



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 06:24 am BST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.11
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) : 2.11

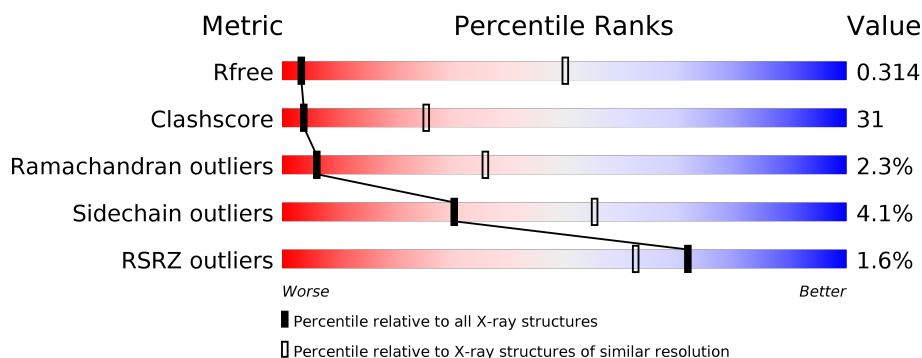
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.92 Å.

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



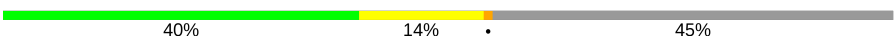


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1135 (6.02-3.80)
Clashscore	141614	1210 (6.02-3.80)
Ramachandran outliers	138981	1141 (6.02-3.80)
Sidechain outliers	138945	1118 (6.02-3.80)
RSRZ outliers	127900	1007 (6.10-3.72)

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

Mol	Chain	Length	Quality of chain
1	A	755	<div> <div>3%</div> <div> <div></div> <div>57%</div> <div>38%</div> <div>••</div> </div> </div>
2	B	740	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>36%</div> <div>•</div> </div> </div>
3	C	80	<div> <div></div> <div> <div></div> <div>79%</div> <div>19%</div> <div>•</div> </div> </div>
4	D	138	<div> <div></div> <div> <div></div> <div>70%</div> <div>27%</div> <div>•</div> </div> </div>
5	E	75	<div> <div>%</div> <div> <div></div> <div>57%</div> <div>31%</div> <div>•</div> <div>8%</div> </div> </div>
6	F	164	<div> <div>%</div> <div> <div></div> <div>51%</div> <div>31%</div> <div>•</div> <div>14%</div> </div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	801	X	-	-	-
13	CLA	A	802	X	-	-	-
13	CLA	A	803	X	-	X	-
13	CLA	A	804	X	-	-	-
13	CLA	A	805	X	-	-	-
13	CLA	A	806	X	-	-	-
13	CLA	A	807	X	-	-	-
13	CLA	A	808	X	-	-	-
13	CLA	A	809	X	-	-	-
13	CLA	A	810	X	-	-	X
13	CLA	A	811	X	-	-	-
13	CLA	A	812	X	-	-	X
13	CLA	A	813	X	-	-	-
13	CLA	A	814	X	-	-	-
13	CLA	A	815	X	-	-	X
13	CLA	A	816	X	-	-	X
13	CLA	A	817	X	-	-	-
13	CLA	A	818	X	-	-	-
13	CLA	A	819	X	-	-	-
13	CLA	A	820	X	-	-	-
13	CLA	A	821	X	-	-	-
13	CLA	A	822	X	-	-	-
13	CLA	A	823	X	-	-	-
13	CLA	A	824	X	-	-	-
13	CLA	A	825	X	-	X	-
13	CLA	A	826	X	-	-	-
13	CLA	A	827	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	828	X	-	-	-
13	CLA	A	829	X	-	-	-
13	CLA	A	830	X	-	-	-
13	CLA	A	831	X	-	-	-
13	CLA	A	832	X	-	X	-
13	CLA	A	833	X	-	-	-
13	CLA	A	834	X	-	-	-
13	CLA	A	835	X	-	-	-
13	CLA	A	836	X	-	-	X
13	CLA	A	837	X	-	-	-
13	CLA	A	838	X	-	-	-
13	CLA	A	839	X	-	-	-
13	CLA	A	840	X	-	-	-
13	CLA	A	841	X	-	-	-
13	CLA	A	842	X	-	X	-
13	CLA	A	843	X	-	-	-
13	CLA	A	844	X	-	-	-
13	CLA	A	845	X	-	-	-
13	CLA	A	855	X	-	-	-
13	CLA	B	801	X	-	-	-
13	CLA	B	802	X	-	-	-
13	CLA	B	803	X	-	-	-
13	CLA	B	804	X	-	-	-
13	CLA	B	805	X	-	-	-
13	CLA	B	806	X	-	-	-
13	CLA	B	807	X	-	-	-
13	CLA	B	808	X	-	-	-
13	CLA	B	809	X	-	-	-
13	CLA	B	810	X	-	-	-
13	CLA	B	811	X	-	-	-
13	CLA	B	812	X	-	-	-
13	CLA	B	813	X	-	-	-
13	CLA	B	814	X	-	-	-
13	CLA	B	815	X	-	-	-
13	CLA	B	816	X	-	-	-
13	CLA	B	817	X	-	-	-
13	CLA	B	818	X	-	-	-
13	CLA	B	819	X	-	-	-
13	CLA	B	820	X	-	-	-
13	CLA	B	821	X	-	-	-
13	CLA	B	822	X	-	X	-
13	CLA	B	823	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	B	824	X	-	-	-
13	CLA	B	825	X	-	-	-
13	CLA	B	826	X	-	-	-
13	CLA	B	827	X	-	-	-
13	CLA	B	828	X	-	-	-
13	CLA	B	829	X	-	-	-
13	CLA	B	830	X	-	X	-
13	CLA	B	831	X	-	-	-
13	CLA	B	832	X	-	-	-
13	CLA	B	833	X	-	-	-
13	CLA	B	834	X	-	-	-
13	CLA	B	835	X	-	-	-
13	CLA	B	836	X	-	-	-
13	CLA	B	837	X	-	-	-
13	CLA	B	838	X	-	-	-
13	CLA	B	839	X	-	-	-
13	CLA	F	1301	X	-	-	-
13	CLA	I	101	X	-	-	-
13	CLA	J	1101	X	-	-	-
13	CLA	J	1102	X	-	-	-
13	CLA	J	1103	X	-	-	-
13	CLA	L	1002	X	-	-	-
13	CLA	L	1003	X	-	-	-
13	CLA	L	1004	X	-	-	-
13	CLA	M	1201	X	-	-	-
13	CLA	M	1202	X	-	-	X
13	CLA	X	102	X	-	-	-
15	BCR	A	847	-	-	-	X
15	BCR	A	848	-	-	-	X
15	BCR	A	849	-	-	-	X
15	BCR	B	841	-	-	-	X

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 23997 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	740	Total	C	N	O	S	0	0	0
			5784	3794	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	N	O	S	0	0	0
			5879	3867	986	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	N	O	S	0	0	0
			598	367	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	N	O	S	0	0	0
			1075	682	186	204	3			

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

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

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

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

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

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

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

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

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

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

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

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

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	N	O	S	0	0	0
			241	161	36	43	1			

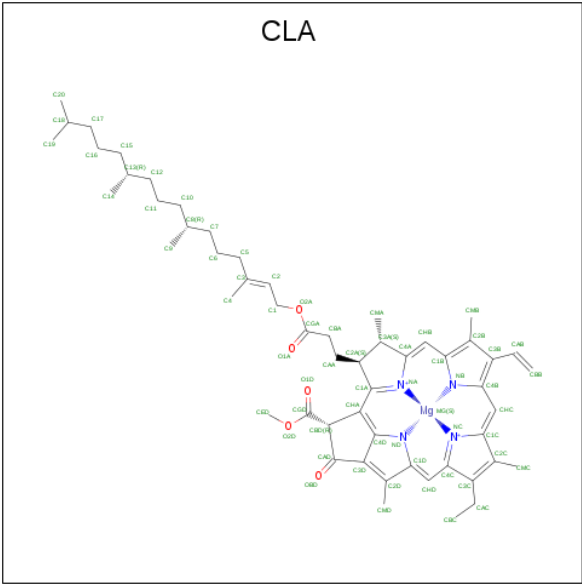
- Molecule 12 is a protein called Photosystem I 4.8K protein.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	32	ALA	-	EXPRESSION TAG	UNP Q8DKP6
X	33	ALA	-	EXPRESSION TAG	UNP Q8DKP6
X	34	ALA	-	EXPRESSION TAG	UNP Q8DKP6
X	35	ALA	-	EXPRESSION TAG	UNP Q8DKP6

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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

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

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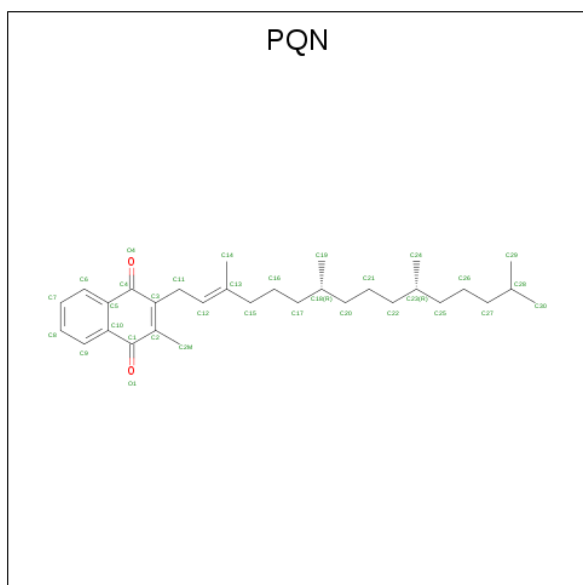
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 58	C 48	Mg 1	N 4	O 5	0	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	F	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	I	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	J	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	J	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	J	1	Total 37	C 31	Mg 1	N 4	O 1	0	0
13	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	M	1	Total 54	C 44	Mg 1	N 4	O 5	0	0

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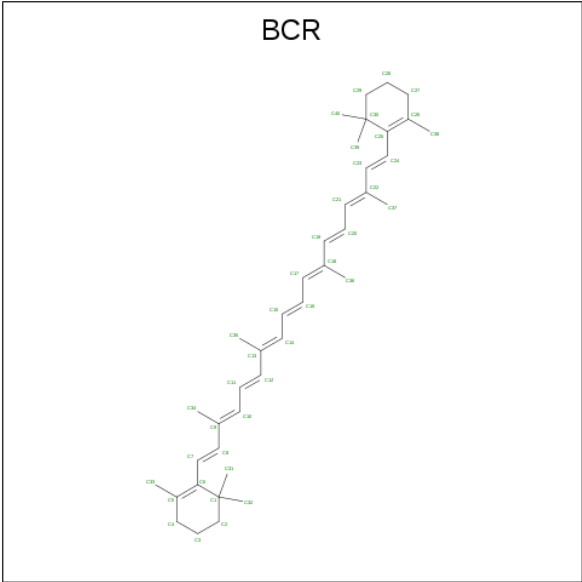
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	M	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	X	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

- Molecule 14 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 15 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



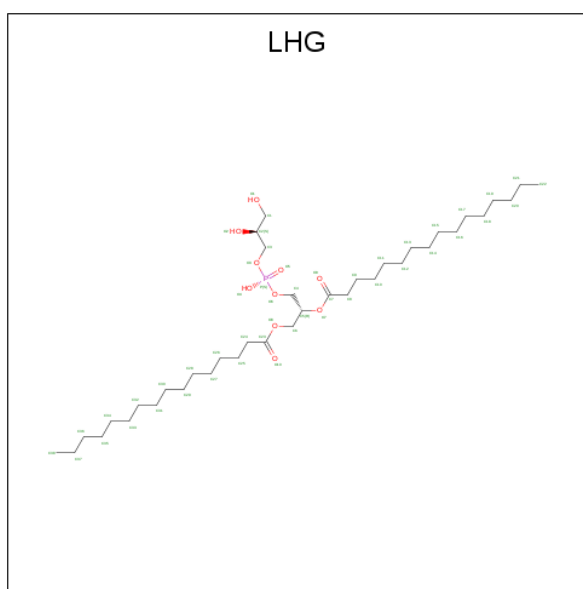
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 25 25	0	0
15	B	1	Total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

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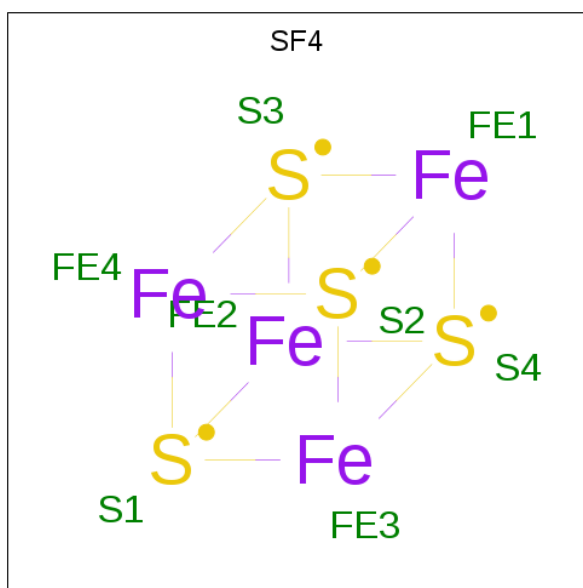
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total C 40 40	0	0
15	F	1	Total C 40 40	0	0
15	I	1	Total C 40 40	0	0
15	J	1	Total C 40 40	0	0
15	J	1	Total C 40 40	0	0
15	L	1	Total C 40 40	0	0
15	L	1	Total C 40 40	0	0
15	M	1	Total C 40 40	0	0

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



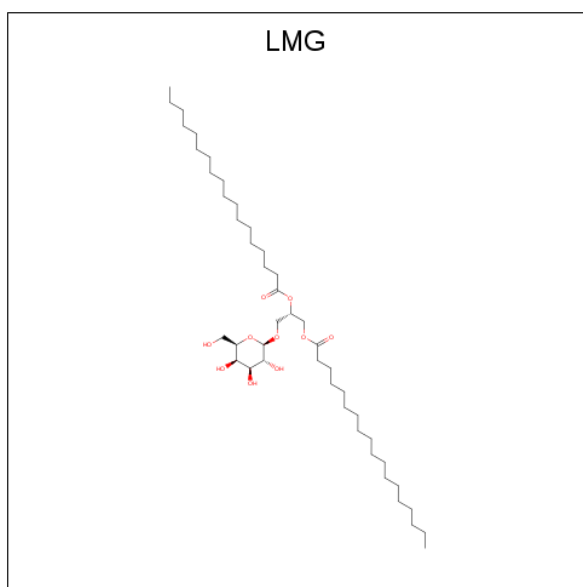
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total C O P 49 38 10 1	0	0
16	A	1	Total C O P 27 16 10 1	0	0
16	X	1	Total C O P 23 12 10 1	0	0

- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $\text{C}_{45}\text{H}_{86}\text{O}_{10}$).



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

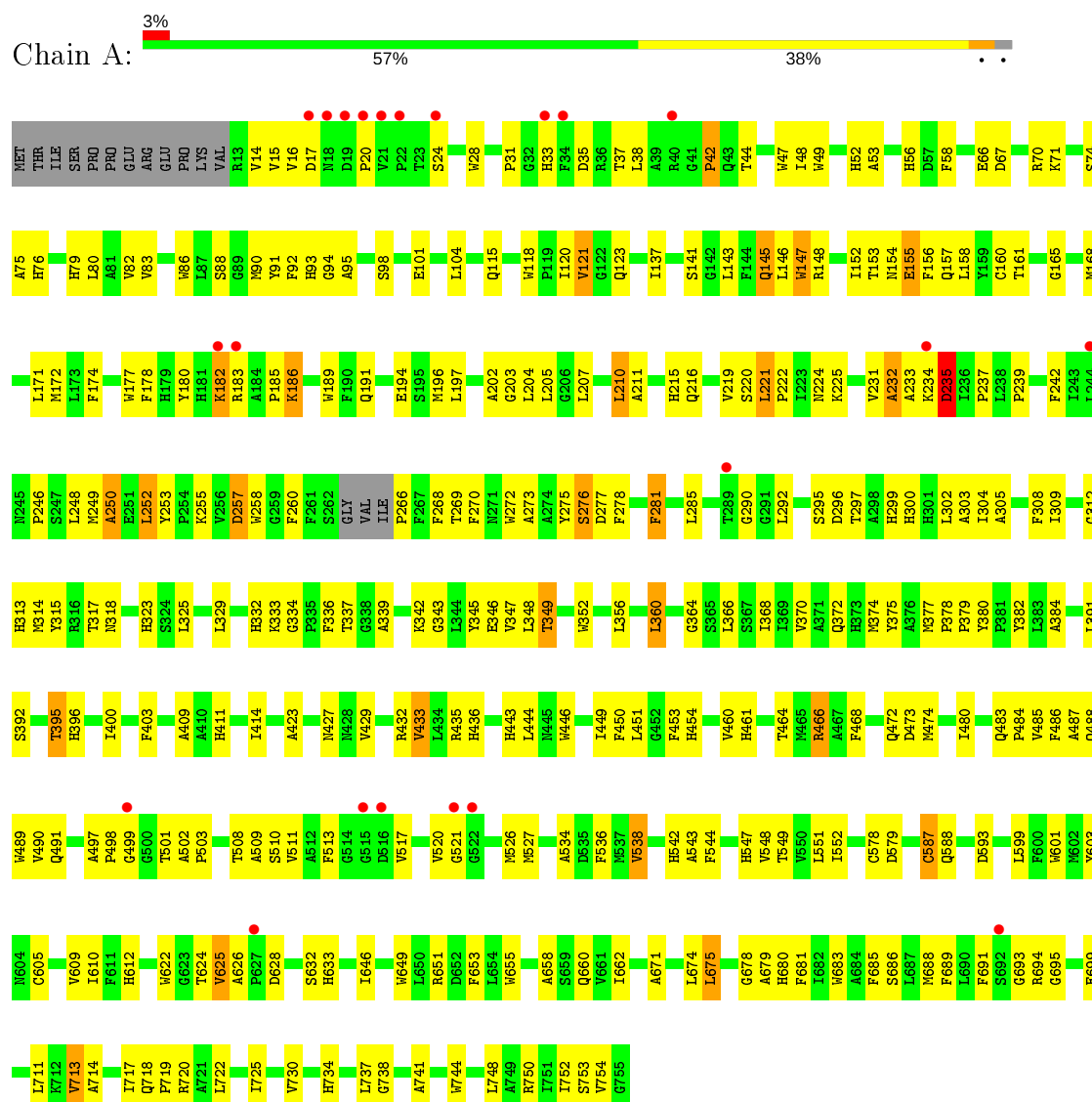
- Molecule 19 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

3 Residue-property plots

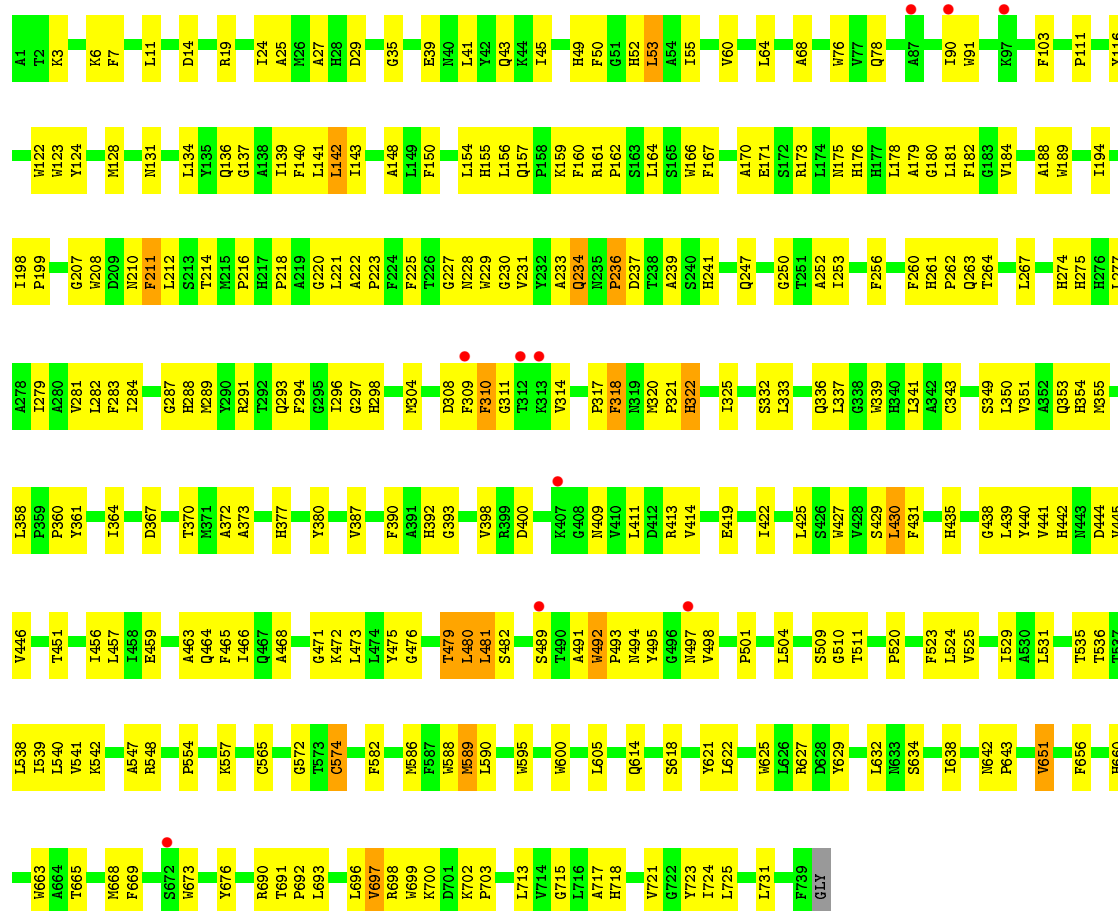
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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



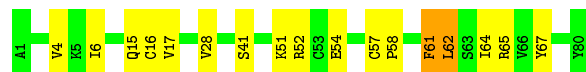
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





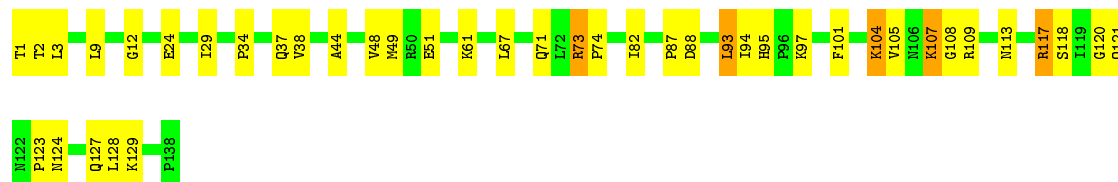
• Molecule 3: Photosystem I iron-sulfur center

Chain C: 79% 19%



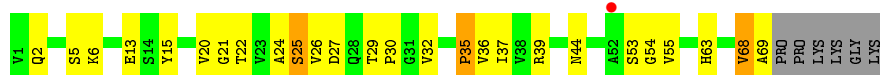
• Molecule 4: Photosystem I reaction center subunit II

Chain D: 70% 27%



• Molecule 5: Photosystem I reaction center subunit IV

Chain E: 57% 31% 8%



- Molecule 6: Photosystem I reaction center subunit III



- Molecule 7: Photosystem I reaction center subunit VIII



- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 9: Photosystem I reaction center subunit PsaK



- Molecule 10: Photosystem I reaction center subunit XI



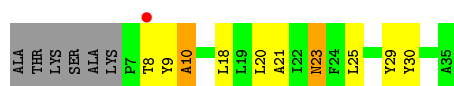
- Molecule 11: Photosystem I reaction center subunit XII

Chain M:  61% 32% 6%



- Molecule 12: Photosystem I 4.8K protein

Chain X: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	281.00Å 281.00Å 165.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.97 – 4.92 97.97 – 4.92	Depositor EDS
% Data completeness (in resolution range)	96.4 (97.97-4.92) 96.3 (97.97-4.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.35 (at 4.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1058)	Depositor
R, R_{free}	0.274 , 0.315 0.274 , 0.314	Depositor DCC
R_{free} test set	1534 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 23.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.13$	Xtriage
Estimated twinning fraction	0.175 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.69	EDS
Total number of atoms	23997	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.38	0/5983	0.69	3/8158 (0.0%)
2	B	0.40	0/6096	0.68	2/8332 (0.0%)
3	C	0.39	0/608	0.76	0/824
4	D	0.35	0/1101	0.78	0/1492
5	E	0.42	0/551	0.85	1/750 (0.1%)
6	F	0.41	0/1087	0.76	0/1476
7	I	0.38	0/312	0.80	1/425 (0.2%)
8	J	0.40	0/350	0.80	1/477 (0.2%)
9	K	0.40	0/220	0.91	0/300
10	L	0.39	0/1148	0.79	2/1558 (0.1%)
11	M	0.47	0/244	0.91	1/332 (0.3%)
12	X	0.41	0/242	0.66	0/332
All	All	0.39	0/17942	0.72	11/24456 (0.0%)

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

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

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	ASP	CB-CG-OD2	-8.44	110.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	ASP	CB-CG-OD1	8.11	125.60	118.30
10	L	76	LEU	CB-CG-CD2	7.19	123.22	111.00
7	I	26	VAL	CG1-CB-CG2	6.87	121.90	110.90
10	L	48	LEU	CB-CG-CD2	6.78	122.52	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5784	0	5639	350	0
2	B	5879	0	5632	345	0
3	C	598	0	580	15	0
4	D	1075	0	1077	30	0
5	E	539	0	528	13	0
6	F	1065	0	1077	51	0
7	I	301	0	306	23	0
8	J	338	0	347	23	0
9	K	222	0	111	9	0
10	L	1119	0	1125	50	1
11	M	241	0	264	22	0
12	X	233	0	231	11	0
13	A	2667	0	2635	478	0
13	B	2230	0	2182	427	0
13	F	45	0	33	5	0
13	I	65	0	72	15	0
13	J	147	0	129	17	0
13	L	195	0	216	28	0
13	M	99	0	81	18	0
13	X	45	0	33	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A	33	0	46	7	0
14	B	33	0	46	7	0
15	A	240	0	336	39	0
15	B	345	0	481	83	0
15	F	40	0	56	13	0
15	I	40	0	56	11	0
15	J	80	0	112	11	0
15	L	80	0	112	16	0
15	M	40	0	56	13	0
16	A	76	0	98	12	0
16	X	23	0	16	1	0
17	A	8	0	0	0	0
17	C	16	0	0	0	0
18	B	55	0	86	18	0
19	L	1	0	0	0	0
All	All	23997	0	23799	1470	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

The worst 5 of 1470 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:806:CLA:H12	7:I:18:VAL:HG21	1.35	1.08
13:A:803:CLA:H151	13:A:842:CLA:HAB	1.36	1.08
13:B:831:CLA:HED1	8:J:36:LEU:H	1.06	1.07
13:B:808:CLA:HMA1	13:I:101:CLA:HAB	1.31	1.06
13:B:817:CLA:HBD	13:B:821:CLA:HED2	1.37	1.06

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:40:GLY:O	10:L:114:SER:OG[3_665]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	736/755 (98%)	685 (93%)	39 (5%)	12 (2%)	9	44
2	B	737/740 (100%)	691 (94%)	37 (5%)	9 (1%)	13	50
3	C	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	12	48
4	D	136/138 (99%)	123 (90%)	8 (6%)	5 (4%)	3	27
5	E	67/75 (89%)	53 (79%)	6 (9%)	8 (12%)	0	6
6	F	139/164 (85%)	127 (91%)	8 (6%)	4 (3%)	4	31
7	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	K	42/83 (51%)	30 (71%)	5 (12%)	7 (17%)	0	3
10	L	149/154 (97%)	138 (93%)	9 (6%)	2 (1%)	12	48
11	M	29/31 (94%)	26 (90%)	2 (7%)	1 (3%)	3	29
12	X	27/35 (77%)	21 (78%)	5 (18%)	1 (4%)	3	27
All	All	2215/2334 (95%)	2039 (92%)	126 (6%)	50 (2%)	6	36

5 of 50 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	589/603 (98%)	567 (96%)	22 (4%)	34	58
2	B	595/597 (100%)	572 (96%)	23 (4%)	32	57
3	C	67/67 (100%)	65 (97%)	2 (3%)	41	63
4	D	115/115 (100%)	109 (95%)	6 (5%)	23	49
5	E	59/64 (92%)	58 (98%)	1 (2%)	60	78
6	F	109/128 (85%)	105 (96%)	4 (4%)	34	58
7	I	32/32 (100%)	31 (97%)	1 (3%)	40	62
8	J	36/36 (100%)	35 (97%)	1 (3%)	43	65
10	L	117/119 (98%)	109 (93%)	8 (7%)	16	42
11	M	26/26 (100%)	24 (92%)	2 (8%)	13	39
12	X	20/24 (83%)	18 (90%)	2 (10%)	7	28
All	All	1765/1811 (98%)	1693 (96%)	72 (4%)	30	55

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	349	SER
2	B	605	LEU
10	L	134	VAL
2	B	411	LEU
2	B	525	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	136	GLN
6	F	95	ASN
2	B	261	HIS
1	A	542	HIS
6	F	40	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 128 ligands modelled in this entry, 1 is monoatomic - leaving 127 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
13	CLA	B	832	-	36,53,73	1.58	7 (19%)	39,89,113	2.67	9 (23%)
13	CLA	A	806	-	59,73,73	1.43	10 (16%)	67,113,113	2.01	11 (16%)
13	CLA	B	837	-	41,55,73	1.57	9 (21%)	45,91,113	2.45	8 (17%)
13	CLA	B	825	-	59,73,73	1.48	9 (15%)	67,113,113	1.99	8 (11%)
15	BCR	A	850	-	41,41,41	2.29	23 (56%)	56,56,56	2.19	22 (39%)
15	BCR	A	847	-	41,41,41	2.23	24 (58%)	56,56,56	2.05	23 (41%)
13	CLA	M	1201	-	48,62,73	1.62	12 (25%)	53,99,113	2.43	12 (22%)
13	CLA	A	822	-	43,57,73	1.58	8 (18%)	46,93,113	2.73	9 (19%)
13	CLA	A	805	-	59,73,73	1.47	11 (18%)	67,113,113	2.00	10 (14%)
13	CLA	A	845	16	46,60,73	1.60	11 (23%)	51,97,113	2.56	13 (25%)
13	CLA	B	817	-	59,73,73	1.43	11 (18%)	67,113,113	2.05	9 (13%)
17	SF4	C	101	3	0,12,12	0.00	-	-	-	-
13	CLA	B	812	-	59,73,73	1.43	11 (18%)	67,113,113	2.27	11 (16%)
13	CLA	B	831	-	52,66,73	1.54	10 (19%)	58,104,113	2.67	12 (20%)
13	CLA	A	828	-	59,73,73	1.46	10 (16%)	67,113,113	2.16	10 (14%)
13	CLA	A	802	-	59,73,73	1.46	10 (16%)	67,113,113	1.89	9 (13%)
13	CLA	A	815	-	36,53,73	1.54	6 (16%)	39,89,113	2.64	10 (25%)
13	CLA	A	810	-	36,53,73	1.56	7 (19%)	39,89,113	2.81	8 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	814	-	49,63,73	1.55	10 (20%)	55,101,113	2.45	11 (20%)
15	BCR	J	1104	-	41,41,41	2.23	24 (58%)	56,56,56	2.24	24 (42%)
13	CLA	A	801	-	59,73,73	1.47	11 (18%)	67,113,113	2.30	12 (17%)
15	BCR	A	851	-	41,41,41	2.21	24 (58%)	56,56,56	2.17	17 (30%)
15	BCR	B	841	-	41,41,41	2.20	24 (58%)	56,56,56	2.11	23 (41%)
13	CLA	B	816	-	54,68,73	1.50	11 (20%)	61,107,113	2.18	14 (22%)
15	BCR	B	846	-	41,41,41	2.22	24 (58%)	56,56,56	2.08	21 (37%)
13	CLA	B	835	-	54,68,73	1.52	10 (18%)	61,107,113	2.41	15 (24%)
13	CLA	B	813	-	36,53,73	1.53	6 (16%)	39,89,113	2.65	10 (25%)
13	CLA	B	808	2	59,73,73	1.44	10 (16%)	67,113,113	2.26	11 (16%)
13	CLA	B	811	-	59,73,73	1.48	10 (16%)	67,113,113	2.25	11 (16%)
13	CLA	B	827	-	59,73,73	1.43	10 (16%)	67,113,113	2.33	12 (17%)
15	BCR	F	1302	-	41,41,41	2.19	25 (60%)	56,56,56	2.20	21 (37%)
13	CLA	J	1102	8	36,53,73	1.56	7 (19%)	39,89,113	2.79	8 (20%)
13	CLA	A	811	13	59,73,73	1.46	10 (16%)	67,113,113	2.19	10 (14%)
13	CLA	A	834	-	59,73,73	1.44	12 (20%)	67,113,113	1.91	9 (13%)
15	BCR	B	842	-	41,41,41	2.26	24 (58%)	56,56,56	2.27	21 (37%)
13	CLA	A	818	-	48,62,73	1.58	11 (22%)	53,99,113	2.40	12 (22%)
13	CLA	A	820	-	55,69,73	1.50	11 (20%)	62,108,113	2.10	12 (19%)
13	CLA	B	803	-	59,73,73	1.46	11 (18%)	67,113,113	2.22	12 (17%)
13	CLA	A	842	-	59,73,73	1.48	11 (18%)	67,113,113	1.90	9 (13%)
15	BCR	B	850	-	41,41,41	2.21	25 (60%)	56,56,56	2.36	25 (44%)
13	CLA	B	821	-	36,53,73	1.61	7 (19%)	39,89,113	2.49	8 (20%)
13	CLA	A	813	-	54,68,73	1.49	9 (16%)	61,107,113	2.30	12 (19%)
13	CLA	J	1101	-	59,73,73	1.42	9 (15%)	67,113,113	2.15	15 (22%)
13	CLA	A	823	-	45,59,73	1.63	9 (20%)	50,96,113	2.08	10 (20%)
13	CLA	B	823	-	40,54,73	1.62	8 (20%)	44,90,113	2.40	10 (22%)
13	CLA	L	1003	-	59,73,73	1.43	10 (16%)	67,113,113	2.38	14 (20%)
16	LHG	A	854	13	26,26,48	1.23	2 (7%)	29,32,54	1.19	2 (6%)
13	CLA	A	838	-	59,73,73	1.44	10 (16%)	67,113,113	2.17	13 (19%)
13	CLA	A	808	1	59,73,73	1.47	9 (15%)	67,113,113	2.39	14 (20%)
13	CLA	B	824	-	59,73,73	1.45	9 (15%)	67,113,113	2.24	13 (19%)
13	CLA	A	807	-	45,59,73	1.65	10 (22%)	50,96,113	2.44	9 (18%)
18	LMG	B	848	-	55,55,55	1.05	8 (14%)	63,63,63	1.23	3 (4%)
13	CLA	A	840	-	59,73,73	1.46	11 (18%)	67,113,113	2.15	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	824	-	53,67,73	1.52	11 (20%)	59,105,113	2.63	14 (23%)
14	PQN	A	846	-	34,34,34	0.97	1 (2%)	42,45,45	1.18	4 (9%)
15	BCR	L	1006	-	41,41,41	2.22	24 (58%)	56,56,56	2.03	19 (33%)
15	BCR	B	843	-	41,41,41	2.18	24 (58%)	56,56,56	2.39	26 (46%)
13	CLA	A	827	-	59,73,73	1.43	10 (16%)	67,113,113	2.19	12 (17%)
13	CLA	A	843	-	59,73,73	1.41	10 (16%)	67,113,113	2.23	14 (20%)
13	CLA	I	101	-	59,73,73	1.45	11 (18%)	67,113,113	2.19	13 (19%)
15	BCR	J	1105	-	41,41,41	2.23	24 (58%)	56,56,56	2.15	23 (41%)
15	BCR	A	849	-	41,41,41	2.10	22 (53%)	56,56,56	2.23	24 (42%)
13	CLA	A	814	-	36,53,73	1.56	6 (16%)	39,89,113	2.62	9 (23%)
13	CLA	X	102	12	36,53,73	1.55	7 (19%)	39,89,113	2.97	8 (20%)
13	CLA	B	839	-	59,73,73	1.44	10 (16%)	67,113,113	2.07	11 (16%)
13	CLA	L	1004	-	59,73,73	1.44	10 (16%)	67,113,113	2.14	12 (17%)
13	CLA	B	829	-	43,57,73	1.57	8 (18%)	46,93,113	2.22	9 (19%)
13	CLA	B	801	-	59,73,73	1.46	11 (18%)	67,113,113	2.20	12 (17%)
15	BCR	A	852	-	41,41,41	2.26	24 (58%)	56,56,56	2.28	20 (35%)
17	SF4	A	856	1,2	0,12,12	0.00	-	-	-	-
13	CLA	B	833	-	36,53,73	1.54	6 (16%)	39,89,113	2.64	8 (20%)
13	CLA	A	829	-	59,73,73	1.44	11 (18%)	67,113,113	2.26	13 (19%)
13	CLA	B	838	-	59,73,73	1.44	10 (16%)	67,113,113	2.23	14 (20%)
13	CLA	A	803	-	59,73,73	1.44	9 (15%)	67,113,113	2.05	12 (17%)
13	CLA	B	807	-	59,73,73	1.47	12 (20%)	67,113,113	2.13	12 (17%)
13	CLA	B	820	-	49,63,73	1.57	11 (22%)	55,101,113	2.10	12 (21%)
13	CLA	B	805	-	59,73,73	1.43	11 (18%)	67,113,113	1.99	11 (16%)
15	BCR	L	1005	-	41,41,41	2.18	23 (56%)	56,56,56	2.26	23 (41%)
13	CLA	B	809	-	36,53,73	1.58	7 (19%)	39,89,113	2.80	8 (20%)
13	CLA	A	839	-	41,55,73	1.57	8 (19%)	45,91,113	2.44	10 (22%)
13	CLA	A	833	-	59,73,73	1.47	10 (16%)	67,113,113	2.01	8 (11%)
13	CLA	B	802	-	59,73,73	1.45	9 (15%)	67,113,113	2.49	11 (16%)
13	CLA	A	821	-	59,73,73	1.45	10 (16%)	67,113,113	2.14	12 (17%)
13	CLA	A	831	-	44,58,73	1.65	11 (25%)	49,95,113	2.35	9 (18%)
14	PQN	B	840	-	34,34,34	0.89	1 (2%)	42,45,45	1.36	4 (9%)
17	SF4	C	102	3	0,12,12	0.00	-	-	-	-
13	CLA	A	837	-	45,59,73	1.66	8 (17%)	50,96,113	2.62	13 (26%)
13	CLA	A	819	-	59,73,73	1.40	11 (18%)	67,113,113	2.29	17 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	816	-	43,57,73	1.55	9 (20%)	46,93,113	2.40	8 (17%)
13	CLA	B	822	-	48,62,73	1.59	10 (20%)	53,99,113	2.42	11 (20%)
16	LHG	A	853	-	48,48,48	0.90	2 (4%)	51,54,54	1.06	2 (3%)
15	BCR	A	848	-	41,41,41	2.24	23 (56%)	56,56,56	2.14	21 (37%)
13	CLA	B	830	-	59,73,73	1.47	10 (16%)	67,113,113	2.08	12 (17%)
13	CLA	B	828	-	36,53,73	1.57	8 (22%)	39,89,113	2.59	7 (17%)
13	CLA	A	844	-	32,49,73	1.56	7 (21%)	32,83,113	1.99	5 (15%)
13	CLA	A	835	-	48,62,73	1.60	9 (18%)	53,99,113	2.10	12 (22%)
13	CLA	J	1103	-	31,45,73	1.77	8 (25%)	31,78,113	2.01	3 (9%)
13	CLA	F	1301	-	36,53,73	1.58	7 (19%)	39,89,113	2.60	10 (25%)
13	CLA	B	836	-	59,73,73	1.45	11 (18%)	67,113,113	2.05	10 (14%)
15	BCR	B	847	-	41,41,41	2.21	24 (58%)	56,56,56	2.27	23 (41%)
13	CLA	A	825	-	59,73,73	1.46	9 (15%)	67,113,113	2.16	10 (14%)
13	CLA	B	806	-	59,73,73	1.44	12 (20%)	67,113,113	2.15	11 (16%)
13	CLA	A	832	-	59,73,73	1.46	11 (18%)	67,113,113	2.24	11 (16%)
13	CLA	A	812	-	48,62,73	1.56	10 (20%)	53,99,113	2.44	12 (22%)
13	CLA	A	804	13	53,67,73	1.55	9 (16%)	59,105,113	2.09	10 (16%)
13	CLA	A	836	1	36,53,73	1.57	6 (16%)	39,89,113	2.42	9 (23%)
15	BCR	I	102	-	41,41,41	2.10	21 (51%)	56,56,56	2.32	23 (41%)
16	LHG	X	101	-	22,22,48	1.31	2 (9%)	25,28,54	1.01	1 (4%)
13	CLA	B	826	-	59,73,73	1.45	10 (16%)	67,113,113	1.87	8 (11%)
13	CLA	A	855	-	36,53,73	1.54	7 (19%)	39,89,113	2.65	9 (23%)
15	BCR	M	1203	-	41,41,41	2.18	22 (53%)	56,56,56	2.27	21 (37%)
13	CLA	M	1202	-	36,53,73	1.57	6 (16%)	39,89,113	2.71	7 (17%)
15	BCR	B	845	-	41,41,41	2.18	23 (56%)	56,56,56	2.35	22 (39%)
15	BCR	B	844	-	25,25,41	2.30	14 (56%)	33,33,56	2.14	13 (39%)
13	CLA	A	841	-	45,59,73	1.61	9 (20%)	50,96,113	2.21	10 (20%)
13	CLA	B	810	-	36,53,73	1.54	8 (22%)	39,89,113	2.39	7 (17%)
13	CLA	A	809	1	59,73,73	1.46	10 (16%)	67,113,113	2.28	17 (25%)
13	CLA	B	815	-	53,67,73	1.53	10 (18%)	59,105,113	2.02	9 (15%)
13	CLA	A	826	-	59,73,73	1.49	11 (18%)	67,113,113	2.10	14 (20%)
13	CLA	A	817	-	48,62,73	1.61	10 (20%)	53,99,113	2.20	10 (18%)
13	CLA	A	830	-	59,73,73	1.43	9 (15%)	67,113,113	2.29	13 (19%)
13	CLA	B	804	-	59,73,73	1.44	10 (16%)	67,113,113	2.06	11 (16%)
13	CLA	L	1002	10	59,73,73	1.43	10 (16%)	67,113,113	2.28	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	818	-	41,55,73	1.58	7 (17%)	45,91,113	2.32	7 (15%)
13	CLA	B	834	-	36,53,73	1.57	7 (19%)	39,89,113	2.67	8 (20%)
13	CLA	B	819	-	36,53,73	1.58	7 (19%)	39,89,113	2.76	8 (20%)
15	BCR	B	849	-	41,41,41	2.13	21 (51%)	56,56,56	2.34	22 (39%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	832	-	3/3/16/25	2/11/111/135	-
13	CLA	A	806	-	2/2/20/25	8/37/135/135	-
13	CLA	B	837	-	3/3/16/25	4/16/114/135	-
13	CLA	B	825	-	3/3/20/25	11/37/135/135	-
15	BCR	A	850	-	-	6/29/63/63	0/2/2/2
15	BCR	A	847	-	-	8/29/63/63	0/2/2/2
13	CLA	M	1201	-	2/2/17/25	5/24/122/135	-
13	CLA	A	822	-	3/3/16/25	4/18/116/135	-
13	CLA	A	805	-	1/1/20/25	10/37/135/135	-
13	CLA	A	845	16	3/3/17/25	3/22/120/135	-
13	CLA	B	817	-	2/2/20/25	10/37/135/135	-
17	SF4	C	101	3	-	-	0/6/5/5
13	CLA	B	812	-	3/3/20/25	11/37/135/135	-
13	CLA	B	831	-	3/3/18/25	6/29/127/135	-
13	CLA	A	828	-	2/2/20/25	18/37/135/135	-
13	CLA	A	802	-	2/2/20/25	3/37/135/135	-
13	CLA	A	815	-	2/2/16/25	0/11/111/135	-
13	CLA	A	810	-	3/3/16/25	3/11/111/135	-
13	CLA	B	814	-	3/3/18/25	4/25/123/135	-
15	BCR	J	1104	-	-	11/29/63/63	0/2/2/2
13	CLA	A	801	-	2/2/20/25	7/37/135/135	-
15	BCR	A	851	-	-	8/29/63/63	0/2/2/2
15	BCR	B	841	-	-	10/29/63/63	0/2/2/2
13	CLA	B	816	-	2/2/19/25	4/31/129/135	-
15	BCR	B	846	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	835	-	2/2/19/25	8/31/129/135	-
13	CLA	B	813	-	1/1/16/25	1/11/111/135	-
13	CLA	B	808	2	1/1/20/25	7/37/135/135	-
13	CLA	B	811	-	2/2/20/25	10/37/135/135	-
13	CLA	B	827	-	3/3/20/25	8/37/135/135	-
15	BCR	F	1302	-	-	10/29/63/63	0/2/2/2
13	CLA	J	1102	8	2/2/16/25	3/11/111/135	-
13	CLA	A	811	13	3/3/20/25	13/37/135/135	-
13	CLA	A	834	-	2/2/20/25	12/37/135/135	-
15	BCR	B	842	-	-	12/29/63/63	0/2/2/2
13	CLA	A	818	-	3/3/17/25	7/24/122/135	-
13	CLA	A	820	-	3/3/19/25	9/33/131/135	-
13	CLA	B	803	-	1/1/20/25	12/37/135/135	-
13	CLA	A	842	-	3/3/20/25	14/37/135/135	-
15	BCR	B	850	-	-	8/29/63/63	0/2/2/2
13	CLA	B	821	-	3/3/16/25	2/11/111/135	-
13	CLA	A	813	-	3/3/19/25	7/31/129/135	-
13	CLA	J	1101	-	3/3/20/25	5/37/135/135	-
13	CLA	A	823	-	3/3/17/25	4/21/119/135	-
13	CLA	B	823	-	2/2/16/25	1/15/113/135	-
13	CLA	L	1003	-	3/3/20/25	14/37/135/135	-
16	LHG	A	854	13	-	10/31/31/53	-
13	CLA	A	838	-	2/2/20/25	13/37/135/135	-
13	CLA	A	808	1	3/3/20/25	10/37/135/135	-
13	CLA	B	824	-	1/1/20/25	9/37/135/135	-
13	CLA	A	807	-	3/3/17/25	5/21/119/135	-
18	LMG	B	848	-	-	11/50/70/70	0/1/1/1
13	CLA	A	840	-	3/3/20/25	10/37/135/135	-
13	CLA	A	824	-	3/3/18/25	9/30/128/135	-
14	PQN	A	846	-	-	7/23/43/43	0/2/2/2
15	BCR	L	1006	-	-	8/29/63/63	0/2/2/2
15	BCR	B	843	-	-	9/29/63/63	0/2/2/2
13	CLA	A	827	-	3/3/20/25	8/37/135/135	-
13	CLA	A	843	-	3/3/20/25	6/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	I	101	-	2/2/20/25	10/37/135/135	-
15	BCR	J	1105	-	-	14/29/63/63	0/2/2/2
15	BCR	A	849	-	-	5/29/63/63	0/2/2/2
13	CLA	A	814	-	3/3/16/25	1/11/111/135	-
13	CLA	X	102	12	2/2/16/25	1/11/111/135	-
13	CLA	B	839	-	3/3/20/25	5/37/135/135	-
13	CLA	L	1004	-	3/3/20/25	9/37/135/135	-
13	CLA	B	829	-	3/3/16/25	3/18/116/135	-
13	CLA	B	801	-	2/2/20/25	10/37/135/135	-
15	BCR	A	852	-	-	13/29/63/63	0/2/2/2
17	SF4	A	856	1,2	-	-	0/6/5/5
13	CLA	B	833	-	2/2/16/25	2/11/111/135	-
13	CLA	A	829	-	2/2/20/25	9/37/135/135	-
13	CLA	B	838	-	3/3/20/25	13/37/135/135	-
13	CLA	A	803	-	3/3/20/25	9/37/135/135	-
13	CLA	B	807	-	3/3/20/25	14/37/135/135	-
13	CLA	B	820	-	3/3/18/25	6/25/123/135	-
13	CLA	B	805	-	3/3/20/25	5/37/135/135	-
15	BCR	L	1005	-	-	9/29/63/63	0/2/2/2
13	CLA	B	809	-	3/3/16/25	1/11/111/135	-
13	CLA	A	839	-	3/3/16/25	3/16/114/135	-
13	CLA	A	833	-	2/2/20/25	6/37/135/135	-
13	CLA	B	802	-	1/1/20/25	10/37/135/135	-
13	CLA	A	821	-	2/2/20/25	14/37/135/135	-
13	CLA	A	831	-	3/3/17/25	2/19/117/135	-
14	PQN	B	840	-	-	7/23/43/43	0/2/2/2
17	SF4	C	102	3	-	-	0/6/5/5
13	CLA	A	837	-	1/1/17/25	2/21/119/135	-
13	CLA	A	819	-	3/3/20/25	11/37/135/135	-
13	CLA	A	816	-	2/2/16/25	3/18/116/135	-
13	CLA	B	822	-	2/2/17/25	9/24/122/135	-
16	LHG	A	853	-	-	22/53/53/53	-
15	BCR	A	848	-	-	13/29/63/63	0/2/2/2
13	CLA	B	830	-	2/2/20/25	11/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	828	-	2/2/16/25	4/11/111/135	-
13	CLA	A	844	-	1/1/14/25	0/5/101/135	-
13	CLA	A	835	-	3/3/17/25	5/24/122/135	-
13	CLA	J	1103	-	2/2/13/25	0/2/96/135	-
13	CLA	F	1301	-	1/1/16/25	3/11/111/135	-
13	CLA	B	836	-	3/3/20/25	9/37/135/135	-
15	BCR	B	847	-	-	12/29/63/63	0/2/2/2
13	CLA	A	825	-	2/2/20/25	6/37/135/135	-
13	CLA	B	806	-	2/2/20/25	9/37/135/135	-
13	CLA	A	832	-	2/2/20/25	16/37/135/135	-
13	CLA	A	812	-	2/2/17/25	9/24/122/135	-
13	CLA	A	804	13	3/3/18/25	8/30/128/135	-
13	CLA	A	836	1	2/2/16/25	2/11/111/135	-
15	BCR	I	102	-	-	16/29/63/63	0/2/2/2
16	LHG	X	101	-	-	9/26/26/53	-
13	CLA	B	826	-	2/2/20/25	13/37/135/135	-
13	CLA	A	855	-	2/2/16/25	1/11/111/135	-
15	BCR	M	1203	-	-	15/29/63/63	0/2/2/2
13	CLA	M	1202	-	2/2/16/25	1/11/111/135	-
15	BCR	B	845	-	-	10/29/63/63	0/2/2/2
15	BCR	B	844	-	-	6/18/35/63	0/1/1/2
13	CLA	A	841	-	3/3/17/25	3/21/119/135	-
13	CLA	B	810	-	2/2/16/25	1/11/111/135	-
13	CLA	A	809	1	1/1/20/25	9/37/135/135	-
13	CLA	B	815	-	3/3/18/25	7/30/128/135	-
13	CLA	A	826	-	2/2/20/25	9/37/135/135	-
13	CLA	A	817	-	3/3/17/25	3/24/122/135	-
13	CLA	A	830	-	3/3/20/25	9/37/135/135	-
13	CLA	B	804	-	2/2/20/25	7/37/135/135	-
13	CLA	L	1002	10	3/3/20/25	11/37/135/135	-
13	CLA	B	818	-	2/2/16/25	2/16/114/135	-
13	CLA	B	834	-	2/2/16/25	2/11/111/135	-
13	CLA	B	819	-	3/3/16/25	1/11/111/135	-
15	BCR	B	849	-	-	14/29/63/63	0/2/2/2

The worst 5 of 1421 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J	1103	CLA	C3A-C2A	-4.26	1.50	1.54
13	A	824	CLA	C1B-CHB	-3.99	1.29	1.41
13	A	834	CLA	C1B-CHB	-3.95	1.30	1.41
13	B	816	CLA	C1B-CHB	-3.92	1.30	1.41
13	L	1002	CLA	C1B-CHB	-3.91	1.30	1.41

The worst 5 of 1514 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	809	CLA	C4A-NA-C1A	11.51	111.88	106.71
13	A	808	CLA	C4A-NA-C1A	11.40	111.83	106.71
13	A	830	CLA	C4A-NA-C1A	11.31	111.79	106.71
13	M	1202	CLA	C4A-NA-C1A	11.22	111.75	106.71
13	B	827	CLA	C4A-NA-C1A	11.19	111.74	106.71

5 of 229 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	B	832	CLA	NC
13	B	832	CLA	ND
13	B	832	CLA	NA
13	A	806	CLA	ND
13	A	806	CLA	NA

5 of 930 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	850	BCR	C36-C18-C19-C20
15	A	850	BCR	C37-C22-C23-C24
15	A	850	BCR	C23-C24-C25-C26
15	A	850	BCR	C23-C24-C25-C30
15	A	847	BCR	C7-C8-C9-C34

There are no ring outliers.

123 monomers are involved in 1092 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	832	CLA	12	0
13	A	806	CLA	9	0
13	B	837	CLA	8	0
13	B	825	CLA	18	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	850	BCR	4	0
15	A	847	BCR	5	0
13	M	1201	CLA	17	0
13	A	822	CLA	7	0
13	A	805	CLA	13	0
13	A	845	CLA	11	0
13	B	817	CLA	12	0
13	B	812	CLA	15	0
13	B	831	CLA	12	0
13	A	828	CLA	16	0
13	A	802	CLA	12	0
13	A	815	CLA	7	0
13	A	810	CLA	8	0
13	B	814	CLA	10	0
15	J	1104	BCR	4	0
13	A	801	CLA	8	0
15	A	851	BCR	3	0
15	B	841	BCR	5	0
13	B	816	CLA	16	0
15	B	846	BCR	7	0
13	B	835	CLA	16	0
13	B	813	CLA	10	0
13	B	808	CLA	14	0
13	B	811	CLA	18	0
13	B	827	CLA	14	0
15	F	1302	BCR	13	0
13	J	1102	CLA	4	0
13	A	811	CLA	14	0
13	A	834	CLA	18	0
15	B	842	BCR	4	0
13	A	818	CLA	11	0
13	A	820	CLA	10	0
13	B	803	CLA	16	0
13	A	842	CLA	22	0
15	B	850	BCR	6	0
13	B	821	CLA	13	0
13	A	813	CLA	19	0
13	J	1101	CLA	13	0
13	A	823	CLA	13	0
13	B	823	CLA	8	0
13	L	1003	CLA	16	0
16	A	854	LHG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	838	CLA	14	0
13	A	808	CLA	17	0
13	B	824	CLA	20	0
13	A	807	CLA	13	0
18	B	848	LMG	18	0
13	A	840	CLA	16	0
13	A	824	CLA	8	0
14	A	846	PQN	7	0
15	L	1006	BCR	4	0
15	B	843	BCR	18	0
13	A	827	CLA	15	0
13	A	843	CLA	10	0
13	I	101	CLA	15	0
15	J	1105	BCR	7	0
15	A	849	BCR	4	0
13	A	814	CLA	8	0
13	X	102	CLA	5	0
13	B	839	CLA	7	0
13	L	1004	CLA	7	0
13	B	829	CLA	7	0
13	B	801	CLA	13	0
15	A	852	BCR	19	0
13	B	833	CLA	3	0
13	A	829	CLA	10	0
13	B	838	CLA	18	0
13	A	803	CLA	27	0
13	B	807	CLA	12	0
13	B	820	CLA	12	0
13	B	805	CLA	9	0
15	L	1005	BCR	12	0
13	B	809	CLA	8	0
13	A	839	CLA	17	0
13	A	833	CLA	19	0
13	B	802	CLA	18	0
13	A	821	CLA	12	0
13	A	831	CLA	11	0
14	B	840	PQN	7	0
13	A	837	CLA	14	0
13	A	819	CLA	16	0
13	A	816	CLA	3	0
13	B	822	CLA	21	0
16	A	853	LHG	10	0

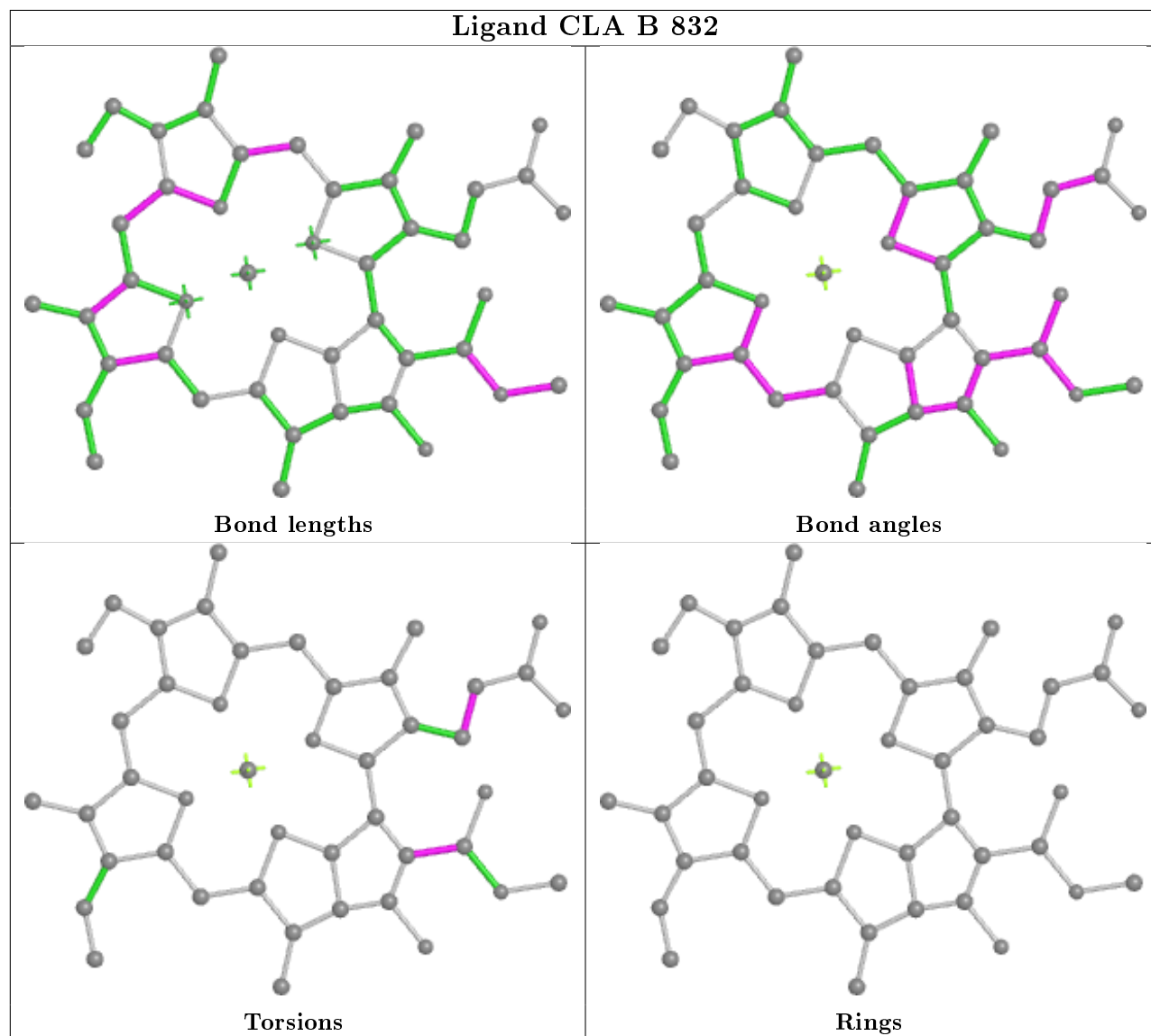
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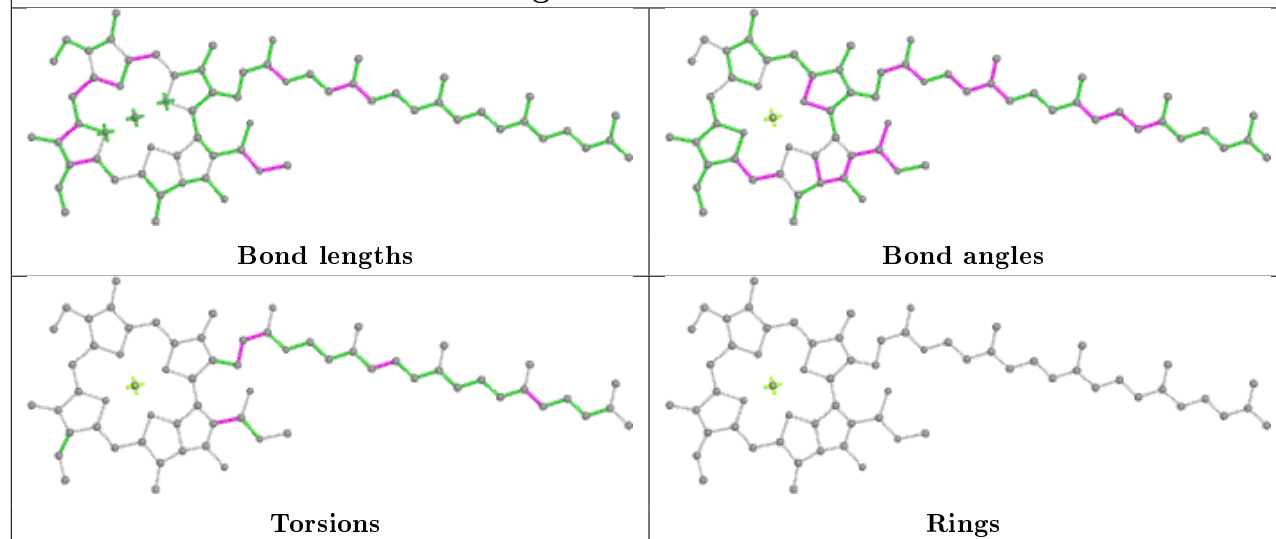
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	848	BCR	5	0
13	B	830	CLA	24	0
13	B	828	CLA	6	0
13	A	844	CLA	3	0
13	A	835	CLA	8	0
13	F	1301	CLA	5	0
13	B	836	CLA	10	0
15	B	847	BCR	12	0
13	A	825	CLA	22	0
13	B	806	CLA	15	0
13	A	832	CLA	21	0
13	A	812	CLA	7	0
13	A	804	CLA	10	0
13	A	836	CLA	11	0
15	I	102	BCR	11	0
16	X	101	LHG	1	0
13	B	826	CLA	19	0
13	A	855	CLA	2	0
15	M	1203	BCR	13	0
13	M	1202	CLA	1	0
15	B	845	BCR	9	0
15	B	844	BCR	6	0
13	A	841	CLA	6	0
13	B	810	CLA	5	0
13	A	809	CLA	16	0
13	B	815	CLA	15	0
13	A	826	CLA	17	0
13	A	817	CLA	9	0
13	A	830	CLA	14	0
13	B	804	CLA	17	0
13	L	1002	CLA	5	0
13	B	818	CLA	4	0
13	B	834	CLA	7	0
13	B	819	CLA	1	0
15	B	849	BCR	16	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

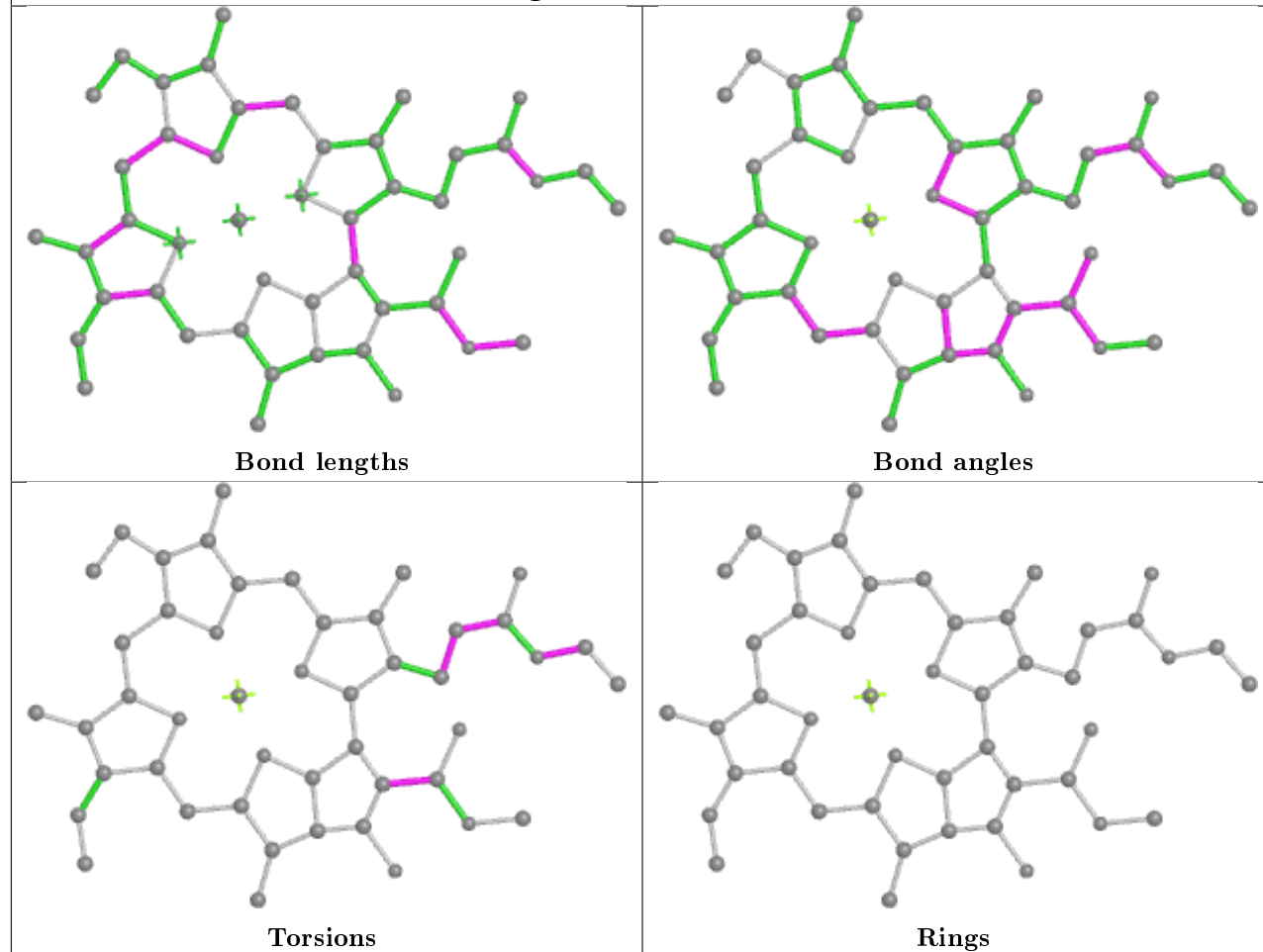
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

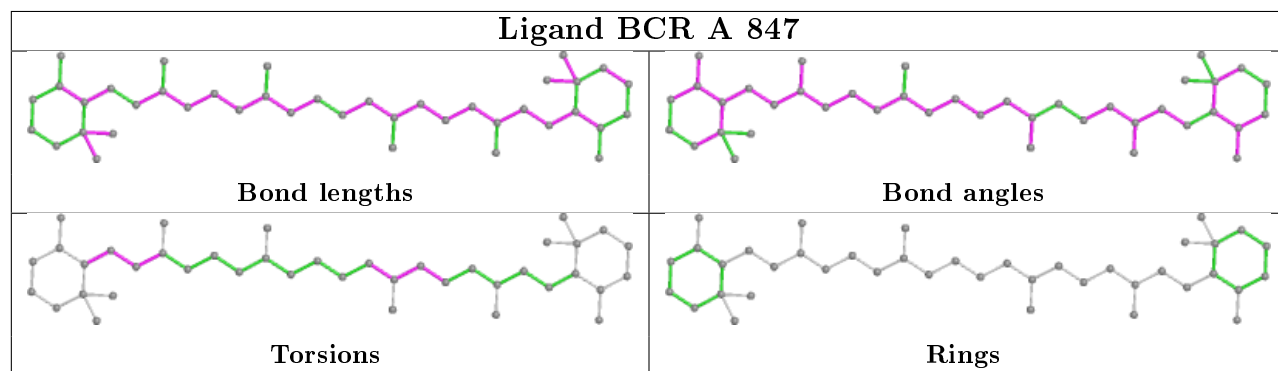
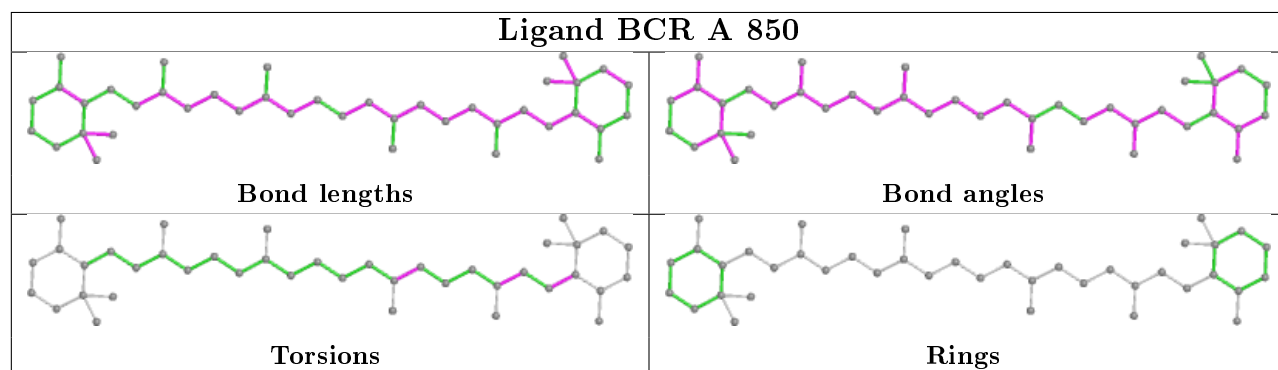
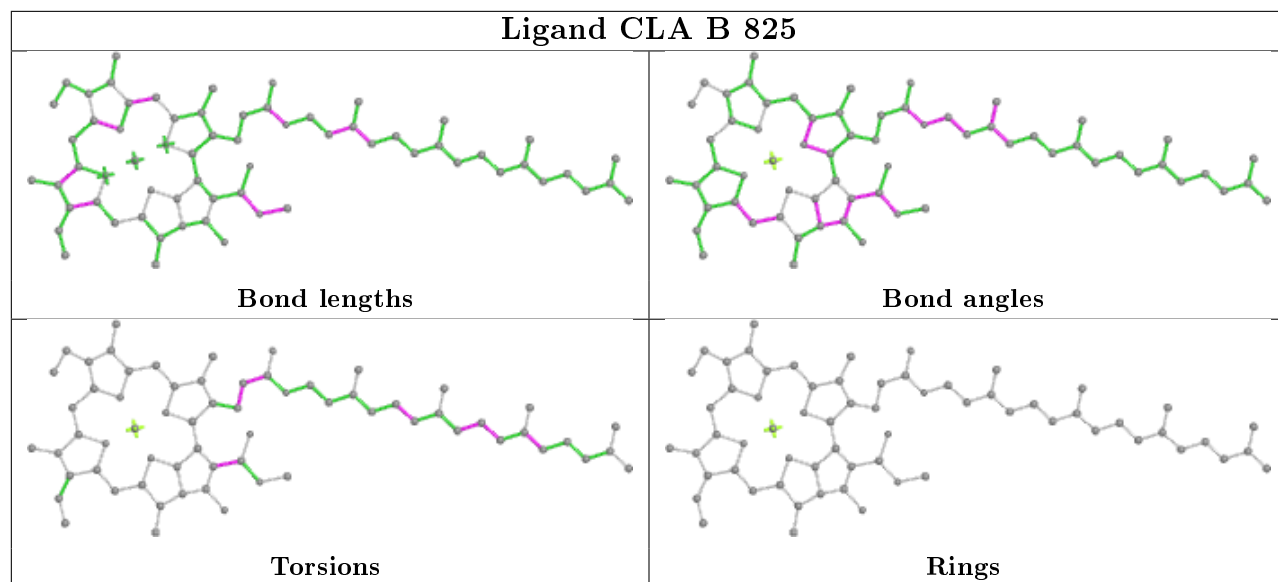


Ligand CLA A 806

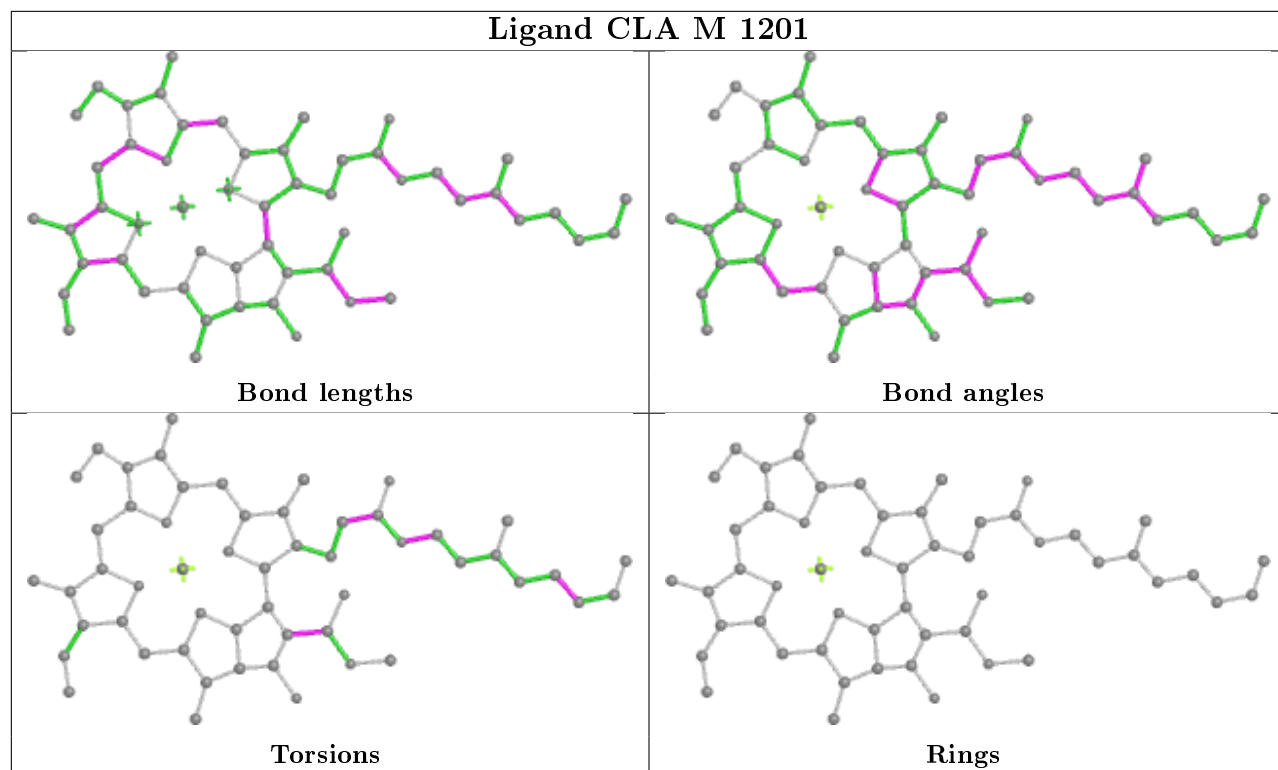


Ligand CLA B 837

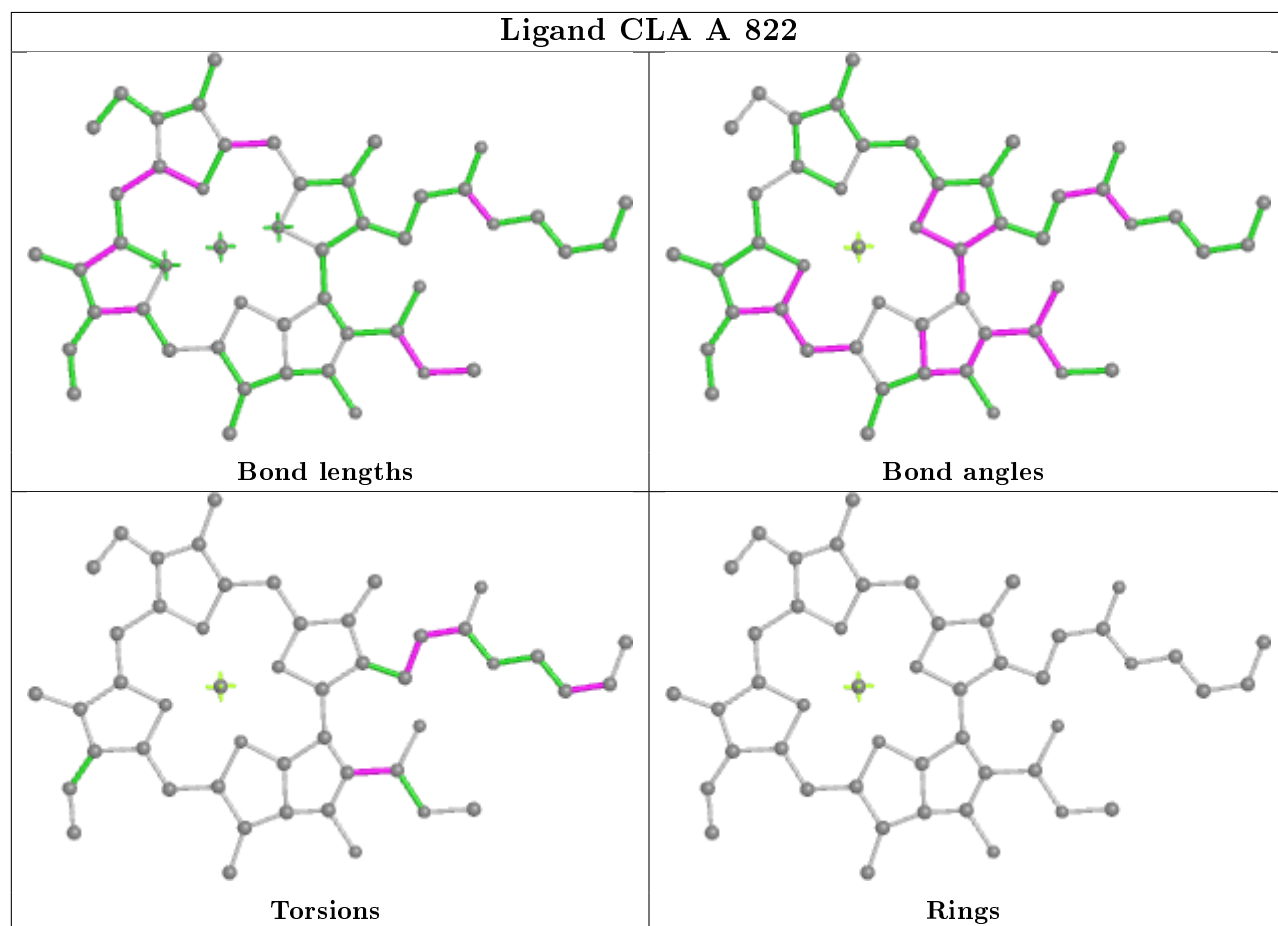




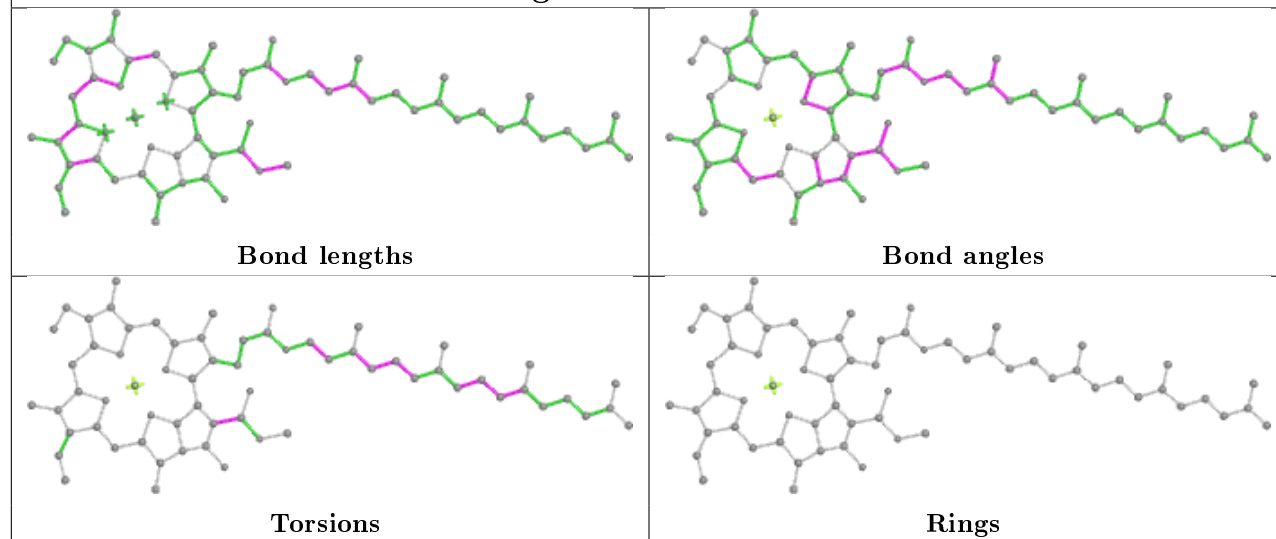
Ligand CLA M 1201



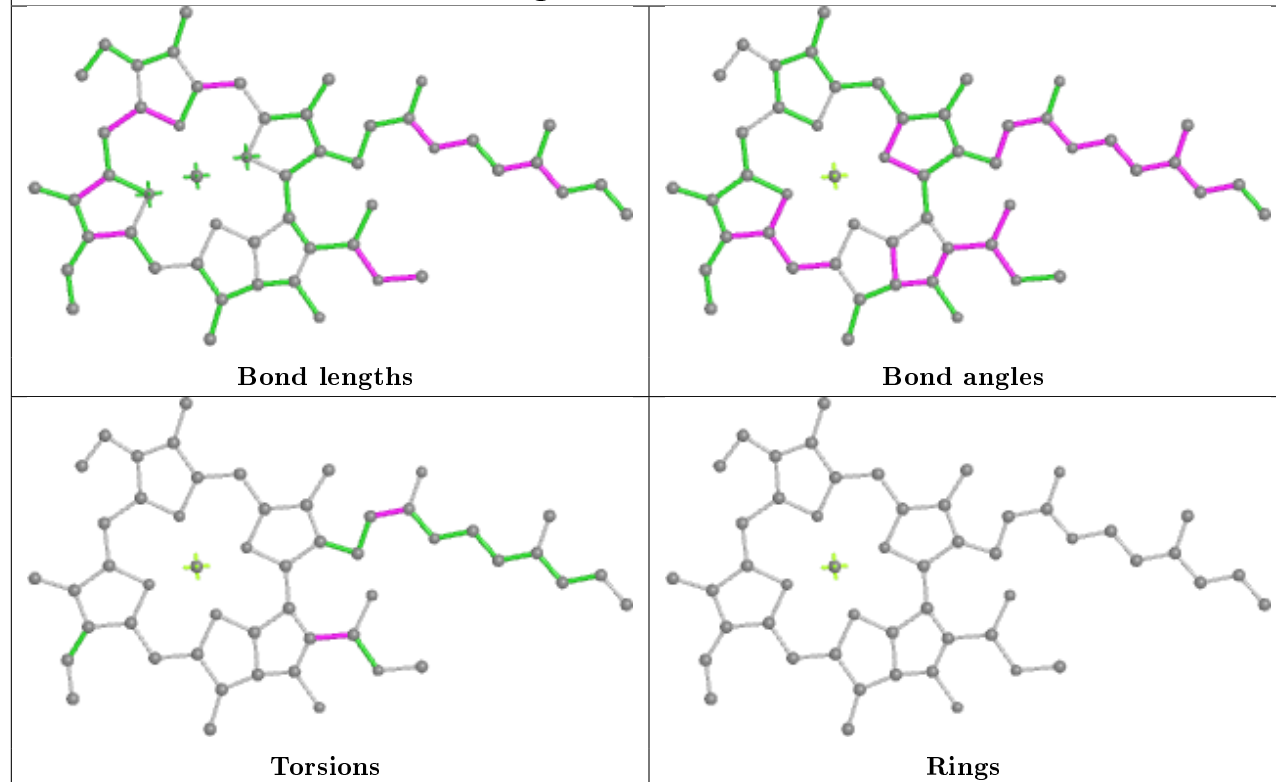
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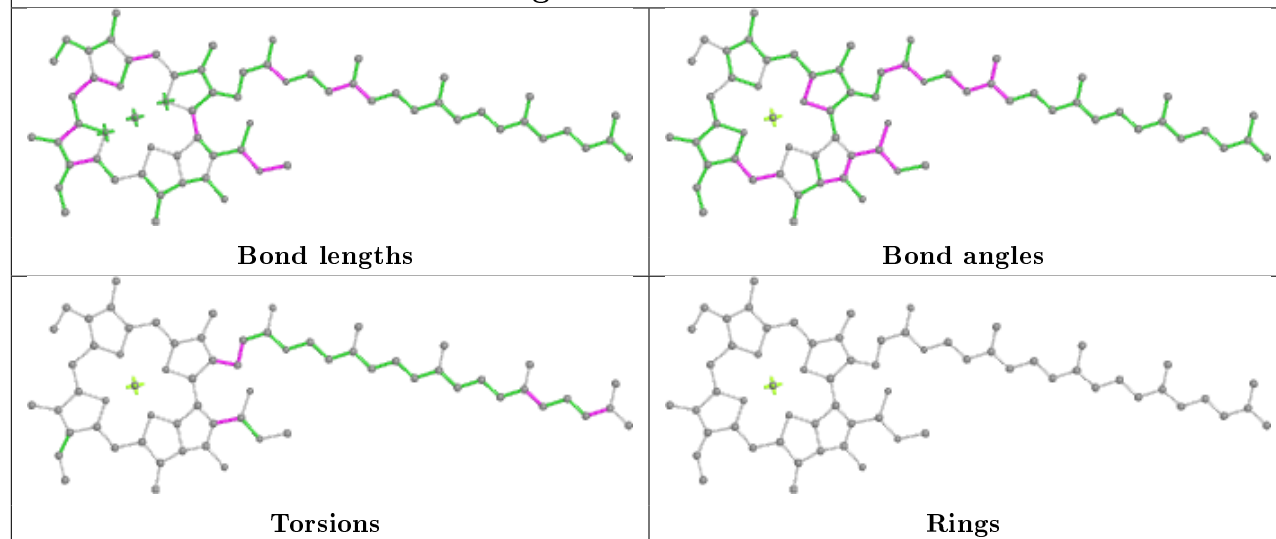
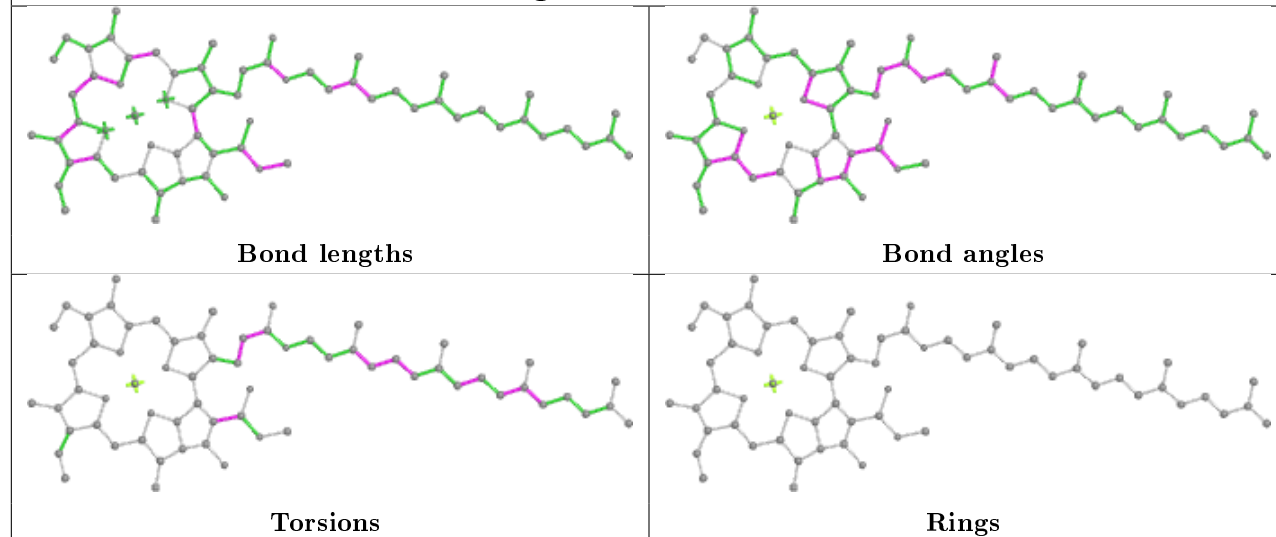


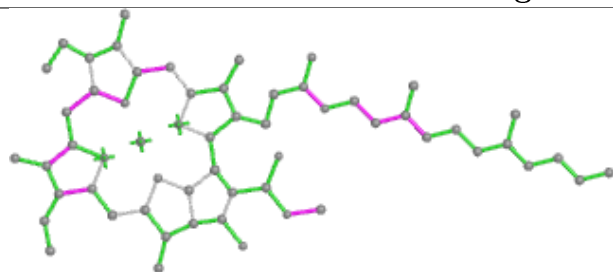
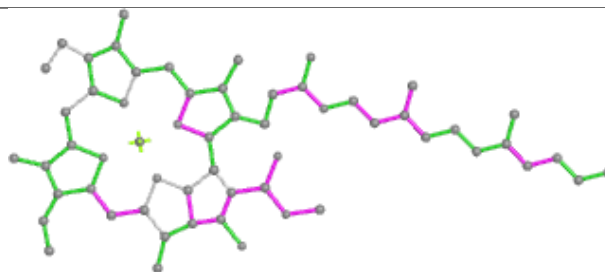
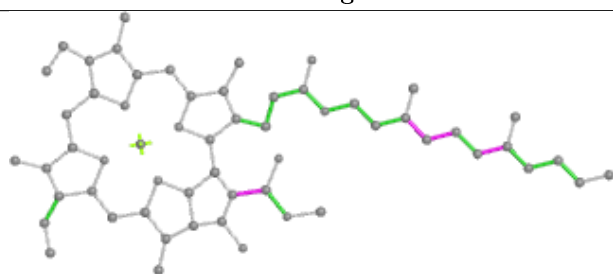
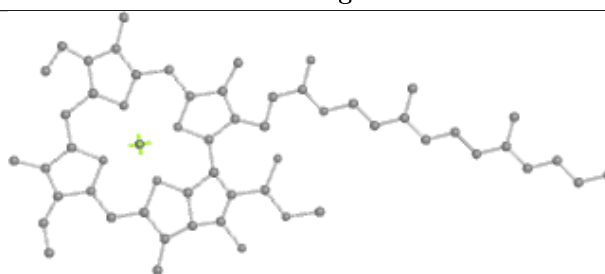
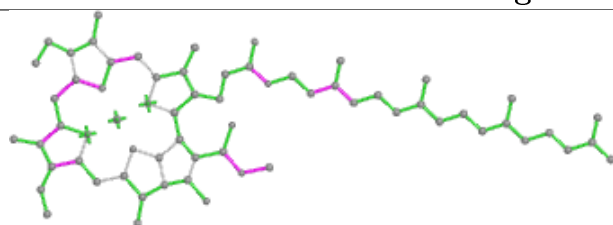
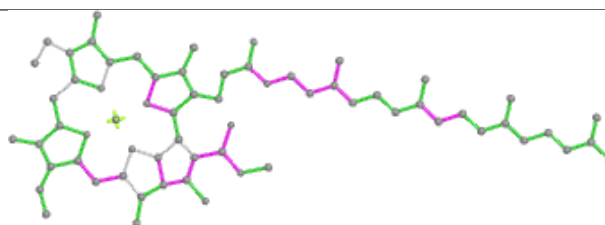
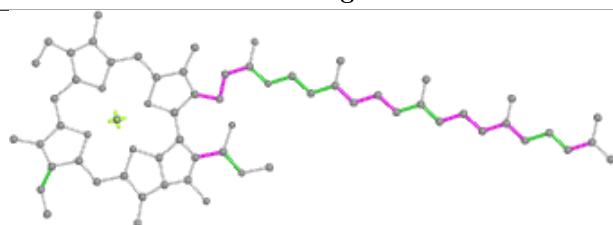
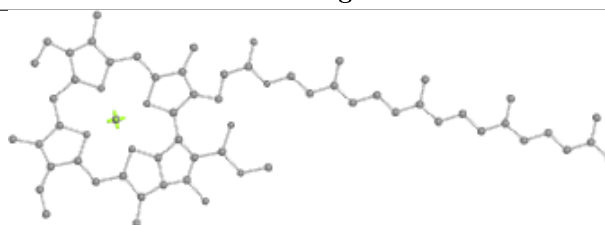
Ligand CLA A 805



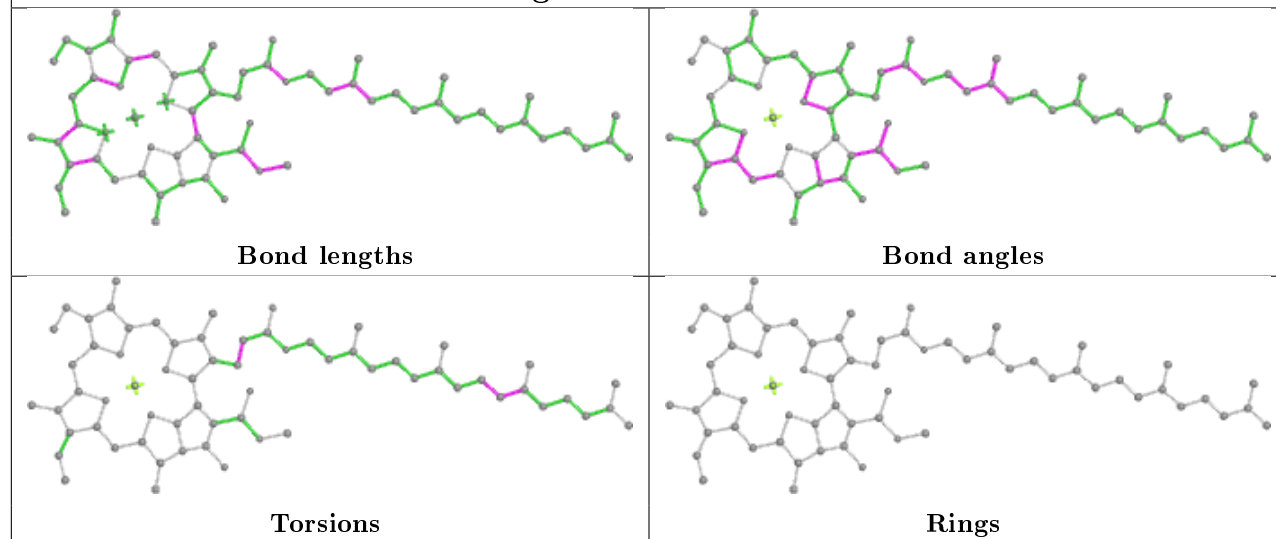
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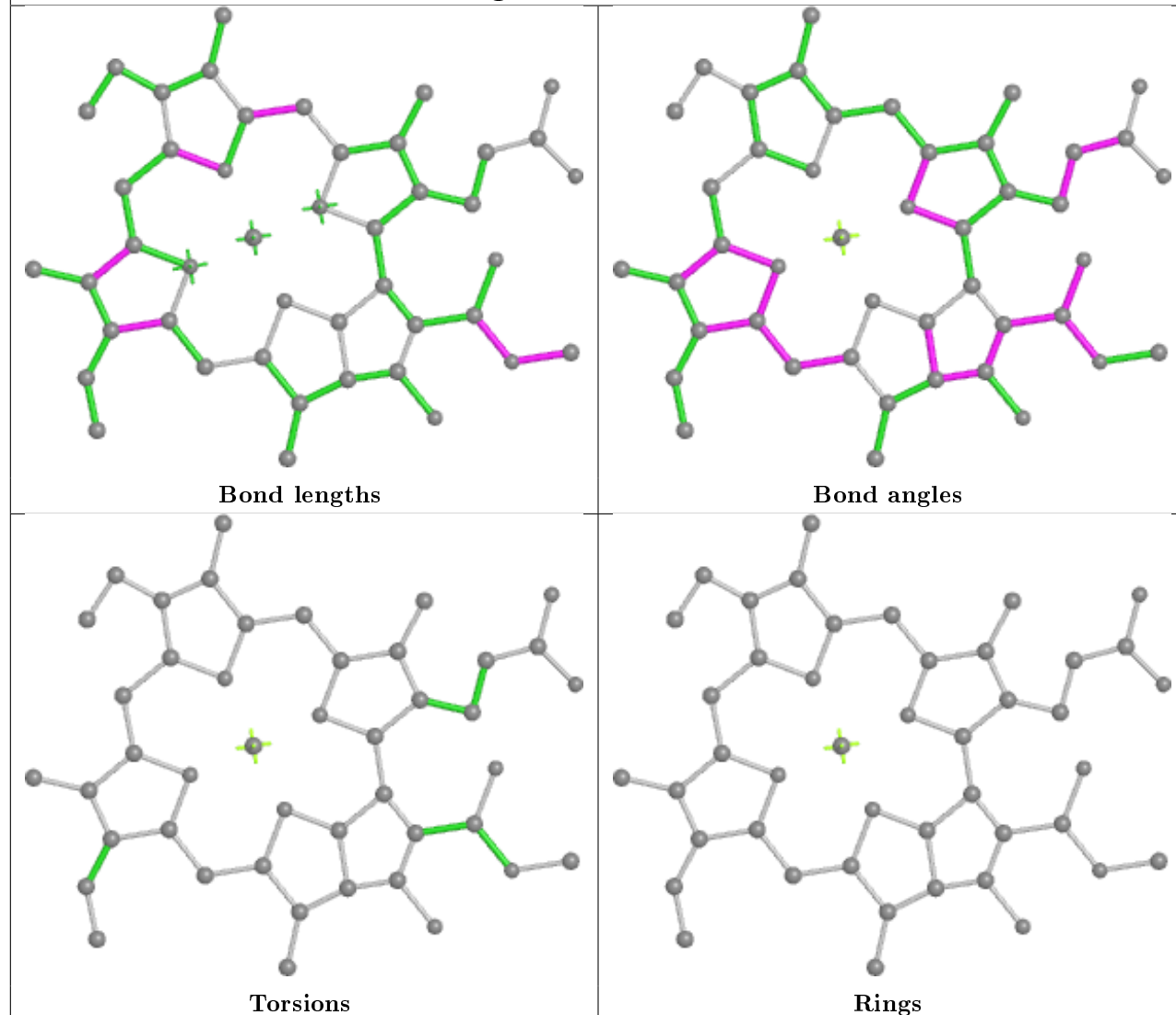
Ligand CLA B 817**Ligand CLA B 812**

Ligand CLA B 831**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 828****Bond lengths****Bond angles****Torsions****Rings**

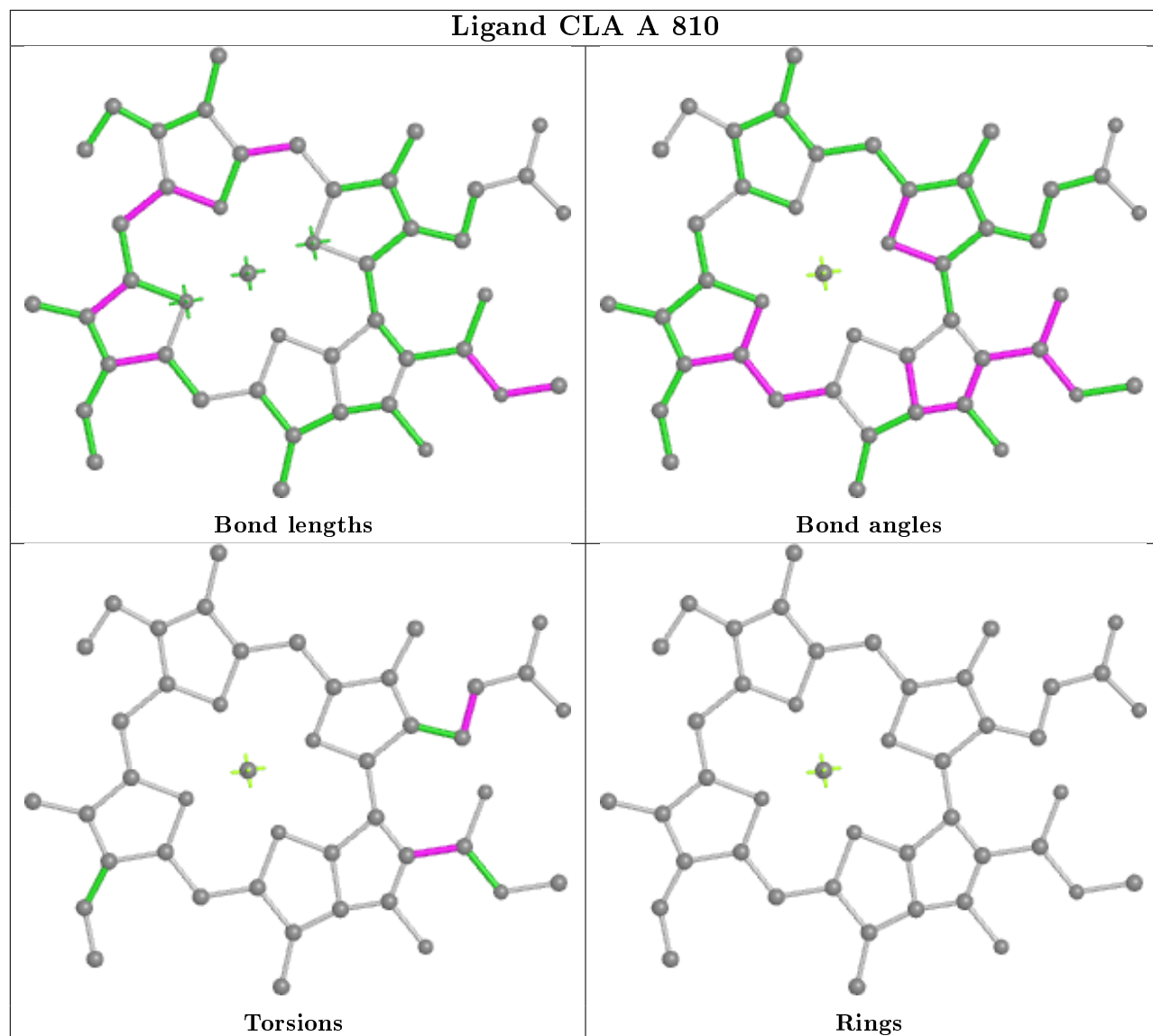
Ligand CLA A 802



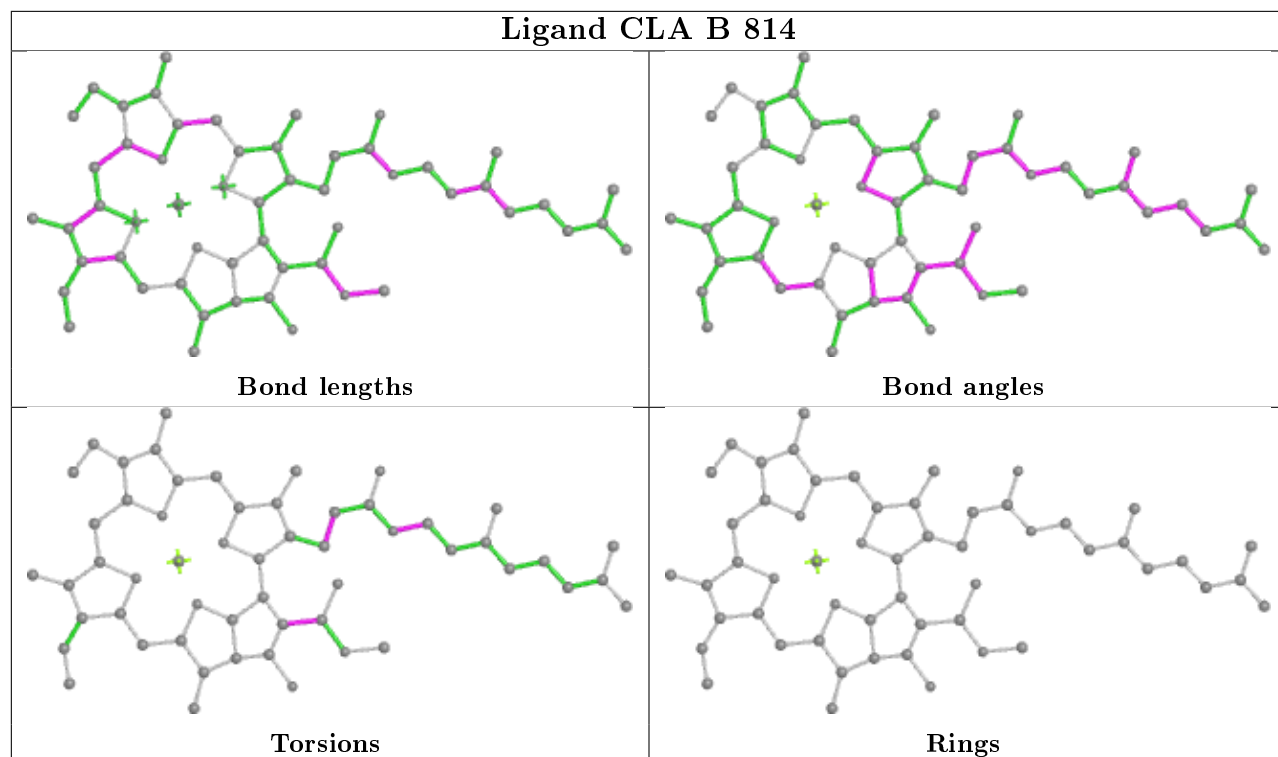
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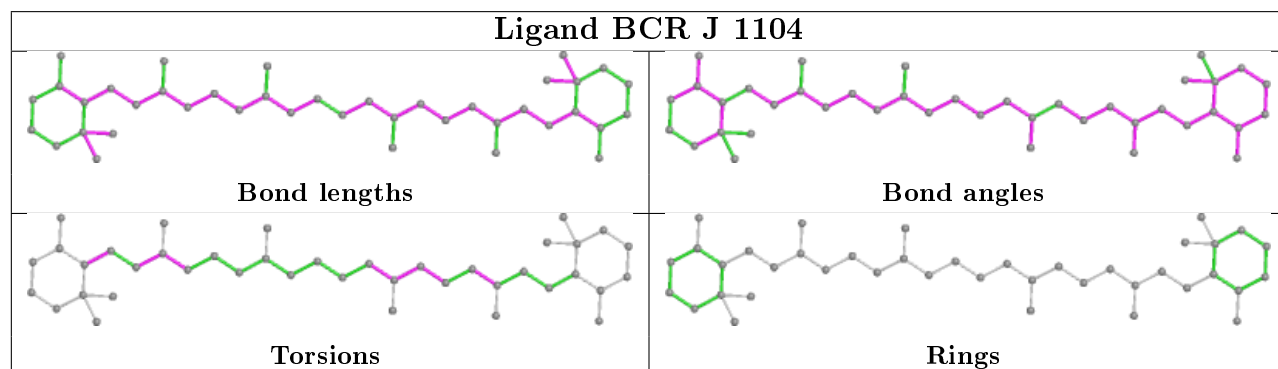
Ligand CLA A 810



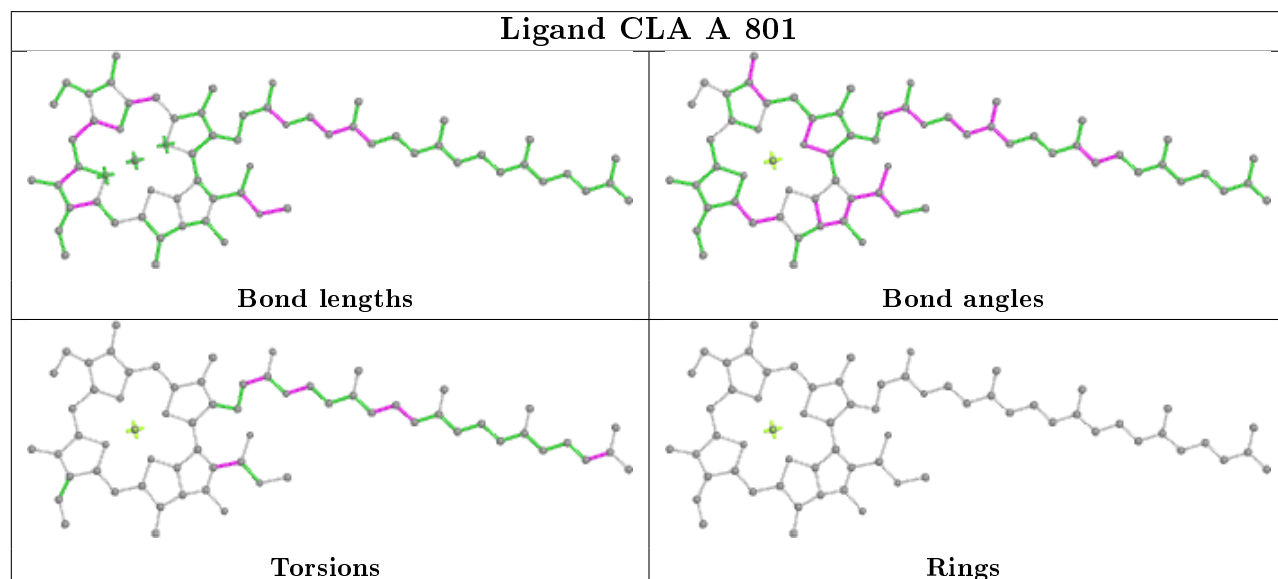
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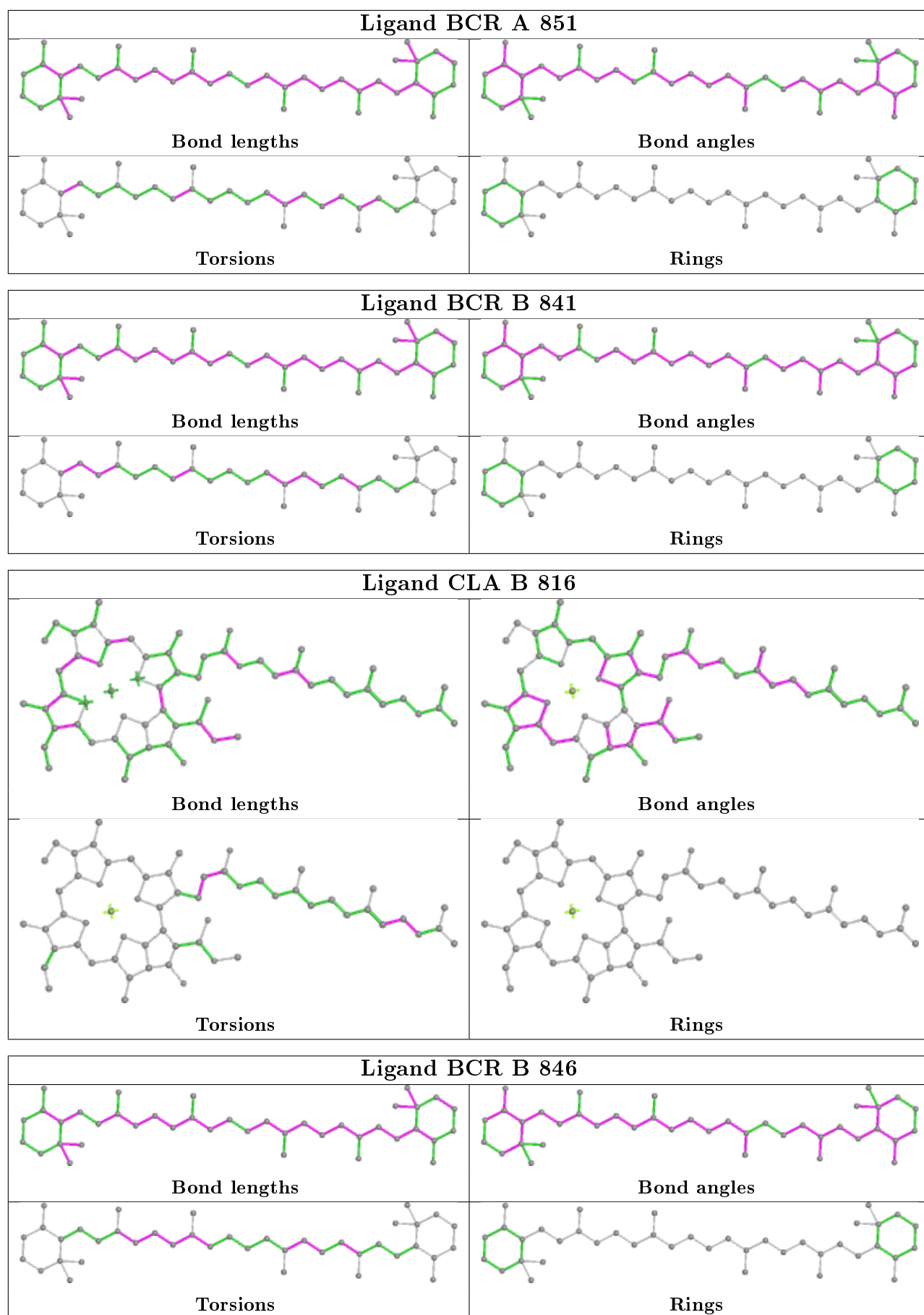


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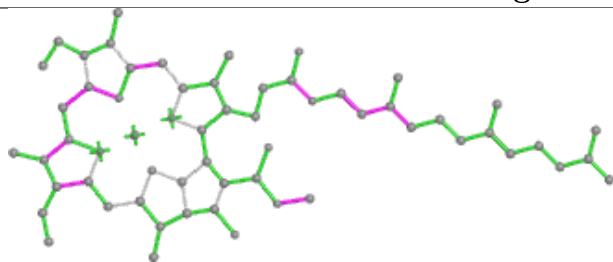


Ligand CLA A 801

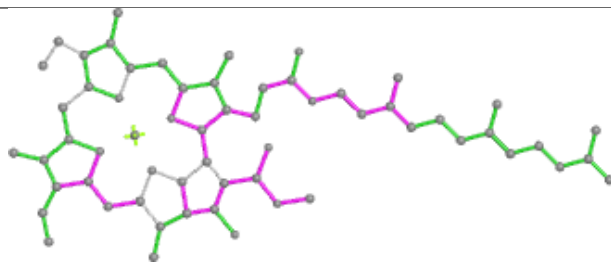




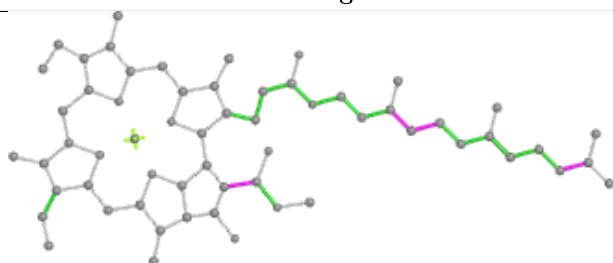
Ligand CLA B 835



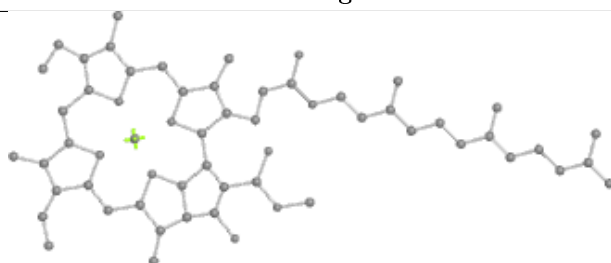
Bond lengths



Bond angles

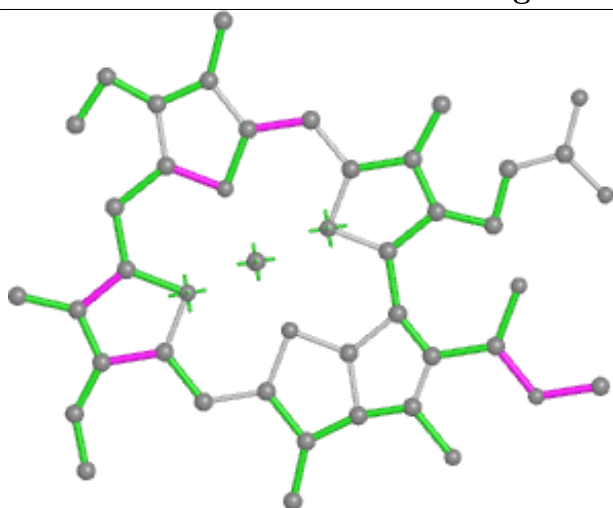


Torsions

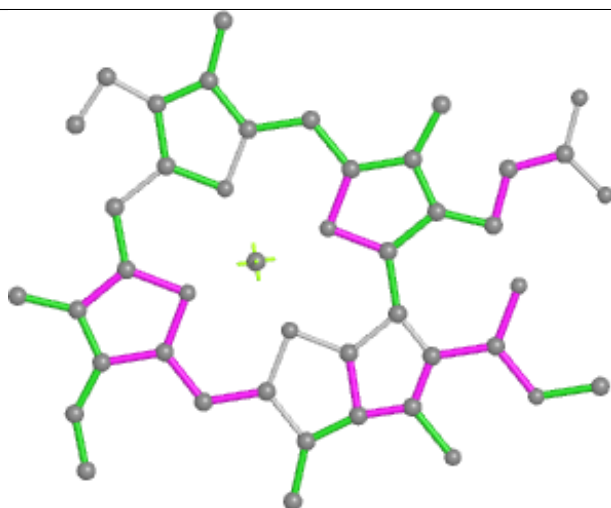


Rings

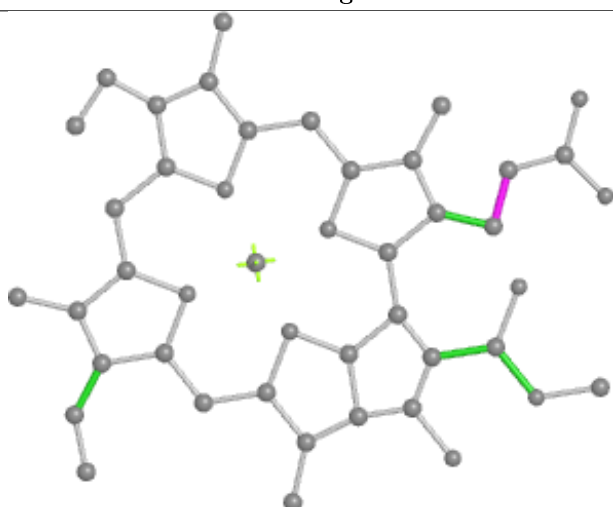
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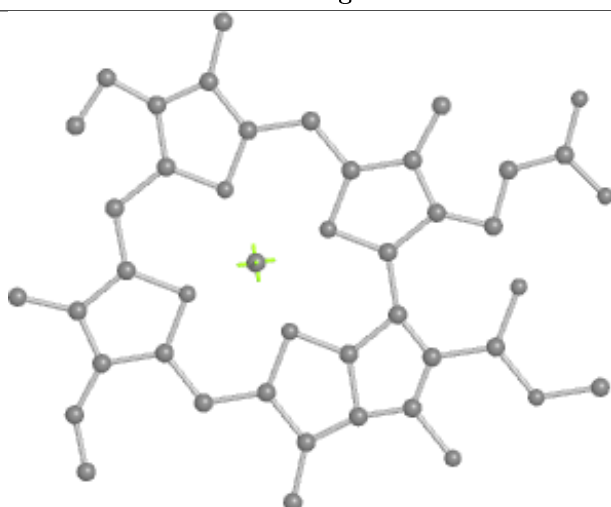
Bond lengths



Bond angles

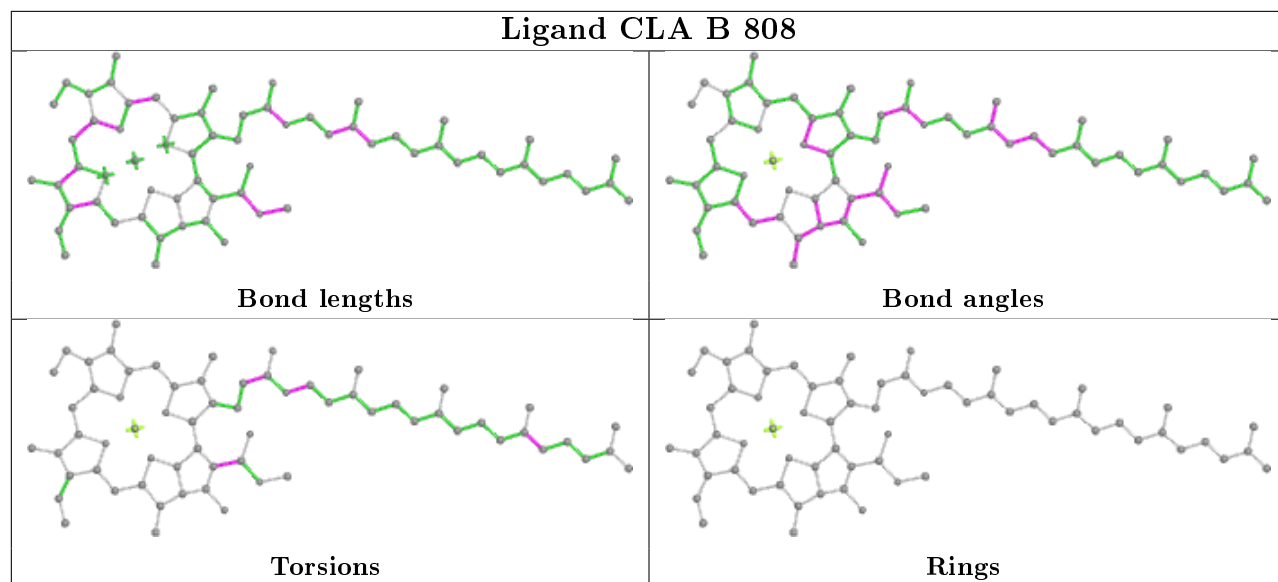


Torsions

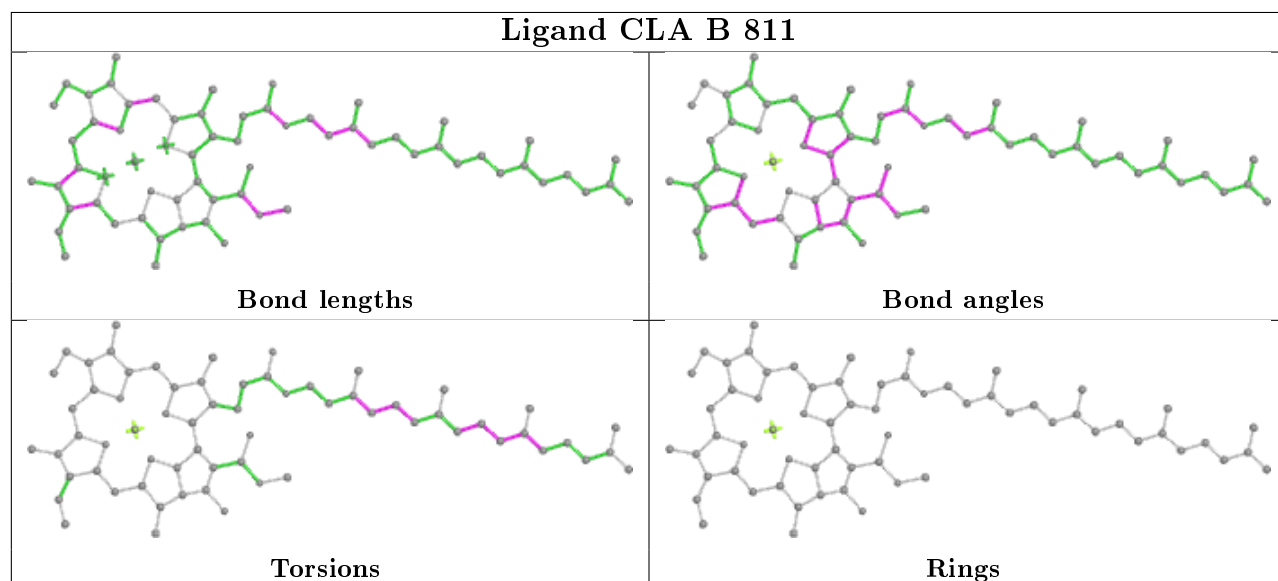


Rings

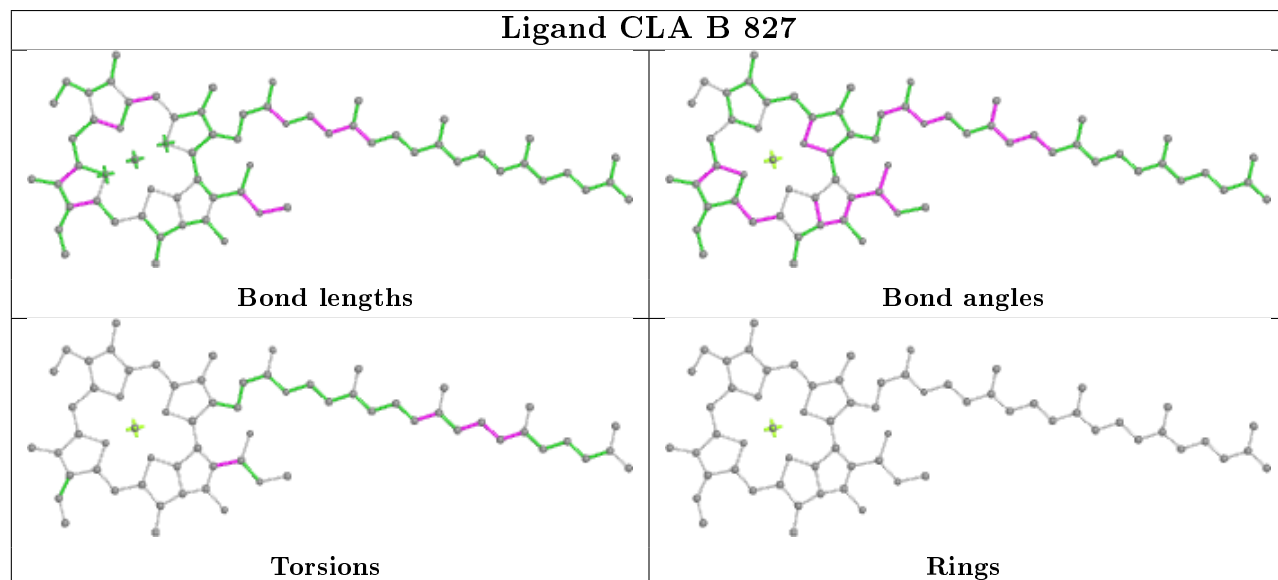
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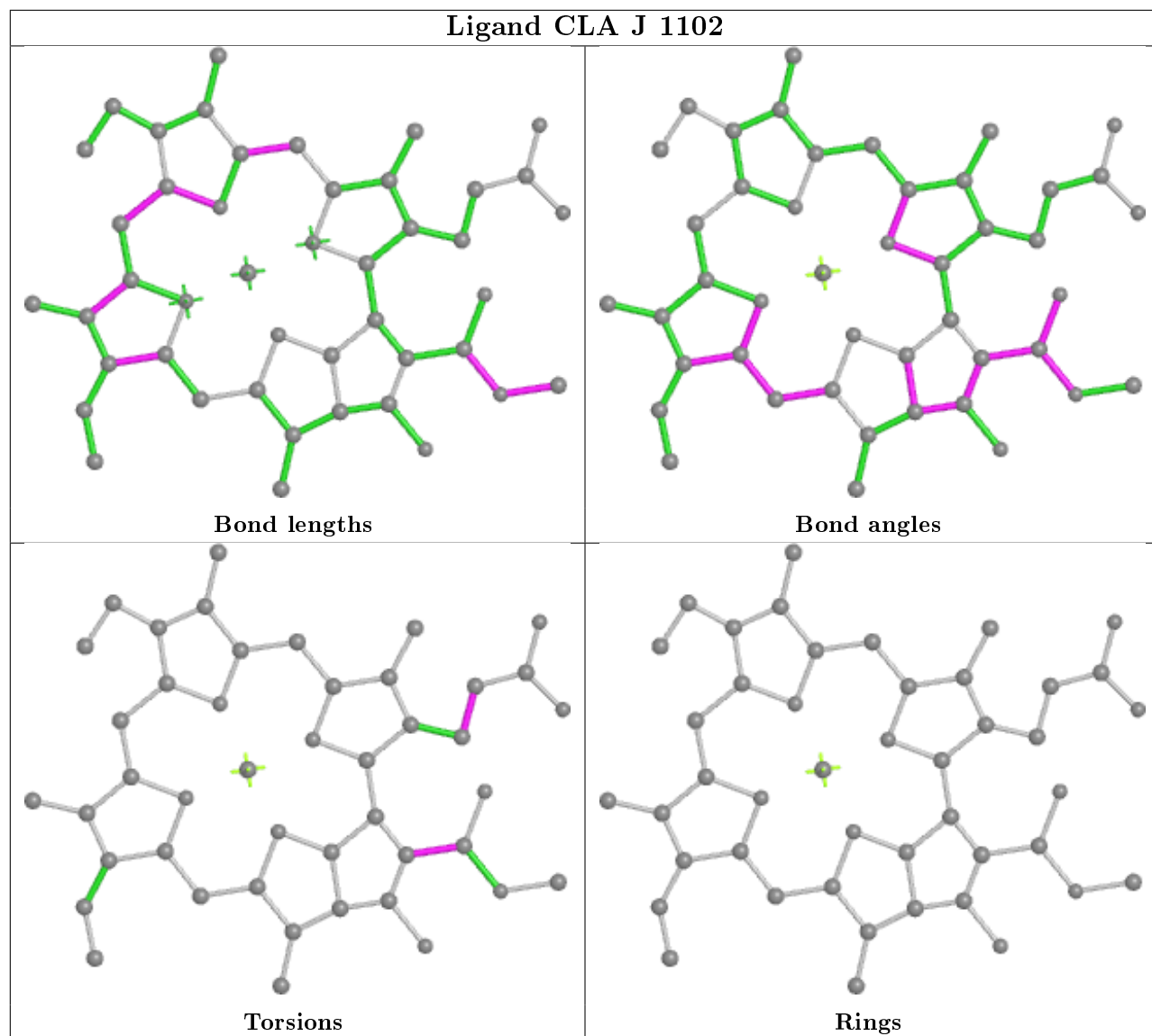
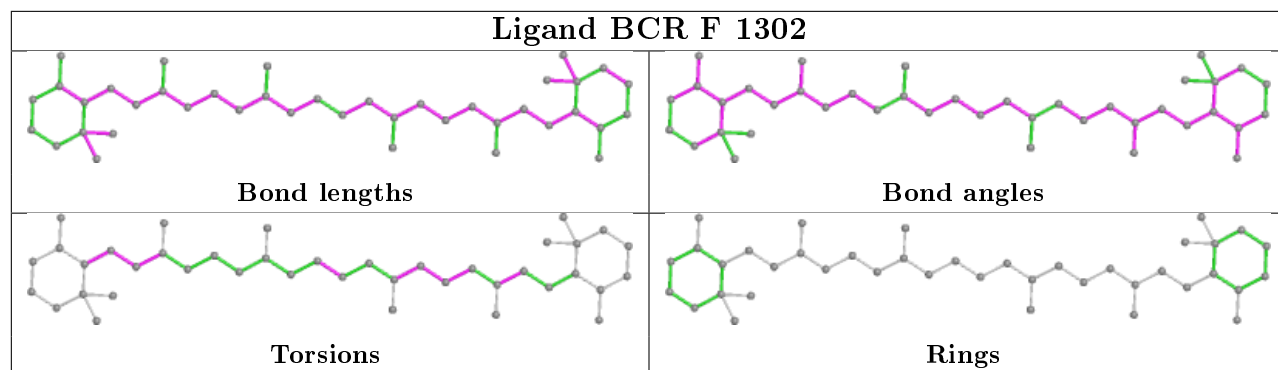


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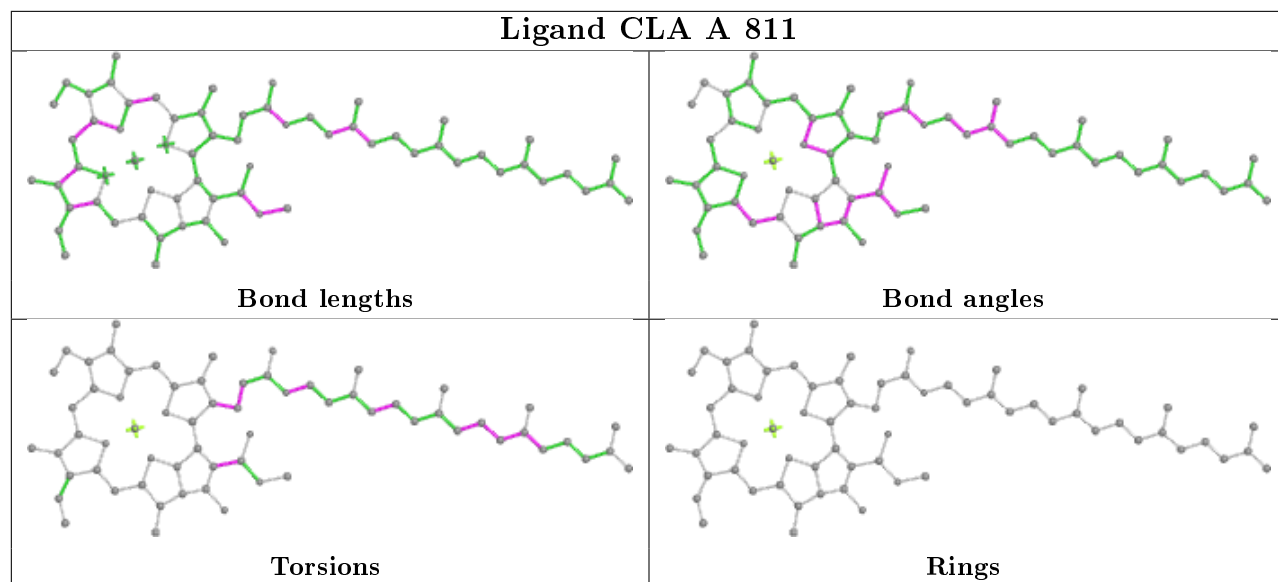


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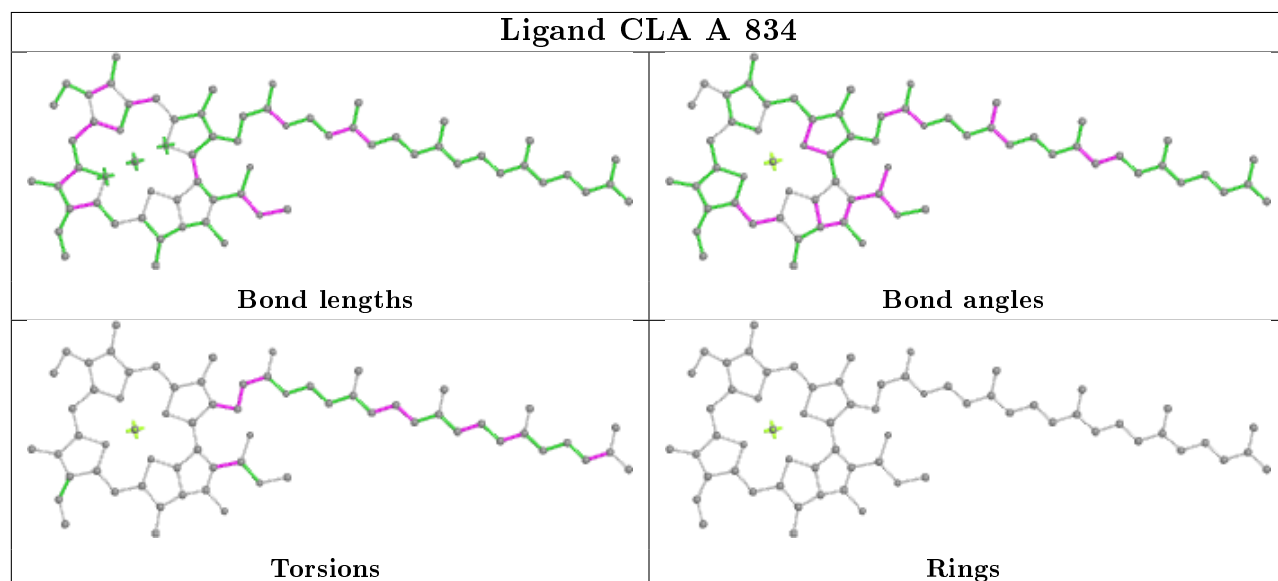




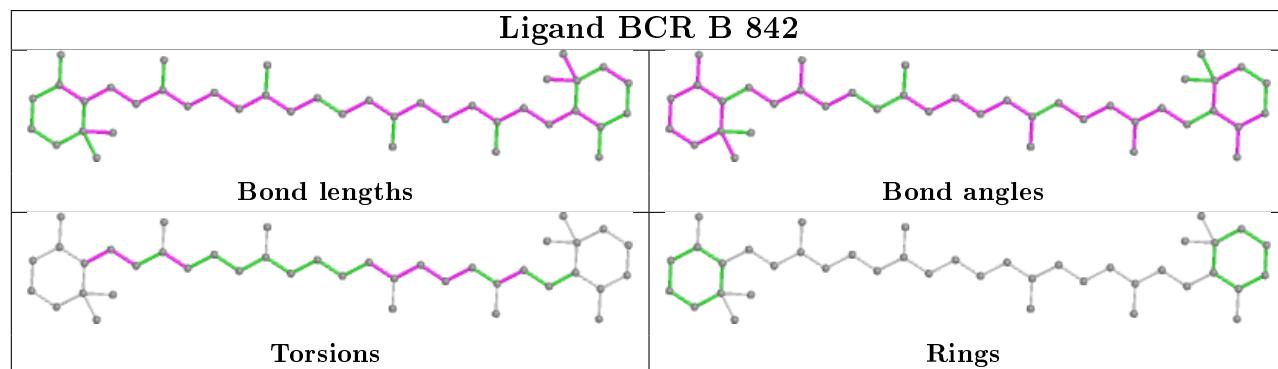
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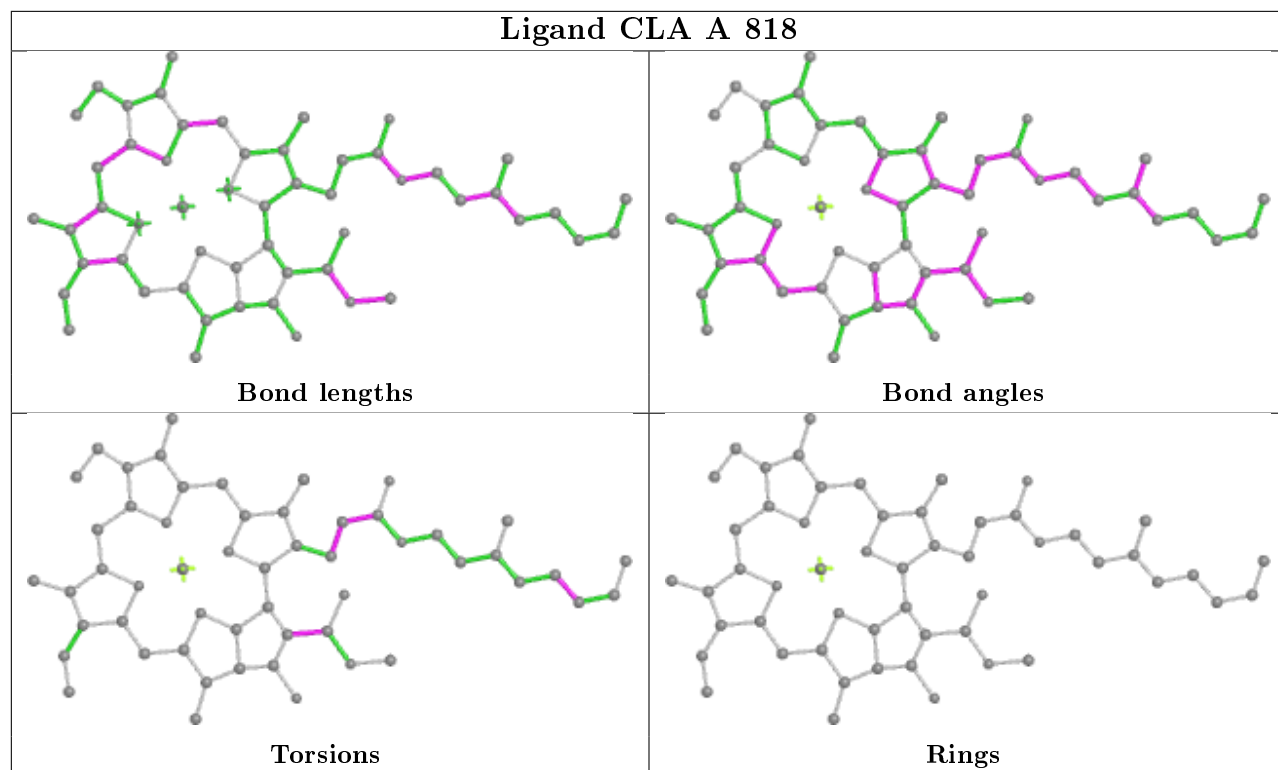
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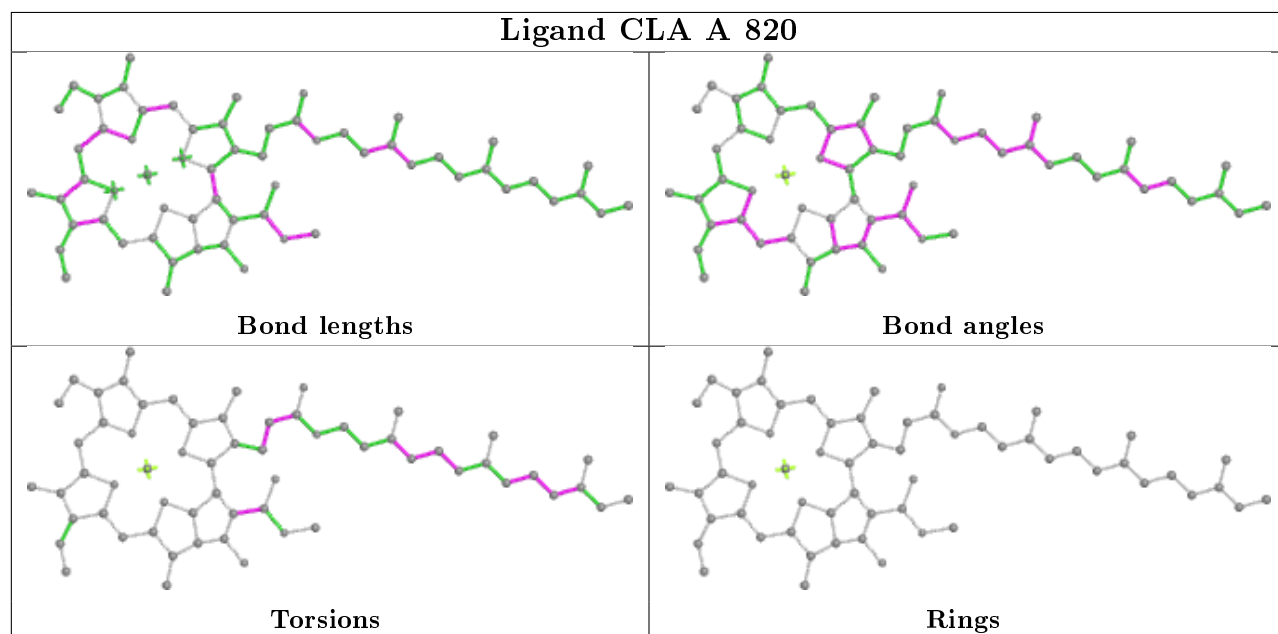
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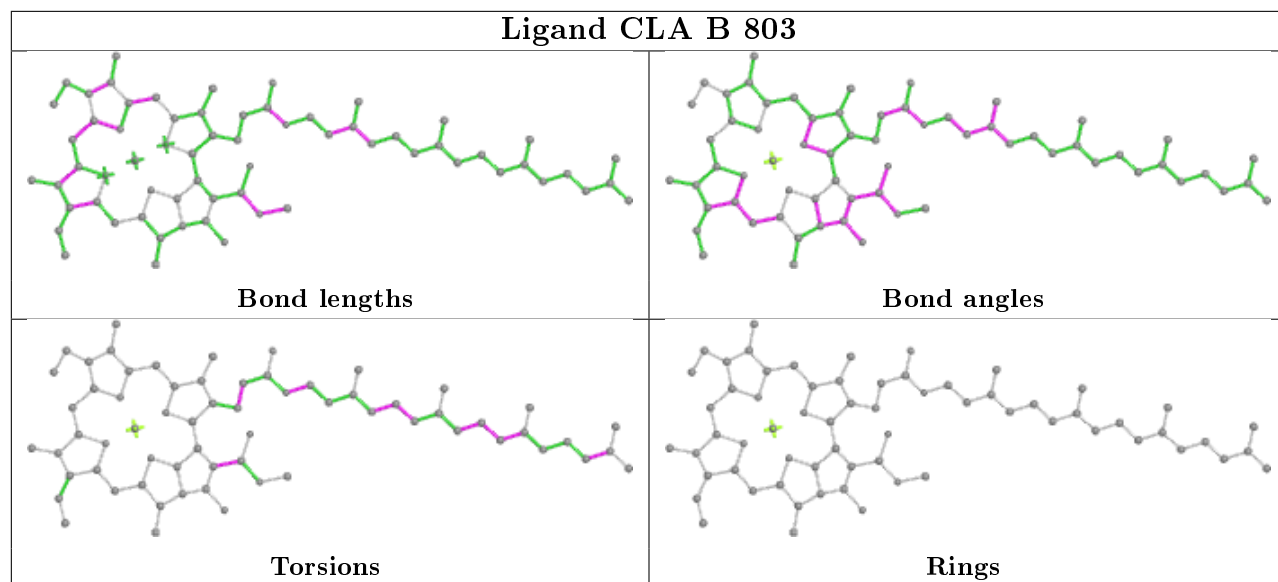
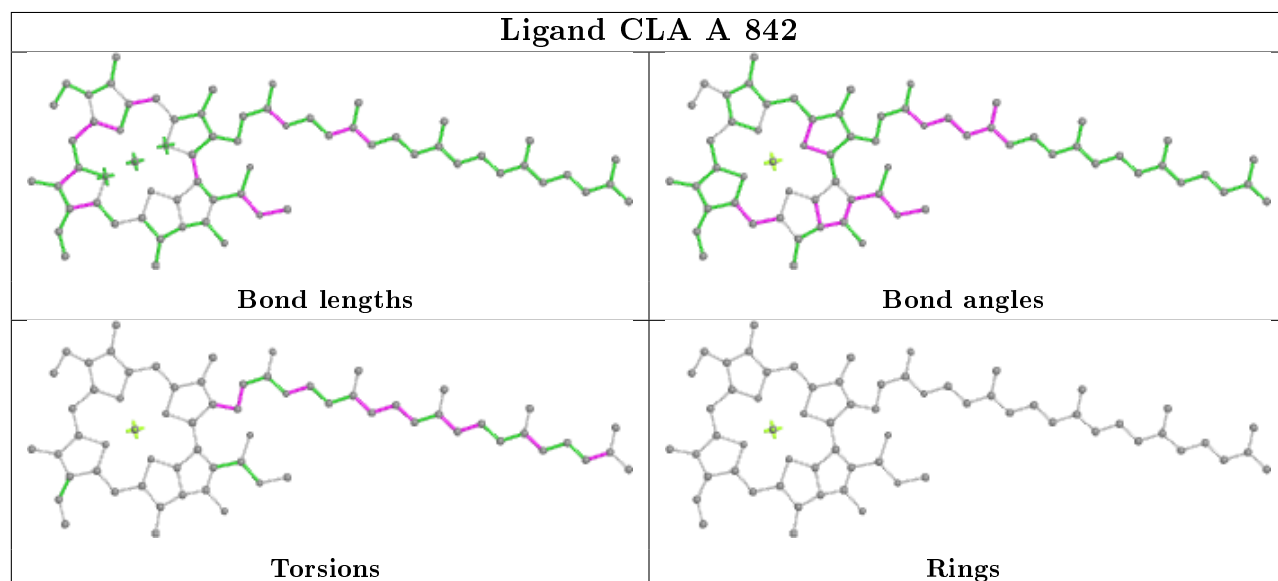
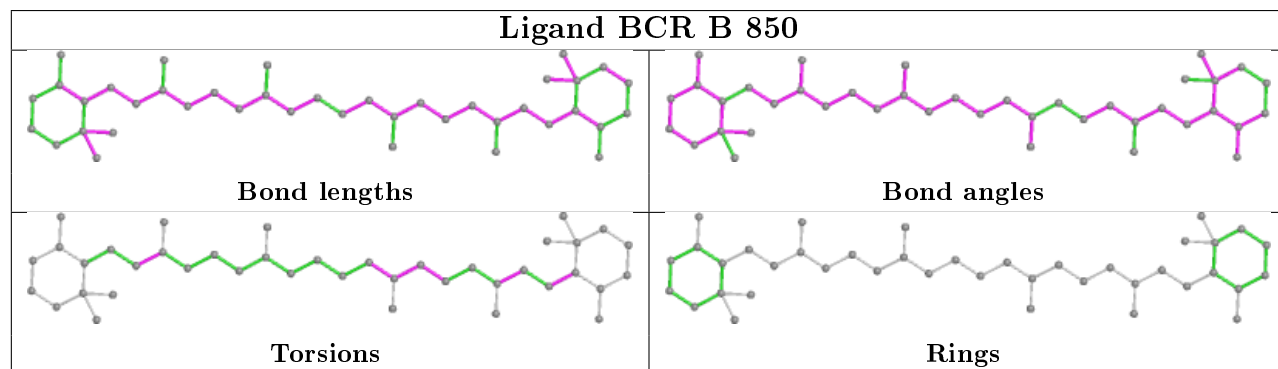


Ligand CLA A 818

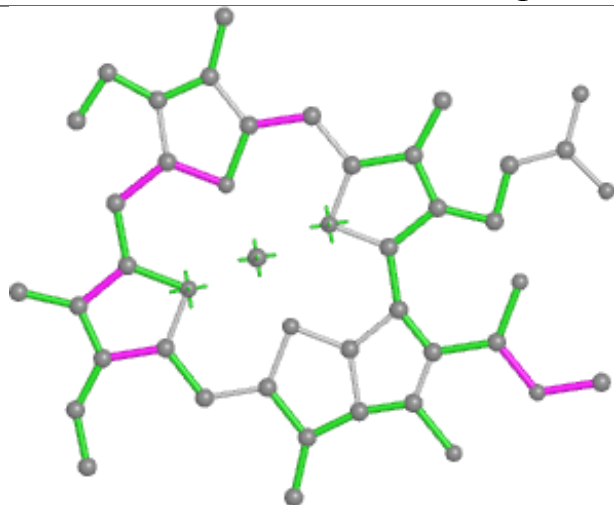


Ligand CLA A 820

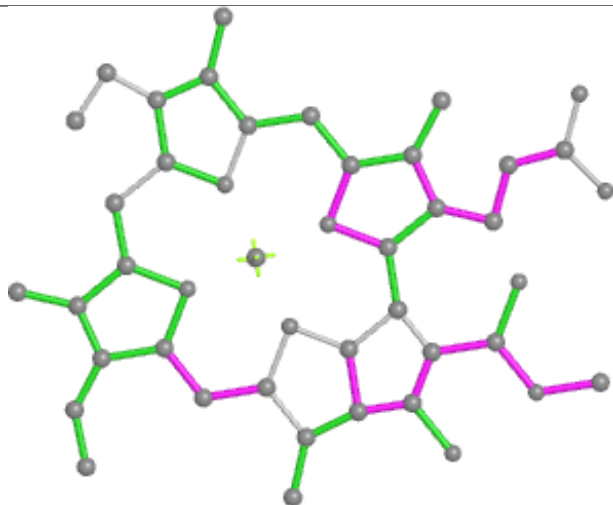


Ligand CLA B 803**Ligand CLA A 842****Ligand BCR B 850**

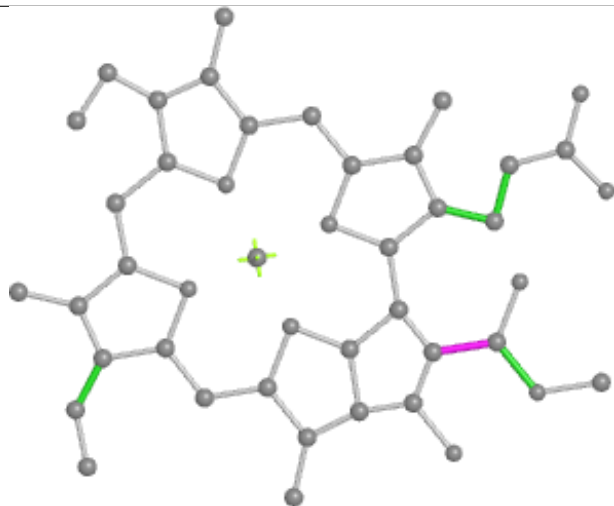
Ligand CLA B 821



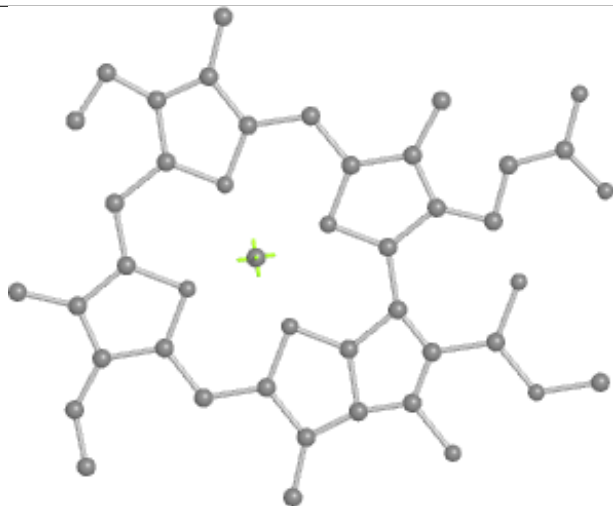
Bond lengths



Bond angles

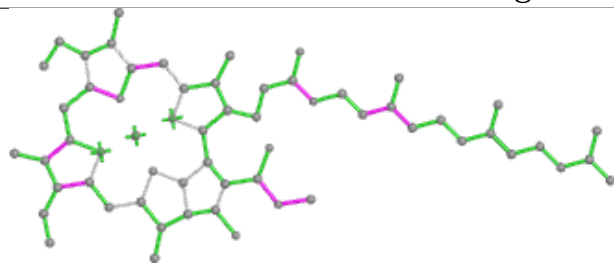


Torsions

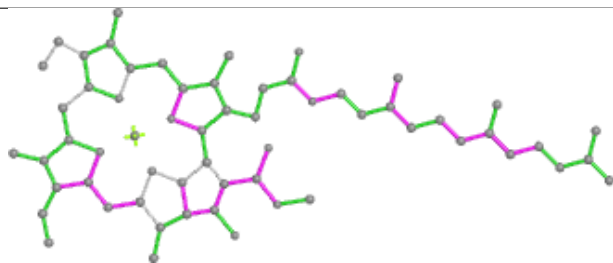


Rings

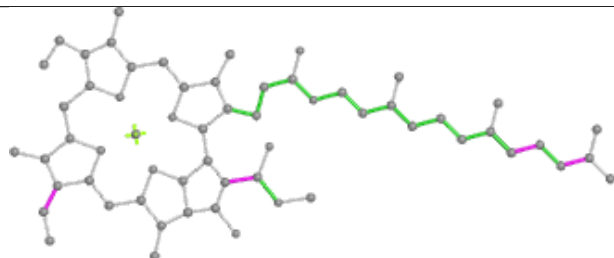
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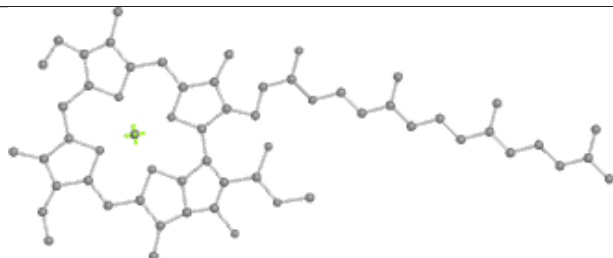
Bond lengths



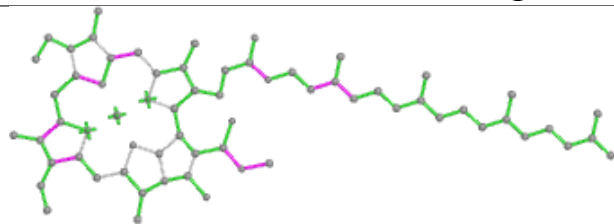
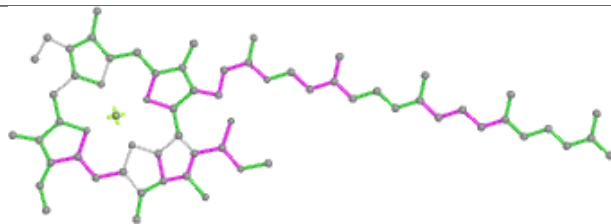
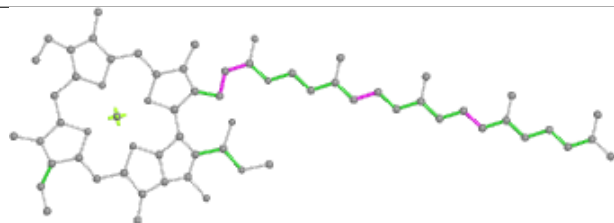
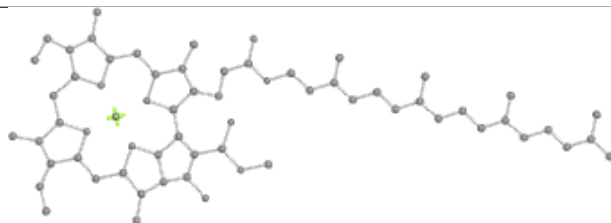
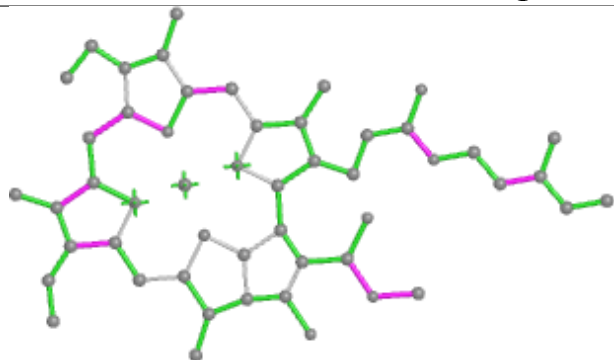
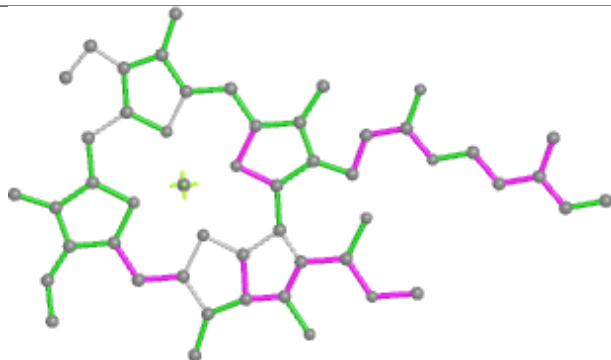
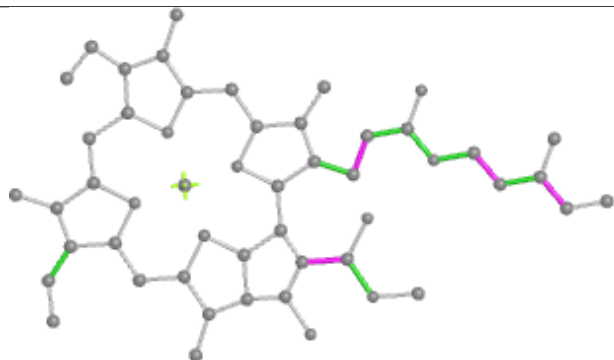
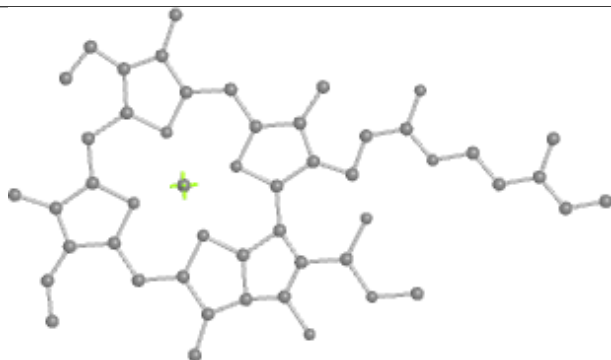
Bond angles



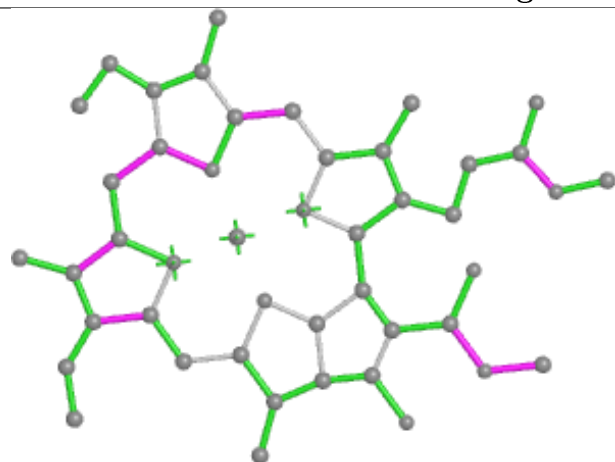
Torsions



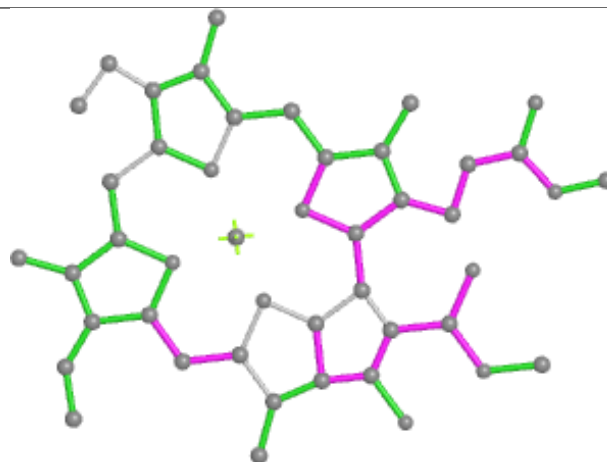
Rings

Ligand CLA J 1101**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 823****Bond lengths****Bond angles****Torsions****Rings**

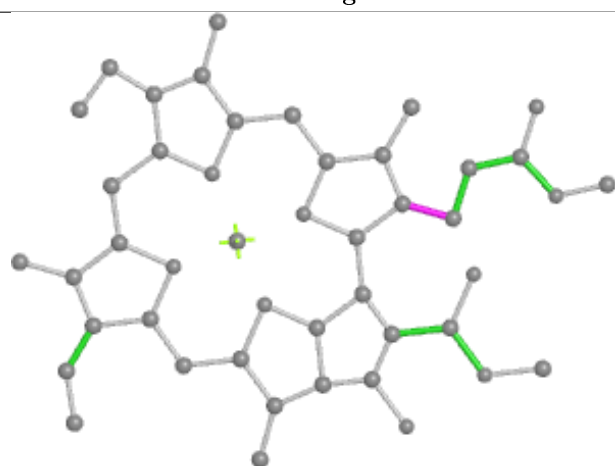
Ligand CLA B 823



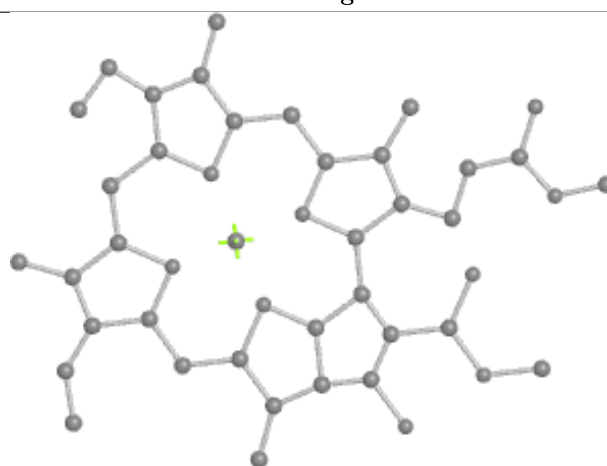
Bond lengths



Bond angles

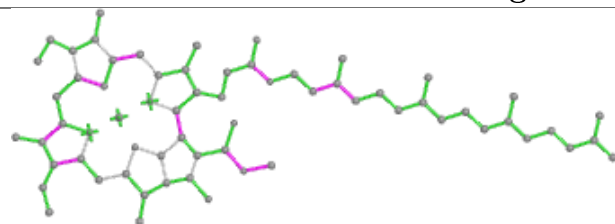


Torsions

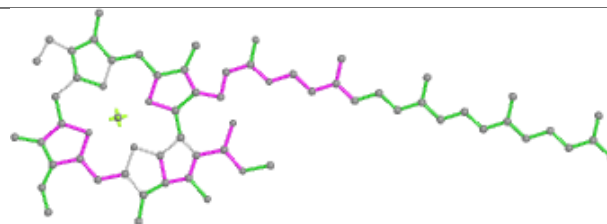


Rings

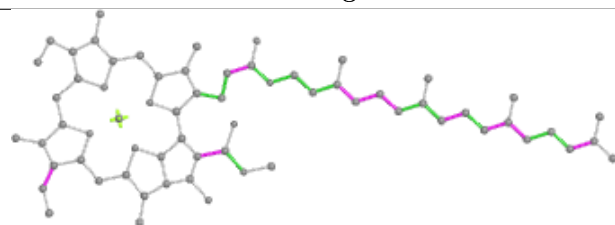
Ligand CLA L 1003



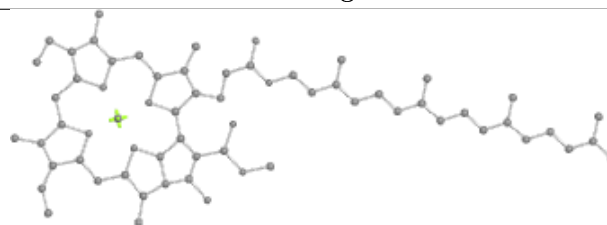
Bond lengths



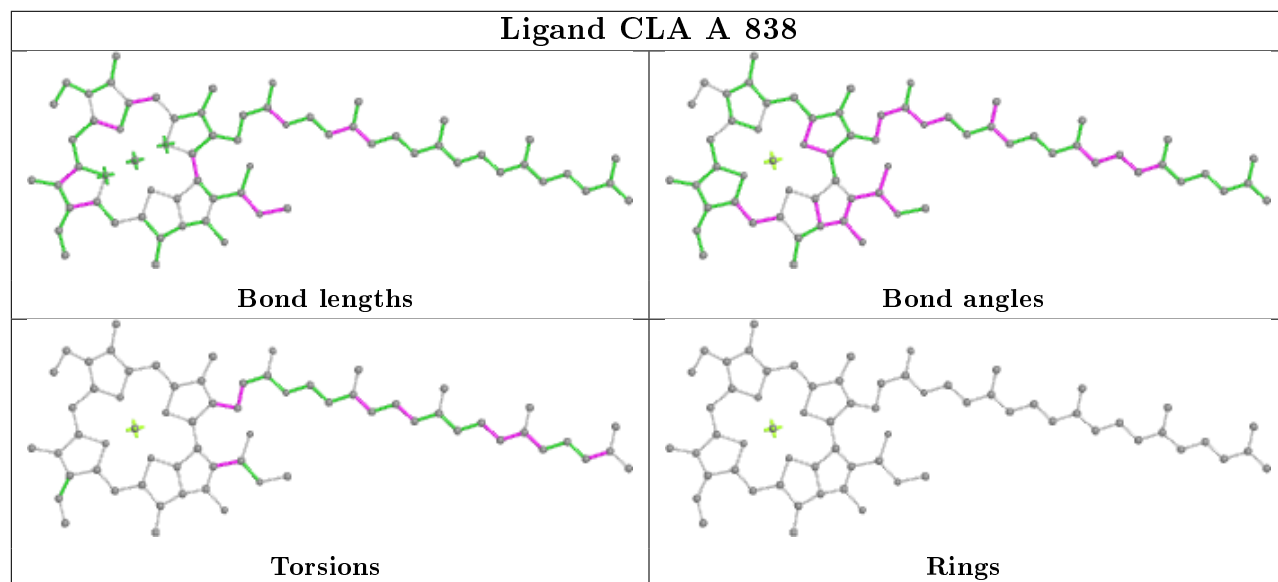
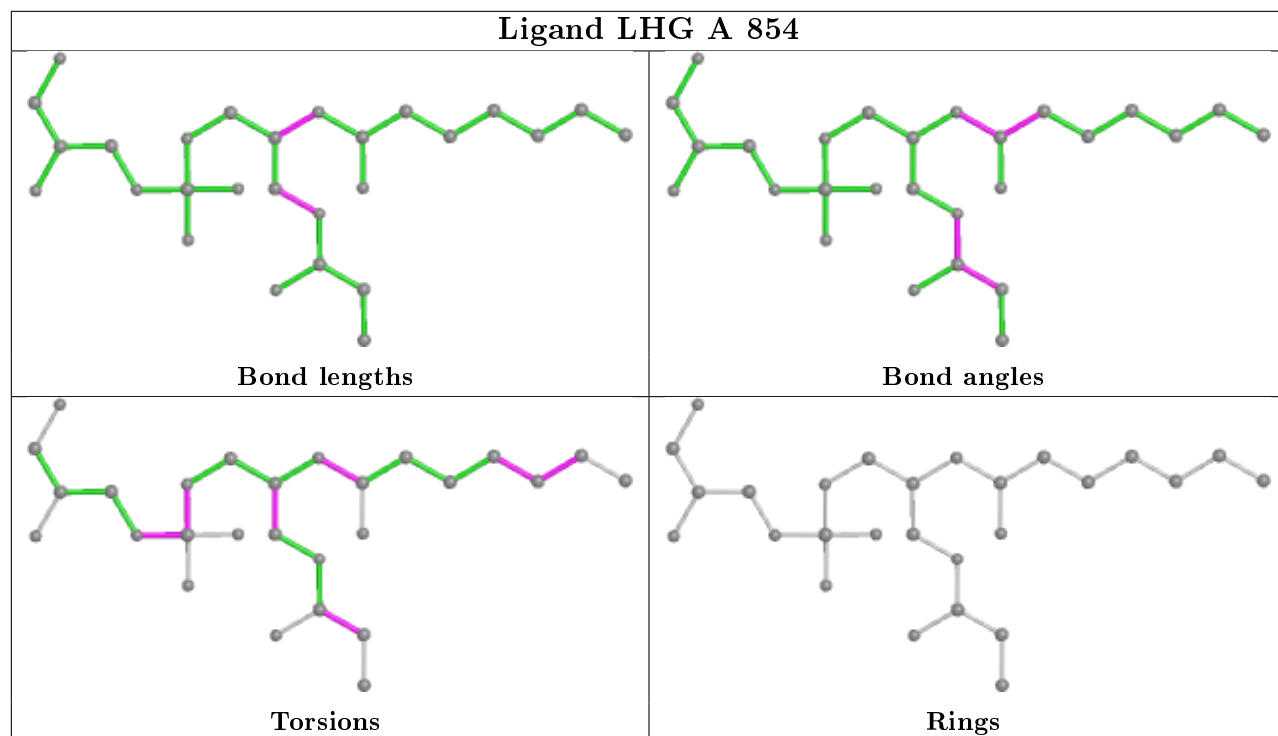
Bond angles

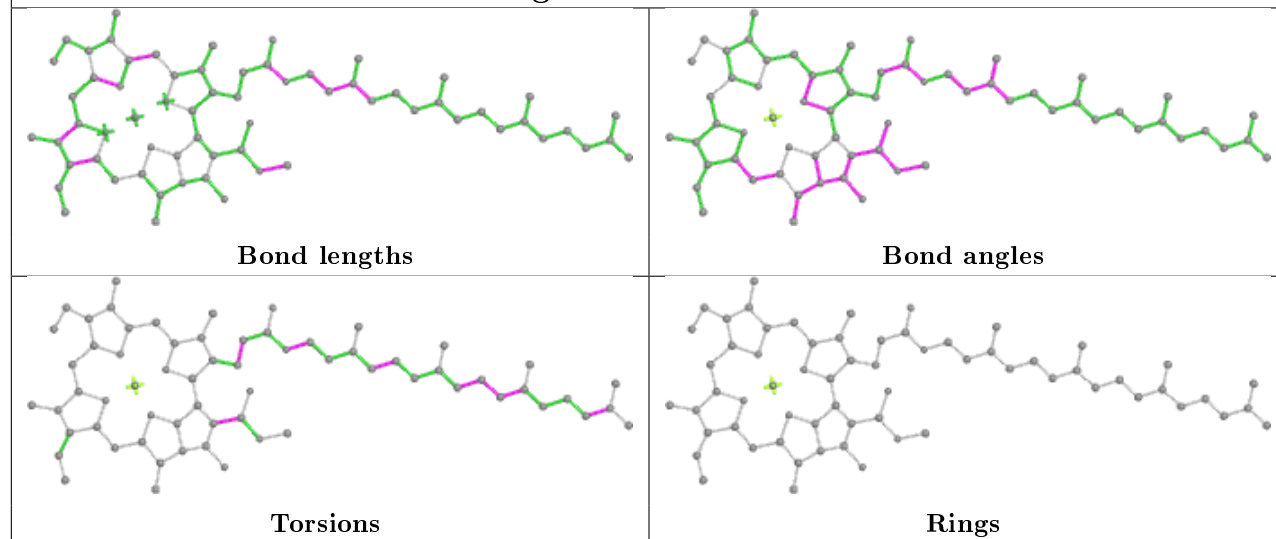
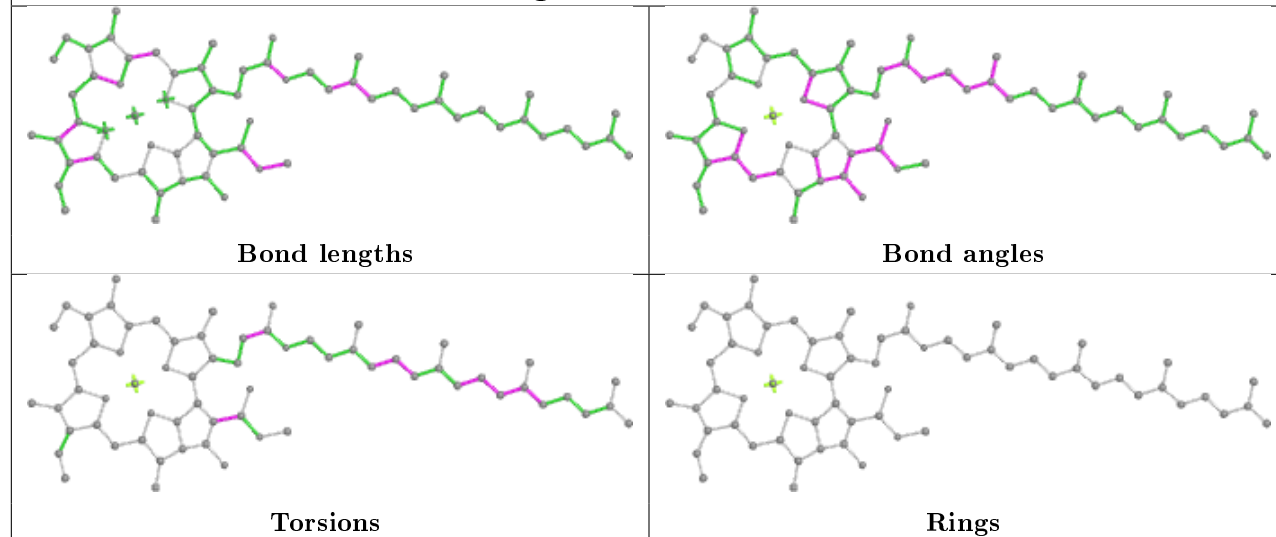


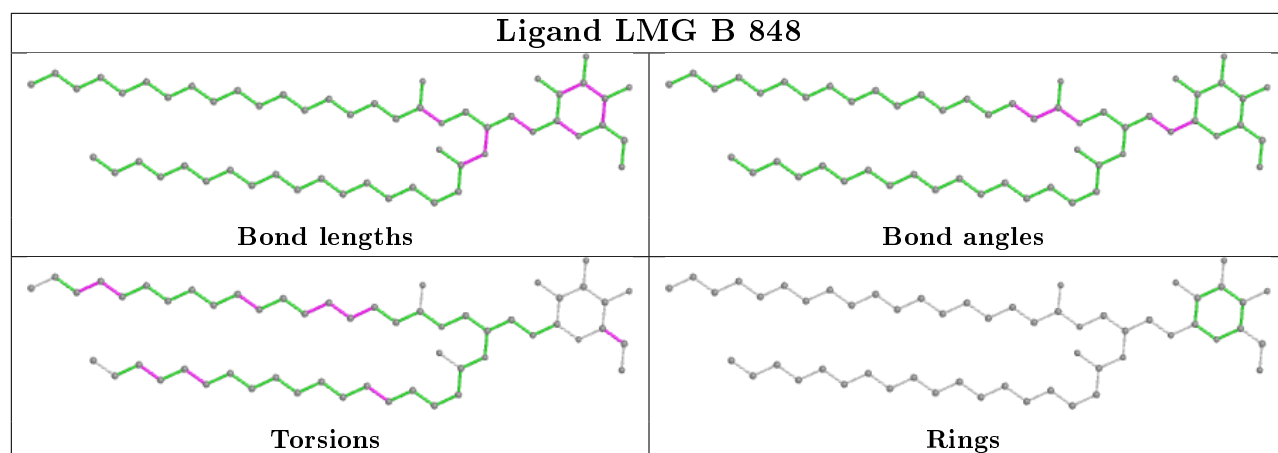
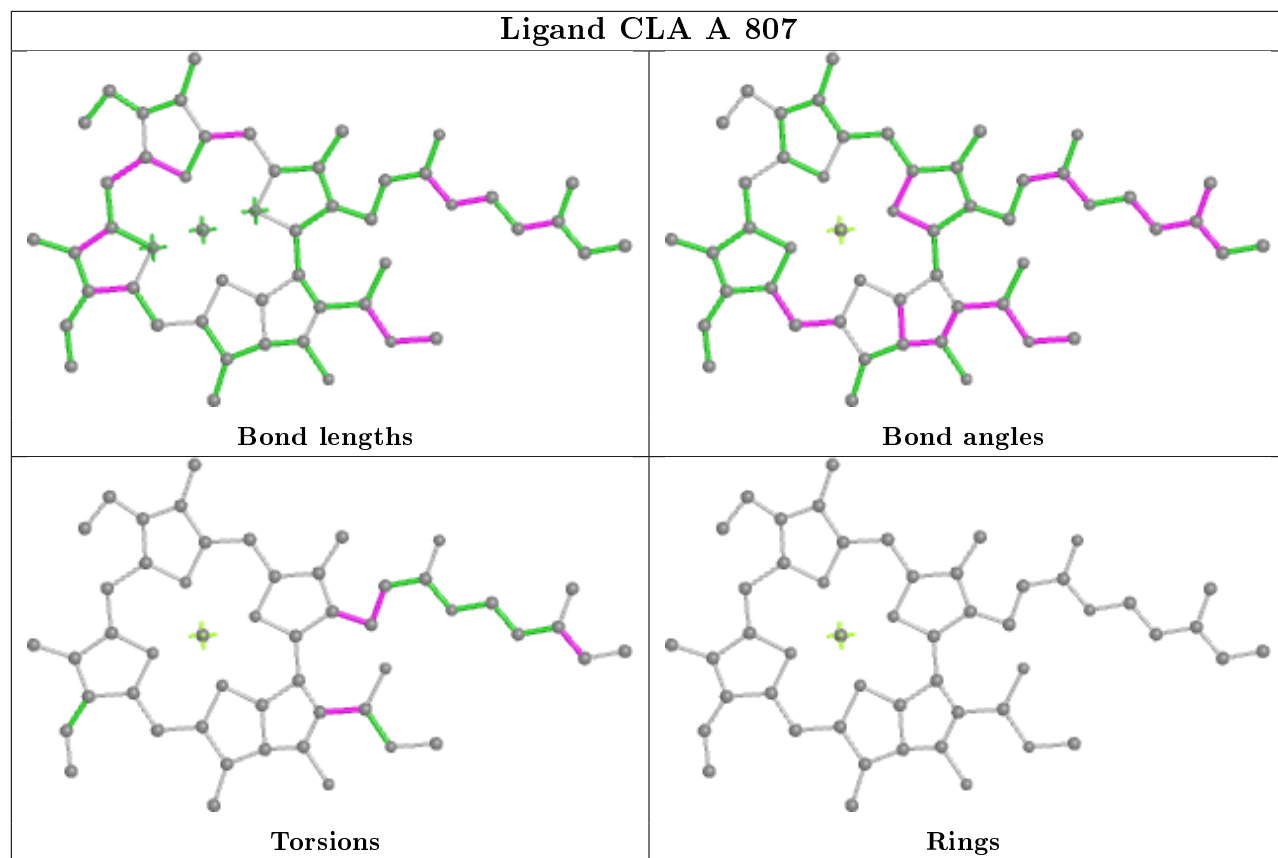
Torsions



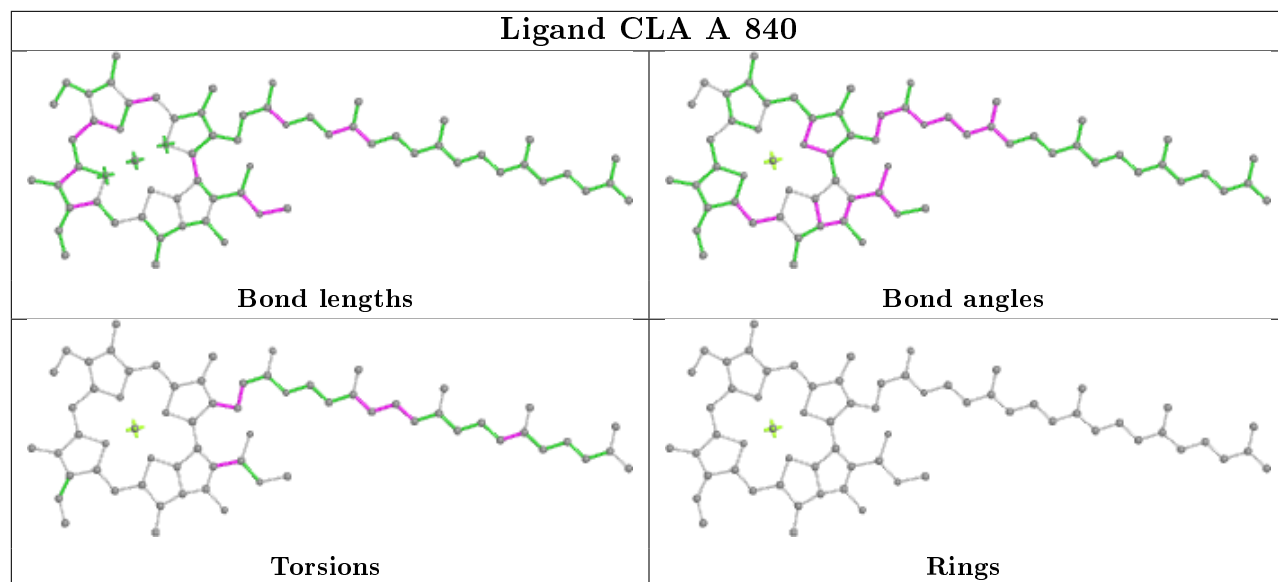
Rings



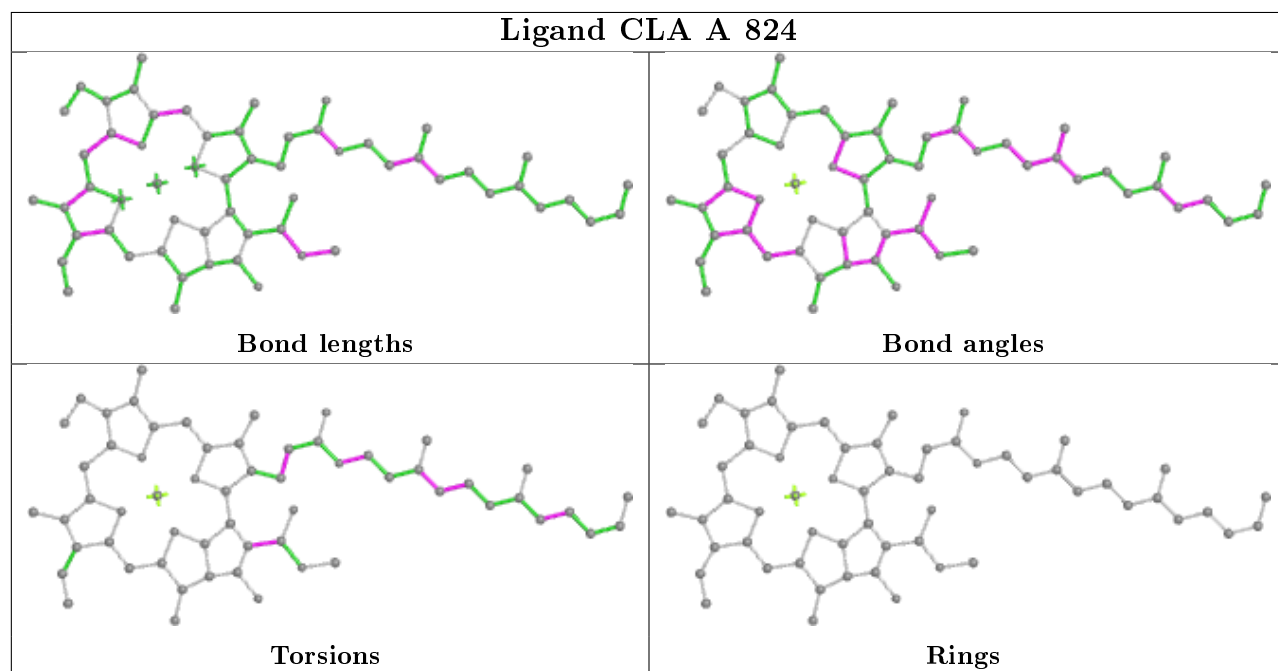
Ligand CLA A 808**Ligand CLA B 824**



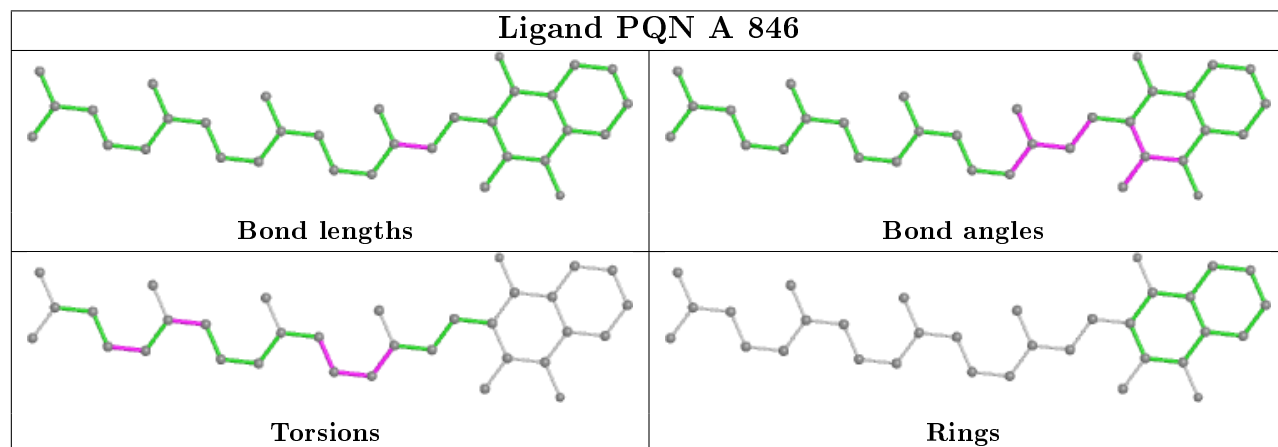
Ligand CLA A 840

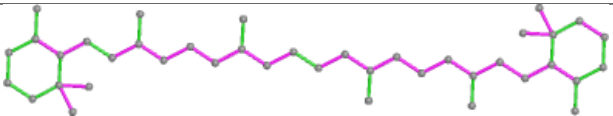
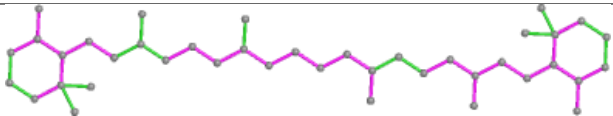
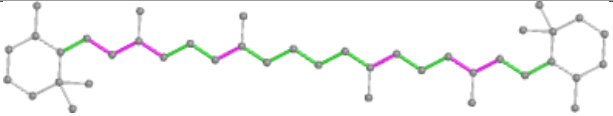
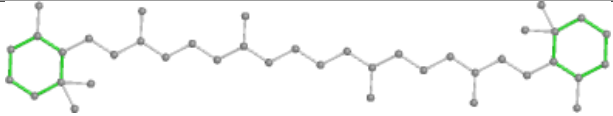


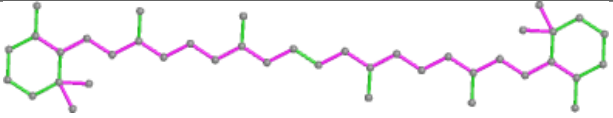
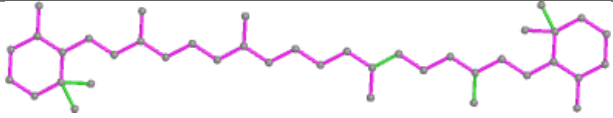
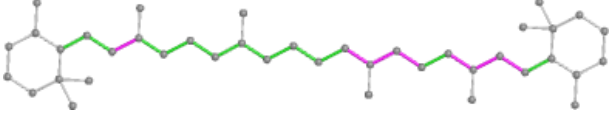
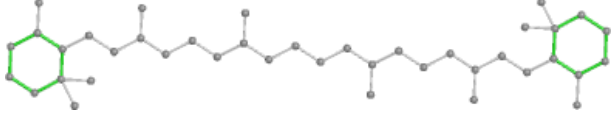
Ligand CLA A 824

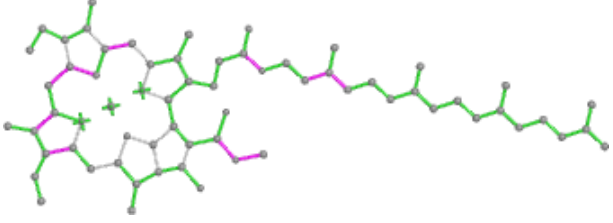
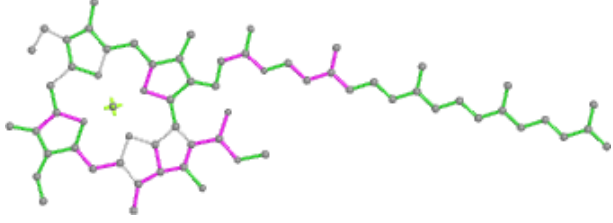
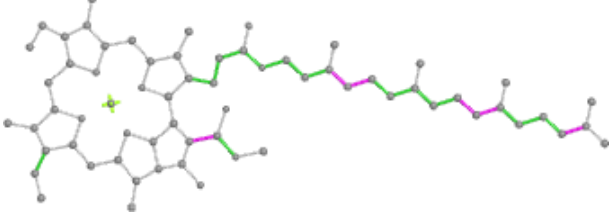
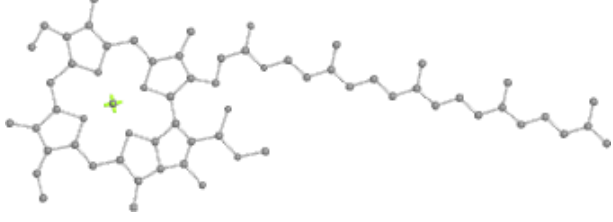


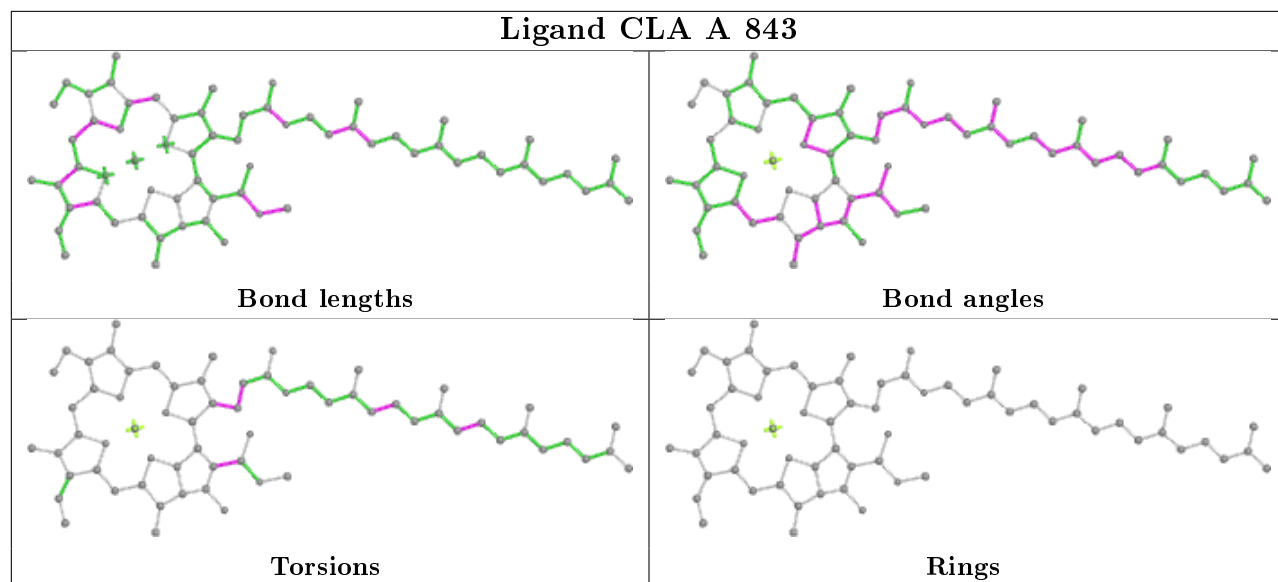
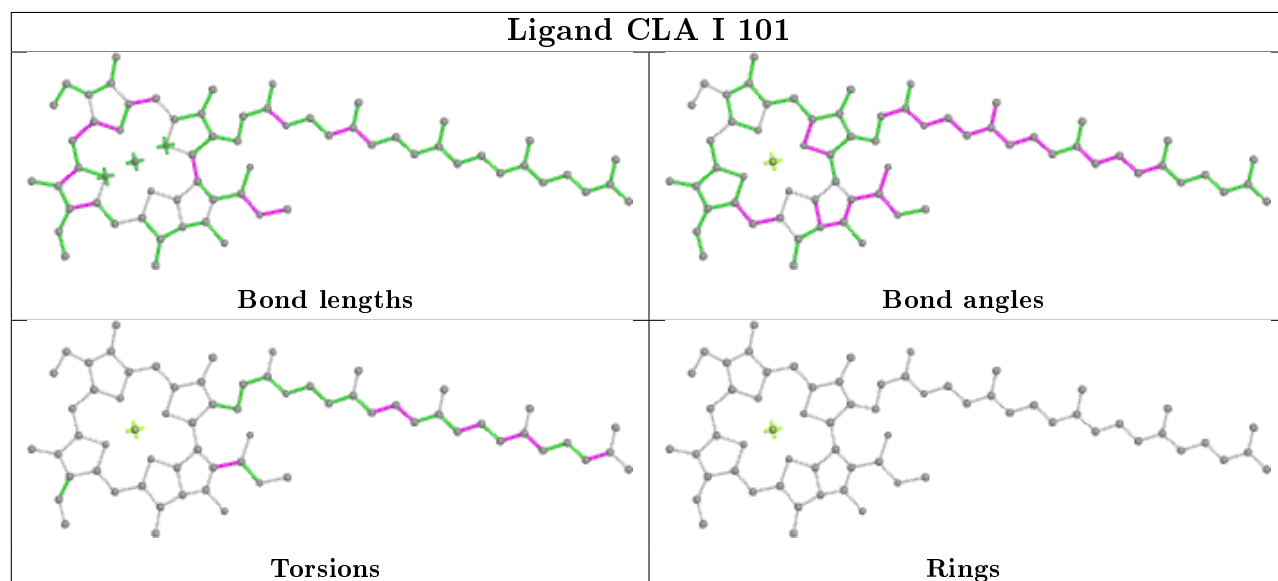
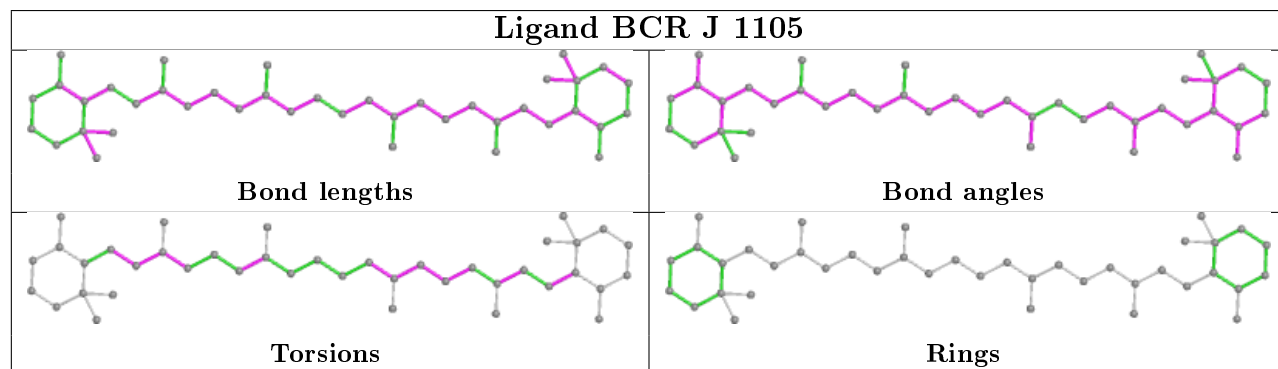
Ligand PQN A 846

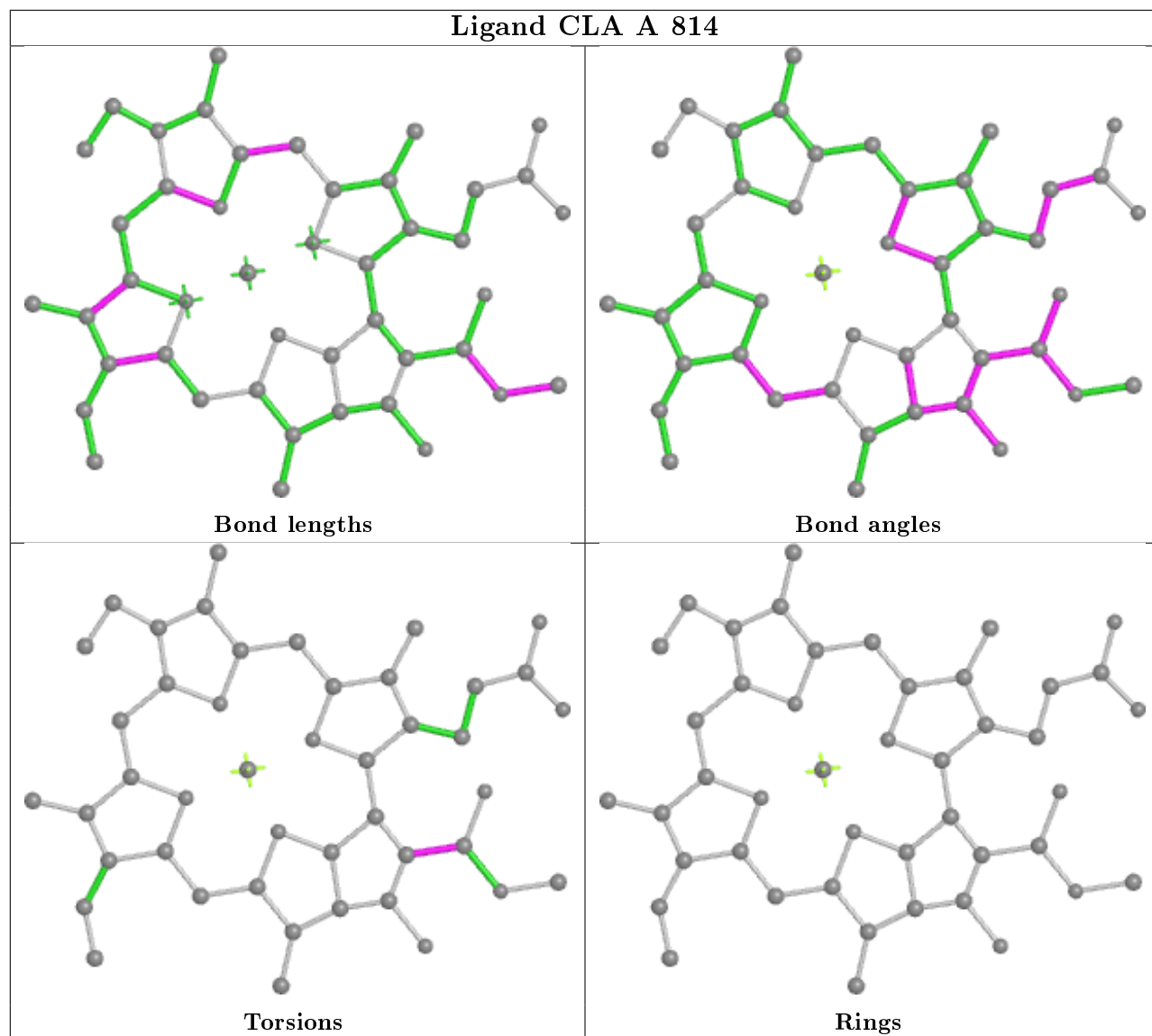
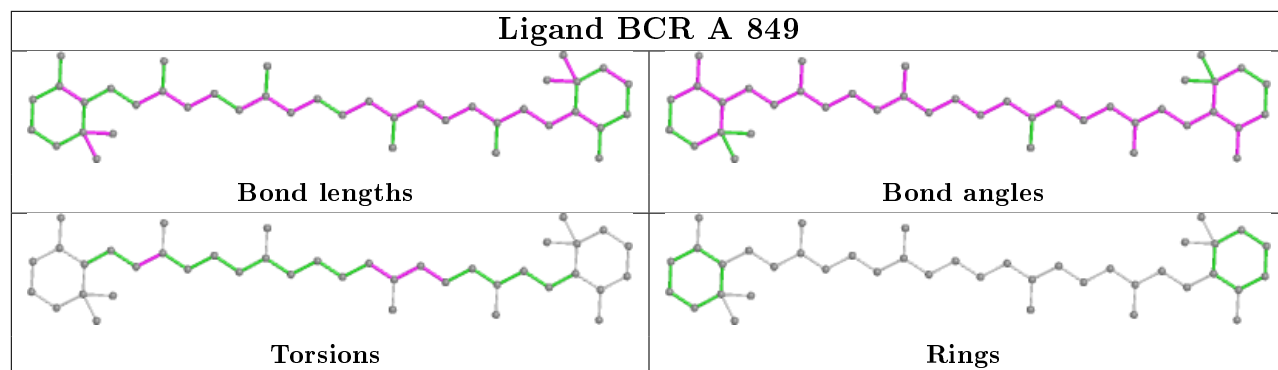


Ligand BCR L 1006	
	
Bond lengths	Bond angles
	
Torsions	Rings

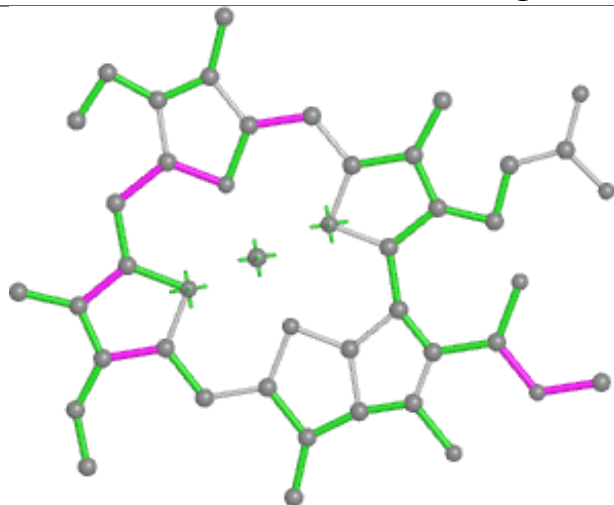
Ligand BCR B 843	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

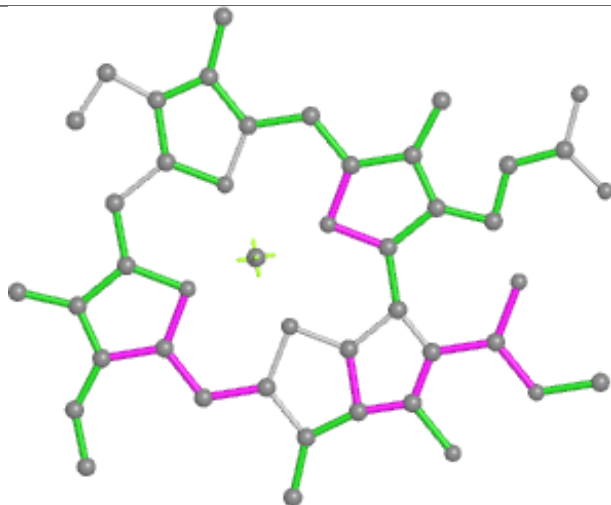
Ligand CLA A 843**Ligand CLA I 101****Ligand BCR J 1105**



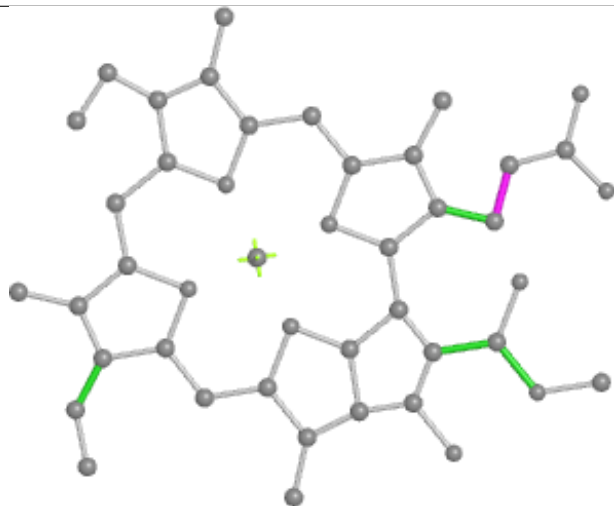
Ligand CLA X 102



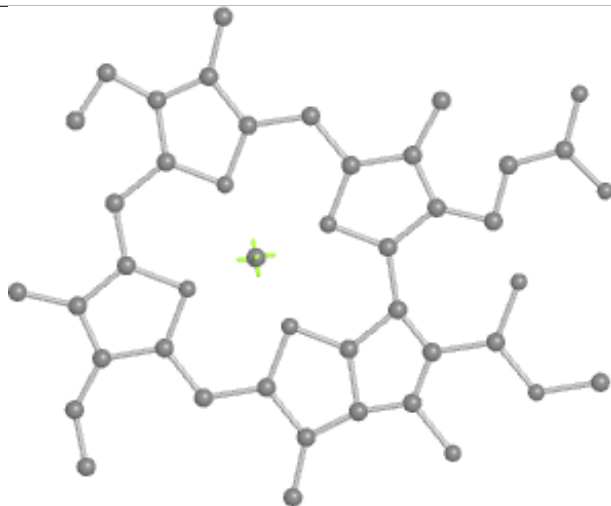
Bond lengths



Bond angles

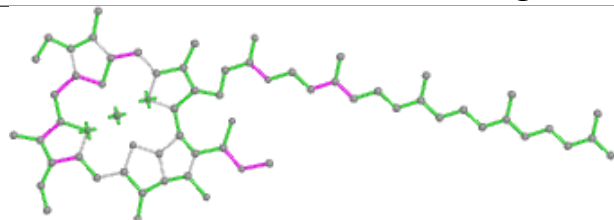


Torsions

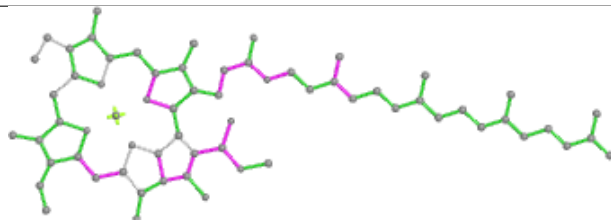


Rings

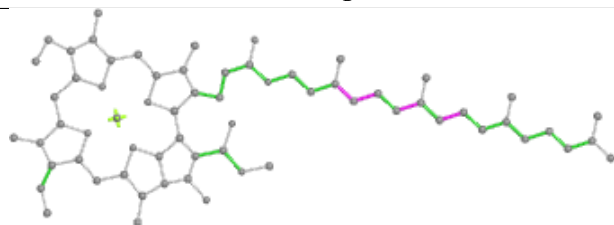
Ligand CLA B 839



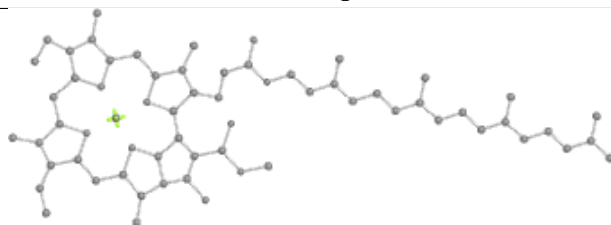
Bond lengths



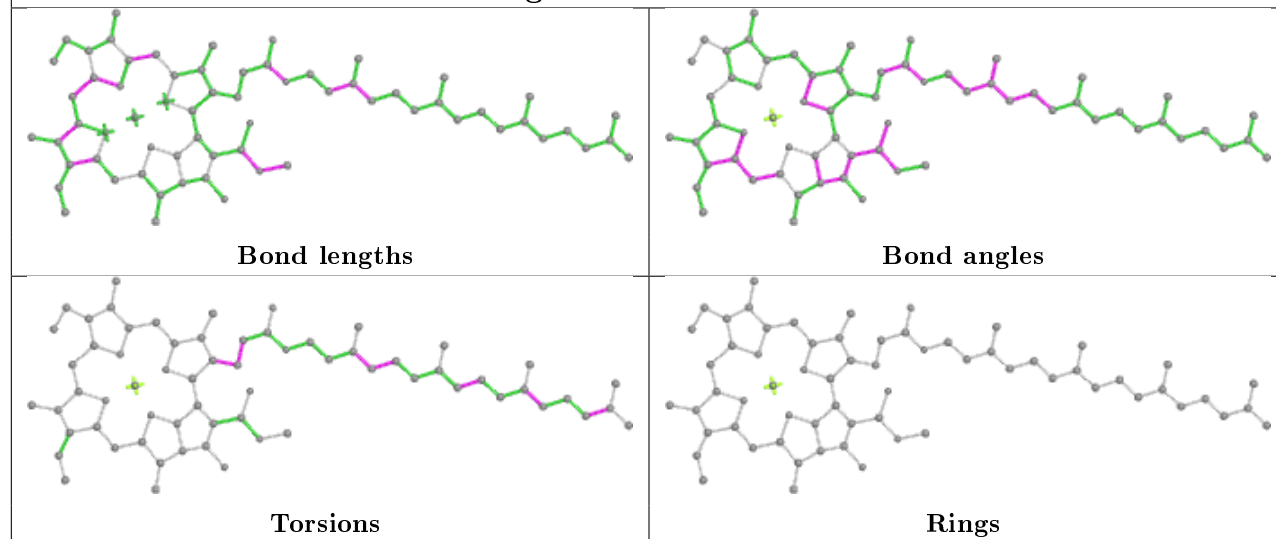
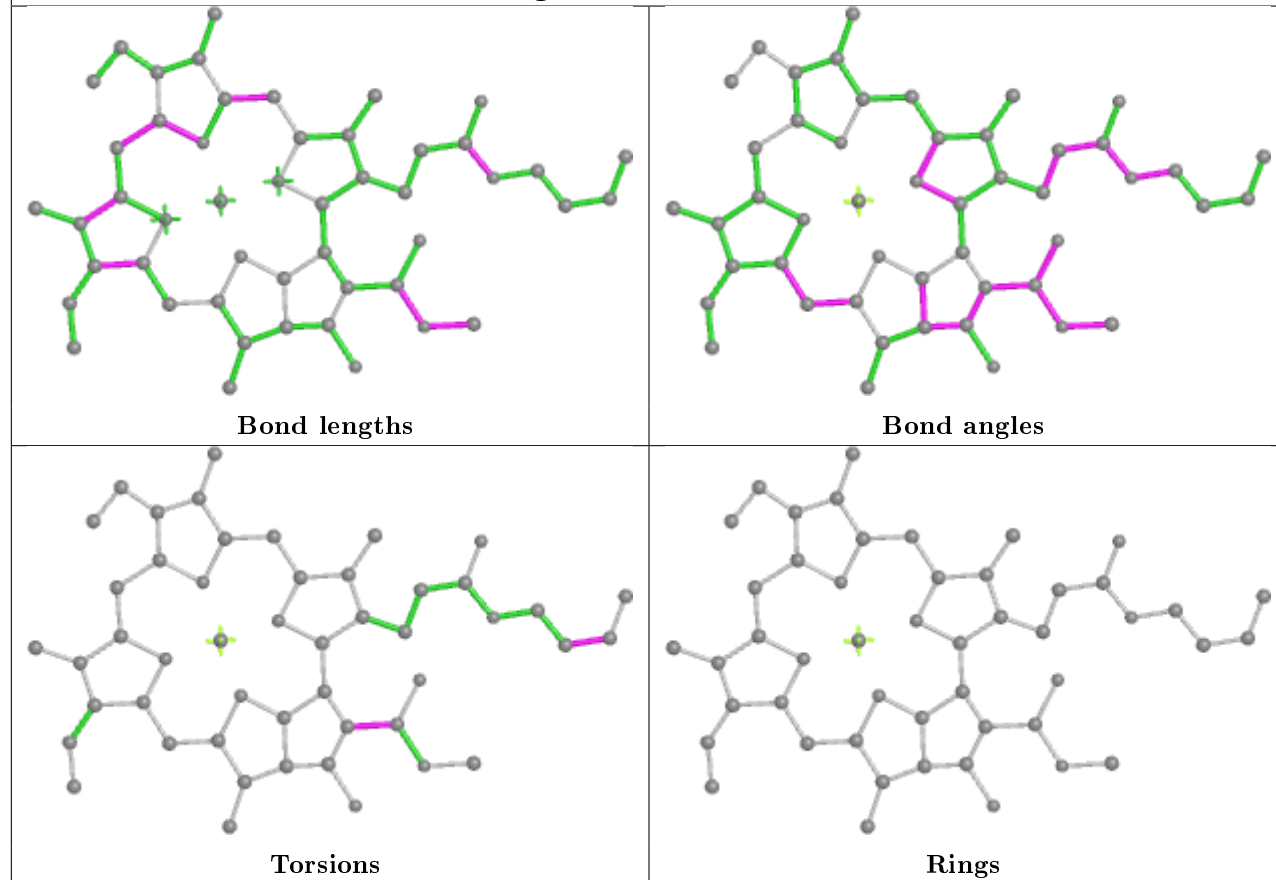
Bond angles

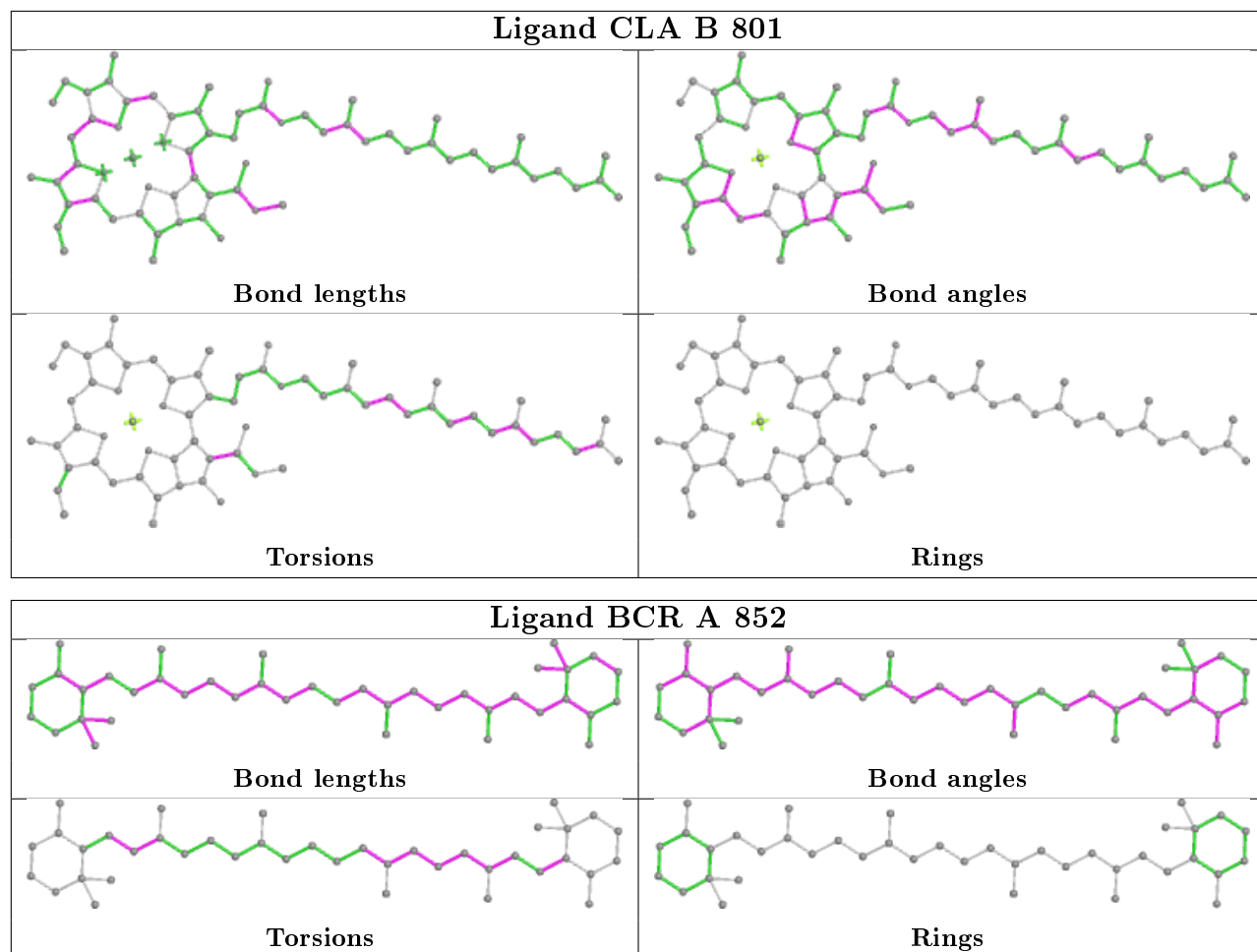


Torsions

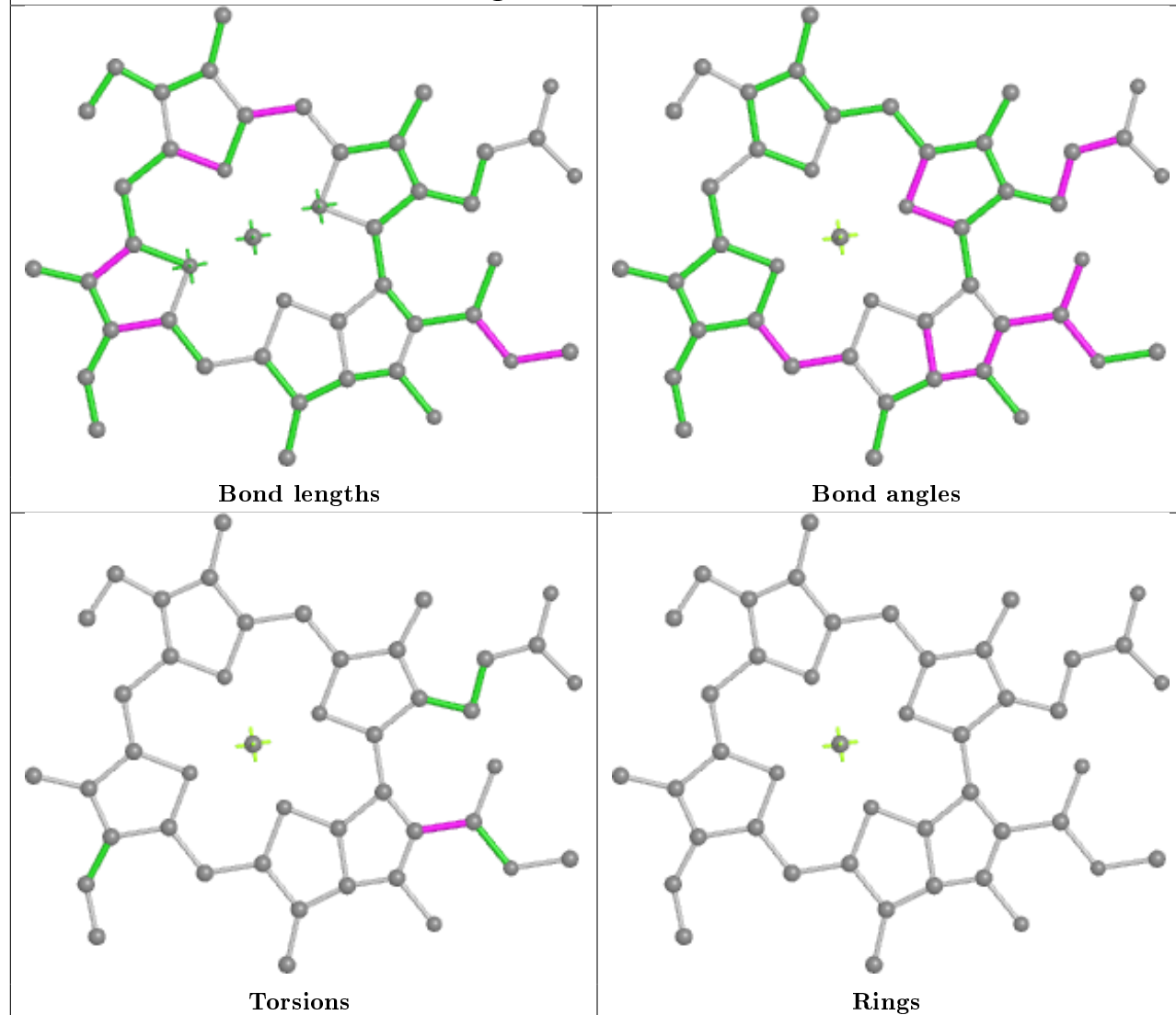


Rings

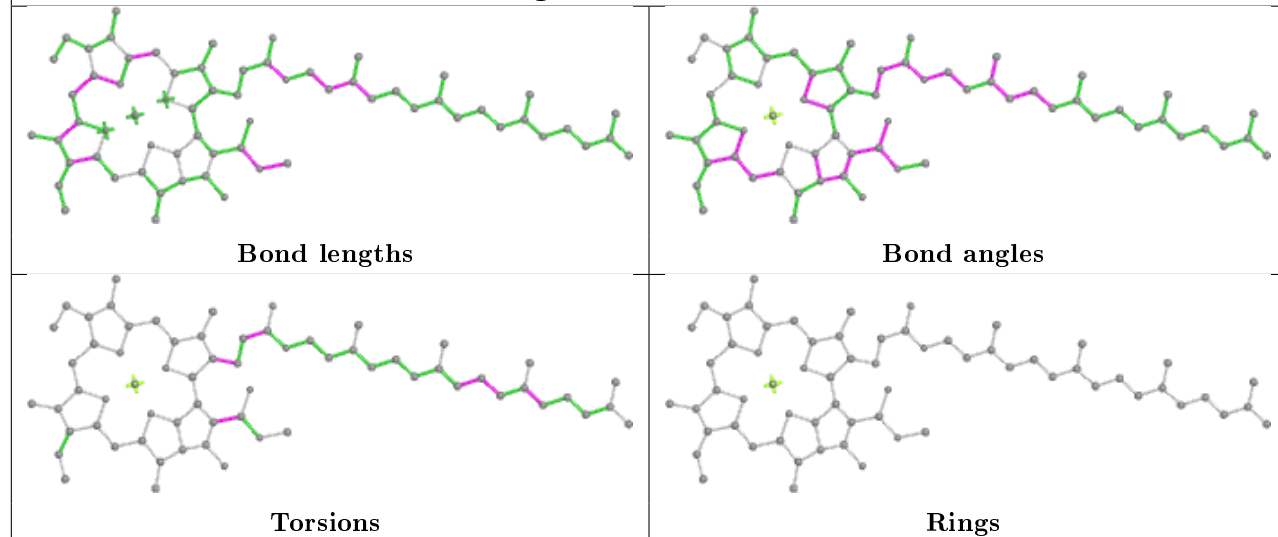
Ligand CLA L 1004**Ligand CLA B 829**



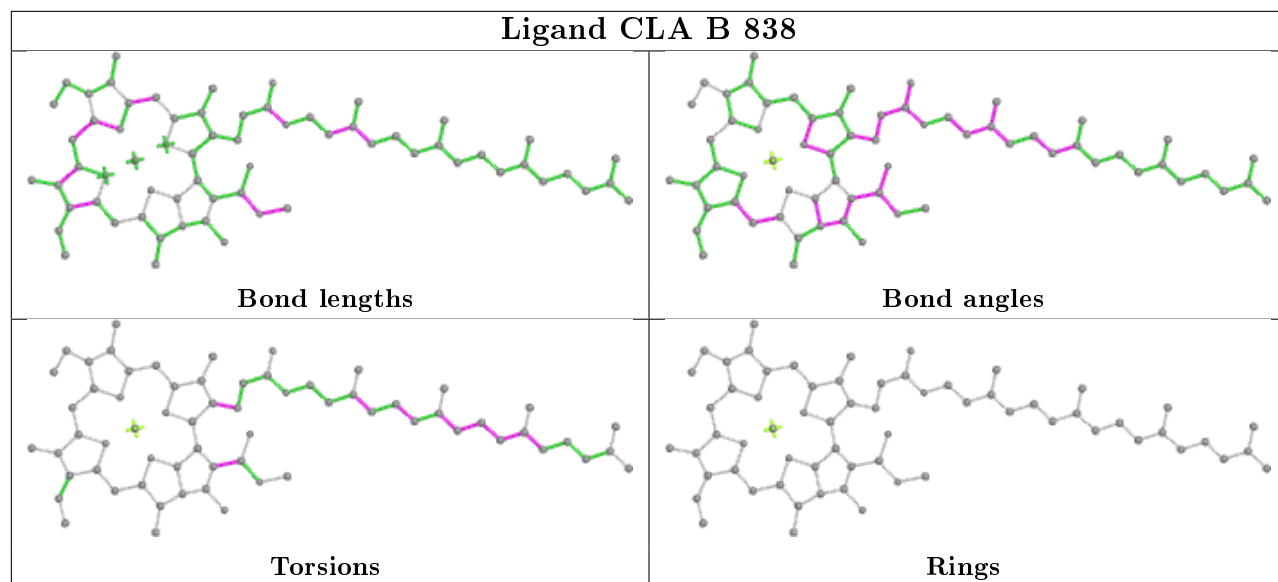
Ligand CLA B 833



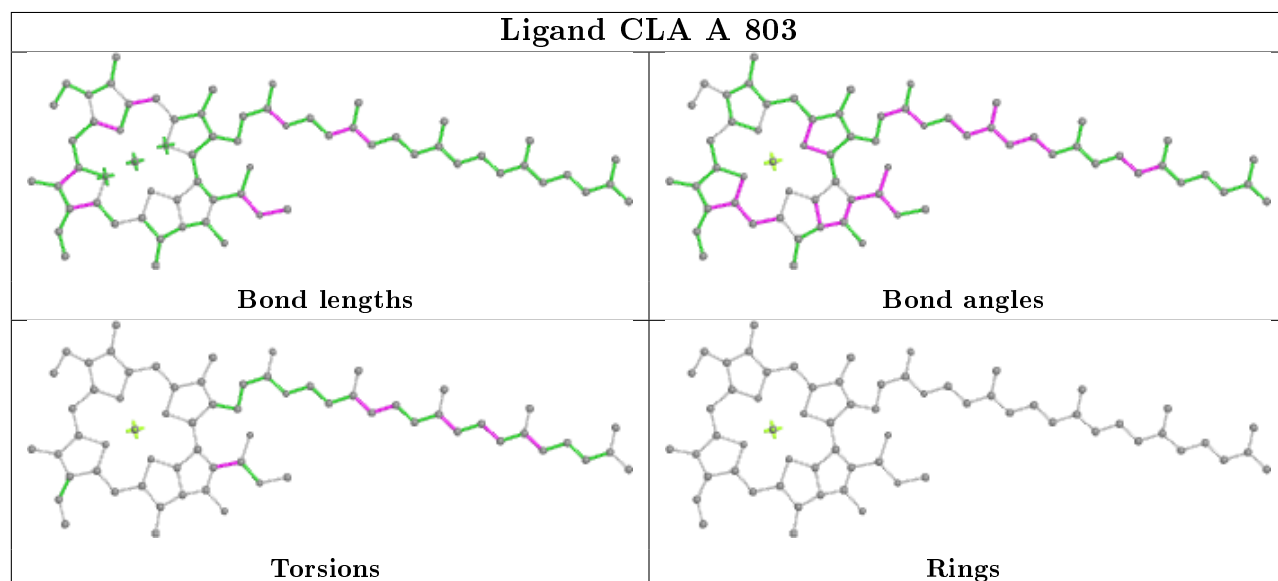
Ligand CLA A 829



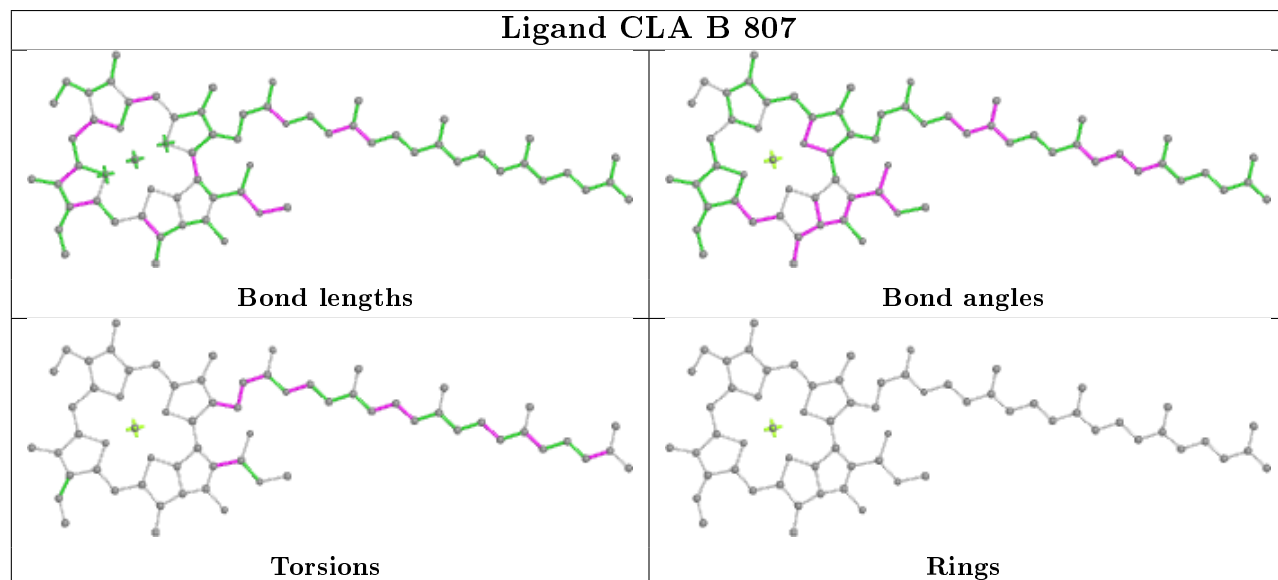
Ligand CLA B 838



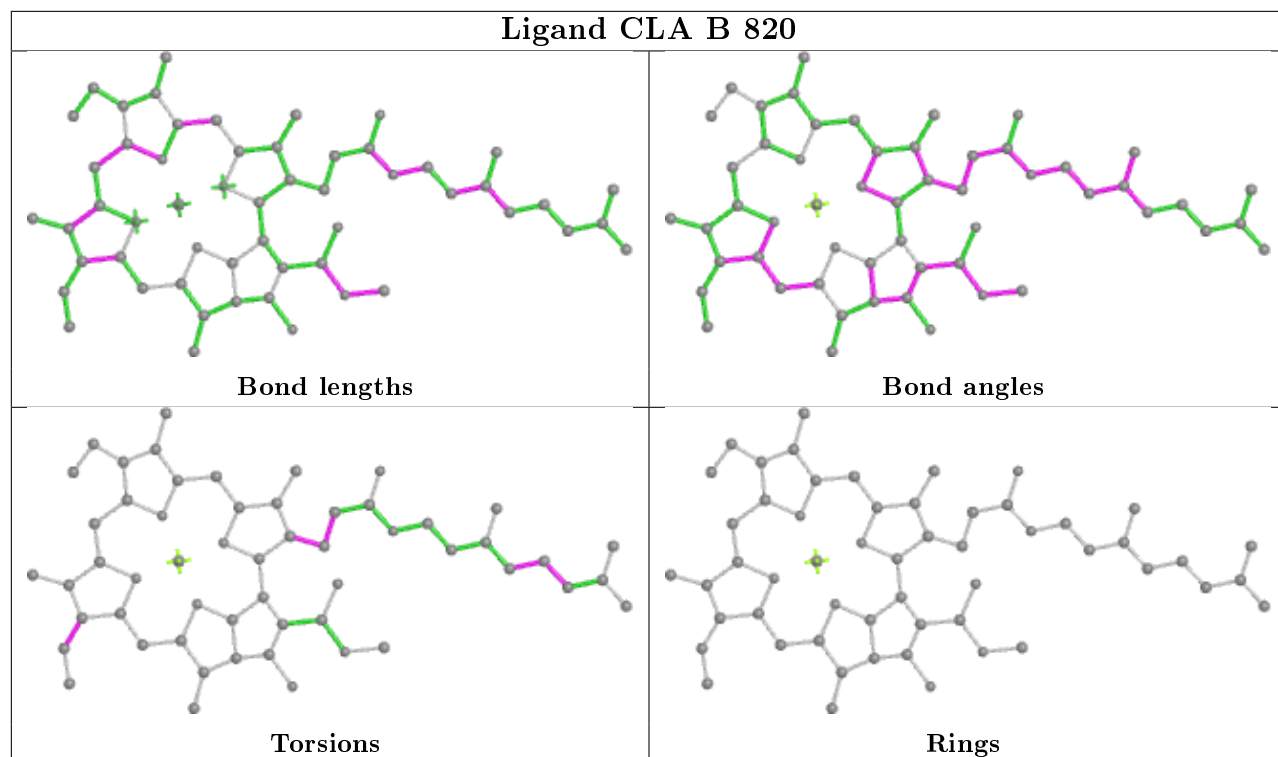
Ligand CLA A 803



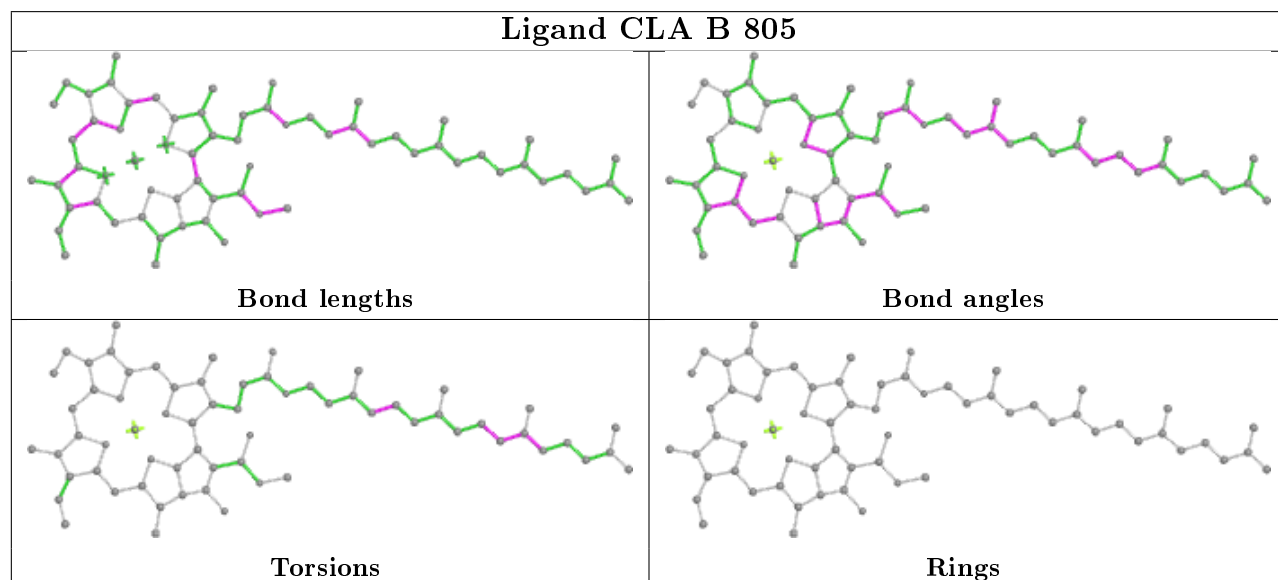
Ligand CLA B 807



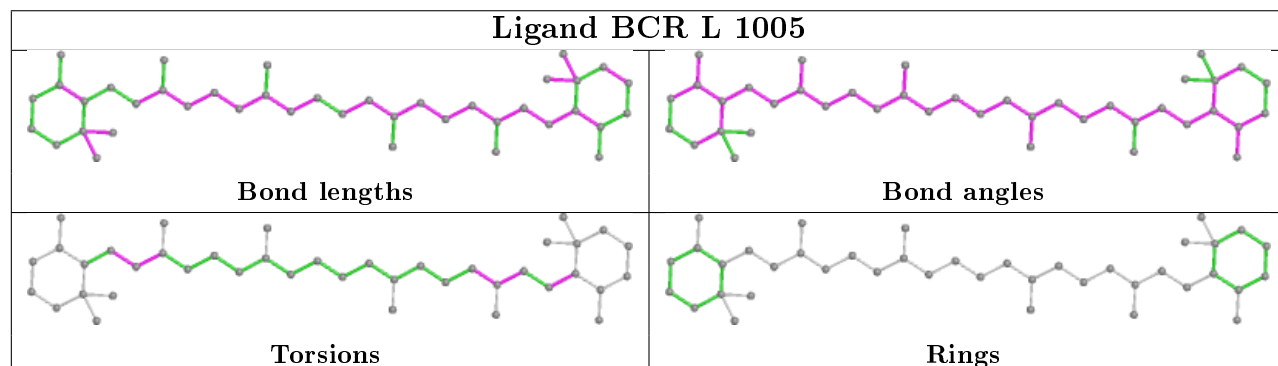
Ligand CLA B 820



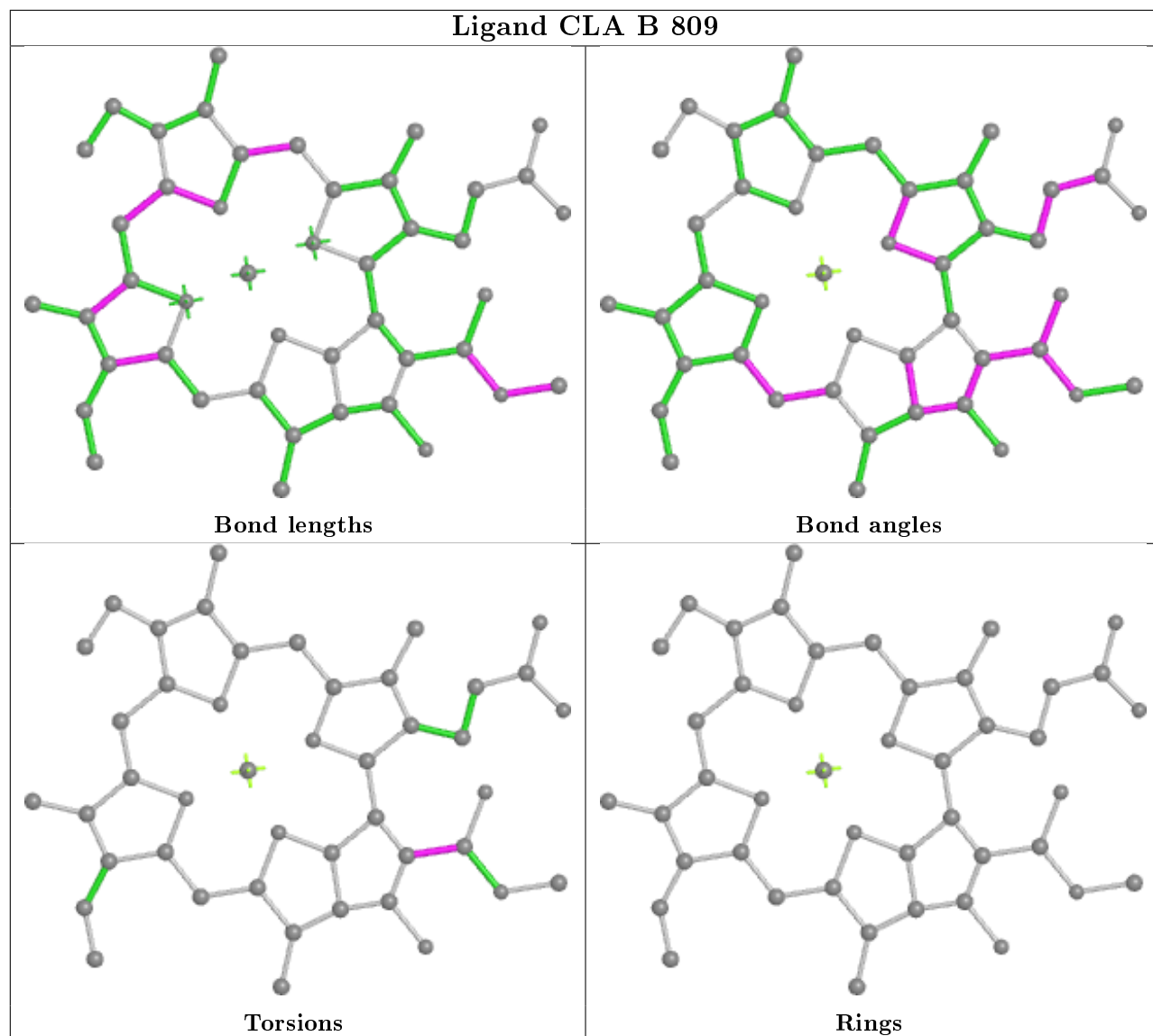
Ligand CLA B 805



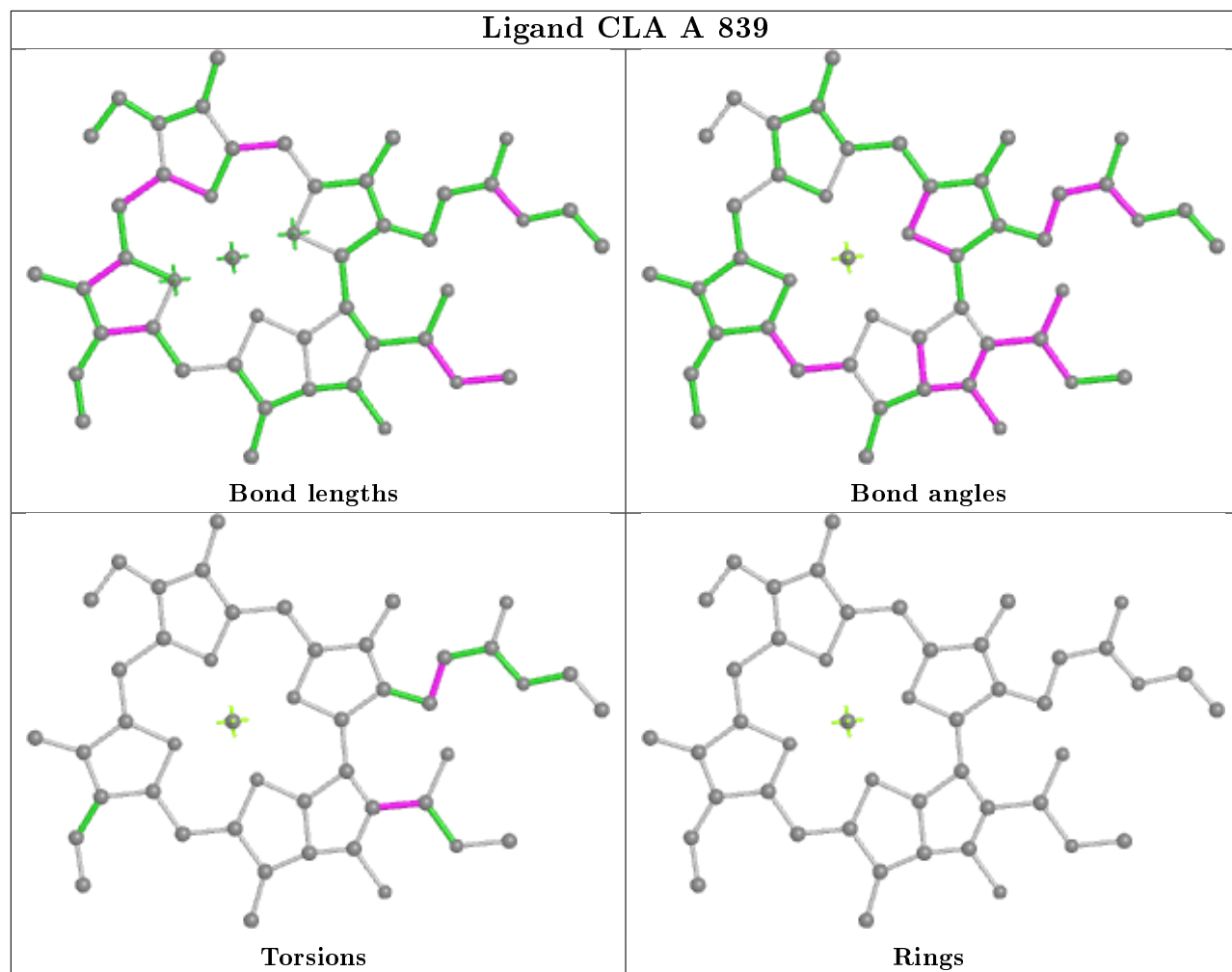
Ligand BCR L 1005



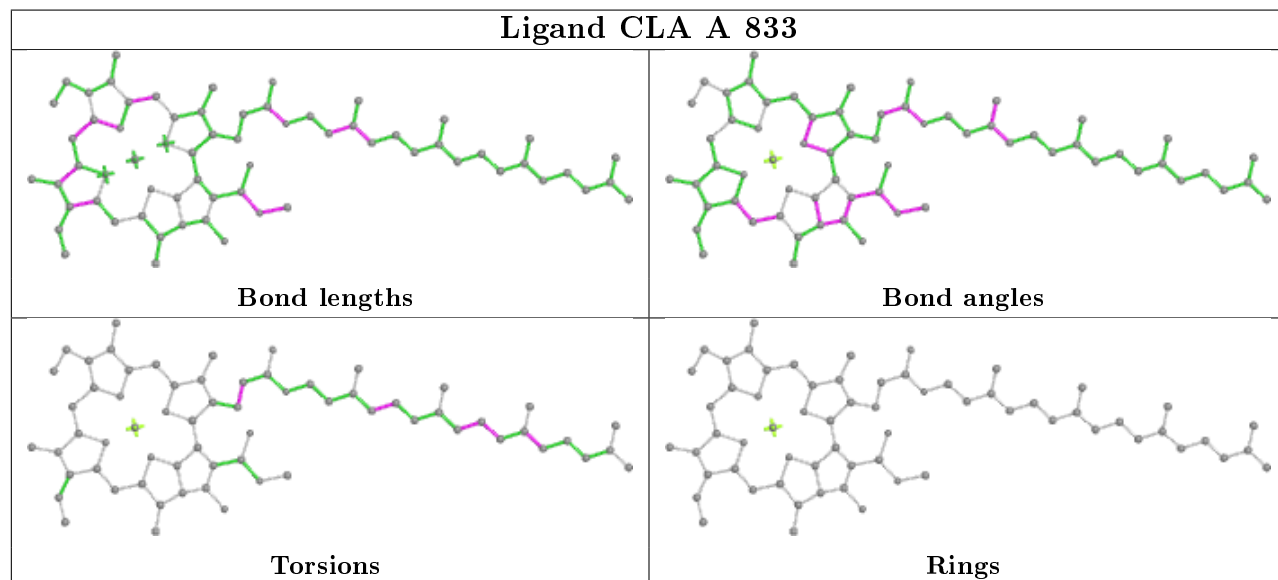
Ligand CLA B 809

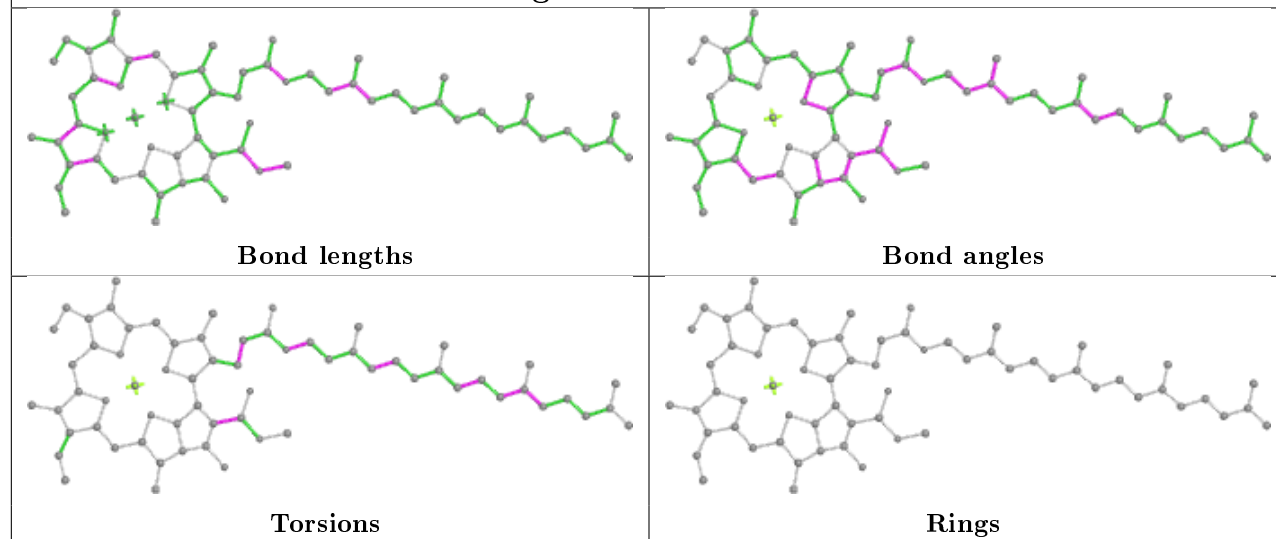
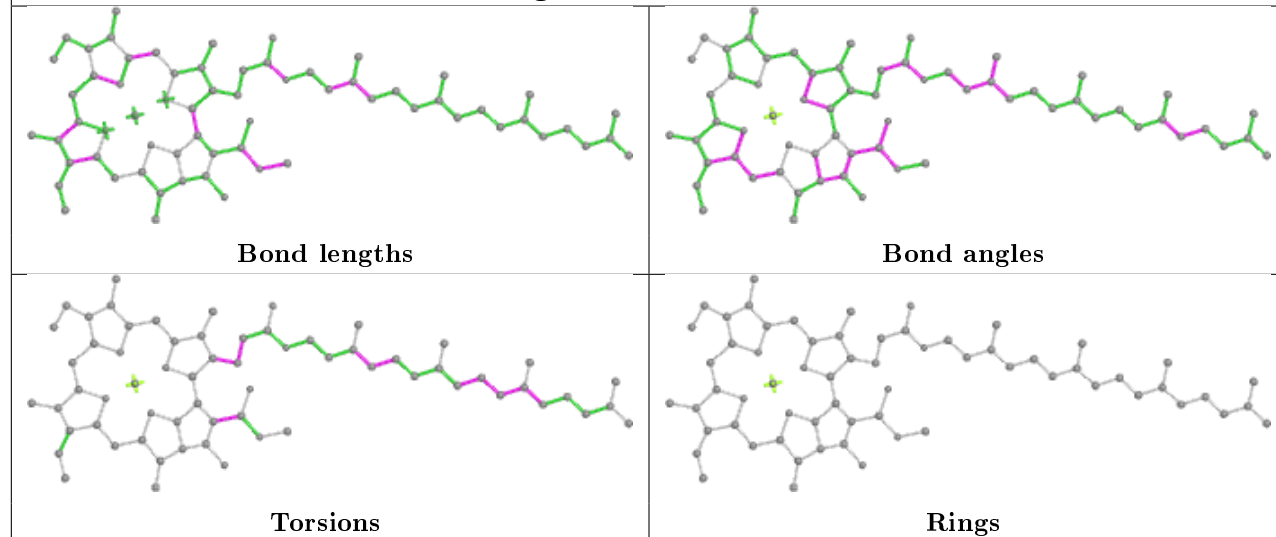


Ligand CLA A 839

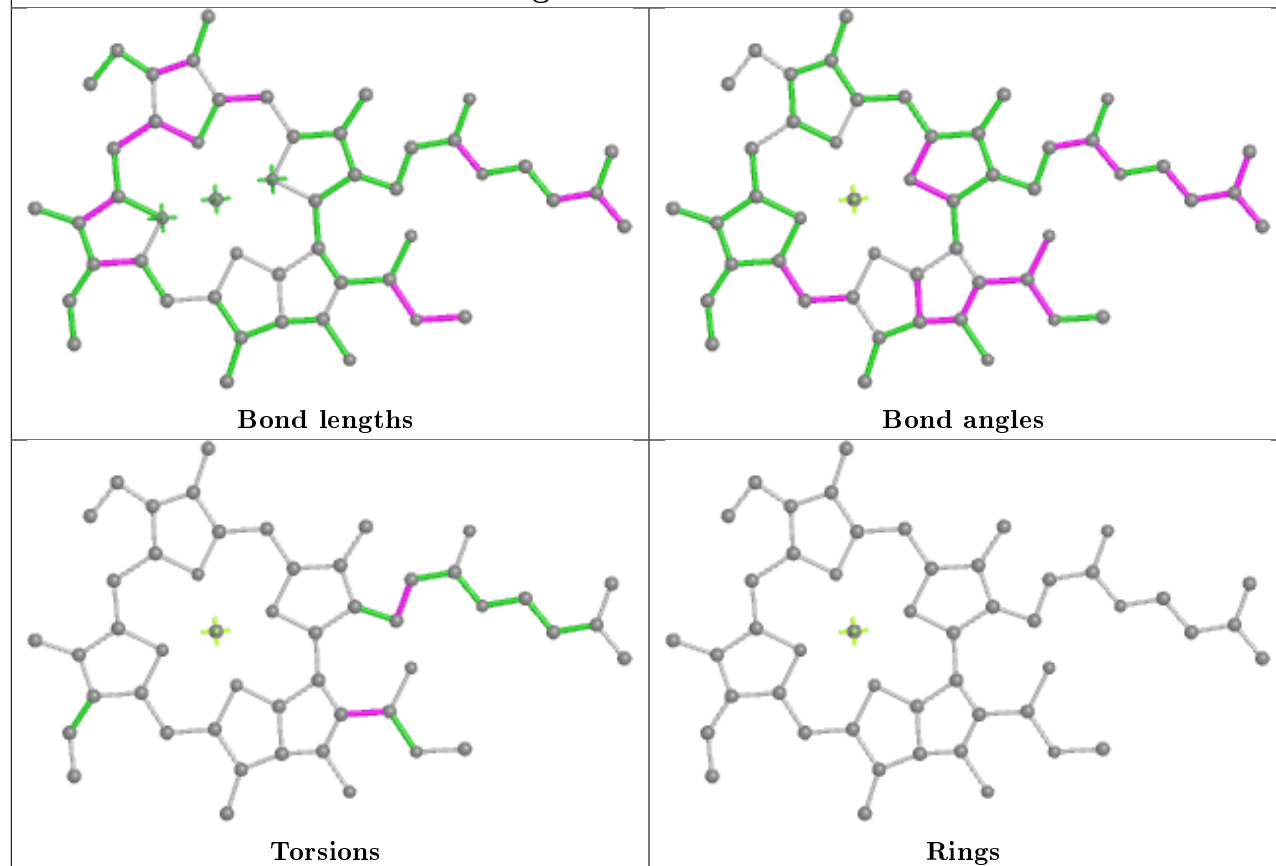


Ligand CLA A 833

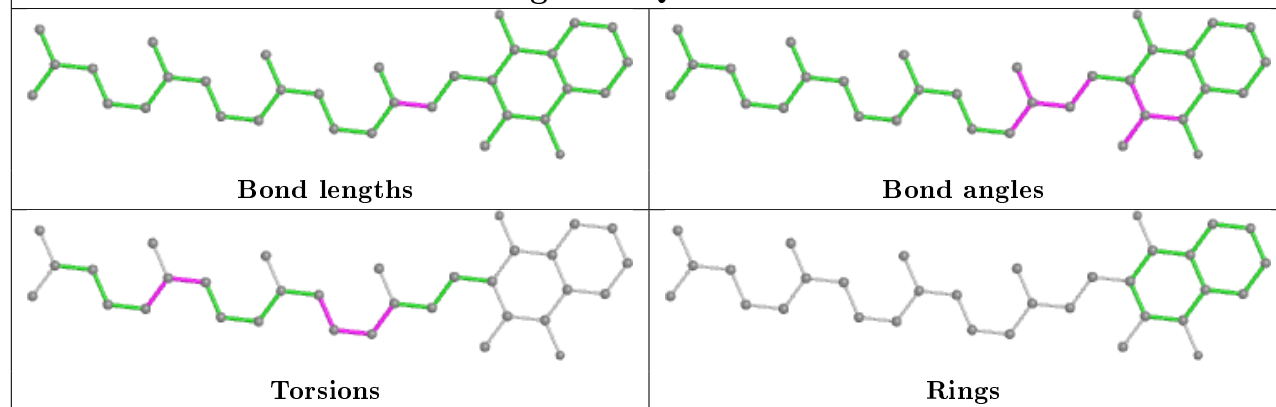


Ligand CLA B 802**Ligand CLA A 821**

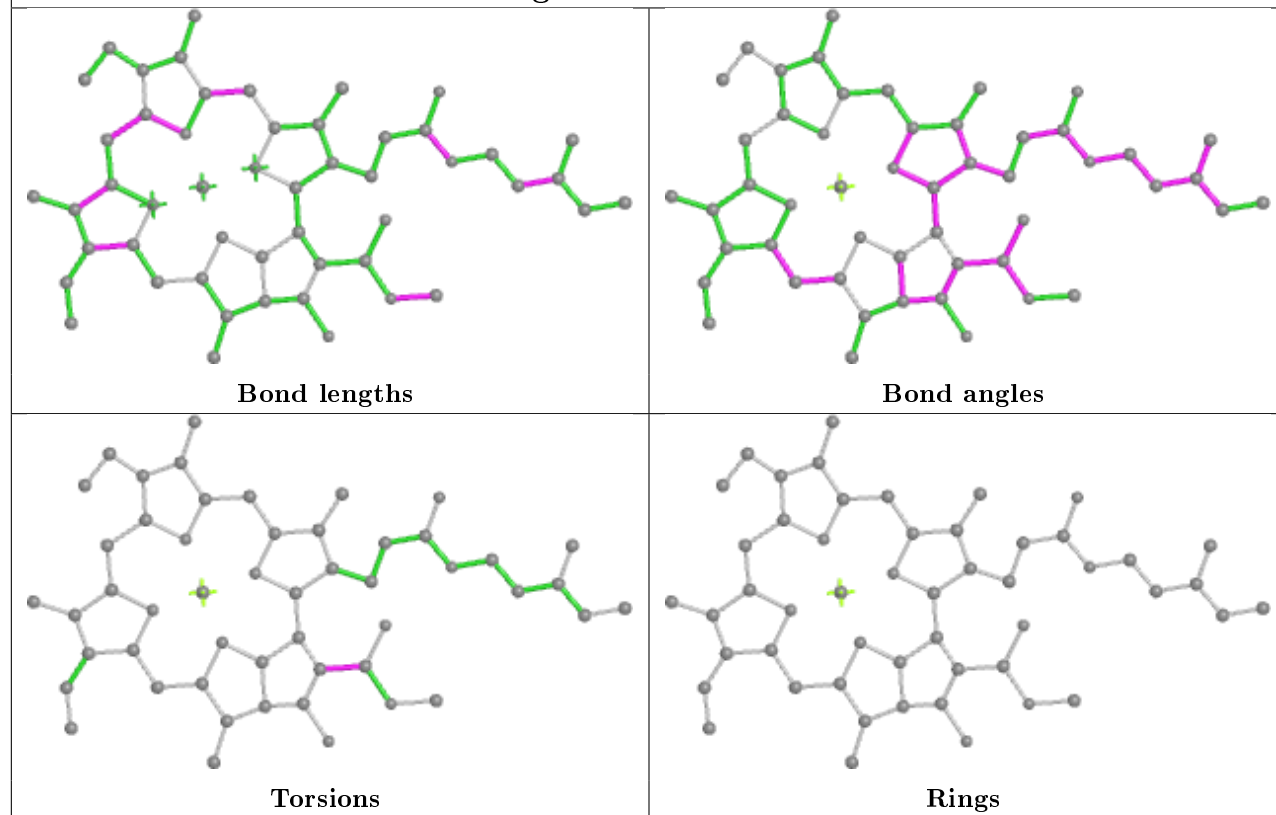
Ligand CLA A 831



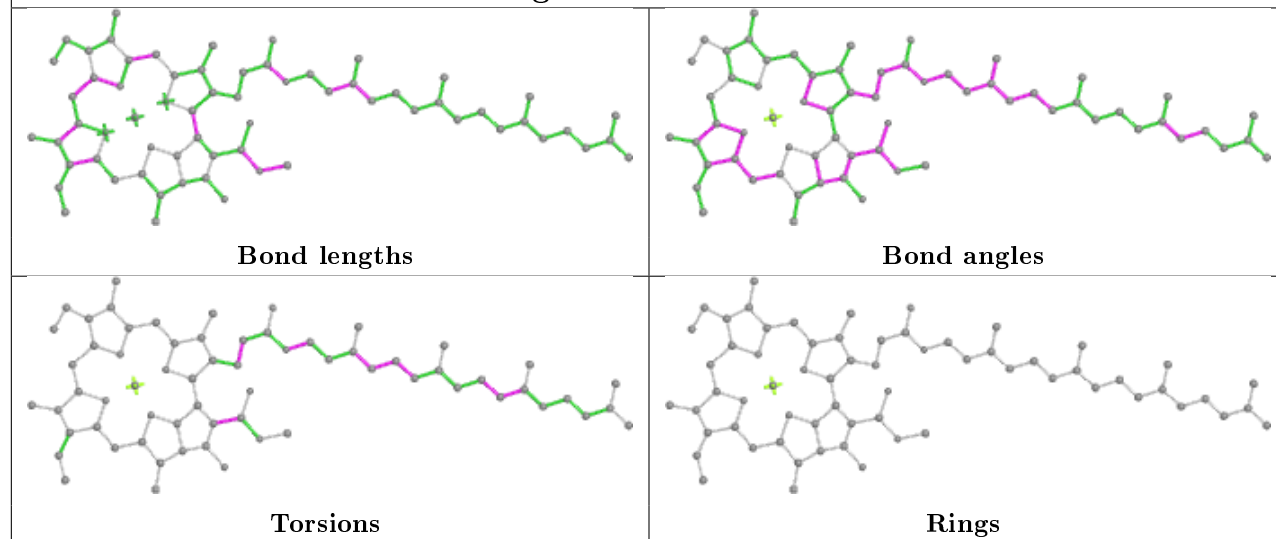
Ligand PQN B 840



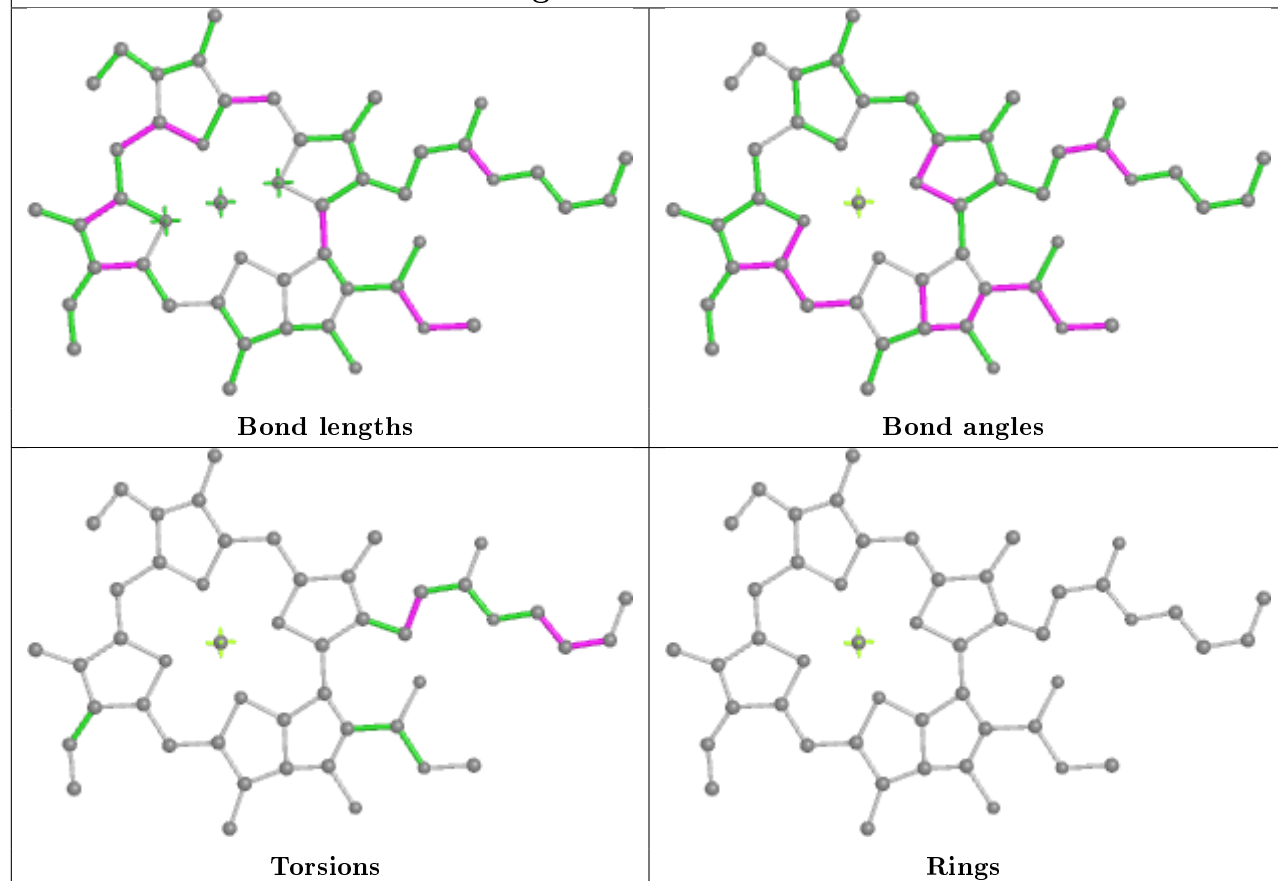
Ligand CLA A 837



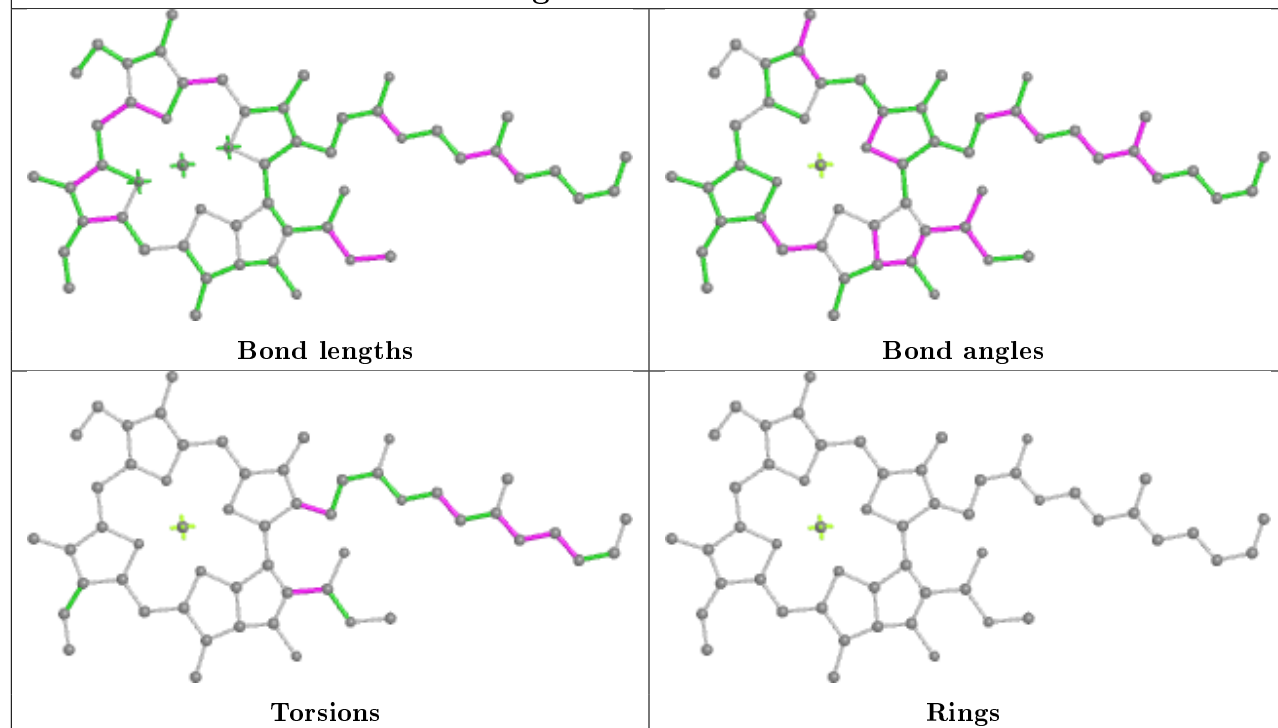
Ligand CLA A 819

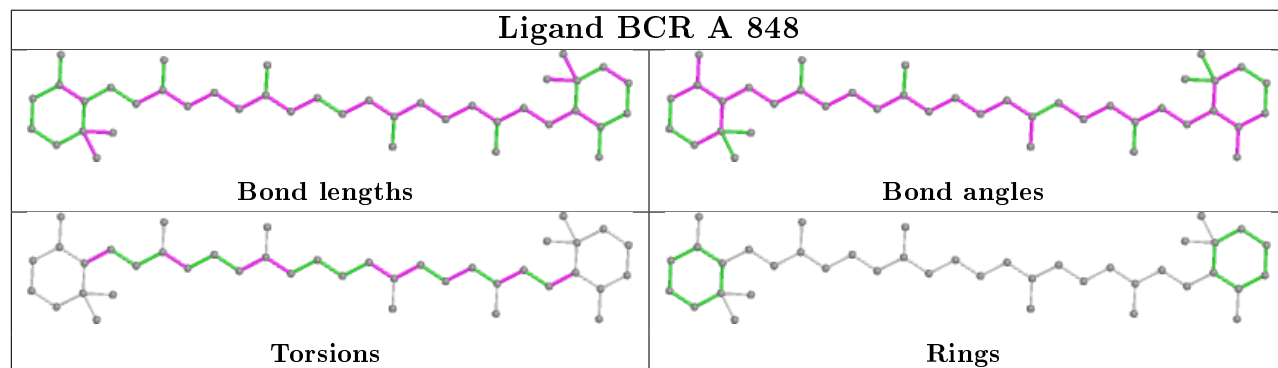
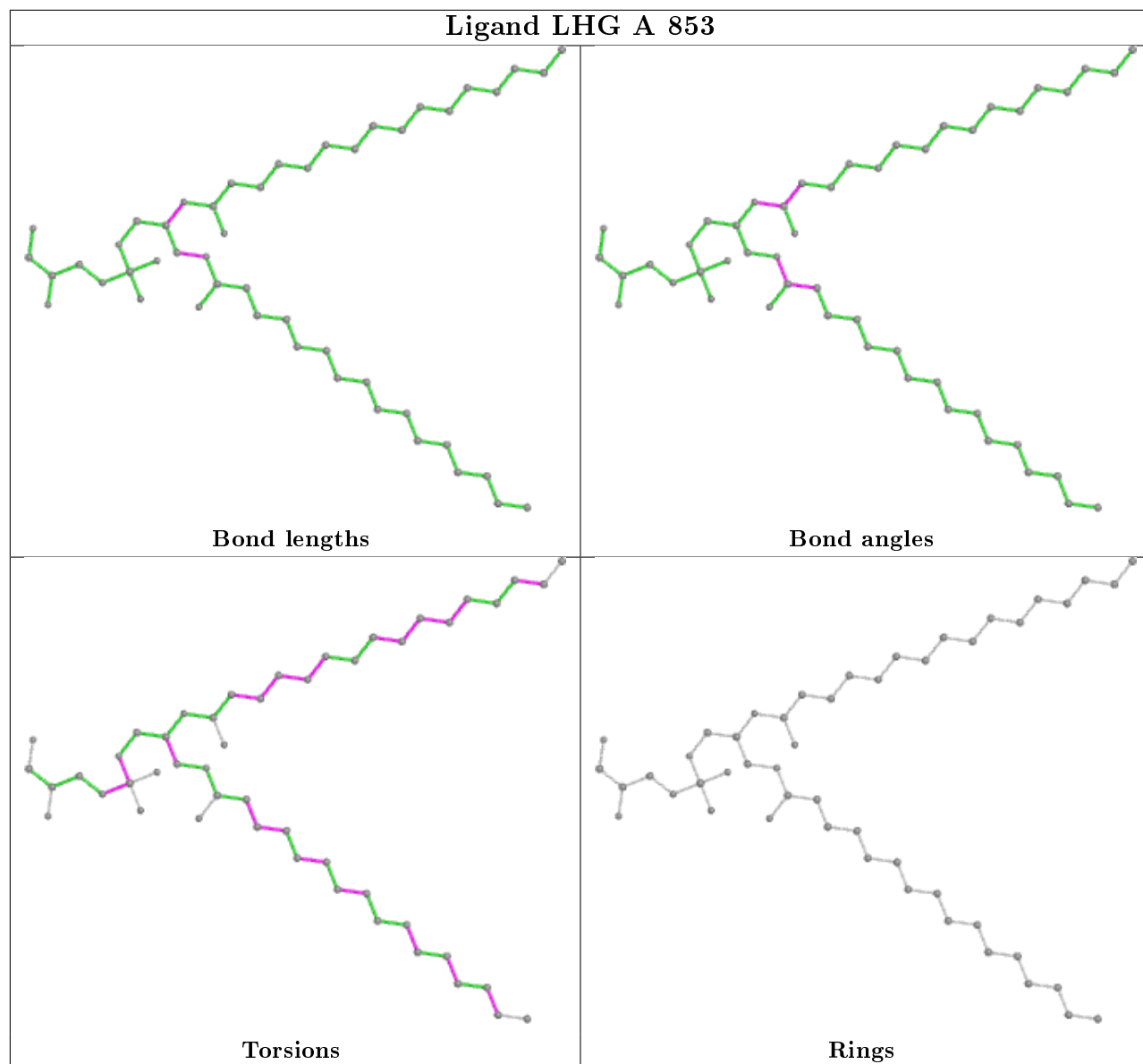


Ligand CLA A 816

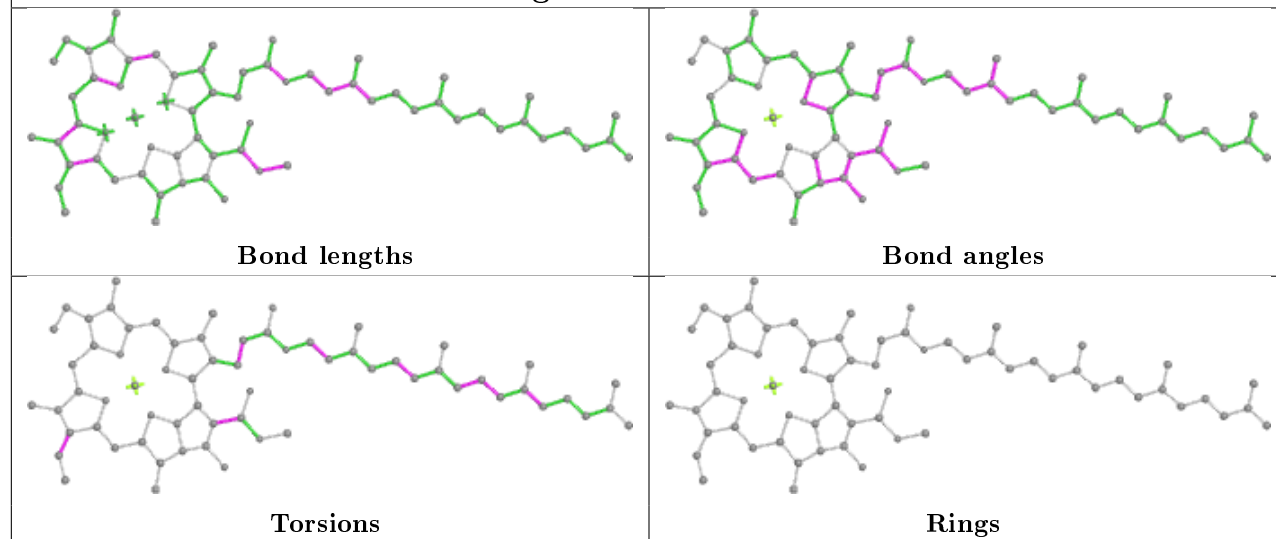


Ligand CLA B 822

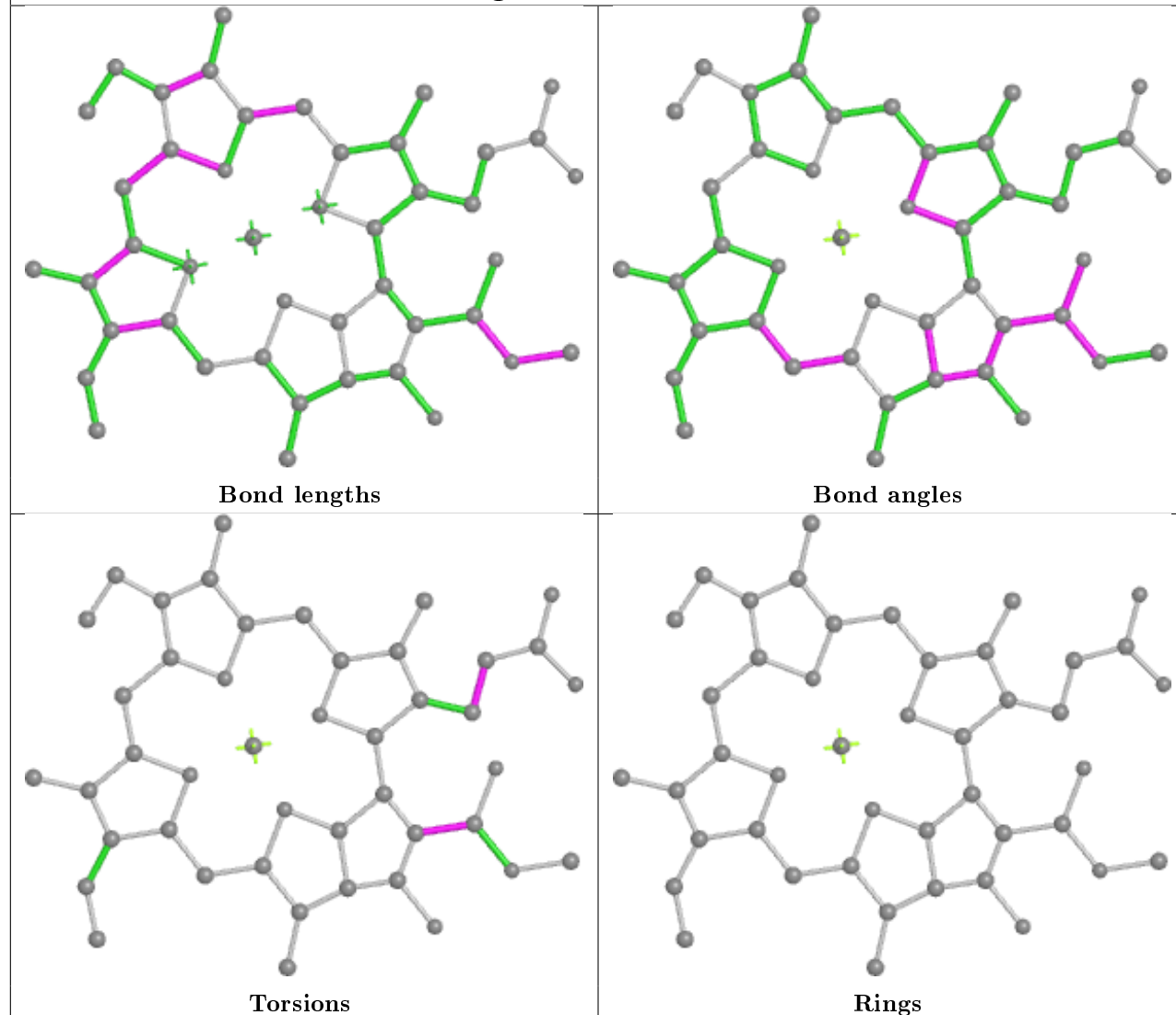


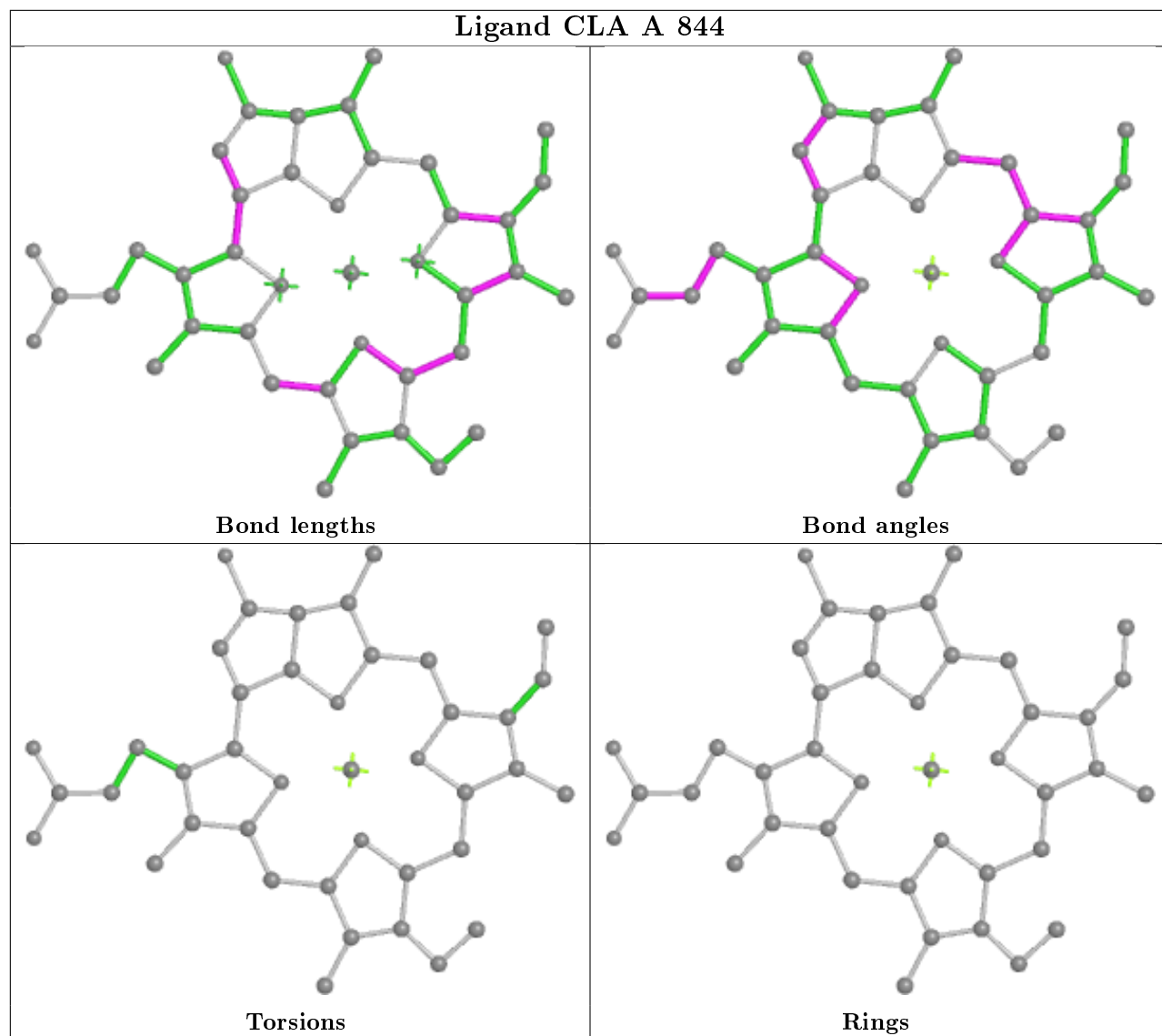


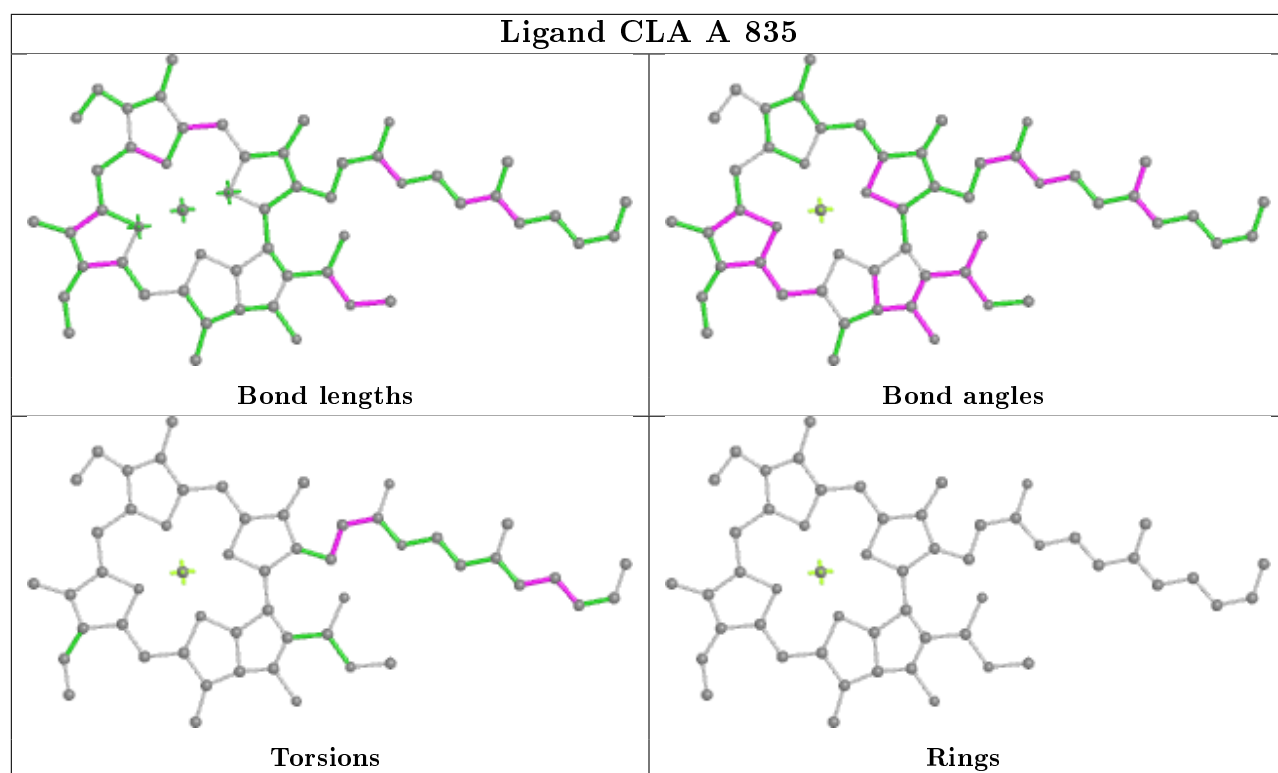
Ligand CLA B 830

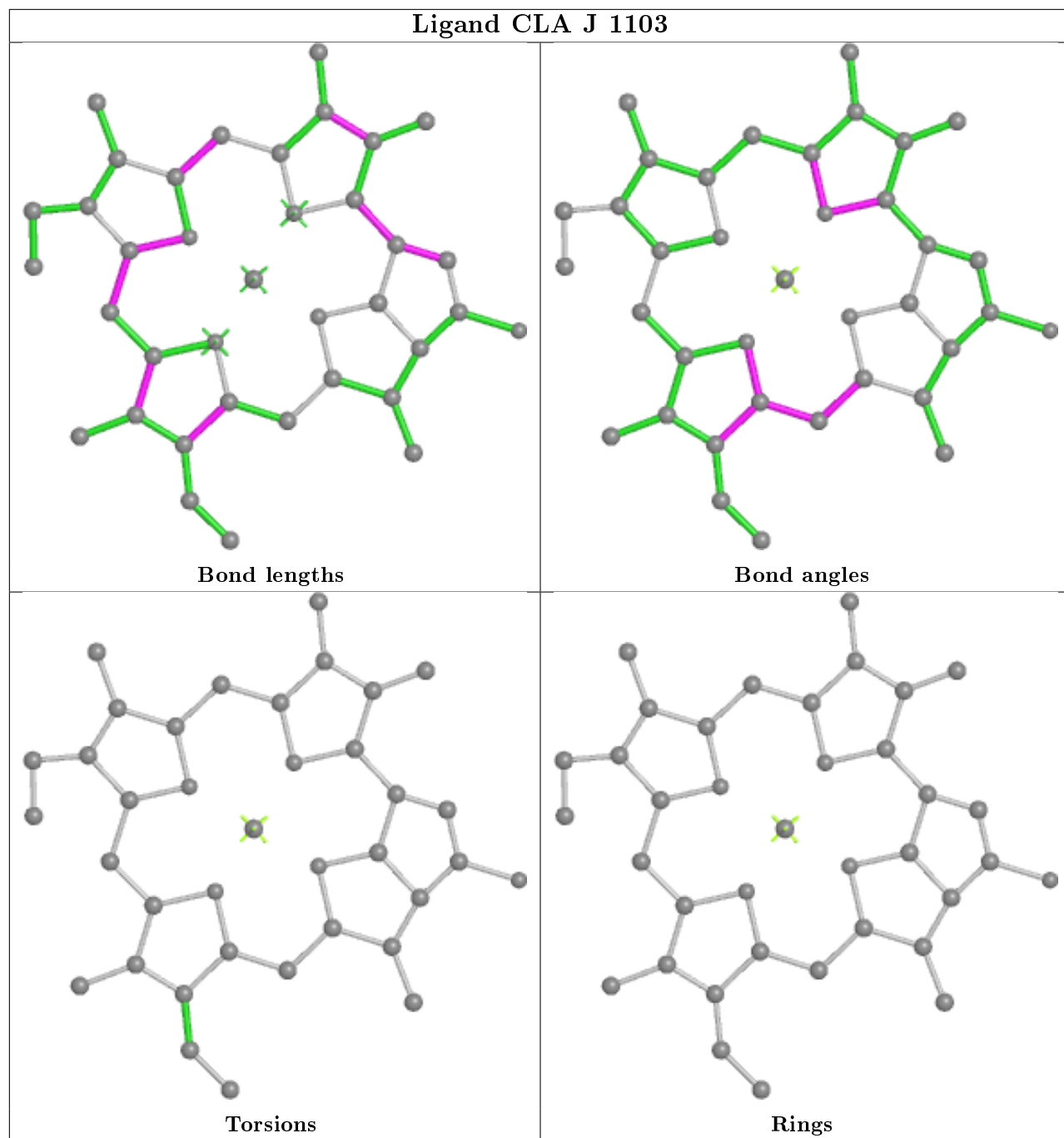


Ligand CLA B 828

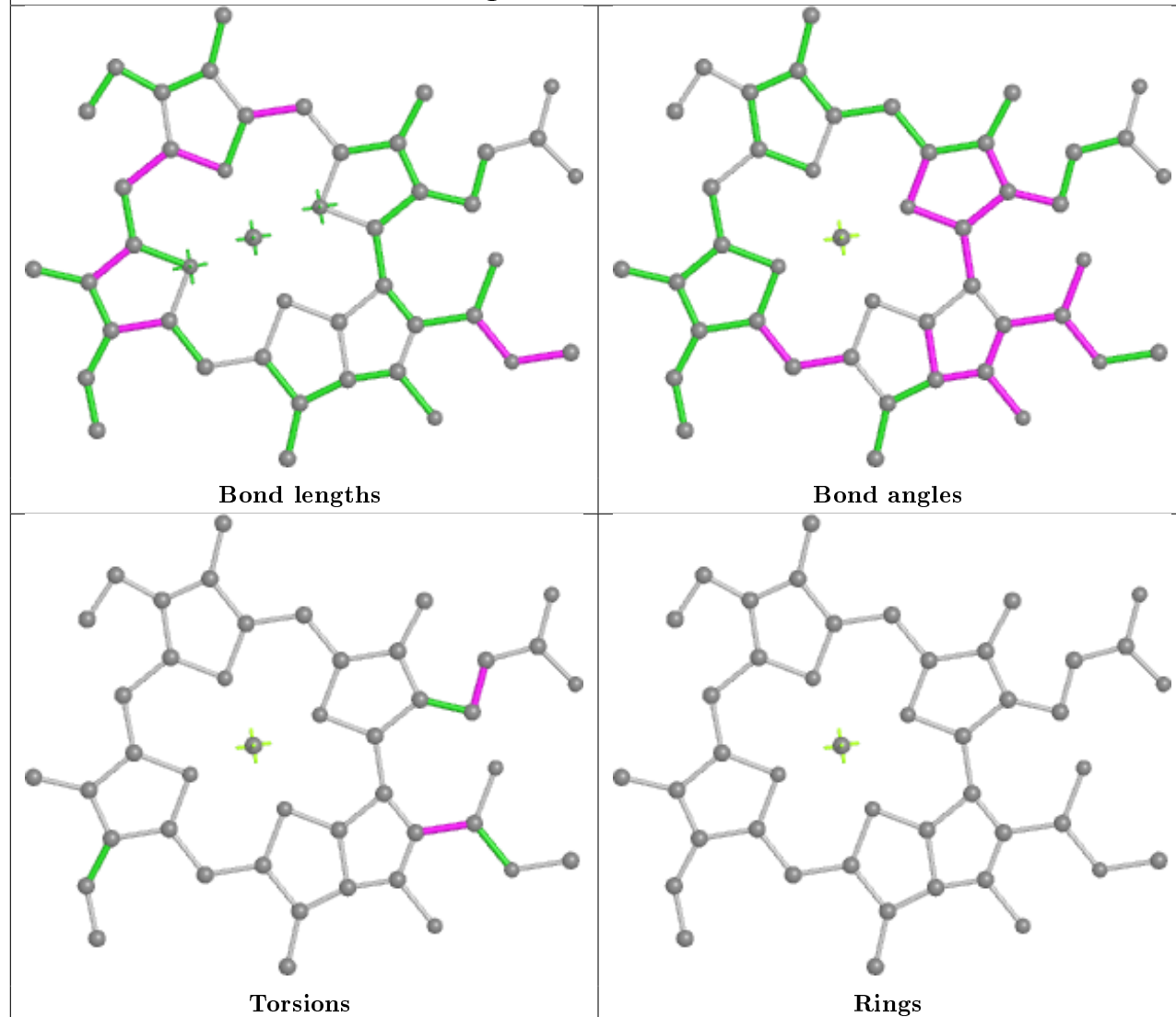




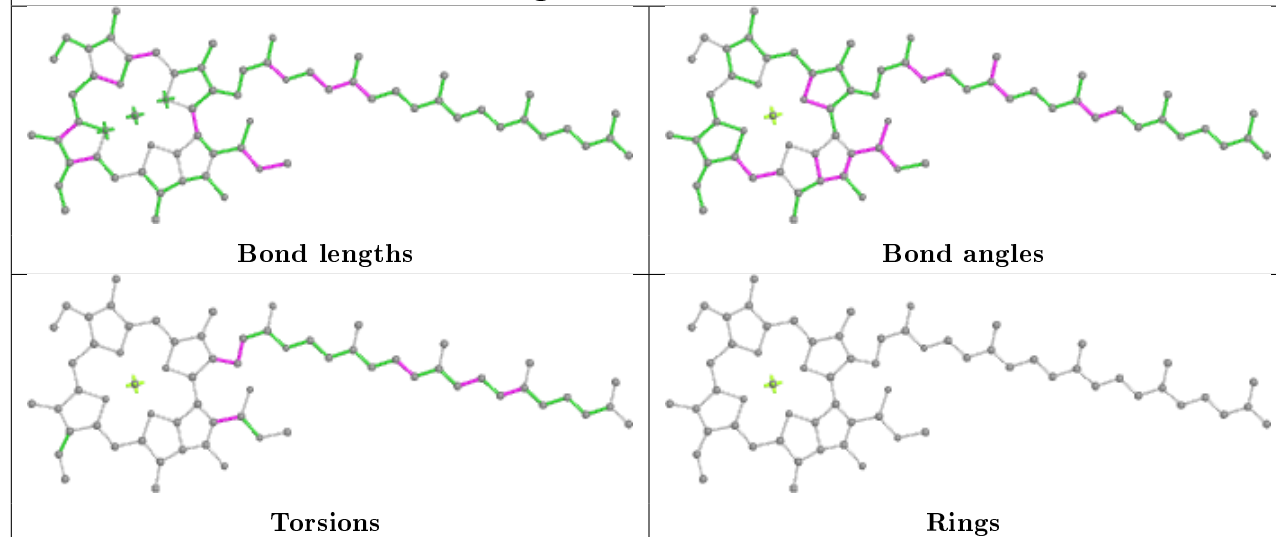


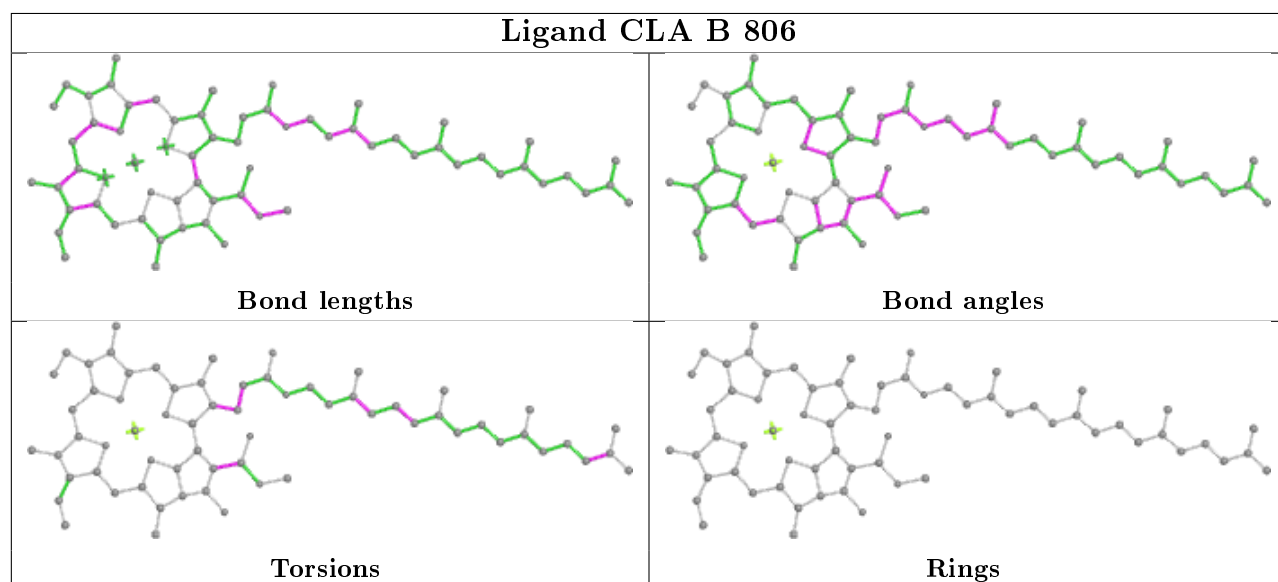
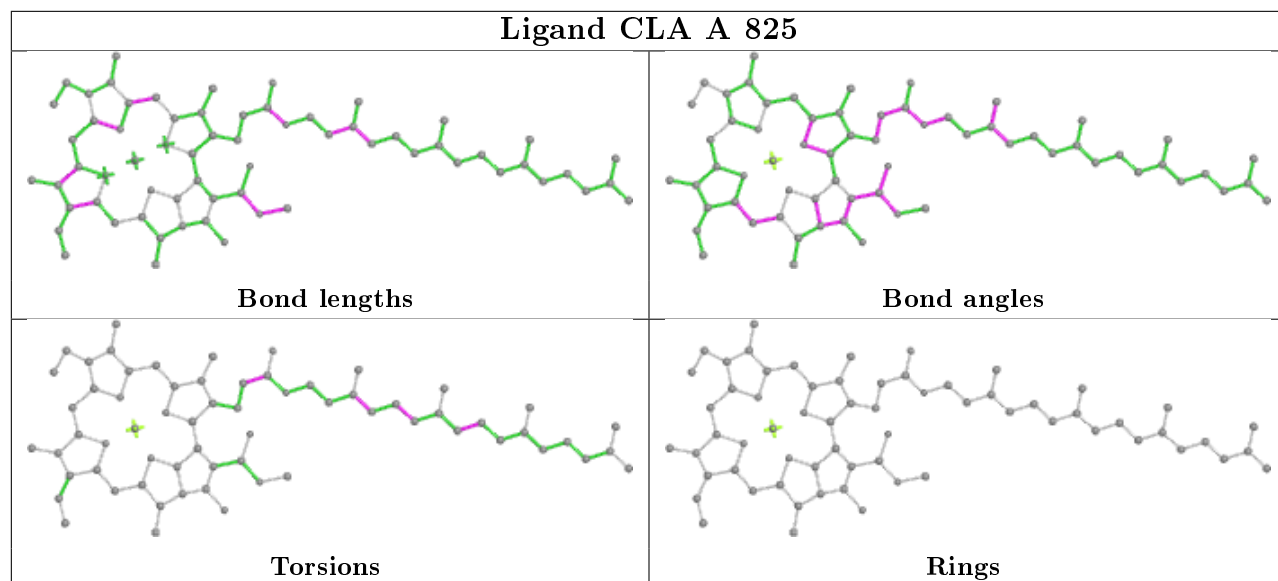
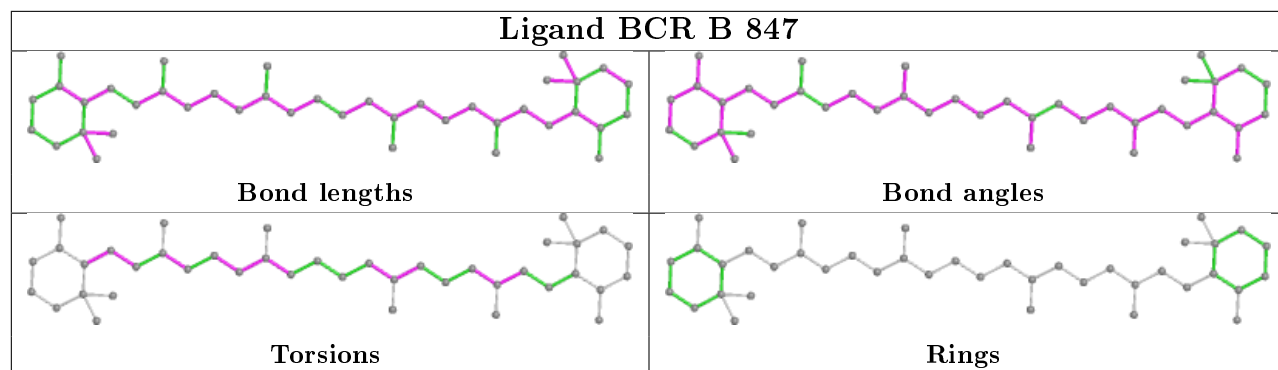


Ligand CLA F 1301

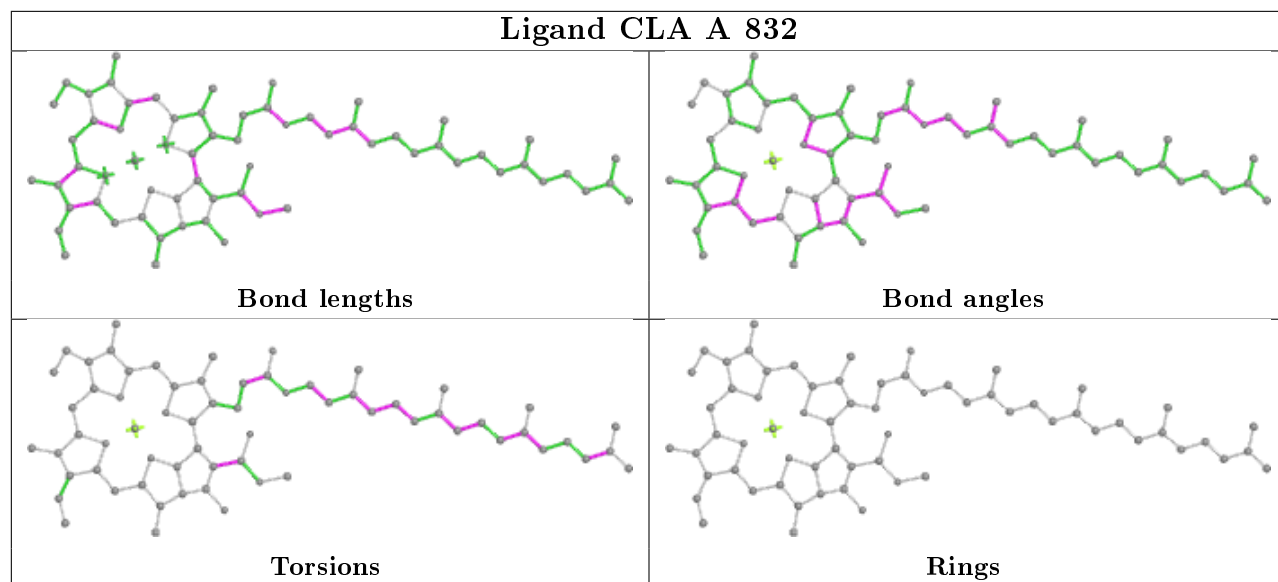


Ligand CLA B 836

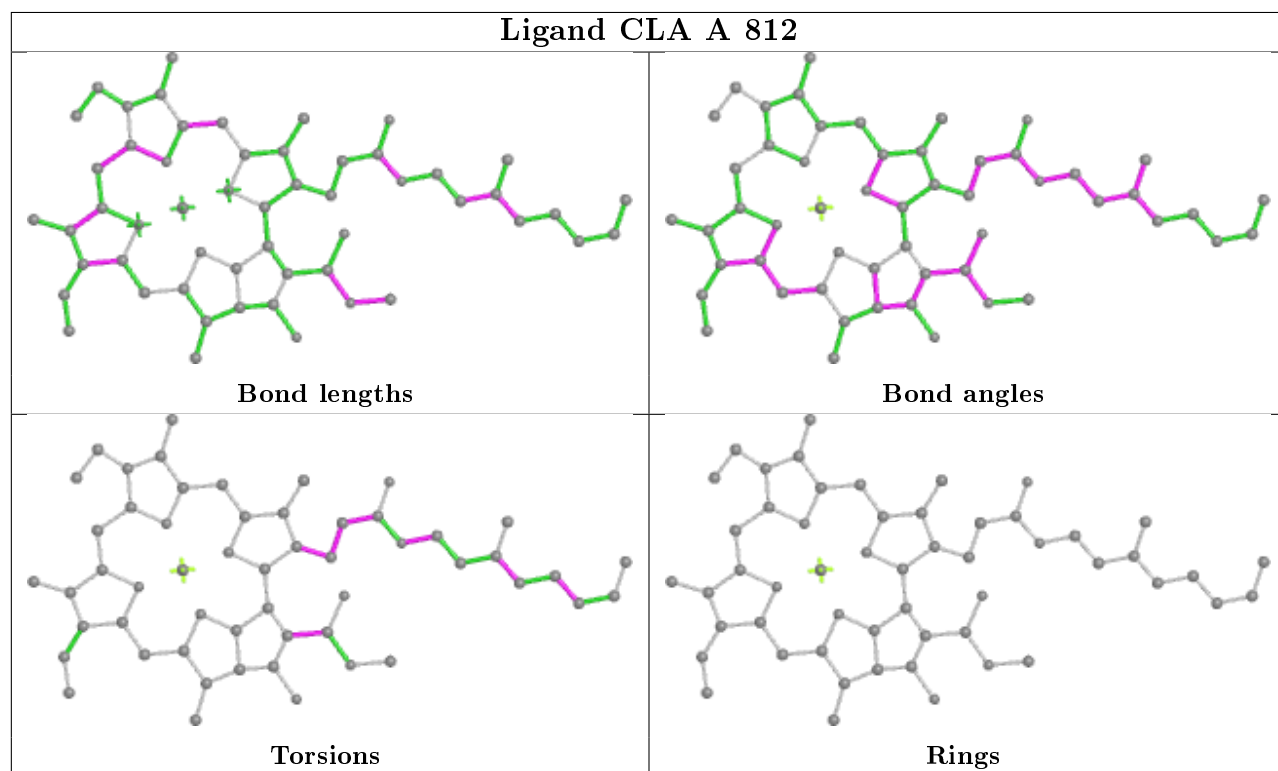


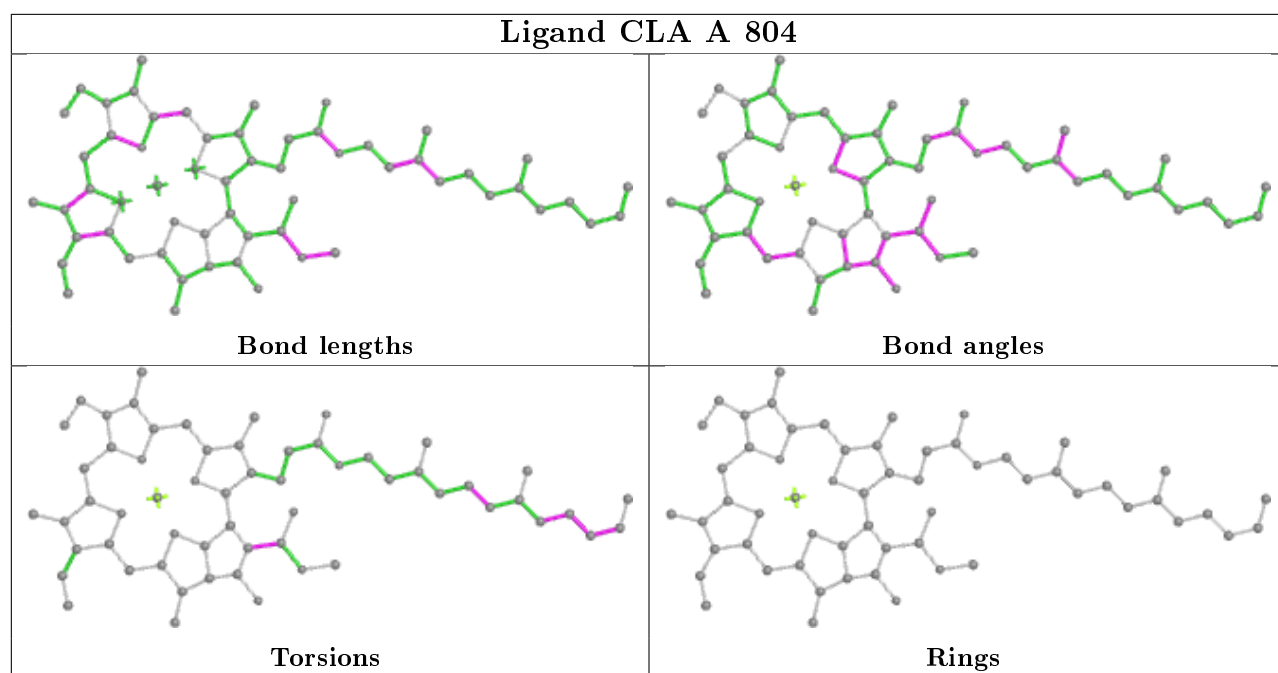


Ligand CLA A 832

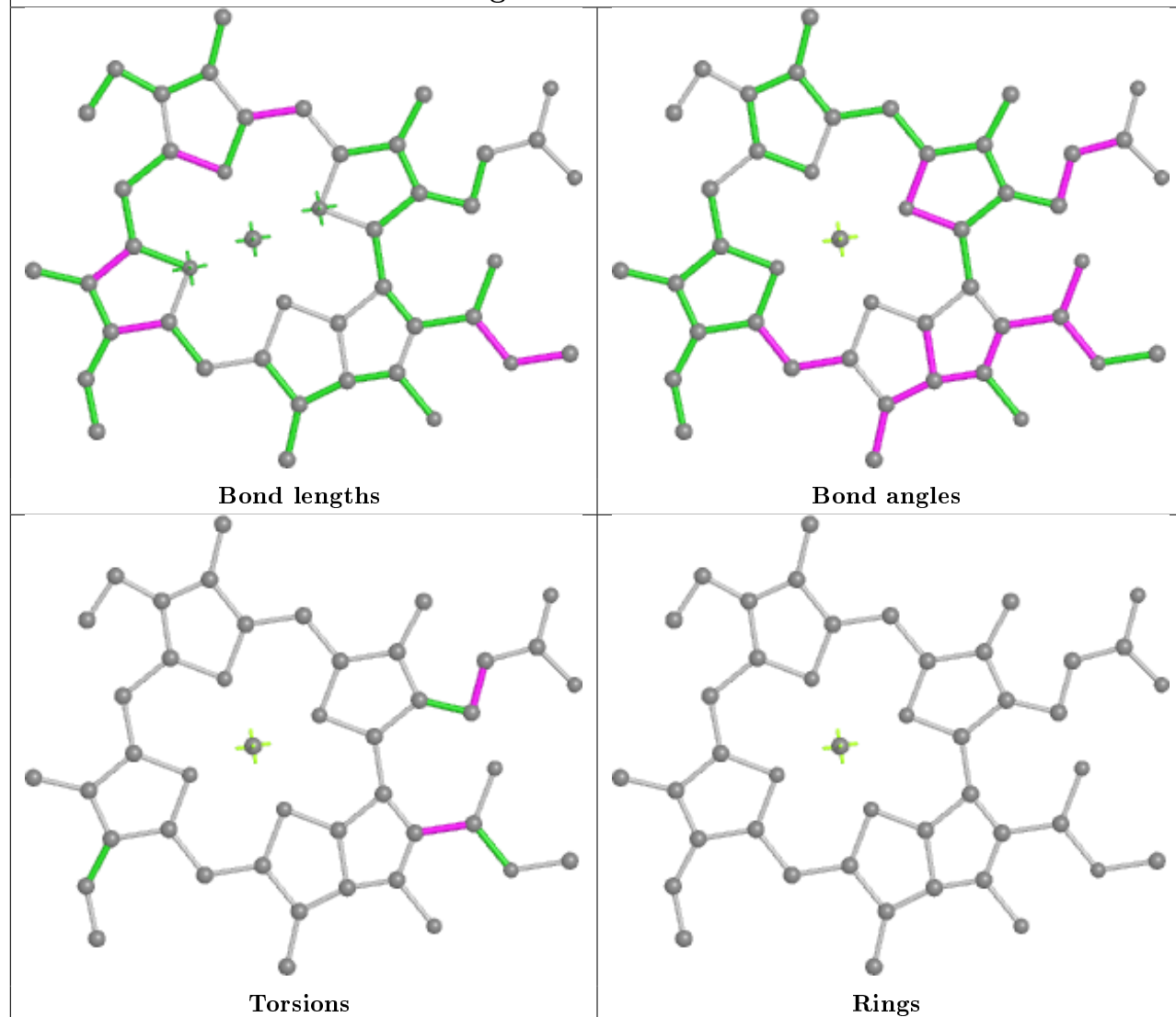


Ligand CLA A 812

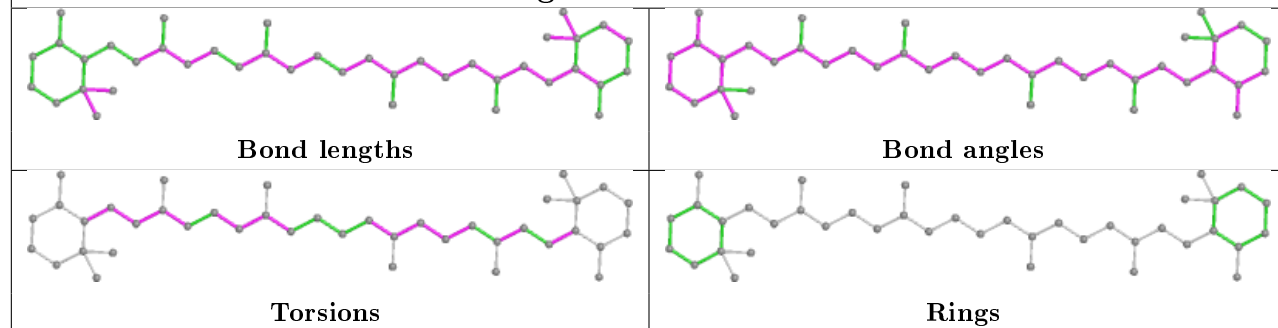


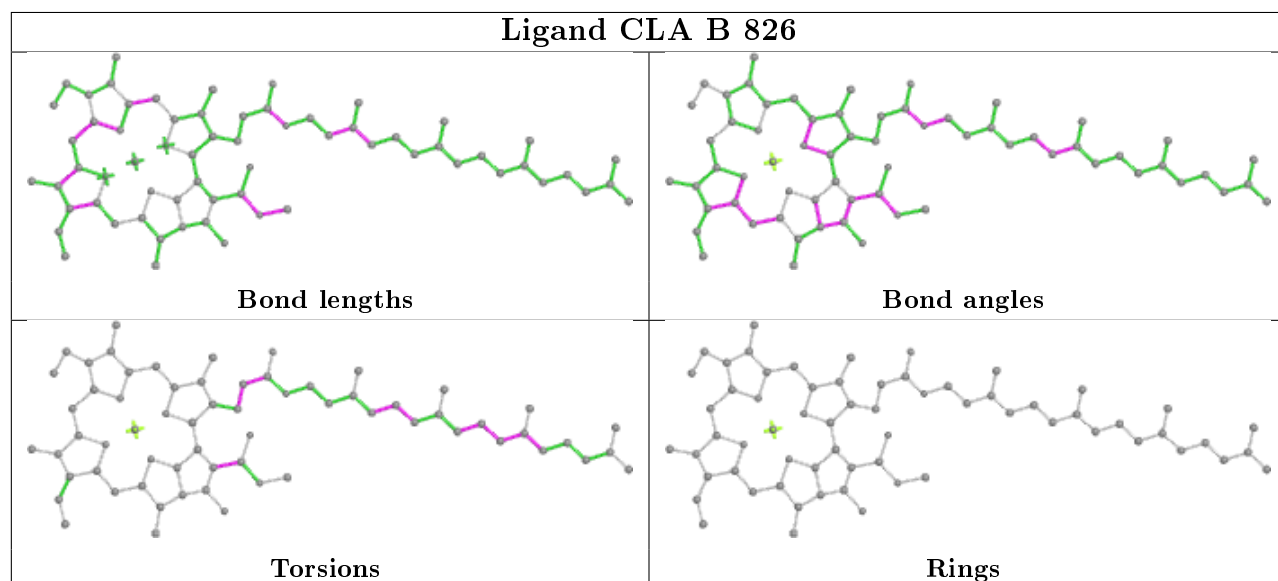
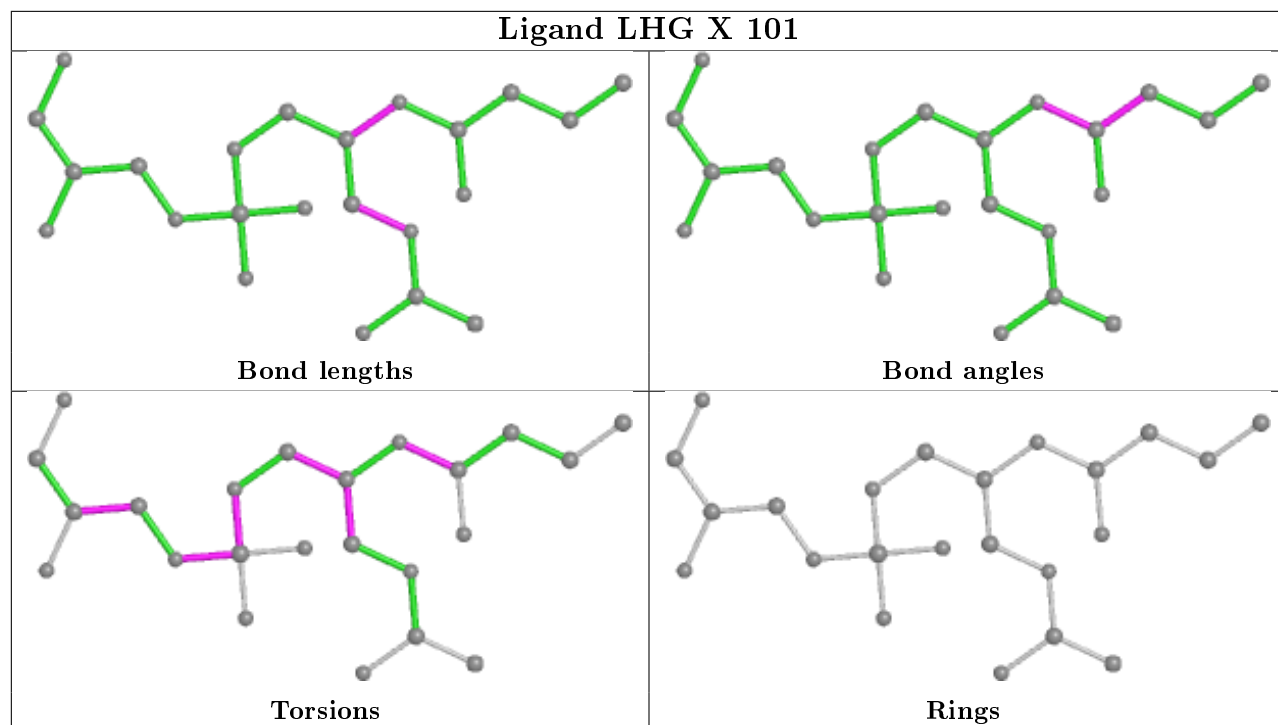


Ligand CLA A 836

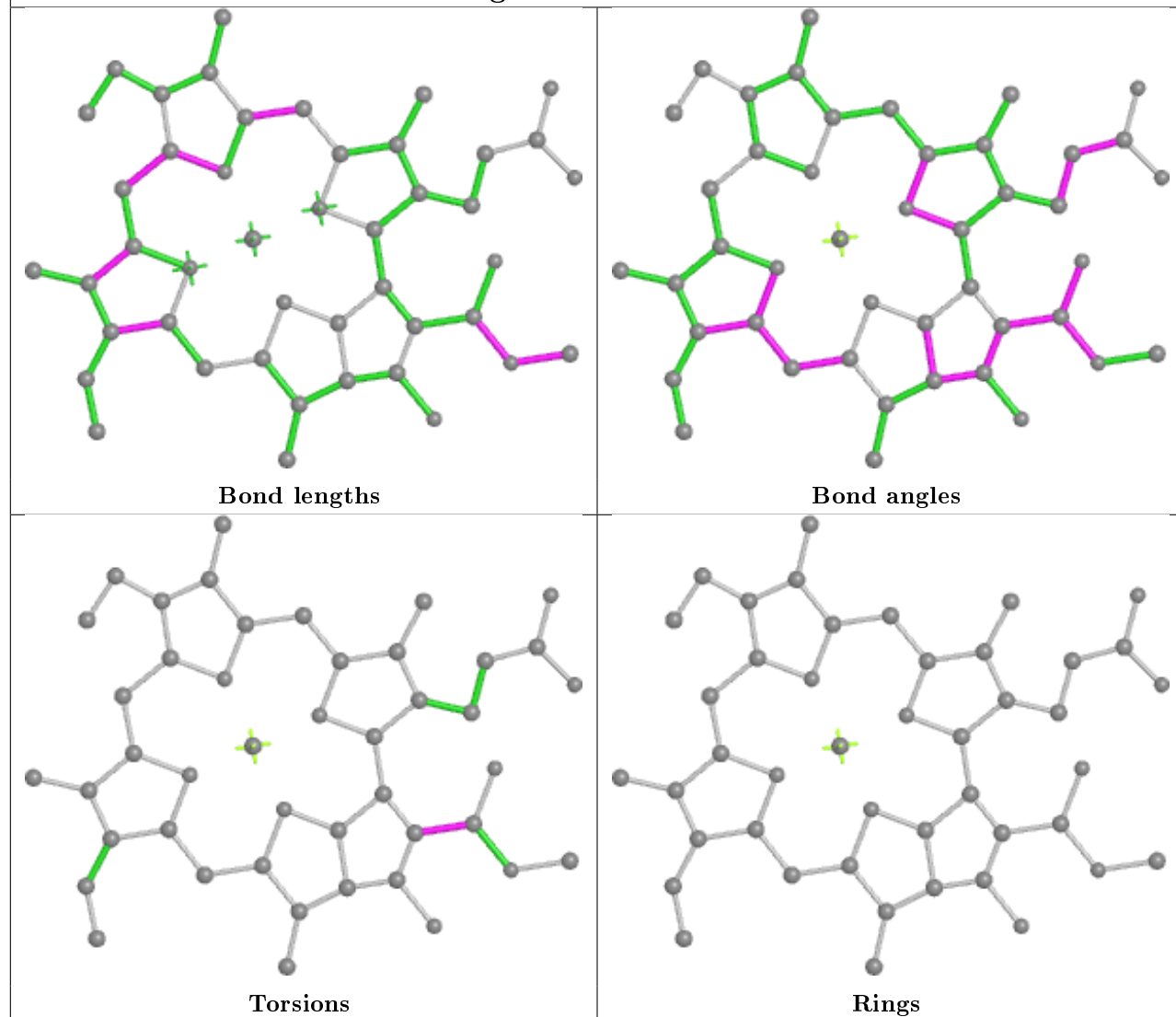


Ligand BCR I 102

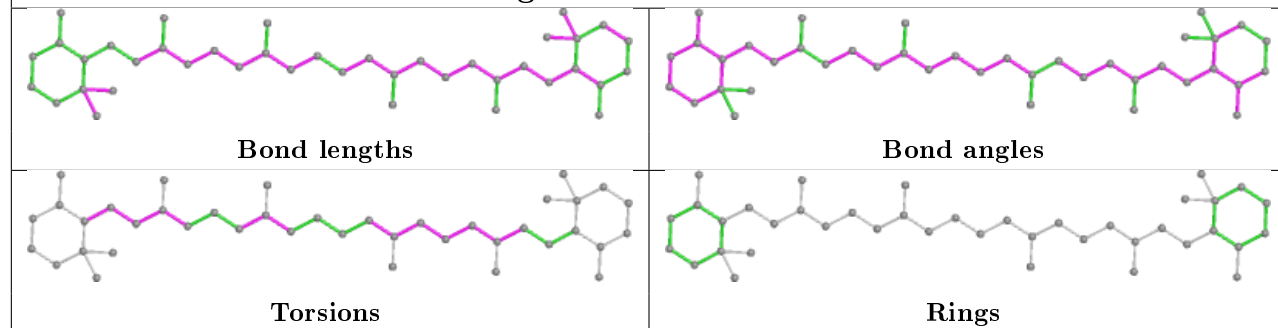




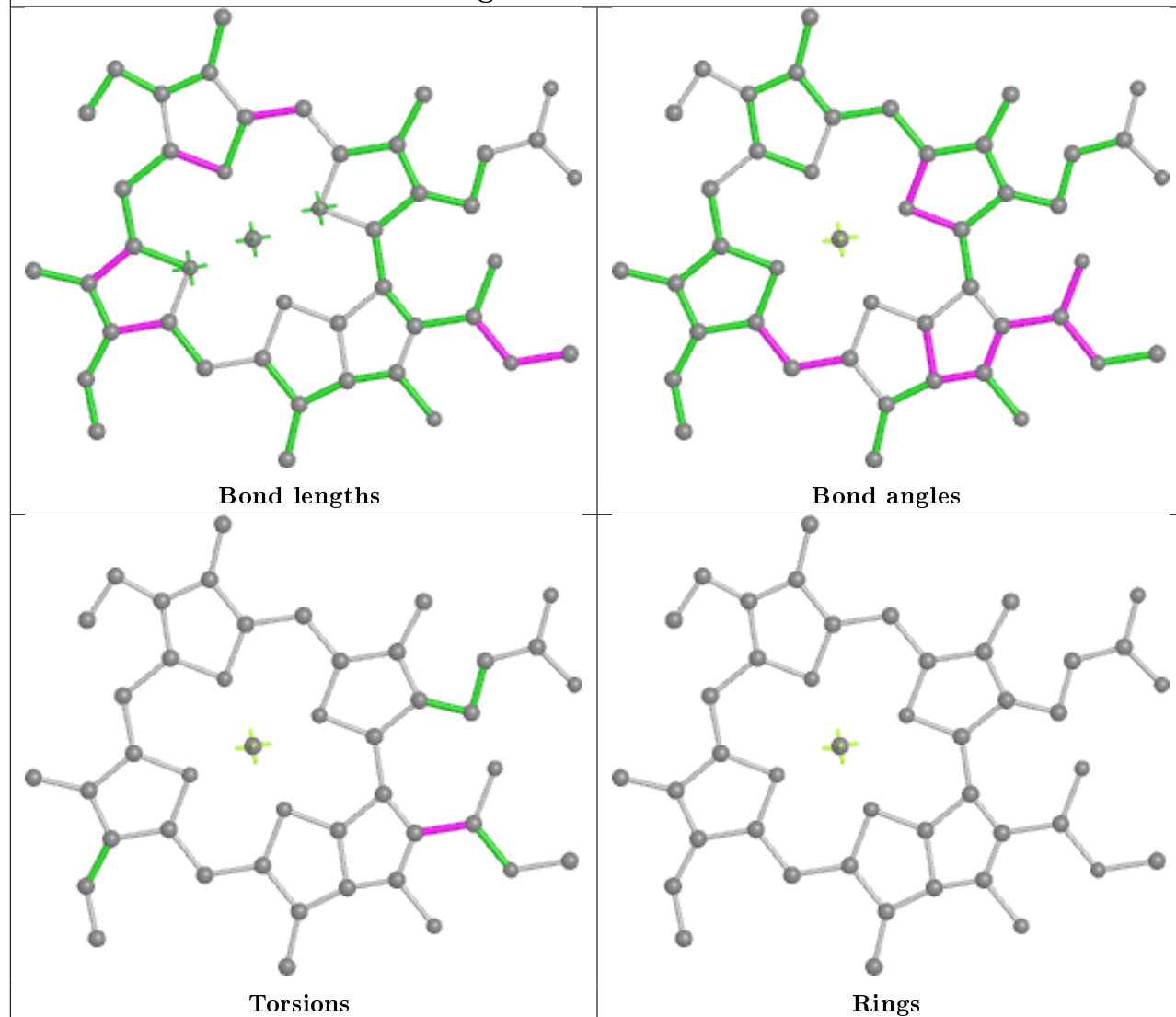
Ligand CLA A 855



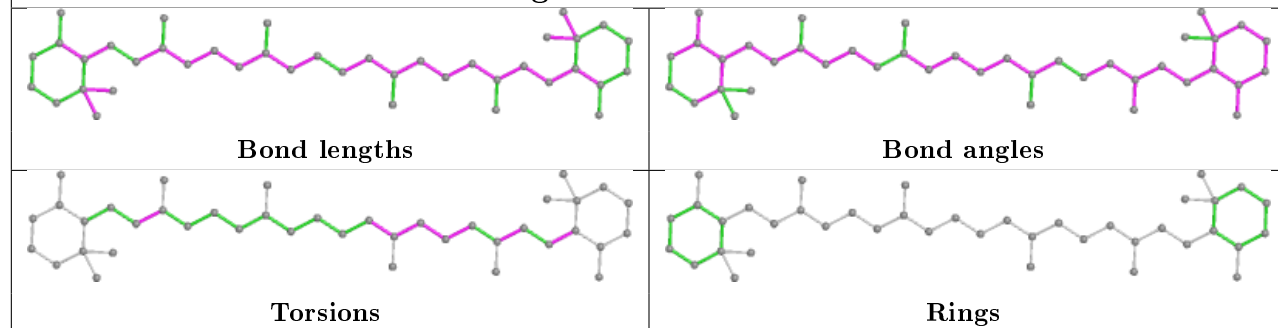
Ligand BCR M 1203

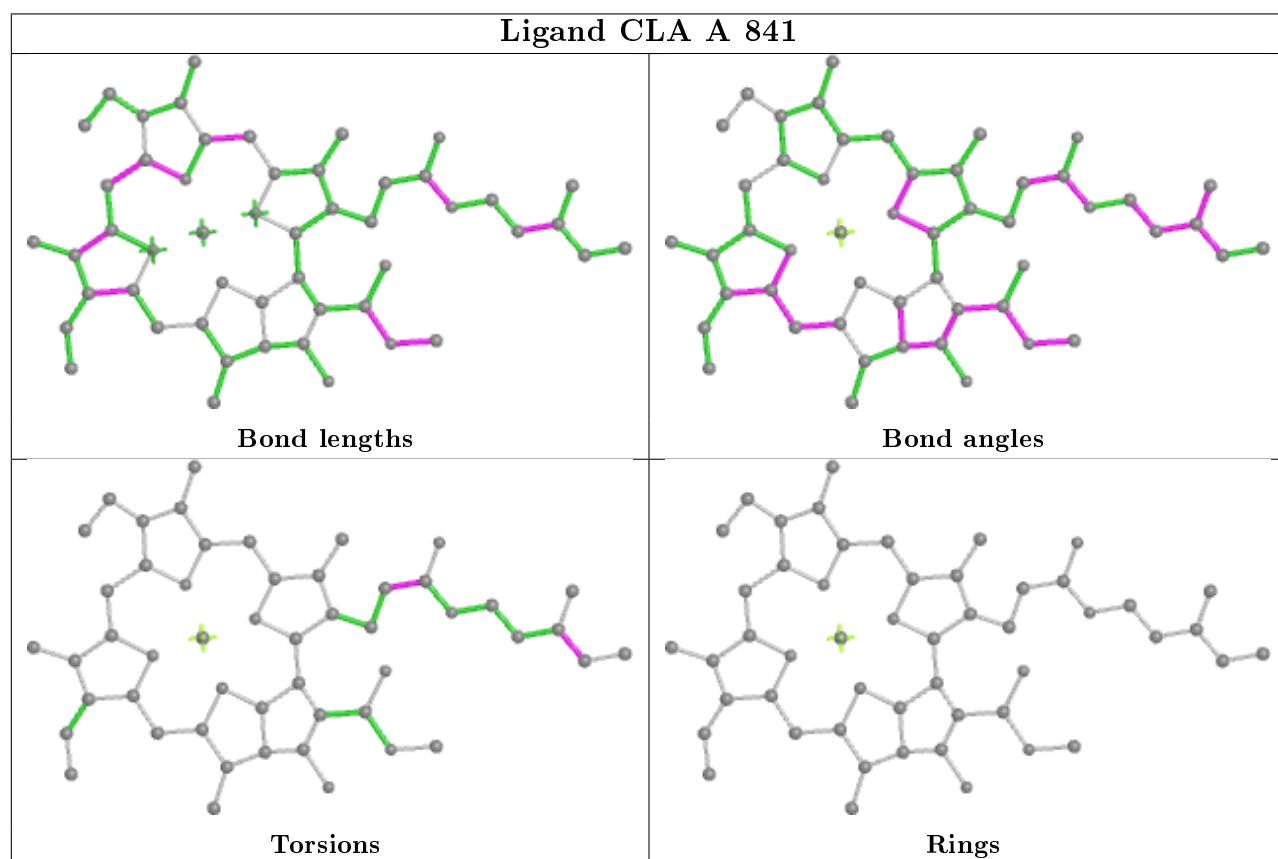
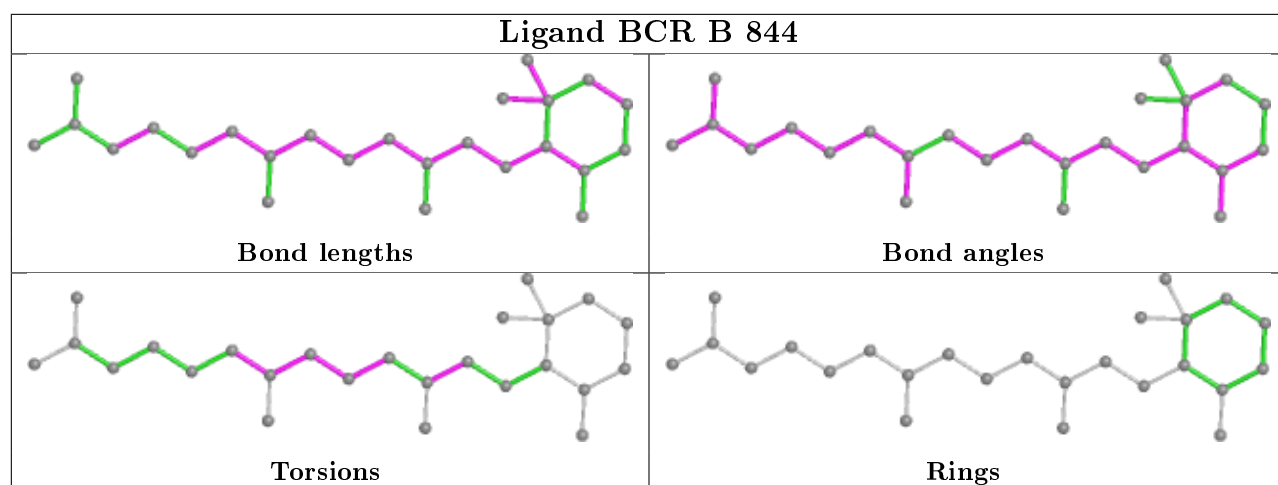


Ligand CLA M 1202

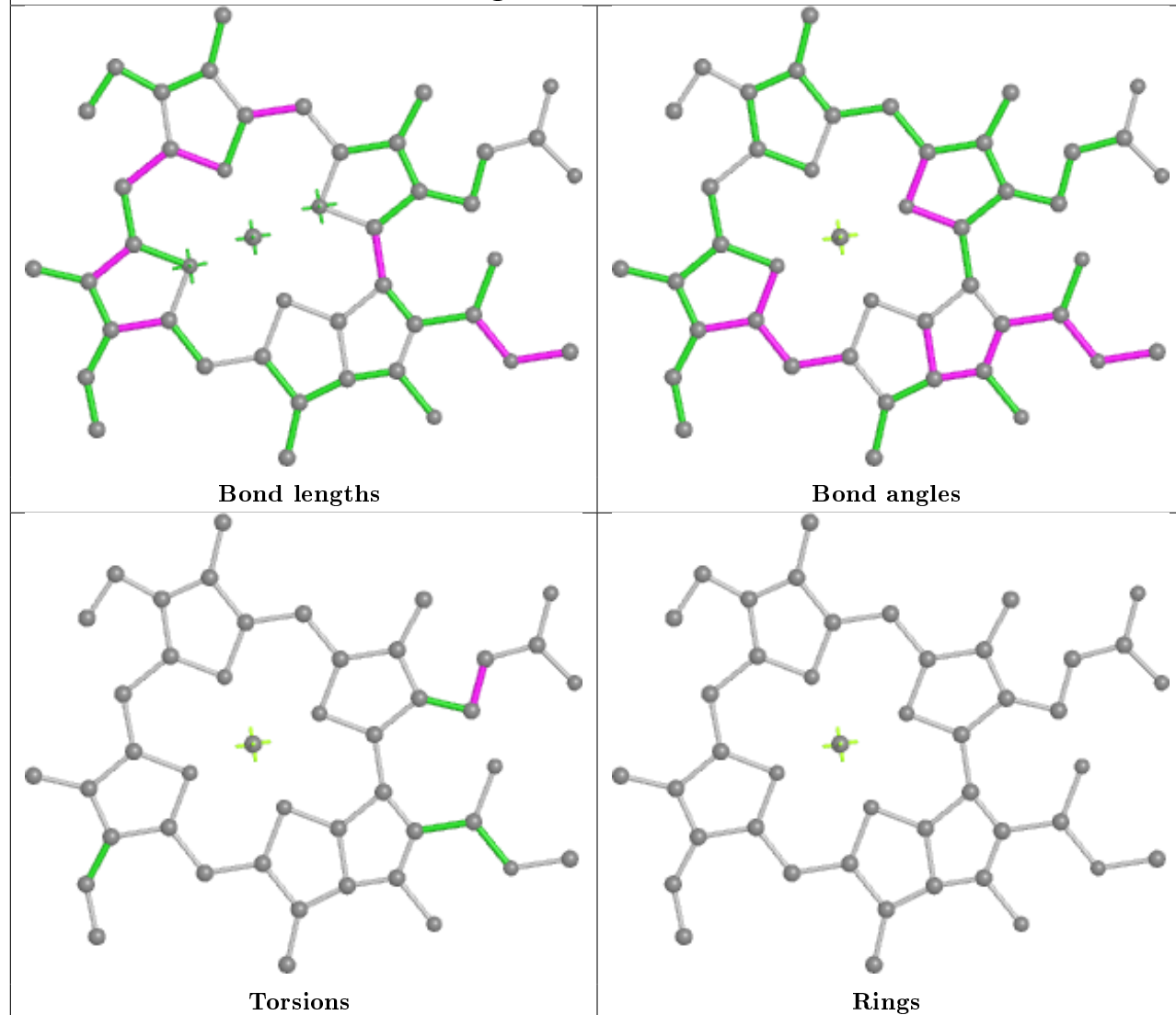


Ligand BCR B 845

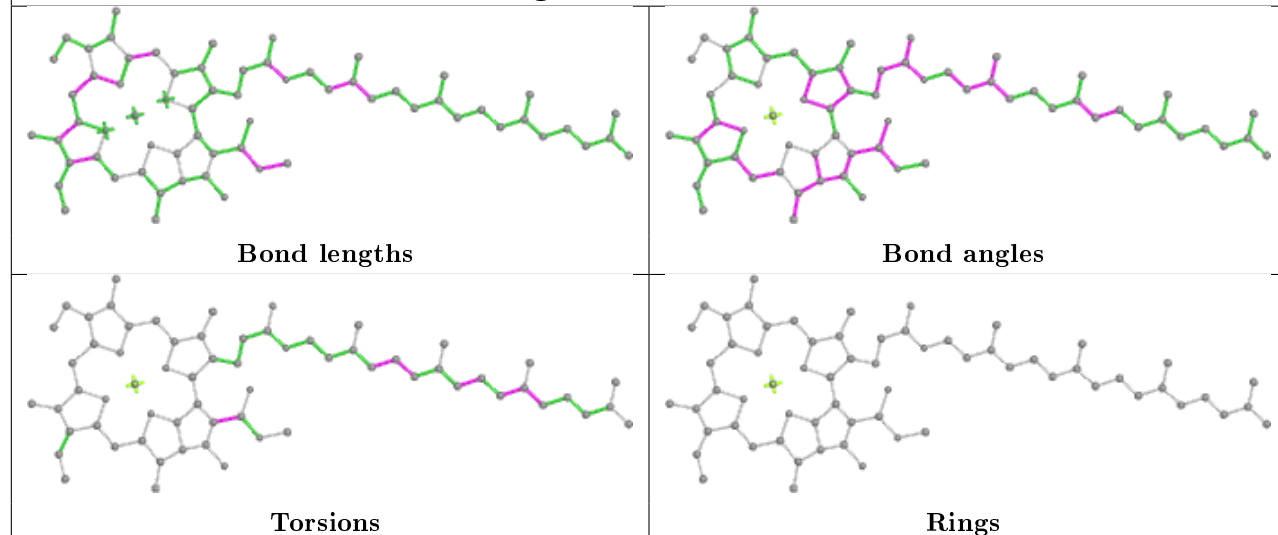




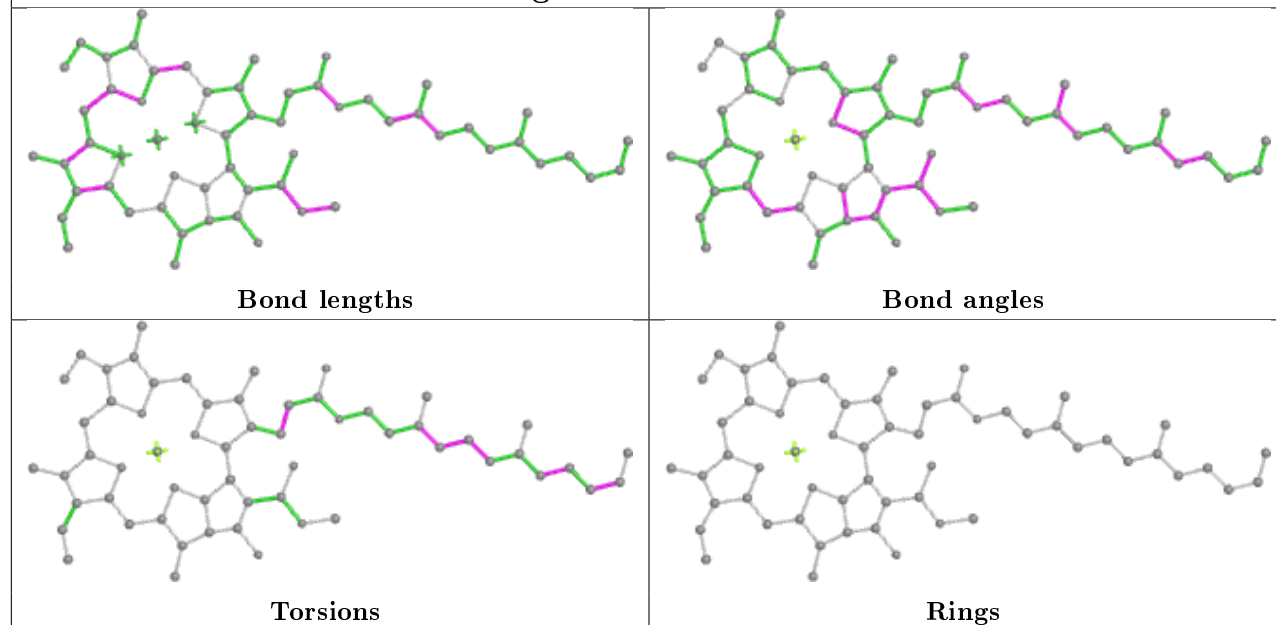
Ligand CLA B 810



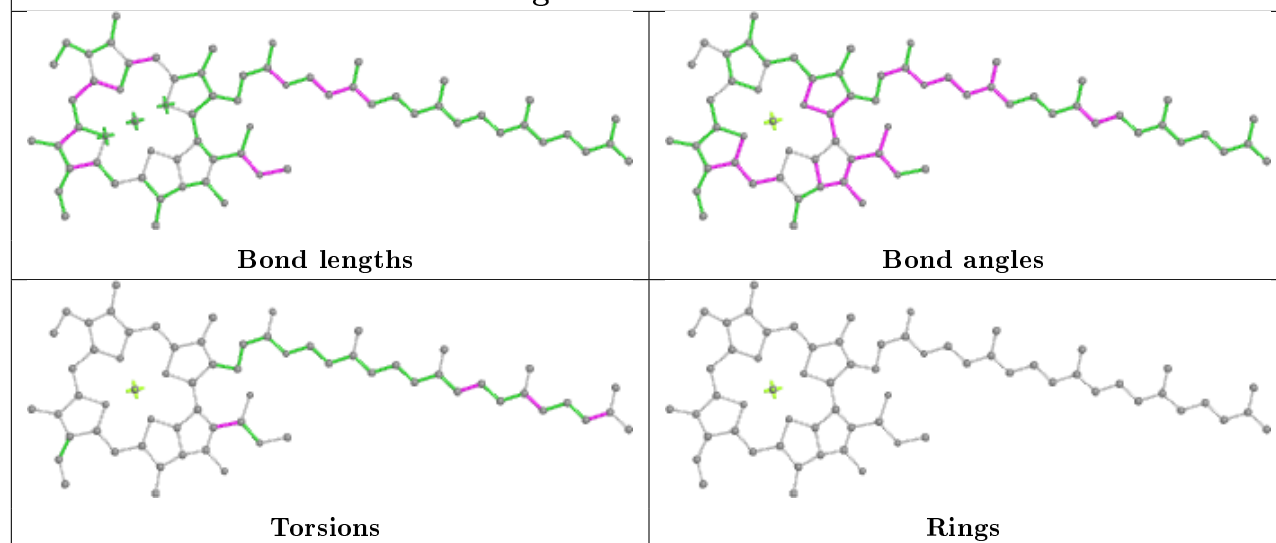
Ligand CLA A 809



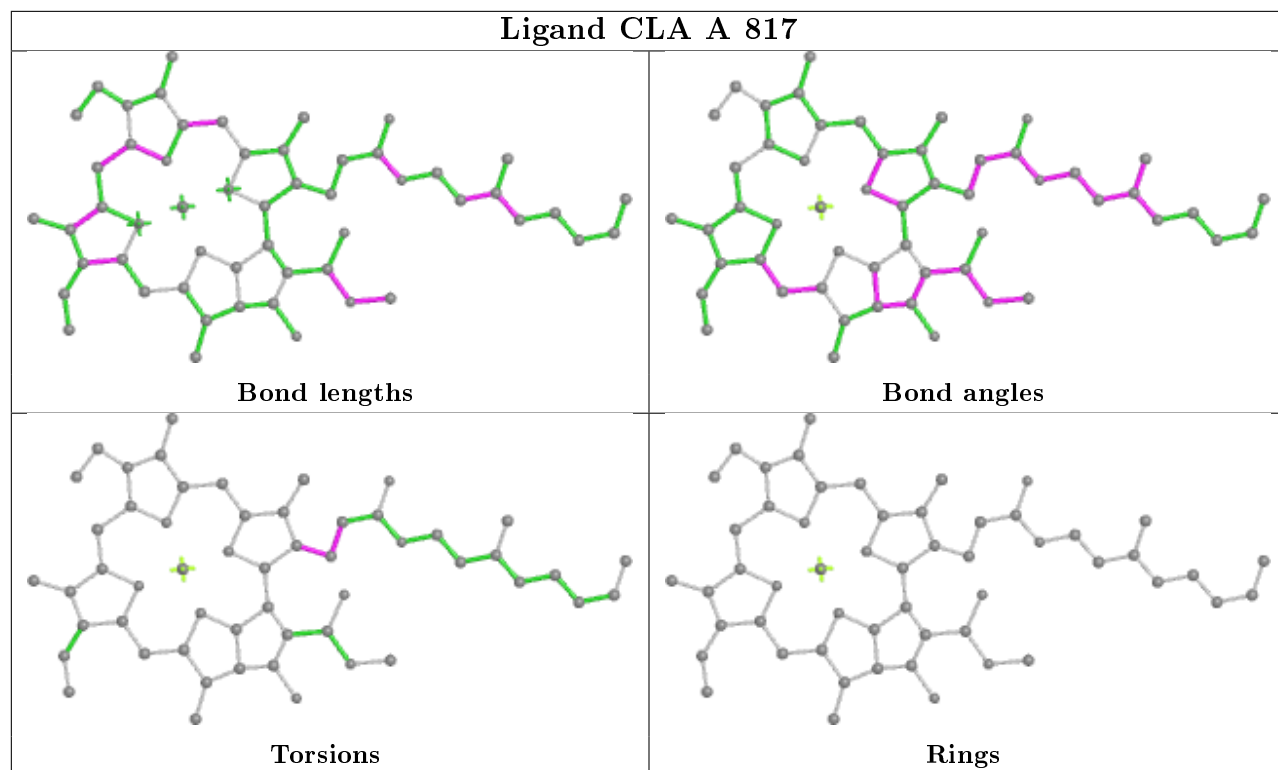
Ligand CLA B 815



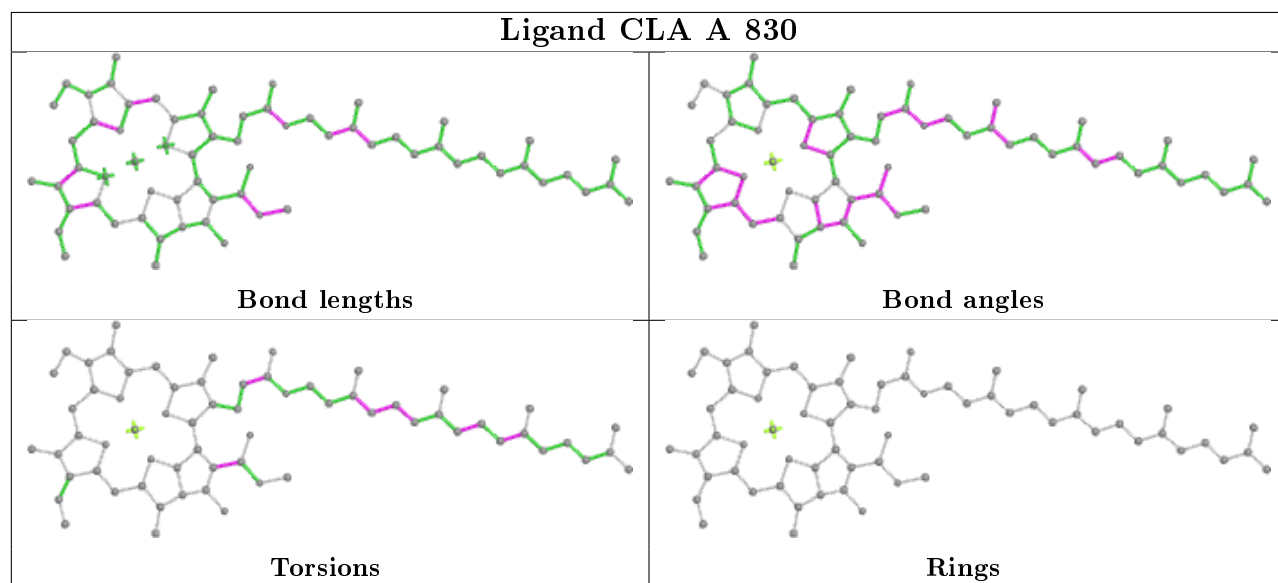
Ligand CLA A 826

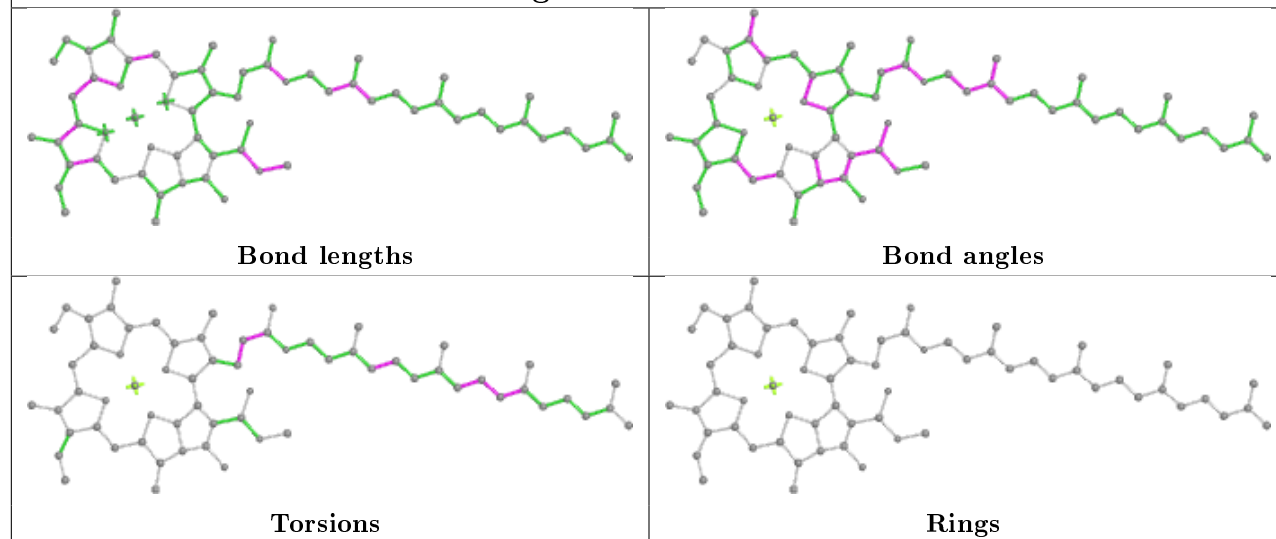
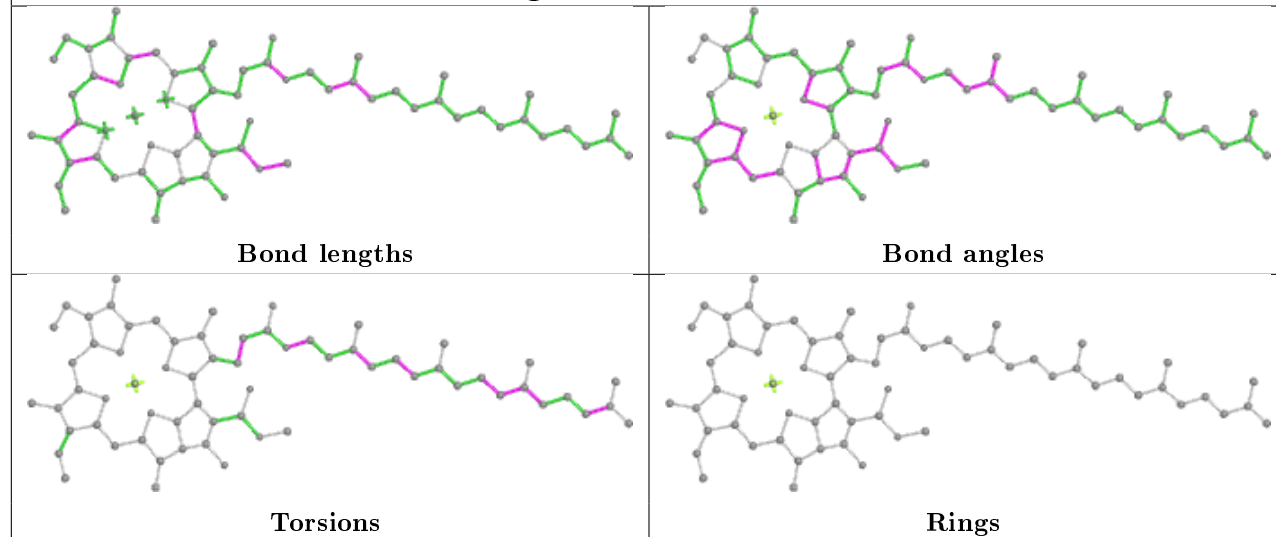


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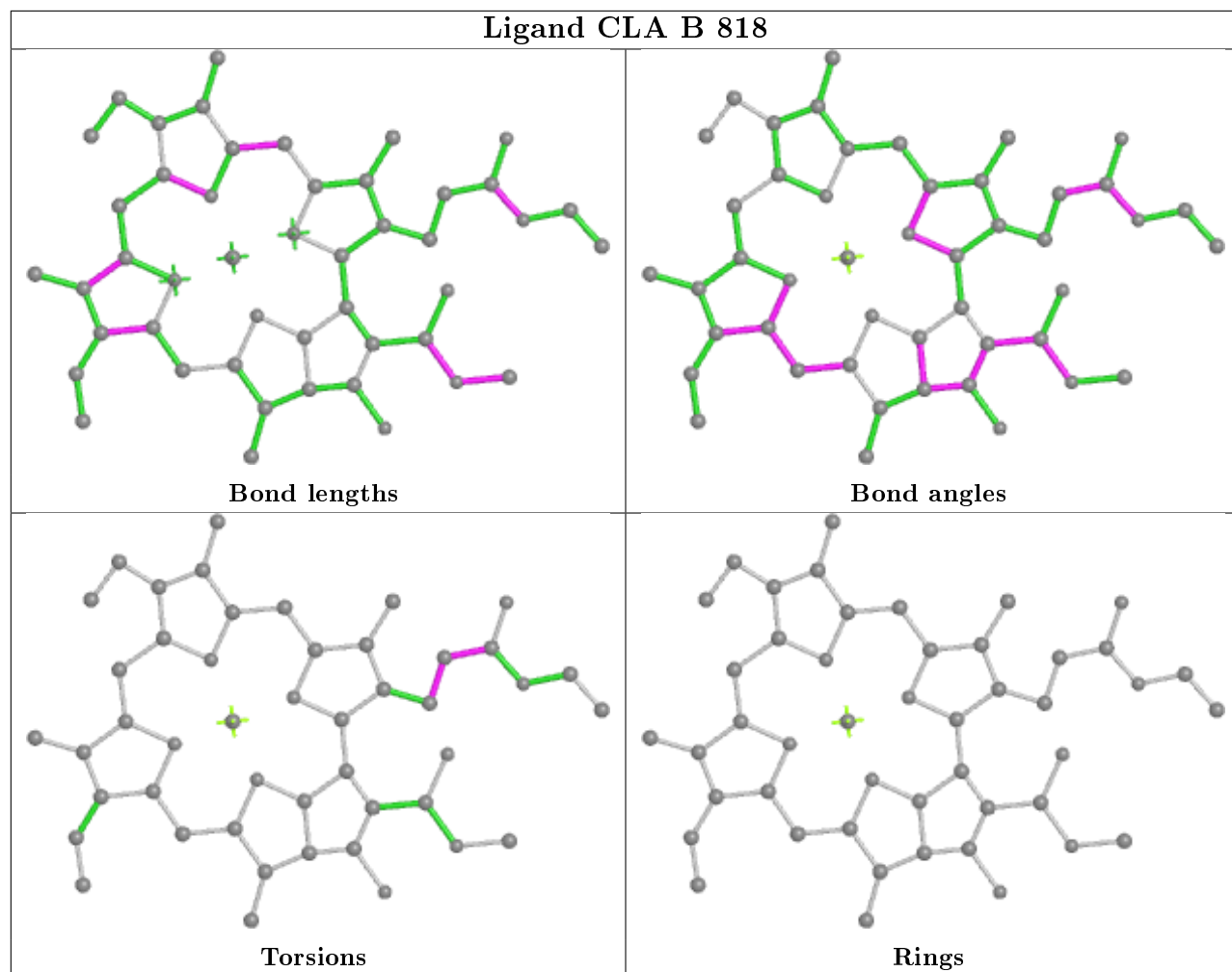


Ligand CLA A 830

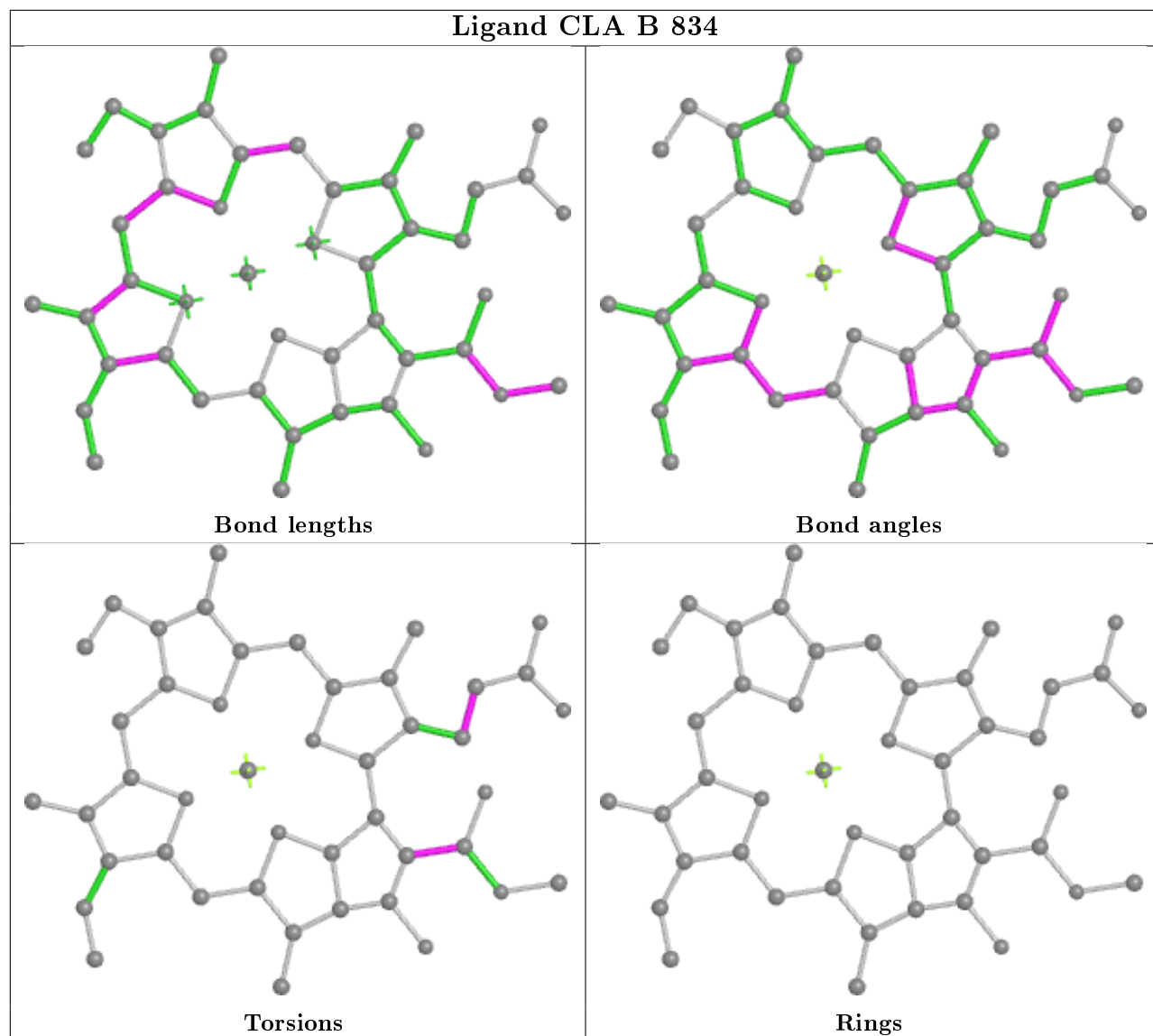


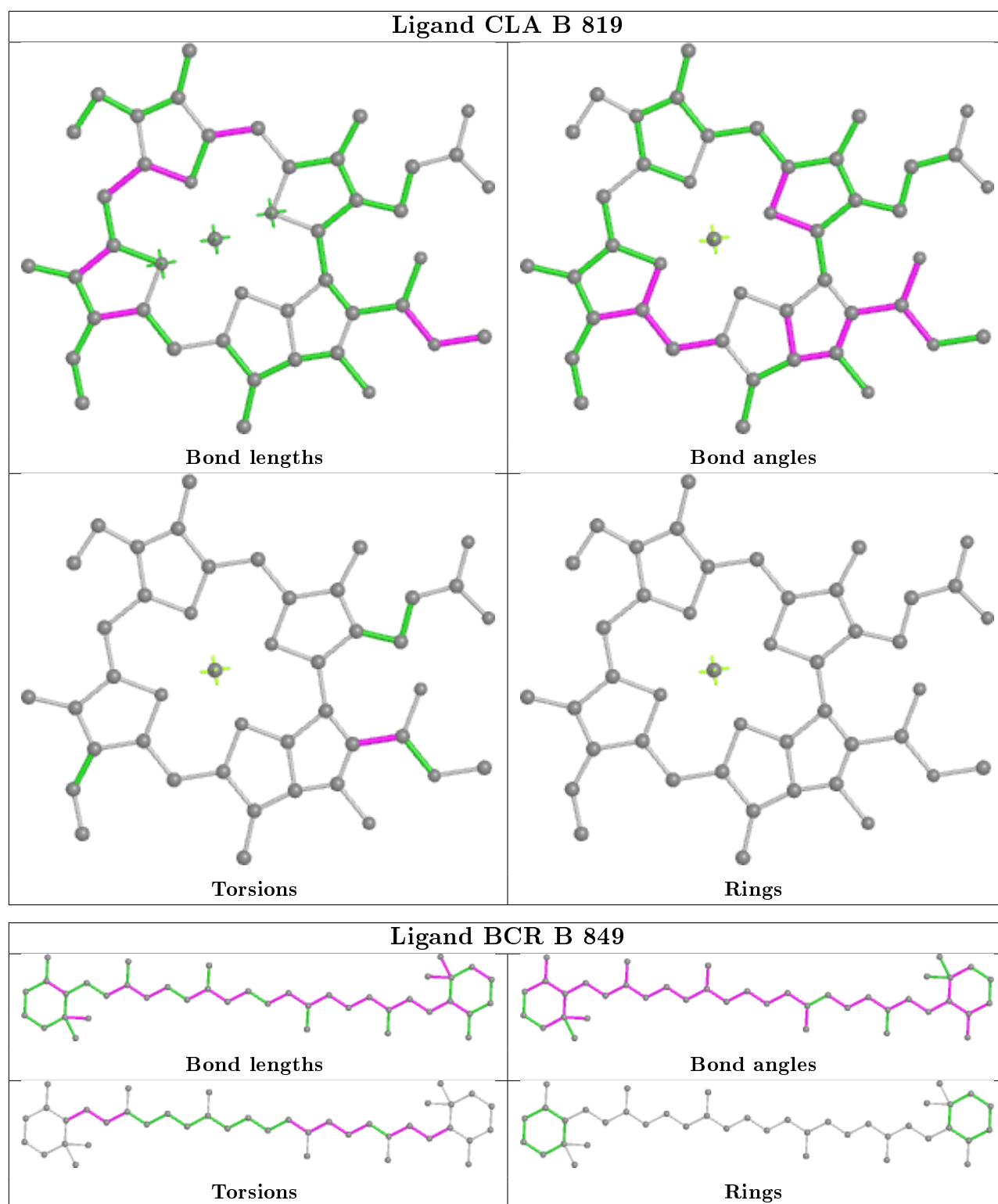
Ligand CLA B 804**Ligand CLA L 1002**

Ligand CLA B 818



Ligand CLA B 834





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	740/755 (98%)	0.11	22 (2%) 50 40	42, 99, 157, 202	0
2	B	739/740 (99%)	0.01	10 (1%) 75 65	34, 76, 126, 215	0
3	C	80/80 (100%)	-0.41	0 100 100	46, 72, 126, 138	0
4	D	138/138 (100%)	0.00	0 100 100	45, 72, 117, 137	0
5	E	69/75 (92%)	0.39	1 (1%) 75 65	77, 100, 148, 194	0
6	F	141/164 (85%)	-0.23	1 (0%) 87 82	54, 83, 136, 158	0
7	I	38/38 (100%)	0.14	0 100 100	10, 36, 74, 78	0
8	J	41/41 (100%)	-0.62	0 100 100	65, 89, 136, 165	0
9	K	46/83 (55%)	-0.41	0 100 100	55, 87, 141, 169	0
10	L	151/154 (98%)	-0.18	1 (0%) 87 82	14, 49, 104, 140	0
11	M	31/31 (100%)	-0.03	0 100 100	31, 51, 80, 92	0
12	X	29/35 (82%)	-0.27	1 (3%) 45 37	59, 80, 120, 155	0
All	All	2243/2334 (96%)	-0.01	36 (1%) 72 62	10, 81, 141, 215	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	19	ASP	4.2
1	A	24	SER	3.5
10	L	146	ASP	3.4
1	A	18	ASN	3.3
2	B	497	ASN	3.3

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
13	CLA	A	844	41/65	0.67	0.40	116,136,148,281	0
13	CLA	A	815	45/65	0.73	0.64	111,150,177,185	0
15	BCR	A	847	40/40	0.73	0.82	98,140,151,162	0
13	CLA	M	1202	45/65	0.73	0.73	51,149,183,198	0
15	BCR	A	848	40/40	0.74	0.95	112,132,147,157	0
15	BCR	A	849	40/40	0.75	1.28	95,136,179,183	0
13	CLA	A	816	49/65	0.76	0.85	119,163,187,193	0
13	CLA	A	812	54/65	0.77	0.63	136,181,240,396	0
15	BCR	B	841	40/40	0.77	0.84	65,105,151,155	0
13	CLA	J	1102	45/65	0.78	0.38	75,111,128,280	0
13	CLA	A	836	45/65	0.79	0.47	63,96,163,234	0
13	CLA	A	810	45/65	0.79	0.50	109,136,151,223	0
16	LHG	X	101	23/49	0.80	0.40	78,81,207,208	0
15	BCR	B	850	40/40	0.80	0.42	83,107,144,146	0
13	CLA	A	827	65/65	0.81	0.72	68,103,137,248	0
15	BCR	A	850	40/40	0.81	0.90	56,96,126,139	0
13	CLA	A	807	51/65	0.81	0.51	87,100,151,177	0
13	CLA	B	834	45/65	0.81	0.54	91,118,151,158	0
13	CLA	A	822	49/65	0.82	0.47	102,126,157,235	0
18	LMG	B	848	55/55	0.82	0.67	42,51,67,114	0
13	CLA	A	813	60/65	0.82	0.60	115,146,178,366	0
13	CLA	B	819	45/65	0.82	0.50	98,131,171,173	0
13	CLA	A	820	61/65	0.83	0.76	119,135,166,198	0
13	CLA	A	855	45/65	0.83	0.40	95,118,140,153	0
13	CLA	A	845	52/65	0.83	0.44	56,78,188,214	0
13	CLA	A	817	54/65	0.83	0.45	83,104,164,172	0
15	BCR	F	1302	40/40	0.83	0.66	70,94,125,128	0
13	CLA	B	814	55/65	0.83	0.70	77,122,182,325	0
13	CLA	A	821	65/65	0.84	0.56	72,100,164,266	0
15	BCR	J	1105	40/40	0.84	0.43	63,67,71,71	0
13	CLA	A	835	54/65	0.85	0.50	54,79,117,204	0
13	CLA	B	831	58/65	0.85	0.46	80,101,148,333	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	CLA	B	810	45/65	0.85	0.49	47,84,145,182	0
16	LHG	A	853	49/49	0.86	0.69	57,74,107,127	0
15	BCR	B	843	40/40	0.86	0.60	45,59,82,86	0
13	CLA	B	828	45/65	0.86	0.43	70,80,132,193	0
13	CLA	B	833	45/65	0.86	0.47	77,104,141,148	0
13	CLA	B	820	55/65	0.86	0.49	77,105,141,146	0
13	CLA	B	818	47/65	0.86	0.61	56,99,146,292	0
13	CLA	B	813	45/65	0.86	0.40	51,86,132,141	0
13	CLA	A	823	51/65	0.86	0.51	74,129,153,156	0
13	CLA	B	829	49/65	0.87	0.47	80,85,125,141	0
15	BCR	A	852	40/40	0.87	0.82	78,107,149,162	0
13	CLA	A	840	65/65	0.87	0.44	77,87,117,198	0
13	CLA	A	842	65/65	0.88	0.57	62,82,149,162	0
13	CLA	B	835	60/65	0.88	0.32	65,106,240,292	0
13	CLA	M	1201	54/65	0.88	0.51	34,42,121,127	0
13	CLA	J	1103	37/65	0.88	0.31	85,117,155,158	0
13	CLA	B	836	65/65	0.88	0.42	69,98,146,234	0
13	CLA	A	825	65/65	0.88	0.32	74,102,152,193	0
15	BCR	J	1104	40/40	0.88	0.82	64,78,113,120	0
15	BCR	A	851	40/40	0.88	0.71	50,58,118,132	0
13	CLA	A	829	65/65	0.88	0.60	83,108,179,197	0
13	CLA	A	811	65/65	0.88	0.65	95,134,173,321	0
15	BCR	M	1203	40/40	0.88	0.53	43,48,87,92	0
13	CLA	B	809	45/65	0.88	0.45	39,95,125,308	0
13	CLA	A	841	51/65	0.88	0.38	80,105,182,204	0
15	BCR	B	842	40/40	0.88	0.66	48,76,129,134	0
13	CLA	A	809	65/65	0.88	0.49	78,117,148,152	0
13	CLA	A	819	65/65	0.88	0.59	97,140,181,328	0
13	CLA	A	824	59/65	0.88	0.54	59,101,164,321	0
13	CLA	A	818	54/65	0.88	0.47	92,136,168,207	0
13	CLA	A	802	65/65	0.88	0.59	40,77,110,230	0
13	CLA	A	828	65/65	0.89	0.49	59,74,127,289	0
13	CLA	B	806	65/65	0.89	0.45	33,63,107,170	0
13	CLA	B	803	65/65	0.89	0.64	40,68,95,180	0
13	CLA	A	804	59/65	0.89	0.59	83,99,117,144	0
13	CLA	A	826	65/65	0.89	0.61	53,80,112,127	0
13	CLA	B	807	65/65	0.89	0.63	38,65,106,122	0
13	CLA	B	832	45/65	0.89	0.39	71,121,142,247	0
13	CLA	F	1301	45/65	0.89	0.45	94,137,167,175	0
13	CLA	A	805	65/65	0.89	0.58	85,98,117,126	0
15	BCR	B	845	40/40	0.90	0.40	60,66,78,82	0
15	BCR	B	844	25/40	0.90	0.44	65,68,113,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	CLA	A	843	65/65	0.90	0.49	56,83,169,197	0
15	BCR	B	846	40/40	0.90	0.70	75,91,131,137	0
13	CLA	A	833	65/65	0.90	0.56	39,45,110,121	0
13	CLA	B	817	65/65	0.90	0.48	57,65,113,125	0
13	CLA	A	831	50/65	0.90	0.39	45,76,105,144	0
13	CLA	A	814	45/65	0.90	0.32	108,150,172,174	0
13	CLA	B	838	65/65	0.90	0.54	35,45,102,125	0
13	CLA	L	1004	65/65	0.90	0.44	21,31,64,72	0
13	CLA	B	839	65/65	0.91	0.49	35,49,151,215	0
13	CLA	J	1101	65/65	0.91	0.52	77,129,178,357	0
13	CLA	A	832	65/65	0.91	0.34	42,45,81,134	0
13	CLA	A	806	65/65	0.91	0.57	63,80,155,164	0
16	LHG	A	854	27/49	0.91	0.37	49,58,88,122	0
13	CLA	B	802	65/65	0.91	0.53	61,82,112,165	0
13	CLA	A	808	65/65	0.91	0.40	72,89,172,177	0
13	CLA	A	830	65/65	0.91	0.51	59,71,105,119	0
13	CLA	B	804	65/65	0.91	0.57	45,51,117,199	0
13	CLA	B	824	65/65	0.91	0.38	58,65,88,96	0
14	PQN	B	840	33/33	0.91	0.73	56,84,105,121	0
13	CLA	X	102	45/65	0.91	0.26	67,104,127,283	0
13	CLA	B	821	45/65	0.92	0.35	63,69,105,191	0
13	CLA	A	838	65/65	0.92	0.37	45,81,109,114	0
13	CLA	A	837	51/65	0.92	0.43	52,56,96,147	0
15	BCR	B	847	40/40	0.92	0.70	40,51,116,126	0
13	CLA	A	803	65/65	0.92	0.57	76,100,142,222	0
14	PQN	A	846	33/33	0.92	0.56	55,64,82,82	0
13	CLA	B	837	47/65	0.92	0.27	65,71,119,193	0
13	CLA	B	815	59/65	0.92	0.48	55,58,76,293	0
13	CLA	B	812	65/65	0.92	0.41	37,42,111,117	0
13	CLA	B	830	65/65	0.92	0.61	82,91,129,139	0
13	CLA	B	808	65/65	0.92	0.60	36,41,97,103	0
15	BCR	I	102	40/40	0.92	0.38	19,20,48,52	0
13	CLA	L	1002	65/65	0.92	0.36	29,65,103,148	0
13	CLA	I	101	65/65	0.92	0.38	33,57,85,338	0
13	CLA	B	826	65/65	0.92	0.51	42,47,127,149	0
13	CLA	L	1003	65/65	0.92	0.35	16,52,179,216	0
13	CLA	B	825	65/65	0.93	0.47	40,60,136,157	0
13	CLA	B	801	65/65	0.93	0.42	57,68,123,322	0
13	CLA	B	811	65/65	0.93	0.58	48,71,108,145	0
15	BCR	L	1005	40/40	0.93	0.45	11,16,81,93	0
13	CLA	B	827	65/65	0.93	0.47	44,66,95,108	0
13	CLA	A	834	65/65	0.93	0.44	39,40,92,96	0

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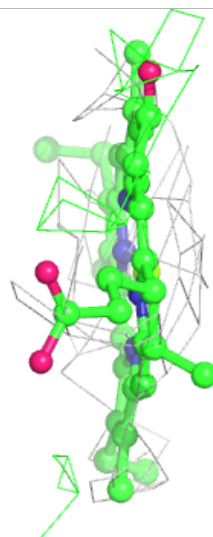
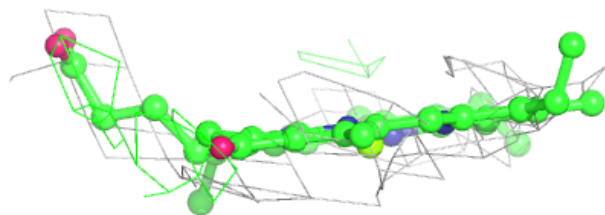
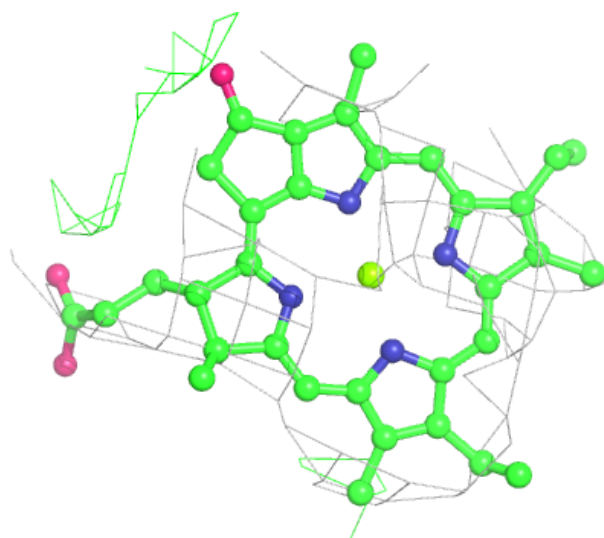
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	BCR	L	1006	40/40	0.93	0.29	16,24,64,78	0
15	BCR	B	849	40/40	0.93	0.41	12,43,147,152	0
13	CLA	B	823	46/65	0.94	0.28	59,68,120,137	0
13	CLA	A	839	47/65	0.94	0.31	48,51,119,202	0
13	CLA	B	816	60/65	0.94	0.54	46,53,111,221	0
19	CA	L	1001	1/1	0.94	0.14	22,22,22,22	0
13	CLA	B	822	54/65	0.94	0.44	61,86,118,158	0
13	CLA	B	805	65/65	0.94	0.41	41,48,97,150	0
13	CLA	A	801	65/65	0.94	0.49	44,53,82,89	0
17	SF4	C	102	8/8	0.99	0.16	47,48,122,359	0
17	SF4	A	856	8/8	0.99	0.22	49,50,150,174	0
17	SF4	C	101	8/8	0.99	0.20	48,48,49,62	0

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

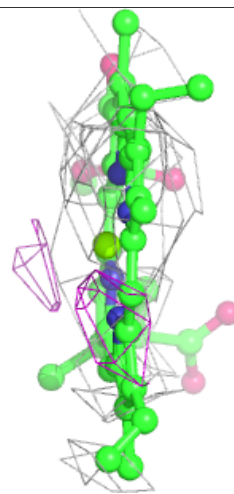
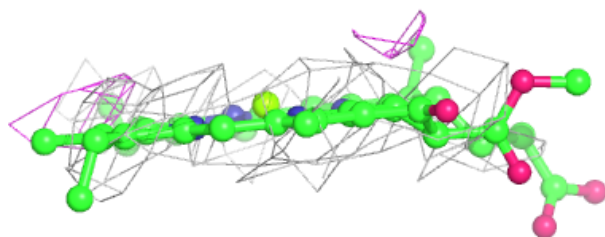
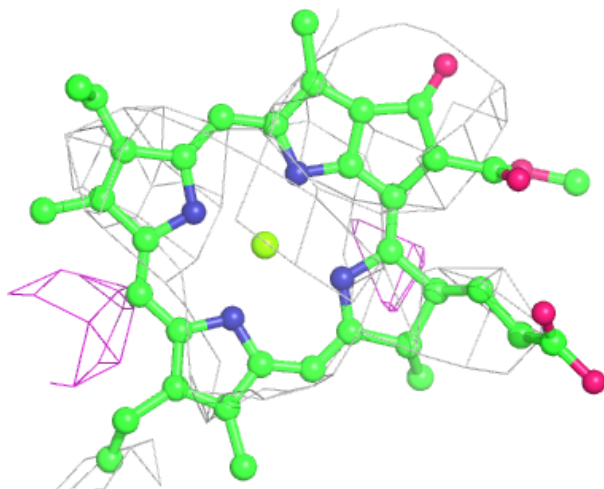
Electron density around CLA A 844:

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



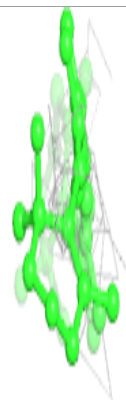
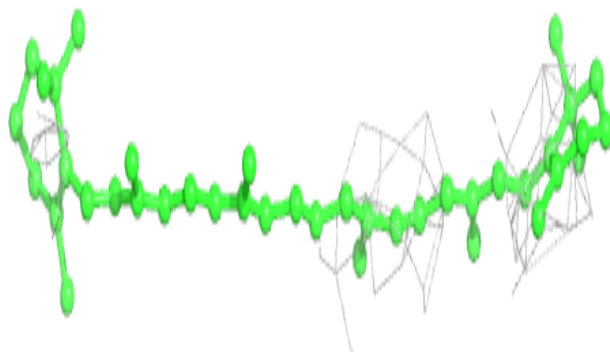
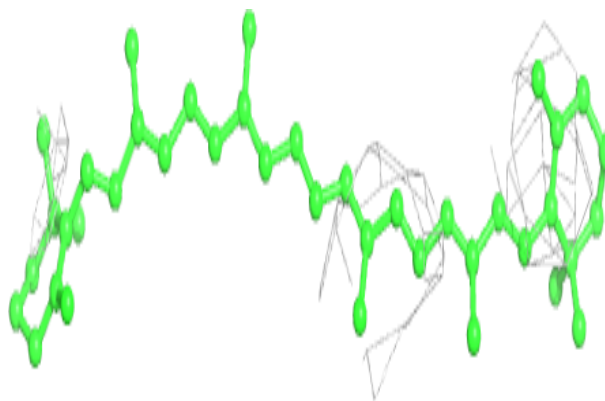
Electron density around CLA A 815:

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



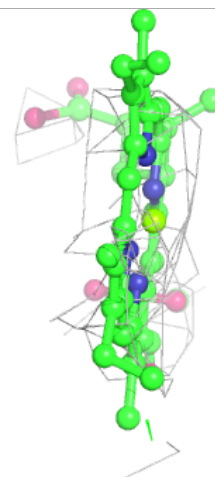
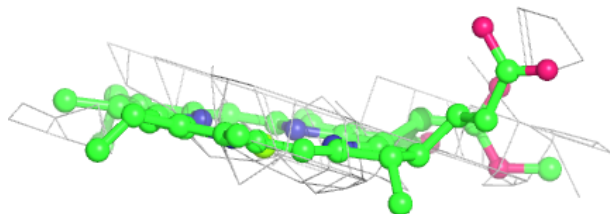
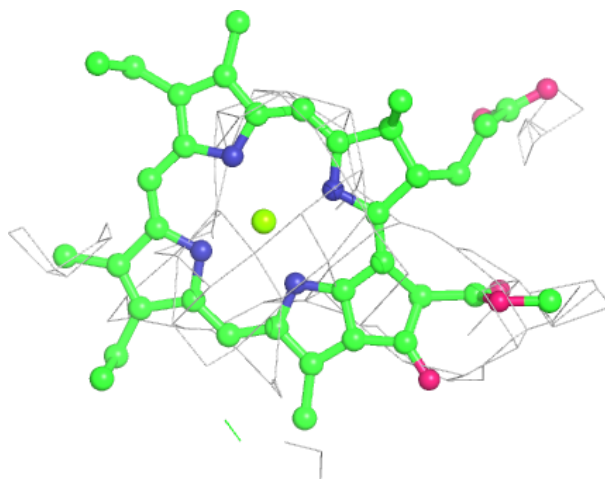
Electron density around BCR A 847:

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



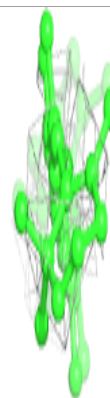
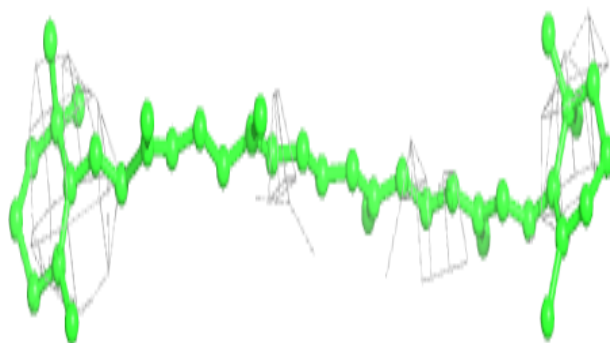
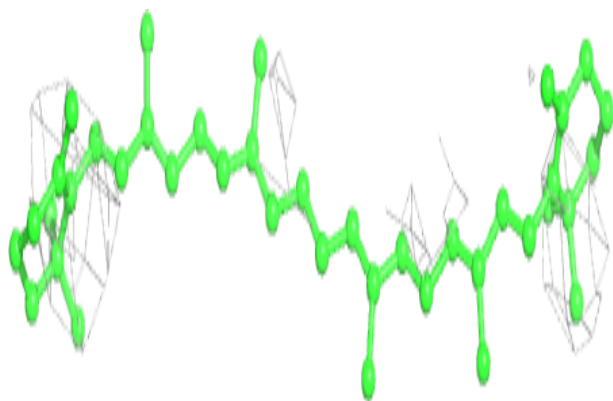
Electron density around CLA M 1202:

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

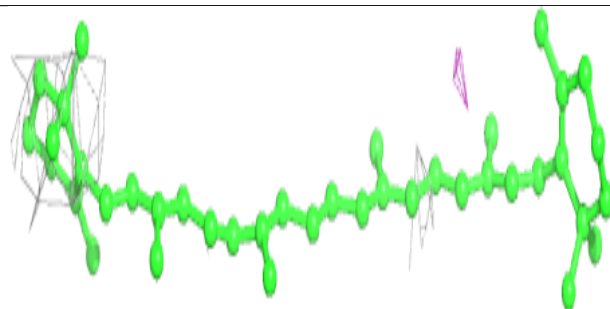
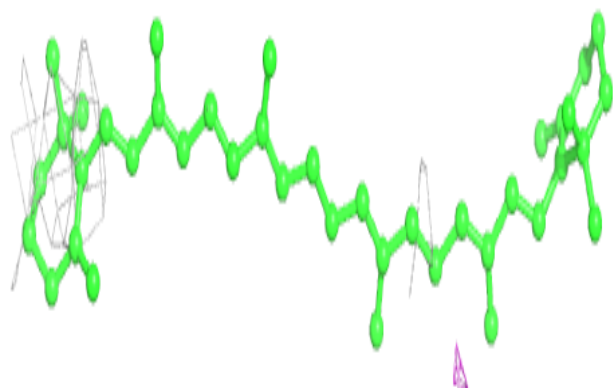


Electron density around BCR A 848:

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

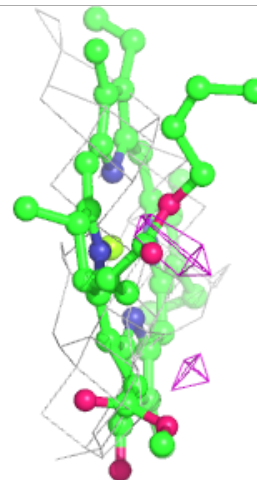
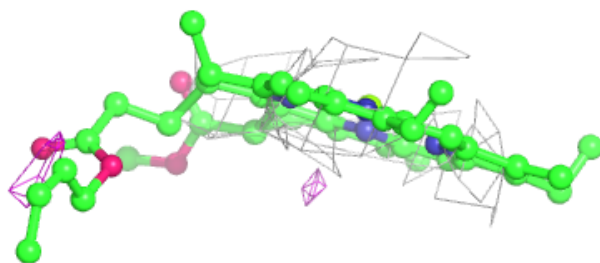
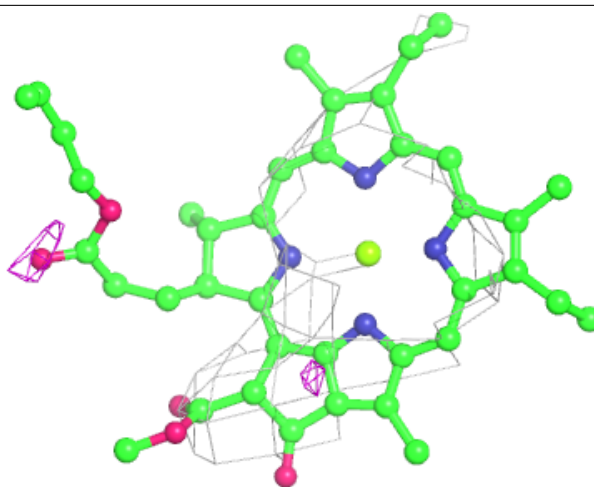
**Electron density around BCR A 849:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



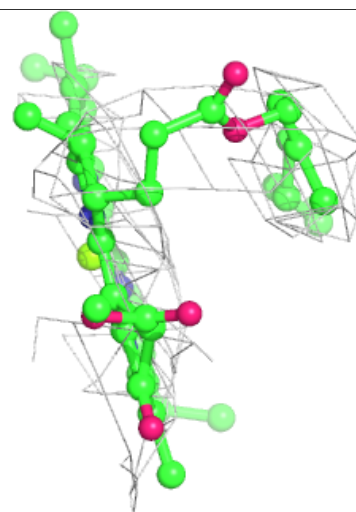
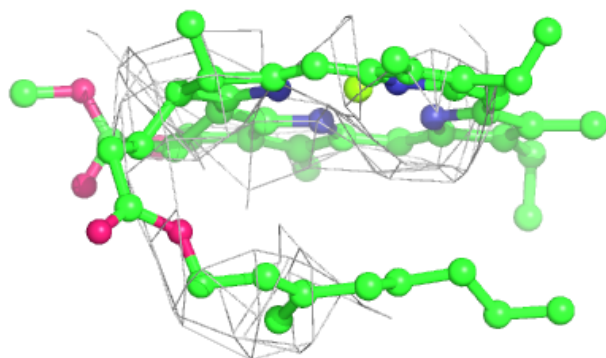
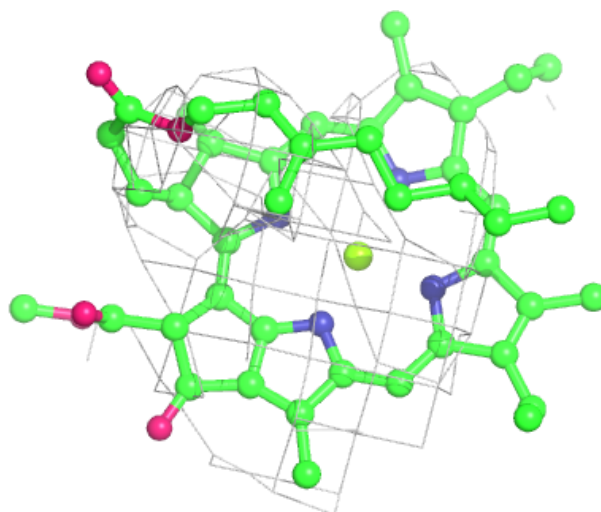
Electron density around CLA A 816:

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



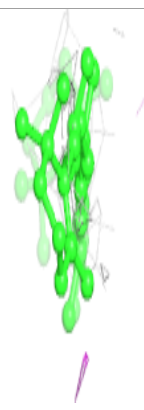
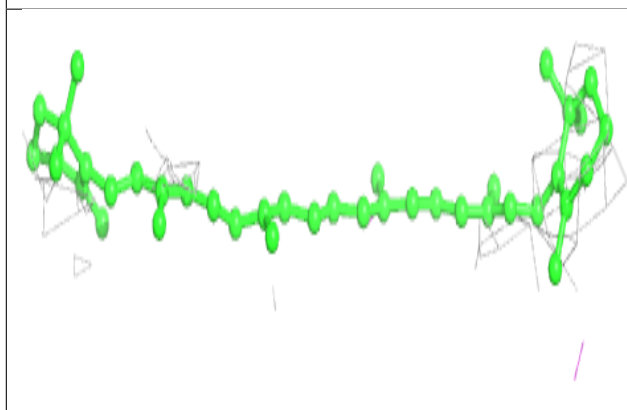
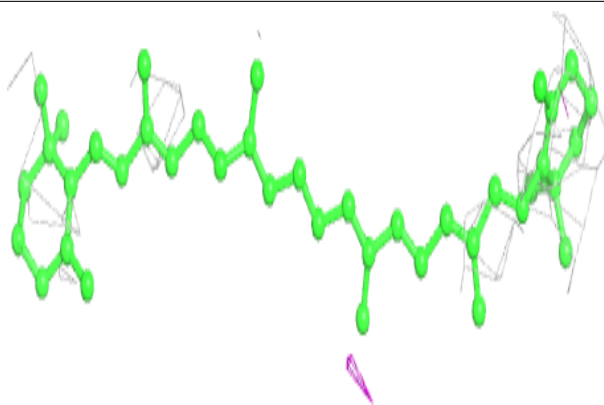
Electron density around CLA A 812:

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



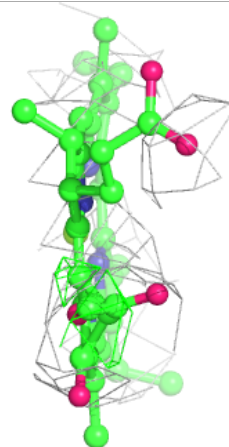
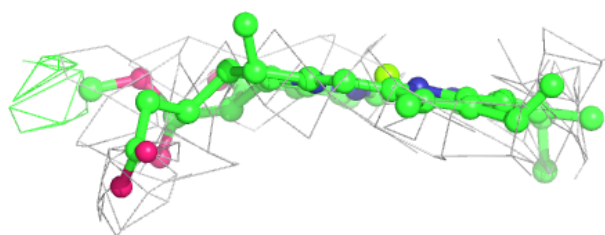
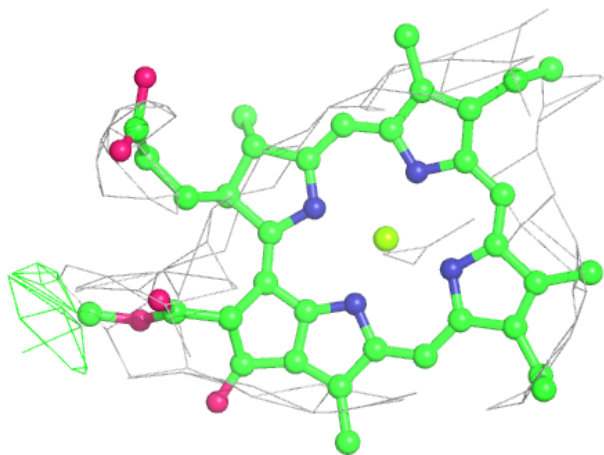
Electron density around BCR B 841:

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



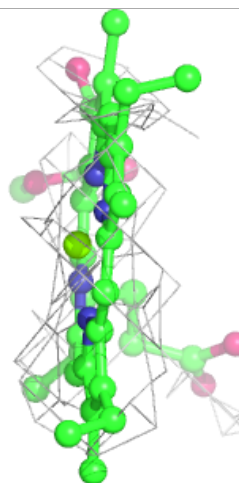
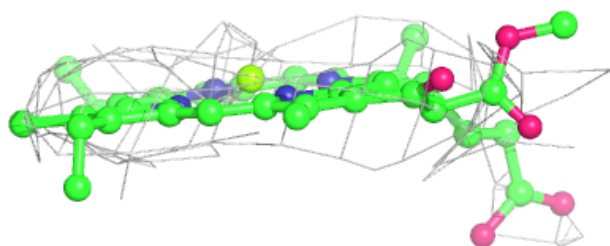
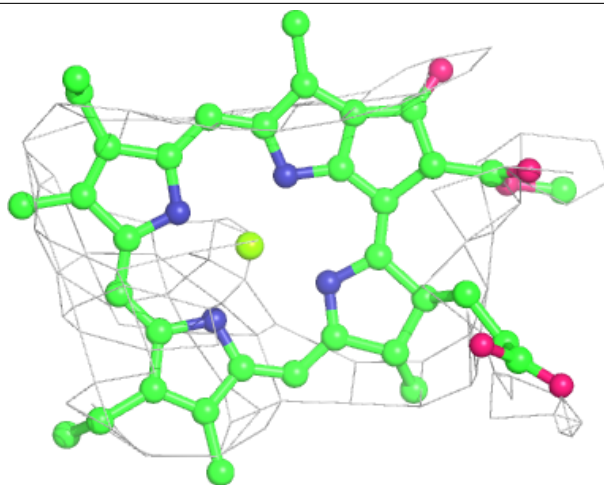
Electron density around CLA J 1102:

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



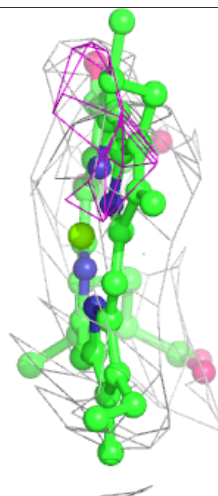
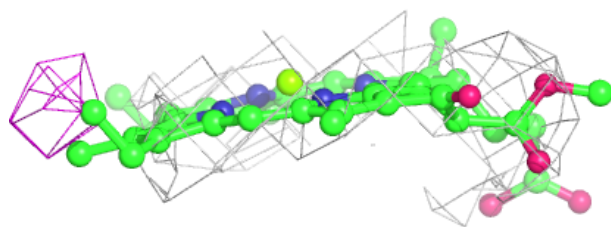
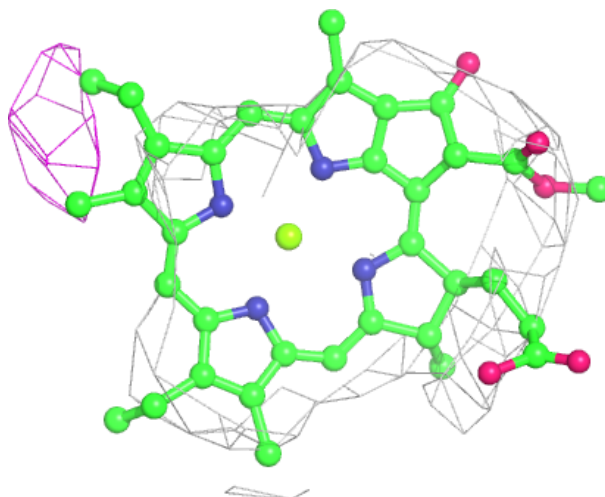
Electron density around CLA A 836:

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



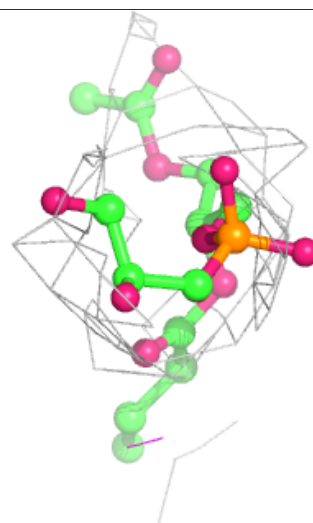
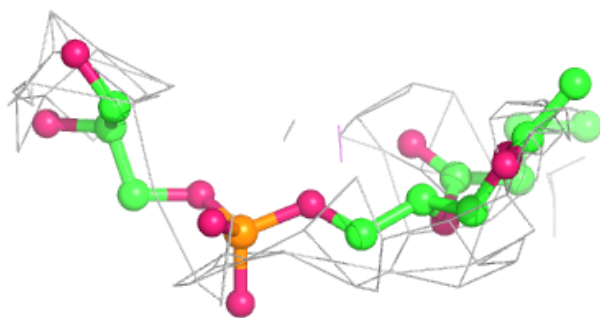
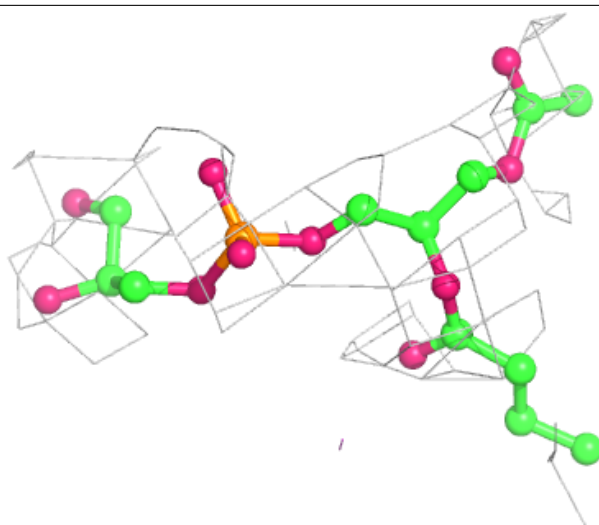
Electron density around CLA A 810:

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



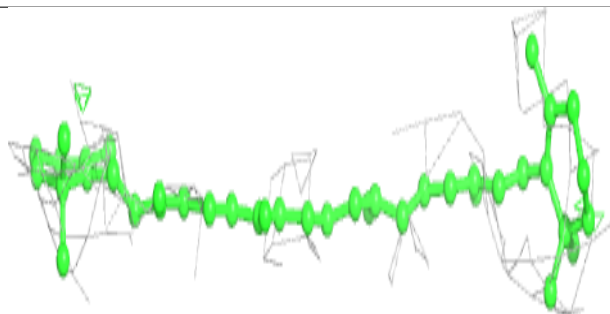
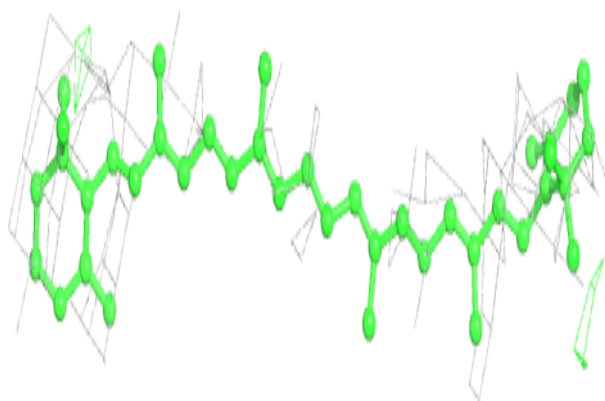
Electron density around LHG X 101:

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

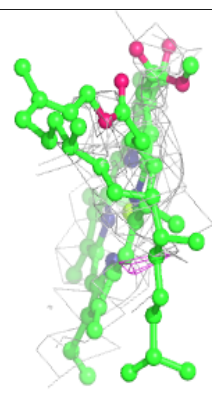
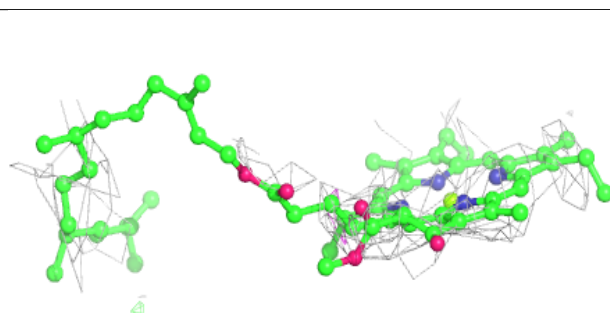
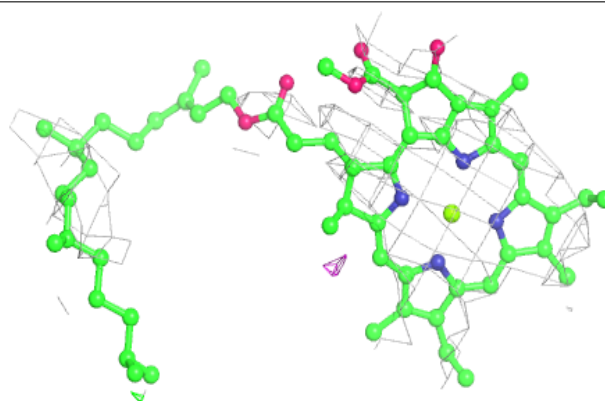


Electron density around BCR B 850:

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

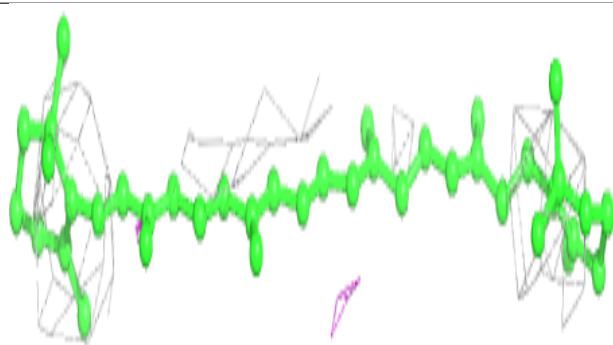
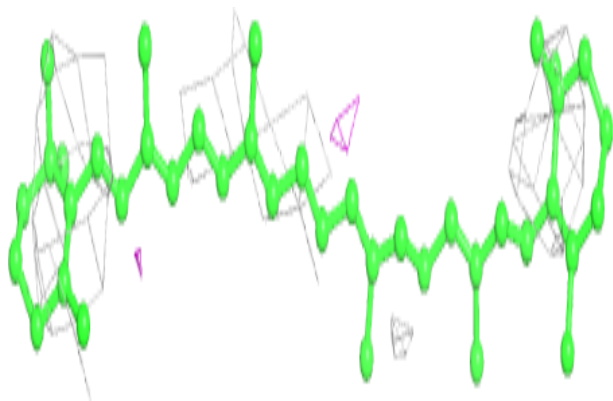
**Electron density around CLA A 827:**

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



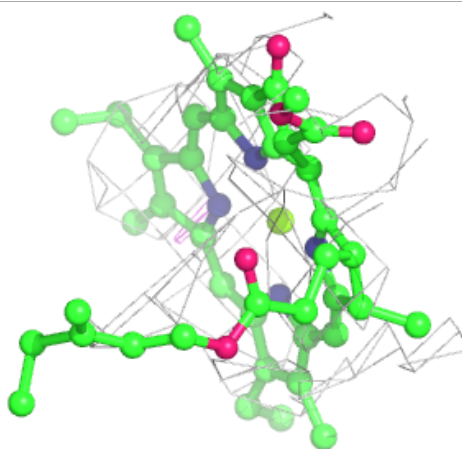
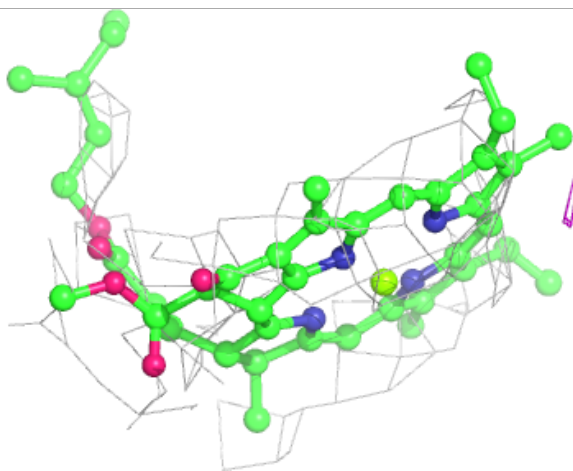
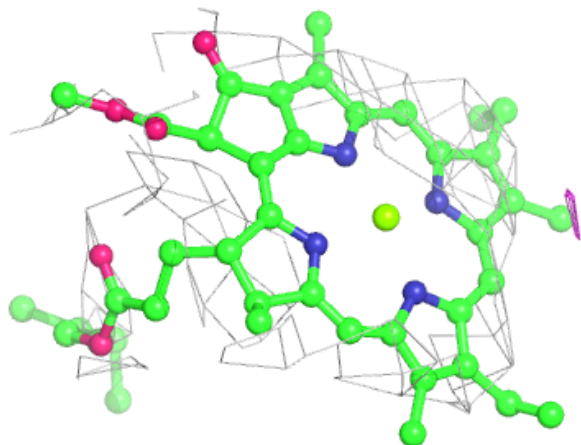
Electron density around BCR A 850:

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



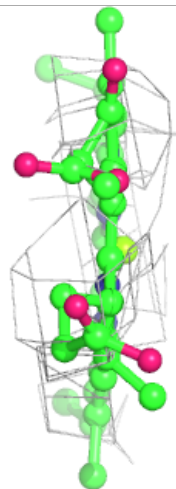
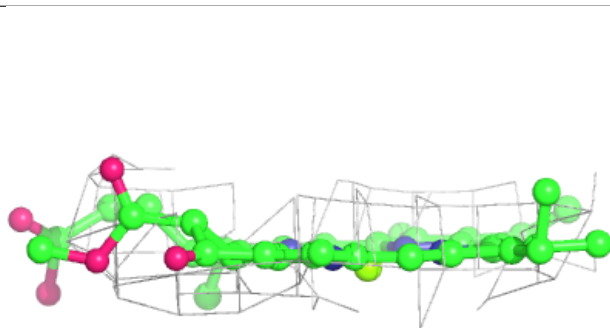
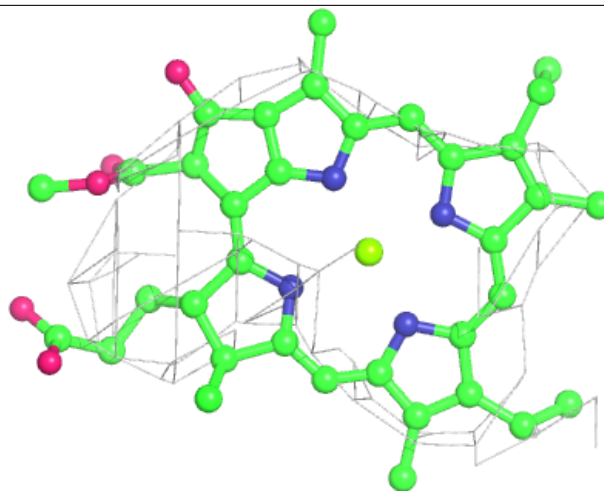
Electron density around CLA A 807:

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



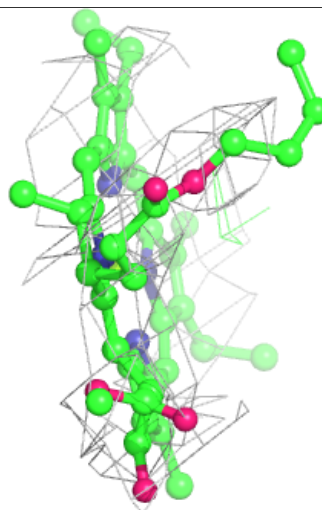
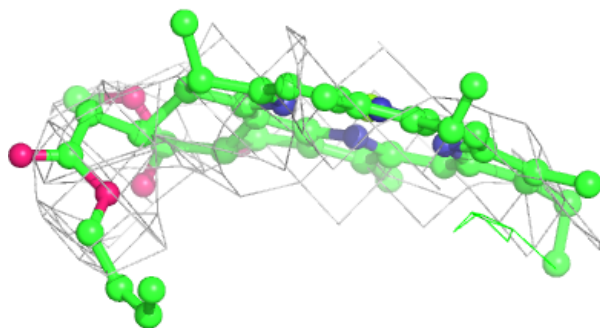
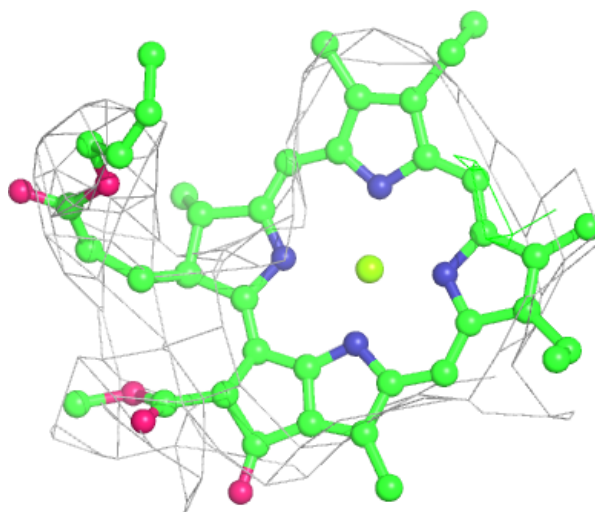
Electron density around CLA B 834:

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



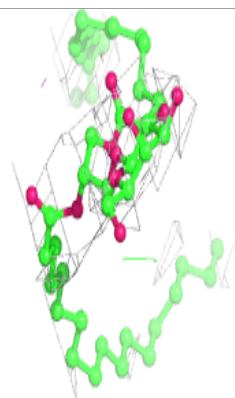
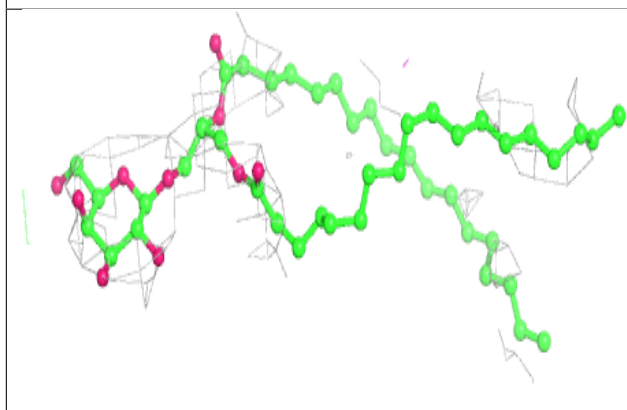
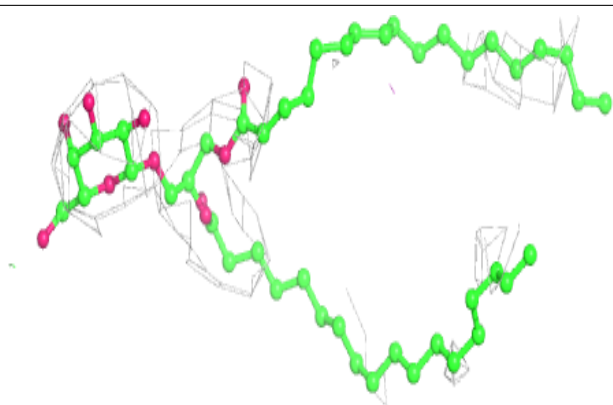
Electron density around CLA A 822:

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



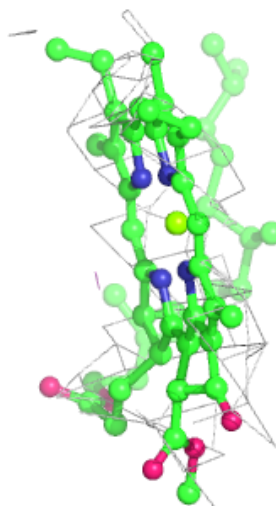
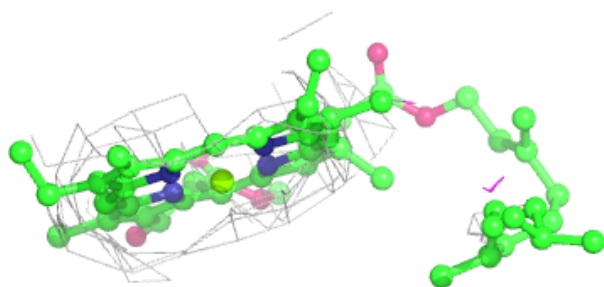
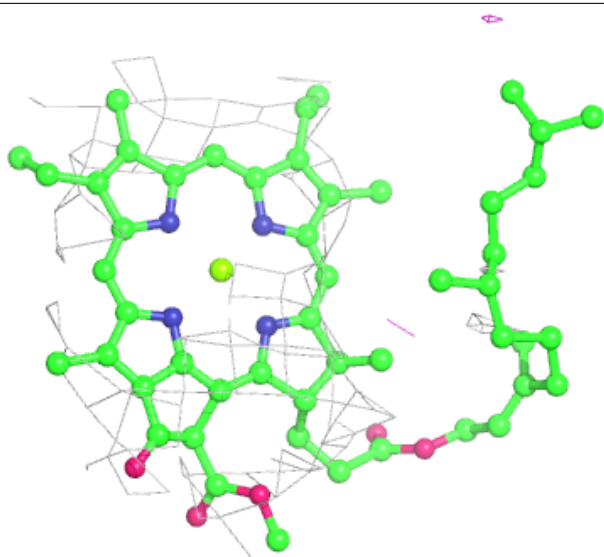
Electron density around LMG B 848:

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



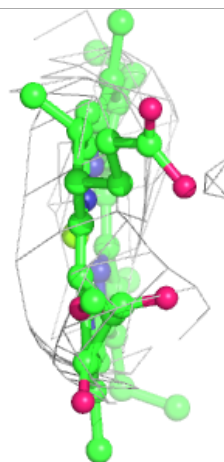
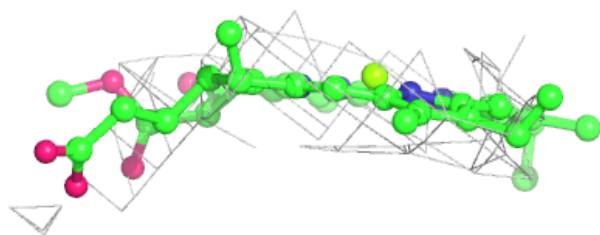
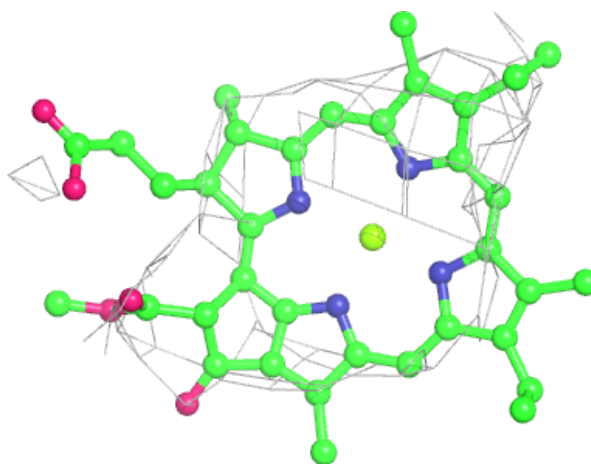
Electron density around CLA A 813:

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



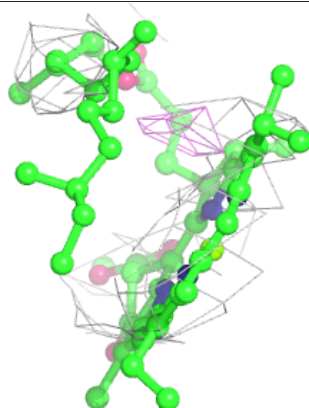
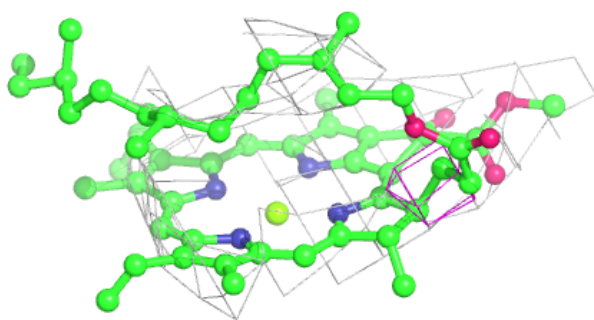
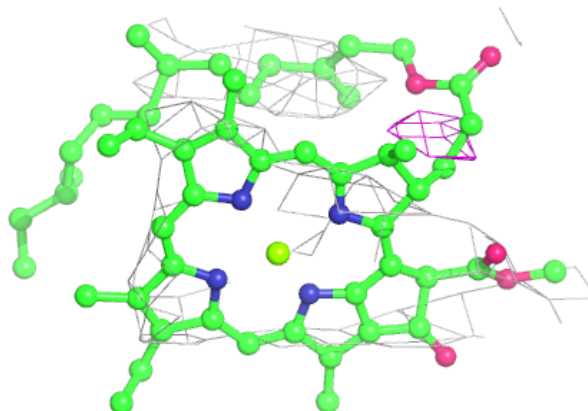
Electron density around CLA B 819:

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



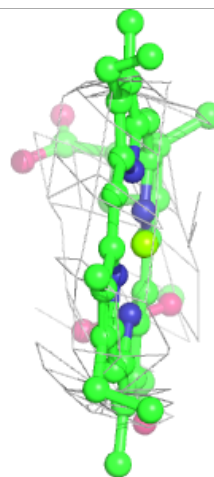
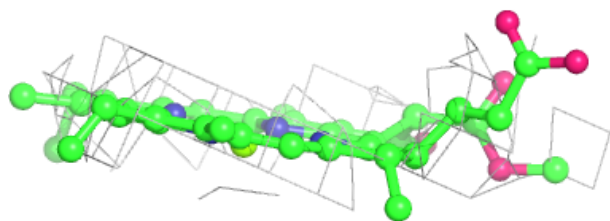
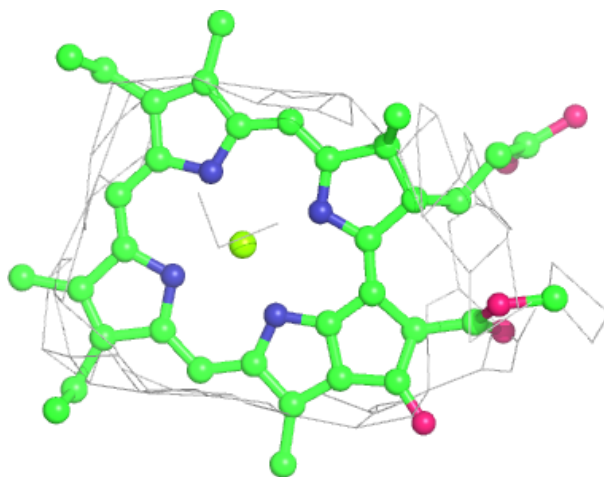
Electron density around CLA A 820:

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



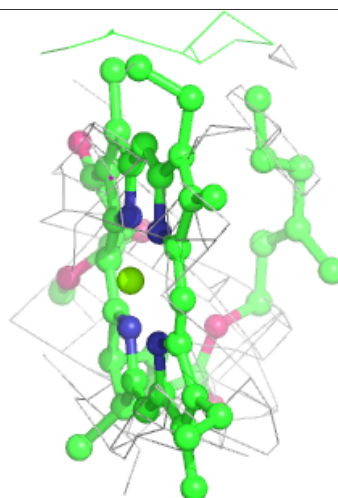
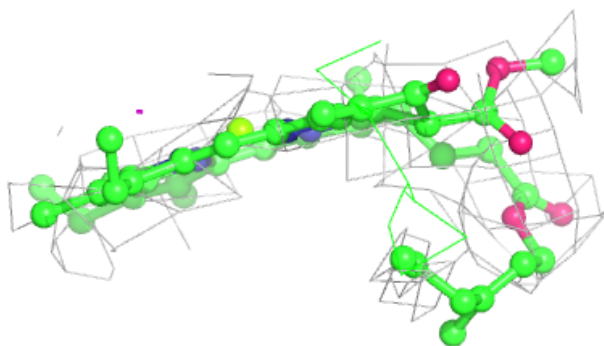
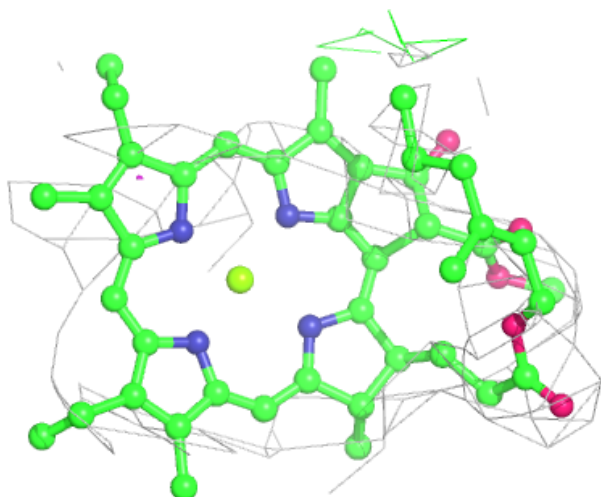
Electron density around CLA A 855:

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



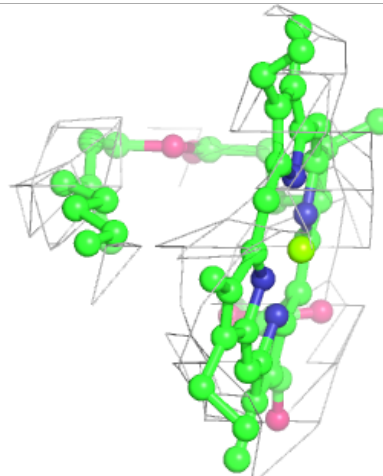
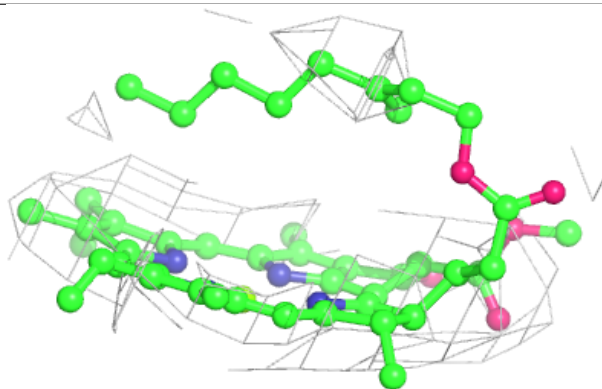
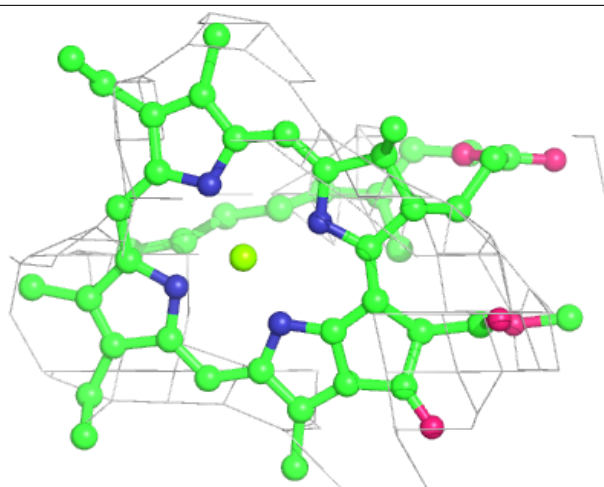
Electron density around CLA A 845:

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



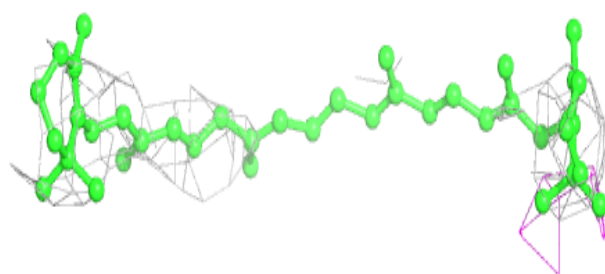
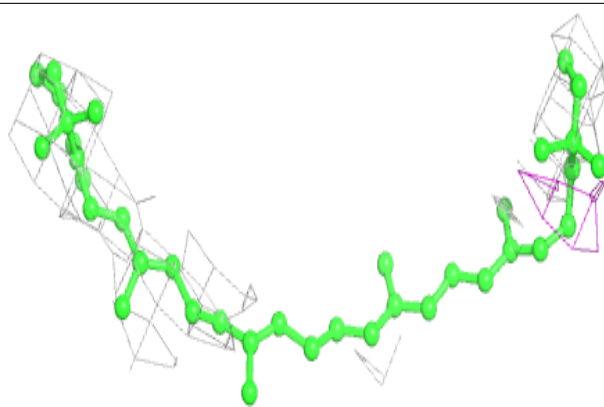
Electron density around CLA A 817:

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



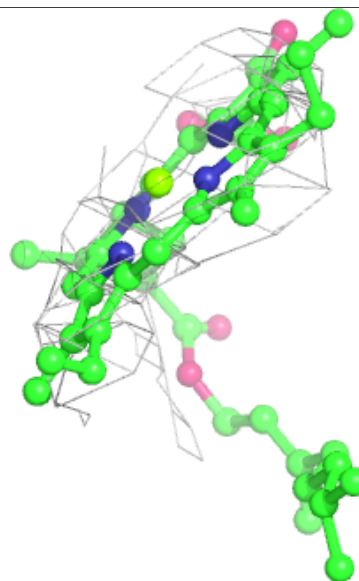
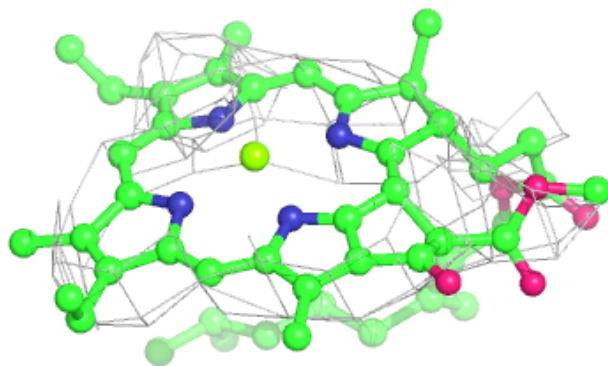
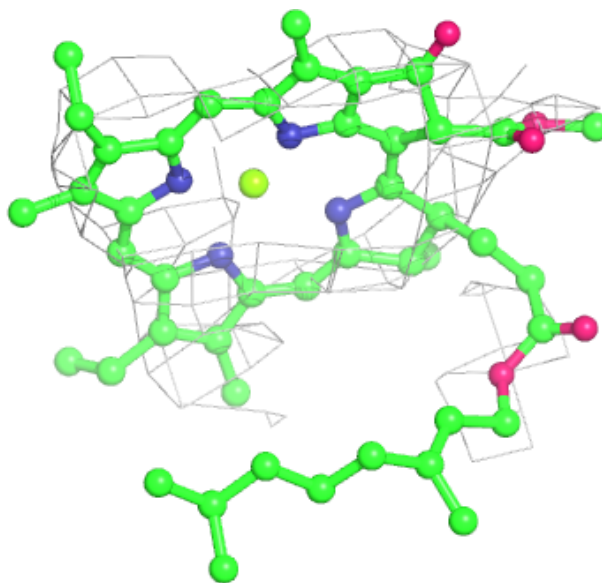
Electron density around BCR F 1302:

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



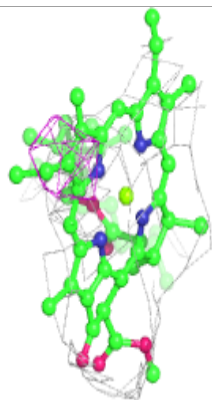
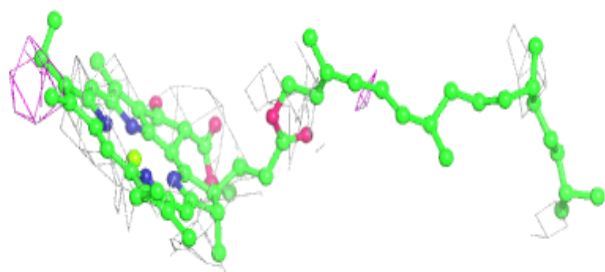
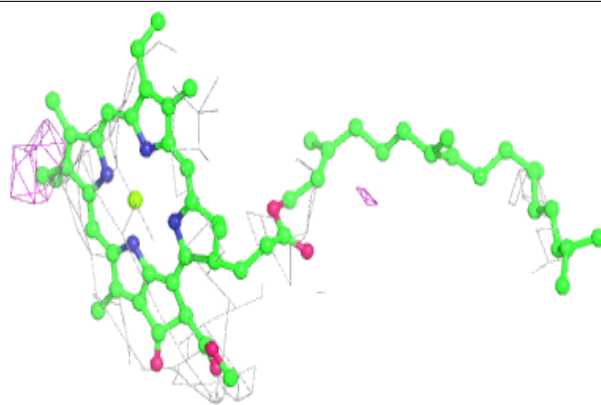
Electron density around CLA B 814:

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

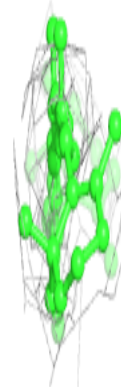
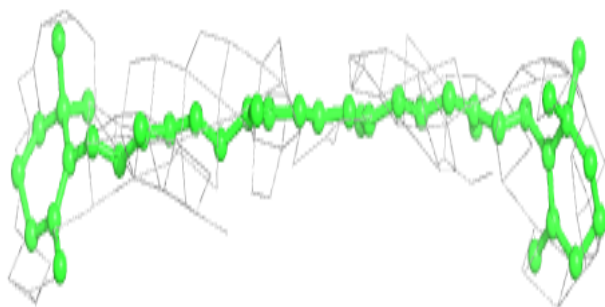
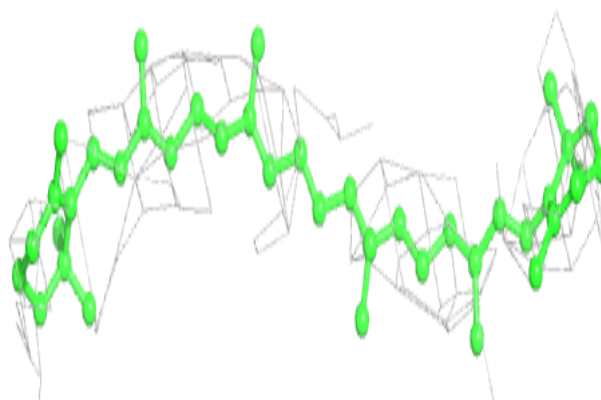


Electron density around CLA A 821:

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

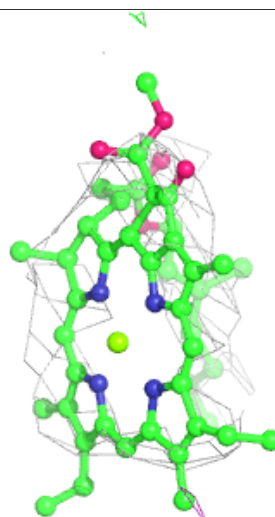
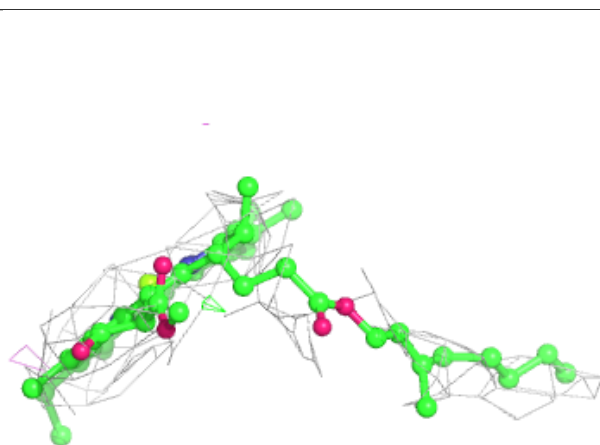
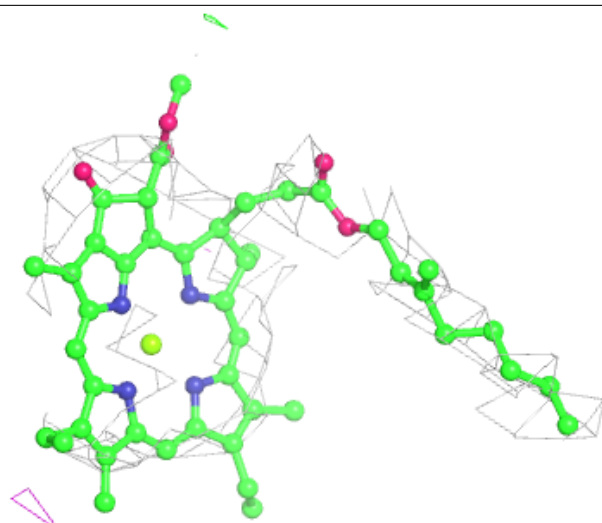
**Electron density around BCR J 1105:**

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



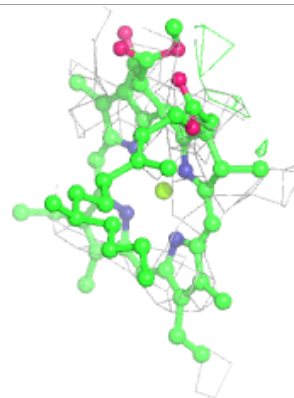
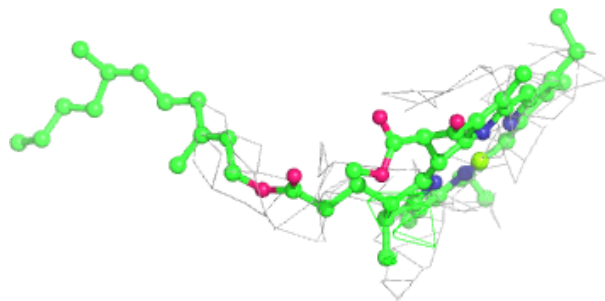
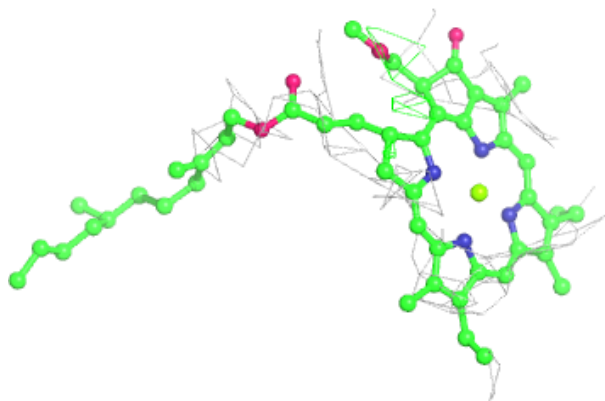
Electron density around CLA A 835:

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



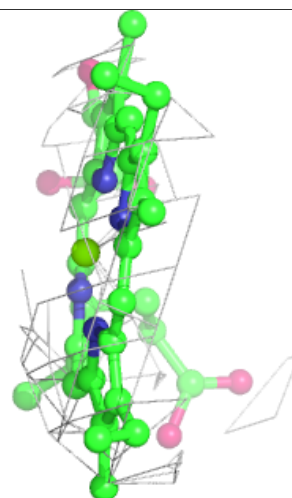
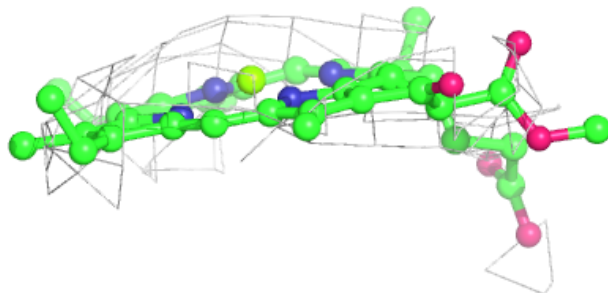
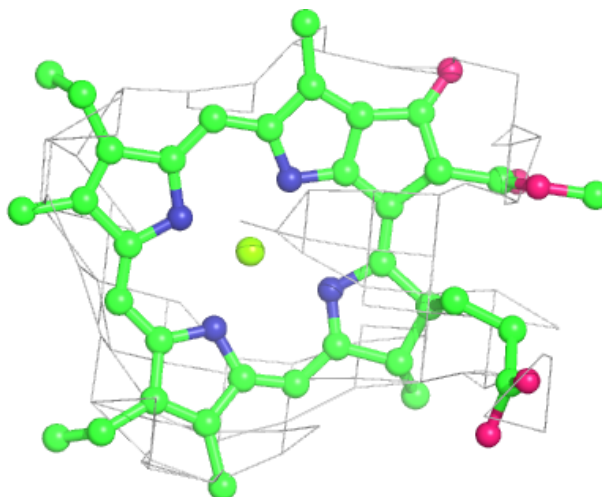
Electron density around CLA B 831:

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



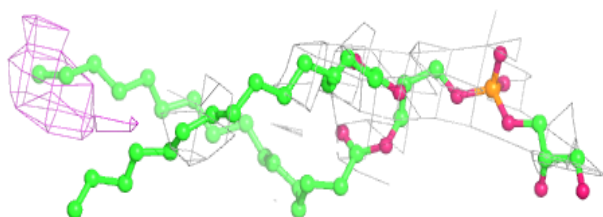
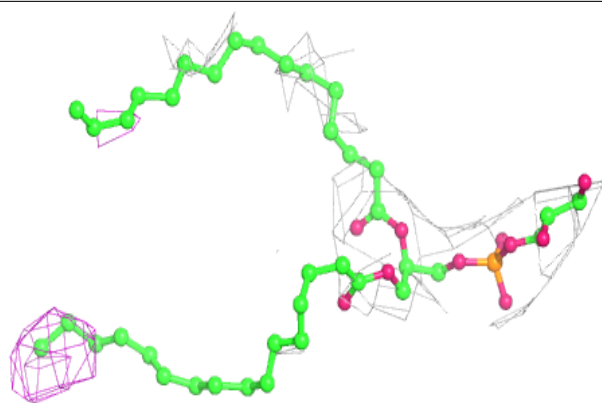
Electron density around CLA B 810:

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

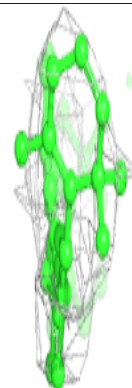
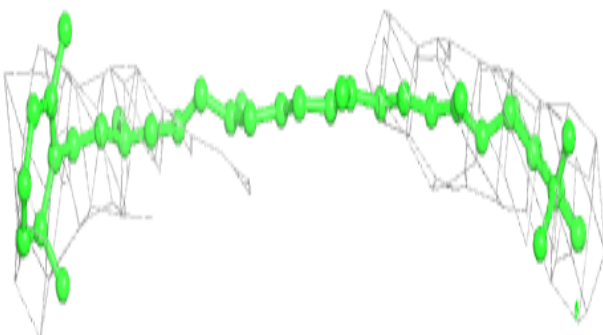
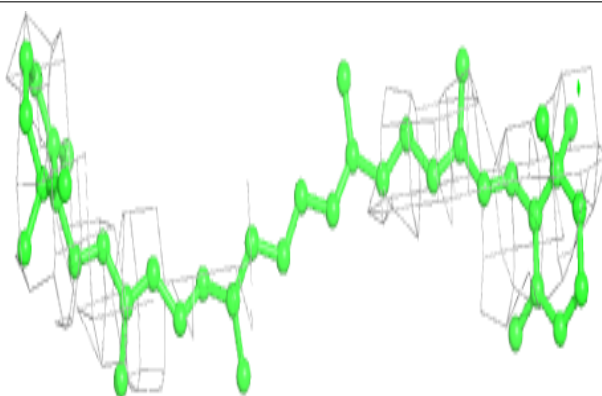


Electron density around LHG A 853:

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

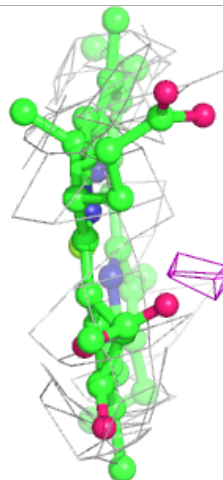
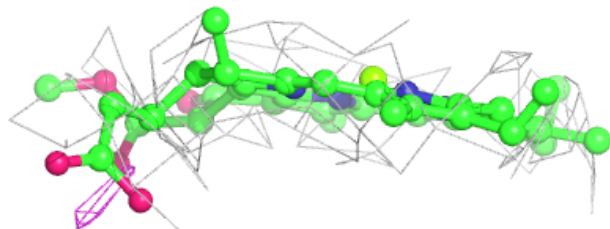
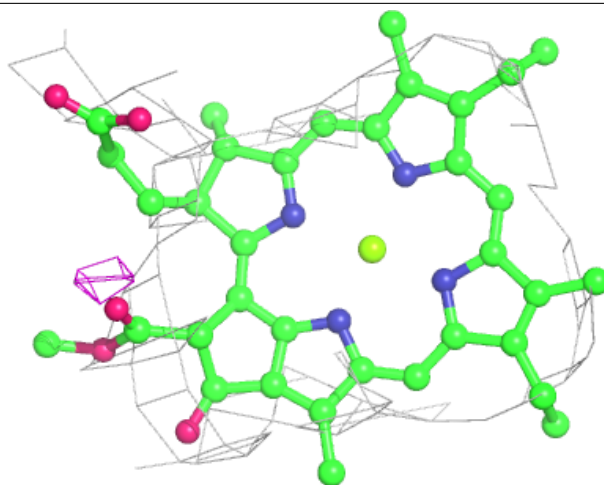
**Electron density around BCR B 843:**

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



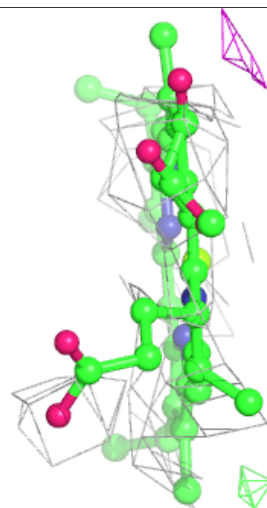
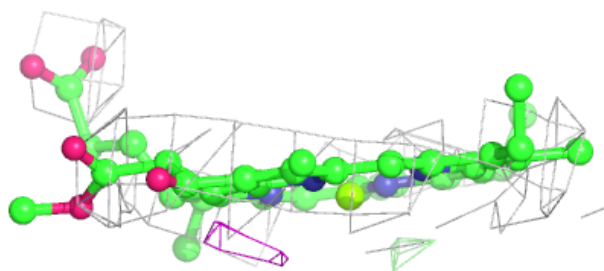
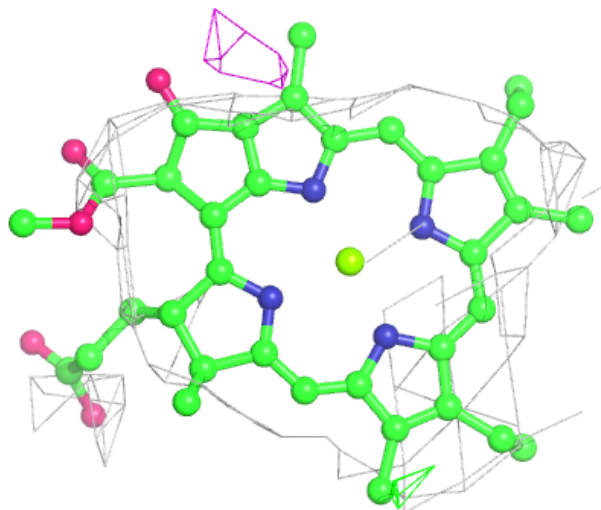
Electron density around CLA B 828:

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



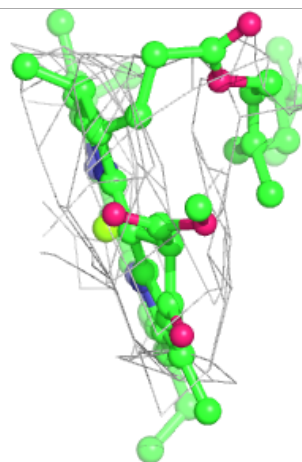
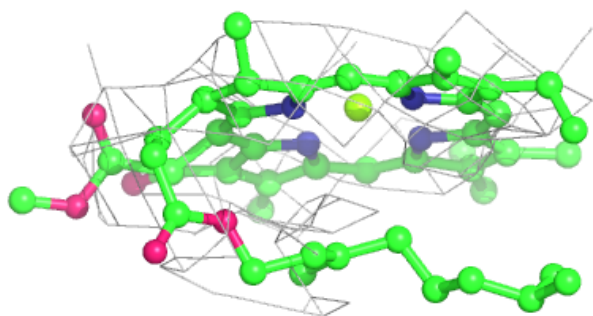
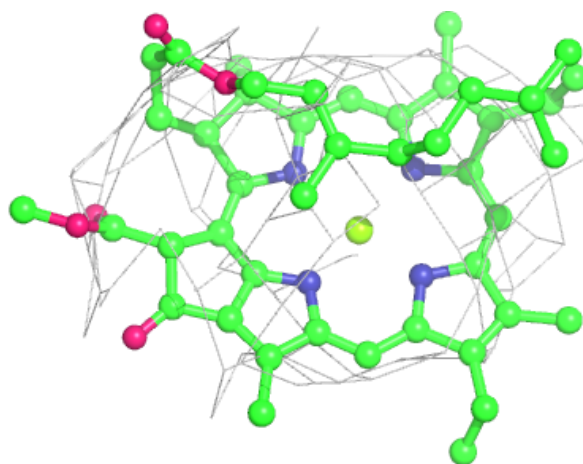
Electron density around CLA B 833:

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



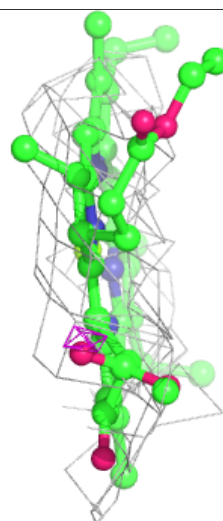
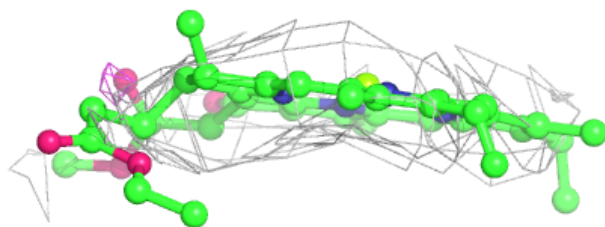
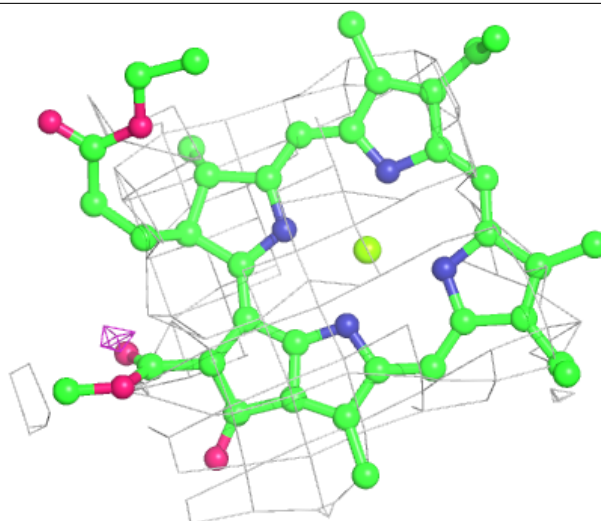
Electron density around CLA B 820:

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



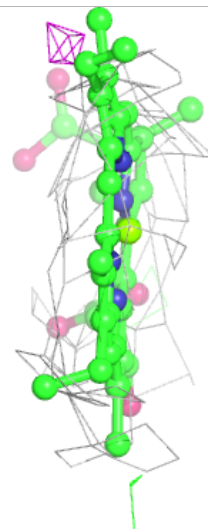
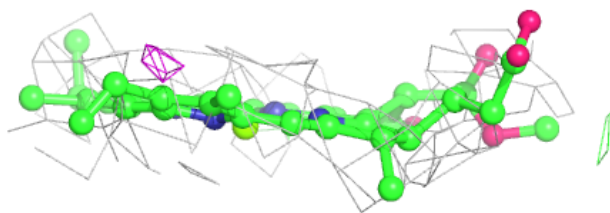
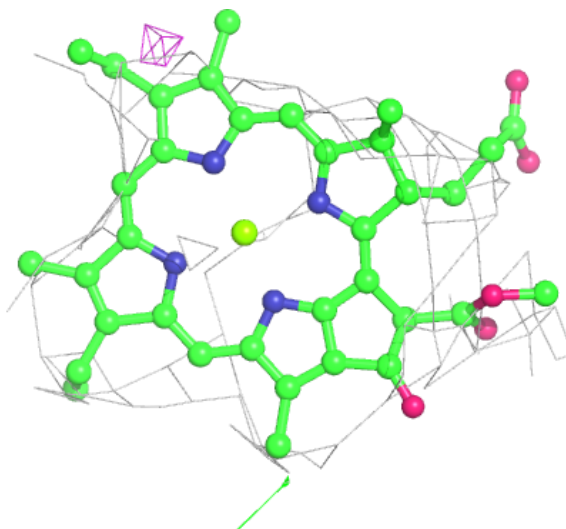
Electron density around CLA B 818:

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



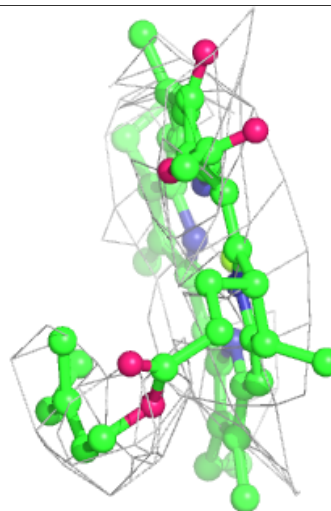
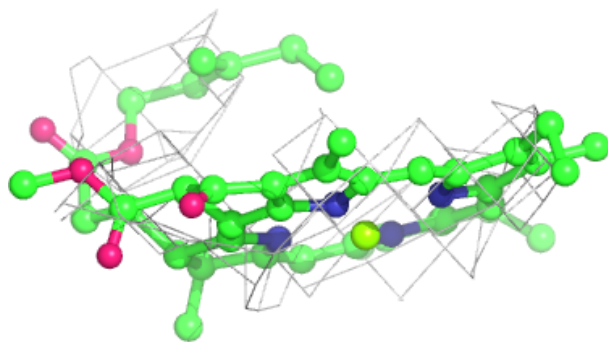
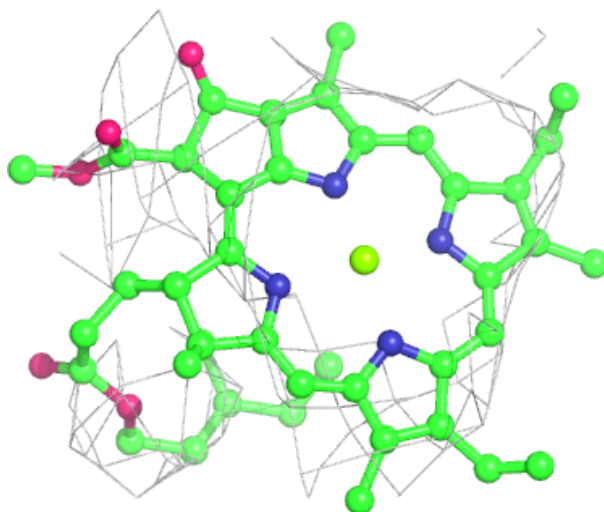
Electron density around CLA B 813:

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



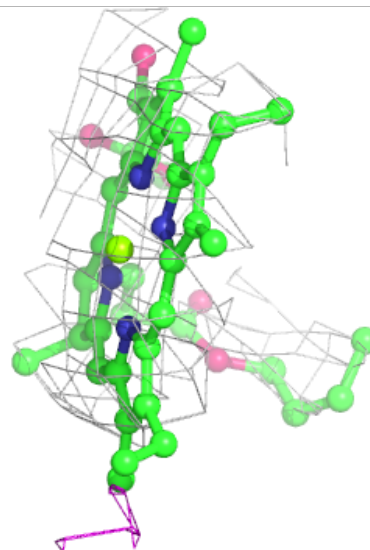
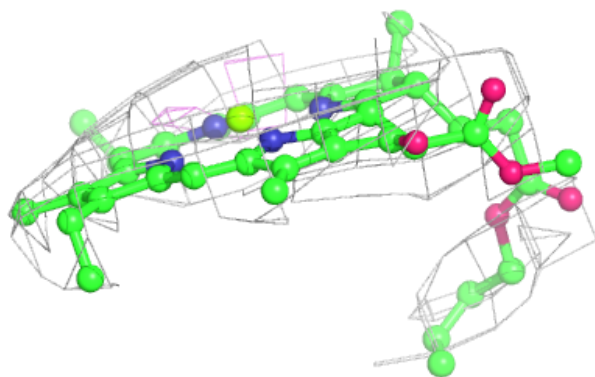
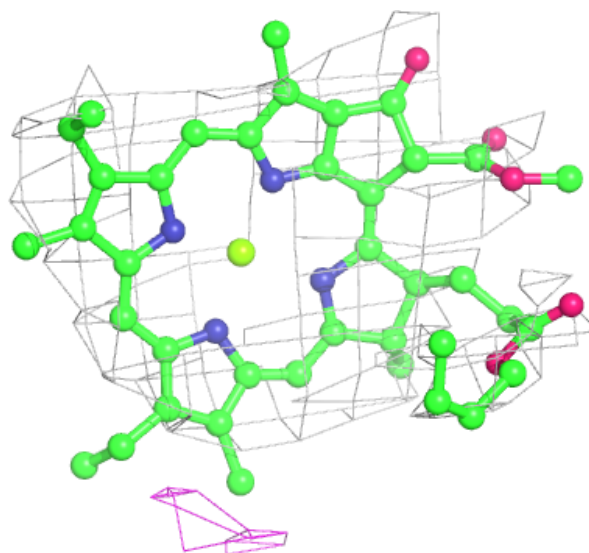
Electron density around CLA A 823:

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



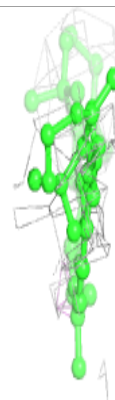
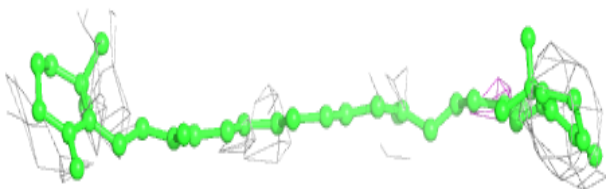
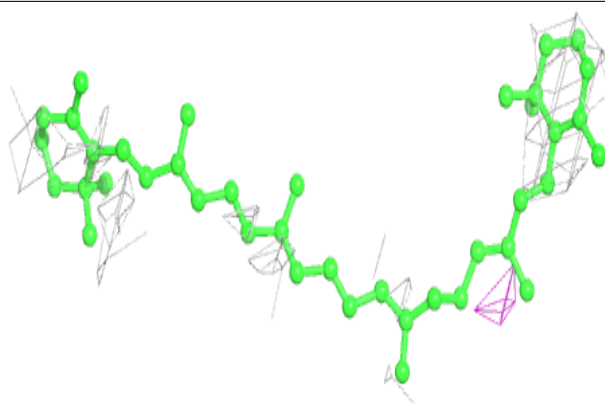
Electron density around CLA B 829:

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

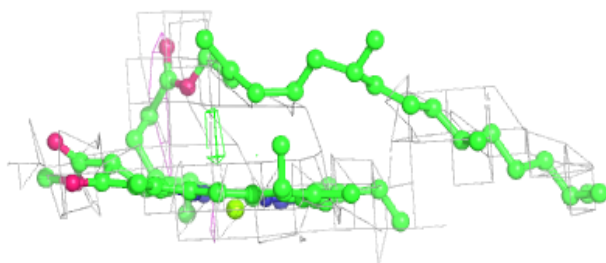
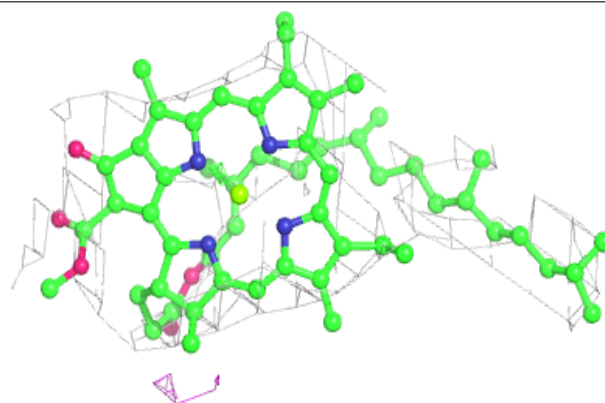


Electron density around BCR A 852:

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

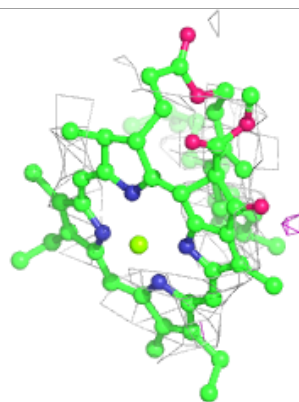
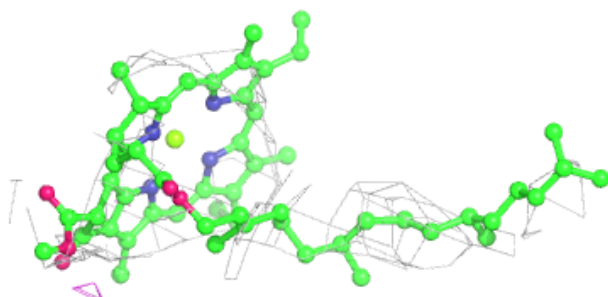
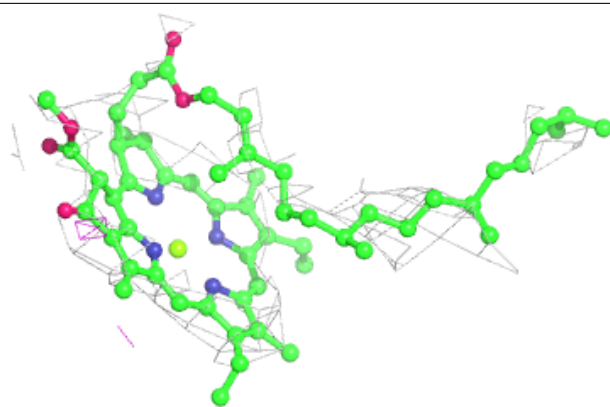
**Electron density around CLA A 840:**

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

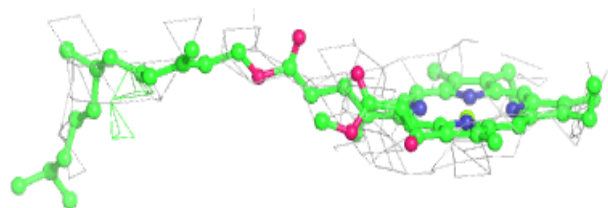
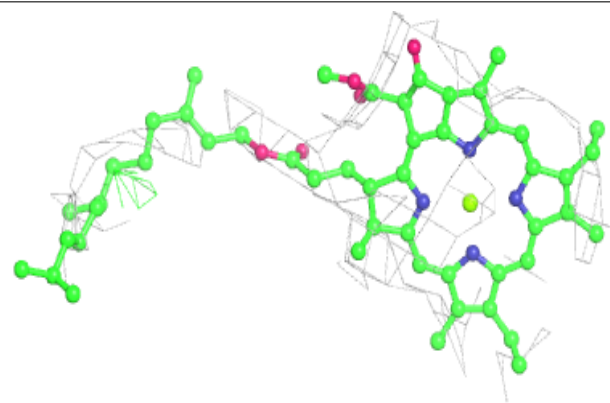


Electron density around CLA A 842:

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

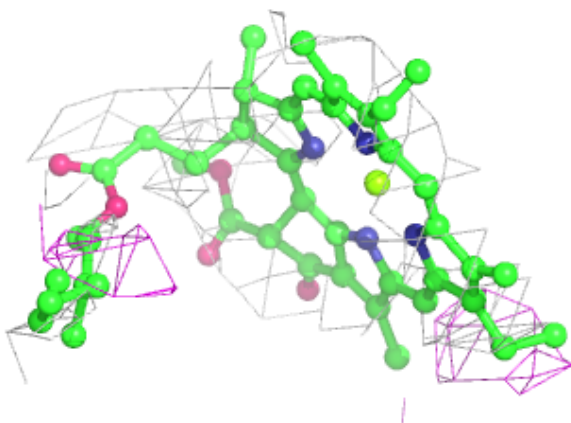
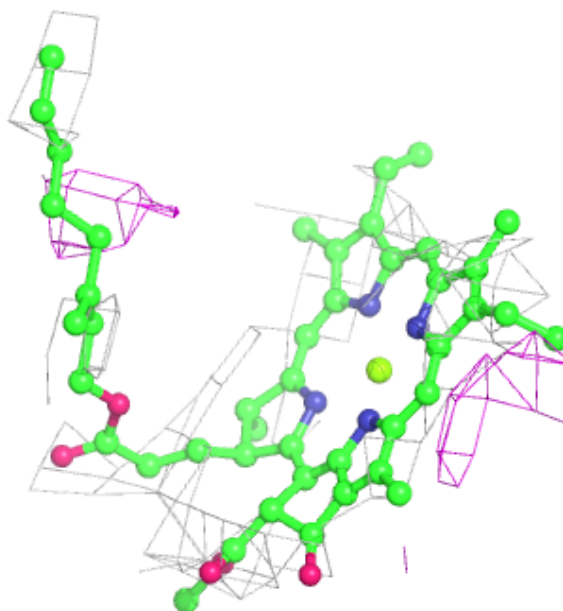
**Electron density around CLA B 835:**

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



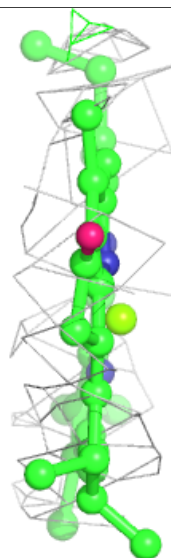
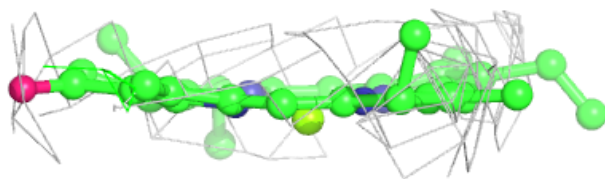
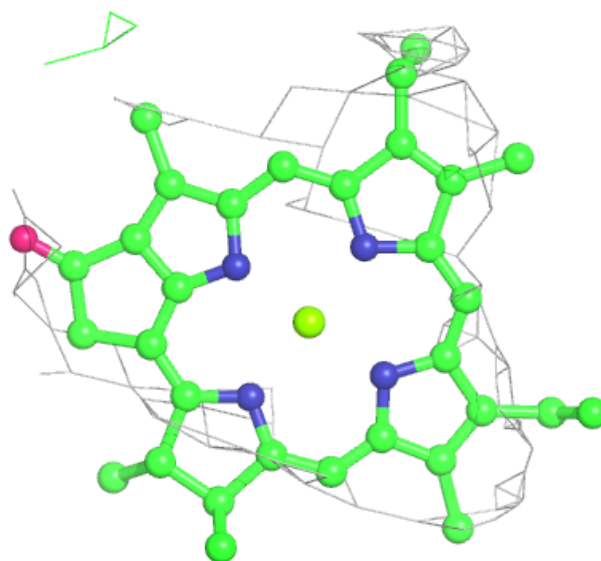
Electron density around CLA M 1201:

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



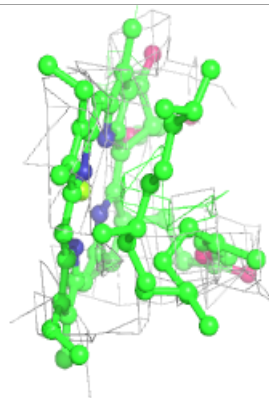
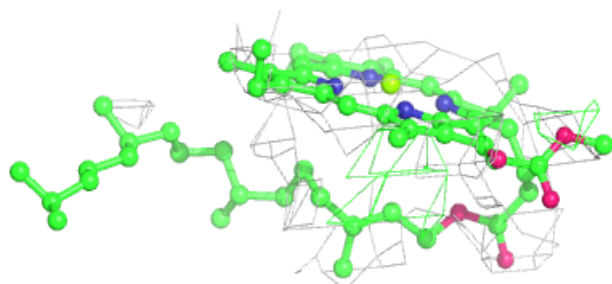
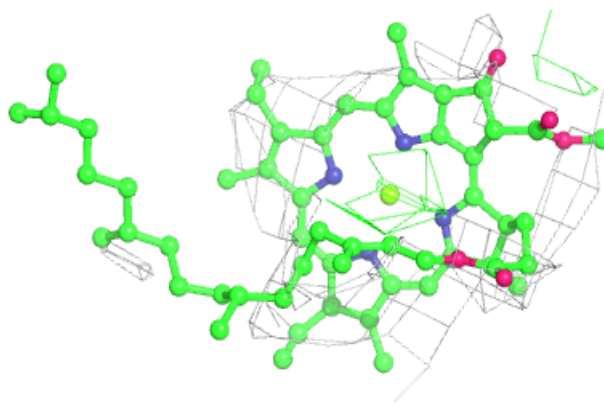
Electron density around CLA J 1103:

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



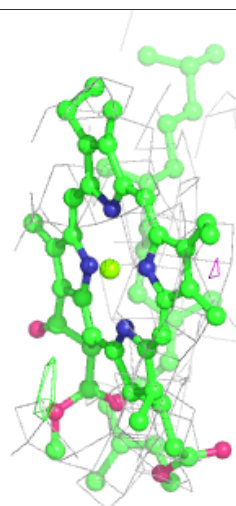
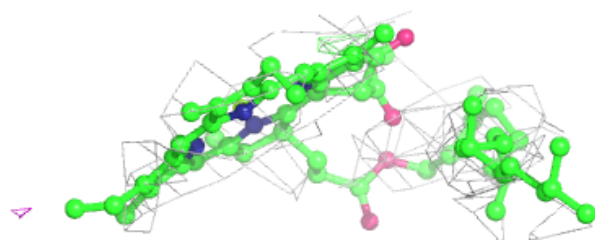
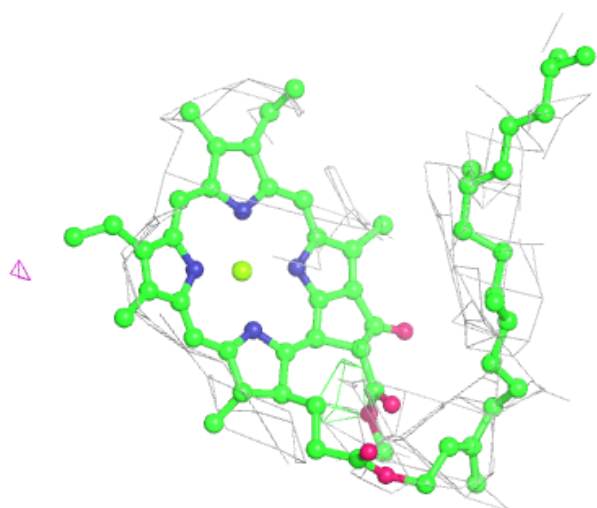
Electron density around CLA B 836:

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



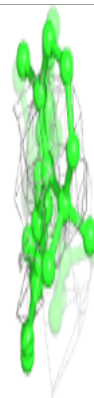
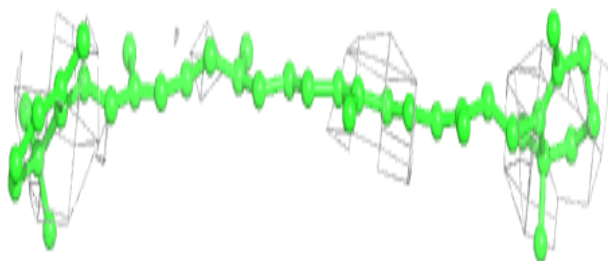
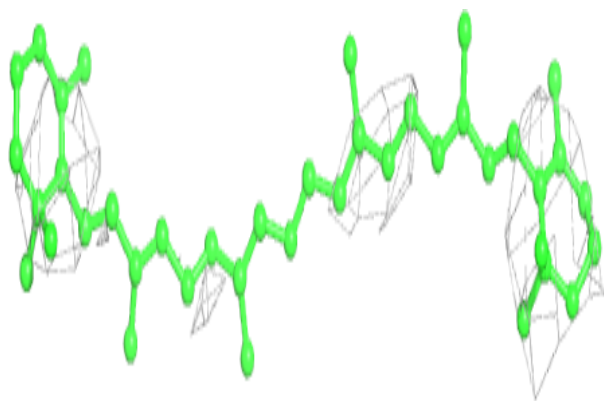
Electron density around CLA A 825:

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

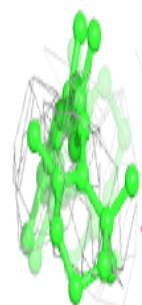
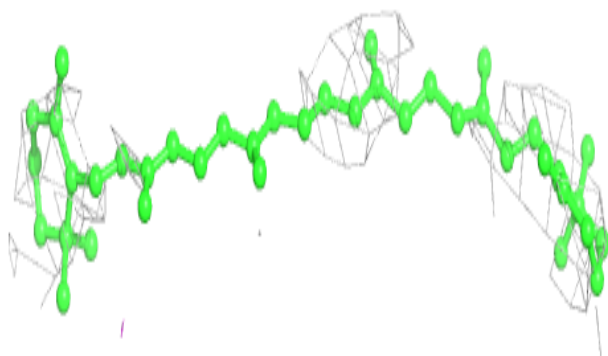
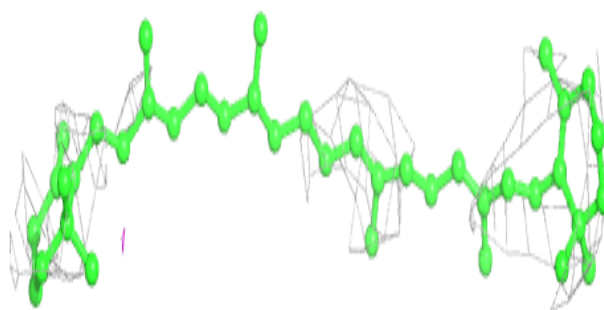


Electron density around BCR J 1104:

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

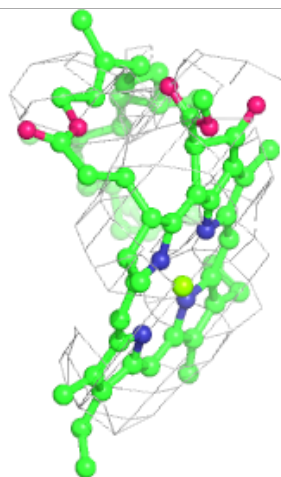
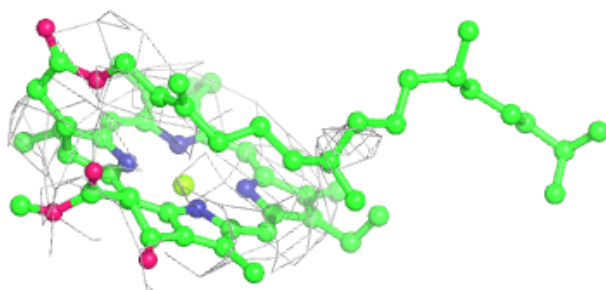
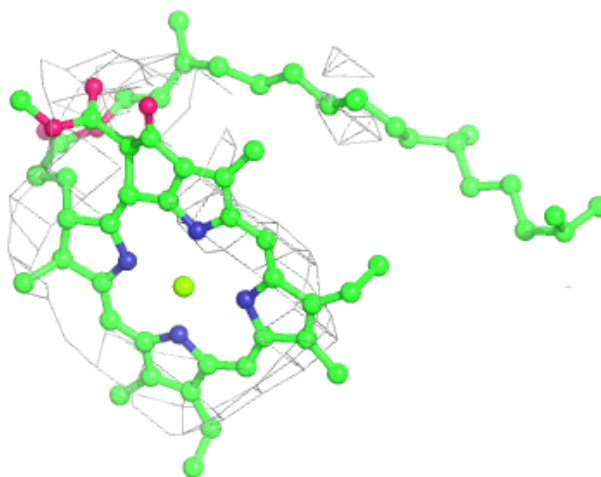
**Electron density around BCR A 851:**

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



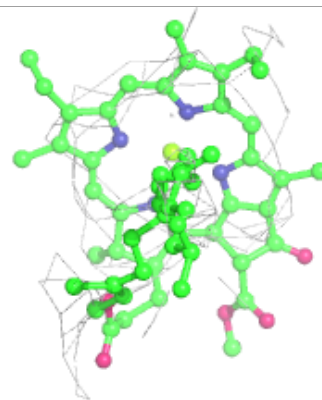
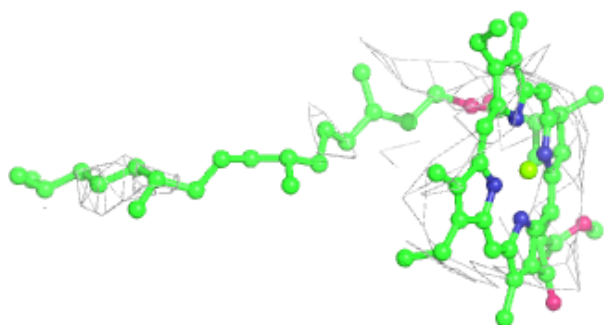
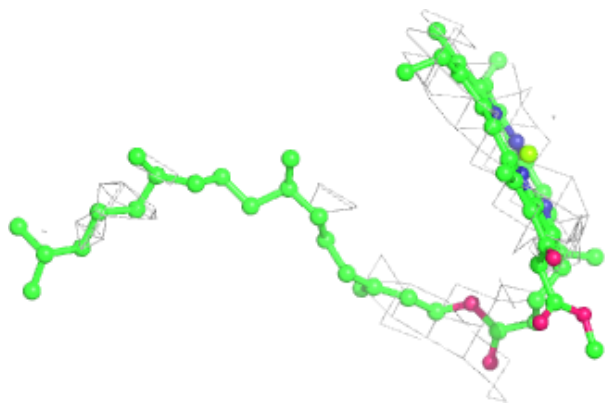
Electron density around CLA A 829:

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

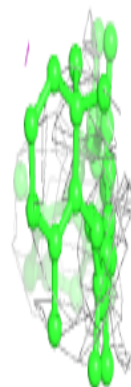
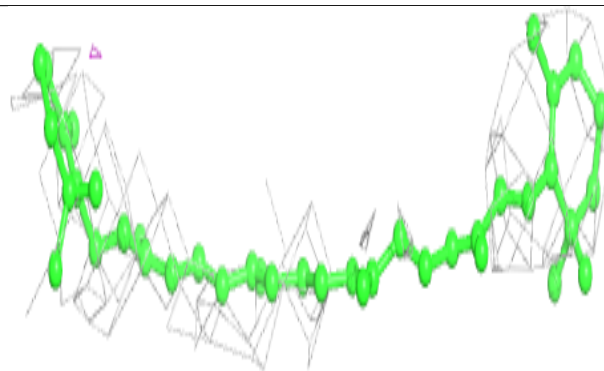
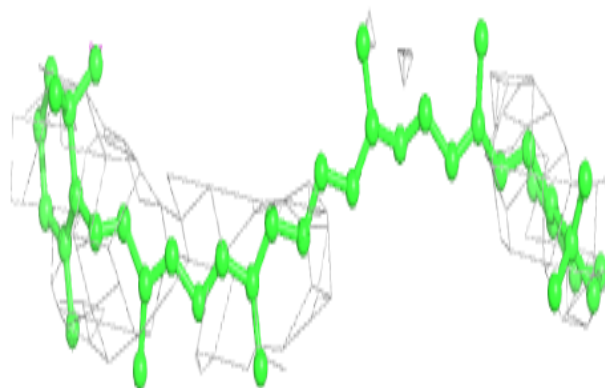


Electron density around CLA A 811:

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

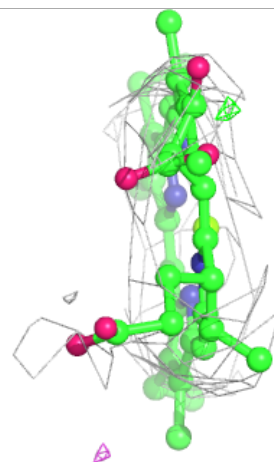
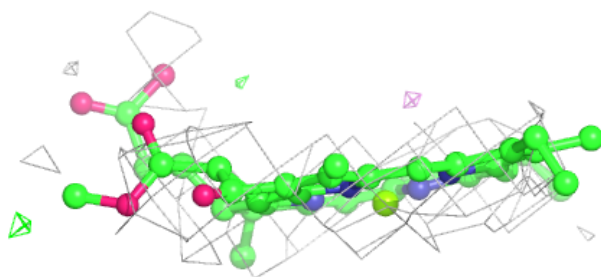
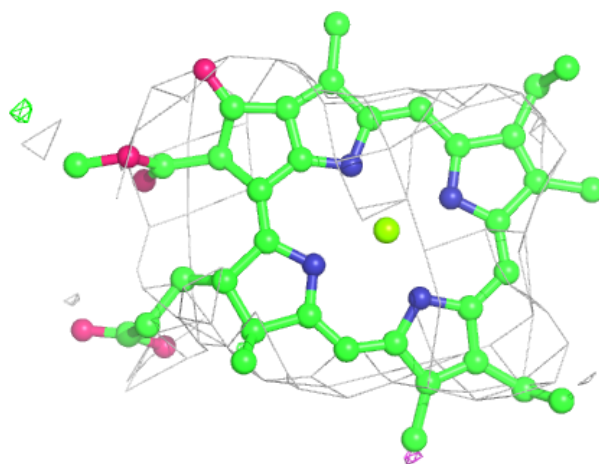
**Electron density around BCR M 1203:**

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



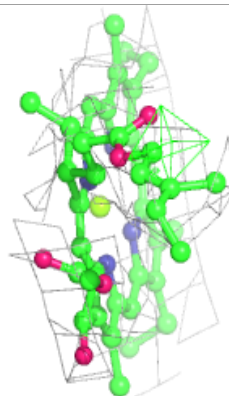
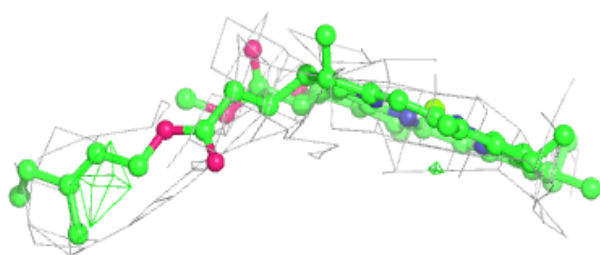
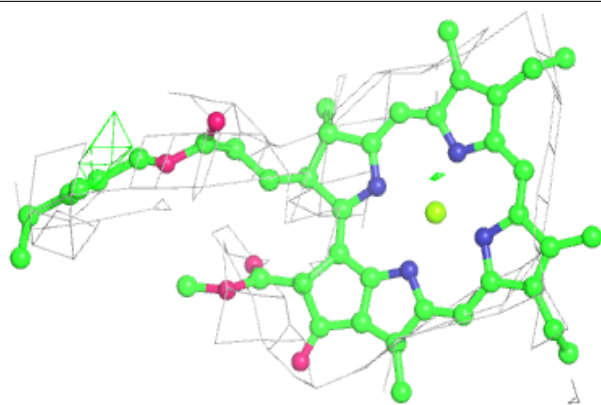
Electron density around CLA B 809:

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

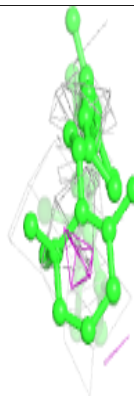
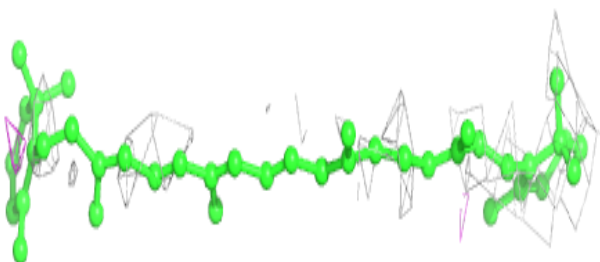
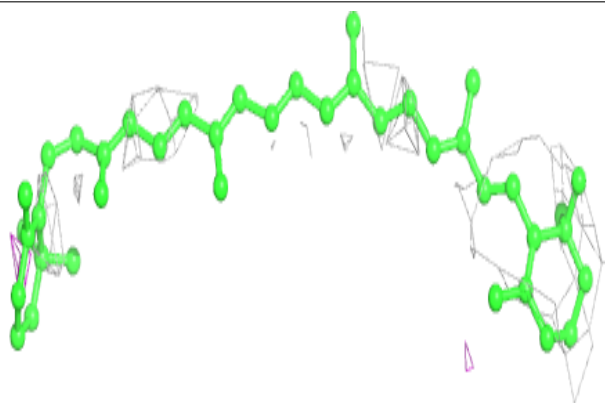


Electron density around CLA A 841:

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

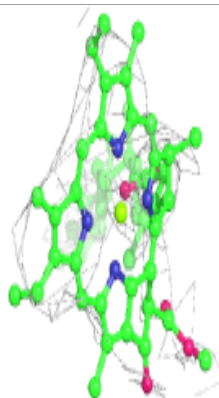
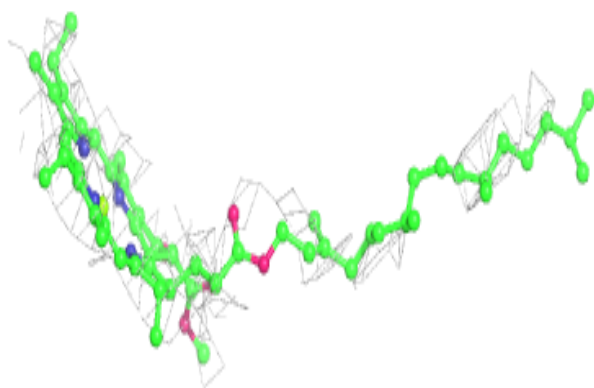
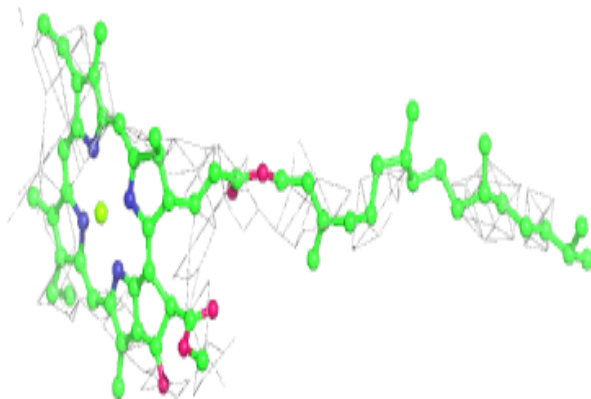
**Electron density around BCR B 842:**

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

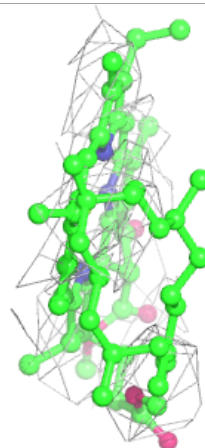
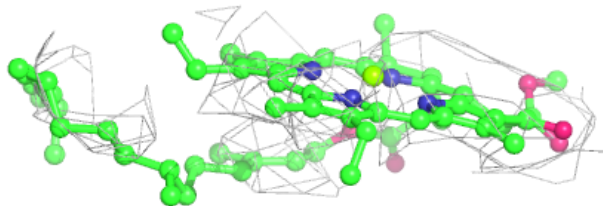
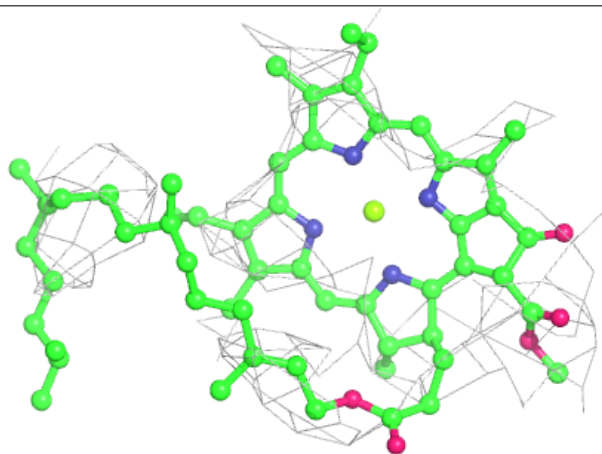


Electron density around CLA A 809:

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

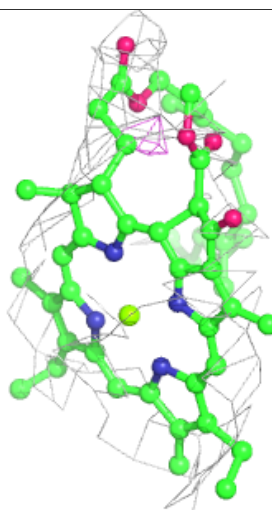
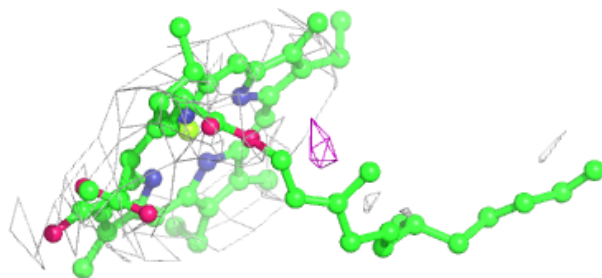
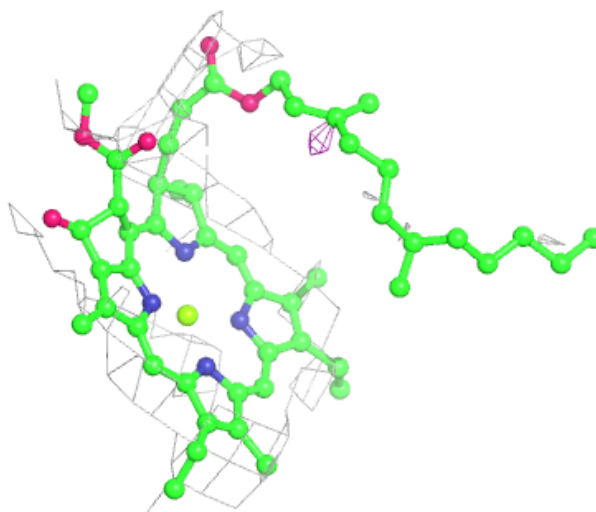
**Electron density around CLA A 819:**

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



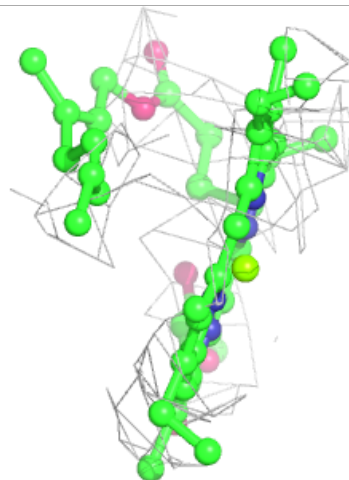
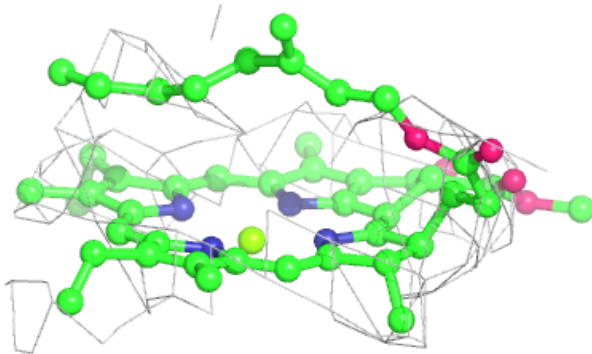
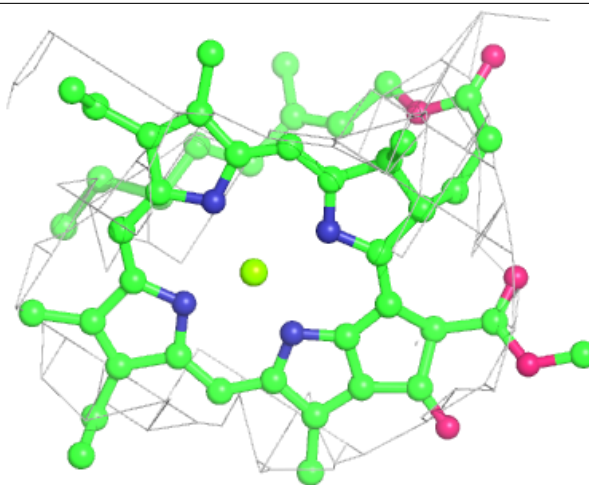
Electron density around CLA A 824:

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



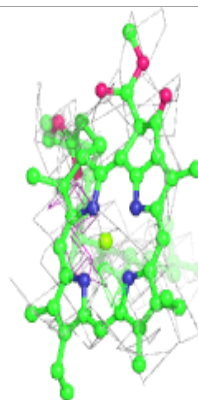
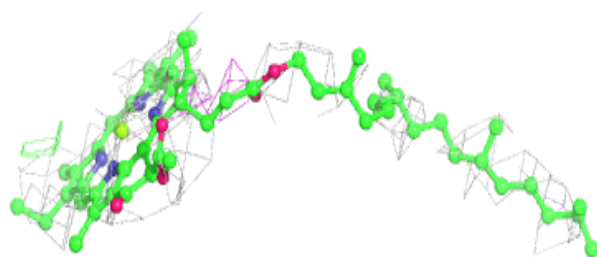
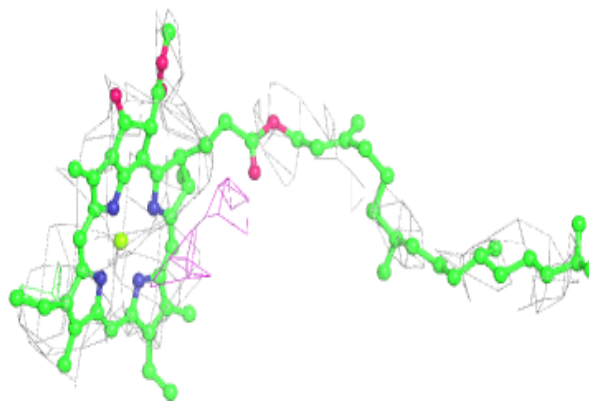
Electron density around CLA A 818:

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



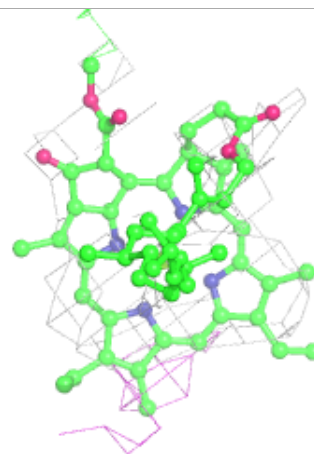
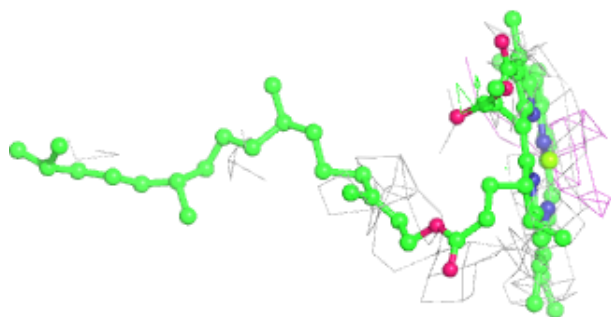
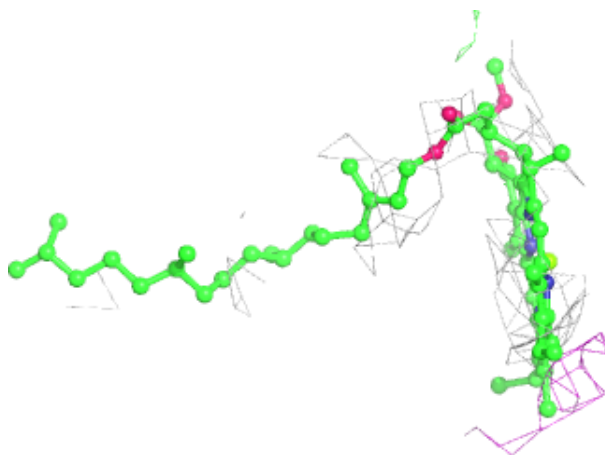
Electron density around CLA A 802:

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



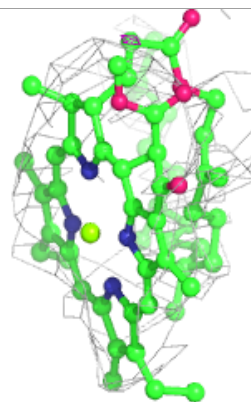
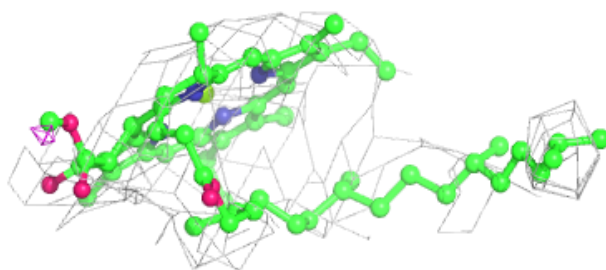
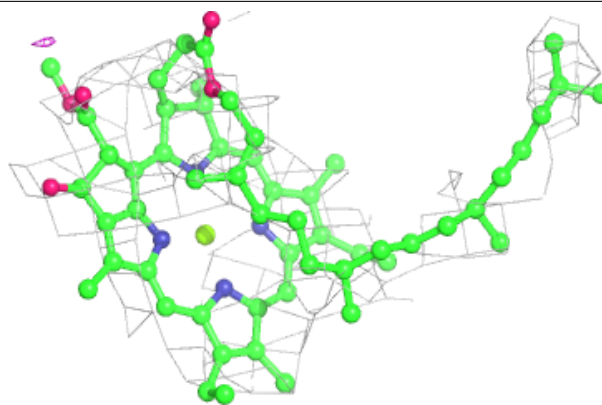
Electron density around CLA A 828:

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

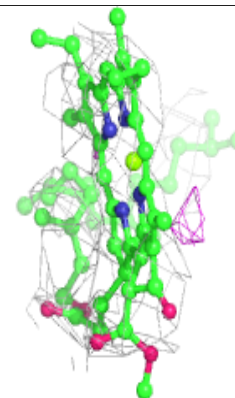
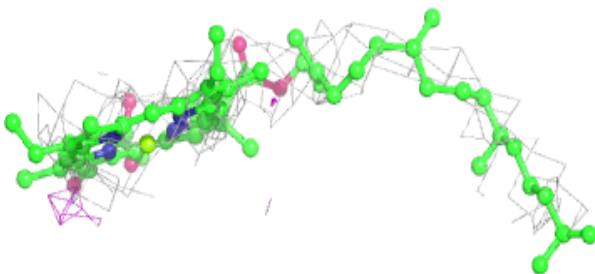
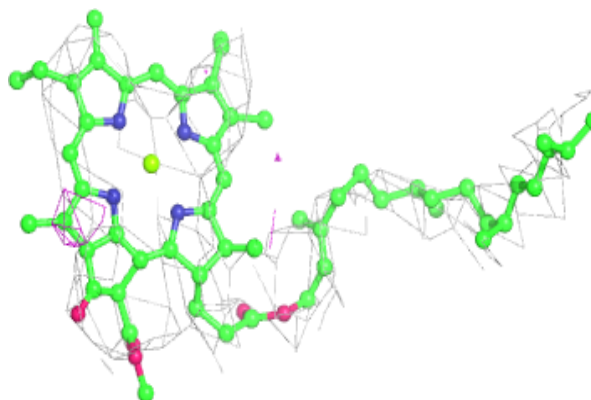


Electron density around CLA B 806:

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

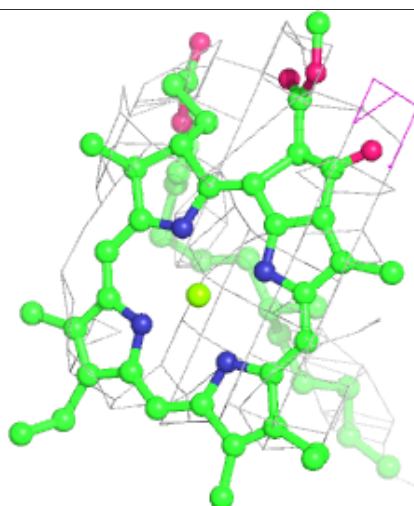
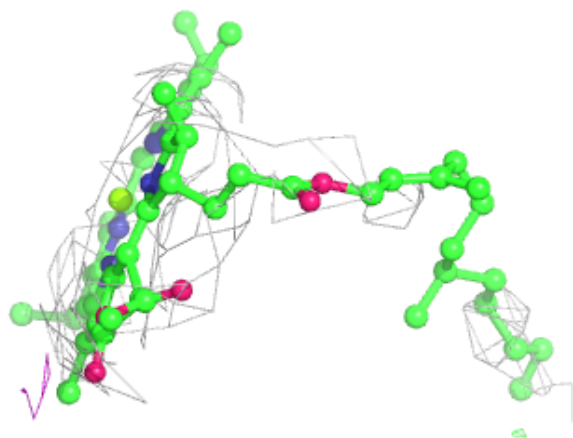
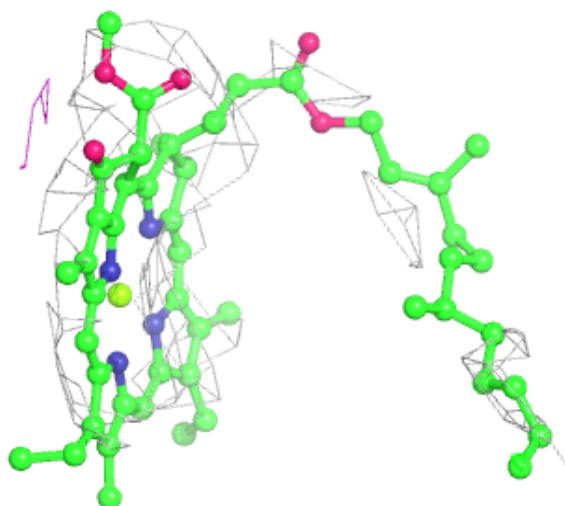
**Electron density around CLA B 803:**

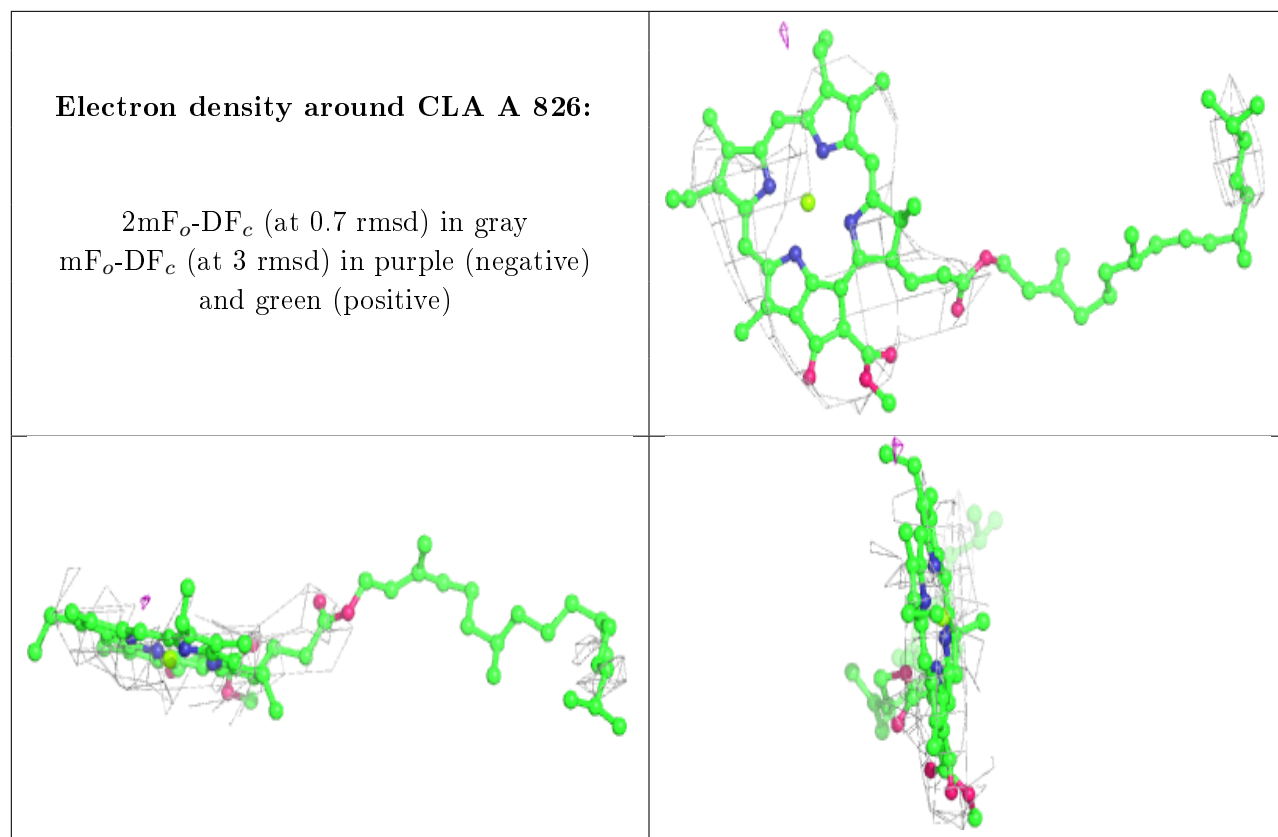
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA A 804:

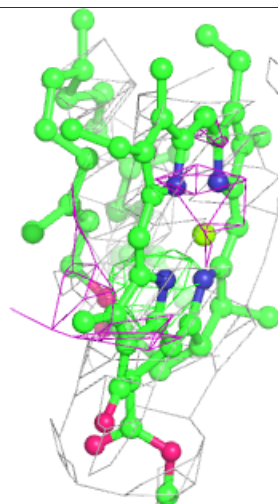
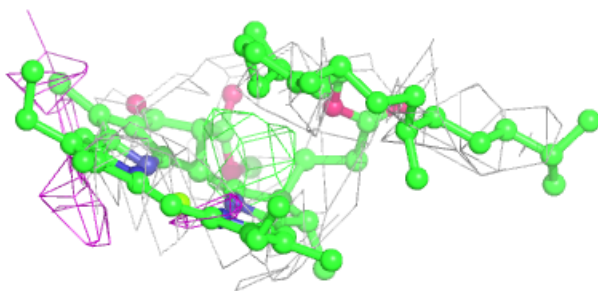
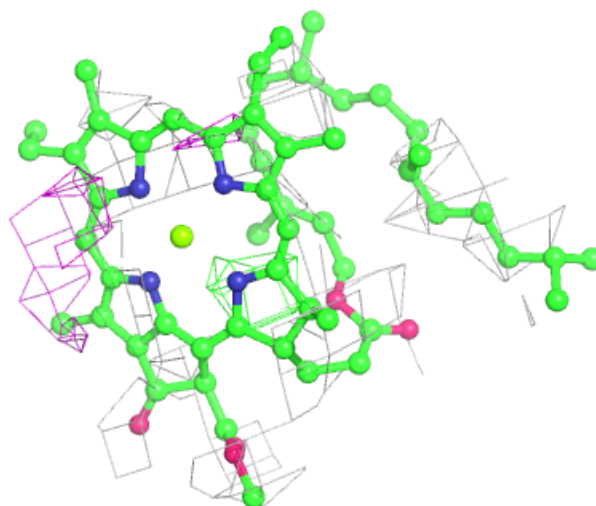
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





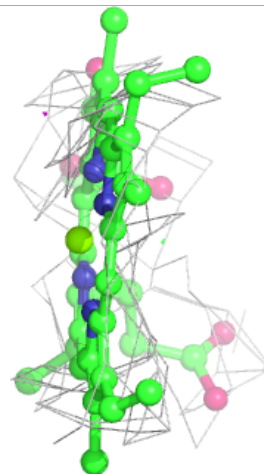
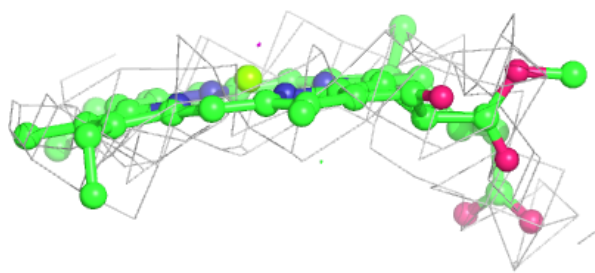
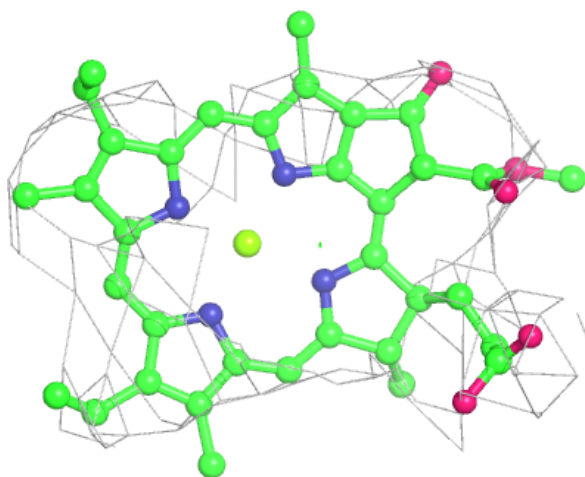
Electron density around CLA B 807:

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



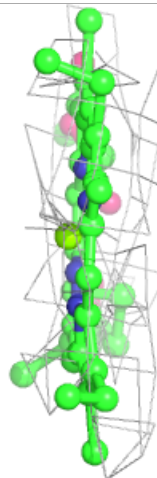
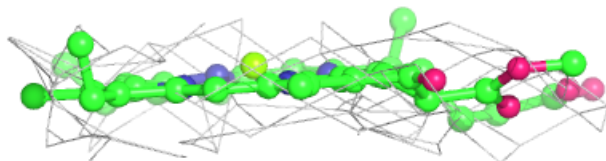
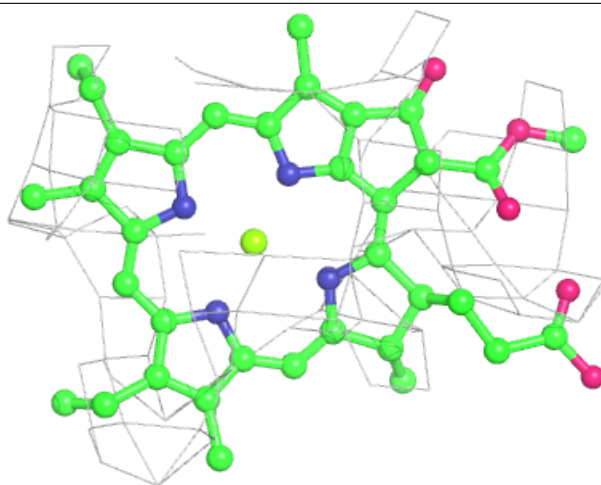
Electron density around CLA B 832:

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



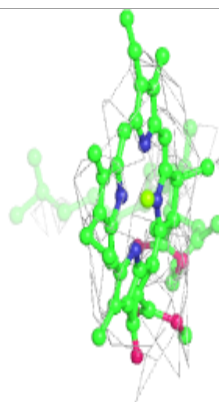
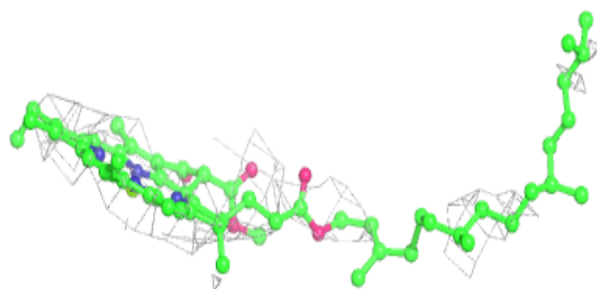
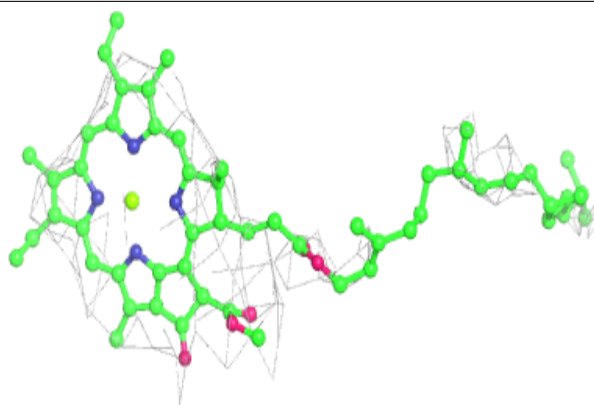
Electron density around CLA F 1301:

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

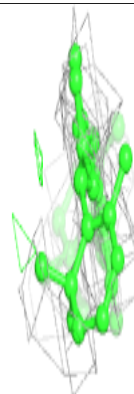
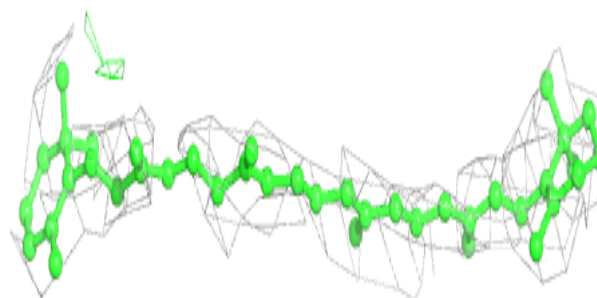
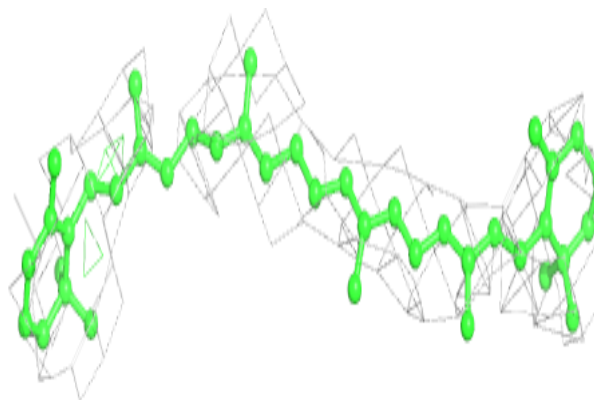


Electron density around CLA A 805:

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

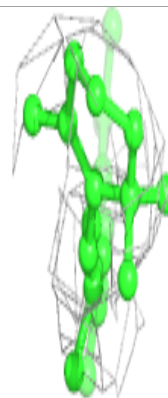
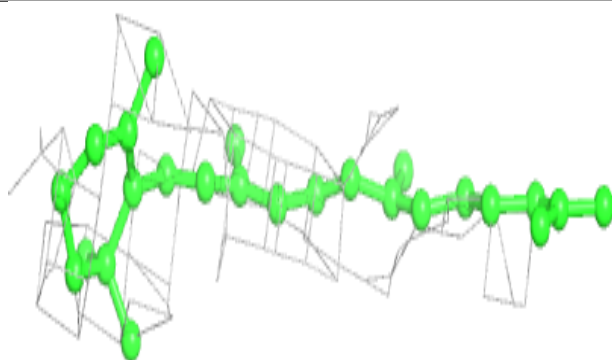
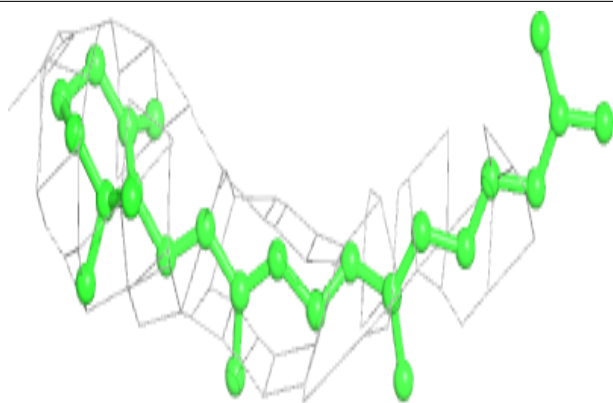
**Electron density around BCR B 845:**

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

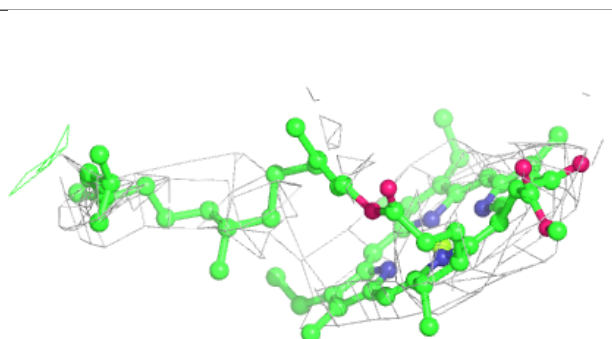
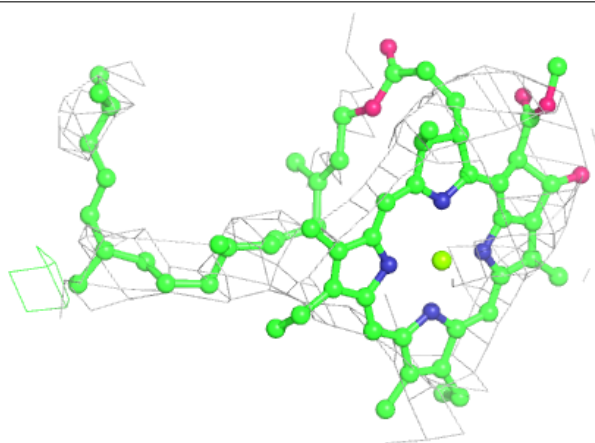


Electron density around BCR B 844:

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

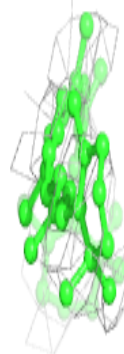
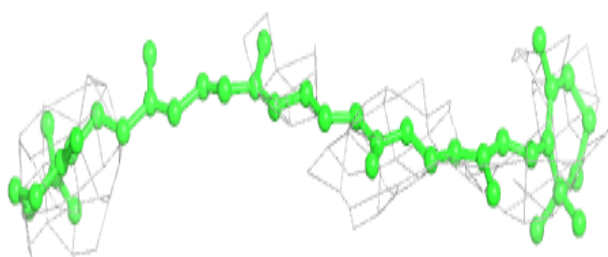
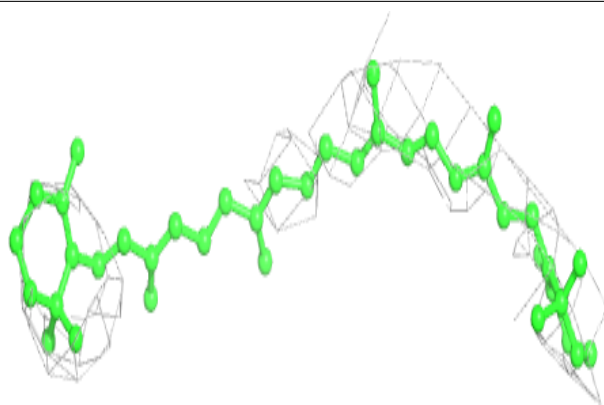
**Electron density around CLA A 843:**

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

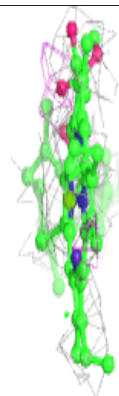
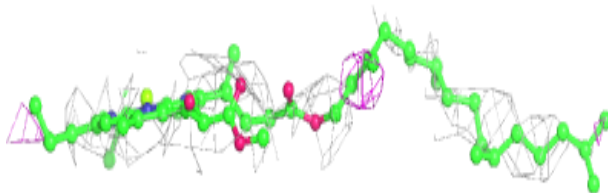
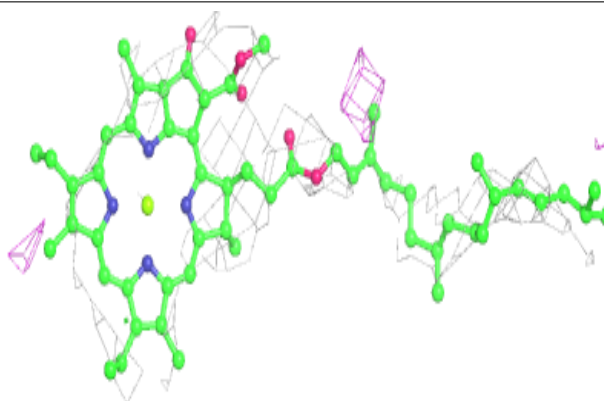


Electron density around BCR B 846:

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

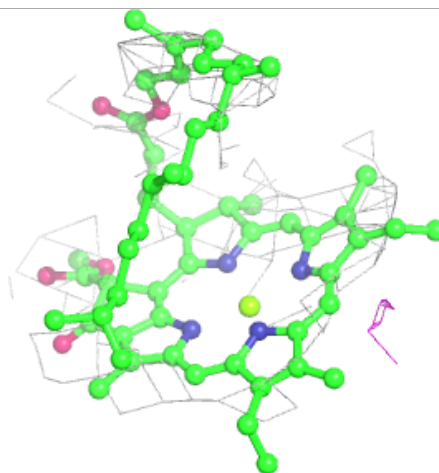
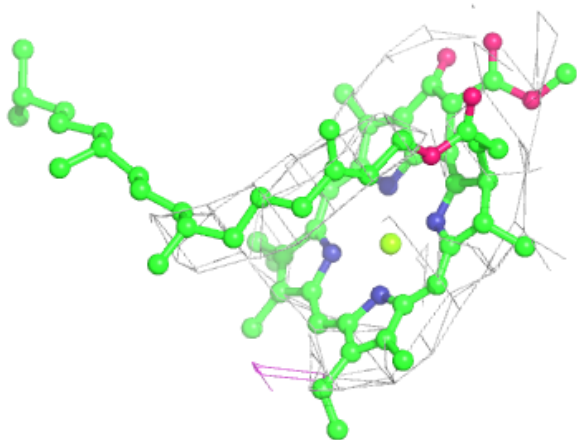
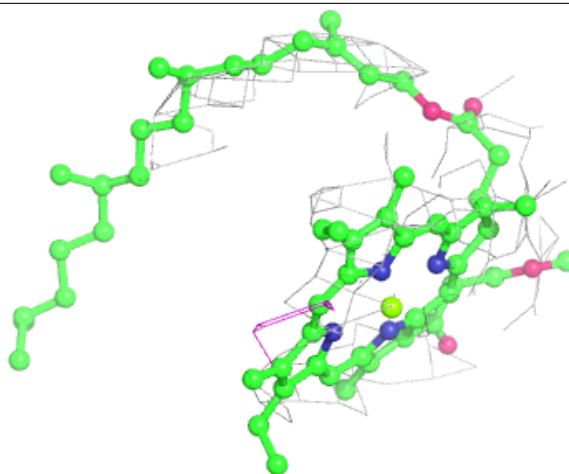
**Electron density around CLA A 833:**

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



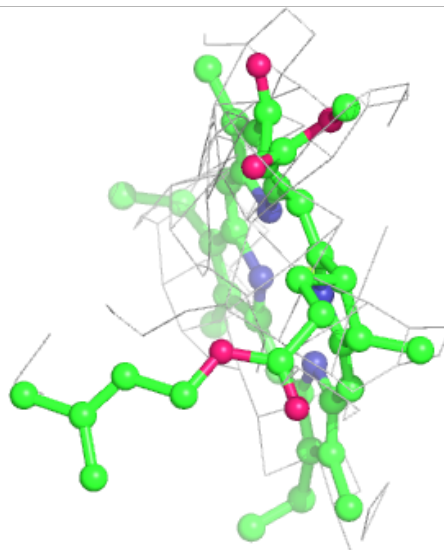
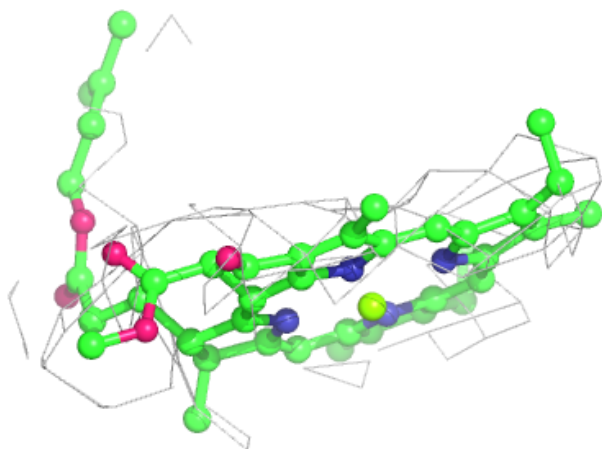
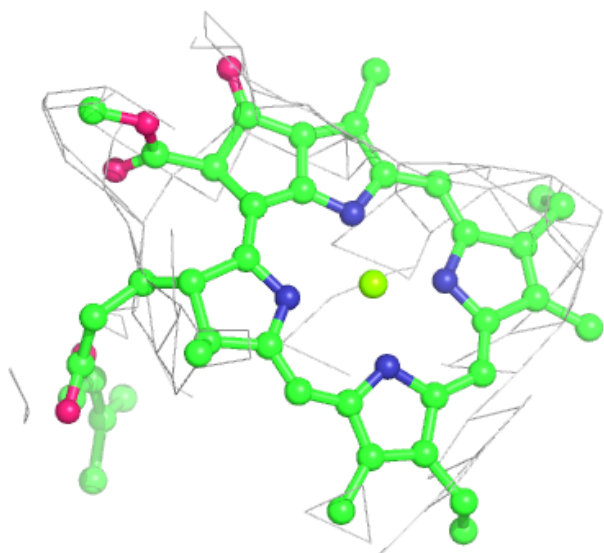
Electron density around CLA B 817:

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



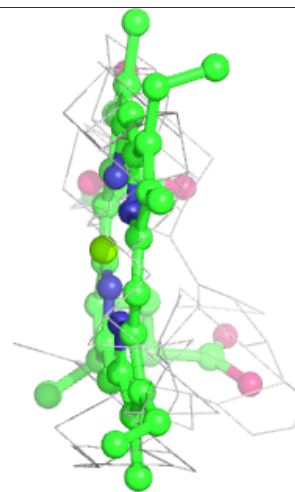
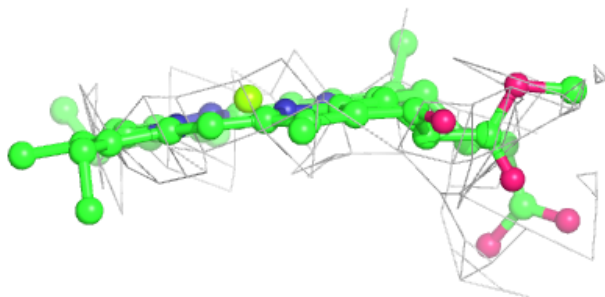
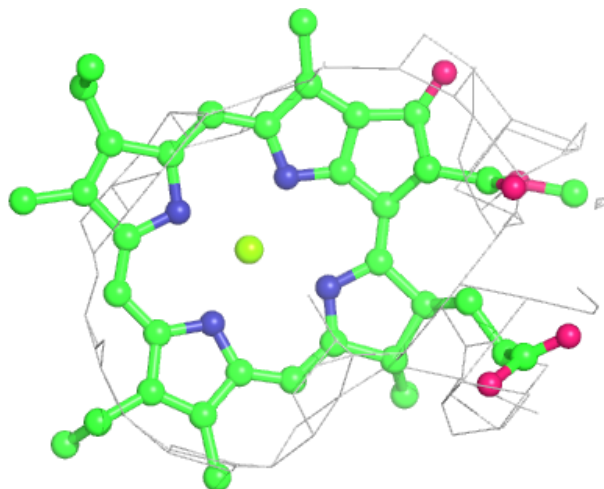
Electron density around CLA A 831:

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



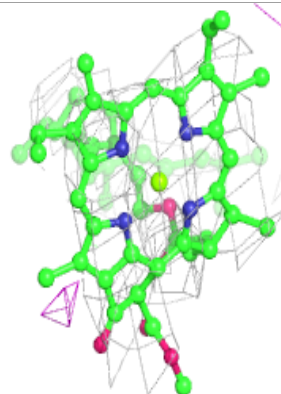
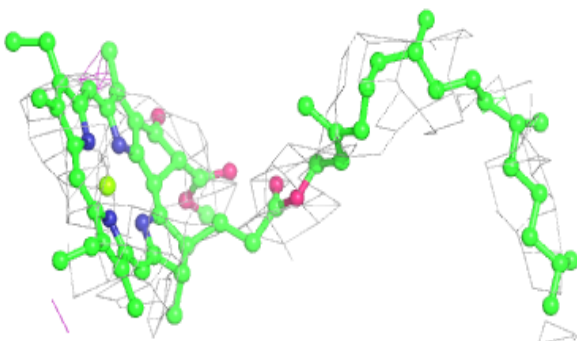
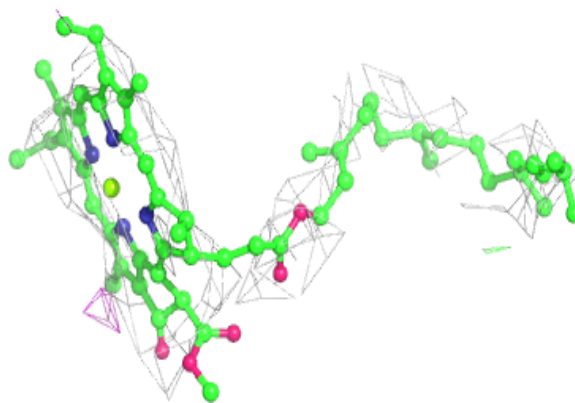
Electron density around CLA A 814:

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

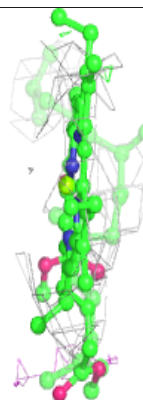
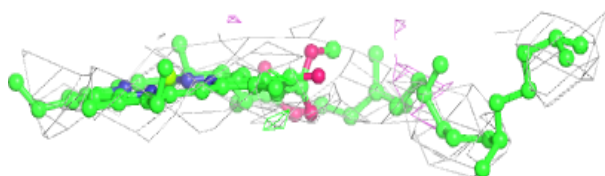
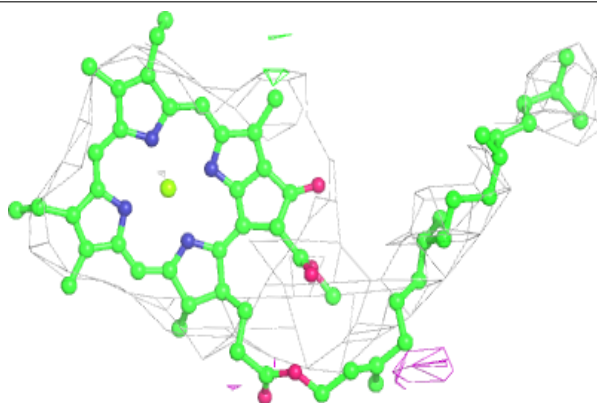


Electron density around CLA B 838:

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

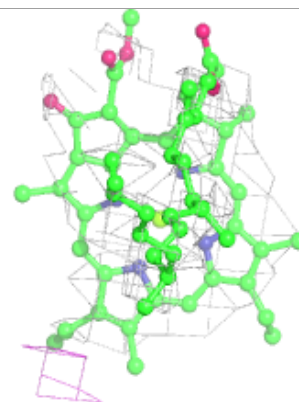
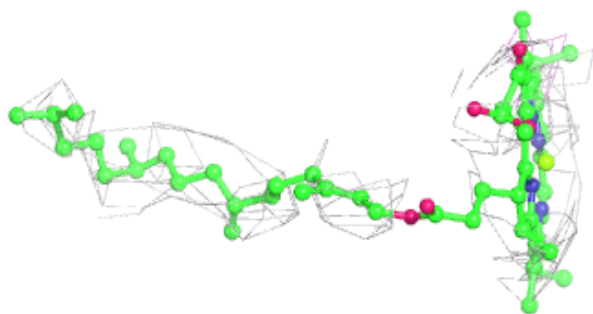
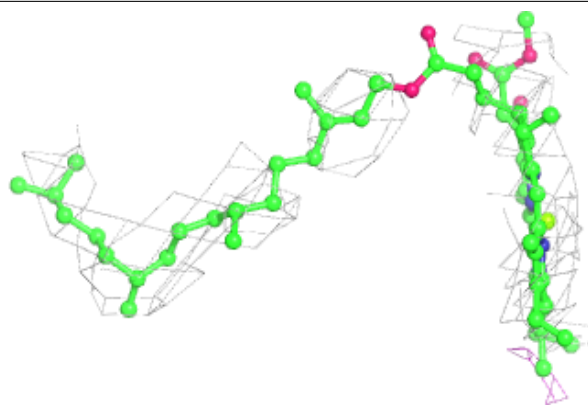
**Electron density around CLA L 1004:**

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

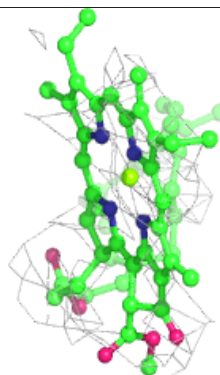
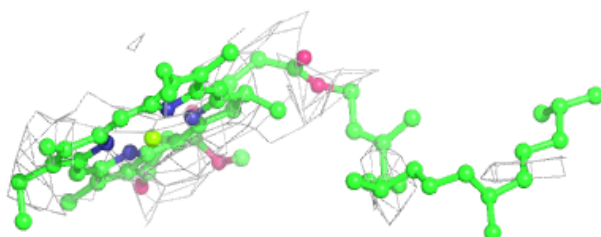
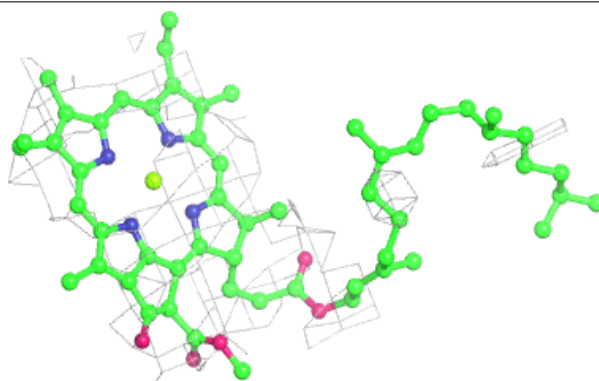


Electron density around CLA B 839:

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

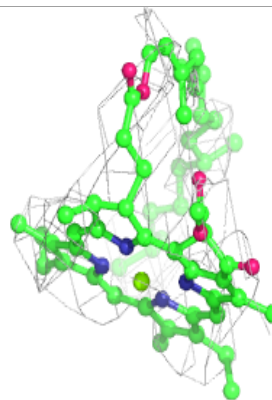
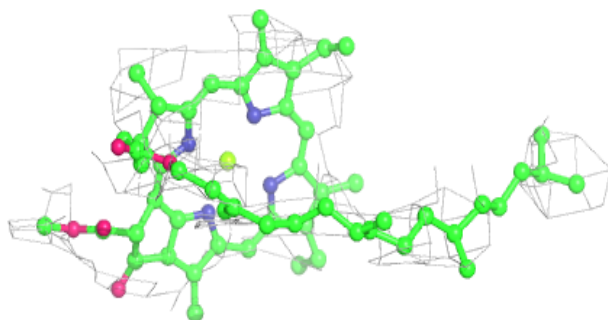
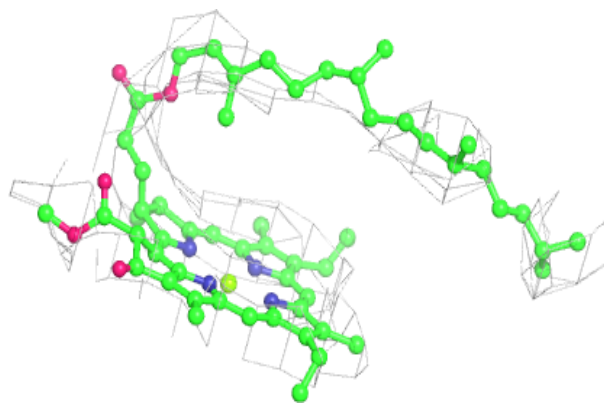
**Electron density around CLA J 1101:**

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



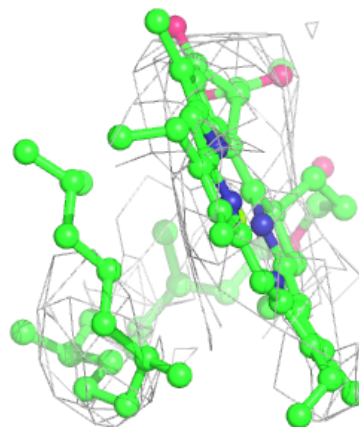
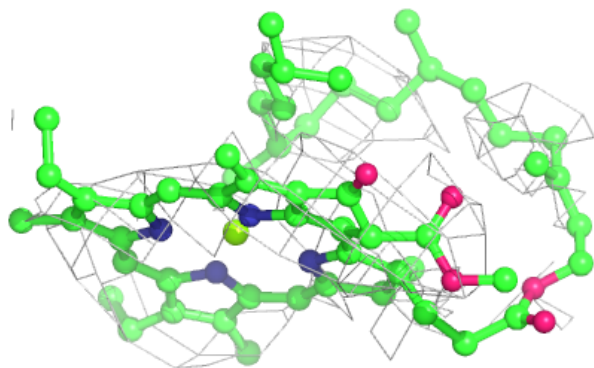
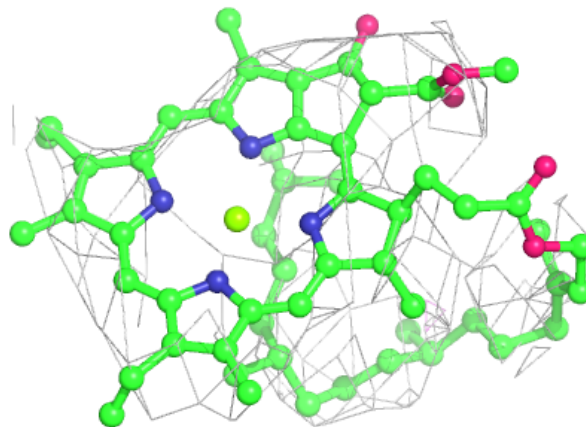
Electron density around CLA A 832:

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



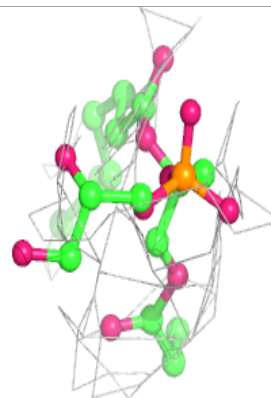
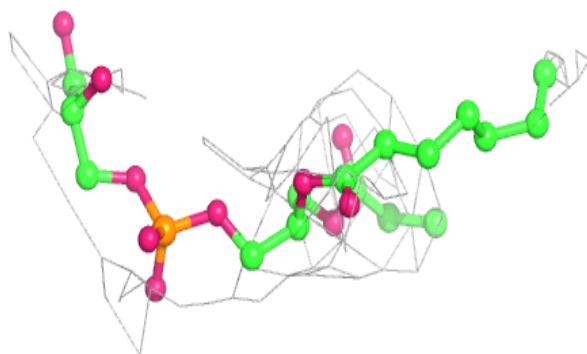
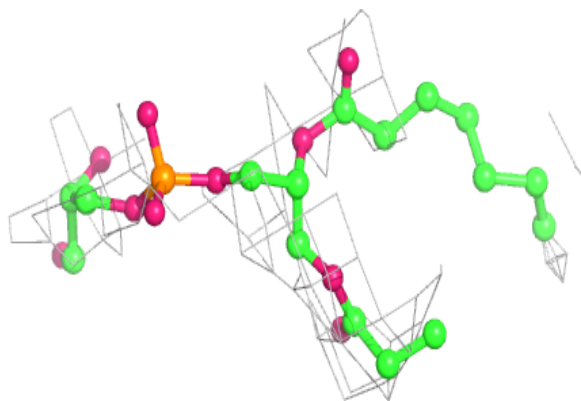
Electron density around CLA A 806:

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

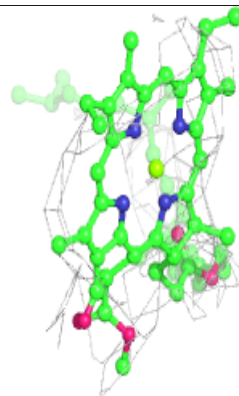
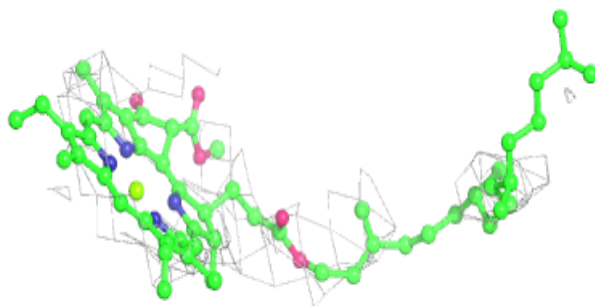
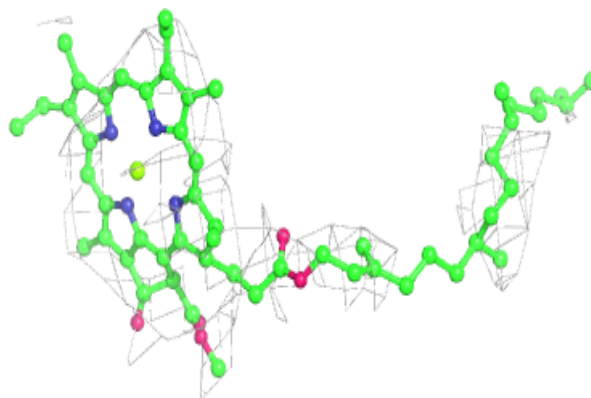


Electron density around LHG A 854:

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

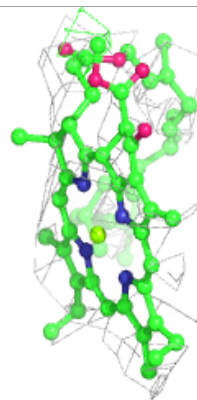
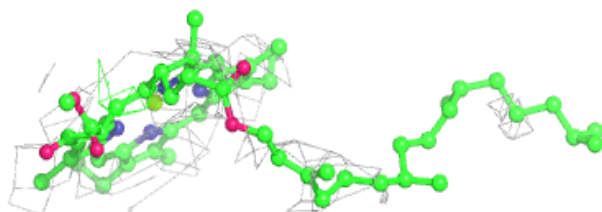
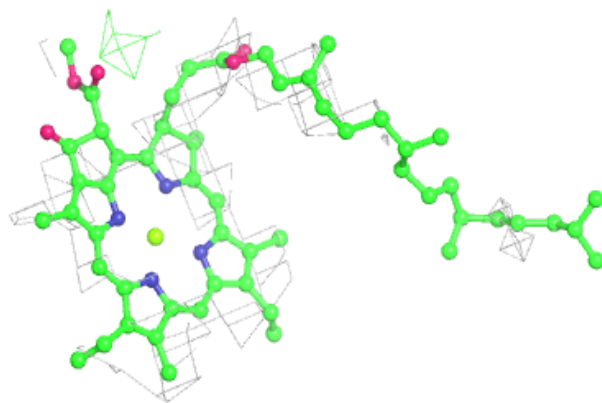
**Electron density around CLA B 802:**

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

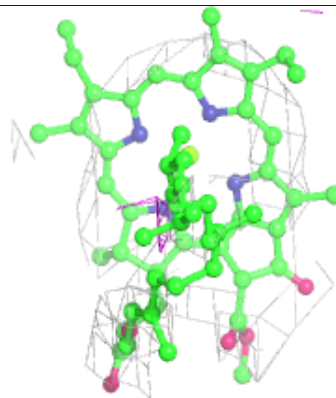
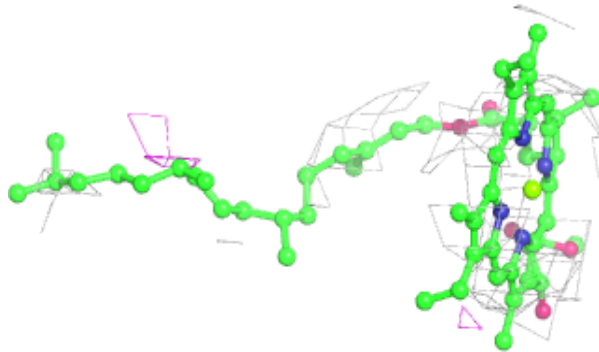
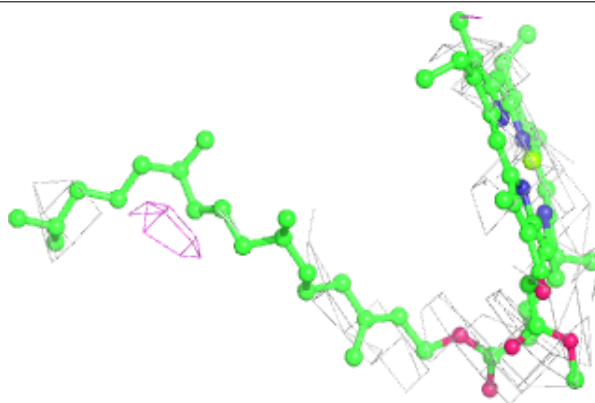


Electron density around CLA A 808:

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

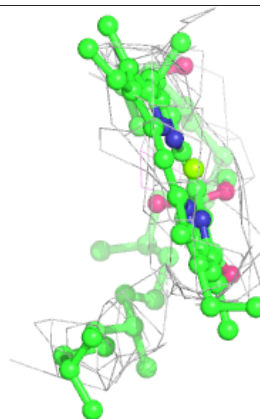
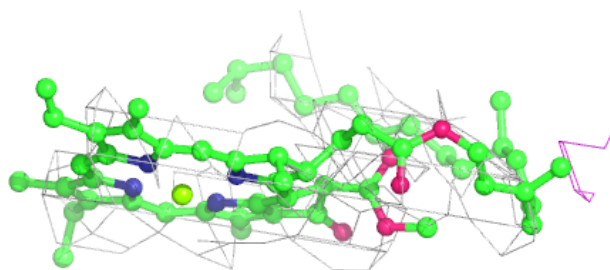
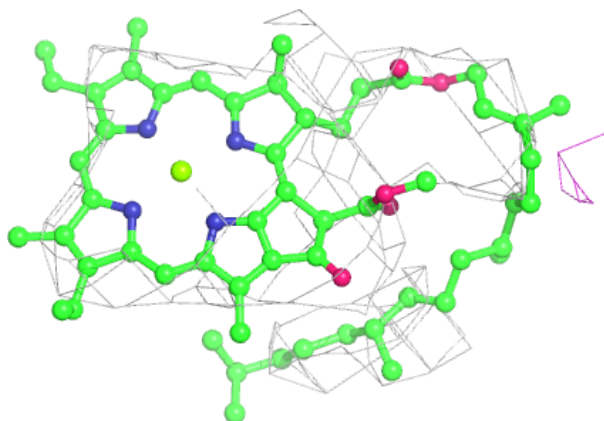
**Electron density around CLA A 830:**

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

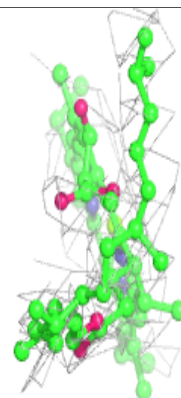
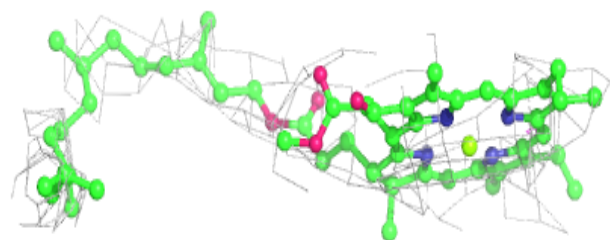
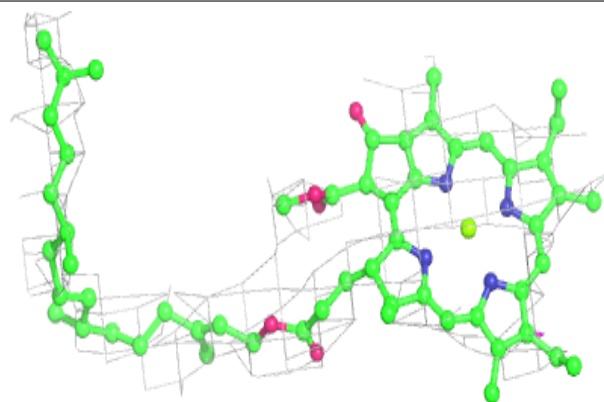


Electron density around CLA B 804:

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

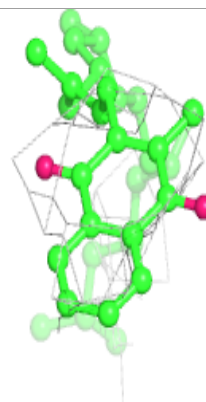
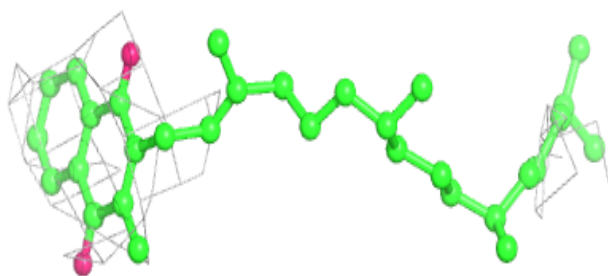
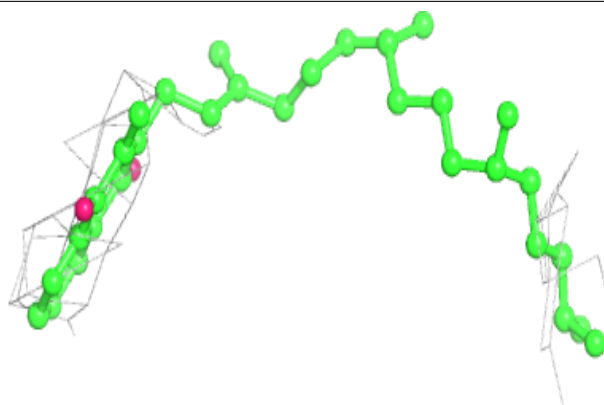
**Electron density around CLA B 824:**

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



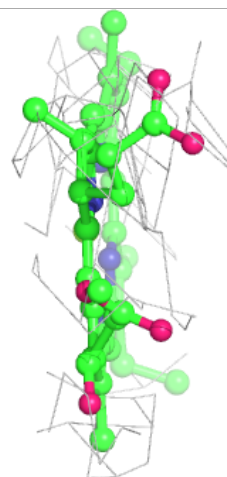
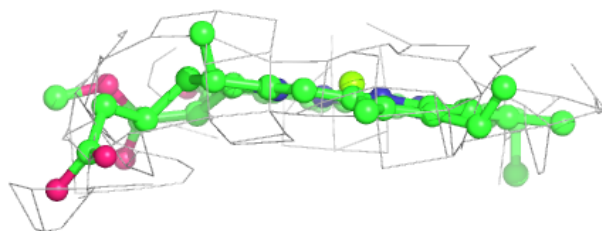
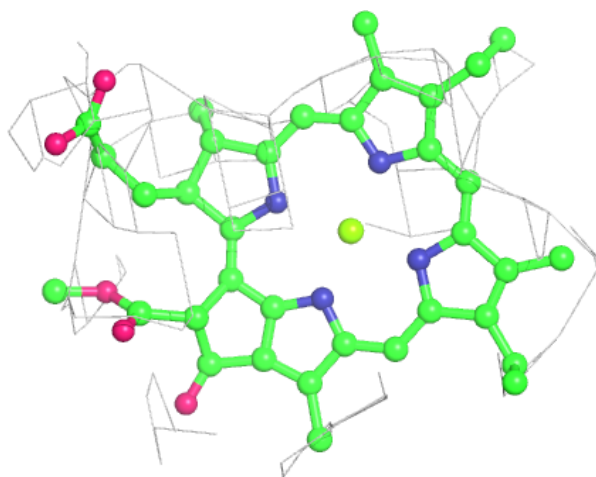
Electron density around PQN B 840:

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



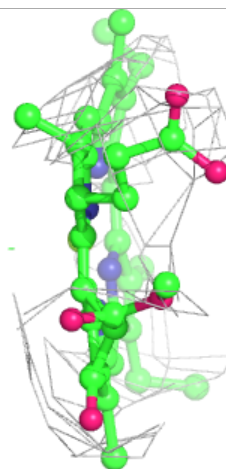
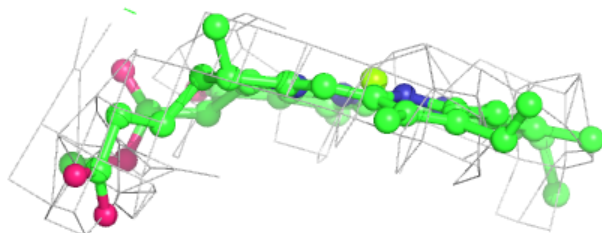
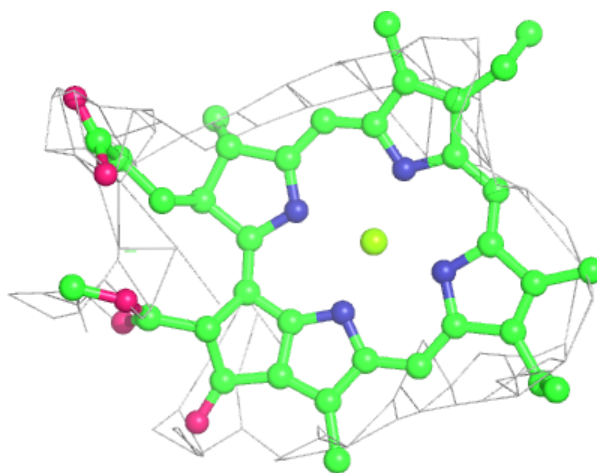
Electron density around CLA X 102:

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



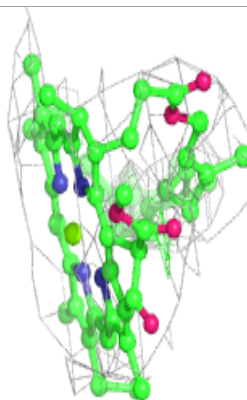
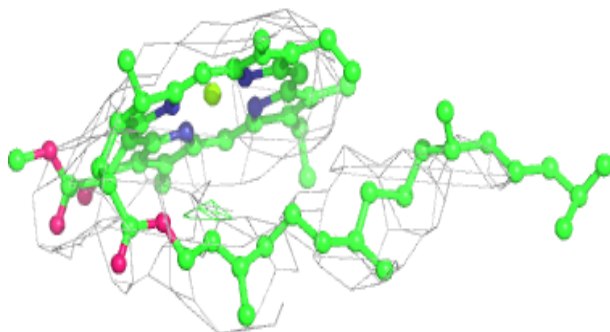
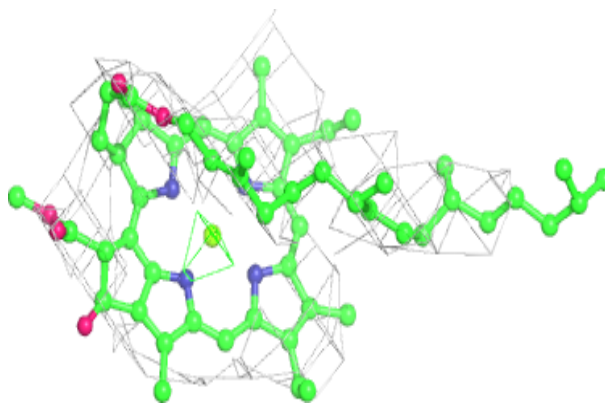
Electron density around CLA B 821:

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

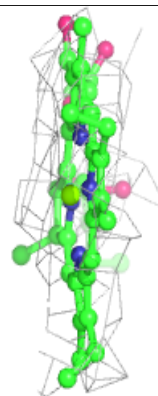
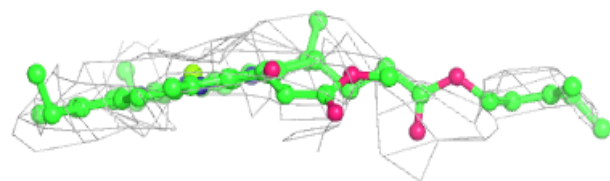
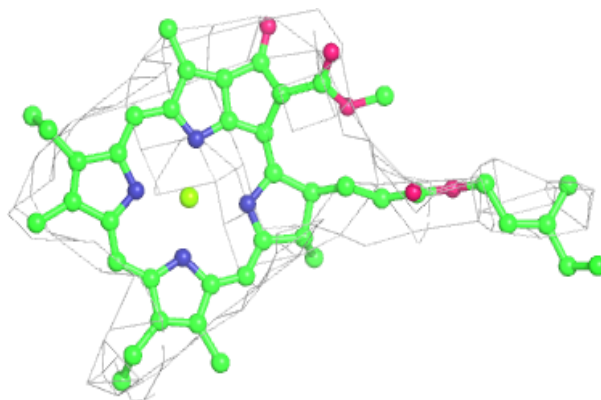


Electron density around CLA A 838:

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

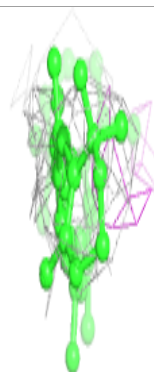
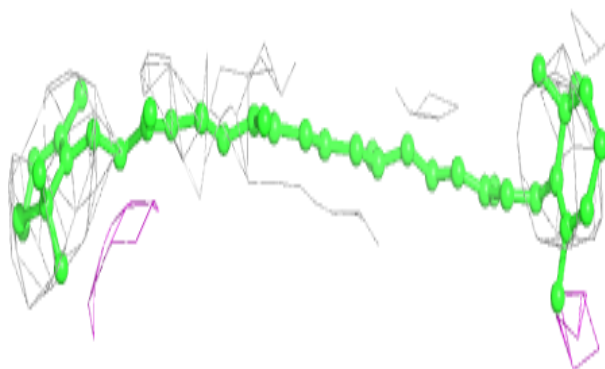
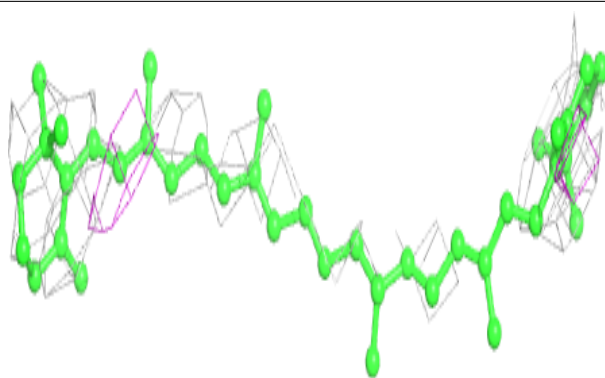
**Electron density around CLA A 837:**

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

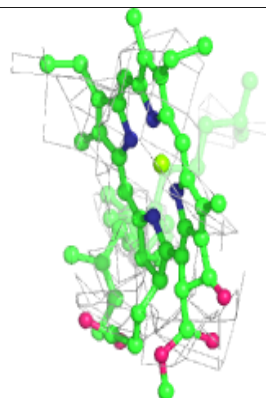
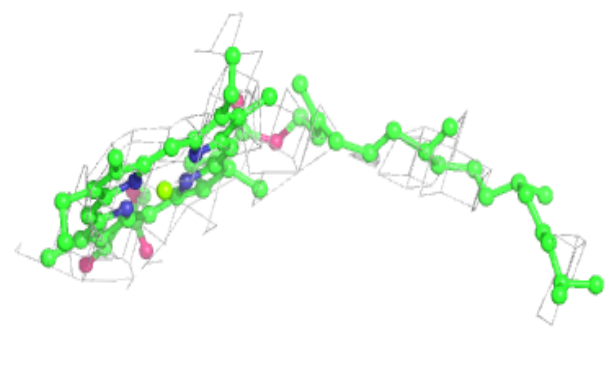
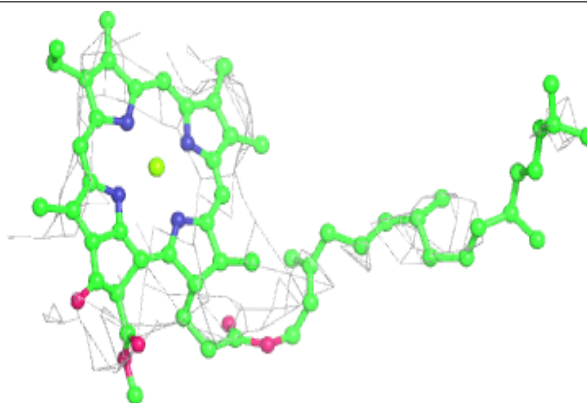


Electron density around BCR B 847:

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

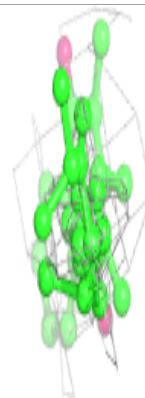
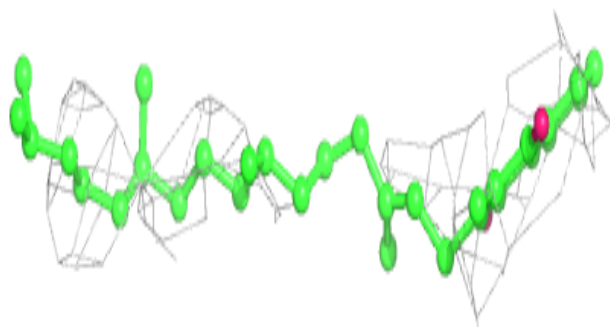
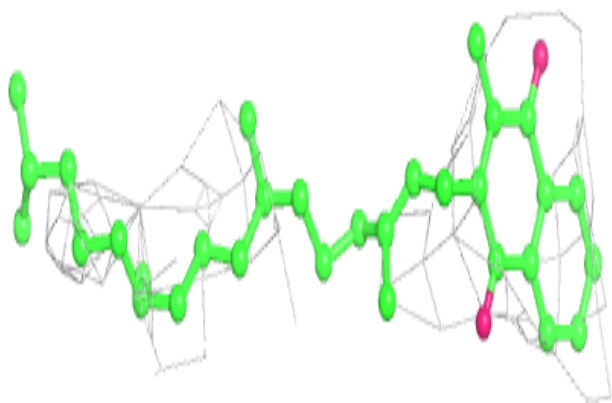
**Electron density around CLA A 803:**

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



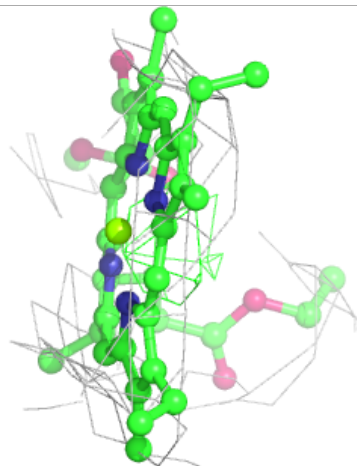
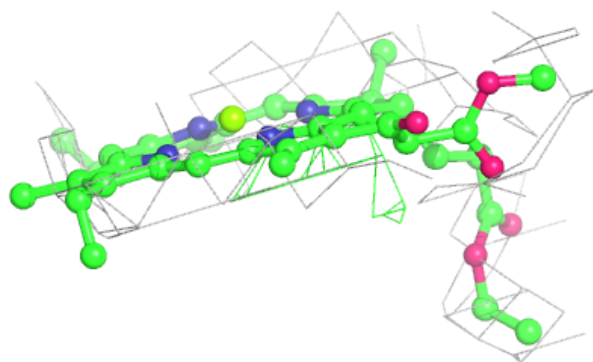
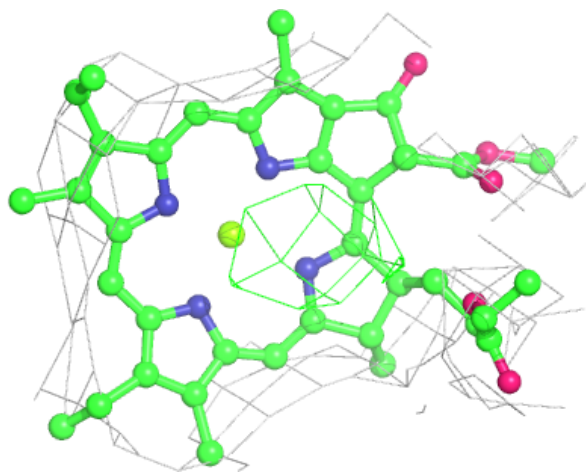
Electron density around PQN A 846:

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



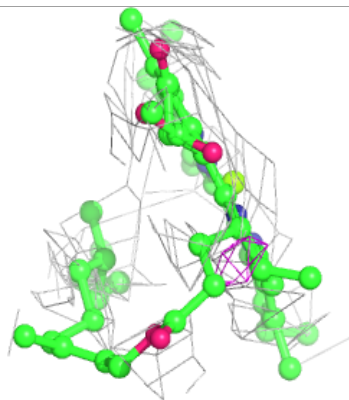
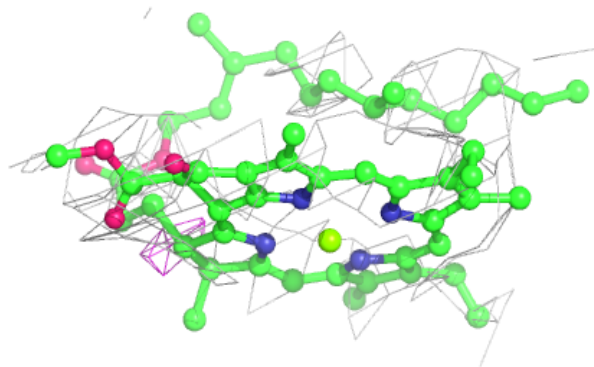
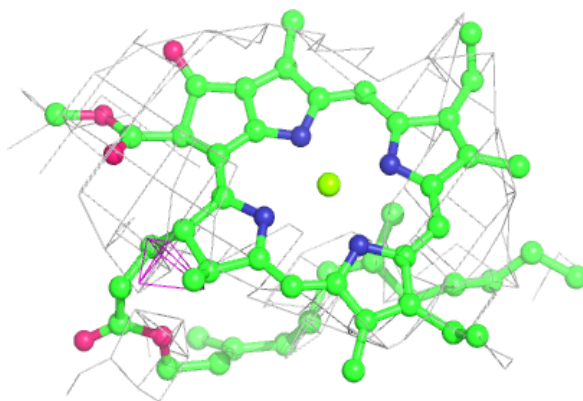
Electron density around CLA B 837:

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

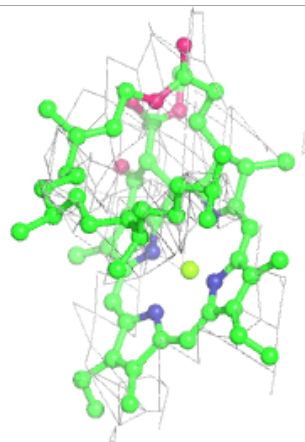
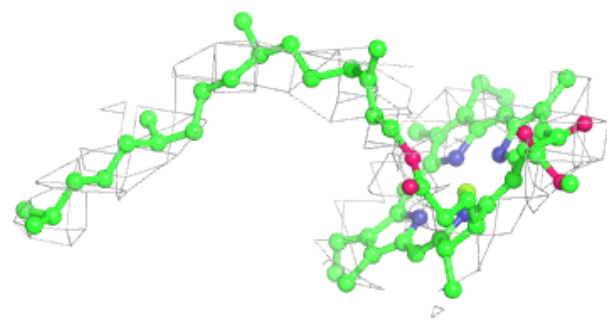
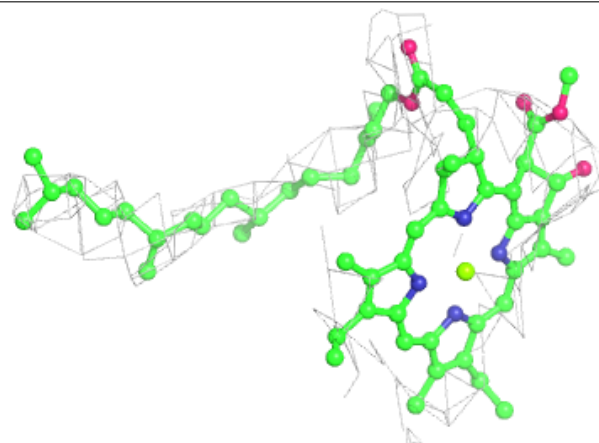


Electron density around CLA B 815:

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

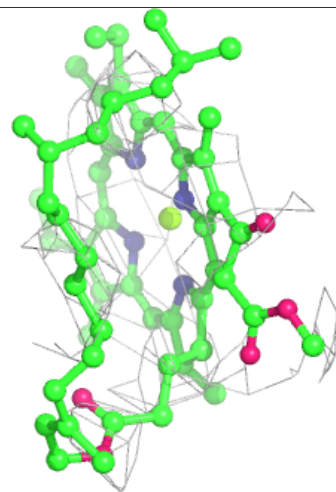
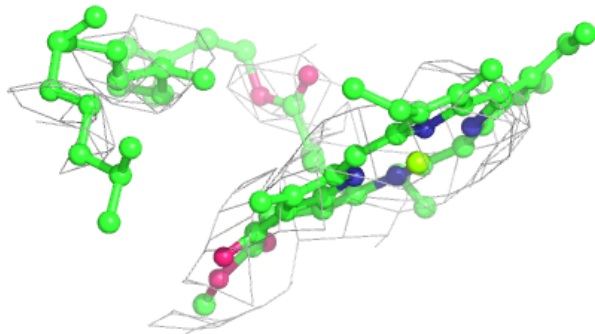
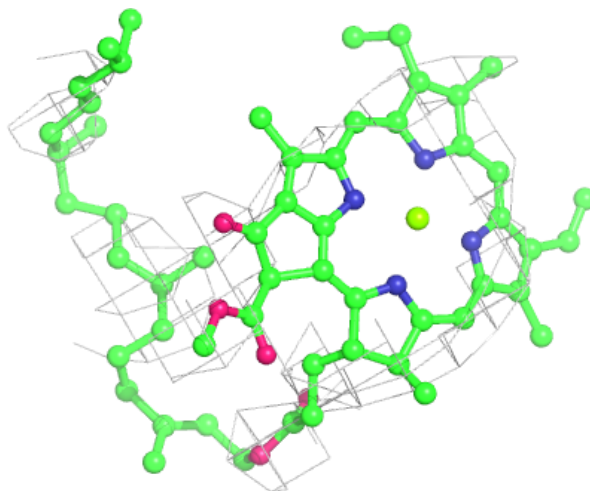
**Electron density around CLA B 812:**

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



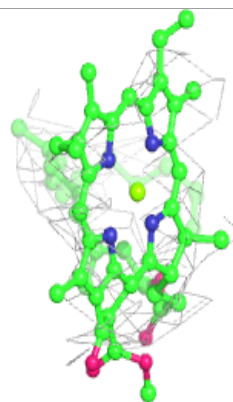
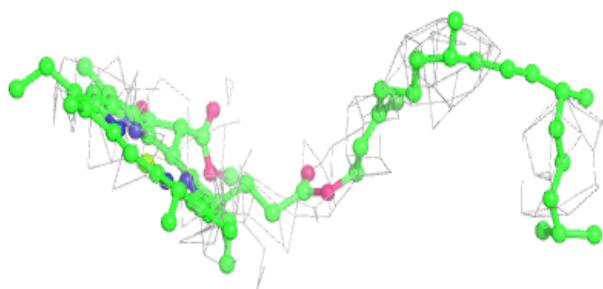
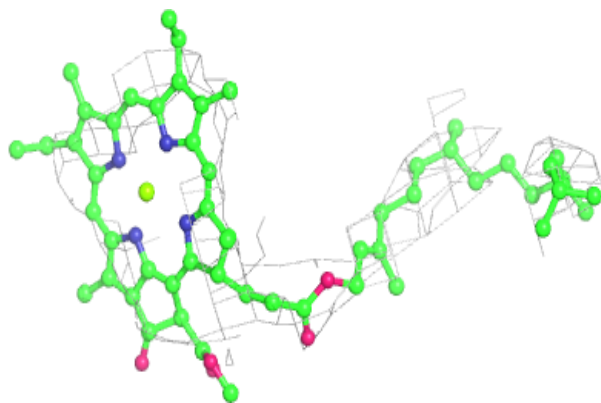
Electron density around CLA B 830:

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

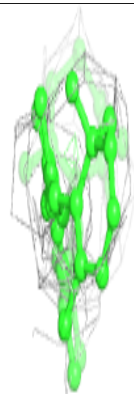
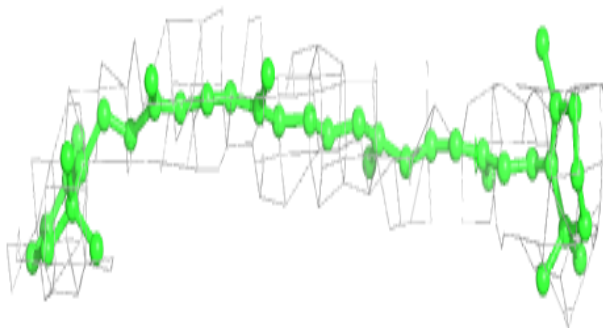
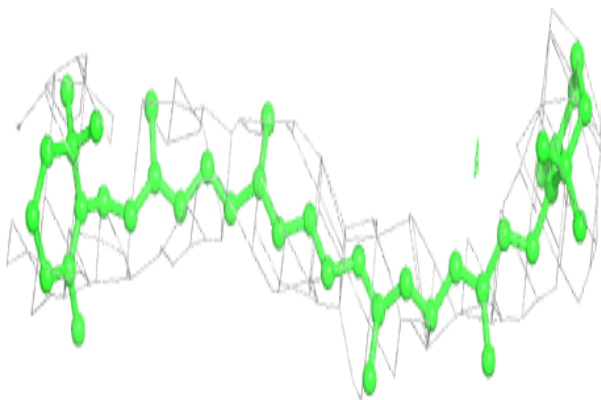


Electron density around CLA B 808:

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

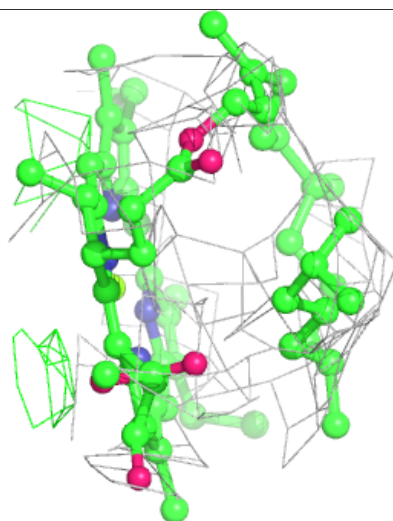
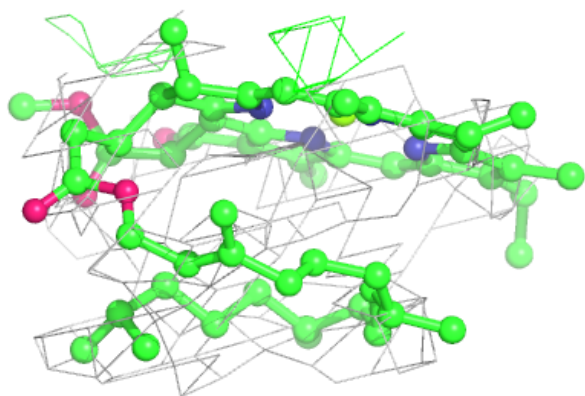
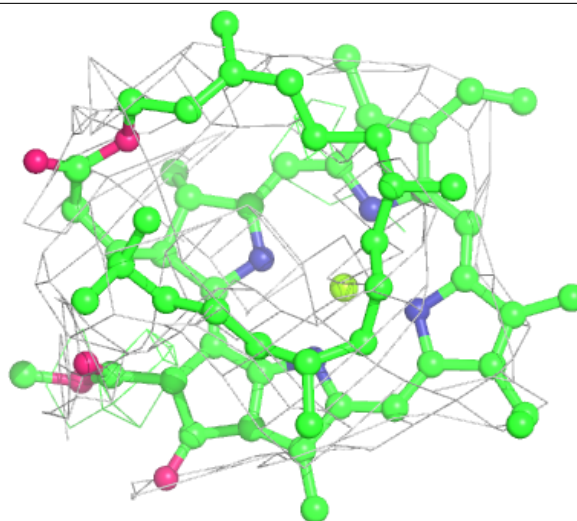
**Electron density around BCR I 102:**

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



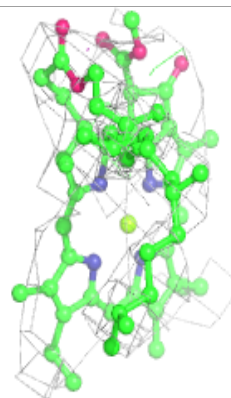
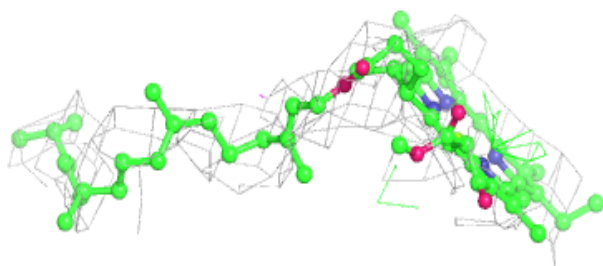
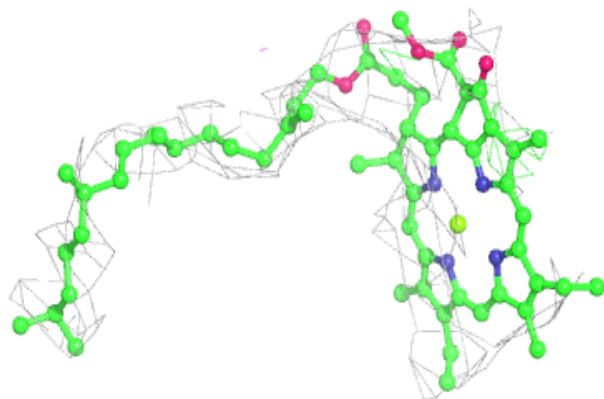
Electron density around CLA L 1002:

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

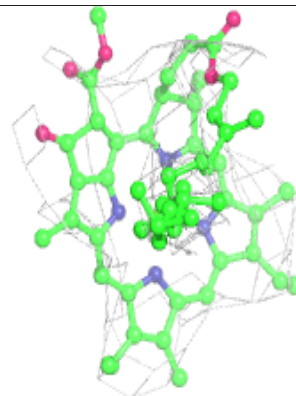
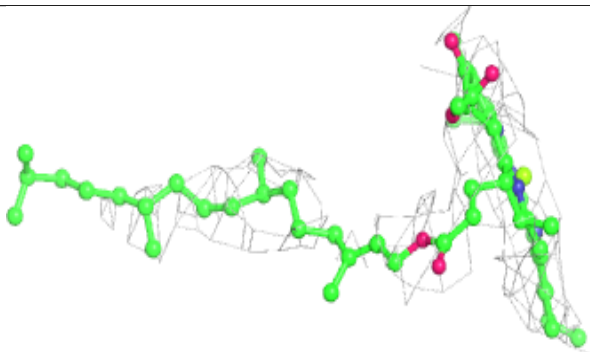
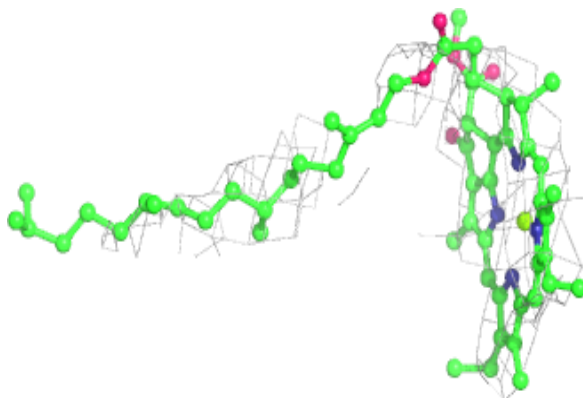


Electron density around CLA I 101:

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

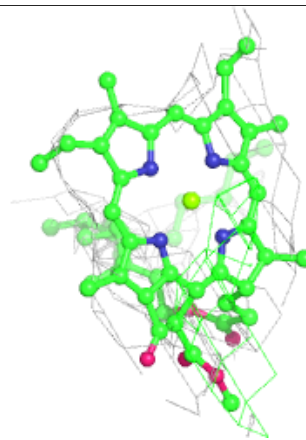
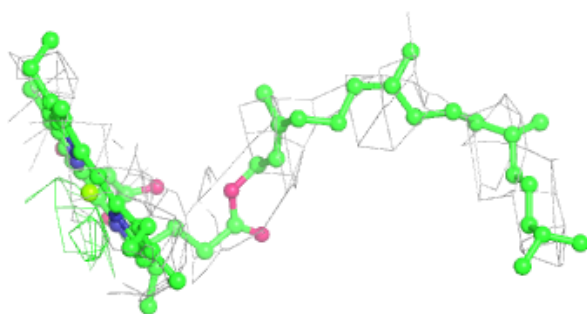
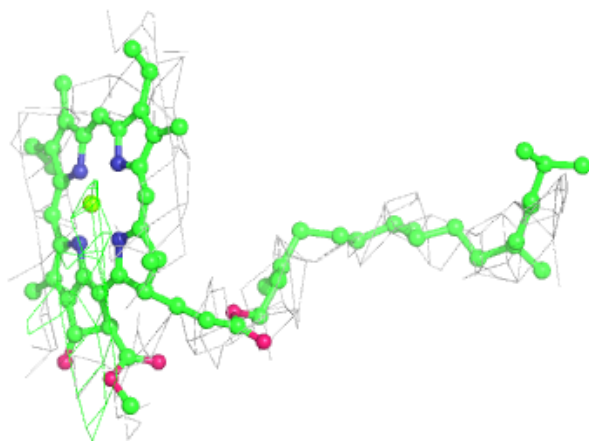
**Electron density around CLA B 826:**

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



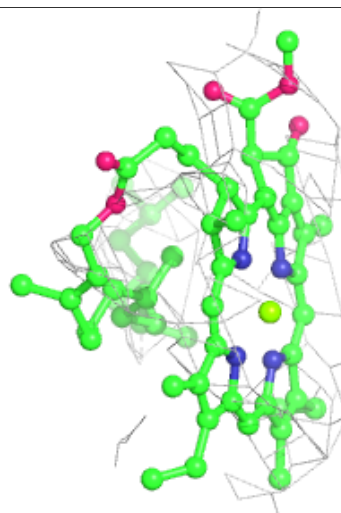
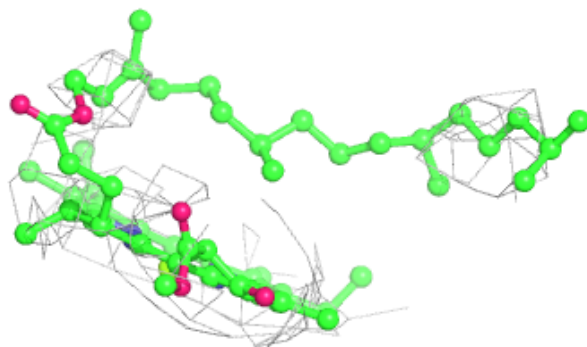
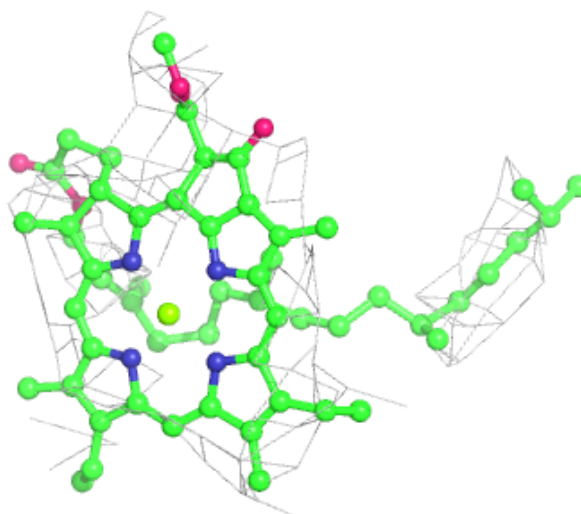
Electron density around CLA L 1003:

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



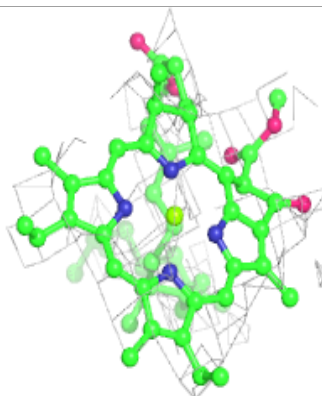
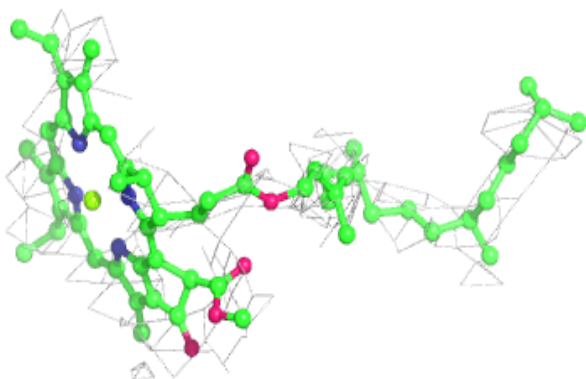
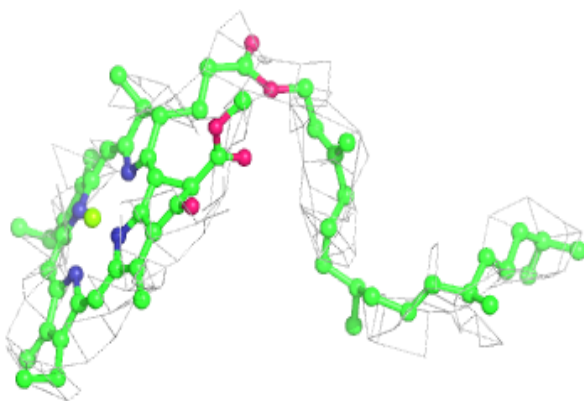
Electron density around CLA B 825:

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

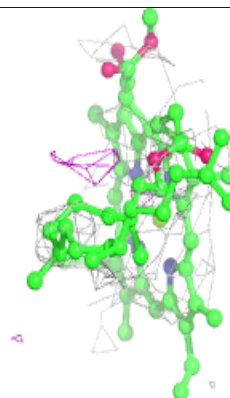
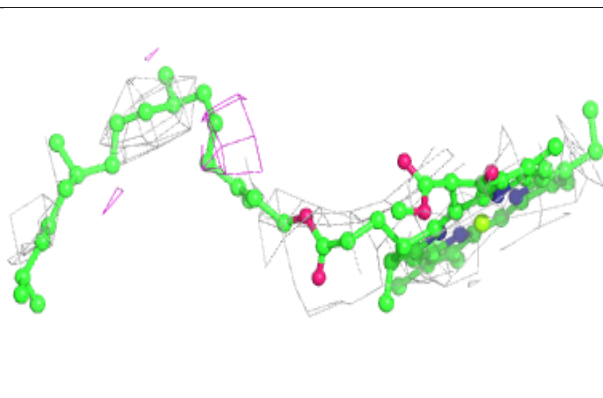
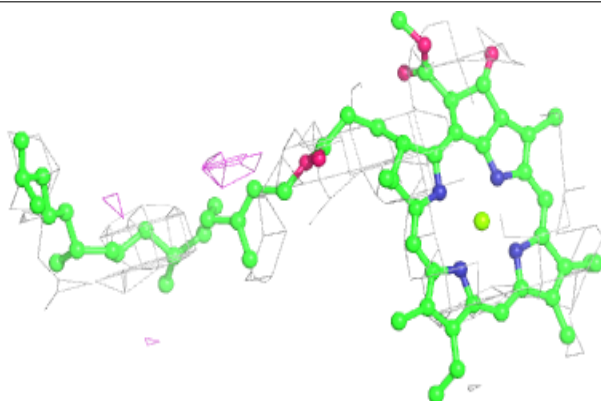


Electron density around CLA B 801:

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

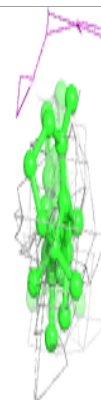
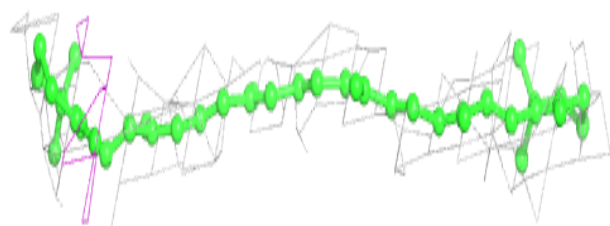
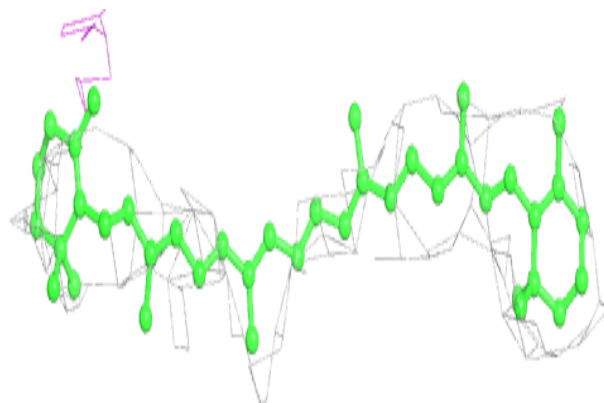
**Electron density around CLA B 811:**

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

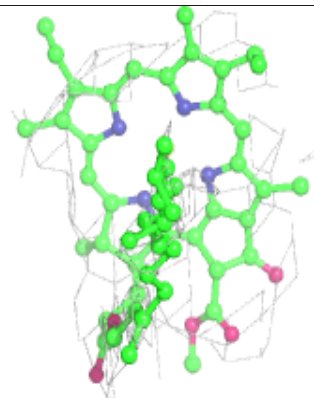
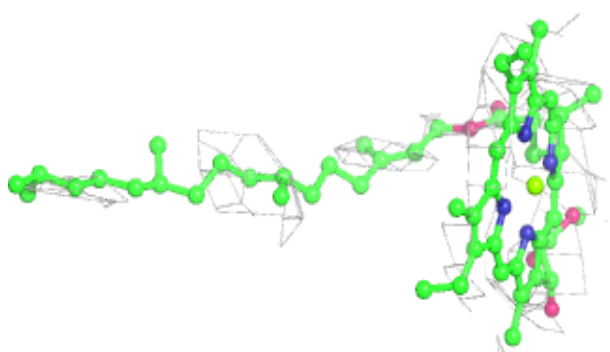
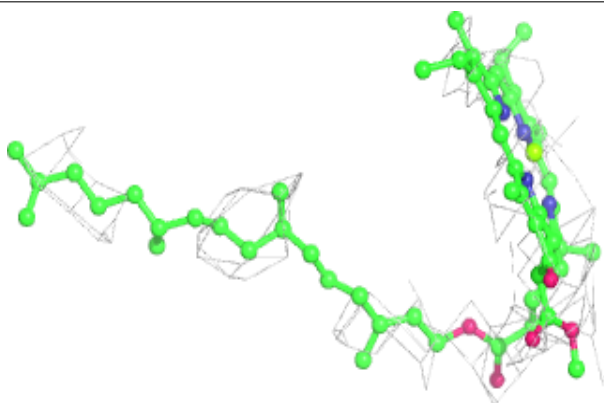


Electron density around BCR L 1005:

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

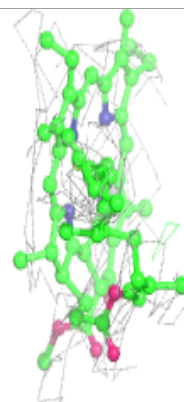
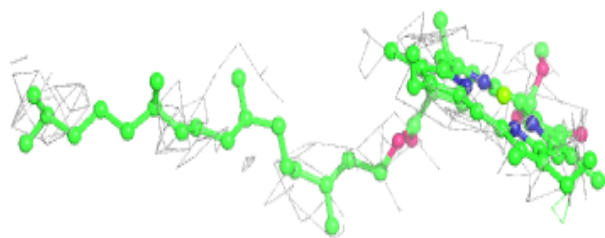
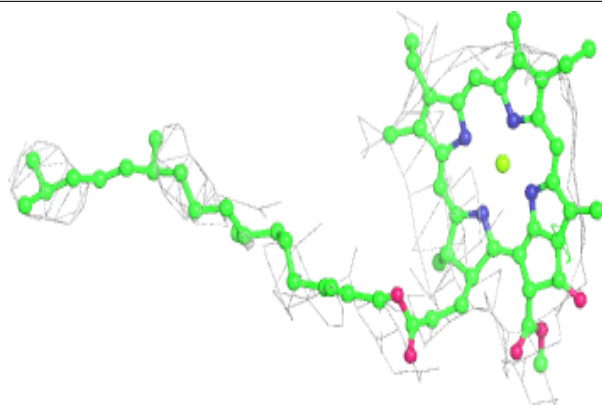
**Electron density around CLA B 827:**

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

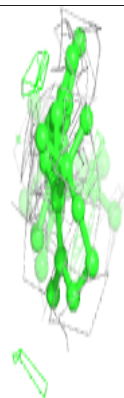
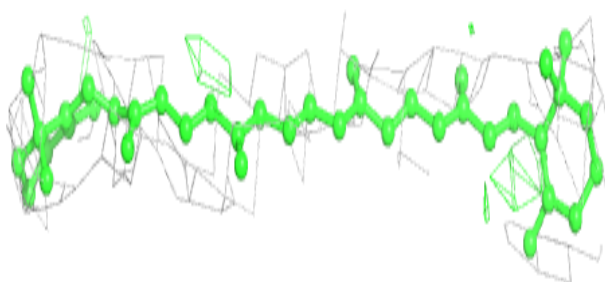
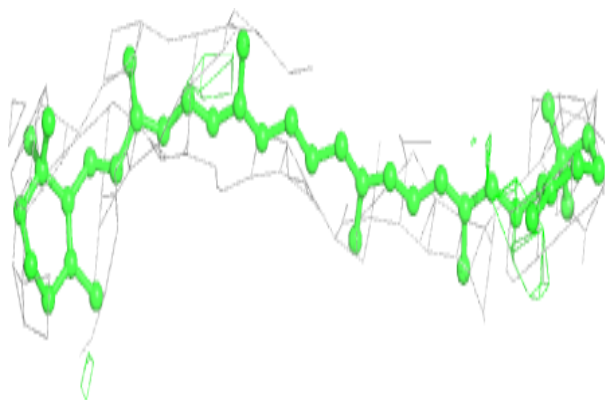


Electron density around CLA A 834:

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

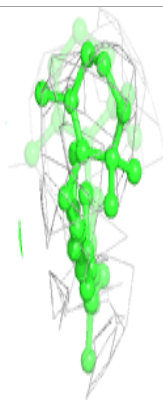
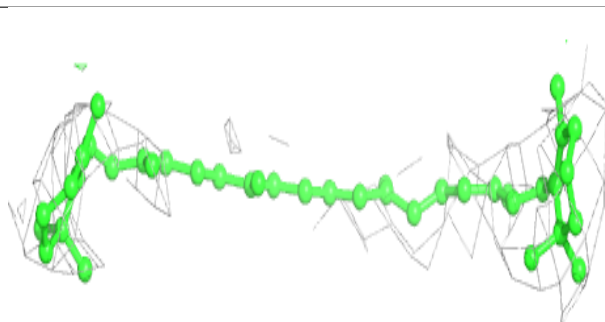
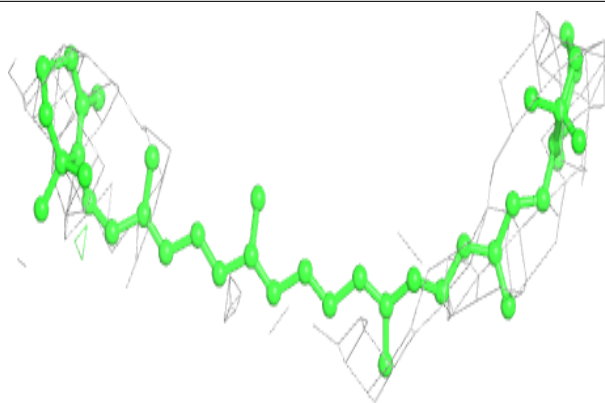
**Electron density around BCR L 1006:**

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



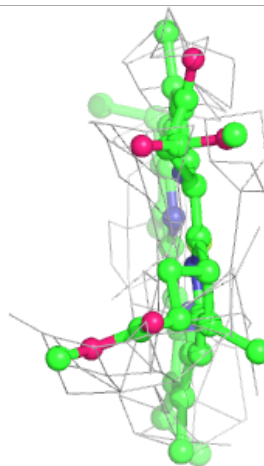
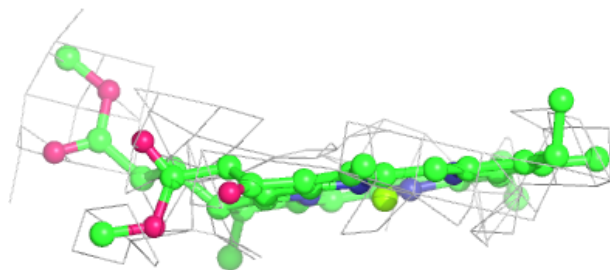
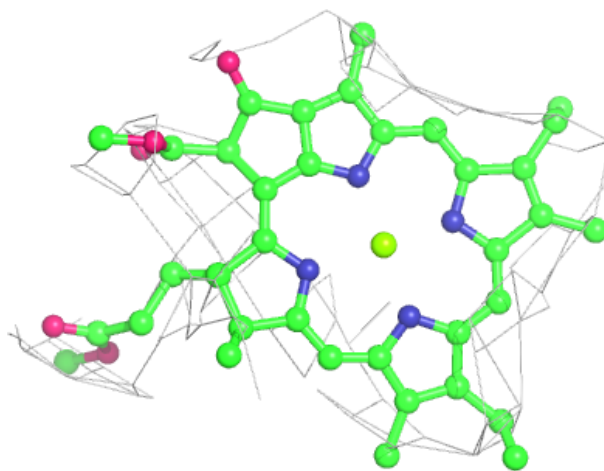
Electron density around BCR B 849:

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



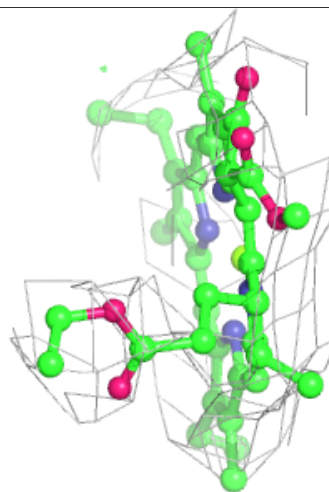
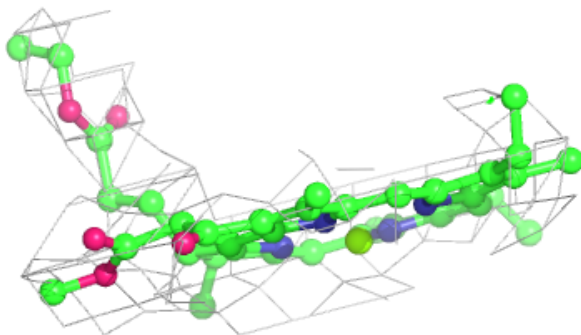
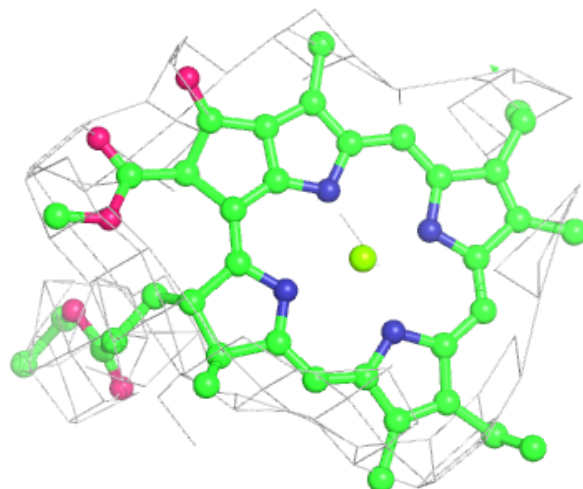
Electron density around CLA B 823:

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



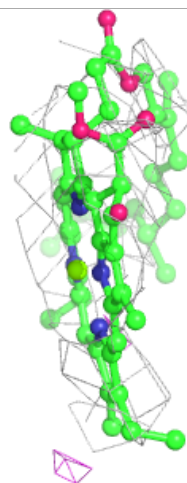
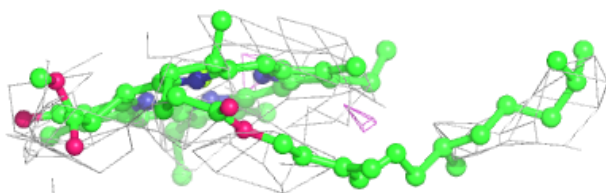
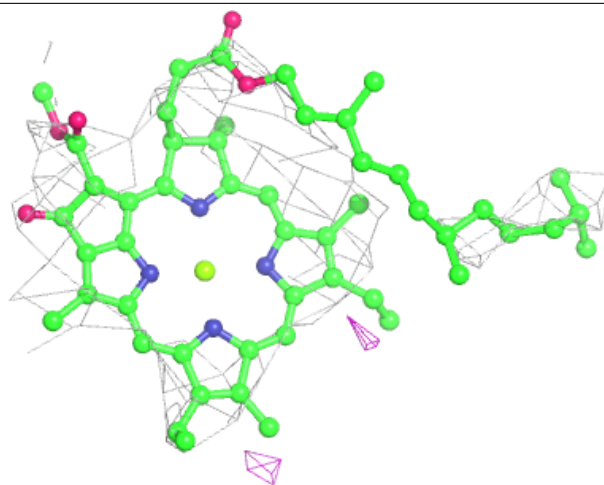
Electron density around CLA A 839:

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



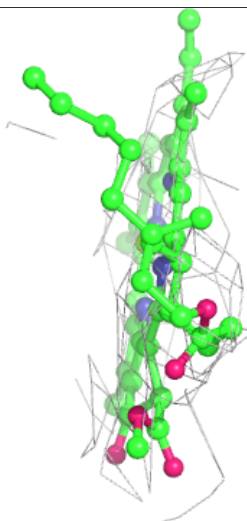
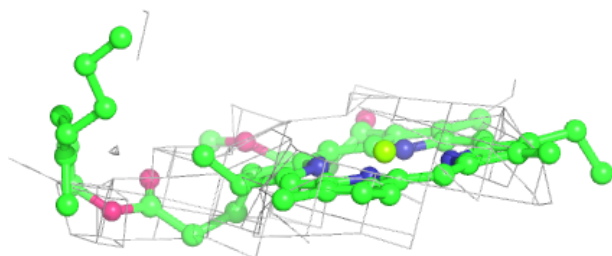
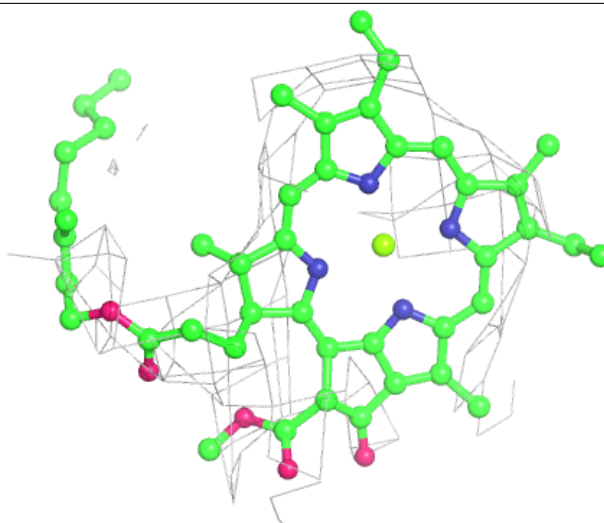
Electron density around CLA B 816:

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



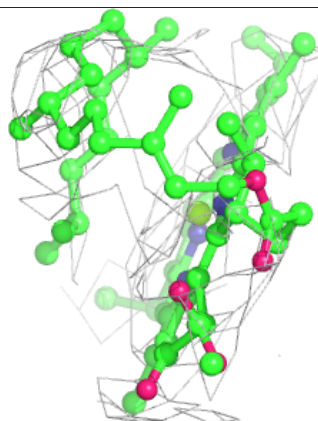
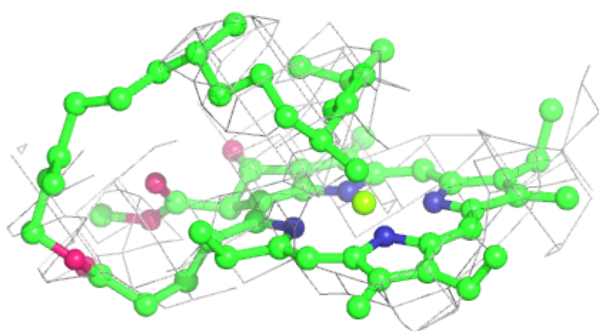
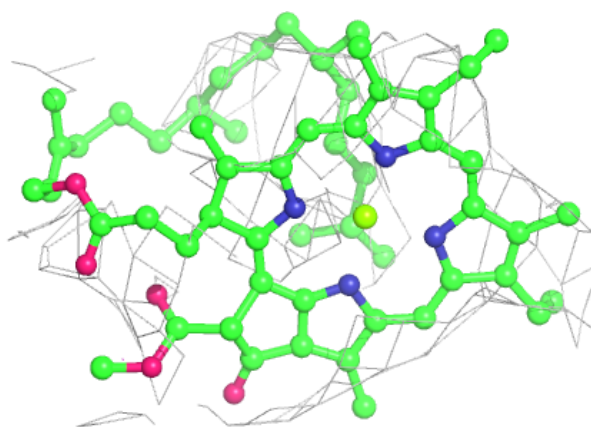
Electron density around CLA B 822:

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

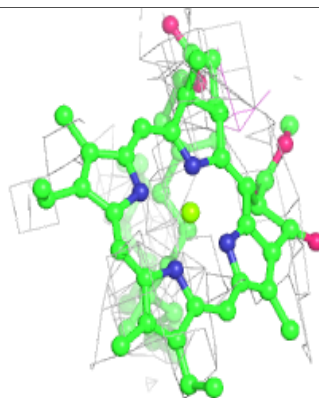
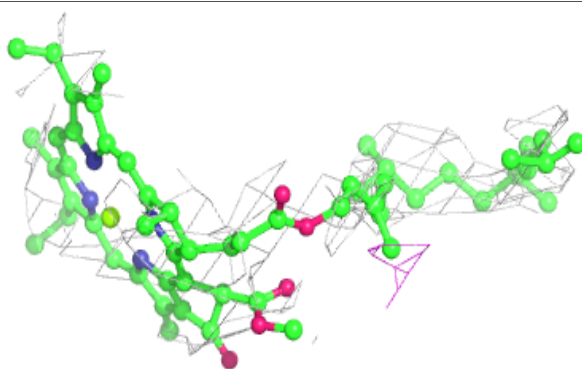
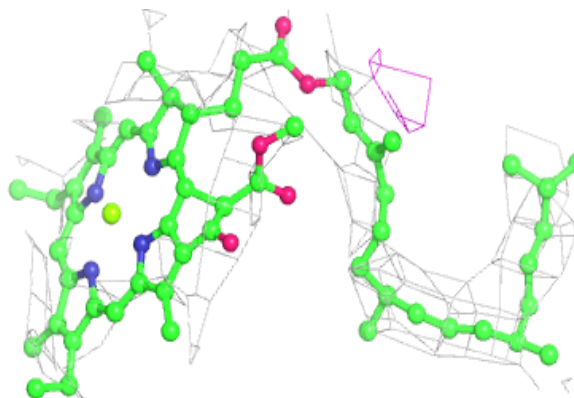


Electron density around CLA B 805:

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

**Electron density around CLA A 801:**

$2mF_o-DF_c$ (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.