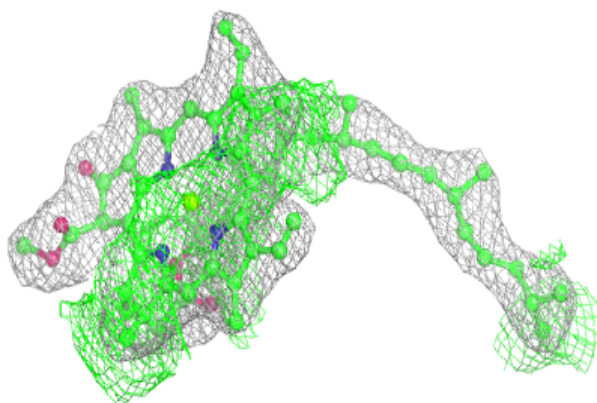
**Electron density around CLA A 839:**

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

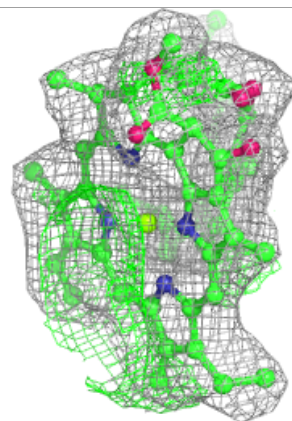
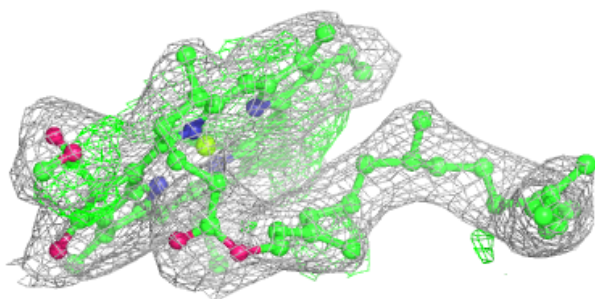
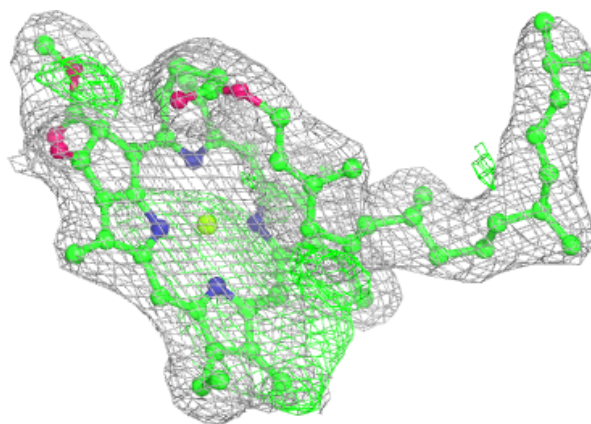


**Electron density around CLA A 840:**

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

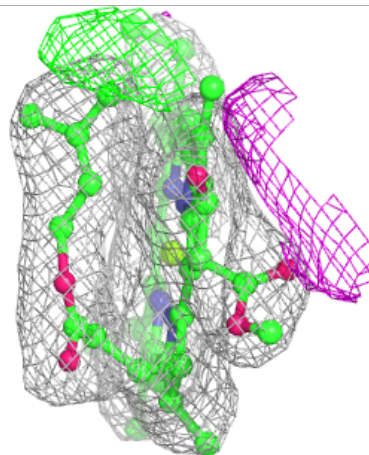
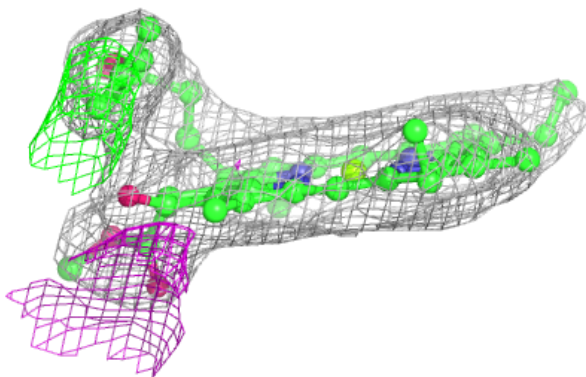
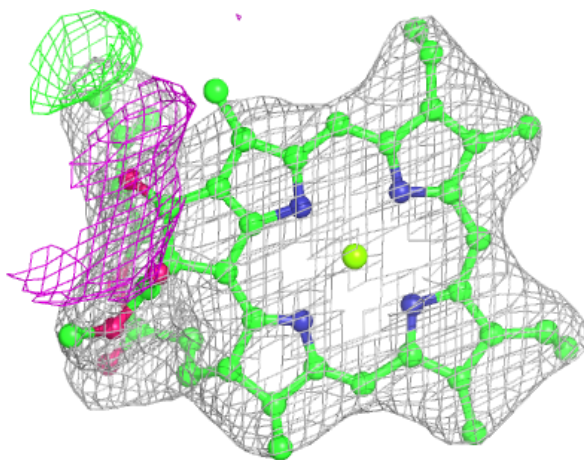
**Electron density around CLA A 841:**

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



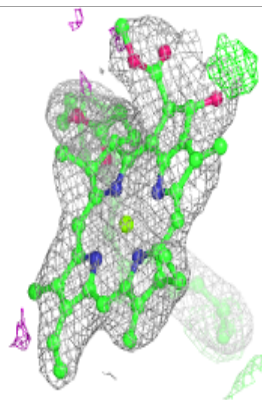
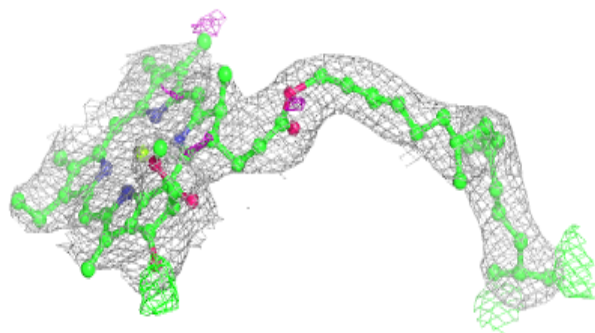
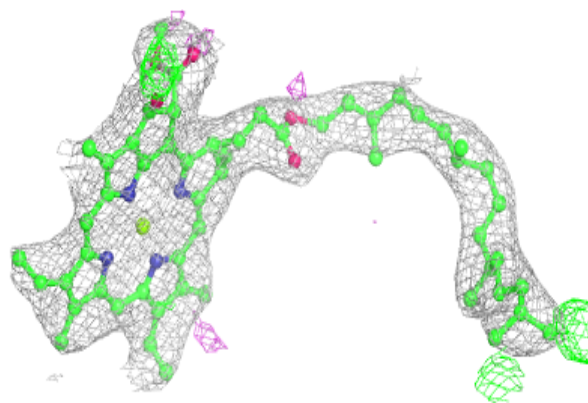
**Electron density around CLA A 842:**

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

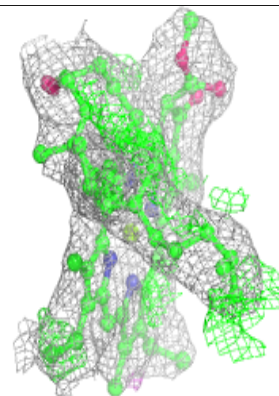
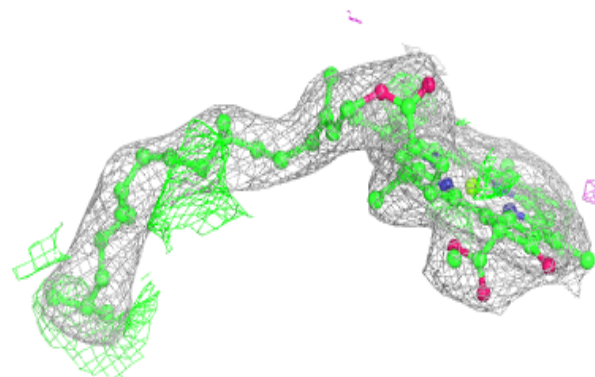
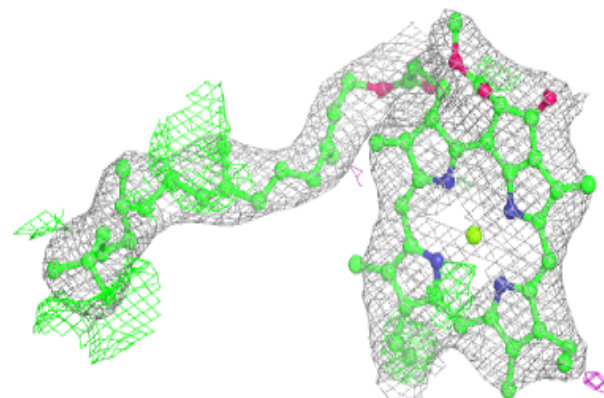


**Electron density around CLA A 852:**

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

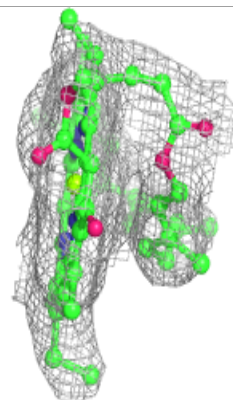
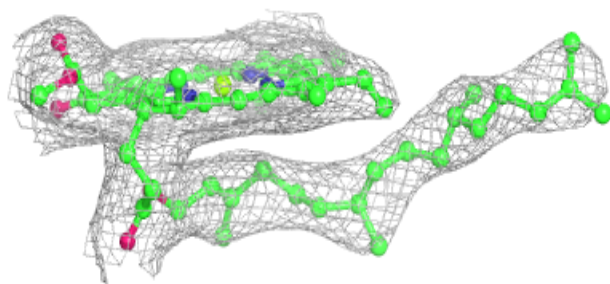
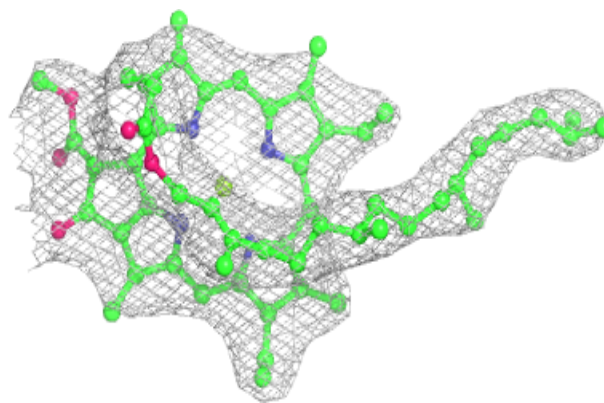
**Electron density around CLA B 801:**

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

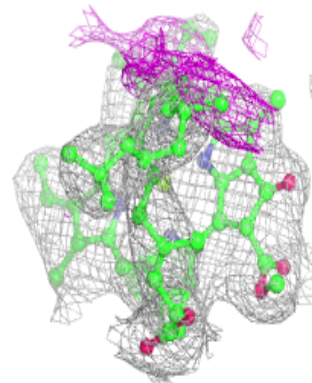
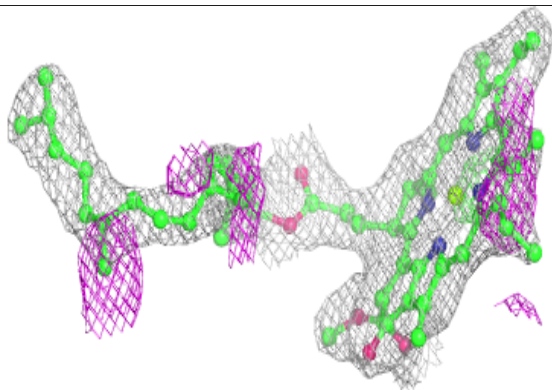
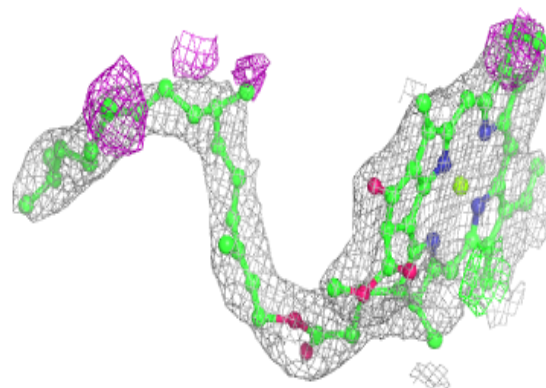


**Electron density around CLA B 802:**

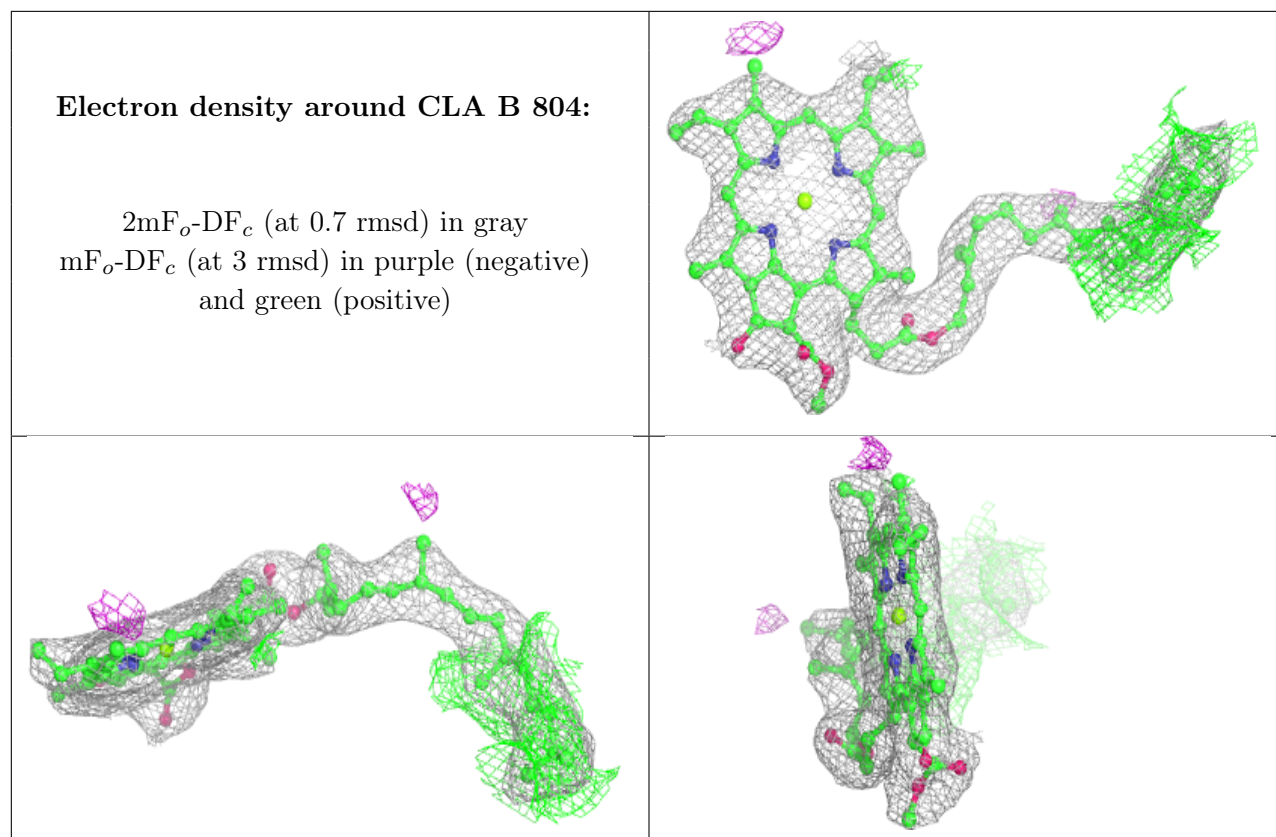
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**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)

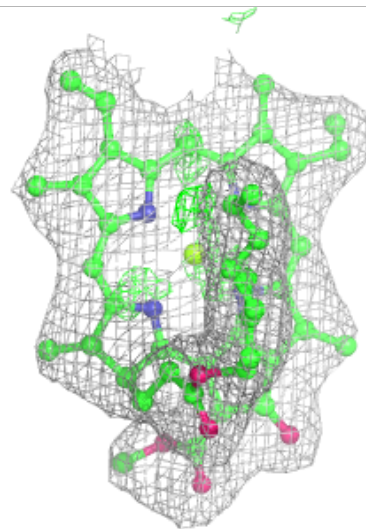
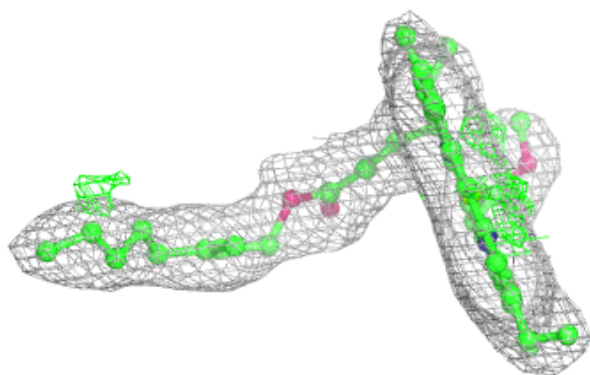
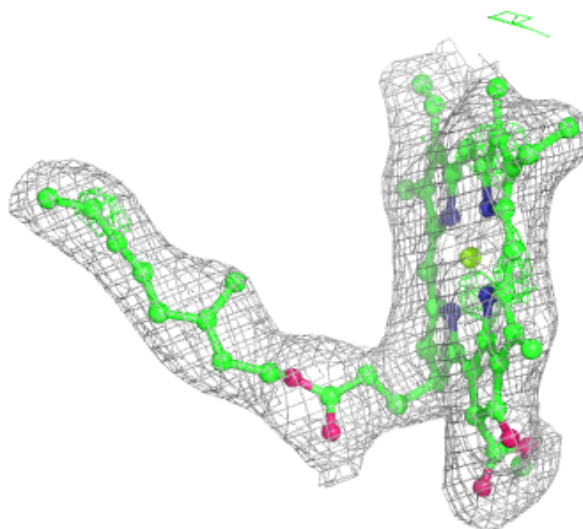






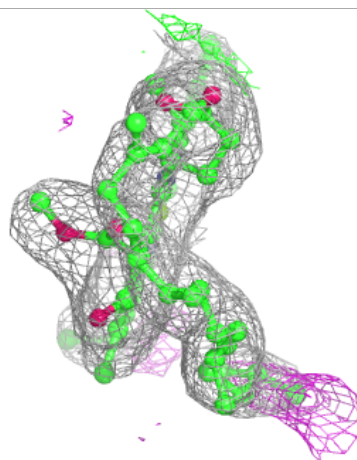
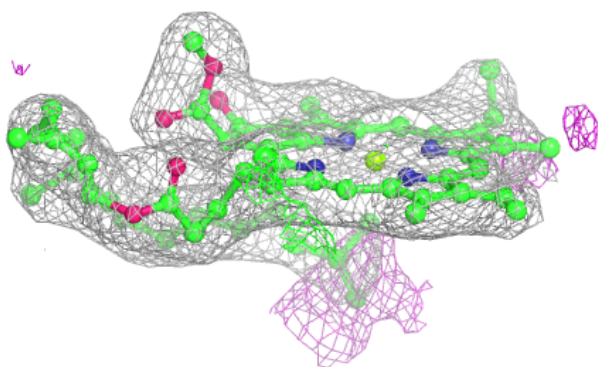
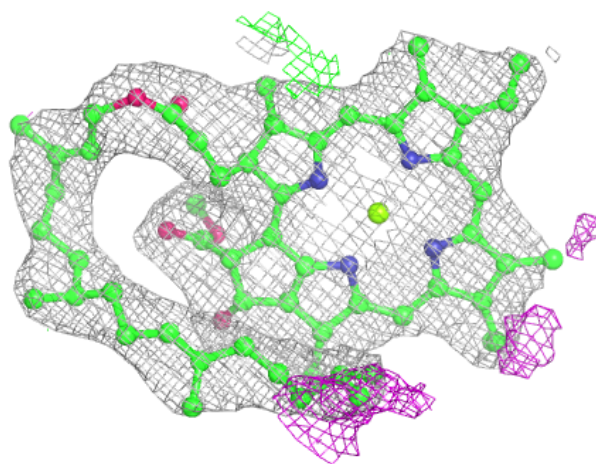
**Electron density around CLA B 805:**

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



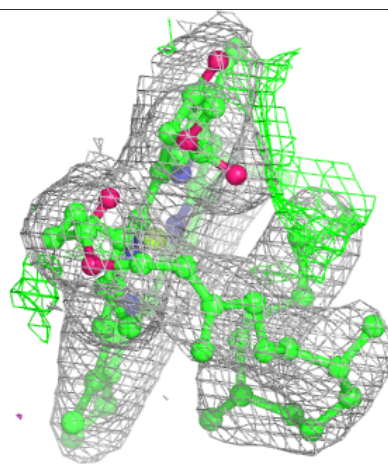
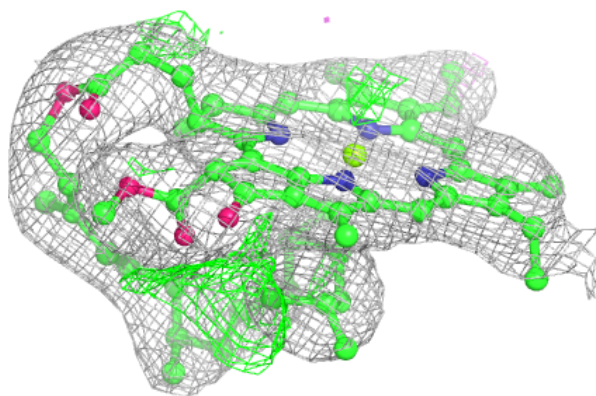
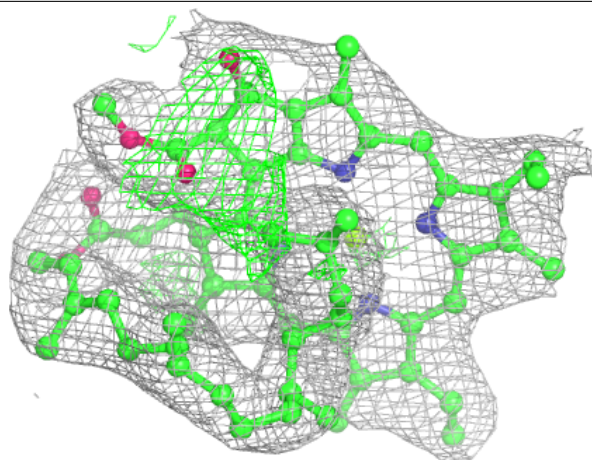
**Electron density around CLA B 806:**

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



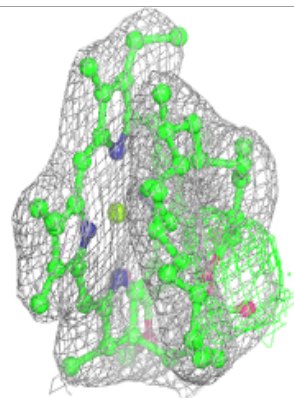
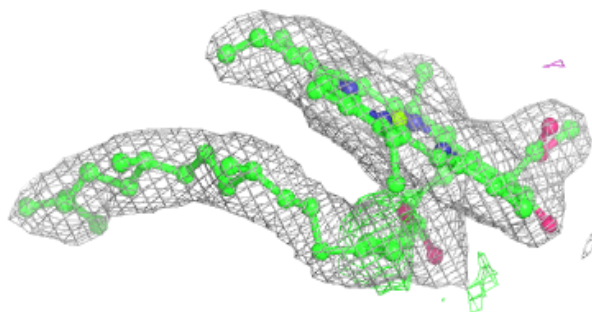
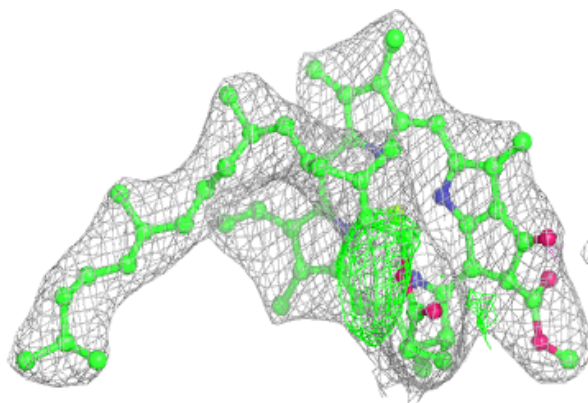
**Electron density around CLA B 807:**

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



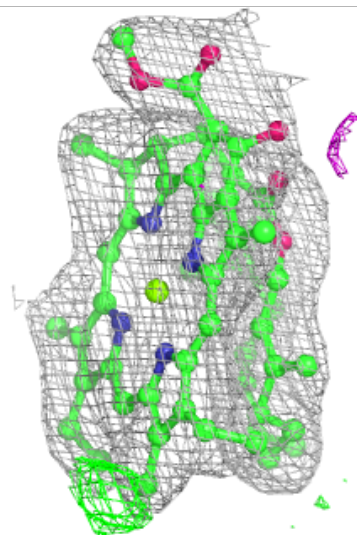
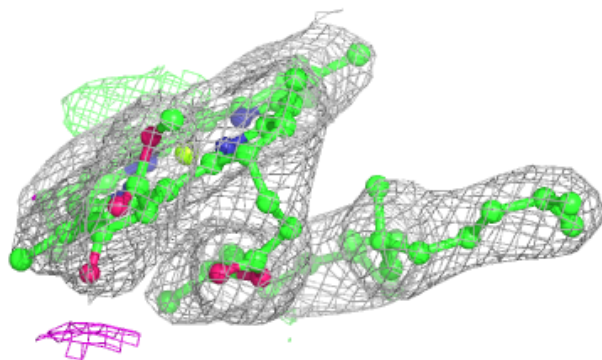
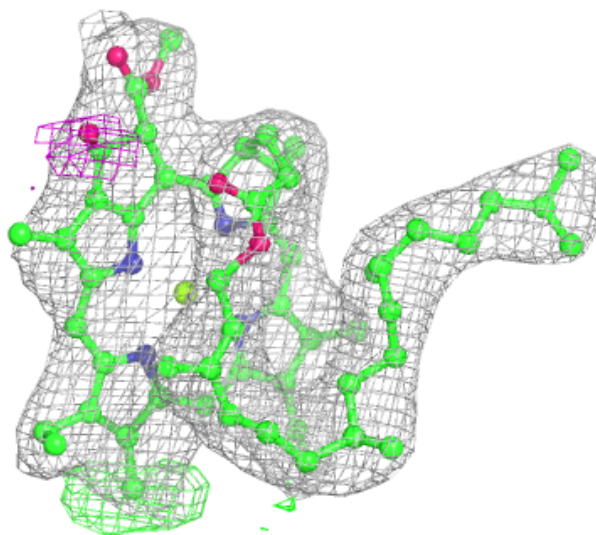
**Electron density around CLA B 808:**

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



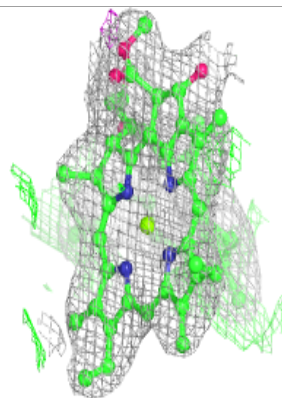
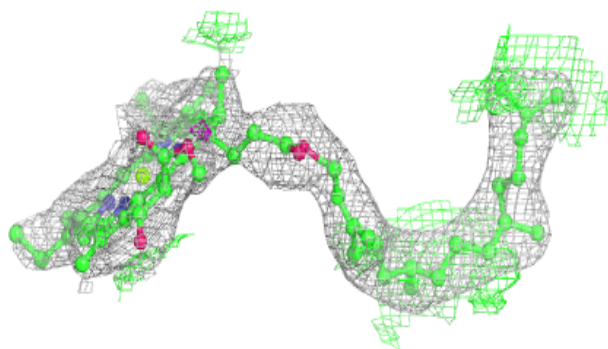
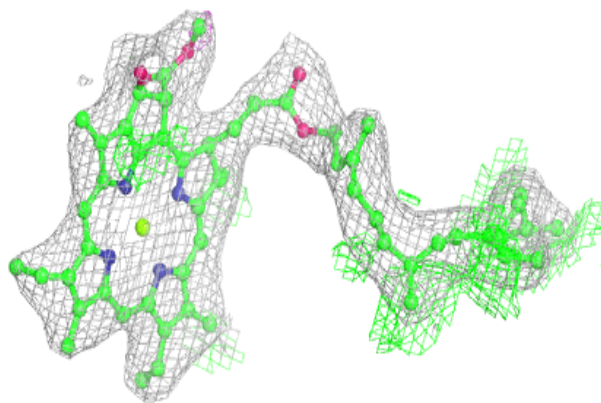
**Electron density around CLA B 809:**

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



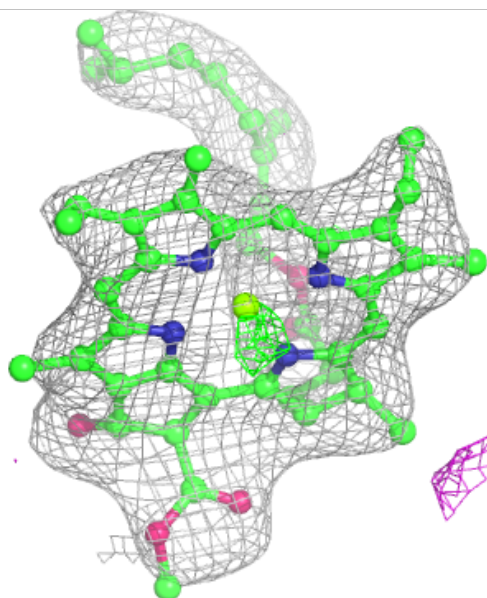
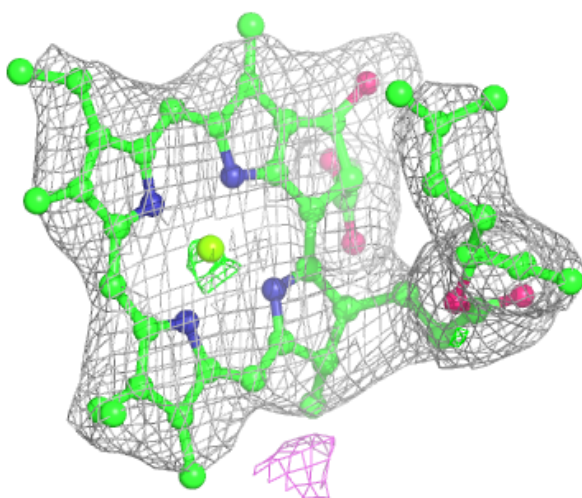
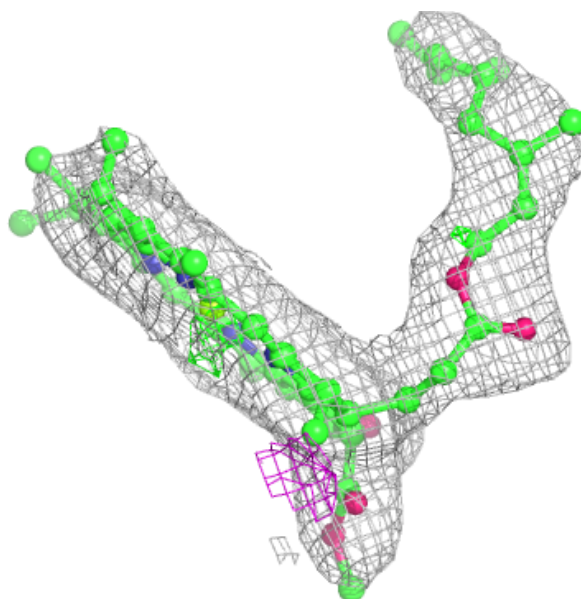
**Electron density around CLA B 810:**

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



**Electron density around CLA B 811:**

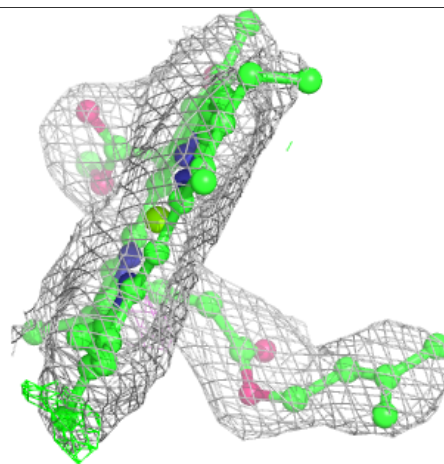
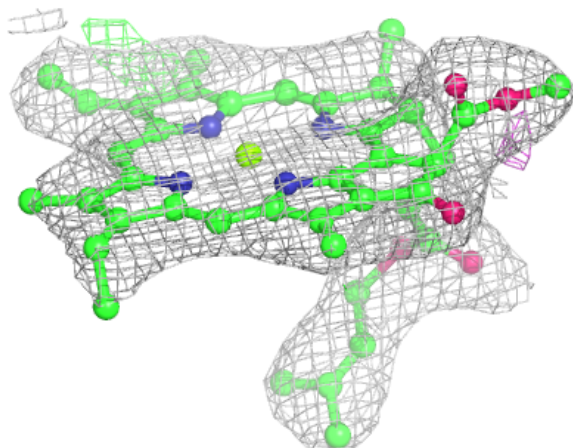
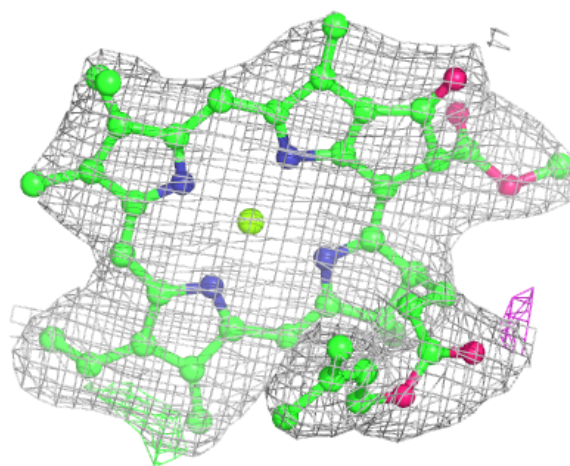
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





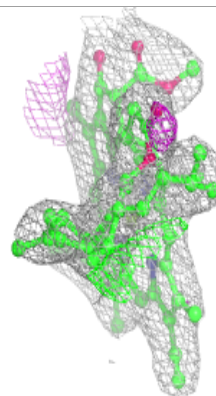
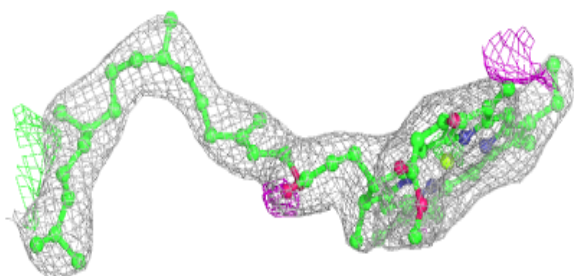
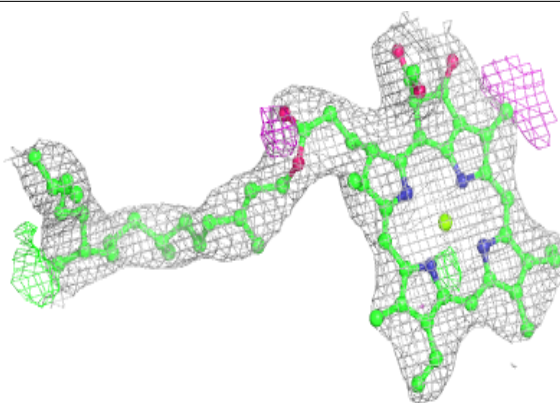
**Electron density around CLA B 812:**

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

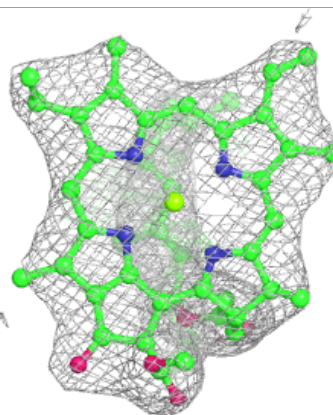
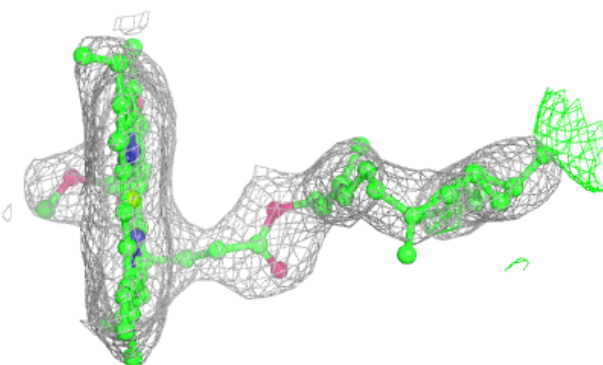
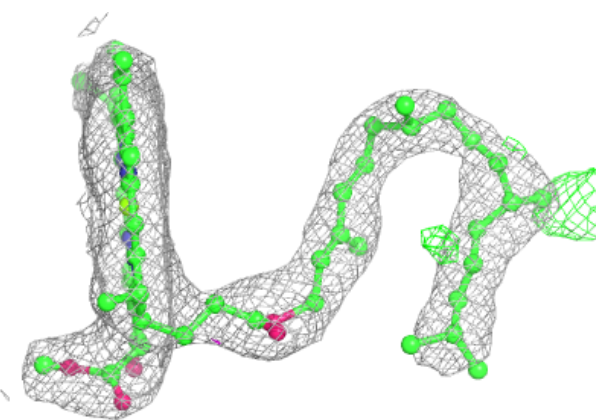


**Electron density around CLA B 813:**

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

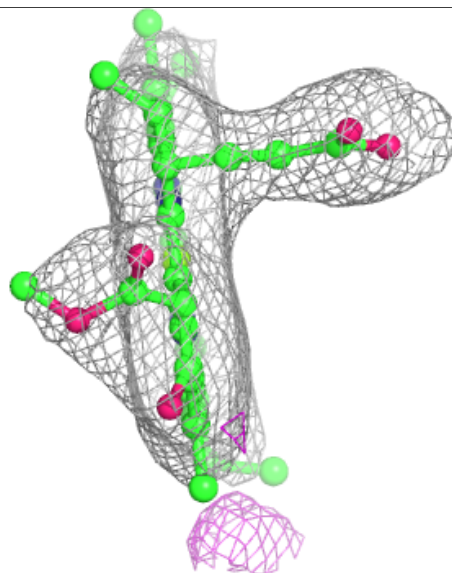
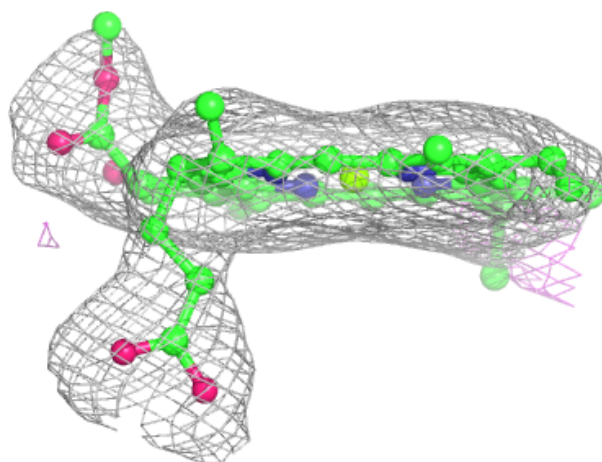
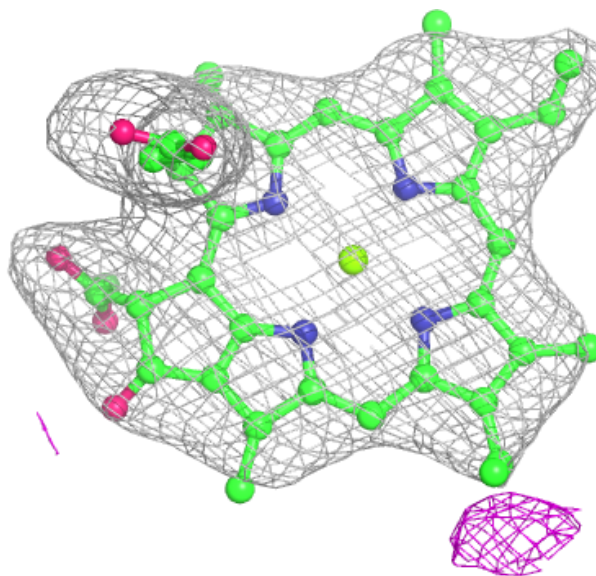
**Electron density around CLA B 814:**

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



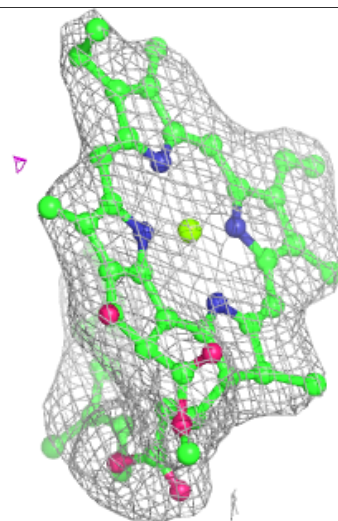
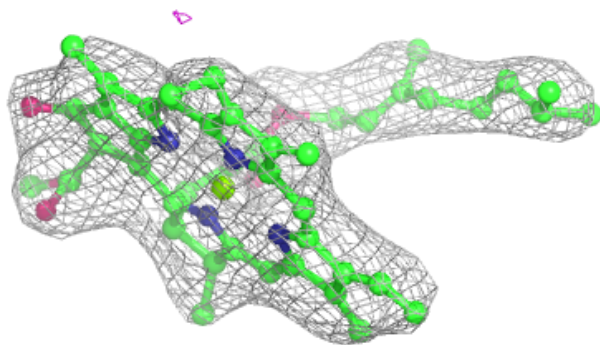
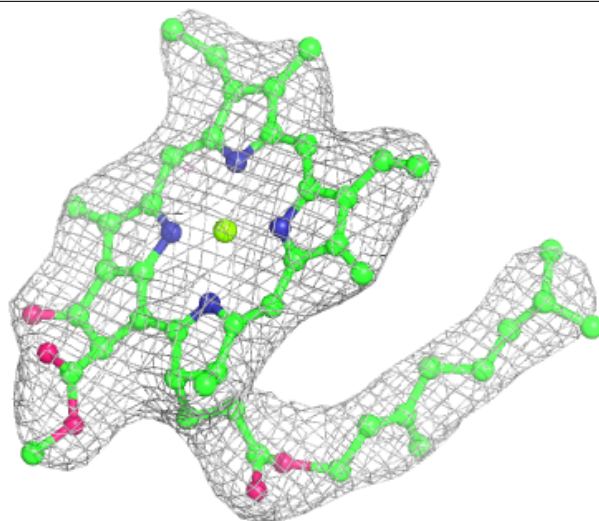
**Electron density around CLA B 815:**

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



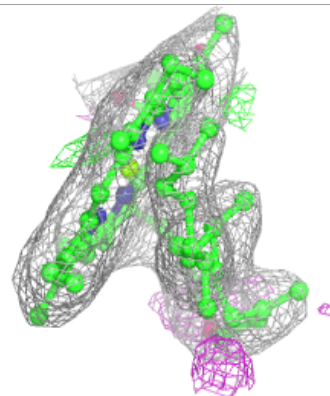
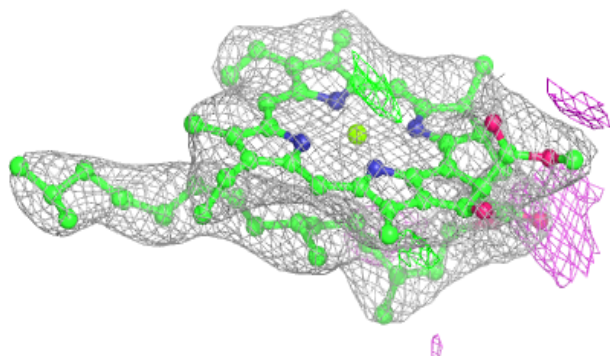
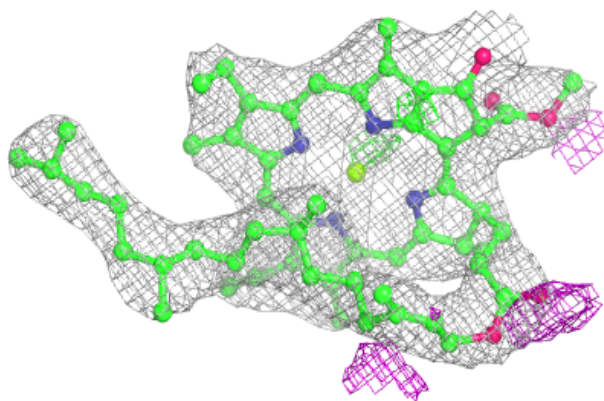
**Electron density around CLA B 816:**

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

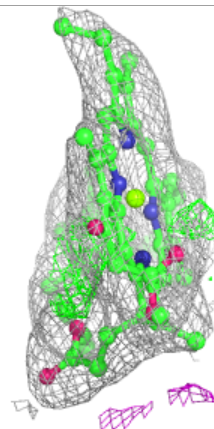
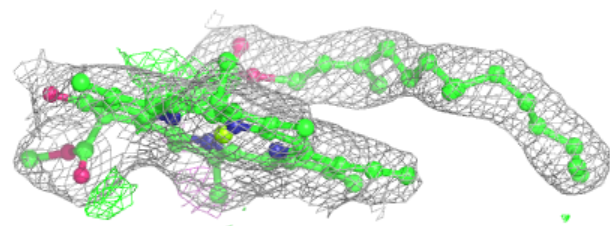
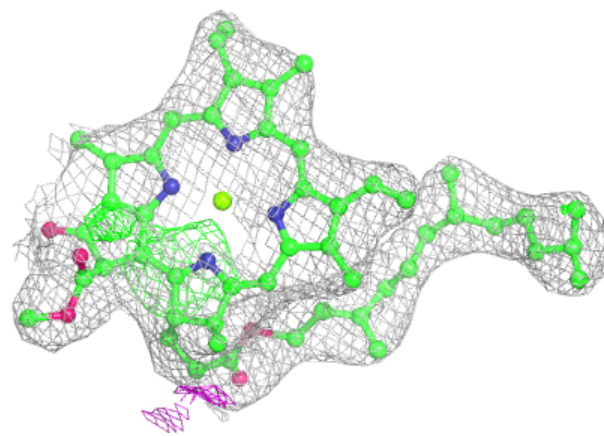


**Electron density around CLA B 817:**

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

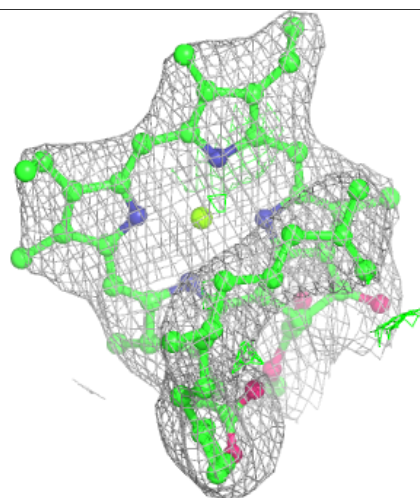
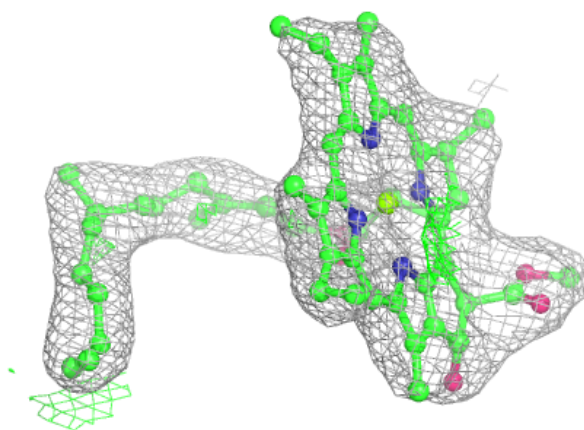
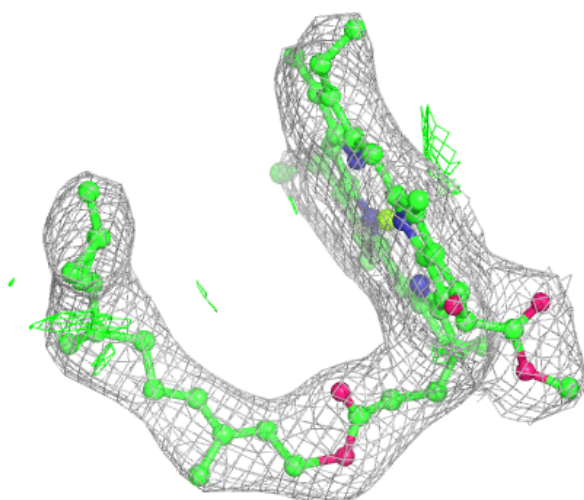
**Electron density around CLA B 818:**

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



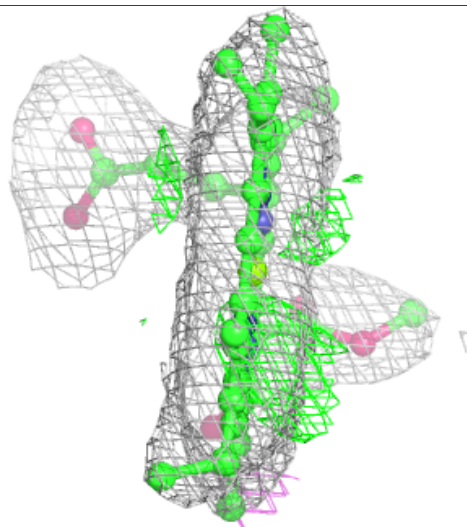
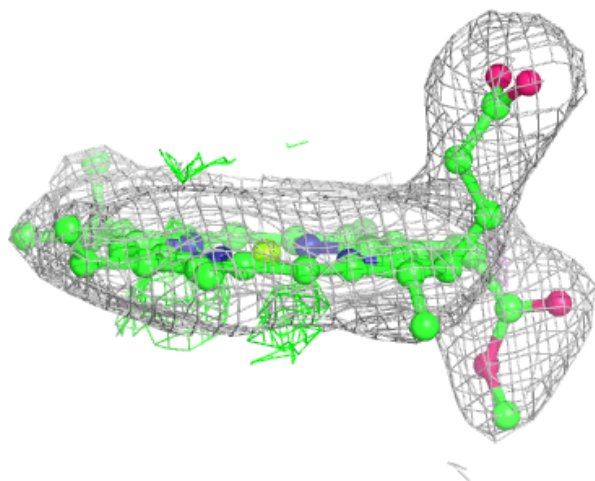
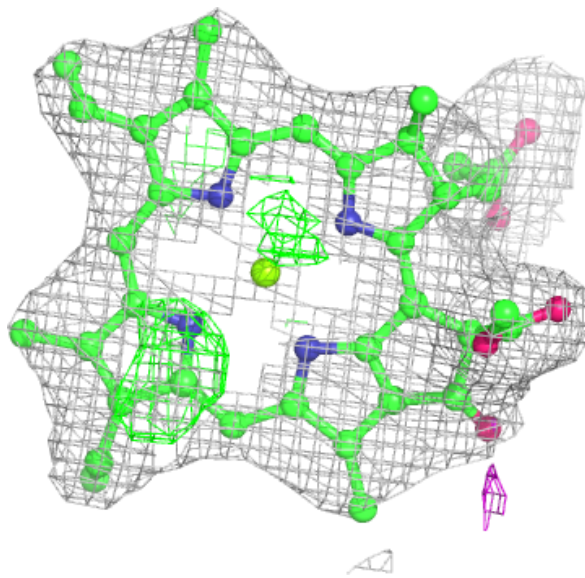
**Electron density around CLA B 819:**

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



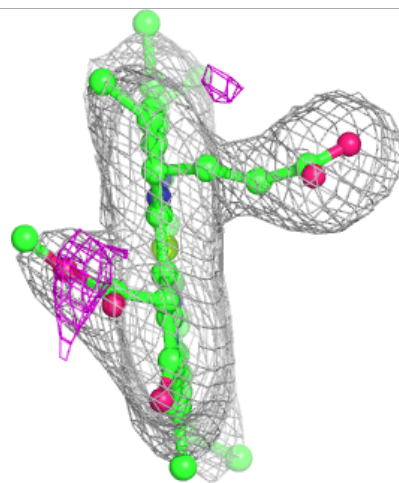
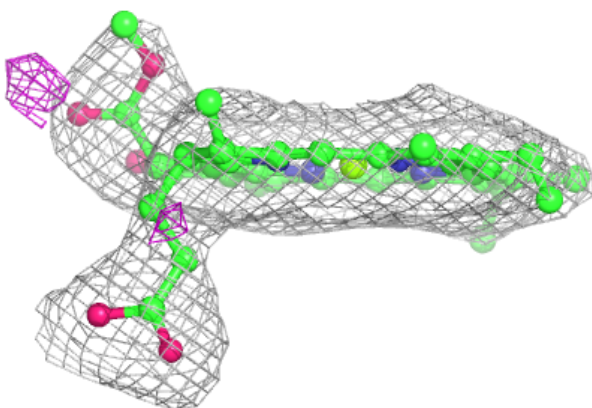
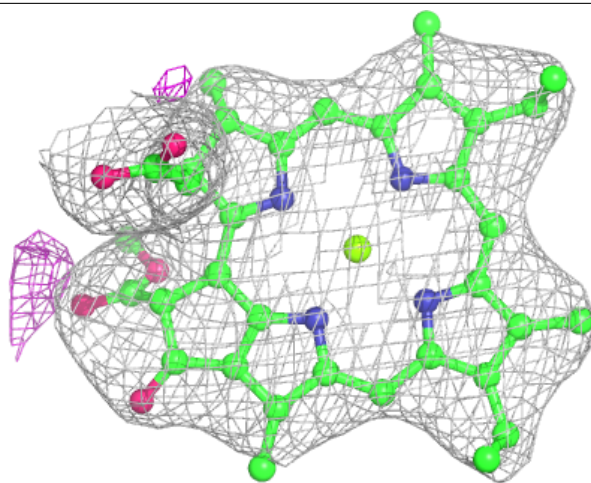
**Electron density around CLA B 820:**

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



**Electron density around CLA B 821:**

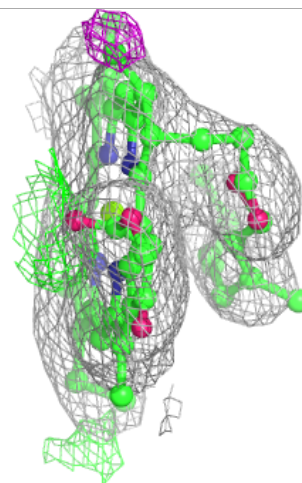
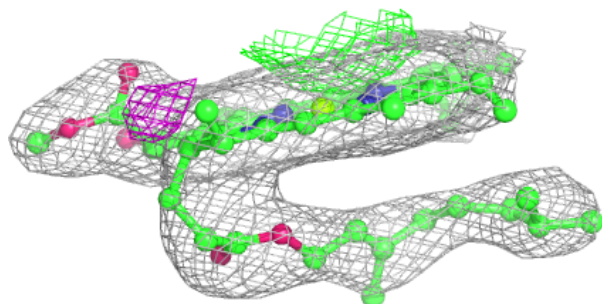
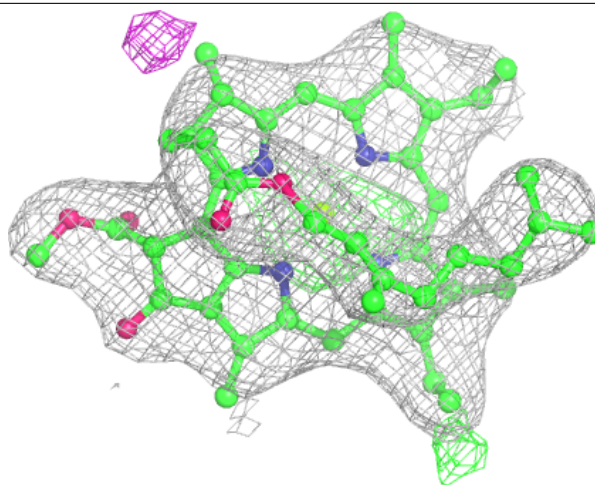
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





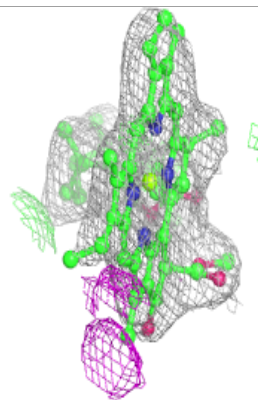
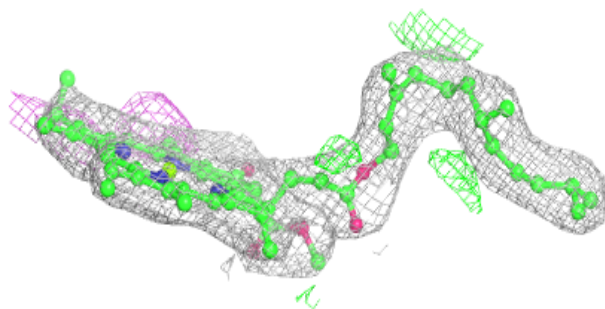
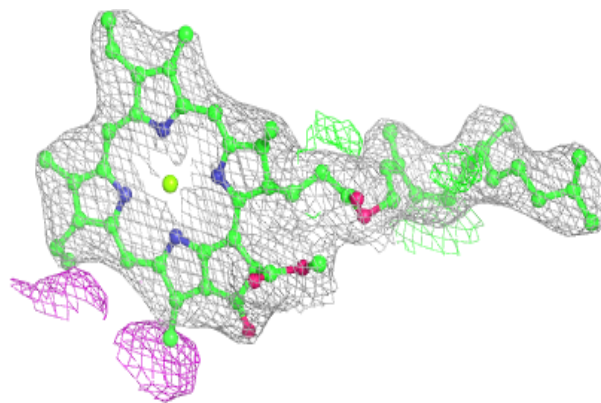
**Electron density around CLA B 822:**

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



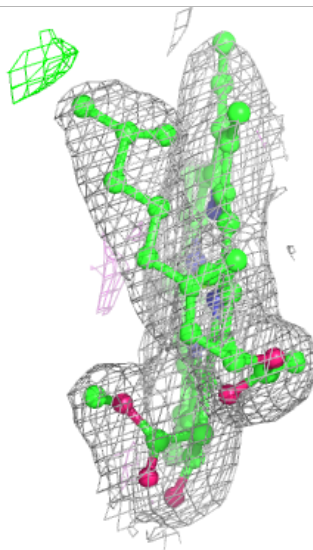
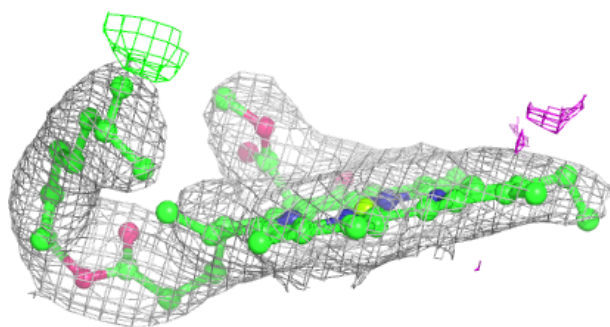
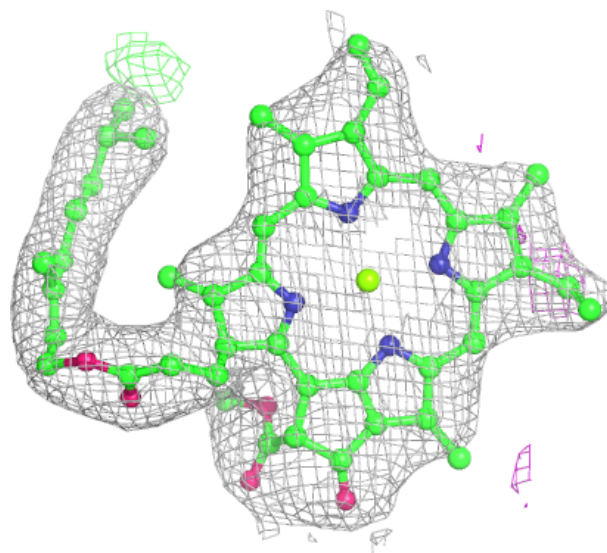
**Electron density around CLA B 823:**

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



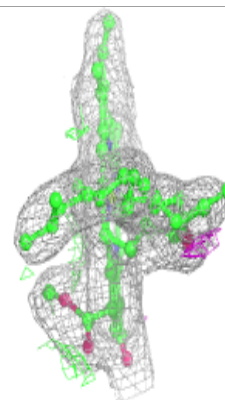
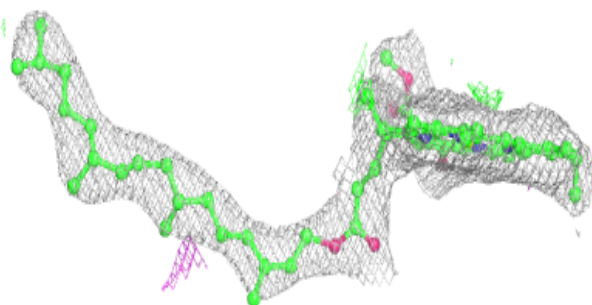
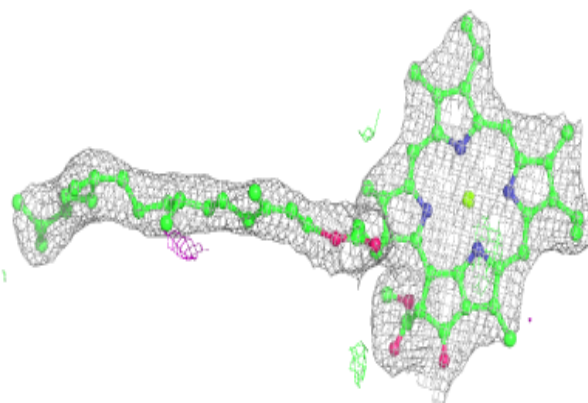
**Electron density around CLA B 824:**

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

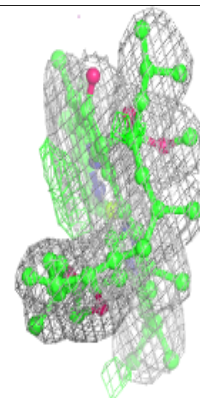
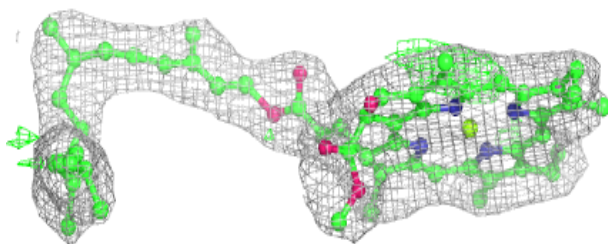
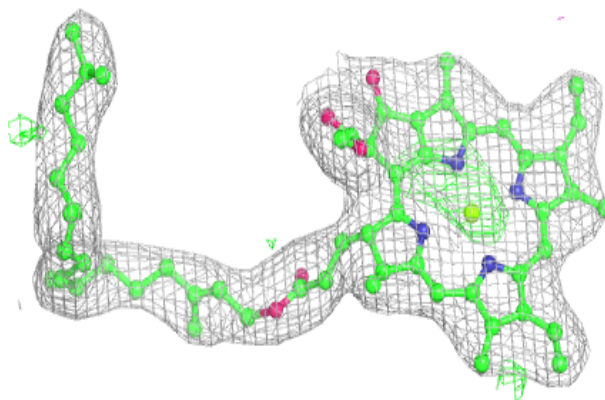


**Electron density around CLA B 825:**

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

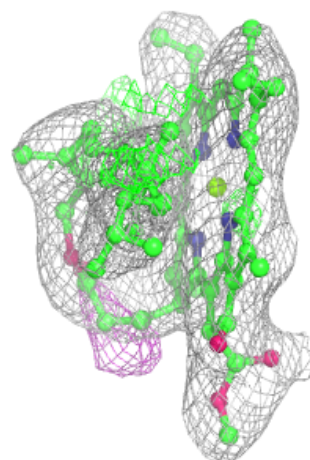
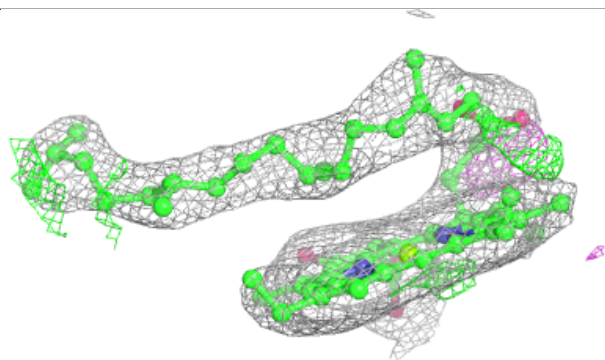
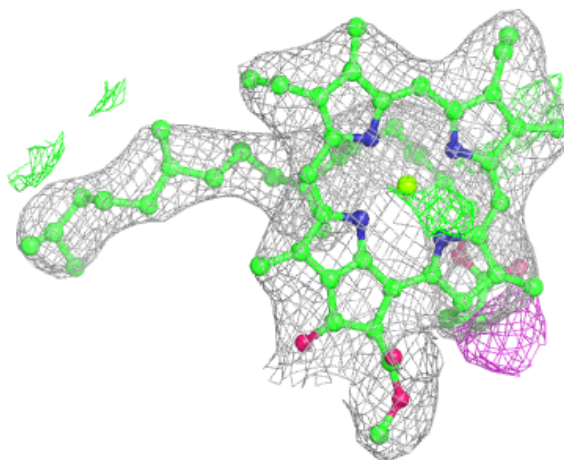
**Electron density around CLA B 826:**

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



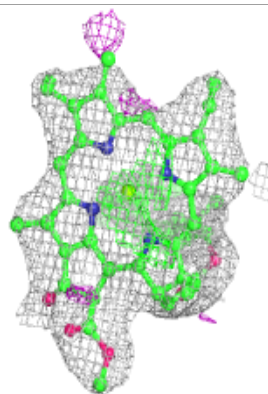
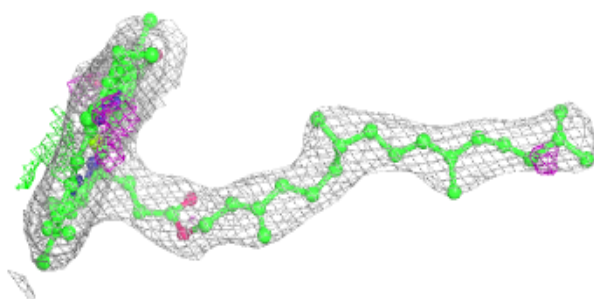
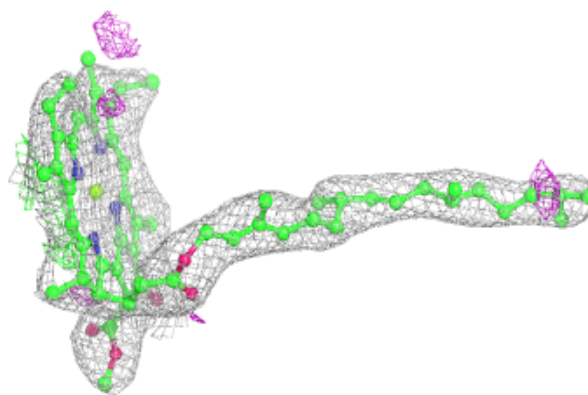
**Electron density around CLA B 827:**

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

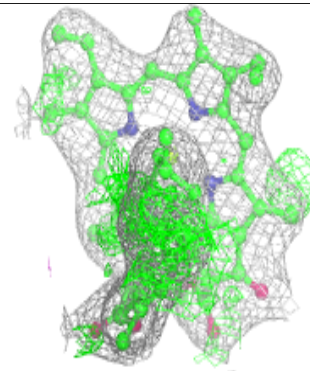
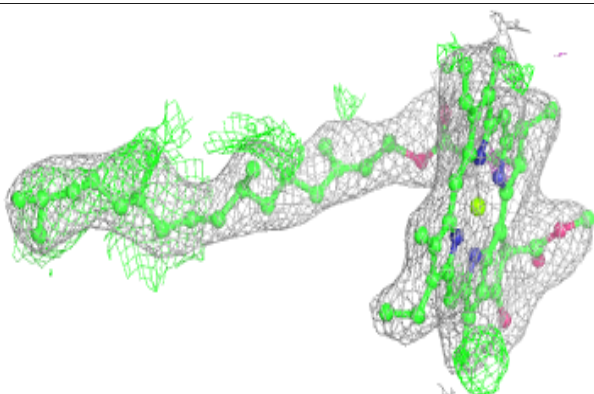
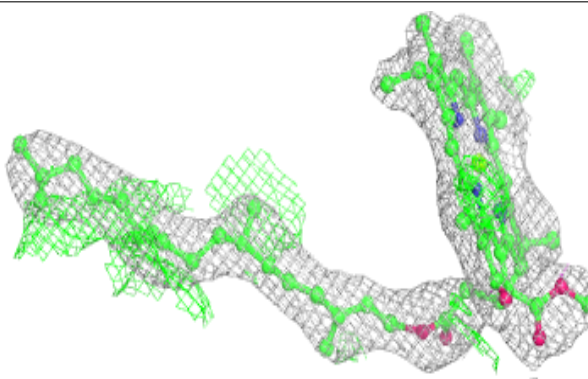


**Electron density around CLA B 828:**

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

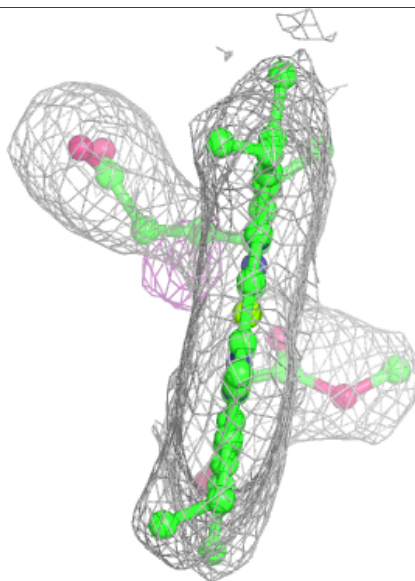
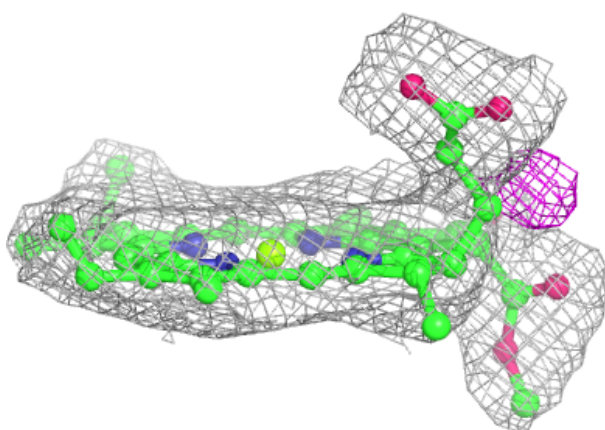
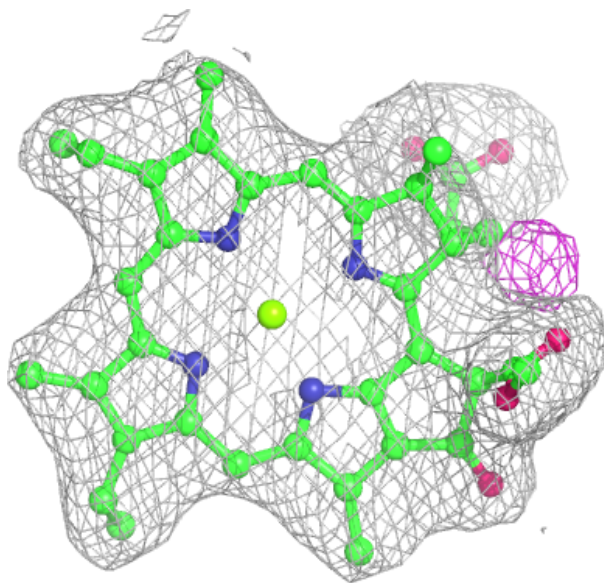
**Electron density around CLA B 829:**

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



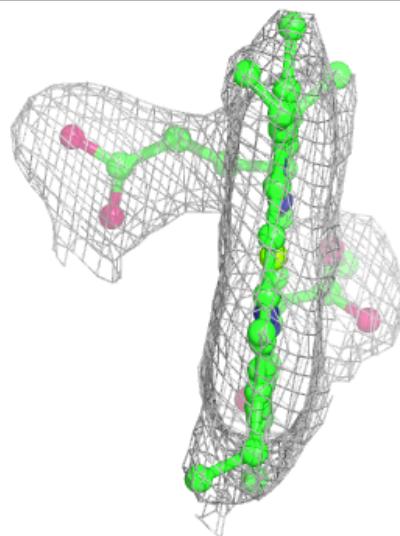
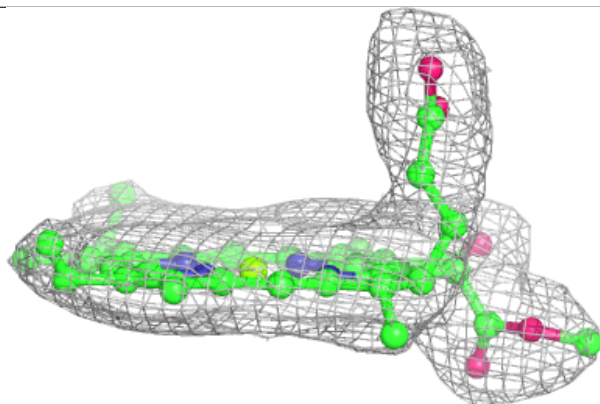
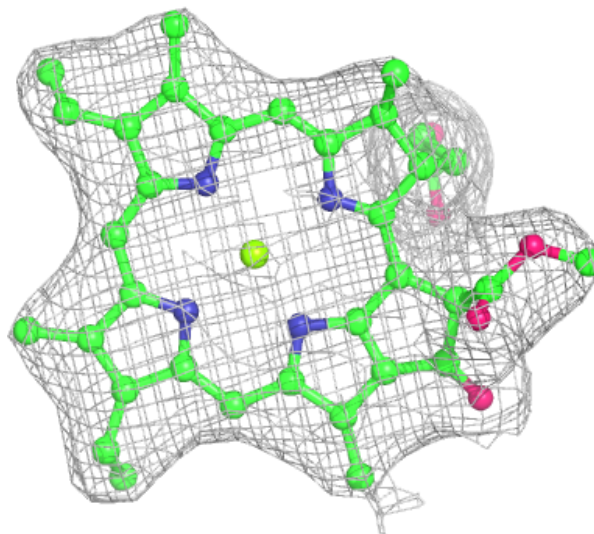
**Electron density around CLA B 830:**

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



**Electron density around CLA B 831:**

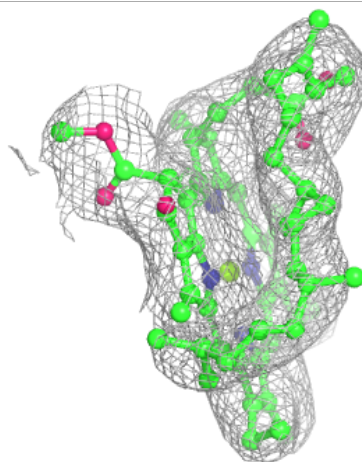
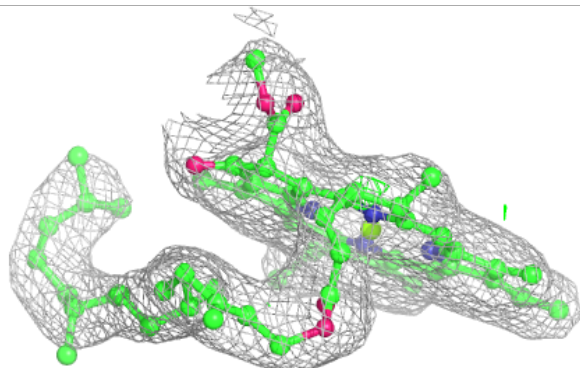
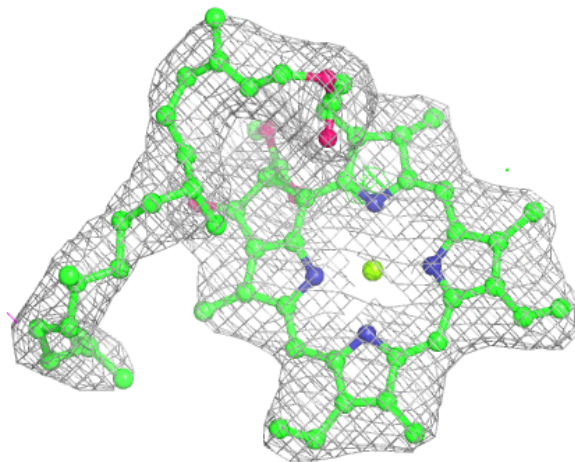
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

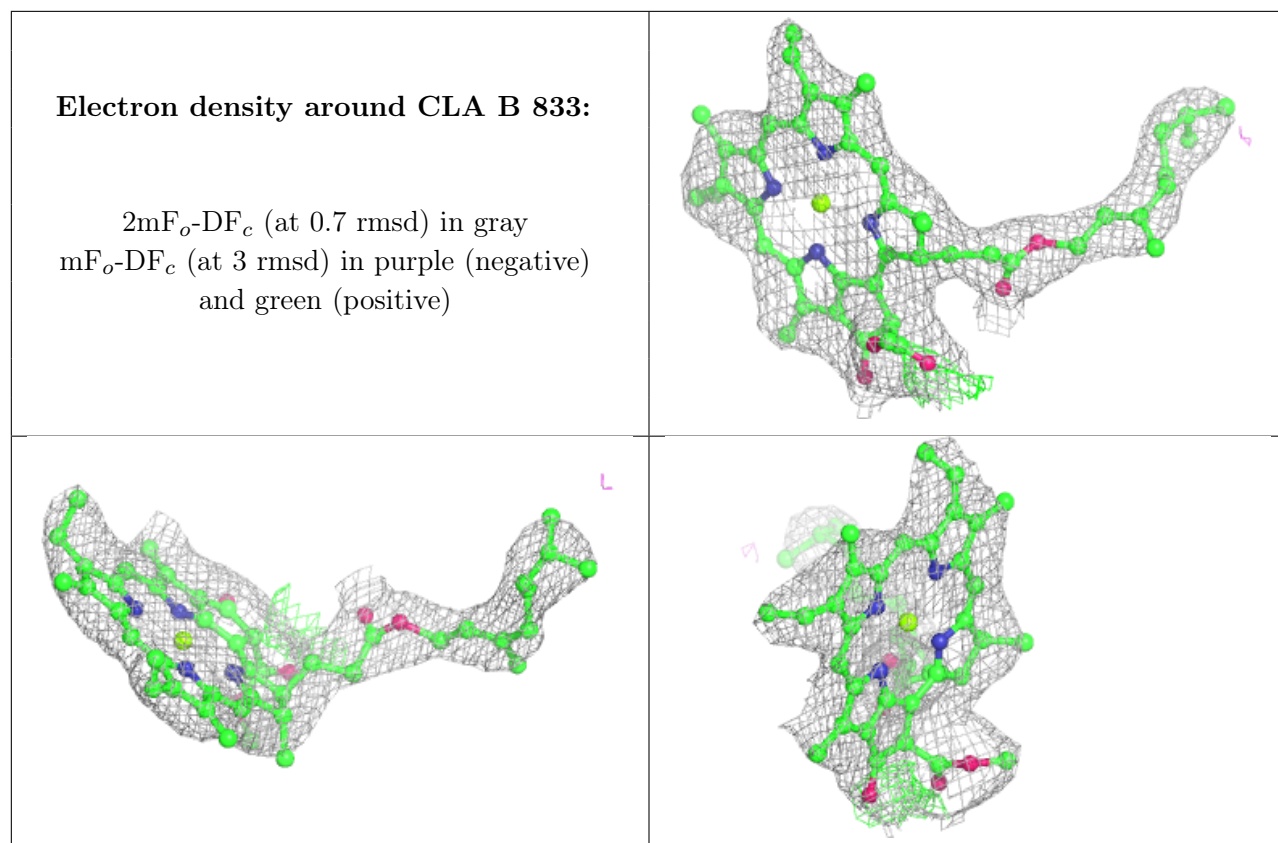




**Electron density around CLA B 832:**

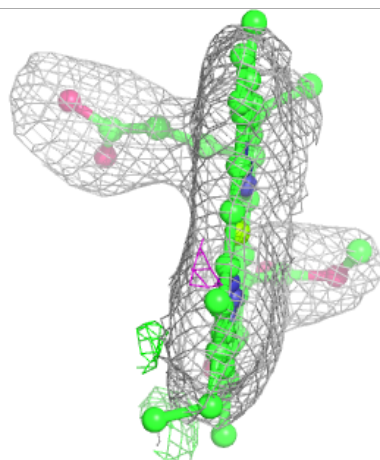
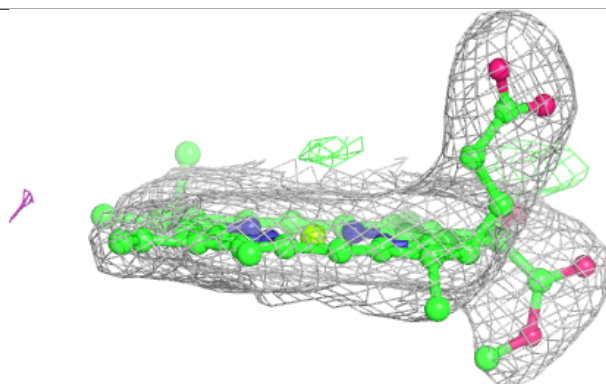
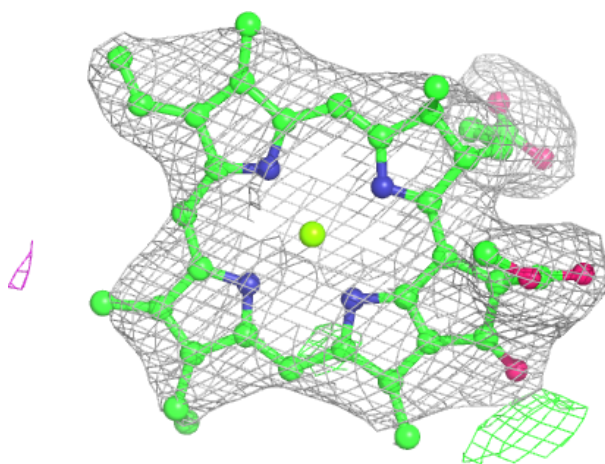
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





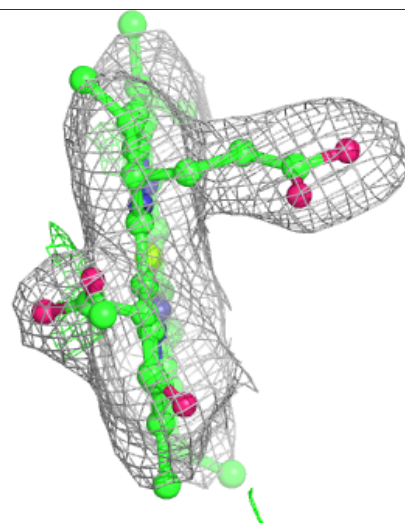
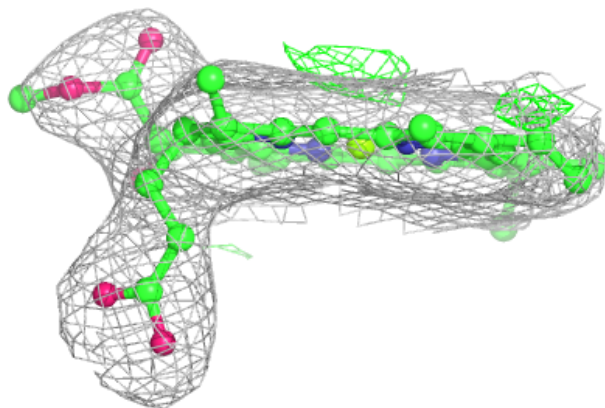
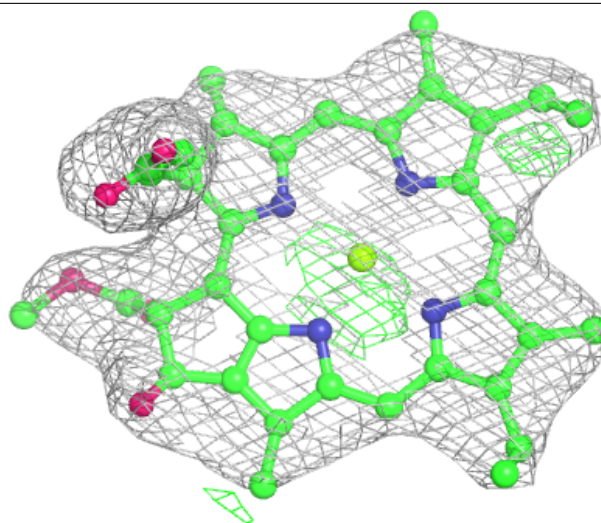
**Electron density around CLA B 834:**

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



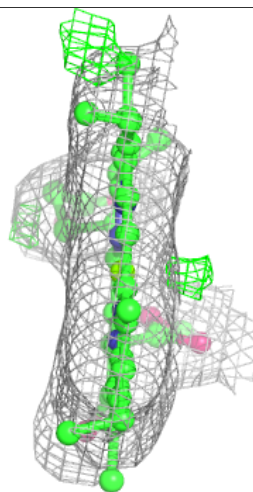
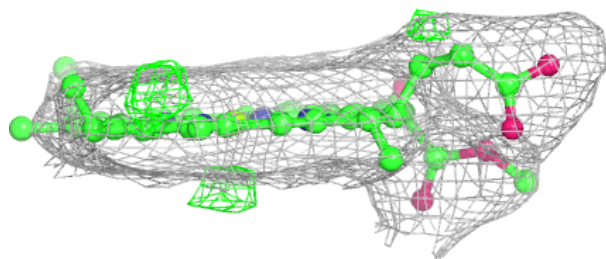
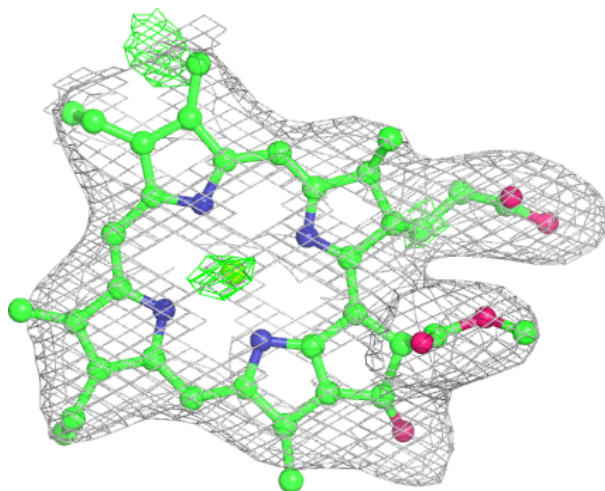
**Electron density around CLA B 835:**

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



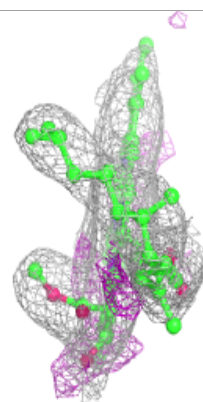
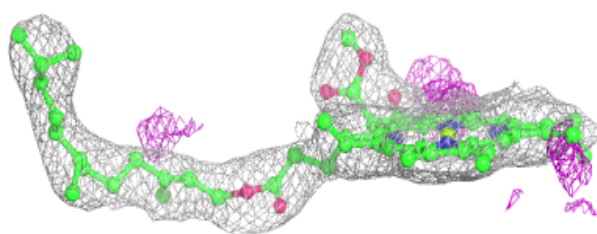
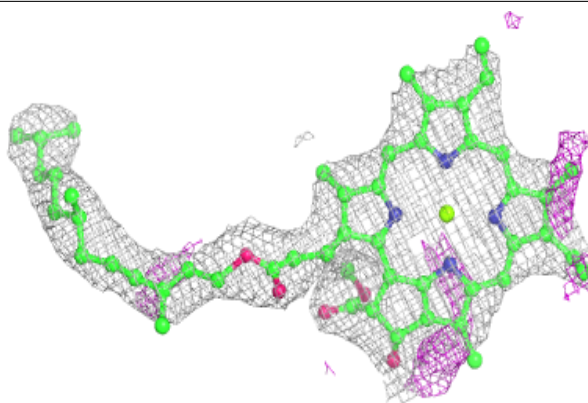
**Electron density around CLA B 836:**

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

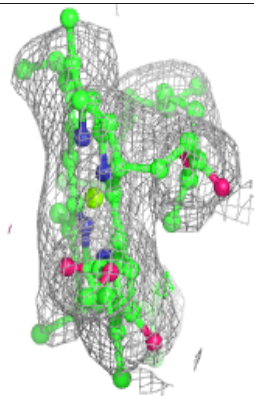
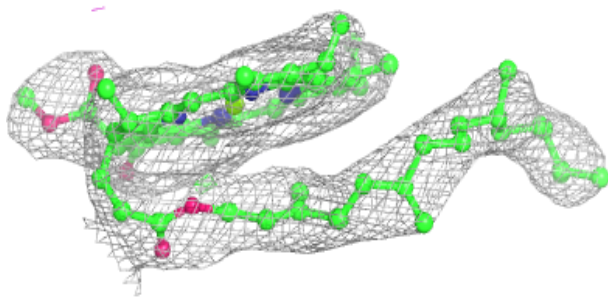
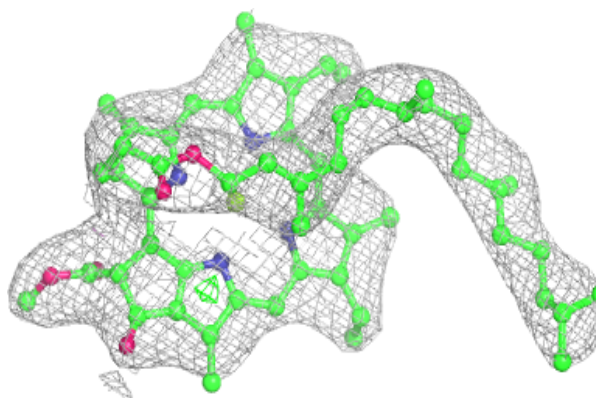


**Electron density around CLA B 837:**

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

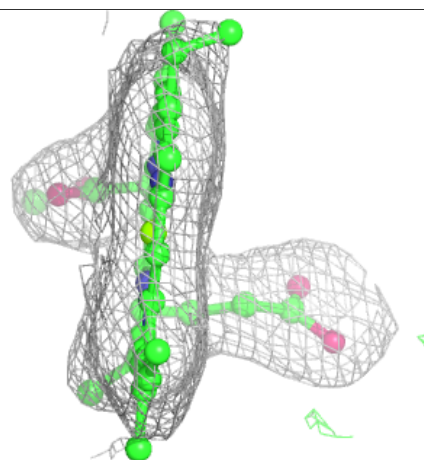
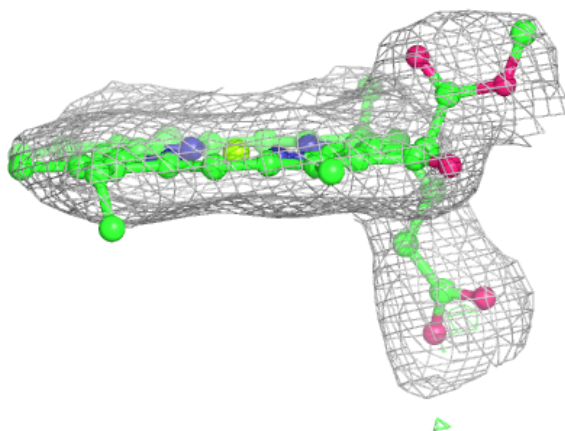
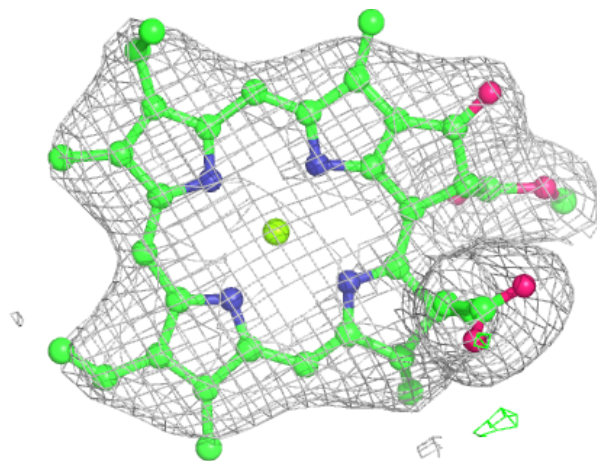
**Electron density around CLA B 838:**

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



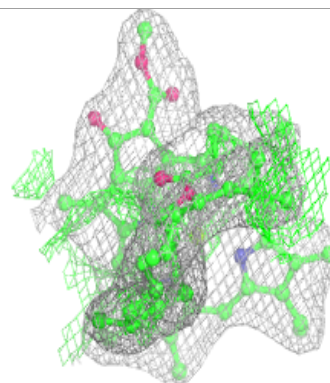
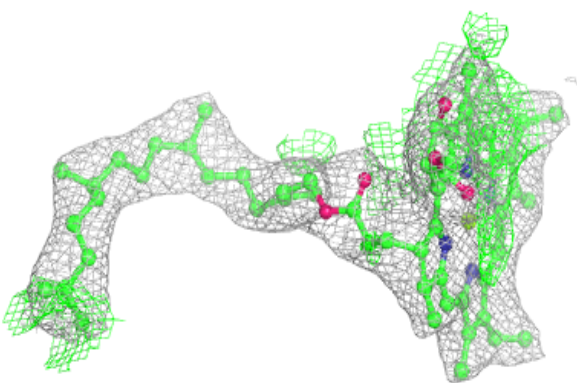
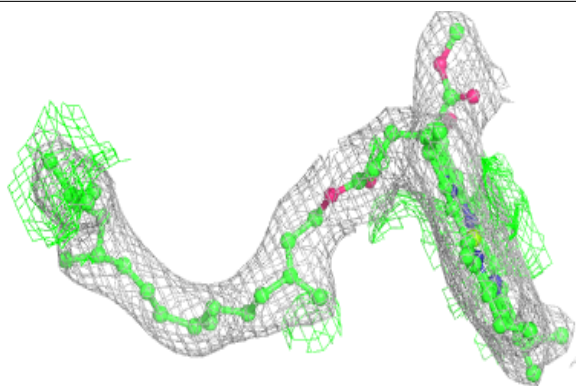
**Electron density around CLA B 839:**

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

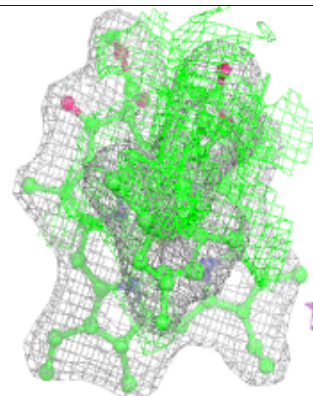
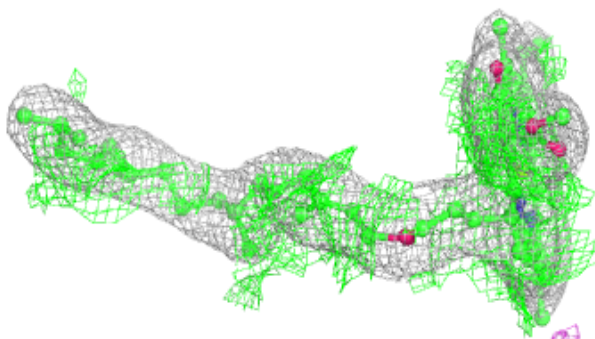
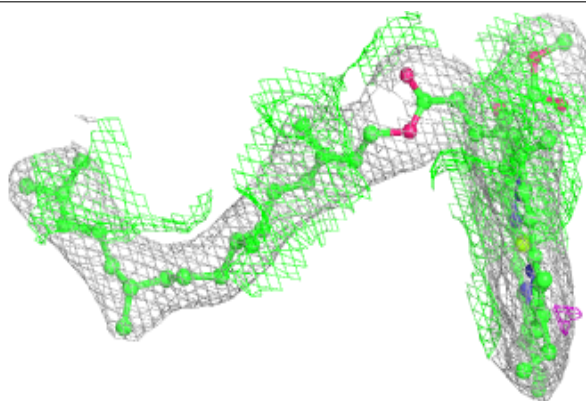


**Electron density around CLA B 840:**

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

**Electron density around CLA B 841:**

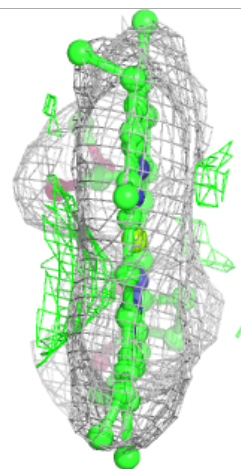
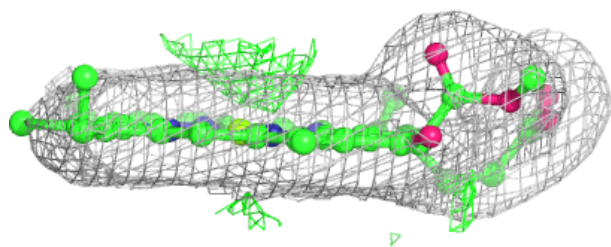
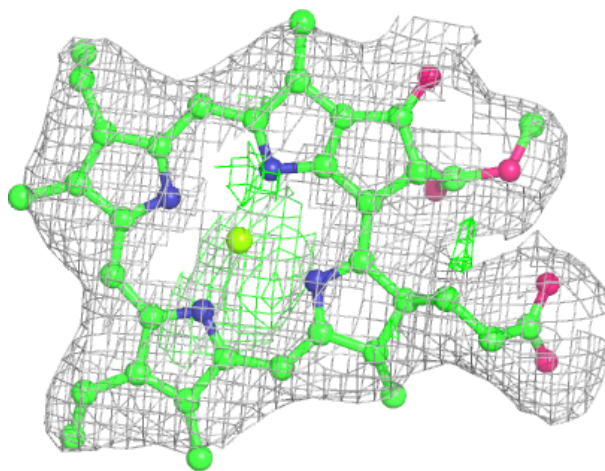
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





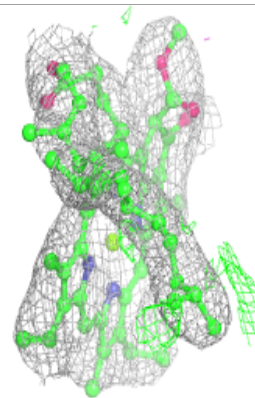
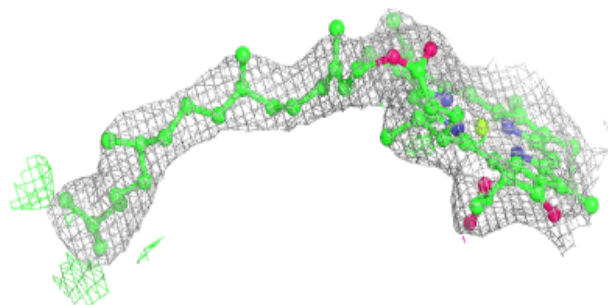
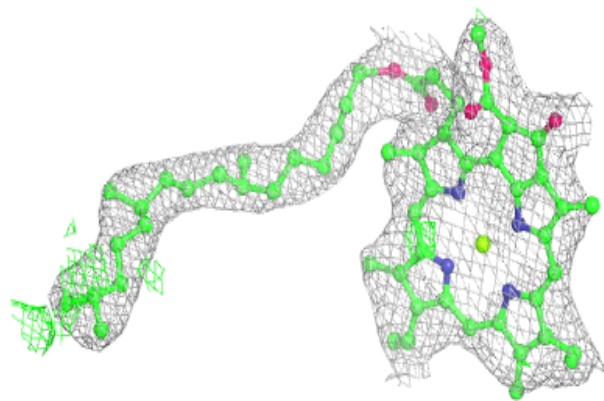
**Electron density around CLA F 202:**

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

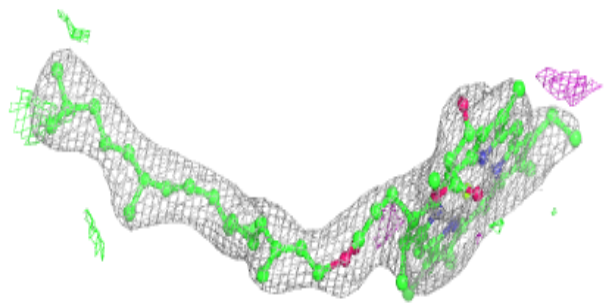
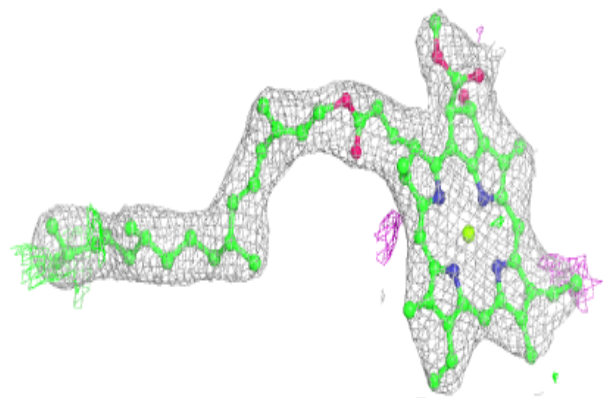


**Electron density around CLA G 802:**

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

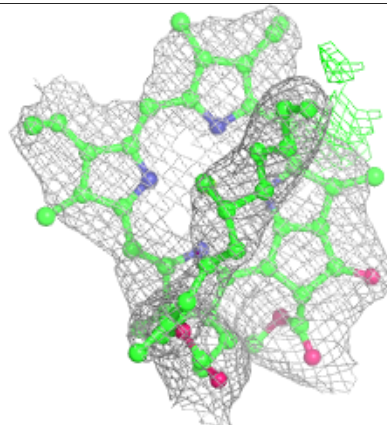
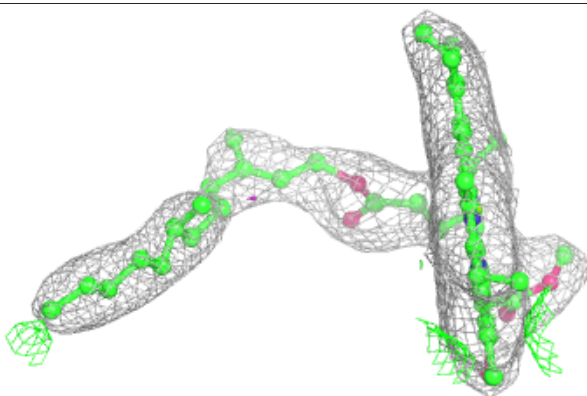
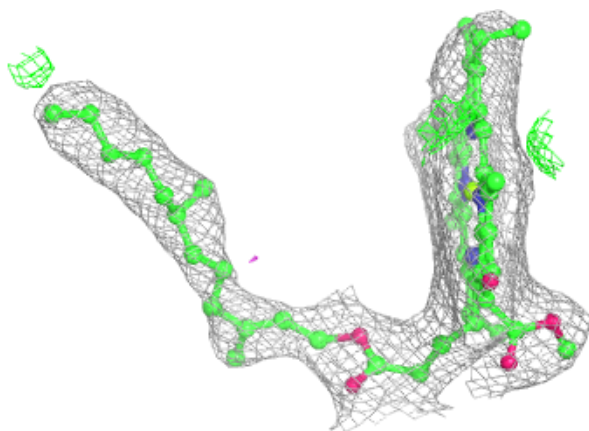
**Electron density around CLA G 803:**

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

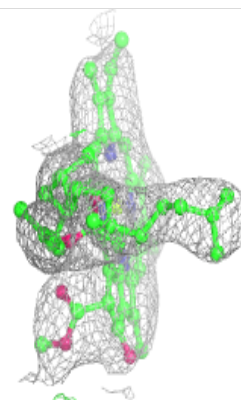
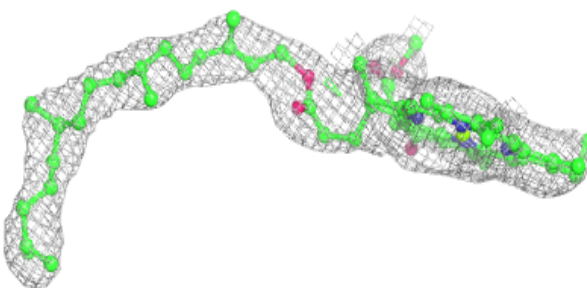
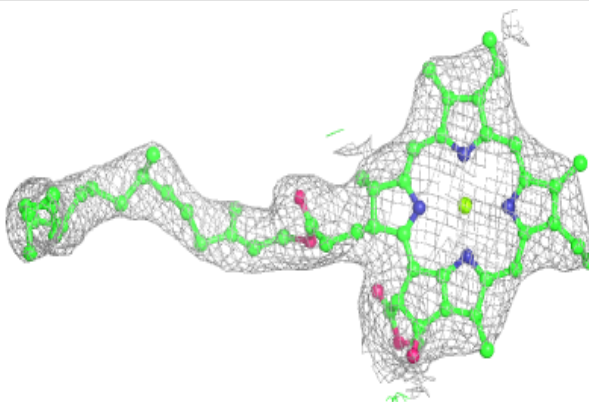


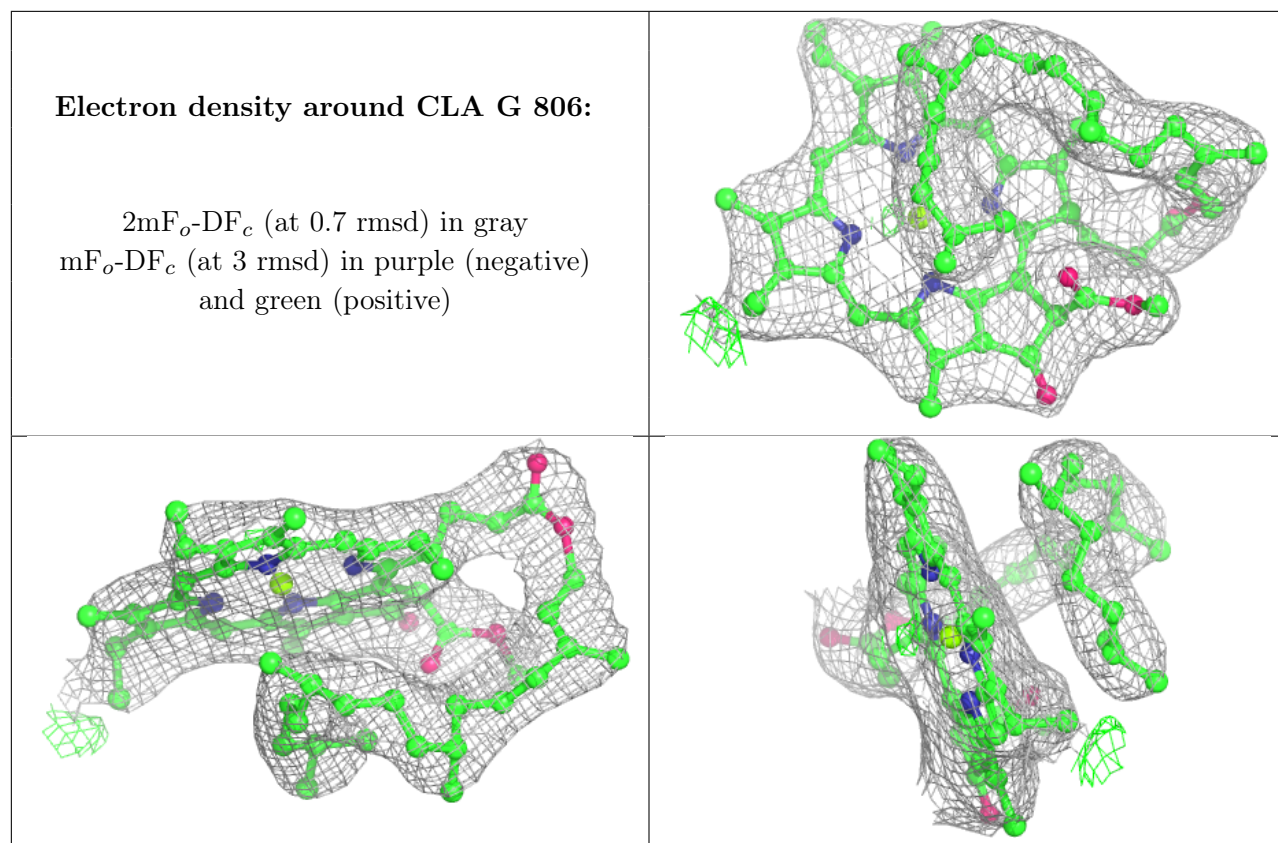
**Electron density around CLA G 804:**

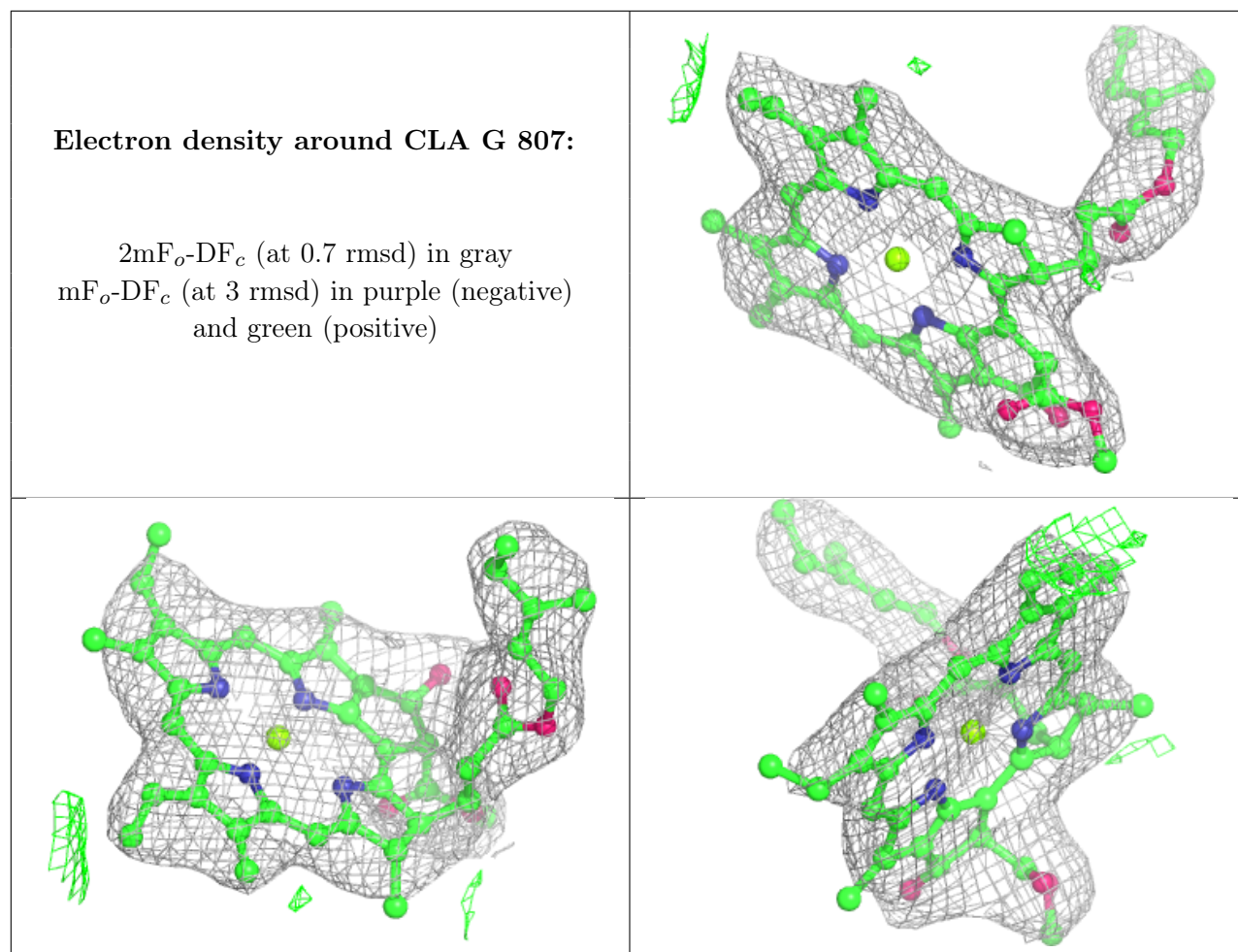
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA G 805:**

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

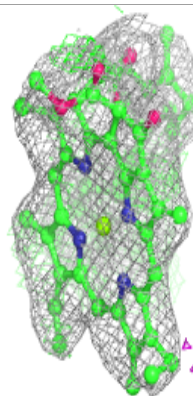
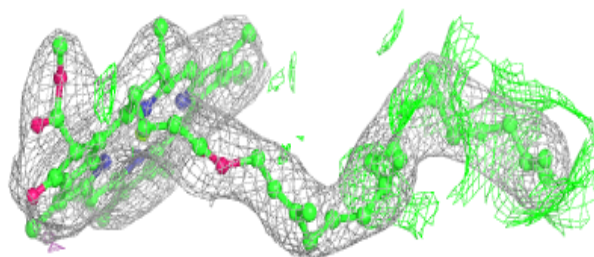
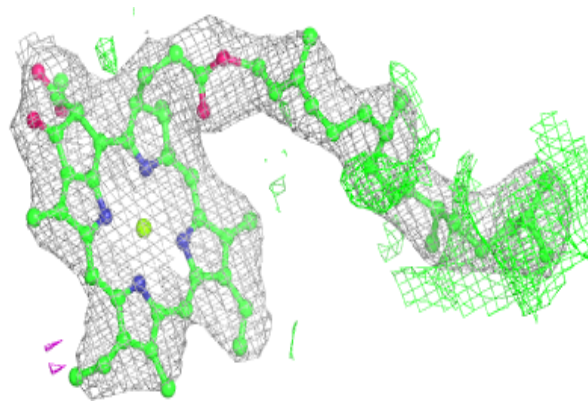




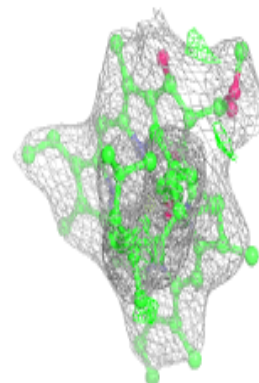
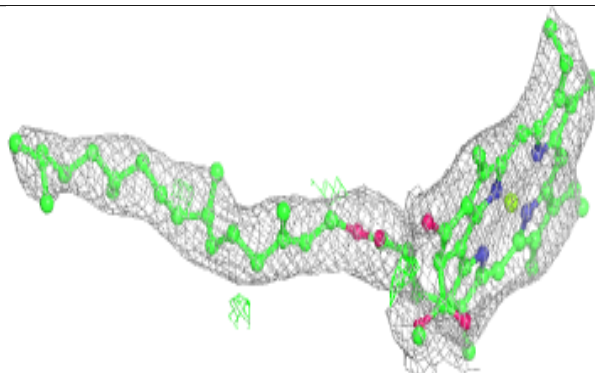
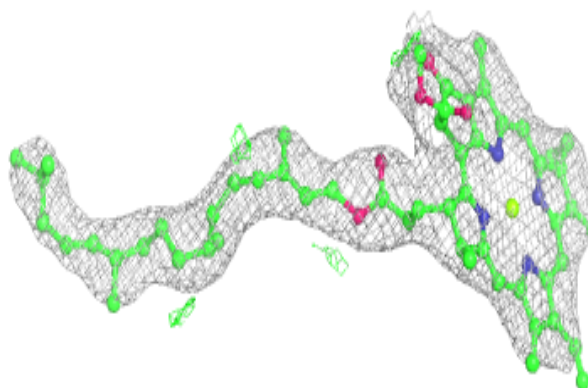


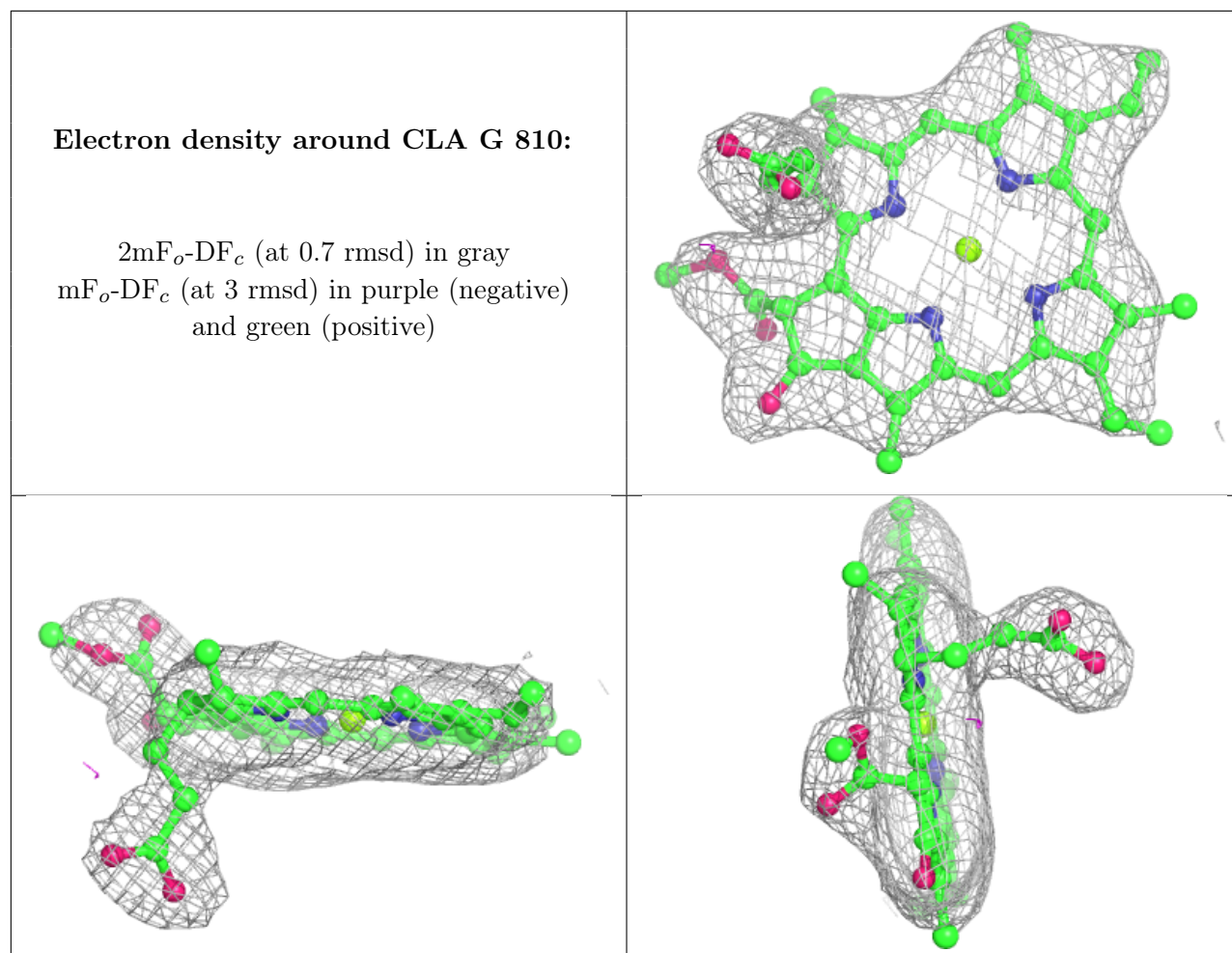
**Electron density around CLA G 808:**

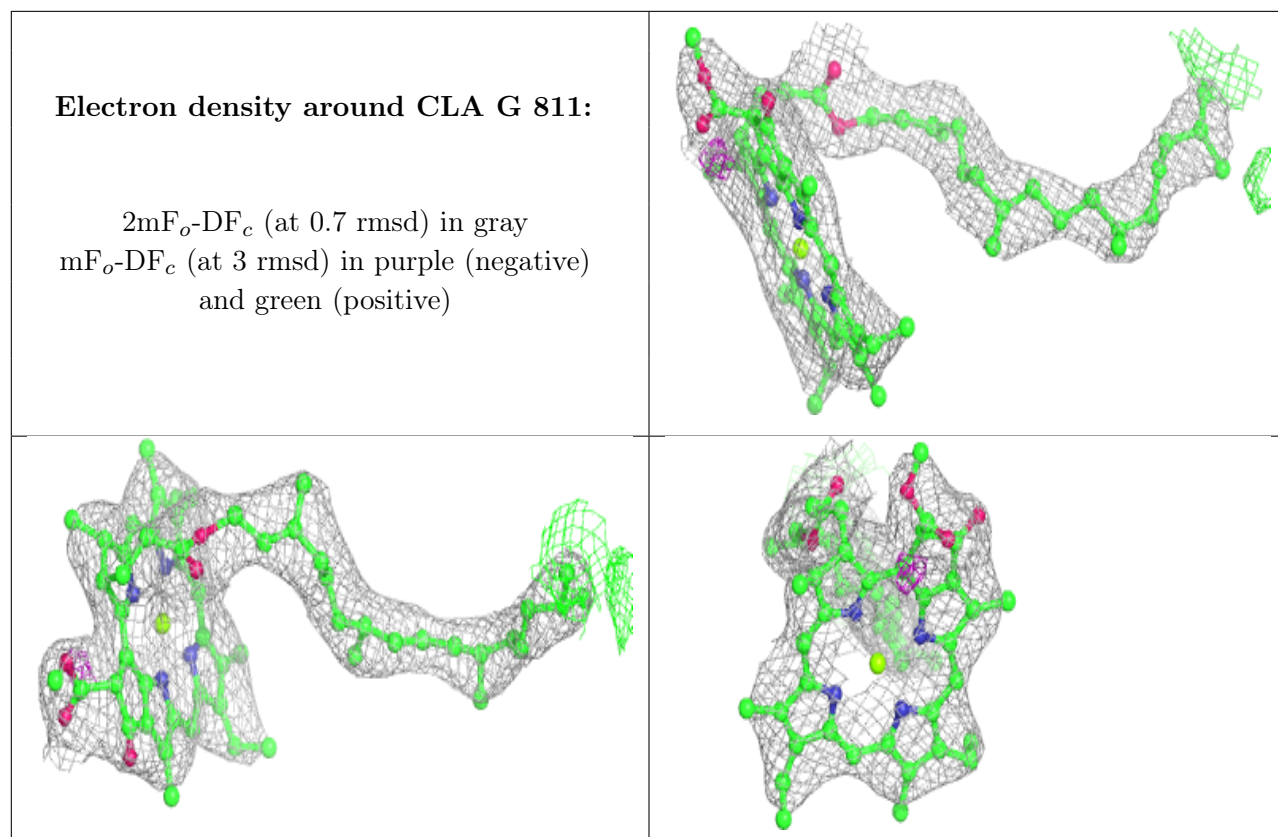
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA G 809:**

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



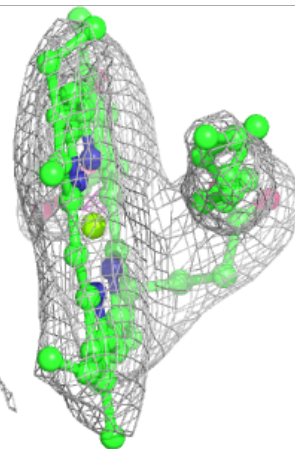
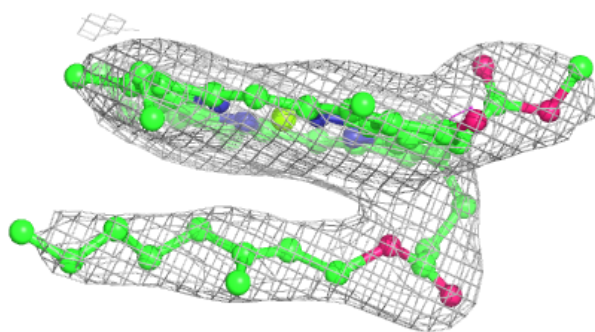
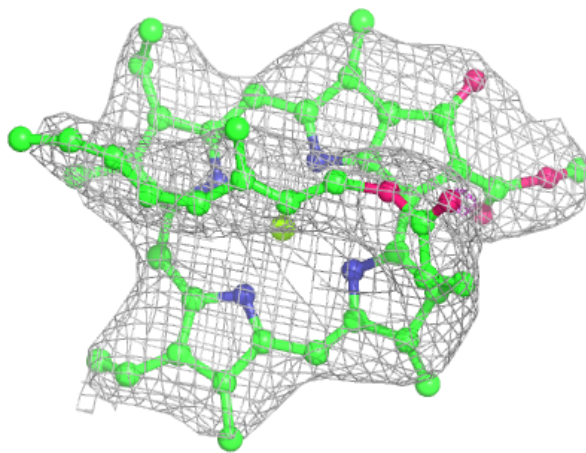


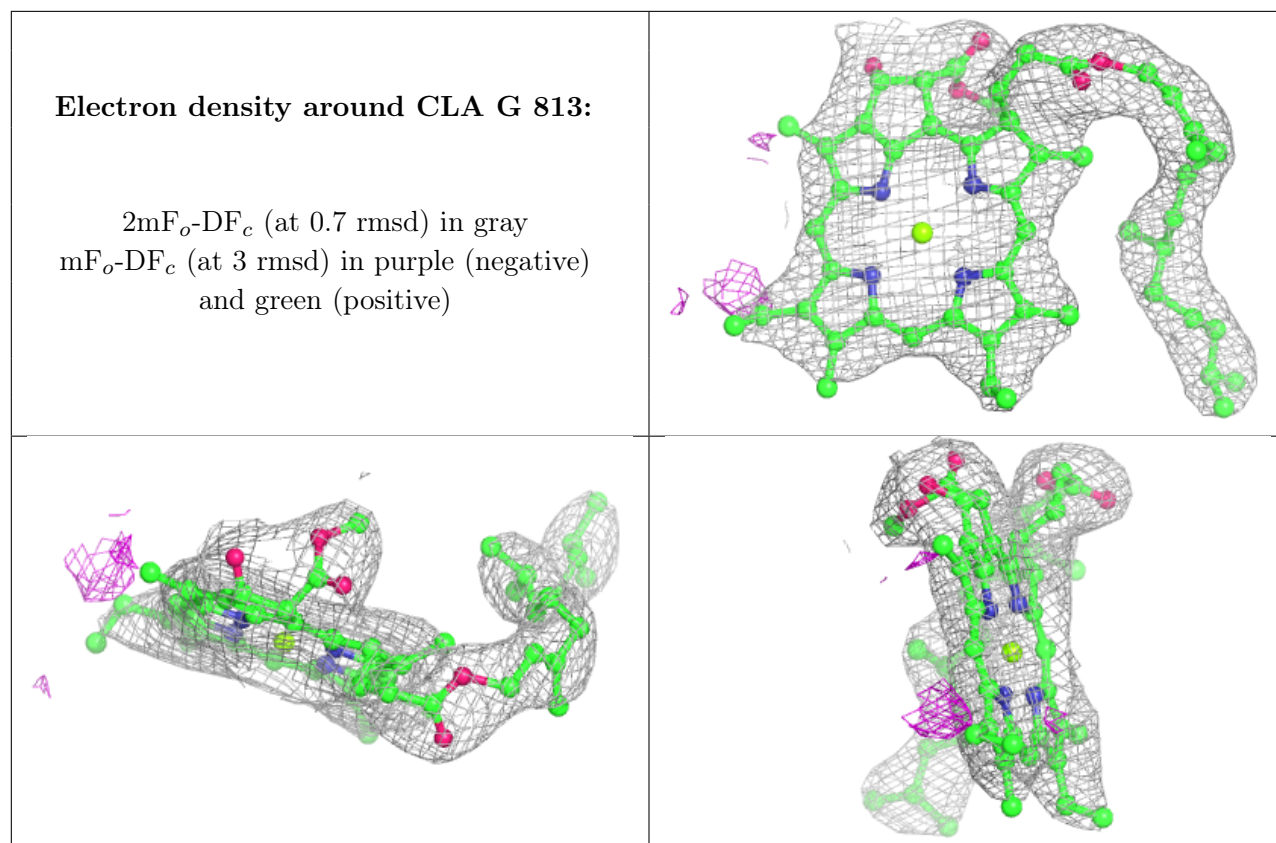




**Electron density around CLA G 812:**

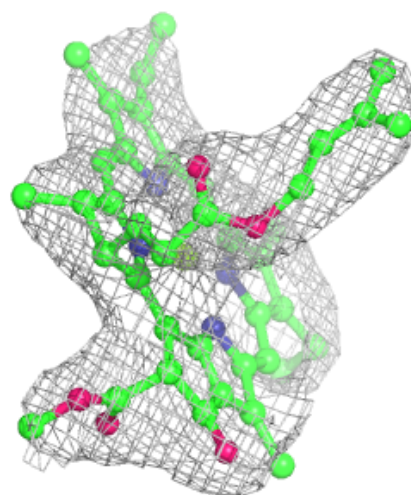
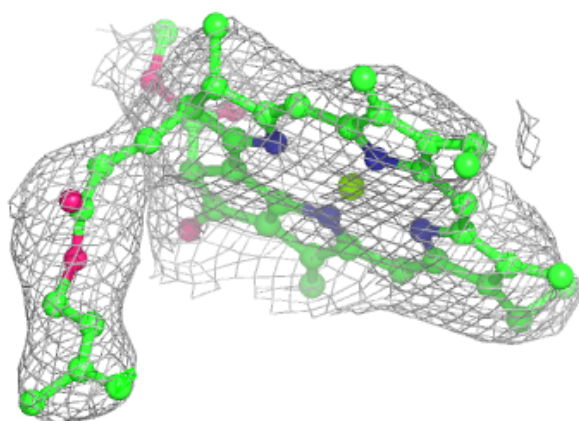
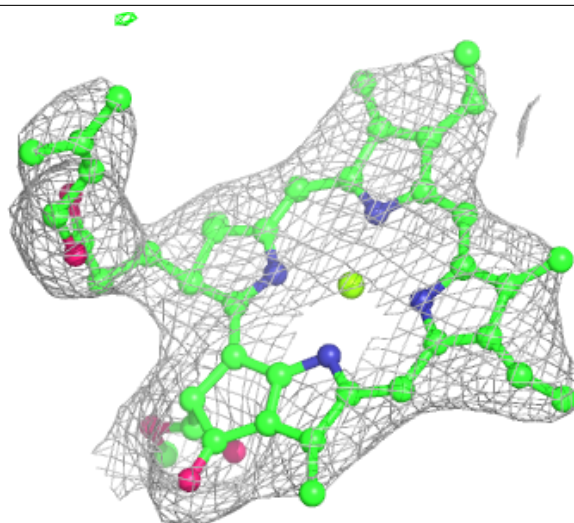
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





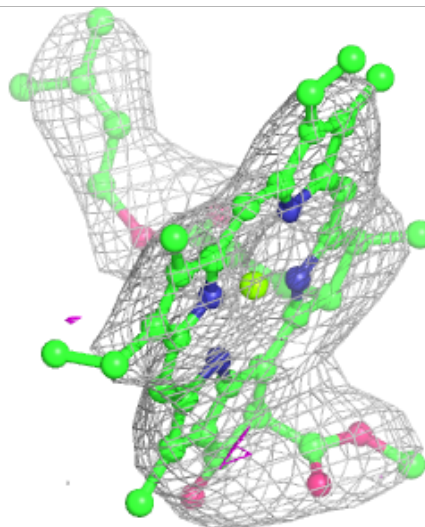
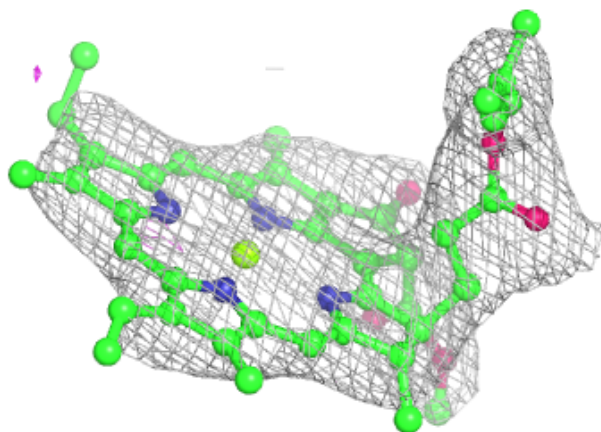
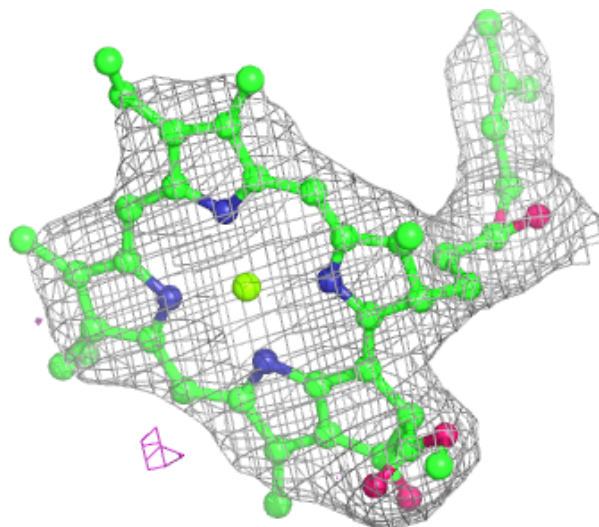
**Electron density around CLA G 814:**

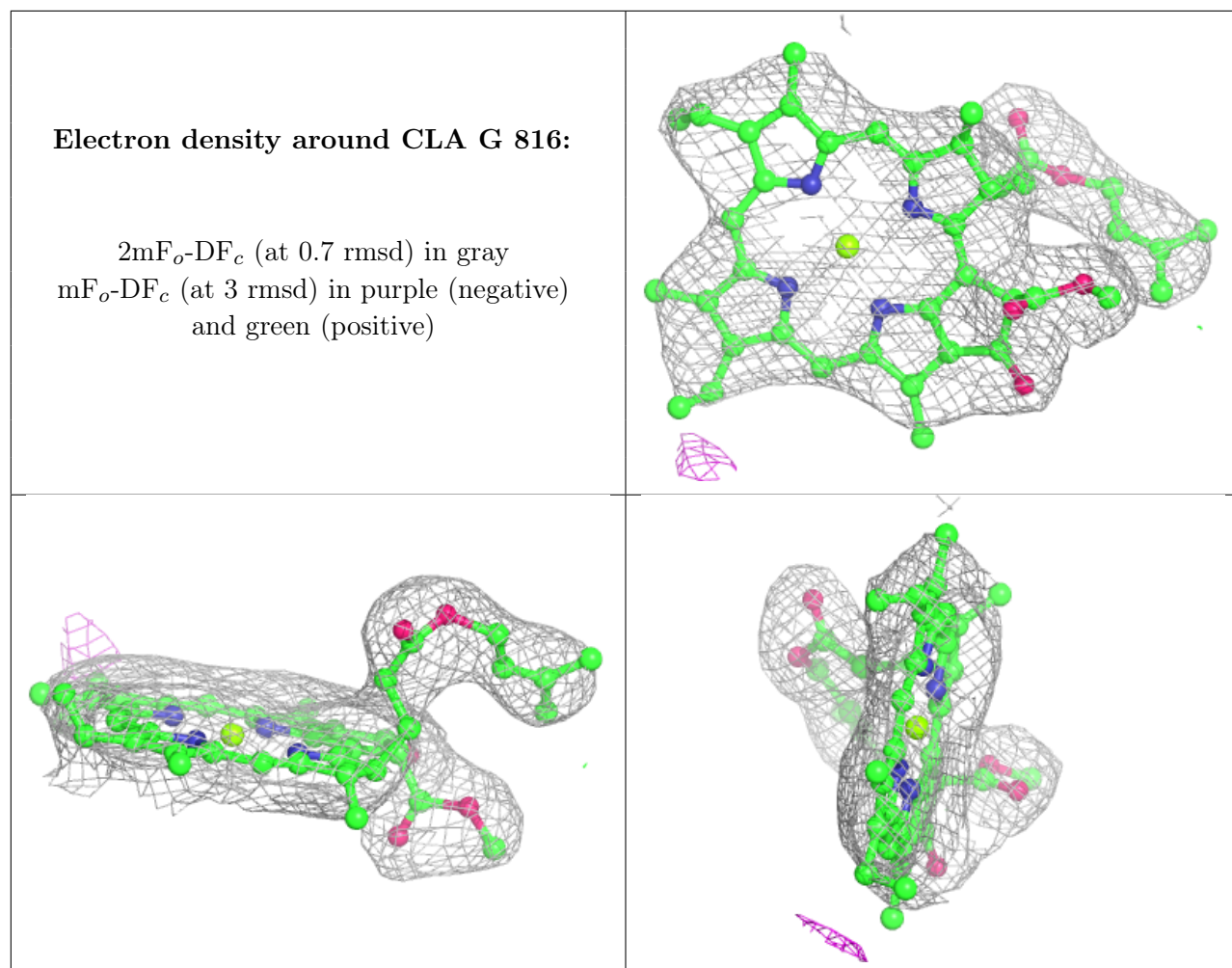
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA G 815:**

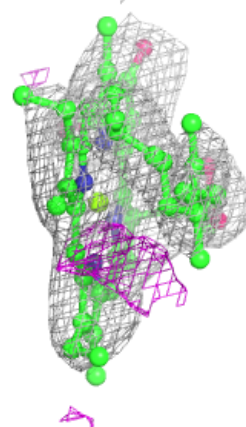
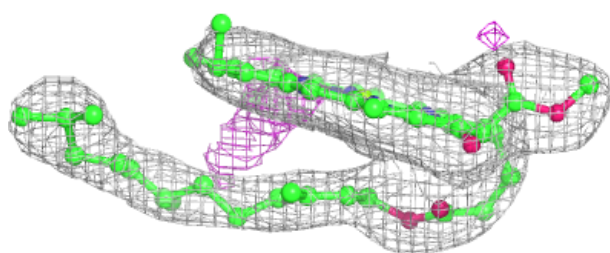
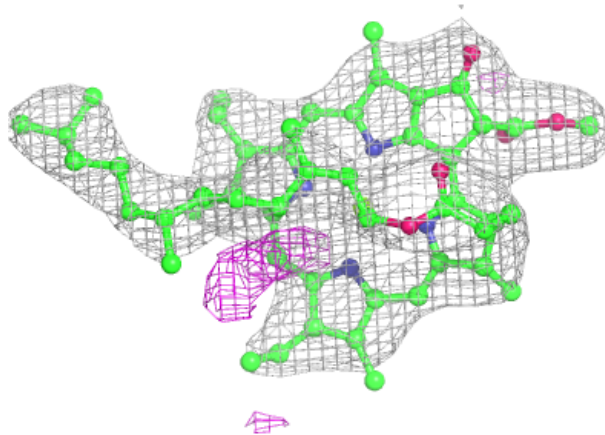
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



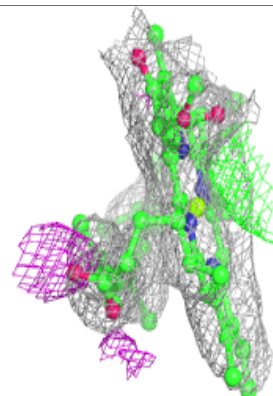
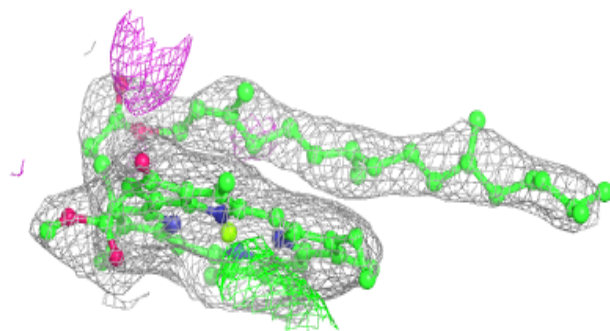
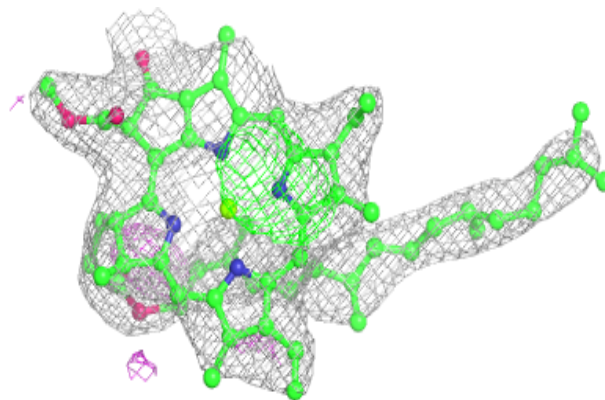


**Electron density around CLA G 817:**

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

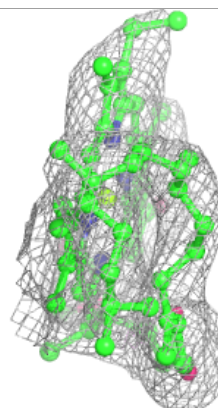
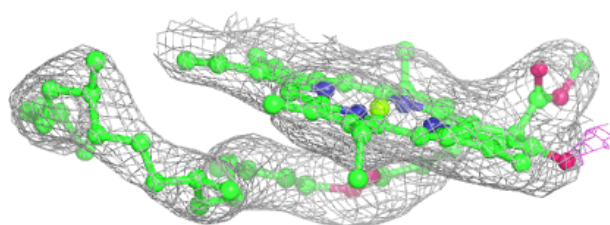
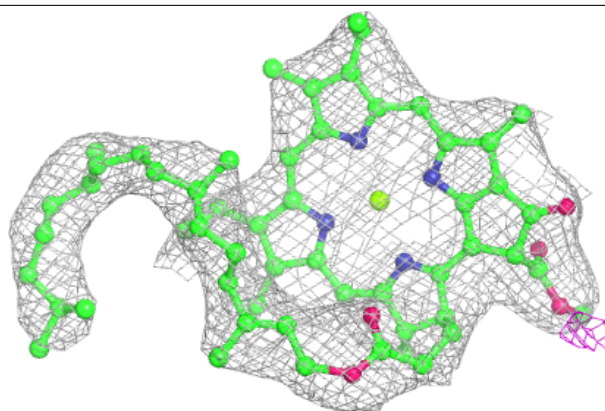
**Electron density around CLA G 818:**

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

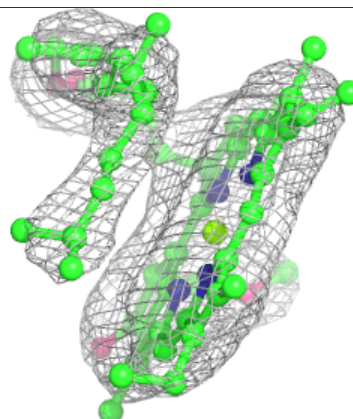
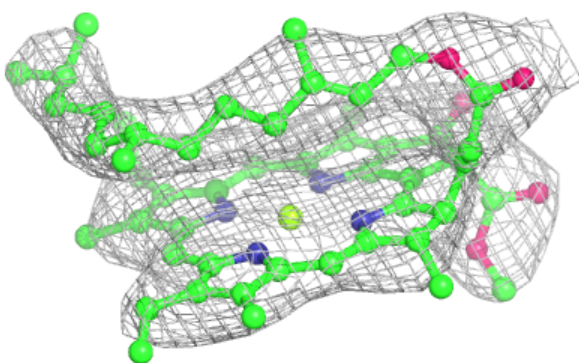
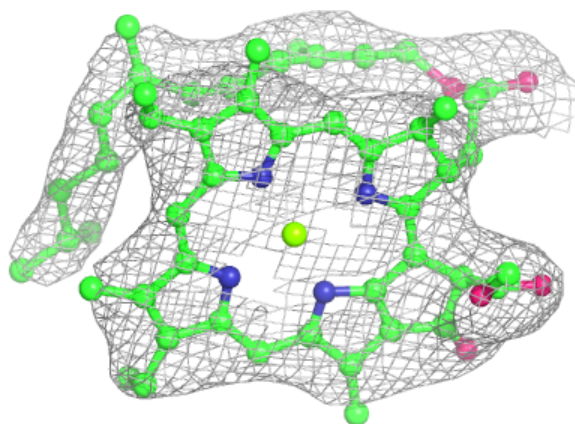


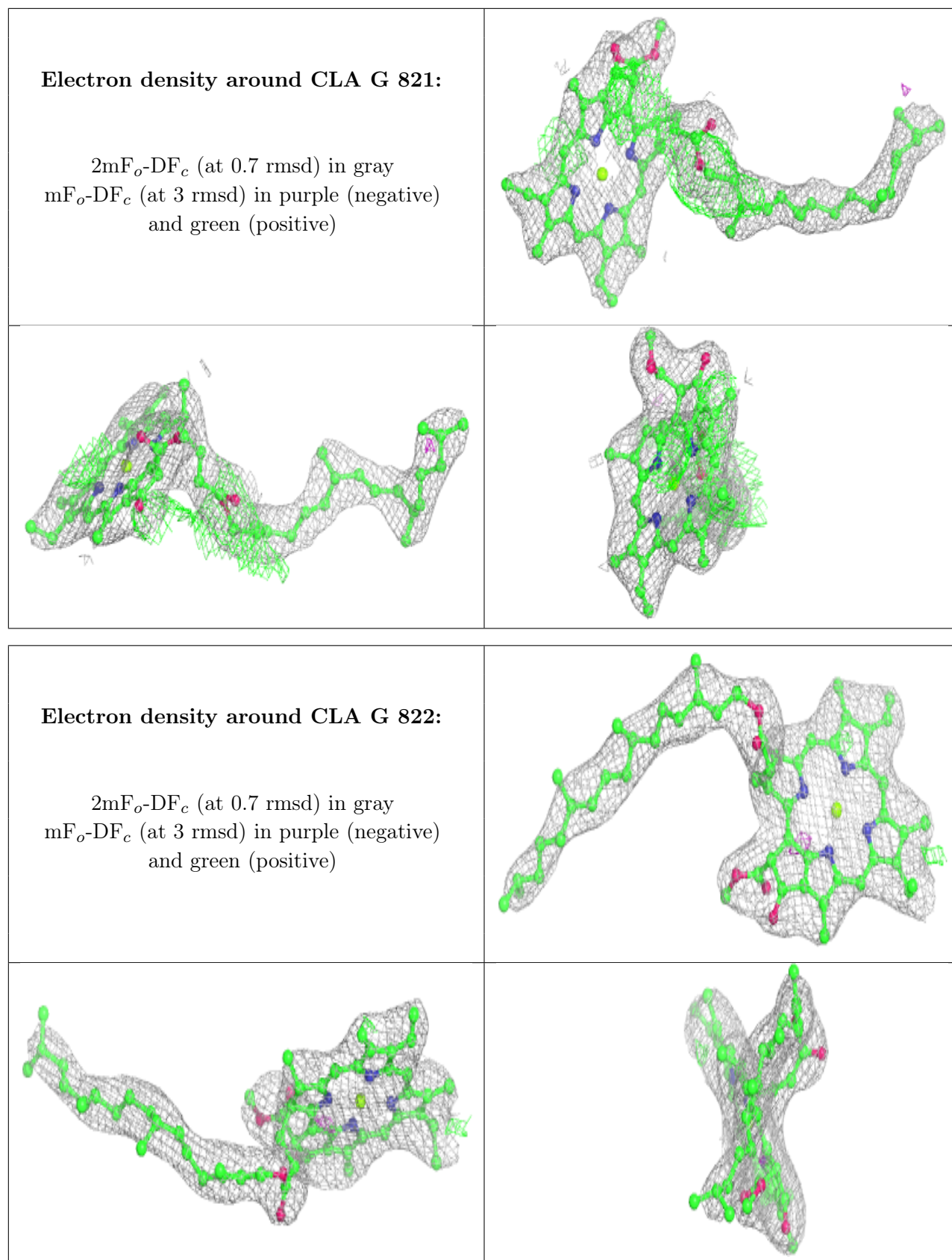
**Electron density around CLA G 819:**

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

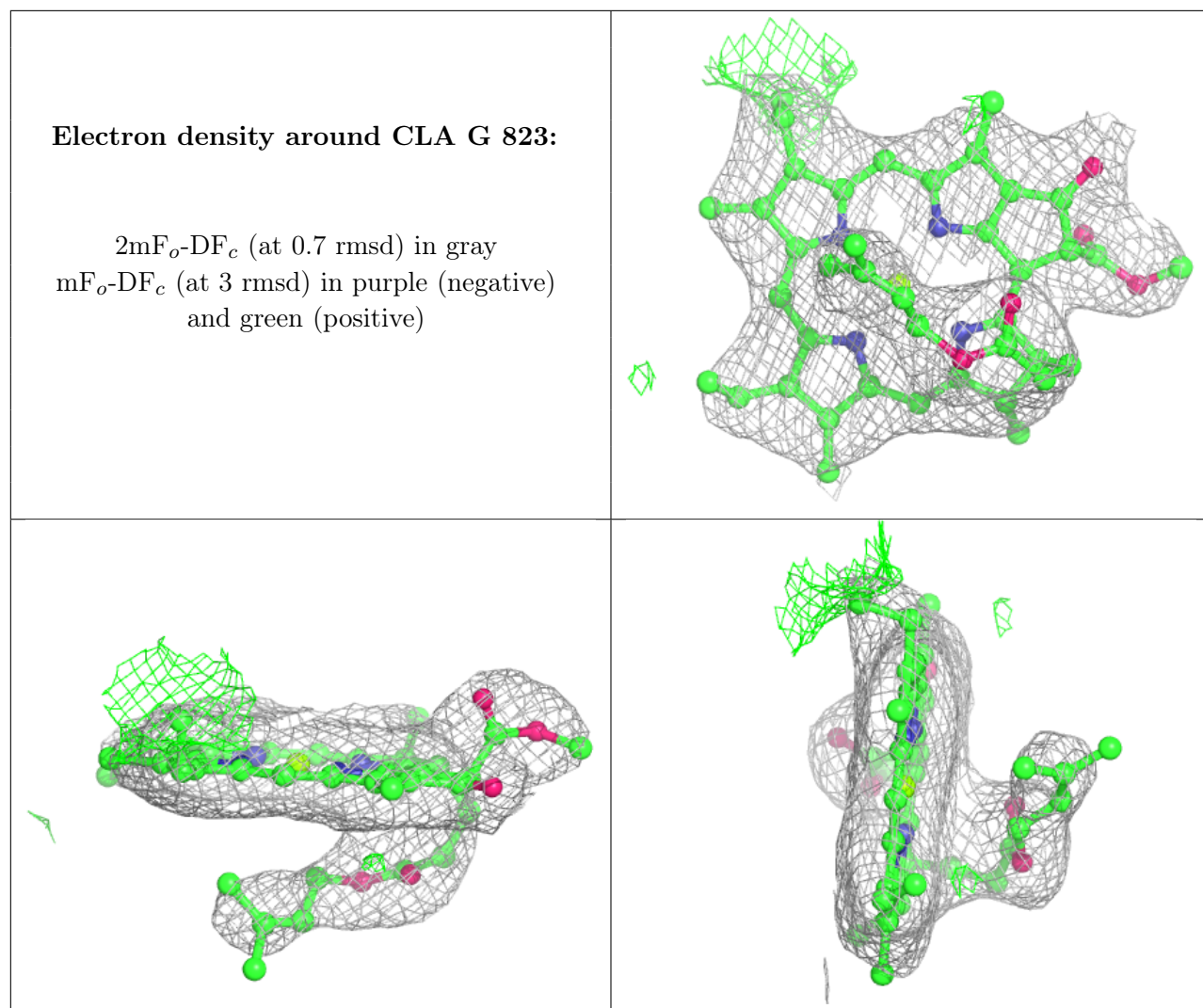
**Electron density around CLA G 820:**

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



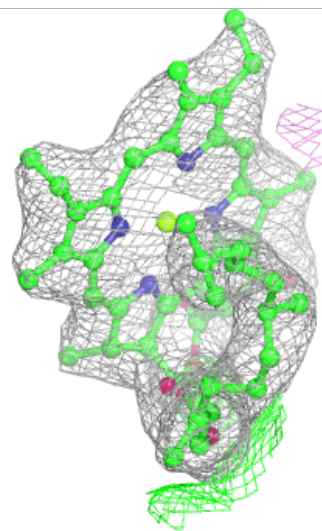
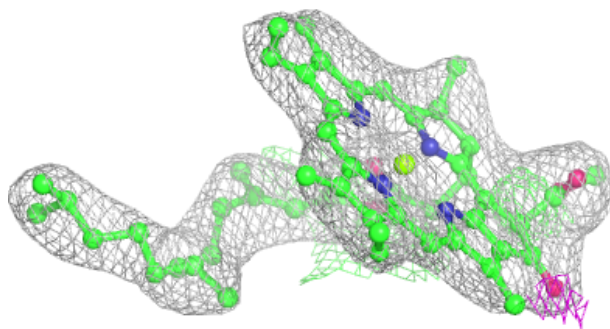
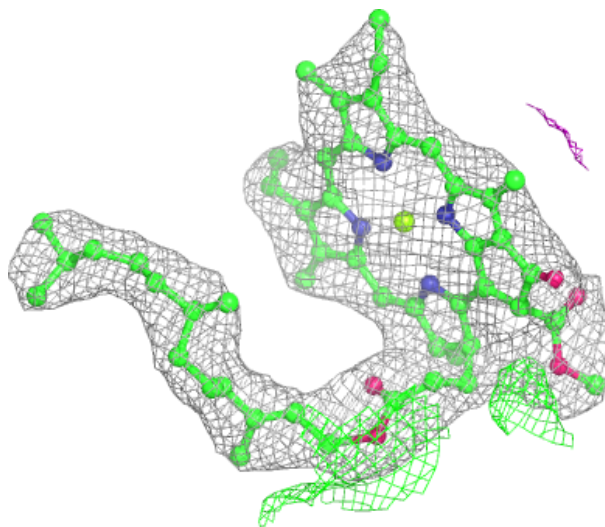






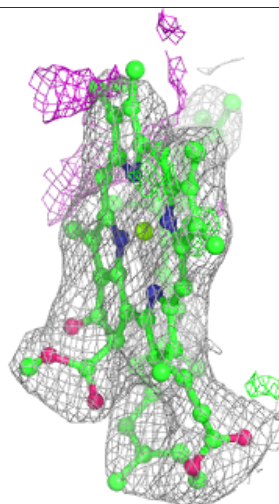
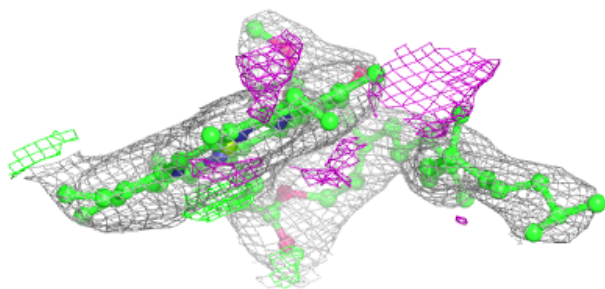
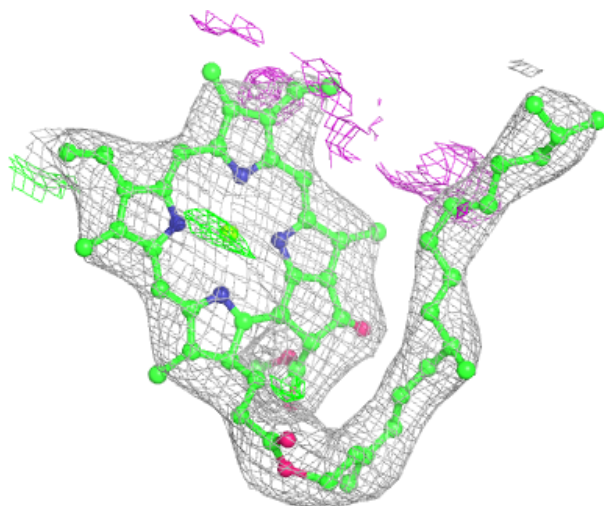
**Electron density around CLA G 824:**

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



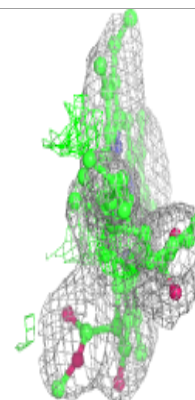
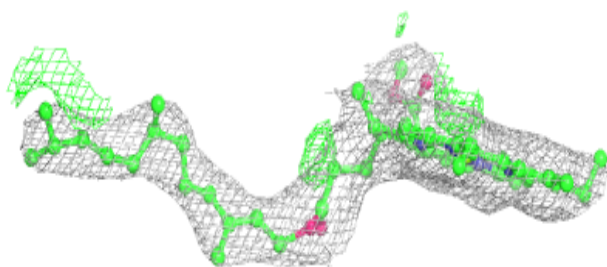
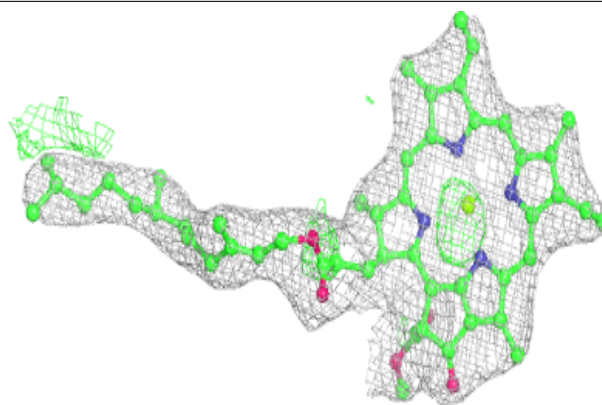
**Electron density around CLA G 825:**

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

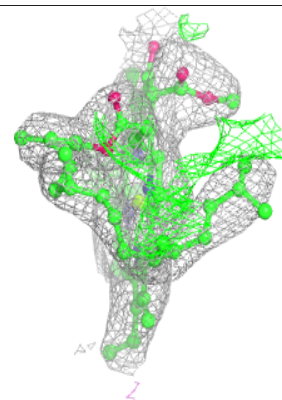
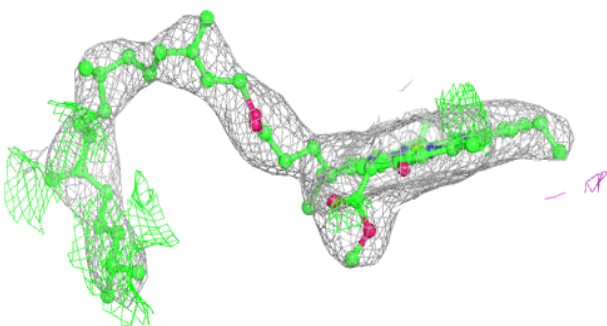
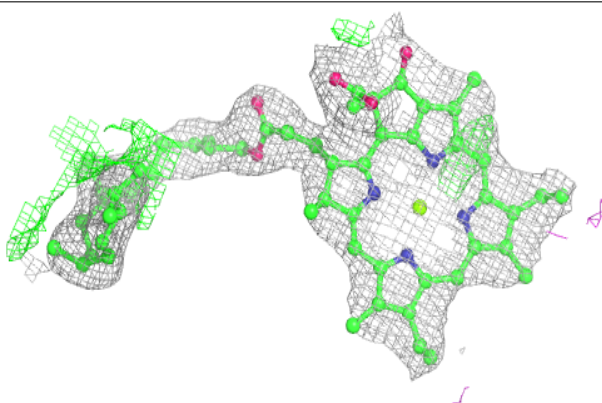


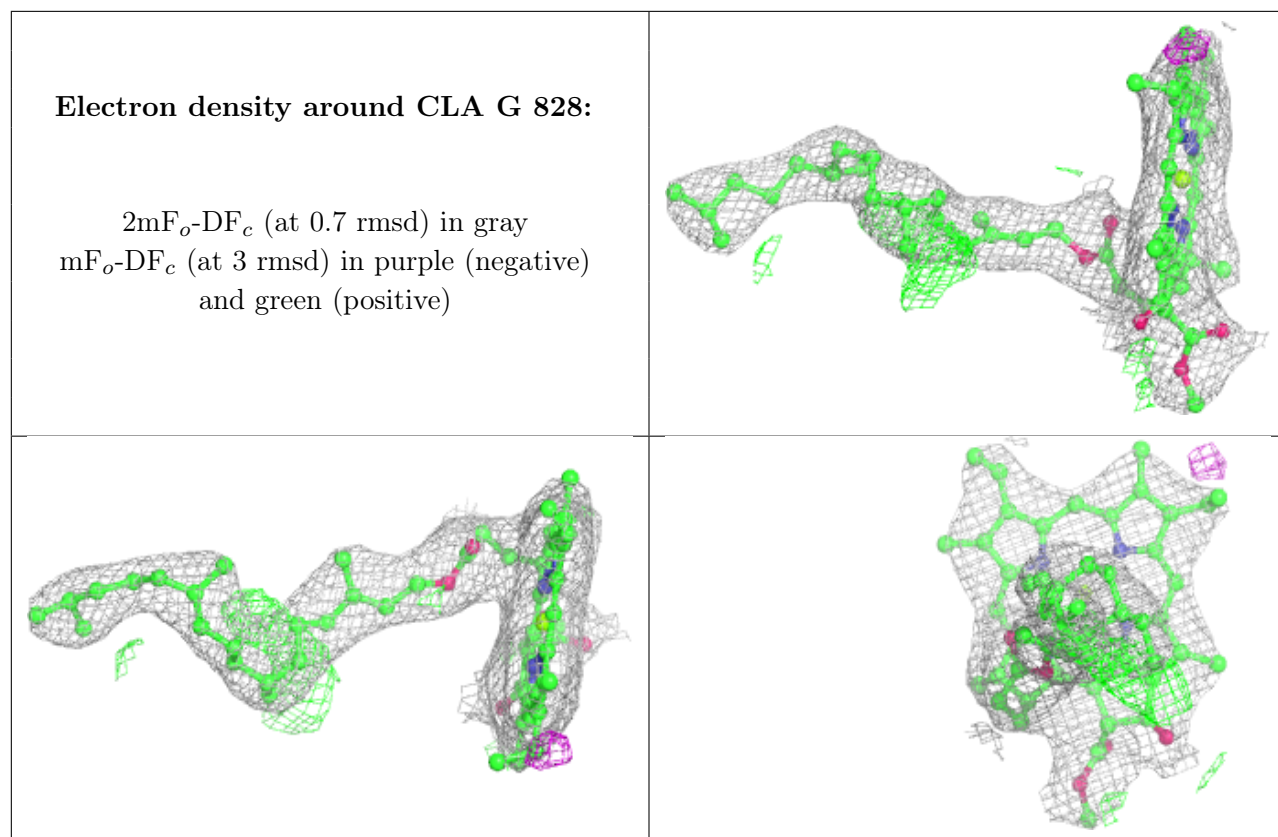
**Electron density around CLA G 826:**

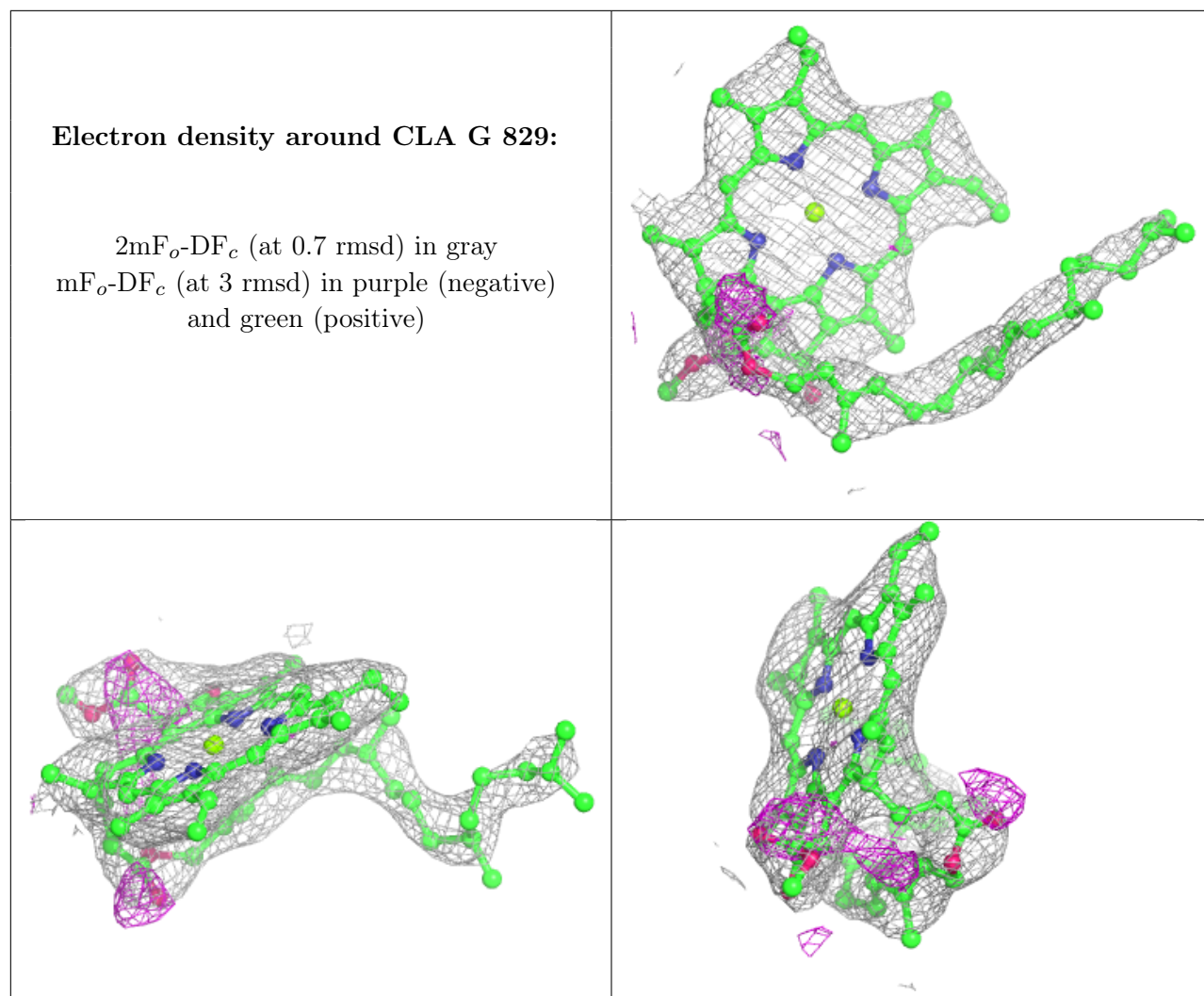
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

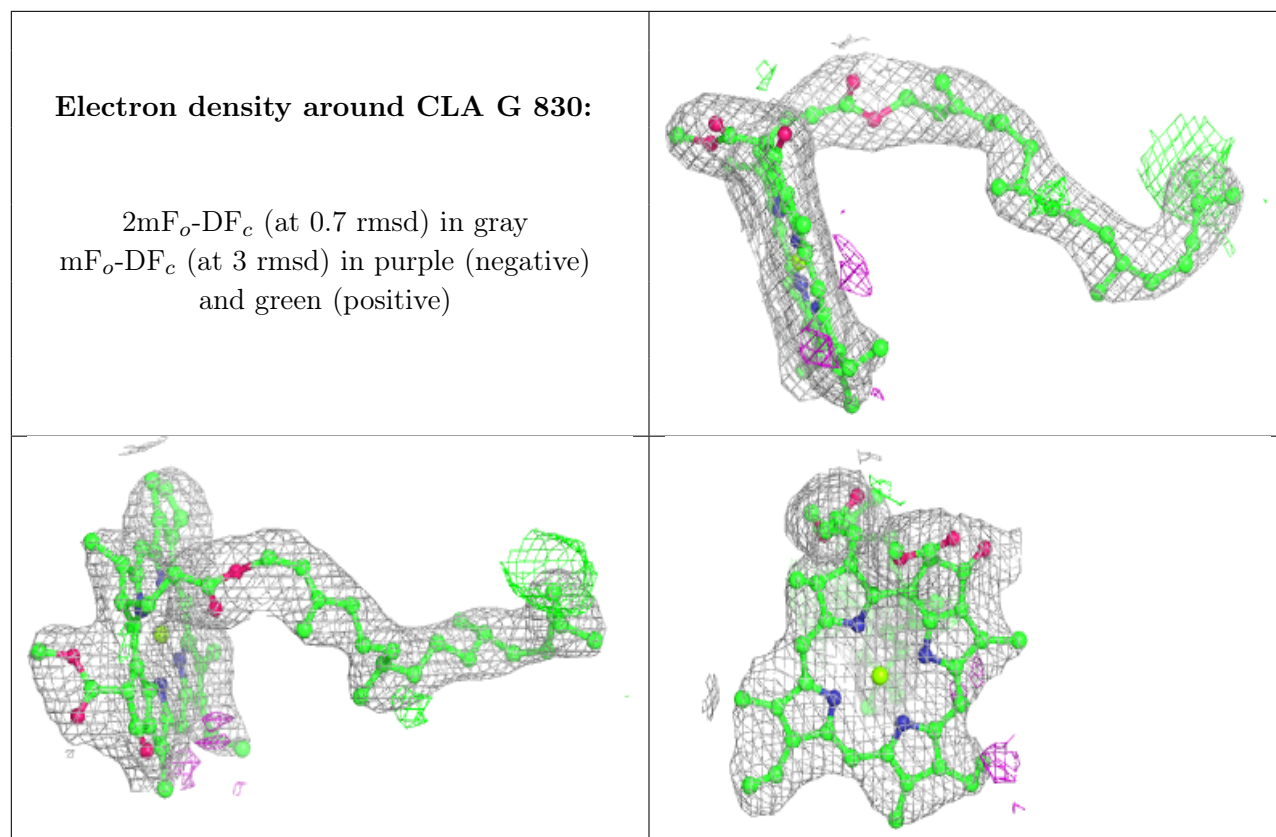
**Electron density around CLA G 827:**

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



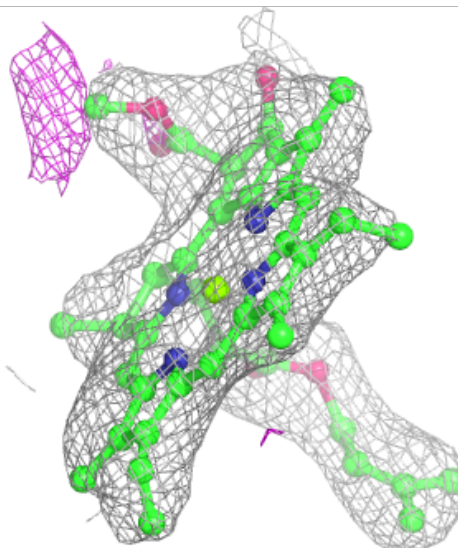
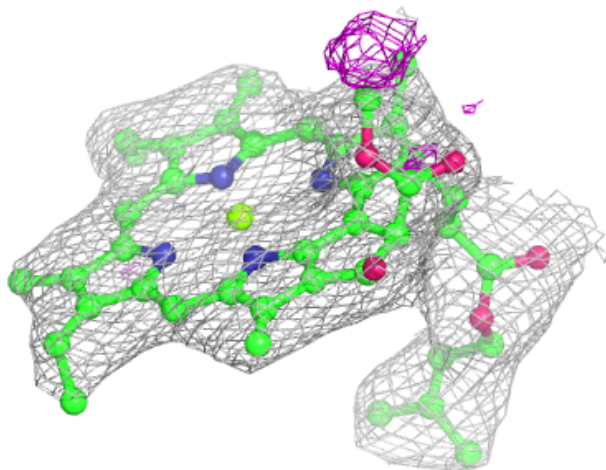
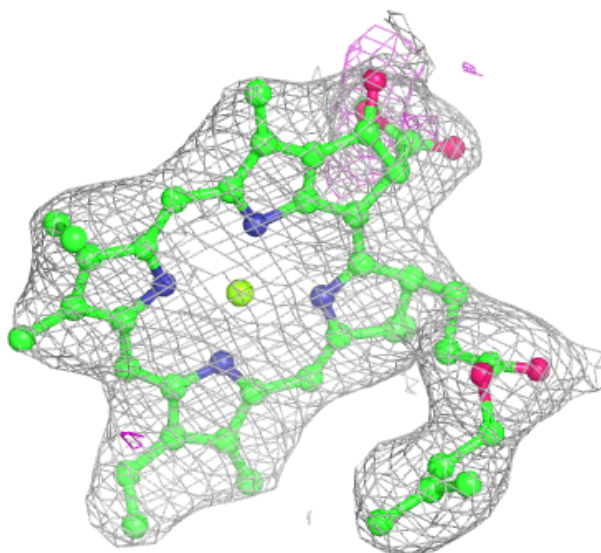




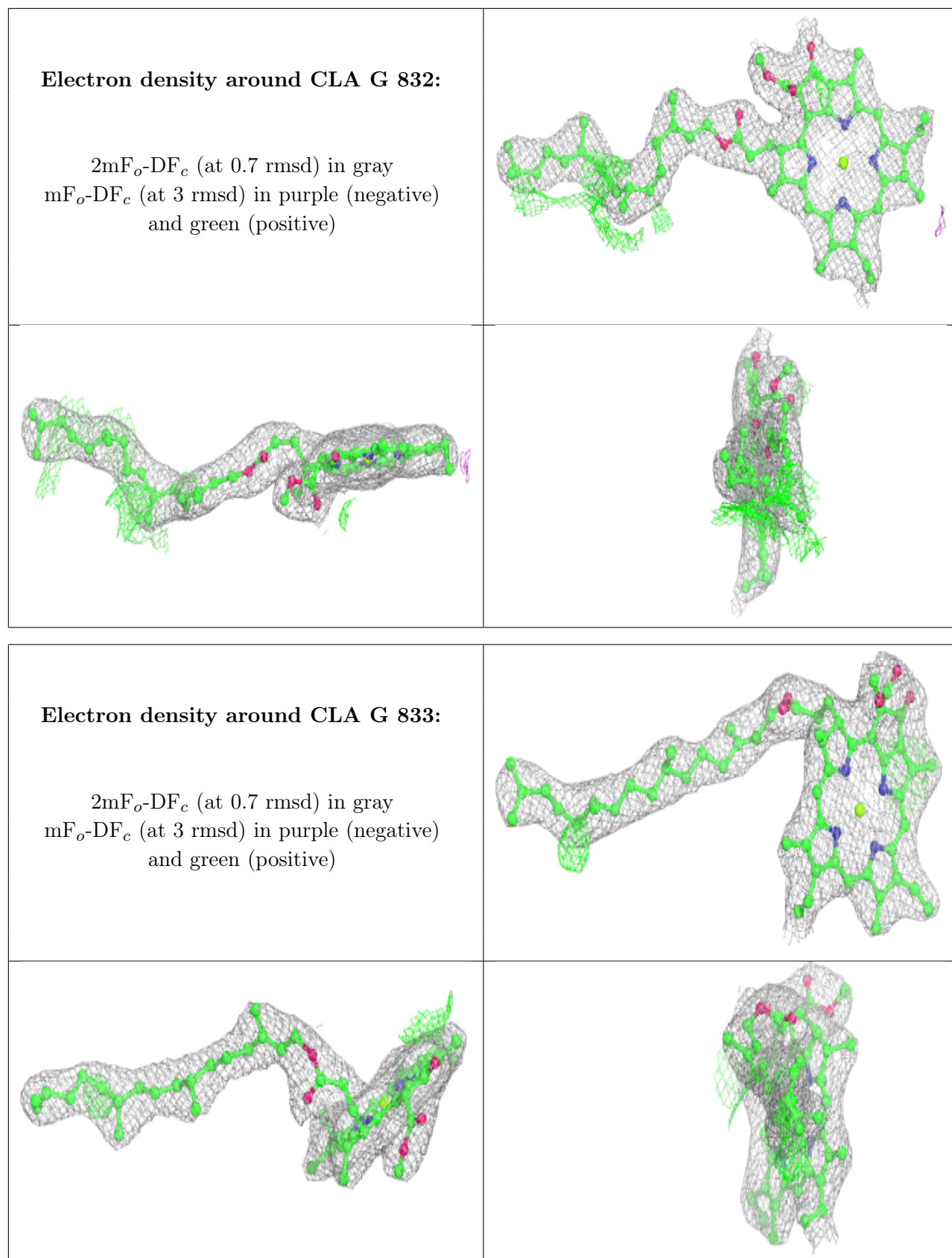


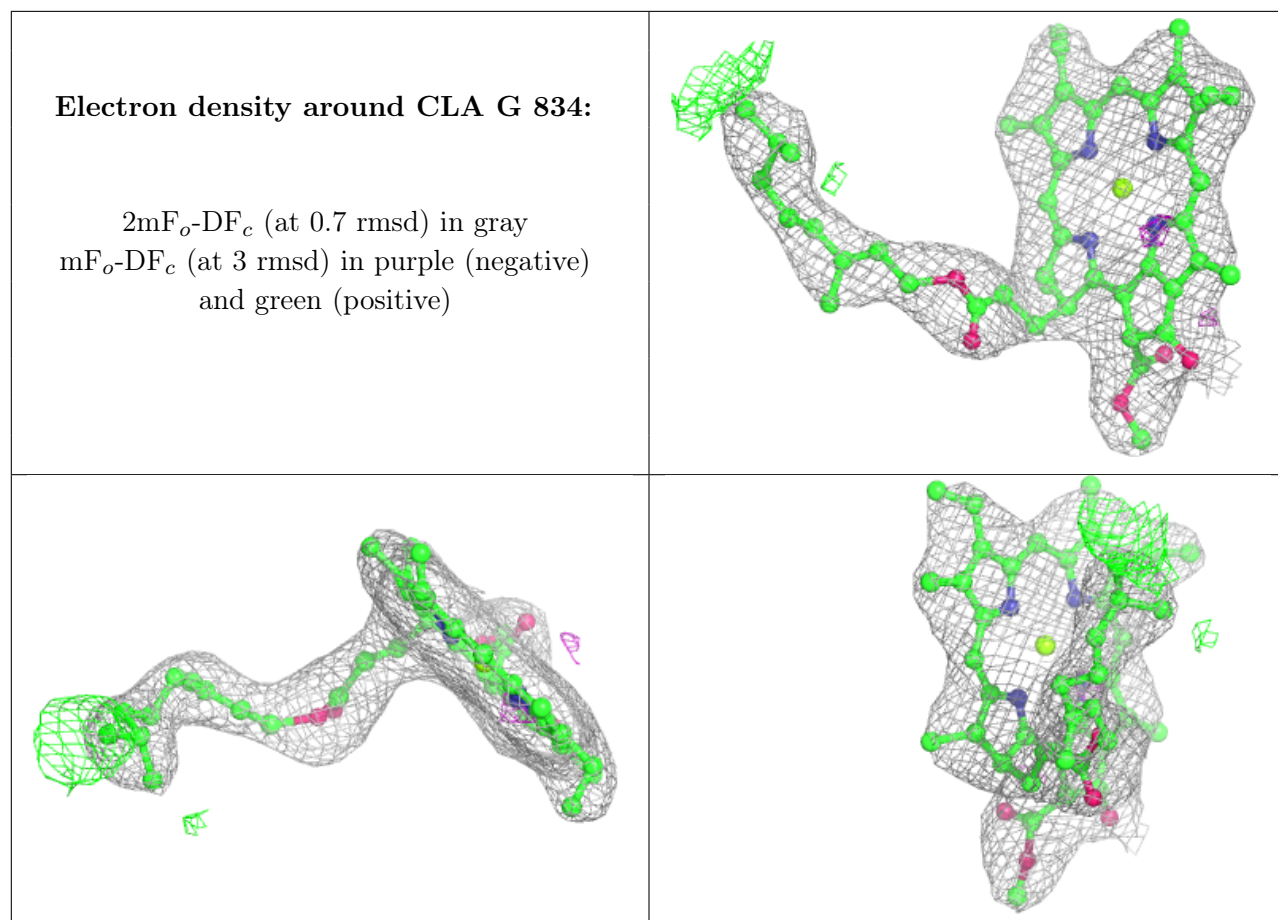
**Electron density around CLA G 831:**

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



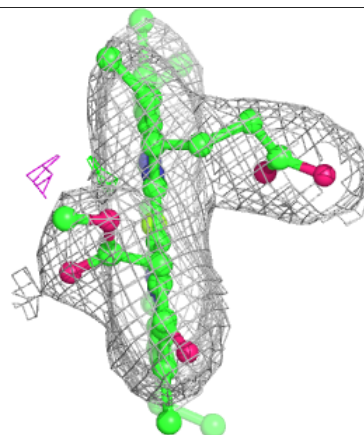
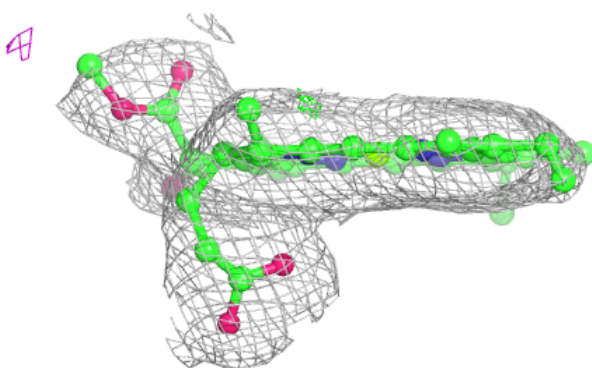
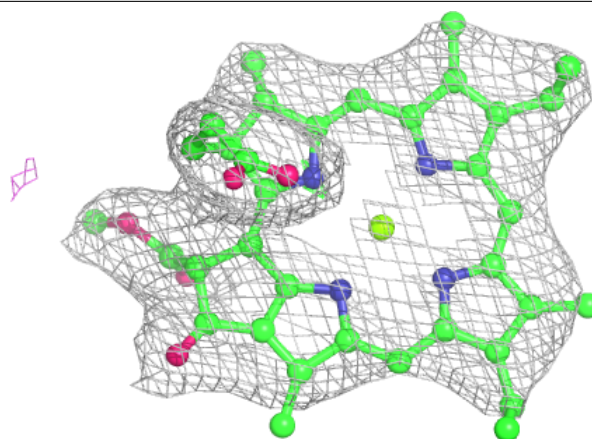




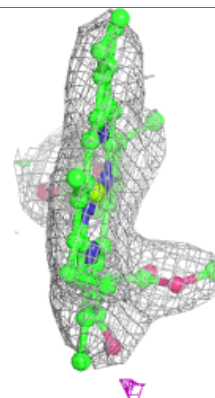
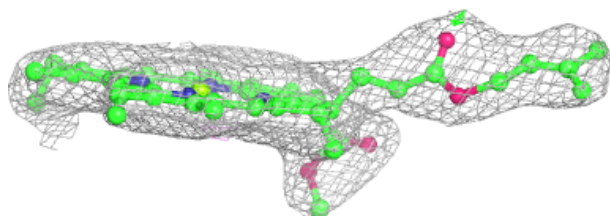
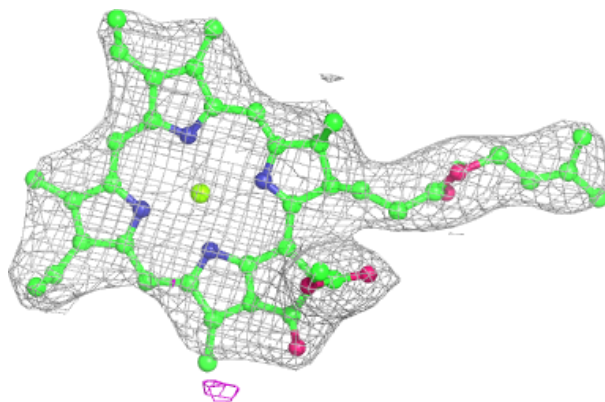


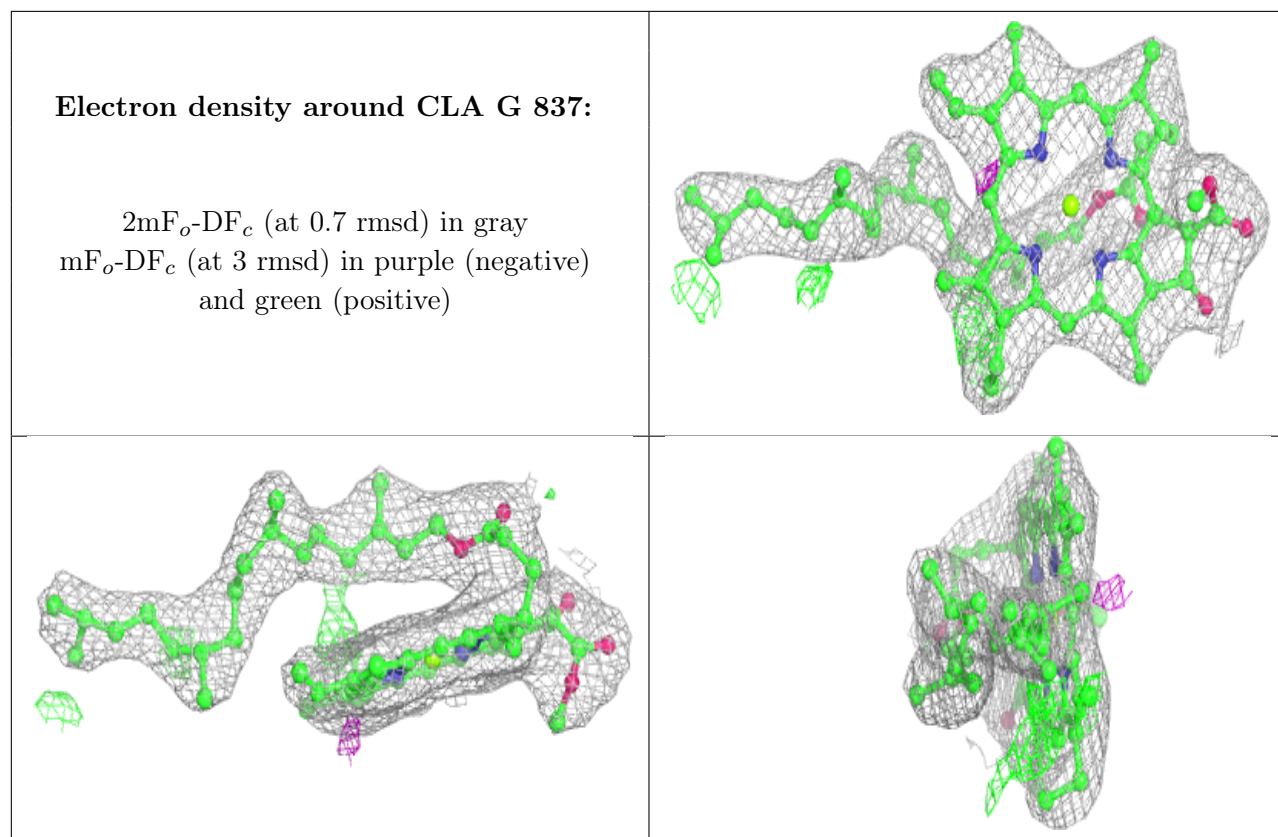
**Electron density around CLA G 835:**

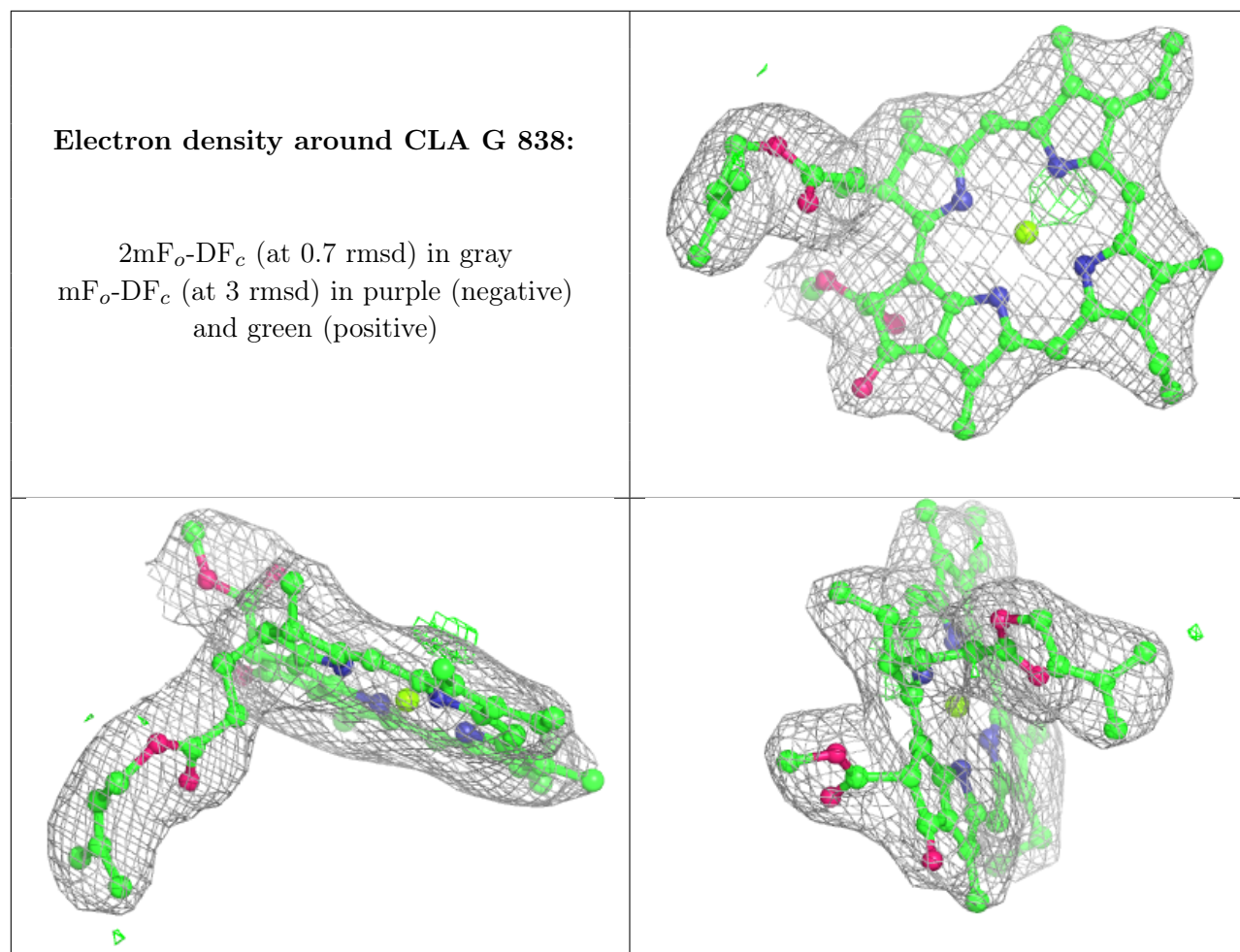
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

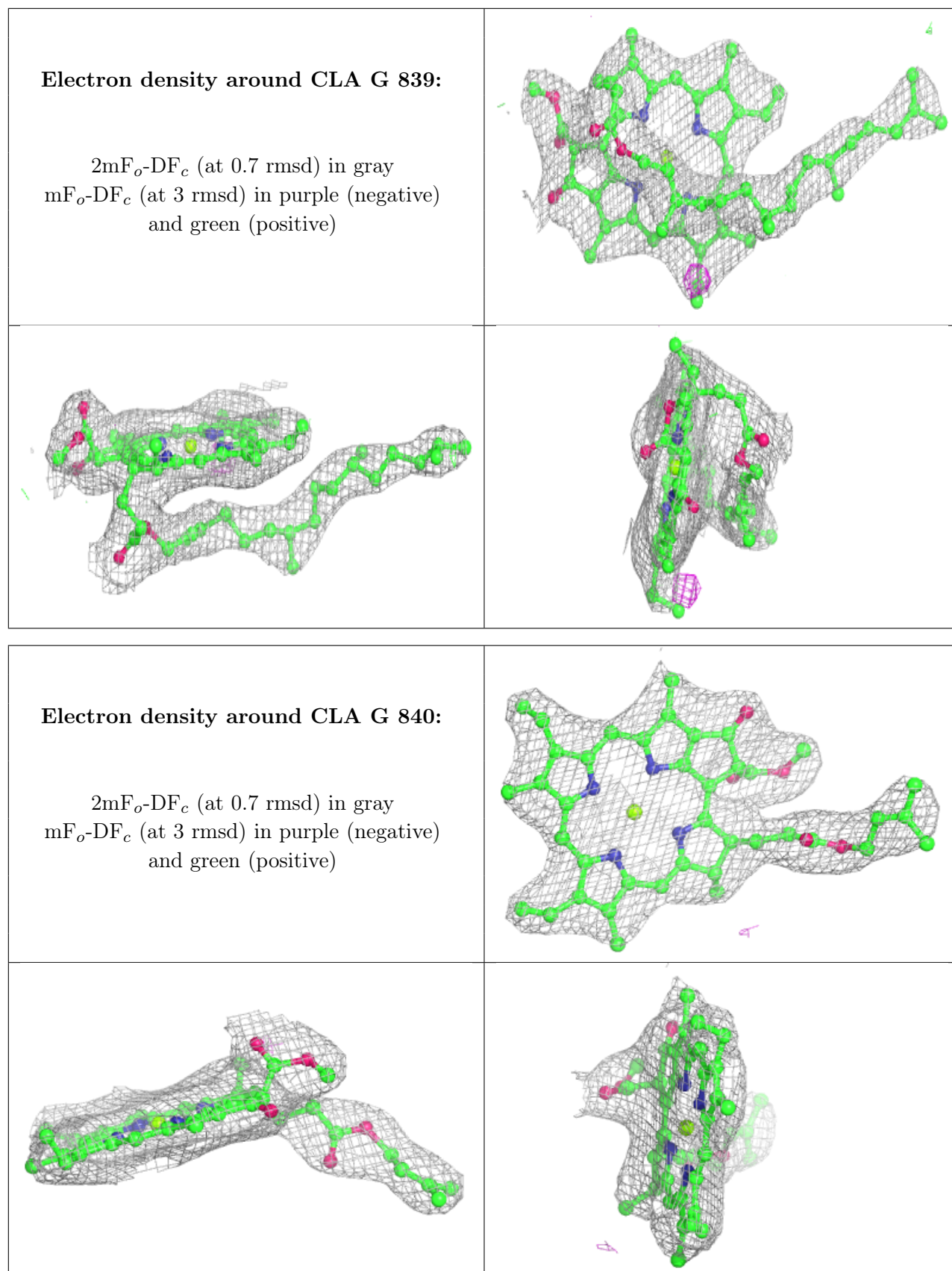
**Electron density around CLA G 836:**

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



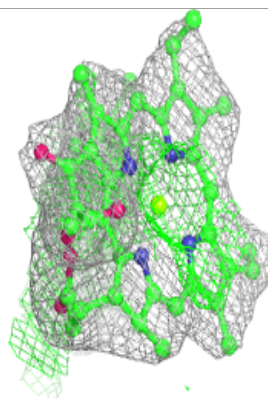
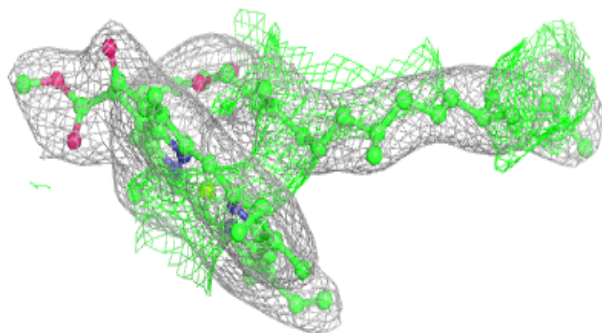
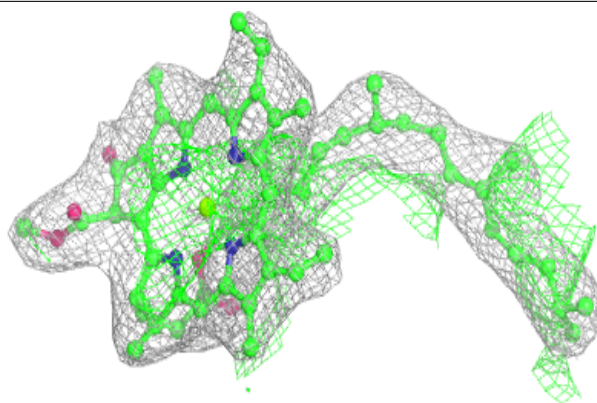




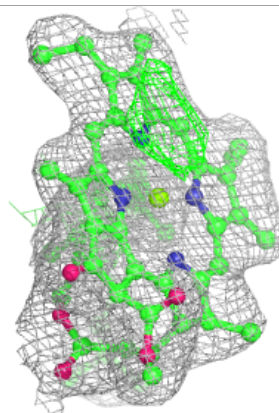
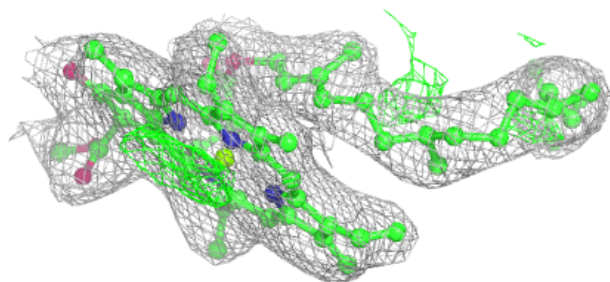
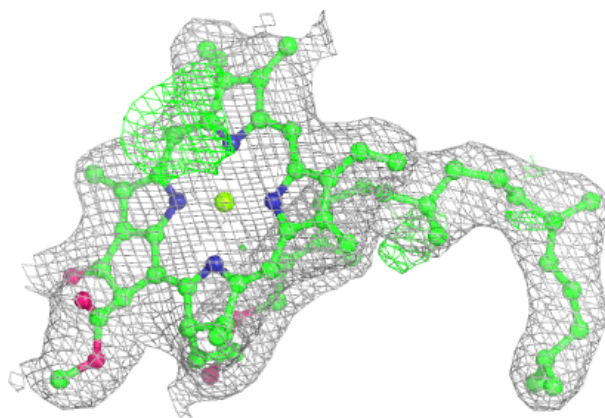


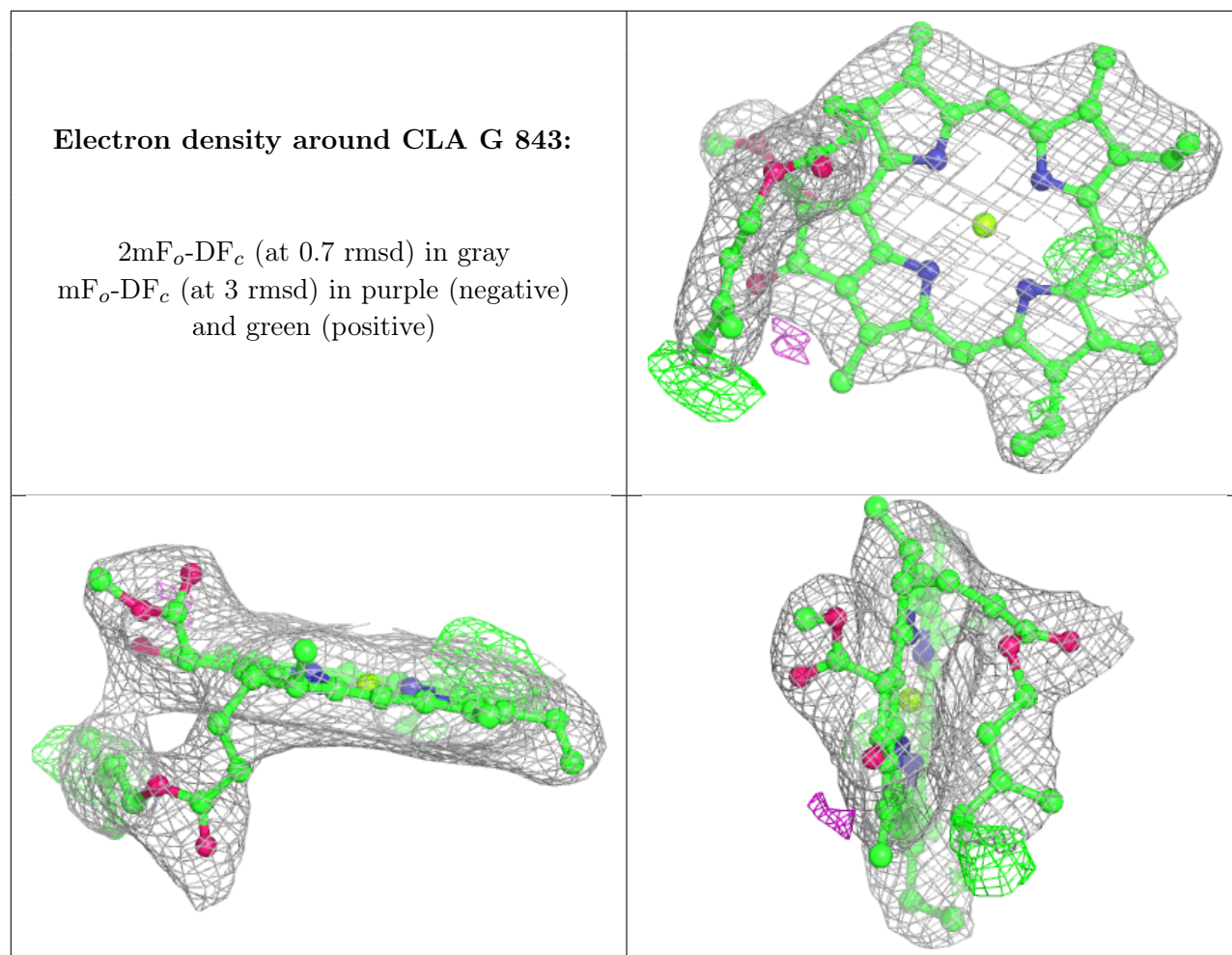
**Electron density around CLA G 841:**

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

**Electron density around CLA G 842:**

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

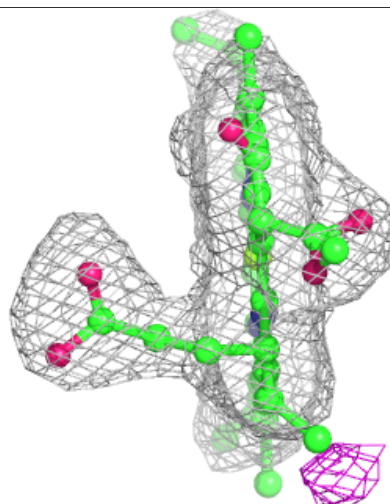
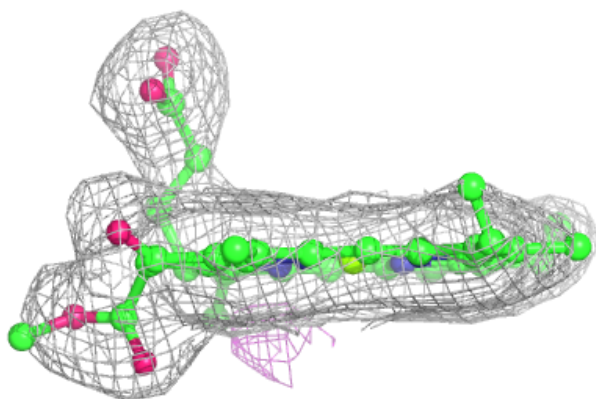
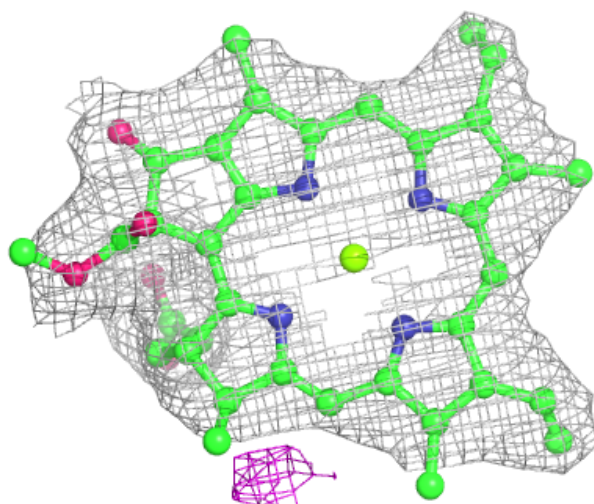






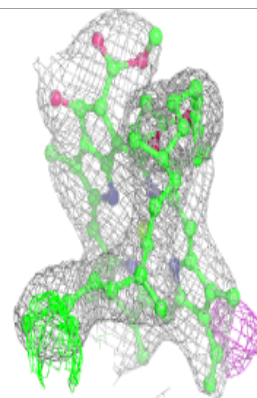
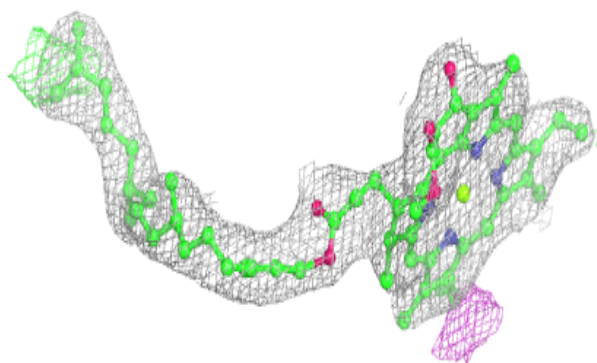
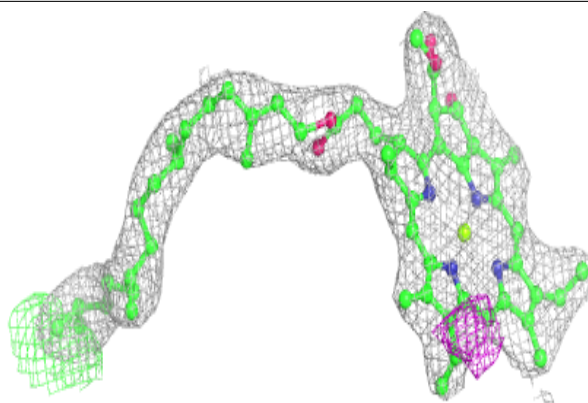
**Electron density around CLA G 853:**

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

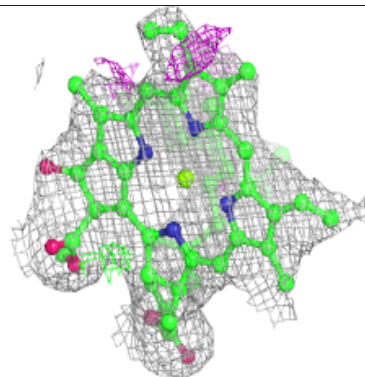
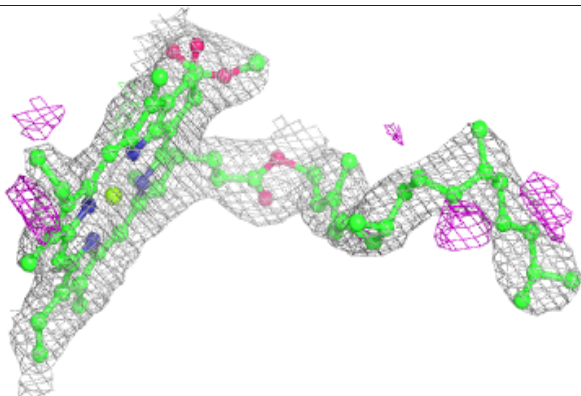
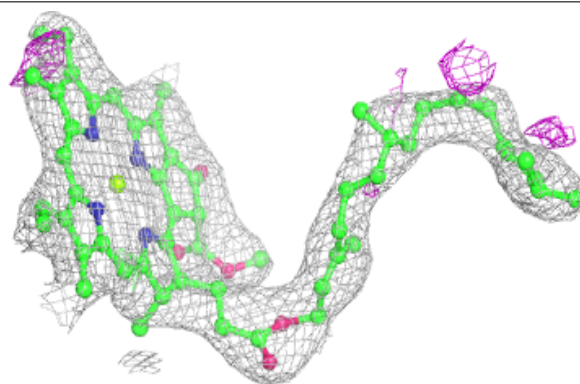


**Electron density around CLA H 801:**

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

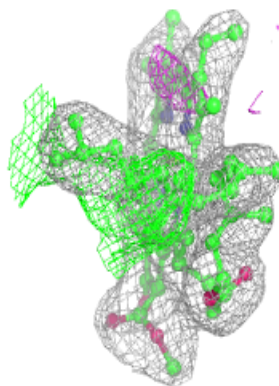
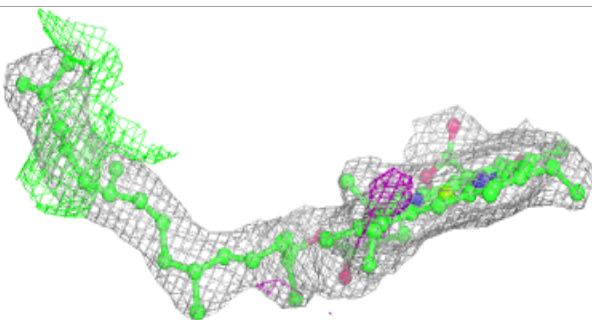
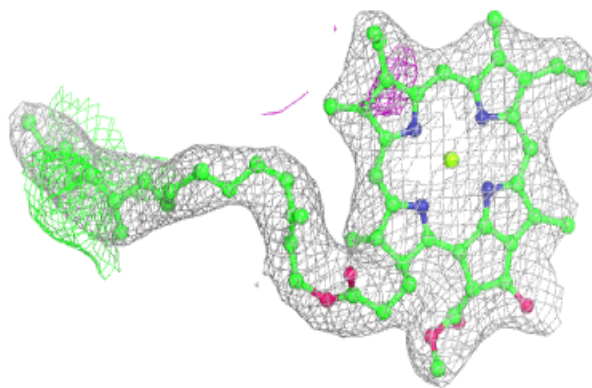
**Electron density around CLA H 802:**

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

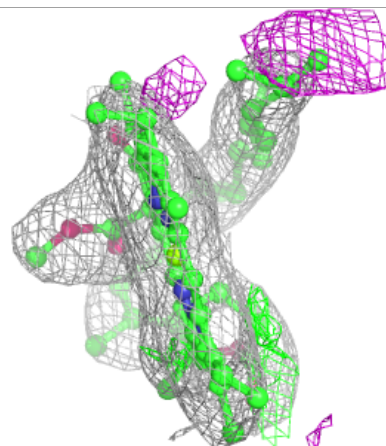
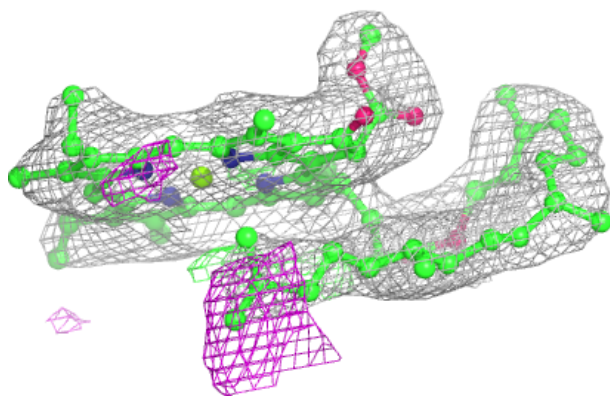
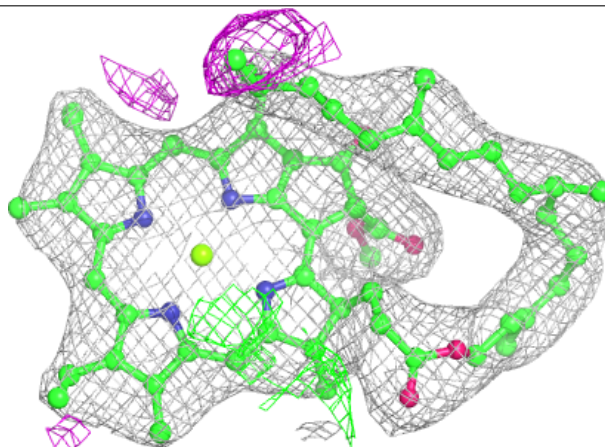


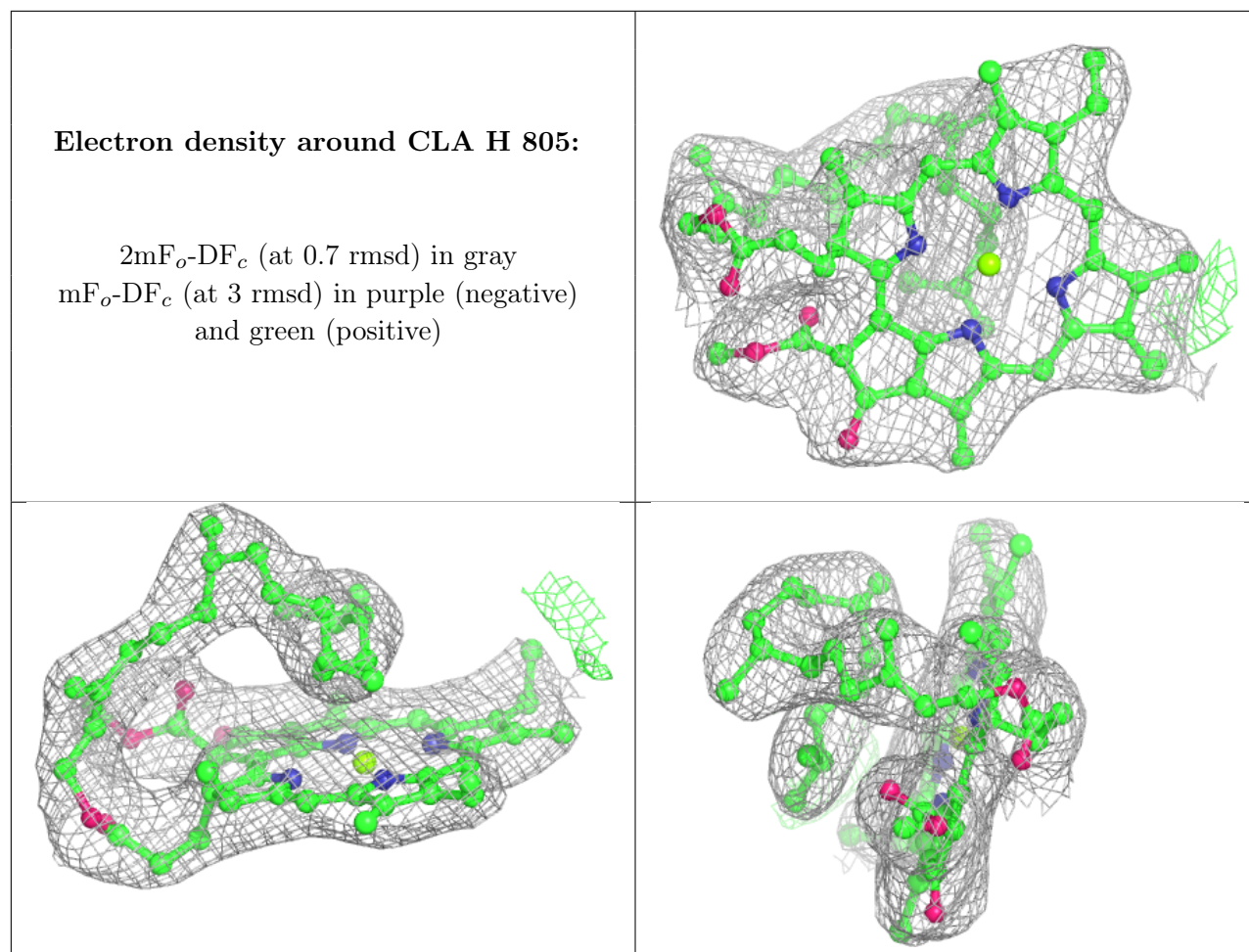
**Electron density around CLA H 803:**

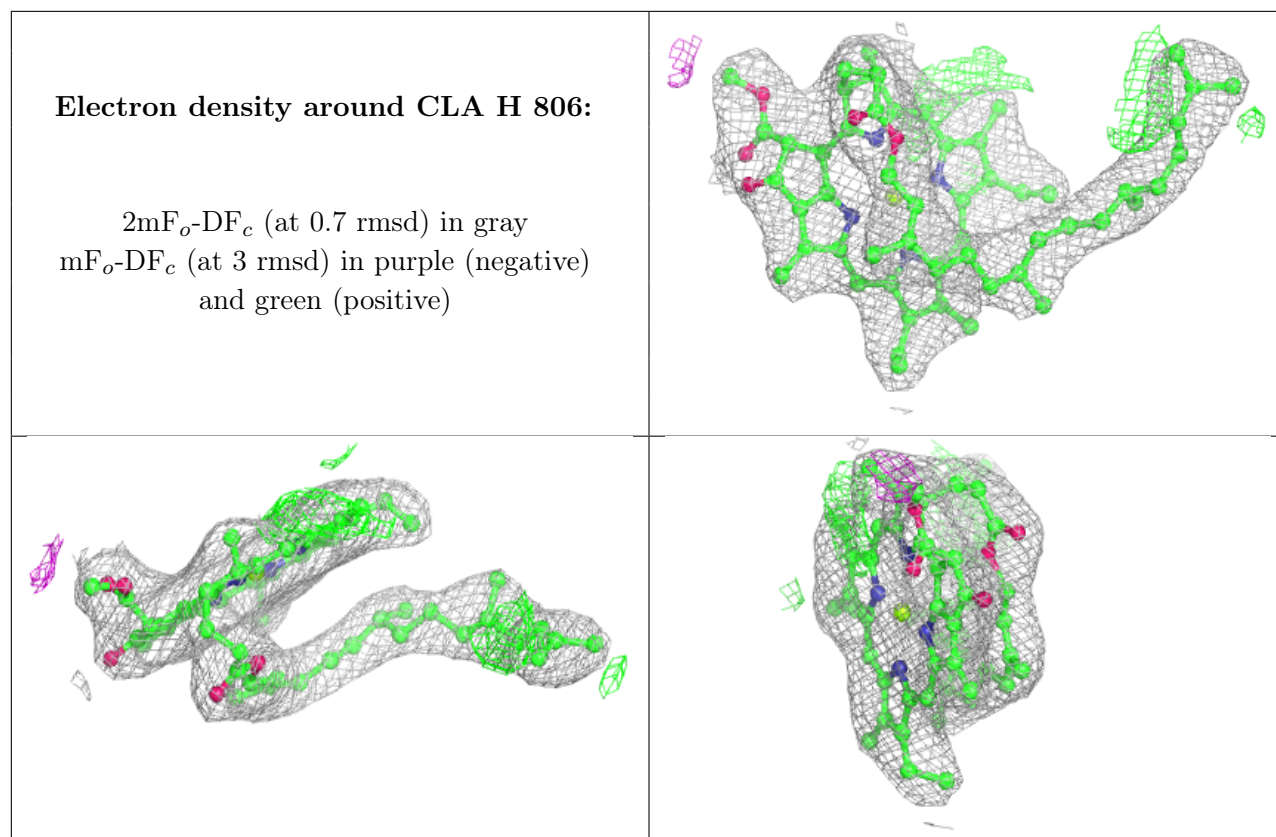
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

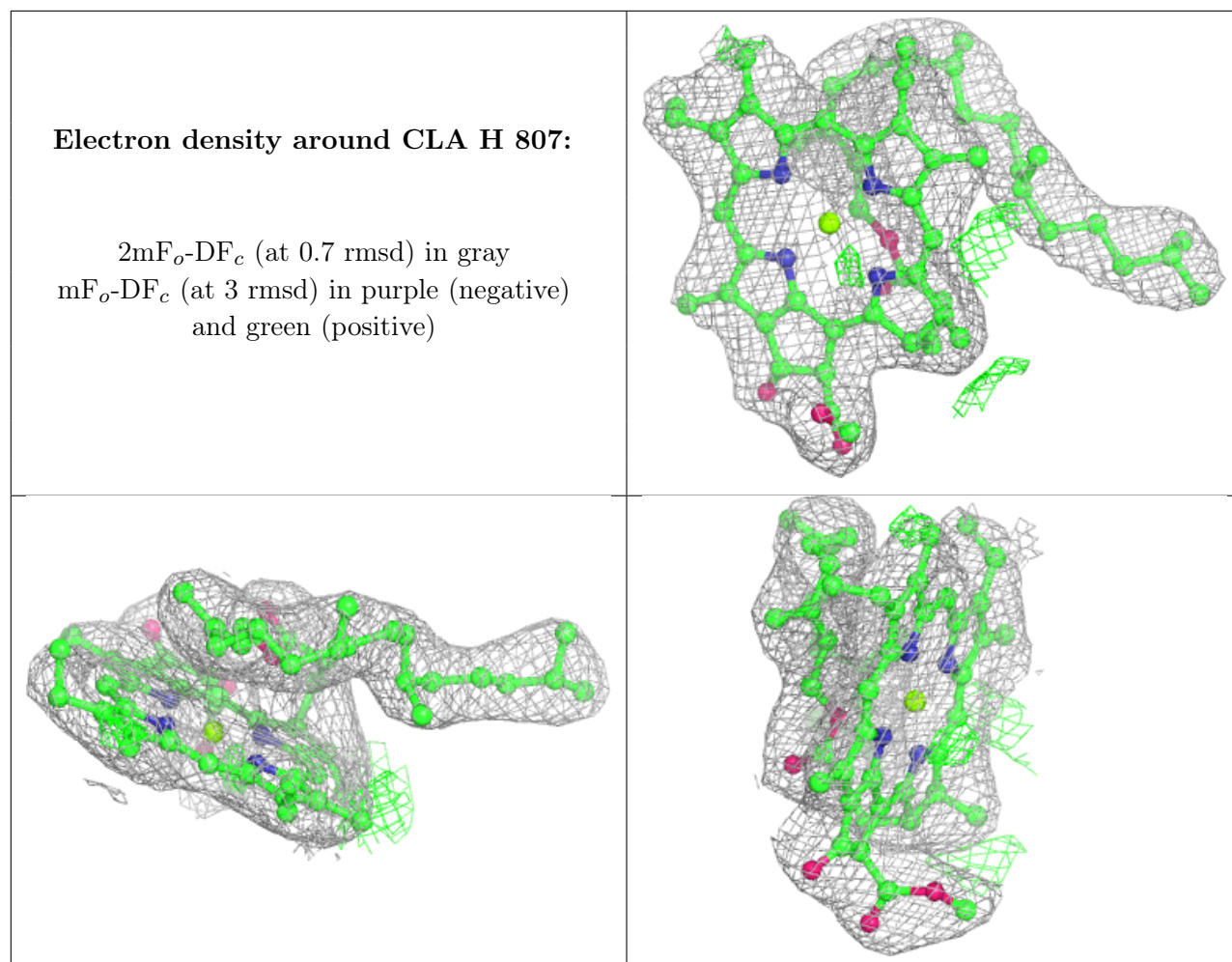
**Electron density around CLA H 804:**

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



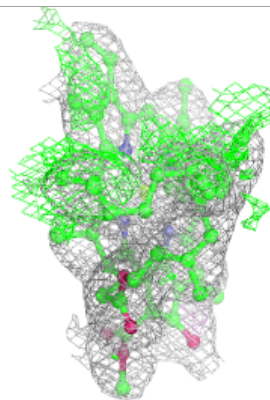
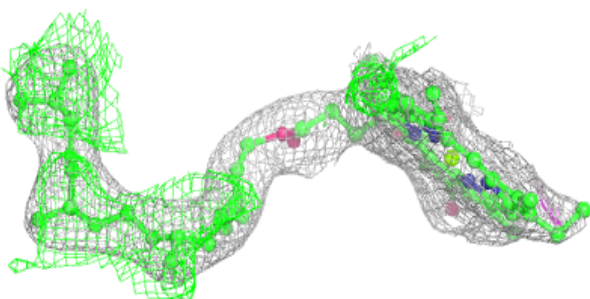
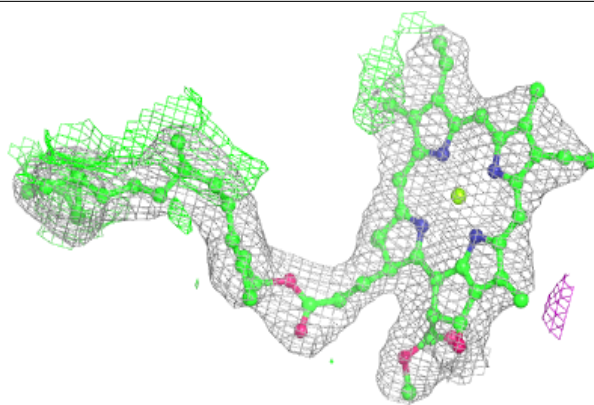




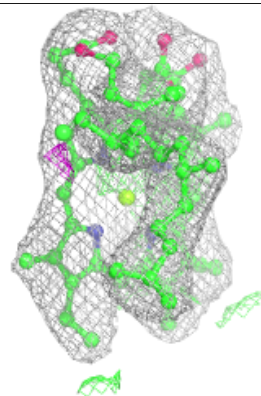
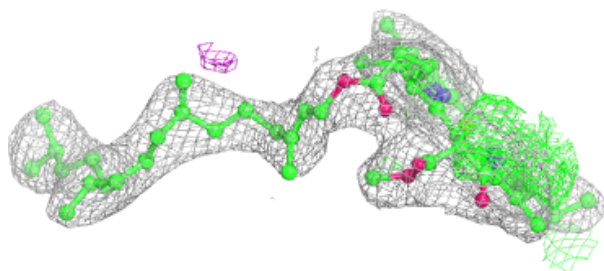
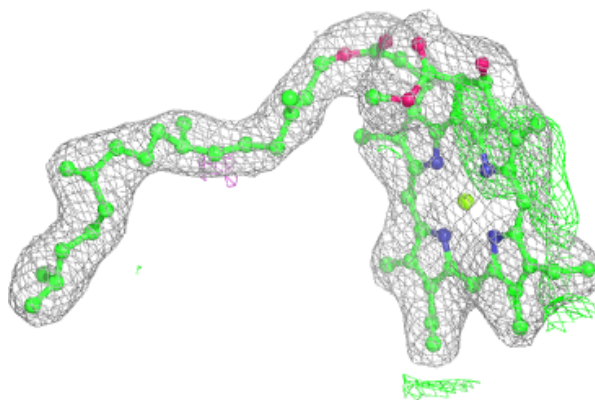


**Electron density around CLA H 808:**

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

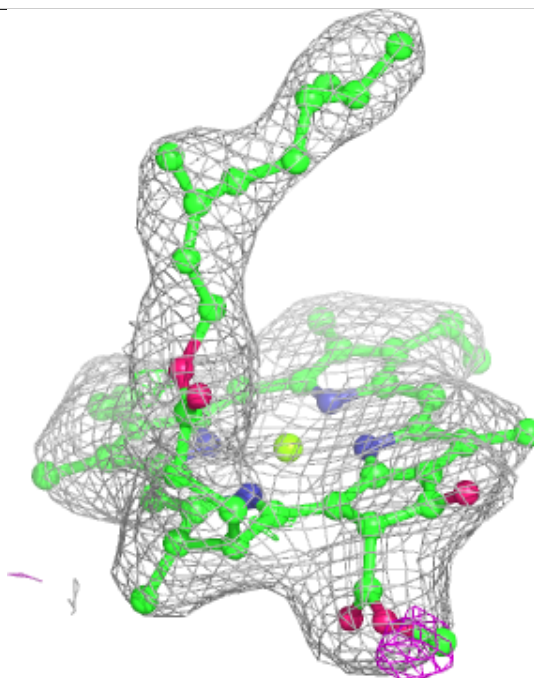
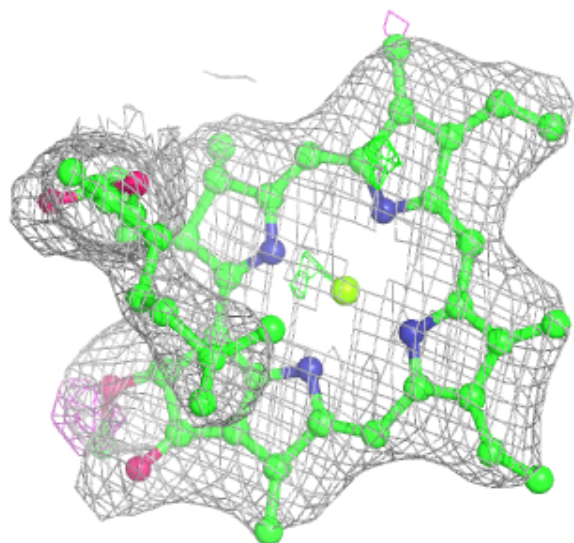
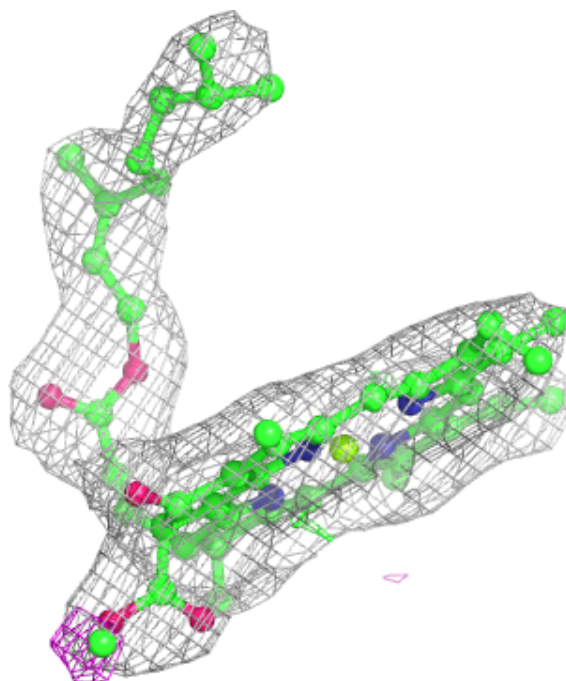
**Electron density around CLA H 809:**

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



**Electron density around CLA H 810:**

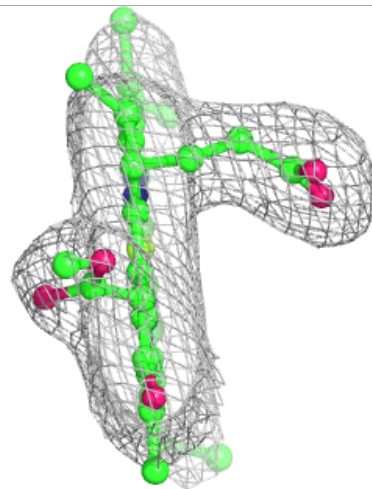
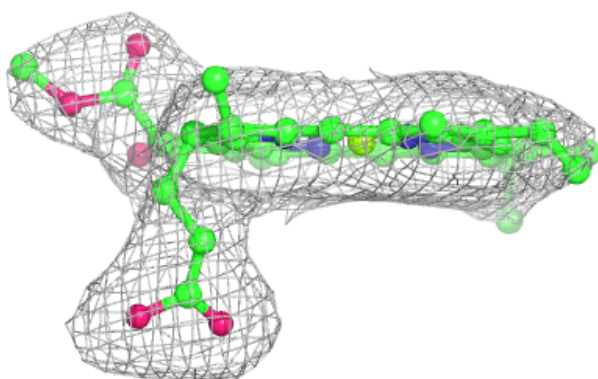
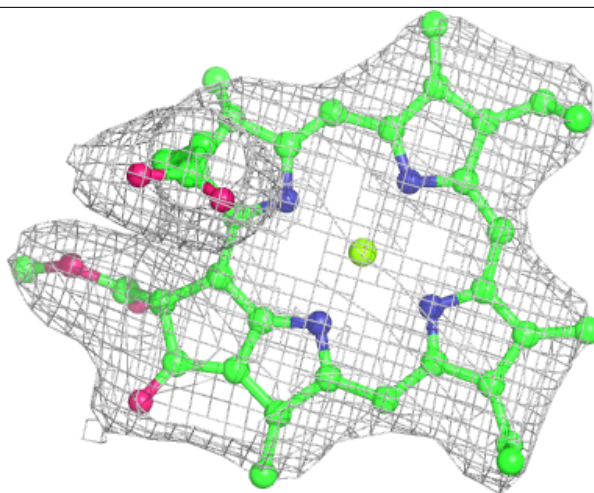
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





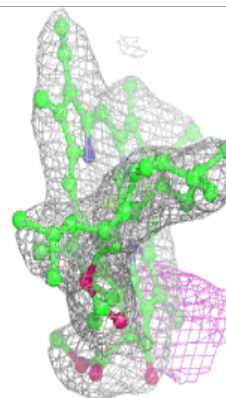
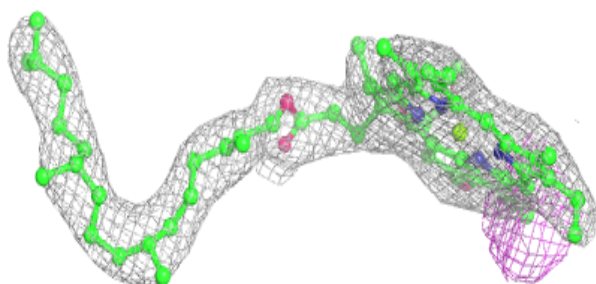
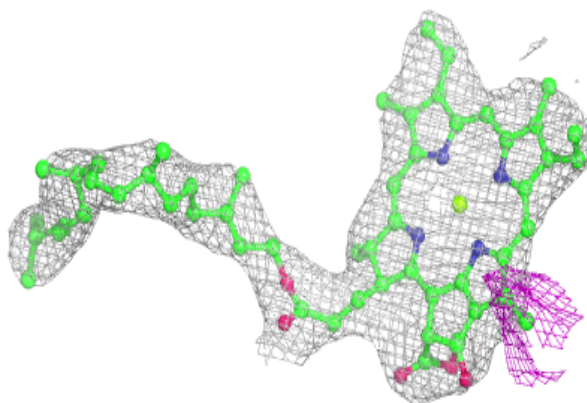
**Electron density around CLA H 811:**

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

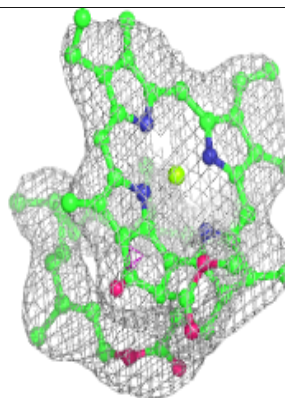
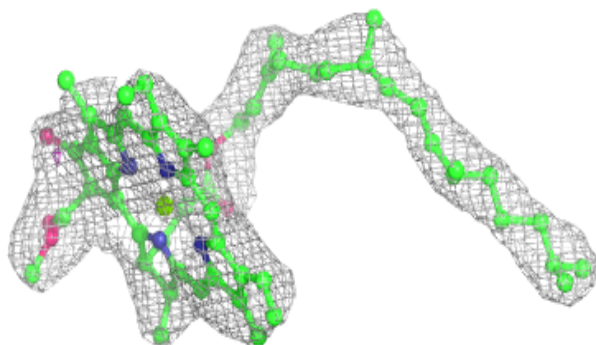
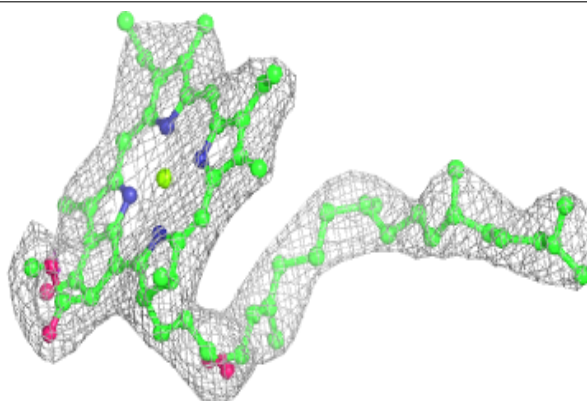


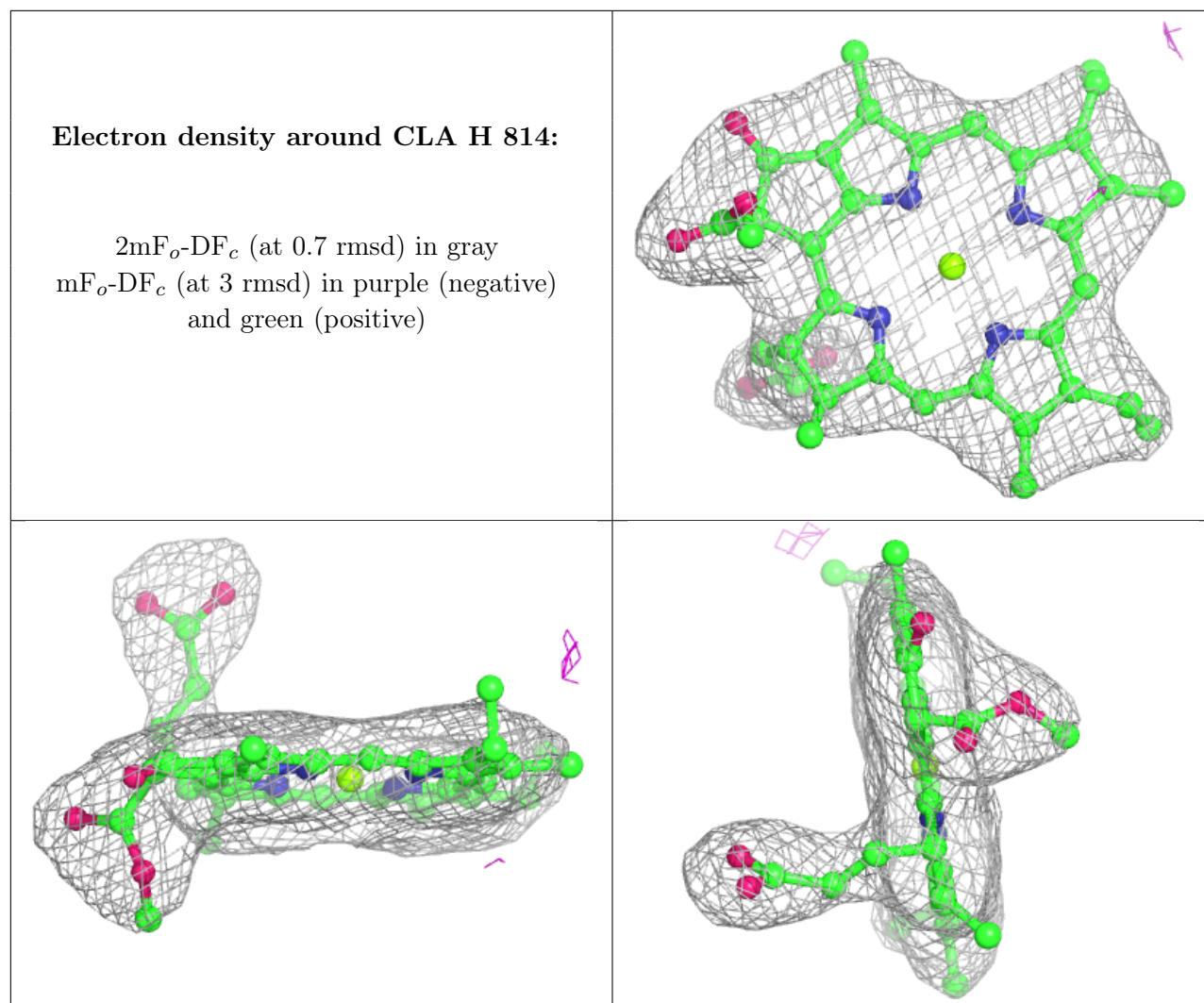
**Electron density around CLA H 812:**

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

**Electron density around CLA H 813:**

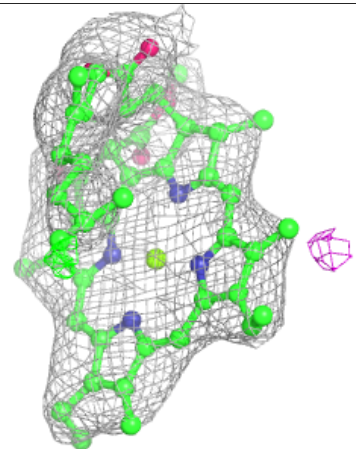
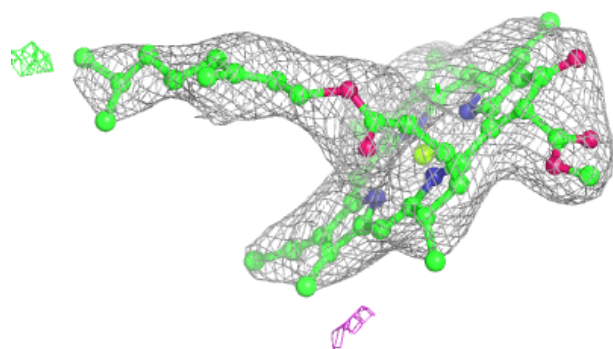
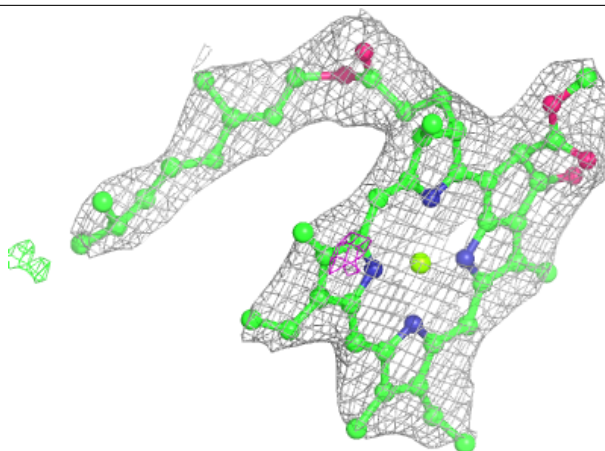
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



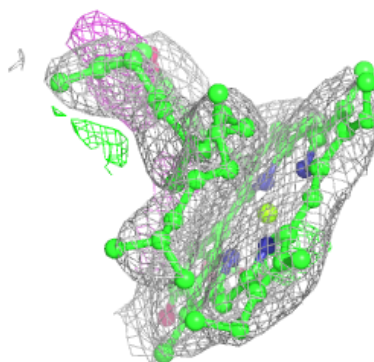
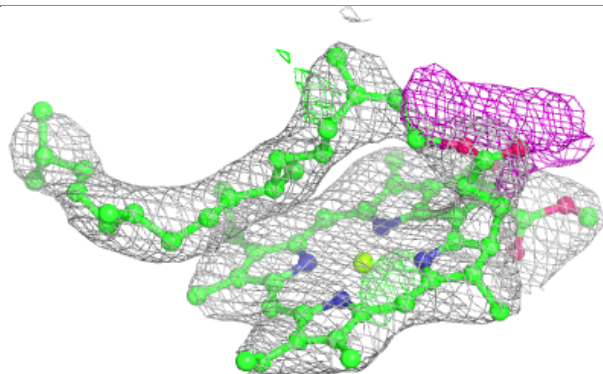
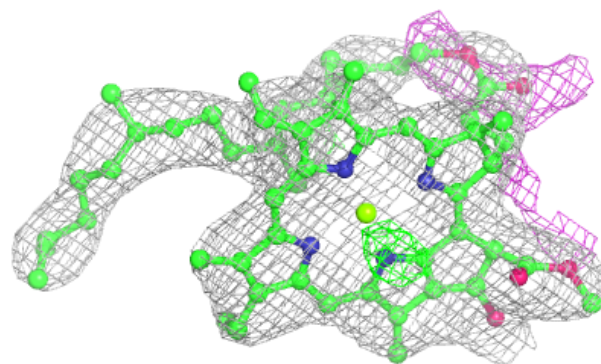


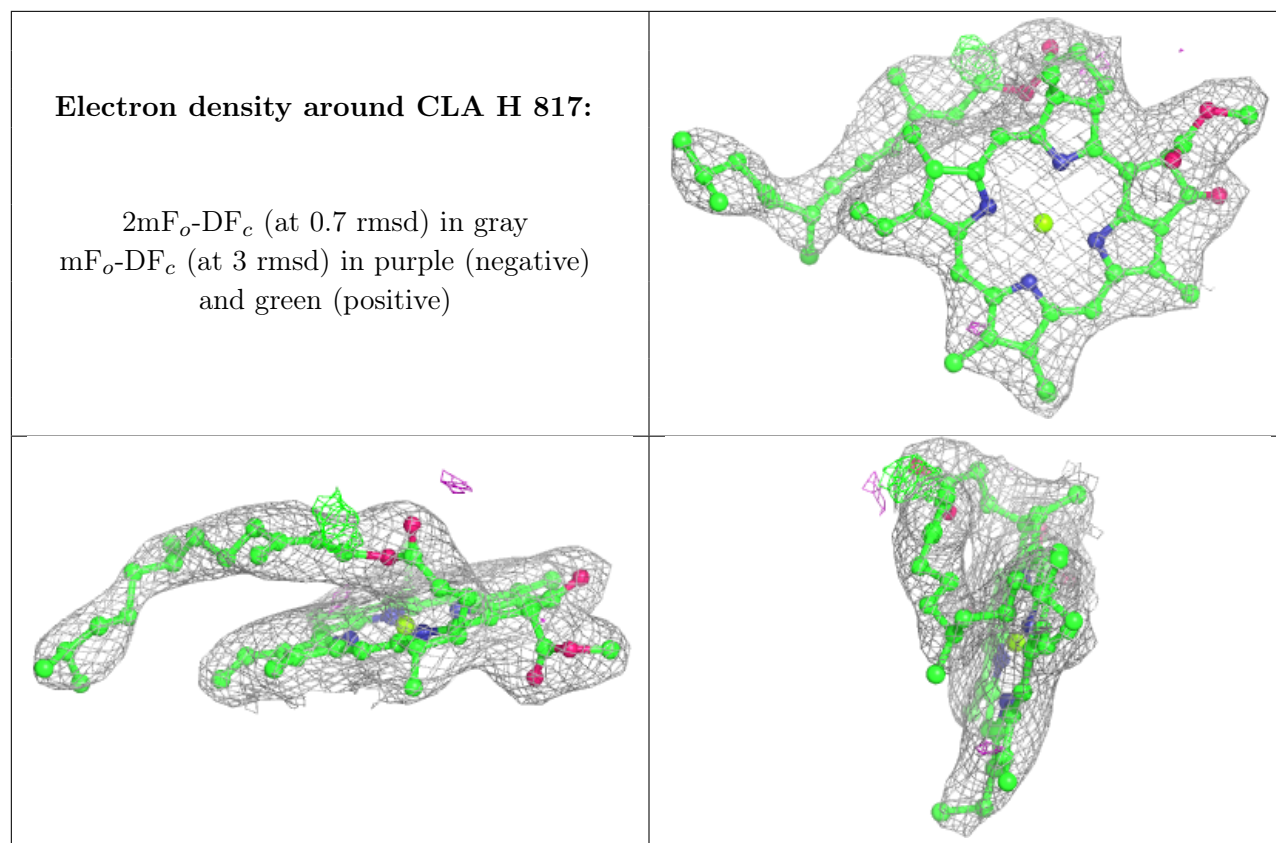
**Electron density around CLA H 815:**

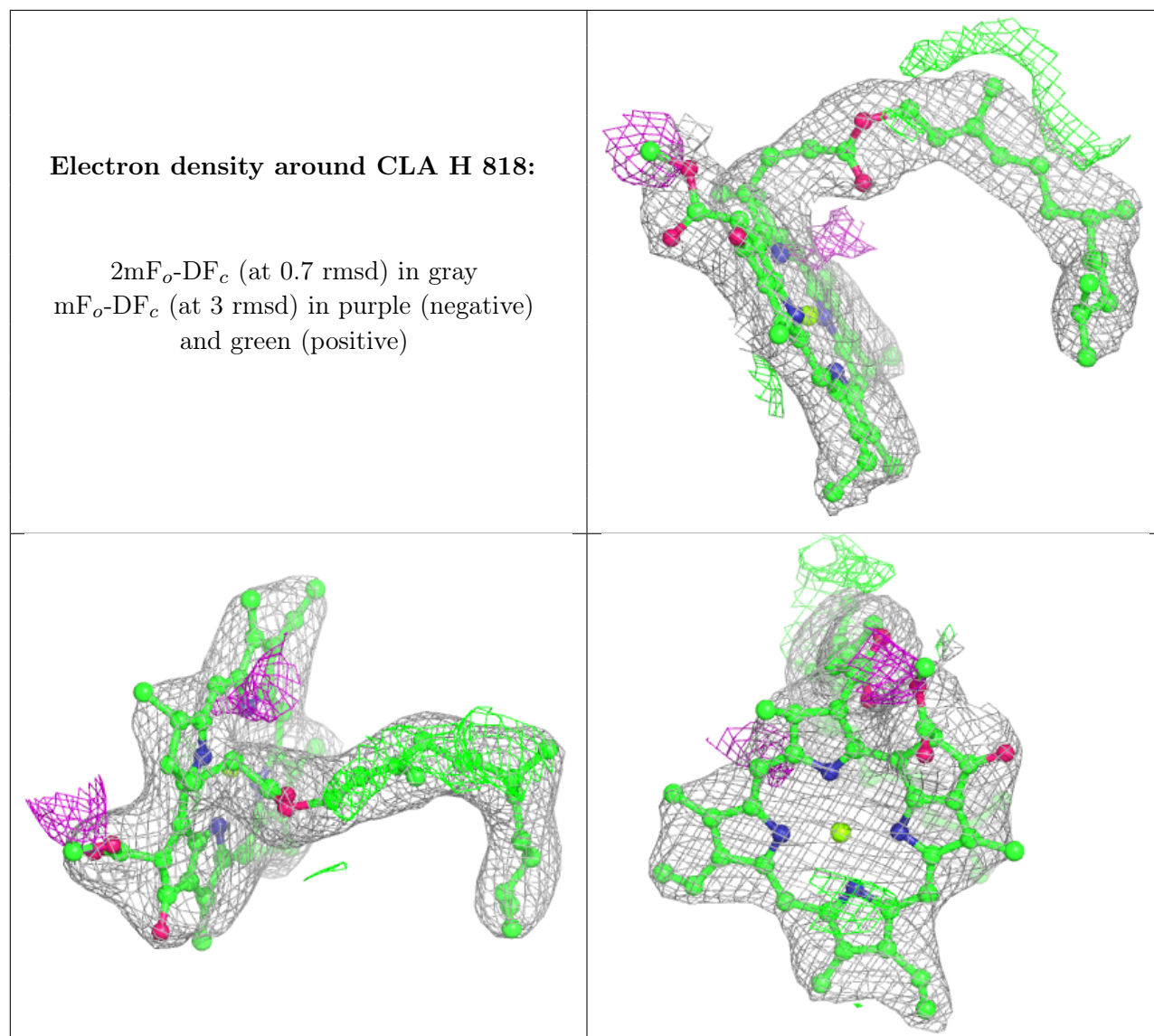
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA H 816:**

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

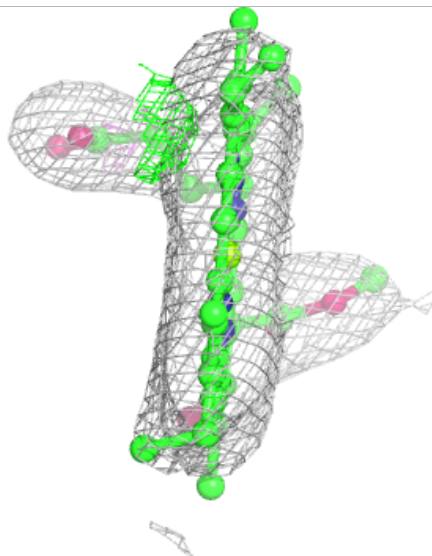
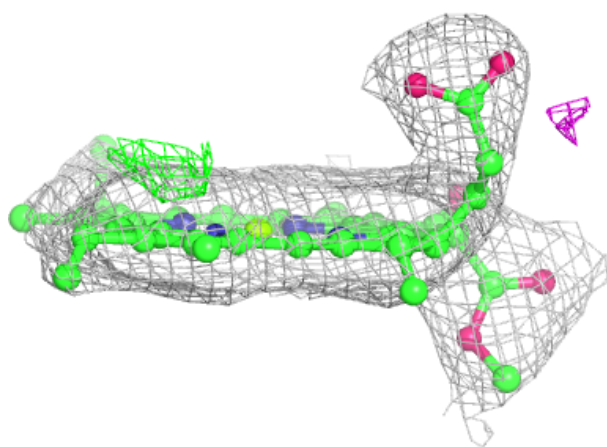
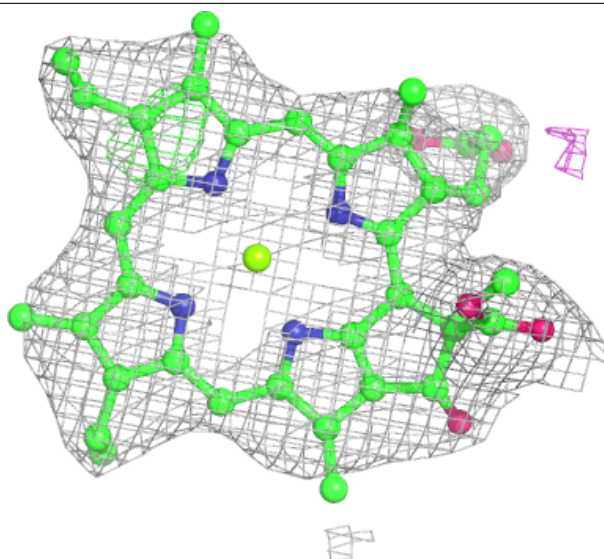


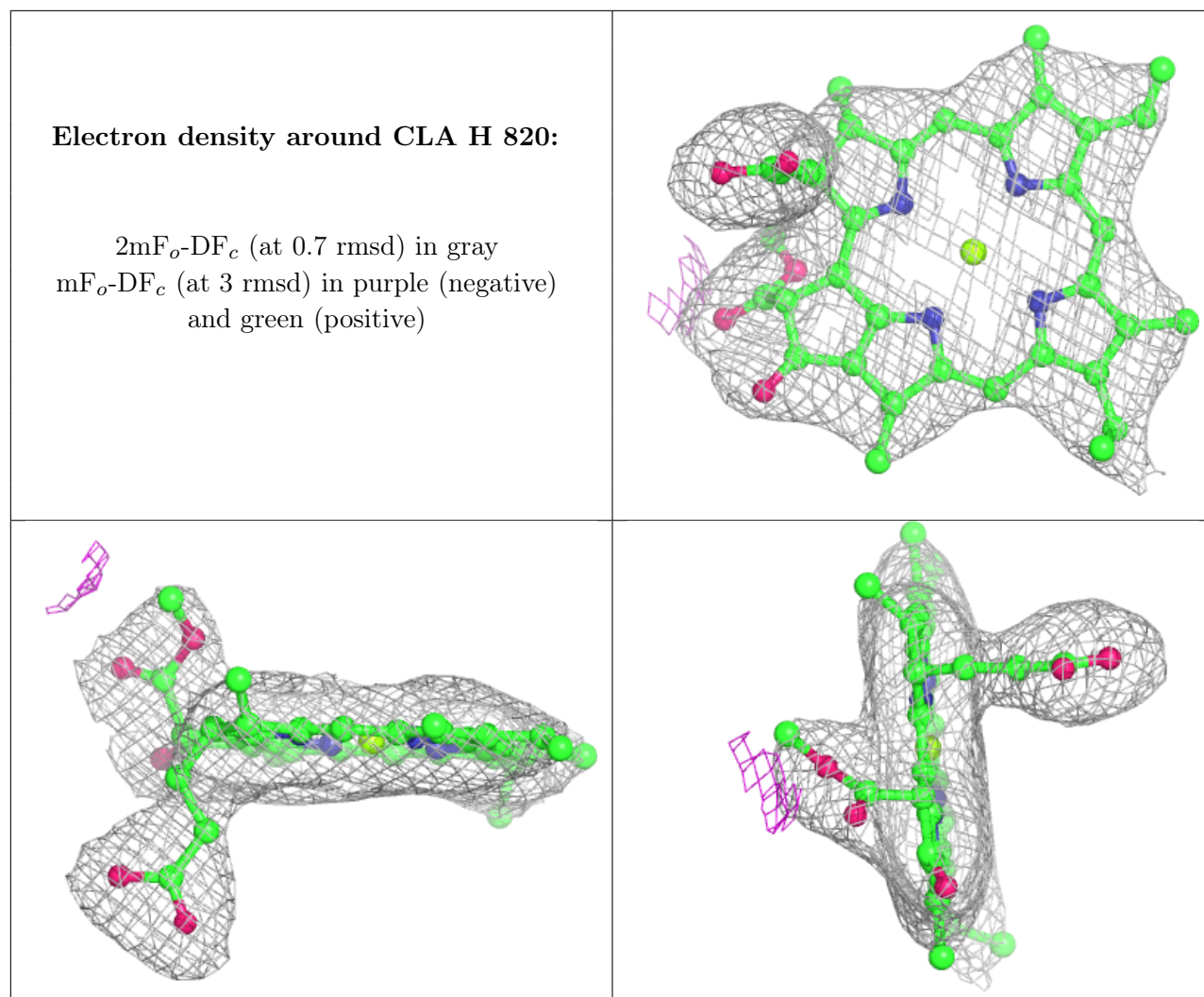




**Electron density around CLA H 819:**

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

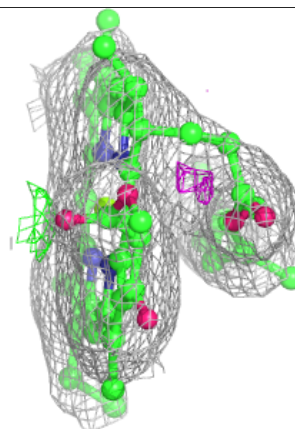
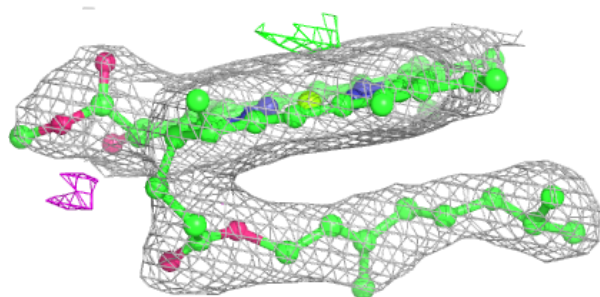
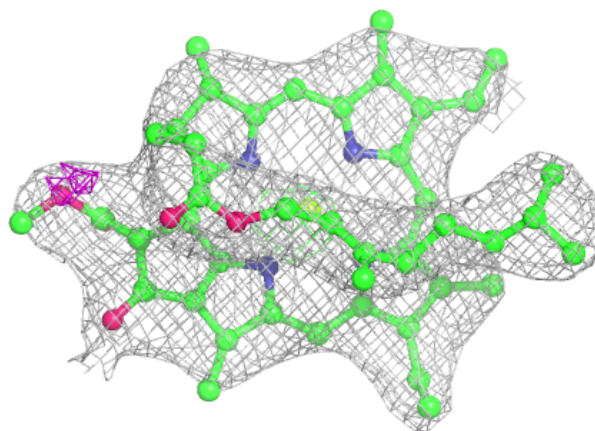




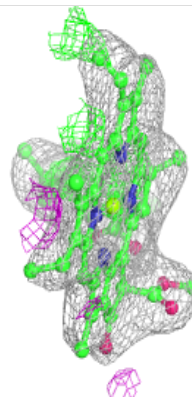
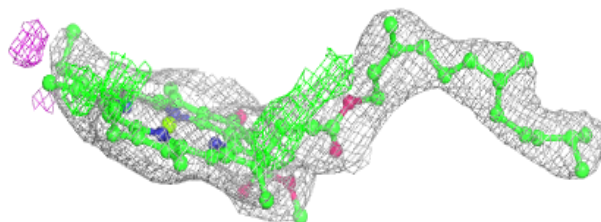
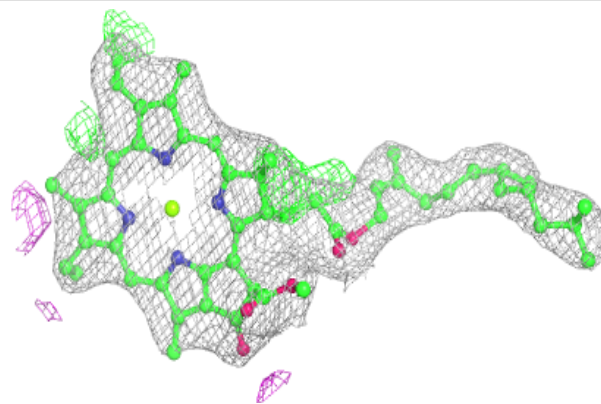


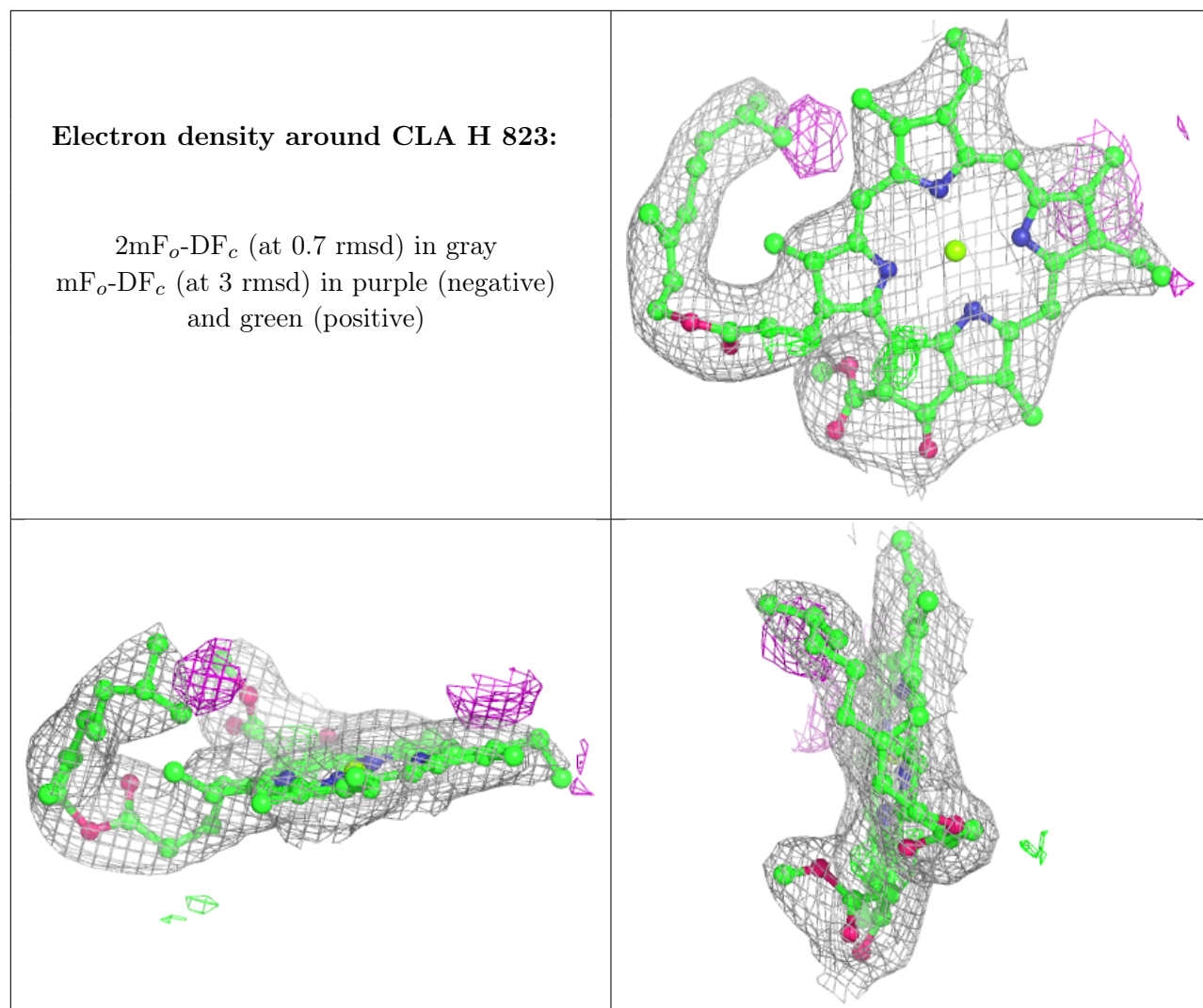
**Electron density around CLA H 821:**

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

**Electron density around CLA H 822:**

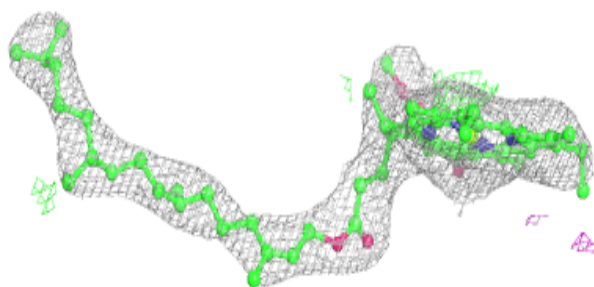
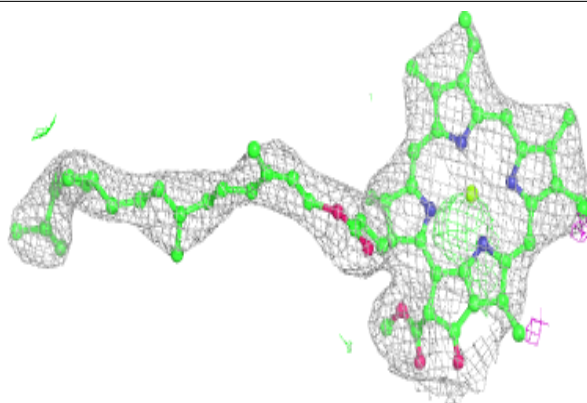
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



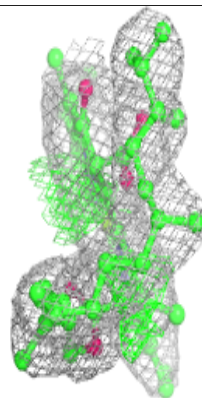
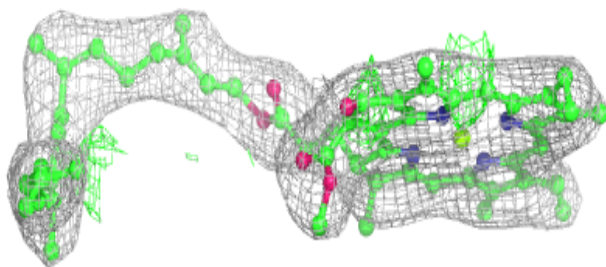
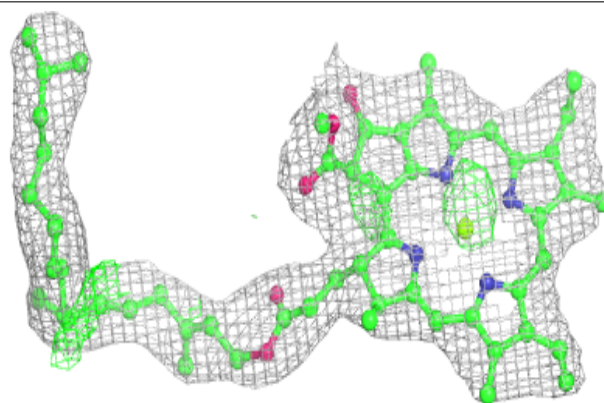


**Electron density around CLA H 824:**

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

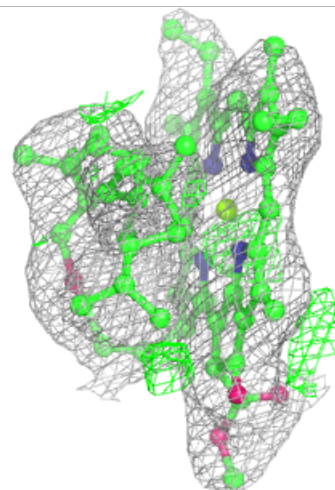
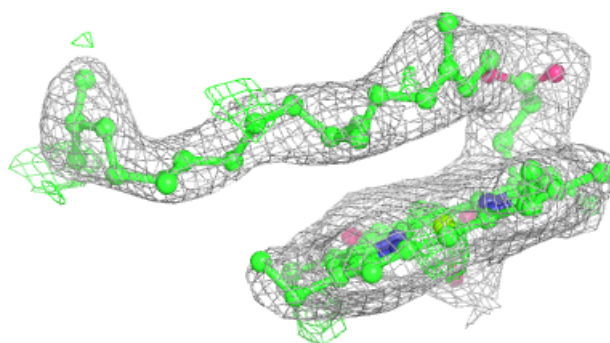
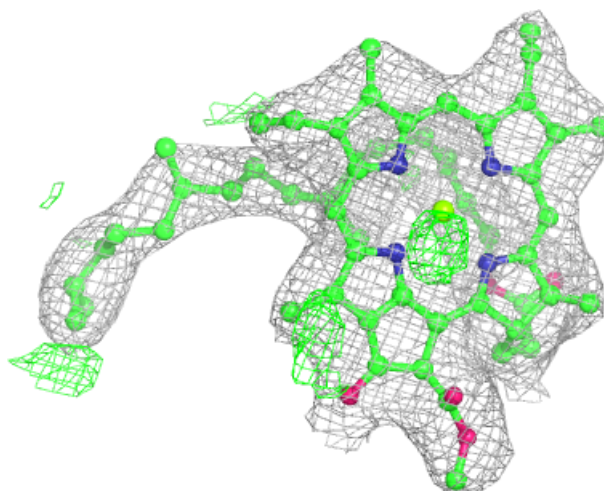
**Electron density around CLA H 825:**

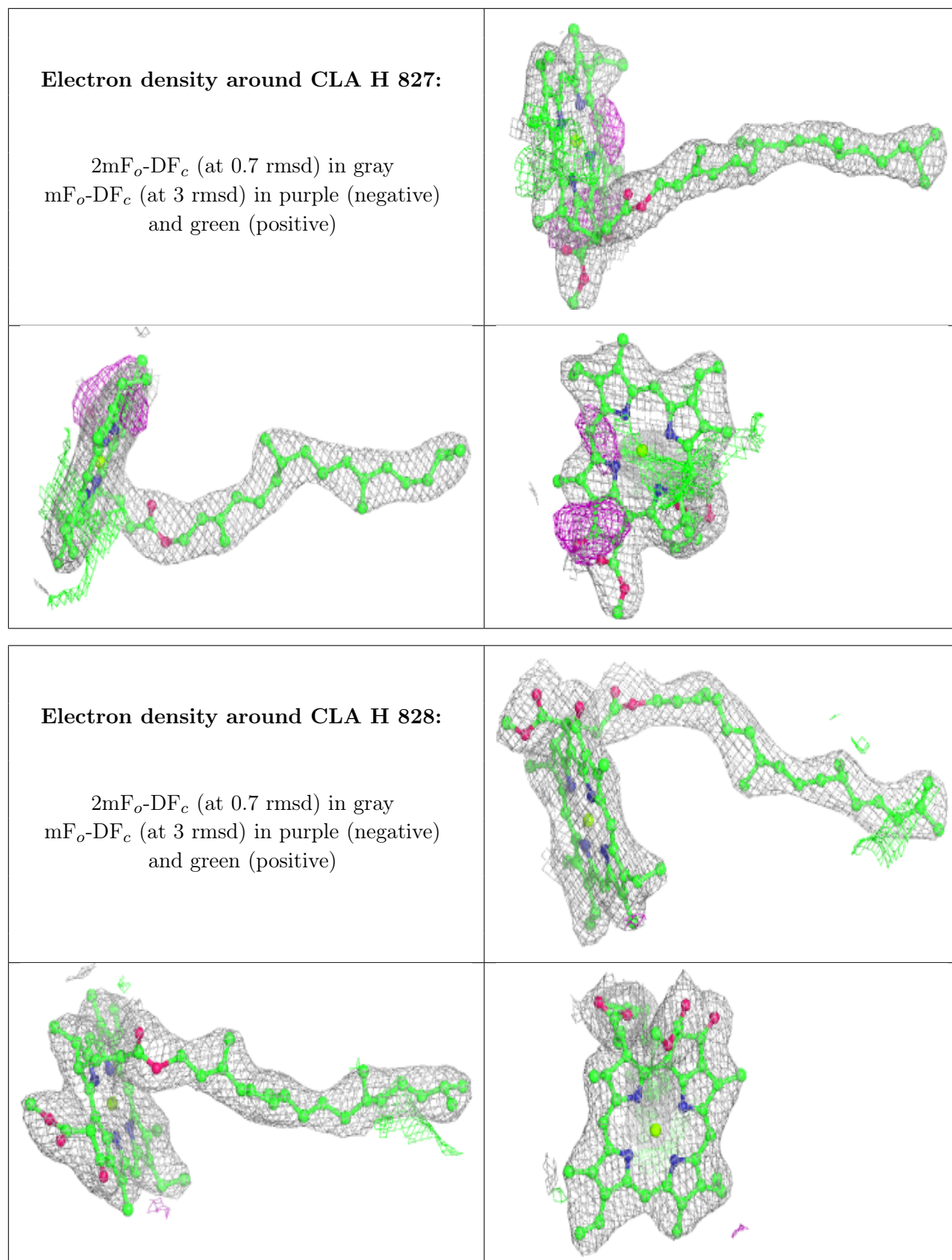
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

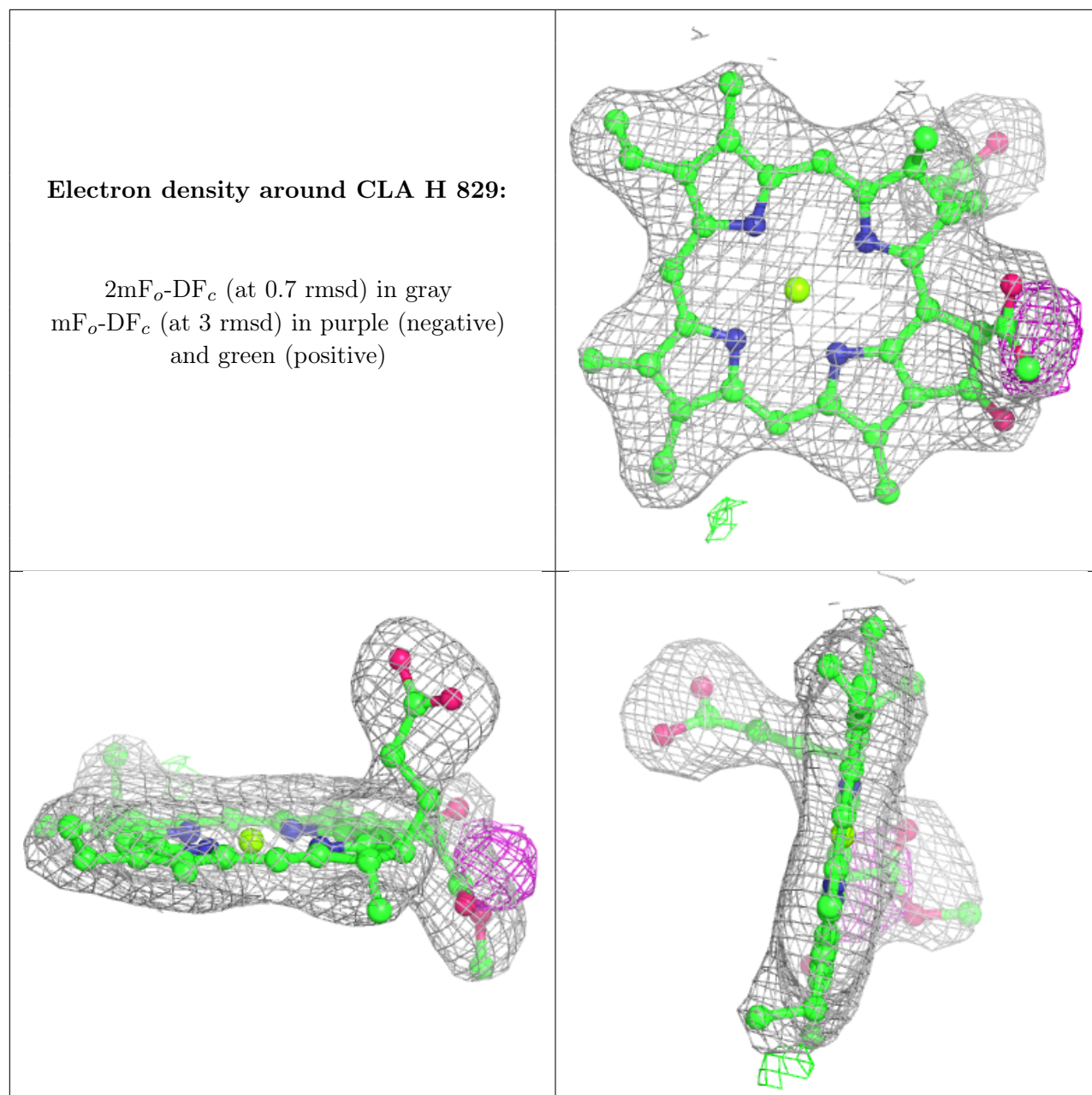


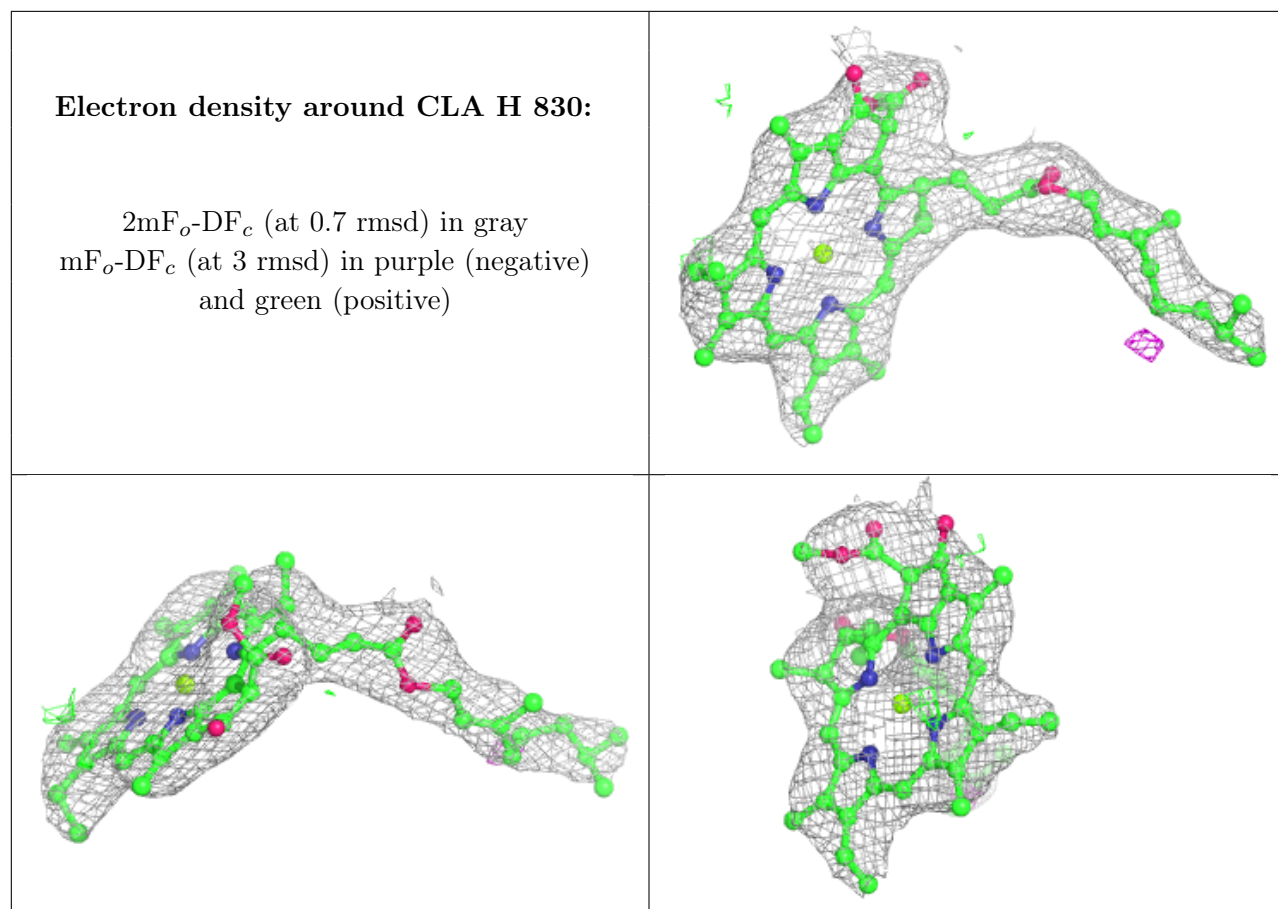
**Electron density around CLA H 826:**

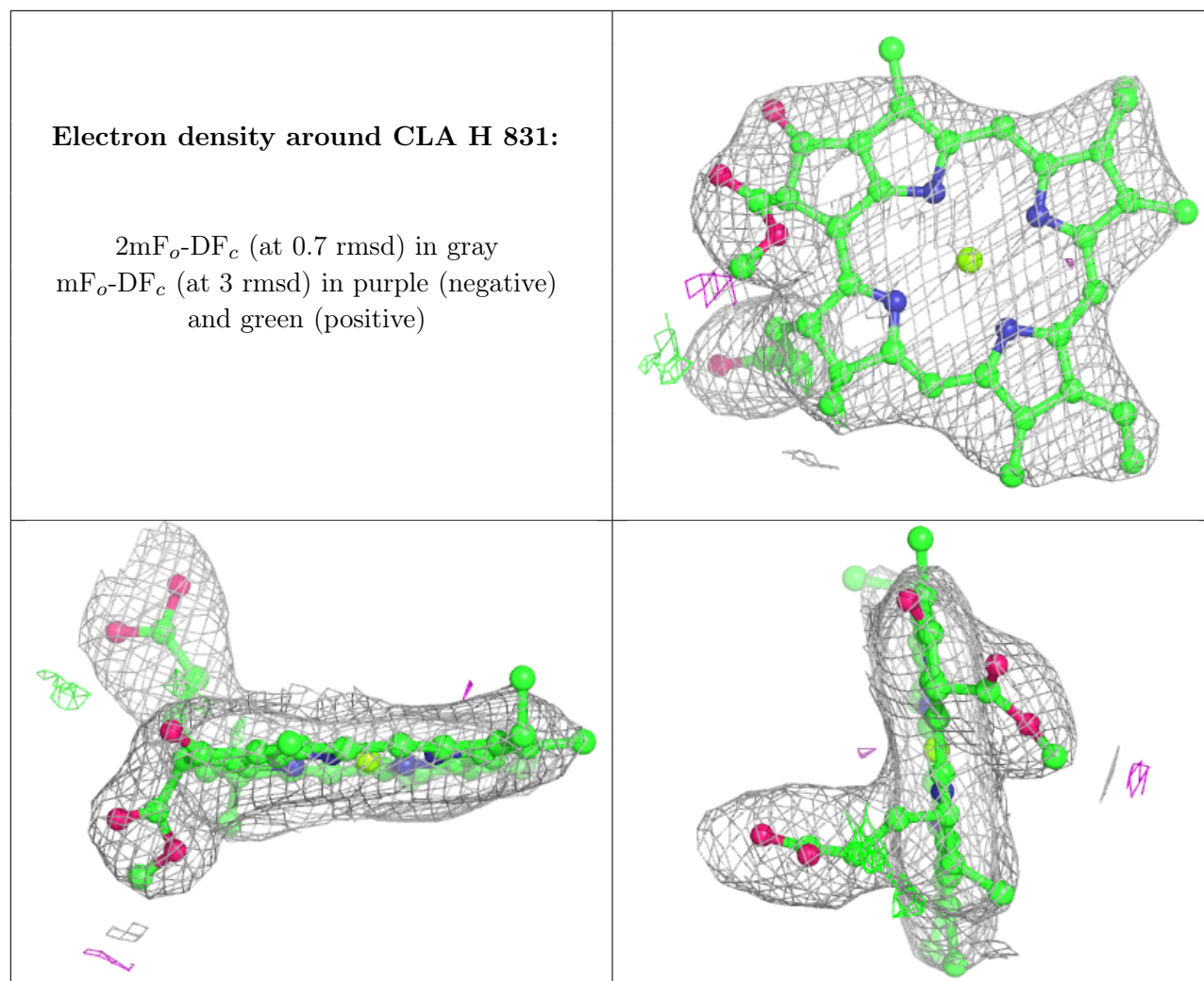
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)







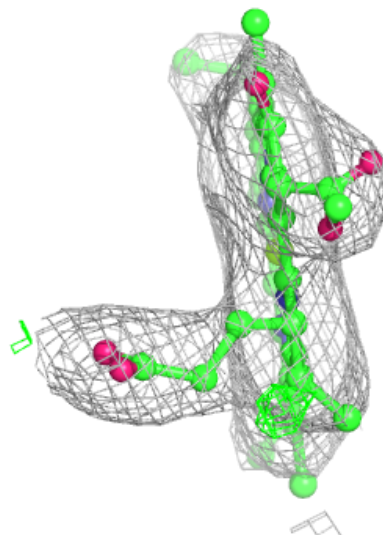
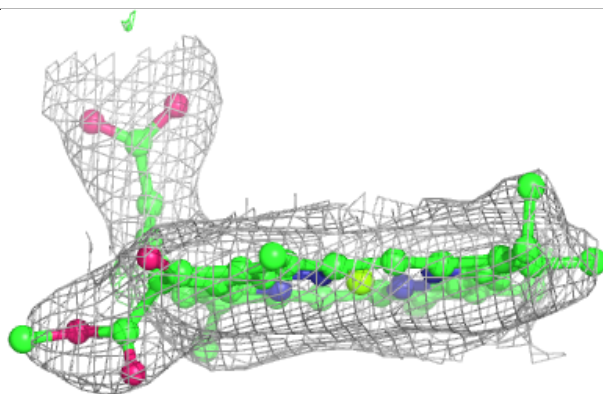
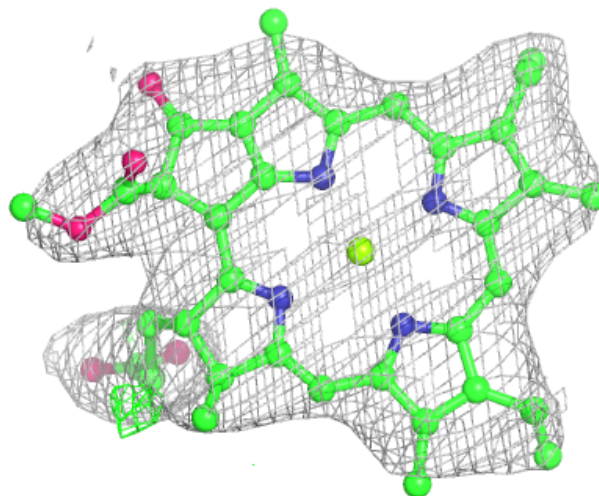


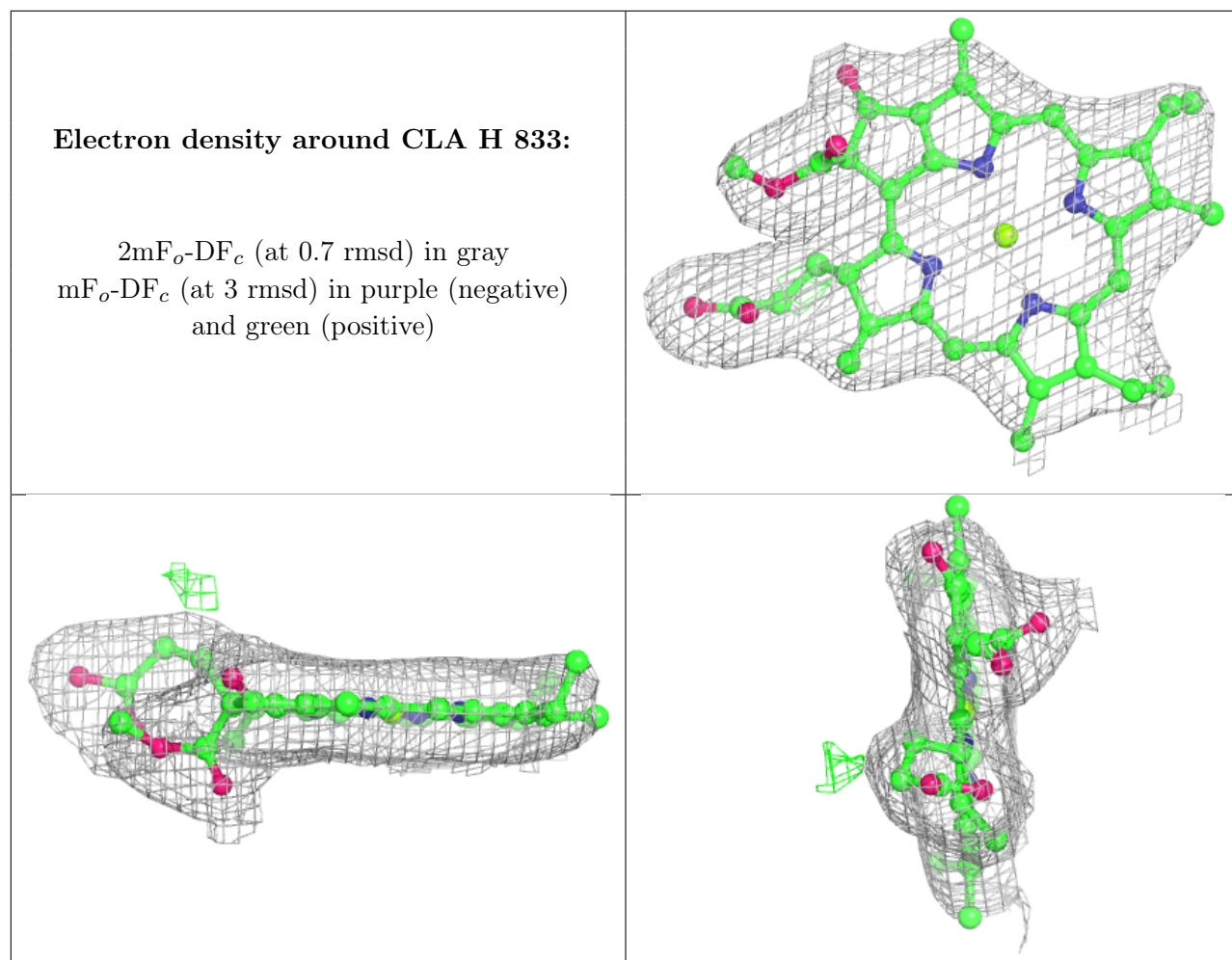




**Electron density around CLA H 832:**

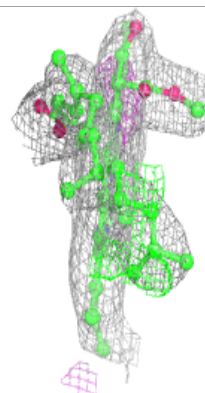
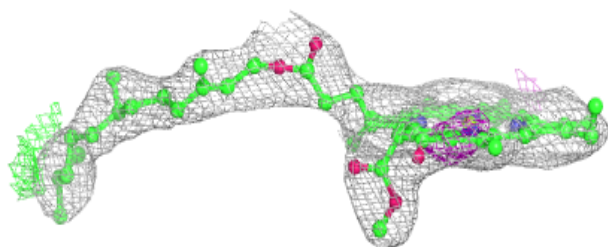
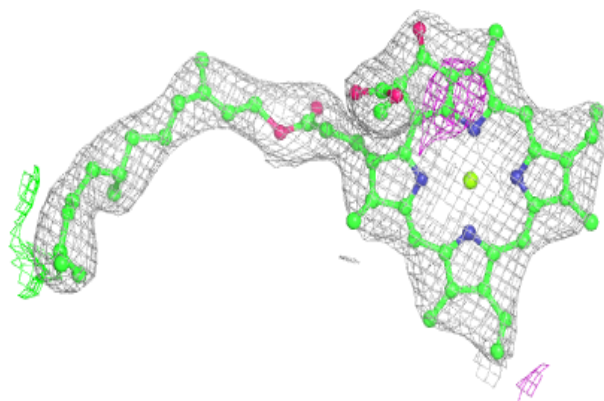
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



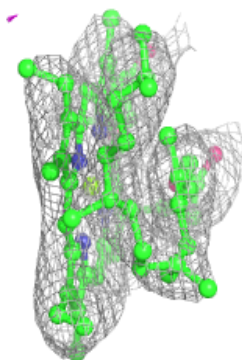
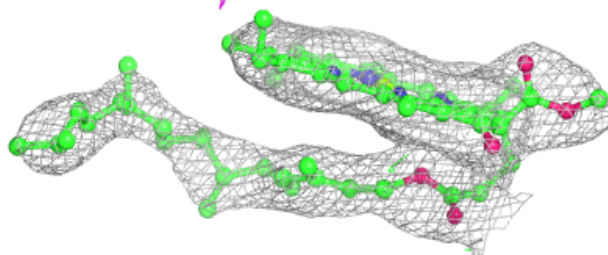
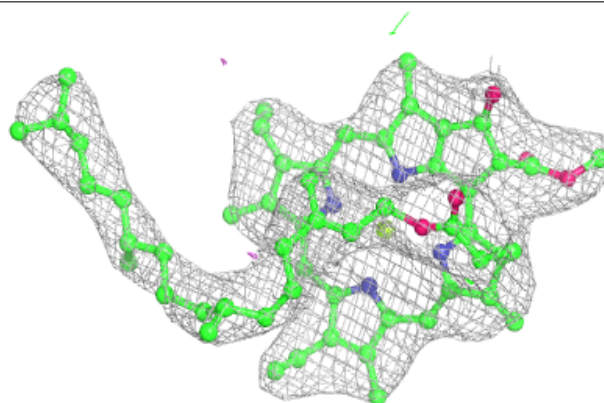


**Electron density around CLA H 834:**

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

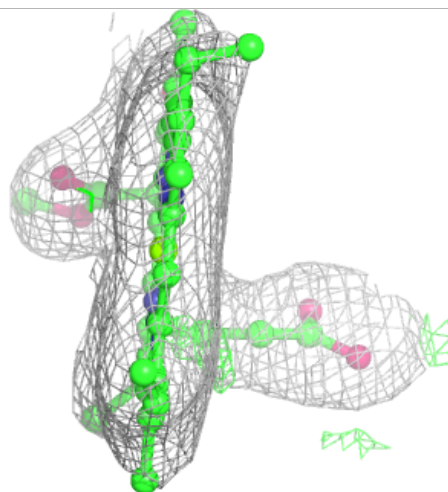
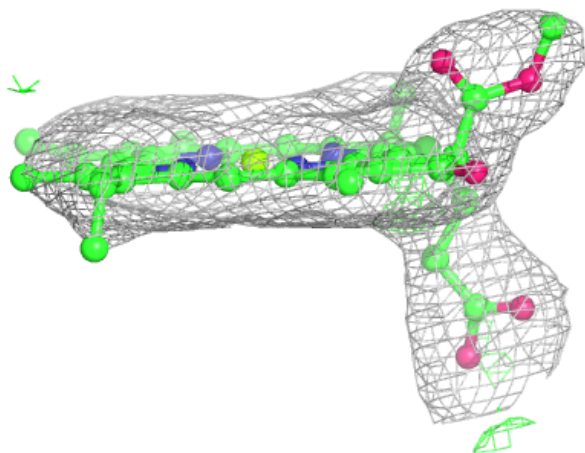
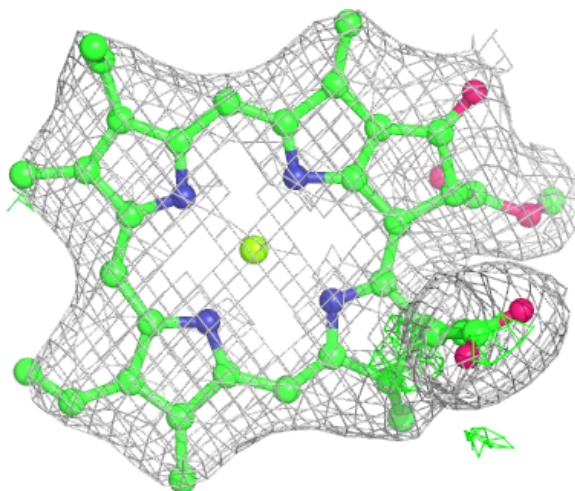
**Electron density around CLA H 835:**

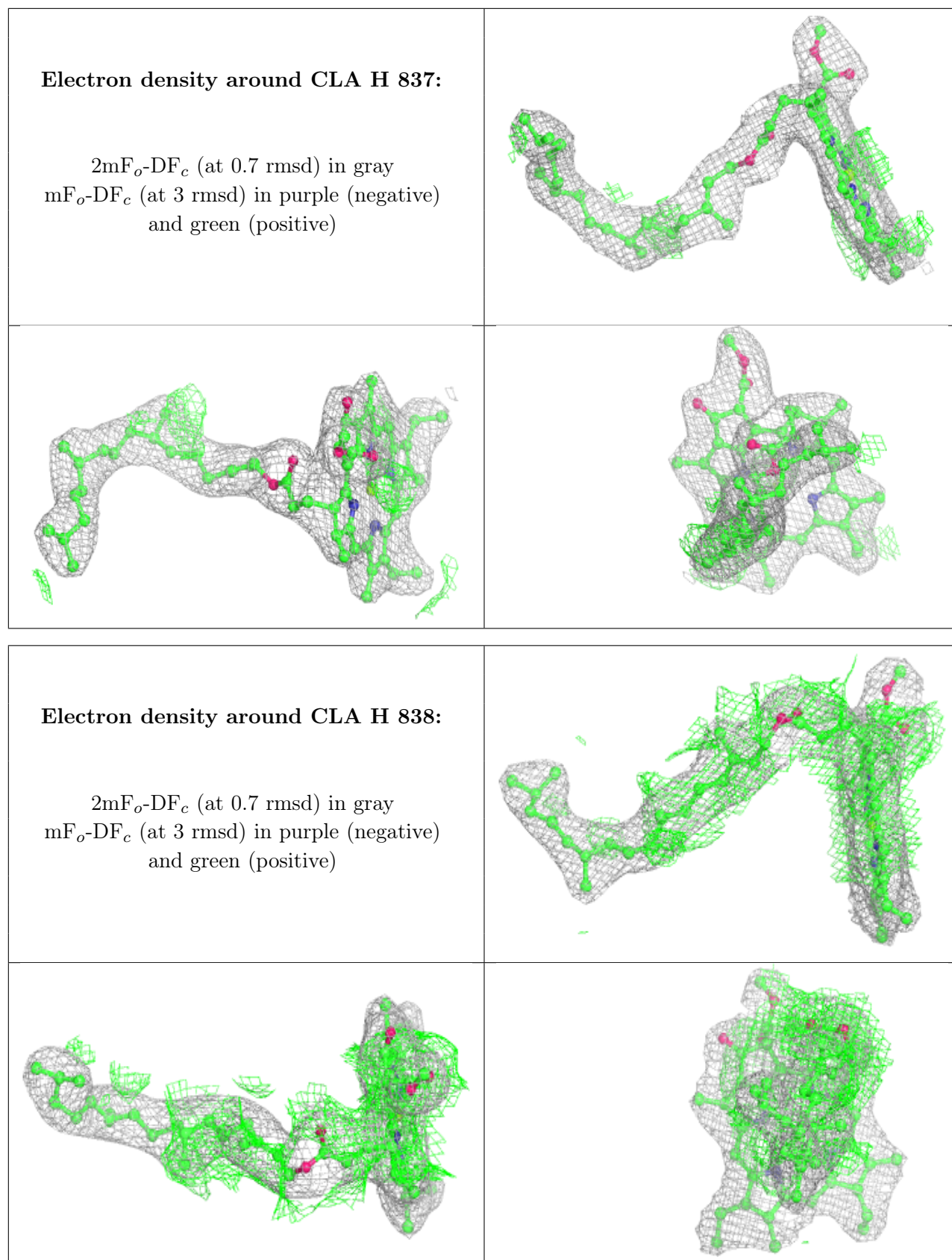
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA H 836:**

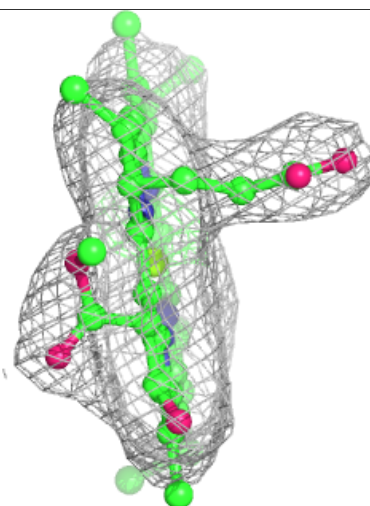
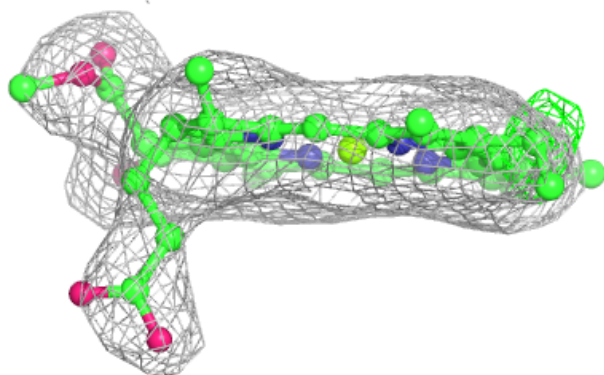
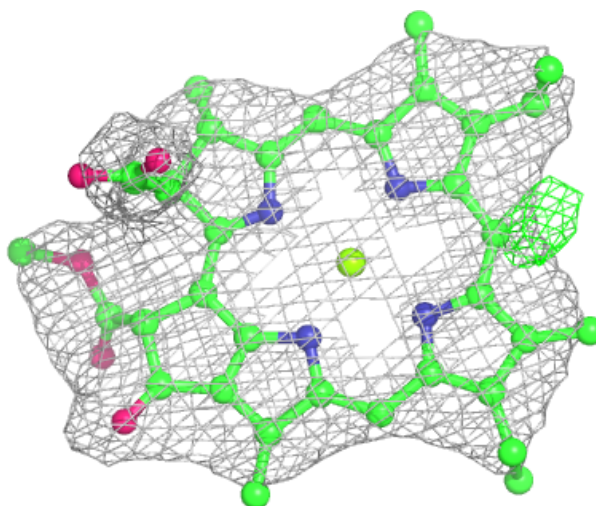
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





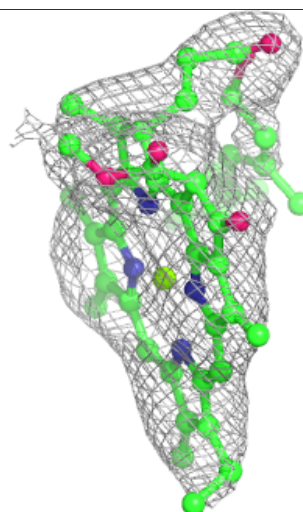
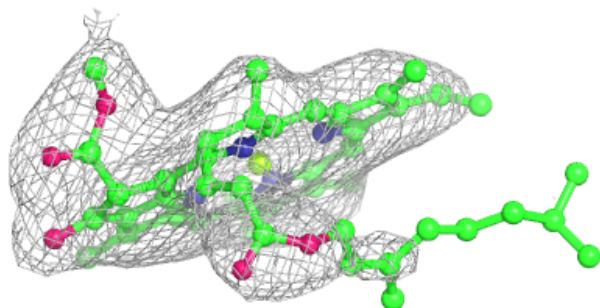
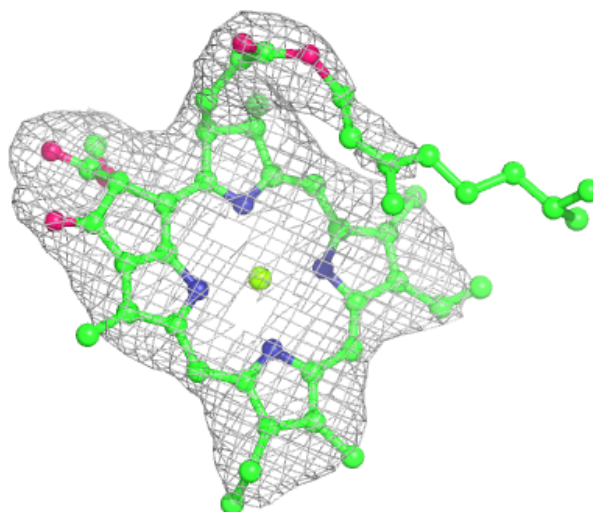
**Electron density around CLA J 101:**

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



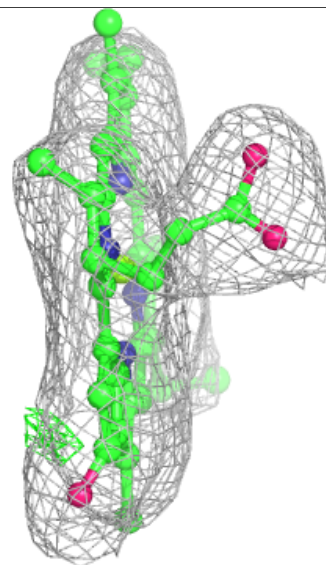
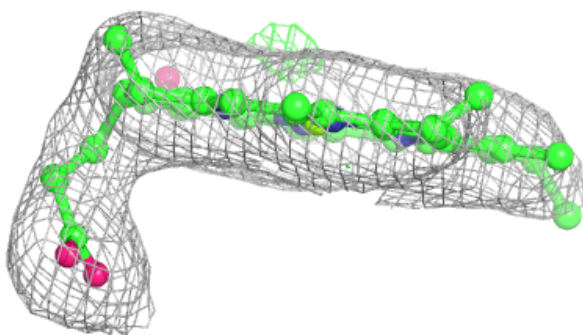
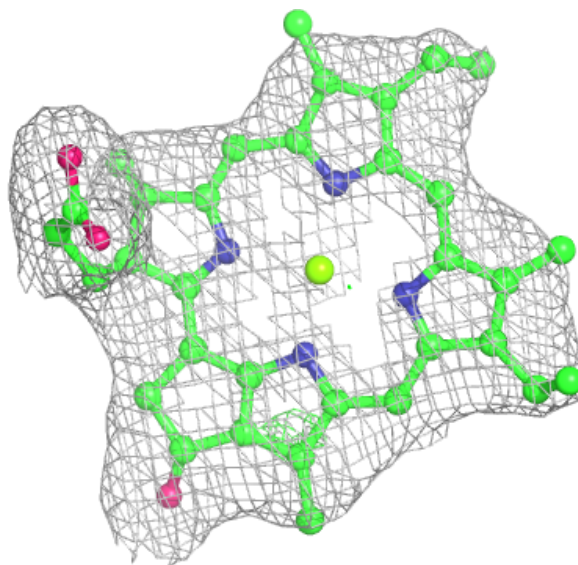
**Electron density around CLA J 102:**

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



**Electron density around CLA K 101:**

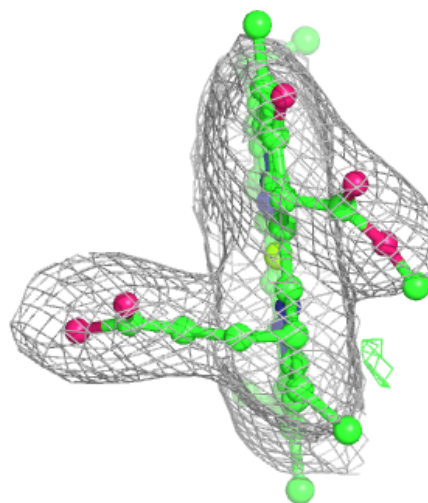
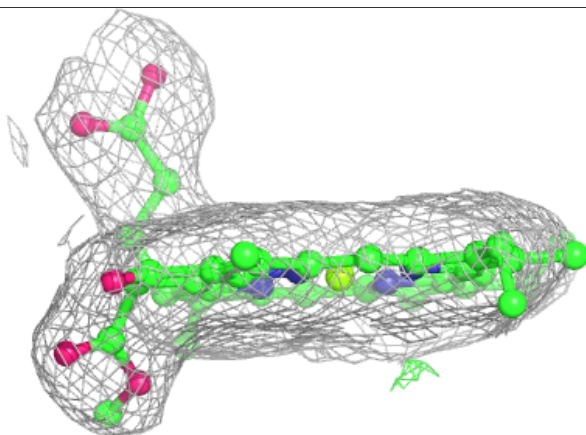
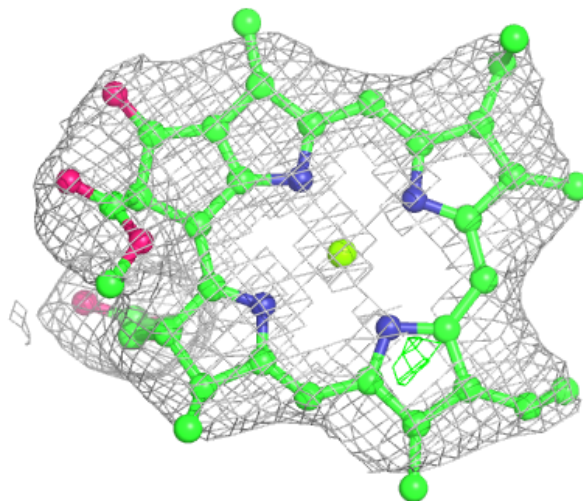
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





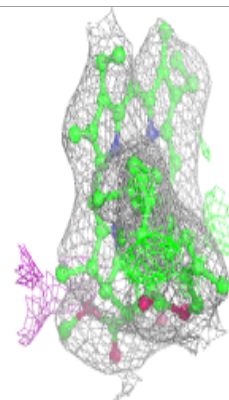
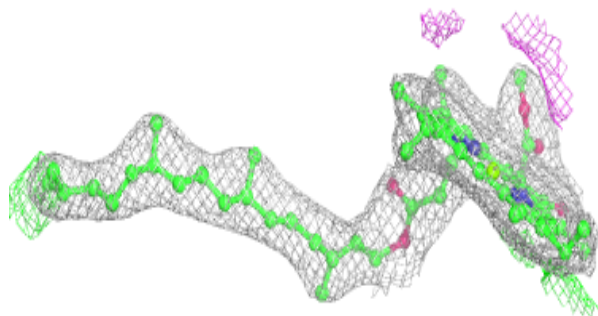
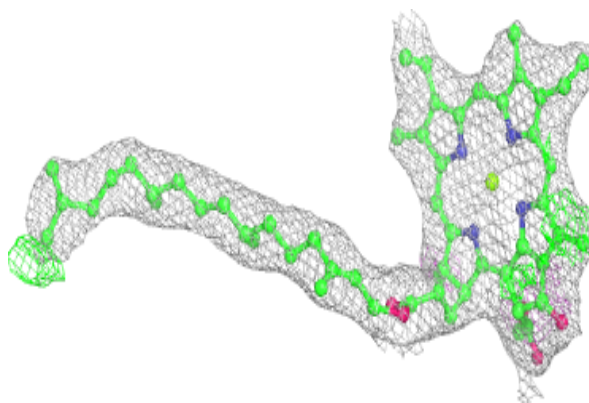
**Electron density around CLA K 103:**

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

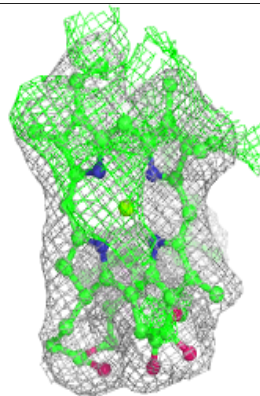
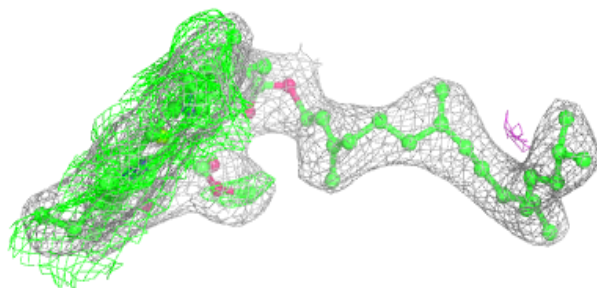
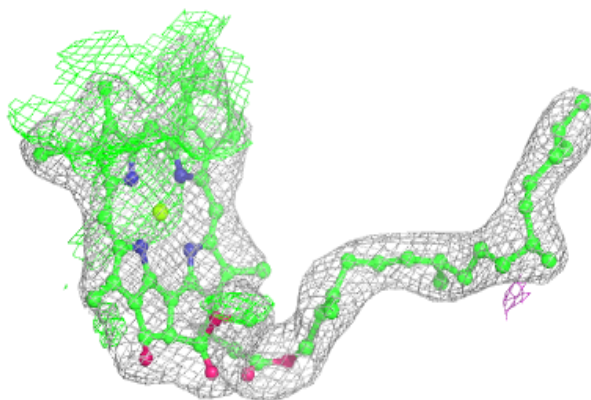


**Electron density around CLA L 201:**

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

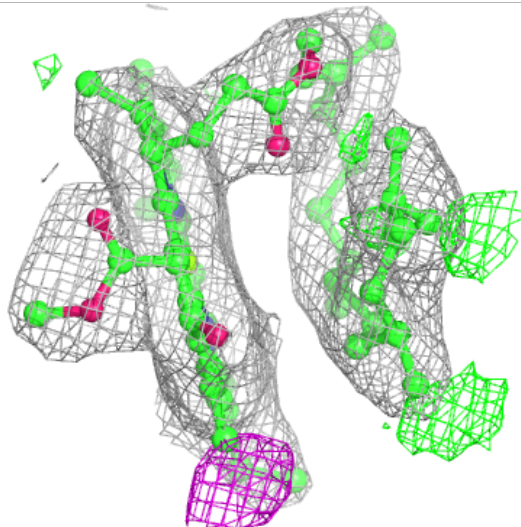
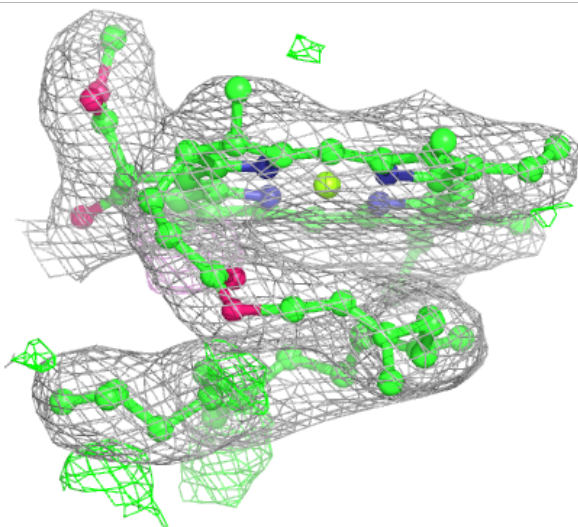
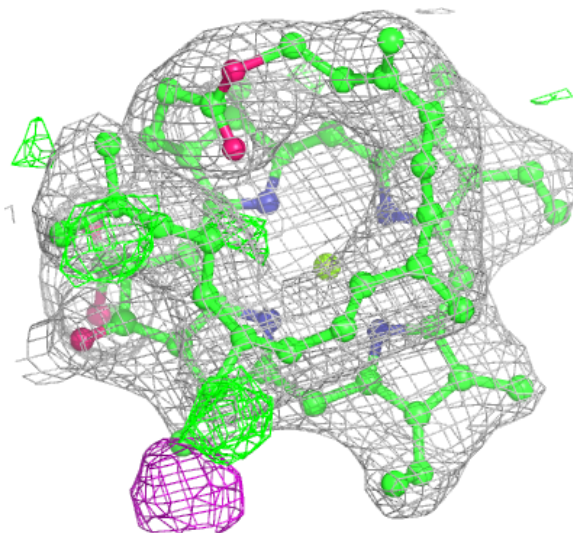
**Electron density around CLA L 202:**

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



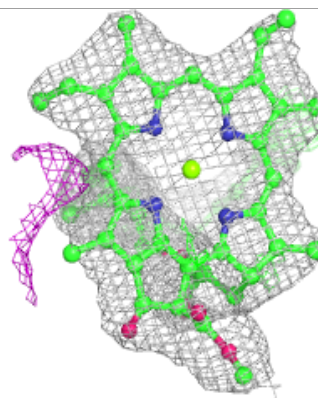
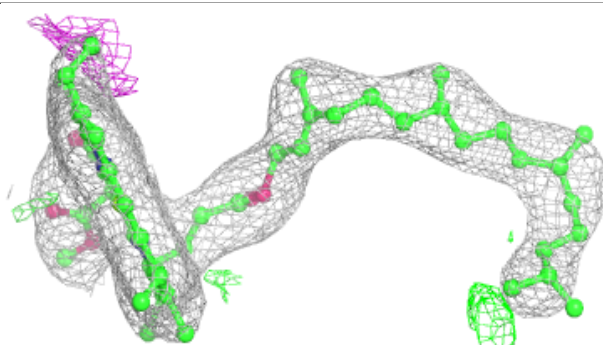
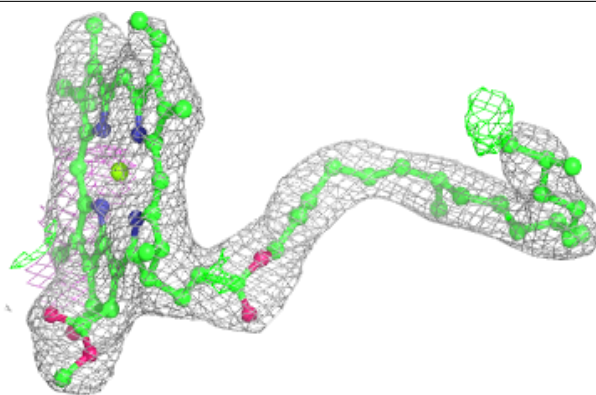
**Electron density around CLA L 205:**

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

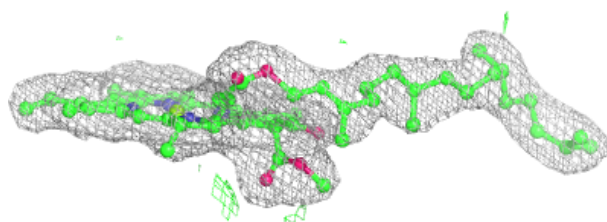
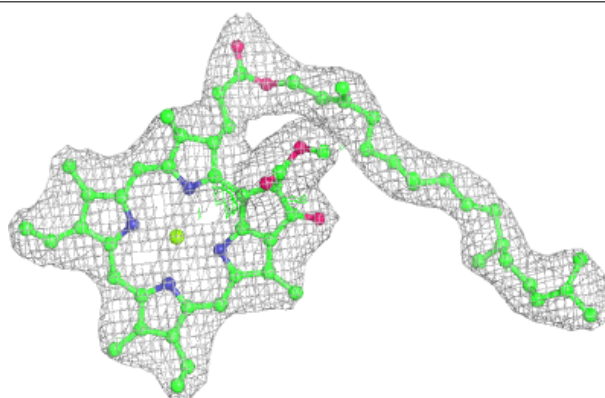


**Electron density around CLA L 206:**

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

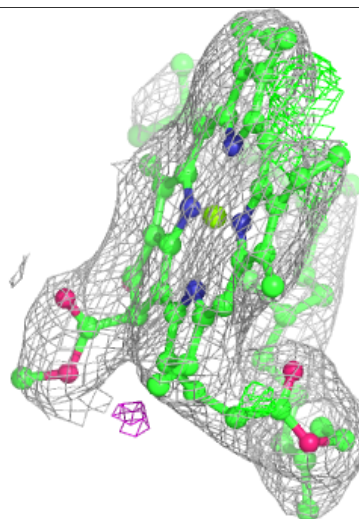
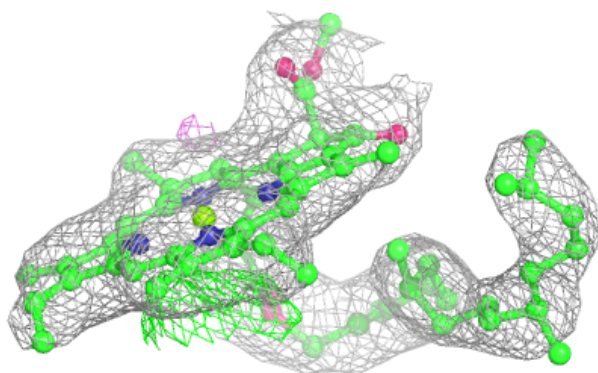
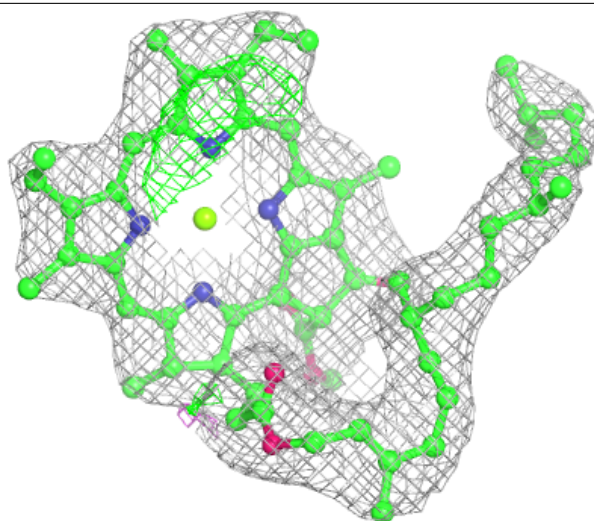
**Electron density around CLA L 207:**

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



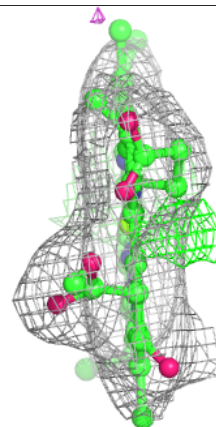
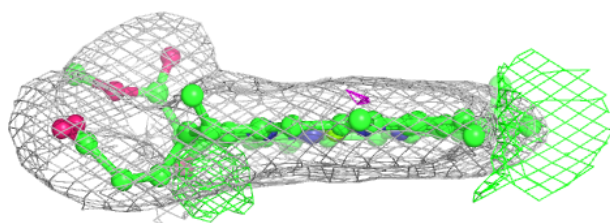
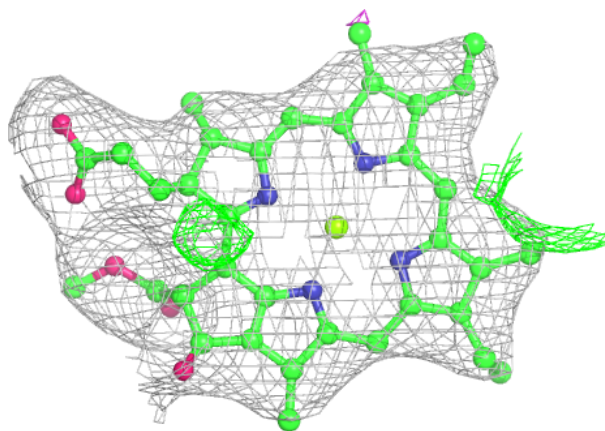
**Electron density around CLA Q 201:**

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

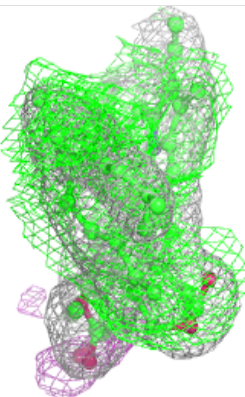
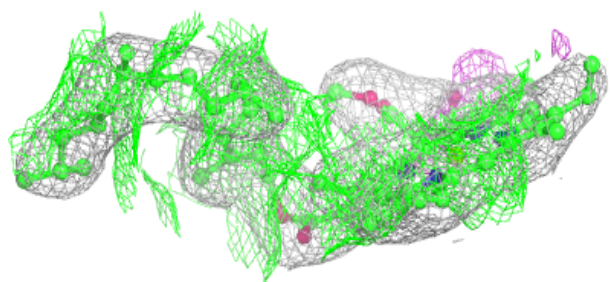
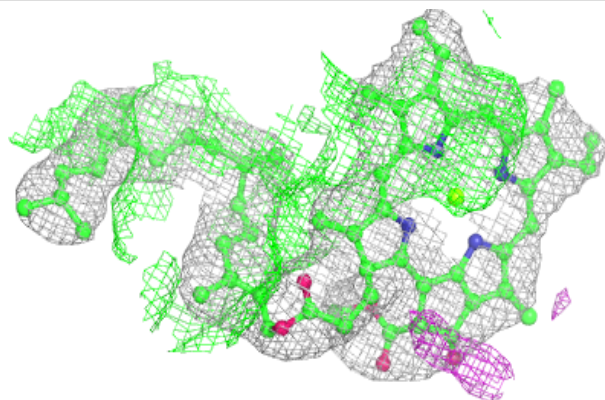


**Electron density around CLA Q 203:**

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

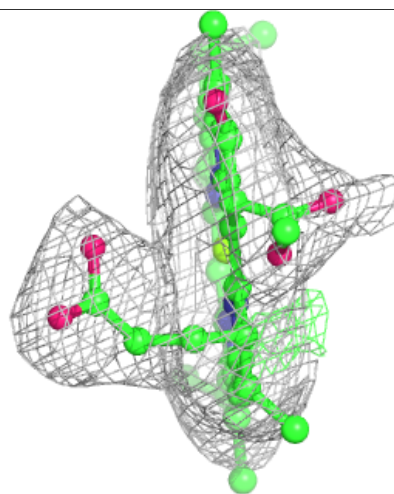
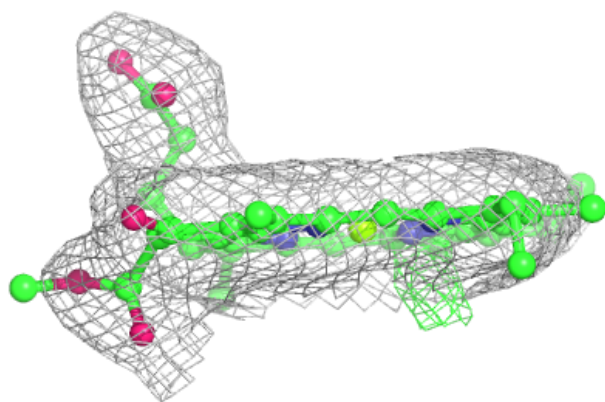
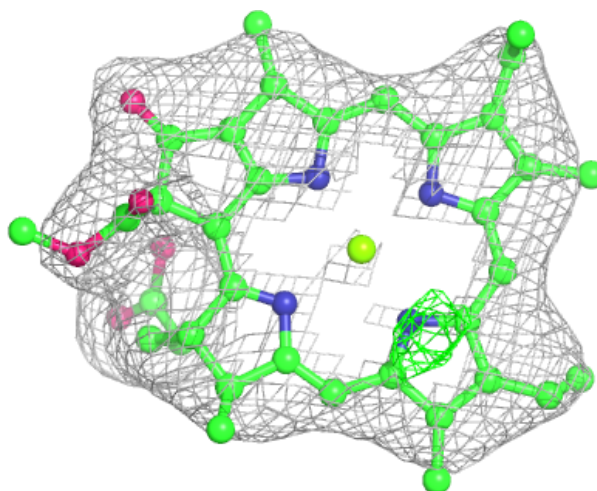
**Electron density around CLA S 1101:**

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



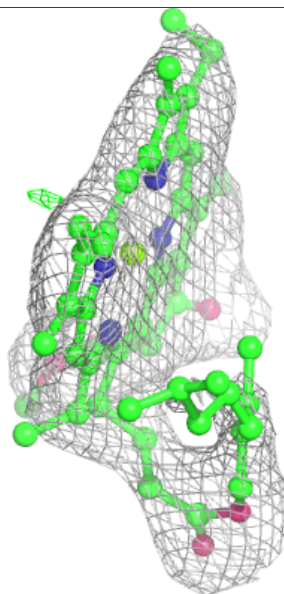
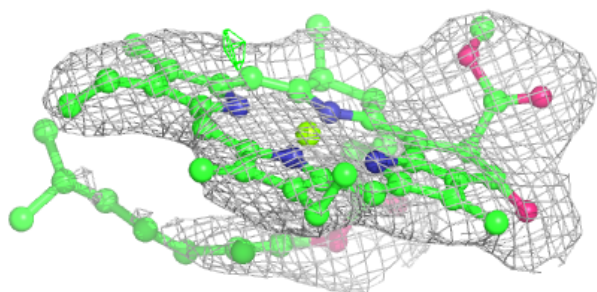
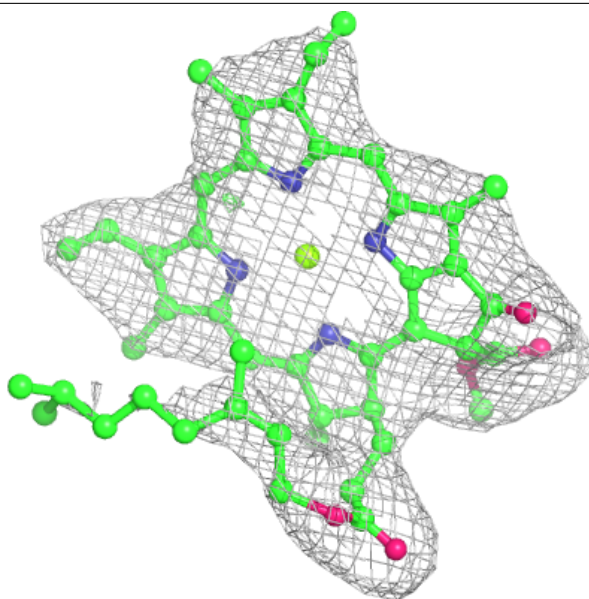
**Electron density around CLA S 1102:**

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



**Electron density around CLA S 1103:**

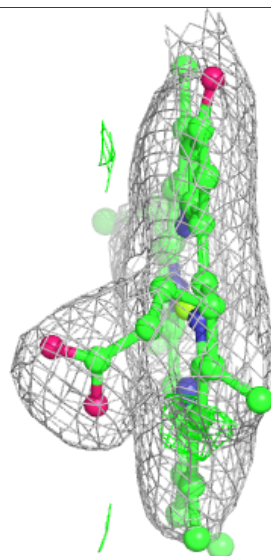
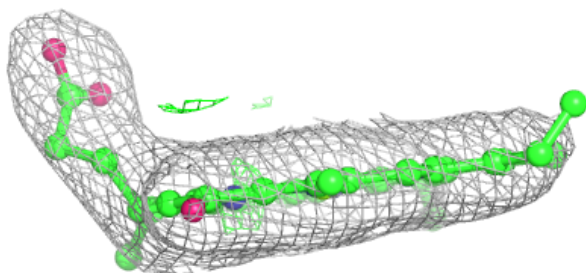
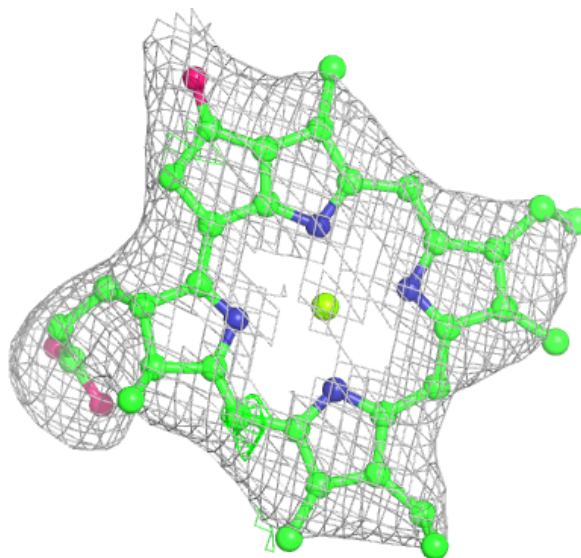
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





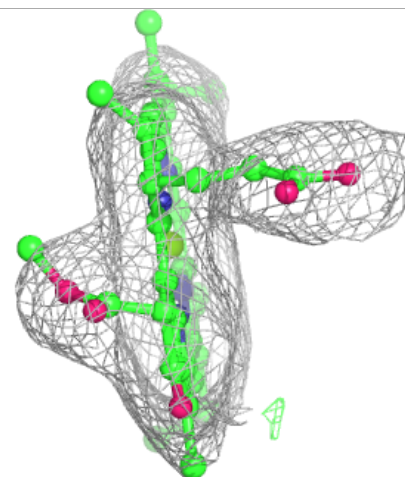
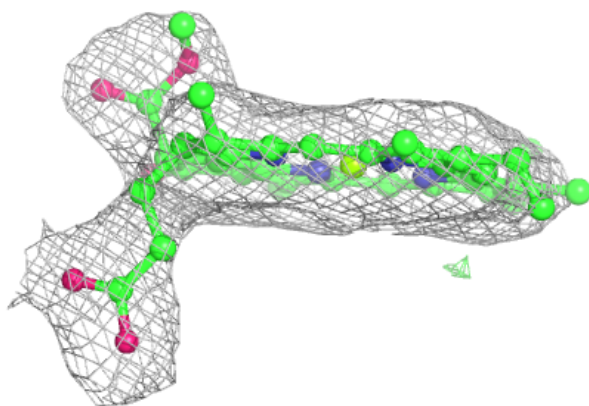
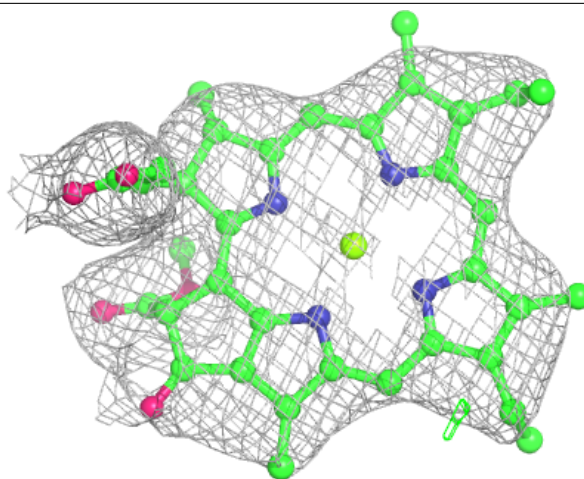
**Electron density around CLA T 101:**

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



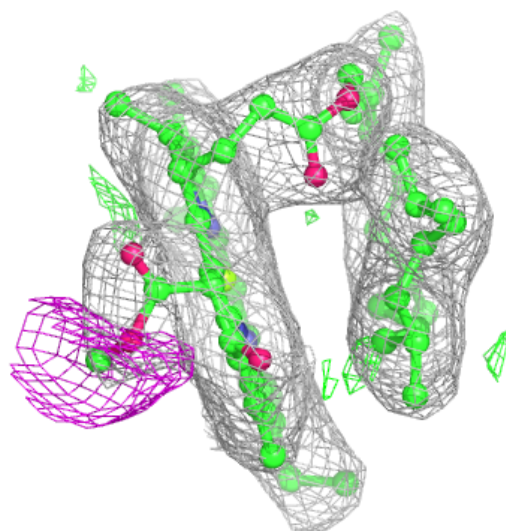
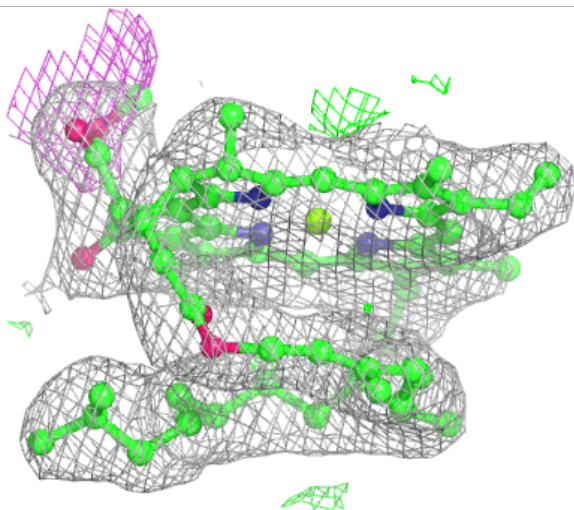
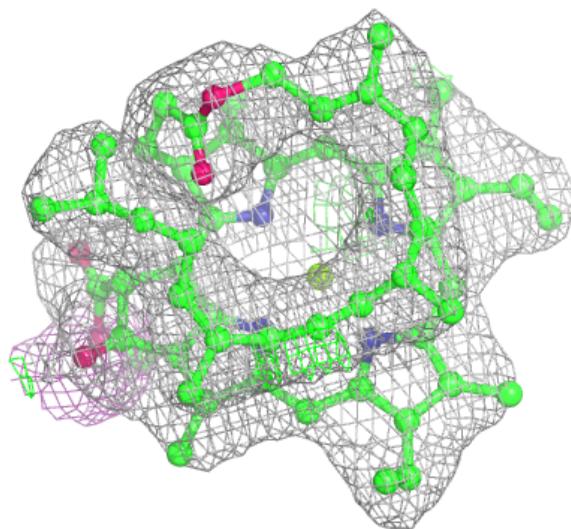
**Electron density around CLA T 103:**

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



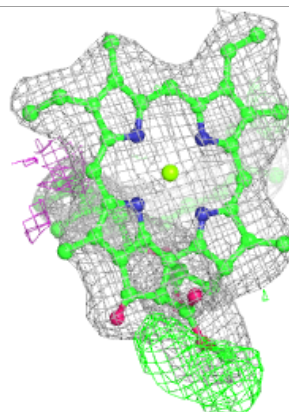
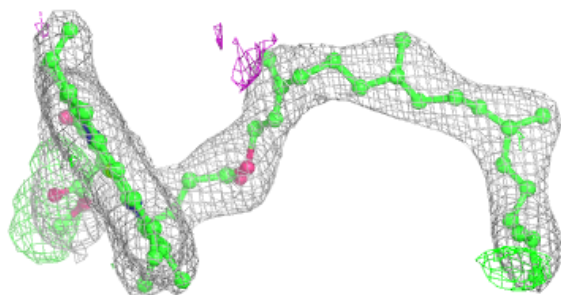
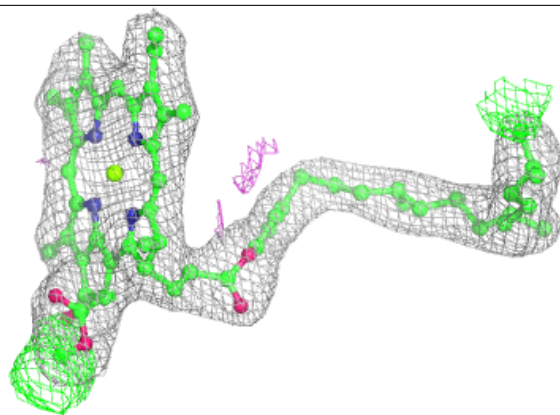
**Electron density around CLA U 1002:**

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

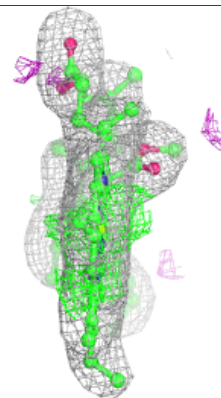
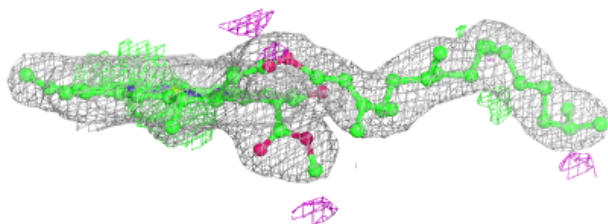
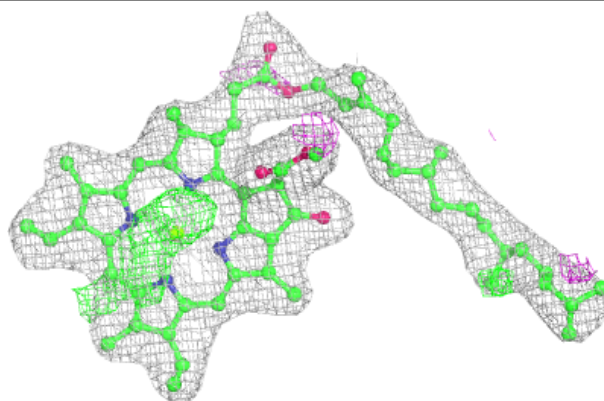


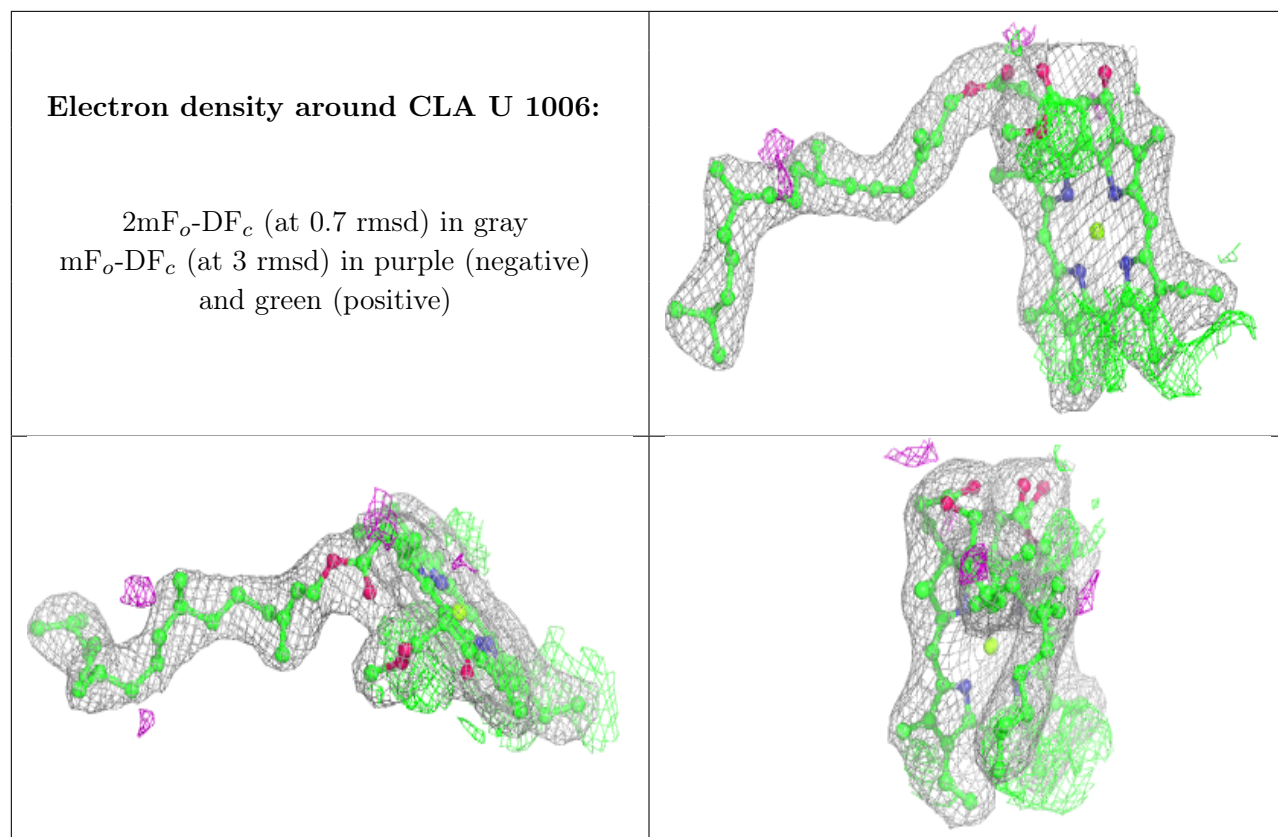
**Electron density around CLA U 1003:**

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

**Electron density around CLA U 1004:**

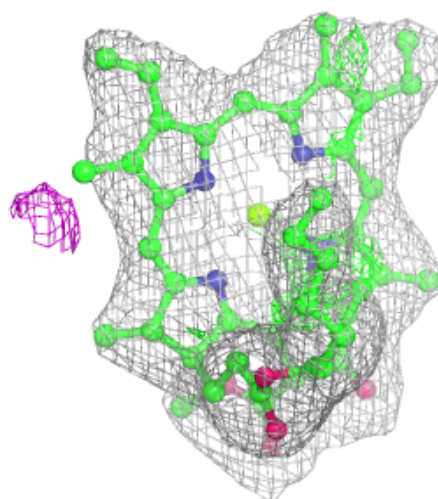
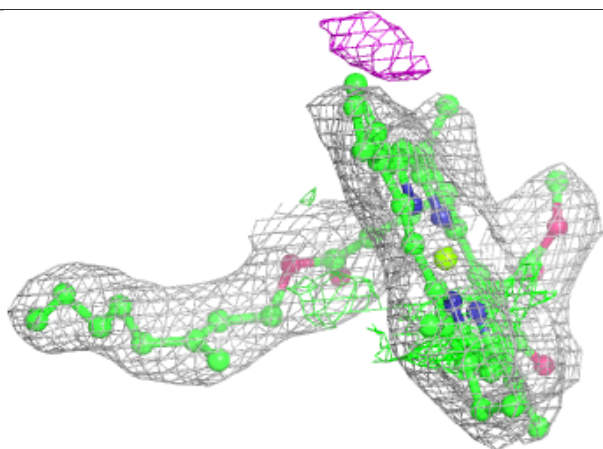
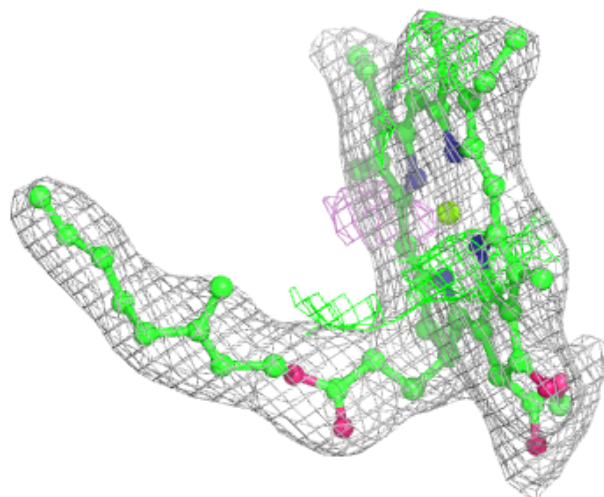
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





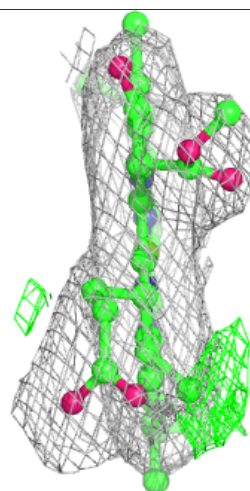
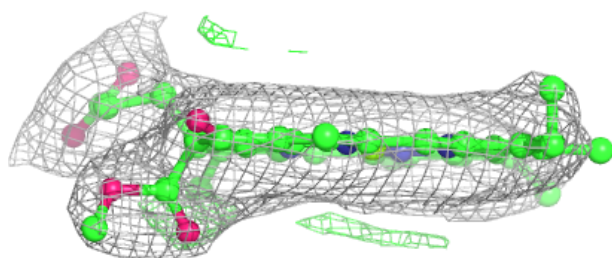
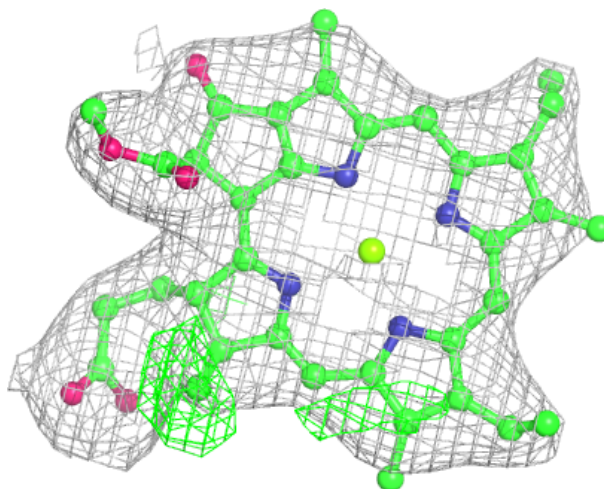
**Electron density around CLA V 1201:**

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



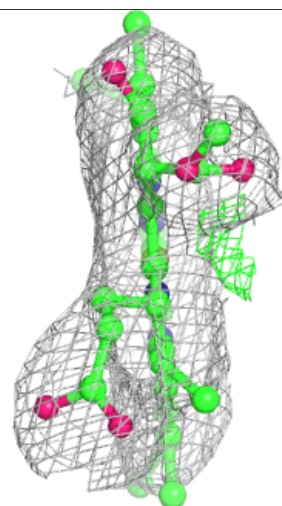
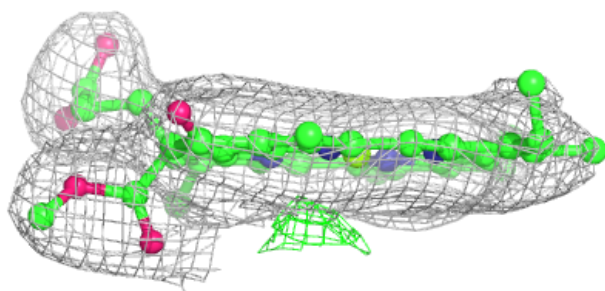
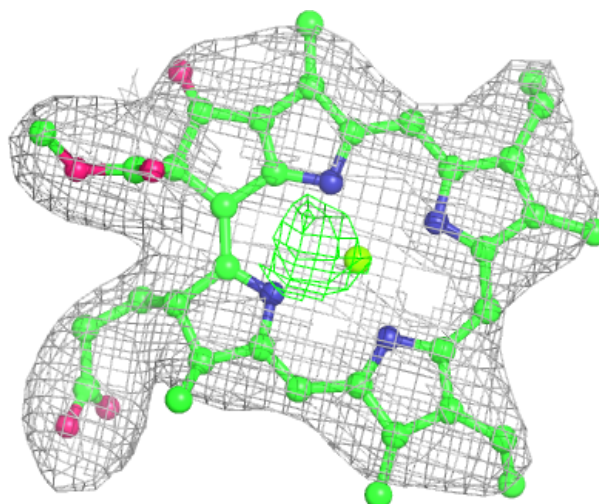
**Electron density around CLA W 1701:**

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



**Electron density around CLA X 1701:**

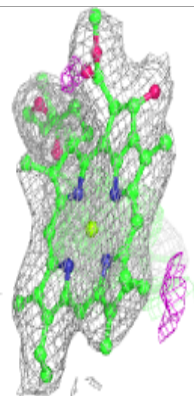
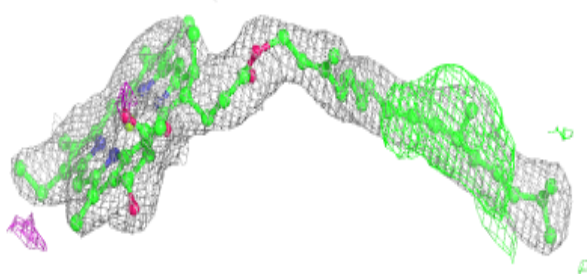
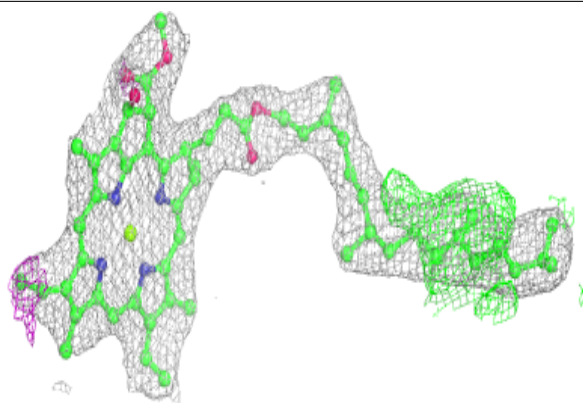
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



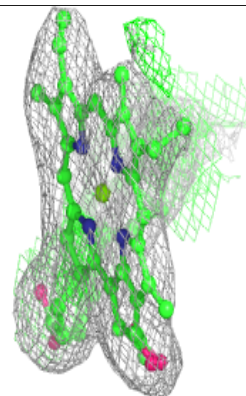
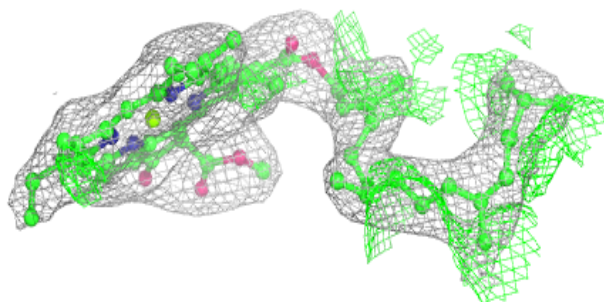
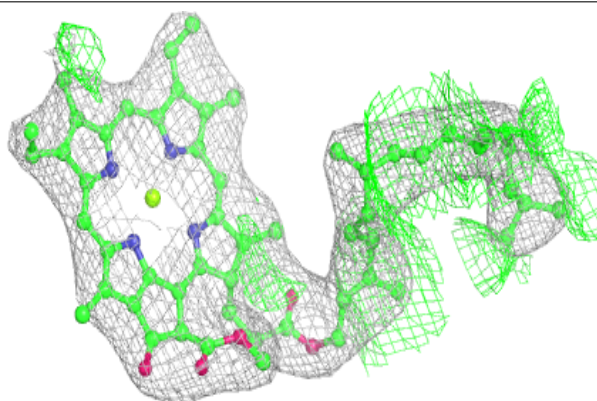


**Electron density around CLA Y 802:**

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

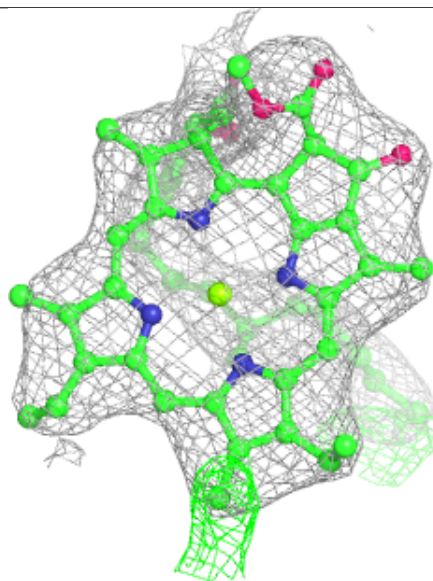
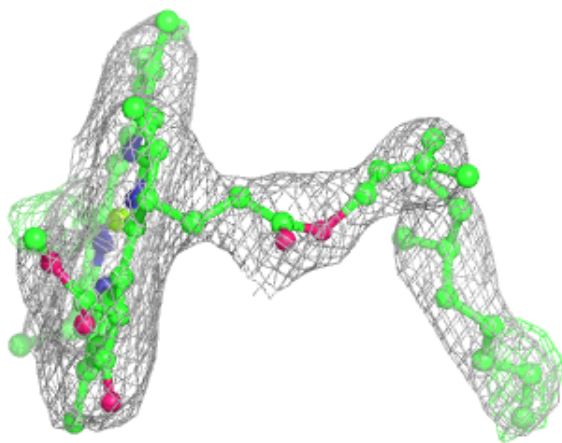
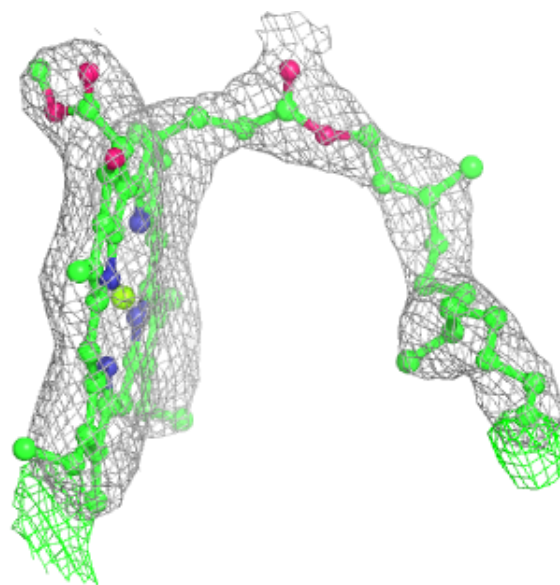
**Electron density around CLA Y 803:**

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



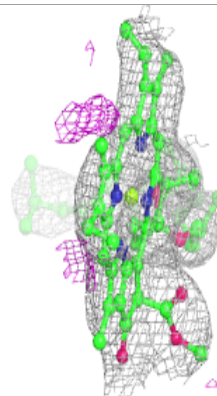
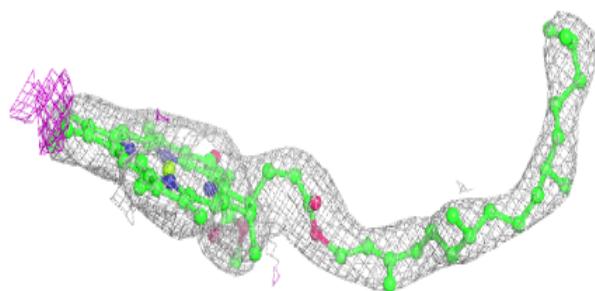
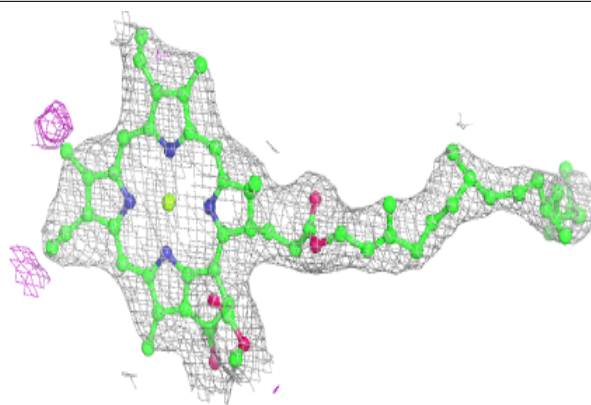
**Electron density around CLA Y 804:**

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

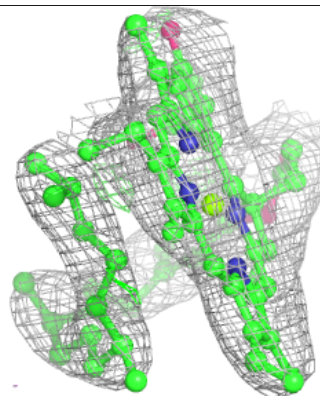
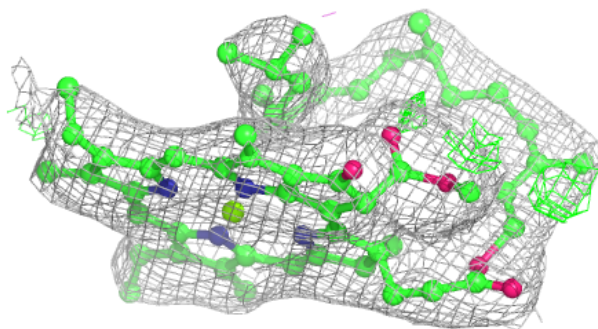
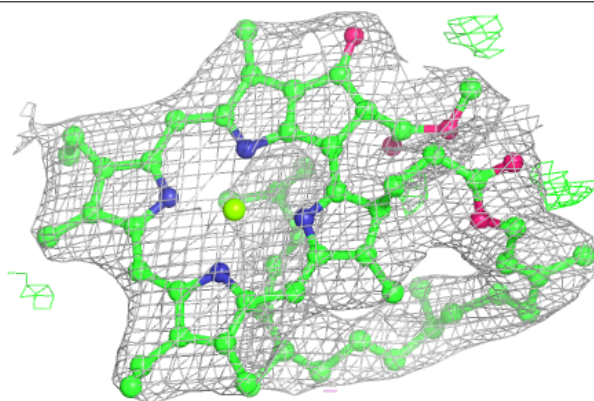


**Electron density around CLA Y 805:**

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

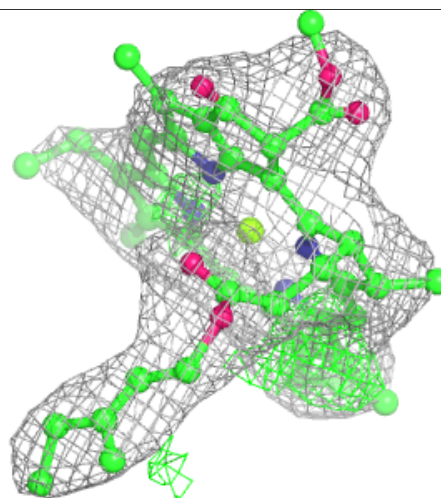
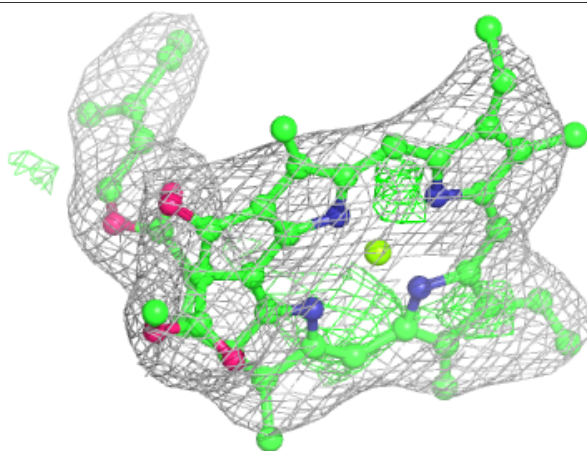
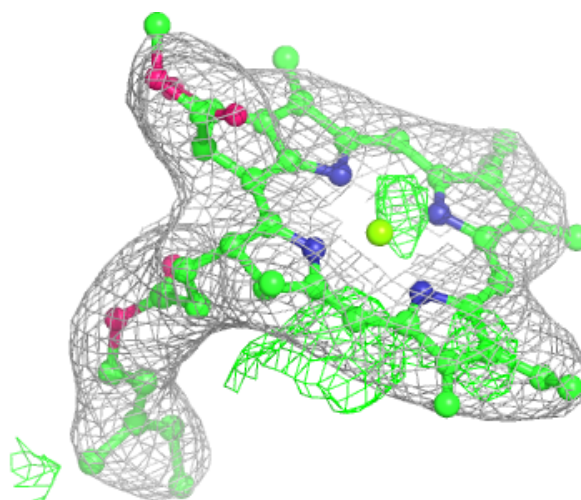
**Electron density around CLA Y 806:**

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



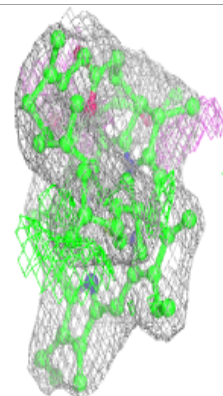
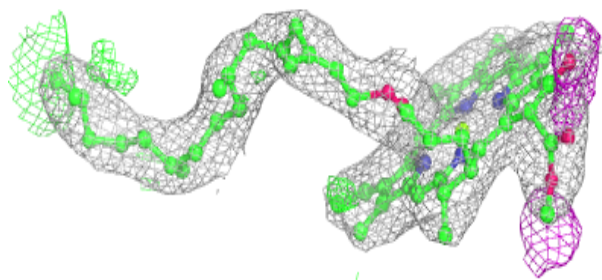
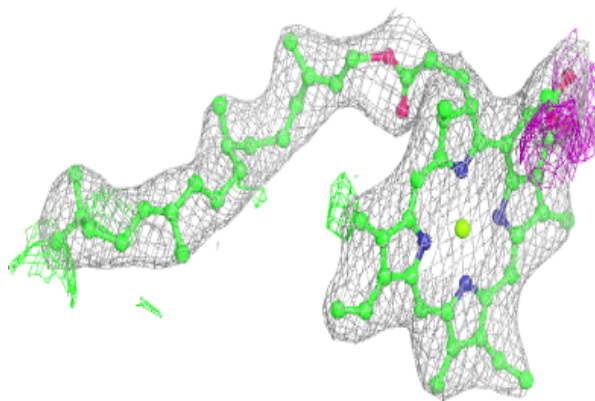
**Electron density around CLA Y 807:**

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

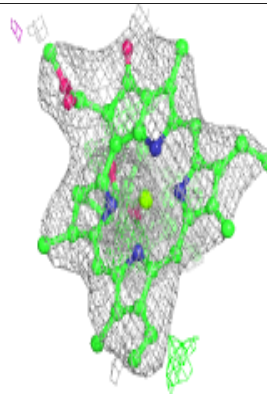
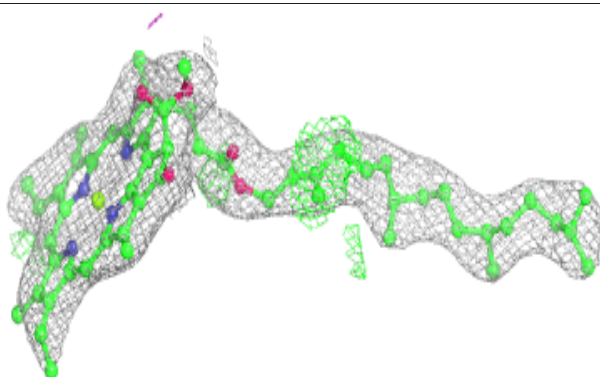
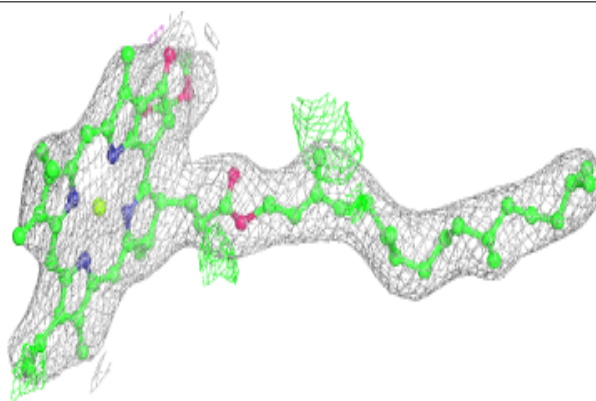


**Electron density around CLA Y 808:**

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

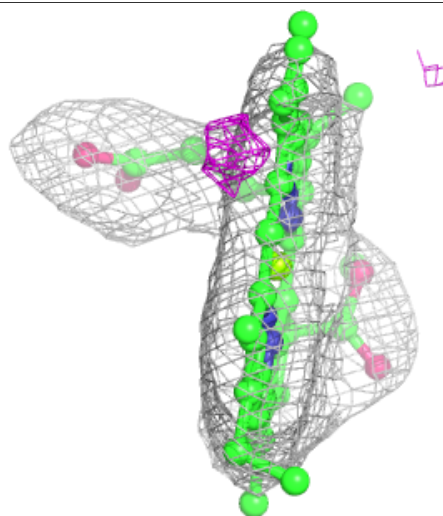
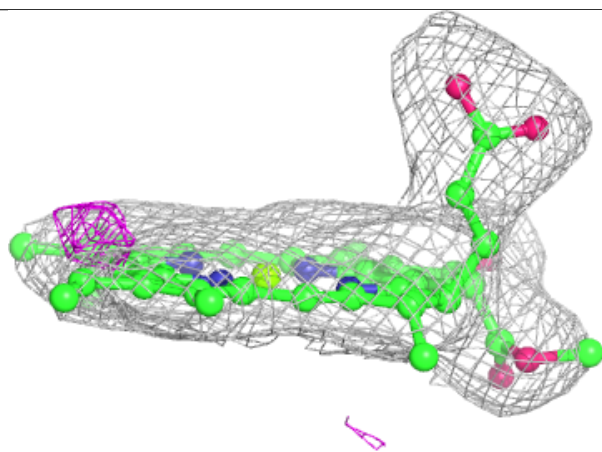
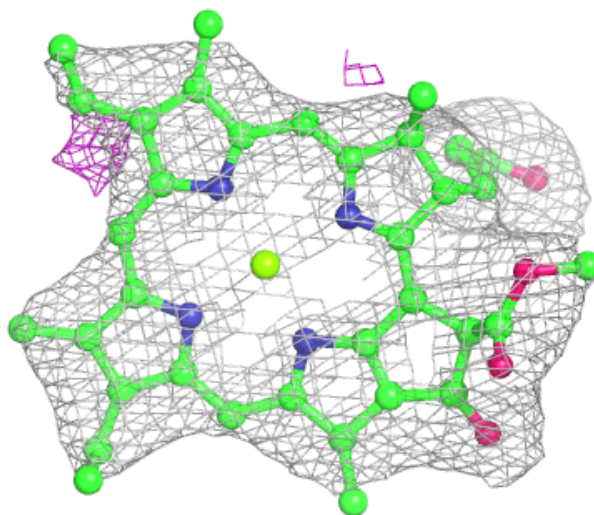
**Electron density around CLA Y 809:**

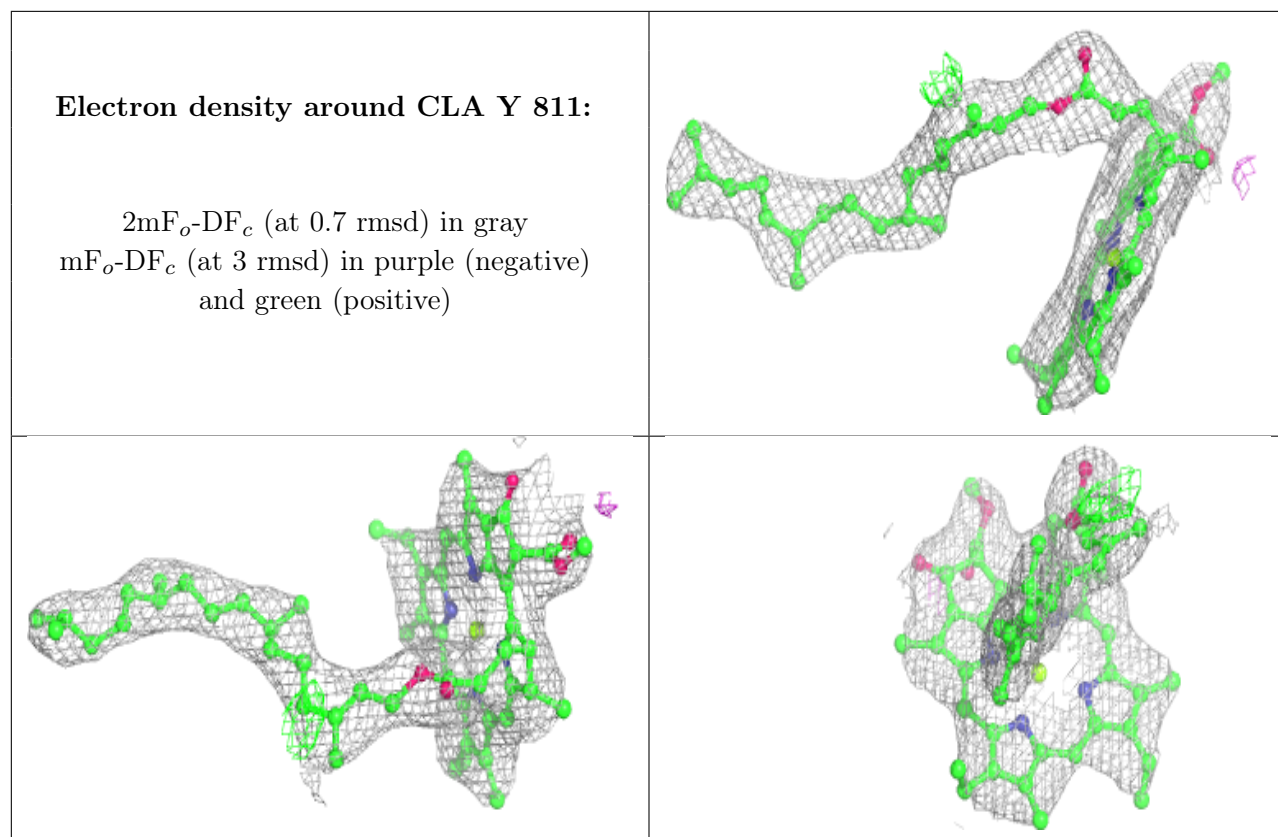
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

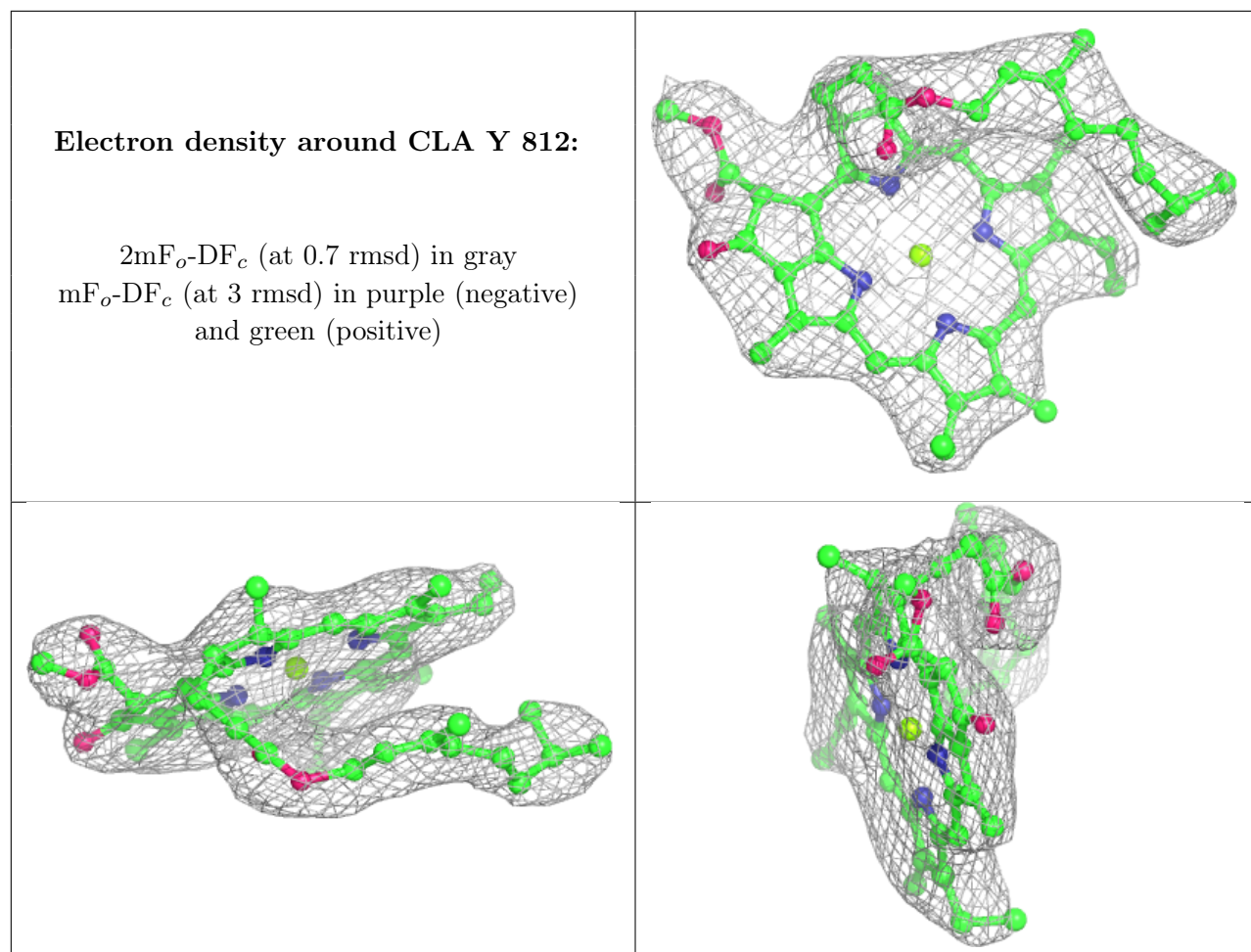


**Electron density around CLA Y 810:**

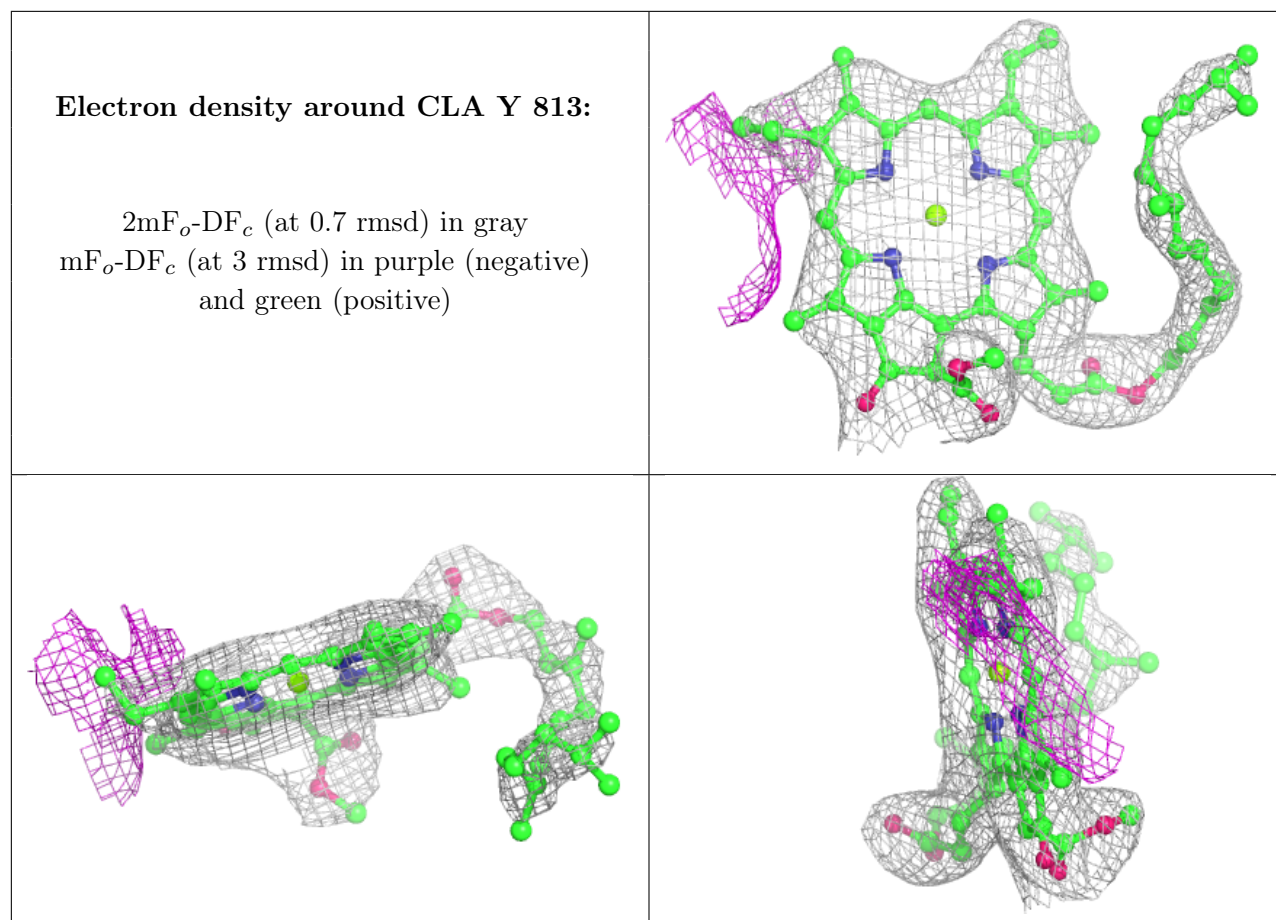
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

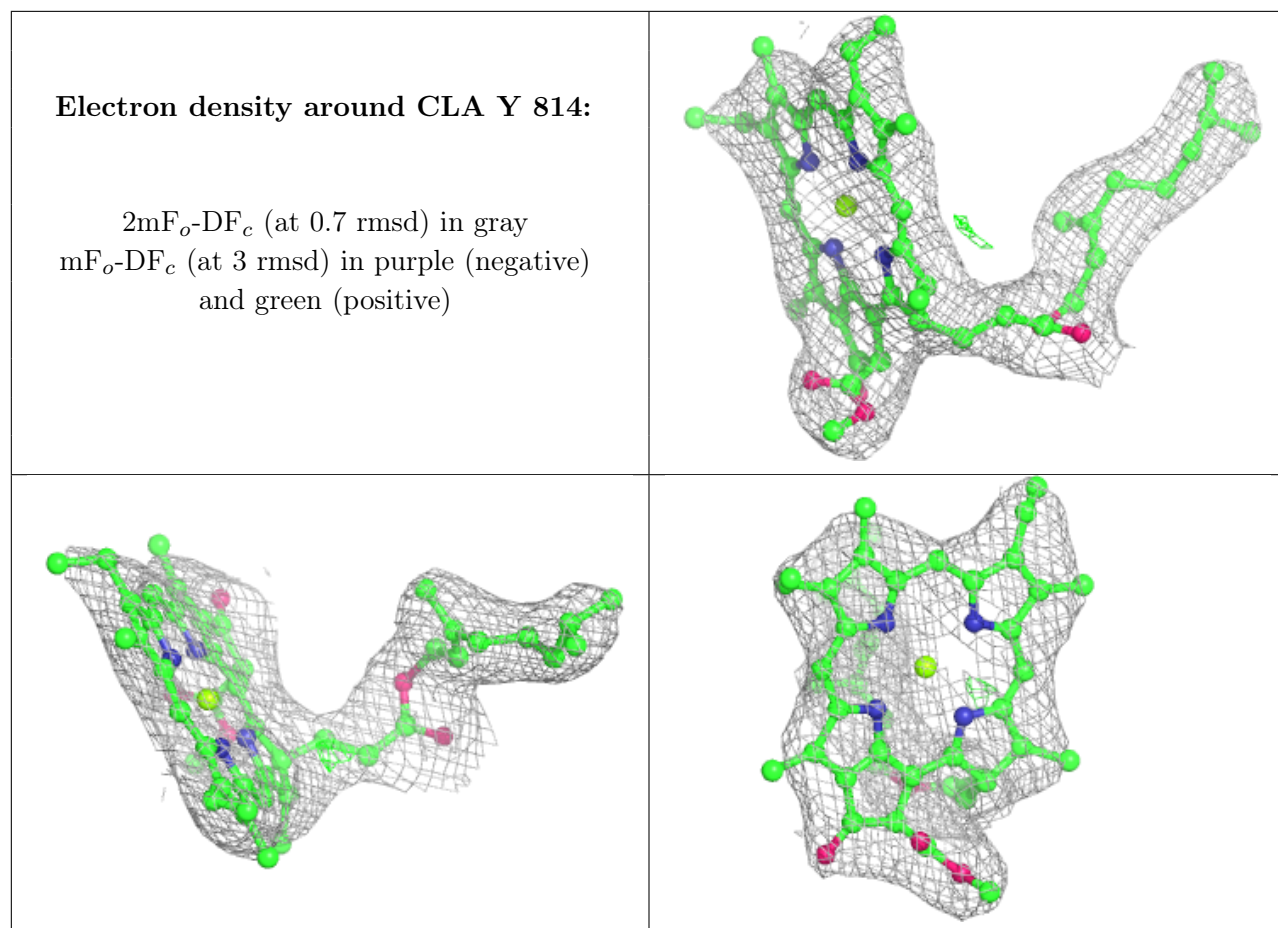






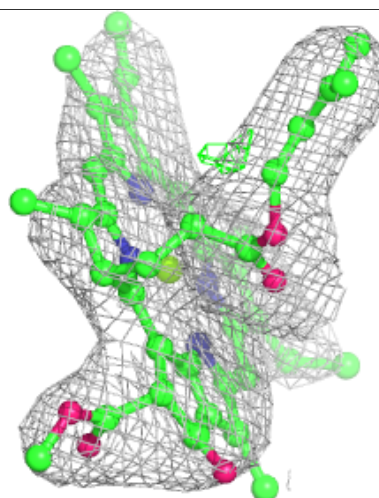
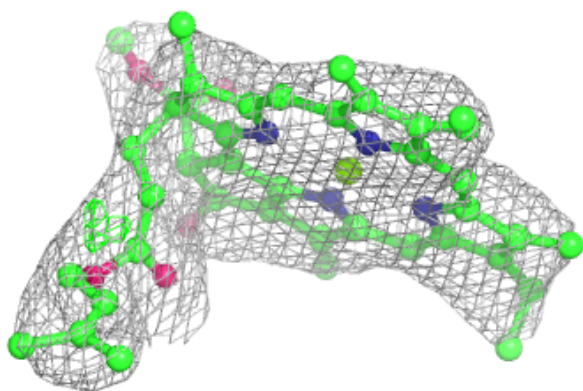
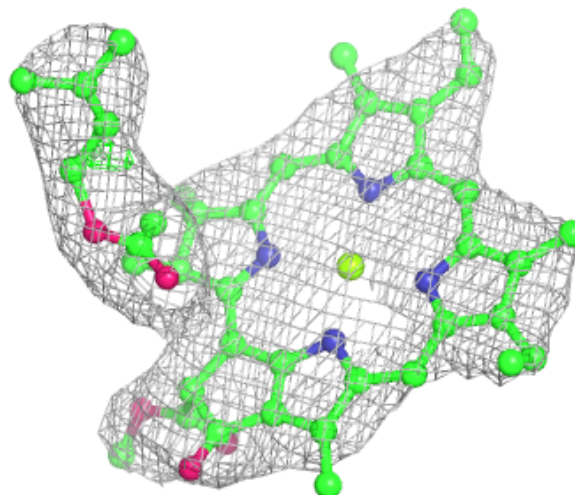






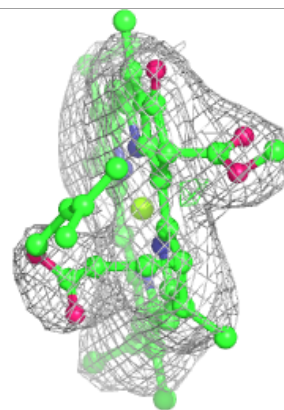
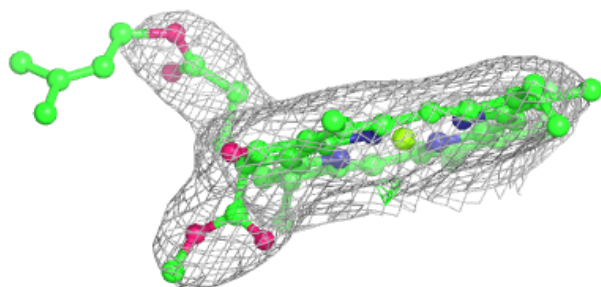
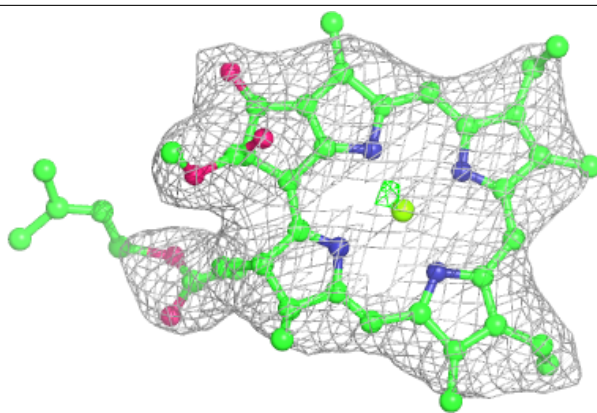
**Electron density around CLA Y 815:**

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

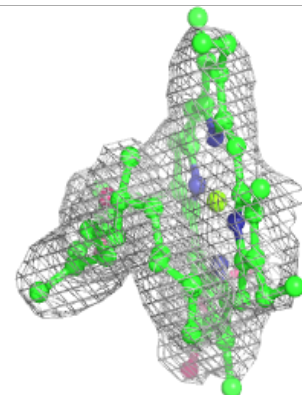
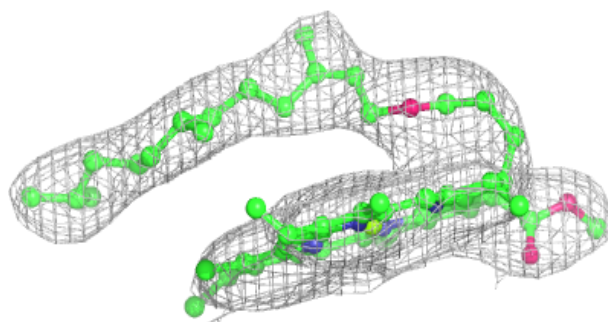
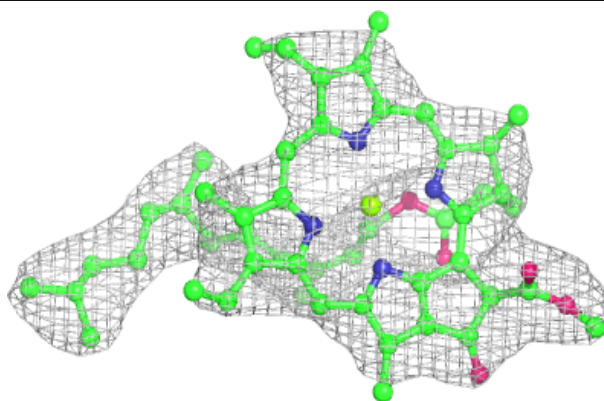


**Electron density around CLA Y 816:**

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

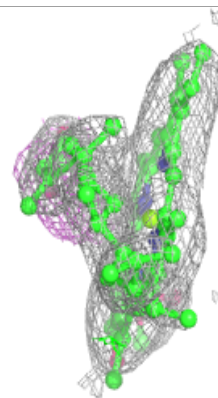
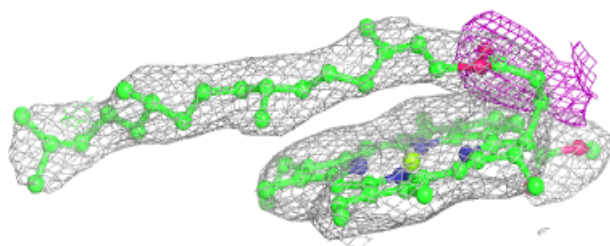
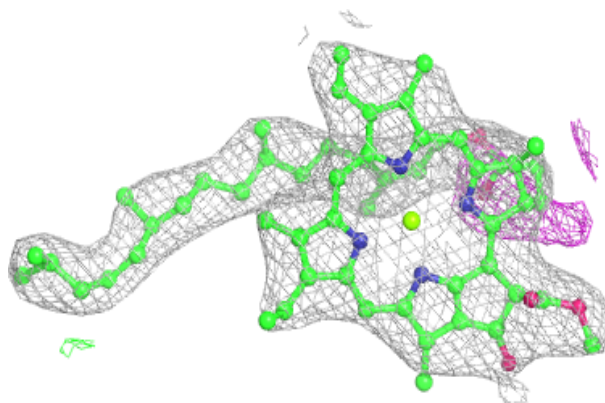
**Electron density around CLA Y 817:**

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

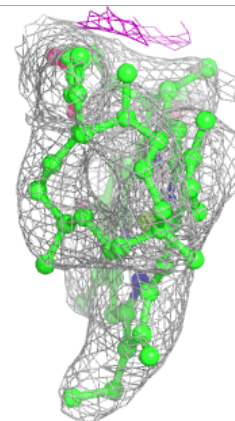
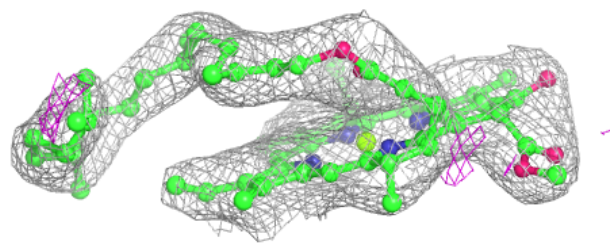
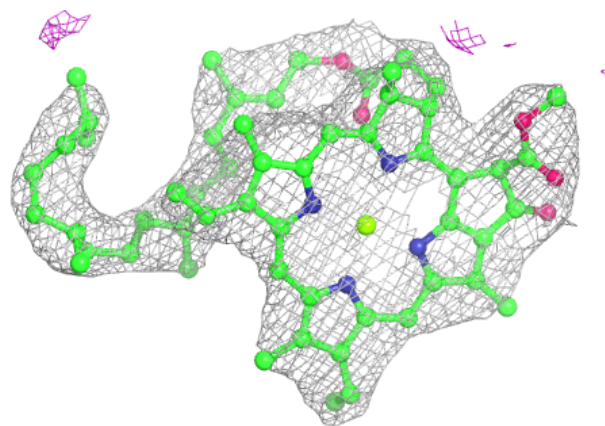


**Electron density around CLA Y 818:**

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

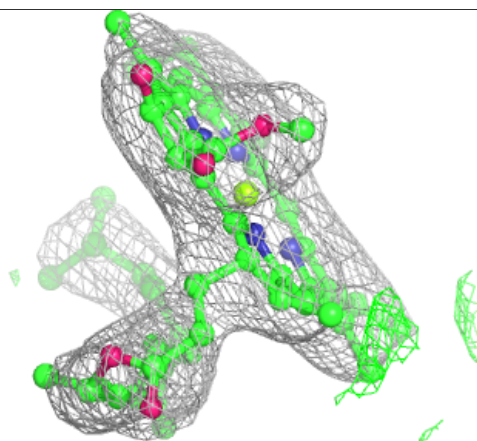
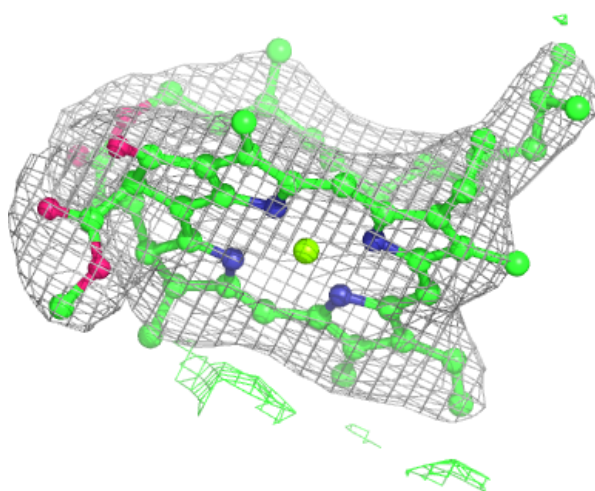
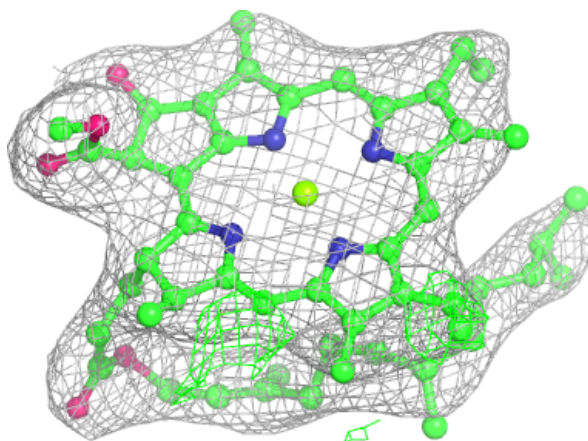
**Electron density around CLA Y 819:**

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



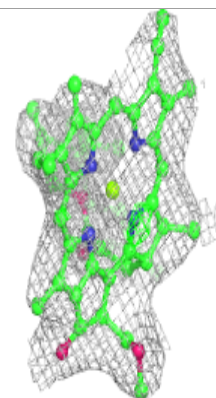
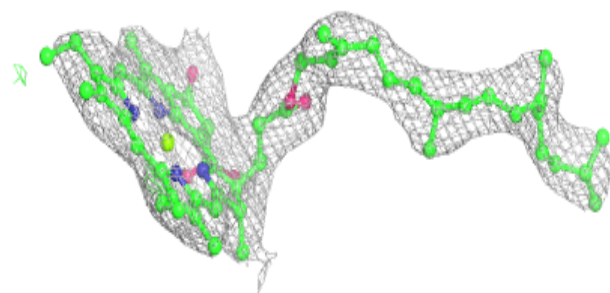
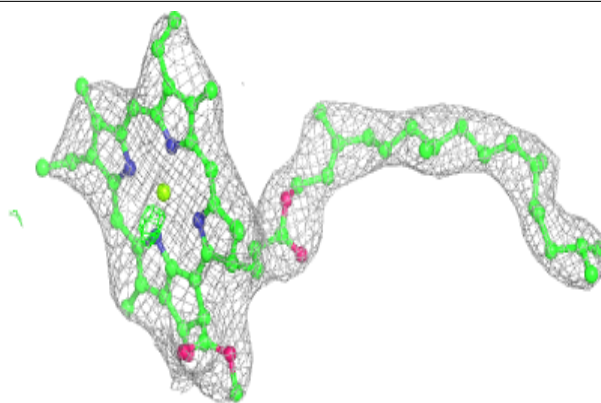
**Electron density around CLA Y 820:**

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

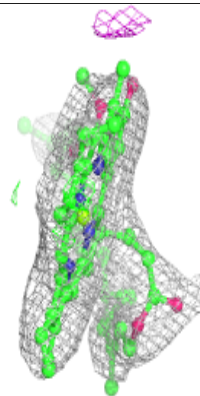
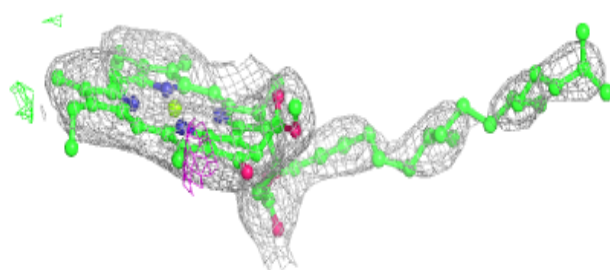
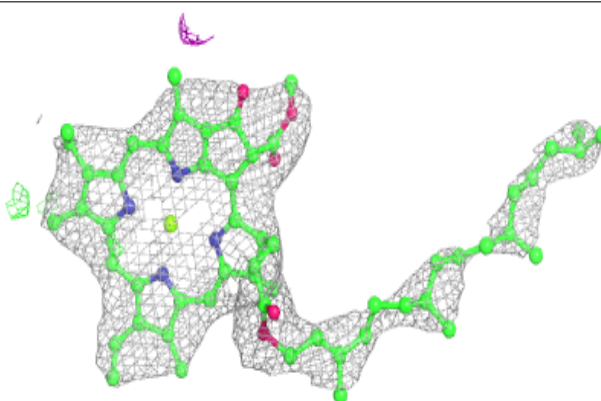


**Electron density around CLA Y 821:**

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

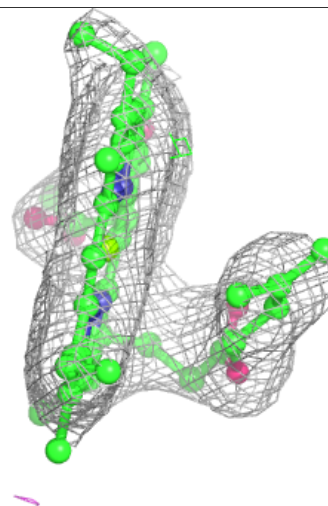
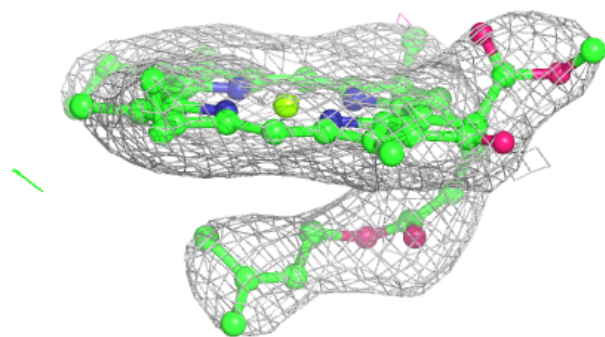
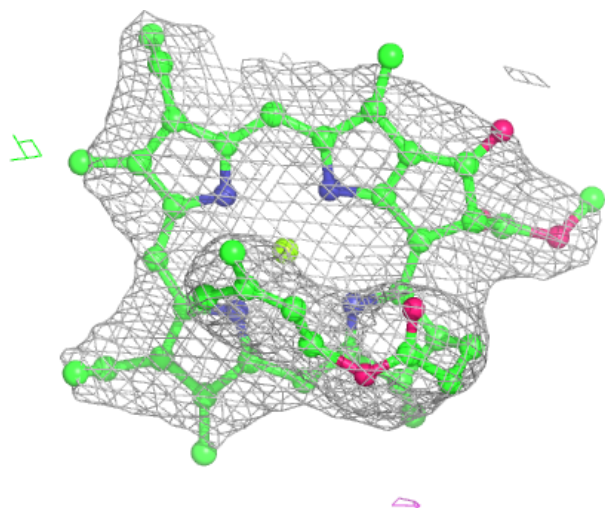
**Electron density around CLA Y 822:**

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



**Electron density around CLA Y 823:**

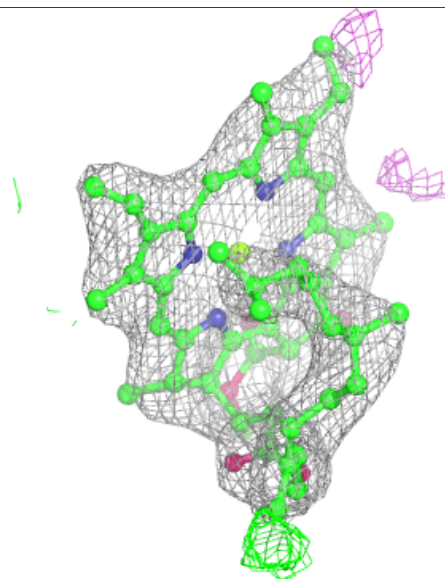
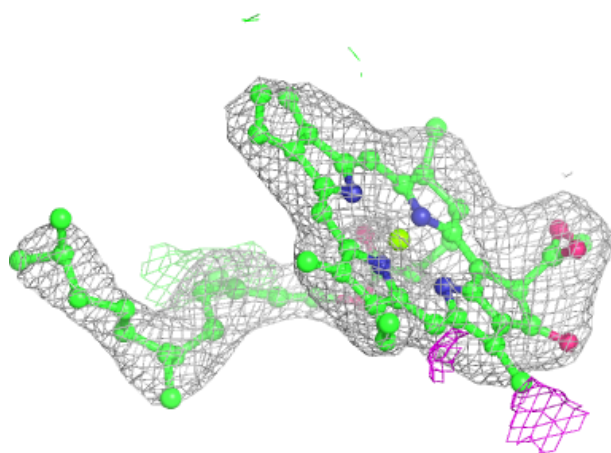
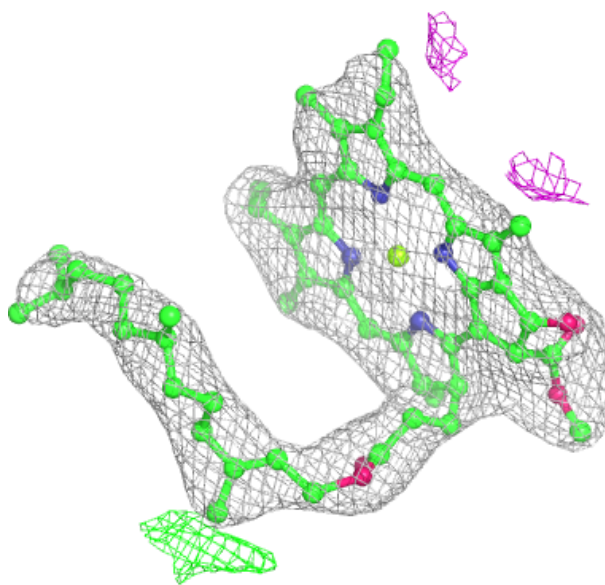
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

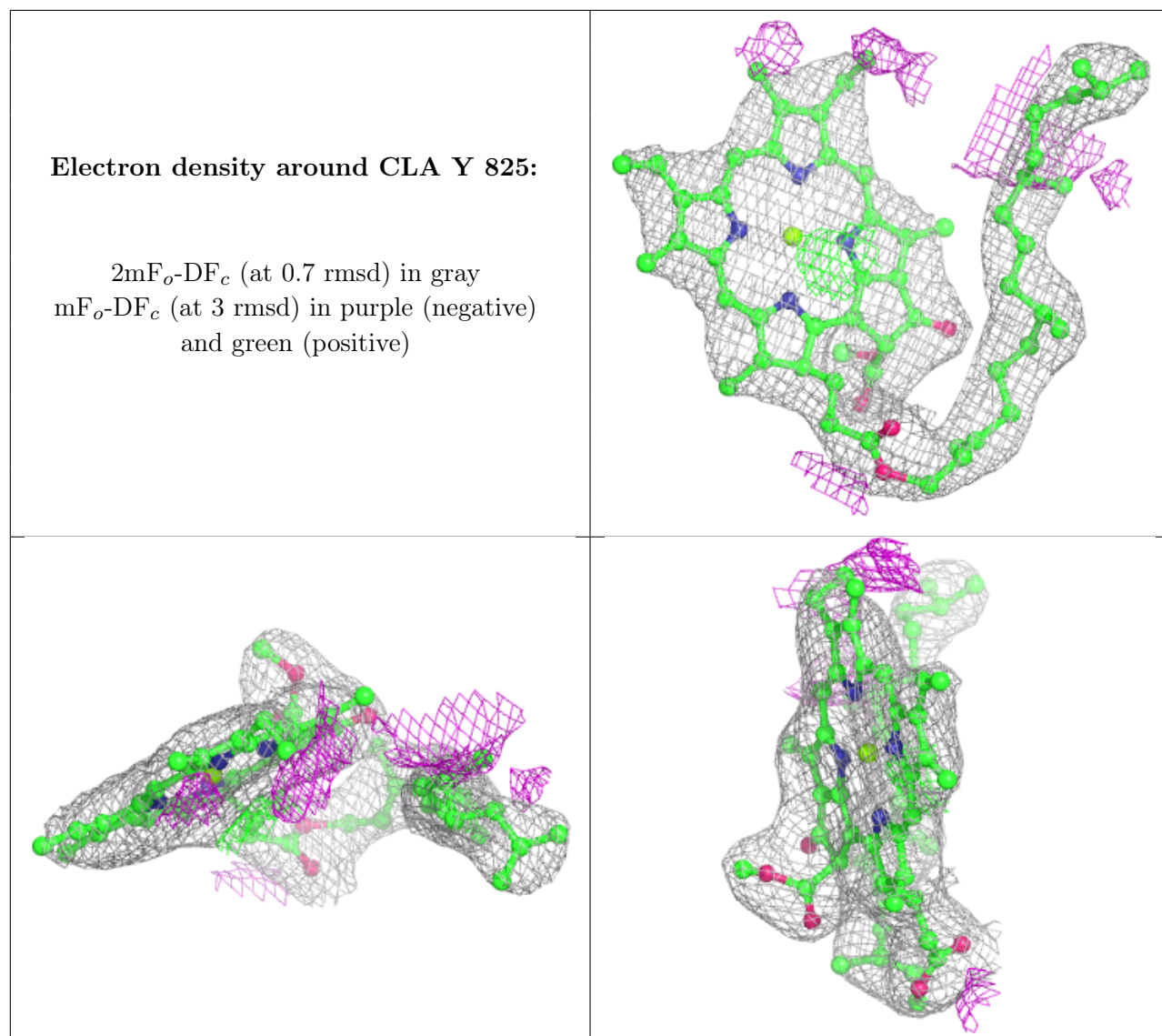




**Electron density around CLA Y 824:**

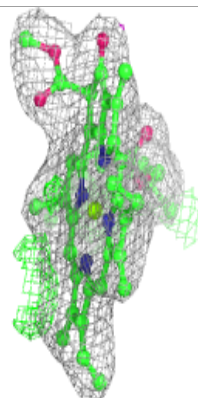
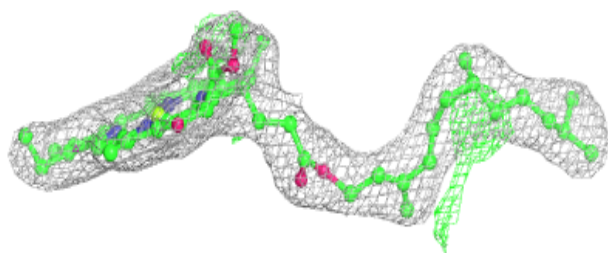
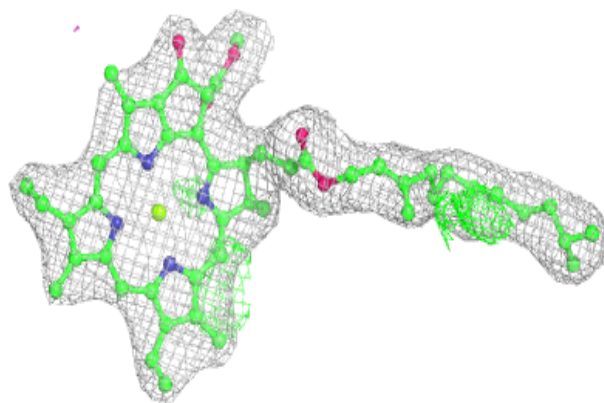
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



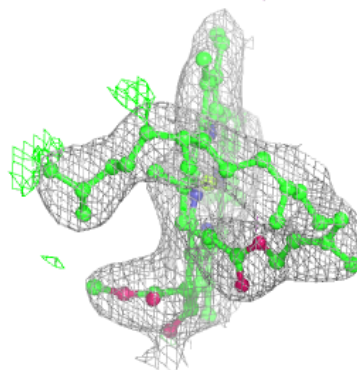
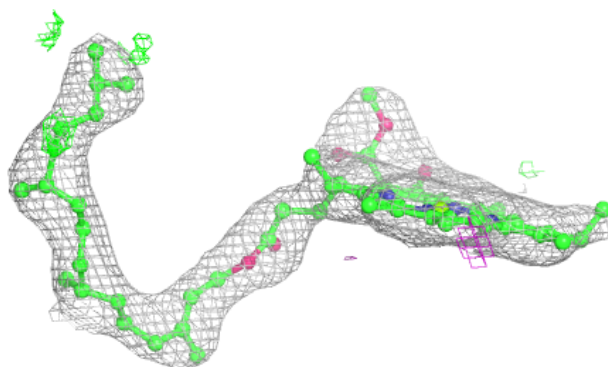
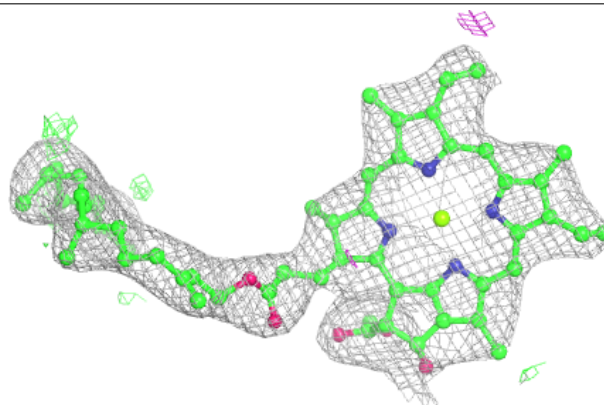


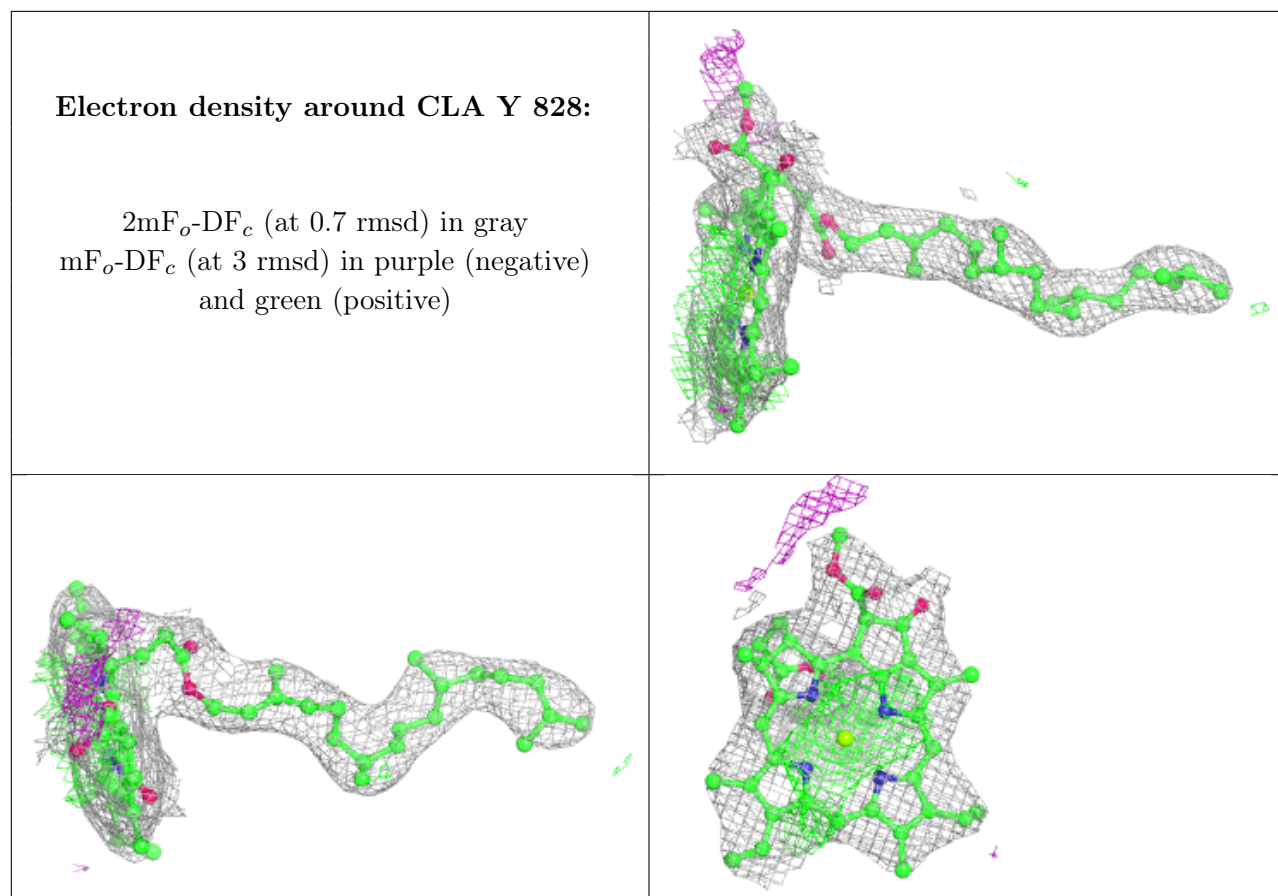
**Electron density around CLA Y 826:**

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

**Electron density around CLA Y 827:**

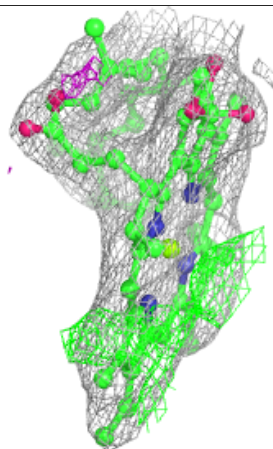
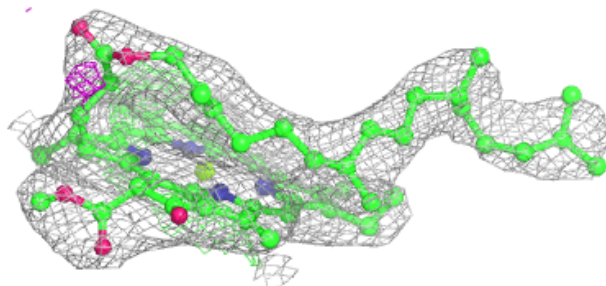
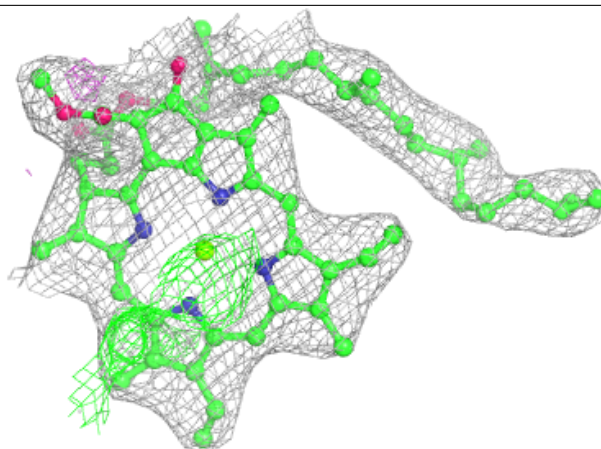
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



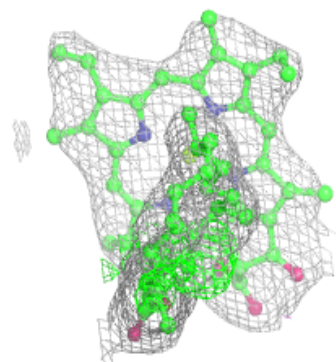
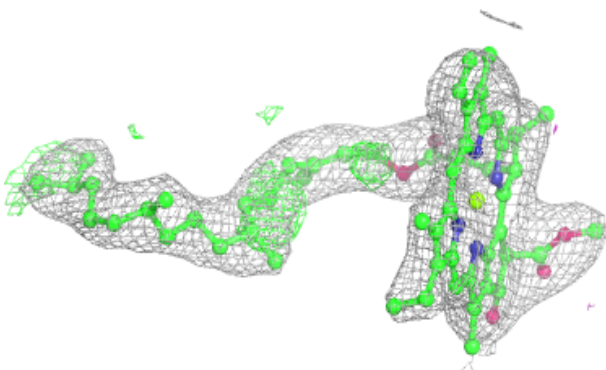
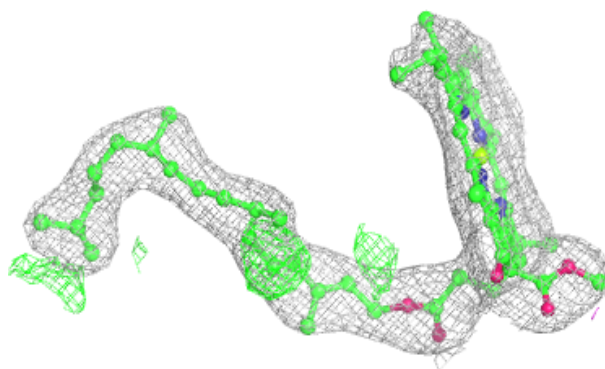


**Electron density around CLA Y 829:**

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

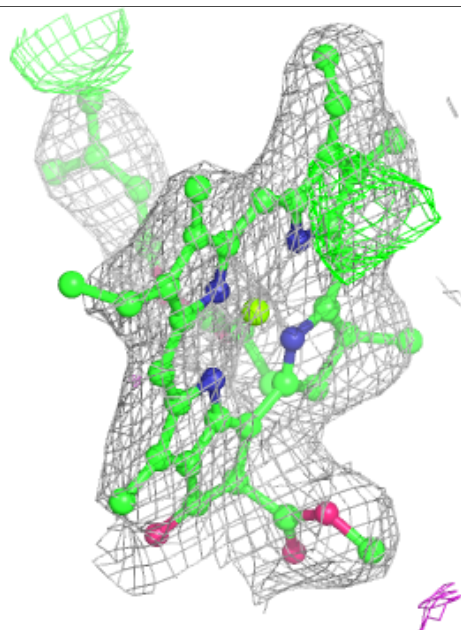
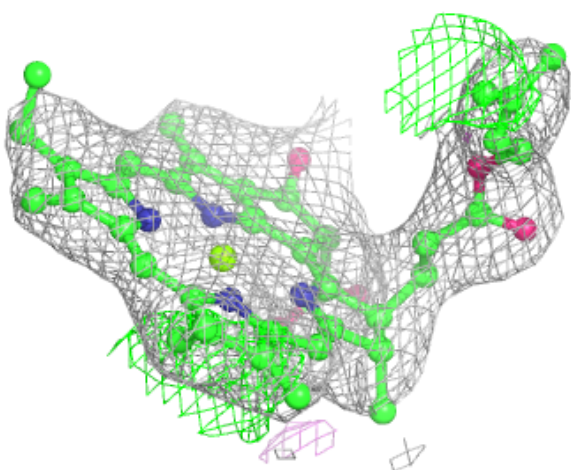
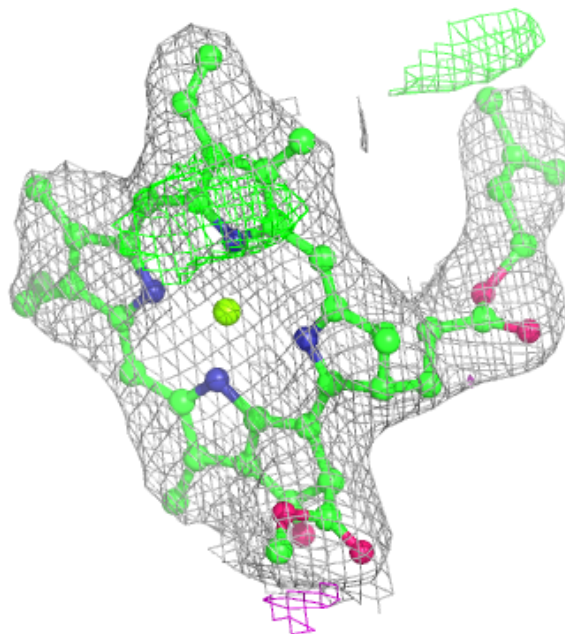
**Electron density around CLA Y 830:**

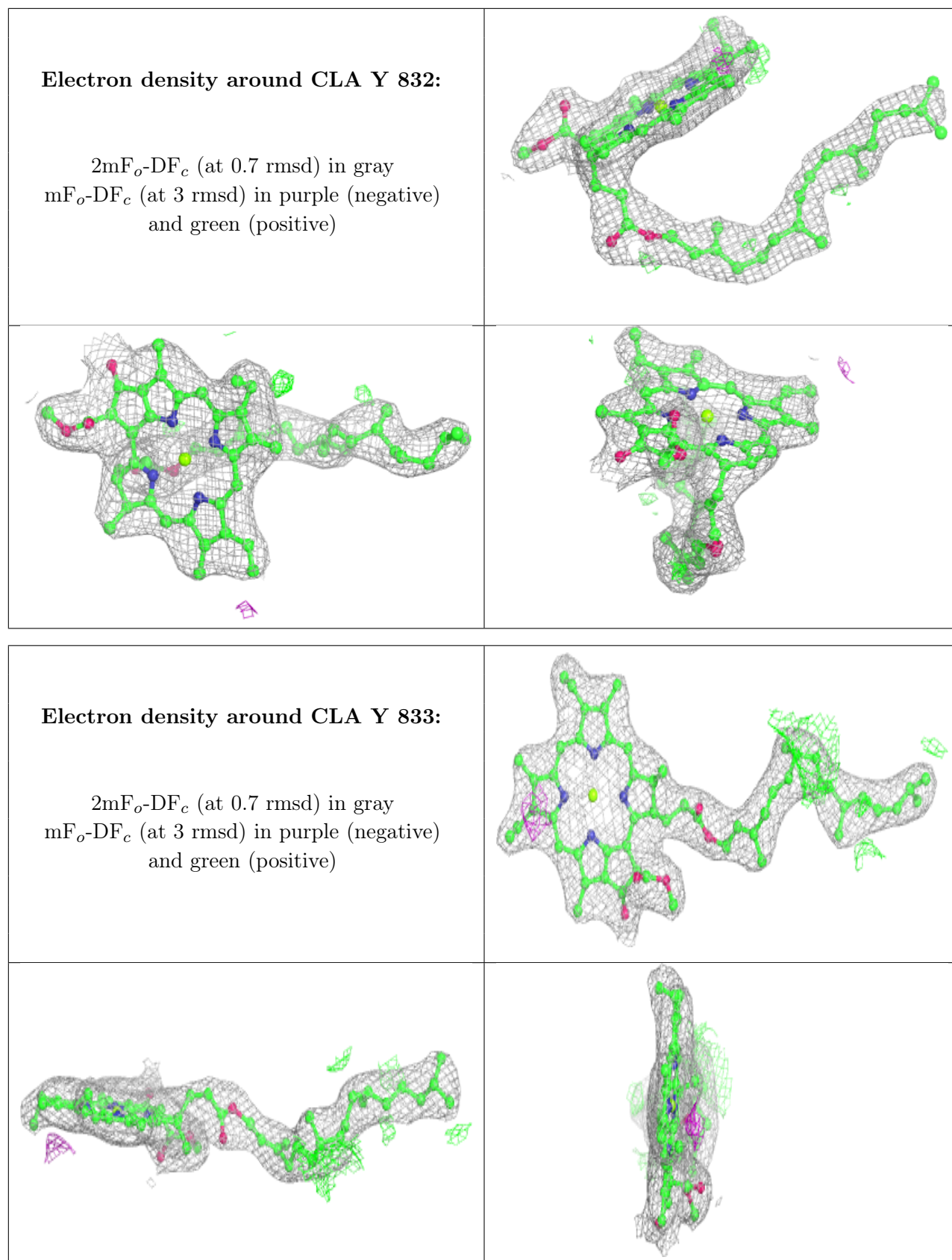
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA Y 831:**

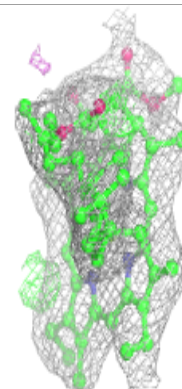
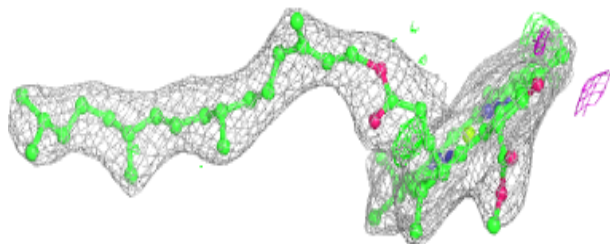
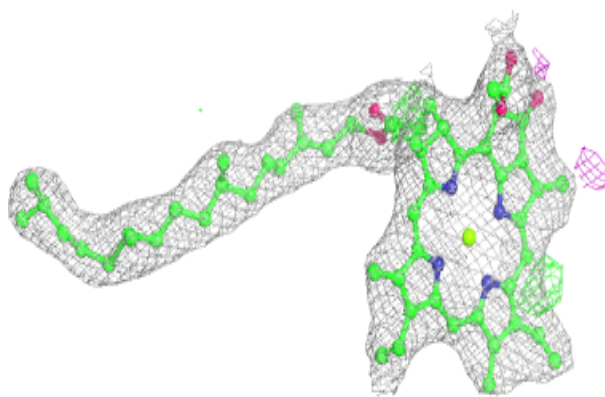
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



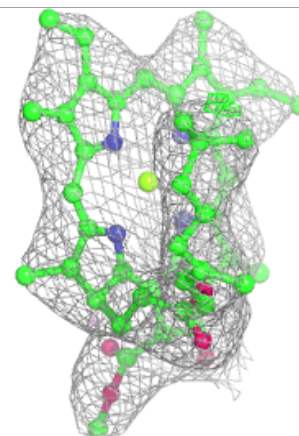
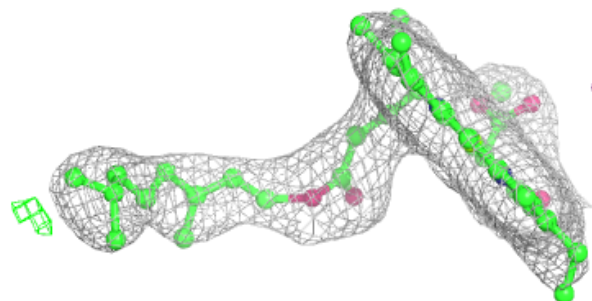
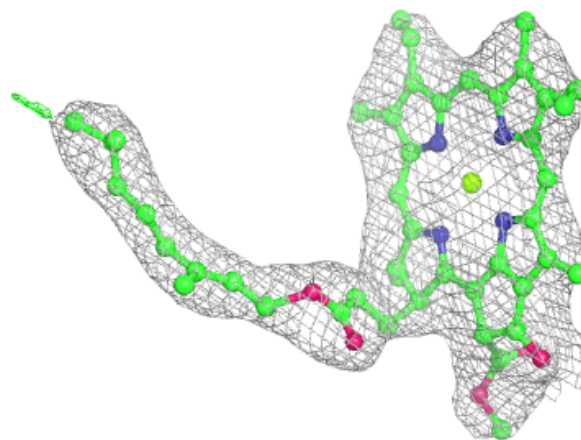


**Electron density around CLA Y 834:**

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

**Electron density around CLA Y 835:**

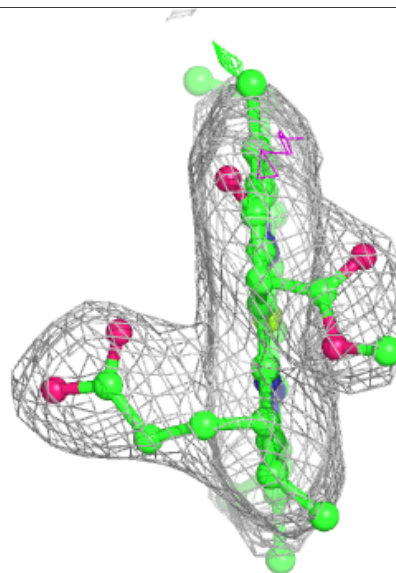
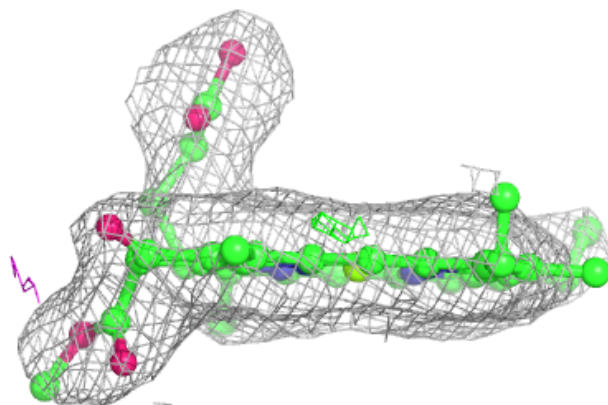
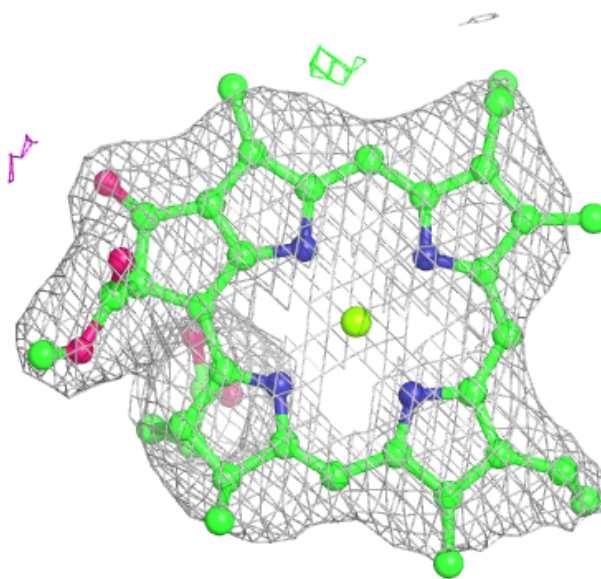
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





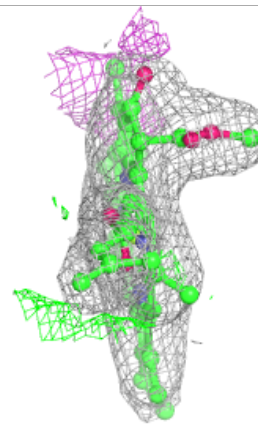
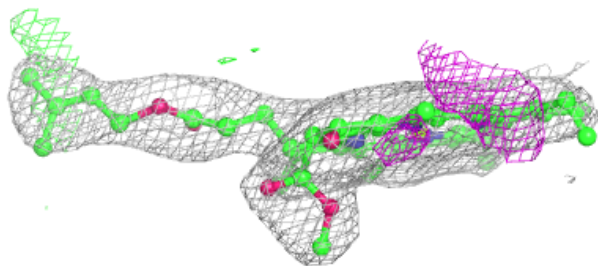
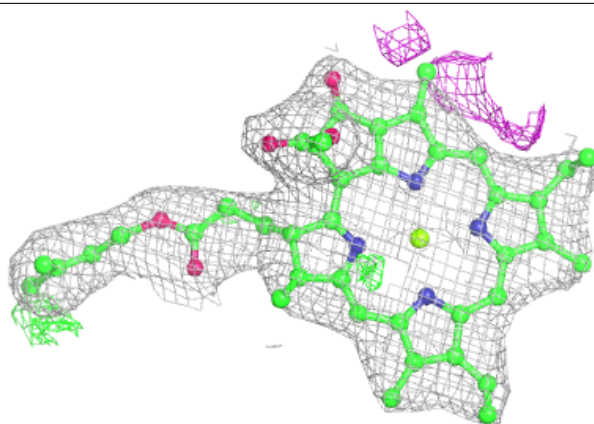
**Electron density around CLA Y 836:**

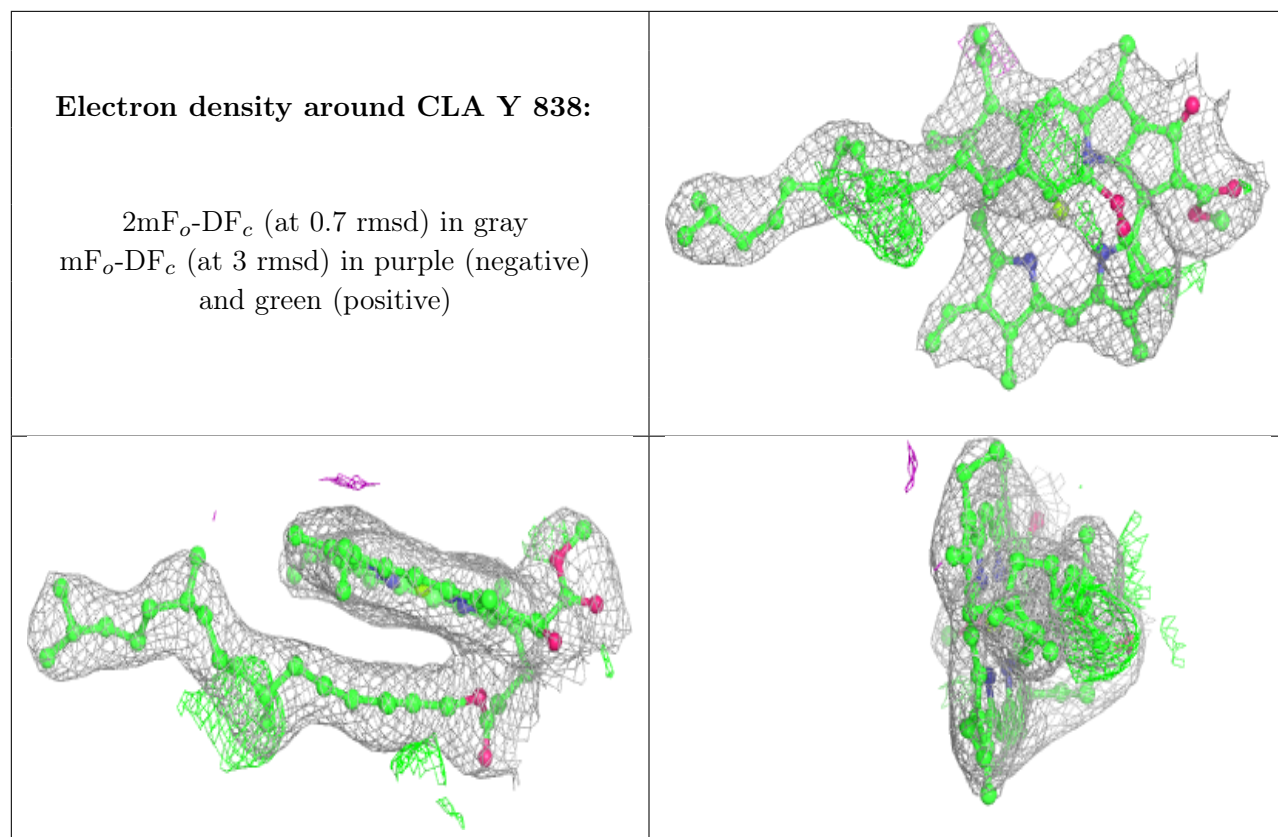
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA Y 837:**

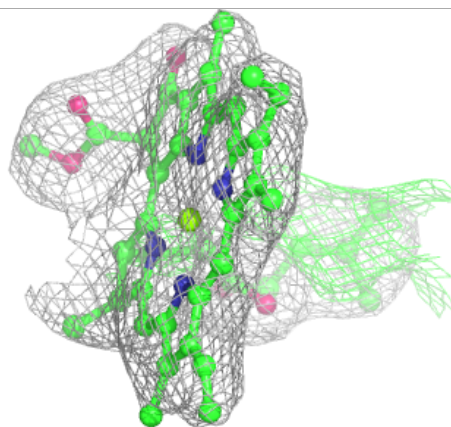
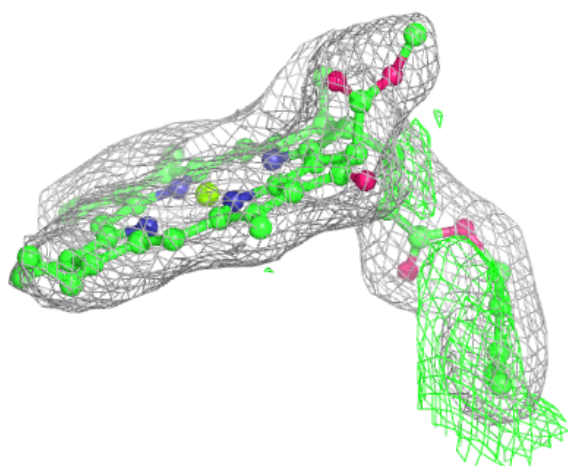
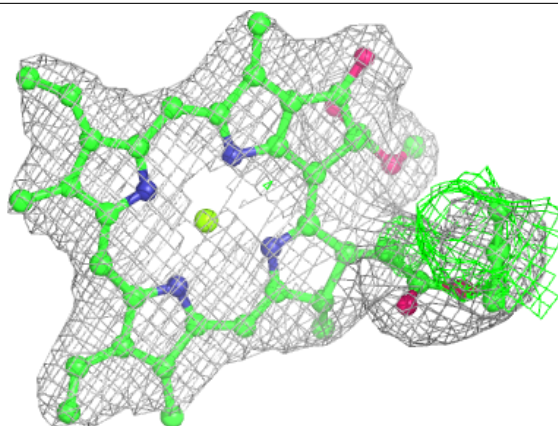
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





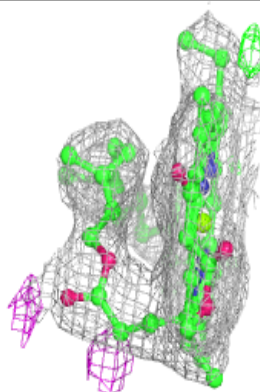
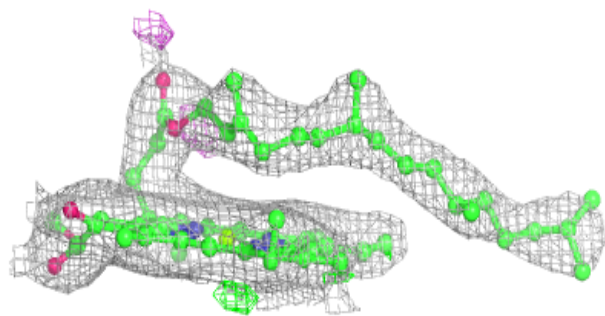
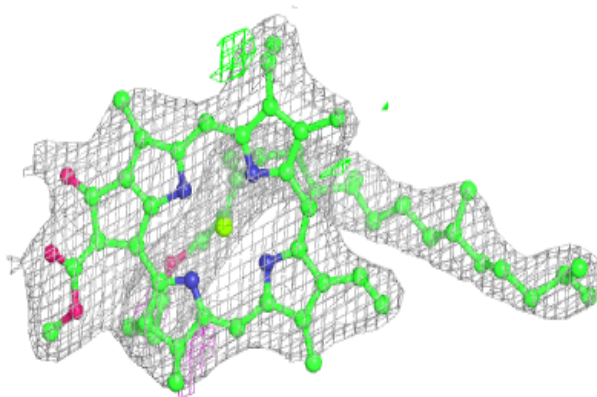
**Electron density around CLA Y 839:**

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

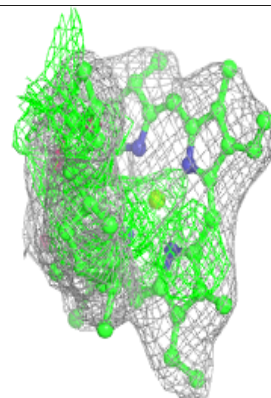
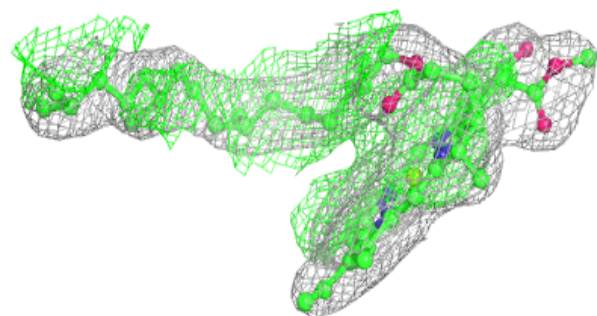
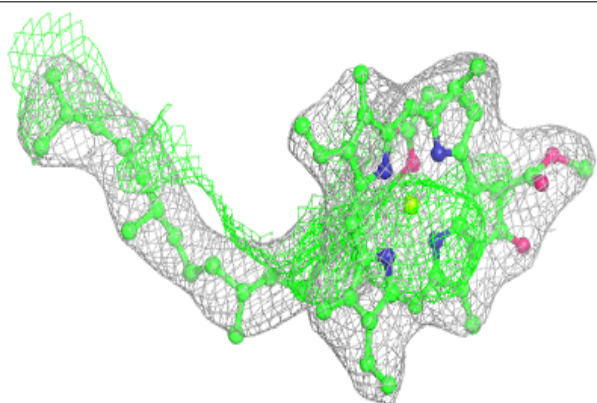


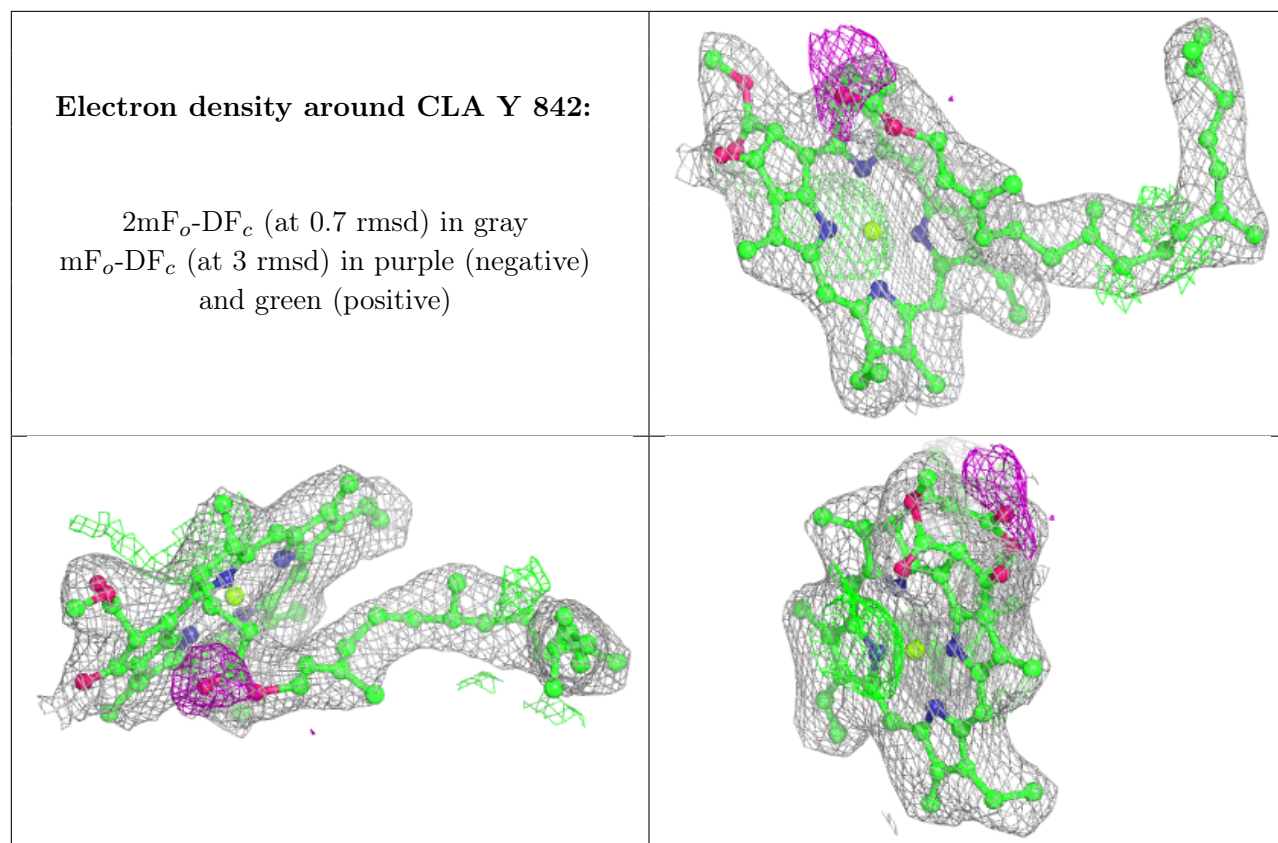
**Electron density around CLA Y 840:**

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

**Electron density around CLA Y 841:**

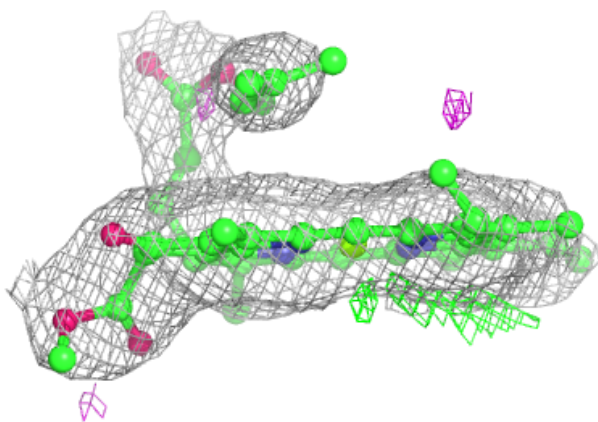
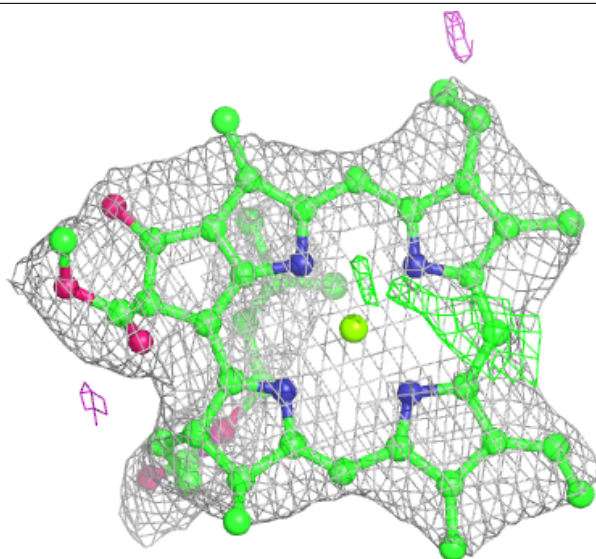
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





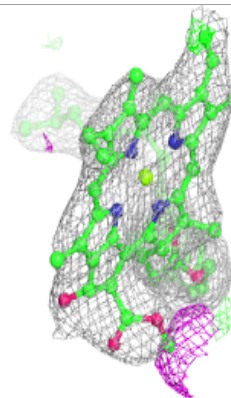
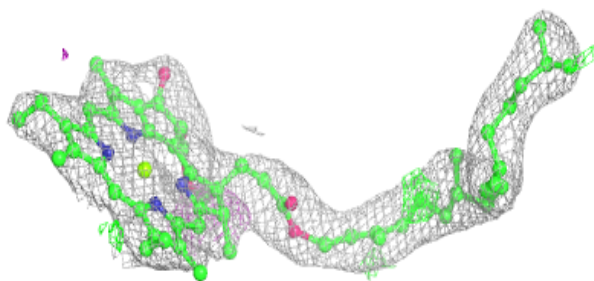
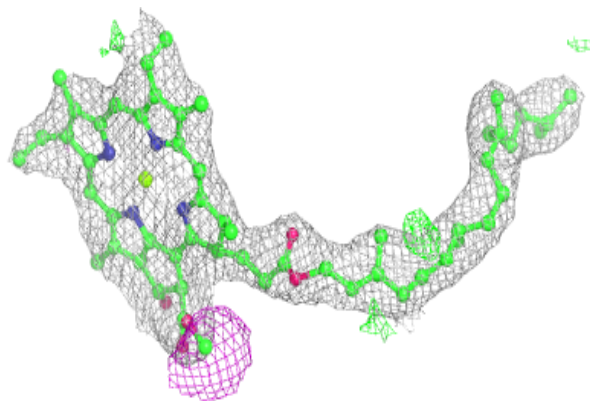
**Electron density around CLA Y 843:**

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

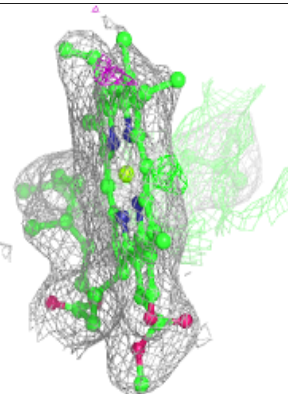
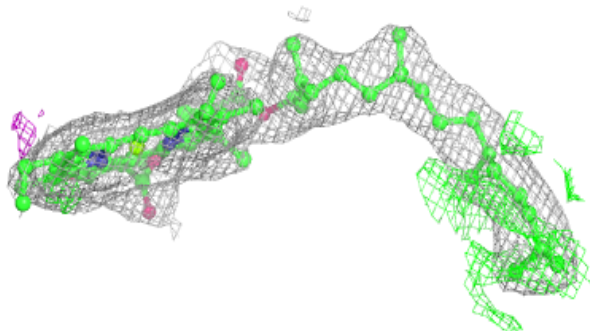
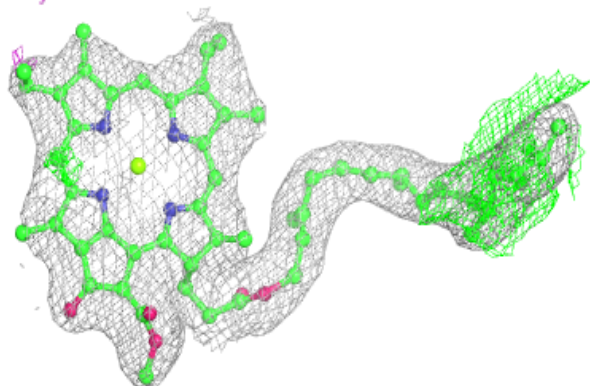


**Electron density around CLA Y 854:**

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

**Electron density around CLA Y 855:**

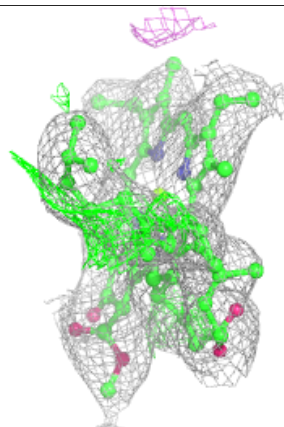
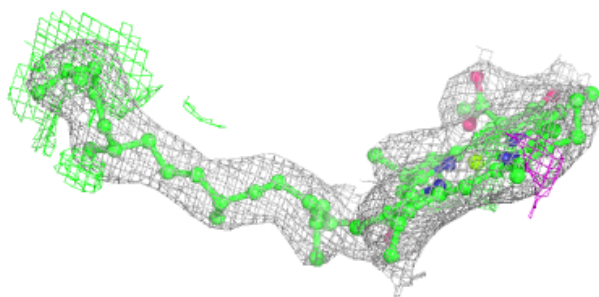
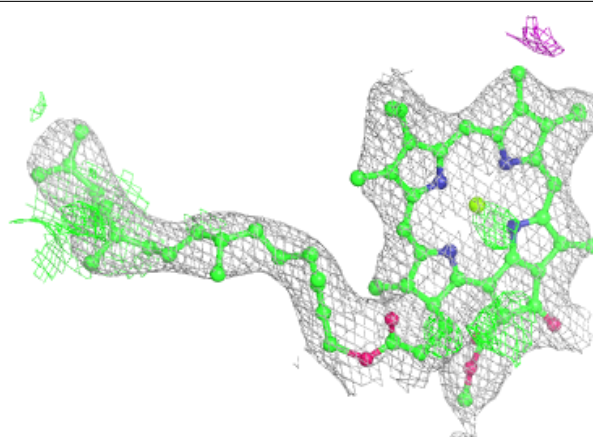
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



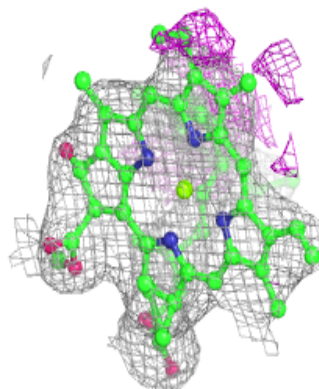
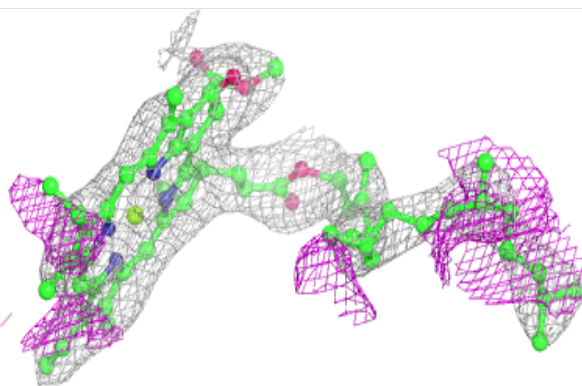
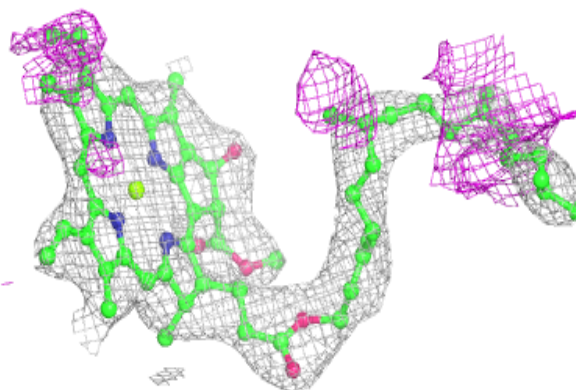


**Electron density around CLA Z 801:**

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

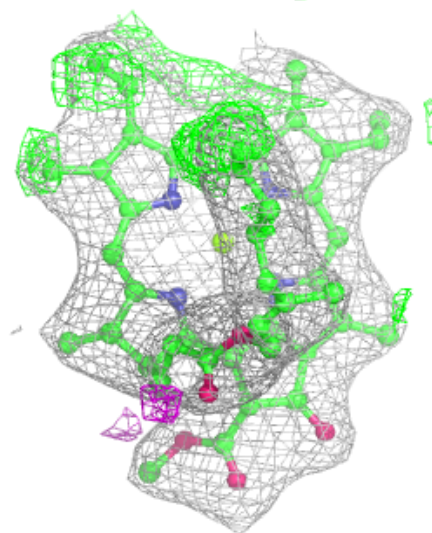
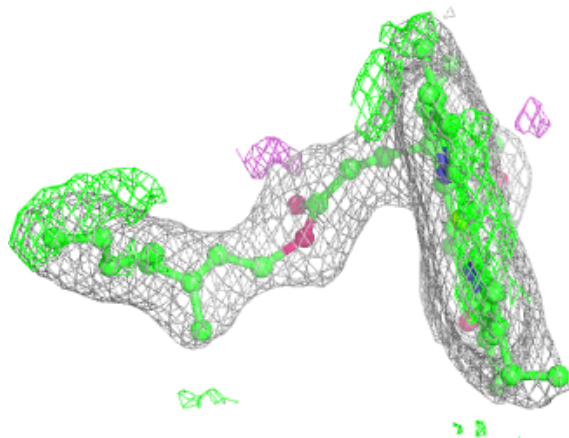
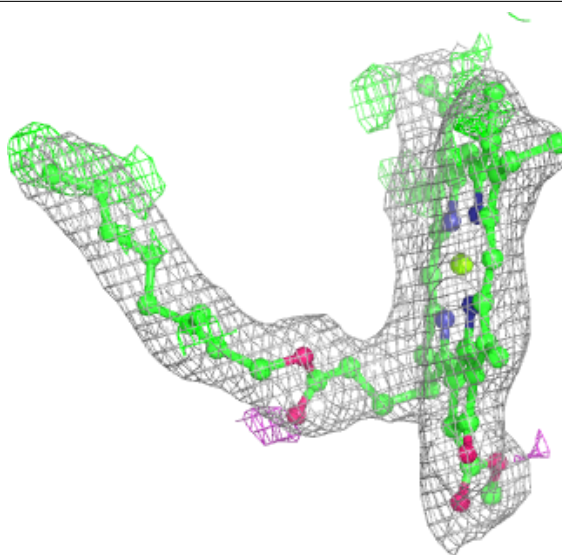
**Electron density around CLA Z 802:**

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



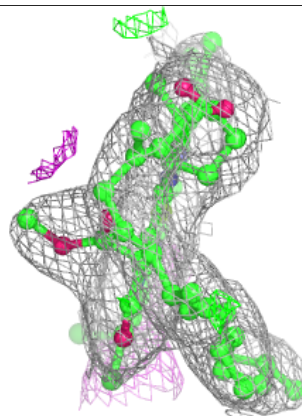
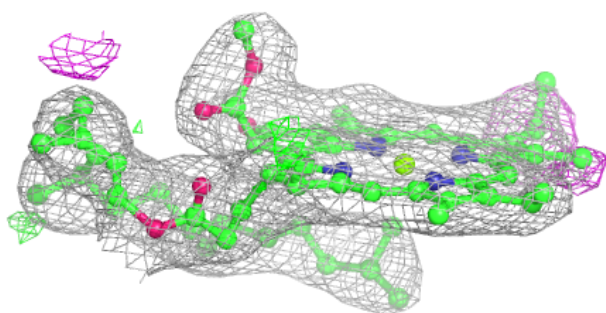
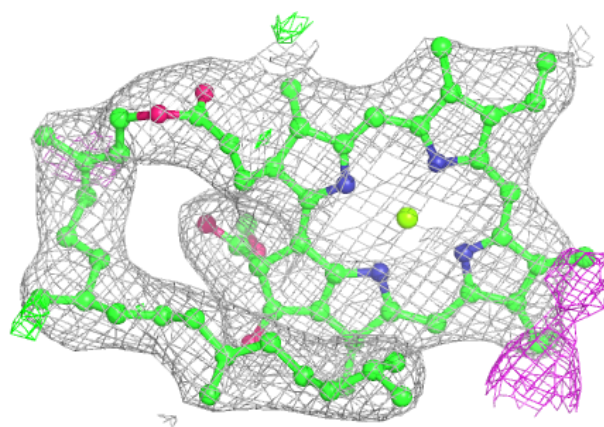
**Electron density around CLA Z 803:**

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



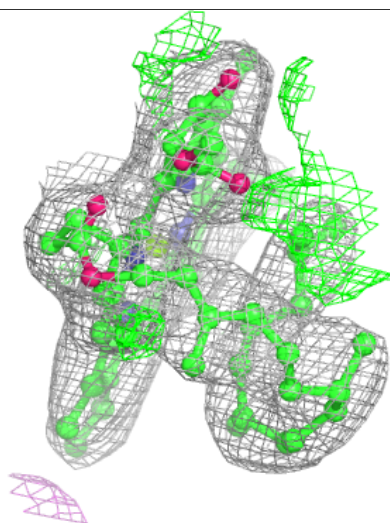
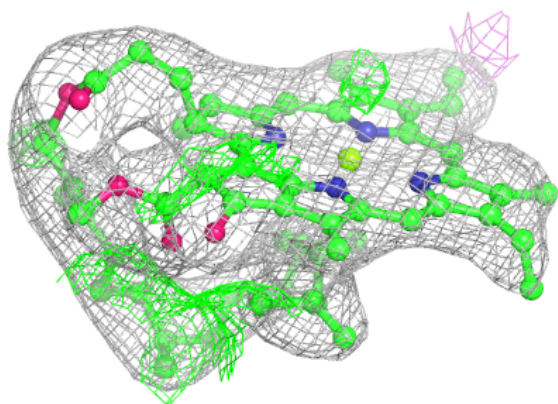
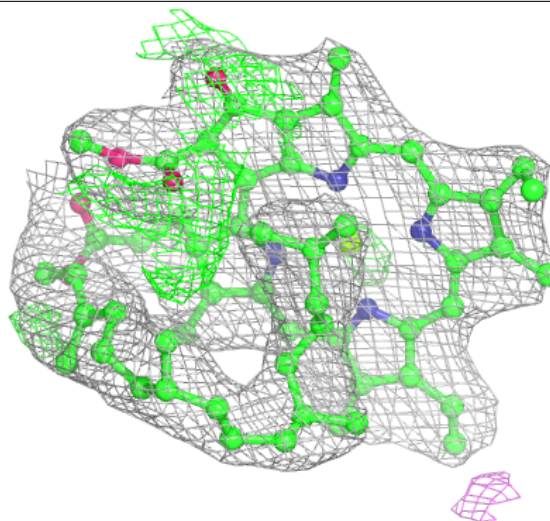
**Electron density around CLA Z 804:**

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



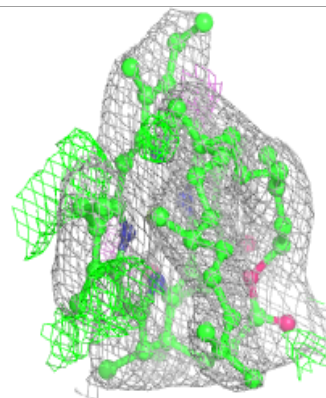
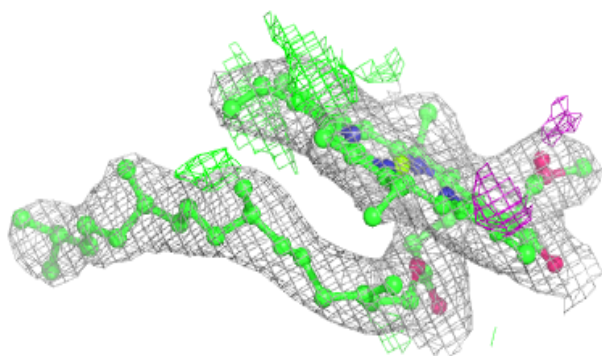
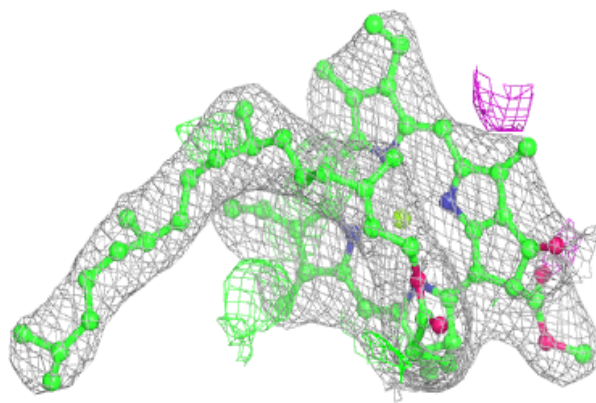
**Electron density around CLA Z 805:**

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



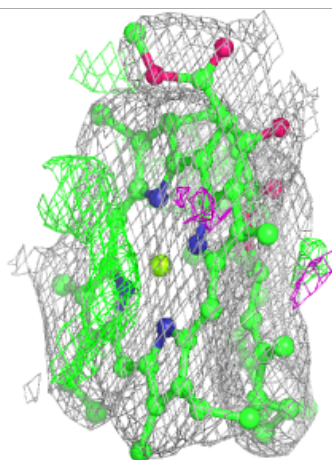
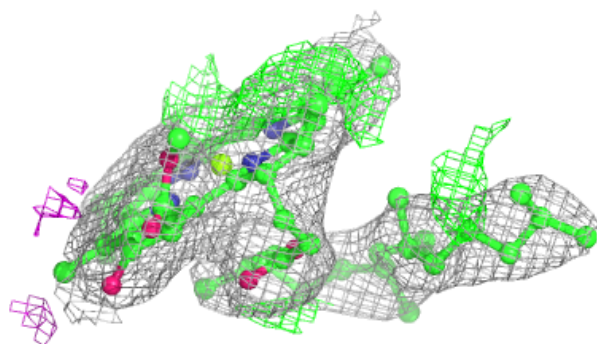
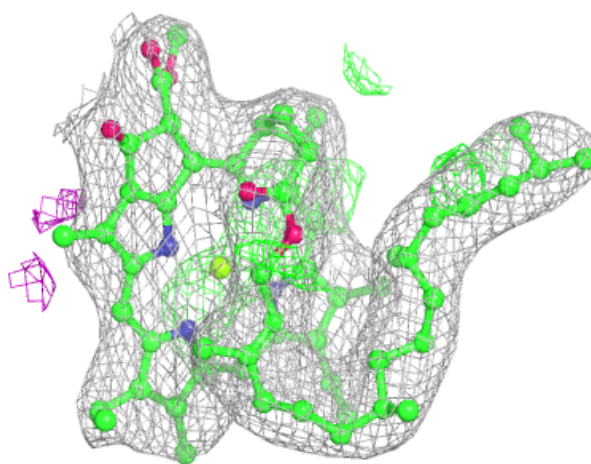
**Electron density around CLA Z 806:**

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



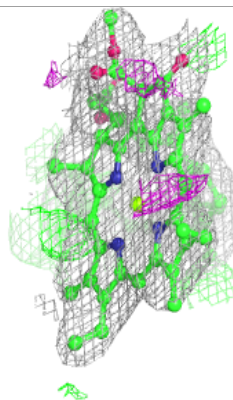
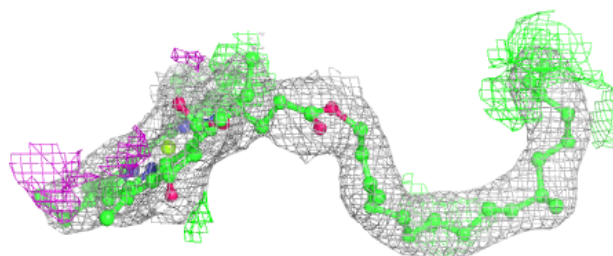
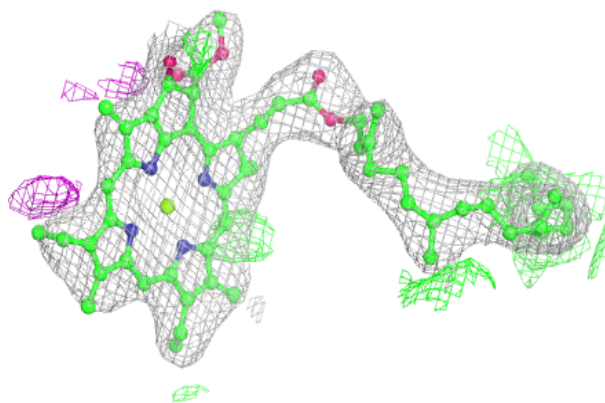
**Electron density around CLA Z 807:**

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



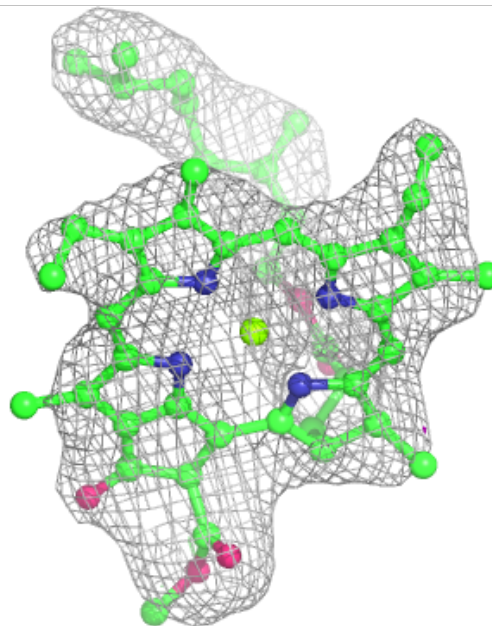
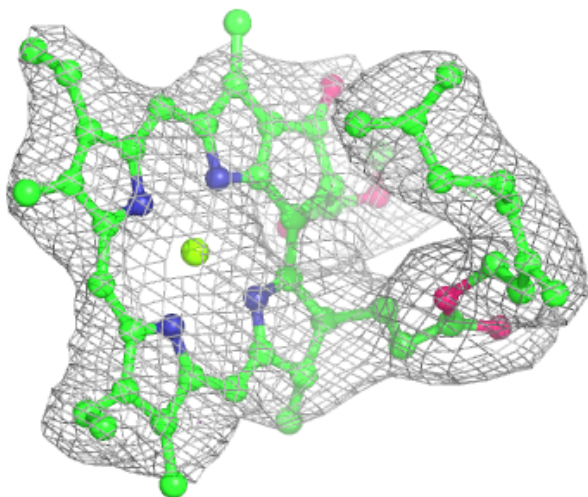
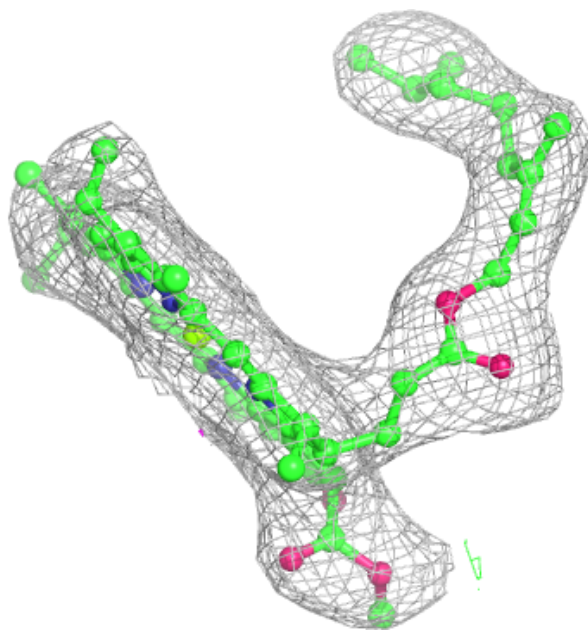
**Electron density around CLA Z 808:**

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



**Electron density around CLA Z 809:**

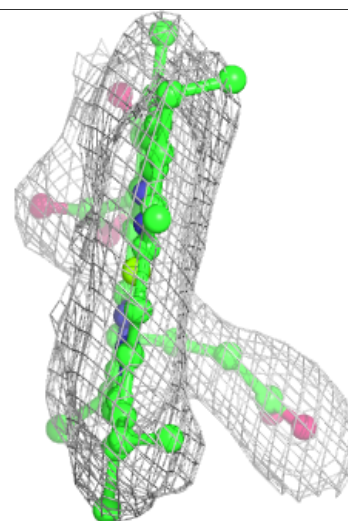
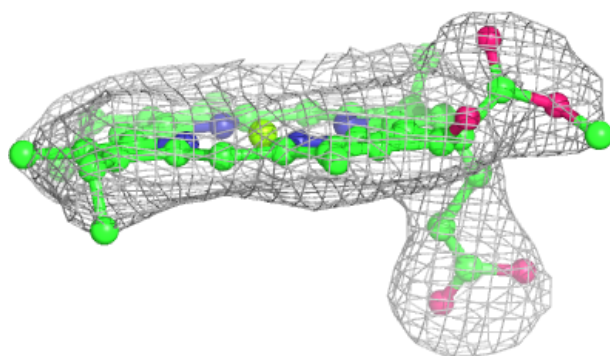
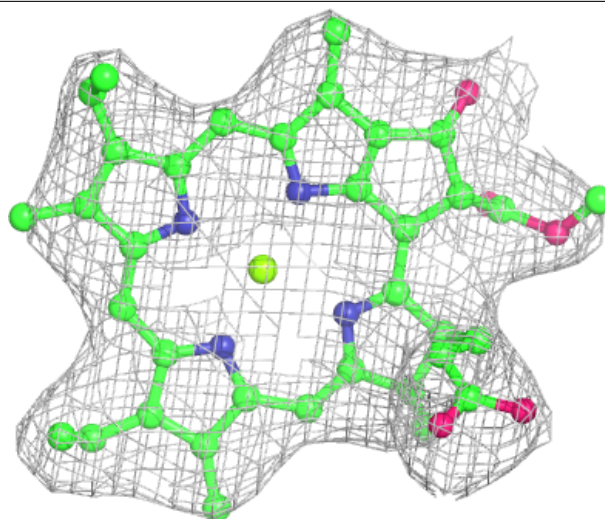
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





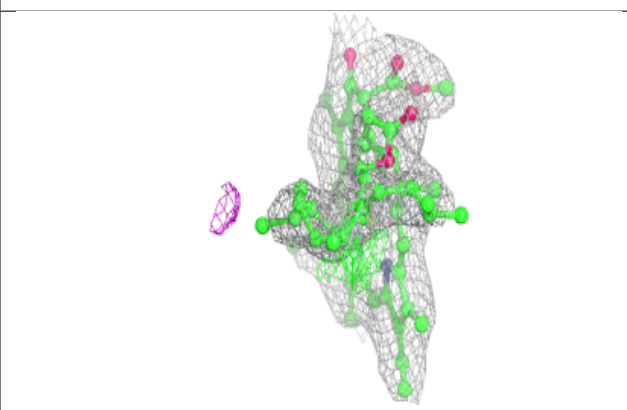
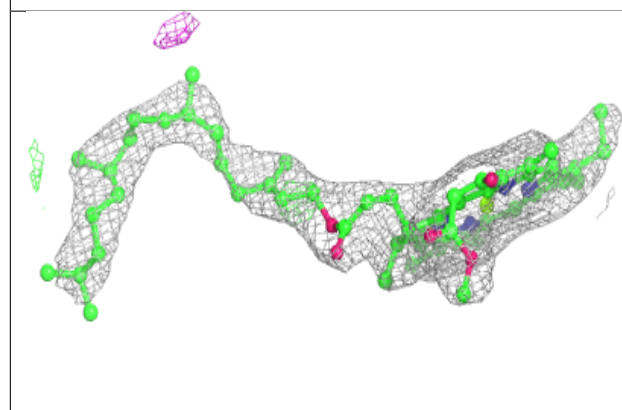
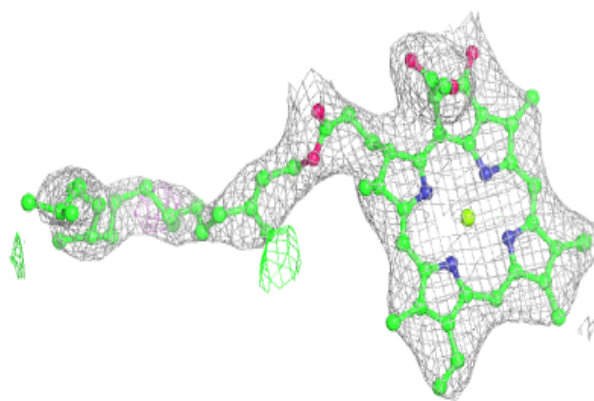
**Electron density around CLA Z 810:**

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

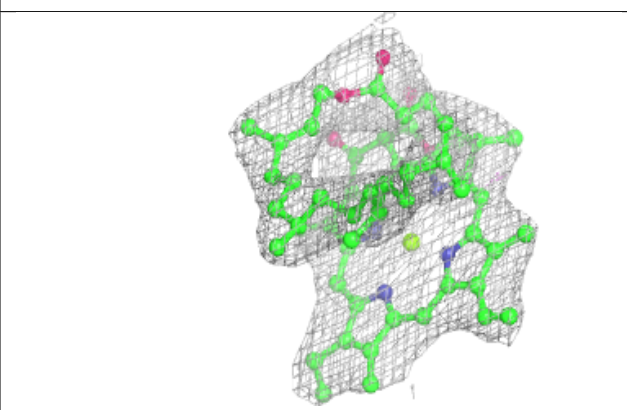
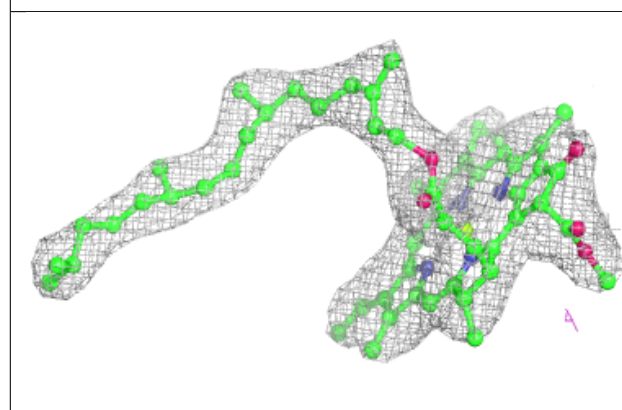
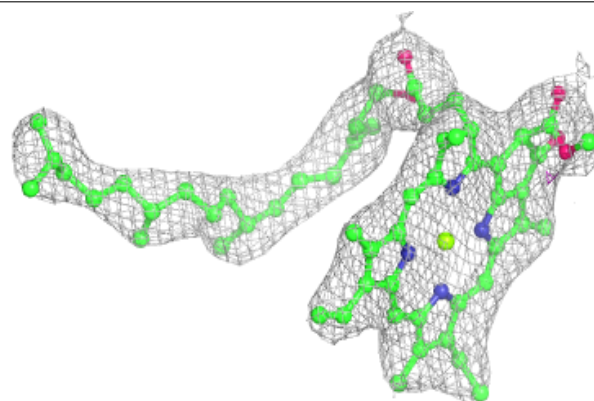


**Electron density around CLA Z 811:**

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

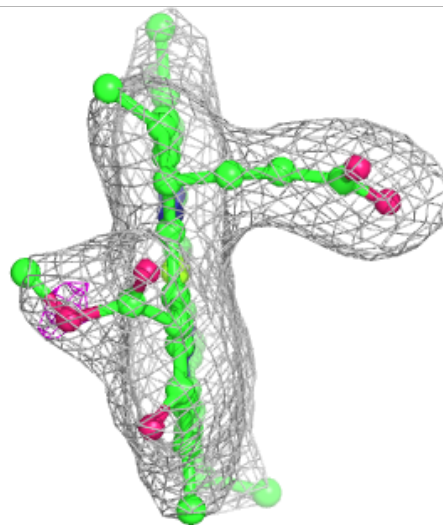
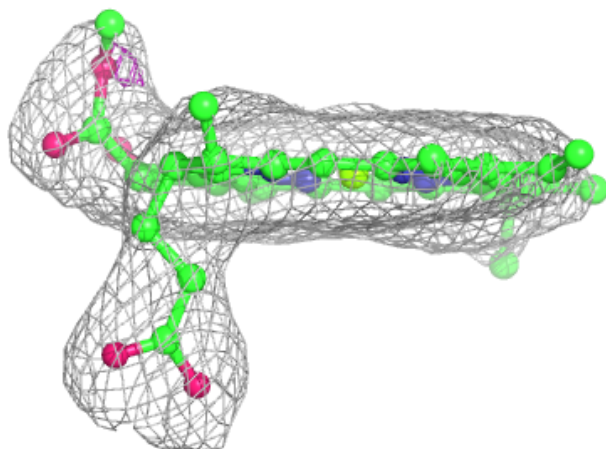
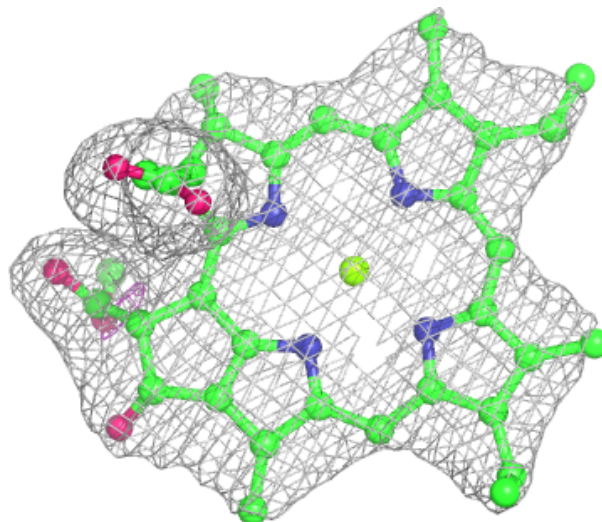
**Electron density around CLA Z 812:**

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



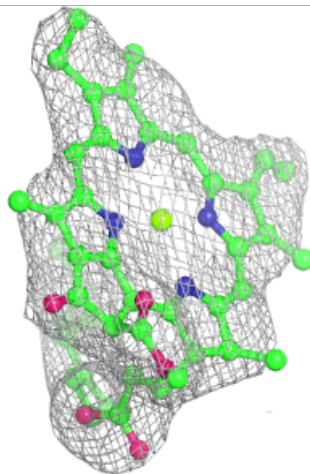
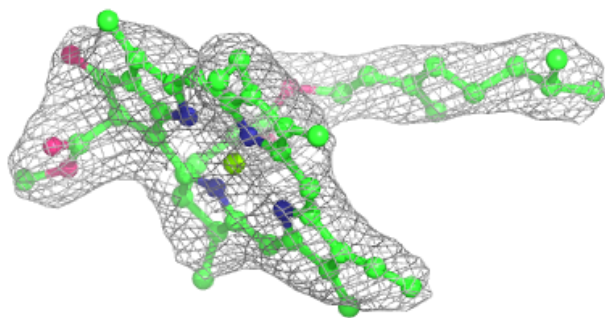
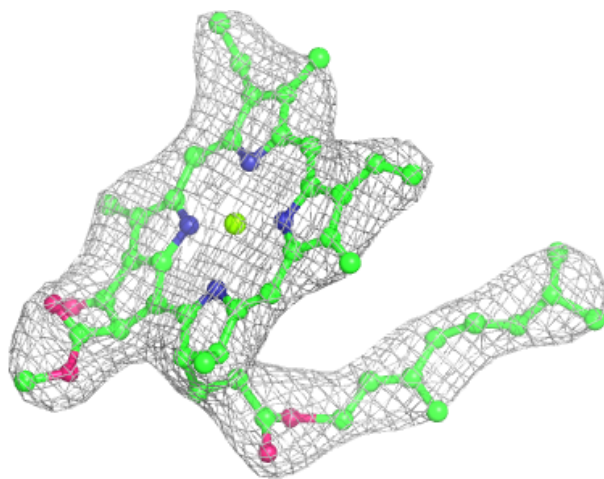
**Electron density around CLA Z 813:**

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



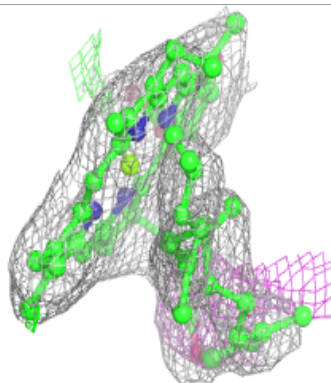
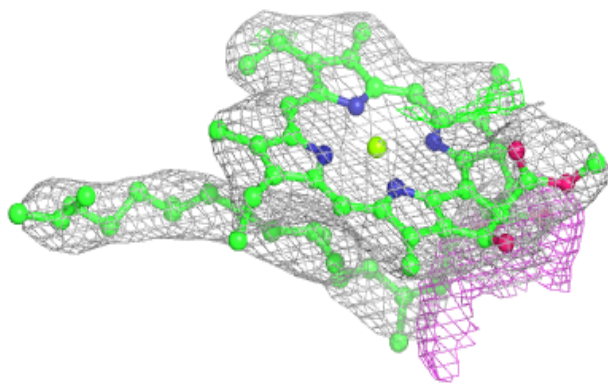
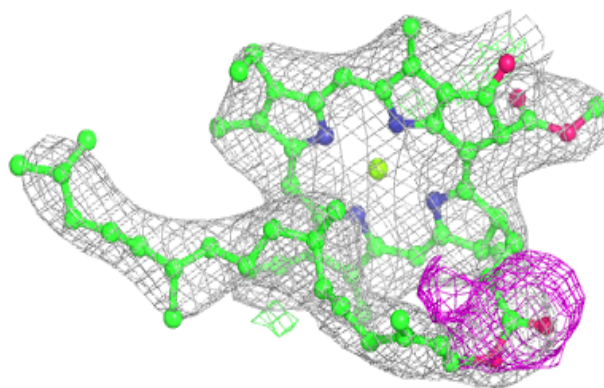
**Electron density around CLA Z 814:**

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

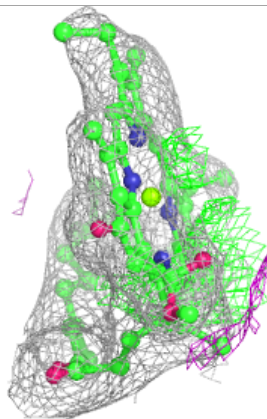
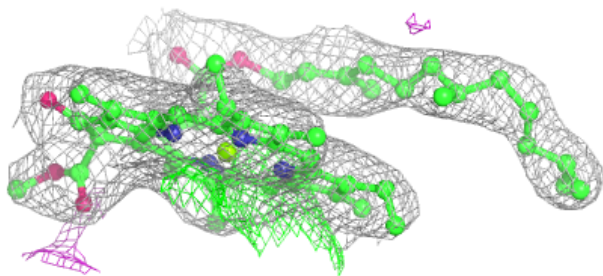
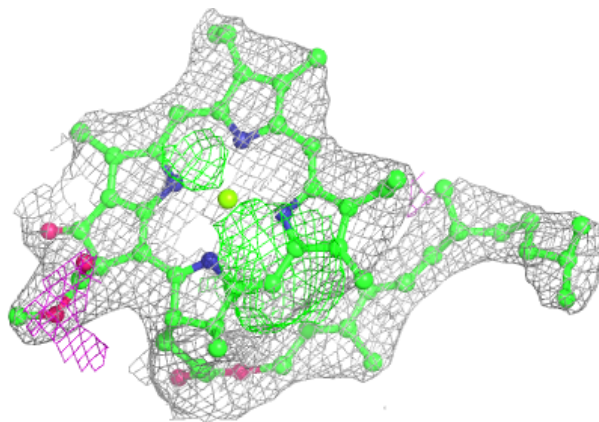


**Electron density around CLA Z 815:**

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

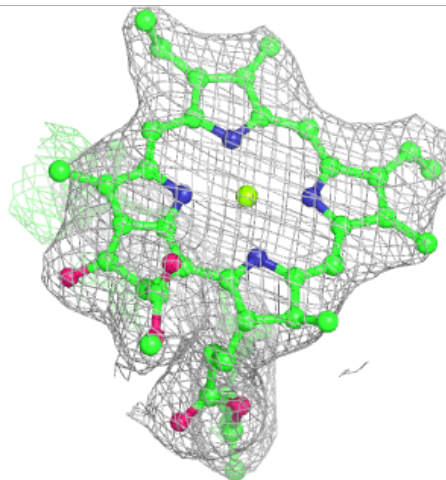
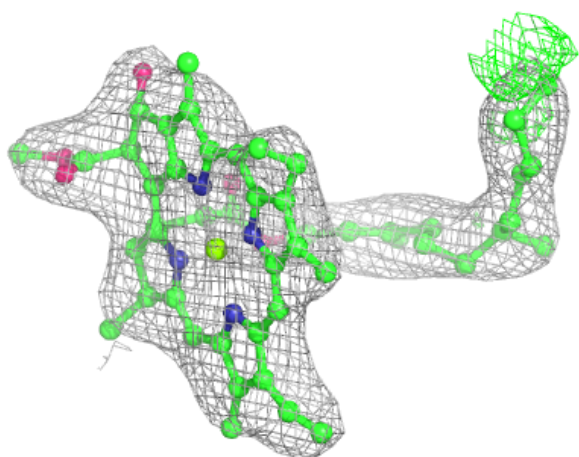
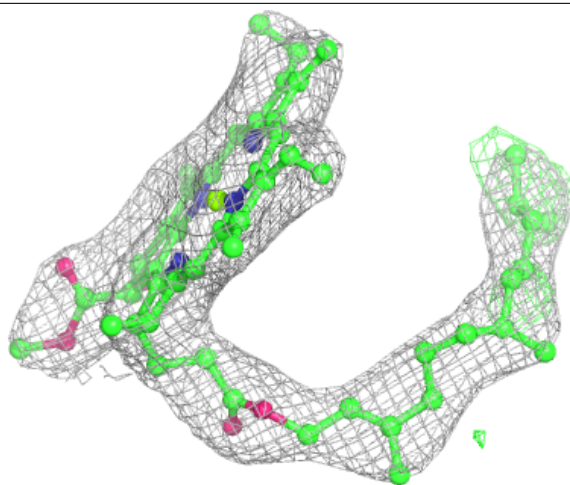
**Electron density around CLA Z 816:**

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



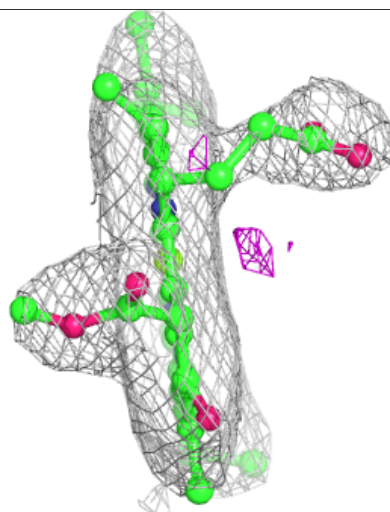
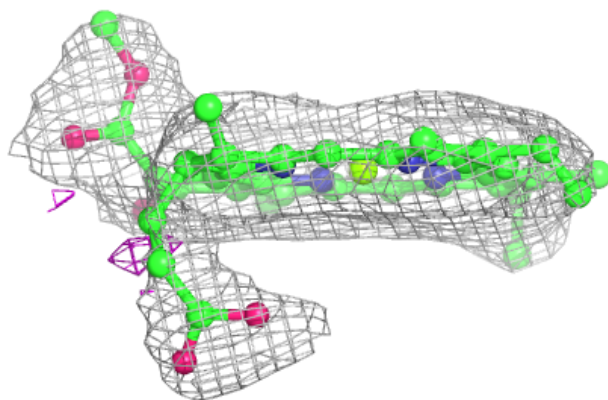
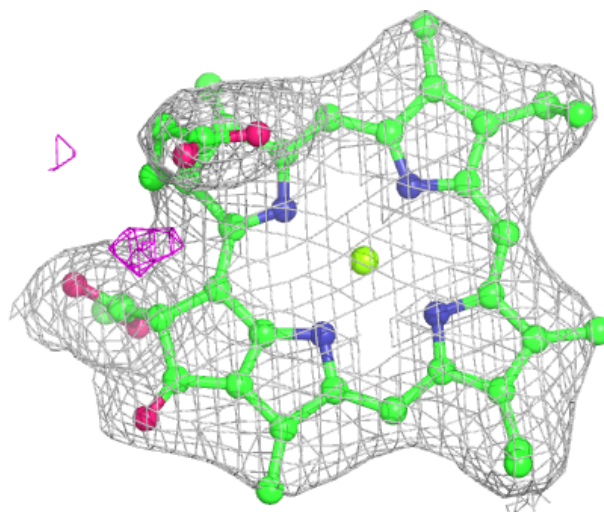
**Electron density around CLA Z 817:**

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



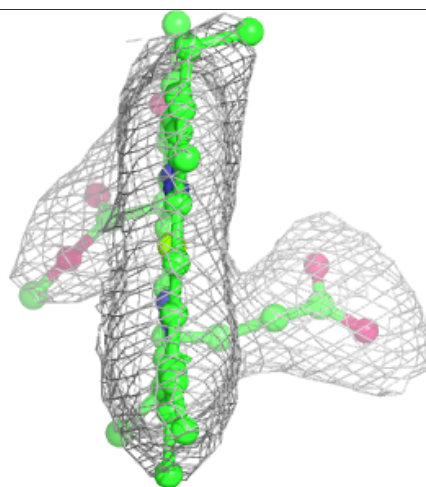
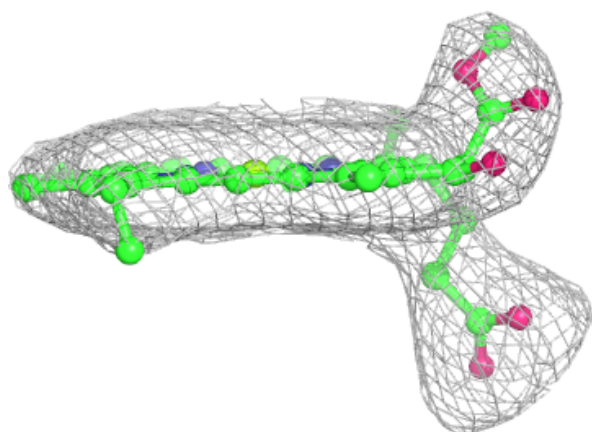
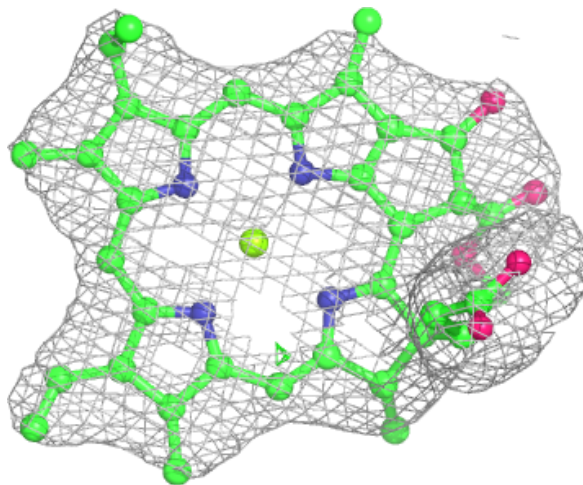
**Electron density around CLA Z 818:**

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



**Electron density around CLA Z 819:**

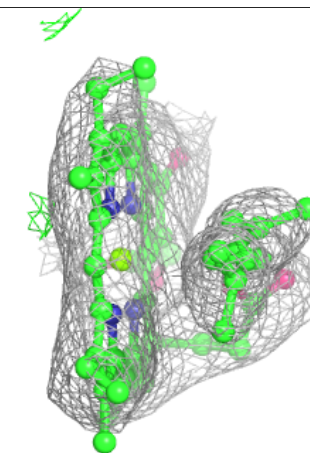
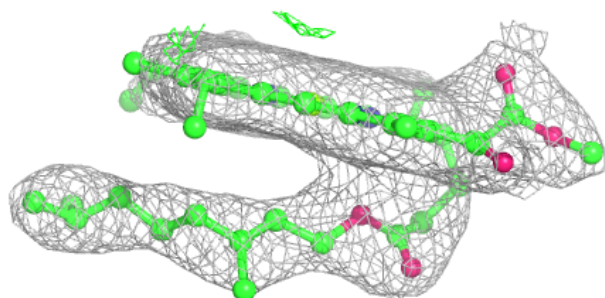
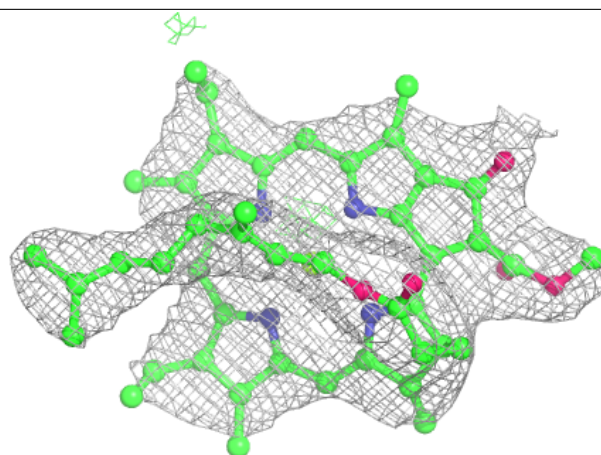
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



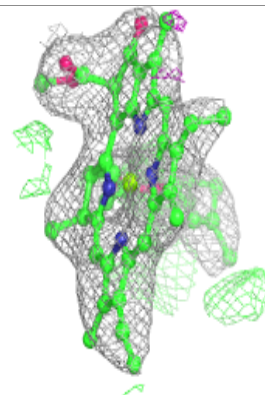
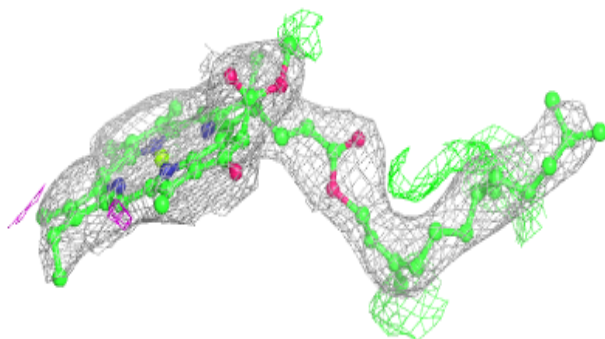
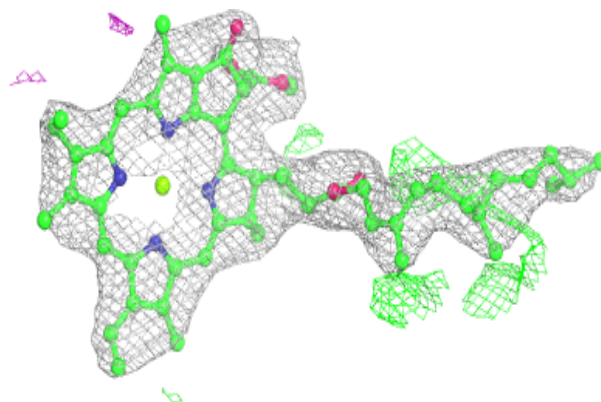


**Electron density around CLA Z 820:**

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

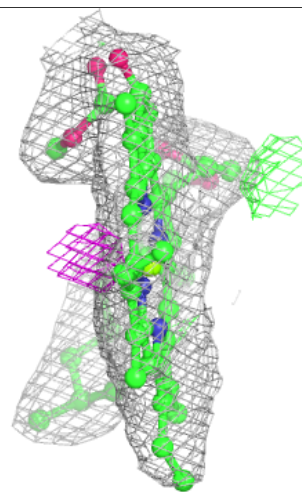
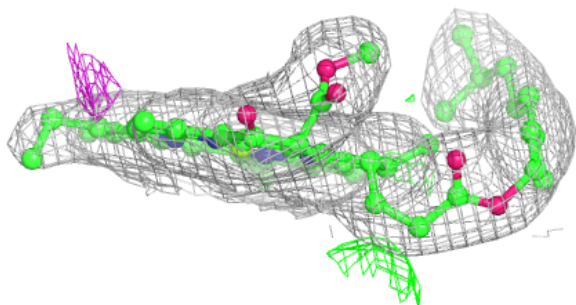
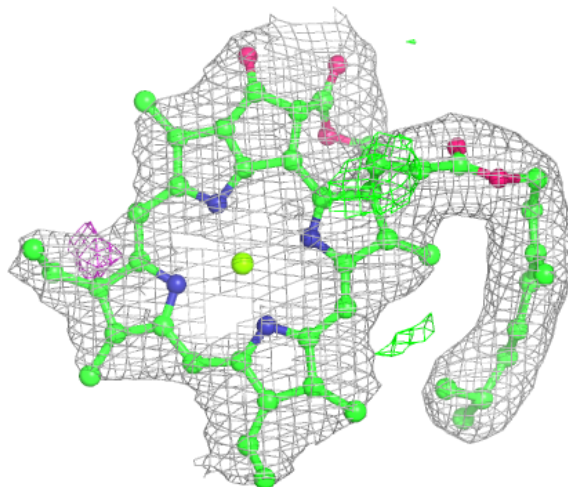
**Electron density around CLA Z 821:**

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



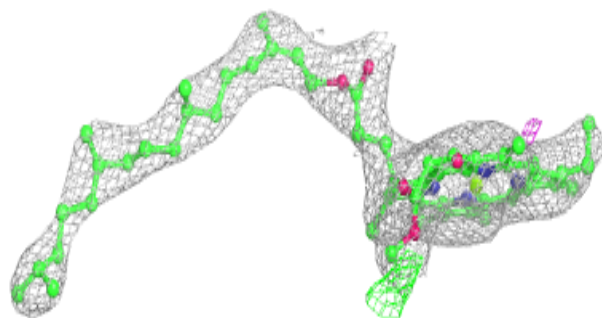
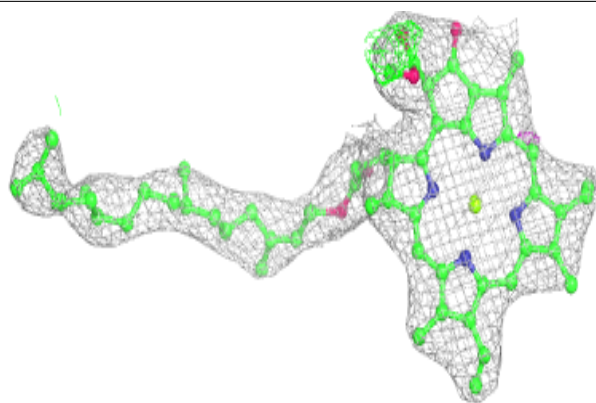
**Electron density around CLA Z 822:**

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

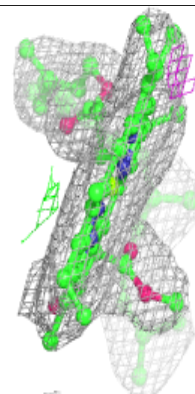
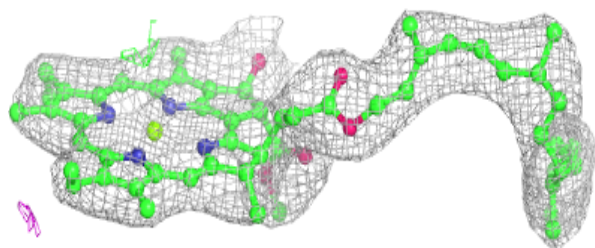
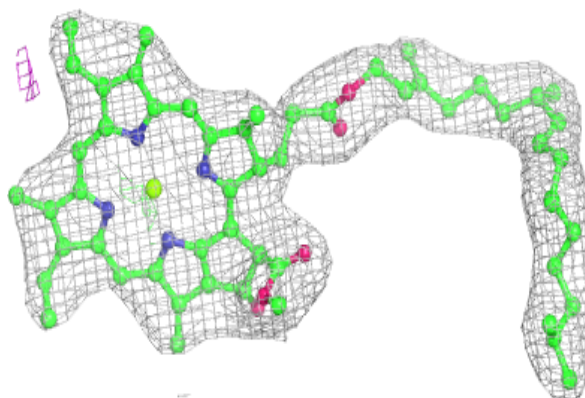


**Electron density around CLA Z 823:**

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

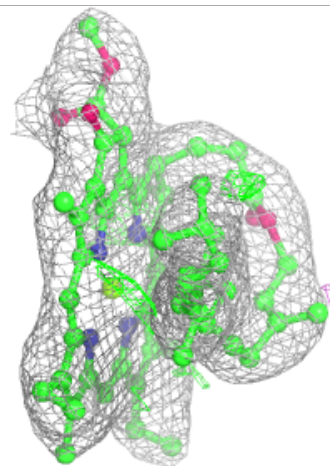
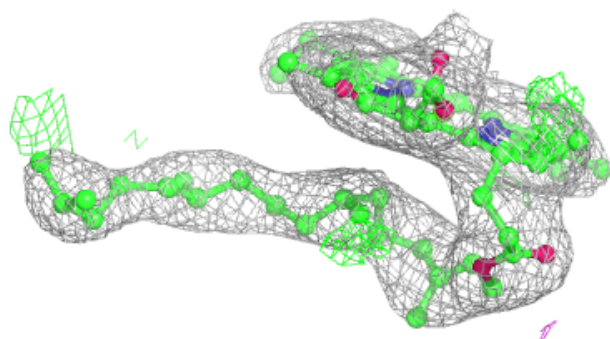
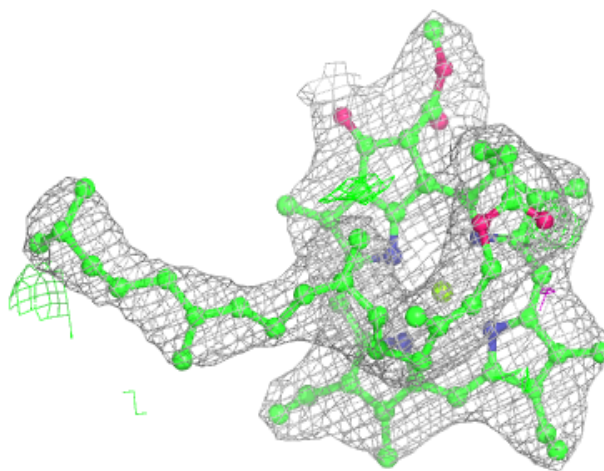
**Electron density around CLA Z 824:**

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



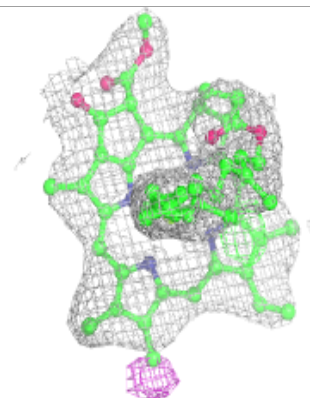
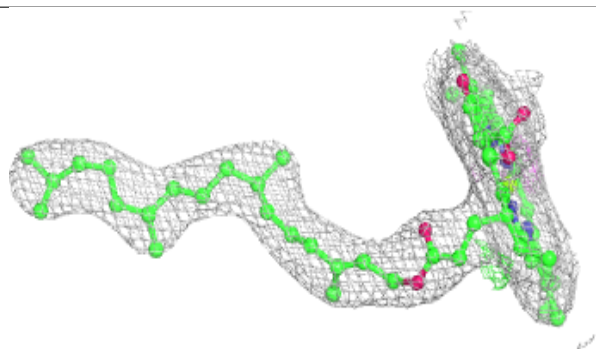
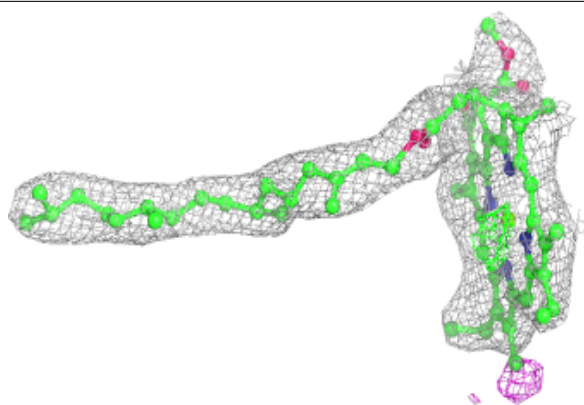
**Electron density around CLA Z 825:**

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

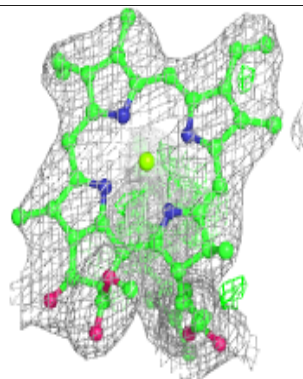
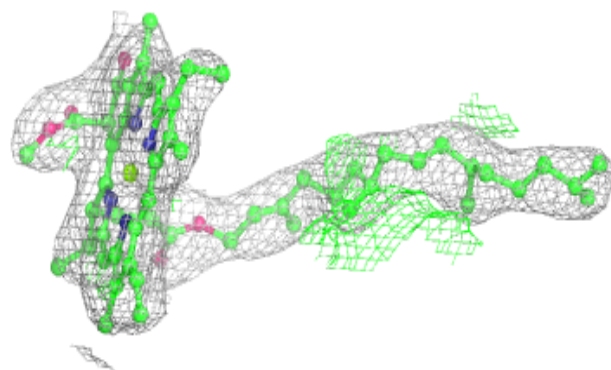
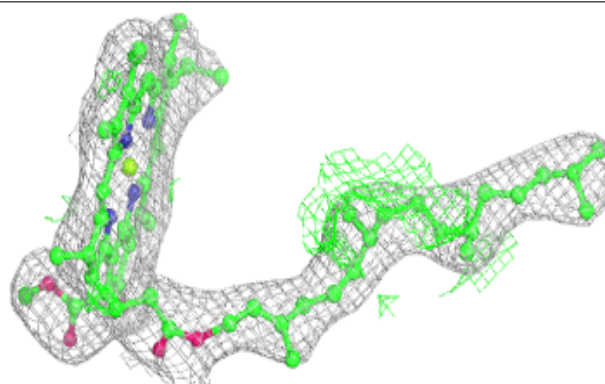


**Electron density around CLA Z 826:**

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

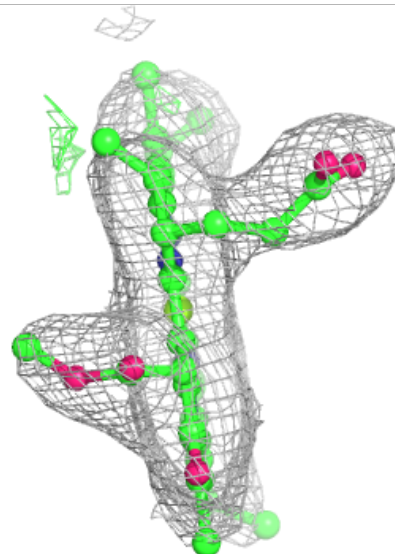
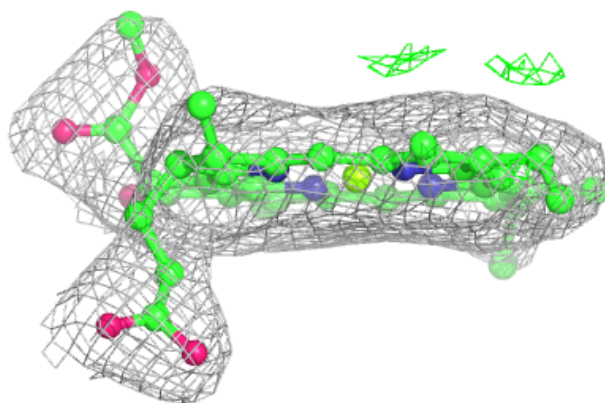
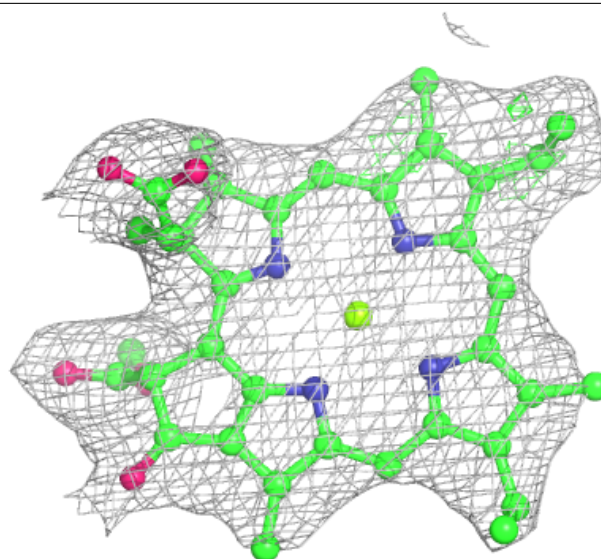
**Electron density around CLA Z 827:**

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



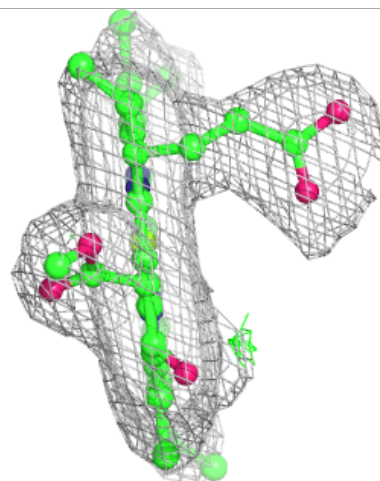
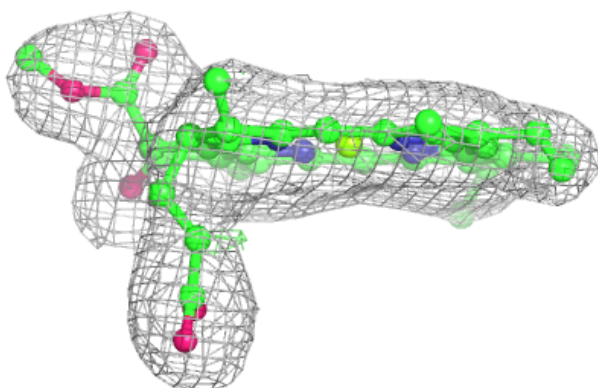
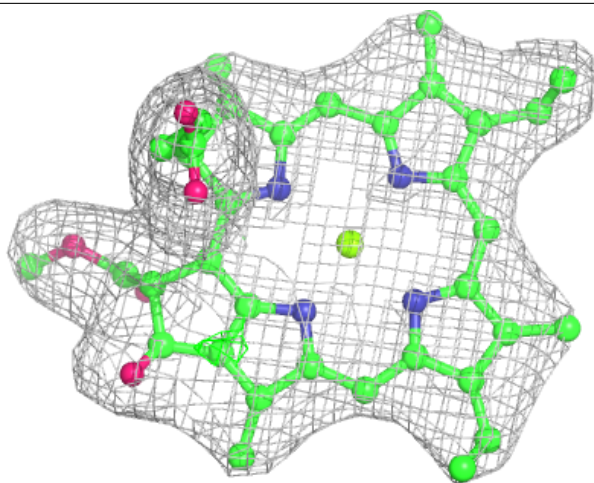
**Electron density around CLA Z 828:**

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



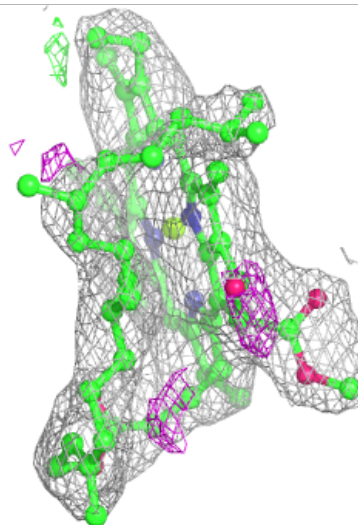
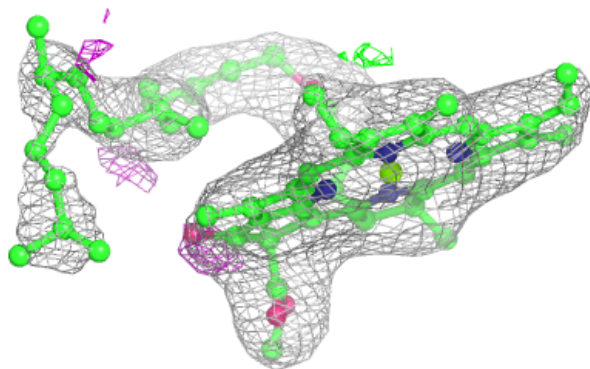
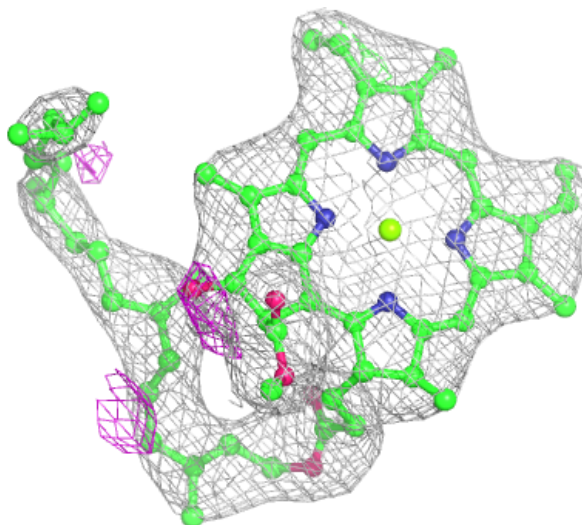
**Electron density around CLA Z 829:**

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



**Electron density around CLA Z 830:**

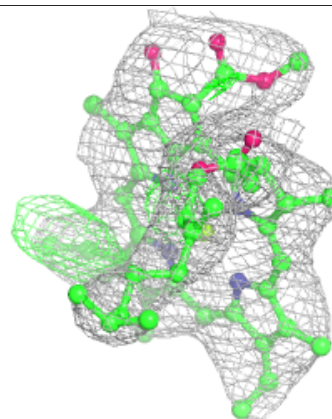
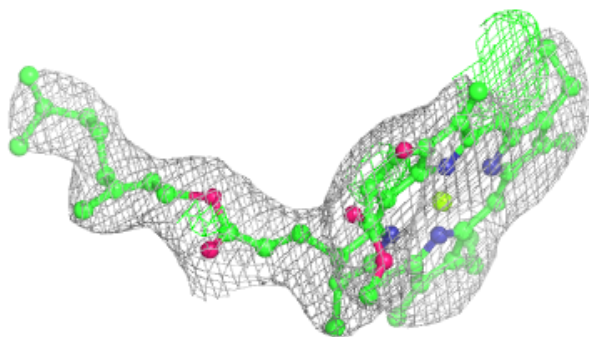
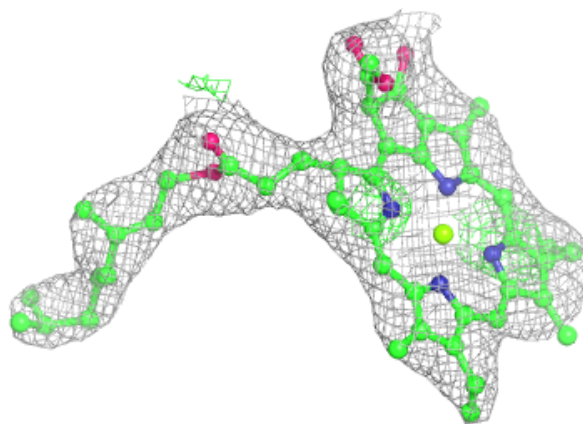
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





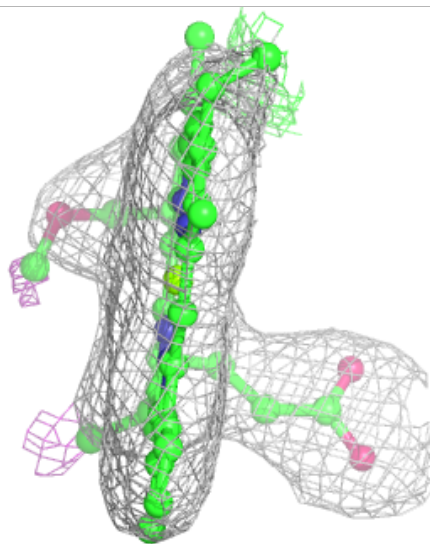
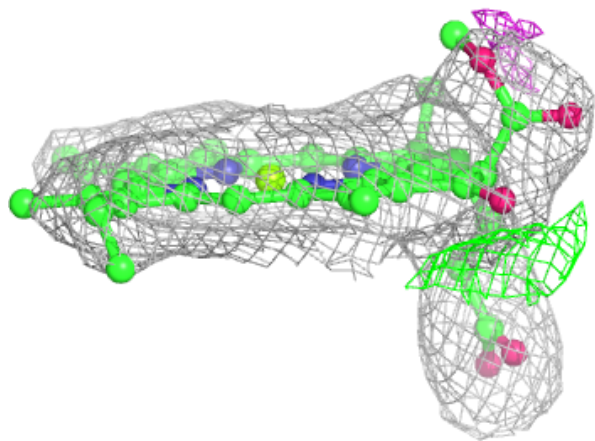
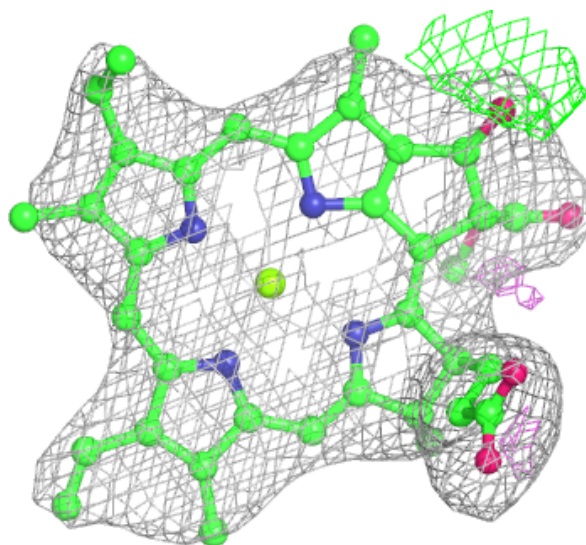
**Electron density around CLA Z 831:**

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



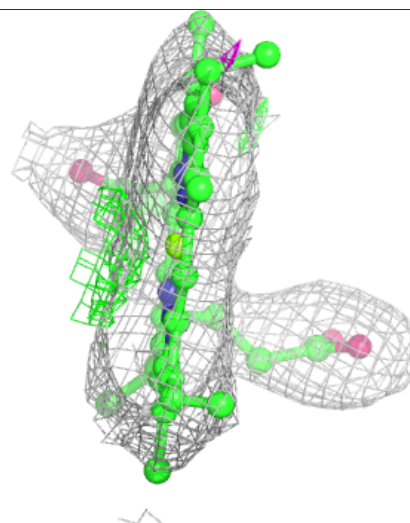
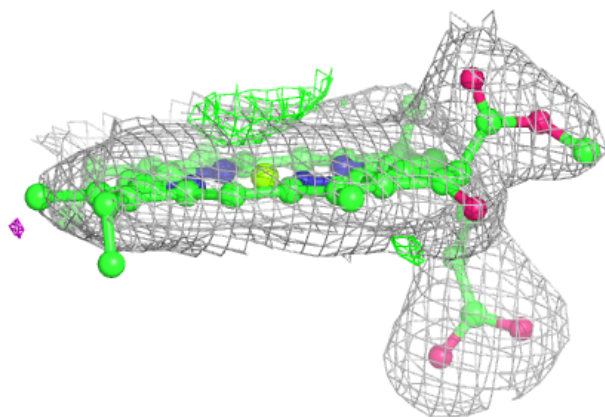
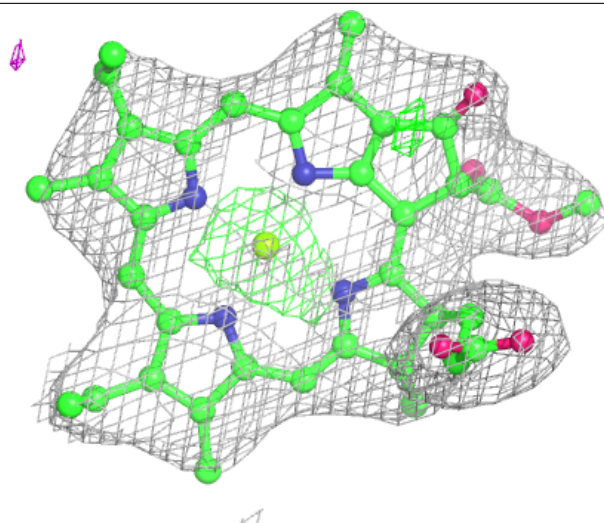
**Electron density around CLA Z 832:**

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



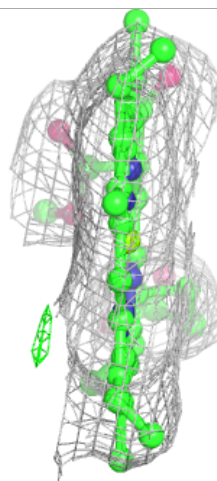
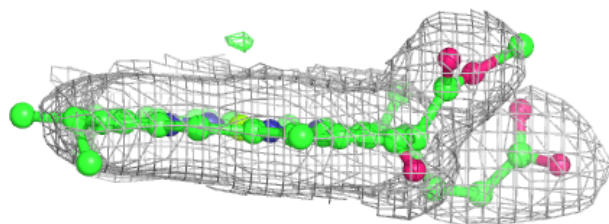
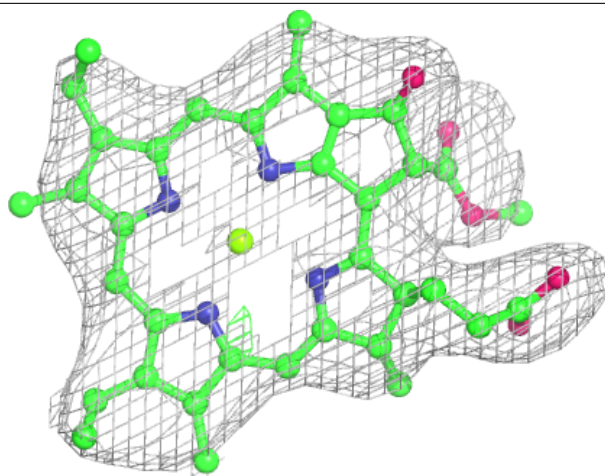
**Electron density around CLA Z 833:**

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



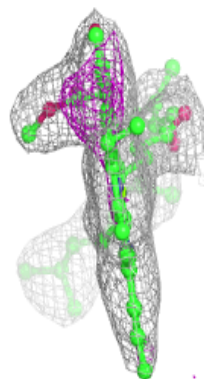
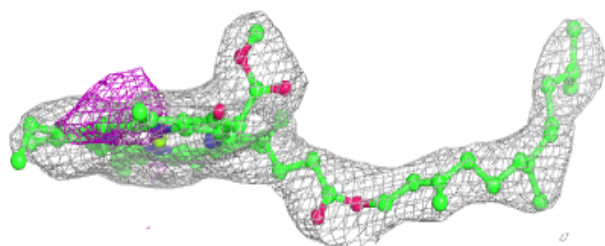
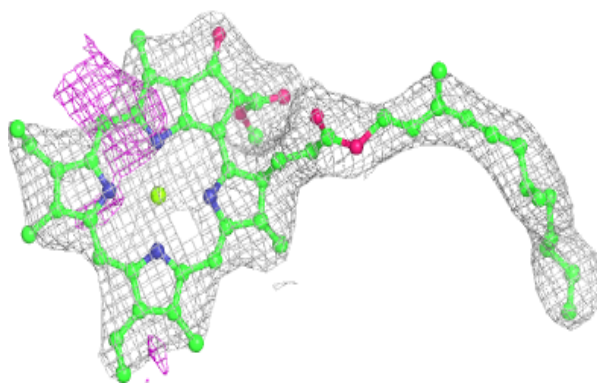
**Electron density around CLA Z 834:**

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

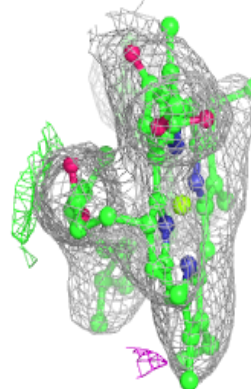
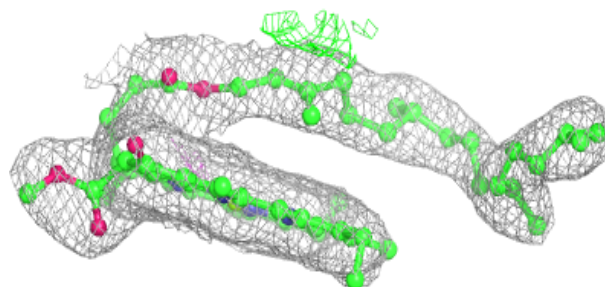
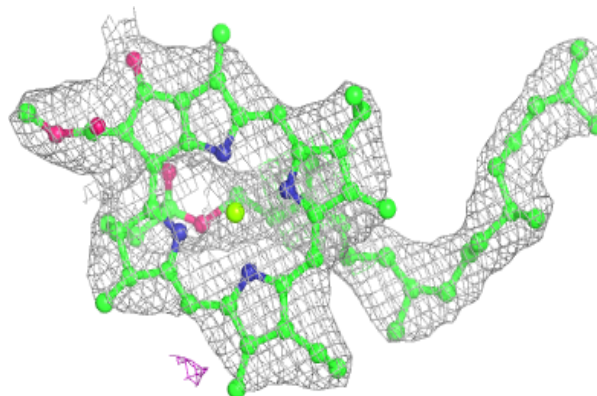


**Electron density around CLA Z 835:**

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

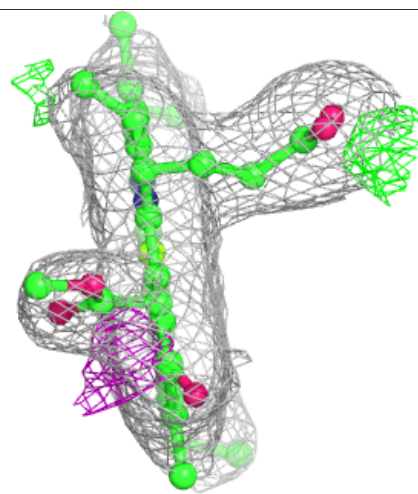
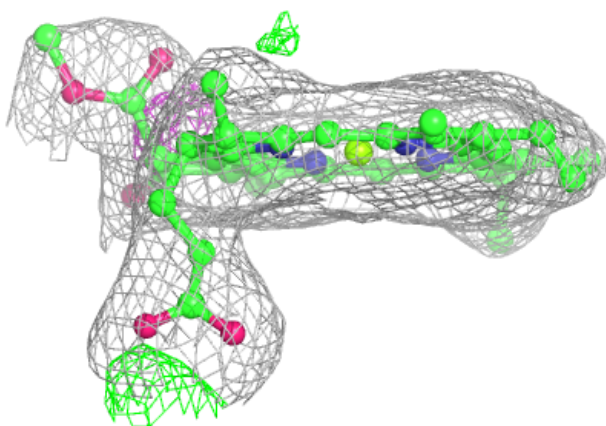
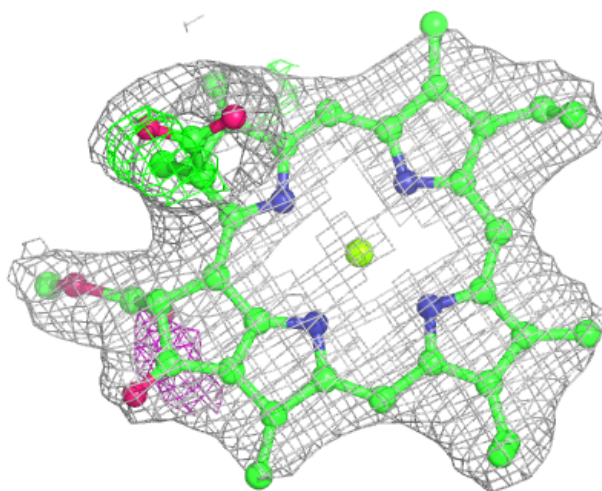
**Electron density around CLA Z 836:**

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



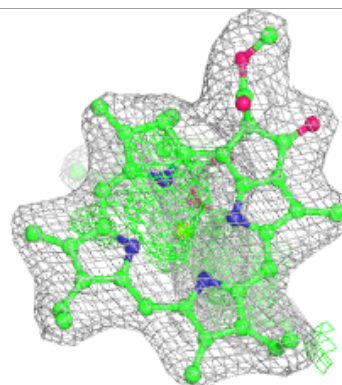
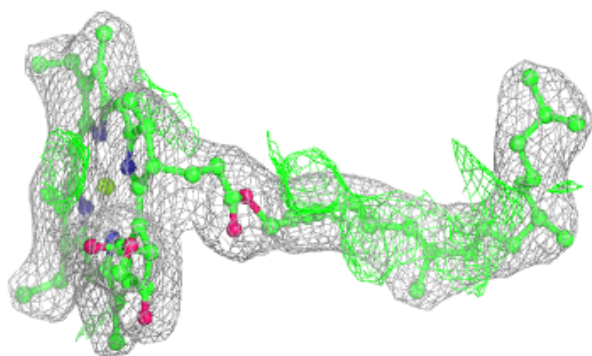
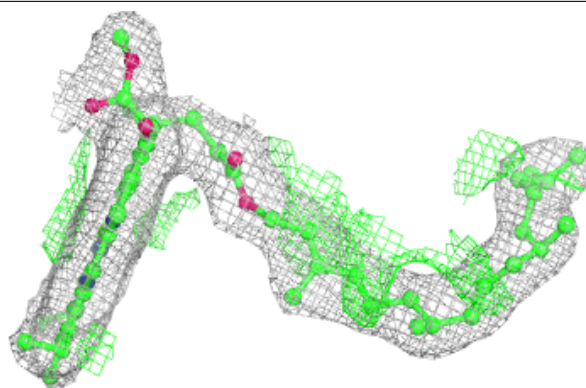
**Electron density around CLA Z 837:**

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

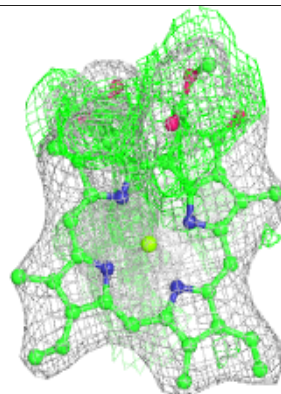
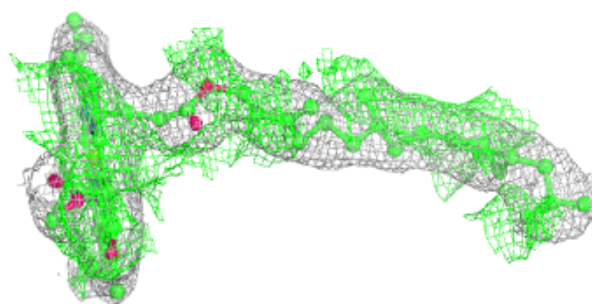
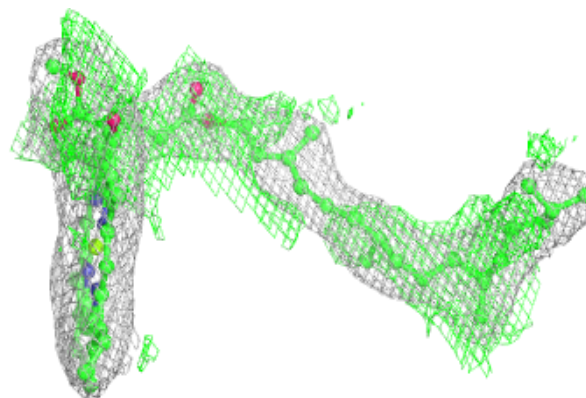


**Electron density around CLA Z 838:**

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

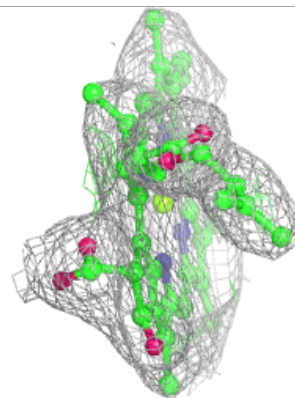
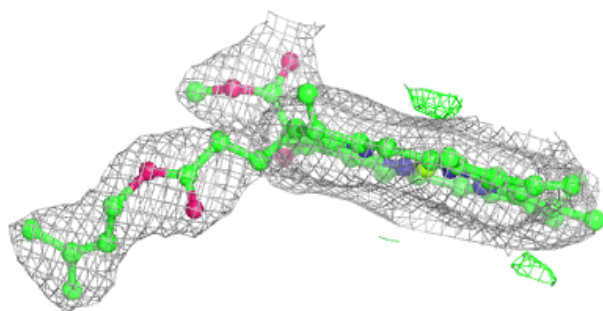
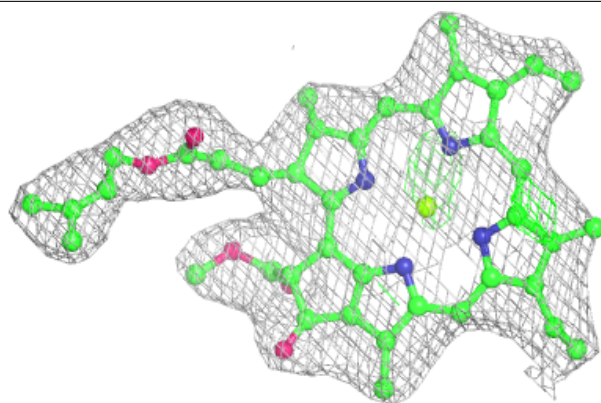
**Electron density around CLA Z 839:**

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



**Electron density around CLA d 201:**

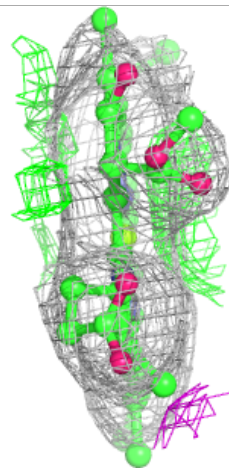
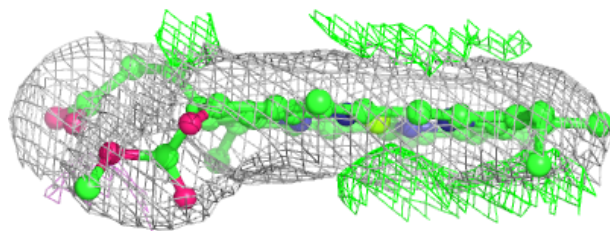
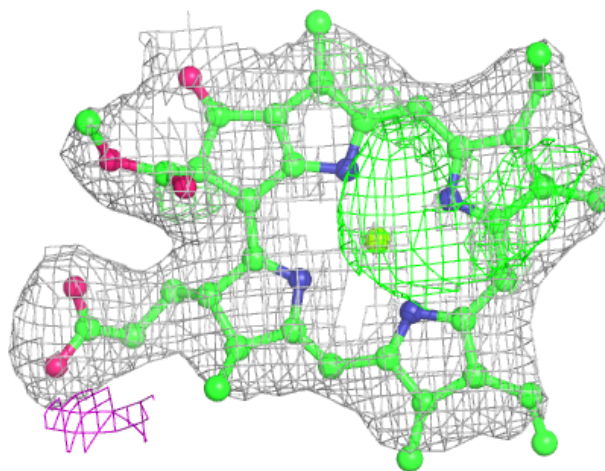
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





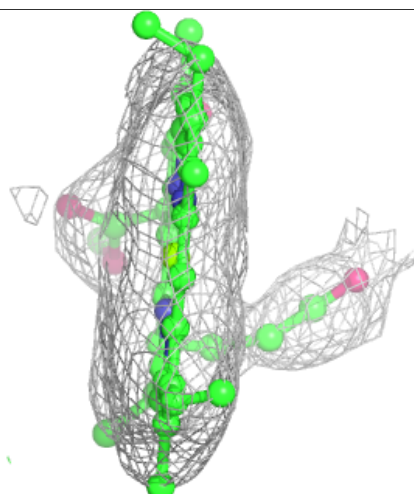
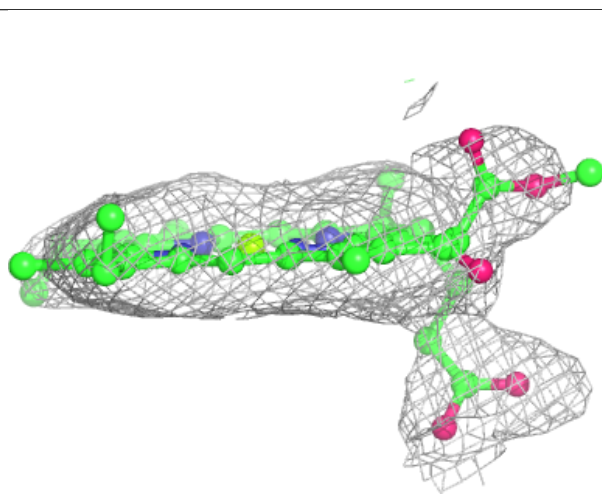
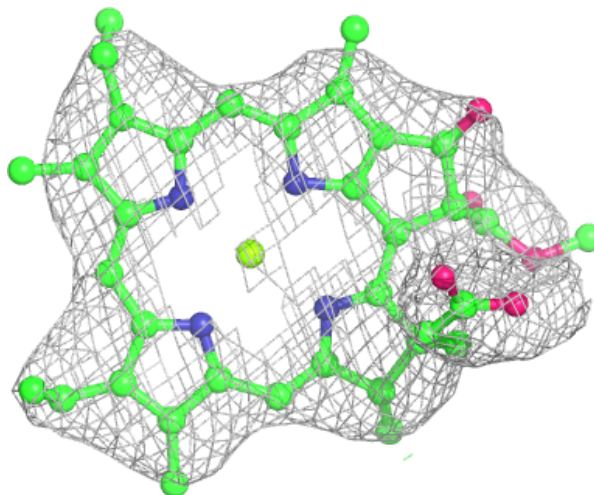
**Electron density around CLA d 202:**

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



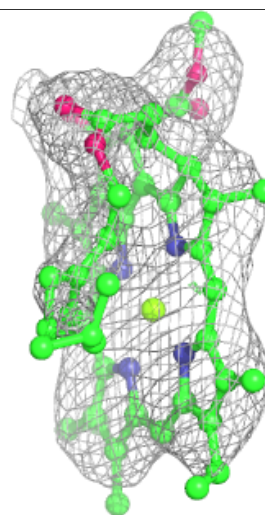
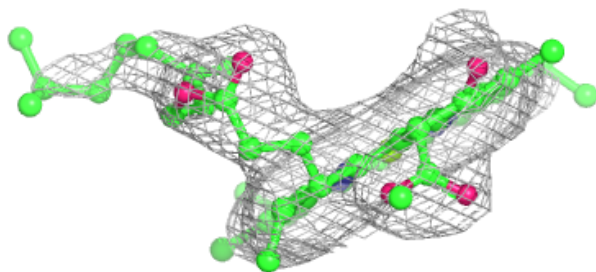
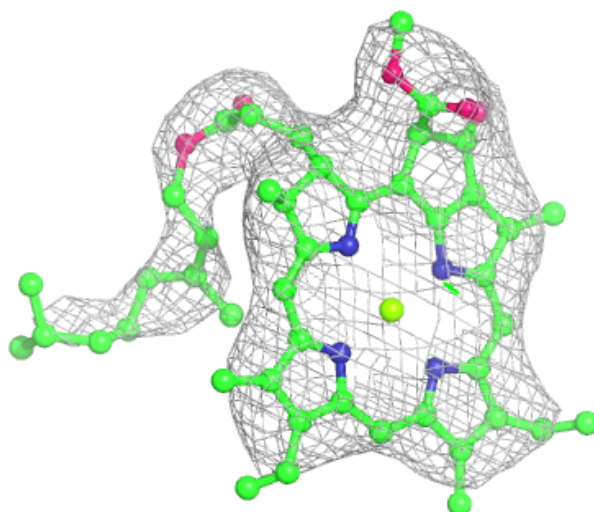
**Electron density around CLA f 101:**

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



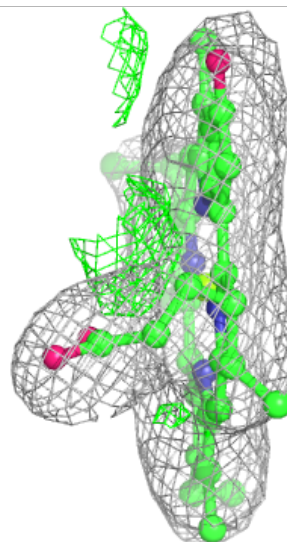
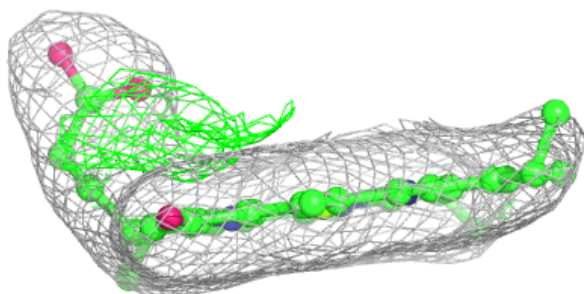
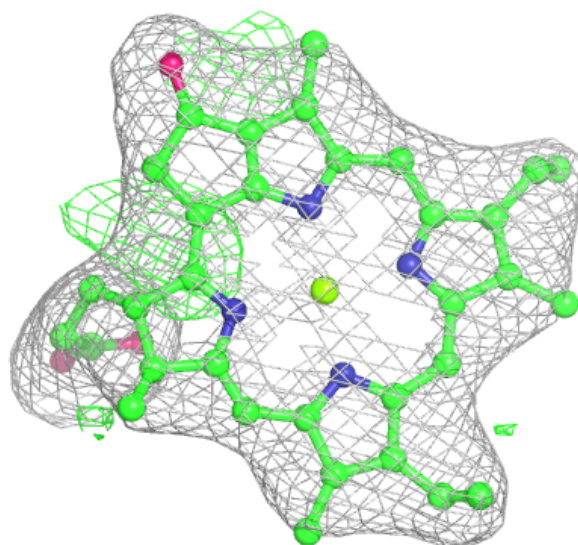
**Electron density around CLA f 102:**

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



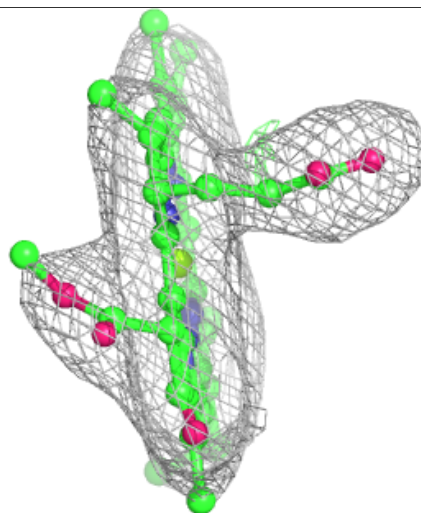
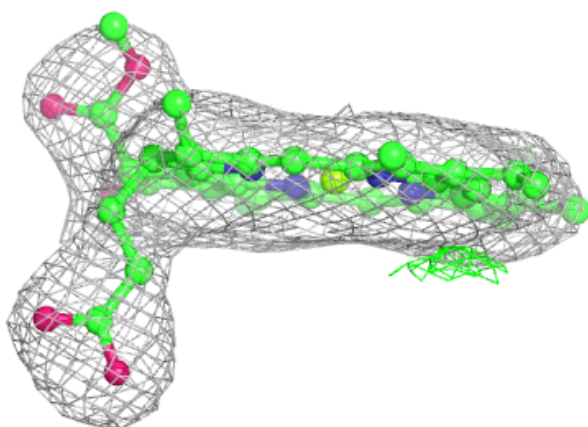
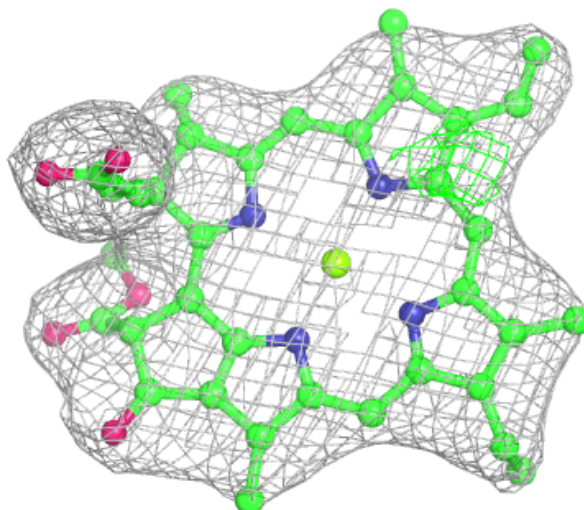
**Electron density around CLA g 101:**

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



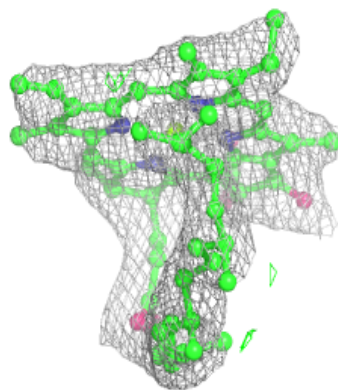
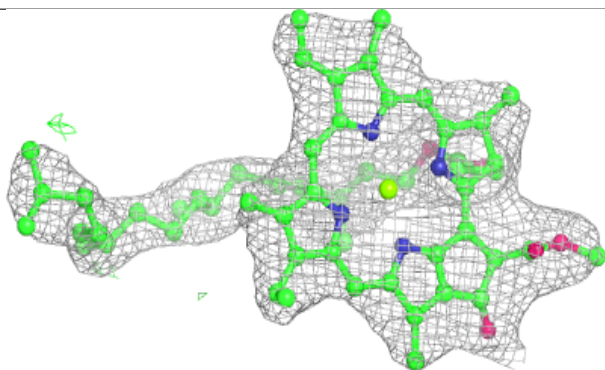
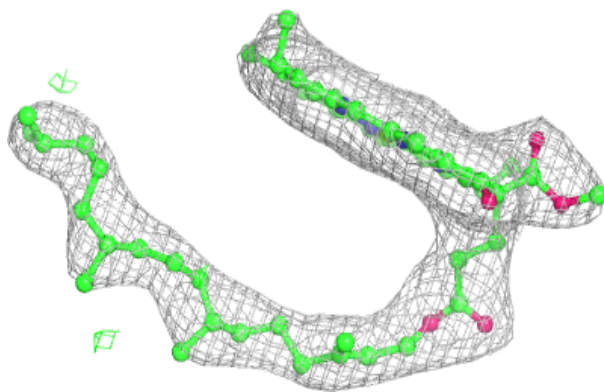
**Electron density around CLA g 102:**

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



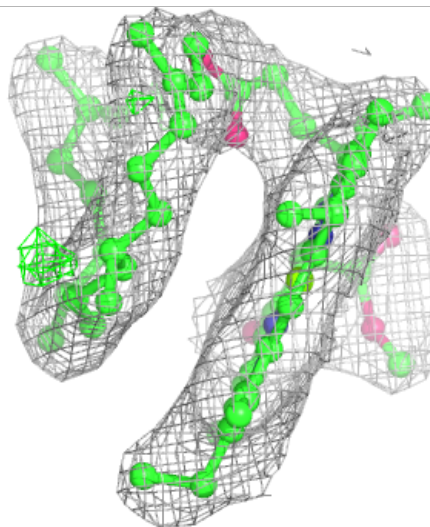
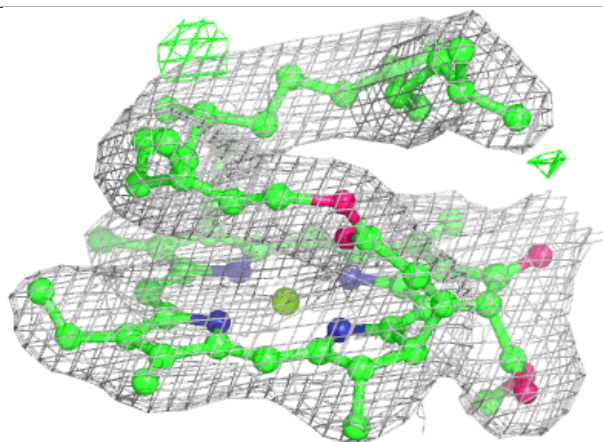
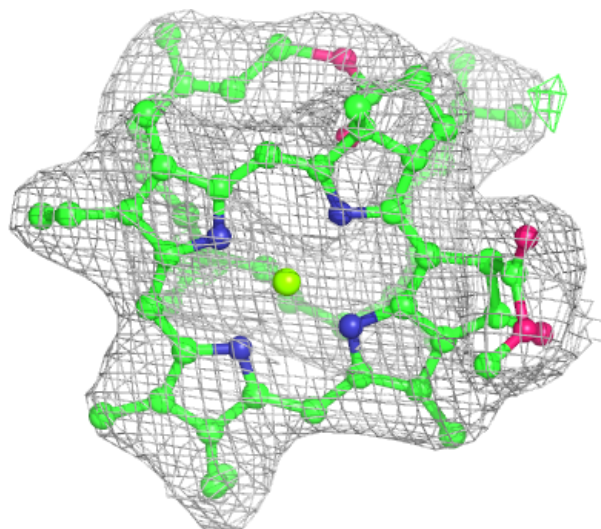
**Electron density around CLA h 201:**

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



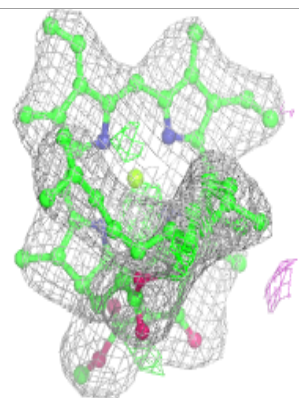
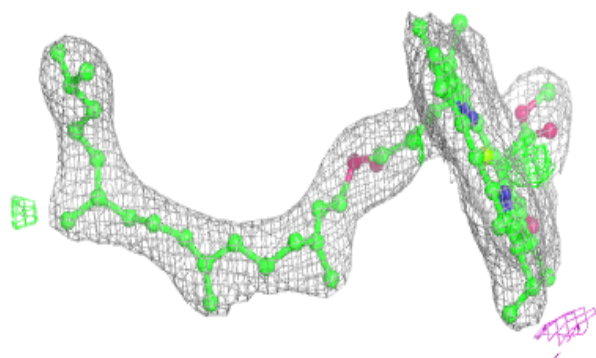
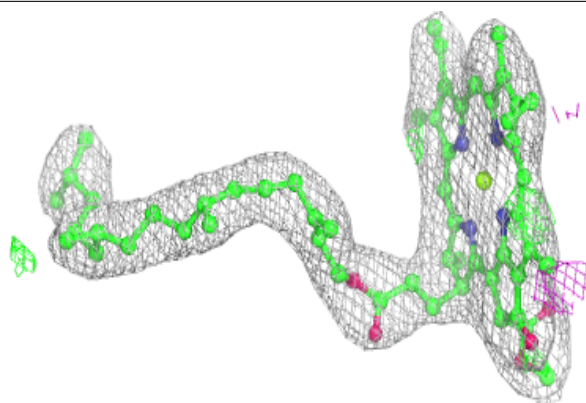
**Electron density around CLA h 205:**

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

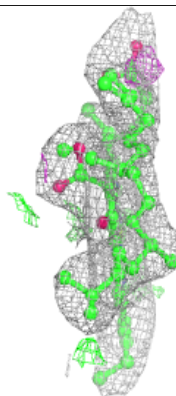
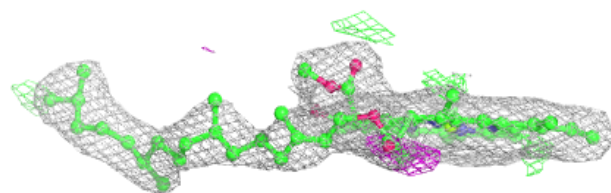
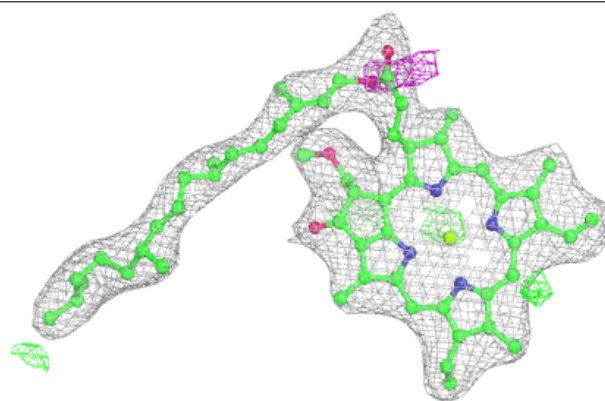


**Electron density around CLA h 206:**

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

**Electron density around CLA h 207:**

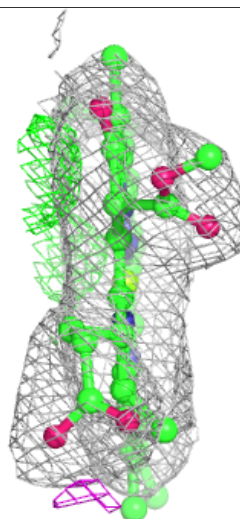
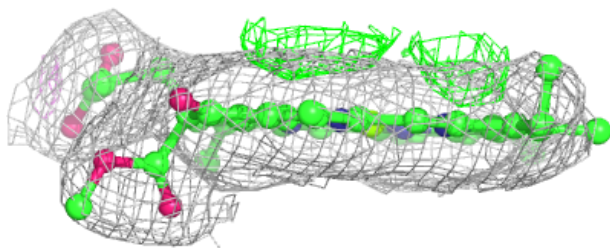
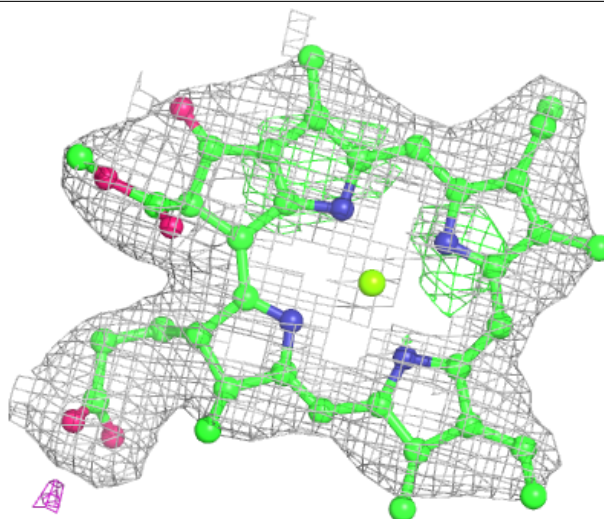
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





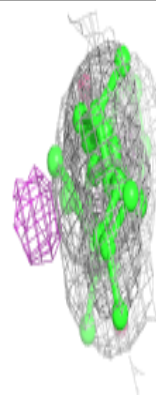
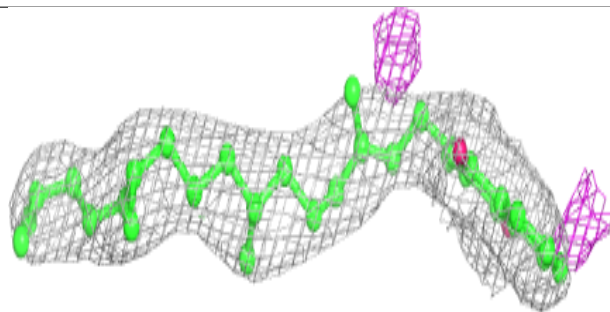
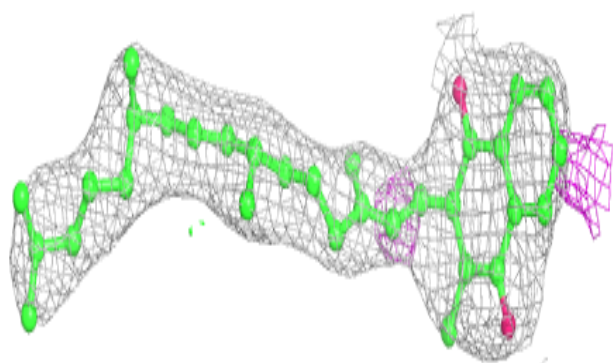
**Electron density around CLA j 102:**

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

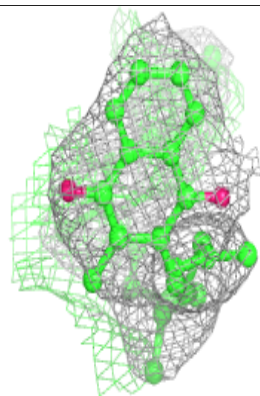
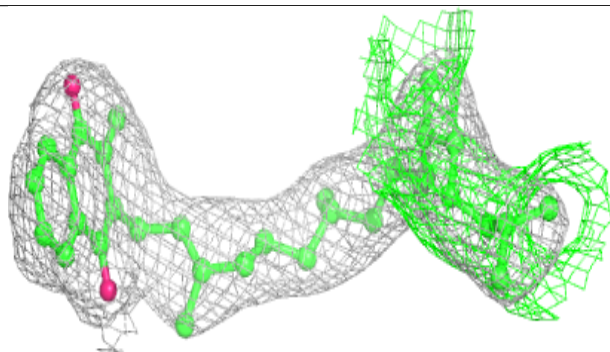
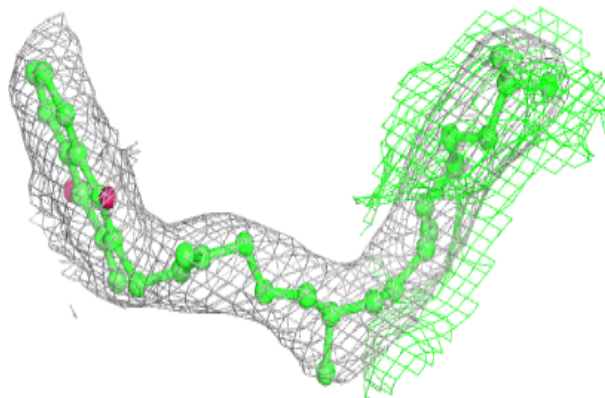


**Electron density around PQN A 843:**

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

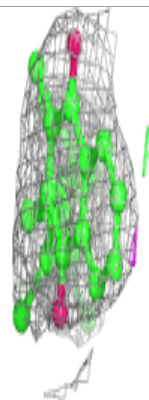
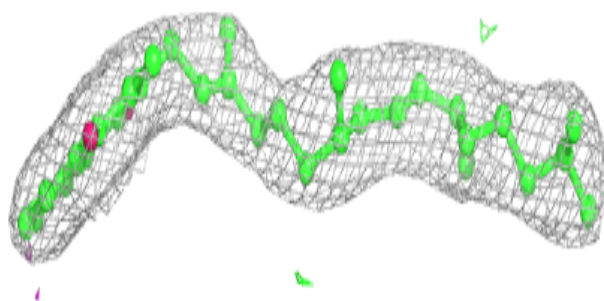
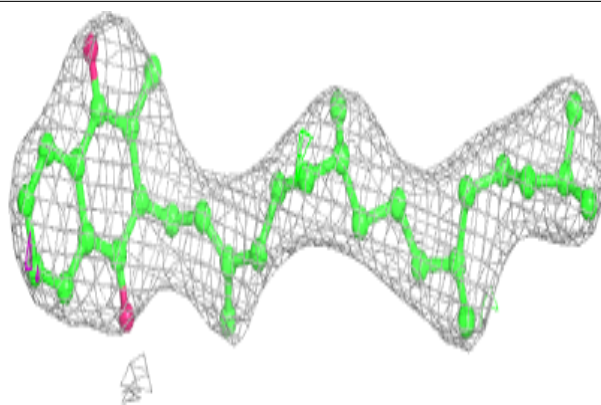
**Electron density around PQN B 842:**

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

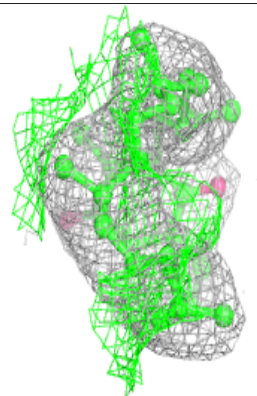
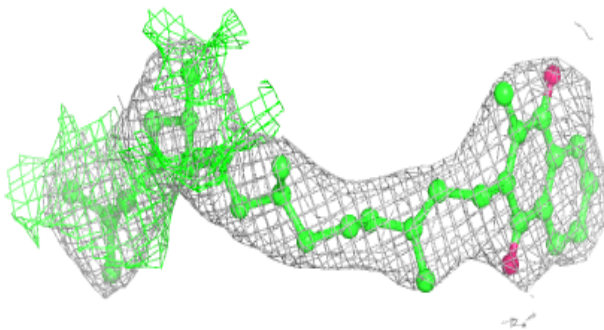
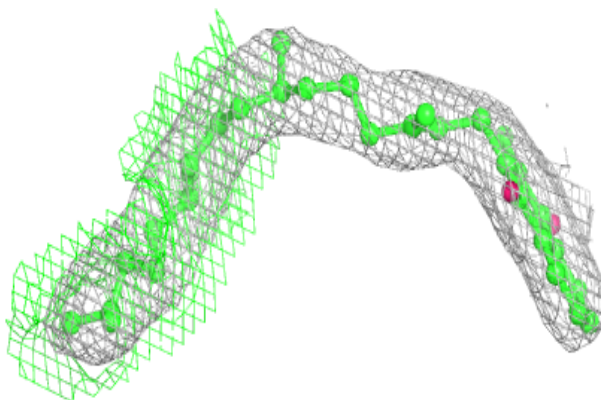


**Electron density around PQN G 844:**

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

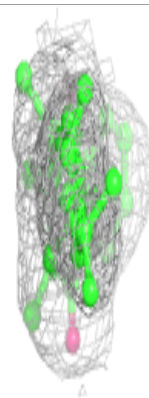
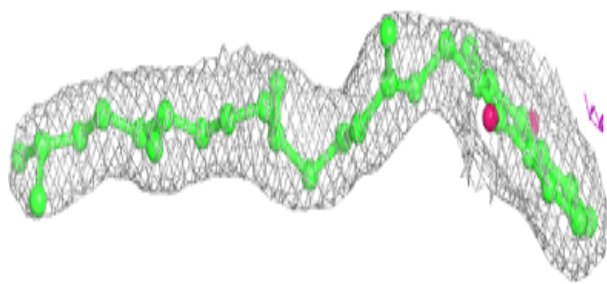
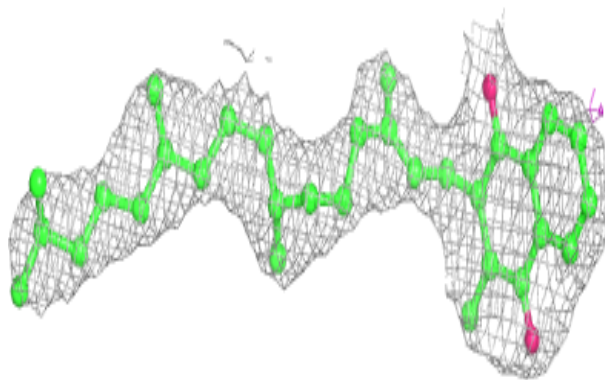
**Electron density around PQN H 839:**

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

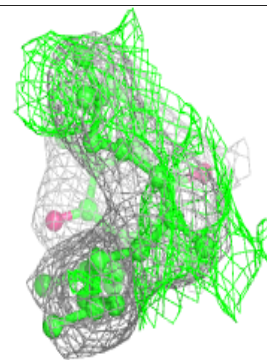
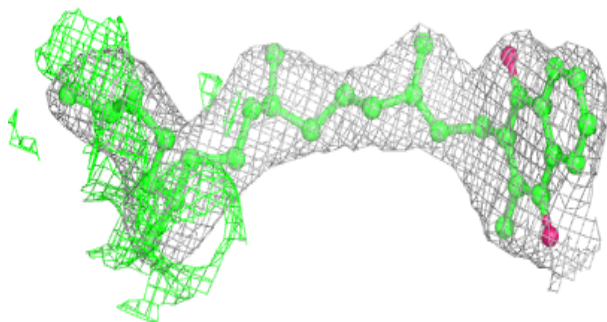
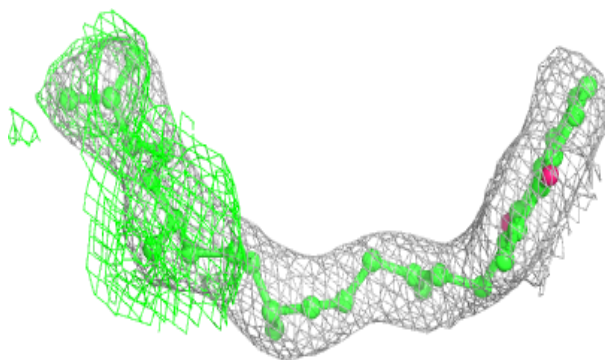


**Electron density around PQN Y 844:**

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

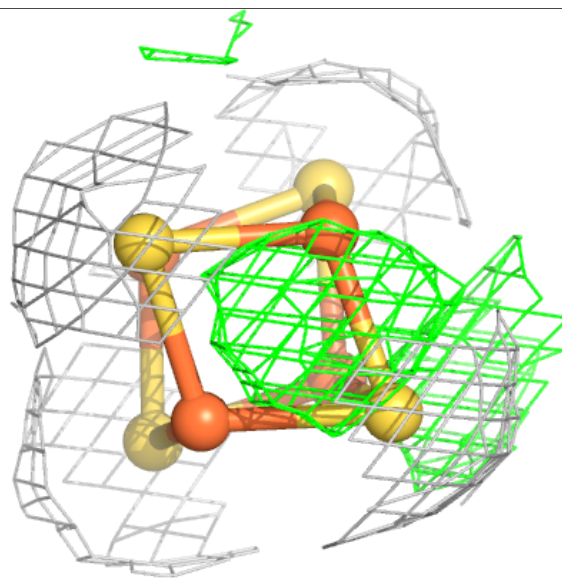
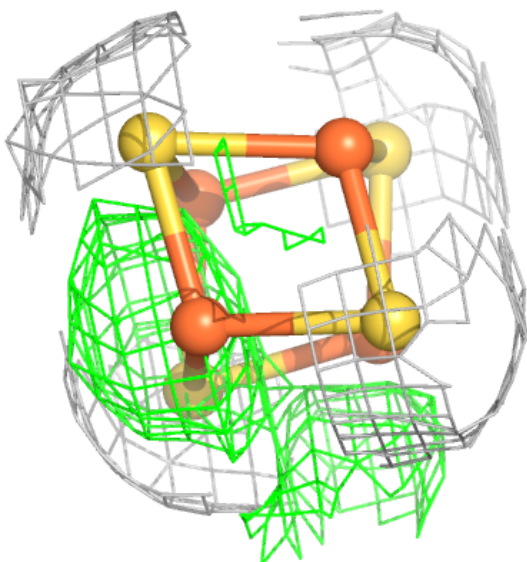
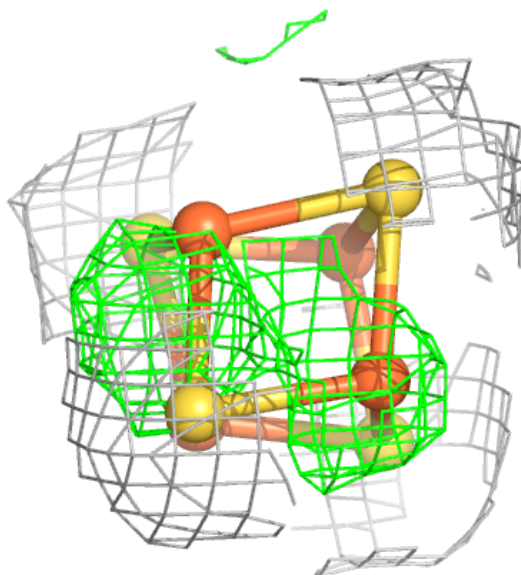
**Electron density around PQN Z 840:**

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



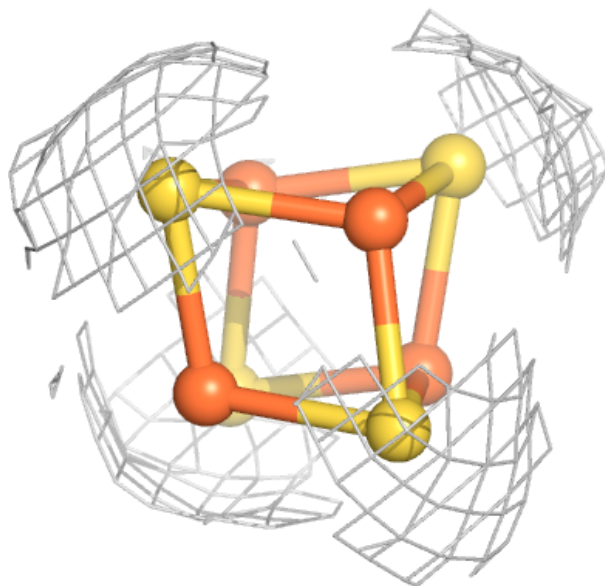
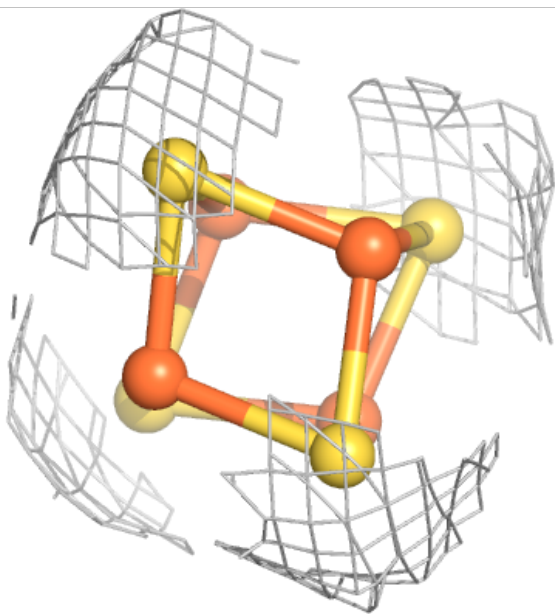
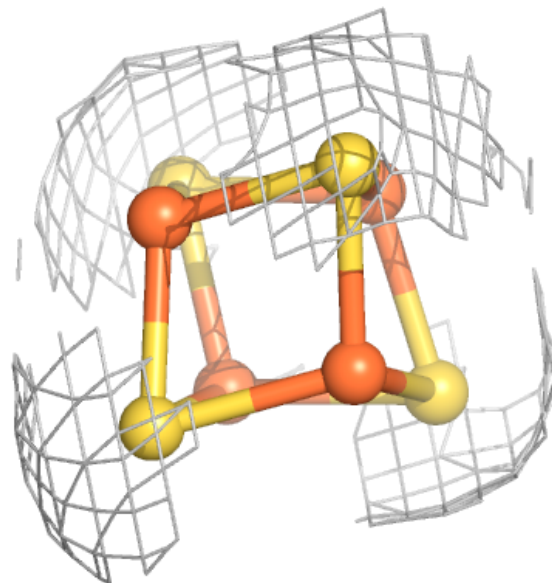
**Electron density around SF4 A 844:**

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



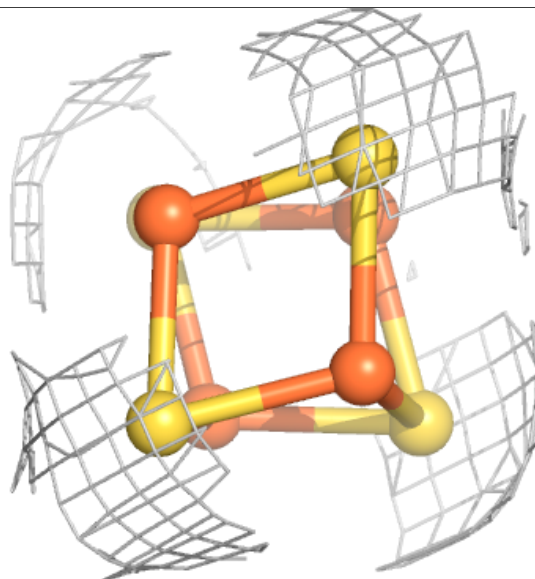
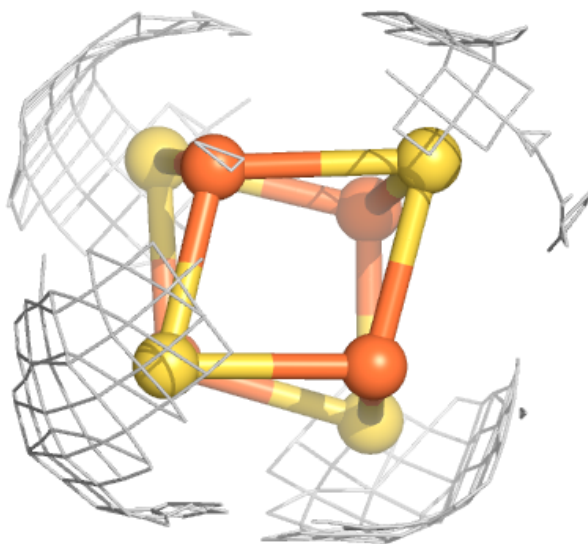
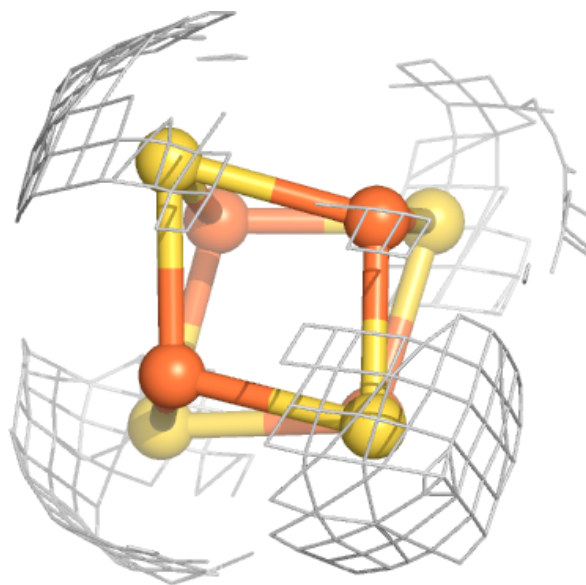
**Electron density around SF4 C 101:**

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



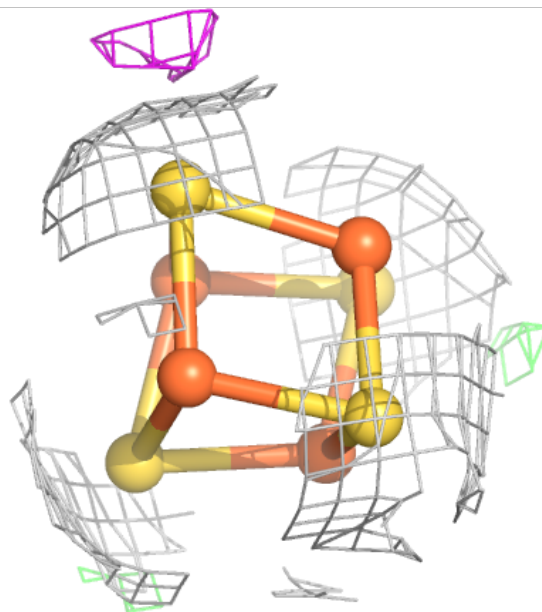
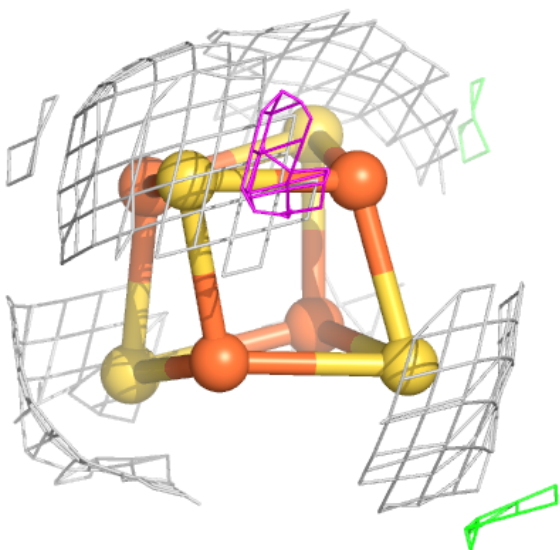
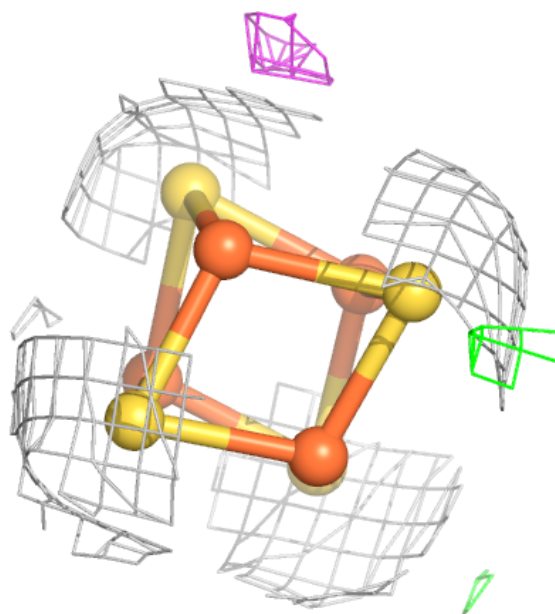
**Electron density around SF4 C 102:**

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



**Electron density around SF4 G 845:**

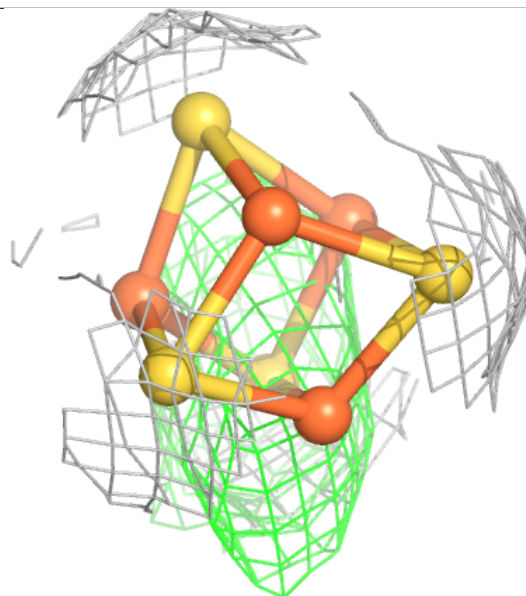
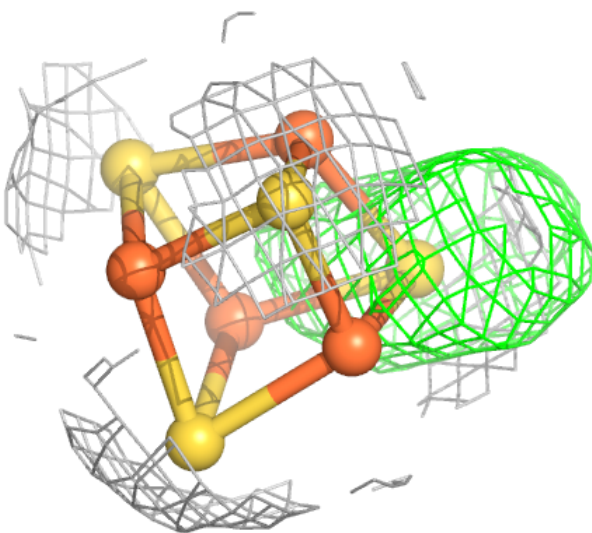
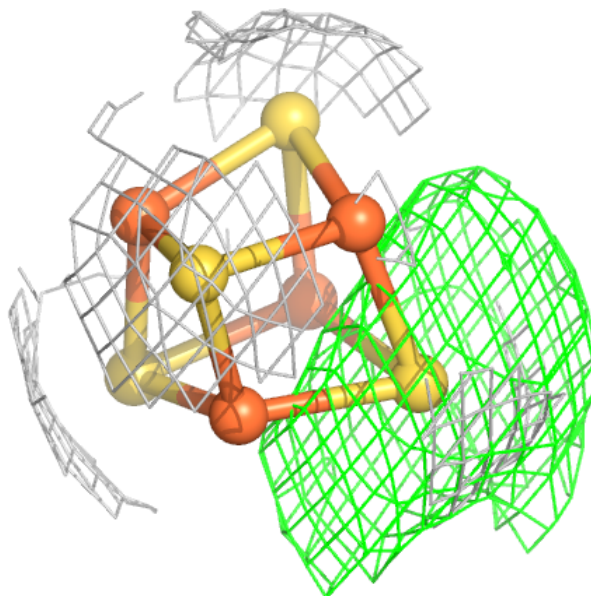
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





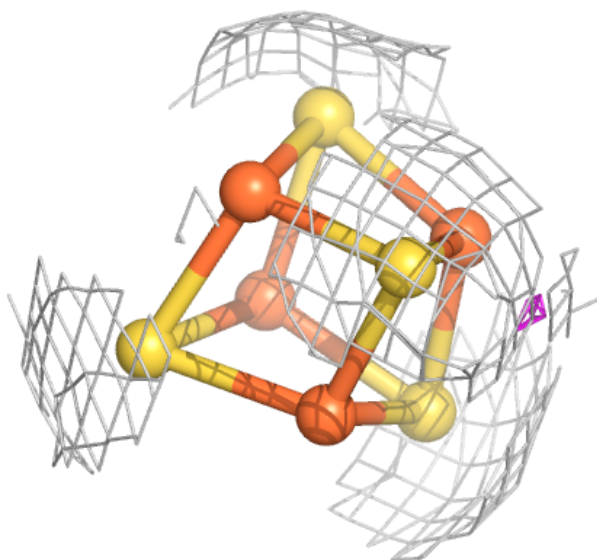
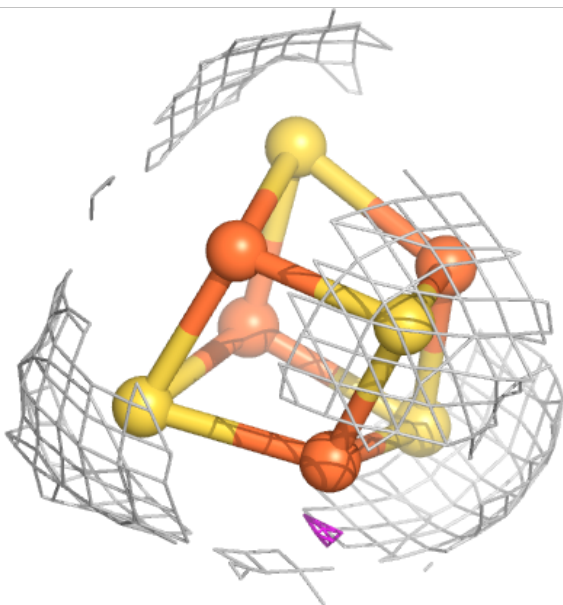
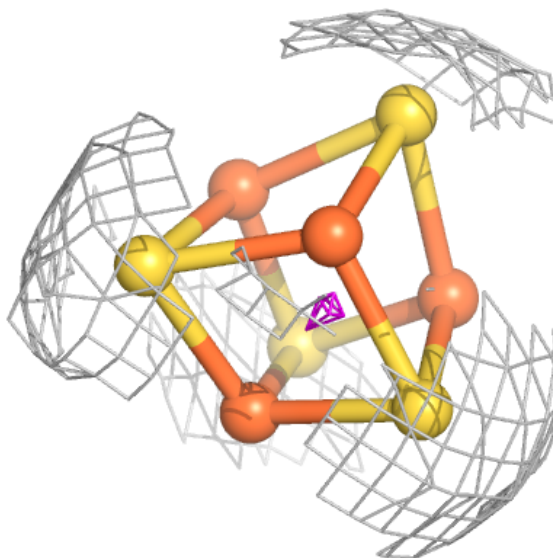
**Electron density around SF4 N 101:**

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



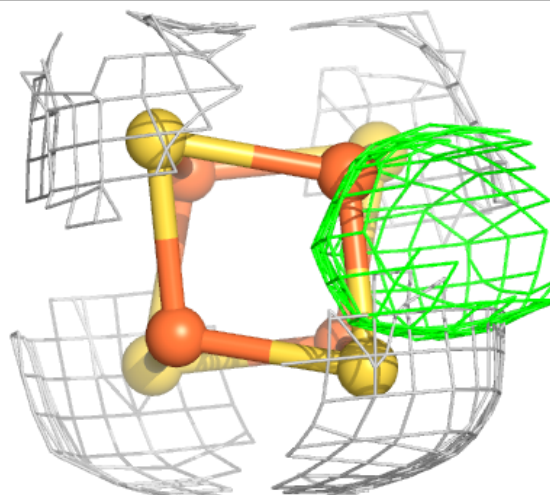
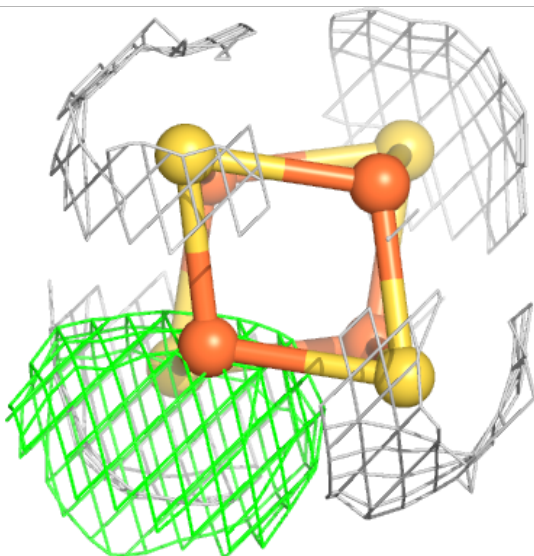
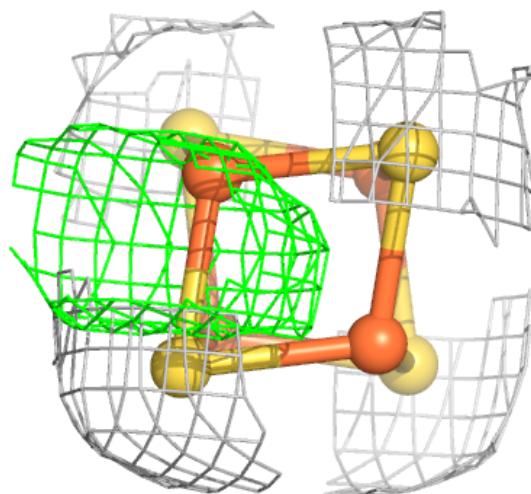
**Electron density around SF4 N 102:**

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



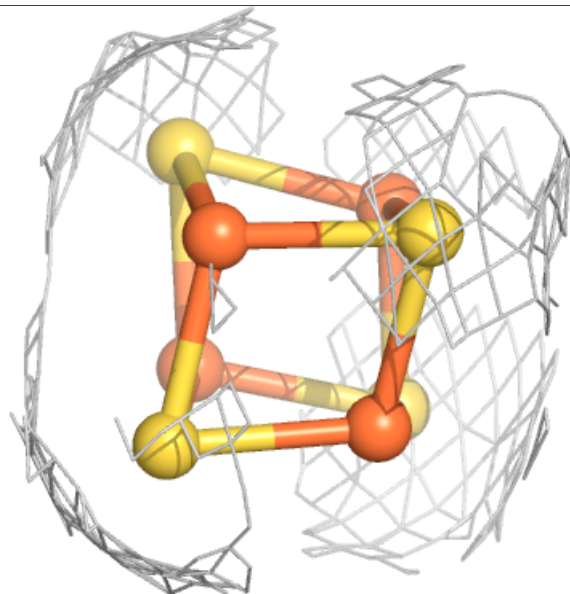
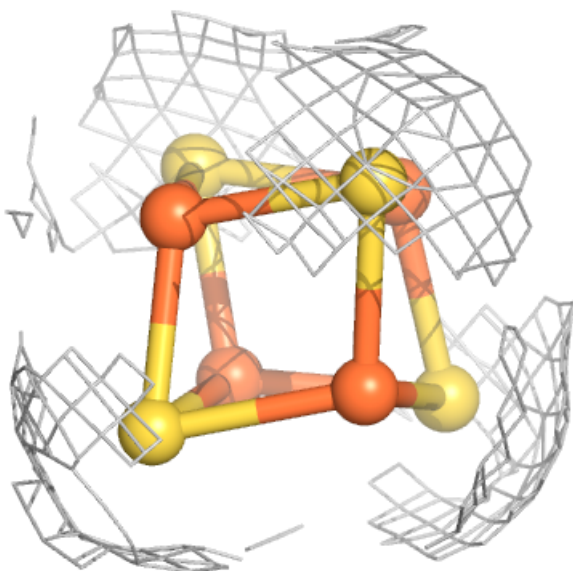
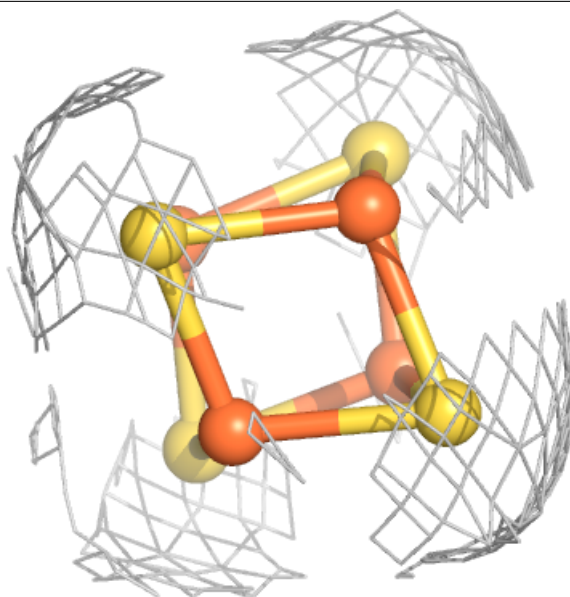
**Electron density around SF4 Y 845:**

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



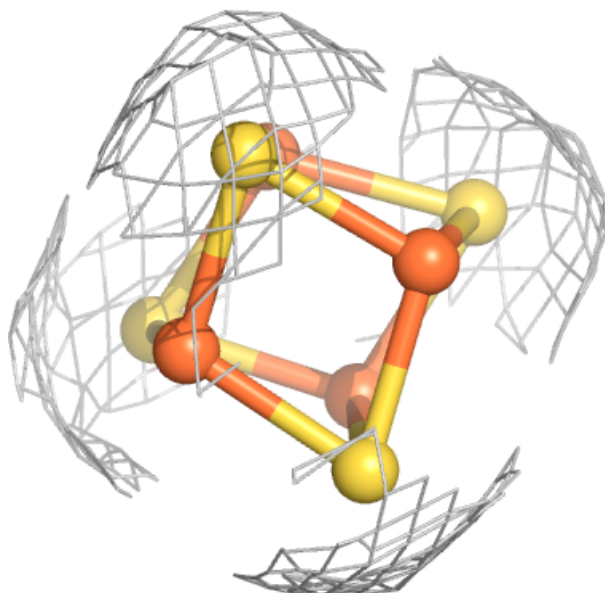
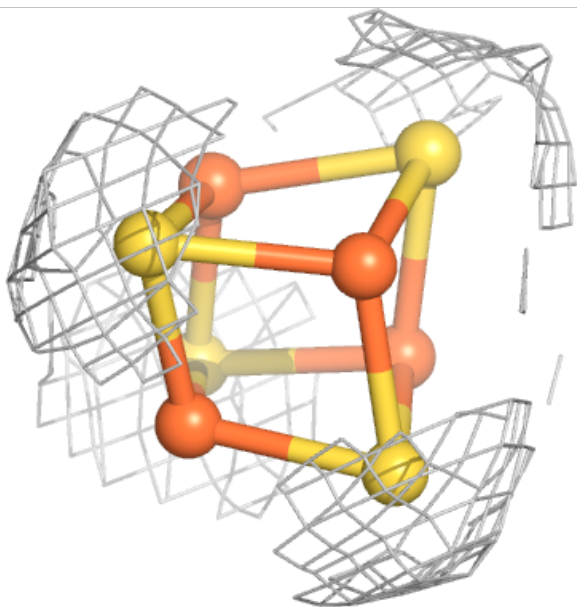
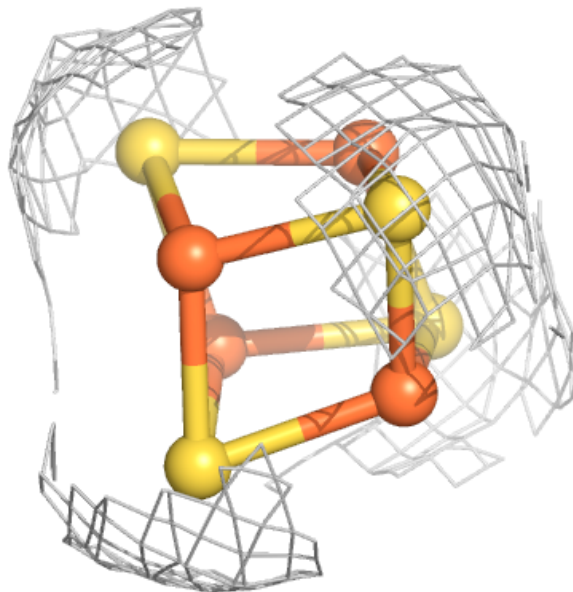
**Electron density around SF4 a 101:**

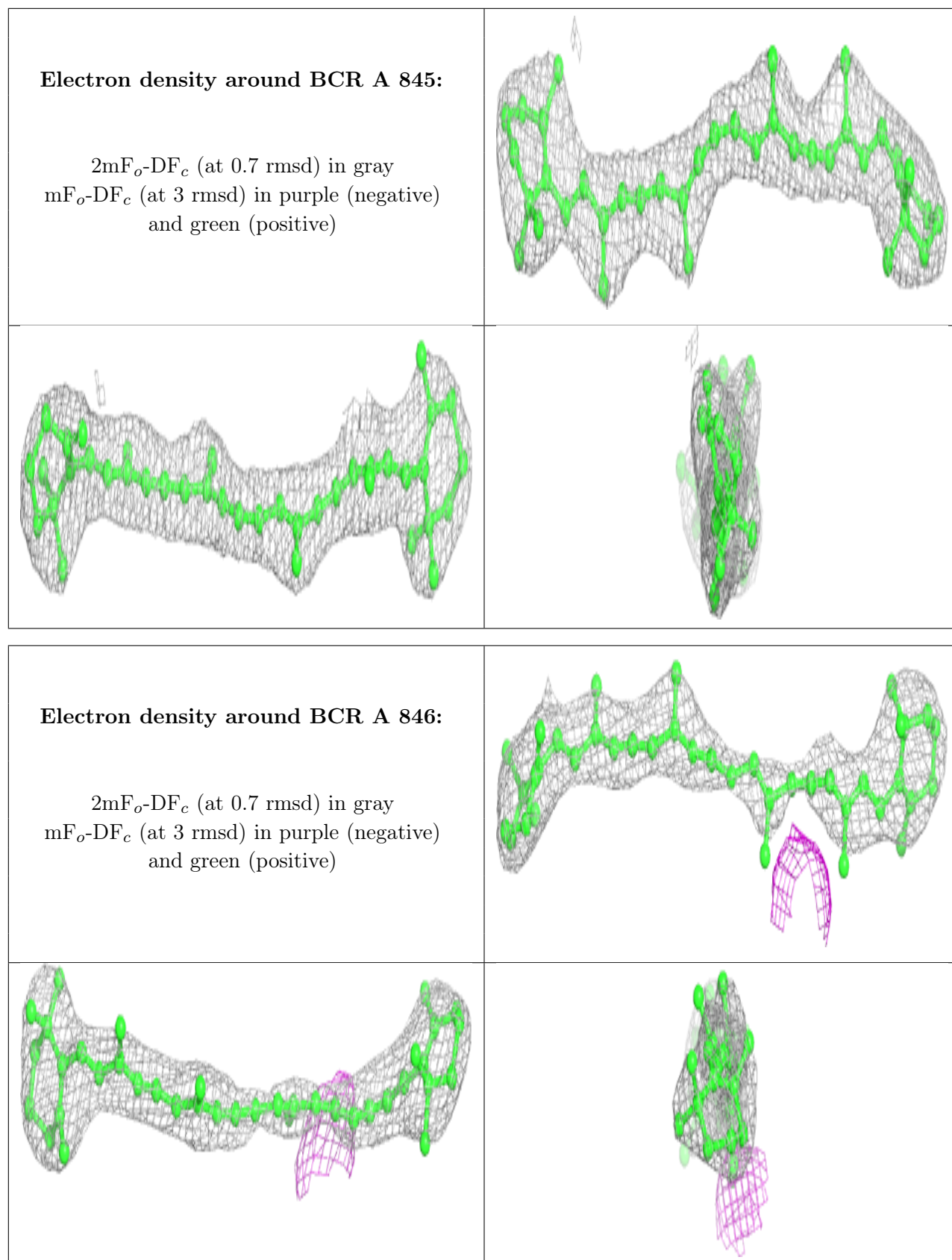
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

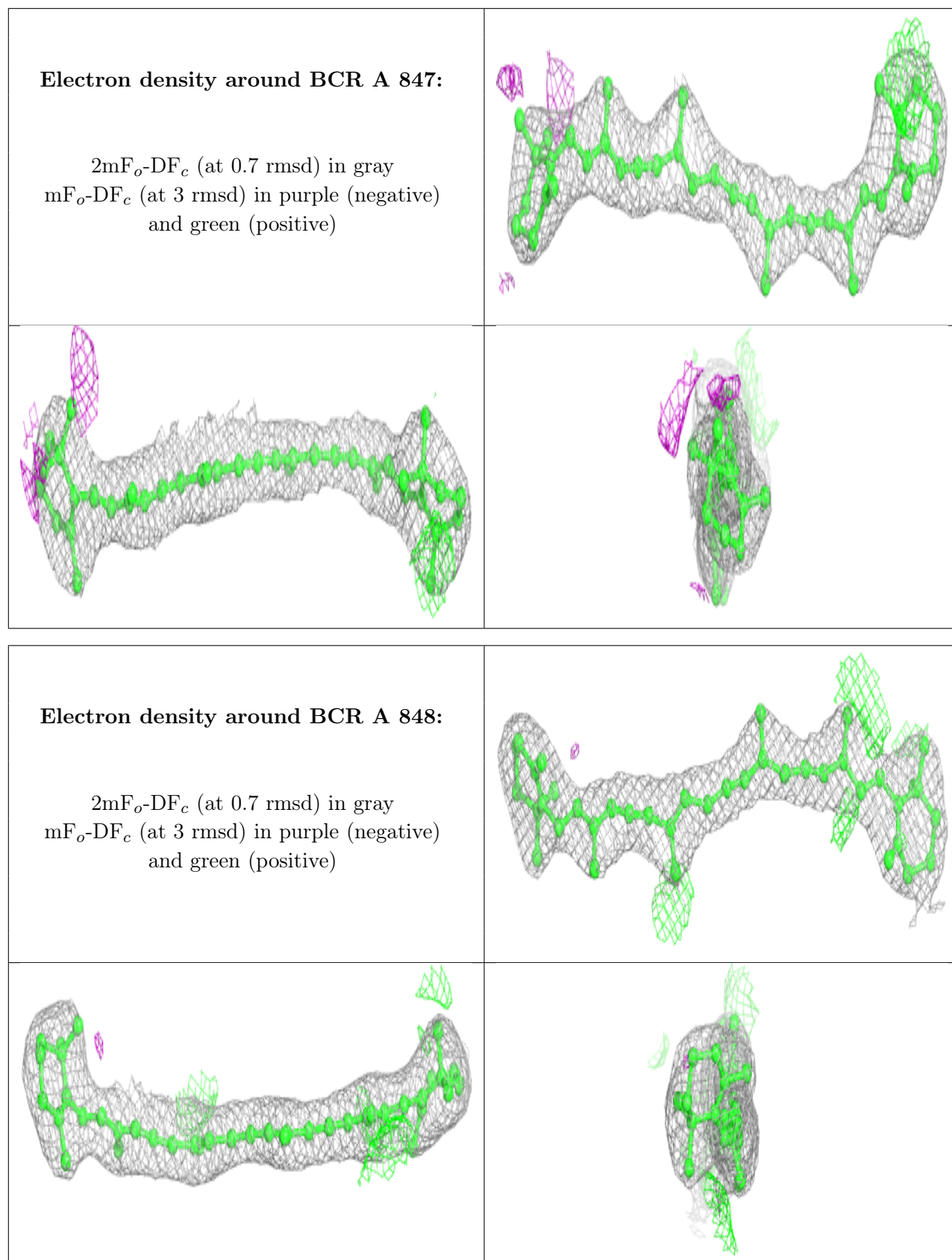


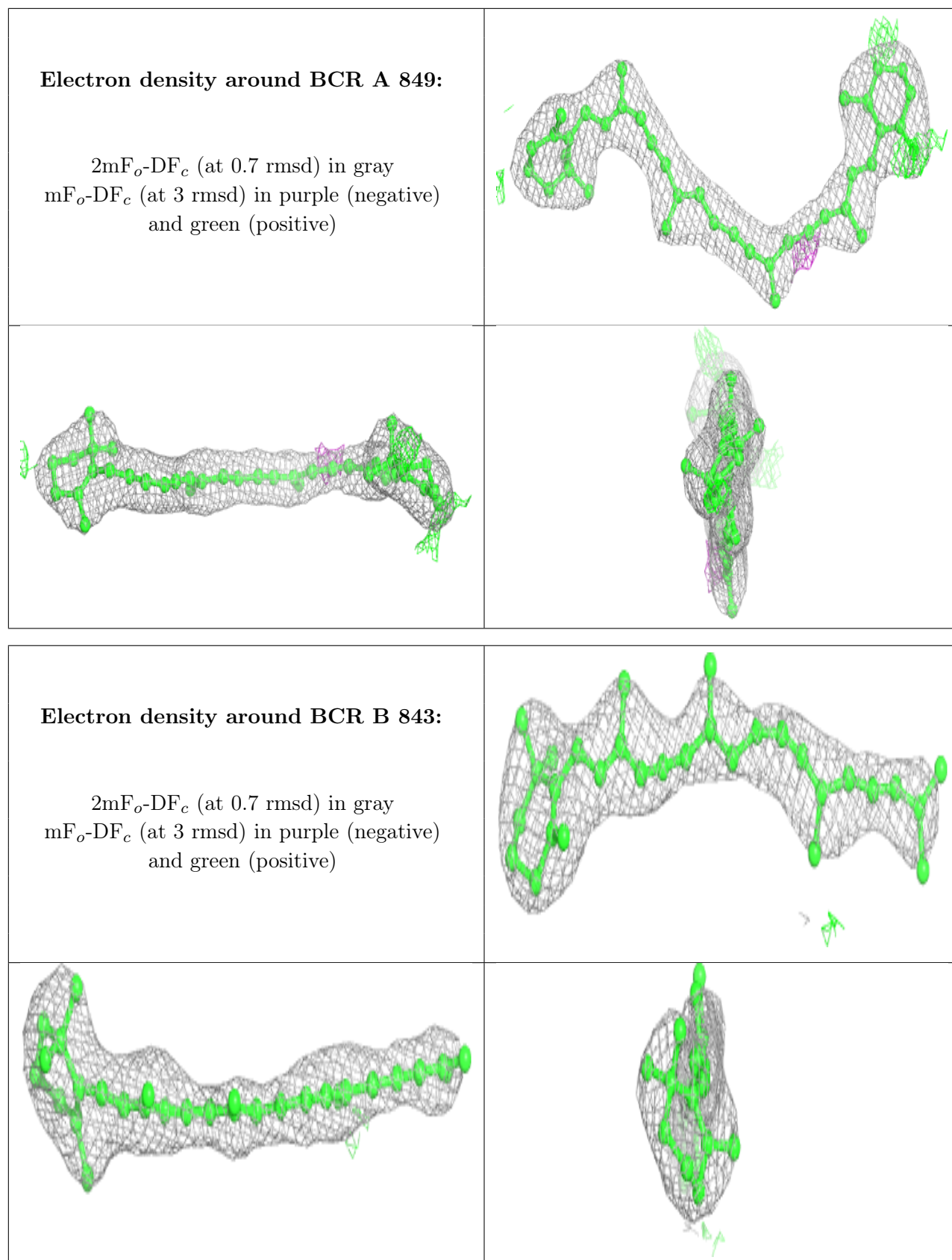
**Electron density around SF4 a 102:**

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

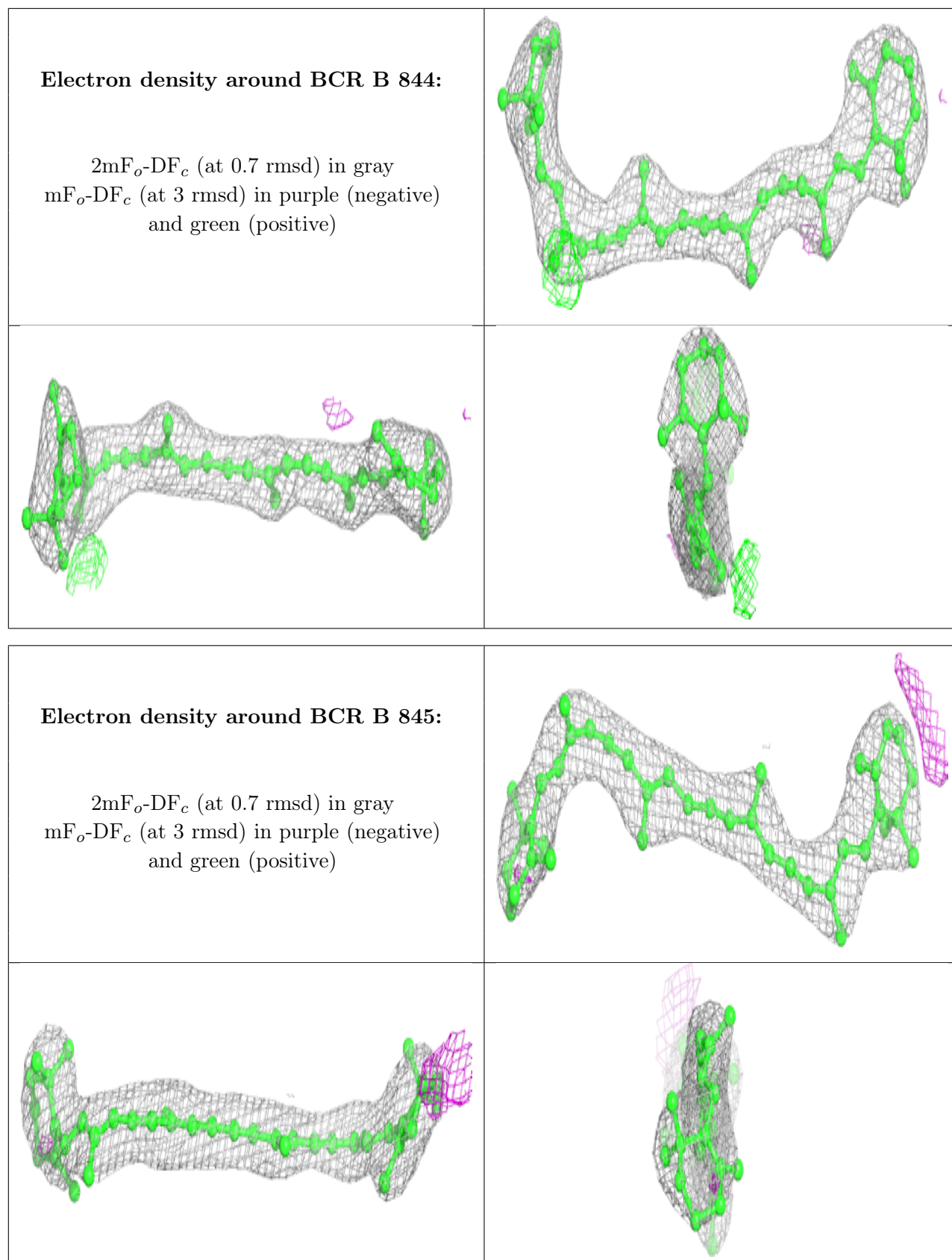


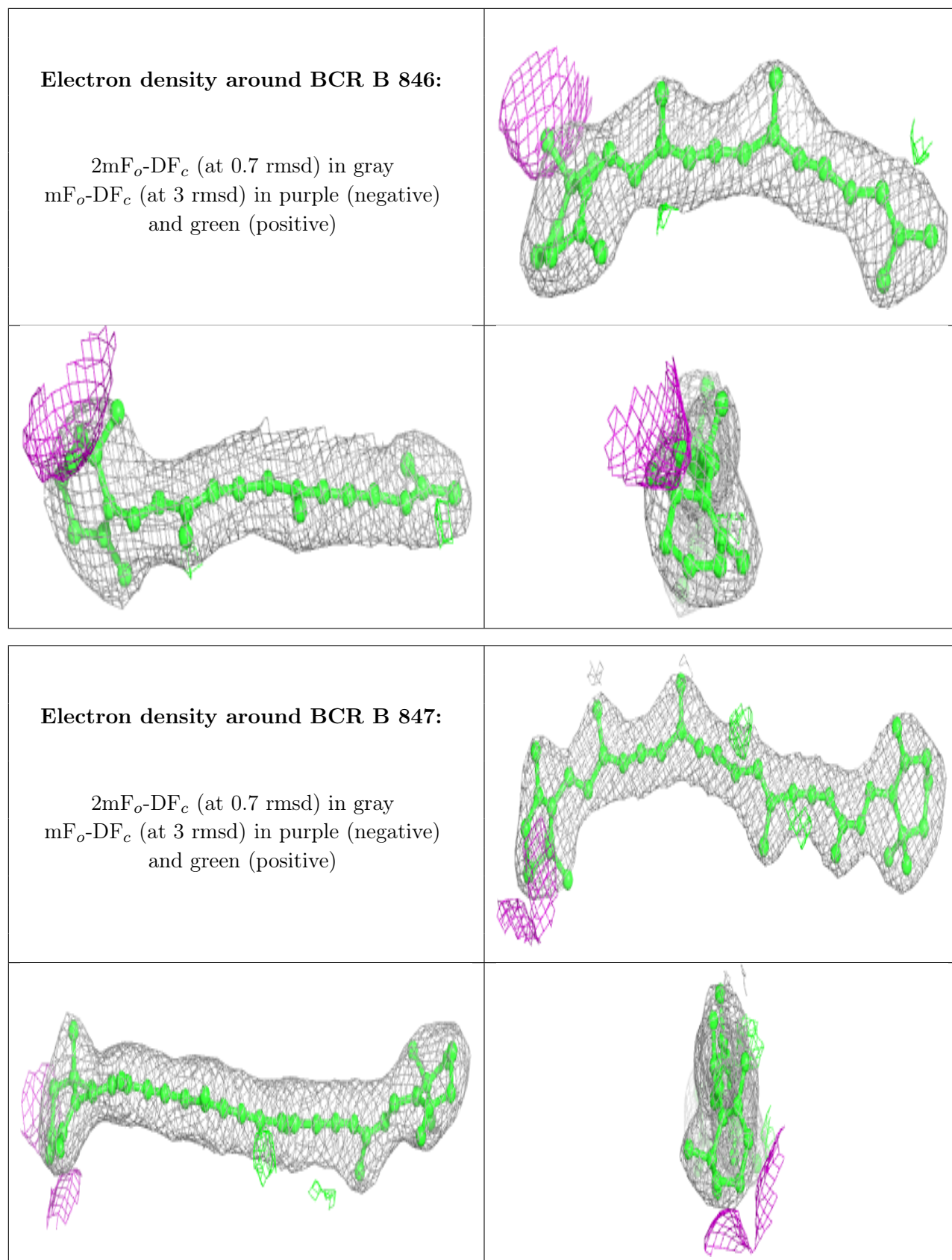


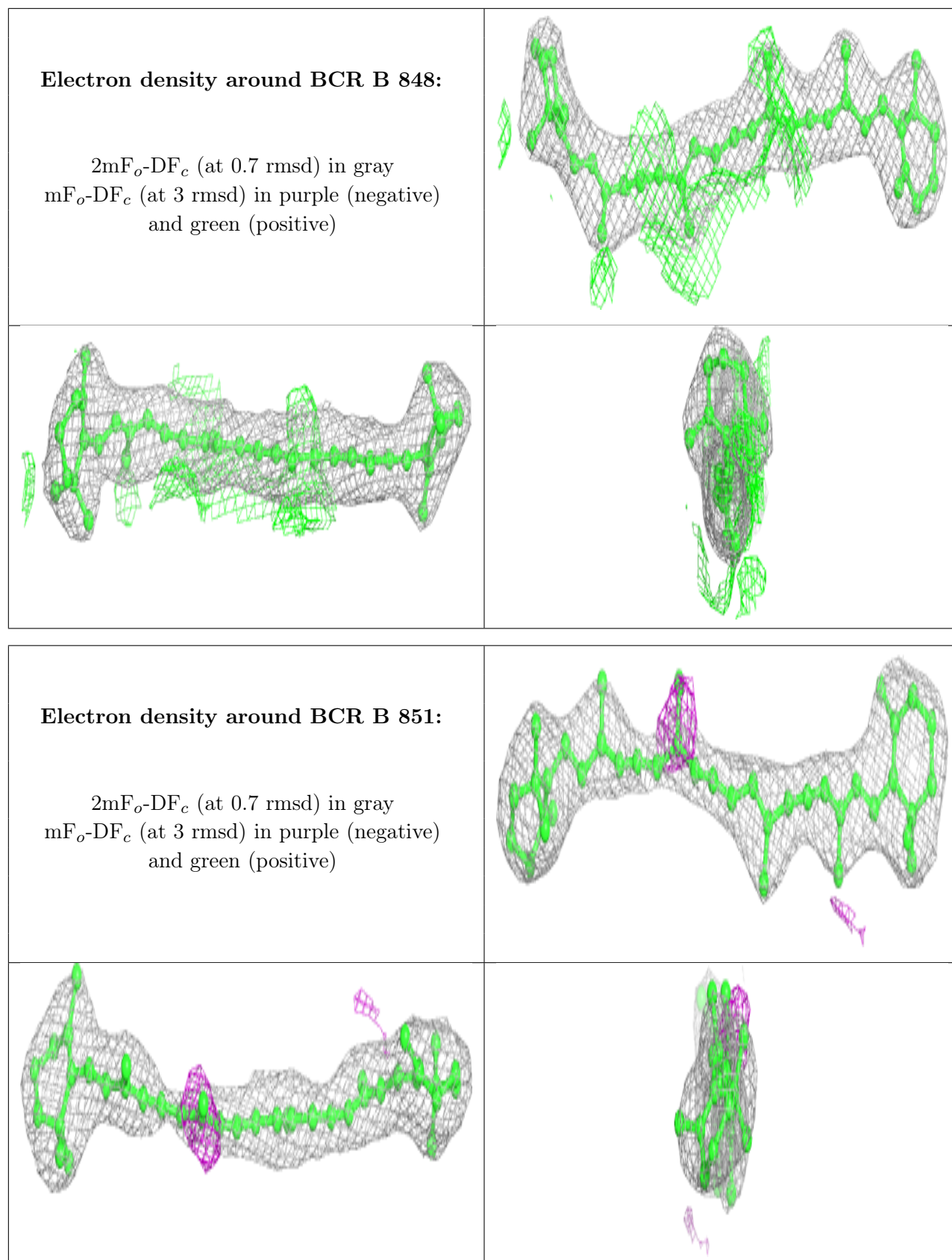






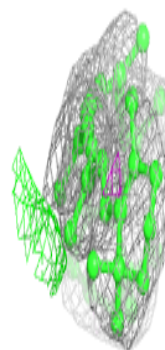
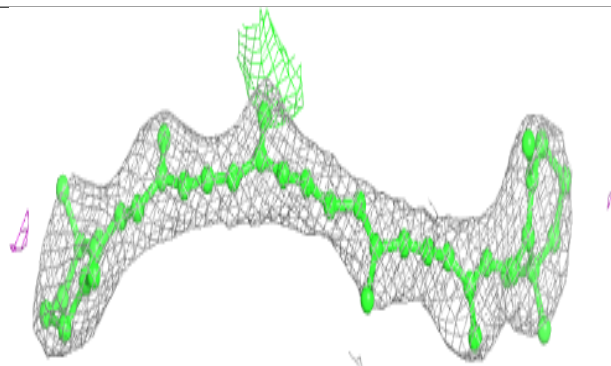
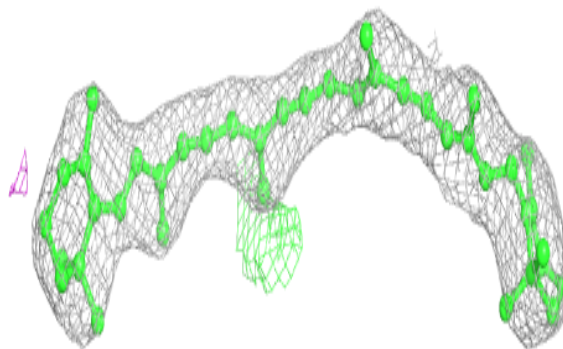




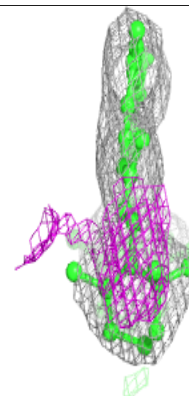
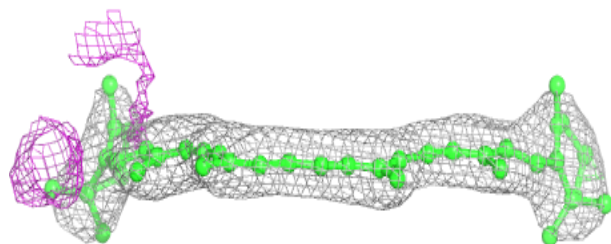
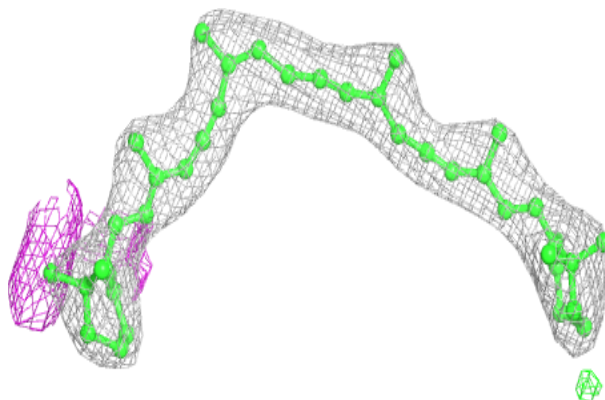


**Electron density around BCR F 201:**

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

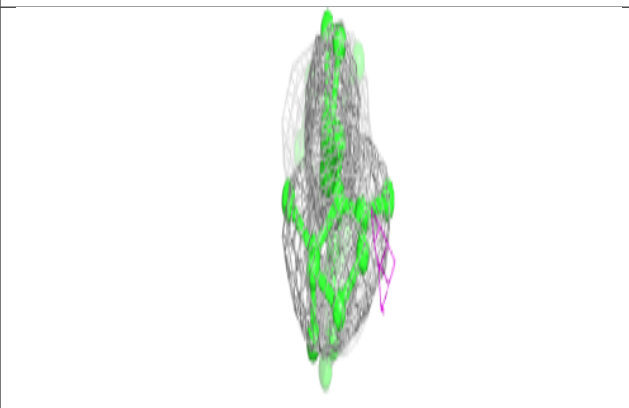
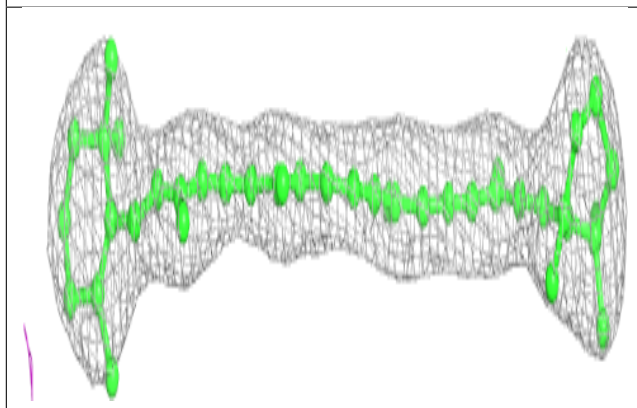
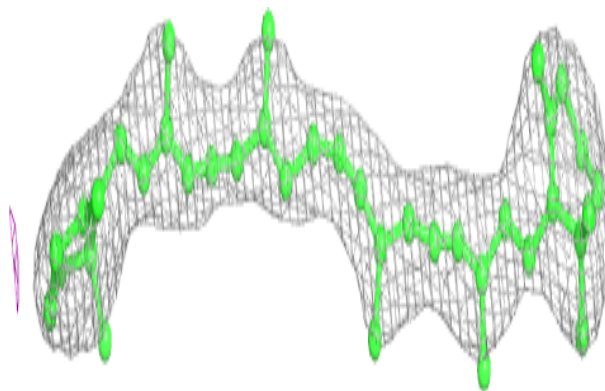
**Electron density around BCR F 203:**

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

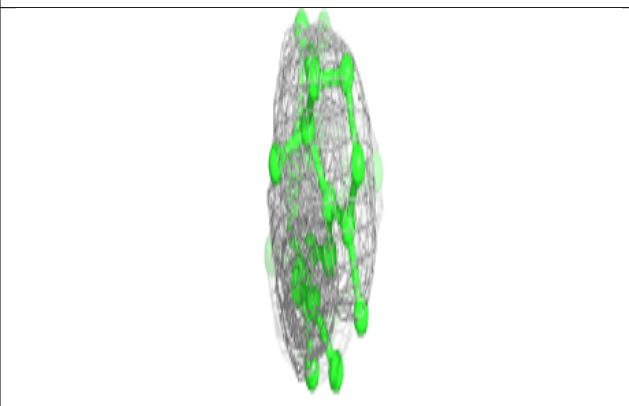
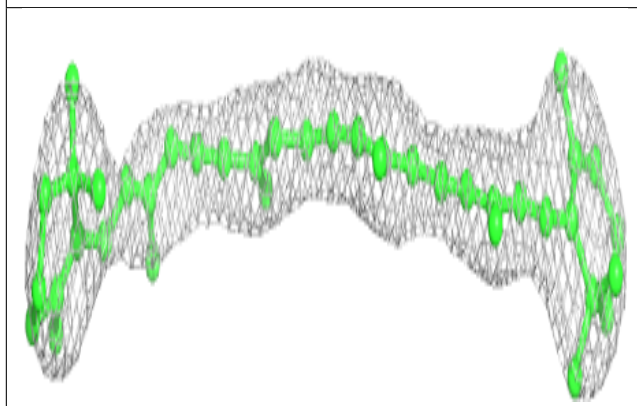
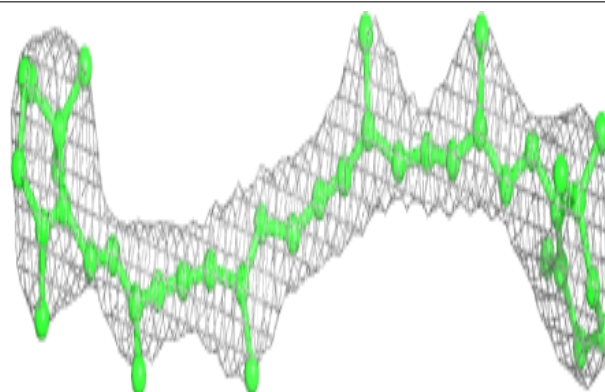


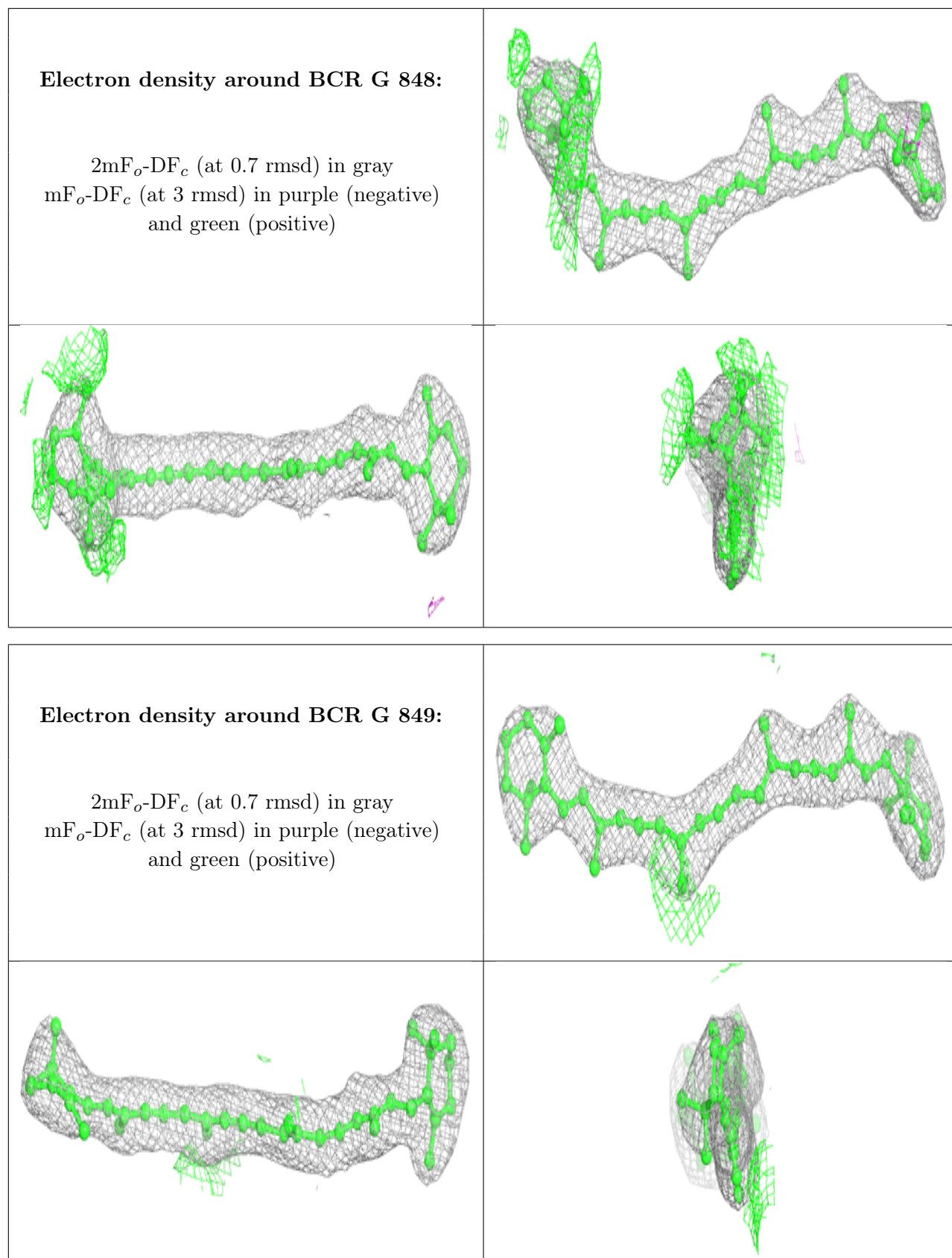
**Electron density around BCR G 846:**

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

**Electron density around BCR G 847:**

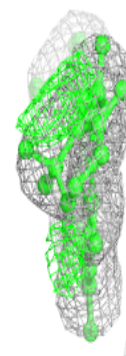
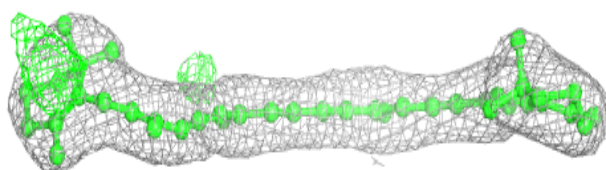
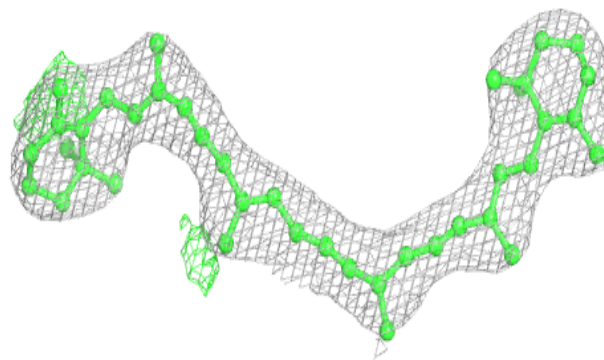
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



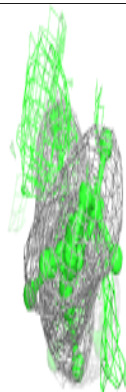
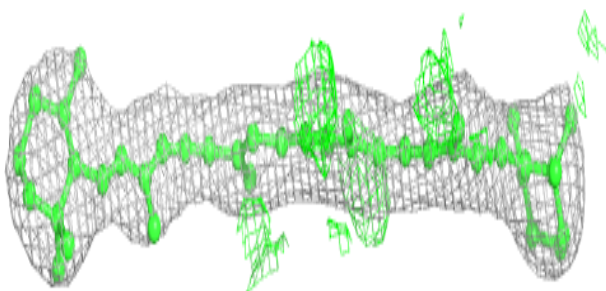
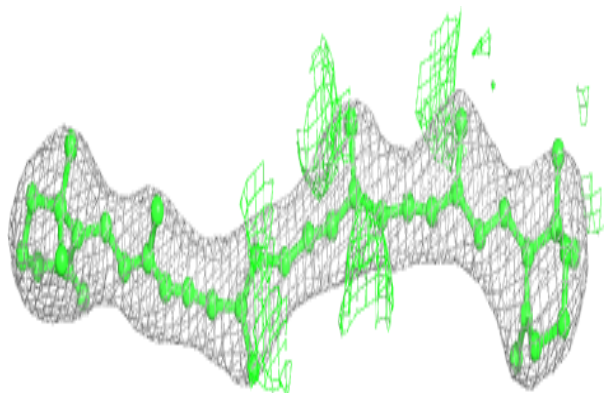


**Electron density around BCR G 850:**

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

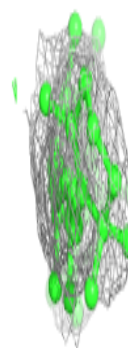
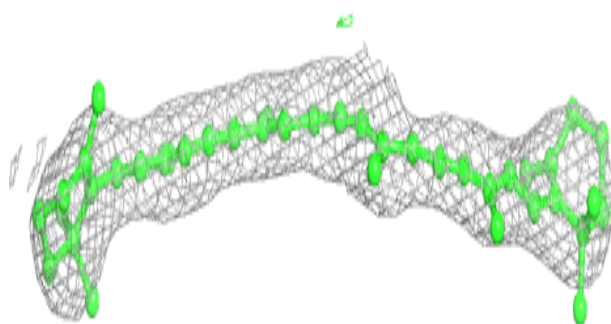
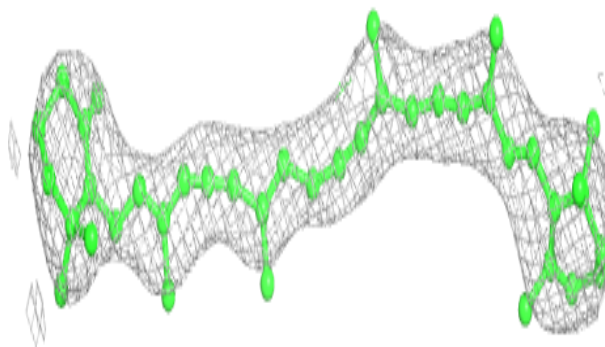
**Electron density around BCR G 854:**

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

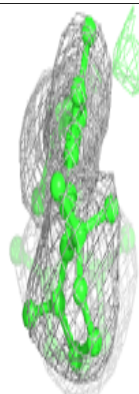
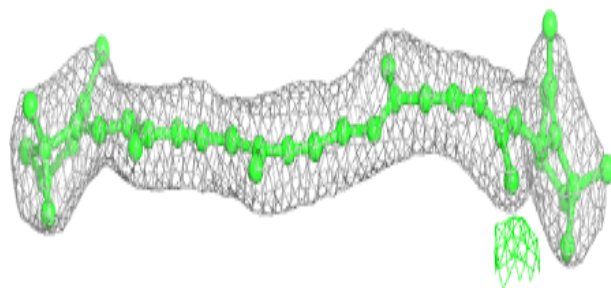
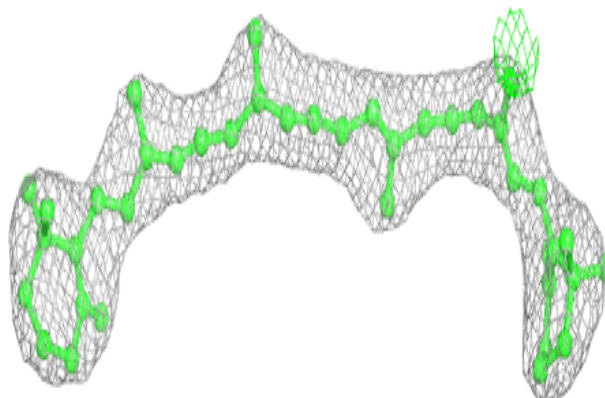


**Electron density around BCR H 840:**

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

**Electron density around BCR H 841:**

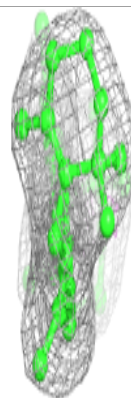
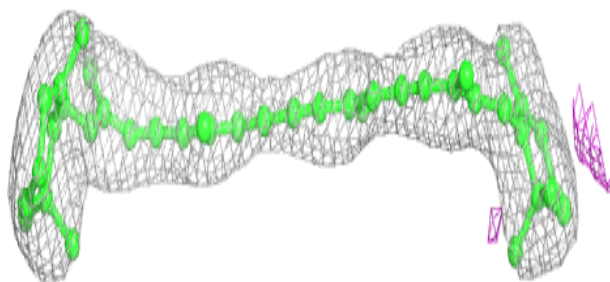
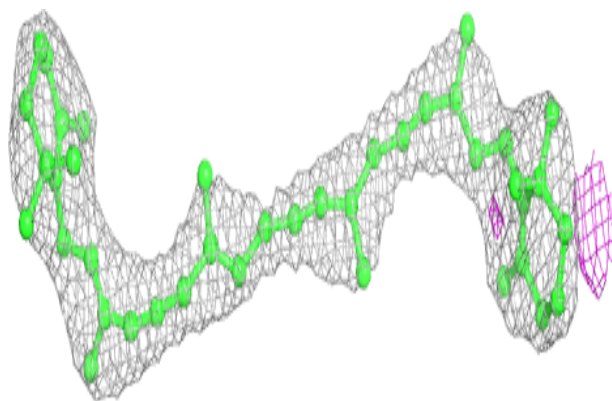
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



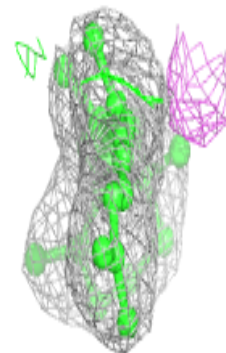
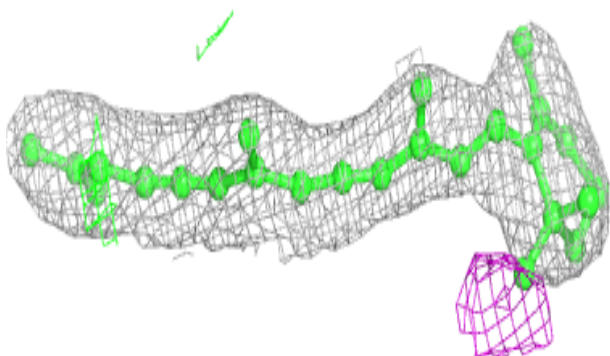
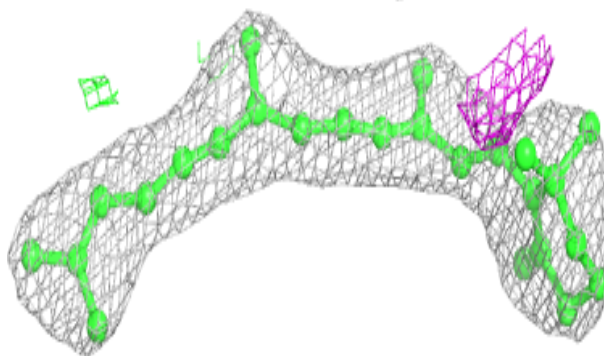


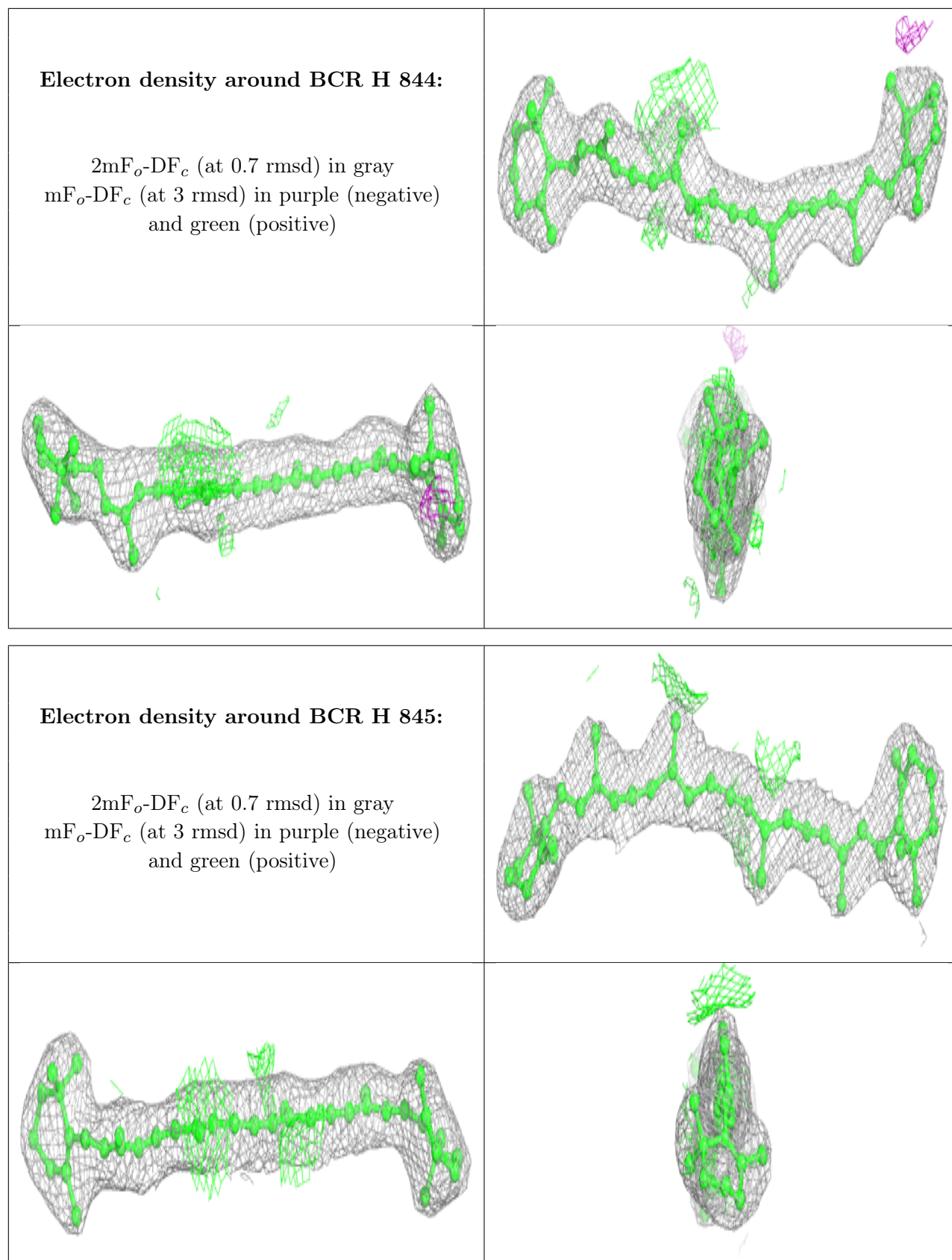
**Electron density around BCR H 842:**

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

**Electron density around BCR H 843:**

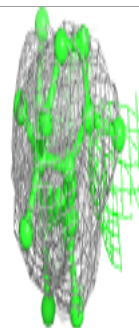
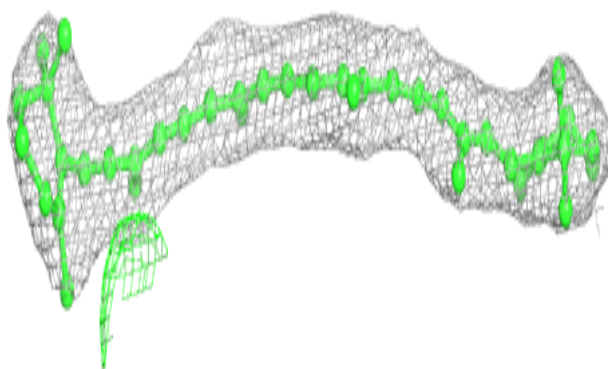
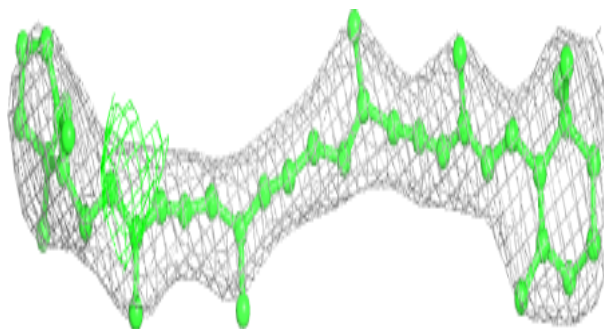
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



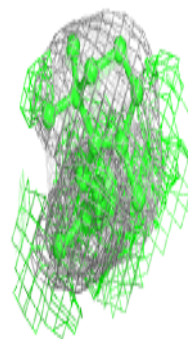
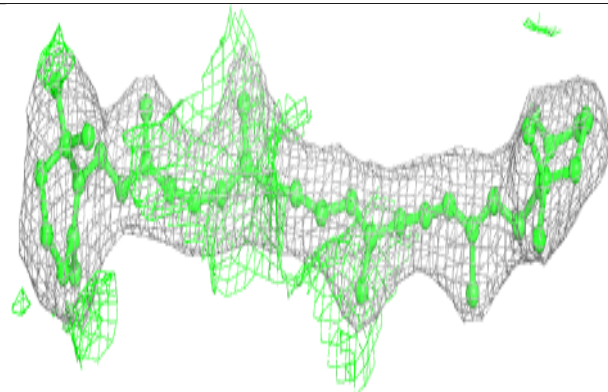
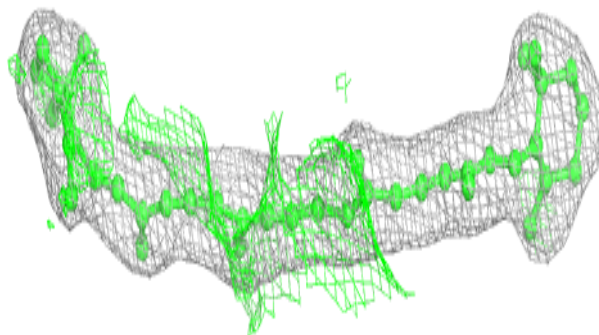


**Electron density around BCR H 848:**

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

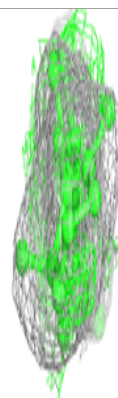
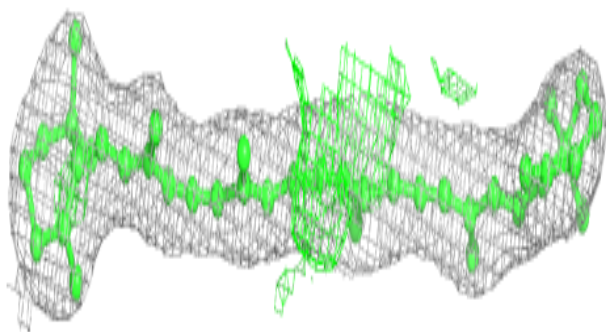
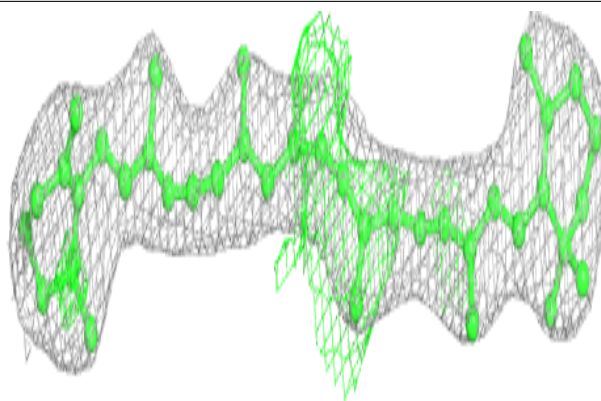
**Electron density around BCR I 101:**

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

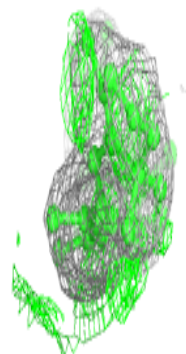
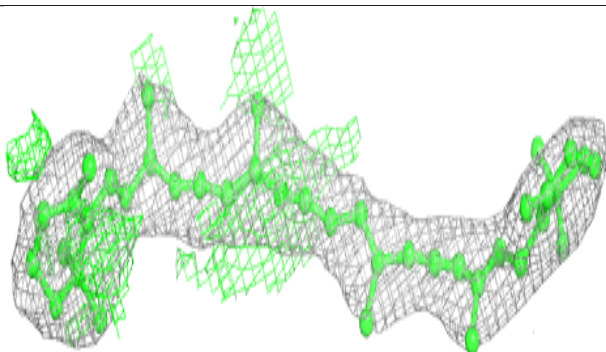
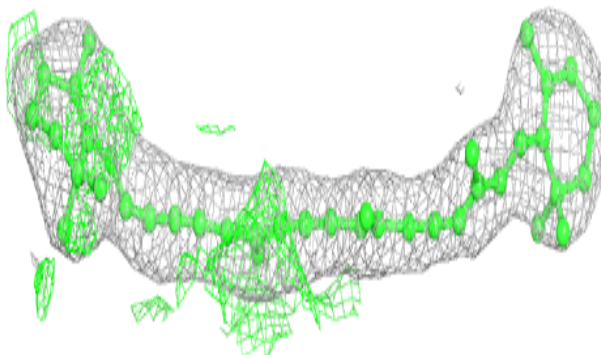


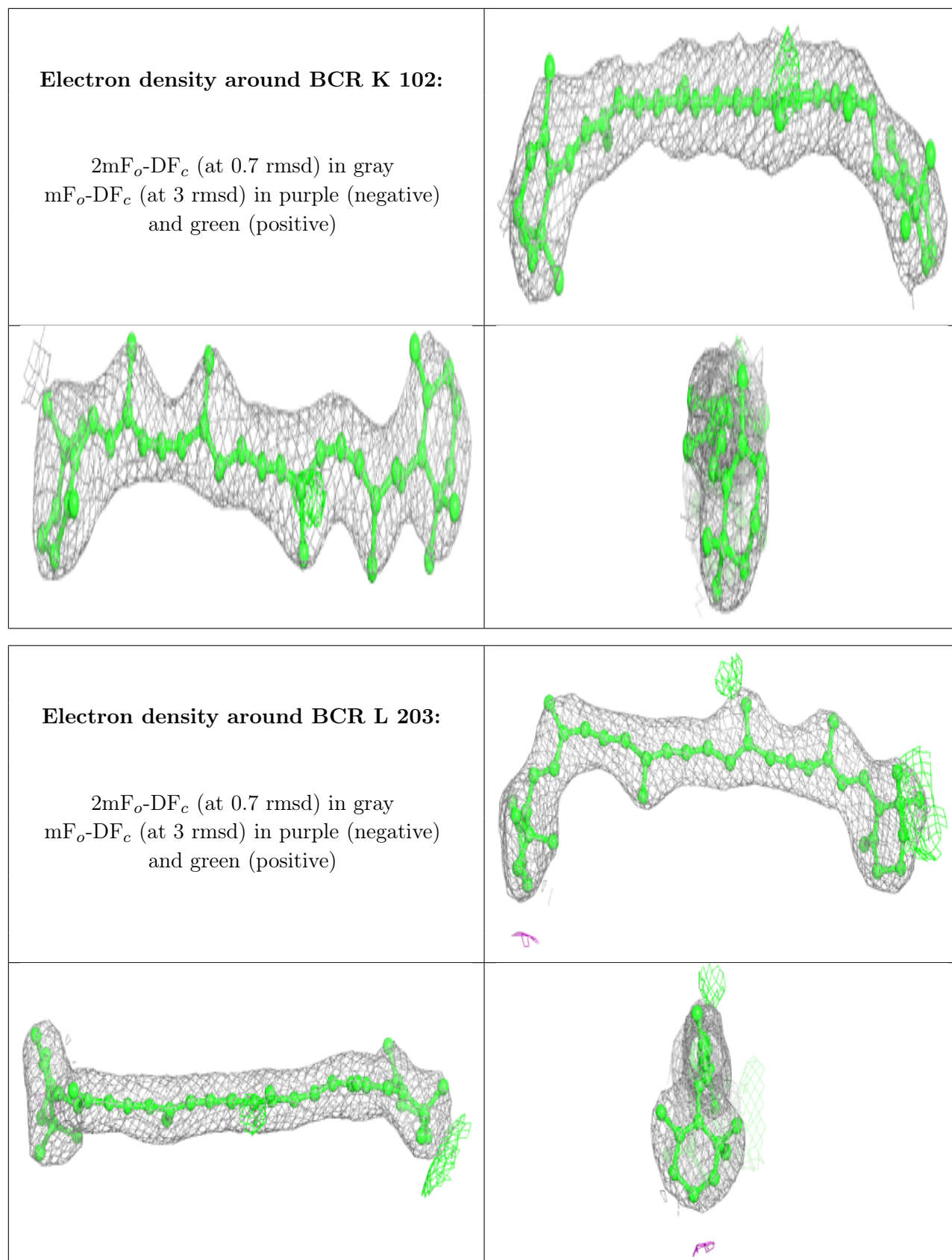
**Electron density around BCR J 103:**

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

**Electron density around BCR J 104:**

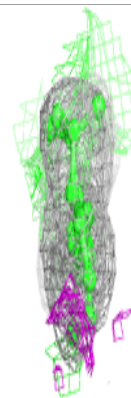
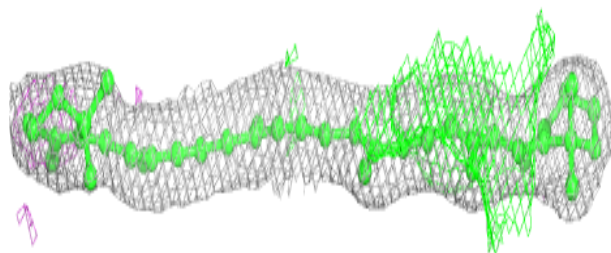
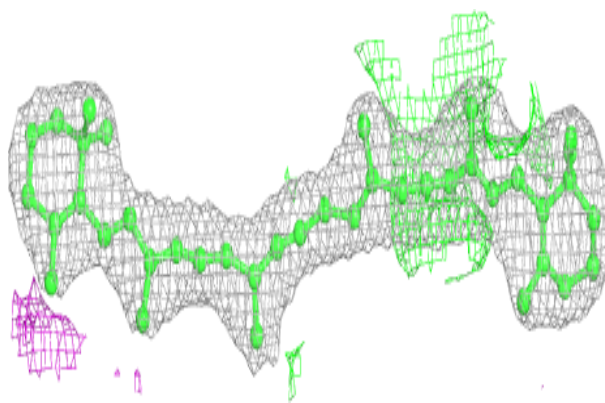
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



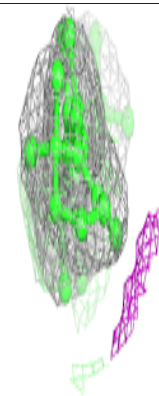
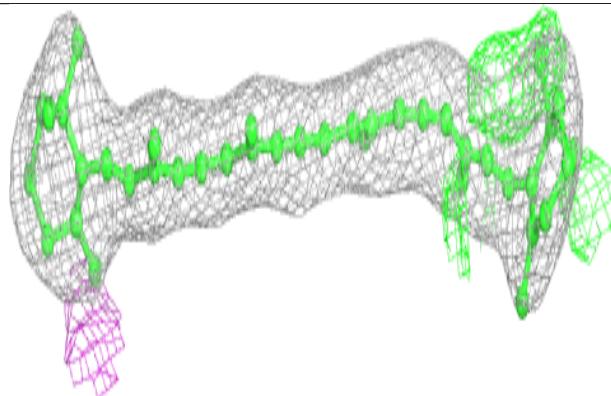
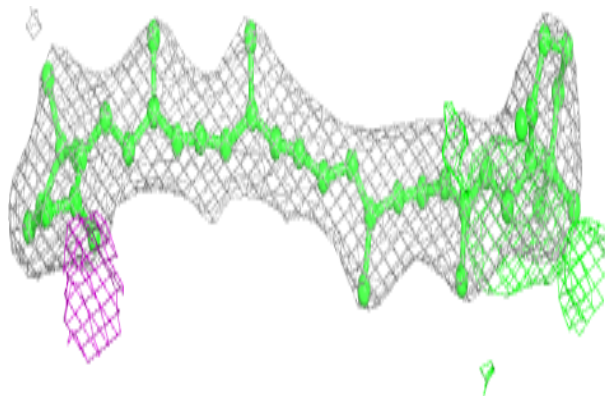


**Electron density around BCR L 208:**

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

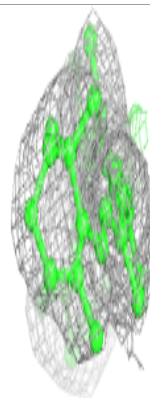
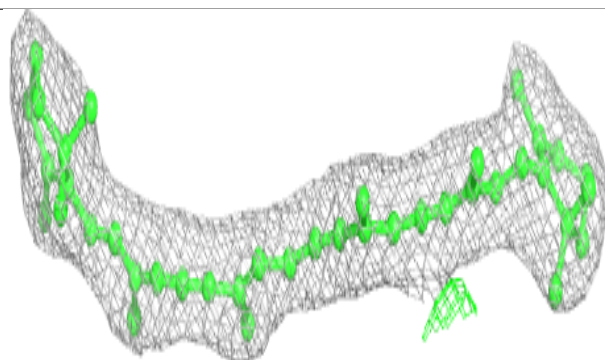
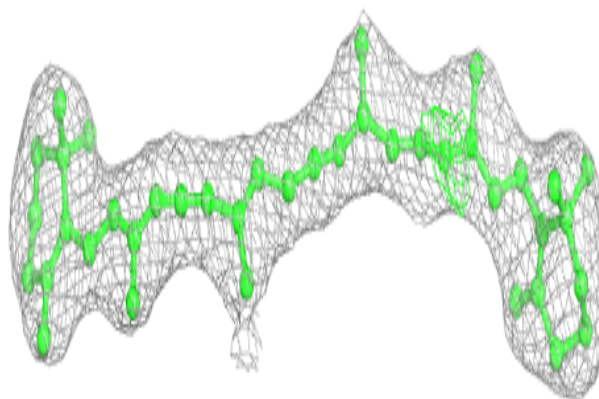
**Electron density around BCR L 209:**

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

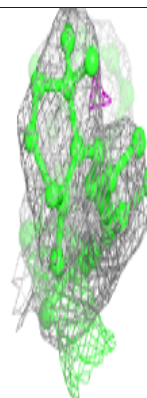
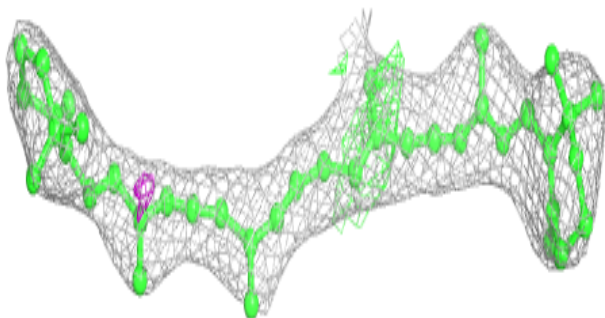
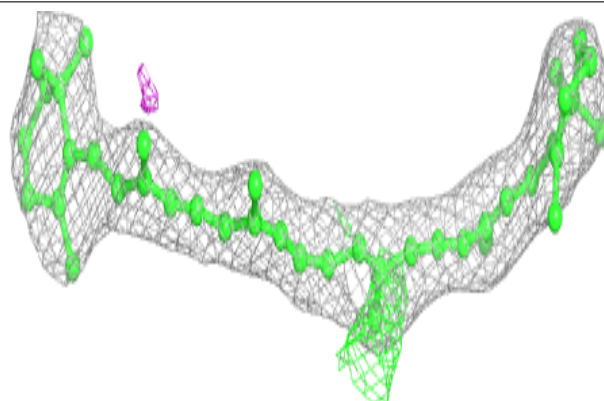


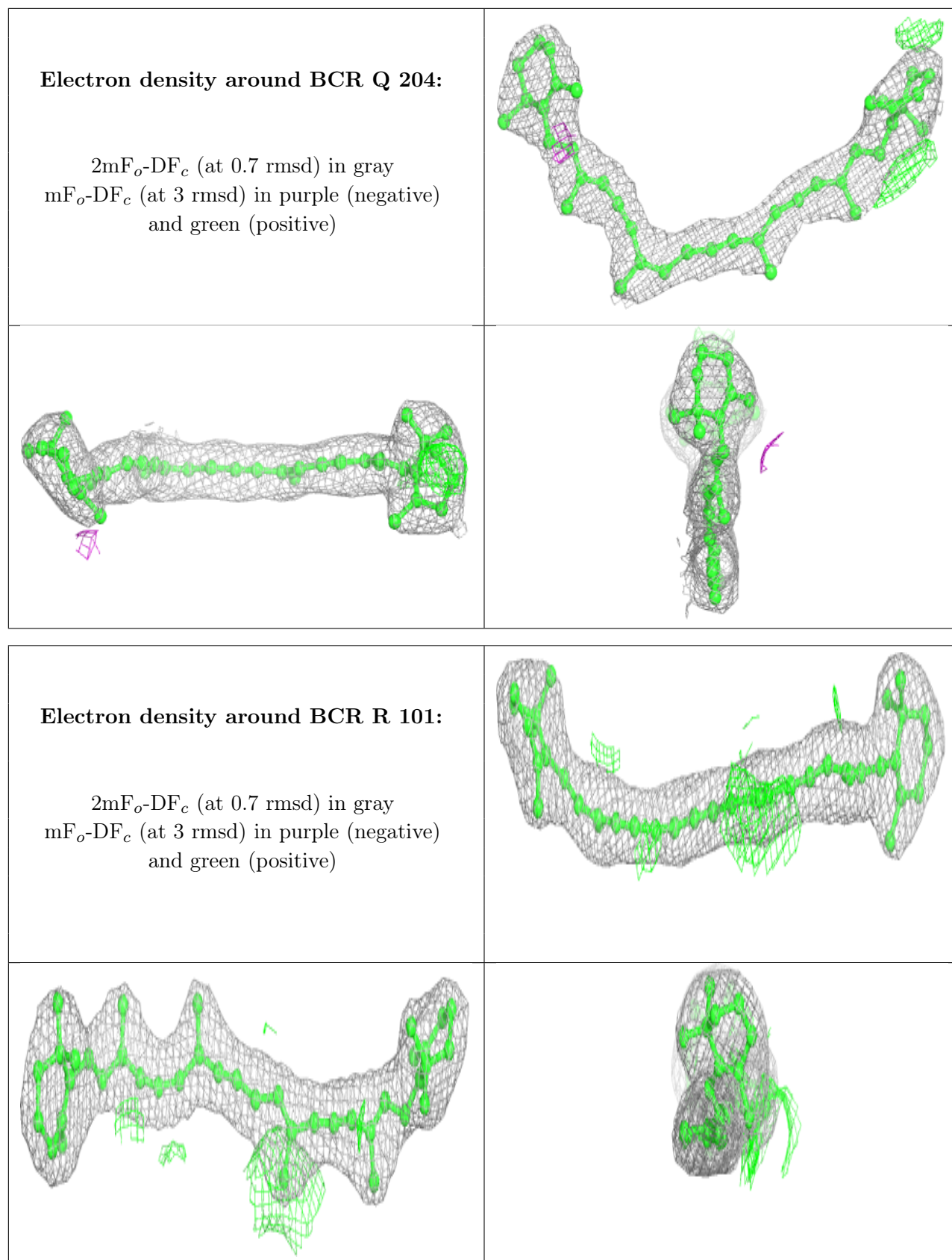
**Electron density around BCR M 101:**

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

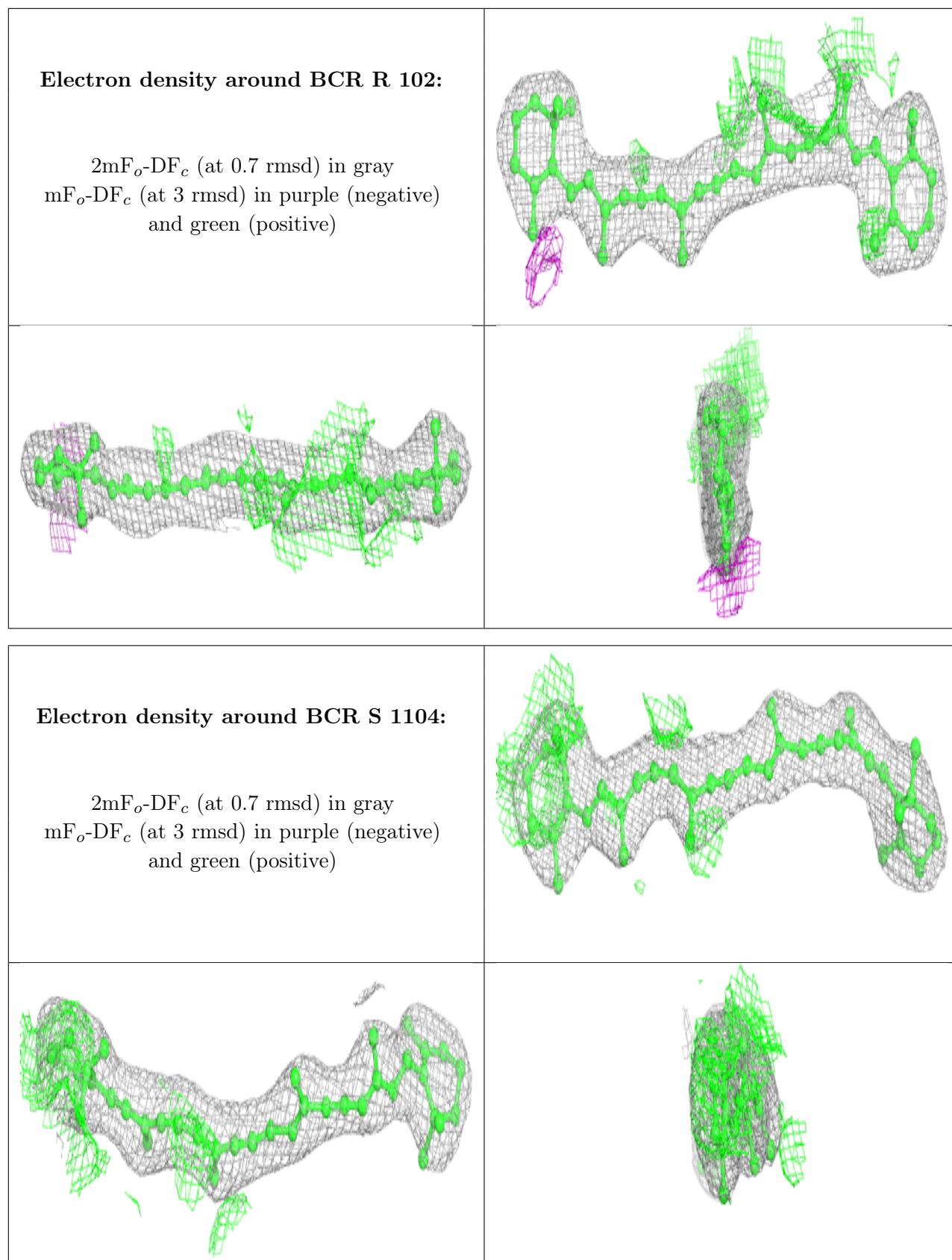
**Electron density around BCR Q 202:**

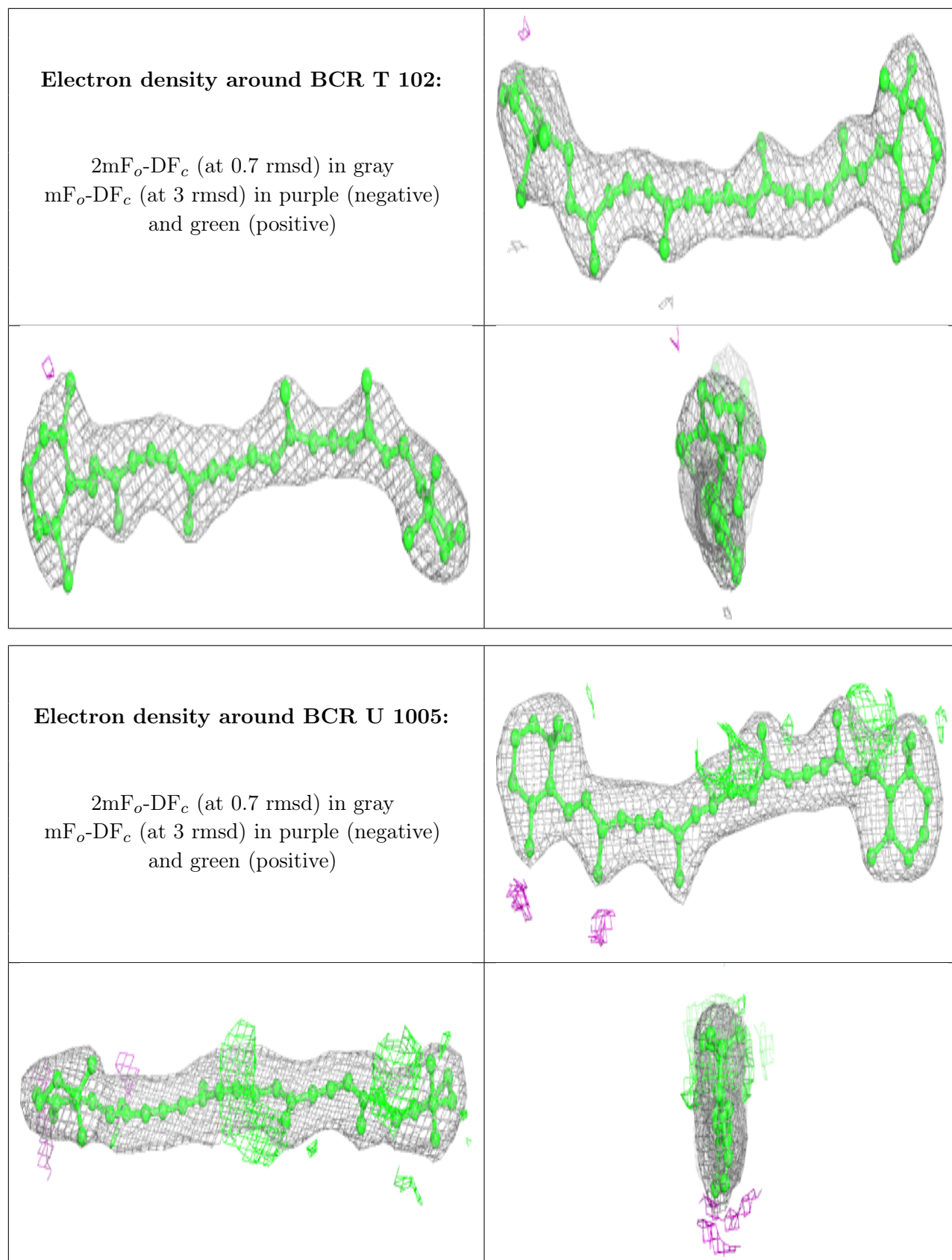
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





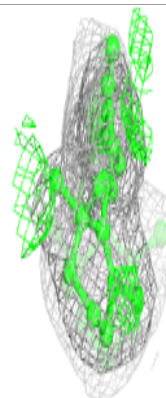
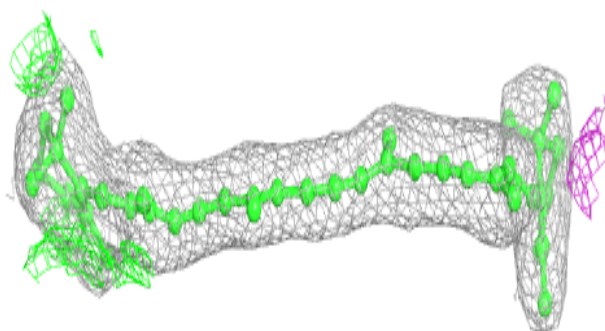
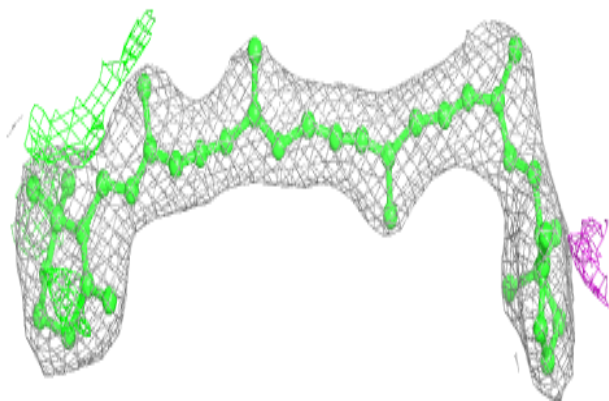




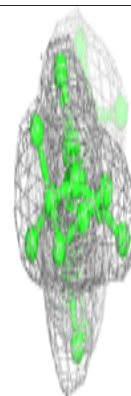
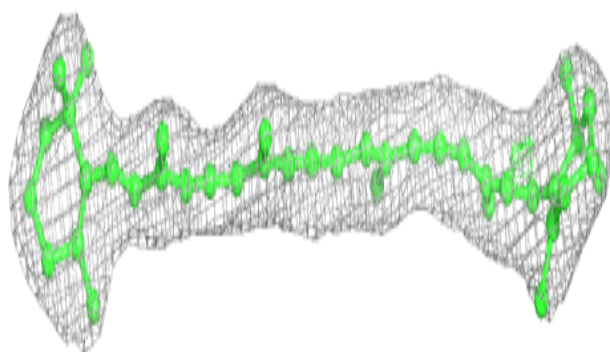
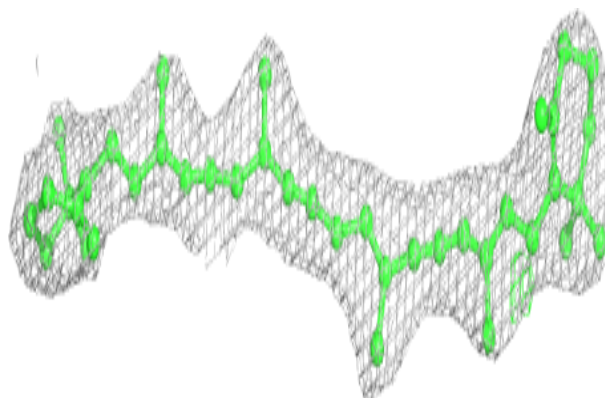


**Electron density around BCR U 1007:**

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

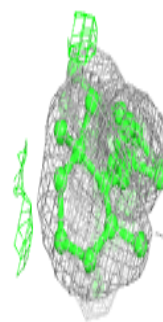
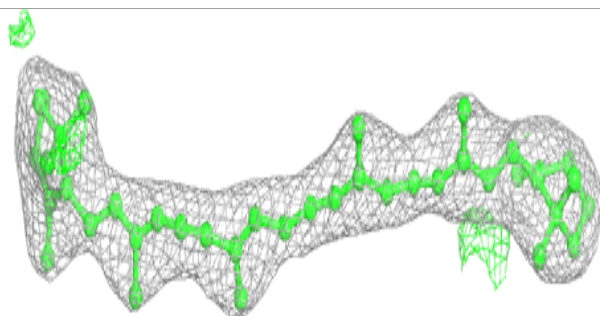
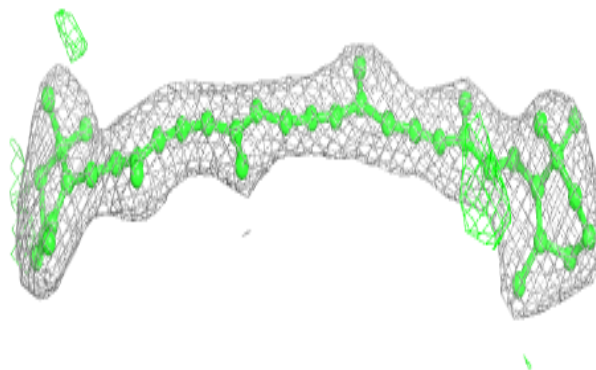
**Electron density around BCR U 1008:**

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

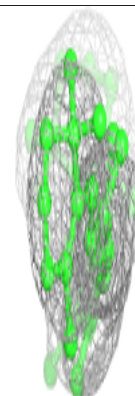
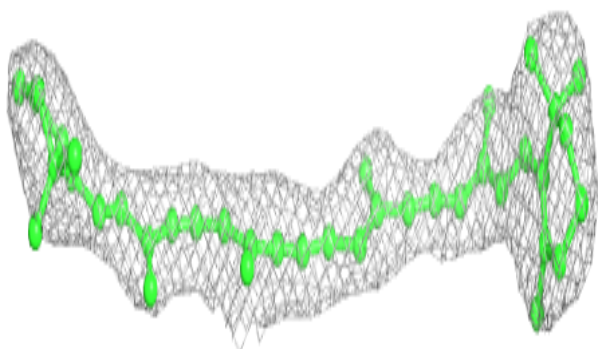
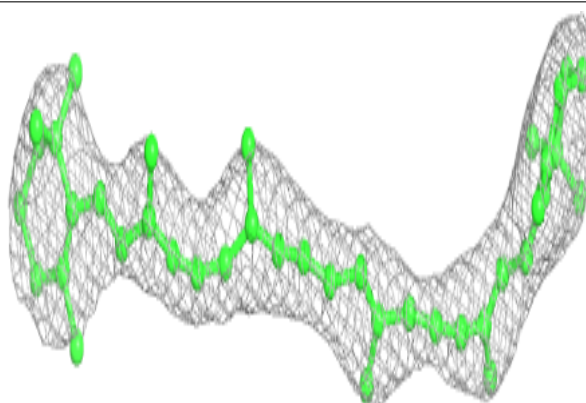


**Electron density around BCR V 1202:**

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

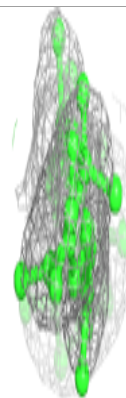
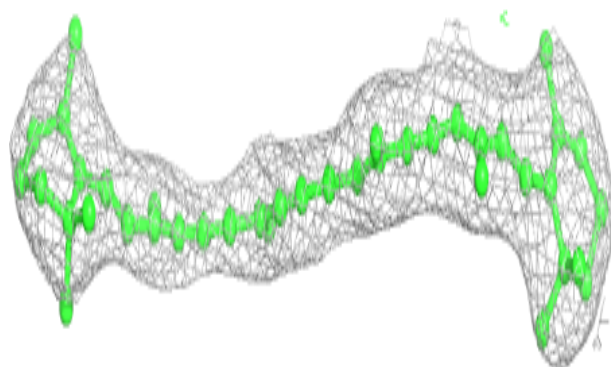
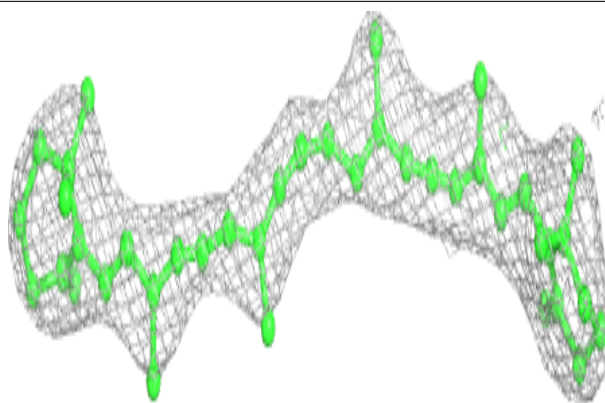
**Electron density around BCR Y 846:**

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

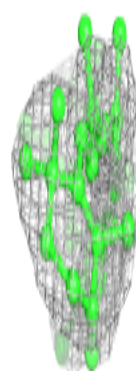
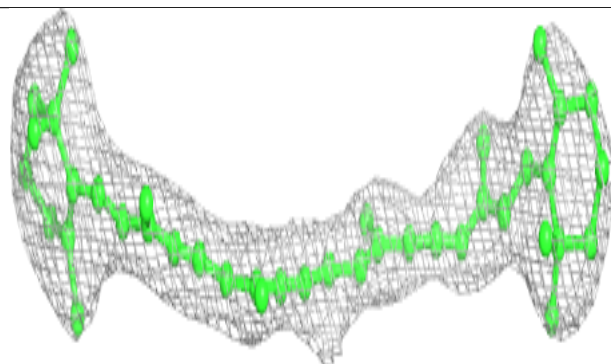
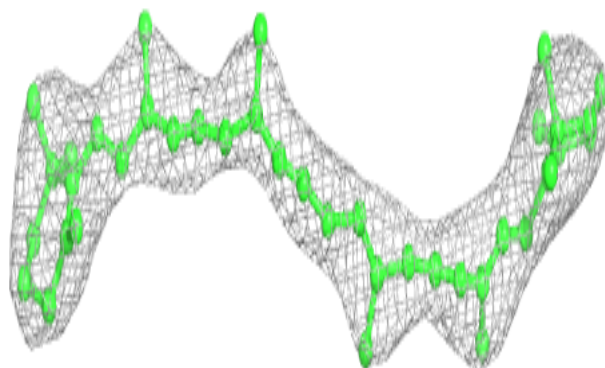


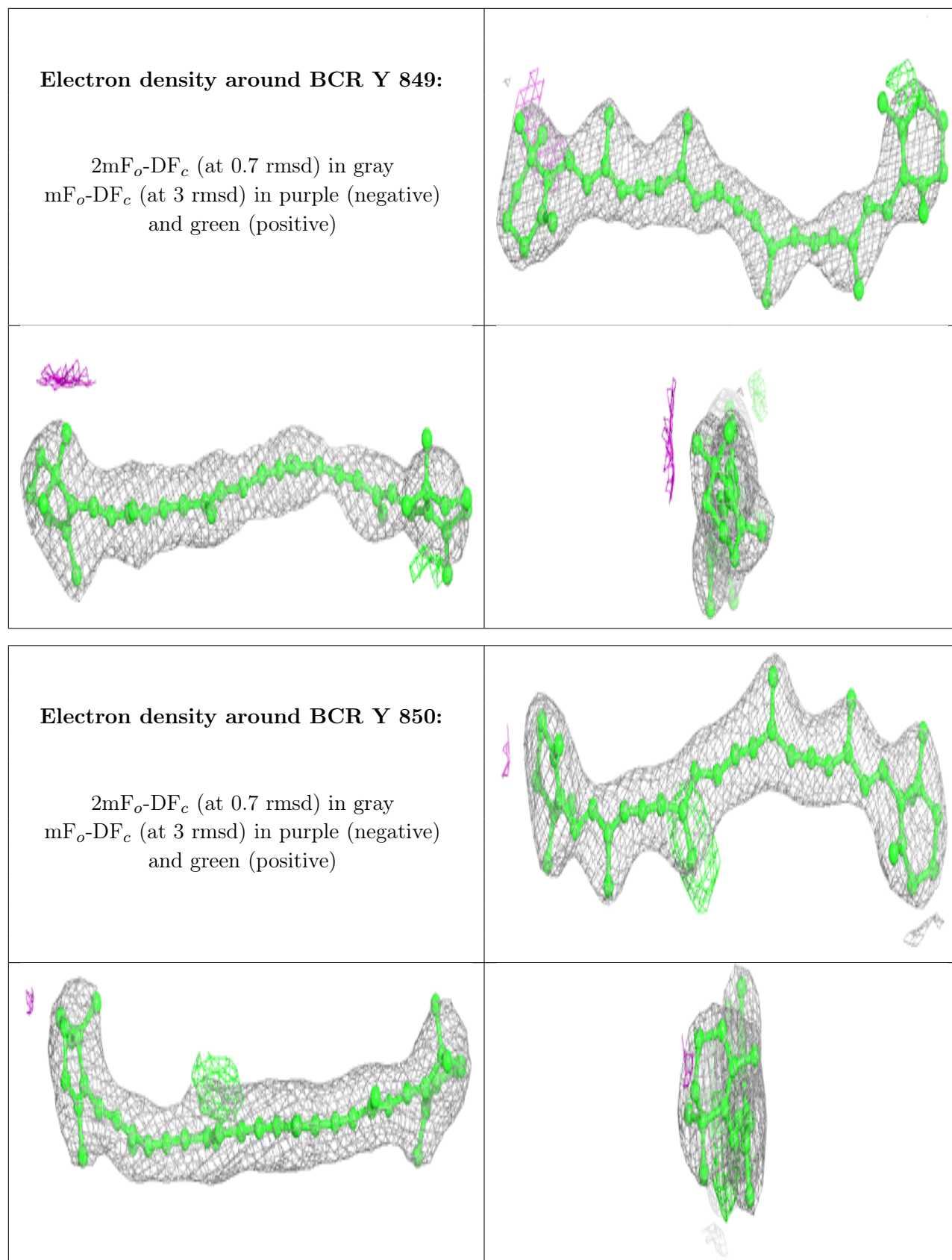
**Electron density around BCR Y 847:**

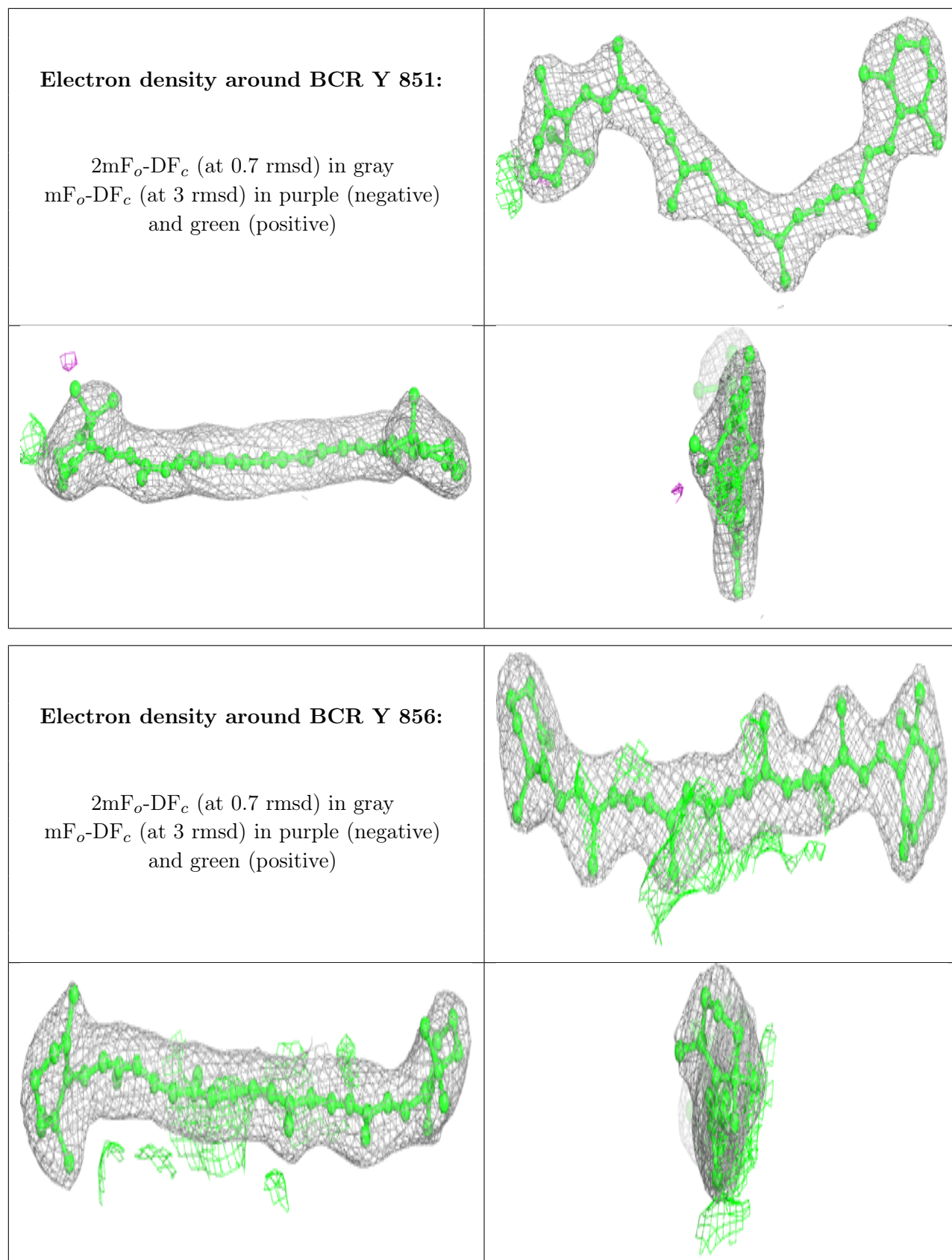
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR Y 848:**

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

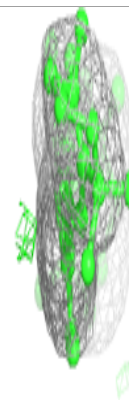
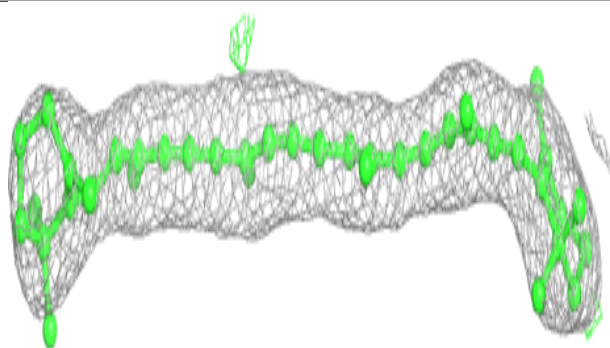
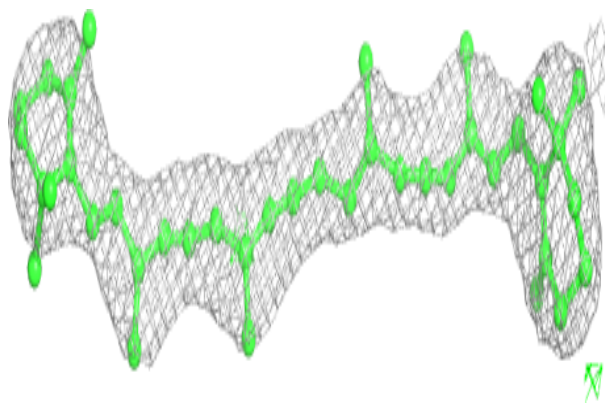




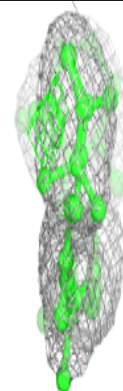
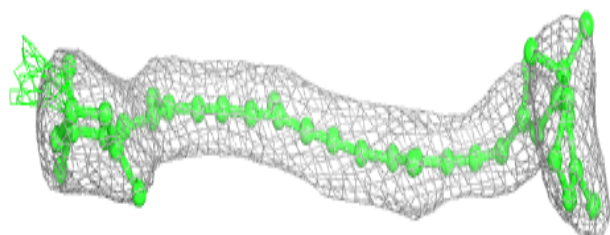
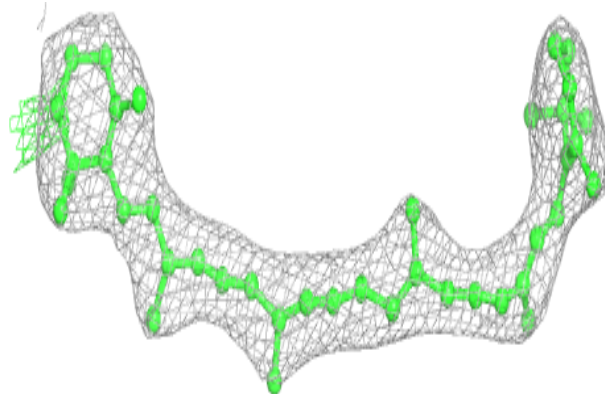


**Electron density around BCR Z 841:**

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

**Electron density around BCR Z 842:**

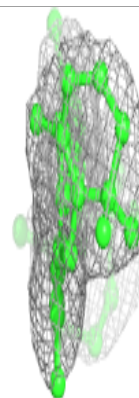
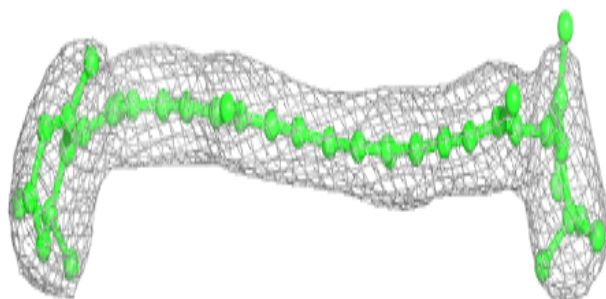
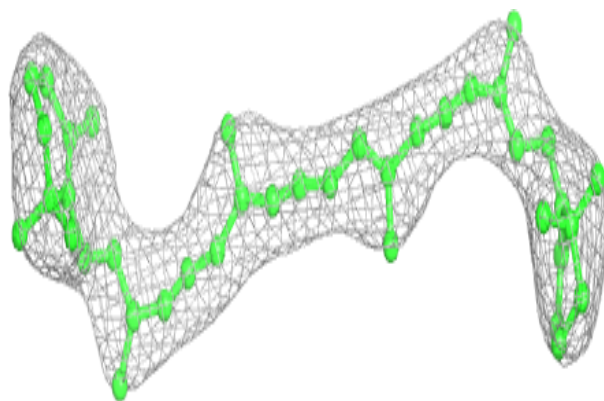
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



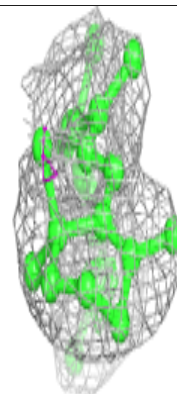
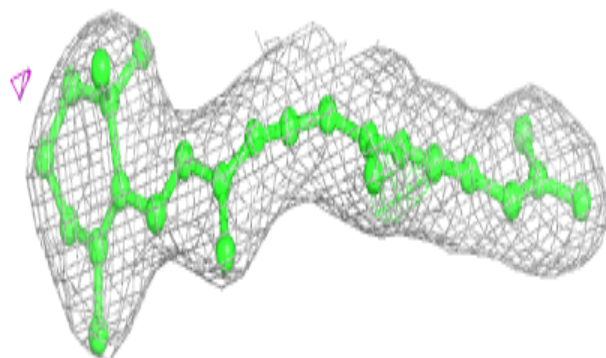
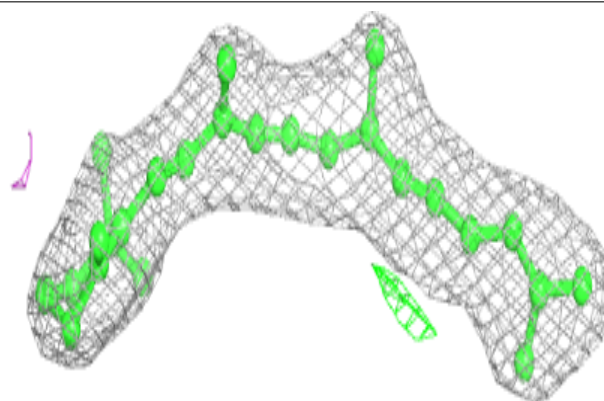


**Electron density around BCR Z 843:**

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

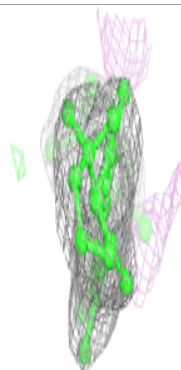
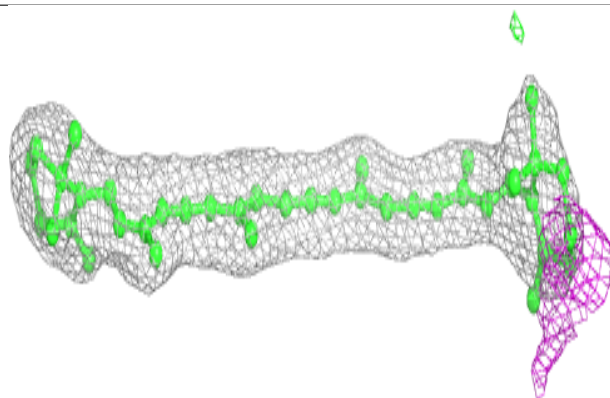
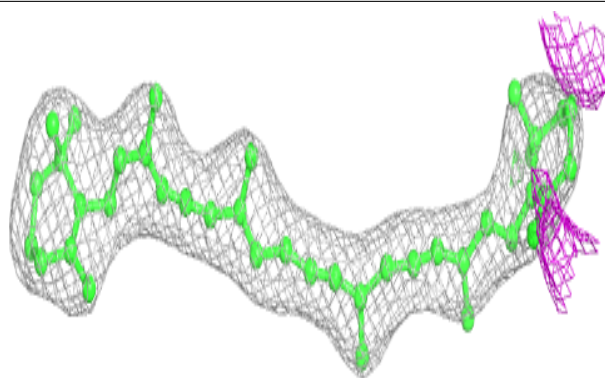
**Electron density around BCR Z 844:**

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

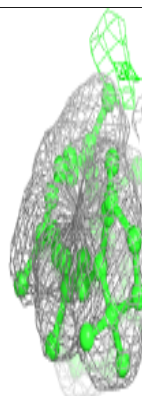
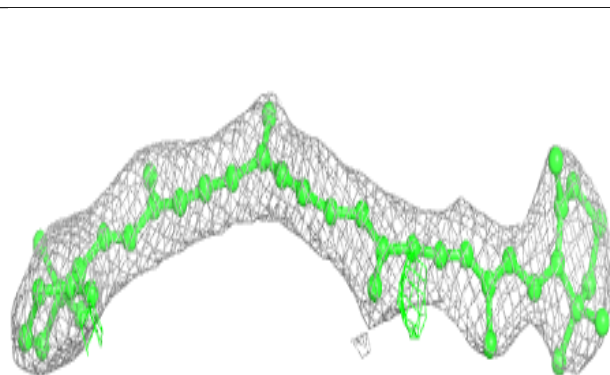
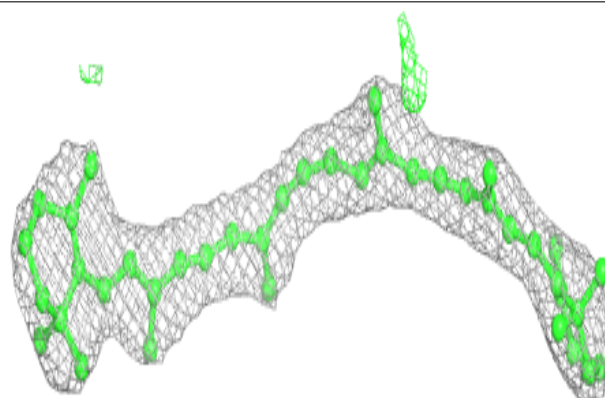


**Electron density around BCR Z 845:**

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

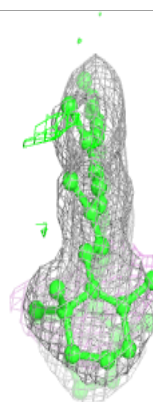
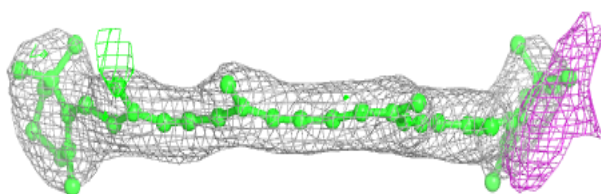
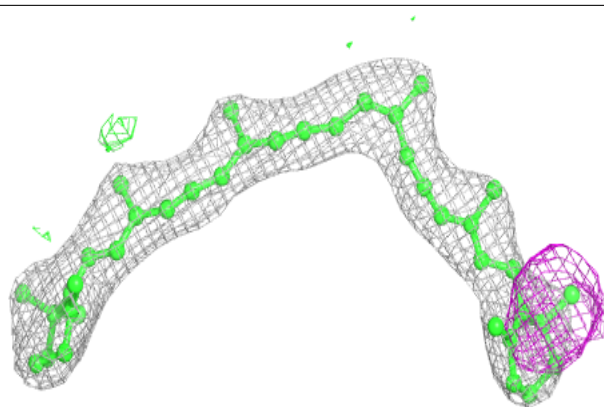
**Electron density around BCR Z 846:**

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

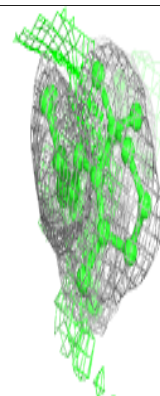
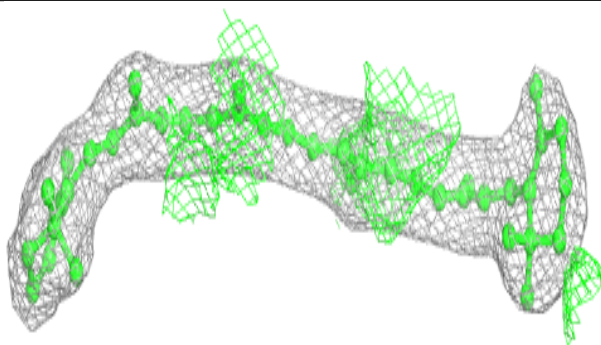
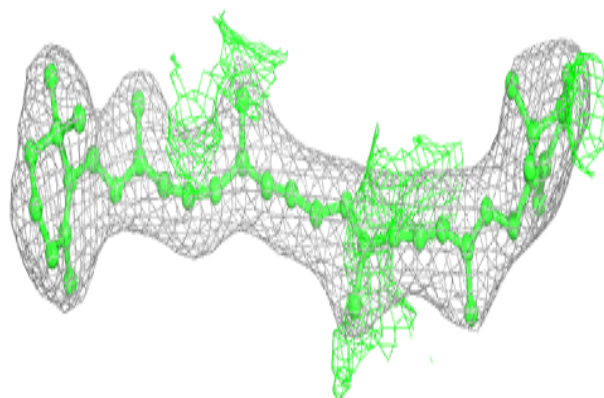


**Electron density around BCR d 203:**

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

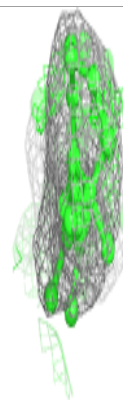
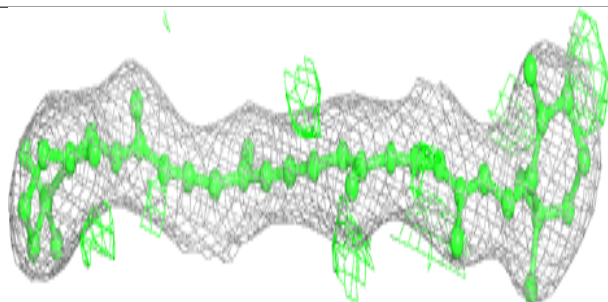
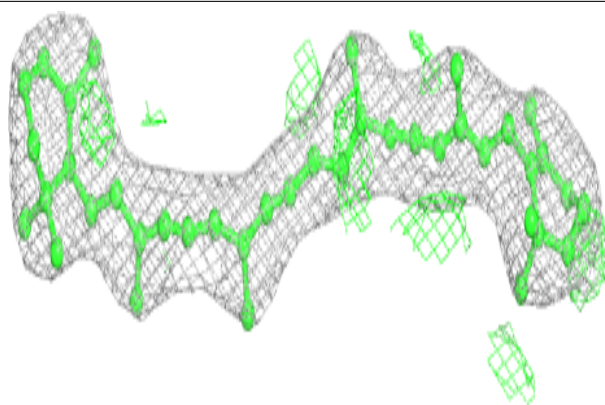
**Electron density around BCR e 101:**

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

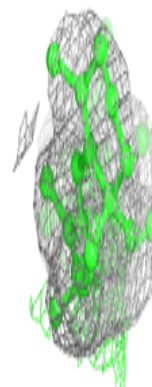
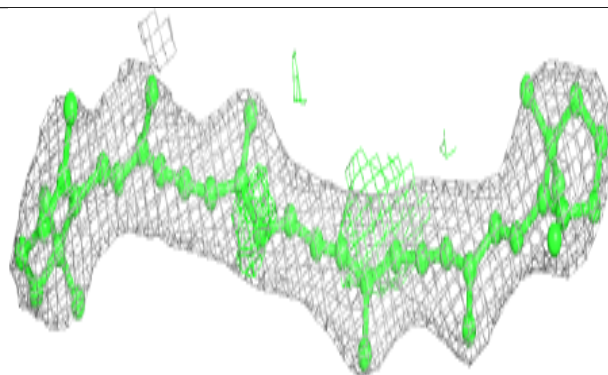
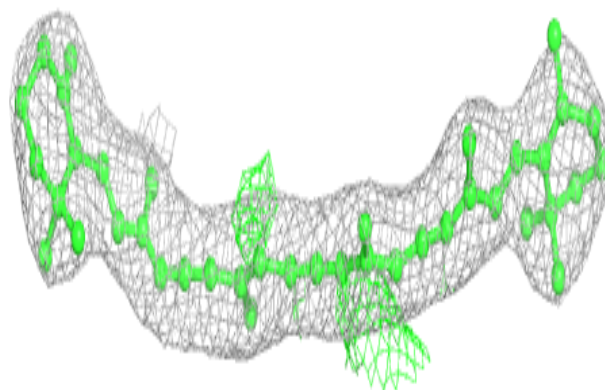


**Electron density around BCR f 103:**

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

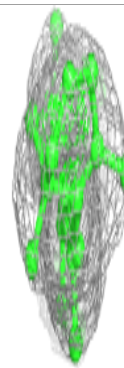
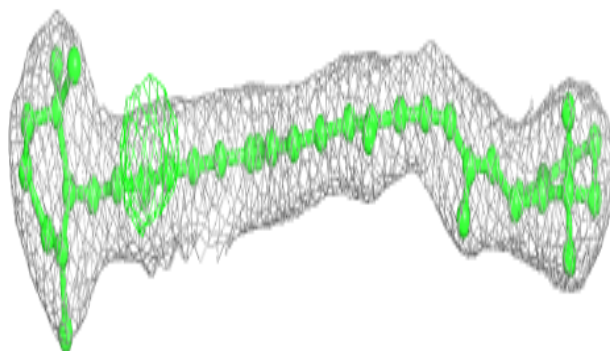
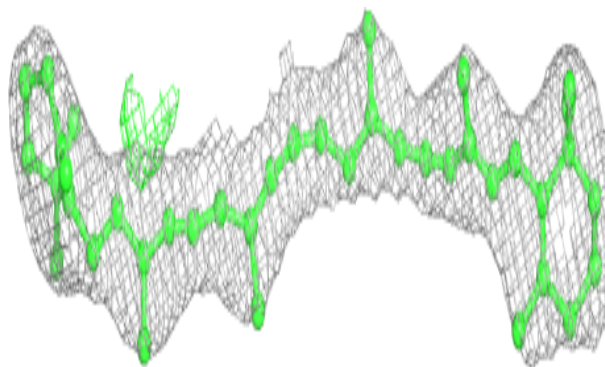
**Electron density around BCR f 104:**

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

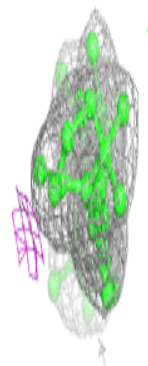
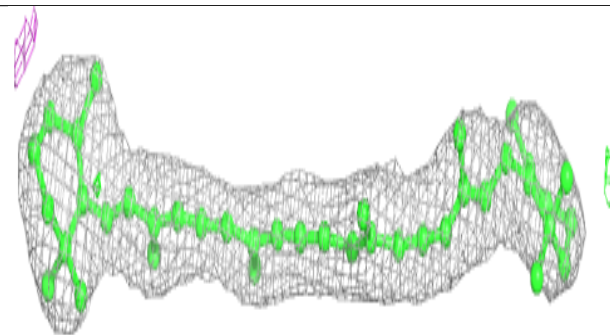
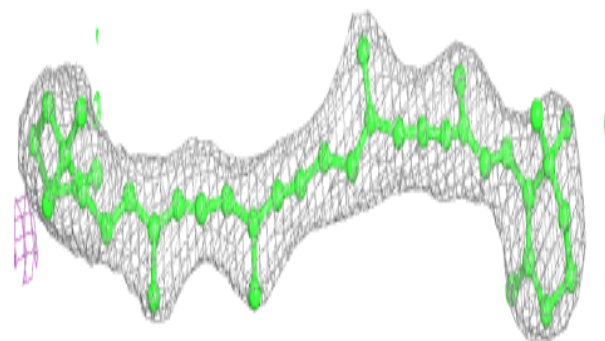


**Electron density around BCR f 105:**

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

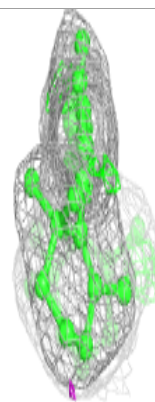
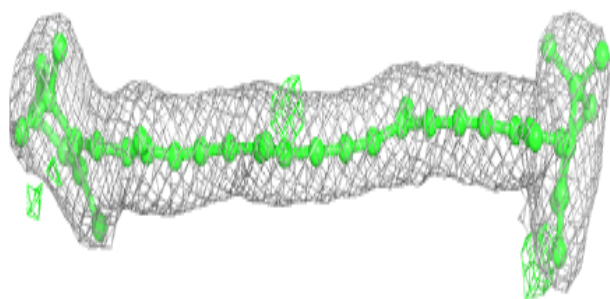
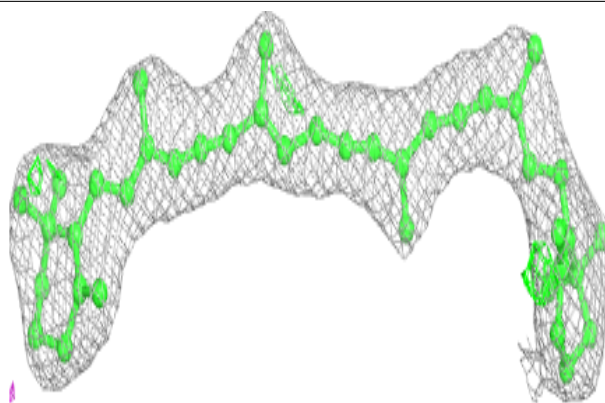
**Electron density around BCR h 202:**

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

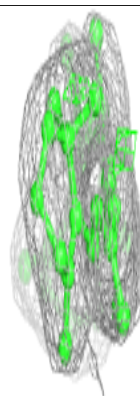
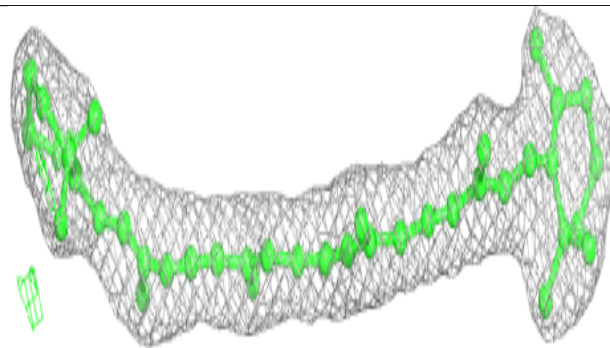
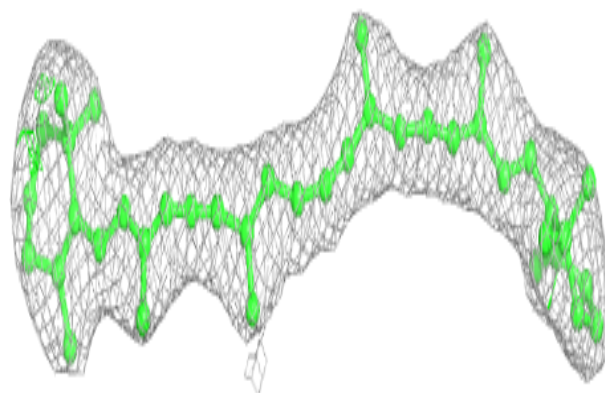


**Electron density around BCR h 203:**

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

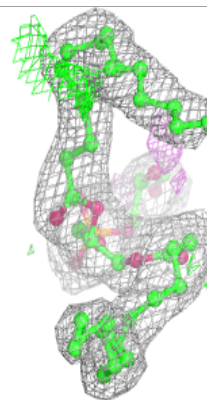
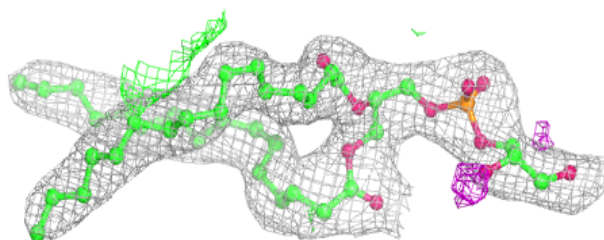
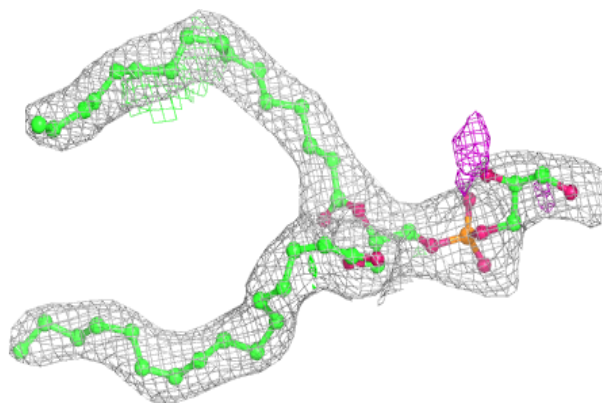
**Electron density around BCR i 101:**

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

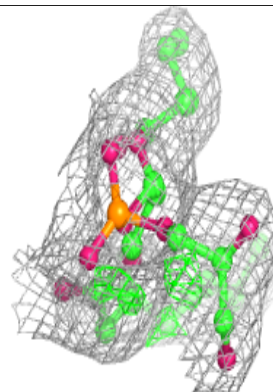
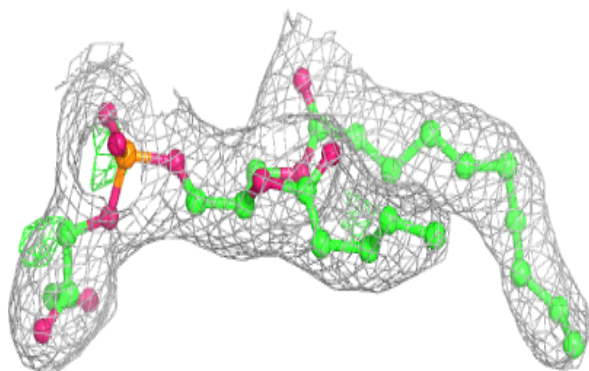
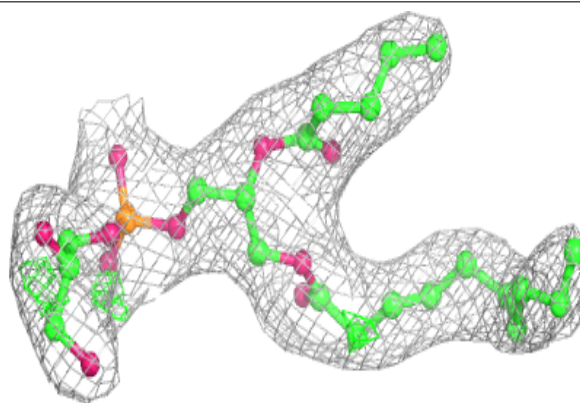


**Electron density around LHG A 850:**

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

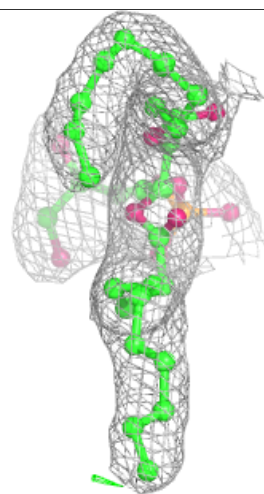
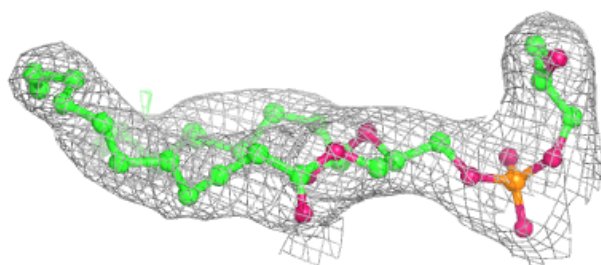
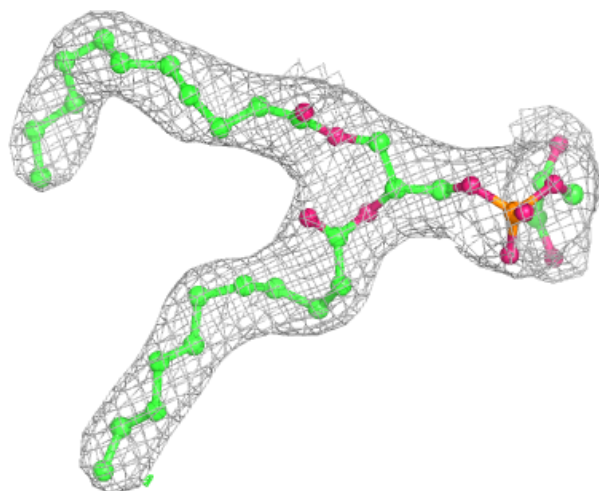
**Electron density around LHG A 851:**

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



**Electron density around LHG B 850:**

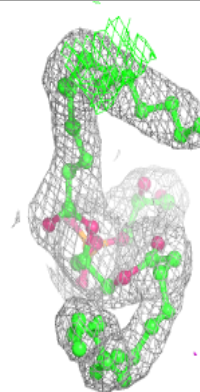
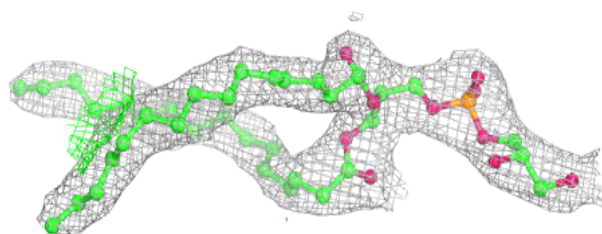
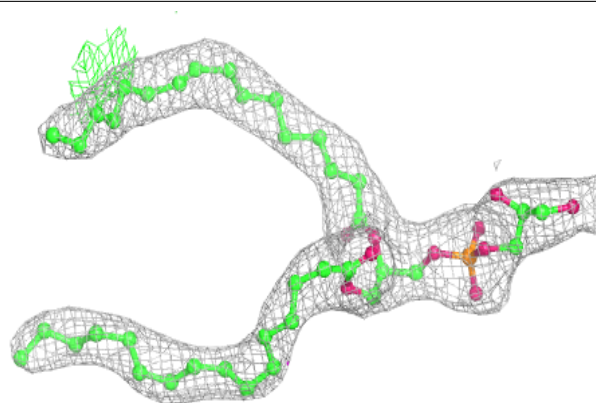
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



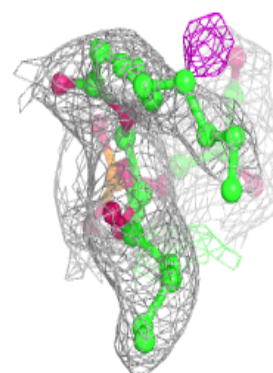
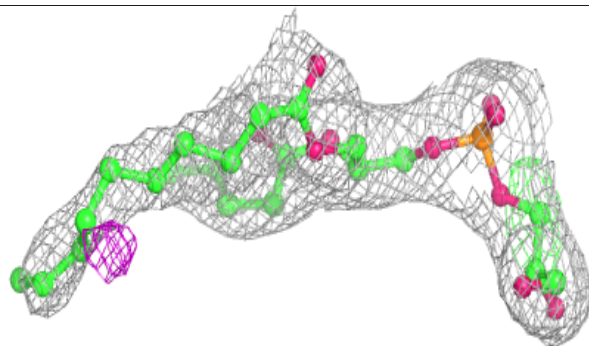
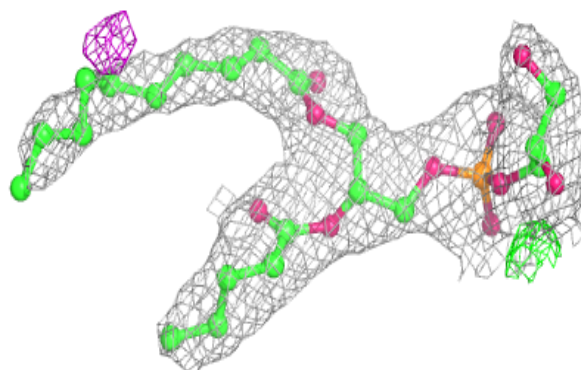


**Electron density around LHG G 851:**

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

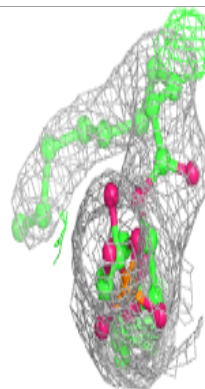
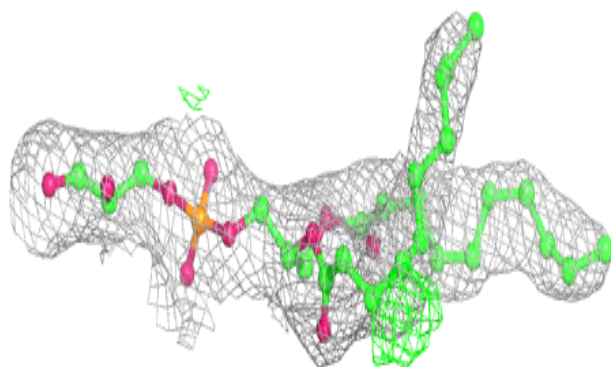
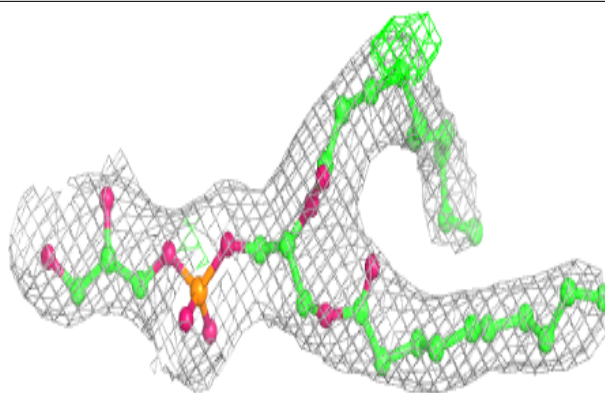
**Electron density around LHG G 852:**

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

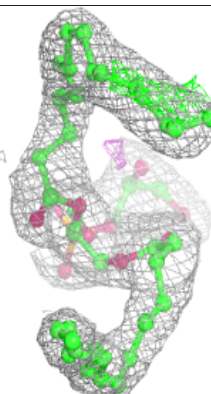
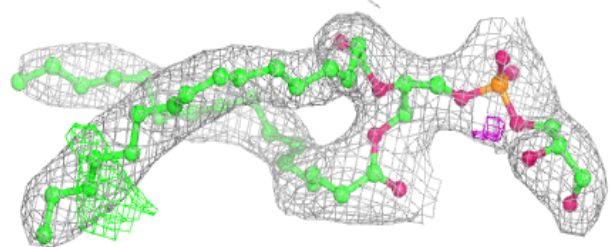
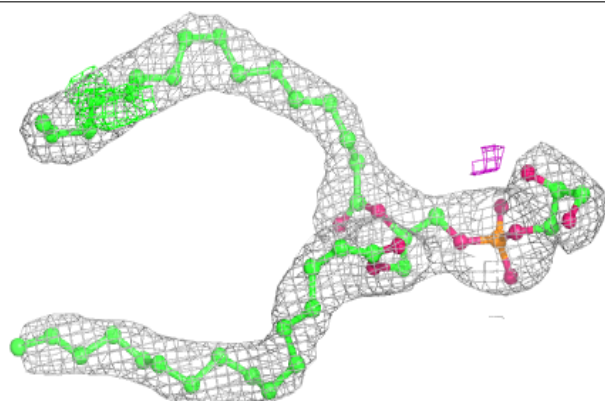


**Electron density around LHG H 847:**

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

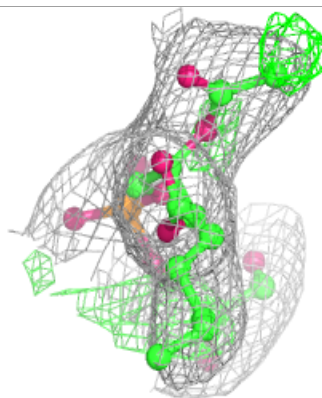
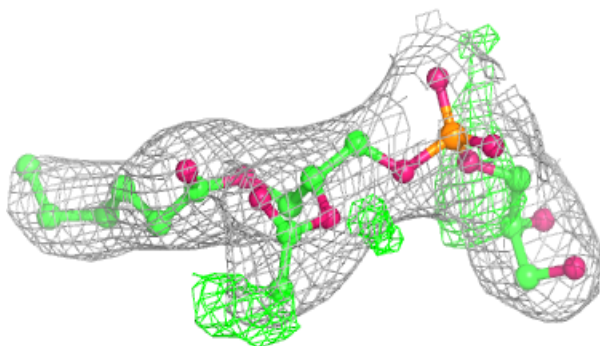
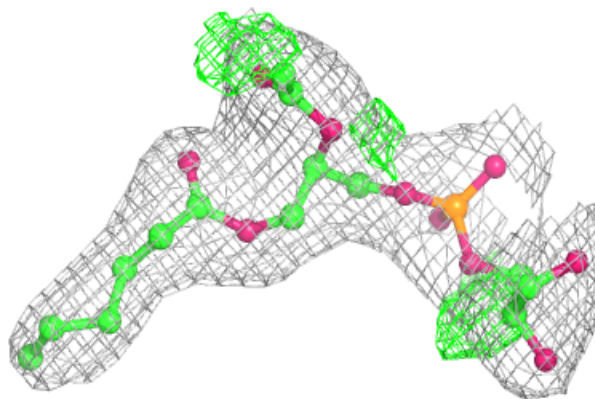
**Electron density around LHG Y 852:**

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

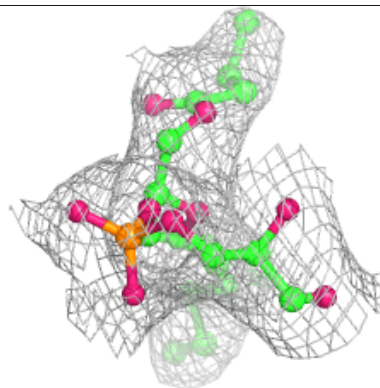
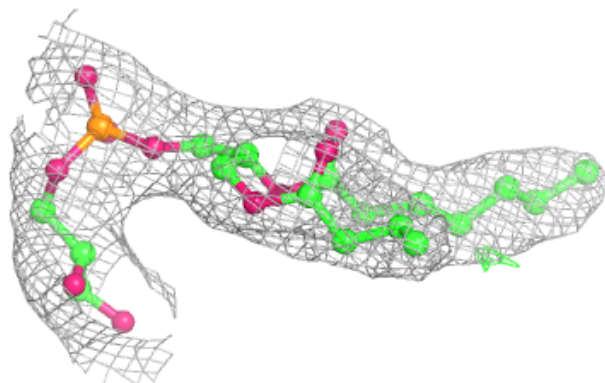
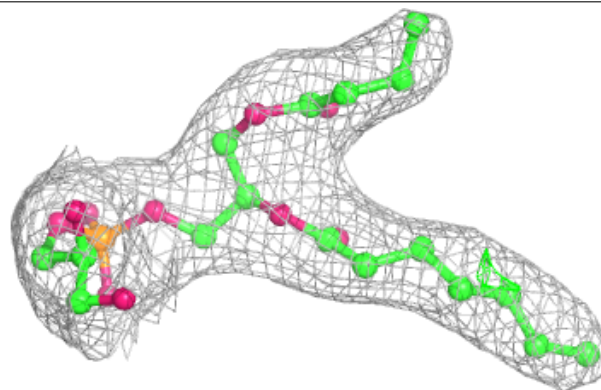


**Electron density around LHG Y 853:**

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

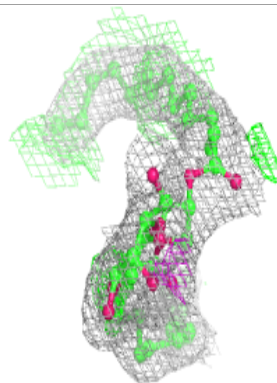
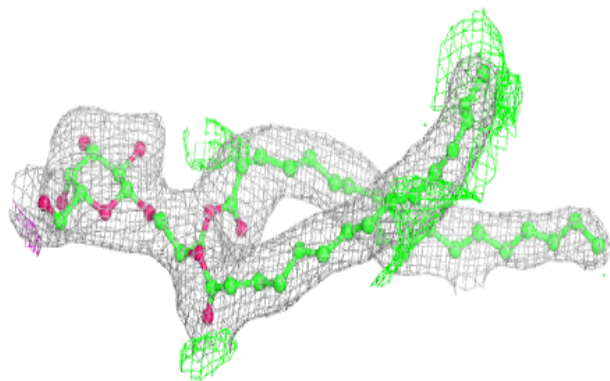
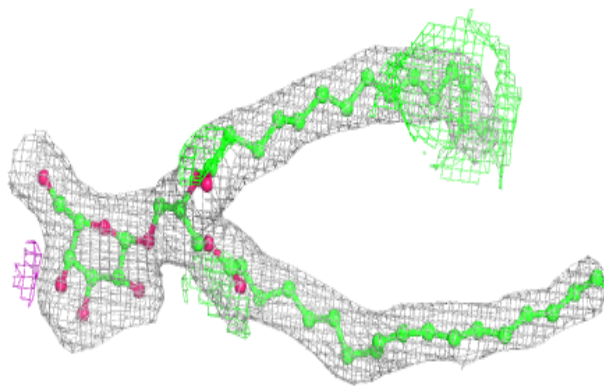
**Electron density around LHG j 101:**

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

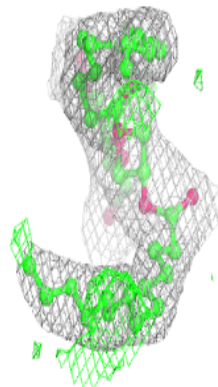
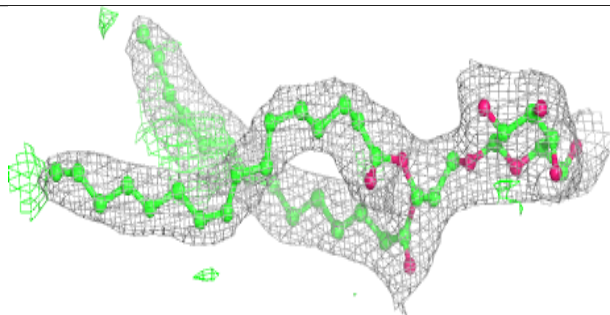
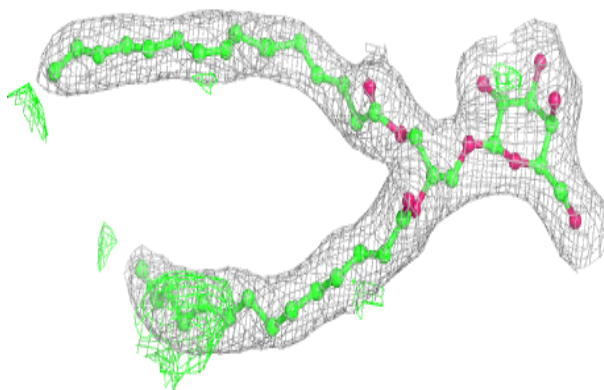


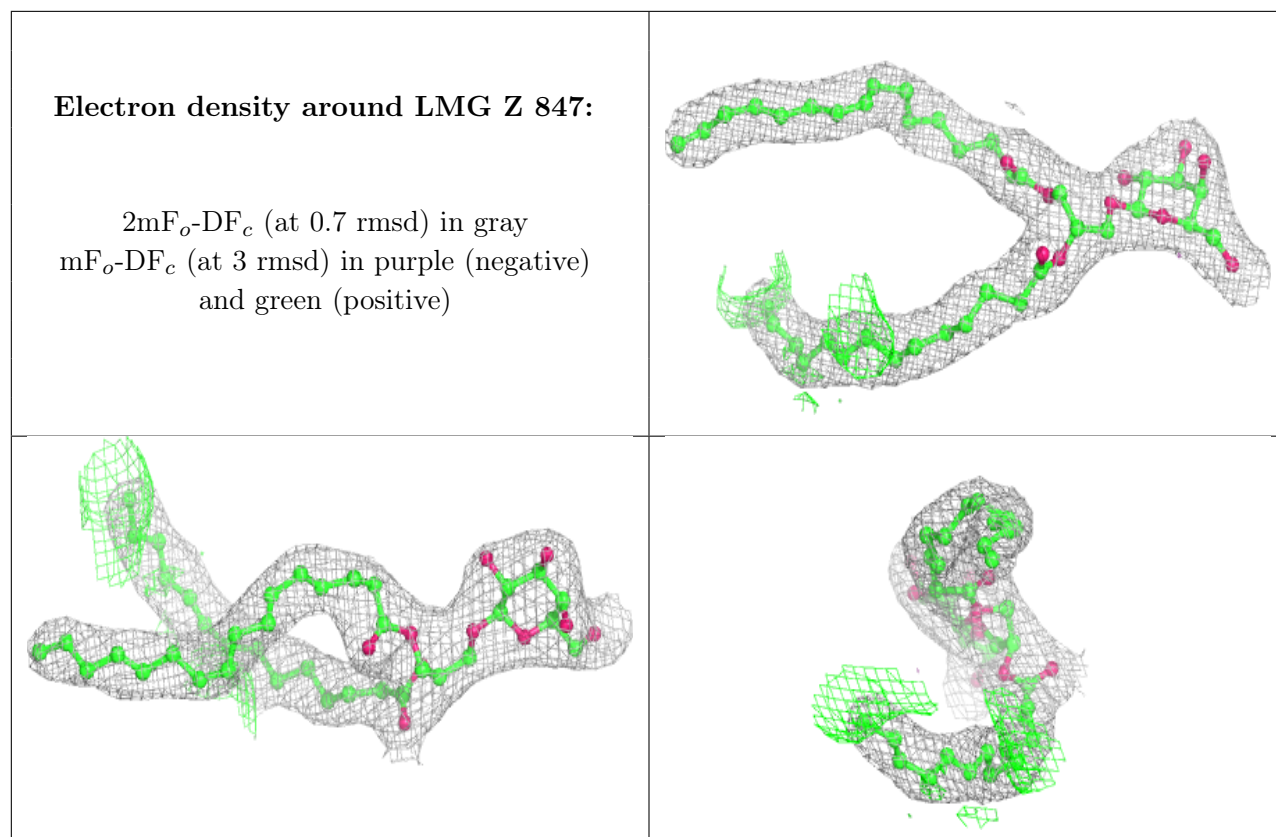
**Electron density around LMG B 849:**

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

**Electron density around LMG H 846:**

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





## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.