



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 15, 2021 – 12:44 PM EST

PDB ID : 7M78  
Title : Room Temperature XFEL Crystallography reveals asymmetry in the vicinity of the two phylloquinones in Photosystem I  
Authors : Keable, S.M.; Simon, P.S.; Kolsch, A.; Kern, J.; Yachandra, V.K.; Zouni, A.; Yano, J.  
Deposited on : 2021-03-26  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

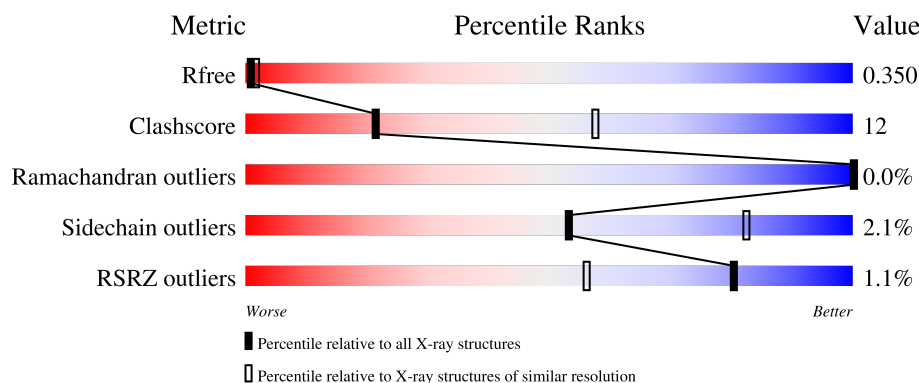
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	755	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>.</div> </div> </div>
2	B	740	<div> <div></div> <div>73%</div> <div>26%</div> </div>
3	C	80	<div> <div></div> <div>74%</div> <div>24%</div> <div>.</div> </div>
4	D	138	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>22%</div> </div> </div>
5	E	75	<div> <div></div> <div>73%</div> <div>16%</div> <div>.</div> <div>8%</div> </div>

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CL0	A	801	X	-	-	-
14	CLA	A	802	X	-	-	-
14	CLA	A	803	X	-	-	-
14	CLA	A	804	X	-	-	-
14	CLA	A	805	X	-	-	-
14	CLA	A	806	X	-	-	-
14	CLA	A	807	X	-	-	-
14	CLA	A	808	X	-	-	-
14	CLA	A	809	X	-	-	-
14	CLA	A	810	X	-	-	-
14	CLA	A	811	X	-	-	-
14	CLA	A	812	X	-	-	-
14	CLA	A	813	X	-	-	-
14	CLA	A	814	X	-	-	-
14	CLA	A	815	X	-	-	-
14	CLA	A	816	X	-	-	-
14	CLA	A	817	X	-	-	-
14	CLA	A	818	X	-	-	-
14	CLA	A	819	X	-	-	-
14	CLA	A	820	X	-	-	-
14	CLA	A	821	X	-	-	-
14	CLA	A	822	X	-	-	-
14	CLA	A	823	X	-	-	-
14	CLA	A	824	X	-	-	-
14	CLA	A	825	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	826	X	-	-	-
14	CLA	A	827	X	-	-	-
14	CLA	A	828	X	-	-	-
14	CLA	A	829	X	-	-	-
14	CLA	A	830	X	-	-	-
14	CLA	A	831	X	-	-	-
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	839	X	-	-	-
14	CLA	A	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	842	X	-	-	-
14	CLA	A	843	X	-	-	-
14	CLA	A	844	X	-	-	-
14	CLA	A	857	X	-	-	-
14	CLA	B	802	X	-	-	-
14	CLA	B	803	X	-	-	-
14	CLA	B	804	X	-	-	-
14	CLA	B	805	X	-	-	-
14	CLA	B	806	X	-	-	-
14	CLA	B	807	X	-	-	-
14	CLA	B	808	X	-	-	-
14	CLA	B	809	X	-	-	-
14	CLA	B	810	X	-	-	-
14	CLA	B	811	X	-	-	-
14	CLA	B	812	X	-	-	-
14	CLA	B	813	X	-	-	-
14	CLA	B	814	X	-	-	-
14	CLA	B	815	X	-	-	-
14	CLA	B	816	X	-	-	-
14	CLA	B	817	X	-	-	-
14	CLA	B	818	X	-	-	-
14	CLA	B	819	X	-	-	-
14	CLA	B	820	X	-	-	-
14	CLA	B	821	X	-	-	-
14	CLA	B	822	X	-	-	-
14	CLA	B	823	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	824	X	-	-	-
14	CLA	B	825	X	-	-	-
14	CLA	B	826	X	-	-	-
14	CLA	B	827	X	-	-	-
14	CLA	B	828	X	-	-	-
14	CLA	B	829	X	-	-	-
14	CLA	B	830	X	-	-	-
14	CLA	B	831	X	-	-	-
14	CLA	B	832	X	-	-	-
14	CLA	B	833	X	-	-	-
14	CLA	B	834	X	-	-	-
14	CLA	B	835	X	-	-	-
14	CLA	B	836	X	-	-	-
14	CLA	B	837	X	-	-	-
14	CLA	B	838	X	-	-	-
14	CLA	B	839	X	-	-	-
14	CLA	B	840	X	-	-	-
14	CLA	B	841	X	-	-	-
14	CLA	F	201	X	-	-	-
14	CLA	F	202	X	-	-	-
14	CLA	J	101	X	-	-	-
14	CLA	J	102	X	-	-	-
14	CLA	K	101	X	-	-	-
14	CLA	K	102	X	-	-	-
14	CLA	L	204	X	-	-	-
14	CLA	L	205	X	-	-	-
14	CLA	L	206	X	-	-	-
14	CLA	M	102	X	-	-	-
14	CLA	X	1701	X	-	-	-
17	BCR	A	849	-	-	-	X
18	LMG	A	853	-	-	-	X

## 2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 48797 atoms, of which 24384 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
1	A	740	Total	C	H	N	O	S	0	0	0
			11422	3794	5638	988	976	26			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	739	Total	C	H	N	O	S	0	0	0
			11507	3876	5618	987	1005	21			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	80	Total	C	H	N	O	S	0	0	0
			1174	367	576	103	117	11			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	138	Total	C	H	N	O	S	0	0	0
			2152	682	1077	186	204	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	69	Total	C	H	N	O	0	0	0
			1067	342	528	93	104			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	F	141	Total	C	H	N	O	S	0	0	0
			2141	680	1076	184	197	4			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	I	38	Total	C	H	N	O	S	0	0	0
			607	208	306	40	48	5			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	J	41	Total	C	H	N	O	S	0	0	0
			685	231	347	51	54	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
9	K	47	Total	C	H	N	O	S	0	0	0
			687	217	354	58	57	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
10	L	151	Total	C	H	N	O	S	0	0	0
			2244	735	1125	179	201	4			

There is a discrepancy between the modelled and reference sequences:

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

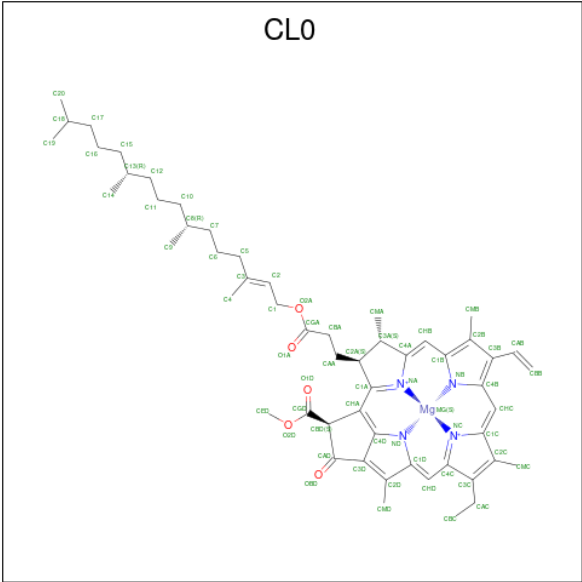
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
11	M	31	Total	C	H	N	O	S	0	0	0
			505	161	264	36	43	1			

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

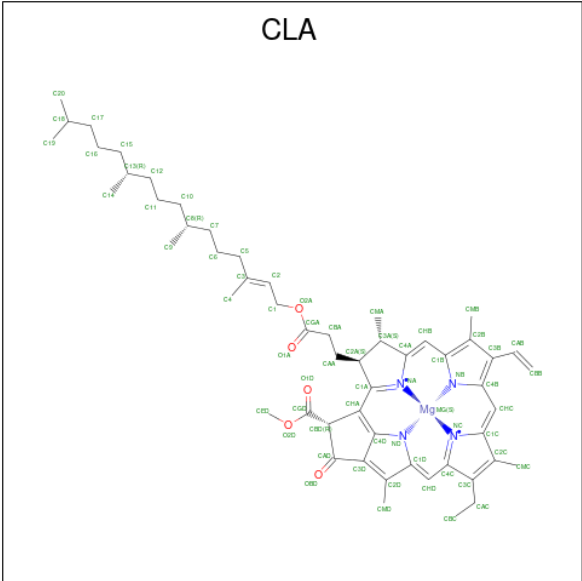
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	X	29	Total	C	H	N	O	0	0	0
			459	172	217	35	35			

- Molecule 13 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			92	41	41	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			88	39	39	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			72	35	29	1	4	3		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			88	39	39	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			92	41	41	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	A	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			89	40	39	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			92	41	41	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			82	37	35	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			95	42	43	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			104	45	49	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			82	37	35	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			104	45	49	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			79	36	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			88	39	39	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			113	48	55	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			82	37	35	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	F	1	Total	C	H	Mg	N	O	0	0
			92	41	41	1	4	5		
14	F	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		

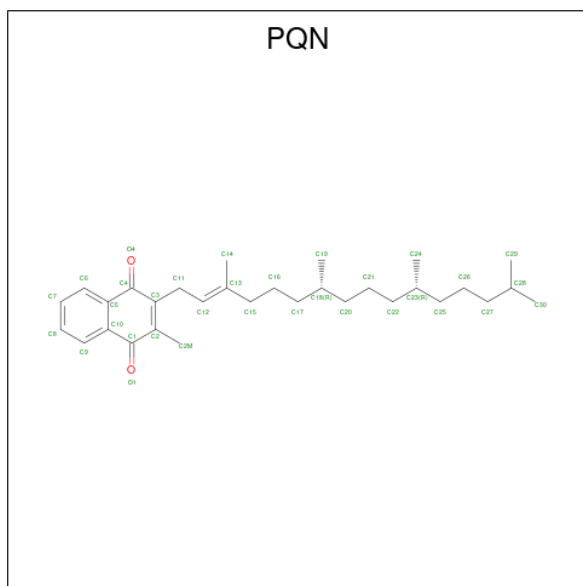
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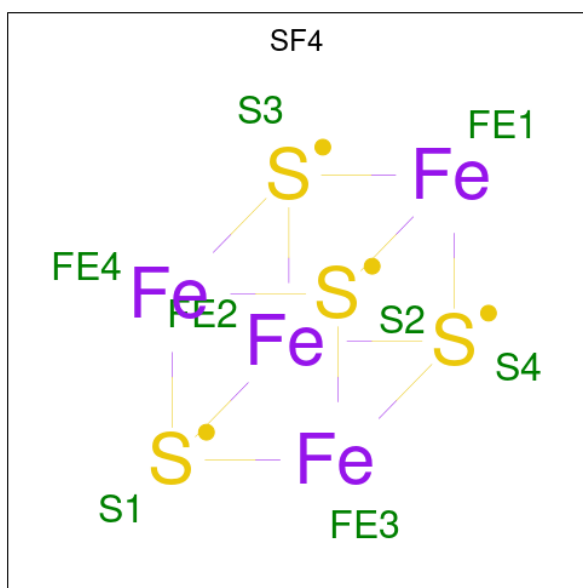
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	J	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	J	1	Total	C	H	Mg	N	O	0	0
			62	31	25	1	4	1		
14	K	1	Total	C	H	Mg	N	O	0	0
			70	33	29	1	4	3		
14	K	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	L	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	L	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	L	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	M	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	X	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		

- Molecule 15 is PHYLLOQUINONE (three-letter code: PQN) (formula:  $C_{31}H_{46}O_2$ ).



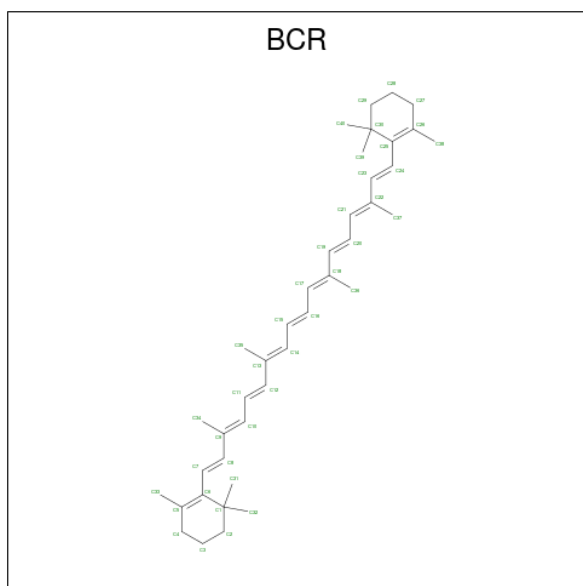
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	A	1	Total	C	H	O	0	0
			79	31	46	2		
15	B	1	Total	C	H	O	0	0
			79	31	46	2		

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



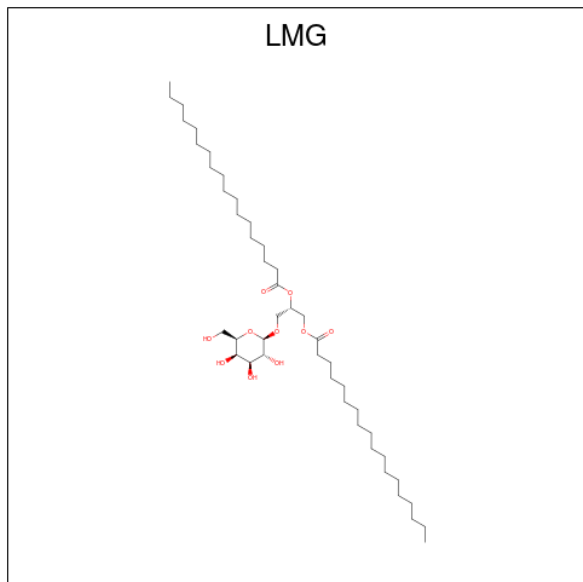
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	A	1	Total	Fe	S	0	0
			8	4	4		
16	C	1	Total	Fe	S	0	0
			8	4	4		
16	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula:  $\text{C}_{40}\text{H}_{56}$ ).



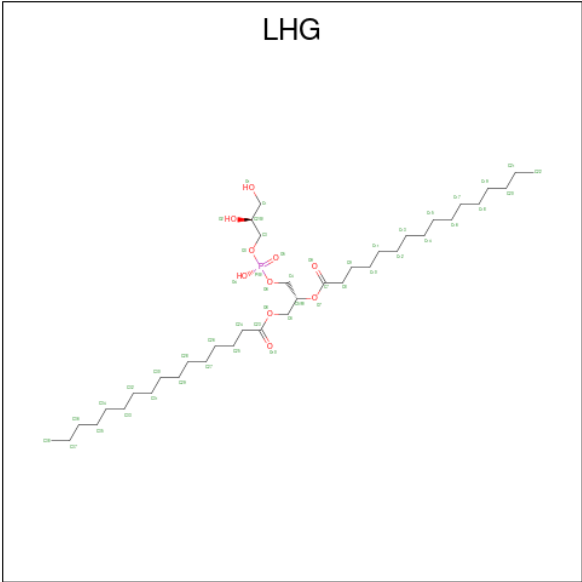
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	A	1	Total	C	H	0	0
			96	40	56		
17	A	1	Total	C	H	0	0
			96	40	56		
17	A	1	Total	C	H	0	0
			96	40	56		
17	A	1	Total	C	H	0	0
			96	40	56		
17	A	1	Total	C	H	0	0
			96	40	56		
17	B	1	Total	C	H	0	0
			96	40	56		
17	B	1	Total	C	H	0	0
			96	40	56		
17	B	1	Total	C	H	0	0
			96	40	56		
17	B	1	Total	C	H	0	0
			96	40	56		
17	B	1	Total	C	H	0	0
			96	40	56		
17	B	1	Total	C	H	0	0
			96	40	56		
17	F	1	Total	C	H	0	0
			96	40	56		
17	I	1	Total	C	H	0	0
			96	40	56		
17	I	1	Total	C	H	0	0
			96	40	56		
17	J	1	Total	C	H	0	0
			96	40	56		
17	J	1	Total	C	H	0	0
			96	40	56		
17	J	1	Total	C	H	0	0
			96	40	56		
17	L	1	Total	C	H	0	0
			96	40	56		
17	L	1	Total	C	H	0	0
			96	40	56		
17	M	1	Total	C	H	0	0
			96	40	56		

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	H	O	0	0
			118	38	70	10		
18	A	1	Total	C	H	O	0	0
			67	22	37	8		
18	B	1	Total	C	H	O	0	0
			141	45	86	10		
18	I	1	Total	C	H	O	0	0
			91	30	51	10		

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).

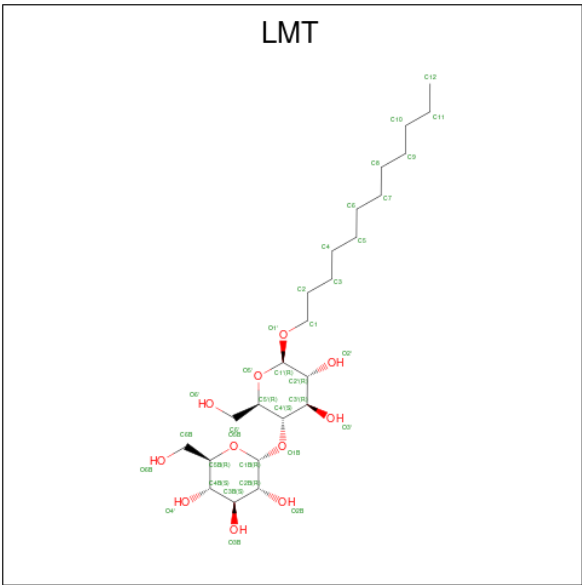


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
19	A	1	Total	C	H	O	P	0	0
			53	16	26	10	1		
19	B	1	Total	C	H	O	P	0	0
			43	12	20	10	1		
19	M	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

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

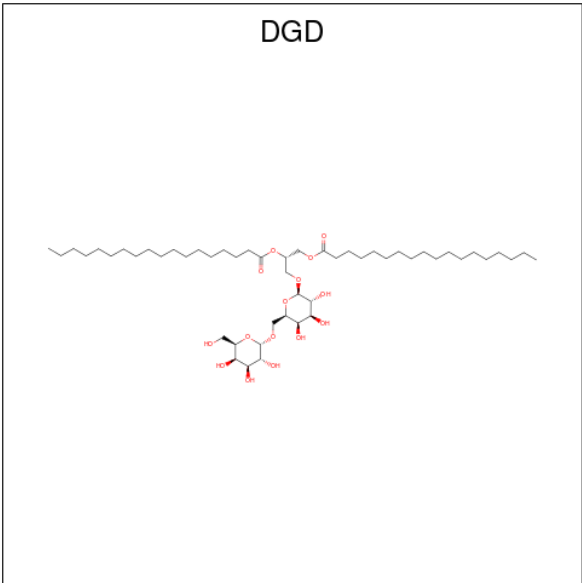
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	B	1	Total	Ca	0	0
			1	1		
20	L	1	Total	Ca	0	0
			1	1		

- Molecule 21 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	L	1	Total	C	H	O	0	0
			81	24	46	11		

- Molecule 22 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	L	1	Total	C	H	O	0	0
			162	51	96	15		

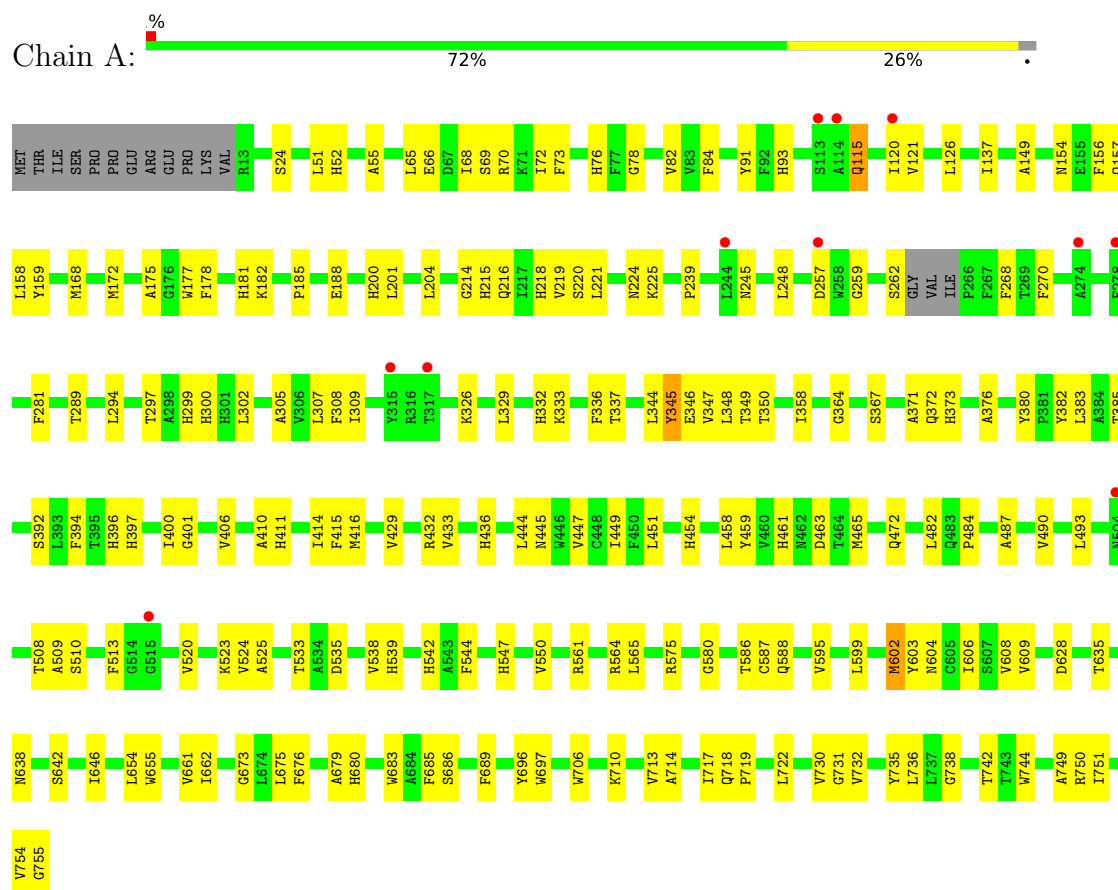
- Molecule 23 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	6	Total 6	O 6	0	0
23	B	8	Total 8	O 8	0	0
23	F	1	Total 1	O 1	0	0
23	J	1	Total 1	O 1	0	0
23	L	3	Total 3	O 3	0	0
23	M	1	Total 1	O 1	0	0

### 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.

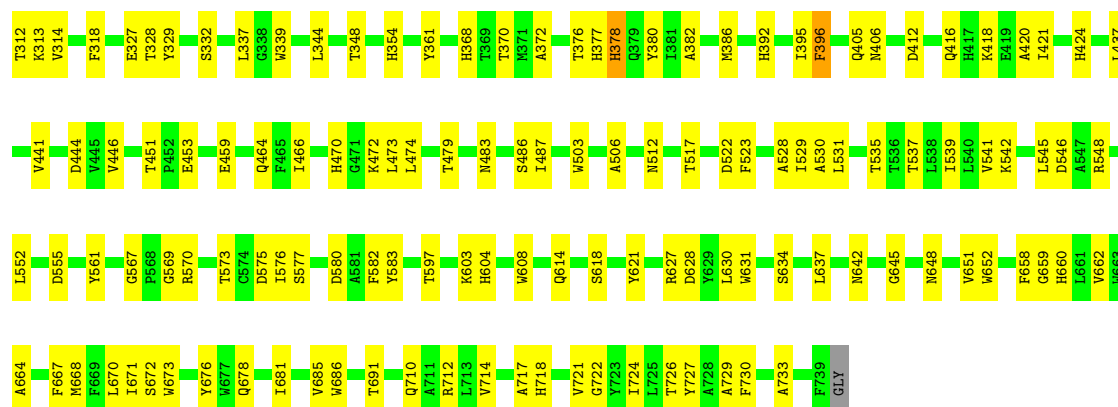
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

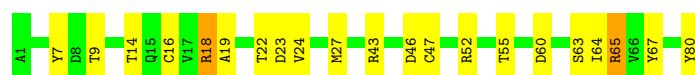






• Molecule 3: Photosystem I iron-sulfur center

Chain C: 74% 24% .



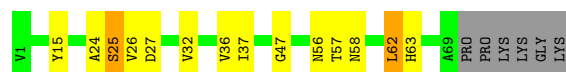
• Molecule 4: Photosystem I reaction center subunit II

Chain D: 78% 22%



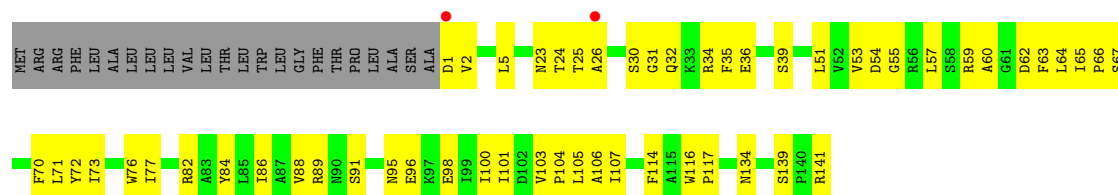
• Molecule 5: Photosystem I reaction center subunit IV

Chain E: 73% 16% 8%



• Molecule 6: Photosystem I reaction center subunit III

Chain F: 52% 34% 14%



• Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 82% 18%



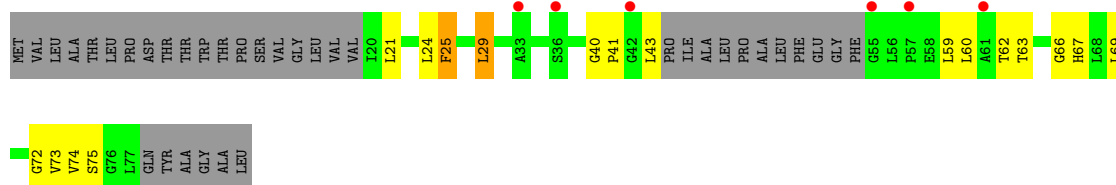
- Molecule 8: Photosystem I reaction center subunit IX

Chain J: 61% 39%



- Molecule 9: Photosystem I reaction center subunit PsaK

Chain K: 7% 35% 19% 43%



- Molecule 10: Photosystem I reaction center subunit XI

Chain L: 81% 16% 3%



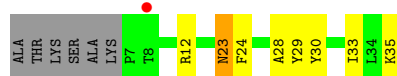
- Molecule 11: Photosystem I reaction center subunit XII

Chain M: 68% 32%



- Molecule 12: Photosystem I 4.8K protein

Chain X: 3% 60% 20% 17%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	284.86Å 284.86Å 166.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.63 – 3.00 31.63 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.63-3.00) 94.3 (31.63-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.88 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, $R_{free}$	0.334 , 0.350 0.334 , 0.350	Depositor DCC
$R_{free}$ test set	1995 reflections (1.30%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.5	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.17 , -97.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.146 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.69	EDS
Total number of atoms	48797	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, LMG, LMT, BCR, CA, LHG, DGD, PQN, CL0, 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	0.26	0/5983	0.47	0/8158
2	B	0.26	0/6107	0.45	0/8345
3	C	0.25	0/608	0.49	0/824
4	D	0.27	0/1101	0.52	0/1492
5	E	0.26	0/551	0.50	0/750
6	F	0.26	0/1087	0.51	0/1476
7	I	0.29	0/312	0.48	0/425
8	J	0.27	0/350	0.43	0/477
9	K	0.26	0/337	0.51	0/454
10	L	0.28	0/1148	0.45	0/1558
11	M	0.30	0/244	0.49	0/332
12	X	0.27	0/251	0.44	0/342
All	All	0.26	0/18079	0.47	0/24633

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	5638	5639	159	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5889	5618	5649	158	0
3	C	598	576	580	16	0
4	D	1075	1077	1077	20	0
5	E	539	528	528	10	0
6	F	1065	1076	1077	41	0
7	I	301	306	306	7	0
8	J	338	347	347	21	0
9	K	333	354	354	16	0
10	L	1119	1125	1125	16	1
11	M	241	264	264	8	0
12	X	242	217	249	10	0
13	A	65	72	72	4	0
14	A	2577	2574	2574	117	0
14	B	2284	2232	2232	87	0
14	F	96	74	74	5	0
14	J	82	58	58	7	0
14	K	86	62	62	5	0
14	L	195	216	216	3	0
14	M	45	33	33	0	0
14	X	45	33	33	4	0
15	A	33	46	46	5	0
15	B	33	46	46	2	0
16	A	8	0	0	0	0
16	C	16	0	0	1	0
17	A	240	336	336	13	0
17	B	280	392	392	17	0
17	F	40	56	56	3	0
17	I	80	112	112	8	0
17	J	120	168	168	14	0
17	L	80	112	112	4	0
17	M	40	56	56	0	0
18	A	78	107	105	2	0
18	B	55	86	86	1	0
18	I	40	51	50	0	0
19	A	76	100	98	1	0
19	B	23	20	16	1	0
19	M	49	74	74	0	0
20	B	1	0	0	0	0
20	L	1	0	0	0	0
21	L	35	46	46	0	0
22	L	66	96	96	2	0
23	A	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	B	8	0	0	0	0
23	F	1	0	0	0	0
23	J	1	0	0	0	0
23	L	3	0	0	1	2
23	M	1	0	0	0	0
All	All	24413	24384	24444	588	2

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 12.

The worst 5 of 588 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)
10:L:153:PHE:O	23:L:302:HOH:O	1.68	1.10
2:B:583:TYR:OH	2:B:670:LEU:HD22	1.60	1.00
2:B:506:ALA:O	2:B:512:ASN:ND2	1.97	0.98
1:A:336:PHE:O	1:A:432:ARG:NH1	2.10	0.85
6:F:1:ASP:N	6:F:5:LEU:O	2.12	0.83

All (2) 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)
23:L:301:HOH:O	23:L:302:HOH:O[3_455]	1.08	1.12
10:L:67:PRO:O	23:L:302:HOH:O[3_455]	2.05	0.15

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	736/755 (98%)	688 (94%)	48 (6%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	737/740 (100%)	695 (94%)	42 (6%)	0	100	100
3	C	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
4	D	136/138 (99%)	124 (91%)	12 (9%)	0	100	100
5	E	67/75 (89%)	60 (90%)	6 (9%)	1 (2%)	10	42
6	F	139/164 (85%)	128 (92%)	11 (8%)	0	100	100
7	I	36/38 (95%)	30 (83%)	6 (17%)	0	100	100
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	K	43/83 (52%)	38 (88%)	5 (12%)	0	100	100
10	L	149/154 (97%)	146 (98%)	3 (2%)	0	100	100
11	M	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
12	X	27/35 (77%)	26 (96%)	1 (4%)	0	100	100
All	All	2216/2334 (95%)	2074 (94%)	141 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	25	SER

### 5.3.2 Protein sidechains ⓘ

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%)	579 (98%)	10 (2%)	60	85
2	B	597/597 (100%)	586 (98%)	11 (2%)	59	85
3	C	67/67 (100%)	64 (96%)	3 (4%)	27	64
4	D	115/115 (100%)	115 (100%)	0	100	100
5	E	59/64 (92%)	57 (97%)	2 (3%)	37	72
6	F	109/128 (85%)	107 (98%)	2 (2%)	59	85
7	I	32/32 (100%)	32 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	J	36/36 (100%)	36 (100%)	0	100	100
9	K	33/61 (54%)	30 (91%)	3 (9%)	9	34
10	L	117/119 (98%)	112 (96%)	5 (4%)	29	66
11	M	26/26 (100%)	26 (100%)	0	100	100
12	X	23/27 (85%)	21 (91%)	2 (9%)	10	37
All	All	1803/1875 (96%)	1765 (98%)	38 (2%)	53	82

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	K	25	PHE
10	L	101	PHE
9	K	29	LEU
10	L	57	PHE
12	X	30	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	66	GLN
10	L	16	HIS
11	M	7	GLN
10	L	75	ASN
8	J	30	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.



## 5.6 Ligand geometry

Of 135 ligands modelled in this entry, 2 are monoatomic - leaving 133 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
14	CLA	A	843	23	56,73,73	1.63	6 (10%)	55,113,113	1.55	8 (14%)
17	BCR	I	103	-	41,41,41	1.10	2 (4%)	56,56,56	1.29	7 (12%)
14	CLA	A	838	-	42,59,73	1.87	5 (11%)	38,96,113	1.77	8 (21%)
18	LMG	A	856	-	30,30,55	1.01	2 (6%)	37,37,63	1.29	5 (13%)
14	CLA	A	810	1	56,73,73	1.63	6 (10%)	55,113,113	1.56	9 (16%)
14	CLA	B	813	-	56,73,73	1.59	6 (10%)	55,113,113	1.50	8 (14%)
14	CLA	B	817	-	50,67,73	1.70	5 (10%)	47,105,113	1.61	8 (17%)
14	CLA	A	836	-	45,62,73	1.84	5 (11%)	41,99,113	1.62	9 (21%)
14	CLA	B	828	-	56,73,73	1.61	6 (10%)	55,113,113	1.46	8 (14%)
14	CLA	B	833	-	49,66,73	1.72	6 (12%)	46,104,113	1.63	9 (19%)
14	CLA	A	816	-	33,53,73	2.09	6 (18%)	27,89,113	2.01	8 (29%)
14	CLA	B	809	2	56,73,73	1.58	6 (10%)	55,113,113	1.63	11 (20%)
14	CLA	A	841	-	56,73,73	1.60	7 (12%)	55,113,113	1.50	8 (14%)
14	CLA	A	811	-	33,53,73	2.06	5 (15%)	27,89,113	2.03	9 (33%)
19	LHG	M	101	-	48,48,48	0.62	0	51,54,54	1.20	6 (11%)
14	CLA	M	102	23	33,53,73	2.09	5 (15%)	27,89,113	1.98	7 (25%)
14	CLA	B	816	-	46,63,73	1.78	5 (10%)	43,101,113	1.65	7 (16%)
14	CLA	B	838	-	56,73,73	1.62	5 (8%)	55,113,113	1.53	9 (16%)
17	BCR	A	851	-	41,41,41	1.07	2 (4%)	56,56,56	1.25	6 (10%)
14	CLA	B	826	-	56,73,73	1.59	6 (10%)	55,113,113	1.54	8 (14%)
17	BCR	F	203	-	41,41,41	1.05	2 (4%)	56,56,56	1.24	7 (12%)
14	CLA	B	805	-	56,73,73	1.60	5 (8%)	55,113,113	1.54	8 (14%)
14	CLA	A	839	-	56,73,73	1.56	5 (8%)	55,113,113	1.53	9 (16%)
14	CLA	B	829	-	56,73,73	1.59	5 (8%)	55,113,113	1.58	9 (16%)
17	BCR	B	851	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	5 (8%)
14	CLA	J	102	-	28,45,73	2.22	6 (21%)	19,78,113	2.14	6 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	B	803	-	56,73,73	1.60	5 (8%)	55,113,113	1.49	7 (12%)
14	CLA	A	807	-	56,73,73	1.63	5 (8%)	55,113,113	1.48	8 (14%)
14	CLA	A	844	19	43,60,73	1.82	6 (13%)	39,97,113	1.81	10 (25%)
14	CLA	A	822	23	56,73,73	1.60	5 (8%)	55,113,113	1.55	9 (16%)
14	CLA	A	815	-	33,53,73	2.10	6 (18%)	27,89,113	1.92	8 (29%)
14	CLA	A	832	-	41,58,73	1.86	5 (12%)	37,95,113	1.77	9 (24%)
17	BCR	B	847	-	41,41,41	1.11	2 (4%)	56,56,56	1.25	8 (14%)
14	CLA	F	201	23	42,59,73	1.87	5 (11%)	38,96,113	1.77	9 (23%)
17	BCR	A	850	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	7 (12%)
14	CLA	A	825	-	50,67,73	1.68	5 (10%)	47,105,113	1.62	8 (17%)
14	CLA	A	818	-	45,62,73	1.79	6 (13%)	41,99,113	1.73	9 (21%)
14	CLA	A	813	-	45,62,73	1.79	5 (11%)	41,99,113	1.69	8 (19%)
14	CLA	A	830	-	56,73,73	1.59	5 (8%)	55,113,113	1.54	7 (12%)
14	CLA	B	814	-	56,73,73	1.61	5 (8%)	55,113,113	1.50	9 (16%)
14	CLA	B	831	-	40,57,73	1.90	6 (15%)	34,93,113	1.88	10 (29%)
14	CLA	A	803	-	56,73,73	1.57	5 (8%)	55,113,113	1.54	9 (16%)
14	CLA	B	823	-	33,53,73	2.10	5 (15%)	27,89,113	2.02	9 (33%)
17	BCR	L	208	-	41,41,41	1.07	2 (4%)	56,56,56	1.26	7 (12%)
14	CLA	B	837	-	51,68,73	1.69	6 (11%)	49,107,113	1.63	9 (18%)
14	CLA	A	835	-	56,73,73	1.65	6 (10%)	55,113,113	1.47	8 (14%)
14	CLA	A	857	23	56,73,73	1.59	5 (8%)	55,113,113	1.61	9 (16%)
14	CLA	X	1701	12	33,53,73	2.08	5 (15%)	27,89,113	1.97	9 (33%)
15	PQN	A	845	-	34,34,34	2.07	7 (20%)	42,45,45	1.20	6 (14%)
22	DGD	L	207	-	67,67,67	0.93	3 (4%)	81,81,81	1.40	14 (17%)
14	CLA	B	804	-	45,62,73	1.77	6 (13%)	41,99,113	1.76	11 (26%)
14	CLA	K	101	-	29,49,73	2.16	5 (17%)	20,83,113	2.14	7 (35%)
17	BCR	J	103	-	41,41,41	1.13	2 (4%)	56,56,56	1.27	7 (12%)
17	BCR	B	848	-	41,41,41	1.09	2 (4%)	56,56,56	1.21	6 (10%)
18	LMG	A	853	-	48,48,55	0.77	0	56,56,63	1.29	5 (8%)
17	BCR	A	848	-	41,41,41	1.13	2 (4%)	56,56,56	1.35	7 (12%)
17	BCR	J	104	-	41,41,41	1.09	2 (4%)	56,56,56	1.30	9 (16%)
14	CLA	A	812	14	56,73,73	1.60	5 (8%)	55,113,113	1.47	8 (14%)
14	CLA	A	829	-	56,73,73	1.60	6 (10%)	55,113,113	1.46	7 (12%)
14	CLA	B	822	23	46,63,73	1.75	6 (13%)	43,101,113	1.62	7 (16%)
16	SF4	C	102	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	B	808	-	56,73,73	1.60	6 (10%)	55,113,113	1.49	9 (16%)
18	LMG	B	849	-	55,55,55	0.71	1 (1%)	63,63,63	1.36	7 (11%)
14	CLA	B	835	23	33,53,73	2.09	5 (15%)	27,89,113	1.99	8 (29%)
14	CLA	B	810	2	56,73,73	1.58	6 (10%)	55,113,113	1.64	10 (18%)
19	LHG	A	855	14	26,26,48	0.83	1 (3%)	29,32,54	1.32	3 (10%)
14	CLA	A	814	-	51,68,73	1.68	5 (9%)	49,107,113	1.59	10 (20%)
14	CLA	L	204	10	56,73,73	1.57	6 (10%)	55,113,113	1.64	10 (18%)
17	BCR	A	852	-	41,41,41	1.10	2 (4%)	56,56,56	1.37	8 (14%)
19	LHG	B	850	-	22,22,48	0.91	2 (9%)	25,28,54	1.19	1 (4%)
14	CLA	A	821	-	33,50,73	2.05	6 (18%)	26,84,113	2.11	7 (26%)
14	CLA	A	809	1	56,73,73	1.60	5 (8%)	55,113,113	1.60	8 (14%)
14	CLA	B	836	23	33,53,73	2.16	5 (15%)	27,89,113	2.01	8 (29%)
14	CLA	F	202	23	33,53,73	2.08	5 (15%)	27,89,113	1.92	8 (29%)
17	BCR	B	845	-	41,41,41	1.08	2 (4%)	56,56,56	1.22	6 (10%)
18	LMG	I	102	-	40,40,55	0.90	1 (2%)	48,48,63	1.26	6 (12%)
17	BCR	A	849	-	41,41,41	1.08	2 (4%)	56,56,56	1.19	4 (7%)
14	CLA	B	841	-	56,73,73	1.65	5 (8%)	55,113,113	1.52	9 (16%)
15	PQN	B	842	-	34,34,34	2.06	7 (20%)	42,45,45	1.17	5 (11%)
21	LMT	L	202	-	36,36,36	1.15	4 (11%)	47,47,47	1.03	2 (4%)
14	CLA	K	102	-	33,53,73	2.06	5 (15%)	27,89,113	2.04	8 (29%)
19	LHG	A	854	-	48,48,48	0.62	1 (2%)	51,54,54	1.24	6 (11%)
14	CLA	B	839	-	38,55,73	1.97	5 (13%)	33,91,113	1.85	10 (30%)
17	BCR	M	103	-	41,41,41	1.10	2 (4%)	56,56,56	1.27	8 (14%)
14	CLA	B	834	-	33,53,73	2.06	5 (15%)	27,89,113	2.05	8 (29%)
14	CLA	A	805	14	50,67,73	1.70	5 (10%)	47,105,113	1.58	10 (21%)
14	CLA	A	820	-	56,73,73	1.59	6 (10%)	55,113,113	1.59	10 (18%)
14	CLA	B	807	-	56,73,73	1.60	5 (8%)	55,113,113	1.56	10 (18%)
14	CLA	B	815	-	33,53,73	2.08	6 (18%)	27,89,113	1.97	9 (33%)
14	CLA	B	832	-	56,73,73	1.60	5 (8%)	55,113,113	1.51	9 (16%)
14	CLA	B	840	23	56,73,73	1.60	4 (7%)	55,113,113	1.52	9 (16%)
14	CLA	A	819	-	45,62,73	1.81	6 (13%)	41,99,113	1.65	8 (19%)
14	CLA	B	818	-	51,68,73	1.65	5 (9%)	49,107,113	1.61	8 (16%)
17	BCR	A	847	-	41,41,41	1.10	2 (4%)	56,56,56	1.28	8 (14%)
14	CLA	A	840	-	38,55,73	1.95	5 (13%)	33,91,113	1.84	9 (27%)
14	CLA	B	812	-	33,53,73	2.10	5 (15%)	27,89,113	2.02	8 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	B	825	23	37,54,73	1.93	6 (16%)	32,90,113	1.85	8 (25%)
17	BCR	L	201	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	8 (14%)
14	CLA	A	837	1	33,53,73	2.08	5 (15%)	27,89,113	2.05	9 (33%)
14	CLA	A	834	-	56,73,73	1.64	4 (7%)	55,113,113	1.45	8 (14%)
14	CLA	B	824	2	45,62,73	1.78	5 (11%)	41,99,113	1.71	8 (19%)
17	BCR	B	846	-	41,41,41	1.03	2 (4%)	56,56,56	1.27	8 (14%)
14	CLA	A	808	-	42,59,73	1.91	6 (14%)	38,96,113	1.75	9 (23%)
14	CLA	A	831	-	56,73,73	1.60	5 (8%)	55,113,113	1.57	11 (20%)
17	BCR	B	844	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	9 (16%)
14	CLA	A	823	-	40,57,73	1.90	6 (15%)	34,93,113	1.88	9 (26%)
14	CLA	A	804	-	56,73,73	1.61	5 (8%)	55,113,113	1.48	7 (12%)
16	SF4	C	101	3	0,12,12	-	-	-	-	-
14	CLA	B	827	-	56,73,73	1.59	7 (12%)	55,113,113	1.43	9 (16%)
14	CLA	L	206	23	56,73,73	1.58	6 (10%)	55,113,113	1.75	10 (18%)
16	SF4	A	846	2,1	0,12,12	-	-	-	-	-
17	BCR	B	843	-	41,41,41	1.06	2 (4%)	56,56,56	1.24	9 (16%)
17	BCR	I	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.29	6 (10%)
14	CLA	A	802	23	56,73,73	1.62	6 (10%)	55,113,113	1.49	6 (10%)
14	CLA	A	817	23	40,57,73	1.87	5 (12%)	34,93,113	1.81	9 (26%)
14	CLA	B	806	-	56,73,73	1.63	6 (10%)	55,113,113	1.48	7 (12%)
14	CLA	B	821	-	33,53,73	2.05	5 (15%)	27,89,113	2.04	8 (29%)
17	BCR	J	105	-	41,41,41	1.07	2 (4%)	56,56,56	1.25	9 (16%)
14	CLA	A	806	-	56,73,73	1.60	7 (12%)	55,113,113	1.58	10 (18%)
14	CLA	J	101	8	33,53,73	2.04	5 (15%)	27,89,113	2.07	8 (29%)
14	CLA	B	820	-	38,55,73	1.93	5 (13%)	33,91,113	1.84	7 (21%)
14	CLA	A	842	-	56,73,73	1.63	6 (10%)	55,113,113	1.60	8 (14%)
14	CLA	B	819	23	56,73,73	1.58	6 (10%)	55,113,113	1.55	8 (14%)
14	CLA	B	802	-	56,73,73	1.58	6 (10%)	55,113,113	1.57	8 (14%)
14	CLA	A	824	-	42,59,73	1.82	5 (11%)	38,96,113	1.74	8 (21%)
13	CL0	A	801	-	59,73,73	1.42	5 (8%)	67,113,113	1.45	9 (13%)
14	CLA	A	826	23	56,73,73	1.61	5 (8%)	55,113,113	1.54	7 (12%)
14	CLA	A	827	23	56,73,73	1.60	5 (8%)	55,113,113	1.50	9 (16%)
14	CLA	B	811	-	33,53,73	2.06	5 (15%)	27,89,113	2.19	9 (33%)
14	CLA	A	828	-	56,73,73	1.63	5 (8%)	55,113,113	1.47	9 (16%)
14	CLA	L	205	-	56,73,73	1.59	5 (8%)	55,113,113	1.59	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	A	833	-	56,73,73	1.56	5 (8%)	55,113,113	1.47	8 (14%)
14	CLA	B	830	-	33,53,73	2.08	6 (18%)	27,89,113	2.01	7 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	843	23	1/1/20/20	9/37/115/115	-
17	BCR	I	103	-	-	14/29/63/63	0/2/2/2
14	CLA	A	838	-	1/1/17/20	6/21/99/115	-
18	LMG	A	856	-	-	12/23/43/70	0/1/1/1
14	CLA	A	810	1	1/1/20/20	11/37/115/115	-
14	CLA	B	813	-	1/1/20/20	19/37/115/115	-
14	CLA	B	817	-	1/1/18/20	10/30/108/115	-
14	CLA	A	836	-	1/1/17/20	6/24/102/115	-
14	CLA	B	828	-	1/1/20/20	18/37/115/115	-
14	CLA	B	833	-	1/1/18/20	4/29/107/115	-
14	CLA	A	816	-	1/1/15/20	5/11/91/115	-
14	CLA	B	809	2	1/1/20/20	14/37/115/115	-
14	CLA	A	841	-	1/1/20/20	6/37/115/115	-
14	CLA	A	811	-	1/1/15/20	8/11/91/115	-
19	LHG	M	101	-	-	26/53/53/53	-
14	CLA	M	102	23	1/1/15/20	4/11/91/115	-
14	CLA	B	816	-	1/1/18/20	6/25/103/115	-
14	CLA	B	838	-	1/1/20/20	12/37/115/115	-
17	BCR	A	851	-	-	7/29/63/63	0/2/2/2
14	CLA	B	826	-	1/1/20/20	20/37/115/115	-
17	BCR	F	203	-	-	9/29/63/63	0/2/2/2
14	CLA	B	805	-	1/1/20/20	15/37/115/115	-
14	CLA	A	839	-	1/1/20/20	13/37/115/115	-
14	CLA	B	829	-	1/1/20/20	9/37/115/115	-
17	BCR	B	851	-	-	8/29/63/63	0/2/2/2
14	CLA	J	102	-	1/1/12/20	1/2/76/115	-
14	CLA	B	803	-	1/1/20/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	807	-	1/1/20/20	16/37/115/115	-
14	CLA	A	844	19	1/1/17/20	6/22/100/115	-
14	CLA	A	822	23	1/1/20/20	14/37/115/115	-
14	CLA	A	815	-	1/1/15/20	5/11/91/115	-
14	CLA	A	832	-	1/1/17/20	8/19/97/115	-
17	BCR	B	847	-	-	14/29/63/63	0/2/2/2
14	CLA	F	201	23	1/1/17/20	4/21/99/115	-
17	BCR	A	850	-	-	11/29/63/63	0/2/2/2
14	CLA	A	825	-	1/1/18/20	12/30/108/115	-
14	CLA	A	818	-	1/1/17/20	4/24/102/115	-
14	CLA	A	813	-	1/1/17/20	7/24/102/115	-
14	CLA	A	830	-	1/1/20/20	15/37/115/115	-
14	CLA	B	814	-	1/1/20/20	13/37/115/115	-
14	CLA	B	831	-	1/1/16/20	7/18/96/115	-
14	CLA	A	803	-	1/1/20/20	6/37/115/115	-
14	CLA	B	823	-	1/1/15/20	4/11/91/115	-
17	BCR	L	208	-	-	11/29/63/63	0/2/2/2
14	CLA	B	837	-	1/1/19/20	6/31/109/115	-
14	CLA	A	835	-	1/1/20/20	12/37/115/115	-
14	CLA	A	857	23	1/1/20/20	19/37/115/115	-
14	CLA	X	1701	12	1/1/15/20	4/11/91/115	-
15	PQN	A	845	-	-	11/23/43/43	0/2/2/2
22	DGD	L	207	-	-	23/55/95/95	0/2/2/2
14	CLA	B	804	-	1/1/17/20	7/24/102/115	-
14	CLA	K	101	-	1/1/13/20	1/5/81/115	-
17	BCR	J	103	-	-	18/29/63/63	0/2/2/2
17	BCR	B	848	-	-	6/29/63/63	0/2/2/2
18	LMG	A	853	-	-	25/43/63/70	0/1/1/1
17	BCR	A	848	-	-	17/29/63/63	0/2/2/2
17	BCR	J	104	-	-	13/29/63/63	0/2/2/2
14	CLA	A	812	14	1/1/20/20	7/37/115/115	-
14	CLA	A	829	-	1/1/20/20	13/37/115/115	-
14	CLA	B	822	23	1/1/18/20	8/25/103/115	-
16	SF4	C	102	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	808	-	1/1/20/20	8/37/115/115	-
18	LMG	B	849	-	-	18/50/70/70	0/1/1/1
14	CLA	B	835	23	1/1/15/20	4/11/91/115	-
14	CLA	B	810	2	1/1/20/20	15/37/115/115	-
19	LHG	A	855	14	-	12/31/31/53	-
14	CLA	A	814	-	1/1/19/20	9/31/109/115	-
14	CLA	L	204	10	1/1/20/20	13/37/115/115	-
17	BCR	A	852	-	-	19/29/63/63	0/2/2/2
19	LHG	B	850	-	-	14/26/26/53	-
14	CLA	A	821	-	1/1/14/20	0/8/86/115	-
14	CLA	A	809	1	1/1/20/20	11/37/115/115	-
14	CLA	B	836	23	1/1/15/20	4/11/91/115	-
14	CLA	F	202	23	1/1/15/20	2/11/91/115	-
17	BCR	B	845	-	-	9/29/63/63	0/2/2/2
18	LMG	I	102	-	-	9/35/55/70	0/1/1/1
17	BCR	A	849	-	-	12/29/63/63	0/2/2/2
14	CLA	B	841	-	1/1/20/20	6/37/115/115	-
15	PQN	B	842	-	-	8/23/43/43	0/2/2/2
21	LMT	L	202	-	-	12/21/61/61	0/2/2/2
14	CLA	K	102	-	1/1/15/20	4/11/91/115	-
19	LHG	A	854	-	-	22/53/53/53	-
14	CLA	B	839	-	1/1/15/20	4/16/94/115	-
17	BCR	M	103	-	-	18/29/63/63	0/2/2/2
14	CLA	B	834	-	1/1/15/20	4/11/91/115	-
14	CLA	A	805	14	1/1/18/20	9/30/108/115	-
14	CLA	A	820	-	1/1/20/20	17/37/115/115	-
14	CLA	B	807	-	1/1/20/20	10/37/115/115	-
14	CLA	B	815	-	1/1/15/20	5/11/91/115	-
14	CLA	B	832	-	1/1/20/20	14/37/115/115	-
14	CLA	B	840	23	1/1/20/20	8/37/115/115	-
14	CLA	A	819	-	1/1/17/20	7/24/102/115	-
14	CLA	B	818	-	1/1/19/20	8/31/109/115	-
17	BCR	A	847	-	-	11/29/63/63	0/2/2/2
14	CLA	A	840	-	1/1/15/20	4/16/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	812	-	1/1/15/20	3/11/91/115	-
14	CLA	B	825	23	1/1/15/20	5/15/93/115	-
17	BCR	L	201	-	-	12/29/63/63	0/2/2/2
14	CLA	A	837	1	1/1/15/20	5/11/91/115	-
14	CLA	A	834	-	1/1/20/20	7/37/115/115	-
14	CLA	B	824	2	1/1/17/20	8/24/102/115	-
17	BCR	B	846	-	-	13/29/63/63	0/2/2/2
14	CLA	A	808	-	1/1/17/20	7/21/99/115	-
14	CLA	A	831	-	1/1/20/20	10/37/115/115	-
17	BCR	B	844	-	-	9/29/63/63	0/2/2/2
14	CLA	A	823	-	1/1/16/20	11/18/96/115	-
14	CLA	A	804	-	1/1/20/20	12/37/115/115	-
16	SF4	C	101	3	-	-	0/6/5/5
14	CLA	B	827	-	1/1/20/20	14/37/115/115	-
14	CLA	L	206	23	1/1/20/20	8/37/115/115	-
17	BCR	B	843	-	-	7/29/63/63	0/2/2/2
16	SF4	A	846	2,1	-	-	0/6/5/5
17	BCR	I	101	-	-	15/29/63/63	0/2/2/2
14	CLA	A	802	23	1/1/20/20	11/37/115/115	-
14	CLA	A	817	23	1/1/16/20	8/18/96/115	-
14	CLA	B	806	-	1/1/20/20	8/37/115/115	-
14	CLA	B	821	-	1/1/15/20	6/11/91/115	-
17	BCR	J	105	-	-	10/29/63/63	0/2/2/2
14	CLA	A	806	-	1/1/20/20	17/37/115/115	-
14	CLA	J	101	8	1/1/15/20	3/11/91/115	-
14	CLA	B	820	-	1/1/15/20	9/16/94/115	-
14	CLA	A	842	-	1/1/20/20	9/37/115/115	-
14	CLA	B	819	23	1/1/20/20	12/37/115/115	-
14	CLA	B	802	-	1/1/20/20	14/37/115/115	-
14	CLA	A	824	-	1/1/17/20	5/21/99/115	-
13	CL0	A	801	-	3/3/25/25	17/37/135/135	-
14	CLA	A	826	23	1/1/20/20	12/37/115/115	-
14	CLA	A	827	23	1/1/20/20	6/37/115/115	-
14	CLA	B	811	-	1/1/15/20	4/11/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	828	-	1/1/20/20	14/37/115/115	-
14	CLA	L	205	-	1/1/20/20	12/37/115/115	-
14	CLA	A	833	-	1/1/20/20	12/37/115/115	-
14	CLA	B	830	-	1/1/15/20	7/11/91/115	-

The worst 5 of 592 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	836	CLA	C4B-NB	8.46	1.42	1.35
14	A	843	CLA	C4B-NB	8.12	1.42	1.35
14	B	841	CLA	C4B-NB	8.10	1.42	1.35
14	A	834	CLA	C4B-NB	8.08	1.42	1.35
14	A	808	CLA	C4B-NB	8.06	1.42	1.35

The worst 5 of 1042 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	842	CLA	C4A-NA-C1A	7.34	110.00	106.71
14	B	802	CLA	C4A-NA-C1A	7.25	109.97	106.71
14	B	810	CLA	C4A-NA-C1A	7.14	109.92	106.71
14	B	811	CLA	C4A-NA-C1A	6.95	109.83	106.71
14	L	204	CLA	C4A-NA-C1A	6.86	109.79	106.71

5 of 98 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	801	CL0	NA
13	A	801	CL0	ND
13	A	801	CL0	NC
14	A	802	CLA	ND
14	A	803	CLA	ND

5 of 1302 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	801	CL0	CHA-CBD-CGD-O1D
13	A	801	CL0	CHA-CBD-CGD-O2D
13	A	801	CL0	CBD-CGD-O2D-CED
14	A	804	CLA	C1A-C2A-CAA-CBA
14	A	804	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

117 monomers are involved in 270 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	843	CLA	3	0
17	I	103	BCR	4	0
14	A	838	CLA	2	0
18	A	856	LMG	2	0
14	A	810	CLA	7	0
14	B	813	CLA	6	0
14	B	817	CLA	4	0
14	B	828	CLA	3	0
14	B	833	CLA	4	0
14	B	809	CLA	2	0
14	A	841	CLA	4	0
14	A	811	CLA	4	0
14	B	816	CLA	2	0
14	B	838	CLA	3	0
17	A	851	BCR	1	0
14	B	826	CLA	4	0
17	F	203	BCR	3	0
14	B	805	CLA	2	0
14	A	839	CLA	3	0
14	B	829	CLA	3	0
17	B	851	BCR	1	0
14	J	102	CLA	1	0
14	B	803	CLA	6	0
14	A	807	CLA	1	0
14	A	844	CLA	3	0
14	A	822	CLA	5	0
14	A	815	CLA	3	0
14	A	832	CLA	3	0
17	B	847	BCR	5	0
14	F	201	CLA	2	0
17	A	850	BCR	1	0
14	A	825	CLA	4	0
14	A	818	CLA	1	0
14	A	813	CLA	2	0
14	A	830	CLA	3	0
14	B	814	CLA	3	0
14	B	831	CLA	3	0
14	A	803	CLA	6	0
14	B	823	CLA	2	0
17	L	208	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	837	CLA	3	0
14	A	835	CLA	2	0
14	A	857	CLA	9	0
14	X	1701	CLA	4	0
15	A	845	PQN	5	0
22	L	207	DGD	2	0
14	B	804	CLA	3	0
14	K	101	CLA	4	0
17	J	103	BCR	2	0
17	B	848	BCR	3	0
17	A	848	BCR	5	0
17	J	104	BCR	4	0
14	A	812	CLA	5	0
14	A	829	CLA	7	0
14	B	822	CLA	1	0
16	C	102	SF4	1	0
14	B	808	CLA	1	0
18	B	849	LMG	1	0
14	B	835	CLA	2	0
14	B	810	CLA	1	0
14	A	814	CLA	2	0
14	L	204	CLA	1	0
17	A	852	BCR	5	0
19	B	850	LHG	1	0
14	A	809	CLA	2	0
14	B	836	CLA	1	0
14	F	202	CLA	3	0
17	B	845	BCR	2	0
17	A	849	BCR	1	0
14	B	841	CLA	2	0
15	B	842	PQN	2	0
14	K	102	CLA	1	0
19	A	854	LHG	1	0
14	B	839	CLA	4	0
14	B	834	CLA	3	0
14	A	805	CLA	8	0
14	A	820	CLA	4	0
14	B	815	CLA	1	0
14	B	832	CLA	3	0
14	B	840	CLA	2	0
14	A	819	CLA	1	0
14	B	818	CLA	1	0

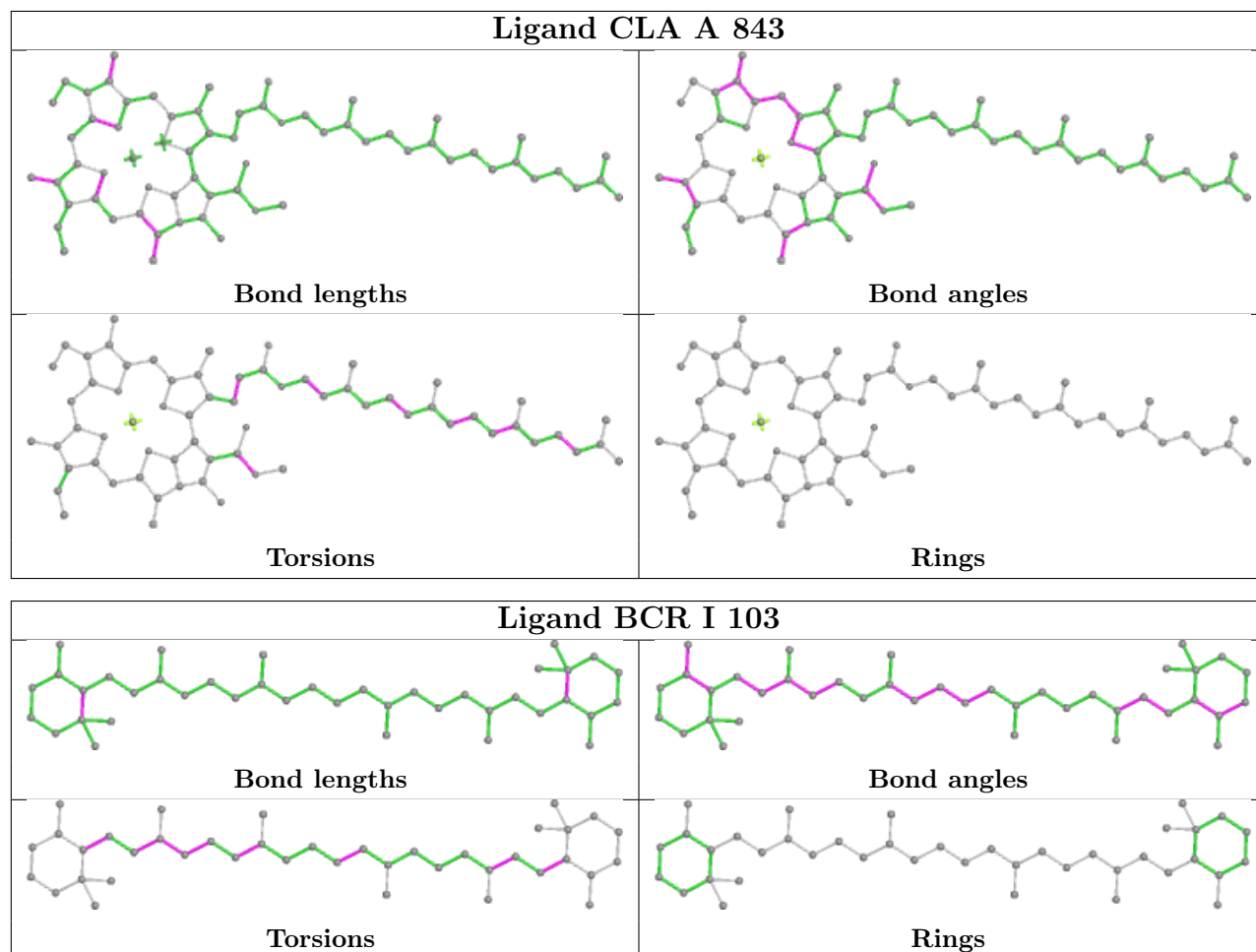
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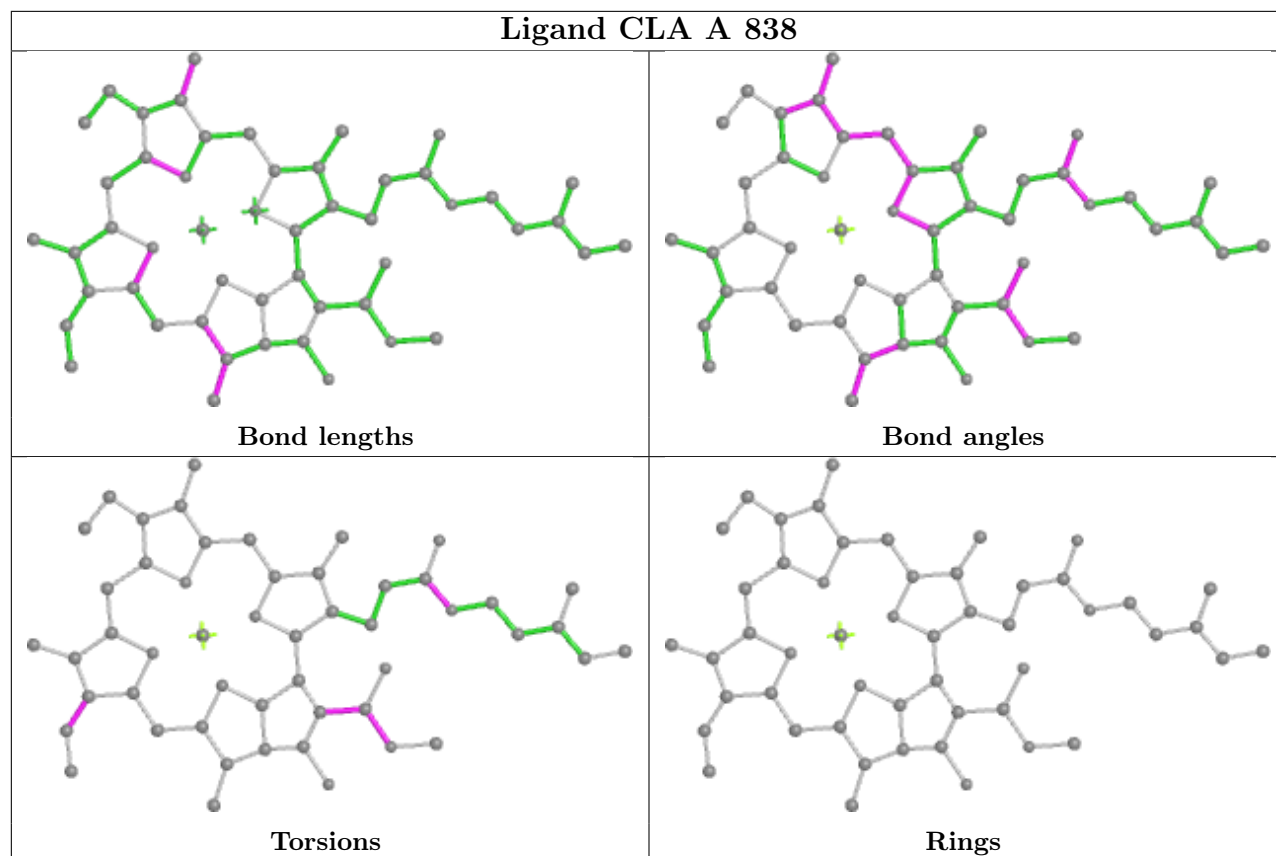
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	847	BCR	1	0
14	A	840	CLA	3	0
14	B	812	CLA	2	0
14	B	825	CLA	3	0
17	L	201	BCR	3	0
14	A	834	CLA	1	0
14	B	824	CLA	2	0
17	B	846	BCR	3	0
14	A	808	CLA	2	0
14	A	831	CLA	4	0
17	B	844	BCR	1	0
14	A	804	CLA	3	0
14	B	827	CLA	3	0
14	L	206	CLA	1	0
17	B	843	BCR	2	0
17	I	101	BCR	4	0
14	A	802	CLA	3	0
14	A	817	CLA	2	0
14	B	806	CLA	1	0
17	J	105	BCR	8	0
14	A	806	CLA	4	0
14	J	101	CLA	6	0
14	B	820	CLA	2	0
14	A	842	CLA	3	0
14	B	819	CLA	1	0
14	B	802	CLA	6	0
14	A	824	CLA	2	0
13	A	801	CL0	4	0
14	A	826	CLA	4	0
14	A	827	CLA	3	0
14	B	811	CLA	1	0
14	A	828	CLA	3	0
14	L	205	CLA	1	0
14	A	833	CLA	3	0
14	B	830	CLA	1	0

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

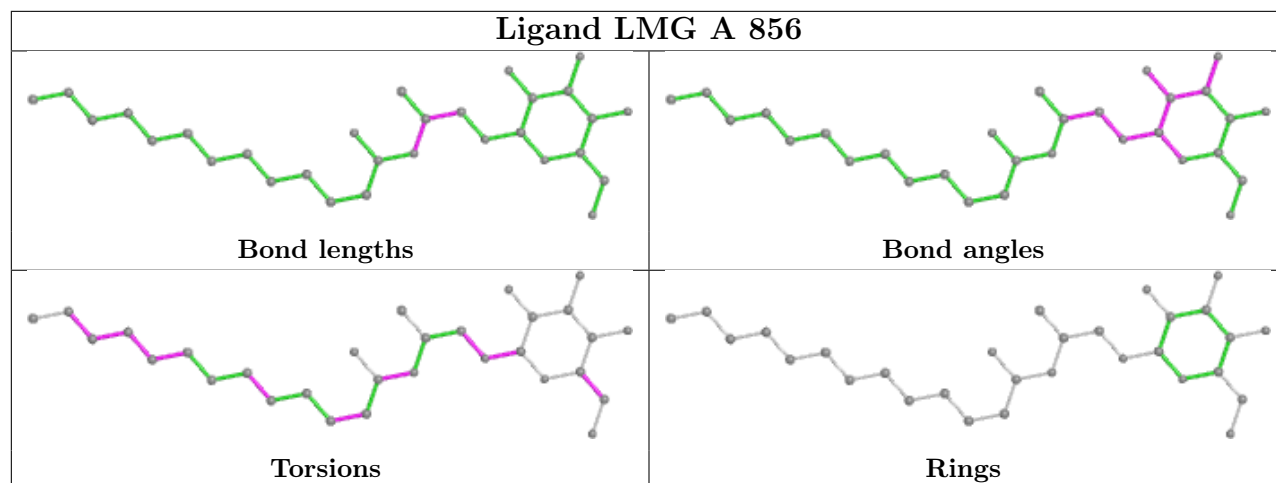
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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



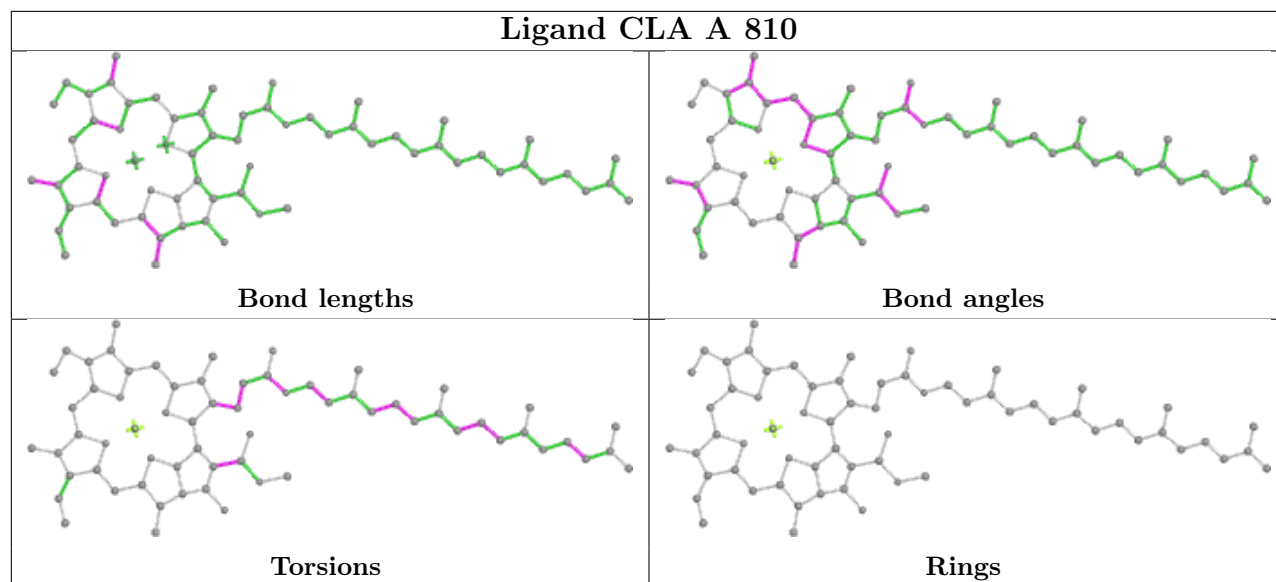
## Ligand CLA A 838



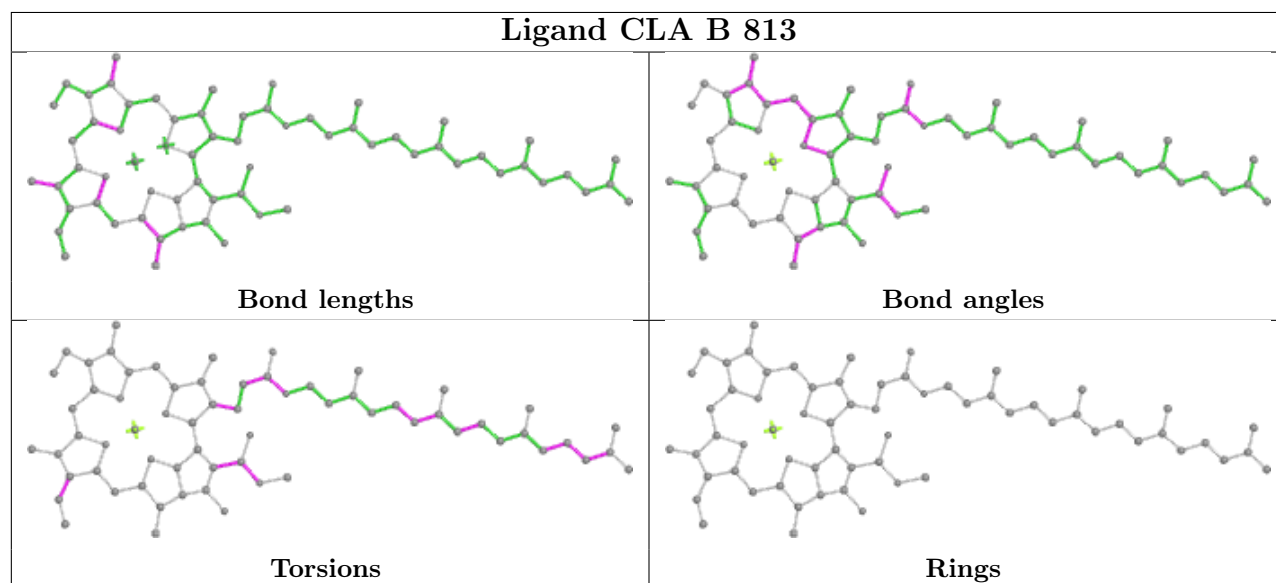
## Ligand LMG A 856



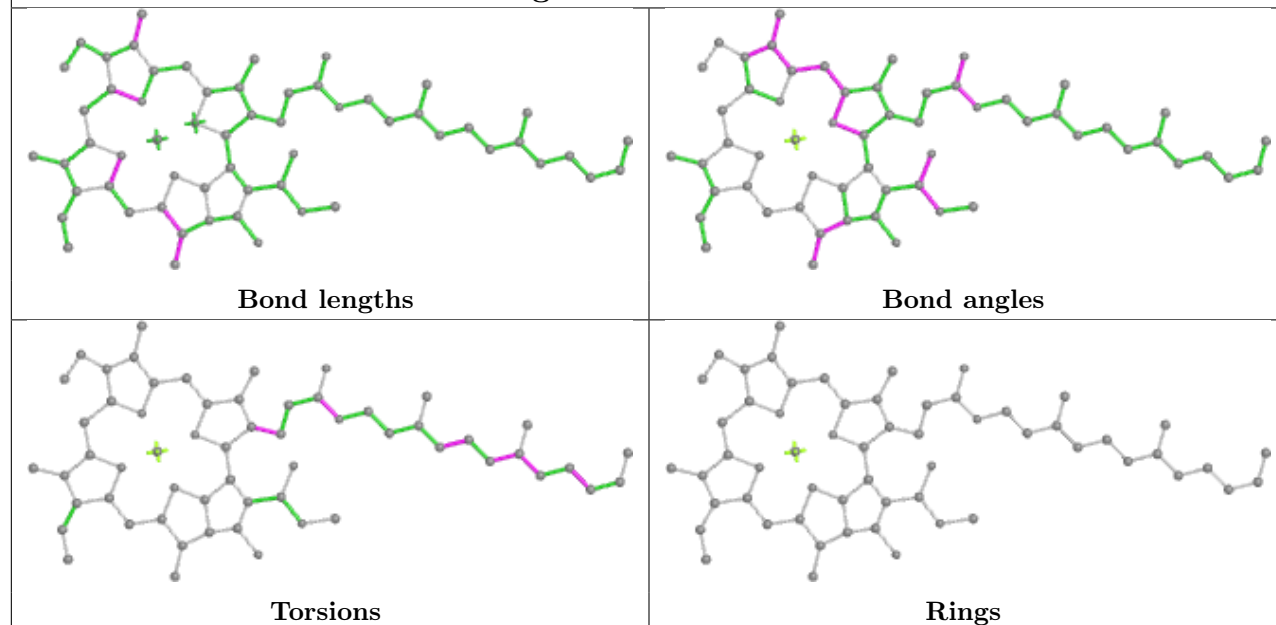
## Ligand CLA A 810



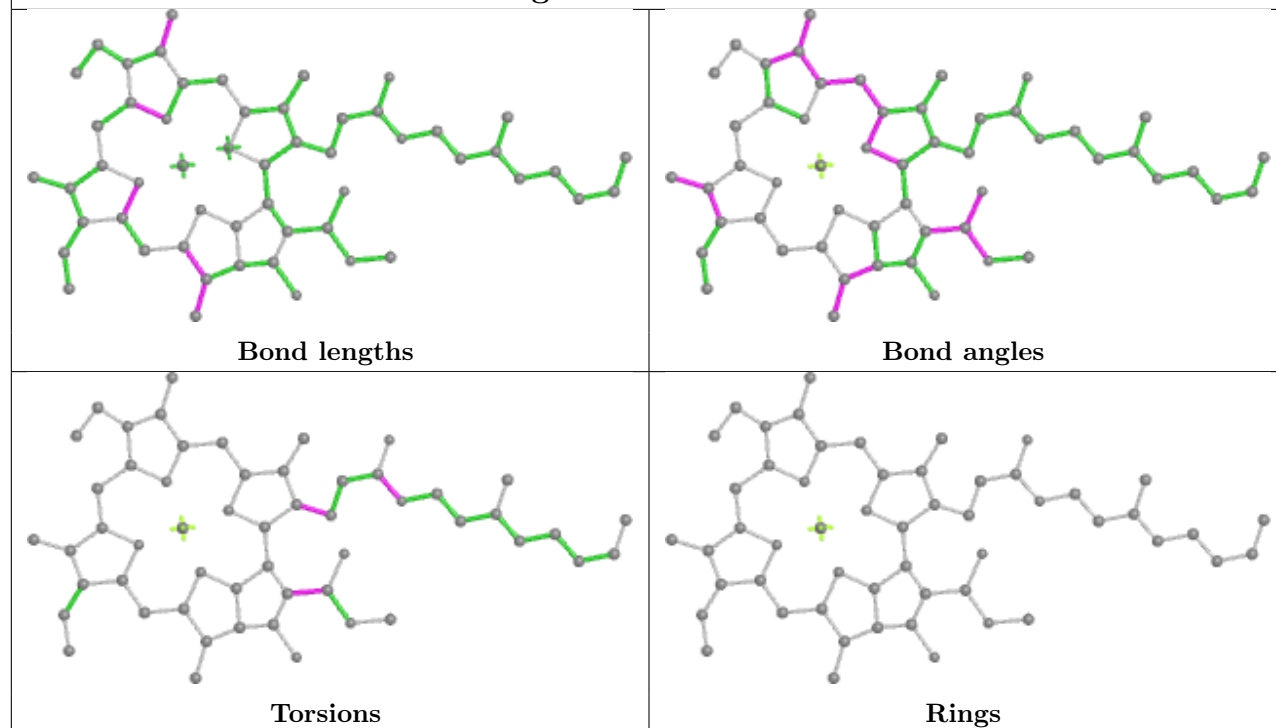
## Ligand CLA B 813



## Ligand CLA B 817

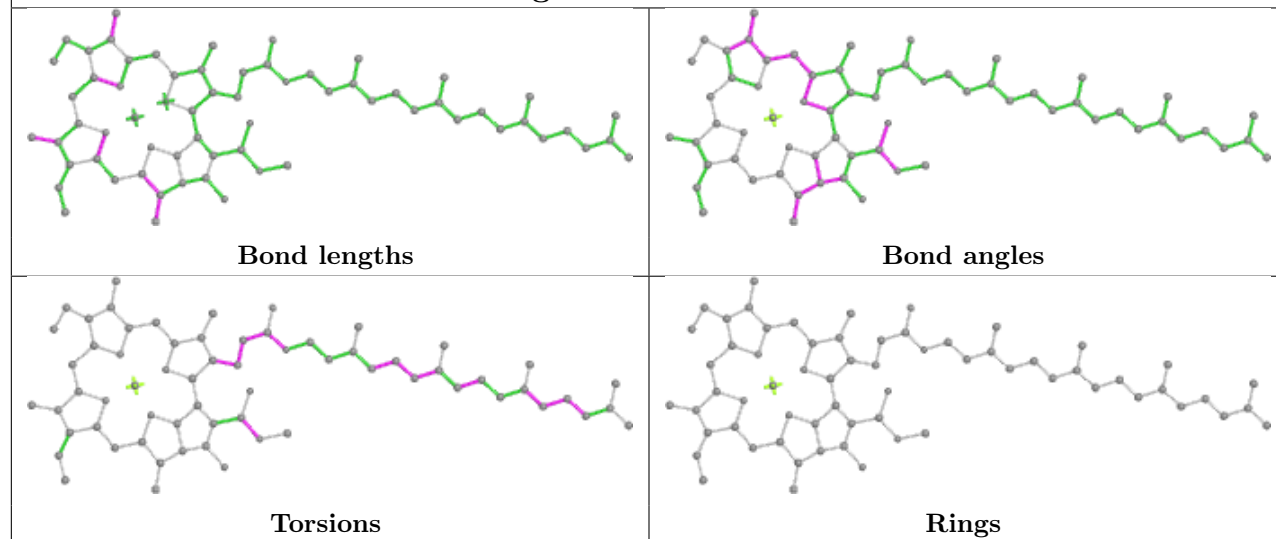


## Ligand CLA A 836

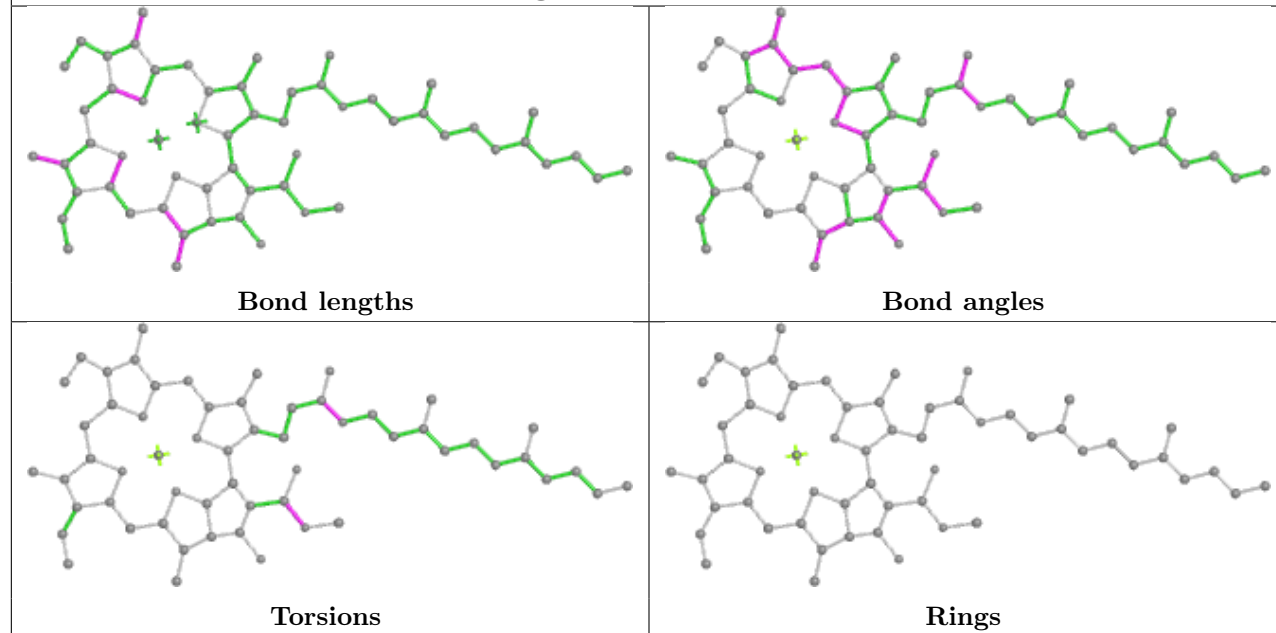




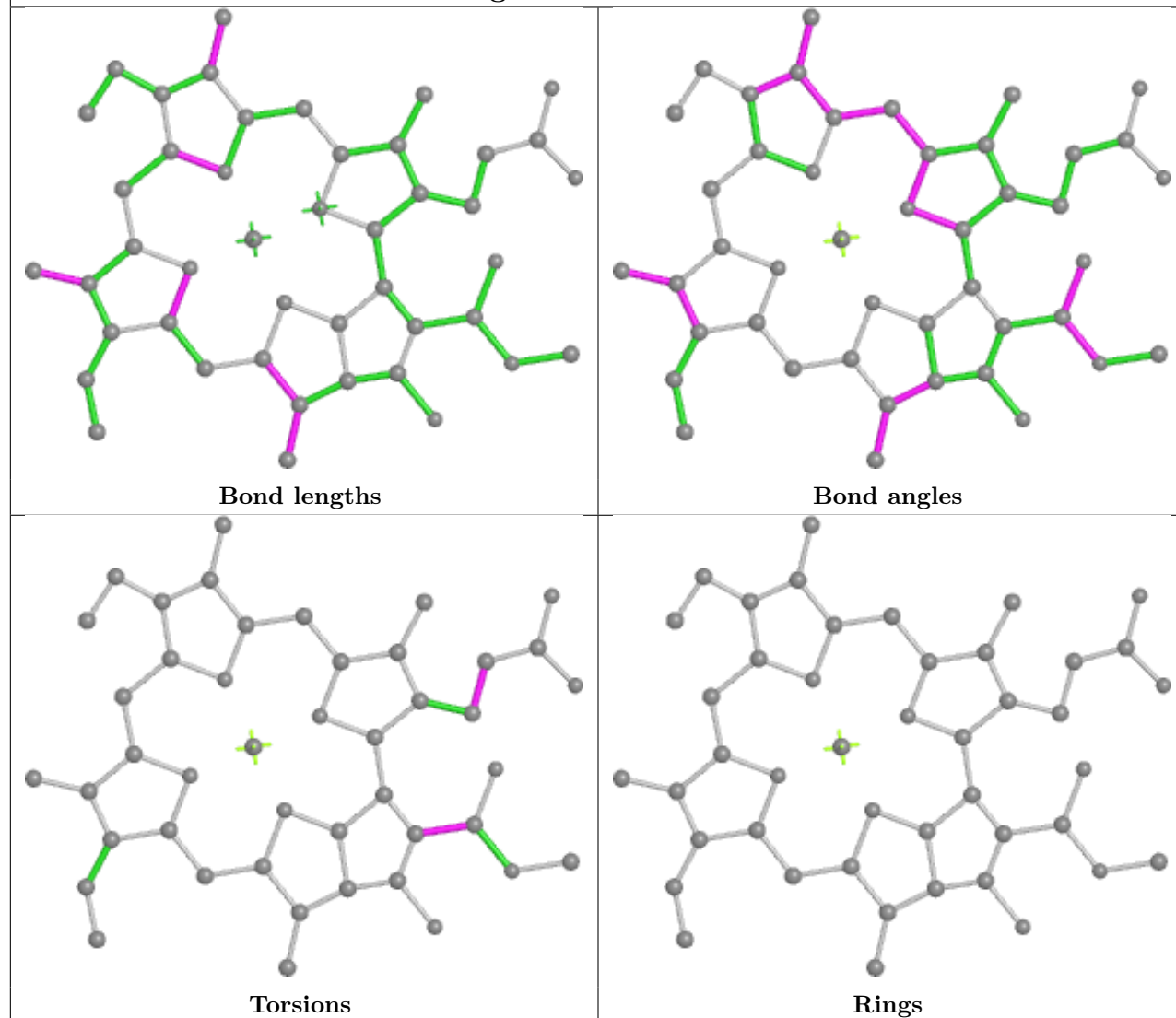
## Ligand CLA B 828



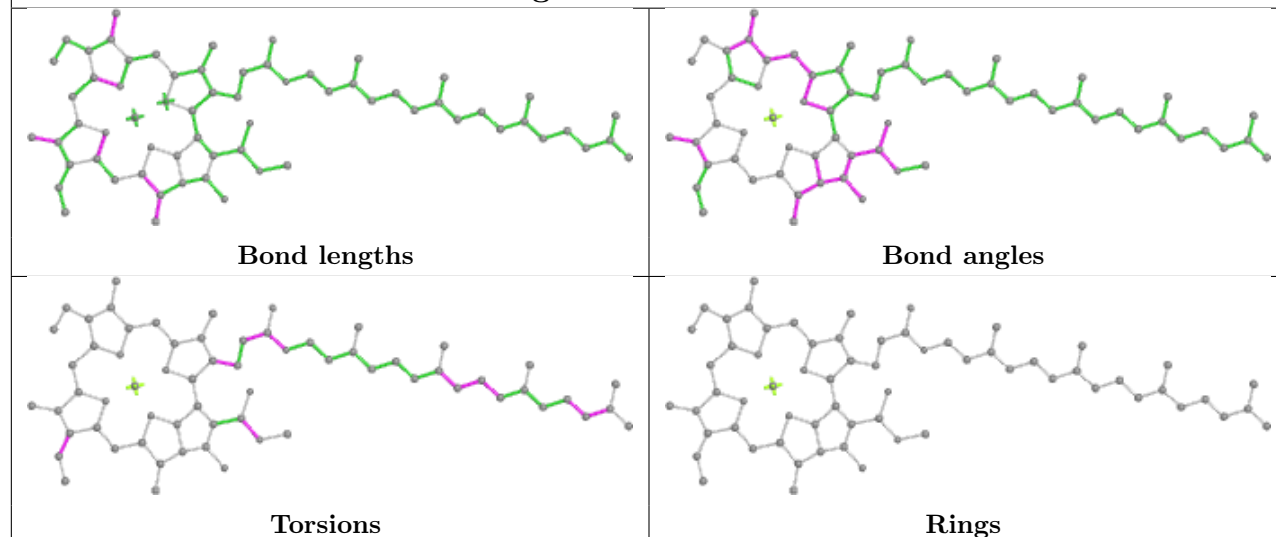
## Ligand CLA B 833



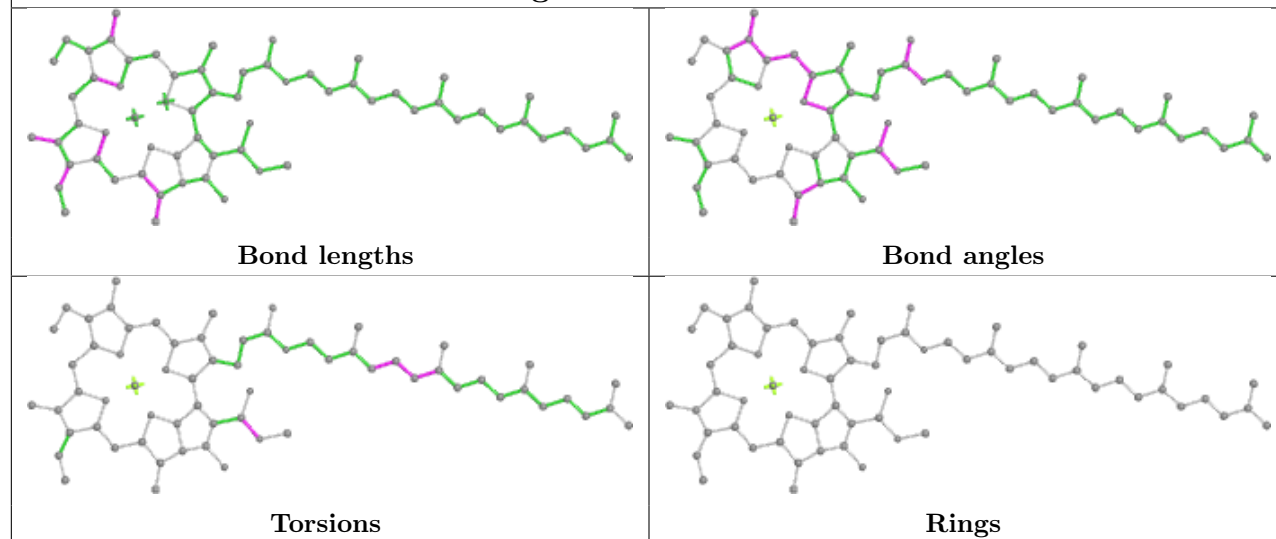
## Ligand CLA A 816



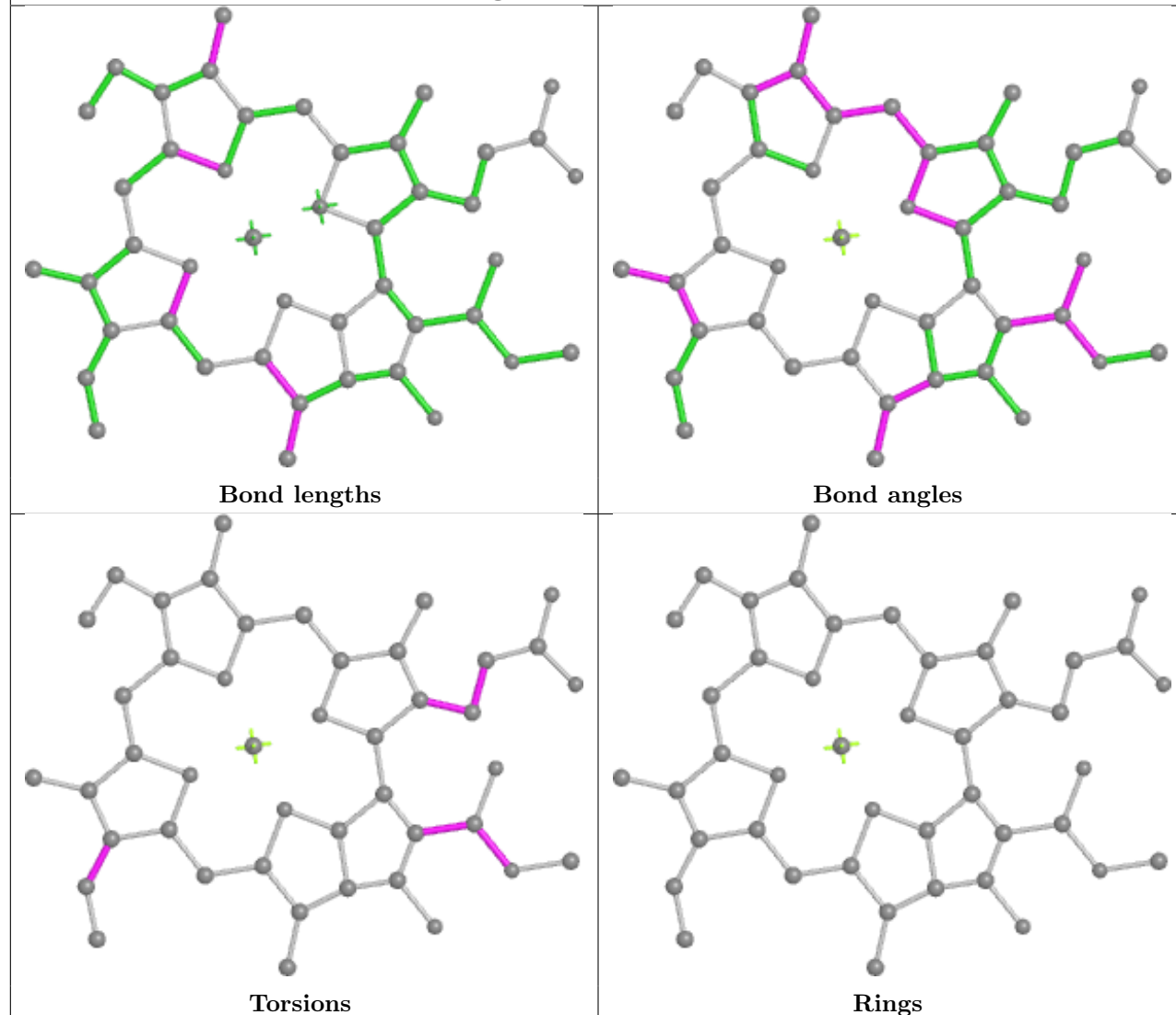
## Ligand CLA B 809

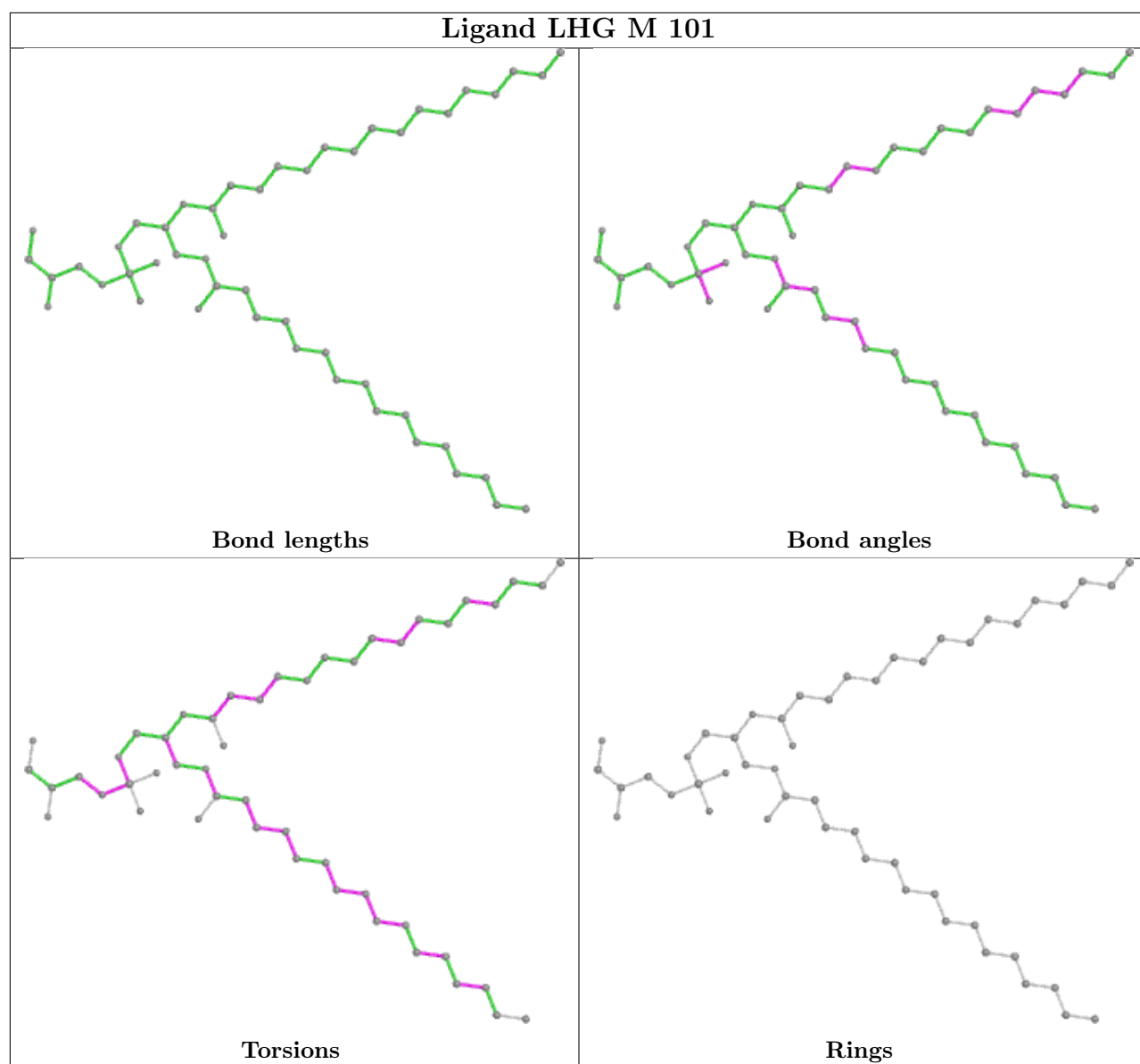


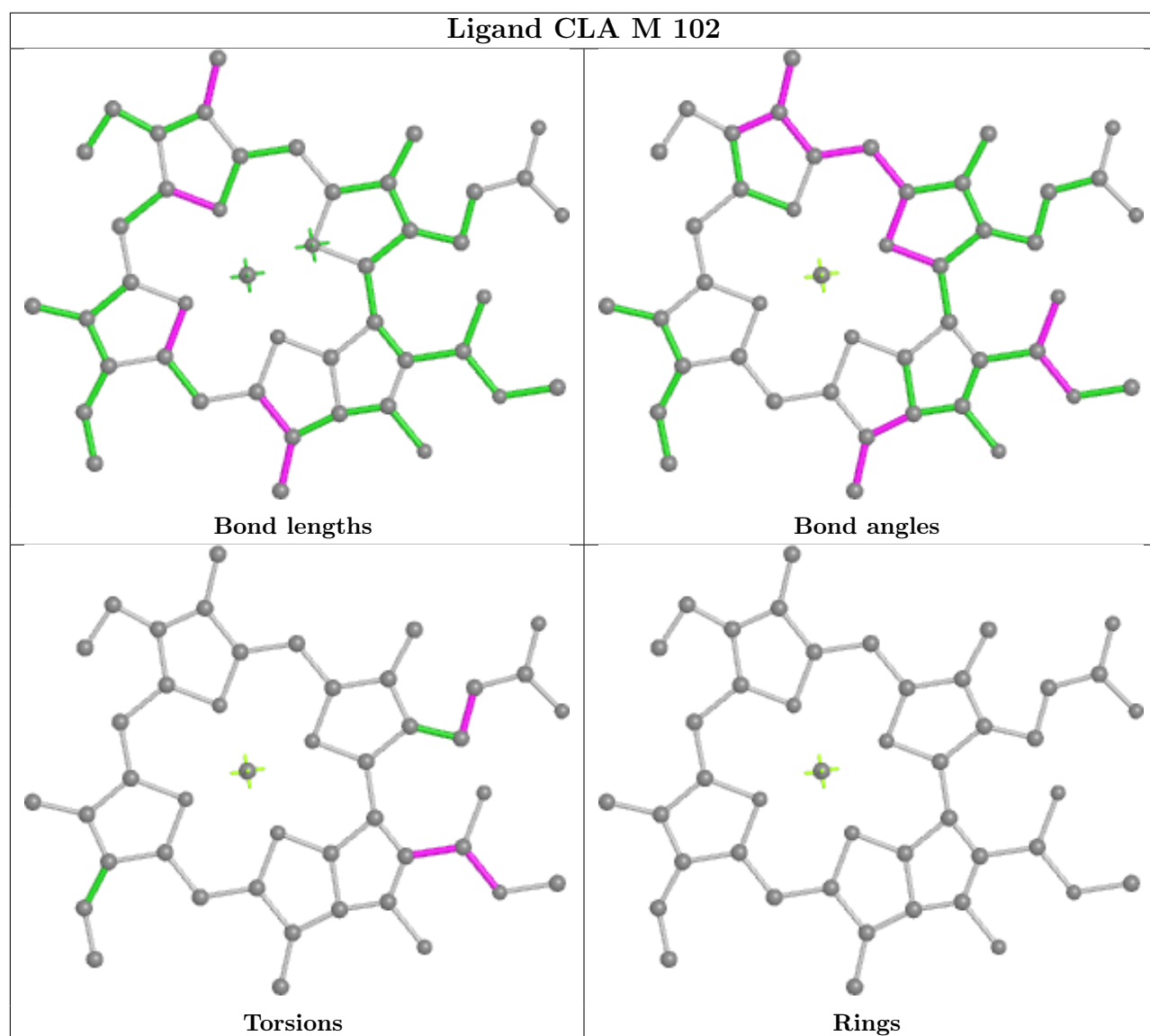
## Ligand CLA A 841



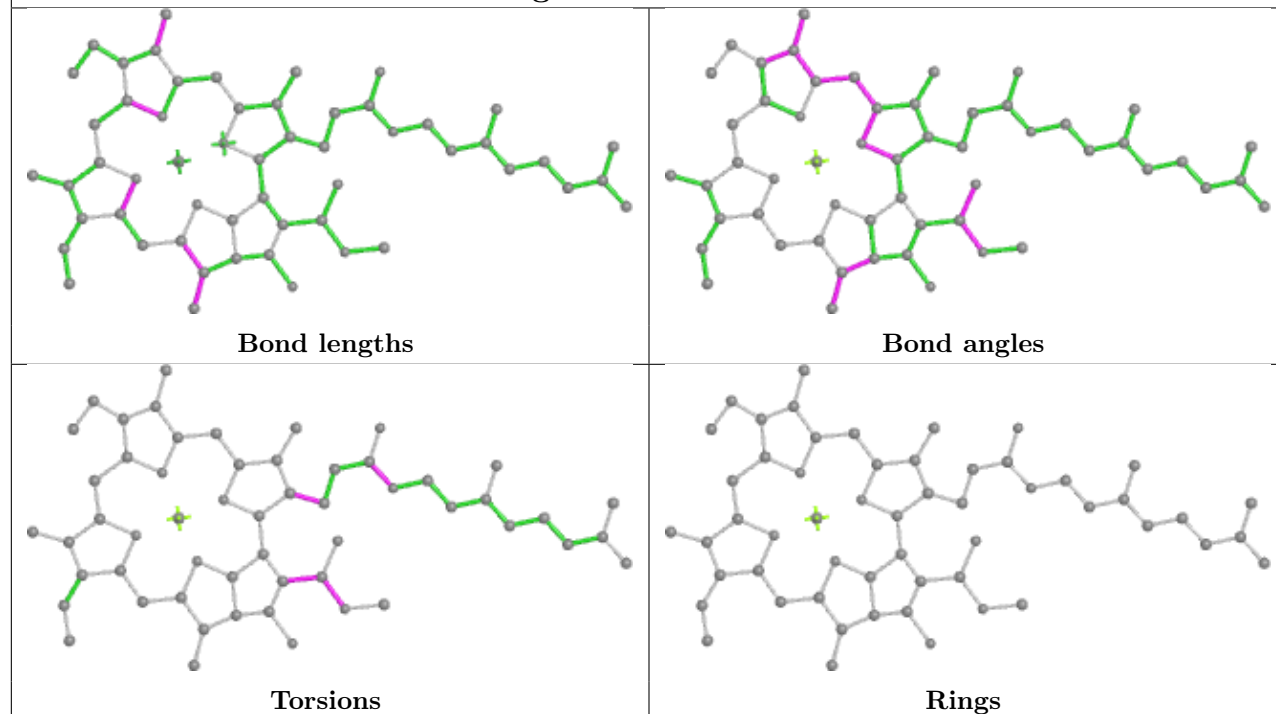
## Ligand CLA A 811



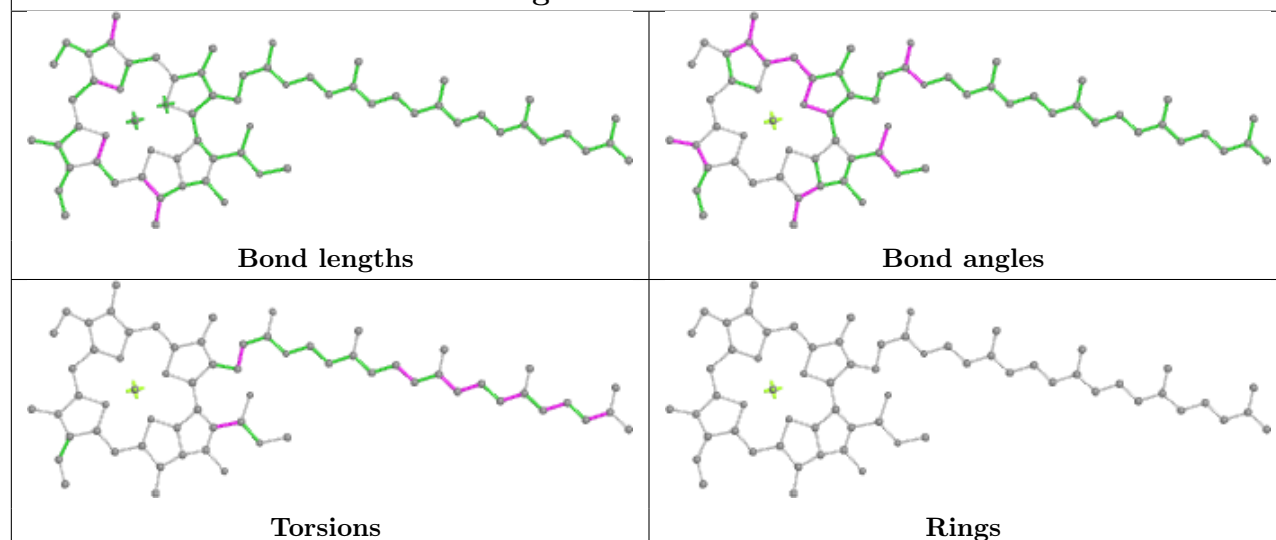




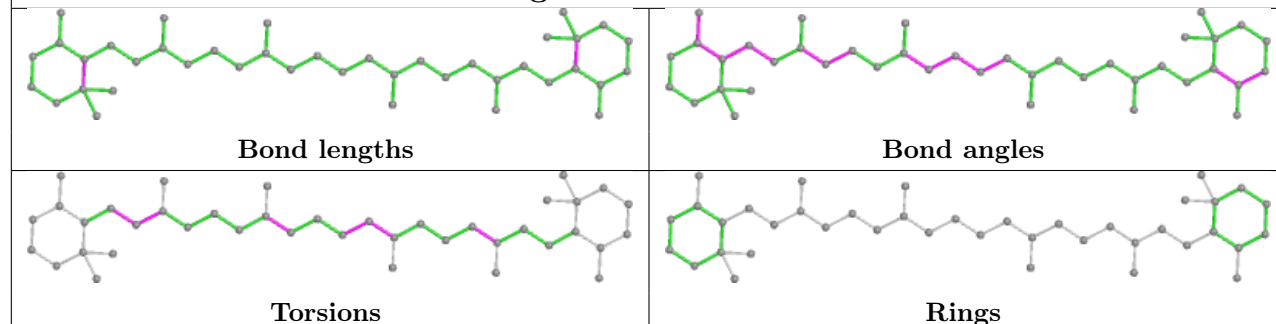
## Ligand CLA B 816

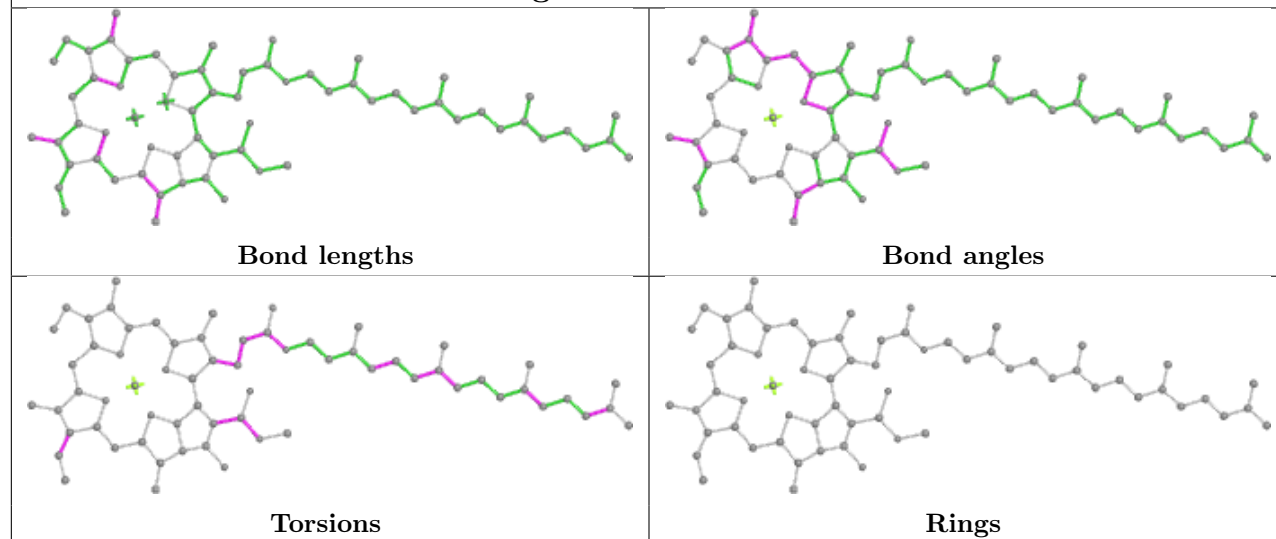
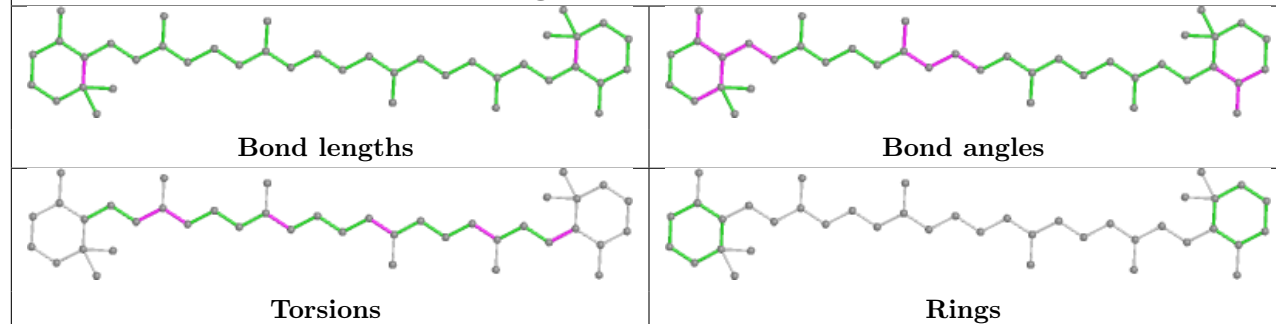
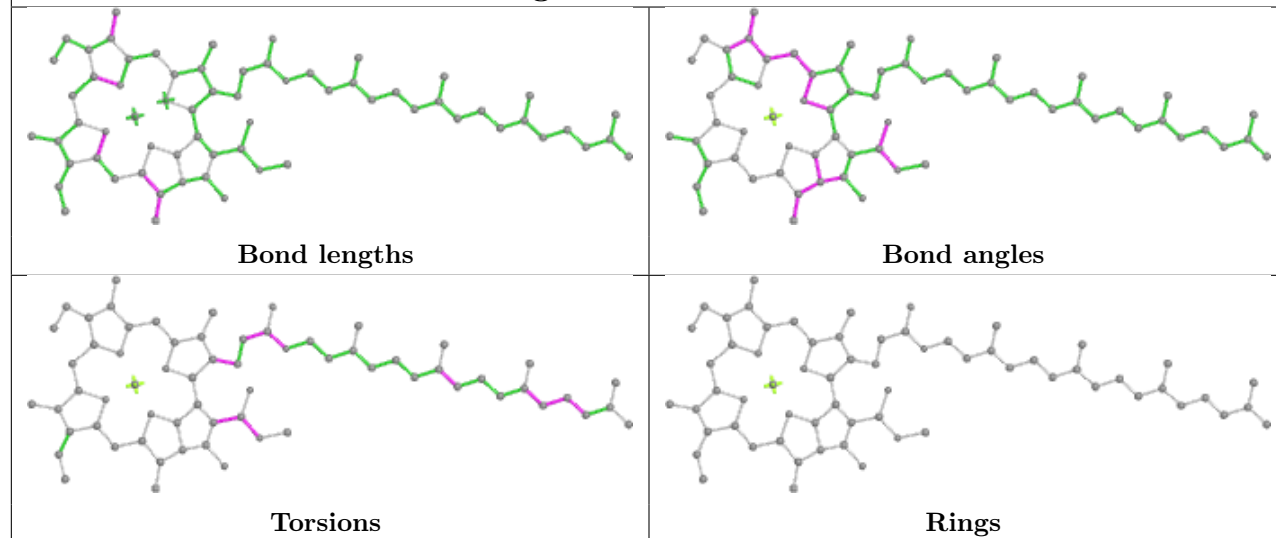


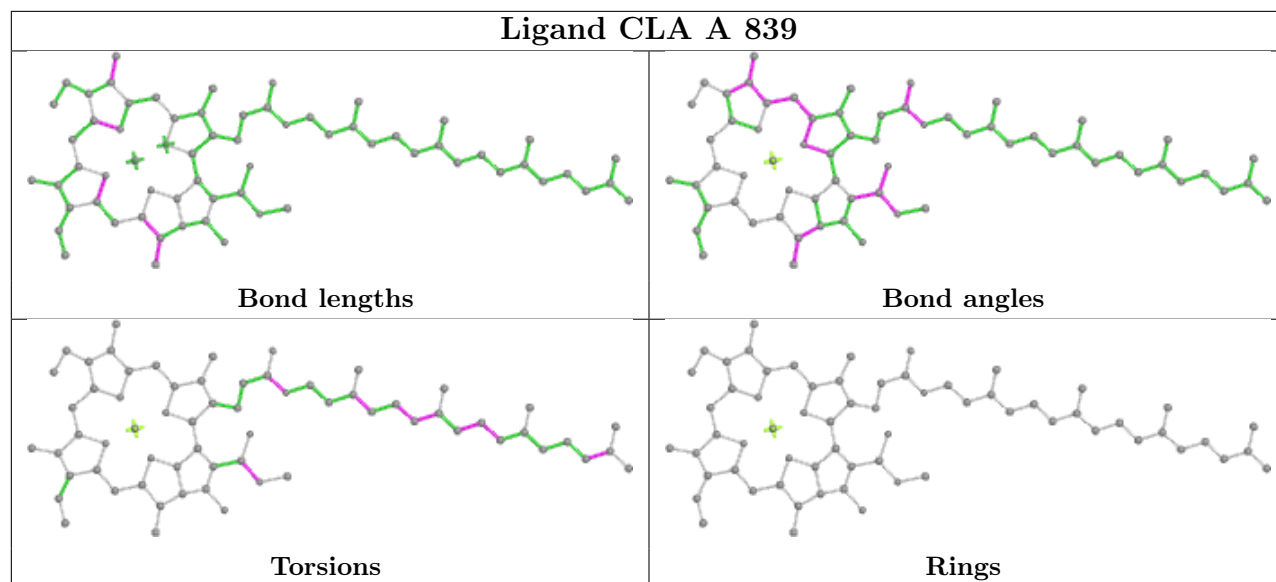
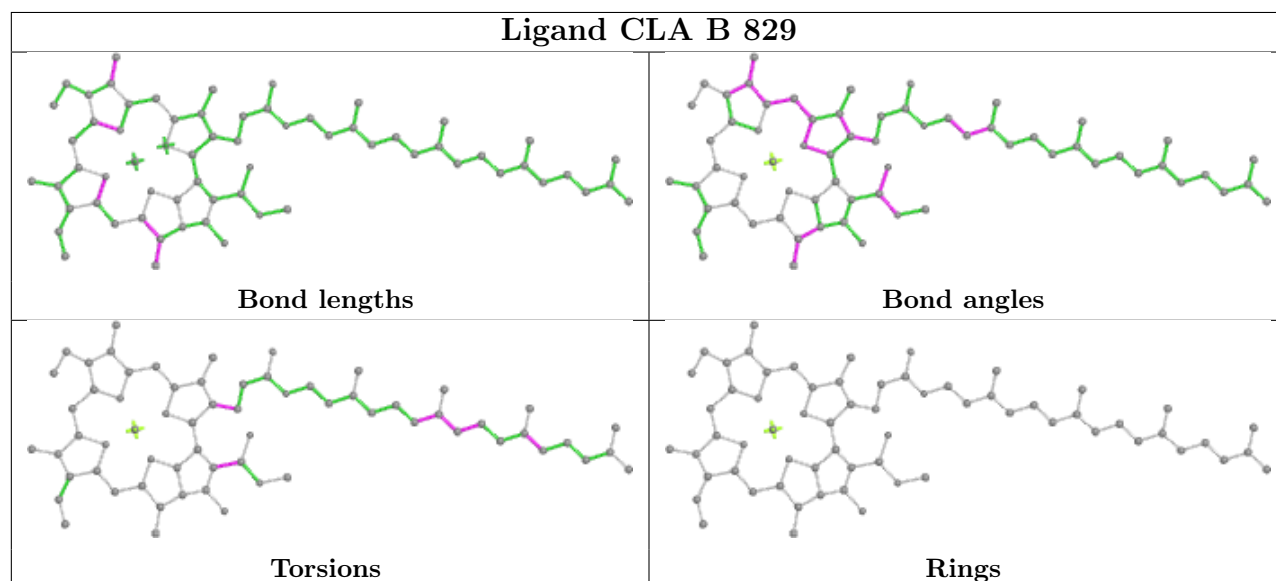
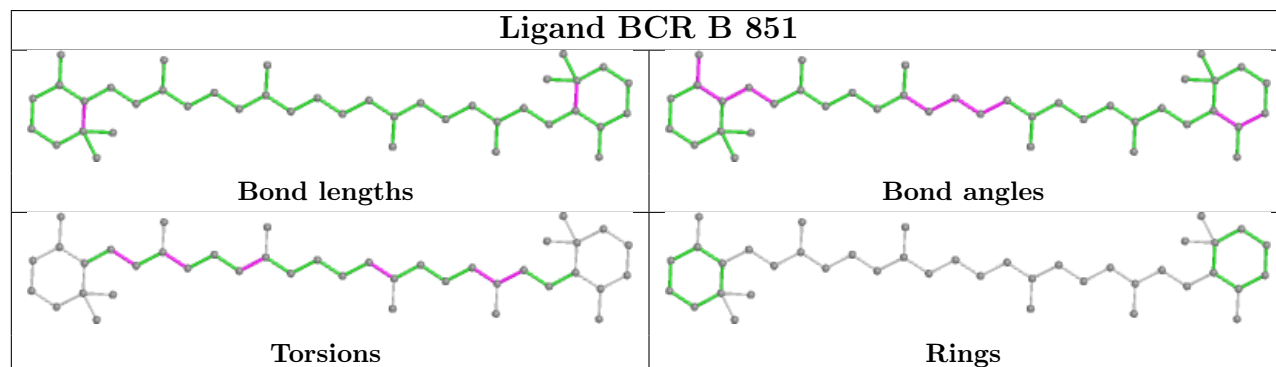
## Ligand CLA B 838



## Ligand BCR A 851

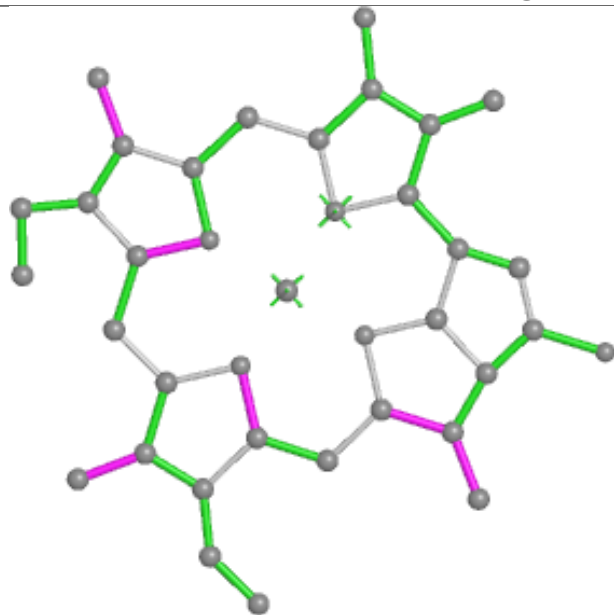


**Ligand CLA B 826****Ligand BCR F 203****Ligand CLA B 805**

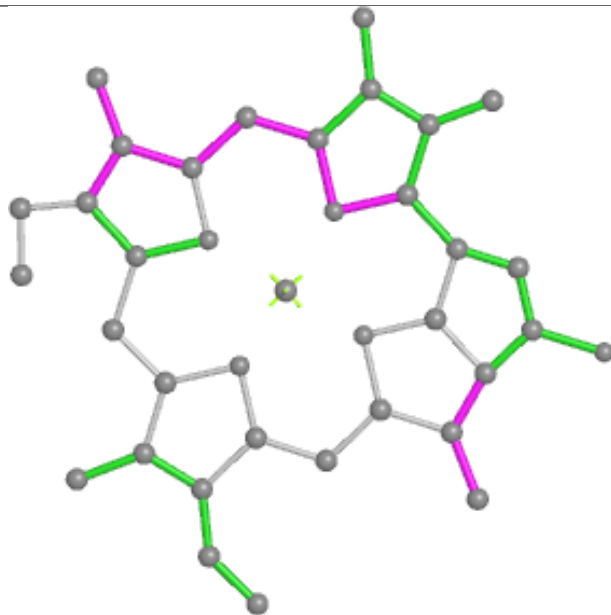
**Ligand CLA A 839****Ligand CLA B 829****Ligand BCR B 851**



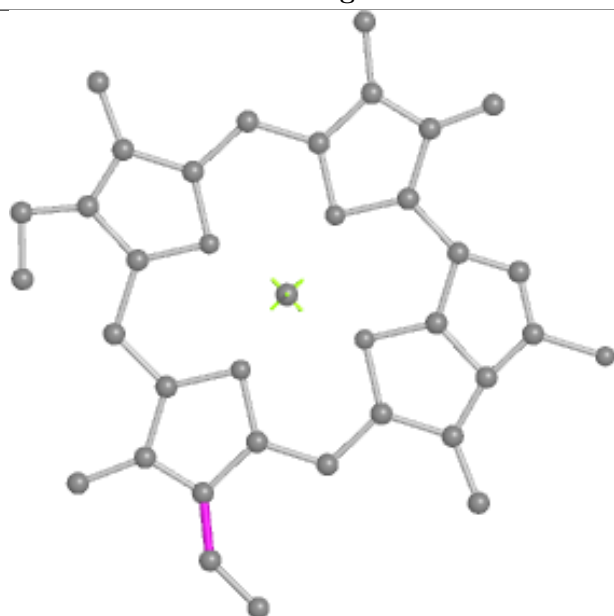
## Ligand CLA J 102



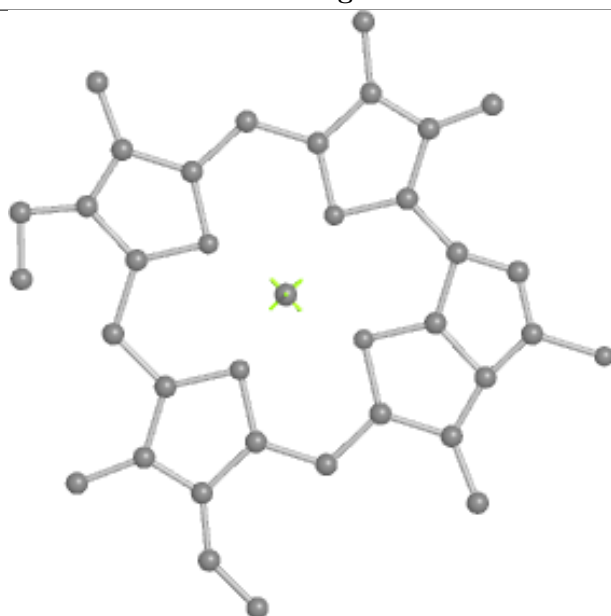
Bond lengths



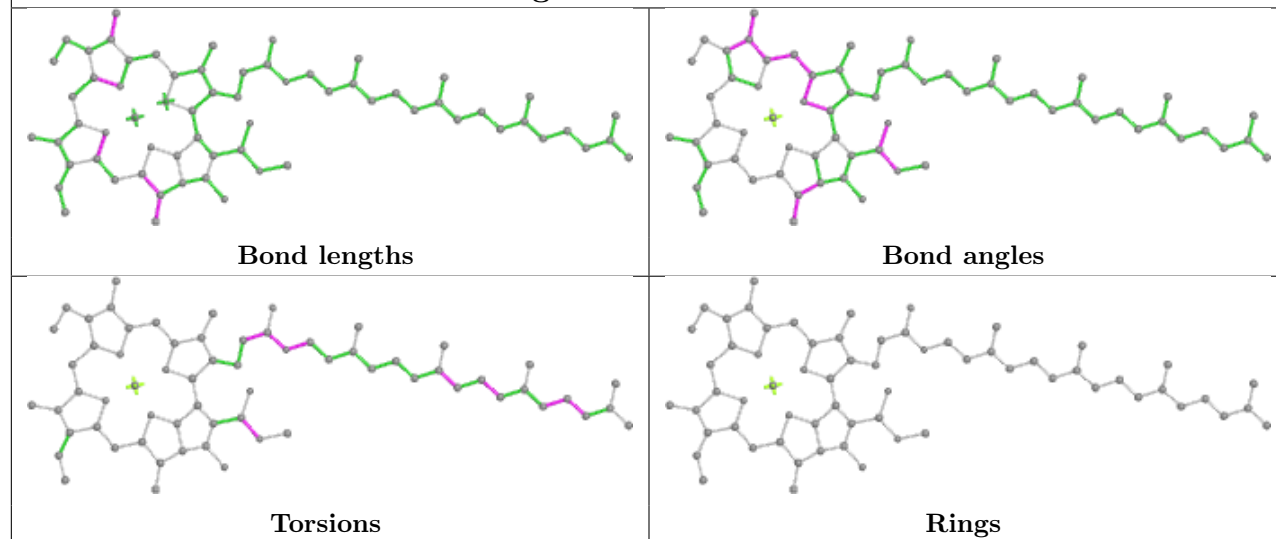
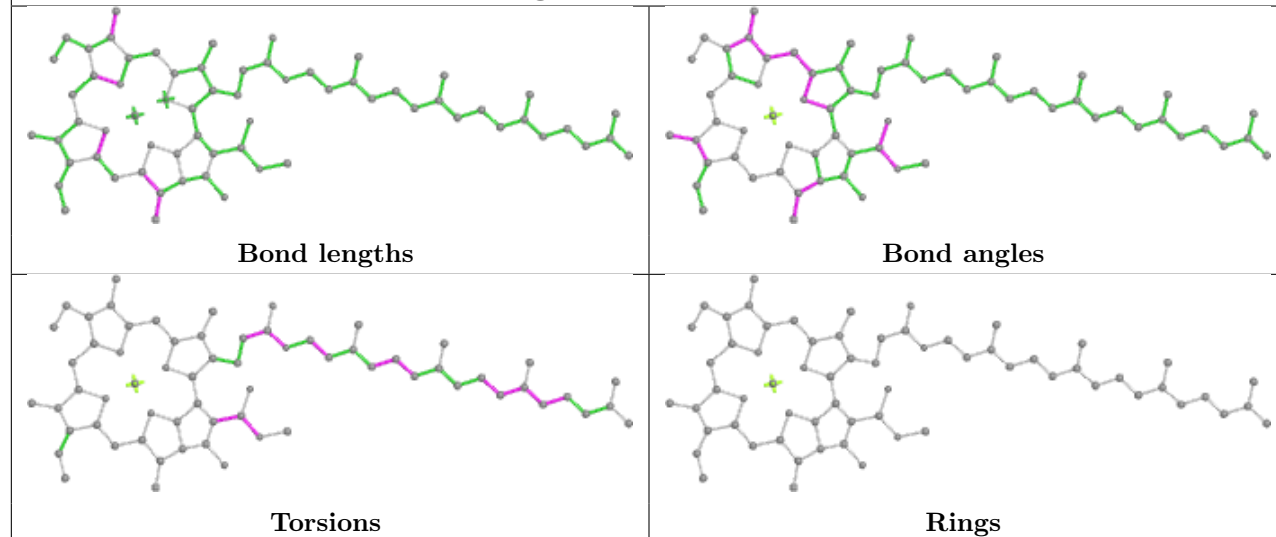
Bond angles

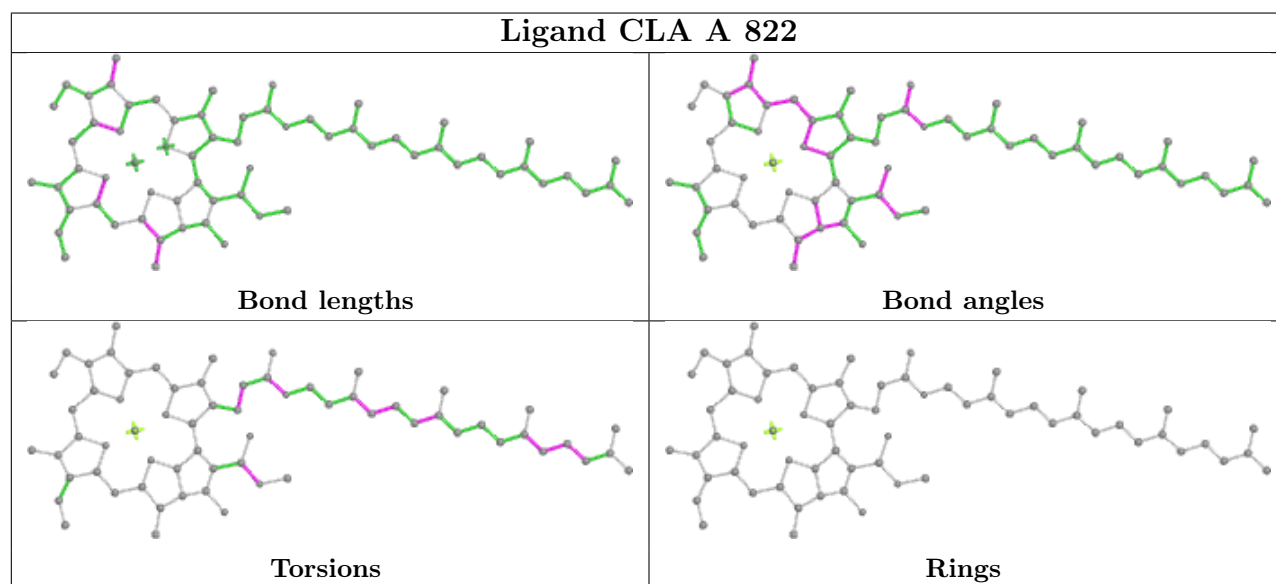
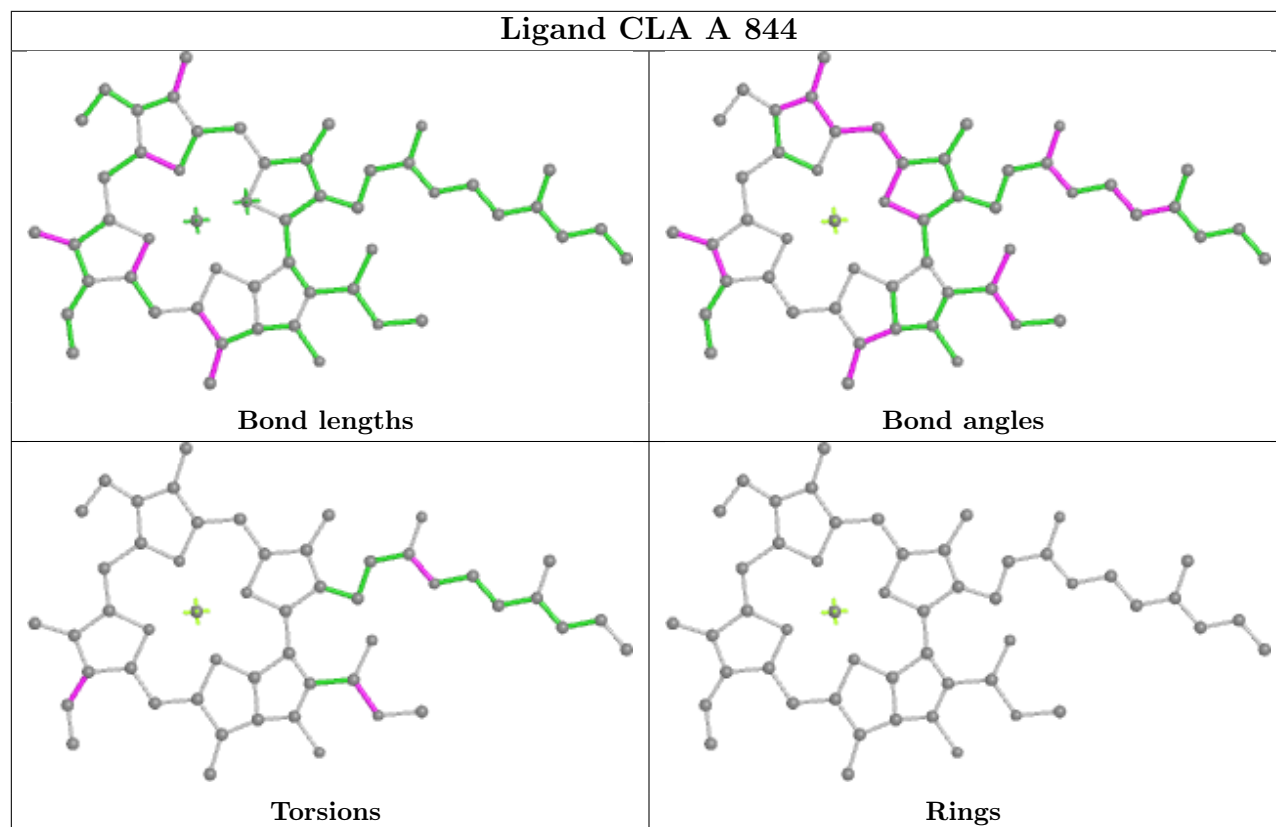


Torsions

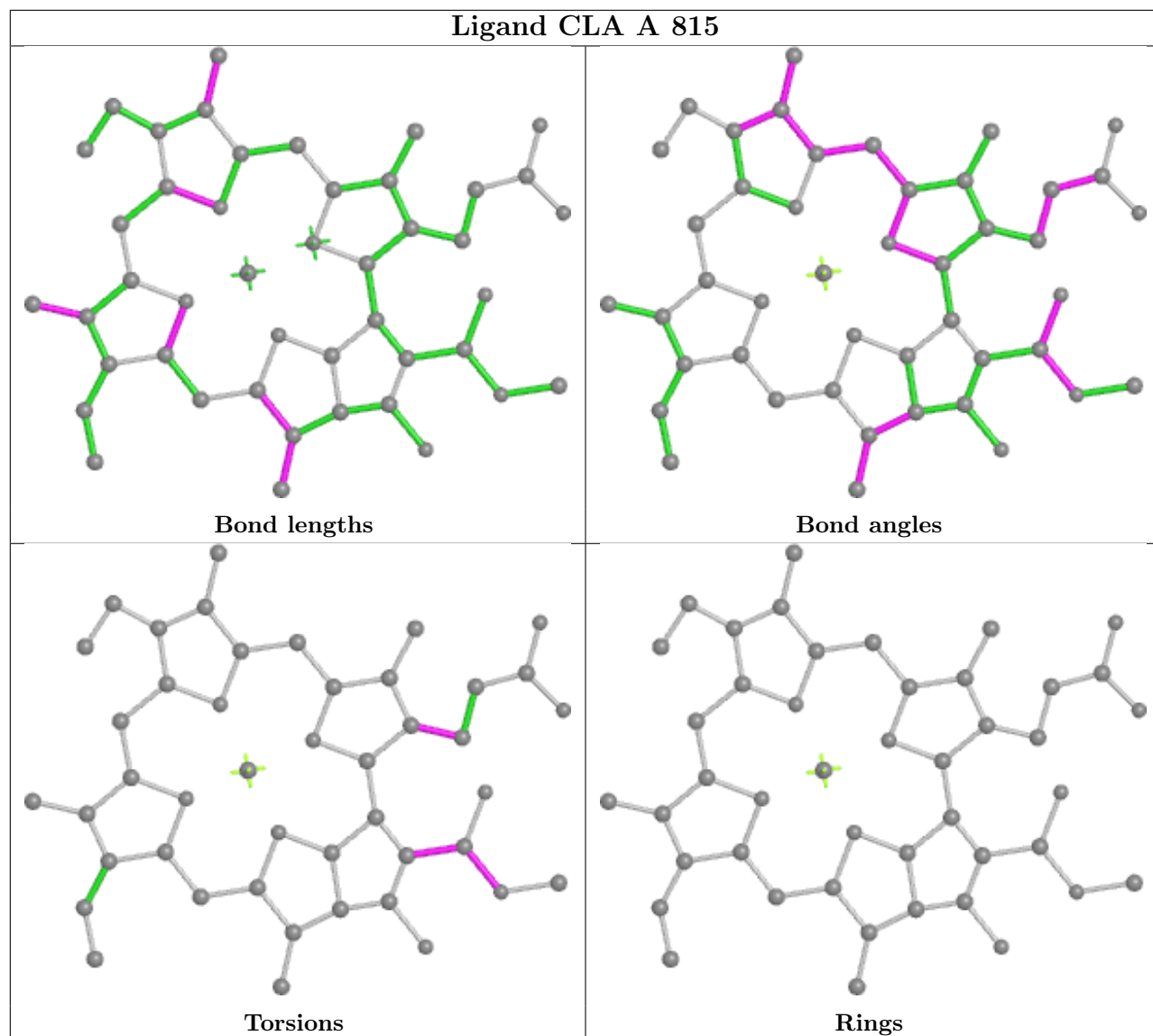


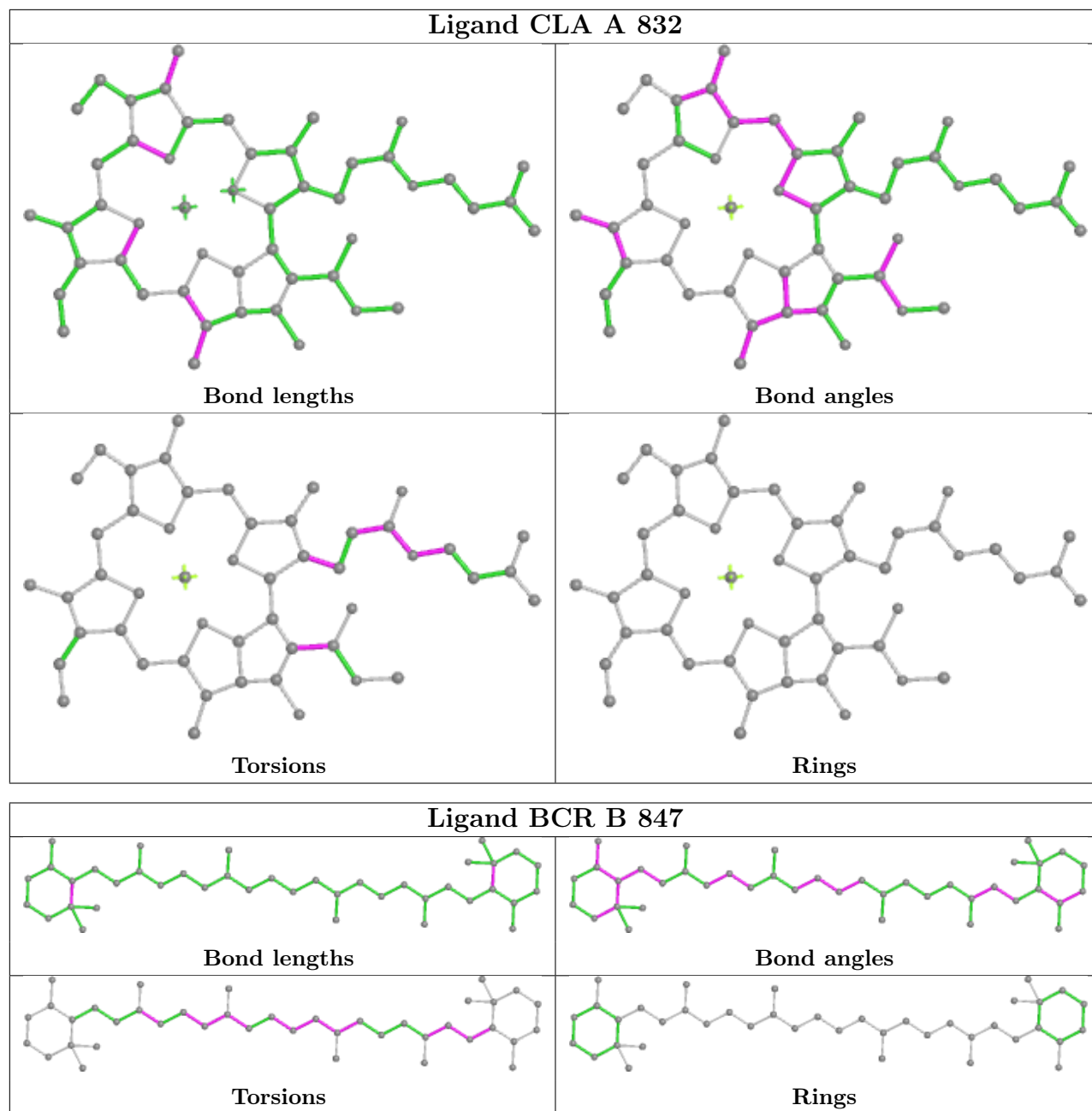
Rings

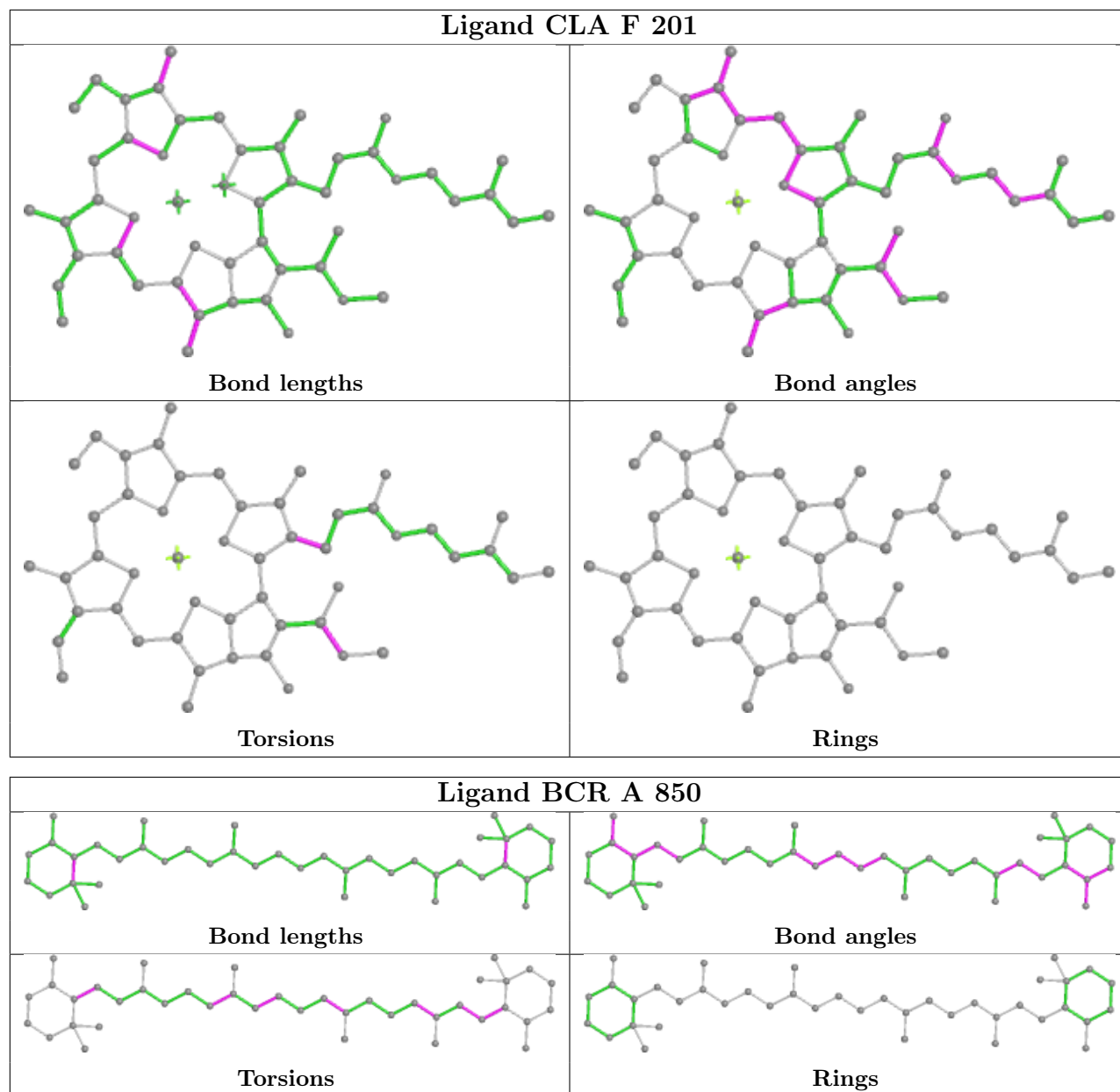
**Ligand CLA B 803****Ligand CLA A 807**



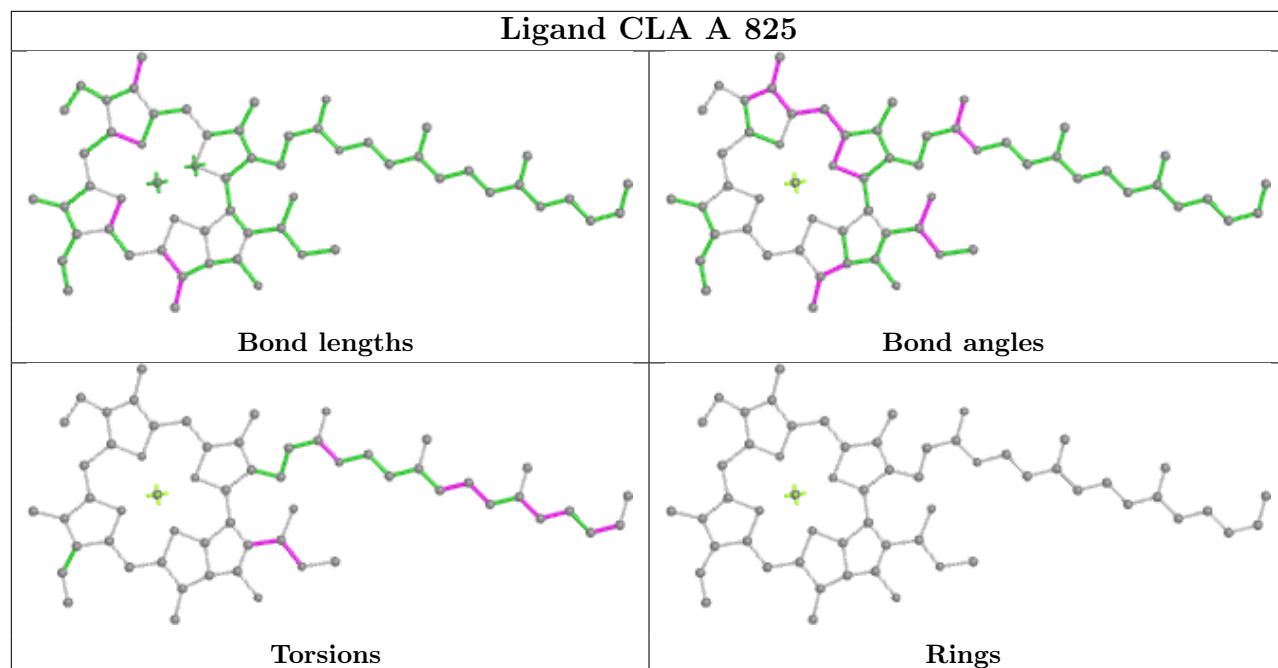
## Ligand CLA A 815



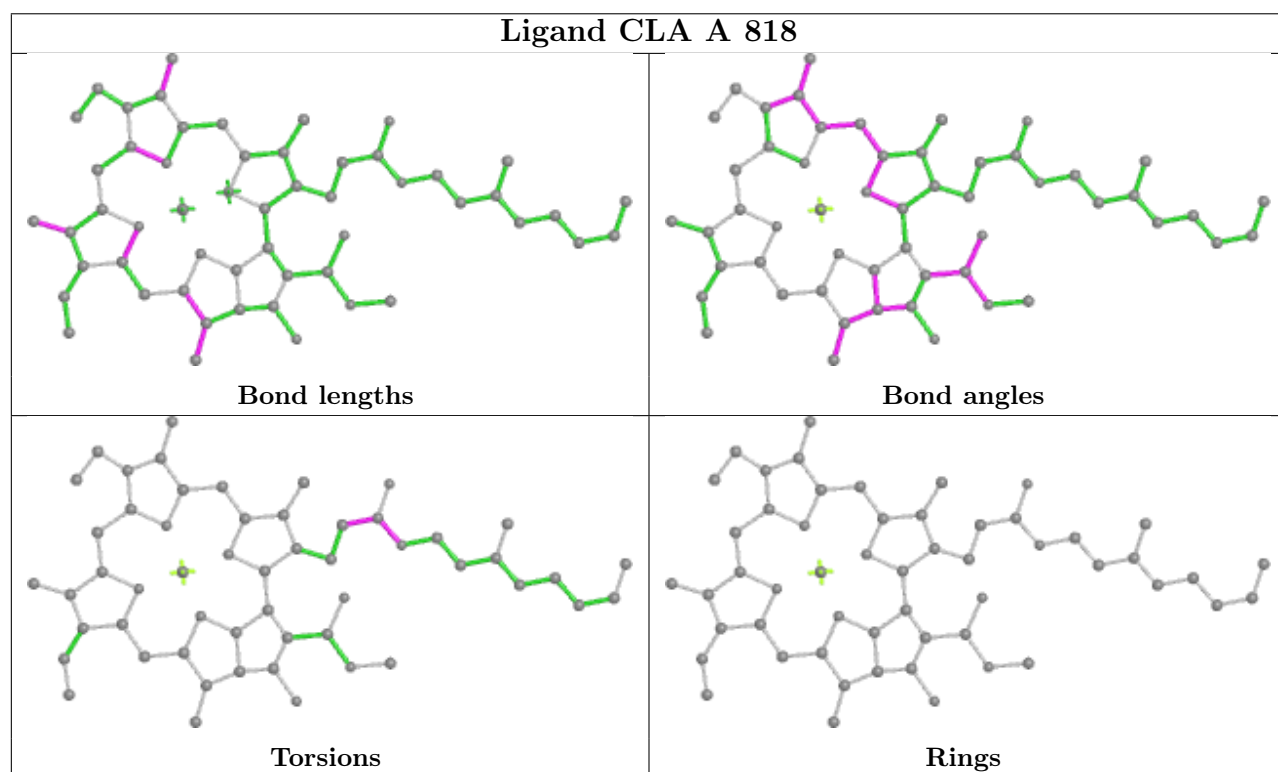




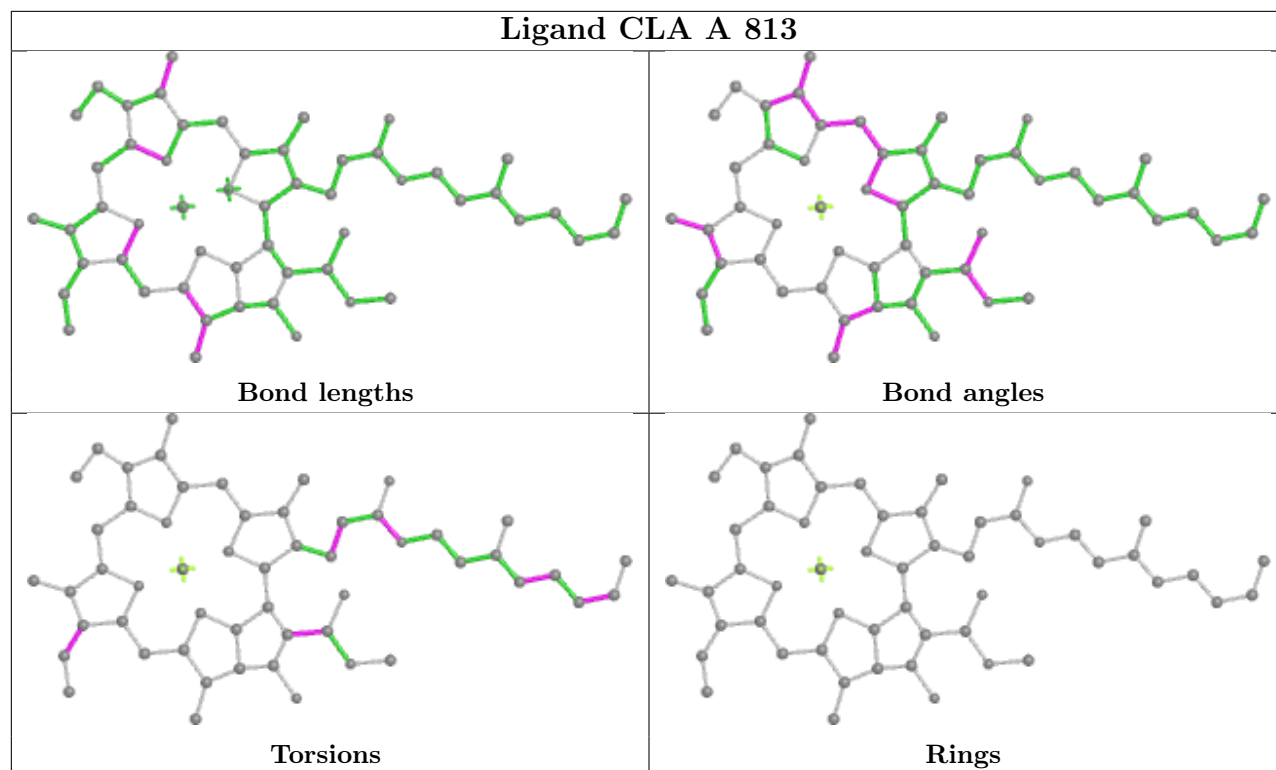
## Ligand CLA A 825



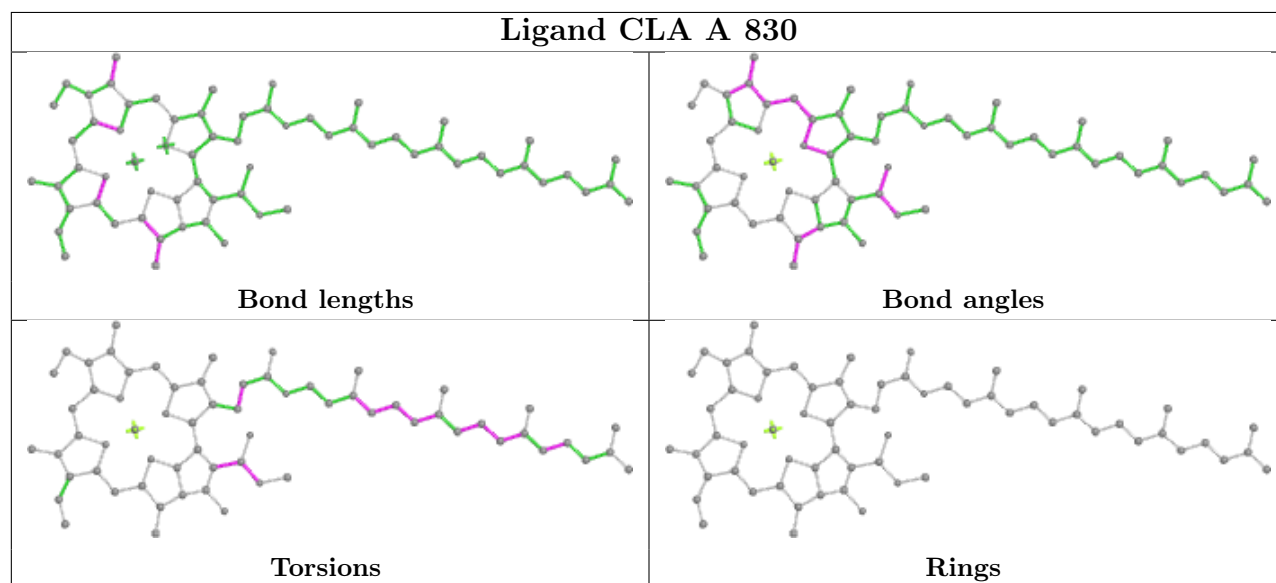
## Ligand CLA A 818



## Ligand CLA A 813

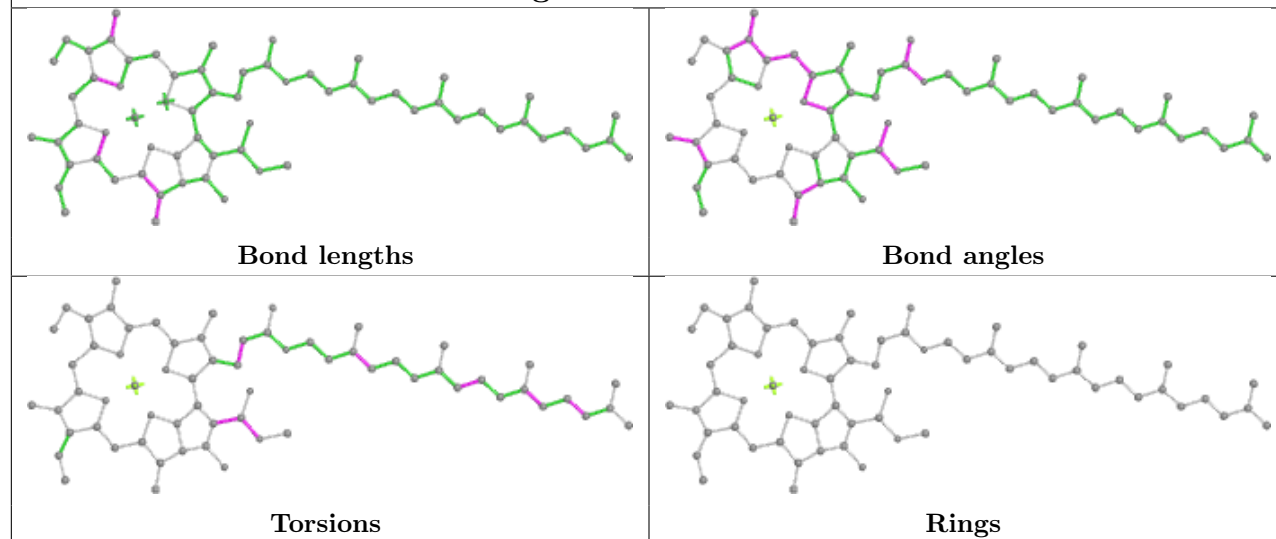


## Ligand CLA A 830

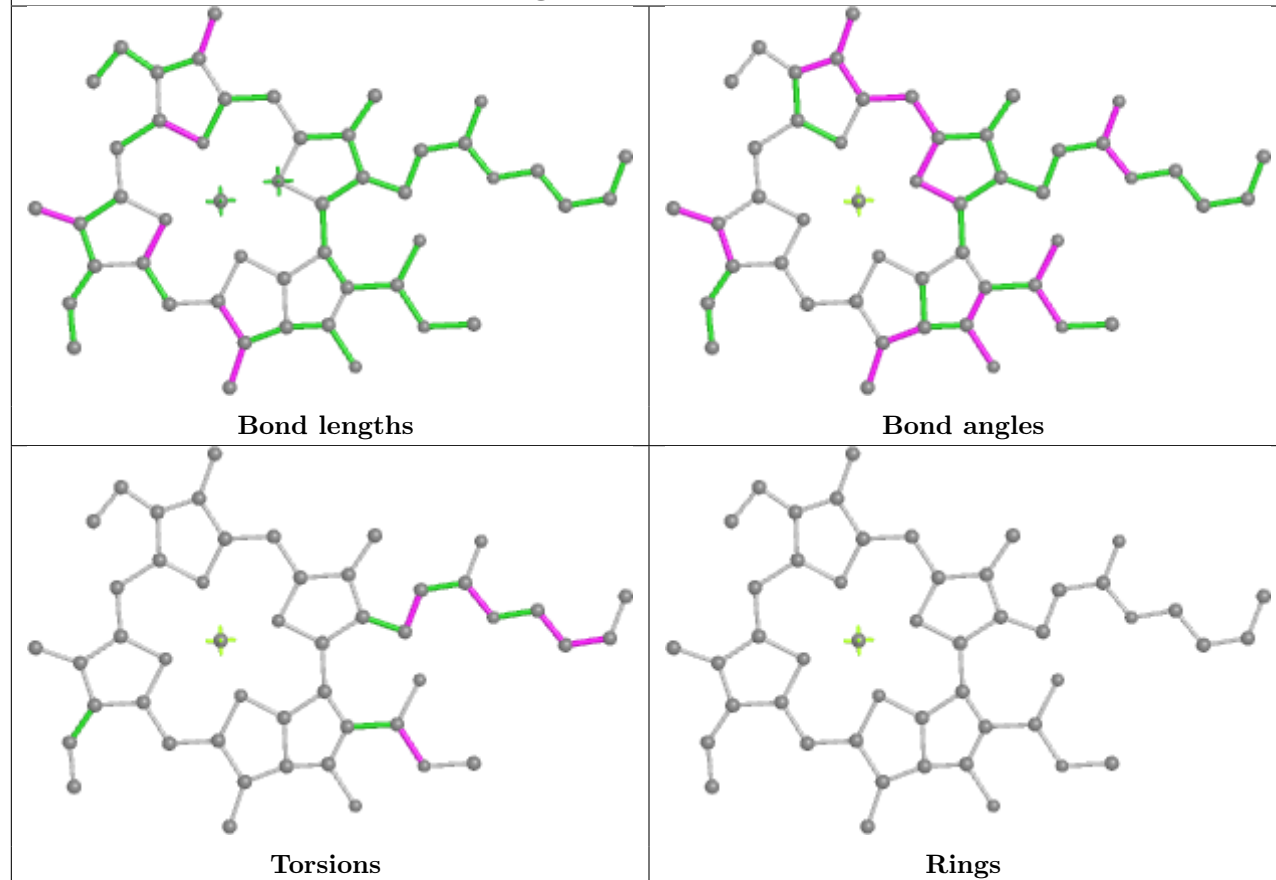




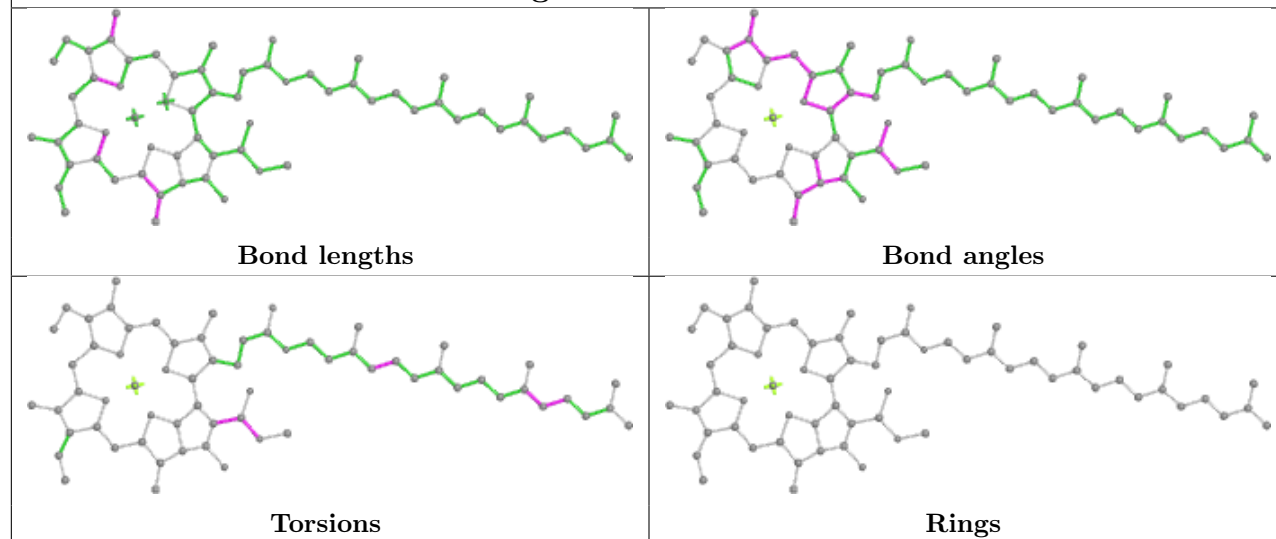
## Ligand CLA B 814



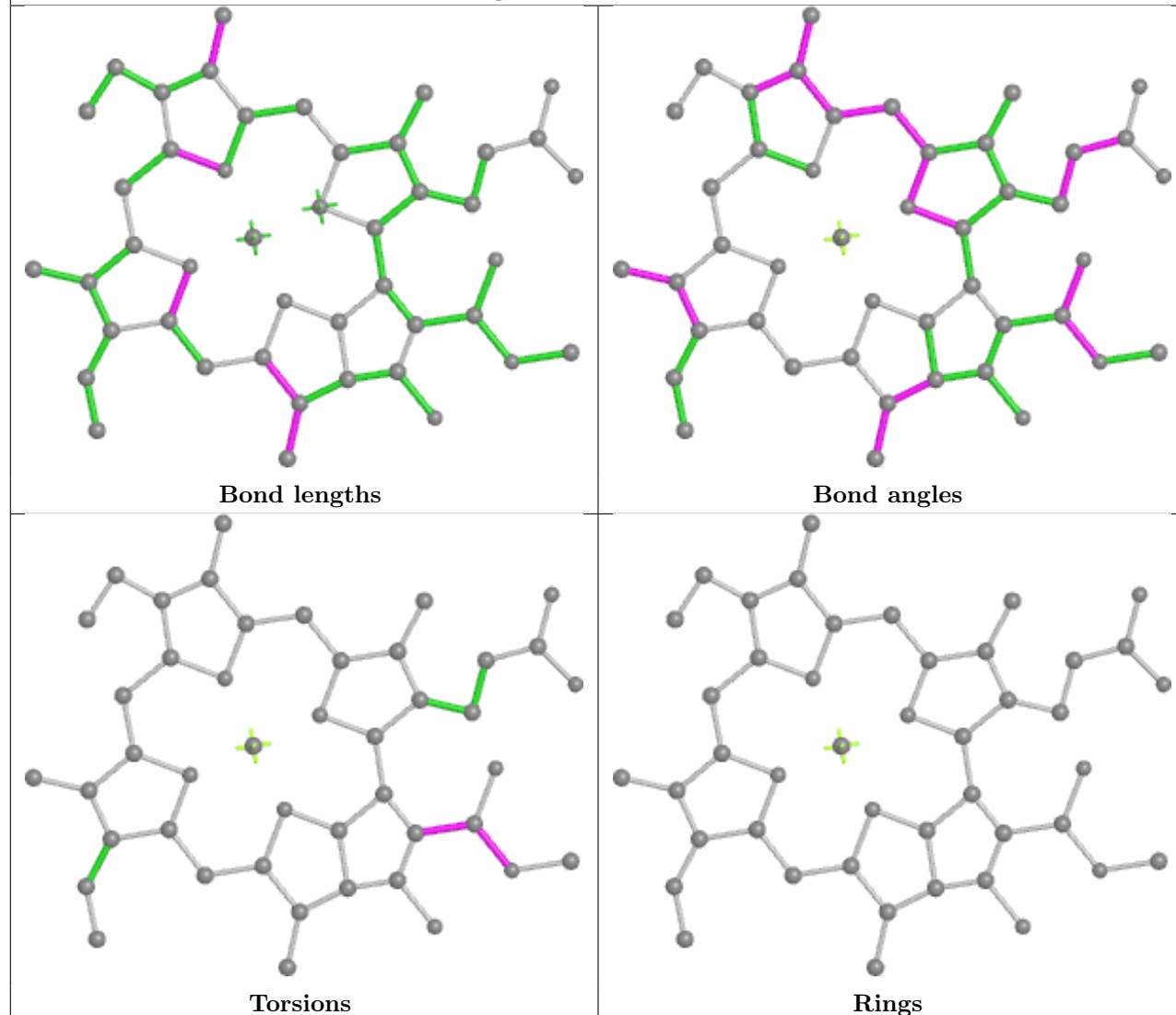
## Ligand CLA B 831

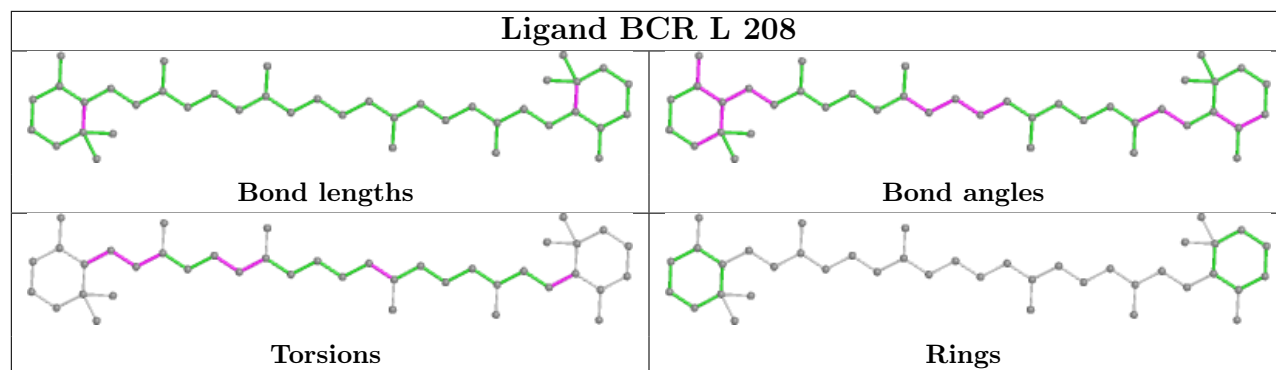
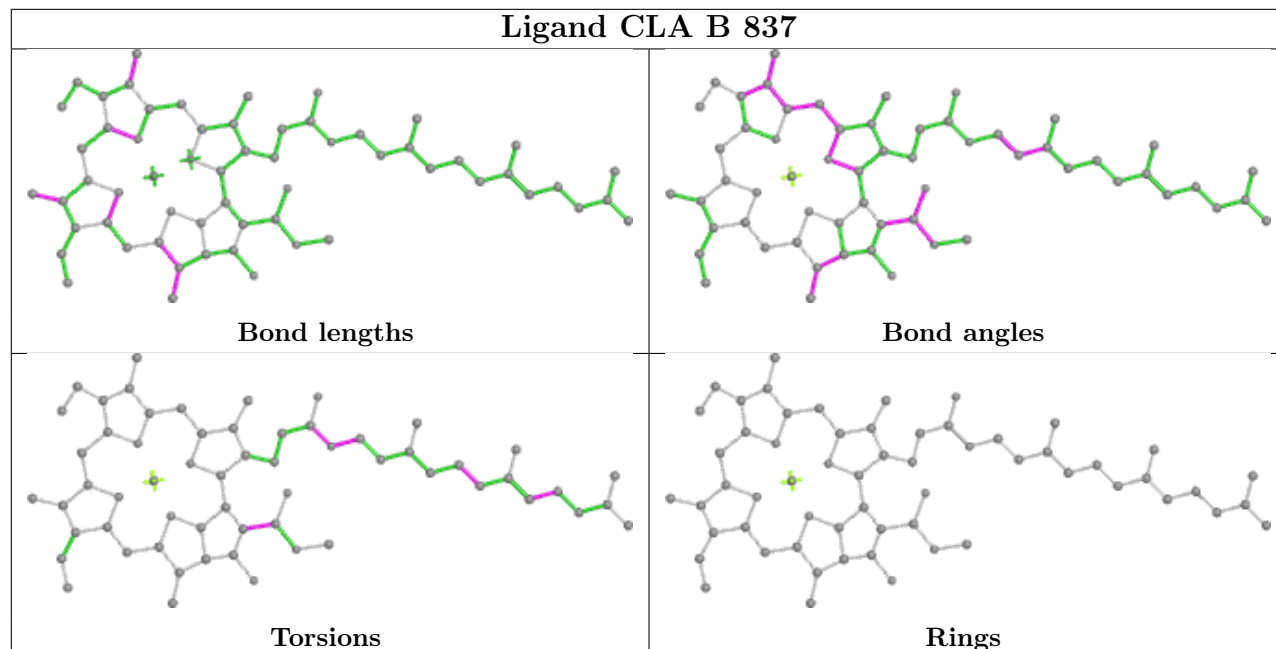
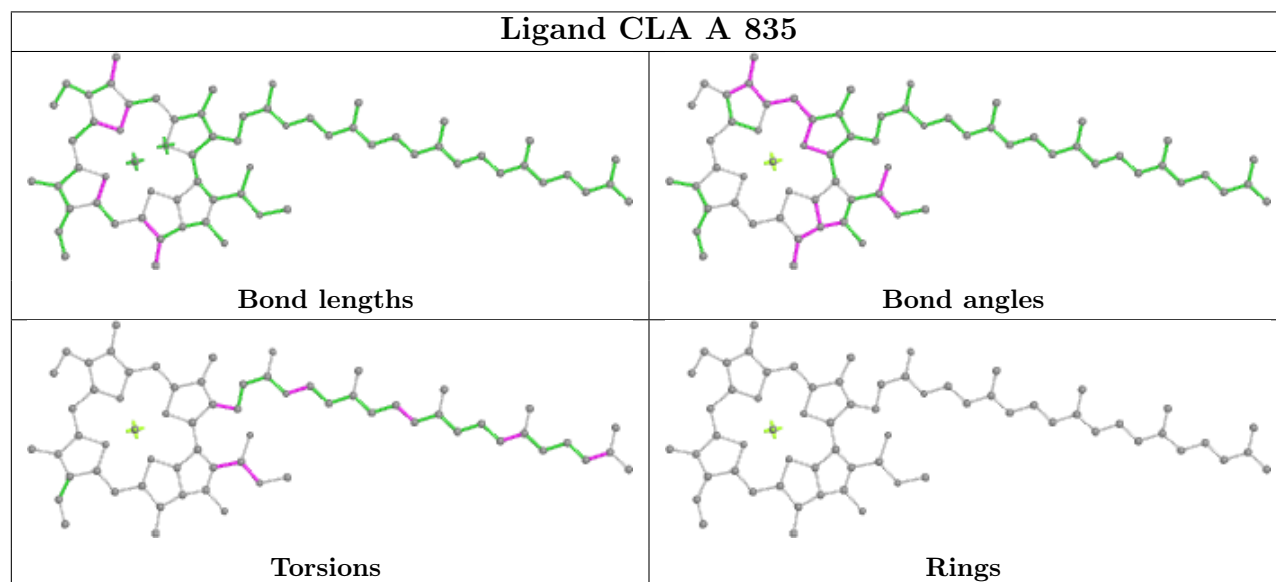


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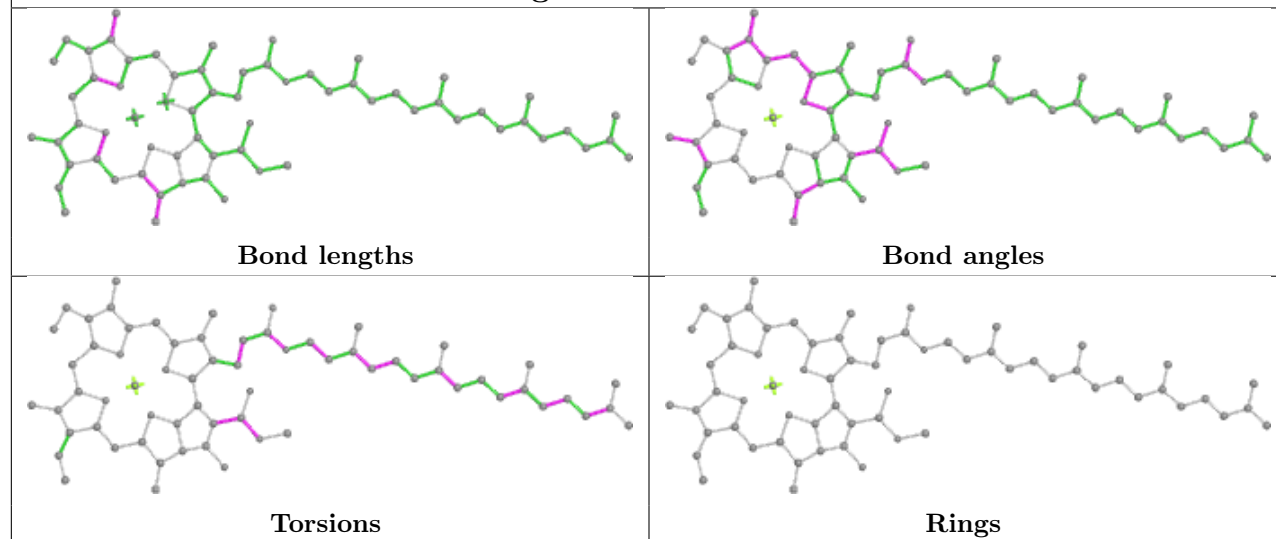


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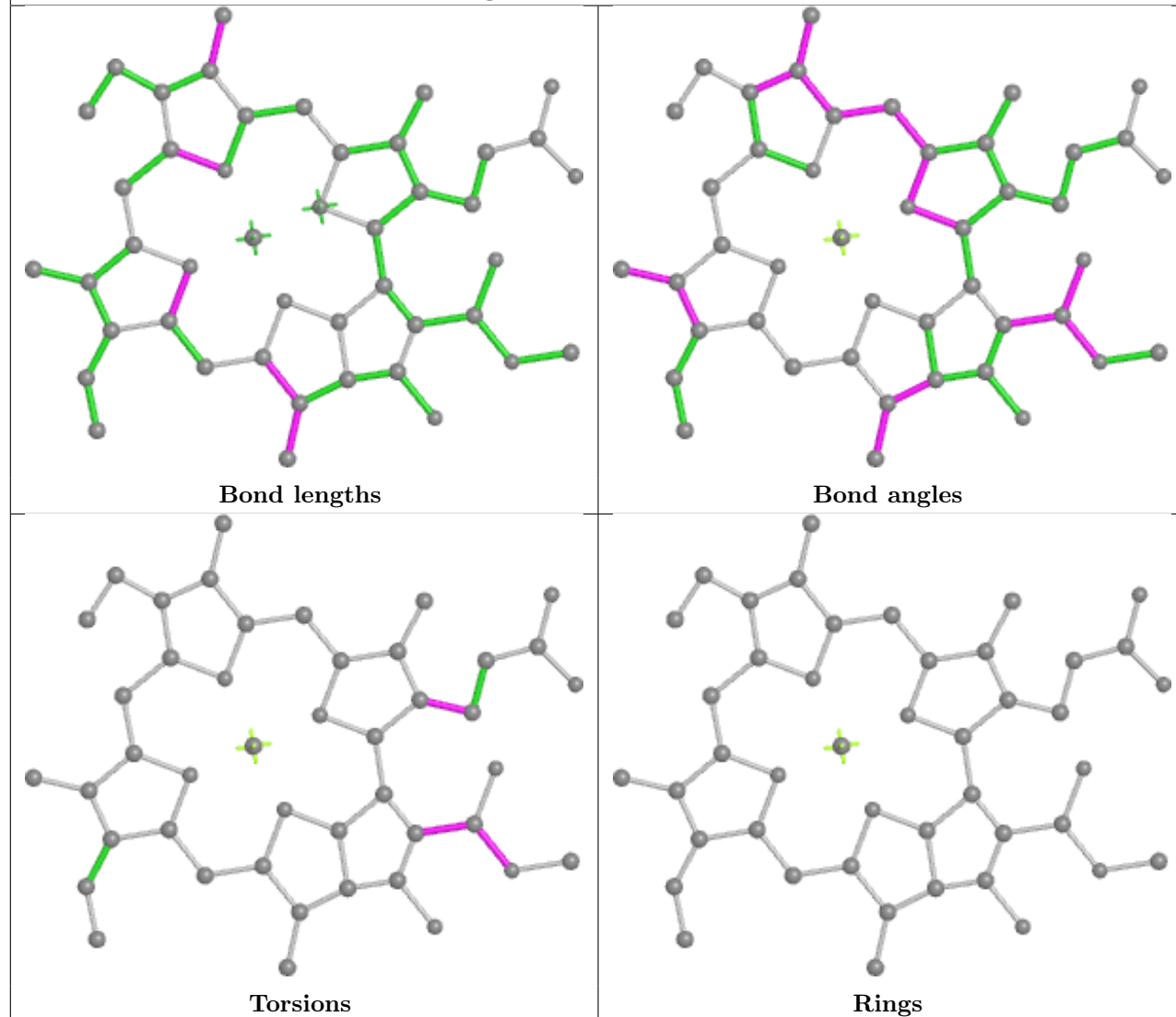


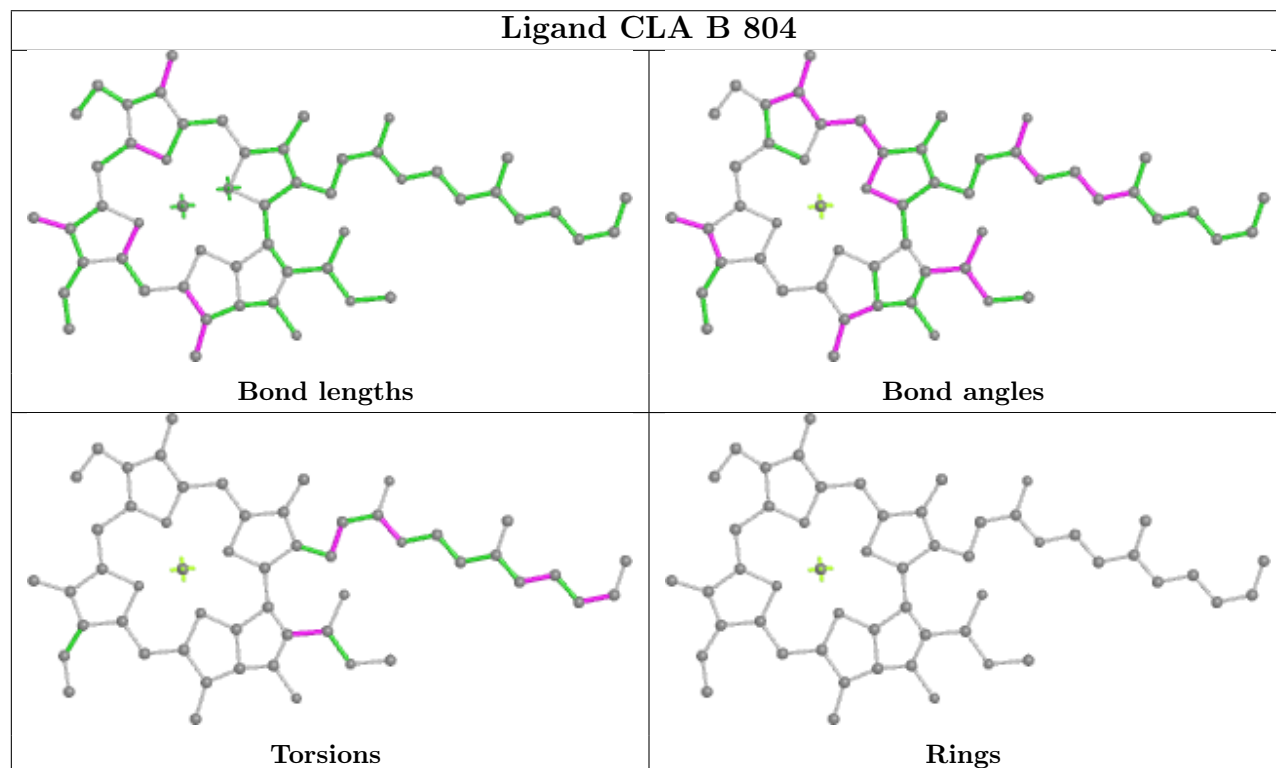
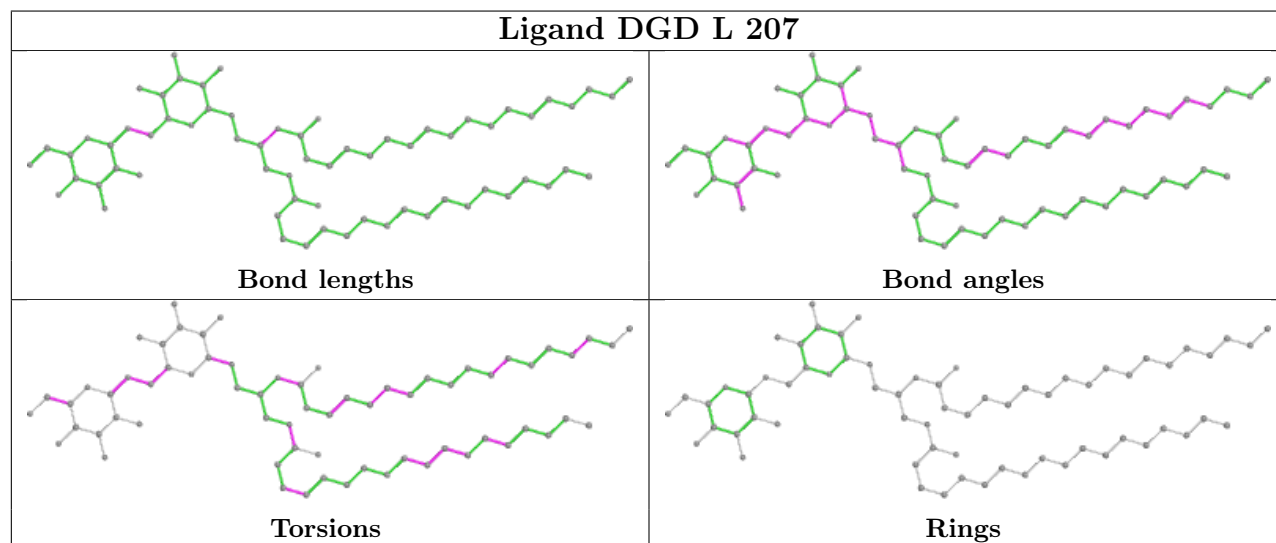
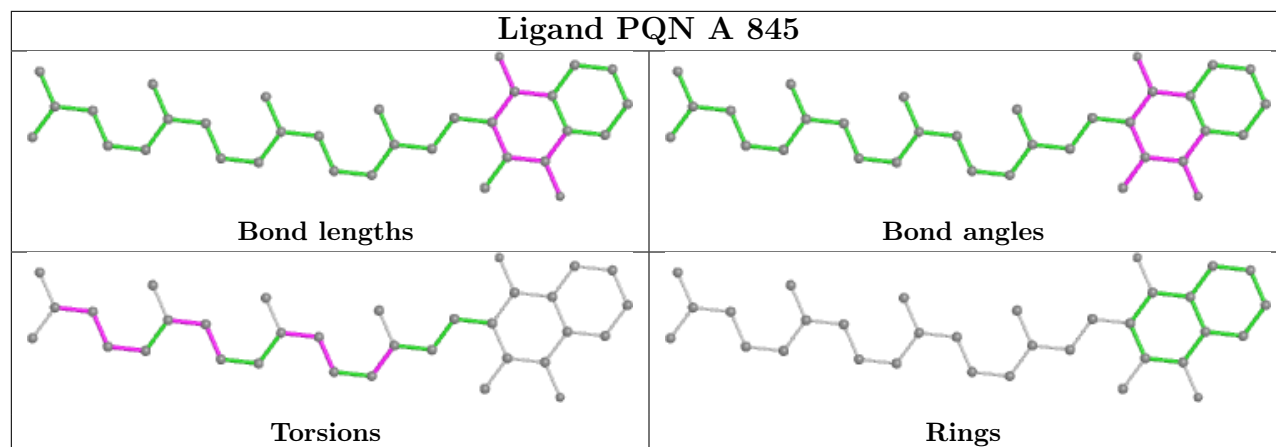
**Ligand BCR L 208****Ligand CLA B 837****Ligand CLA A 835**

## Ligand CLA A 857

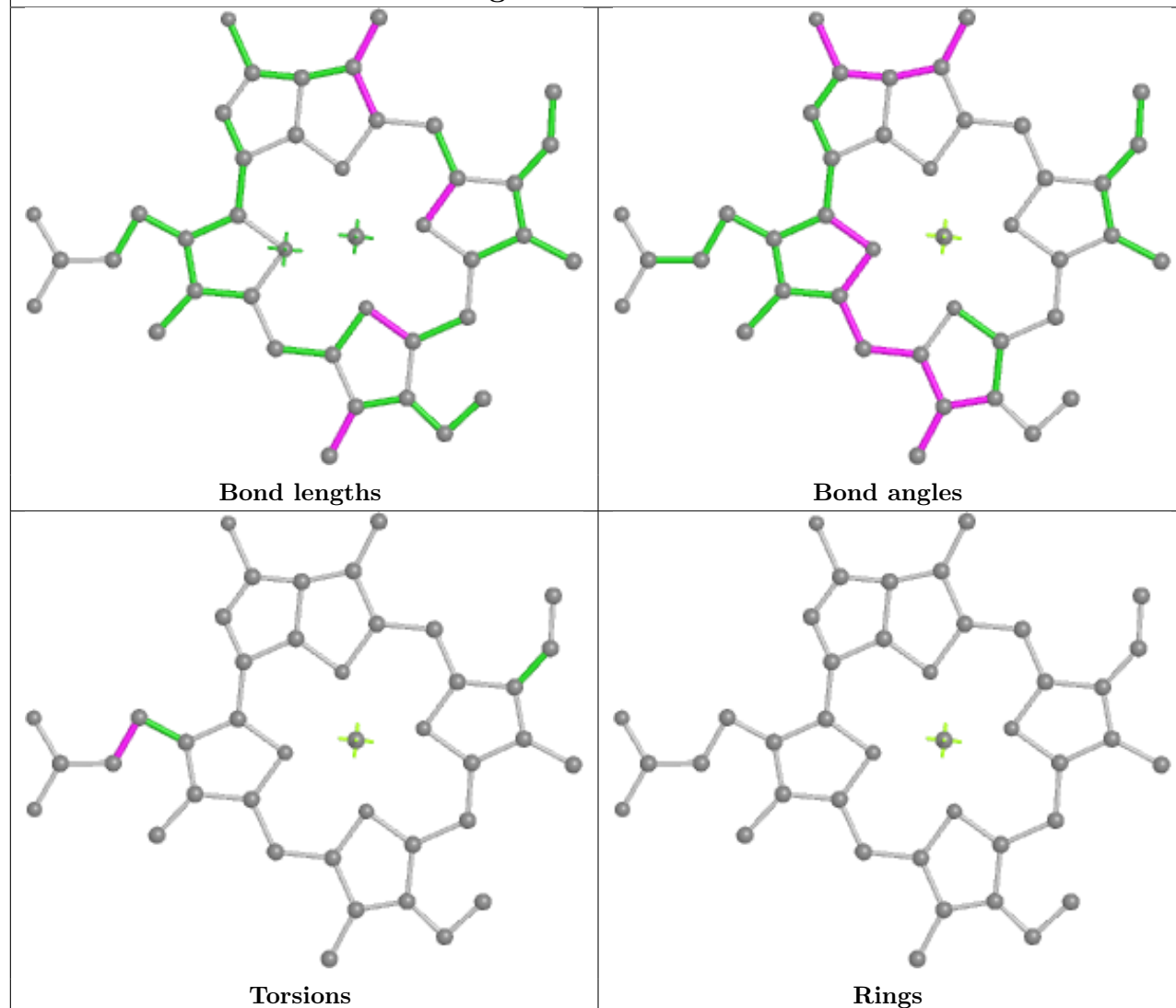


## Ligand CLA X 1701

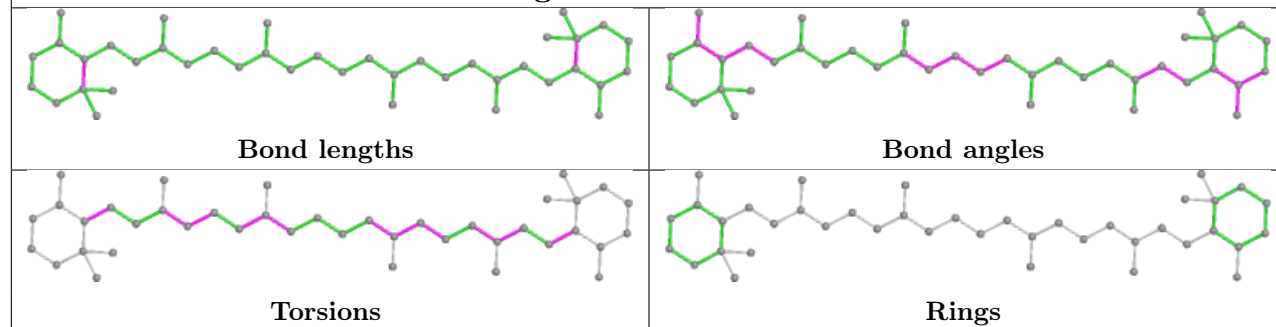


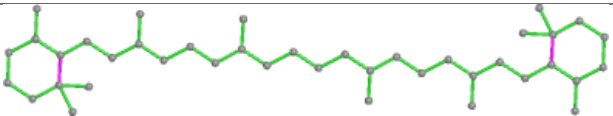
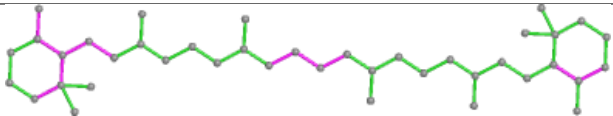
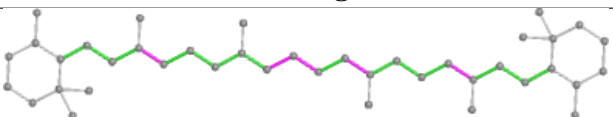
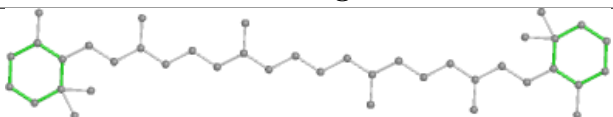


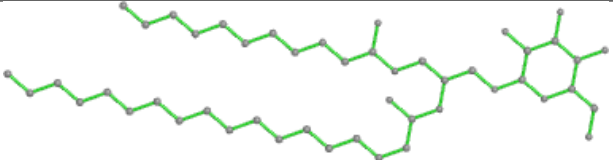
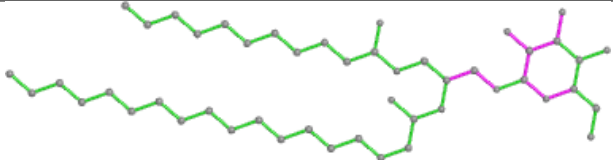
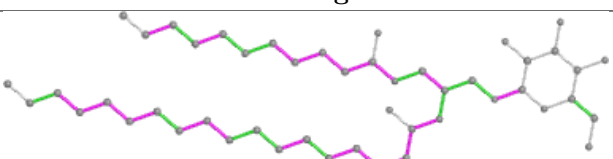
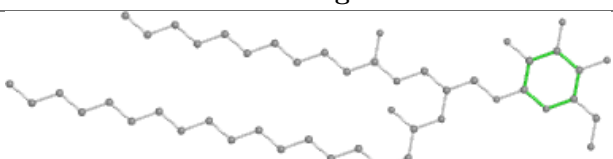
## Ligand CLA K 101

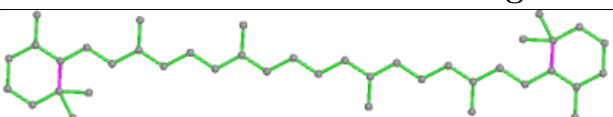
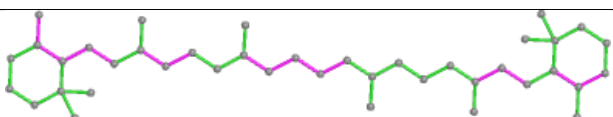
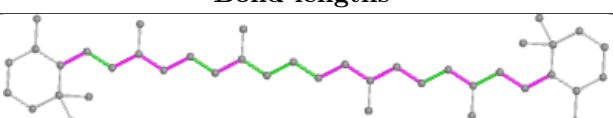
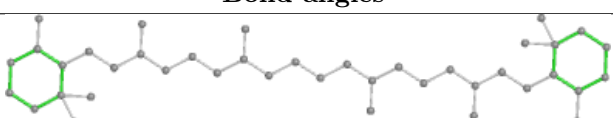


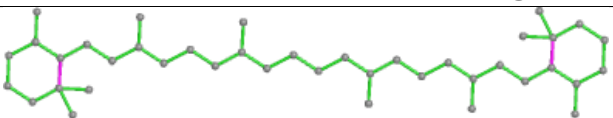
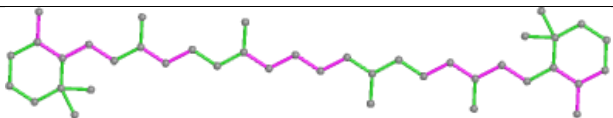
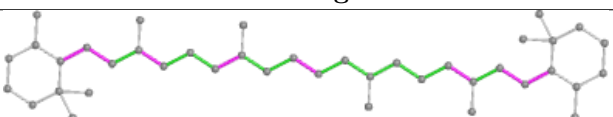
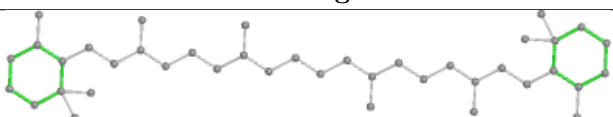
## Ligand BCR J 103

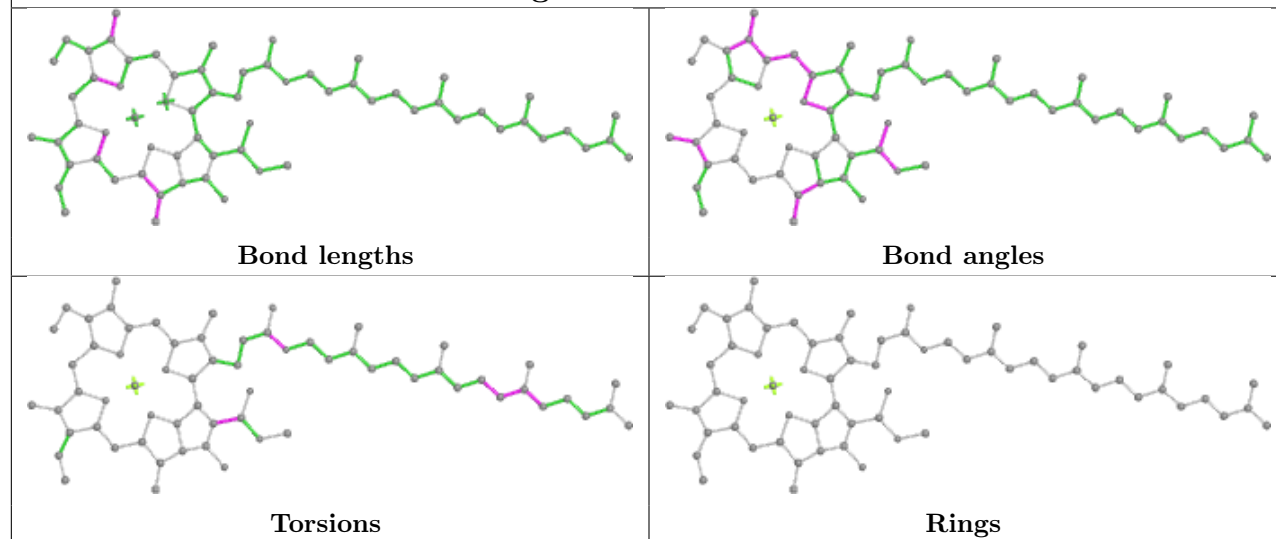
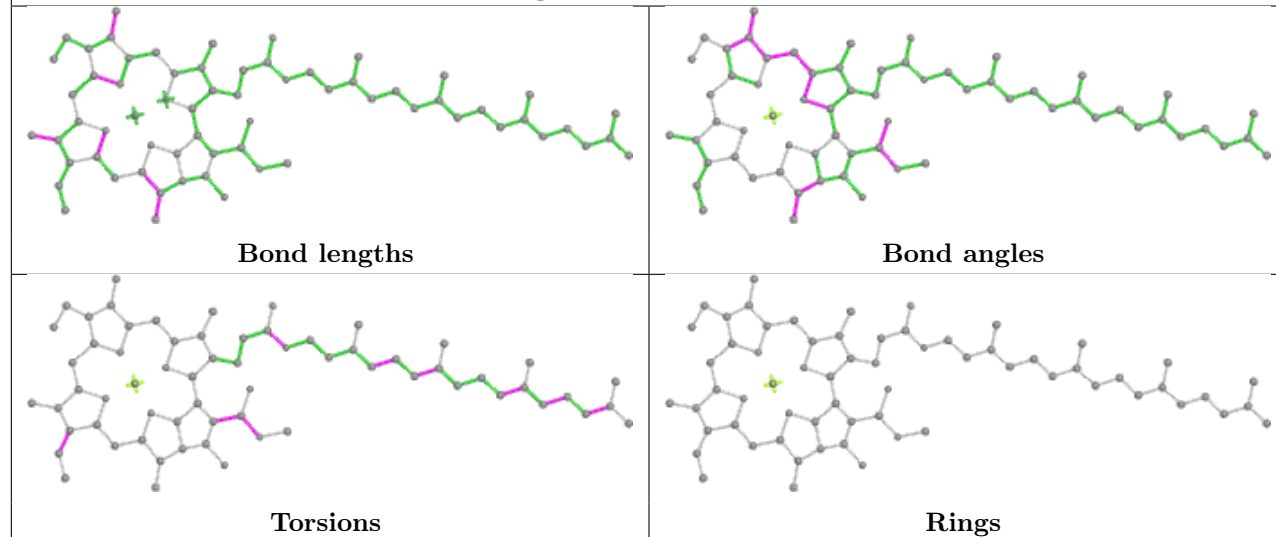


Ligand BCR B 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

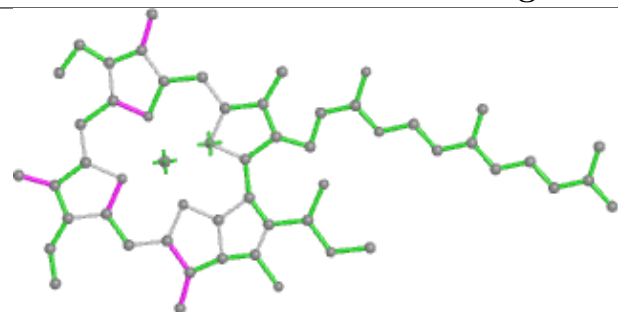
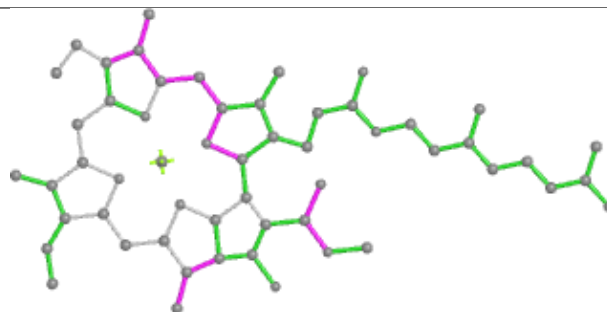
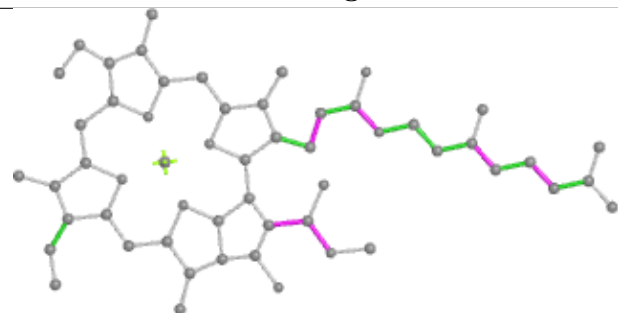
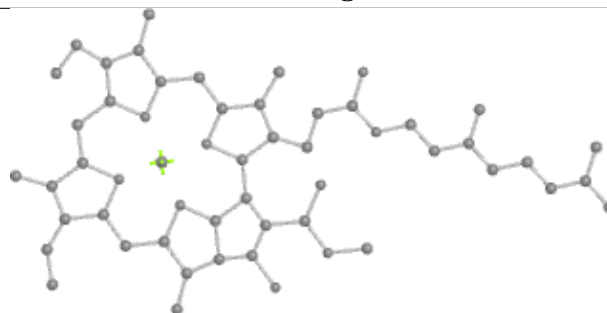
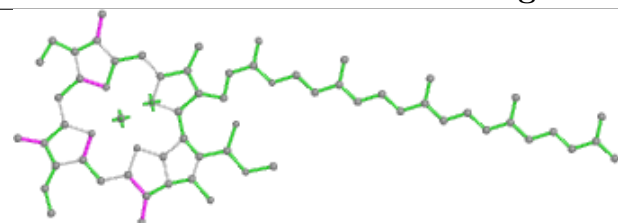
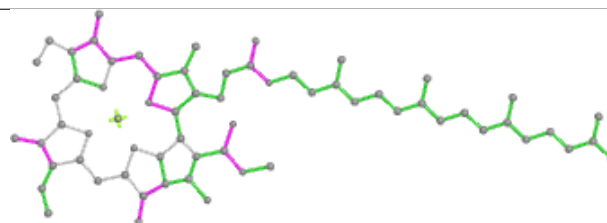
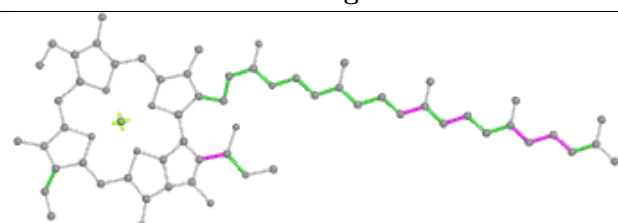
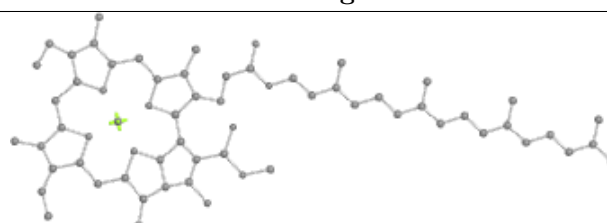
Ligand LMG A 853	
	
Bond lengths	Bond angles
	
Torsions	Rings

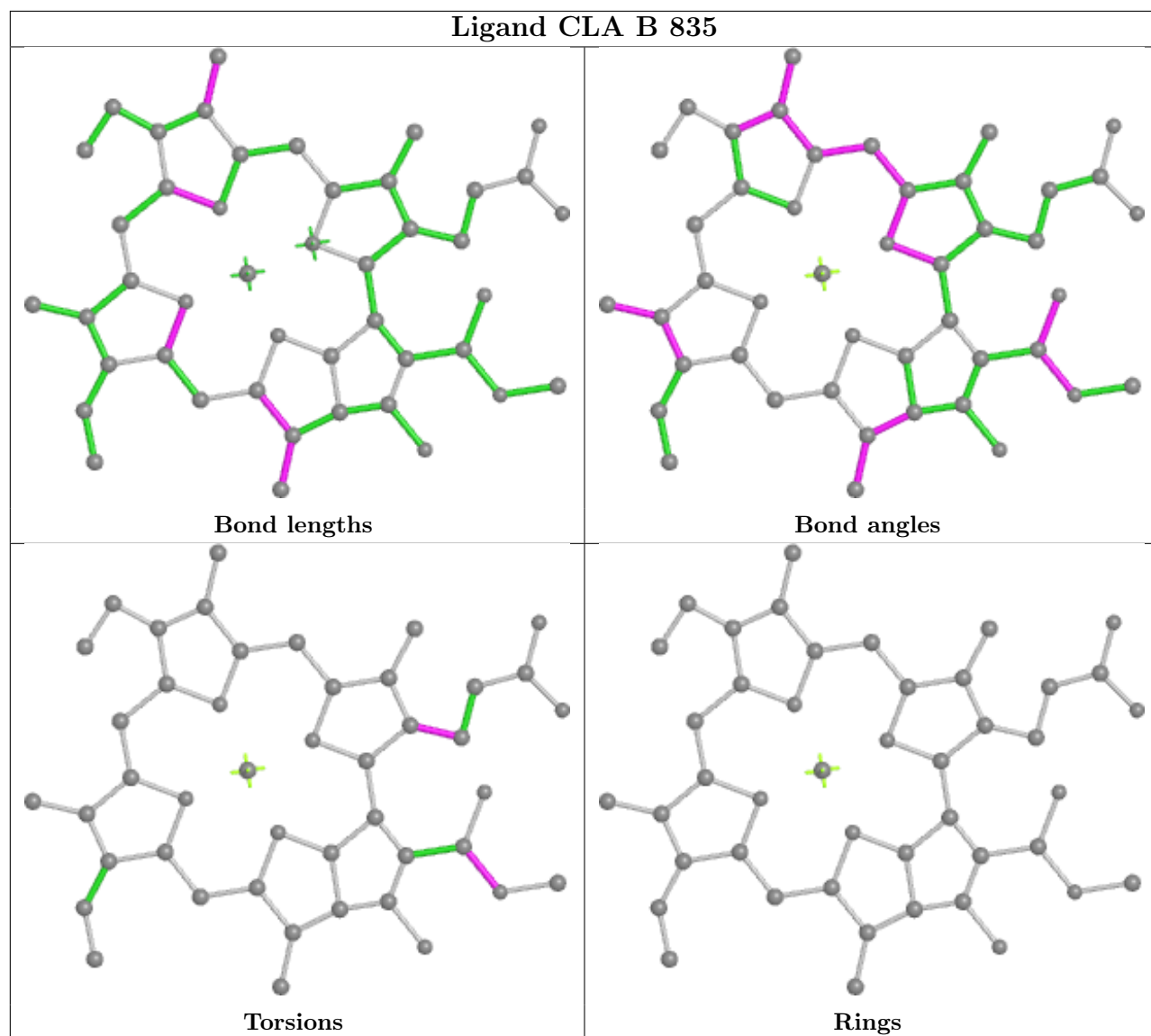
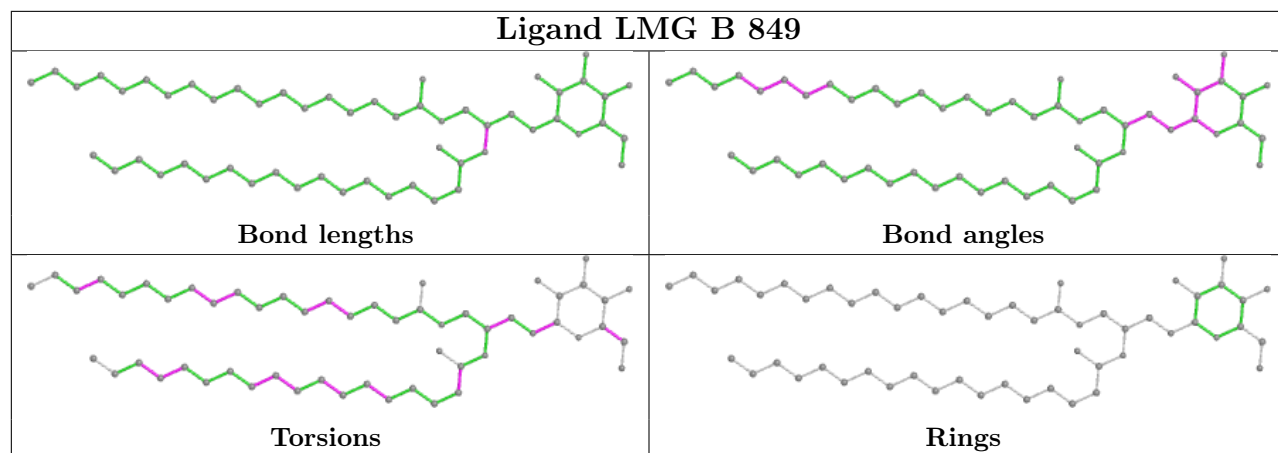
Ligand BCR A 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR J 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

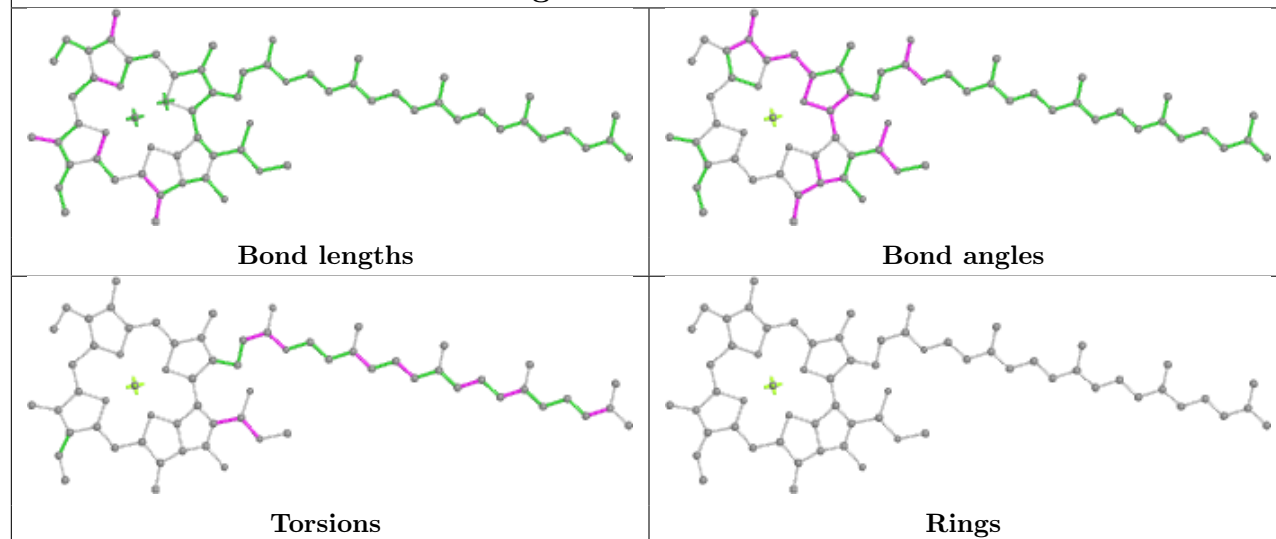
**Ligand CLA A 812****Ligand CLA A 829**



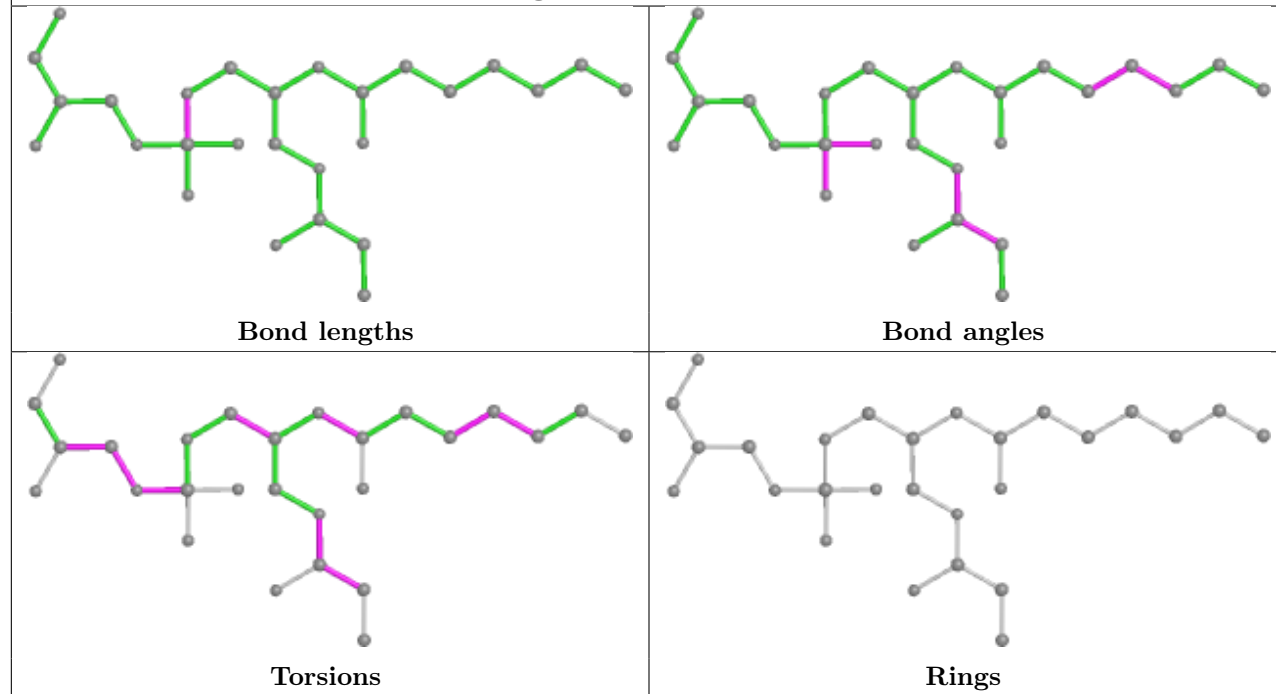
**Ligand CLA B 822****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 808****Bond lengths****Bond angles****Torsions****Rings**



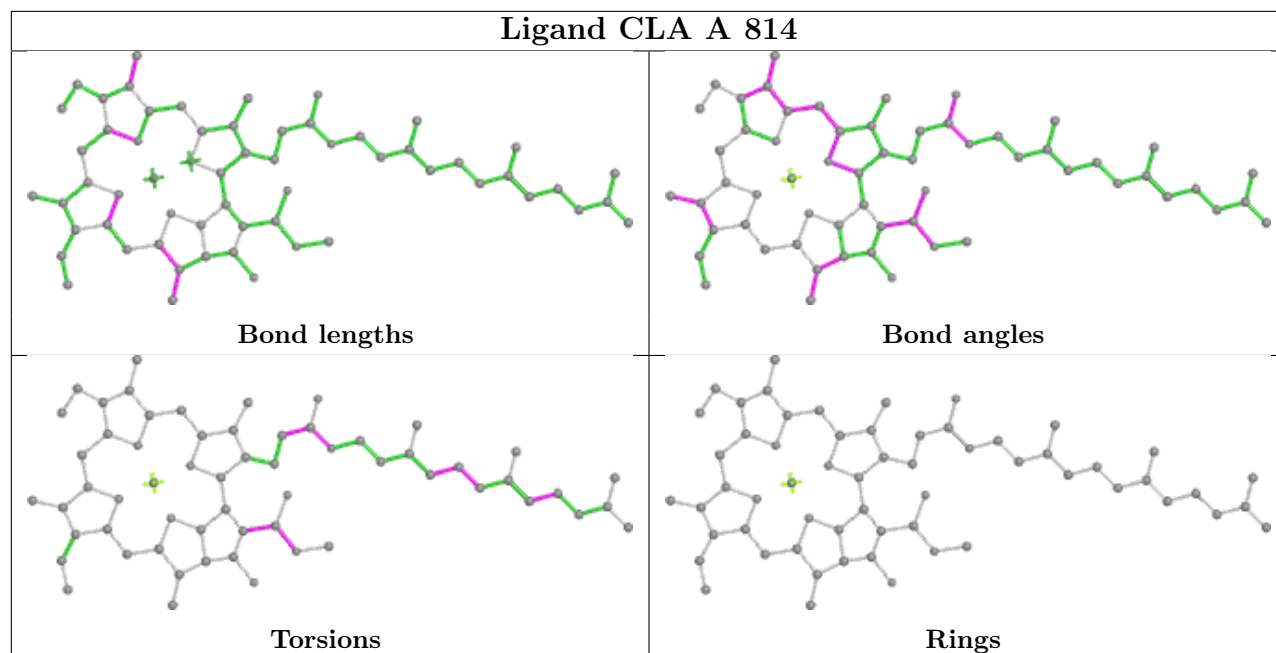
## Ligand CLA B 810



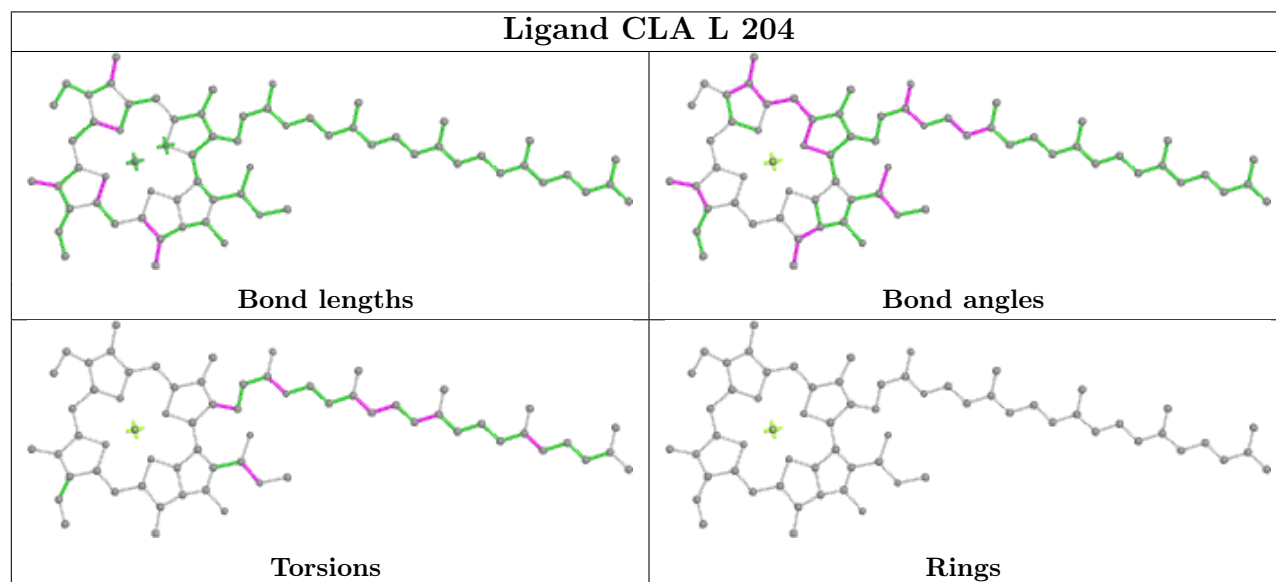
## Ligand LHG A 855



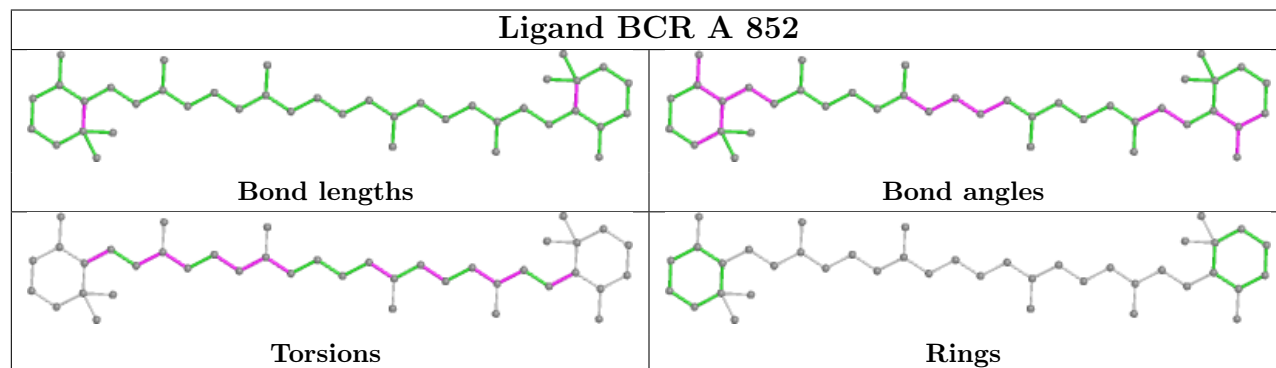
## Ligand CLA A 814

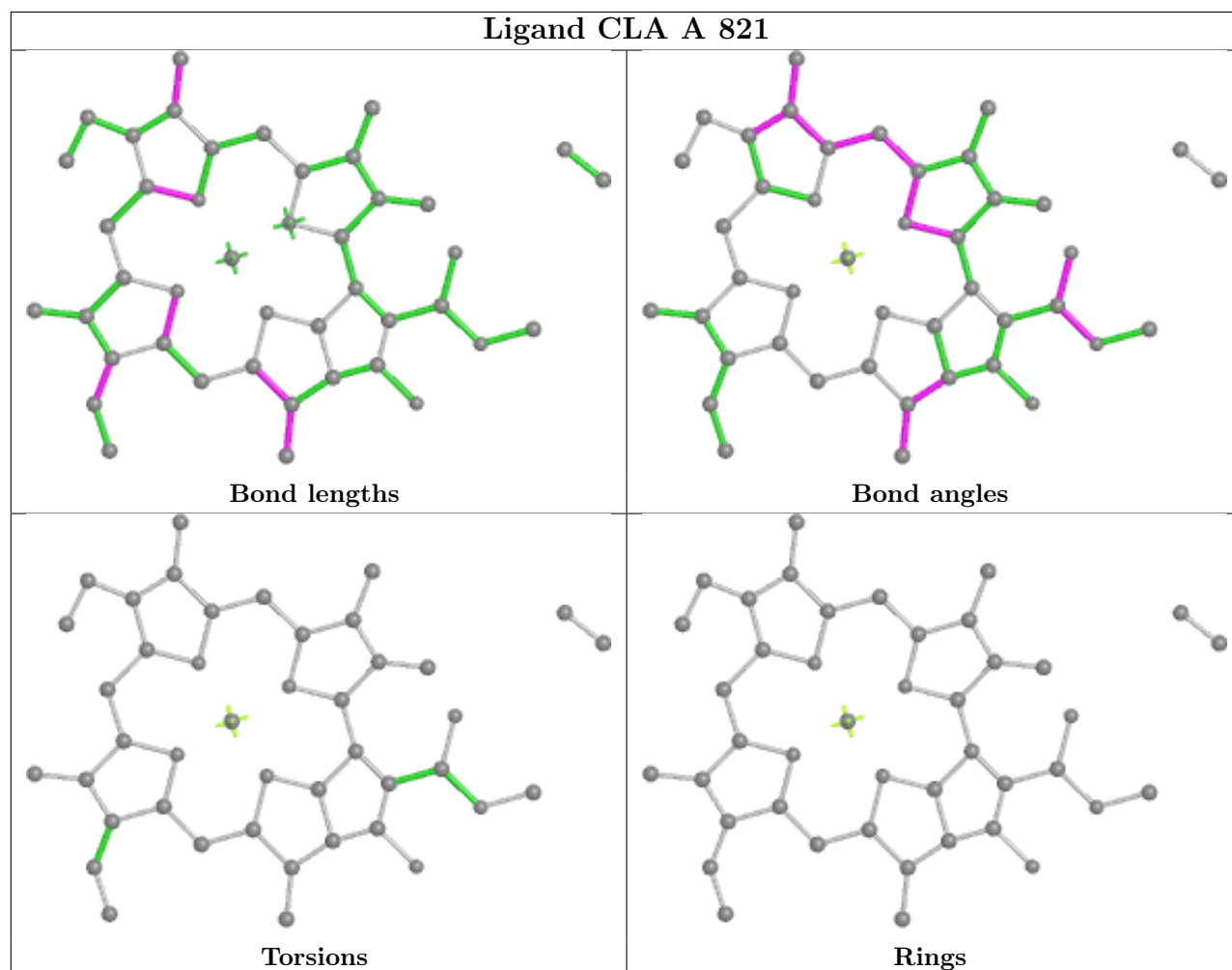
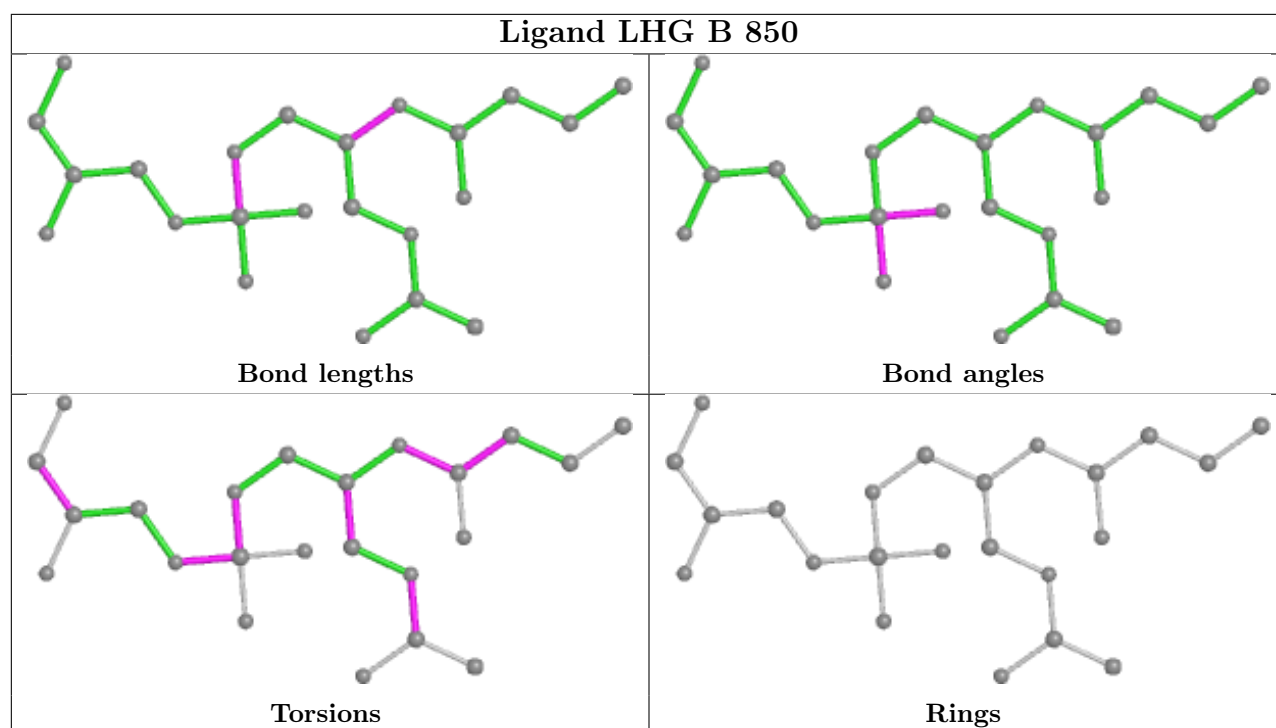


## Ligand CLA L 204

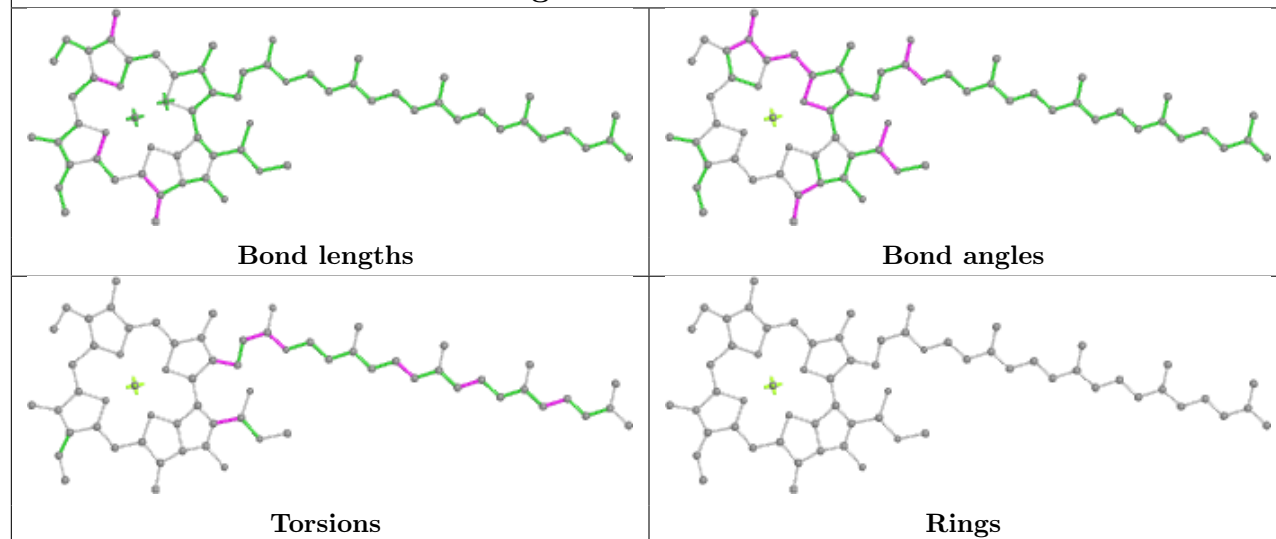


## Ligand BCR A 852

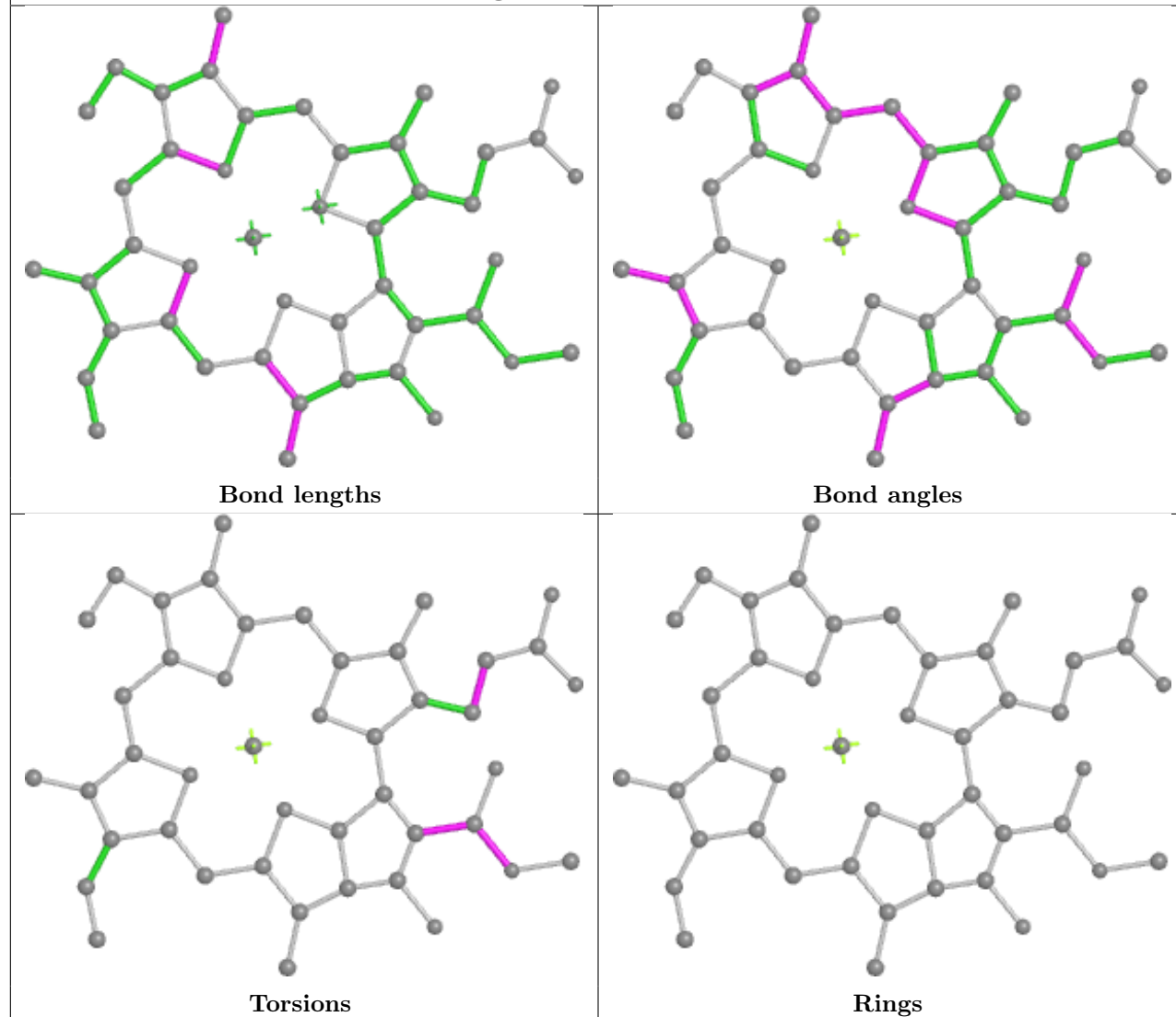




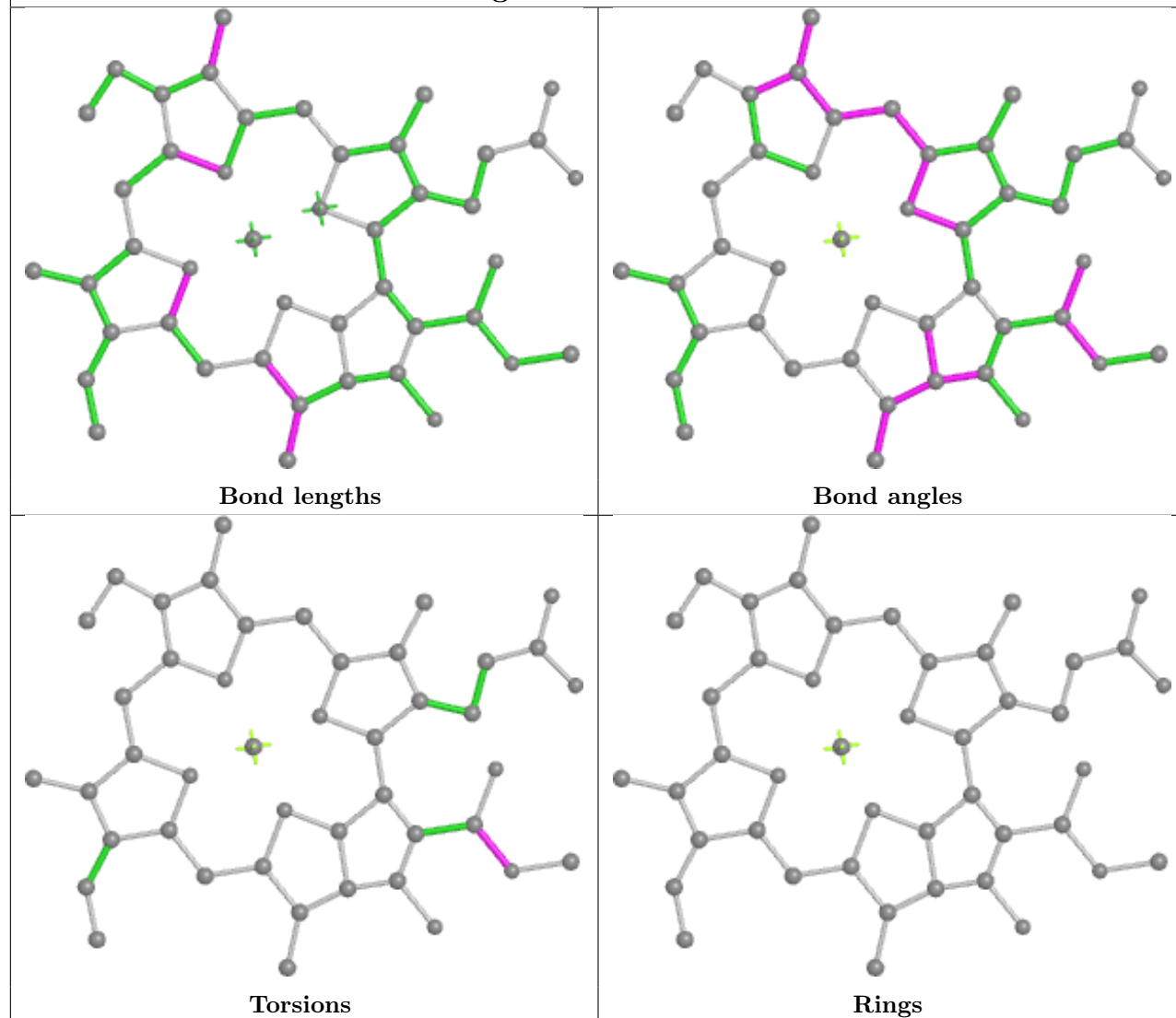
## Ligand CLA A 809



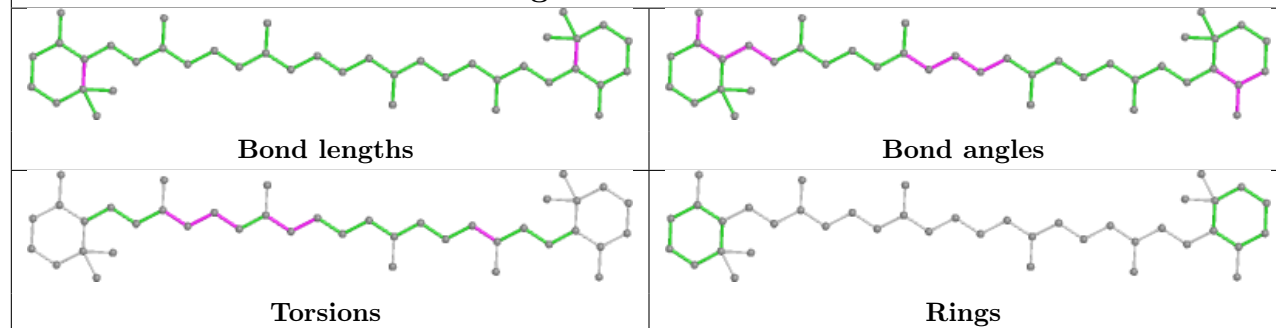
## Ligand CLA B 836

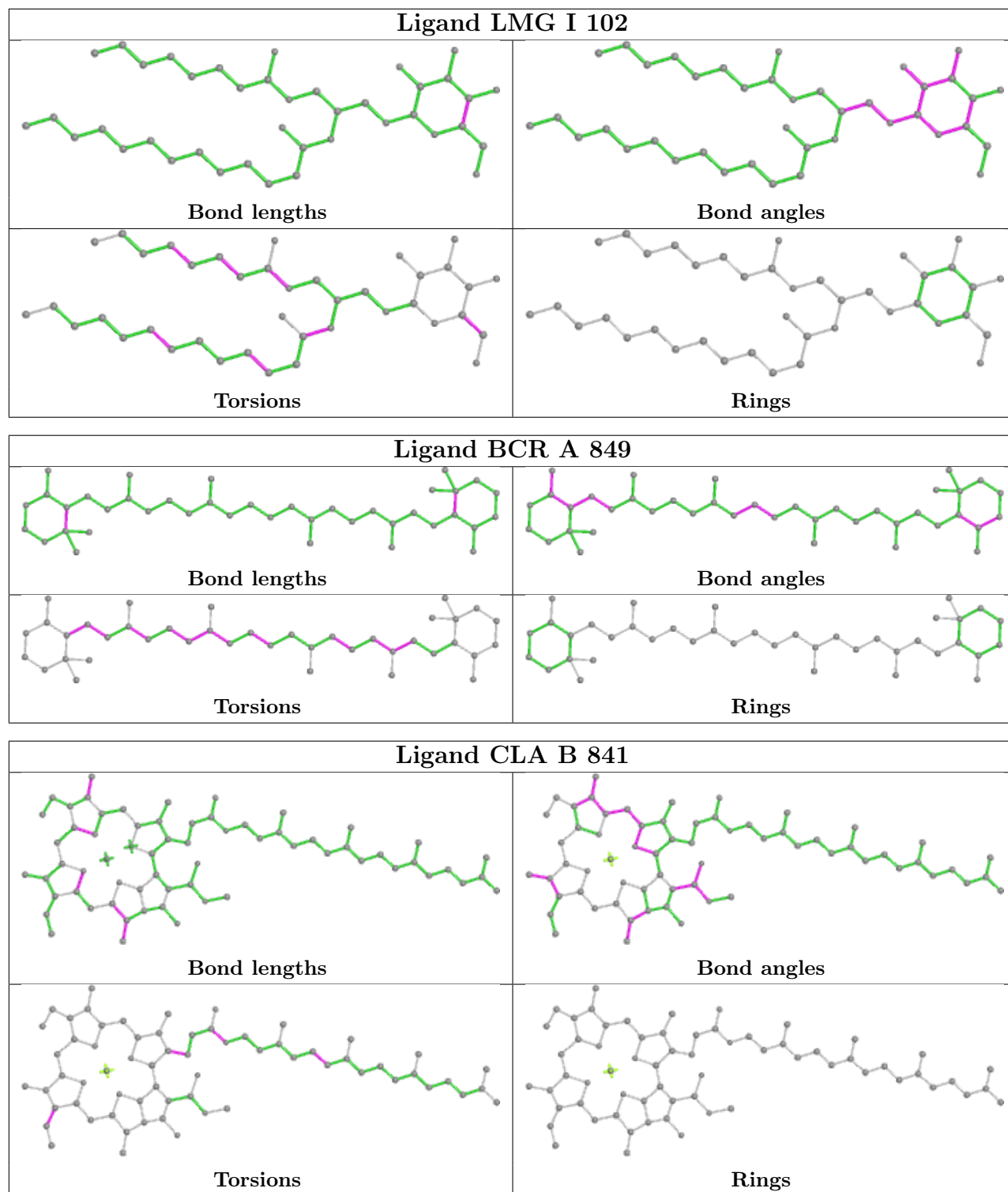


## Ligand CLA F 202

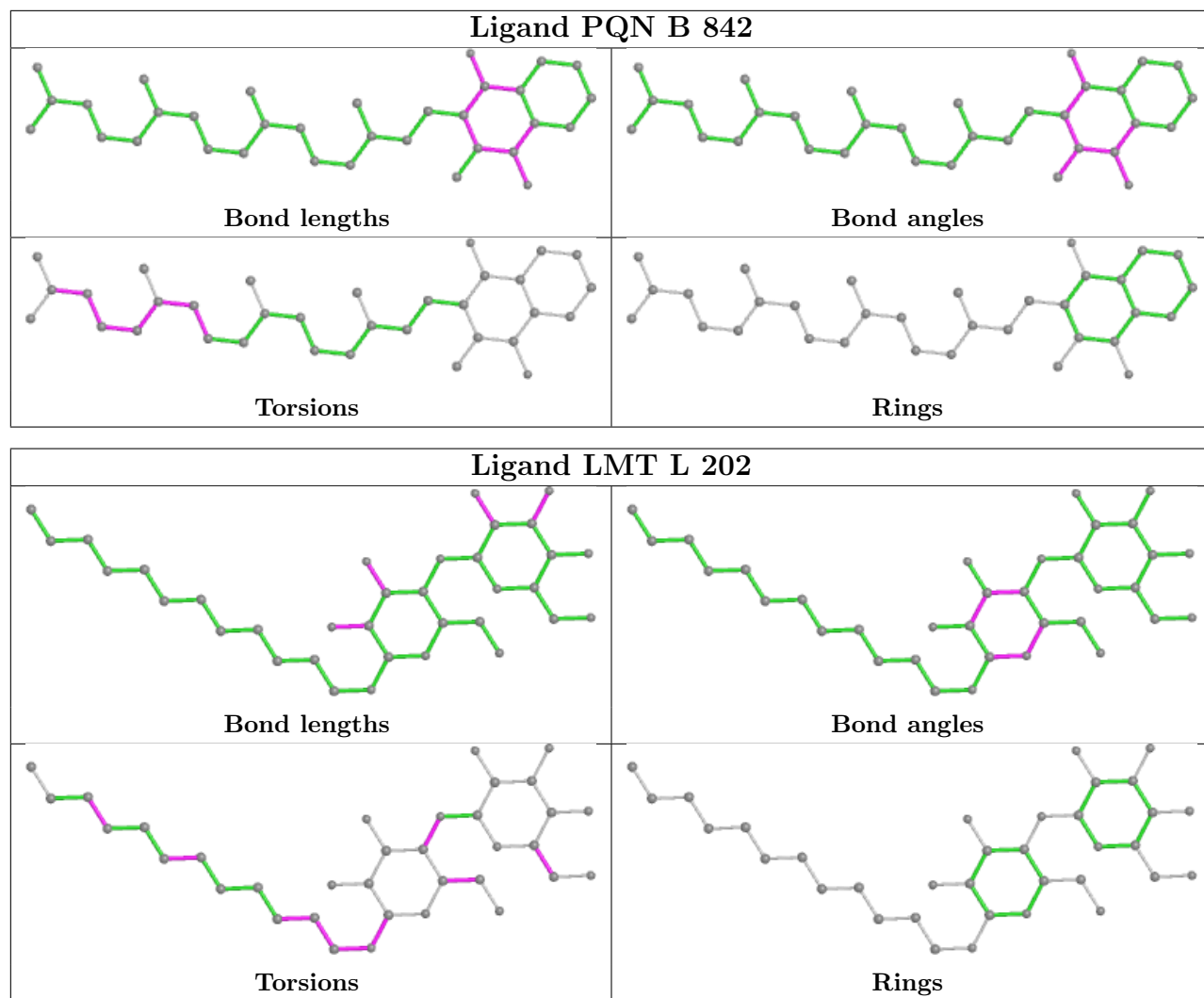


## Ligand BCR B 845

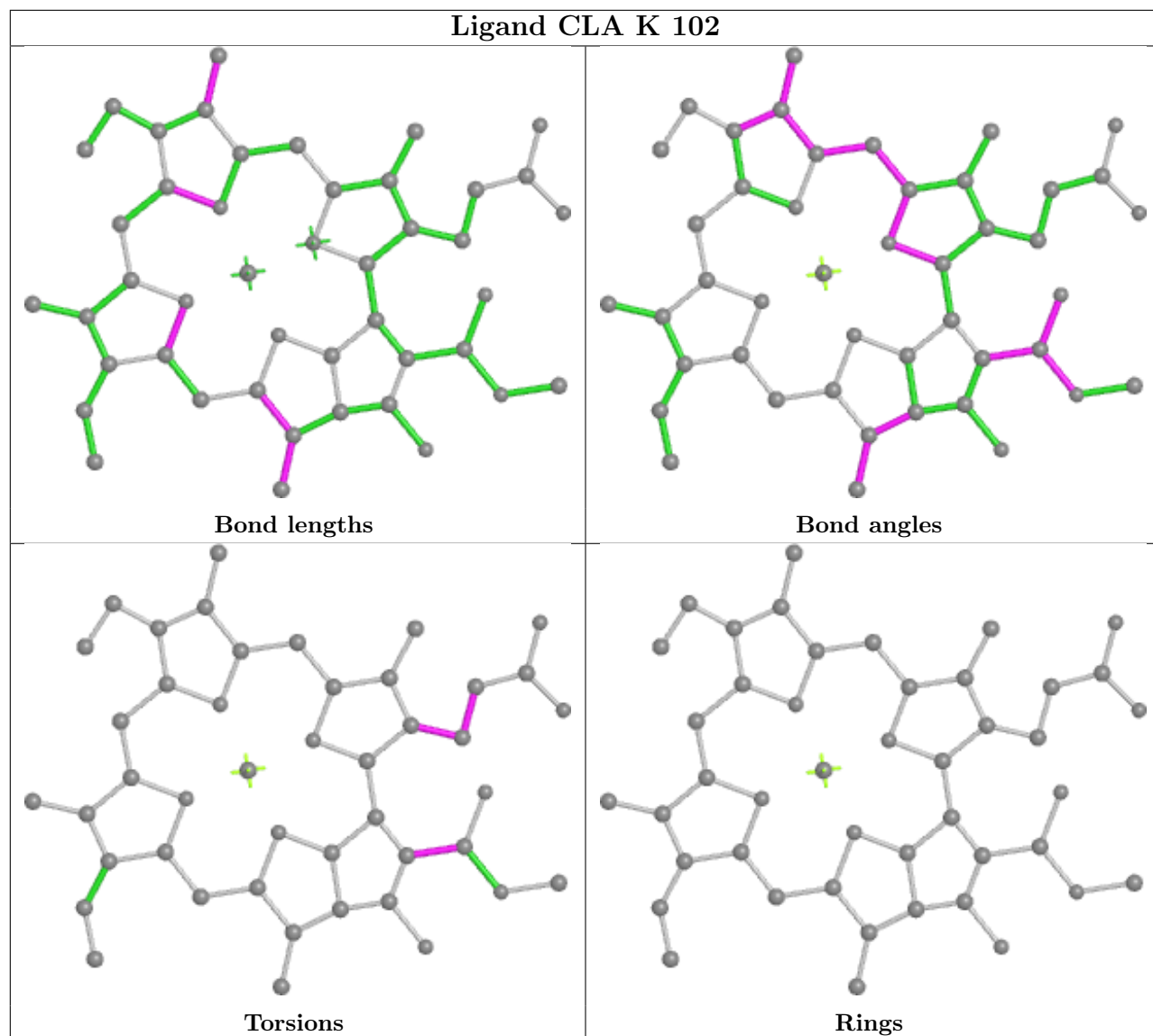


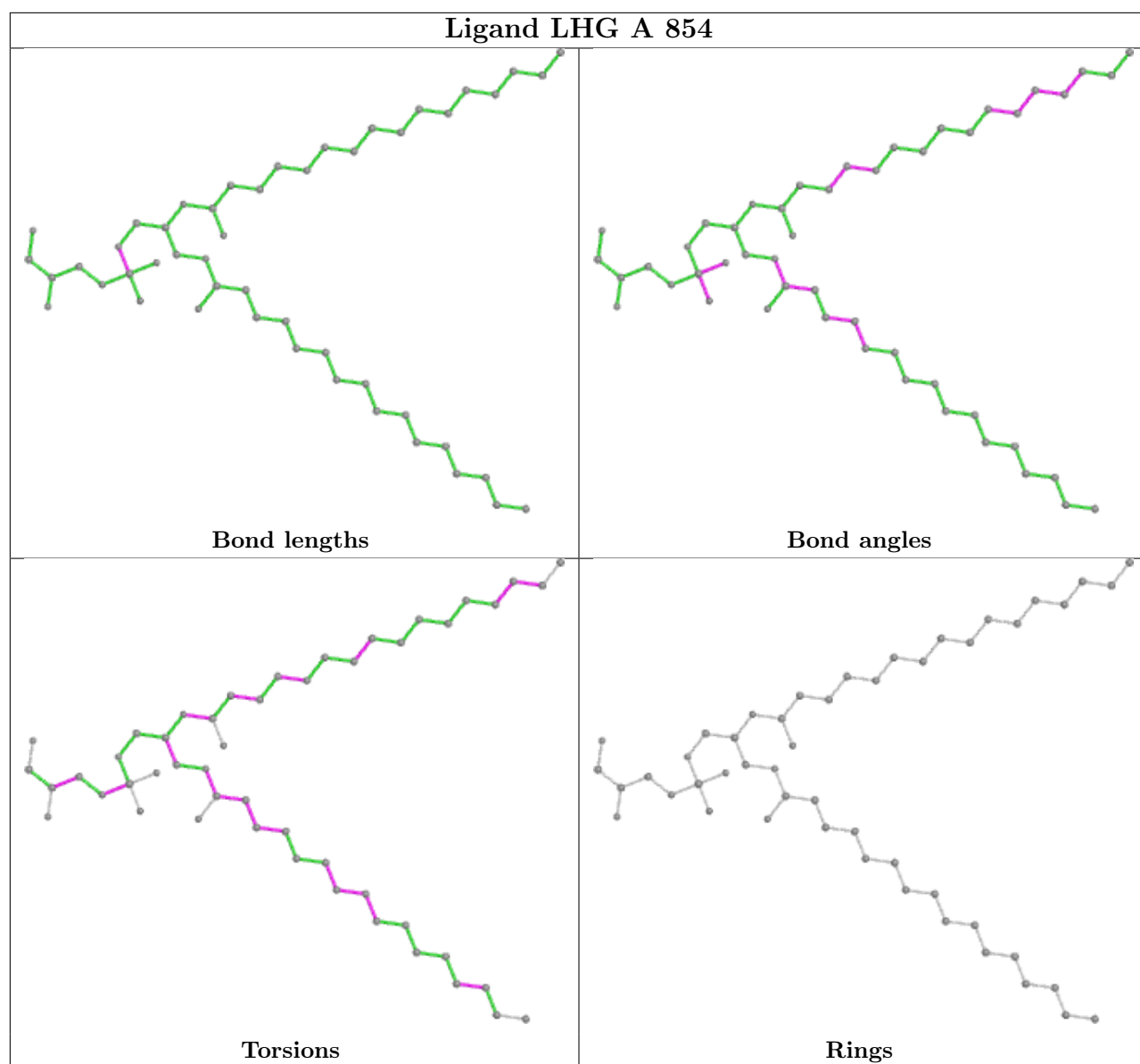




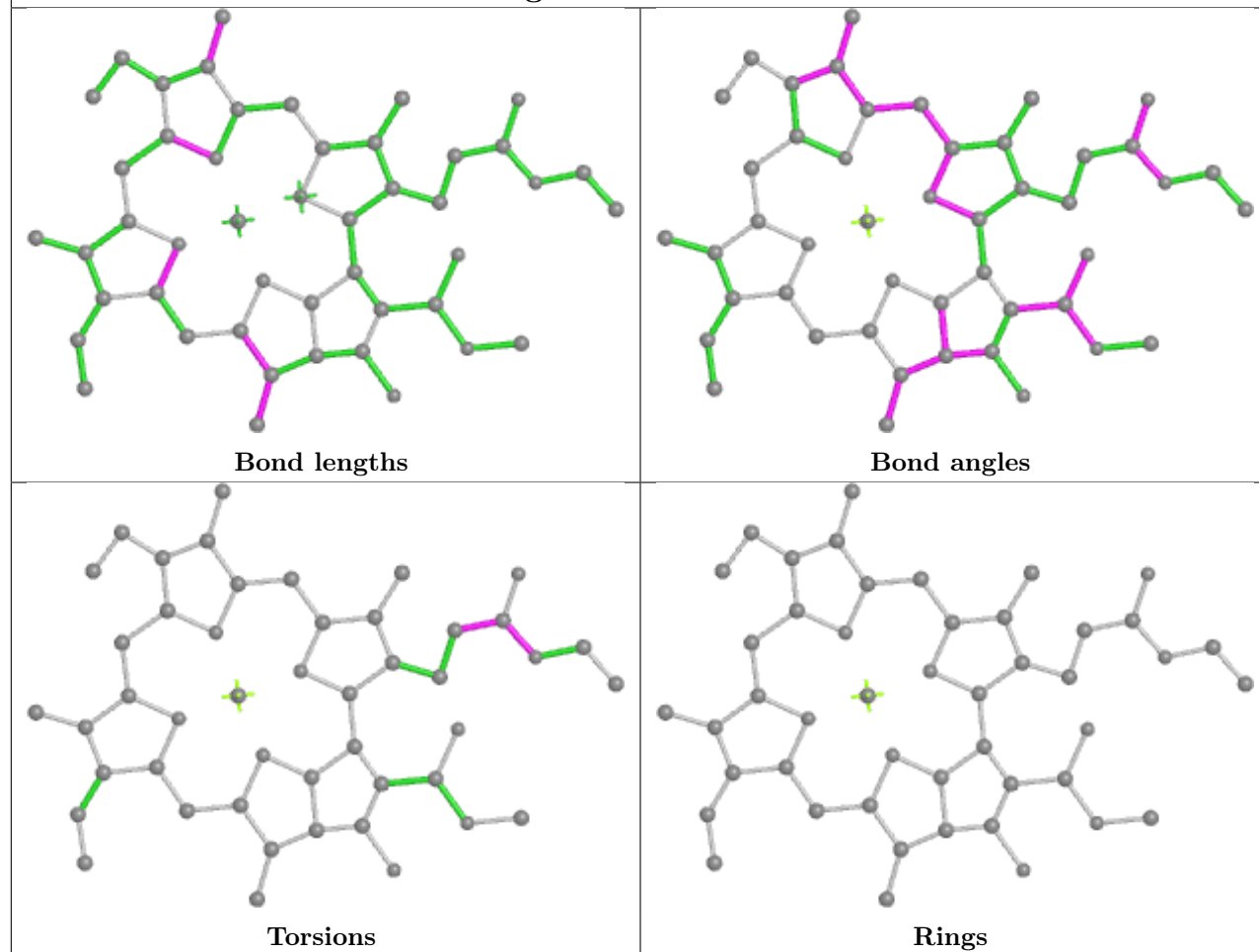


## Ligand CLA K 102

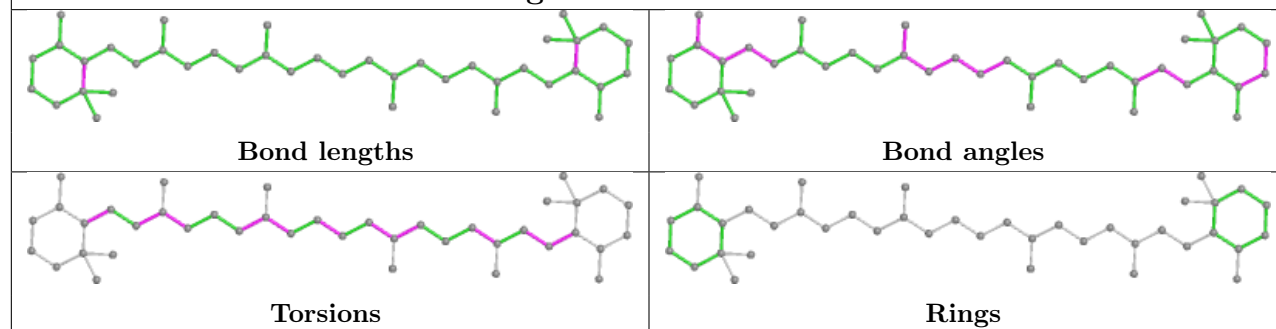




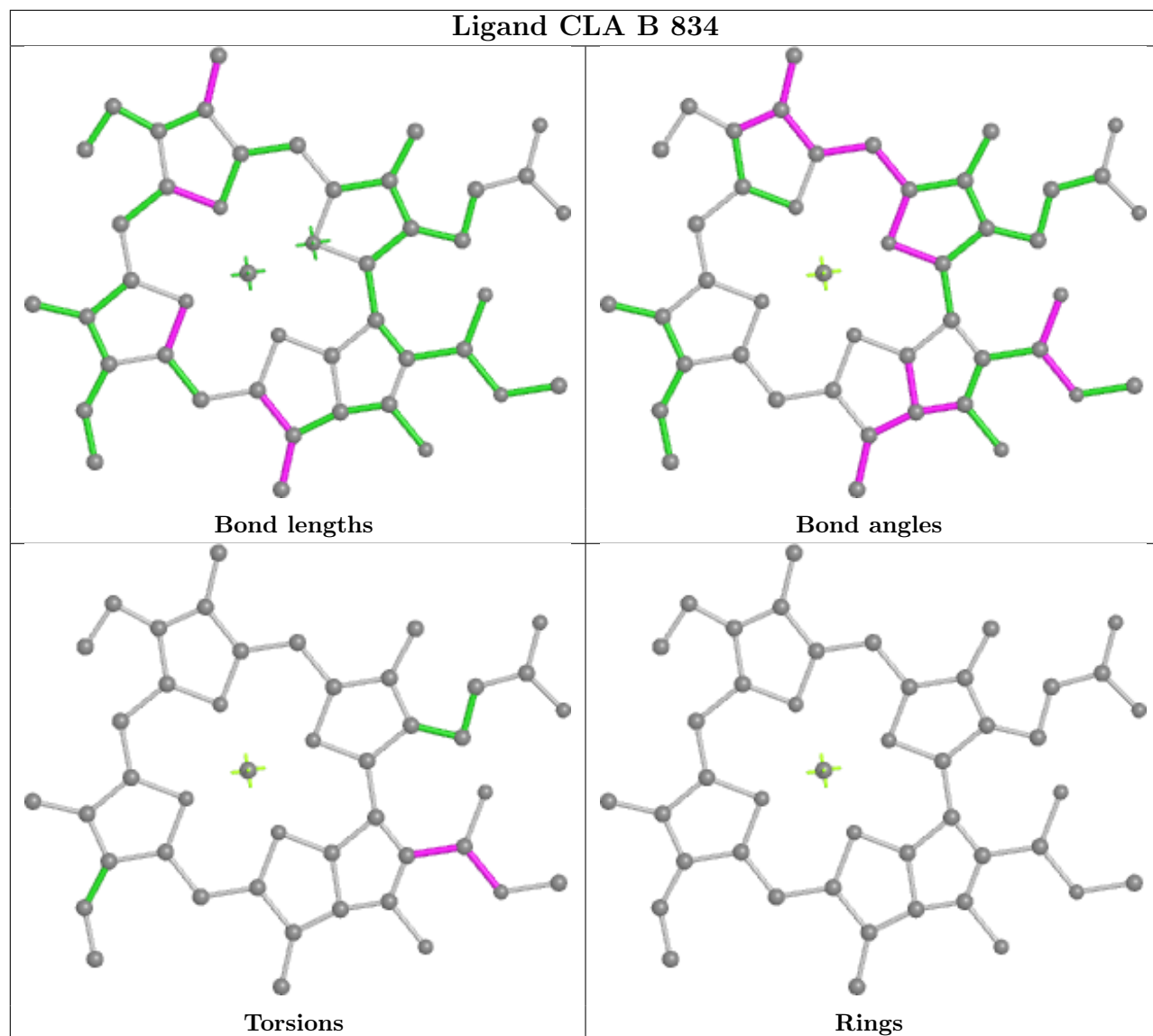
## Ligand CLA B 839



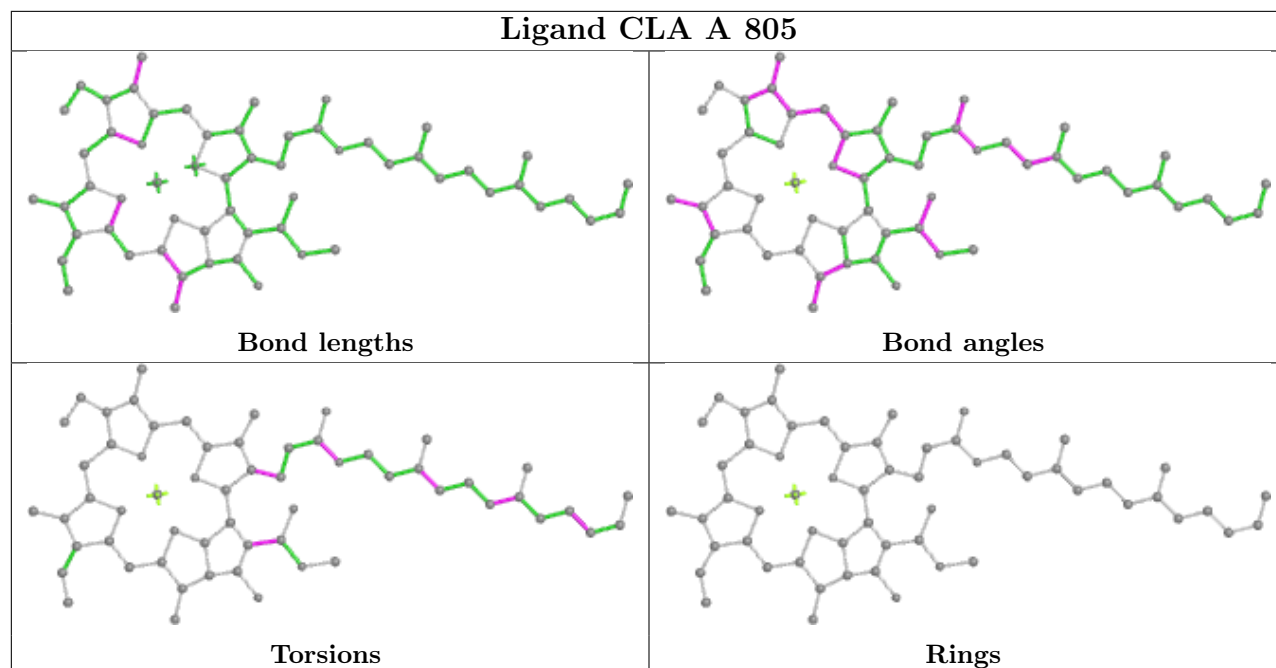
## Ligand BCR M 103



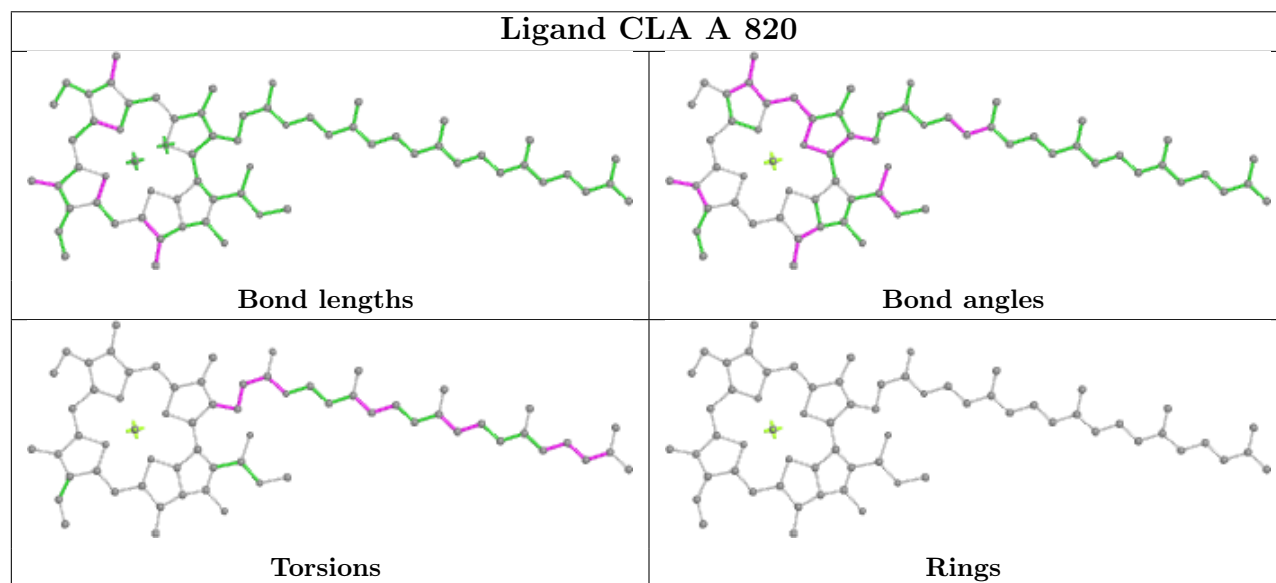
## Ligand CLA B 834



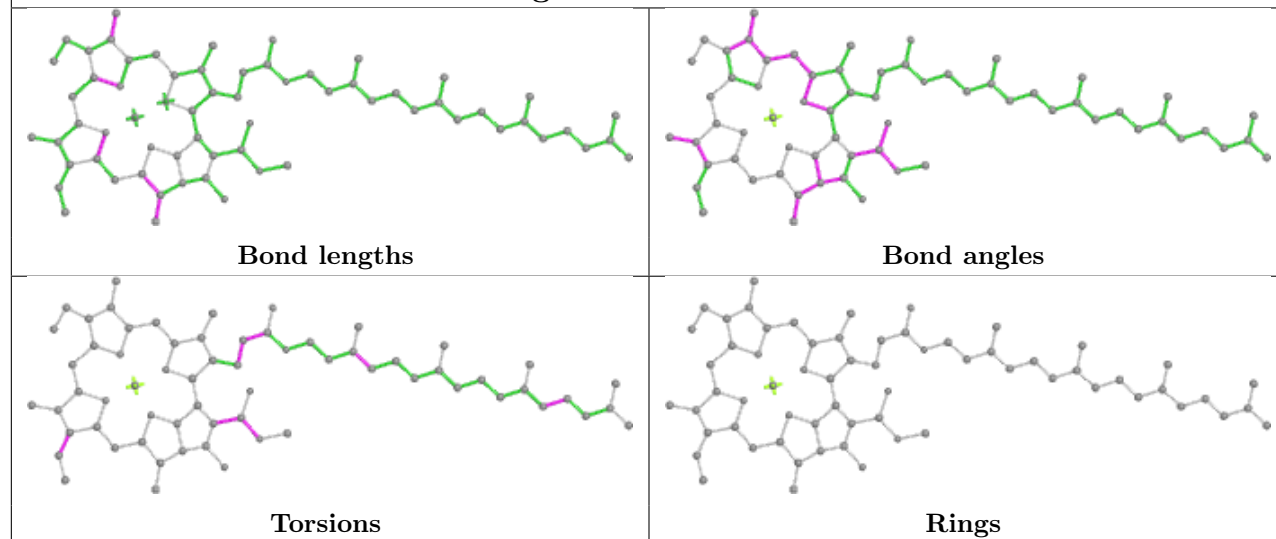
## Ligand CLA A 805



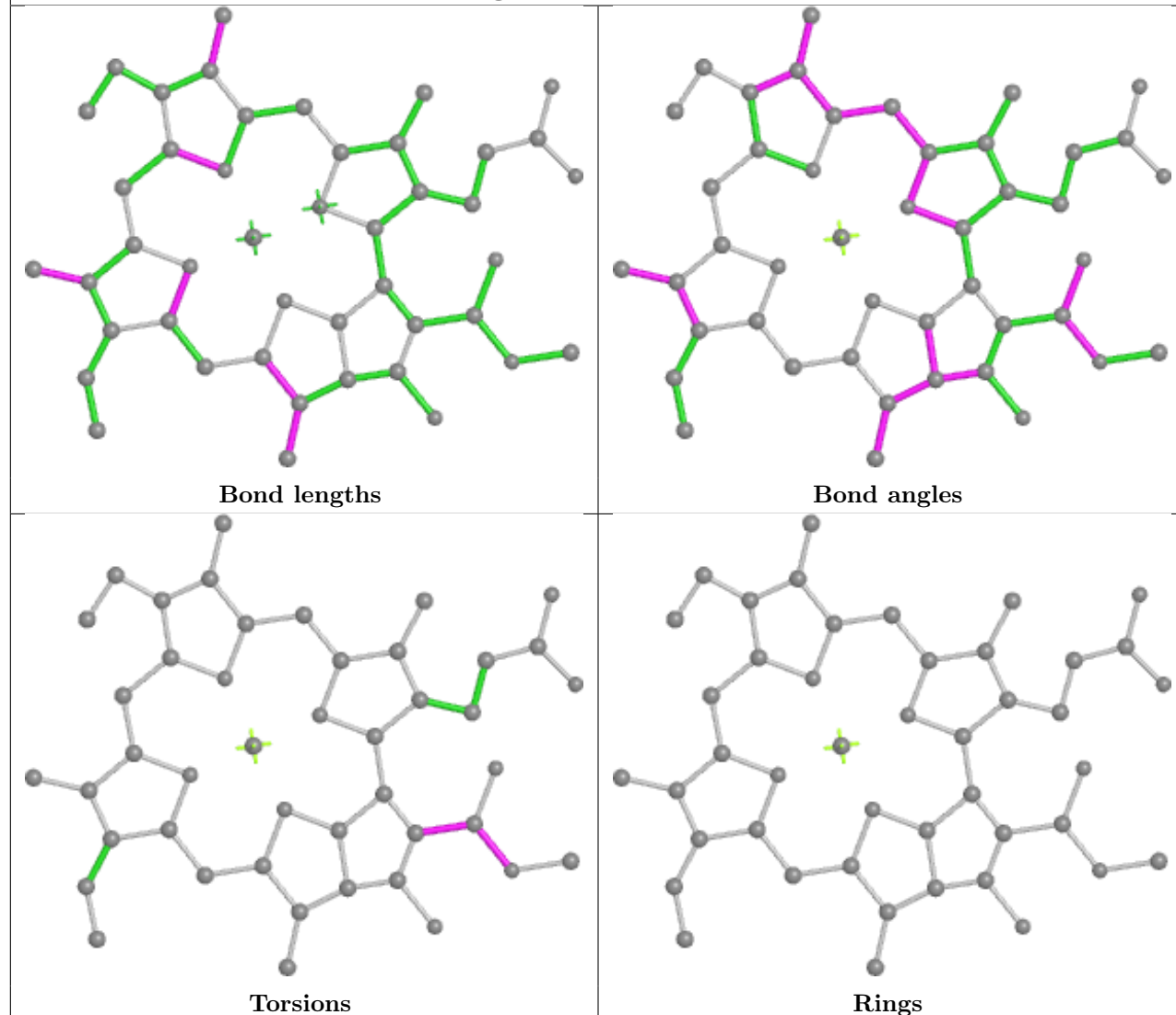
## Ligand CLA A 820

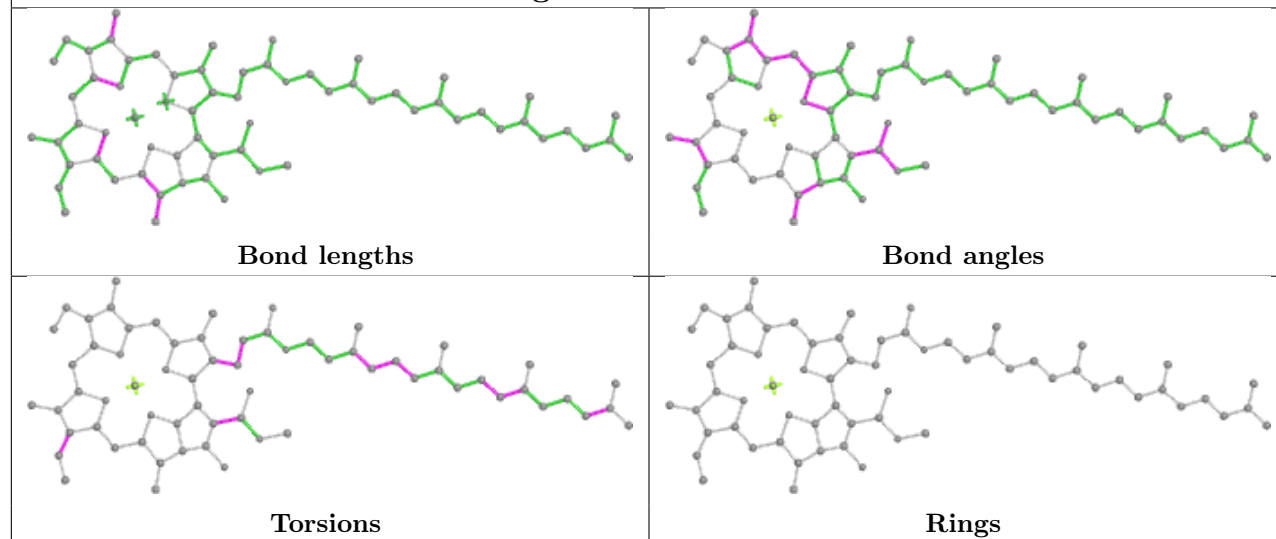
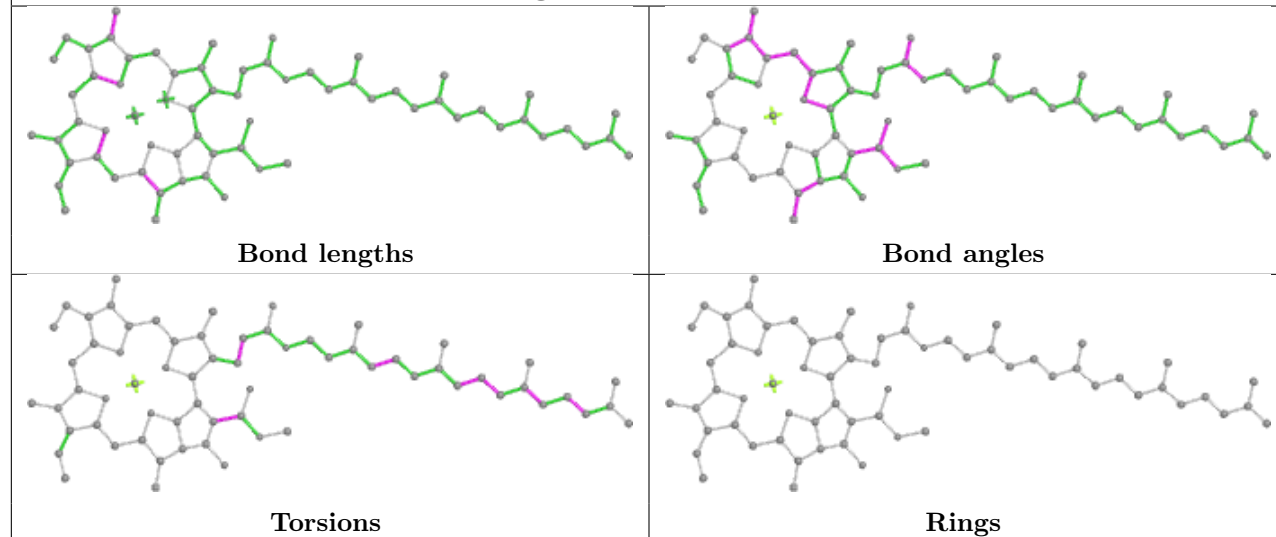


## Ligand CLA B 807



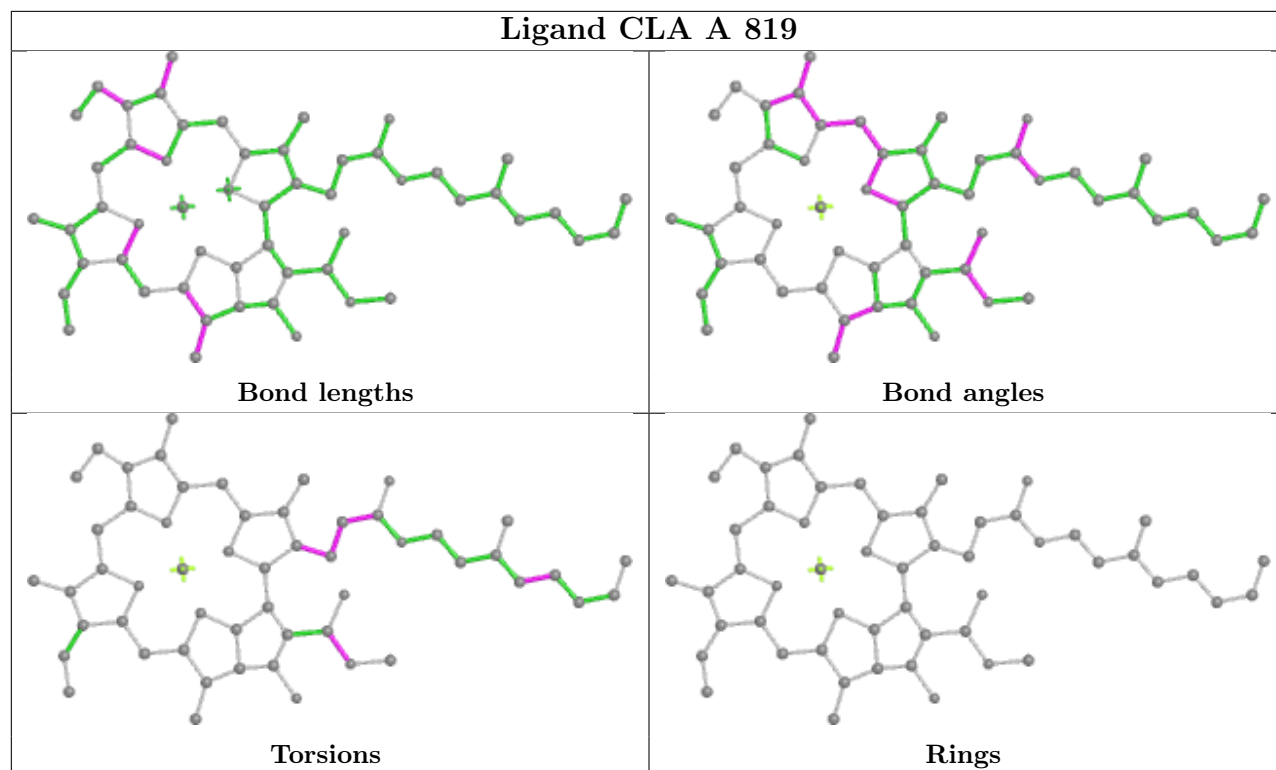
## Ligand CLA B 815



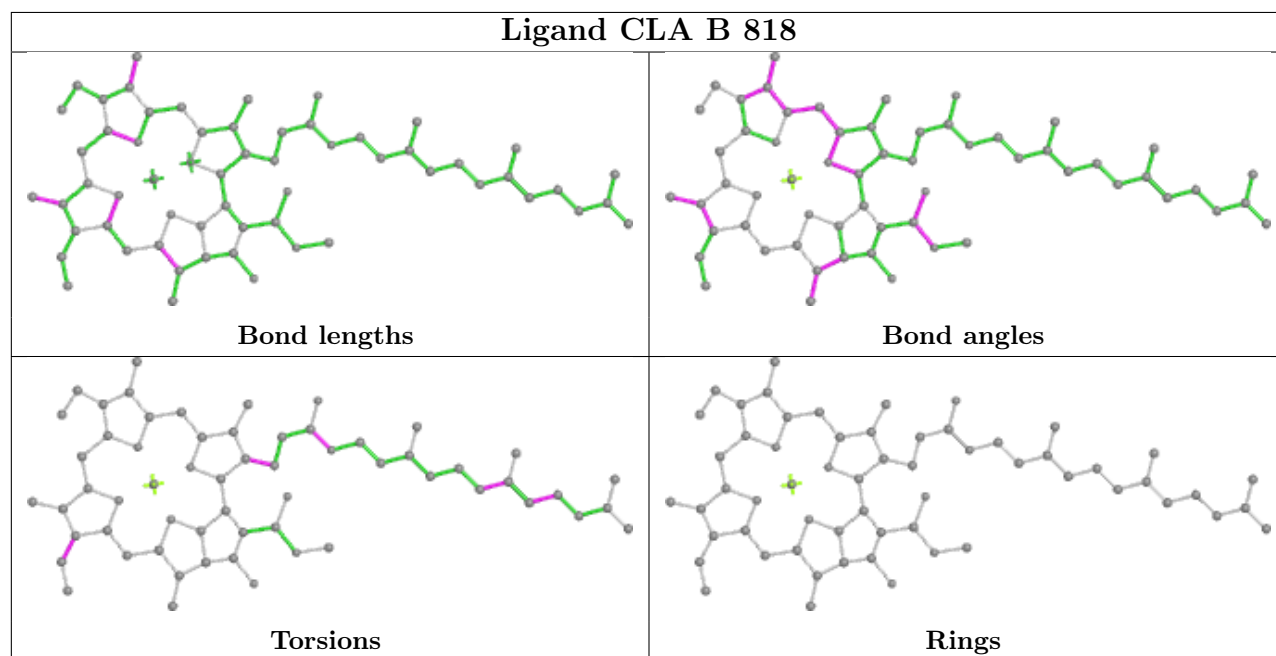
**Ligand CLA B 832****Ligand CLA B 840**

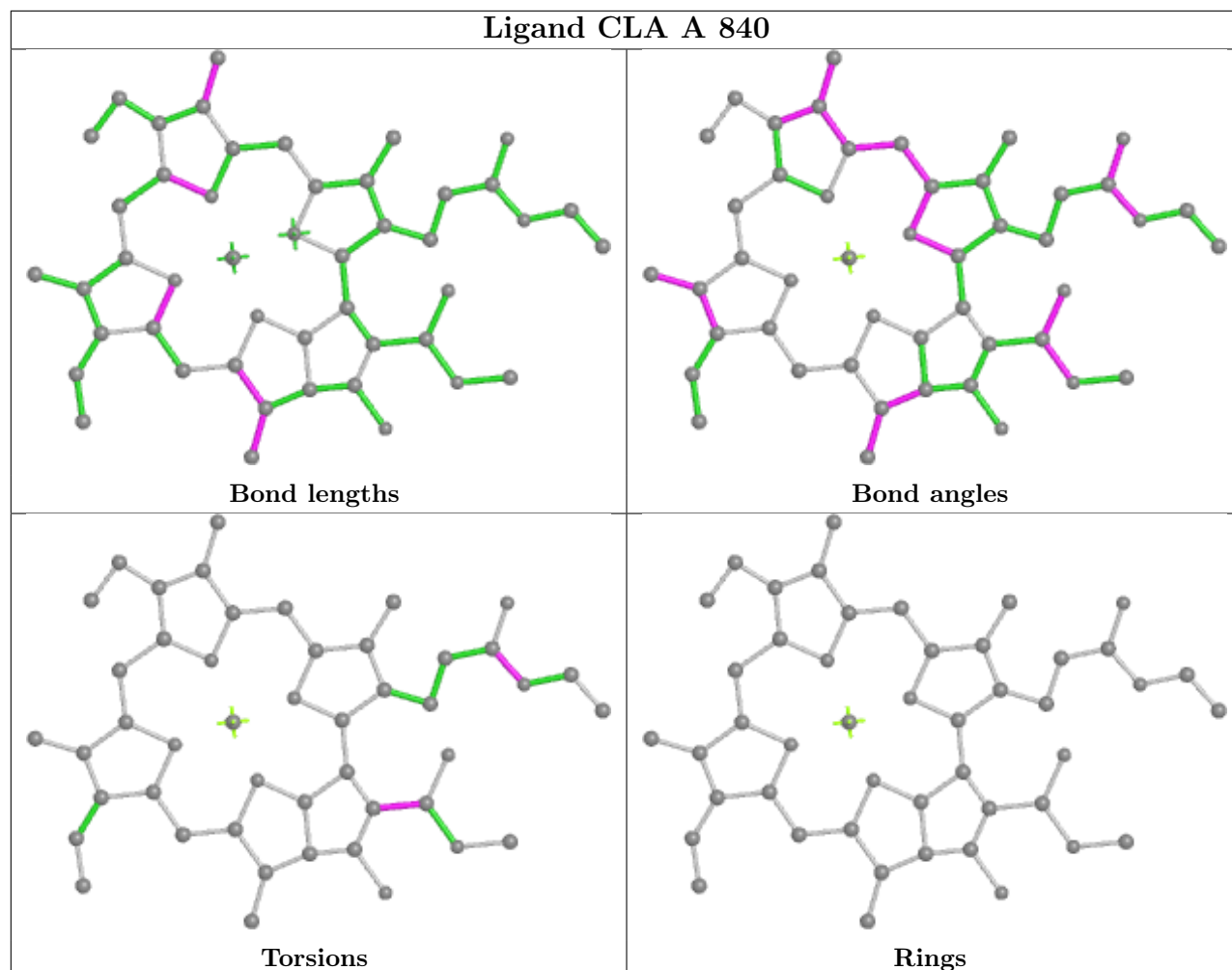
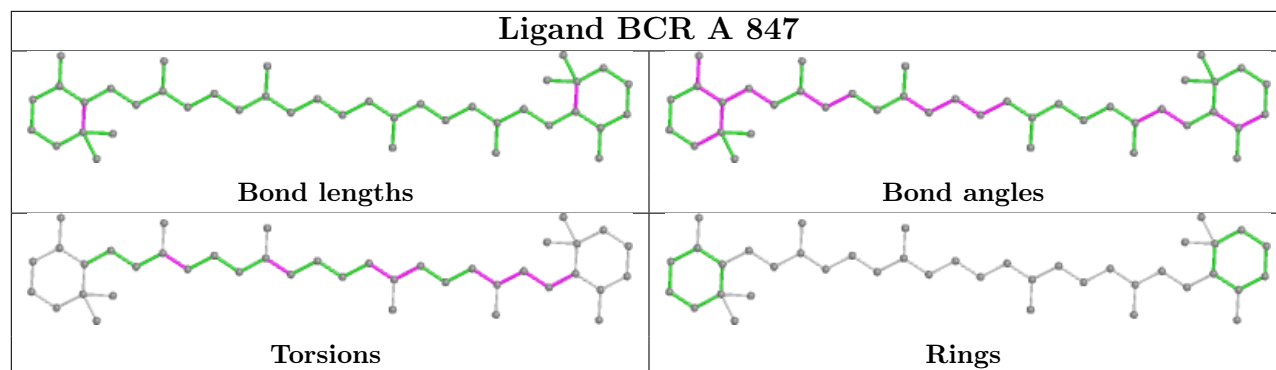


## Ligand CLA A 819

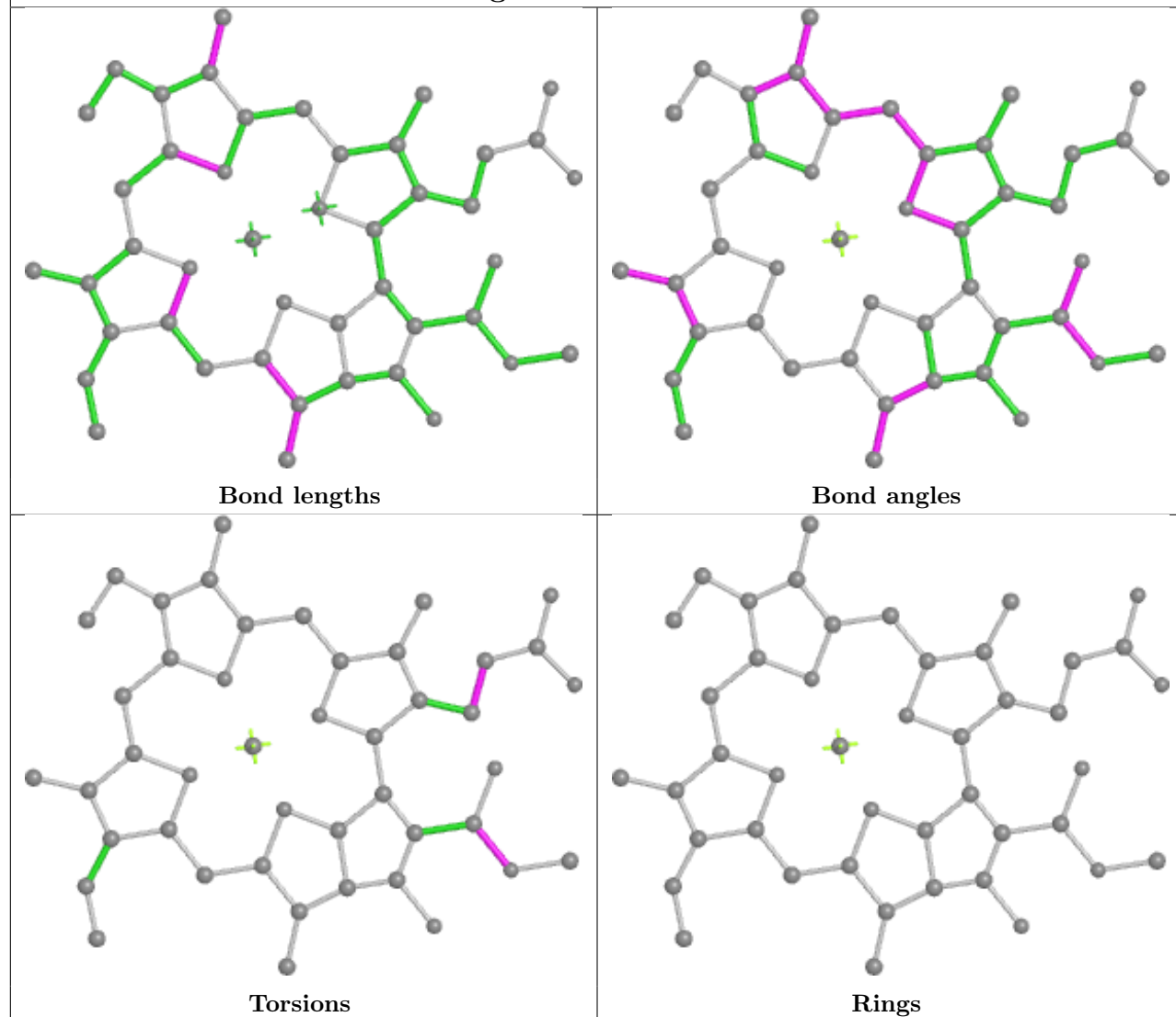


## Ligand CLA B 818

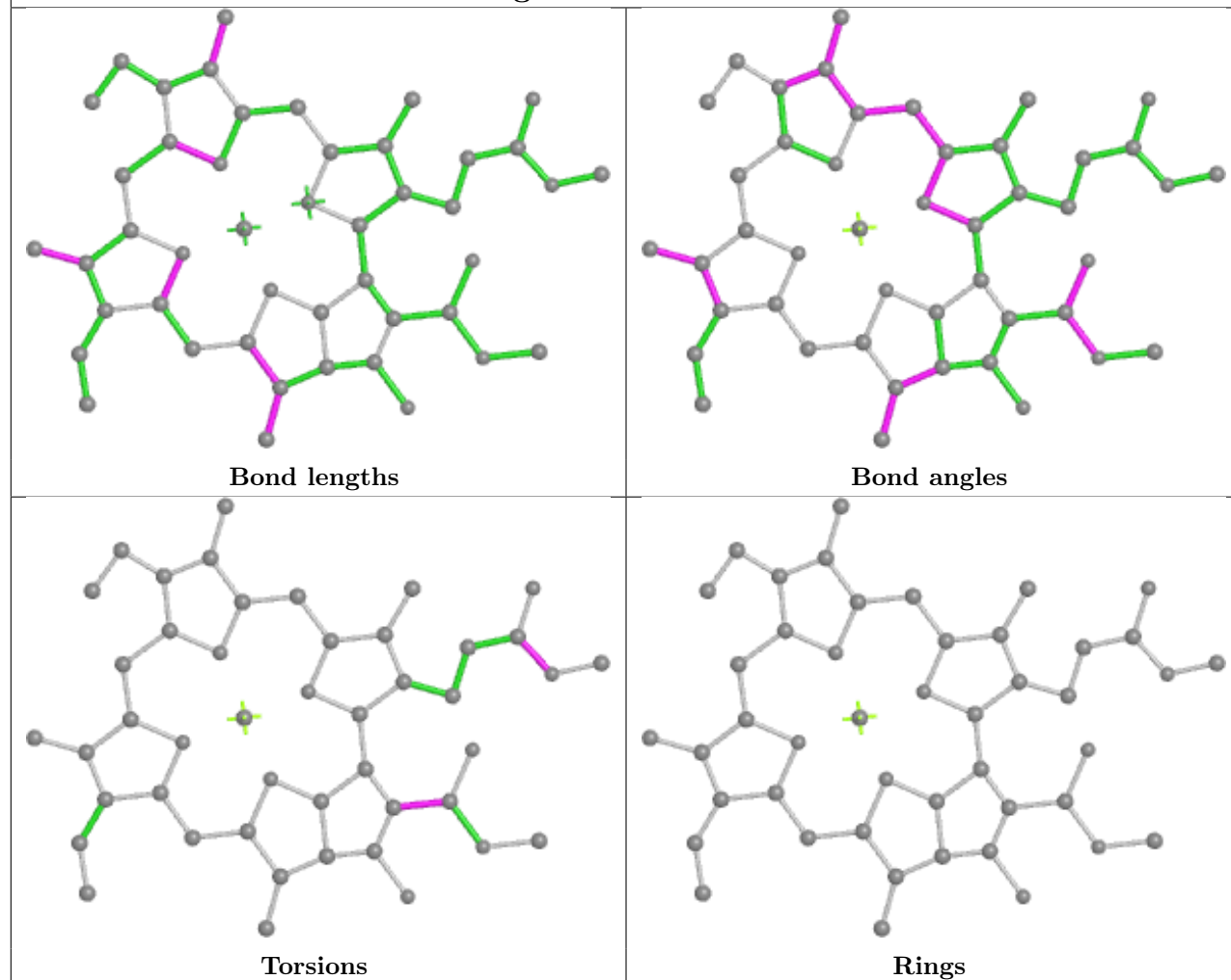




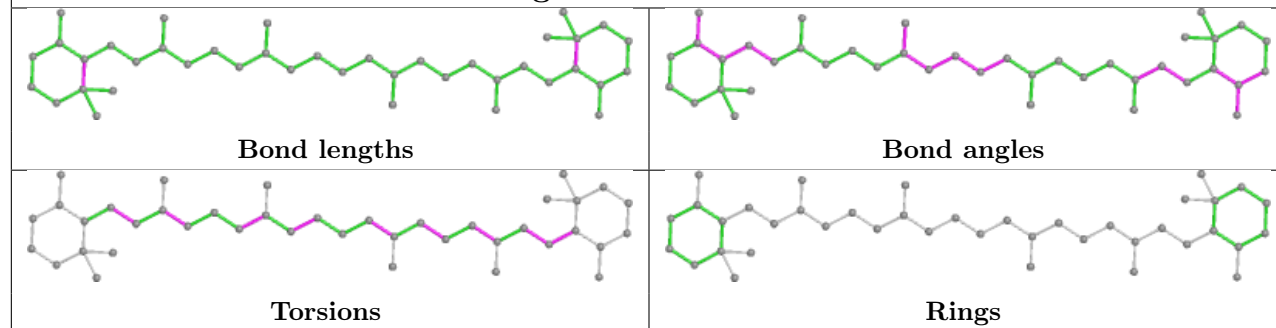
## Ligand CLA B 812



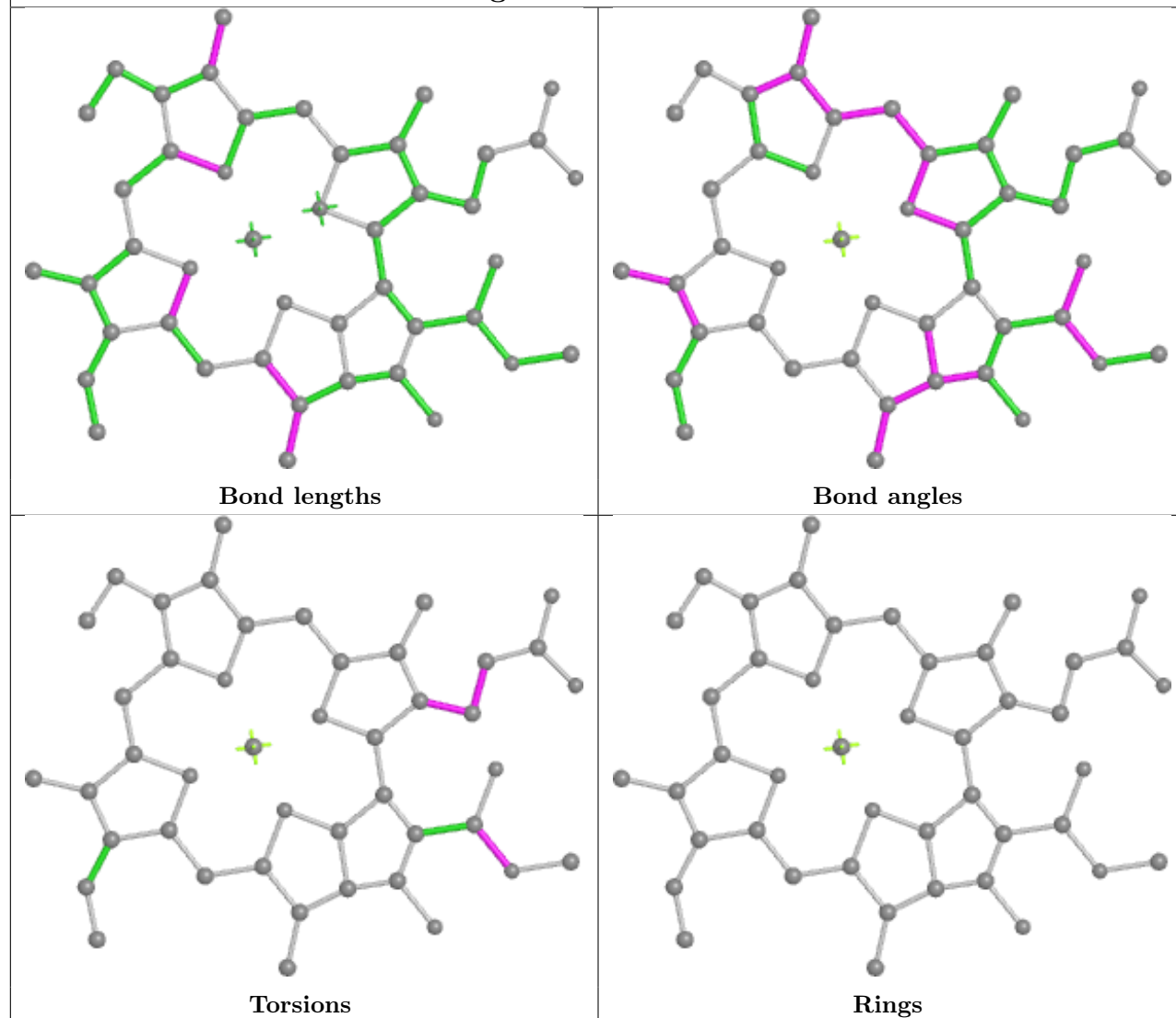
## Ligand CLA B 825



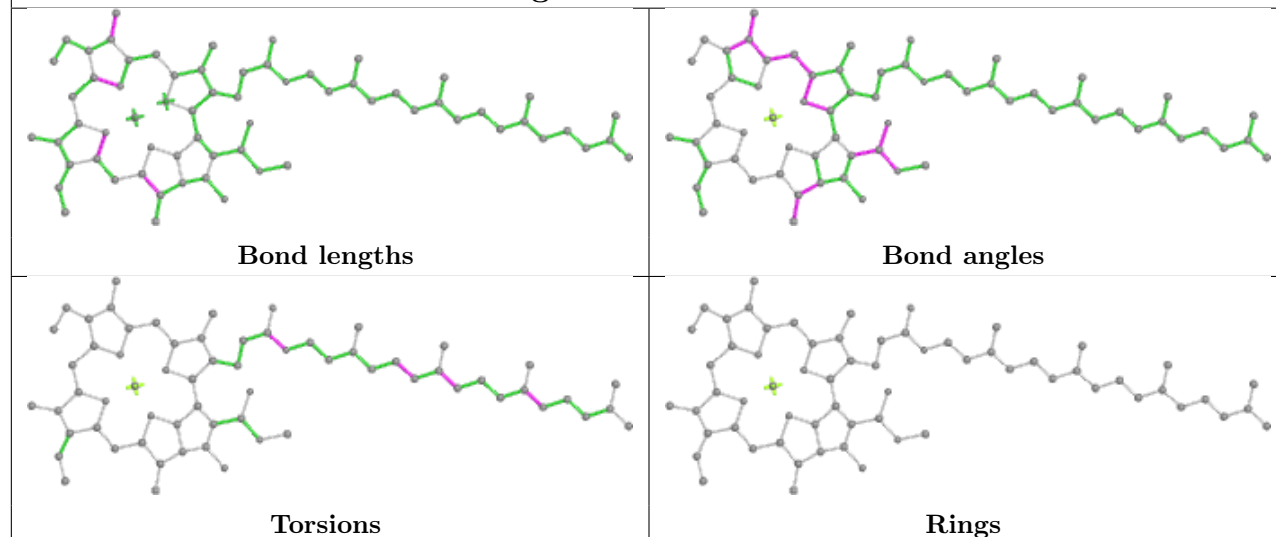
## Ligand BCR L 201

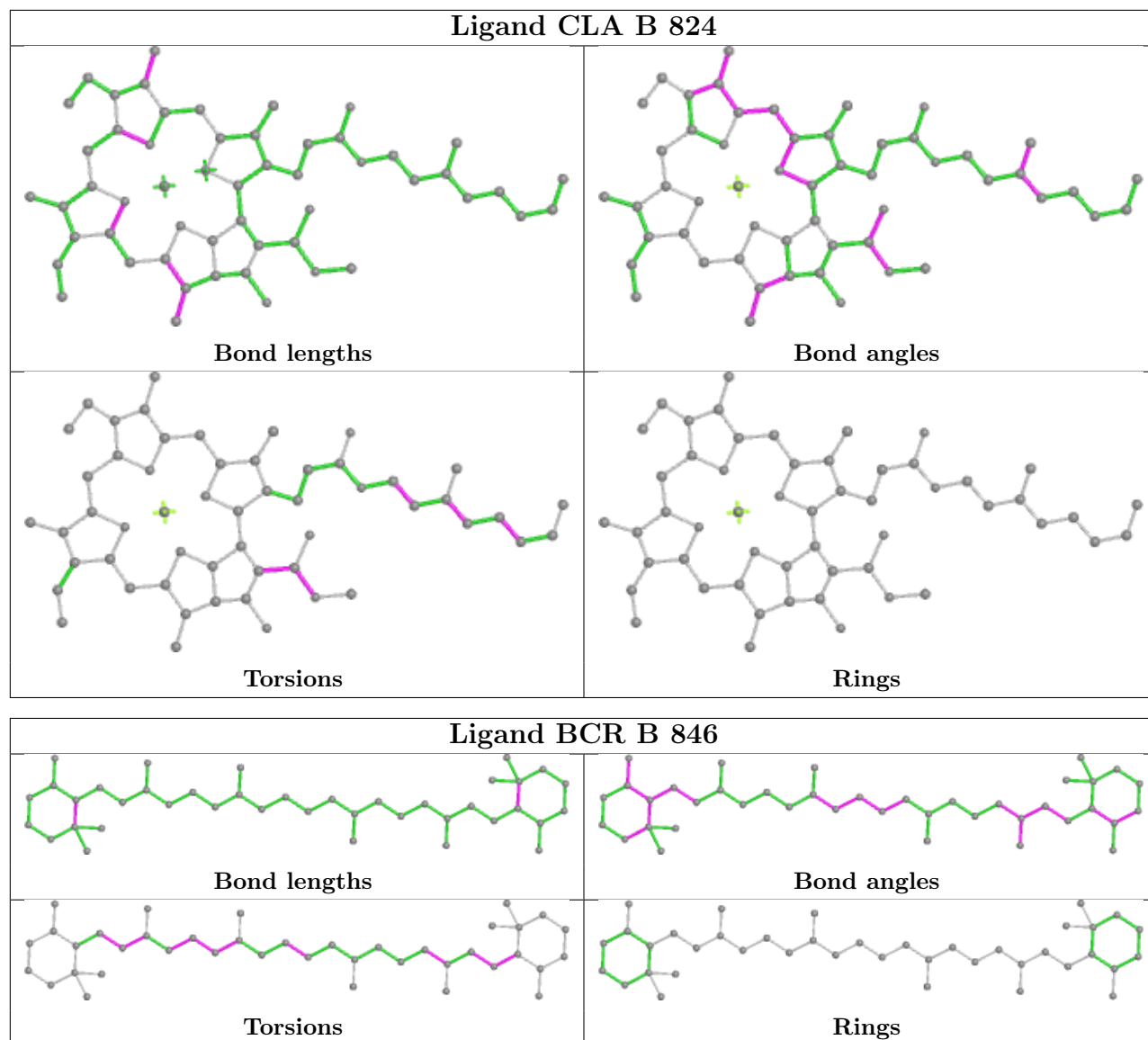


## Ligand CLA A 837

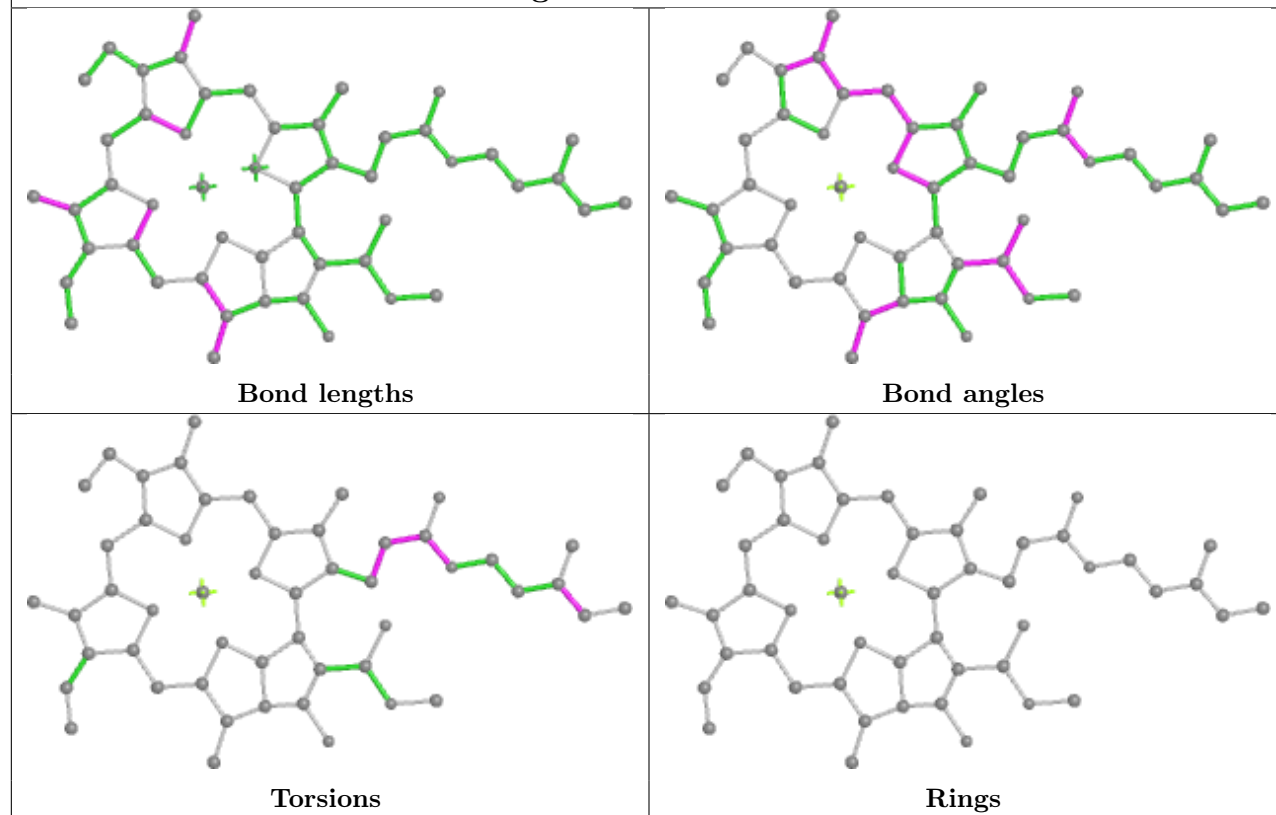


## Ligand CLA A 834

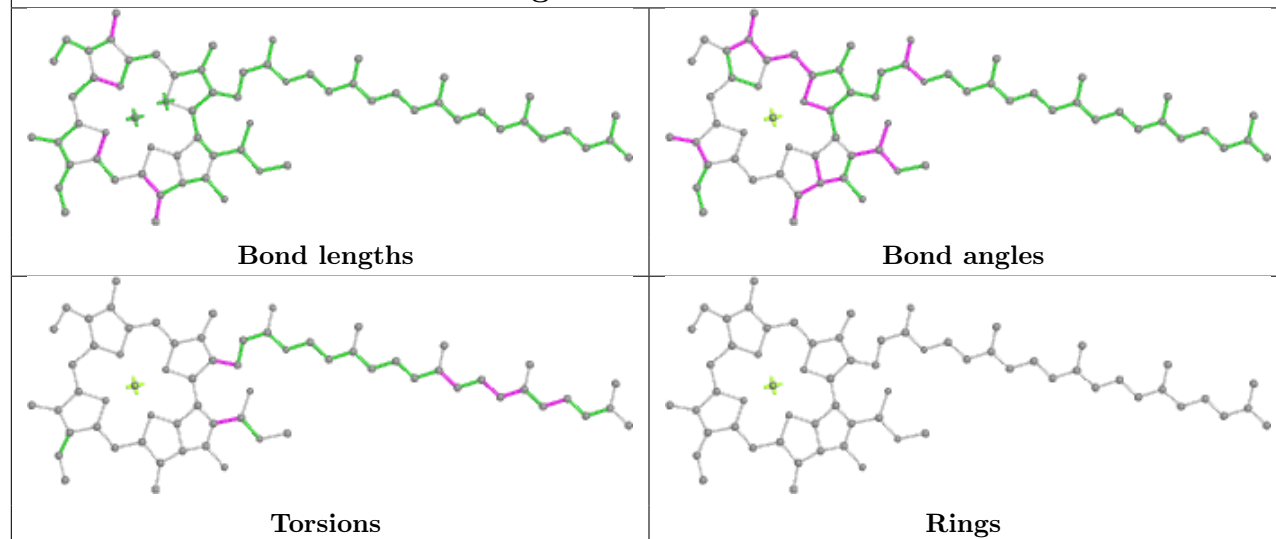


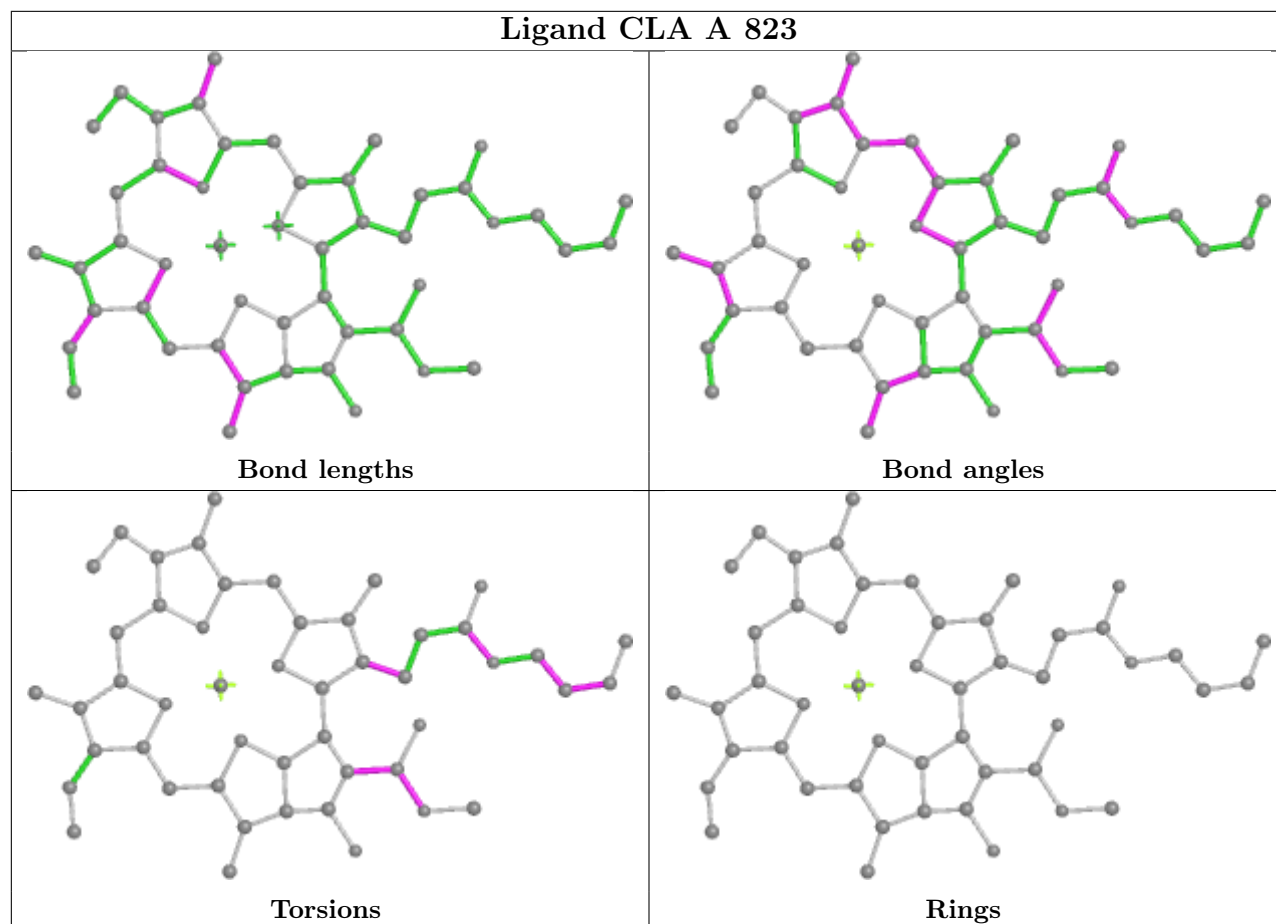
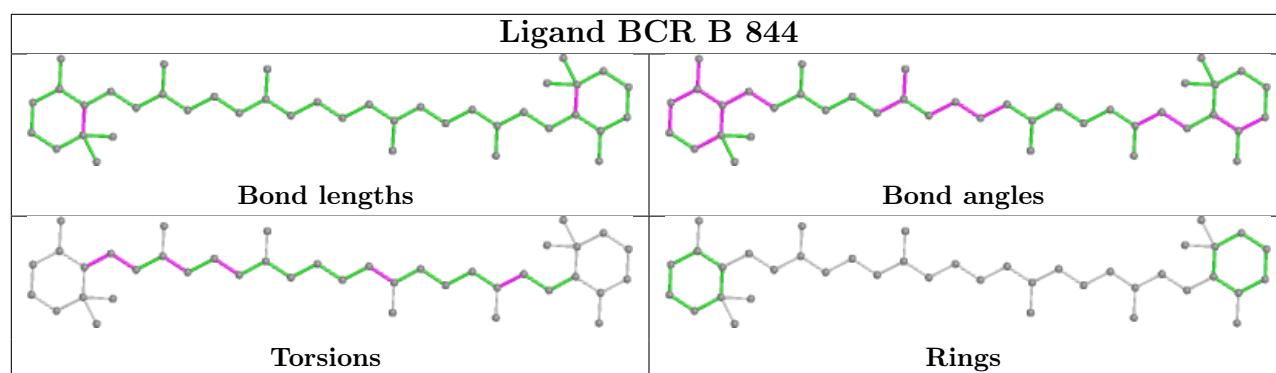


## Ligand CLA A 808



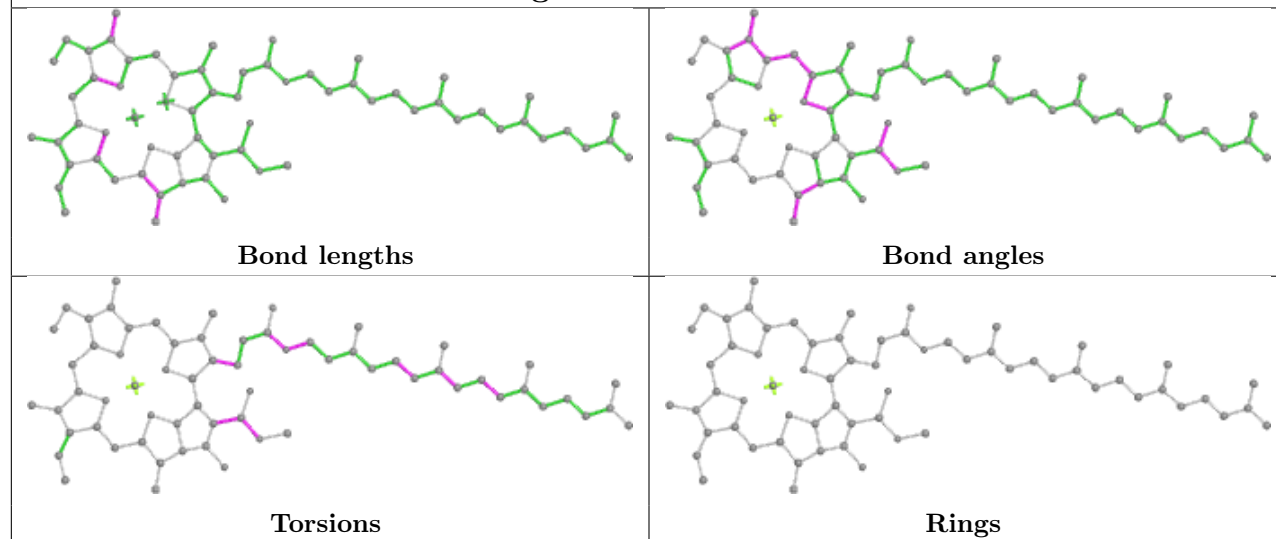
## Ligand CLA A 831



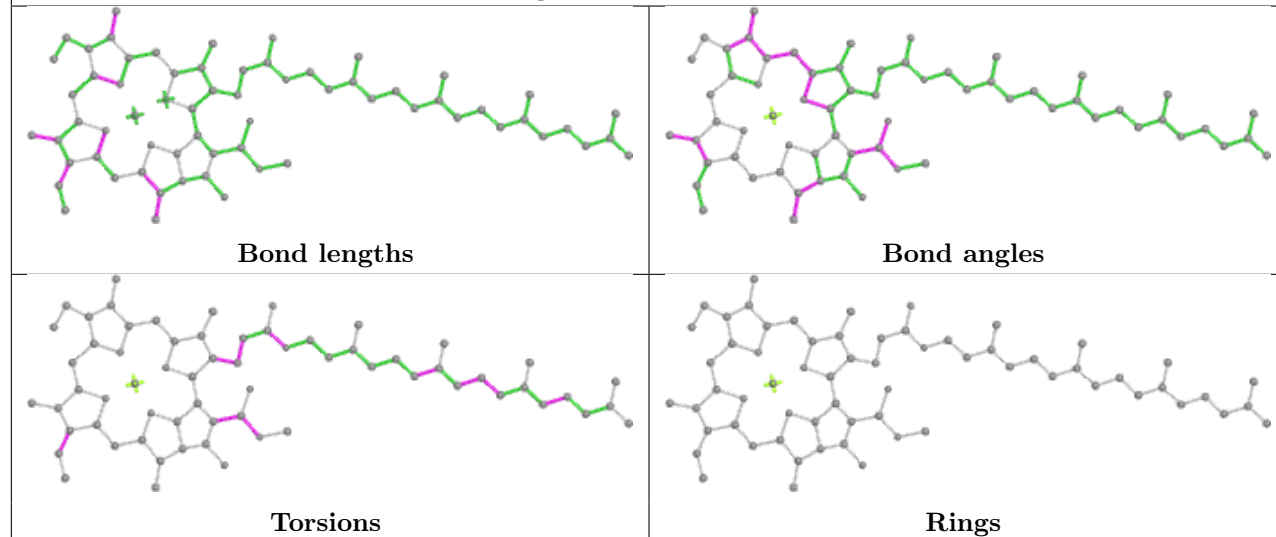




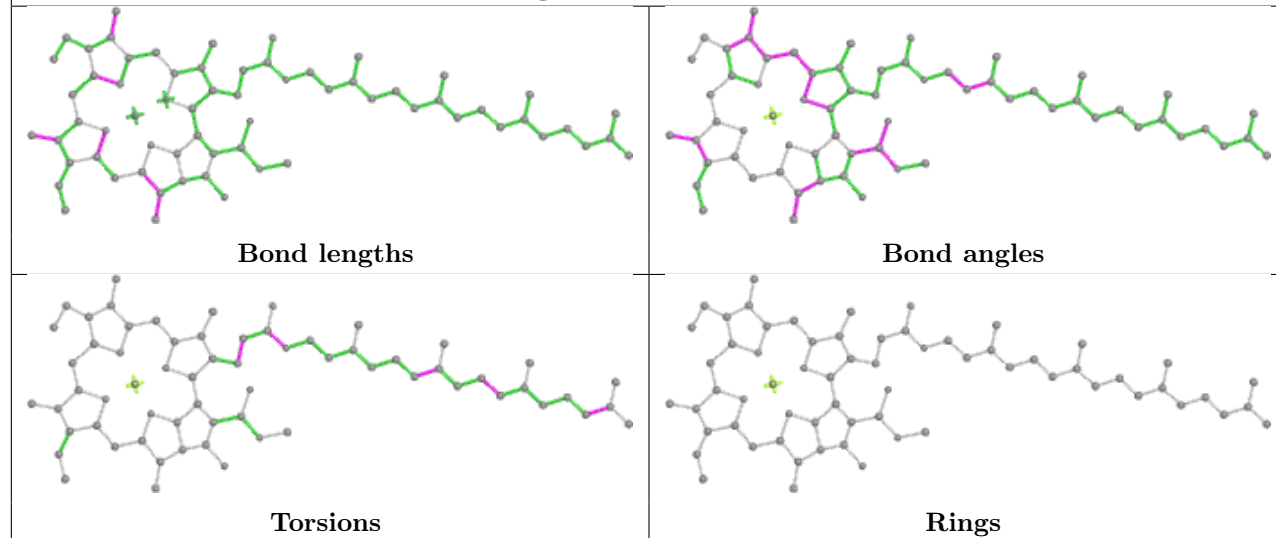
## Ligand CLA A 804

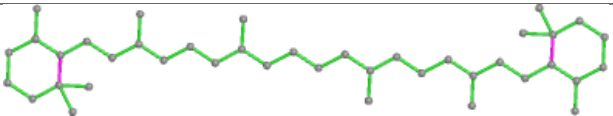
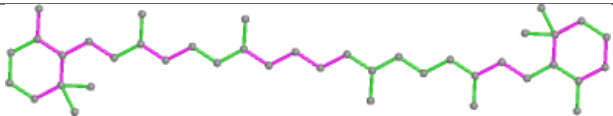
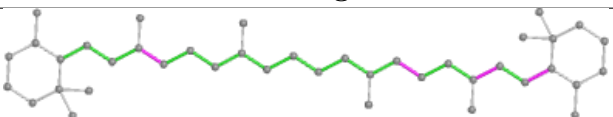
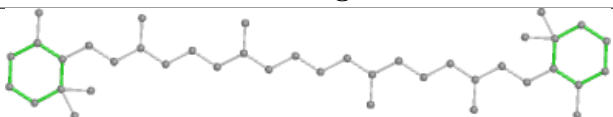


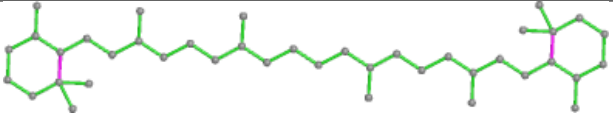
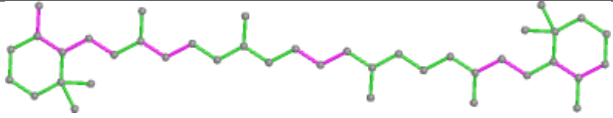
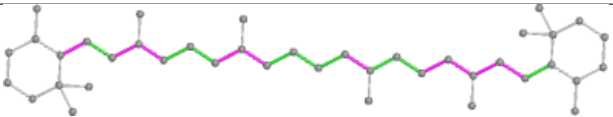
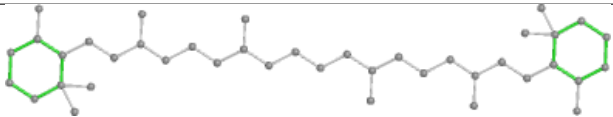
## Ligand CLA B 827

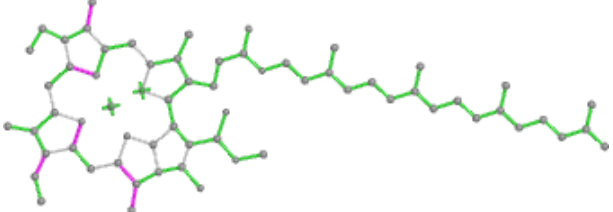
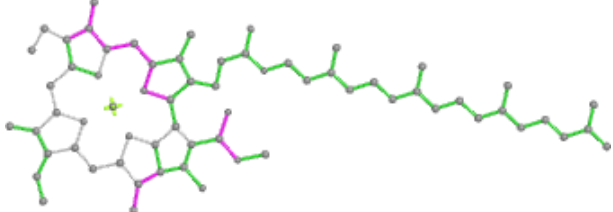
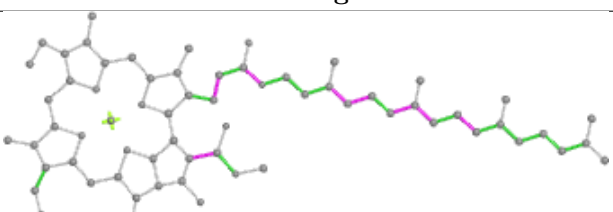
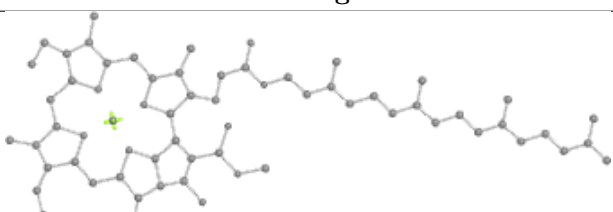


## Ligand CLA L 206

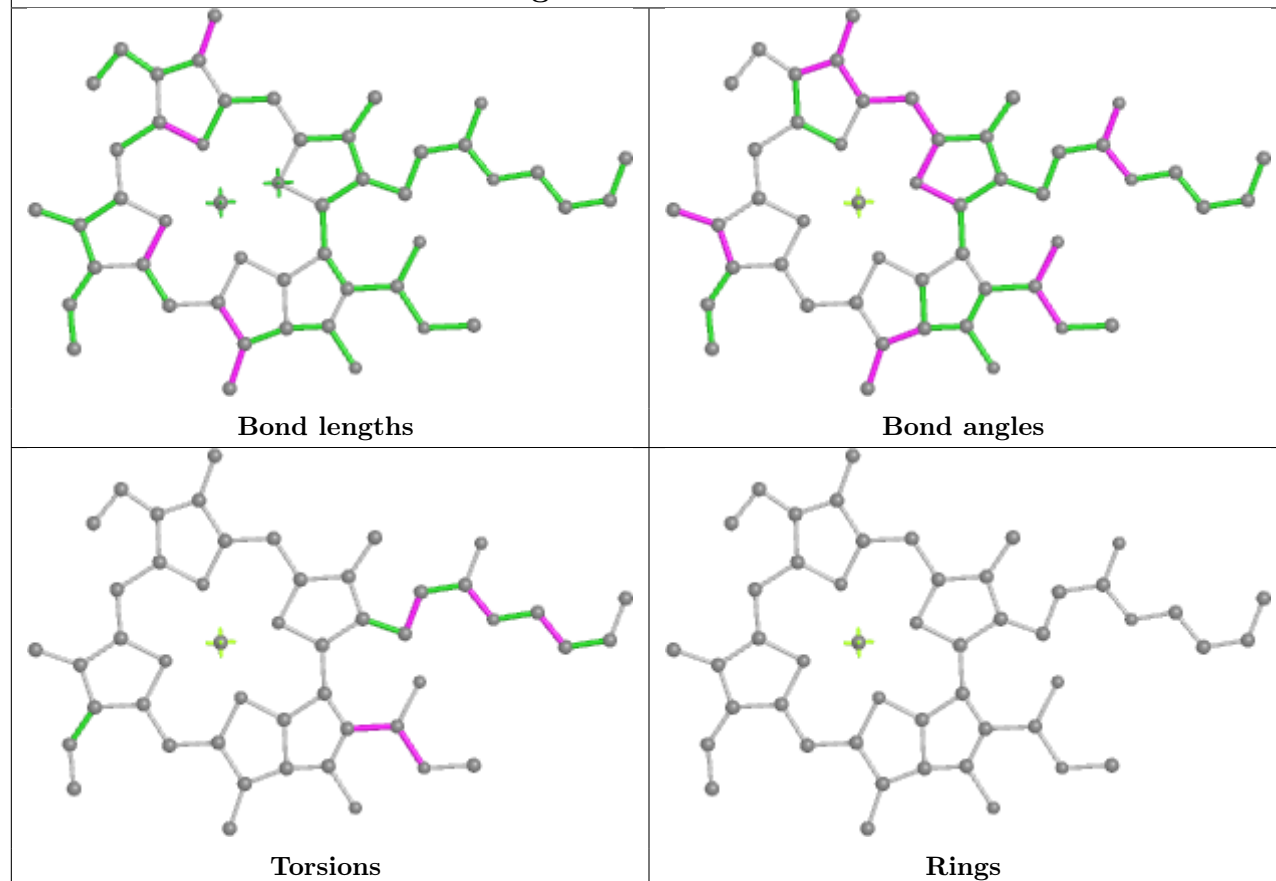


Ligand BCR B 843	
	
Bond lengths	Bond angles
	
Torsions	Rings

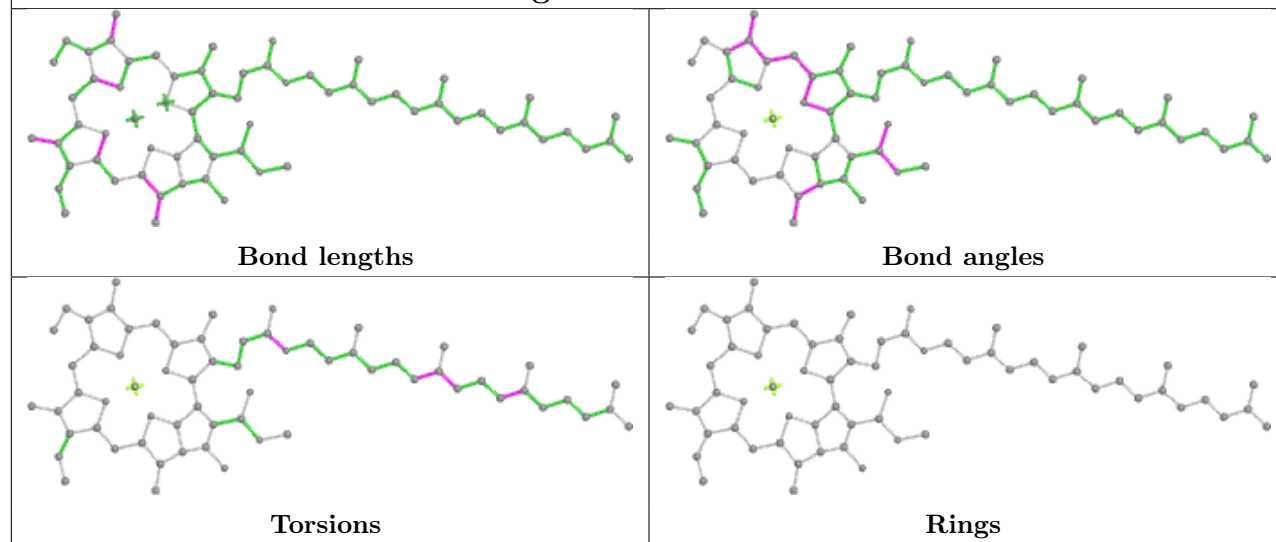
Ligand BCR I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

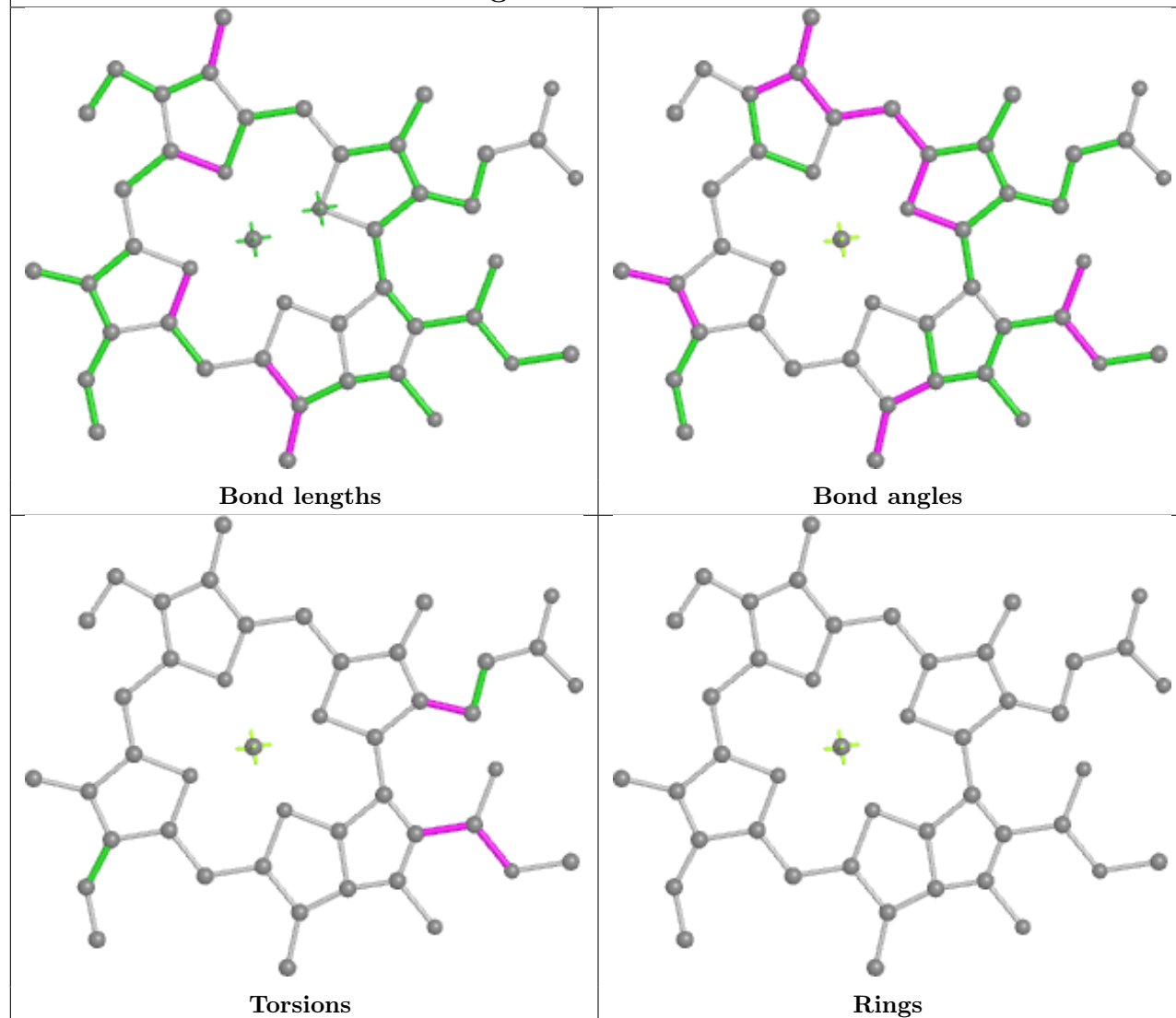
## Ligand CLA A 817



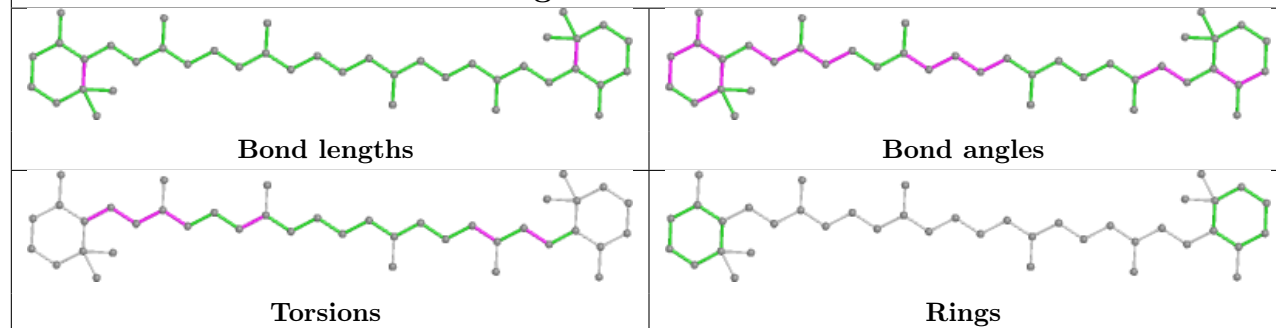
## Ligand CLA B 806



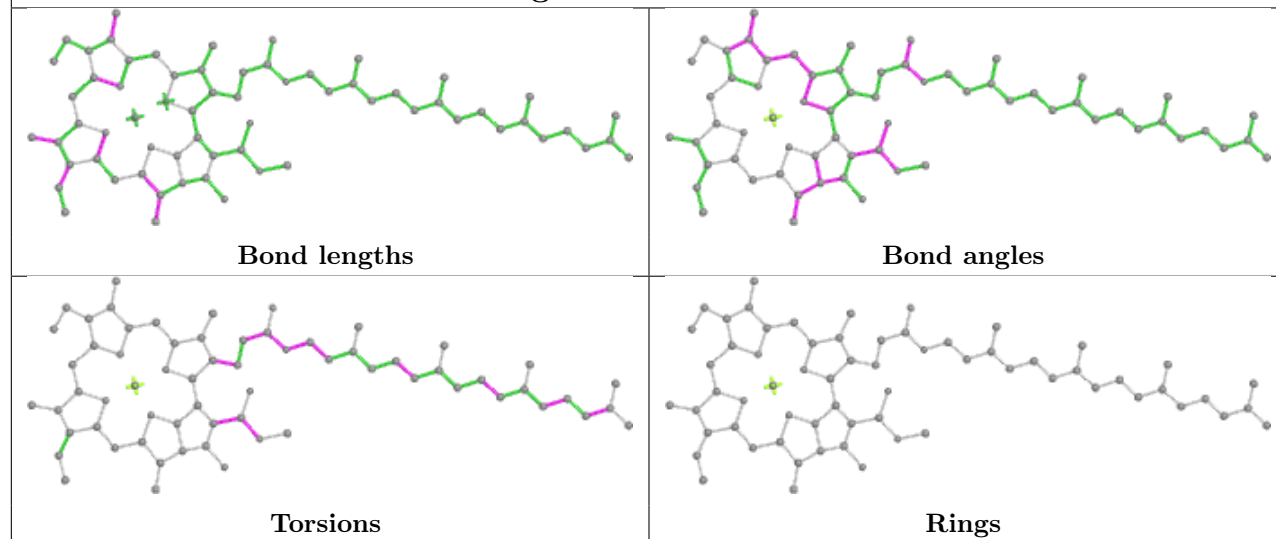
## Ligand CLA B 821



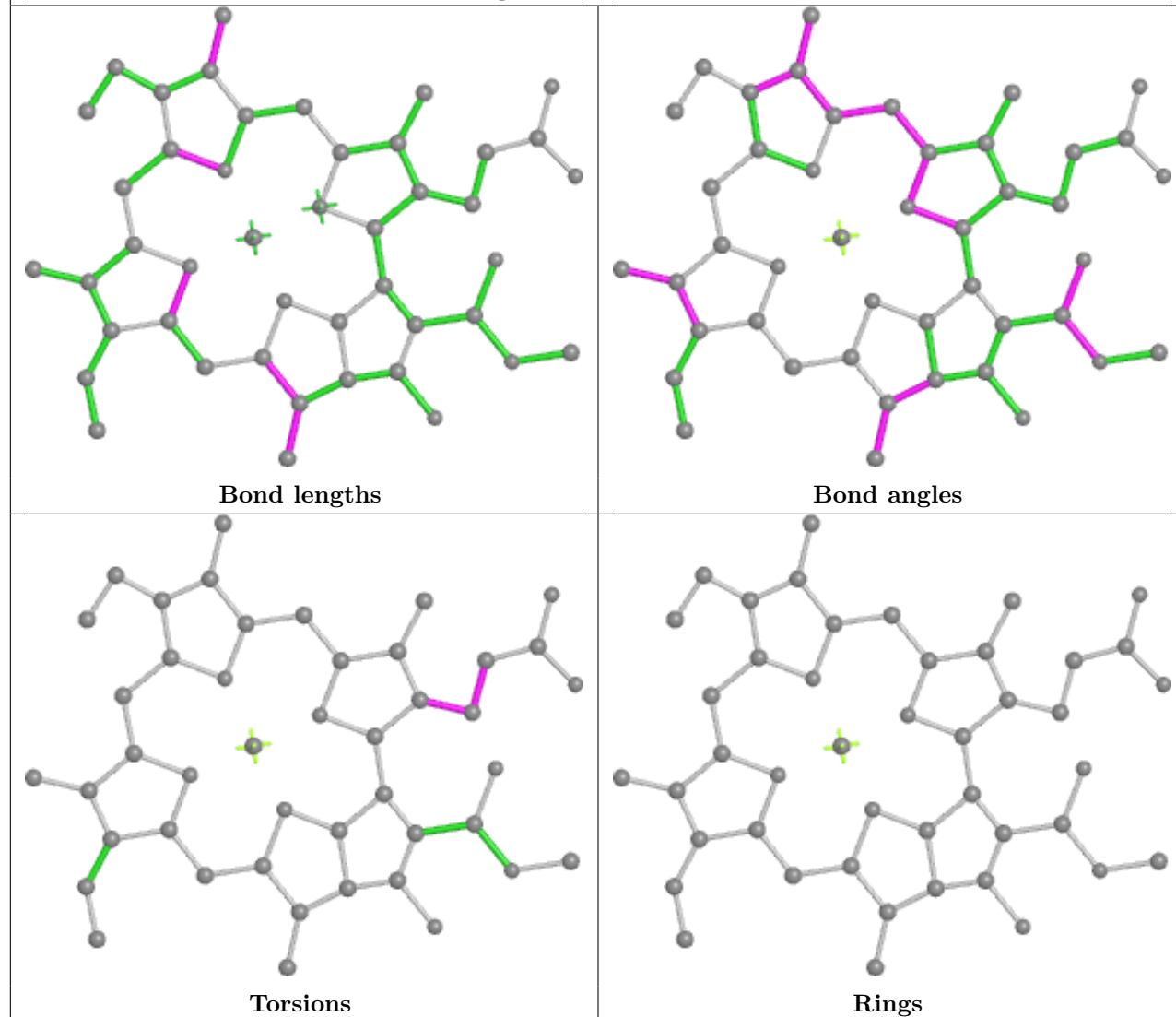
## Ligand BCR J 105



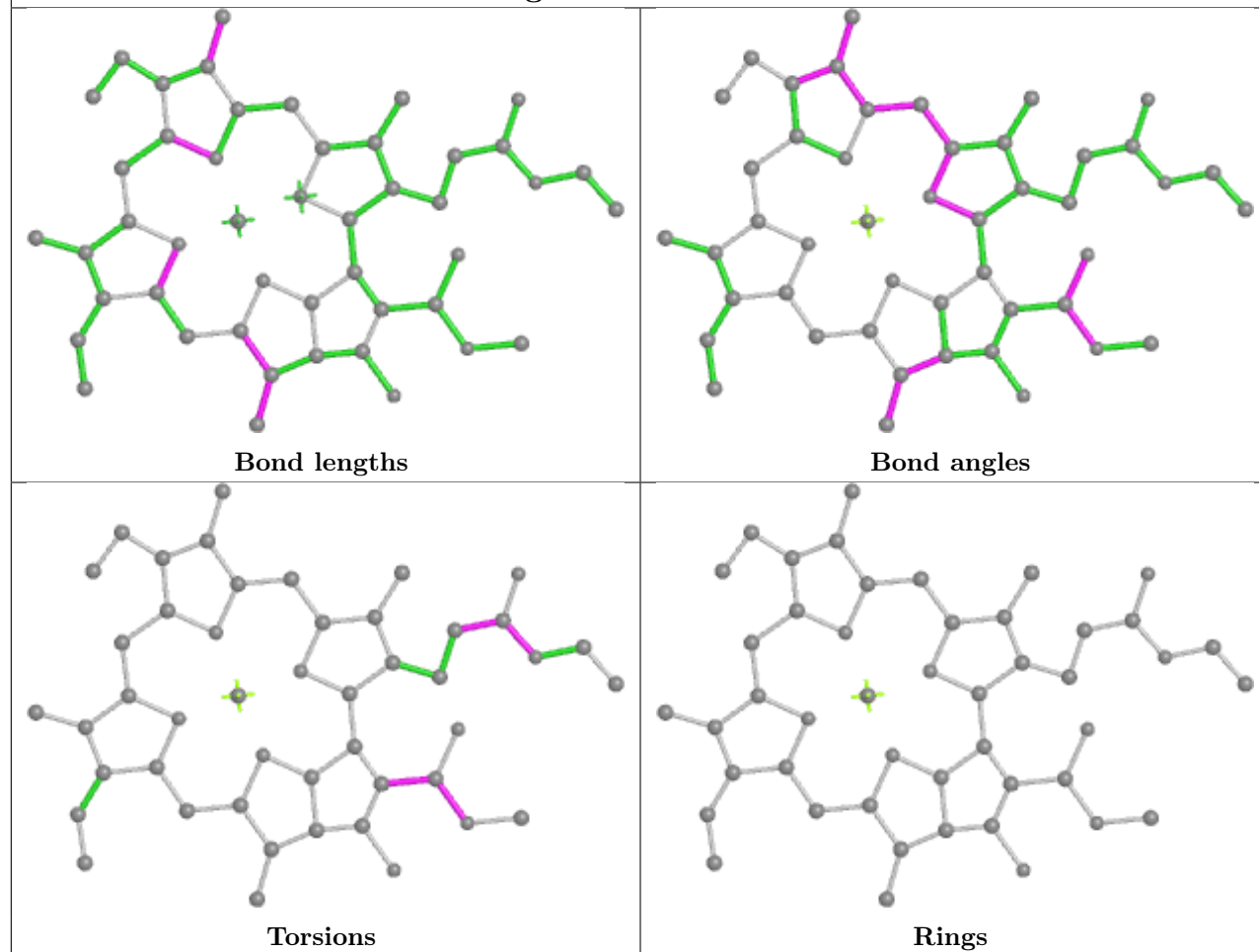
## Ligand CLA A 806



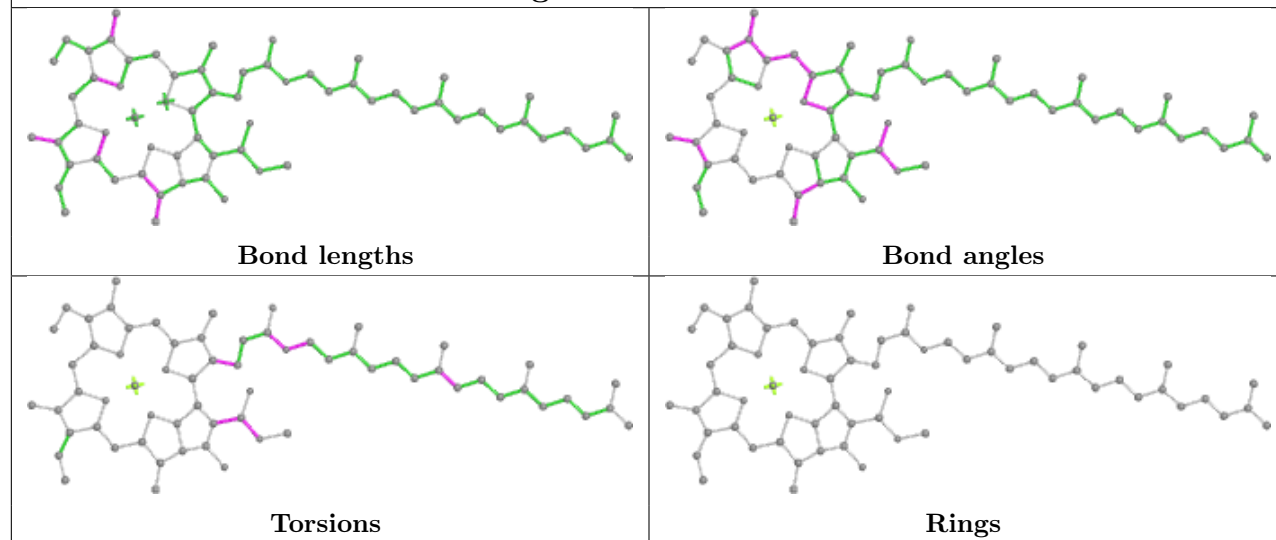
## Ligand CLA J 101

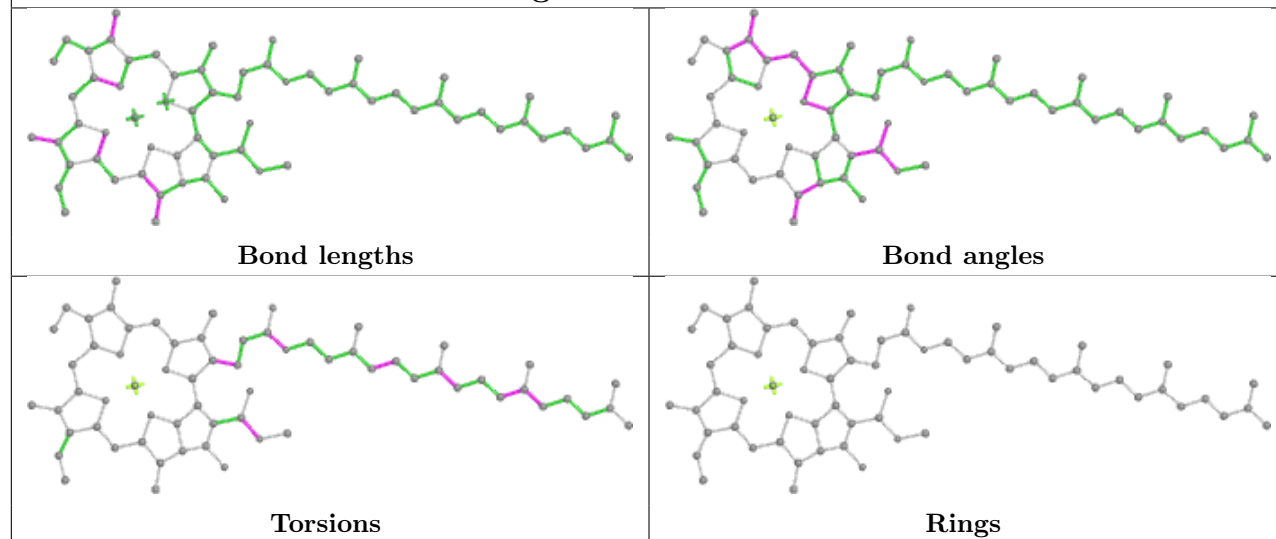
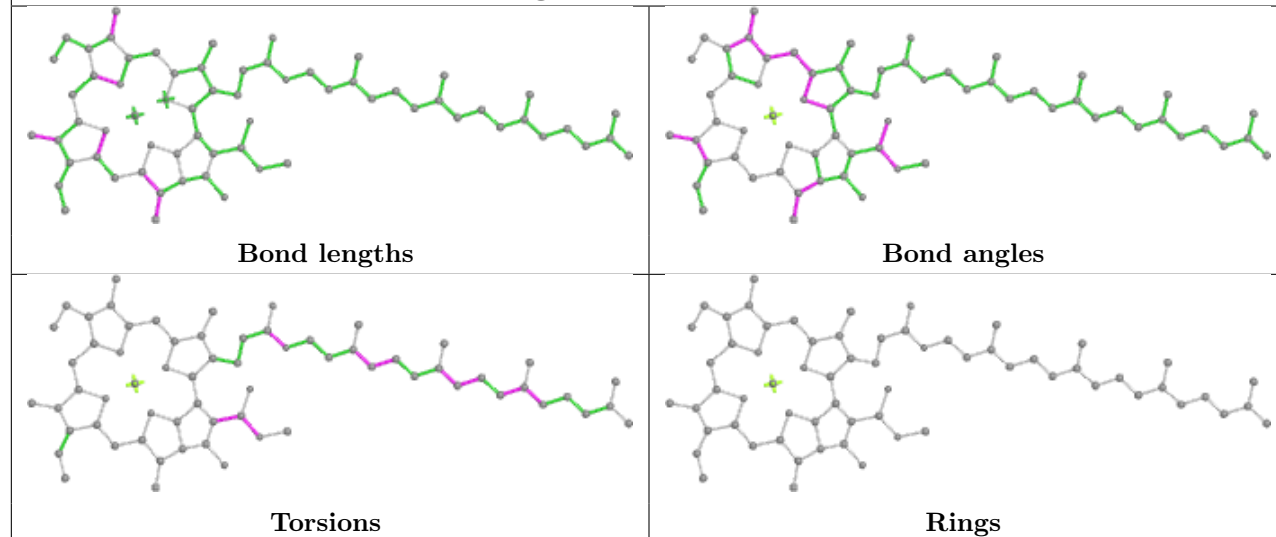


## Ligand CLA B 820

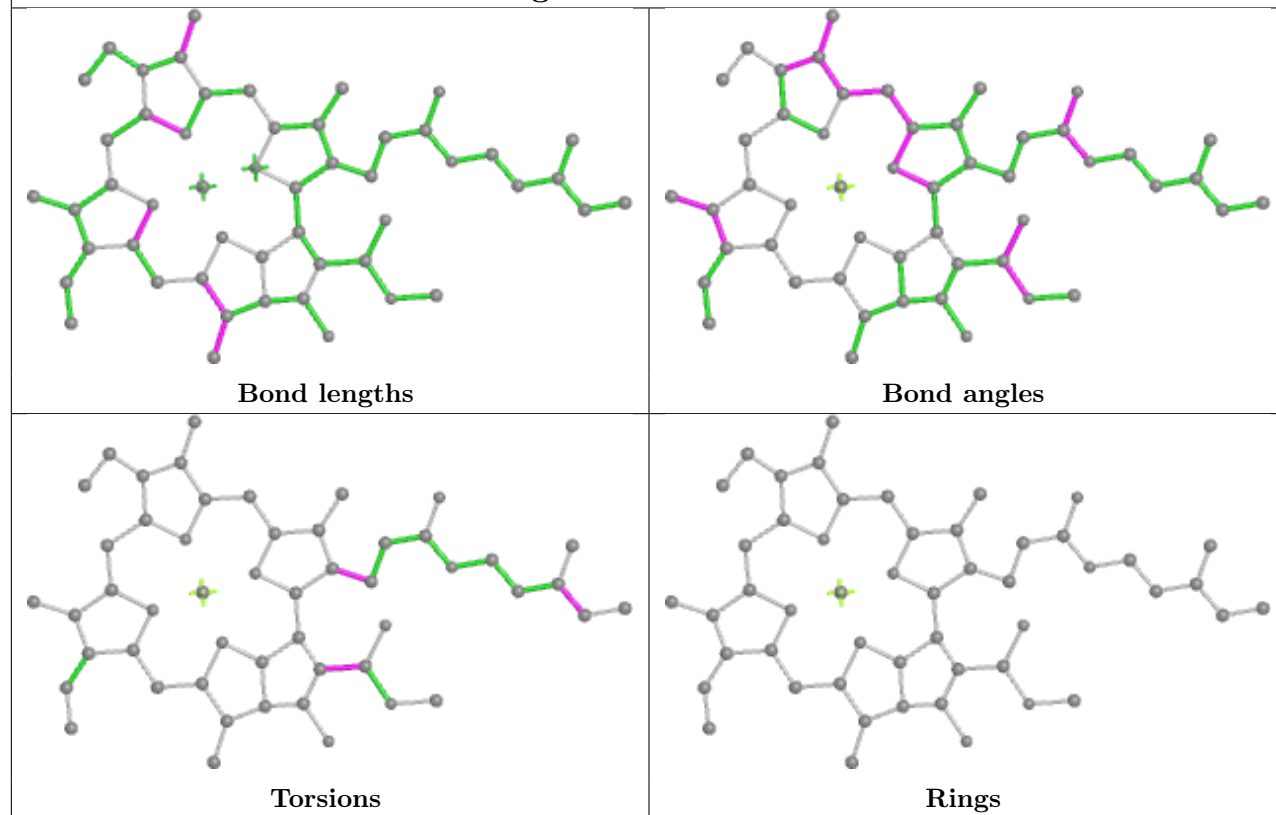


## Ligand CLA A 842

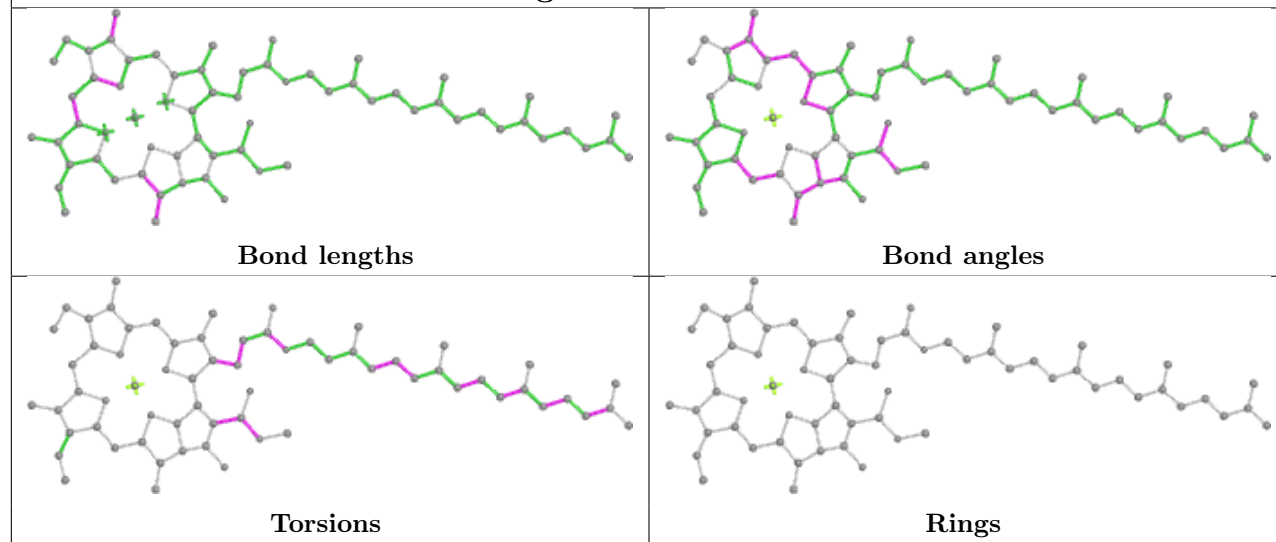


**Ligand CLA B 819****Ligand CLA B 802**

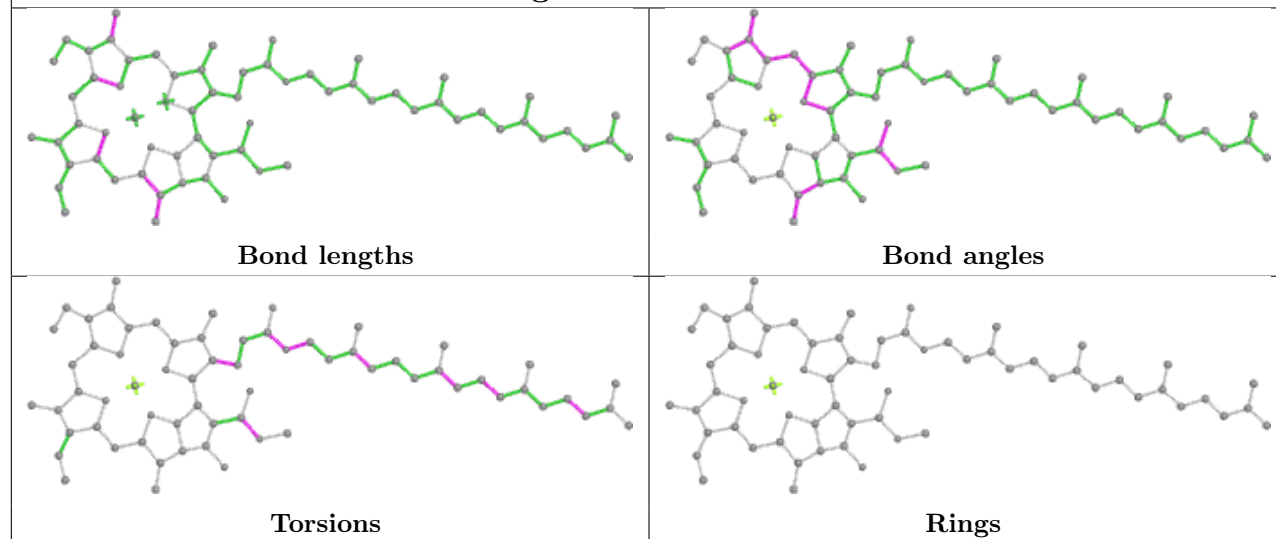
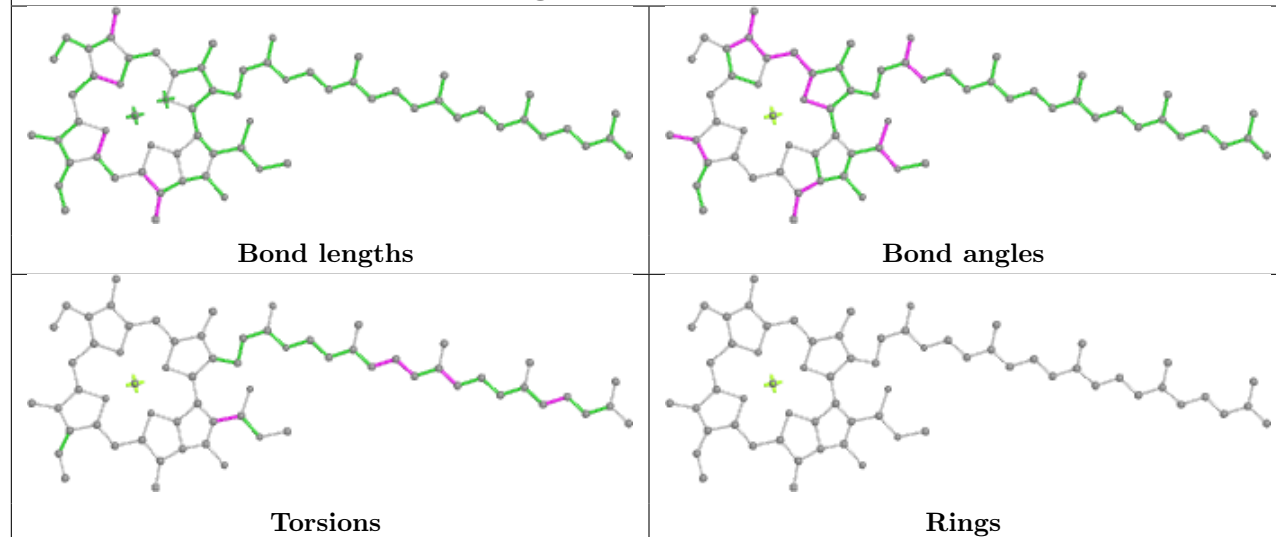
## Ligand CLA A 824



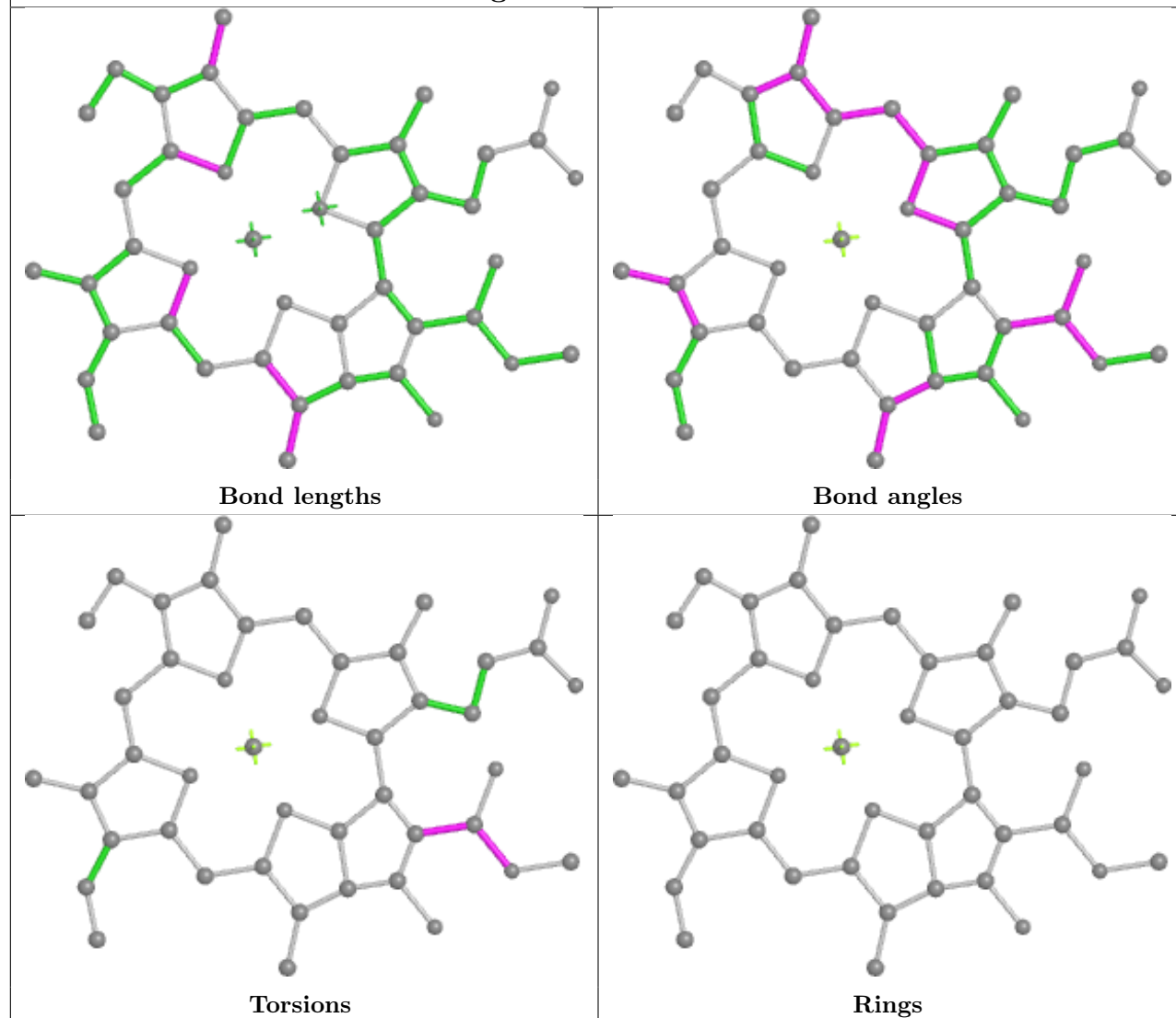
## Ligand CL0 A 801



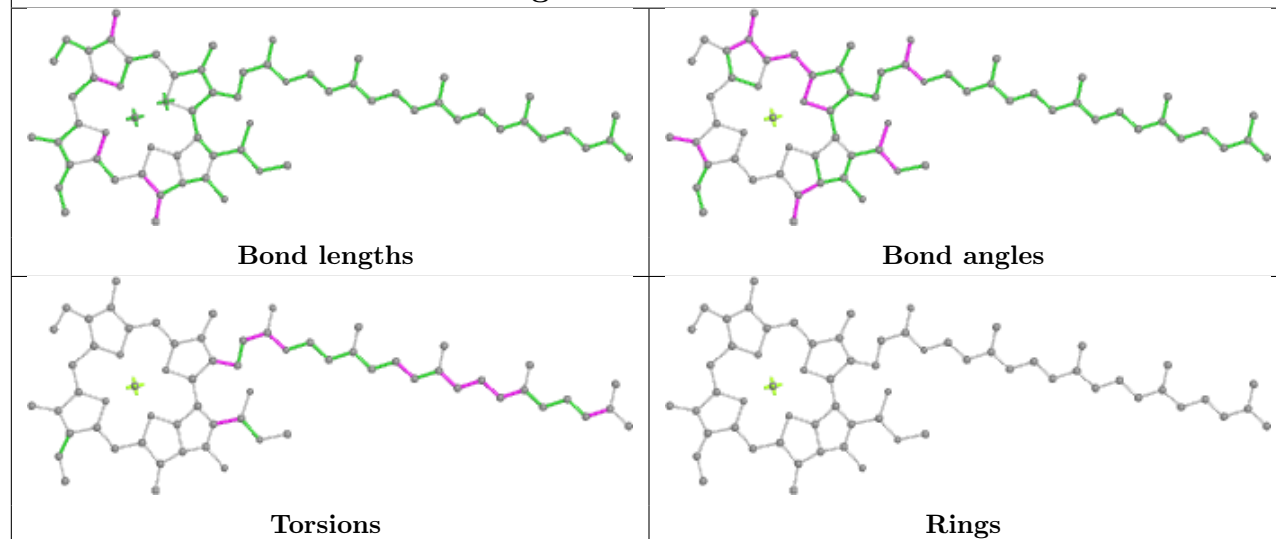


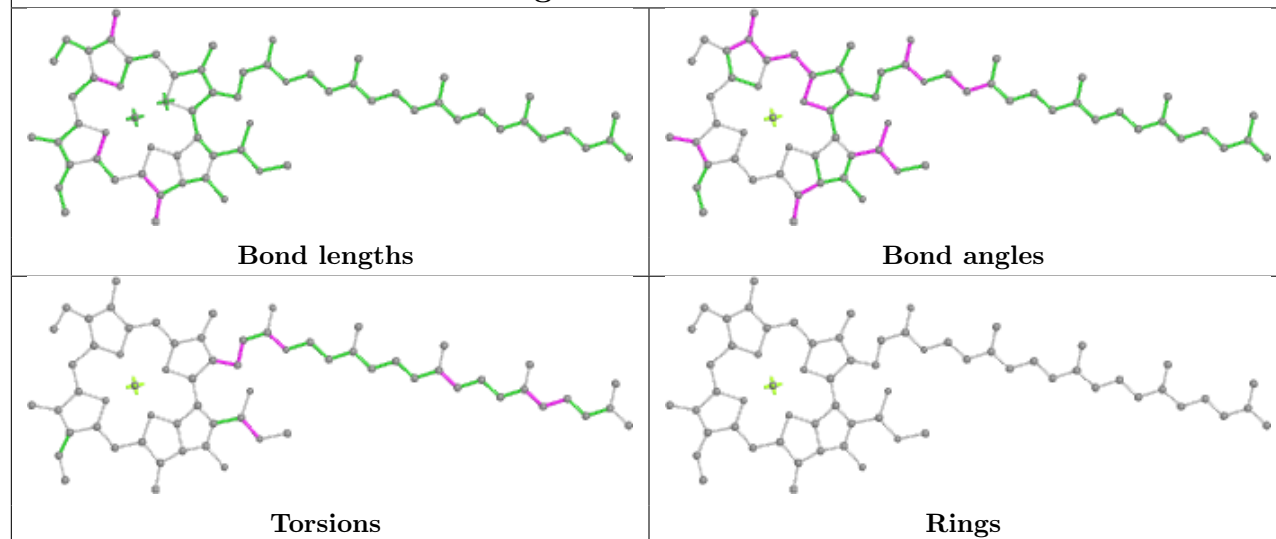
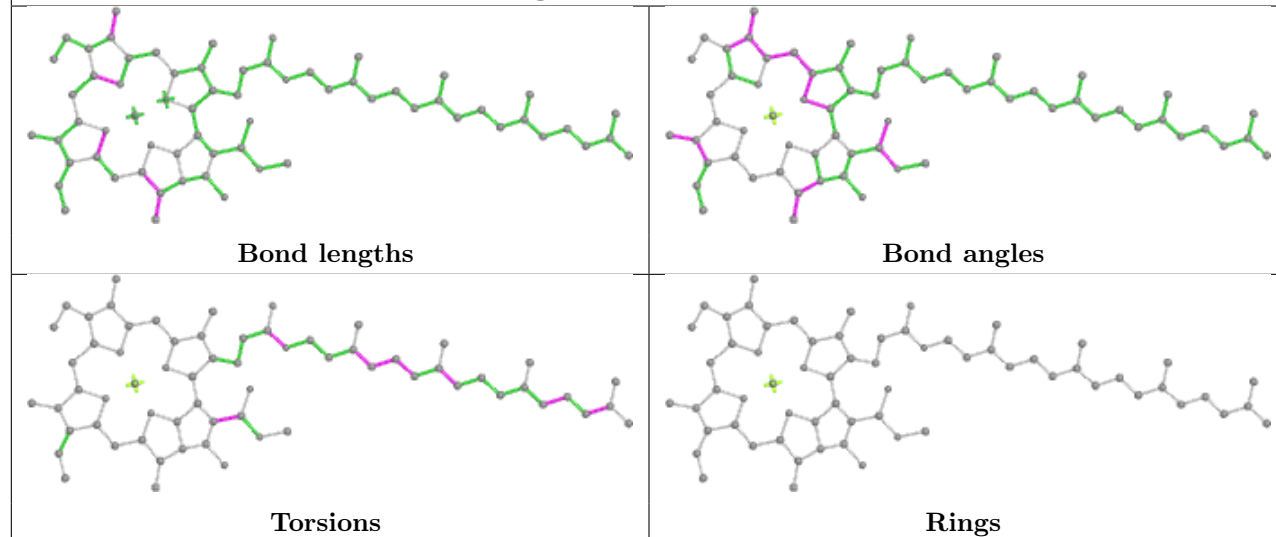
**Ligand CLA A 826****Ligand CLA A 827**

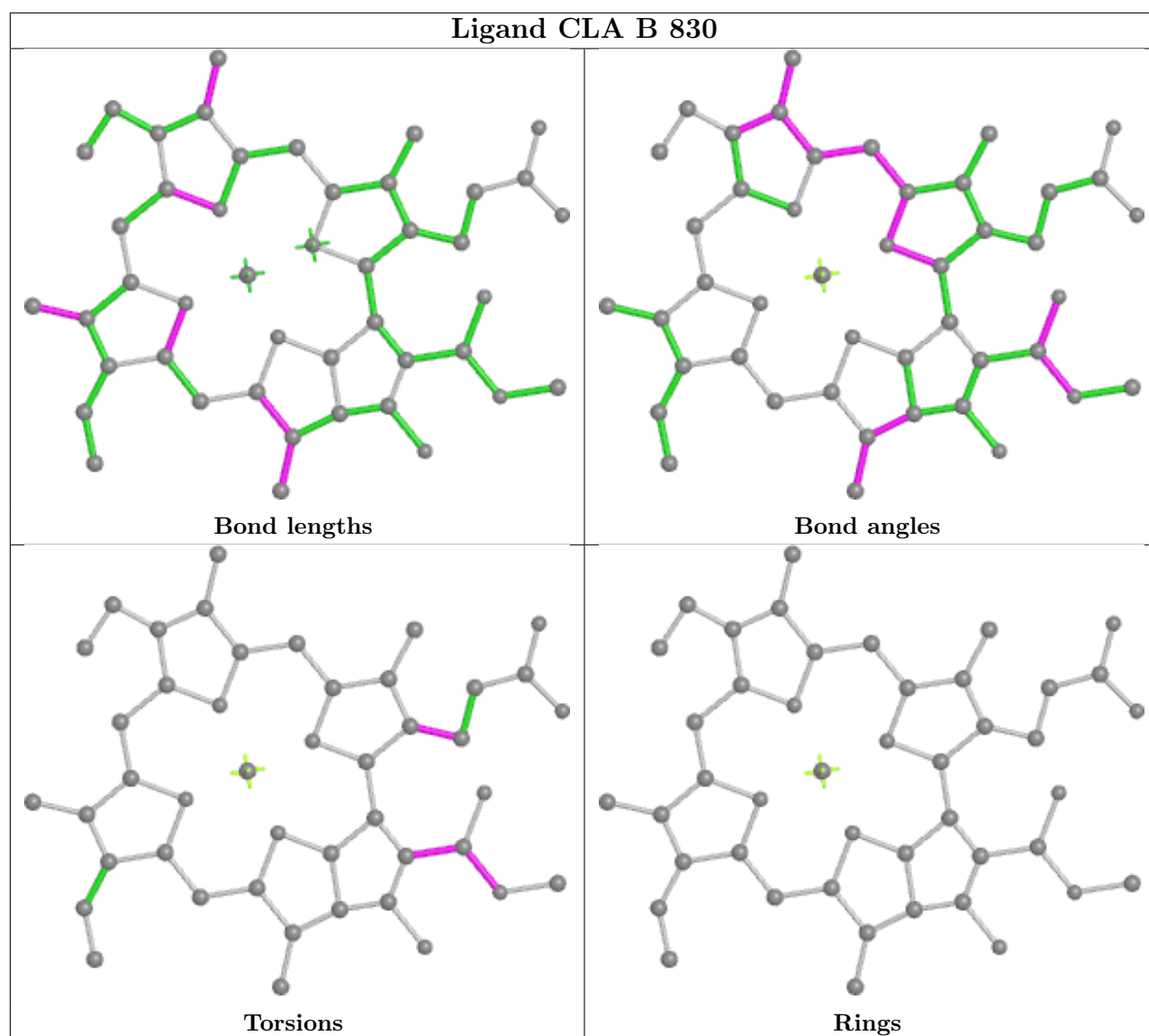
## Ligand CLA B 811



## Ligand CLA A 828



**Ligand CLA L 205****Ligand CLA A 833**



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	740/755 (98%)	-0.40	11 (1%) 73 46	2, 50, 98, 135	0
2	B	739/740 (99%)	-0.54	2 (0%) 94 84	2, 26, 68, 102	0
3	C	80/80 (100%)	-0.55	0 100 100	2, 20, 44, 49	0
4	D	138/138 (100%)	-0.47	1 (0%) 87 69	3, 30, 54, 101	0
5	E	69/75 (92%)	-0.36	0 100 100	22, 44, 65, 79	0
6	F	141/164 (85%)	-0.28	2 (1%) 75 49	20, 68, 85, 92	0
7	I	38/38 (100%)	-0.58	0 100 100	2, 6, 29, 53	0
8	J	41/41 (100%)	-0.51	0 100 100	62, 78, 91, 105	0
9	K	47/83 (56%)	0.32	6 (12%) 3 1	87, 123, 138, 154	0
10	L	151/154 (98%)	-0.57	1 (0%) 87 69	2, 4, 34, 84	0
11	M	31/31 (100%)	-0.49	0 100 100	4, 16, 38, 65	0
12	X	29/35 (82%)	-0.16	1 (3%) 45 19	40, 52, 78, 92	0
All	All	2244/2334 (96%)	-0.45	24 (1%) 80 56	2, 35, 92, 154	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	315	TYR	5.1
4	D	1	THR	4.4
2	B	212	LEU	3.6
1	A	244	LEU	3.5
6	F	26	ALA	3.4

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	CLA	M	102	45/65	0.61	0.31	57,105,140,154	0
14	CLA	A	816	45/65	0.69	0.30	79,117,143,153	0
17	BCR	A	847	40/40	0.72	0.36	81,120,140,149	0
17	BCR	A	848	40/40	0.73	0.37	70,105,135,149	0
18	LMG	A	853	48/55	0.73	0.42	30,87,126,134	0
17	BCR	J	105	40/40	0.74	0.30	41,87,128,135	0
14	CLA	A	823	49/65	0.75	0.20	52,90,119,131	0
18	LMG	I	102	40/55	0.76	0.32	23,59,94,118	0
21	LMT	L	202	35/35	0.76	0.33	48,116,152,165	0
17	BCR	A	849	40/40	0.77	0.41	51,93,145,150	0
17	BCR	B	843	40/40	0.77	0.36	49,84,117,135	0
17	BCR	B	847	40/40	0.78	0.25	19,65,98,106	0
17	BCR	F	203	40/40	0.78	0.32	17,68,100,121	0
18	LMG	A	856	30/55	0.79	0.27	6,57,119,135	0
14	CLA	A	828	65/65	0.80	0.22	33,66,102,109	0
19	LHG	M	101	49/49	0.80	0.20	21,63,138,155	0
14	CLA	K	102	45/65	0.80	0.22	75,105,138,139	0
14	CLA	B	837	60/65	0.81	0.27	15,55,86,96	0
14	CLA	A	812	65/65	0.81	0.22	55,87,118,120	0
14	CLA	A	818	54/65	0.81	0.21	69,98,125,135	0
22	DGD	L	207	66/66	0.81	0.28	19,73,129,142	0
14	CLA	A	817	49/65	0.82	0.29	37,101,133,134	0
17	BCR	J	103	40/40	0.82	0.23	34,76,98,103	0
14	CLA	B	817	59/65	0.82	0.22	21,55,83,91	0
14	CLA	A	837	45/65	0.83	0.23	54,78,101,111	0
14	CLA	K	101	41/65	0.83	0.20	86,123,158,168	0
14	CLA	A	844	52/65	0.83	0.22	18,57,85,93	0
17	BCR	A	850	40/40	0.83	0.27	35,65,129,131	0
14	CLA	A	815	45/65	0.83	0.19	59,88,123,130	0
17	BCR	B	846	40/40	0.84	0.25	27,53,73,79	0
14	CLA	J	101	45/65	0.84	0.37	91,111,145,149	0
17	BCR	B	851	40/40	0.84	0.34	20,58,101,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	CLA	A	805	59/65	0.85	0.19	48,72,99,115	0
14	CLA	A	824	51/65	0.85	0.27	41,74,106,112	0
19	LHG	A	854	49/49	0.85	0.29	12,58,82,92	0
14	CLA	A	826	65/65	0.85	0.16	45,74,105,108	0
14	CLA	A	814	60/65	0.85	0.23	47,88,113,115	0
14	CLA	A	836	54/65	0.85	0.22	20,61,102,109	0
14	CLA	B	833	58/65	0.86	0.27	36,72,110,115	0
14	CLA	A	831	65/65	0.86	0.21	29,61,84,92	0
14	CLA	A	811	45/65	0.86	0.16	66,99,125,133	0
14	CLA	A	807	65/65	0.86	0.18	30,58,84,90	0
14	CLA	A	813	54/65	0.86	0.18	47,74,102,110	0
14	CLA	B	811	45/65	0.86	0.27	18,41,61,84	0
14	CLA	A	810	65/65	0.86	0.20	18,73,122,135	0
14	CLA	B	820	47/65	0.86	0.20	43,72,103,108	0
14	CLA	A	830	65/65	0.87	0.19	29,62,92,95	0
14	CLA	B	812	45/65	0.87	0.16	31,63,89,93	0
14	CLA	A	820	65/65	0.87	0.21	39,74,99,107	0
17	BCR	J	104	40/40	0.87	0.19	52,90,119,124	0
15	PQN	B	842	33/33	0.87	0.21	27,47,66,70	0
14	CLA	A	832	50/65	0.87	0.19	6,35,65,91	0
14	CLA	B	822	55/65	0.87	0.21	42,68,95,96	0
14	CLA	A	825	59/65	0.87	0.26	23,57,97,109	0
14	CLA	A	821	43/65	0.87	0.22	46,104,144,150	0
19	LHG	B	850	23/49	0.87	0.20	46,85,113,119	0
14	CLA	F	202	45/65	0.87	0.24	60,89,119,125	0
14	CLA	A	809	65/65	0.87	0.20	12,58,97,102	0
14	CLA	J	102	37/65	0.87	0.27	76,99,123,137	0
14	CLA	B	834	45/65	0.88	0.19	28,47,69,71	0
14	CLA	B	836	45/65	0.88	0.33	37,62,94,95	0
14	CLA	A	804	65/65	0.88	0.17	33,72,99,106	0
14	CLA	A	808	51/65	0.88	0.16	55,76,104,107	0
14	CLA	X	1701	45/65	0.88	0.20	49,78,108,114	0
17	BCR	B	844	40/40	0.88	0.25	22,48,88,97	0
14	CLA	B	819	65/65	0.88	0.23	22,65,95,106	0
14	CLA	B	816	55/65	0.89	0.23	35,70,107,140	0
14	CLA	B	804	54/65	0.89	0.19	2,22,41,48	0
14	CLA	A	822	65/65	0.89	0.20	25,61,95,101	0
14	CLA	A	829	65/65	0.89	0.20	33,59,84,91	0
14	CLA	B	821	45/65	0.89	0.17	40,67,93,94	0
17	BCR	A	851	40/40	0.89	0.23	15,47,82,98	0
14	CLA	B	813	65/65	0.89	0.22	15,46,72,76	0
14	CLA	B	828	65/65	0.89	0.21	2,35,53,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
17	BCR	B	845	40/40	0.89	0.23	16,50,105,117	0
14	CLA	B	814	65/65	0.89	0.20	19,51,86,91	0
14	CLA	B	815	45/65	0.89	0.18	35,56,89,92	0
15	PQN	A	845	33/33	0.89	0.21	61,89,118,121	0
14	CLA	L	205	65/65	0.90	0.18	2,19,91,104	0
14	CLA	B	823	45/65	0.90	0.19	4,35,68,80	0
17	BCR	M	103	40/40	0.90	0.22	2,22,50,56	0
14	CLA	B	825	46/65	0.90	0.21	10,38,62,64	0
14	CLA	B	838	65/65	0.90	0.20	16,62,101,117	0
14	CLA	A	834	65/65	0.90	0.20	2,11,39,45	0
14	CLA	B	832	65/65	0.90	0.27	29,60,86,95	0
14	CLA	A	819	54/65	0.90	0.17	35,68,90,106	0
14	CLA	A	857	65/65	0.90	0.21	12,39,65,76	0
17	BCR	I	101	40/40	0.90	0.23	2,2,24,41	0
14	CLA	B	835	45/65	0.90	0.22	18,53,81,85	0
14	CLA	L	206	65/65	0.91	0.19	2,20,49,59	0
14	CLA	A	839	65/65	0.91	0.19	2,32,71,94	0
19	LHG	A	855	27/49	0.91	0.20	20,53,90,91	0
14	CLA	B	824	54/65	0.91	0.17	21,38,60,61	0
14	CLA	A	806	65/65	0.91	0.20	40,74,110,115	0
14	CLA	F	201	51/65	0.91	0.15	10,49,98,117	0
14	CLA	A	838	51/65	0.91	0.18	10,33,53,76	0
17	BCR	A	852	40/40	0.92	0.18	2,37,64,66	0
14	CLA	B	826	65/65	0.92	0.17	11,39,65,70	0
14	CLA	B	827	65/65	0.92	0.20	2,22,74,76	0
14	CLA	A	841	65/65	0.92	0.21	6,42,97,106	0
18	LMG	B	849	55/55	0.92	0.20	2,31,57,61	0
14	CLA	B	830	45/65	0.92	0.18	19,47,69,87	0
14	CLA	B	807	65/65	0.92	0.22	2,9,40,63	0
14	CLA	A	843	65/65	0.92	0.21	2,2,24,33	0
14	CLA	A	803	65/65	0.92	0.17	16,41,61,82	0
14	CLA	B	818	60/65	0.92	0.20	23,44,74,81	0
14	CLA	L	204	65/65	0.92	0.18	2,15,46,67	0
14	CLA	A	827	65/65	0.92	0.18	3,42,119,141	0
14	CLA	B	808	65/65	0.93	0.17	2,13,45,50	0
17	BCR	B	848	40/40	0.93	0.20	2,8,34,35	0
14	CLA	B	829	65/65	0.93	0.17	2,21,53,72	0
14	CLA	B	809	65/65	0.93	0.18	2,12,40,63	0
14	CLA	B	810	65/65	0.93	0.18	2,2,33,43	0
17	BCR	I	103	40/40	0.93	0.17	2,2,21,39	0
14	CLA	B	840	65/65	0.93	0.19	2,2,26,31	0
14	CLA	B	806	65/65	0.93	0.16	2,24,51,64	0

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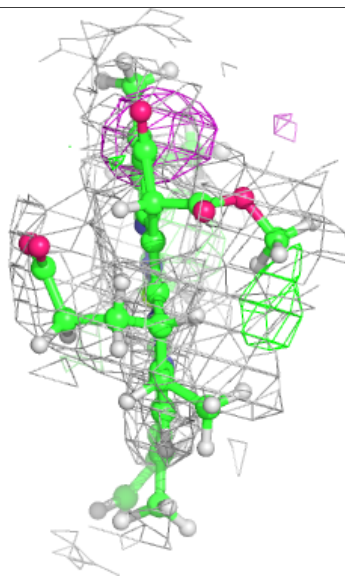
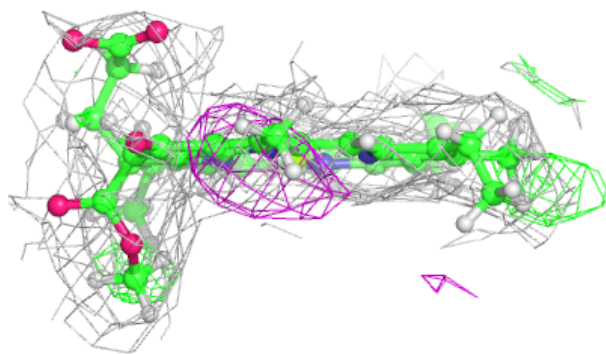
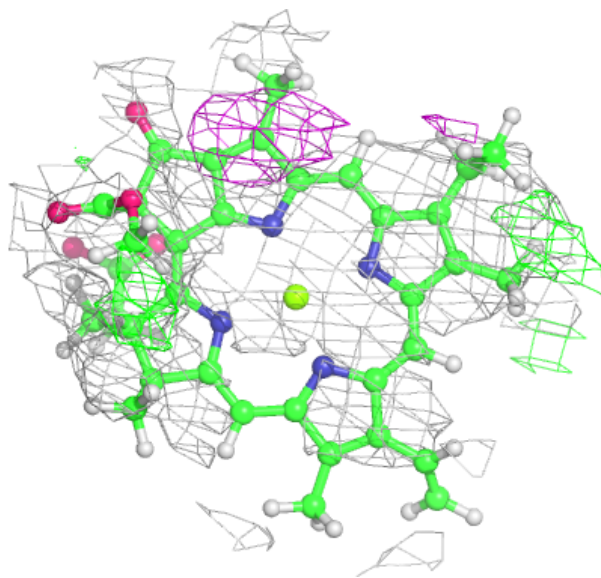
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	CLA	B	802	65/65	0.93	0.15	2,23,44,50	0
17	BCR	L	201	40/40	0.93	0.16	2,8,33,35	0
17	BCR	L	208	40/40	0.93	0.21	2,12,60,72	0
14	CLA	A	840	47/65	0.94	0.16	2,28,49,67	0
13	CL0	A	801	65/65	0.94	0.17	2,20,45,48	0
14	CLA	A	842	65/65	0.94	0.16	11,47,91,109	0
14	CLA	B	805	65/65	0.94	0.18	2,30,63,75	0
14	CLA	A	835	65/65	0.94	0.18	2,6,35,63	0
14	CLA	B	831	49/65	0.94	0.18	8,43,70,96	0
14	CLA	B	839	47/65	0.94	0.22	23,48,67,79	0
20	CA	B	801	1/1	0.94	0.10	43,43,43,43	0
14	CLA	A	833	65/65	0.94	0.20	2,37,109,114	0
14	CLA	B	841	65/65	0.94	0.18	2,3,26,29	0
14	CLA	A	802	65/65	0.95	0.17	2,12,28,48	0
14	CLA	B	803	65/65	0.95	0.15	2,7,27,38	0
16	SF4	A	846	8/8	0.98	0.17	3,20,62,92	0
16	SF4	C	101	8/8	0.98	0.16	2,25,32,45	0
16	SF4	C	102	8/8	0.98	0.15	12,19,36,38	0
20	CA	L	203	1/1	0.99	0.09	2,2,2,2	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.

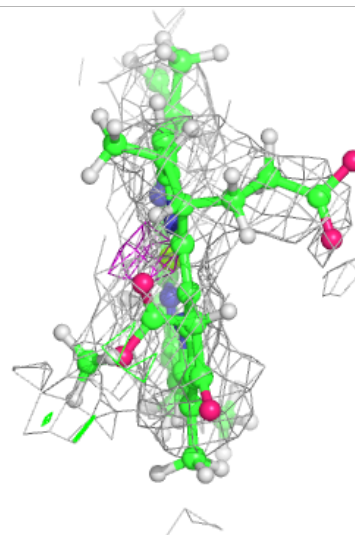
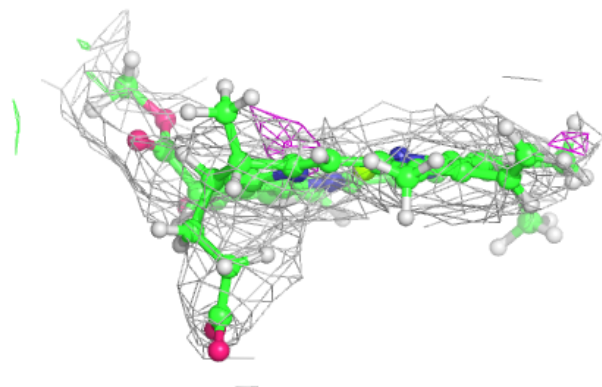
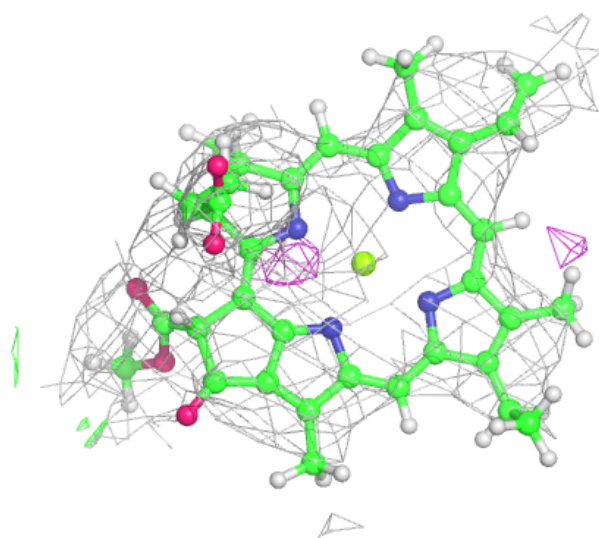
**Electron density around CLA M 102:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



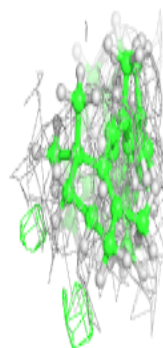
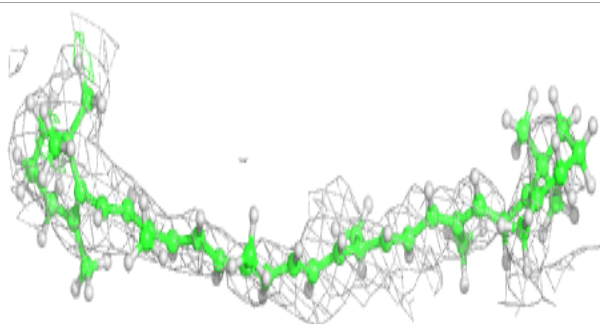
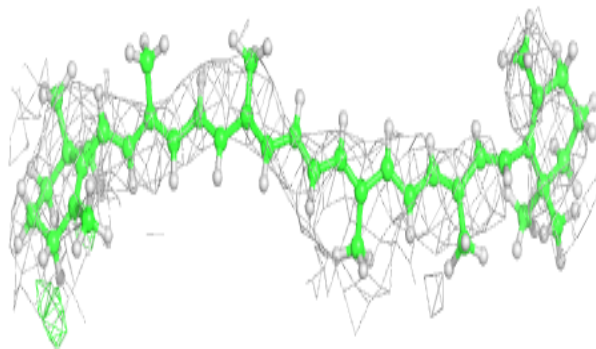
**Electron density around CLA A 816:**

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

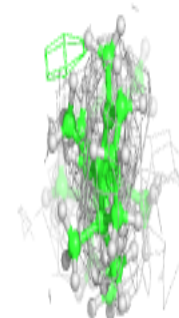
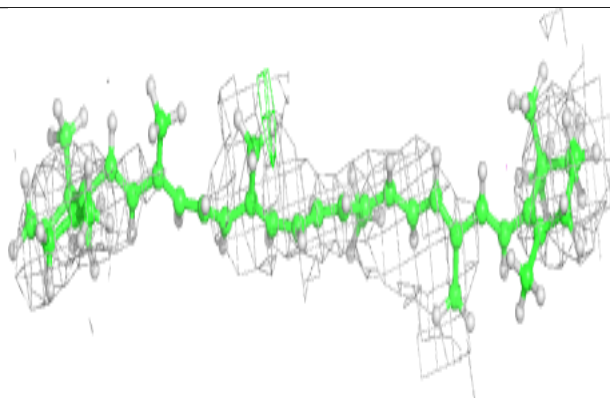
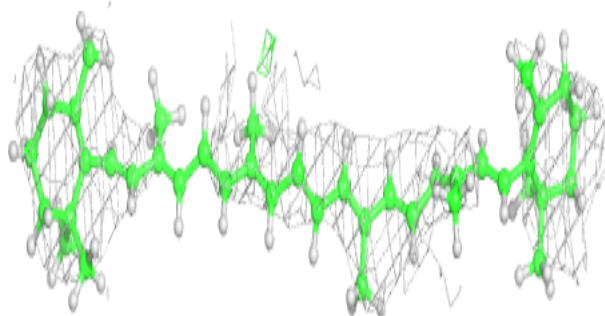


**Electron density around BCR A 847:**

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

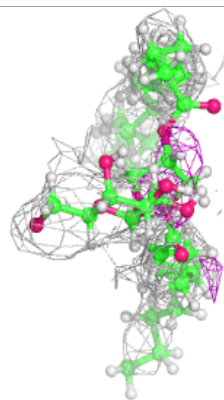
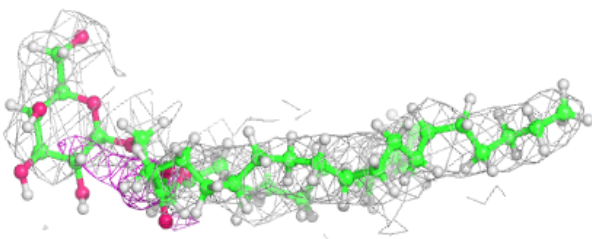
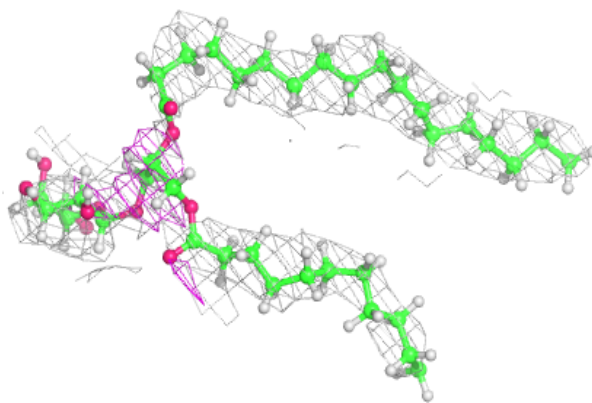
**Electron density around BCR A 848:**

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

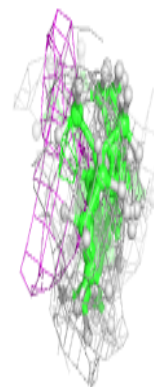
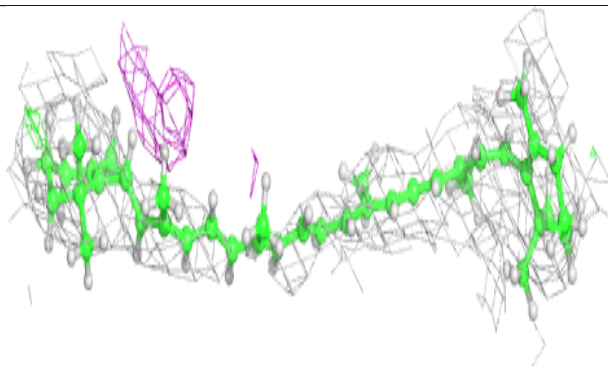
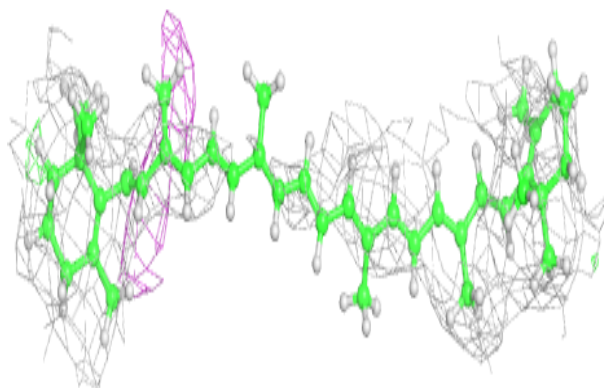


**Electron density around LMG A 853:**

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

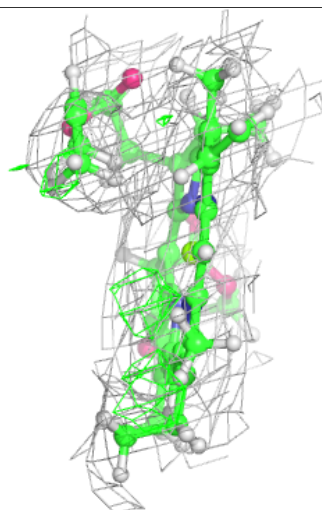
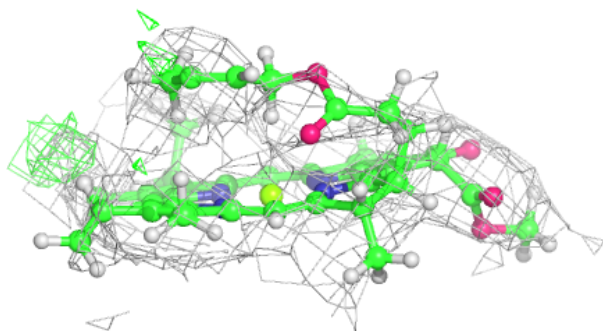
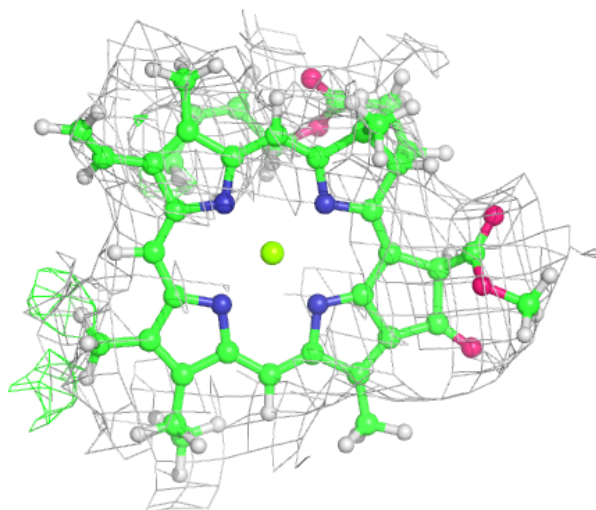
**Electron density around BCR J 105:**

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



**Electron density around CLA A 823:**

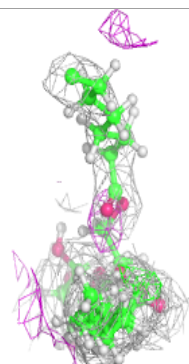
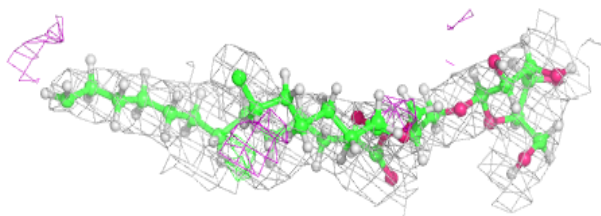
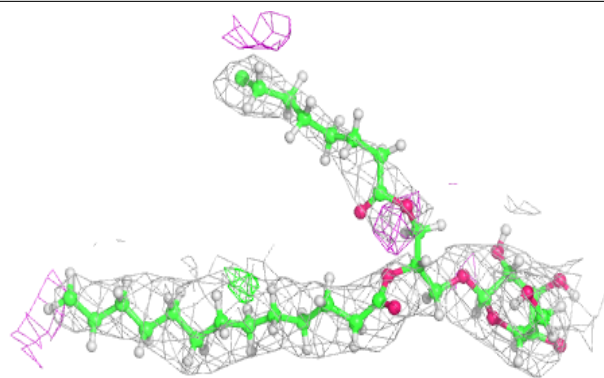
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



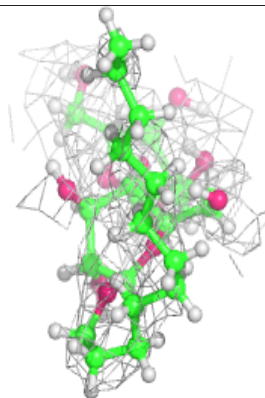
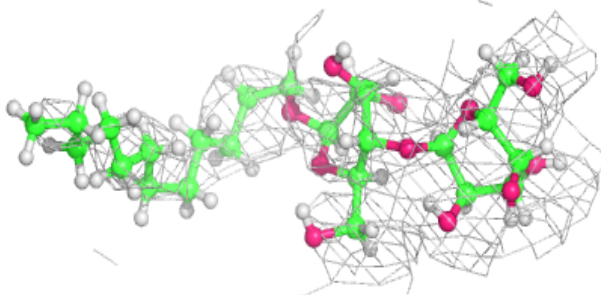
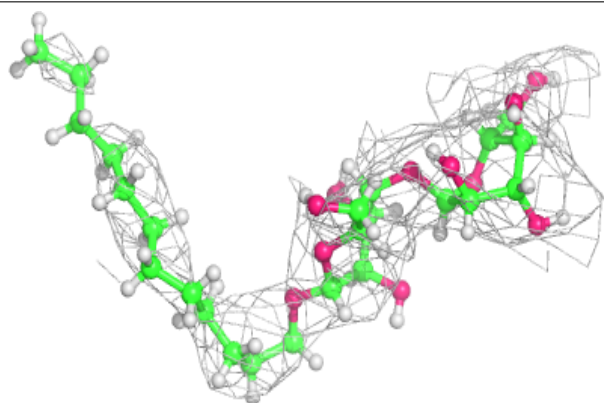


**Electron density around LMG I 102:**

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

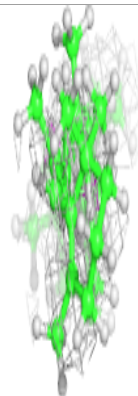
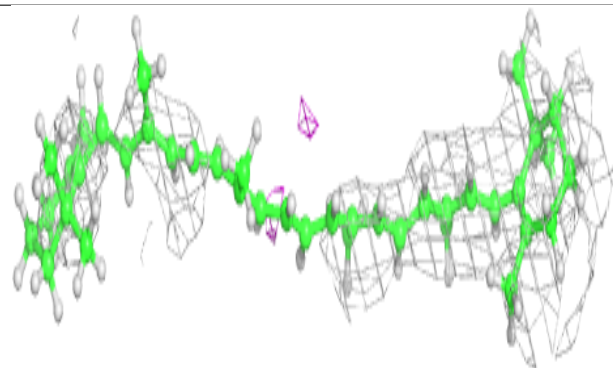
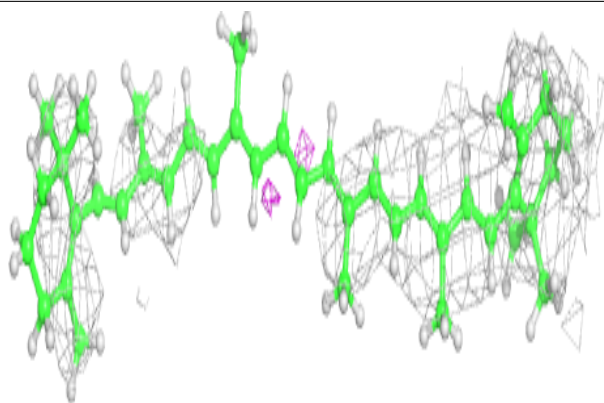
**Electron density around LMT L 202:**

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

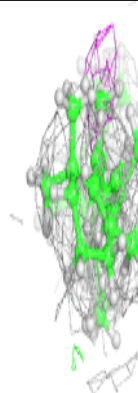
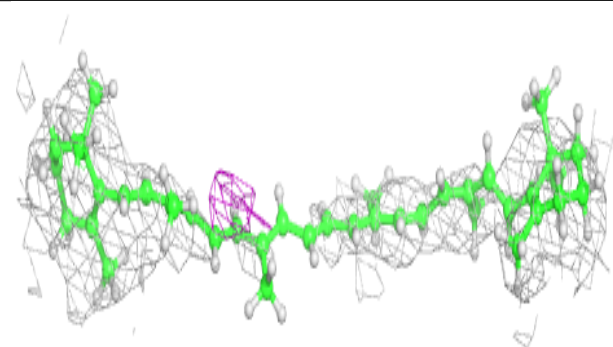
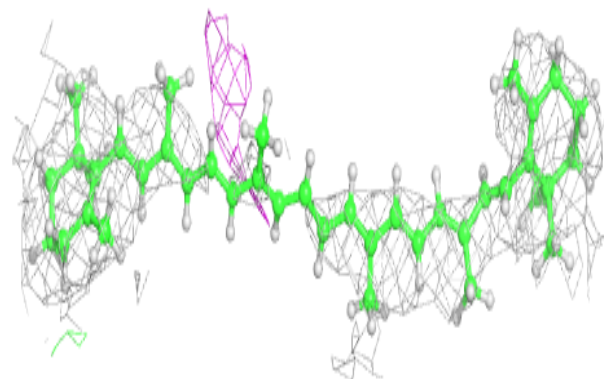


**Electron density around BCR A 849:**

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

**Electron density around BCR B 843:**

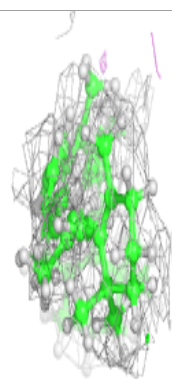
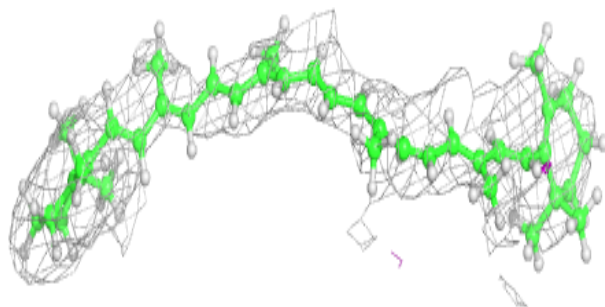
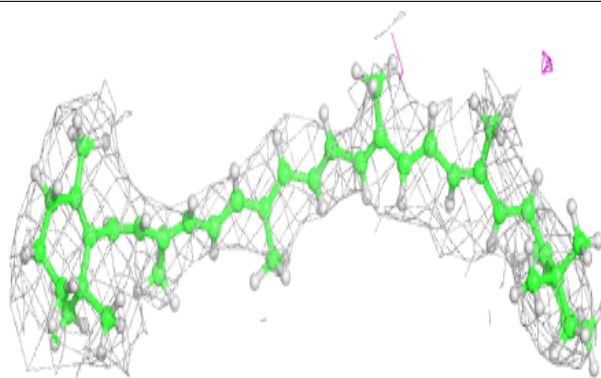
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



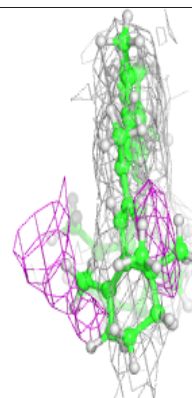
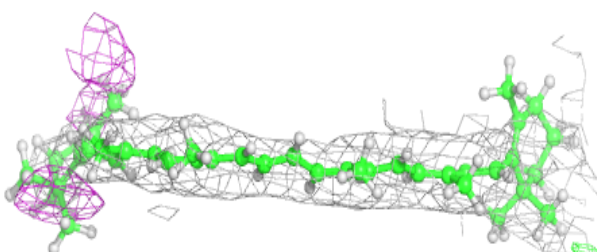
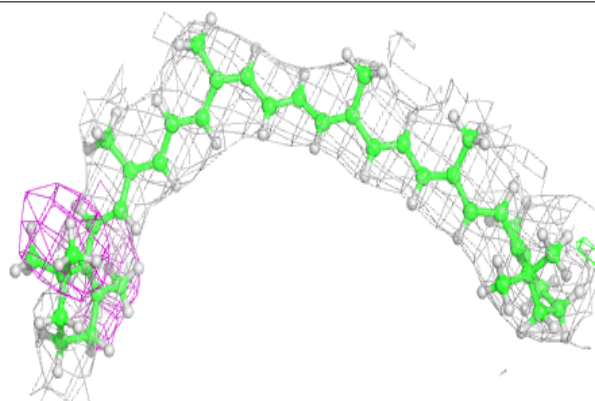


**Electron density around BCR B 847:**

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

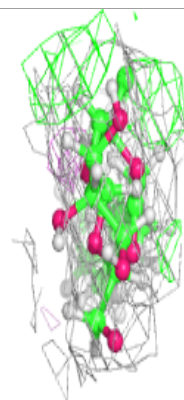
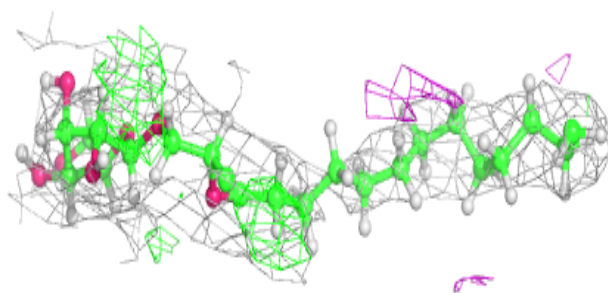
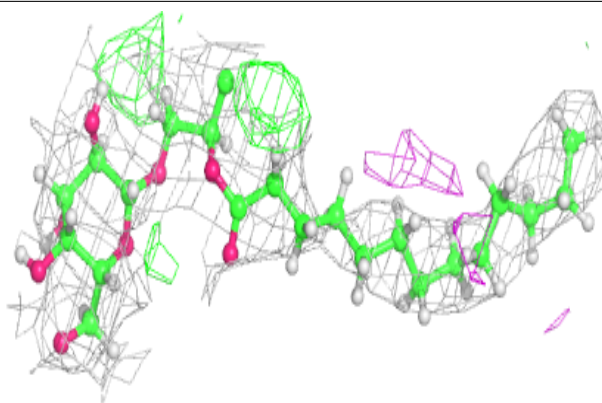
**Electron density around BCR F 203:**

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

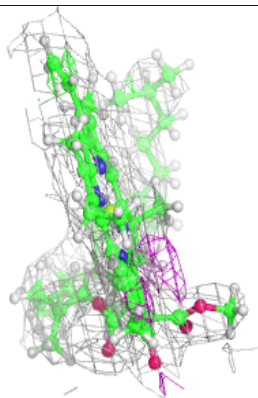
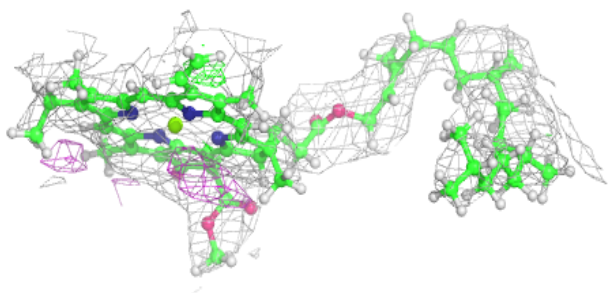
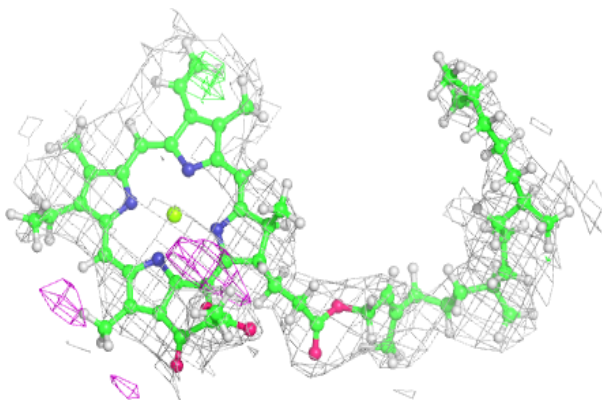


**Electron density around LMG A 856:**

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

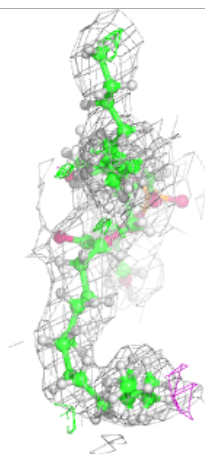
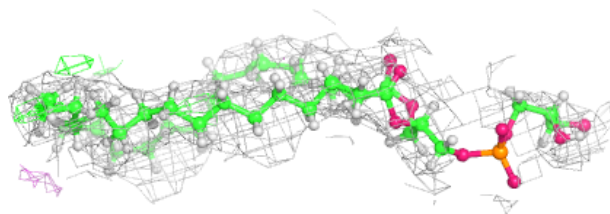
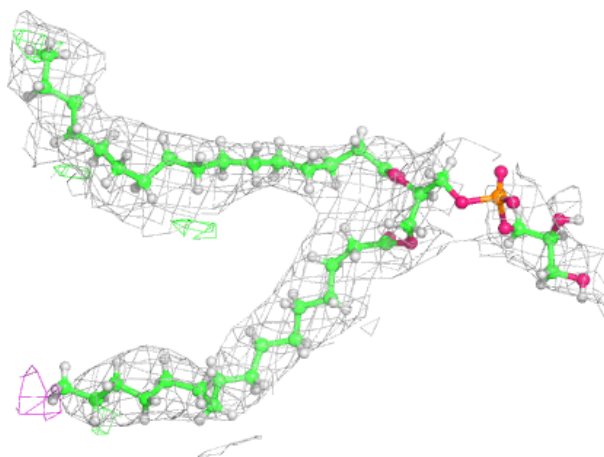
**Electron density around CLA A 828:**

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



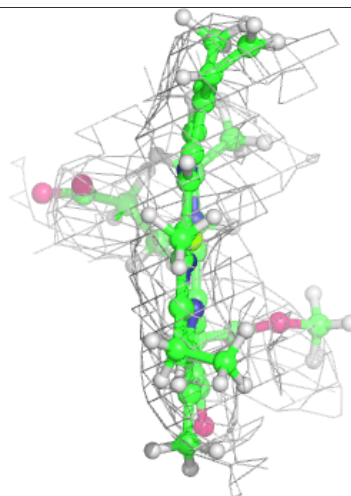
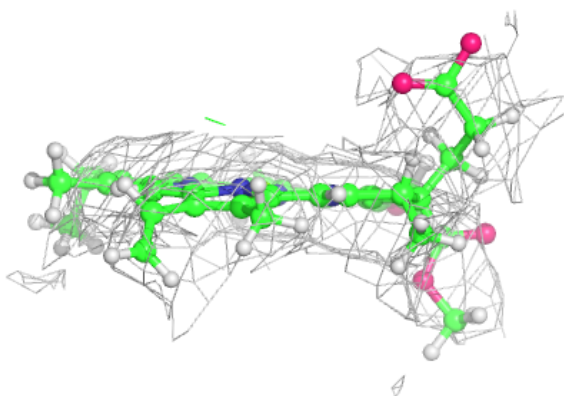
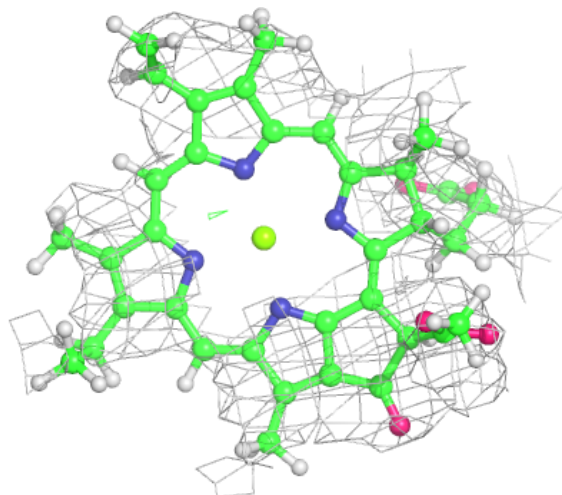
**Electron density around LHG M 101:**

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



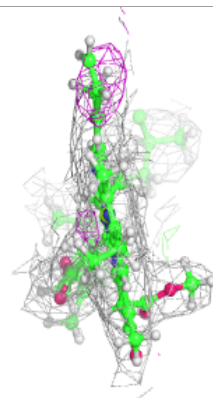
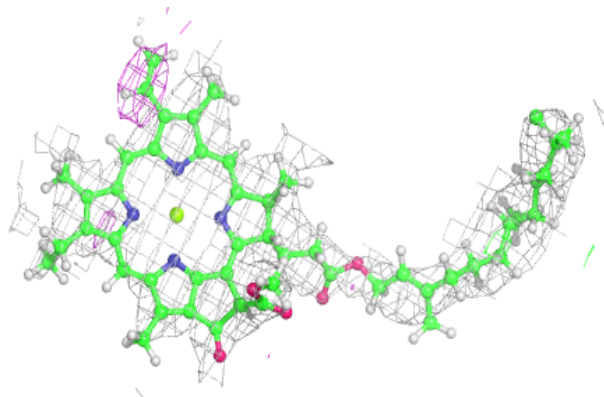
**Electron density around CLA K 102:**

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

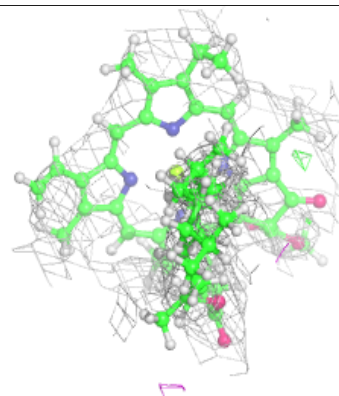
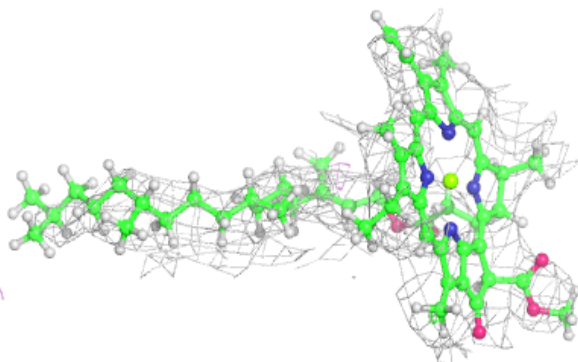
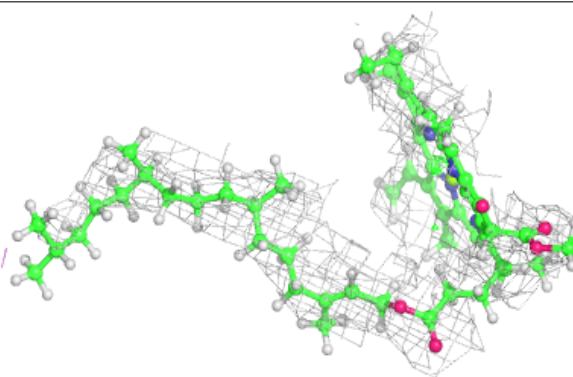


**Electron density around CLA B 837:**

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

**Electron density around CLA A 812:**

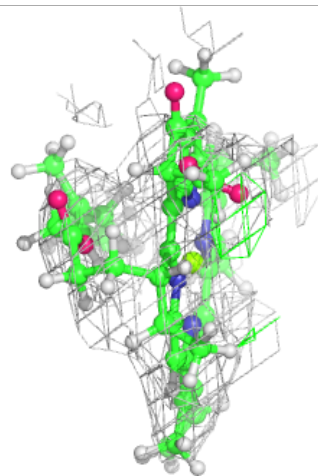
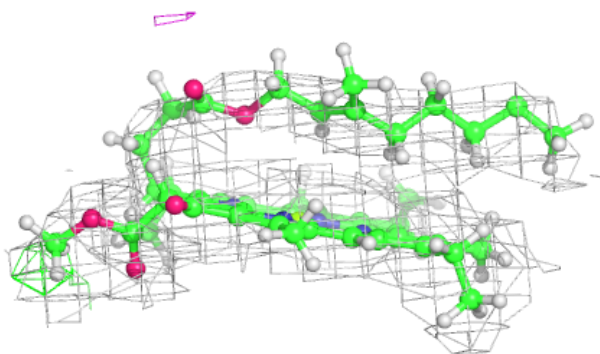
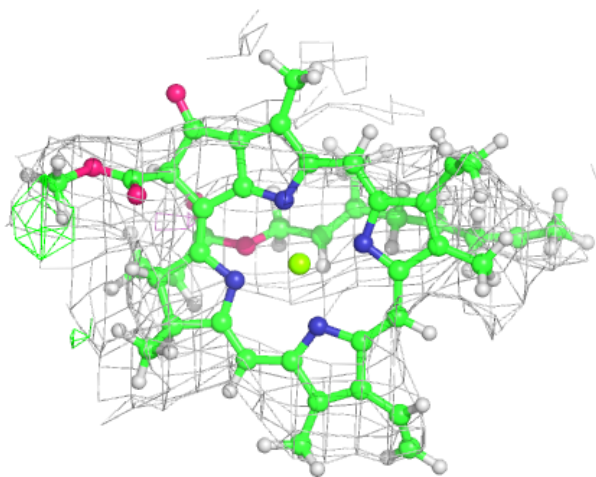
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





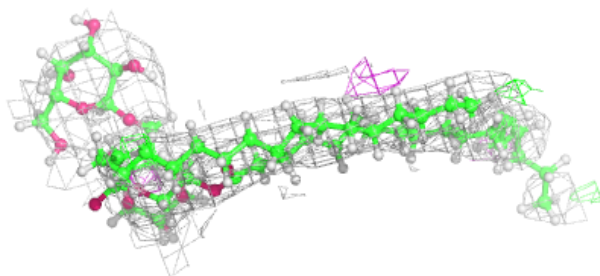
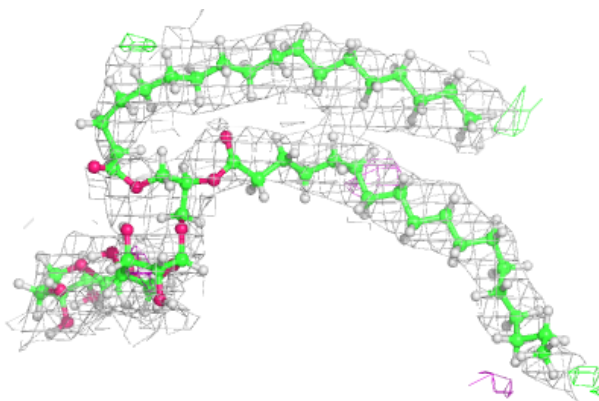
**Electron density around CLA A 818:**

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



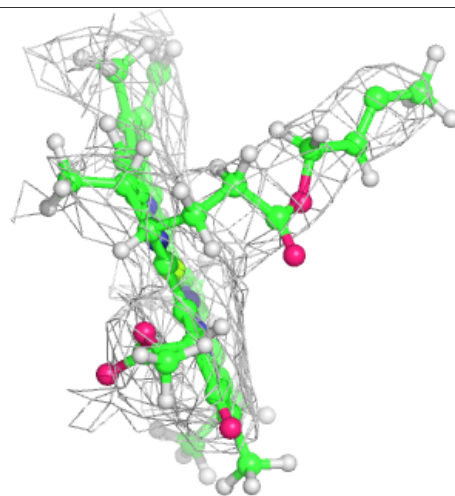
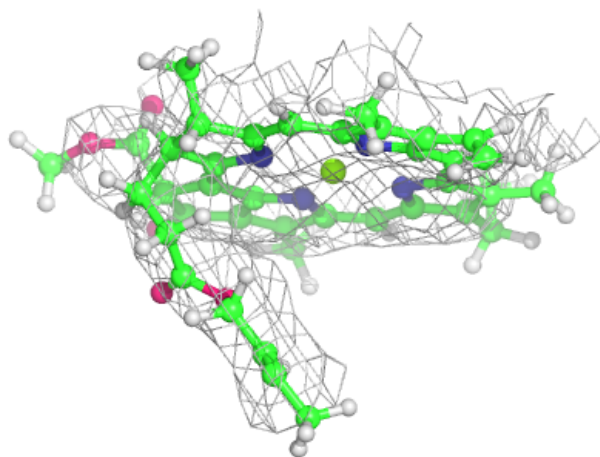
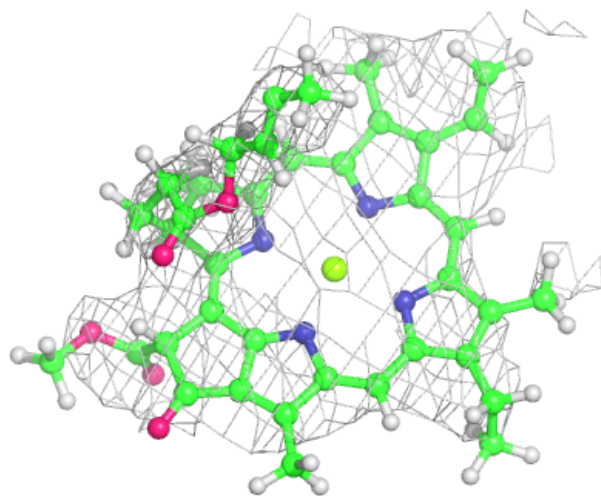
**Electron density around DGD L 207:**

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



**Electron density around CLA A 817:**

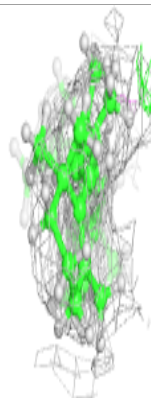
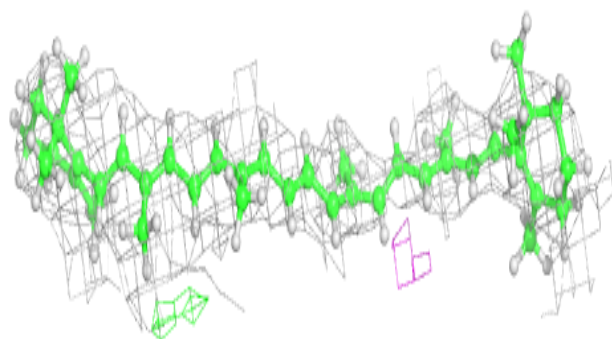
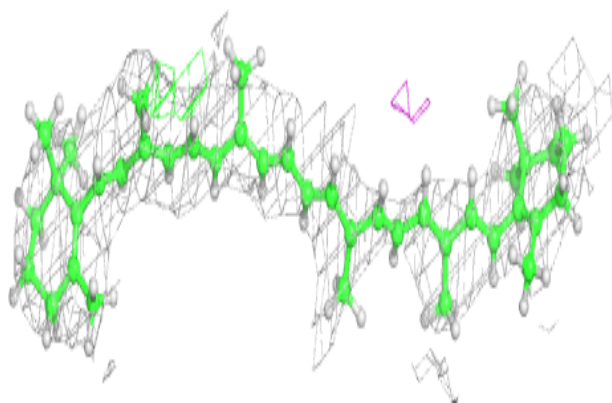
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





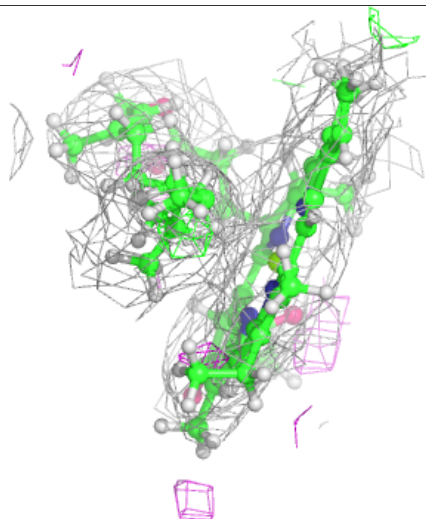
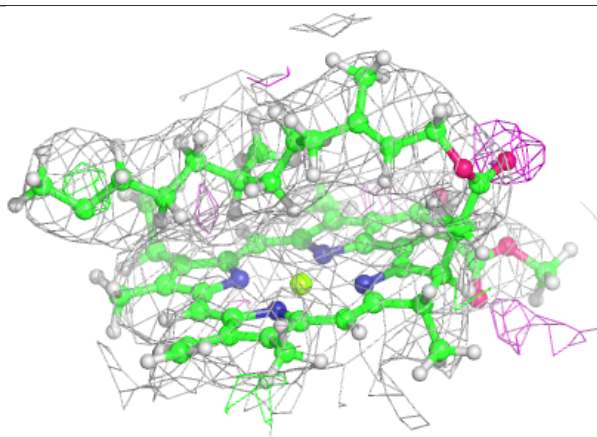
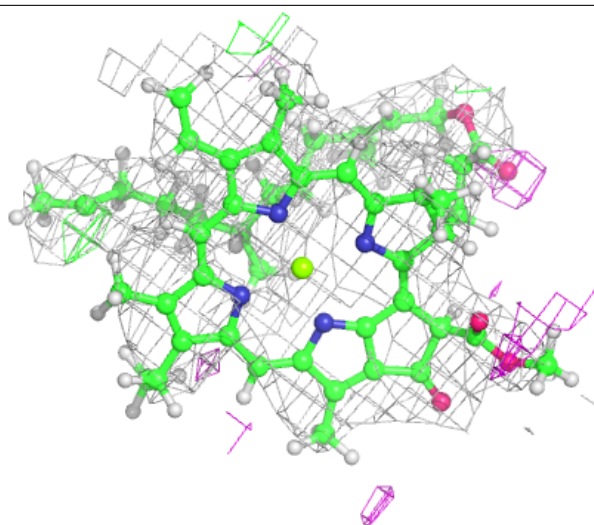
**Electron density around BCR J 103:**

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



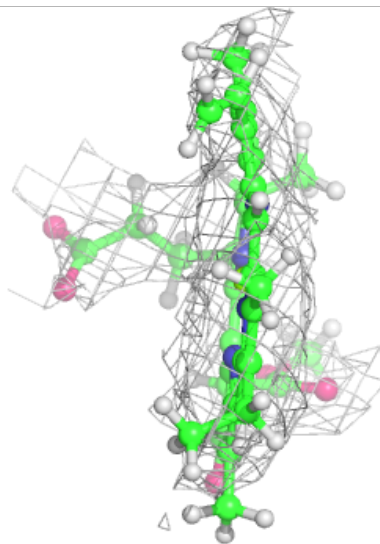
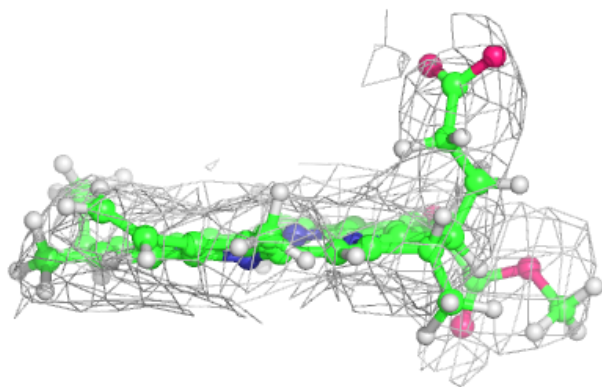
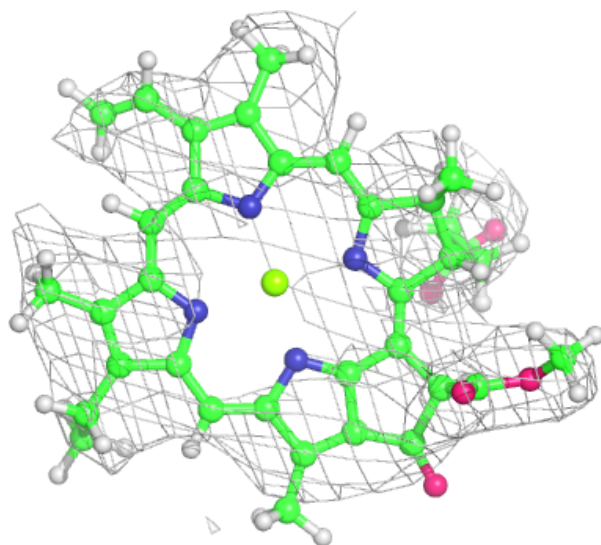
**Electron density around CLA B 817:**

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



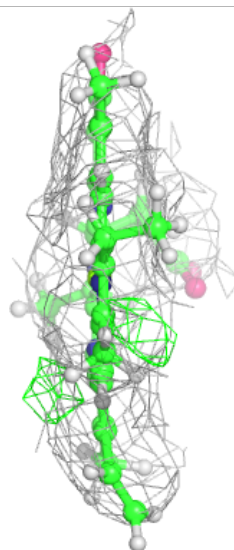
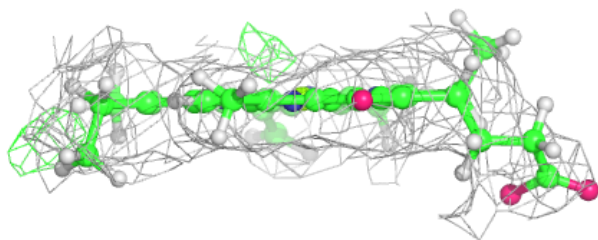
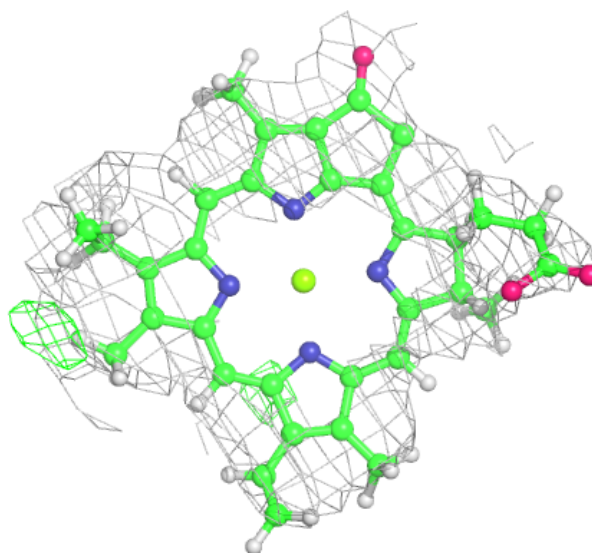
**Electron density around CLA A 837:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



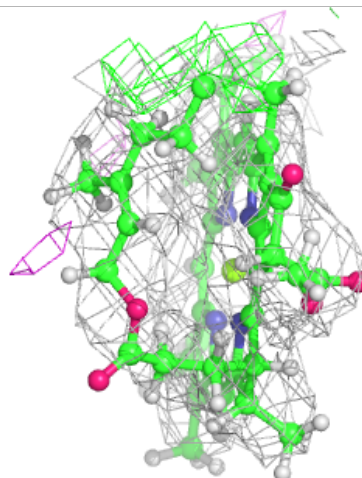
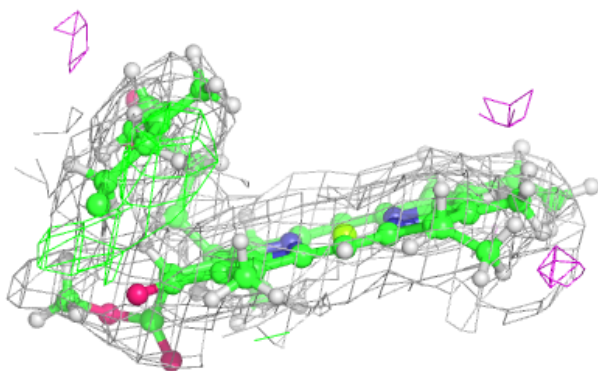
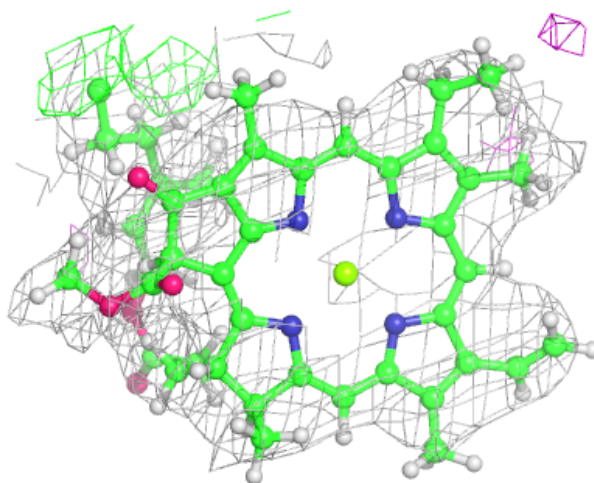
**Electron density around CLA K 101:**

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



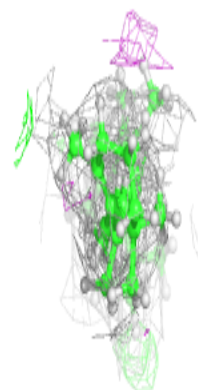
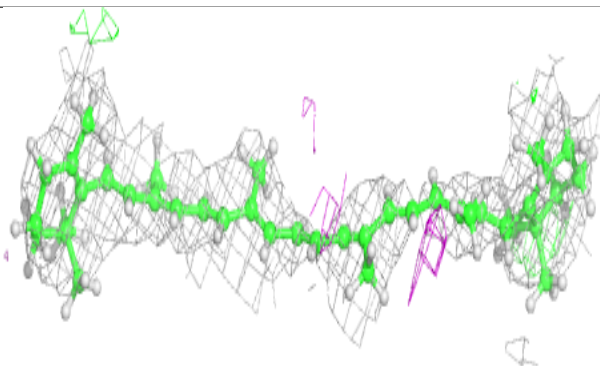
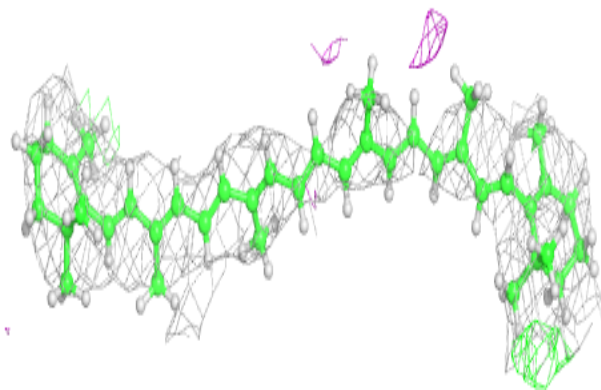
**Electron density around CLA A 844:**

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



**Electron density around BCR A 850:**

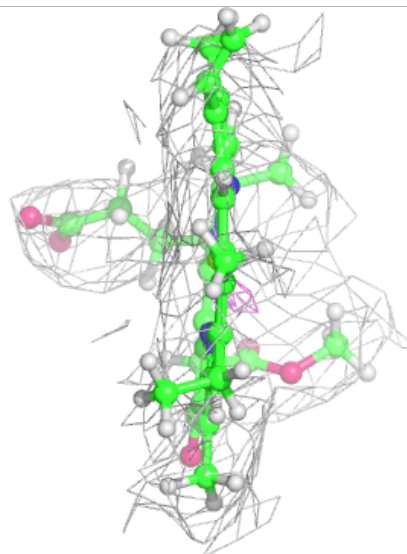
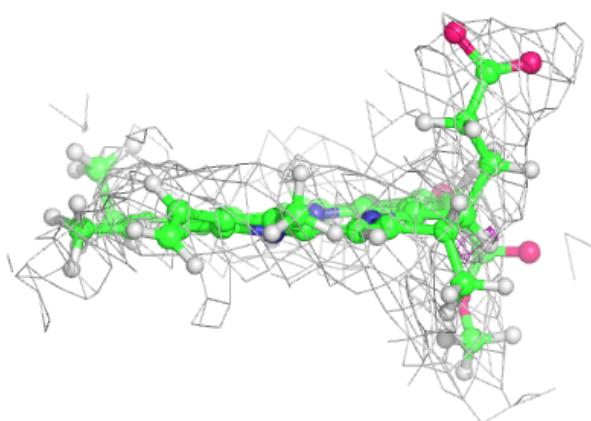
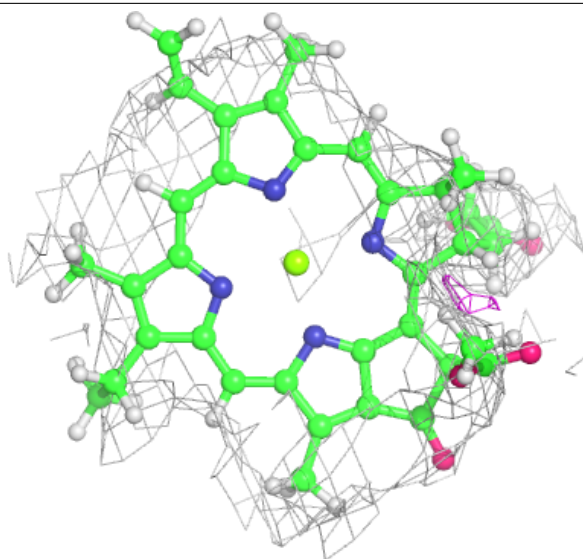
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





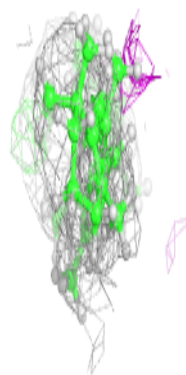
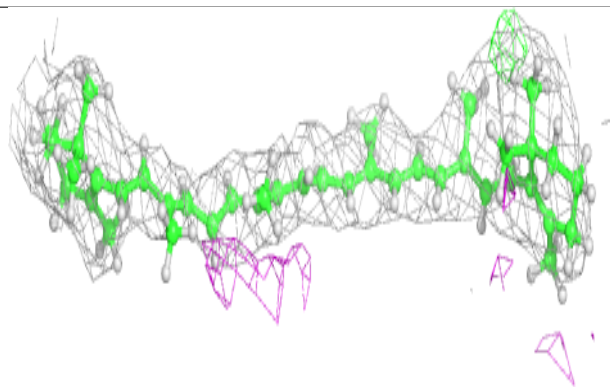
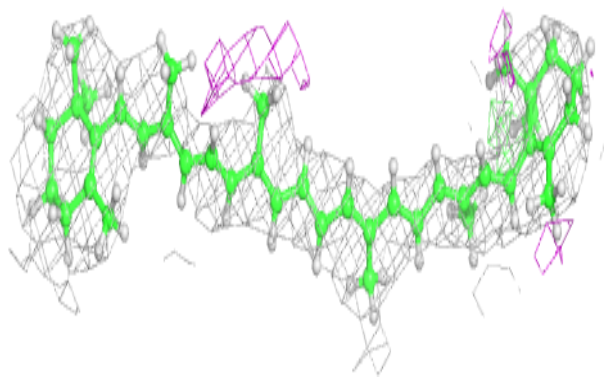
**Electron density around CLA A 815:**

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



**Electron density around BCR B 846:**

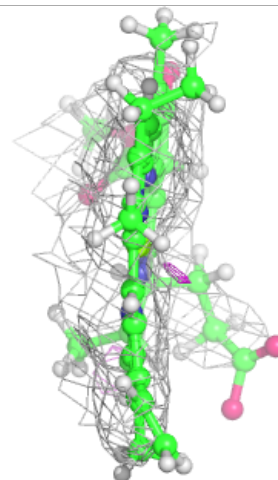
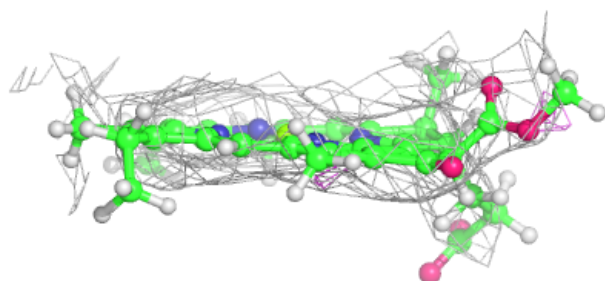
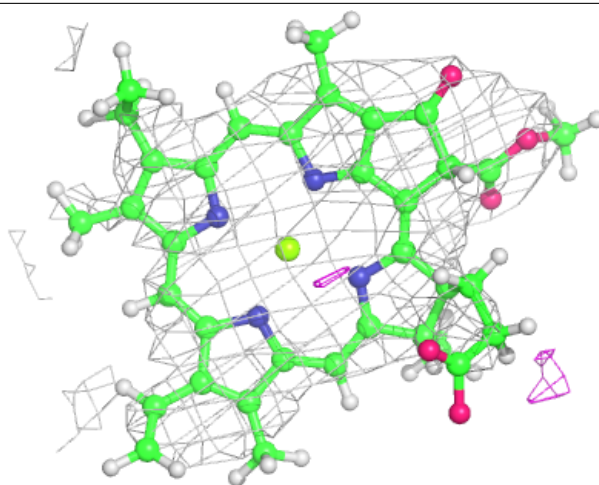
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





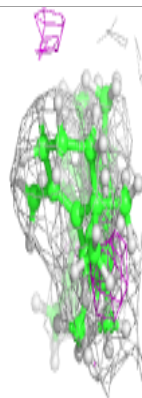
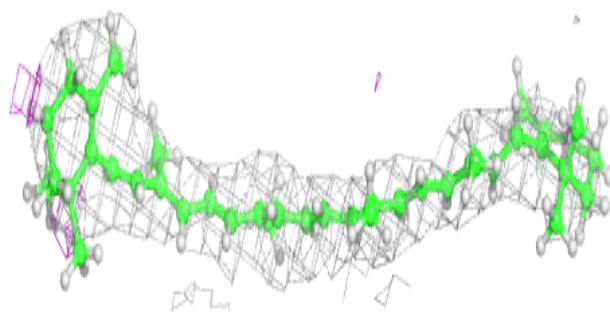
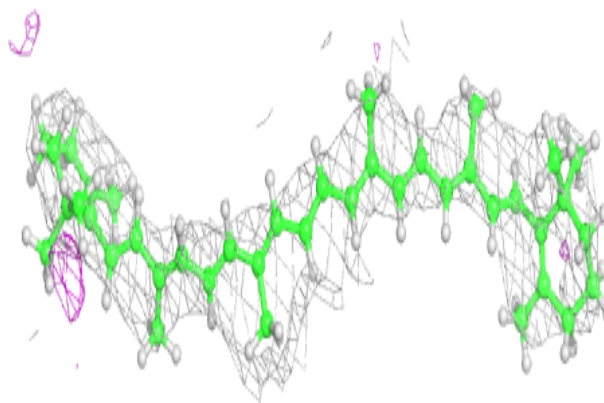
**Electron density around CLA J 101:**

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



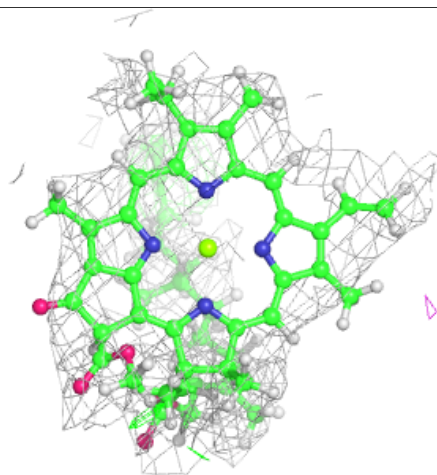
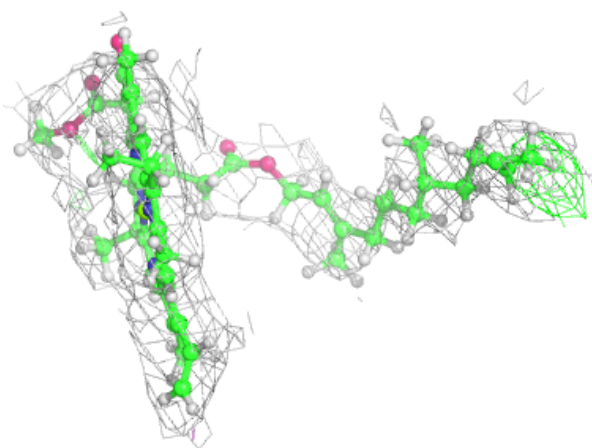
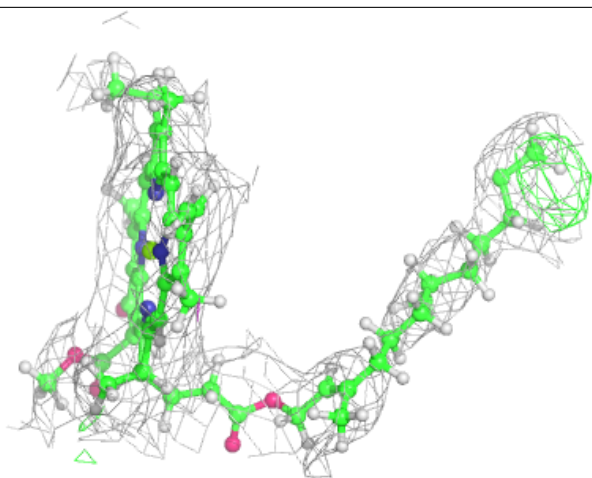
**Electron density around BCR B 851:**

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



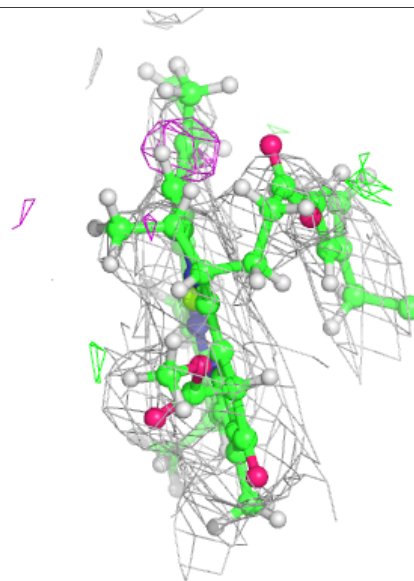
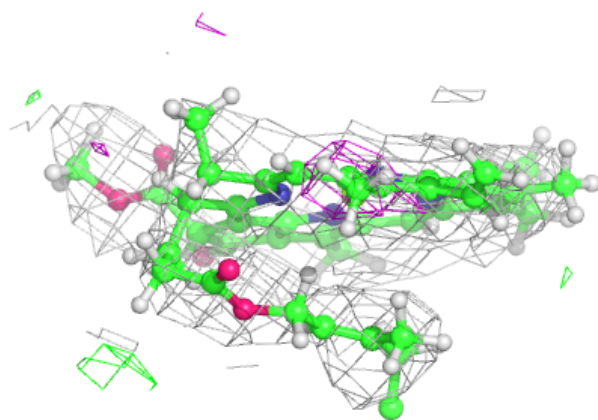
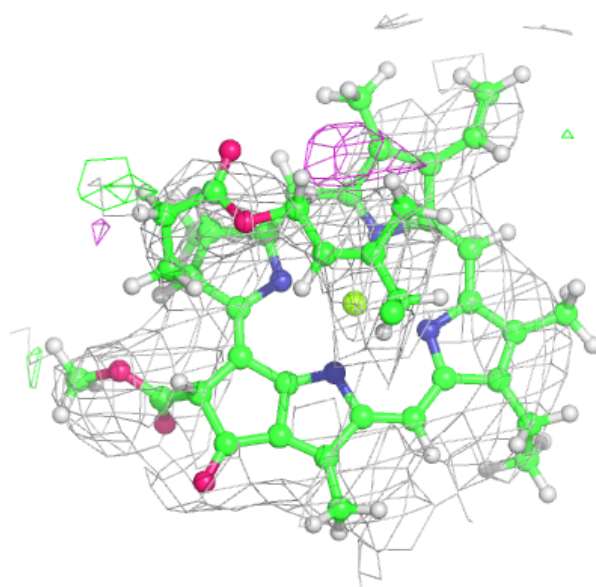
**Electron density around CLA A 805:**

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



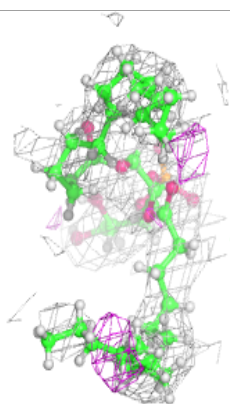
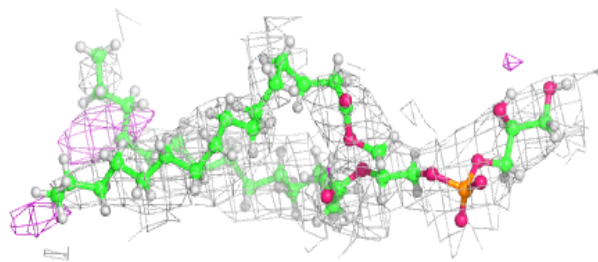
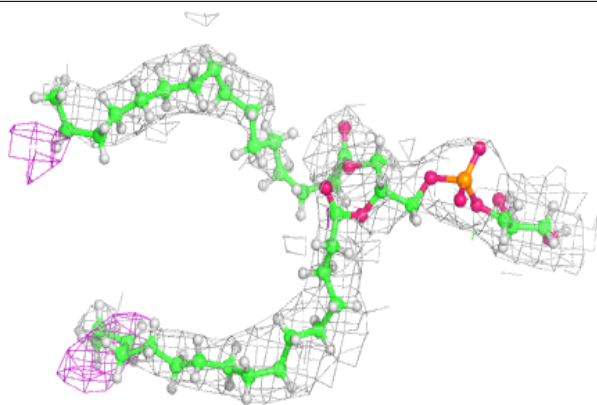
**Electron density around CLA A 824:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



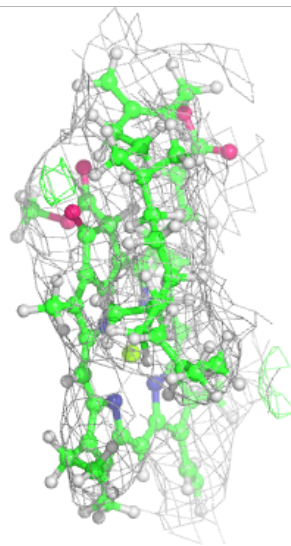
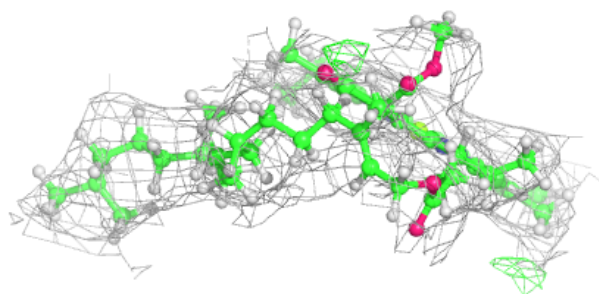
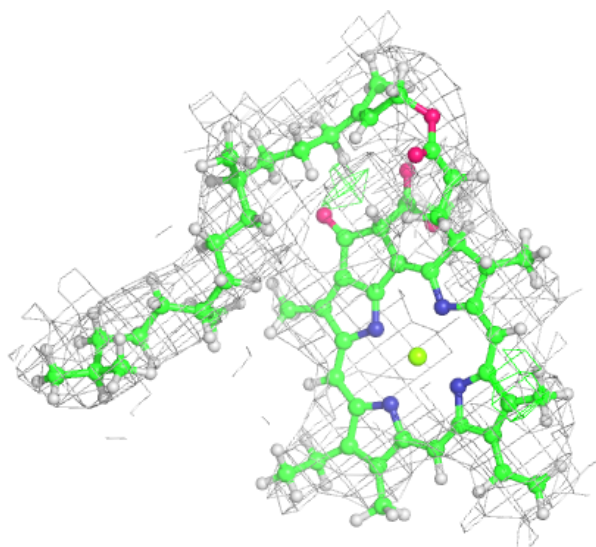
**Electron density around LHG A 854:**

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



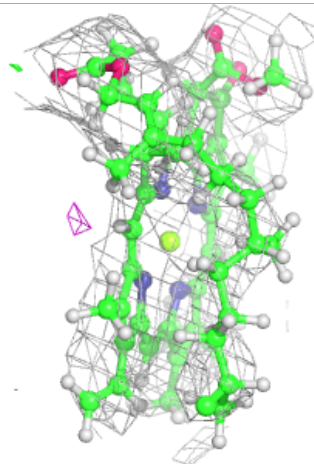
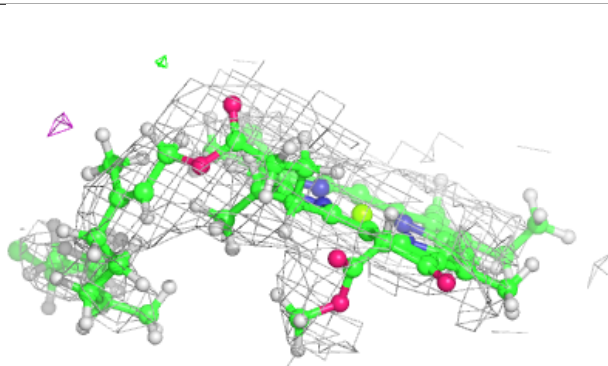
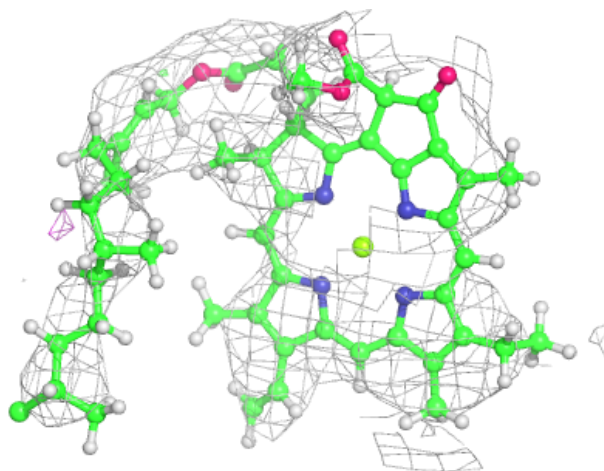
**Electron density around CLA A 826:**

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



**Electron density around CLA A 814:**

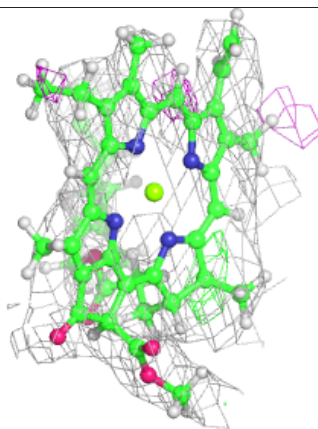
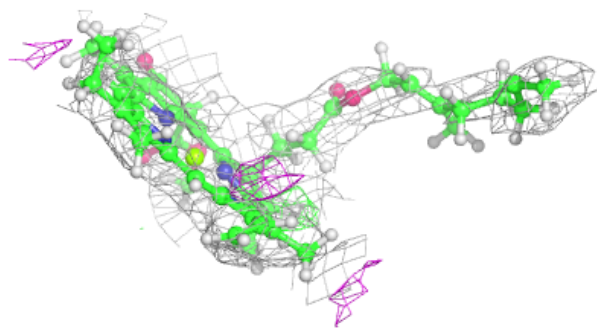
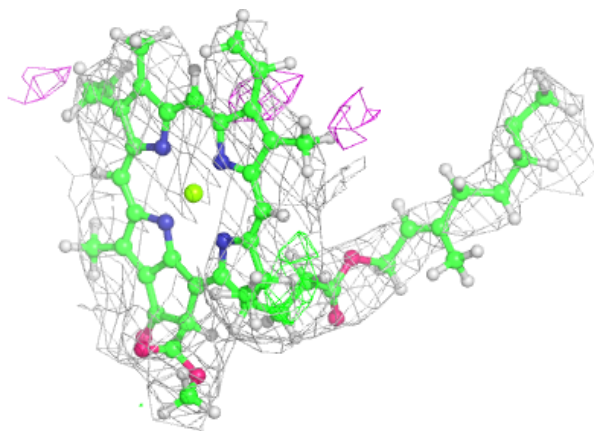
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA A 836:**

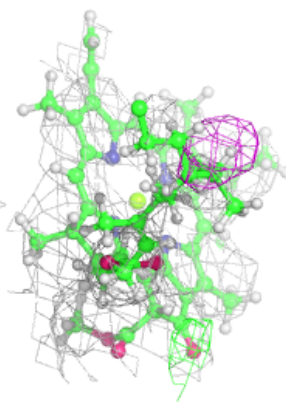
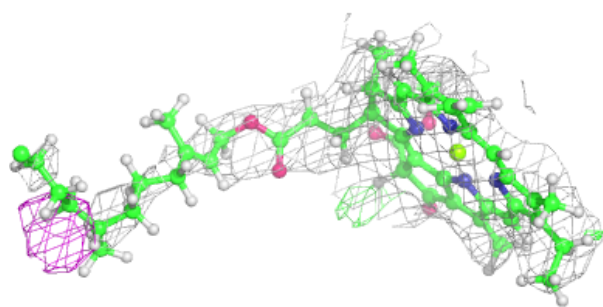
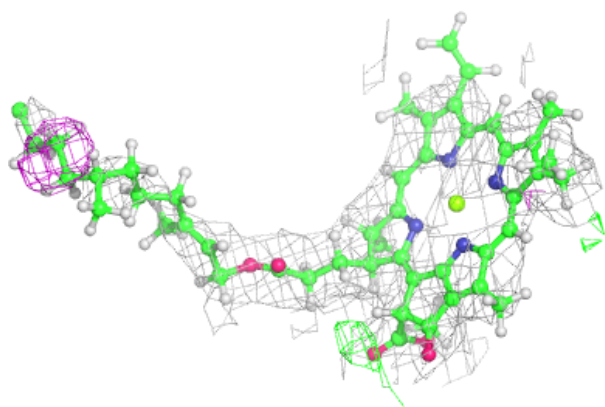
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



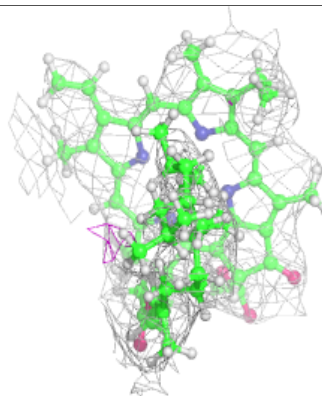
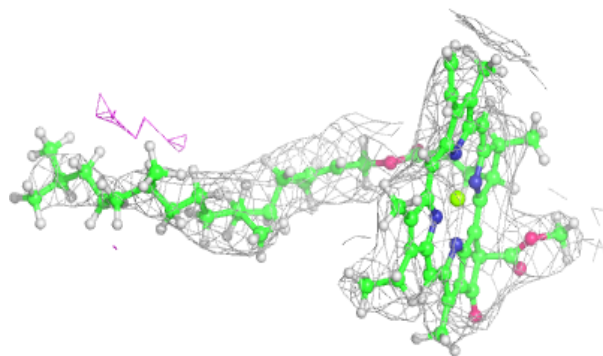
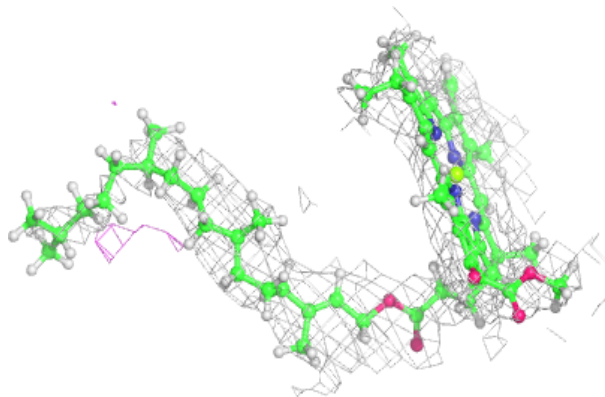


**Electron density around CLA B 833:**

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

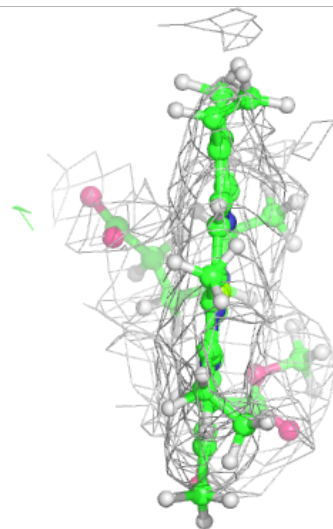
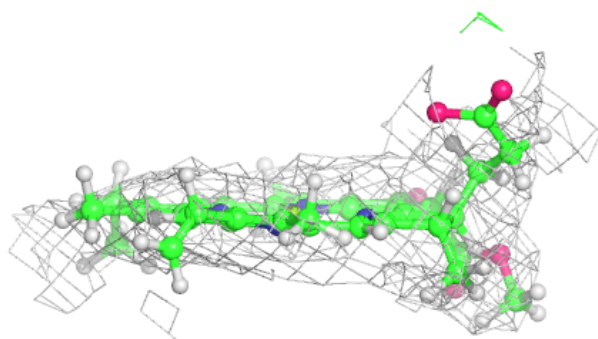
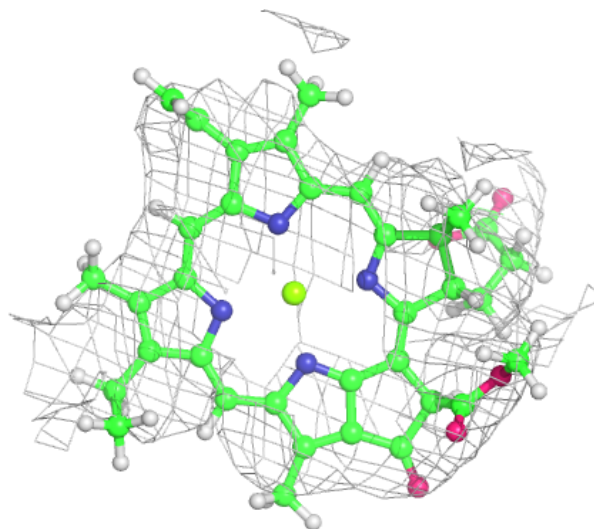
**Electron density around CLA A 831:**

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



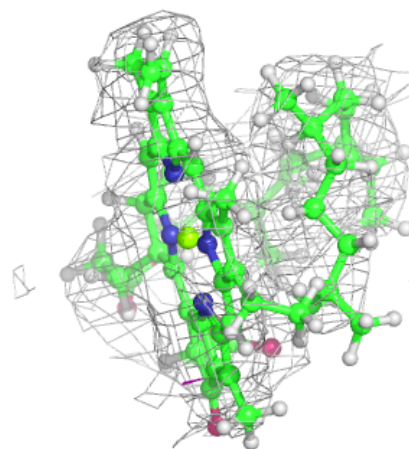
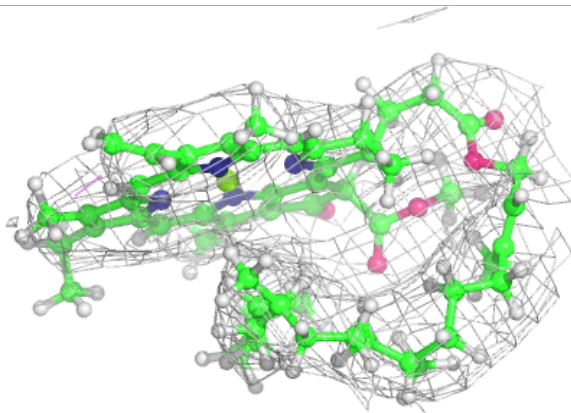
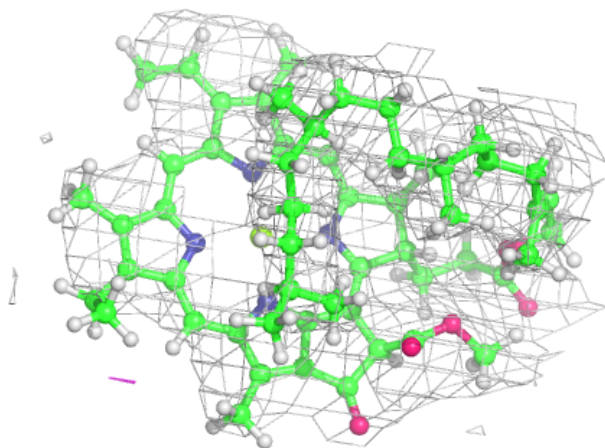
**Electron density around CLA A 811:**

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



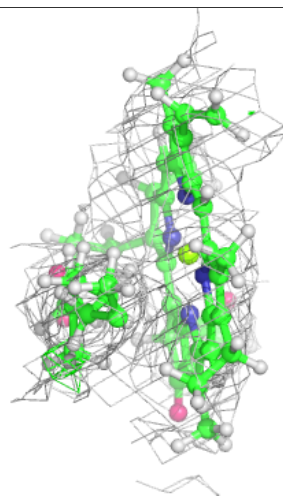
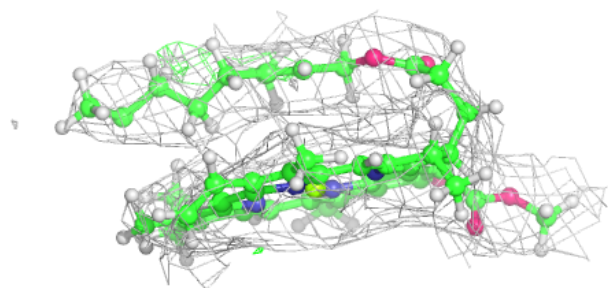
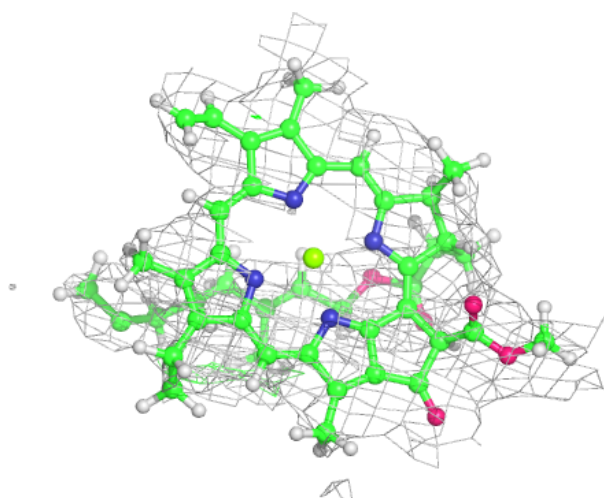
**Electron density around CLA A 807:**

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



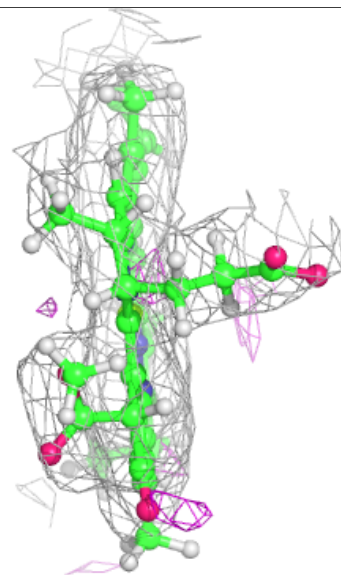
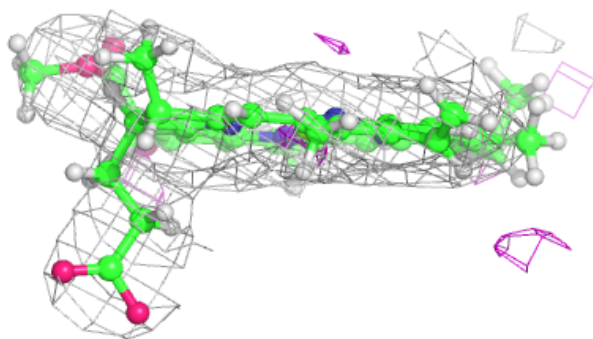
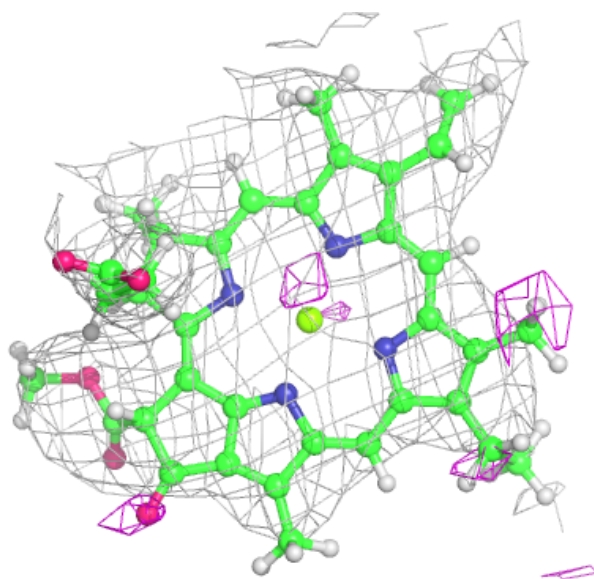
**Electron density around CLA A 813:**

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



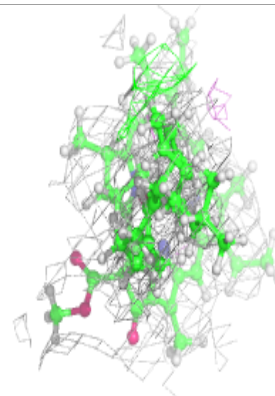
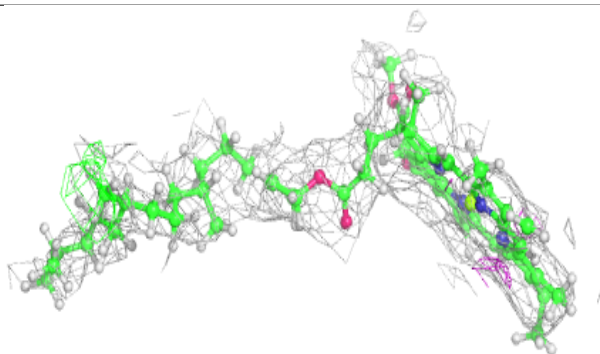
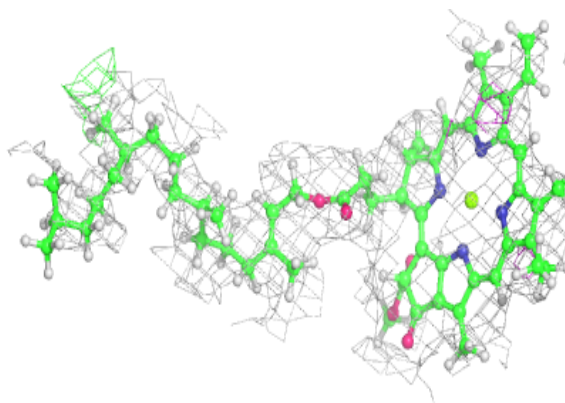
**Electron density around CLA B 811:**

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



**Electron density around CLA A 810:**

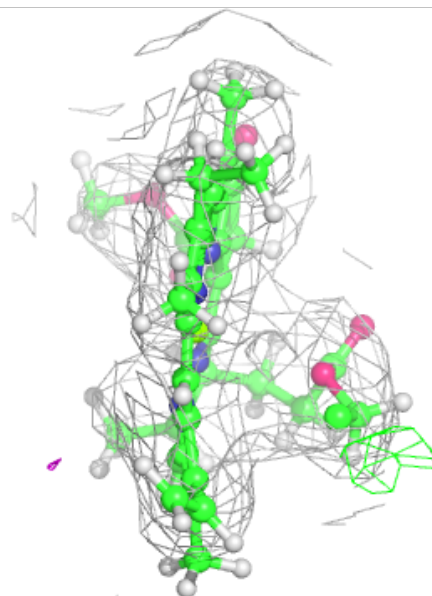
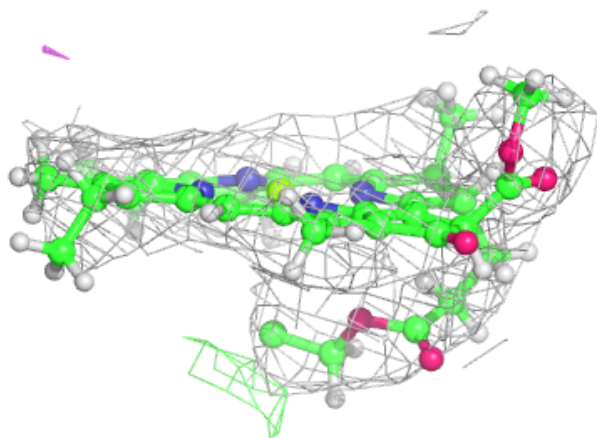
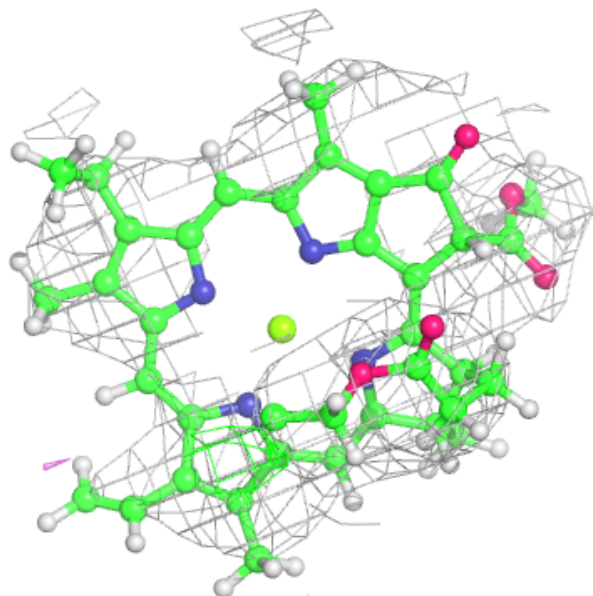
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





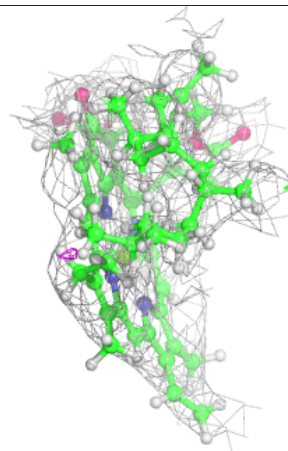
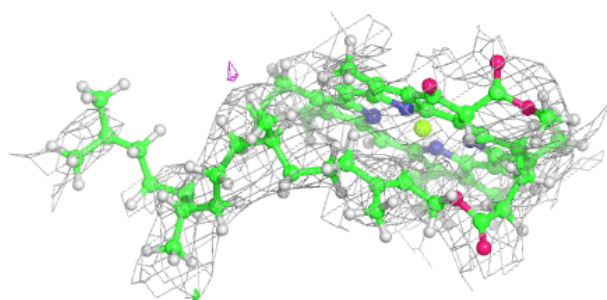
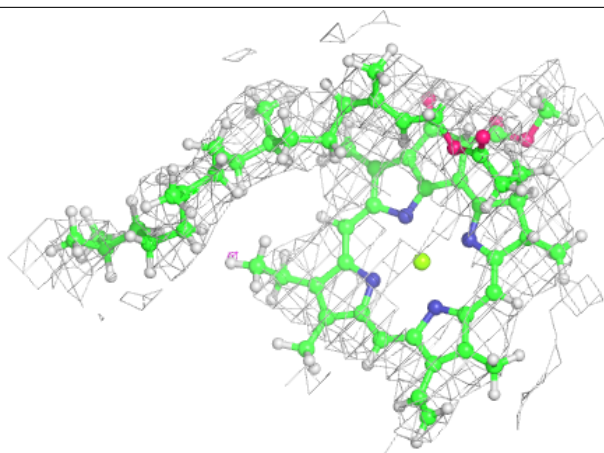
**Electron density around CLA B 820:**

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



**Electron density around CLA A 830:**

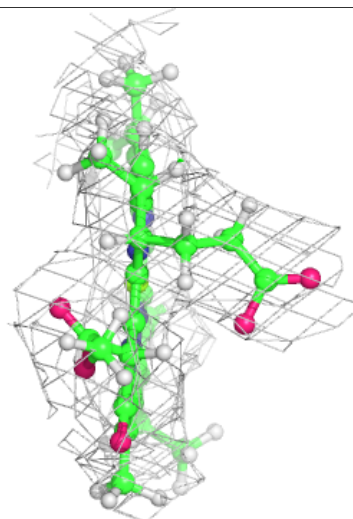
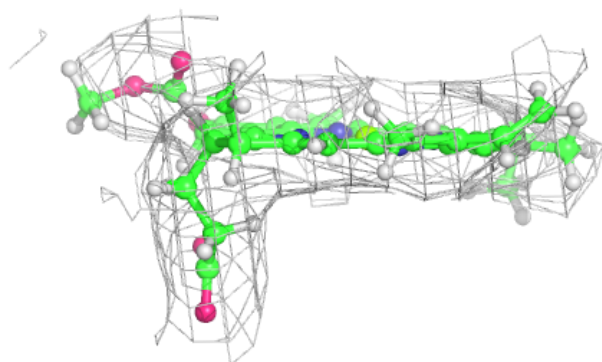
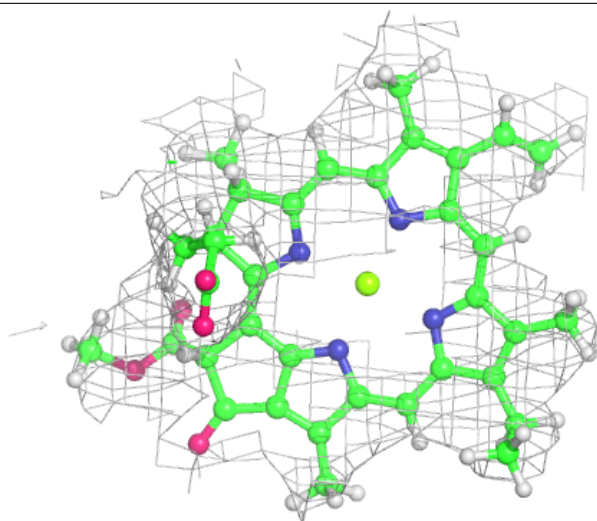
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





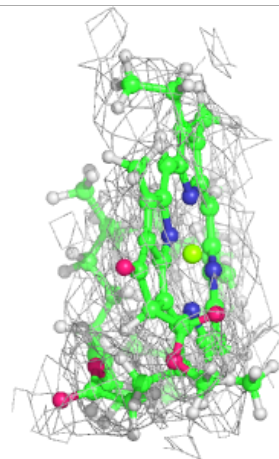
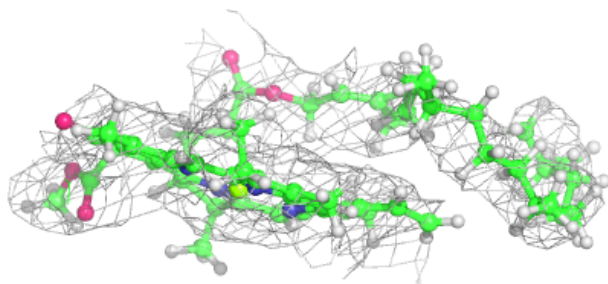
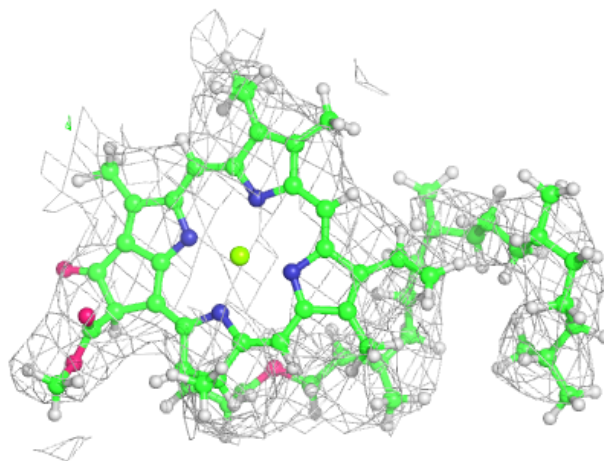
**Electron density around CLA B 812:**

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



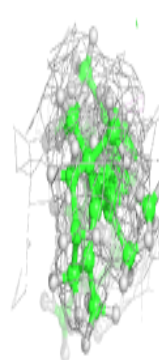
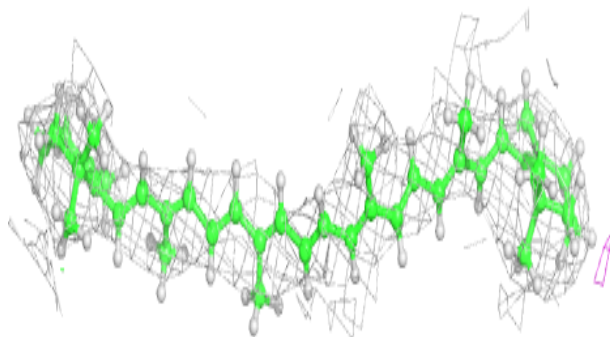
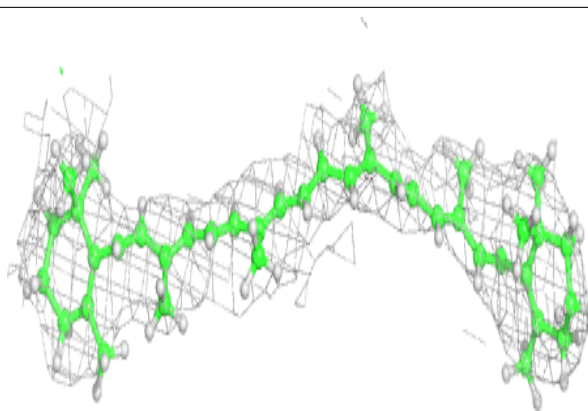
**Electron density around CLA A 820:**

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

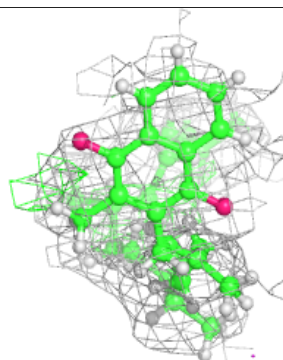
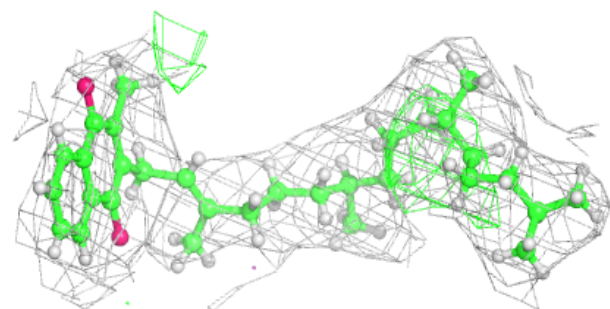
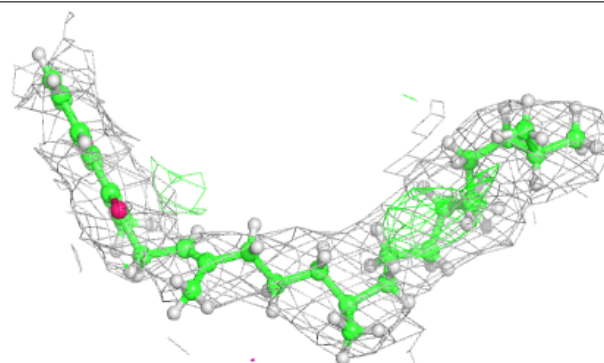


**Electron density around BCR J 104:**

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

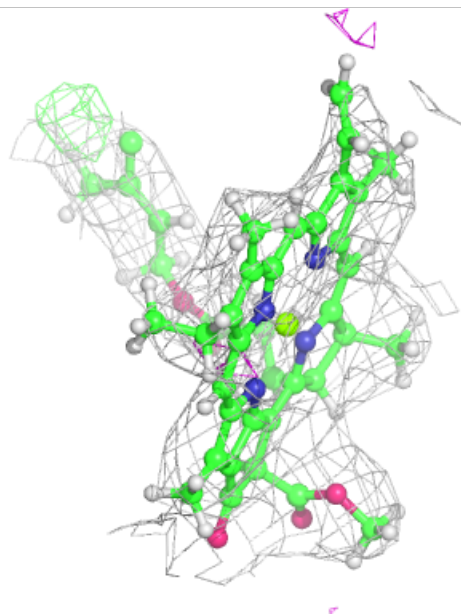
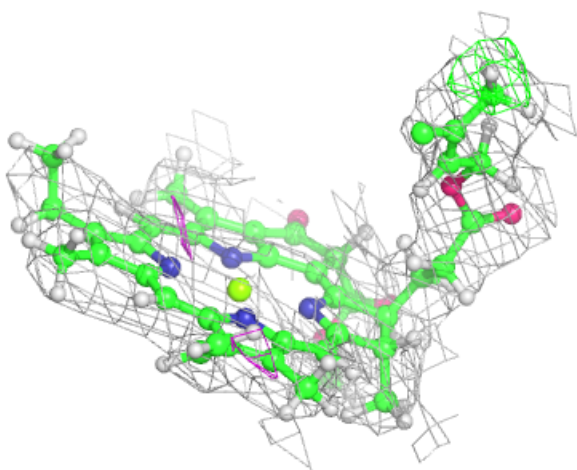
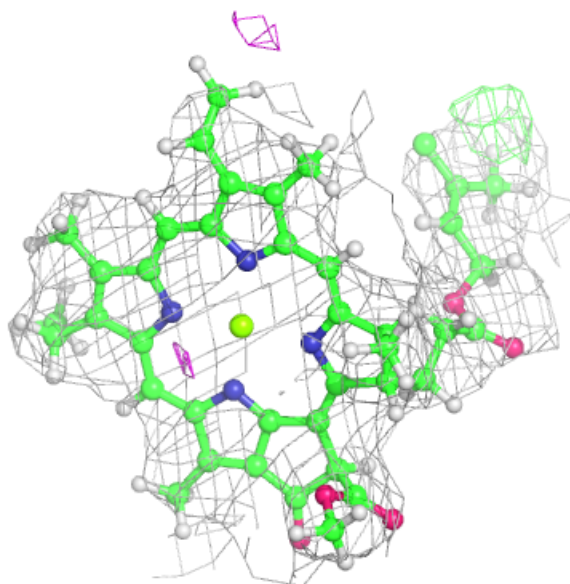
**Electron density around PQN B 842:**

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



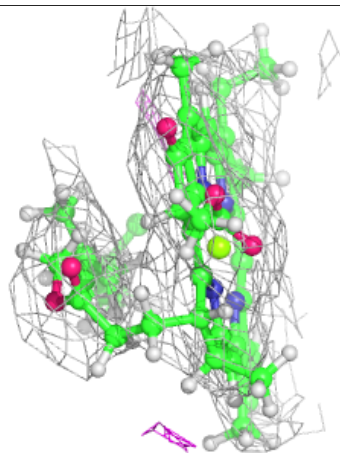
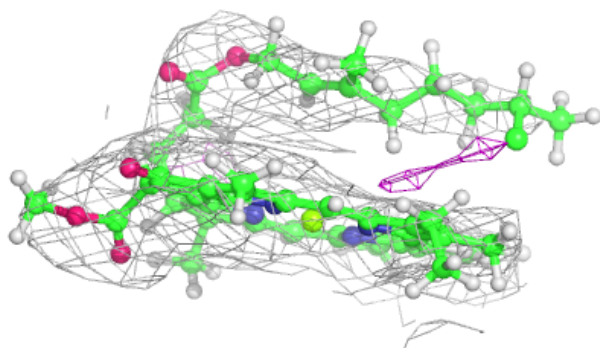
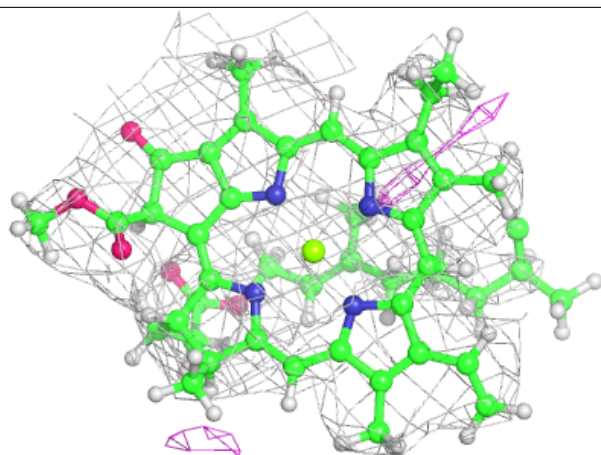
**Electron density around CLA A 832:**

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



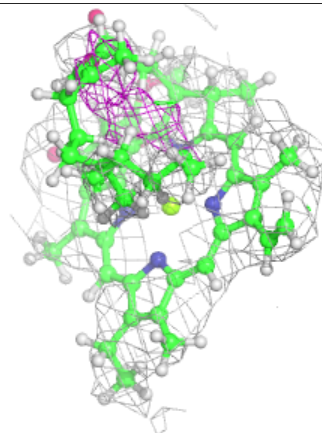
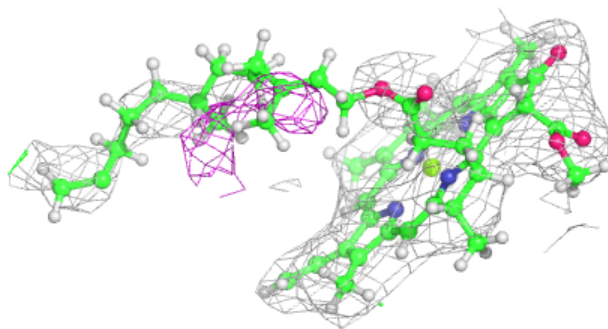
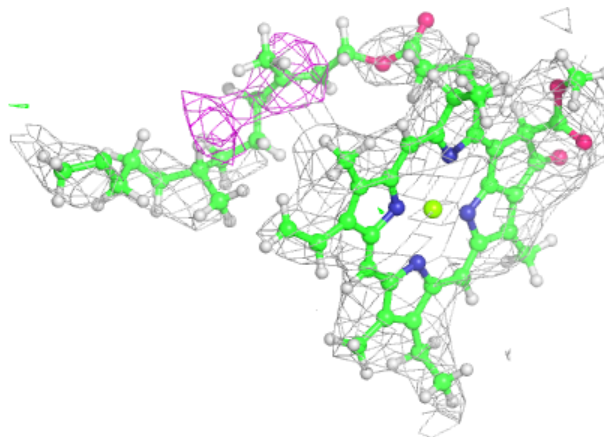
**Electron density around CLA B 822:**

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



**Electron density around CLA A 825:**

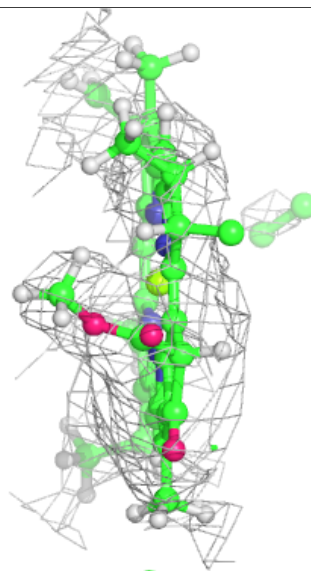
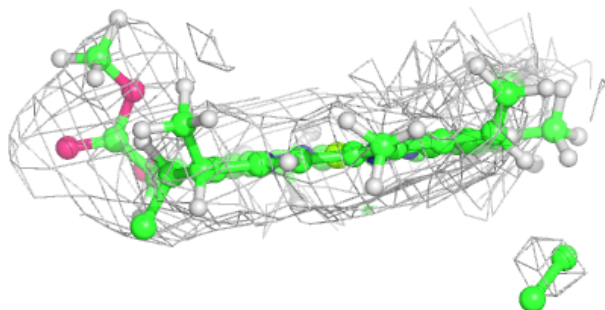
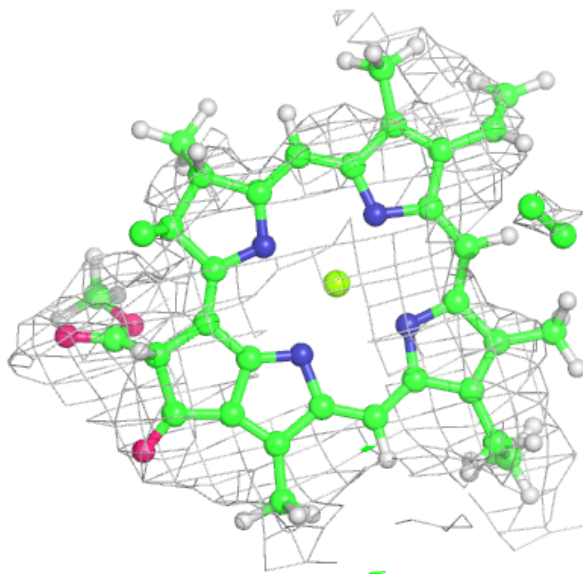
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





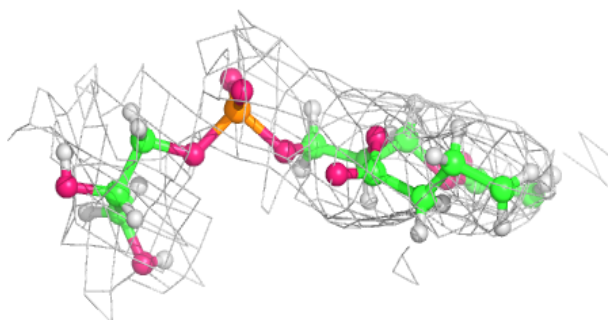
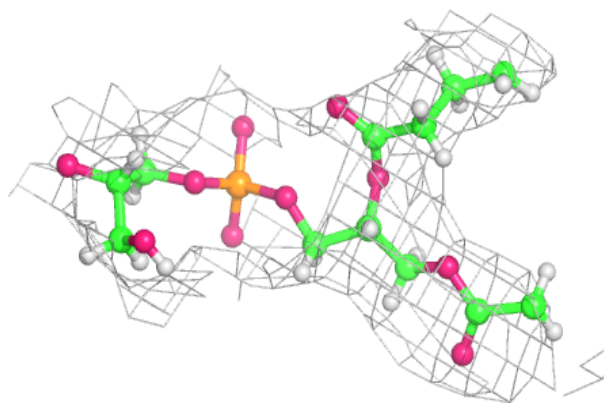
**Electron density around CLA A 821:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LHG B 850:**

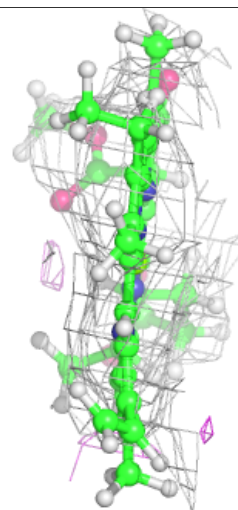
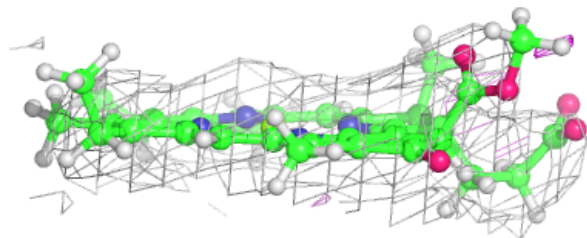
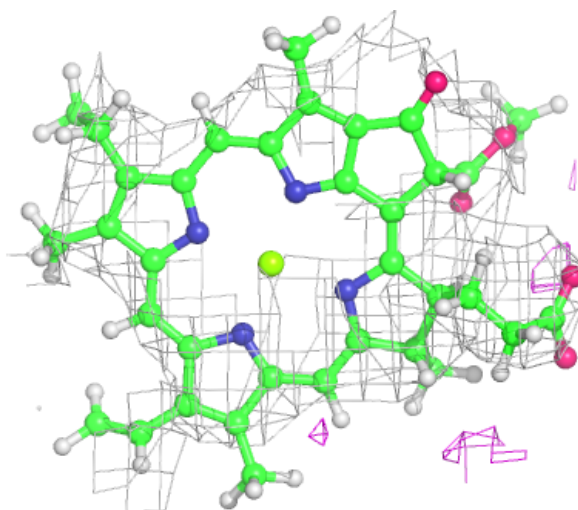
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





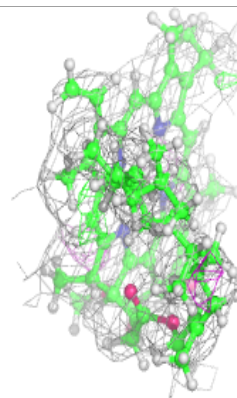
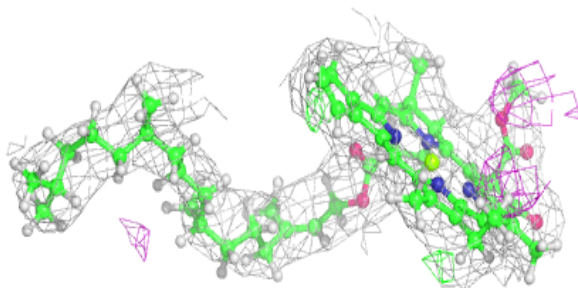
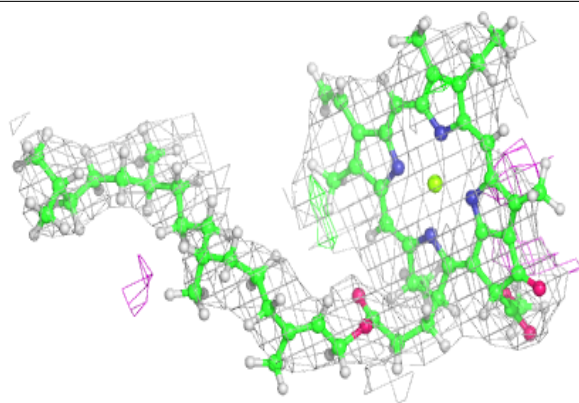
**Electron density around CLA F 202:**

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



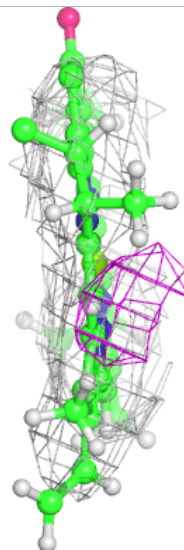
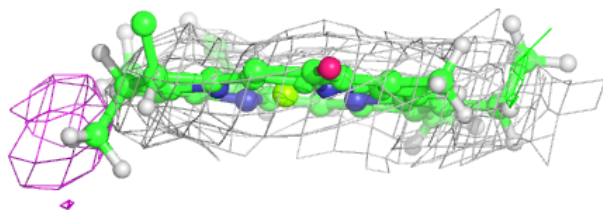
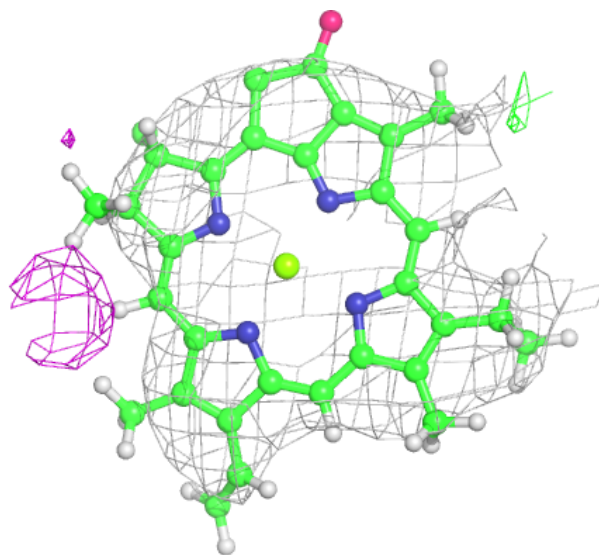
**Electron density around CLA A 809:**

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



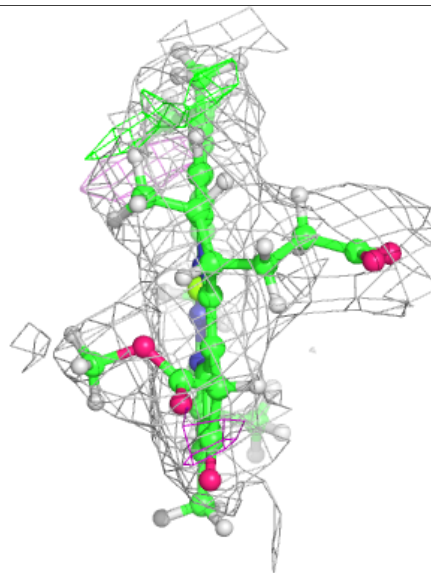
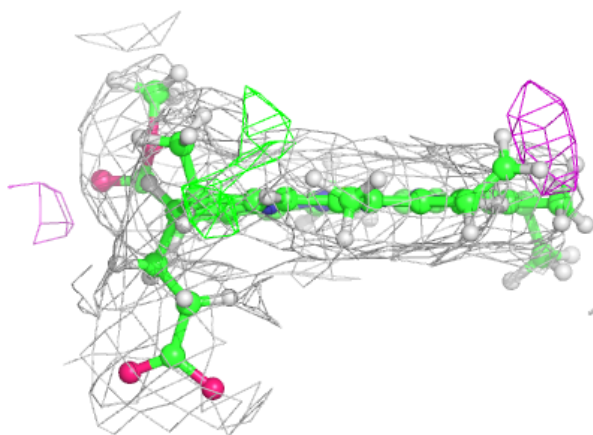
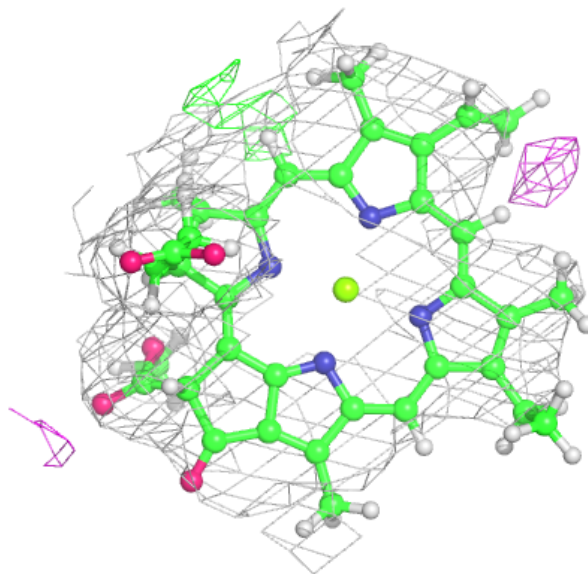
**Electron density around CLA J 102:**

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



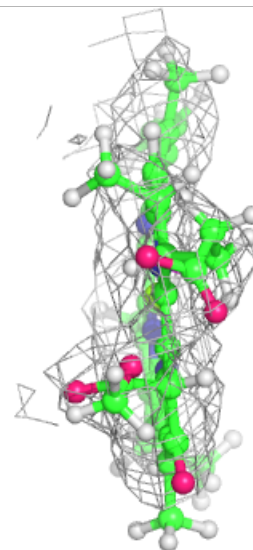
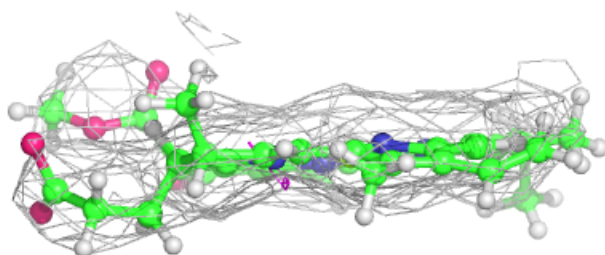
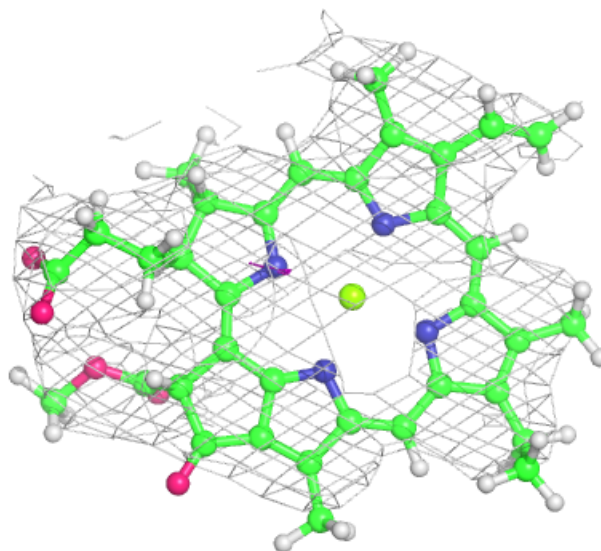
**Electron density around CLA B 834:**

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



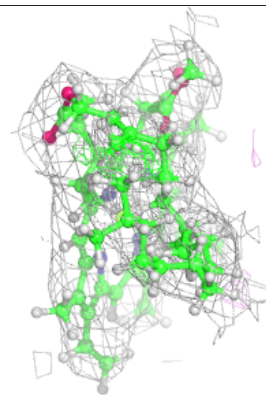
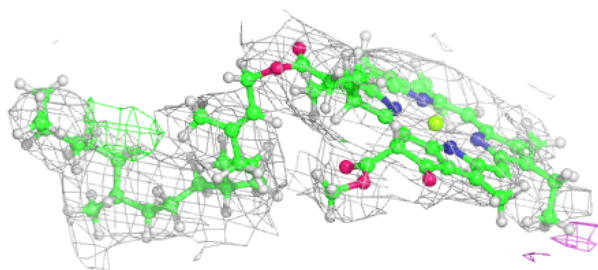
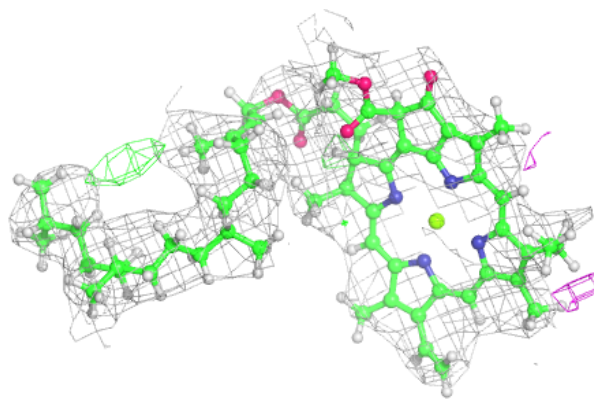
**Electron density around CLA B 836:**

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



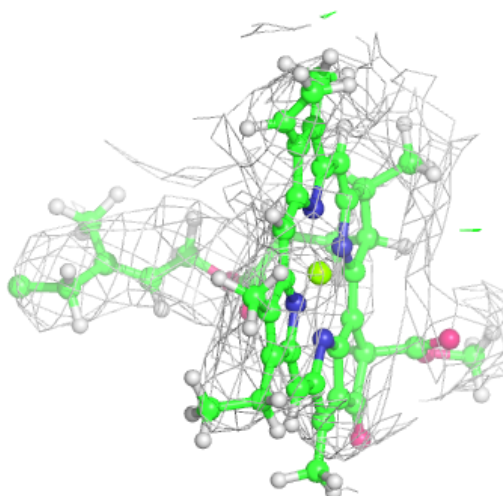
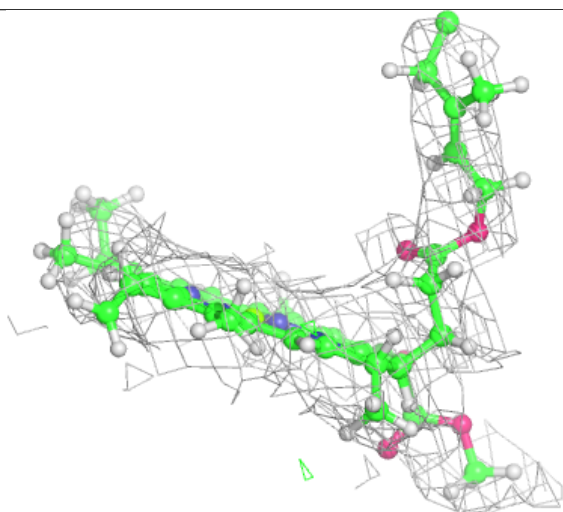
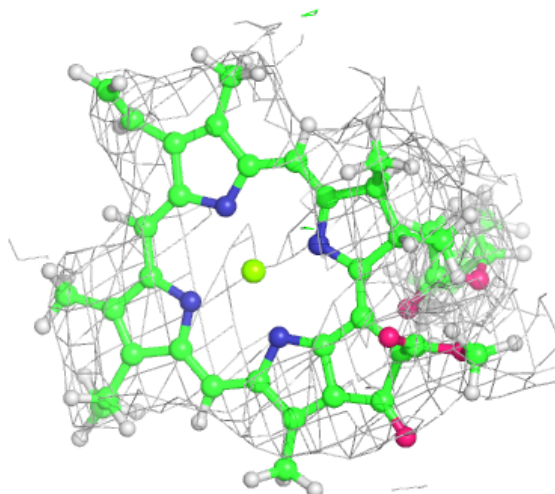
**Electron density around CLA A 804:**

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



**Electron density around CLA A 808:**

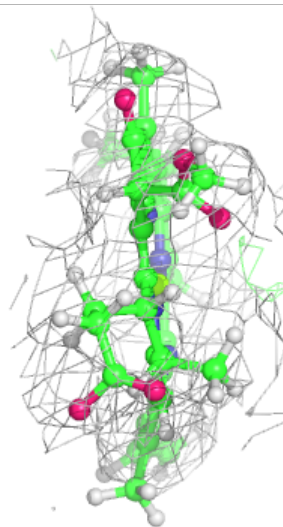
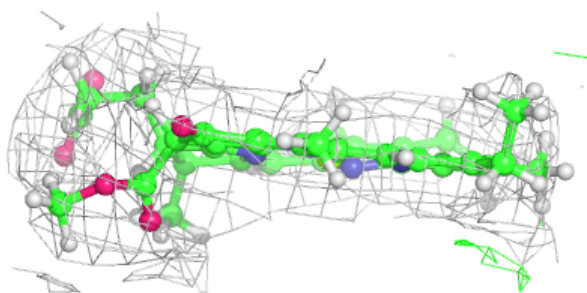
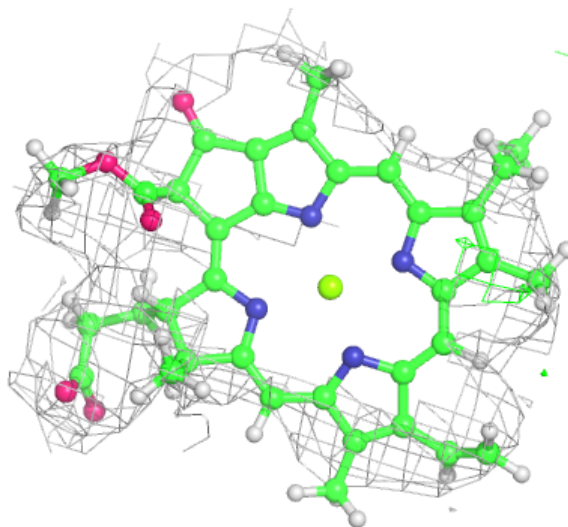
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA X 1701:**

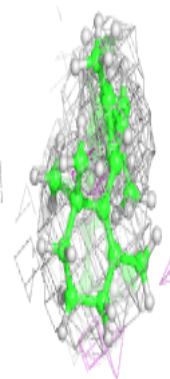
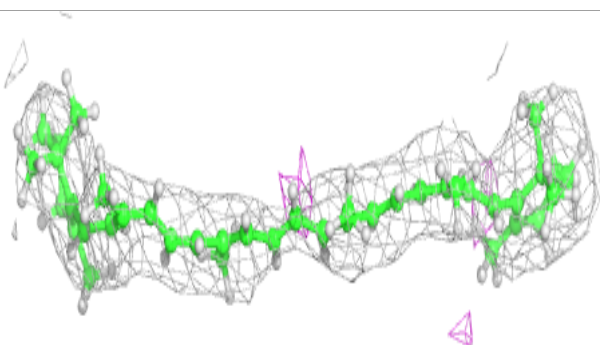
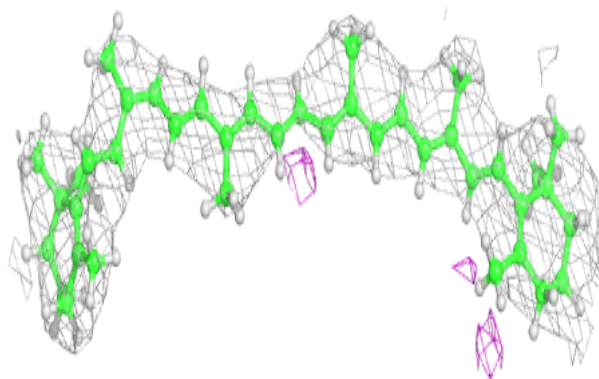
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



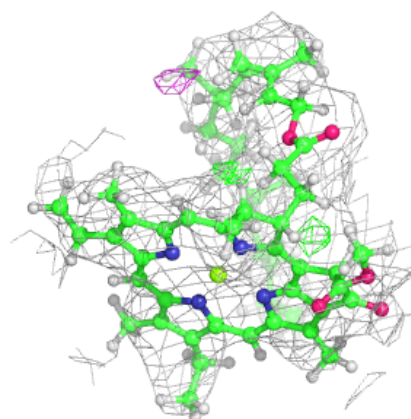
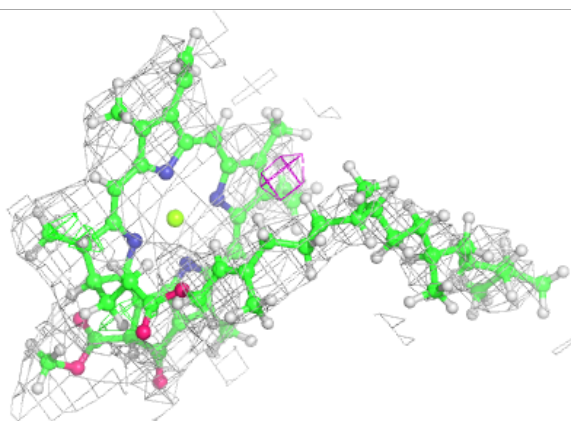
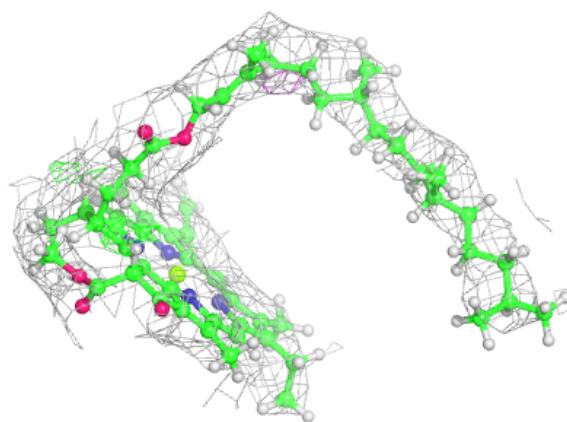


**Electron density around BCR B 844:**

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

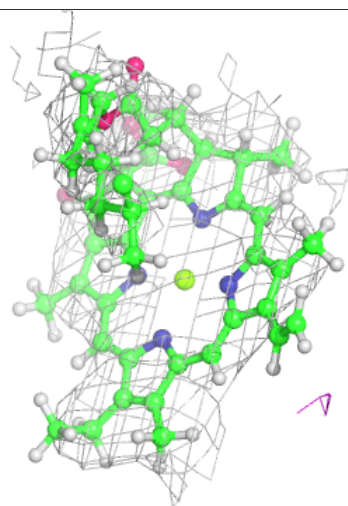
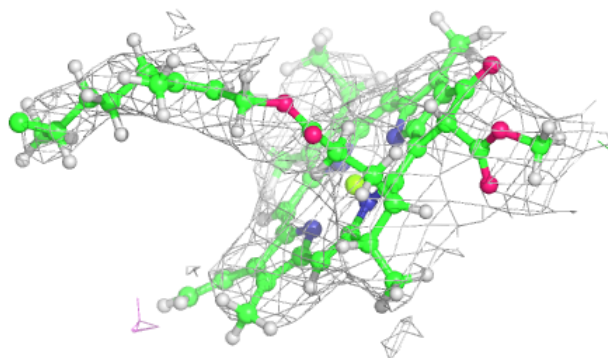
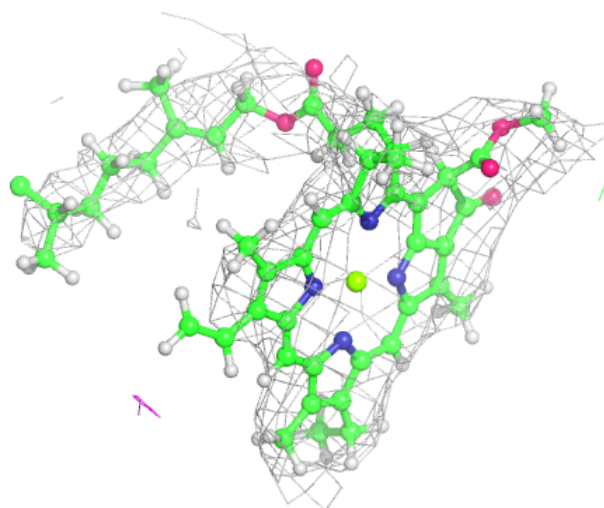
**Electron density around CLA B 819:**

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



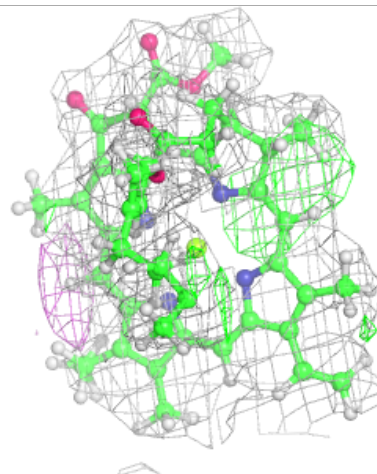
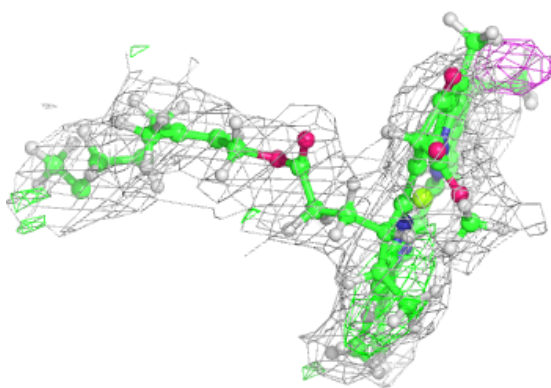
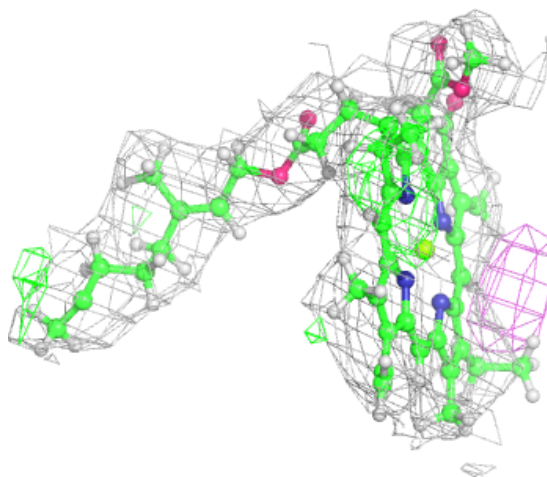
**Electron density around CLA B 816:**

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



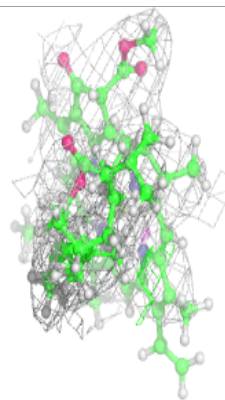
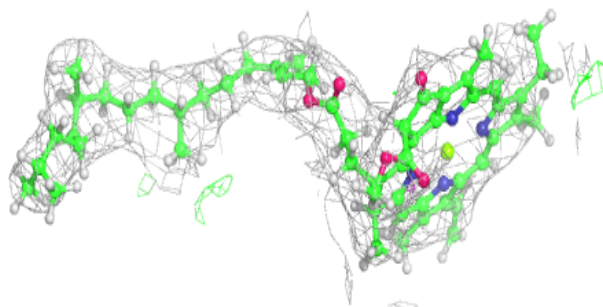
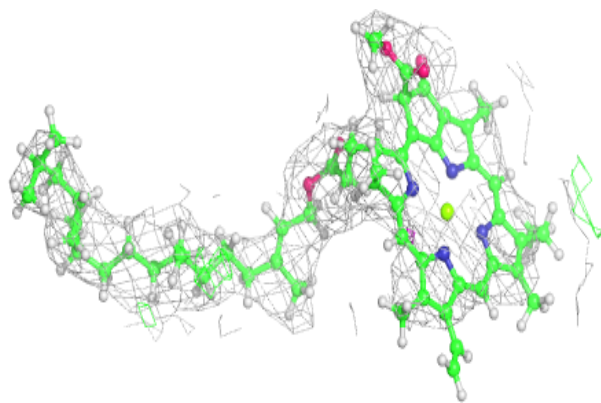
**Electron density around CLA B 804:**

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

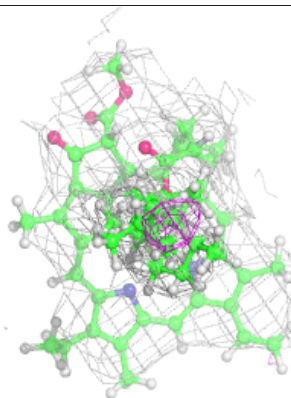
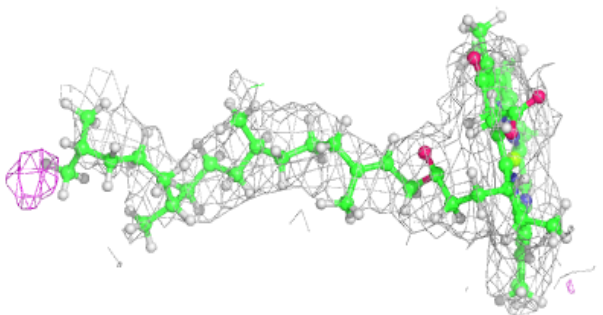
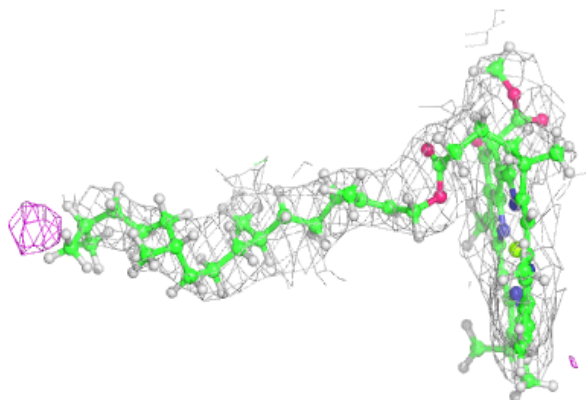


**Electron density around CLA A 822:**

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

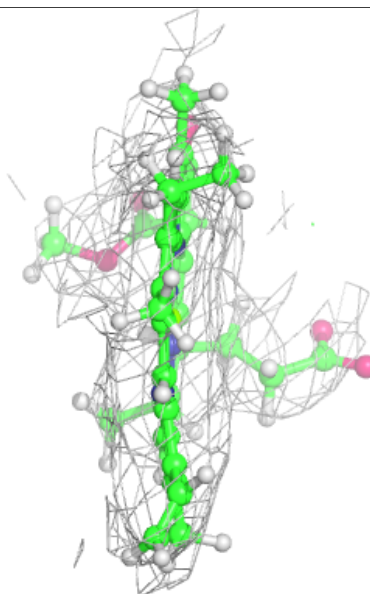
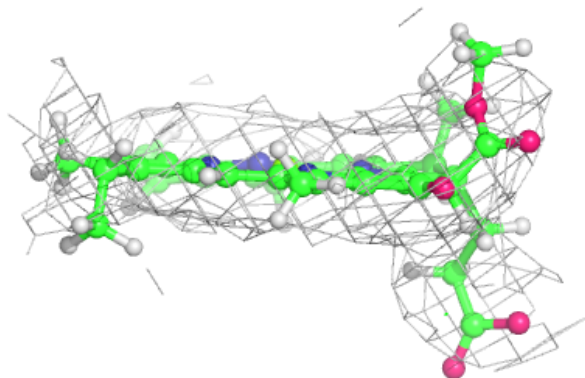
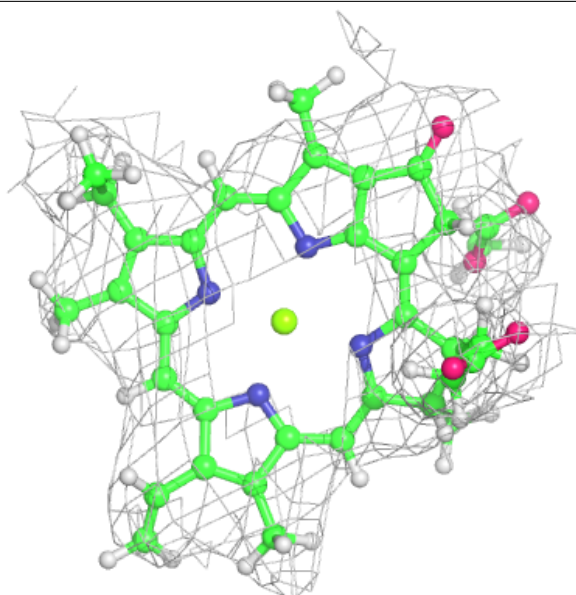
**Electron density around CLA A 829:**

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



**Electron density around CLA B 821:**

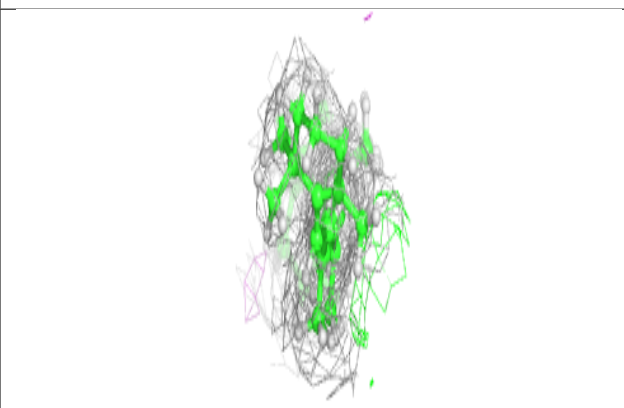
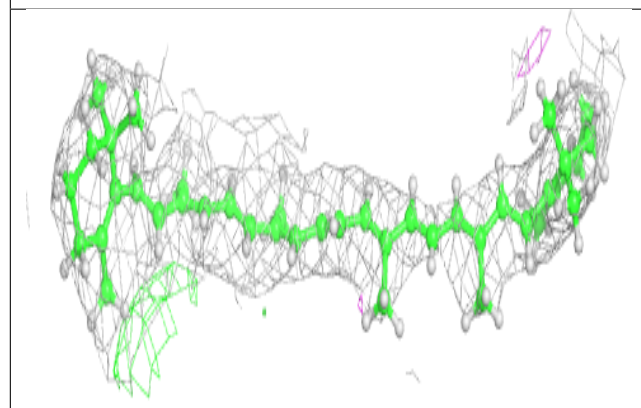
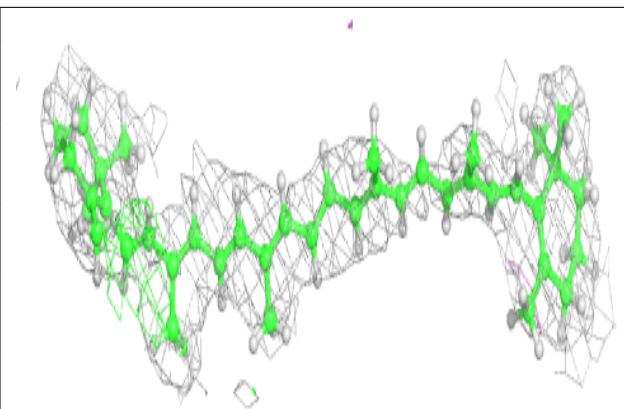
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



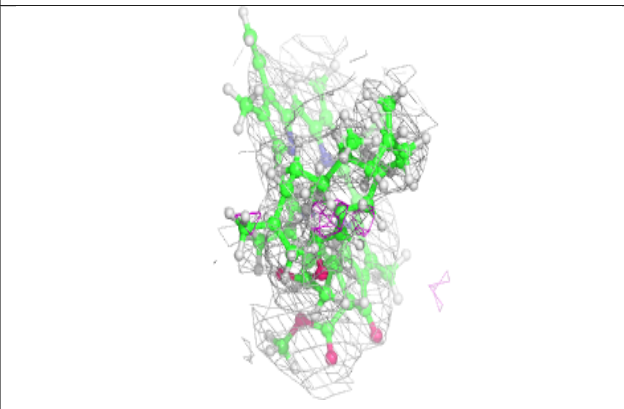
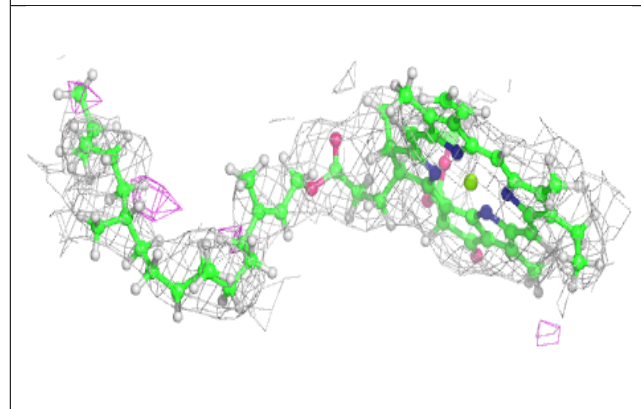
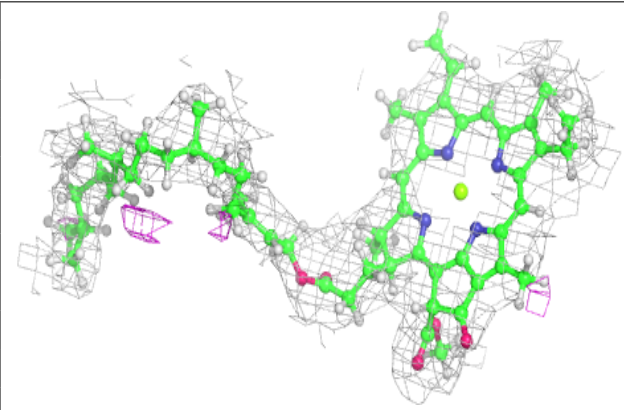


**Electron density around BCR A 851:**

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

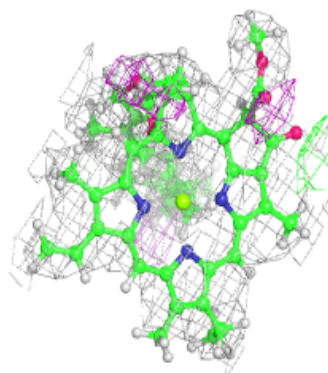
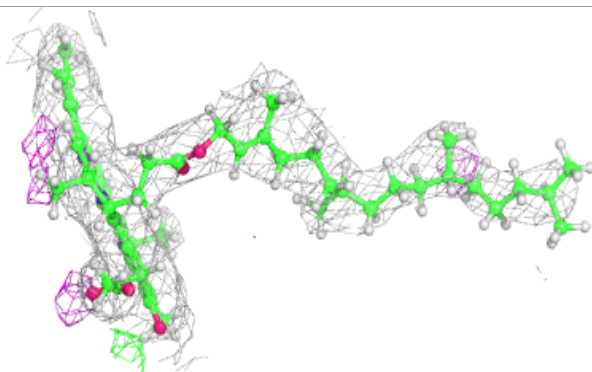
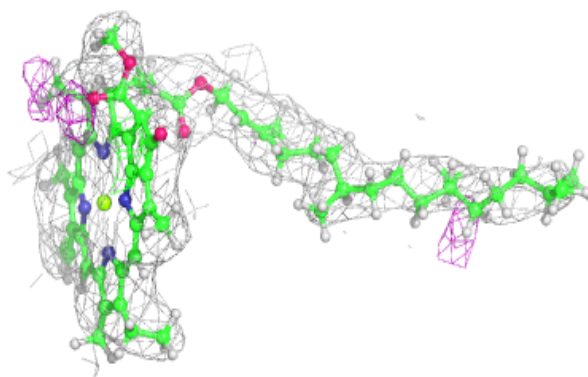
**Electron density around CLA B 813:**

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

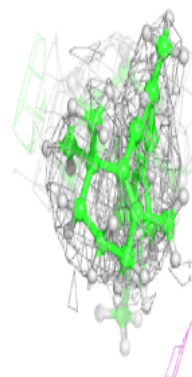
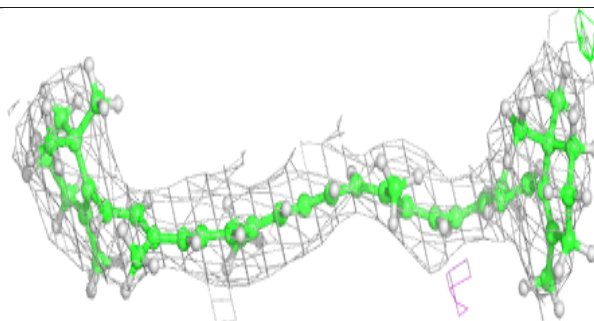
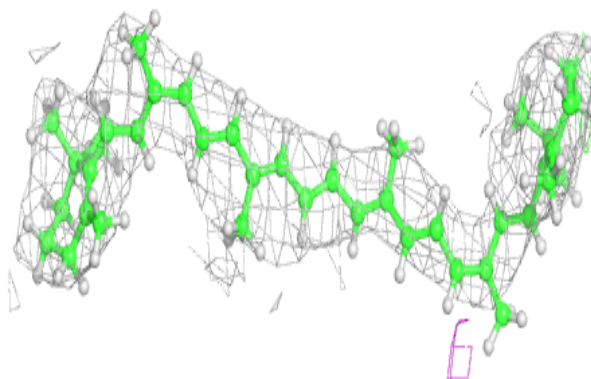


**Electron density around CLA B 828:**

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

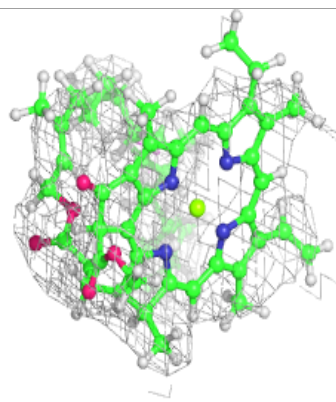
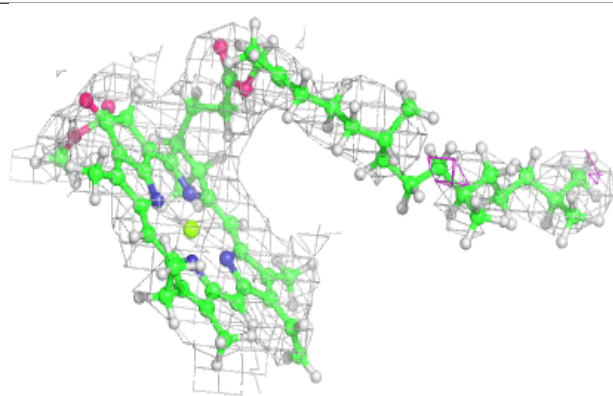
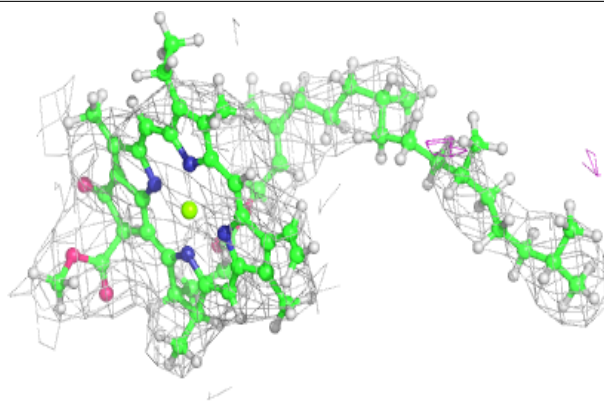
**Electron density around BCR B 845:**

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



**Electron density around CLA B 814:**

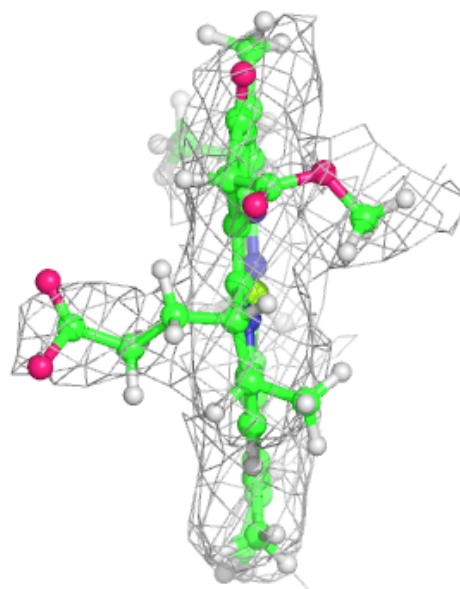
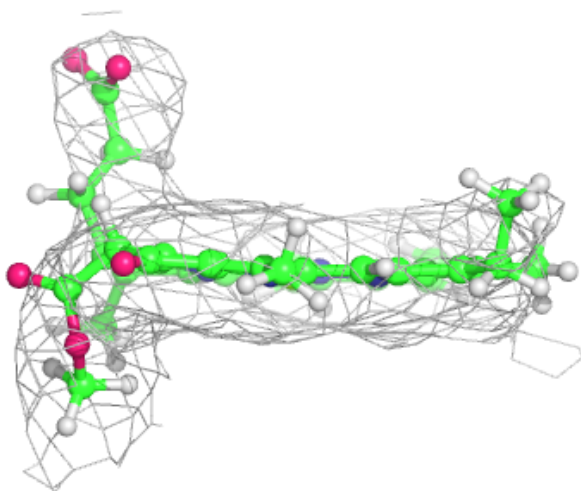
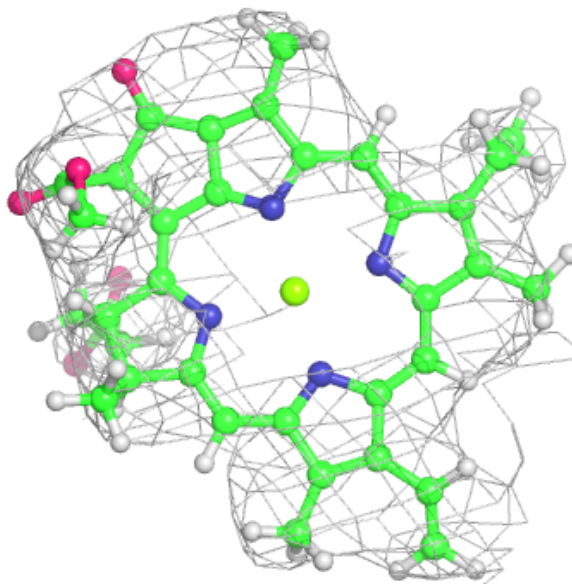
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





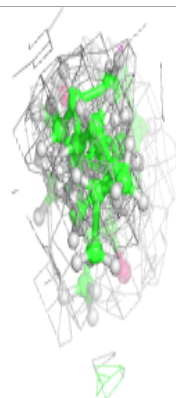
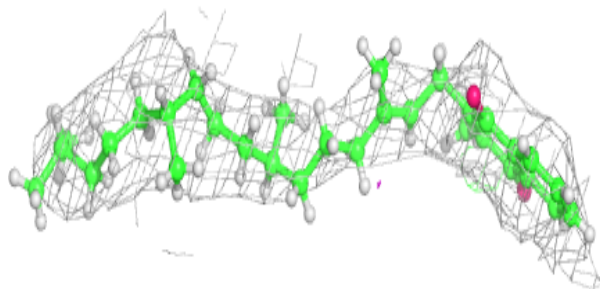
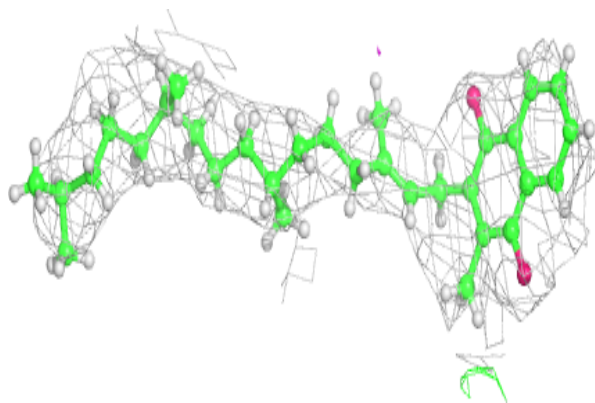
**Electron density around CLA B 815:**

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

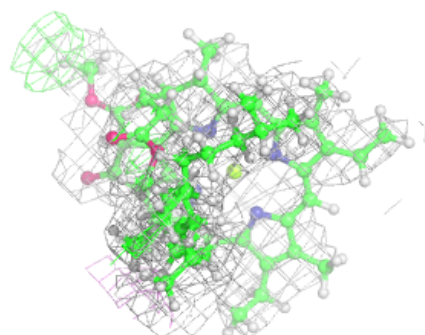
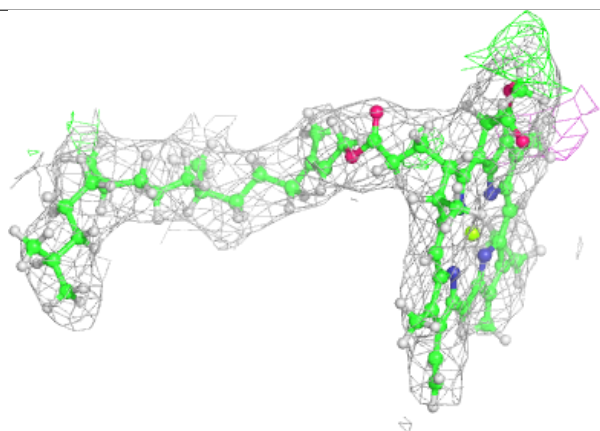
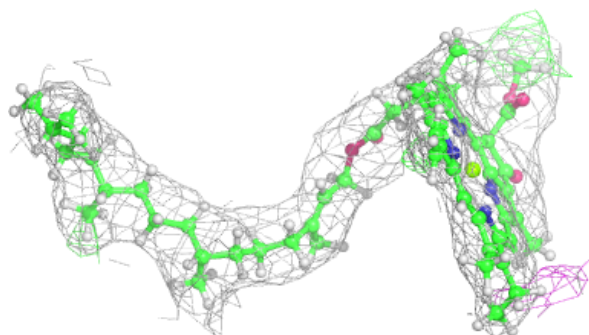


**Electron density around PQN A 845:**

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

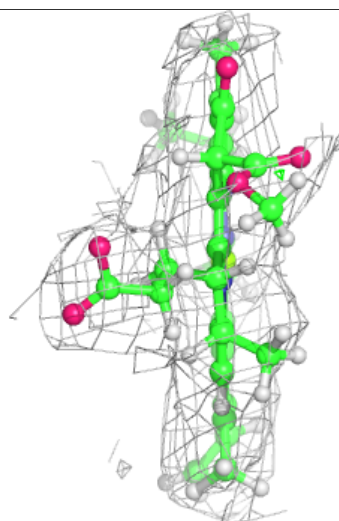
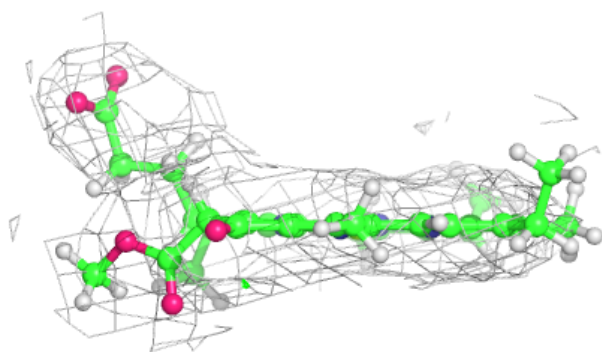
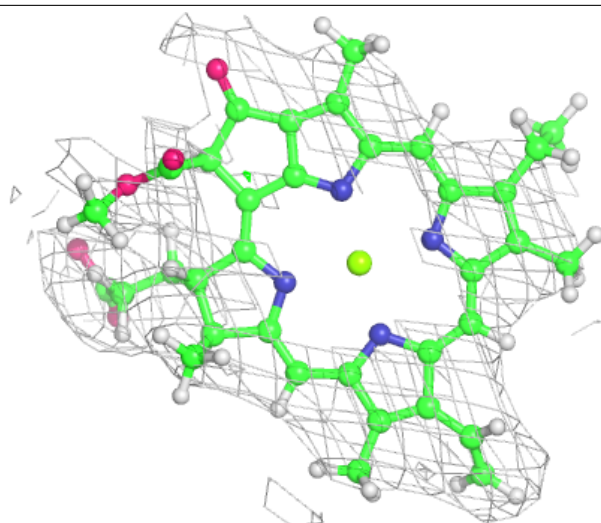
**Electron density around CLA L 205:**

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



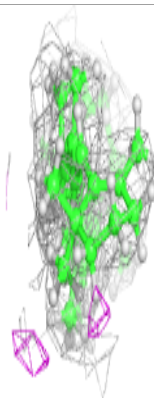
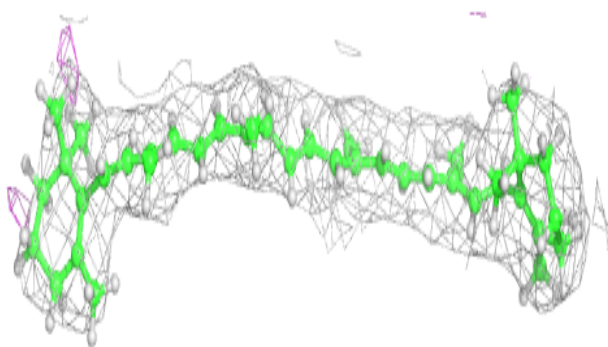
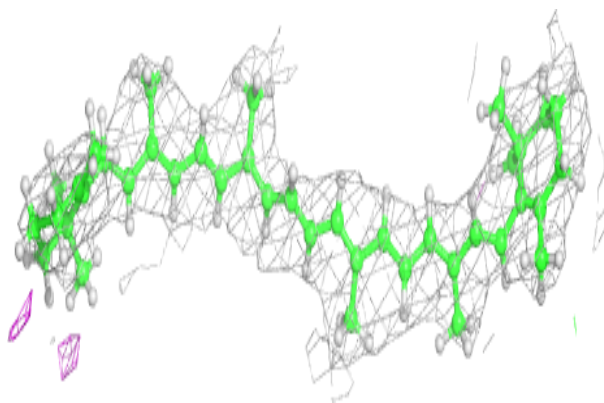
**Electron density around CLA B 823:**

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



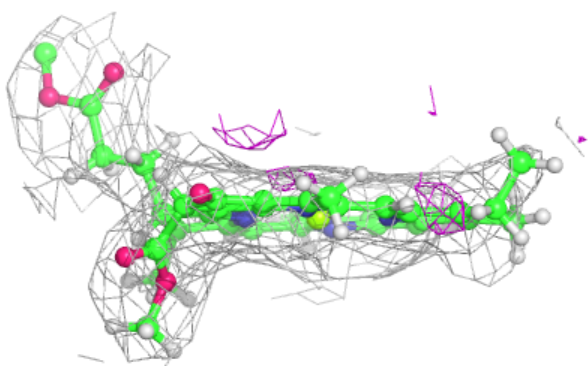
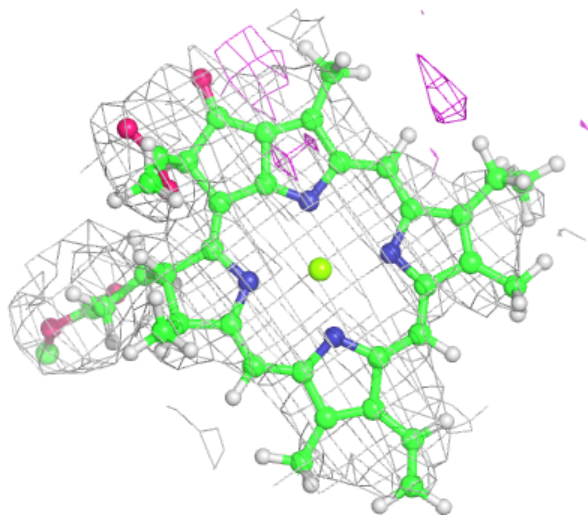
**Electron density around BCR M 103:**

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



**Electron density around CLA B 825:**

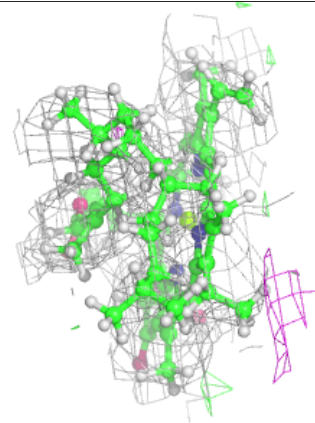
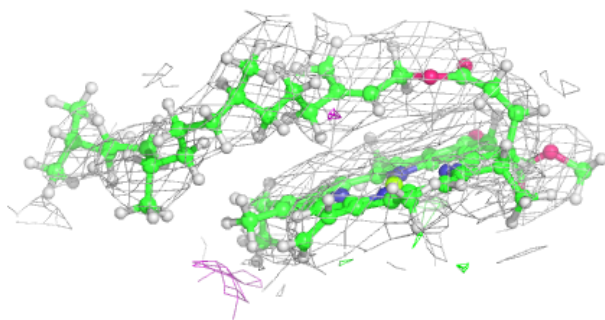
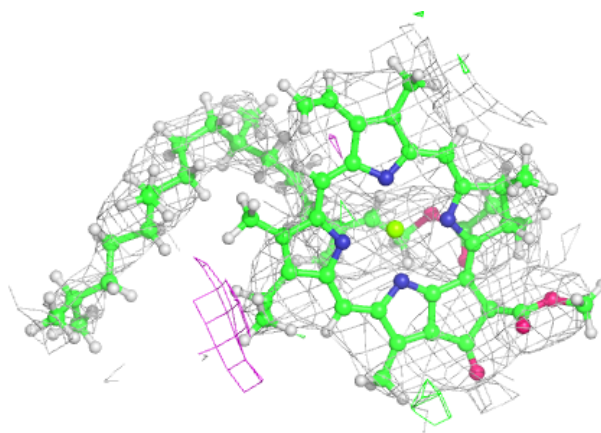
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



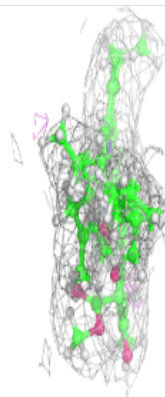
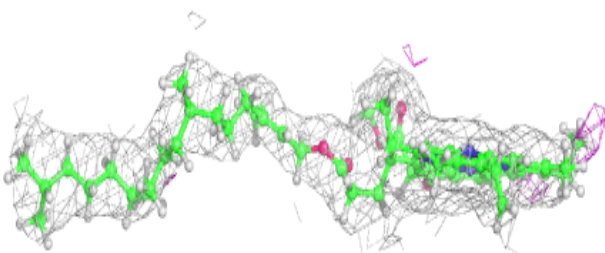
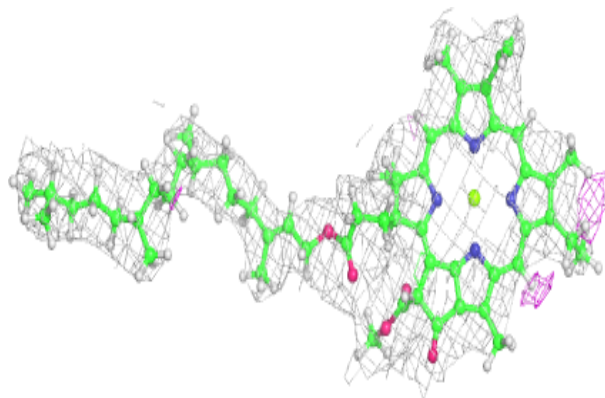


**Electron density around CLA B 838:**

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

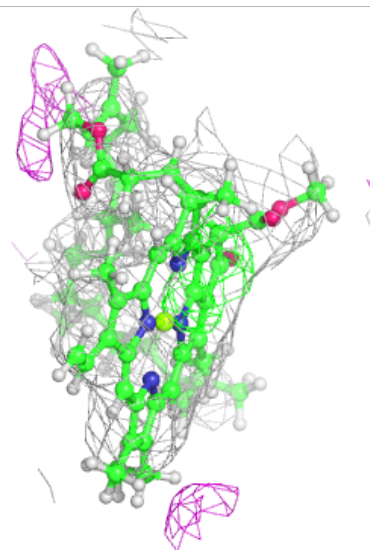
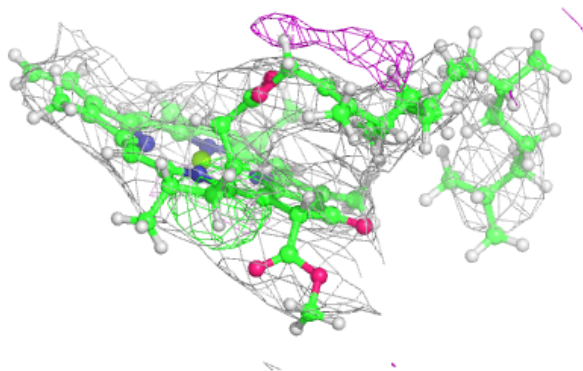
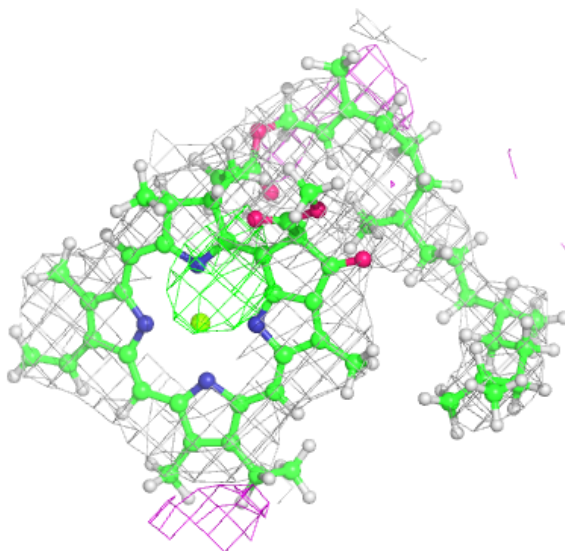
**Electron density around CLA A 834:**

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



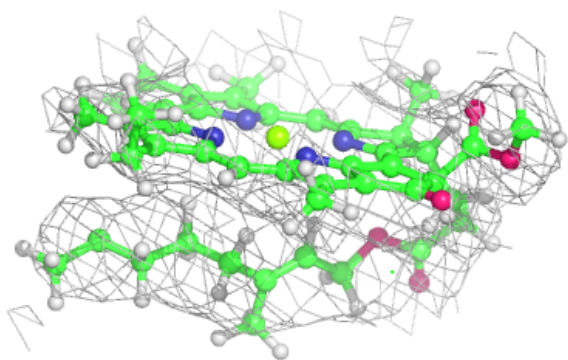
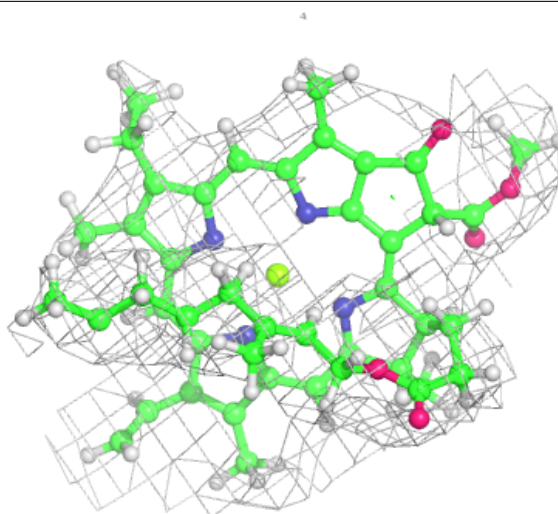
**Electron density around CLA B 832:**

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



**Electron density around CLA A 819:**

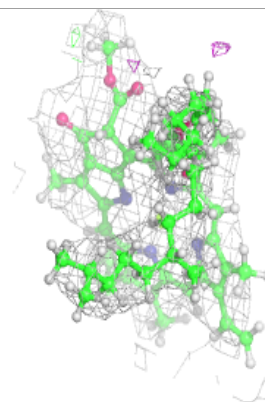
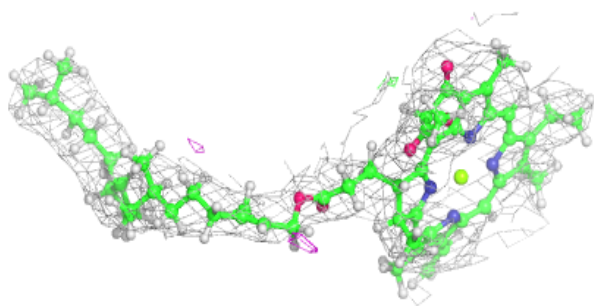
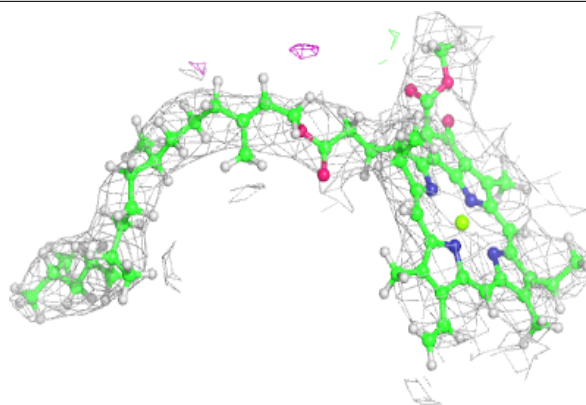
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



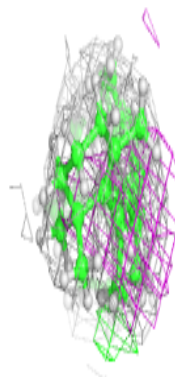
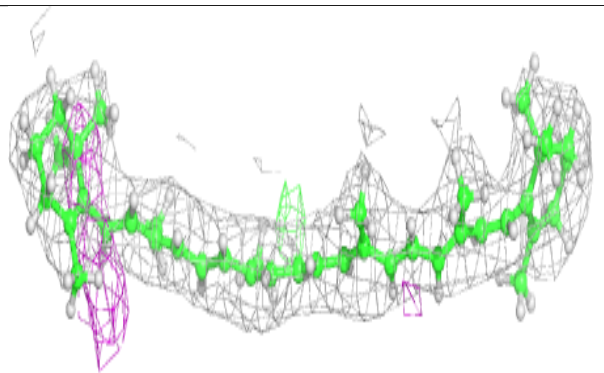
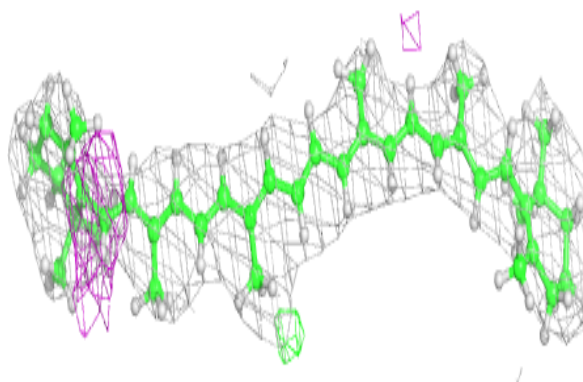


**Electron density around CLA A 857:**

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

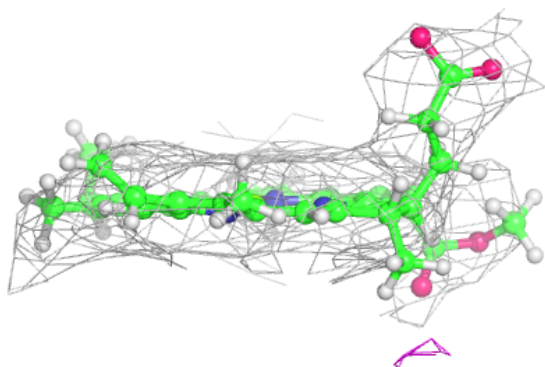
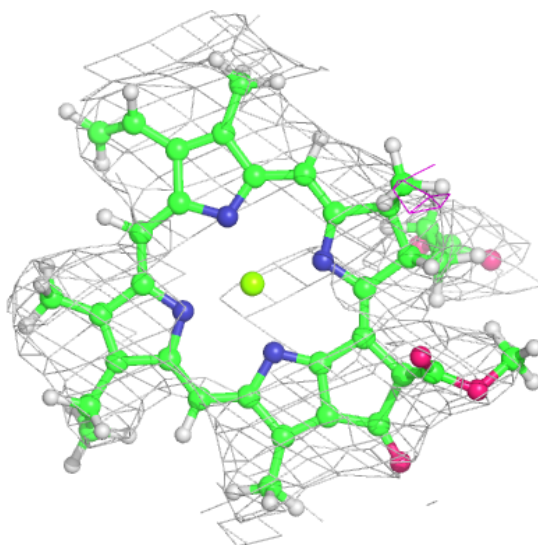
**Electron density around BCR I 101:**

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



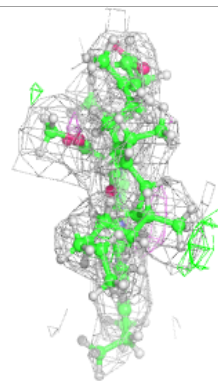
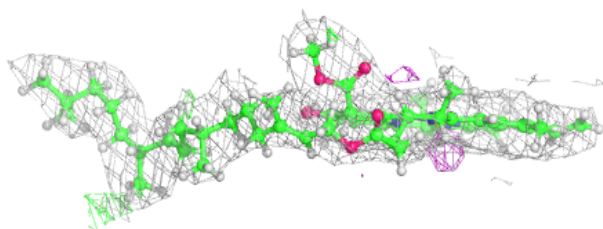
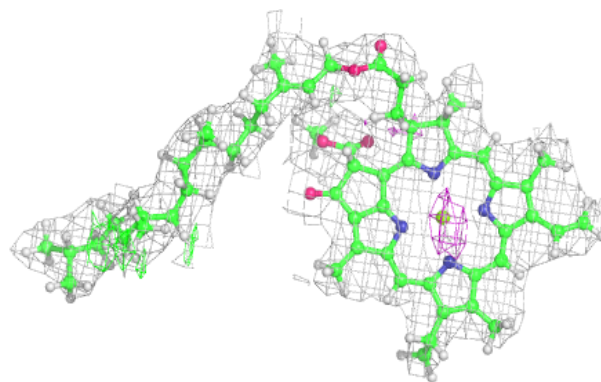
**Electron density around CLA B 835:**

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

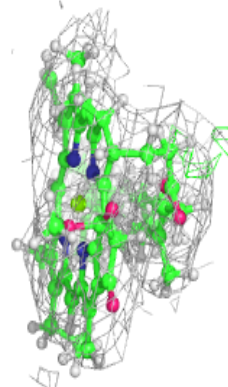
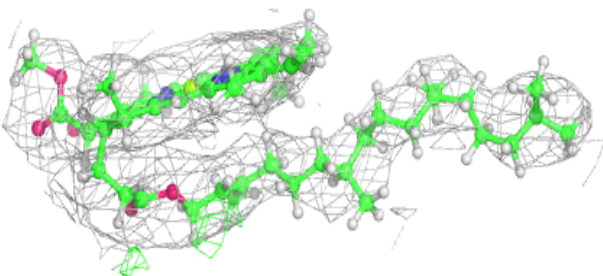
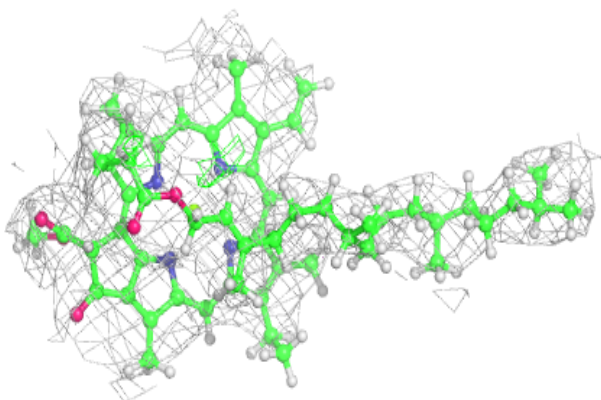


**Electron density around CLA L 206:**

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

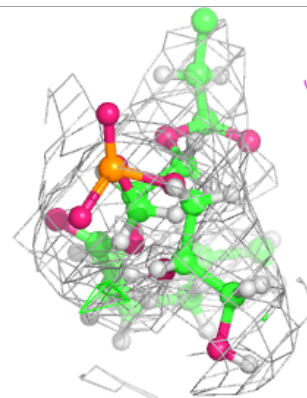
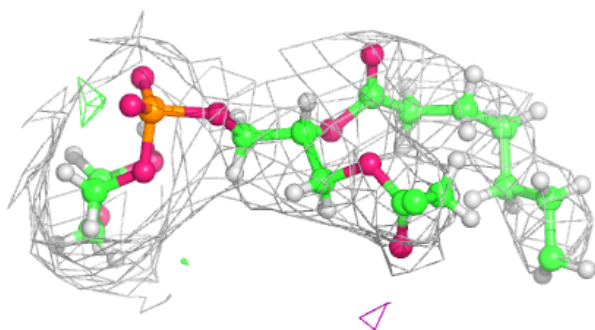
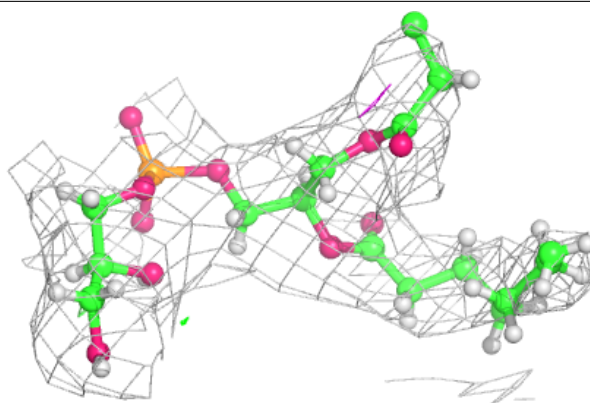
**Electron density around CLA A 839:**

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



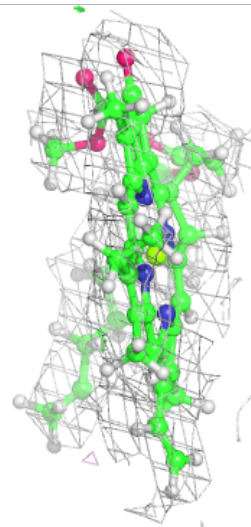
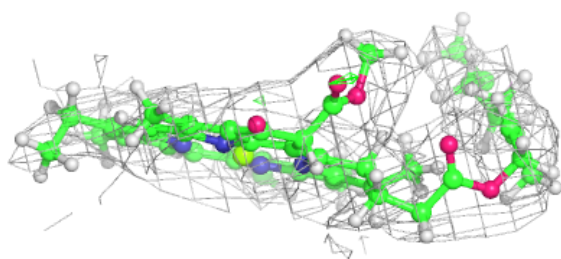
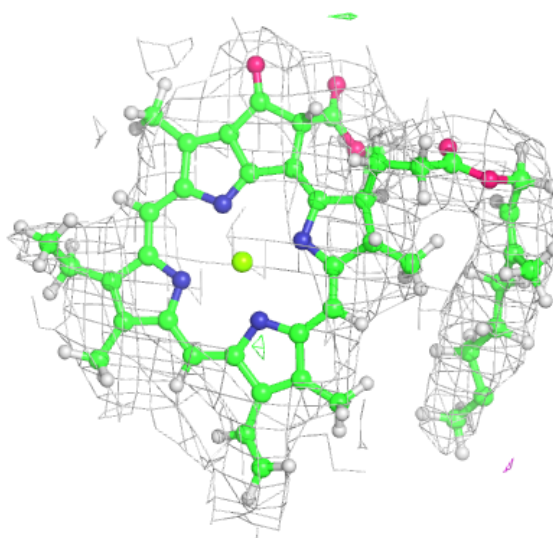
**Electron density around LHG A 855:**

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



**Electron density around CLA B 824:**

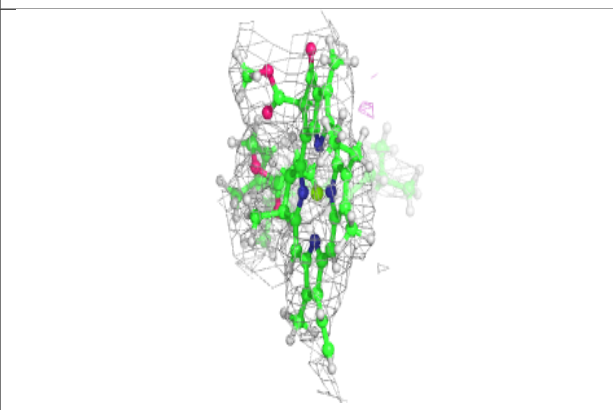
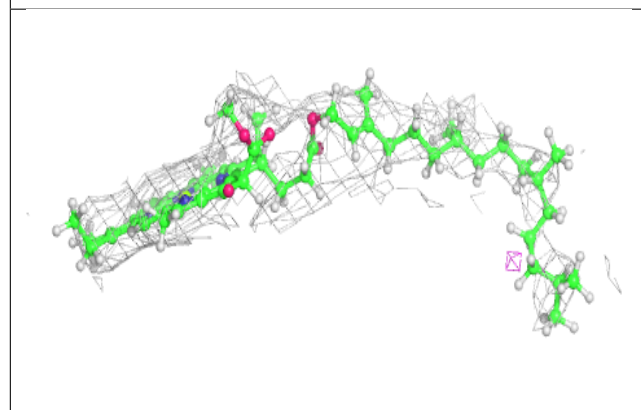
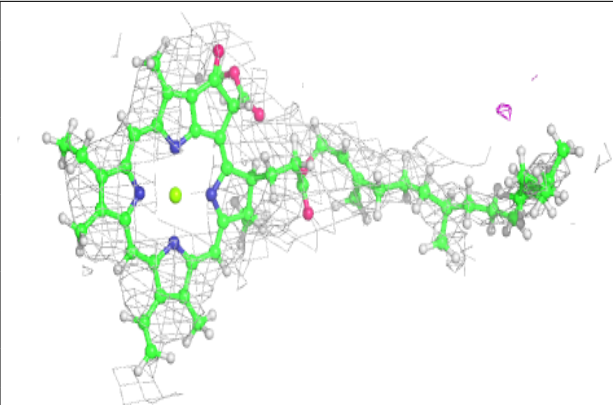
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



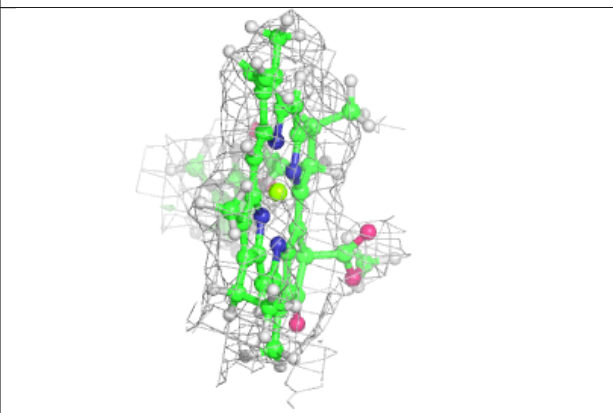
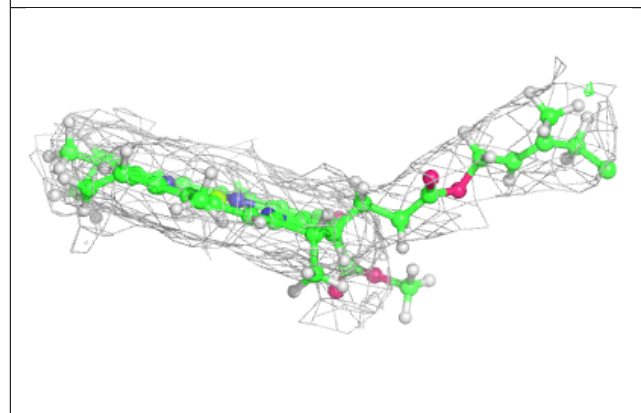
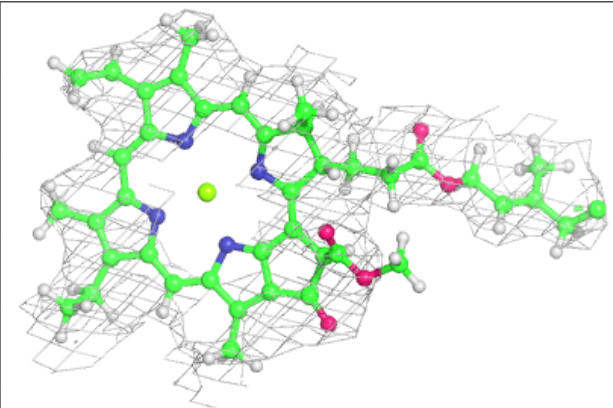


**Electron density around CLA A 806:**

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

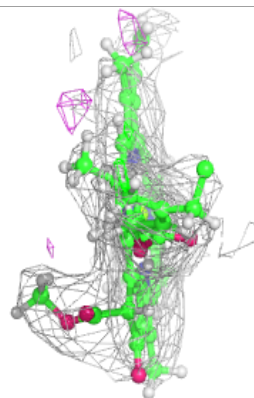
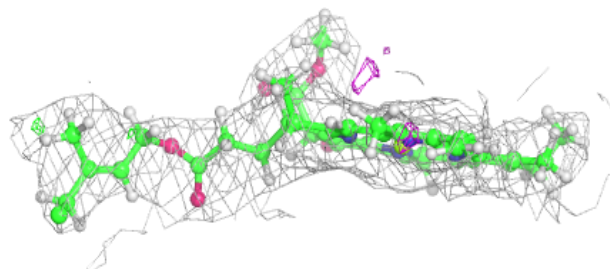
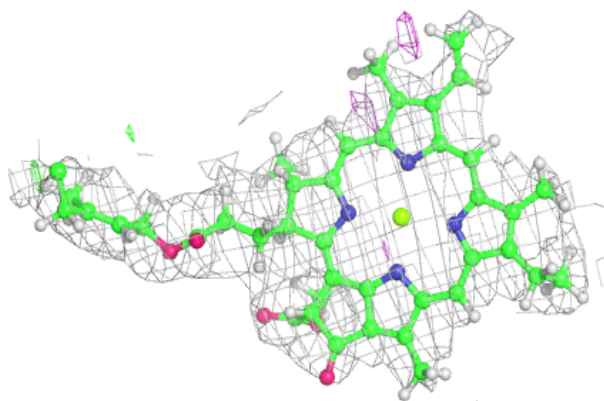
**Electron density around CLA F 201:**

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

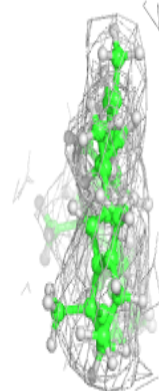
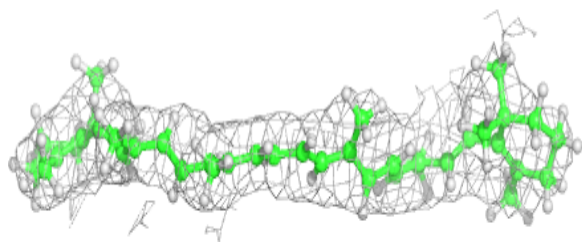
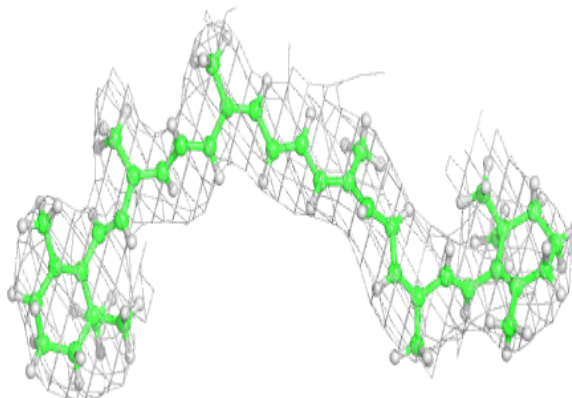


**Electron density around CLA A 838:**

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

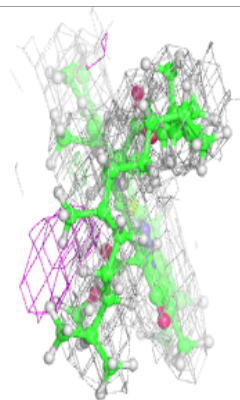
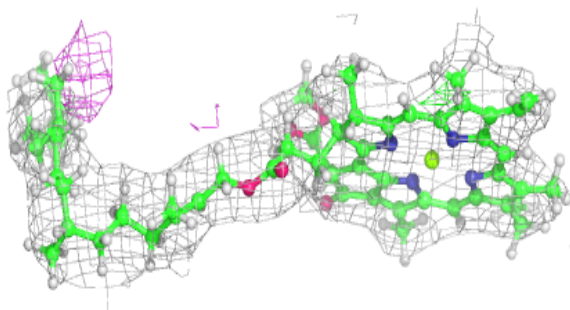
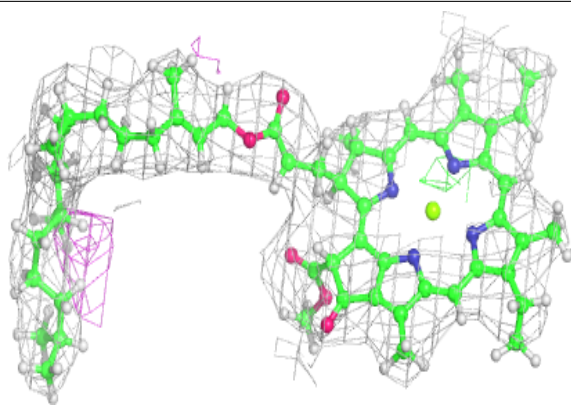
**Electron density around BCR A 852:**

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



**Electron density around CLA B 826:**

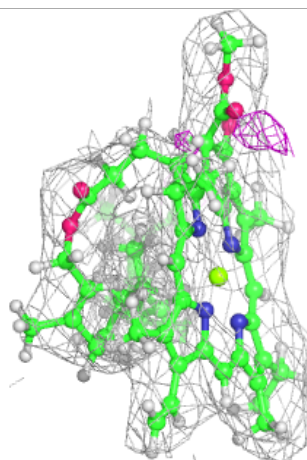
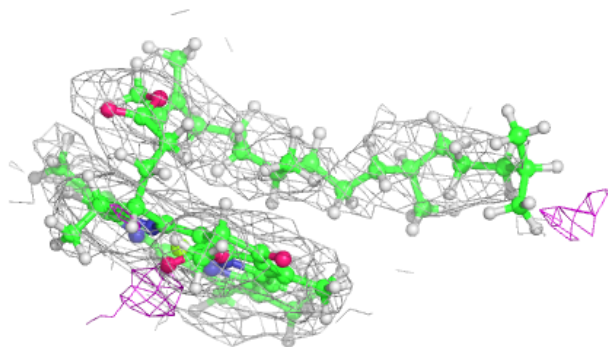
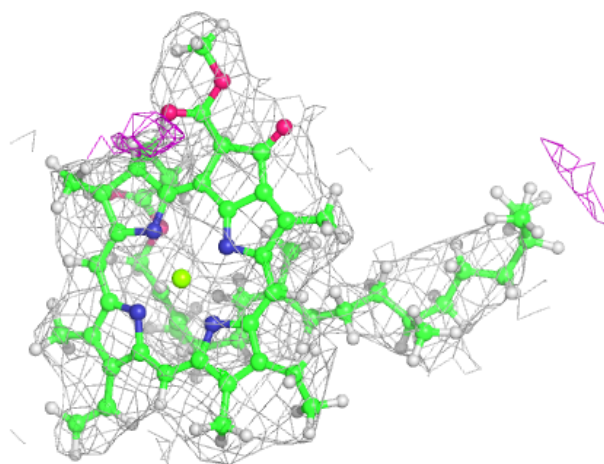
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





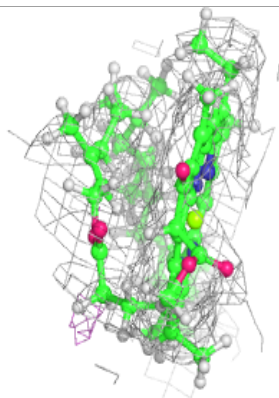
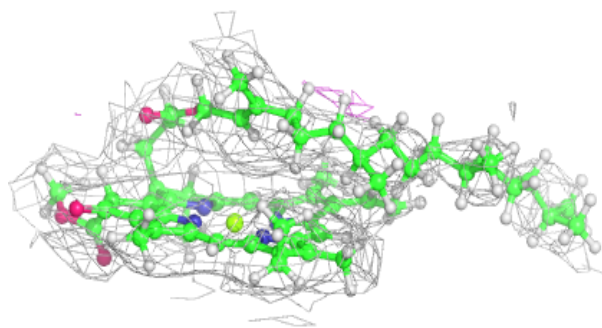
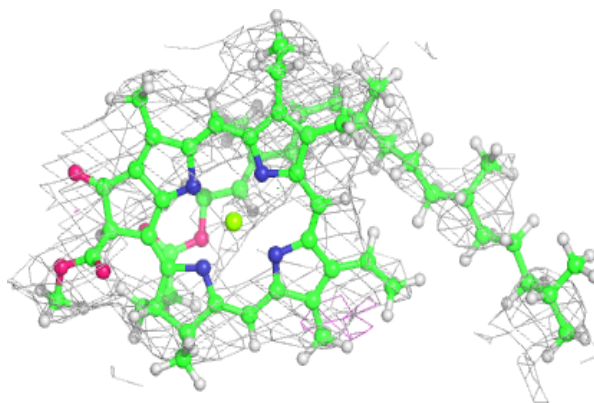
**Electron density around CLA B 827:**

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

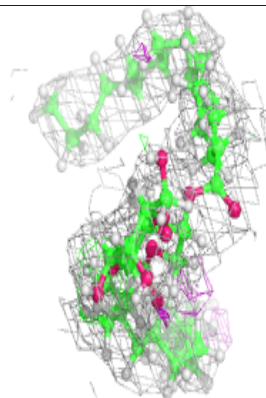
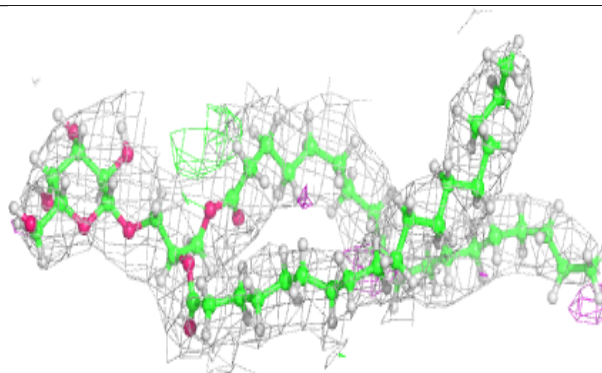
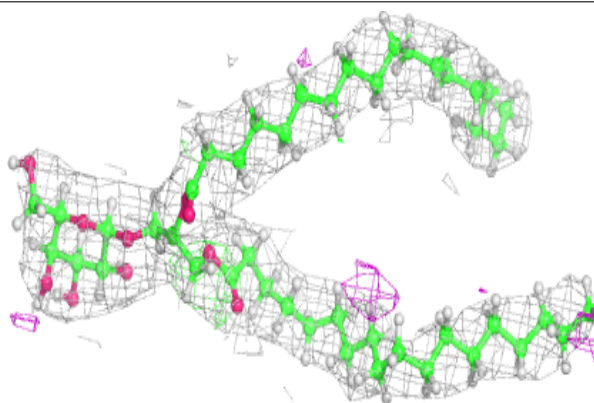


**Electron density around CLA A 841:**

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

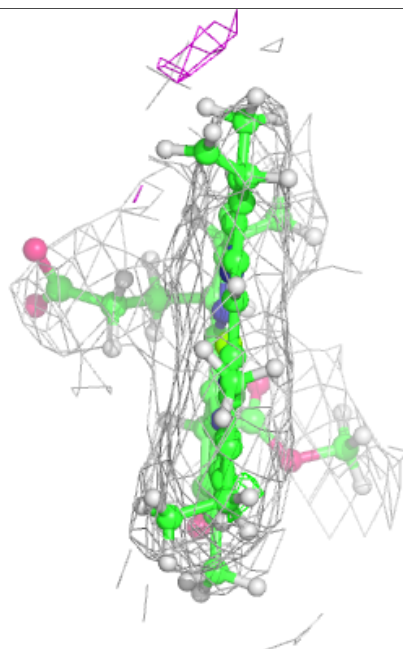
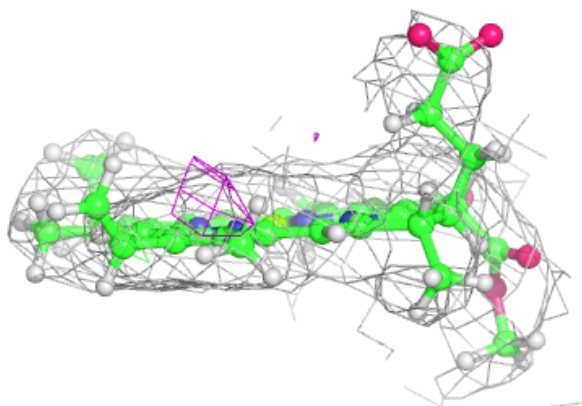
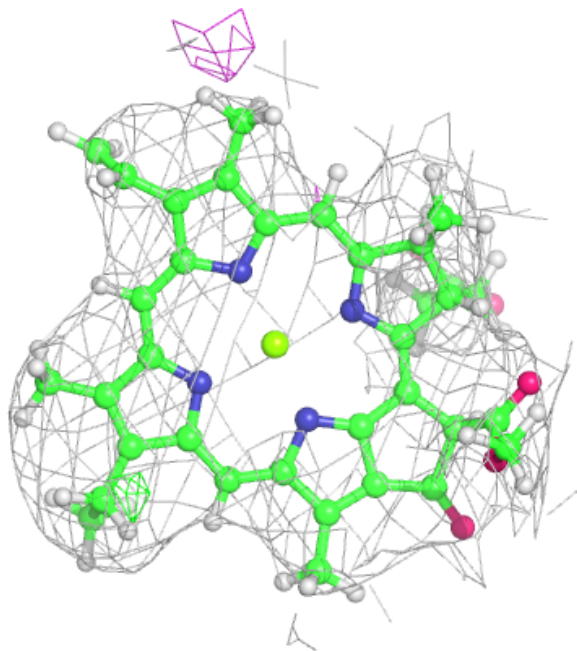
**Electron density around LMG B 849:**

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



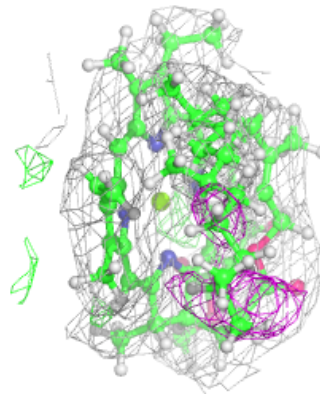
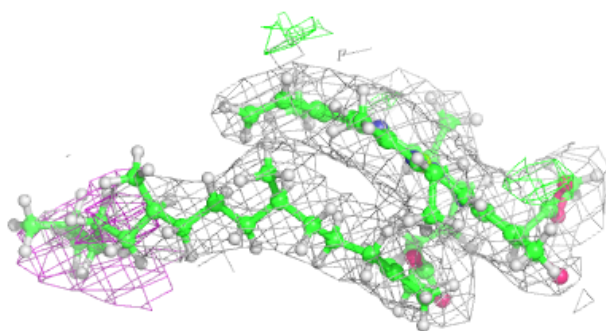
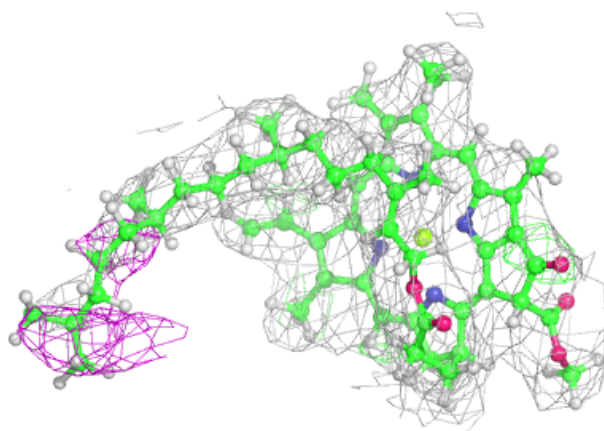
**Electron density around CLA B 830:**

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

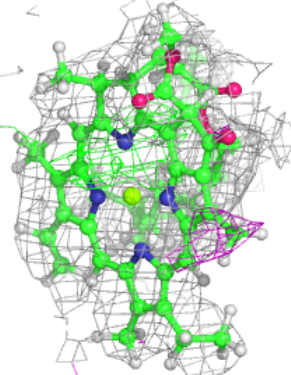
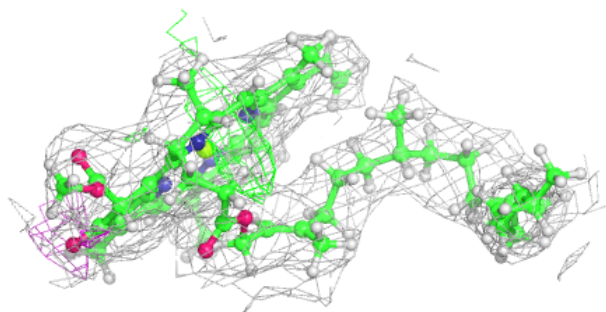
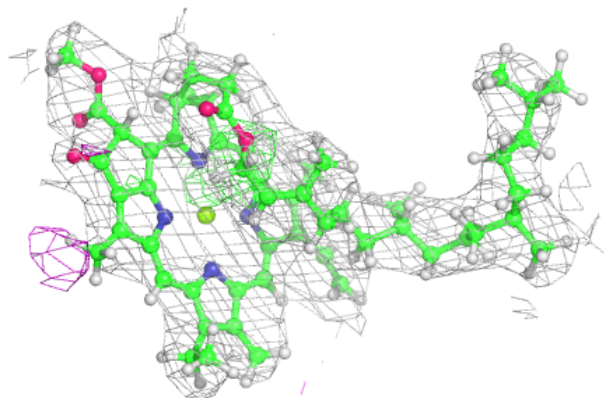


**Electron density around CLA B 807:**

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

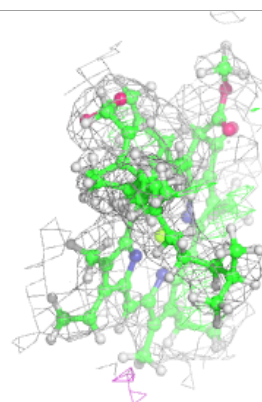
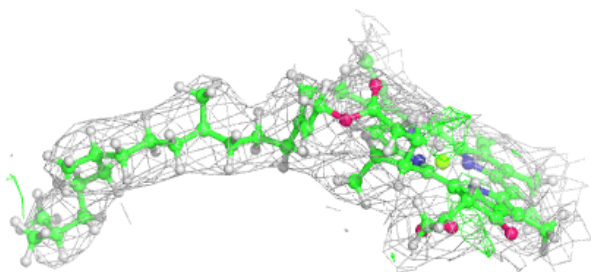
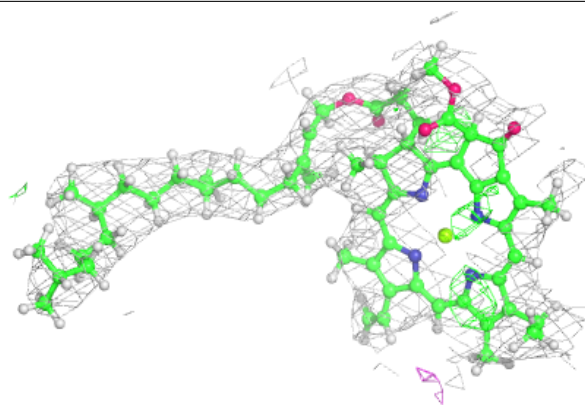
**Electron density around CLA A 843:**

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



**Electron density around CLA A 803:**

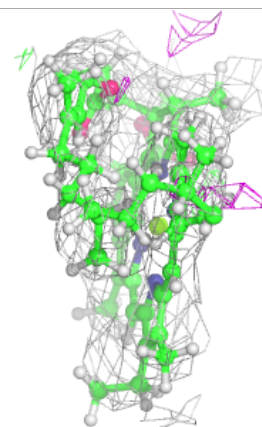
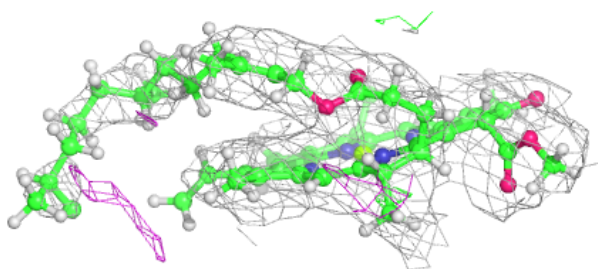
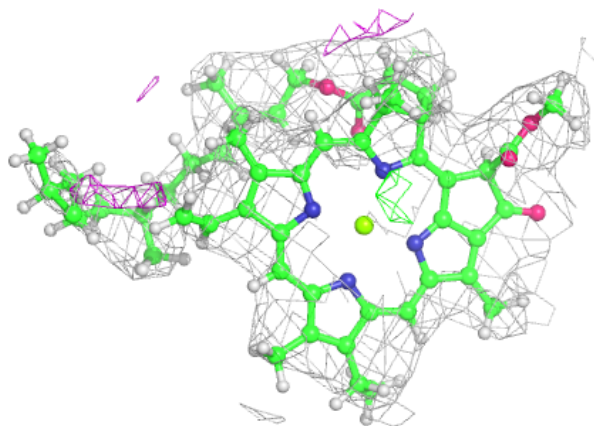
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





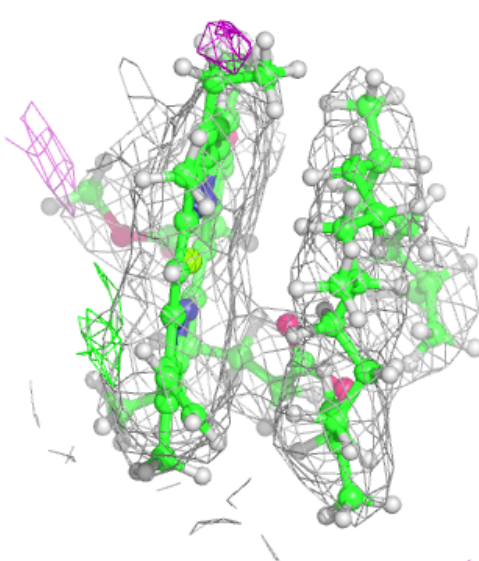
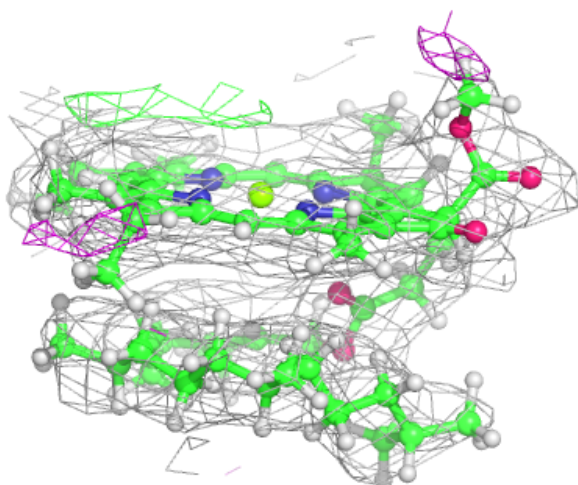
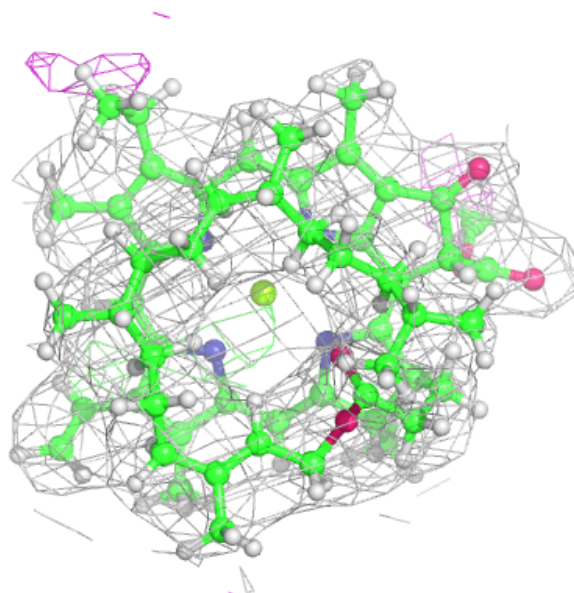
**Electron density around CLA B 818:**

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



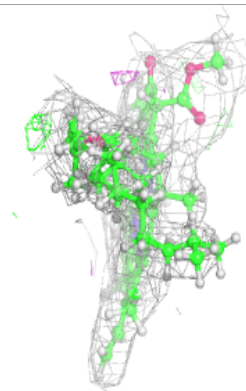
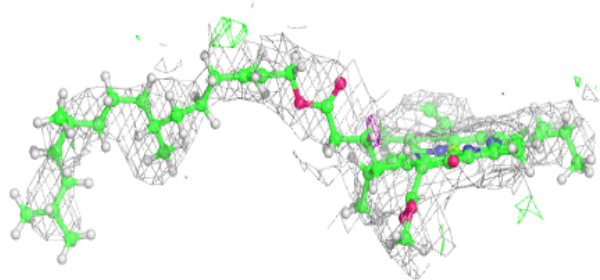
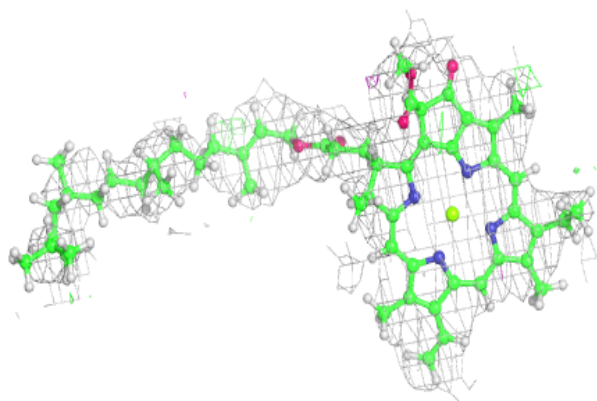
**Electron density around CLA L 204:**

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



**Electron density around CLA A 827:**

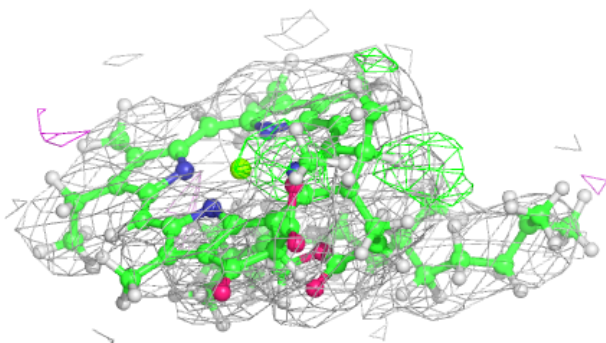
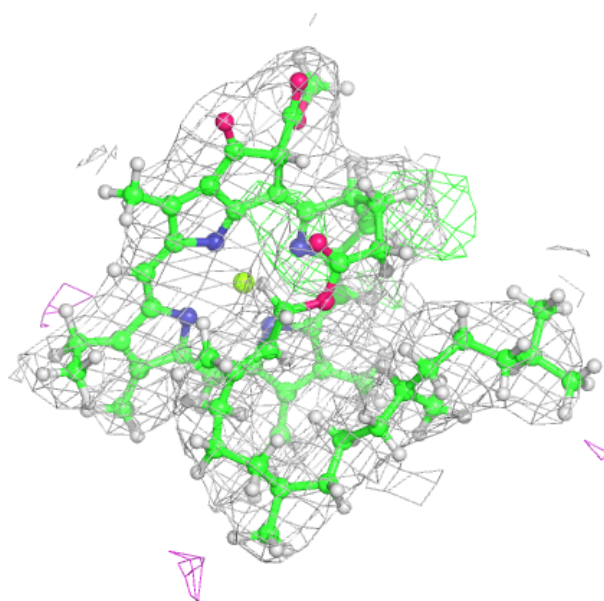
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





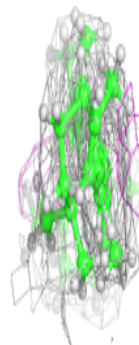
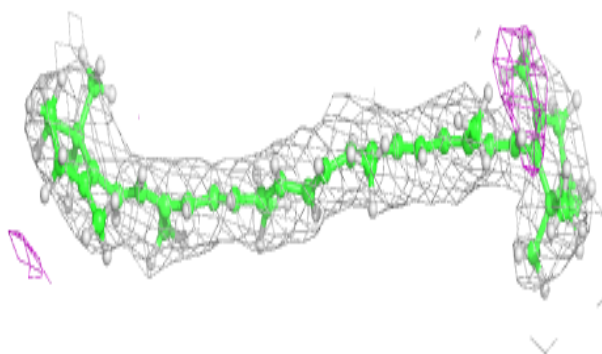
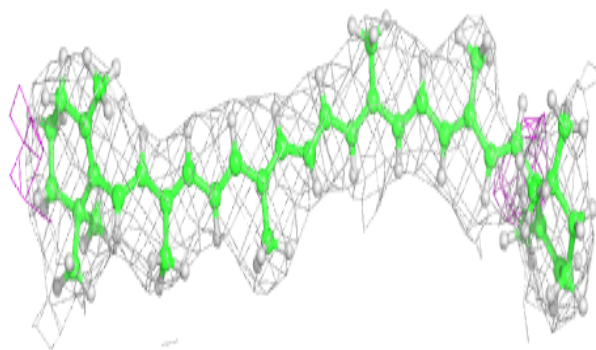
**Electron density around CLA B 808:**

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

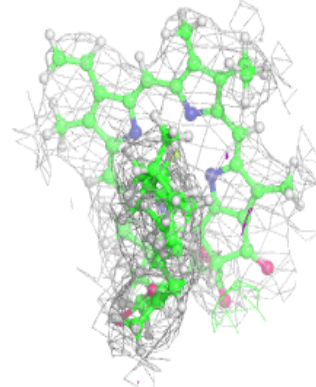
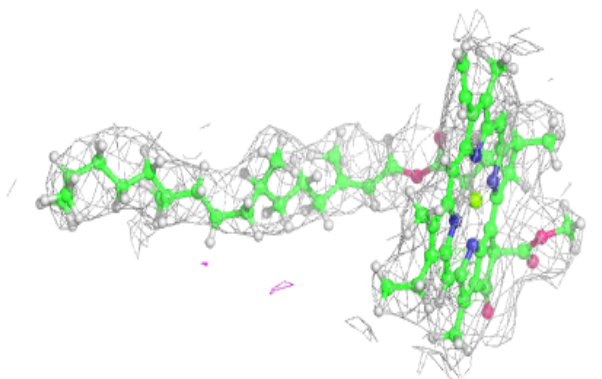
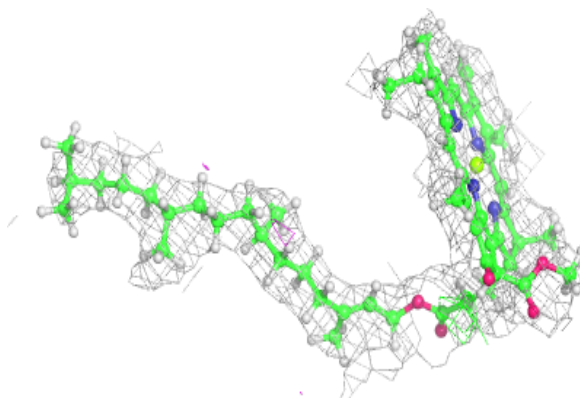


**Electron density around BCR B 848:**

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

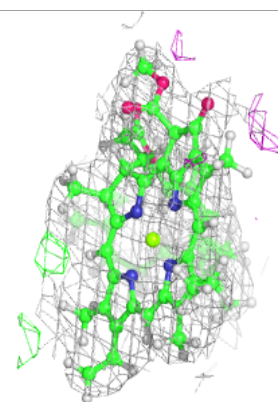
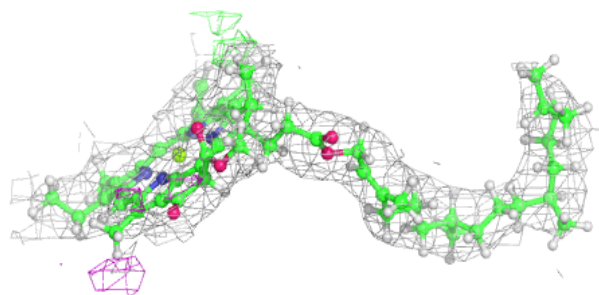
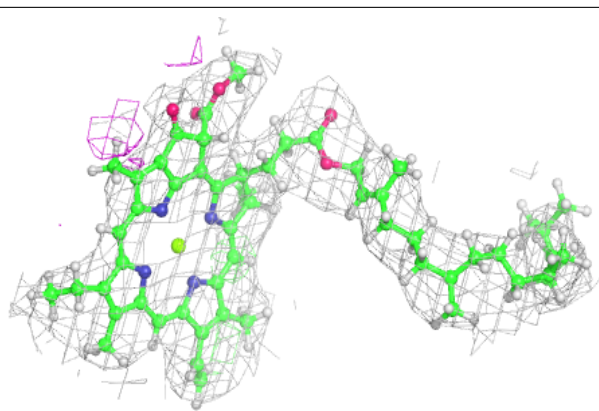
**Electron density around CLA B 829:**

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

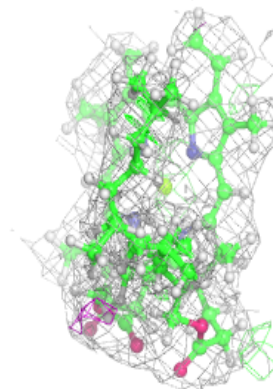
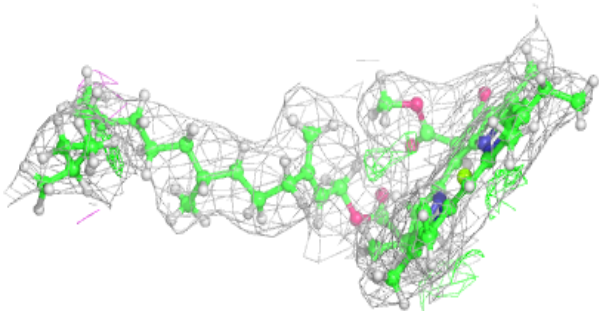
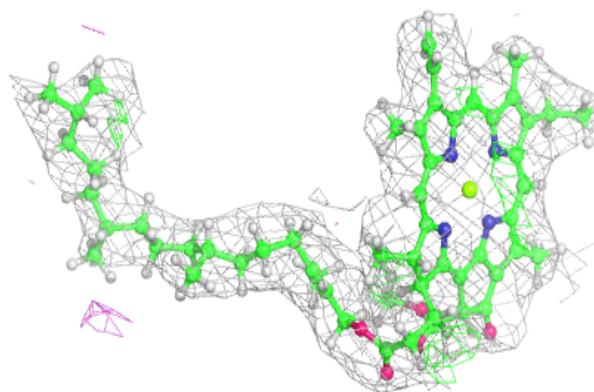


**Electron density around CLA B 809:**

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

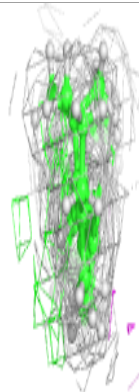
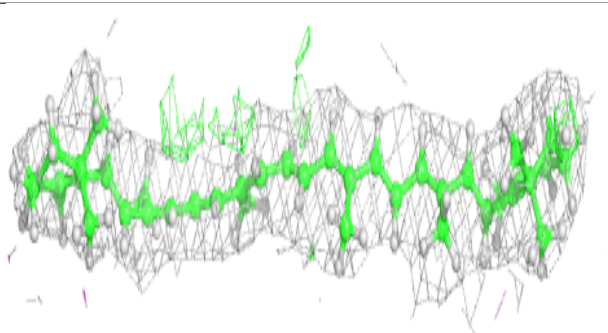
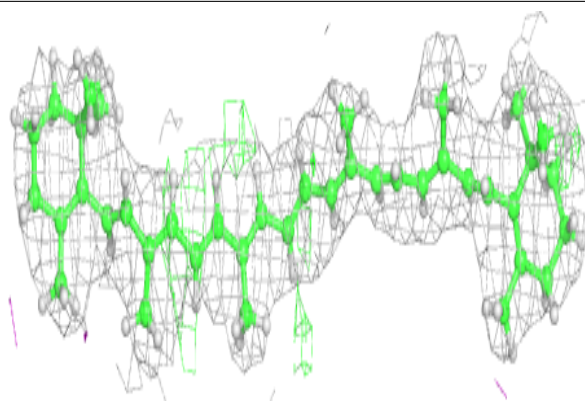
**Electron density around CLA B 810:**

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

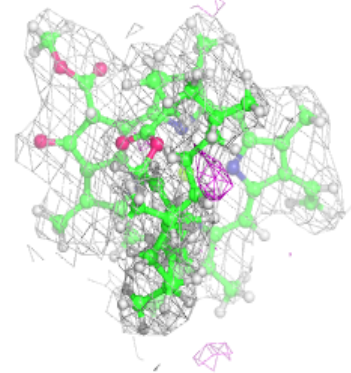
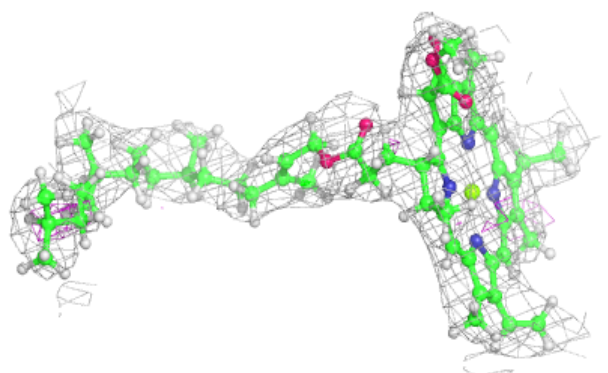
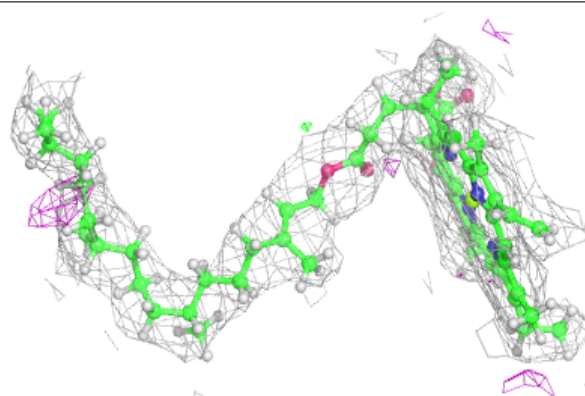


**Electron density around BCR I 103:**

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

**Electron density around CLA B 840:**

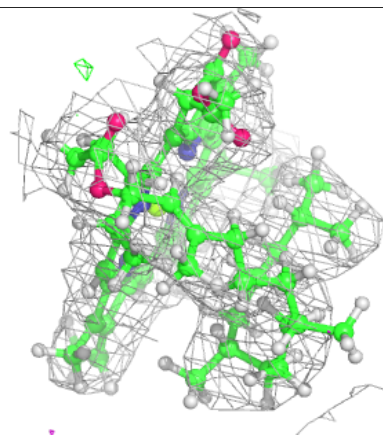
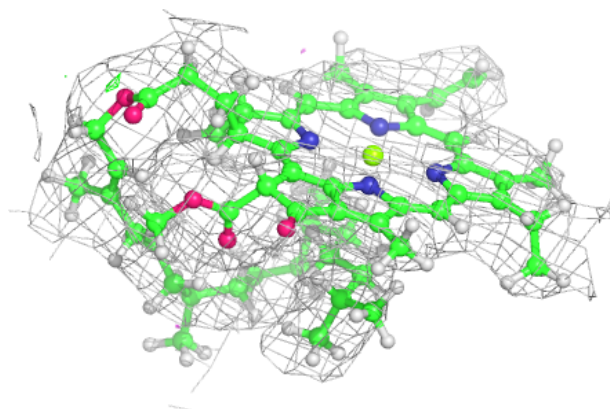
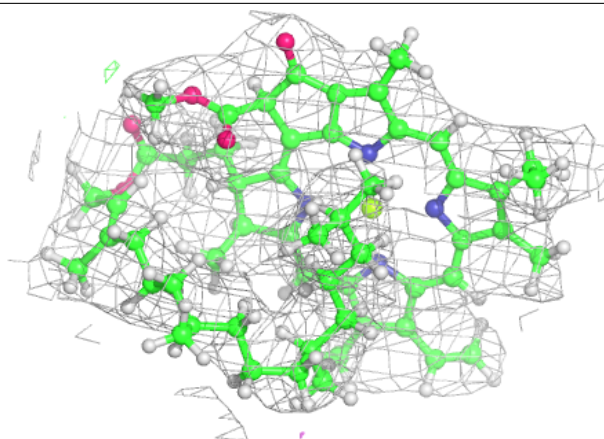
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



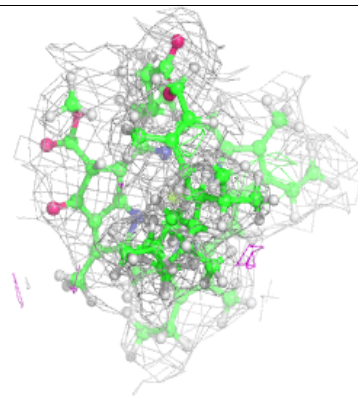
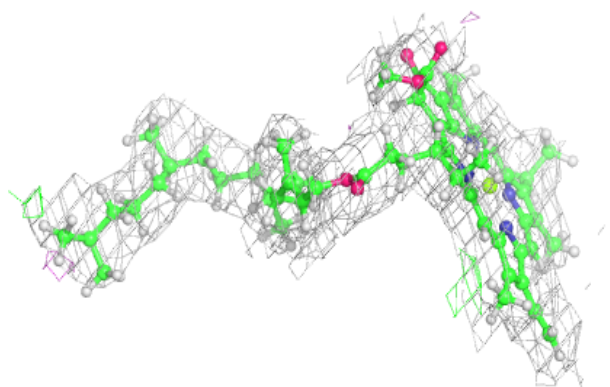
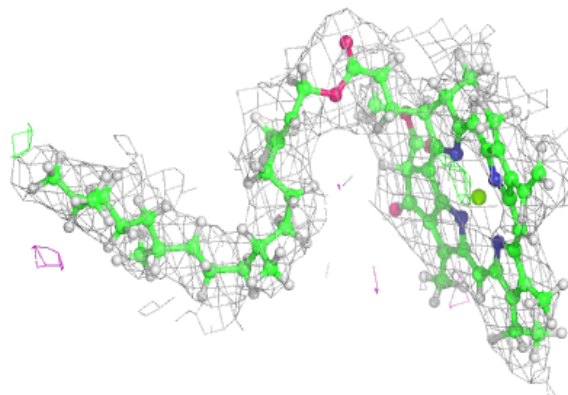


**Electron density around CLA B 806:**

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

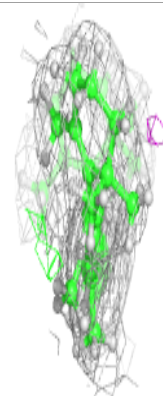
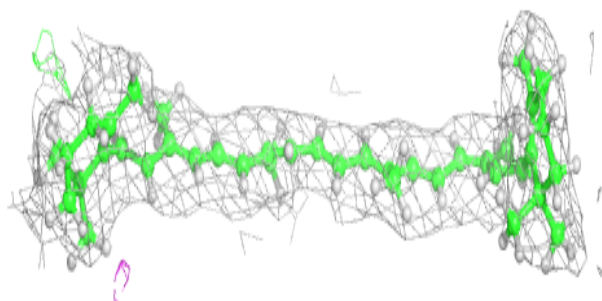
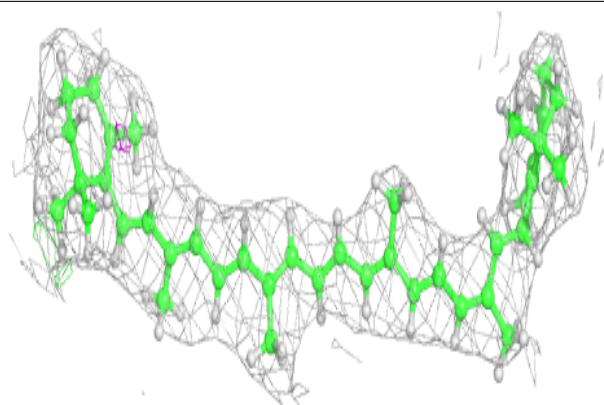
**Electron density around CLA B 802:**

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

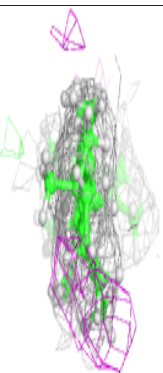
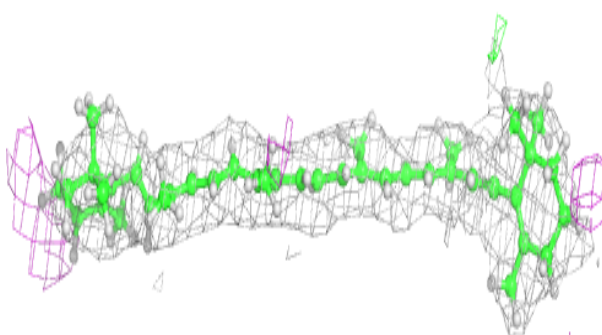
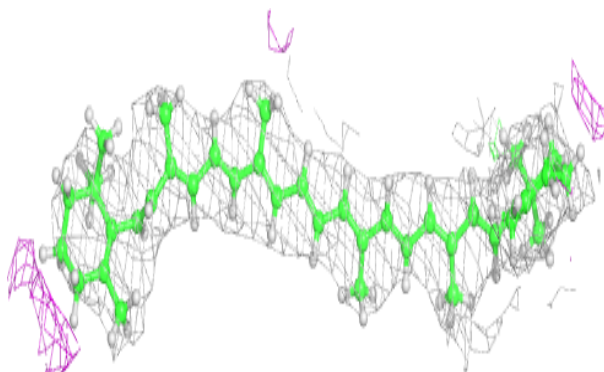


**Electron density around BCR L 201:**

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

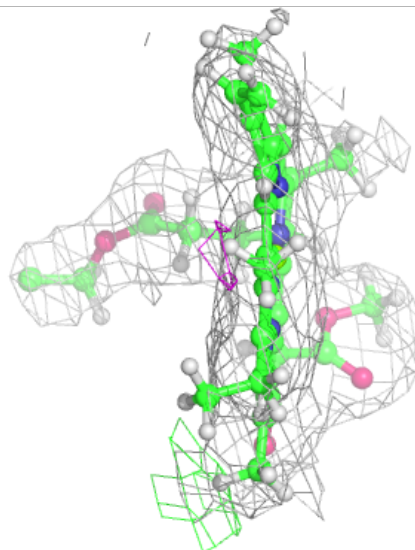
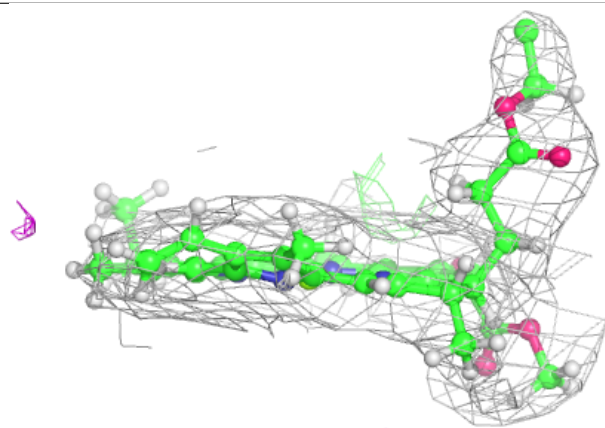
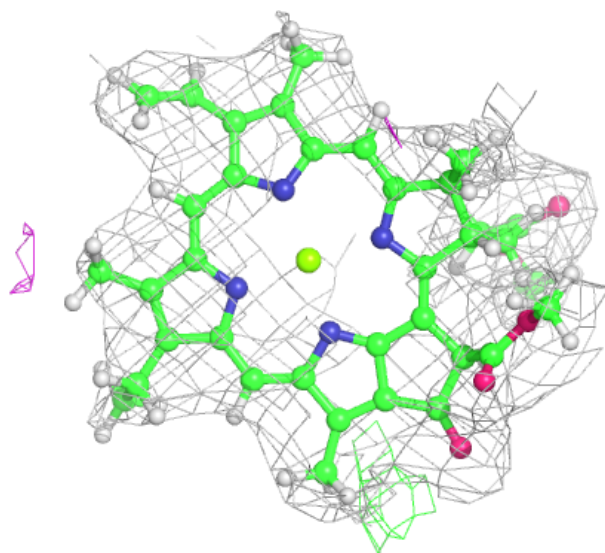
**Electron density around BCR L 208:**

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



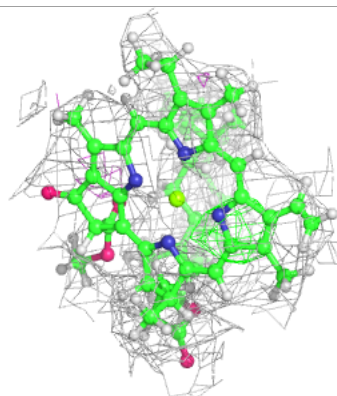
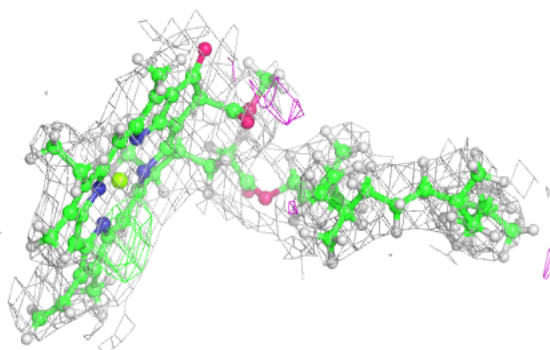
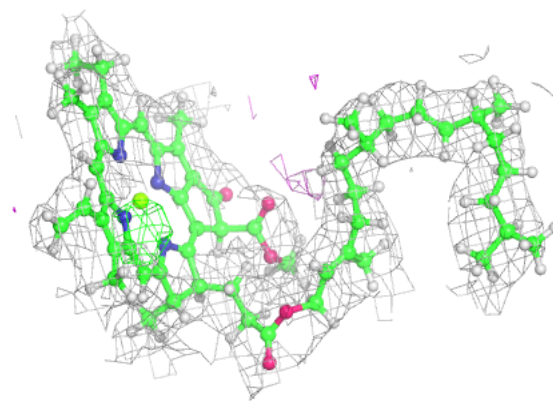
**Electron density around CLA A 840:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

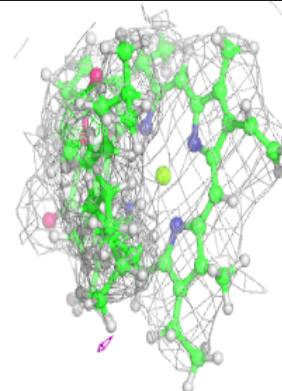
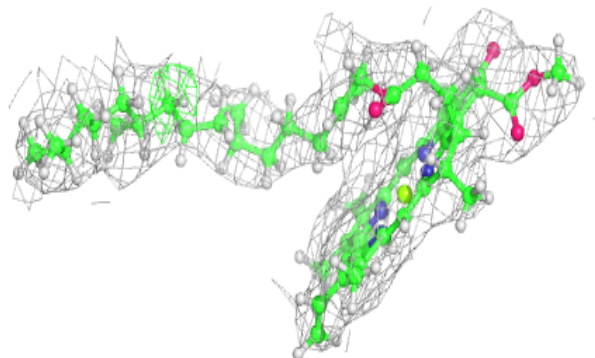
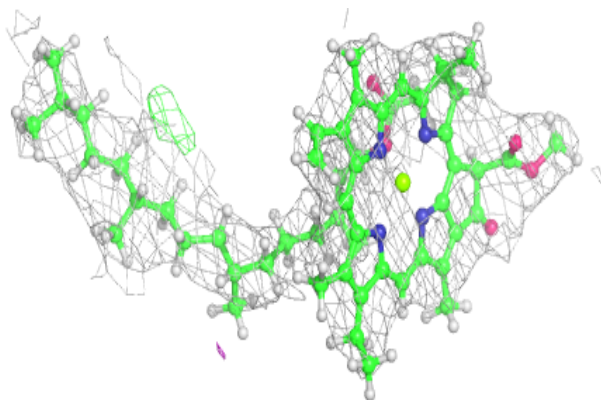


**Electron density around CL0 A 801:**

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

**Electron density around CLA A 842:**

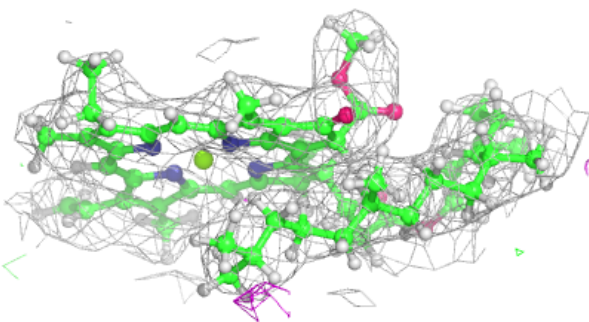
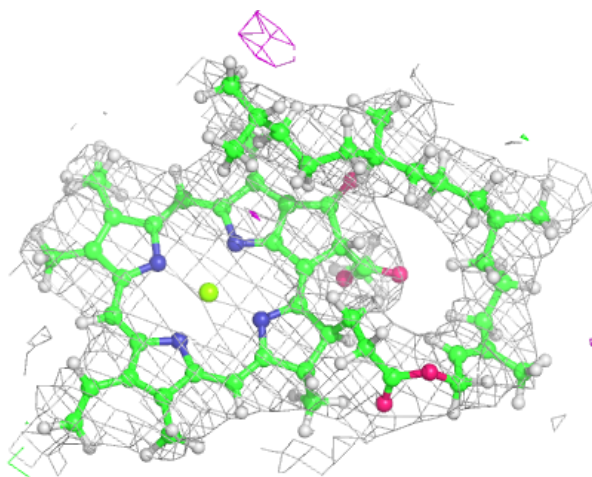
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





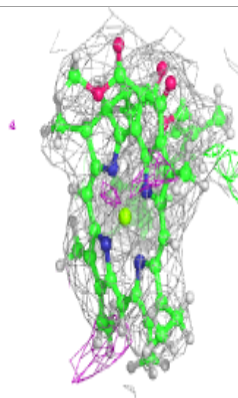
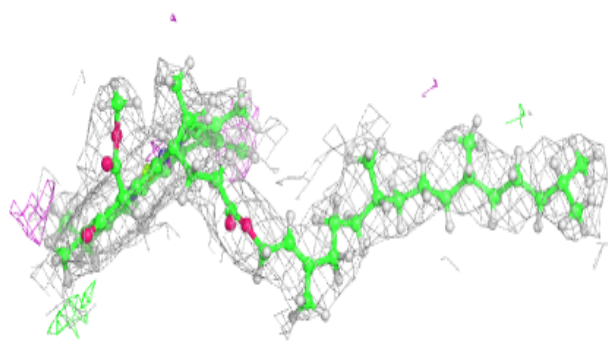
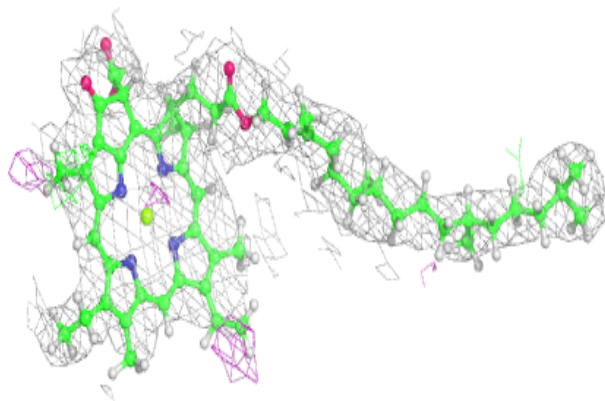
**Electron density around CLA B 805:**

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



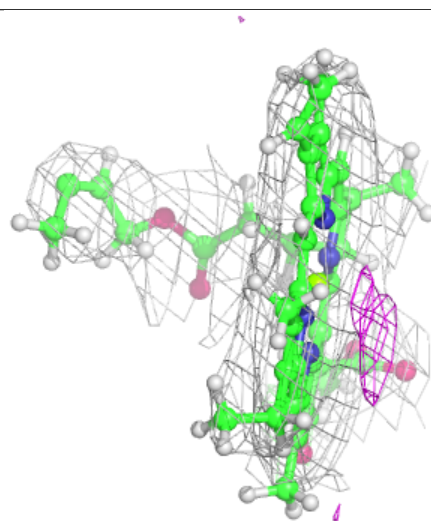
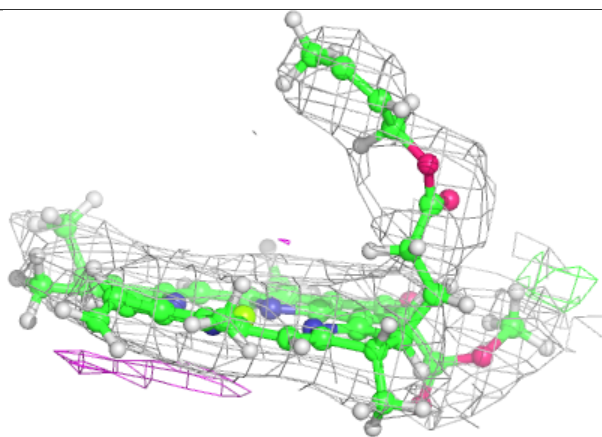
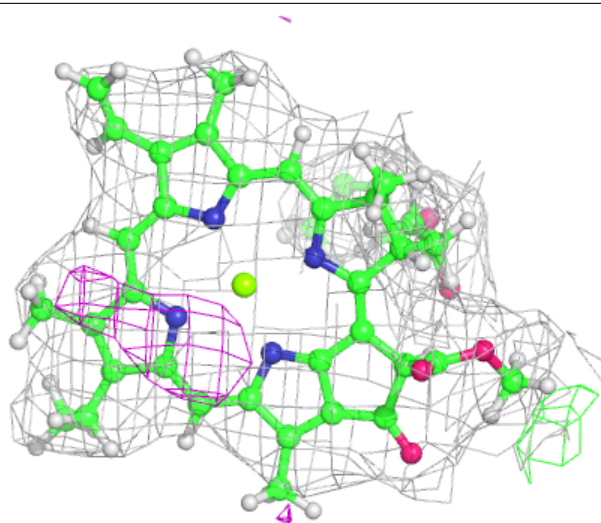
**Electron density around CLA A 835:**

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



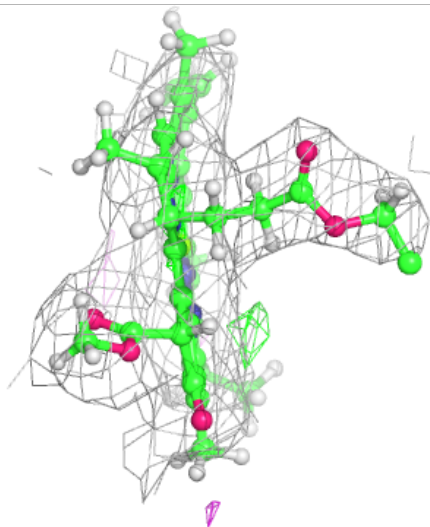
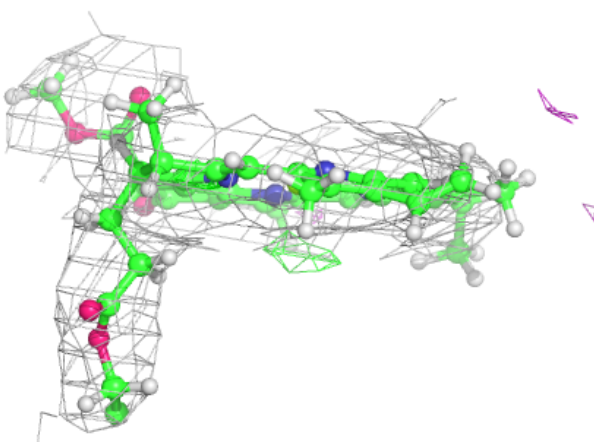
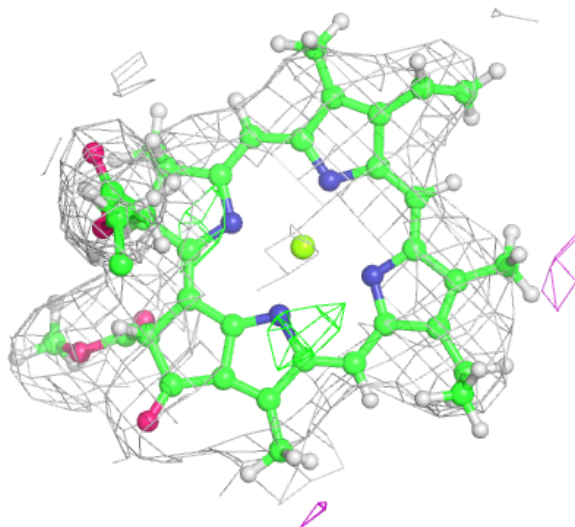
**Electron density around CLA B 831:**

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



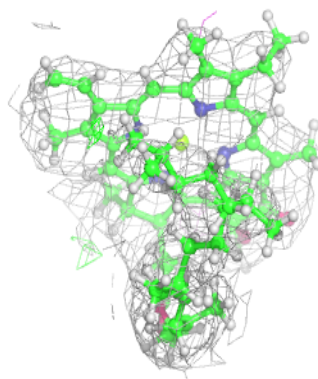
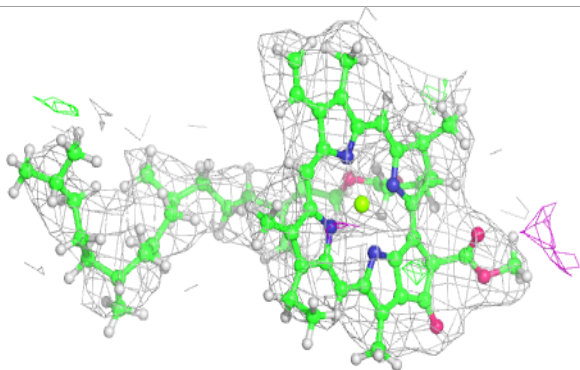
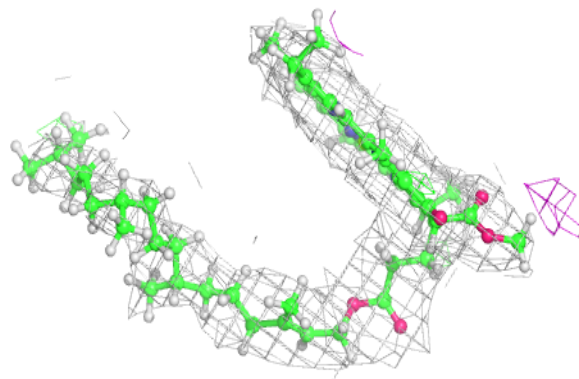
**Electron density around CLA B 839:**

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

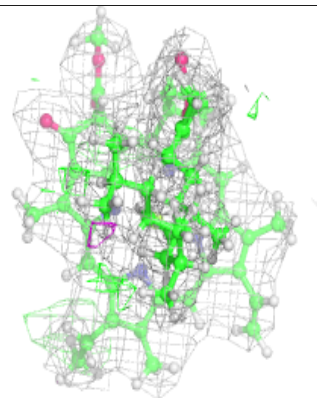
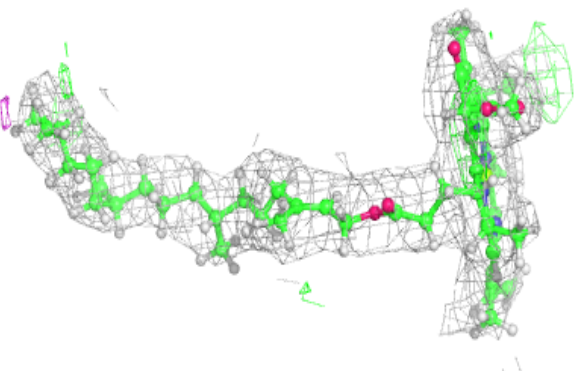
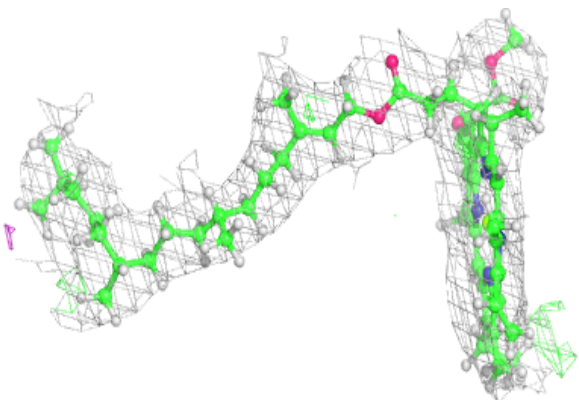


**Electron density around CLA A 833:**

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

**Electron density around CLA B 841:**

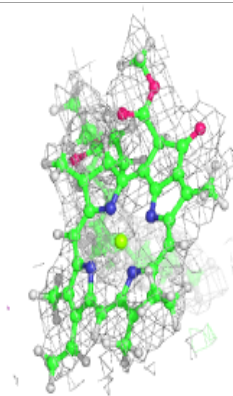
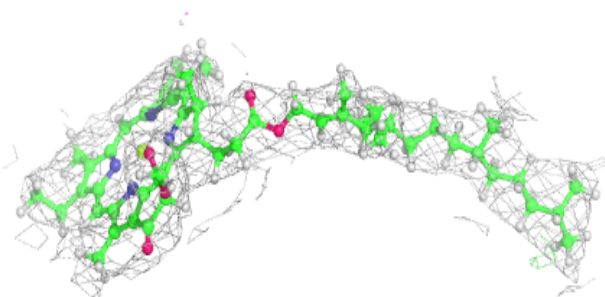
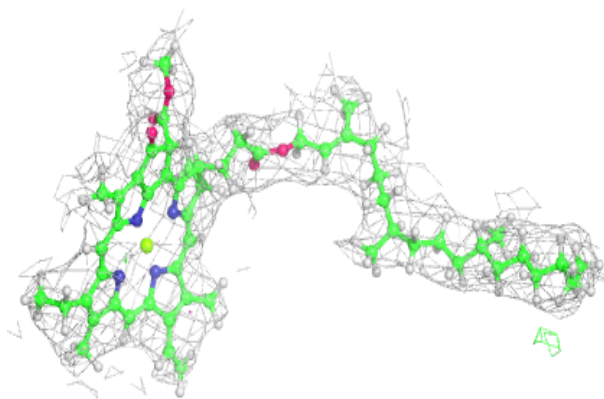
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



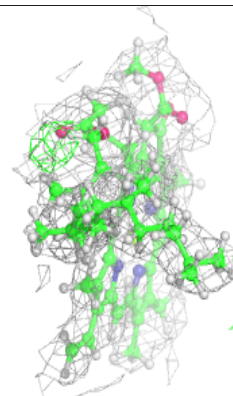
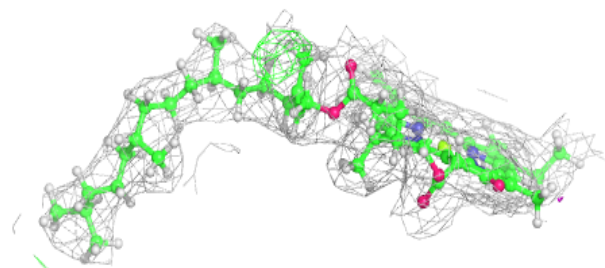
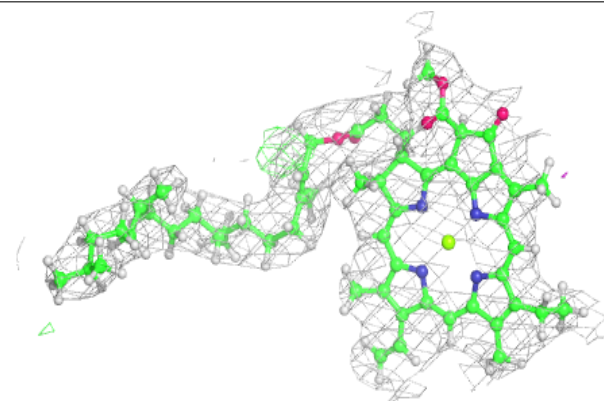


**Electron density around CLA A 802:**

$2mF_o-DF_c$  (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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.