



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2023 – 10:03 AM EDT

PDB ID : 3PCQ  
Title : Femtosecond X-ray protein Nanocrystallography  
Authors : Chapman, H.N.; Fromme, P.; Barty, A.; White, T.A.; Kirian, R.A.; Aquila, A.; Hunter, M.S.; Schulz, J.; Deponte, D.P.; Weierstall, U.; Doak, R.B.; Maia, F.R.N.C.; Martin, A.V.; Schlichting, I.; Lomb, L.; Coppola, N.; Shoeman, R.L.; Epp, S.W.; Hartmann, R.; Rolles, D.; Rudenko, A.; Foucar, L.; Kimmel, N.; Weidenspointner, G.; Holl, P.; Liang, M.; Barthelmess, M.; Caleman, C.; Boutet, S.; Bogan, M.J.; Krzywinski, J.; Bostedt, C.; Bajt, S.; Gumprecht, L.; Rudek, B.; Erk, B.; Schmidt, C.; Homke, A.; Reich, C.; Pietschner, D.; Struder, L.; Hauser, G.; Gorke, H.; Ullrich, J.; Herrmann, S.; Schaller, G.; Schopper, F.; Soltau, H.; Kuhnel, K.-U.; Messerschmidt, M.; Bozek, J.D.; Hau-Riege, S.P.; Frank, M.; Hampton, C.Y.; Sierra, R.; Starodub, D.; Williams, G.J.; Hajdu, J.; Timneanu, N.; Seibert, M.M.; Andreasson, J.; Rocker, A.; Jonsson, O.; Svenda, M.; Stern, S.; Nass, K.; Andritschke, R.; Schroter, C.-D.; Krasniqi, F.; Bott, M.; Schmidt, K.E.; Wang, X.; Grotjohann, I.; Holton, J.M.; Barends, T.R.M.; Neutze, R.; Marchesini, S.; Fromme, R.; Schorb, S.; Rupp, D.; Adolph, M.; Gorkhover, T.; Andersson, I.; Hirsemann, H.; Potdevin, G.; Graafsma, H.; Nilsson, B.; Spence, J.C.H.  
Deposited on : 2010-10-21  
Resolution : 8.98 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>.

---

The following versions of software and data (see [references](#) ①) 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

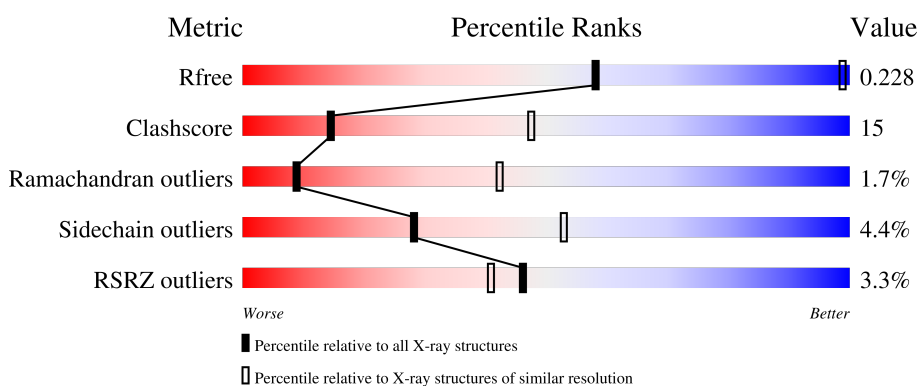
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 8.98 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.






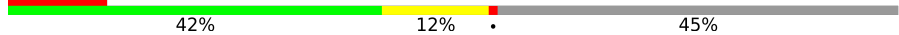



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1005 (11.50-3.90)
Clashscore	141614	1070 (11.50-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	755	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2%      71%      24%      • •</p>
2	B	740	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 26%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="text-align: center;">3%      71%      26%      •</p>
3	C	80	<div style="display: flex; align-items: center;"> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> </div> <p style="text-align: center;">74%      25%      •</p>
4	D	138	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 68%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 28%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="text-align: center;">5%      68%      28%      •</p>
5	E	75	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">8%      71%      17%      • 8%</p>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	164	
7	I	38	
8	J	41	
9	K	83	
10	L	154	
11	M	31	
12	X	35	

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	CLA	A	801	X	-	-	-
13	CLA	A	802	X	-	-	-
13	CLA	A	803	X	-	-	-
13	CLA	A	804	X	-	-	-
13	CLA	A	805	X	-	-	-
13	CLA	A	806	X	-	-	-
13	CLA	A	807	X	-	-	-
13	CLA	A	808	X	-	-	-
13	CLA	A	809	X	-	-	-
13	CLA	A	810	X	-	-	-
13	CLA	A	812	X	-	-	-
13	CLA	A	813	X	-	-	-
13	CLA	A	814	X	-	-	-
13	CLA	A	815	X	-	-	-
13	CLA	A	816	X	-	-	X
13	CLA	A	817	X	-	-	-
13	CLA	A	819	X	-	-	-
13	CLA	A	820	X	-	-	-
13	CLA	A	821	X	-	-	-
13	CLA	A	822	X	-	-	X
13	CLA	A	823	X	-	-	X
13	CLA	A	824	X	-	-	X
13	CLA	A	825	X	-	-	-
13	CLA	A	826	X	-	-	-
13	CLA	A	827	X	-	-	X

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	828	X	-	-	-
13	CLA	A	829	X	-	-	-
13	CLA	A	830	X	-	-	-
13	CLA	A	831	X	-	-	-
13	CLA	A	832	X	-	-	-
13	CLA	A	833	X	-	-	-
13	CLA	A	835	X	-	-	-
13	CLA	A	836	X	-	-	-
13	CLA	A	837	X	-	-	-
13	CLA	A	838	X	-	-	-
13	CLA	A	839	X	-	-	-
13	CLA	A	840	X	-	-	-
13	CLA	A	841	X	-	-	-
13	CLA	A	842	X	-	-	-
13	CLA	A	843	X	-	-	-
13	CLA	A	844	X	-	-	X
13	CLA	A	845	X	-	-	X
13	CLA	A	846	X	-	-	-
13	CLA	B	801	X	-	-	-
13	CLA	B	802	X	-	-	-
13	CLA	B	804	X	-	-	-
13	CLA	B	805	X	-	-	-
13	CLA	B	806	X	-	-	-
13	CLA	B	807	X	-	-	-
13	CLA	B	808	X	-	-	-
13	CLA	B	809	X	-	-	-
13	CLA	B	810	X	-	-	-
13	CLA	B	811	X	-	-	-
13	CLA	B	812	X	-	-	X
13	CLA	B	813	X	-	-	-
13	CLA	B	814	X	-	-	-
13	CLA	B	815	-	-	-	X
13	CLA	B	816	X	-	-	X
13	CLA	B	817	X	-	-	-
13	CLA	B	818	X	-	-	-
13	CLA	B	819	X	-	-	-
13	CLA	B	820	X	-	-	X
13	CLA	B	821	X	-	-	X
13	CLA	B	822	X	-	-	-
13	CLA	B	823	X	-	-	-
13	CLA	B	824	X	-	-	-
13	CLA	B	825	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	B	826	X	-	-	-
13	CLA	B	827	X	-	-	-
13	CLA	B	829	X	-	-	-
13	CLA	B	830	X	-	-	-
13	CLA	B	831	X	-	-	-
13	CLA	B	832	X	-	-	-
13	CLA	B	833	X	-	-	X
13	CLA	B	834	X	-	-	-
13	CLA	B	835	X	-	-	-
13	CLA	B	836	X	-	-	-
13	CLA	B	837	X	-	-	-
13	CLA	B	838	X	-	-	-
13	CLA	B	840	X	-	-	X
13	CLA	F	1301	X	-	-	-
13	CLA	J	101	X	-	-	X
13	CLA	J	102	X	-	-	X
13	CLA	K	1401	-	-	-	X
13	CLA	L	1002	X	-	-	-
13	CLA	L	1004	X	-	-	-
13	CLA	M	1601	X	-	-	X
13	CLA	X	1701	X	-	-	-
16	BCR	A	850	-	-	-	X
16	BCR	A	851	-	-	-	X
16	BCR	A	852	-	-	-	X
16	BCR	A	853	-	-	-	X
16	BCR	B	843	-	-	-	X
16	BCR	B	844	-	-	-	X
16	BCR	B	845	-	-	-	X
16	BCR	J	105	-	-	-	X
17	LHG	A	855	-	-	-	X
17	LHG	A	856	X	-	-	-
18	LMG	B	850	-	-	-	X

## 2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 24196 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	740	5784	3794	988	976	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	5879	3867	986	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

- 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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	K	46	222	130	46	46	0	0	0

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

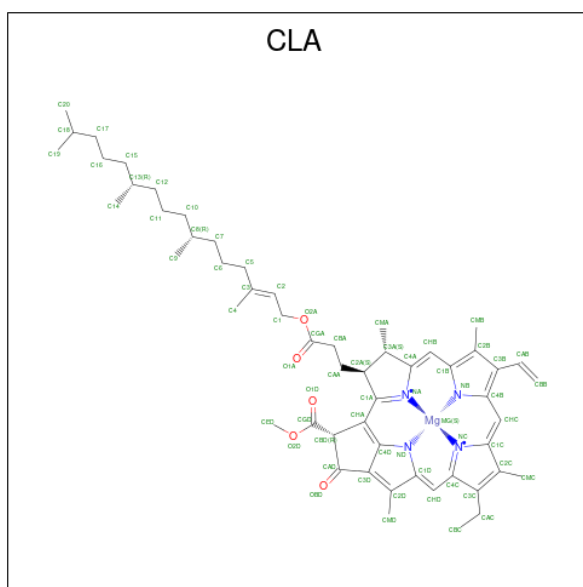
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	M	31	241	161	36	43	1	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	X	29	232	163	34	35	0	0	0

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).





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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
13	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

*Continued on next page...*

*Continued from previous page...*

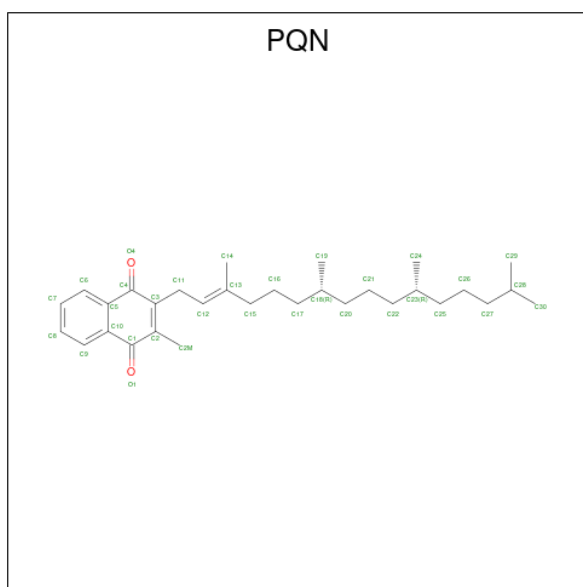
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

*Continued on next page...*

*Continued from previous page...*

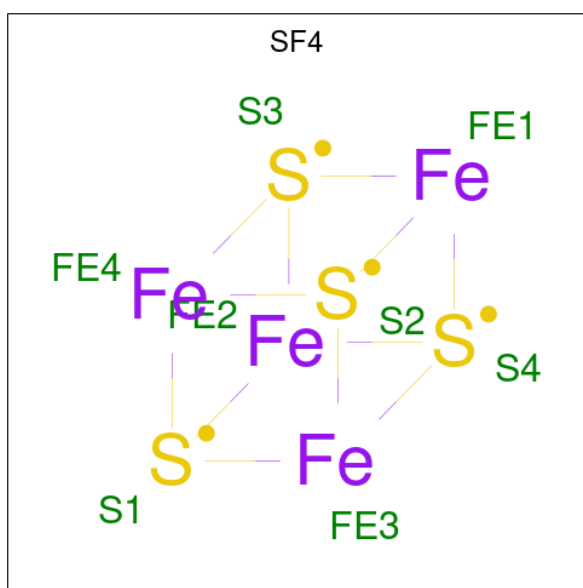
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	J	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	J	1	Total	C	Mg	N	O	0	0
			37	31	1	4	1		
13	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	M	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	X	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

- Molecule 14 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



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

- Molecule 15 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



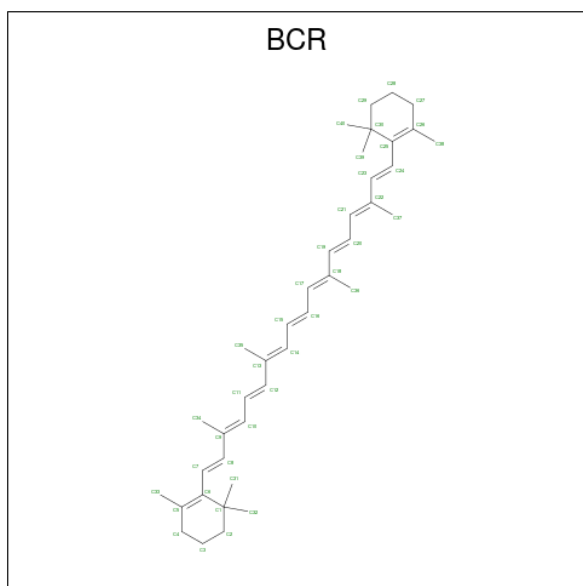
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Fe S	0	0
			8	4 4		
15	C	1	Total	Fe S	0	0
			8	4 4		

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 16 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



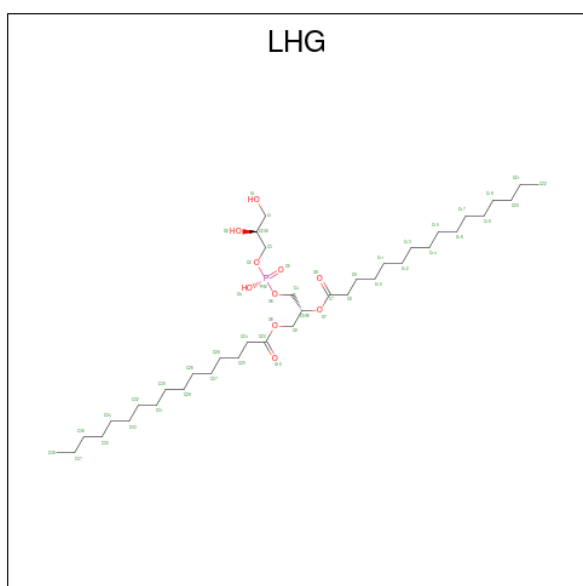
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	C	0	0
			40	40		
16	A	1	Total	C	0	0
			40	40		
16	A	1	Total	C	0	0
			40	40		
16	A	1	Total	C	0	0
			40	40		
16	A	1	Total	C	0	0
			40	40		
16	A	1	Total	C	0	0
			40	40		
16	B	1	Total	C	0	0
			40	40		
16	B	1	Total	C	0	0
			40	40		
16	B	1	Total	C	0	0
			40	40		
16	B	1	Total	C	0	0
			25	25		

*Continued on next page...*

Continued from previous page...

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

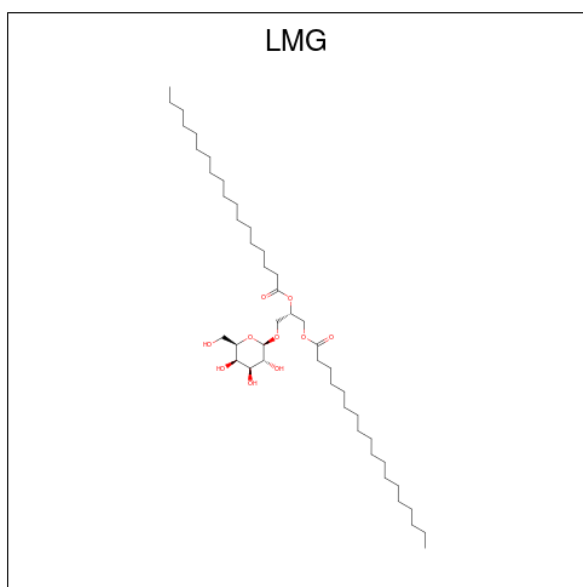
- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
17	A	1	Total	C	O	P	0	0
			49	38	10	1		
17	A	1	Total	C	O	P	0	0
			27	16	10	1		
17	B	1	Total	C	O	P	0	0
			23	12	10	1		

- Molecule 18 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	
18	B	1	Total	C	O		0	0
			55	45	10			

- Molecule 19 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	L	1	Total	Ca	0	0
			1	1		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	53	Total	O	0	0
			53	53		
20	B	65	Total	O	0	0
			65	65		

*Continued on next page...*

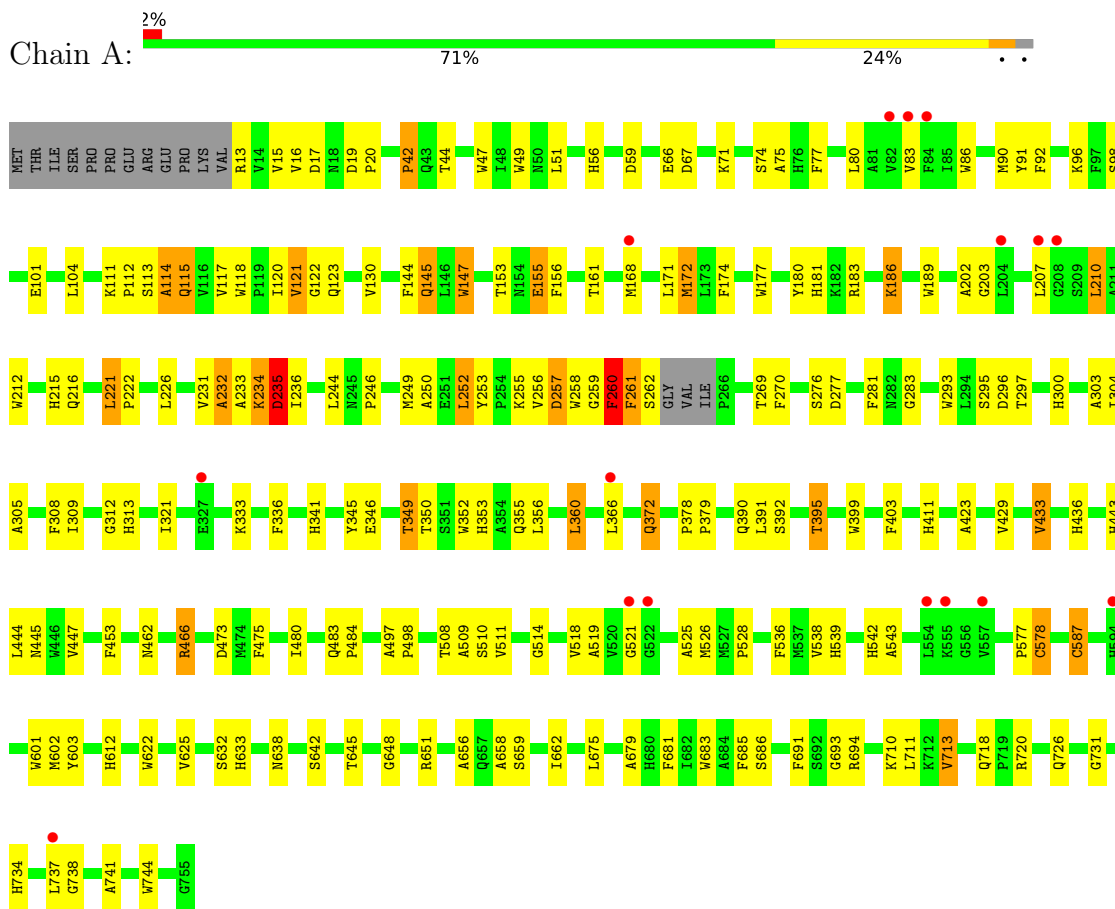
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
20	C	21	Total 21	O 21	0	0
20	D	17	Total 17	O 17	0	0
20	E	5	Total 5	O 5	0	0
20	F	6	Total 6	O 6	0	0
20	I	3	Total 3	O 3	0	0
20	J	1	Total 1	O 1	0	0
20	L	27	Total 27	O 27	0	0
20	M	2	Total 2	O 2	0	0

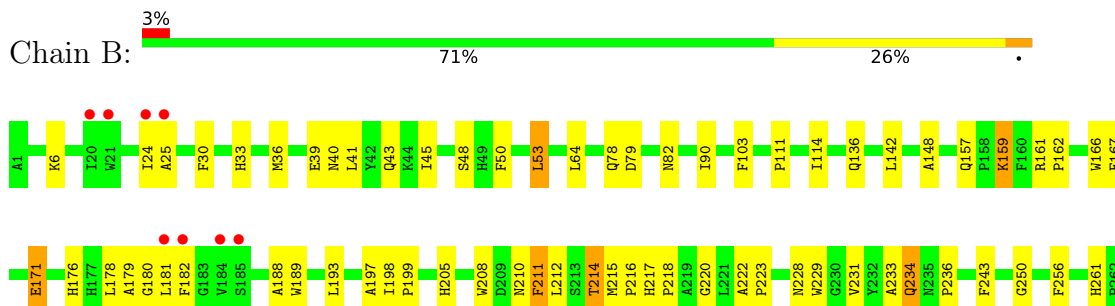
### 3 Residue-property plots [i](#)

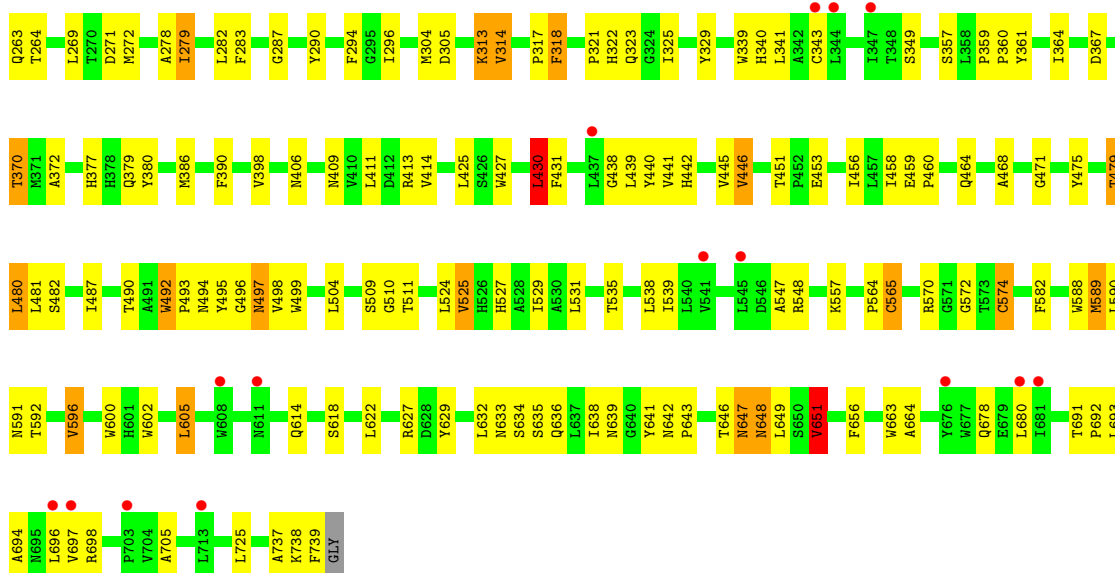
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



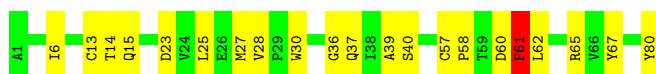
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





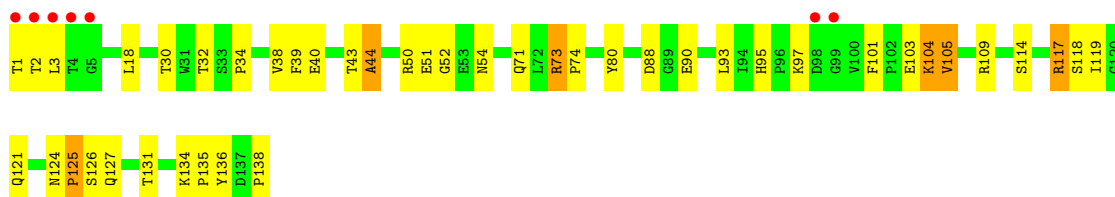
- Molecule 3: Photosystem I iron-sulfur center

Chain C: 74% 25%



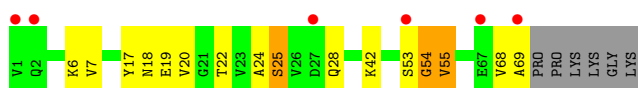
- Molecule 4: Photosystem I reaction center subunit II

Chain D: 5% 68% 28%



- Molecule 5: Photosystem I reaction center subunit IV

Chain E: 8% 71% 17% 8%



- Molecule 6: Photosystem I reaction center subunit III

Chain F: 57% 28% 14%





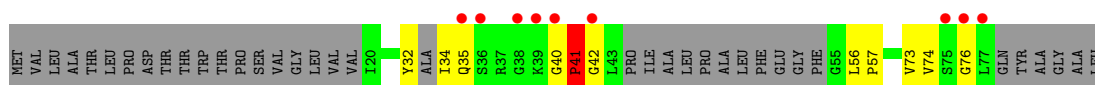
- Molecule 7: Photosystem I reaction center subunit VIII



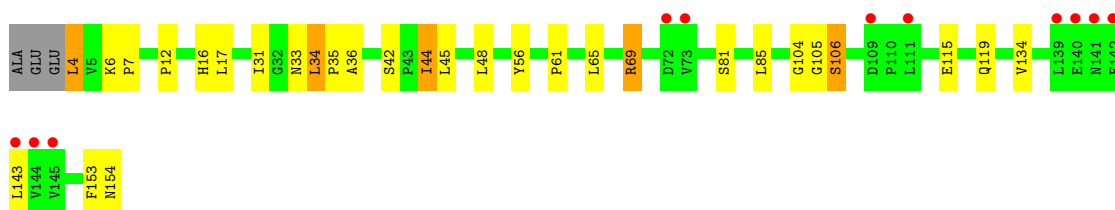
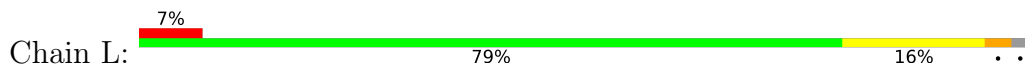
- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 9: Photosystem I reaction center subunit PsaK



- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 12: Photosystem I 4.8K protein



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	281.00Å 281.00Å 165.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	81.12 – 8.98 81.12 – 9.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (81.12-8.98) 99.1 (81.12-9.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.89 (at 8.41Å)	Xtrriage
Refinement program	REFMAC 5.6.0076	Depositor
R, $R_{free}$	0.252 , 0.232 0.246 , 0.228	Depositor DCC
$R_{free}$ test set	187 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	203.6	Xtrriage
Anisotropy	0.356	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 73.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.16$ , $\langle L^2 \rangle = 0.04$	Xtrriage
Estimated twinning fraction	0.499 for h,-h-k,-l	Xtrriage
Reported twinning fraction	0.500 for H, K, L 0.500 for K, H, -L	Depositor
Outliers	0 of 5591 reflections	Xtrriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	24196	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.40% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, BCR, CLA, SF4, LMG, CA, 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	0.51	0/5983	0.66	2/8158 (0.0%)
2	B	0.56	0/6096	0.67	2/8332 (0.0%)
3	C	0.74	0/608	0.96	4/824 (0.5%)
4	D	0.57	0/1101	0.81	1/1492 (0.1%)
5	E	0.57	0/551	0.84	2/750 (0.3%)
6	F	0.47	0/1087	0.66	0/1476
7	I	0.67	0/312	0.75	0/425
8	J	0.45	0/350	0.65	0/477
9	K	0.52	0/219	0.86	3/297 (1.0%)
10	L	0.67	0/1148	0.75	0/1558
11	M	0.63	0/244	0.85	1/332 (0.3%)
12	X	0.54	0/241	0.67	0/330
All	All	0.55	0/17940	0.70	15/24451 (0.1%)

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
3	C	0	1

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	80	TYR	CA-C-O	9.93	140.96	120.10
11	M	30	TYR	N-CA-C	7.84	132.17	111.00
4	D	131	THR	N-CA-C	-7.83	89.86	111.00
5	E	54	GLY	N-CA-C	7.51	131.88	113.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed( <sup>o</sup> )	Ideal( <sup>o</sup> )
1	A	521	GLY	N-CA-C	-6.42	97.05	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	61	PHE	Sidechain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5784	0	5639	214	0
2	B	5879	0	5632	238	0
3	C	598	0	580	16	0
4	D	1075	0	1077	39	0
5	E	539	0	528	10	1
6	F	1065	0	1079	41	1
7	I	301	0	306	7	0
8	J	338	0	347	23	0
9	K	222	0	110	4	0
10	L	1119	0	1125	22	2
11	M	241	0	264	13	0
12	X	232	0	220	6	0
13	A	2687	0	2675	139	0
13	B	2349	0	2304	151	0
13	F	45	0	33	1	0
13	J	82	0	58	1	0
13	K	45	0	33	1	0
13	L	195	0	216	11	0
13	M	45	0	33	1	0
13	X	45	0	33	1	0
14	A	33	0	46	1	0
14	B	33	0	46	1	0
15	A	8	0	0	0	0
15	C	16	0	0	0	0
16	A	240	0	336	22	0

*Continued on next page...*



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	B	265	0	369	17	0
16	F	40	0	56	2	0
16	I	80	0	112	3	0
16	J	120	0	168	16	0
16	L	80	0	112	1	0
16	M	40	0	56	2	0
17	A	76	0	98	6	0
17	B	23	0	16	1	0
18	B	55	0	86	5	0
19	L	1	0	0	0	1
20	A	53	0	0	5	1
20	B	65	0	0	3	0
20	C	21	0	0	3	0
20	D	17	0	0	1	0
20	E	5	0	0	0	0
20	F	6	0	0	1	0
20	I	3	0	0	0	0
20	J	1	0	0	0	0
20	L	27	0	0	1	2
20	M	2	0	0	1	0
All	All	24196	0	23793	736	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 736 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:31:ARG:HD3	16:J:104:BCR:H312	1.26	1.17
2:B:622:LEU:HD12	13:B:802:CLA:H11	1.28	1.15
1:A:508:THR:HG22	1:A:510:SER:H	1.18	1.07
2:B:159:LYS:H	2:B:159:LYS:HD2	1.18	1.04
4:D:50:ARG:H	4:D:54:ASN:HD21	1.06	1.01

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:1126:HOH:O	20:L:1126:HOH:O[2_655]	1.08	1.12
10:L:153:PHE:O	19:L:1001:CA:CA[3_665]	1.57	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:28:GLN:OE1	6:F:1:ASP:N[4_664]	2.00	0.20
10:L:154:ASN:OXT	20:A:950:HOH:O[3_665]	2.07	0.13
20:L:1108:HOH:O	20:L:1117:HOH:O[2_655]	2.07	0.13

## 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	736/755 (98%)	695 (94%)	31 (4%)	10 (1%)	11	46
2	B	737/740 (100%)	691 (94%)	37 (5%)	9 (1%)	13	50
3	C	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	12	48
4	D	136/138 (99%)	125 (92%)	8 (6%)	3 (2%)	6	35
5	E	67/75 (89%)	59 (88%)	4 (6%)	4 (6%)	1	17
6	F	139/164 (85%)	128 (92%)	8 (6%)	3 (2%)	6	35
7	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	K	40/83 (48%)	32 (80%)	5 (12%)	3 (8%)	1	13
10	L	149/154 (97%)	140 (94%)	7 (5%)	2 (1%)	12	48
11	M	29/31 (94%)	28 (97%)	0	1 (3%)	3	26
12	X	27/35 (77%)	22 (82%)	4 (15%)	1 (4%)	3	24
All	All	2213/2334 (95%)	2065 (93%)	111 (5%)	37 (2%)	9	42

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	235	ASP
1	A	260	PHE
1	A	261	PHE

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	234	GLN

### 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	589/603 (98%)	565 (96%)	24 (4%)	30	55
2	B	595/597 (100%)	567 (95%)	28 (5%)	26	51
3	C	67/67 (100%)	66 (98%)	1 (2%)	65	80
4	D	115/115 (100%)	107 (93%)	8 (7%)	15	40
5	E	59/64 (92%)	59 (100%)	0	100	100
6	F	109/128 (85%)	107 (98%)	2 (2%)	59	77
7	I	32/32 (100%)	30 (94%)	2 (6%)	18	43
8	J	36/36 (100%)	34 (94%)	2 (6%)	21	46
10	L	117/119 (98%)	109 (93%)	8 (7%)	16	41
11	M	26/26 (100%)	25 (96%)	1 (4%)	33	57
12	X	20/27 (74%)	18 (90%)	2 (10%)	7	26
All	All	1765/1814 (97%)	1687 (96%)	78 (4%)	28	53

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	105	VAL
10	L	48	LEU
4	D	125	PRO
8	J	1	MET
11	M	17	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	688	HIS
6	F	95	ASN
3	C	37	GLN
4	D	95	HIS
1	A	718	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

Of 128 ligands modelled in this entry, 1 is monoatomic - leaving 127 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$
13	CLA	A	845	-	42,49,73	1.66	9 (21%)	48,83,113	2.00	7 (14%)
13	CLA	A	819	-	54,62,73	1.57	10 (18%)	62,99,113	1.90	12 (19%)
16	BCR	A	854	-	41,41,41	1.38	6 (14%)	56,56,56	2.03	19 (33%)
13	CLA	A	829	-	65,73,73	1.28	7 (10%)	76,113,113	1.67	11 (14%)
13	CLA	B	813	-	65,73,73	1.43	7 (10%)	76,113,113	1.69	11 (14%)
13	CLA	A	826	20	65,73,73	1.42	7 (10%)	76,113,113	1.71	12 (15%)
13	CLA	A	830	-	65,73,73	1.42	7 (10%)	76,113,113	1.73	7 (9%)
13	CLA	B	839	-	47,55,73	1.56	8 (17%)	54,91,113	1.84	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	CLA	B	826	-	65,73,73	1.44	7 (10%)	76,113,113	1.81	11 (14%)
13	CLA	A	824	-	51,59,73	1.57	9 (17%)	59,96,113	1.95	10 (16%)
15	SF4	A	848	2,1	0,12,12	-	-	-	-	-
13	CLA	A	827	20	65,73,73	1.24	7 (10%)	76,113,113	1.76	9 (11%)
16	BCR	B	844	-	41,41,41	1.56	7 (17%)	56,56,56	2.10	19 (33%)
13	CLA	A	817	20	49,57,73	1.48	8 (16%)	55,93,113	2.06	9 (16%)
13	CLA	B	829	-	65,73,73	1.41	9 (13%)	76,113,113	1.79	12 (15%)
13	CLA	B	805	-	65,73,73	1.33	7 (10%)	76,113,113	1.70	10 (13%)
13	CLA	A	838	-	51,59,73	1.35	4 (7%)	59,96,113	2.07	13 (22%)
13	CLA	M	1601	20	45,53,73	1.59	7 (15%)	52,89,113	2.19	8 (15%)
13	CLA	A	833	-	65,73,73	1.22	6 (9%)	76,113,113	1.89	10 (13%)
13	CLA	A	809	1	65,73,73	1.35	7 (10%)	76,113,113	1.80	10 (13%)
13	CLA	A	837	1	45,53,73	1.52	8 (17%)	52,89,113	2.13	9 (17%)
13	CLA	A	805	13	59,67,73	1.40	7 (11%)	68,105,113	1.88	12 (17%)
16	BCR	J	103	-	41,41,41	1.29	5 (12%)	56,56,56	1.90	16 (28%)
13	CLA	L	1002	10	65,73,73	1.51	9 (13%)	76,113,113	1.76	10 (13%)
13	CLA	B	806	-	65,73,73	1.29	6 (9%)	76,113,113	1.65	10 (13%)
13	CLA	A	807	-	65,73,73	1.39	8 (12%)	76,113,113	1.90	14 (18%)
16	BCR	A	849	-	41,41,41	1.36	5 (12%)	56,56,56	1.88	16 (28%)
13	CLA	B	822	20	55,63,73	1.46	7 (12%)	64,101,113	1.96	10 (15%)
13	CLA	B	801	-	65,73,73	1.39	6 (9%)	76,113,113	1.71	10 (13%)
16	BCR	I	101	-	41,41,41	1.31	7 (17%)	56,56,56	1.79	15 (26%)
13	CLA	J	101	8	45,53,73	1.65	7 (15%)	52,89,113	2.14	10 (19%)
14	PQN	A	847	-	34,34,34	3.54	17 (50%)	42,45,45	2.21	3 (7%)
13	CLA	A	828	-	65,73,73	1.39	6 (9%)	76,113,113	1.78	11 (14%)
15	SF4	C	101	3	0,12,12	-	-	-	-	-
13	CLA	J	102	-	38,45,73	1.78	7 (18%)	43,78,113	2.15	8 (18%)
13	CLA	B	835	20	45,53,73	1.70	8 (17%)	52,89,113	1.98	11 (21%)
13	CLA	B	816	-	55,63,73	1.57	10 (18%)	64,101,113	1.85	9 (14%)
13	CLA	A	802	20	65,73,73	1.40	10 (15%)	76,113,113	1.63	8 (10%)
13	CLA	A	811	-	45,53,73	1.59	7 (15%)	52,89,113	1.98	10 (19%)
13	CLA	B	825	20	46,54,73	1.43	8 (17%)	53,90,113	2.14	13 (24%)
17	LHG	A	856	13	26,26,48	2.32	5 (19%)	29,32,54	1.58	5 (17%)
13	CLA	A	801	-	65,73,73	1.41	8 (12%)	76,113,113	2.04	17 (22%)
13	CLA	A	841	-	65,73,73	1.35	7 (10%)	76,113,113	1.76	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	BCR	B	846	-	25,25,41	1.36	4 (16%)	33,33,56	1.85	11 (33%)
13	CLA	B	831	-	49,57,73	1.52	8 (16%)	55,93,113	1.99	7 (12%)
13	CLA	A	818	-	54,62,73	1.57	10 (18%)	62,99,113	1.83	9 (14%)
16	BCR	B	847	-	41,41,41	1.24	5 (12%)	56,56,56	1.88	19 (33%)
13	CLA	A	835	-	65,73,73	1.37	9 (13%)	76,113,113	1.70	11 (14%)
13	CLA	B	804	-	54,62,73	1.46	8 (14%)	62,99,113	2.03	12 (19%)
13	CLA	B	802	20	65,73,73	1.45	6 (9%)	76,113,113	1.72	12 (15%)
13	CLA	X	1701	12	45,53,73	1.61	5 (11%)	52,89,113	2.13	9 (17%)
18	LMG	B	850	-	55,55,55	0.87	2 (3%)	63,63,63	1.30	3 (4%)
13	CLA	B	814	-	65,73,73	1.34	8 (12%)	76,113,113	1.80	12 (15%)
13	CLA	L	1004	20	65,73,73	1.43	7 (10%)	76,113,113	1.69	8 (10%)
13	CLA	B	827	-	65,73,73	1.54	10 (15%)	76,113,113	1.83	14 (18%)
13	CLA	A	808	-	51,59,73	1.61	10 (19%)	59,96,113	1.98	10 (16%)
13	CLA	A	823	-	49,57,73	1.47	6 (12%)	55,93,113	2.12	12 (21%)
13	CLA	B	821	-	45,53,73	1.62	8 (17%)	52,89,113	2.19	12 (23%)
13	CLA	A	806	-	65,73,73	1.19	4 (6%)	76,113,113	1.82	15 (19%)
16	BCR	M	1602	-	41,41,41	1.33	6 (14%)	56,56,56	1.78	14 (25%)
13	CLA	A	846	17	52,60,73	1.62	10 (19%)	60,97,113	2.14	12 (20%)
13	CLA	A	836	-	54,62,73	1.41	10 (18%)	62,99,113	1.99	11 (17%)
13	CLA	A	834	-	65,73,73	1.20	5 (7%)	76,113,113	1.69	13 (17%)
13	CLA	B	815	-	45,53,73	1.58	8 (17%)	52,89,113	2.03	9 (17%)
13	CLA	A	820	-	65,73,73	1.39	12 (18%)	76,113,113	1.90	14 (18%)
13	CLA	A	822	20	65,73,73	1.33	8 (12%)	76,113,113	1.84	12 (15%)
13	CLA	B	809	2	65,73,73	1.36	6 (9%)	76,113,113	1.71	10 (13%)
13	CLA	B	837	-	60,68,73	1.48	8 (13%)	70,107,113	1.75	11 (15%)
13	CLA	B	840	20	65,73,73	1.31	8 (12%)	76,113,113	1.66	12 (15%)
13	CLA	A	816	-	45,53,73	1.51	6 (13%)	52,89,113	2.22	14 (26%)
13	CLA	A	821	-	61,69,73	1.46	9 (14%)	71,108,113	1.95	11 (15%)
16	BCR	F	1302	-	41,41,41	1.28	4 (9%)	56,56,56	1.81	17 (30%)
16	BCR	A	853	-	41,41,41	1.28	8 (19%)	56,56,56	1.90	18 (32%)
13	CLA	A	812	13	65,73,73	1.30	8 (12%)	76,113,113	1.79	10 (13%)
16	BCR	J	104	-	41,41,41	1.27	4 (9%)	56,56,56	1.83	19 (33%)
16	BCR	I	102	-	41,41,41	1.28	6 (14%)	56,56,56	1.82	17 (30%)
13	CLA	K	1401	-	45,53,73	1.61	8 (17%)	52,89,113	1.96	7 (13%)
16	BCR	A	851	-	41,41,41	1.41	6 (14%)	56,56,56	1.94	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	CLA	A	844	20	65,73,73	1.34	10 (15%)	76,113,113	1.68	11 (14%)
13	CLA	F	1301	20	45,53,73	1.66	7 (15%)	52,89,113	2.04	7 (13%)
13	CLA	B	828	-	65,73,73	1.54	13 (20%)	76,113,113	1.70	12 (15%)
13	CLA	A	813	-	54,62,73	1.47	9 (16%)	62,99,113	2.02	11 (17%)
13	CLA	B	803	-	65,73,73	1.50	9 (13%)	76,113,113	1.64	7 (9%)
13	CLA	A	839	-	65,73,73	1.37	8 (12%)	76,113,113	1.64	8 (10%)
16	BCR	L	1006	-	41,41,41	1.60	8 (19%)	56,56,56	1.72	12 (21%)
13	CLA	A	810	1	65,73,73	1.38	8 (12%)	76,113,113	1.83	13 (17%)
13	CLA	B	819	20	65,73,73	1.36	7 (10%)	76,113,113	1.74	11 (14%)
13	CLA	A	842	20	51,59,73	1.48	8 (15%)	59,96,113	1.92	10 (16%)
13	CLA	A	832	-	50,58,73	1.53	7 (14%)	58,95,113	2.07	12 (20%)
13	CLA	B	811	-	45,53,73	1.54	8 (17%)	52,89,113	2.02	10 (19%)
16	BCR	B	843	-	41,41,41	1.51	5 (12%)	56,56,56	2.02	16 (28%)
17	LHG	A	855	-	48,48,48	1.76	5 (10%)	51,54,54	1.30	3 (5%)
13	CLA	B	830	-	45,53,73	1.55	8 (17%)	52,89,113	2.15	11 (21%)
13	CLA	B	838	-	65,73,73	1.32	9 (13%)	76,113,113	1.80	12 (15%)
13	CLA	B	824	2	54,62,73	1.74	12 (22%)	62,99,113	1.92	10 (16%)
13	CLA	B	818	-	60,68,73	1.43	8 (13%)	70,107,113	1.97	11 (15%)
13	CLA	B	817	-	59,67,73	1.44	8 (13%)	68,105,113	1.84	12 (17%)
13	CLA	B	820	-	47,55,73	1.53	7 (14%)	54,91,113	2.23	11 (20%)
16	BCR	A	850	-	41,41,41	1.27	4 (9%)	56,56,56	1.77	17 (30%)
13	CLA	L	1003	-	65,73,73	1.43	9 (13%)	76,113,113	1.76	11 (14%)
13	CLA	B	834	-	45,53,73	1.57	9 (20%)	52,89,113	2.05	11 (21%)
14	PQN	B	842	-	34,34,34	3.47	16 (47%)	42,45,45	2.10	4 (9%)
13	CLA	A	803	-	65,73,73	1.36	9 (13%)	76,113,113	1.78	14 (18%)
16	BCR	B	848	-	41,41,41	1.24	5 (12%)	56,56,56	1.99	20 (35%)
16	BCR	B	849	-	41,41,41	1.28	4 (9%)	56,56,56	1.74	17 (30%)
13	CLA	B	836	20	45,53,73	1.52	5 (11%)	52,89,113	2.07	10 (19%)
13	CLA	B	823	-	45,53,73	1.57	5 (11%)	52,89,113	2.00	9 (17%)
16	BCR	B	845	-	41,41,41	1.26	5 (12%)	56,56,56	2.01	20 (35%)
16	BCR	J	105	-	41,41,41	1.41	5 (12%)	56,56,56	1.88	13 (23%)
13	CLA	A	840	-	47,55,73	1.65	7 (14%)	54,91,113	1.92	9 (16%)
13	CLA	A	825	-	59,67,73	1.36	7 (11%)	68,105,113	1.80	13 (19%)
13	CLA	A	843	-	65,73,73	1.38	9 (13%)	76,113,113	1.80	14 (18%)
13	CLA	A	815	-	45,53,73	1.65	8 (17%)	52,89,113	2.02	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	CLA	A	831	-	65,73,73	1.57	10 (15%)	76,113,113	1.69	10 (13%)
13	CLA	B	841	-	65,73,73	1.17	9 (13%)	76,113,113	1.73	10 (13%)
13	CLA	B	833	-	58,66,73	1.46	10 (17%)	67,104,113	1.96	11 (16%)
13	CLA	B	807	-	65,73,73	1.25	8 (12%)	76,113,113	1.78	9 (11%)
13	CLA	B	832	-	65,73,73	1.36	7 (10%)	76,113,113	1.75	8 (10%)
13	CLA	A	814	-	60,68,73	1.31	7 (11%)	70,107,113	1.89	13 (18%)
17	LHG	B	851	-	22,22,48	2.80	5 (22%)	25,28,54	1.13	1 (4%)
13	CLA	B	808	-	65,73,73	1.32	7 (10%)	76,113,113	1.72	13 (17%)
13	CLA	B	812	-	45,53,73	1.54	6 (13%)	52,89,113	2.16	10 (19%)
16	BCR	L	1005	-	41,41,41	1.42	8 (19%)	56,56,56	1.81	15 (26%)
15	SF4	C	102	3	0,12,12	-	-	-	-	-
13	CLA	B	810	2	65,73,73	1.43	9 (13%)	76,113,113	1.78	14 (18%)
13	CLA	A	804	-	65,73,73	1.32	6 (9%)	76,113,113	1.74	9 (11%)
16	BCR	A	852	-	41,41,41	1.37	6 (14%)	56,56,56	1.78	14 (25%)

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
13	CLA	A	845	-	1/1/9/20	3/7/81/115	-
13	CLA	A	819	-	1/1/12/20	9/24/102/115	-
16	BCR	A	854	-	-	8/29/63/63	0/2/2/2
13	CLA	A	829	-	1/1/15/20	8/37/115/115	-
13	CLA	B	813	-	1/1/15/20	13/37/115/115	-
13	CLA	A	826	20	1/1/15/20	11/37/115/115	-
13	CLA	A	830	-	1/1/15/20	9/37/115/115	-
13	CLA	B	839	-	-	4/16/94/115	-
13	CLA	B	826	-	1/1/15/20	12/37/115/115	-
13	CLA	A	824	-	1/1/12/20	10/21/99/115	-
16	BCR	B	844	-	-	6/29/63/63	0/2/2/2
13	CLA	A	827	20	1/1/15/20	12/37/115/115	-
15	SF4	A	848	2,1	-	-	0/6/5/5
13	CLA	A	817	20	1/1/11/20	9/18/96/115	-
13	CLA	B	829	-	1/1/15/20	9/37/115/115	-

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	805	-	1/1/15/20	13/37/115/115	-
13	CLA	A	838	-	1/1/12/20	6/21/99/115	-
13	CLA	M	1601	20	1/1/11/20	9/13/91/115	-
13	CLA	A	833	-	1/1/15/20	7/37/115/115	-
13	CLA	A	809	1	1/1/15/20	16/37/115/115	-
13	CLA	A	837	1	1/1/11/20	5/13/91/115	-
13	CLA	A	805	13	1/1/13/20	12/30/108/115	-
16	BCR	J	103	-	-	3/29/63/63	0/2/2/2
13	CLA	L	1002	10	1/1/15/20	11/37/115/115	-
13	CLA	B	806	-	1/1/15/20	15/37/115/115	-
13	CLA	A	807	-	1/1/15/20	14/37/115/115	-
16	BCR	A	849	-	-	0/29/63/63	0/2/2/2
13	CLA	B	822	20	1/1/13/20	8/25/103/115	-
13	CLA	B	801	-	1/1/15/20	10/37/115/115	-
16	BCR	I	101	-	-	0/29/63/63	0/2/2/2
13	CLA	J	101	8	1/1/11/20	11/13/91/115	-
14	PQN	A	847	-	-	6/23/43/43	0/2/2/2
13	CLA	A	828	-	1/1/15/20	7/37/115/115	-
15	SF4	C	101	3	-	-	0/6/5/5
13	CLA	J	102	-	1/1/8/20	0/2/76/115	-
13	CLA	B	835	20	1/1/11/20	0/13/91/115	-
13	CLA	B	816	-	1/1/13/20	8/25/103/115	-
13	CLA	A	802	20	1/1/15/20	4/37/115/115	-
13	CLA	A	811	-	-	9/13/91/115	-
13	CLA	B	825	20	1/1/11/20	6/15/93/115	-
17	LHG	A	856	13	1/1/5/5	10/31/31/53	-
13	CLA	A	801	-	1/1/15/20	2/37/115/115	-
13	CLA	A	841	-	1/1/15/20	7/37/115/115	-
16	BCR	B	846	-	-	6/18/35/63	0/1/1/2
13	CLA	B	831	-	1/1/11/20	9/18/96/115	-
13	CLA	A	818	-	-	1/24/102/115	-
16	BCR	B	847	-	-	2/29/63/63	0/2/2/2
13	CLA	A	835	-	1/1/15/20	8/37/115/115	-
13	CLA	B	804	-	1/1/12/20	4/24/102/115	-
13	CLA	B	802	20	1/1/15/20	7/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	X	1701	12	1/1/11/20	5/13/91/115	-
18	LMG	B	850	-	-	8/50/70/70	0/1/1/1
13	CLA	B	814	-	1/1/15/20	11/37/115/115	-
13	CLA	L	1004	20	1/1/15/20	8/37/115/115	-
13	CLA	B	827	-	1/1/15/20	14/37/115/115	-
13	CLA	A	808	-	1/1/12/20	6/21/99/115	-
13	CLA	A	823	-	1/1/11/20	10/18/96/115	-
13	CLA	B	821	-	1/1/11/20	5/13/91/115	-
13	CLA	A	806	-	1/1/15/20	16/37/115/115	-
16	BCR	M	1602	-	-	4/29/63/63	0/2/2/2
13	CLA	A	846	17	1/1/12/20	15/22/100/115	-
13	CLA	A	836	-	1/1/12/20	6/24/102/115	-
13	CLA	A	834	-	-	5/37/115/115	-
13	CLA	B	815	-	-	8/13/91/115	-
13	CLA	A	820	-	1/1/15/20	14/37/115/115	-
13	CLA	A	822	20	1/1/15/20	6/37/115/115	-
13	CLA	B	809	2	1/1/15/20	14/37/115/115	-
13	CLA	B	837	-	1/1/14/20	9/31/109/115	-
13	CLA	B	840	20	1/1/15/20	2/37/115/115	-
13	CLA	A	816	-	1/1/11/20	4/13/91/115	-
13	CLA	A	821	-	1/1/14/20	14/33/111/115	-
16	BCR	F	1302	-	-	5/29/63/63	0/2/2/2
16	BCR	A	853	-	-	2/29/63/63	0/2/2/2
13	CLA	A	812	13	1/1/15/20	12/37/115/115	-
16	BCR	J	104	-	-	4/29/63/63	0/2/2/2
16	BCR	I	102	-	-	4/29/63/63	0/2/2/2
13	CLA	K	1401	-	-	6/13/91/115	-
16	BCR	A	851	-	-	0/29/63/63	0/2/2/2
13	CLA	A	844	20	1/1/15/20	10/37/115/115	-
13	CLA	F	1301	20	1/1/11/20	4/13/91/115	-
13	CLA	B	828	-	-	10/37/115/115	-
13	CLA	A	813	-	1/1/12/20	8/24/102/115	-
13	CLA	B	803	-	-	2/37/115/115	-
13	CLA	A	839	-	1/1/15/20	8/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	L	1006	-	-	1/29/63/63	0/2/2/2
13	CLA	A	810	1	1/1/15/20	13/37/115/115	-
13	CLA	B	819	20	1/1/15/20	4/37/115/115	-
13	CLA	A	842	20	1/1/12/20	8/21/99/115	-
13	CLA	A	832	-	1/1/12/20	3/19/97/115	-
13	CLA	B	811	-	1/1/11/20	3/13/91/115	-
16	BCR	B	843	-	-	0/29/63/63	0/2/2/2
17	LHG	A	855	-	-	18/53/53/53	-
13	CLA	B	830	-	1/1/11/20	8/13/91/115	-
13	CLA	B	838	-	1/1/15/20	0/37/115/115	-
13	CLA	B	824	2	1/1/12/20	7/24/102/115	-
13	CLA	B	818	-	1/1/14/20	10/31/109/115	-
13	CLA	B	817	-	1/1/13/20	7/30/108/115	-
13	CLA	B	820	-	1/1/11/20	6/16/94/115	-
16	BCR	A	850	-	-	4/29/63/63	0/2/2/2
13	CLA	L	1003	-	-	7/37/115/115	-
13	CLA	B	834	-	1/1/11/20	4/13/91/115	-
14	PQN	B	842	-	-	4/23/43/43	0/2/2/2
13	CLA	A	803	-	1/1/15/20	10/37/115/115	-
16	BCR	B	848	-	-	1/29/63/63	0/2/2/2
16	BCR	B	849	-	-	2/29/63/63	0/2/2/2
13	CLA	B	836	20	1/1/11/20	4/13/91/115	-
13	CLA	B	823	-	1/1/11/20	3/13/91/115	-
16	BCR	B	845	-	-	6/29/63/63	0/2/2/2
16	BCR	J	105	-	-	2/29/63/63	0/2/2/2
13	CLA	A	840	-	1/1/11/20	5/16/94/115	-
13	CLA	A	825	-	1/1/13/20	12/30/108/115	-
13	CLA	A	843	-	1/1/15/20	8/37/115/115	-
13	CLA	A	815	-	1/1/11/20	1/13/91/115	-
13	CLA	A	831	-	1/1/15/20	6/37/115/115	-
13	CLA	B	841	-	-	8/37/115/115	-
13	CLA	B	833	-	1/1/13/20	6/29/107/115	-
13	CLA	B	807	-	1/1/15/20	2/37/115/115	-
13	CLA	B	832	-	1/1/15/20	16/37/115/115	-
13	CLA	A	814	-	1/1/14/20	11/31/109/115	-

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	LHG	B	851	-	-	7/26/26/53	-
13	CLA	B	808	-	1/1/15/20	9/37/115/115	-
13	CLA	B	812	-	1/1/11/20	3/13/91/115	-
16	BCR	L	1005	-	-	1/29/63/63	0/2/2/2
15	SF4	C	102	3	-	-	0/6/5/5
13	CLA	B	810	2	1/1/15/20	7/37/115/115	-
13	CLA	A	804	-	1/1/15/20	6/37/115/115	-
16	BCR	A	852	-	-	2/29/63/63	0/2/2/2

The worst 5 of 926 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	847	PQN	O4-C4	9.27	1.42	1.23
14	B	842	PQN	O4-C4	8.96	1.42	1.23
14	A	847	PQN	O1-C1	8.94	1.42	1.23
17	B	851	LHG	P-O5	8.61	1.81	1.50
14	B	842	PQN	O1-C1	8.43	1.41	1.23

The worst 5 of 1410 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	820	CLA	C4A-NA-C1A	12.37	112.27	106.71
13	A	833	CLA	C4A-NA-C1A	12.20	112.19	106.71
13	M	1601	CLA	C4A-NA-C1A	12.08	112.14	106.71
13	A	813	CLA	C4A-NA-C1A	11.91	112.06	106.71
13	A	821	CLA	C4A-NA-C1A	11.90	112.06	106.71

5 of 87 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	801	CLA	ND
13	A	802	CLA	ND
13	A	803	CLA	ND
13	A	804	CLA	ND
13	A	805	CLA	ND

5 of 863 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	803	CLA	O2A-C1-C2-C3

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	A	805	CLA	C3A-C2A-CAA-CBA
13	A	806	CLA	C1A-C2A-CAA-CBA
13	A	806	CLA	C3A-C2A-CAA-CBA
13	A	806	CLA	CBA-CGA-O2A-C1

There are no ring outliers.

114 monomers are involved in 334 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	845	CLA	1	0
13	A	819	CLA	4	0
16	A	854	BCR	13	0
13	A	829	CLA	13	0
13	B	813	CLA	6	0
13	A	826	CLA	4	0
13	A	830	CLA	1	0
13	B	839	CLA	4	0
13	B	826	CLA	3	0
13	A	824	CLA	1	0
13	A	827	CLA	5	0
16	B	844	BCR	1	0
13	A	817	CLA	2	0
13	B	829	CLA	7	0
13	B	805	CLA	3	0
13	A	838	CLA	2	0
13	M	1601	CLA	1	0
13	A	833	CLA	1	0
13	A	809	CLA	6	0
13	A	837	CLA	2	0
13	A	805	CLA	1	0
16	J	103	BCR	4	0
13	L	1002	CLA	2	0
13	B	806	CLA	6	0
13	A	807	CLA	4	0
16	A	849	BCR	2	0
13	B	822	CLA	4	0
13	B	801	CLA	8	0
16	I	101	BCR	3	0
13	J	101	CLA	1	0
14	A	847	PQN	1	0
13	A	828	CLA	3	0
13	B	835	CLA	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	816	CLA	3	0
13	A	802	CLA	3	0
13	A	811	CLA	4	0
13	B	825	CLA	2	0
17	A	856	LHG	2	0
13	A	801	CLA	9	0
13	A	841	CLA	2	0
16	B	846	BCR	5	0
13	B	831	CLA	2	0
16	B	847	BCR	3	0
13	A	835	CLA	4	0
13	B	804	CLA	2	0
13	B	802	CLA	17	0
13	X	1701	CLA	1	0
18	B	850	LMG	5	0
13	B	814	CLA	6	0
13	L	1004	CLA	2	0
13	B	827	CLA	5	0
13	A	808	CLA	2	0
13	A	823	CLA	2	0
13	B	821	CLA	1	0
13	A	806	CLA	6	0
16	M	1602	BCR	2	0
13	A	846	CLA	5	0
13	A	836	CLA	4	0
13	B	815	CLA	2	0
13	A	820	CLA	6	0
13	A	822	CLA	4	0
13	B	809	CLA	2	0
13	B	837	CLA	3	0
13	B	840	CLA	3	0
13	A	821	CLA	5	0
16	F	1302	BCR	2	0
16	A	853	BCR	1	0
13	A	812	CLA	1	0
16	J	104	BCR	7	0
13	K	1401	CLA	1	0
16	A	851	BCR	1	0
13	A	844	CLA	5	0
13	F	1301	CLA	1	0
13	B	828	CLA	8	0
13	B	803	CLA	4	0

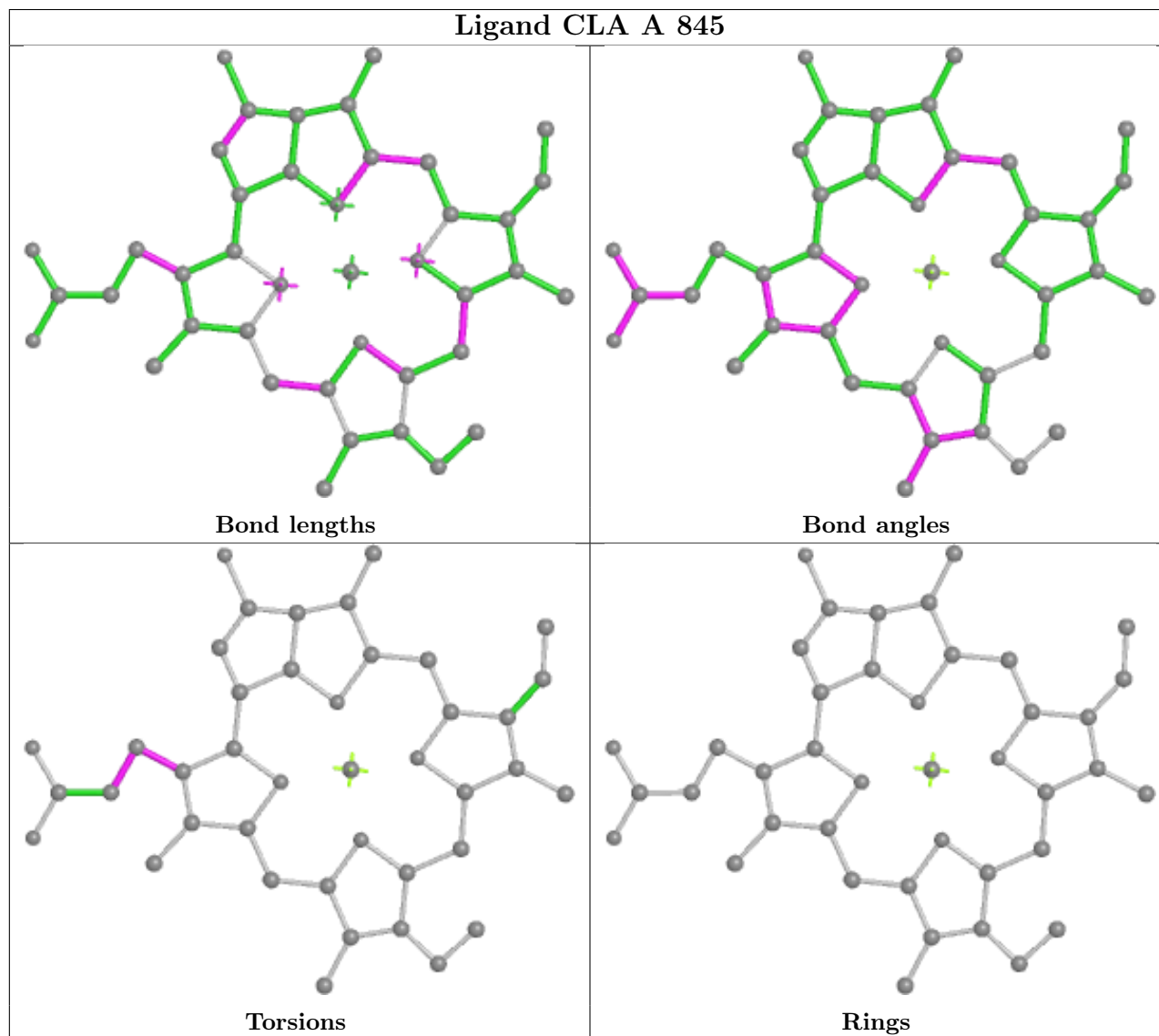
*Continued on next page...*

*Continued from previous page...*

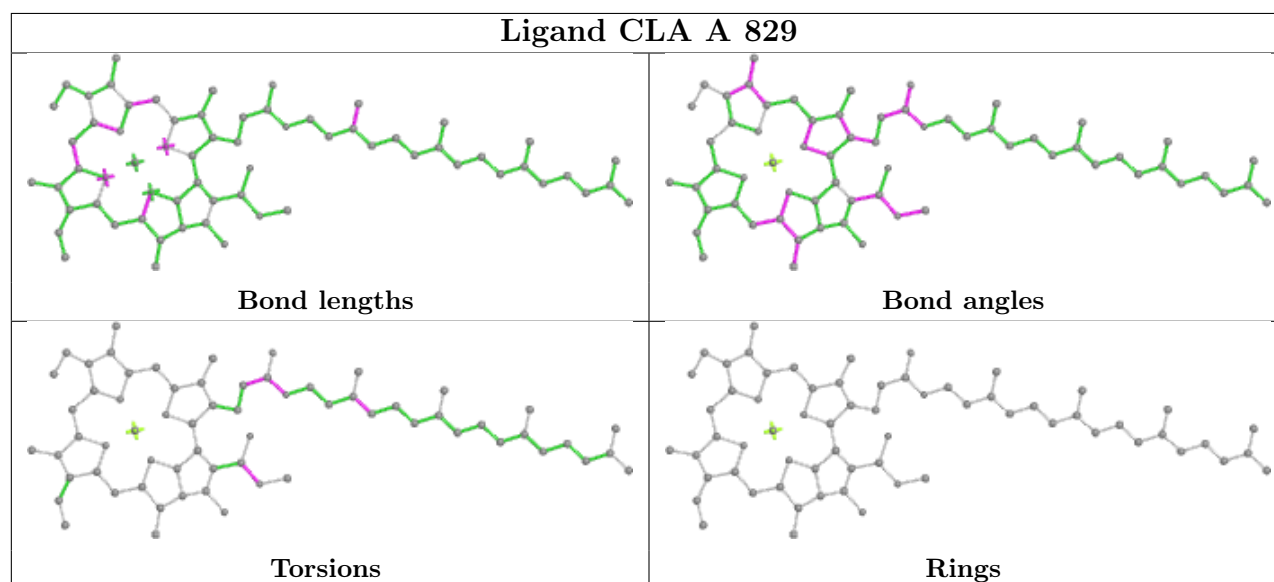
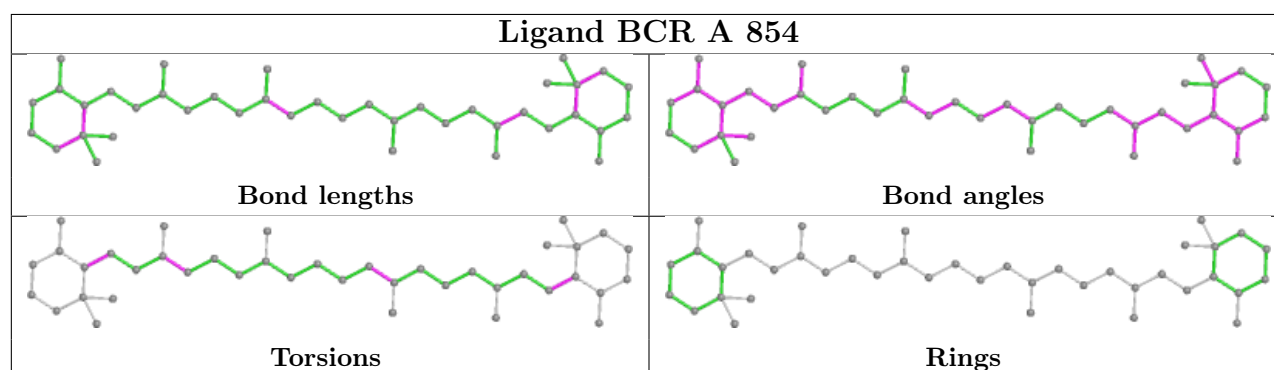
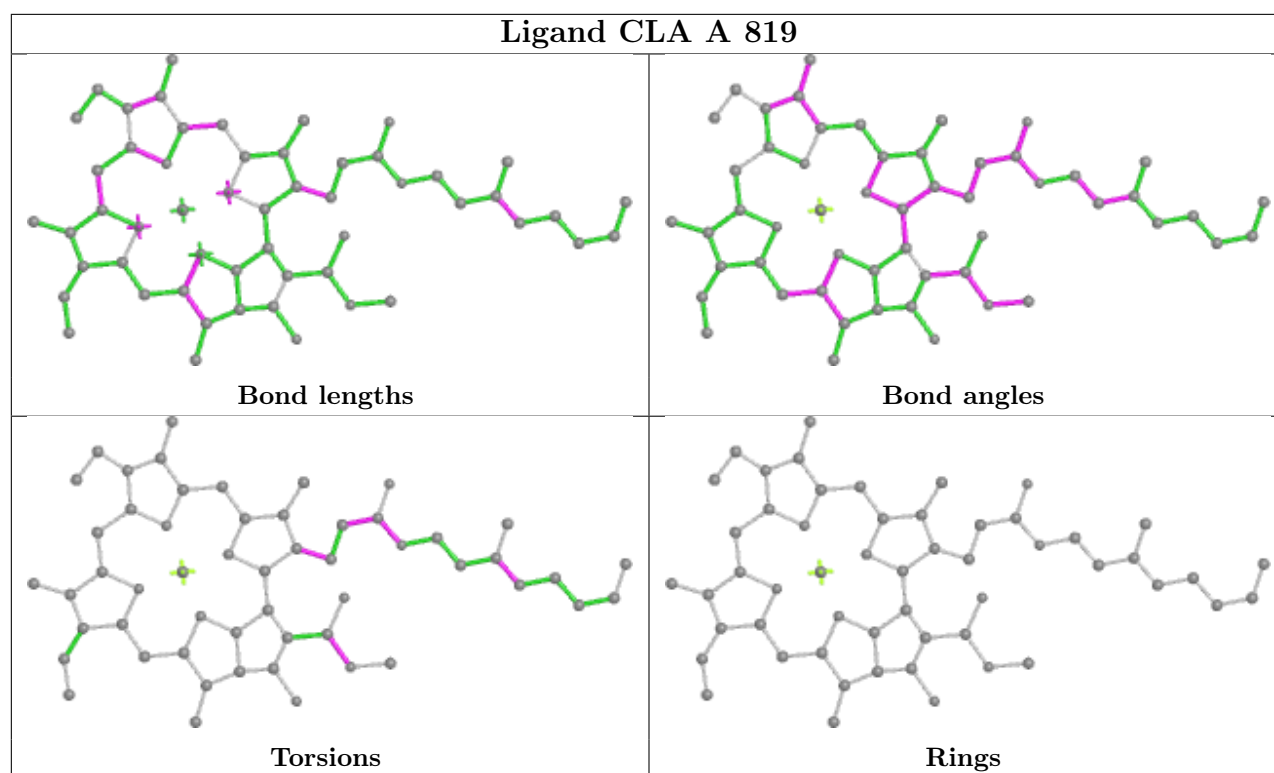
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	839	CLA	6	0
16	L	1006	BCR	1	0
13	A	810	CLA	4	0
13	B	819	CLA	5	0
13	A	832	CLA	1	0
13	B	811	CLA	1	0
16	B	843	BCR	1	0
17	A	855	LHG	4	0
13	B	830	CLA	5	0
13	B	838	CLA	2	0
13	B	824	CLA	10	0
13	B	818	CLA	5	0
13	B	817	CLA	8	0
13	B	820	CLA	2	0
16	A	850	BCR	2	0
13	L	1003	CLA	8	0
14	B	842	PQN	1	0
13	A	803	CLA	10	0
16	B	848	BCR	1	0
16	B	849	BCR	1	0
13	B	836	CLA	2	0
13	B	823	CLA	3	0
16	B	845	BCR	5	0
16	J	105	BCR	5	0
13	A	840	CLA	3	0
13	A	825	CLA	2	0
13	A	843	CLA	8	0
13	A	815	CLA	5	0
13	A	831	CLA	6	0
13	B	833	CLA	7	0
13	B	807	CLA	1	0
13	B	832	CLA	6	0
13	A	814	CLA	1	0
17	B	851	LHG	1	0
13	B	808	CLA	3	0
13	B	812	CLA	1	0
13	B	810	CLA	5	0
13	A	804	CLA	2	0
16	A	852	BCR	4	0

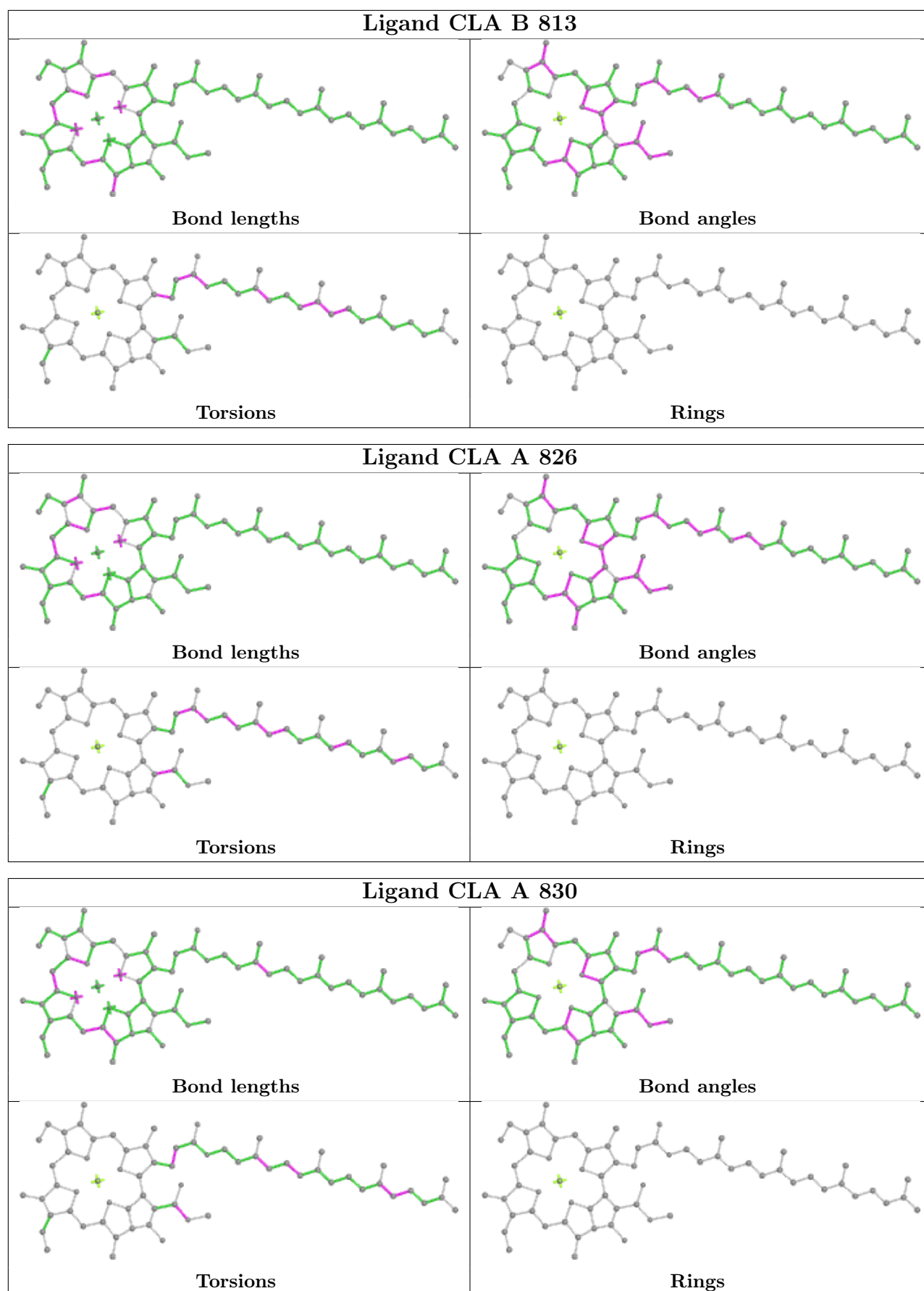
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

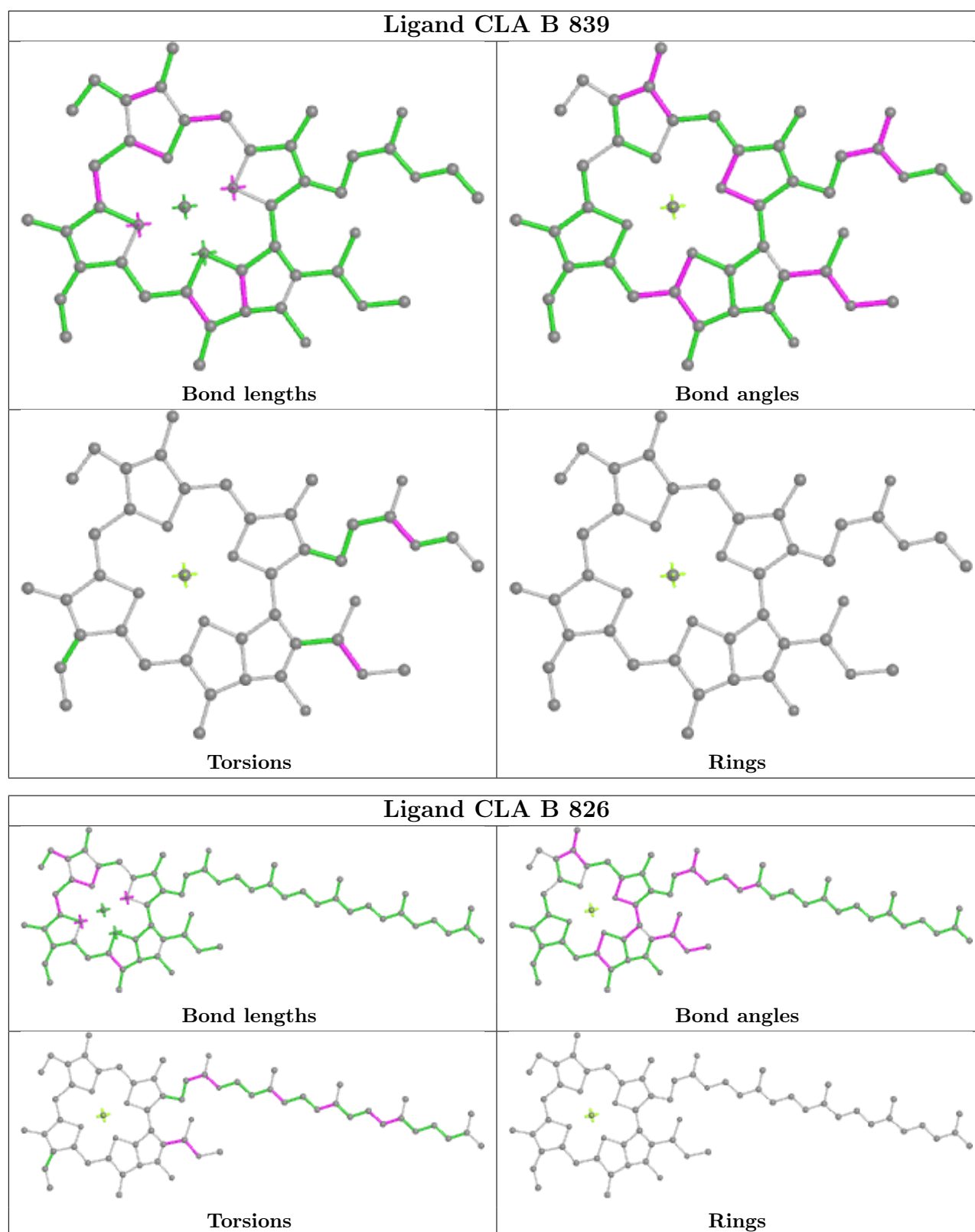
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted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

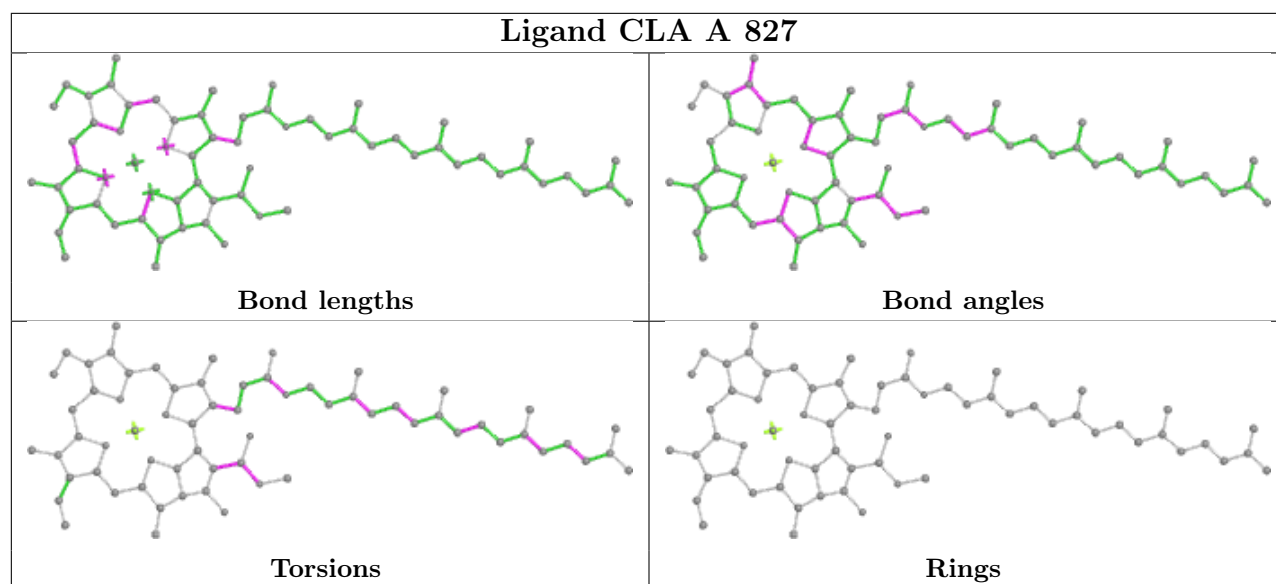
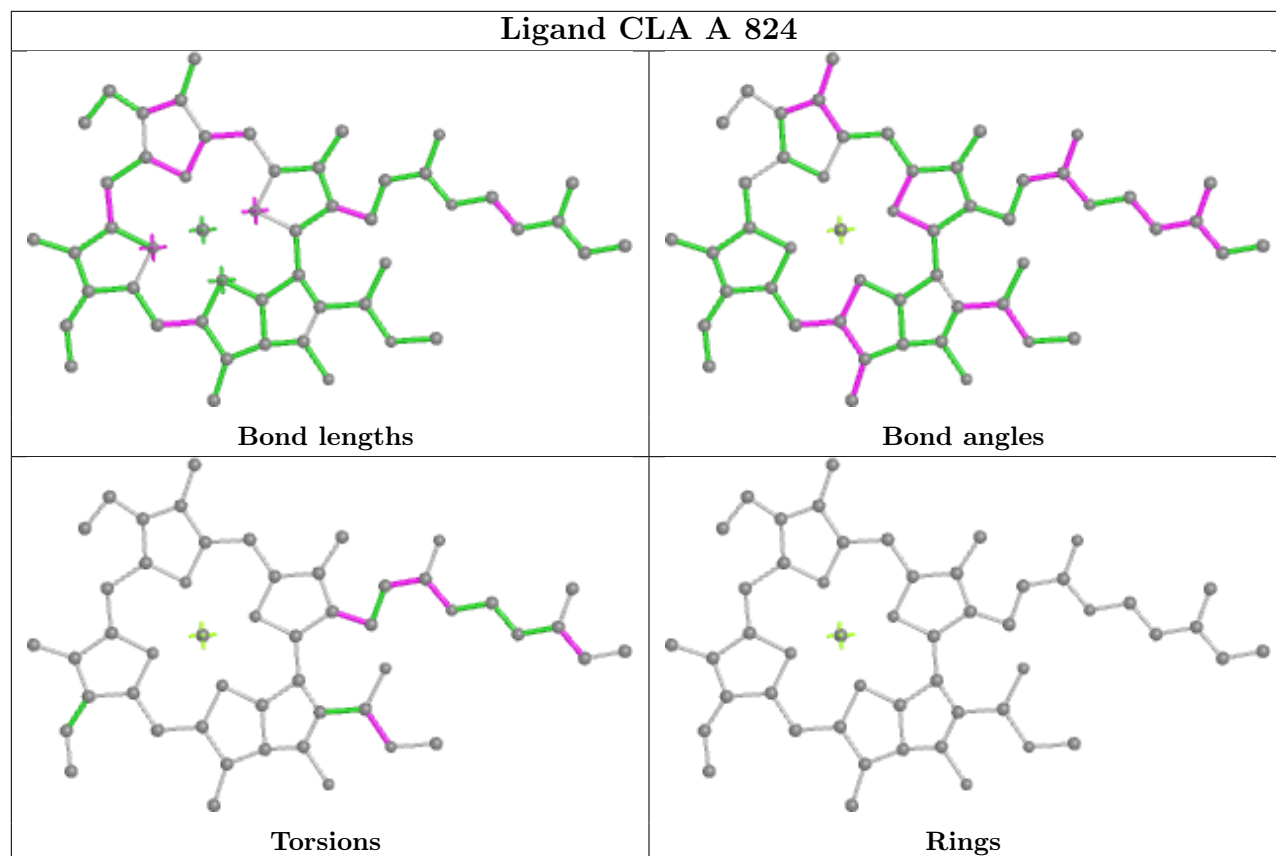


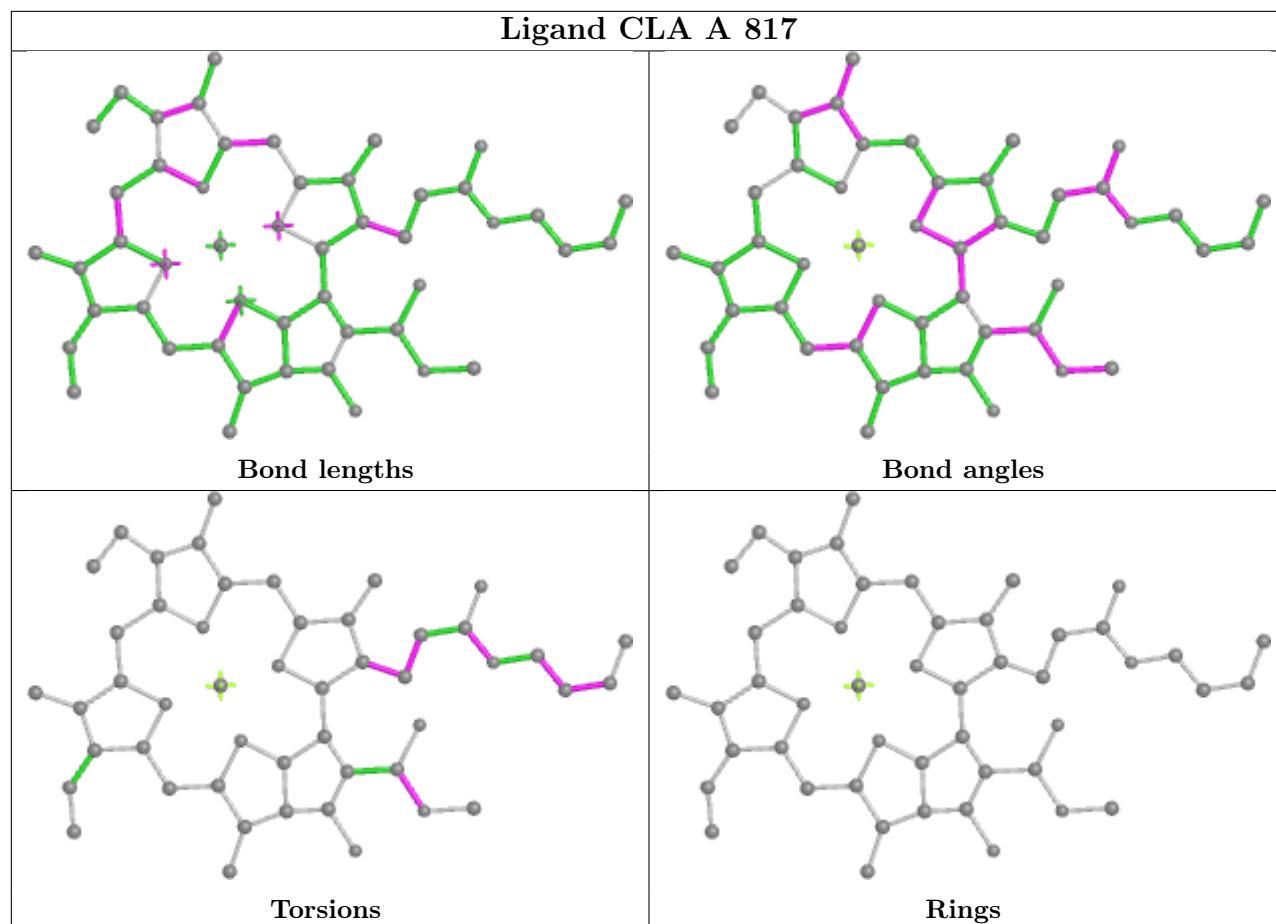
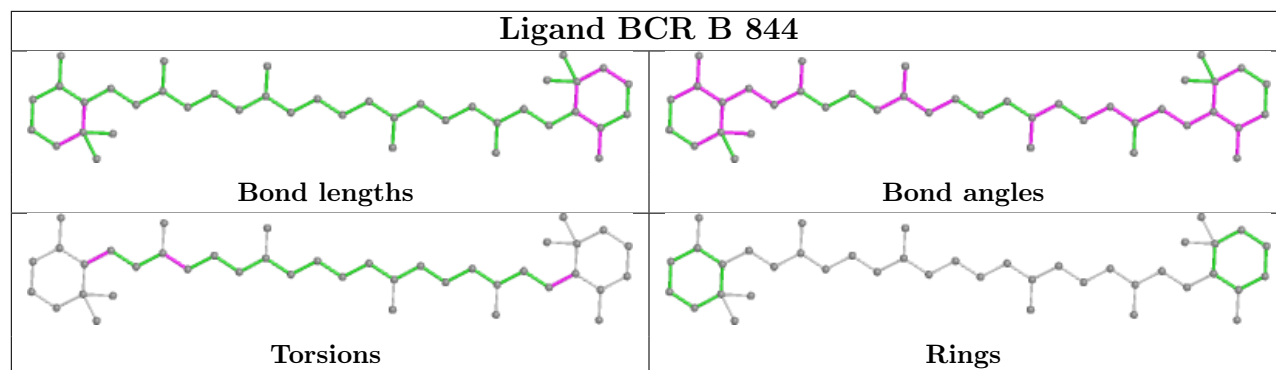


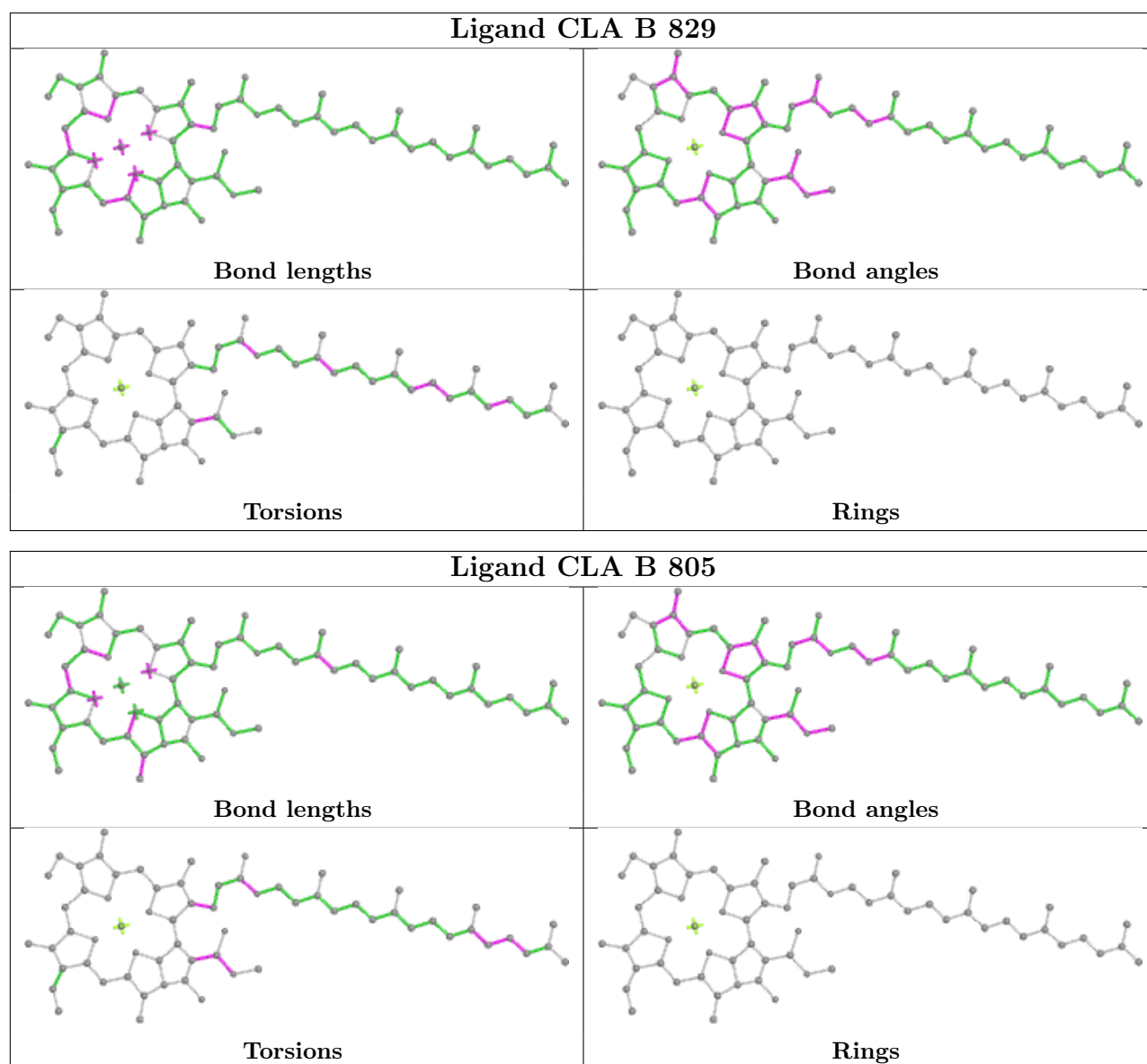


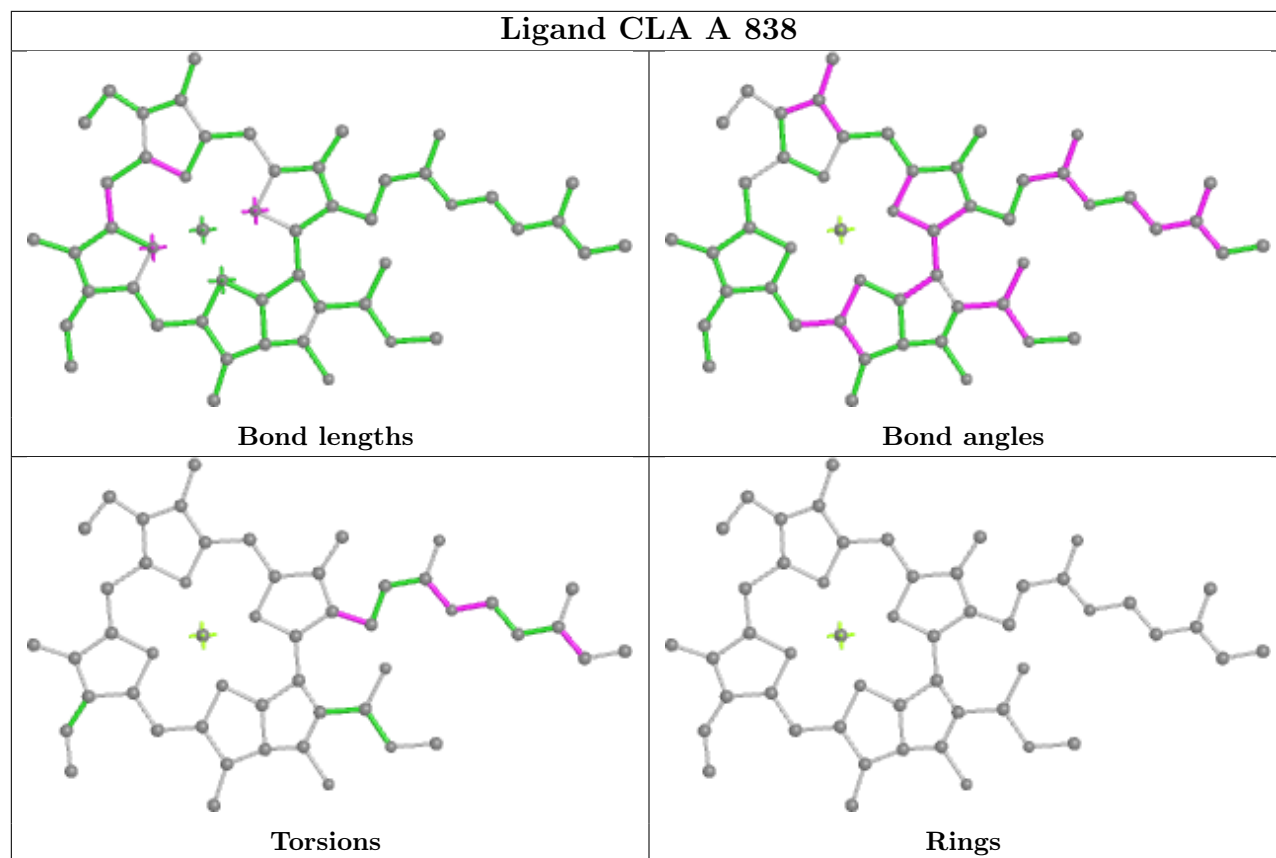


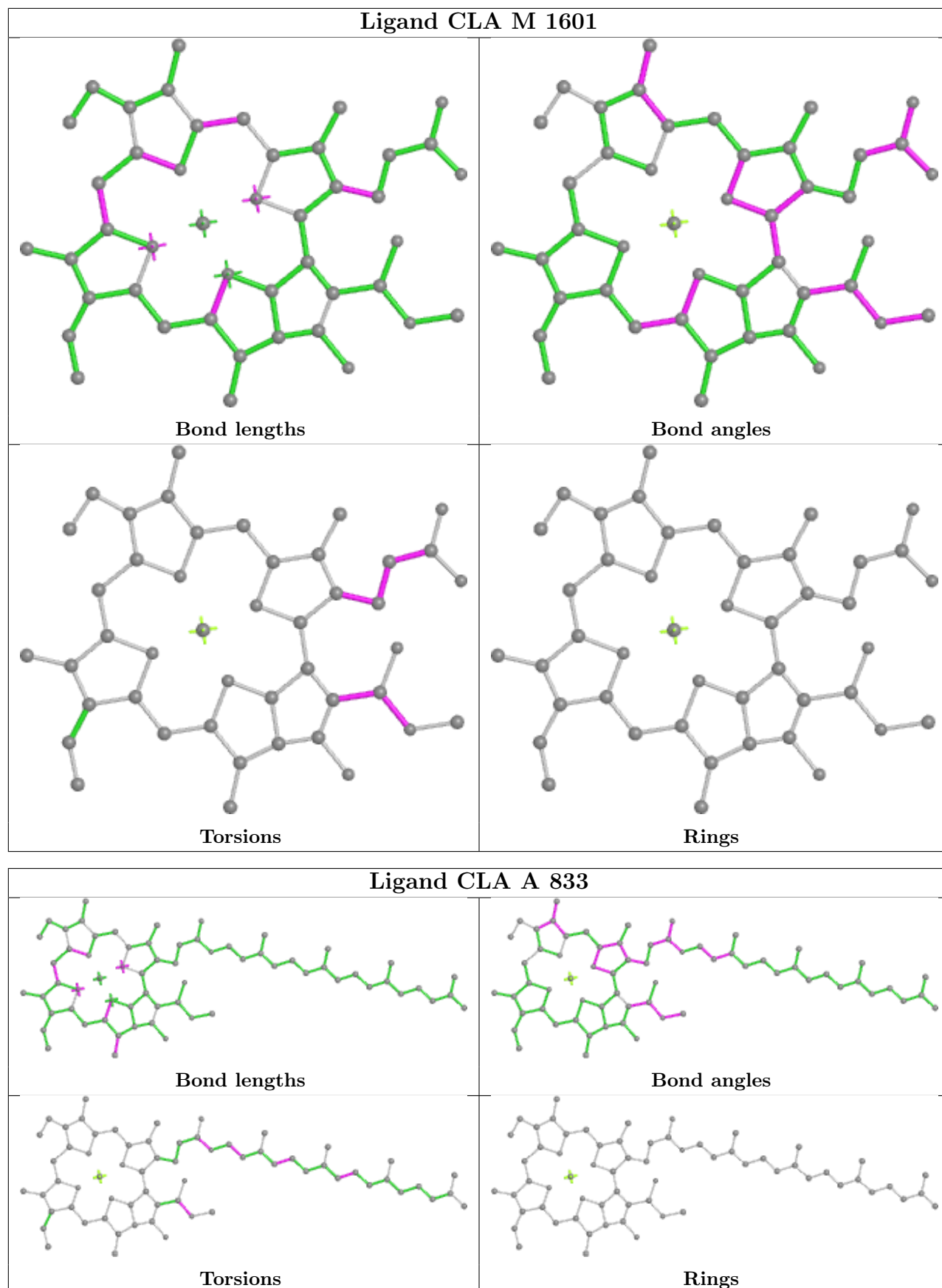




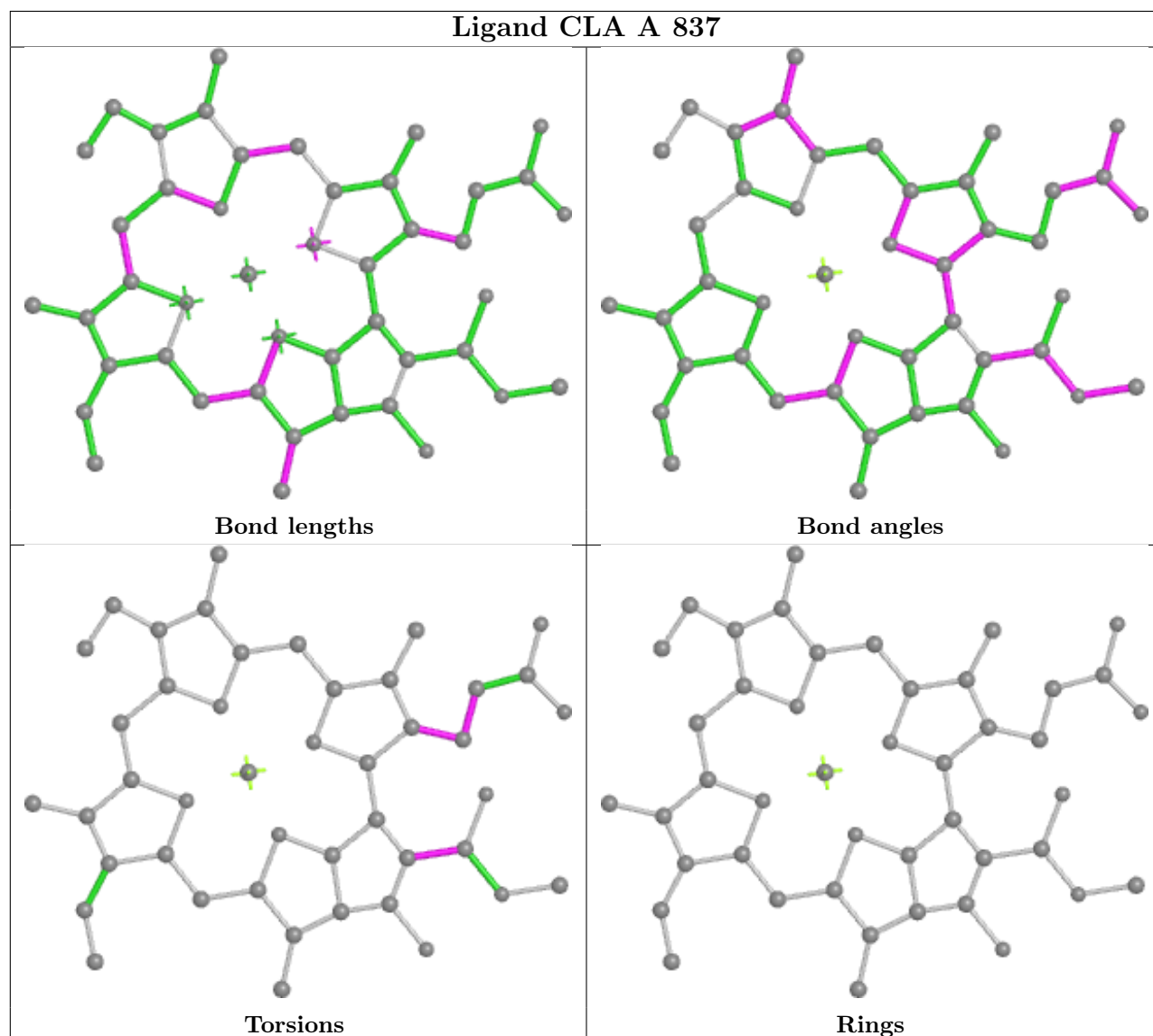
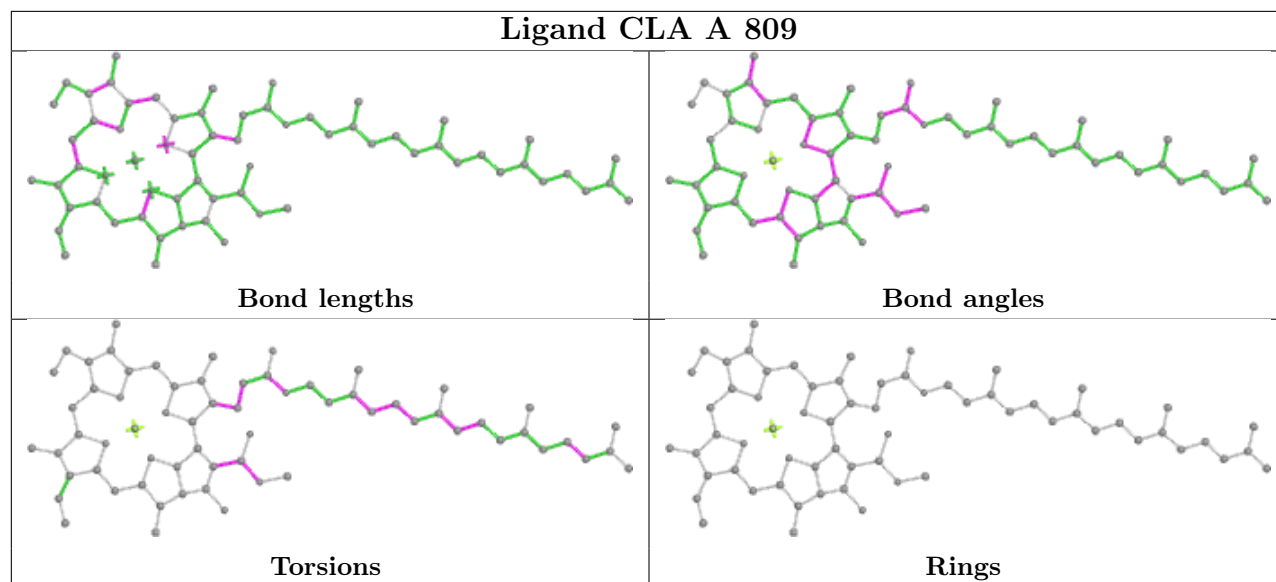


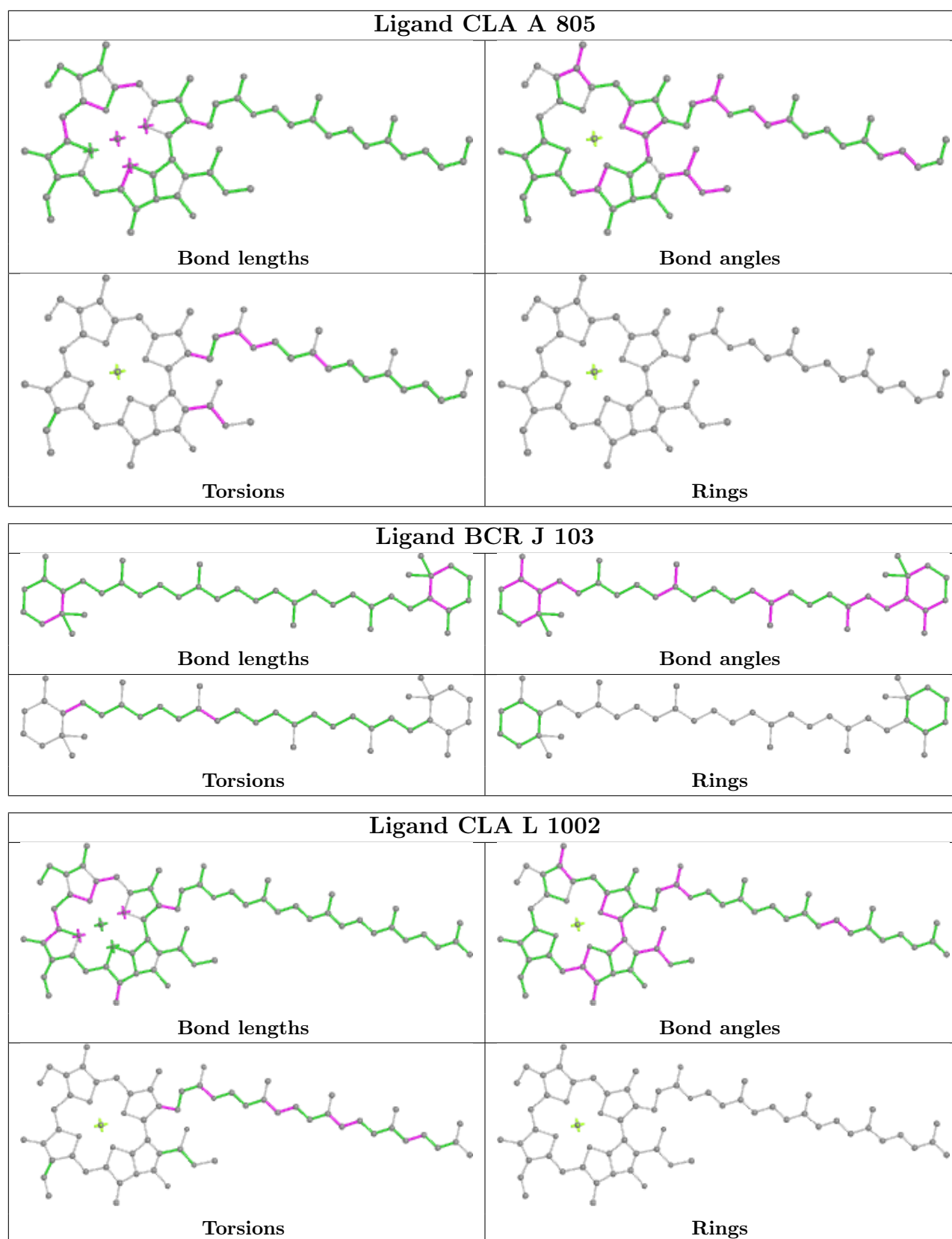


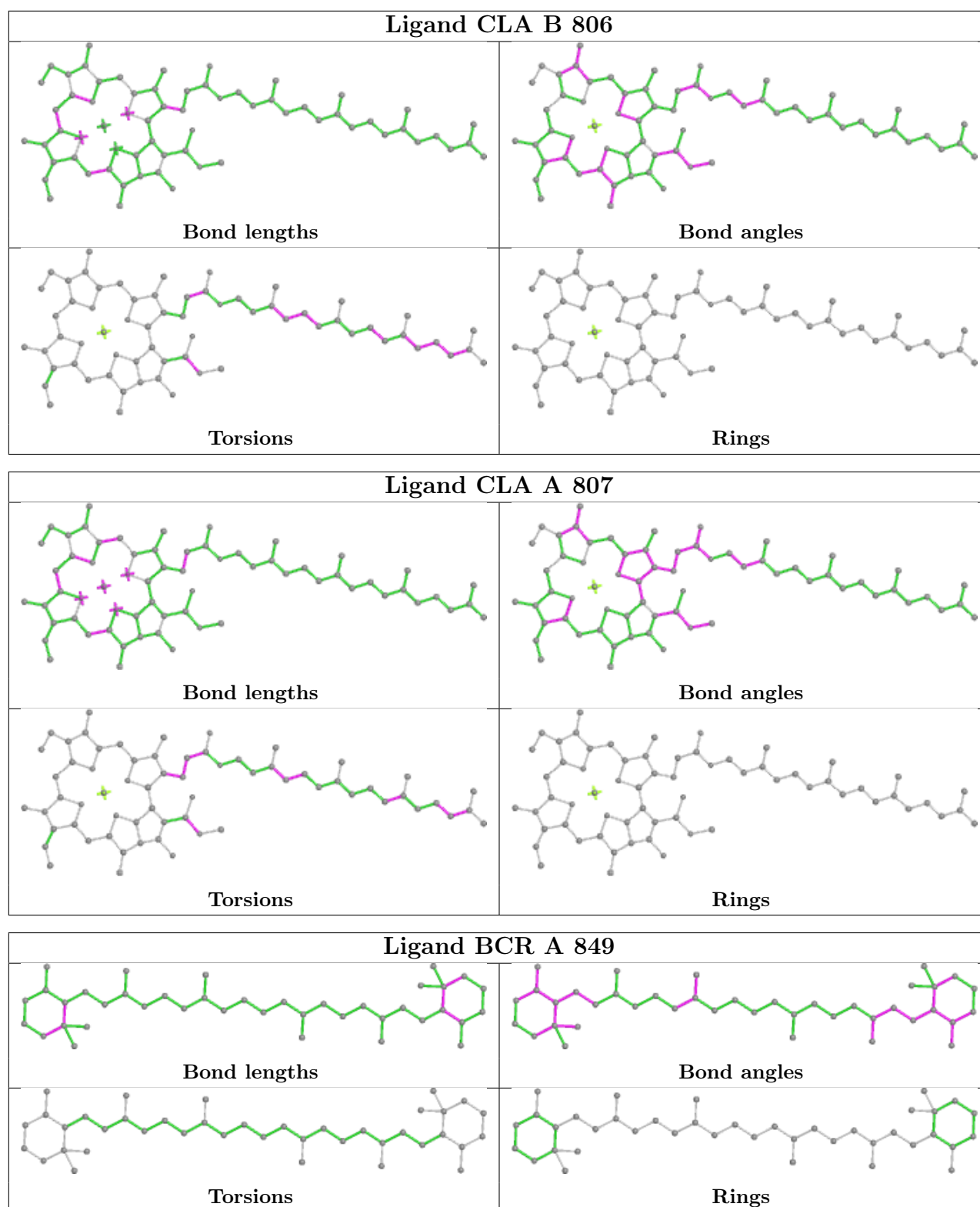


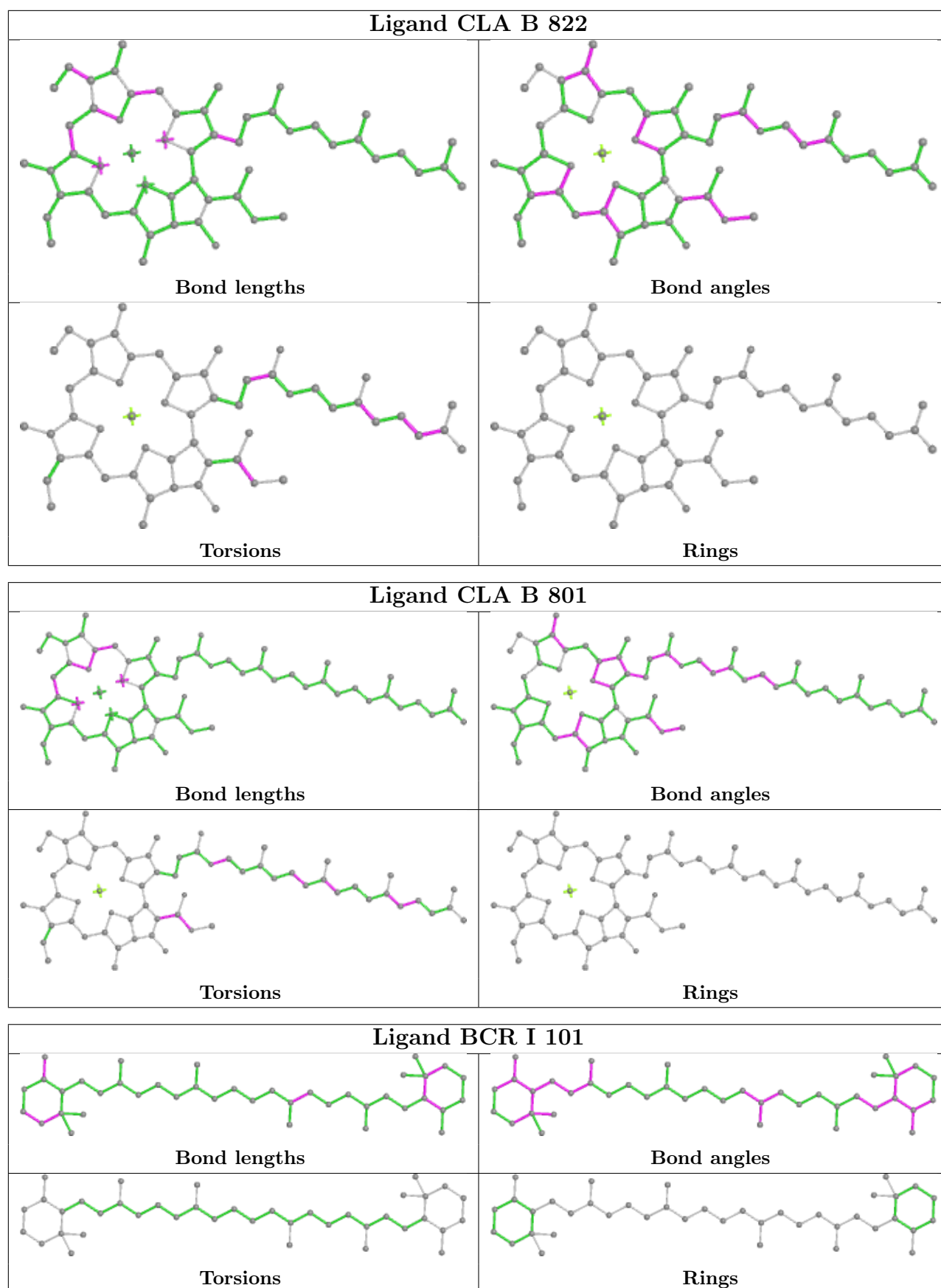


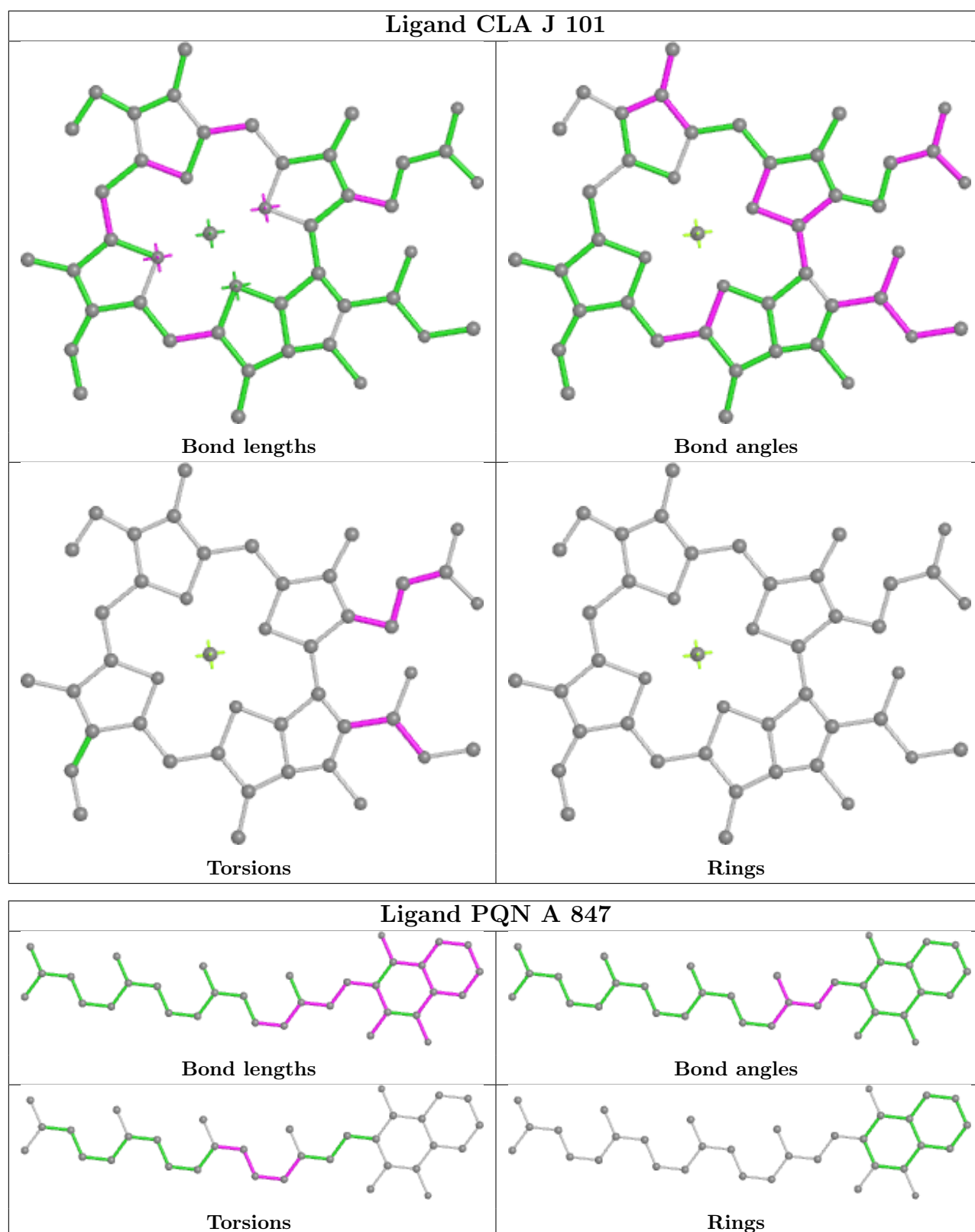


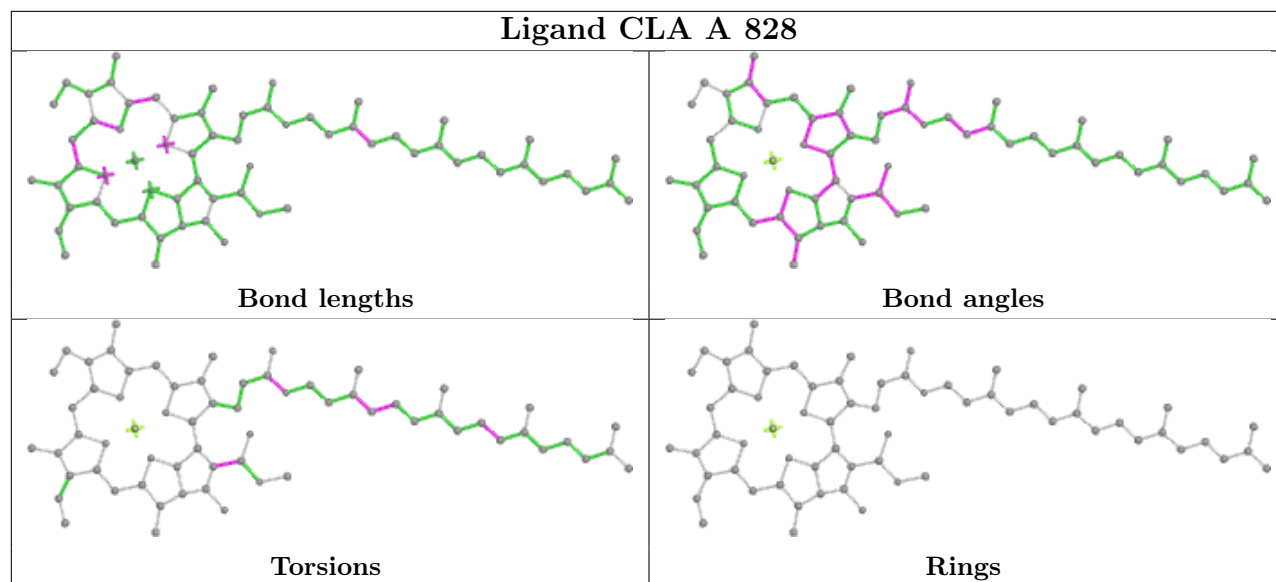




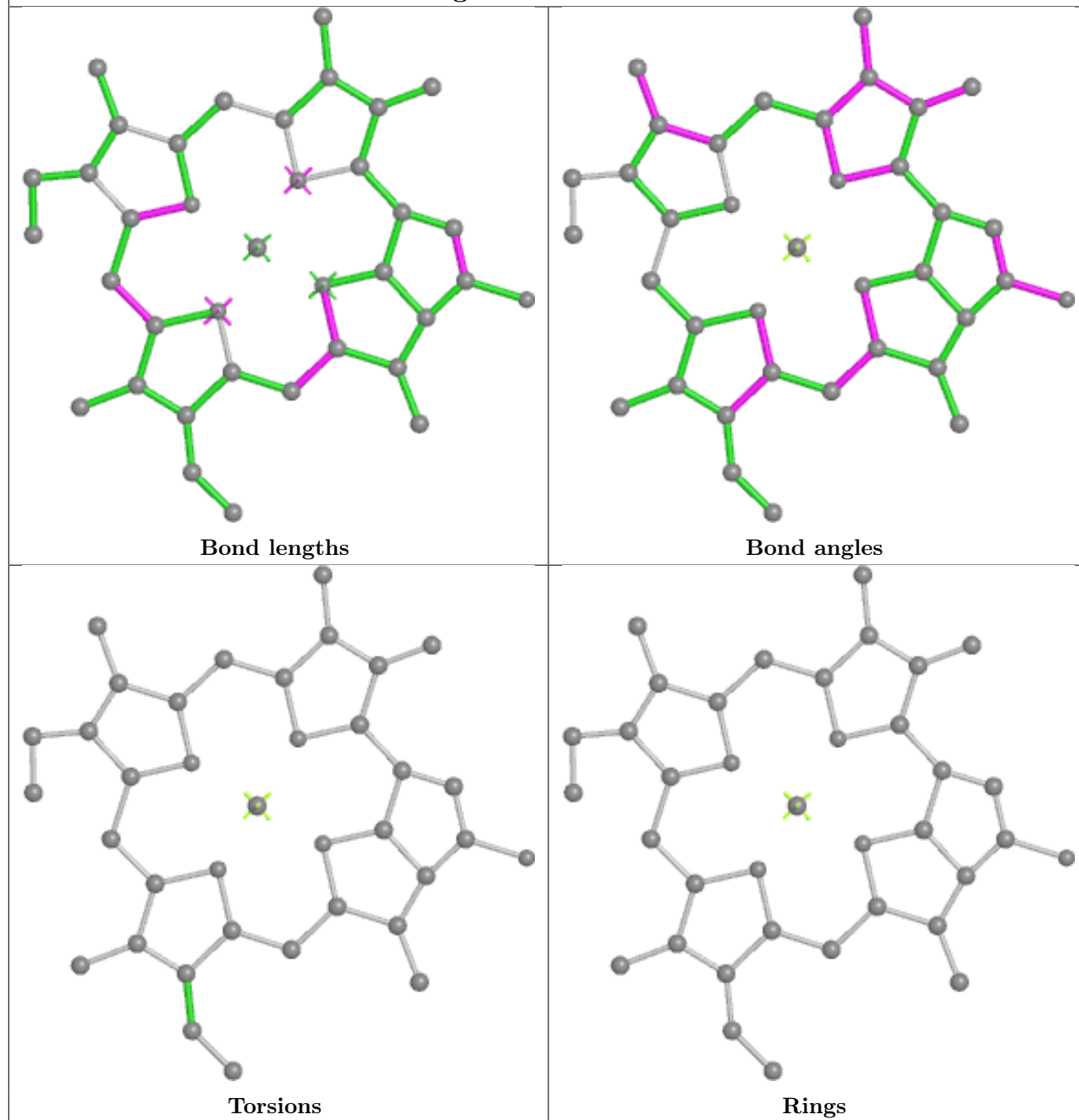


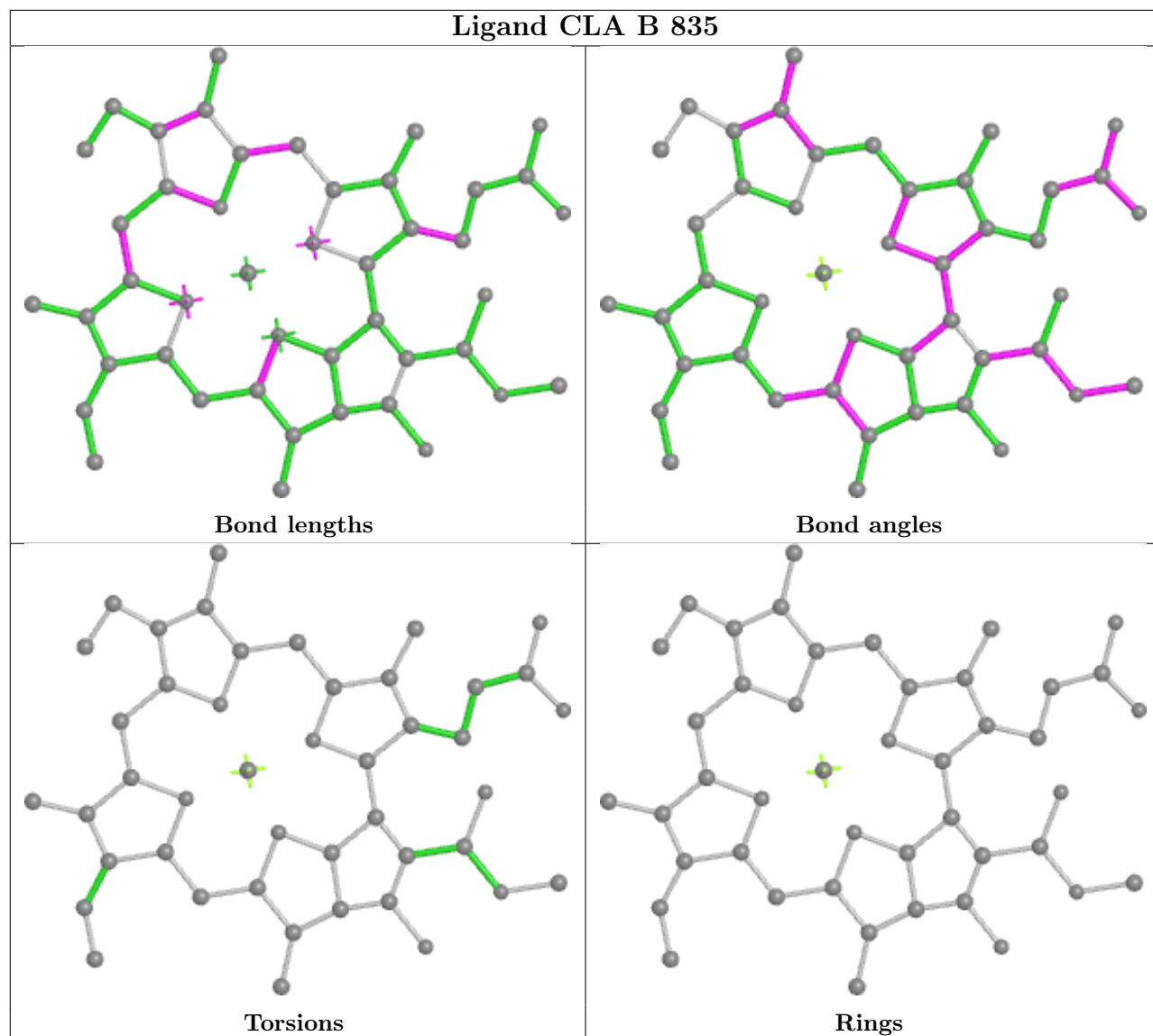




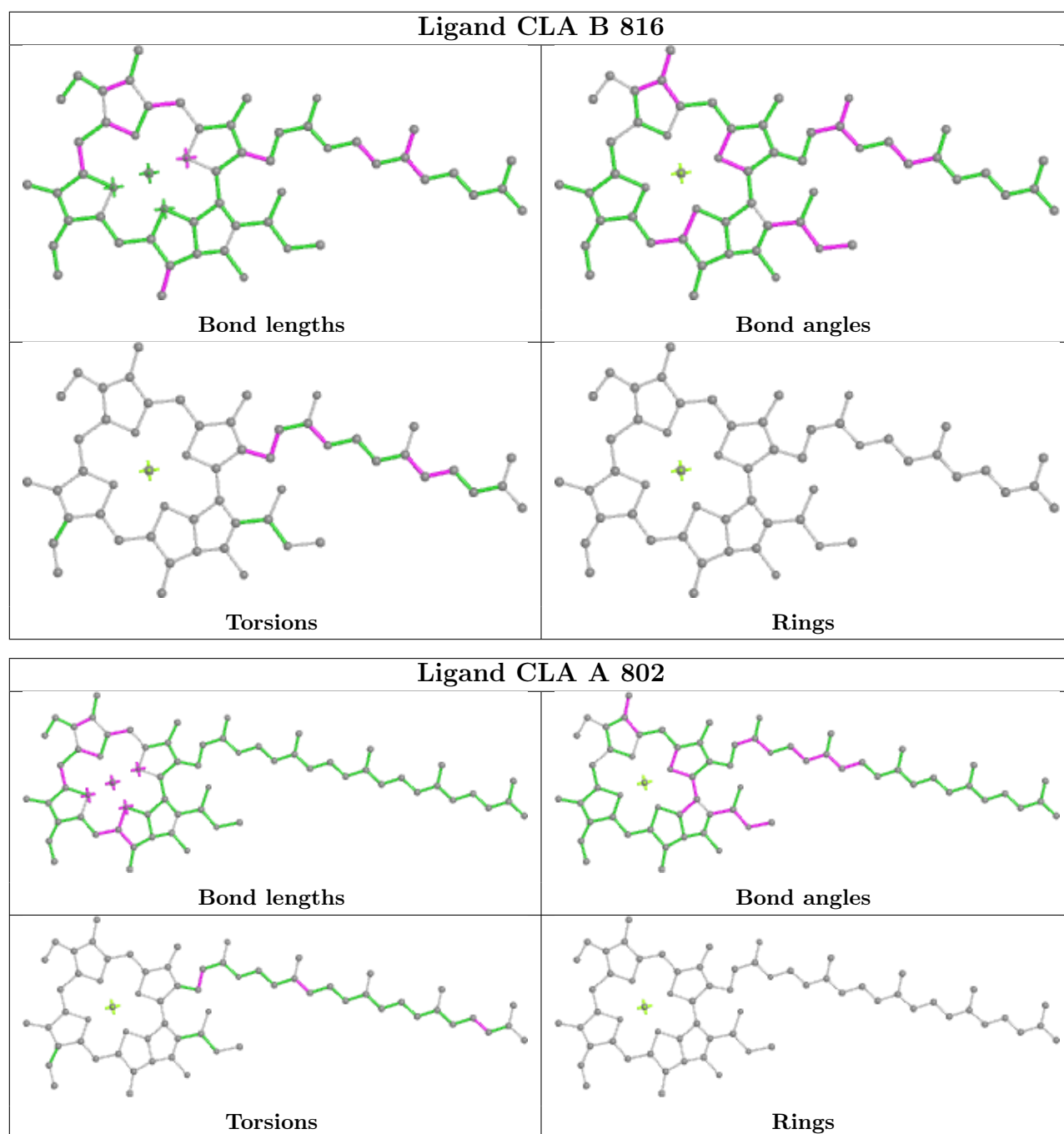


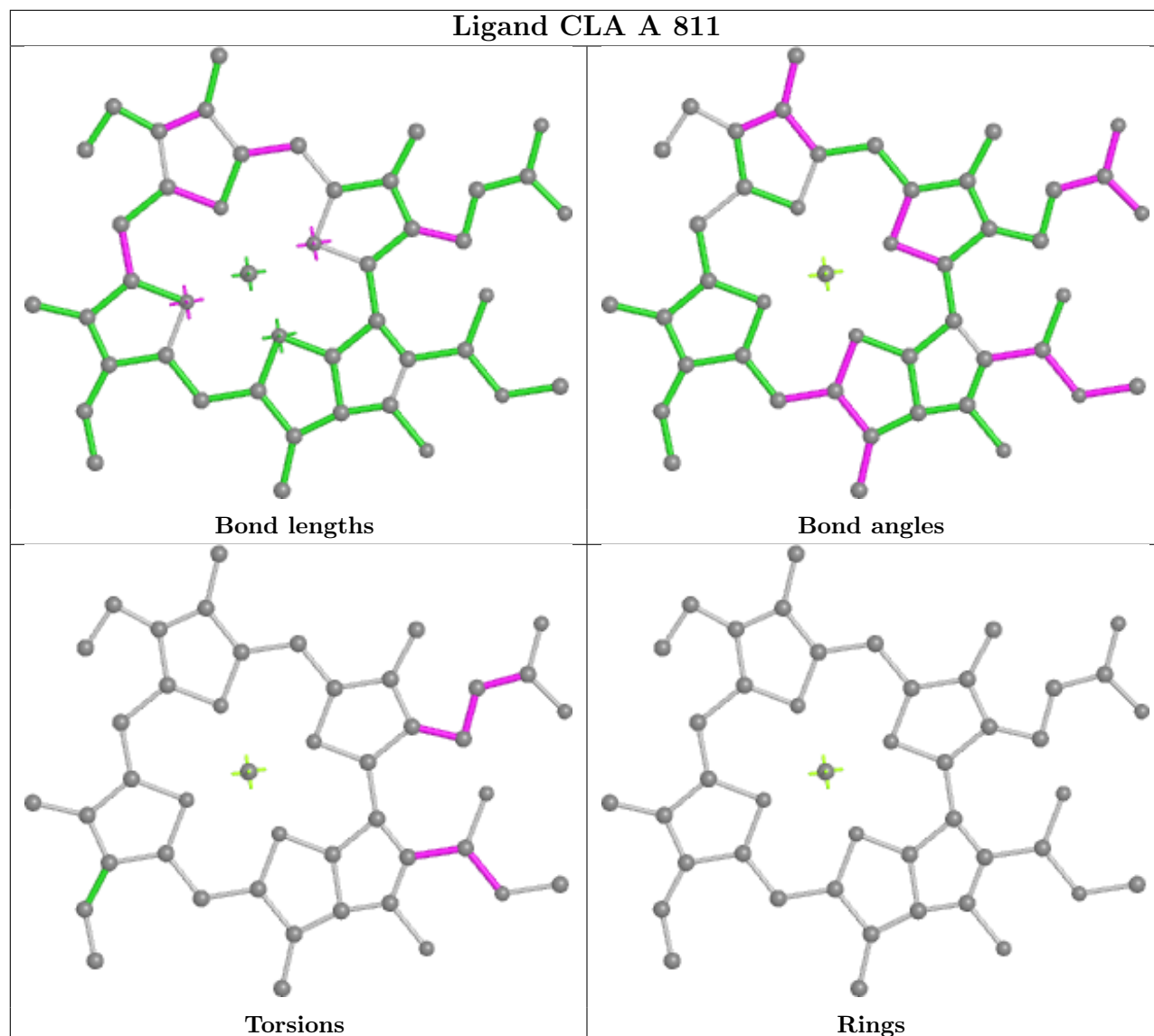
## Ligand CLA J 102

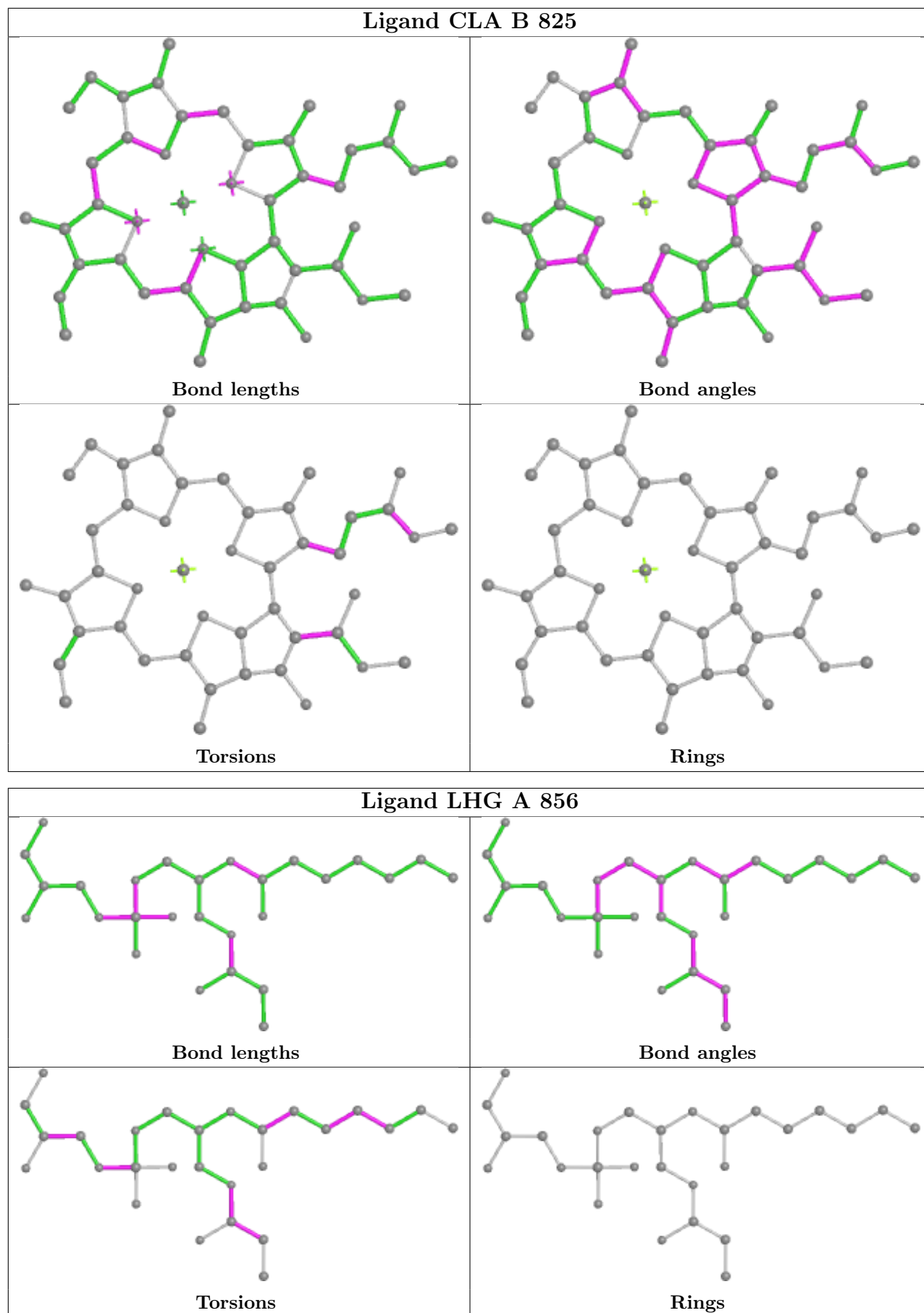


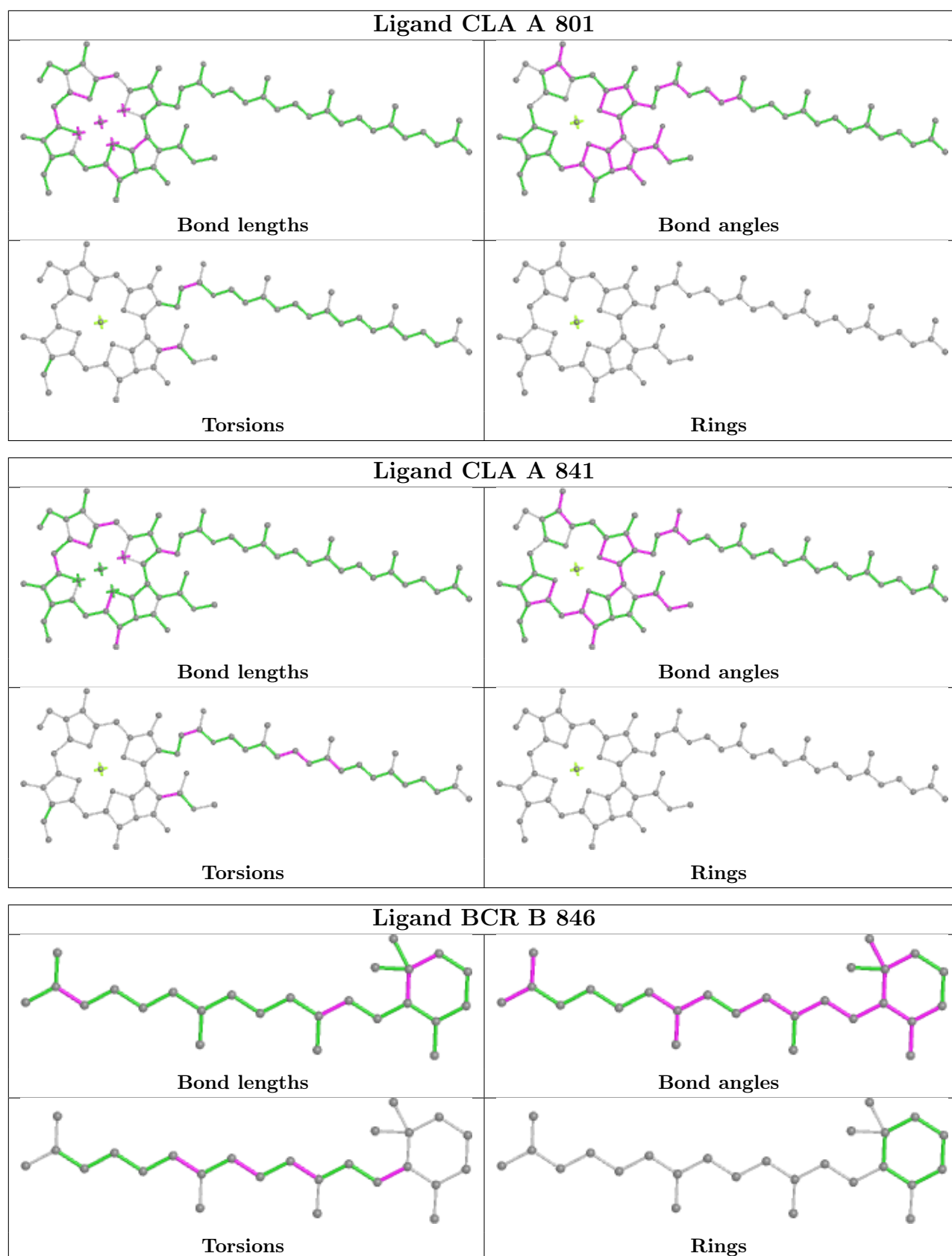


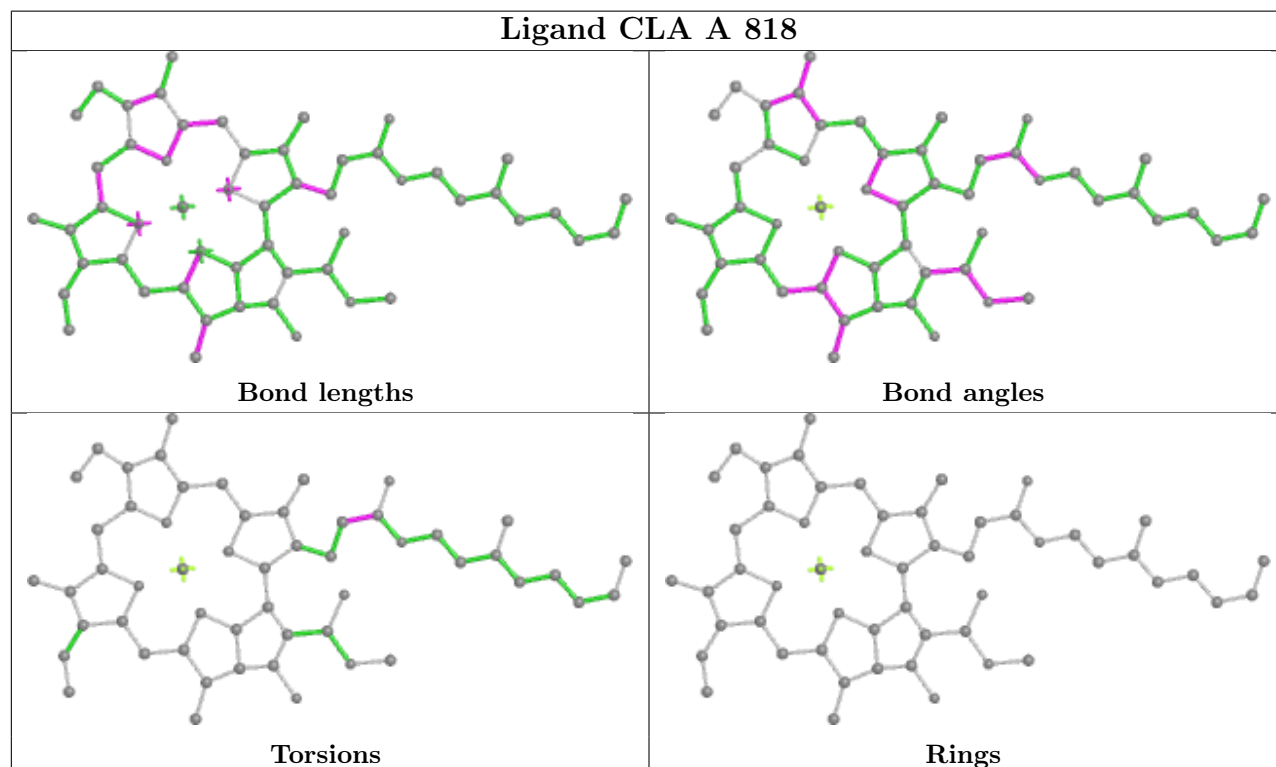
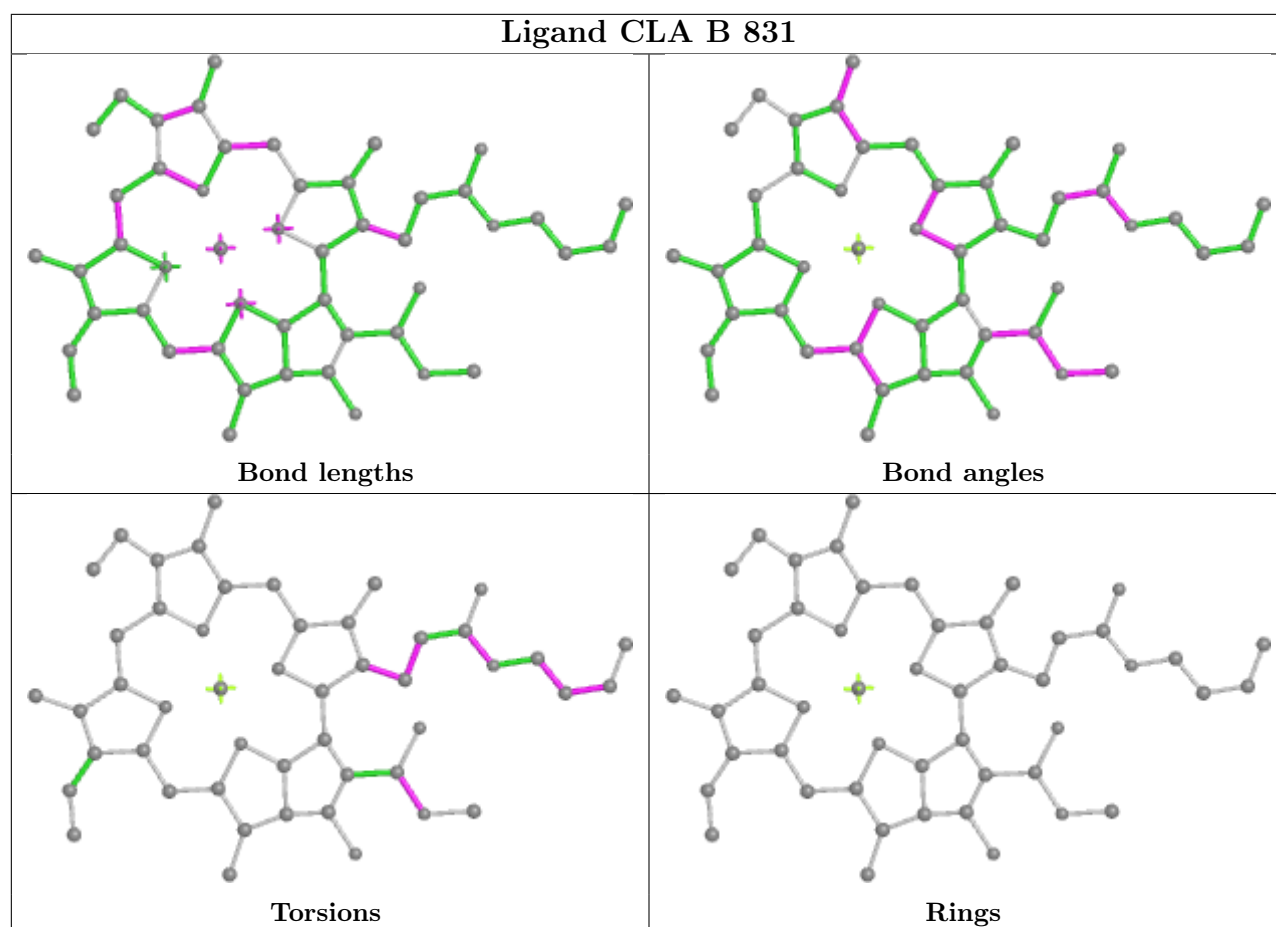


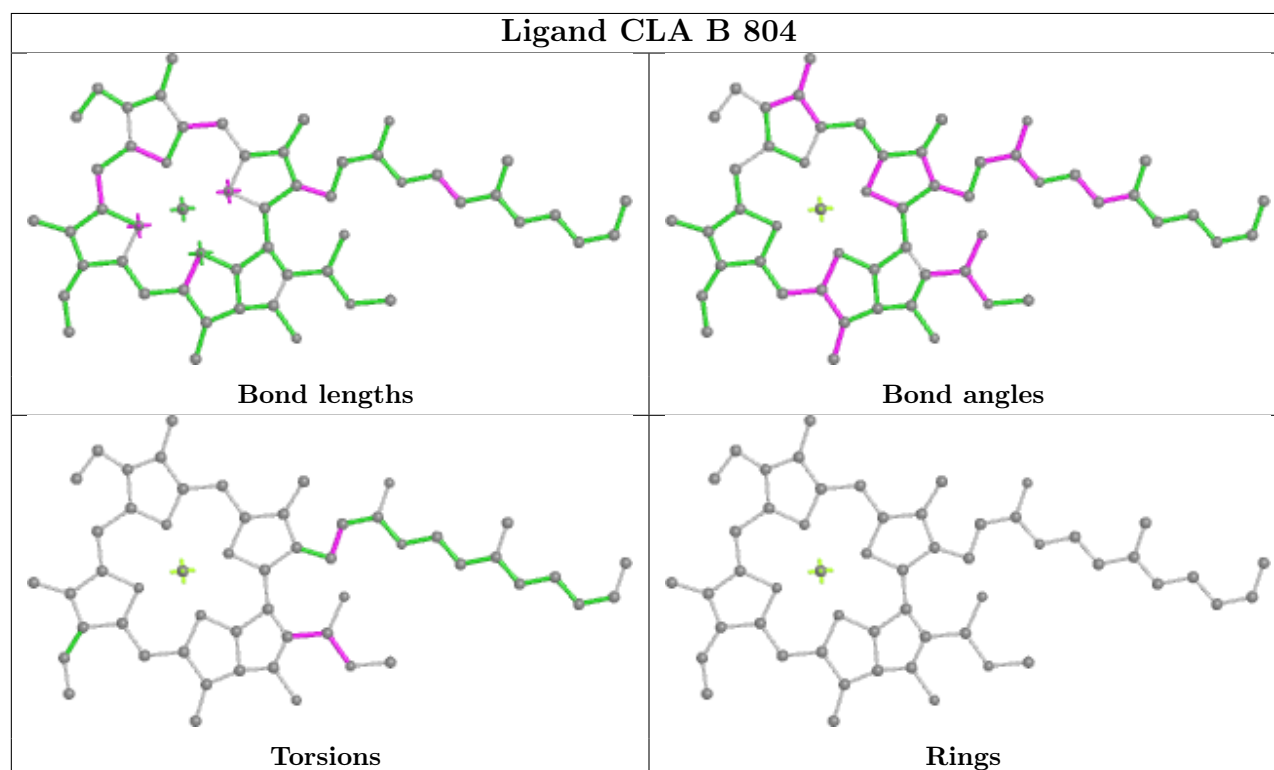
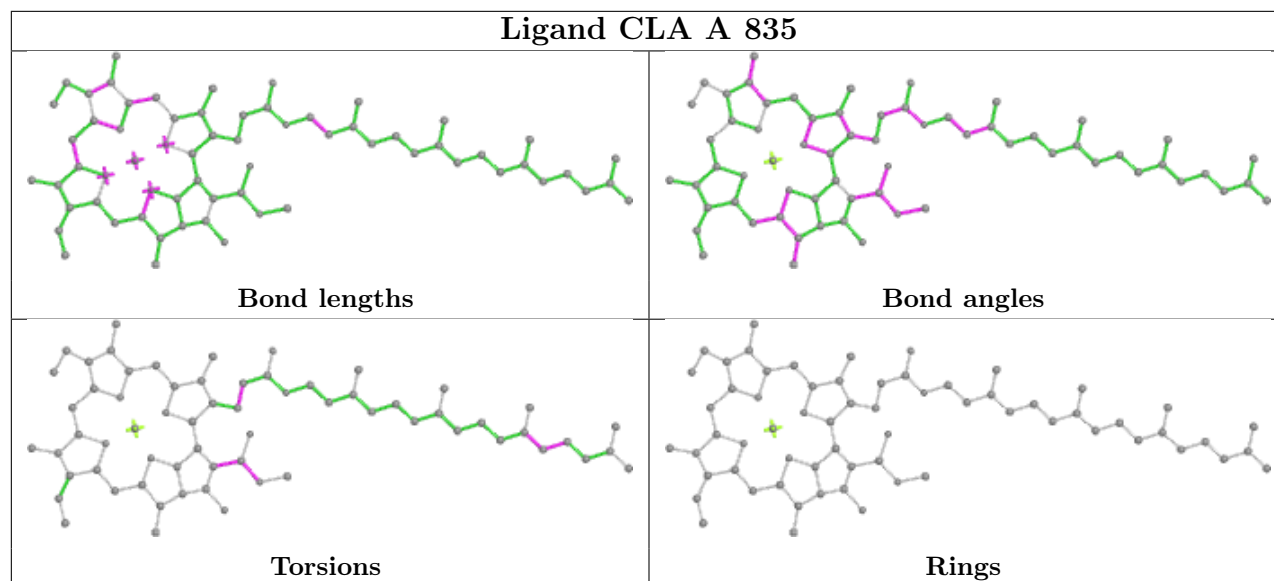
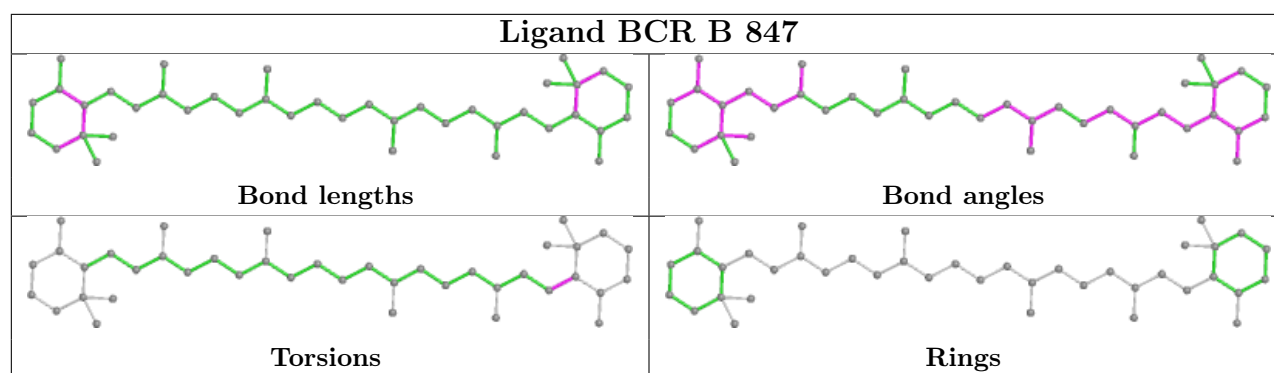


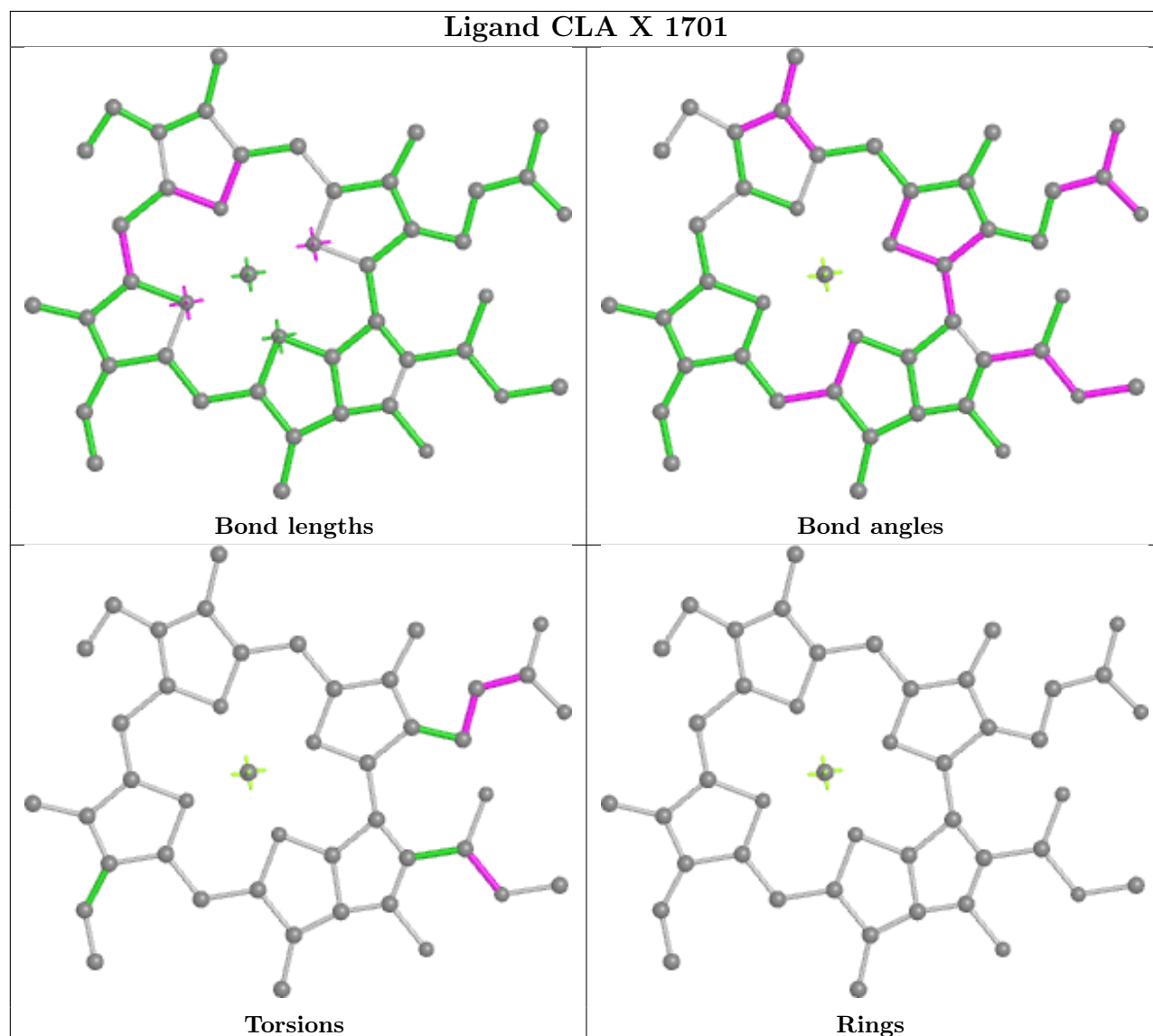
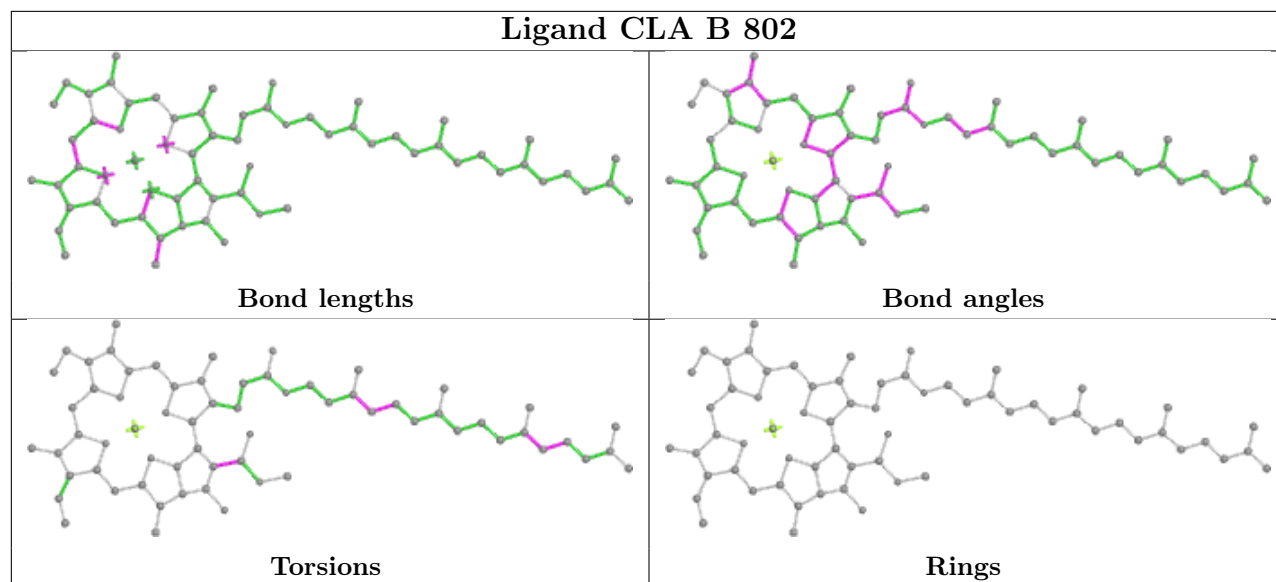


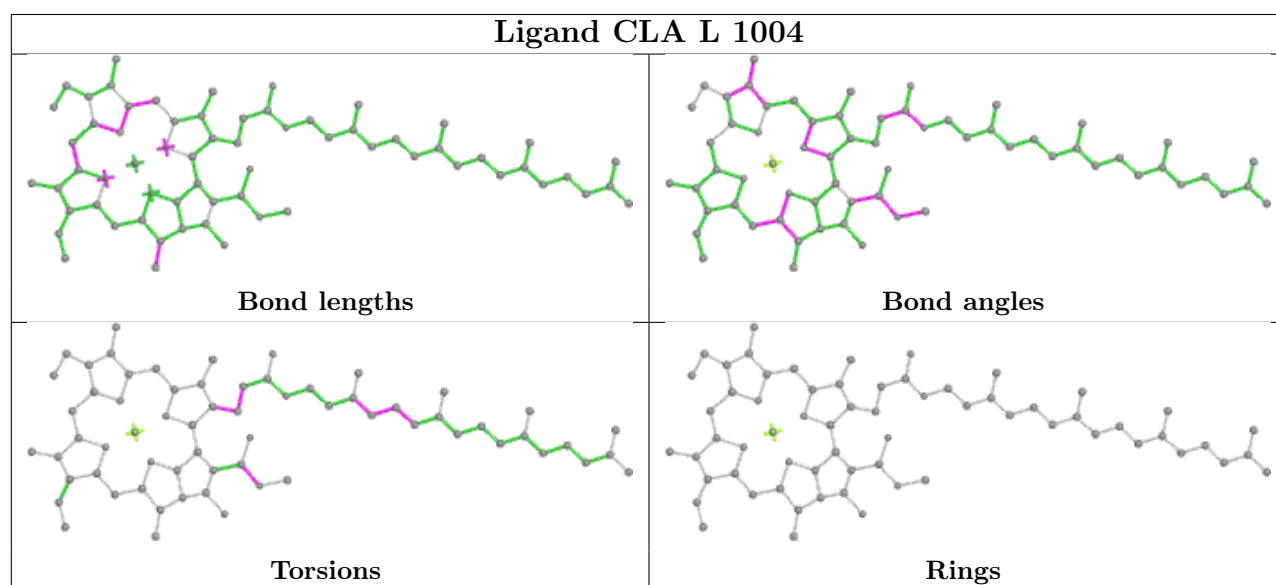
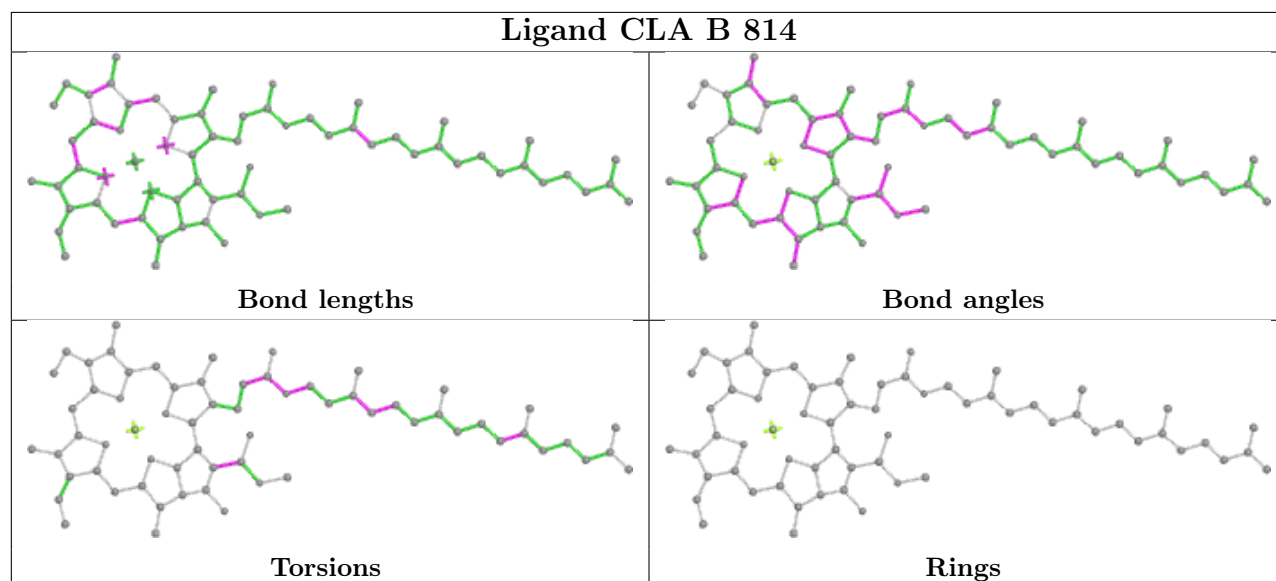
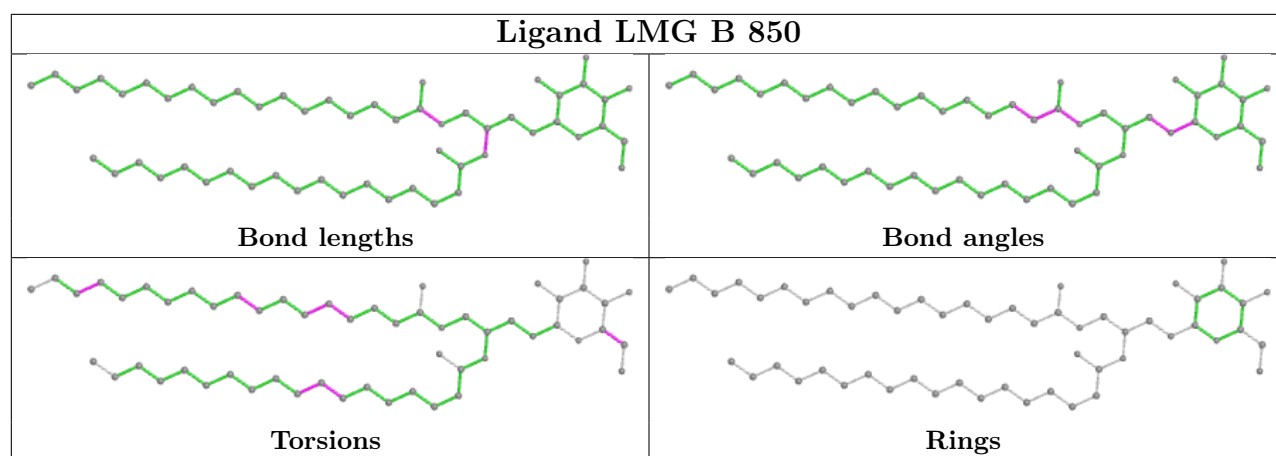




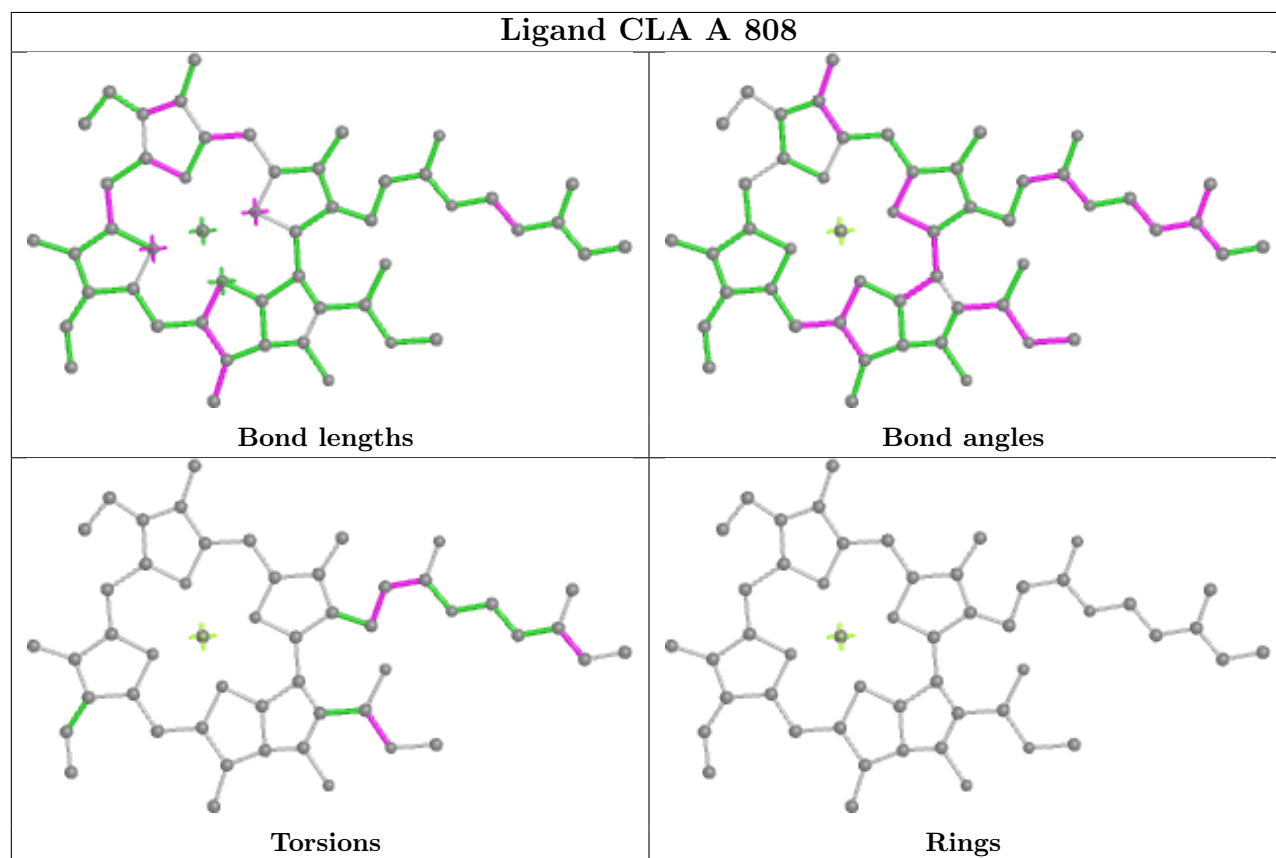
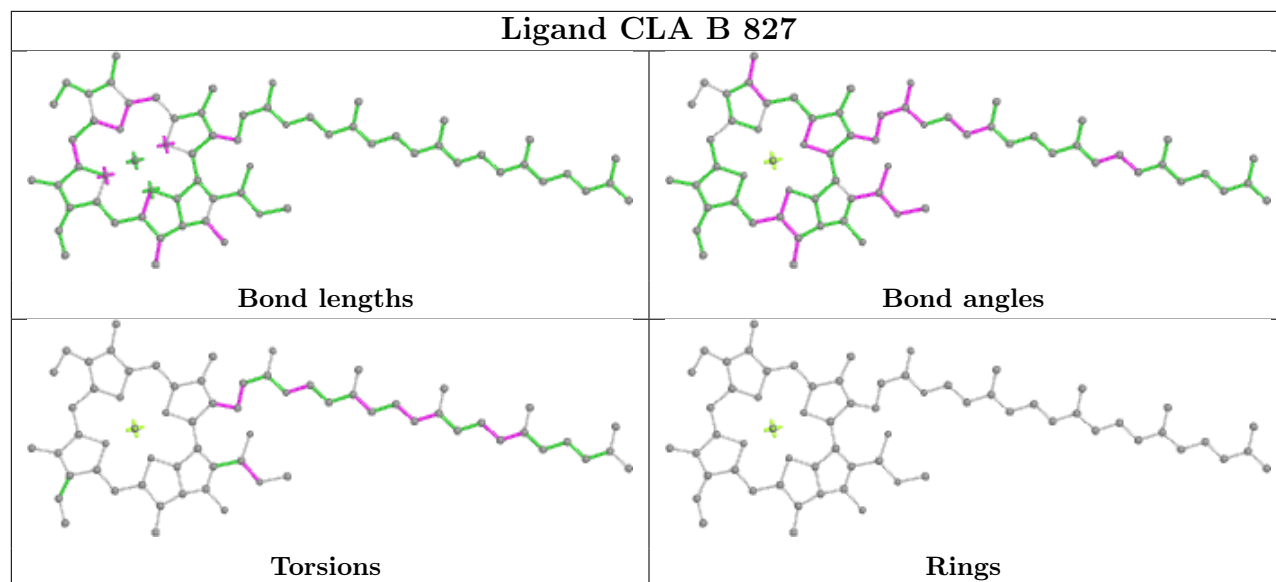


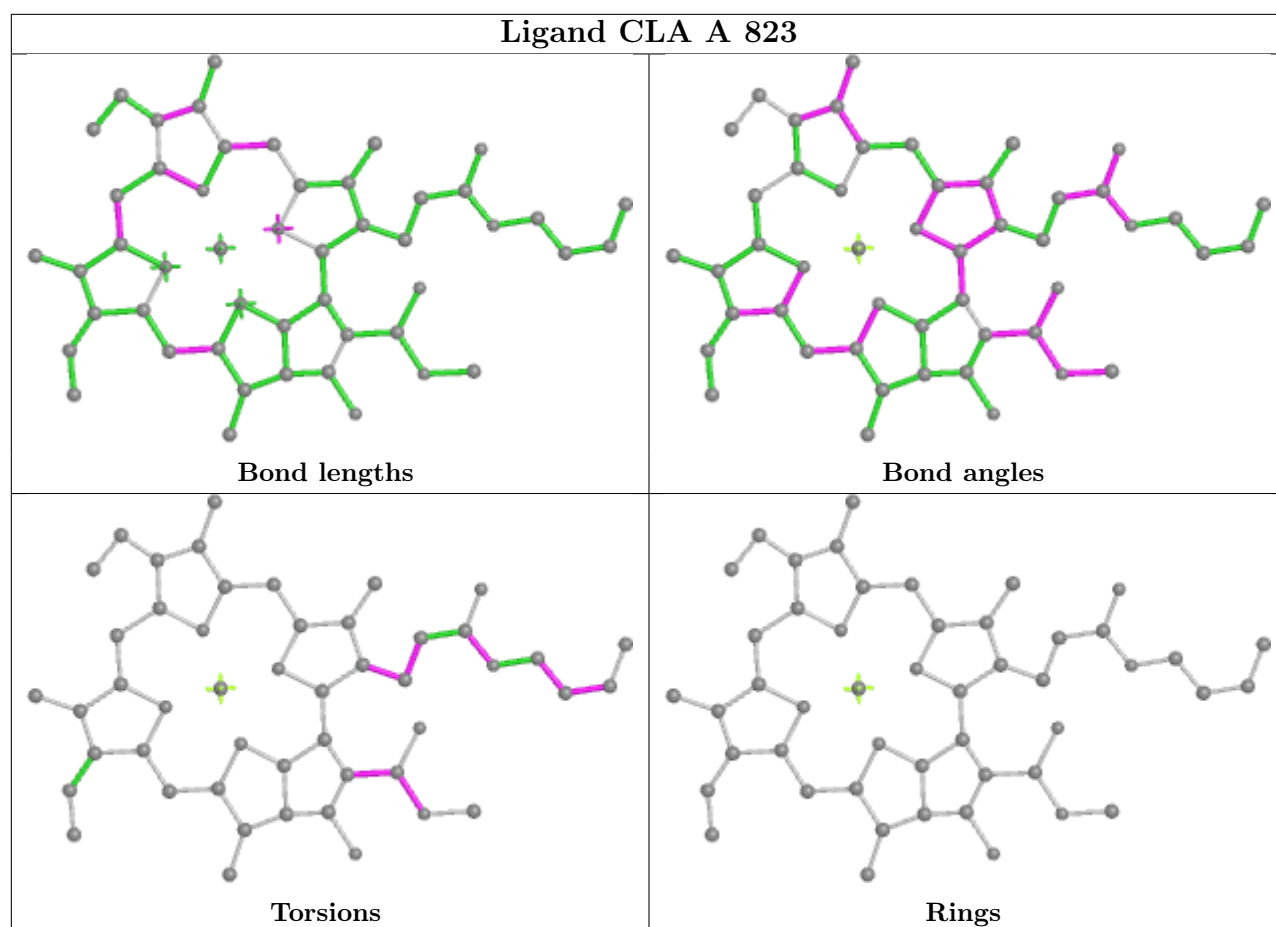




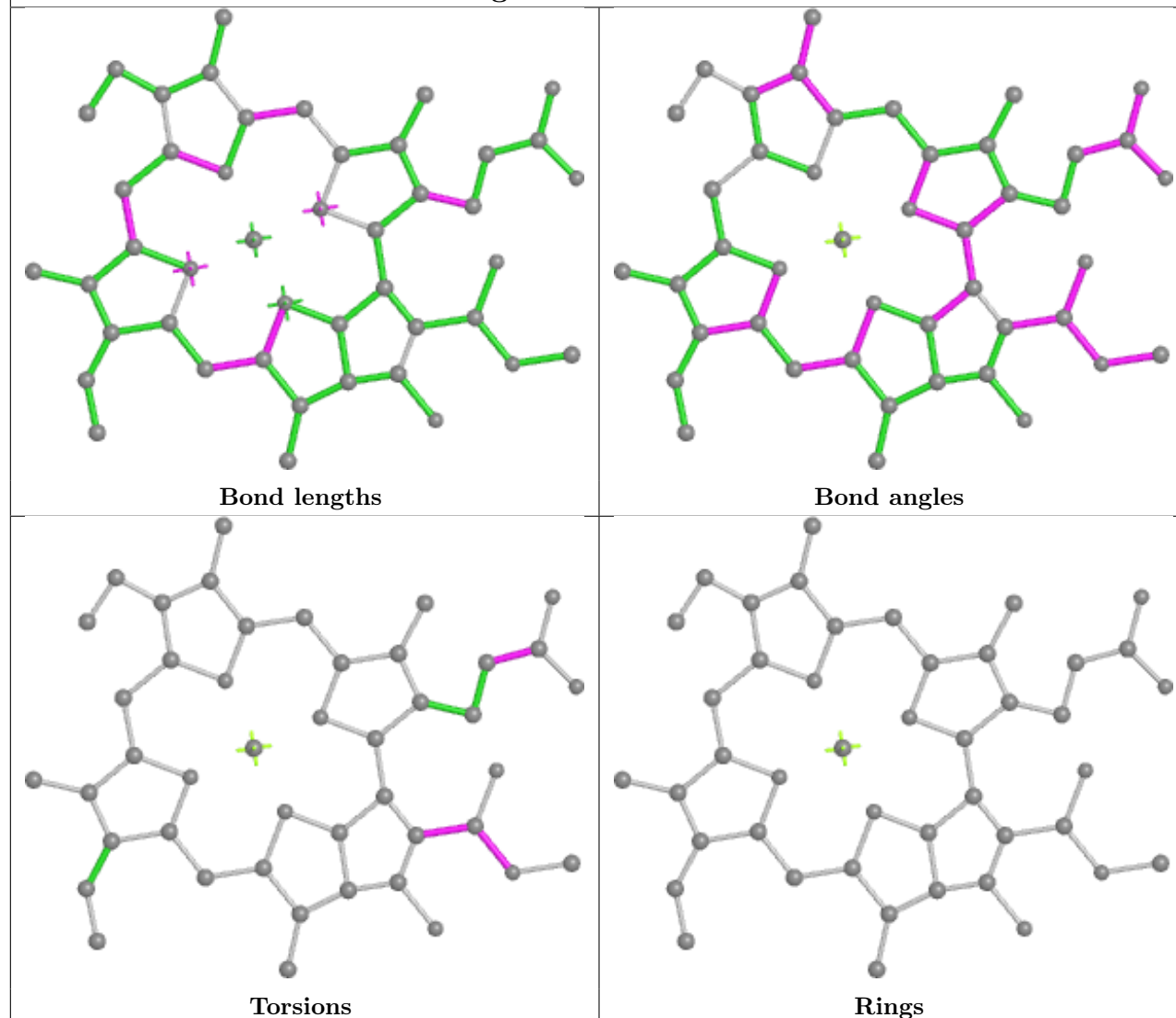




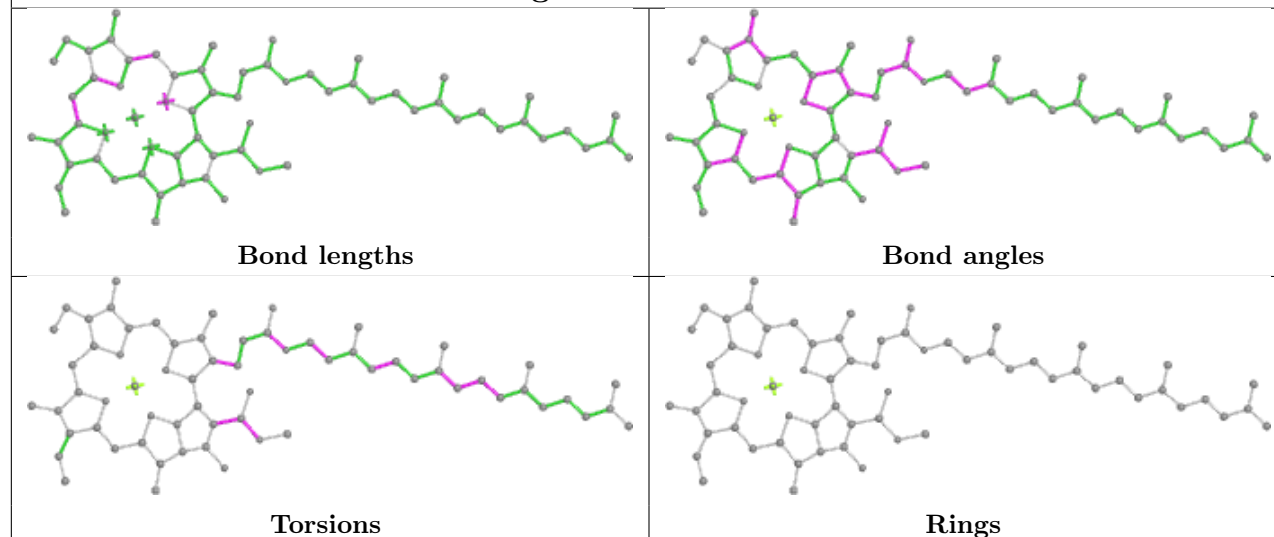


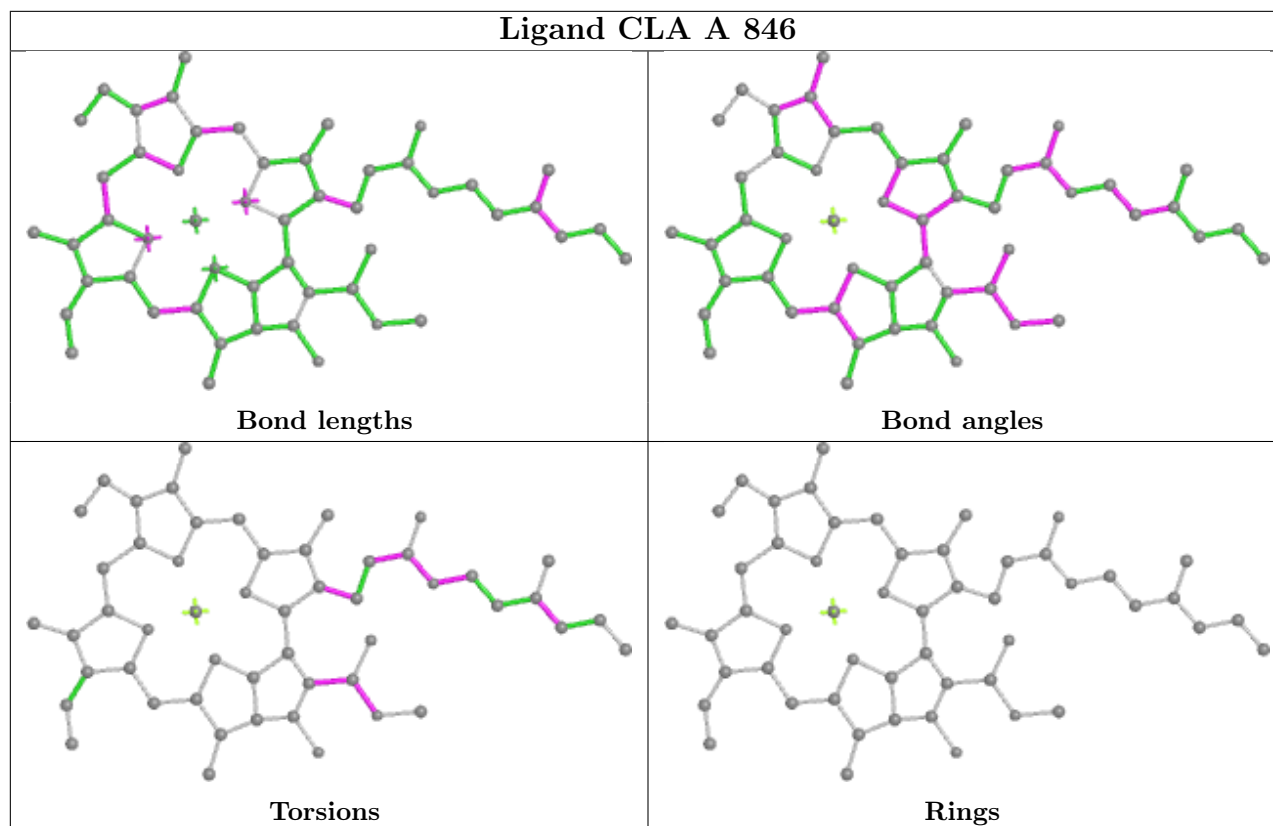
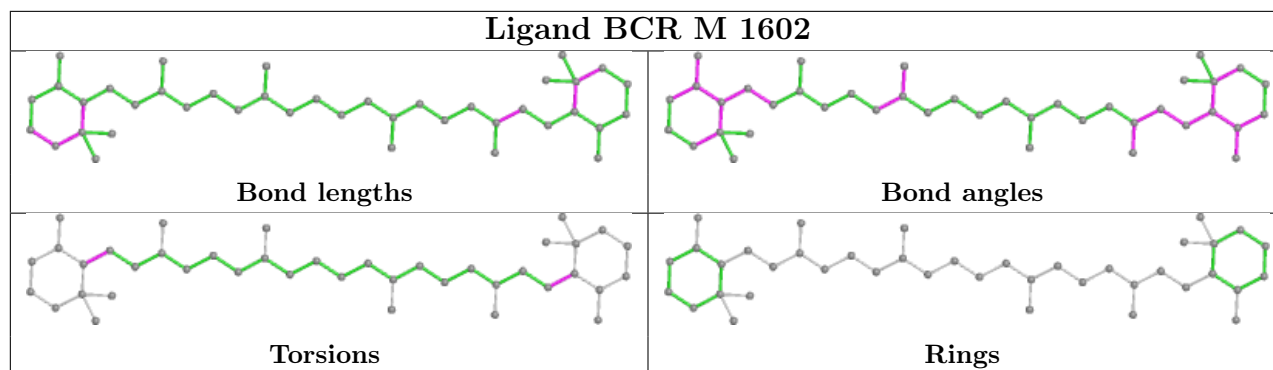


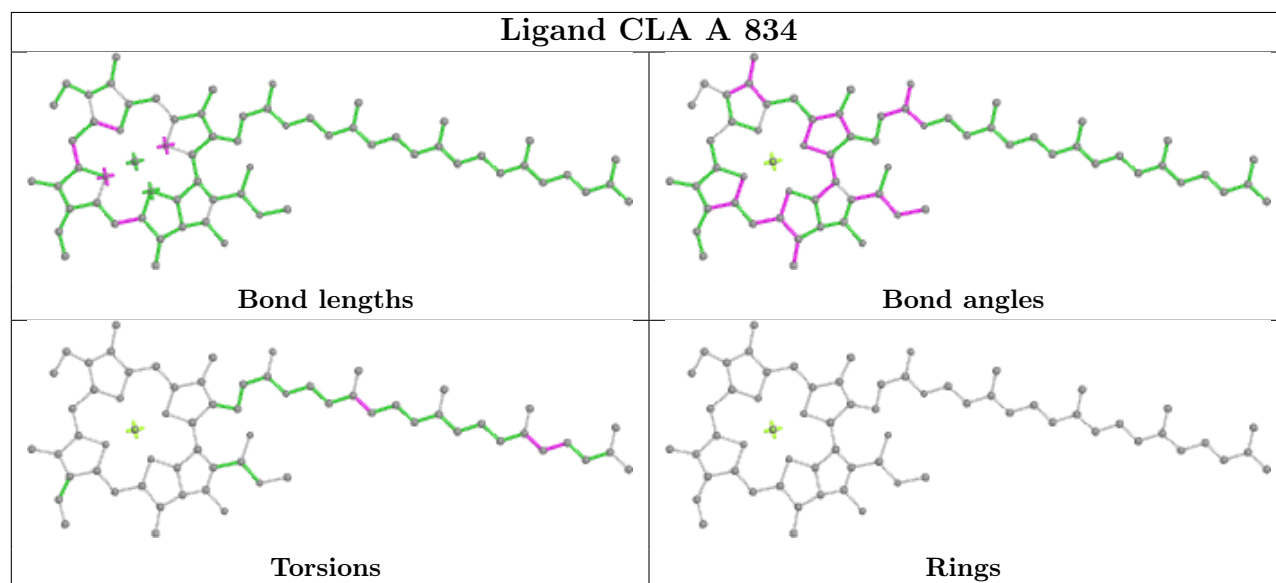
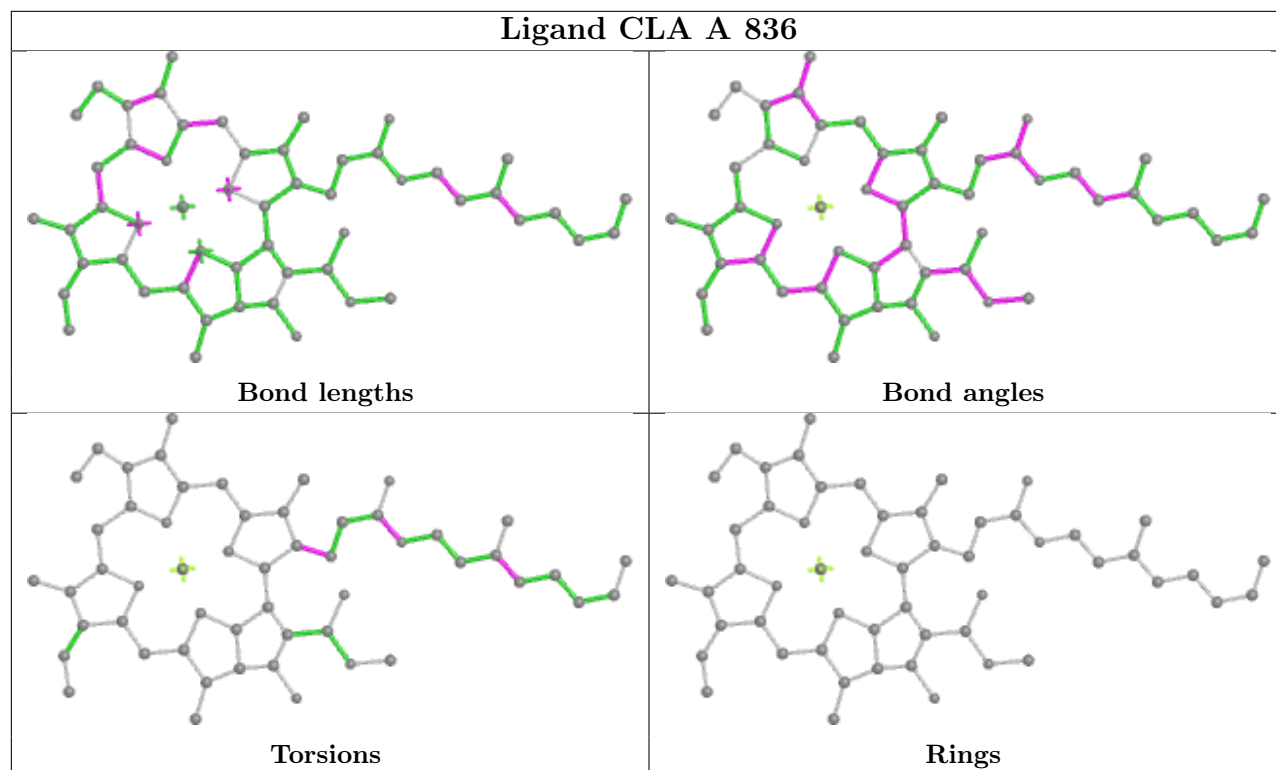
## Ligand CLA B 821



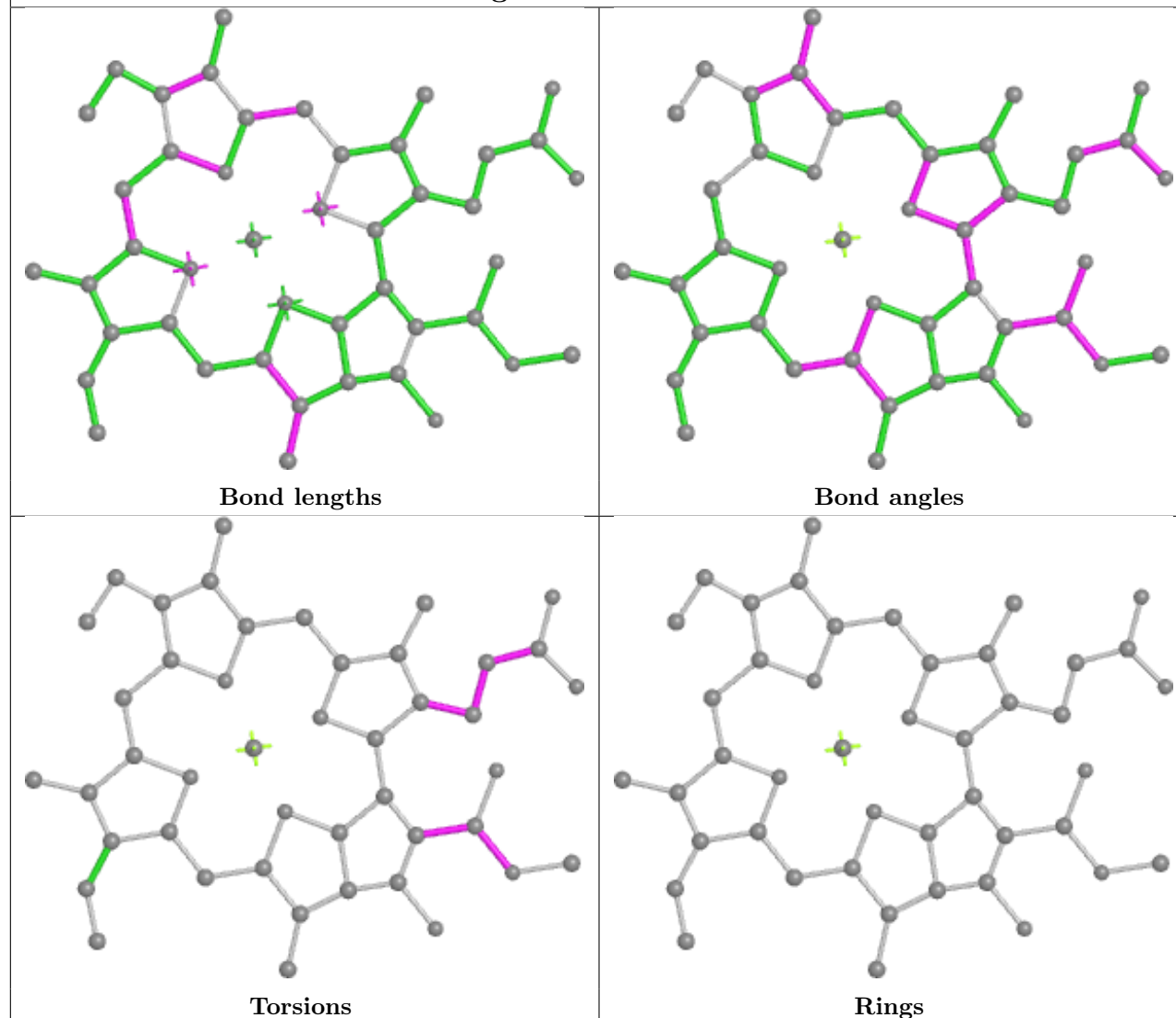
## Ligand CLA A 806



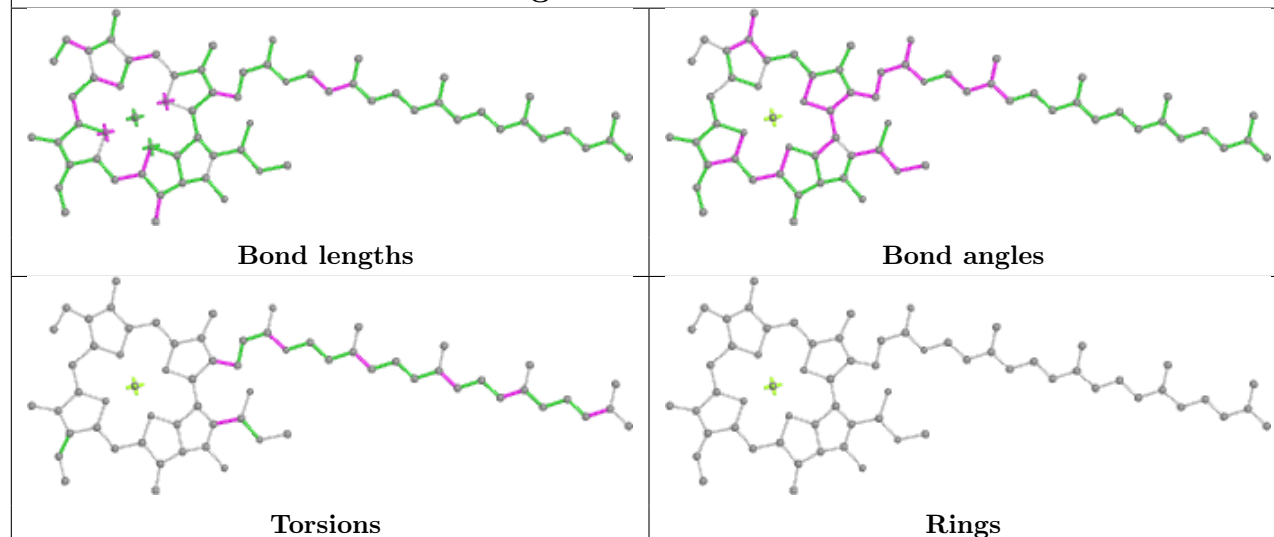


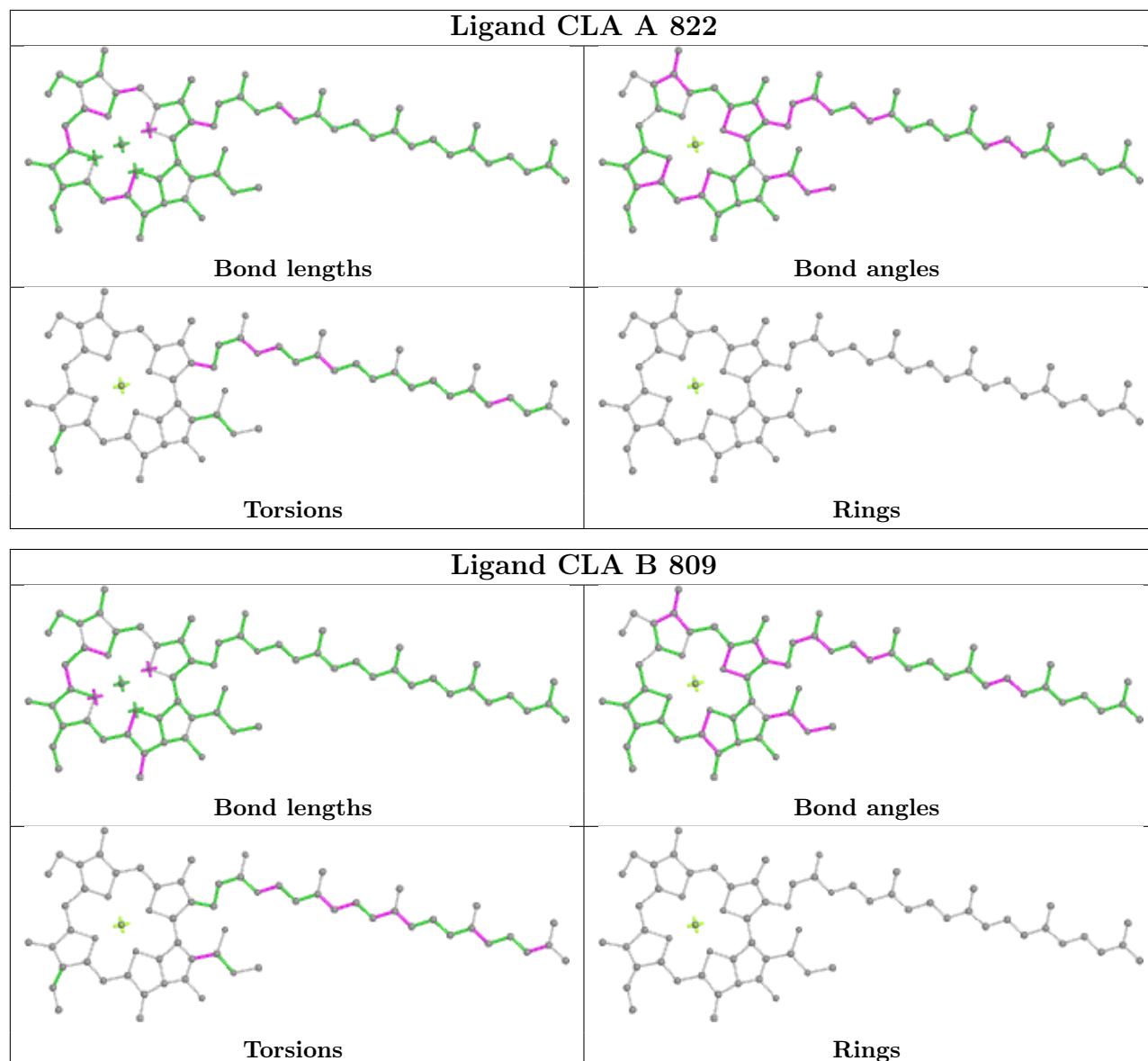


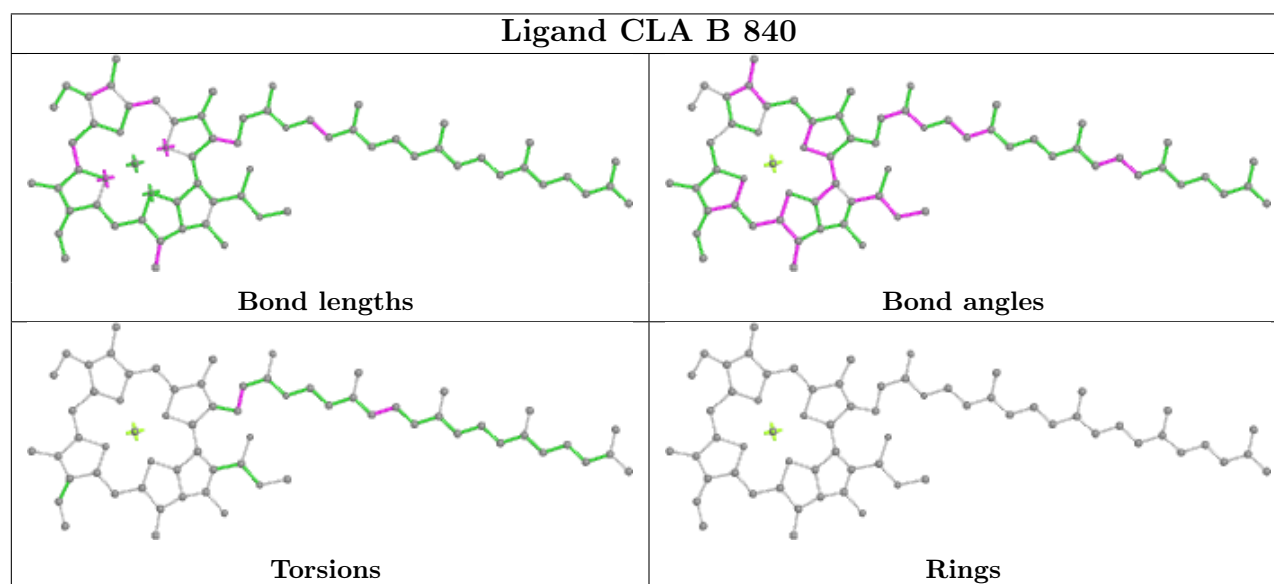
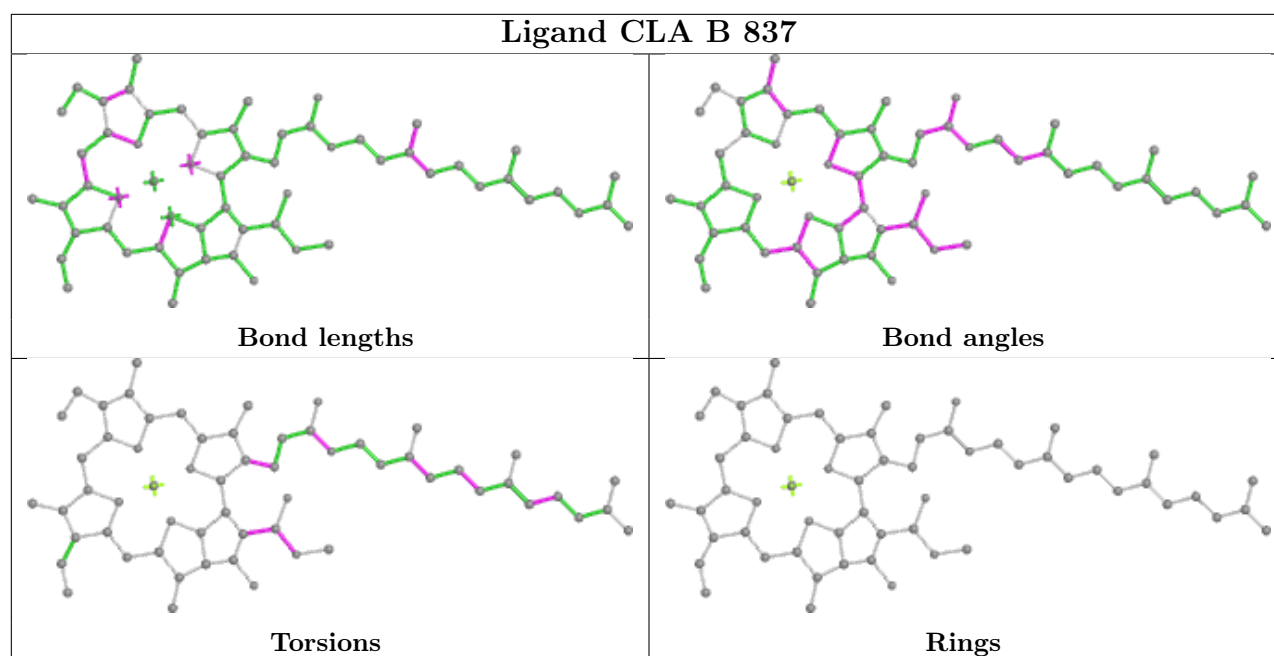
## Ligand CLA B 815



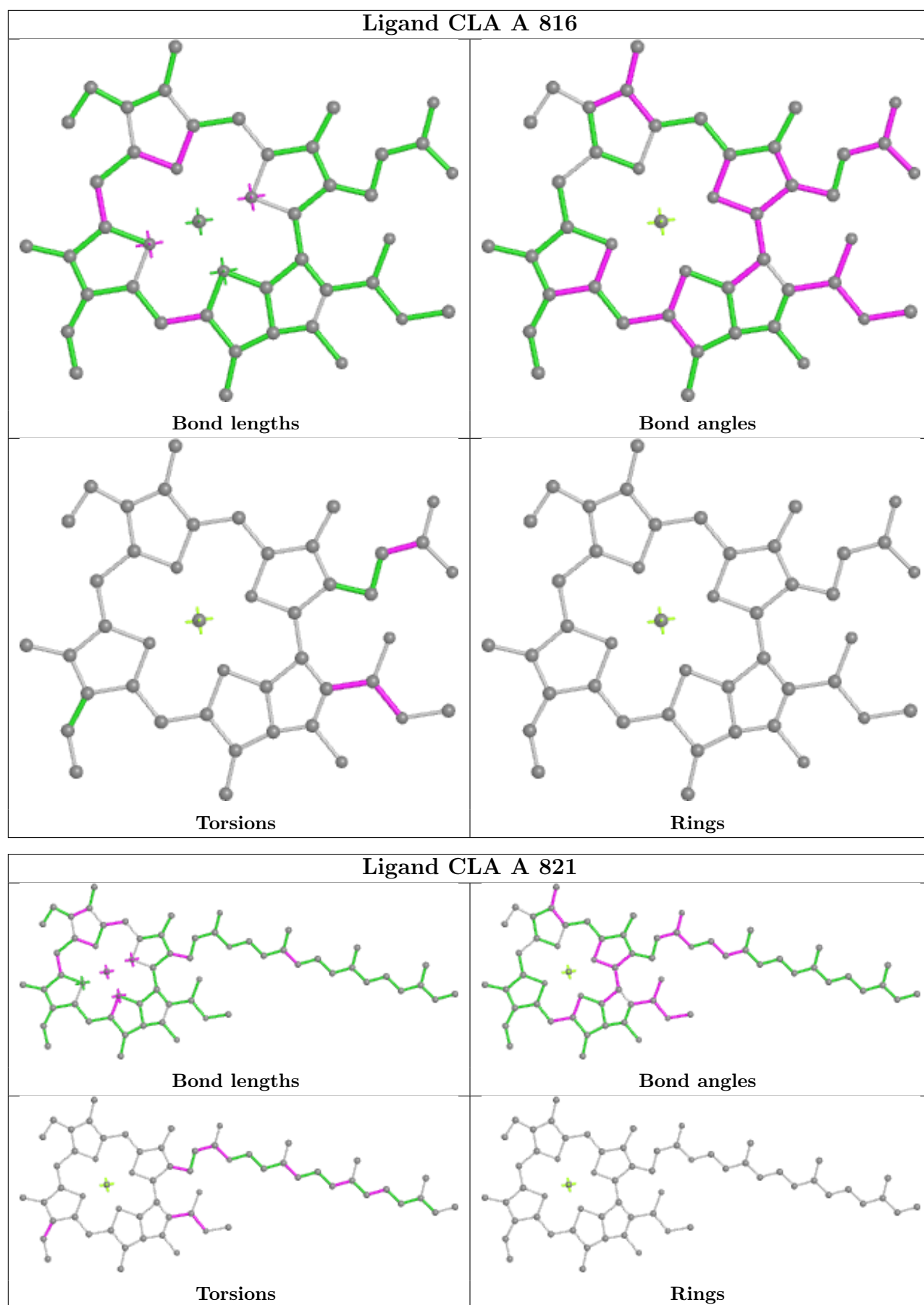
## Ligand CLA A 820

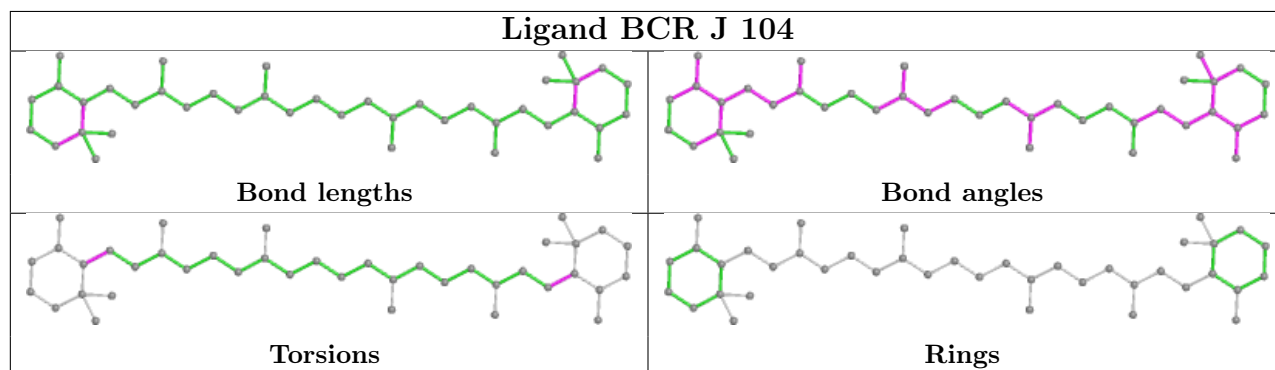
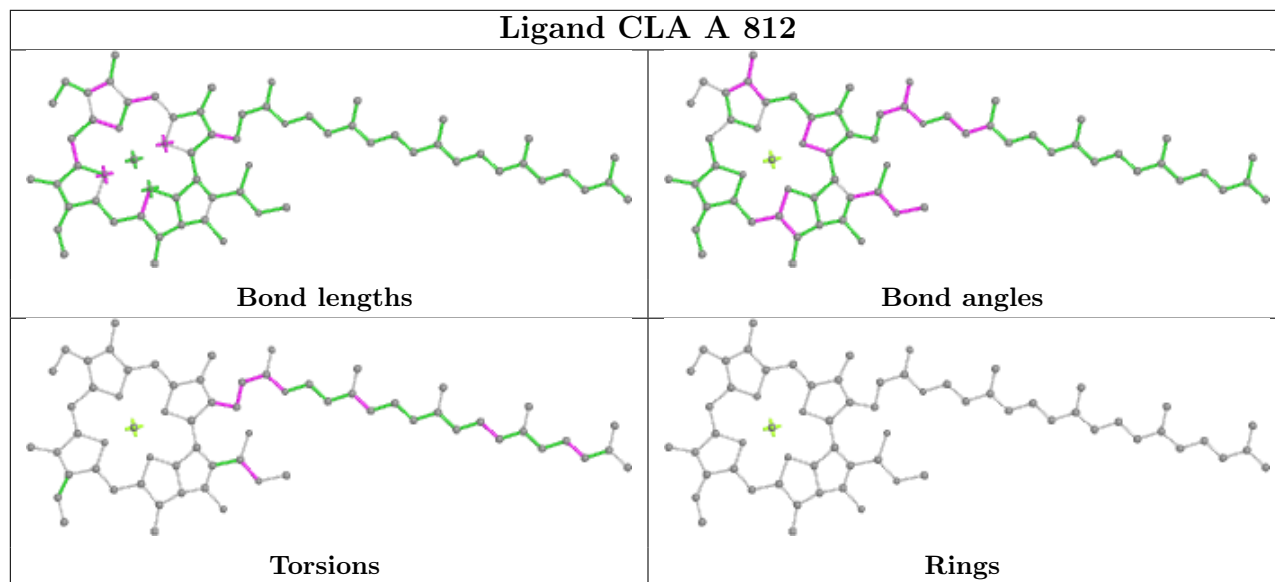
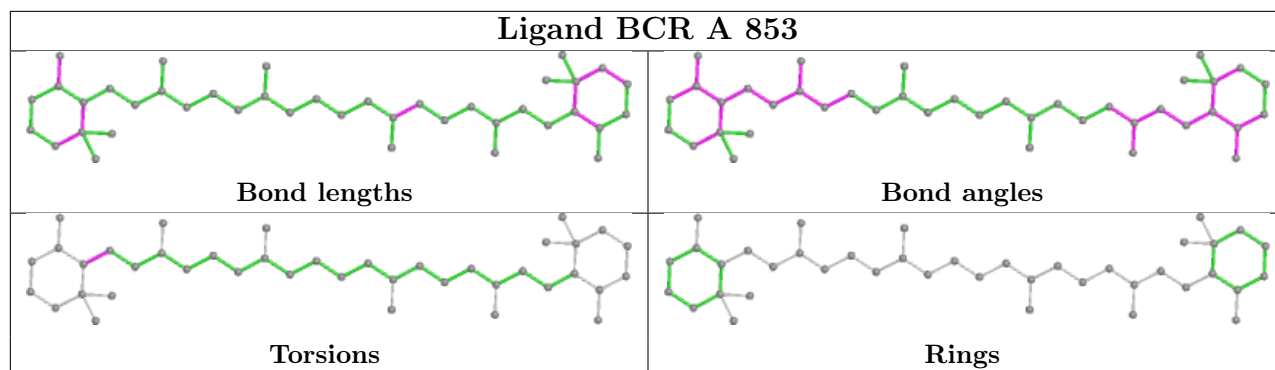
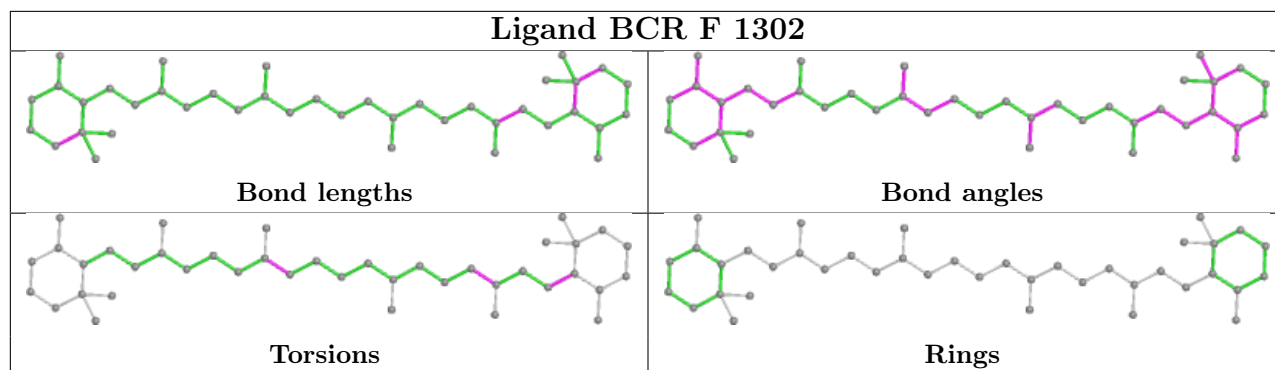


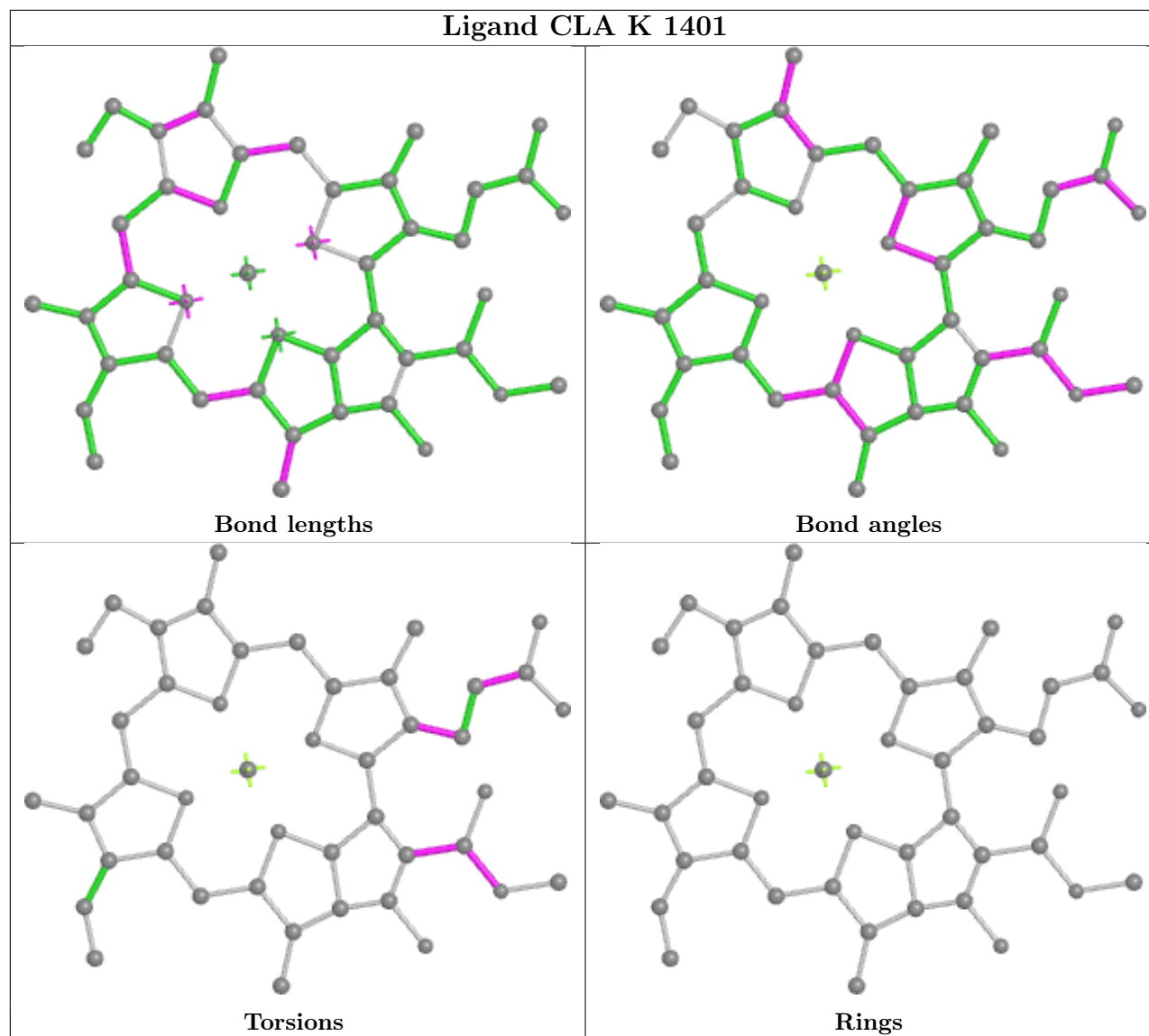
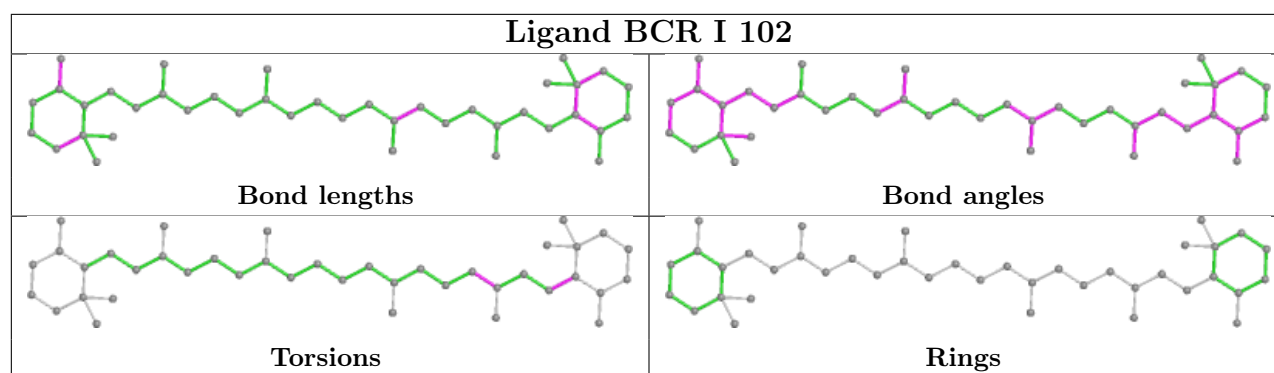


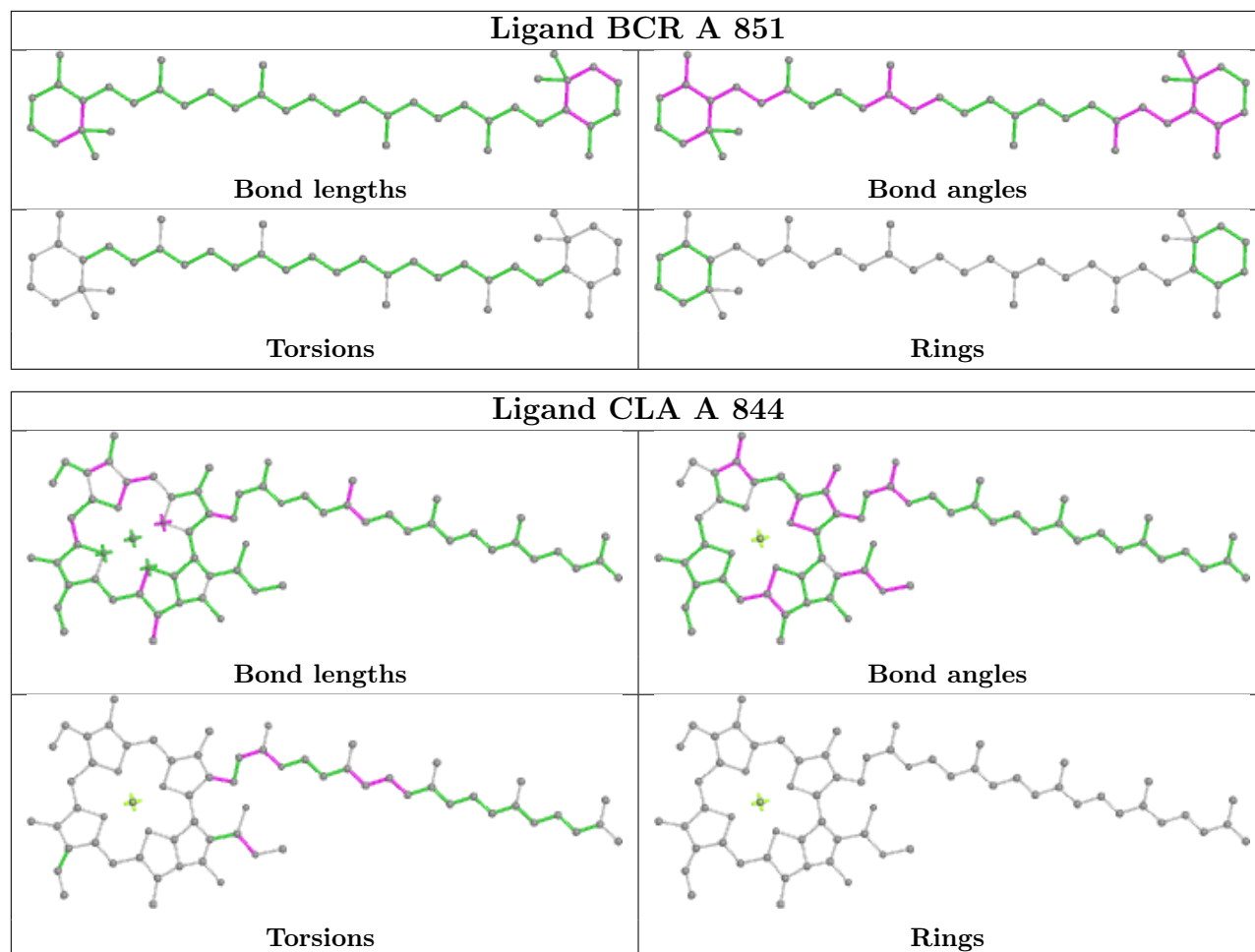


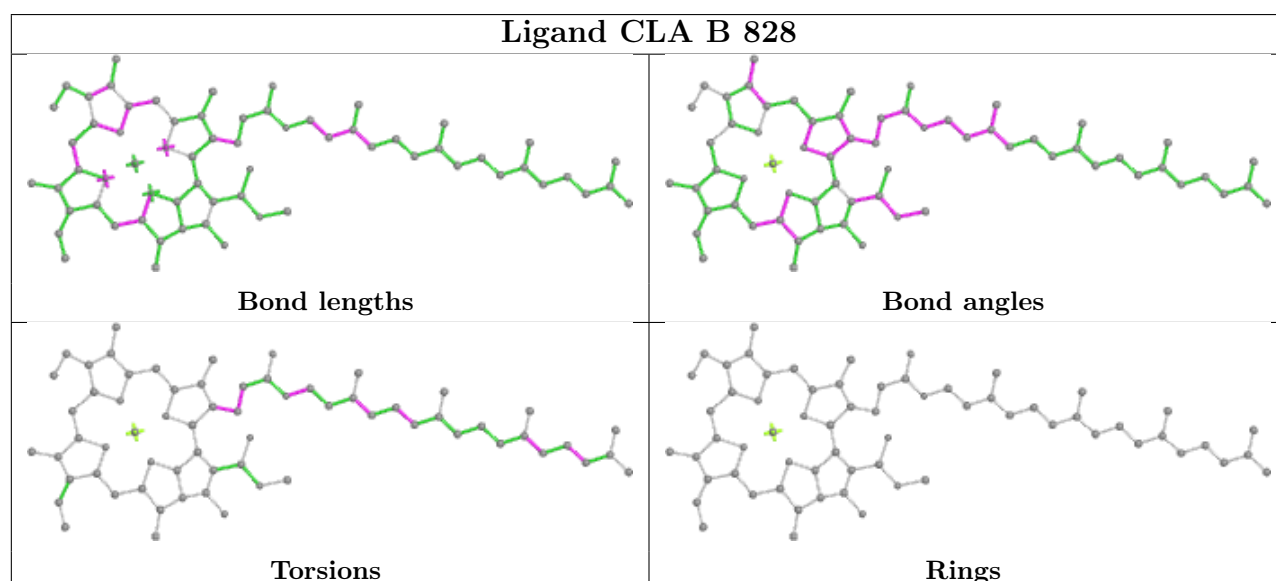
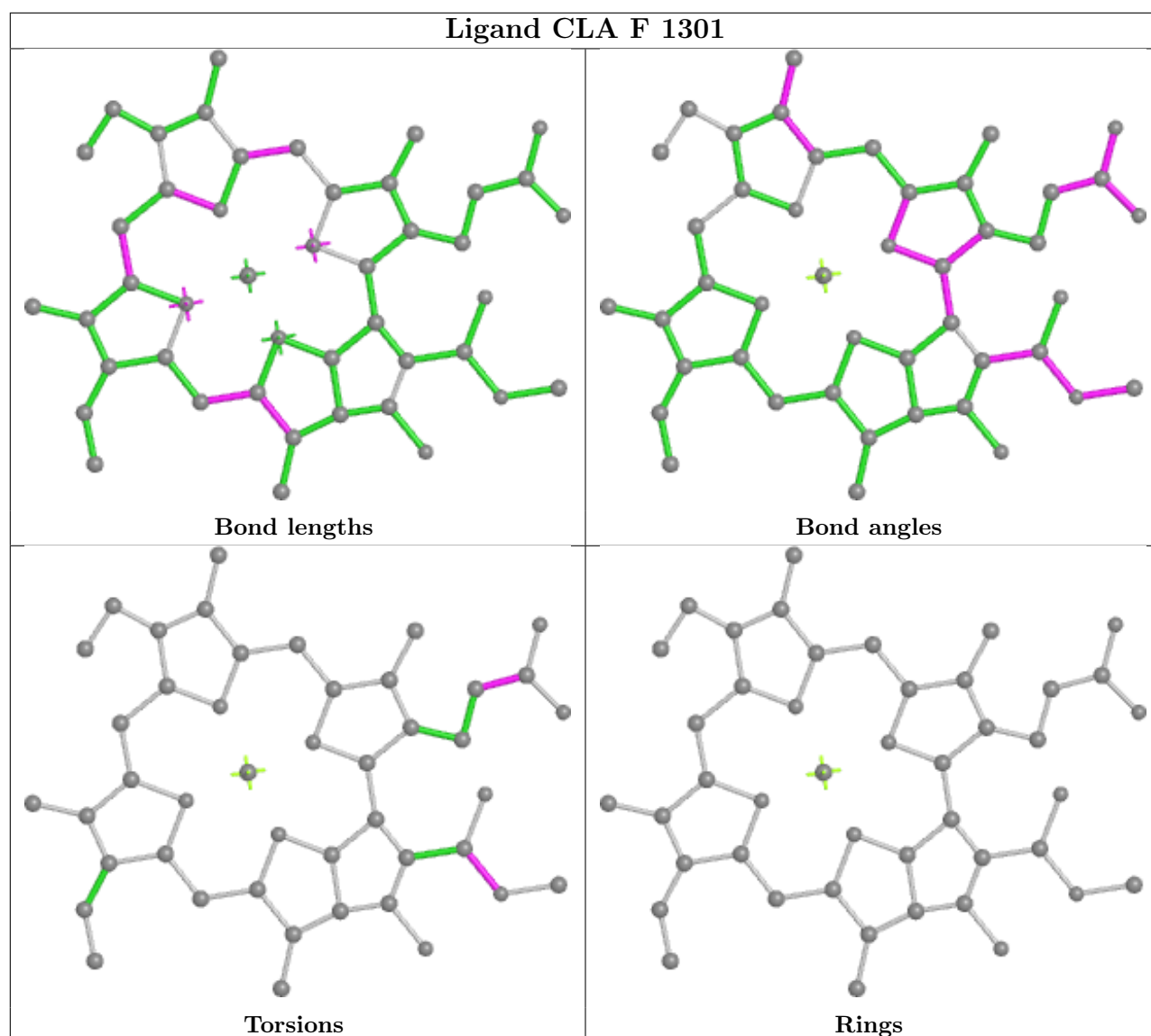


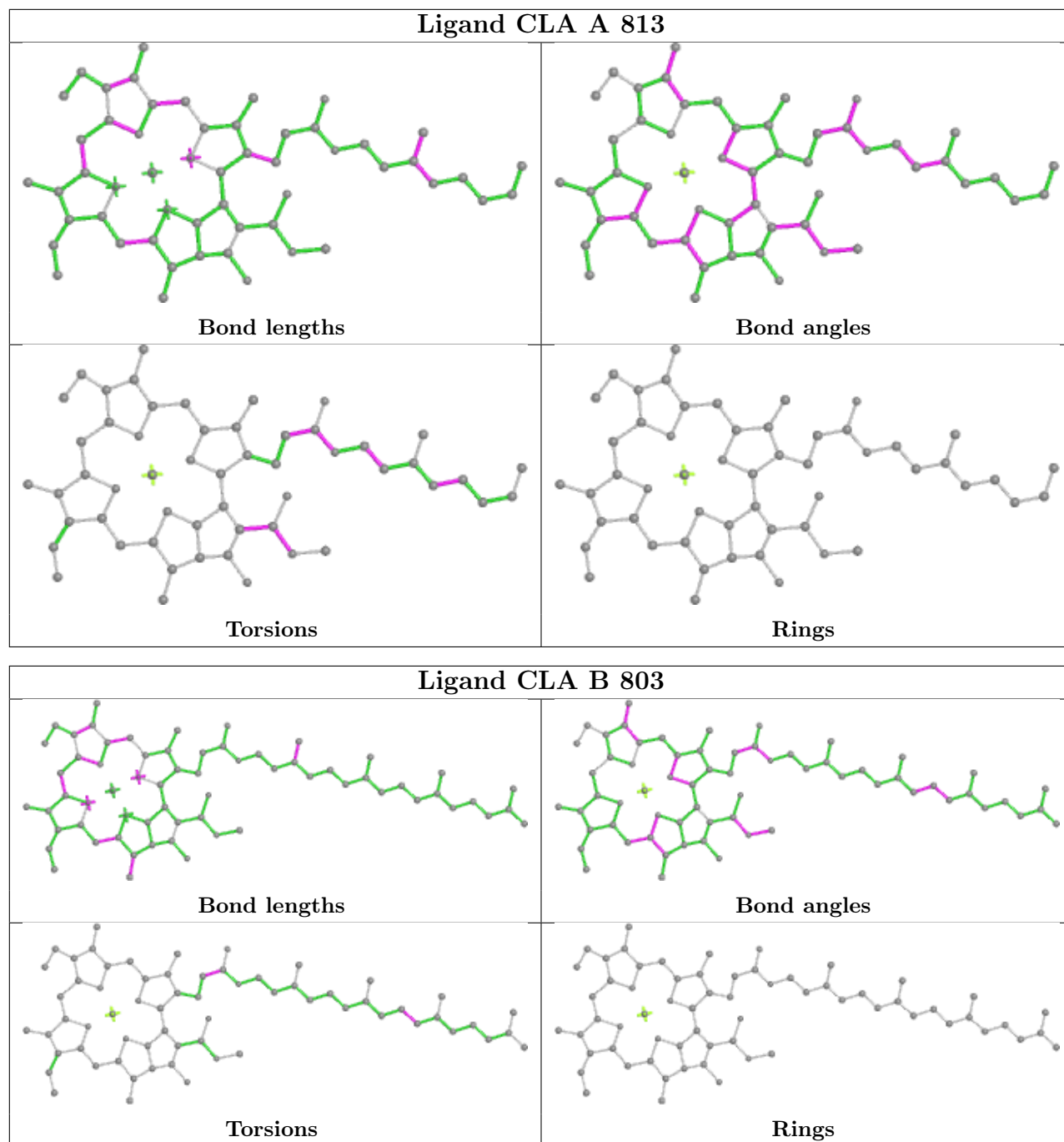


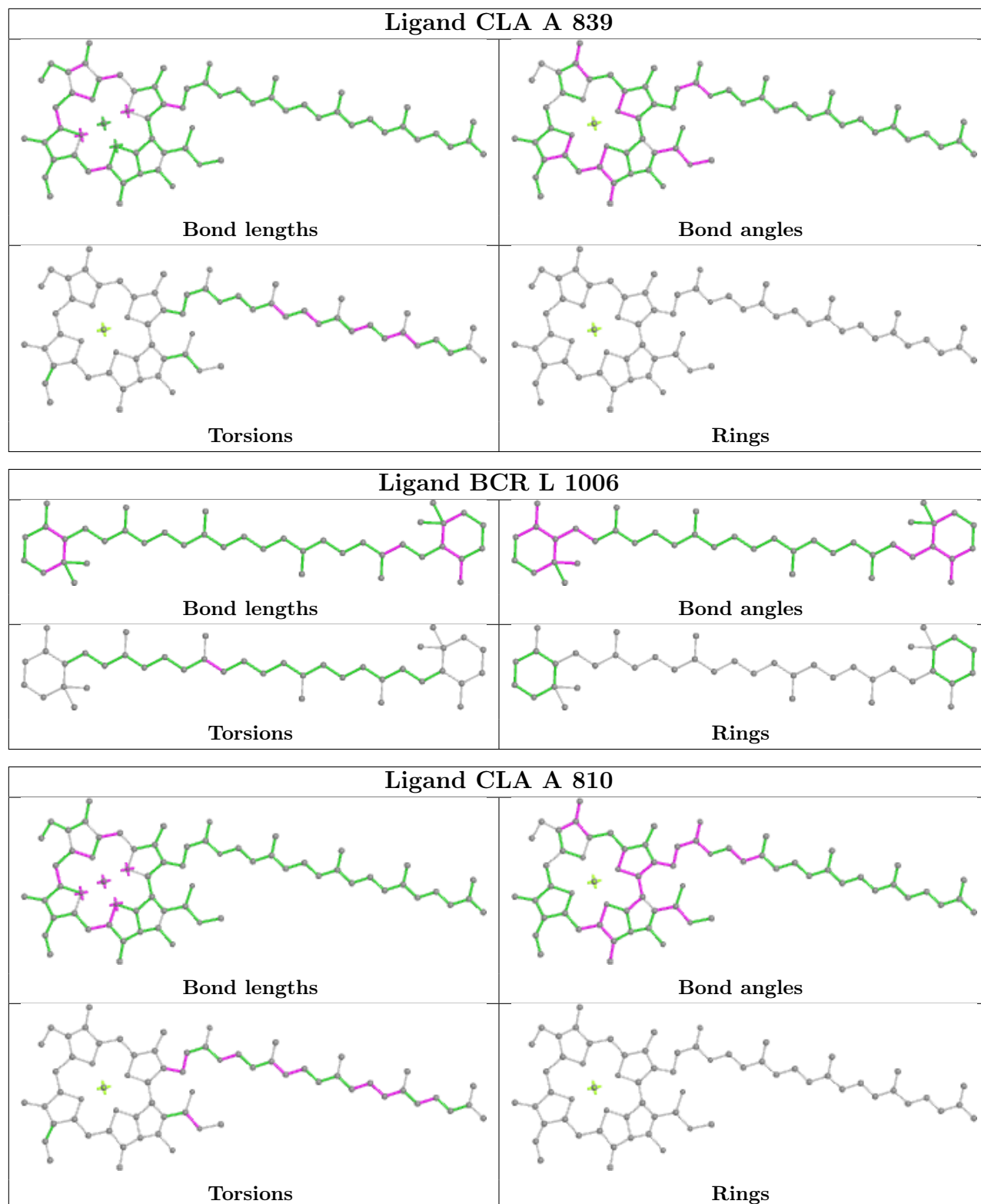


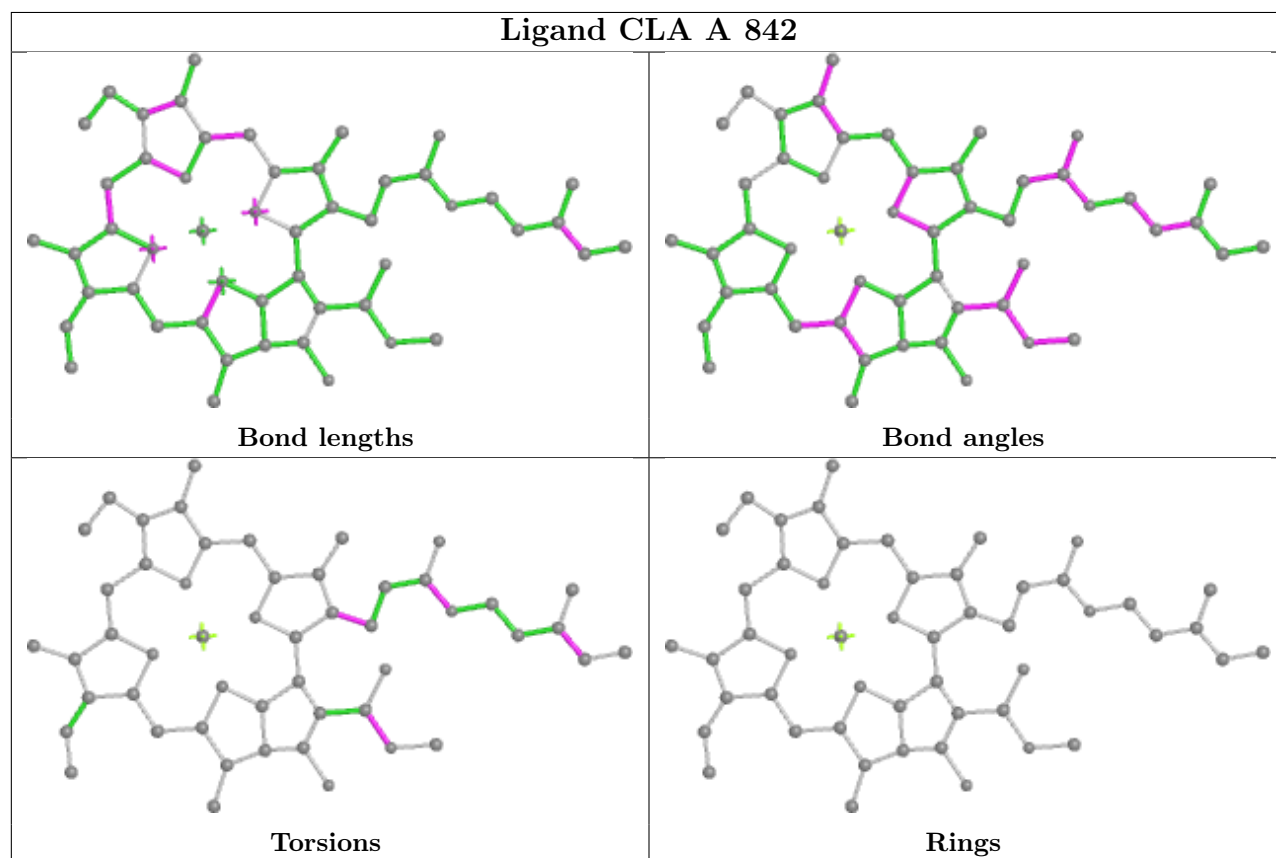
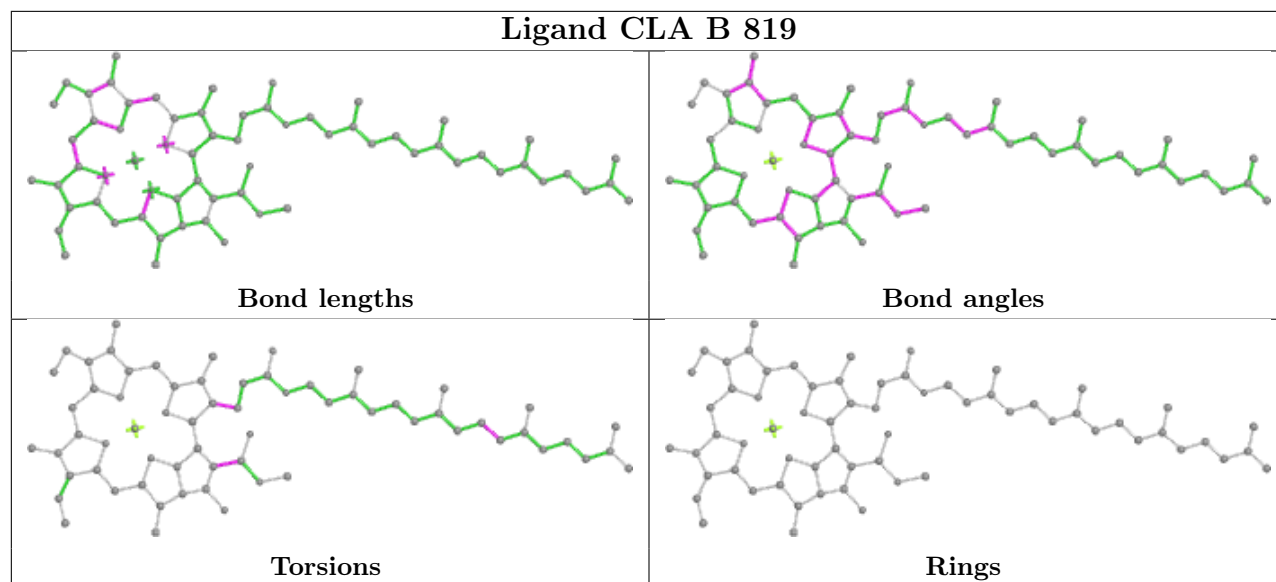




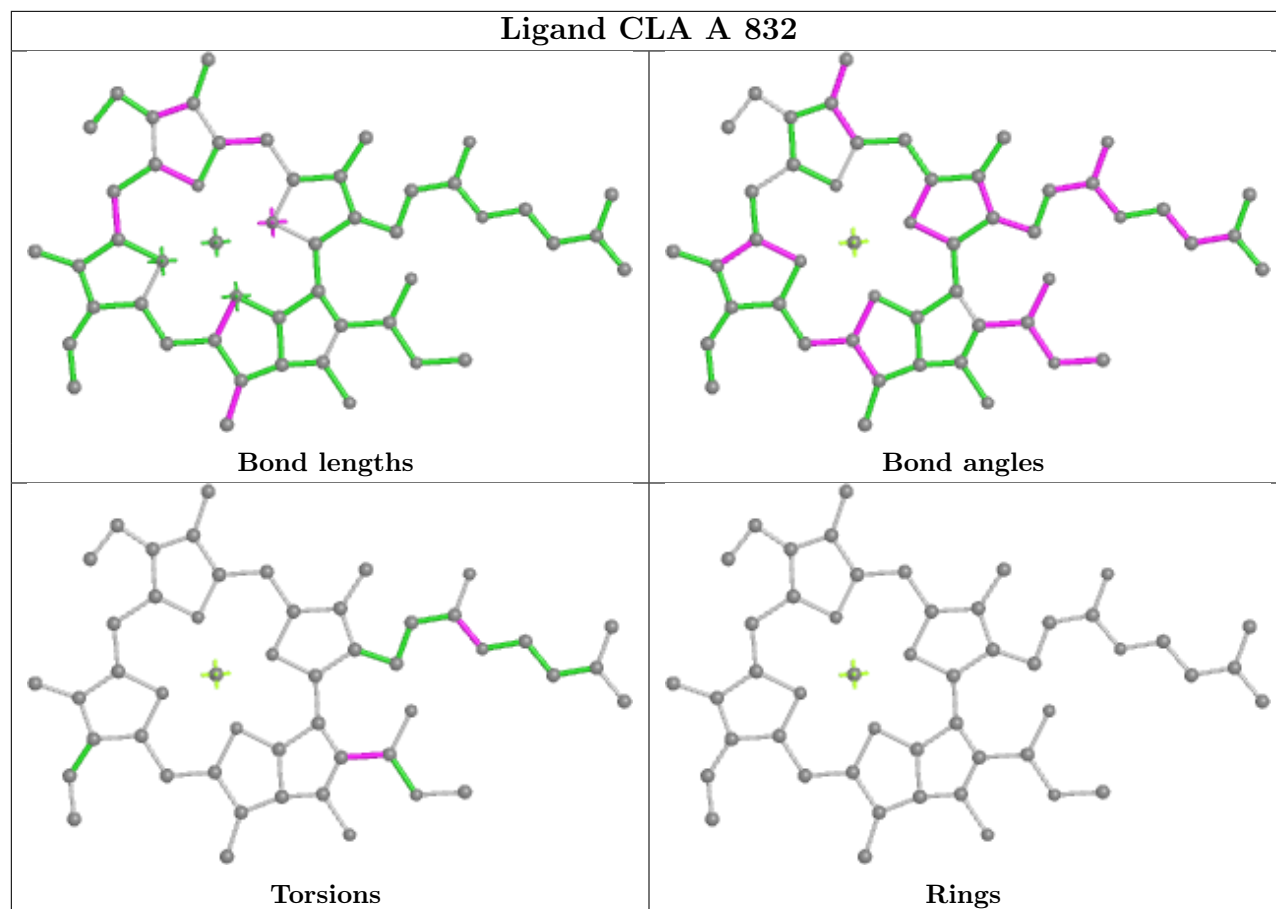


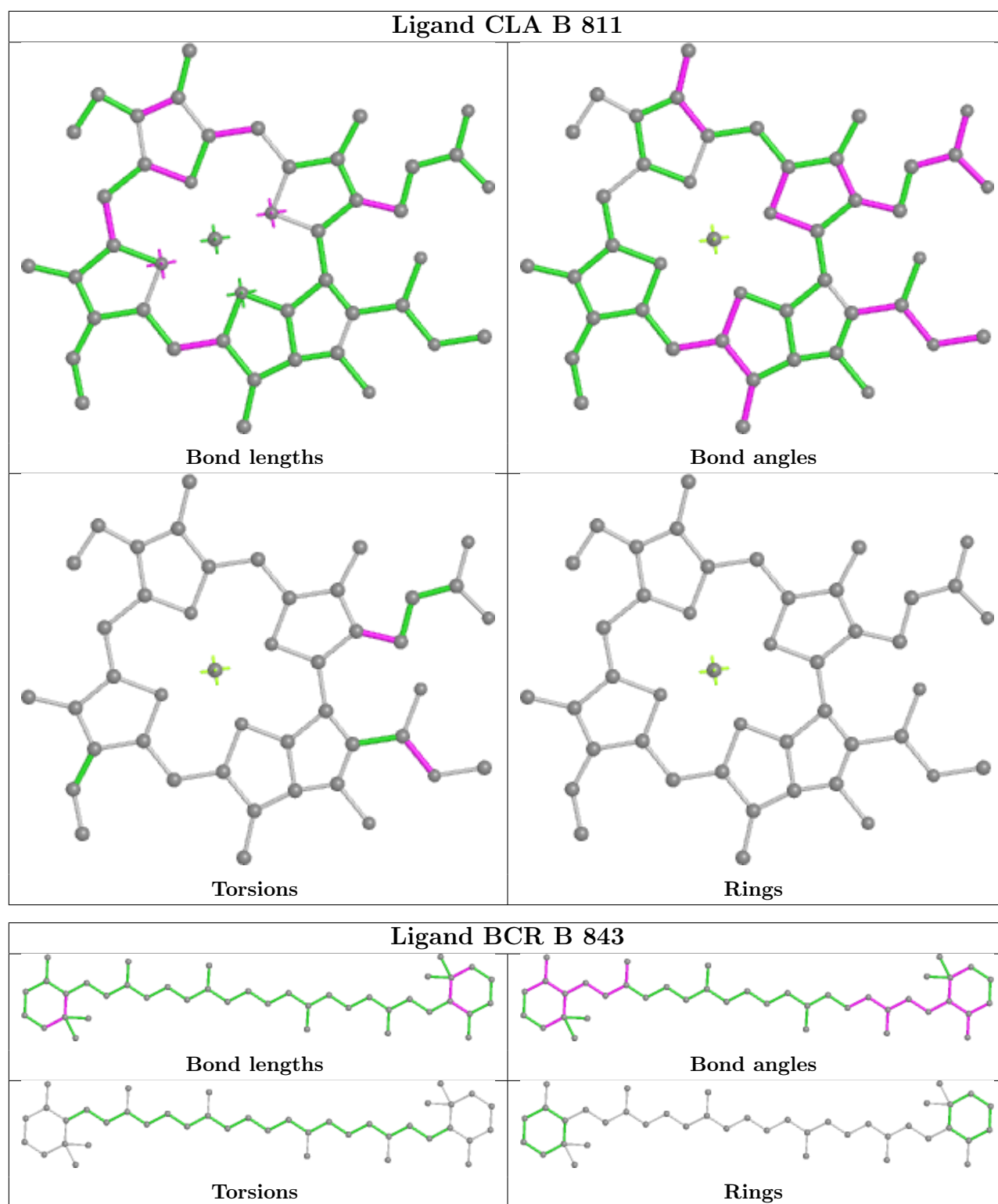


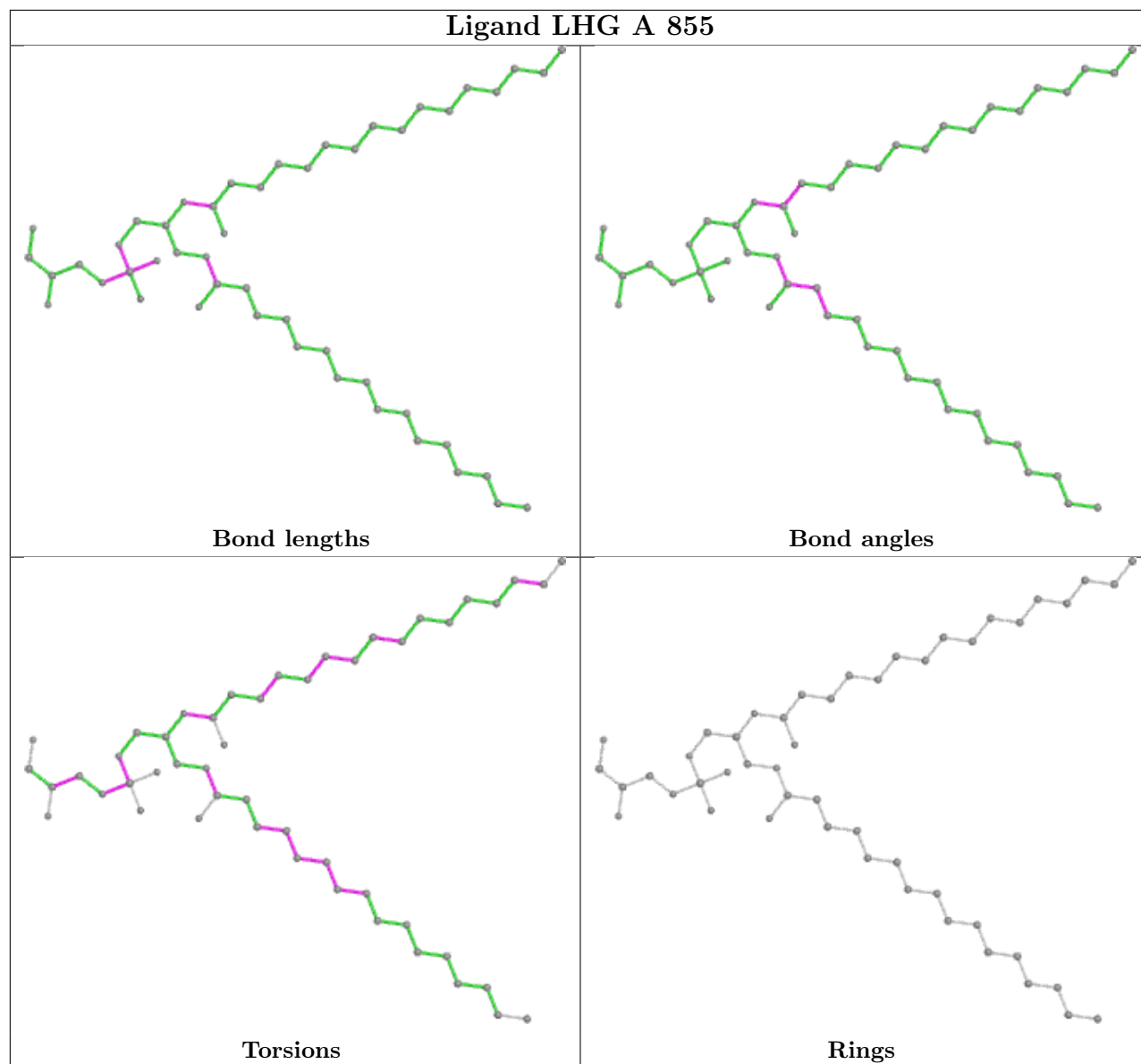




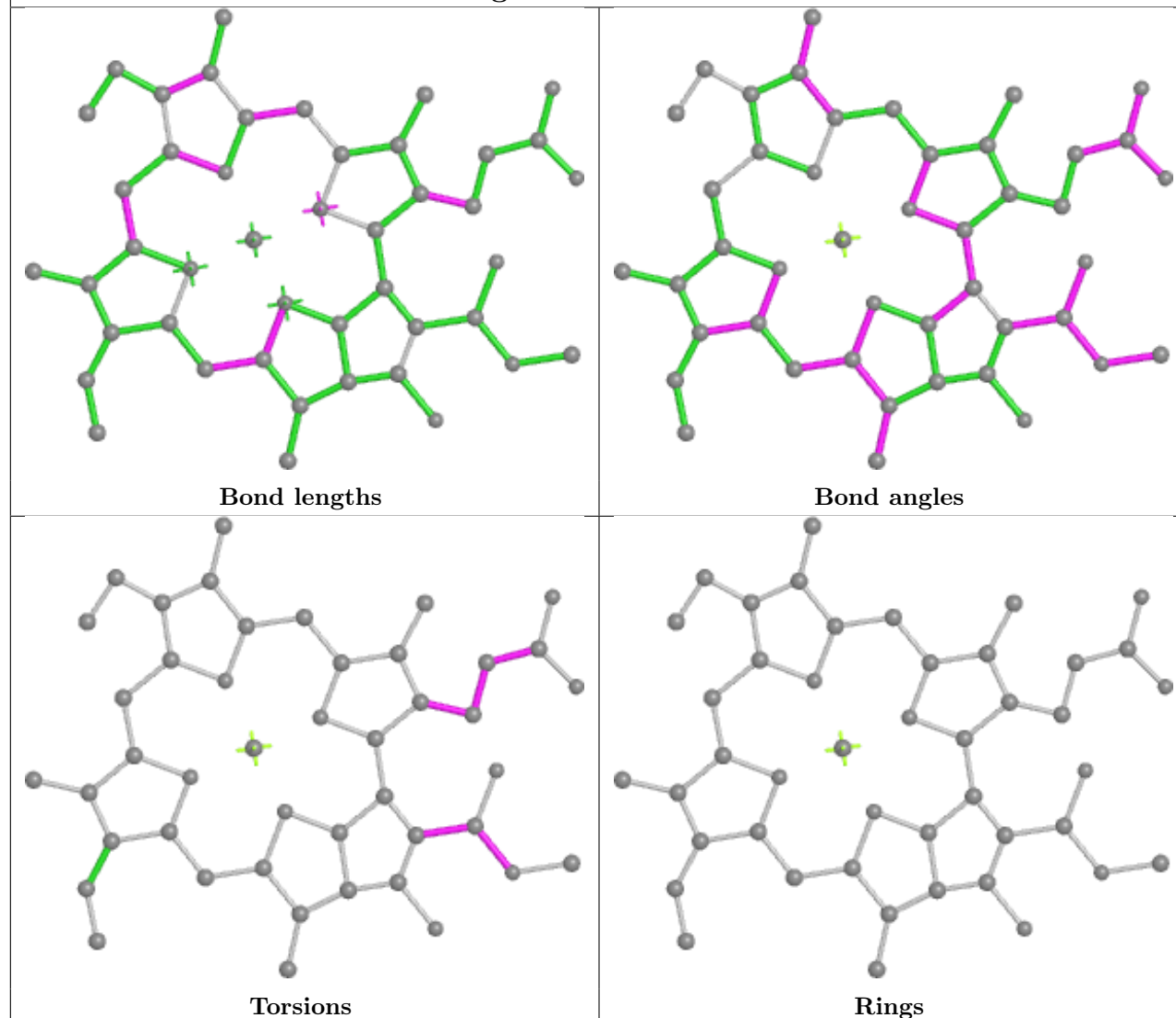




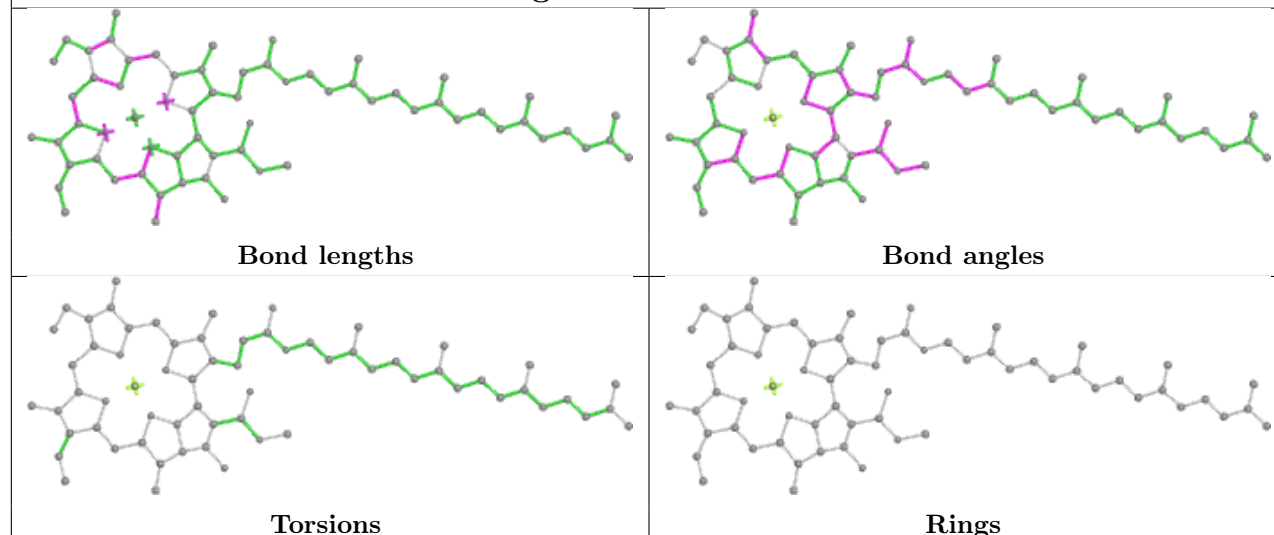


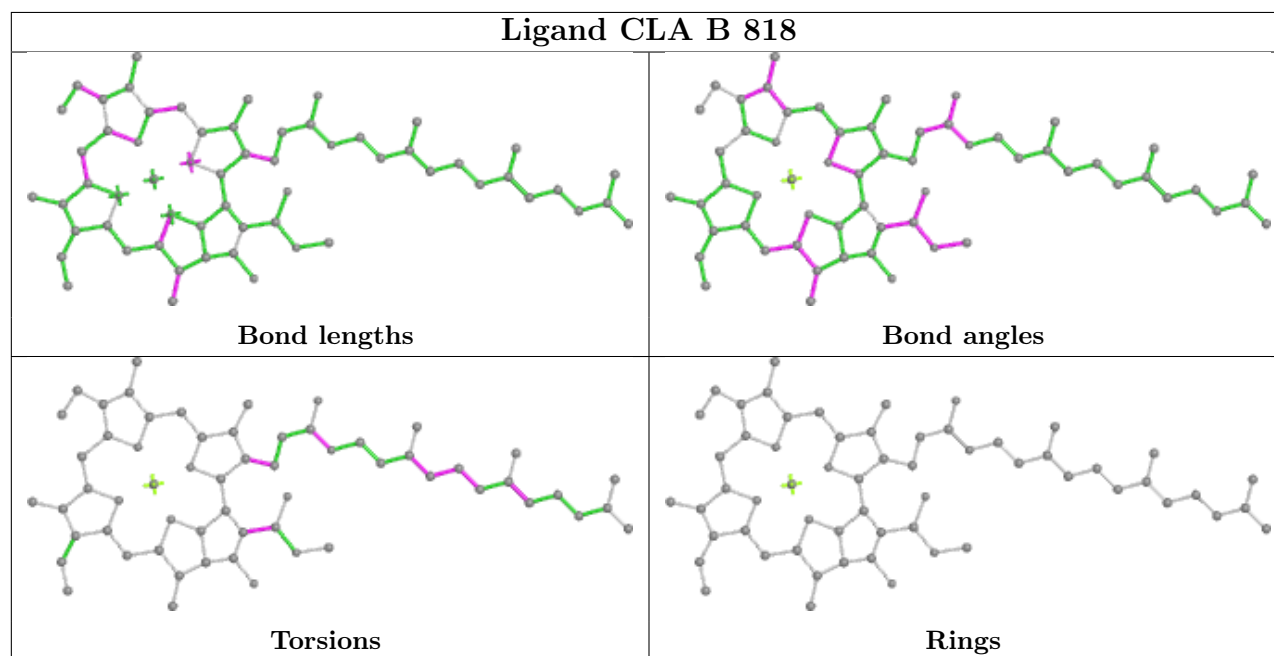
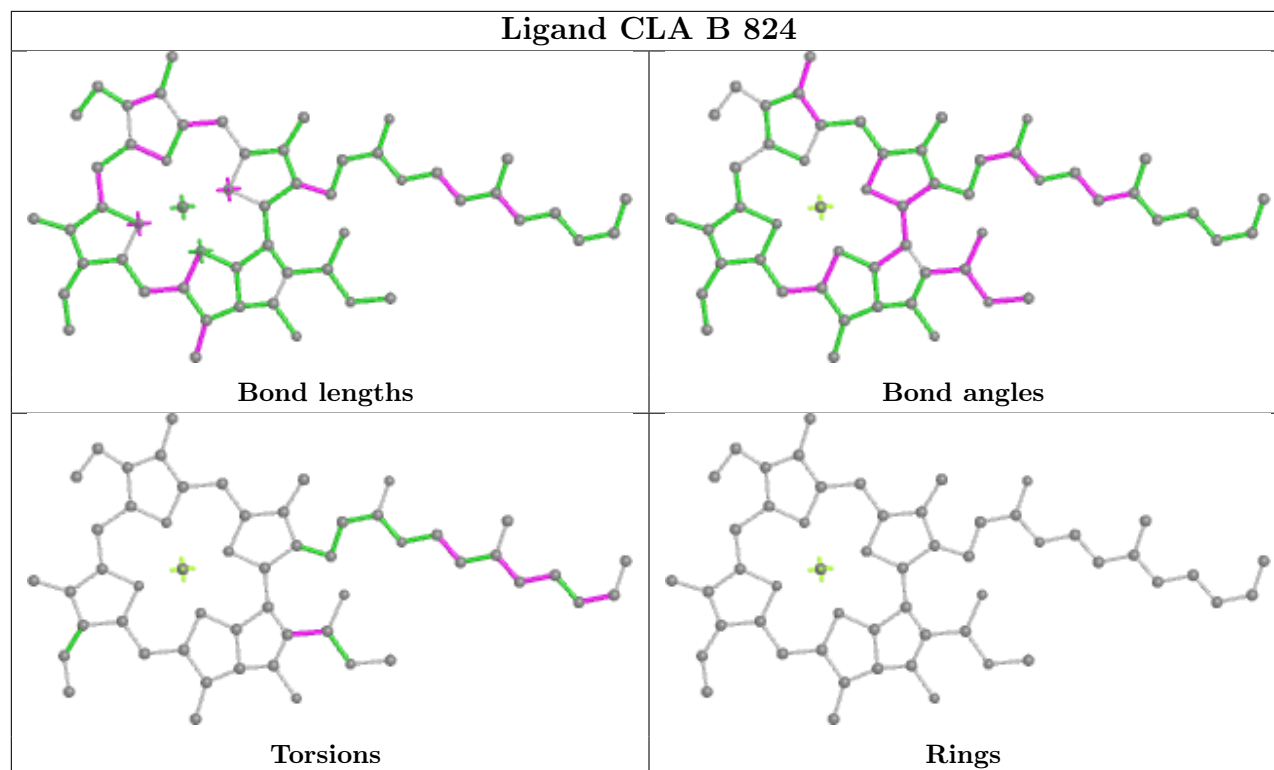


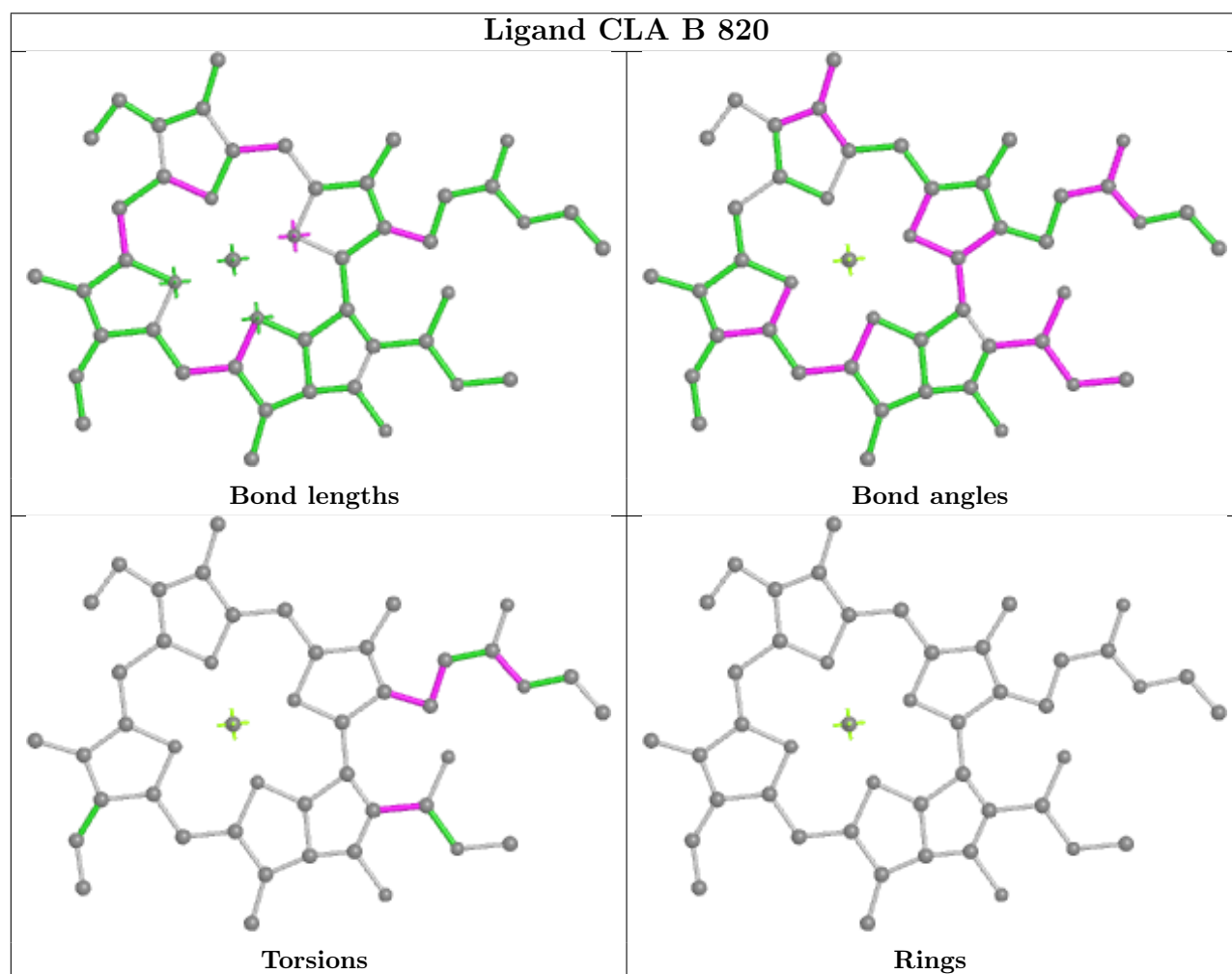
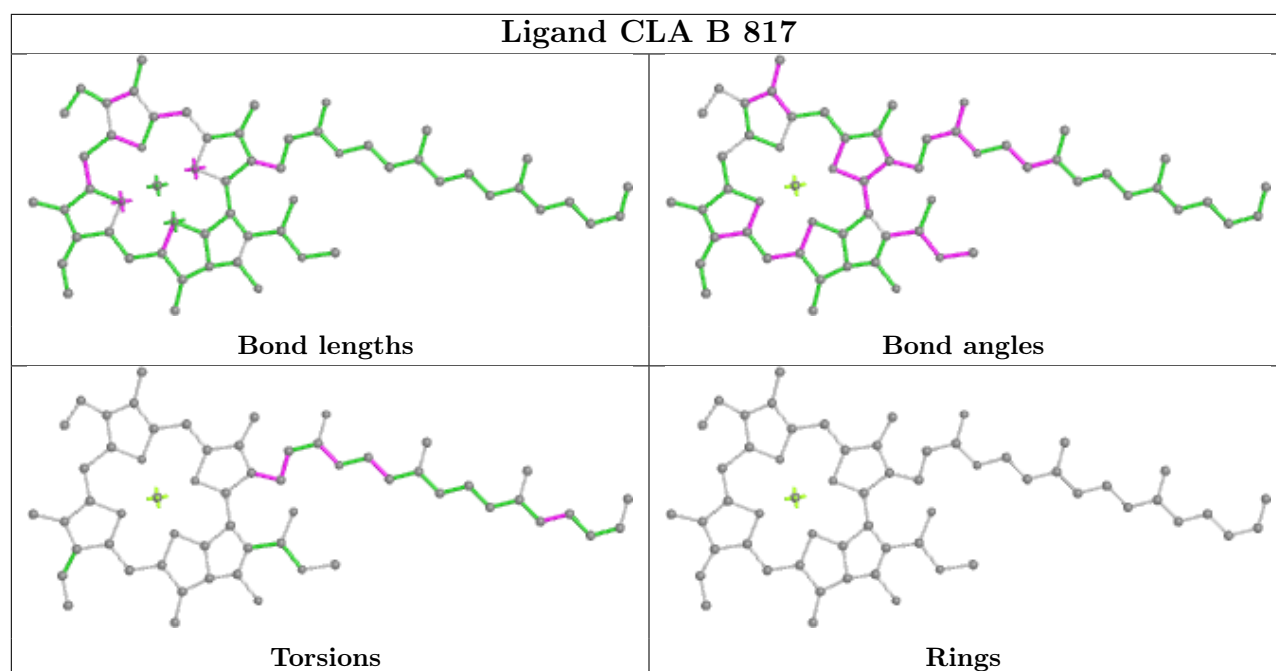
## Ligand CLA B 830

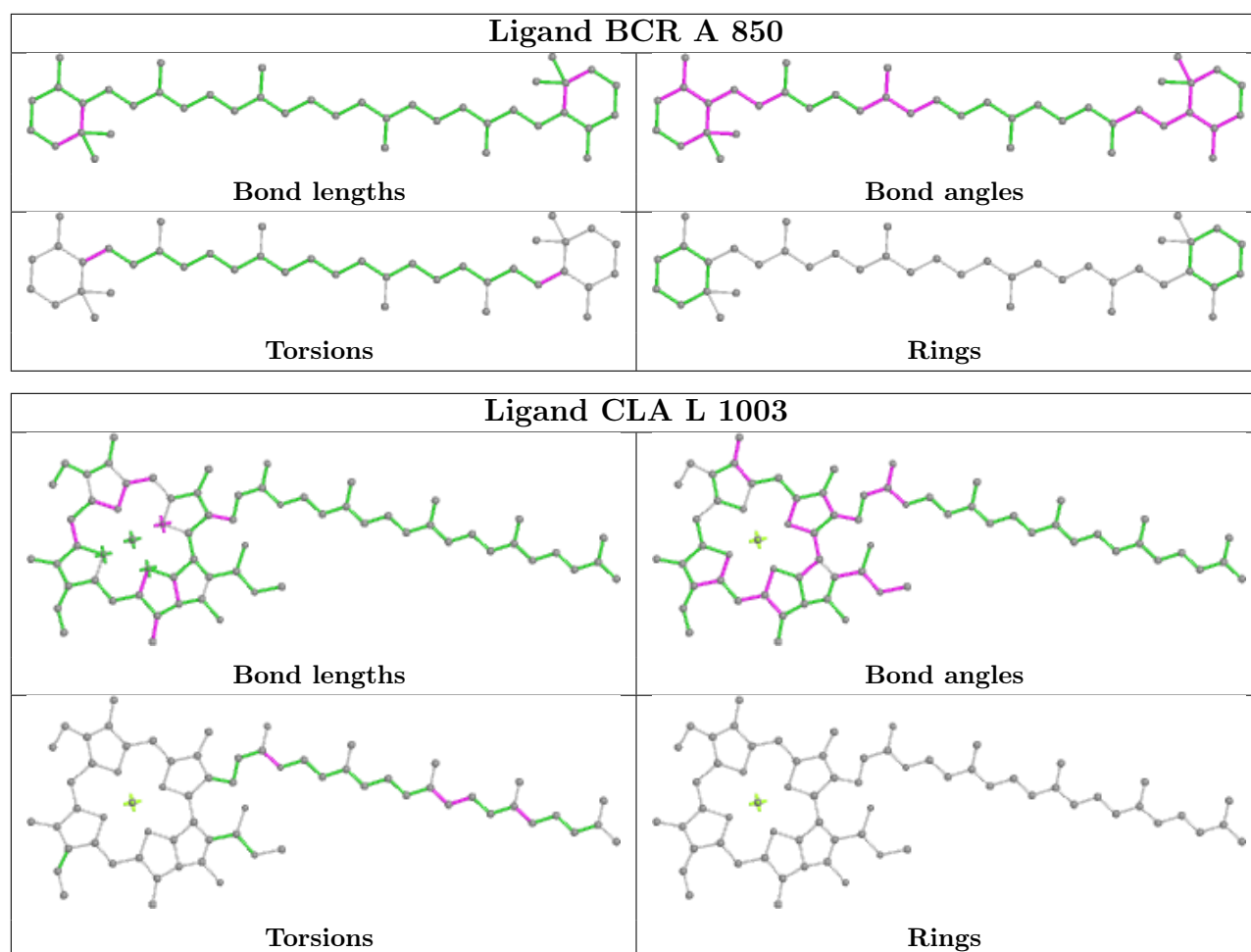


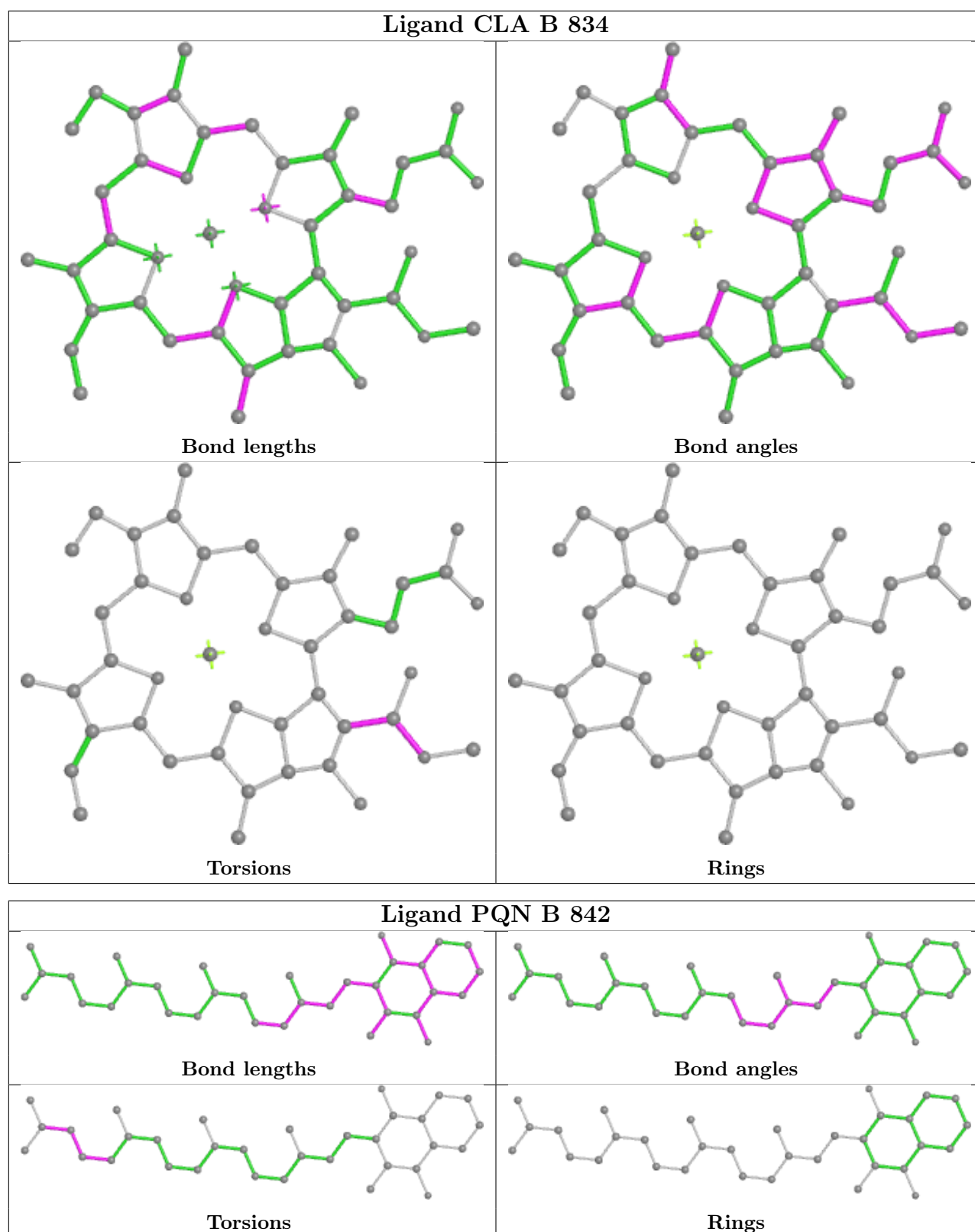
## Ligand CLA B 838



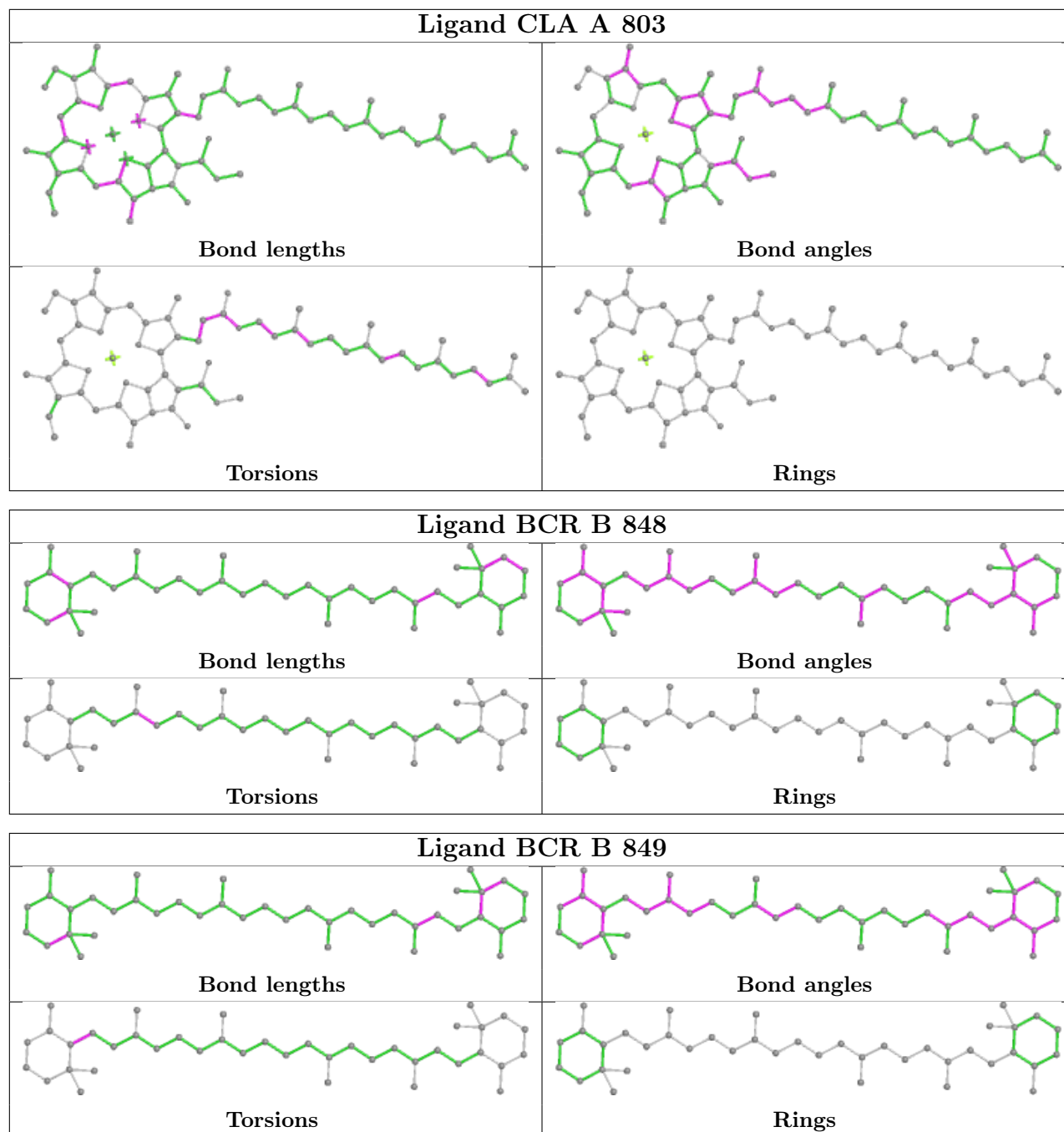


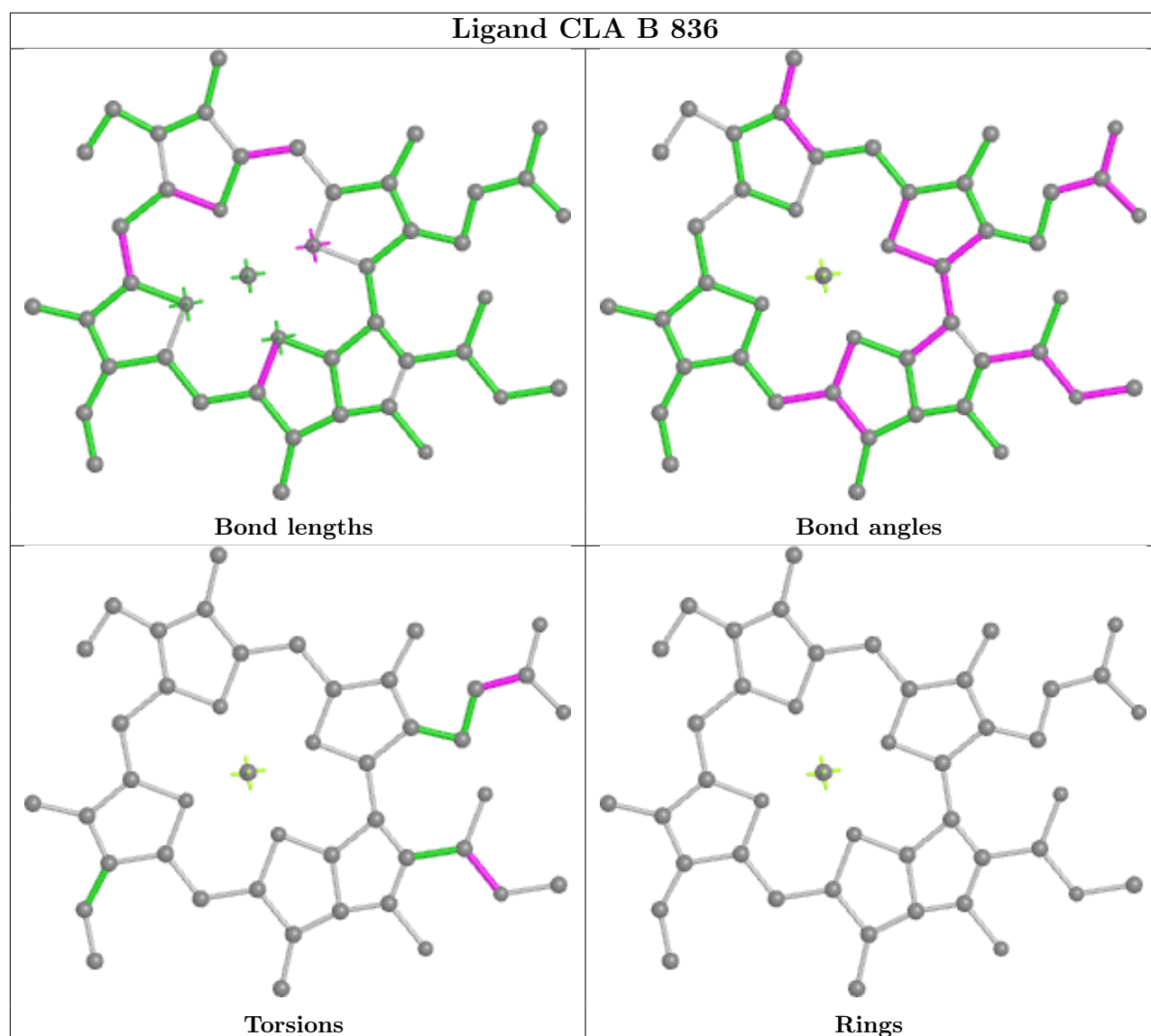


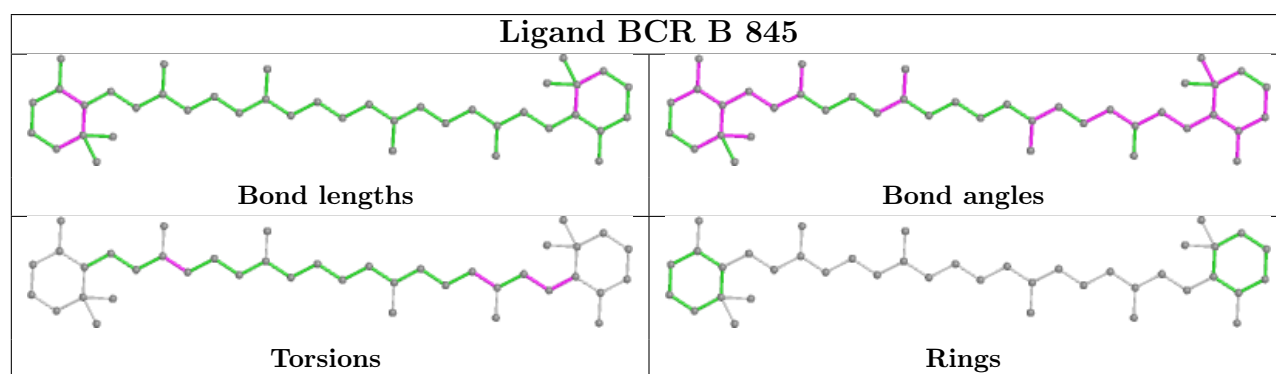
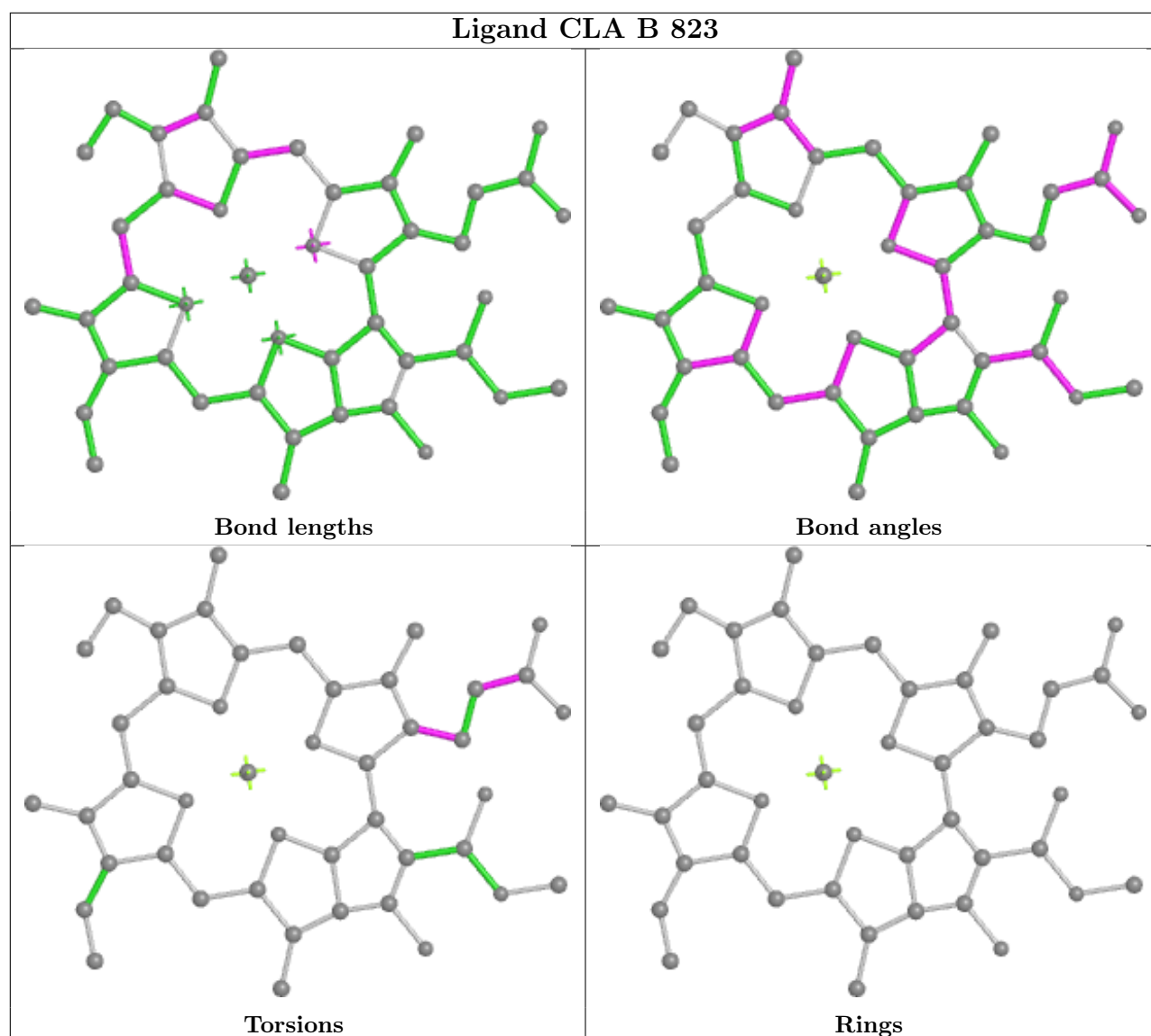


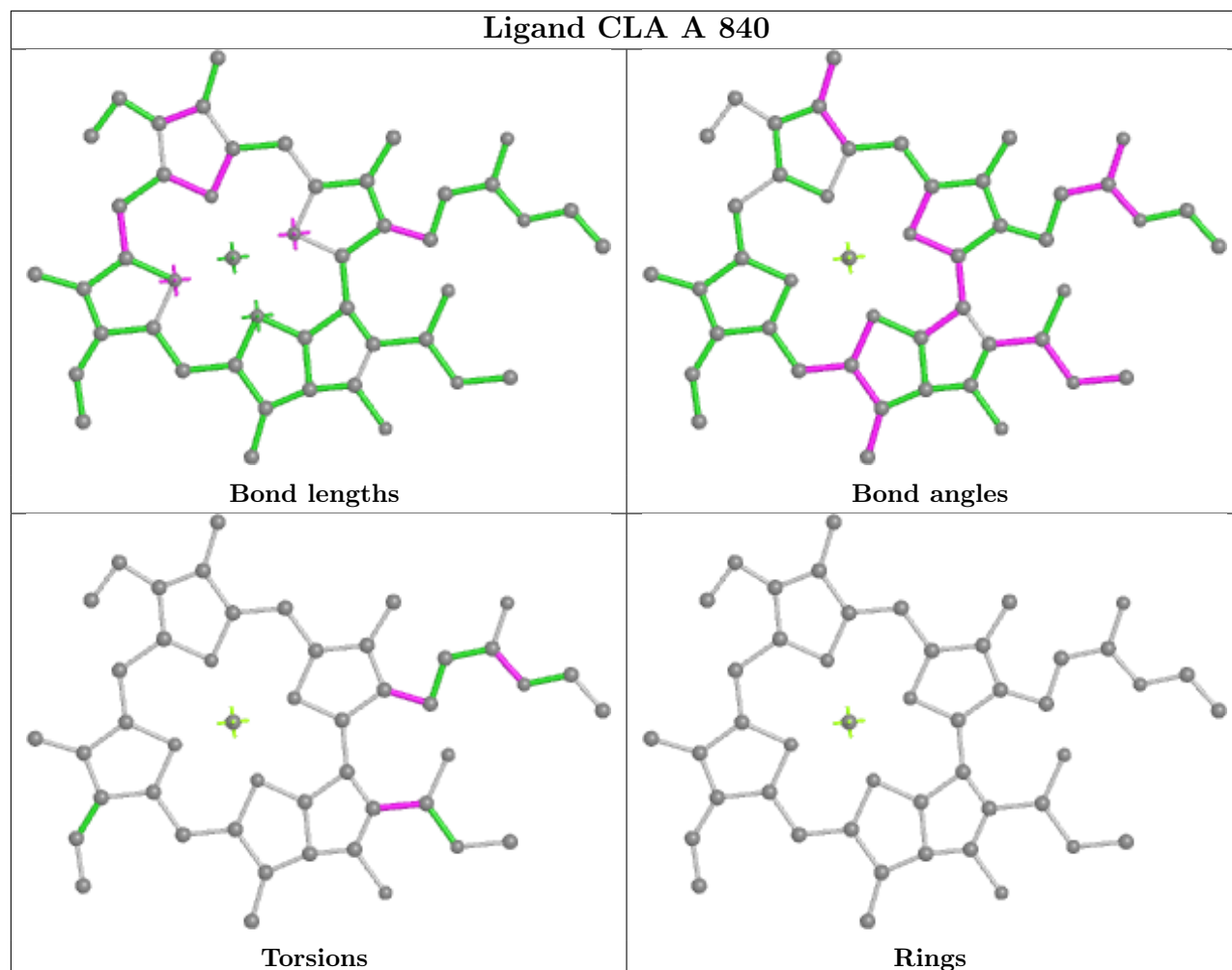
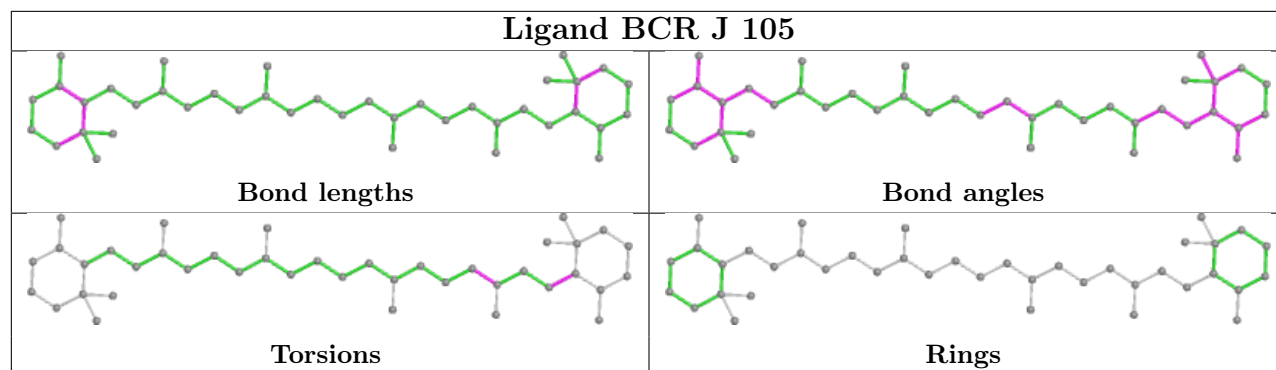


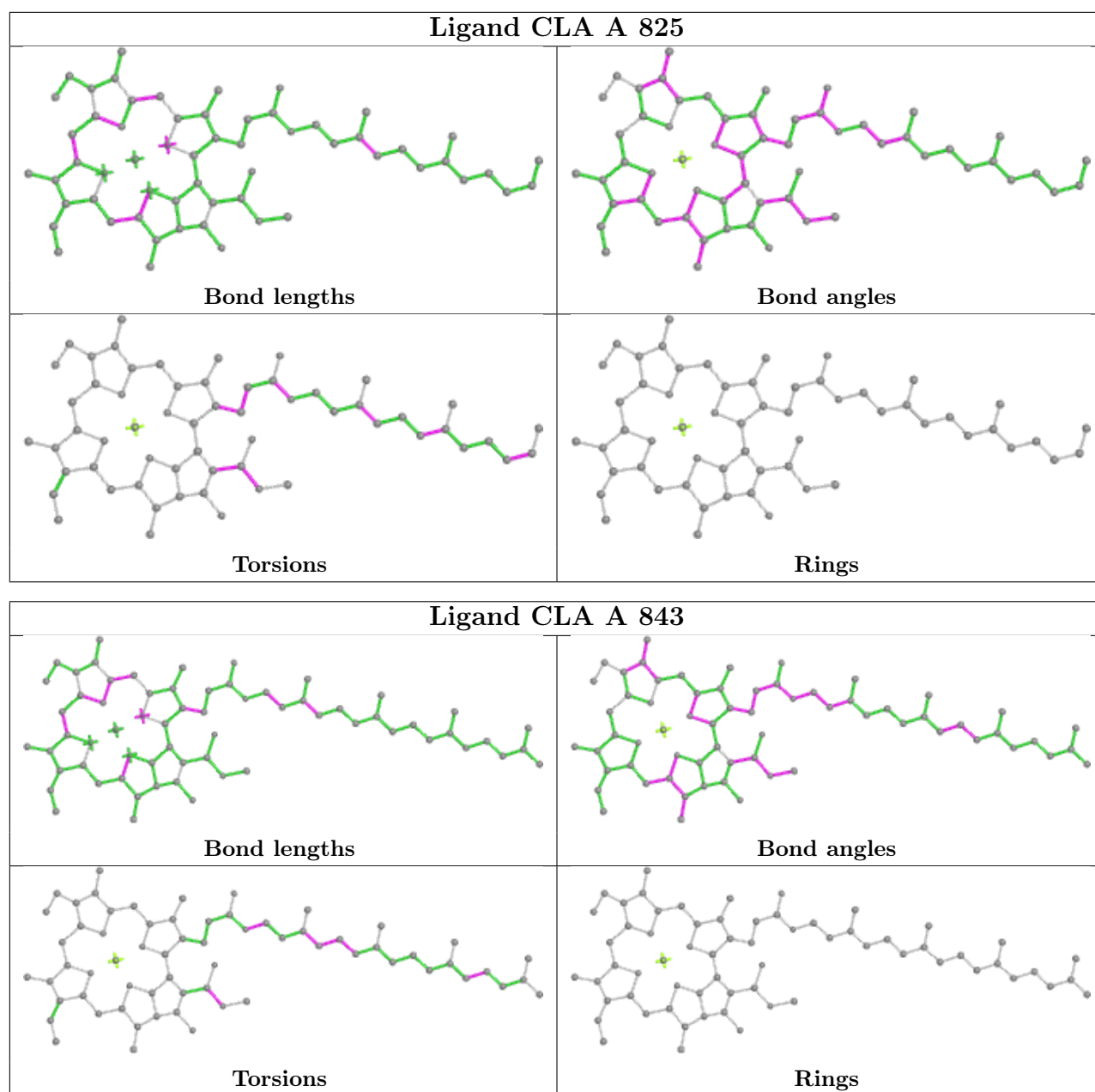


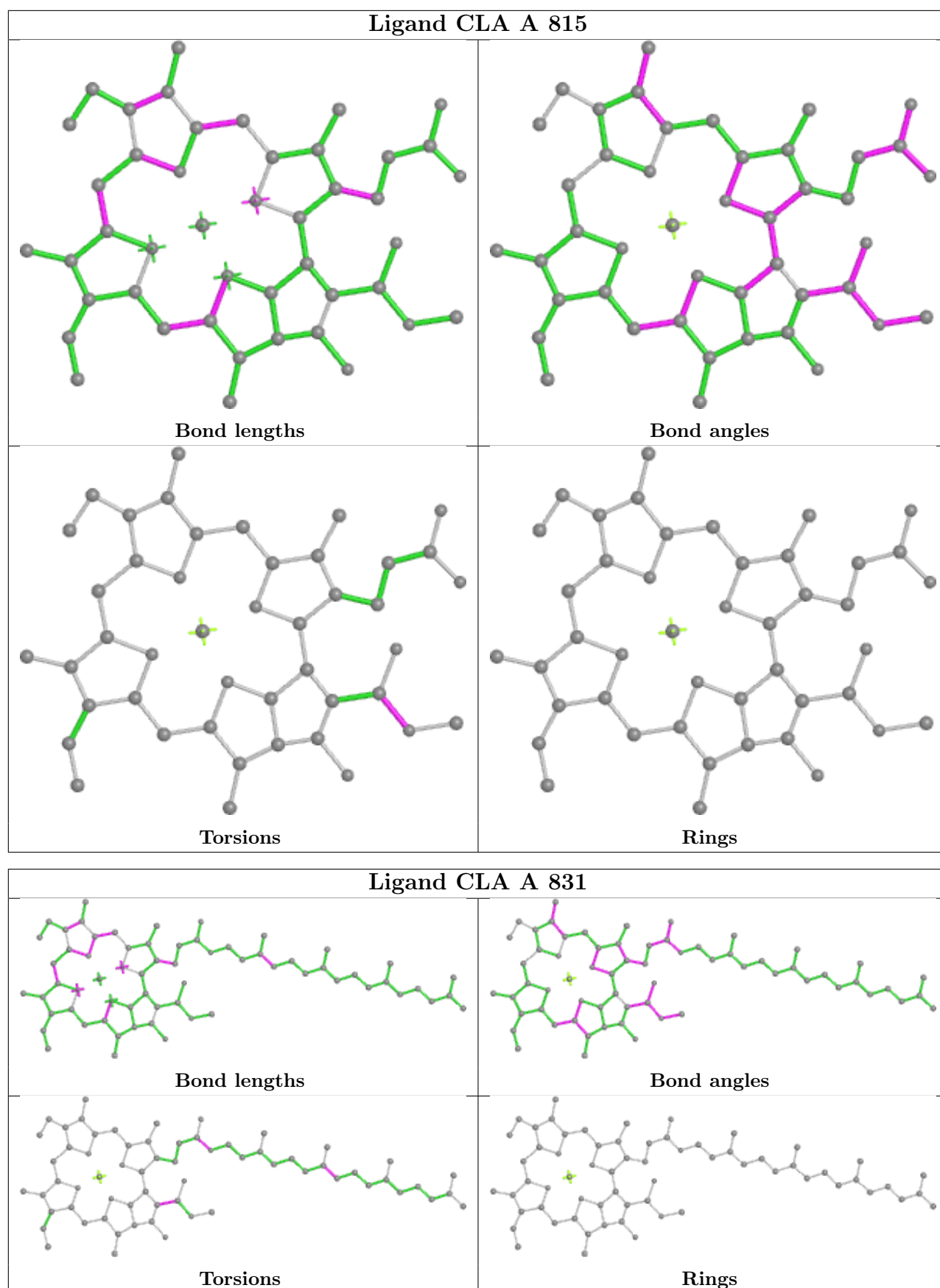


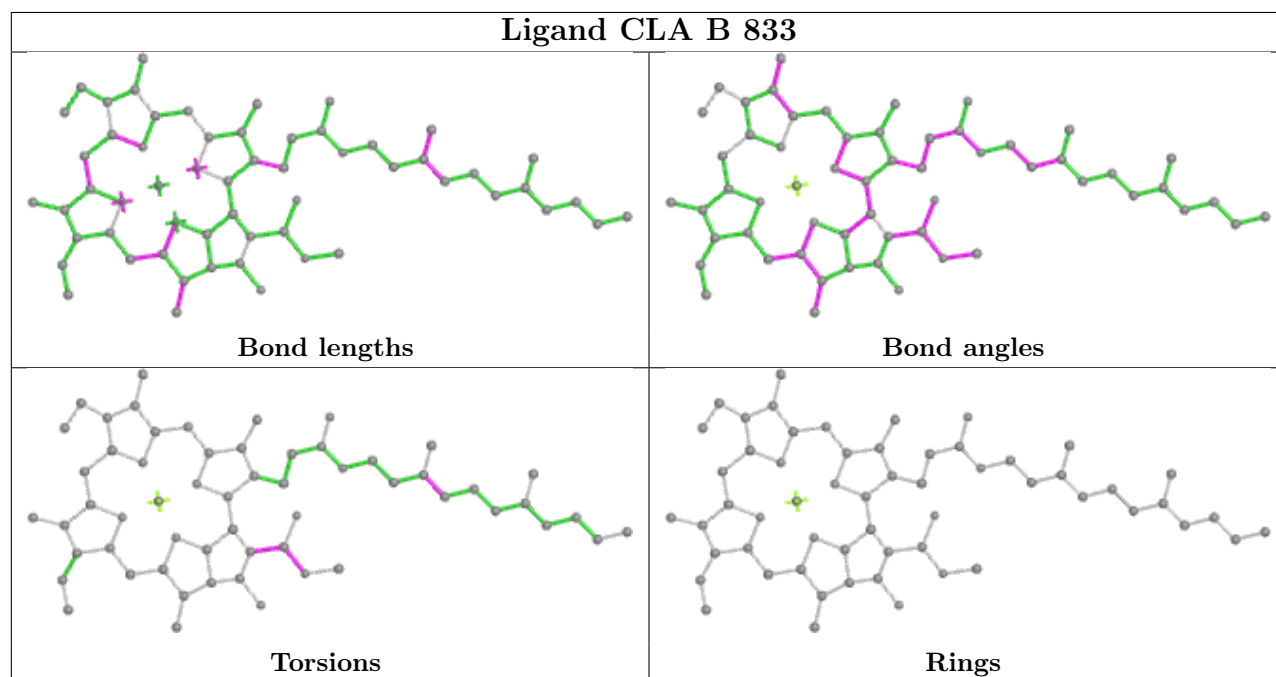
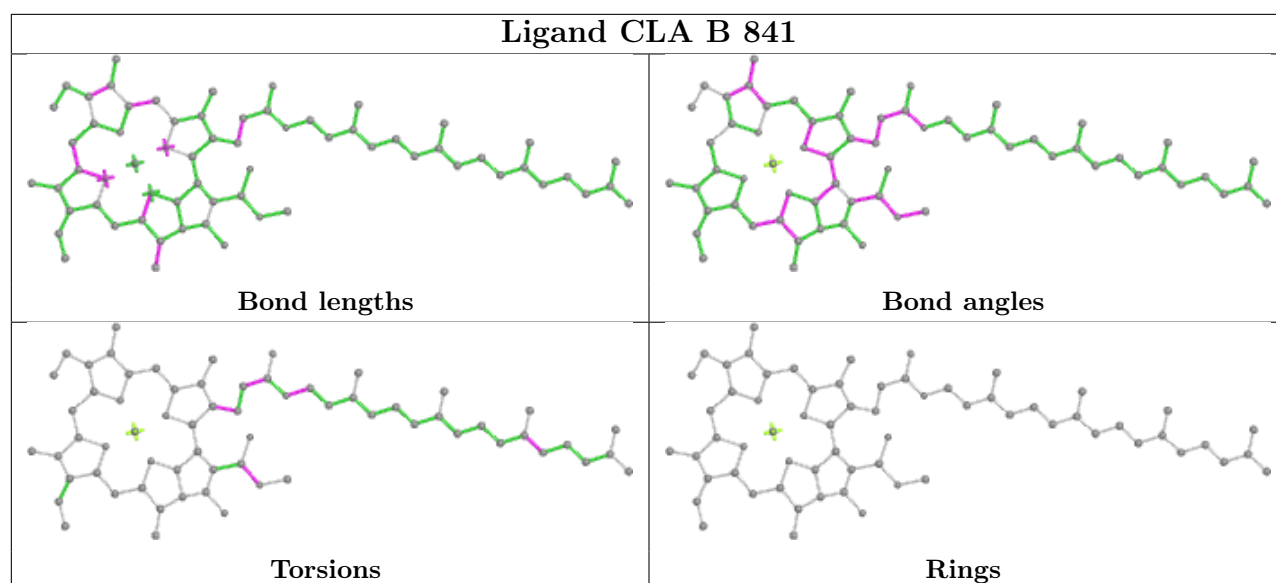


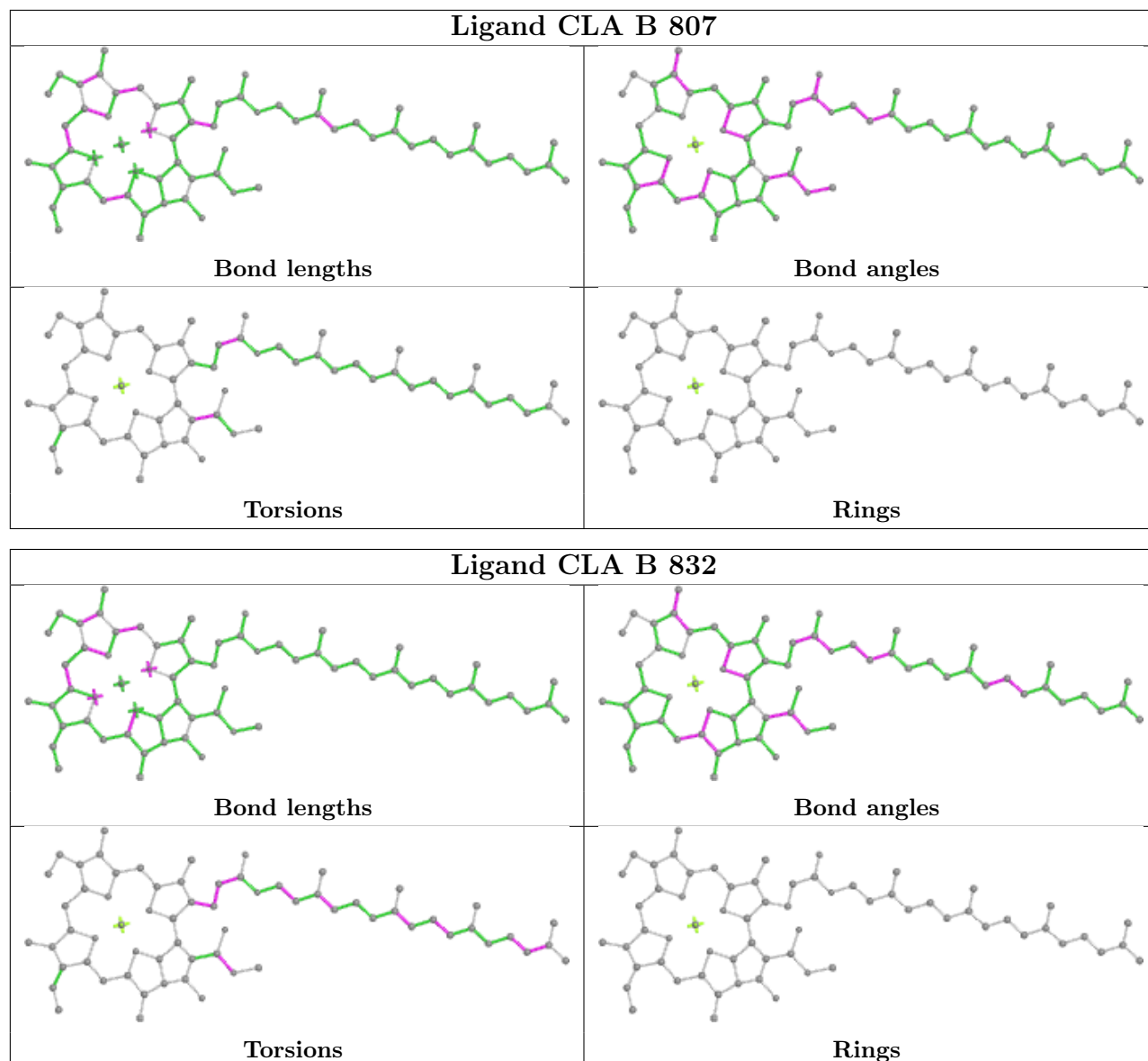




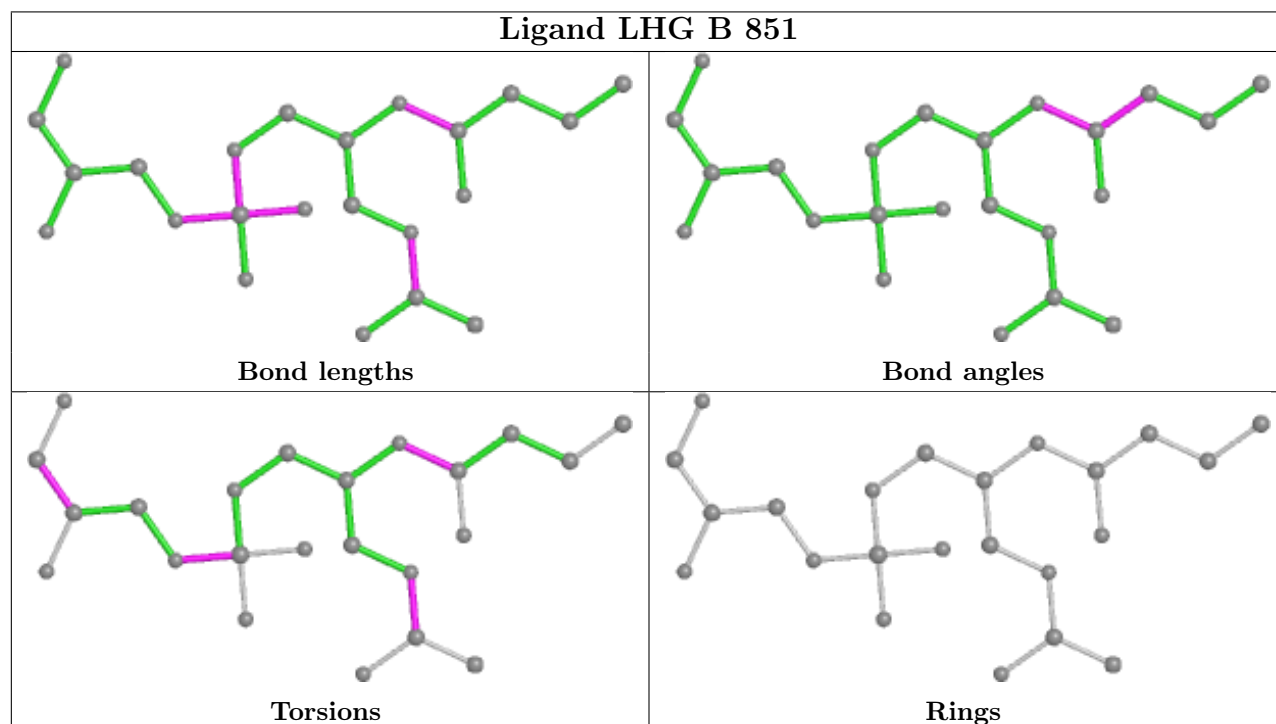
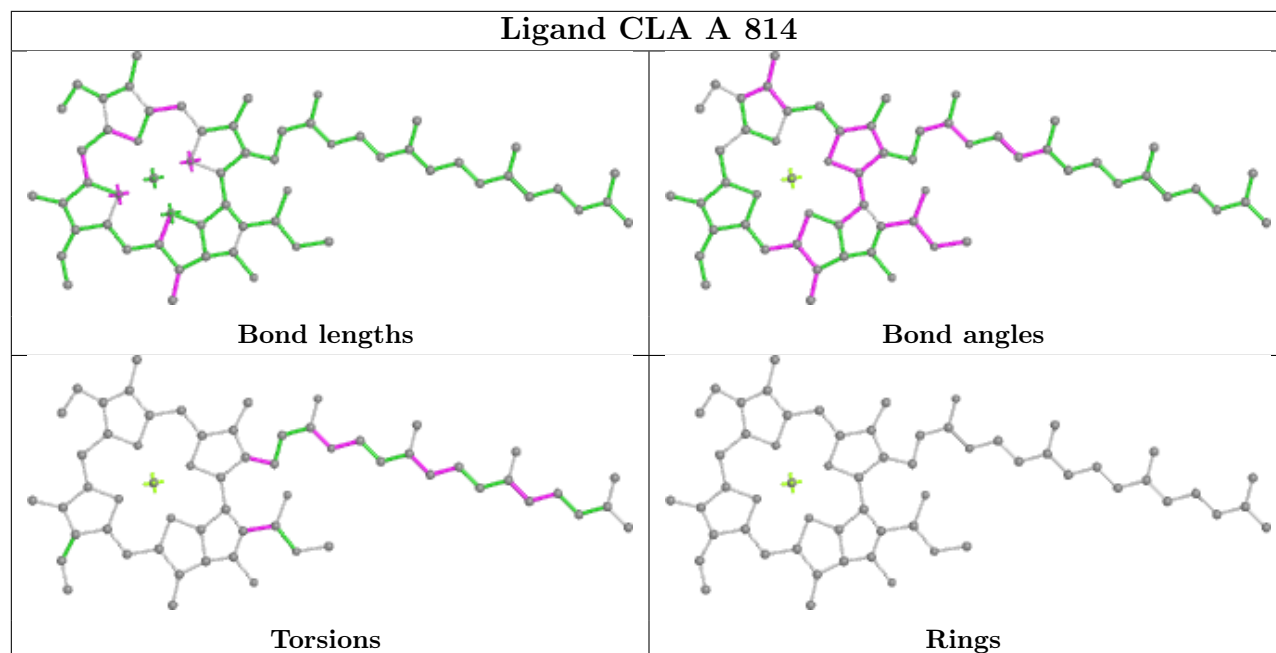


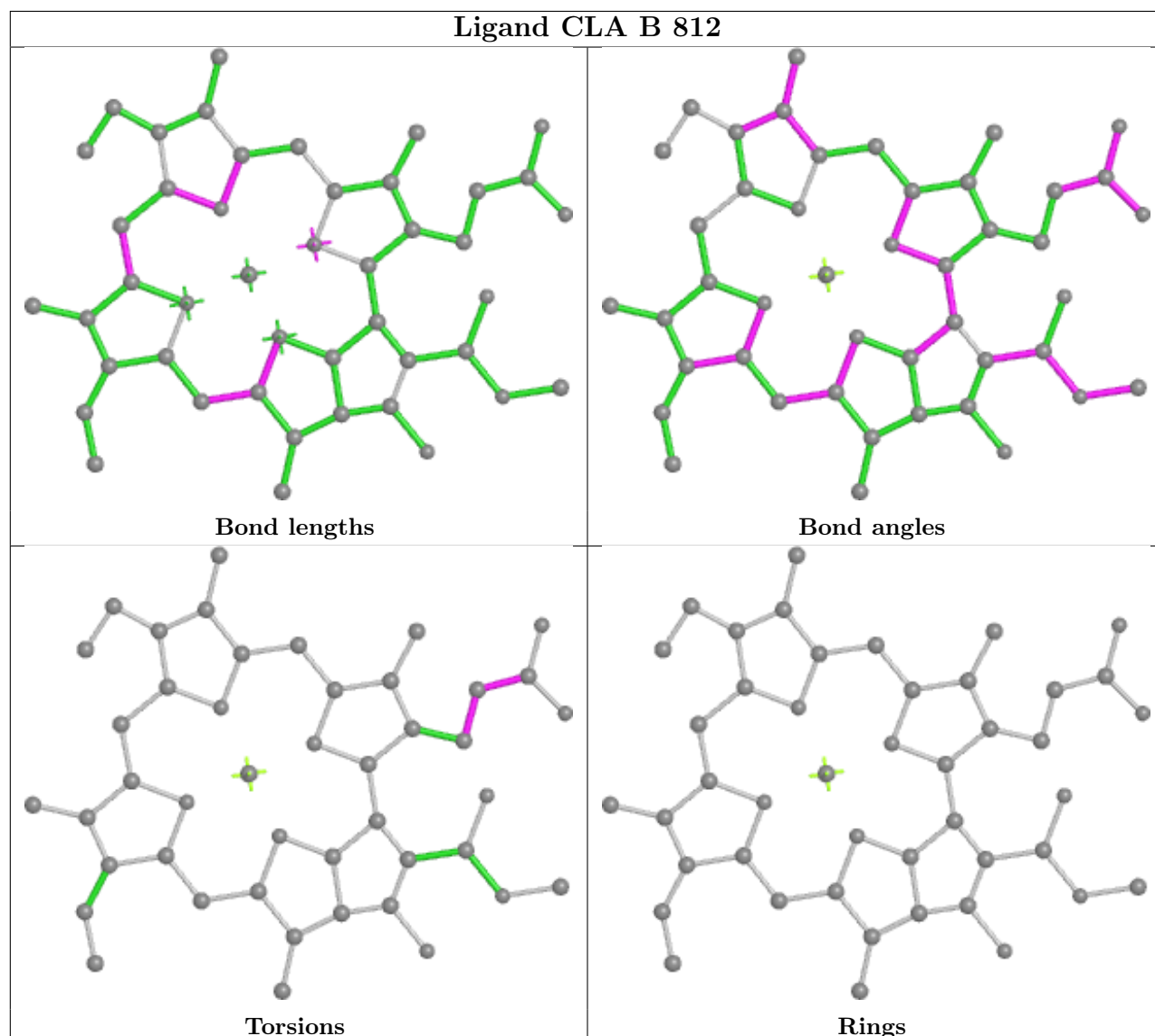
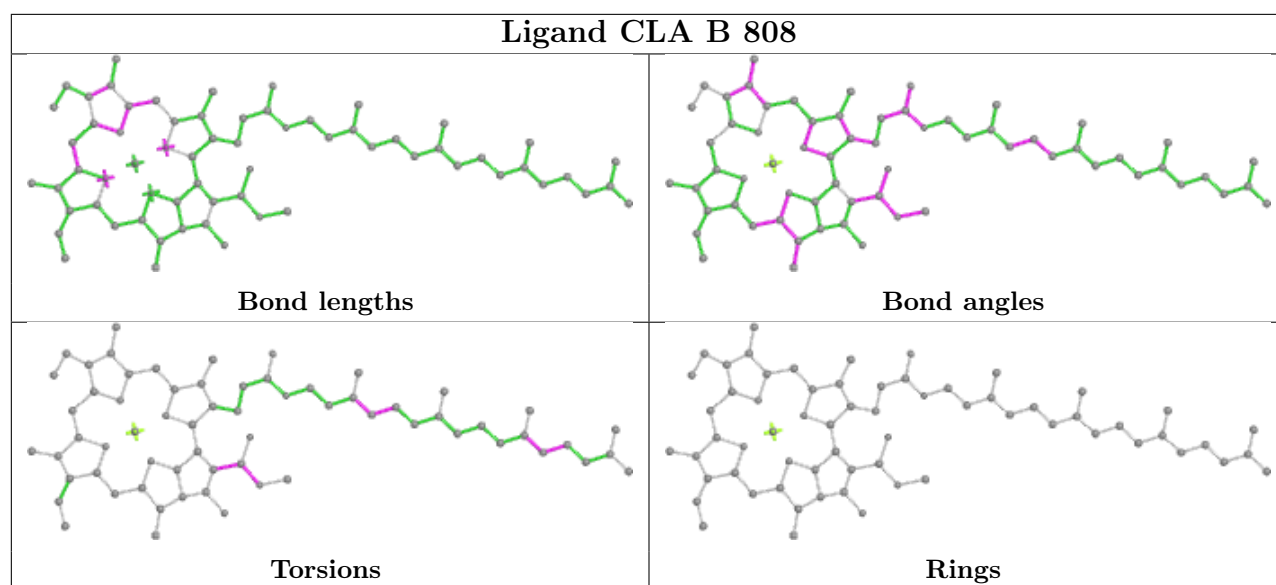


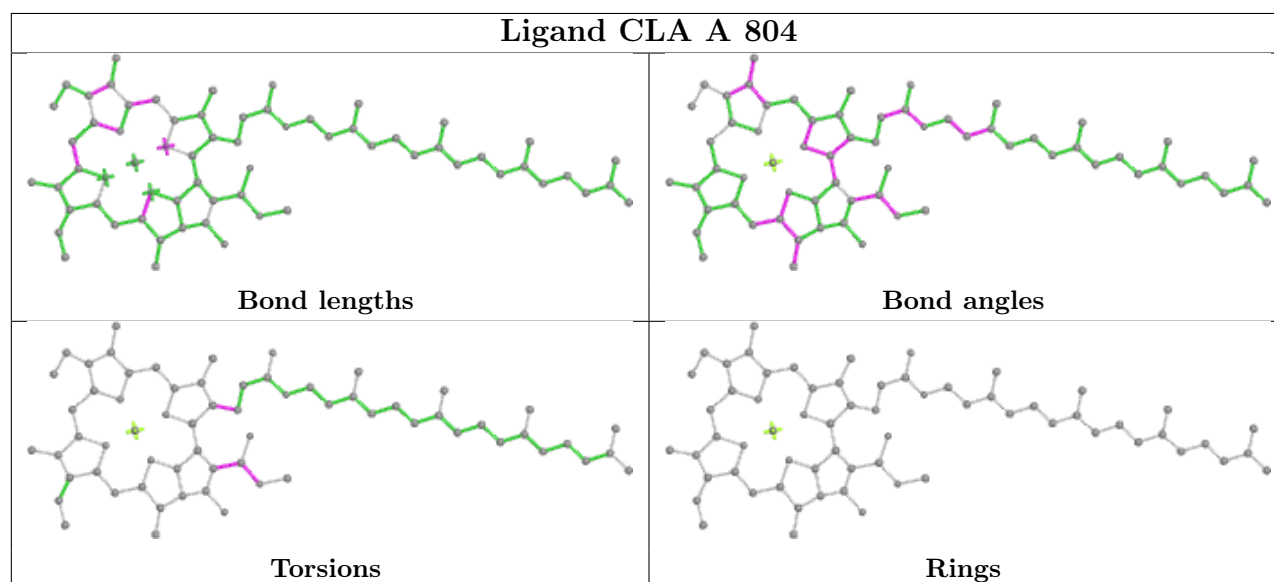
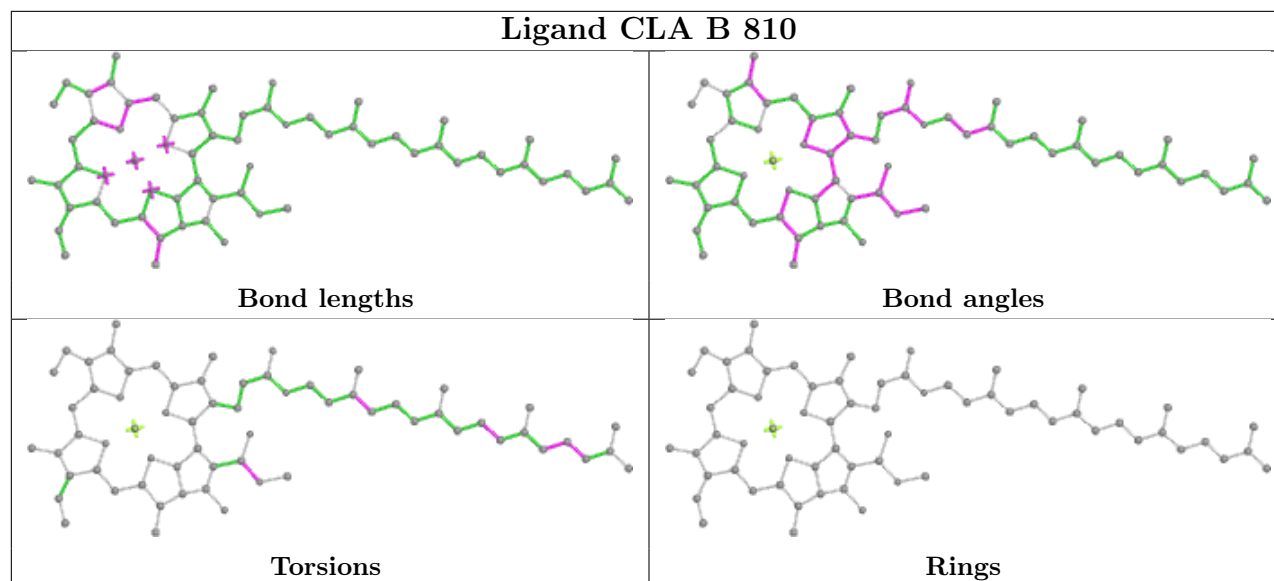
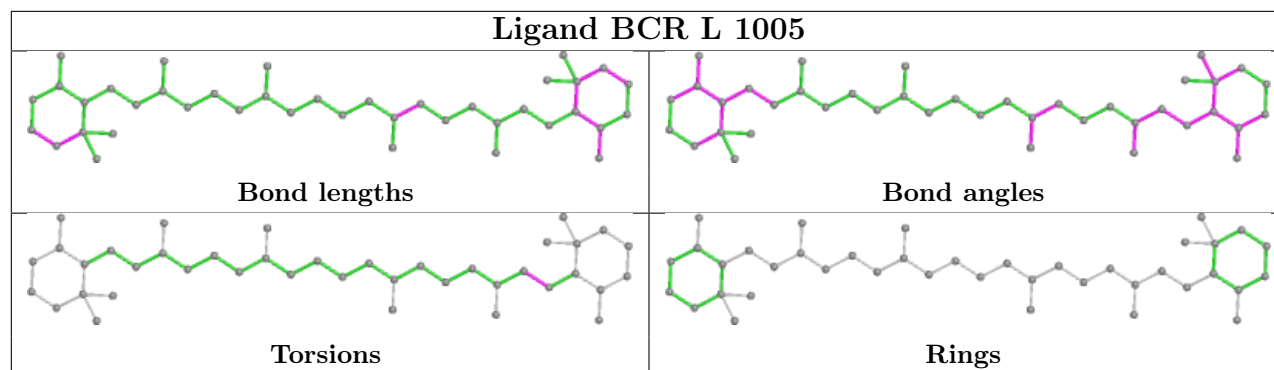


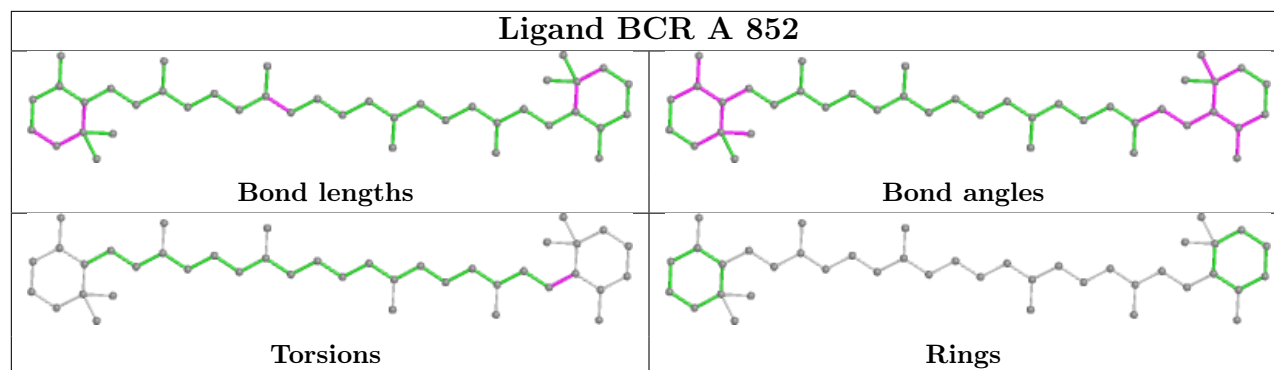












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	740/755 (98%)	-0.24	16 (2%) 62 54	22, 45, 71, 93	0
2	B	739/740 (99%)	-0.14	23 (3%) 49 42	20, 38, 71, 89	0
3	C	80/80 (100%)	-0.61	0 100 100	22, 33, 45, 54	0
4	D	138/138 (100%)	-0.07	7 (5%) 28 27	27, 41, 56, 84	0
5	E	69/75 (92%)	0.41	6 (8%) 10 12	29, 46, 62, 76	0
6	F	141/164 (85%)	-0.24	0 100 100	37, 57, 68, 72	0
7	I	38/38 (100%)	0.34	0 100 100	20, 33, 47, 53	0
8	J	41/41 (100%)	0.01	0 100 100	53, 60, 77, 86	0
9	K	46/83 (55%)	0.98	9 (19%) 1 3	72, 81, 96, 99	0
10	L	151/154 (98%)	0.25	11 (7%) 15 16	19, 26, 47, 67	0
11	M	31/31 (100%)	0.25	0 100 100	30, 38, 52, 62	0
12	X	29/35 (82%)	-0.06	1 (3%) 45 40	58, 63, 81, 88	0
All	All	2243/2334 (96%)	-0.11	73 (3%) 46 41	19, 42, 74, 99	0

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	2	THR	7.3
4	D	3	LEU	5.9
4	D	4	THR	5.5
1	A	207	LEU	5.4
10	L	144	VAL	4.5

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
16	BCR	A	852	40/40	0.57	1.14	47,60,96,96	0
13	CLA	J	102	37/65	0.61	0.94	95,96,97,97	0
13	CLA	B	812	45/65	0.62	0.57	66,69,80,85	0
16	BCR	B	844	40/40	0.69	1.82	56,68,93,93	0
18	LMG	B	850	55/55	0.69	1.11	34,40,57,60	0
13	CLA	A	823	49/65	0.71	0.50	64,68,82,83	0
13	CLA	J	101	45/65	0.72	0.70	98,99,100,100	0
16	BCR	A	851	40/40	0.73	1.46	47,61,89,89	0
16	BCR	J	105	40/40	0.73	0.78	53,67,93,94	0
13	CLA	A	845	41/65	0.73	0.82	87,90,92,93	0
13	CLA	B	820	47/65	0.74	0.67	88,92,97,97	0
16	BCR	B	845	40/40	0.74	1.29	33,51,87,88	0
13	CLA	B	840	65/65	0.74	1.10	13,18,41,42	0
13	CLA	B	816	55/65	0.74	0.63	54,60,85,87	0
16	BCR	A	850	40/40	0.76	1.29	57,61,79,79	0
13	CLA	B	815	45/65	0.76	0.55	57,62,73,77	0
13	CLA	A	822	65/65	0.76	0.83	41,45,55,57	0
16	BCR	A	853	40/40	0.76	1.16	30,37,59,60	0
13	CLA	A	811	45/65	0.77	0.39	68,71,75,76	0
16	BCR	B	843	40/40	0.77	0.86	88,90,97,98	0
13	CLA	B	833	58/65	0.77	0.70	36,47,77,78	0
13	CLA	A	844	65/65	0.78	0.93	17,22,43,47	0
13	CLA	A	824	51/65	0.78	0.66	53,59,77,77	0
13	CLA	M	1601	45/65	0.78	0.87	96,97,99,100	0
13	CLA	A	816	45/65	0.79	0.63	78,82,83,83	0
17	LHG	A	855	49/49	0.79	0.76	39,50,60,63	0
13	CLA	A	827	65/65	0.79	0.64	24,31,83,85	0
19	CA	L	1001	1/1	0.79	0.17	27,27,27,27	0
13	CLA	B	811	45/65	0.80	0.39	42,49,62,66	0
13	CLA	B	821	45/65	0.80	0.49	80,81,90,93	0
13	CLA	K	1401	45/65	0.80	0.66	70,74,81,84	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
13	CLA	A	812	65/65	0.81	0.45	63,65,72,74	0
13	CLA	B	836	45/65	0.81	0.41	78,82,85,87	0
13	CLA	A	808	51/65	0.81	0.46	55,58,79,79	0
16	BCR	B	846	25/40	0.82	0.98	64,66,69,70	0
13	CLA	F	1301	45/65	0.82	0.53	75,77,82,83	0
13	CLA	A	846	52/65	0.82	0.54	69,75,97,99	0
13	CLA	B	814	65/65	0.82	0.65	34,43,68,69	0
13	CLA	A	821	61/65	0.82	0.74	56,62,85,85	0
16	BCR	M	1602	40/40	0.83	0.88	28,37,59,62	0
13	CLA	B	830	45/65	0.83	0.69	51,54,67,72	0
17	LHG	B	851	23/49	0.83	0.46	79,89,92,93	0
13	CLA	B	831	49/65	0.83	0.82	36,40,63,65	0
16	BCR	A	849	40/40	0.83	0.80	62,69,79,79	0
13	CLA	A	828	65/65	0.84	0.56	32,42,66,68	0
16	BCR	B	849	40/40	0.84	1.07	23,27,30,31	0
13	CLA	A	834	65/65	0.84	1.04	24,28,43,44	0
16	BCR	L	1005	40/40	0.84	1.37	20,24,29,30	0
13	CLA	B	819	65/65	0.84	0.74	78,82,99,100	0
13	CLA	A	818	54/65	0.84	0.51	63,66,68,69	0
13	CLA	L	1004	65/65	0.84	0.82	22,31,61,62	0
13	CLA	B	839	47/65	0.84	0.55	41,47,55,60	0
13	CLA	A	813	54/65	0.84	0.56	44,47,76,77	0
13	CLA	B	841	65/65	0.85	1.14	22,29,44,50	0
13	CLA	A	817	49/65	0.85	0.47	87,90,92,94	0
13	CLA	A	810	65/65	0.85	0.89	39,43,77,78	0
13	CLA	A	825	59/65	0.85	0.74	34,43,76,76	0
13	CLA	B	826	65/65	0.85	0.65	31,39,63,65	0
13	CLA	A	840	47/65	0.85	0.70	30,35,52,57	0
16	BCR	J	104	40/40	0.86	0.87	61,69,75,76	0
13	CLA	A	838	51/65	0.86	0.34	30,35,45,46	0
13	CLA	B	803	65/65	0.86	0.62	24,29,35,36	0
16	BCR	I	101	40/40	0.86	0.77	19,27,40,40	0
13	CLA	A	833	65/65	0.87	0.80	20,31,85,88	0
13	CLA	A	839	65/65	0.87	0.70	32,38,58,59	0
13	CLA	A	837	45/65	0.87	0.56	60,68,76,80	0
16	BCR	B	847	40/40	0.88	0.97	46,53,61,61	0
13	CLA	A	814	60/65	0.88	0.69	49,53,80,81	0
16	BCR	F	1302	40/40	0.88	0.77	43,49,60,60	0
13	CLA	B	832	65/65	0.88	0.63	37,43,65,66	0
13	CLA	A	805	59/65	0.89	0.46	40,46,85,86	0
16	BCR	L	1006	40/40	0.89	0.45	26,35,66,67	0
13	CLA	L	1003	65/65	0.89	0.78	17,23,66,67	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
13	CLA	A	815	45/65	0.89	0.36	64,66,67,68	0
16	BCR	J	103	40/40	0.89	1.36	55,58,60,60	0
13	CLA	B	825	46/65	0.89	0.49	29,36,46,48	0
13	CLA	X	1701	45/65	0.89	0.46	77,83,86,88	0
13	CLA	B	828	65/65	0.90	1.11	31,35,48,52	0
13	CLA	A	806	65/65	0.90	0.61	33,39,68,70	0
13	CLA	B	810	65/65	0.90	0.53	15,23,43,44	0
13	CLA	A	826	65/65	0.90	0.45	45,49,62,63	0
13	CLA	A	843	65/65	0.90	1.48	29,35,60,60	0
13	CLA	A	807	65/65	0.91	0.77	38,43,51,52	0
13	CLA	B	824	54/65	0.91	0.51	54,59,69,71	0
13	CLA	B	801	65/65	0.92	0.31	22,30,38,46	0
14	PQN	A	847	33/33	0.92	0.77	41,43,67,68	0
13	CLA	B	813	65/65	0.92	0.90	49,59,68,70	0
16	BCR	I	102	40/40	0.92	0.59	19,26,31,32	0
13	CLA	A	836	54/65	0.92	0.59	46,50,64,64	0
13	CLA	B	804	54/65	0.92	0.84	20,29,48,52	0
13	CLA	B	805	65/65	0.92	0.65	28,37,66,69	0
13	CLA	B	817	59/65	0.92	0.54	39,47,66,70	0
13	CLA	B	807	65/65	0.92	0.52	21,24,50,53	0
13	CLA	L	1002	65/65	0.92	0.57	21,27,58,61	0
13	CLA	A	804	65/65	0.92	0.83	45,50,80,83	0
17	LHG	A	856	27/49	0.92	0.40	51,56,60,61	0
13	CLA	A	802	65/65	0.92	0.53	23,26,35,39	0
13	CLA	B	838	65/65	0.92	0.46	38,44,74,78	0
16	BCR	B	848	40/40	0.92	0.95	40,52,58,58	0
13	CLA	A	819	54/65	0.93	0.39	44,50,54,56	0
13	CLA	B	822	55/65	0.93	0.35	69,70,88,89	0
13	CLA	B	823	45/65	0.93	0.36	58,62,70,73	0
13	CLA	A	830	65/65	0.93	0.72	33,40,52,55	0
13	CLA	A	820	65/65	0.93	0.59	43,48,56,58	0
16	BCR	A	854	40/40	0.93	1.45	29,39,50,53	0
13	CLA	B	835	45/65	0.93	0.46	58,61,70,75	0
13	CLA	A	801	65/65	0.93	0.39	22,27,36,38	0
15	SF4	C	102	8/8	0.93	0.21	33,34,35,35	0
13	CLA	A	809	65/65	0.94	0.75	33,40,66,67	0
14	PQN	B	842	33/33	0.94	0.96	24,29,36,36	0
13	CLA	B	806	65/65	0.94	0.98	30,34,53,54	0
13	CLA	A	831	65/65	0.94	0.53	35,43,52,53	0
13	CLA	B	809	65/65	0.94	0.71	20,26,61,62	0
13	CLA	A	842	51/65	0.94	0.45	38,43,70,71	0
13	CLA	B	818	60/65	0.94	0.86	33,39,64,66	0

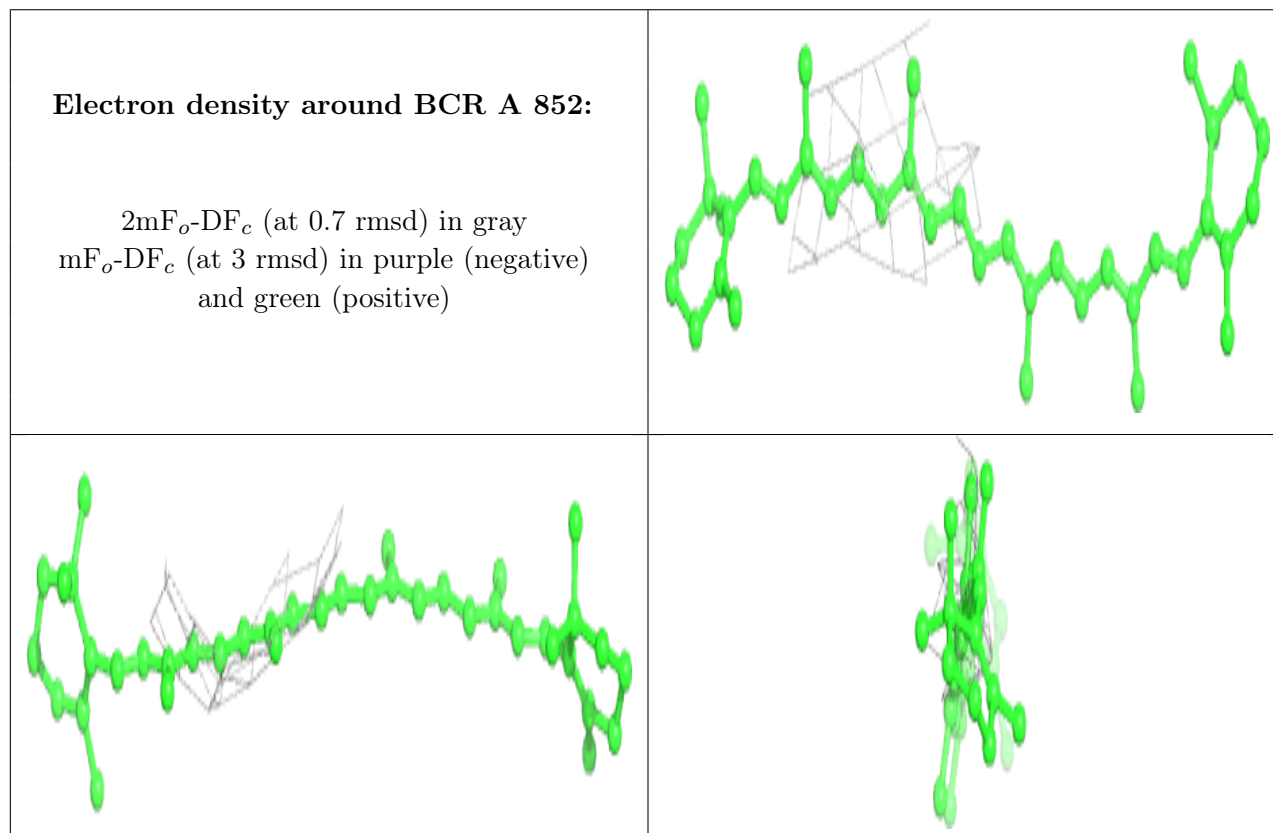
*Continued on next page...*



Continued from previous page...

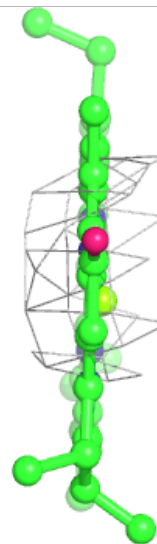
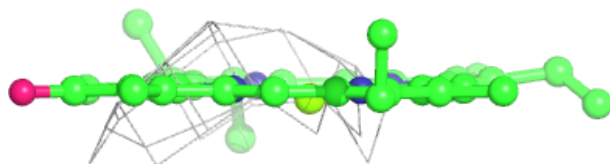
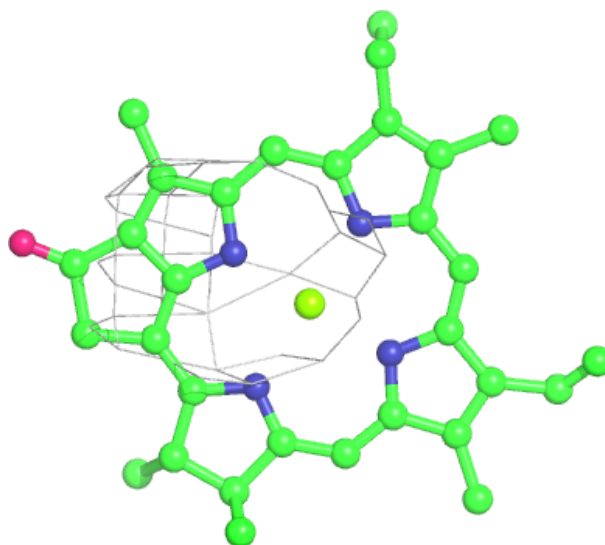
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
13	CLA	A	832	50/65	0.94	0.43	32,37,58,59	0
13	CLA	B	829	65/65	0.94	0.88	18,29,63,65	0
13	CLA	A	803	65/65	0.94	0.71	33,41,51,54	0
13	CLA	B	837	60/65	0.95	0.33	42,48,70,71	0
13	CLA	A	835	65/65	0.95	0.49	14,19,36,40	0
13	CLA	B	827	65/65	0.96	0.63	24,31,77,80	0
13	CLA	B	834	45/65	0.96	0.47	40,47,53,56	0
13	CLA	B	802	65/65	0.96	0.53	28,39,55,59	0
13	CLA	B	808	65/65	0.96	0.56	21,28,49,50	0
13	CLA	A	841	65/65	0.97	0.42	33,38,55,55	0
15	SF4	C	101	8/8	0.97	0.24	24,25,26,26	0
13	CLA	A	829	65/65	0.98	0.61	38,46,74,75	0
15	SF4	A	848	8/8	0.99	0.18	25,26,27,27	0

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



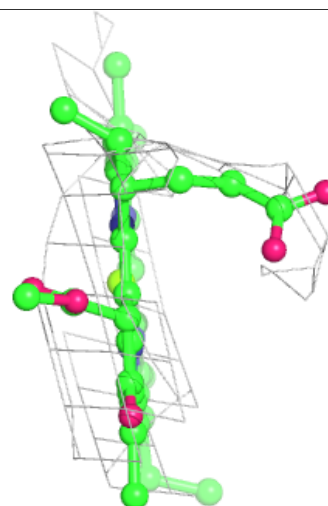
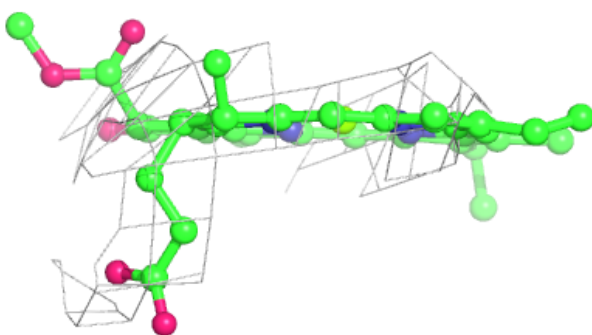
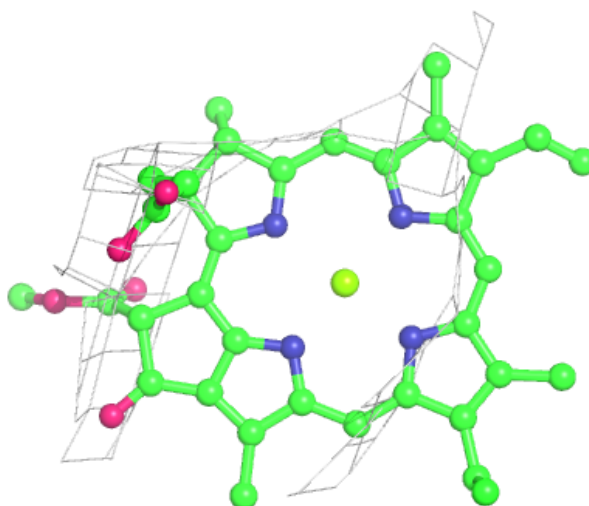
**Electron density around CLA J 102:**

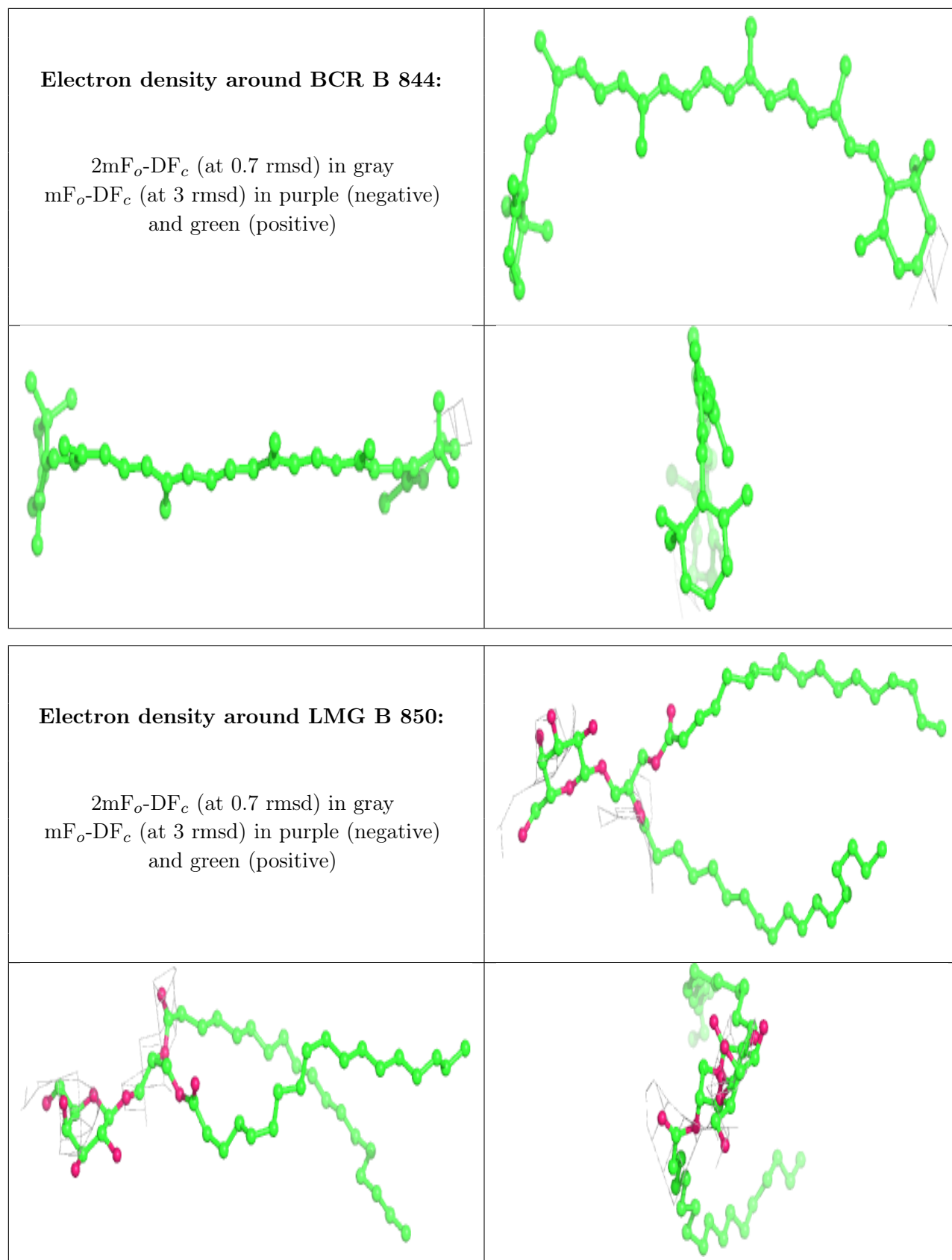
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 812:**

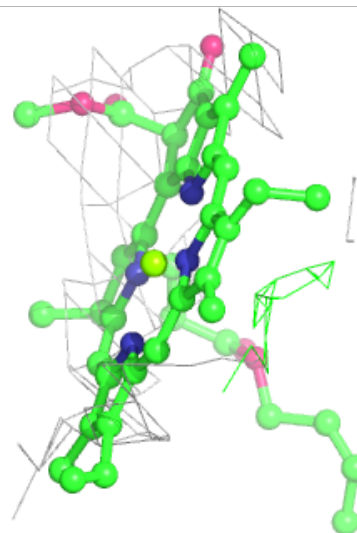
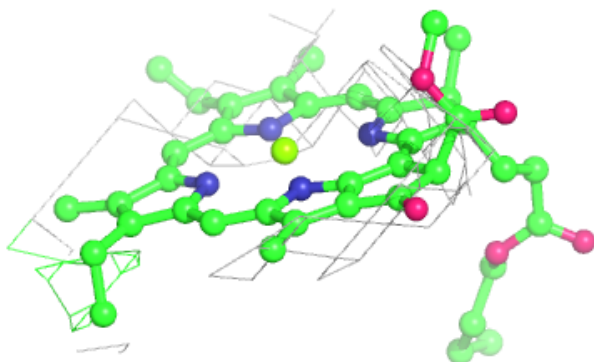
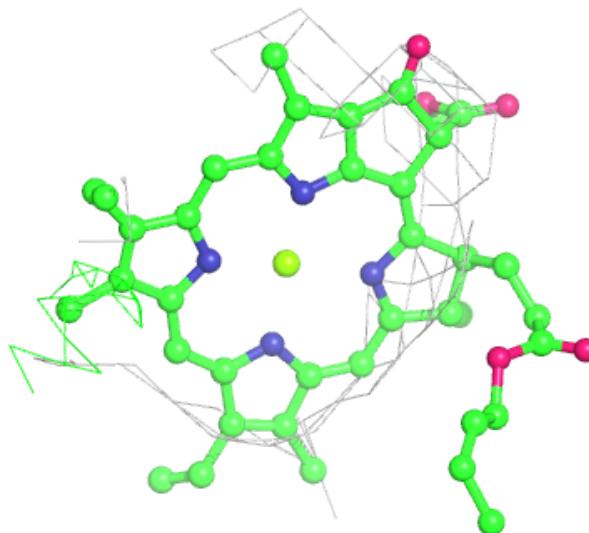
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





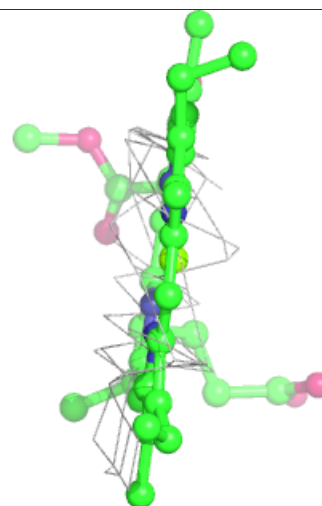
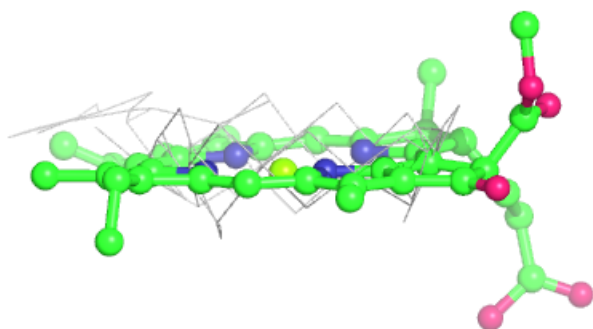
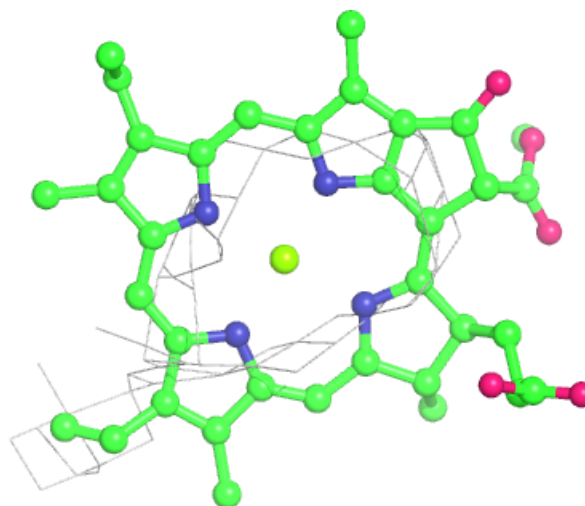
**Electron density around CLA A 823:**

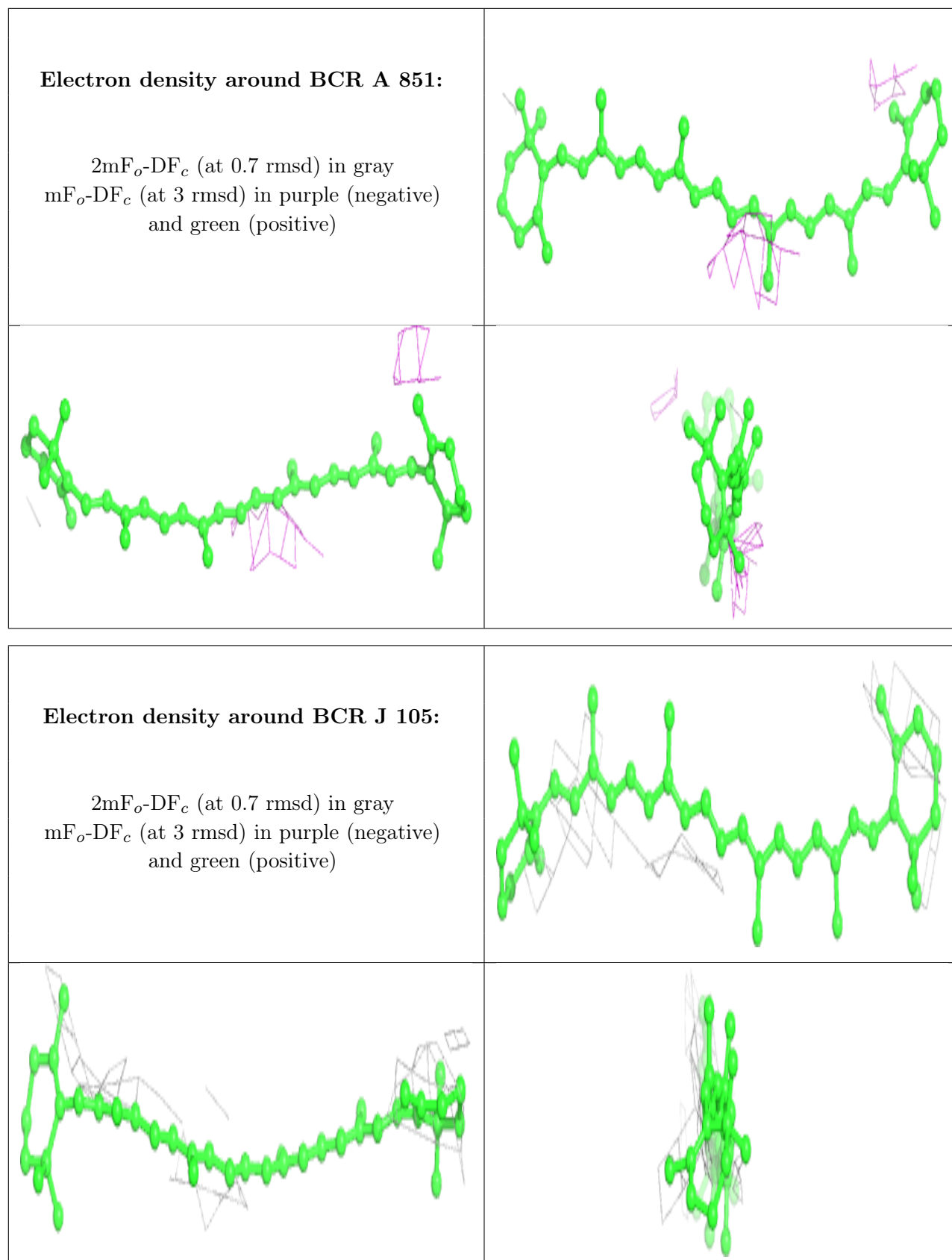
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

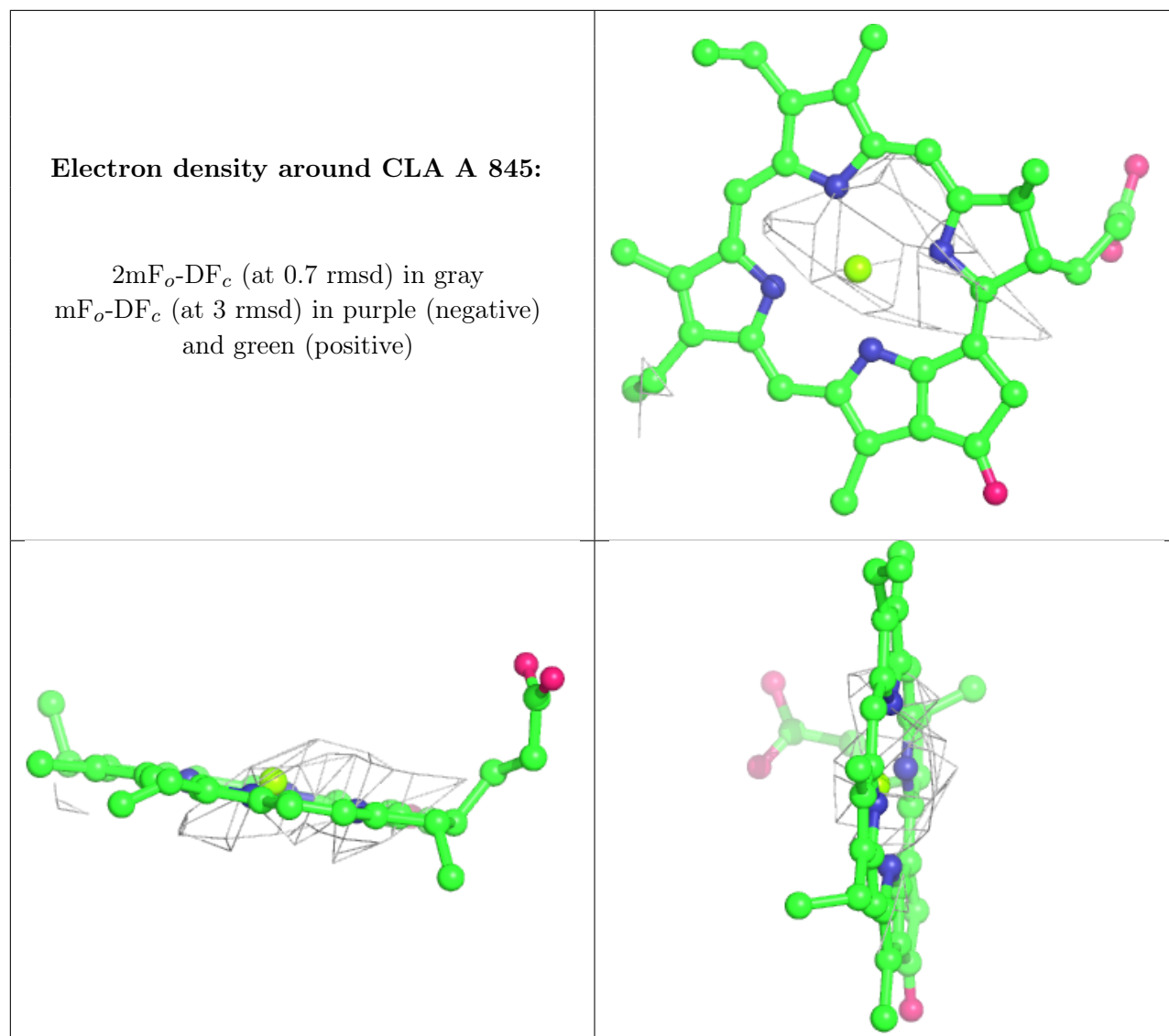


**Electron density around CLA J 101:**

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



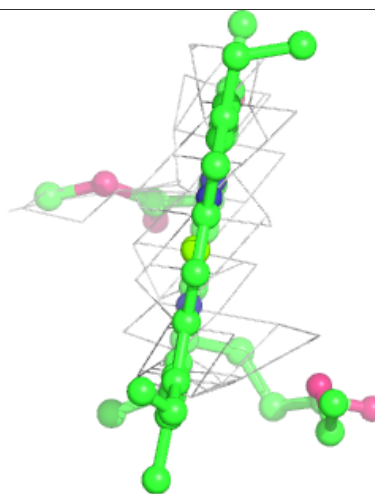
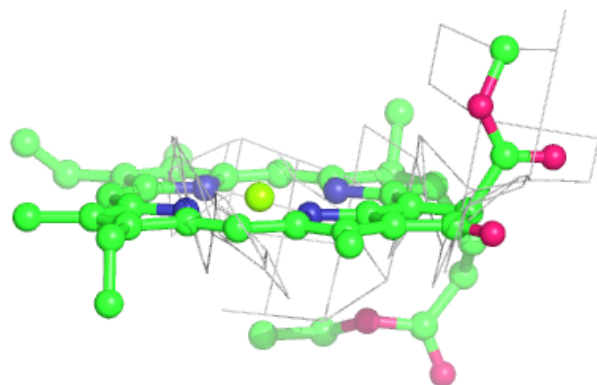
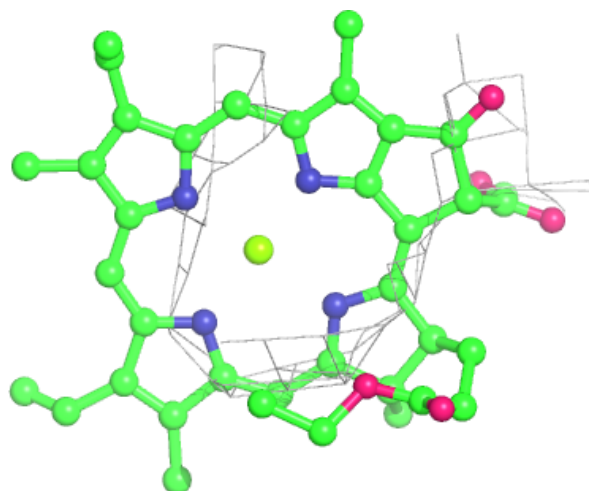


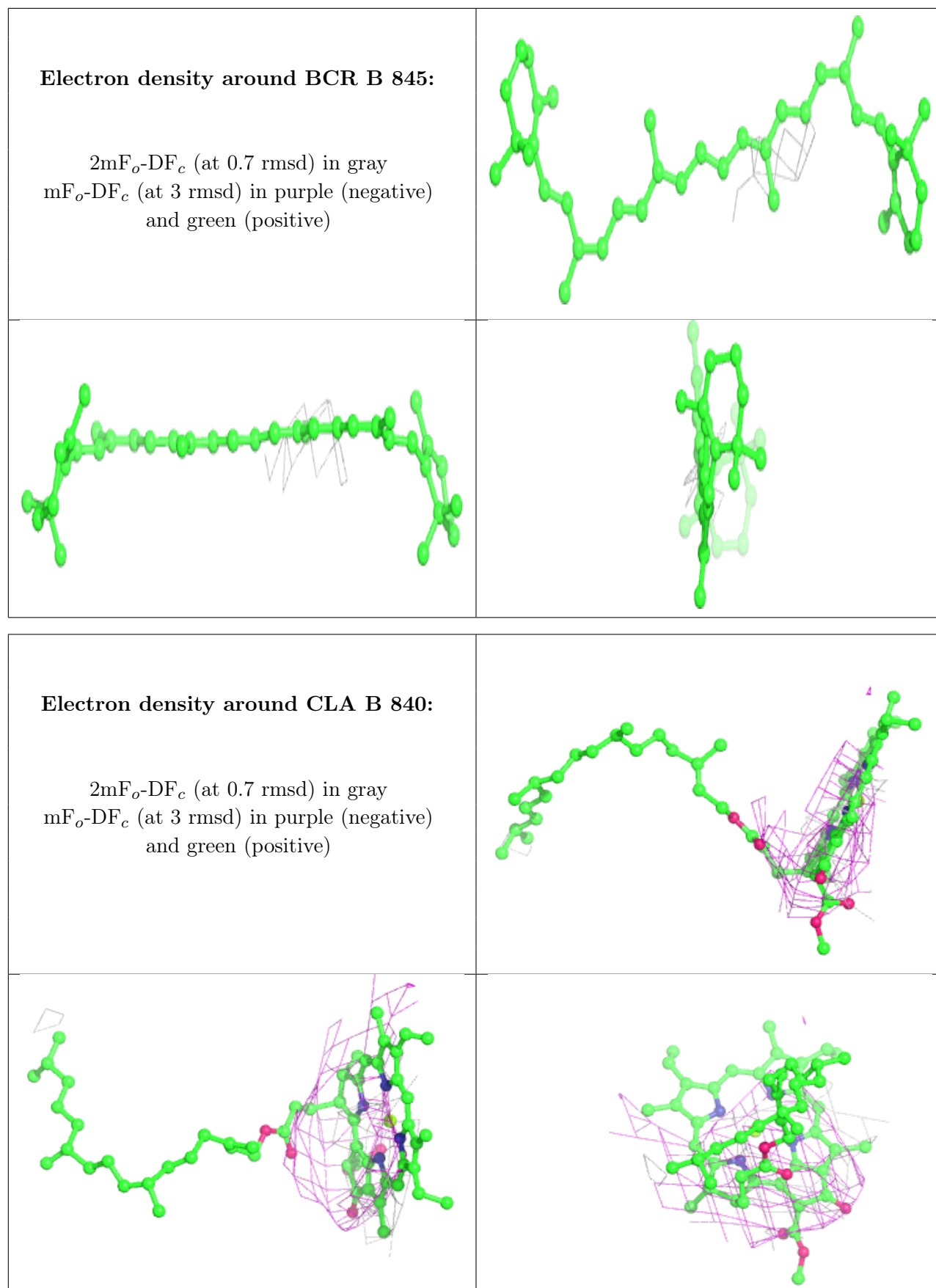




**Electron density around CLA B 820:**

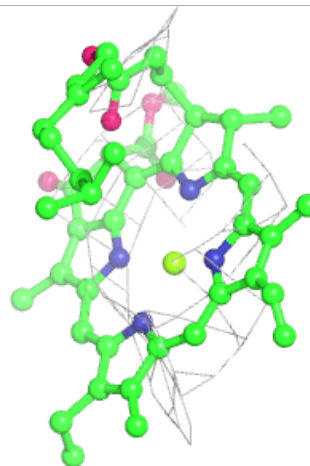
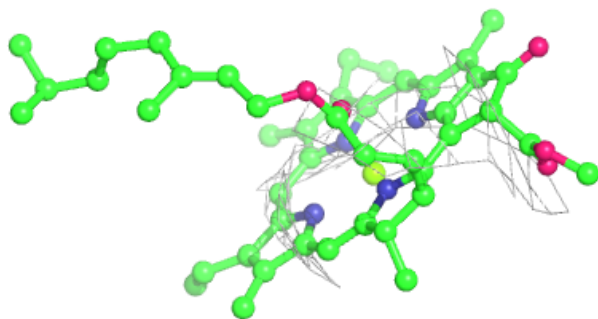
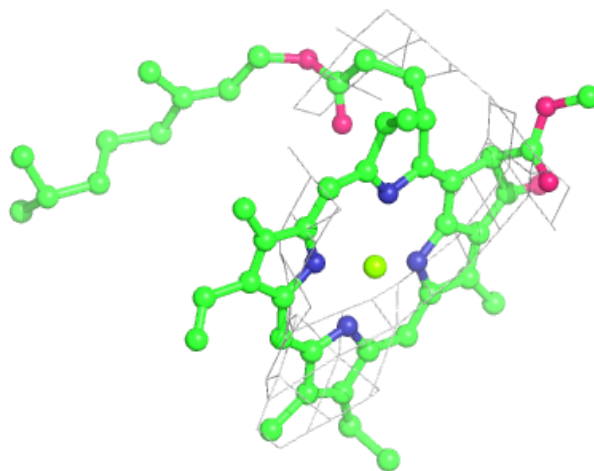
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

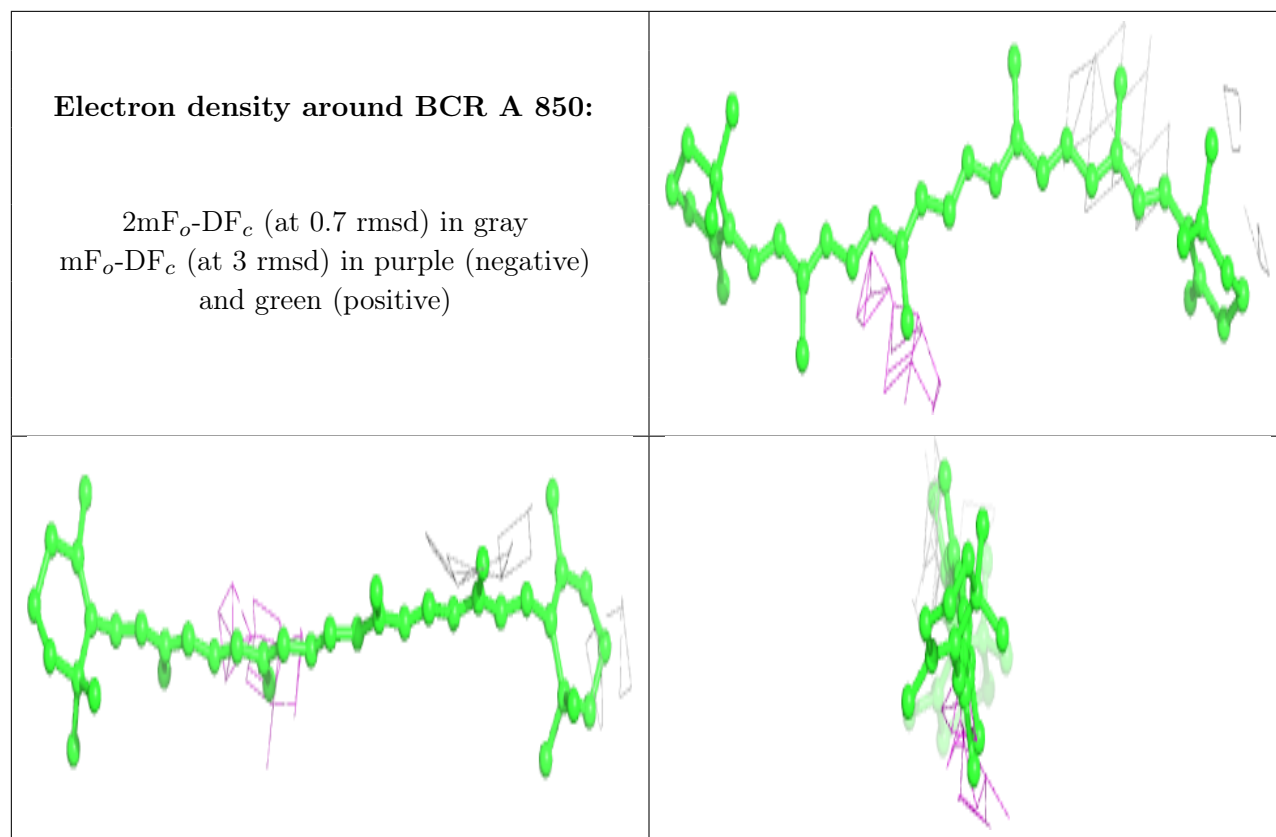




**Electron density around CLA B 816:**

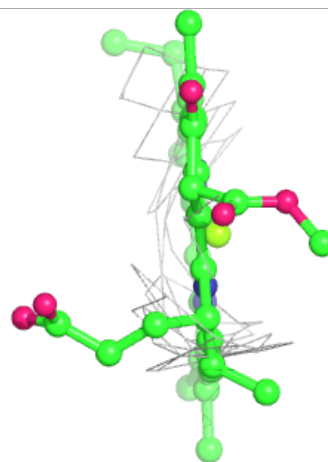
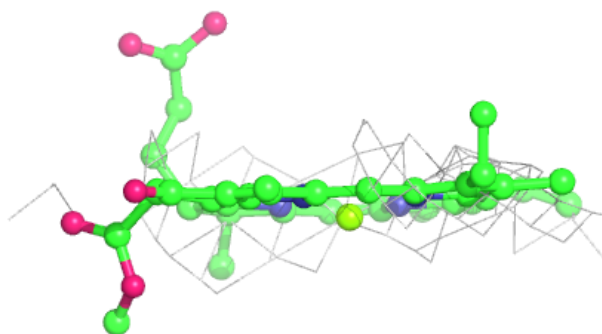
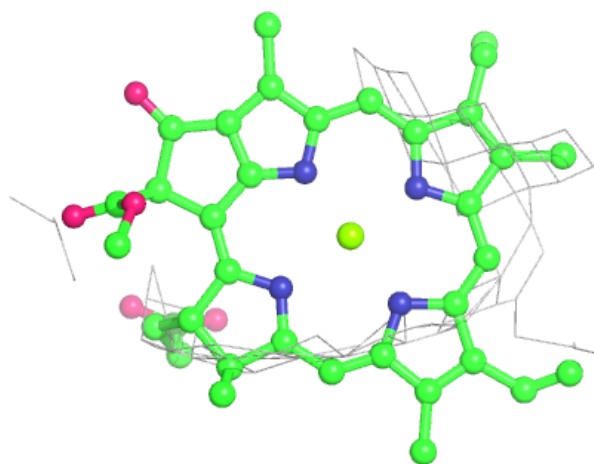
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





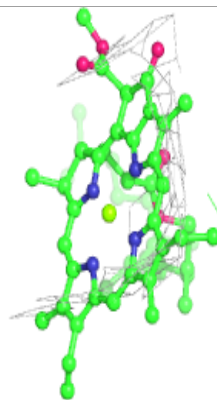
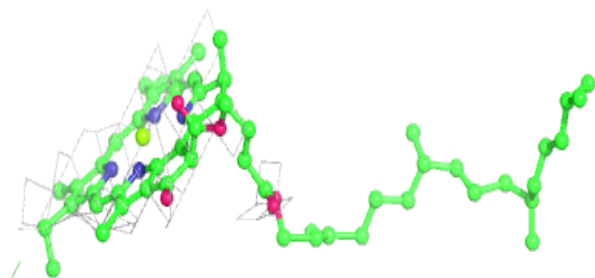
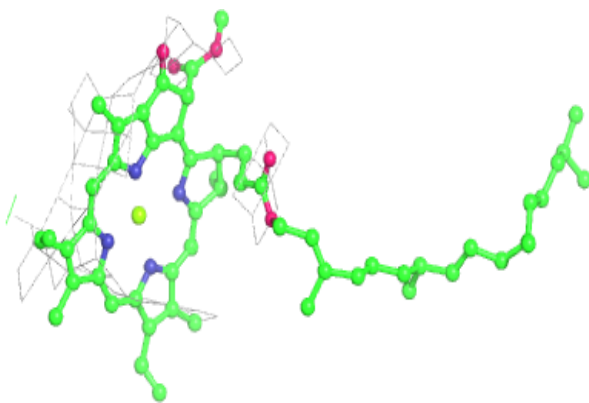
**Electron density around CLA B 815:**

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

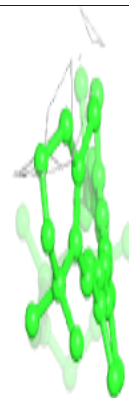
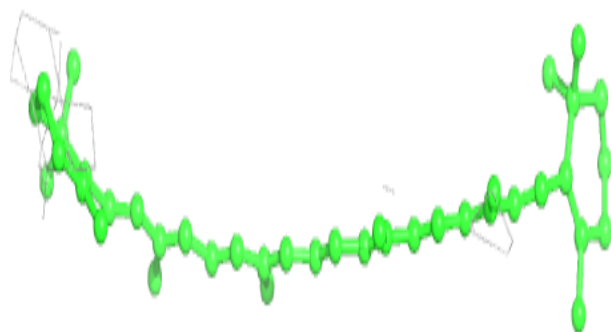
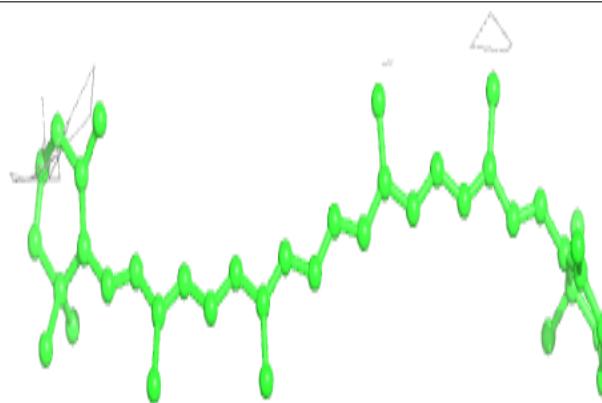


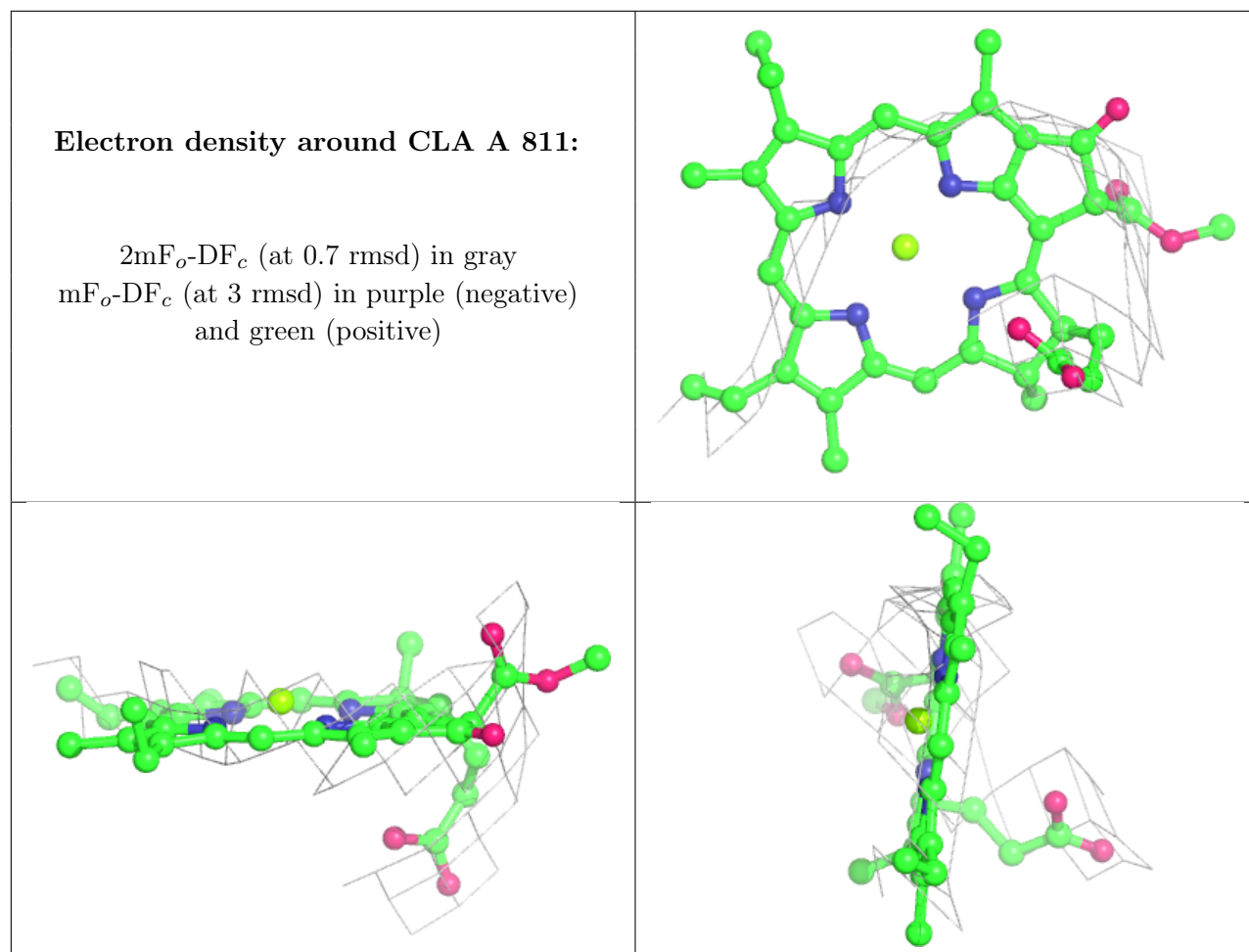
**Electron density around CLA A 822:**

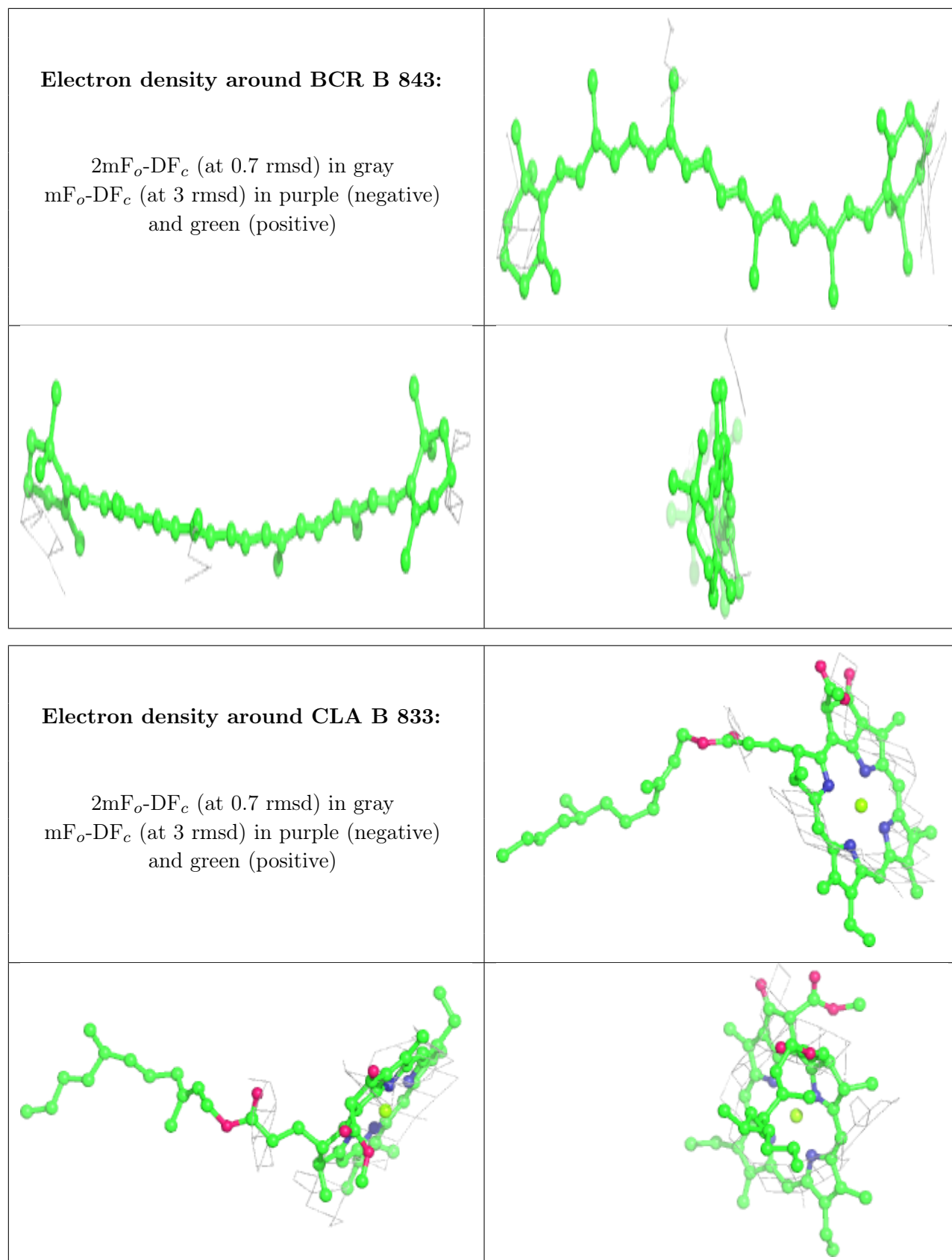
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR A 853:**

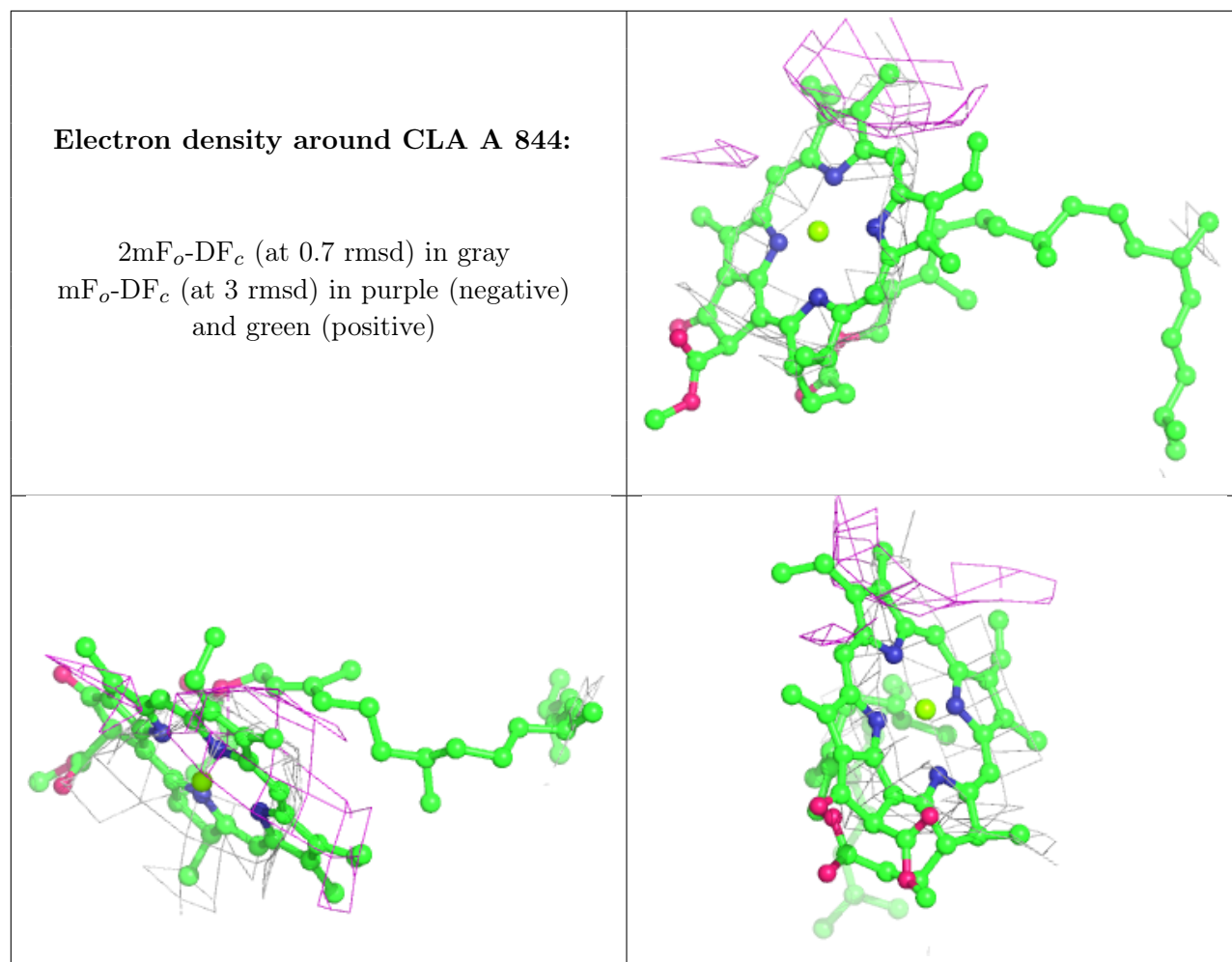
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

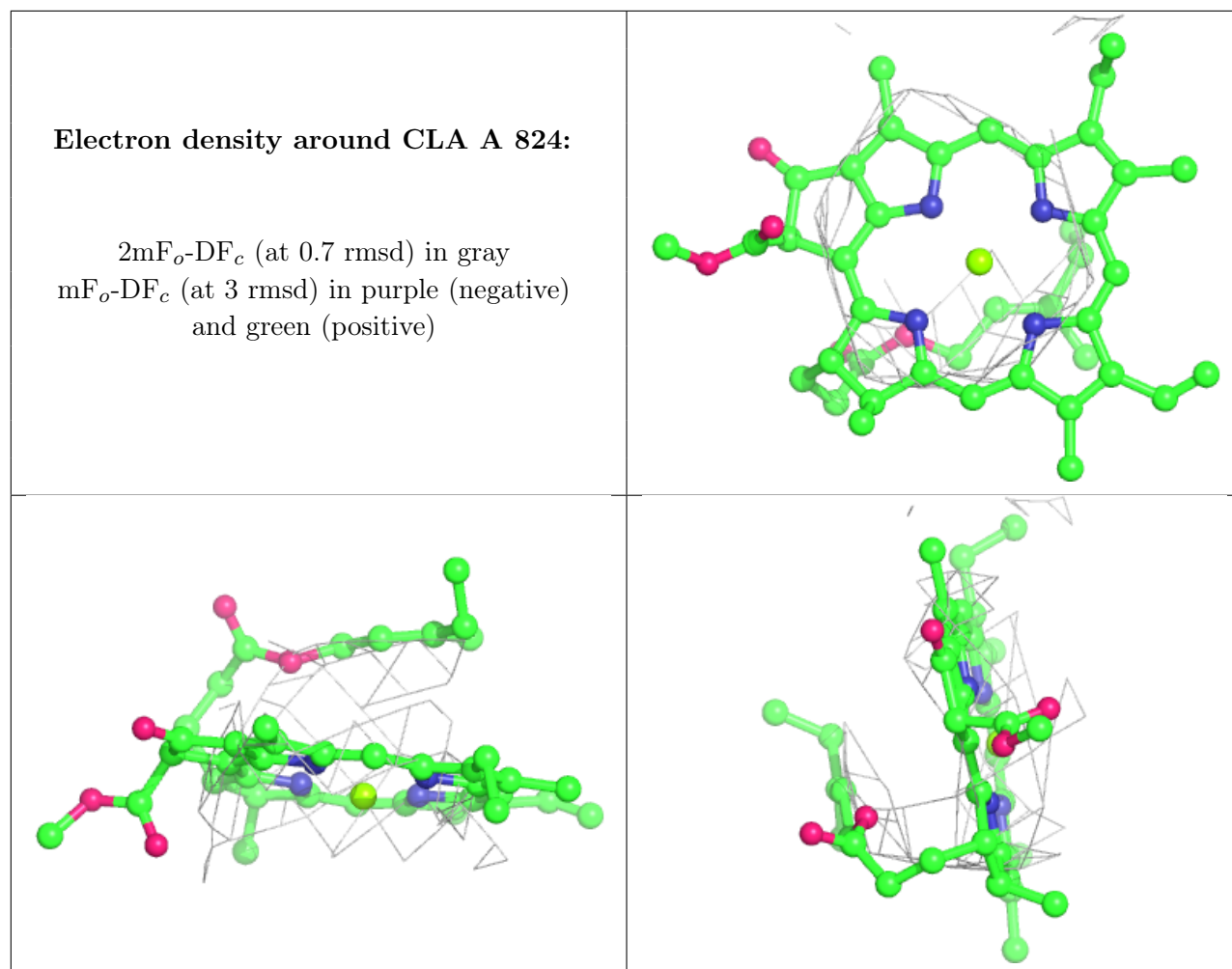






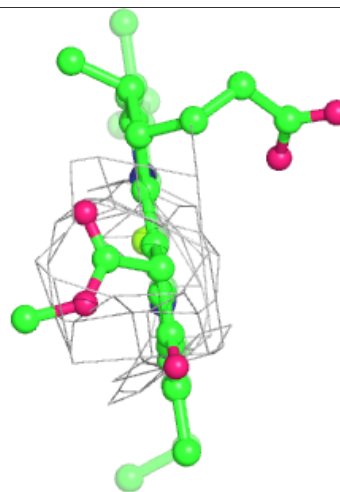
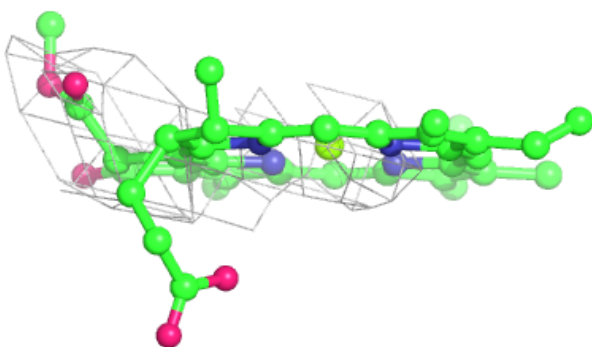
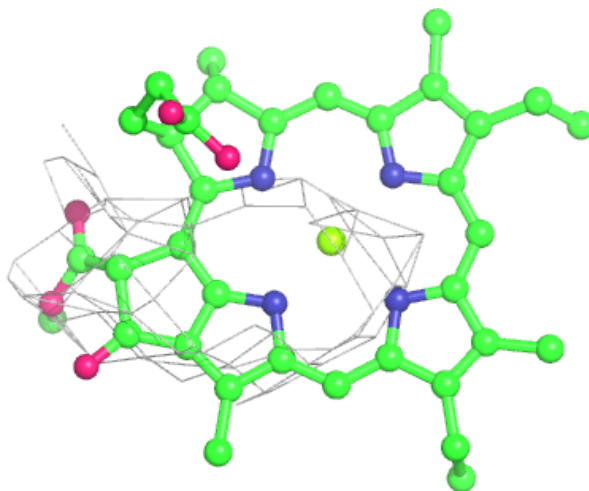


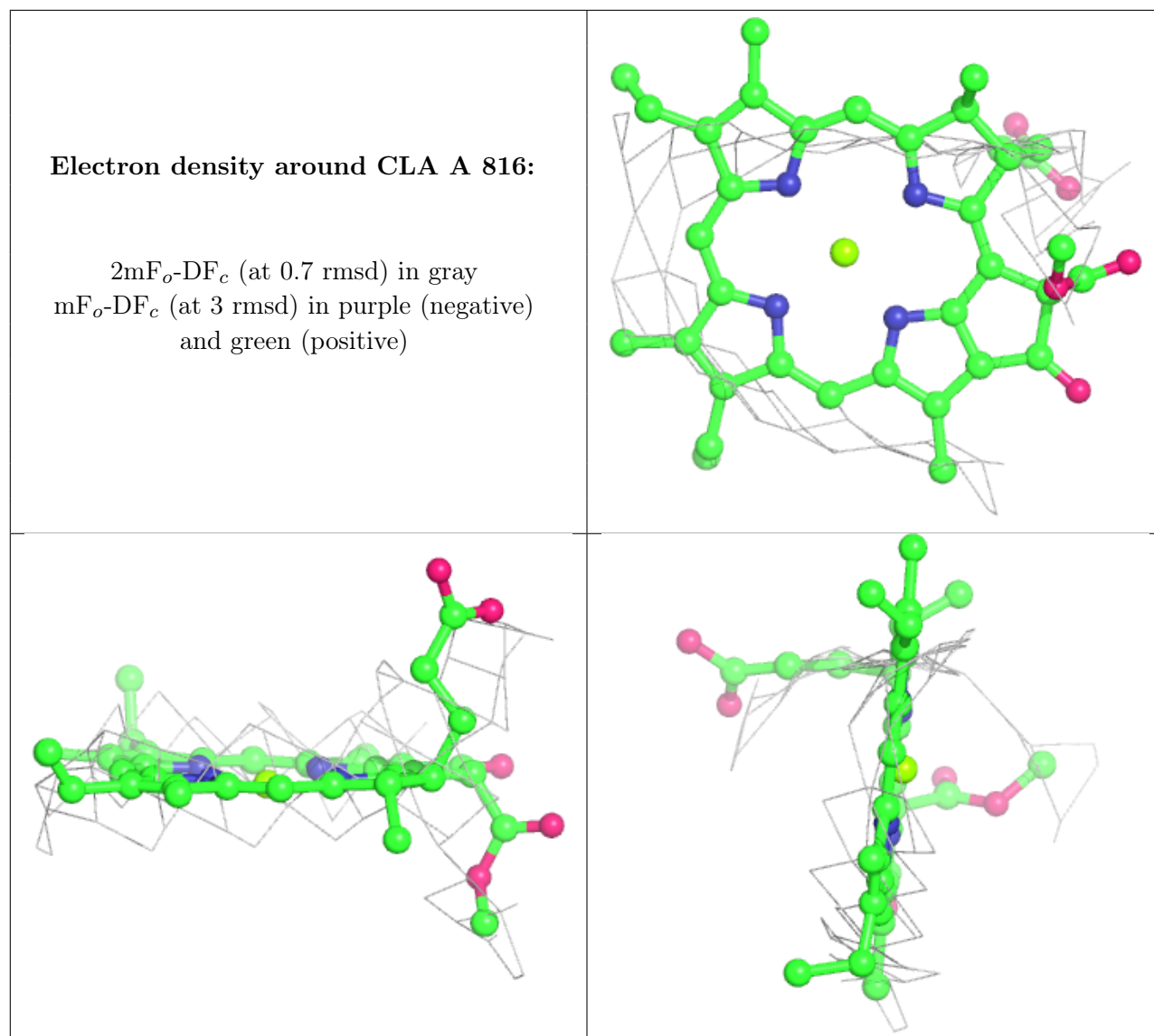


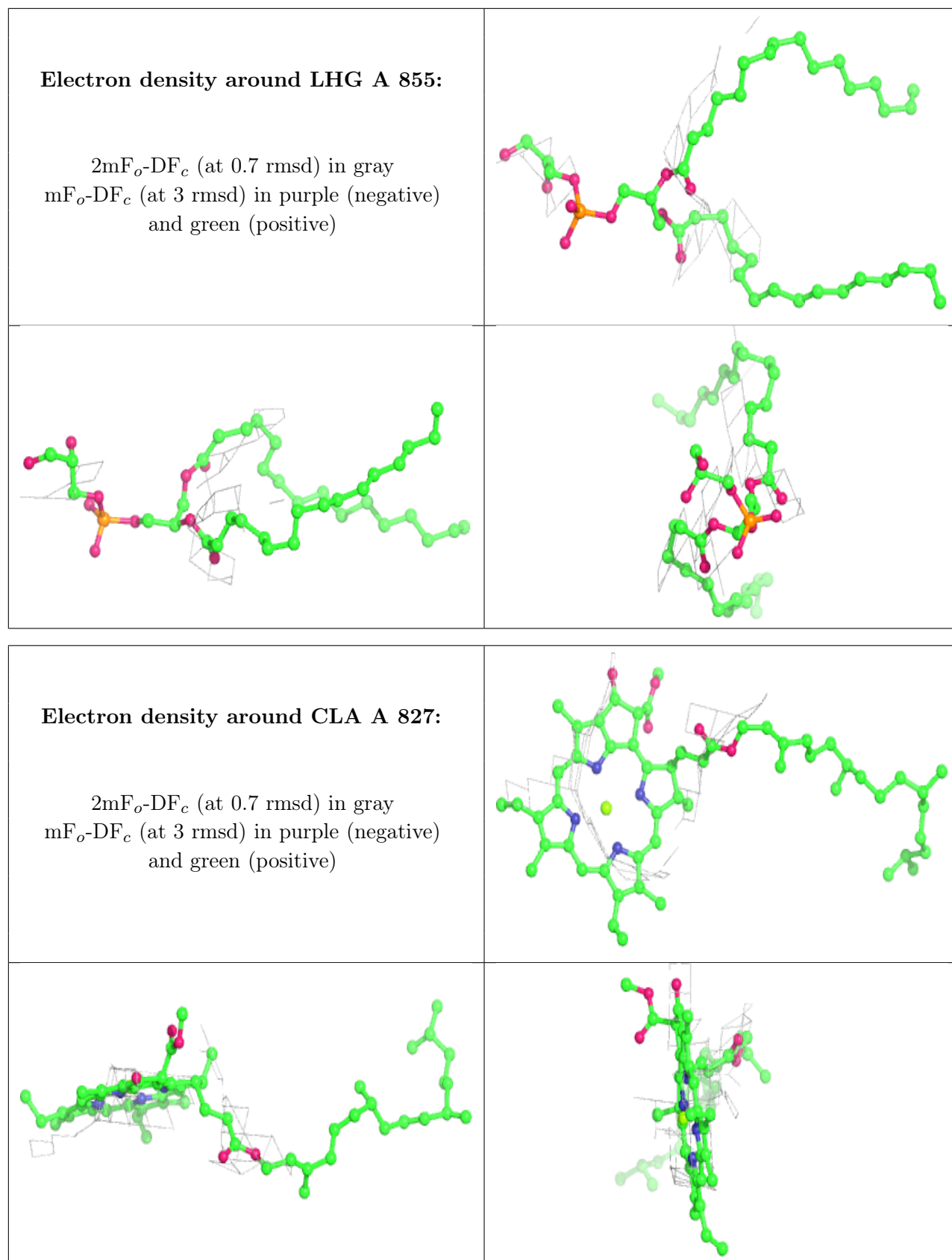


**Electron density around CLA M 1601:**

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

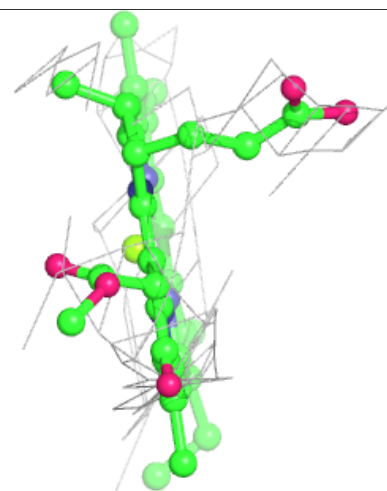
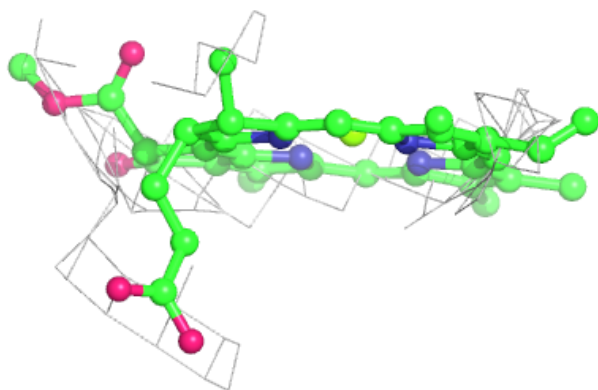
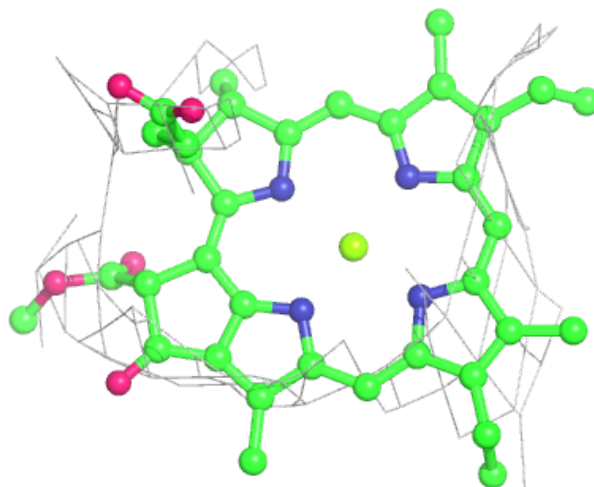






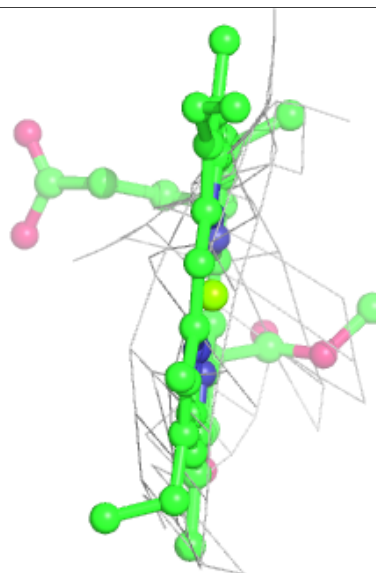
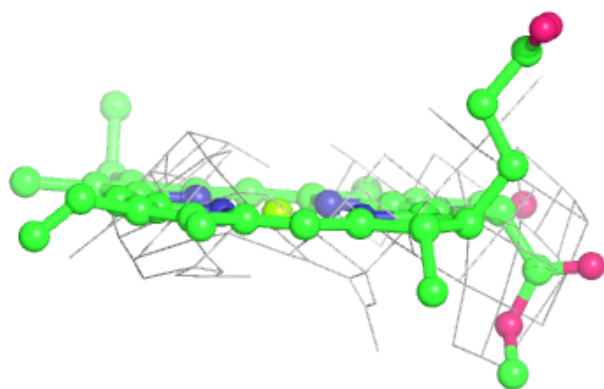
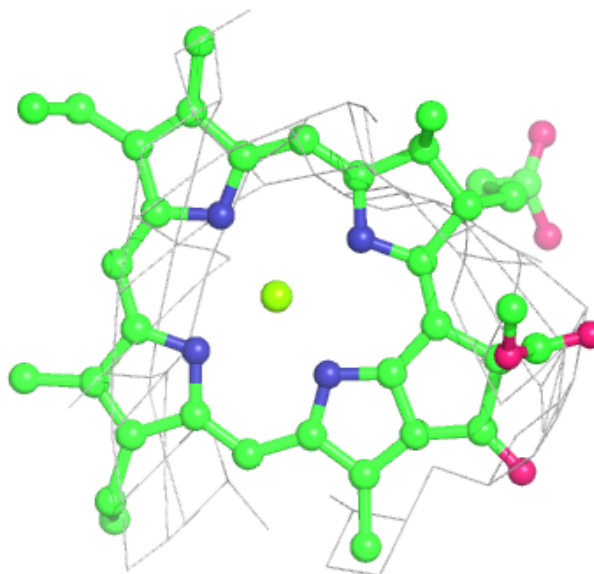
**Electron density around CLA B 811:**

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



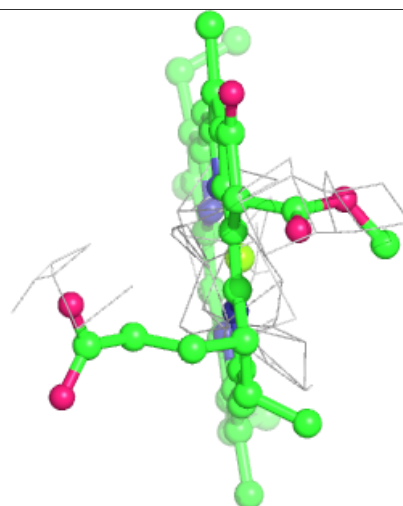
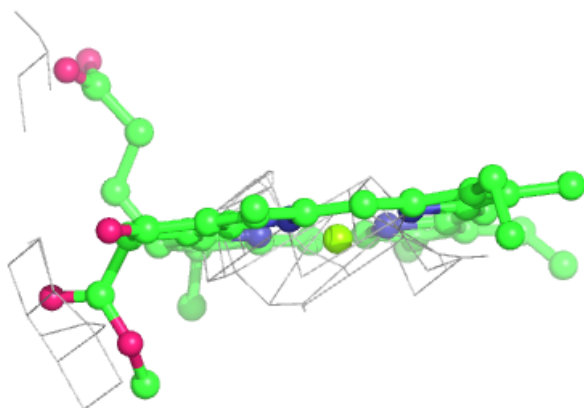
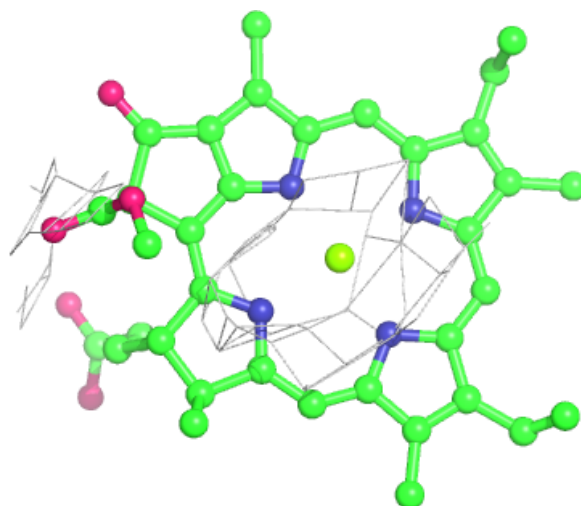
**Electron density around CLA B 821:**

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

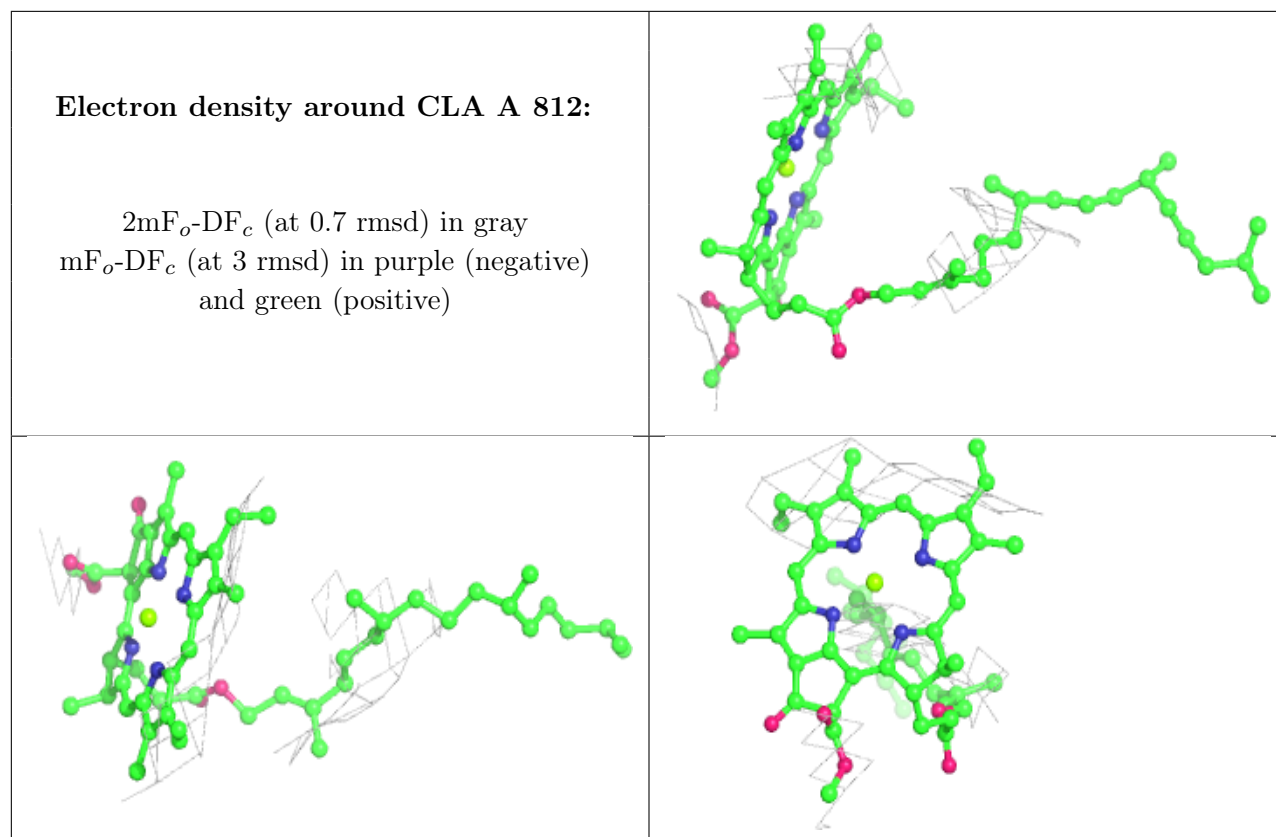


**Electron density around CLA K 1401:**

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

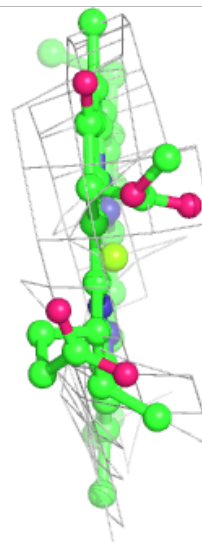
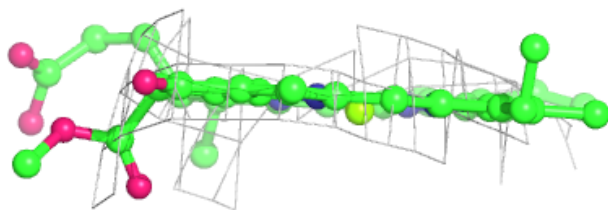
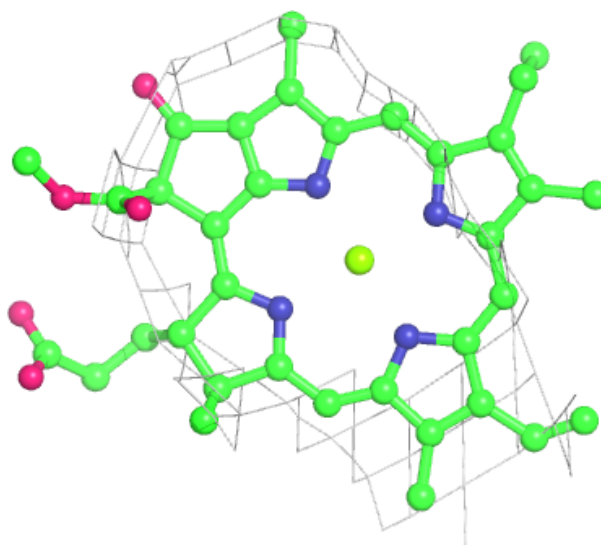






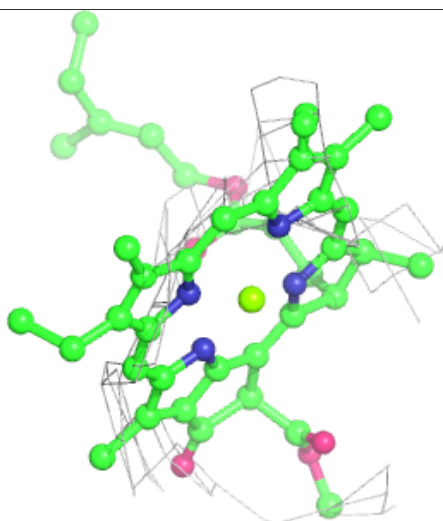
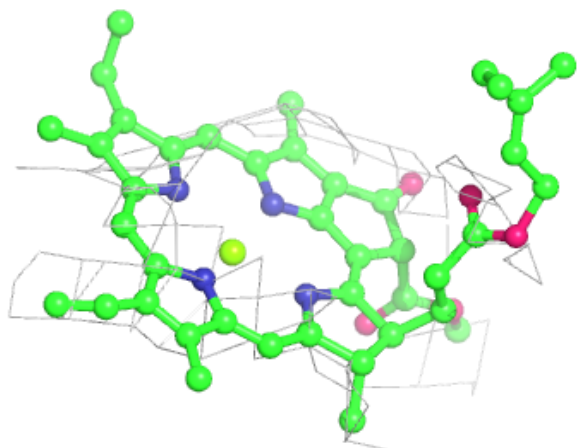
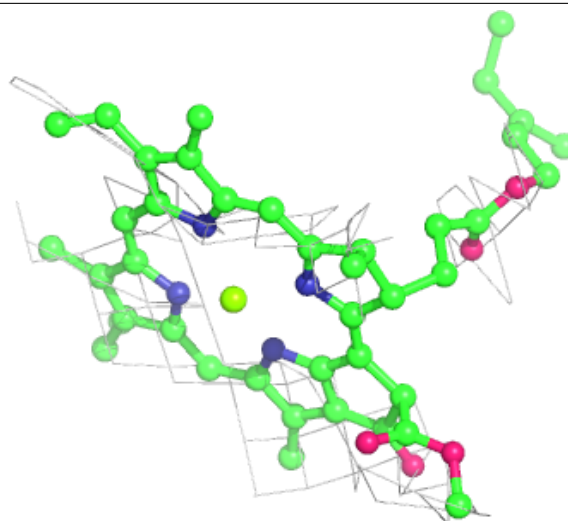
**Electron density around CLA B 836:**

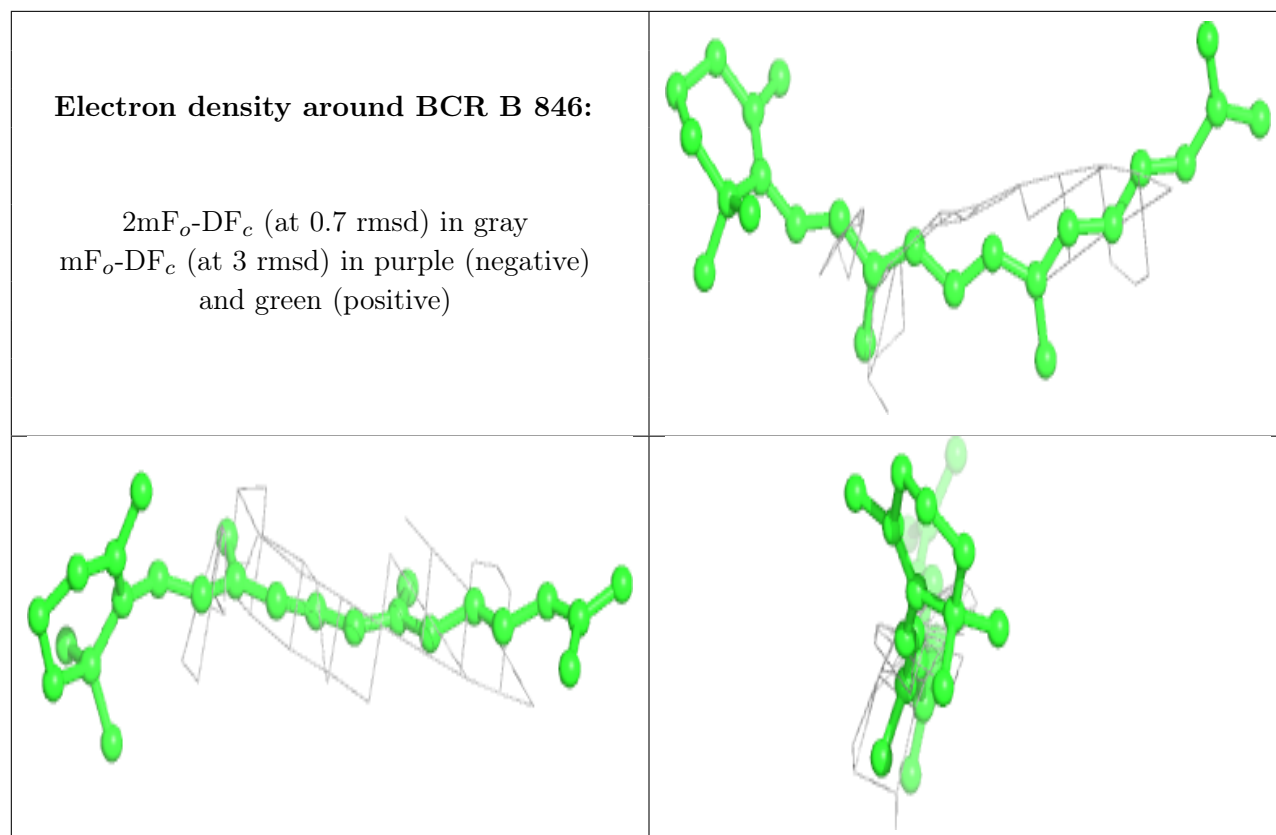
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

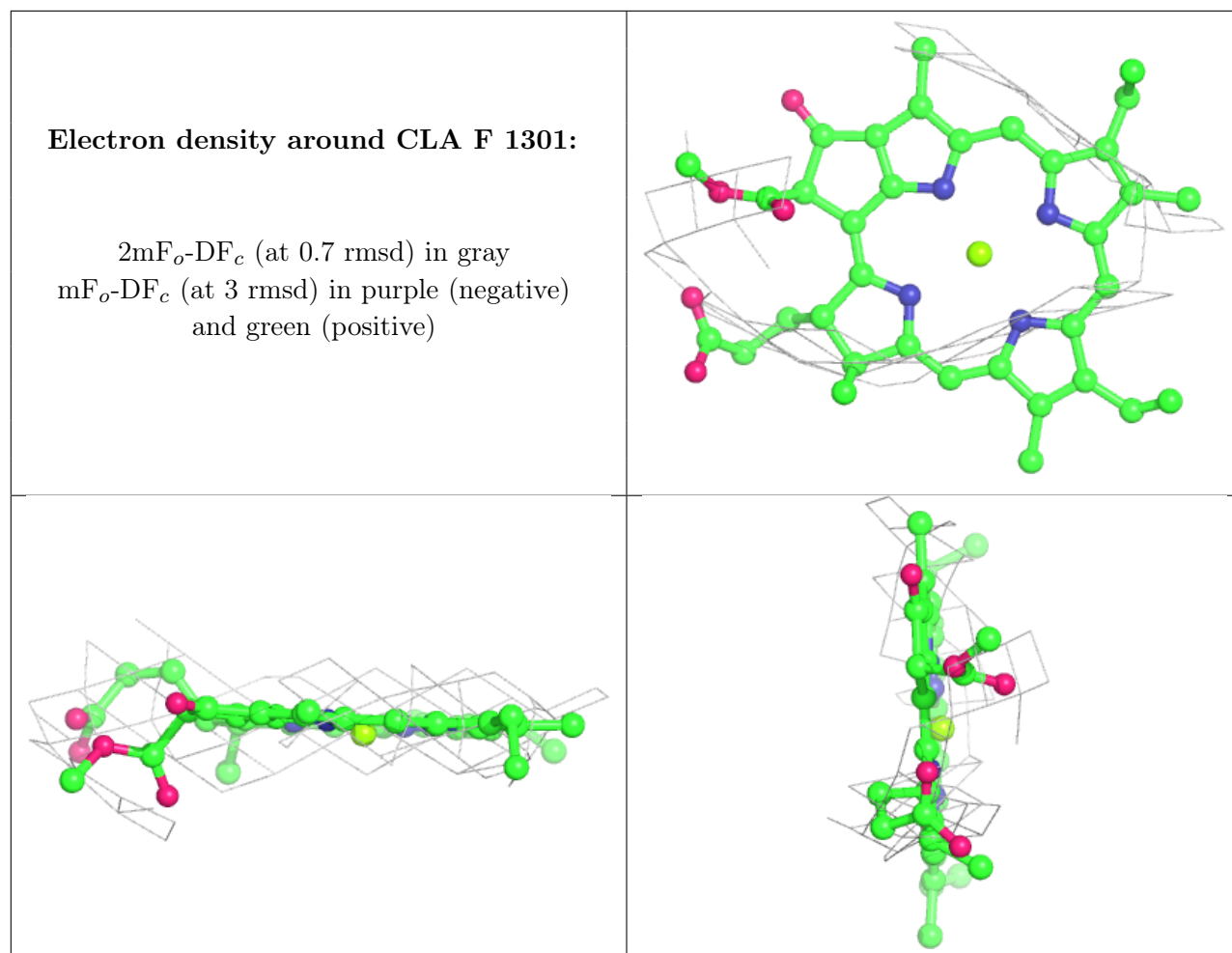


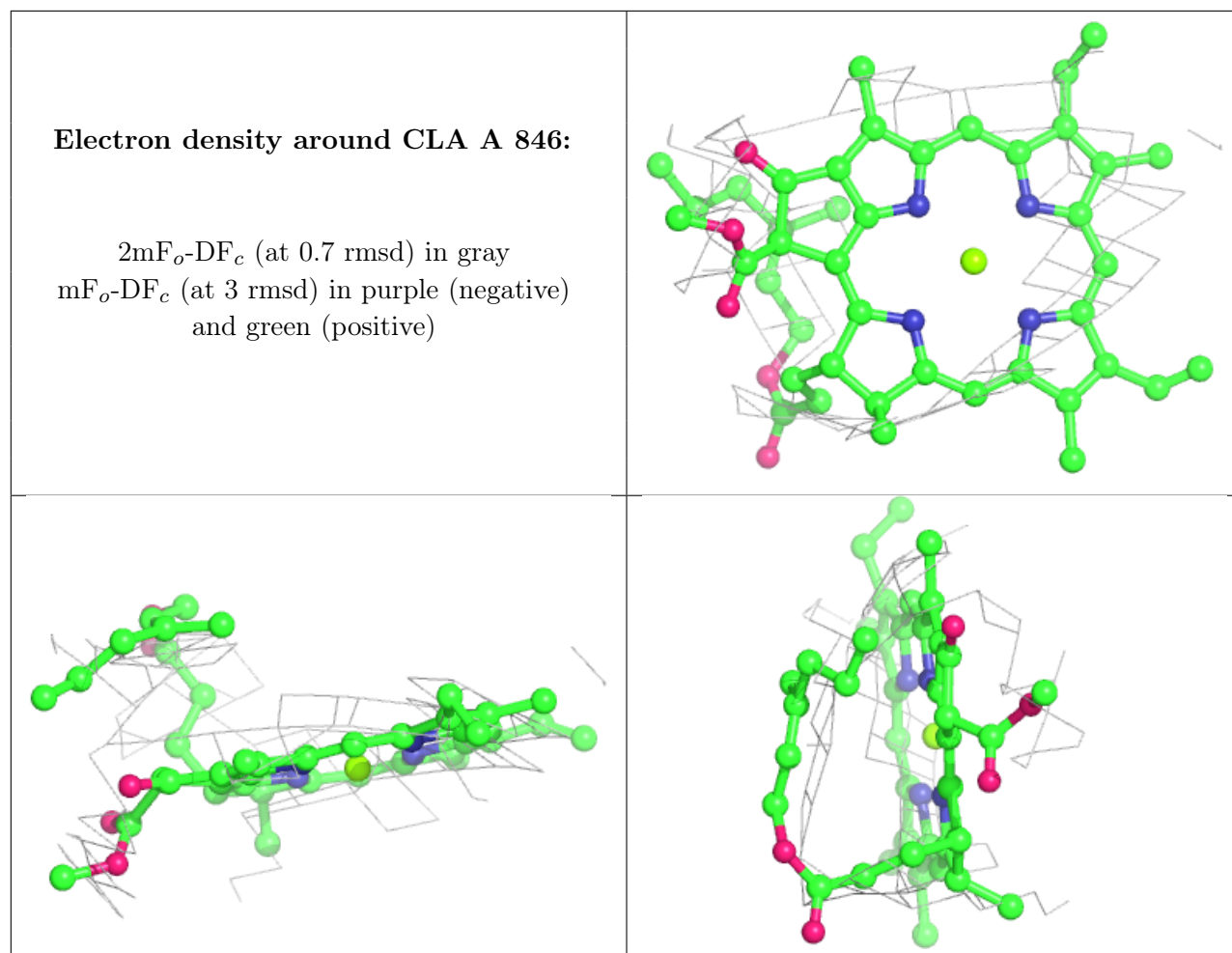
**Electron density around CLA A 808:**

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



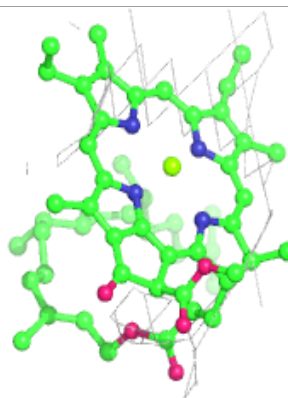
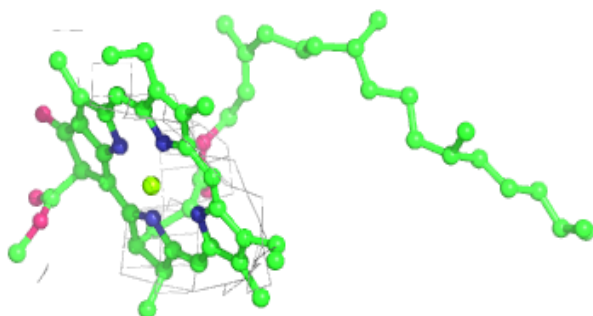
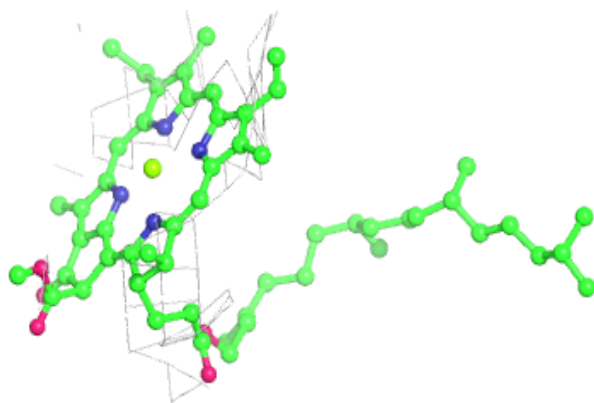




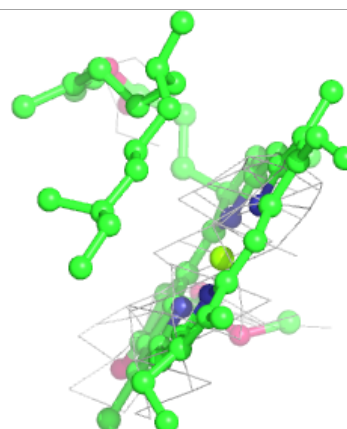
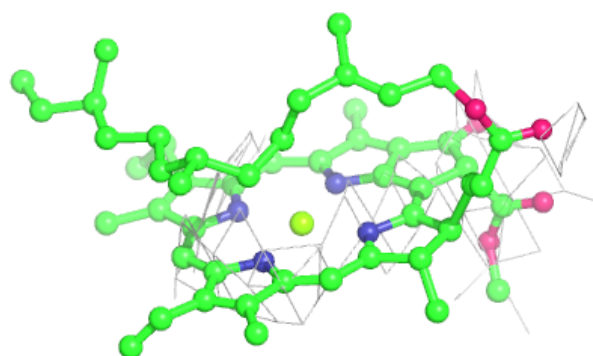
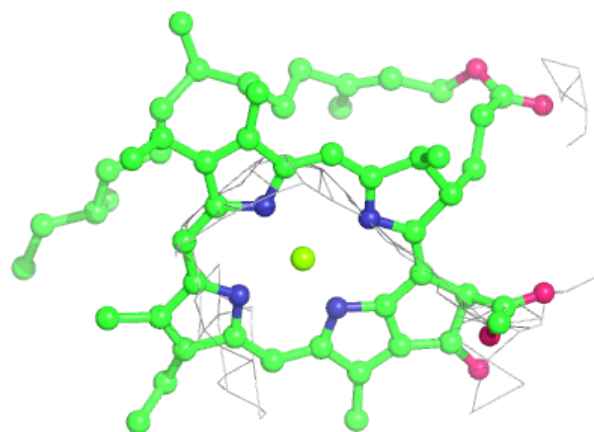


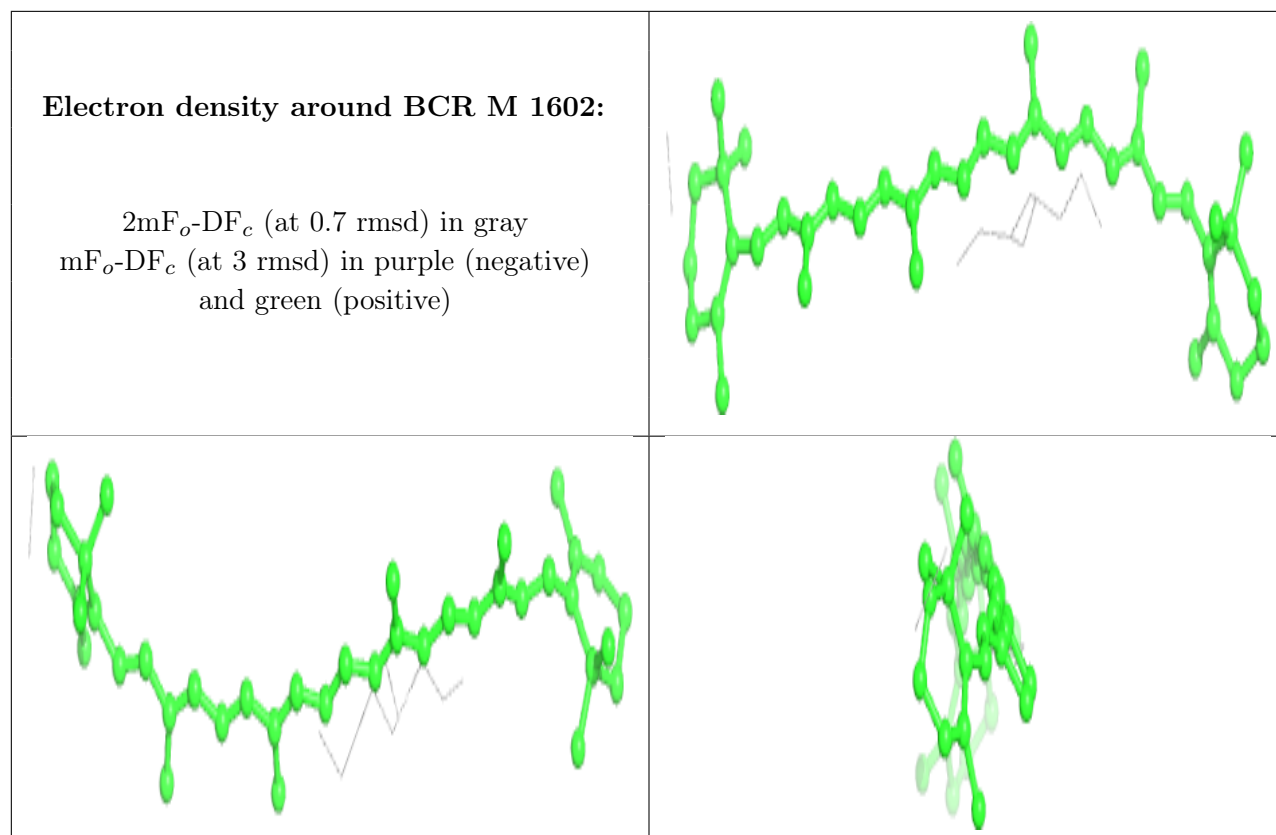
**Electron density around CLA B 814:**

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

**Electron density around CLA 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)

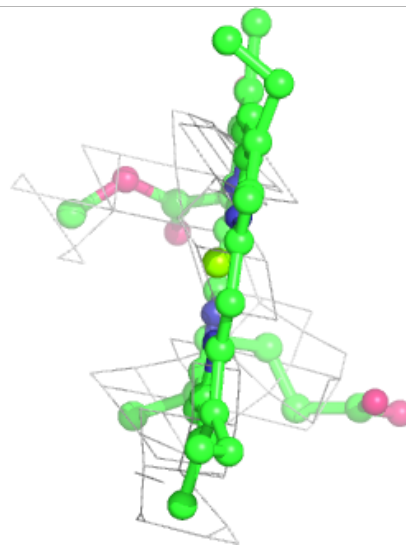
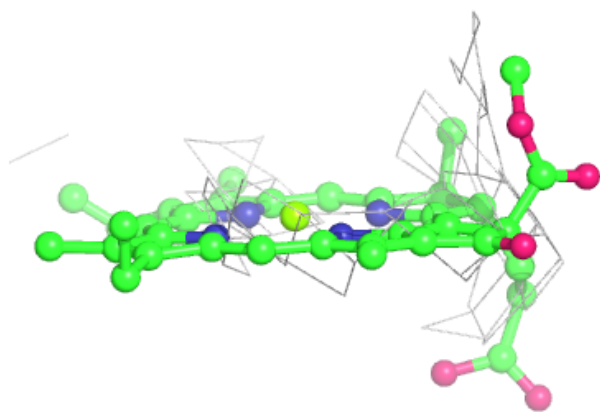
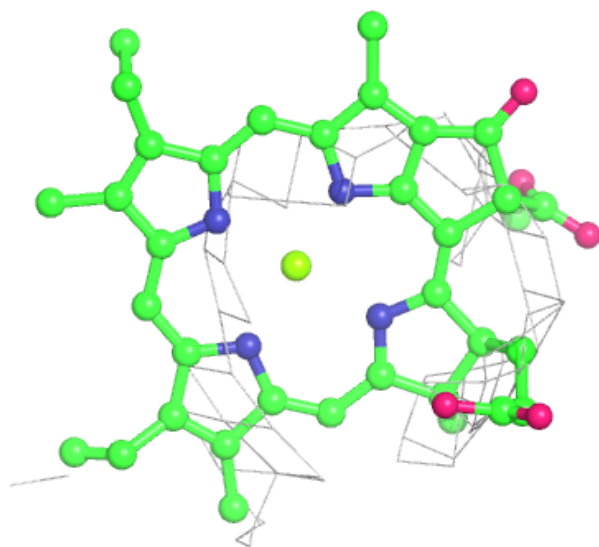


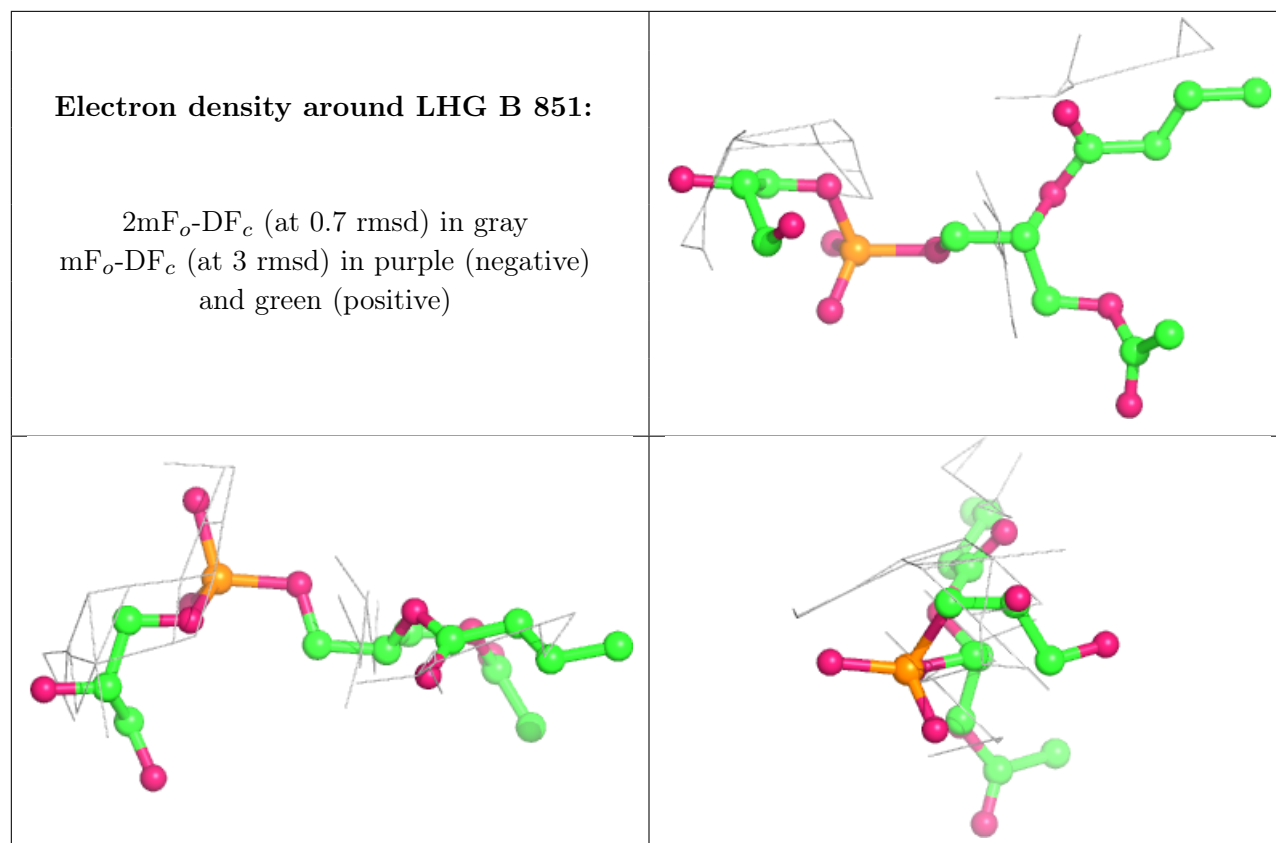




**Electron density around CLA B 830:**

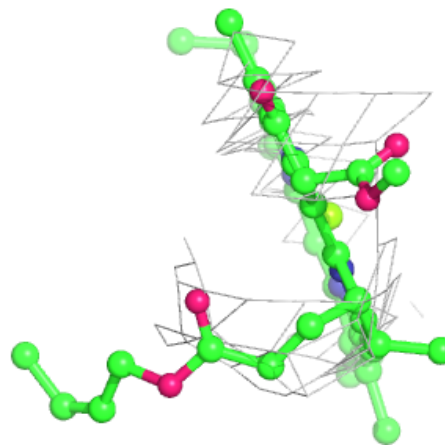
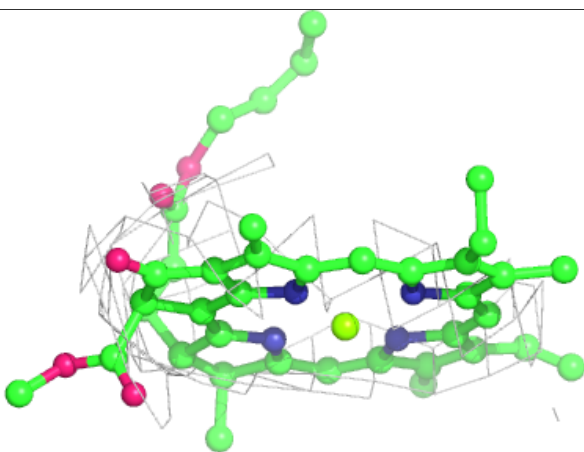
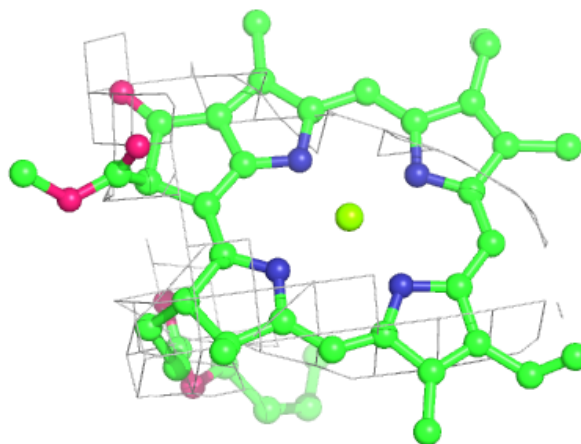
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

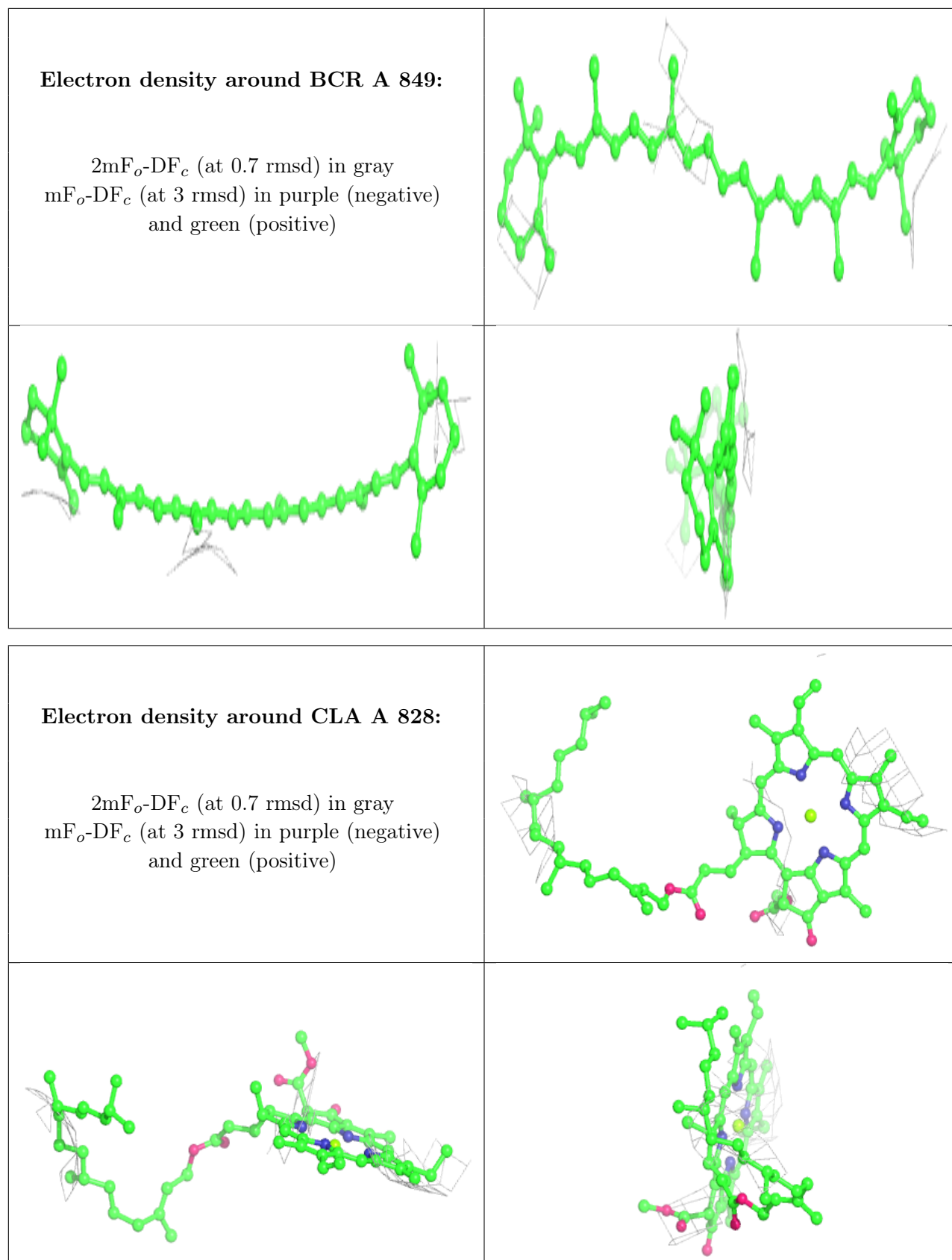


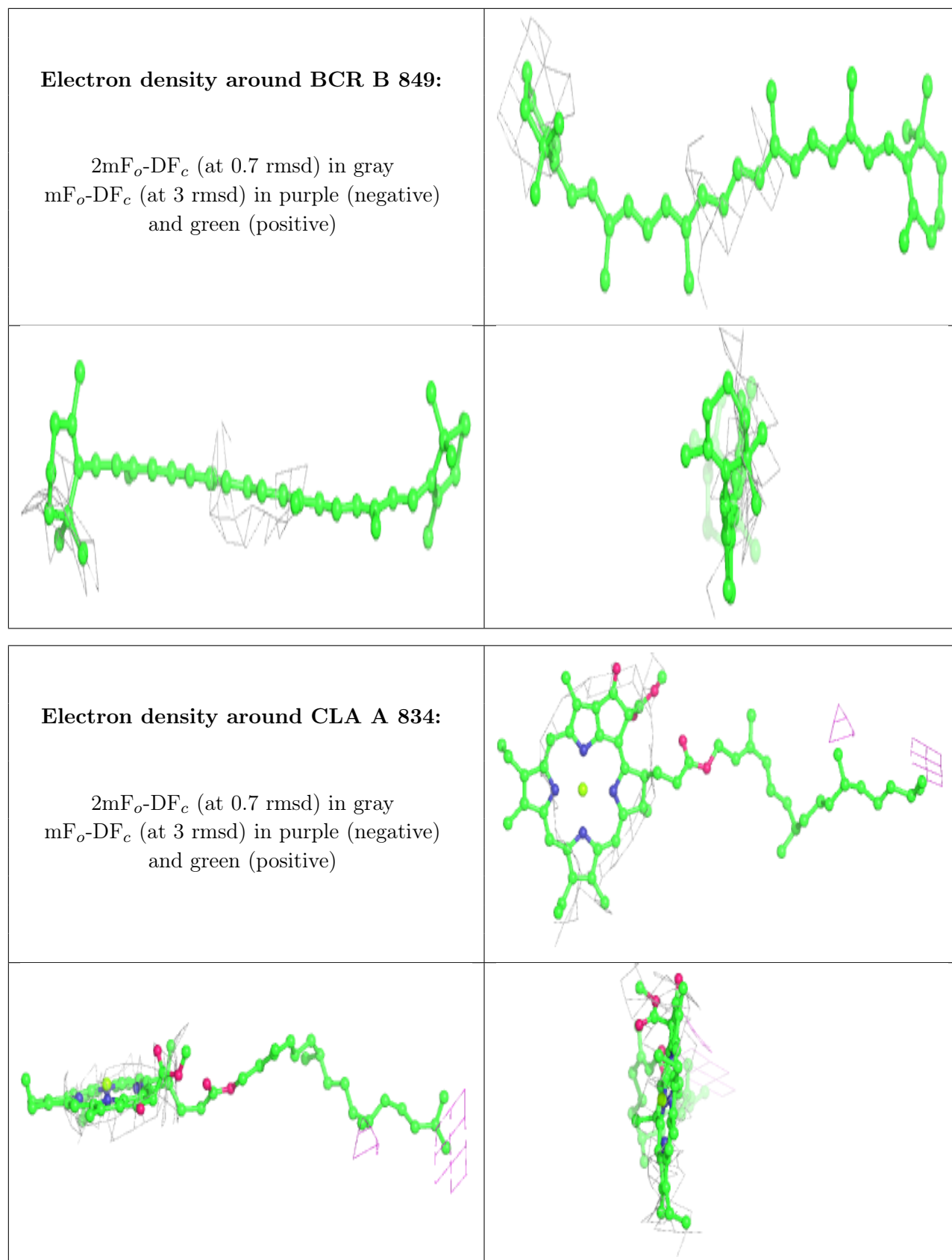


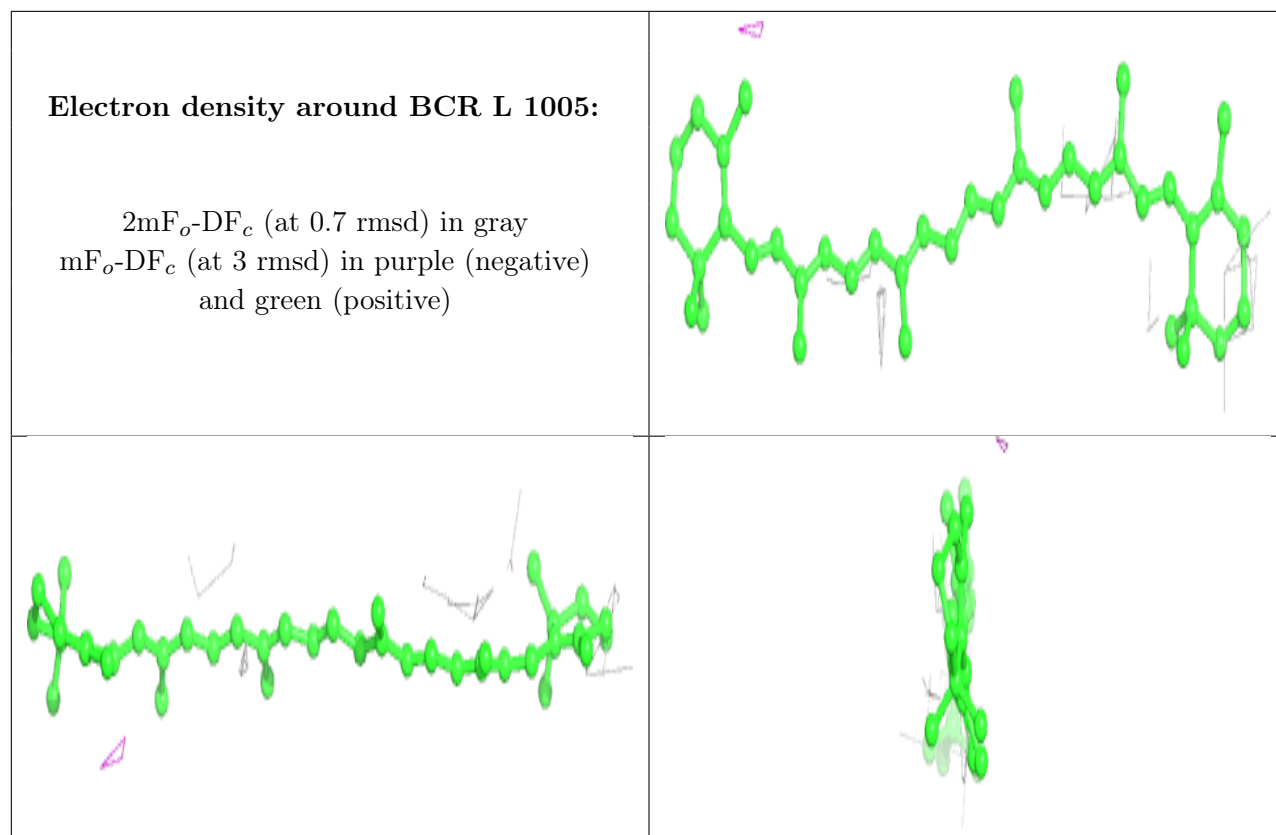
**Electron density around CLA B 831:**

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



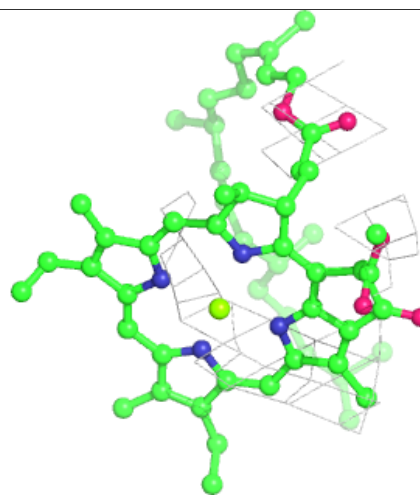
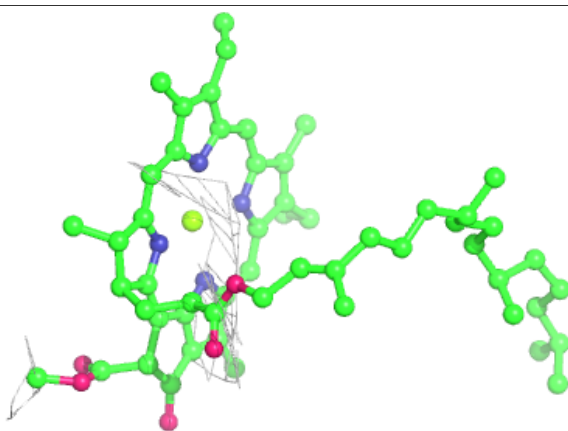
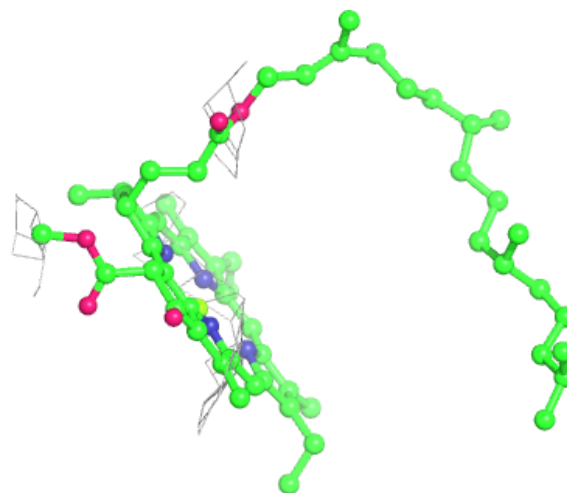


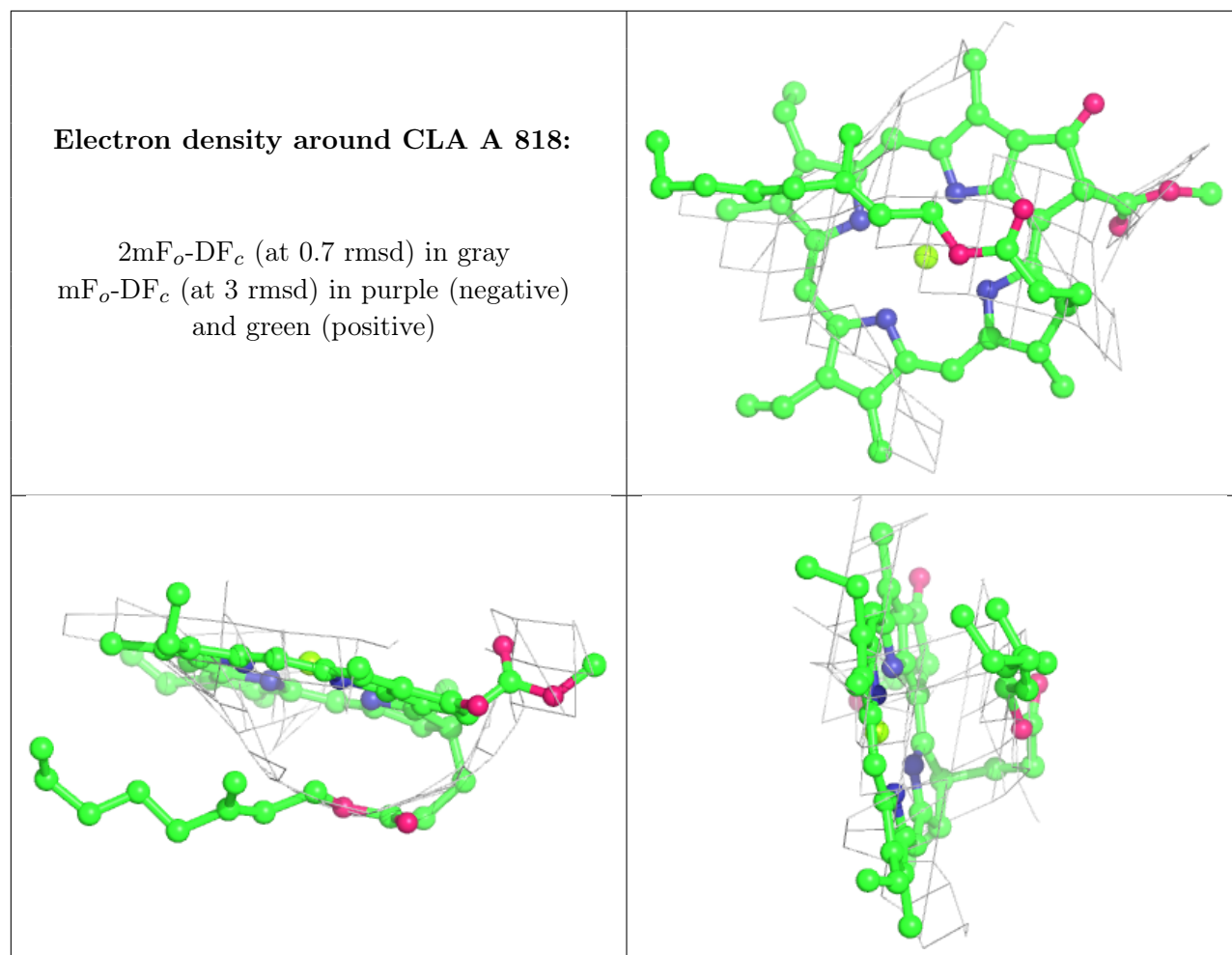




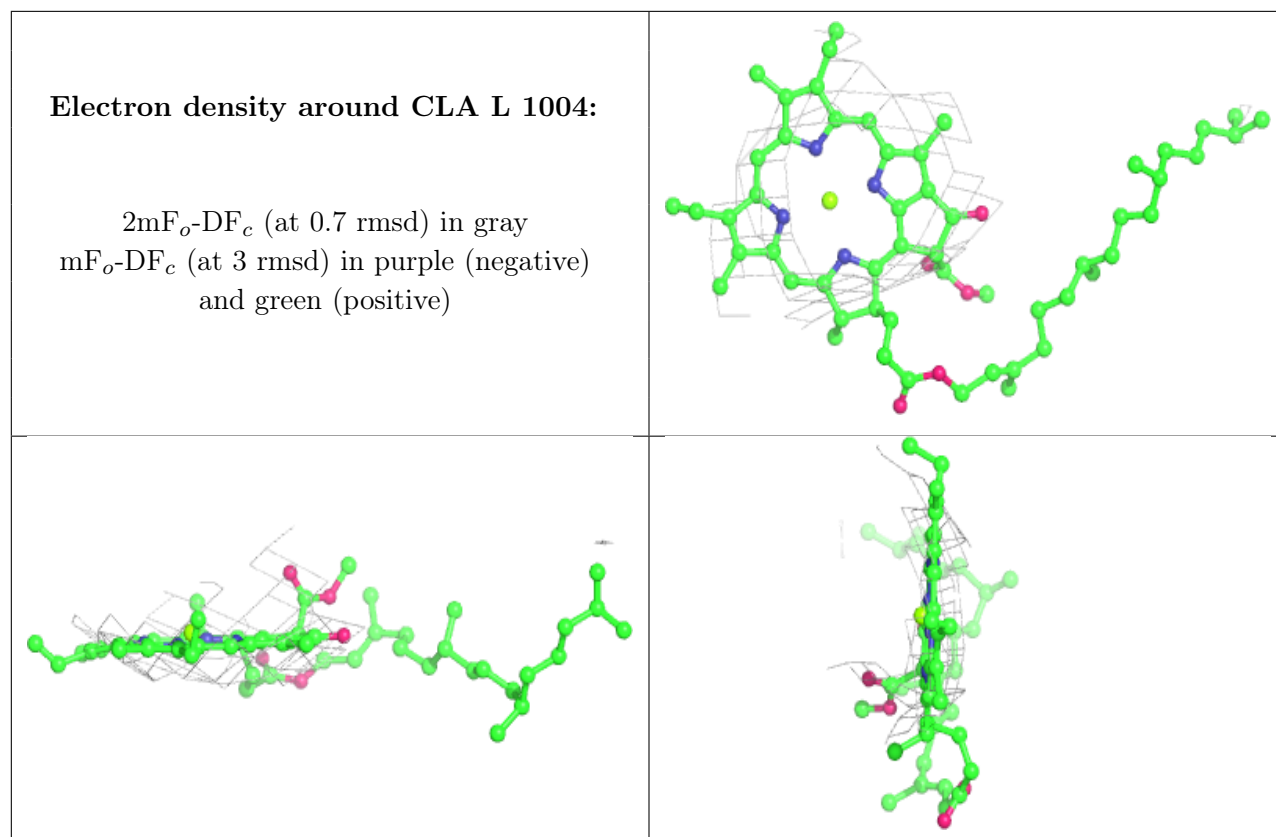
**Electron density around CLA B 819:**

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



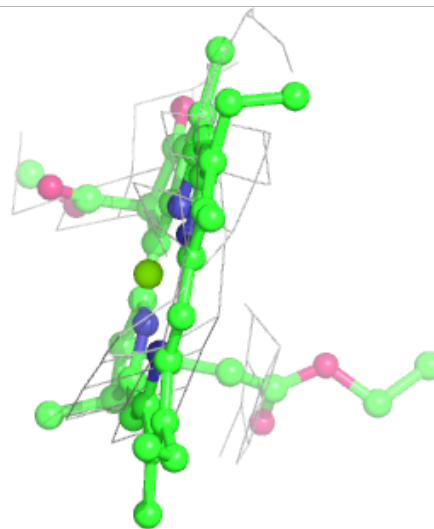
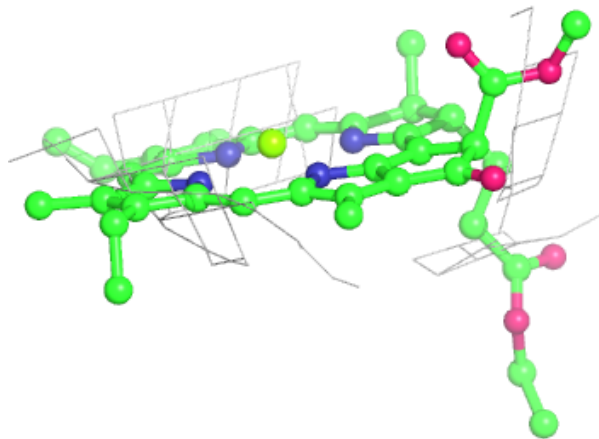
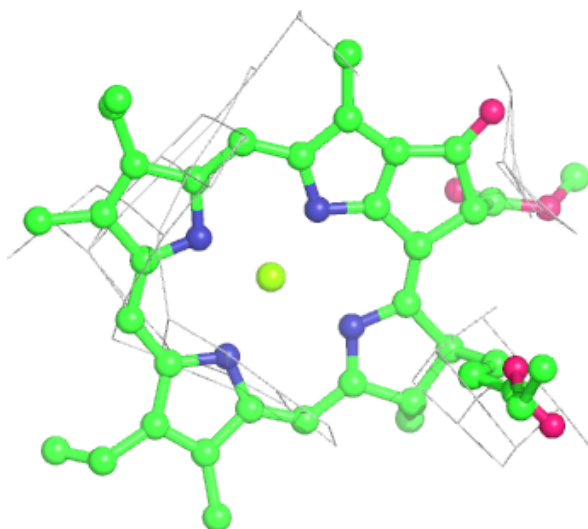






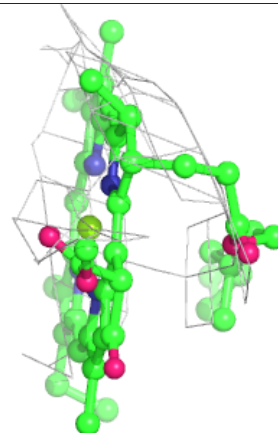
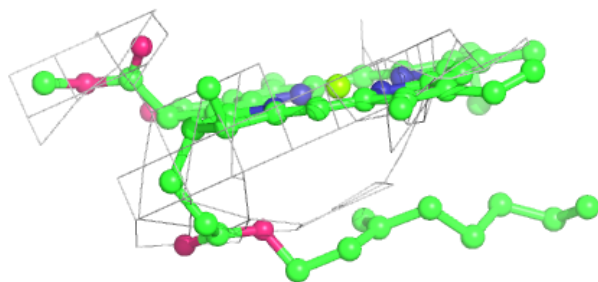
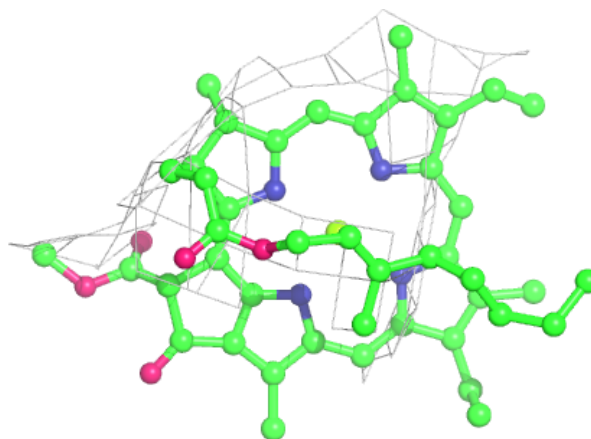
**Electron density around CLA B 839:**

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

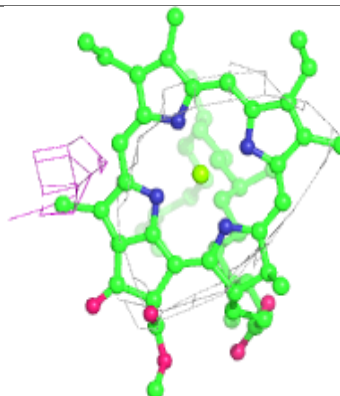
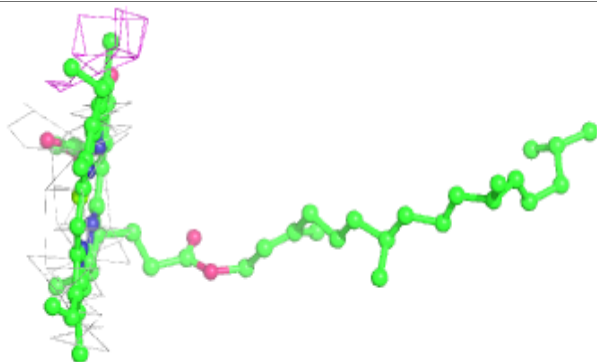
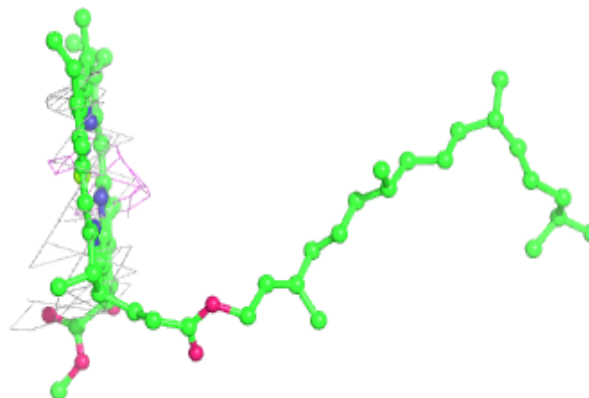


**Electron density around CLA A 813:**

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

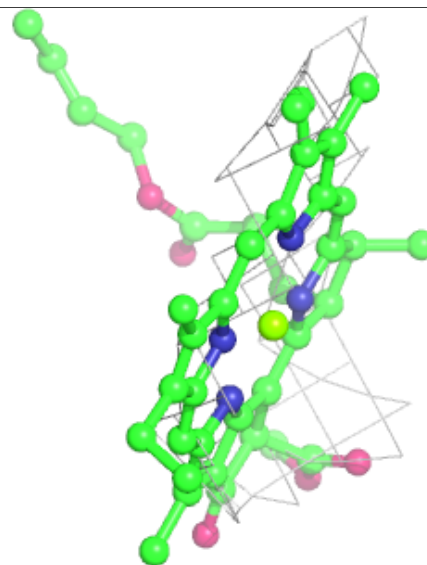
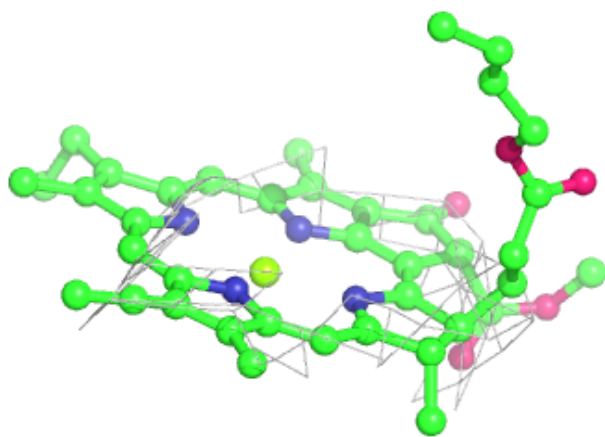
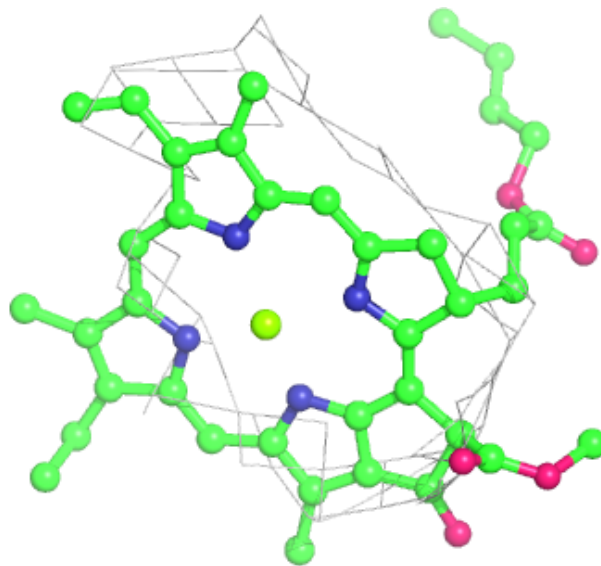
**Electron density around CLA B 841:**

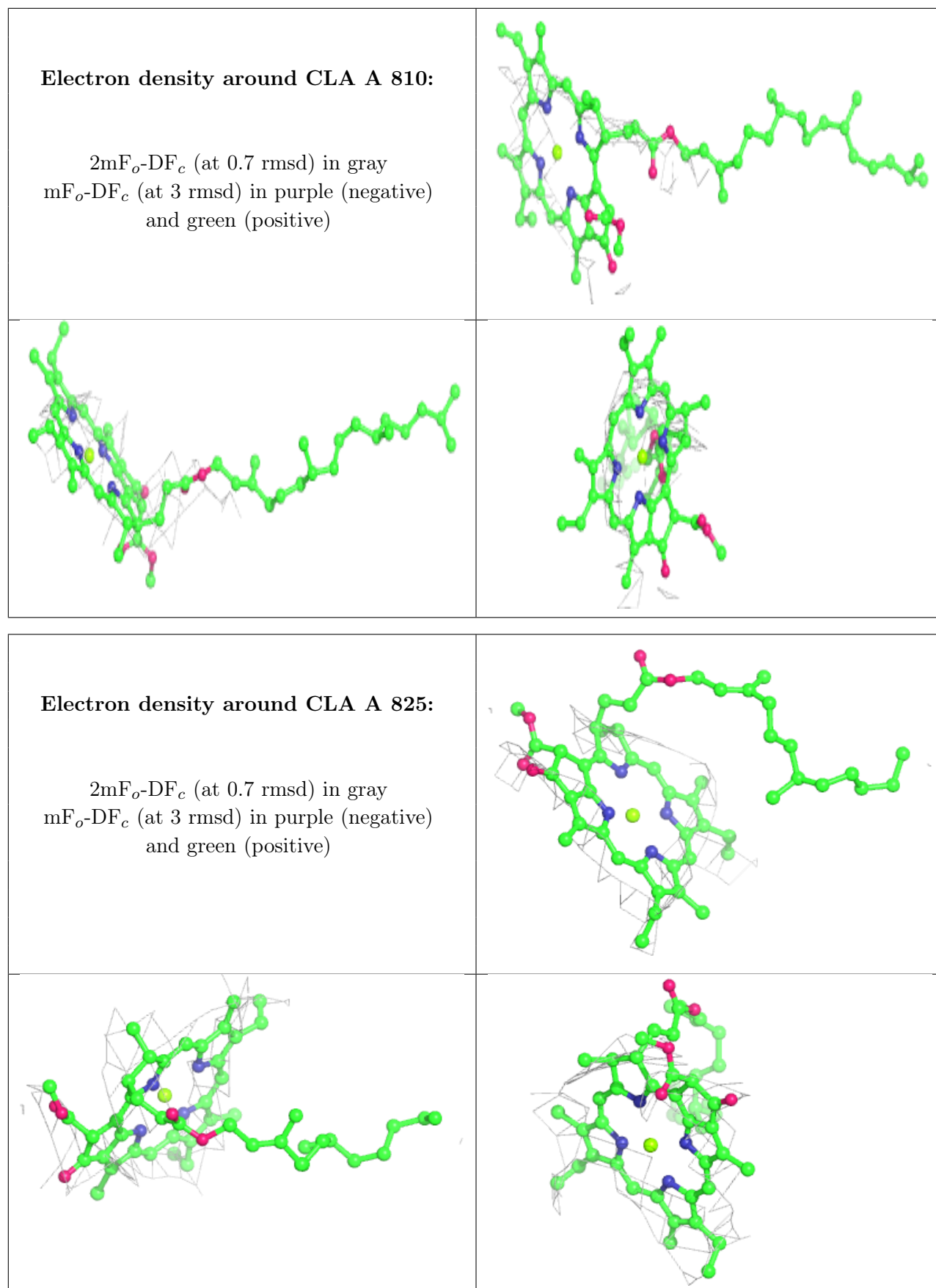
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

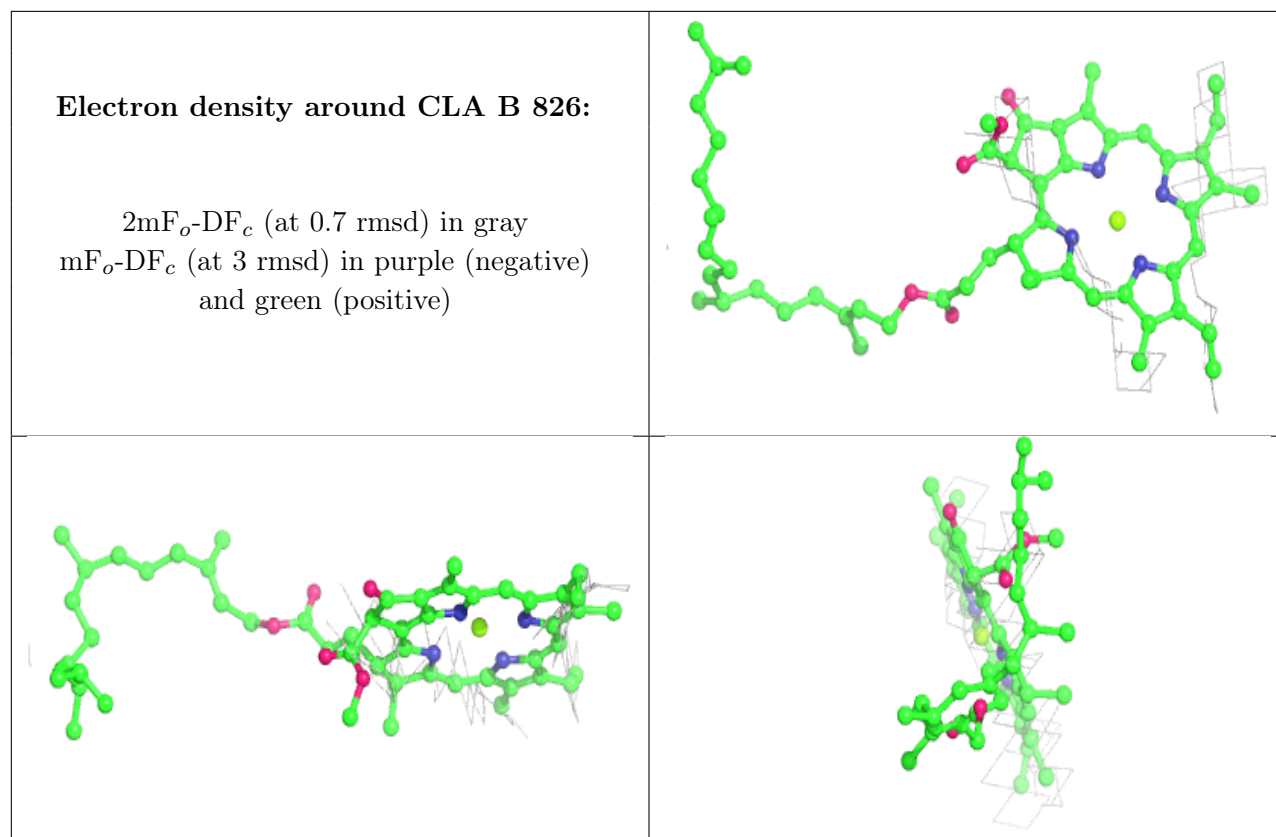


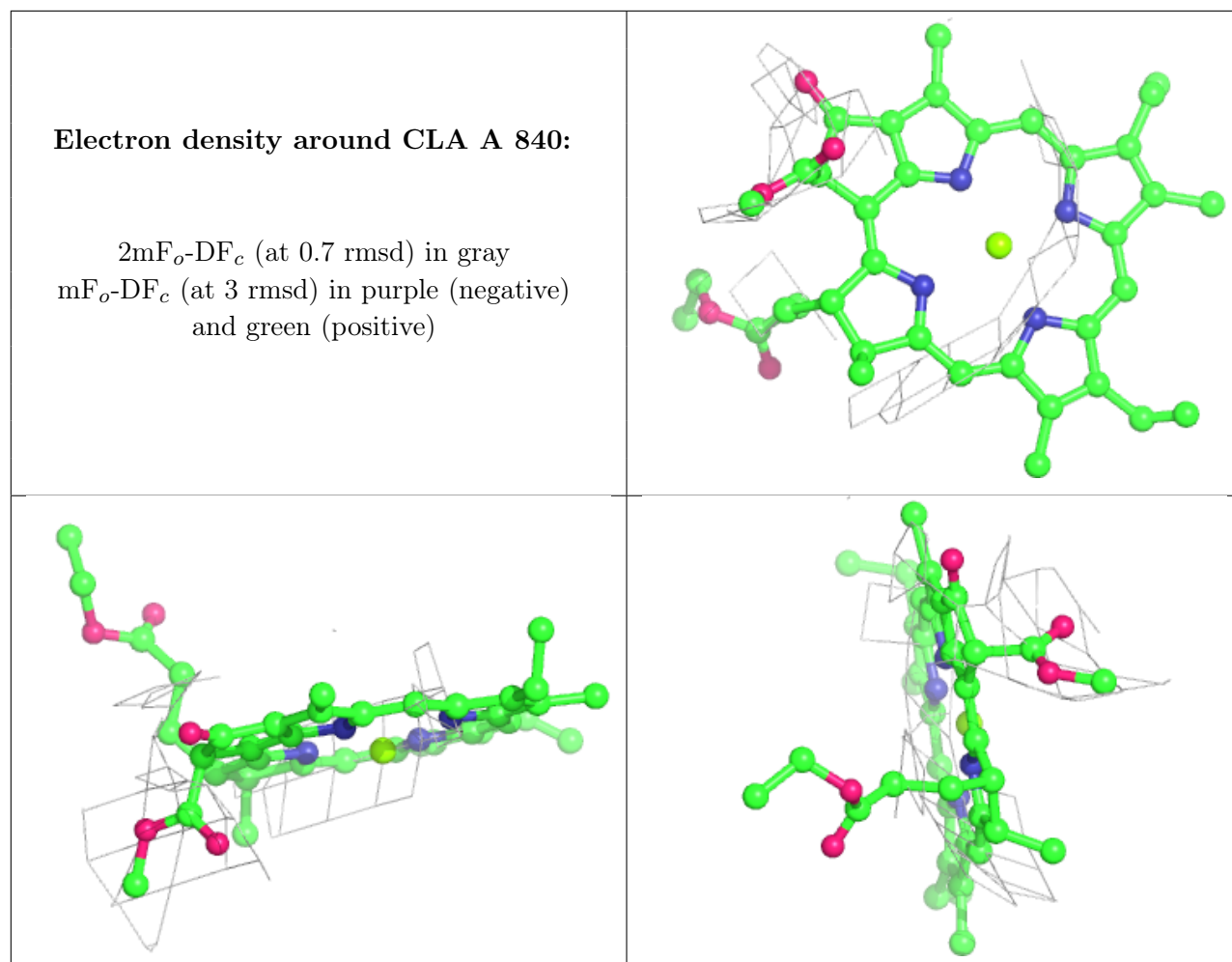
**Electron density around CLA A 817:**

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



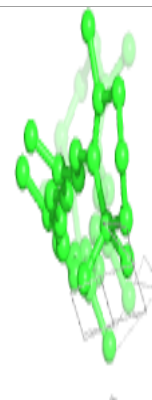
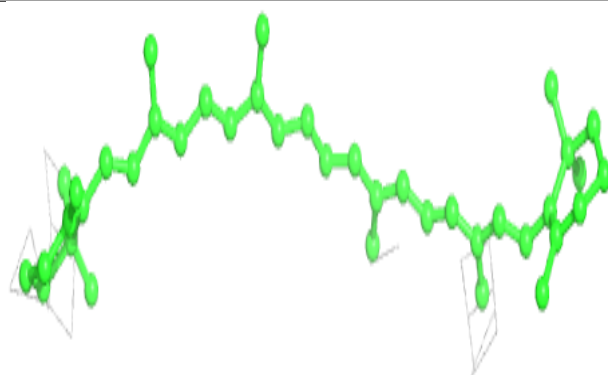
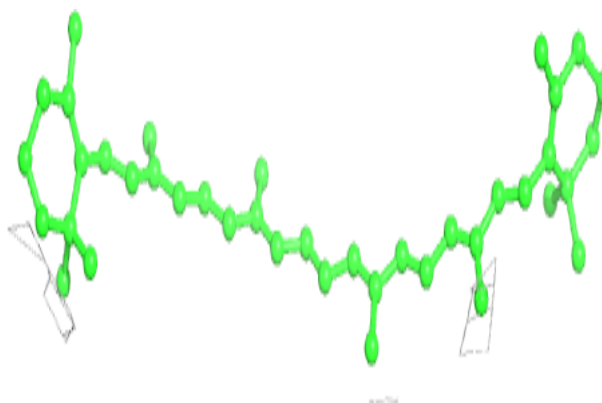




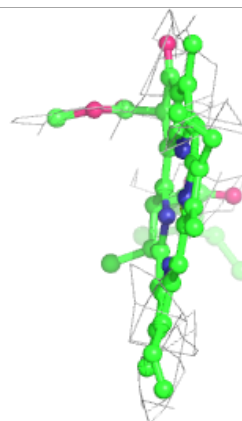
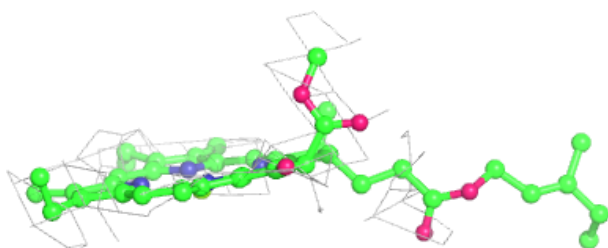
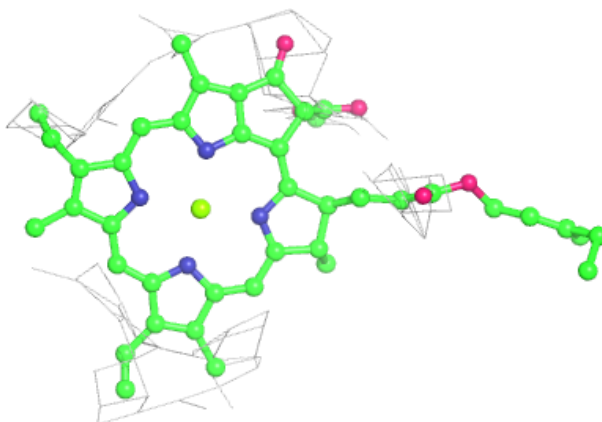


**Electron density around BCR J 104:**

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

**Electron density around CLA A 838:**

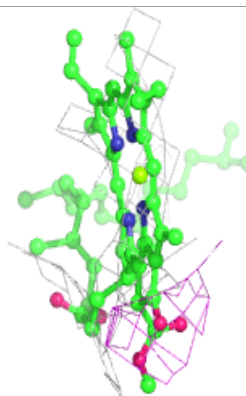
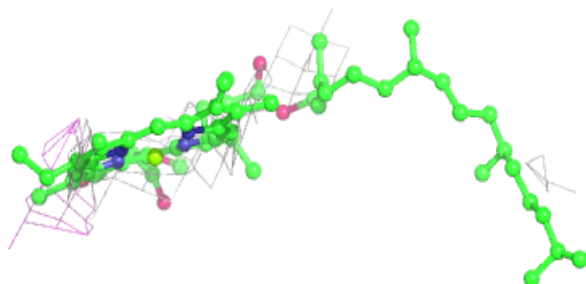
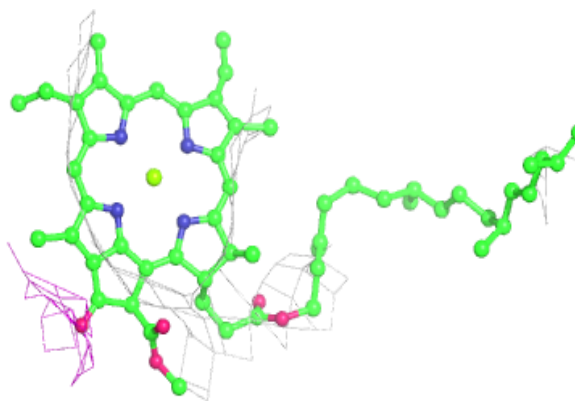
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



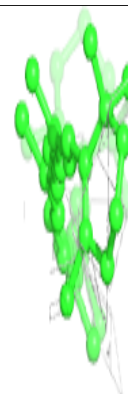
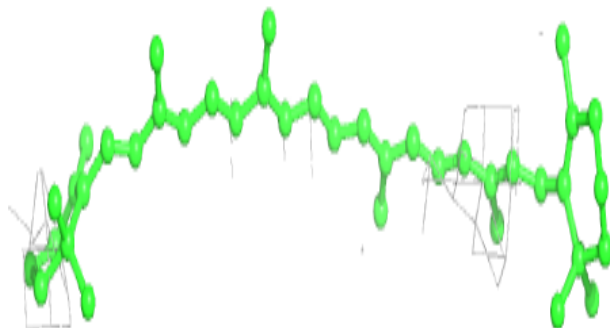
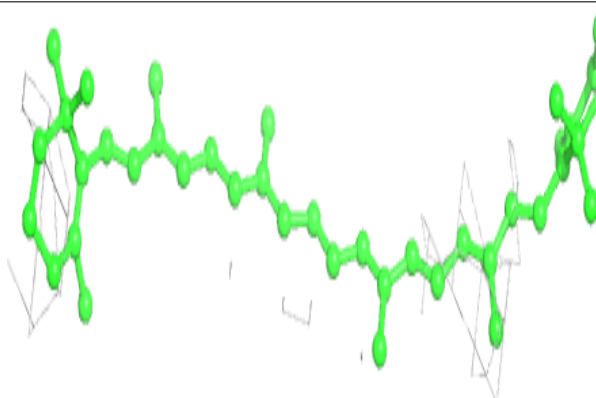


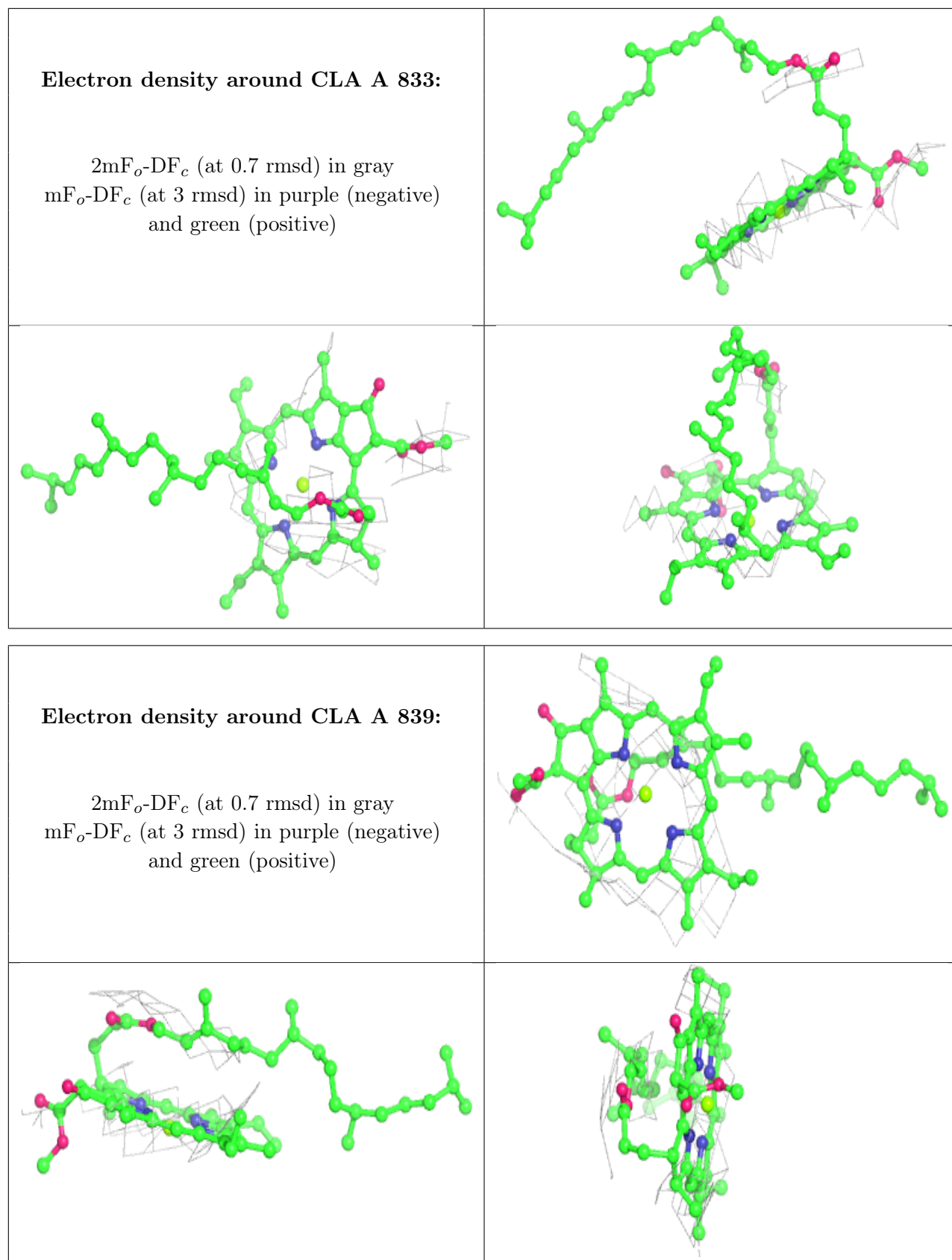
**Electron density around CLA B 803:**

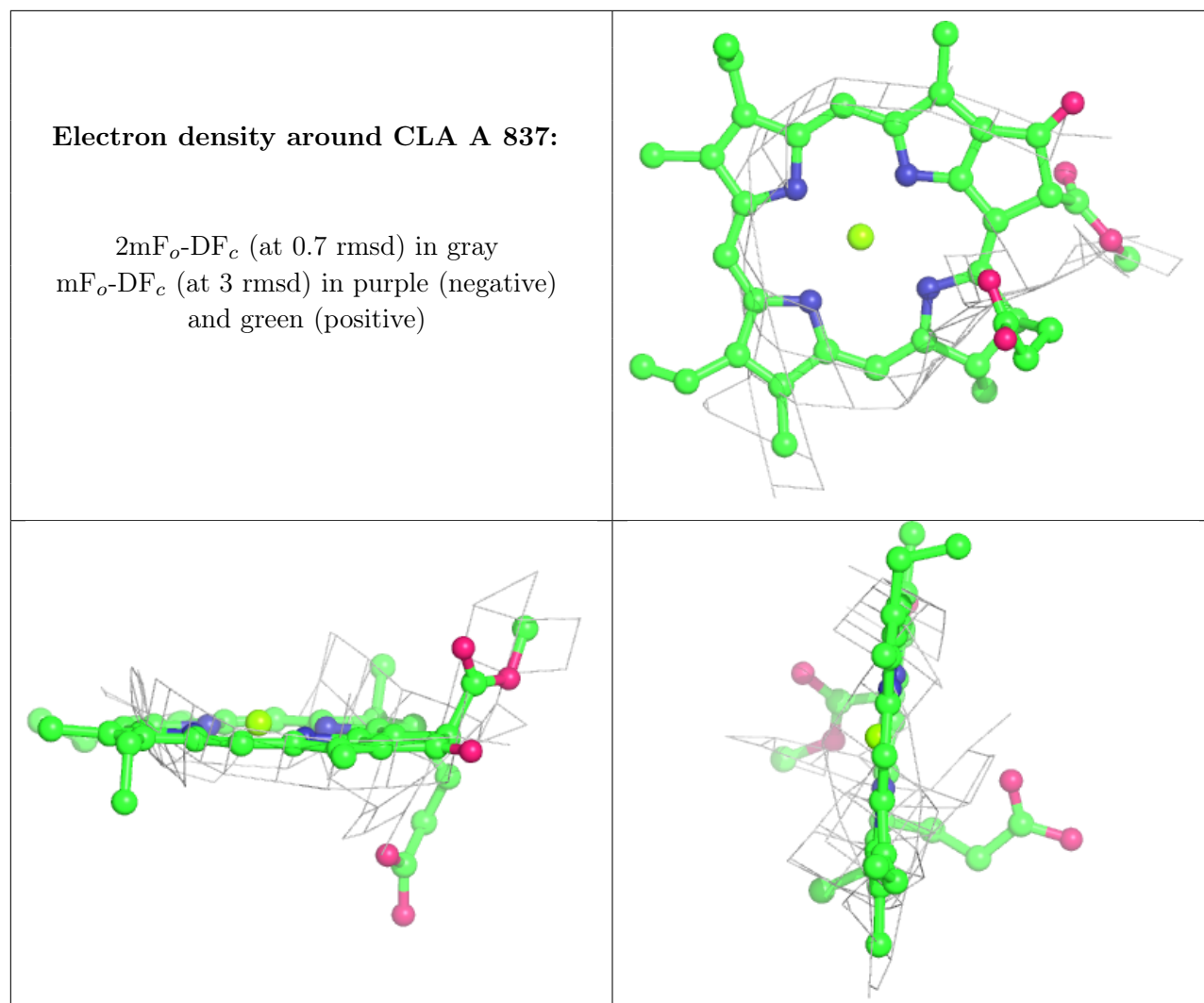
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

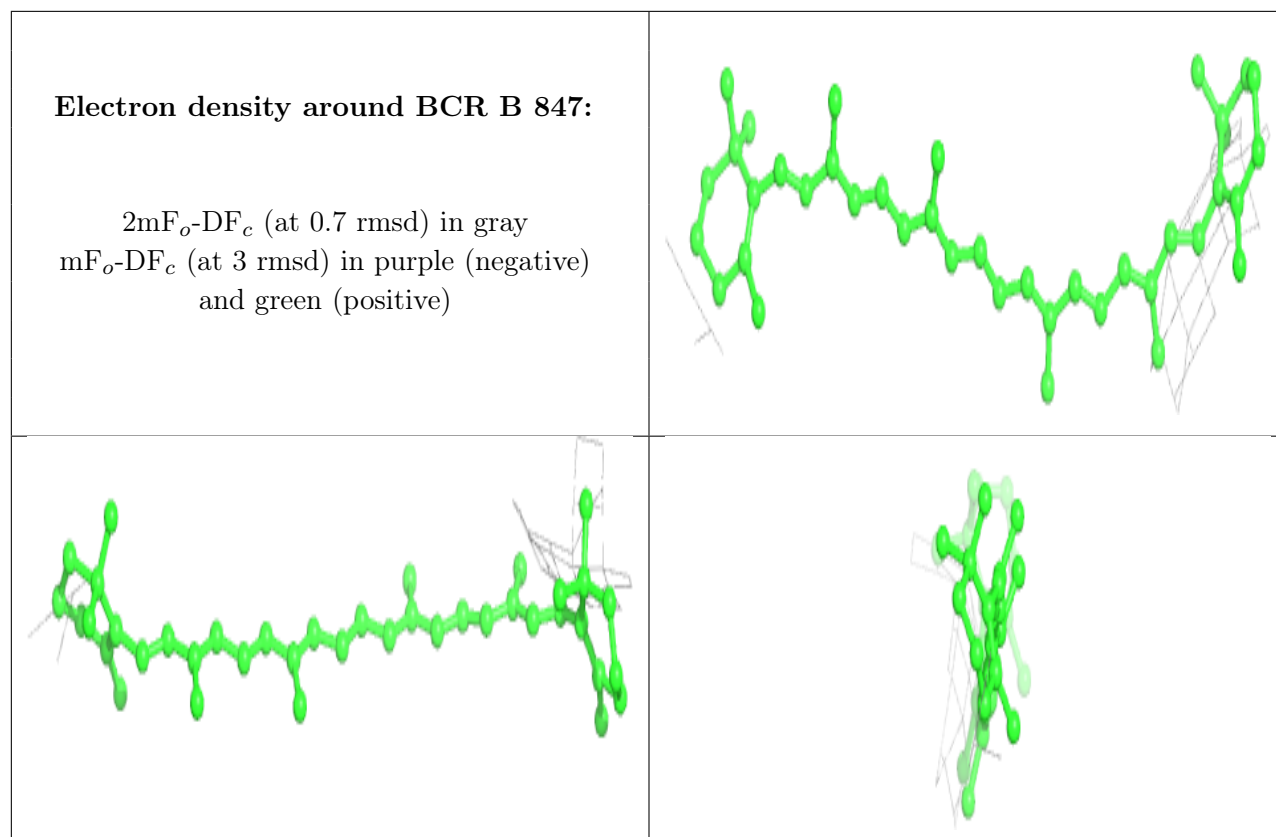
**Electron density around BCR I 101:**

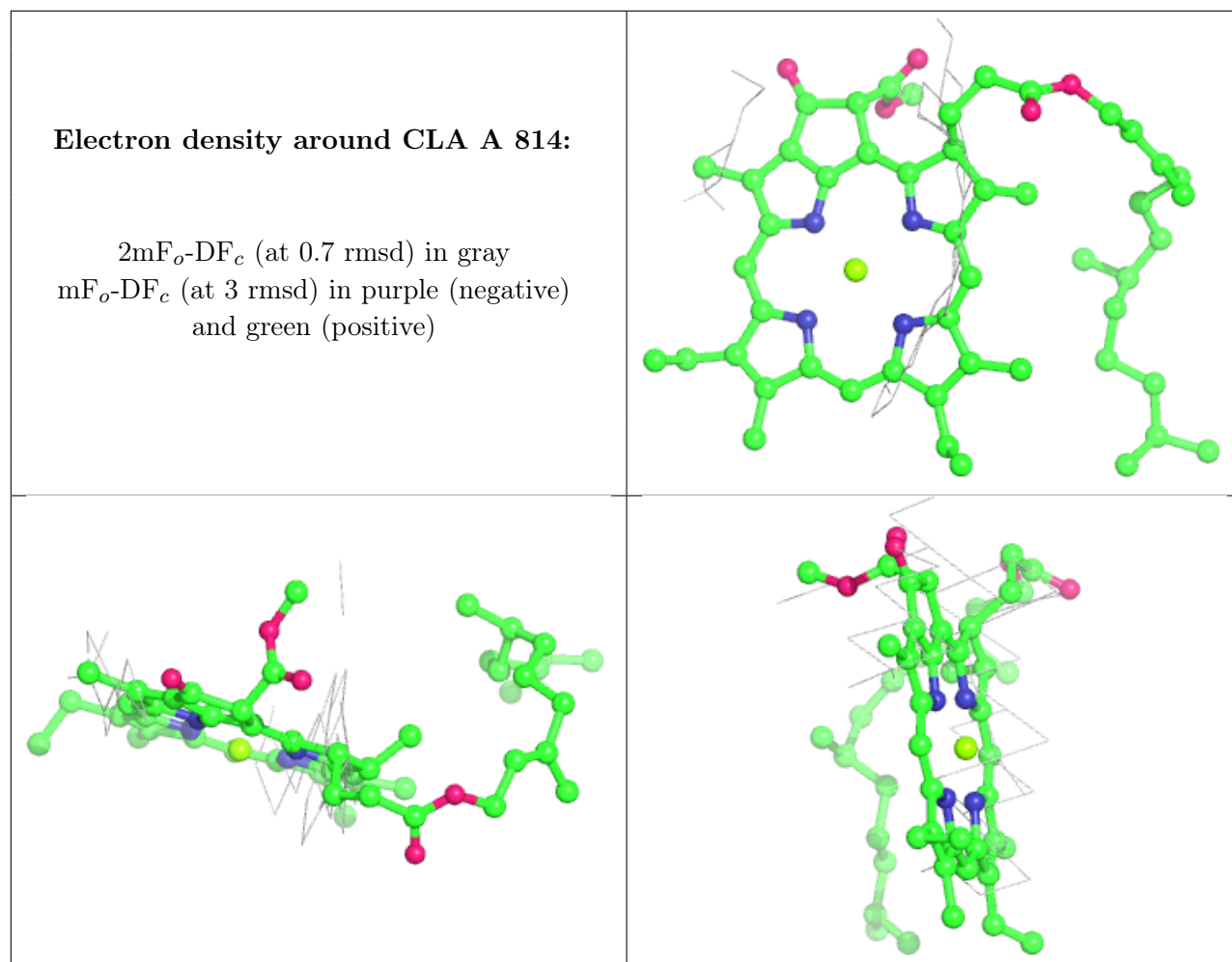
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

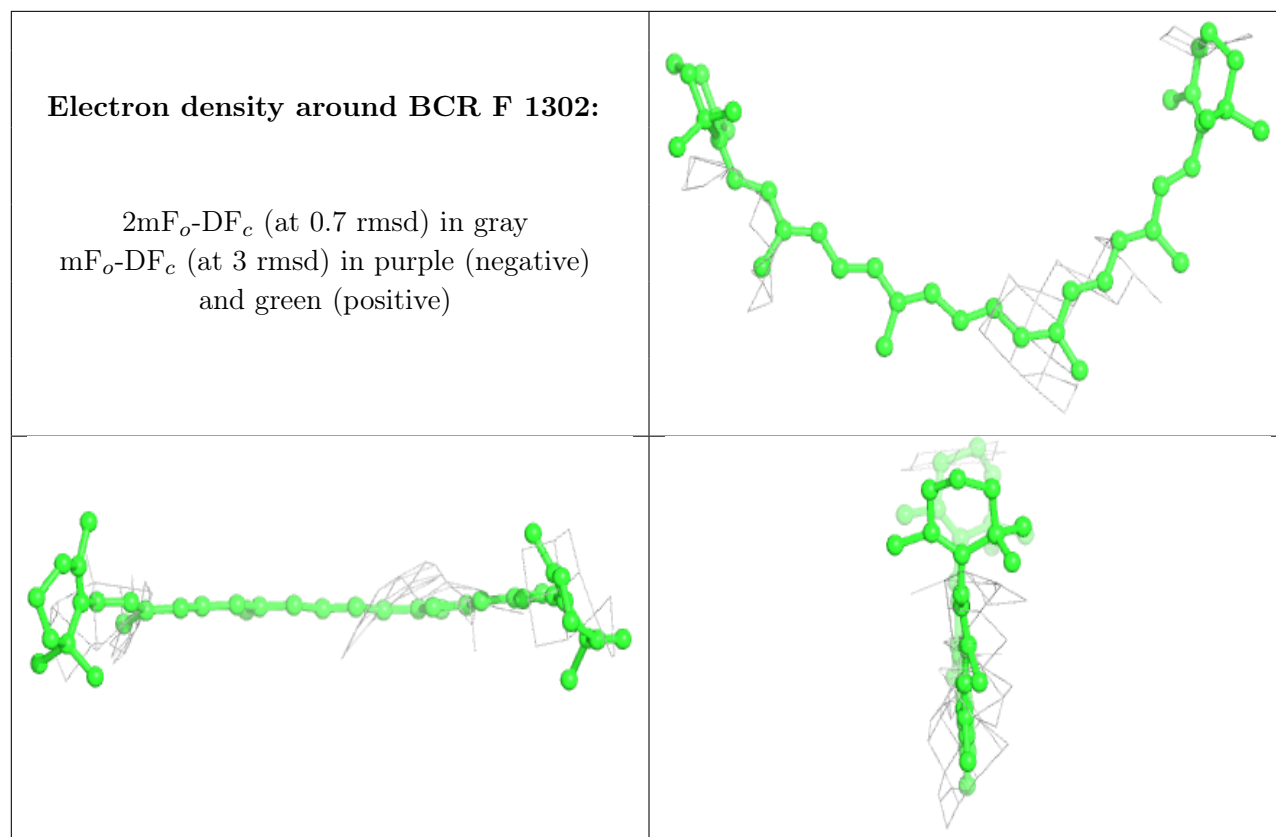






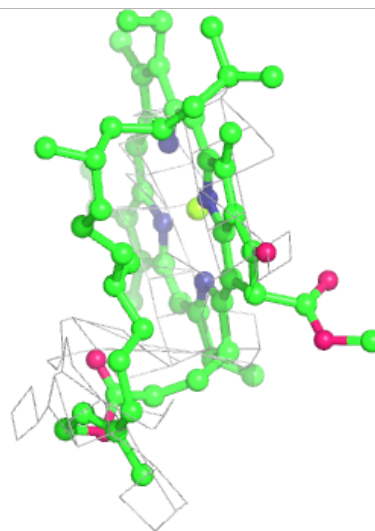
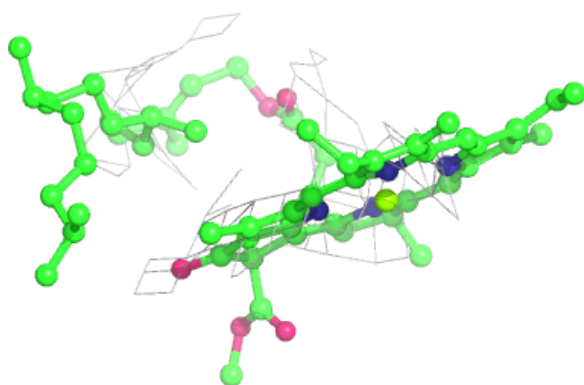
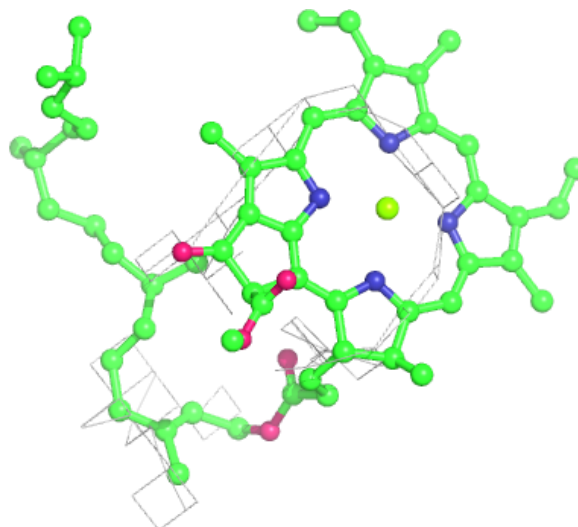


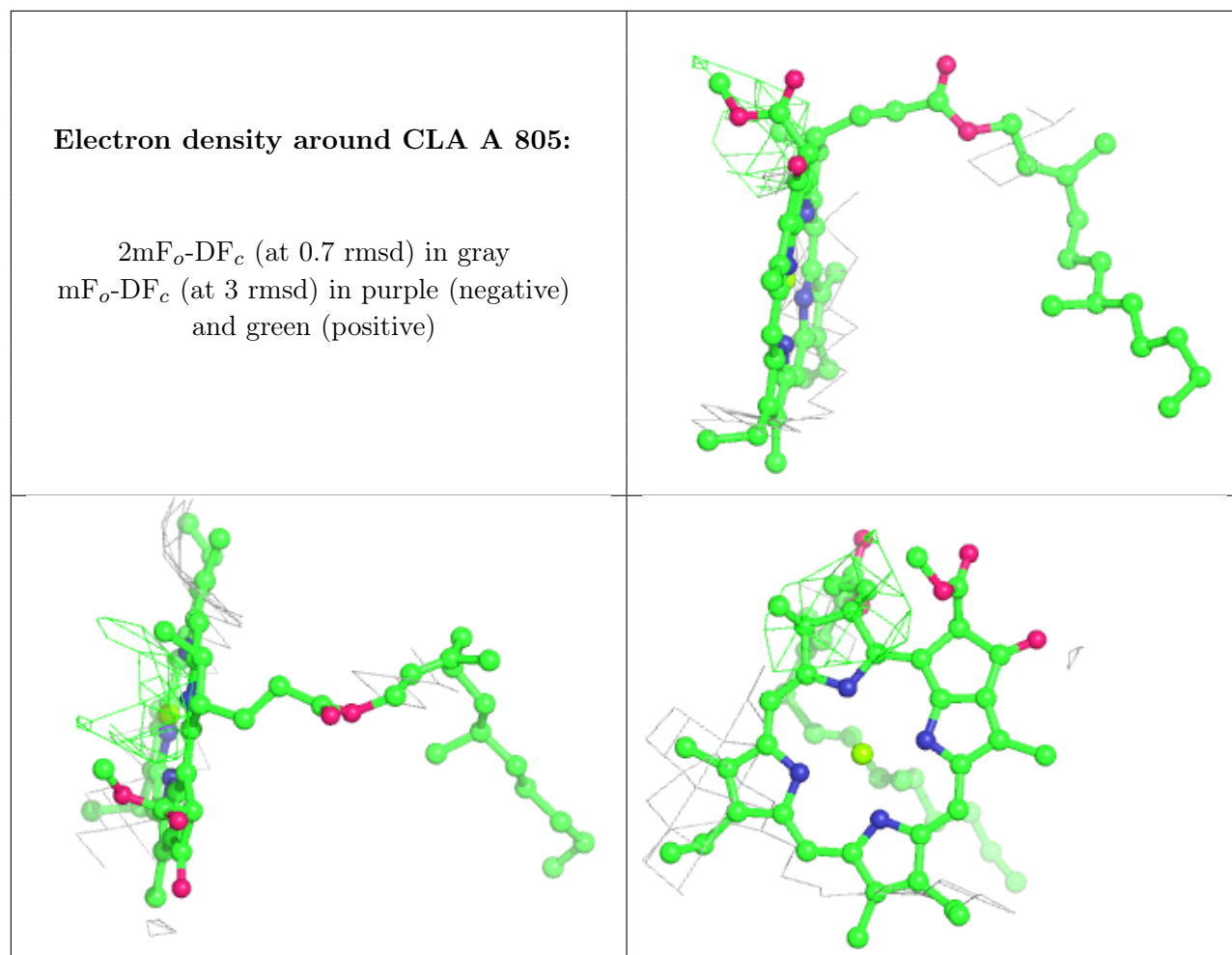




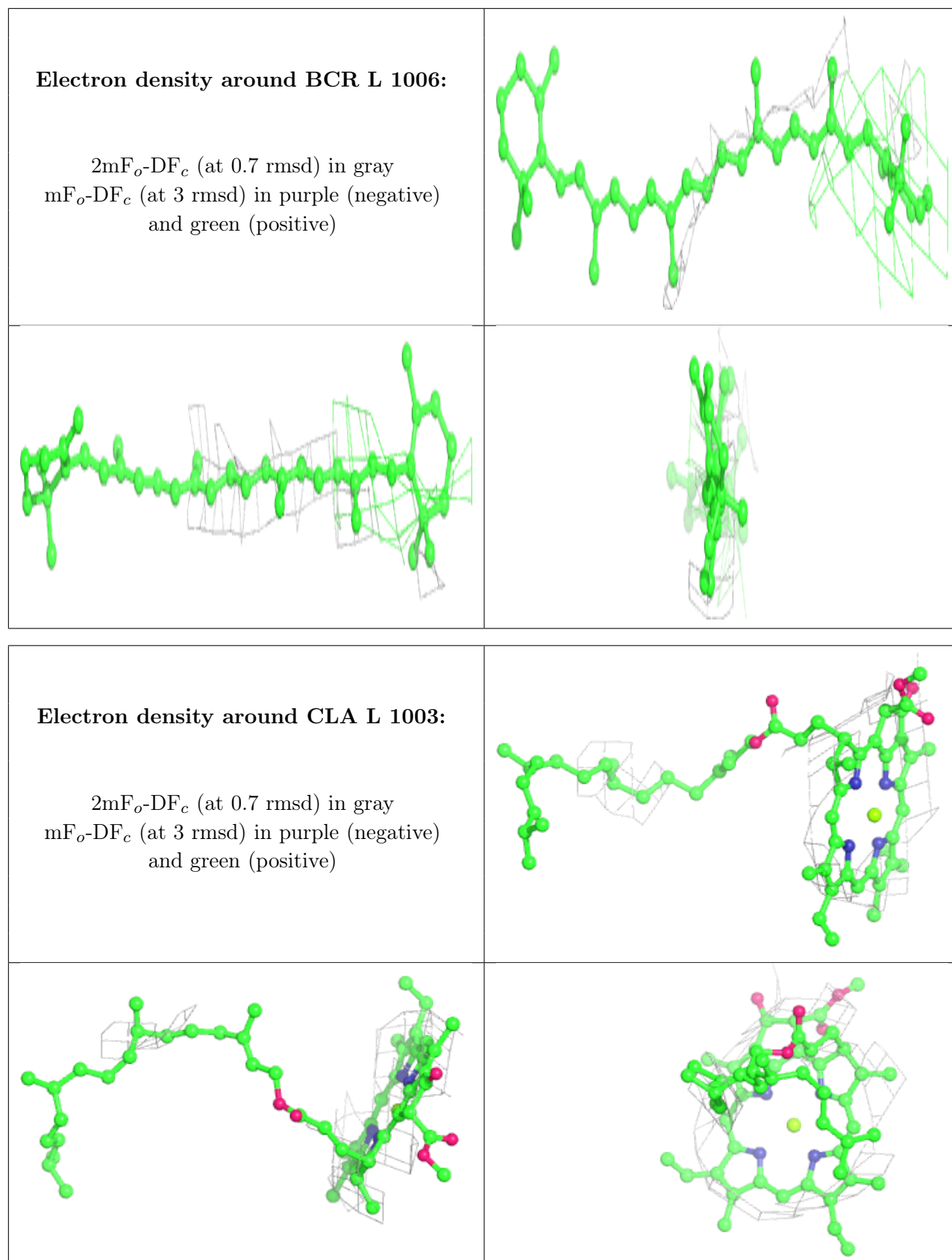
**Electron density around CLA B 832:**

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



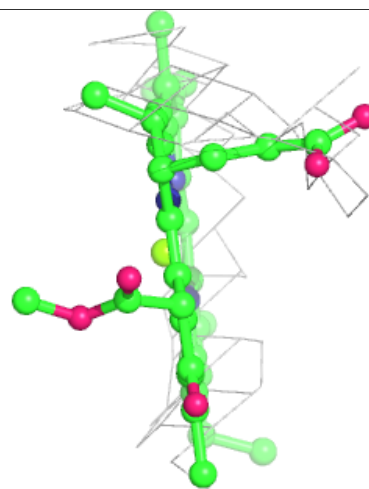
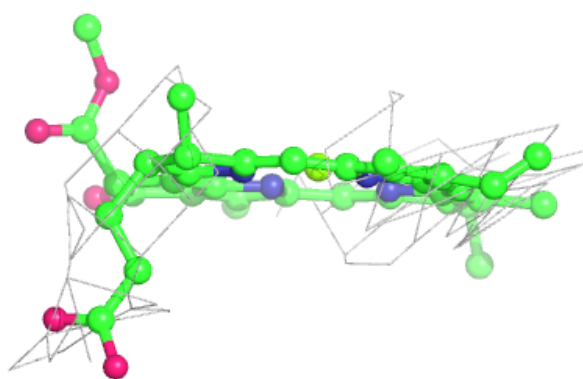
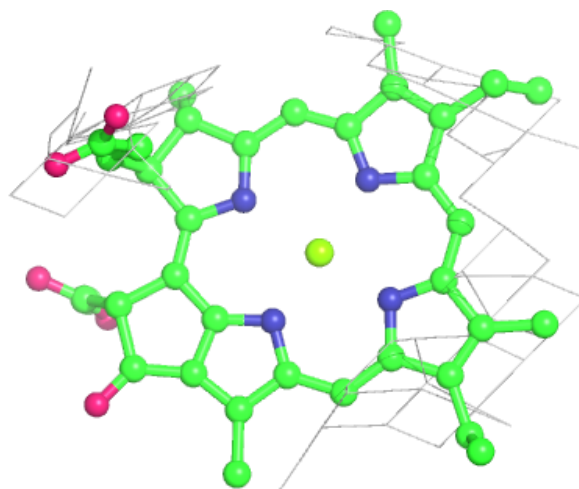


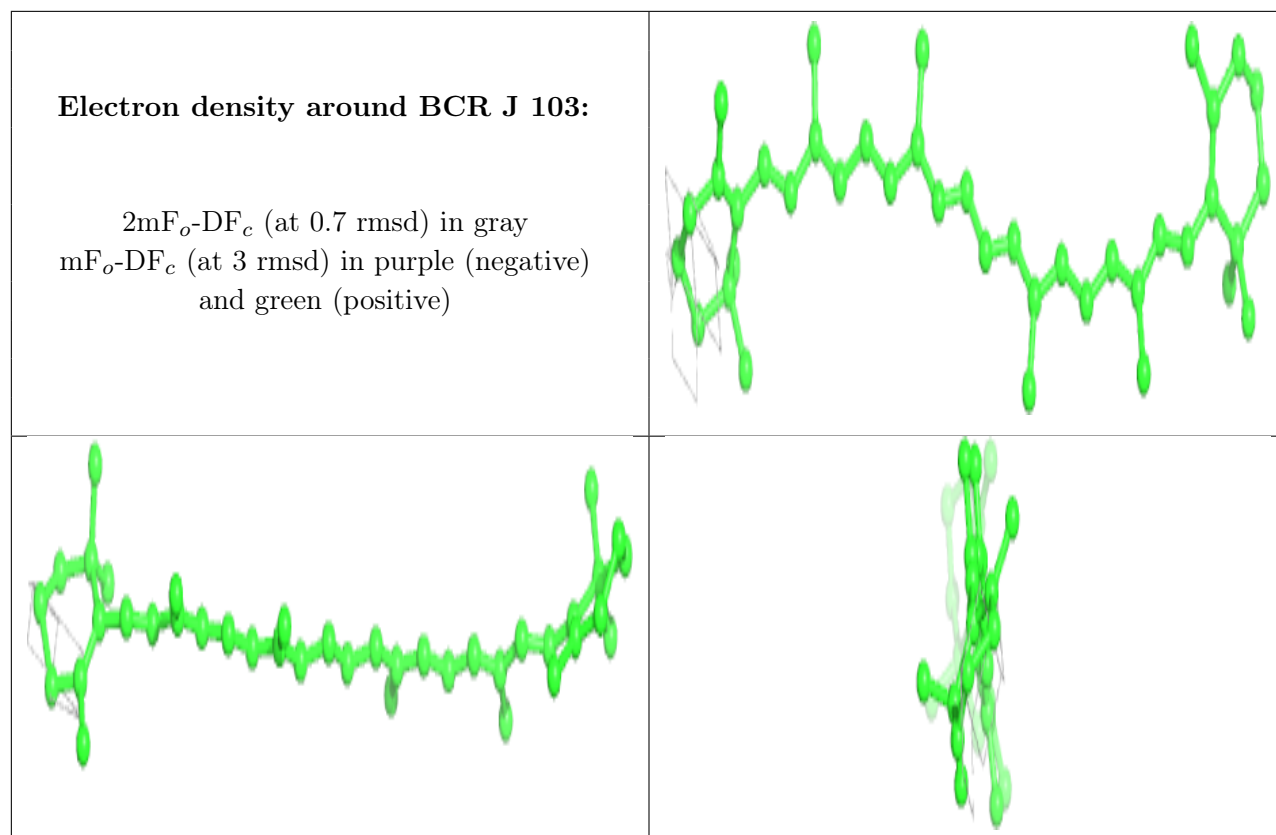




**Electron density around CLA A 815:**

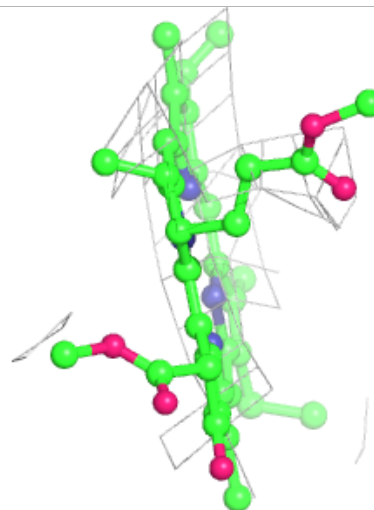
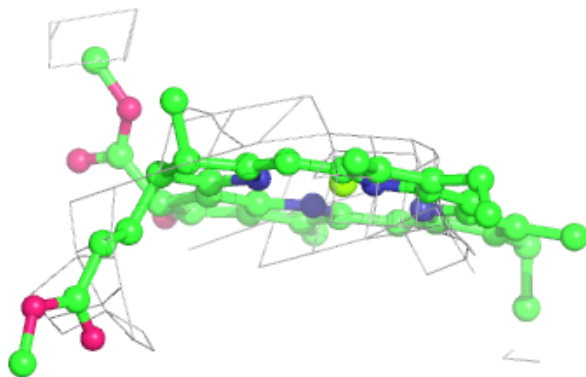
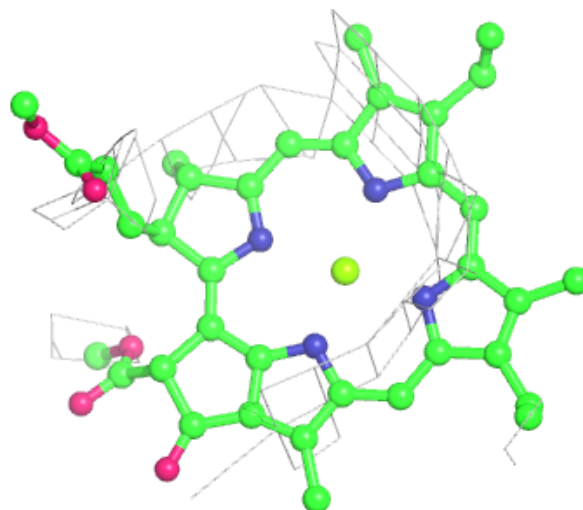
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





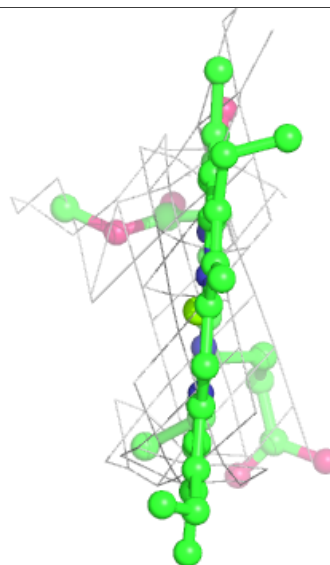
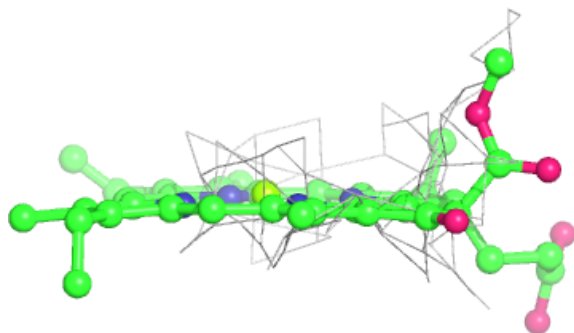
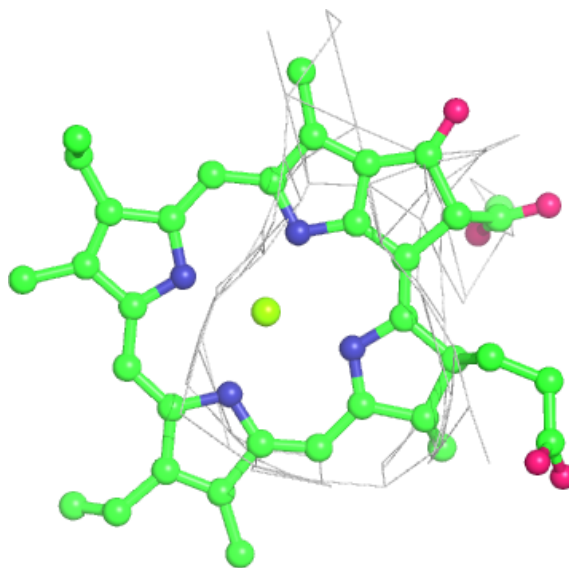
**Electron density around CLA B 825:**

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



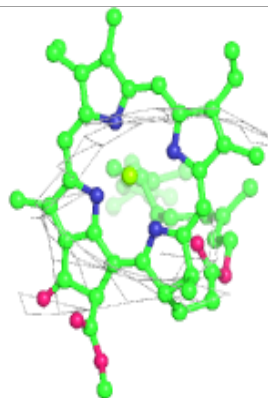
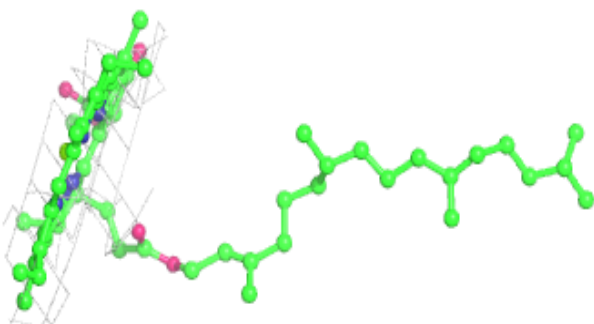
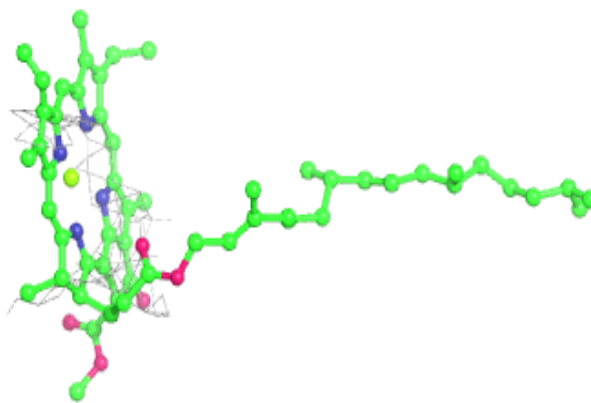
**Electron density around CLA X 1701:**

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

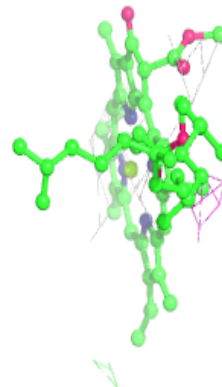
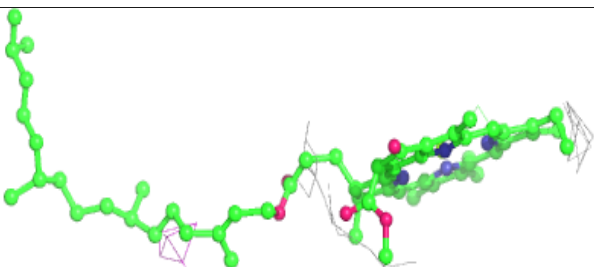
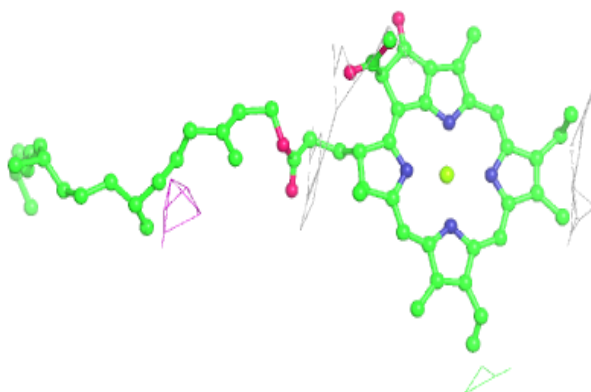


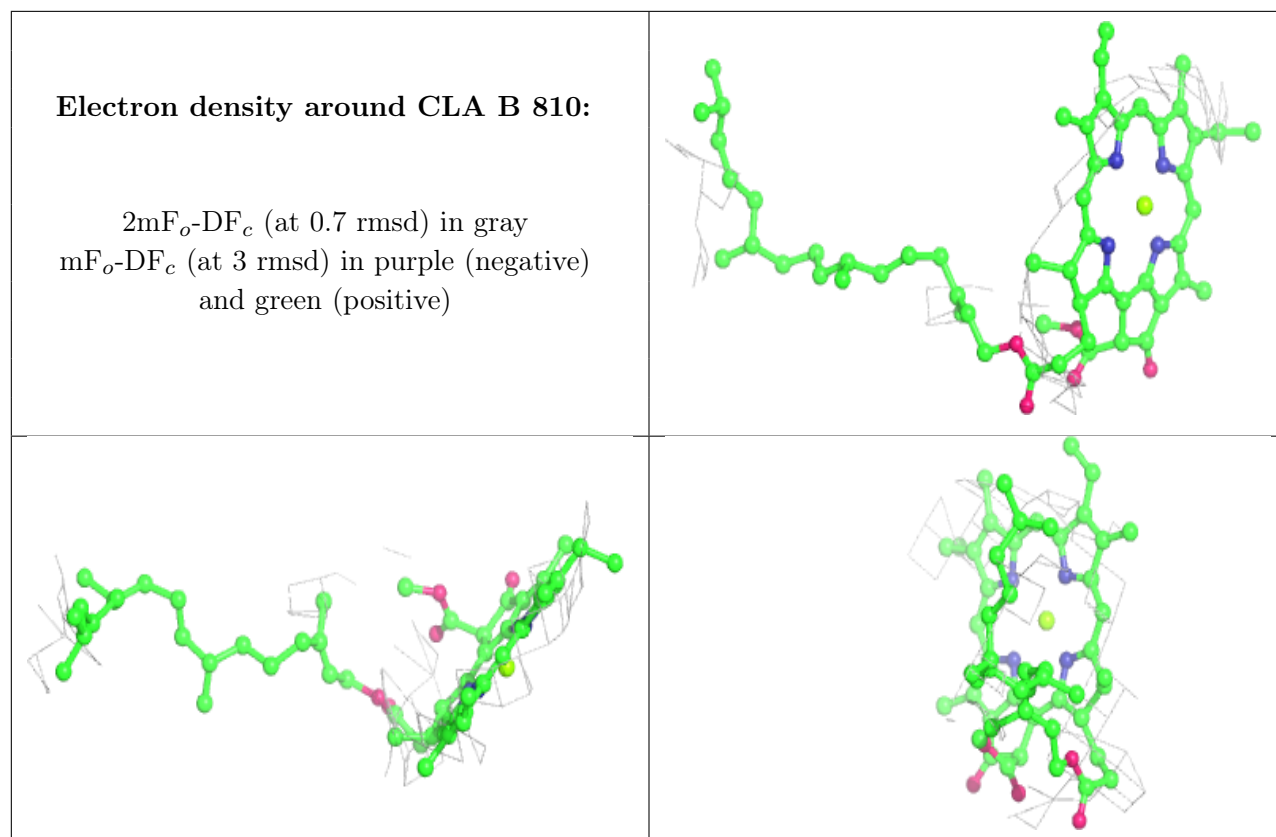
**Electron density around CLA B 828:**

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

**Electron density around CLA A 806:**

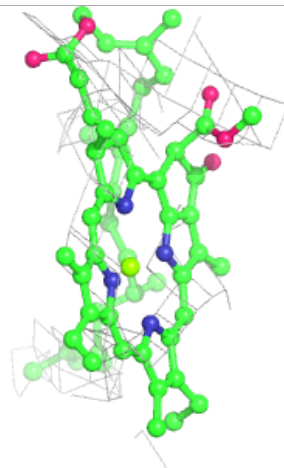
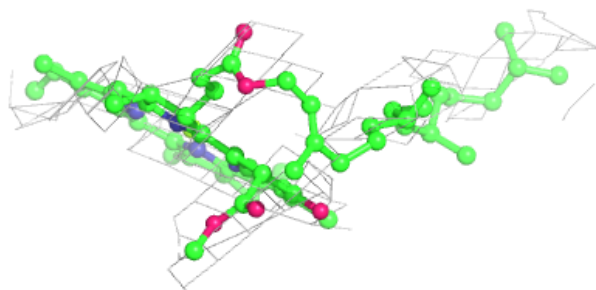
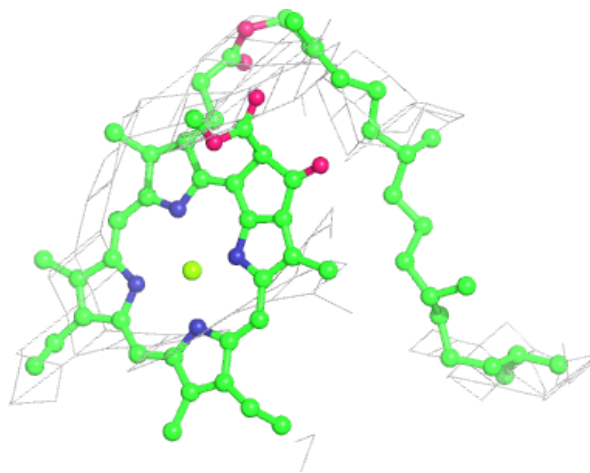
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA A 826:**

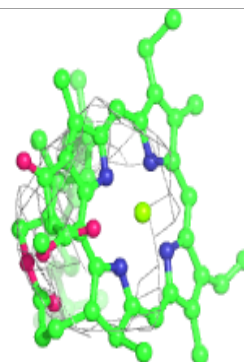
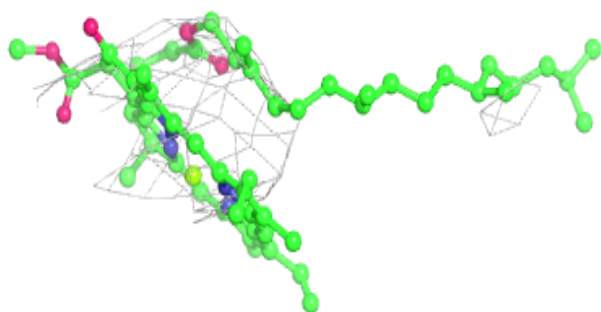
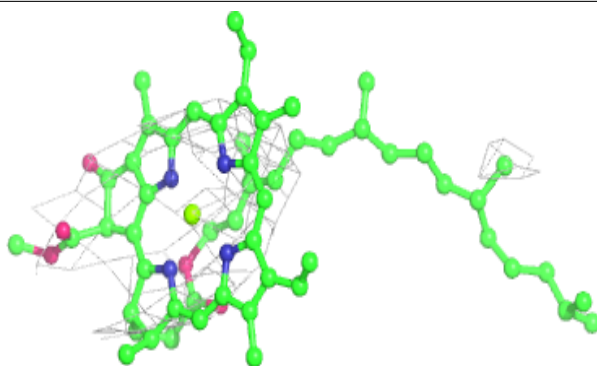
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



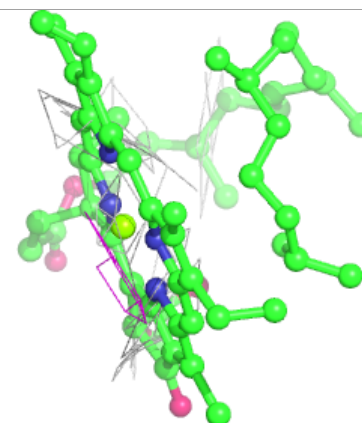
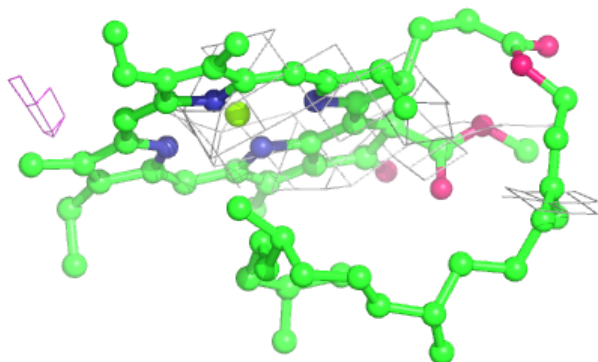
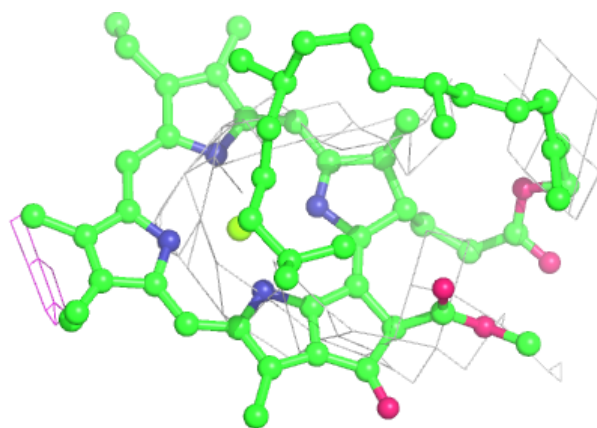


**Electron density around CLA A 843:**

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

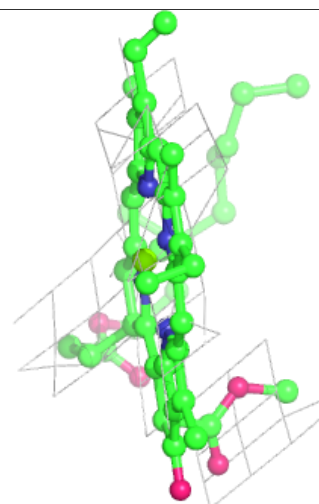
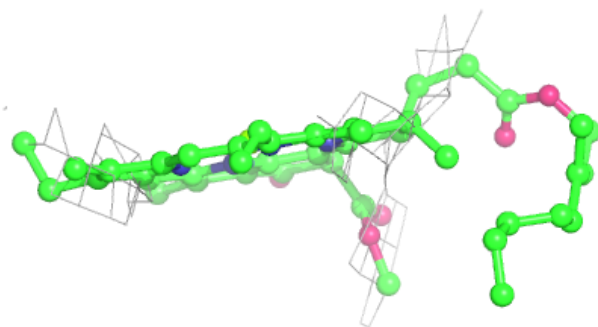
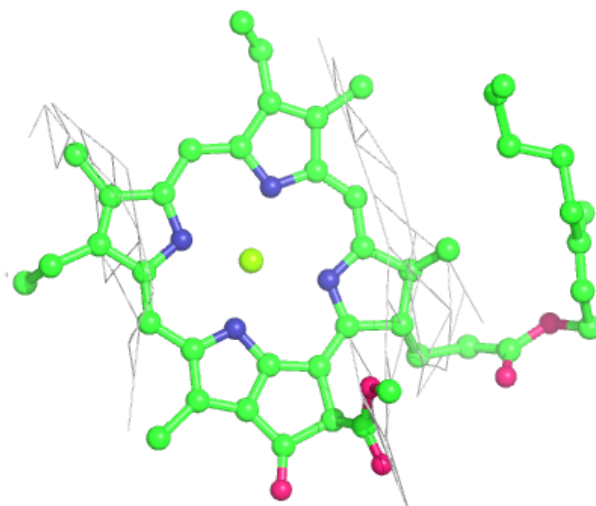
**Electron density around CLA A 807:**

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



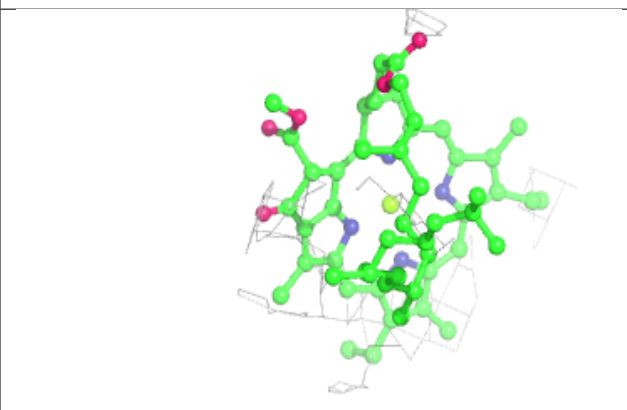
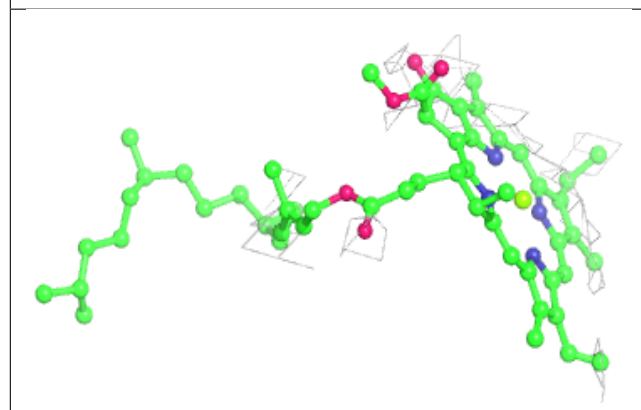
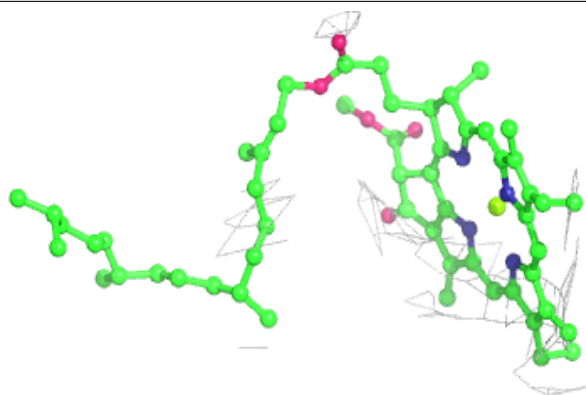
**Electron density around CLA B 824:**

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

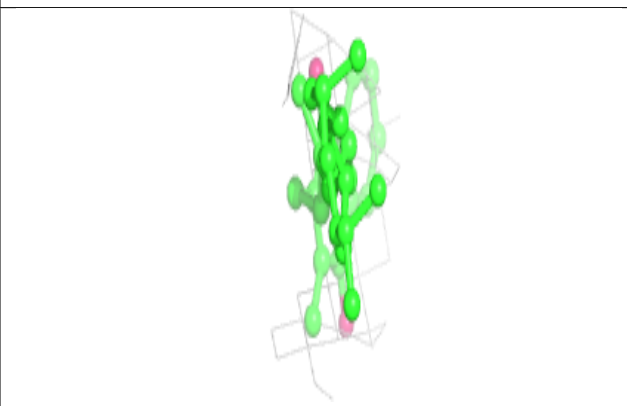
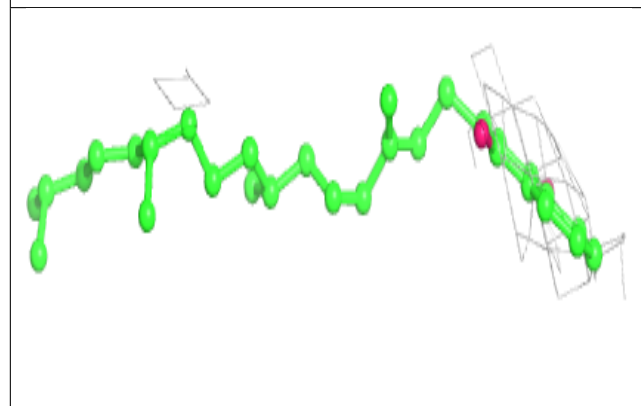
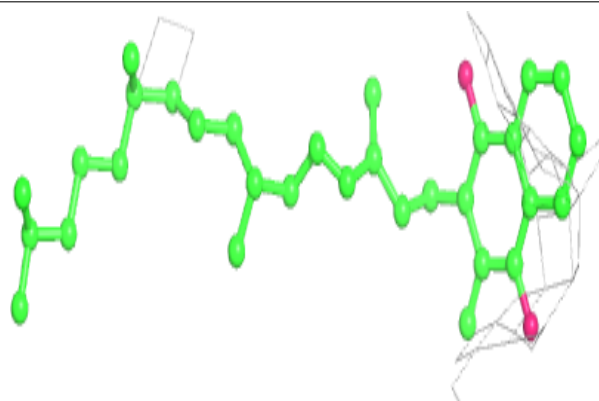


**Electron density around CLA B 801:**

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

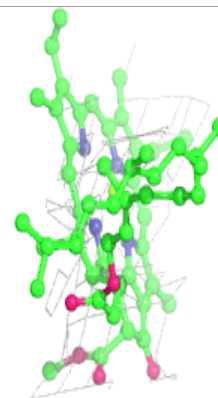
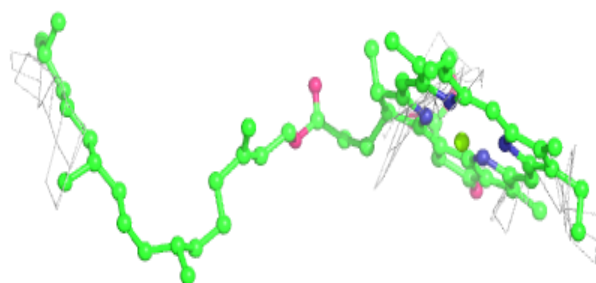
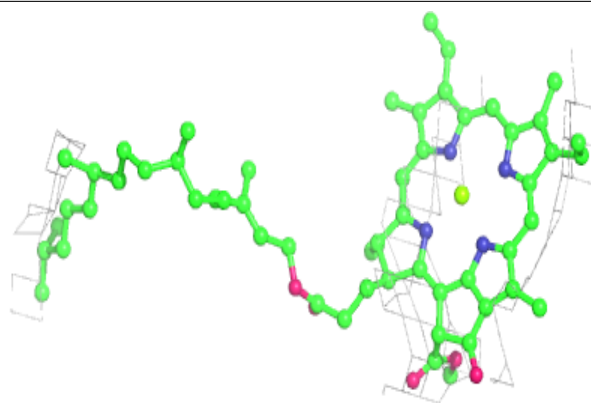
**Electron density around PQN A 847:**

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

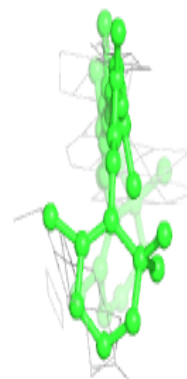
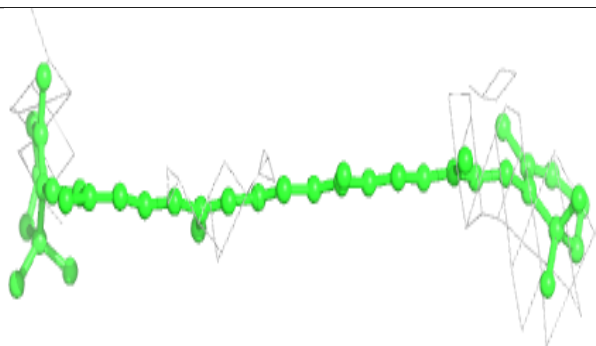
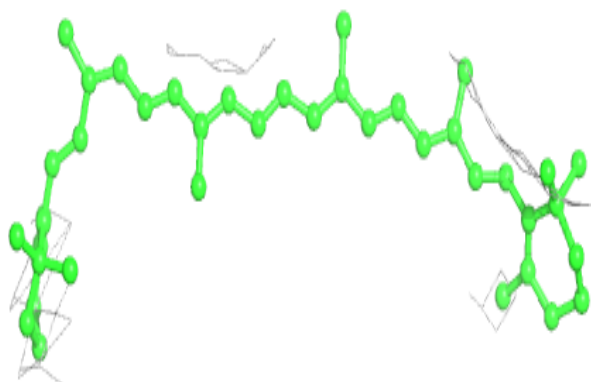


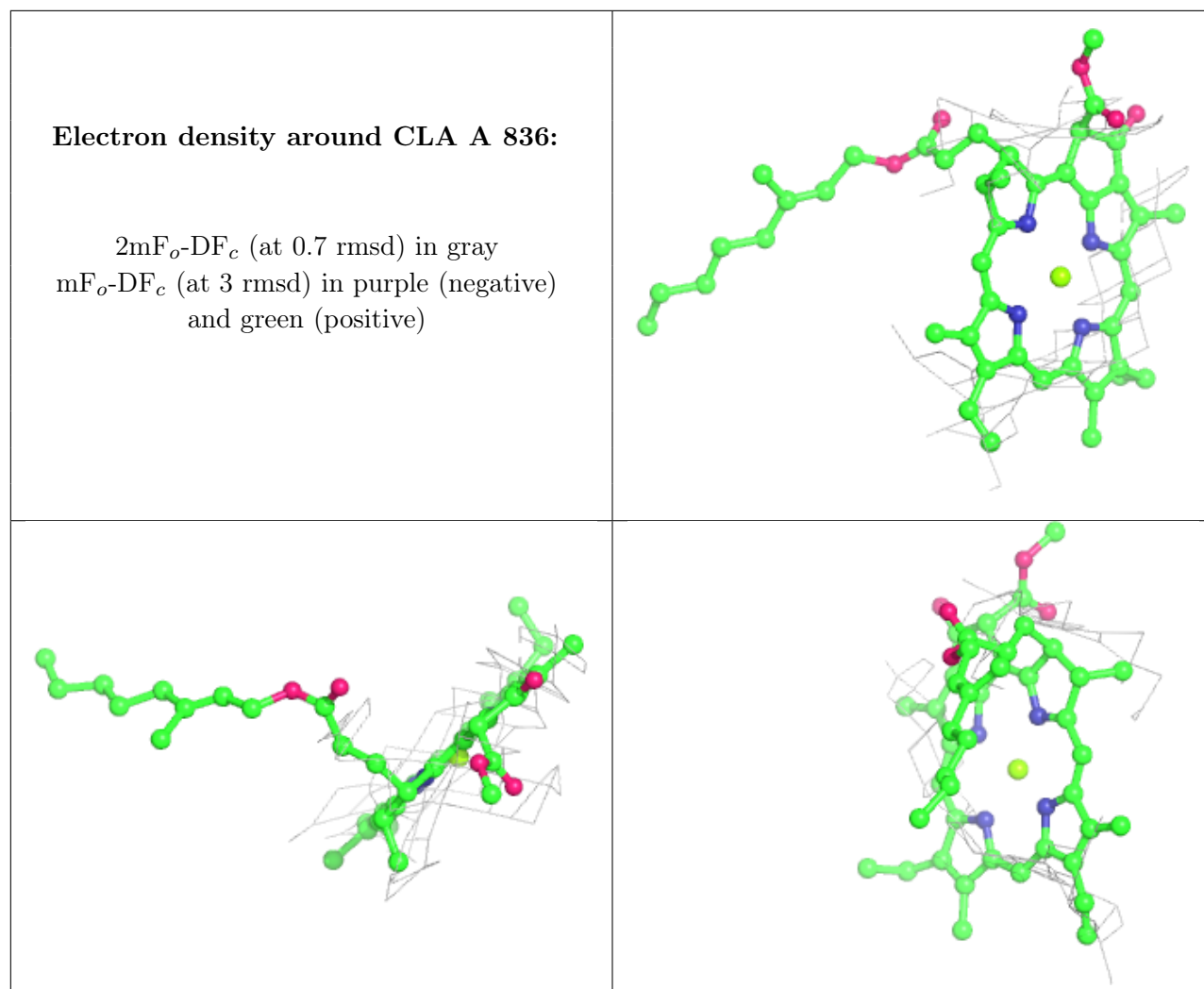
**Electron density around CLA B 813:**

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

**Electron density around BCR I 102:**

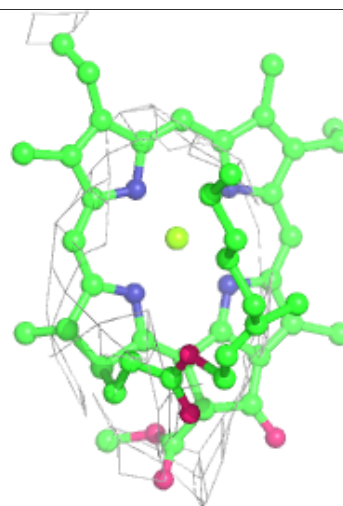
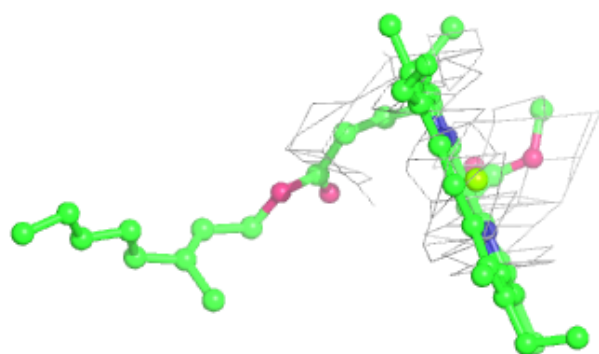
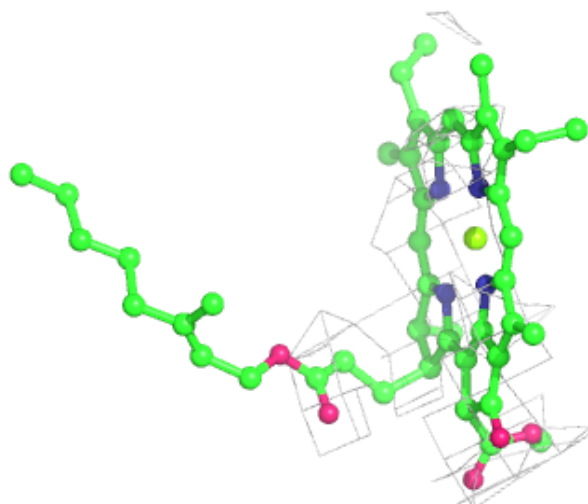
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





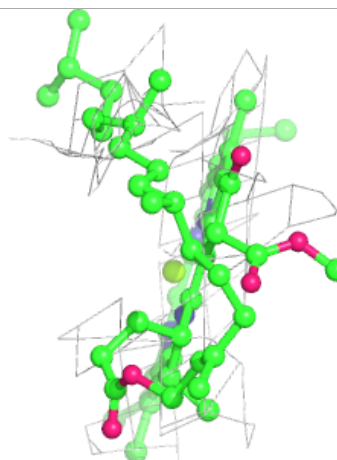
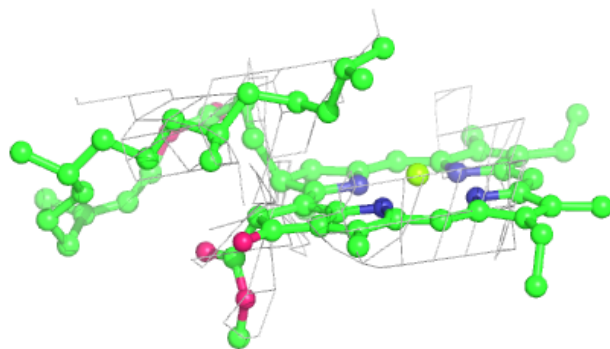
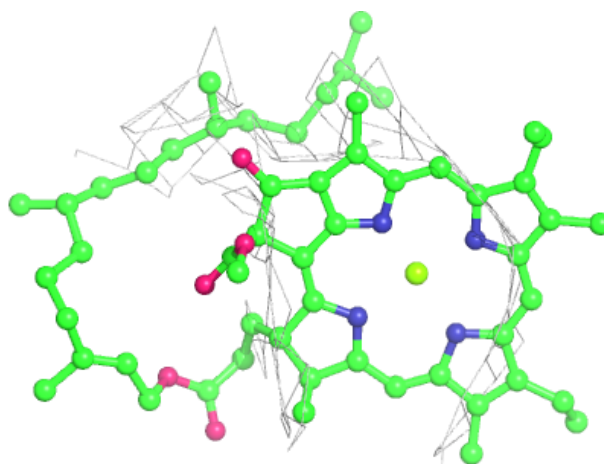
**Electron density around CLA B 804:**

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



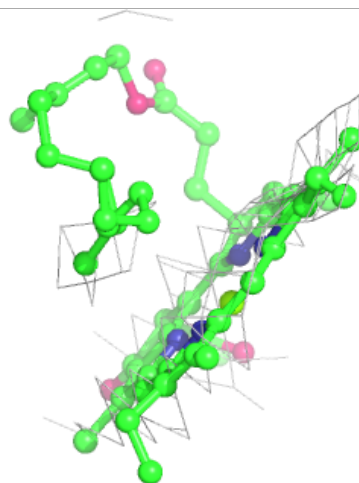
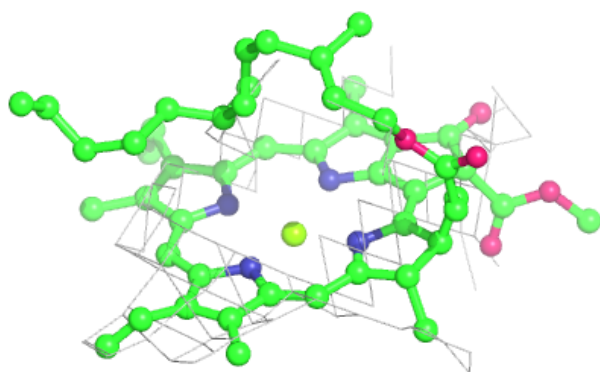
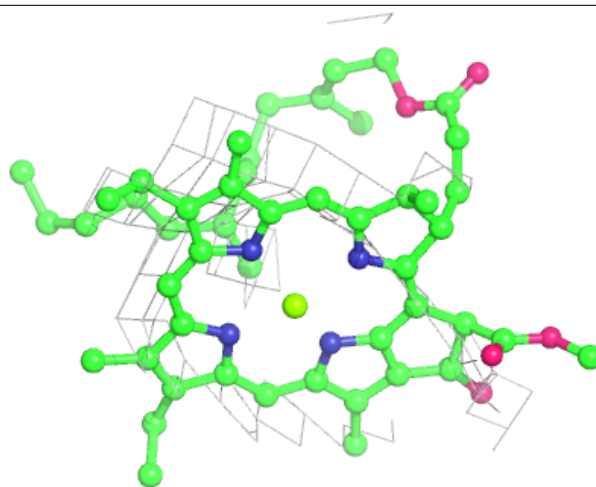
**Electron density around CLA B 805:**

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

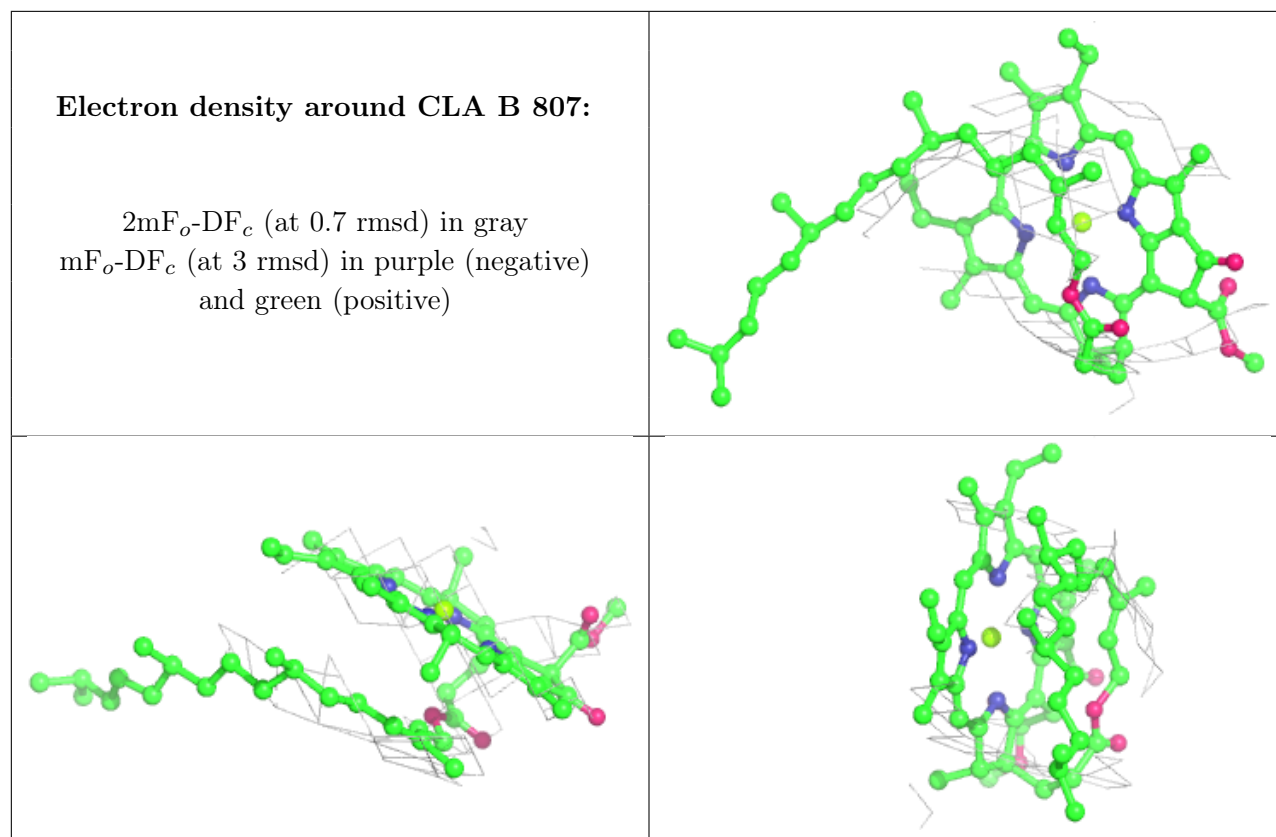


**Electron density around CLA B 817:**

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

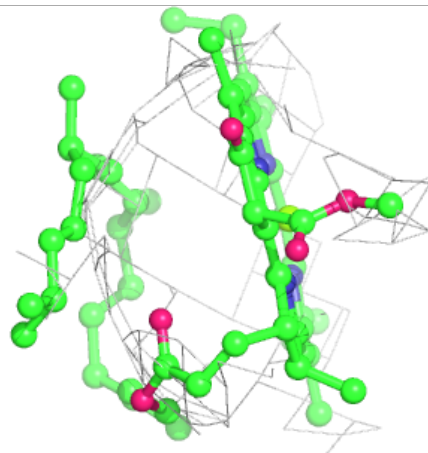
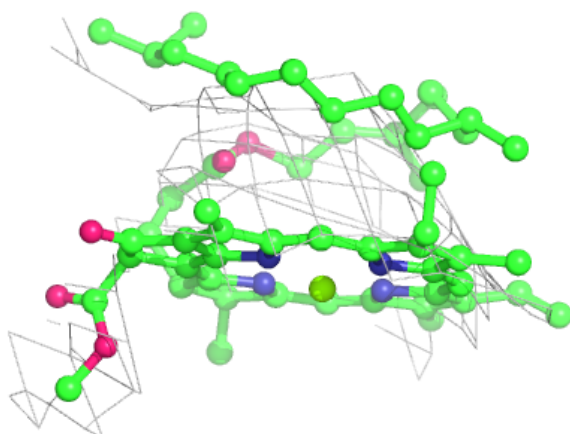
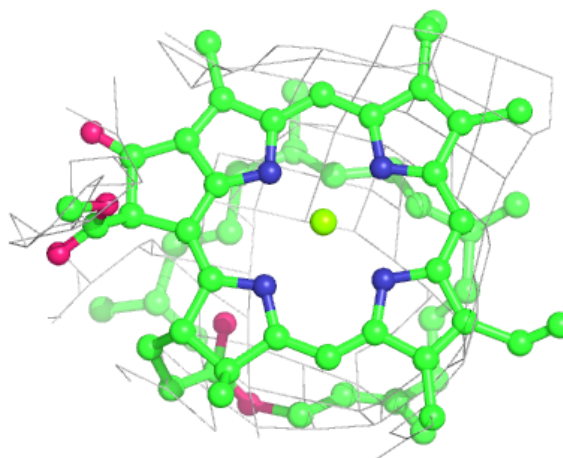






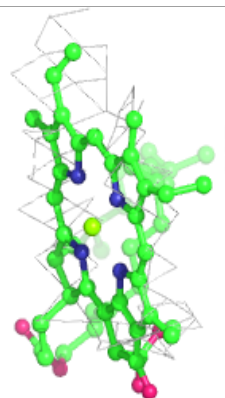
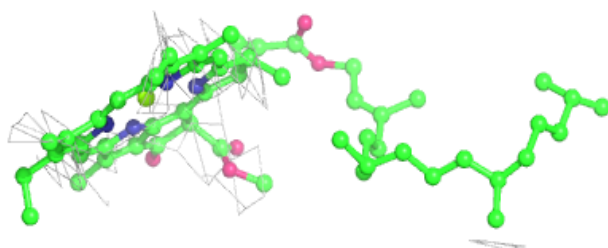
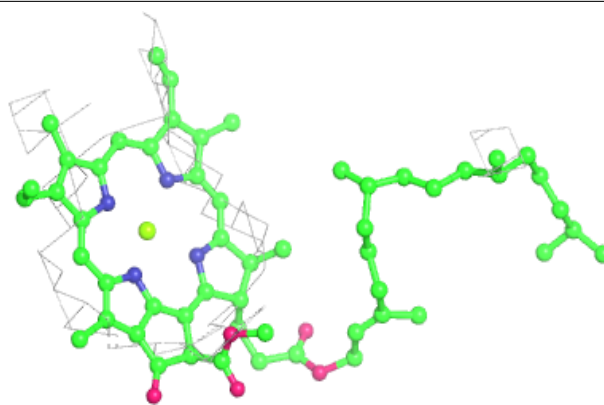
**Electron density around CLA L 1002:**

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

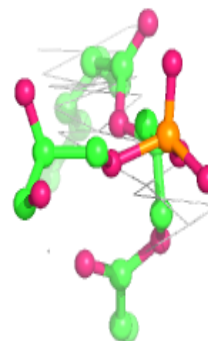
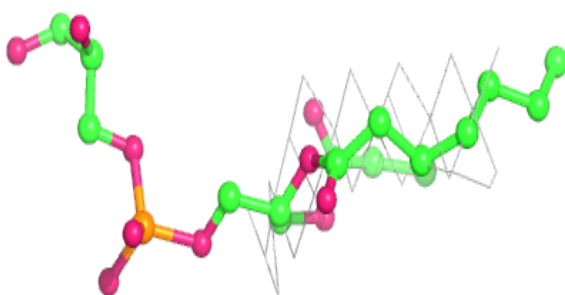
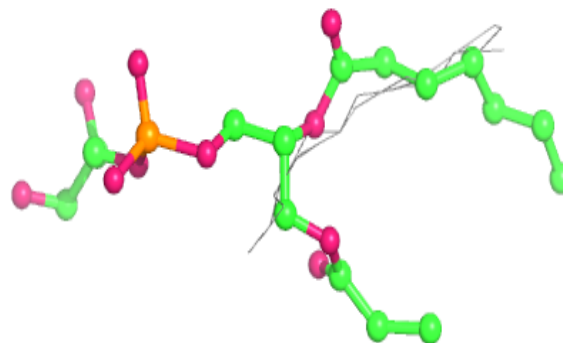


**Electron density around CLA A 804:**

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

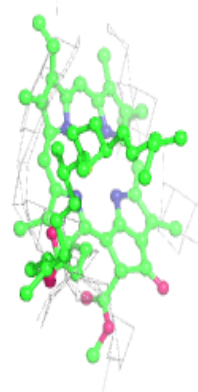
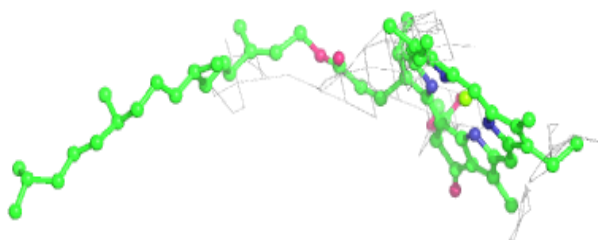
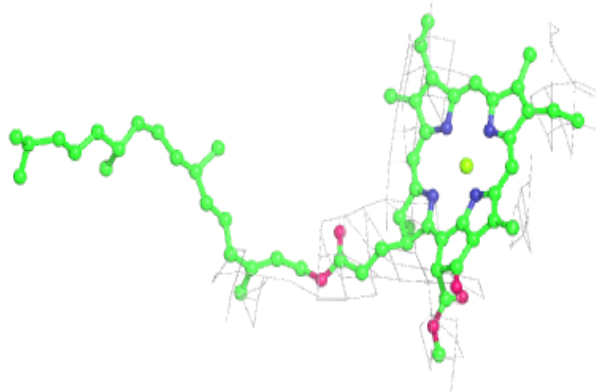
**Electron density around LHG A 856:**

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

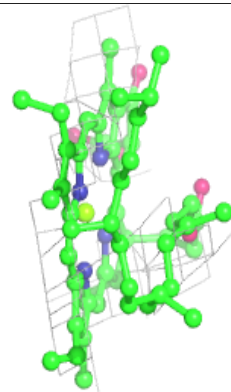
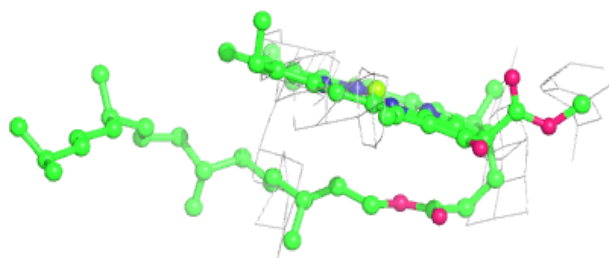
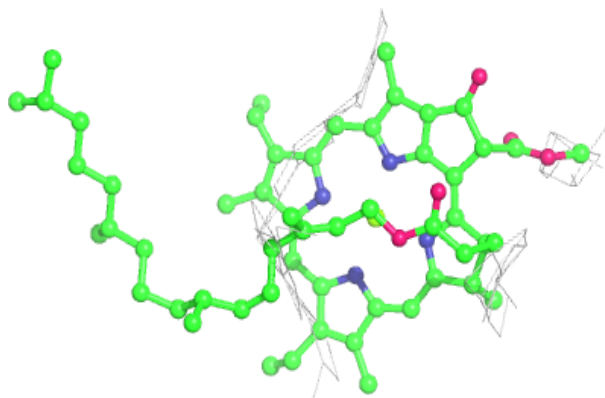


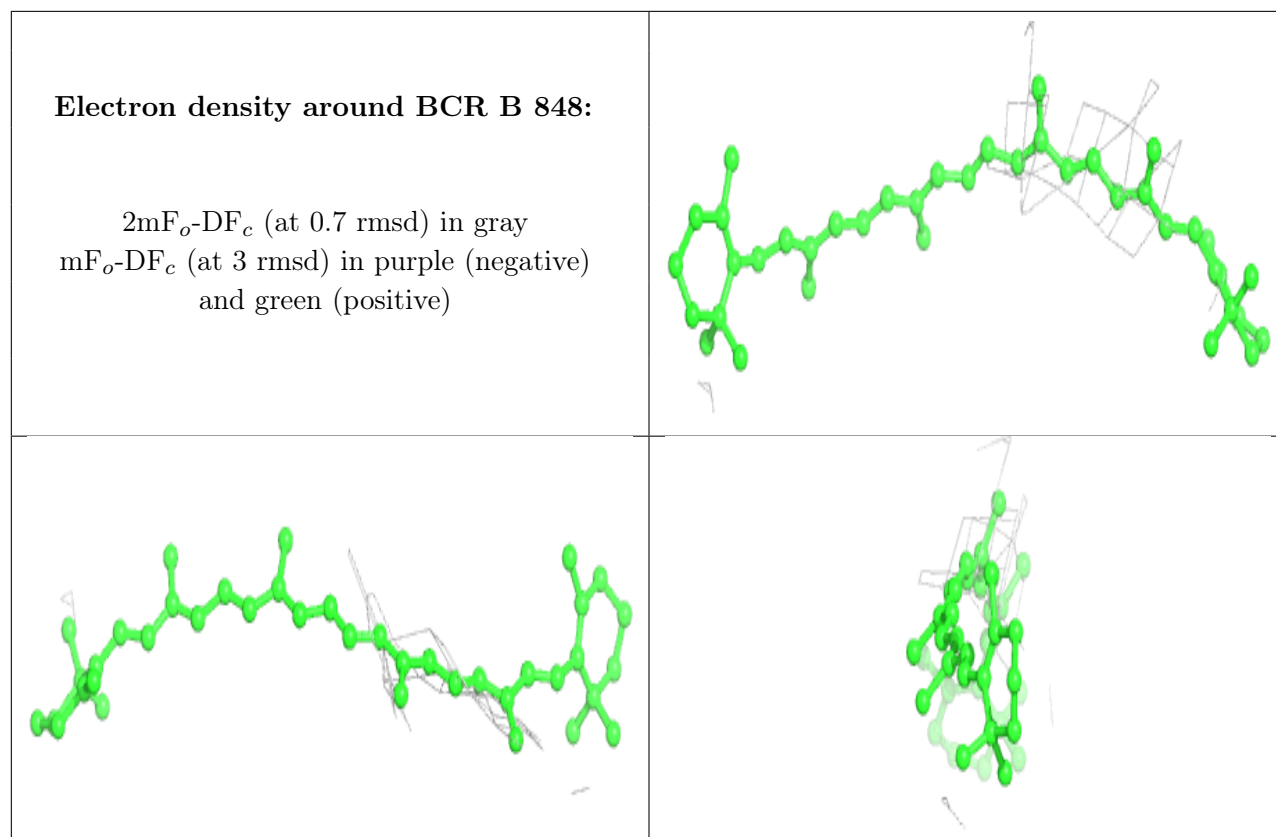
**Electron density around CLA A 802:**

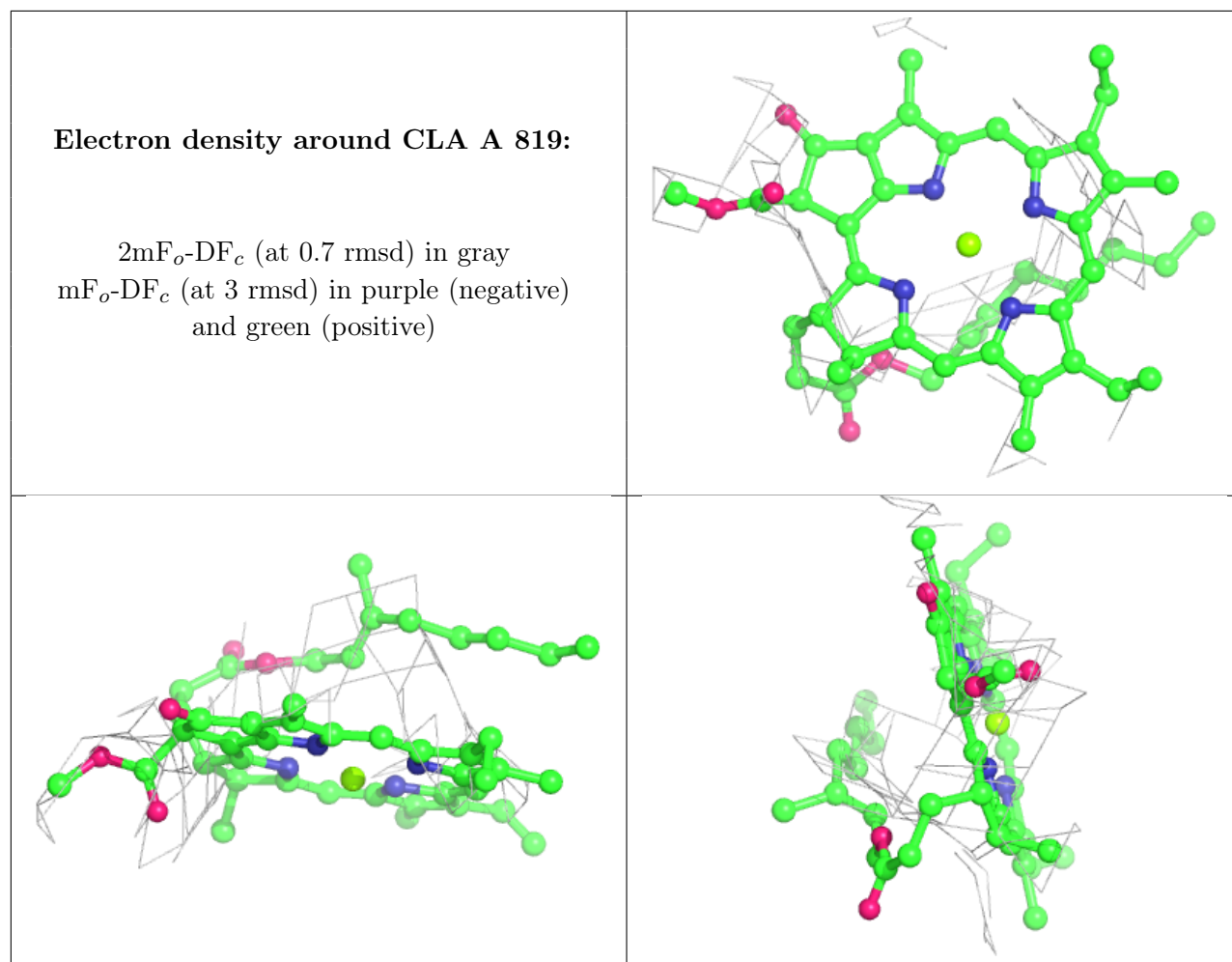
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

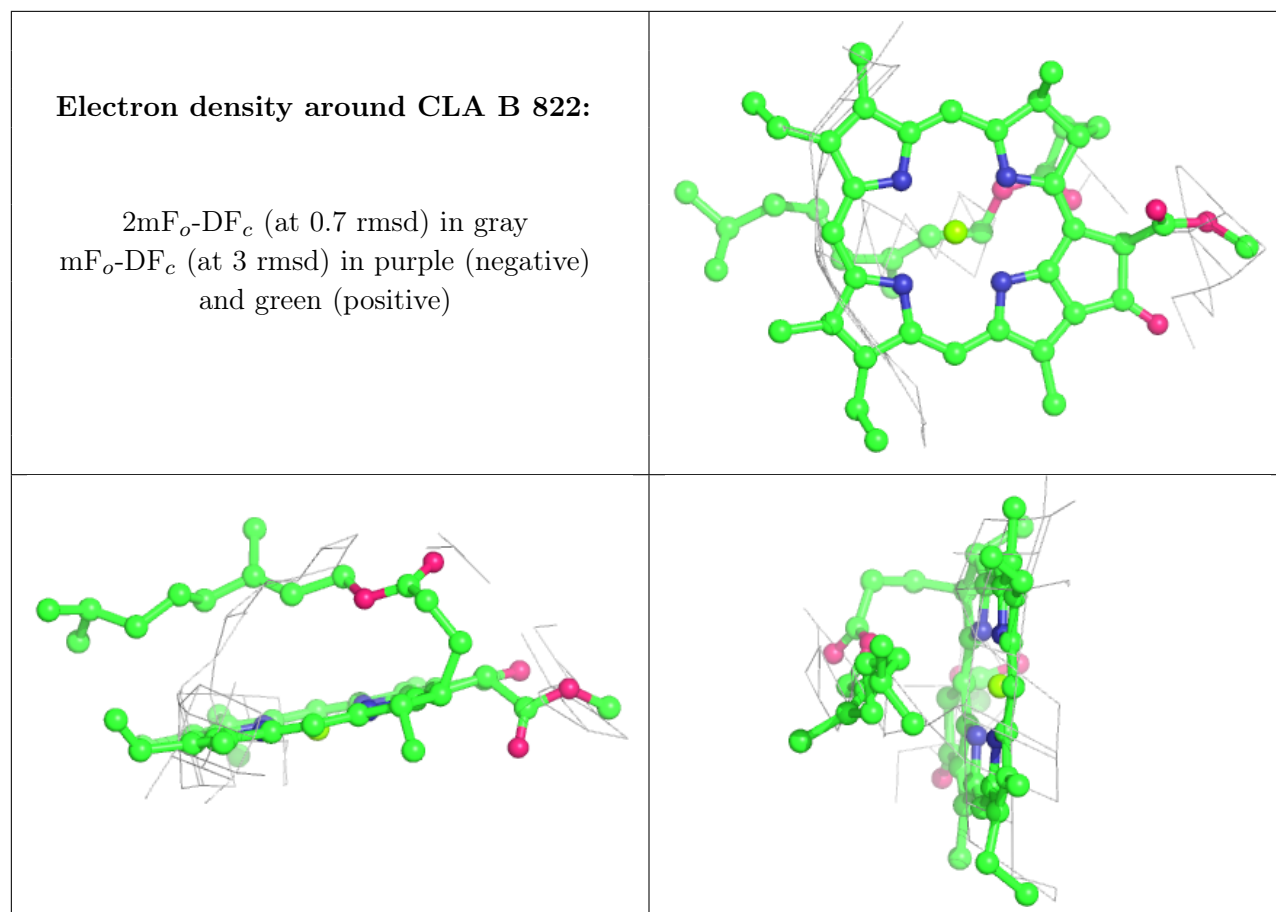
**Electron density around CLA B 838:**

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



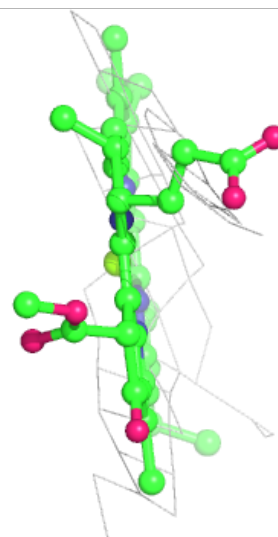
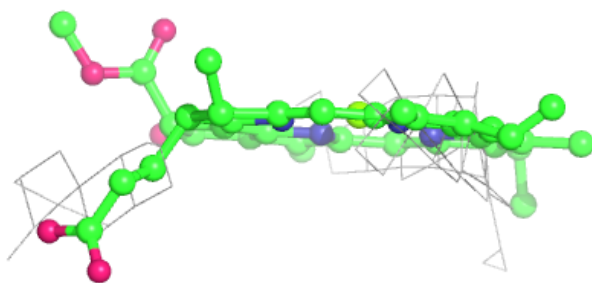
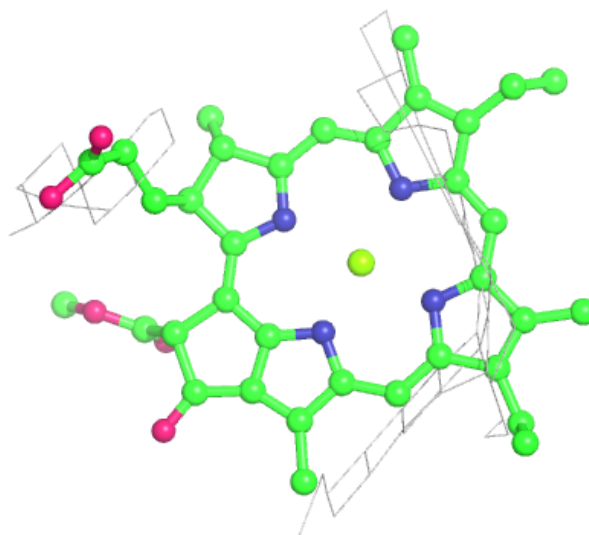




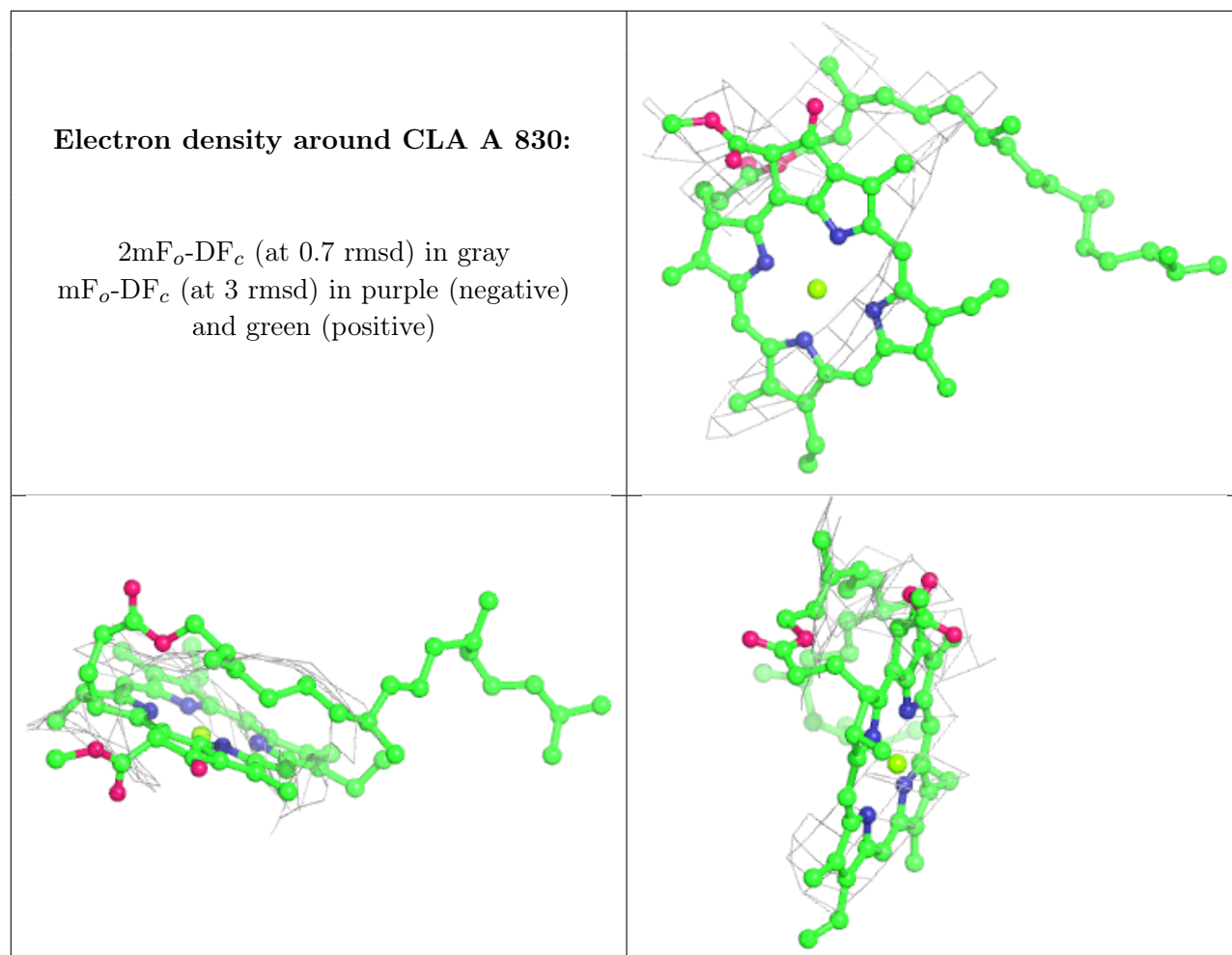


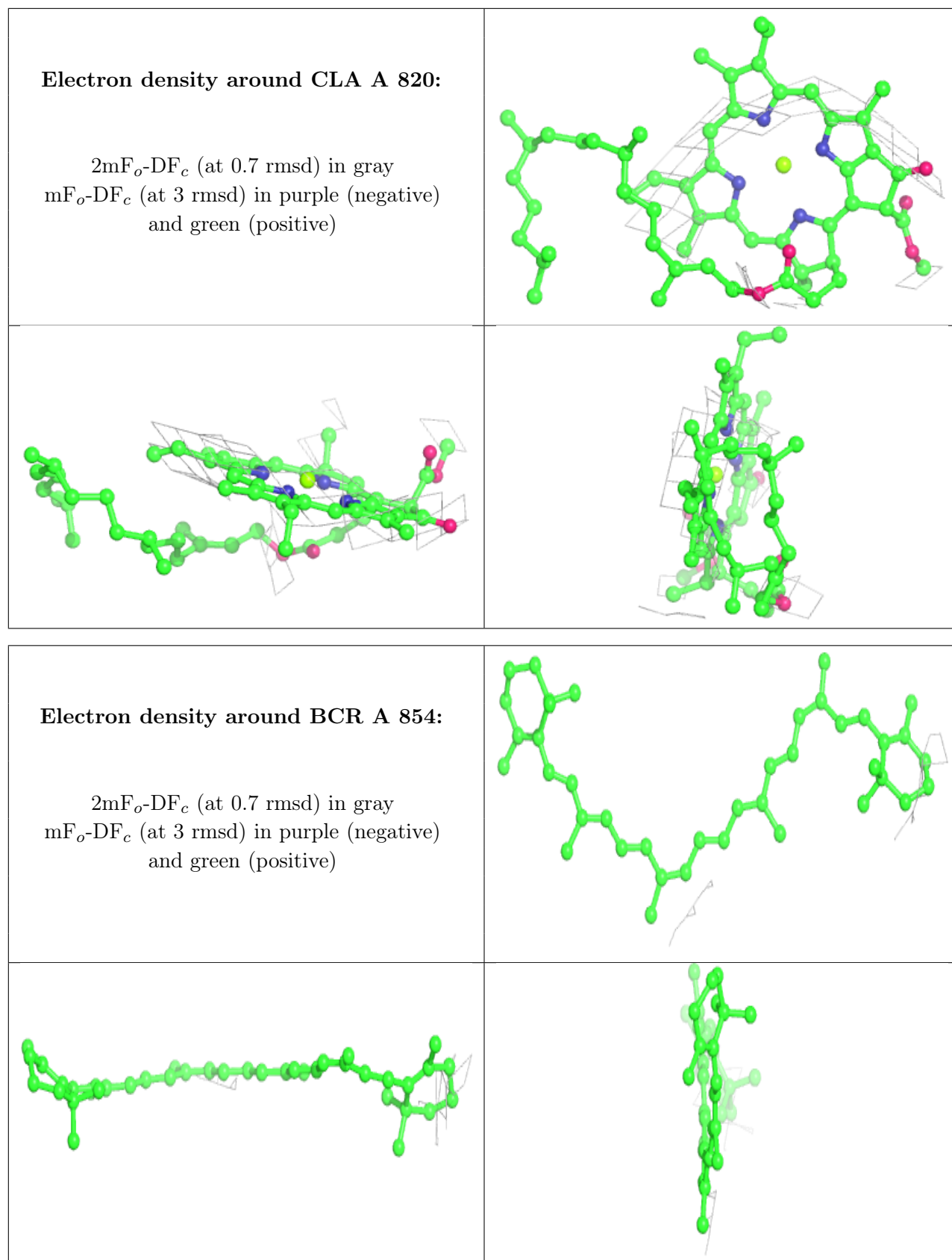
**Electron density around CLA B 823:**

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



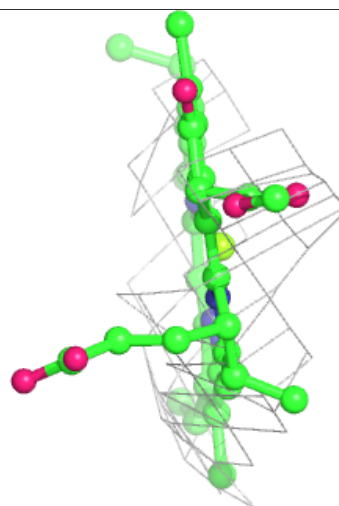
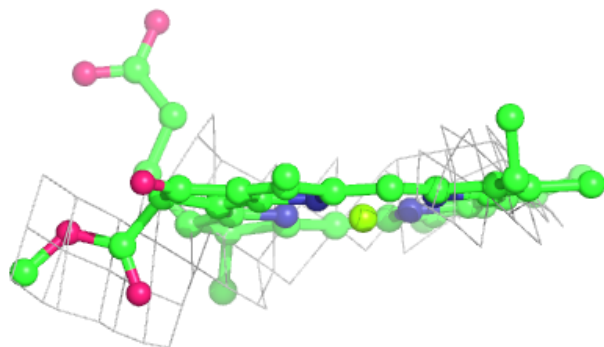
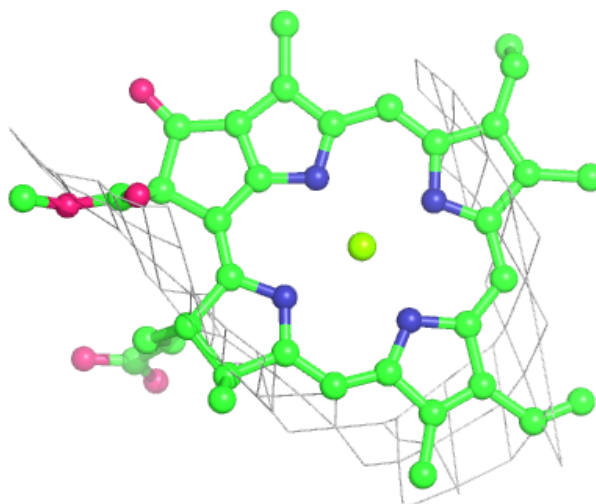


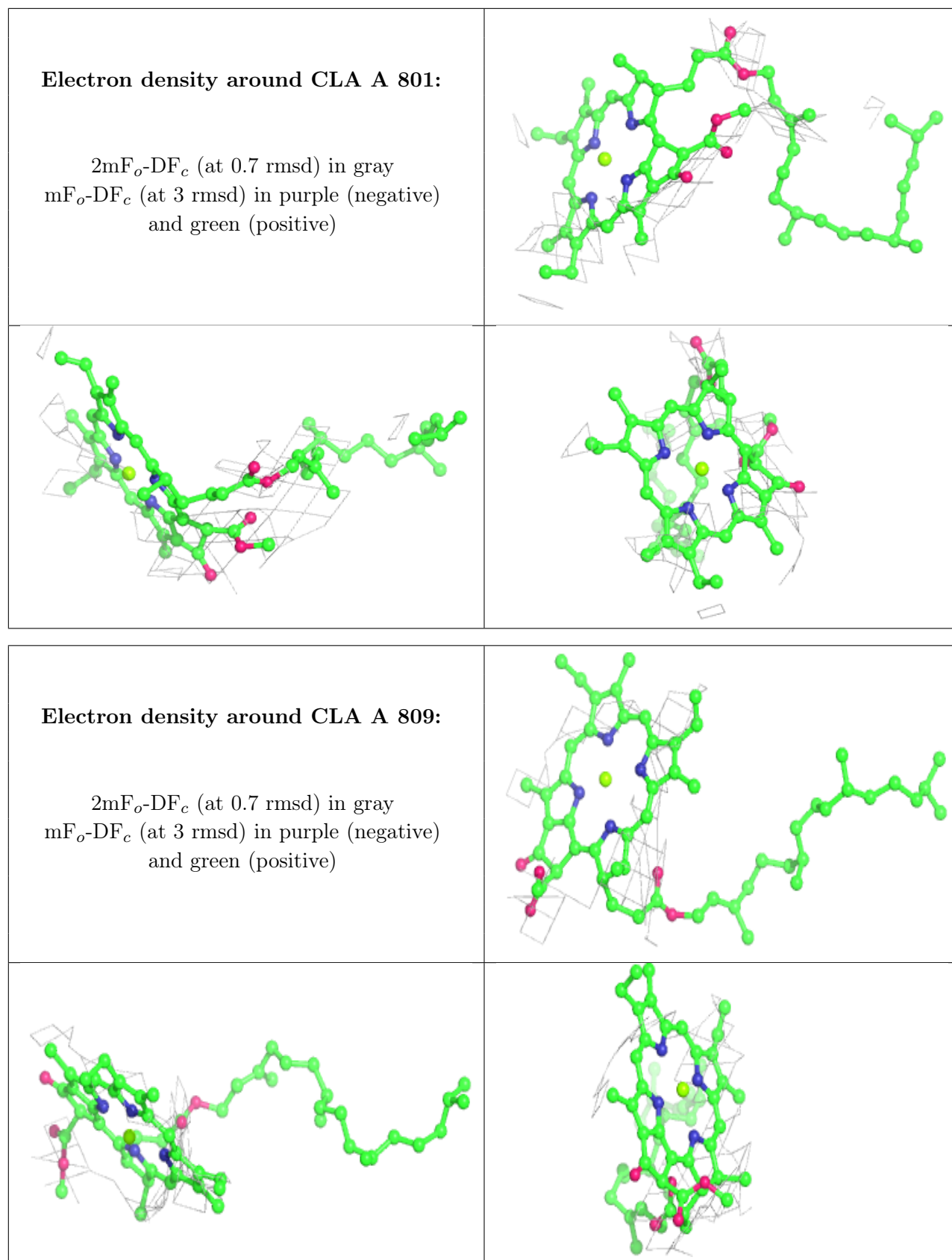


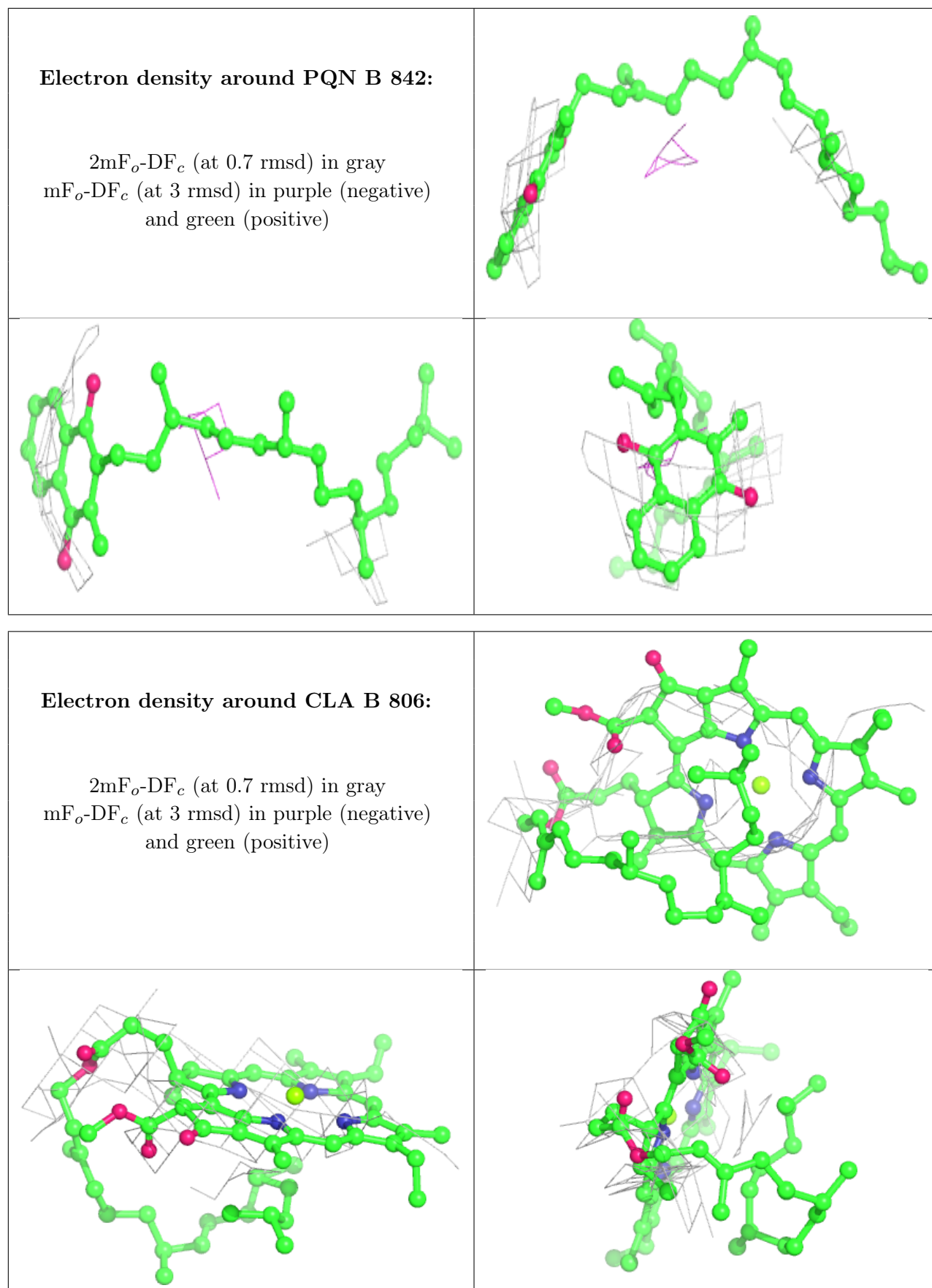


**Electron density around CLA B 835:**

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

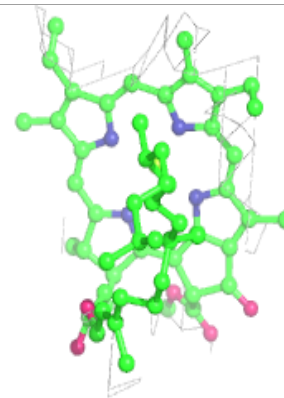
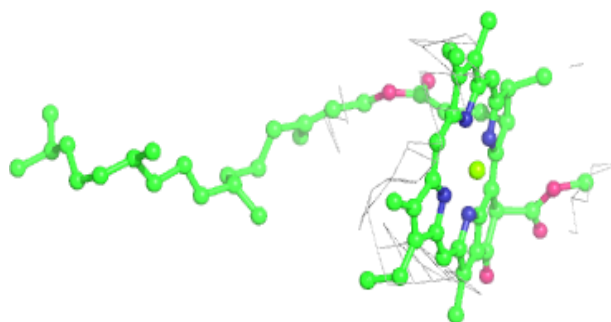
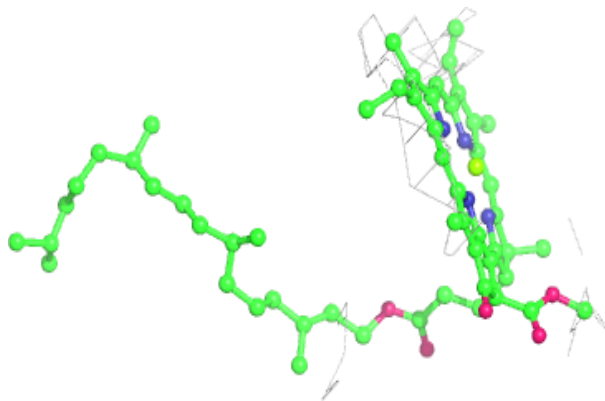




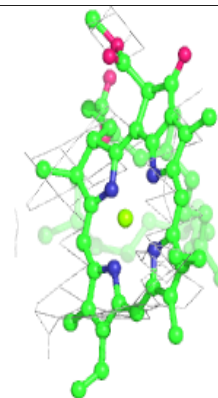
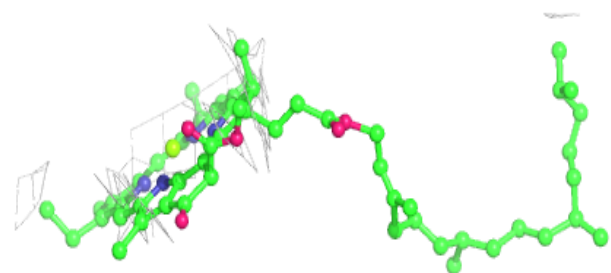
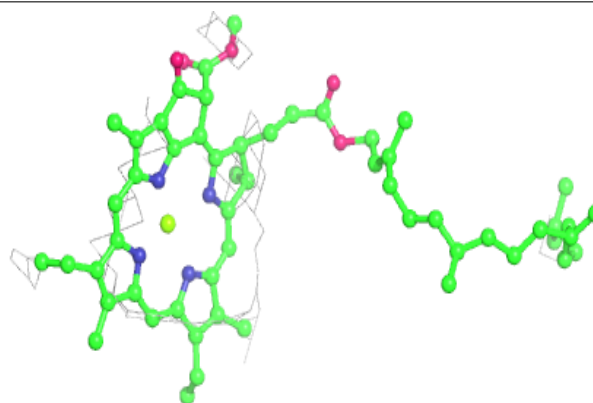


**Electron density around CLA A 831:**

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

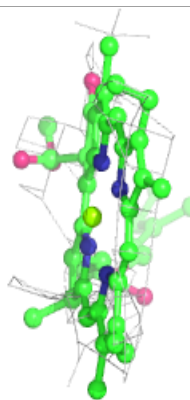
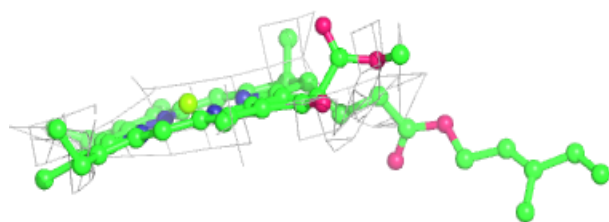
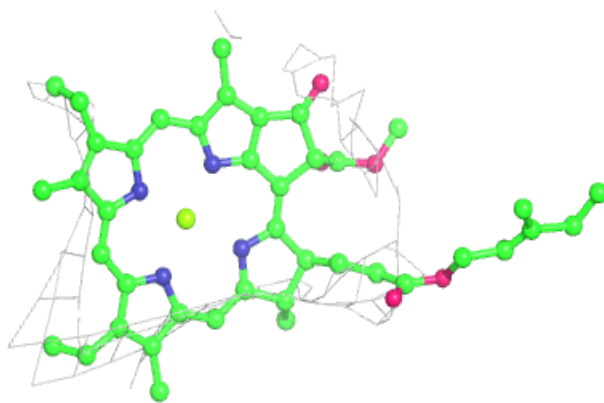
**Electron density around CLA B 809:**

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

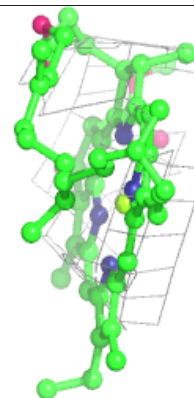
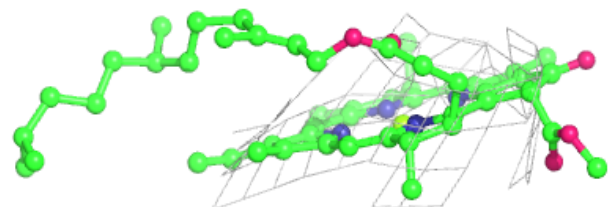
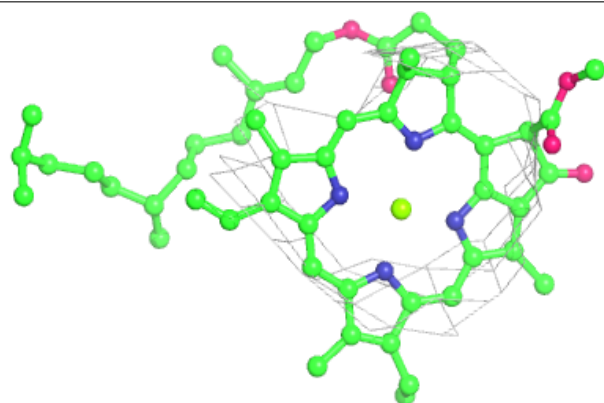


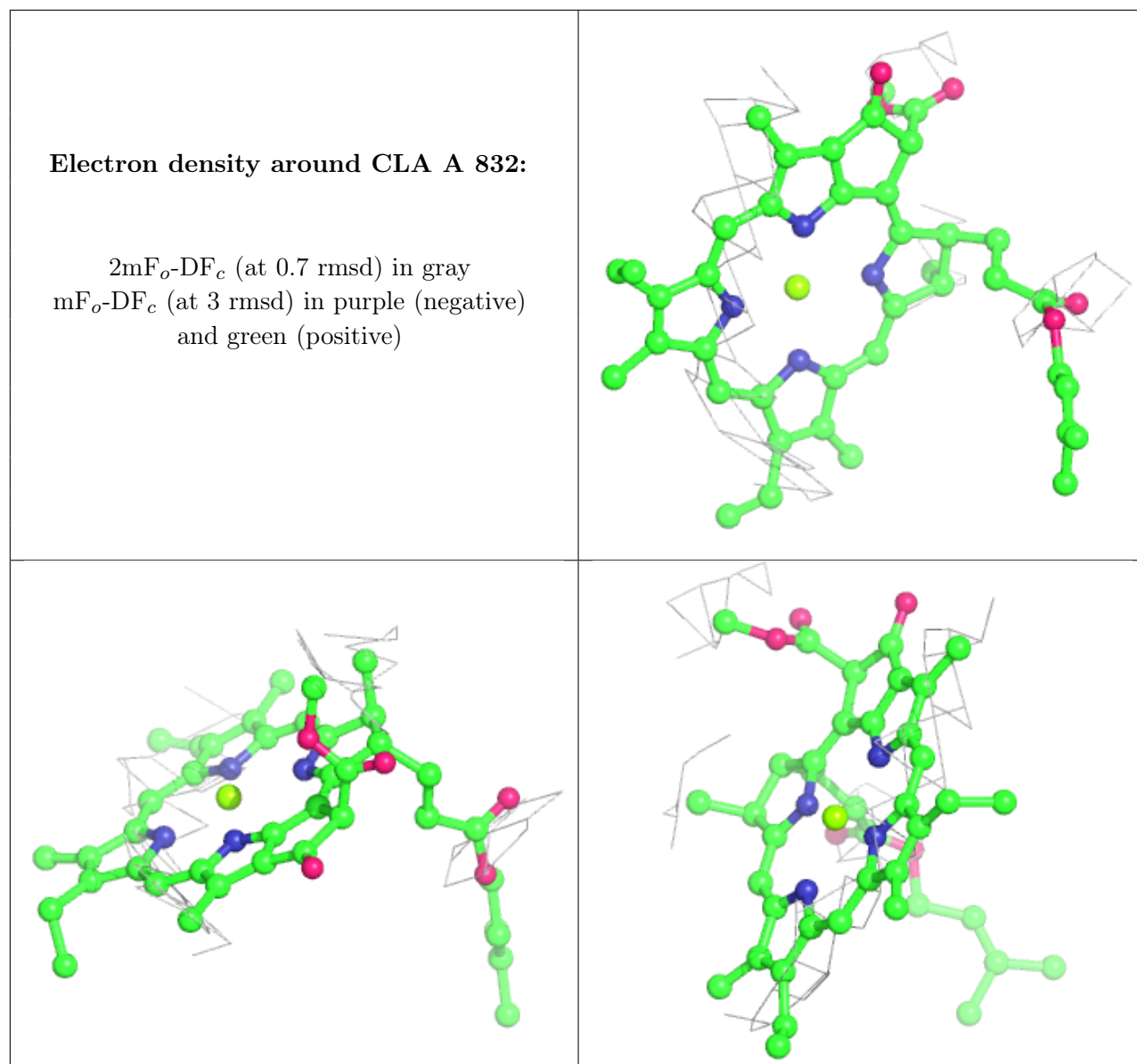
**Electron density around CLA A 842:**

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

**Electron density around CLA 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)

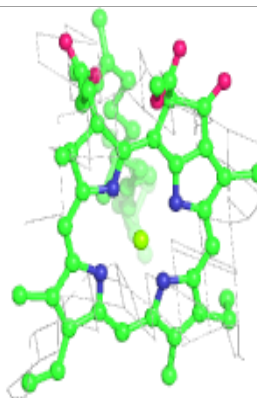
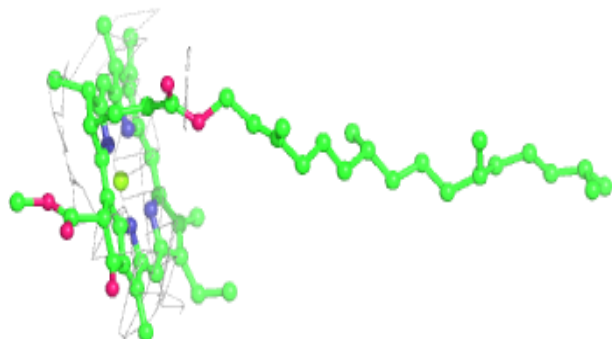
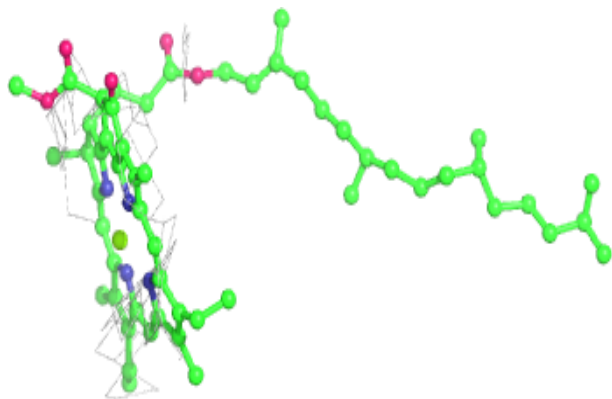




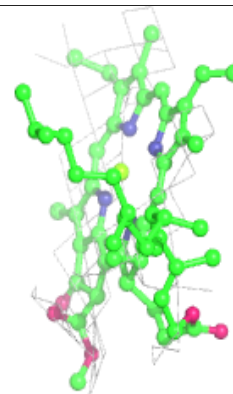
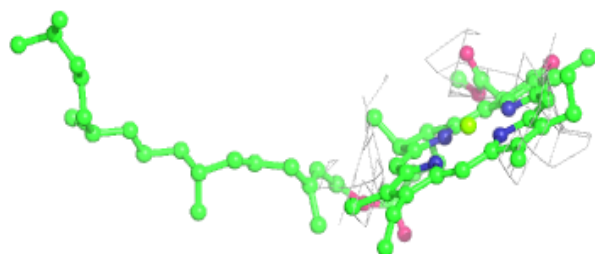
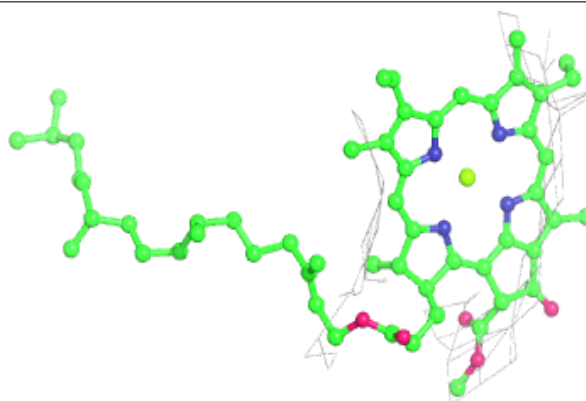


**Electron density around CLA B 829:**

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

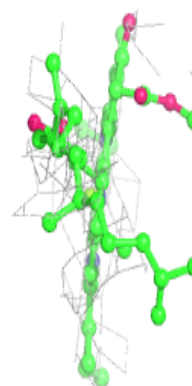
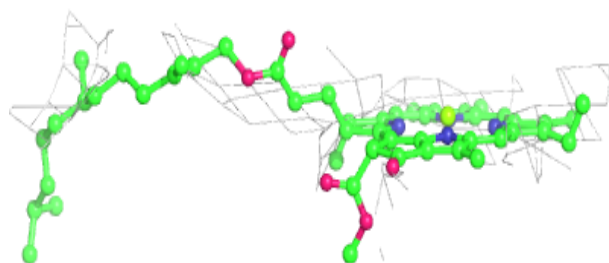
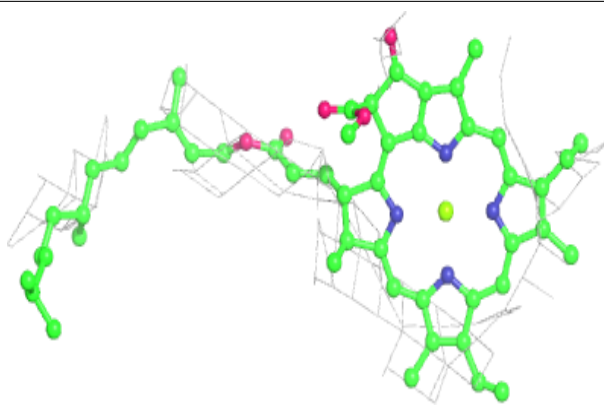
**Electron density around CLA A 803:**

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

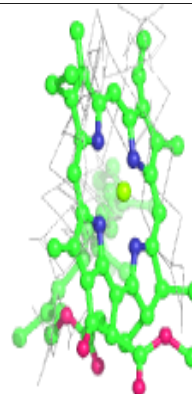
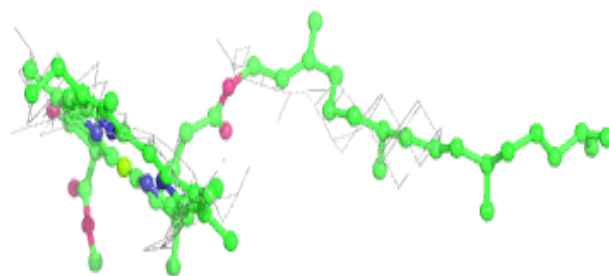
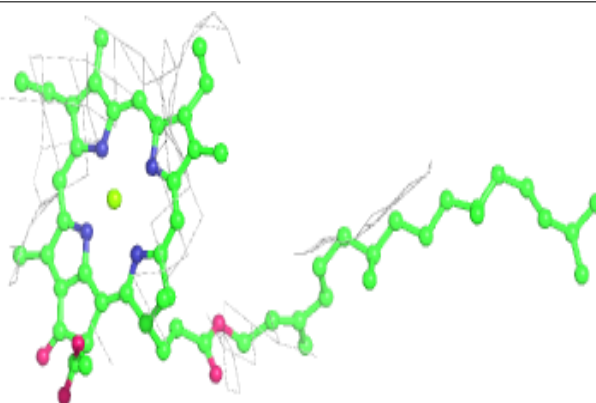


**Electron density around CLA B 837:**

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

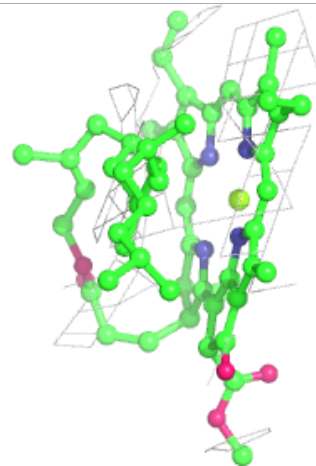
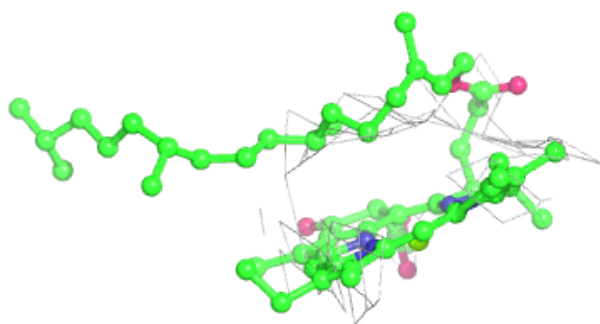
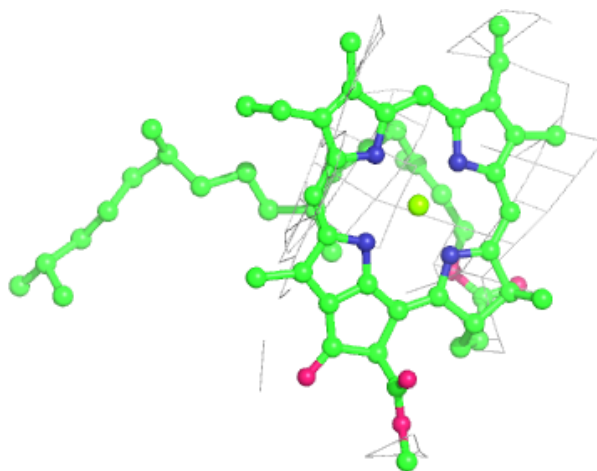
**Electron density around CLA A 835:**

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



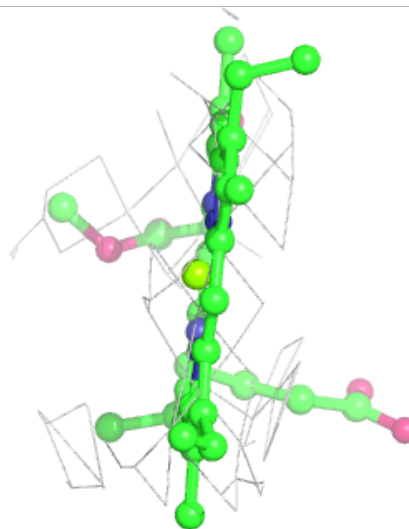
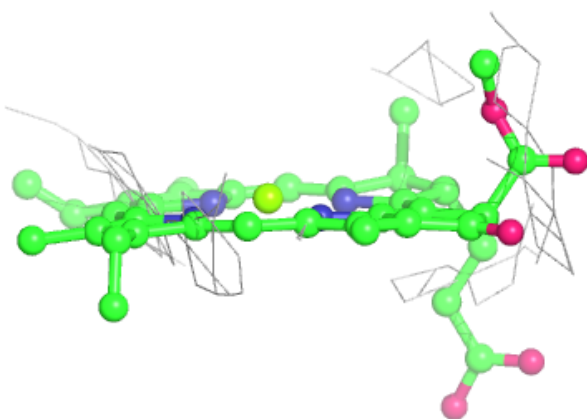
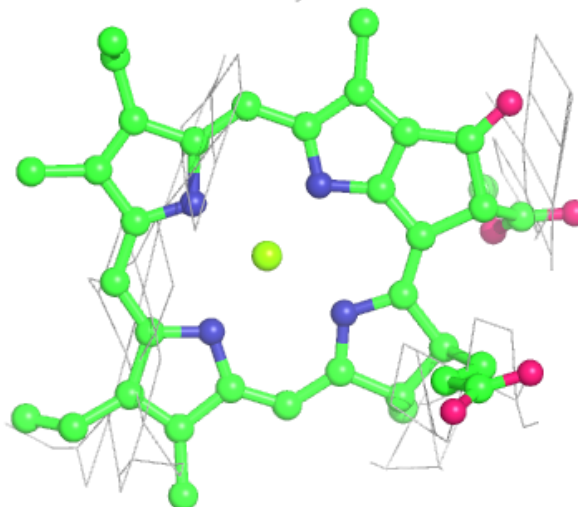
**Electron density around CLA B 827:**

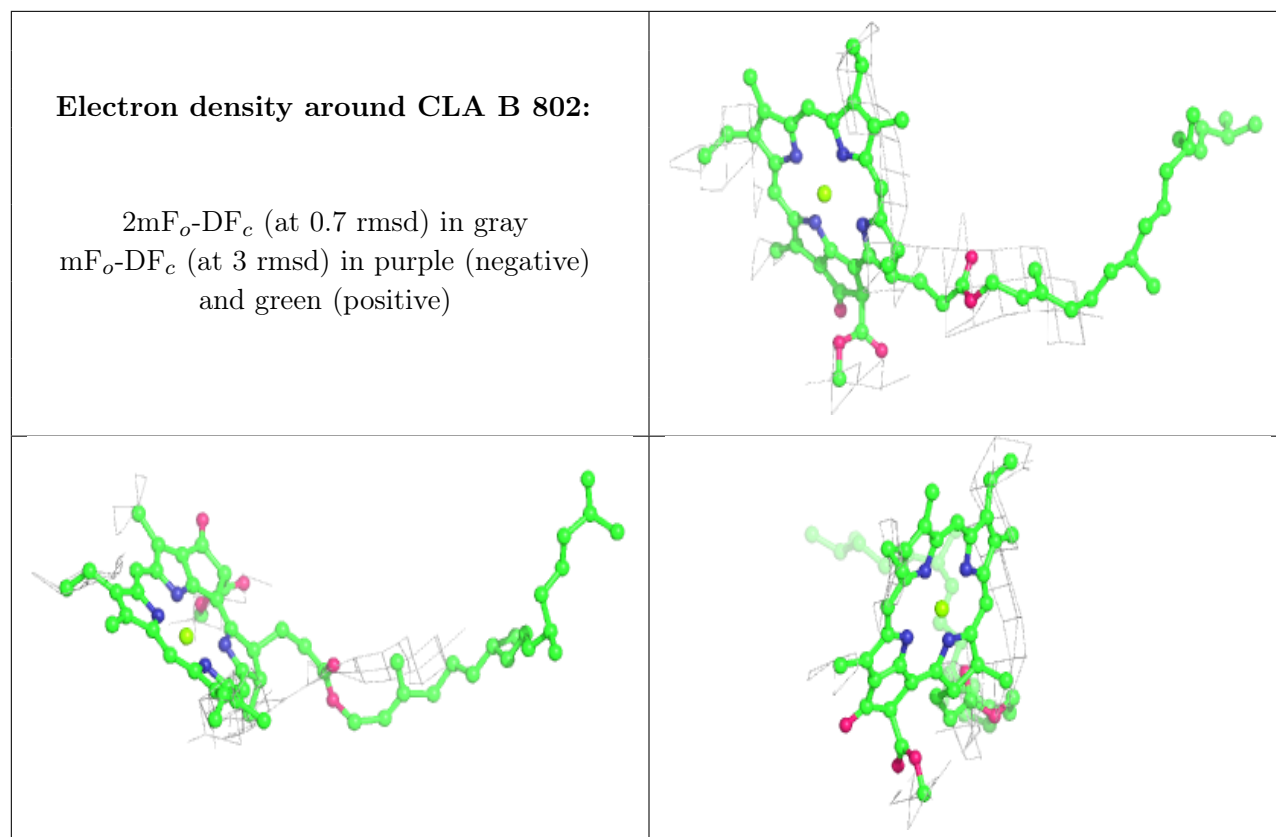
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 834:**

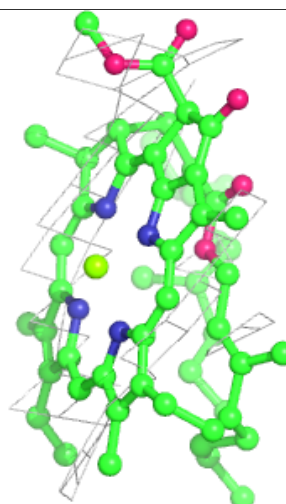
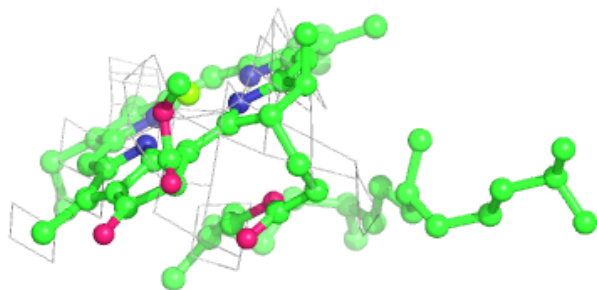
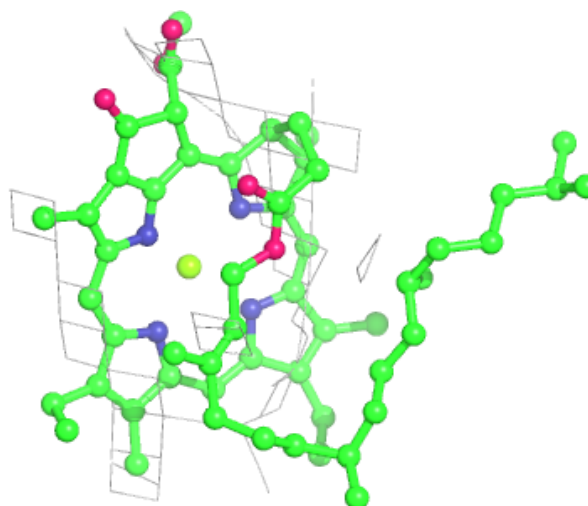
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

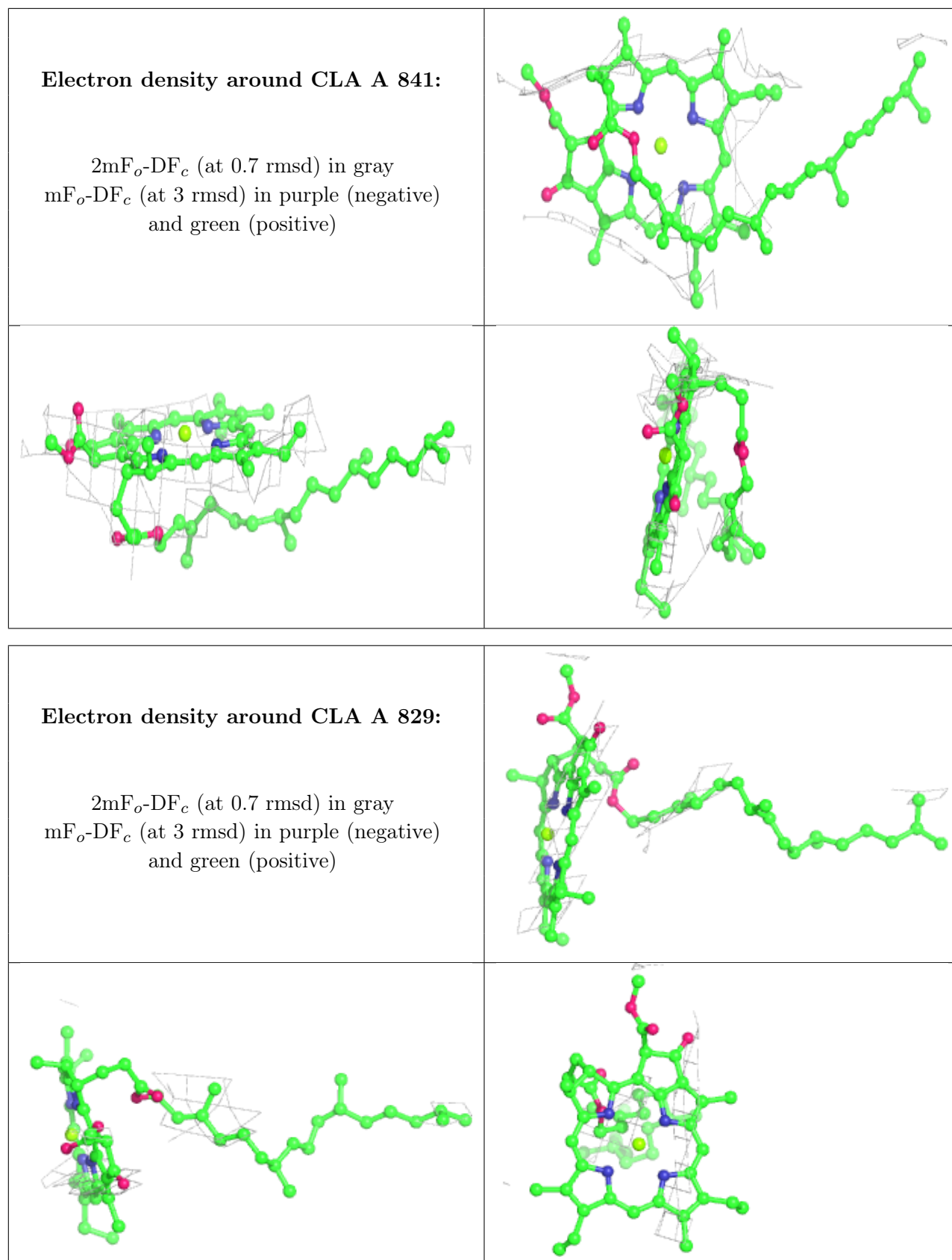




**Electron density around CLA B 808:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.