



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 11:27 PM UTC

PDB ID : 4FE1 / pdb_00004fe1
Title : Improving the Accuracy of Macromolecular Structure Refinement at 7 Å Resolution
Authors : Fromme, R.; Adams, P.D.; Fromme, P.; Levitt, M.; Schroeder, G.F.; Brunger, A.T.
Deposited on : 2012-05-29
Resolution : 4.92 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

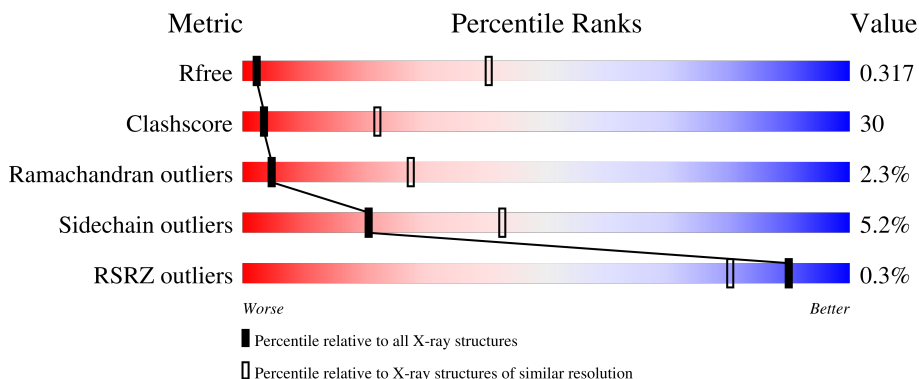
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.92 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}	180053	1008 (5.88-3.96)
Clashscore	190562	1020 (5.82-3.98)
Ramachandran outliers	187476	1125 (5.94-3.90)
Sidechain outliers	187428	1105 (5.94-3.90)
RSRZ outliers	180081	1003 (5.88-3.96)

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

Mol	Chain	Length	Quality of chain
1	A	755	
2	B	740	
3	C	80	
4	D	138	

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Mol	Chain	Length	Quality of chain
5	E	75	
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	-	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	810	X	-	-	-
13	CLA	A	811	X	-	-	-
13	CLA	A	812	X	-	-	-
13	CLA	A	813	X	-	-	-
13	CLA	A	814	X	-	-	-
13	CLA	A	815	X	-	-	-
13	CLA	A	817	X	-	-	-
13	CLA	A	818	X	-	-	-
13	CLA	A	819	X	-	-	-
13	CLA	A	820	X	-	-	-
13	CLA	A	821	X	-	-	-
13	CLA	A	822	X	-	-	-
13	CLA	A	823	X	-	-	-
13	CLA	A	824	X	-	-	-
13	CLA	A	825	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	827	X	-	-	-
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	834	X	-	-	-
13	CLA	A	835	X	-	-	-
13	CLA	A	836	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	845	X	-	-	-
13	CLA	A	855	X	-	-	-
13	CLA	B	801	X	-	-	-
13	CLA	B	802	X	-	-	-
13	CLA	B	803	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	-	-	-
13	CLA	B	814	X	-	-	-
13	CLA	B	815	X	-	-	-
13	CLA	B	816	X	-	-	-
13	CLA	B	817	X	-	-	-
13	CLA	B	818	X	-	-	-
13	CLA	B	819	X	-	-	-
13	CLA	B	820	X	-	-	-
13	CLA	B	821	X	-	-	-
13	CLA	B	822	X	-	-	-
13	CLA	B	823	X	-	-	-
13	CLA	B	824	X	-	-	-
13	CLA	B	825	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	B	826	X	-	-	-
13	CLA	B	827	X	-	-	-
13	CLA	B	828	X	-	-	-
13	CLA	B	829	X	-	-	-
13	CLA	B	830	X	-	X	-
13	CLA	B	831	X	-	-	-
13	CLA	B	832	X	-	-	-
13	CLA	B	833	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	839	X	-	-	-
13	CLA	I	101	X	-	-	-
13	CLA	J	1101	X	-	-	-
13	CLA	J	1102	X	-	-	-
13	CLA	J	1103	X	-	-	-
13	CLA	L	1002	X	-	-	-
13	CLA	L	1003	X	-	-	-
13	CLA	L	1004	X	-	-	-
13	CLA	M	1201	X	-	-	-
13	CLA	X	102	X	-	-	-

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 23997 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

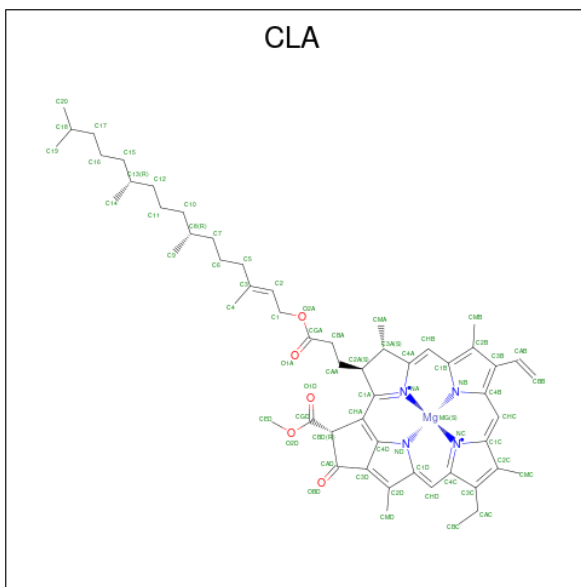
- Molecule 12 is a protein called Photosystem I 4.8K protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	X	29	233	164	34	35	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	32	ALA	-	expression tag	UNP Q8DKP6
X	33	ALA	-	expression tag	UNP Q8DKP6
X	34	ALA	-	expression tag	UNP Q8DKP6
X	35	ALA	-	expression tag	UNP Q8DKP6

- Molecule 13 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
13	A	1	65	55	1	4	5	0	0
13	A	1	54	44	1	4	5	0	0
13	A	1	60	50	1	4	5	0	0
13	A	1	45	35	1	4	5	0	0
13	A	1	45	35	1	4	5	0	0
13	A	1	49	39	1	4	5	0	0
13	A	1	54	44	1	4	5	0	0
13	A	1	54	44	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0
13	A	1	61	51	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0
13	A	1	49	39	1	4	5	0	0
13	A	1	51	41	1	4	5	0	0
13	A	1	59	49	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0
13	A	1	65	55	1	4	5	0	0
13	A	1	50	40	1	4	5	0	0

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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
			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	A	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
			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		

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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
			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
			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
			65	55	1	4	5		

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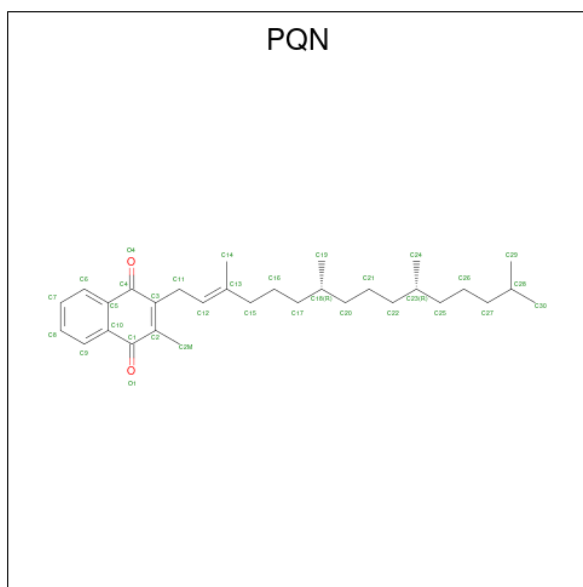
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			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	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	J	1	Total	C	Mg	N	O	0	0
			65	55	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	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
			54	44	1	4	5		

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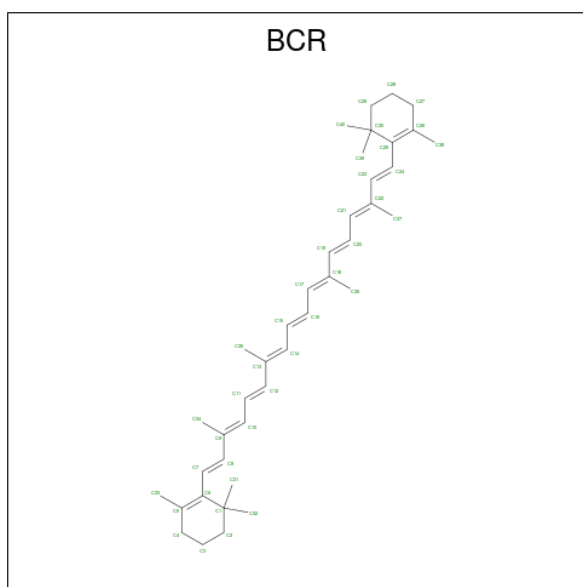
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	M	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	X	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

- Molecule 14 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



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



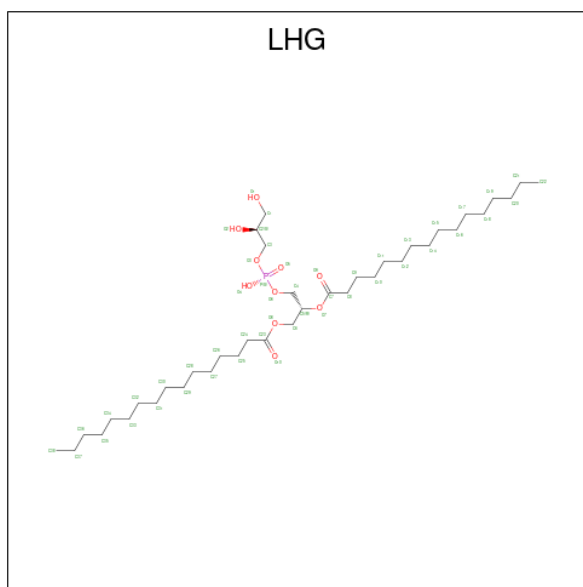
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 25 25	0	0
15	B	1	Total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

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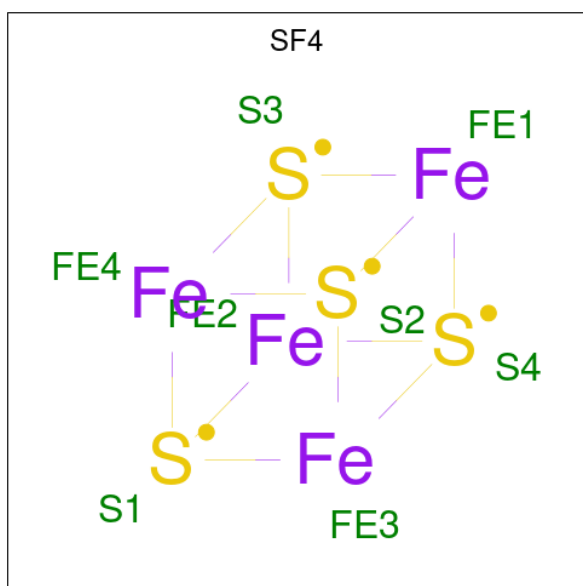
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total C 40 40	0	0
15	F	1	Total C 40 40	0	0
15	I	1	Total C 40 40	0	0
15	J	1	Total C 40 40	0	0
15	J	1	Total C 40 40	0	0
15	L	1	Total C 40 40	0	0
15	L	1	Total C 40 40	0	0
15	M	1	Total C 40 40	0	0

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



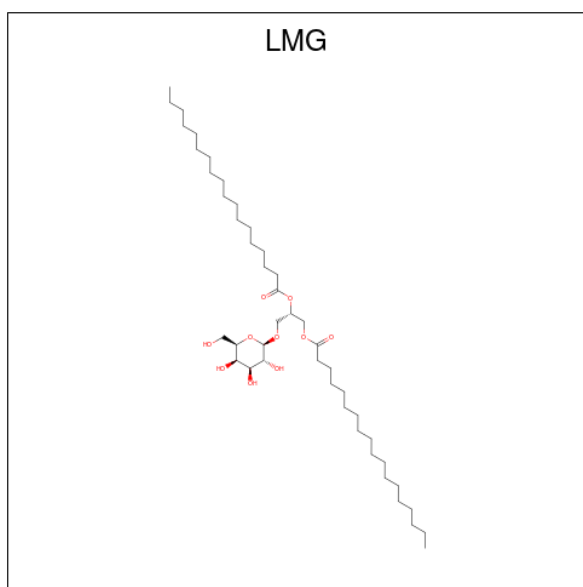
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total C O P 49 38 10 1	0	0
16	A	1	Total C O P 27 16 10 1	0	0
16	X	1	Total C O P 23 12 10 1	0	0

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	B	1	Total	C	O	0	0
			55	45	10		

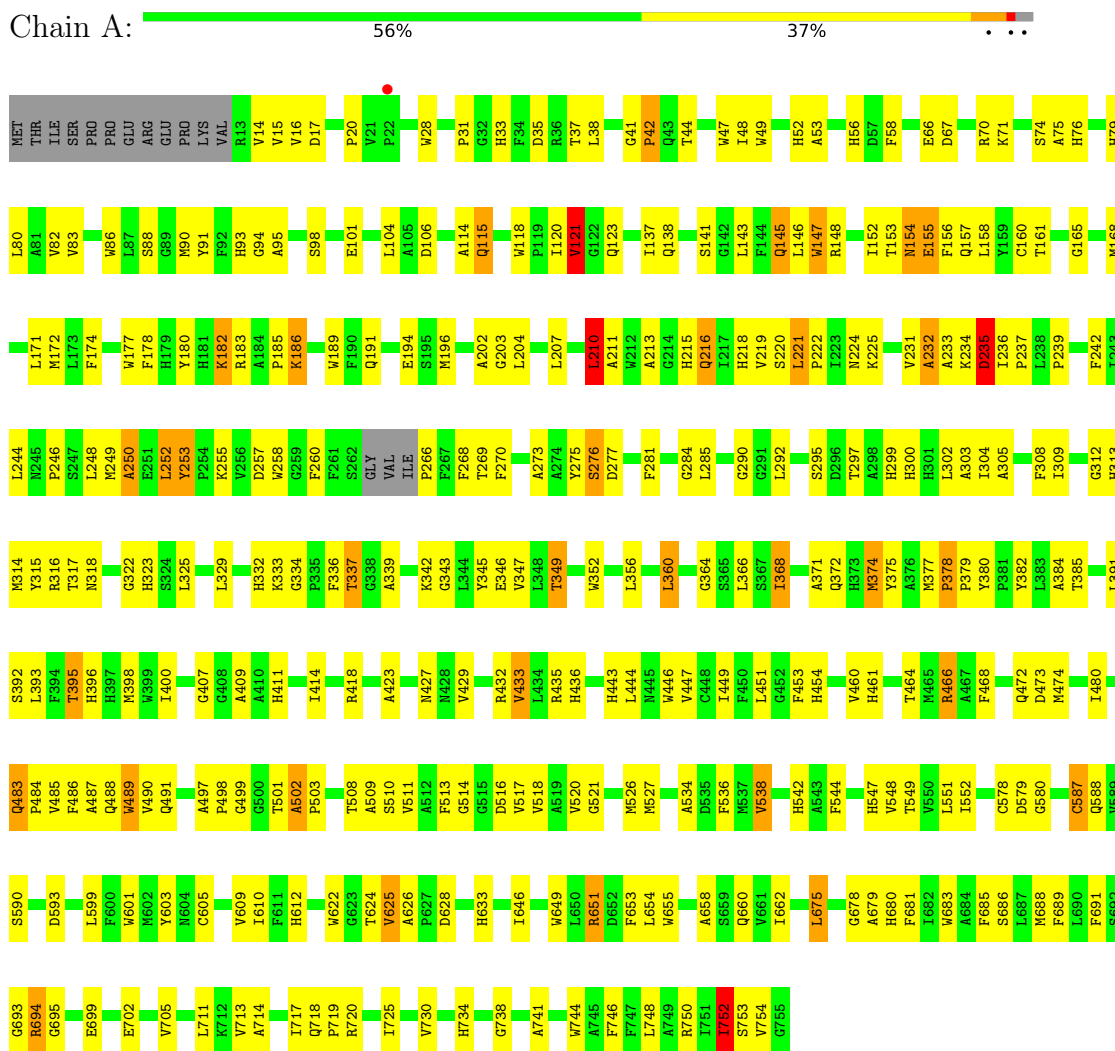
- Molecule 19 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

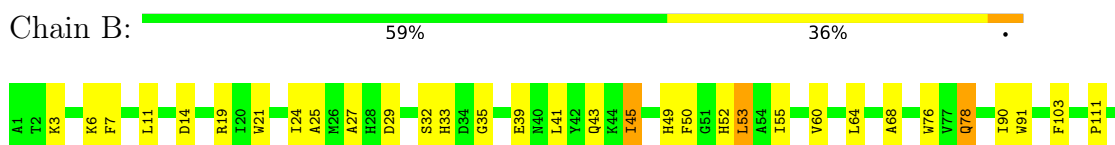
3 Residue-property plots

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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

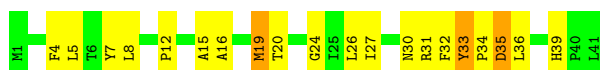




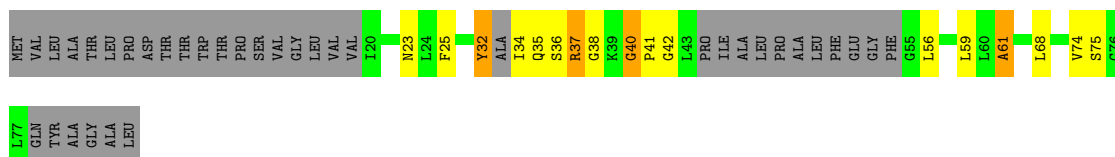
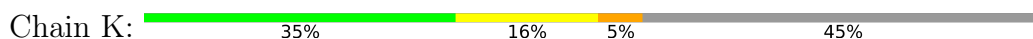
- Molecule 7: Photosystem I reaction center subunit VIII



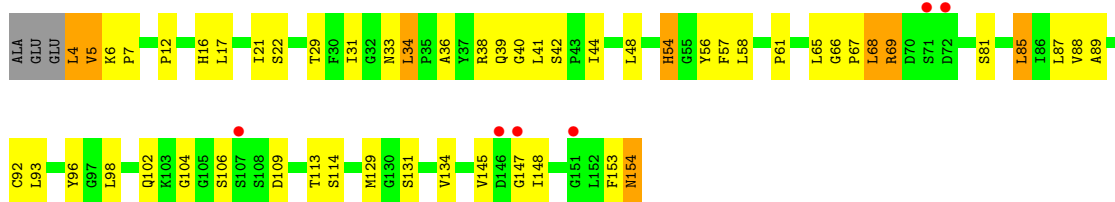
- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 9: Photosystem I reaction center subunit Psak



- Molecule 10: Photosystem I reaction center subunit XI

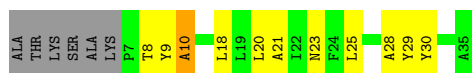


- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 12: Photosystem I 4.8K protein

Chain X:  51% 29% 0% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	281.00Å 281.00Å 165.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.97 – 4.92 97.97 – 4.92	Depositor EDS
% Data completeness (in resolution range)	96.4 (97.97-4.92) 96.3 (97.97-4.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.35 (at 4.87Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8_1058)	Depositor
R, R_{free}	0.274 , 0.315 0.276 , 0.317	Depositor DCC
R_{free} test set	1534 reflections (4.37%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtrriage
Anisotropy	0.569	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 258.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.13$	Xtrriage
Estimated twinning fraction	0.175 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	23997	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.11	34/8158 (0.4%)
2	B	0.52	0/6096	1.08	31/8332 (0.4%)
3	C	0.50	0/608	1.25	7/824 (0.8%)
4	D	0.47	0/1101	1.06	3/1492 (0.2%)
5	E	0.52	0/551	1.16	2/750 (0.3%)
6	F	0.59	0/1087	1.15	6/1476 (0.4%)
7	I	0.51	0/312	1.10	2/425 (0.5%)
8	J	0.52	0/350	1.26	6/477 (1.3%)
9	K	0.61	0/220	1.71	10/300 (3.3%)
10	L	0.50	0/1148	1.16	12/1558 (0.8%)
11	M	0.73	0/244	1.37	2/332 (0.6%)
12	X	0.50	0/242	1.02	1/332 (0.3%)
All	All	0.52	0/17942	1.12	116/24456 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
4	D	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	PRO	CA-C-N	11.32	131.07	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	PRO	C-N-CA	11.32	131.07	119.64
2	B	217	HIS	CA-C-N	11.03	133.62	119.84
2	B	217	HIS	C-N-CA	11.03	133.62	119.84
1	A	580	GLY	CA-C-N	10.30	129.91	119.82

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	337	THR	Mainchain
2	B	35	GLY	Mainchain
4	D	88	ASP	Mainchain

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	340	0
2	B	5879	0	5632	344	0
3	C	598	0	580	16	0
4	D	1075	0	1077	31	0
5	E	539	0	528	14	0
6	F	1065	0	1077	53	0
7	I	301	0	306	24	0
8	J	338	0	347	24	0
9	K	222	0	111	9	0
10	L	1119	0	1125	49	1
11	M	241	0	264	23	0
12	X	233	0	231	11	0
13	A	2667	0	2635	435	0
13	B	2230	0	2182	406	0
13	F	45	0	33	4	0
13	I	65	0	72	15	0
13	J	147	0	129	15	0
13	L	195	0	216	26	0
13	M	99	0	81	16	0
13	X	45	0	33	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A	33	0	46	7	0
14	B	33	0	46	6	0
15	A	240	0	336	38	0
15	B	345	0	481	82	0
15	F	40	0	56	12	0
15	I	40	0	56	9	0
15	J	80	0	112	9	0
15	L	80	0	112	16	0
15	M	40	0	56	11	0
16	A	76	0	98	11	0
16	X	23	0	16	1	0
17	A	8	0	0	0	0
17	C	16	0	0	0	0
18	B	55	0	86	18	0
19	L	1	0	0	0	0
All	All	23997	0	23799	1418	1

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 30.

The worst 5 of 1418 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)
13:B:806:CLA:H12	7:I:18:VAL:HG21	1.35	1.08
13:A:803:CLA:H151	13:A:842:CLA:HAB	1.36	1.08
13:B:831:CLA:HED1	8:J:36:LEU:H	1.06	1.07
13:B:817:CLA:HBD	13:B:821:CLA:HED2	1.37	1.06
13:A:828:CLA:H51	15:A:852:BCR:H312	1.33	1.05

All (1) 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)
10:L:40:GLY:O	10:L:114:SER:OG[3_665]	2.17	0.03

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%)	685 (93%)	39 (5%)	12 (2%)	7	37
2	B	737/740 (100%)	691 (94%)	37 (5%)	9 (1%)	10	42
3	C	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	9	41
4	D	136/138 (99%)	123 (90%)	8 (6%)	5 (4%)	2	19
5	E	67/75 (89%)	53 (79%)	6 (9%)	8 (12%)	0	5
6	F	139/164 (85%)	127 (91%)	8 (6%)	4 (3%)	3	23
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	42/83 (51%)	30 (71%)	5 (12%)	7 (17%)	0	3
10	L	149/154 (97%)	138 (93%)	9 (6%)	2 (1%)	9	41
11	M	29/31 (94%)	26 (90%)	2 (7%)	1 (3%)	3	20
12	X	27/35 (77%)	21 (78%)	5 (18%)	1 (4%)	2	19
All	All	2215/2334 (95%)	2039 (92%)	126 (6%)	50 (2%)	5	28

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	VAL
1	A	235	ASP
2	B	211	PHE
2	B	234	GLN
2	B	480	LEU

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%)	561 (95%)	28 (5%)	23	45
2	B	595/597 (100%)	565 (95%)	30 (5%)	22	43
3	C	67/67 (100%)	64 (96%)	3 (4%)	24	46
4	D	115/115 (100%)	107 (93%)	8 (7%)	14	36
5	E	59/64 (92%)	57 (97%)	2 (3%)	32	54
6	F	109/128 (85%)	105 (96%)	4 (4%)	30	51
7	I	32/32 (100%)	30 (94%)	2 (6%)	16	38
8	J	36/36 (100%)	35 (97%)	1 (3%)	38	59
10	L	117/119 (98%)	108 (92%)	9 (8%)	12	32
11	M	26/26 (100%)	23 (88%)	3 (12%)	5	19
12	X	20/24 (83%)	19 (95%)	1 (5%)	22	43
All	All	1765/1811 (98%)	1674 (95%)	91 (5%)	21	43

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	698	ARG
6	F	1	ASP
3	C	65	ARG
4	D	104	LYS
7	I	10	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	228	ASN
2	B	261	HIS
10	L	119	GLN
4	D	127	GLN
5	E	18	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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	J	1102	8	49,53,73	1.77	12 (24%)	58,89,113	2.04	7 (12%)
13	CLA	B	828	-	49,53,73	1.80	16 (32%)	58,89,113	1.96	7 (12%)
15	BCR	L	1006	-	41,41,41	2.13	21 (51%)	56,56,56	2.04	22 (39%)
15	BCR	L	1005	-	41,41,41	2.10	20 (48%)	56,56,56	2.28	24 (42%)
15	BCR	B	841	-	41,41,41	2.12	20 (48%)	56,56,56	2.13	22 (39%)
13	CLA	A	855	-	49,53,73	1.79	13 (26%)	58,89,113	2.03	9 (15%)
18	LMG	B	848	-	55,55,55	1.06	8 (14%)	63,63,63	1.22	3 (4%)
13	CLA	A	842	-	69,73,73	1.66	18 (26%)	82,113,113	1.63	9 (10%)
13	CLA	B	802	-	69,73,73	1.65	18 (26%)	82,113,113	2.08	13 (15%)
13	CLA	A	803	-	69,73,73	1.62	16 (23%)	82,113,113	1.74	12 (14%)
13	CLA	A	833	-	69,73,73	1.62	17 (24%)	82,113,113	1.71	8 (9%)
14	PQN	B	840	-	34,34,34	0.92	1 (2%)	43,45,45	1.40	5 (11%)
13	CLA	A	835	-	58,62,73	1.76	18 (31%)	68,99,113	1.81	7 (10%)
13	CLA	B	816	-	64,68,73	1.69	17 (26%)	76,107,113	1.84	13 (17%)
13	CLA	F	1301	-	49,53,73	1.84	13 (26%)	58,89,113	2.11	11 (18%)
13	CLA	A	823	-	55,59,73	1.79	16 (29%)	64,96,113	1.84	9 (14%)
13	CLA	B	820	-	59,63,73	1.74	16 (27%)	70,101,113	1.83	10 (14%)
15	BCR	A	847	-	41,41,41	2.14	21 (51%)	56,56,56	2.07	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	806	-	69,73,73	1.60	15 (21%)	82,113,113	1.76	12 (14%)
16	LHG	A	853	-	48,48,48	0.94	2 (4%)	51,54,54	1.07	2 (3%)
13	CLA	A	836	1	49,53,73	1.79	13 (26%)	58,89,113	1.94	6 (10%)
15	BCR	B	845	-	41,41,41	2.10	18 (43%)	56,56,56	2.39	22 (39%)
15	BCR	J	1104	-	41,41,41	2.14	20 (48%)	56,56,56	2.27	23 (41%)
13	CLA	B	836	-	69,73,73	1.63	18 (26%)	82,113,113	1.81	11 (13%)
13	CLA	B	814	-	59,63,73	1.70	15 (25%)	70,101,113	2.02	12 (17%)
13	CLA	B	818	-	51,55,73	1.80	15 (29%)	60,91,113	1.84	5 (8%)
13	CLA	A	811	13	69,73,73	1.62	16 (23%)	82,113,113	1.90	11 (13%)
13	CLA	A	839	-	51,55,73	1.73	11 (21%)	60,91,113	2.10	8 (13%)
13	CLA	A	827	-	69,73,73	1.61	16 (23%)	82,113,113	1.84	11 (13%)
13	CLA	B	823	-	50,54,73	1.81	13 (26%)	59,90,113	1.99	11 (18%)
13	CLA	B	822	-	58,62,73	1.80	18 (31%)	68,99,113	2.03	10 (14%)
13	CLA	A	830	-	69,73,73	1.57	16 (23%)	82,113,113	1.90	12 (14%)
16	LHG	X	101	-	22,22,48	1.35	2 (9%)	25,28,54	1.03	1 (4%)
13	CLA	B	827	-	69,73,73	1.60	16 (23%)	82,113,113	1.95	13 (15%)
15	BCR	M	1203	-	41,41,41	2.09	18 (43%)	56,56,56	2.30	21 (37%)
13	CLA	A	808	1	69,73,73	1.66	15 (21%)	82,113,113	2.06	12 (14%)
17	SF4	C	101	3	0,12,12	-	-	-	-	-
15	BCR	B	842	-	41,41,41	2.16	21 (51%)	56,56,56	2.29	19 (33%)
15	BCR	B	849	-	41,41,41	2.04	18 (43%)	56,56,56	2.36	20 (35%)
13	CLA	B	809	-	49,53,73	1.78	14 (28%)	58,89,113	2.05	9 (15%)
13	CLA	B	837	-	51,55,73	1.75	15 (29%)	60,91,113	1.98	8 (13%)
15	BCR	A	848	-	41,41,41	2.14	20 (48%)	56,56,56	2.15	21 (37%)
13	CLA	A	841	-	55,59,73	1.79	13 (23%)	64,96,113	1.86	8 (12%)
17	SF4	C	102	3	0,12,12	-	-	-	-	-
13	CLA	A	809	1	69,73,73	1.64	17 (24%)	82,113,113	2.01	16 (19%)
13	CLA	A	825	-	69,73,73	1.62	16 (23%)	82,113,113	1.86	11 (13%)
17	SF4	A	856	1,2	0,12,12	-	-	-	-	-
13	CLA	A	826	-	69,73,73	1.65	15 (21%)	82,113,113	1.83	13 (15%)
13	CLA	L	1003	-	69,73,73	1.62	17 (24%)	82,113,113	1.95	14 (17%)
13	CLA	A	818	-	58,62,73	1.75	16 (27%)	68,99,113	2.06	10 (14%)
15	BCR	A	851	-	41,41,41	2.12	20 (48%)	56,56,56	2.18	19 (33%)
15	BCR	A	852	-	41,41,41	2.15	21 (51%)	56,56,56	2.29	19 (33%)
13	CLA	A	844	-	45,49,73	1.82	13 (28%)	54,83,113	1.67	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	812	-	69,73,73	1.63	18 (26%)	82,113,113	1.90	10 (12%)
15	BCR	I	102	-	41,41,41	2.02	17 (41%)	56,56,56	2.35	24 (42%)
13	CLA	B	825	-	69,73,73	1.64	15 (21%)	82,113,113	1.73	8 (9%)
14	PQN	A	846	-	34,34,34	0.99	1 (2%)	43,45,45	1.21	4 (9%)
15	BCR	B	847	-	41,41,41	2.12	20 (48%)	56,56,56	2.29	21 (37%)
13	CLA	A	843	-	69,73,73	1.60	16 (23%)	82,113,113	1.87	12 (14%)
13	CLA	J	1101	-	69,73,73	1.61	14 (20%)	82,113,113	1.88	14 (17%)
13	CLA	A	832	-	69,73,73	1.62	17 (24%)	82,113,113	1.93	11 (13%)
13	CLA	A	812	-	58,62,73	1.74	16 (27%)	68,99,113	2.09	12 (17%)
15	BCR	A	849	-	41,41,41	2.03	18 (43%)	56,56,56	2.25	23 (41%)
13	CLA	A	829	-	69,73,73	1.60	18 (26%)	82,113,113	1.93	12 (14%)
13	CLA	B	833	-	49,53,73	1.78	13 (26%)	58,89,113	2.10	5 (8%)
13	CLA	X	102	12	49,53,73	1.81	15 (30%)	58,89,113	2.21	8 (13%)
13	CLA	B	813	-	49,53,73	1.81	14 (28%)	58,89,113	2.05	9 (15%)
13	CLA	B	826	-	69,73,73	1.62	17 (24%)	82,113,113	1.66	7 (8%)
13	CLA	B	808	2	69,73,73	1.63	15 (21%)	82,113,113	1.88	10 (12%)
13	CLA	B	804	-	69,73,73	1.61	16 (23%)	82,113,113	1.80	11 (13%)
13	CLA	B	815	-	63,67,73	1.70	17 (26%)	74,105,113	1.75	10 (13%)
13	CLA	A	831	-	54,58,73	1.80	16 (29%)	64,95,113	1.92	9 (14%)
15	BCR	F	1302	-	41,41,41	2.10	21 (51%)	56,56,56	2.22	21 (37%)
13	CLA	B	831	-	62,66,73	1.71	16 (25%)	73,104,113	2.10	12 (16%)
13	CLA	A	819	-	69,73,73	1.59	17 (24%)	82,113,113	2.03	13 (15%)
13	CLA	L	1002	10	69,73,73	1.62	18 (26%)	82,113,113	1.86	11 (13%)
13	CLA	A	821	-	69,73,73	1.61	17 (24%)	82,113,113	1.93	11 (13%)
13	CLA	B	819	-	49,53,73	1.79	15 (30%)	58,89,113	2.03	8 (13%)
13	CLA	A	801	-	69,73,73	1.65	18 (26%)	82,113,113	1.83	13 (15%)
13	CLA	A	845	16	56,60,73	1.74	16 (28%)	65,97,113	2.12	14 (21%)
13	CLA	I	101	-	69,73,73	1.65	18 (26%)	82,113,113	1.91	14 (17%)
15	BCR	B	843	-	41,41,41	2.09	21 (51%)	56,56,56	2.42	26 (46%)
13	CLA	B	801	-	69,73,73	1.63	18 (26%)	82,113,113	1.80	11 (13%)
13	CLA	A	805	-	69,73,73	1.61	17 (24%)	82,113,113	1.77	9 (10%)
13	CLA	B	824	-	69,73,73	1.62	15 (21%)	82,113,113	1.84	11 (13%)
13	CLA	B	835	-	64,68,73	1.72	15 (23%)	76,107,113	1.89	15 (19%)
13	CLA	B	810	-	49,53,73	1.80	15 (30%)	58,89,113	1.87	7 (12%)
13	CLA	A	837	-	55,59,73	1.84	15 (27%)	64,96,113	2.08	14 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	805	-	69,73,73	1.59	16 (23%)	82,113,113	1.77	10 (12%)
13	CLA	B	838	-	69,73,73	1.63	15 (21%)	82,113,113	1.92	13 (15%)
13	CLA	M	1201	-	58,62,73	1.76	17 (29%)	68,99,113	2.09	13 (19%)
15	BCR	A	850	-	41,41,41	2.18	21 (51%)	56,56,56	2.20	20 (35%)
13	CLA	A	804	13	63,67,73	1.71	16 (25%)	74,105,113	1.82	10 (13%)
13	CLA	A	807	-	55,59,73	1.80	15 (27%)	64,96,113	2.12	11 (17%)
15	BCR	B	850	-	41,41,41	2.13	21 (51%)	56,56,56	2.38	23 (41%)
13	CLA	A	840	-	69,73,73	1.61	17 (24%)	82,113,113	1.89	12 (14%)
13	CLA	B	829	-	53,57,73	1.73	14 (26%)	61,93,113	1.84	11 (18%)
13	CLA	B	832	-	49,53,73	1.79	14 (28%)	58,89,113	2.01	9 (15%)
13	CLA	A	816	-	53,57,73	1.74	13 (24%)	61,93,113	1.89	8 (13%)
13	CLA	B	830	-	69,73,73	1.61	16 (23%)	82,113,113	1.87	9 (10%)
13	CLA	M	1202	-	49,53,73	1.77	13 (26%)	58,89,113	2.12	9 (15%)
13	CLA	B	806	-	69,73,73	1.63	17 (24%)	82,113,113	1.88	12 (14%)
13	CLA	A	820	-	65,69,73	1.70	18 (27%)	77,108,113	1.82	13 (16%)
13	CLA	L	1004	-	69,73,73	1.61	16 (23%)	82,113,113	1.86	10 (12%)
13	CLA	A	813	-	64,68,73	1.66	15 (23%)	76,107,113	1.91	11 (14%)
13	CLA	B	821	-	49,53,73	1.81	13 (26%)	58,89,113	1.85	9 (15%)
13	CLA	J	1103	-	41,45,73	1.96	13 (31%)	50,78,113	1.68	4 (8%)
15	BCR	B	844	-	25,25,41	2.19	13 (52%)	33,33,56	2.12	12 (36%)
13	CLA	B	807	-	69,73,73	1.64	18 (26%)	82,113,113	1.92	11 (13%)
15	BCR	J	1105	-	41,41,41	2.14	20 (48%)	56,56,56	2.16	22 (39%)
13	CLA	A	814	-	49,53,73	1.80	15 (30%)	58,89,113	1.92	9 (15%)
13	CLA	A	824	-	63,67,73	1.70	18 (28%)	74,105,113	1.99	13 (17%)
13	CLA	A	810	-	49,53,73	1.76	13 (26%)	58,89,113	2.12	8 (13%)
13	CLA	A	817	-	58,62,73	1.75	15 (25%)	68,99,113	1.83	11 (16%)
16	LHG	A	854	13	26,26,48	1.27	2 (7%)	29,32,54	1.17	2 (6%)
13	CLA	B	839	-	69,73,73	1.61	17 (24%)	82,113,113	1.78	11 (13%)
13	CLA	A	834	-	69,73,73	1.66	19 (27%)	82,113,113	1.75	9 (10%)
13	CLA	B	817	-	69,73,73	1.62	17 (24%)	82,113,113	1.88	9 (10%)
15	BCR	B	846	-	41,41,41	2.13	20 (48%)	56,56,56	2.09	19 (33%)
13	CLA	A	828	-	69,73,73	1.60	15 (21%)	82,113,113	1.84	11 (13%)
13	CLA	A	822	-	53,57,73	1.78	13 (24%)	61,93,113	2.21	9 (14%)
13	CLA	B	834	-	49,53,73	1.78	13 (26%)	58,89,113	2.04	8 (13%)
13	CLA	A	838	-	69,73,73	1.64	19 (27%)	82,113,113	1.89	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	803	-	69,73,73	1.63	18 (26%)	82,113,113	1.78	10 (12%)
13	CLA	A	802	-	69,73,73	1.65	18 (26%)	82,113,113	1.71	7 (8%)
13	CLA	A	815	-	49,53,73	1.77	14 (28%)	58,89,113	2.06	11 (18%)
13	CLA	B	811	-	69,73,73	1.65	16 (23%)	82,113,113	1.85	9 (10%)

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	J	1102	8	1/1/11/20	5/15/91/115	-
13	CLA	B	828	-	1/1/11/20	5/15/91/115	-
15	BCR	L	1006	-	-	8/29/63/63	0/2/2/2
15	BCR	L	1005	-	-	9/29/63/63	0/2/2/2
15	BCR	B	841	-	-	8/29/63/63	0/2/2/2
13	CLA	A	855	-	1/1/11/20	2/15/91/115	-
18	LMG	B	848	-	-	11/50/70/70	0/1/1/1
13	CLA	A	842	-	1/1/15/20	16/39/115/115	-
13	CLA	B	802	-	1/1/15/20	12/39/115/115	-
13	CLA	A	803	-	1/1/15/20	8/39/115/115	-
13	CLA	A	833	-	1/1/15/20	8/39/115/115	-
14	PQN	B	840	-	-	5/23/43/43	0/2/2/2
13	CLA	A	835	-	1/1/12/20	7/26/102/115	-
13	CLA	B	816	-	1/1/14/20	6/33/109/115	-
13	CLA	F	1301	-	-	5/15/91/115	-
13	CLA	A	823	-	1/1/12/20	4/23/99/115	-
13	CLA	B	820	-	1/1/13/20	8/27/103/115	-
15	BCR	A	847	-	-	8/29/63/63	0/2/2/2
13	CLA	A	806	-	1/1/15/20	8/39/115/115	-
16	LHG	A	853	-	-	20/53/53/53	-
13	CLA	A	836	1	1/1/11/20	6/15/91/115	-
15	BCR	B	845	-	-	10/29/63/63	0/2/2/2
15	BCR	J	1104	-	-	11/29/63/63	0/2/2/2
13	CLA	B	836	-	1/1/15/20	11/39/115/115	-
13	CLA	B	814	-	1/1/13/20	6/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	818	-	1/1/11/20	4/18/94/115	-
13	CLA	A	811	13	1/1/15/20	15/39/115/115	-
13	CLA	A	839	-	1/1/11/20	5/18/94/115	-
13	CLA	A	827	-	1/1/15/20	10/39/115/115	-
13	CLA	B	823	-	1/1/11/20	3/17/93/115	-
13	CLA	B	822	-	1/1/12/20	9/26/102/115	-
13	CLA	A	830	-	1/1/15/20	10/39/115/115	-
16	LHG	X	101	-	-	8/26/26/53	-
13	CLA	B	827	-	1/1/15/20	8/39/115/115	-
15	BCR	M	1203	-	-	15/29/63/63	0/2/2/2
13	CLA	A	808	1	1/1/15/20	12/39/115/115	-
17	SF4	C	101	3	-	-	0/6/5/5
15	BCR	B	842	-	-	12/29/63/63	0/2/2/2
15	BCR	B	849	-	-	14/29/63/63	0/2/2/2
13	CLA	B	809	-	1/1/11/20	4/15/91/115	-
13	CLA	B	837	-	1/1/11/20	5/18/94/115	-
15	BCR	A	848	-	-	11/29/63/63	0/2/2/2
13	CLA	A	841	-	1/1/12/20	5/23/99/115	-
17	SF4	C	102	3	-	-	0/6/5/5
13	CLA	A	809	1	-	10/39/115/115	-
13	CLA	A	825	-	1/1/15/20	6/39/115/115	-
17	SF4	A	856	1,2	-	-	0/6/5/5
13	CLA	A	826	-	-	8/39/115/115	-
13	CLA	L	1003	-	1/1/15/20	15/39/115/115	-
13	CLA	A	818	-	1/1/12/20	7/26/102/115	-
15	BCR	A	851	-	-	8/29/63/63	0/2/2/2
15	BCR	A	852	-	-	12/29/63/63	0/2/2/2
13	CLA	A	844	-	-	4/9/81/115	-
13	CLA	B	812	-	1/1/15/20	12/39/115/115	-
15	BCR	I	102	-	-	15/29/63/63	0/2/2/2
13	CLA	B	825	-	1/1/15/20	11/39/115/115	-
14	PQN	A	846	-	-	6/23/43/43	0/2/2/2
15	BCR	B	847	-	-	12/29/63/63	0/2/2/2
13	CLA	A	843	-	1/1/15/20	8/39/115/115	-
13	CLA	J	1101	-	1/1/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	832	-	1/1/15/20	17/39/115/115	-
13	CLA	A	812	-	1/1/12/20	9/26/102/115	-
15	BCR	A	849	-	-	5/29/63/63	0/2/2/2
13	CLA	A	829	-	1/1/15/20	10/39/115/115	-
13	CLA	B	833	-	1/1/11/20	6/15/91/115	-
13	CLA	X	102	12	1/1/11/20	7/15/91/115	-
13	CLA	B	813	-	-	5/15/91/115	-
13	CLA	B	826	-	1/1/15/20	13/39/115/115	-
13	CLA	B	808	2	1/1/15/20	9/39/115/115	-
13	CLA	B	804	-	1/1/15/20	6/39/115/115	-
13	CLA	B	815	-	1/1/13/20	9/32/108/115	-
13	CLA	A	831	-	1/1/12/20	3/21/97/115	-
15	BCR	F	1302	-	-	10/29/63/63	0/2/2/2
13	CLA	B	831	-	1/1/13/20	8/31/107/115	-
13	CLA	A	819	-	1/1/15/20	13/39/115/115	-
13	CLA	L	1002	10	1/1/15/20	10/39/115/115	-
13	CLA	A	821	-	1/1/15/20	15/39/115/115	-
13	CLA	B	819	-	1/1/11/20	2/15/91/115	-
13	CLA	A	801	-	1/1/15/20	8/39/115/115	-
13	CLA	A	845	16	1/1/12/20	5/24/100/115	-
13	CLA	I	101	-	1/1/15/20	11/39/115/115	-
15	BCR	B	843	-	-	9/29/63/63	0/2/2/2
13	CLA	B	801	-	1/1/15/20	11/39/115/115	-
13	CLA	A	805	-	1/1/15/20	9/39/115/115	-
13	CLA	B	824	-	1/1/15/20	9/39/115/115	-
13	CLA	B	835	-	1/1/14/20	9/33/109/115	-
13	CLA	B	810	-	1/1/11/20	5/15/91/115	-
13	CLA	B	805	-	1/1/15/20	7/39/115/115	-
13	CLA	B	838	-	1/1/15/20	14/39/115/115	-
13	CLA	M	1201	-	1/1/12/20	7/26/102/115	-
13	CLA	A	837	-	-	4/23/99/115	-
15	BCR	A	850	-	-	6/29/63/63	0/2/2/2
13	CLA	A	804	13	1/1/13/20	8/32/108/115	-
13	CLA	A	807	-	1/1/12/20	6/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	B	850	-	-	7/29/63/63	0/2/2/2
13	CLA	A	840	-	1/1/15/20	12/39/115/115	-
13	CLA	B	829	-	1/1/11/20	3/20/96/115	-
13	CLA	B	832	-	1/1/11/20	3/15/91/115	-
13	CLA	A	816	-	-	5/20/96/115	-
13	CLA	B	830	-	1/1/15/20	11/39/115/115	-
13	CLA	M	1202	-	-	4/15/91/115	-
13	CLA	B	806	-	1/1/15/20	12/39/115/115	-
13	CLA	A	820	-	1/1/14/20	10/35/111/115	-
13	CLA	L	1004	-	1/1/15/20	11/39/115/115	-
13	CLA	A	813	-	1/1/14/20	9/33/109/115	-
13	CLA	B	821	-	1/1/11/20	3/15/91/115	-
13	CLA	J	1103	-	1/1/8/20	2/4/76/115	-
15	BCR	B	844	-	-	6/18/35/63	0/1/1/2
13	CLA	B	807	-	1/1/15/20	16/39/115/115	-
15	BCR	J	1105	-	-	14/29/63/63	0/2/2/2
13	CLA	A	814	-	1/1/11/20	4/15/91/115	-
13	CLA	A	824	-	1/1/13/20	9/32/108/115	-
13	CLA	A	810	-	1/1/11/20	7/15/91/115	-
13	CLA	A	817	-	1/1/12/20	4/26/102/115	-
16	LHG	A	854	13	-	8/31/31/53	-
13	CLA	B	839	-	1/1/15/20	8/39/115/115	-
13	CLA	A	834	-	1/1/15/20	12/39/115/115	-
13	CLA	B	817	-	1/1/15/20	10/39/115/115	-
15	BCR	B	846	-	-	8/29/63/63	0/2/2/2
13	CLA	A	828	-	1/1/15/20	16/39/115/115	-
13	CLA	A	822	-	1/1/11/20	7/20/96/115	-
13	CLA	B	834	-	1/1/11/20	3/15/91/115	-
13	CLA	A	838	-	1/1/15/20	16/39/115/115	-
13	CLA	B	803	-	1/1/15/20	13/39/115/115	-
13	CLA	A	802	-	1/1/15/20	5/39/115/115	-
13	CLA	A	815	-	1/1/11/20	2/15/91/115	-
13	CLA	B	811	-	1/1/15/20	12/39/115/115	-

The worst 5 of 1952 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J	1103	CLA	C3A-C2A	-4.48	1.50	1.54
13	A	808	CLA	MG-ND	-4.34	1.97	2.05
13	B	802	CLA	MG-ND	-4.27	1.97	2.05
13	A	824	CLA	CHB-C1B	-4.25	1.29	1.39
13	B	822	CLA	MG-ND	-4.23	1.97	2.05

The worst 5 of 1470 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	809	CLA	C4A-NA-C1A	11.40	111.88	106.68
13	A	808	CLA	C4A-NA-C1A	11.29	111.83	106.68
13	A	830	CLA	C4A-NA-C1A	11.20	111.79	106.68
13	M	1202	CLA	C4A-NA-C1A	11.11	111.75	106.68
13	B	827	CLA	C4A-NA-C1A	11.09	111.74	106.68

5 of 88 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 1055 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	801	CLA	C2B-C3B-CAB-CBB
13	A	801	CLA	C4B-C3B-CAB-CBB
13	A	802	CLA	C4B-C3B-CAB-CBB
13	A	804	CLA	C2B-C3B-CAB-CBB
13	A	804	CLA	C4B-C3B-CAB-CBB

There are no ring outliers.

123 monomers are involved in 1016 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	J	1102	CLA	3	0
13	B	828	CLA	5	0
15	L	1006	BCR	4	0
15	L	1005	BCR	12	0
15	B	841	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	855	CLA	2	0
18	B	848	LMG	18	0
13	A	842	CLA	20	0
13	B	802	CLA	17	0
13	A	803	CLA	26	0
13	A	833	CLA	15	0
14	B	840	PQN	6	0
13	A	835	CLA	7	0
13	B	816	CLA	15	0
13	F	1301	CLA	4	0
13	A	823	CLA	13	0
13	B	820	CLA	11	0
15	A	847	BCR	5	0
13	A	806	CLA	10	0
16	A	853	LHG	9	0
13	A	836	CLA	9	0
15	B	845	BCR	7	0
15	J	1104	BCR	3	0
13	B	836	CLA	10	0
13	B	814	CLA	8	0
13	B	818	CLA	4	0
13	A	811	CLA	13	0
13	A	839	CLA	13	0
13	A	827	CLA	13	0
13	B	823	CLA	8	0
13	B	822	CLA	20	0
13	A	830	CLA	13	0
16	X	101	LHG	1	0
13	B	827	CLA	13	0
15	M	1203	BCR	11	0
13	A	808	CLA	19	0
15	B	842	BCR	4	0
15	B	849	BCR	16	0
13	B	809	CLA	6	0
13	B	837	CLA	6	0
15	A	848	BCR	5	0
13	A	841	CLA	5	0
13	A	809	CLA	12	0
13	A	825	CLA	20	0
13	A	826	CLA	16	0
13	L	1003	CLA	16	0
13	A	818	CLA	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	851	BCR	2	0
15	A	852	BCR	19	0
13	A	844	CLA	2	0
13	B	812	CLA	14	0
15	I	102	BCR	9	0
13	B	825	CLA	18	0
14	A	846	PQN	7	0
15	B	847	BCR	13	0
13	A	843	CLA	10	0
13	J	1101	CLA	12	0
13	A	832	CLA	19	0
13	A	812	CLA	3	0
15	A	849	BCR	4	0
13	A	829	CLA	9	0
13	B	833	CLA	3	0
13	X	102	CLA	4	0
13	B	813	CLA	9	0
13	B	826	CLA	17	0
13	B	808	CLA	15	0
13	B	804	CLA	16	0
13	B	815	CLA	16	0
13	A	831	CLA	9	0
15	F	1302	BCR	12	0
13	B	831	CLA	12	0
13	A	819	CLA	16	0
13	L	1002	CLA	5	0
13	A	821	CLA	12	0
13	B	819	CLA	2	0
13	A	801	CLA	12	0
13	A	845	CLA	11	0
13	I	101	CLA	15	0
15	B	843	BCR	17	0
13	B	801	CLA	12	0
13	A	805	CLA	10	0
13	B	824	CLA	18	0
13	B	835	CLA	15	0
13	B	810	CLA	6	0
13	A	837	CLA	12	0
13	B	805	CLA	8	0
13	B	838	CLA	15	0
13	M	1201	CLA	15	0
15	A	850	BCR	4	0

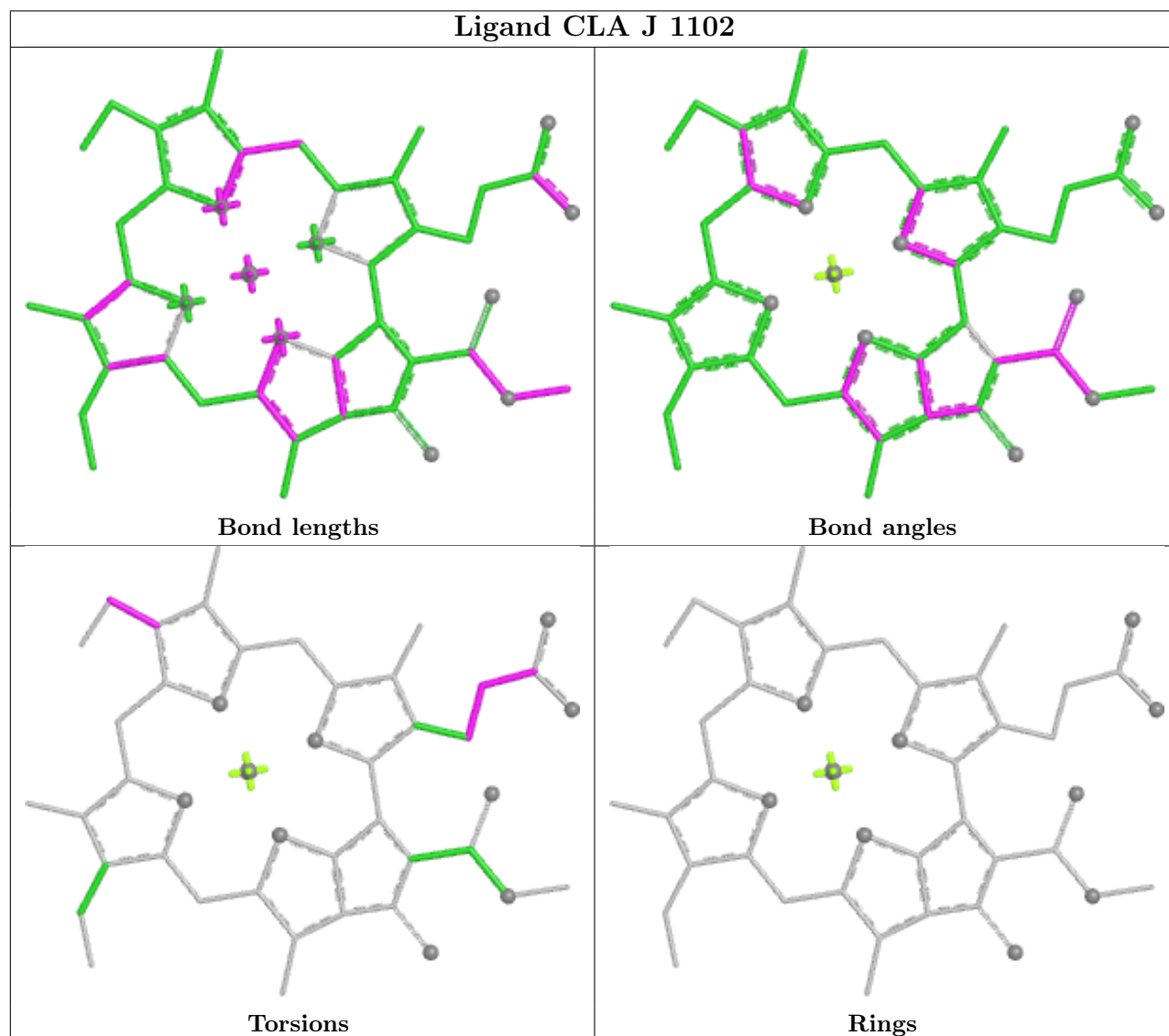
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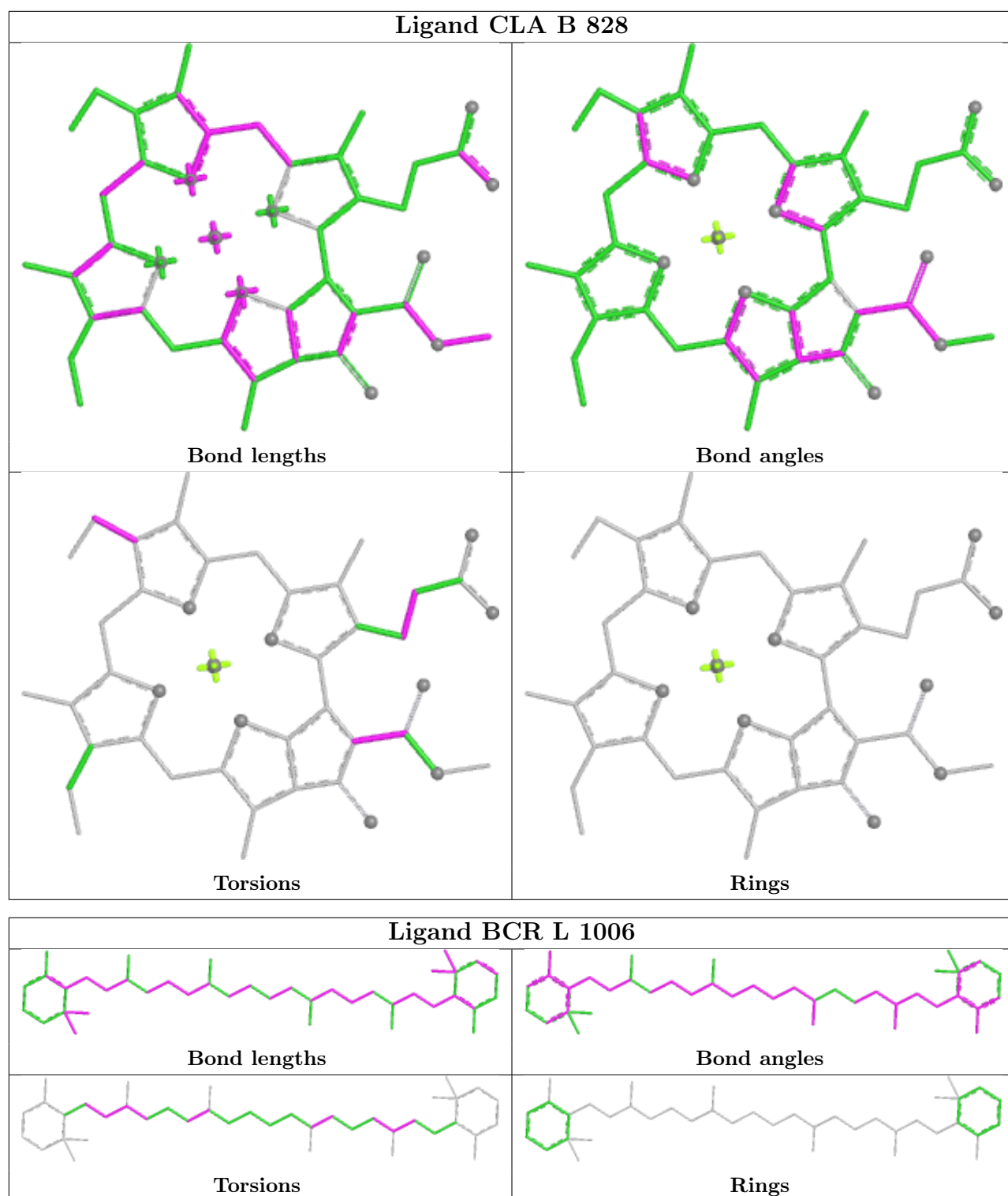
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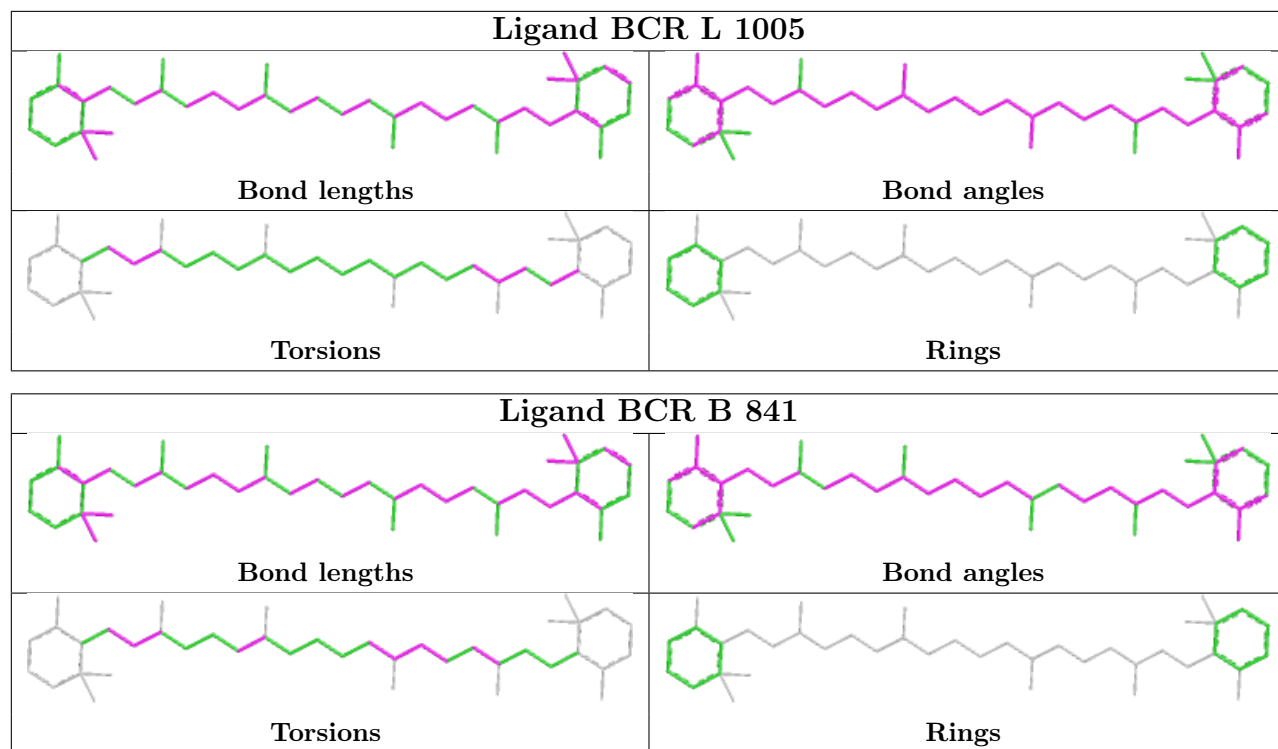
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	804	CLA	10	0
13	A	807	CLA	11	0
15	B	850	BCR	6	0
13	A	840	CLA	16	0
13	B	829	CLA	6	0
13	B	832	CLA	9	0
13	A	816	CLA	4	0
13	B	830	CLA	23	0
13	M	1202	CLA	1	0
13	B	806	CLA	14	0
13	A	820	CLA	7	0
13	L	1004	CLA	5	0
13	A	813	CLA	14	0
13	B	821	CLA	11	0
15	B	844	BCR	6	0
13	B	807	CLA	13	0
15	J	1105	BCR	6	0
13	A	814	CLA	9	0
13	A	824	CLA	6	0
13	A	810	CLA	5	0
13	A	817	CLA	8	0
16	A	854	LHG	2	0
13	B	839	CLA	7	0
13	A	834	CLA	18	0
13	B	817	CLA	14	0
15	B	846	BCR	7	0
13	A	828	CLA	15	0
13	A	822	CLA	7	0
13	B	834	CLA	4	0
13	A	838	CLA	8	0
13	B	803	CLA	16	0
13	A	802	CLA	13	0
13	A	815	CLA	6	0
13	B	811	CLA	15	0

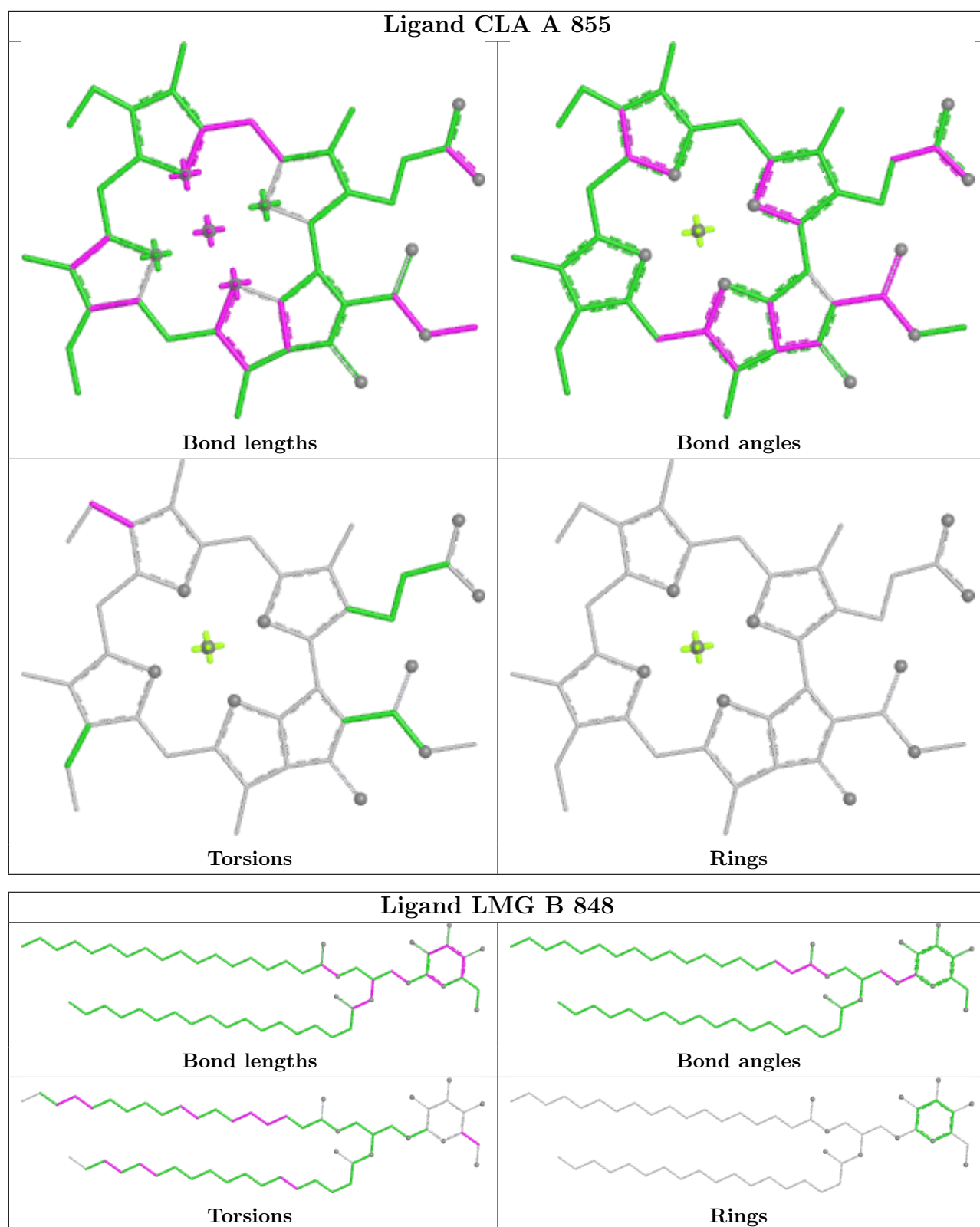
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

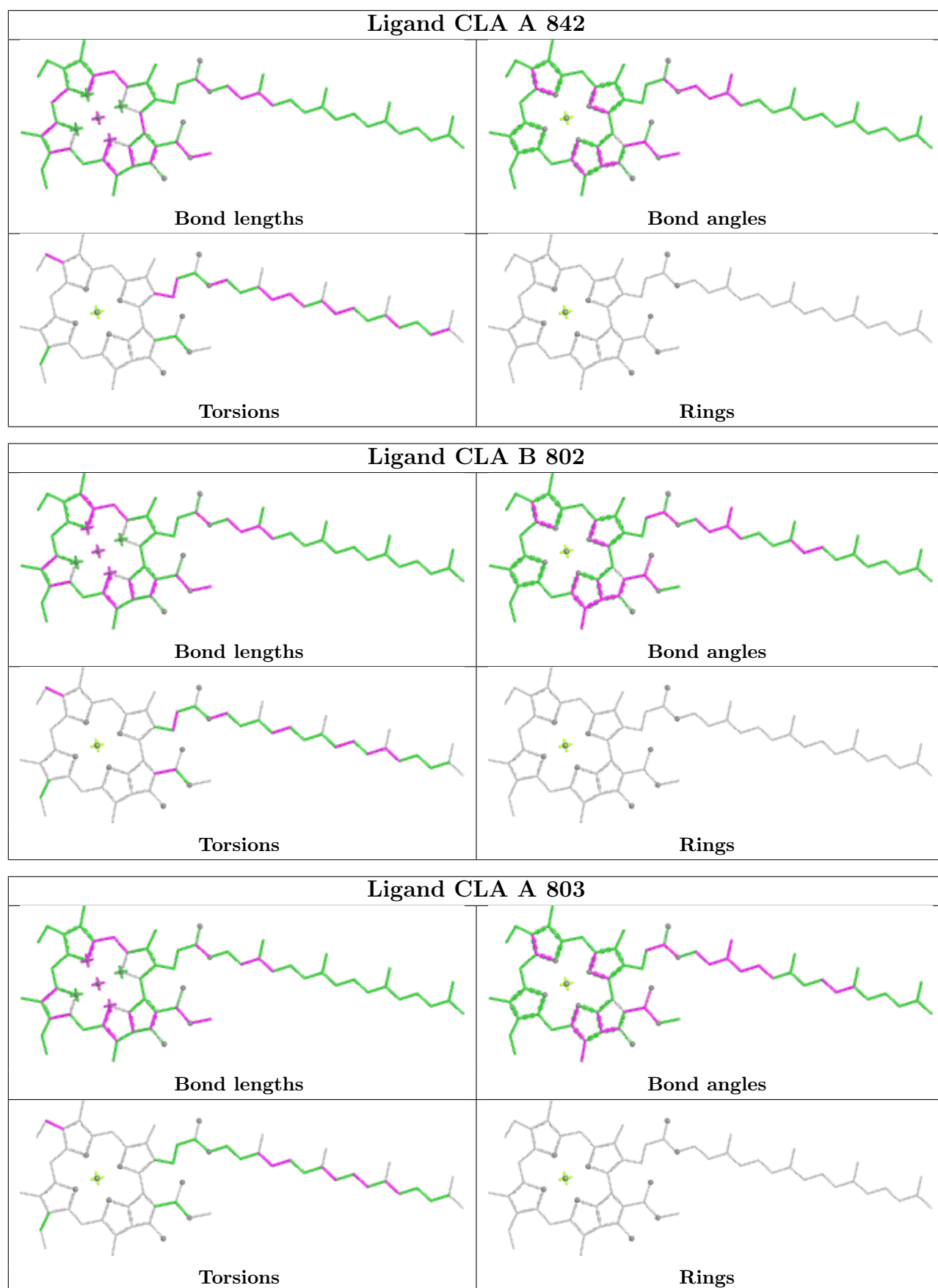
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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

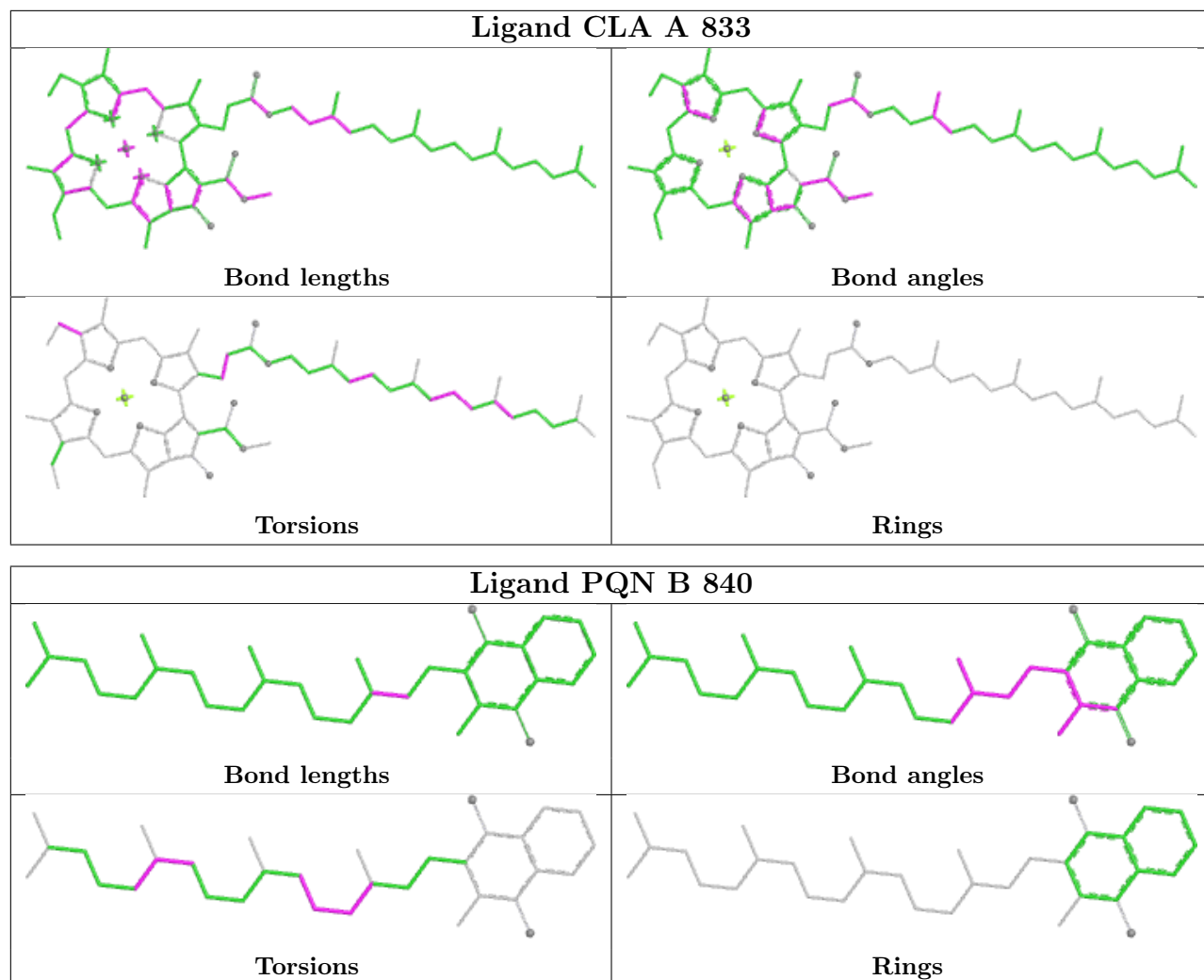


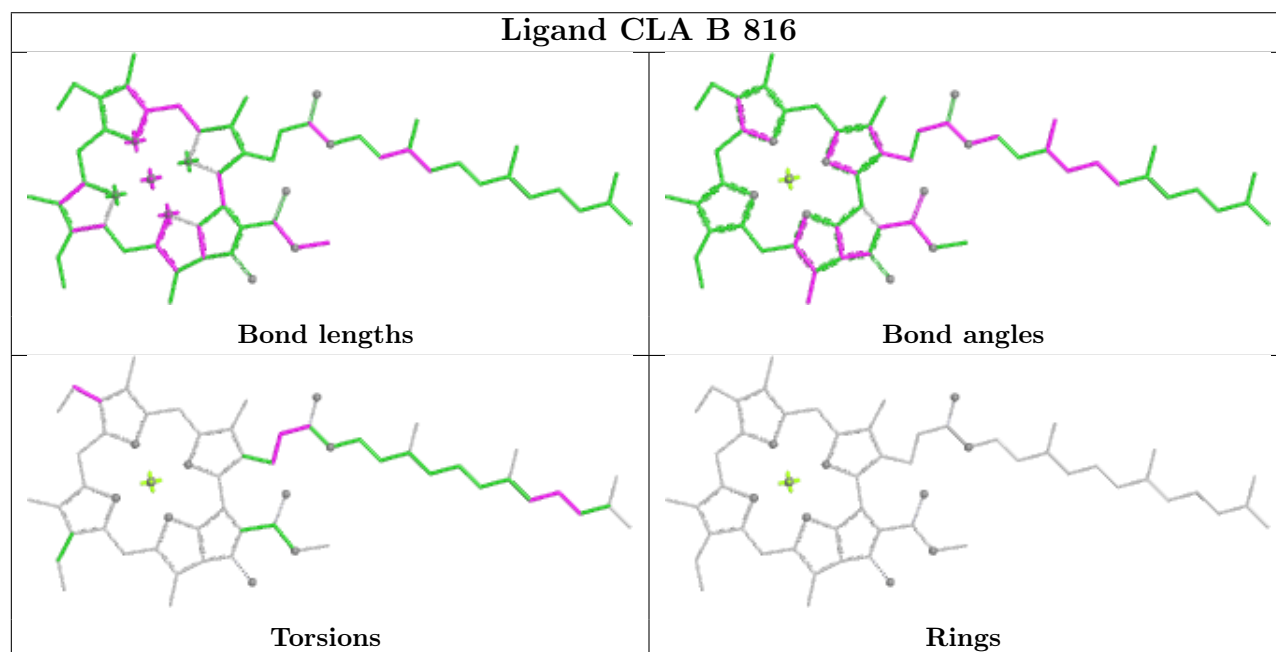
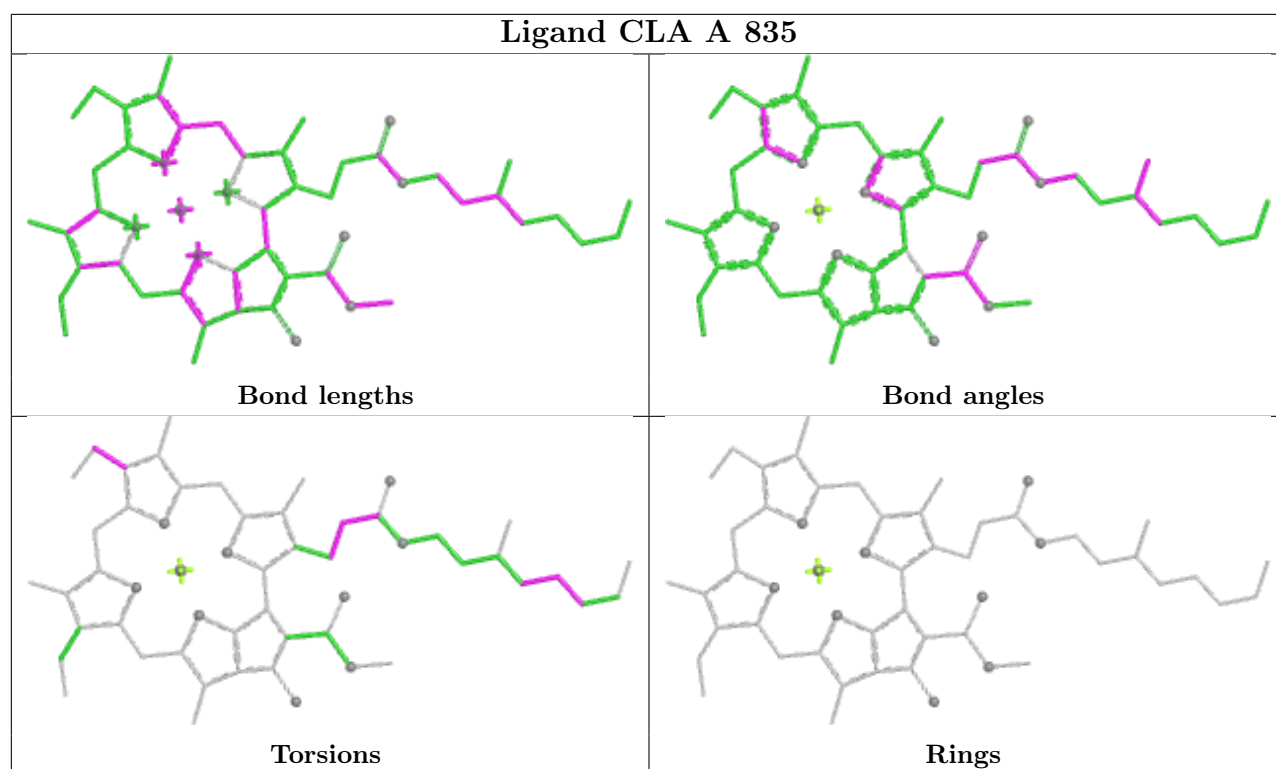


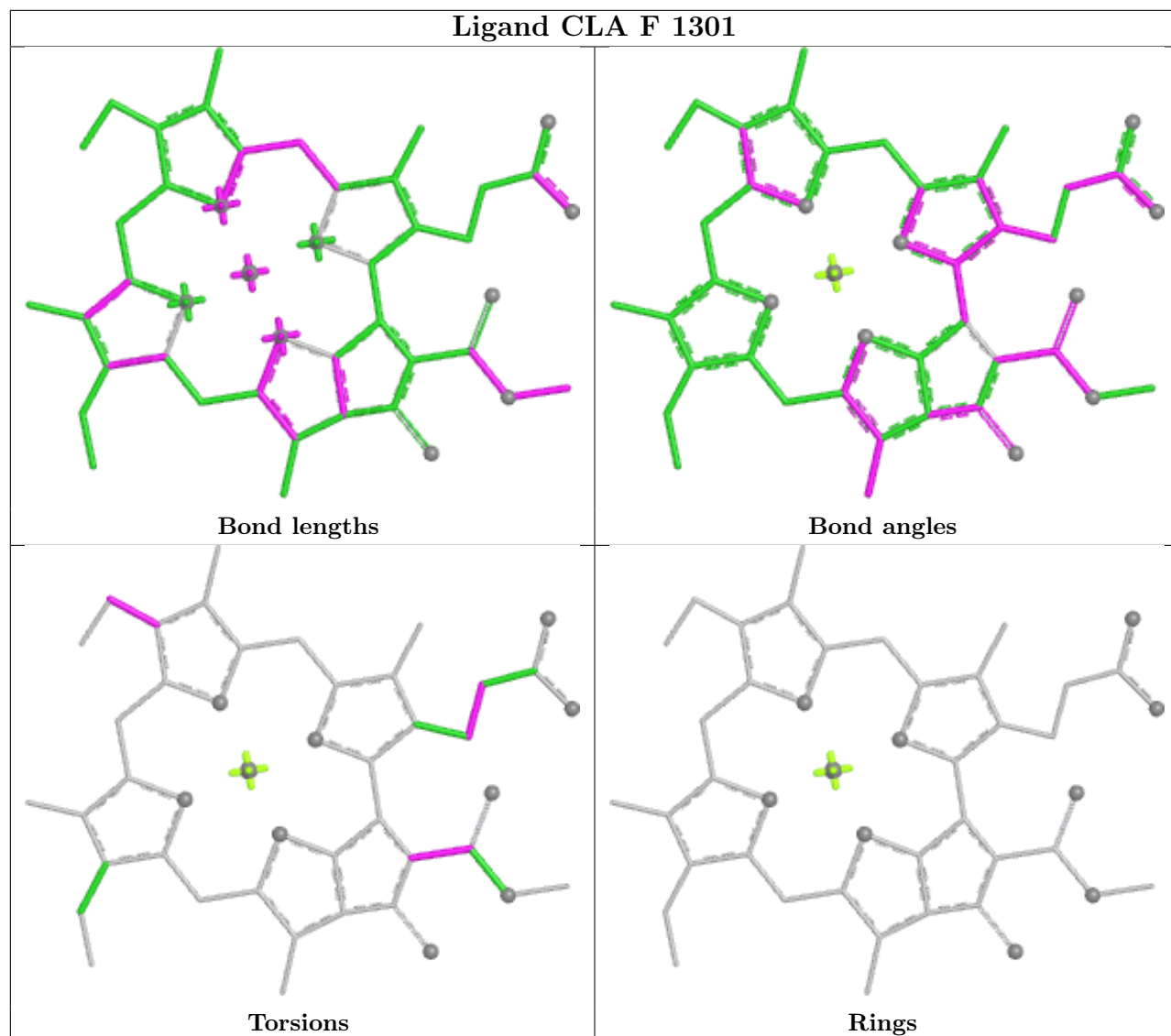


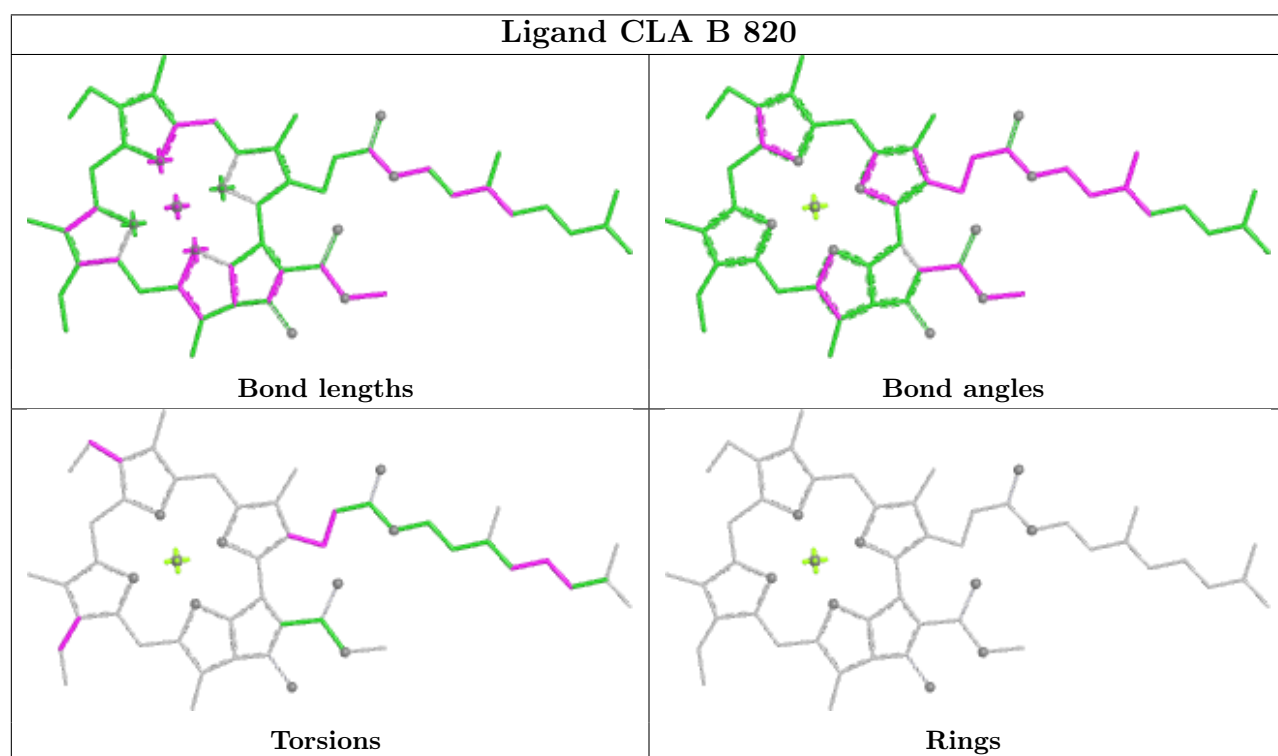
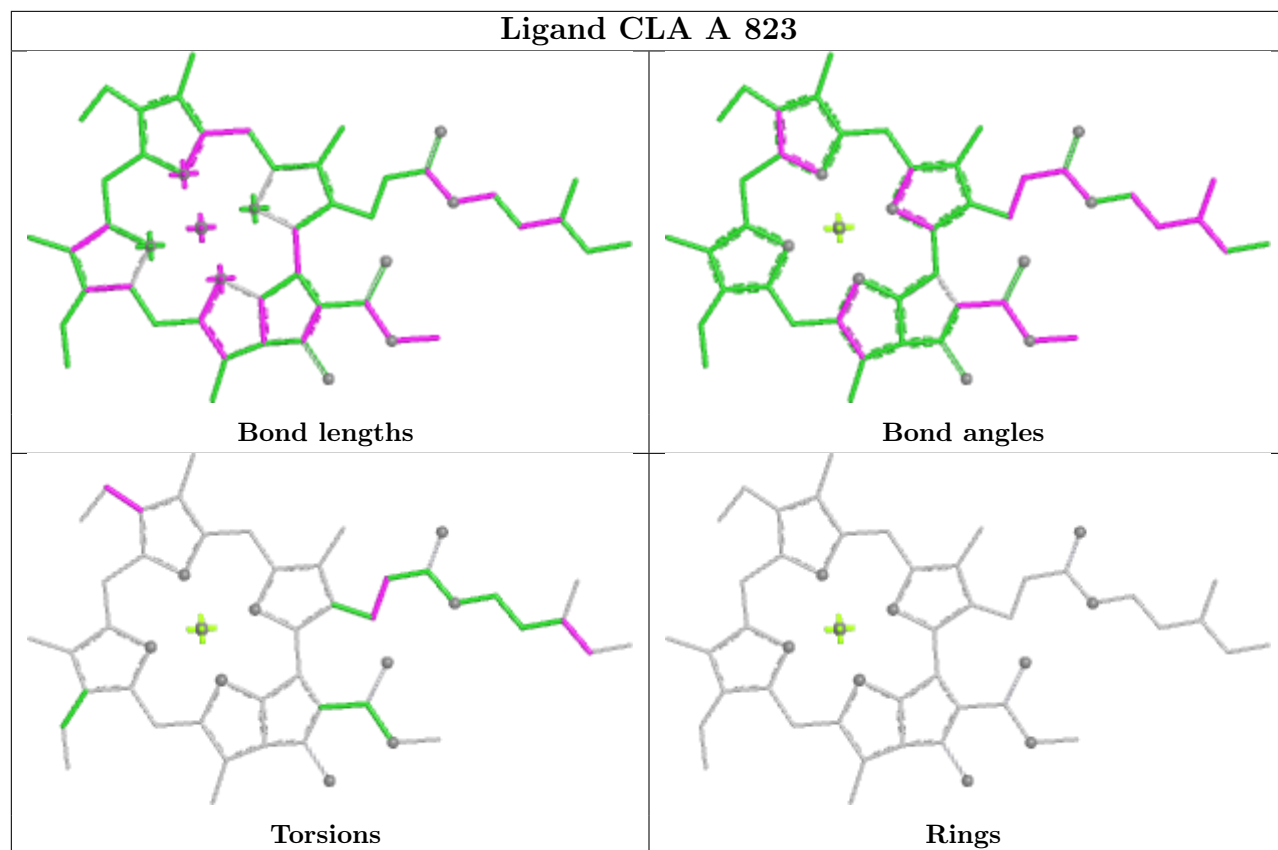


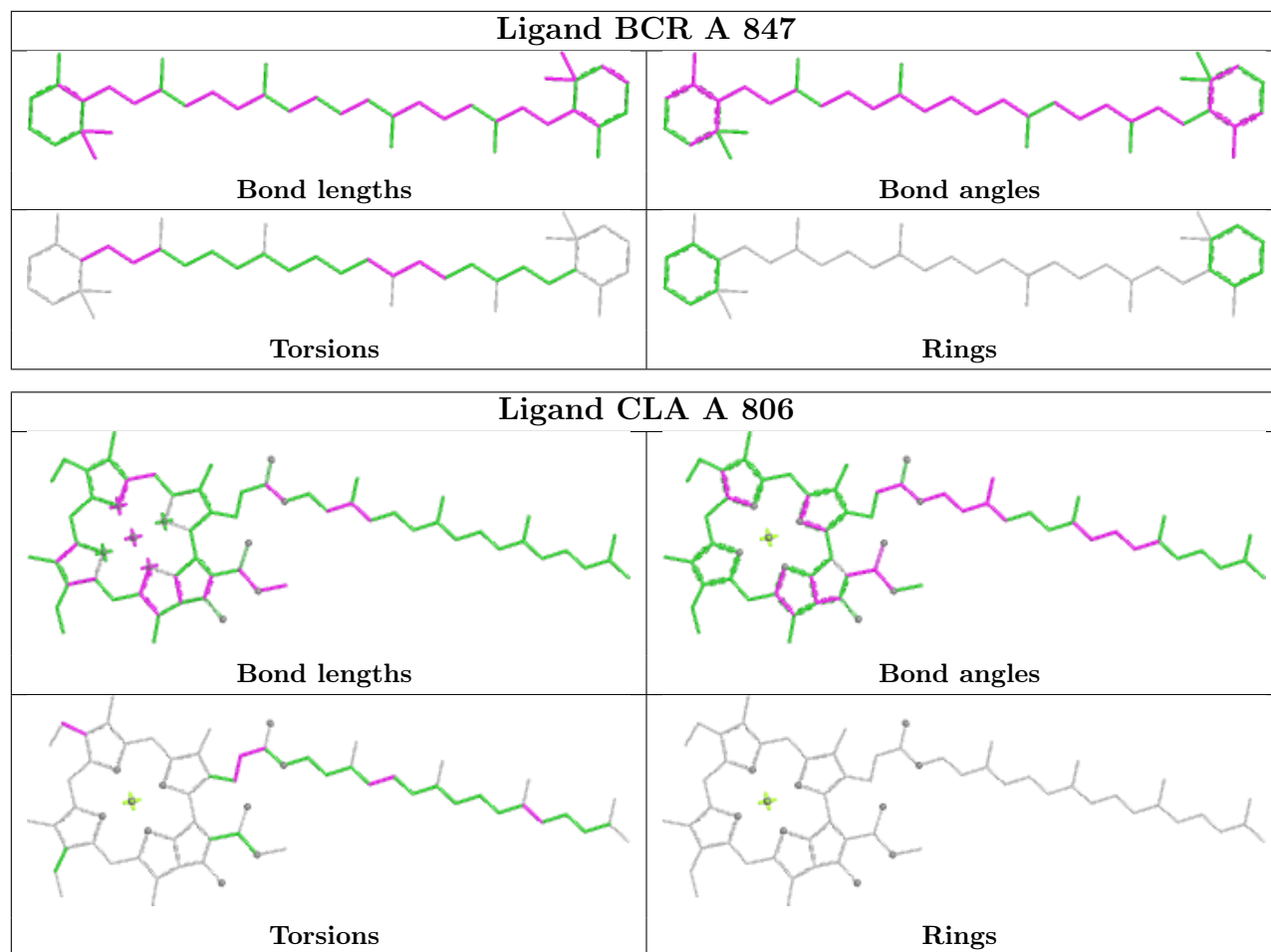


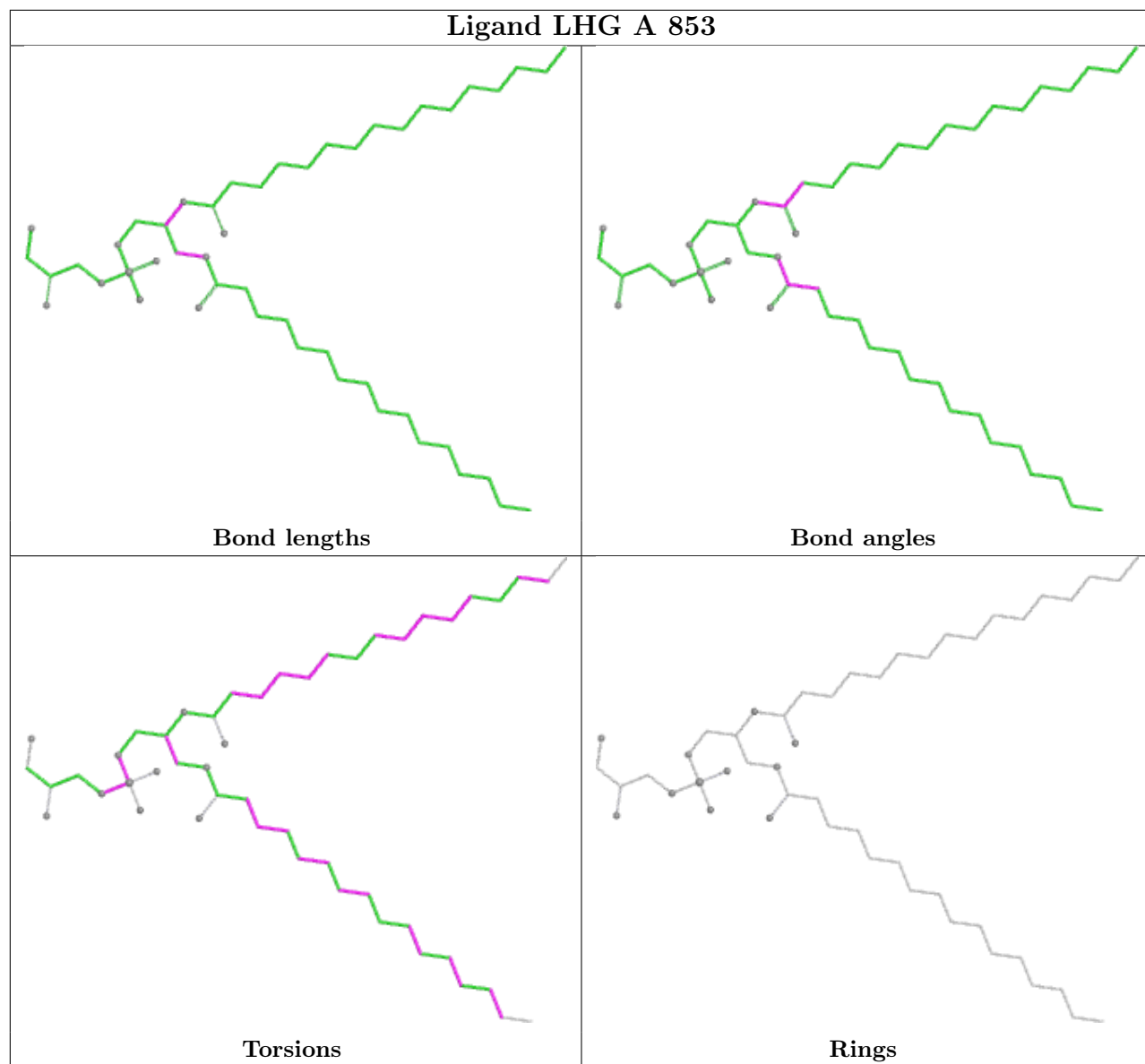


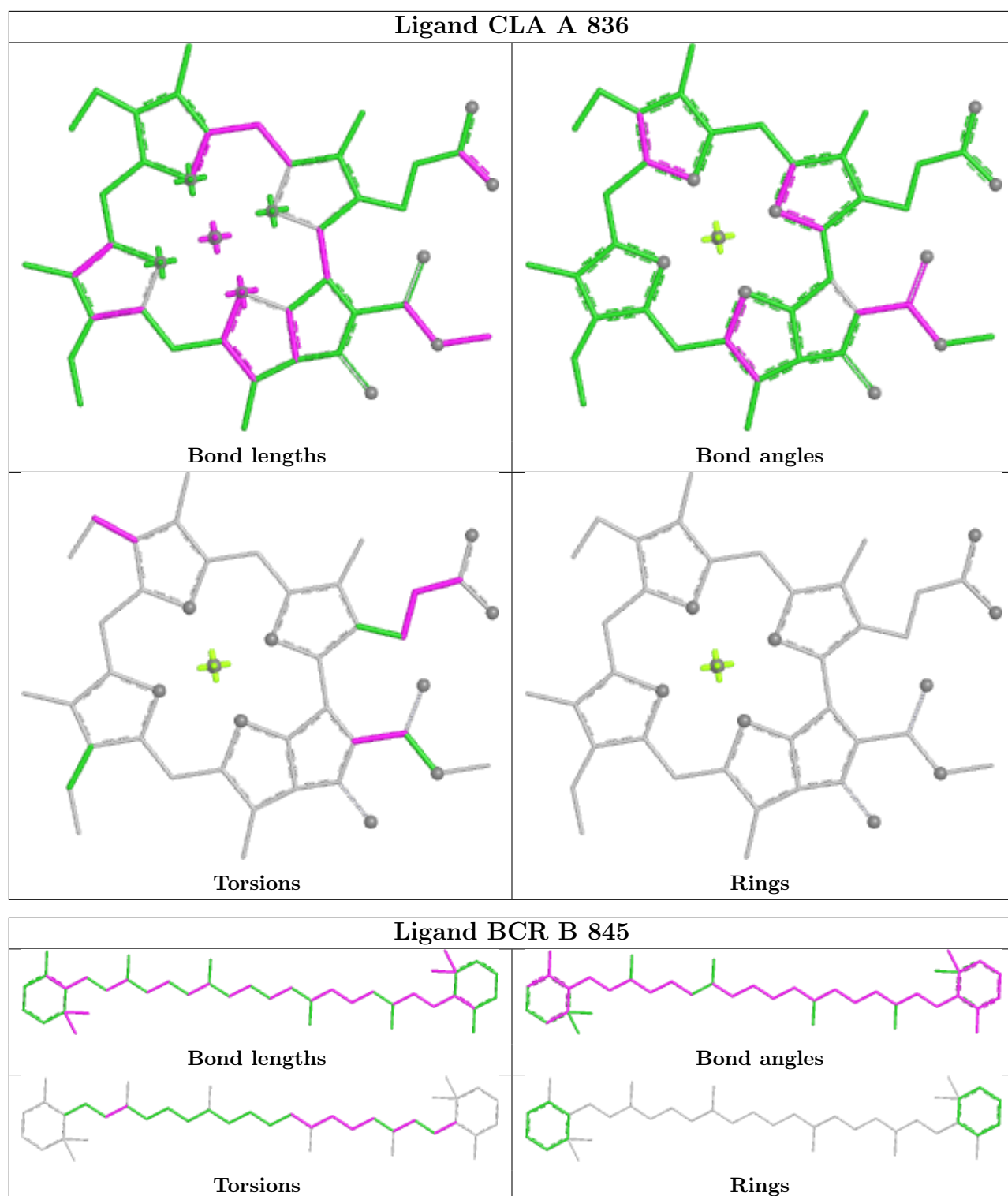


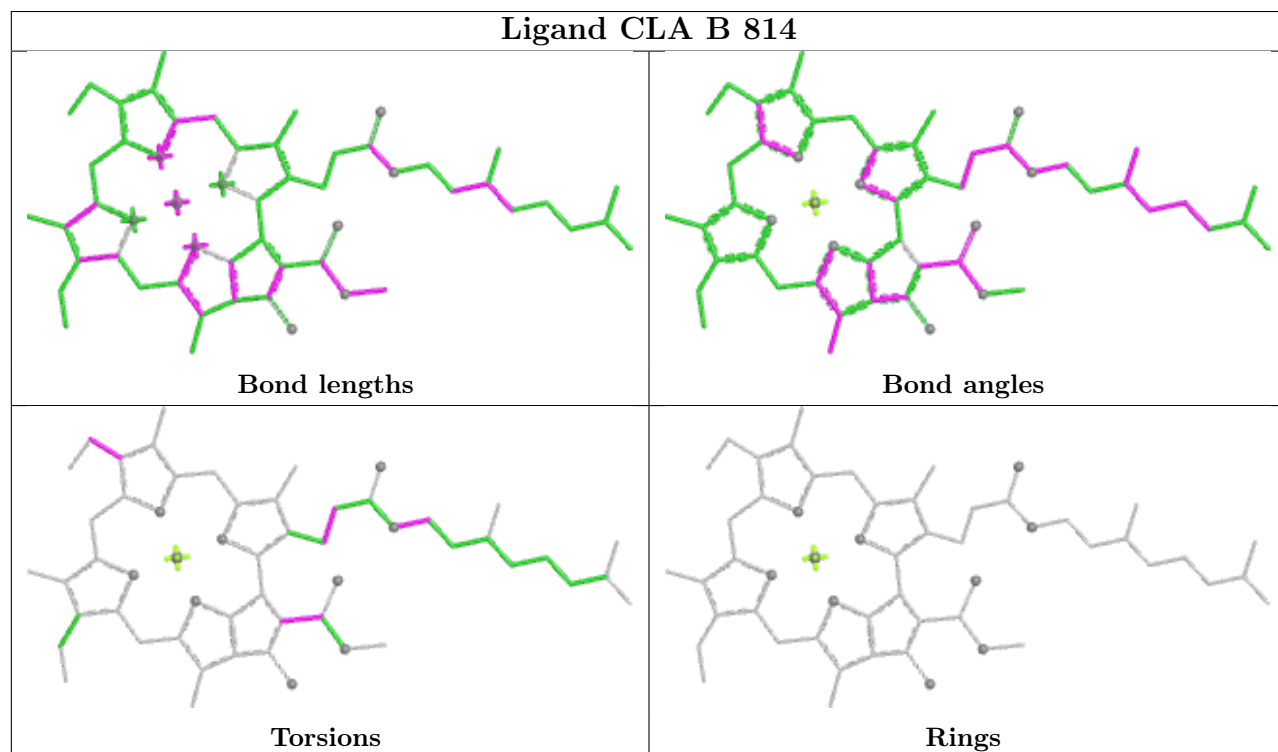
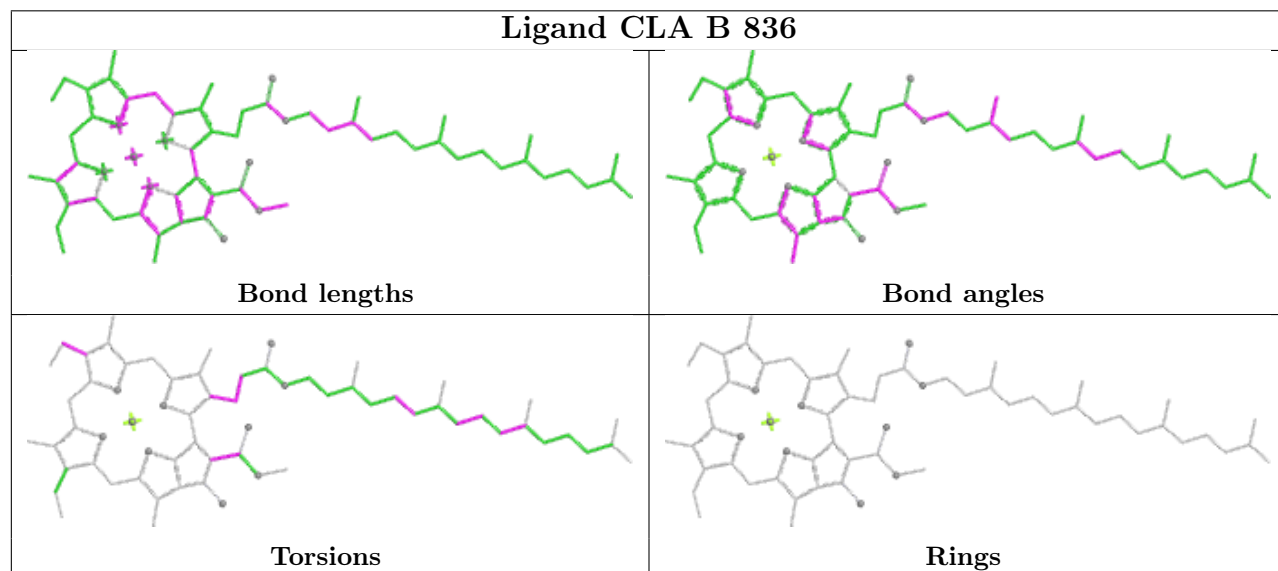
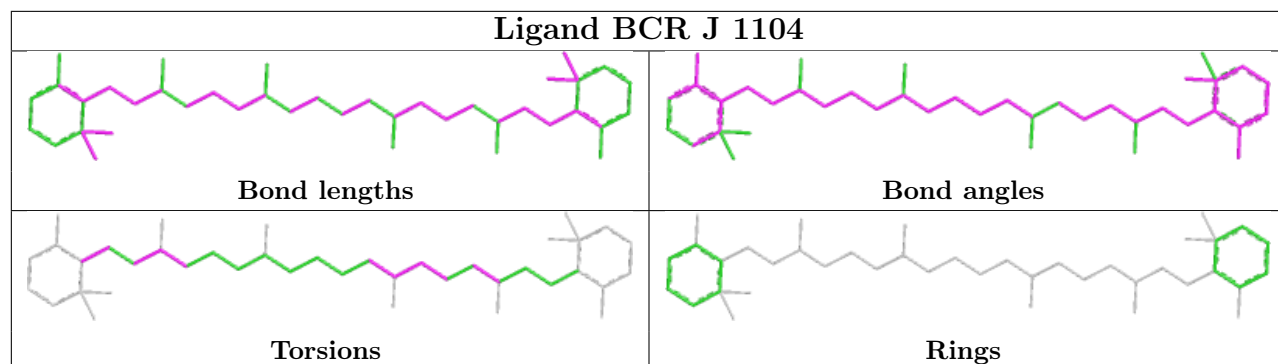


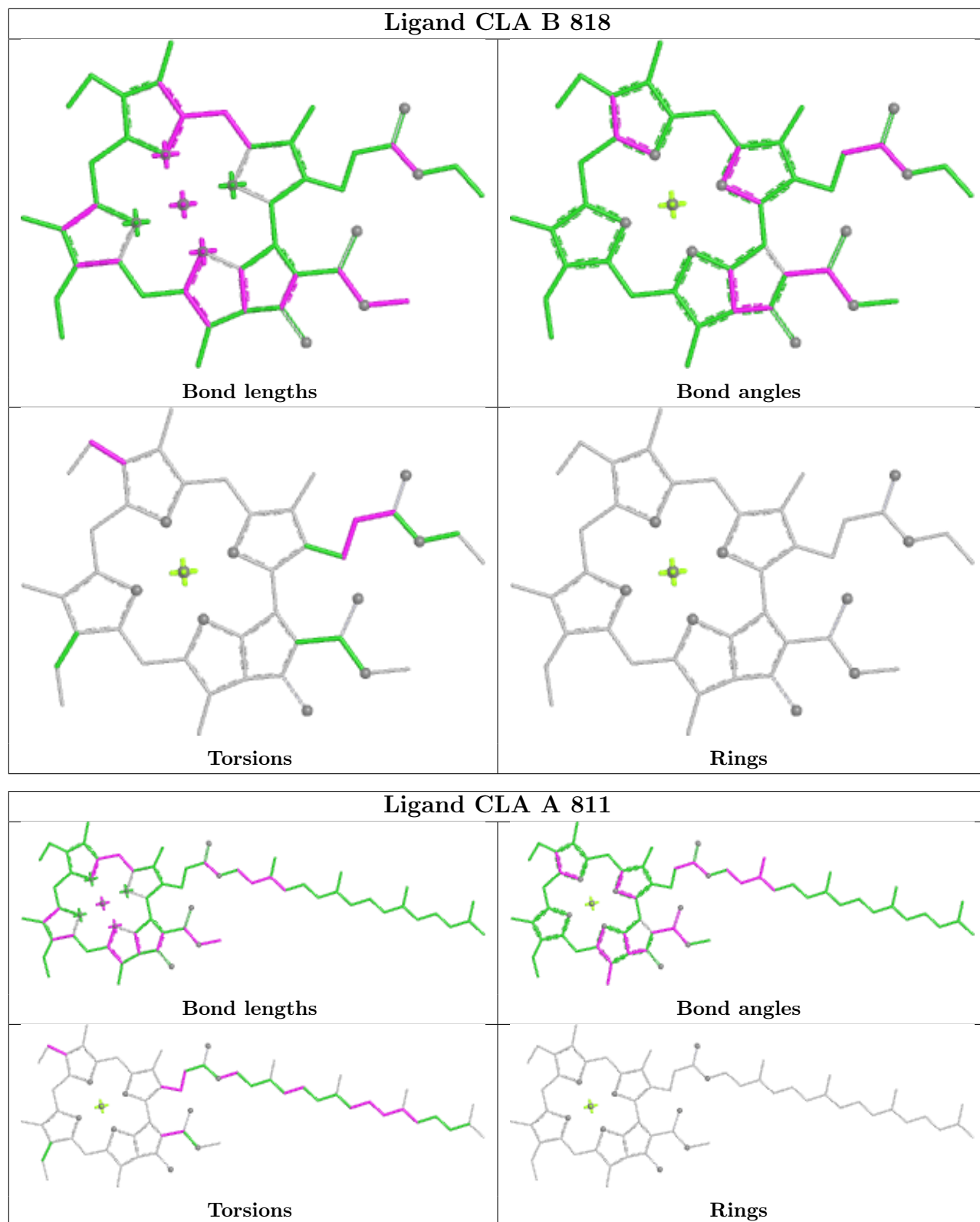


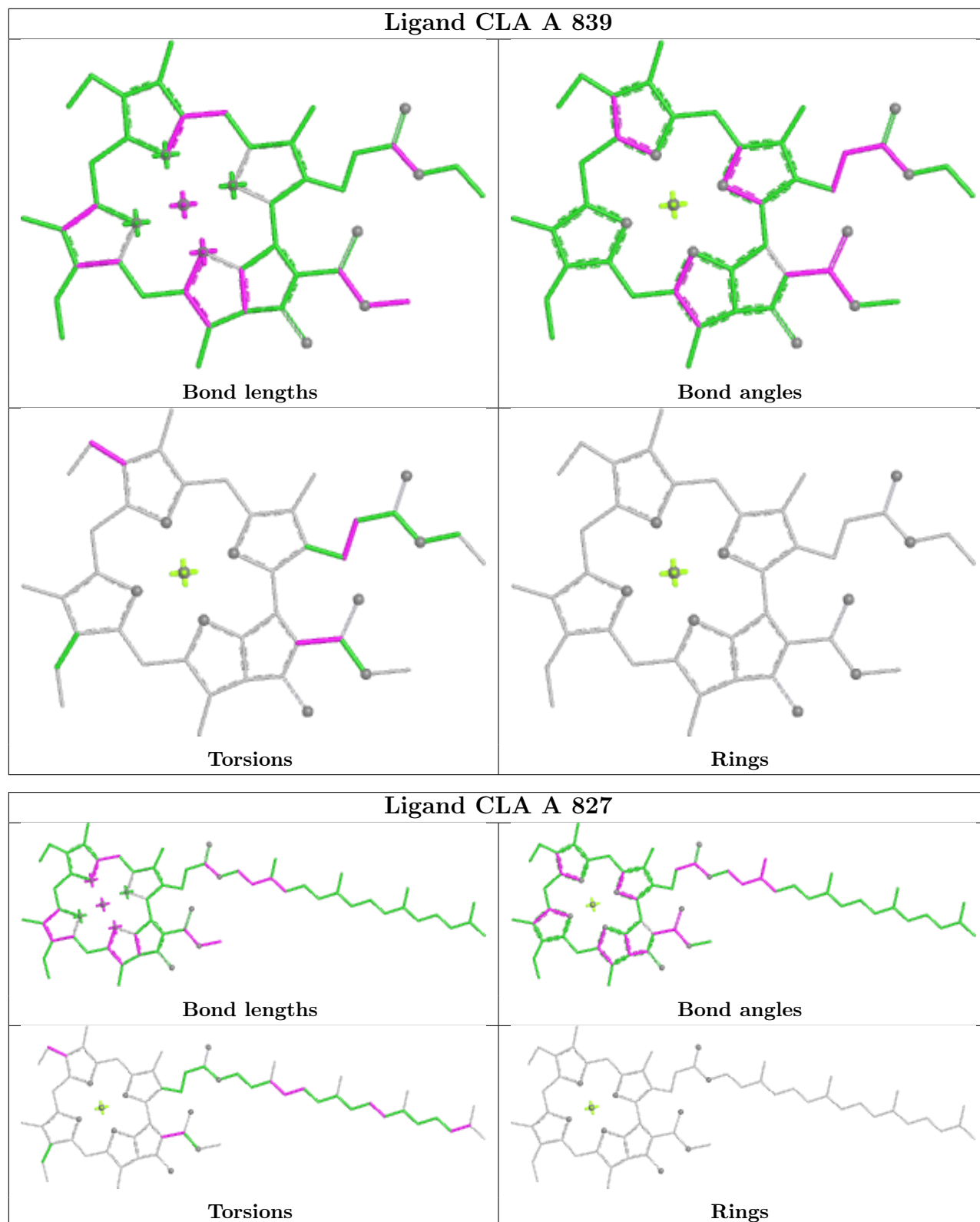


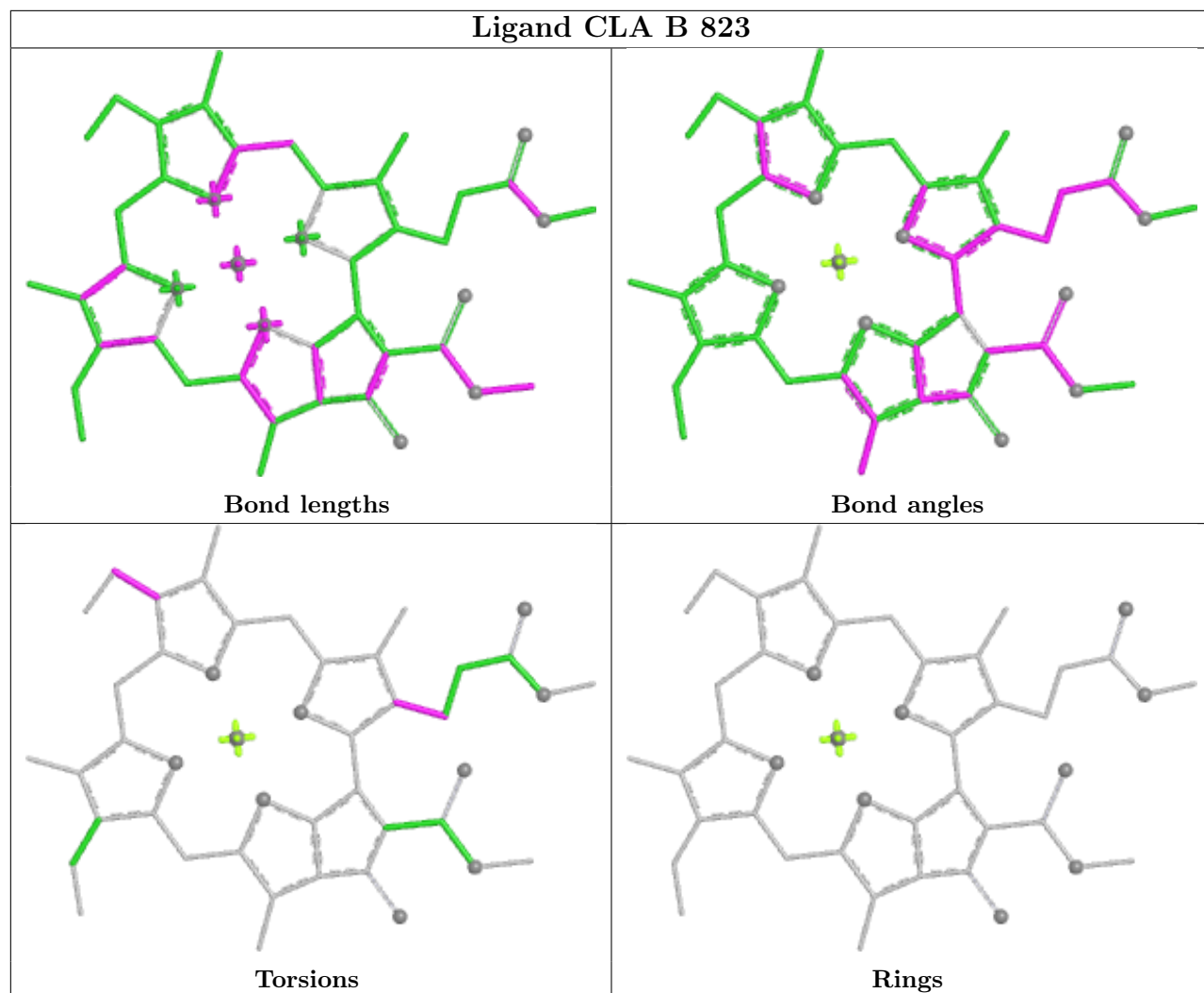


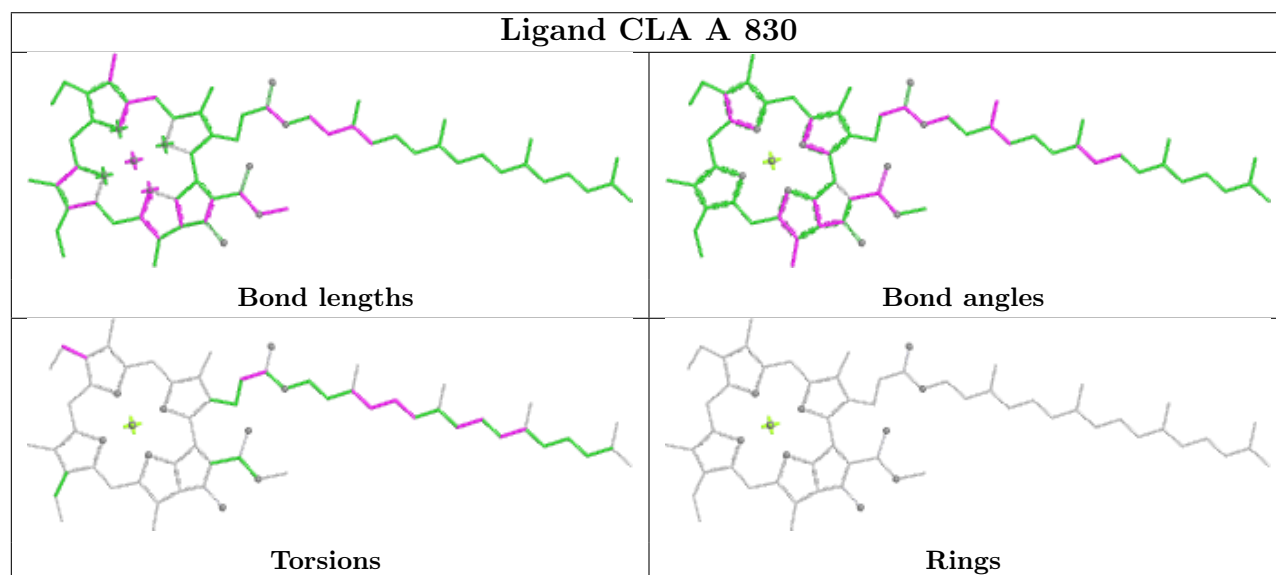
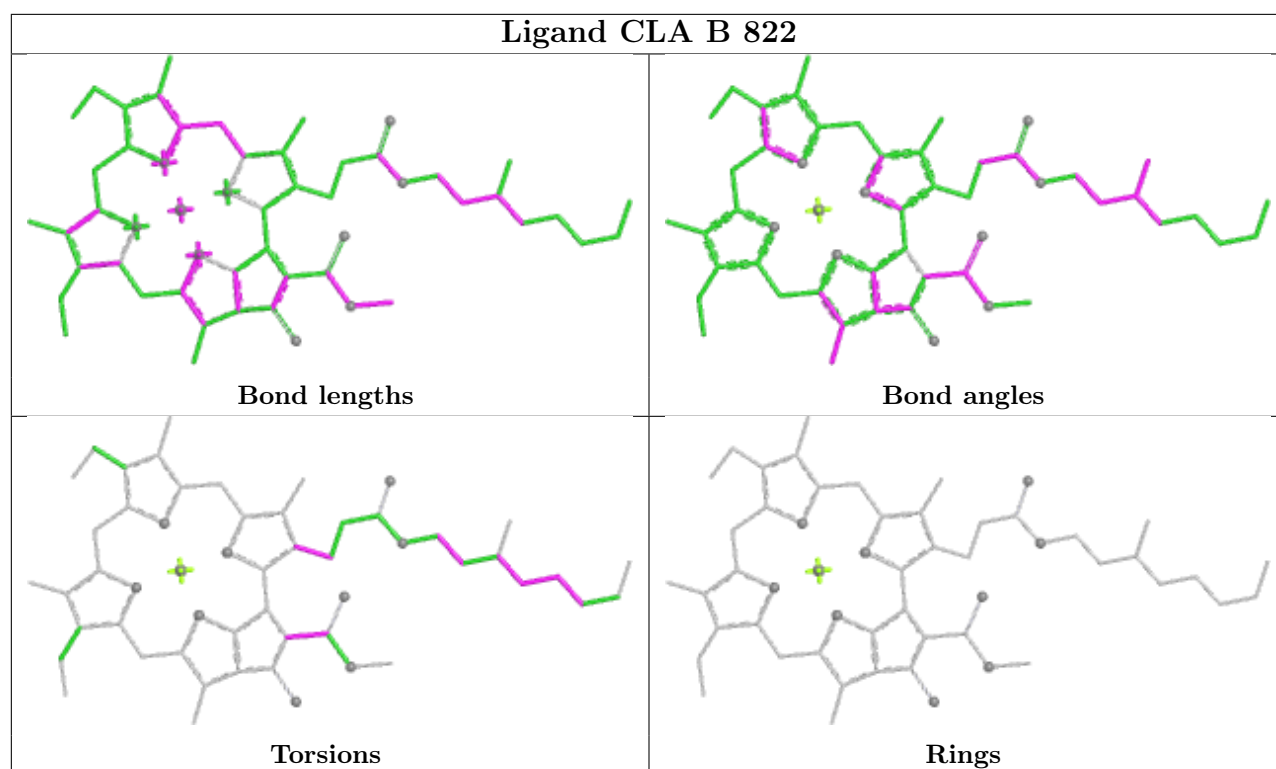


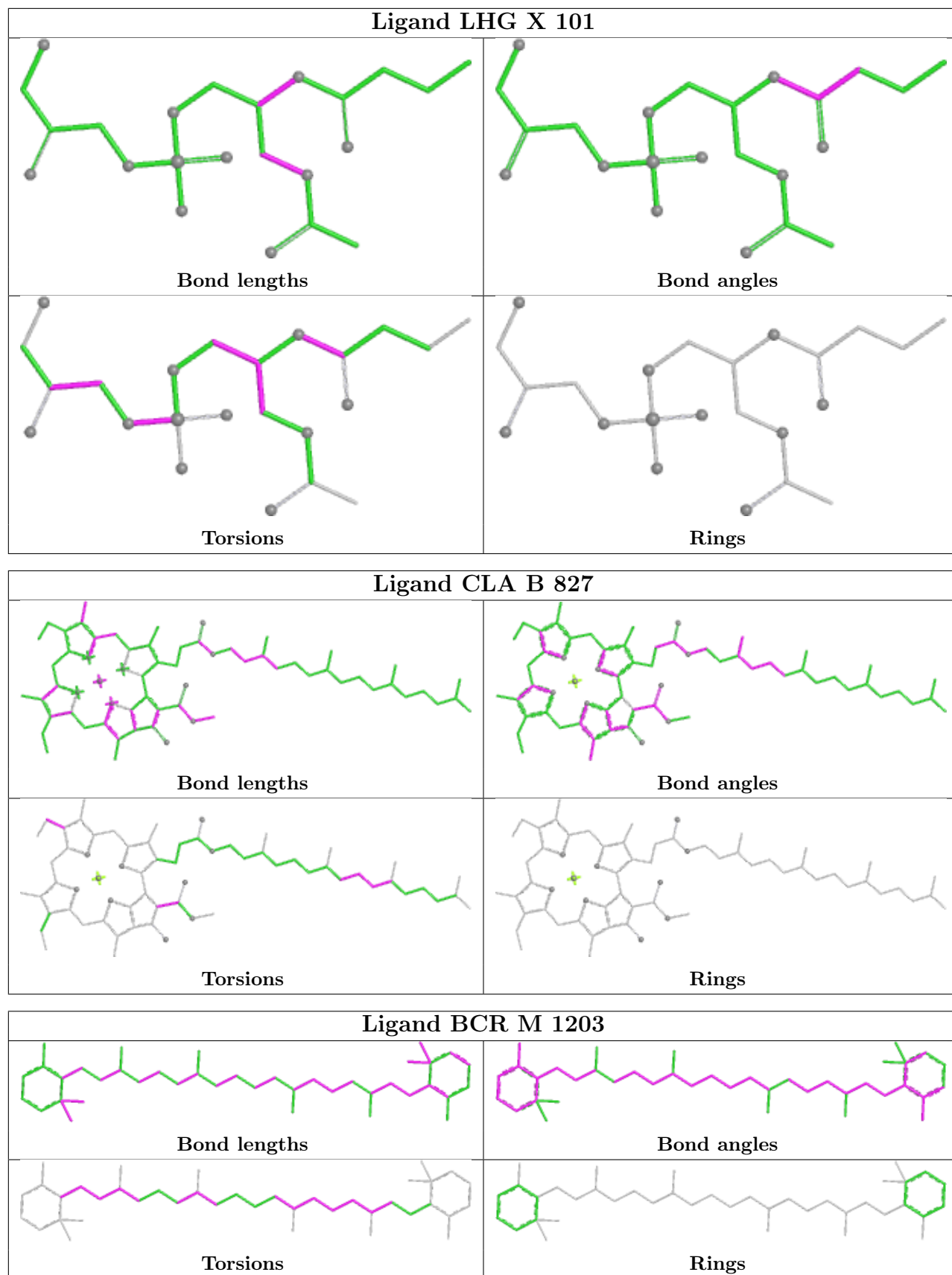


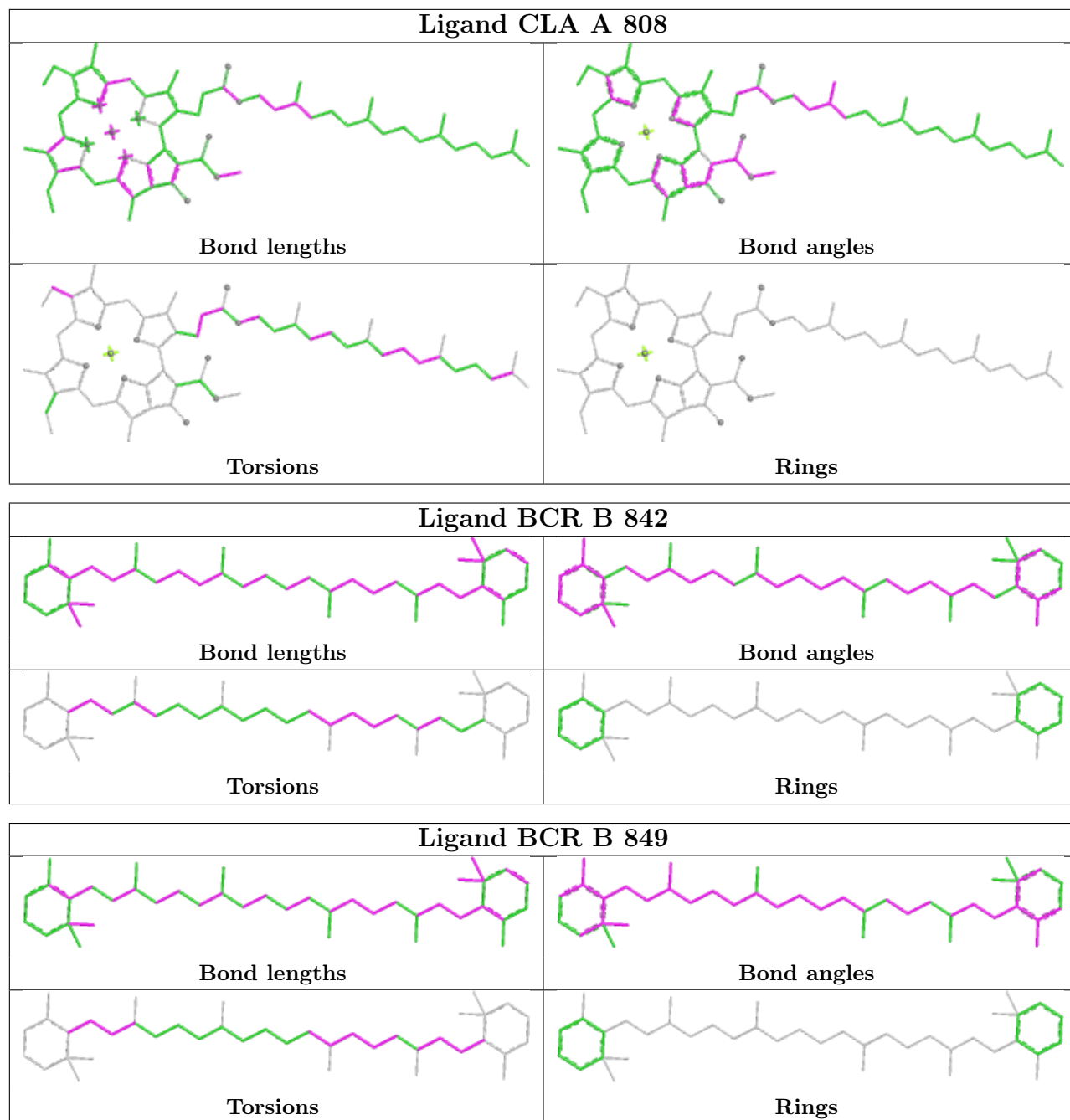


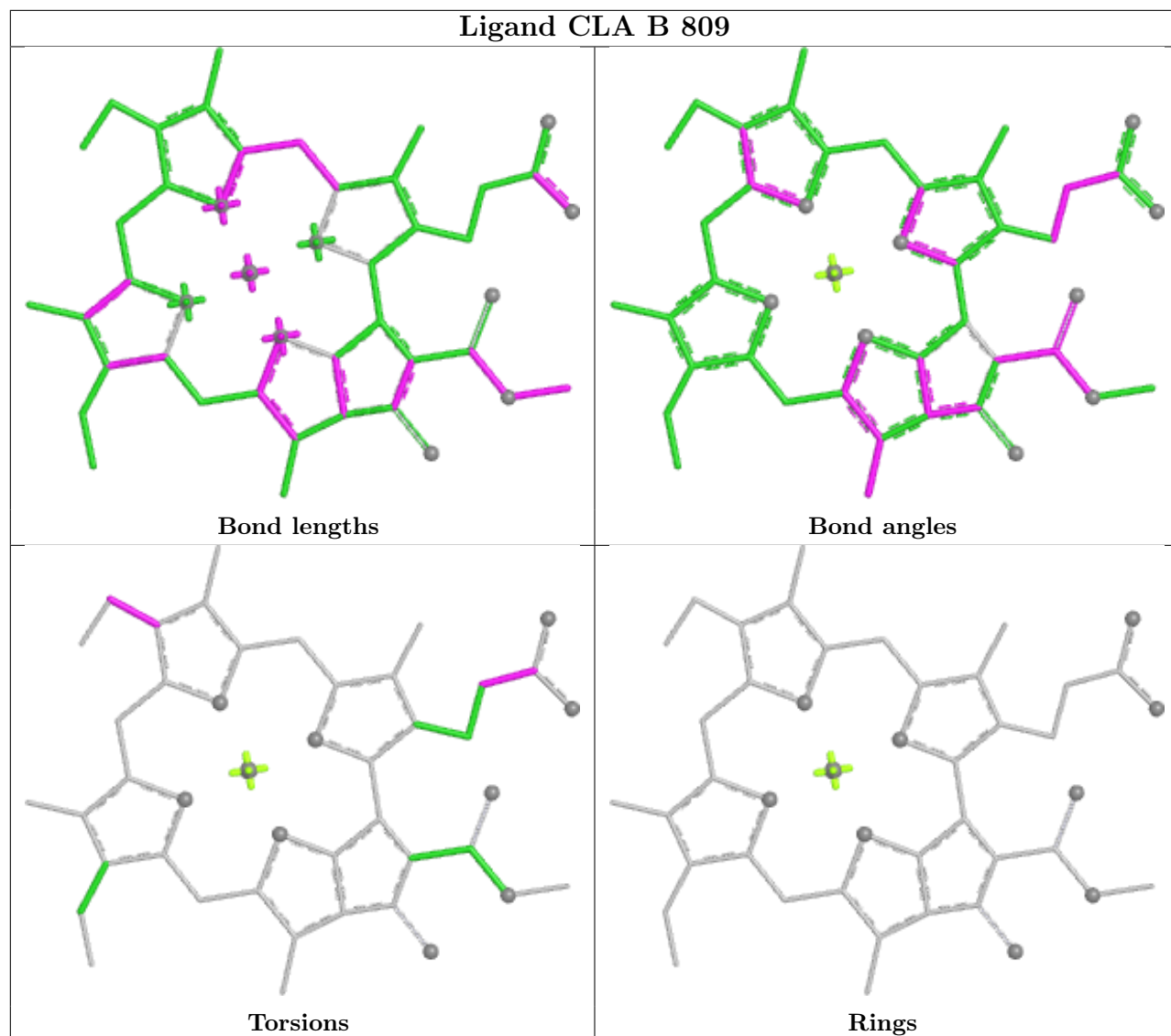


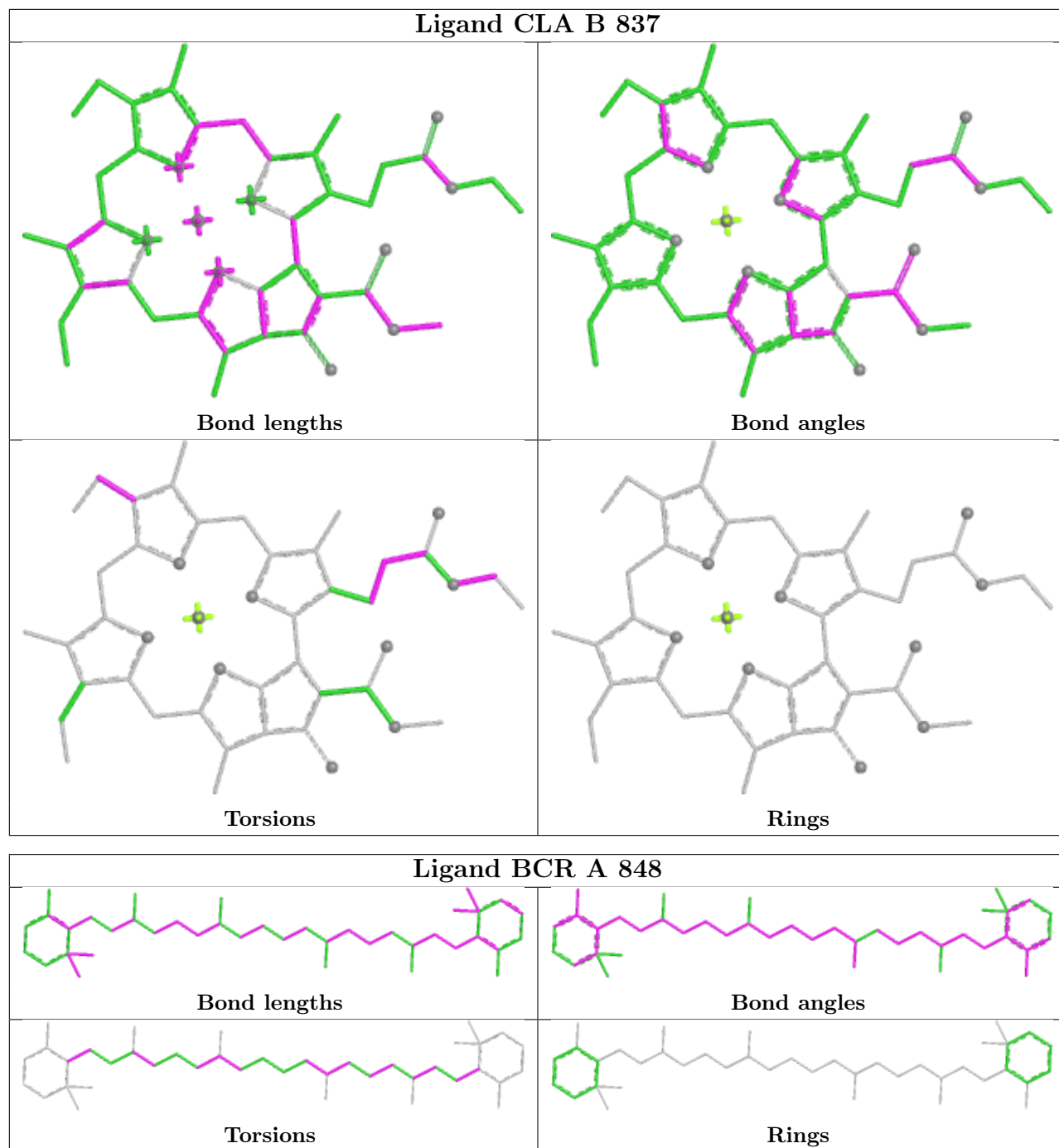


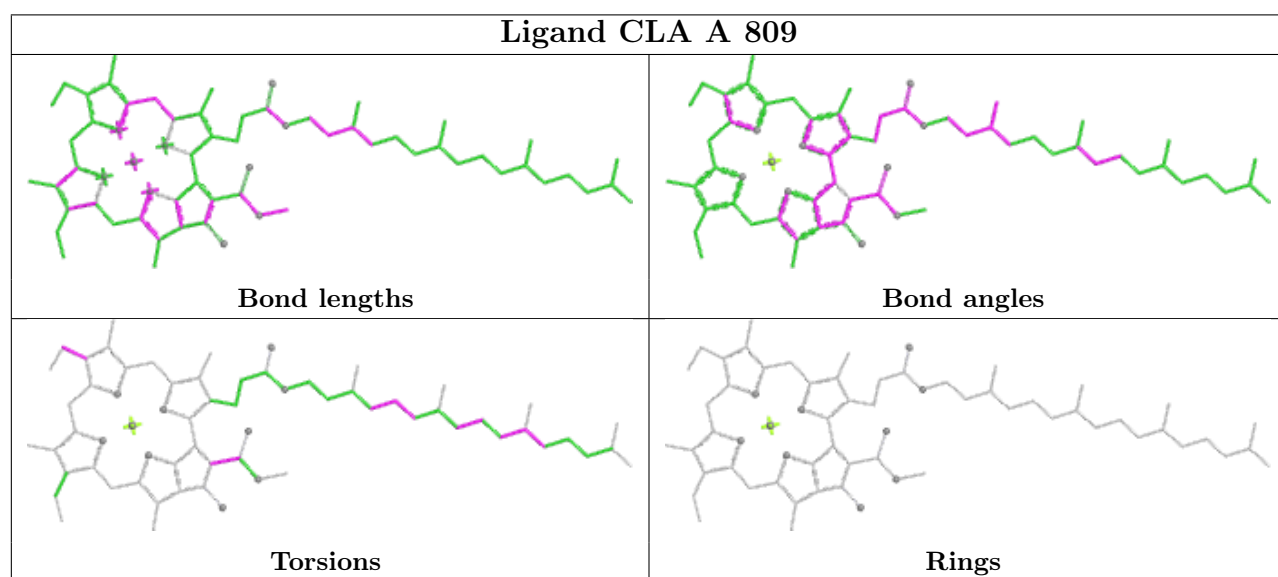
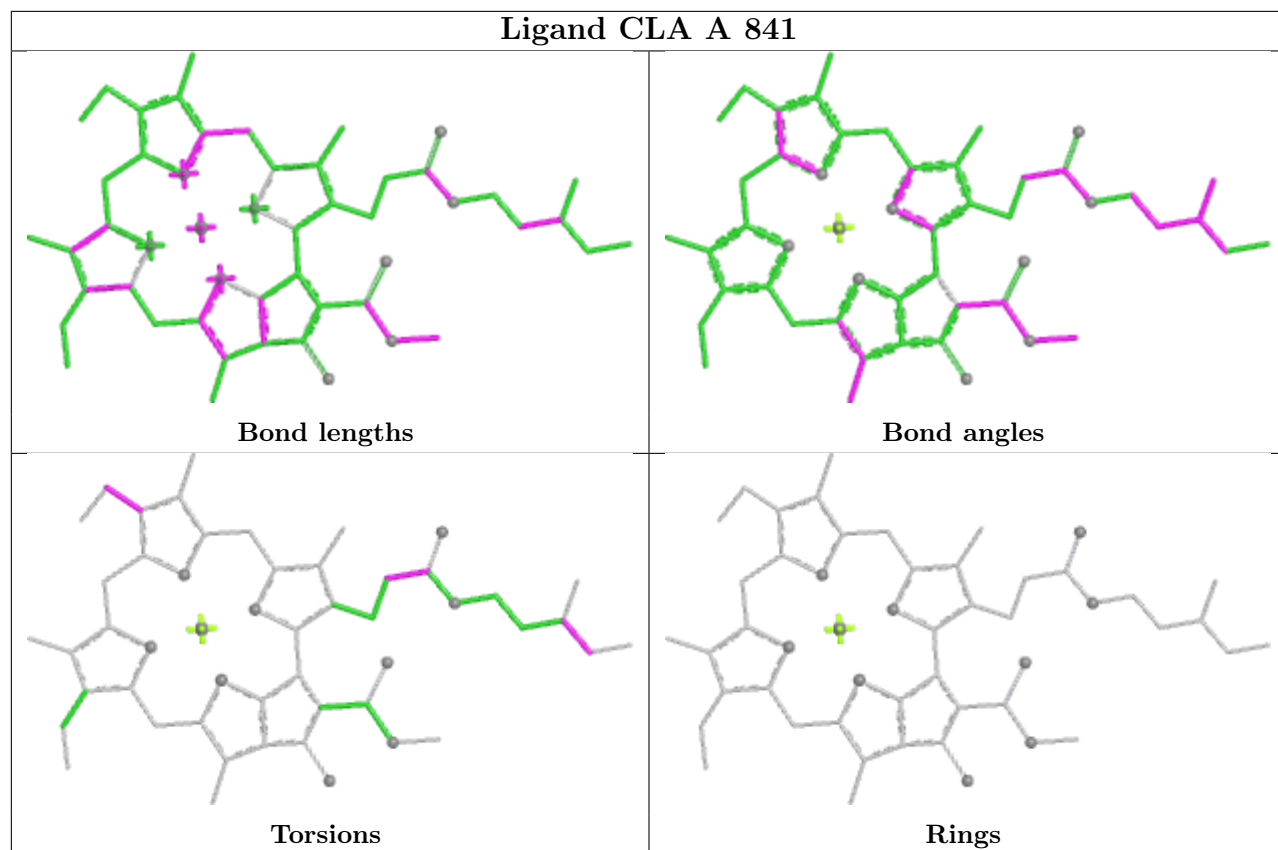


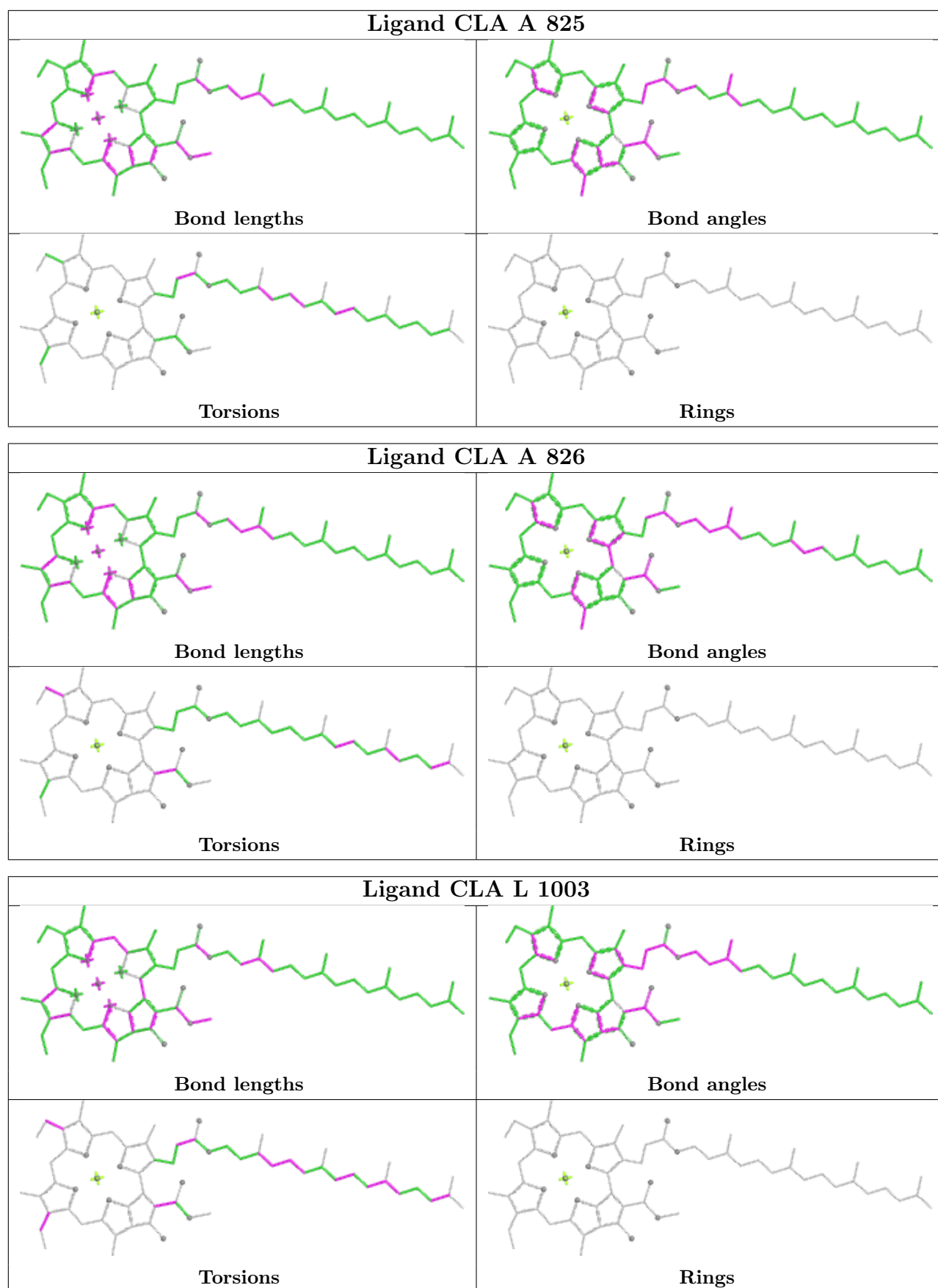


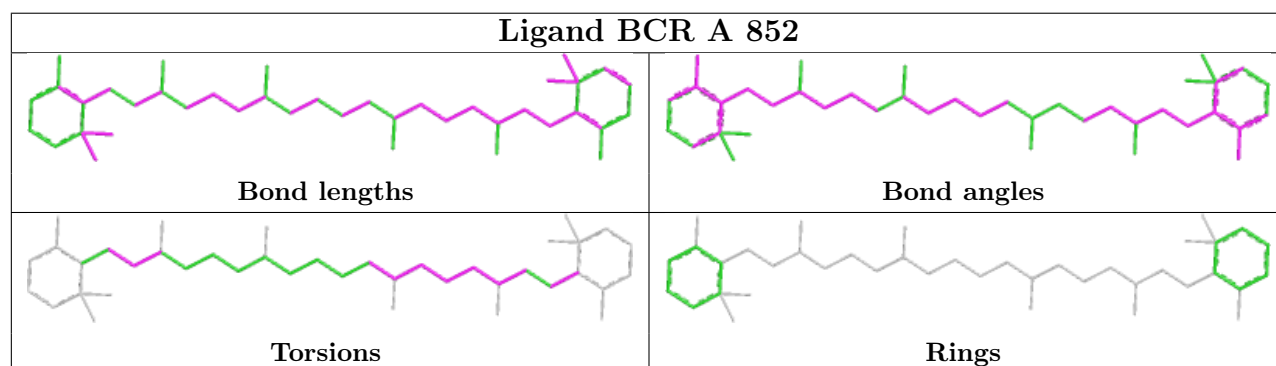
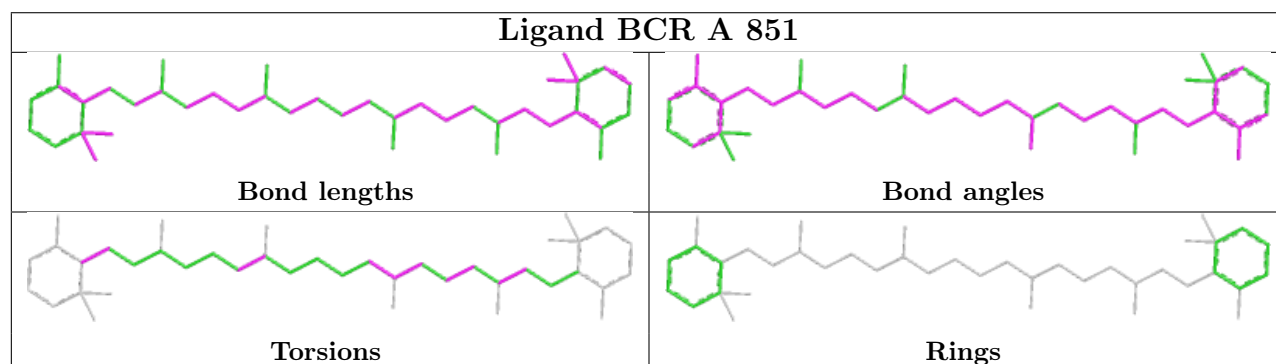
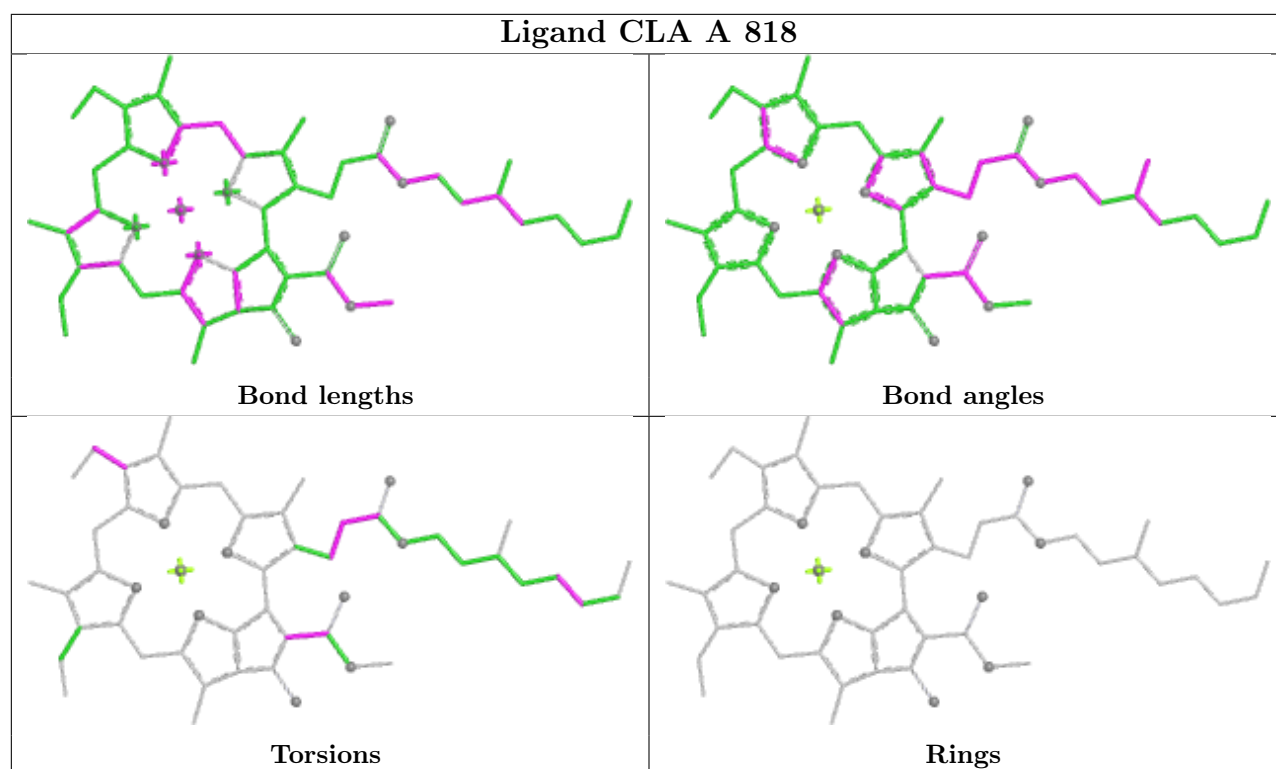


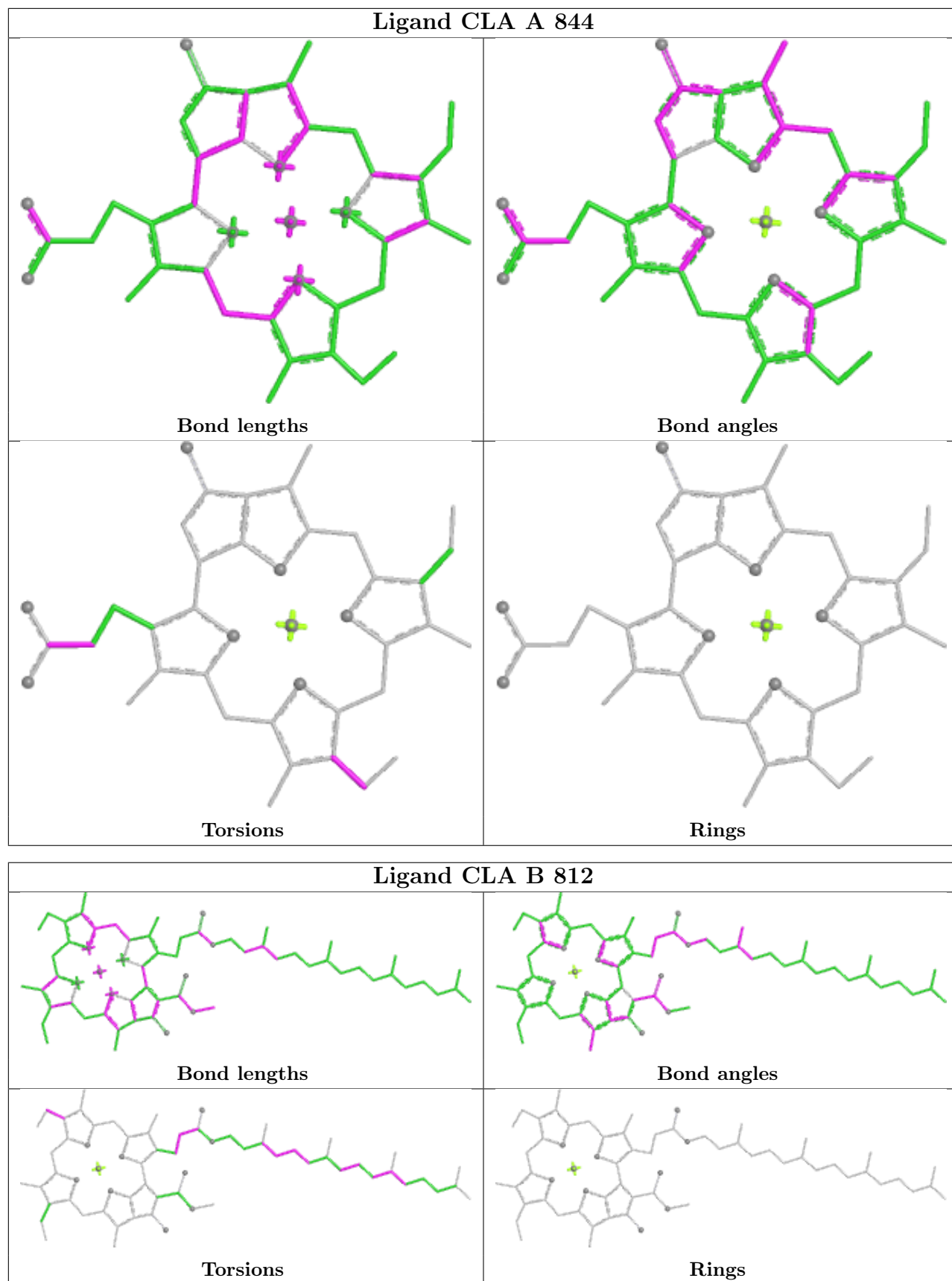


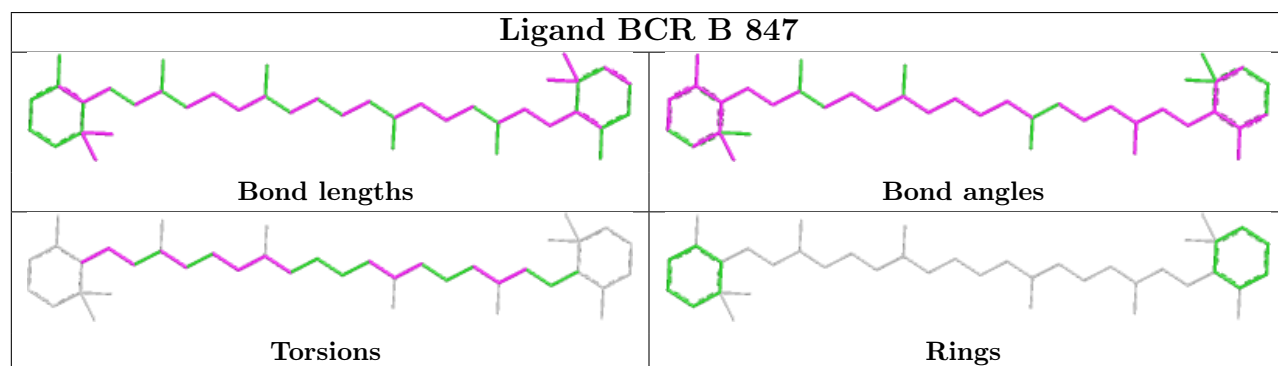
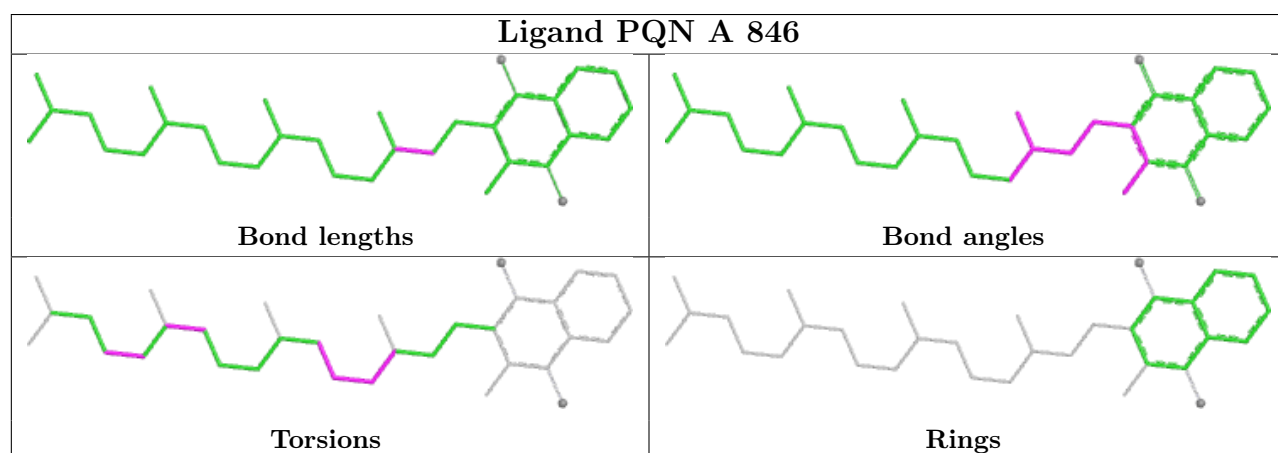
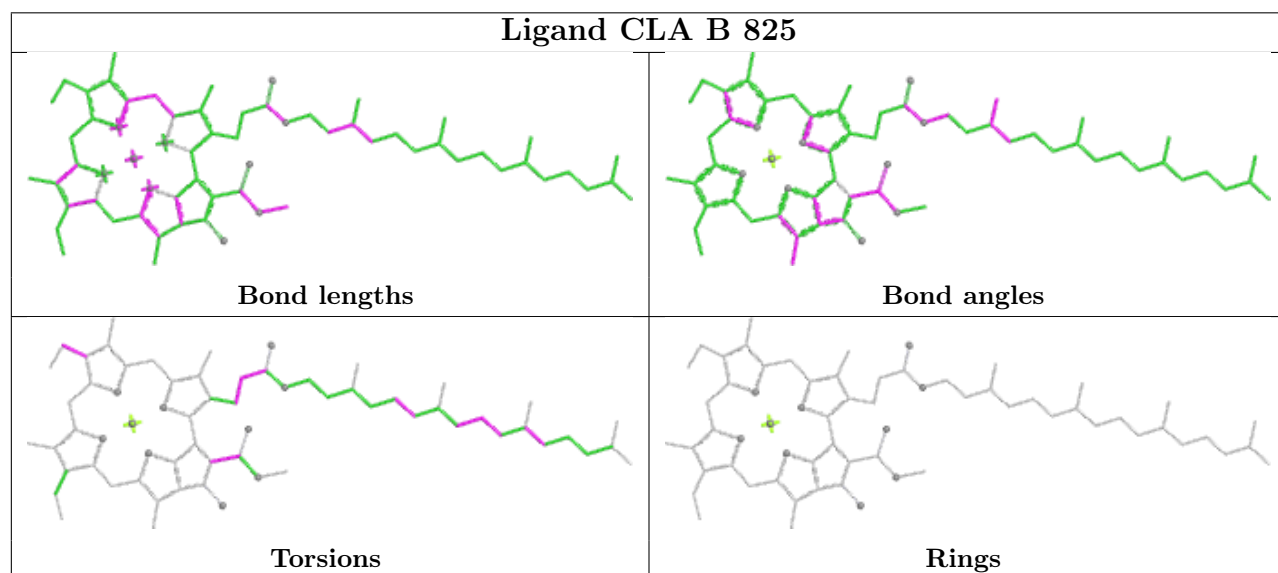
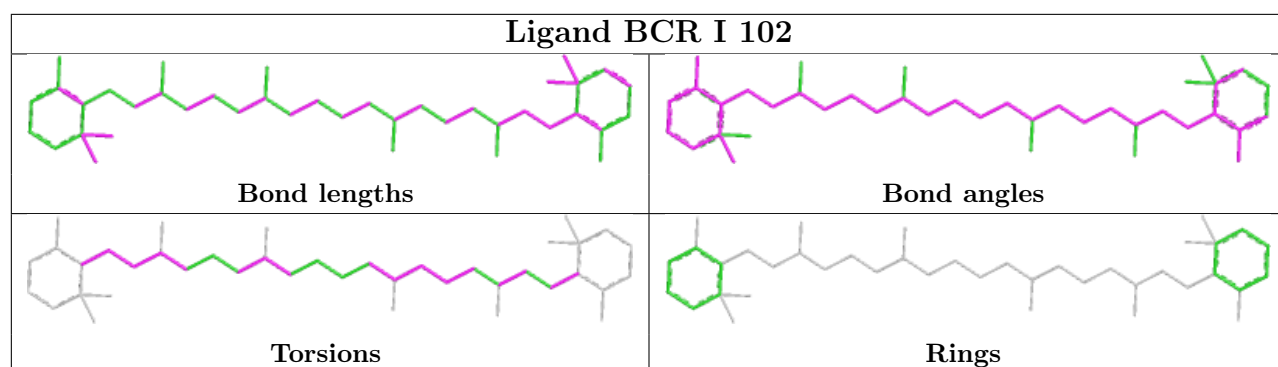


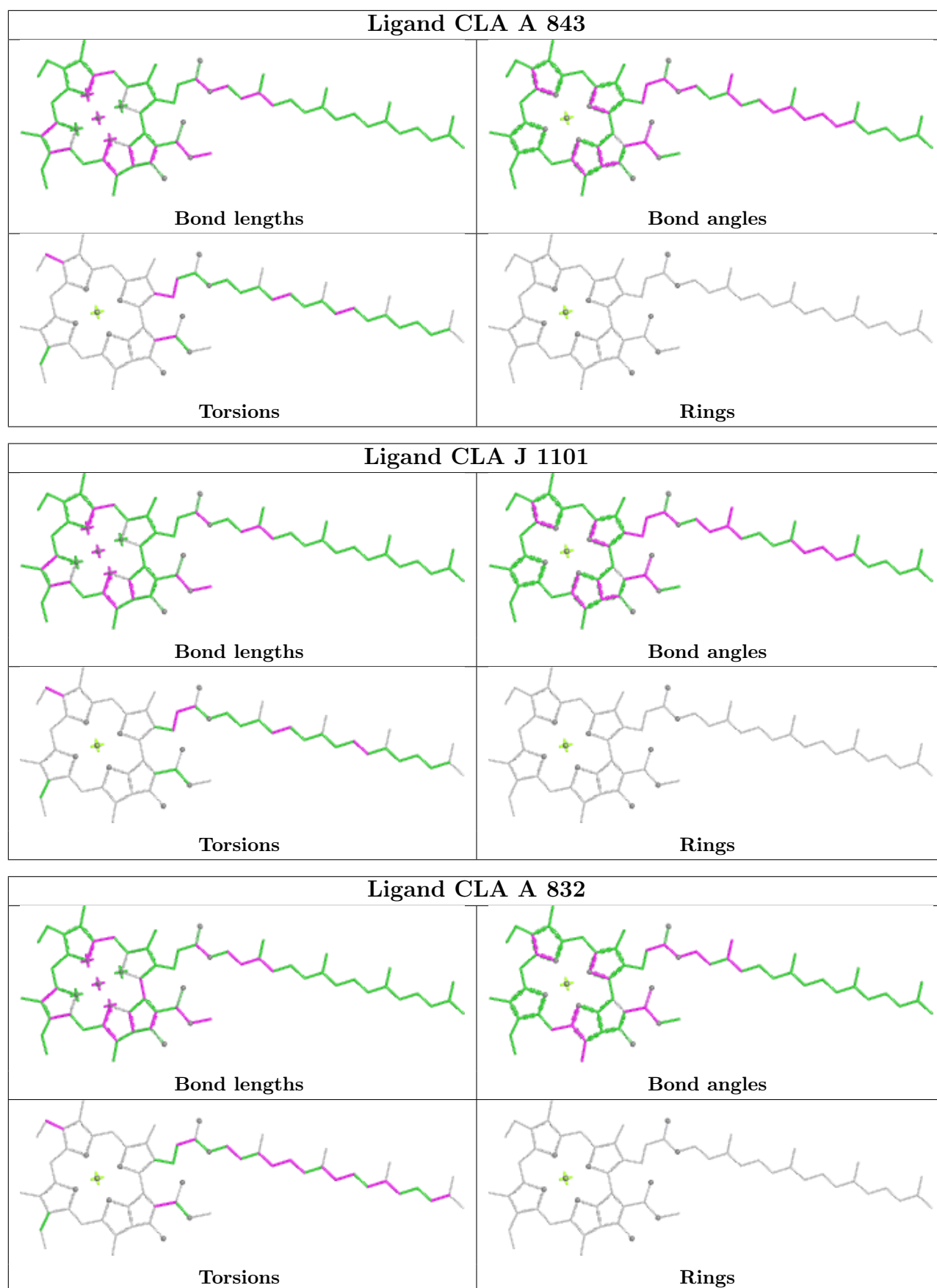


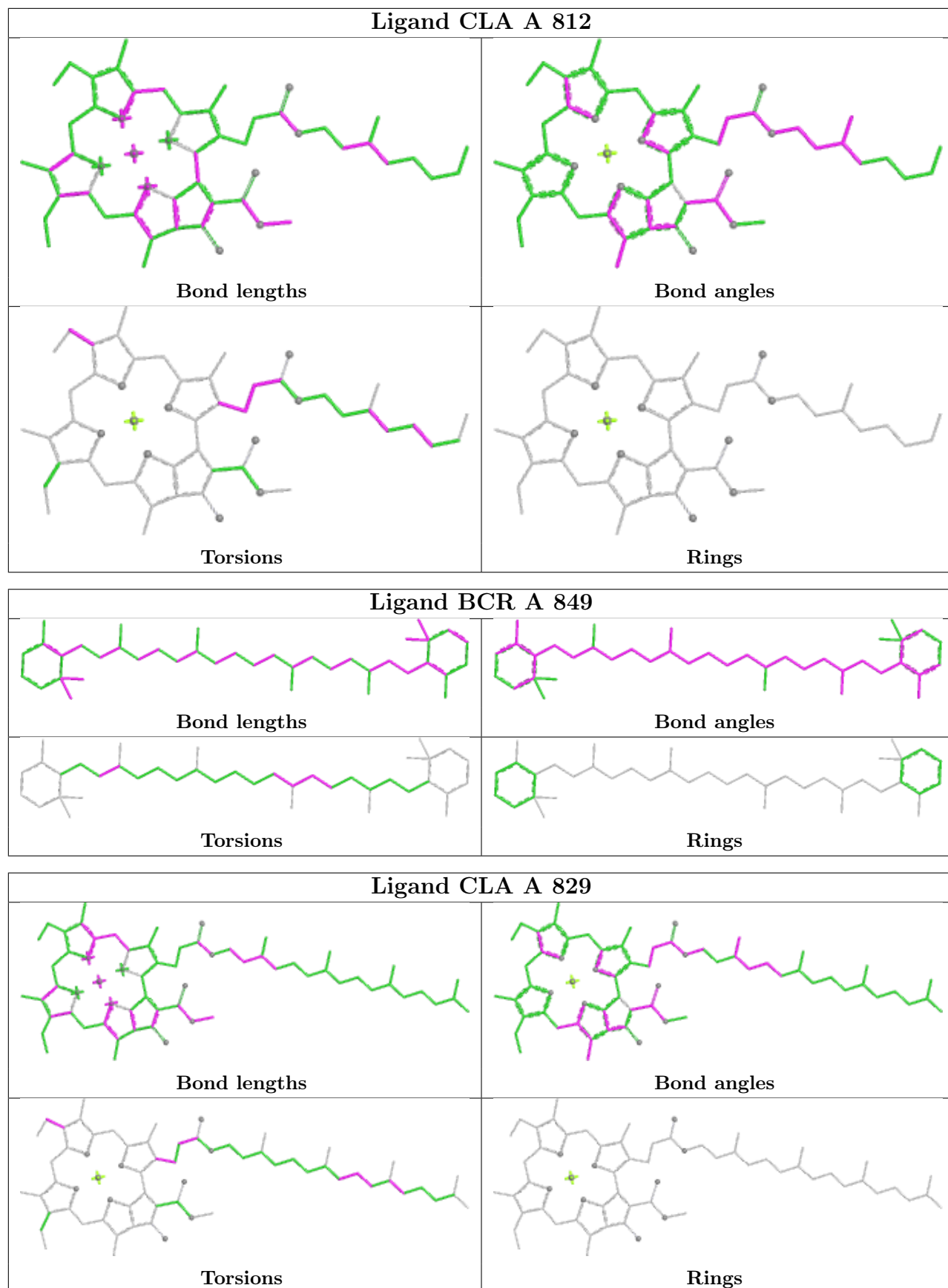


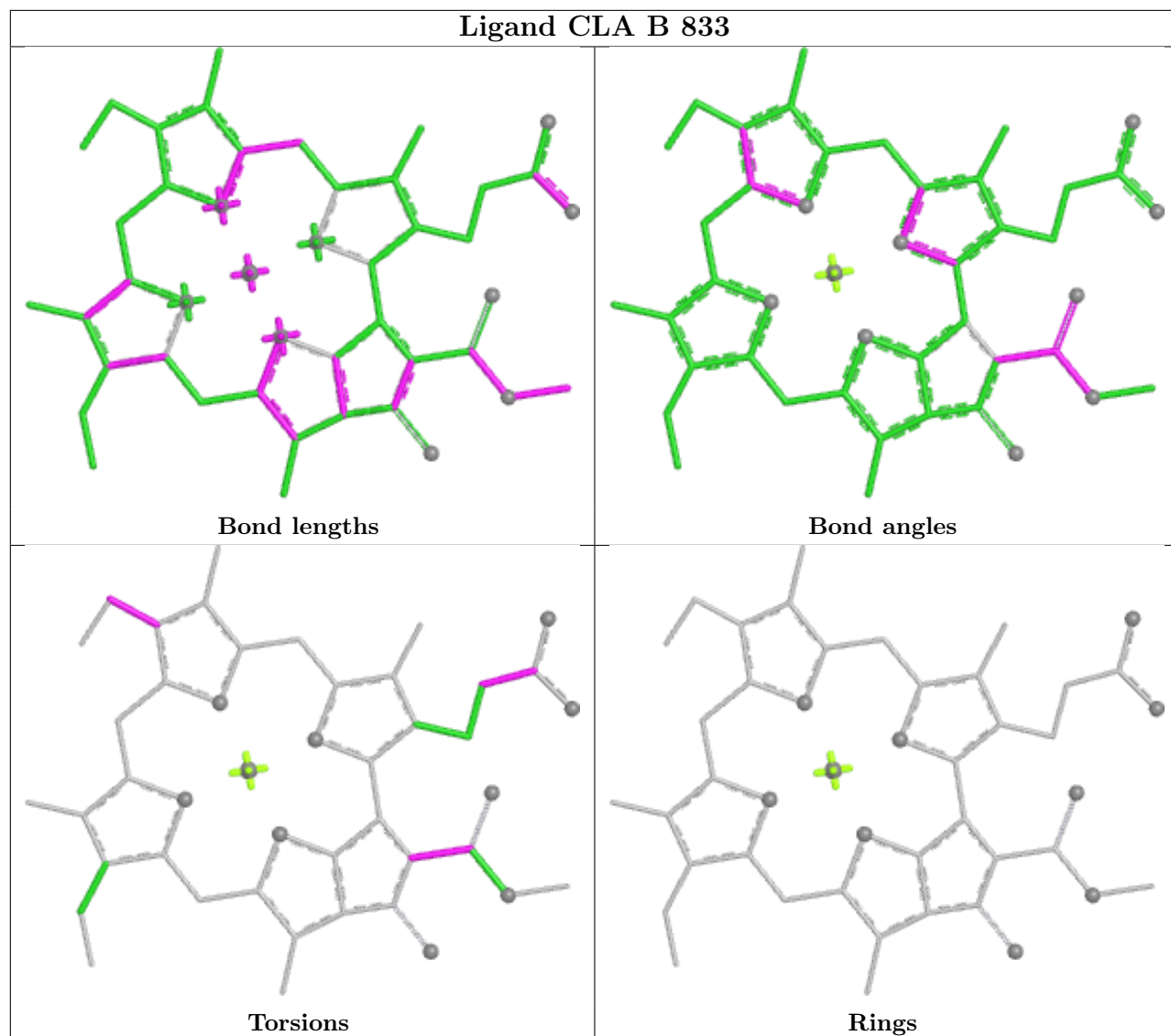


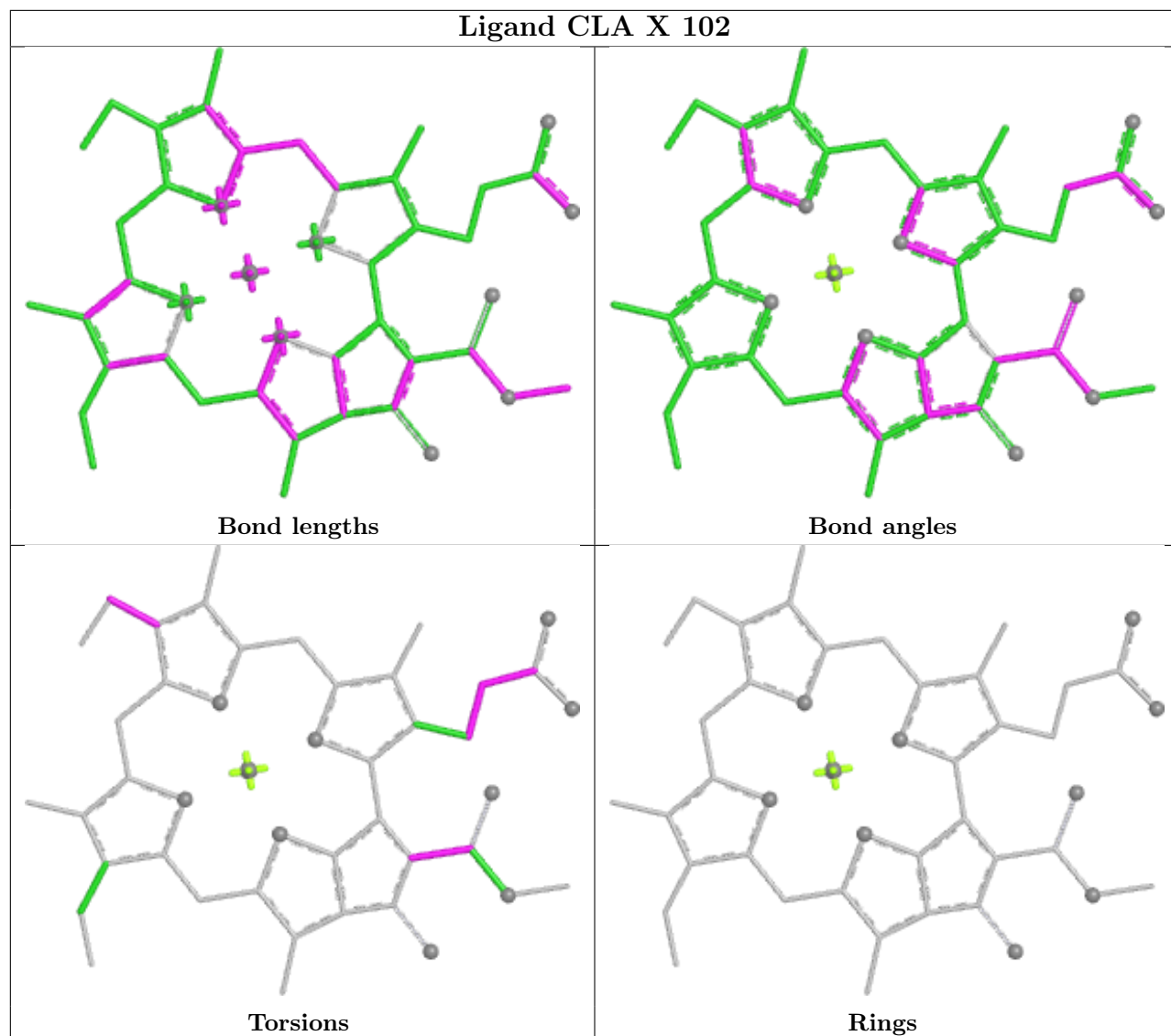


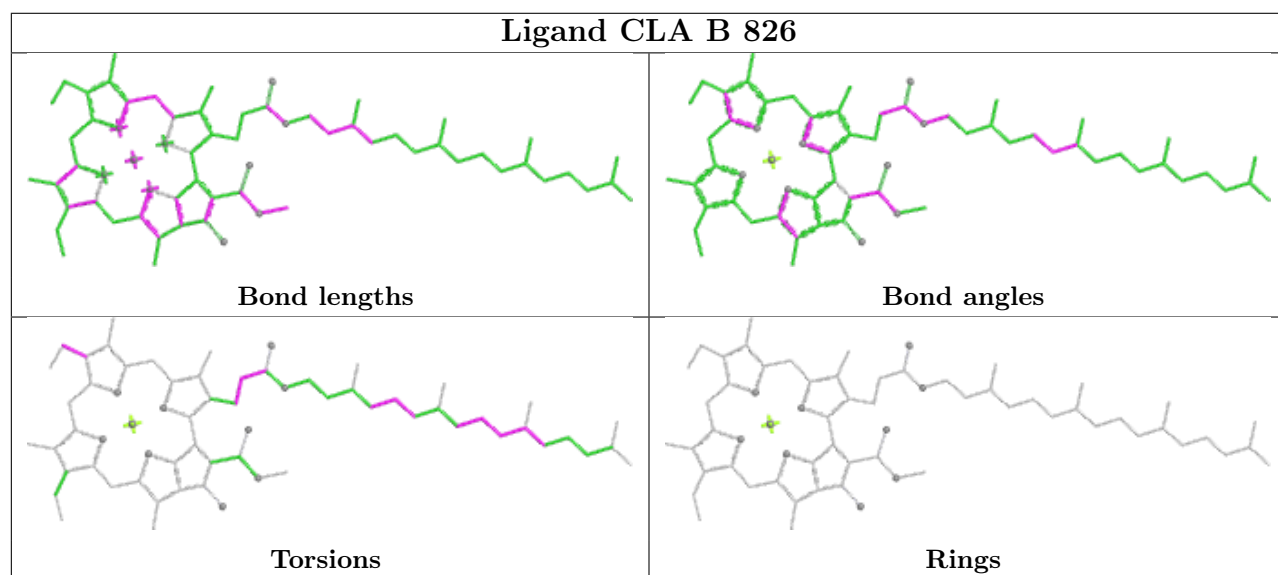
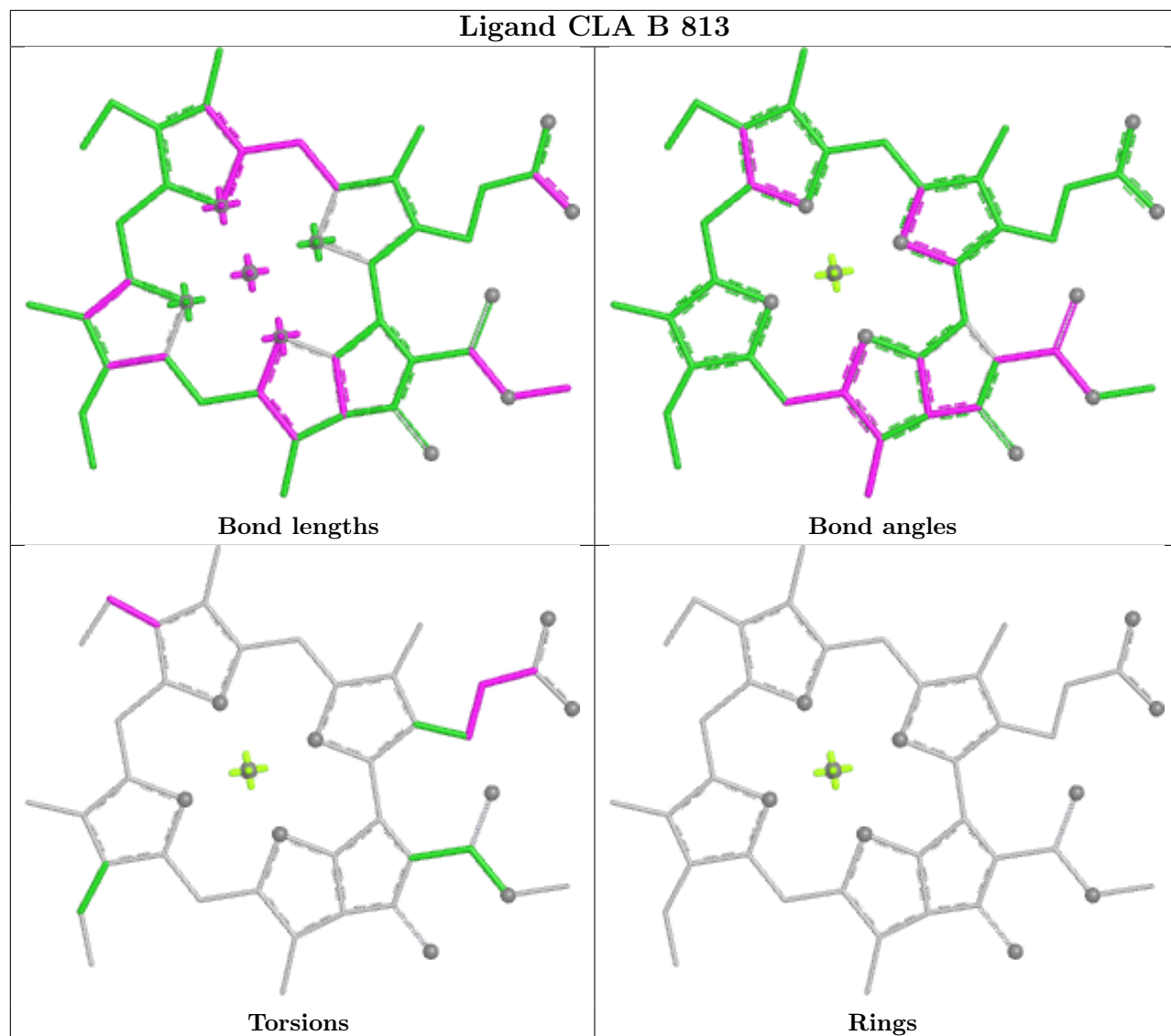


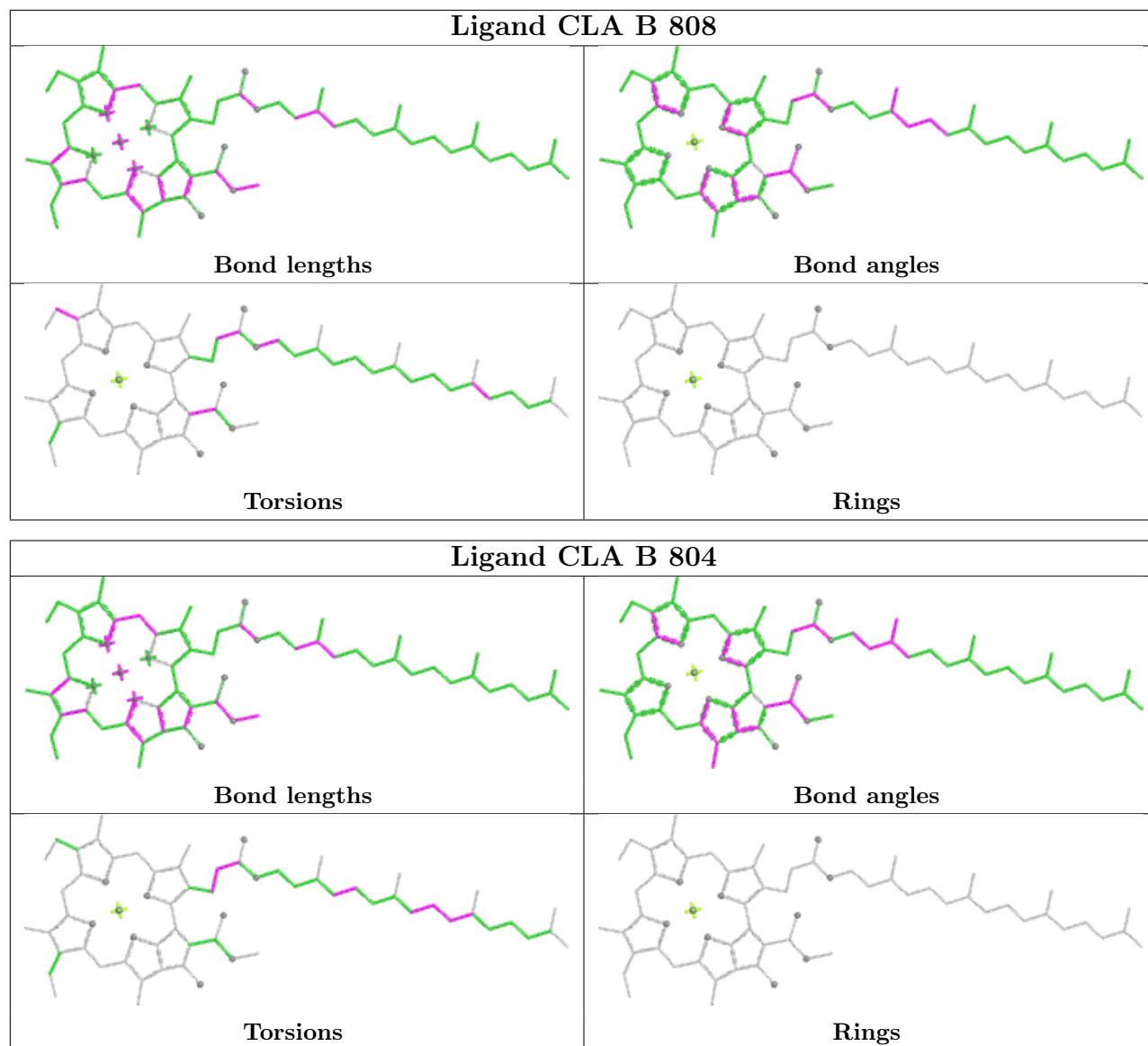


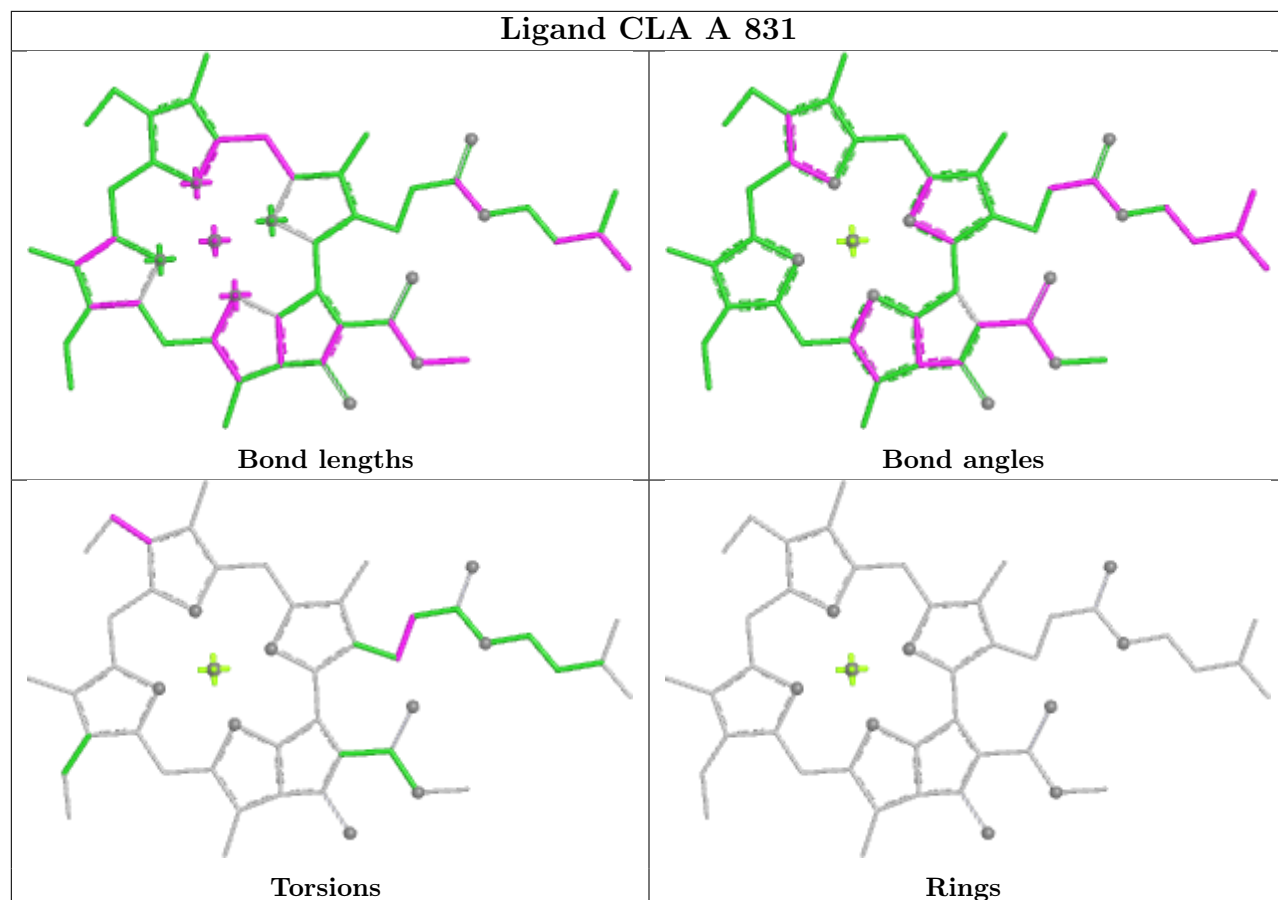
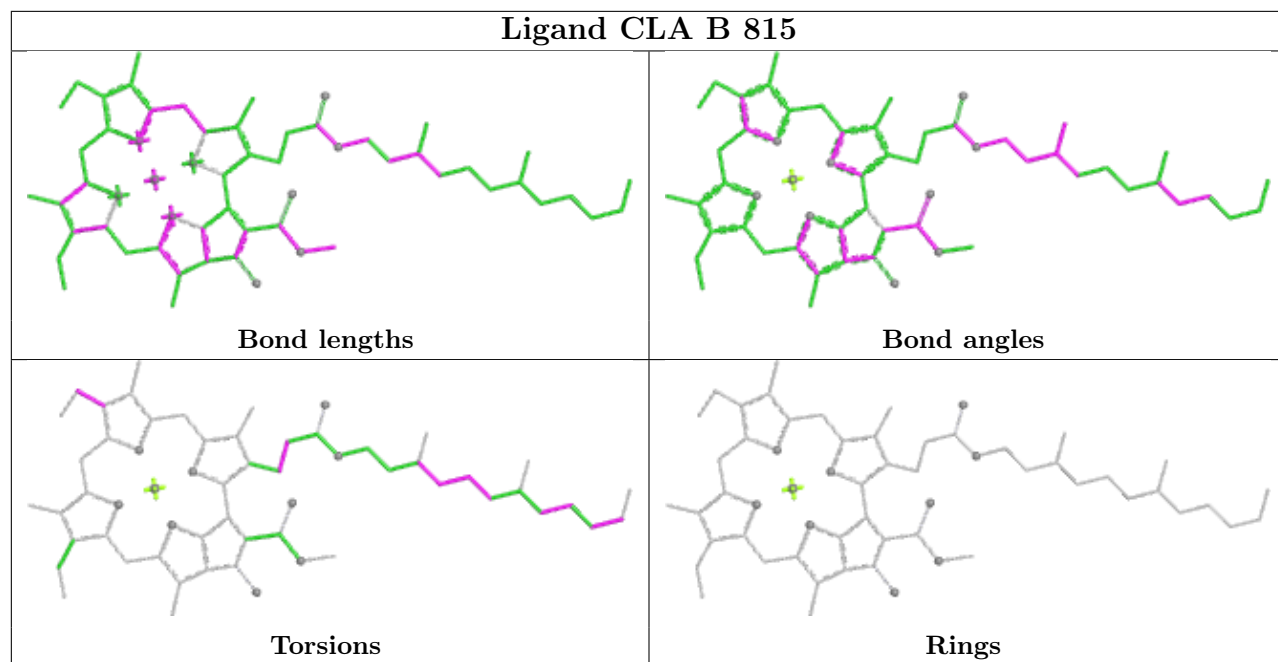


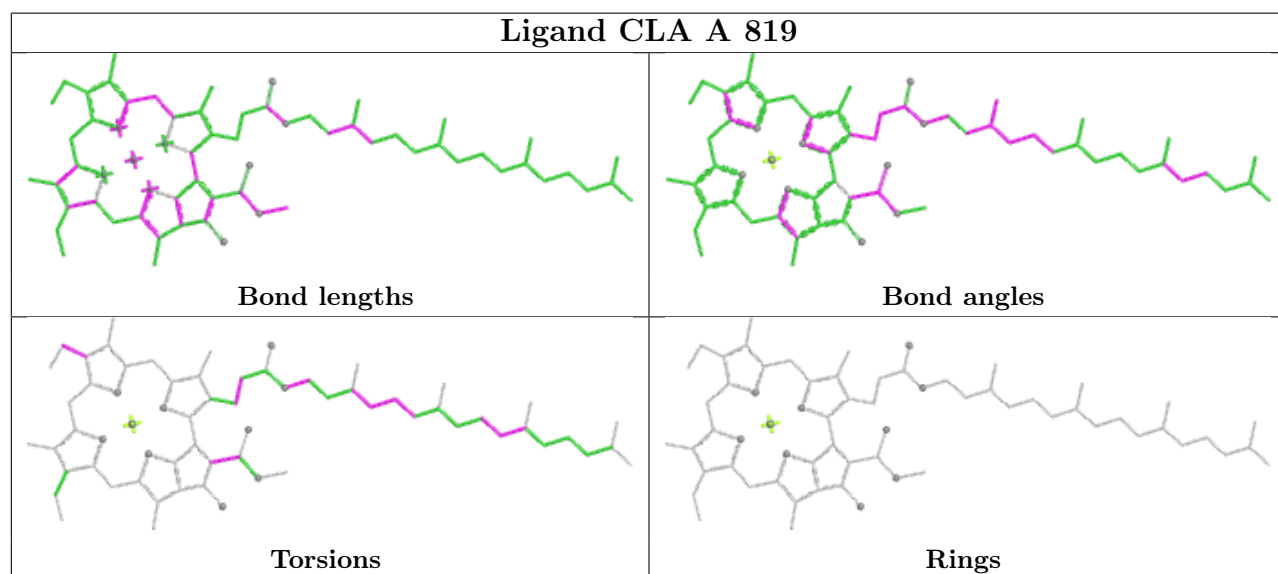
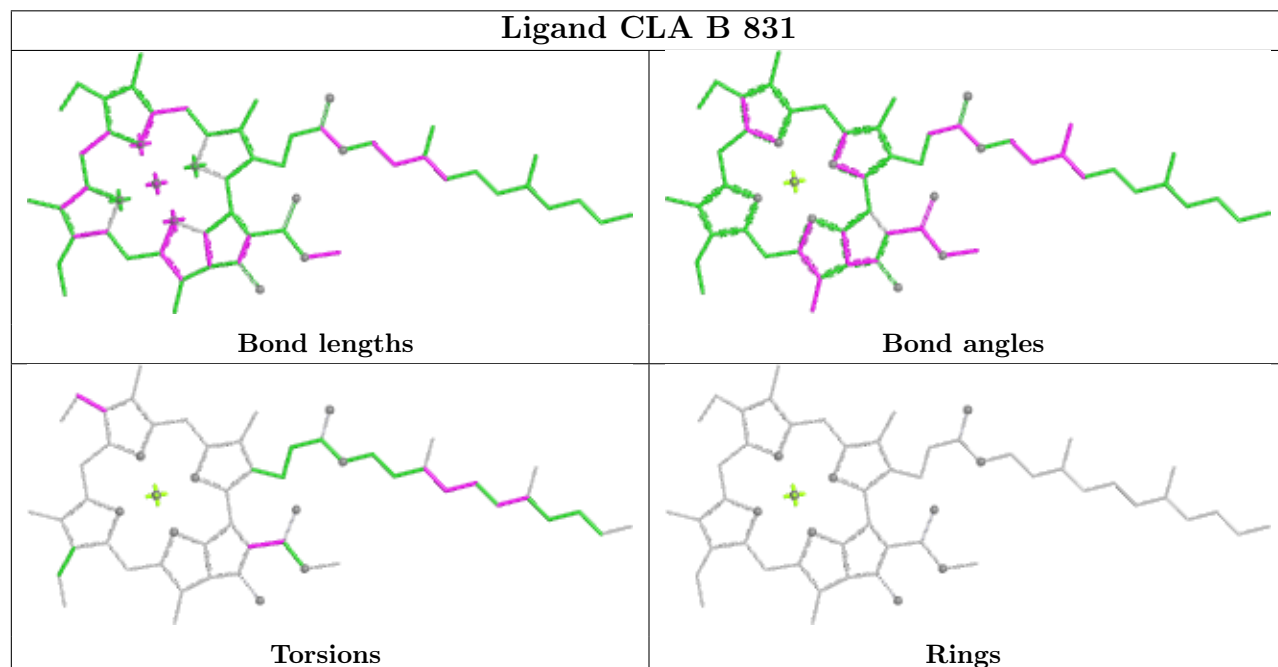
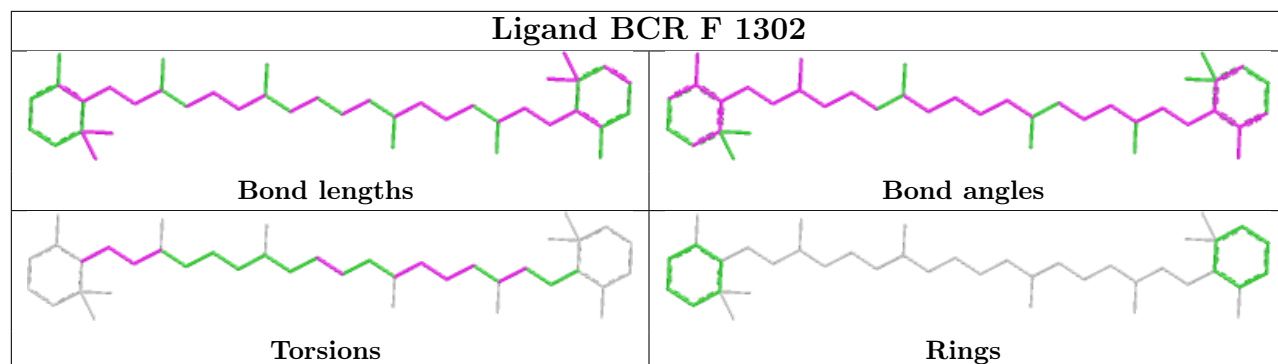


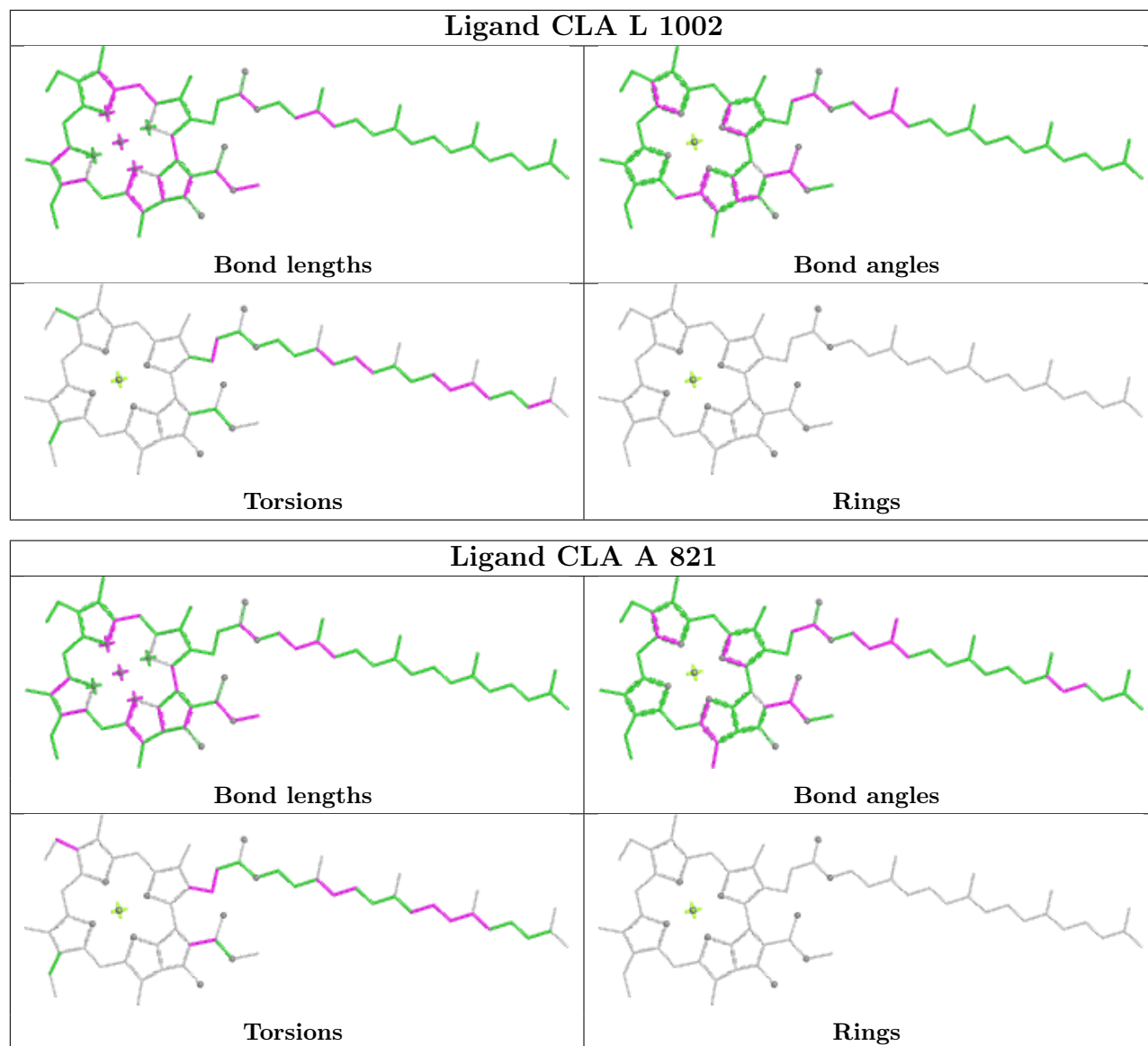


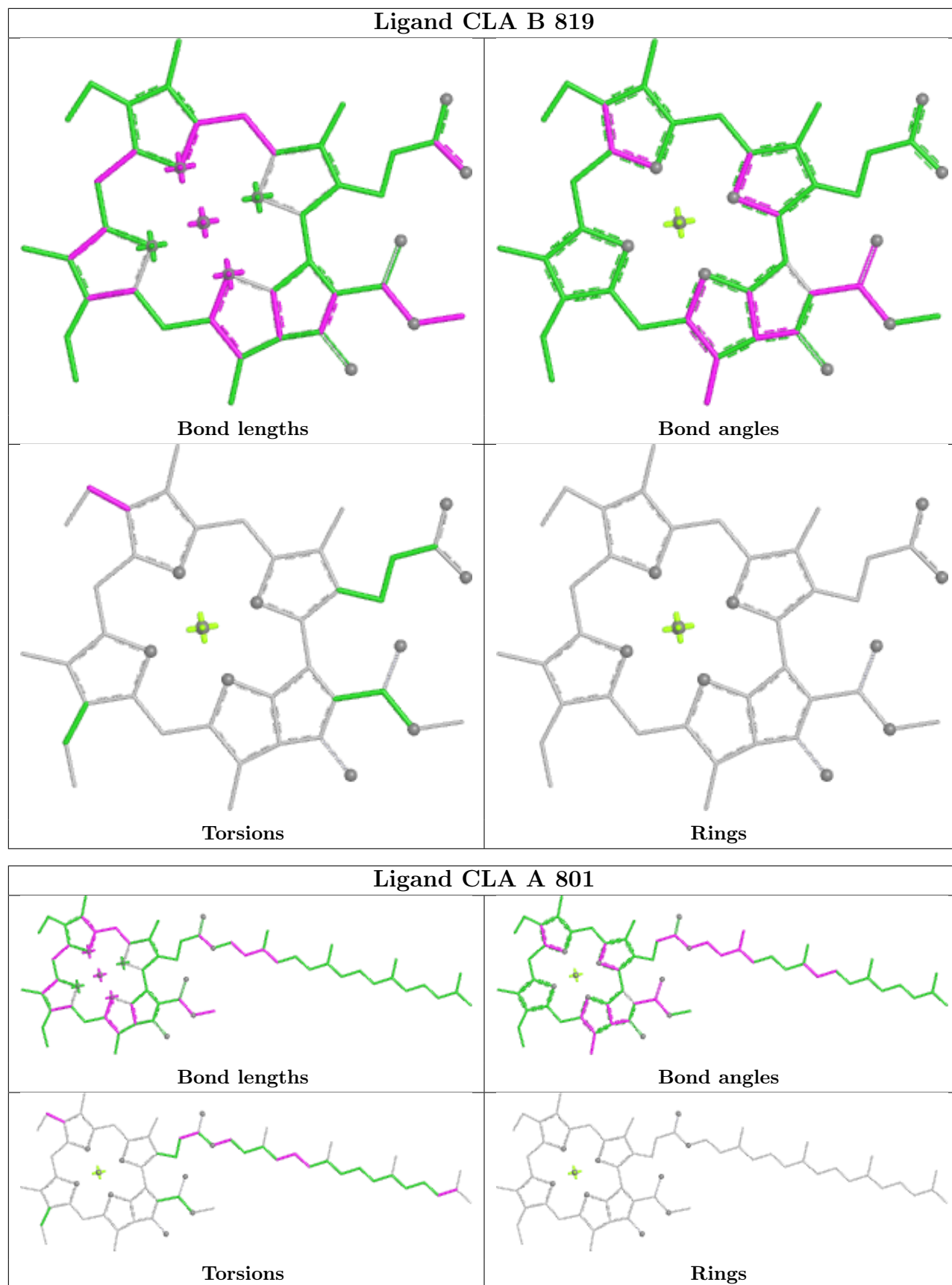


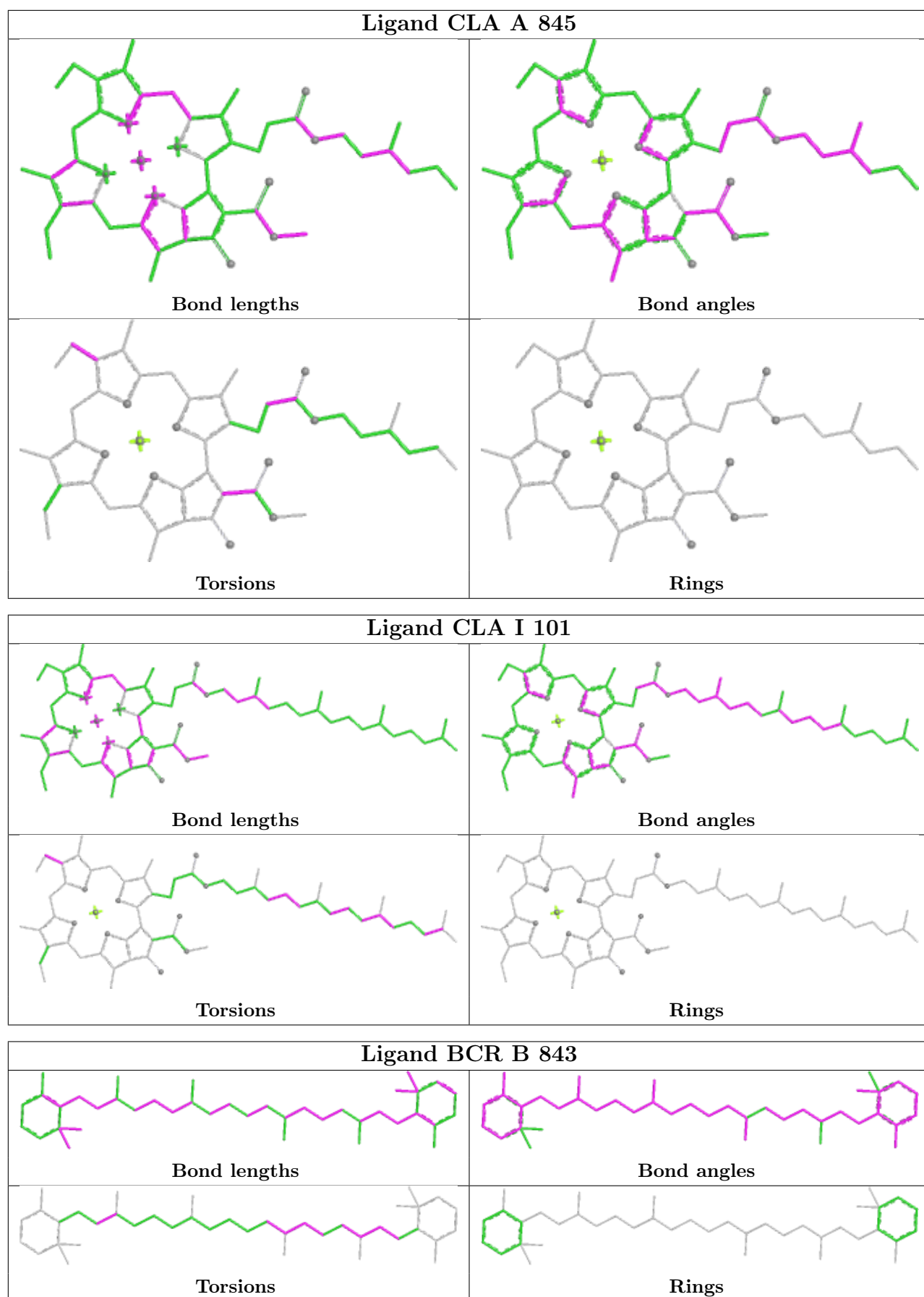


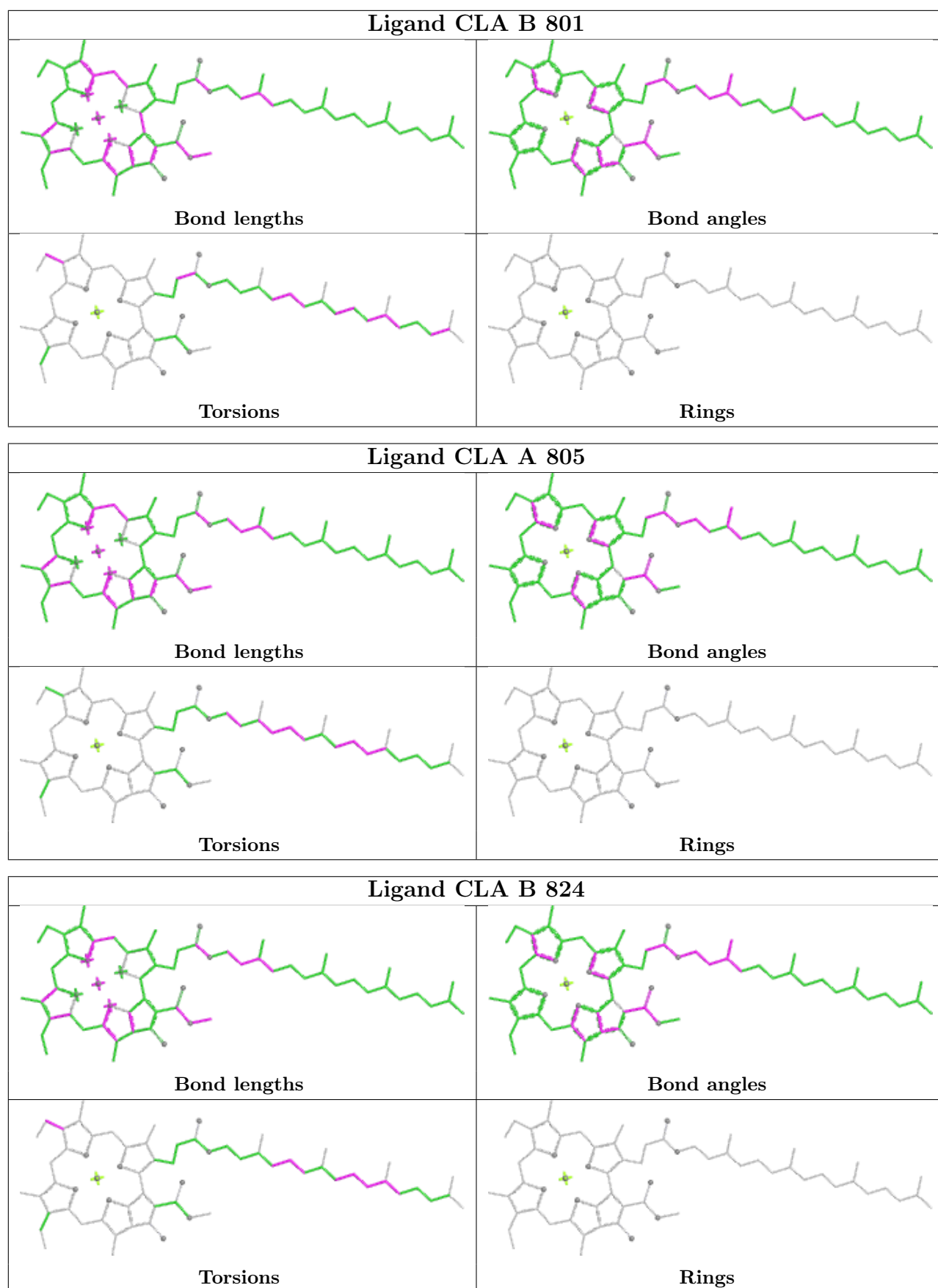


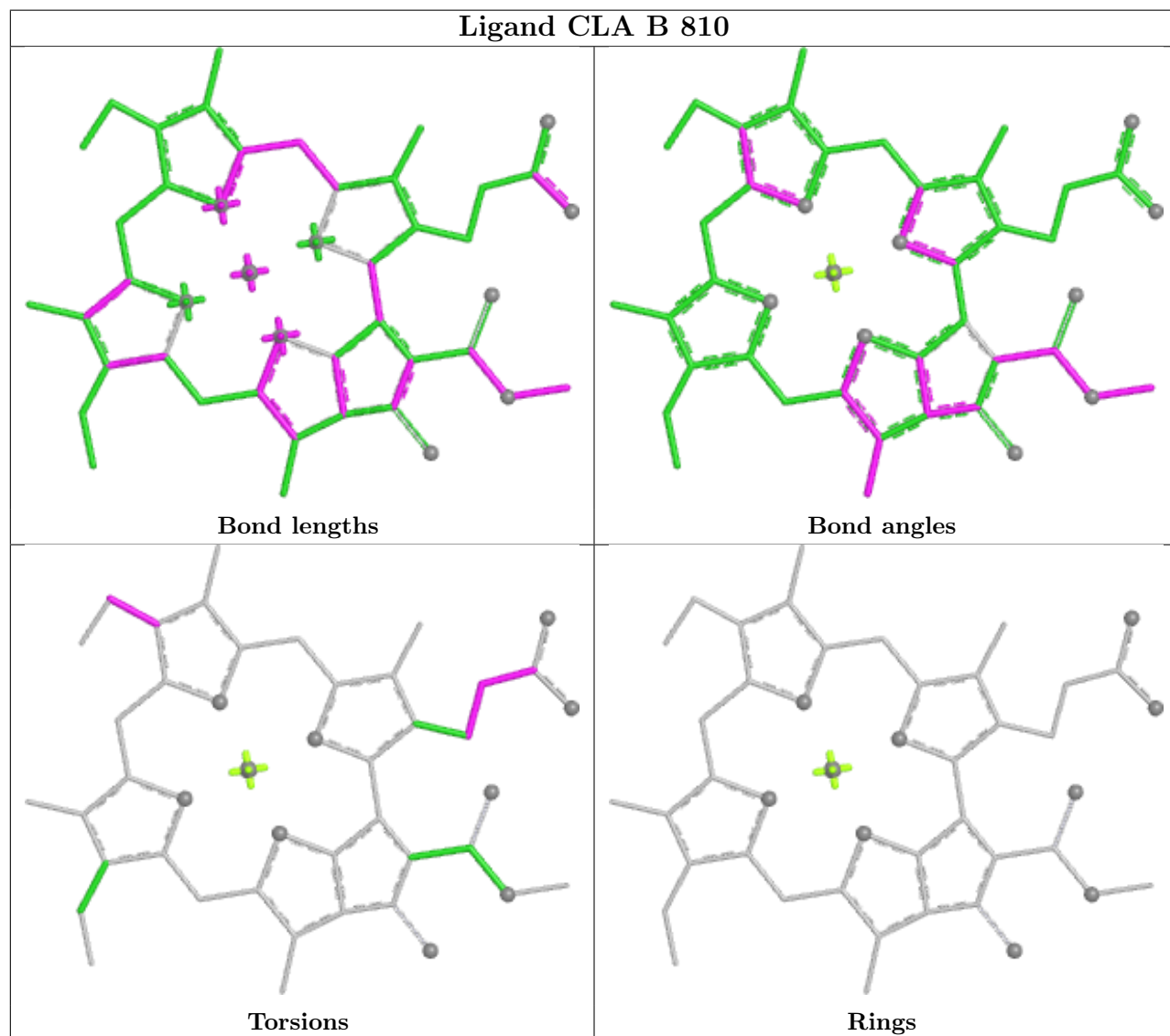
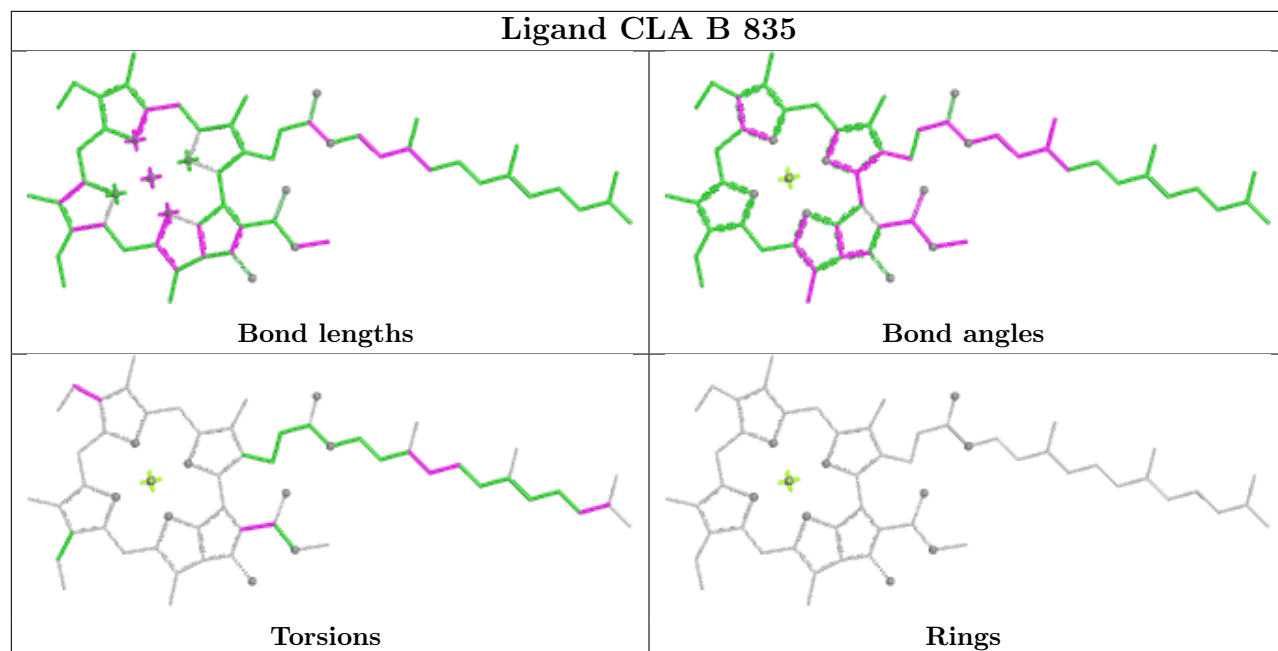


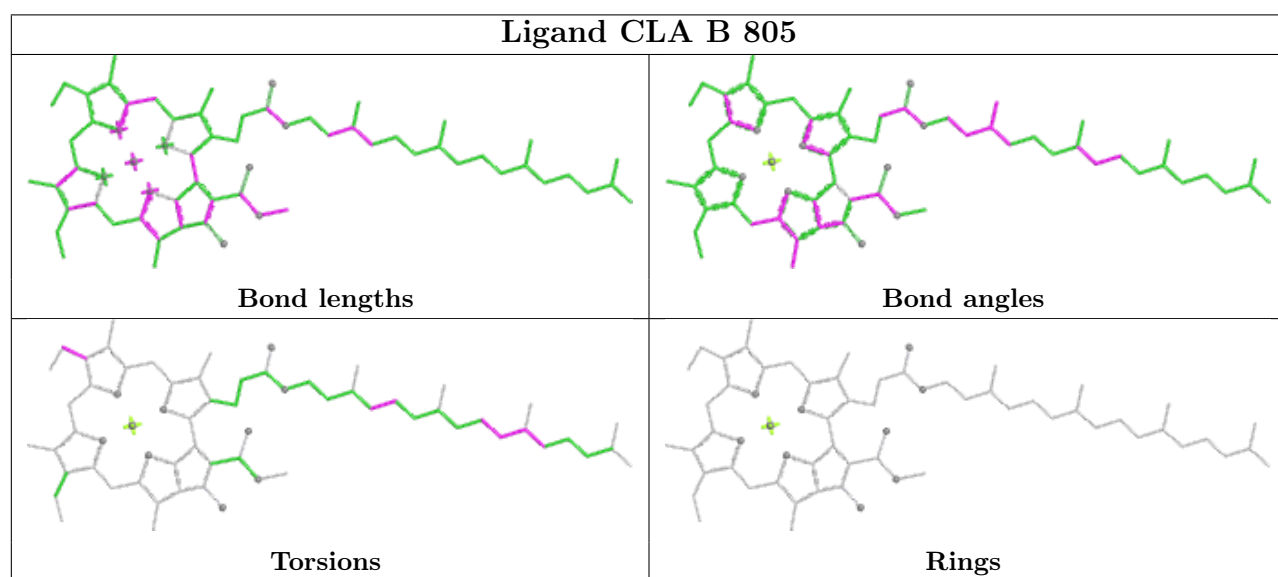
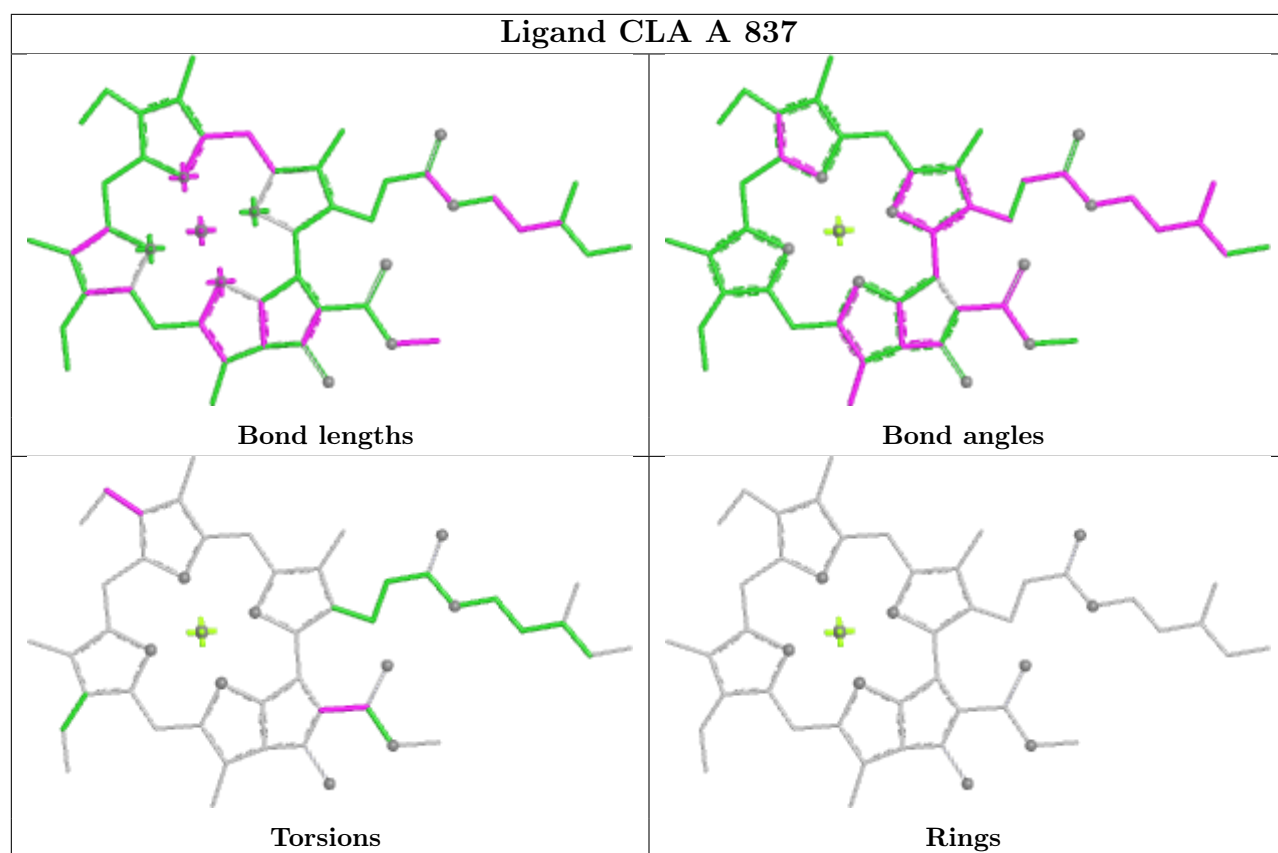


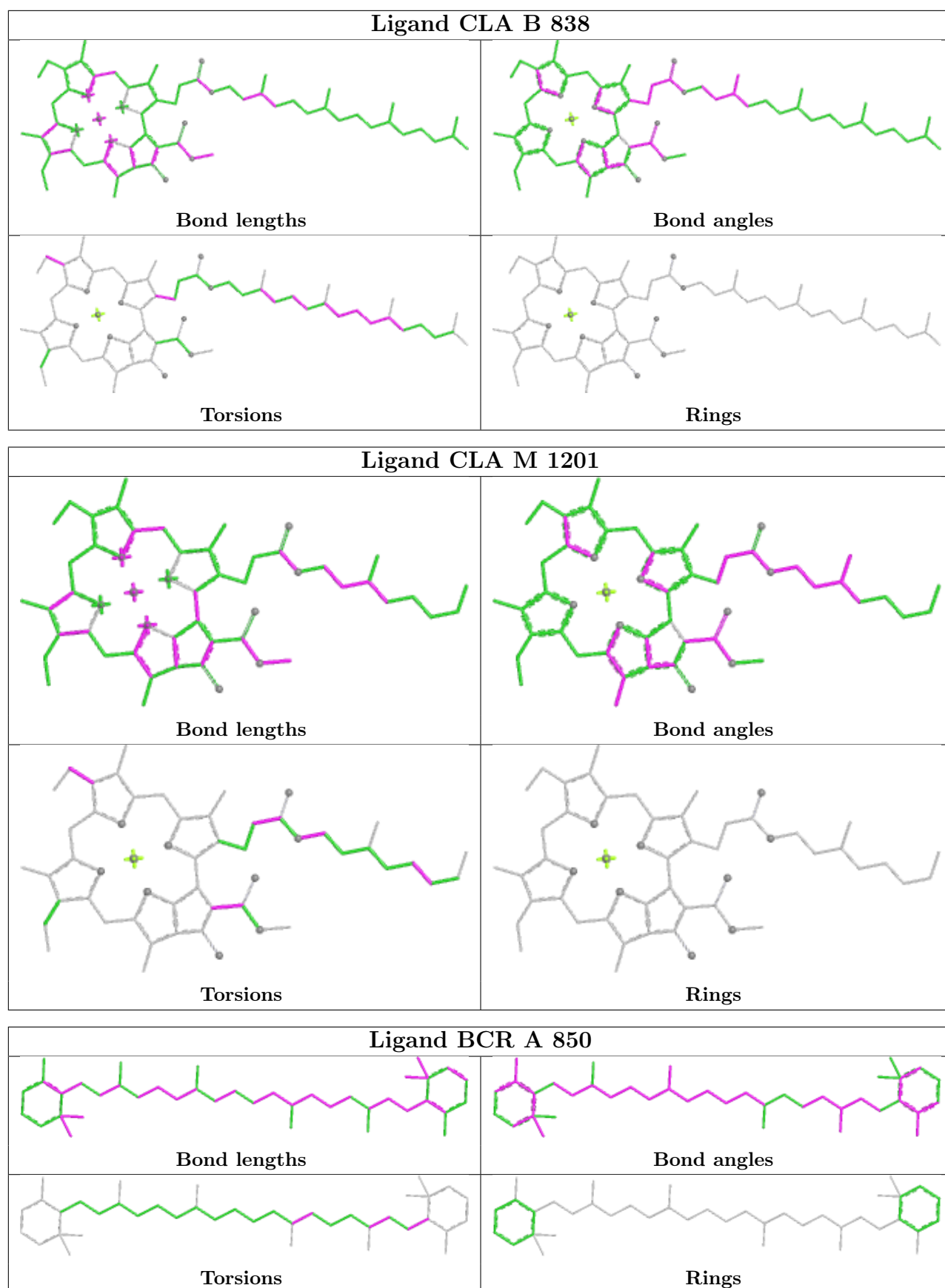


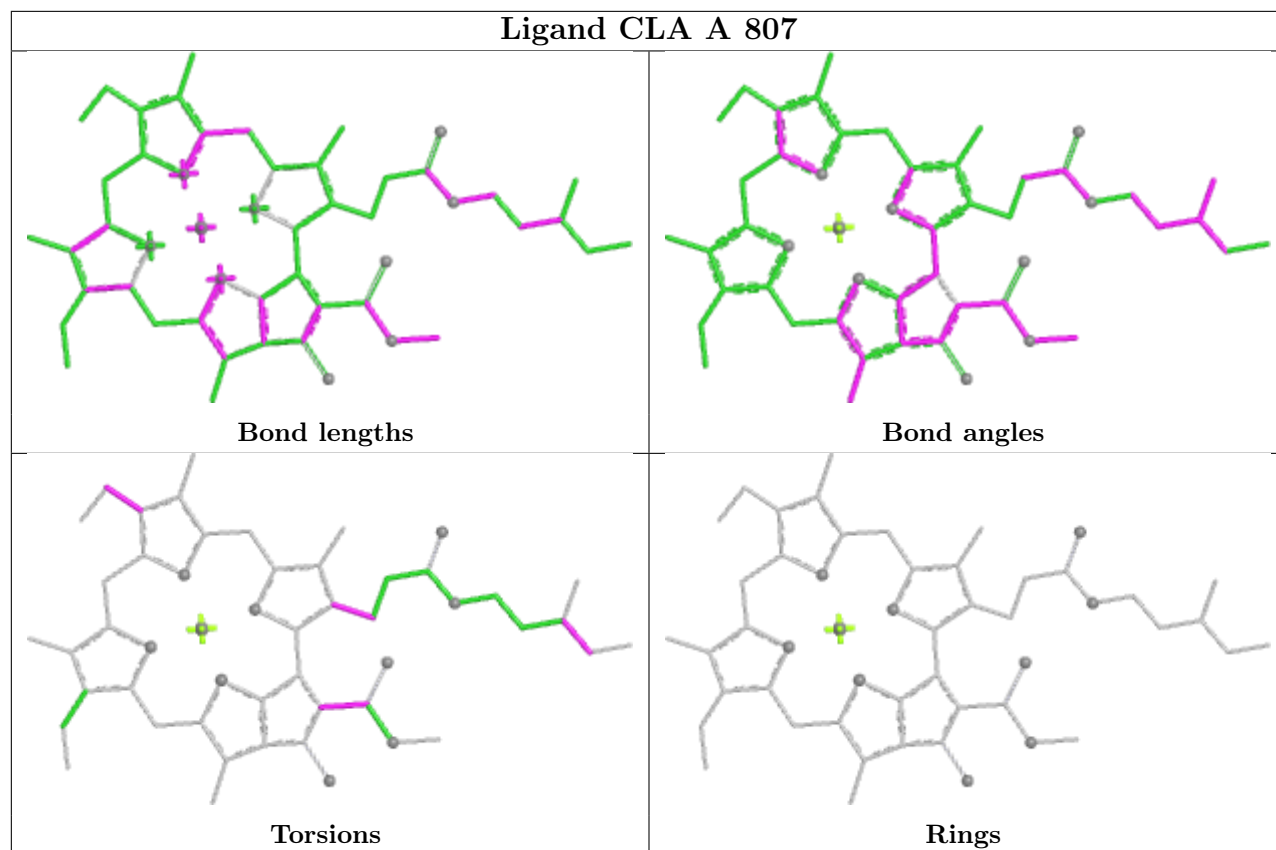
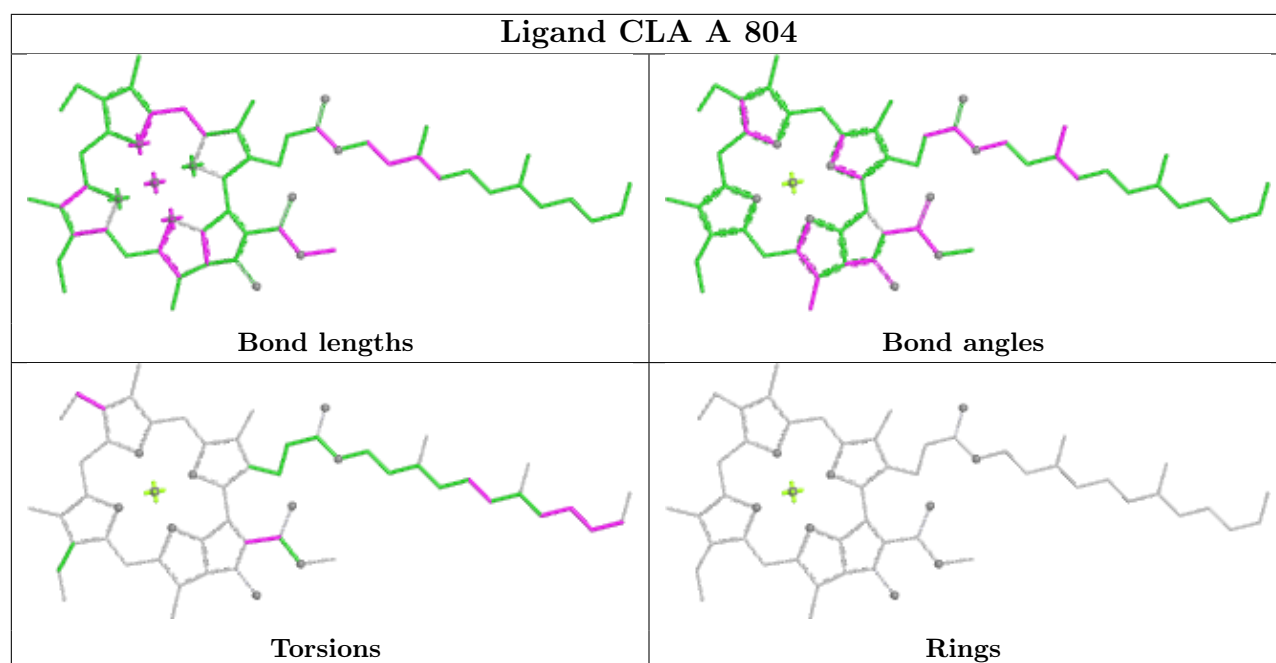


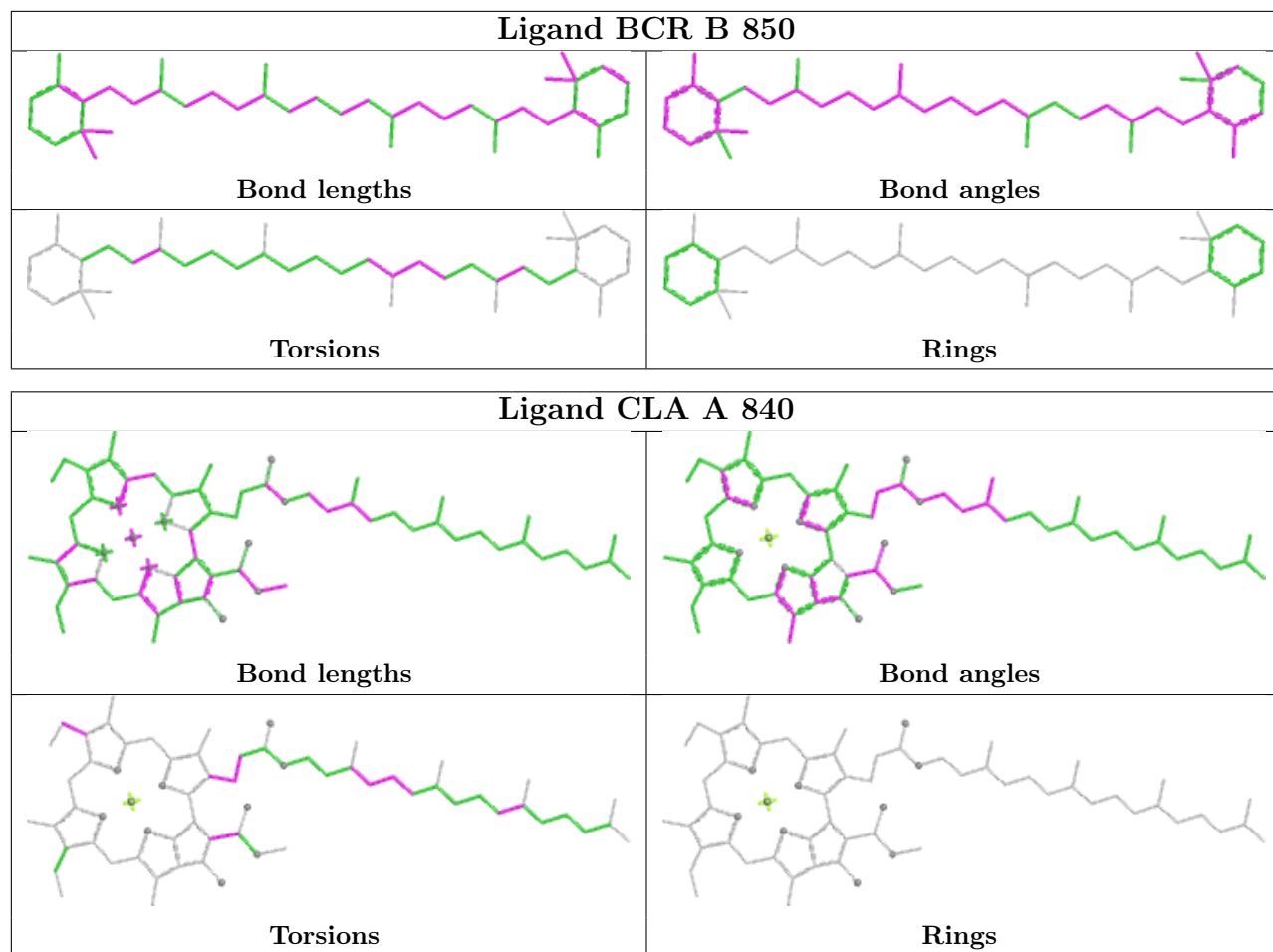


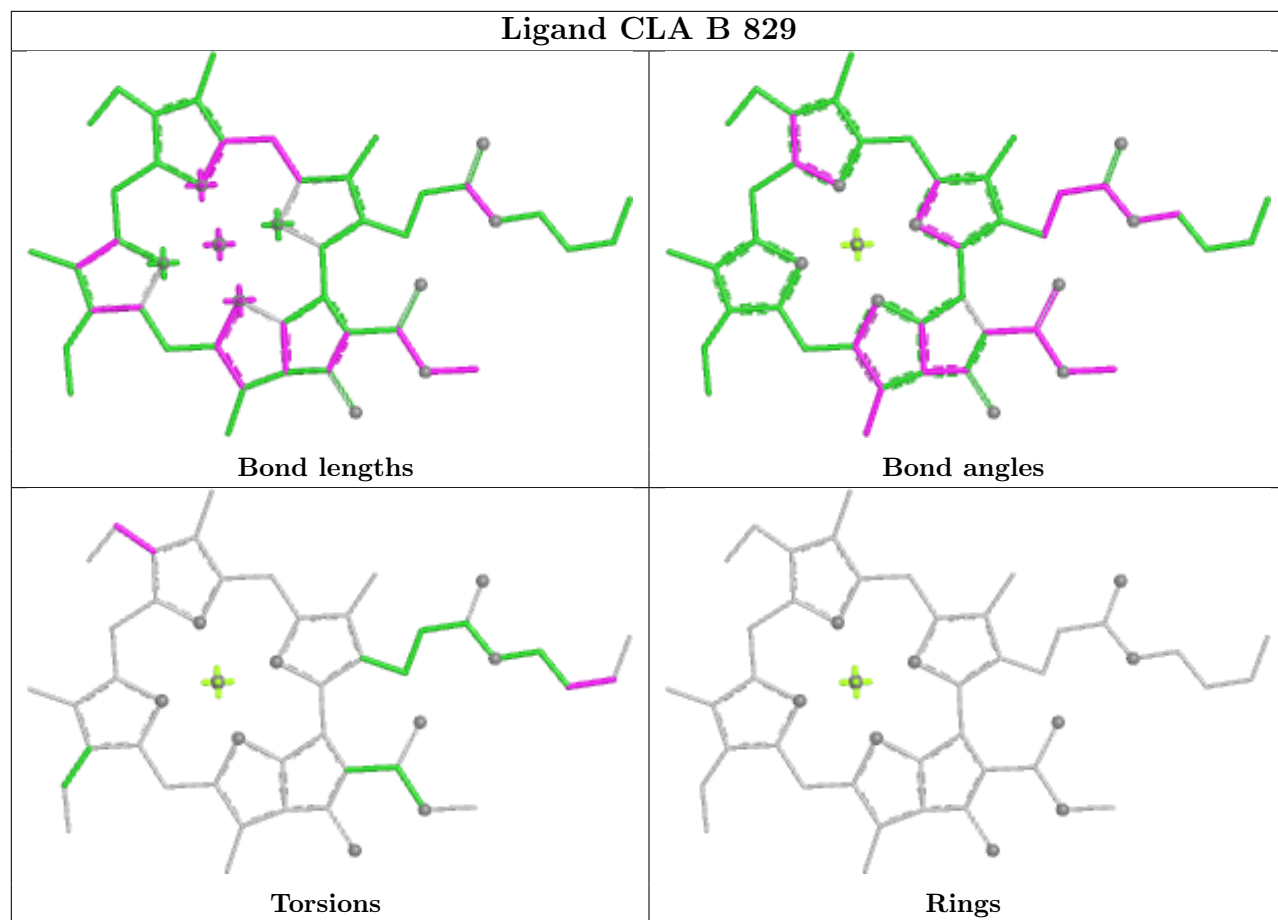


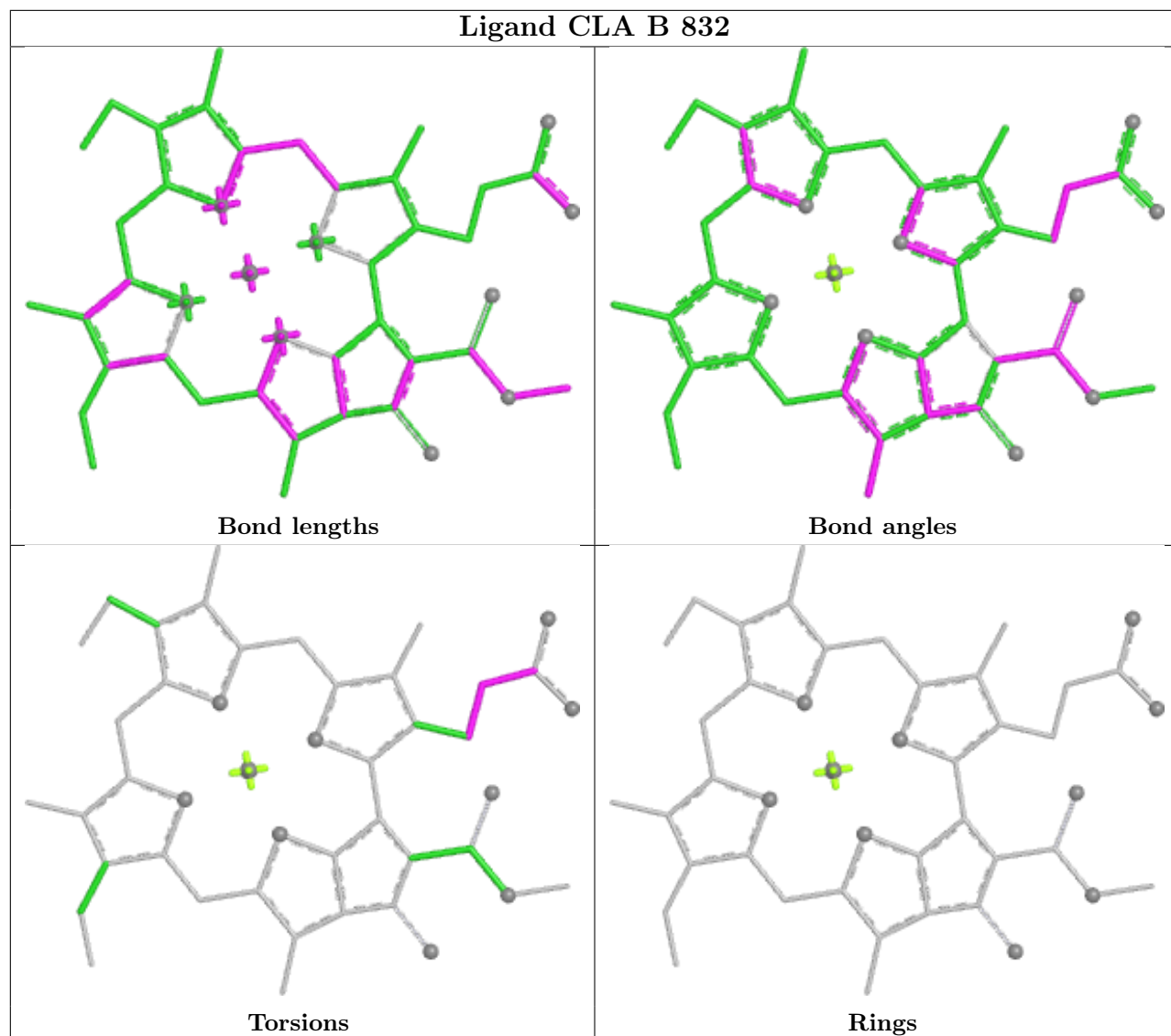


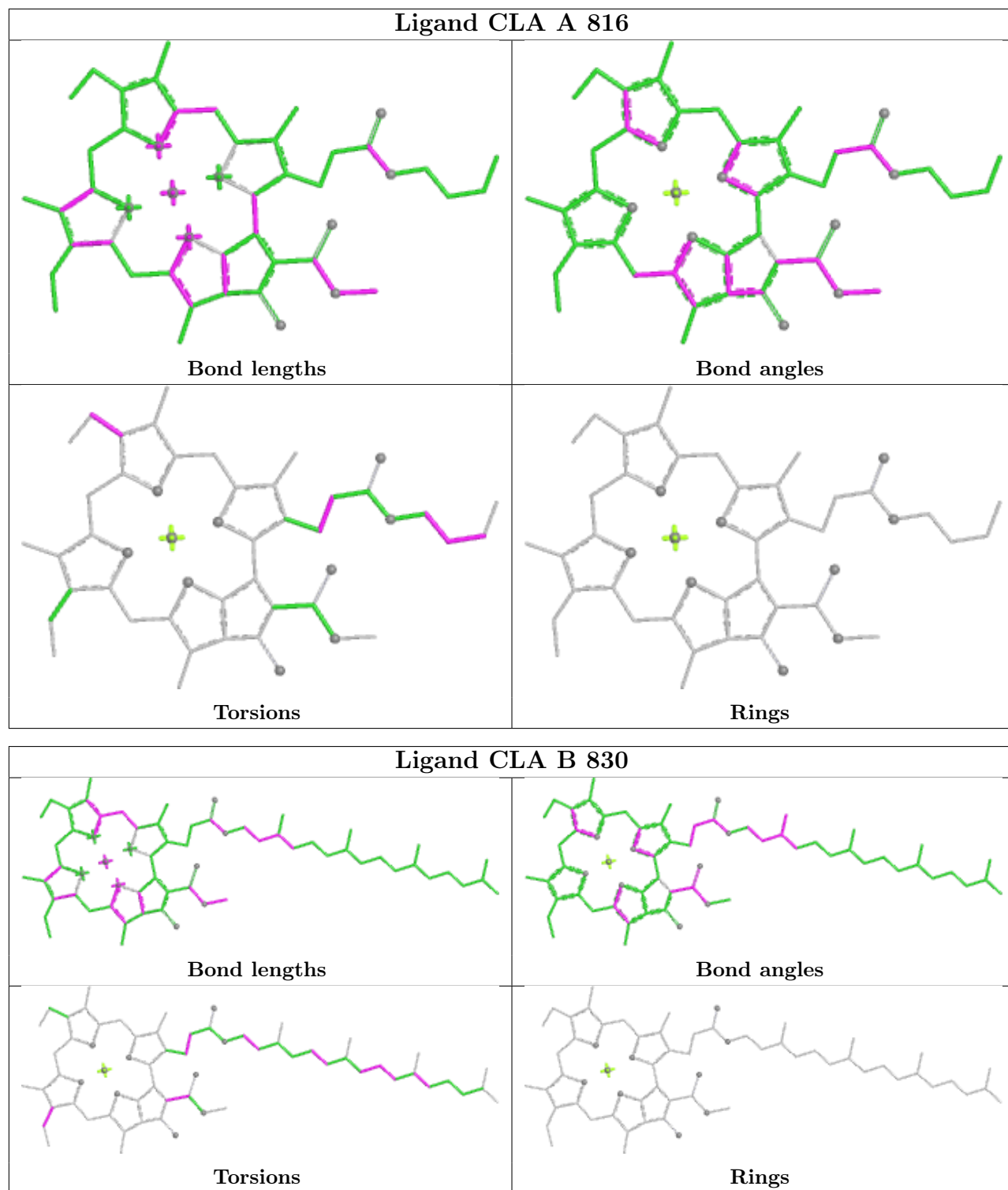


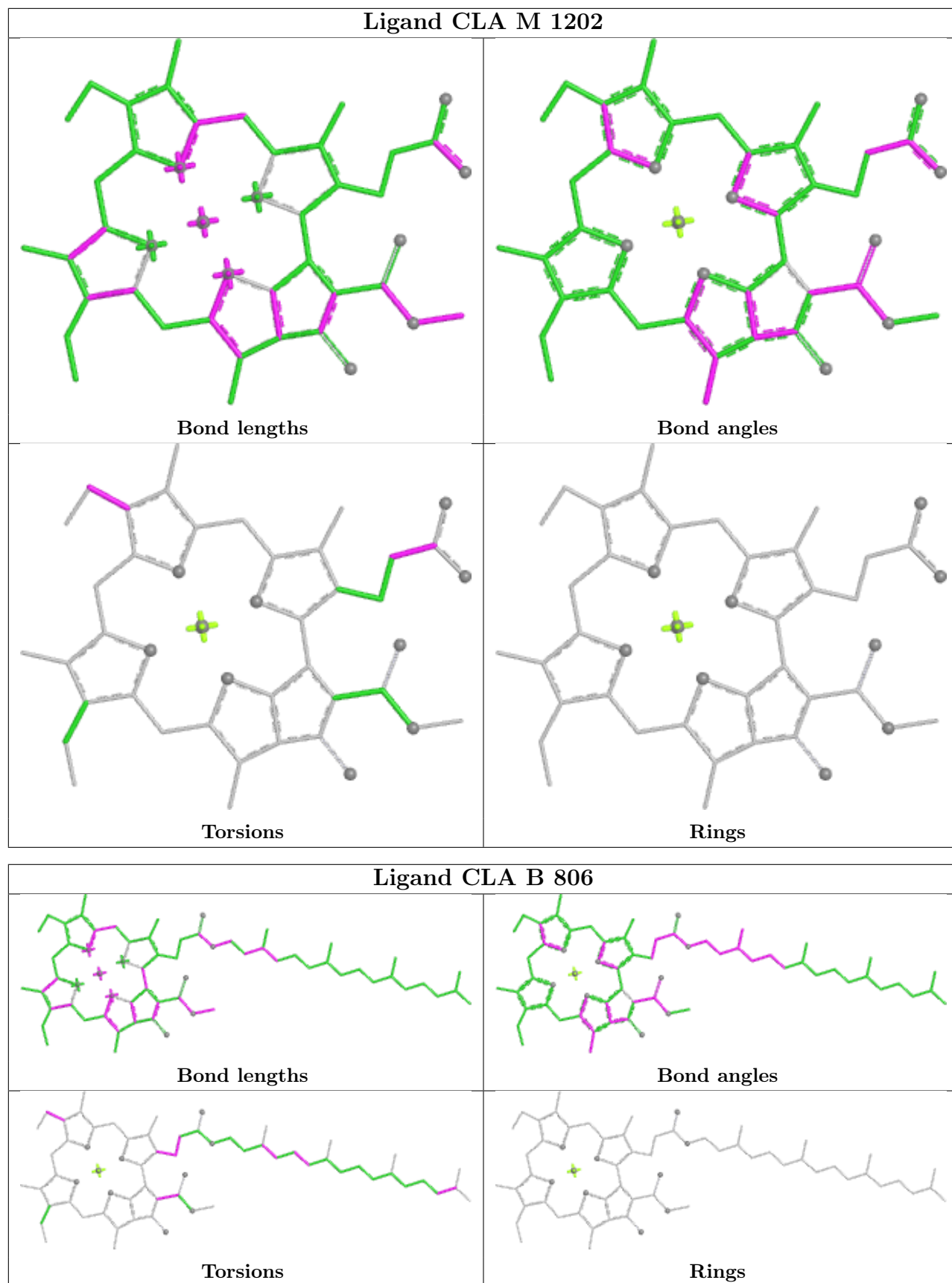


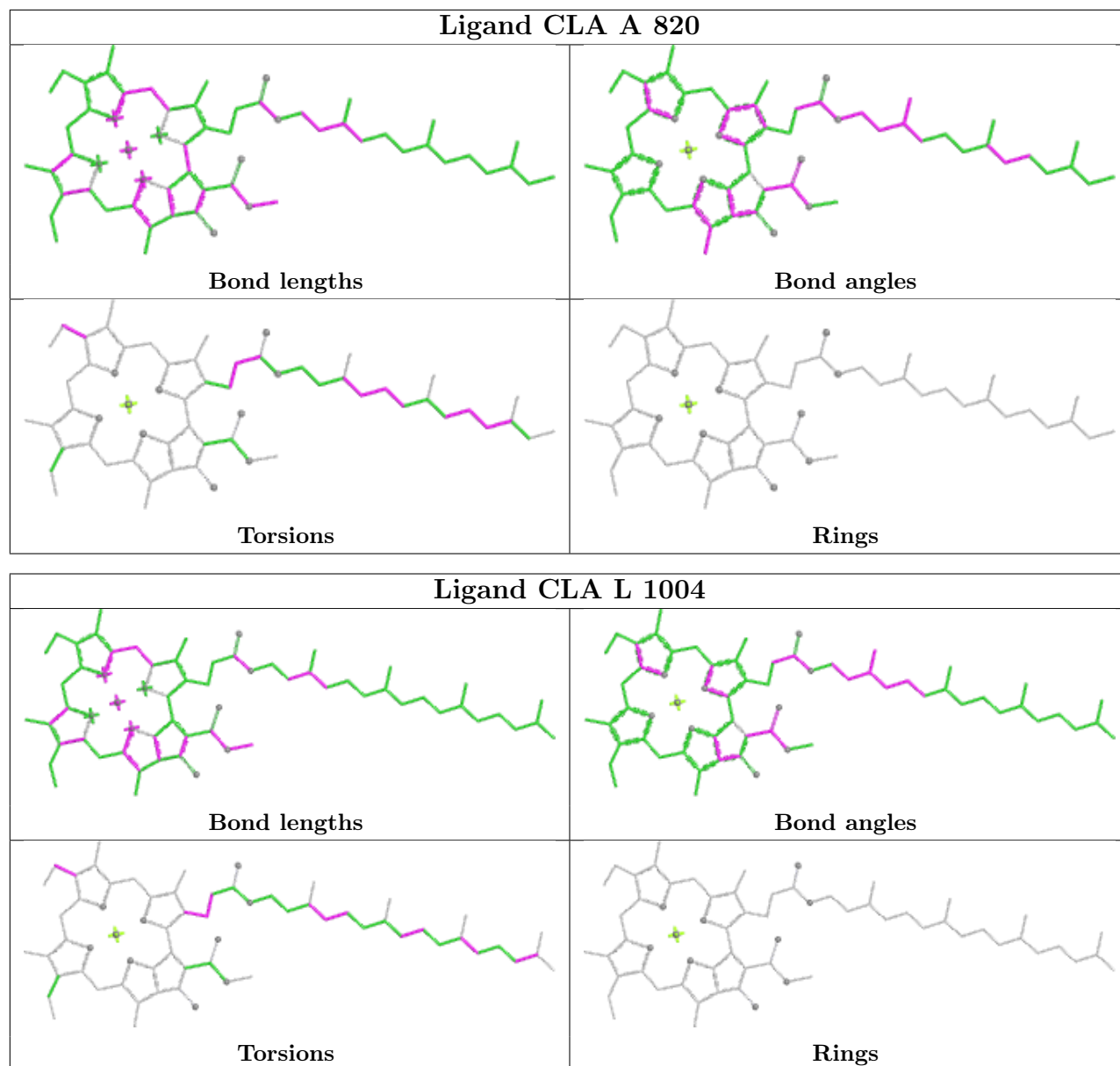


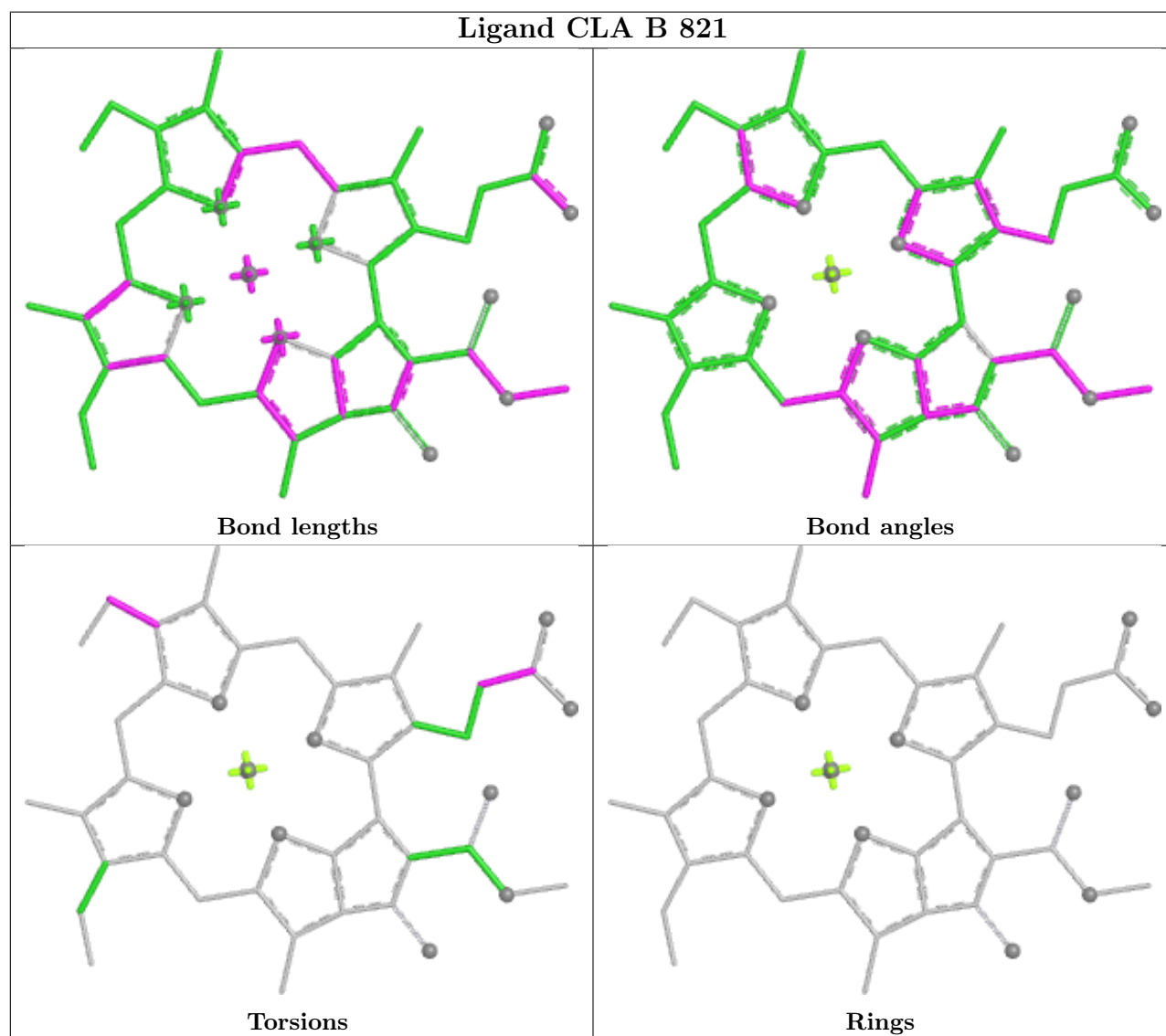
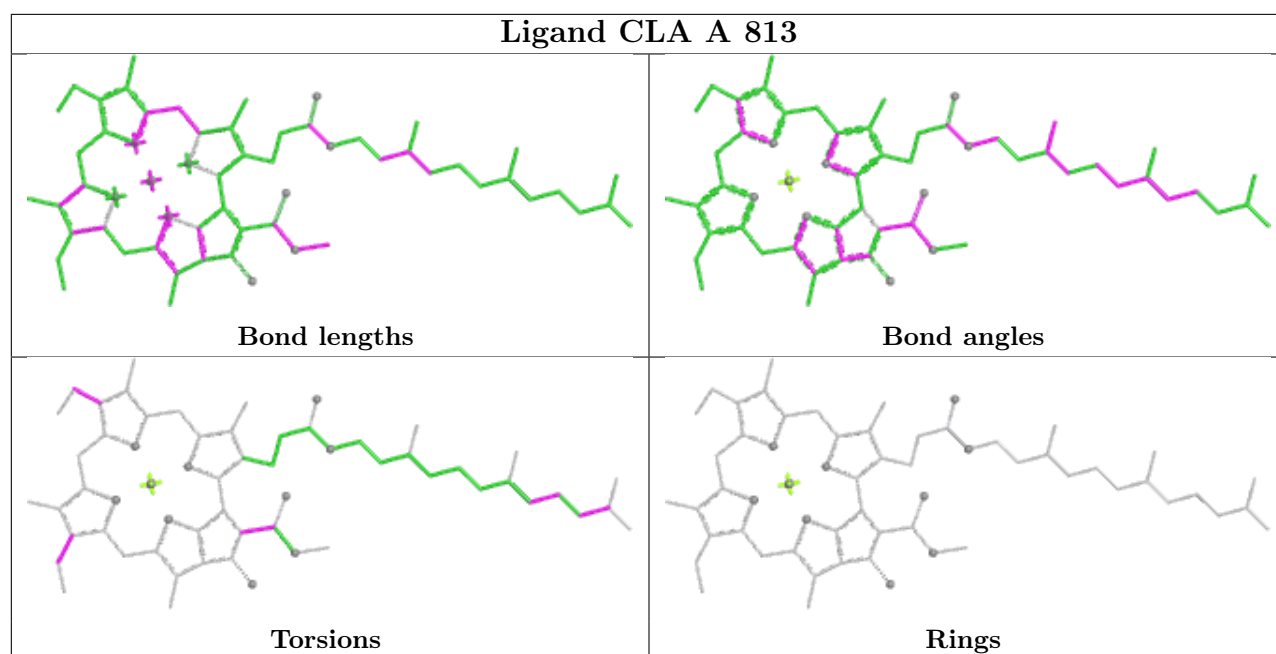


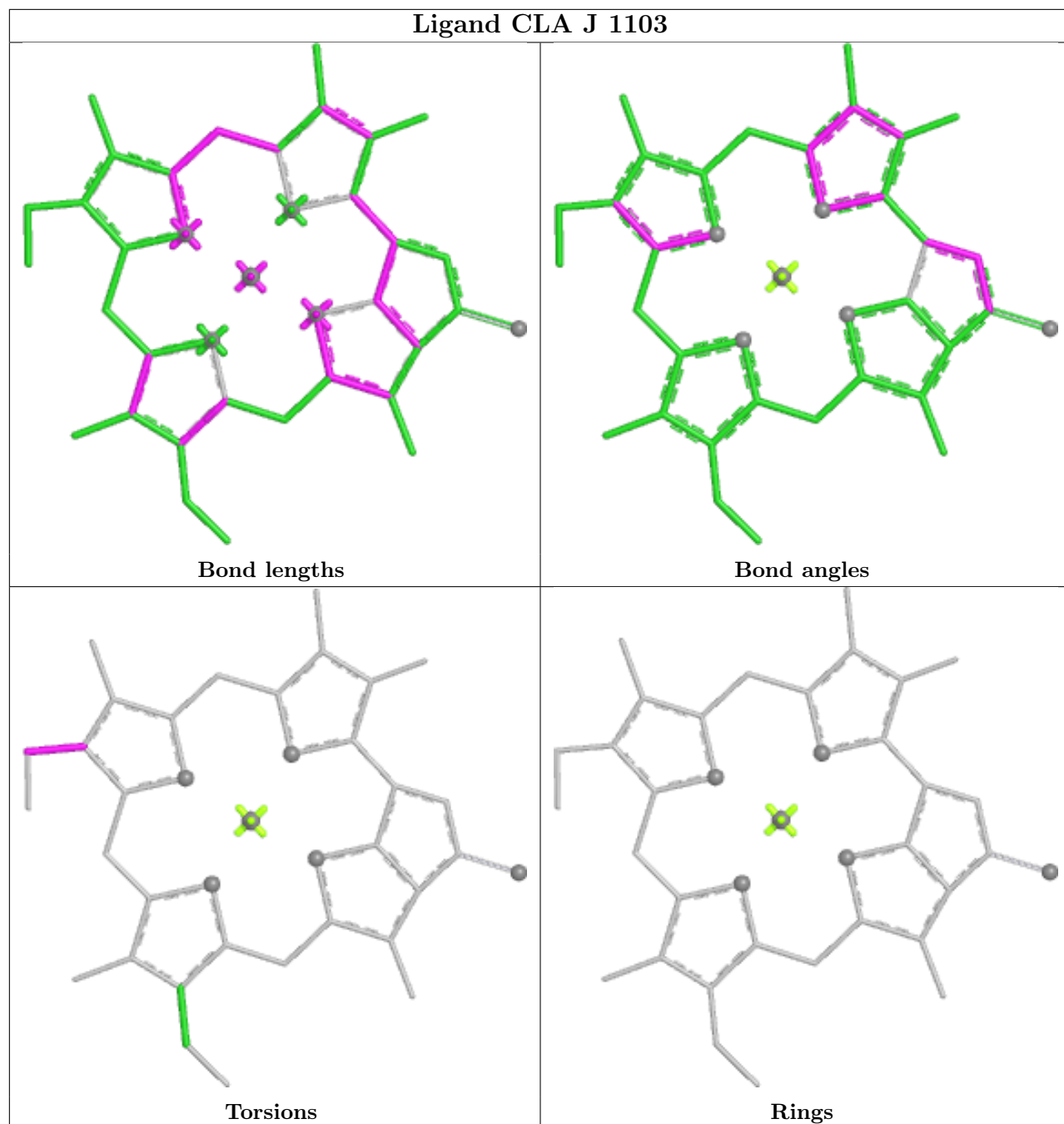


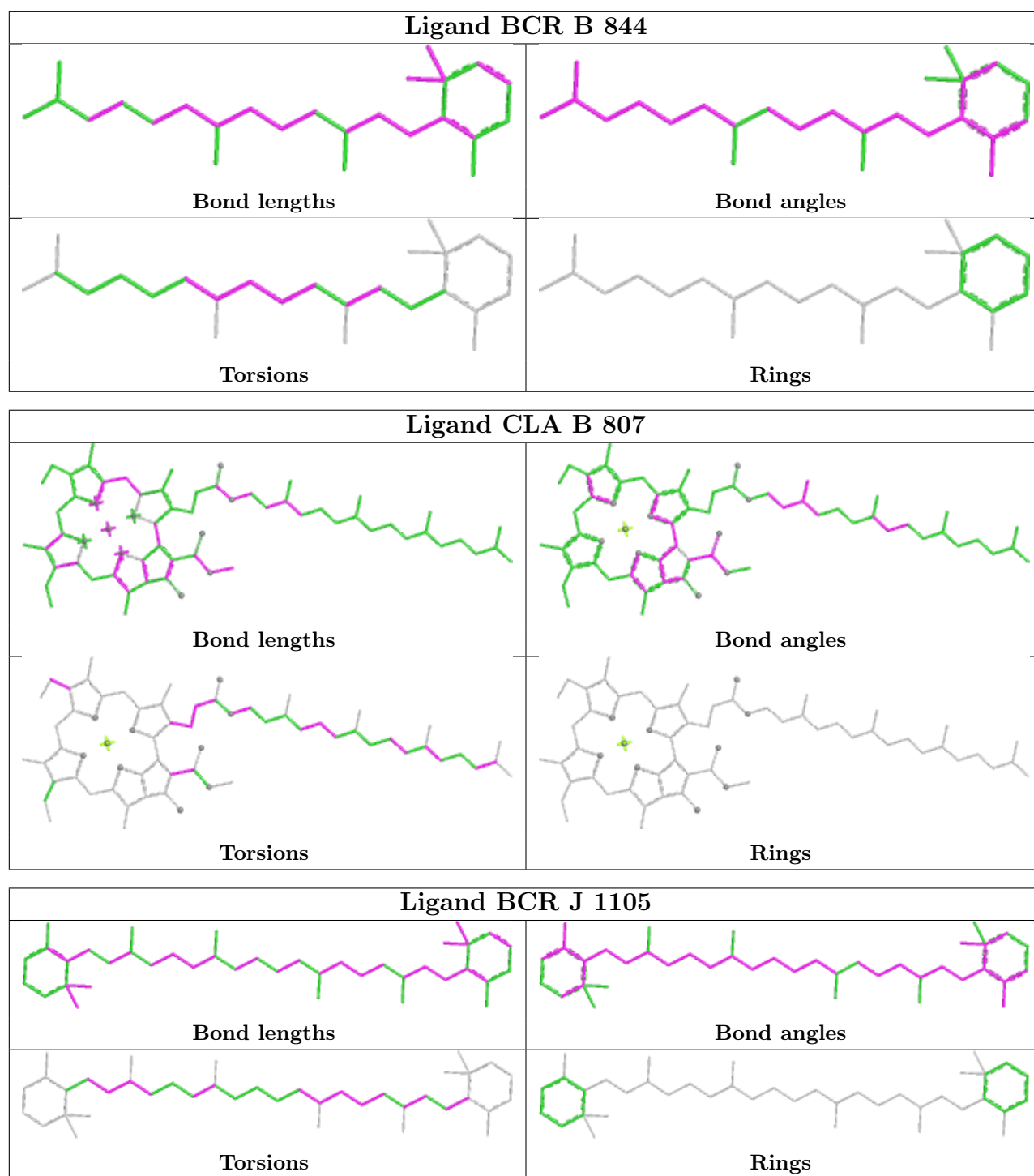


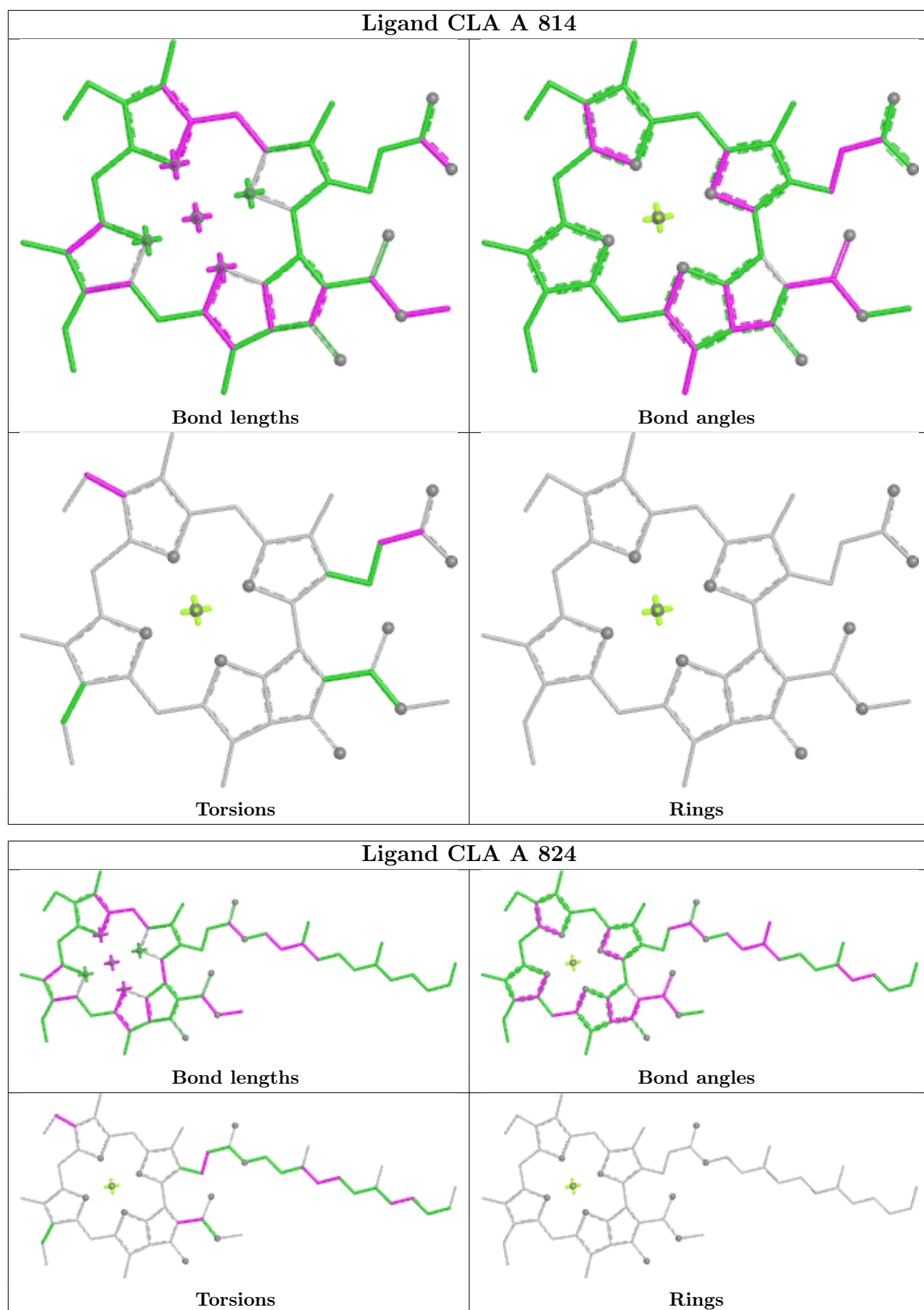


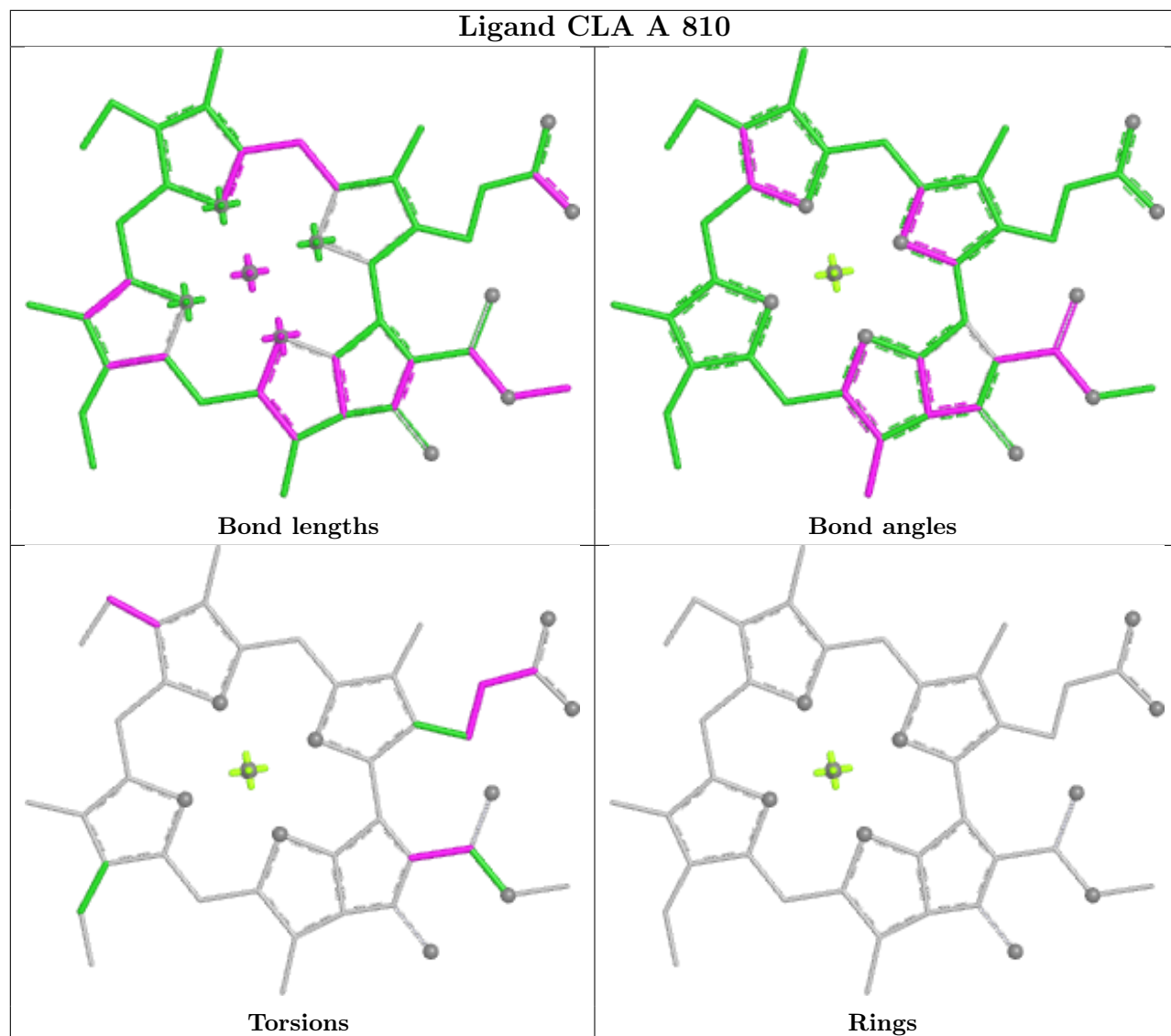


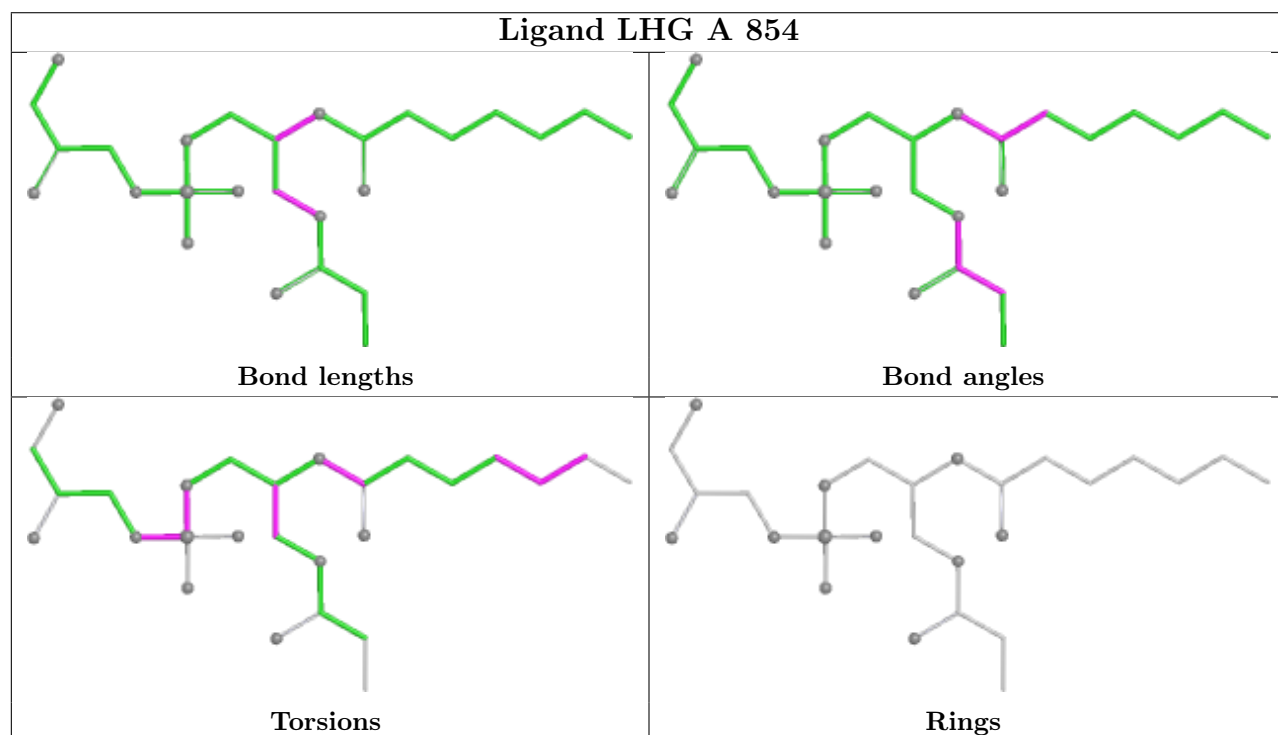
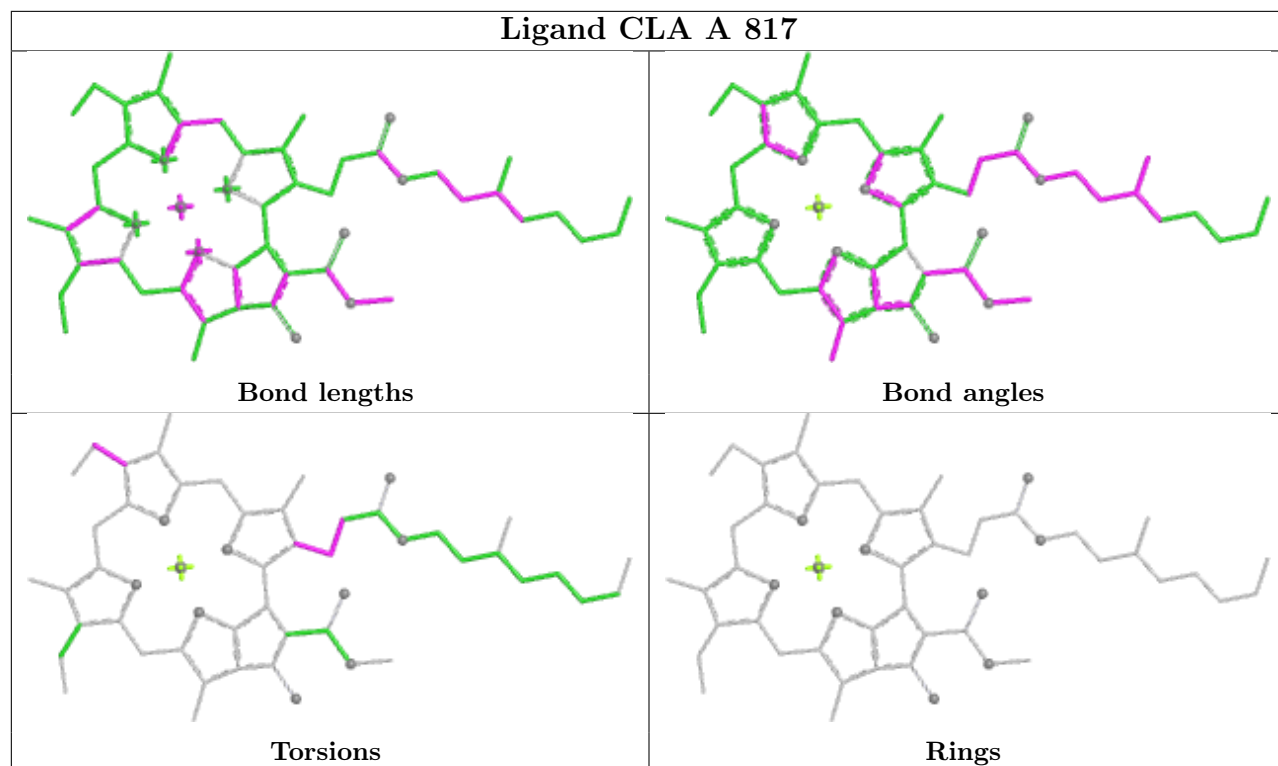


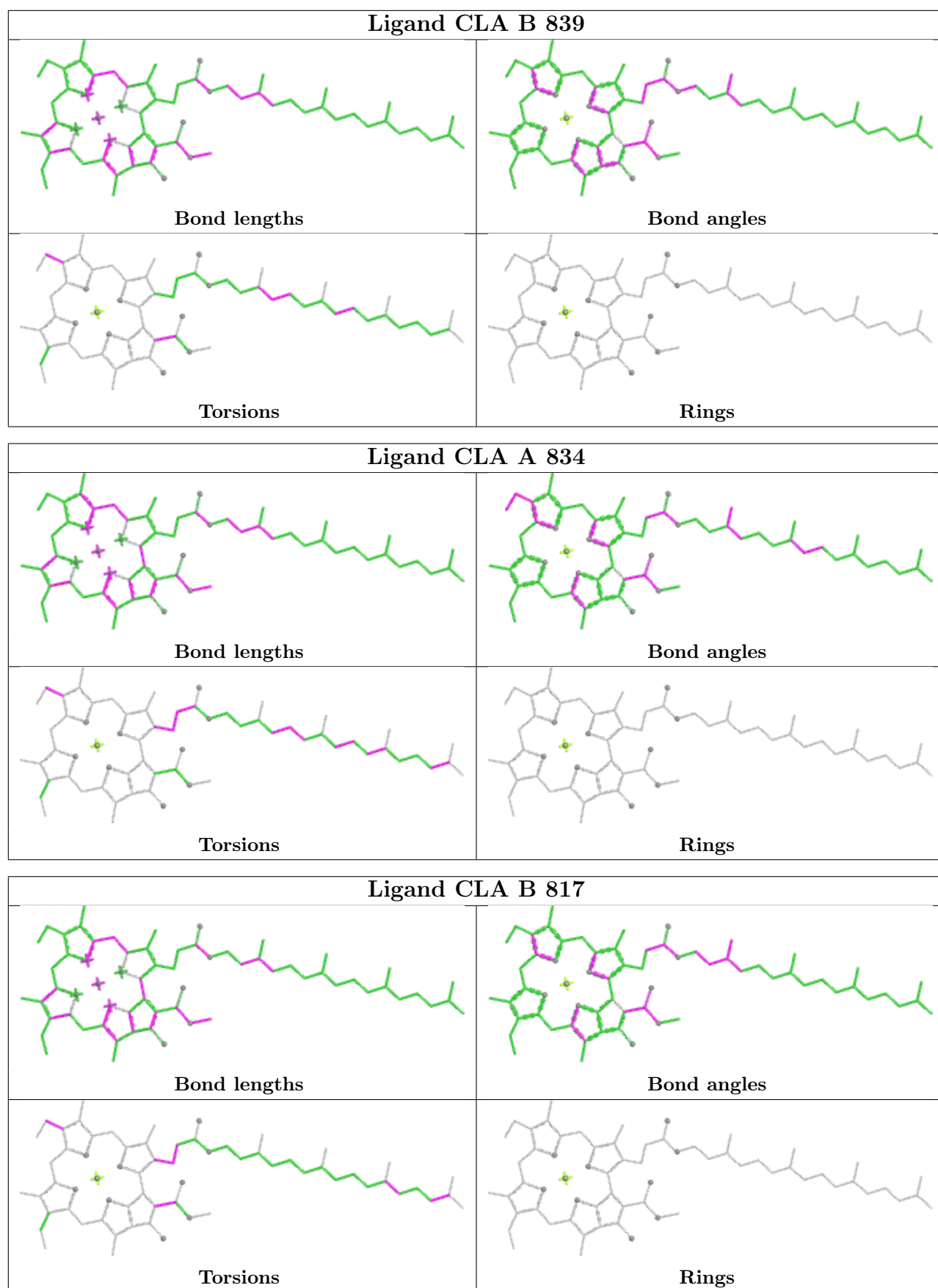


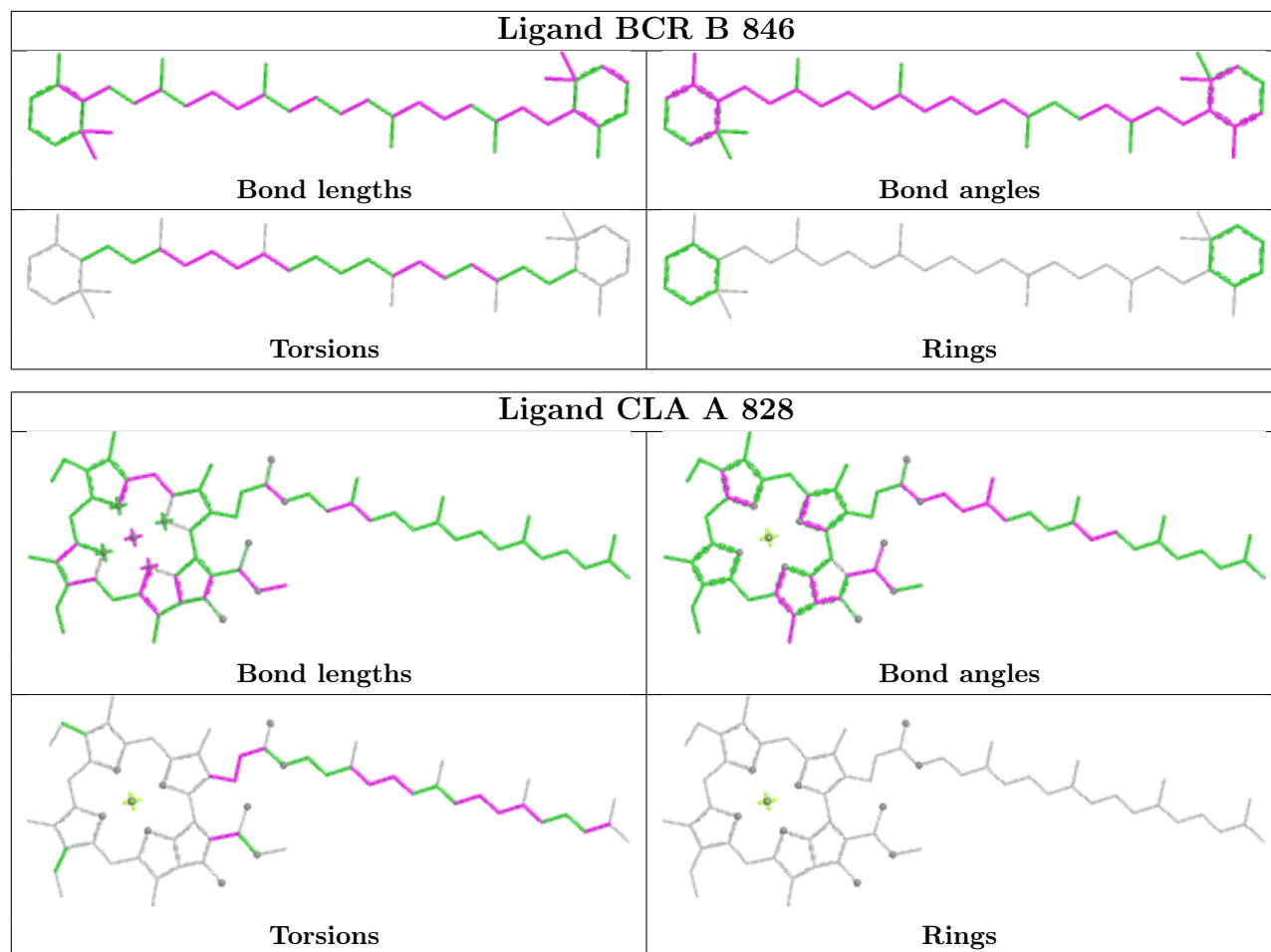


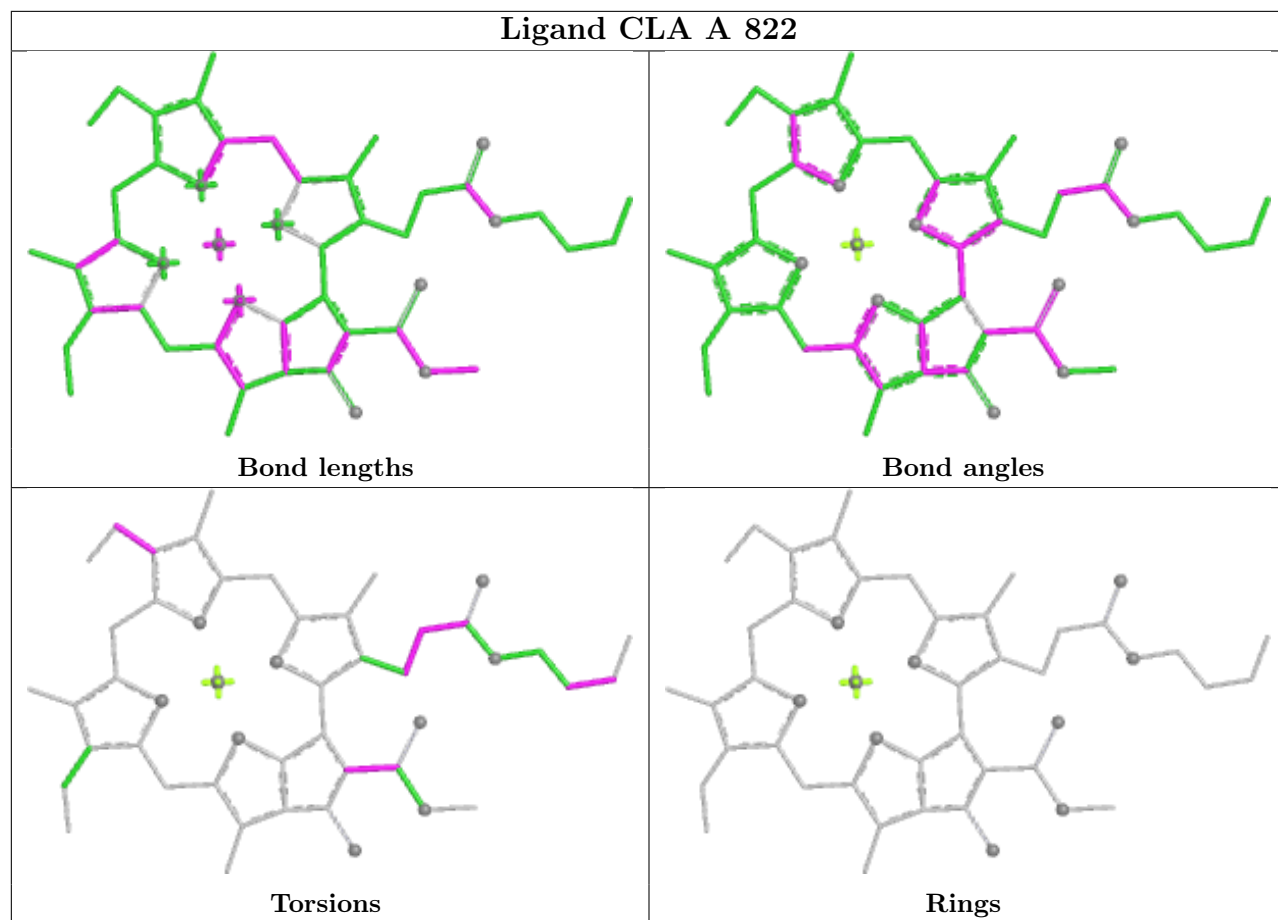


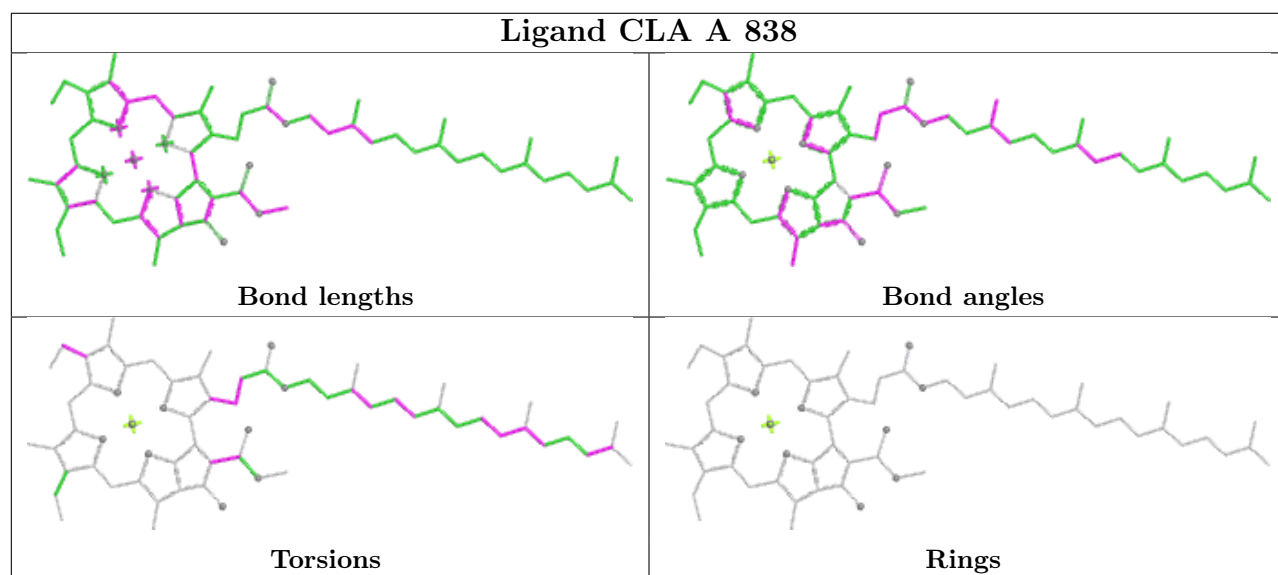
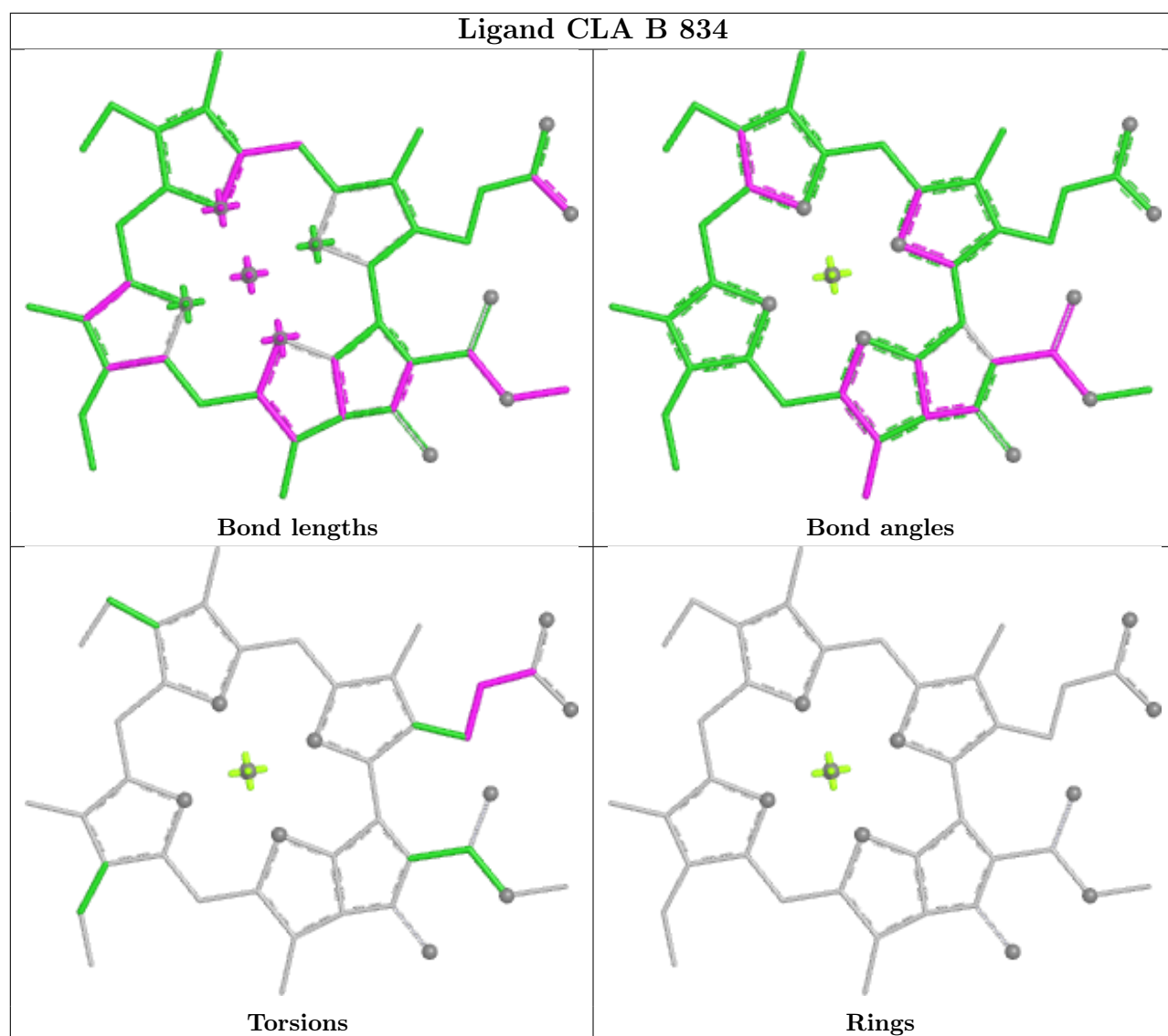


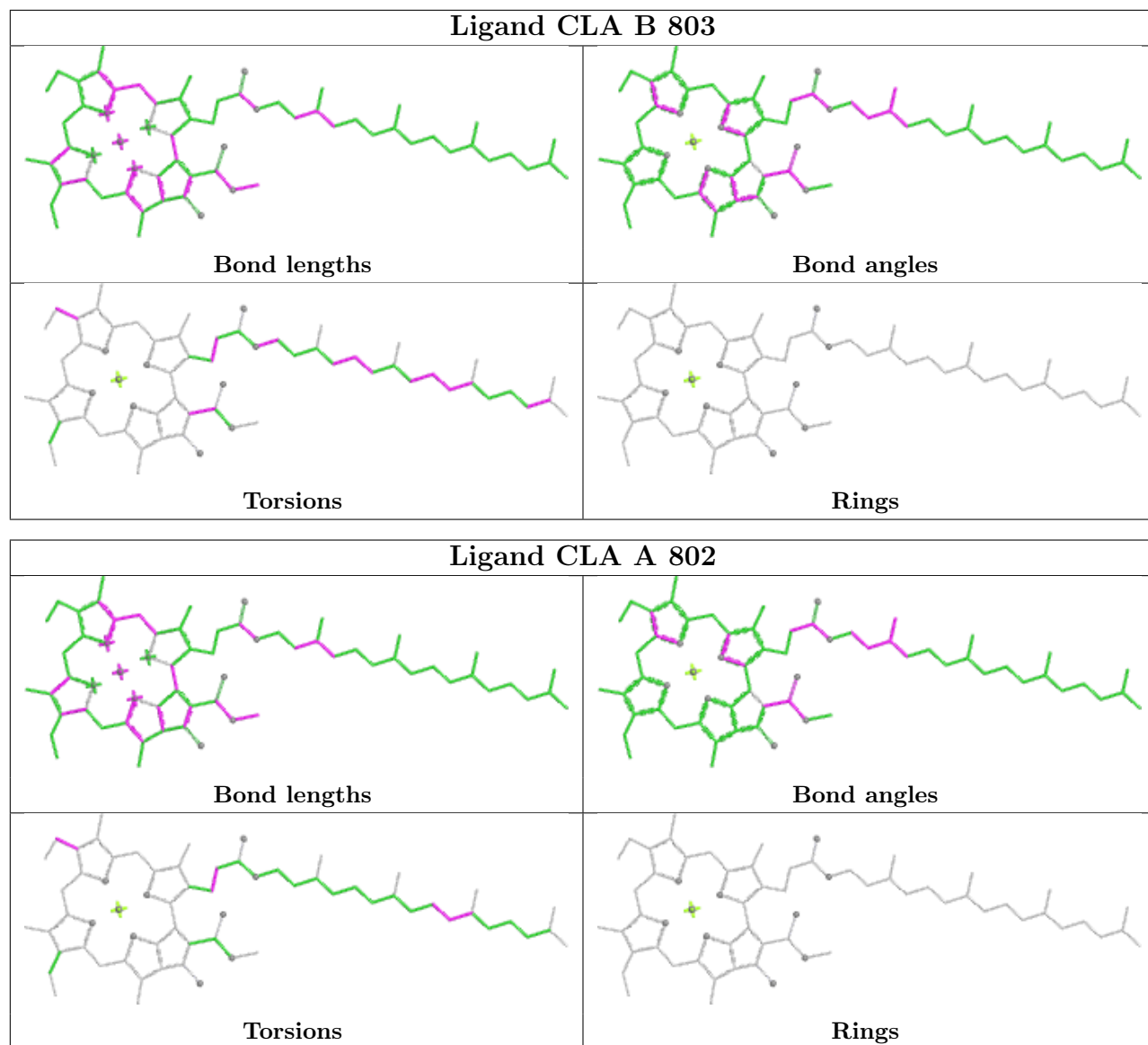


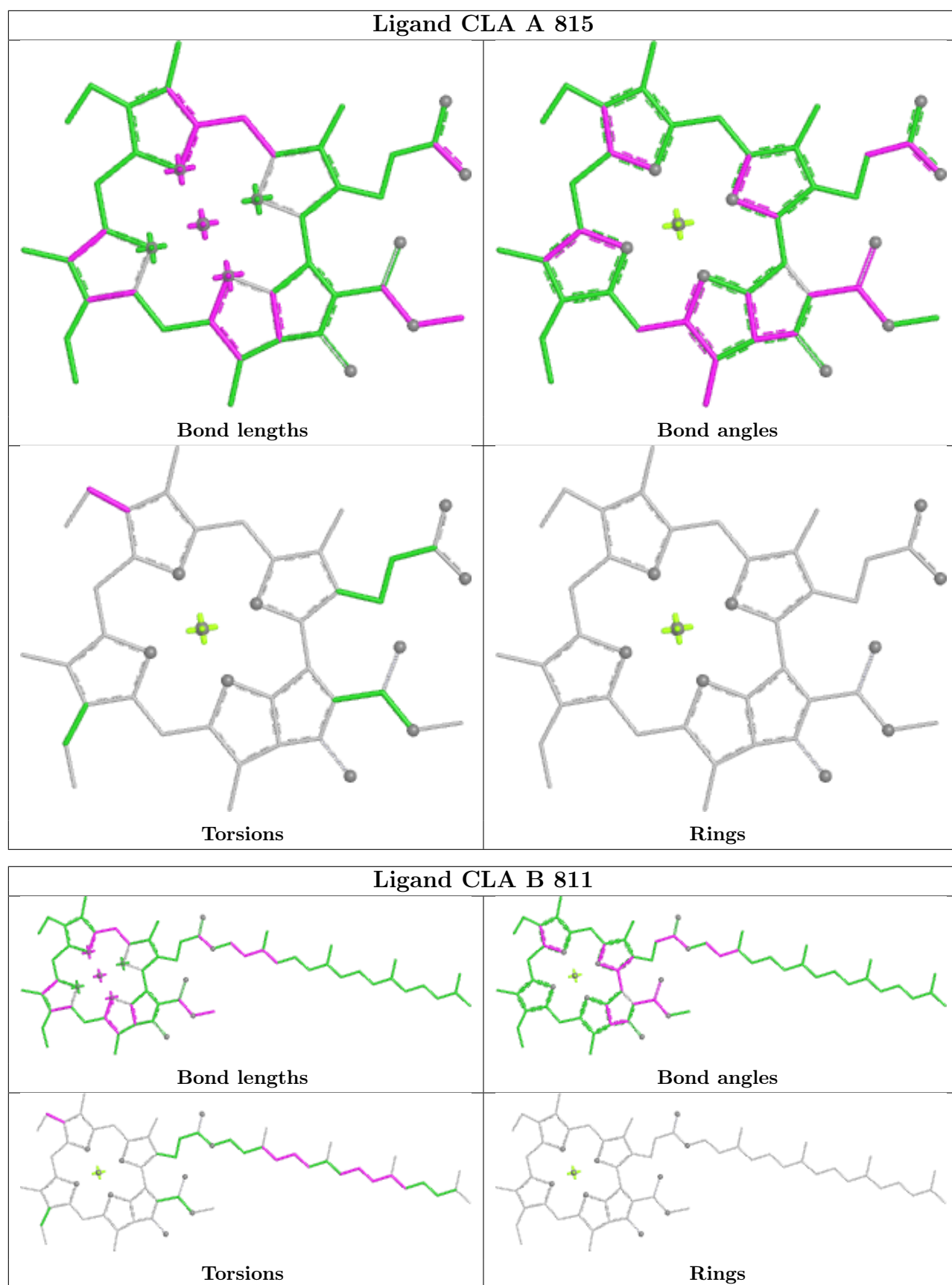












5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	740/755 (98%)	-0.50	1 (0%) 92 87	42, 99, 157, 202	0
2	B	739/740 (99%)	-0.56	0 100 100	34, 76, 126, 215	0
3	C	80/80 (100%)	-0.70	0 100 100	46, 72, 126, 138	0
4	D	138/138 (100%)	-0.62	0 100 100	45, 72, 117, 137	0
5	E	69/75 (92%)	-0.58	0 100 100	77, 100, 148, 194	0
6	F	141/164 (85%)	-0.62	0 100 100	54, 83, 136, 158	0
7	I	38/38 (100%)	-0.65	0 100 100	10, 36, 74, 78	0
8	J	41/41 (100%)	-0.77	0 100 100	65, 89, 136, 165	0
9	K	46/83 (55%)	-0.68	0 100 100	55, 87, 141, 169	0
10	L	151/154 (98%)	-0.23	6 (3%) 42 37	14, 49, 104, 140	0
11	M	31/31 (100%)	-0.71	0 100 100	31, 51, 80, 92	0
12	X	29/35 (82%)	-0.56	0 100 100	59, 80, 120, 155	0
All	All	2243/2334 (96%)	-0.54	7 (0%) 90 80	10, 81, 141, 215	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	L	107	SER	3.9
10	L	146	ASP	3.8
1	A	22	PRO	3.3
10	L	147	GLY	3.1
10	L	72	ASP	2.6

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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
13	CLA	A	812	54/65	0.97	0.11	136,181,240,396	0
13	CLA	B	832	45/65	0.97	0.12	71,121,142,247	0
13	CLA	B	834	45/65	0.97	0.10	91,118,151,158	0
15	BCR	A	847	40/40	0.97	0.12	98,140,151,162	0
15	BCR	A	849	40/40	0.97	0.12	95,136,179,183	0
18	LMG	B	848	55/55	0.97	0.12	42,51,67,114	0
13	CLA	A	801	65/65	0.98	0.09	44,53,82,89	0
13	CLA	A	813	60/65	0.98	0.08	115,146,178,366	0
13	CLA	A	816	49/65	0.98	0.12	119,163,187,193	0
13	CLA	A	817	54/65	0.98	0.08	83,104,164,172	0
13	CLA	A	820	61/65	0.98	0.08	119,135,166,198	0
13	CLA	A	822	49/65	0.98	0.10	102,126,157,235	0
13	CLA	A	823	51/65	0.98	0.09	74,129,153,156	0
13	CLA	A	827	65/65	0.98	0.10	68,103,137,248	0
13	CLA	A	829	65/65	0.98	0.10	83,108,179,197	0
13	CLA	A	835	54/65	0.98	0.11	54,79,117,204	0
13	CLA	A	839	47/65	0.98	0.08	48,51,119,202	0
13	CLA	A	840	65/65	0.98	0.10	77,87,117,198	0
13	CLA	A	841	51/65	0.98	0.09	80,105,182,204	0
13	CLA	A	843	65/65	0.98	0.10	56,83,169,197	0
13	CLA	A	844	41/65	0.98	0.08	116,136,148,281	0
13	CLA	A	845	52/65	0.98	0.09	56,78,188,214	0
13	CLA	A	855	45/65	0.98	0.08	95,118,140,153	0
13	CLA	B	802	65/65	0.98	0.09	61,82,112,165	0
13	CLA	B	803	65/65	0.98	0.11	40,68,95,180	0
13	CLA	B	808	65/65	0.98	0.10	36,41,97,103	0
13	CLA	B	810	45/65	0.98	0.09	47,84,145,182	0
13	CLA	B	812	65/65	0.98	0.10	37,42,111,117	0
13	CLA	B	813	45/65	0.98	0.09	51,86,132,141	0
13	CLA	B	814	55/65	0.98	0.10	77,122,182,325	0
13	CLA	B	815	59/65	0.98	0.09	55,58,76,293	0
13	CLA	B	817	65/65	0.98	0.09	57,65,113,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
13	CLA	B	820	55/65	0.98	0.09	77,105,141,146	0
13	CLA	B	821	45/65	0.98	0.09	63,69,105,191	0
13	CLA	B	823	46/65	0.98	0.09	59,68,120,137	0
13	CLA	B	824	65/65	0.98	0.10	58,65,88,96	0
13	CLA	B	828	45/65	0.98	0.09	70,80,132,193	0
13	CLA	B	829	49/65	0.98	0.11	80,85,125,141	0
13	CLA	A	804	59/65	0.98	0.09	83,99,117,144	0
13	CLA	B	833	45/65	0.98	0.09	77,104,141,148	0
13	CLA	A	807	51/65	0.98	0.09	87,100,151,177	0
13	CLA	B	835	60/65	0.98	0.08	65,106,240,292	0
13	CLA	B	838	65/65	0.98	0.11	35,45,102,125	0
13	CLA	B	839	65/65	0.98	0.09	35,49,151,215	0
13	CLA	F	1301	45/65	0.98	0.09	94,137,167,175	0
13	CLA	J	1102	45/65	0.98	0.08	75,111,128,280	0
14	PQN	A	846	33/33	0.98	0.09	55,64,82,82	0
14	PQN	B	840	33/33	0.98	0.10	56,84,105,121	0
13	CLA	A	809	65/65	0.98	0.11	78,117,148,152	0
15	BCR	A	848	40/40	0.98	0.11	112,132,147,157	0
13	CLA	A	810	45/65	0.98	0.10	109,136,151,223	0
15	BCR	B	841	40/40	0.98	0.13	65,105,151,155	0
15	BCR	B	843	40/40	0.98	0.10	45,59,82,86	0
15	BCR	B	845	40/40	0.98	0.09	60,66,78,82	0
15	BCR	B	846	40/40	0.98	0.10	75,91,131,137	0
15	BCR	B	847	40/40	0.98	0.11	40,51,116,126	0
15	BCR	B	849	40/40	0.98	0.09	12,43,147,152	0
15	BCR	B	850	40/40	0.98	0.09	83,107,144,146	0
15	BCR	J	1104	40/40	0.98	0.10	64,78,113,120	0
15	BCR	L	1005	40/40	0.98	0.10	11,16,81,93	0
15	BCR	L	1006	40/40	0.98	0.10	16,24,64,78	0
15	BCR	M	1203	40/40	0.98	0.09	43,48,87,92	0
16	LHG	X	101	23/49	0.98	0.08	78,81,207,208	0
13	CLA	A	811	65/65	0.98	0.11	95,134,173,321	0
19	CA	L	1001	1/1	0.98	0.10	22,22,22,22	0
13	CLA	A	833	65/65	0.99	0.09	39,45,110,121	0
13	CLA	A	834	65/65	0.99	0.08	39,40,92,96	0
13	CLA	B	822	54/65	0.99	0.08	61,86,118,158	0
13	CLA	A	802	65/65	0.99	0.08	40,77,110,230	0
13	CLA	A	836	45/65	0.99	0.08	63,96,163,234	0
13	CLA	B	825	65/65	0.99	0.08	40,60,136,157	0
13	CLA	B	826	65/65	0.99	0.08	42,47,127,149	0
13	CLA	B	827	65/65	0.99	0.08	44,66,95,108	0
13	CLA	A	837	51/65	0.99	0.07	52,56,96,147	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	CLA	A	838	65/65	0.99	0.08	45,81,109,114	0
13	CLA	B	830	65/65	0.99	0.08	82,91,129,139	0
13	CLA	B	831	58/65	0.99	0.10	80,101,148,333	0
13	CLA	A	805	65/65	0.99	0.08	85,98,117,126	0
13	CLA	A	818	54/65	0.99	0.07	92,136,168,207	0
13	CLA	A	819	65/65	0.99	0.08	97,140,181,328	0
13	CLA	A	842	65/65	0.99	0.09	62,82,149,162	0
13	CLA	B	836	65/65	0.99	0.09	69,98,146,234	0
13	CLA	B	837	47/65	0.99	0.07	65,71,119,193	0
13	CLA	A	806	65/65	0.99	0.09	63,80,155,164	0
13	CLA	A	821	65/65	0.99	0.08	72,100,164,266	0
13	CLA	A	803	65/65	0.99	0.09	76,100,142,222	0
13	CLA	I	101	65/65	0.99	0.08	33,57,85,338	0
13	CLA	J	1101	65/65	0.99	0.09	77,129,178,357	0
13	CLA	A	808	65/65	0.99	0.08	72,89,172,177	0
13	CLA	J	1103	37/65	0.99	0.07	85,117,155,158	0
13	CLA	L	1002	65/65	0.99	0.09	29,65,103,148	0
13	CLA	L	1003	65/65	0.99	0.08	16,52,179,216	0
13	CLA	L	1004	65/65	0.99	0.08	21,31,64,72	0
13	CLA	M	1201	54/65	0.99	0.07	34,42,121,127	0
13	CLA	M	1202	45/65	0.99	0.09	51,149,183,198	0
13	CLA	X	102	45/65	0.99	0.08	67,104,127,283	0
13	CLA	B	801	65/65	0.99	0.08	57,68,123,322	0
13	CLA	A	824	59/65	0.99	0.08	59,101,164,321	0
13	CLA	A	825	65/65	0.99	0.07	74,102,152,193	0
13	CLA	B	804	65/65	0.99	0.08	45,51,117,199	0
13	CLA	B	805	65/65	0.99	0.07	41,48,97,150	0
15	BCR	A	850	40/40	0.99	0.09	56,96,126,139	0
15	BCR	A	851	40/40	0.99	0.07	50,58,118,132	0
15	BCR	A	852	40/40	0.99	0.10	78,107,149,162	0
13	CLA	B	806	65/65	0.99	0.08	33,63,107,170	0
15	BCR	B	842	40/40	0.99	0.07	48,76,129,134	0
13	CLA	B	807	65/65	0.99	0.08	38,65,106,122	0
15	BCR	B	844	25/40	0.99	0.08	65,68,113,118	0
13	CLA	A	826	65/65	0.99	0.08	53,80,112,127	0
13	CLA	B	809	45/65	0.99	0.08	39,95,125,308	0
13	CLA	A	814	45/65	0.99	0.07	108,150,172,174	0
13	CLA	B	811	65/65	0.99	0.08	48,71,108,145	0
13	CLA	A	828	65/65	0.99	0.08	59,74,127,289	0
15	BCR	F	1302	40/40	0.99	0.10	70,94,125,128	0
15	BCR	I	102	40/40	0.99	0.08	19,20,48,52	0
13	CLA	A	815	45/65	0.99	0.09	111,150,177,185	0

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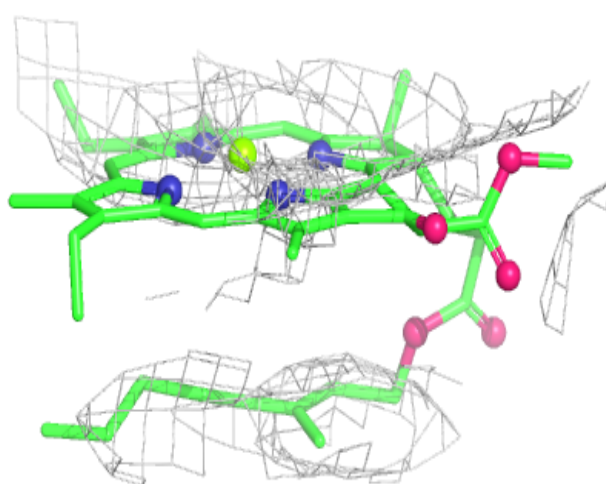
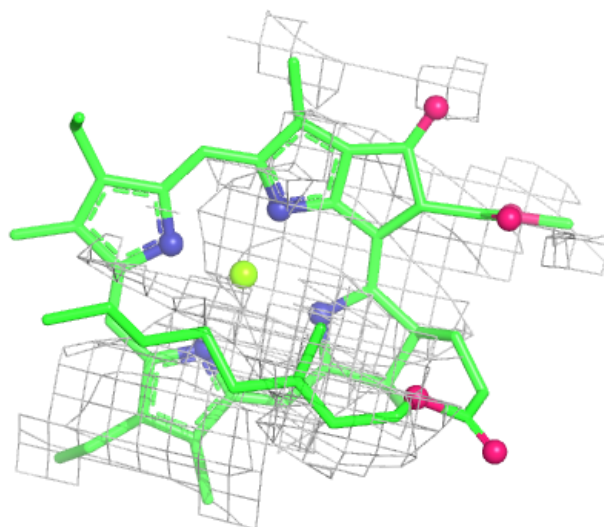
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	BCR	J	1105	40/40	0.99	0.07	63,67,71,71	0
13	CLA	A	830	65/65	0.99	0.07	59,71,105,119	0
13	CLA	A	831	50/65	0.99	0.08	45,76,105,144	0
13	CLA	B	816	60/65	0.99	0.09	46,53,111,221	0
16	LHG	A	853	49/49	0.99	0.09	57,74,107,127	0
16	LHG	A	854	27/49	0.99	0.06	49,58,88,122	0
13	CLA	A	832	65/65	0.99	0.07	42,45,81,134	0
13	CLA	B	818	47/65	0.99	0.09	56,99,146,292	0
13	CLA	B	819	45/65	0.99	0.10	98,131,171,173	0
17	SF4	C	102	8/8	1.00	0.03	47,48,122,359	0
17	SF4	A	856	8/8	1.00	0.04	49,50,150,174	0
17	SF4	C	101	8/8	1.00	0.03	48,48,49,62	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.

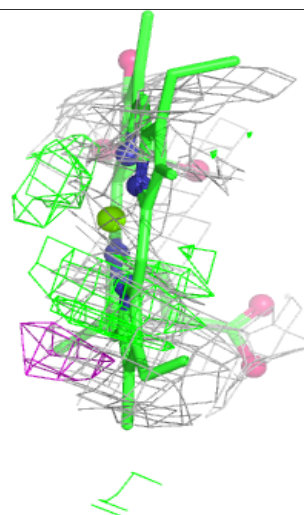
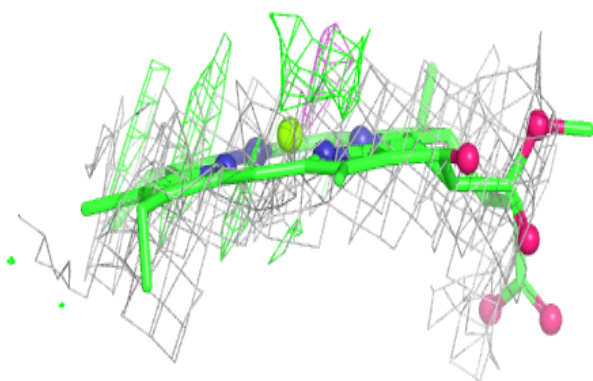
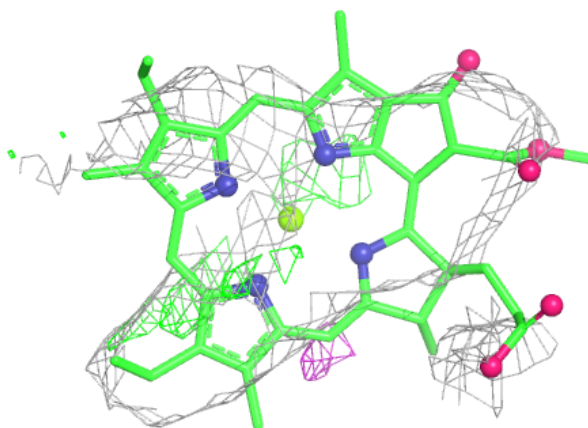
Electron density around CLA A 812:

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



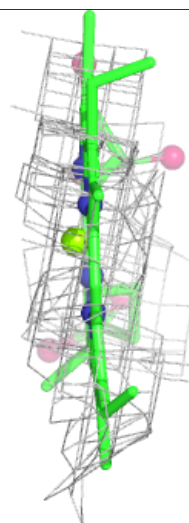
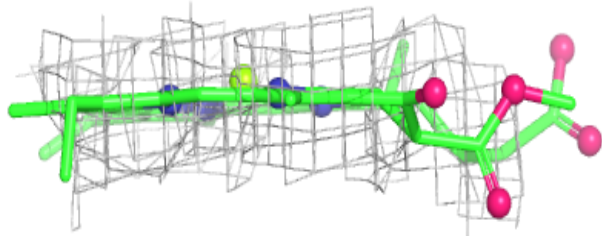
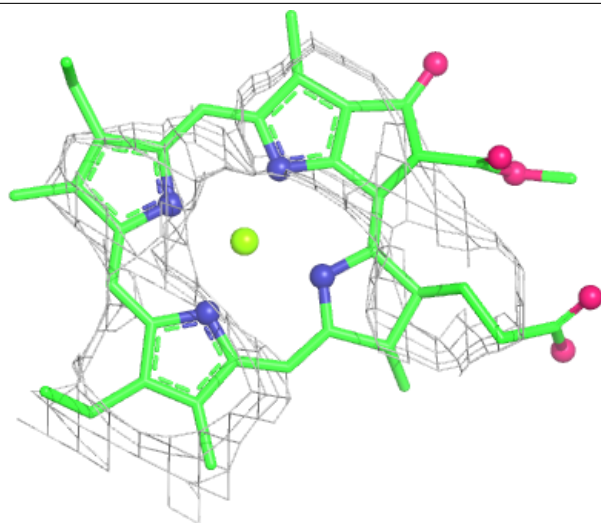
Electron density around CLA B 832:

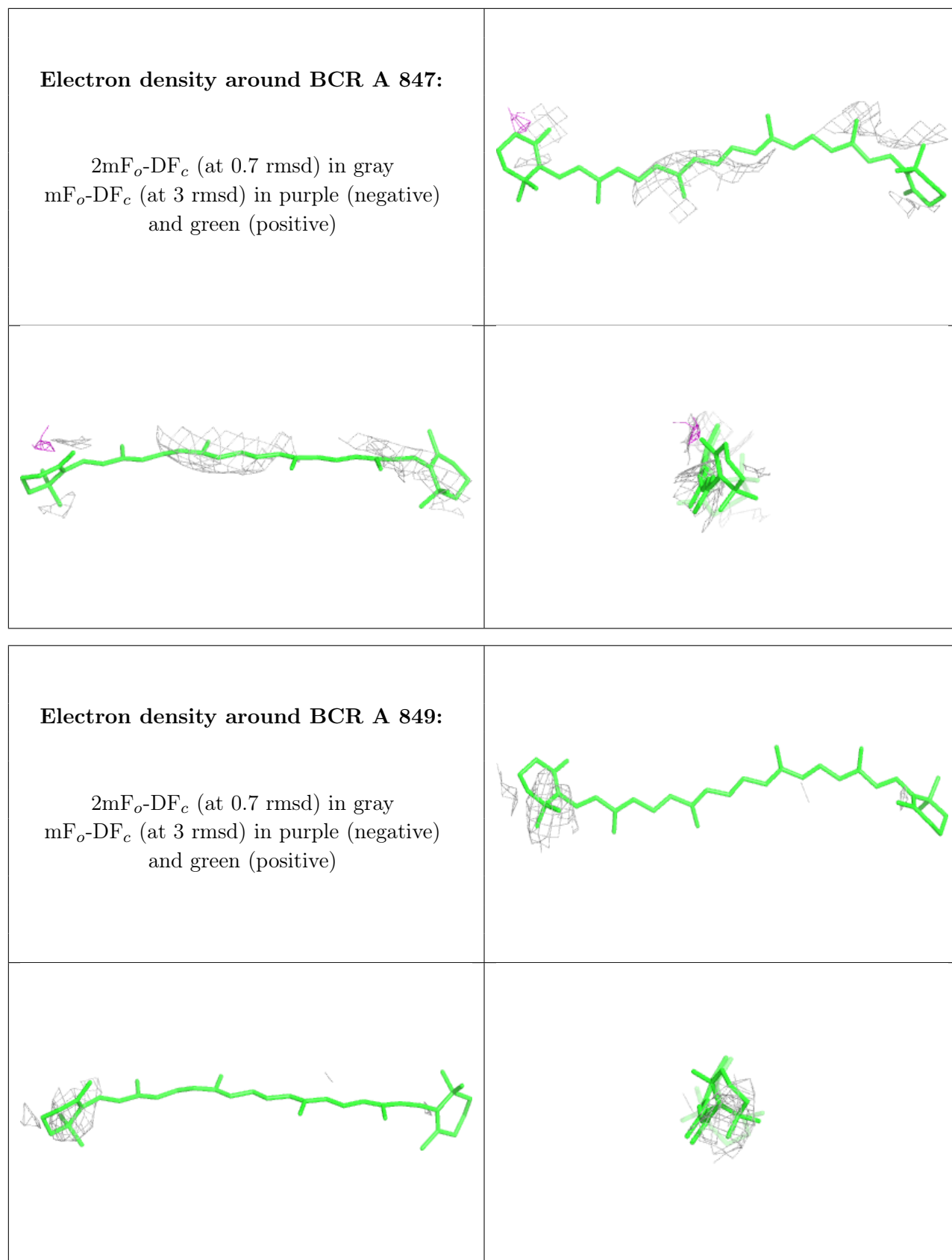
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 834:

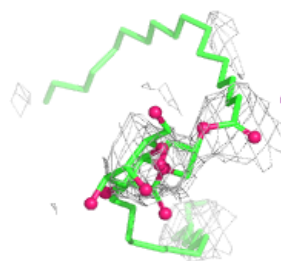
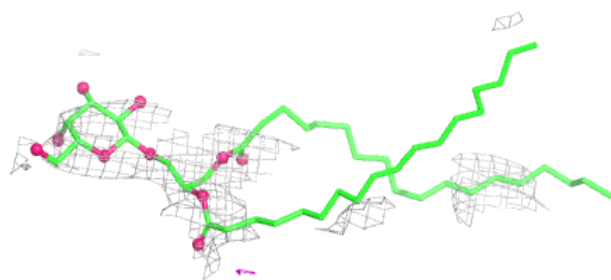
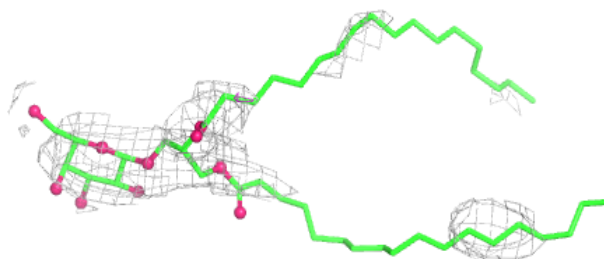
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



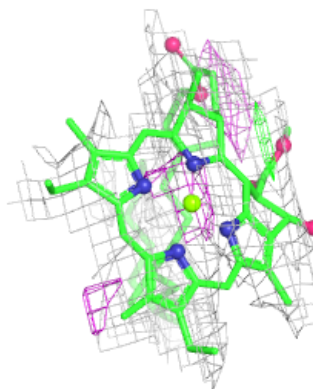
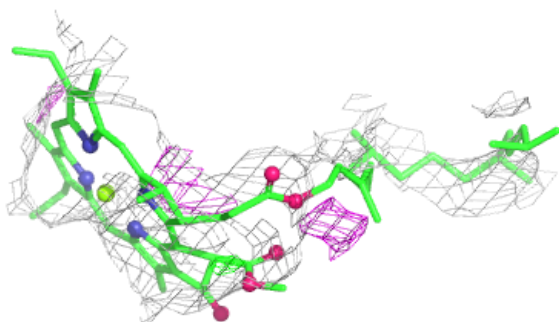
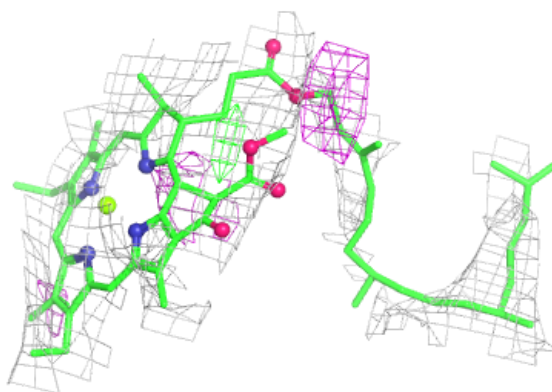


Electron density around LMG B 848:

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

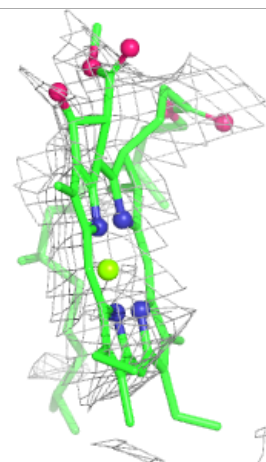
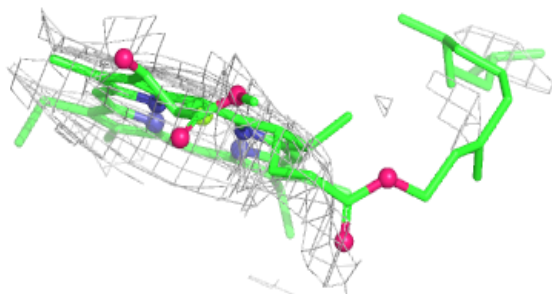
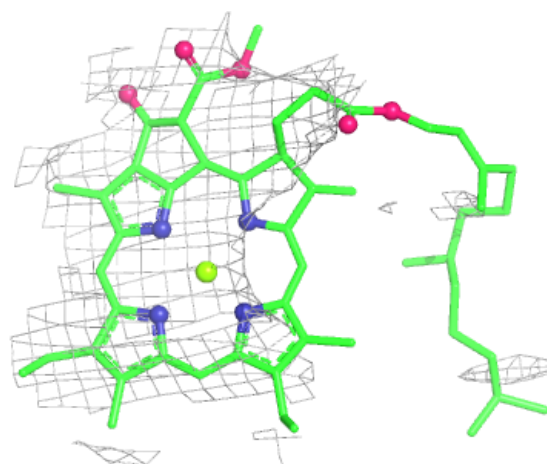
**Electron density around CLA A 801:**

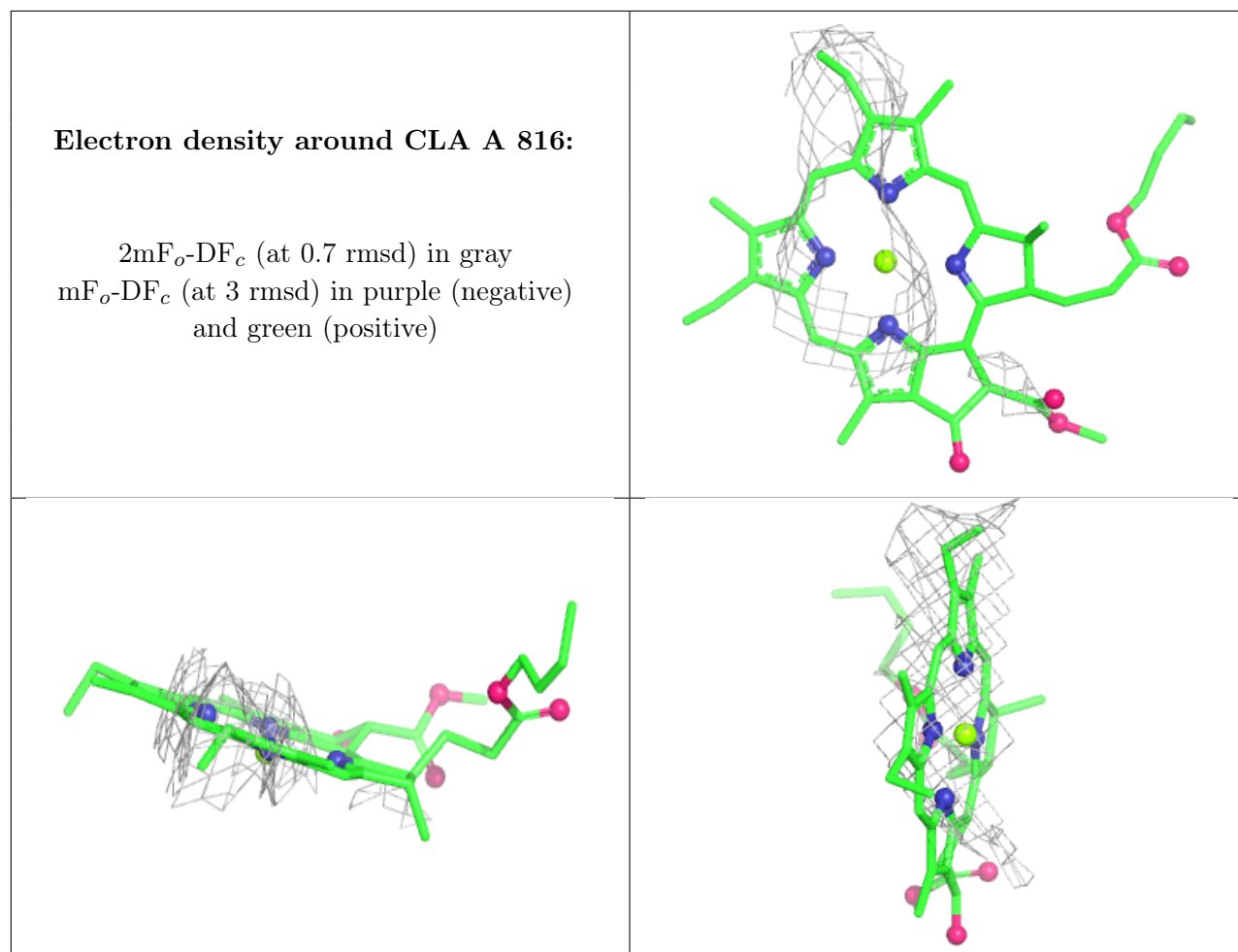
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA A 813:

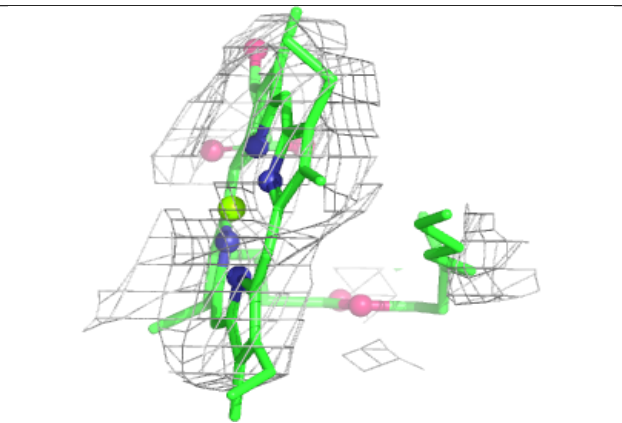
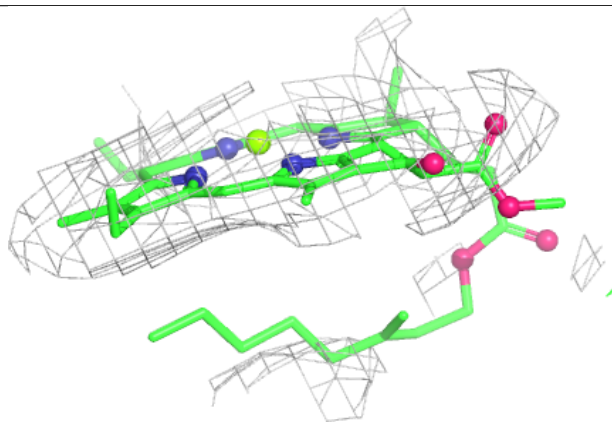
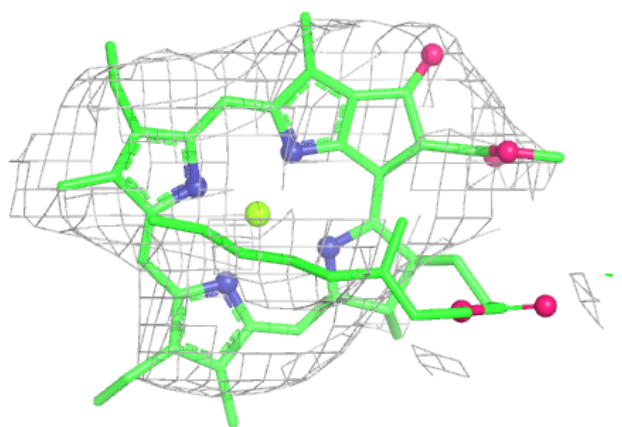
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



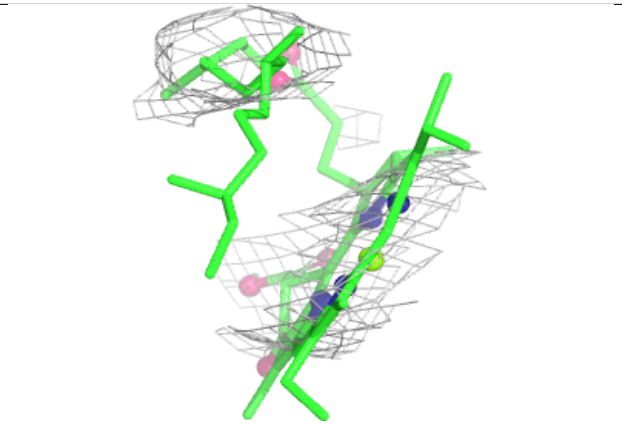
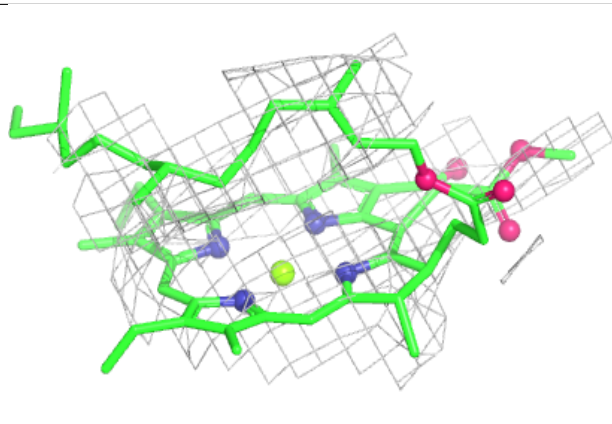
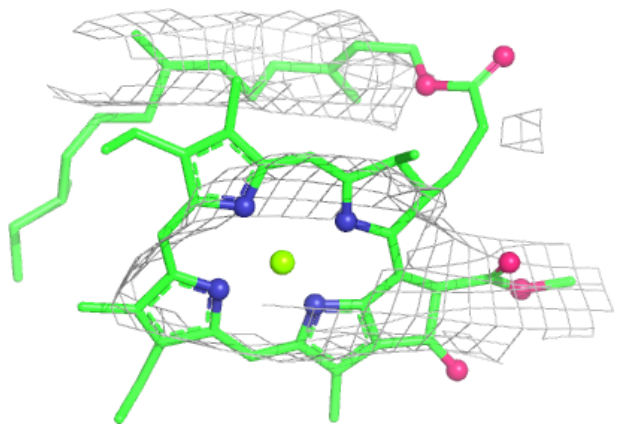


Electron density around CLA A 817:

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

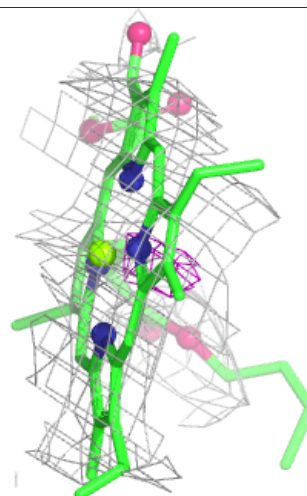
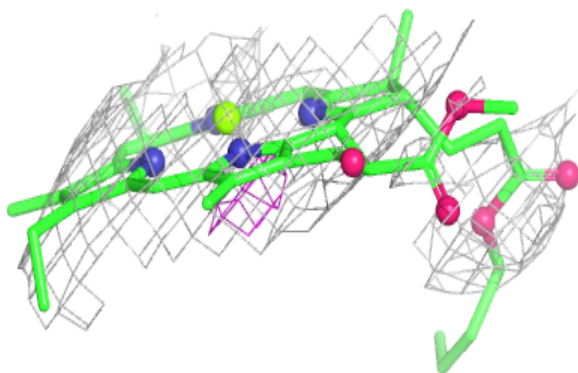
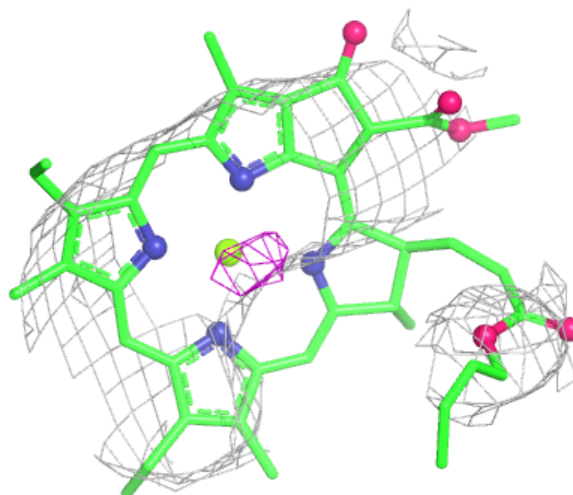
**Electron density around CLA A 820:**

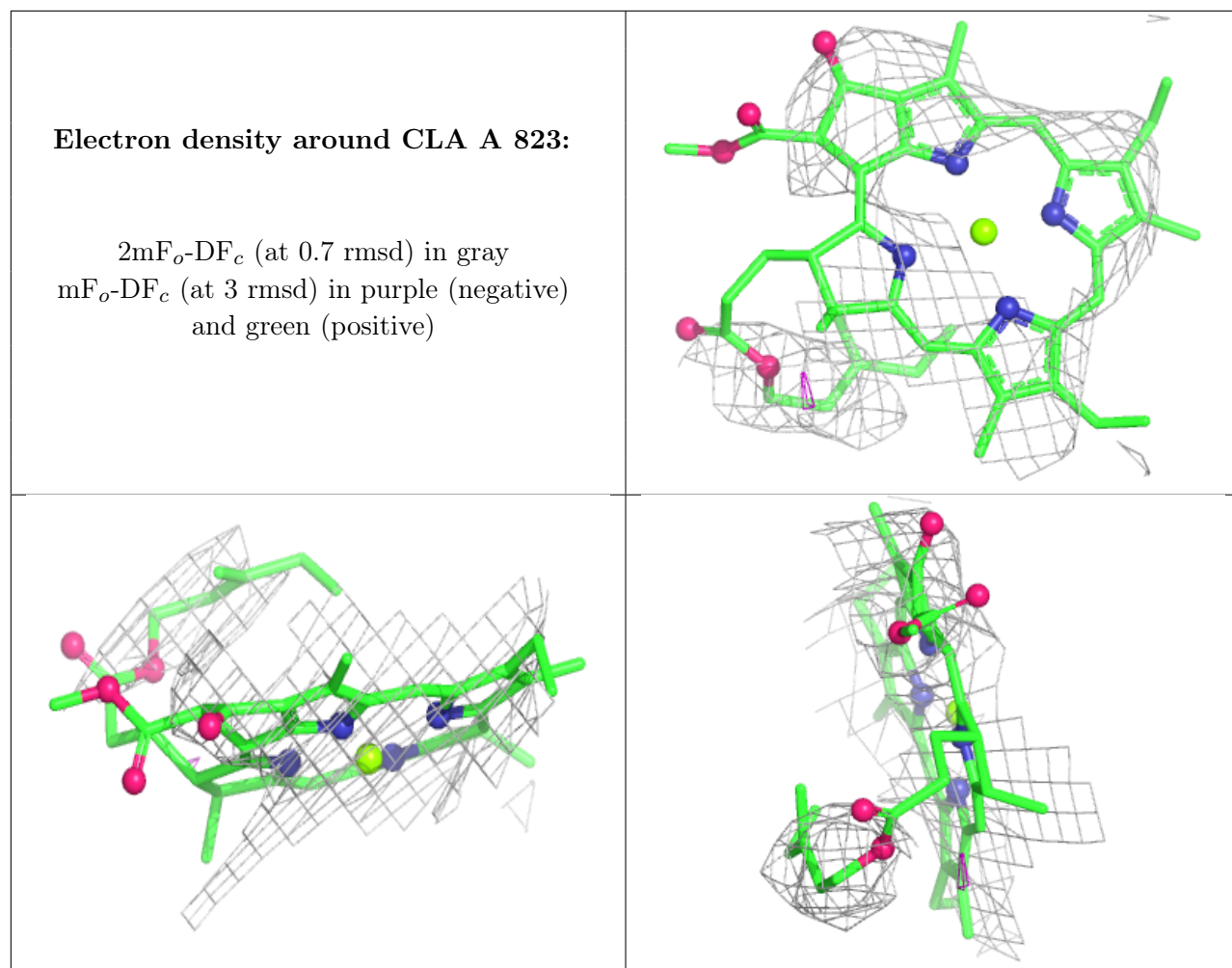
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

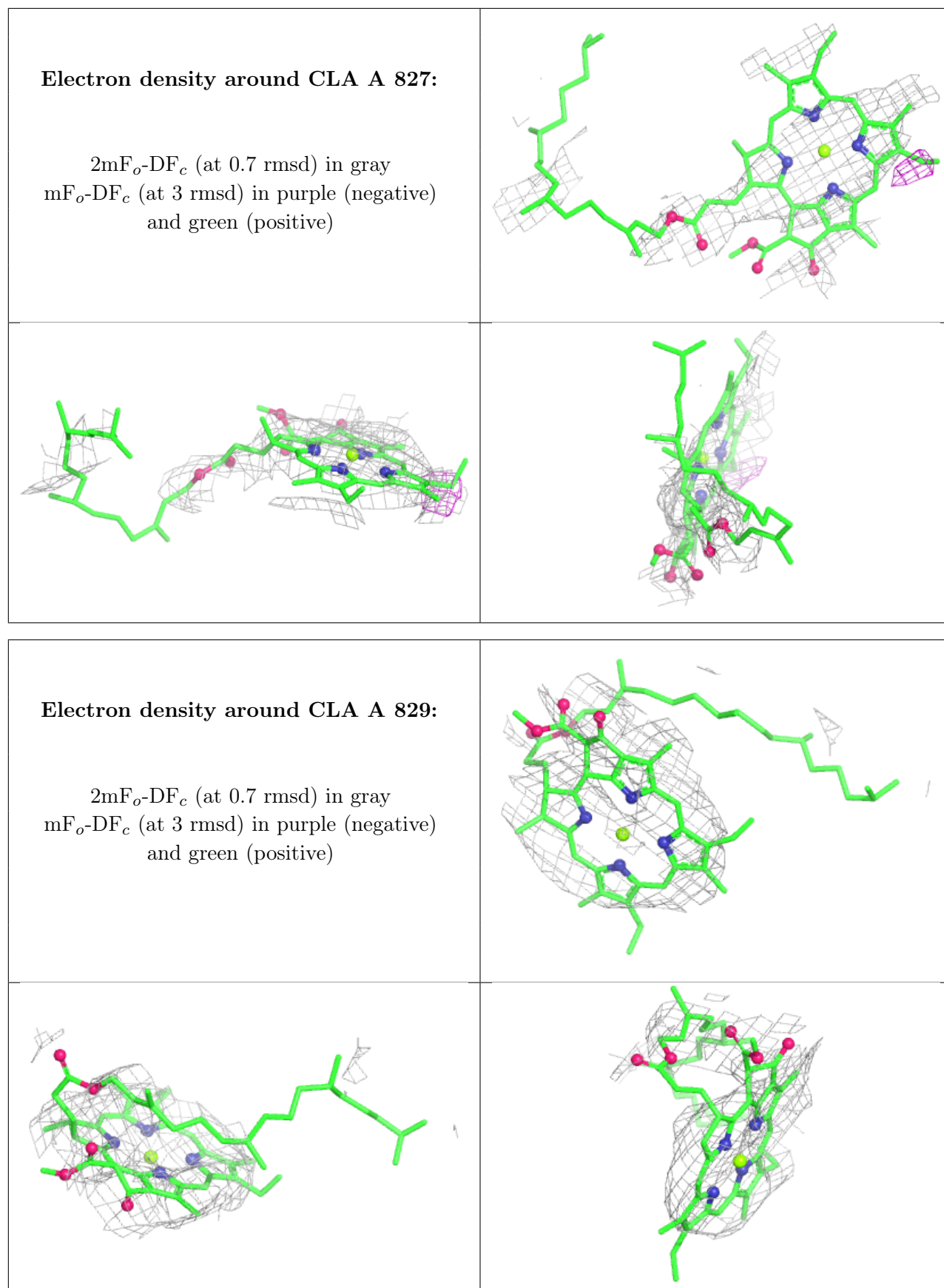


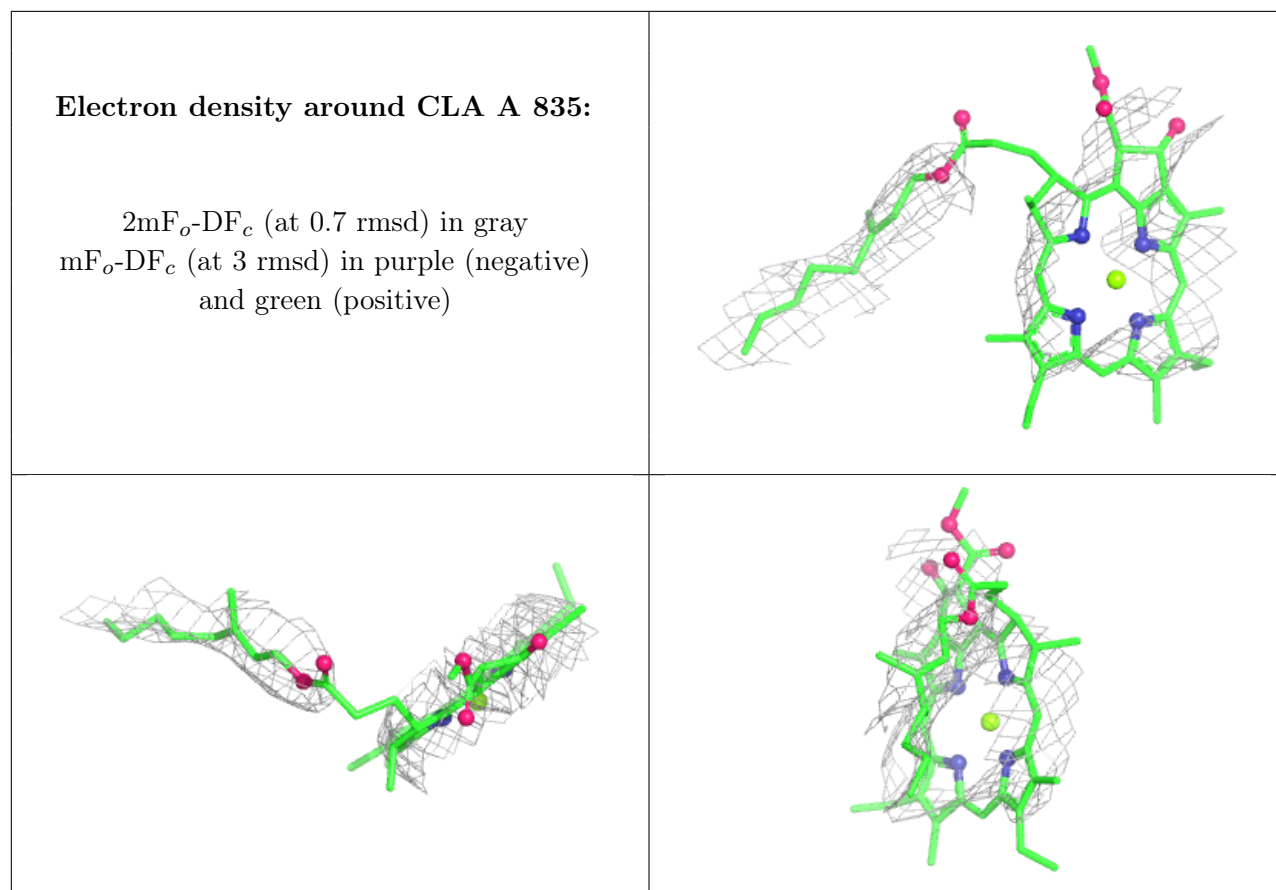
Electron density around CLA A 822:

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



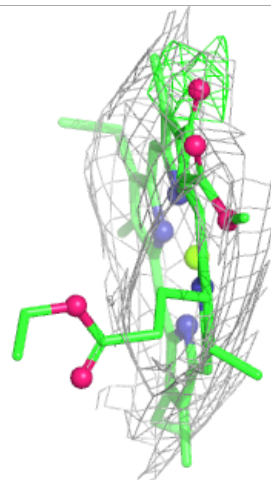
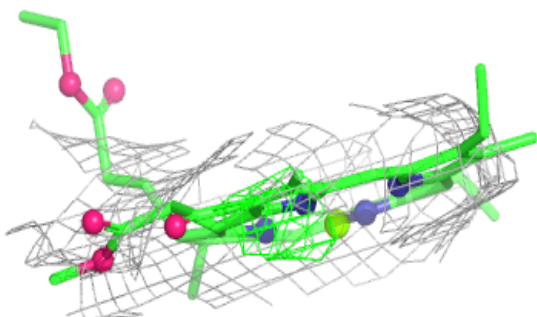
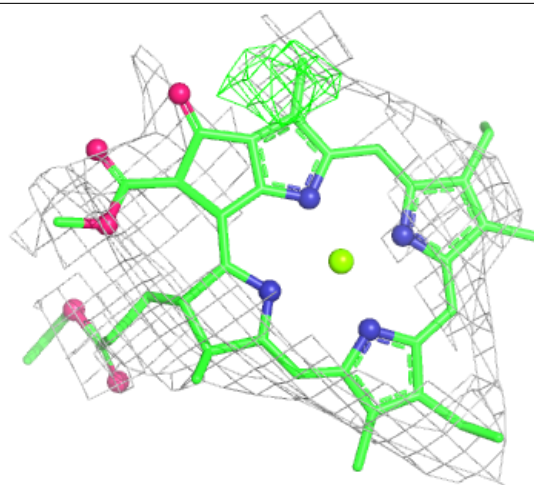






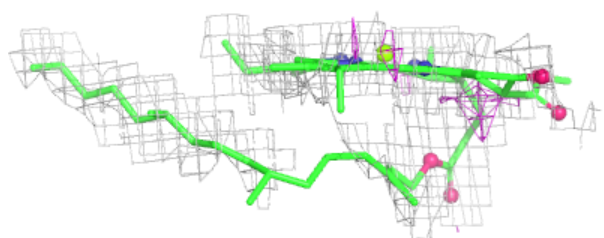
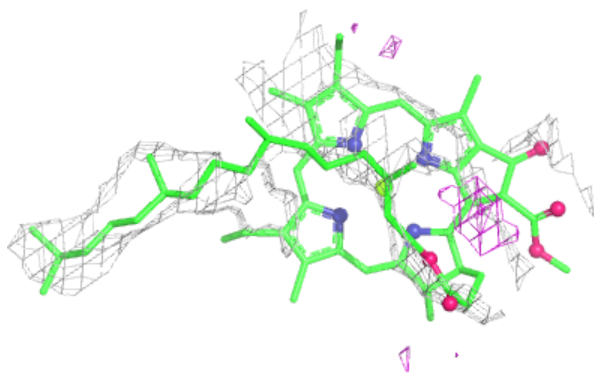
Electron density around CLA A 839:

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

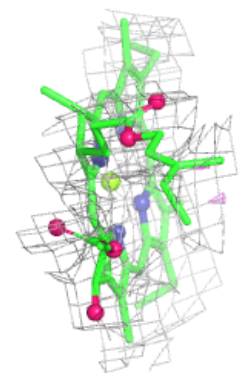
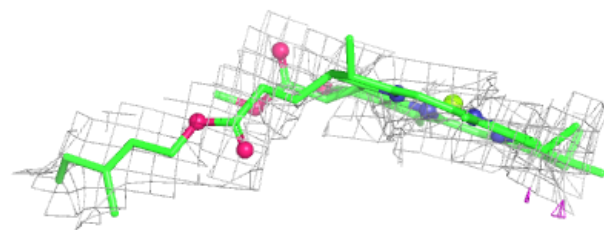
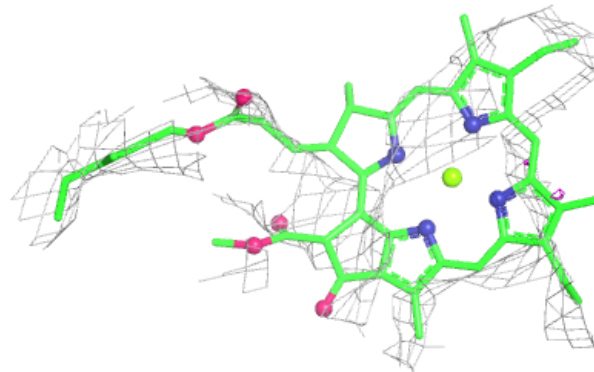


Electron density around CLA A 840:

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

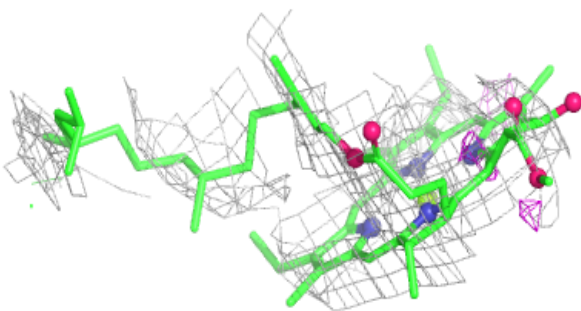
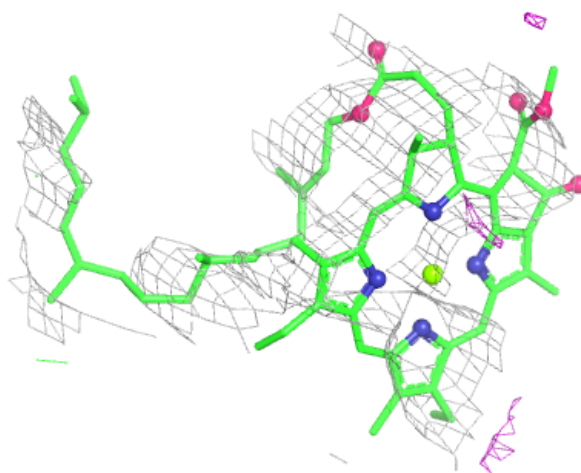
**Electron density around CLA A 841:**

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



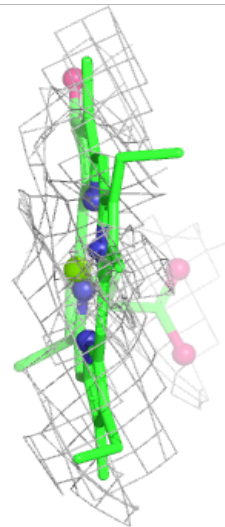
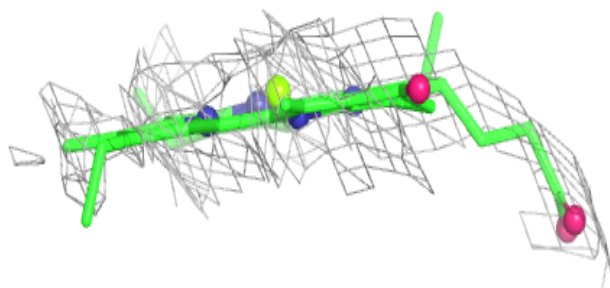
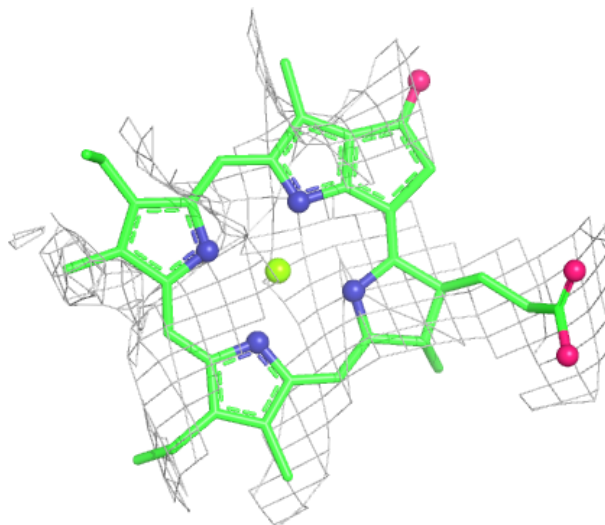
Electron density around CLA A 843:

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



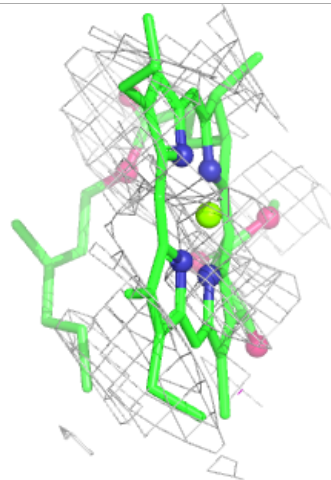
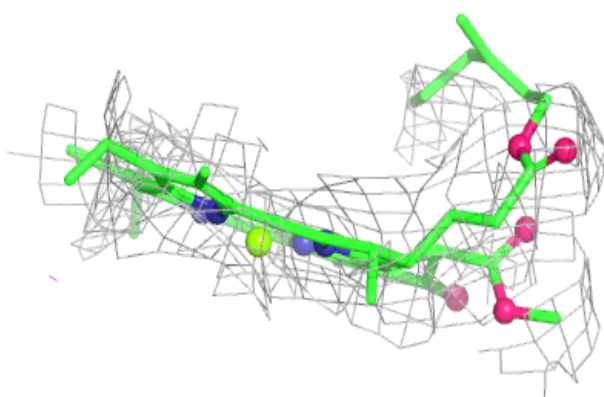
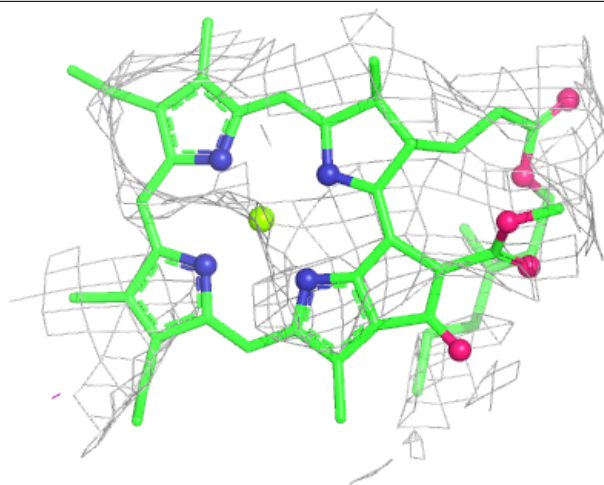
Electron density around CLA A 844:

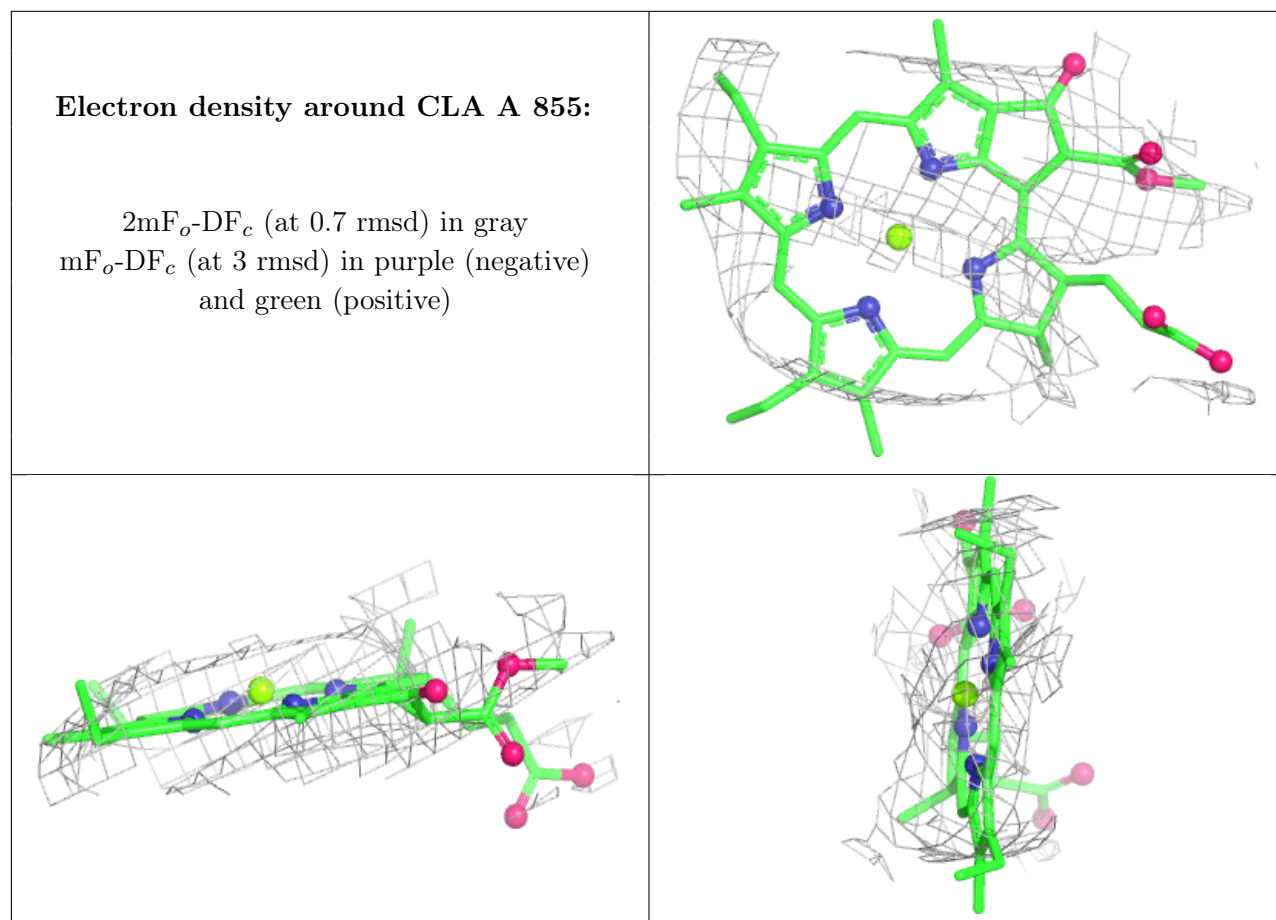
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA A 845:

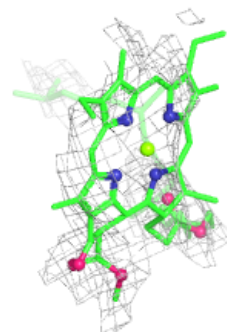
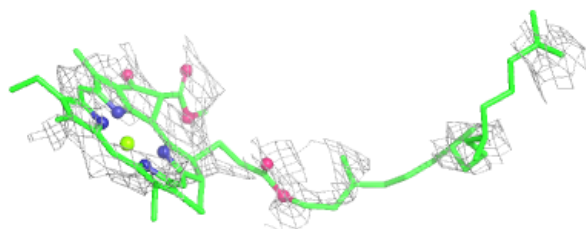
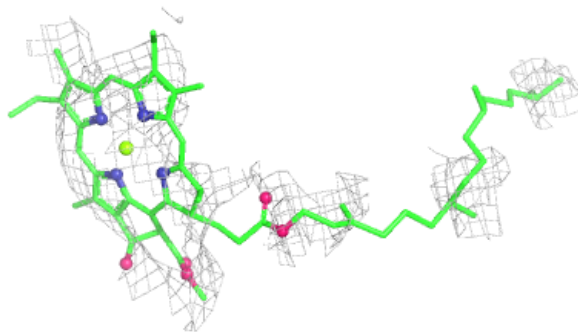
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



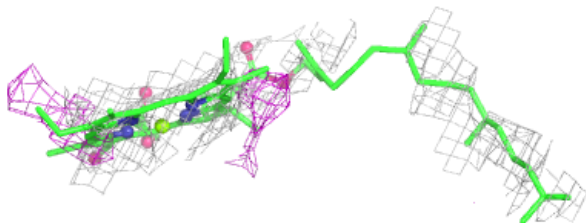
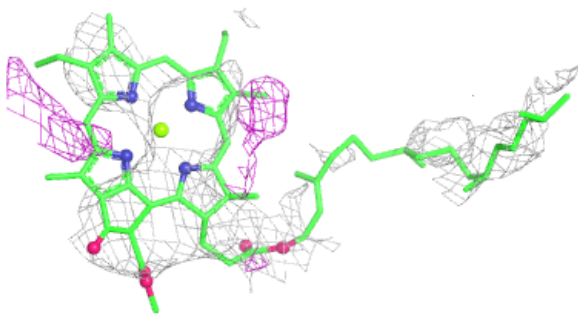


Electron density around CLA B 802:

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

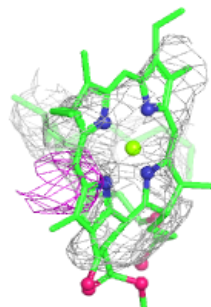
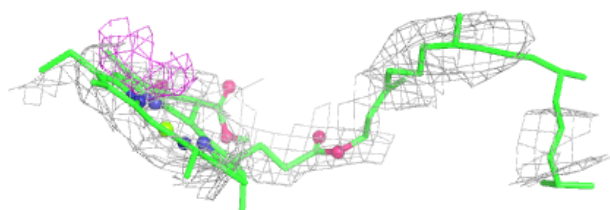
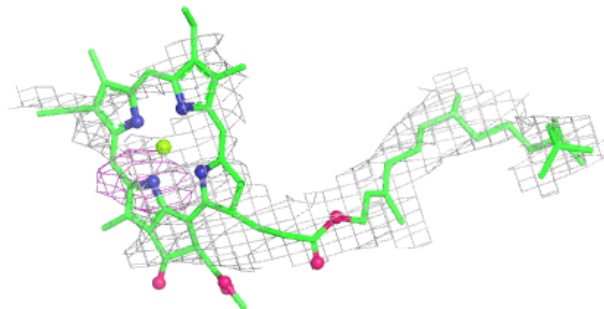
**Electron density around CLA B 803:**

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



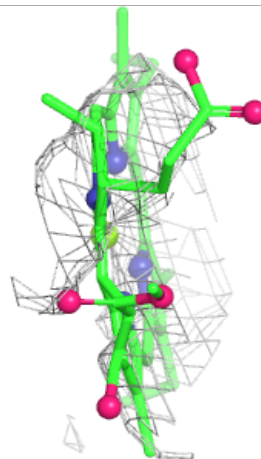
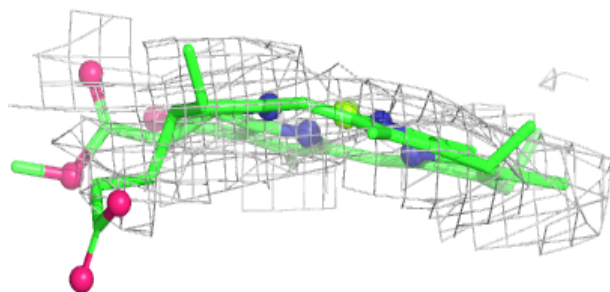
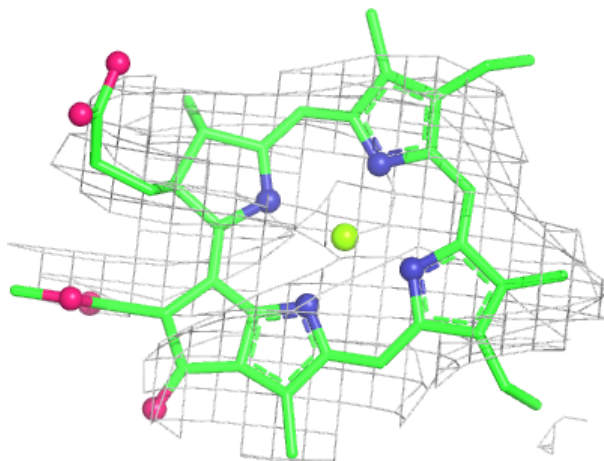
Electron density around CLA B 808:

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



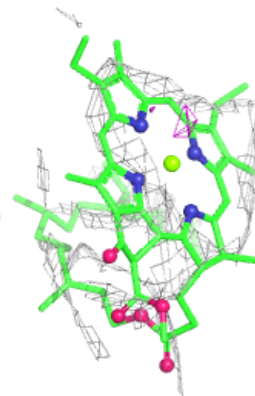
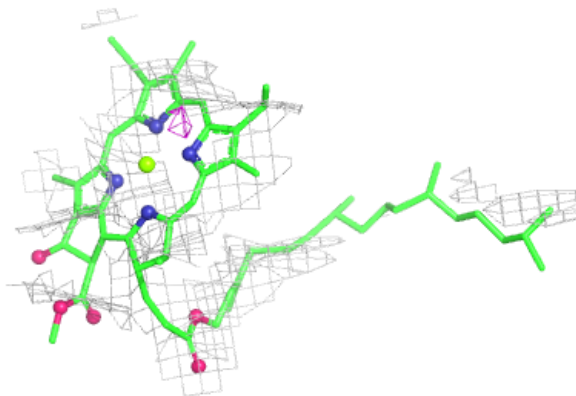
Electron density around CLA B 810:

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



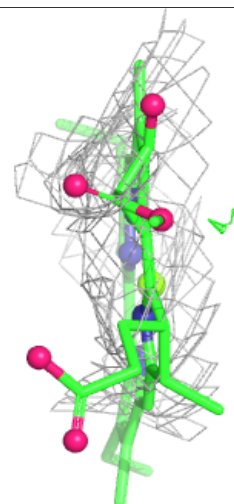
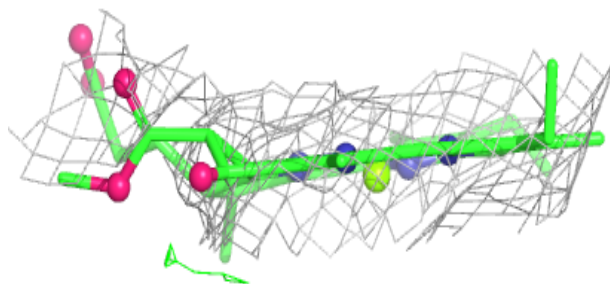
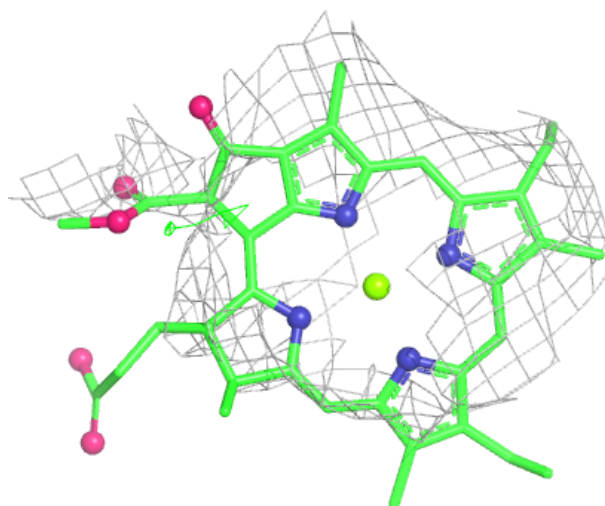
Electron density around CLA B 812:

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



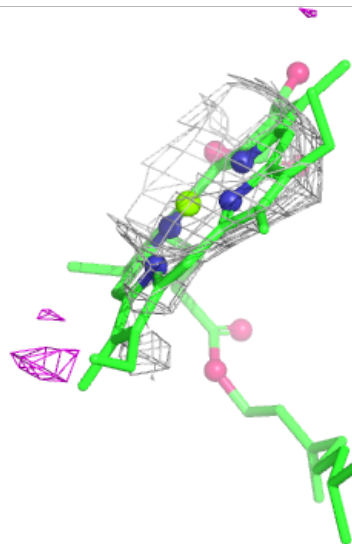
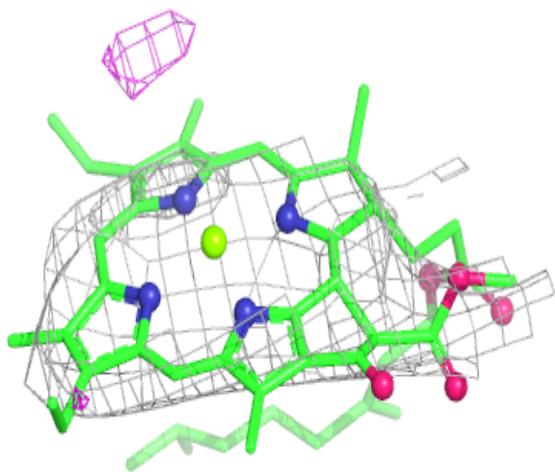
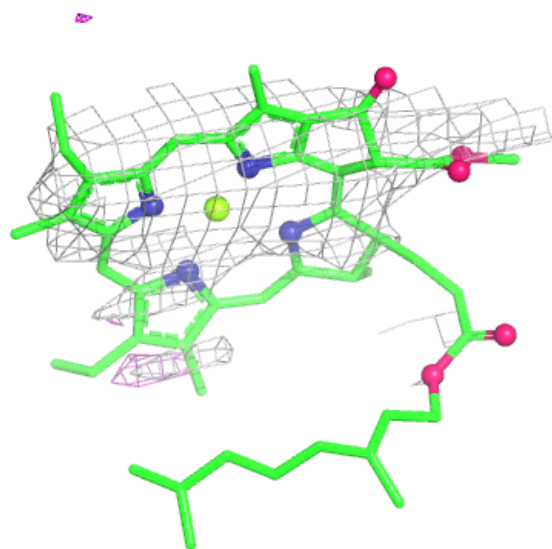
Electron density around CLA B 813:

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



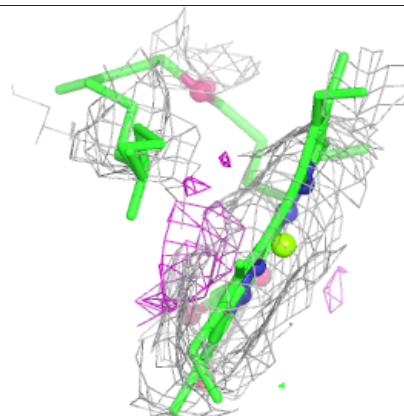
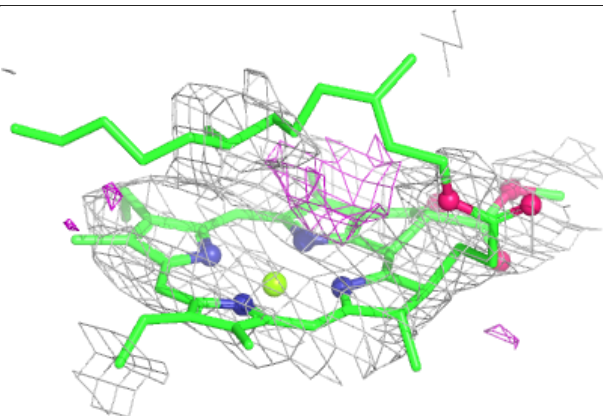
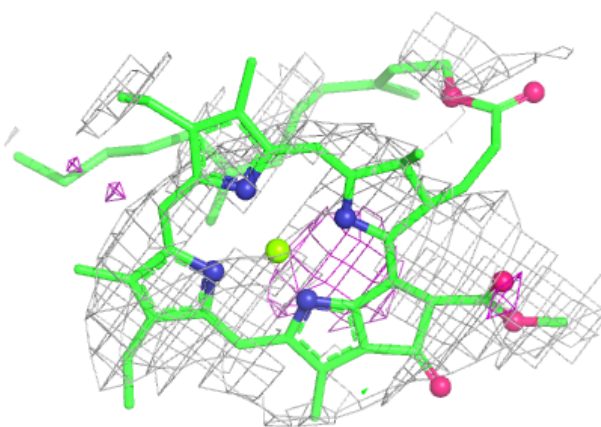
Electron density around CLA B 814:

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



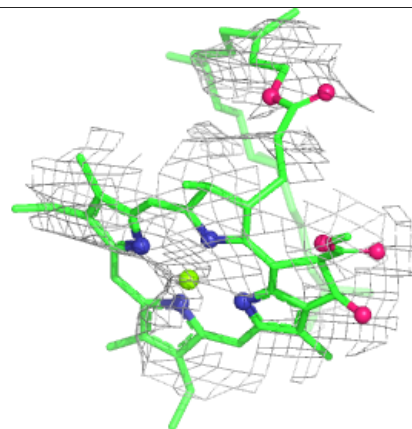
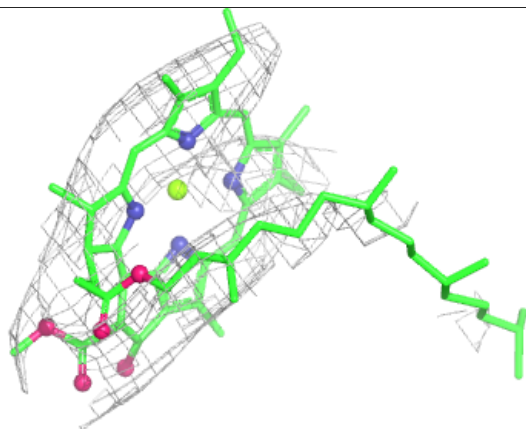
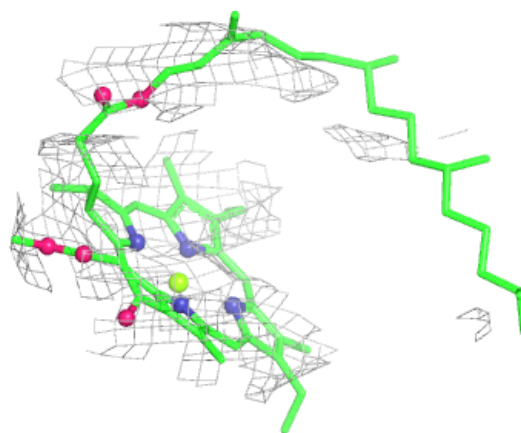
Electron density around CLA B 815:

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



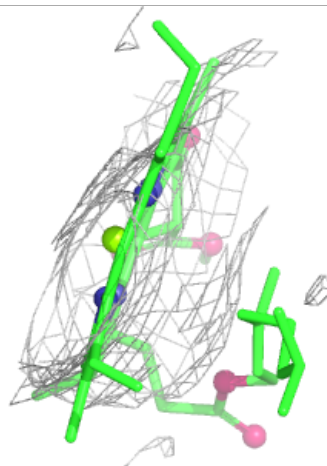
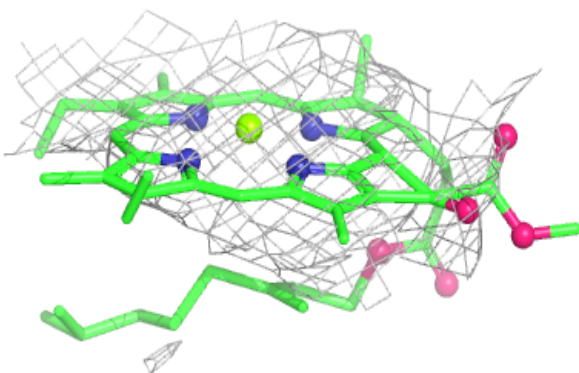
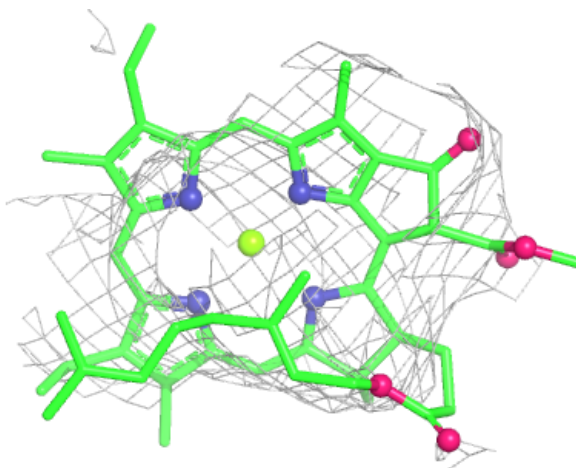
Electron density around CLA B 817:

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



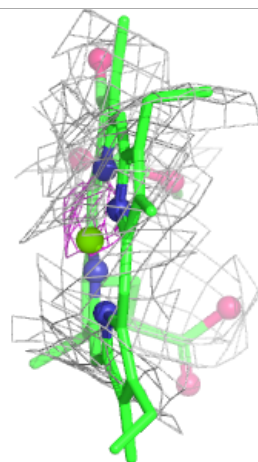
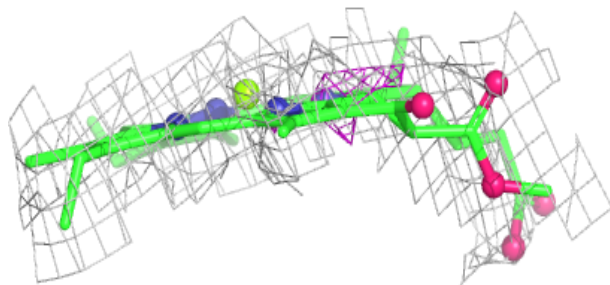
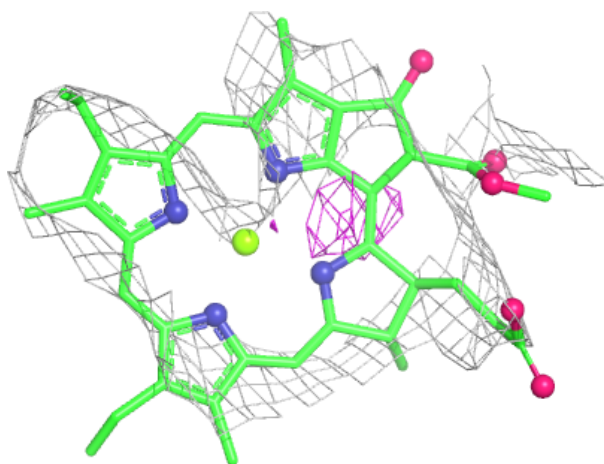
Electron density around CLA B 820:

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



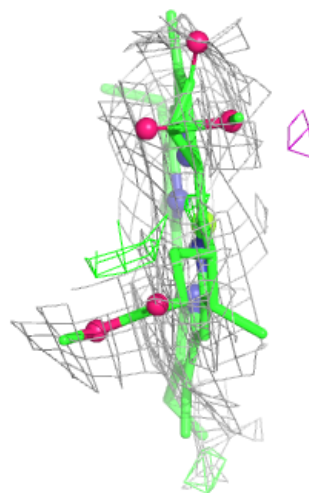
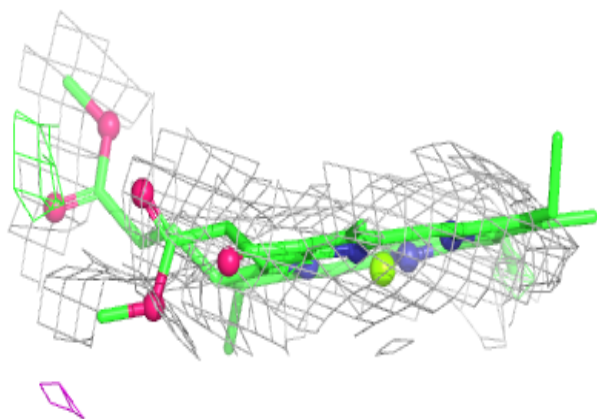
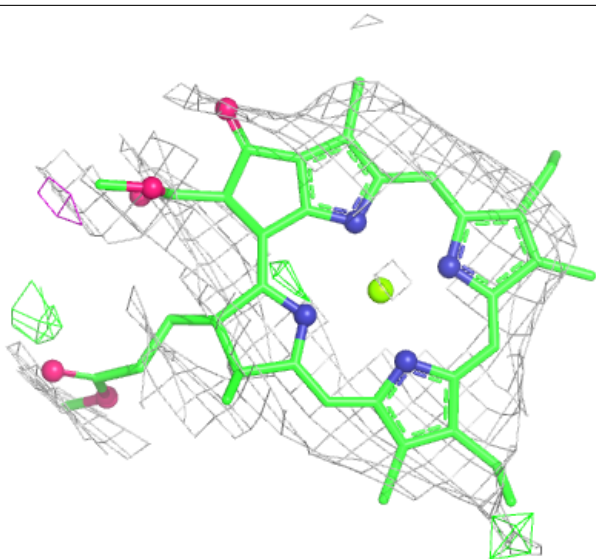
Electron density around CLA B 821:

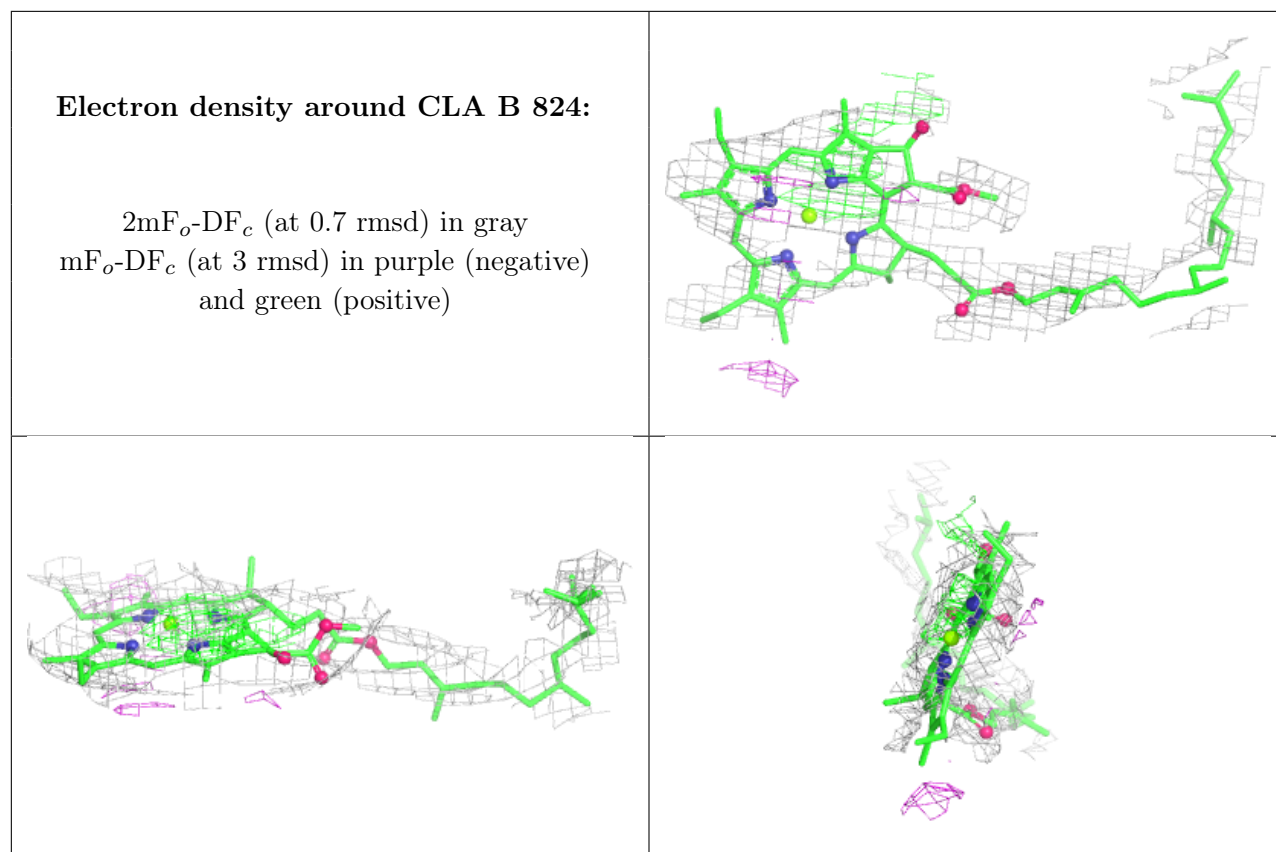
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 823:

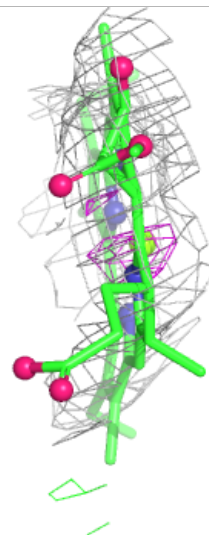
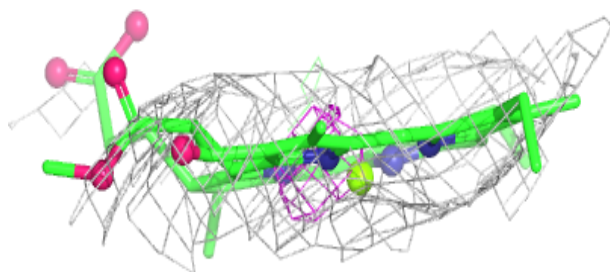
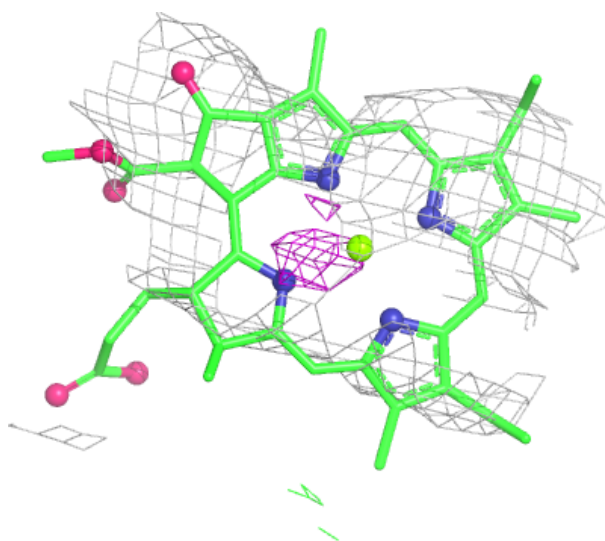
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





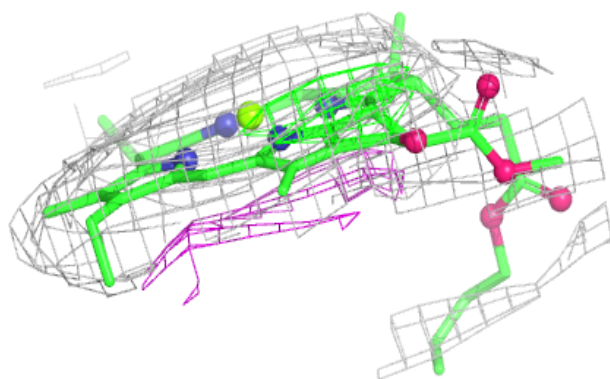
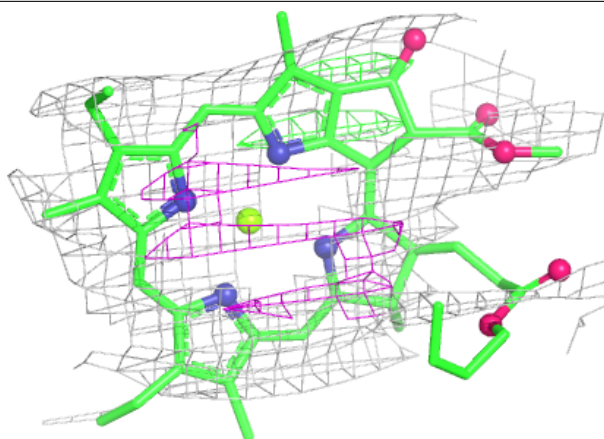
Electron density around CLA B 828:

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



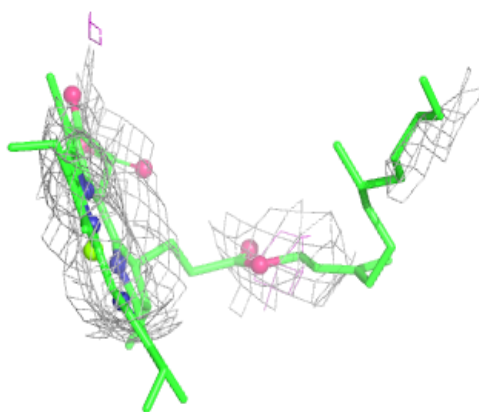
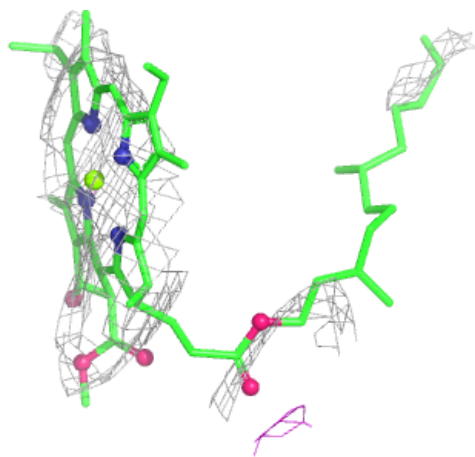
Electron density around CLA B 829:

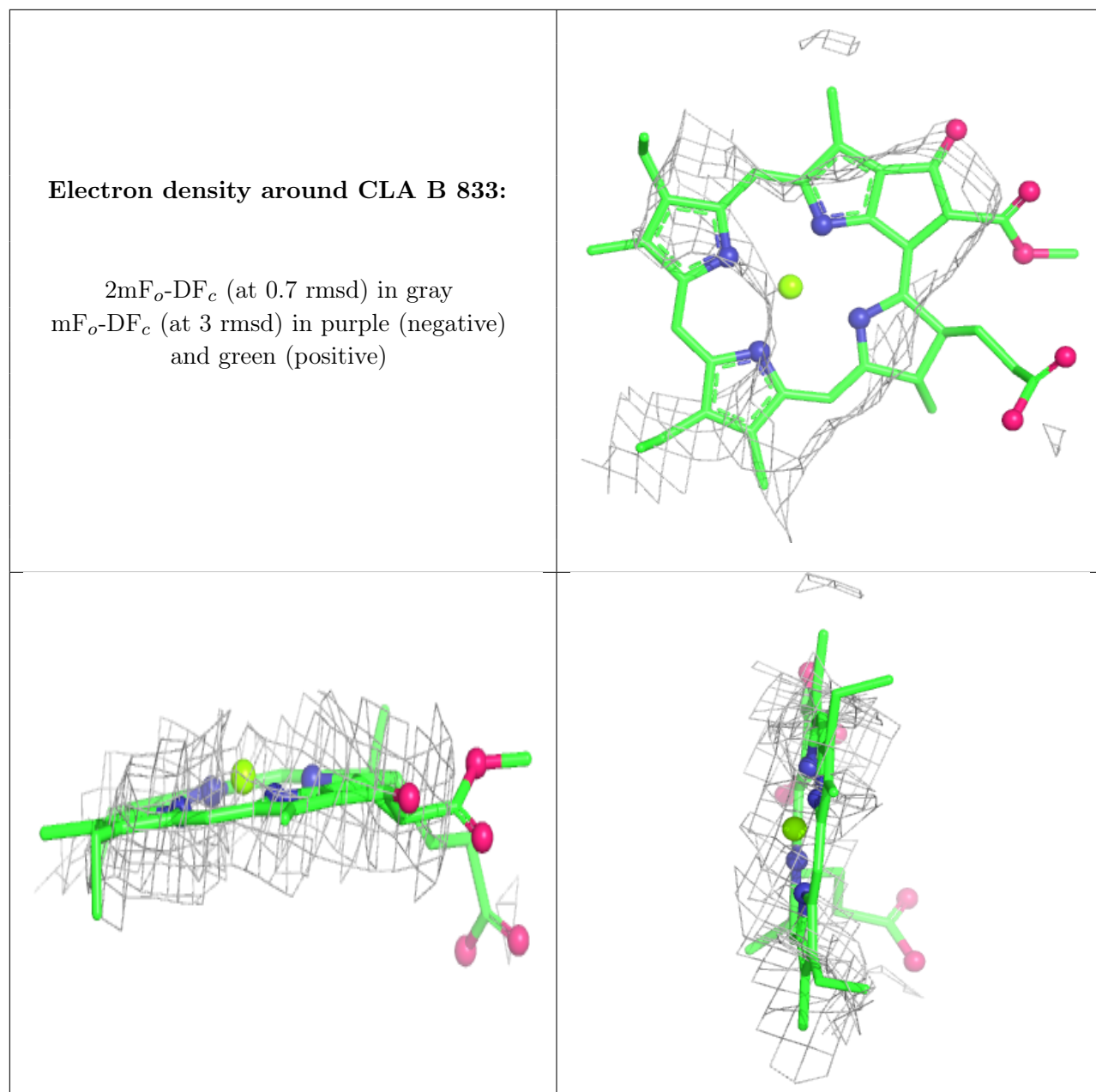
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA A 804:

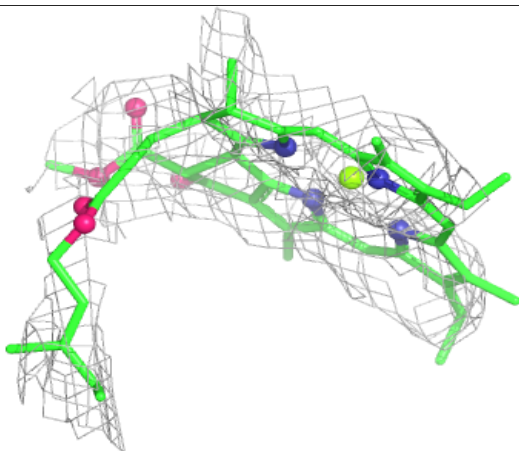
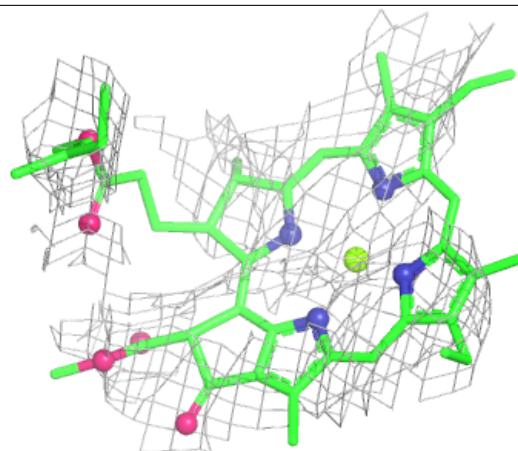
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





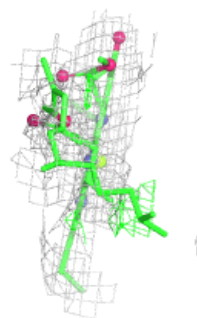
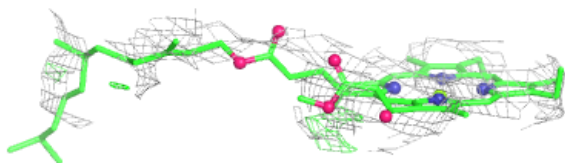
Electron density around CLA A 807:

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

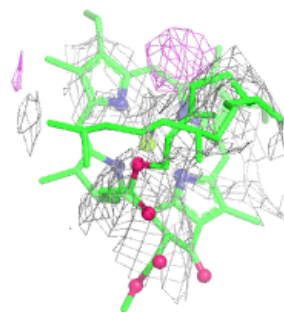
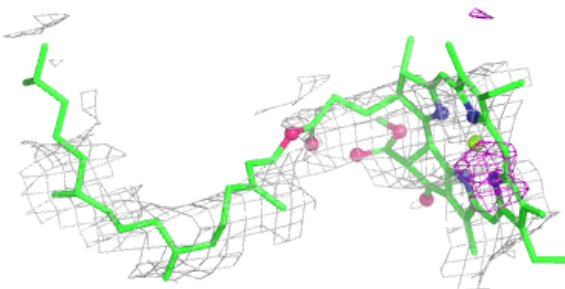
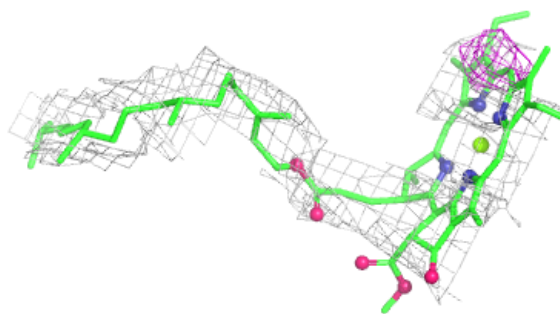


Electron density around CLA B 835:

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

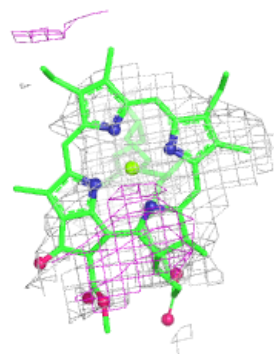
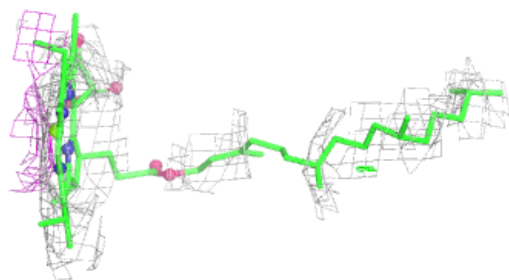
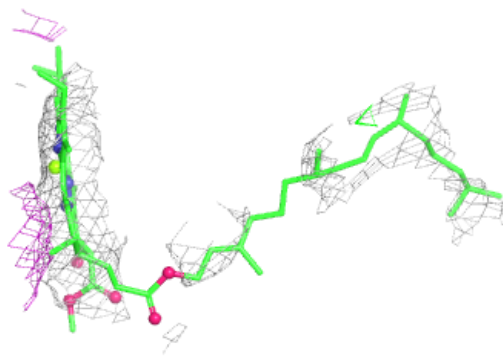
**Electron density around CLA B 838:**

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



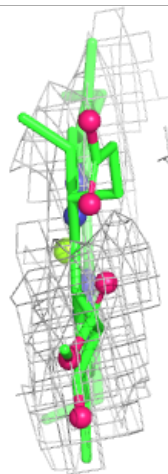
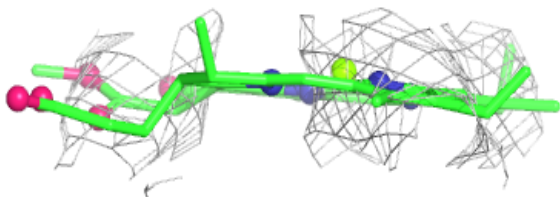
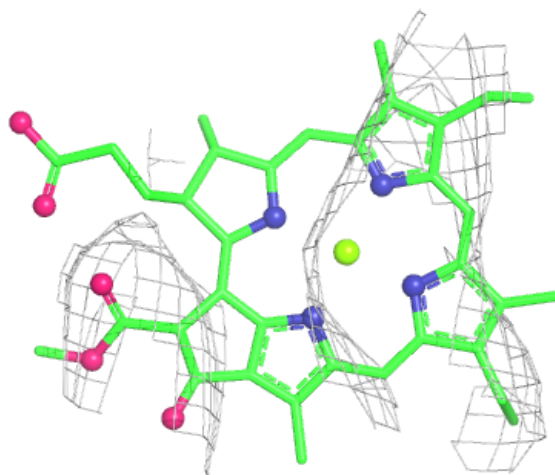
Electron density around CLA B 839:

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



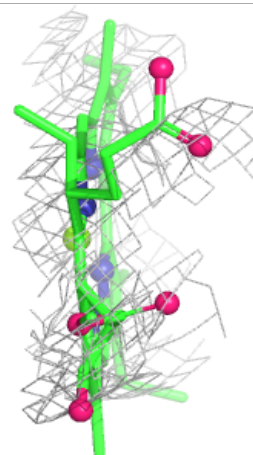
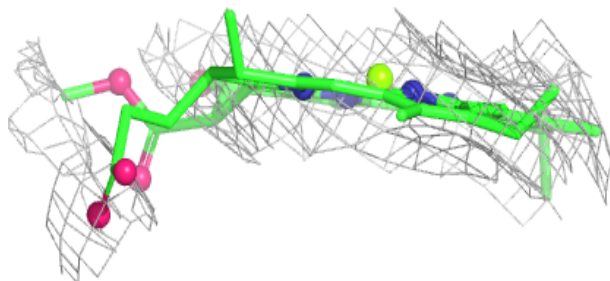
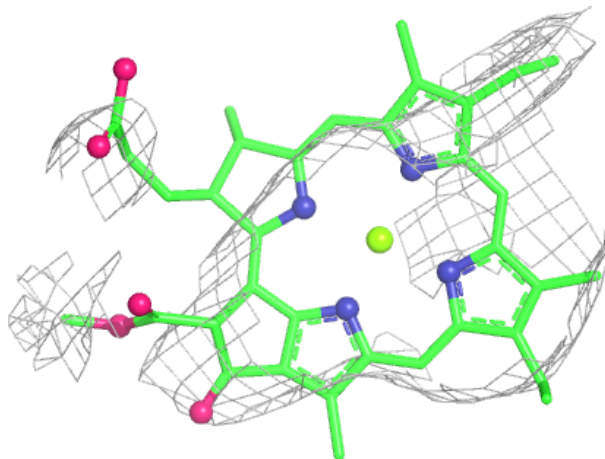
Electron density around CLA F 1301:

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



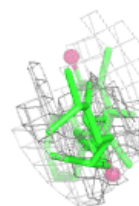
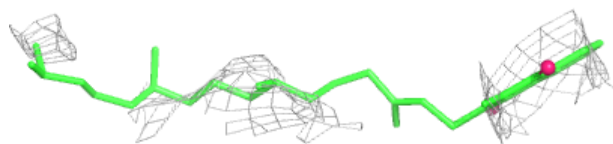
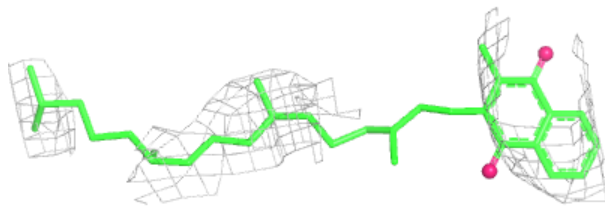
Electron density around CLA J 1102:

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

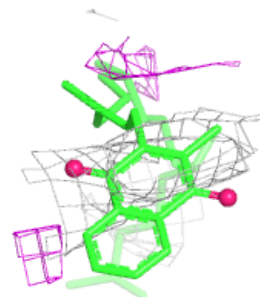
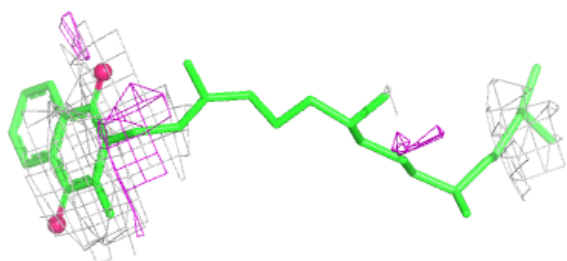
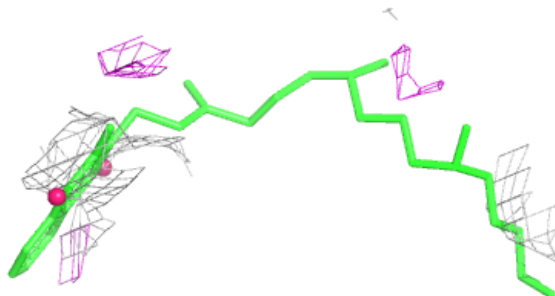


Electron density around PQN A 846:

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

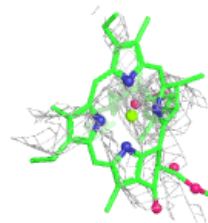
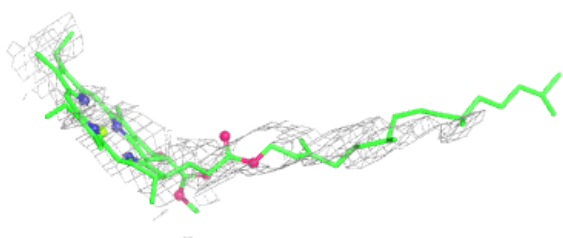
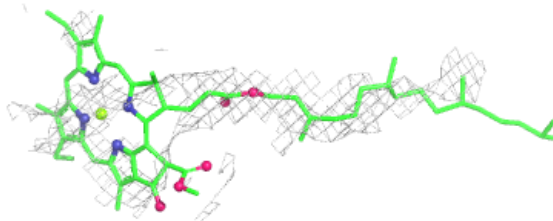
**Electron density around PQN B 840:**

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

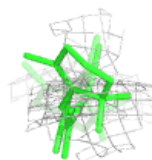
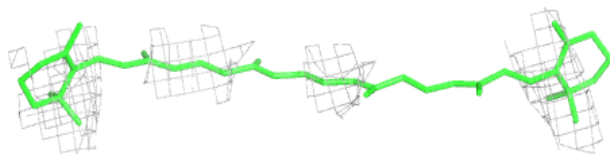
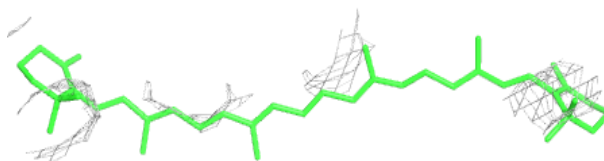


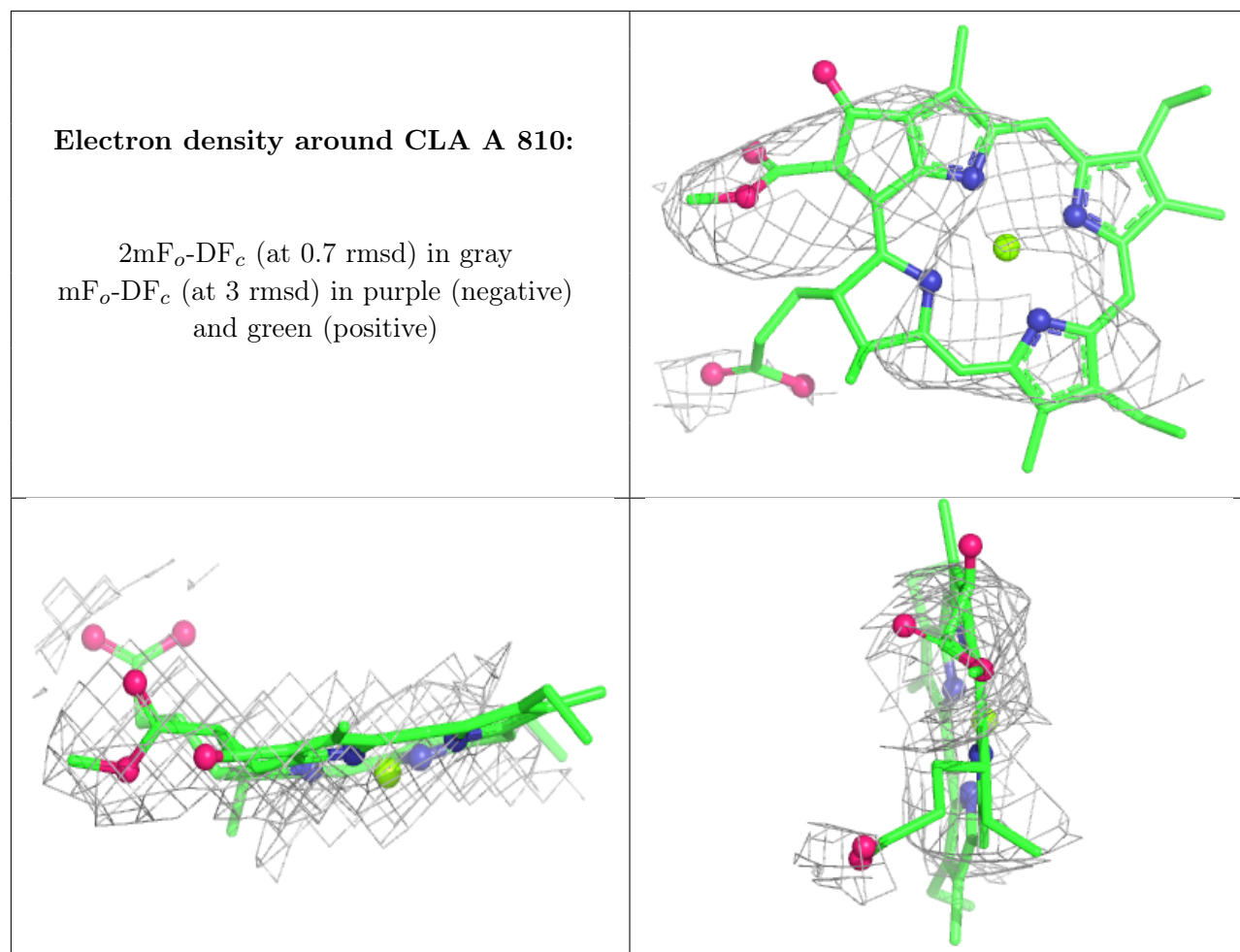
Electron density around CLA A 809:

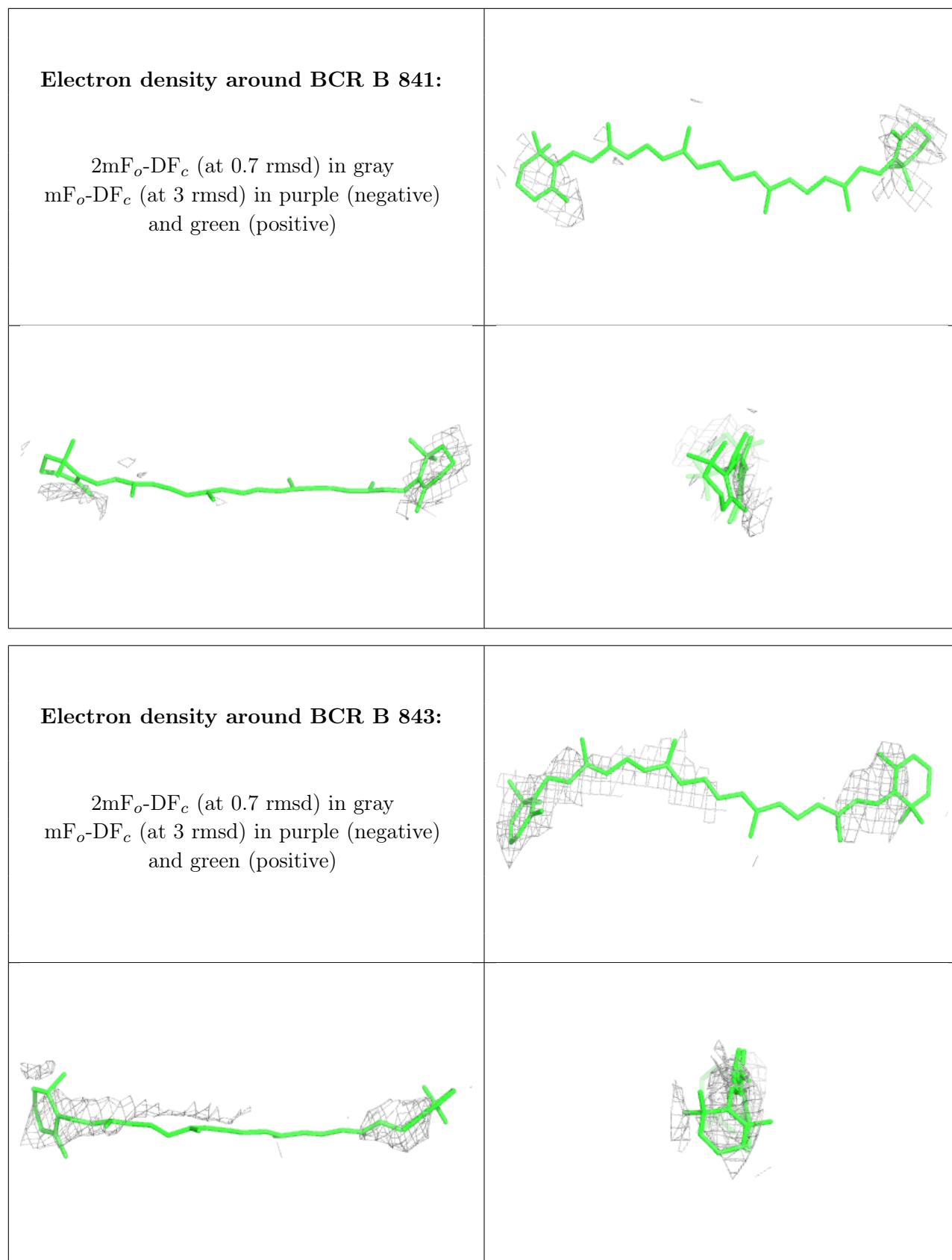
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

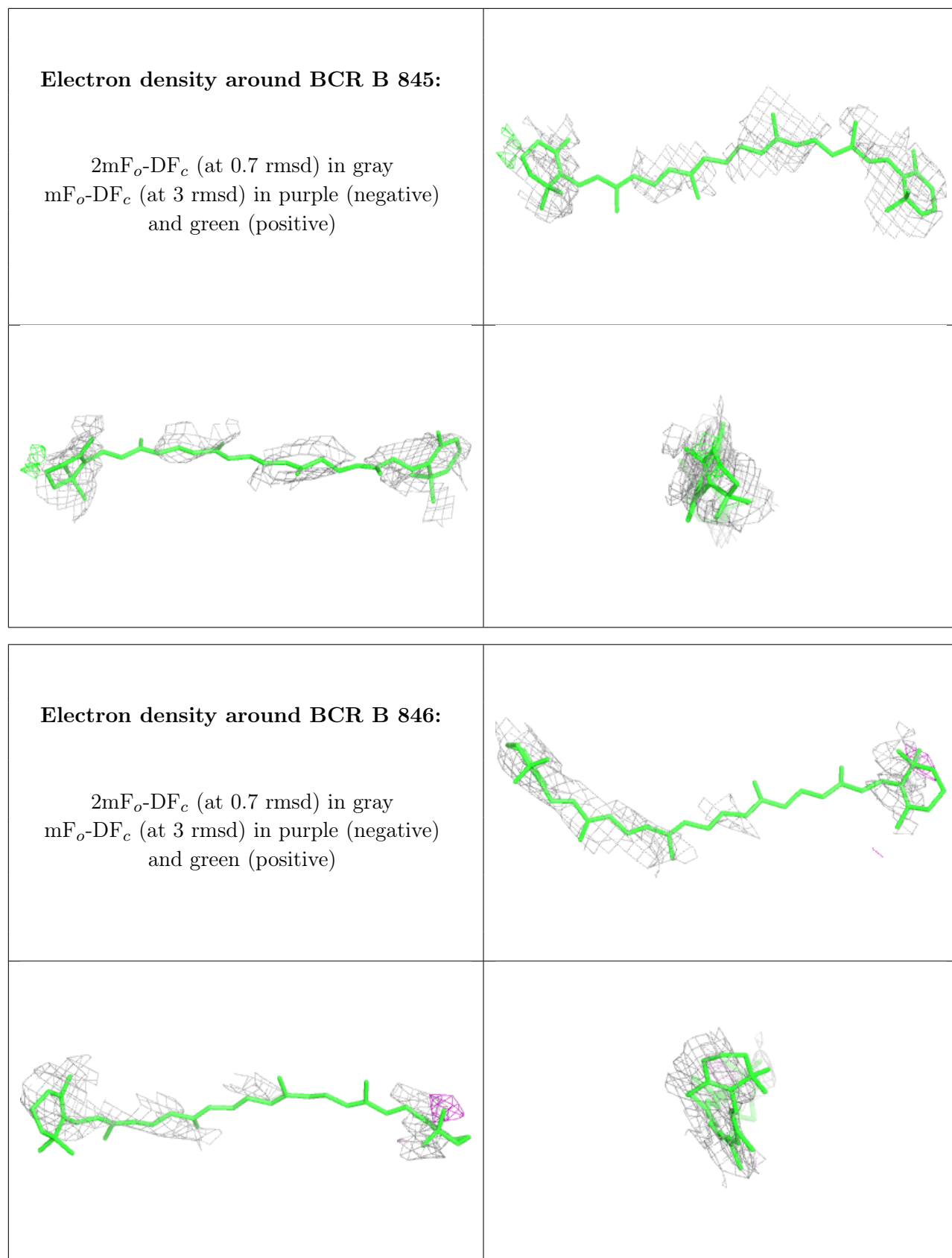
**Electron density around BCR A 848:**

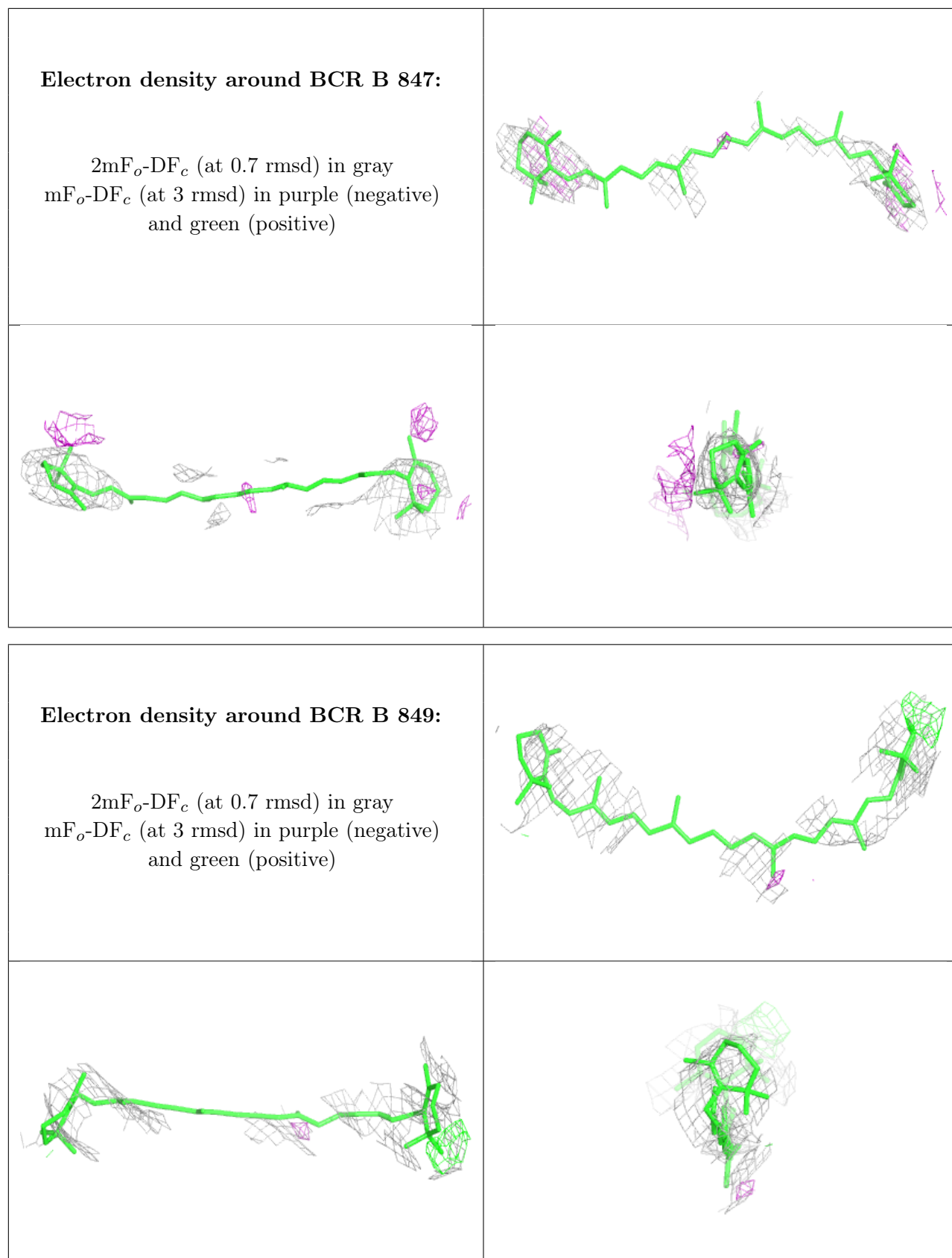
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

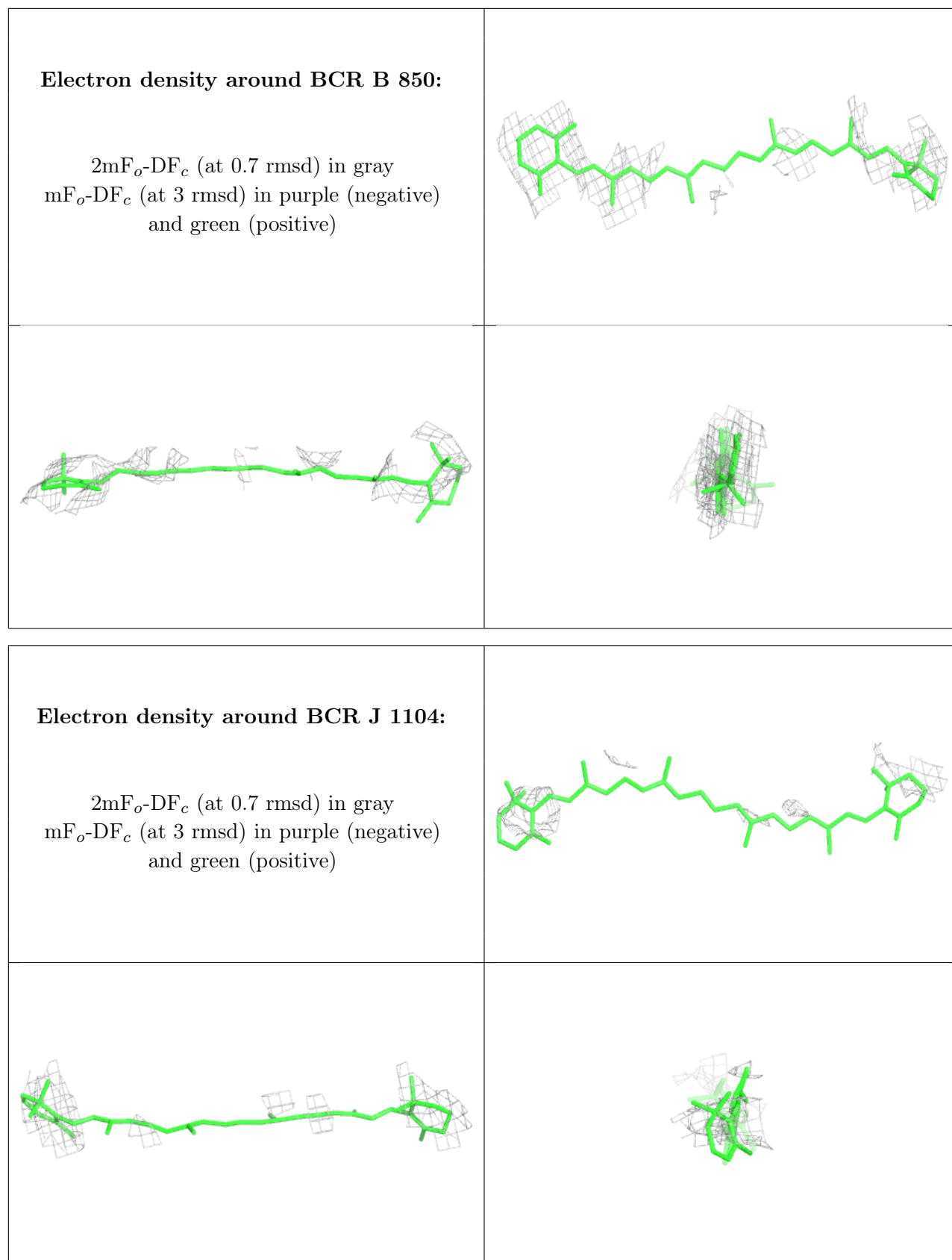






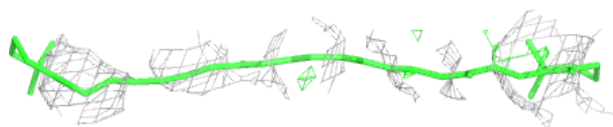
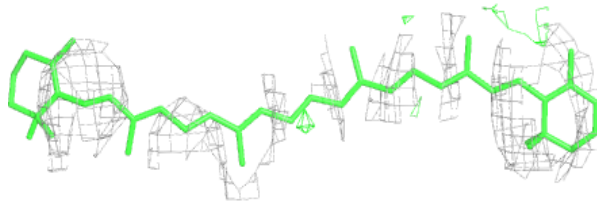




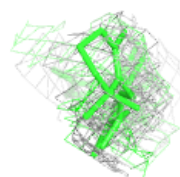
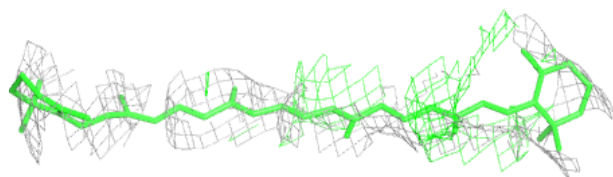
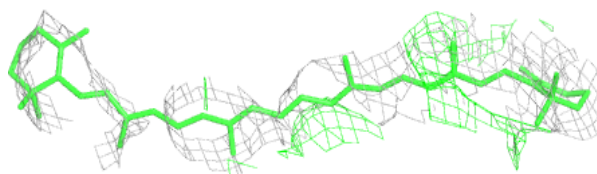


Electron density around BCR L 1005:

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

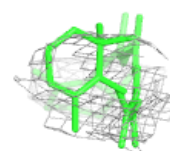
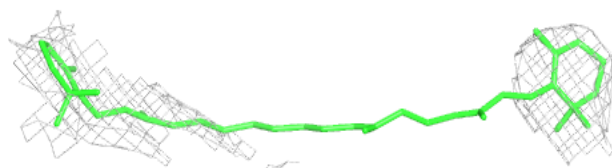
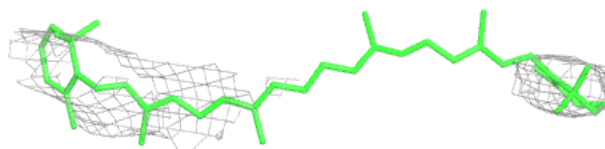
**Electron density around BCR L 1006:**

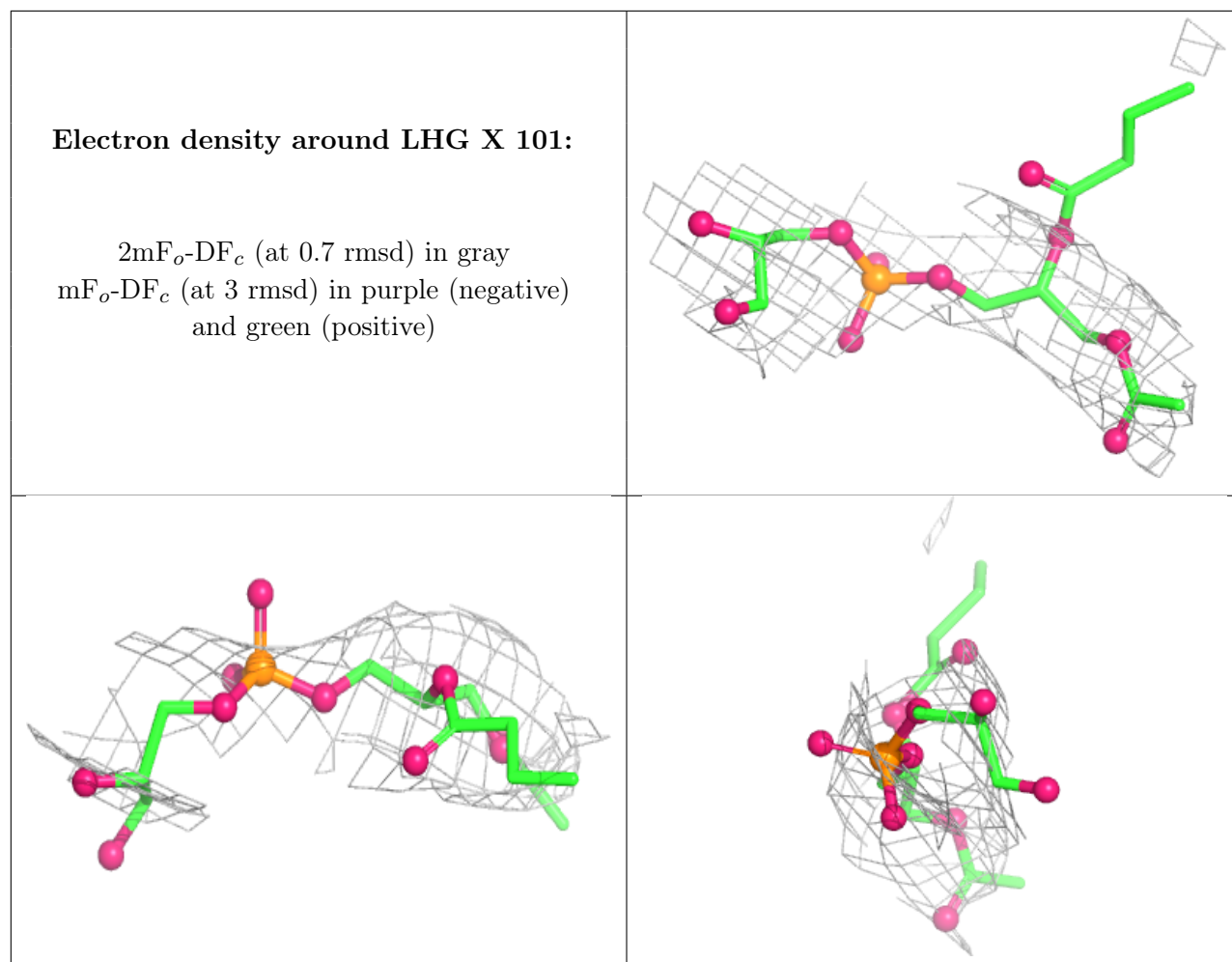
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BCR M 1203:

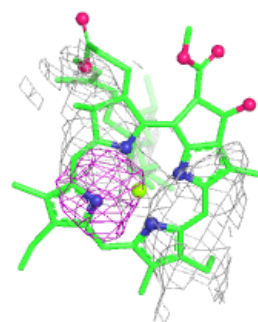
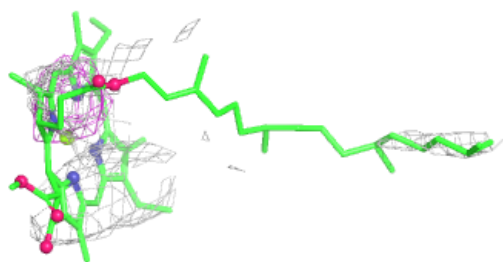
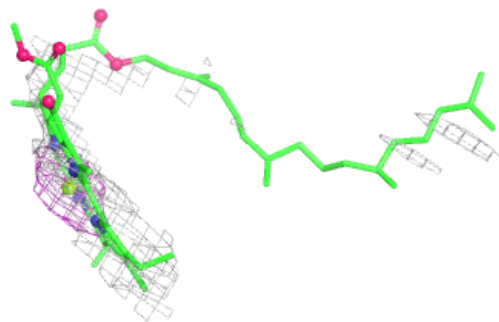
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



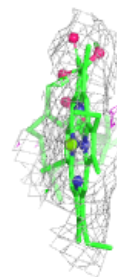


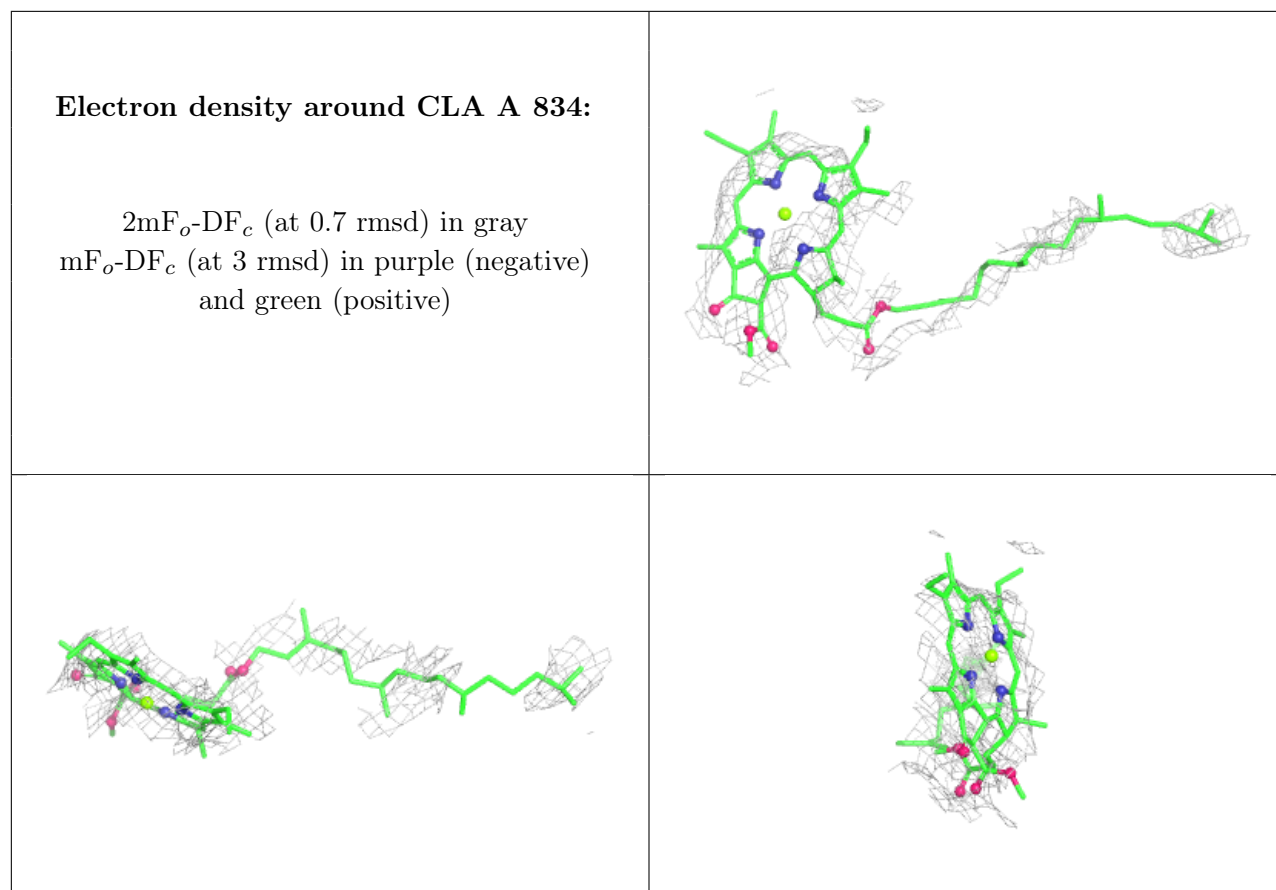
Electron density around CLA A 811:

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

**Electron density around CLA A 833:**

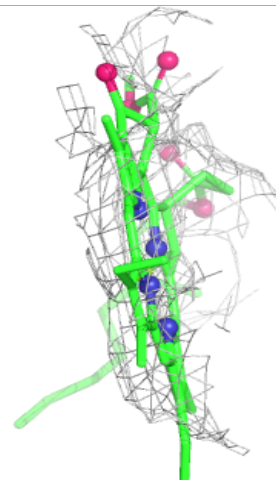
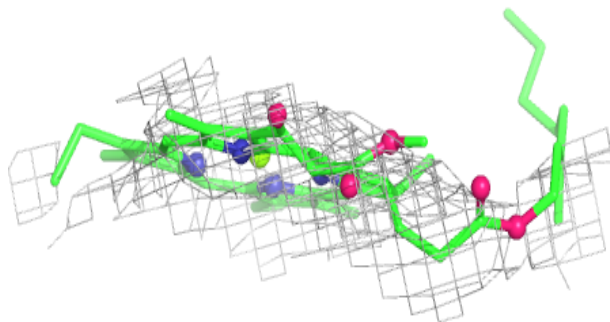
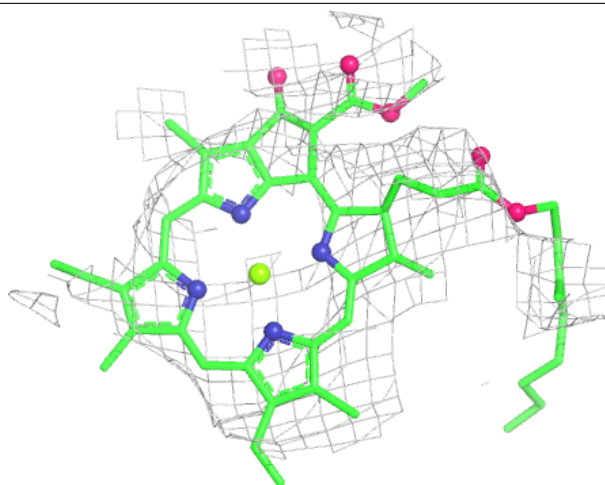
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

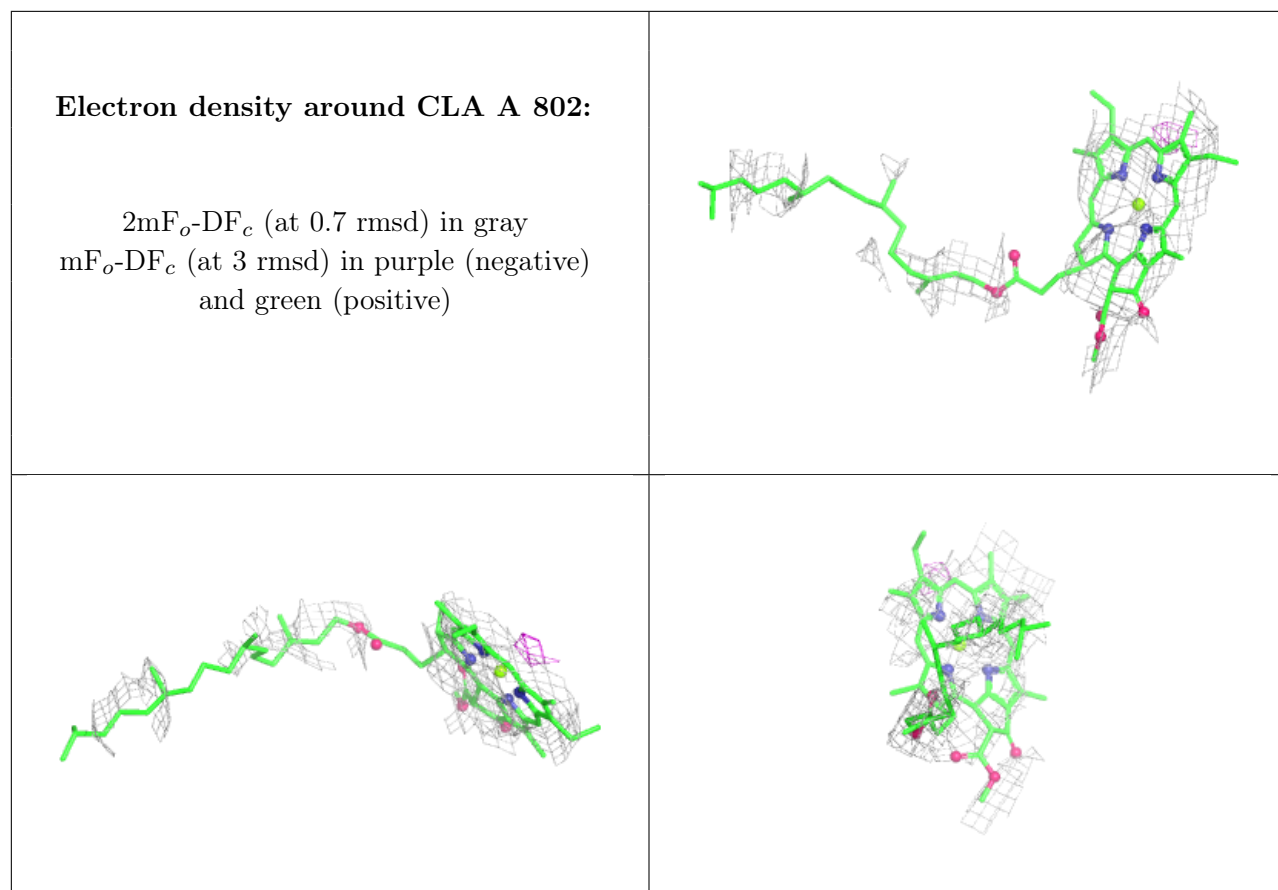




Electron density around CLA B 822:

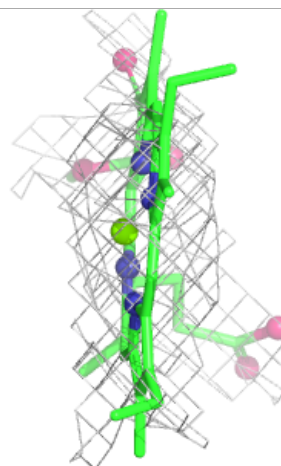
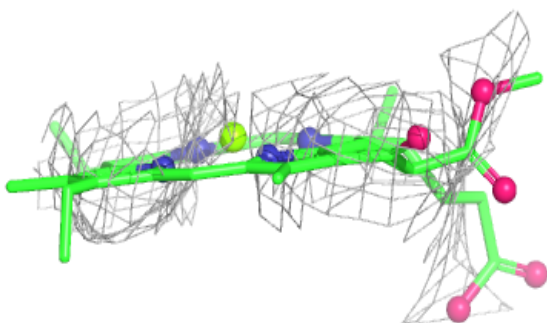
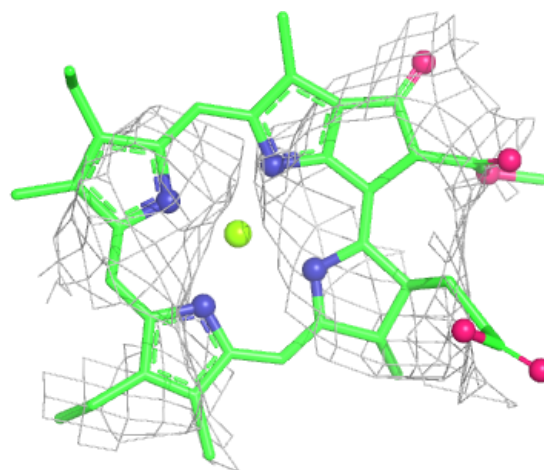
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





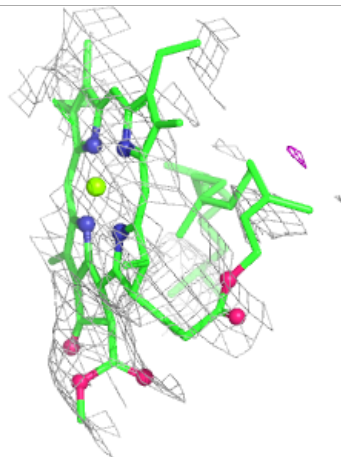
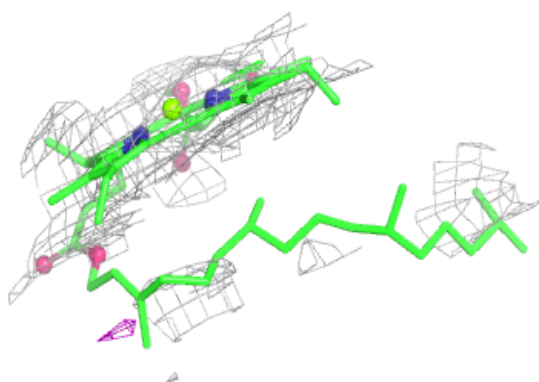
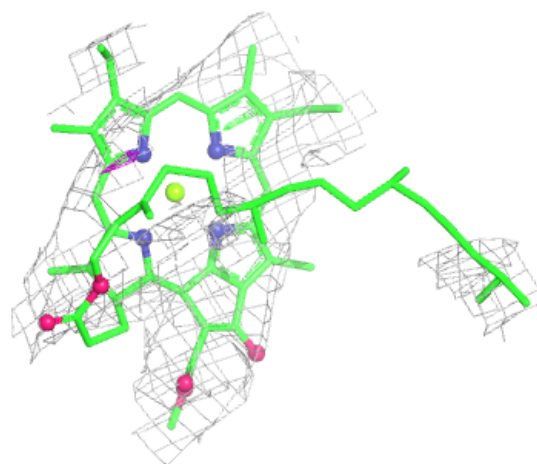
Electron density around CLA A 836:

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



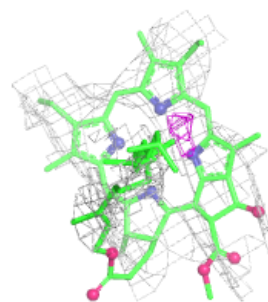
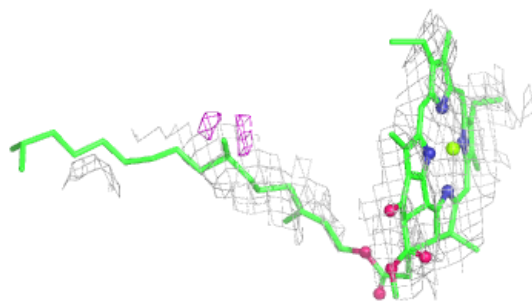
Electron density around CLA B 825:

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

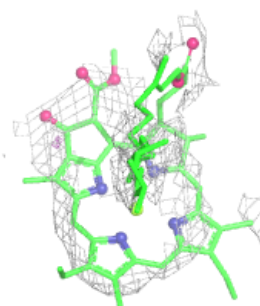
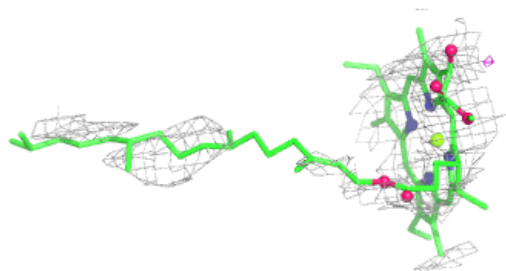
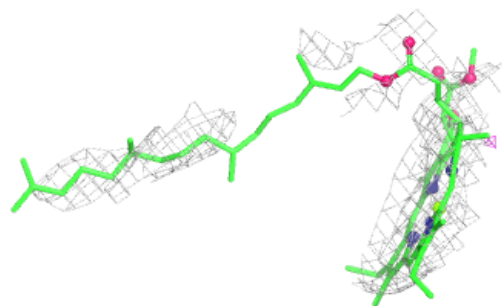


Electron density around CLA B 826:

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

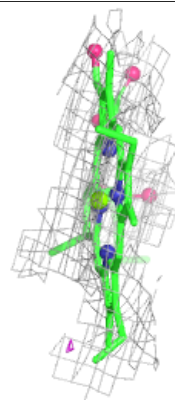
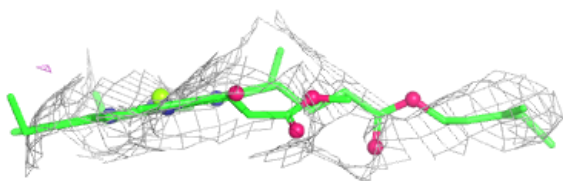
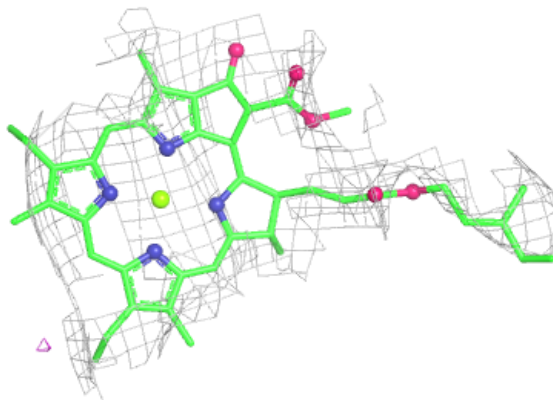
**Electron density around CLA B 827:**

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

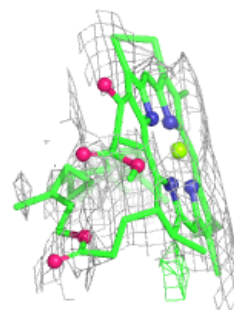
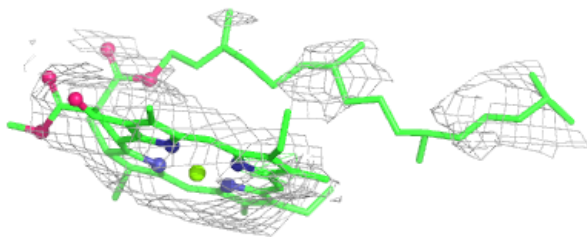
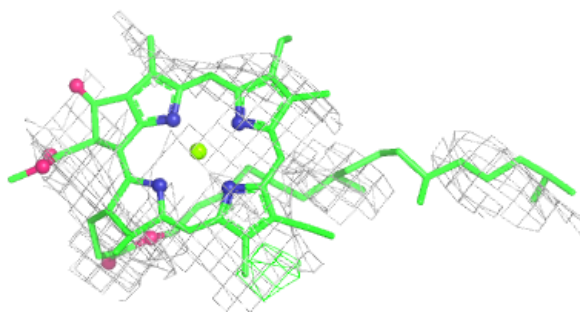


Electron density around CLA A 837:

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

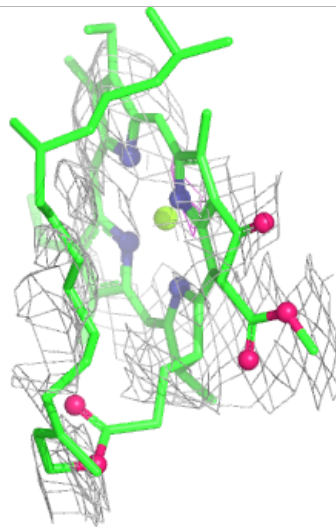
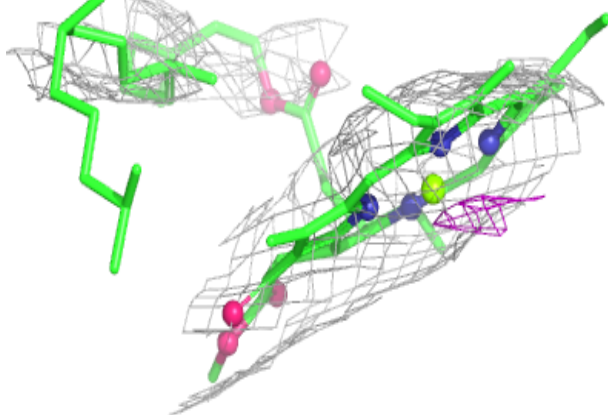
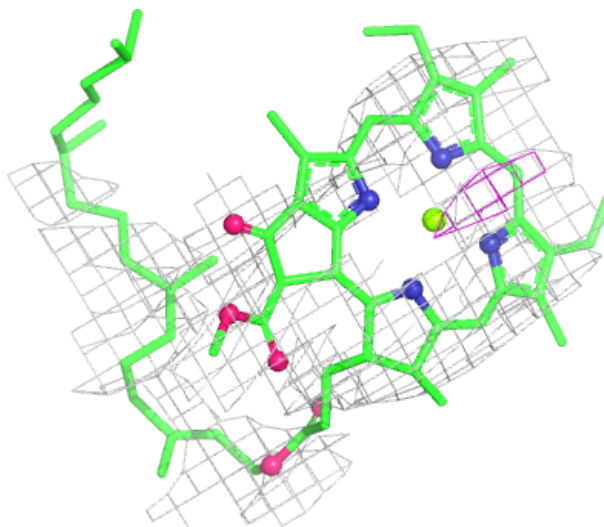
**Electron density around CLA A 838:**

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



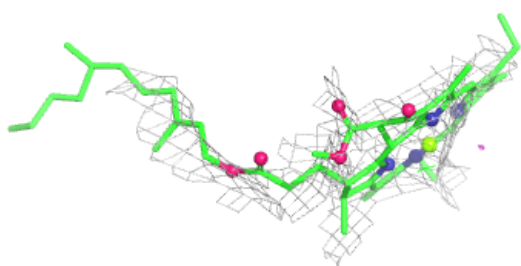
Electron density around CLA B 830:

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

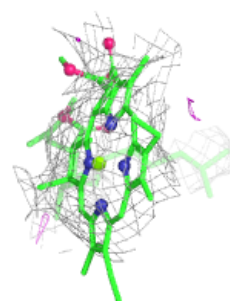
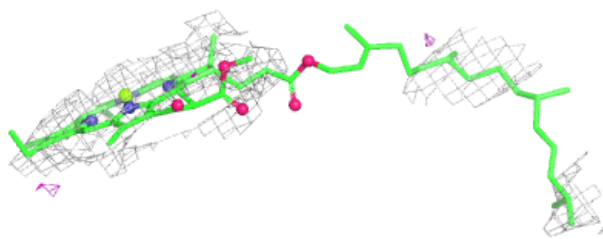
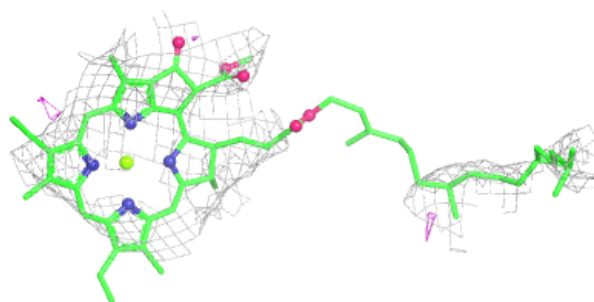


Electron density around CLA B 831:

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

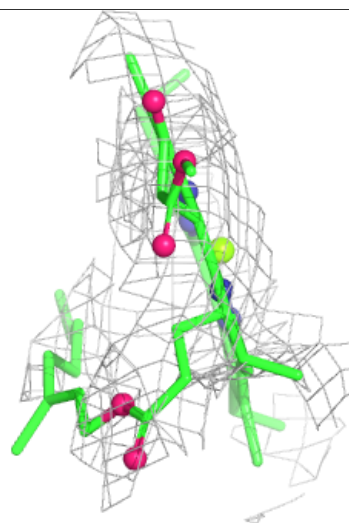
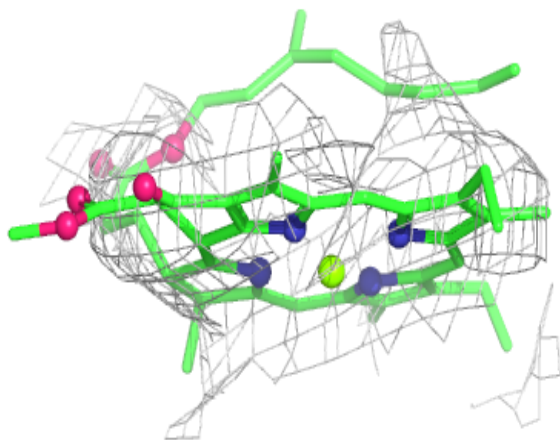
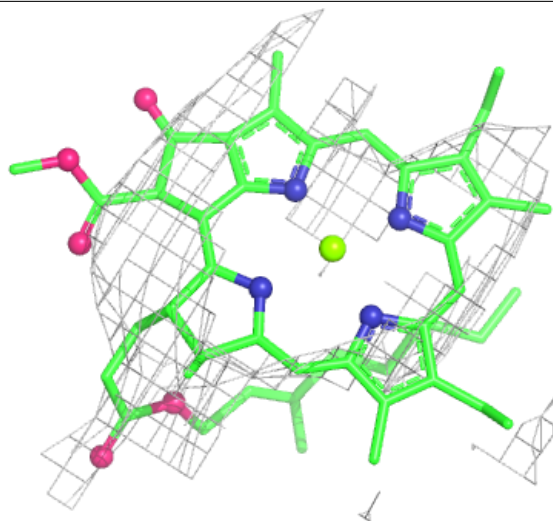
**Electron density around CLA A 805:**

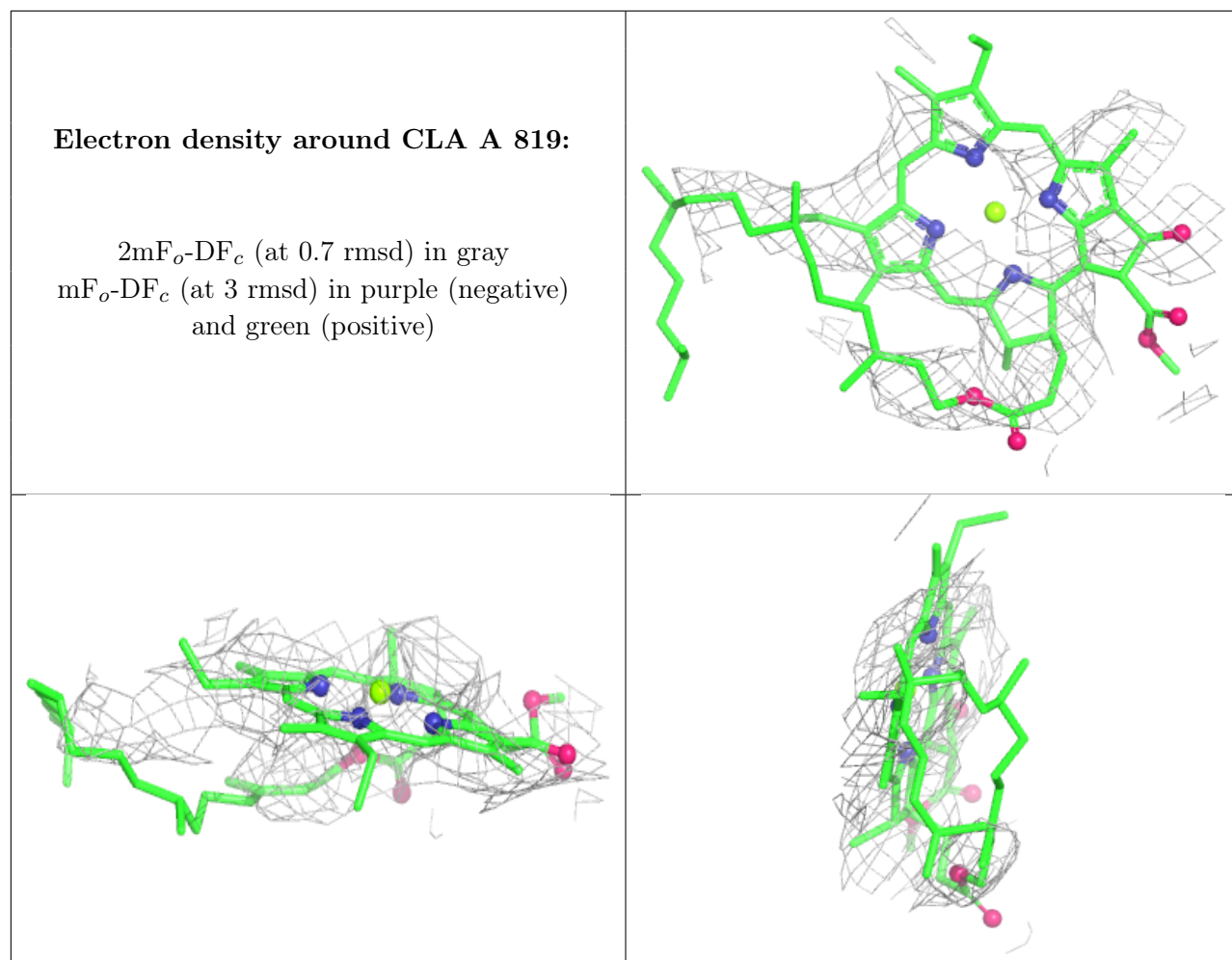
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA A 818:

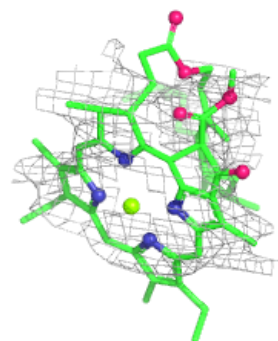
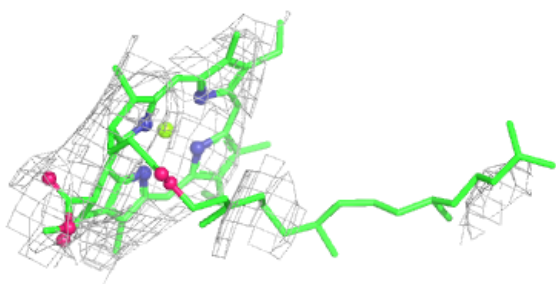
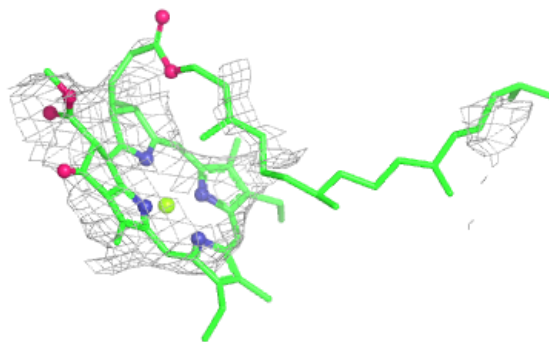
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



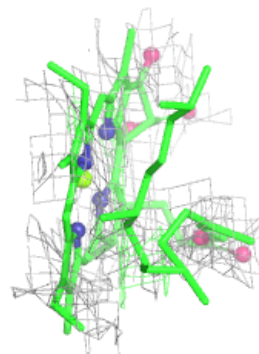
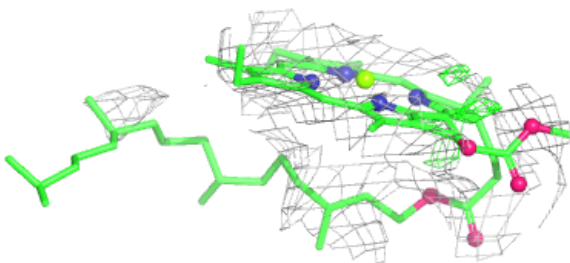
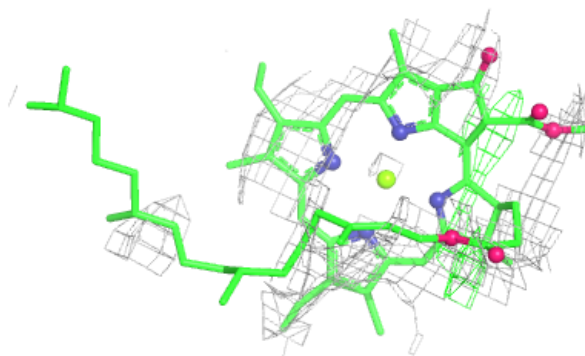


Electron density around CLA A 842:

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

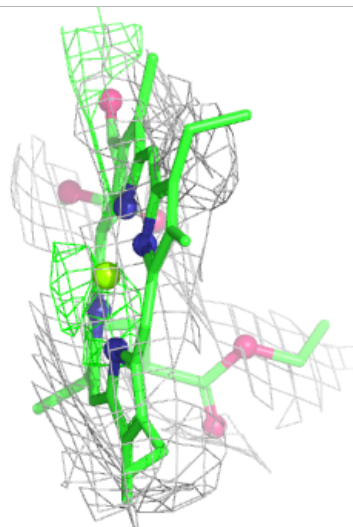
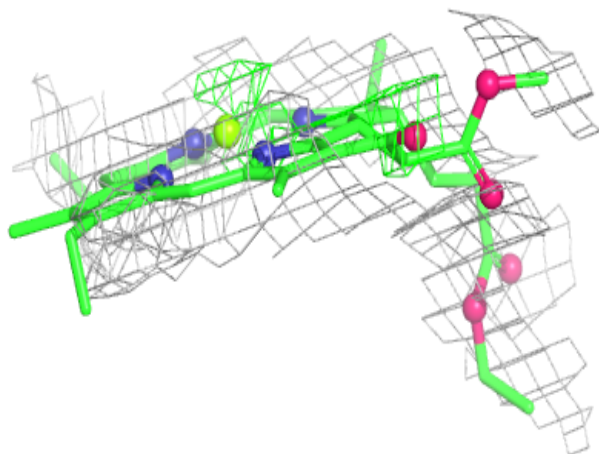
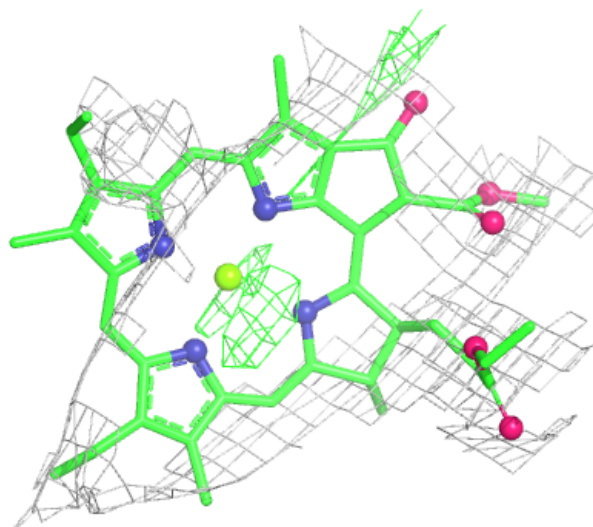
**Electron density around CLA B 836:**

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



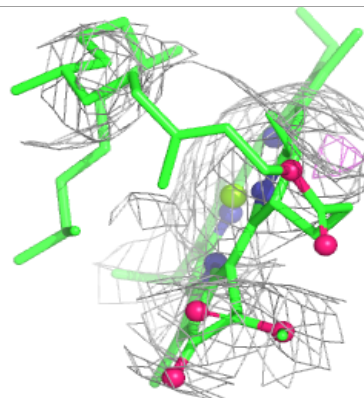
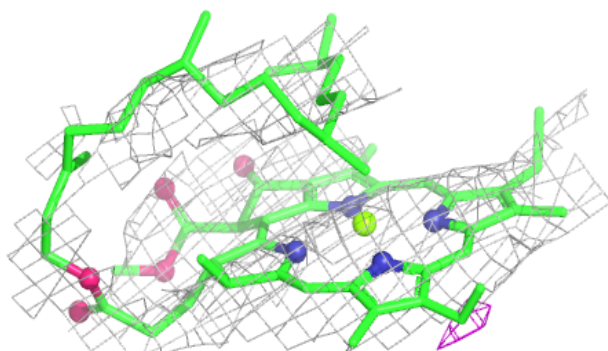
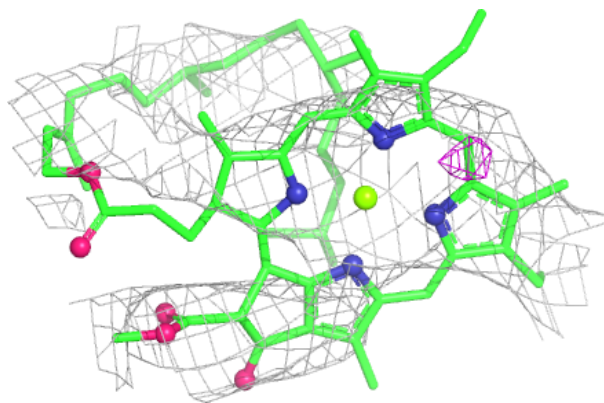
Electron density around CLA B 837:

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

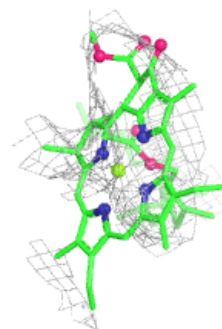
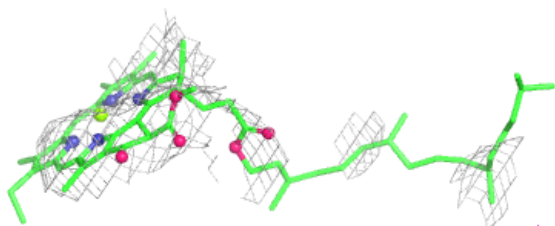
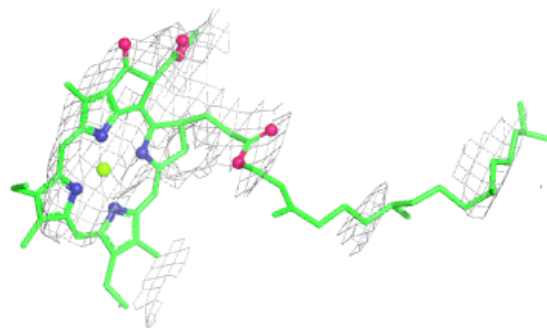


Electron density around CLA A 806:

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

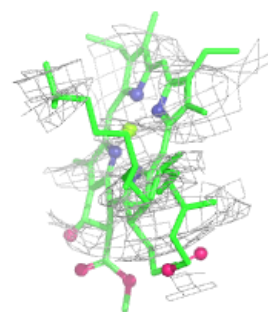
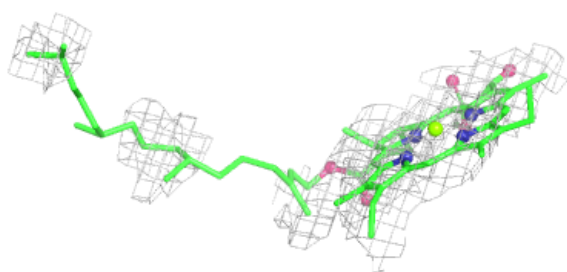
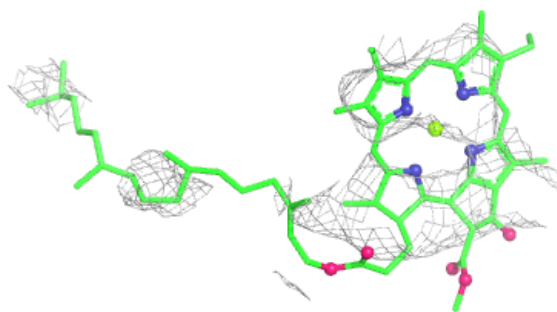
**Electron density around CLA A 821:**

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

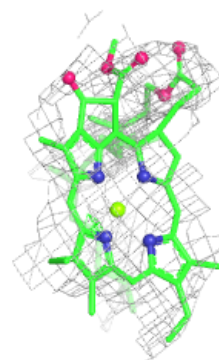
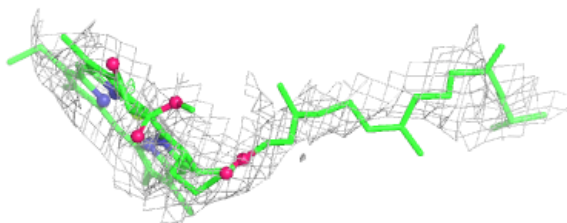
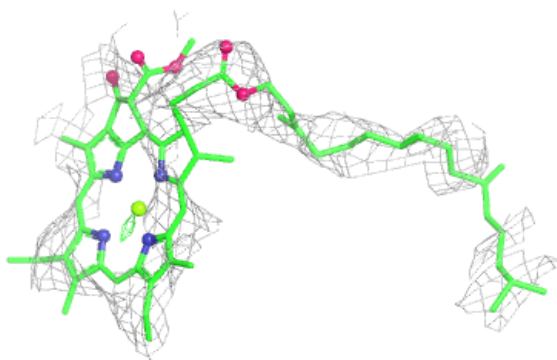


Electron density around CLA A 803:

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

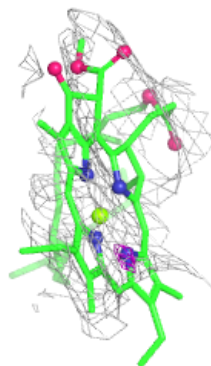
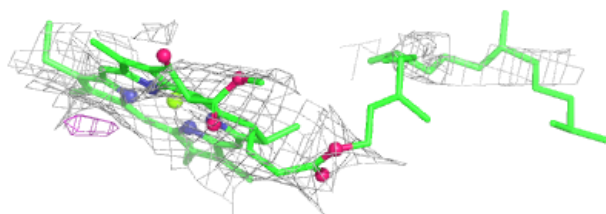
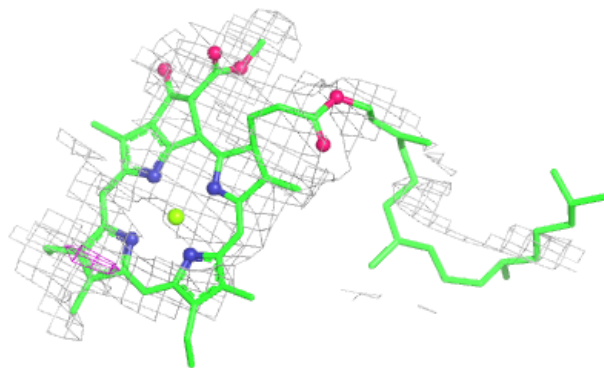
**Electron density around CLA I 101:**

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

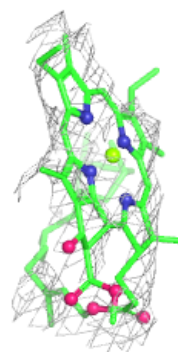
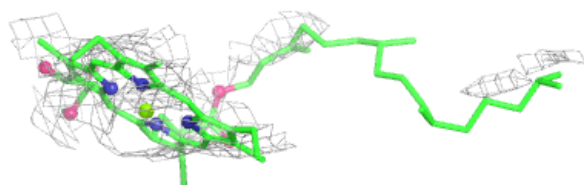
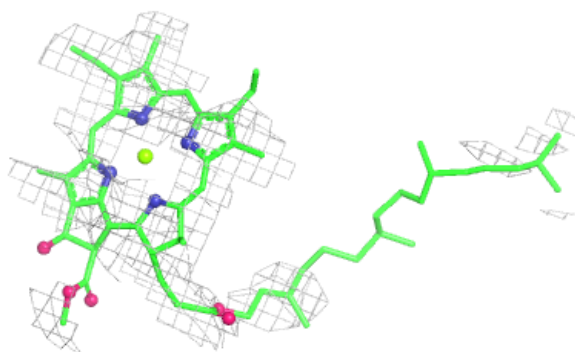


Electron density around CLA J 1101:

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

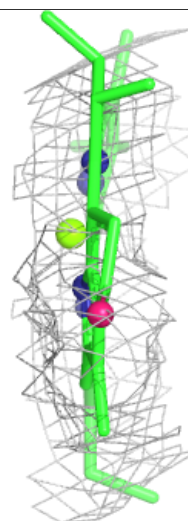
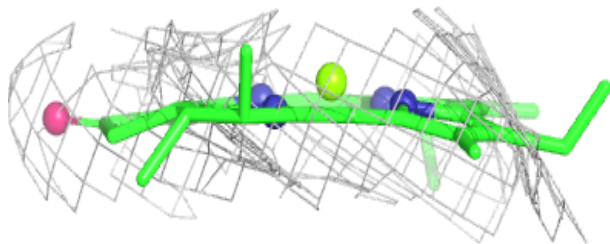
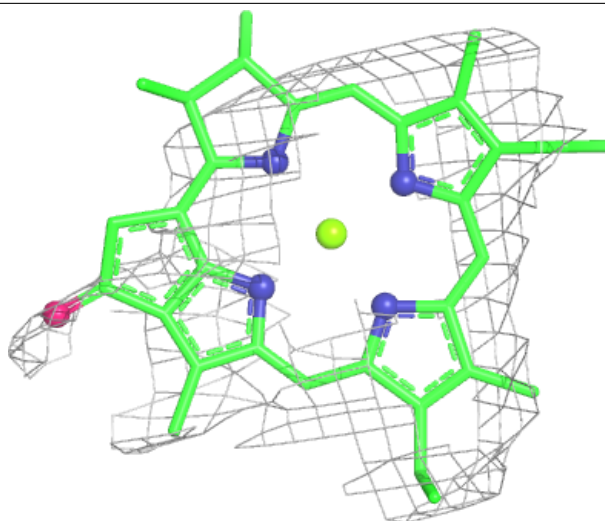
**Electron density around CLA A 808:**

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



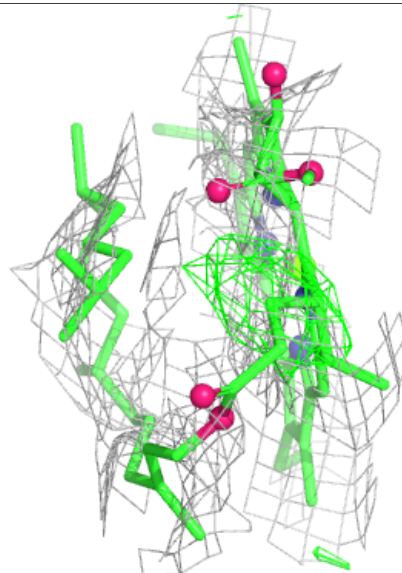
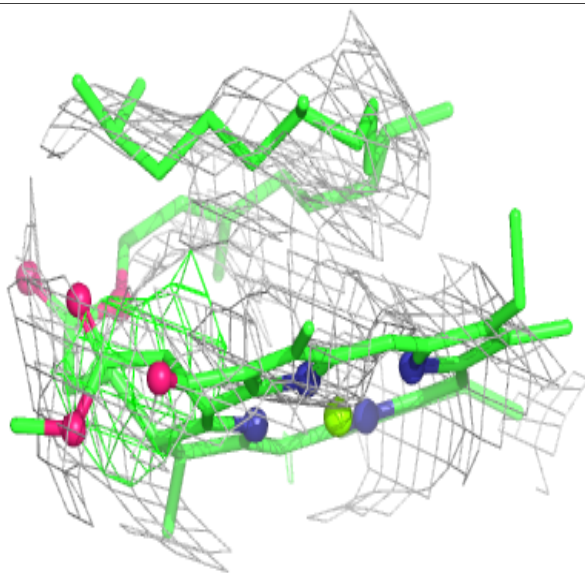
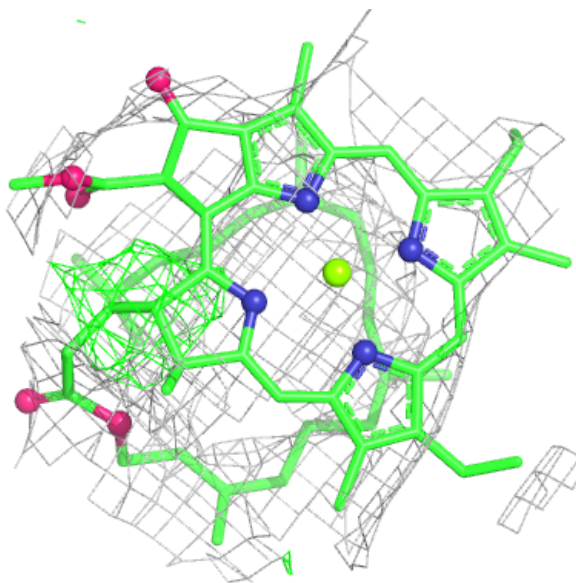
Electron density around CLA J 1103:

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



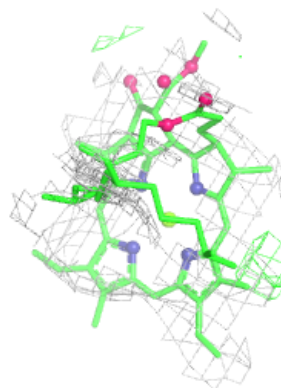
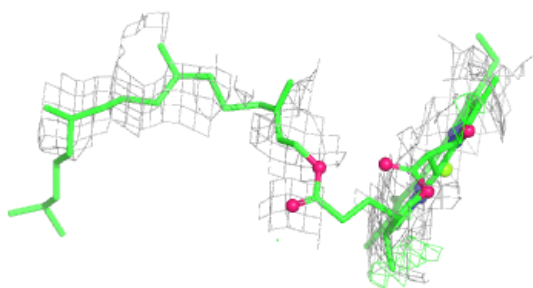
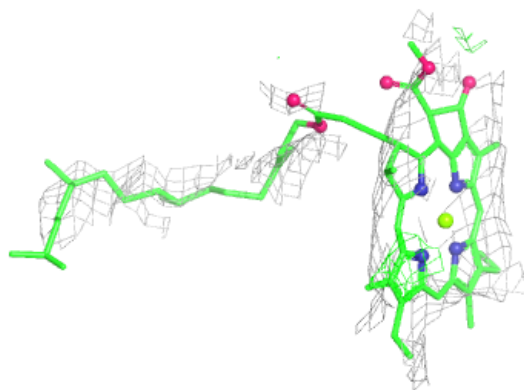
Electron density around CLA L 1002:

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

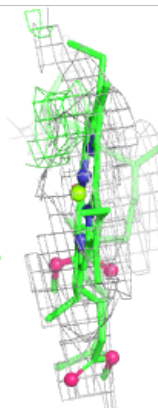
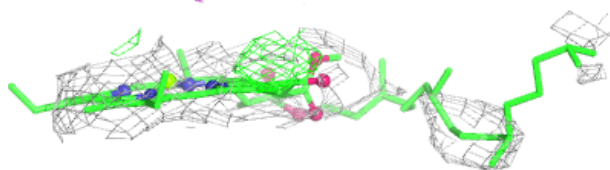
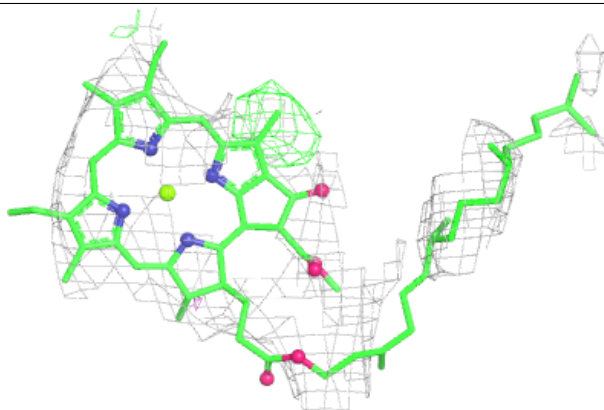


Electron density around CLA L 1003:

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

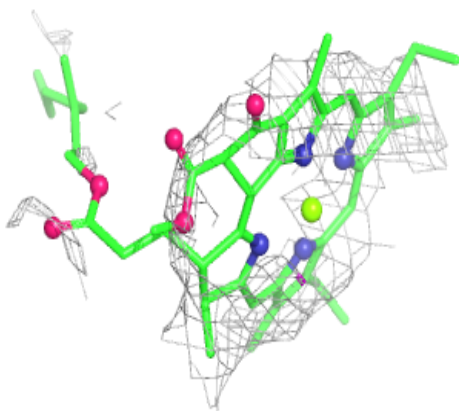
**Electron density around CLA L 1004:**

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



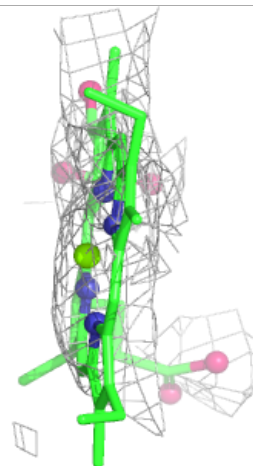
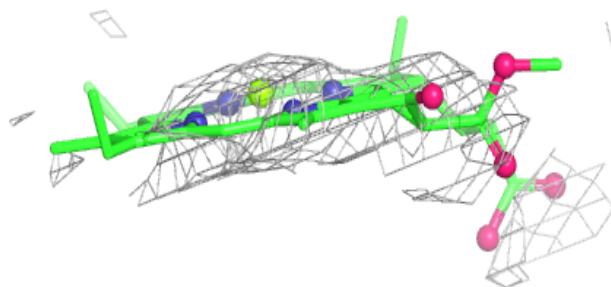
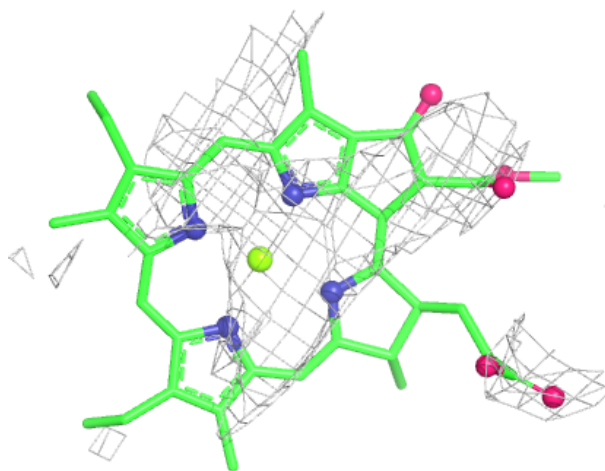
Electron density around CLA M 1201:

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



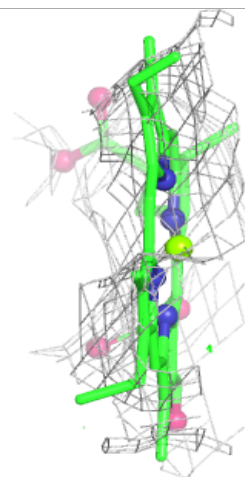
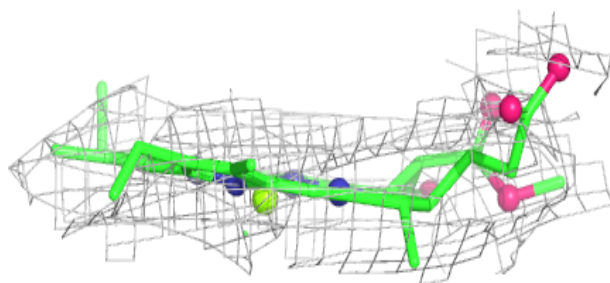
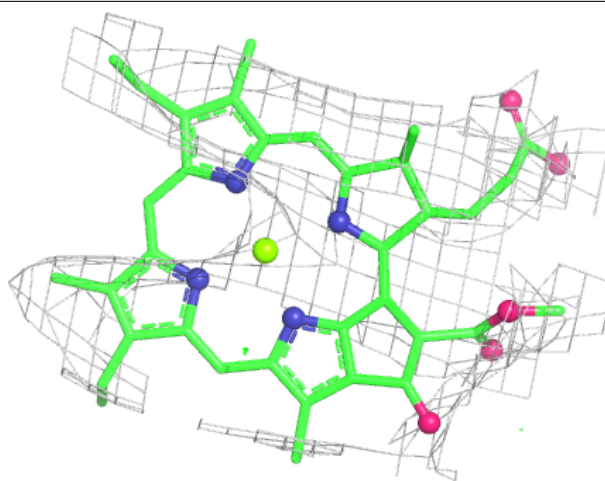
Electron density around CLA M 1202:

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



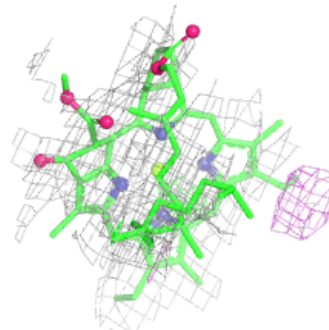
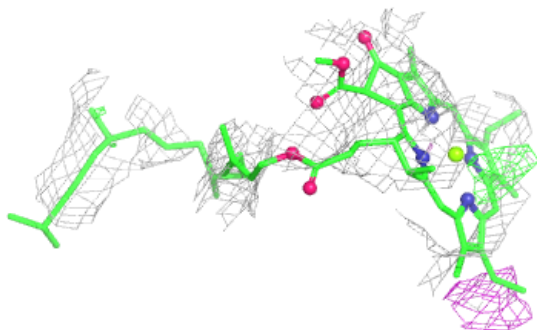
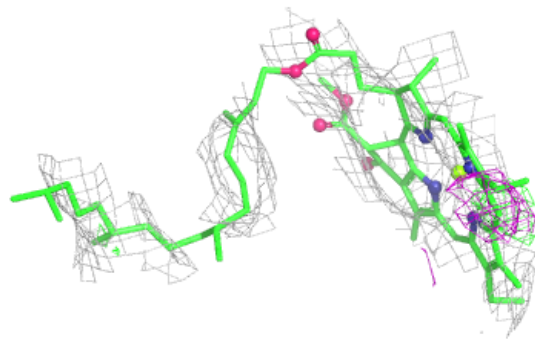
Electron density around CLA X 102:

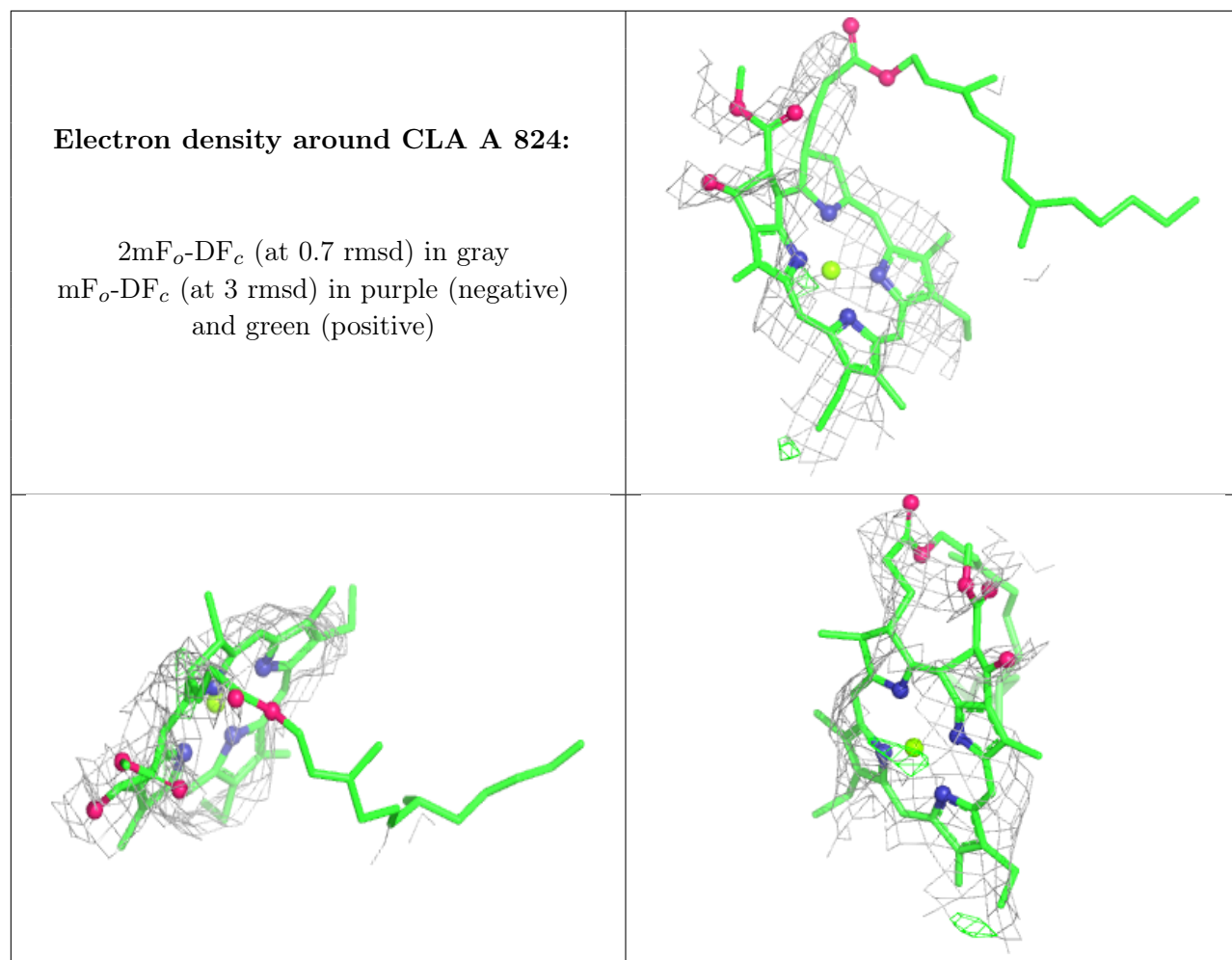
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 801:

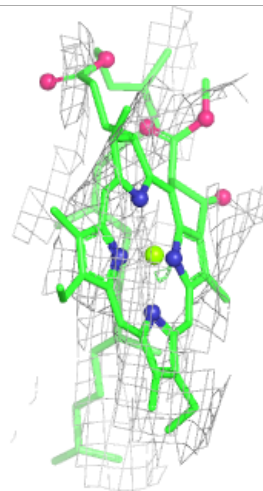
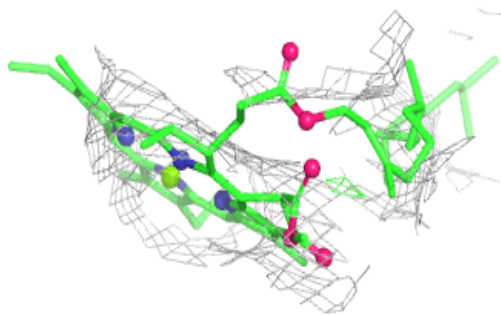
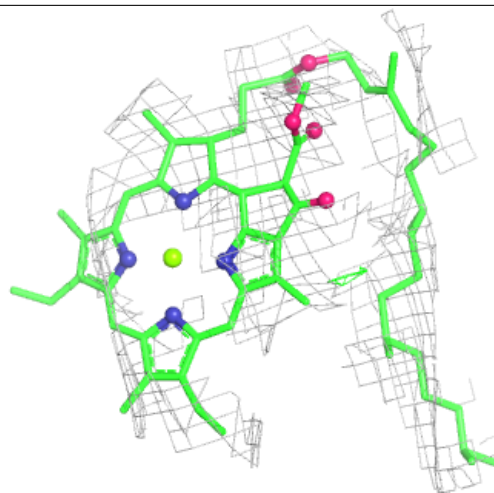
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





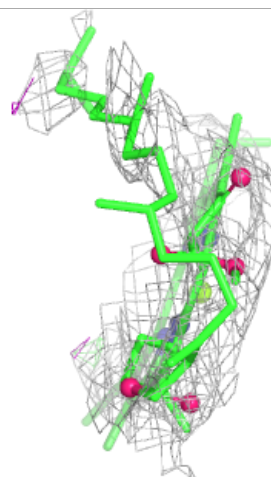
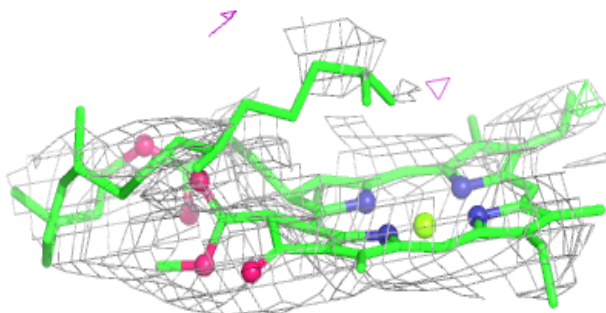
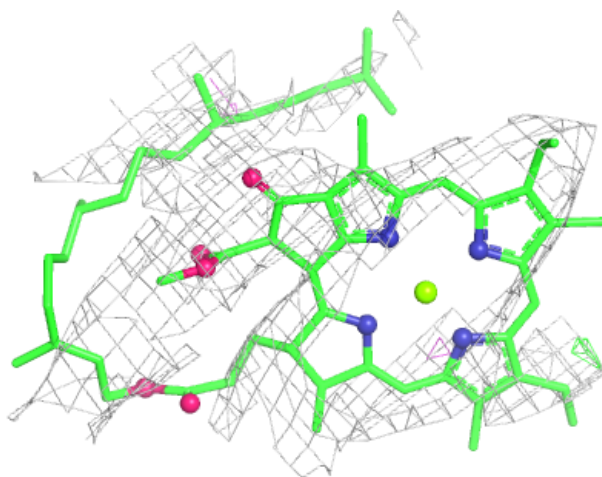
Electron density around CLA A 825:

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



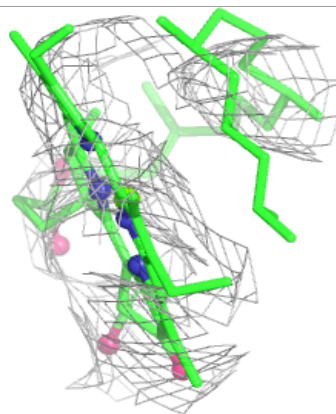
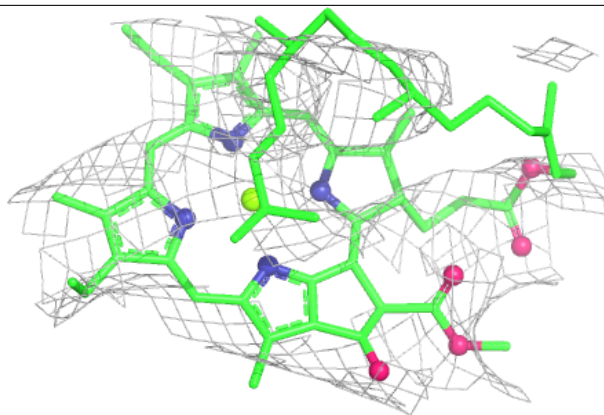
Electron density around CLA B 804:

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

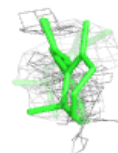
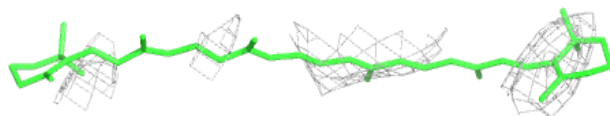
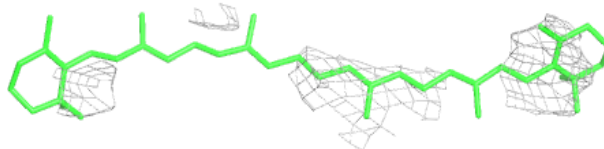


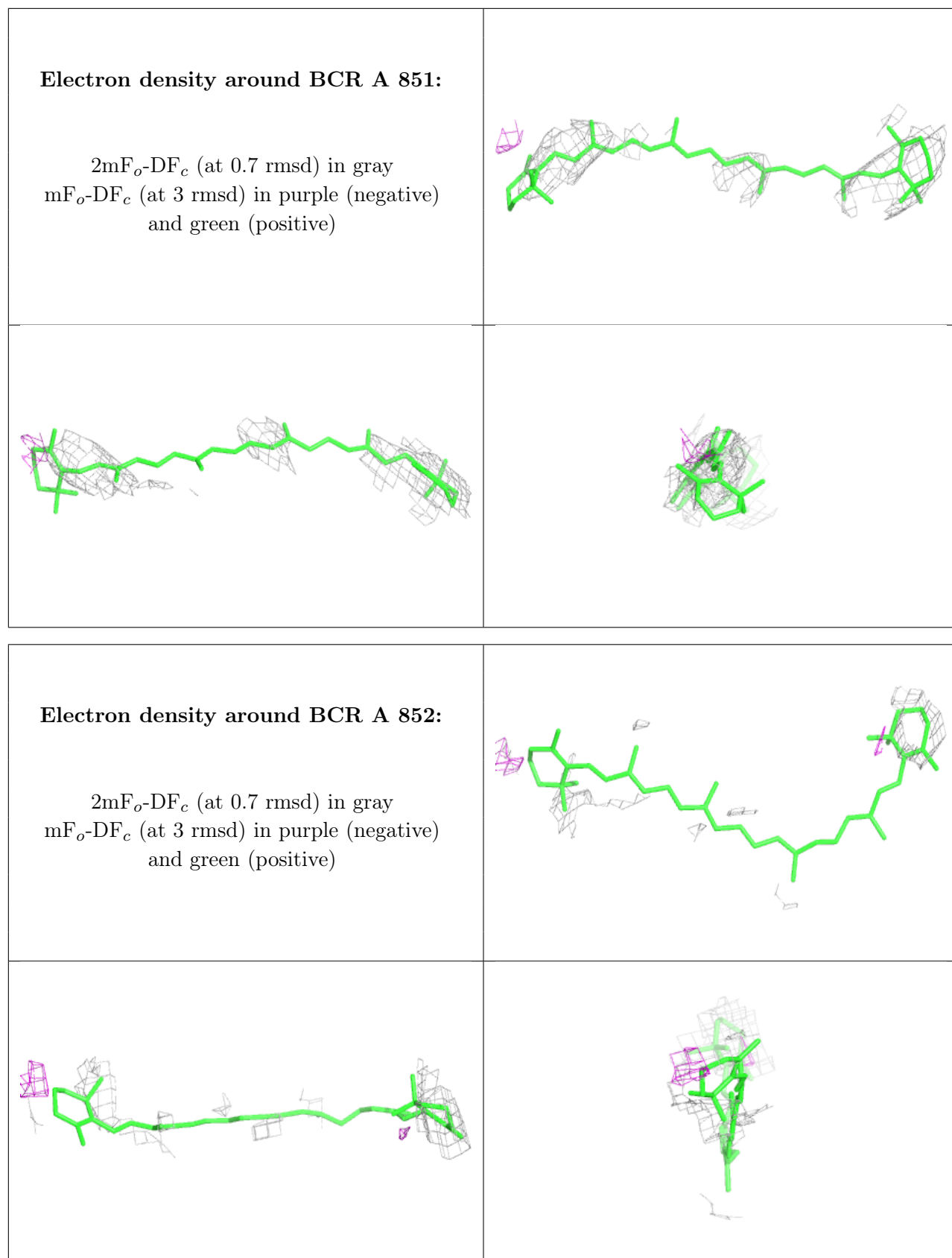
Electron density around CLA B 805:

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

**Electron density around BCR A 850:**

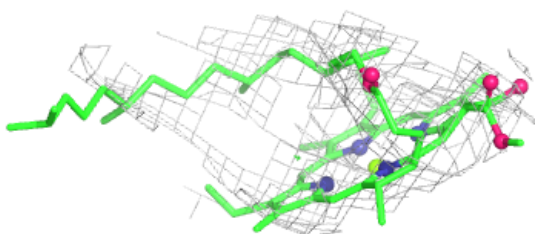
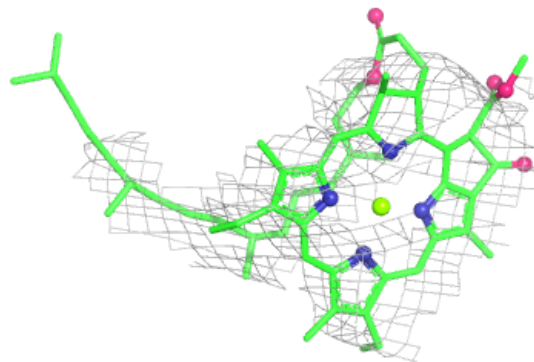
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



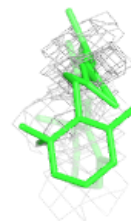
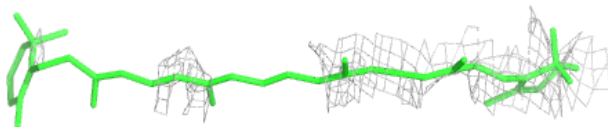
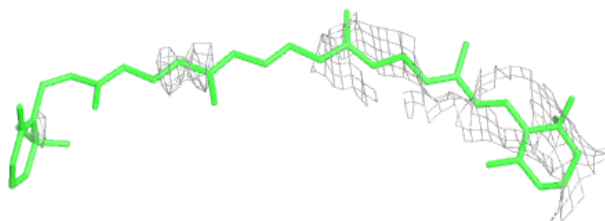


Electron density around CLA B 806:

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

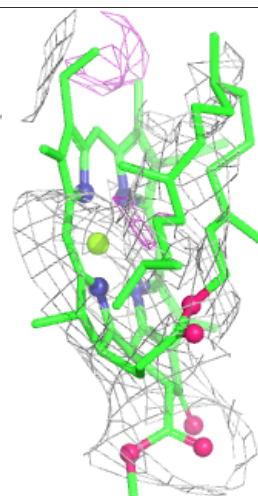
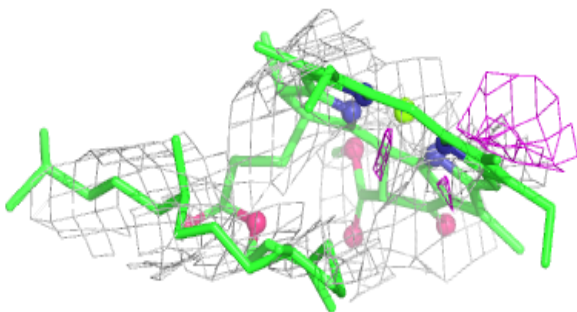
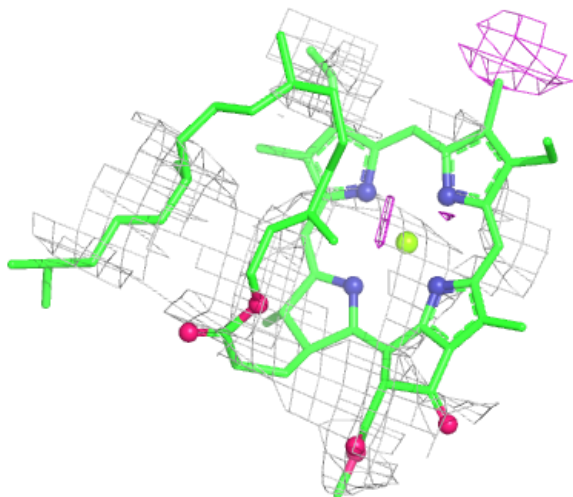
**Electron density around BCR B 842:**

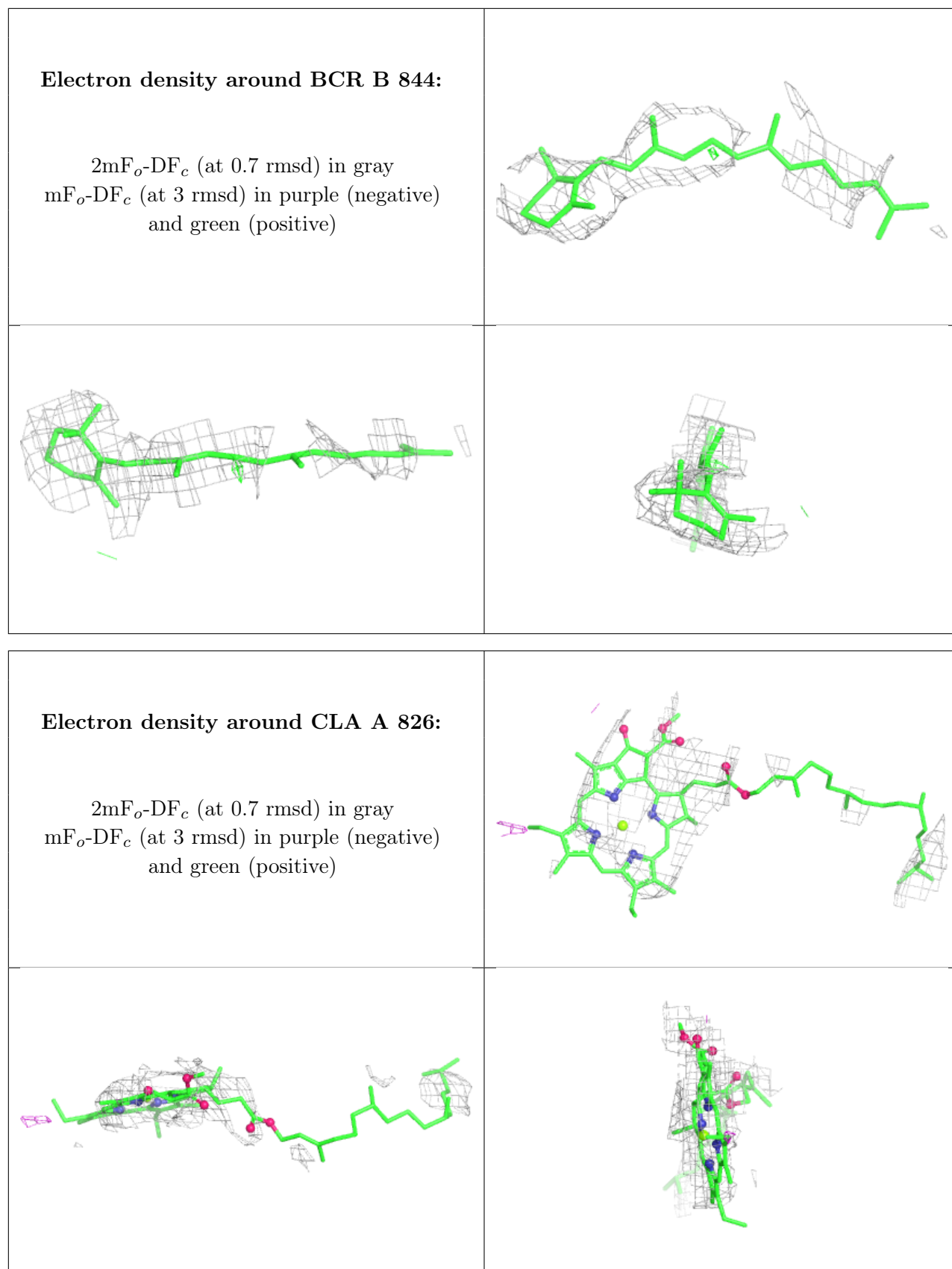
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 807:

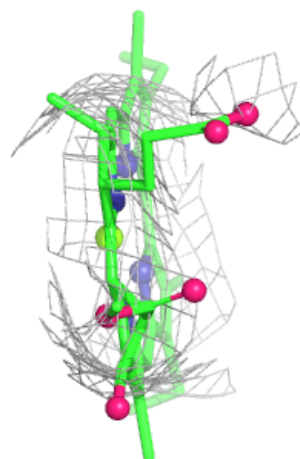
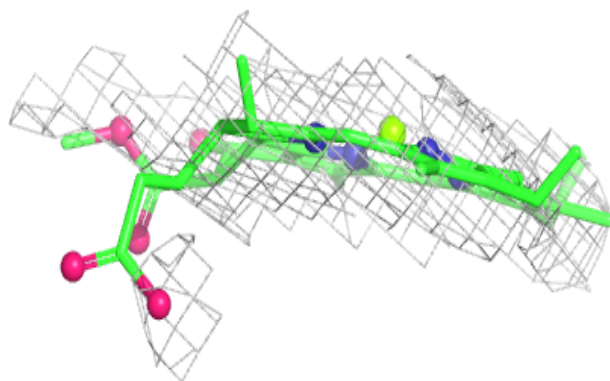
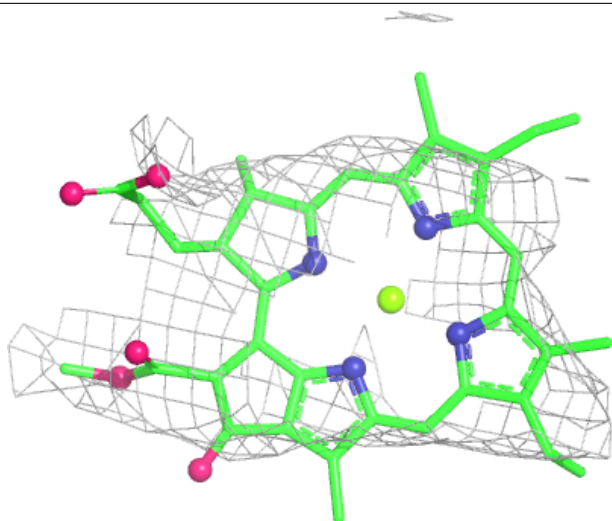
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





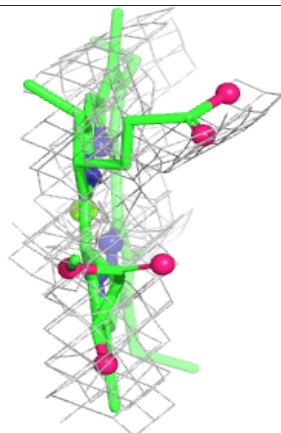
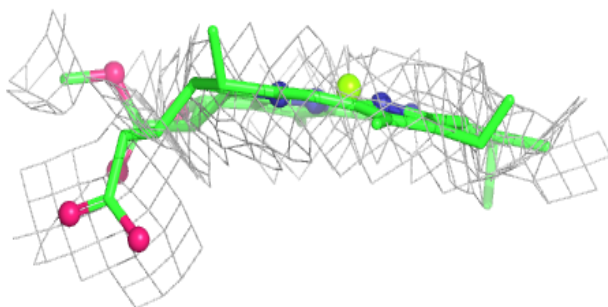
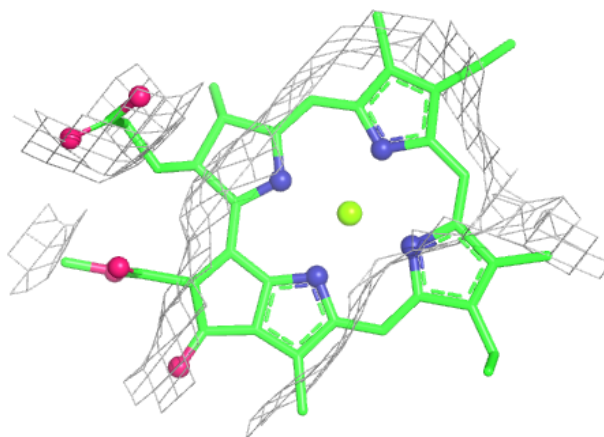
Electron density around CLA B 809:

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

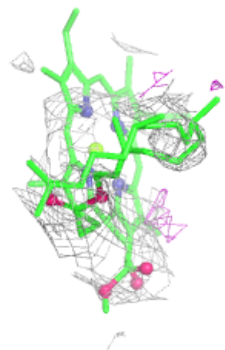
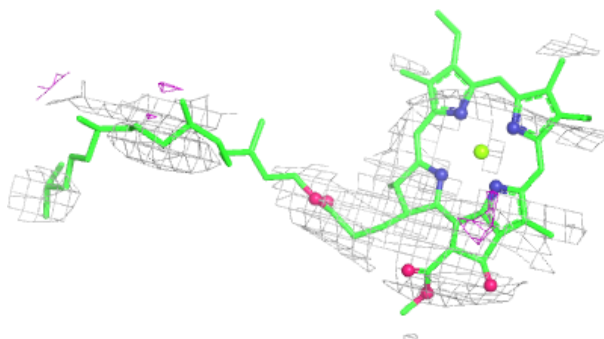


Electron density around CLA A 814:

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

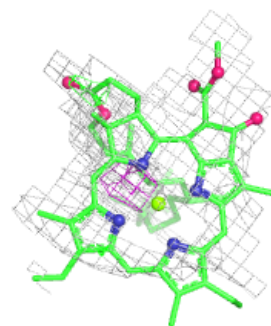
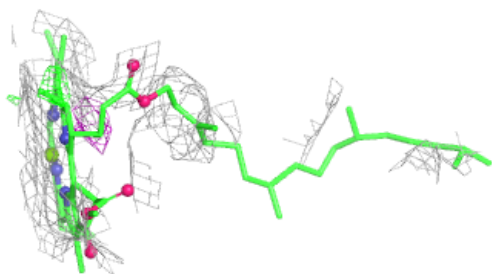
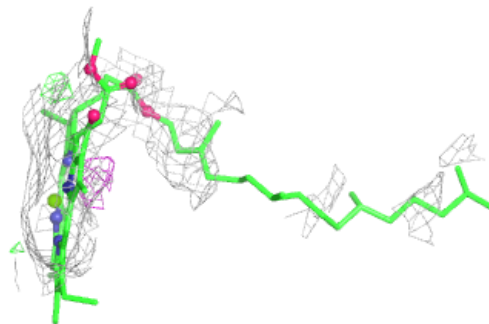
**Electron density around CLA B 811:**

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

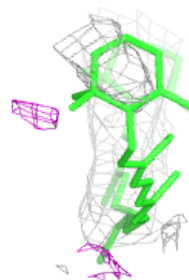
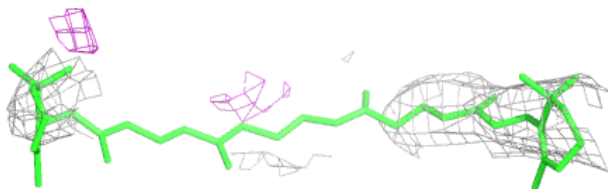
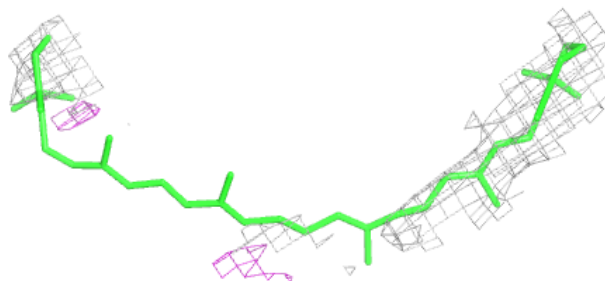


Electron density around CLA A 828:

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

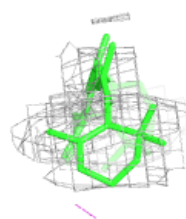
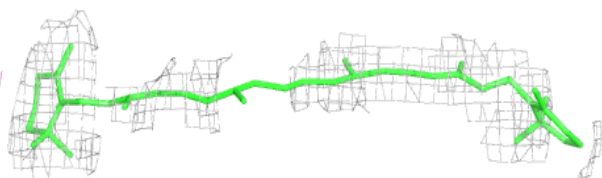
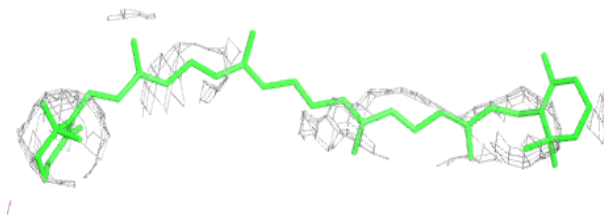
**Electron density around BCR F 1302:**

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



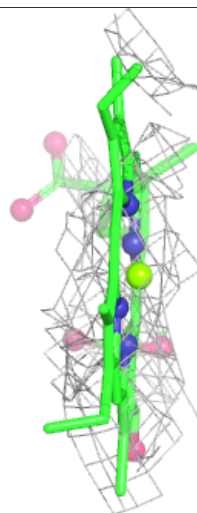
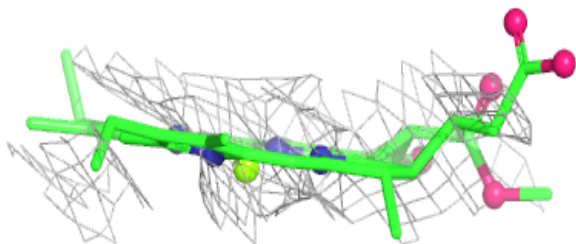
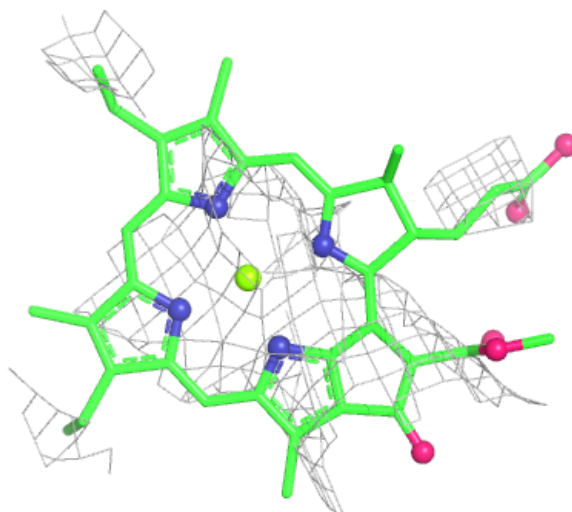
Electron density around BCR I 102:

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



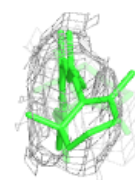
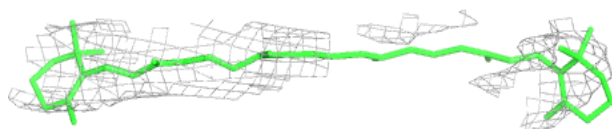
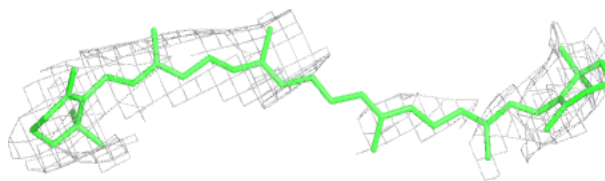
Electron density around CLA A 815:

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

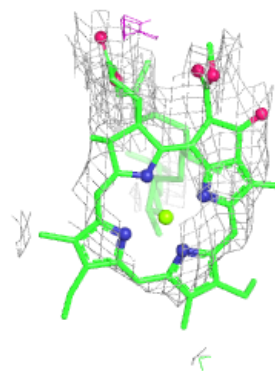
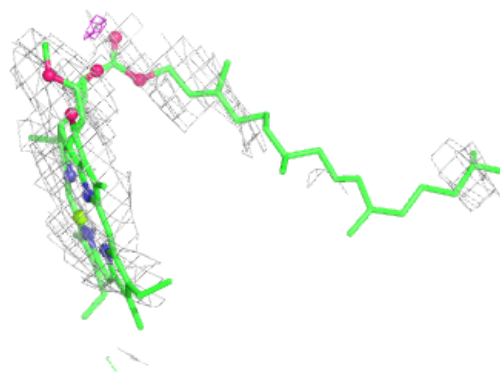


Electron density around BCR J 1105:

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

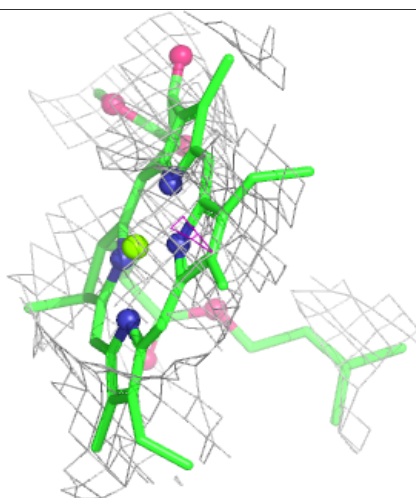
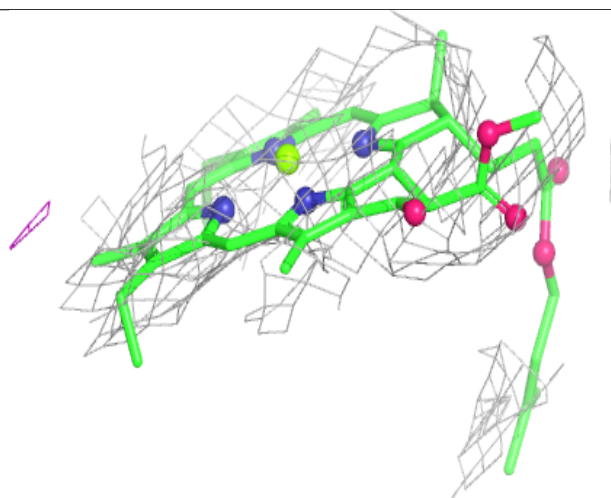
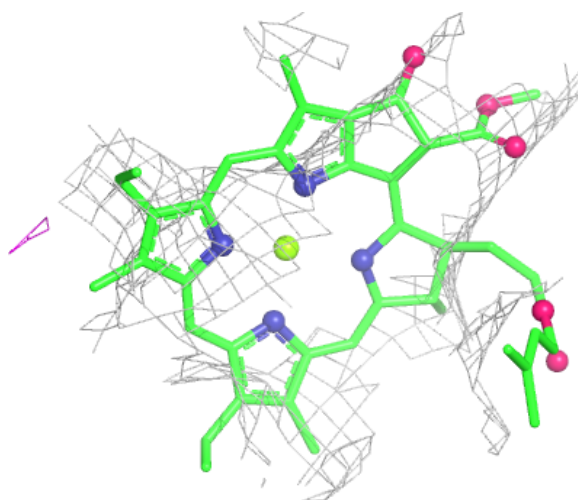
**Electron density around CLA A 830:**

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



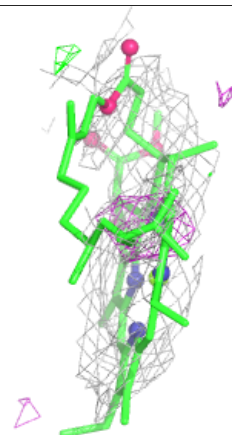
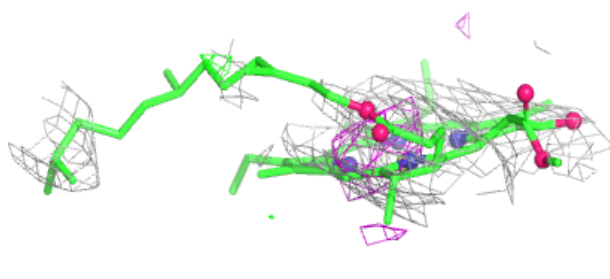
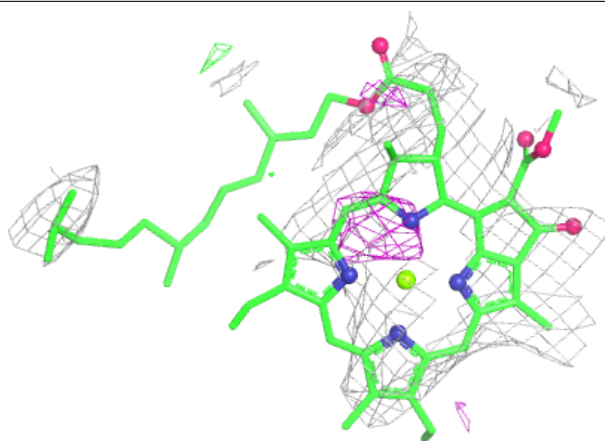
Electron density around CLA A 831:

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

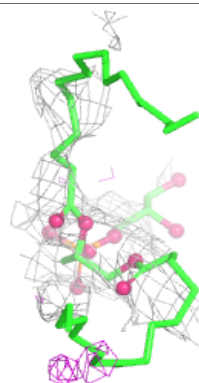
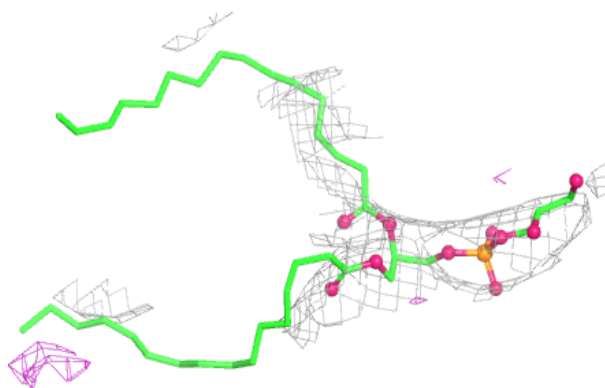


Electron density around CLA B 816:

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

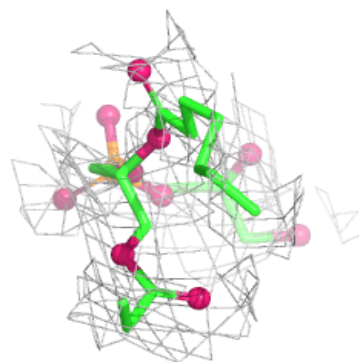
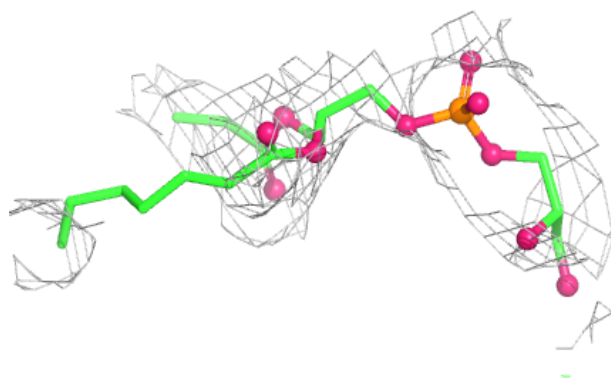
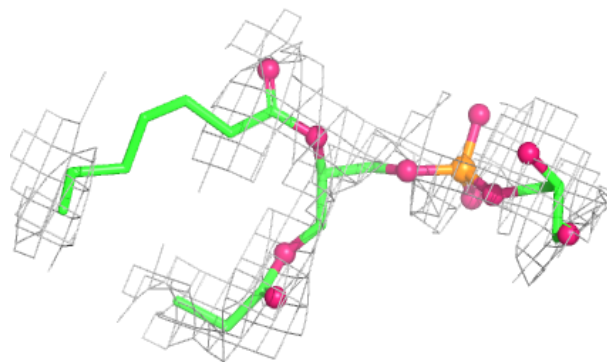
**Electron density around LHG A 853:**

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

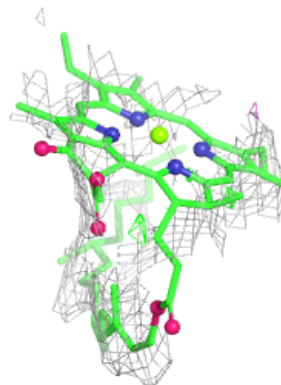
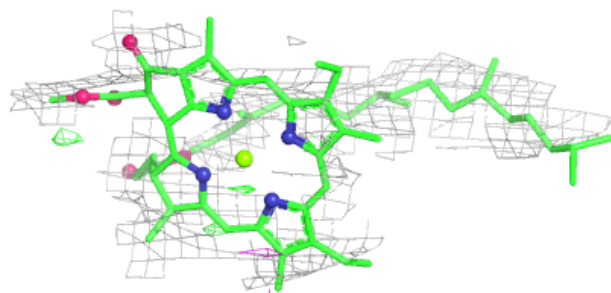
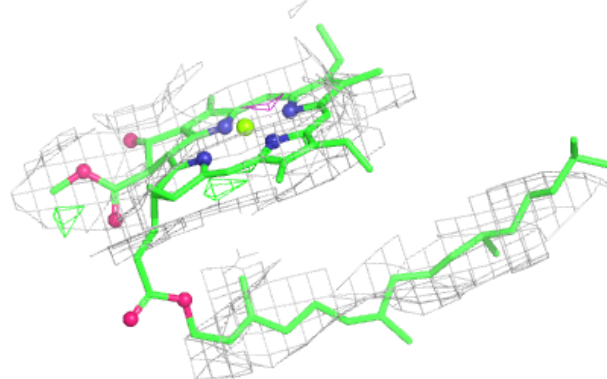


Electron density around LHG A 854:

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

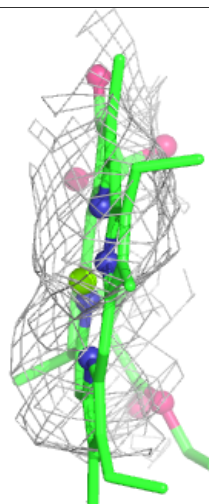
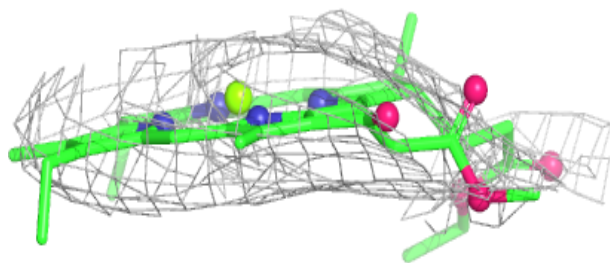
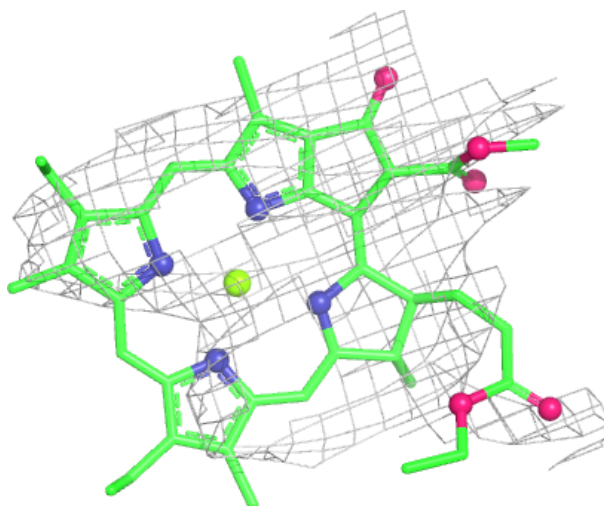
**Electron density around CLA A 832:**

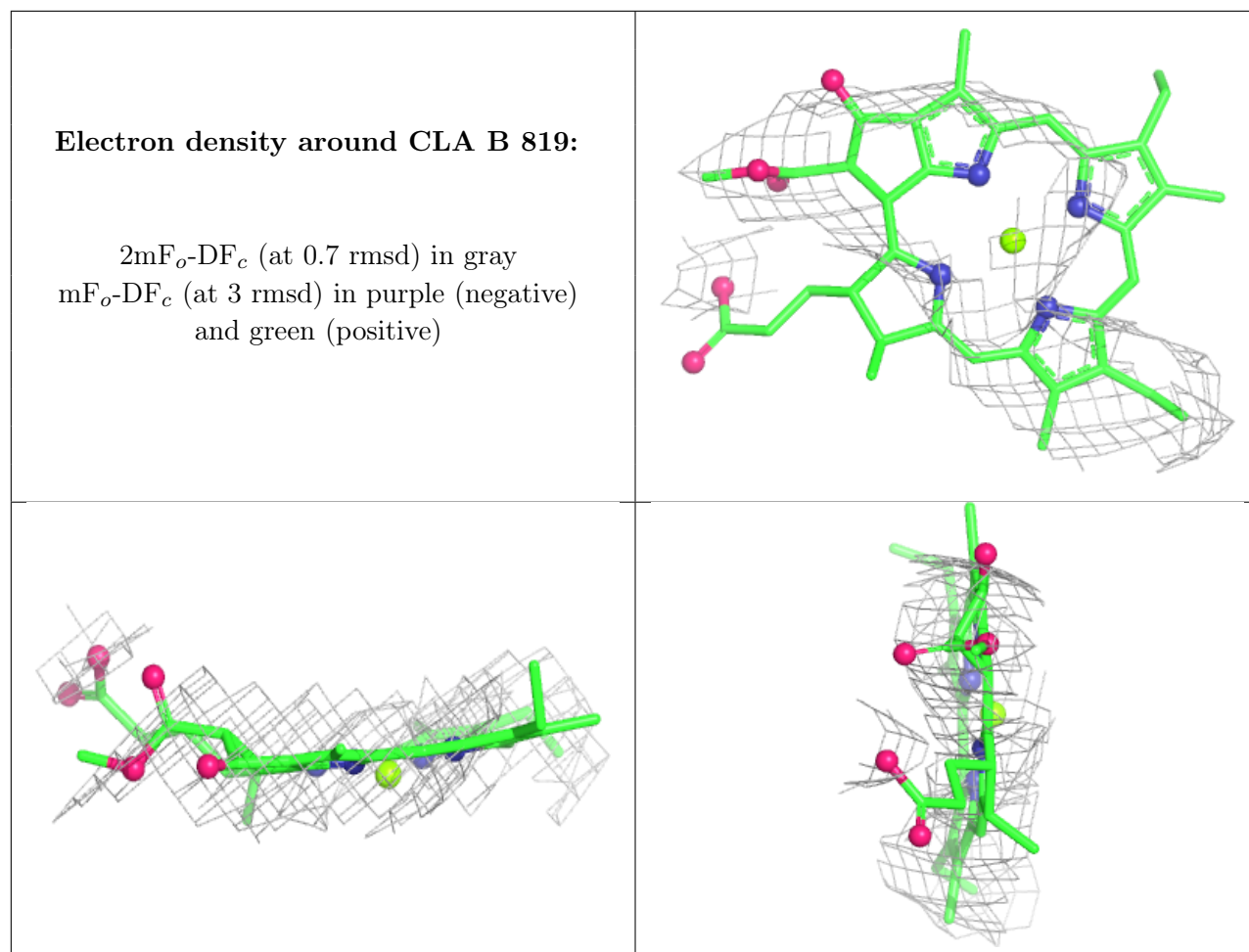
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.