



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 02:36 pm BST

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

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

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

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

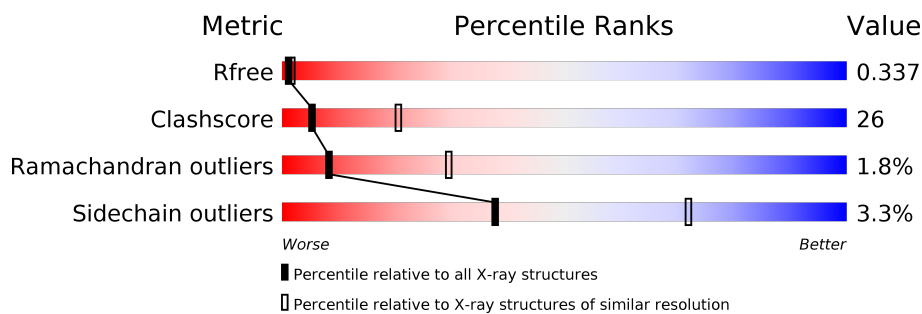
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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




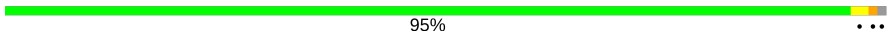









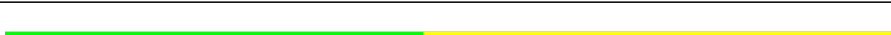


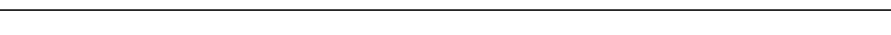
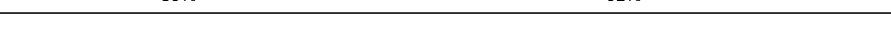

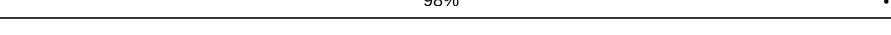


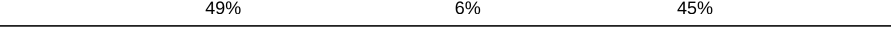




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	755	55% 42% ..
1	G	755	52% 45% ..
1	Y	755	50% 46% ..
2	B	741	53% 44% .
2	H	741	54% 43% .
2	Z	741	54% 44% .
3	C	81	56% 40% ...

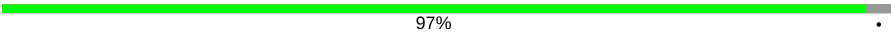
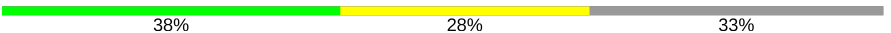


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Mol	Chain	Length	Quality of chain
3	N	81	
3	a	81	
4	D	139	
4	O	139	
4	b	139	
5	E	76	
5	P	76	
5	c	76	
6	F	164	
6	Q	164	
6	d	164	
7	I	38	
7	R	38	
7	e	38	
8	J	41	
8	S	41	
8	f	41	
9	K	83	
9	T	83	
9	g	83	
10	L	155	
10	U	155	
10	h	155	
11	M	31	
11	V	31	

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Mol	Chain	Length	Quality of chain
11	i	31	 97%
12	W	39	 38% 28% 33%
12	X	39	 49% 15% 33%
12	j	39	 64% 33%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CL0	A	801	X	-	-	-
13	CL0	G	801	X	-	-	-
13	CL0	Y	801	X	-	-	-
14	CLA	A	802	X	-	-	-
14	CLA	A	803	X	-	-	-
14	CLA	A	804	X	-	-	-
14	CLA	A	805	X	-	-	-
14	CLA	A	806	X	-	-	-
14	CLA	A	807	X	-	-	-
14	CLA	A	808	X	-	-	-
14	CLA	A	809	X	-	-	-
14	CLA	A	810	X	-	-	-
14	CLA	A	811	X	-	-	-
14	CLA	A	812	X	-	-	-
14	CLA	A	813	X	-	-	-
14	CLA	A	814	X	-	-	-
14	CLA	A	815	X	-	-	-
14	CLA	A	816	X	-	-	-
14	CLA	A	817	X	-	-	-
14	CLA	A	818	X	-	-	-
14	CLA	A	819	X	-	-	-
14	CLA	A	820	X	-	-	-
14	CLA	A	821	X	-	-	-
14	CLA	A	822	X	-	-	-
14	CLA	A	823	X	-	-	-
14	CLA	A	824	X	-	-	-
14	CLA	A	825	X	-	-	-
14	CLA	A	826	X	-	-	-
14	CLA	A	827	X	-	-	-
14	CLA	A	828	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	829	X	-	-	-
14	CLA	A	830	X	-	-	-
14	CLA	A	831	X	-	-	-
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	839	X	-	-	-
14	CLA	A	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	842	X	-	-	-
14	CLA	A	852	X	-	-	-
14	CLA	B	801	X	-	-	-
14	CLA	B	802	X	-	-	-
14	CLA	B	803	X	-	-	-
14	CLA	B	804	X	-	-	-
14	CLA	B	805	X	-	-	-
14	CLA	B	806	X	-	-	-
14	CLA	B	807	X	-	-	-
14	CLA	B	808	X	-	-	-
14	CLA	B	809	X	-	-	-
14	CLA	B	810	X	-	-	-
14	CLA	B	811	X	-	-	-
14	CLA	B	812	X	-	-	-
14	CLA	B	813	X	-	-	-
14	CLA	B	814	X	-	-	-
14	CLA	B	815	X	-	-	-
14	CLA	B	816	X	-	-	-
14	CLA	B	817	X	-	-	-
14	CLA	B	818	X	-	-	-
14	CLA	B	819	X	-	-	-
14	CLA	B	820	X	-	-	-
14	CLA	B	821	X	-	-	-
14	CLA	B	822	X	-	-	-
14	CLA	B	823	X	-	-	-
14	CLA	B	824	X	-	-	-
14	CLA	B	825	X	-	-	-
14	CLA	B	826	X	-	-	-
14	CLA	B	827	X	-	-	-

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	G	829	X	-	-	-
14	CLA	G	830	X	-	-	-
14	CLA	G	831	X	-	-	-
14	CLA	G	832	X	-	-	-
14	CLA	G	833	X	-	-	-
14	CLA	G	834	X	-	-	-
14	CLA	G	835	X	-	-	-
14	CLA	G	836	X	-	-	-
14	CLA	G	837	X	-	-	-
14	CLA	G	838	X	-	-	-
14	CLA	G	839	X	-	-	-
14	CLA	G	840	X	-	-	-
14	CLA	G	841	X	-	-	-
14	CLA	G	842	X	-	-	-
14	CLA	G	843	X	-	-	-
14	CLA	G	853	X	-	-	-
14	CLA	H	801	X	-	X	-
14	CLA	H	802	X	-	-	-
14	CLA	H	803	X	-	-	-
14	CLA	H	804	X	-	-	-
14	CLA	H	805	X	-	-	-
14	CLA	H	806	X	-	-	-
14	CLA	H	807	X	-	-	-
14	CLA	H	808	X	-	-	-
14	CLA	H	809	X	-	-	-
14	CLA	H	810	X	-	-	-
14	CLA	H	811	X	-	-	-
14	CLA	H	812	X	-	-	-
14	CLA	H	813	X	-	-	-
14	CLA	H	814	X	-	-	-
14	CLA	H	815	X	-	-	-
14	CLA	H	816	X	-	-	-
14	CLA	H	817	X	-	-	-
14	CLA	H	818	X	-	-	-
14	CLA	H	819	X	-	-	-
14	CLA	H	820	X	-	-	-
14	CLA	H	821	X	-	-	-
14	CLA	H	822	X	-	-	-
14	CLA	H	823	X	-	-	-
14	CLA	H	824	X	-	-	-
14	CLA	H	825	X	-	-	-
14	CLA	H	826	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	H	827	X	-	-	-
14	CLA	H	828	X	-	-	-
14	CLA	H	829	X	-	-	-
14	CLA	H	830	X	-	-	-
14	CLA	H	831	X	-	-	-
14	CLA	H	832	X	-	-	-
14	CLA	H	833	X	-	-	-
14	CLA	H	834	X	-	-	-
14	CLA	H	835	X	-	-	-
14	CLA	H	836	X	-	-	-
14	CLA	H	837	X	-	-	-
14	CLA	H	838	X	-	-	-
14	CLA	J	101	X	-	-	-
14	CLA	J	102	X	-	-	-
14	CLA	K	101	X	-	-	-
14	CLA	K	103	X	-	-	-
14	CLA	L	201	X	-	-	-
14	CLA	L	202	X	-	-	-
14	CLA	L	205	X	-	-	-
14	CLA	L	206	X	-	-	-
14	CLA	L	207	X	-	-	-
14	CLA	Q	201	X	-	-	-
14	CLA	Q	203	X	-	-	-
14	CLA	S	1101	X	-	-	-
14	CLA	S	1102	X	-	-	-
14	CLA	S	1103	X	-	-	-
14	CLA	T	101	X	-	-	-
14	CLA	T	103	X	-	-	-
14	CLA	U	1002	X	-	-	-
14	CLA	U	1003	X	-	-	-
14	CLA	U	1004	X	-	-	-
14	CLA	U	1006	X	-	-	-
14	CLA	V	1201	X	-	-	-
14	CLA	W	1701	X	-	-	-
14	CLA	X	1701	X	-	-	-
14	CLA	Y	802	X	-	-	-
14	CLA	Y	803	X	-	-	-
14	CLA	Y	804	X	-	-	-
14	CLA	Y	805	X	-	-	-
14	CLA	Y	806	X	-	-	-
14	CLA	Y	807	X	-	-	-
14	CLA	Y	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	Y	809	X	-	-	-
14	CLA	Y	810	X	-	-	-
14	CLA	Y	811	X	-	-	-
14	CLA	Y	812	X	-	-	-
14	CLA	Y	813	X	-	-	-
14	CLA	Y	814	X	-	-	-
14	CLA	Y	815	X	-	-	-
14	CLA	Y	816	X	-	-	-
14	CLA	Y	817	X	-	-	-
14	CLA	Y	818	X	-	-	-
14	CLA	Y	819	X	-	-	-
14	CLA	Y	820	X	-	-	-
14	CLA	Y	821	X	-	-	-
14	CLA	Y	822	X	-	-	-
14	CLA	Y	823	X	-	-	-
14	CLA	Y	824	X	-	-	-
14	CLA	Y	825	X	-	-	-
14	CLA	Y	826	X	-	-	-
14	CLA	Y	827	X	-	-	-
14	CLA	Y	828	X	-	-	-
14	CLA	Y	829	X	-	-	-
14	CLA	Y	830	X	-	-	-
14	CLA	Y	831	X	-	-	-
14	CLA	Y	832	X	-	-	-
14	CLA	Y	833	X	-	-	-
14	CLA	Y	834	X	-	-	-
14	CLA	Y	835	X	-	-	-
14	CLA	Y	836	X	-	-	-
14	CLA	Y	837	X	-	-	-
14	CLA	Y	838	X	-	-	-
14	CLA	Y	839	X	-	-	-
14	CLA	Y	840	X	-	-	-
14	CLA	Y	841	X	-	-	-
14	CLA	Y	842	X	-	-	-
14	CLA	Y	843	X	-	-	-
14	CLA	Y	854	X	-	-	-
14	CLA	Y	855	X	-	-	-
14	CLA	Z	801	X	-	-	-
14	CLA	Z	802	X	-	-	-
14	CLA	Z	803	X	-	-	-
14	CLA	Z	804	X	-	-	-
14	CLA	Z	805	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	Z	806	X	-	-	-
14	CLA	Z	807	X	-	-	-
14	CLA	Z	808	X	-	-	-
14	CLA	Z	809	X	-	-	-
14	CLA	Z	810	X	-	-	-
14	CLA	Z	811	X	-	-	-
14	CLA	Z	812	X	-	-	-
14	CLA	Z	813	X	-	-	-
14	CLA	Z	814	X	-	-	-
14	CLA	Z	815	X	-	-	-
14	CLA	Z	816	X	-	-	-
14	CLA	Z	817	X	-	-	-
14	CLA	Z	818	X	-	-	-
14	CLA	Z	819	X	-	-	-
14	CLA	Z	820	X	-	-	-
14	CLA	Z	821	X	-	-	-
14	CLA	Z	822	X	-	-	-
14	CLA	Z	823	X	-	-	-
14	CLA	Z	824	X	-	-	-
14	CLA	Z	825	X	-	-	-
14	CLA	Z	826	X	-	-	-
14	CLA	Z	827	X	-	-	-
14	CLA	Z	828	X	-	-	-
14	CLA	Z	829	X	-	-	-
14	CLA	Z	830	X	-	-	-
14	CLA	Z	831	X	-	-	-
14	CLA	Z	832	X	-	-	-
14	CLA	Z	833	X	-	-	-
14	CLA	Z	834	X	-	-	-
14	CLA	Z	835	X	-	-	-
14	CLA	Z	836	X	-	-	-
14	CLA	Z	837	X	-	-	-
14	CLA	Z	838	X	-	-	-
14	CLA	Z	839	X	-	-	-
14	CLA	d	201	X	-	-	-
14	CLA	d	202	X	-	-	-
14	CLA	f	101	X	-	-	-
14	CLA	f	102	X	-	-	-
14	CLA	g	101	X	-	-	-
14	CLA	g	102	X	-	-	-
14	CLA	h	201	X	-	-	-
14	CLA	h	205	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	h	206	X	-	-	-
14	CLA	h	207	X	-	-	-
14	CLA	j	102	X	-	-	-
16	SF4	C	101	-	-	X	-
16	SF4	C	102	-	-	X	-
16	SF4	N	102	-	-	X	-

2 Entry composition

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	741	Total	C	N	O	S	0	0	0
			5791	3799	989	977	26			
1	G	741	Total	C	N	O	S	0	0	0
			5791	3799	989	977	26			
1	Y	741	Total	C	N	O	S	0	0	0
			5791	3799	989	977	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
			5889	3876	987	1005	21			
2	H	739	Total	C	N	O	S	0	0	0
			5889	3876	987	1005	21			
2	Z	739	Total	C	N	O	S	0	0	0
			5889	3876	987	1005	21			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

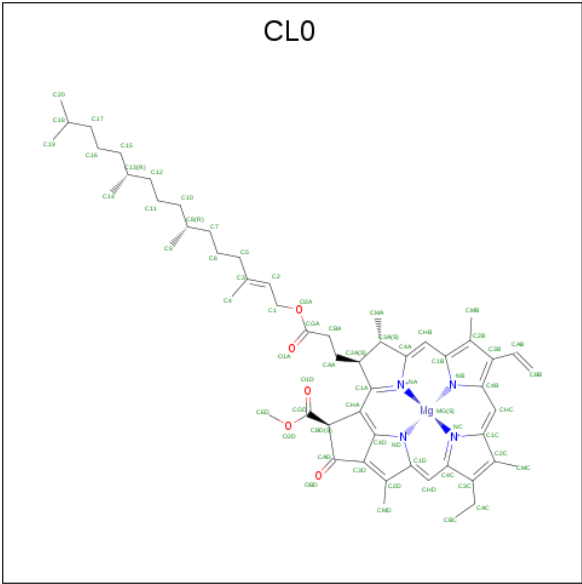
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

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

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

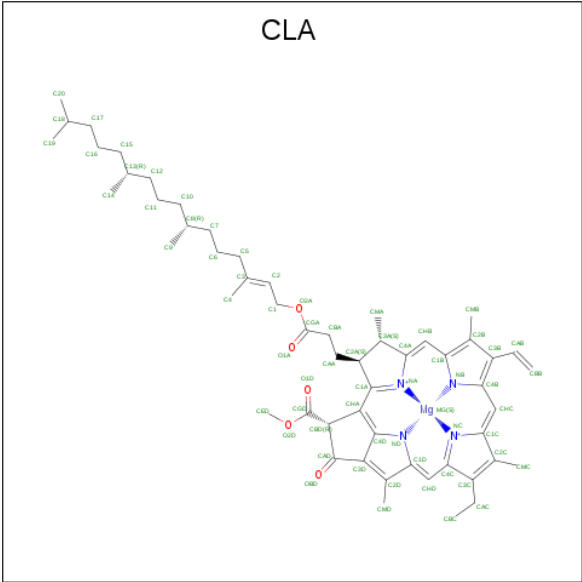
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	W	26	Total	C	N	O	0	0	0
			219	157	31	31			
12	X	26	Total	C	N	O	0	0	0
			219	157	31	31			
12	j	26	Total	C	N	O	0	0	0
			219	157	31	31			

- Molecule 13 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by author).



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

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by author).



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

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

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

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

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

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

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

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

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

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

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

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

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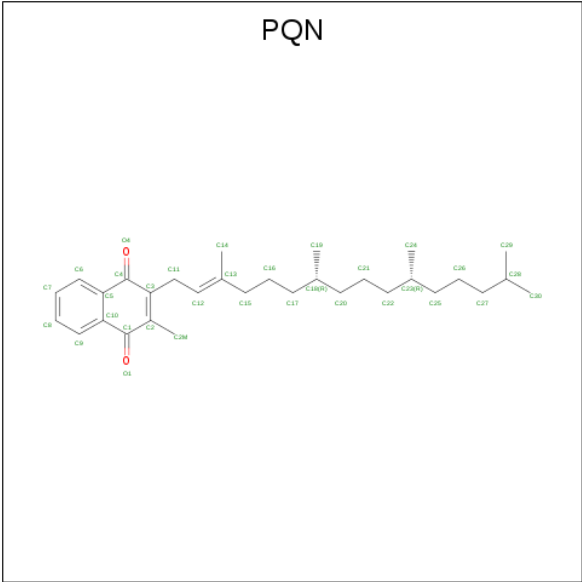
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	Z	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5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

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

- Molecule 15 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by author).



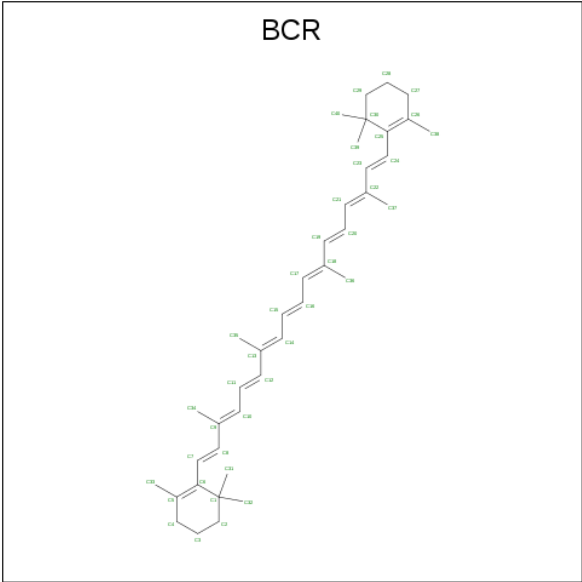
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	A	1	Total	C	O	0	0
			33	31	2		
15	B	1	Total	C	O	0	0
			33	31	2		
15	G	1	Total	C	O	0	0
			33	31	2		
15	H	1	Total	C	O	0	0
			33	31	2		
15	Y	1	Total	C	O	0	0
			33	31	2		
15	Z	1	Total	C	O	0	0
			33	31	2		

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by author).



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

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by author).



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

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

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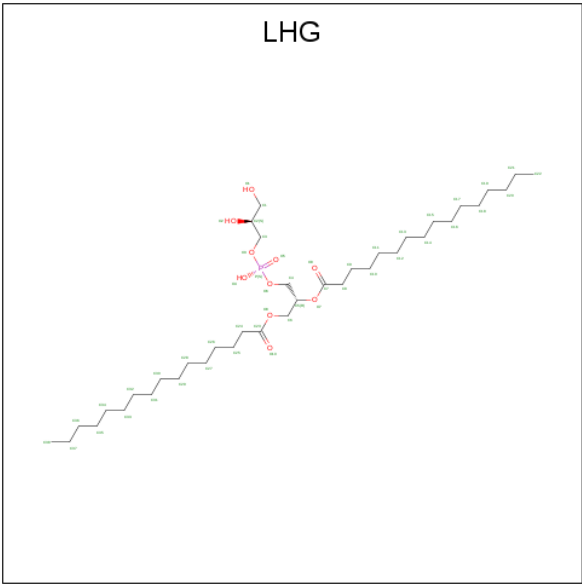
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	Q	1	Total C 40 40	0	0
17	Q	1	Total C 40 40	0	0
17	R	1	Total C 40 40	0	0
17	R	1	Total C 40 40	0	0
17	S	1	Total C 40 40	0	0
17	T	1	Total C 40 40	0	0
17	U	1	Total C 40 40	0	0
17	U	1	Total C 40 40	0	0
17	U	1	Total C 40 40	0	0
17	V	1	Total C 40 40	0	0
17	Y	1	Total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

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

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



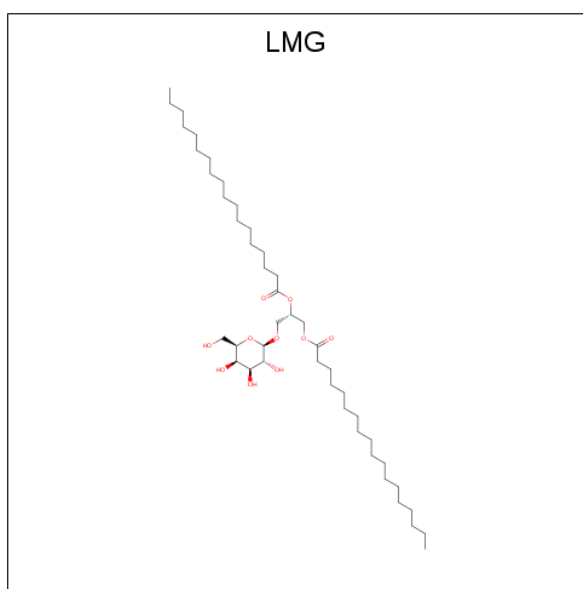
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O P 49 38 10 1	0	0

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

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

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

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

- Molecule 21 is water.

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

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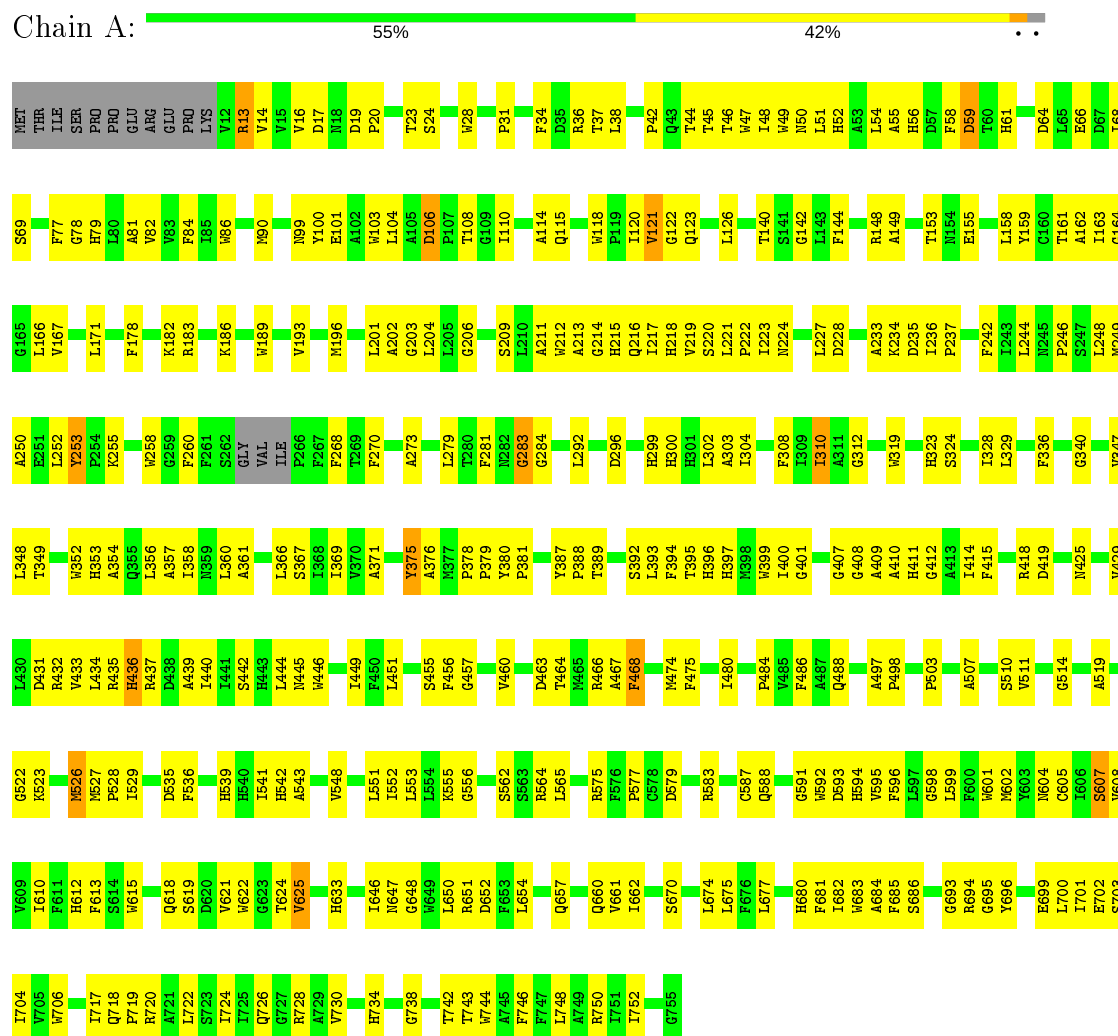
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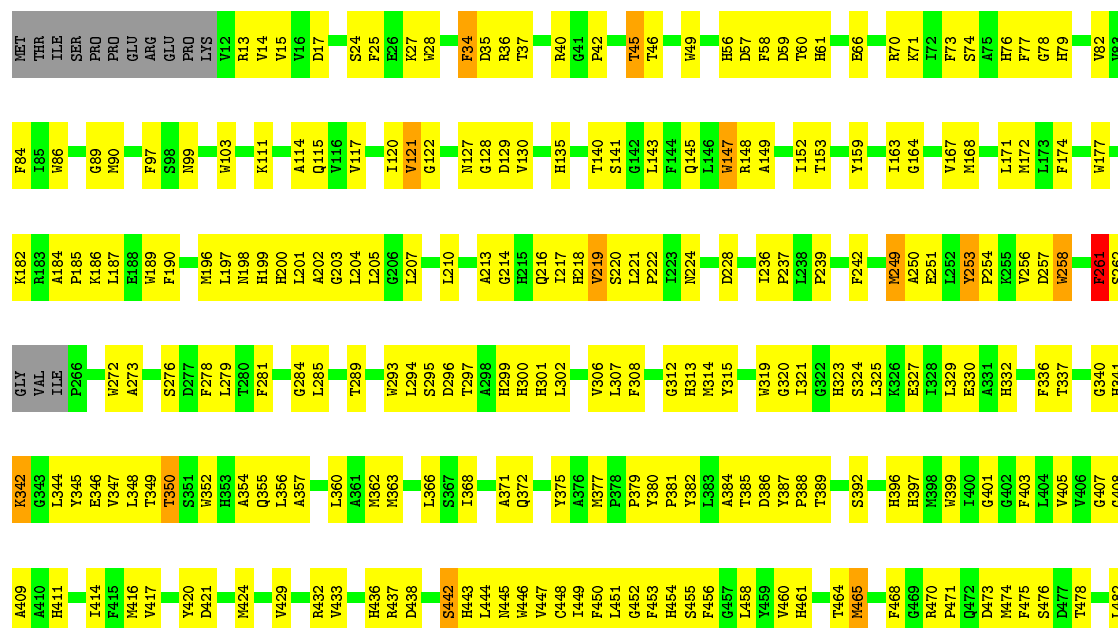
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	Y	8	Total 8	O 8	0	0
21	Z	2	Total 2	O 2	0	0
21	b	4	Total 4	O 4	0	0
21	c	1	Total 1	O 1	0	0
21	d	2	Total 2	O 2	0	0
21	f	1	Total 1	O 1	0	0
21	h	1	Total 1	O 1	0	0
21	j	1	Total 1	O 1	0	0

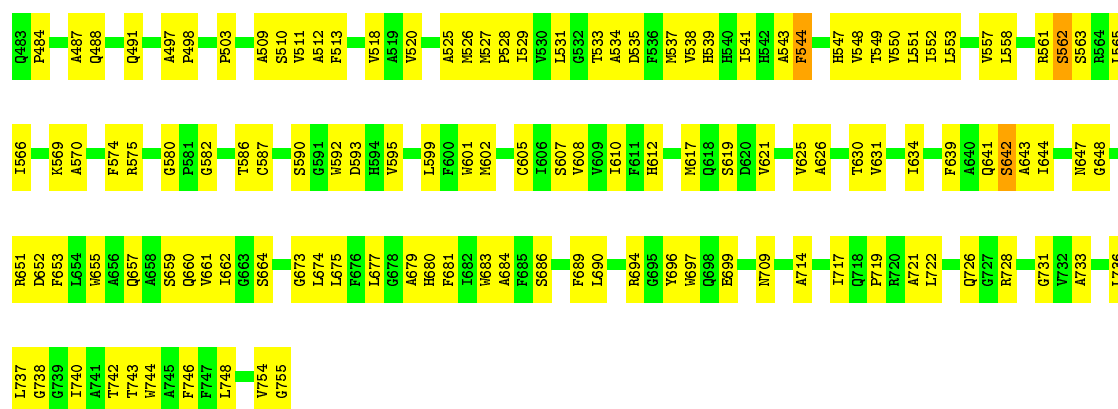
3 Residue-property plots

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

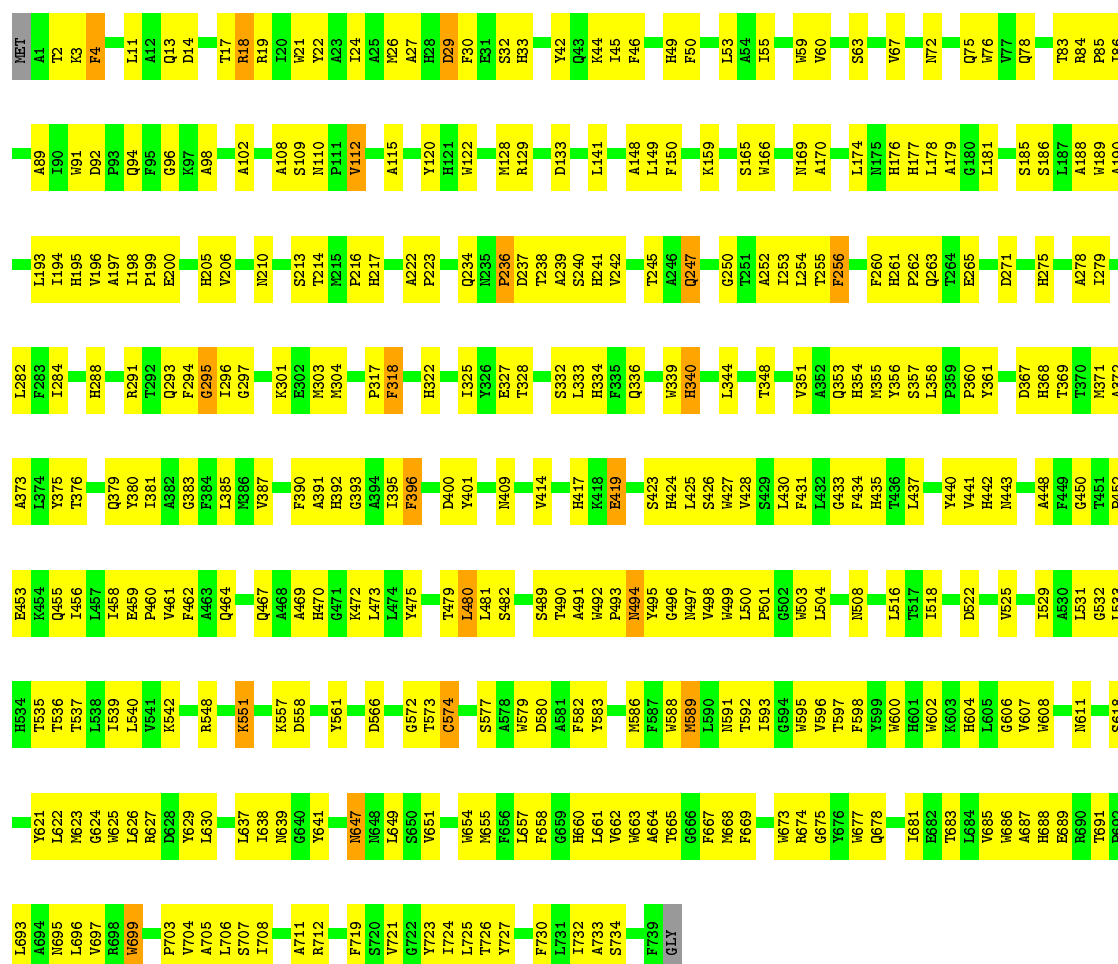






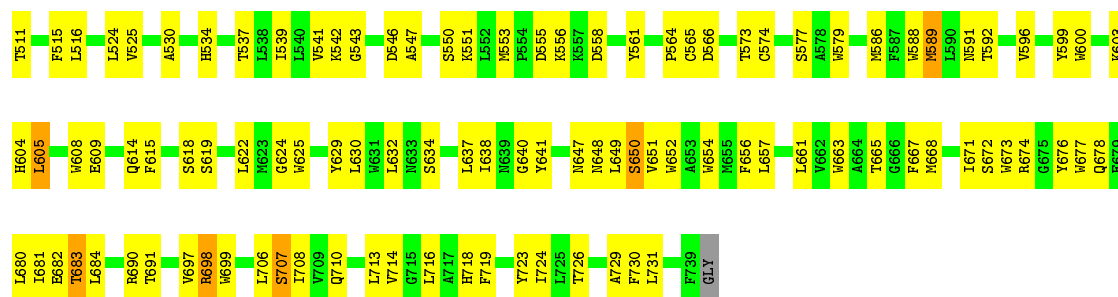
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 53% 44%



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain H: 54% 43%



• Molecule 3: Photosystem I iron-sulfur center



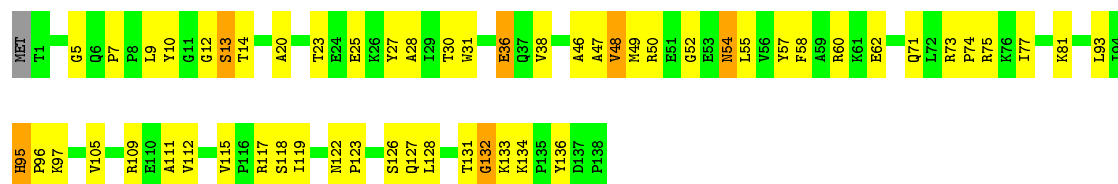
• Molecule 3: Photosystem I iron-sulfur center



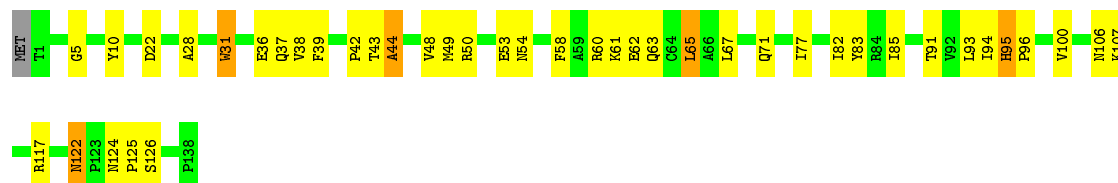
• Molecule 3: Photosystem I iron-sulfur center



• Molecule 4: Photosystem I reaction center subunit II

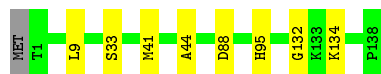


• Molecule 4: Photosystem I reaction center subunit II



- Molecule 4: Photosystem I reaction center subunit II

Chain b:  94% 6%



- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  62% 25% 9%




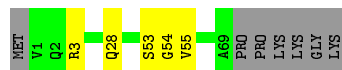
- Molecule 5: Photosystem I reaction center subunit IV

Chain P:  61% 28% 9%



- Molecule 5: Photosystem I reaction center subunit IV

Chain c:  84% 7% 9%



- Molecule 6: Photosystem I reaction center subunit III

Chain F:  54% 30% 14%




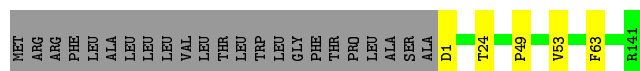
- Molecule 6: Photosystem I reaction center subunit III

Chain Q:  55% 28% 14%



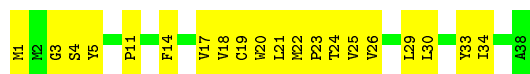
- Molecule 6: Photosystem I reaction center subunit III

Chain d:  83% 14%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:  47% 53%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain R:  63% 37%



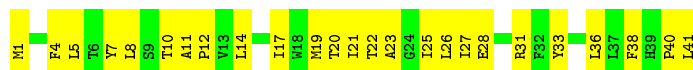
- Molecule 7: Photosystem I reaction center subunit VIII

Chain e:  95% 5%



- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  39% 61%



- Molecule 8: Photosystem I reaction center subunit IX

Chain S:  51% 46%

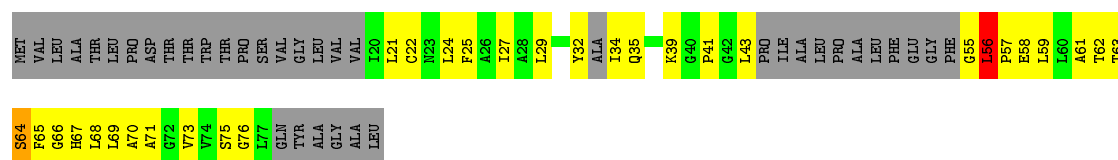


- Molecule 8: Photosystem I reaction center subunit IX

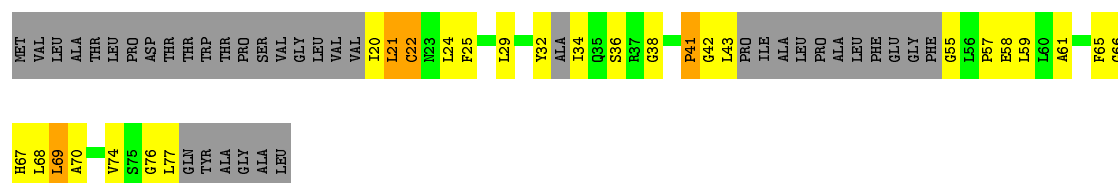
Chain f:  98%



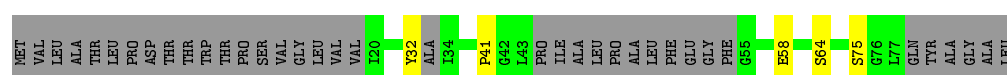
- Molecule 9: Photosystem I reaction center subunit Psak



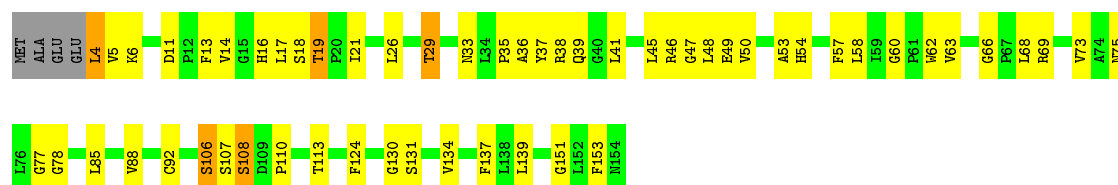
• Molecule 9: Photosystem I reaction center subunit PsaK



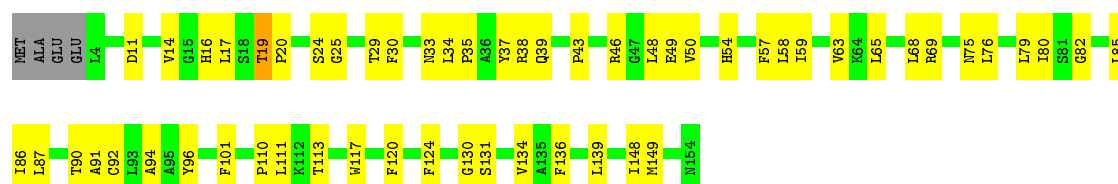
• Molecule 9: Photosystem I reaction center subunit PsaK



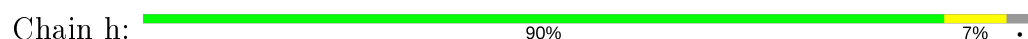
• Molecule 10: Photosystem I reaction center subunit XI



• Molecule 10: Photosystem I reaction center subunit XI



• Molecule 10: Photosystem I reaction center subunit XI





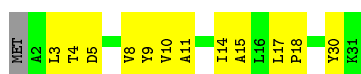
- Molecule 11: Photosystem I reaction center subunit XII

Chain M: 68% 29%



- Molecule 11: Photosystem I reaction center subunit XII

Chain V: 58% 39%



- Molecule 11: Photosystem I reaction center subunit XII

Chain i: 97%



- Molecule 12: Photosystem I 4.8K protein

Chain W: 38% 28% 33%



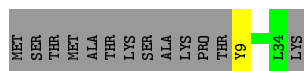
- Molecule 12: Photosystem I 4.8K protein

Chain X: 49% 15% 33%



- Molecule 12: Photosystem I 4.8K protein

Chain j: 64% 33%



4 Data and refinement statistics

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

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

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, CA, CLA, PQN, CL0, SF4, 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	0.66	0/5990	0.74	0/8168
1	G	0.66	0/5990	0.75	0/8168
1	Y	0.66	0/5990	0.75	0/8168
2	B	0.64	0/6107	0.74	0/8345
2	H	0.66	0/6107	0.75	0/8345
2	Z	0.65	0/6107	0.73	0/8345
3	C	0.69	0/608	0.84	0/824
3	N	0.68	0/608	0.85	0/824
3	a	0.69	0/608	0.82	0/824
4	D	0.64	0/1101	0.78	0/1492
4	O	0.63	0/1101	0.77	0/1492
4	b	0.64	0/1101	0.79	0/1492
5	E	0.68	0/551	0.78	0/750
5	P	0.68	0/551	0.76	0/750
5	c	0.67	0/551	0.77	0/750
6	F	0.69	0/1087	0.78	0/1476
6	Q	0.68	0/1087	0.76	0/1476
6	d	0.68	0/1087	0.77	0/1476
7	I	0.66	0/312	0.71	0/425
7	R	0.66	0/312	0.69	0/425
7	e	0.64	0/312	0.76	0/425
8	J	0.64	0/350	0.72	0/477
8	S	0.65	0/350	0.71	0/477
8	f	0.64	0/350	0.71	0/477
9	K	0.72	0/331	0.80	0/444
9	T	0.72	0/331	0.86	0/444
9	g	0.73	0/331	0.82	0/444
10	L	0.68	0/1148	0.78	0/1558
10	U	0.68	0/1148	0.75	0/1558
10	h	0.68	0/1148	0.77	0/1558
11	M	0.68	0/236	0.76	0/322
11	V	0.69	0/236	0.75	0/322

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	K	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	K	56	LEU	Peptide

5.2 Too-close contacts ⓘ

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	5791	0	5648	334	0
1	G	5791	0	5648	363	0
1	Y	5791	0	5649	333	0
2	B	5889	0	5651	350	0
2	H	5889	0	5650	339	0
2	Z	5889	0	5651	322	0
3	C	598	0	582	33	0
3	N	598	0	582	31	0
3	a	598	0	582	0	0
4	D	1075	0	1077	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	O	1075	0	1077	36	0
4	b	1075	0	1077	0	0
5	E	539	0	528	16	0
5	P	539	0	528	11	0
5	c	539	0	528	0	1
6	F	1065	0	1077	45	0
6	Q	1065	0	1077	49	0
6	d	1065	0	1077	0	1
7	I	301	0	306	23	0
7	R	301	0	306	15	0
7	e	301	0	306	0	0
8	J	338	0	347	28	0
8	S	338	0	347	26	0
8	f	338	0	347	0	0
9	K	328	0	348	33	0
9	T	328	0	348	22	0
9	g	328	0	348	0	0
10	L	1119	0	1125	50	0
10	U	1119	0	1125	47	0
10	h	1119	0	1125	0	0
11	M	233	0	252	8	0
11	V	233	0	252	8	0
11	i	233	0	252	0	0
12	W	219	0	221	9	0
12	X	219	0	221	6	0
12	j	219	0	221	0	0
13	A	65	0	72	13	0
13	G	65	0	72	16	0
13	Y	65	0	72	11	0
14	A	2489	0	2488	268	0
14	B	2389	0	2373	250	0
14	F	45	0	32	1	0
14	G	2534	0	2522	287	0
14	H	2220	0	2211	258	0
14	J	100	0	81	4	0
14	K	86	0	61	7	0
14	L	325	0	360	34	0
14	Q	110	0	104	9	0
14	S	165	0	154	11	0
14	T	86	0	62	6	0
14	U	260	0	287	28	0
14	V	54	0	48	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	W	45	0	33	4	0
14	X	45	0	33	0	0
14	Y	2640	0	2675	276	0
14	Z	2254	0	2219	220	0
14	d	95	0	70	0	0
14	f	100	0	82	0	0
14	g	86	0	62	0	0
14	h	260	0	287	0	0
14	j	45	0	33	0	0
15	A	33	0	46	6	0
15	B	33	0	46	11	0
15	G	33	0	46	3	0
15	H	33	0	46	7	0
15	Y	33	0	46	2	0
15	Z	33	0	46	4	0
16	A	8	0	0	1	0
16	C	16	0	0	5	0
16	G	8	0	0	0	0
16	N	16	0	0	3	0
16	Y	8	0	0	0	0
16	a	16	0	0	0	0
17	A	200	0	243	33	0
17	B	255	0	302	53	0
17	F	80	0	98	8	0
17	G	240	0	288	62	0
17	H	265	0	320	47	0
17	I	40	0	48	11	0
17	J	80	0	96	21	0
17	K	40	0	48	3	0
17	L	120	0	145	22	0
17	M	40	0	48	6	0
17	Q	80	0	98	9	0
17	R	80	0	96	12	0
17	S	40	0	47	10	0
17	T	40	0	49	6	0
17	U	120	0	145	19	0
17	V	40	0	49	6	0
17	Y	280	0	337	58	0
17	Z	225	0	271	33	0
17	d	40	0	48	0	0
17	e	40	0	48	0	0
17	f	120	0	145	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	h	80	0	97	0	0
17	i	40	0	47	0	0
18	A	81	0	108	5	0
18	B	39	0	48	0	0
18	G	81	0	108	12	0
18	H	37	0	44	2	0
18	Y	74	0	94	9	0
18	j	28	0	26	0	0
19	B	52	0	77	6	0
19	H	49	0	68	4	0
19	Z	49	0	68	3	0
20	L	1	0	0	0	0
20	U	1	0	0	0	0
20	h	1	0	0	0	0
21	A	9	0	0	0	0
21	B	9	0	0	0	0
21	C	1	0	0	1	0
21	D	2	0	0	0	0
21	E	1	0	0	0	0
21	G	8	0	0	15	0
21	H	3	0	0	0	0
21	J	1	0	0	0	0
21	K	1	0	0	0	0
21	L	5	0	0	0	0
21	N	1	0	0	1	0
21	O	2	0	0	0	0
21	Q	2	0	0	0	0
21	T	1	0	0	0	0
21	U	4	0	0	0	0
21	W	1	0	0	1	0
21	Y	8	0	0	19	0
21	Z	2	0	0	0	0
21	b	4	0	0	0	0
21	c	1	0	0	0	0
21	d	2	0	0	0	0
21	f	1	0	0	0	0
21	h	1	0	0	0	0
21	j	1	0	0	0	0
All	All	72532	0	72009	3482	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 26.

The worst 5 of 3482 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)
14:G:819:CLA:HBB1	21:G:907:HOH:O	1.23	1.26
1:G:373:HIS:ND1	14:G:818:CLA:OBD	1.80	1.15
14:Y:821:CLA:C3B	21:Y:904:HOH:O	1.92	1.14
1:A:399:TRP:CD1	14:A:828:CLA:HAB	1.84	1.12
2:B:318:PHE:CD1	14:B:822:CLA:HAB	1.84	1.10

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)
5:c:28:GLN:OE1	6:d:1:ASP:N[2_545]	2.13	0.07

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	737/755 (98%)	634 (86%)	89 (12%)	14 (2%)	8	28
1	G	737/755 (98%)	634 (86%)	86 (12%)	17 (2%)	6	23
1	Y	737/755 (98%)	627 (85%)	98 (13%)	12 (2%)	9	32
2	B	737/741 (100%)	639 (87%)	84 (11%)	14 (2%)	8	28
2	H	737/741 (100%)	658 (89%)	69 (9%)	10 (1%)	11	36
2	Z	737/741 (100%)	642 (87%)	86 (12%)	9 (1%)	13	40
3	C	78/81 (96%)	72 (92%)	4 (5%)	2 (3%)	5	20
3	N	78/81 (96%)	69 (88%)	8 (10%)	1 (1%)	12	37
3	a	78/81 (96%)	64 (82%)	12 (15%)	2 (3%)	5	20
4	D	136/139 (98%)	119 (88%)	14 (10%)	3 (2%)	6	24
4	O	136/139 (98%)	122 (90%)	11 (8%)	3 (2%)	6	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	b	136/139 (98%)	117 (86%)	15 (11%)	4 (3%)	4	18
5	E	67/76 (88%)	58 (87%)	6 (9%)	3 (4%)	2	9
5	P	67/76 (88%)	56 (84%)	6 (9%)	5 (8%)	1	2
5	c	67/76 (88%)	56 (84%)	8 (12%)	3 (4%)	2	9
6	F	139/164 (85%)	126 (91%)	12 (9%)	1 (1%)	22	54
6	Q	139/164 (85%)	124 (89%)	14 (10%)	1 (1%)	22	54
6	d	139/164 (85%)	118 (85%)	18 (13%)	3 (2%)	6	24
7	I	36/38 (95%)	30 (83%)	6 (17%)	0	100	100
7	R	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
7	e	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	5	19
8	J	39/41 (95%)	34 (87%)	5 (13%)	0	100	100
8	S	39/41 (95%)	34 (87%)	5 (13%)	0	100	100
8	f	39/41 (95%)	38 (97%)	0	1 (3%)	5	20
9	K	40/83 (48%)	31 (78%)	7 (18%)	2 (5%)	2	7
9	T	40/83 (48%)	33 (82%)	4 (10%)	3 (8%)	1	2
9	g	40/83 (48%)	30 (75%)	8 (20%)	2 (5%)	2	7
10	L	149/155 (96%)	124 (83%)	22 (15%)	3 (2%)	7	27
10	U	149/155 (96%)	138 (93%)	11 (7%)	0	100	100
10	h	149/155 (96%)	129 (87%)	17 (11%)	3 (2%)	7	27
11	M	28/31 (90%)	26 (93%)	2 (7%)	0	100	100
11	V	28/31 (90%)	26 (93%)	2 (7%)	0	100	100
11	i	28/31 (90%)	28 (100%)	0	0	100	100
12	W	24/39 (62%)	23 (96%)	1 (4%)	0	100	100
12	X	24/39 (62%)	24 (100%)	0	0	100	100
12	j	24/39 (62%)	23 (96%)	1 (4%)	0	100	100
All	All	6630/7029 (94%)	5768 (87%)	740 (11%)	122 (2%)	8	29

5 of 122 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	VAL
4	D	95	HIS
5	E	55	VAL

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Mol	Chain	Res	Type
1	G	320	GLY
1	G	508	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	590/603 (98%)	574 (97%)	16 (3%)	44	77
1	G	590/603 (98%)	575 (98%)	15 (2%)	47	78
1	Y	590/603 (98%)	572 (97%)	18 (3%)	40	74
2	B	597/598 (100%)	575 (96%)	22 (4%)	34	68
2	H	597/598 (100%)	577 (97%)	20 (3%)	37	71
2	Z	597/598 (100%)	573 (96%)	24 (4%)	31	65
3	C	67/68 (98%)	64 (96%)	3 (4%)	27	61
3	N	67/68 (98%)	65 (97%)	2 (3%)	41	75
3	a	67/68 (98%)	65 (97%)	2 (3%)	41	75
4	D	115/116 (99%)	110 (96%)	5 (4%)	29	62
4	O	115/116 (99%)	110 (96%)	5 (4%)	29	62
4	b	115/116 (99%)	111 (96%)	4 (4%)	36	70
5	E	59/65 (91%)	56 (95%)	3 (5%)	24	56
5	P	59/65 (91%)	57 (97%)	2 (3%)	37	71
5	c	59/65 (91%)	58 (98%)	1 (2%)	60	86
6	F	109/128 (85%)	106 (97%)	3 (3%)	43	76
6	Q	109/128 (85%)	106 (97%)	3 (3%)	43	76
6	d	109/128 (85%)	108 (99%)	1 (1%)	78	93
7	I	32/32 (100%)	32 (100%)	0	100	100
7	R	32/32 (100%)	32 (100%)	0	100	100
7	e	32/32 (100%)	31 (97%)	1 (3%)	40	74
8	J	36/36 (100%)	36 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	S	36/36 (100%)	35 (97%)	1 (3%)	43	76
8	f	36/36 (100%)	36 (100%)	0	100	100
9	K	33/61 (54%)	32 (97%)	1 (3%)	41	75
9	T	33/61 (54%)	31 (94%)	2 (6%)	18	48
9	g	33/61 (54%)	30 (91%)	3 (9%)	9	28
10	L	117/120 (98%)	112 (96%)	5 (4%)	29	62
10	U	117/120 (98%)	113 (97%)	4 (3%)	37	71
10	h	117/120 (98%)	109 (93%)	8 (7%)	16	42
11	M	25/26 (96%)	25 (100%)	0	100	100
11	V	25/26 (96%)	24 (96%)	1 (4%)	31	65
11	i	25/26 (96%)	25 (100%)	0	100	100
12	W	20/31 (64%)	20 (100%)	0	100	100
12	X	20/31 (64%)	19 (95%)	1 (5%)	24	57
12	j	20/31 (64%)	19 (95%)	1 (5%)	24	57
All	All	5400/5652 (96%)	5223 (97%)	177 (3%)	38	72

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

Mol	Chain	Res	Type
2	H	494	ASN
4	O	126	SER
6	d	24	THR
2	H	575	ASP
10	L	19	THR

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

Mol	Chain	Res	Type
1	G	718	GLN
2	H	455	GLN
2	Z	494	ASN
2	H	78	GLN
2	H	192	HIS

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 381 ligands modelled in this entry, 3 are monoatomic - leaving 378 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
14	CLA	B	811	-	49,63,73	2.35	14 (28%)	55,101,113	2.42	21 (38%)
14	CLA	B	817	-	59,73,73	2.06	15 (25%)	67,113,113	2.13	18 (26%)
14	CLA	B	833	-	49,63,73	2.37	15 (30%)	55,101,113	2.42	22 (40%)
14	CLA	H	820	-	36,53,73	2.71	14 (38%)	39,89,113	2.54	16 (41%)
14	CLA	Y	810	-	36,53,73	2.64	14 (38%)	39,89,113	2.47	12 (30%)
14	CLA	Y	827	-	59,73,73	2.26	15 (25%)	67,113,113	2.33	19 (28%)
14	CLA	A	852	-	59,73,73	2.18	15 (25%)	67,113,113	2.60	20 (29%)
14	CLA	A	826	-	54,68,73	2.23	15 (27%)	61,107,113	2.22	16 (26%)
14	CLA	Y	835	-	49,63,73	2.51	16 (32%)	55,101,113	2.36	16 (29%)
18	LHG	Y	852	-	48,48,48	1.01	2 (4%)	51,54,54	1.00	2 (3%)
14	CLA	Z	808	2	59,73,73	2.11	15 (25%)	67,113,113	2.20	17 (25%)
14	CLA	B	841	-	59,73,73	2.10	14 (23%)	67,113,113	2.46	23 (34%)
17	BCR	M	101	-	41,41,41	2.80	6 (14%)	56,56,56	7.13	27 (48%)
14	CLA	H	817	-	54,68,73	2.27	15 (27%)	61,107,113	2.21	15 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	H	818	-	54,68,73	2.34	16 (29%)	61,107,113	2.18	16 (26%)
14	CLA	H	831	-	36,53,73	2.66	13 (36%)	39,89,113	2.64	15 (38%)
17	BCR	U	1005	-	41,41,41	2.72	6 (14%)	56,56,56	6.90	21 (37%)
14	CLA	A	832	-	59,73,73	2.18	14 (23%)	67,113,113	2.13	17 (25%)
17	BCR	G	846	-	41,41,41	2.81	7 (17%)	56,56,56	7.22	30 (53%)
14	CLA	G	824	-	54,68,73	2.26	14 (25%)	61,107,113	2.16	15 (24%)
14	CLA	d	202	-	36,53,73	2.67	14 (38%)	39,89,113	2.45	14 (35%)
14	CLA	B	802	-	59,73,73	2.10	14 (23%)	67,113,113	2.18	20 (29%)
14	CLA	Z	831	-	49,63,73	2.34	13 (26%)	55,101,113	2.49	22 (40%)
14	CLA	B	838	-	59,73,73	2.11	14 (23%)	67,113,113	2.25	17 (25%)
14	CLA	H	804	-	59,73,73	2.19	14 (23%)	67,113,113	2.08	17 (25%)
17	BCR	e	101	-	41,41,41	2.73	6 (14%)	56,56,56	7.45	26 (46%)
14	CLA	Y	855	-	59,73,73	2.09	13 (22%)	67,113,113	2.11	17 (25%)
14	CLA	G	839	-	59,73,73	2.14	15 (25%)	67,113,113	2.42	21 (31%)
14	CLA	H	813	-	59,73,73	2.20	15 (25%)	67,113,113	2.13	17 (25%)
14	CLA	A	822	-	59,73,73	2.25	16 (27%)	67,113,113	2.34	19 (28%)
14	CLA	H	837	-	59,73,73	2.19	15 (25%)	67,113,113	1.98	18 (26%)
14	CLA	L	205	10	59,73,73	2.19	15 (25%)	67,113,113	2.20	17 (25%)
14	CLA	F	202	-	36,53,73	2.64	13 (36%)	39,89,113	2.40	14 (35%)
14	CLA	Y	830	-	59,73,73	2.12	14 (23%)	67,113,113	2.39	16 (23%)
14	CLA	Y	825	-	59,73,73	2.23	15 (25%)	67,113,113	2.28	17 (25%)
14	CLA	Y	809	-	59,73,73	2.16	15 (25%)	67,113,113	2.05	17 (25%)
14	CLA	A	840	-	59,73,73	2.18	15 (25%)	67,113,113	2.00	16 (23%)
14	CLA	G	813	-	54,68,73	2.19	16 (29%)	61,107,113	2.54	19 (31%)
14	CLA	Y	840	-	59,73,73	2.25	15 (25%)	67,113,113	2.37	18 (26%)
14	CLA	B	837	-	54,68,73	2.28	13 (24%)	61,107,113	2.45	17 (27%)
14	CLA	U	1003	-	59,73,73	2.22	15 (25%)	67,113,113	2.26	18 (26%)
17	BCR	H	845	-	41,41,41	2.78	8 (19%)	56,56,56	7.11	28 (50%)
14	CLA	B	834	-	36,53,73	2.77	15 (41%)	39,89,113	3.14	17 (43%)
18	LHG	G	852	14	31,31,48	1.26	2 (6%)	34,37,54	1.31	4 (11%)
14	CLA	A	836	-	44,58,73	2.61	15 (34%)	49,95,113	2.28	15 (30%)
17	BCR	J	103	-	41,41,41	2.61	6 (14%)	56,56,56	6.88	28 (50%)
14	CLA	U	1002	10	59,73,73	2.13	16 (27%)	67,113,113	2.41	22 (32%)
14	CLA	A	812	-	48,62,73	2.40	15 (31%)	53,99,113	2.26	18 (33%)
17	BCR	A	847	-	41,41,41	2.70	6 (14%)	56,56,56	7.09	26 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	G	854	-	41,41,41	2.96	6 (14%)	56,56,56	7.14	27 (48%)
14	CLA	H	805	-	59,73,73	2.14	15 (25%)	67,113,113	2.06	16 (23%)
17	BCR	Y	846	-	41,41,41	2.50	6 (14%)	56,56,56	7.20	24 (42%)
18	LHG	A	850	-	48,48,48	0.99	2 (4%)	51,54,54	1.05	3 (5%)
14	CLA	G	816	-	44,58,73	2.57	15 (34%)	49,95,113	2.64	15 (30%)
14	CLA	G	836	-	44,58,73	2.48	15 (34%)	49,95,113	2.60	17 (34%)
14	CLA	A	820	-	54,68,73	2.27	16 (29%)	61,107,113	2.33	18 (29%)
17	BCR	d	203	-	41,41,41	2.62	6 (14%)	56,56,56	7.01	27 (48%)
14	CLA	G	817	-	54,68,73	2.37	14 (25%)	61,107,113	2.21	20 (32%)
14	CLA	H	807	-	59,73,73	2.28	16 (27%)	67,113,113	2.45	23 (34%)
14	CLA	Y	811	14	59,73,73	2.26	13 (22%)	67,113,113	2.13	17 (25%)
14	CLA	Y	838	-	59,73,73	2.18	16 (27%)	67,113,113	2.11	18 (26%)
14	CLA	H	815	-	49,63,73	2.36	14 (28%)	55,101,113	2.44	19 (34%)
14	CLA	B	825	-	59,73,73	2.22	15 (25%)	67,113,113	2.29	21 (31%)
14	CLA	Y	812	-	49,63,73	2.35	15 (30%)	55,101,113	2.33	20 (36%)
18	LHG	j	101	-	27,27,48	1.28	2 (7%)	30,33,54	1.36	4 (13%)
14	CLA	Z	821	-	54,68,73	2.34	15 (27%)	61,107,113	2.10	19 (31%)
14	CLA	J	102	-	49,63,73	2.47	15 (30%)	55,101,113	2.46	18 (32%)
17	BCR	B	844	-	41,41,41	2.78	6 (14%)	56,56,56	7.31	25 (44%)
14	CLA	S	1102	8	36,53,73	2.62	13 (36%)	39,89,113	2.31	11 (28%)
17	BCR	H	841	-	41,41,41	3.03	7 (17%)	56,56,56	6.95	26 (46%)
17	BCR	A	845	-	41,41,41	2.55	6 (14%)	56,56,56	7.14	28 (50%)
14	CLA	A	807	-	45,59,73	2.47	14 (31%)	50,96,113	2.41	15 (30%)
14	CLA	Z	815	-	59,73,73	2.12	15 (25%)	67,113,113	2.15	19 (28%)
14	CLA	H	810	-	49,63,73	2.28	14 (28%)	55,101,113	2.35	16 (29%)
18	LHG	A	851	14	31,31,48	1.19	2 (6%)	34,37,54	1.20	3 (8%)
14	CLA	H	802	-	59,73,73	2.16	16 (27%)	67,113,113	2.14	19 (28%)
14	CLA	Y	820	-	54,68,73	2.24	15 (27%)	61,107,113	2.26	19 (31%)
17	BCR	G	849	-	41,41,41	2.83	7 (17%)	56,56,56	6.96	25 (44%)
17	BCR	H	842	-	41,41,41	2.74	6 (14%)	56,56,56	7.14	24 (42%)
17	BCR	Y	851	-	41,41,41	2.94	6 (14%)	56,56,56	7.30	29 (51%)
14	CLA	T	101	-	32,49,73	2.69	13 (40%)	32,83,113	2.33	11 (34%)
14	CLA	U	1006	2	59,73,73	2.22	14 (23%)	67,113,113	2.26	23 (34%)
14	CLA	Y	834	-	59,73,73	2.18	13 (22%)	67,113,113	2.04	20 (29%)
14	CLA	Z	832	-	36,53,73	2.76	14 (38%)	39,89,113	2.53	15 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	Z	833	-	36,53,73	2.74	13 (36%)	39,89,113	2.42	11 (28%)
17	BCR	A	849	-	41,41,41	2.67	6 (14%)	56,56,56	7.34	26 (46%)
17	BCR	Y	856	-	41,41,41	2.71	7 (17%)	56,56,56	7.00	30 (53%)
17	BCR	B	851	-	41,41,41	2.77	6 (14%)	56,56,56	7.08	27 (48%)
14	CLA	H	821	-	49,63,73	2.47	15 (30%)	55,101,113	2.43	17 (30%)
14	CLA	L	207	-	59,73,73	2.20	15 (25%)	67,113,113	2.11	17 (25%)
14	CLA	B	819	-	54,68,73	2.30	16 (29%)	61,107,113	2.27	20 (32%)
14	CLA	G	809	-	59,73,73	2.12	14 (23%)	67,113,113	2.17	20 (29%)
18	LHG	H	847	-	36,36,48	1.10	2 (5%)	39,42,54	0.92	3 (7%)
17	BCR	B	848	-	41,41,41	2.76	7 (17%)	56,56,56	6.90	27 (48%)
16	SF4	a	101	3	0,12,12	0.00	-	-	-	-
14	CLA	A	841	-	59,73,73	2.17	16 (27%)	67,113,113	2.06	18 (26%)
14	CLA	G	834	-	49,63,73	2.43	15 (30%)	55,101,113	2.16	17 (30%)
14	CLA	A	816	-	44,58,73	2.61	15 (34%)	49,95,113	2.45	14 (28%)
14	CLA	Z	837	-	36,53,73	2.69	14 (38%)	39,89,113	2.60	12 (30%)
14	CLA	A	815	-	44,58,73	2.53	14 (31%)	49,95,113	2.73	19 (38%)
14	CLA	H	823	2	49,63,73	2.50	16 (32%)	55,101,113	2.59	20 (36%)
14	CLA	B	801	-	59,73,73	2.04	11 (18%)	67,113,113	2.19	15 (22%)
17	BCR	h	202	-	41,41,41	2.53	8 (19%)	56,56,56	7.31	28 (50%)
14	CLA	H	824	-	59,73,73	2.16	16 (27%)	67,113,113	2.52	24 (35%)
14	CLA	Y	833	-	59,73,73	2.18	13 (22%)	67,113,113	2.26	18 (26%)
14	CLA	H	835	-	59,73,73	2.12	15 (25%)	67,113,113	2.13	17 (25%)
14	CLA	G	806	-	59,73,73	2.12	14 (23%)	67,113,113	2.16	14 (20%)
14	CLA	Z	814	-	49,63,73	2.42	15 (30%)	55,101,113	2.45	19 (34%)
14	CLA	A	804	14	53,67,73	2.29	15 (28%)	59,105,113	2.49	17 (28%)
14	CLA	A	829	-	59,73,73	2.15	15 (25%)	67,113,113	1.98	16 (23%)
14	CLA	G	812	-	48,62,73	2.41	14 (29%)	53,99,113	2.24	14 (26%)
14	CLA	Y	808	1	59,73,73	2.16	14 (23%)	67,113,113	2.32	20 (29%)
14	CLA	H	832	-	36,53,73	2.64	14 (38%)	39,89,113	2.58	13 (33%)
14	CLA	Z	801	-	59,73,73	2.11	14 (23%)	67,113,113	2.08	17 (25%)
14	CLA	Z	807	-	59,73,73	2.21	16 (27%)	67,113,113	2.43	19 (28%)
14	CLA	U	1004	-	59,73,73	2.18	14 (23%)	67,113,113	2.26	14 (20%)
17	BCR	J	104	-	41,41,41	2.91	7 (17%)	56,56,56	7.08	27 (48%)
14	CLA	H	827	-	59,73,73	2.16	15 (25%)	67,113,113	2.13	19 (28%)
17	BCR	Y	848	-	41,41,41	2.60	6 (14%)	56,56,56	7.21	29 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	LMG	Z	847	-	49,49,55	1.26	6 (12%)	57,57,63	1.24	5 (8%)
14	CLA	G	804	-	53,67,73	2.24	15 (28%)	59,105,113	2.34	14 (23%)
14	CLA	Y	802	-	59,73,73	2.05	14 (23%)	67,113,113	2.32	17 (25%)
14	CLA	G	811	-	59,73,73	2.24	16 (27%)	67,113,113	2.06	15 (22%)
14	CLA	H	808	2	59,73,73	2.11	14 (23%)	67,113,113	2.32	21 (31%)
14	CLA	H	838	-	59,73,73	2.14	14 (23%)	67,113,113	2.38	20 (29%)
14	CLA	A	825	-	59,73,73	2.21	16 (27%)	67,113,113	2.33	18 (26%)
17	BCR	L	203	-	41,41,41	2.92	6 (14%)	56,56,56	6.97	29 (51%)
13	CL0	G	801	-	59,73,73	2.35	16 (27%)	67,113,113	2.49	20 (29%)
14	CLA	B	804	-	59,73,73	2.12	16 (27%)	67,113,113	2.09	16 (23%)
17	BCR	f	103	-	41,41,41	2.56	6 (14%)	56,56,56	7.19	28 (50%)
14	CLA	Z	812	-	59,73,73	2.38	14 (23%)	67,113,113	2.00	15 (22%)
14	CLA	j	102	-	36,53,73	2.63	13 (36%)	39,89,113	2.36	12 (30%)
14	CLA	L	206	-	59,73,73	2.22	16 (27%)	67,113,113	2.23	16 (23%)
18	LHG	Y	853	14	24,24,48	1.51	2 (8%)	27,30,54	1.60	4 (14%)
14	CLA	A	838	-	44,58,73	2.43	14 (31%)	49,95,113	2.41	17 (34%)
14	CLA	Z	830	-	59,73,73	2.11	14 (23%)	67,113,113	2.07	14 (20%)
16	SF4	N	102	3,21	0,12,12	0.00	-	-	-	-
14	CLA	B	832	-	59,73,73	2.11	14 (23%)	67,113,113	2.28	16 (23%)
14	CLA	B	810	2	59,73,73	2.14	16 (27%)	67,113,113	2.66	20 (29%)
14	CLA	S	1103	-	49,63,73	2.39	15 (30%)	55,101,113	2.51	18 (32%)
17	BCR	f	104	-	41,41,41	2.95	6 (14%)	56,56,56	6.95	28 (50%)
14	CLA	T	103	-	36,53,73	2.74	15 (41%)	39,89,113	2.26	11 (28%)
14	CLA	H	833	-	36,53,73	2.61	13 (36%)	39,89,113	2.49	15 (38%)
17	BCR	Y	850	-	41,41,41	2.70	6 (14%)	56,56,56	7.10	24 (42%)
17	BCR	R	101	-	41,41,41	2.76	6 (14%)	56,56,56	7.47	24 (42%)
14	CLA	H	809	2	59,73,73	2.14	14 (23%)	67,113,113	2.31	21 (31%)
14	CLA	Y	822	-	59,73,73	2.24	15 (25%)	67,113,113	2.23	15 (22%)
14	CLA	H	803	-	59,73,73	2.11	13 (22%)	67,113,113	2.27	18 (26%)
14	CLA	G	837	-	59,73,73	2.16	15 (25%)	67,113,113	2.20	20 (29%)
14	CLA	J	101	8	36,53,73	2.62	13 (36%)	39,89,113	2.45	13 (33%)
15	PQN	G	844	-	34,34,34	1.53	2 (5%)	42,45,45	1.24	6 (14%)
14	CLA	Y	832	-	59,73,73	2.23	14 (23%)	67,113,113	2.33	17 (25%)
14	CLA	A	827	-	59,73,73	2.12	15 (25%)	67,113,113	2.04	17 (25%)
14	CLA	H	830	-	49,63,73	2.36	15 (30%)	55,101,113	2.23	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	Y	818	-	59,73,73	2.21	15 (25%)	67,113,113	2.38	19 (28%)
14	CLA	A	809	1	59,73,73	2.13	15 (25%)	67,113,113	2.36	19 (28%)
14	CLA	B	813	-	59,73,73	2.14	15 (25%)	67,113,113	2.31	19 (28%)
14	CLA	G	840	-	44,58,73	2.60	13 (29%)	49,95,113	2.19	16 (32%)
14	CLA	Z	806	-	59,73,73	2.12	14 (23%)	67,113,113	2.19	17 (25%)
14	CLA	Z	834	-	36,53,73	2.65	16 (44%)	39,89,113	2.74	16 (41%)
14	CLA	B	806	-	59,73,73	2.00	14 (23%)	67,113,113	2.47	19 (28%)
14	CLA	Z	809	-	49,63,73	2.44	15 (30%)	55,101,113	2.25	17 (30%)
14	CLA	G	808	1	59,73,73	2.16	14 (23%)	67,113,113	2.25	20 (29%)
14	CLA	G	832	-	59,73,73	2.08	14 (23%)	67,113,113	2.17	19 (28%)
14	CLA	H	801	-	59,73,73	2.25	14 (23%)	67,113,113	2.52	20 (29%)
14	CLA	Y	821	-	59,73,73	2.31	15 (25%)	67,113,113	1.99	16 (23%)
14	CLA	Z	828	-	36,53,73	2.55	14 (38%)	39,89,113	2.26	14 (35%)
14	CLA	B	812	-	44,58,73	2.48	15 (34%)	49,95,113	2.45	18 (36%)
14	CLA	H	806	-	59,73,73	2.14	14 (23%)	67,113,113	1.95	14 (20%)
14	CLA	G	810	-	36,53,73	2.64	14 (38%)	39,89,113	2.44	13 (33%)
17	BCR	A	848	-	41,41,41	2.57	6 (14%)	56,56,56	7.07	22 (39%)
14	CLA	G	841	-	59,73,73	2.25	14 (23%)	67,113,113	2.20	18 (26%)
14	CLA	A	805	-	59,73,73	2.07	15 (25%)	67,113,113	2.15	16 (23%)
14	CLA	Z	817	-	54,68,73	2.34	14 (25%)	61,107,113	2.17	18 (29%)
14	CLA	Z	803	-	48,62,73	2.48	15 (31%)	53,99,113	2.69	18 (33%)
14	CLA	Y	814	-	49,63,73	2.44	15 (30%)	55,101,113	2.38	16 (29%)
14	CLA	h	201	-	59,73,73	2.13	16 (27%)	67,113,113	2.08	15 (22%)
14	CLA	Z	819	-	36,53,73	2.76	13 (36%)	39,89,113	2.66	14 (35%)
14	CLA	B	827	-	59,73,73	2.10	15 (25%)	67,113,113	2.17	18 (26%)
17	BCR	B	847	-	41,41,41	2.87	6 (14%)	56,56,56	7.00	24 (42%)
17	BCR	G	847	-	41,41,41	2.78	6 (14%)	56,56,56	6.97	26 (46%)
14	CLA	Y	815	-	44,58,73	2.62	15 (34%)	49,95,113	2.64	17 (34%)
14	CLA	B	803	-	59,73,73	2.04	12 (20%)	67,113,113	2.12	18 (26%)
14	CLA	B	824	2	49,63,73	2.43	14 (28%)	55,101,113	2.50	19 (34%)
14	CLA	B	821	-	36,53,73	2.64	14 (38%)	39,89,113	2.55	15 (38%)
17	BCR	Z	841	-	41,41,41	2.90	6 (14%)	56,56,56	7.13	25 (44%)
16	SF4	Y	845	1,2	0,12,12	0.00	-	-	-	-
14	CLA	Z	804	-	59,73,73	2.11	16 (27%)	67,113,113	2.35	21 (31%)
14	CLA	H	812	-	59,73,73	2.21	15 (25%)	67,113,113	2.20	15 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	821	-	59,73,73	2.19	14 (23%)	67,113,113	2.01	16 (23%)
14	CLA	G	830	-	59,73,73	2.16	14 (23%)	67,113,113	2.29	18 (26%)
15	PQN	H	839	-	34,34,34	1.61	2 (5%)	42,45,45	1.28	6 (14%)
14	CLA	A	842	18	44,58,73	2.55	14 (31%)	49,95,113	2.75	14 (28%)
14	CLA	A	802	-	59,73,73	2.08	16 (27%)	67,113,113	2.47	23 (34%)
18	LHG	B	850	-	38,38,48	1.09	2 (5%)	41,44,54	1.28	4 (9%)
17	BCR	L	208	-	41,41,41	3.06	7 (17%)	56,56,56	6.91	24 (42%)
14	CLA	A	831	-	44,58,73	2.44	14 (31%)	49,95,113	2.50	18 (36%)
14	CLA	Y	823	-	44,58,73	2.61	14 (31%)	49,95,113	2.38	18 (36%)
17	BCR	f	105	-	41,41,41	2.74	6 (14%)	56,56,56	7.07	26 (46%)
17	BCR	Z	846	-	41,41,41	2.70	7 (17%)	56,56,56	7.02	20 (35%)
17	BCR	Y	847	-	41,41,41	2.71	6 (14%)	56,56,56	7.10	29 (51%)
14	CLA	A	839	-	44,58,73	2.56	15 (34%)	49,95,113	2.34	16 (32%)
19	LMG	B	849	-	52,52,55	1.29	7 (13%)	60,60,63	0.99	3 (5%)
17	BCR	Z	845	-	41,41,41	2.59	8 (19%)	56,56,56	7.27	30 (53%)
14	CLA	Y	839	-	44,58,73	2.55	16 (36%)	49,95,113	2.63	18 (36%)
17	BCR	B	845	-	41,41,41	2.72	7 (17%)	56,56,56	7.05	27 (48%)
14	CLA	G	825	-	59,73,73	2.16	15 (25%)	67,113,113	2.22	20 (29%)
14	CLA	Y	816	-	44,58,73	2.43	14 (31%)	49,95,113	2.49	16 (32%)
14	CLA	Q	201	-	59,73,73	2.06	14 (23%)	67,113,113	2.26	16 (23%)
17	BCR	G	850	-	41,41,41	2.70	6 (14%)	56,56,56	7.31	27 (48%)
14	CLA	K	101	-	32,49,73	2.74	13 (40%)	32,83,113	2.47	13 (40%)
14	CLA	L	201	-	59,73,73	2.11	14 (23%)	67,113,113	2.22	20 (29%)
14	CLA	A	833	-	59,73,73	2.12	14 (23%)	67,113,113	2.28	22 (32%)
14	CLA	H	829	-	36,53,73	2.63	13 (36%)	39,89,113	2.45	13 (33%)
14	CLA	A	824	-	54,68,73	2.33	14 (25%)	61,107,113	2.14	17 (27%)
14	CLA	L	202	-	59,73,73	2.12	14 (23%)	67,113,113	2.35	21 (31%)
14	CLA	G	820	-	54,68,73	2.29	16 (29%)	61,107,113	2.32	17 (27%)
14	CLA	G	835	1	36,53,73	2.61	14 (38%)	39,89,113	2.52	15 (38%)
14	CLA	Y	826	-	54,68,73	2.29	15 (27%)	61,107,113	2.24	17 (27%)
14	CLA	Y	804	14	53,67,73	2.29	15 (28%)	59,105,113	2.52	19 (32%)
14	CLA	d	201	-	44,58,73	2.55	15 (34%)	49,95,113	2.46	20 (40%)
17	BCR	Q	204	-	41,41,41	2.72	7 (17%)	56,56,56	7.13	28 (50%)
17	BCR	V	1202	-	41,41,41	2.74	7 (17%)	56,56,56	7.27	30 (53%)
14	CLA	Z	825	-	59,73,73	2.12	14 (23%)	67,113,113	1.91	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	Y	837	-	44,58,73	2.51	15 (34%)	49,95,113	2.48	17 (34%)
14	CLA	Z	818	-	36,53,73	2.67	12 (33%)	39,89,113	2.47	14 (35%)
14	CLA	A	814	-	44,58,73	2.57	15 (34%)	49,95,113	2.63	20 (40%)
17	BCR	U	1008	-	41,41,41	2.56	6 (14%)	56,56,56	7.17	25 (44%)
14	CLA	G	803	-	59,73,73	2.13	14 (23%)	67,113,113	2.39	21 (31%)
14	CLA	Y	813	-	54,68,73	2.20	15 (27%)	61,107,113	2.03	17 (27%)
14	CLA	S	1101	-	59,73,73	2.13	15 (25%)	67,113,113	2.28	16 (23%)
17	BCR	F	203	-	41,41,41	2.71	7 (17%)	56,56,56	7.14	29 (51%)
14	CLA	B	820	-	36,53,73	2.60	14 (38%)	39,89,113	2.60	14 (35%)
17	BCR	U	1007	-	41,41,41	2.80	6 (14%)	56,56,56	7.10	21 (37%)
14	CLA	G	833	-	59,73,73	2.26	14 (23%)	67,113,113	2.14	17 (25%)
14	CLA	Z	838	-	59,73,73	2.22	15 (25%)	67,113,113	2.11	19 (28%)
14	CLA	Z	811	-	59,73,73	2.13	14 (23%)	67,113,113	2.07	17 (25%)
14	CLA	H	822	-	54,68,73	2.19	14 (25%)	61,107,113	2.32	20 (32%)
17	BCR	G	848	-	41,41,41	2.71	6 (14%)	56,56,56	7.23	31 (55%)
14	CLA	G	829	-	59,73,73	2.18	15 (25%)	67,113,113	2.01	19 (28%)
16	SF4	C	101	3,21	0,12,12	0.00	-	-		
17	BCR	H	843	-	25,25,41	2.03	2 (8%)	33,33,56	8.12	17 (51%)
14	CLA	Y	806	-	59,73,73	2.18	13 (22%)	67,113,113	2.25	17 (25%)
14	CLA	h	207	-	59,73,73	2.21	15 (25%)	67,113,113	2.21	19 (28%)
14	CLA	Y	829	-	59,73,73	2.20	15 (25%)	67,113,113	2.12	15 (22%)
14	CLA	G	853	-	36,53,73	2.68	14 (38%)	39,89,113	2.22	10 (25%)
16	SF4	C	102	3	0,12,12	0.00	-	-		
16	SF4	a	102	3	0,12,12	0.00	-	-		
14	CLA	A	828	-	59,73,73	2.12	15 (25%)	67,113,113	2.13	15 (22%)
17	BCR	A	846	-	41,41,41	2.62	6 (14%)	56,56,56	7.05	26 (46%)
14	CLA	A	803	-	59,73,73	2.22	17 (28%)	67,113,113	2.44	19 (28%)
17	BCR	Z	843	-	41,41,41	2.56	6 (14%)	56,56,56	7.31	29 (51%)
14	CLA	B	830	-	36,53,73	2.53	14 (38%)	39,89,113	2.73	15 (38%)
14	CLA	Z	820	-	49,63,73	2.48	15 (30%)	55,101,113	2.20	19 (34%)
14	CLA	G	838	-	44,58,73	2.53	15 (34%)	49,95,113	2.48	19 (38%)
14	CLA	Y	841	-	59,73,73	2.11	15 (25%)	67,113,113	1.93	15 (22%)
17	BCR	B	843	-	30,30,41	3.42	6 (20%)	39,39,56	8.21	19 (48%)
14	CLA	Z	822	2	49,63,73	2.39	15 (30%)	55,101,113	2.60	20 (36%)
15	PQN	B	842	-	34,34,34	1.53	3 (8%)	42,45,45	1.22	6 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	Y	842	-	59,73,73	2.14	14 (23%)	67,113,113	2.15	19 (28%)
14	CLA	A	819	-	59,73,73	2.12	15 (25%)	67,113,113	2.05	17 (25%)
14	CLA	V	1201	-	48,62,73	2.46	14 (29%)	53,99,113	2.29	16 (30%)
14	CLA	W	1701	-	36,53,73	2.59	14 (38%)	39,89,113	2.36	12 (30%)
14	CLA	Z	802	-	59,73,73	2.14	15 (25%)	67,113,113	2.26	20 (29%)
14	CLA	H	834	-	54,68,73	2.22	14 (25%)	61,107,113	2.07	18 (29%)
16	SF4	A	844	1,2	0,12,12	0.00	-	-		
14	CLA	B	814	-	59,73,73	2.30	14 (23%)	67,113,113	2.10	19 (28%)
14	CLA	Y	805	-	59,73,73	2.07	14 (23%)	67,113,113	2.26	21 (31%)
14	CLA	Q	203	-	36,53,73	2.59	13 (36%)	39,89,113	2.64	13 (33%)
14	CLA	Y	854	-	59,73,73	2.12	14 (23%)	67,113,113	2.39	18 (26%)
14	CLA	G	802	-	59,73,73	2.18	14 (23%)	67,113,113	2.20	15 (22%)
16	SF4	N	101	3	0,12,12	0.00	-	-		
14	CLA	A	830	-	59,73,73	2.09	16 (27%)	67,113,113	2.30	16 (23%)
14	CLA	G	828	-	59,73,73	2.12	14 (23%)	67,113,113	2.21	21 (31%)
14	CLA	H	836	-	36,53,73	2.63	16 (44%)	39,89,113	2.57	15 (38%)
17	BCR	Z	842	-	41,41,41	2.69	8 (19%)	56,56,56	7.04	26 (46%)
14	CLA	B	808	-	59,73,73	2.11	15 (25%)	67,113,113	2.12	18 (26%)
14	CLA	B	816	-	49,63,73	2.48	14 (28%)	55,101,113	2.28	18 (32%)
14	CLA	Z	839	-	59,73,73	2.26	16 (27%)	67,113,113	2.29	19 (28%)
14	CLA	G	826	-	54,68,73	2.23	14 (25%)	61,107,113	2.24	17 (27%)
14	CLA	A	823	-	44,58,73	2.56	15 (34%)	49,95,113	2.47	18 (36%)
17	BCR	h	203	-	41,41,41	3.00	7 (17%)	56,56,56	7.05	27 (48%)
14	CLA	G	821	-	59,73,73	2.18	14 (23%)	67,113,113	1.95	15 (22%)
14	CLA	B	822	-	49,63,73	2.42	14 (28%)	55,101,113	2.37	19 (34%)
14	CLA	Y	843	18	44,58,73	2.58	15 (34%)	49,95,113	2.60	18 (36%)
14	CLA	B	839	-	36,53,73	2.61	13 (36%)	39,89,113	2.24	9 (23%)
14	CLA	A	808	1	59,73,73	2.15	14 (23%)	67,113,113	2.29	17 (25%)
14	CLA	H	811	-	36,53,73	2.58	13 (36%)	39,89,113	2.23	13 (33%)
14	CLA	B	823	-	54,68,73	2.34	15 (27%)	61,107,113	2.10	16 (26%)
14	CLA	A	811	14	59,73,73	2.16	15 (25%)	67,113,113	1.99	15 (22%)
14	CLA	Z	810	-	36,53,73	2.60	12 (33%)	39,89,113	2.35	15 (38%)
14	CLA	Y	803	-	59,73,73	2.24	14 (23%)	67,113,113	2.28	18 (26%)
14	CLA	H	826	-	59,73,73	2.12	14 (23%)	67,113,113	2.10	18 (26%)
14	CLA	B	807	-	59,73,73	2.11	14 (23%)	67,113,113	2.18	18 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	LMG	H	846	-	49,49,55	1.36	6 (12%)	57,57,63	1.18	4 (7%)
14	CLA	Z	816	-	54,68,73	2.30	15 (27%)	61,107,113	2.21	19 (31%)
14	CLA	B	836	-	36,53,73	2.58	15 (41%)	39,89,113	2.70	13 (33%)
14	CLA	G	805	-	59,73,73	2.09	14 (23%)	67,113,113	2.19	18 (26%)
17	BCR	i	101	-	41,41,41	2.84	7 (17%)	56,56,56	7.60	32 (57%)
14	CLA	H	828	-	59,73,73	2.20	15 (25%)	67,113,113	2.50	17 (25%)
14	CLA	B	831	-	36,53,73	2.60	14 (38%)	39,89,113	2.53	14 (35%)
14	CLA	f	102	-	49,63,73	2.46	15 (30%)	55,101,113	2.35	19 (34%)
14	CLA	Z	824	-	59,73,73	2.10	13 (22%)	67,113,113	2.07	19 (28%)
14	CLA	Z	835	-	54,68,73	2.23	17 (31%)	61,107,113	2.08	15 (24%)
14	CLA	B	826	-	59,73,73	2.20	16 (27%)	67,113,113	2.35	24 (35%)
15	PQN	A	843	-	34,34,34	1.61	2 (5%)	42,45,45	1.09	3 (7%)
14	CLA	A	835	1	36,53,73	2.62	14 (38%)	39,89,113	2.35	13 (33%)
17	BCR	L	209	-	41,41,41	2.75	6 (14%)	56,56,56	7.10	26 (46%)
14	CLA	B	815	-	36,53,73	2.54	12 (33%)	39,89,113	2.50	15 (38%)
14	CLA	Z	813	-	36,53,73	2.77	15 (41%)	39,89,113	2.85	17 (43%)
17	BCR	F	201	-	41,41,41	2.76	6 (14%)	56,56,56	6.88	24 (42%)
14	CLA	X	1701	-	36,53,73	2.65	15 (41%)	39,89,113	2.58	11 (28%)
14	CLA	A	806	-	59,73,73	2.17	16 (27%)	67,113,113	2.10	16 (23%)
14	CLA	B	829	-	59,73,73	2.16	14 (23%)	67,113,113	2.31	15 (22%)
14	CLA	Y	828	-	59,73,73	2.08	15 (25%)	67,113,113	1.95	17 (25%)
17	BCR	H	844	-	41,41,41	2.75	6 (14%)	56,56,56	7.04	29 (51%)
14	CLA	Z	826	-	59,73,73	2.11	14 (23%)	67,113,113	2.10	18 (26%)
14	CLA	B	805	-	48,62,73	2.40	16 (33%)	53,99,113	2.68	18 (33%)
14	CLA	G	815	-	44,58,73	2.47	14 (31%)	49,95,113	2.82	19 (38%)
14	CLA	g	102	-	36,53,73	2.70	13 (36%)	39,89,113	2.41	12 (30%)
14	CLA	G	831	-	44,58,73	2.44	14 (31%)	49,95,113	2.59	17 (34%)
14	CLA	B	809	-	59,73,73	2.13	14 (23%)	67,113,113	2.55	18 (26%)
17	BCR	H	840	-	41,41,41	2.81	6 (14%)	56,56,56	7.12	21 (37%)
14	CLA	G	823	-	44,58,73	2.49	15 (34%)	49,95,113	2.43	17 (34%)
14	CLA	Y	807	-	45,59,73	2.58	16 (35%)	50,96,113	2.45	16 (32%)
17	BCR	S	1104	-	41,41,41	2.89	7 (17%)	56,56,56	7.21	27 (48%)
14	CLA	K	103	-	36,53,73	2.63	13 (36%)	39,89,113	2.45	11 (28%)
14	CLA	Z	829	-	36,53,73	2.75	15 (41%)	39,89,113	2.77	17 (43%)
14	CLA	B	840	-	59,73,73	2.20	16 (27%)	67,113,113	2.09	21 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	G	822	-	59,73,73	2.16	15 (25%)	67,113,113	2.43	21 (31%)
14	CLA	H	814	-	36,53,73	2.66	15 (41%)	39,89,113	2.59	17 (43%)
14	CLA	Y	824	-	54,68,73	2.35	15 (27%)	61,107,113	2.22	16 (26%)
14	CLA	A	837	-	59,73,73	2.12	14 (23%)	67,113,113	2.07	19 (28%)
17	BCR	Q	202	-	41,41,41	2.79	6 (14%)	56,56,56	6.74	27 (48%)
14	CLA	H	819	-	36,53,73	2.60	14 (38%)	39,89,113	2.82	15 (38%)
15	PQN	Y	844	-	34,34,34	1.82	2 (5%)	42,45,45	0.83	1 (2%)
14	CLA	Z	823	-	59,73,73	2.20	15 (25%)	67,113,113	2.44	21 (31%)
14	CLA	g	101	-	32,49,73	2.73	12 (37%)	32,83,113	2.31	11 (34%)
14	CLA	B	818	-	54,68,73	2.24	15 (27%)	61,107,113	2.20	18 (29%)
14	CLA	H	816	-	59,73,73	2.11	15 (25%)	67,113,113	2.38	23 (34%)
17	BCR	T	102	-	41,41,41	2.46	6 (14%)	56,56,56	7.40	24 (42%)
17	BCR	B	846	-	25,25,41	2.18	2 (8%)	33,33,56	8.00	15 (45%)
14	CLA	G	818	-	59,73,73	2.18	14 (23%)	67,113,113	2.15	20 (29%)
14	CLA	A	818	-	59,73,73	2.18	15 (25%)	67,113,113	2.25	19 (28%)
14	CLA	Z	827	-	59,73,73	2.05	15 (25%)	67,113,113	2.36	17 (25%)
13	CL0	A	801	-	59,73,73	2.33	16 (27%)	67,113,113	2.34	14 (20%)
17	BCR	I	101	-	41,41,41	2.59	7 (17%)	56,56,56	7.30	26 (46%)
14	CLA	f	101	8	36,53,73	2.76	15 (41%)	39,89,113	2.36	13 (33%)
14	CLA	Y	817	-	54,68,73	2.36	15 (27%)	61,107,113	2.09	17 (27%)
13	CL0	Y	801	-	59,73,73	2.26	14 (23%)	67,113,113	2.29	17 (25%)
14	CLA	A	817	-	54,68,73	2.25	15 (27%)	61,107,113	2.26	20 (32%)
14	CLA	Z	836	-	59,73,73	2.11	14 (23%)	67,113,113	2.11	16 (23%)
18	LHG	G	851	-	48,48,48	0.93	2 (4%)	51,54,54	1.10	3 (5%)
14	CLA	G	814	-	44,58,73	2.52	14 (31%)	49,95,113	2.91	23 (46%)
14	CLA	A	810	-	36,53,73	2.65	14 (38%)	39,89,113	2.36	10 (25%)
14	CLA	h	205	10	59,73,73	2.20	14 (23%)	67,113,113	2.30	18 (26%)
14	CLA	Y	836	1	36,53,73	2.67	14 (38%)	39,89,113	2.36	11 (28%)
14	CLA	h	206	-	59,73,73	2.20	15 (25%)	67,113,113	2.50	23 (34%)
14	CLA	H	825	-	59,73,73	2.17	16 (27%)	67,113,113	2.18	21 (31%)
14	CLA	A	834	-	49,63,73	2.37	15 (30%)	55,101,113	2.20	17 (30%)
14	CLA	Y	831	-	44,58,73	2.47	15 (34%)	49,95,113	2.59	18 (36%)
14	CLA	Z	805	-	59,73,73	2.18	16 (27%)	67,113,113	2.28	21 (31%)
15	PQN	Z	840	-	34,34,34	1.66	2 (5%)	42,45,45	1.10	4 (9%)
17	BCR	R	102	-	41,41,41	3.00	8 (19%)	56,56,56	6.94	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	G	807	-	45,59,73	2.54	16 (35%)	50,96,113	2.56	17 (34%)
17	BCR	Z	844	-	25,25,41	2.29	2 (8%)	33,33,56	7.89	20 (60%)
14	CLA	B	828	-	59,73,73	2.10	15 (25%)	67,113,113	2.24	18 (26%)
14	CLA	G	819	-	59,73,73	2.25	15 (25%)	67,113,113	2.35	18 (26%)
14	CLA	B	835	-	36,53,73	2.66	16 (44%)	39,89,113	2.58	14 (35%)
17	BCR	H	848	-	41,41,41	2.77	6 (14%)	56,56,56	7.05	28 (50%)
14	CLA	G	842	-	59,73,73	2.16	16 (27%)	67,113,113	1.93	17 (25%)
17	BCR	K	102	-	41,41,41	2.78	6 (14%)	56,56,56	7.21	24 (42%)
16	SF4	G	845	1,2	0,12,12	0.00	-	-	-	-
14	CLA	Y	819	-	59,73,73	2.18	16 (27%)	67,113,113	2.21	15 (22%)
14	CLA	G	827	-	59,73,73	2.17	15 (25%)	67,113,113	1.92	17 (25%)
14	CLA	A	813	-	54,68,73	2.26	15 (27%)	61,107,113	2.30	18 (29%)
17	BCR	Y	849	-	41,41,41	2.74	6 (14%)	56,56,56	7.20	24 (42%)
14	CLA	G	843	18	44,58,73	2.54	16 (36%)	49,95,113	2.46	18 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	808	2	3/3/20/25	10/37/135/135	-
14	CLA	B	817	-	3/3/20/25	9/37/135/135	-
14	CLA	B	833	-	3/3/18/25	10/25/123/135	-
14	CLA	H	820	-	3/3/16/25	4/11/111/135	-
14	CLA	Y	810	-	3/3/16/25	7/11/111/135	-
14	CLA	Y	827	-	3/3/20/25	19/37/135/135	-
14	CLA	A	852	-	3/3/20/25	11/37/135/135	-
14	CLA	A	826	-	3/3/19/25	11/31/129/135	-
14	CLA	Y	835	-	3/3/18/25	9/25/123/135	-
18	LHG	Y	852	-	-	27/53/53/53	-
14	CLA	Z	808	2	3/3/20/25	13/37/135/135	-
14	CLA	B	841	-	3/3/20/25	20/37/135/135	-
17	BCR	M	101	-	-	9/29/63/63	0/2/2/2
14	CLA	H	817	-	3/3/19/25	13/31/129/135	-
14	CLA	H	818	-	3/3/19/25	16/31/129/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	831	-	3/3/16/25	6/11/111/135	-
17	BCR	U	1005	-	-	13/29/63/63	0/2/2/2
14	CLA	A	832	-	3/3/20/25	15/37/135/135	-
17	BCR	G	846	-	-	7/29/63/63	0/2/2/2
14	CLA	G	824	-	3/3/19/25	16/31/129/135	-
14	CLA	d	202	-	3/3/16/25	3/11/111/135	-
14	CLA	B	802	-	3/3/20/25	19/37/135/135	-
14	CLA	Z	831	-	3/3/18/25	12/25/123/135	-
14	CLA	B	838	-	3/3/20/25	13/37/135/135	-
14	CLA	H	804	-	3/3/20/25	12/37/135/135	-
17	BCR	e	101	-	-	10/29/63/63	0/2/2/2
14	CLA	Y	855	-	3/3/20/25	12/37/135/135	-
14	CLA	G	839	-	3/3/20/25	17/37/135/135	-
14	CLA	H	813	-	3/3/20/25	17/37/135/135	-
17	BCR	Z	846	-	-	10/29/63/63	0/2/2/2
14	CLA	H	837	-	3/3/20/25	12/37/135/135	-
14	CLA	L	205	10	3/3/20/25	24/37/135/135	-
14	CLA	F	202	-	3/3/16/25	2/11/111/135	-
15	PQN	Y	844	-	-	6/23/43/43	0/2/2/2
14	CLA	Y	830	-	3/3/20/25	10/37/135/135	-
14	CLA	Y	825	-	3/3/20/25	15/37/135/135	-
17	BCR	Z	843	-	-	7/29/63/63	0/2/2/2
14	CLA	W	1701	-	3/3/16/25	3/11/111/135	-
14	CLA	G	813	-	3/3/19/25	10/31/129/135	-
14	CLA	Y	840	-	3/3/20/25	13/37/135/135	-
14	CLA	B	837	-	3/3/19/25	8/31/129/135	-
14	CLA	U	1003	-	3/3/20/25	13/37/135/135	-
17	BCR	H	845	-	-	8/29/63/63	0/2/2/2
14	CLA	B	834	-	3/3/16/25	3/11/111/135	-
18	LHG	G	852	14	-	15/36/36/53	-
14	CLA	A	836	-	3/3/17/25	7/19/117/135	-
17	BCR	J	103	-	-	6/29/63/63	0/2/2/2
14	CLA	U	1002	10	3/3/20/25	25/37/135/135	-
14	CLA	A	812	-	3/3/17/25	11/24/122/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	A	847	-	-	4/29/63/63	0/2/2/2
17	BCR	G	854	-	-	8/29/63/63	0/2/2/2
14	CLA	H	805	-	3/3/20/25	19/37/135/135	-
17	BCR	Y	846	-	-	9/29/63/63	0/2/2/2
18	LHG	A	850	-	-	28/53/53/53	-
14	CLA	G	816	-	3/3/17/25	9/19/117/135	-
14	CLA	G	836	-	3/3/17/25	9/19/117/135	-
14	CLA	A	820	-	3/3/19/25	15/31/129/135	-
17	BCR	d	203	-	-	10/29/63/63	0/2/2/2
14	CLA	G	817	-	3/3/19/25	9/31/129/135	-
16	SF4	N	102	3,21	-	-	0/6/5/5
14	CLA	H	807	-	3/3/20/25	9/37/135/135	-
14	CLA	Y	811	14	3/3/20/25	21/37/135/135	-
14	CLA	Y	838	-	3/3/20/25	22/37/135/135	-
14	CLA	H	815	-	3/3/18/25	11/25/123/135	-
14	CLA	B	825	-	3/3/20/25	14/37/135/135	-
14	CLA	Y	812	-	3/3/18/25	12/25/123/135	-
18	LHG	j	101	-	-	16/32/32/53	-
14	CLA	J	102	-	3/3/18/25	14/25/123/135	-
17	BCR	B	844	-	-	8/29/63/63	0/2/2/2
14	CLA	S	1102	8	3/3/16/25	6/11/111/135	-
17	BCR	H	841	-	-	13/29/63/63	0/2/2/2
17	BCR	A	845	-	-	11/29/63/63	0/2/2/2
14	CLA	A	807	-	3/3/17/25	9/21/119/135	-
14	CLA	B	809	-	3/3/20/25	20/37/135/135	-
18	LHG	A	851	14	-	17/36/36/53	-
14	CLA	H	802	-	3/3/20/25	19/37/135/135	-
14	CLA	Y	820	-	3/3/19/25	14/31/129/135	-
17	BCR	G	849	-	-	8/29/63/63	0/2/2/2
17	BCR	H	842	-	-	8/29/63/63	0/2/2/2
17	BCR	Y	851	-	-	10/29/63/63	0/2/2/2
14	CLA	T	101	-	3/3/14/25	5/5/101/135	-
14	CLA	U	1006	2	3/3/20/25	16/37/135/135	-
14	CLA	Y	834	-	3/3/20/25	12/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	Z	832	-	3/3/16/25	7/11/111/135	-
14	CLA	Z	833	-	3/3/16/25	6/11/111/135	-
17	BCR	A	849	-	-	10/29/63/63	0/2/2/2
14	CLA	A	825	-	3/3/20/25	15/37/135/135	-
17	BCR	Y	856	-	-	11/29/63/63	0/2/2/2
14	CLA	H	821	-	3/3/18/25	9/25/123/135	-
14	CLA	L	207	-	3/3/20/25	19/37/135/135	-
14	CLA	B	819	-	3/3/19/25	19/31/129/135	-
14	CLA	G	809	-	3/3/20/25	15/37/135/135	-
17	BCR	B	848	-	-	3/29/63/63	0/2/2/2
16	SF4	a	101	3	-	-	0/6/5/5
14	CLA	A	841	-	3/3/20/25	13/37/135/135	-
14	CLA	G	834	-	3/3/18/25	8/25/123/135	-
14	CLA	A	816	-	3/3/17/25	10/19/117/135	-
14	CLA	Z	837	-	3/3/16/25	2/11/111/135	-
14	CLA	A	815	-	3/3/17/25	9/19/117/135	-
14	CLA	H	823	2	3/3/18/25	10/25/123/135	-
14	CLA	B	801	-	3/3/20/25	21/37/135/135	-
17	BCR	h	202	-	-	8/29/63/63	0/2/2/2
14	CLA	H	824	-	3/3/20/25	18/37/135/135	-
14	CLA	Y	833	-	3/3/20/25	13/37/135/135	-
14	CLA	H	835	-	3/3/20/25	16/37/135/135	-
14	CLA	G	806	-	3/3/20/25	20/37/135/135	-
14	CLA	Z	814	-	3/3/18/25	12/25/123/135	-
14	CLA	A	804	14	3/3/18/25	14/30/128/135	-
14	CLA	A	829	-	3/3/20/25	17/37/135/135	-
14	CLA	G	812	-	3/3/17/25	12/24/122/135	-
14	CLA	Y	808	1	3/3/20/25	21/37/135/135	-
14	CLA	H	832	-	3/3/16/25	6/11/111/135	-
14	CLA	G	822	-	3/3/20/25	12/37/135/135	-
14	CLA	Z	807	-	3/3/20/25	12/37/135/135	-
14	CLA	U	1004	-	3/3/20/25	19/37/135/135	-
17	BCR	J	104	-	-	13/29/63/63	0/2/2/2
14	CLA	H	827	-	3/3/20/25	16/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	Y	848	-	-	10/29/63/63	0/2/2/2
19	LMG	Z	847	-	-	16/44/64/70	0/1/1/1
14	CLA	G	804	-	3/3/18/25	12/30/128/135	-
14	CLA	Y	802	-	3/3/20/25	9/37/135/135	-
14	CLA	G	811	-	3/3/20/25	18/37/135/135	-
14	CLA	B	811	-	3/3/18/25	15/25/123/135	-
14	CLA	H	838	-	3/3/20/25	13/37/135/135	-
17	BCR	L	203	-	-	13/29/63/63	0/2/2/2
13	CL0	G	801	-	3/3/20/25	13/37/135/135	-
14	CLA	B	804	-	3/3/20/25	8/37/135/135	-
17	BCR	f	103	-	-	9/29/63/63	0/2/2/2
14	CLA	Z	812	-	3/3/20/25	10/37/135/135	-
14	CLA	j	102	-	3/3/16/25	5/11/111/135	-
14	CLA	L	206	-	3/3/20/25	14/37/135/135	-
18	LHG	Y	853	14	-	20/28/28/53	-
14	CLA	A	838	-	3/3/17/25	9/19/117/135	-
14	CLA	Z	830	-	3/3/20/25	16/37/135/135	-
18	LHG	H	847	-	-	18/41/41/53	-
14	CLA	B	832	-	3/3/20/25	20/37/135/135	-
14	CLA	H	809	2	3/3/20/25	17/37/135/135	-
14	CLA	S	1103	-	3/3/18/25	14/25/123/135	-
17	BCR	f	104	-	-	6/29/63/63	0/2/2/2
14	CLA	T	103	-	3/3/16/25	4/11/111/135	-
14	CLA	H	833	-	3/3/16/25	4/11/111/135	-
17	BCR	Y	850	-	-	7/29/63/63	0/2/2/2
17	BCR	R	101	-	-	12/29/63/63	0/2/2/2
14	CLA	B	810	2	3/3/20/25	15/37/135/135	-
14	CLA	Y	822	-	3/3/20/25	18/37/135/135	-
14	CLA	H	803	-	3/3/20/25	12/37/135/135	-
17	BCR	B	851	-	-	7/29/63/63	0/2/2/2
14	CLA	G	837	-	3/3/20/25	19/37/135/135	-
14	CLA	J	101	8	3/3/16/25	5/11/111/135	-
15	PQN	G	844	-	-	10/23/43/43	0/2/2/2
14	CLA	Y	832	-	3/3/20/25	22/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	827	-	3/3/20/25	13/37/135/135	-
14	CLA	H	830	-	3/3/18/25	12/25/123/135	-
14	CLA	Y	818	-	3/3/20/25	16/37/135/135	-
14	CLA	A	809	1	3/3/20/25	17/37/135/135	-
14	CLA	B	813	-	3/3/20/25	19/37/135/135	-
14	CLA	G	840	-	3/3/17/25	4/19/117/135	-
14	CLA	Z	806	-	3/3/20/25	19/37/135/135	-
14	CLA	Z	834	-	3/3/16/25	6/11/111/135	-
14	CLA	B	806	-	3/3/20/25	14/37/135/135	-
14	CLA	Z	809	-	3/3/18/25	10/25/123/135	-
14	CLA	G	808	1	3/3/20/25	19/37/135/135	-
14	CLA	G	832	-	3/3/20/25	14/37/135/135	-
14	CLA	B	818	-	3/3/19/25	10/31/129/135	-
14	CLA	Y	821	-	3/3/20/25	18/37/135/135	-
14	CLA	Z	828	-	3/3/16/25	5/11/111/135	-
14	CLA	B	812	-	3/3/17/25	9/19/117/135	-
14	CLA	H	806	-	3/3/20/25	10/37/135/135	-
14	CLA	G	810	-	3/3/16/25	6/11/111/135	-
14	CLA	A	830	-	3/3/20/25	12/37/135/135	-
14	CLA	G	841	-	3/3/20/25	17/37/135/135	-
14	CLA	A	805	-	3/3/20/25	22/37/135/135	-
14	CLA	Z	817	-	3/3/19/25	15/31/129/135	-
14	CLA	G	820	-	3/3/19/25	15/31/129/135	-
14	CLA	Y	814	-	3/3/18/25	11/25/123/135	-
14	CLA	h	201	-	3/3/20/25	12/37/135/135	-
14	CLA	Z	819	-	3/3/16/25	5/11/111/135	-
14	CLA	B	827	-	3/3/20/25	14/37/135/135	-
17	BCR	B	847	-	-	11/29/63/63	0/2/2/2
17	BCR	G	847	-	-	9/29/63/63	0/2/2/2
14	CLA	Y	815	-	3/3/17/25	10/19/117/135	-
14	CLA	B	803	-	3/3/20/25	16/37/135/135	-
14	CLA	B	824	2	3/3/18/25	10/25/123/135	-
14	CLA	B	821	-	3/3/16/25	6/11/111/135	-
17	BCR	Z	841	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	842	-	3/3/20/25	17/37/135/135	-
14	CLA	Z	804	-	3/3/20/25	14/37/135/135	-
14	CLA	H	812	-	3/3/20/25	18/37/135/135	-
14	CLA	A	821	-	3/3/20/25	16/37/135/135	-
14	CLA	G	830	-	3/3/20/25	15/37/135/135	-
15	PQN	H	839	-	-	8/23/43/43	0/2/2/2
13	CL0	A	801	-	3/3/20/25	14/37/135/135	-
14	CLA	A	802	-	3/3/20/25	11/37/135/135	-
18	LHG	B	850	-	-	24/43/43/53	-
17	BCR	L	208	-	-	12/29/63/63	0/2/2/2
14	CLA	A	831	-	3/3/17/25	5/19/117/135	-
14	CLA	Y	823	-	3/3/17/25	6/19/117/135	-
17	BCR	f	105	-	-	6/29/63/63	0/2/2/2
14	CLA	A	822	-	3/3/20/25	15/37/135/135	-
17	BCR	Y	847	-	-	6/29/63/63	0/2/2/2
14	CLA	A	839	-	3/3/17/25	4/19/117/135	-
19	LMG	B	849	-	-	14/47/67/70	0/1/1/1
17	BCR	Z	845	-	-	8/29/63/63	0/2/2/2
14	CLA	Y	839	-	3/3/17/25	11/19/117/135	-
17	BCR	B	845	-	-	9/29/63/63	0/2/2/2
14	CLA	G	825	-	3/3/20/25	19/37/135/135	-
14	CLA	Y	816	-	3/3/17/25	5/19/117/135	-
14	CLA	Q	201	-	3/3/20/25	18/37/135/135	-
17	BCR	G	850	-	-	9/29/63/63	0/2/2/2
14	CLA	K	101	-	3/3/14/25	5/5/101/135	-
14	CLA	L	201	-	3/3/20/25	13/37/135/135	-
14	CLA	A	833	-	3/3/20/25	12/37/135/135	-
14	CLA	H	829	-	3/3/16/25	4/11/111/135	-
14	CLA	A	824	-	3/3/19/25	17/31/129/135	-
14	CLA	L	202	-	3/3/20/25	16/37/135/135	-
14	CLA	Z	803	-	3/3/17/25	9/24/122/135	-
14	CLA	G	835	1	3/3/16/25	5/11/111/135	-
14	CLA	Y	826	-	3/3/19/25	7/31/129/135	-
14	CLA	Y	804	14	3/3/18/25	15/30/128/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	d	201	-	3/3/17/25	4/19/117/135	-
17	BCR	Q	204	-	-	7/29/63/63	0/2/2/2
17	BCR	V	1202	-	-	8/29/63/63	0/2/2/2
14	CLA	Z	825	-	3/3/20/25	15/37/135/135	-
14	CLA	Y	837	-	3/3/17/25	7/19/117/135	-
14	CLA	Z	818	-	3/3/16/25	3/11/111/135	-
14	CLA	A	814	-	3/3/17/25	9/19/117/135	-
17	BCR	U	1008	-	-	5/29/63/63	0/2/2/2
14	CLA	G	803	-	3/3/20/25	12/37/135/135	-
14	CLA	Y	813	-	3/3/19/25	10/31/129/135	-
14	CLA	S	1101	-	3/3/20/25	23/37/135/135	-
17	BCR	F	203	-	-	6/29/63/63	0/2/2/2
14	CLA	B	820	-	3/3/16/25	2/11/111/135	-
17	BCR	U	1007	-	-	16/29/63/63	0/2/2/2
14	CLA	G	833	-	3/3/20/25	15/37/135/135	-
14	CLA	Z	838	-	3/3/20/25	12/37/135/135	-
14	CLA	Z	811	-	3/3/20/25	19/37/135/135	-
14	CLA	H	822	-	3/3/19/25	13/31/129/135	-
17	BCR	G	848	-	-	8/29/63/63	0/2/2/2
14	CLA	G	829	-	3/3/20/25	19/37/135/135	-
16	SF4	C	101	3,21	-	-	0/6/5/5
17	BCR	H	843	-	-	7/18/35/63	0/1/1/2
14	CLA	Y	806	-	3/3/20/25	14/37/135/135	-
14	CLA	h	207	-	3/3/20/25	15/37/135/135	-
14	CLA	Y	829	-	3/3/20/25	17/37/135/135	-
14	CLA	G	853	-	3/3/16/25	3/11/111/135	-
16	SF4	C	102	3	-	-	0/6/5/5
14	CLA	Z	823	-	3/3/20/25	17/37/135/135	-
14	CLA	h	205	10	3/3/20/25	23/37/135/135	-
17	BCR	A	846	-	-	12/29/63/63	0/2/2/2
14	CLA	A	803	-	3/3/20/25	19/37/135/135	-
14	CLA	Y	809	-	3/3/20/25	18/37/135/135	-
14	CLA	B	830	-	3/3/16/25	6/11/111/135	-
14	CLA	Z	820	-	3/3/18/25	8/25/123/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	838	-	3/3/17/25	3/19/117/135	-
14	CLA	Y	841	-	3/3/20/25	14/37/135/135	-
17	BCR	B	843	-	-	3/24/41/63	0/1/1/2
14	CLA	Z	822	2	3/3/18/25	10/25/123/135	-
15	PQN	B	842	-	-	12/23/43/43	0/2/2/2
14	CLA	Y	842	-	3/3/20/25	15/37/135/135	-
14	CLA	A	819	-	3/3/20/25	15/37/135/135	-
14	CLA	V	1201	-	3/3/17/25	9/24/122/135	-
14	CLA	A	840	-	3/3/20/25	14/37/135/135	-
14	CLA	G	821	-	3/3/20/25	16/37/135/135	-
14	CLA	H	834	-	3/3/19/25	11/31/129/135	-
16	SF4	A	844	1,2	-	-	0/6/5/5
14	CLA	B	814	-	3/3/20/25	22/37/135/135	-
14	CLA	Y	805	-	3/3/20/25	13/37/135/135	-
14	CLA	Q	203	-	3/3/16/25	4/11/111/135	-
14	CLA	Y	854	-	3/3/20/25	15/37/135/135	-
14	CLA	Z	821	-	3/3/19/25	14/31/129/135	-
16	SF4	N	101	3	-	-	0/6/5/5
17	BCR	A	848	-	-	7/29/63/63	0/2/2/2
14	CLA	G	828	-	3/3/20/25	11/37/135/135	-
14	CLA	H	836	-	3/3/16/25	1/11/111/135	-
17	BCR	Z	842	-	-	6/29/63/63	0/2/2/2
14	CLA	B	808	-	3/3/20/25	13/37/135/135	-
14	CLA	B	816	-	3/3/18/25	9/25/123/135	-
14	CLA	Z	839	-	3/3/20/25	19/37/135/135	-
14	CLA	G	826	-	3/3/19/25	16/31/129/135	-
14	CLA	A	823	-	3/3/17/25	8/19/117/135	-
17	BCR	h	203	-	-	10/29/63/63	0/2/2/2
14	CLA	Z	802	-	3/3/20/25	22/37/135/135	-
14	CLA	B	822	-	3/3/18/25	9/25/123/135	-
14	CLA	Y	843	18	3/3/17/25	11/19/117/135	-
14	CLA	B	839	-	3/3/16/25	1/11/111/135	-
14	CLA	A	808	1	3/3/20/25	23/37/135/135	-
14	CLA	H	811	-	3/3/16/25	3/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	823	-	3/3/19/25	15/31/129/135	-
14	CLA	A	811	14	3/3/20/25	17/37/135/135	-
14	CLA	Z	810	-	3/3/16/25	3/11/111/135	-
14	CLA	Y	803	-	3/3/20/25	18/37/135/135	-
14	CLA	H	826	-	3/3/20/25	12/37/135/135	-
14	CLA	B	807	-	3/3/20/25	18/37/135/135	-
19	LMG	H	846	-	-	11/44/64/70	0/1/1/1
14	CLA	Z	816	-	3/3/19/25	13/31/129/135	-
14	CLA	B	836	-	3/3/16/25	2/11/111/135	-
14	CLA	G	805	-	3/3/20/25	20/37/135/135	-
17	BCR	i	101	-	-	9/29/63/63	0/2/2/2
14	CLA	H	828	-	3/3/20/25	13/37/135/135	-
14	CLA	B	831	-	3/3/16/25	8/11/111/135	-
14	CLA	f	102	-	3/3/18/25	15/25/123/135	-
14	CLA	Z	824	-	3/3/20/25	15/37/135/135	-
14	CLA	Z	835	-	3/3/19/25	11/31/129/135	-
14	CLA	B	826	-	3/3/20/25	16/37/135/135	-
15	PQN	A	843	-	-	5/23/43/43	0/2/2/2
14	CLA	A	835	1	3/3/16/25	4/11/111/135	-
17	BCR	L	209	-	-	9/29/63/63	0/2/2/2
14	CLA	B	815	-	3/3/16/25	4/11/111/135	-
14	CLA	Z	813	-	3/3/16/25	3/11/111/135	-
17	BCR	F	201	-	-	13/29/63/63	0/2/2/2
14	CLA	X	1701	-	3/3/16/25	3/11/111/135	-
14	CLA	A	806	-	3/3/20/25	21/37/135/135	-
14	CLA	B	829	-	3/3/20/25	11/37/135/135	-
14	CLA	Y	828	-	3/3/20/25	16/37/135/135	-
17	BCR	H	844	-	-	8/29/63/63	0/2/2/2
14	CLA	Z	826	-	3/3/20/25	14/37/135/135	-
14	CLA	B	805	-	3/3/17/25	10/24/122/135	-
14	CLA	G	815	-	3/3/17/25	6/19/117/135	-
14	CLA	g	102	-	3/3/16/25	5/11/111/135	-
14	CLA	G	831	-	3/3/17/25	8/19/117/135	-
14	CLA	H	810	-	3/3/18/25	13/25/123/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	H	840	-	-	8/29/63/63	0/2/2/2
14	CLA	G	823	-	3/3/17/25	6/19/117/135	-
14	CLA	Y	807	-	3/3/17/25	11/21/119/135	-
17	BCR	S	1104	-	-	11/29/63/63	0/2/2/2
14	CLA	K	103	-	3/3/16/25	5/11/111/135	-
14	CLA	Z	829	-	3/3/16/25	7/11/111/135	-
14	CLA	B	840	-	3/3/20/25	12/37/135/135	-
14	CLA	Z	801	-	3/3/20/25	20/37/135/135	-
14	CLA	H	814	-	3/3/16/25	4/11/111/135	-
14	CLA	Y	824	-	3/3/19/25	20/31/129/135	-
14	CLA	A	837	-	3/3/20/25	15/37/135/135	-
17	BCR	Q	202	-	-	11/29/63/63	0/2/2/2
14	CLA	H	819	-	3/3/16/25	7/11/111/135	-
14	CLA	Z	815	-	3/3/20/25	17/37/135/135	-
16	SF4	a	102	3	-	-	0/6/5/5
14	CLA	g	101	-	3/3/14/25	3/5/101/135	-
14	CLA	H	801	-	3/3/20/25	14/37/135/135	-
14	CLA	H	816	-	3/3/20/25	12/37/135/135	-
17	BCR	T	102	-	-	9/29/63/63	0/2/2/2
17	BCR	B	846	-	-	3/18/35/63	0/1/1/2
14	CLA	G	802	-	3/3/20/25	19/37/135/135	-
14	CLA	G	818	-	3/3/20/25	17/37/135/135	-
14	CLA	A	818	-	3/3/20/25	23/37/135/135	-
14	CLA	Z	827	-	3/3/20/25	13/37/135/135	-
14	CLA	A	842	18	3/3/17/25	10/19/117/135	-
17	BCR	I	101	-	-	8/29/63/63	0/2/2/2
14	CLA	f	101	8	3/3/16/25	5/11/111/135	-
14	CLA	Y	817	-	3/3/19/25	9/31/129/135	-
13	CL0	Y	801	-	3/3/20/25	14/37/135/135	-
14	CLA	A	817	-	3/3/19/25	15/31/129/135	-
14	CLA	Z	836	-	3/3/20/25	10/37/135/135	-
18	LHG	G	851	-	-	28/53/53/53	-
14	CLA	G	814	-	3/3/17/25	3/19/117/135	-
14	CLA	A	810	-	3/3/16/25	4/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	828	-	3/3/20/25	15/37/135/135	-
14	CLA	Y	836	1	3/3/16/25	4/11/111/135	-
14	CLA	h	206	-	3/3/20/25	13/37/135/135	-
14	CLA	H	825	-	3/3/20/25	11/37/135/135	-
14	CLA	A	834	-	3/3/18/25	9/25/123/135	-
14	CLA	Y	831	-	3/3/17/25	3/19/117/135	-
14	CLA	Z	805	-	3/3/20/25	19/37/135/135	-
15	PQN	Z	840	-	-	10/23/43/43	0/2/2/2
17	BCR	R	102	-	-	11/29/63/63	0/2/2/2
14	CLA	G	807	-	3/3/17/25	10/21/119/135	-
17	BCR	Z	844	-	-	8/18/35/63	0/1/1/2
14	CLA	B	828	-	3/3/20/25	15/37/135/135	-
14	CLA	G	819	-	3/3/20/25	15/37/135/135	-
14	CLA	B	835	-	3/3/16/25	2/11/111/135	-
17	BCR	H	848	-	-	8/29/63/63	0/2/2/2
16	SF4	Y	845	1,2	-	-	0/6/5/5
17	BCR	K	102	-	-	8/29/63/63	0/2/2/2
16	SF4	G	845	1,2	-	-	0/6/5/5
14	CLA	Y	819	-	3/3/20/25	20/37/135/135	-
14	CLA	G	827	-	3/3/20/25	18/37/135/135	-
14	CLA	A	813	-	3/3/19/25	10/31/129/135	-
17	BCR	Y	849	-	-	11/29/63/63	0/2/2/2
14	CLA	G	843	18	3/3/17/25	8/19/117/135	-

The worst 5 of 4609 bond length outliers are listed below:

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

The worst 5 of 6662 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	i	101	BCR	C16-C17-C18	30.09	170.25	127.31

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

5 of 855 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	B	811	CLA	NC
14	B	811	CLA	ND
14	B	811	CLA	NA
14	B	817	CLA	NC
14	B	817	CLA	ND

5 of 4327 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	B	811	CLA	C3A-C2A-CAA-CBA
14	B	811	CLA	CAD-CBD-CGD-O1D
14	B	811	CLA	CAD-CBD-CGD-O2D
14	B	817	CLA	CBA-CGA-O2A-C1
14	B	817	CLA	O1A-CGA-O2A-C1

There are no ring outliers.

349 monomers are involved in 1963 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	811	CLA	3	0
14	B	817	CLA	7	0
14	B	833	CLA	7	0
14	H	820	CLA	4	0
14	Y	810	CLA	5	0
14	Y	827	CLA	8	0
14	A	852	CLA	14	0
14	A	826	CLA	12	0
14	Y	835	CLA	1	0
18	Y	852	LHG	4	0
14	Z	808	CLA	11	0
14	B	841	CLA	5	0
17	M	101	BCR	6	0
14	H	817	CLA	8	0
14	H	818	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	831	CLA	7	0
17	U	1005	BCR	3	0
14	A	832	CLA	7	0
17	G	846	BCR	6	0
14	G	824	CLA	11	0
14	B	802	CLA	6	0
14	Z	831	CLA	7	0
14	B	838	CLA	6	0
14	H	804	CLA	4	0
14	Y	855	CLA	18	0
14	G	839	CLA	10	0
14	H	813	CLA	5	0
14	A	822	CLA	7	0
14	H	837	CLA	4	0
14	L	205	CLA	8	0
14	F	202	CLA	1	0
14	Y	830	CLA	15	0
14	Y	825	CLA	9	0
14	Y	809	CLA	4	0
14	A	840	CLA	16	0
14	G	813	CLA	11	0
14	Y	840	CLA	6	0
14	B	837	CLA	9	0
14	U	1003	CLA	6	0
17	H	845	BCR	9	0
14	B	834	CLA	7	0
18	G	852	LHG	5	0
14	A	836	CLA	8	0
17	J	103	BCR	11	0
14	U	1002	CLA	8	0
14	A	812	CLA	9	0
17	A	847	BCR	3	0
17	G	854	BCR	11	0
14	H	805	CLA	9	0
17	Y	846	BCR	8	0
18	A	850	LHG	4	0
14	G	816	CLA	1	0
14	G	836	CLA	4	0
14	A	820	CLA	3	0
14	G	817	CLA	6	0
14	H	807	CLA	14	0
14	Y	811	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	Y	838	CLA	6	0
14	H	815	CLA	1	0
14	B	825	CLA	13	0
14	Y	812	CLA	3	0
14	Z	821	CLA	4	0
14	J	102	CLA	4	0
17	B	844	BCR	3	0
14	S	1102	CLA	2	0
17	H	841	BCR	5	0
17	A	845	BCR	3	0
14	A	807	CLA	6	0
14	Z	815	CLA	7	0
14	H	810	CLA	6	0
18	A	851	LHG	1	0
14	H	802	CLA	16	0
14	Y	820	CLA	4	0
17	G	849	BCR	16	0
17	H	842	BCR	6	0
17	Y	851	BCR	14	0
14	T	101	CLA	4	0
14	U	1006	CLA	10	0
14	Y	834	CLA	15	0
14	Z	832	CLA	12	0
14	Z	833	CLA	9	0
17	A	849	BCR	11	0
17	Y	856	BCR	5	0
17	B	851	BCR	12	0
14	H	821	CLA	9	0
14	L	207	CLA	4	0
14	B	819	CLA	7	0
14	G	809	CLA	7	0
18	H	847	LHG	2	0
17	B	848	BCR	10	0
14	A	841	CLA	11	0
14	G	834	CLA	7	0
14	A	816	CLA	1	0
14	Z	837	CLA	8	0
14	A	815	CLA	2	0
14	H	823	CLA	8	0
14	B	801	CLA	11	0
14	H	824	CLA	14	0
14	Y	833	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	835	CLA	10	0
14	G	806	CLA	8	0
14	Z	814	CLA	1	0
14	A	804	CLA	7	0
14	A	829	CLA	10	0
14	G	812	CLA	1	0
14	Y	808	CLA	11	0
14	H	832	CLA	6	0
14	Z	801	CLA	13	0
14	Z	807	CLA	12	0
14	U	1004	CLA	7	0
17	J	104	BCR	10	0
14	H	827	CLA	10	0
17	Y	848	BCR	5	0
19	Z	847	LMG	3	0
14	G	804	CLA	10	0
14	Y	802	CLA	9	0
14	G	811	CLA	11	0
14	H	808	CLA	16	0
14	H	838	CLA	3	0
14	A	825	CLA	9	0
17	L	203	BCR	7	0
13	G	801	CL0	16	0
14	B	804	CLA	12	0
14	Z	812	CLA	4	0
14	L	206	CLA	12	0
18	Y	853	LHG	5	0
14	A	838	CLA	7	0
14	Z	830	CLA	2	0
16	N	102	SF4	2	0
14	B	832	CLA	11	0
14	B	810	CLA	9	0
14	S	1103	CLA	2	0
14	T	103	CLA	2	0
14	H	833	CLA	5	0
17	Y	850	BCR	10	0
17	R	101	BCR	3	0
14	H	809	CLA	11	0
14	Y	822	CLA	2	0
14	H	803	CLA	12	0
14	G	837	CLA	5	0
15	G	844	PQN	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	Y	832	CLA	9	0
14	A	827	CLA	9	0
14	H	830	CLA	9	0
14	Y	818	CLA	7	0
14	A	809	CLA	1	0
14	B	813	CLA	15	0
14	G	840	CLA	4	0
14	Z	806	CLA	14	0
14	Z	834	CLA	5	0
14	B	806	CLA	6	0
14	Z	809	CLA	6	0
14	G	808	CLA	13	0
14	G	832	CLA	2	0
14	H	801	CLA	24	0
14	Y	821	CLA	14	0
14	Z	828	CLA	6	0
14	B	812	CLA	1	0
14	H	806	CLA	8	0
14	G	810	CLA	4	0
17	A	848	BCR	8	0
14	G	841	CLA	6	0
14	A	805	CLA	11	0
14	Z	817	CLA	5	0
14	Z	803	CLA	2	0
14	Y	814	CLA	1	0
14	Z	819	CLA	4	0
14	B	827	CLA	8	0
17	B	847	BCR	17	0
17	G	847	BCR	11	0
14	Y	815	CLA	1	0
14	B	803	CLA	16	0
14	B	824	CLA	7	0
14	B	821	CLA	5	0
17	Z	841	BCR	3	0
14	Z	804	CLA	6	0
14	H	812	CLA	8	0
14	A	821	CLA	7	0
14	G	830	CLA	13	0
15	H	839	PQN	7	0
14	A	842	CLA	2	0
14	A	802	CLA	10	0
17	L	208	BCR	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	831	CLA	5	0
14	Y	823	CLA	2	0
17	Z	846	BCR	6	0
17	Y	847	BCR	9	0
14	A	839	CLA	9	0
19	B	849	LMG	6	0
17	Z	845	BCR	6	0
14	Y	839	CLA	6	0
17	B	845	BCR	7	0
14	G	825	CLA	15	0
14	Y	816	CLA	3	0
14	Q	201	CLA	9	0
17	G	850	BCR	13	0
14	K	101	CLA	3	0
14	L	201	CLA	7	0
14	A	833	CLA	5	0
14	H	829	CLA	6	0
14	A	824	CLA	4	0
14	L	202	CLA	7	0
14	G	820	CLA	5	0
14	G	835	CLA	4	0
14	Y	826	CLA	7	0
14	Y	804	CLA	4	0
17	Q	204	BCR	4	0
17	V	1202	BCR	6	0
14	Z	825	CLA	12	0
14	Y	837	CLA	6	0
14	Z	818	CLA	3	0
14	A	814	CLA	2	0
17	U	1008	BCR	6	0
14	G	803	CLA	15	0
14	Y	813	CLA	6	0
14	S	1101	CLA	7	0
14	B	820	CLA	2	0
17	U	1007	BCR	10	0
14	G	833	CLA	4	0
14	Z	838	CLA	6	0
14	Z	811	CLA	8	0
14	H	822	CLA	4	0
17	G	848	BCR	5	0
14	G	829	CLA	11	0
16	C	101	SF4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	843	BCR	5	0
14	Y	806	CLA	12	0
14	Y	829	CLA	11	0
14	G	853	CLA	4	0
16	C	102	SF4	3	0
14	A	828	CLA	16	0
17	A	846	BCR	9	0
14	A	803	CLA	6	0
17	Z	843	BCR	6	0
14	B	830	CLA	5	0
14	Z	820	CLA	4	0
14	G	838	CLA	4	0
14	Y	841	CLA	10	0
17	B	843	BCR	2	0
14	Z	822	CLA	8	0
15	B	842	PQN	11	0
14	Y	842	CLA	9	0
14	A	819	CLA	11	0
14	V	1201	CLA	6	0
14	W	1701	CLA	4	0
14	Z	802	CLA	11	0
14	H	834	CLA	7	0
16	A	844	SF4	1	0
14	B	814	CLA	3	0
14	Y	805	CLA	15	0
14	Y	854	CLA	12	0
14	G	802	CLA	19	0
16	N	101	SF4	1	0
14	A	830	CLA	8	0
14	G	828	CLA	15	0
14	H	836	CLA	11	0
17	Z	842	BCR	4	0
14	B	808	CLA	10	0
14	B	816	CLA	1	0
14	Z	839	CLA	4	0
14	G	826	CLA	6	0
14	A	823	CLA	1	0
14	G	821	CLA	14	0
14	B	822	CLA	7	0
14	Y	843	CLA	5	0
14	B	839	CLA	8	0
14	A	808	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	811	CLA	3	0
14	B	823	CLA	2	0
14	A	811	CLA	7	0
14	Z	810	CLA	3	0
14	Y	803	CLA	7	0
14	H	826	CLA	10	0
14	B	807	CLA	10	0
19	H	846	LMG	4	0
14	Z	816	CLA	10	0
14	B	836	CLA	7	0
14	G	805	CLA	14	0
14	H	828	CLA	11	0
14	B	831	CLA	3	0
14	Z	824	CLA	7	0
14	Z	835	CLA	9	0
14	B	826	CLA	8	0
15	A	843	PQN	6	0
14	A	835	CLA	9	0
17	L	209	BCR	8	0
14	B	815	CLA	7	0
14	Z	813	CLA	5	0
17	F	201	BCR	8	0
14	A	806	CLA	14	0
14	B	829	CLA	6	0
14	Y	828	CLA	20	0
17	H	844	BCR	10	0
14	Z	826	CLA	7	0
14	B	805	CLA	10	0
14	G	815	CLA	7	0
14	G	831	CLA	5	0
14	B	809	CLA	12	0
17	H	840	BCR	8	0
14	G	823	CLA	3	0
14	Y	807	CLA	3	0
17	S	1104	BCR	10	0
14	K	103	CLA	4	0
14	Z	829	CLA	2	0
14	B	840	CLA	7	0
14	G	822	CLA	2	0
14	H	814	CLA	5	0
14	Y	824	CLA	3	0
14	A	837	CLA	11	0

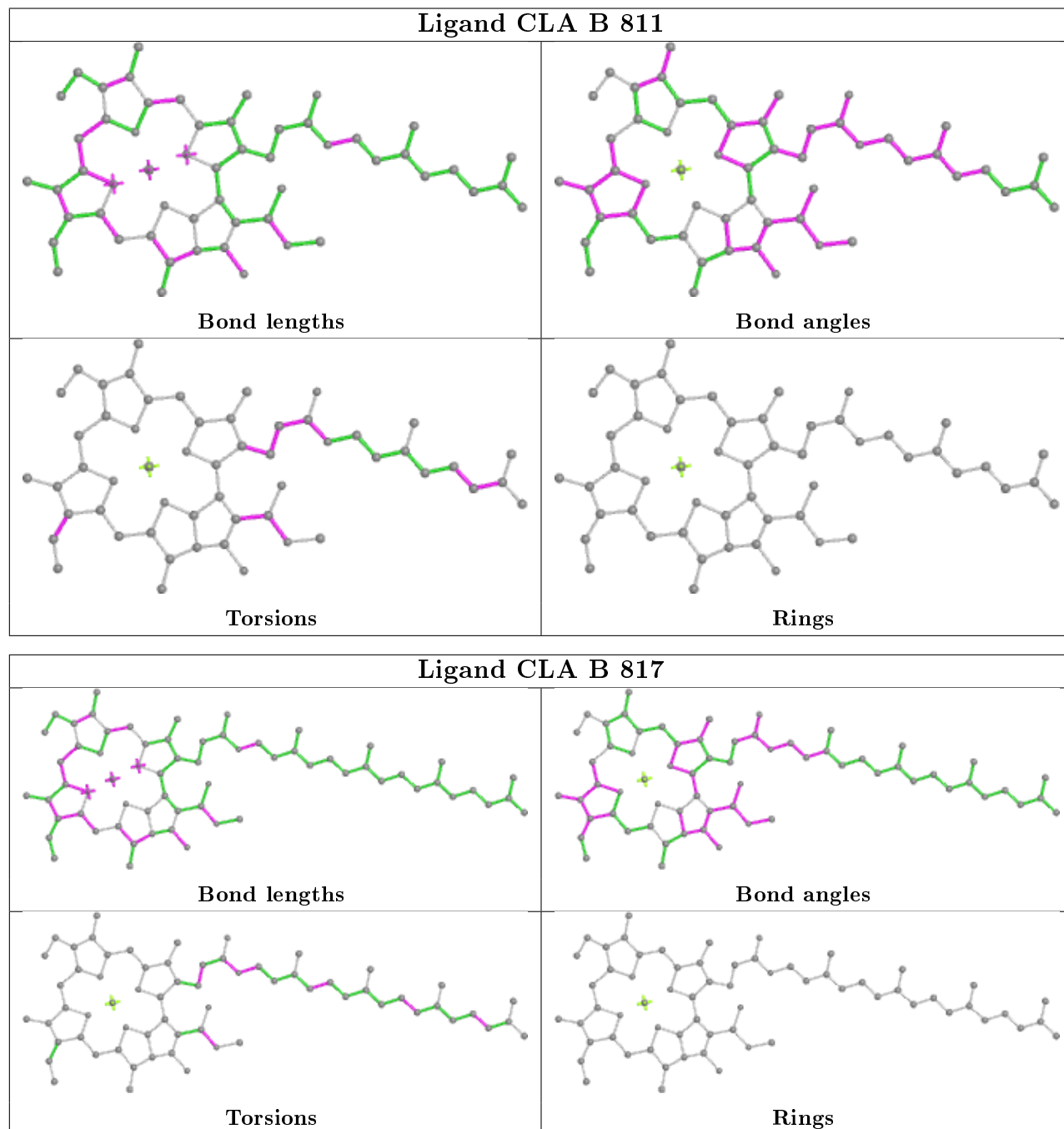
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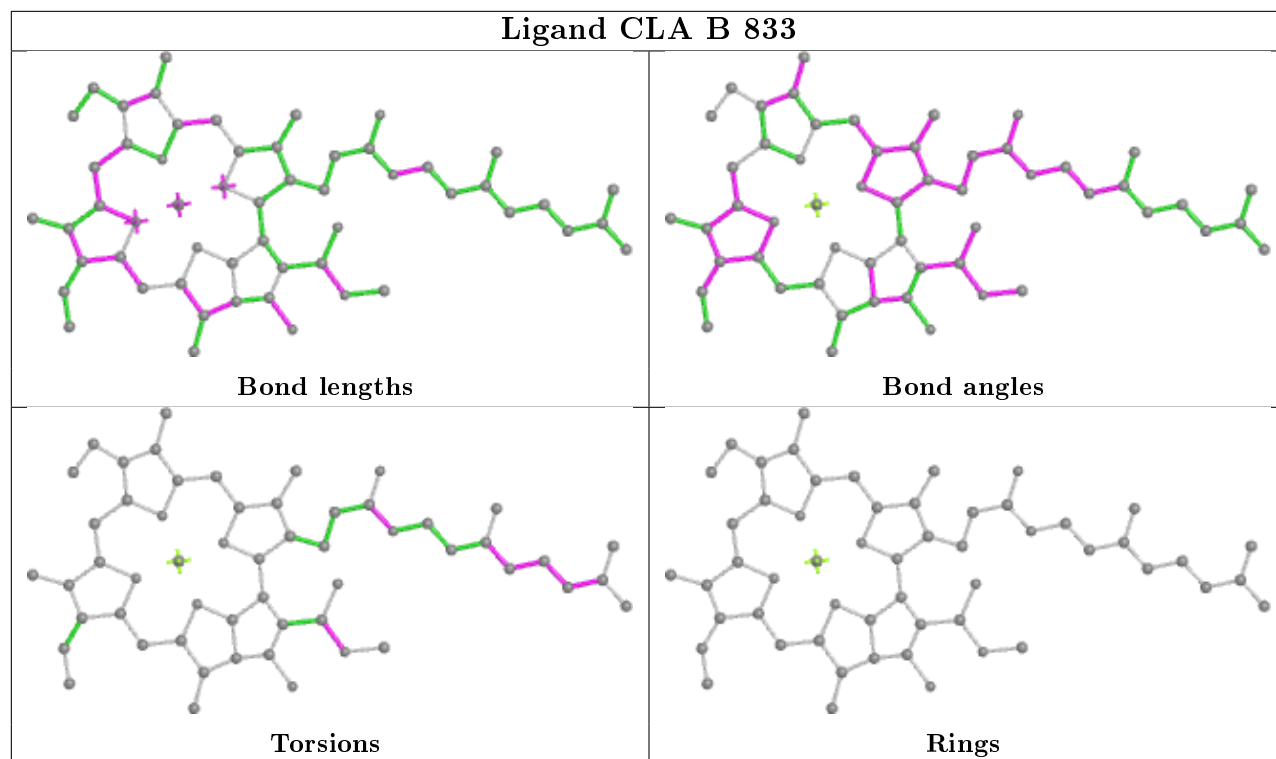
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Q	202	BCR	5	0
14	H	819	CLA	3	0
15	Y	844	PQN	2	0
14	Z	823	CLA	7	0
14	B	818	CLA	8	0
14	H	816	CLA	10	0
17	T	102	BCR	6	0
17	B	846	BCR	2	0
14	G	818	CLA	15	0
14	A	818	CLA	10	0
14	Z	827	CLA	10	0
13	A	801	CL0	13	0
17	I	101	BCR	11	0
14	Y	817	CLA	5	0
13	Y	801	CL0	11	0
14	A	817	CLA	5	0
14	Z	836	CLA	2	0
18	G	851	LHG	7	0
14	G	814	CLA	7	0
14	A	810	CLA	7	0
14	Y	836	CLA	3	0
14	H	825	CLA	4	0
14	A	834	CLA	10	0
14	Y	831	CLA	4	0
14	Z	805	CLA	7	0
15	Z	840	PQN	4	0
17	R	102	BCR	9	0
14	G	807	CLA	4	0
17	Z	844	BCR	8	0
14	B	828	CLA	8	0
14	G	819	CLA	15	0
14	B	835	CLA	8	0
17	H	848	BCR	5	0
14	G	842	CLA	6	0
17	K	102	BCR	3	0
14	Y	819	CLA	12	0
14	G	827	CLA	8	0
14	A	813	CLA	10	0
17	Y	849	BCR	7	0
14	G	843	CLA	4	0

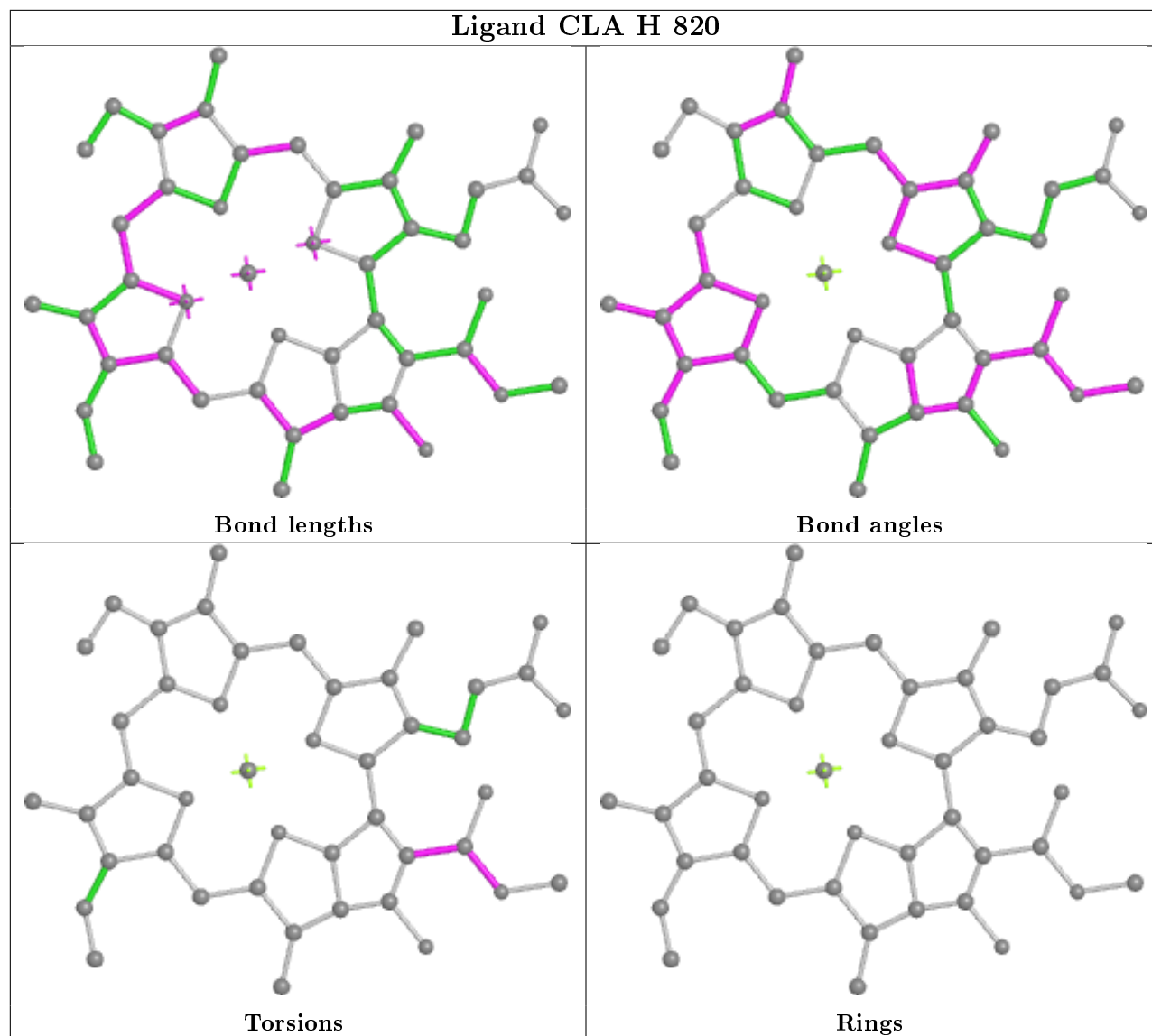
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

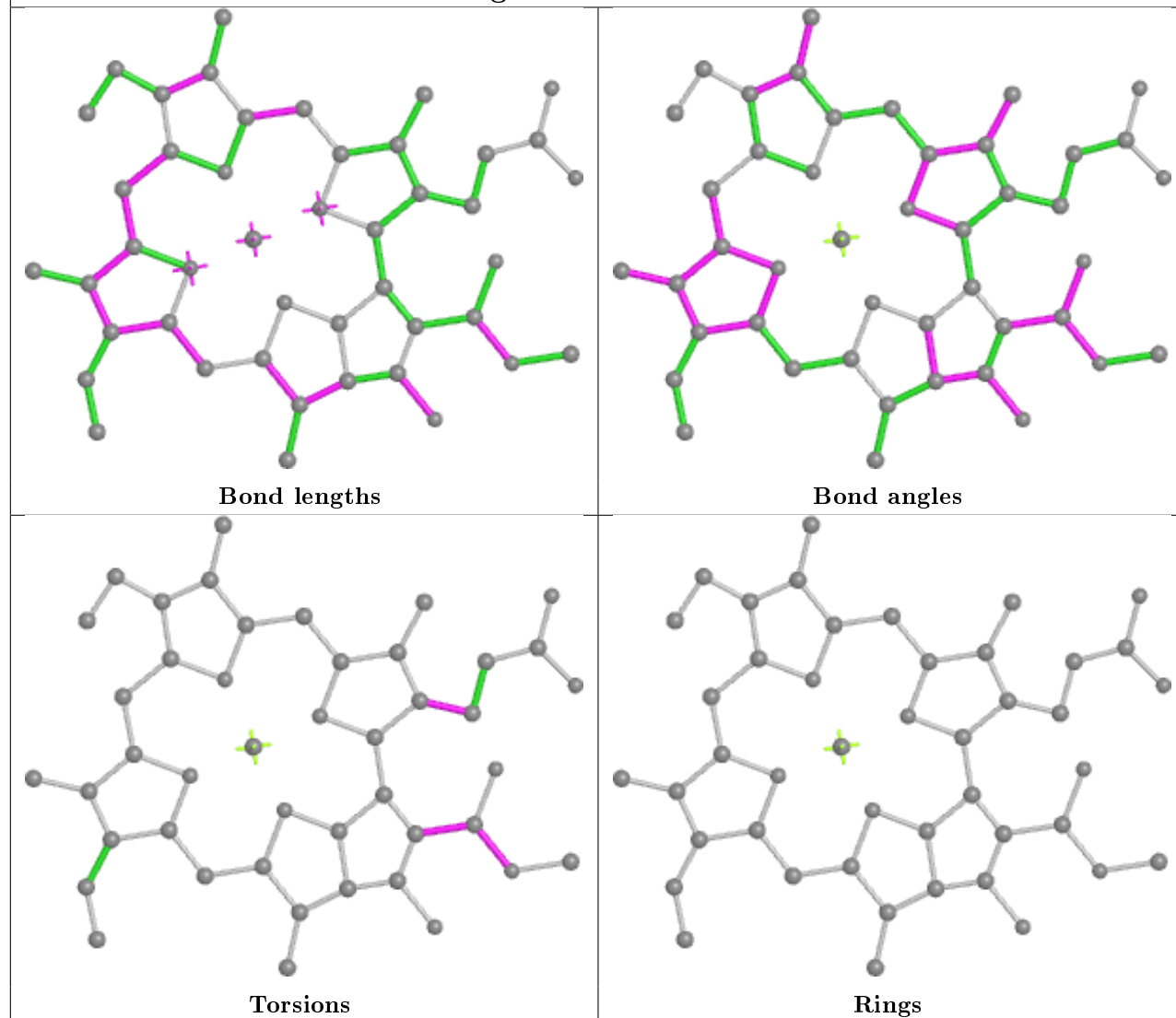




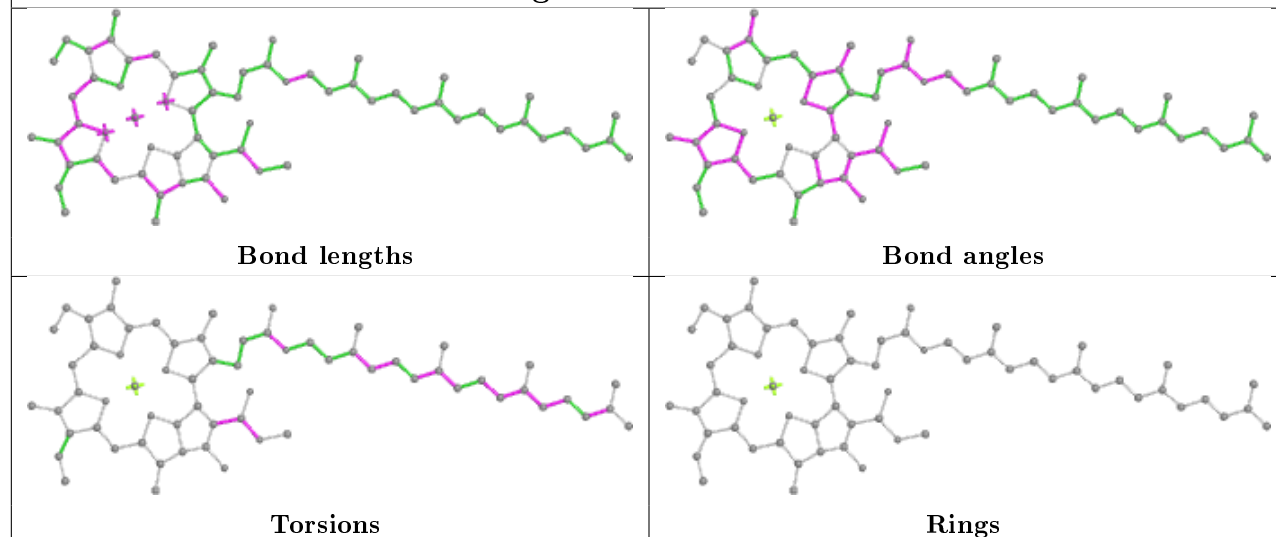
Ligand CLA H 820

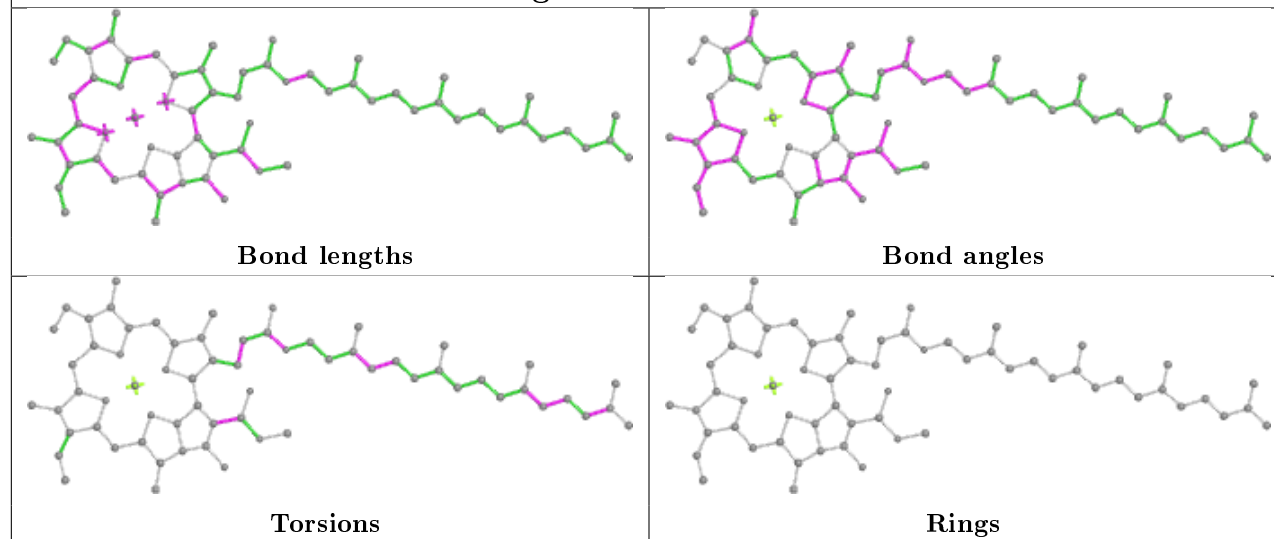
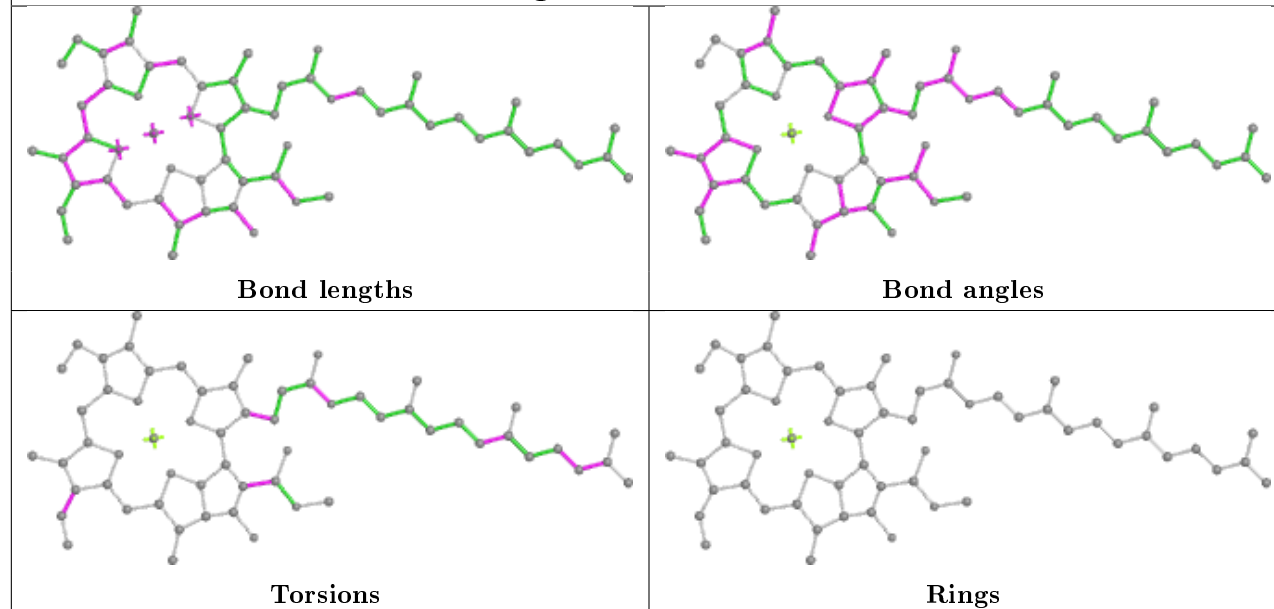


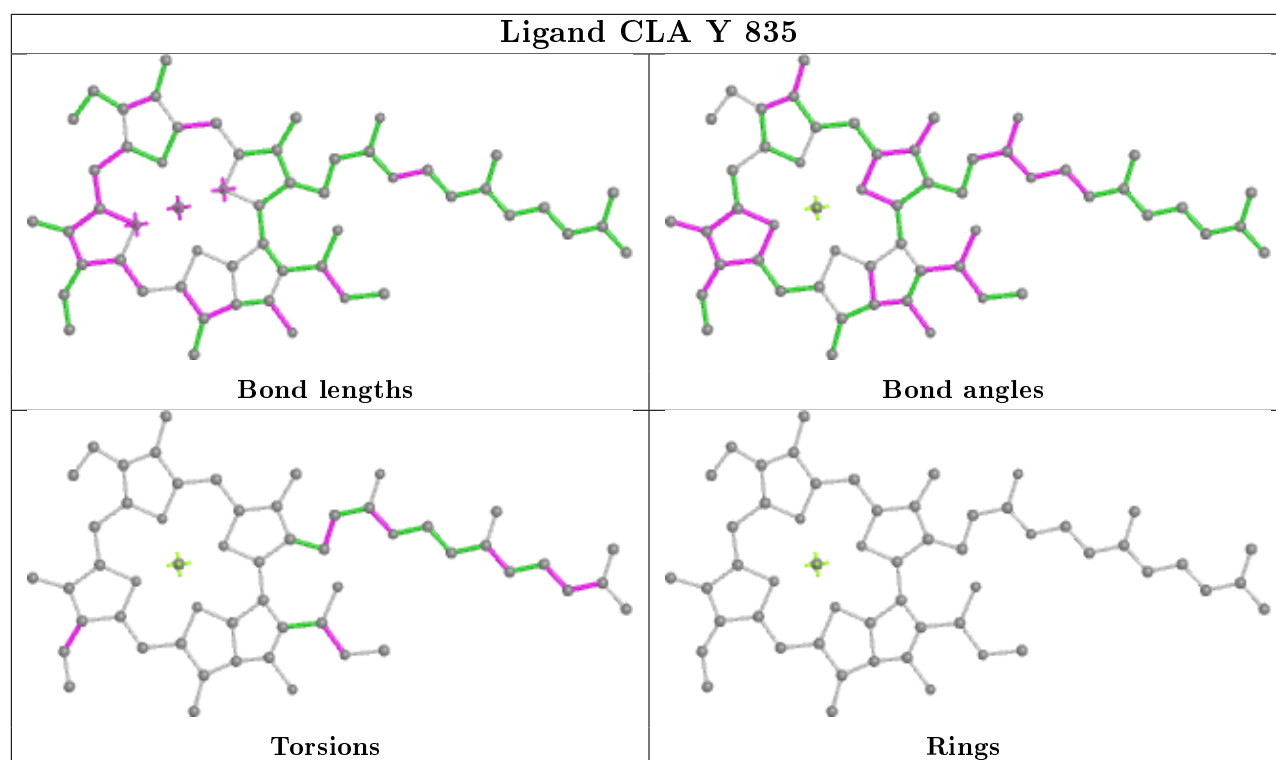
Ligand CLA Y 810

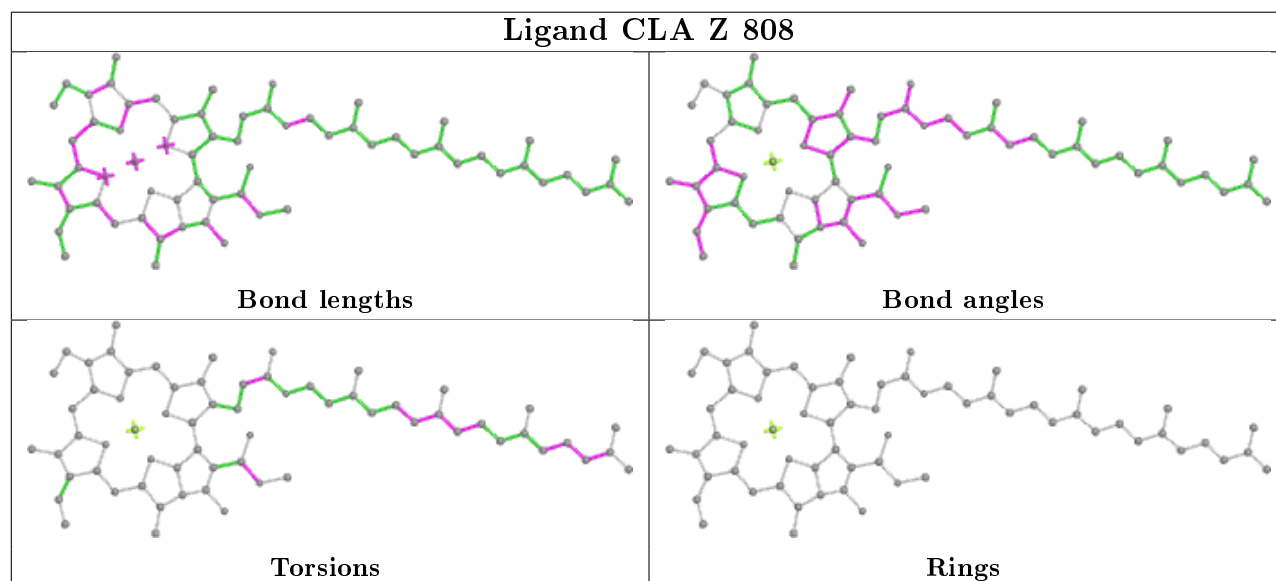
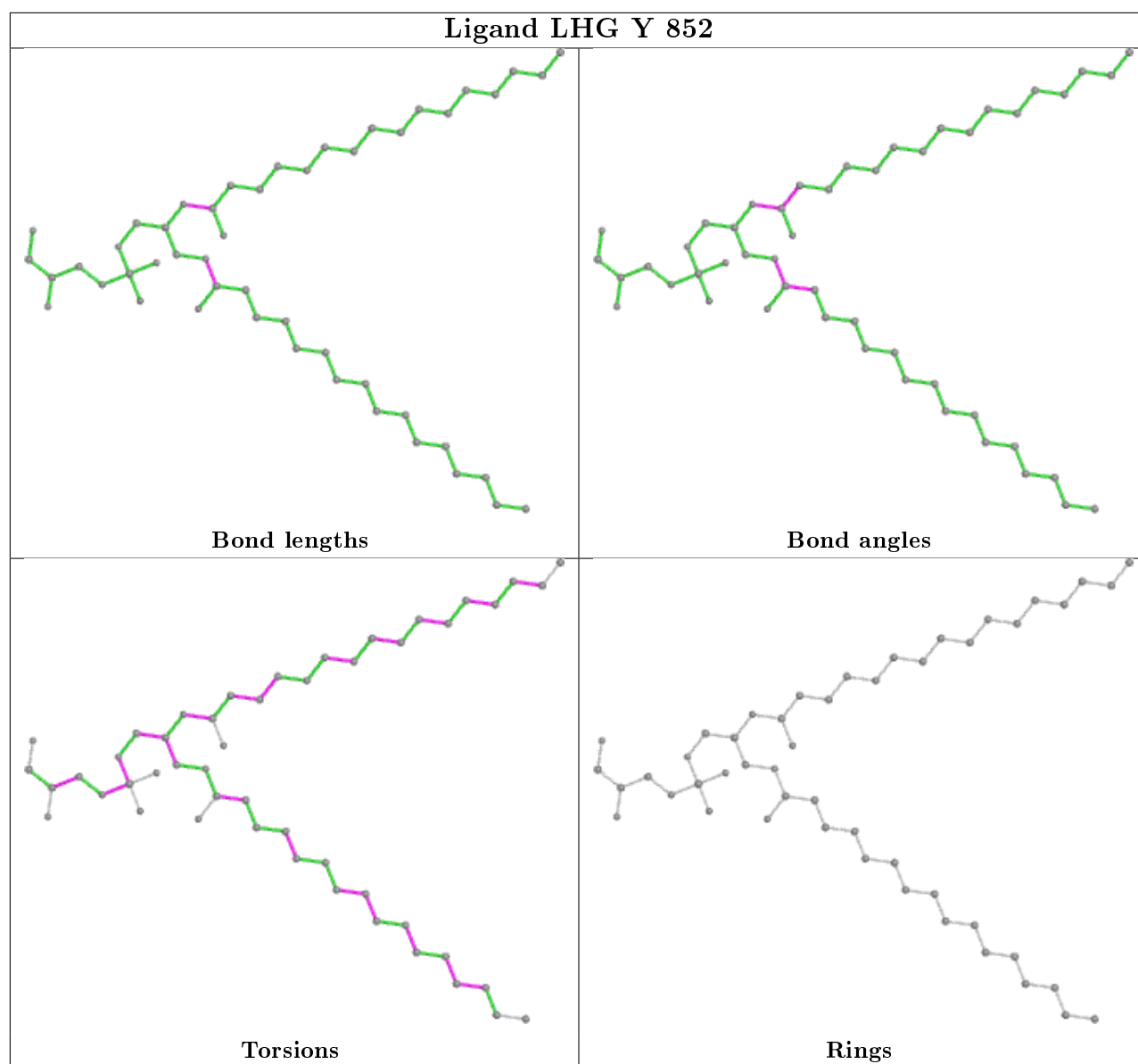


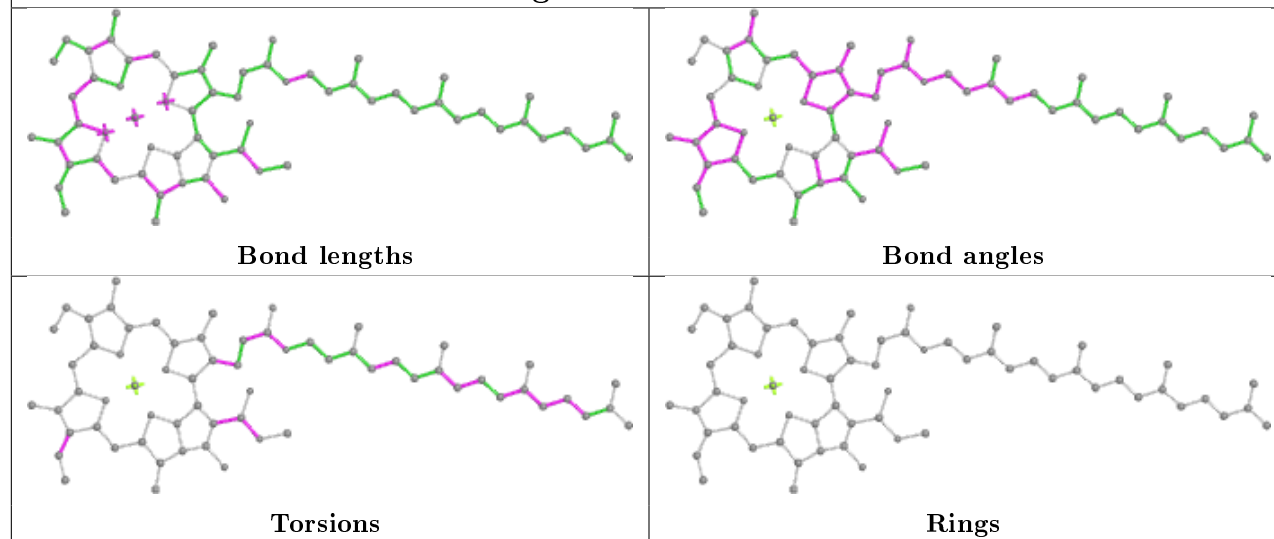
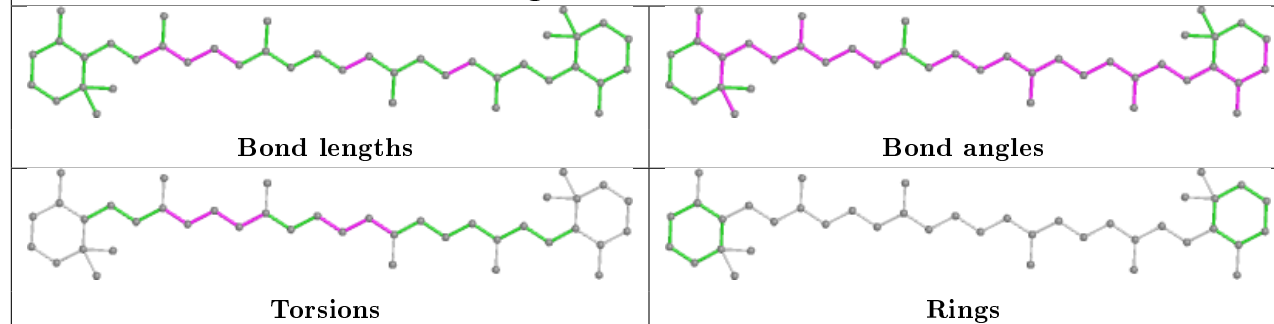
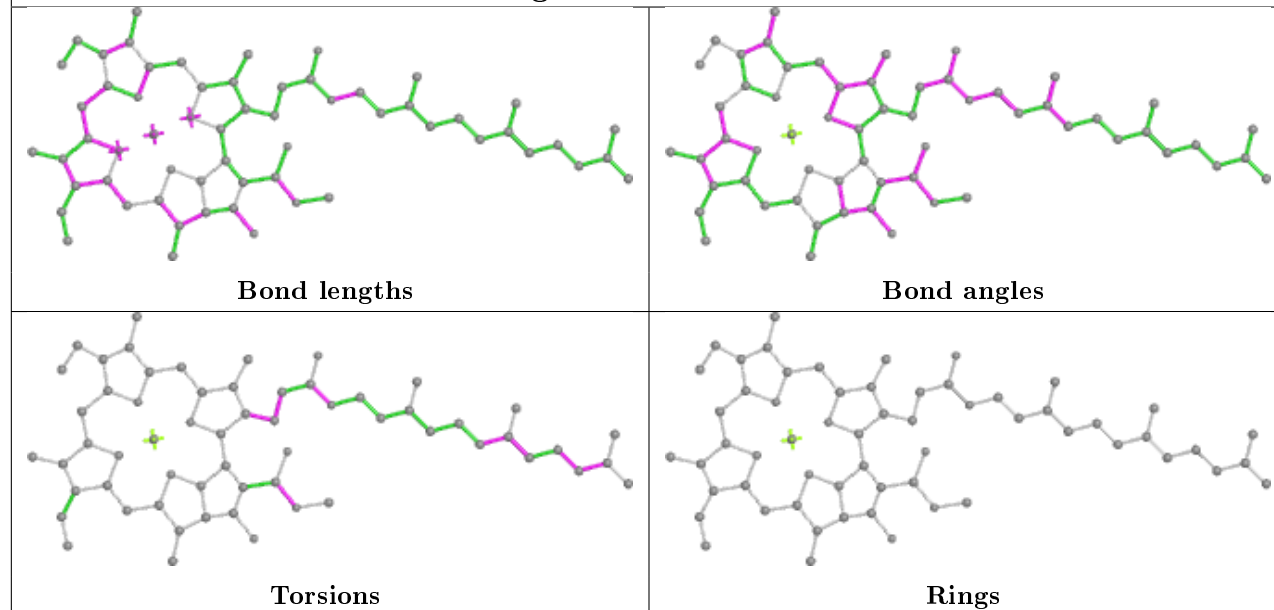
Ligand CLA Y 827



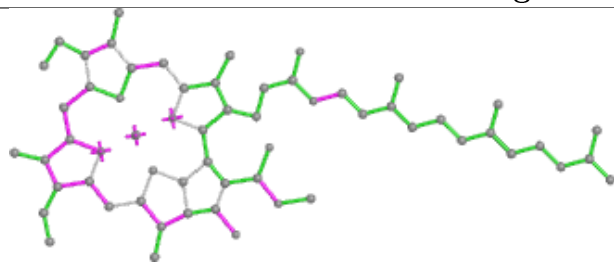
Ligand CLA A 852**Ligand CLA A 826**



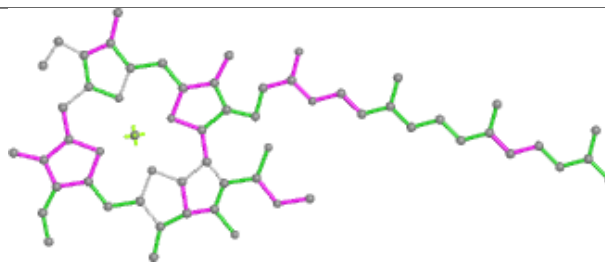


Ligand CLA B 841**Ligand BCR M 101****Ligand CLA H 817**

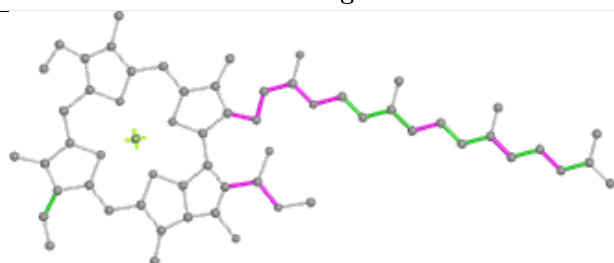
Ligand CLA H 818



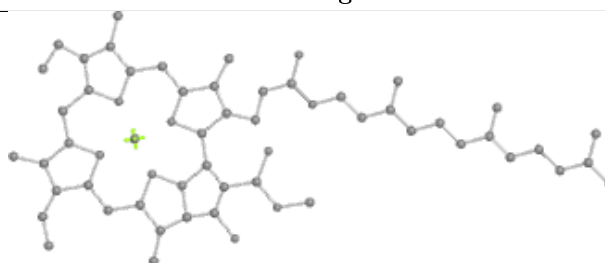
Bond lengths



Bond angles

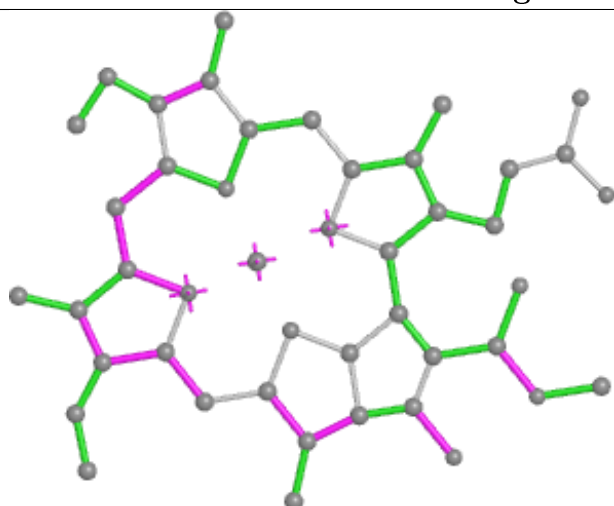


Torsions

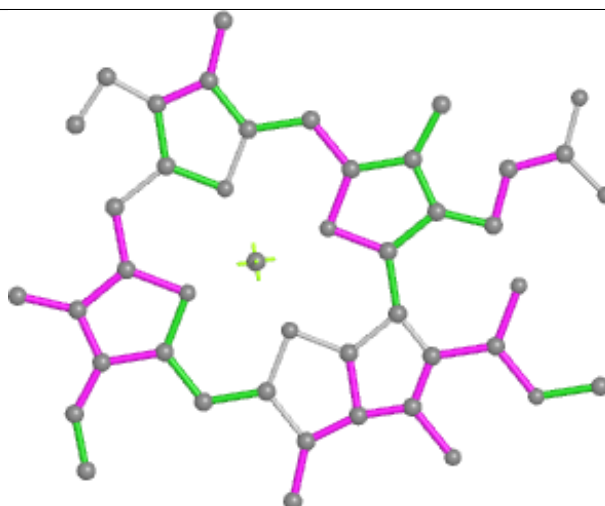


Rings

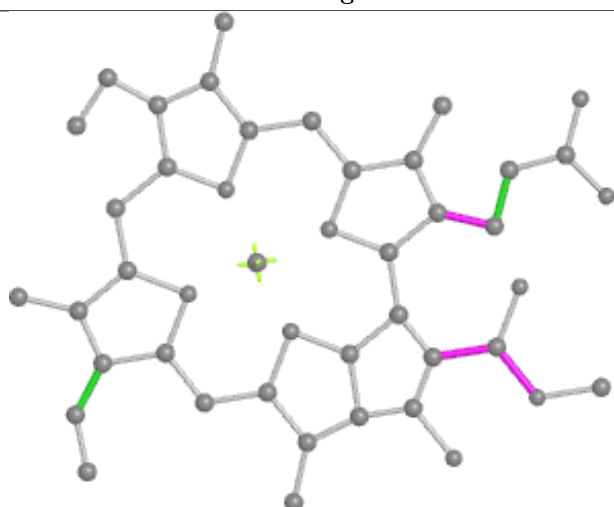
Ligand CLA H 831



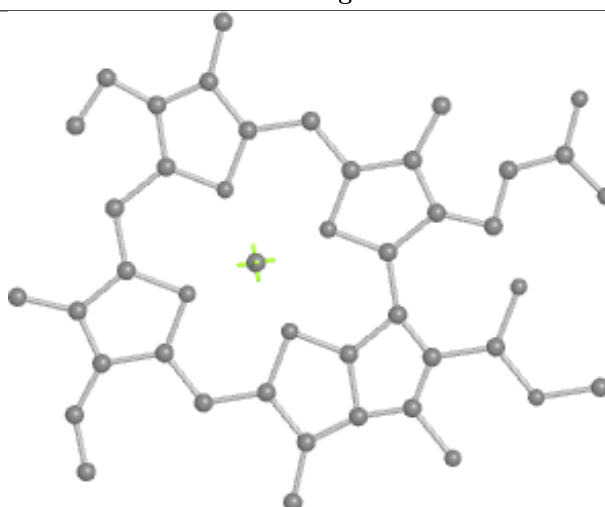
Bond lengths



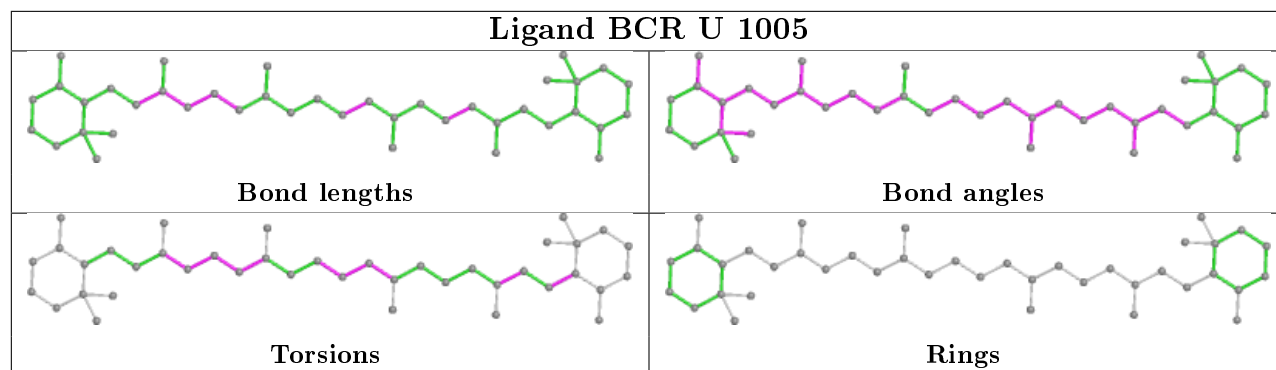
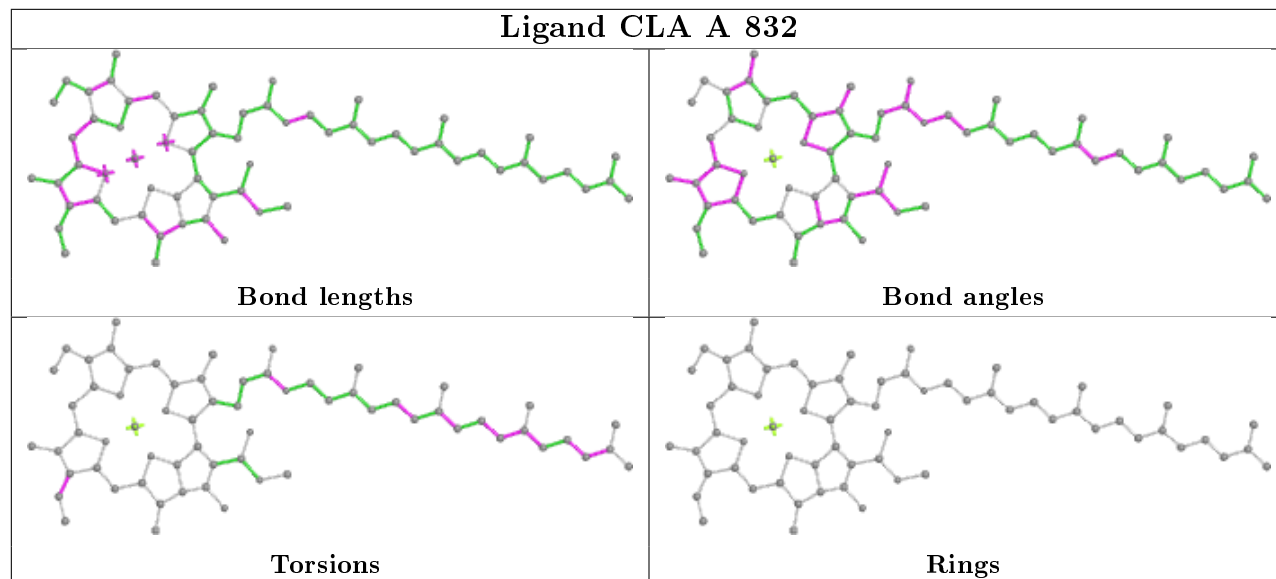
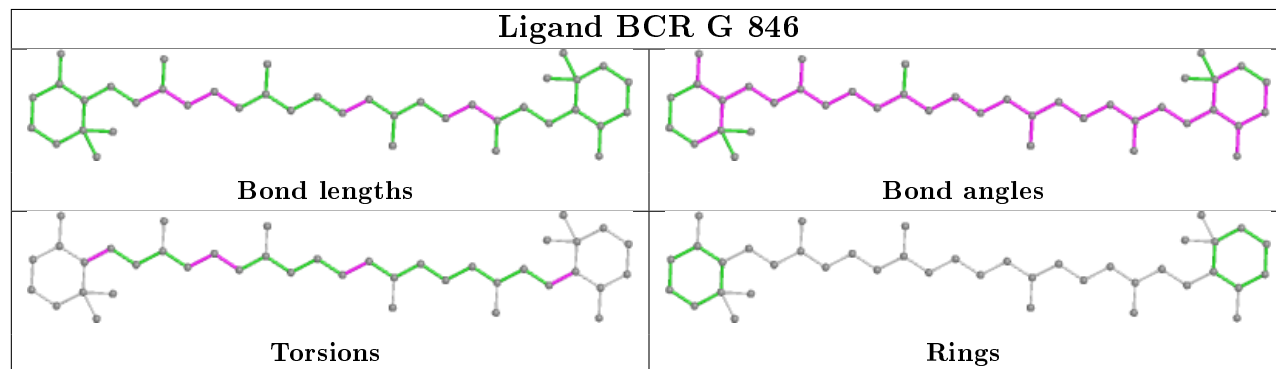
Bond angles



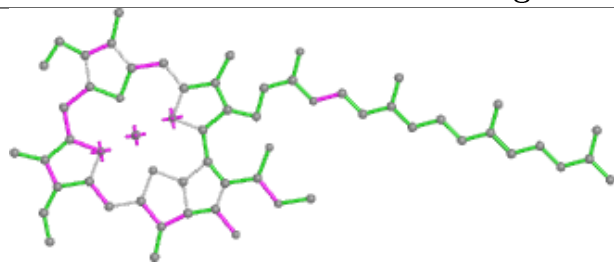
Torsions



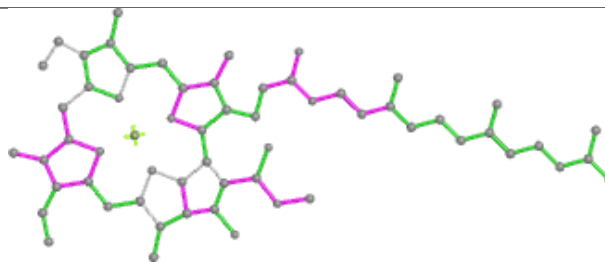
Rings

Ligand BCR U 1005**Ligand CLA A 832****Ligand BCR G 846**

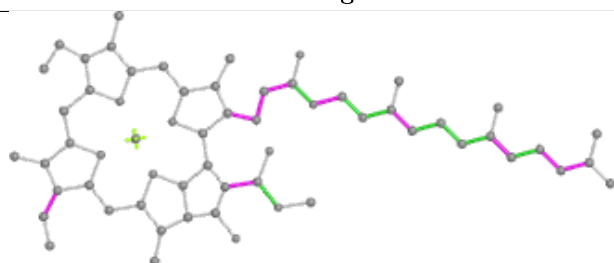
Ligand CLA G 824



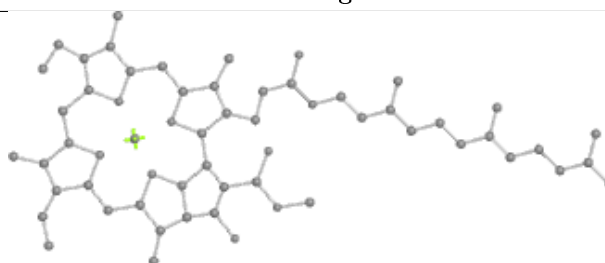
Bond lengths



Bond angles

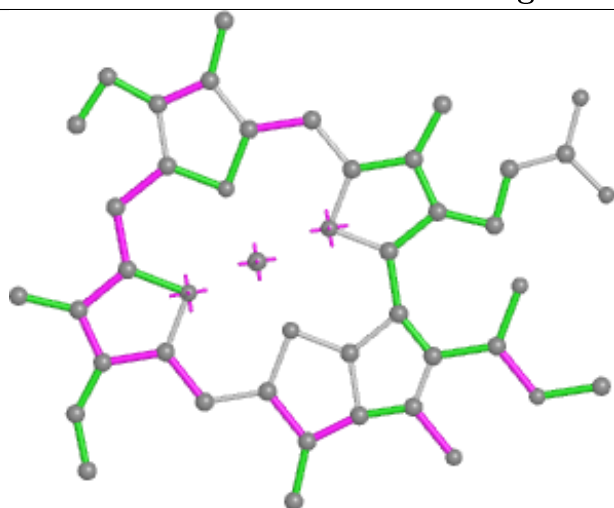


Torsions

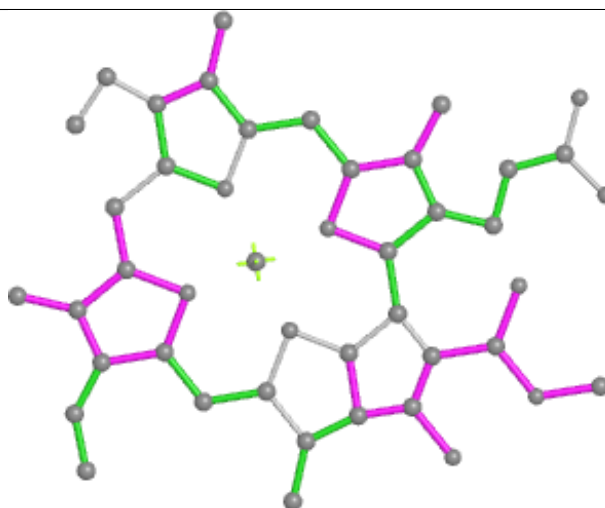


Rings

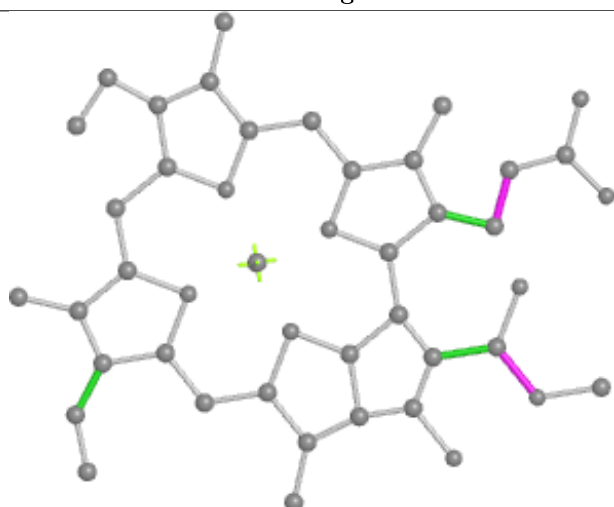
Ligand CLA d 202



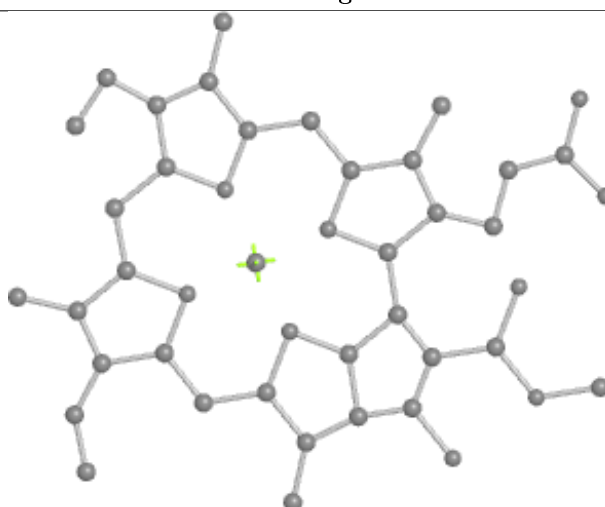
Bond lengths



Bond angles

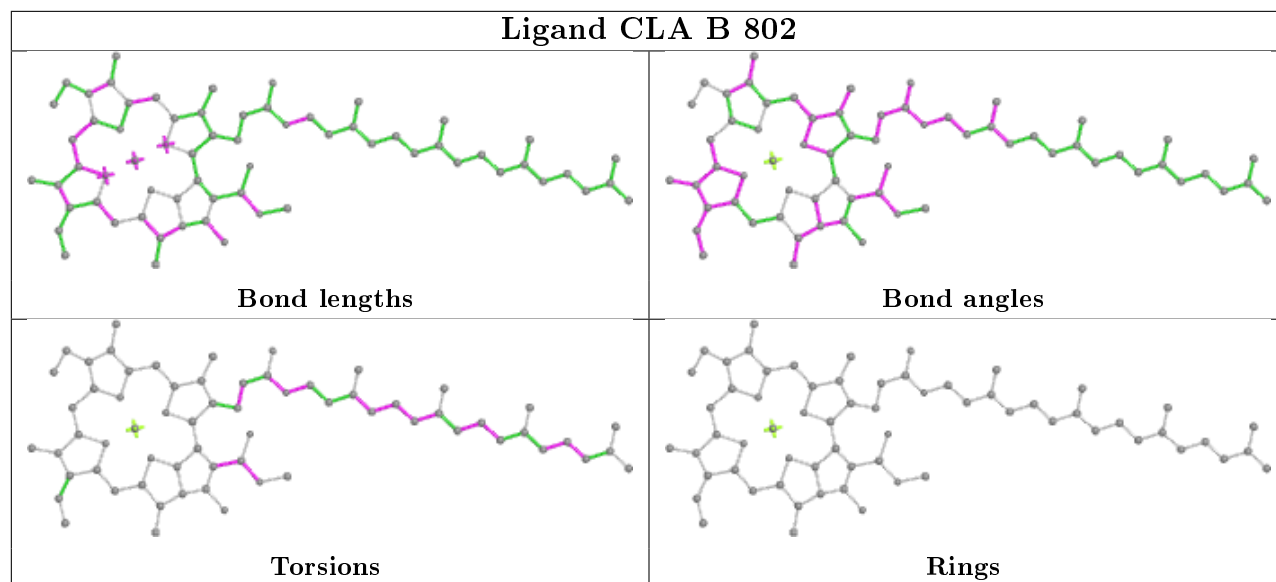


Torsions

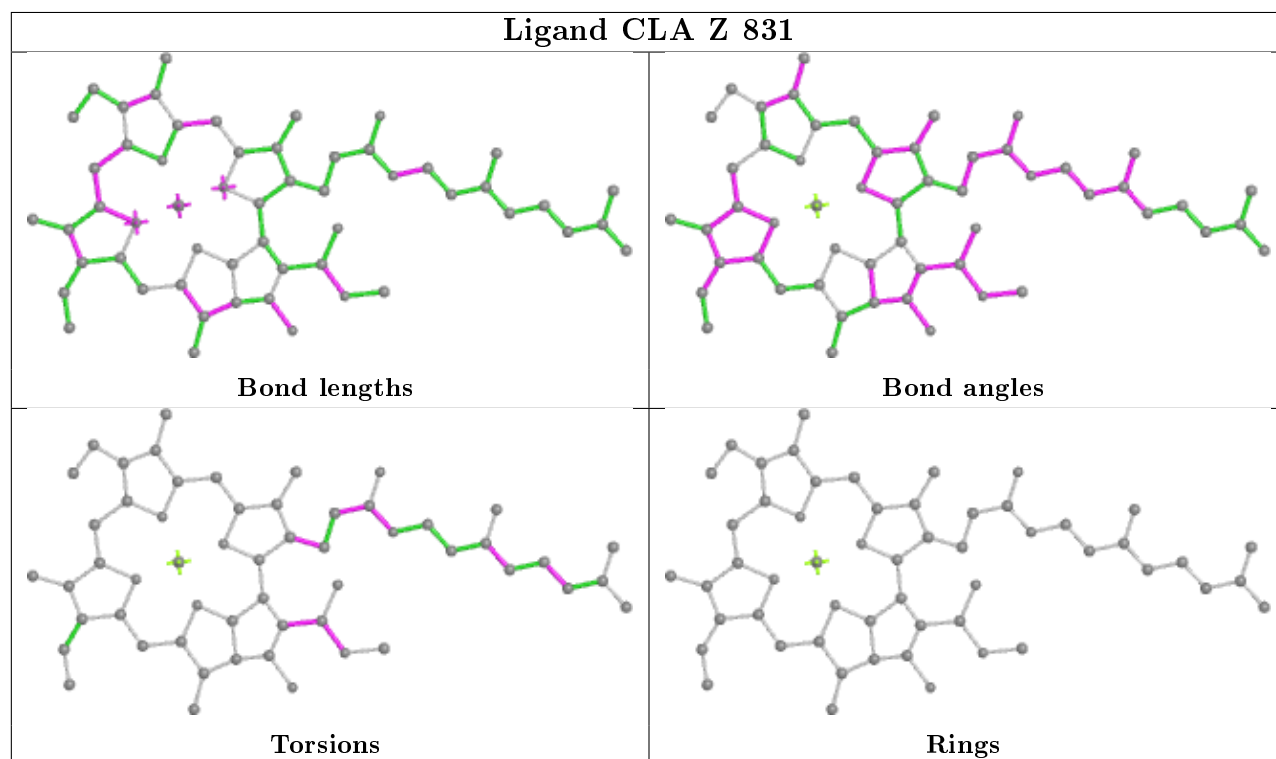


Rings

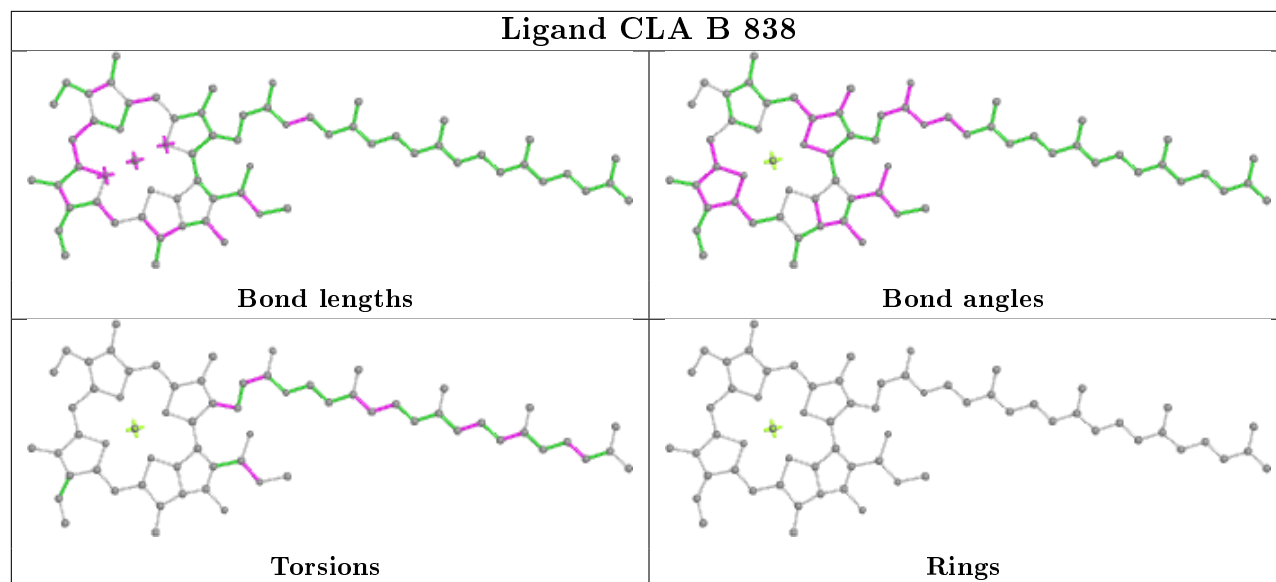
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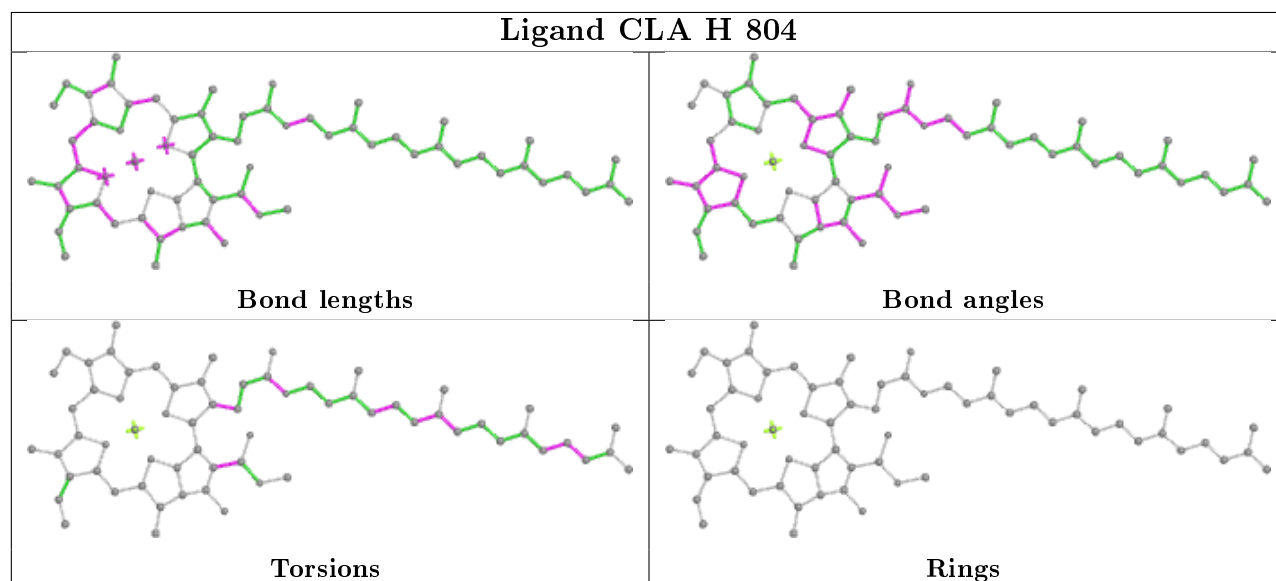
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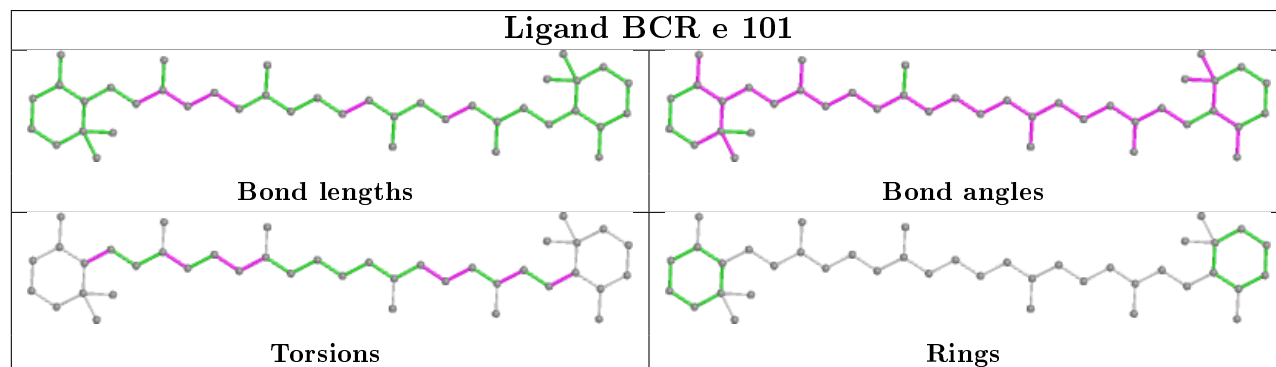
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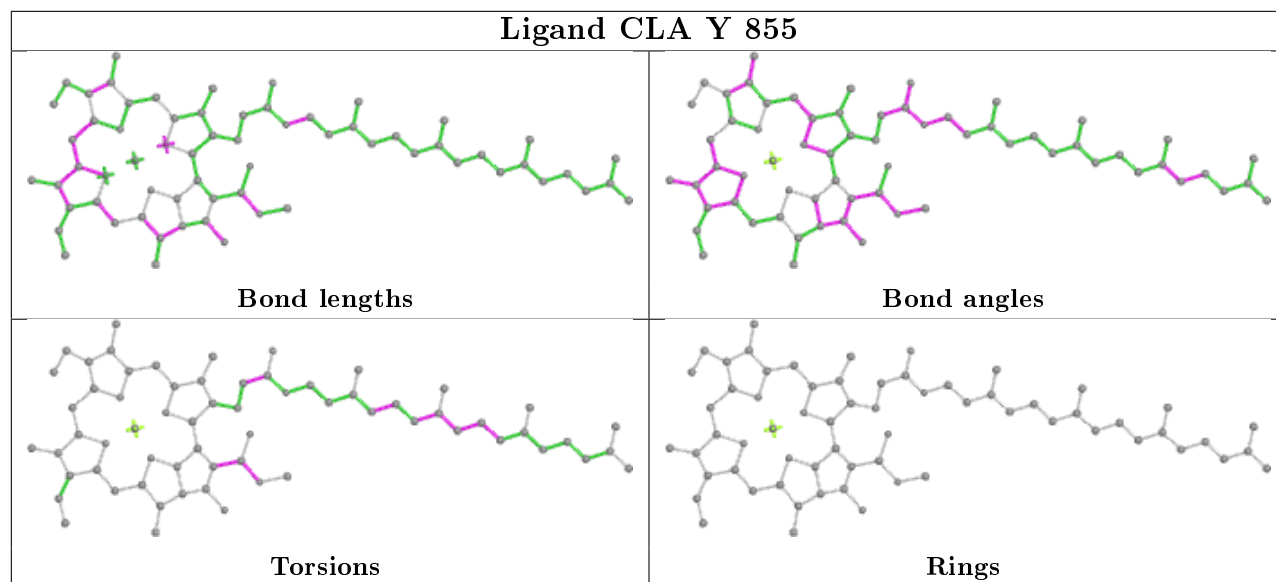
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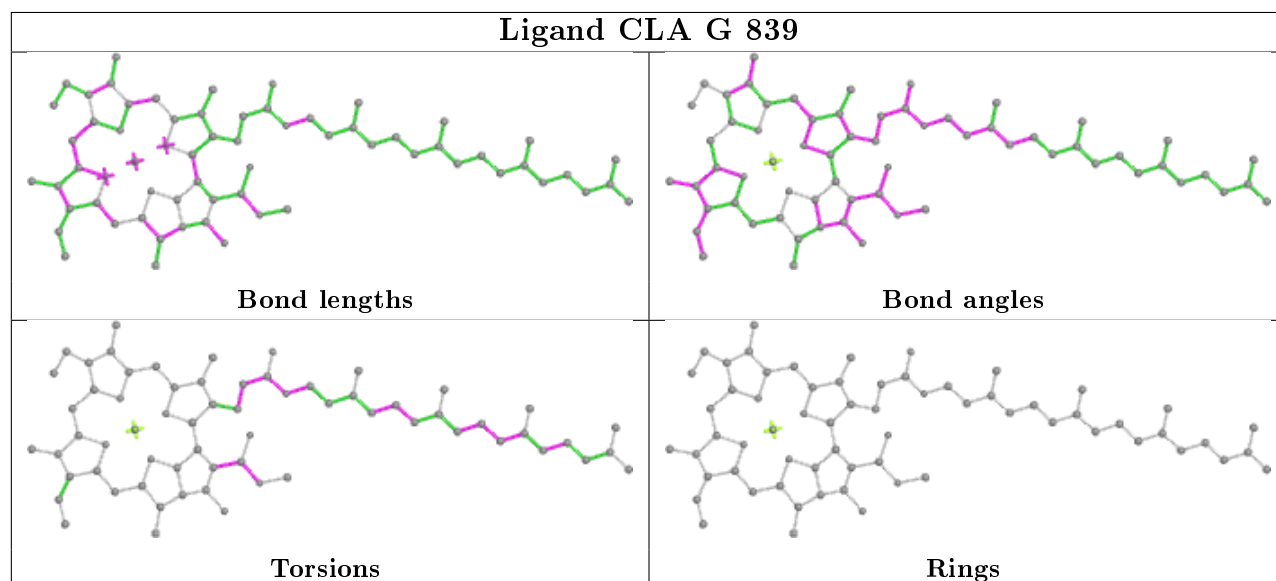
Ligand BCR e 101



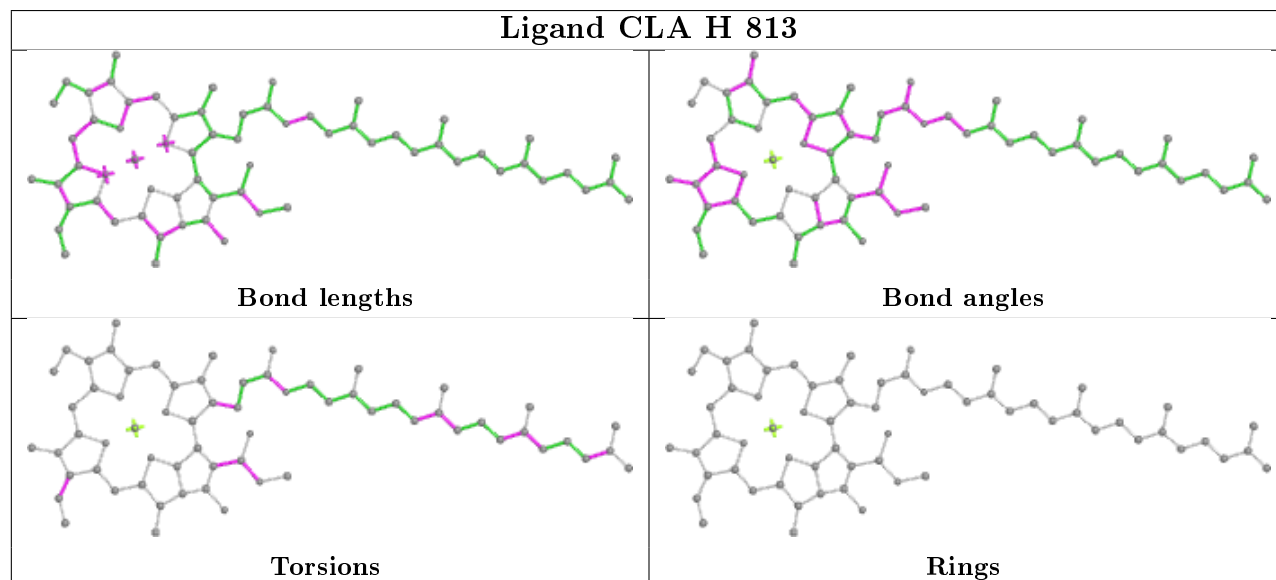
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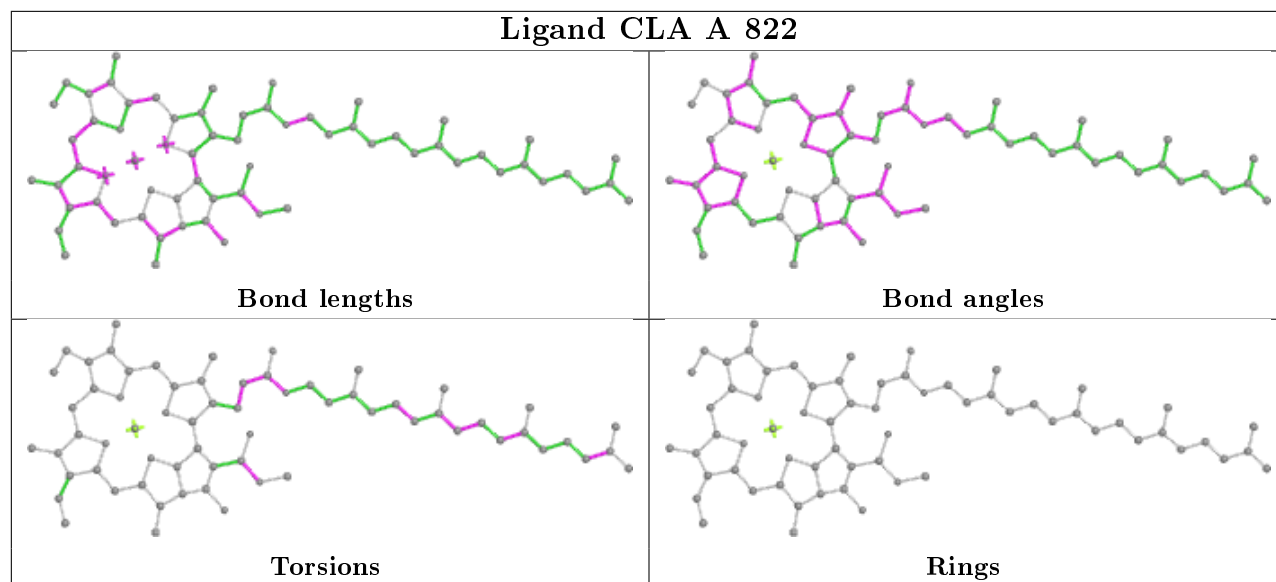
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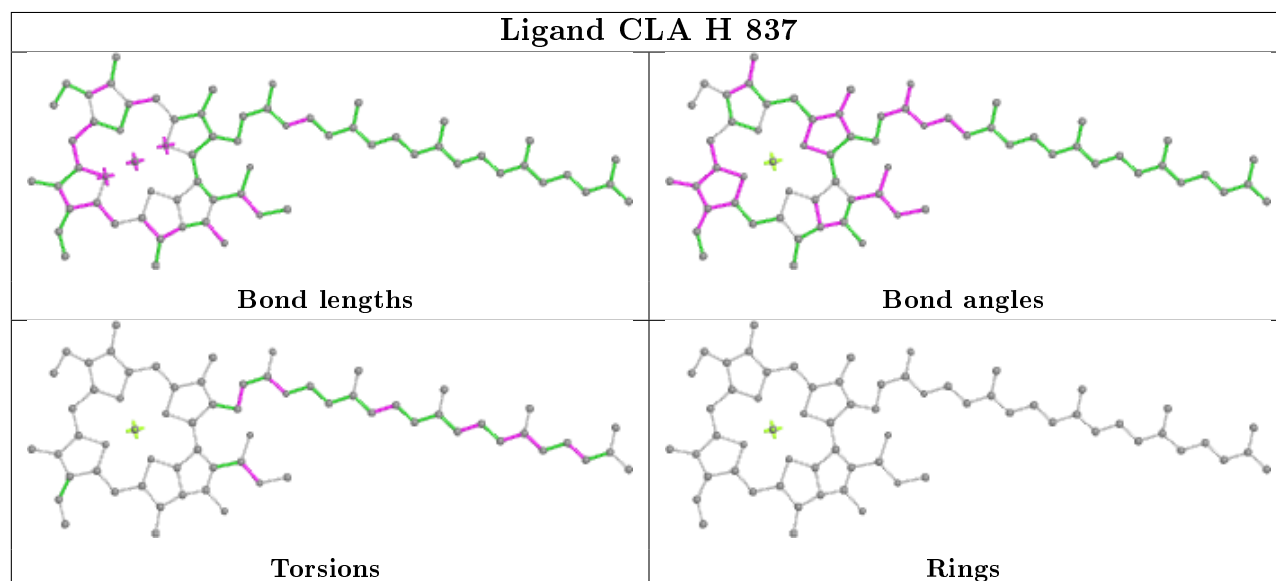
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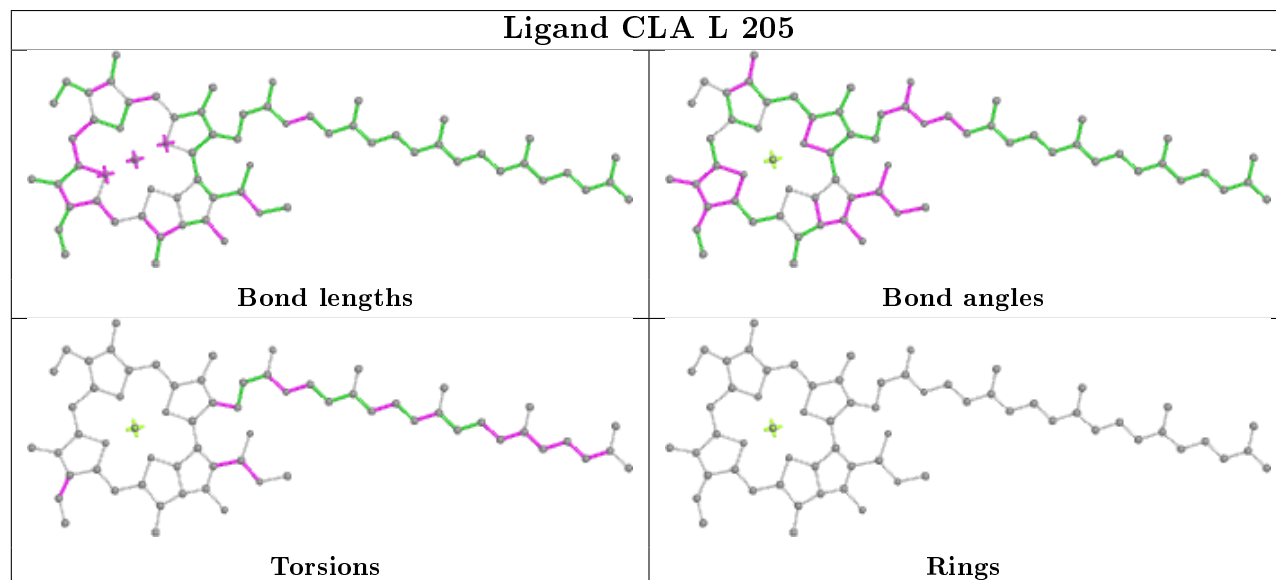
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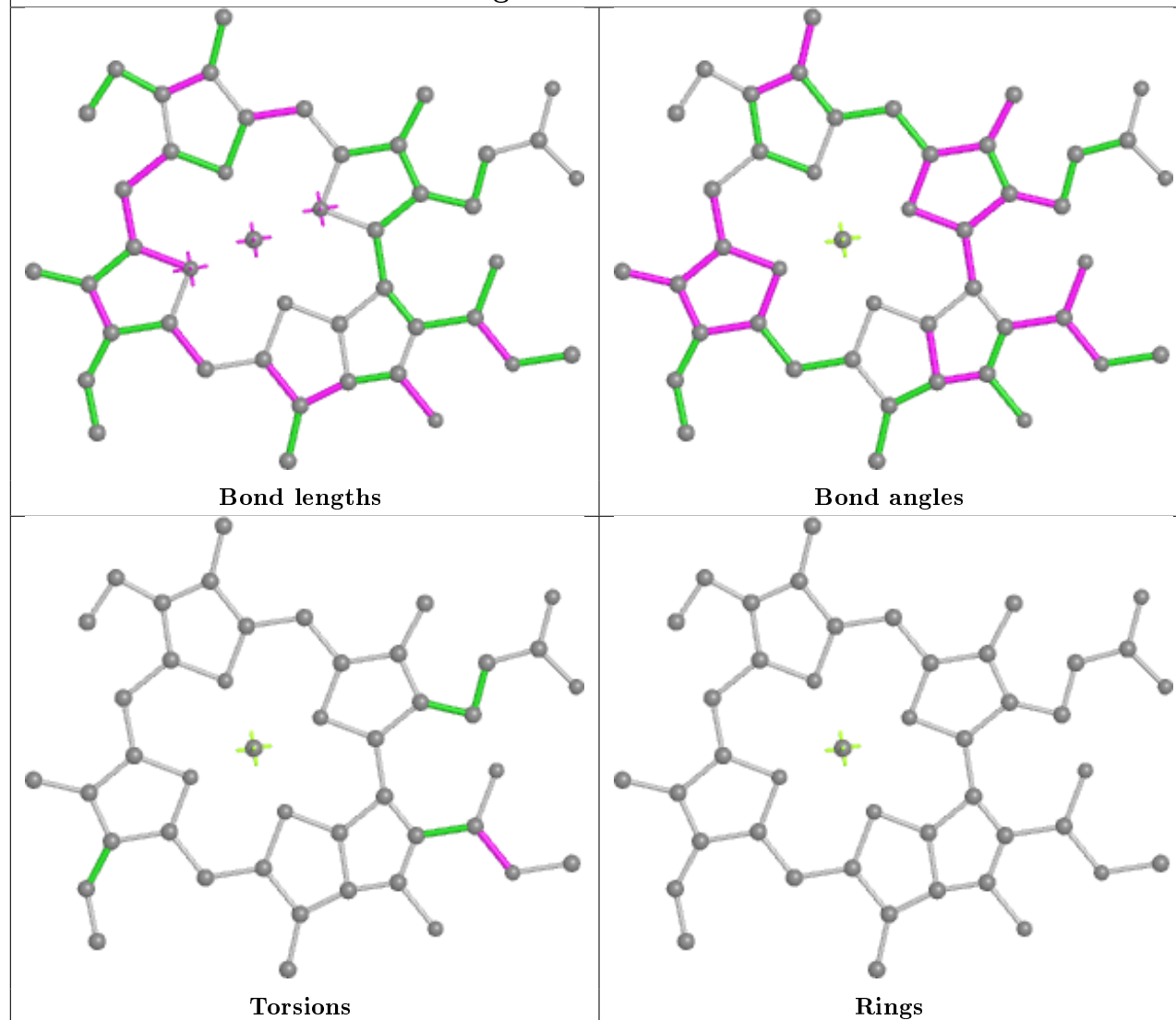
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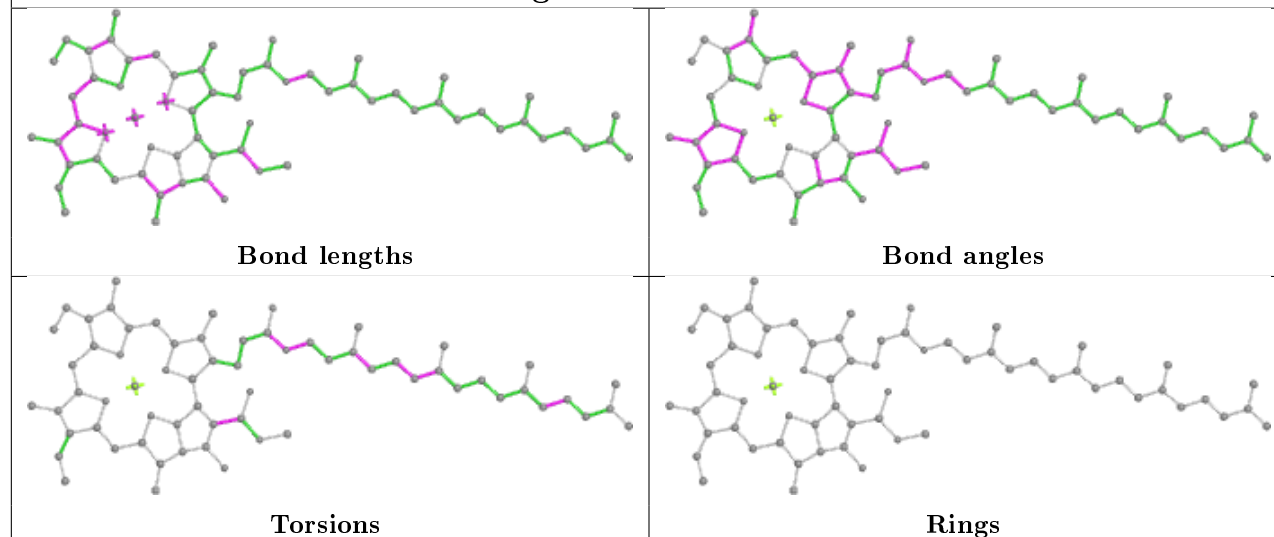
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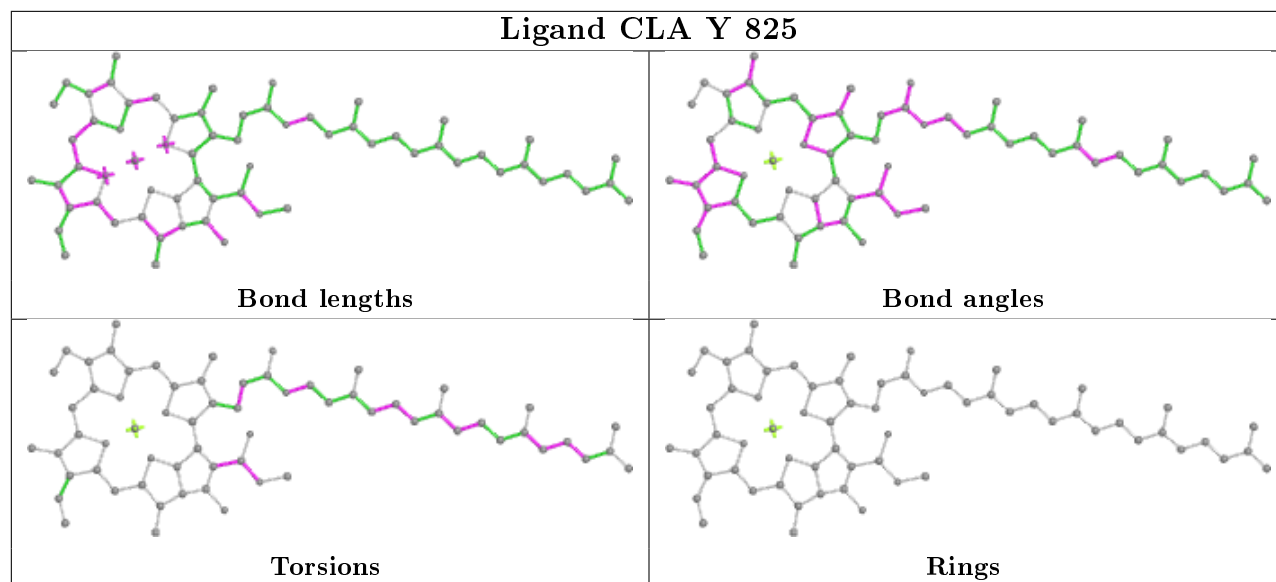
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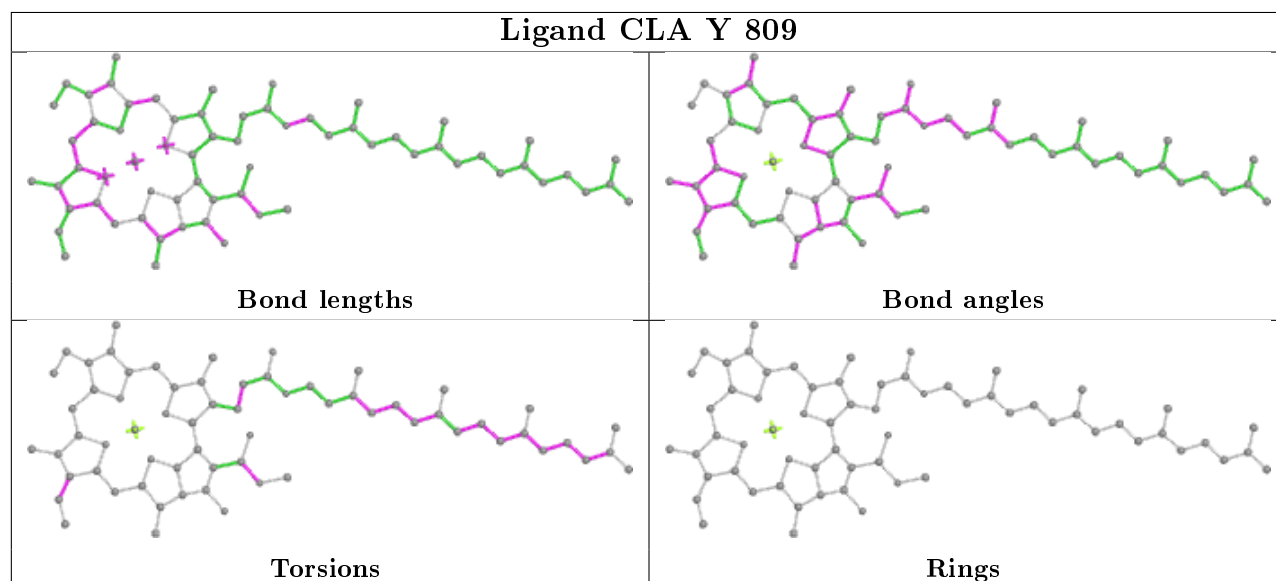
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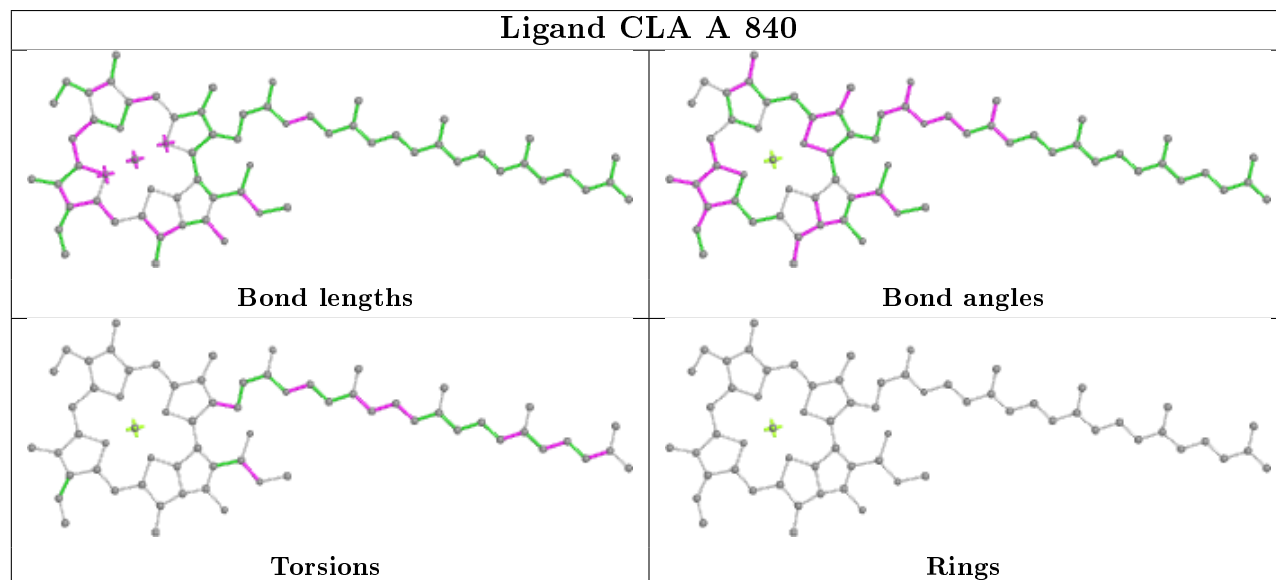
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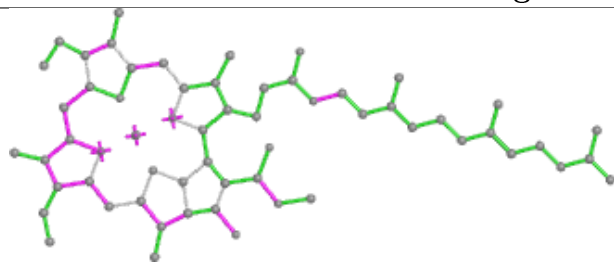
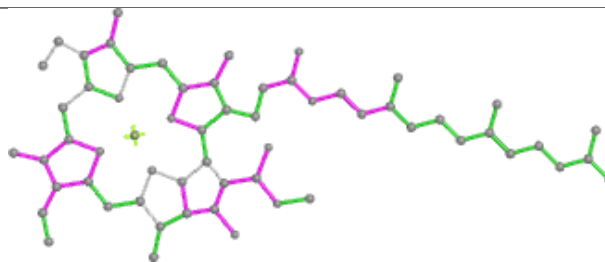
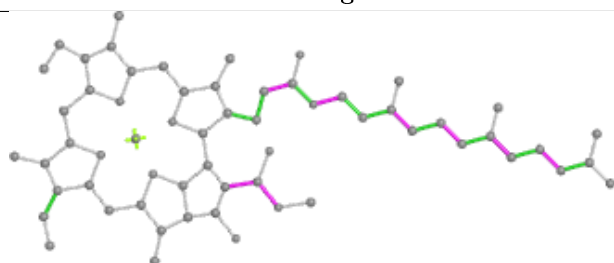
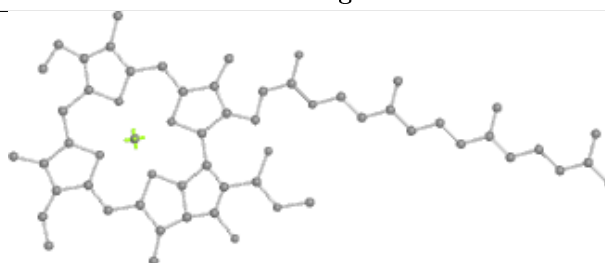
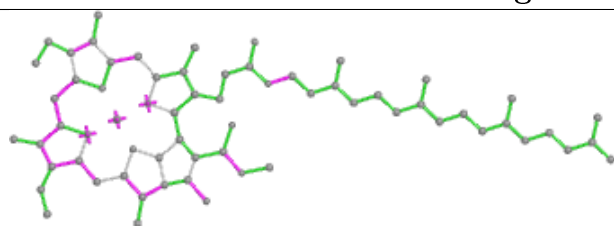
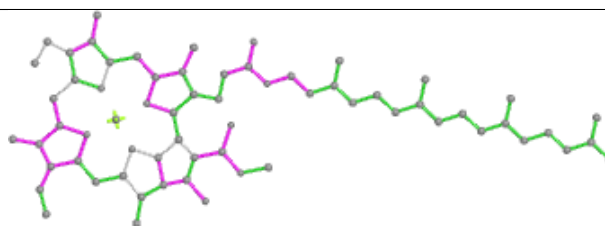
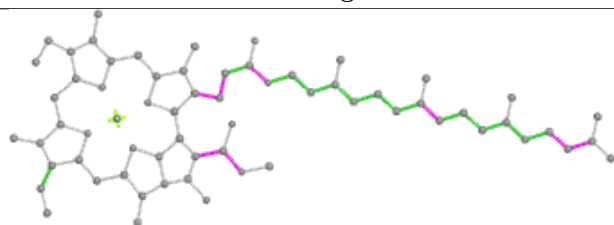
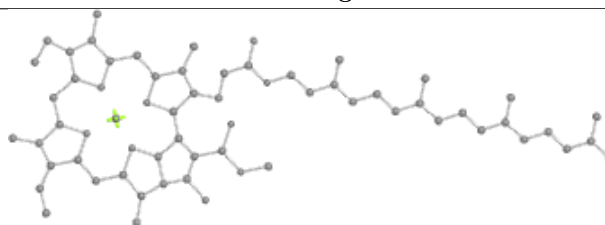


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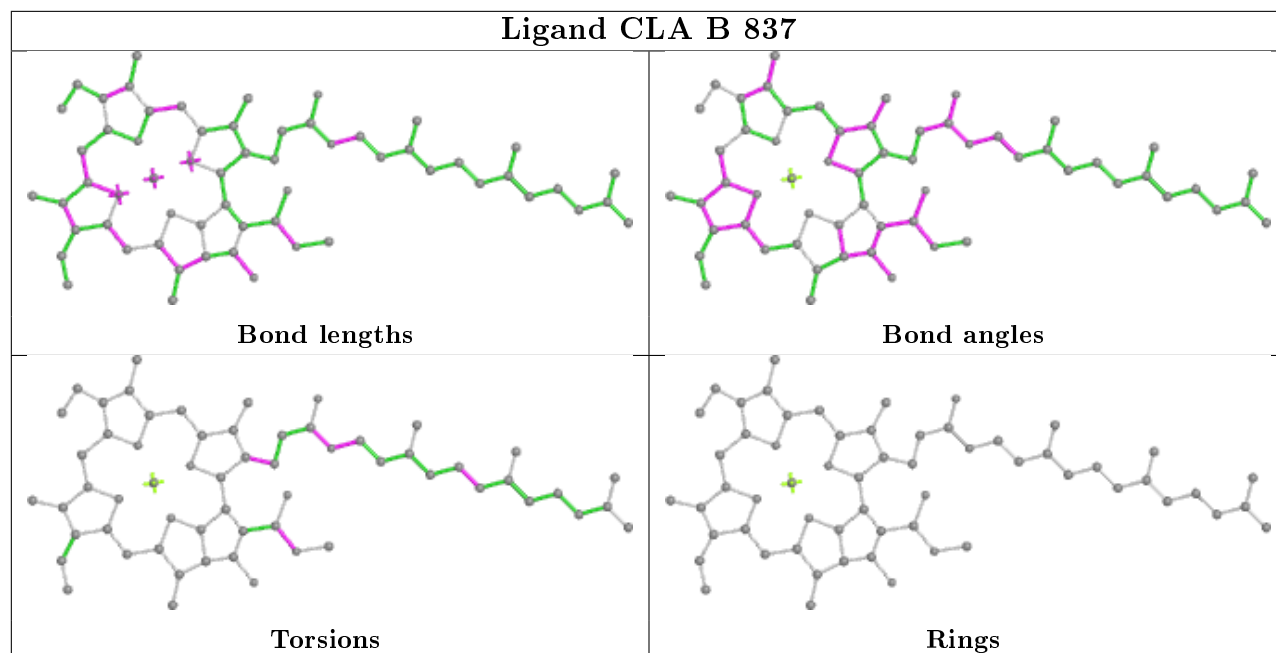


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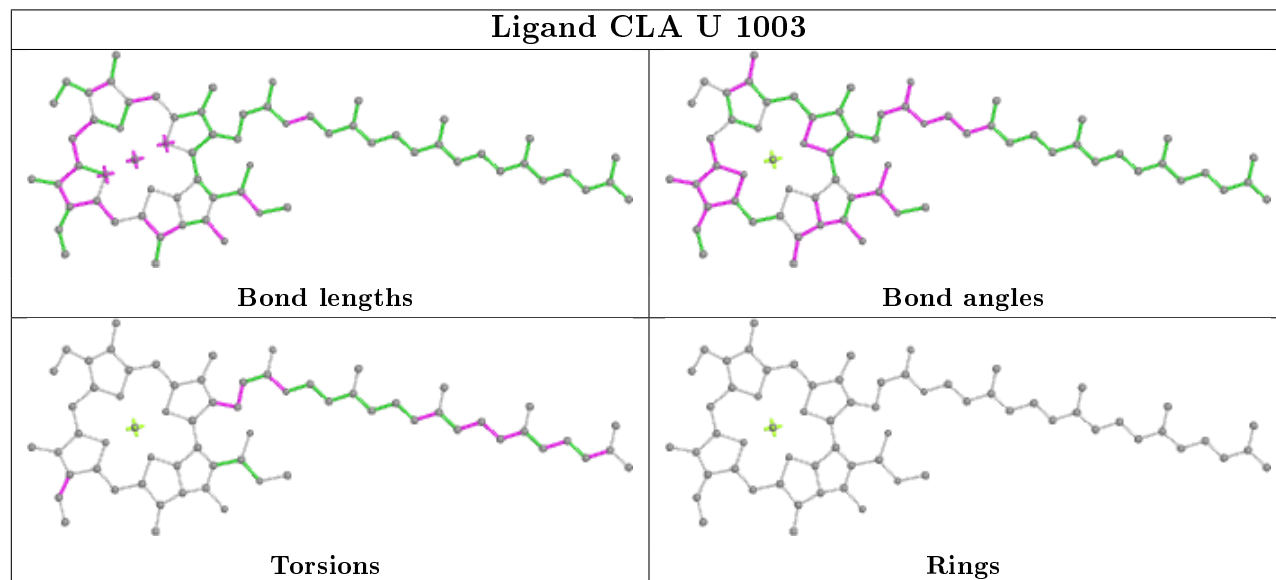


Ligand CLA G 813**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA Y 840****Bond lengths****Bond angles****Torsions****Rings**

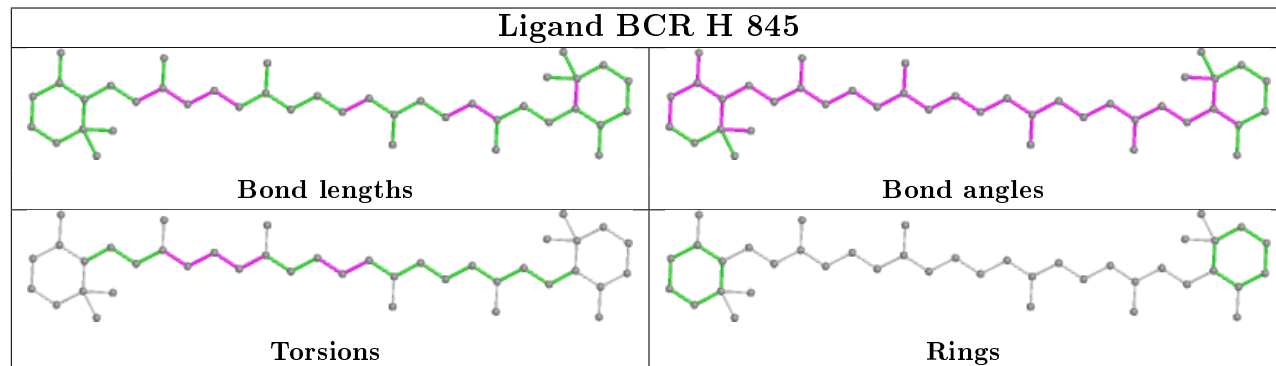
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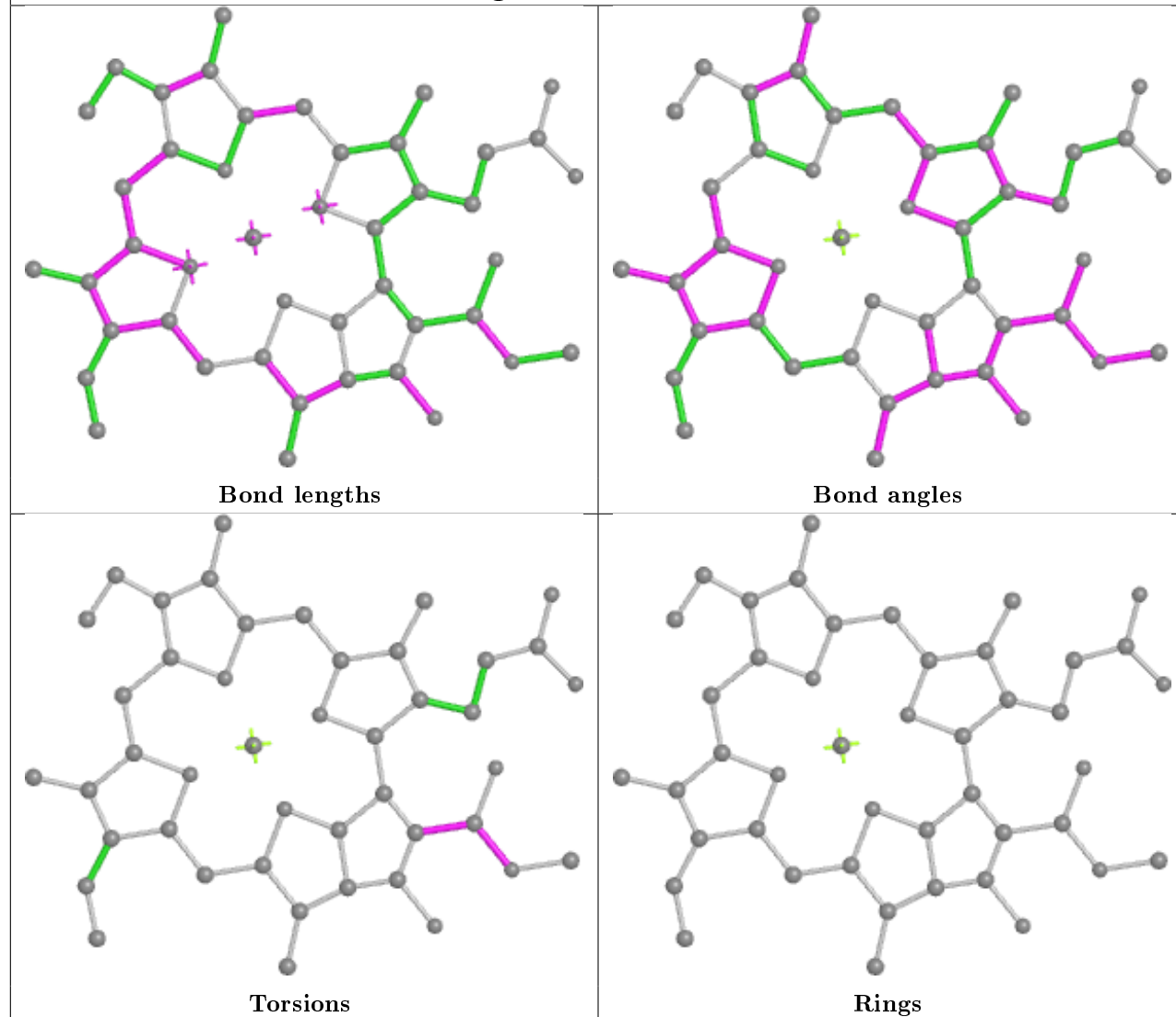
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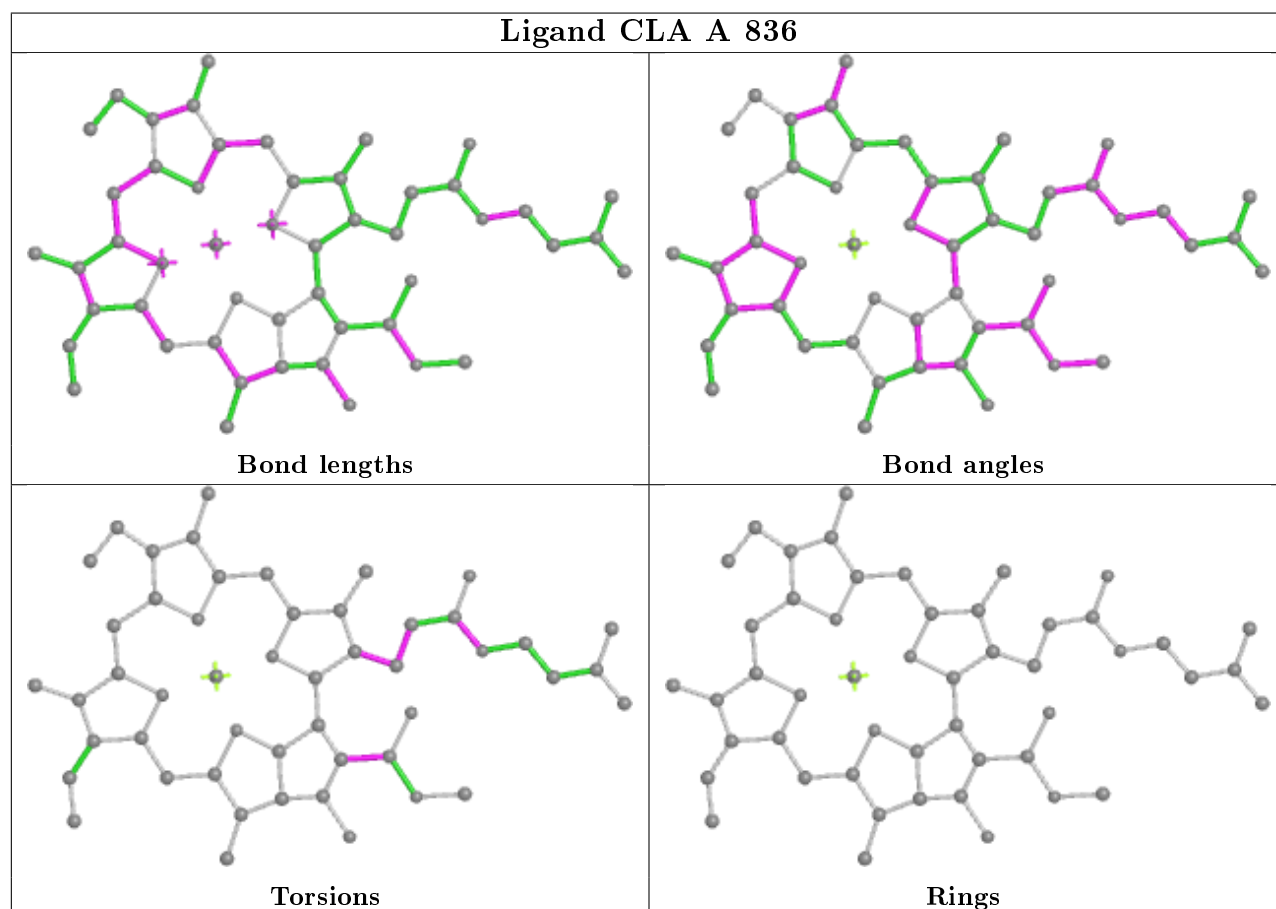
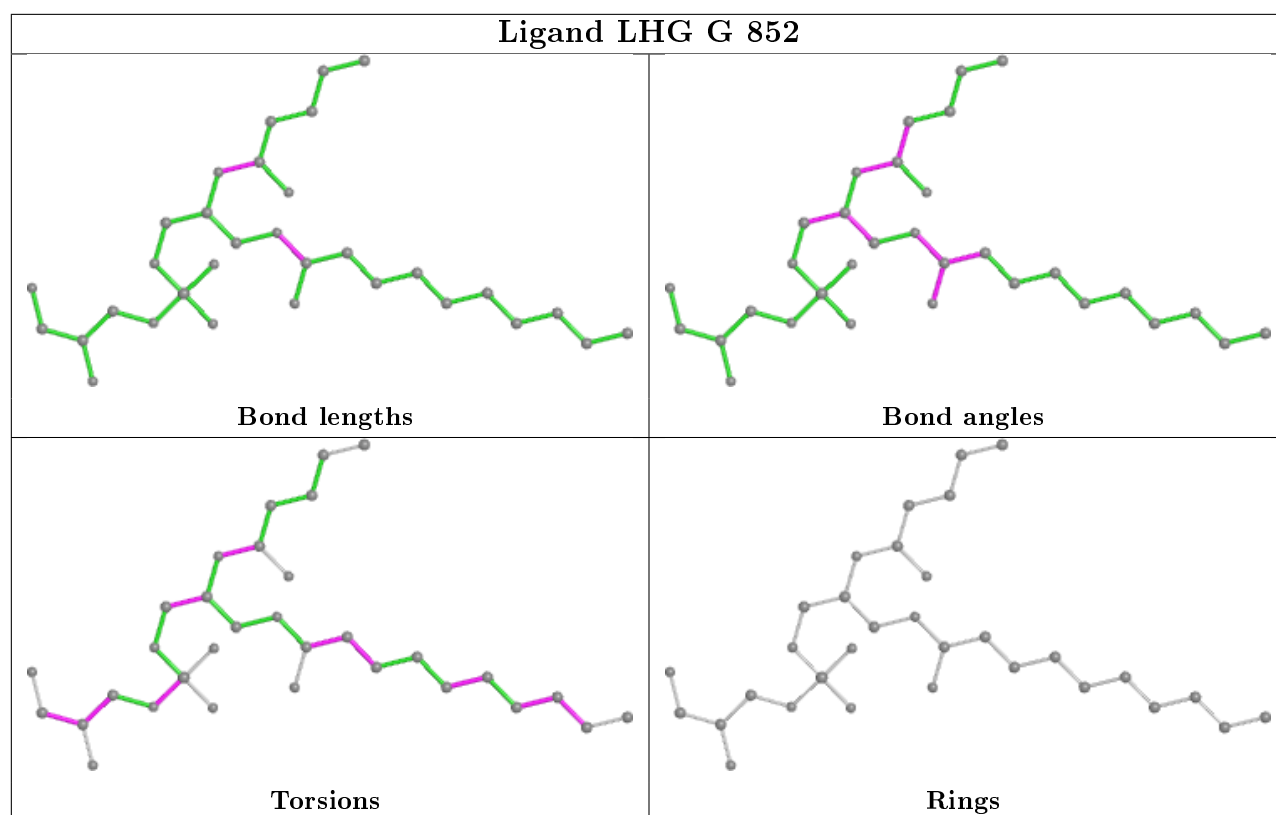


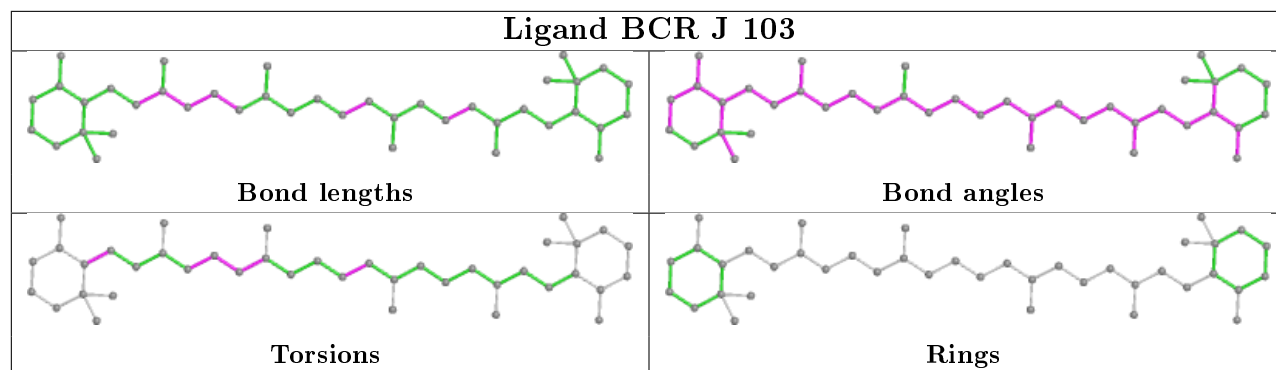
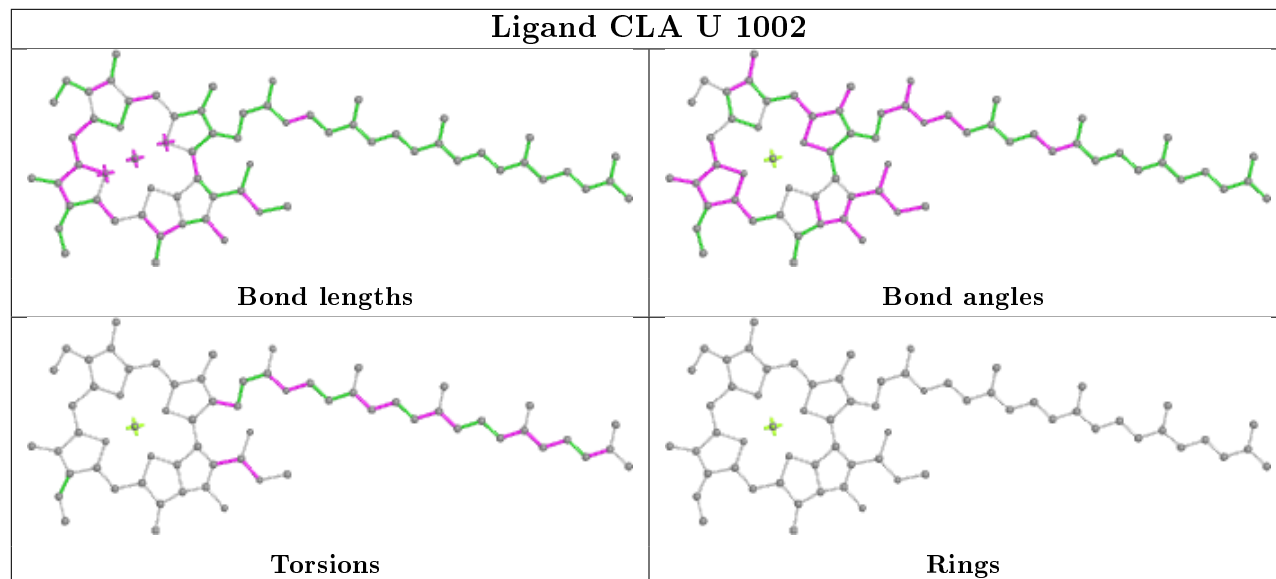
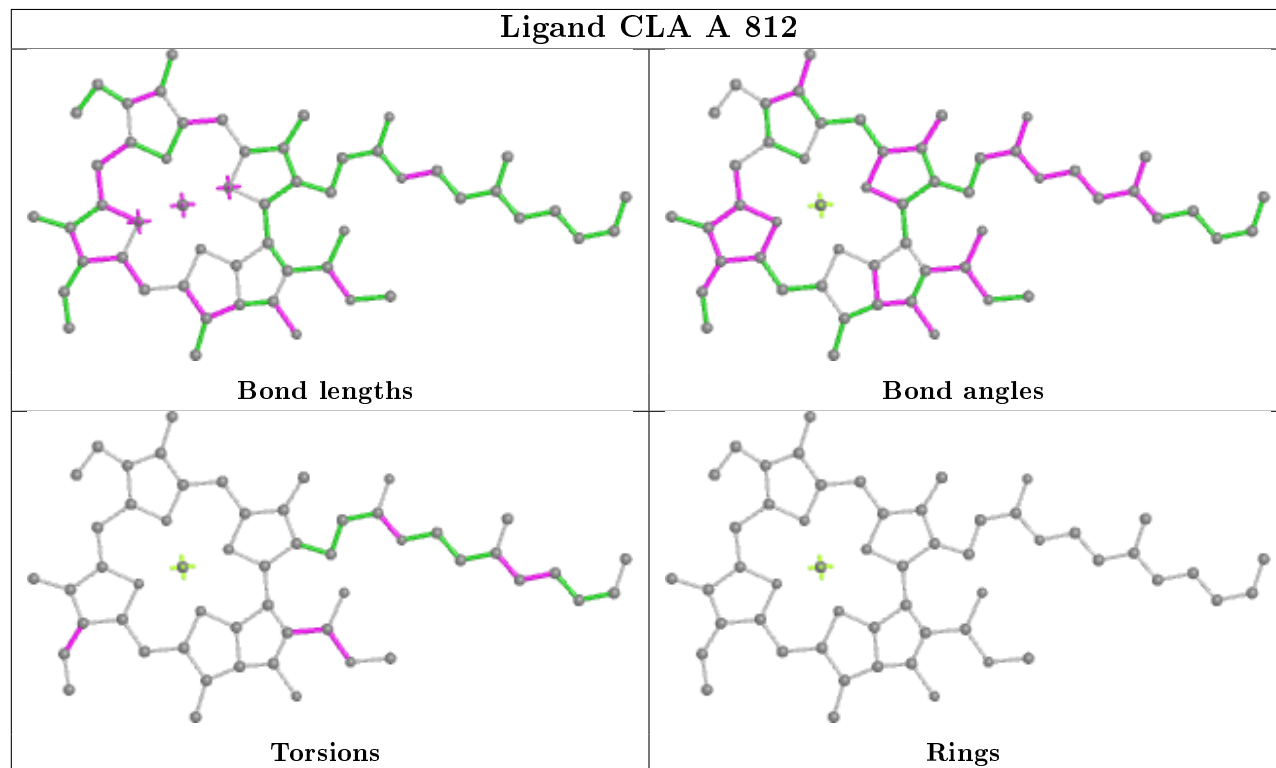
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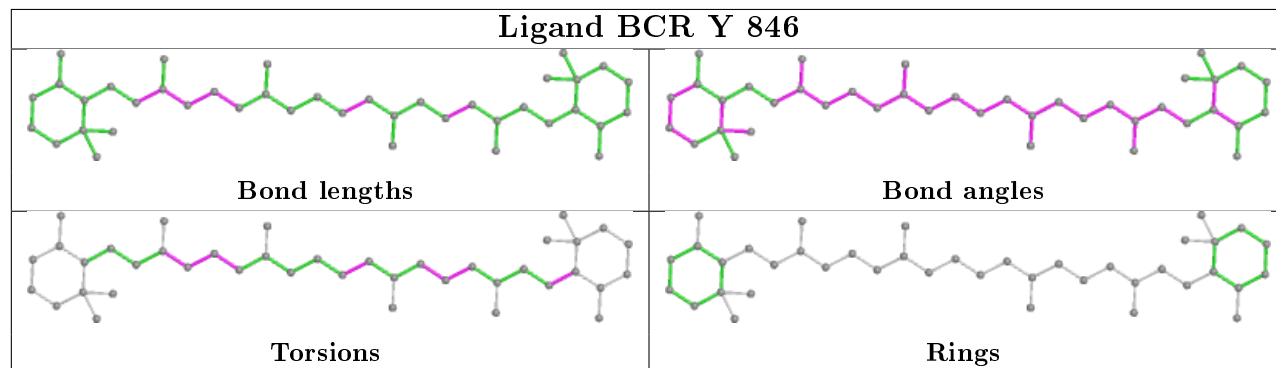
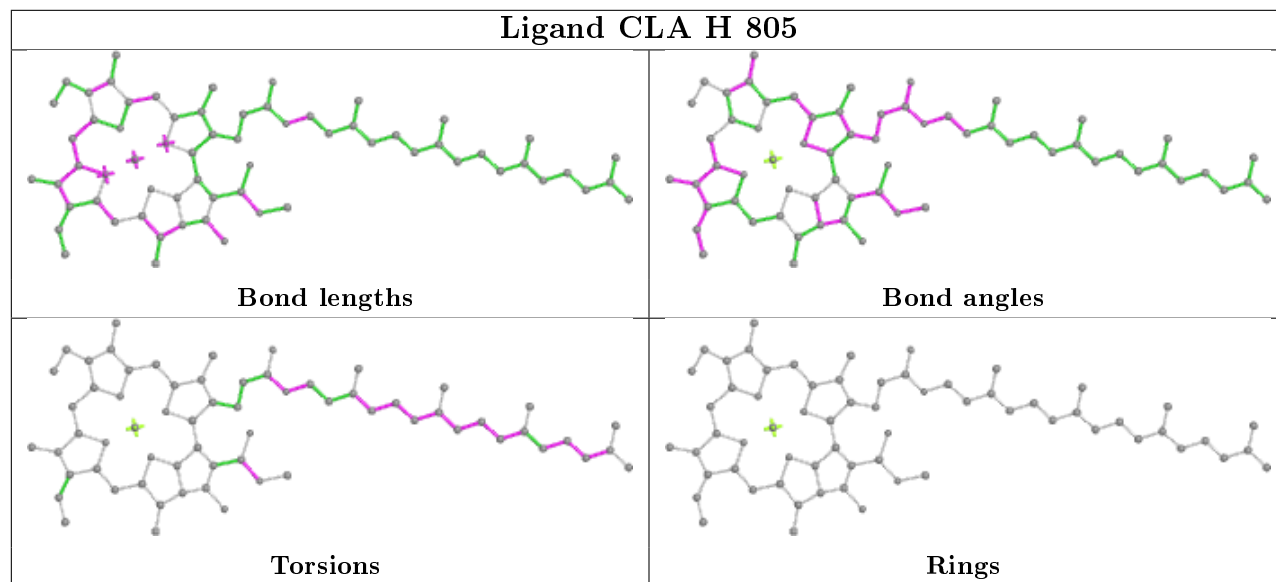
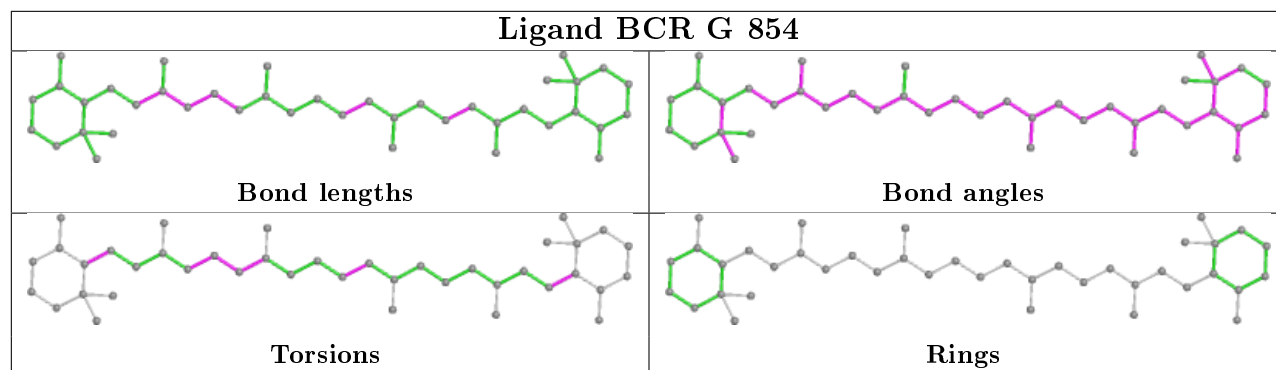
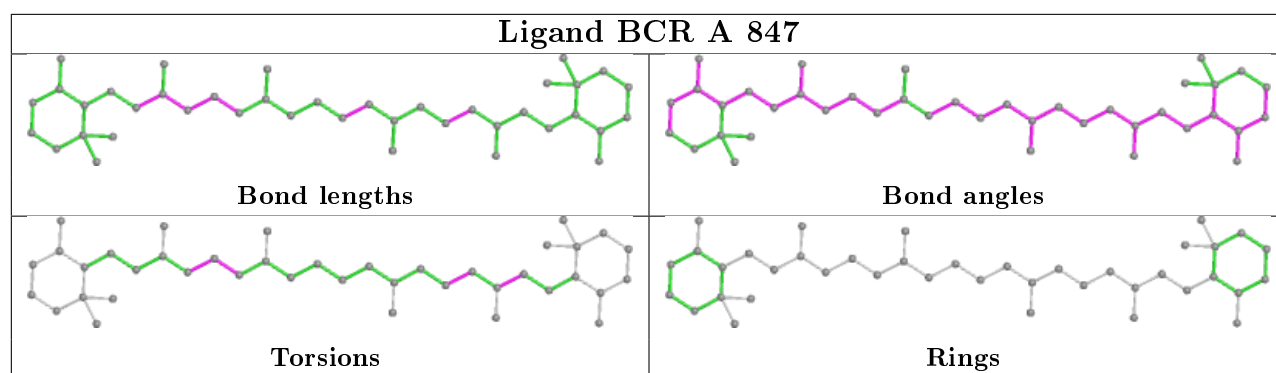


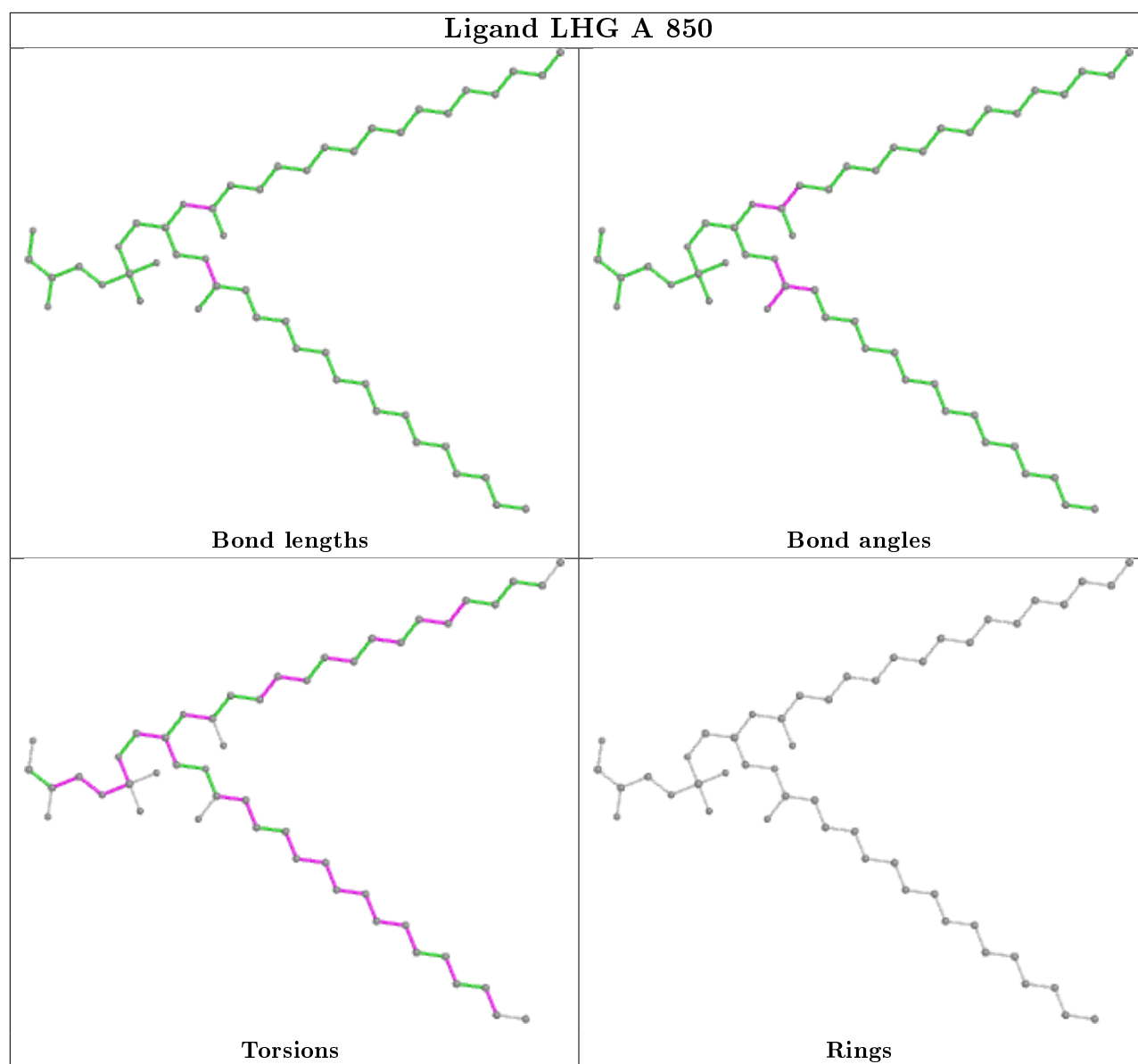
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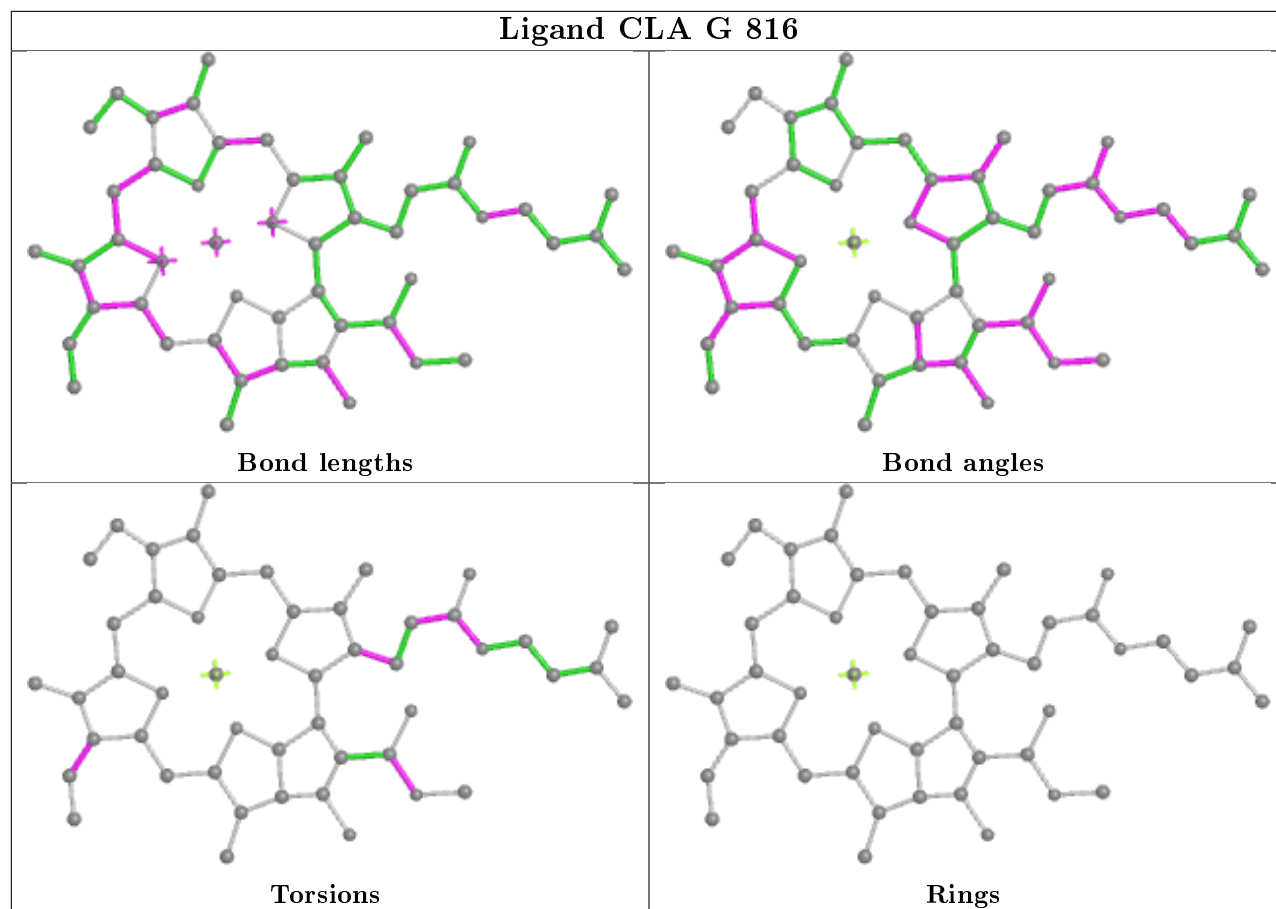




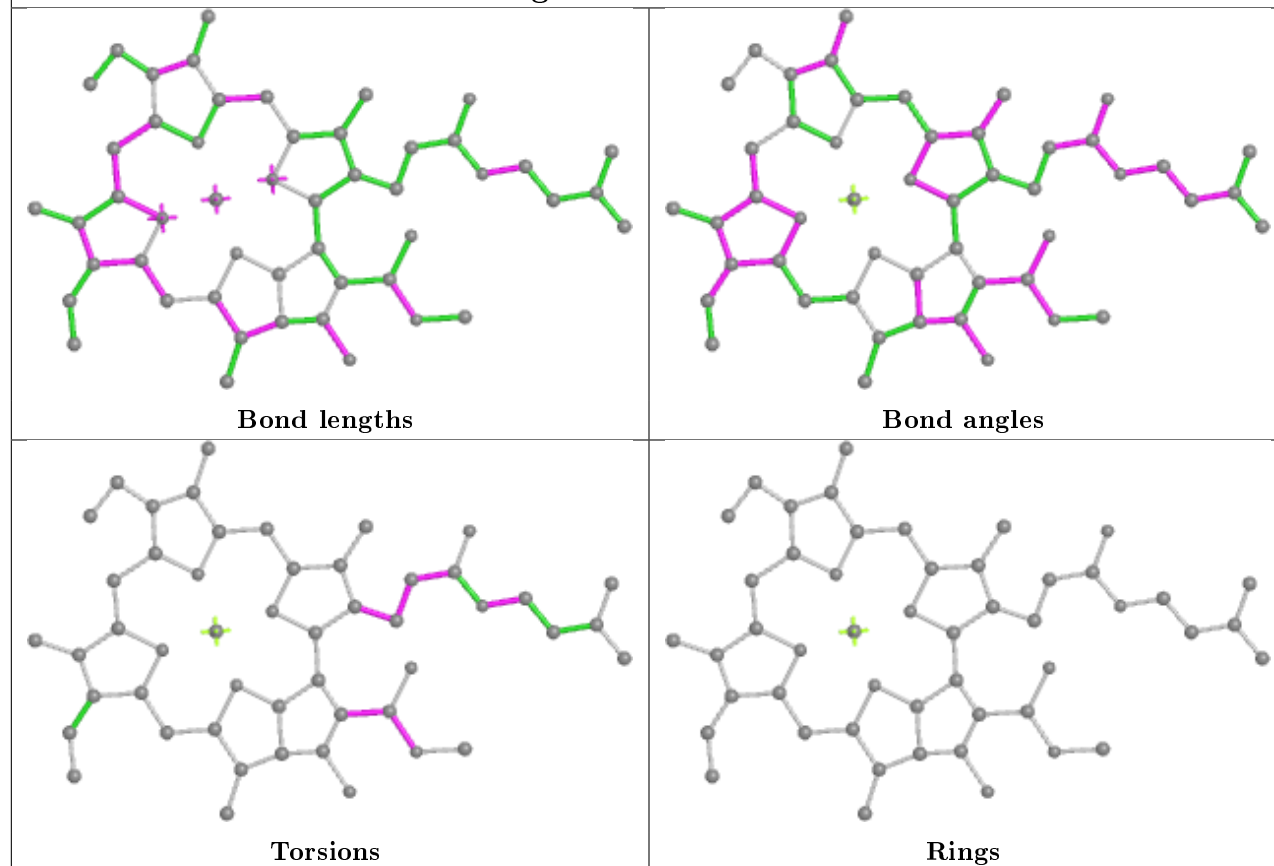
Ligand BCR J 103**Ligand CLA U 1002****Ligand CLA A 812**



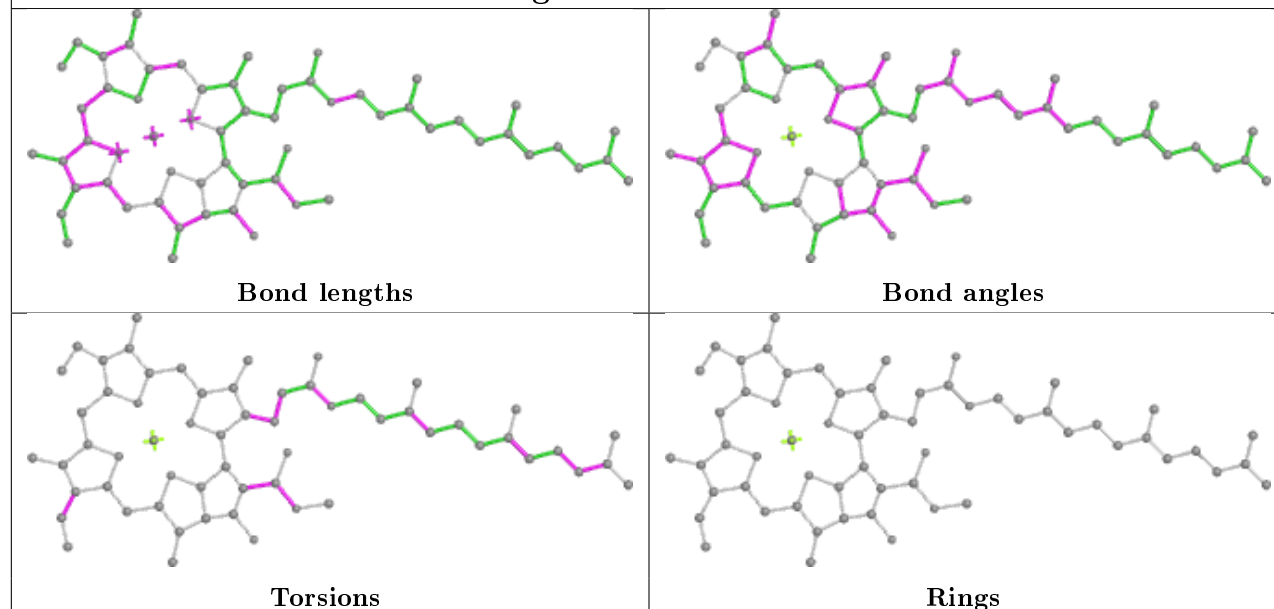




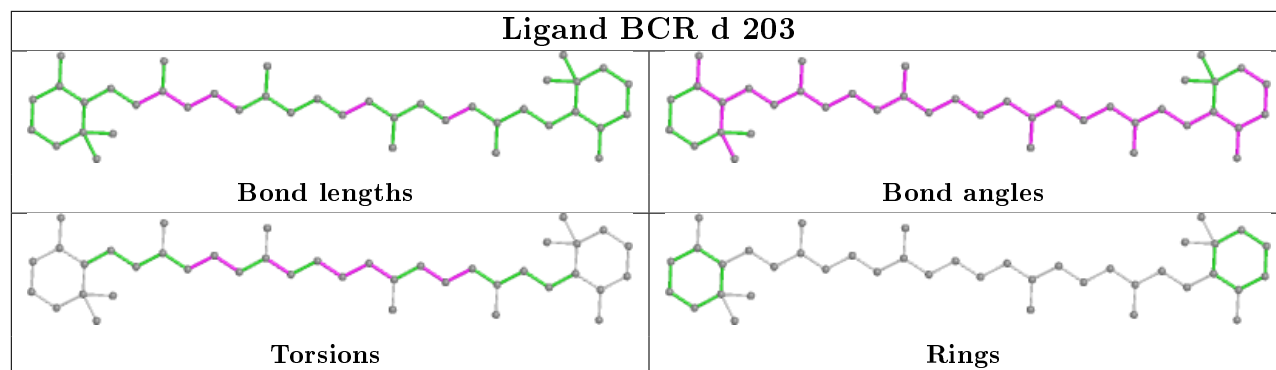
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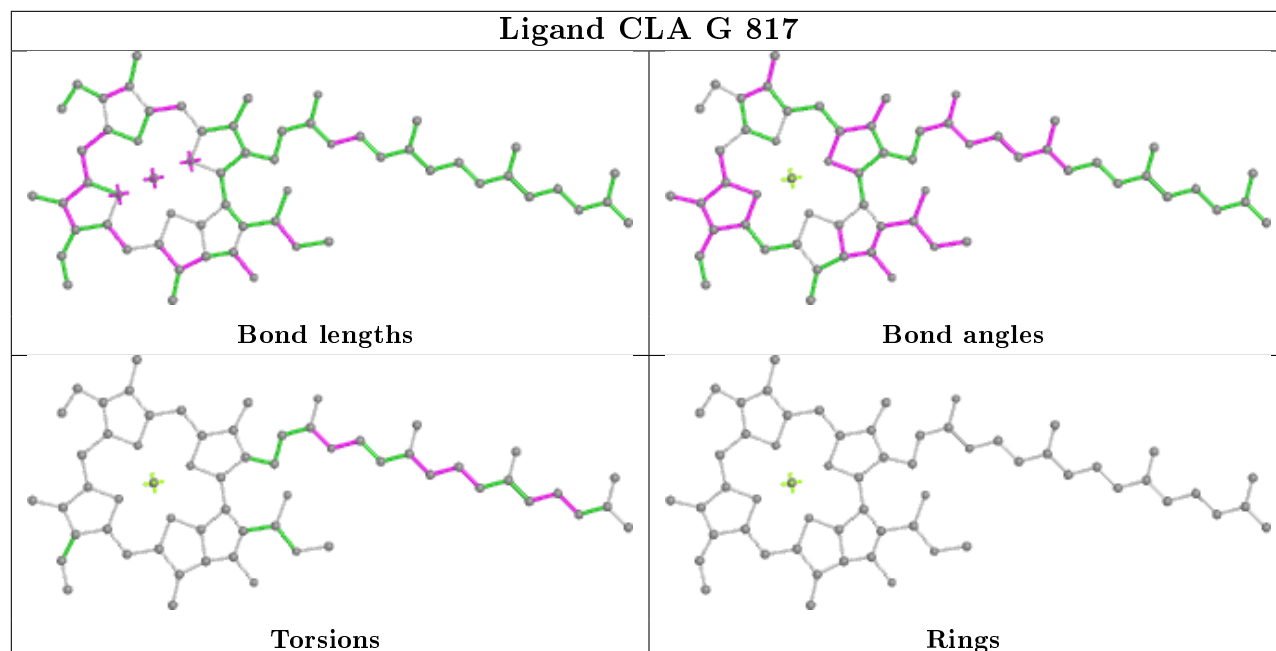
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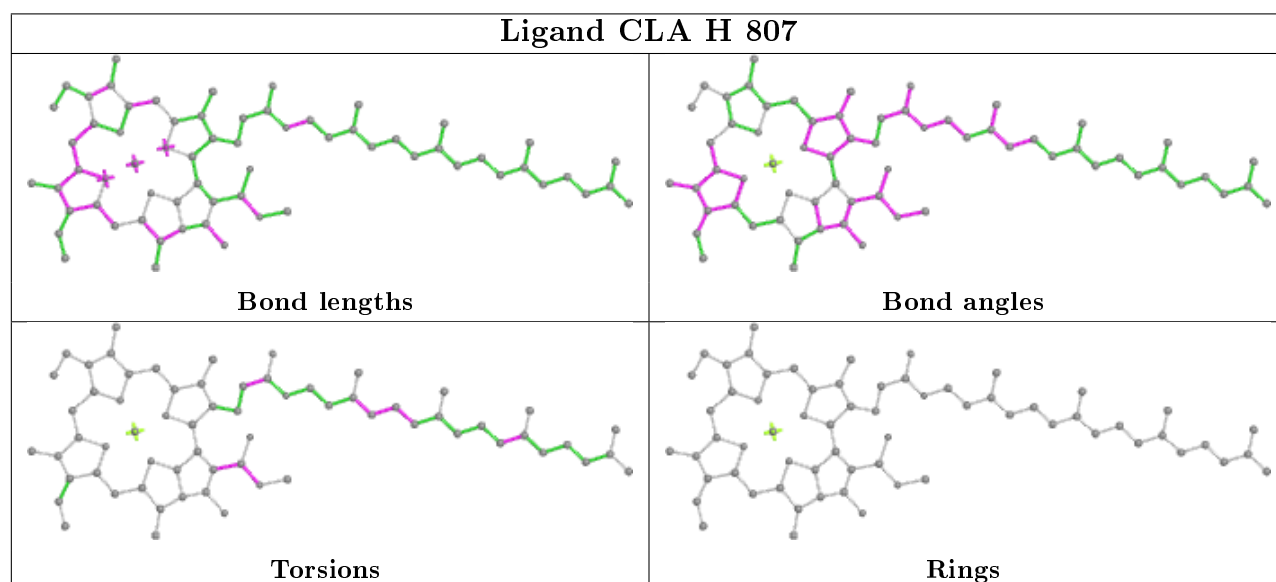
Ligand BCR d 203



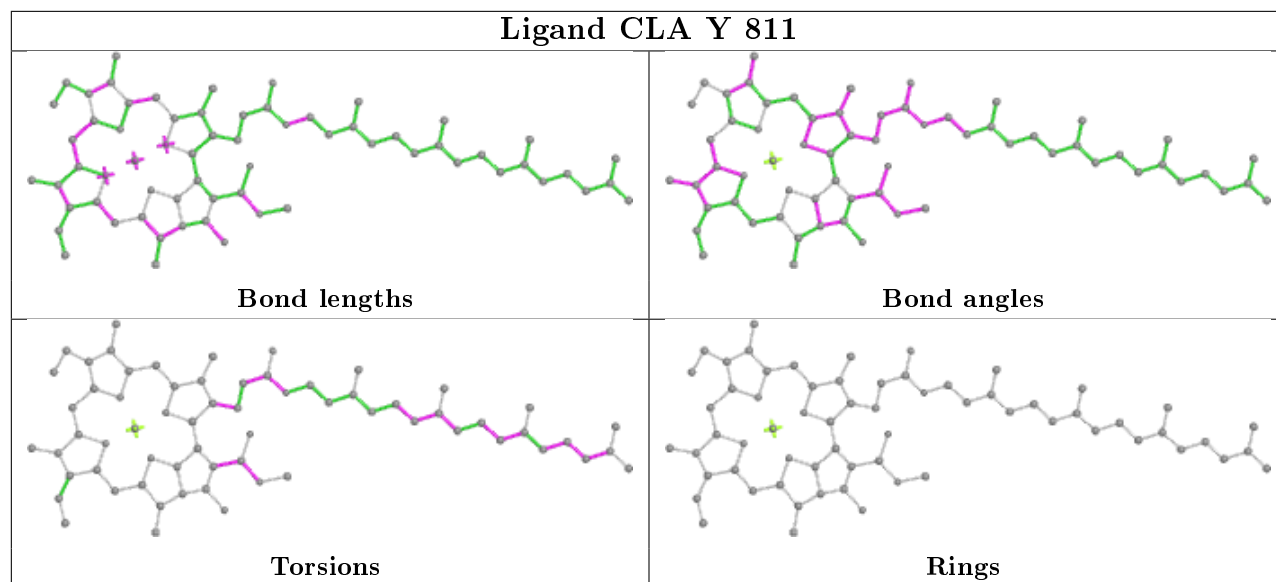
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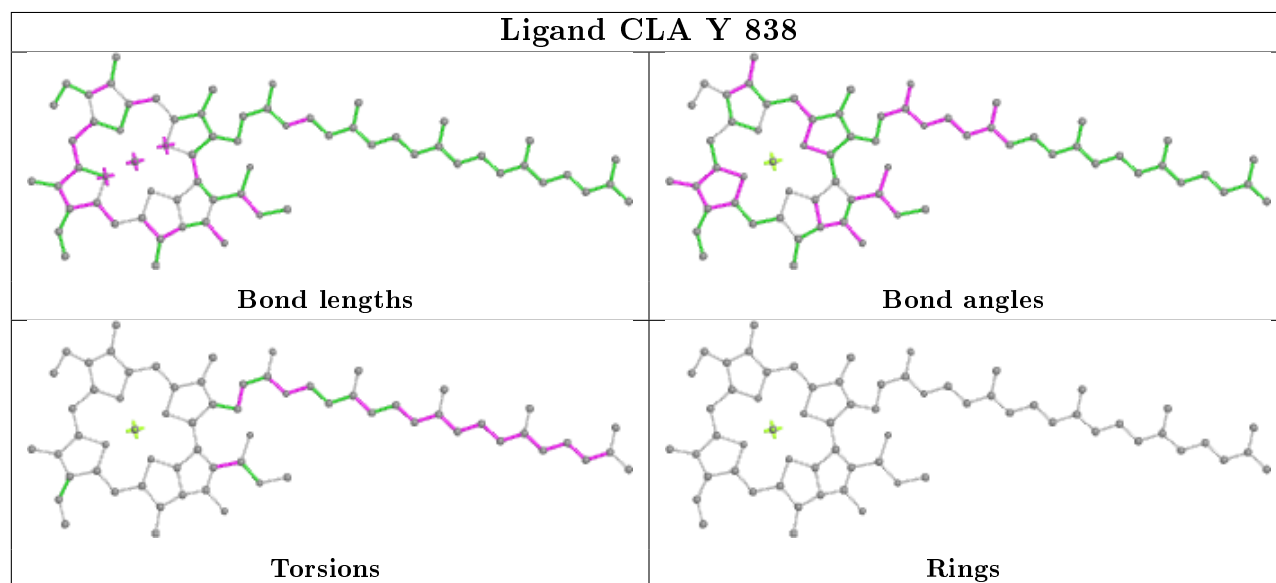
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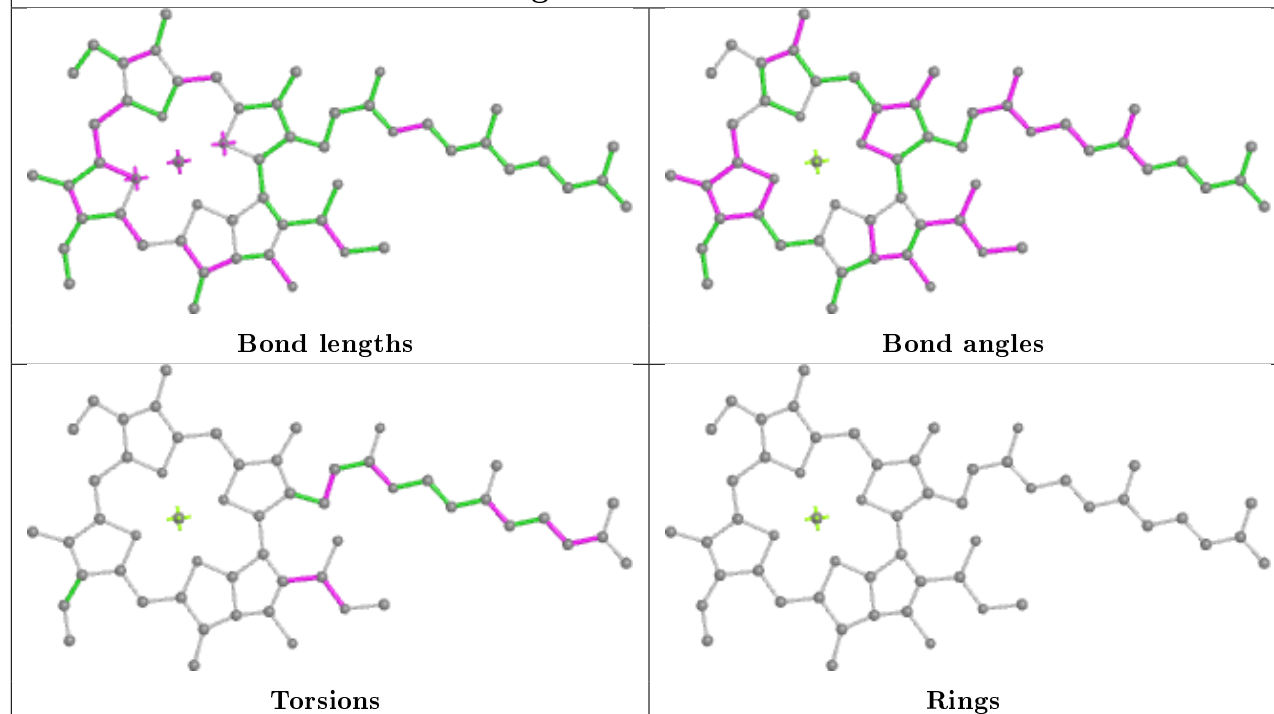
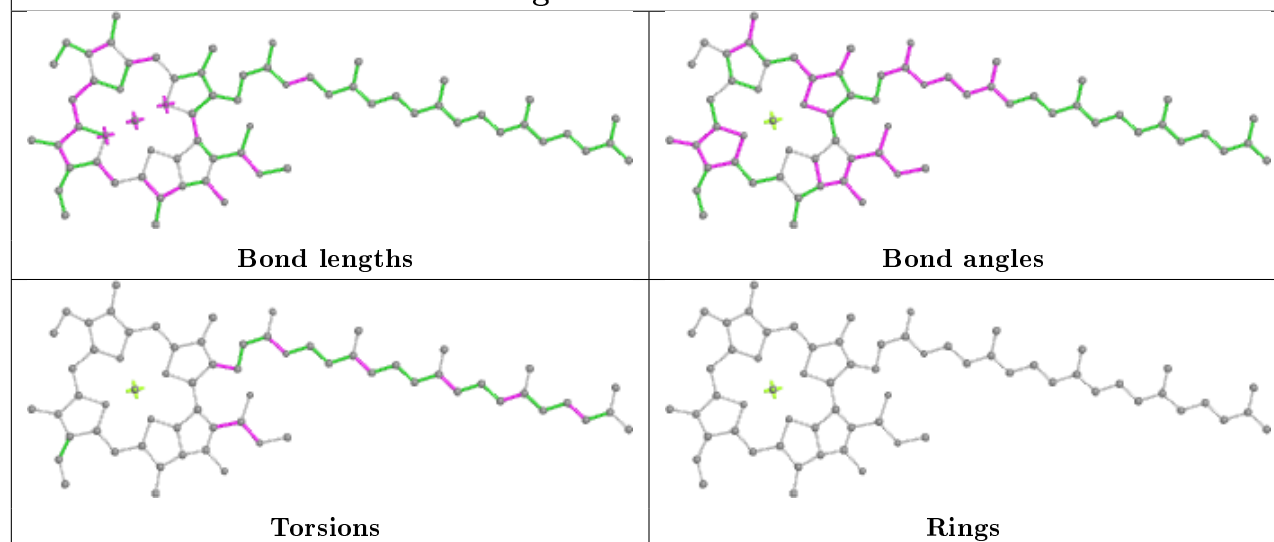


Ligand CLA Y 811

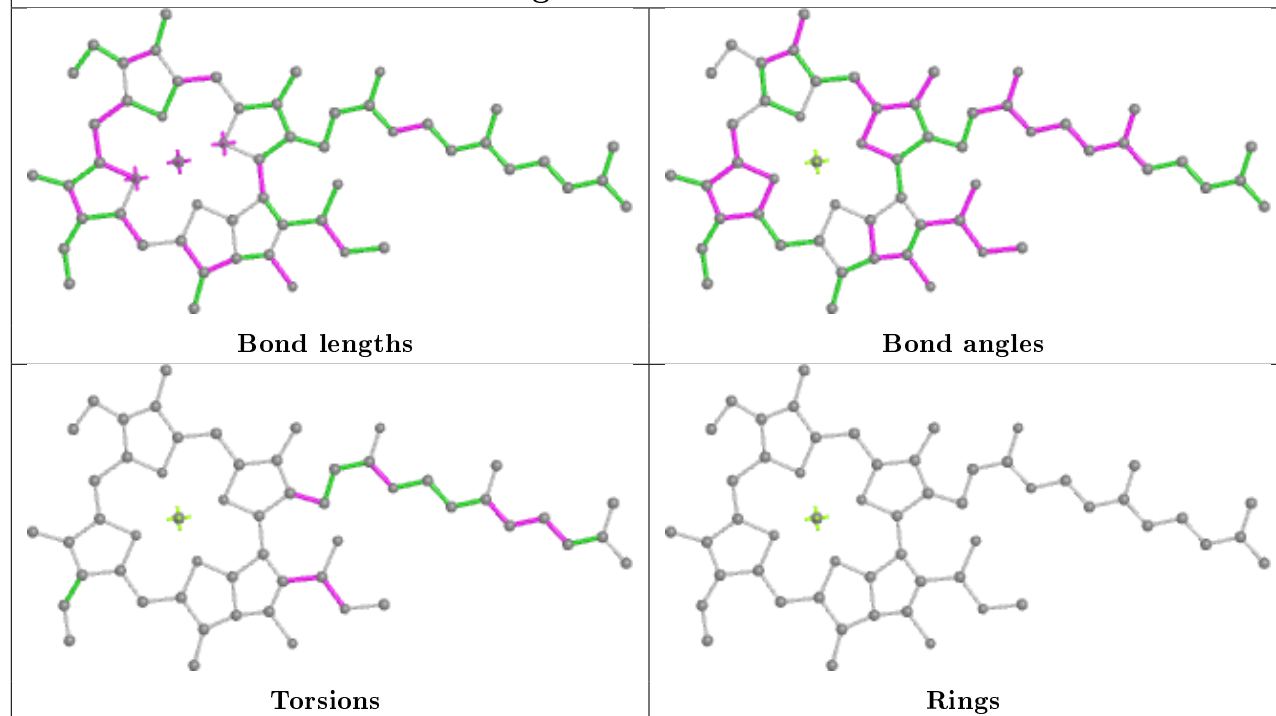


Ligand CLA Y 838

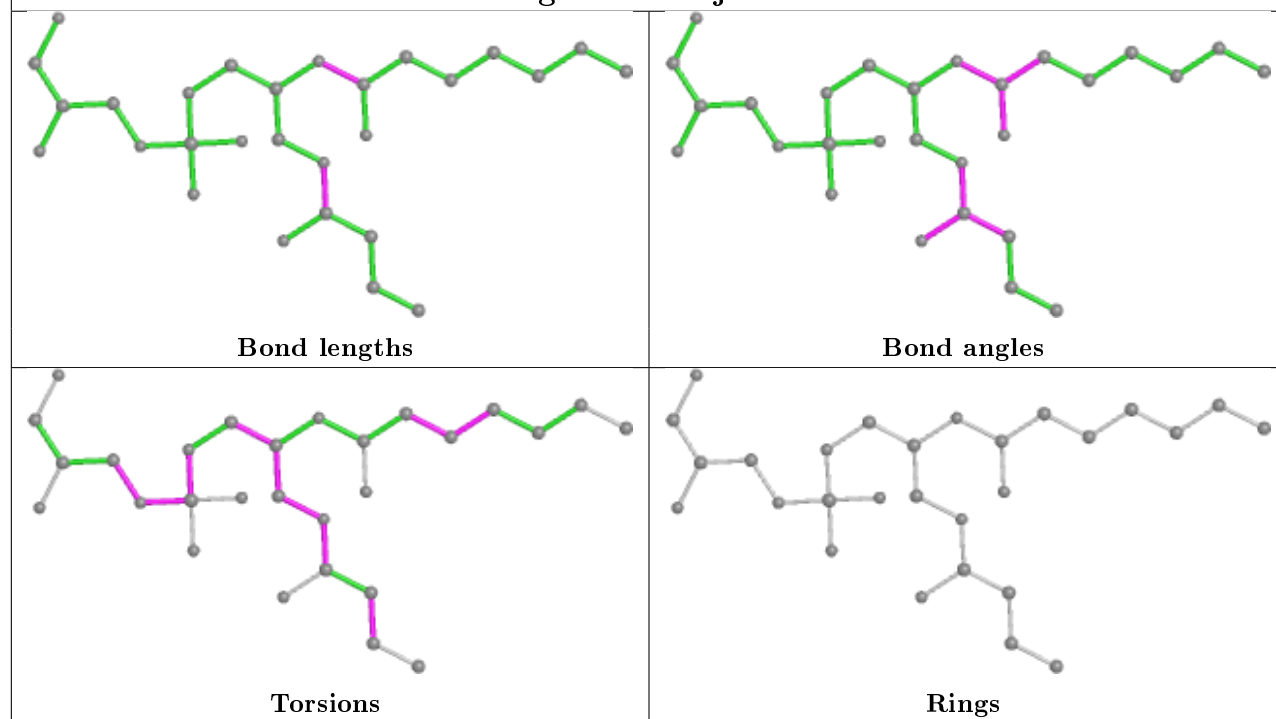


Ligand CLA H 815**Ligand CLA B 825**

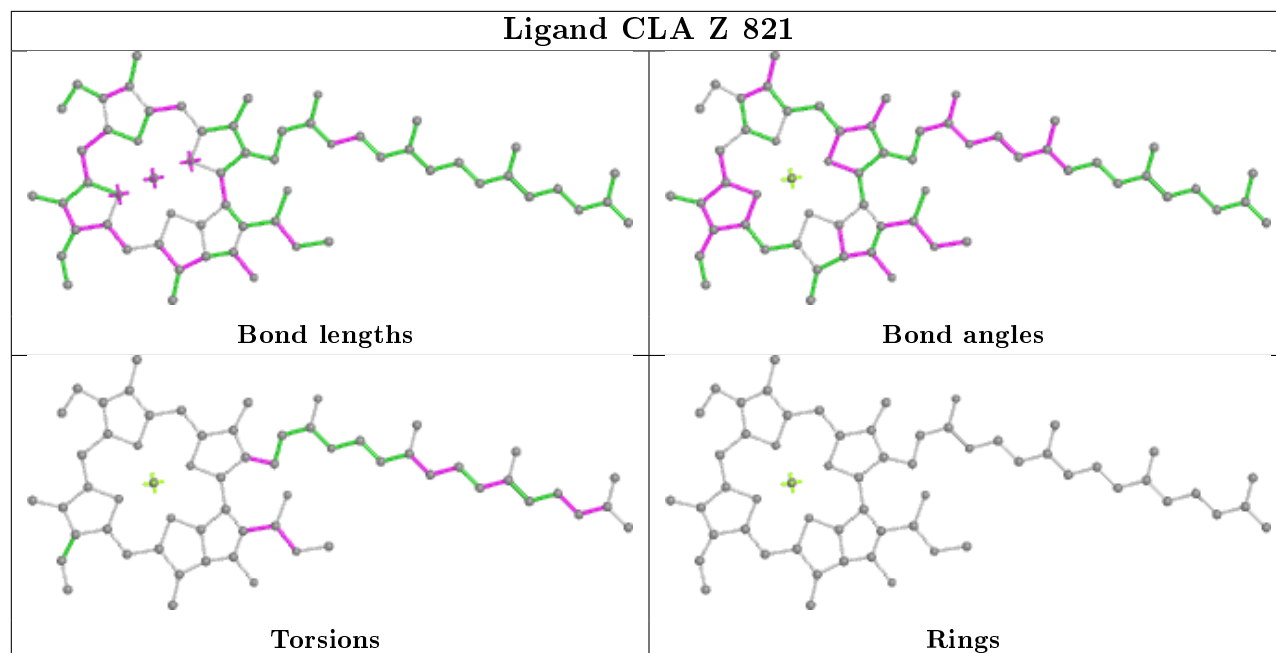
Ligand CLA Y 812



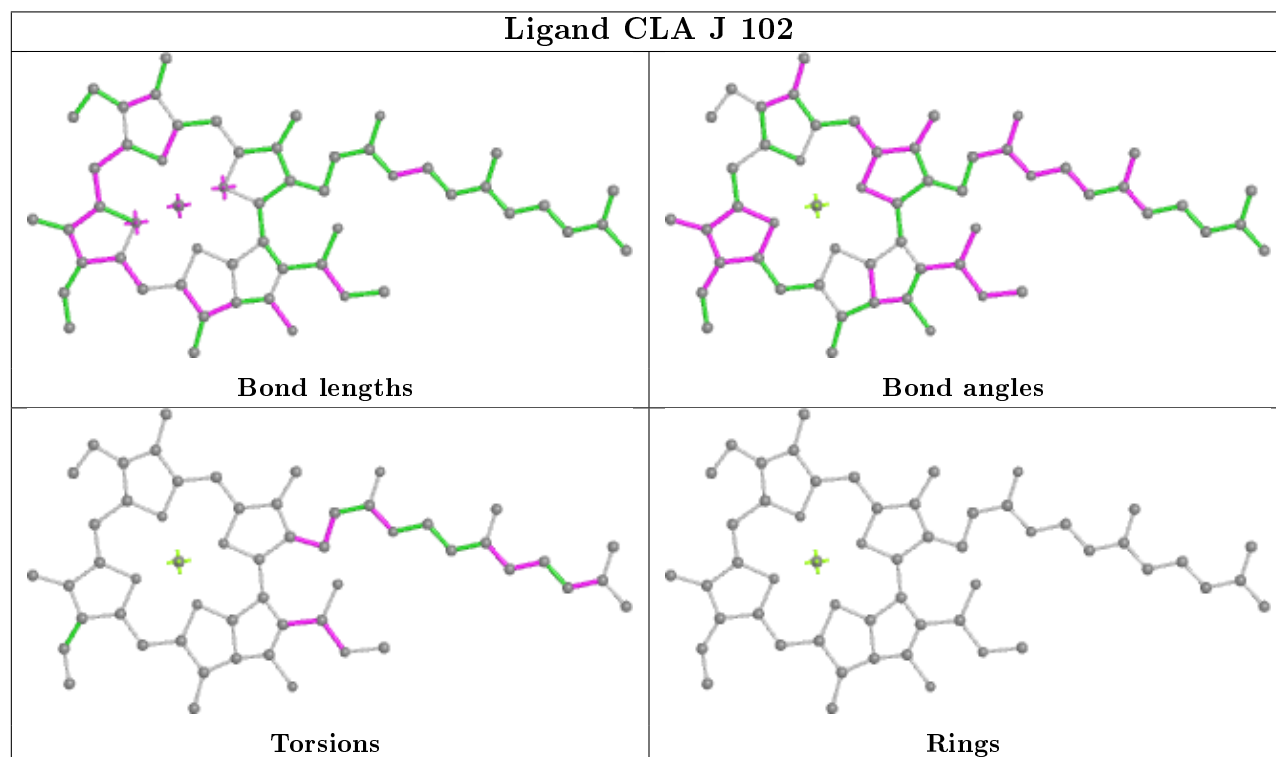
Ligand LHG j 101



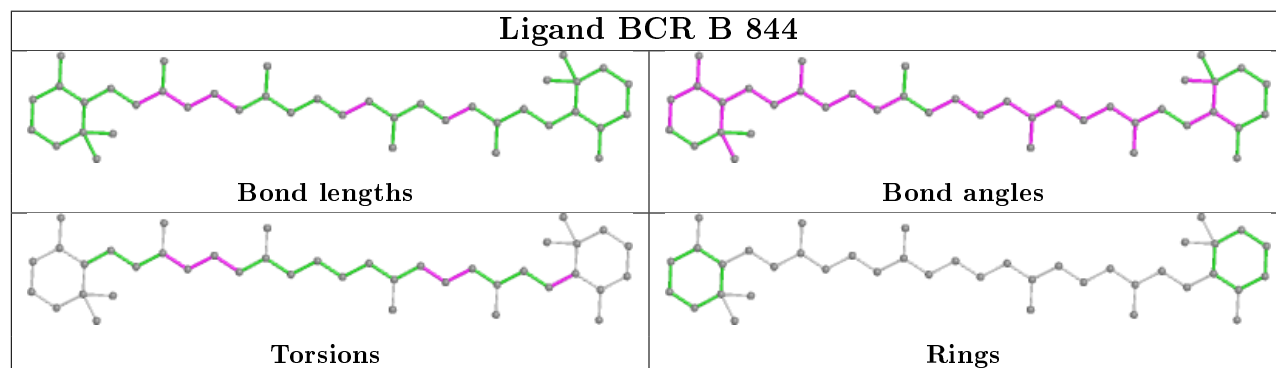
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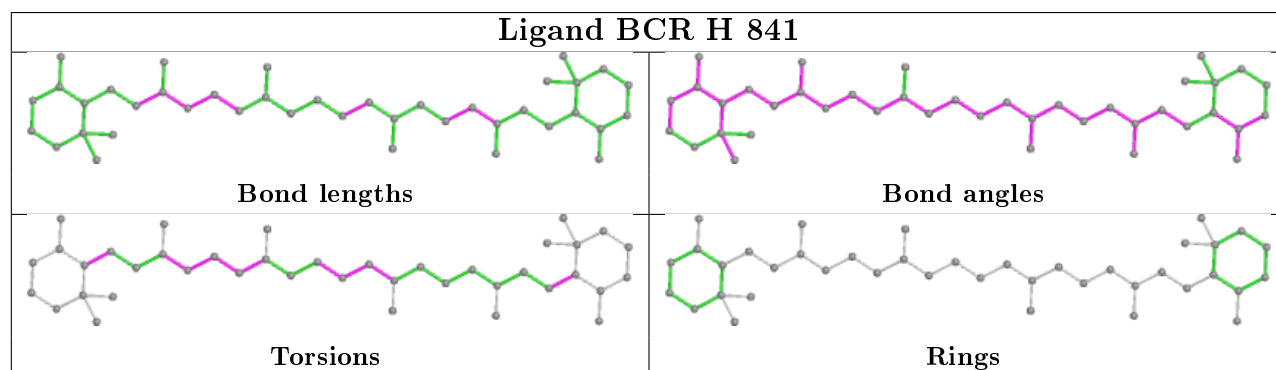
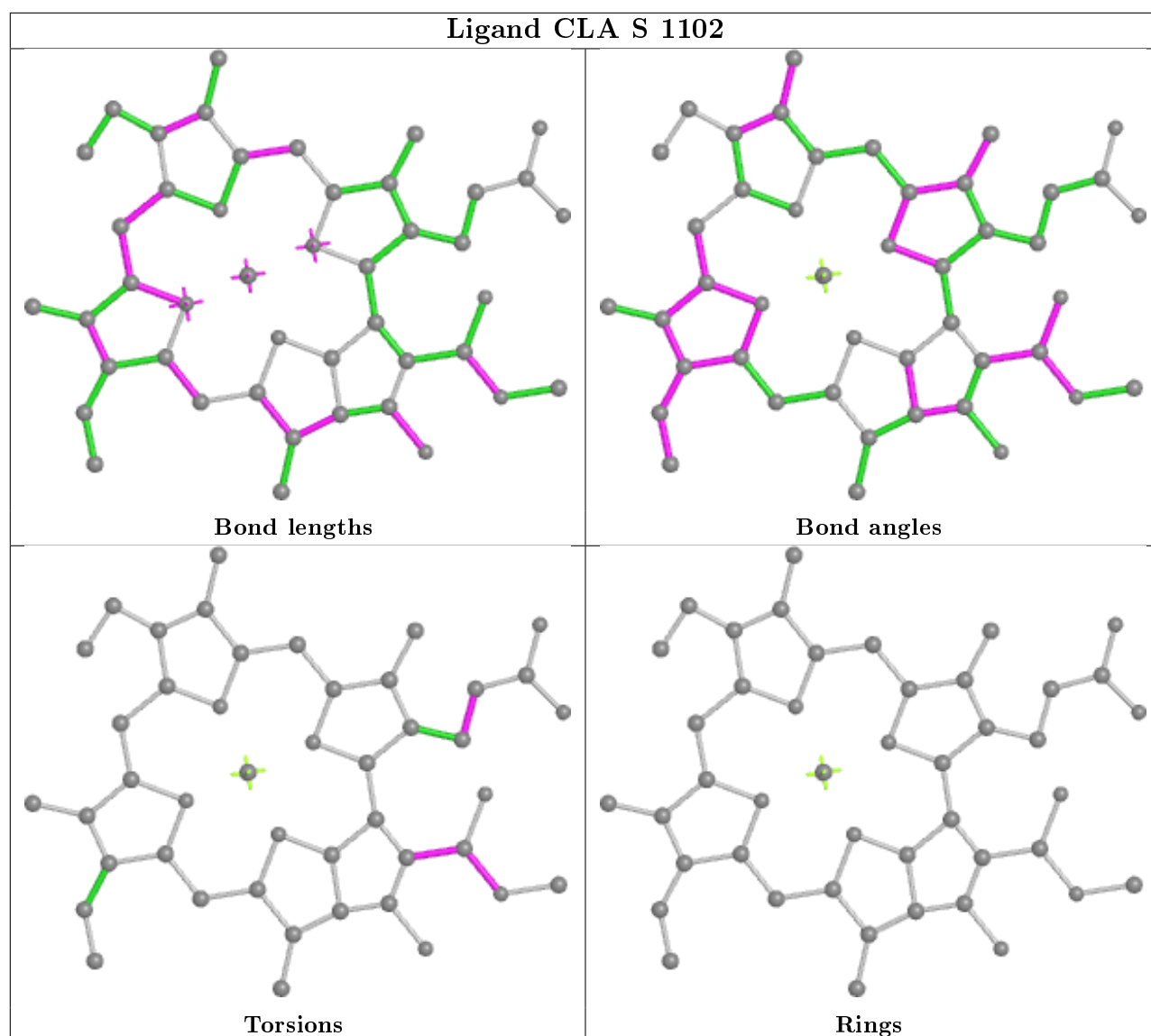


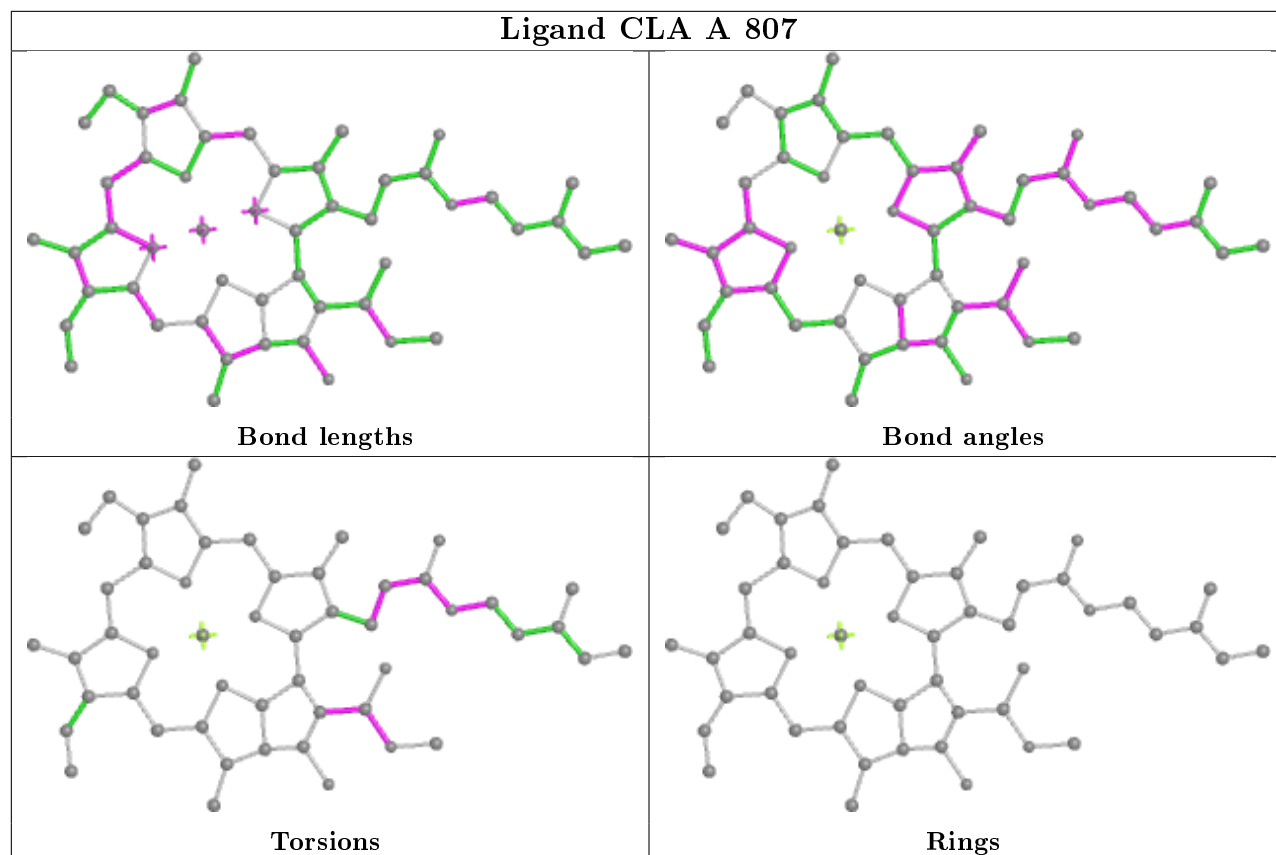
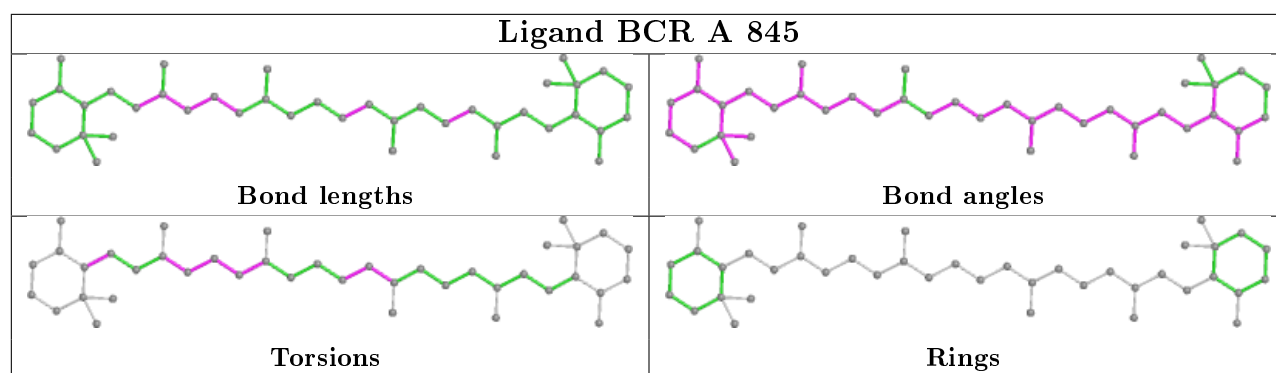
Ligand CLA J 102



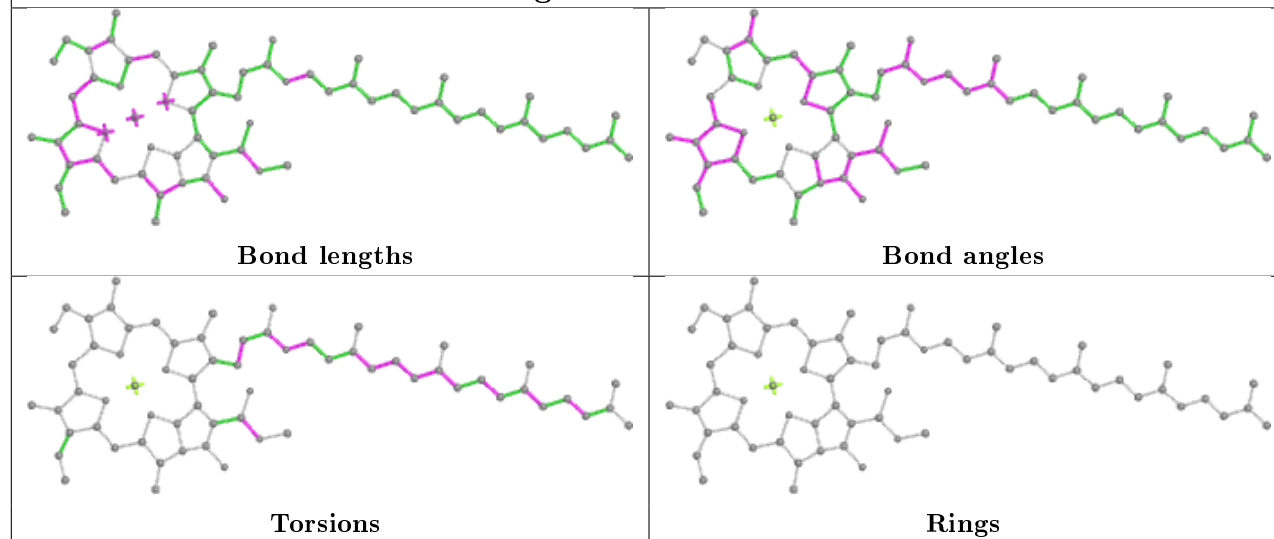
Ligand BCR B 844



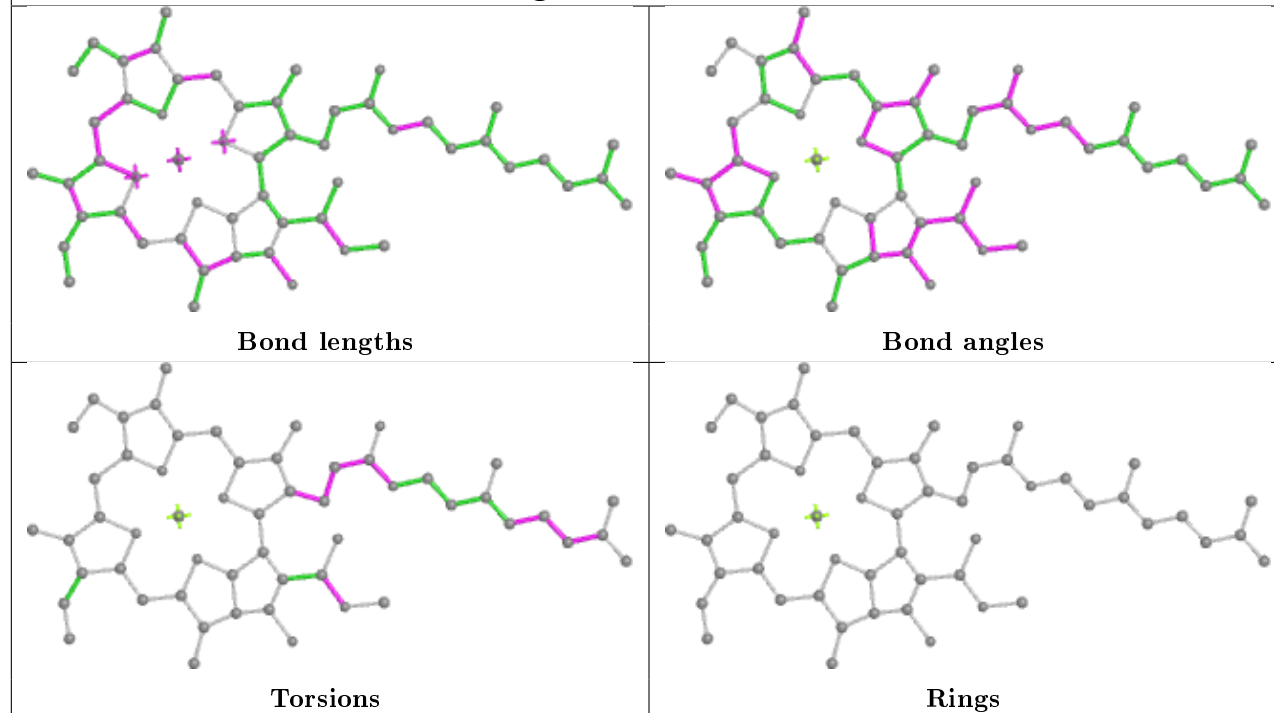


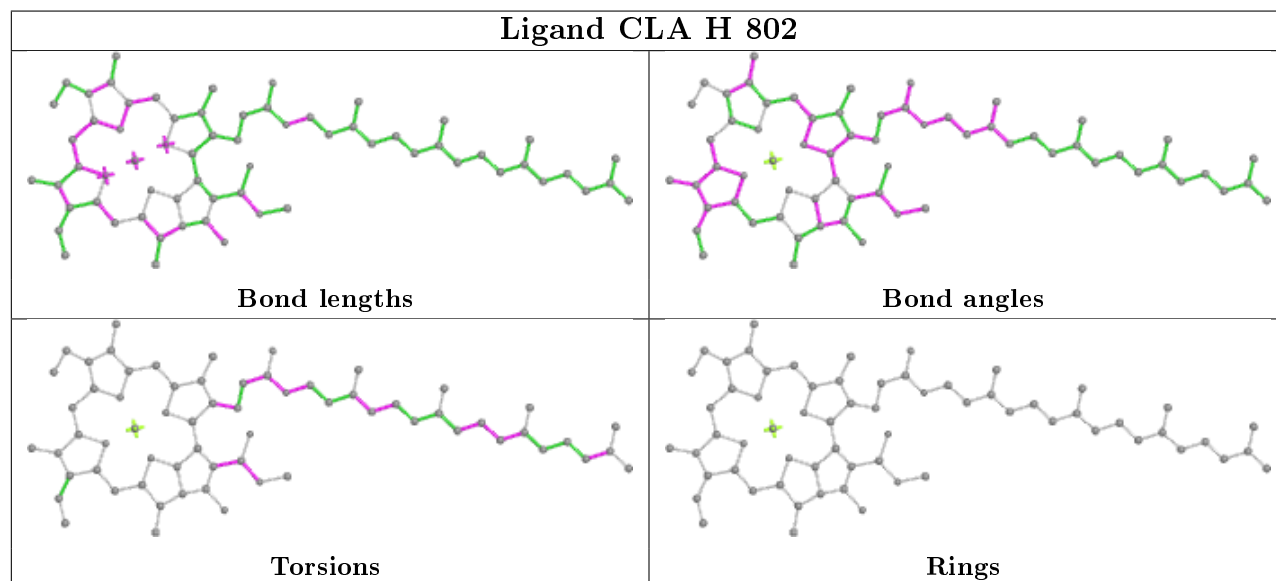
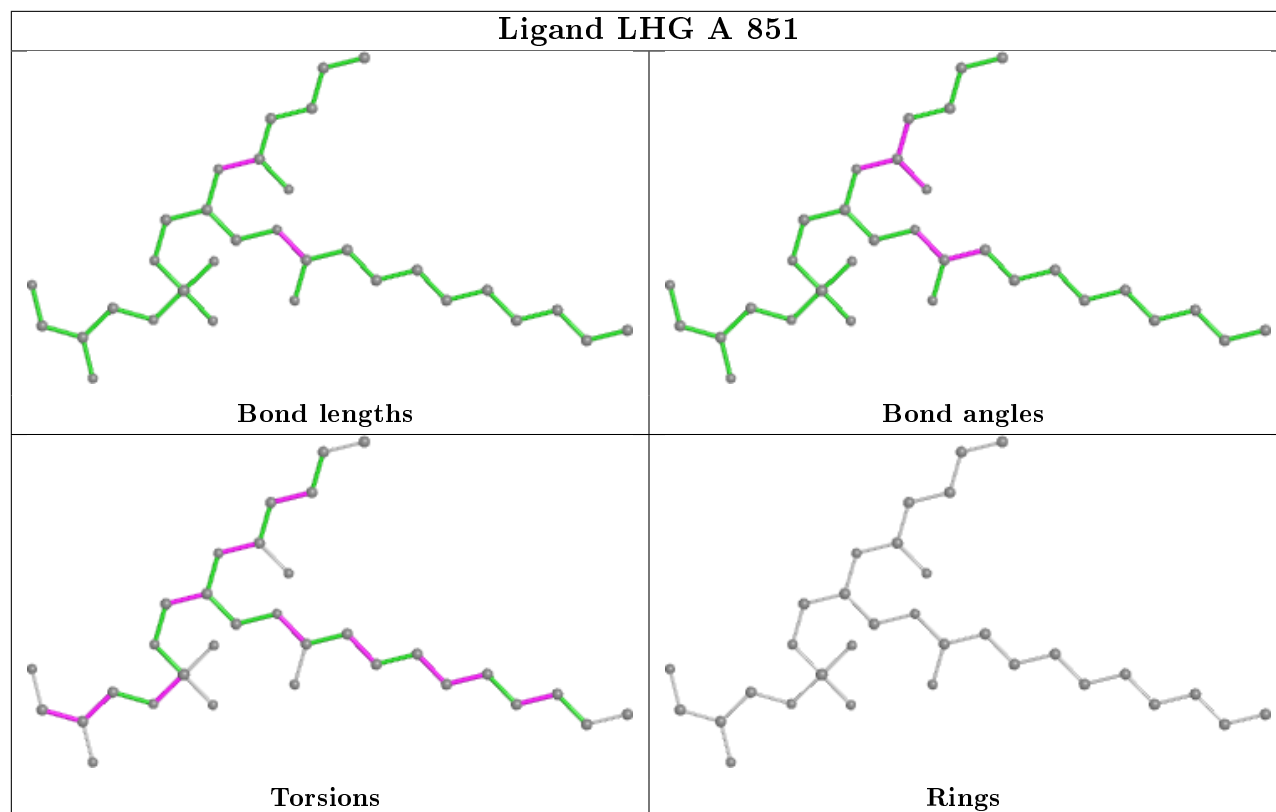


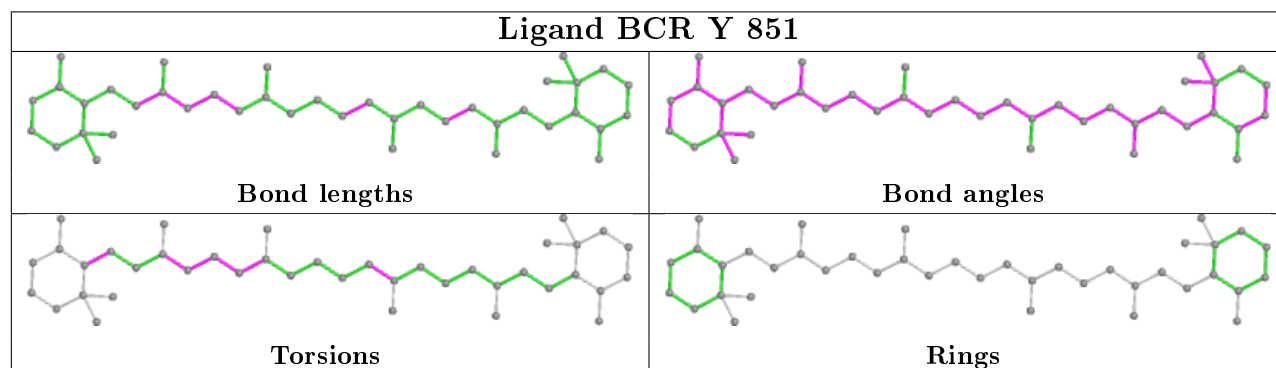
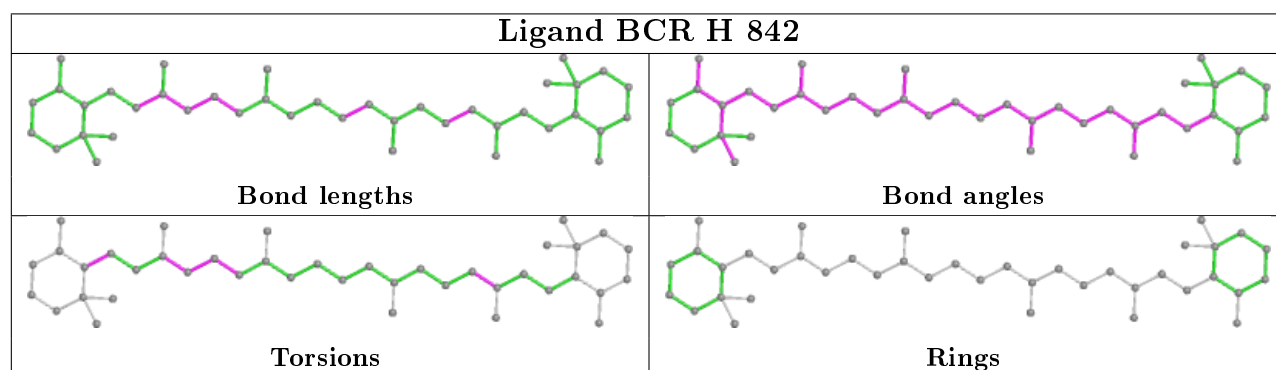
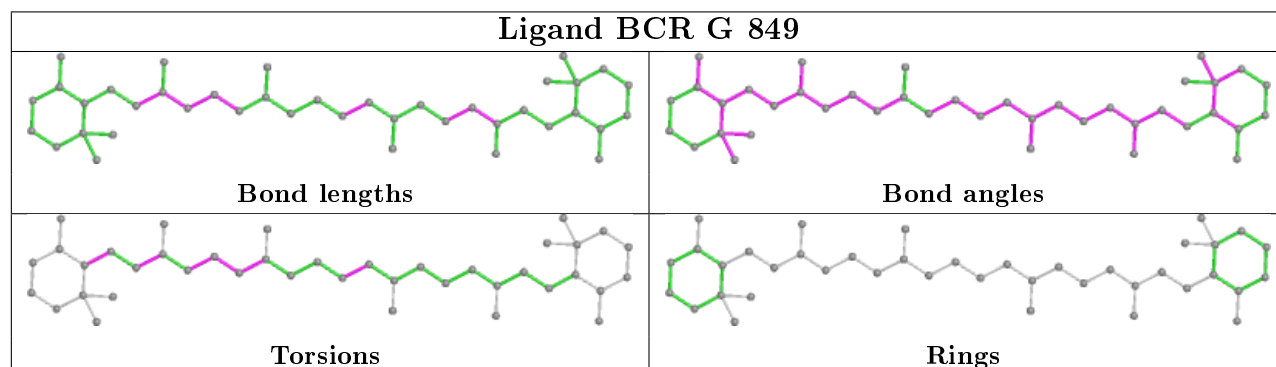
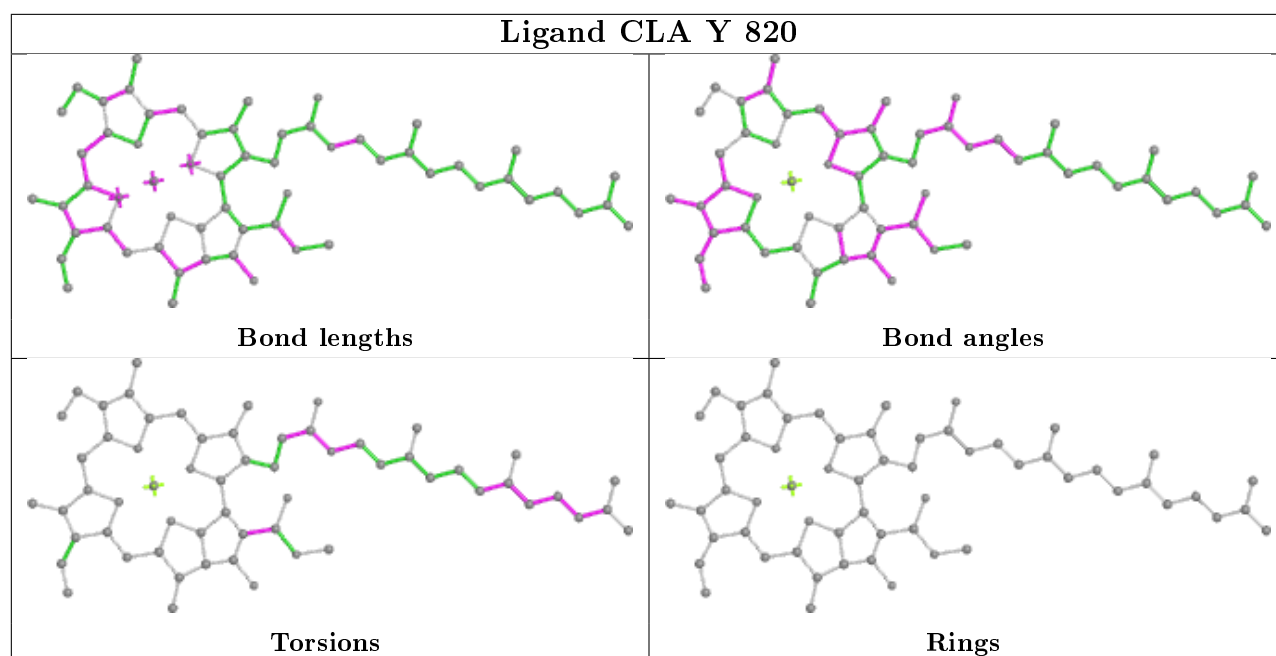
Ligand CLA Z 815



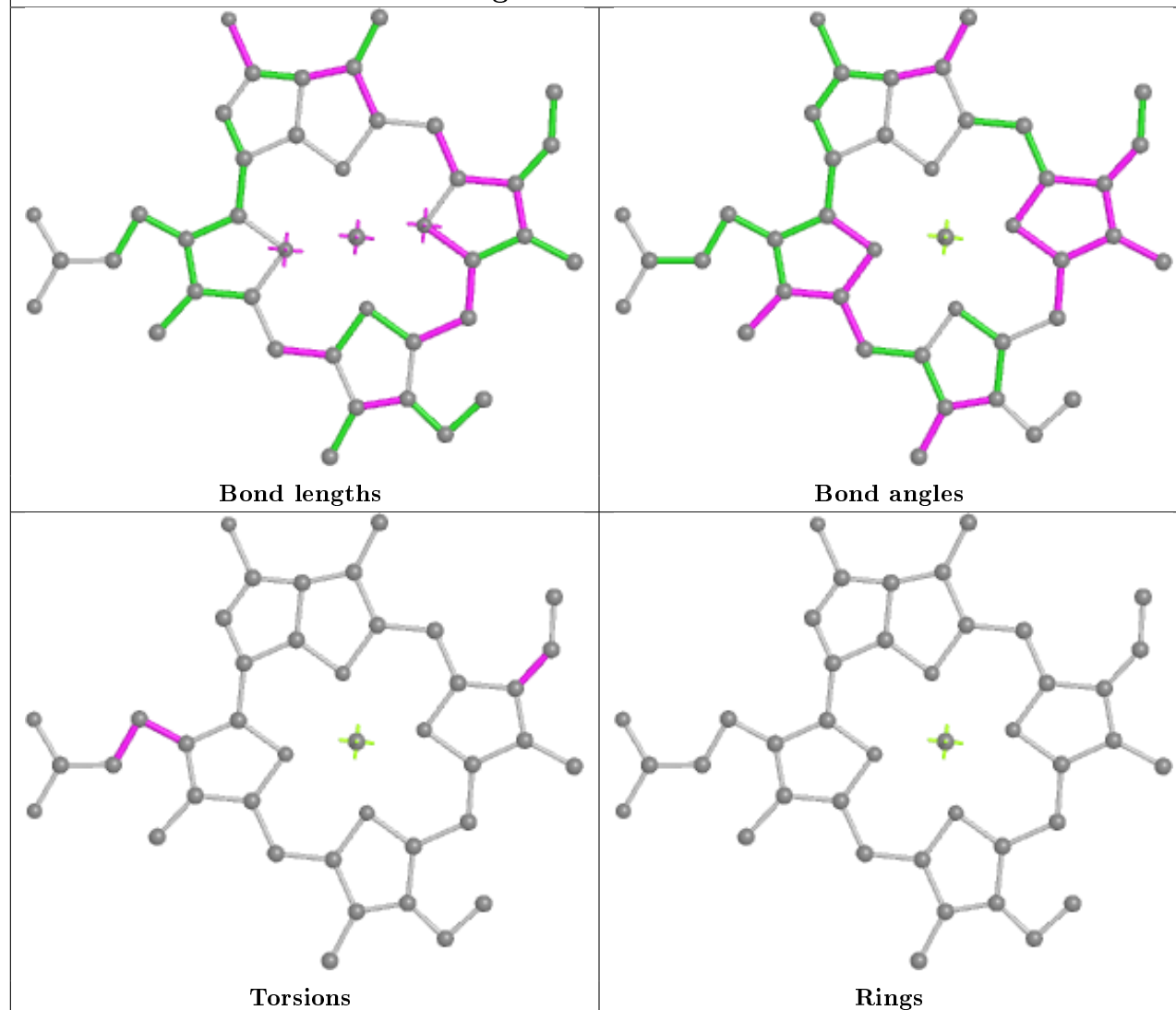
Ligand CLA H 810



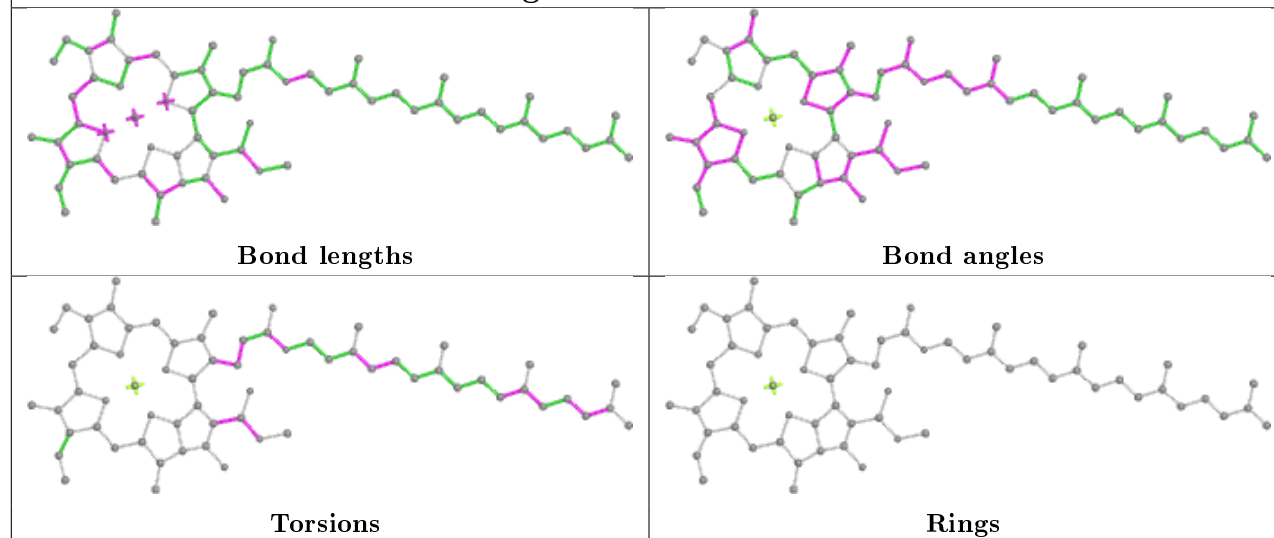




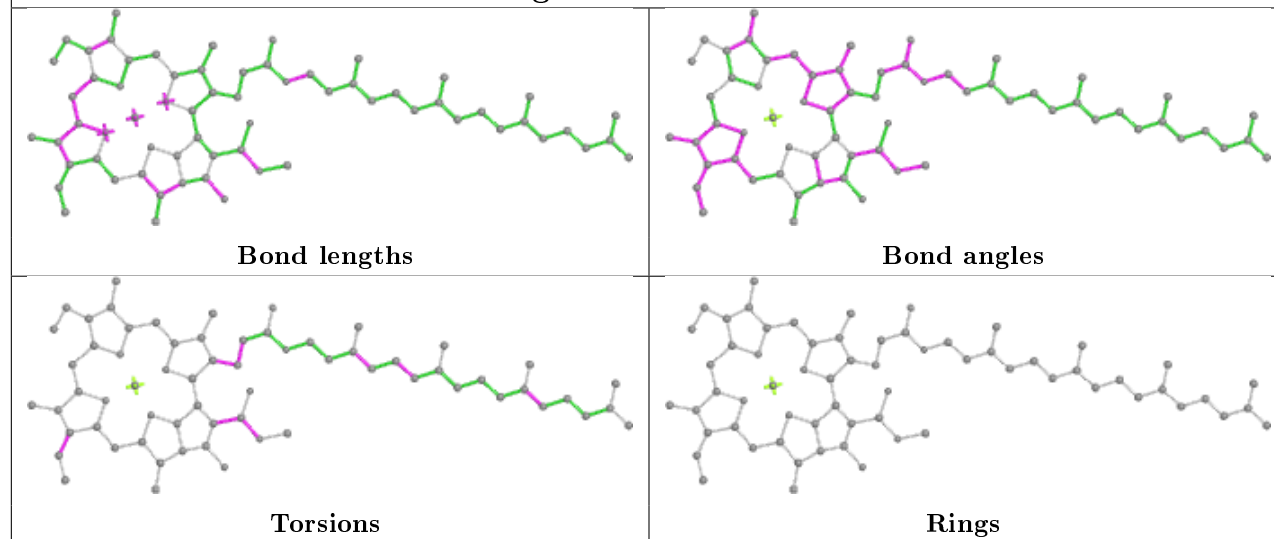
Ligand CLA T 101



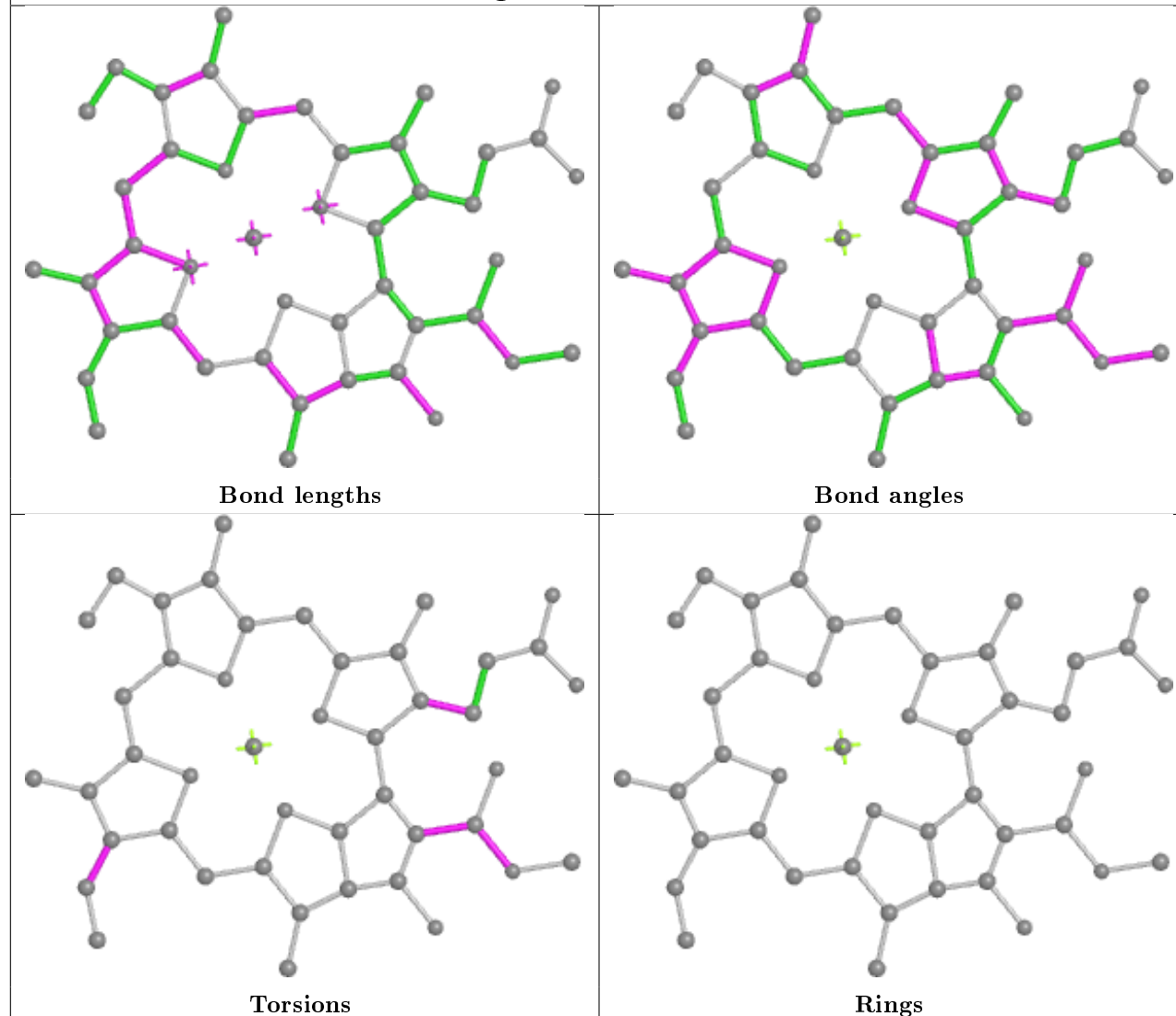
Ligand CLA U 1006



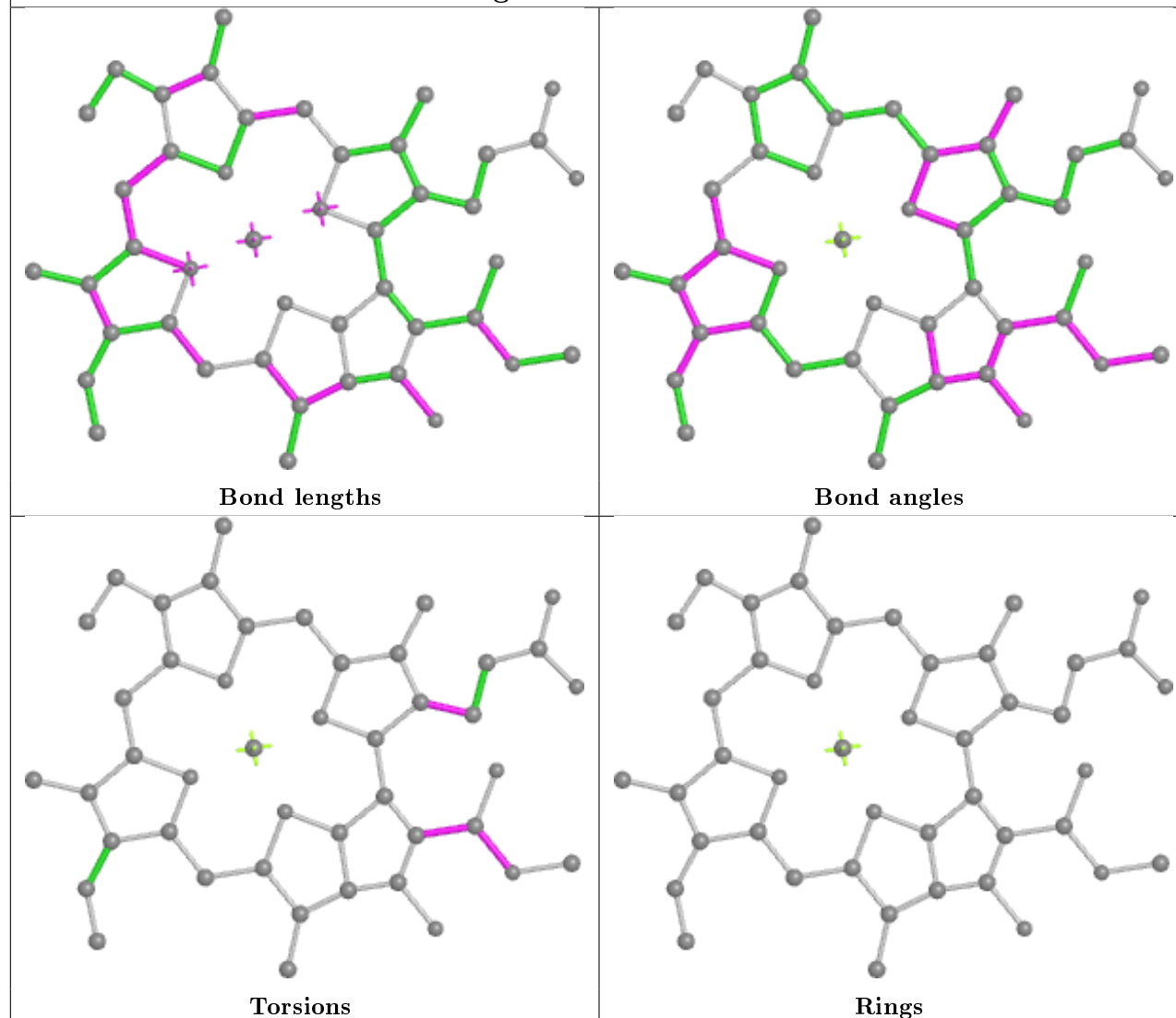
Ligand CLA Y 834



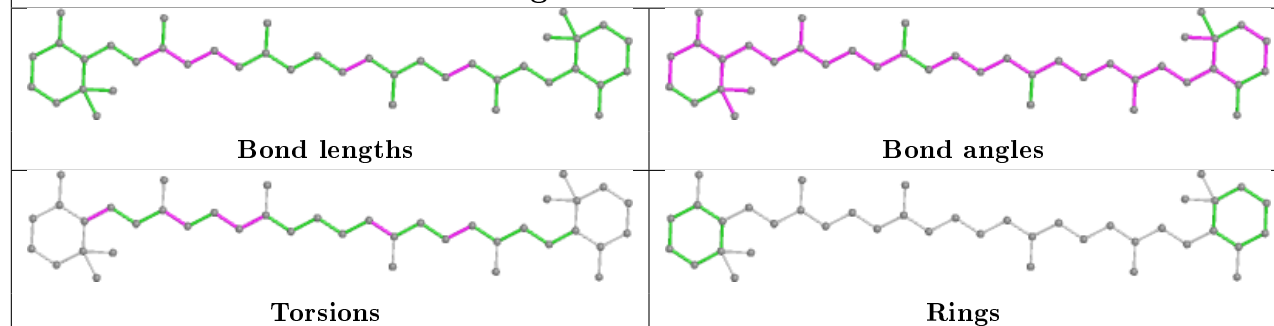
Ligand CLA Z 832

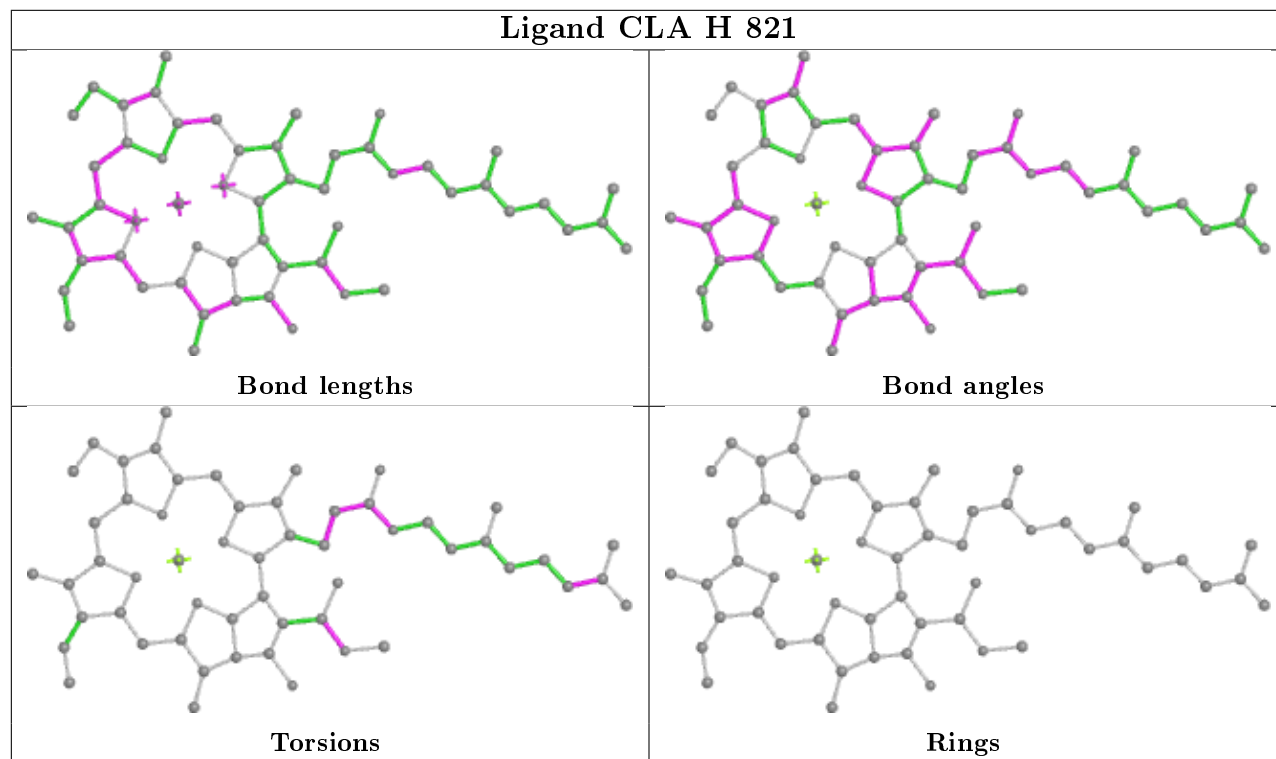
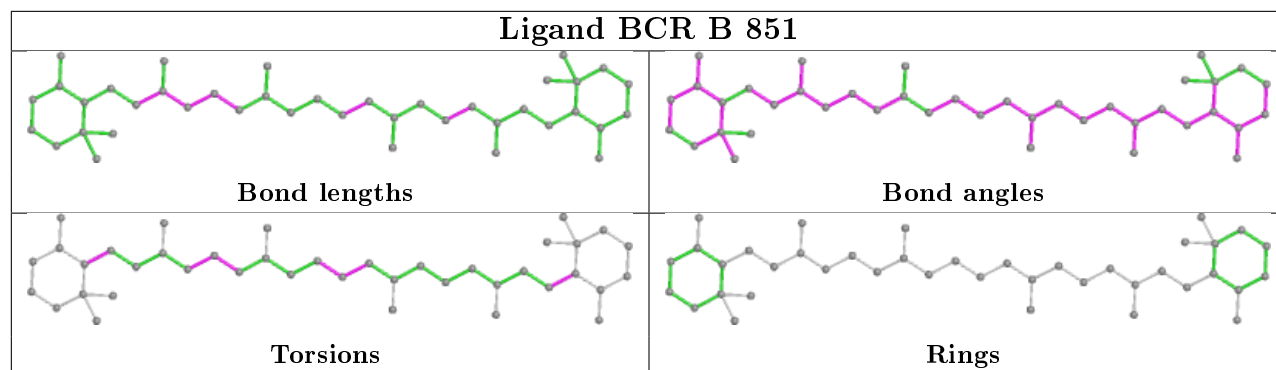
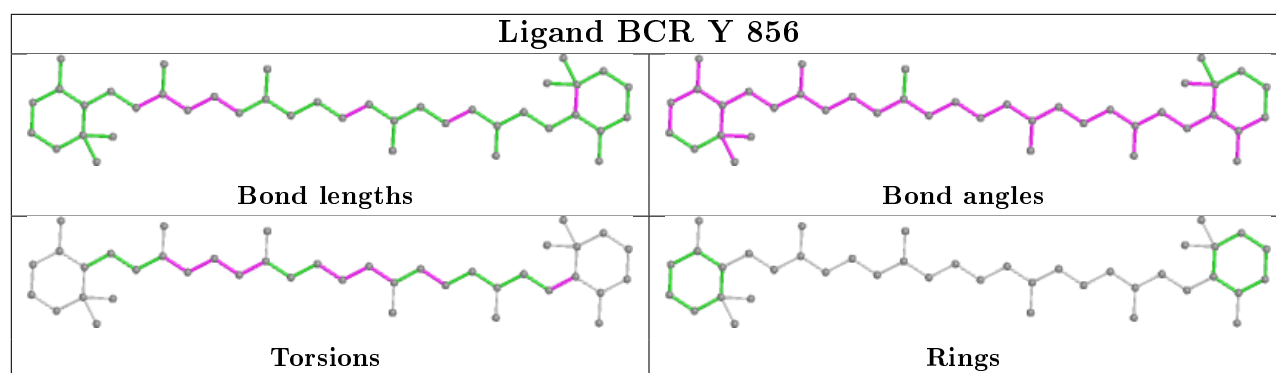


Ligand CLA Z 833

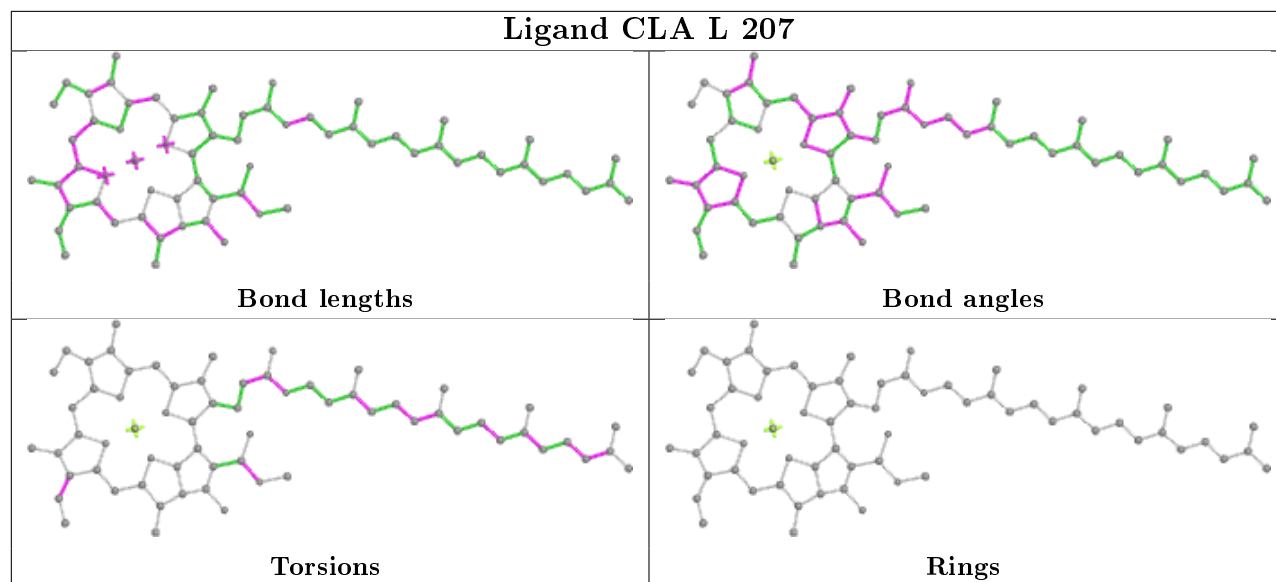


Ligand BCR A 849

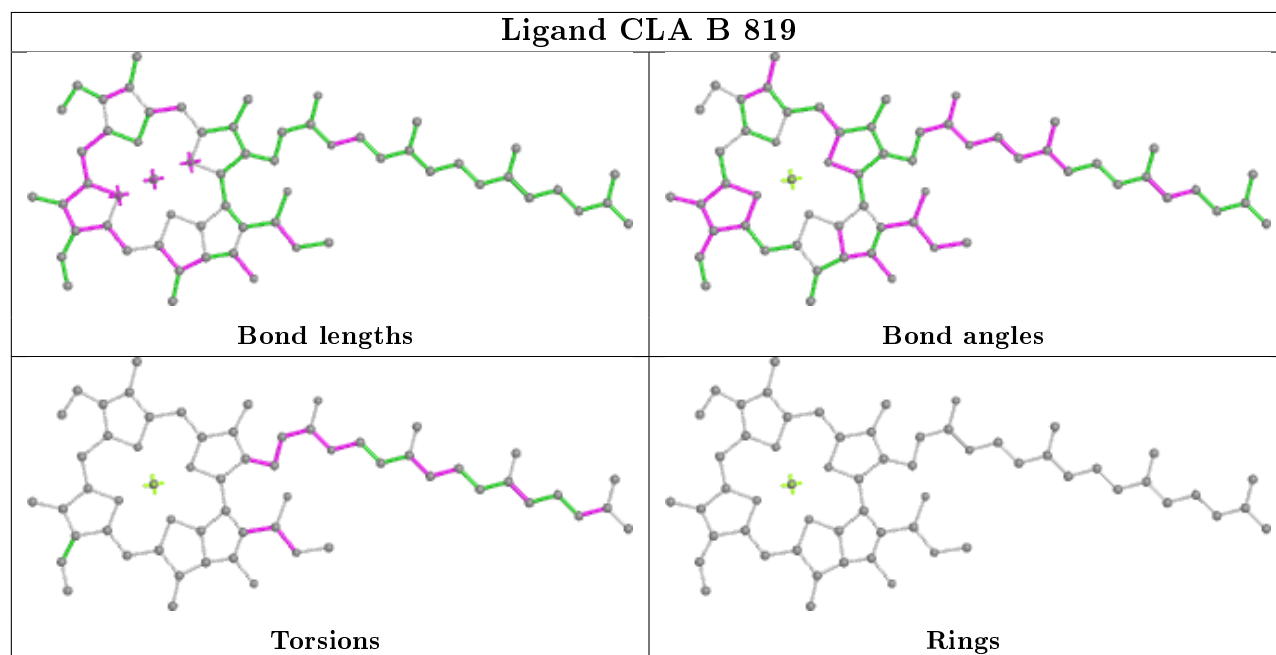




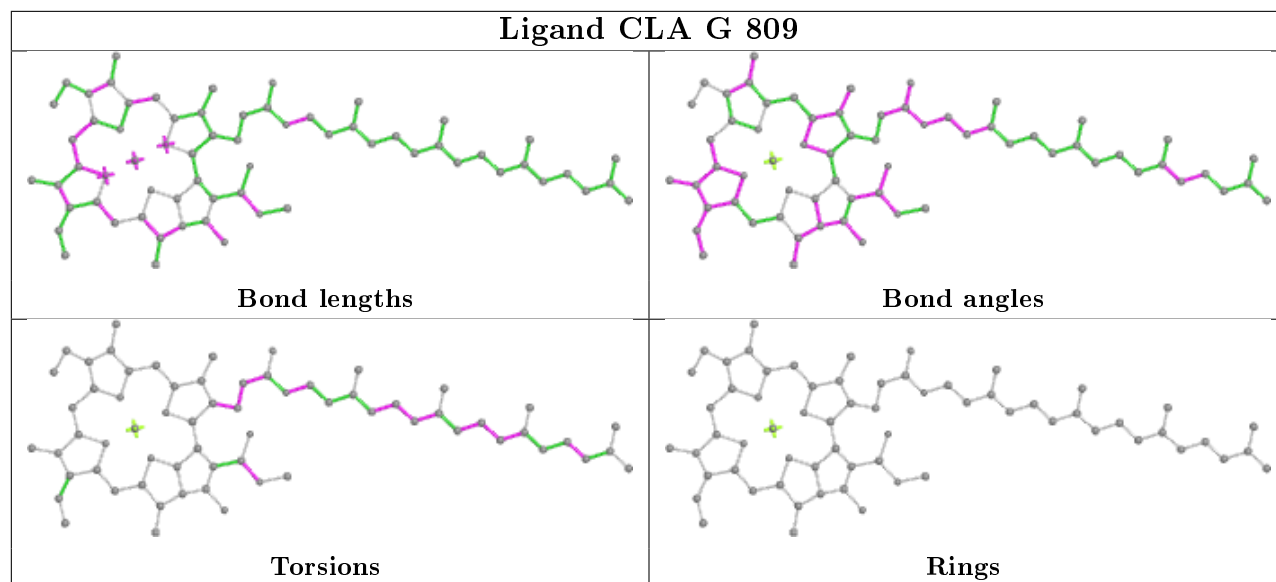
Ligand CLA L 207



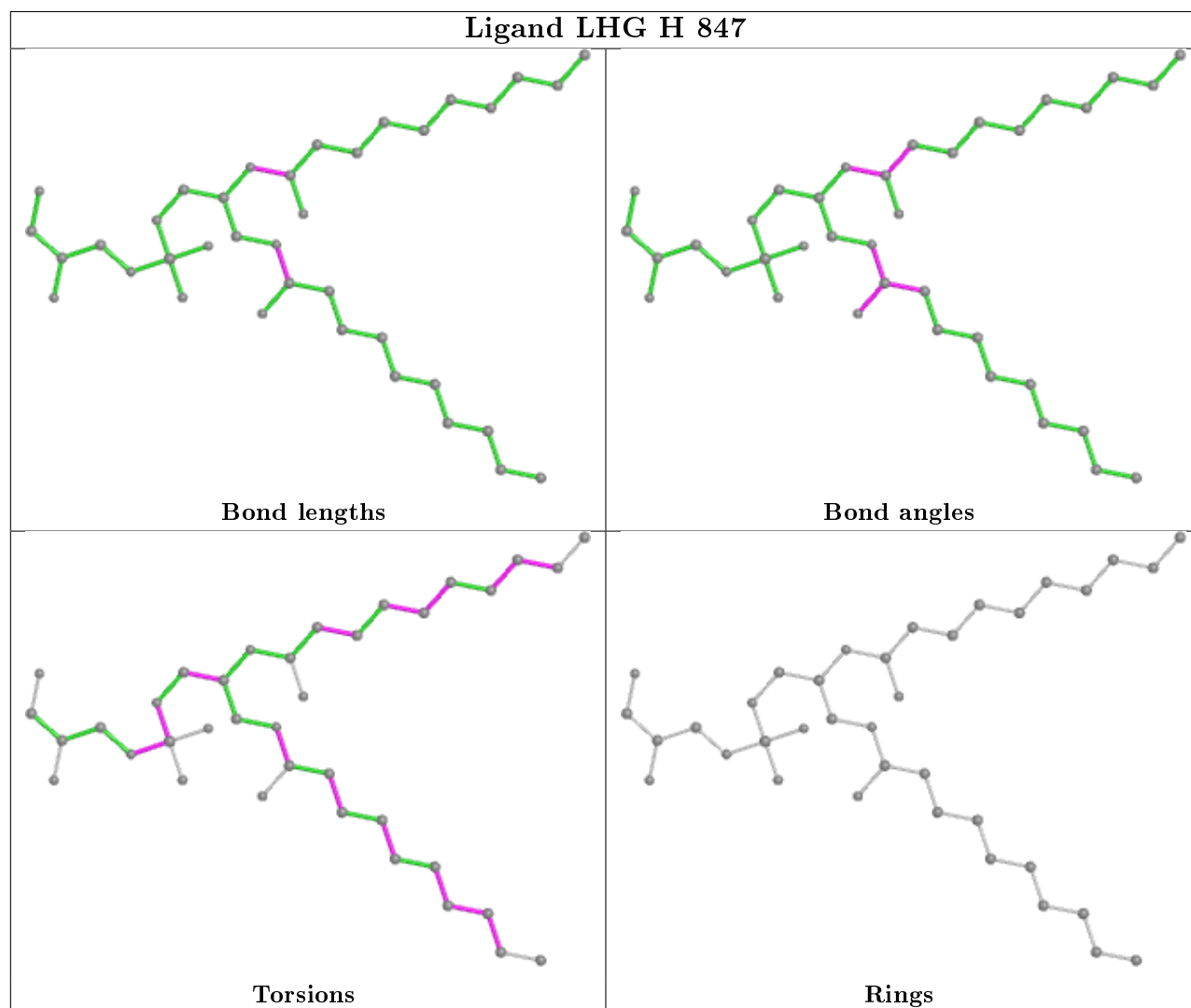
Ligand CLA B 819

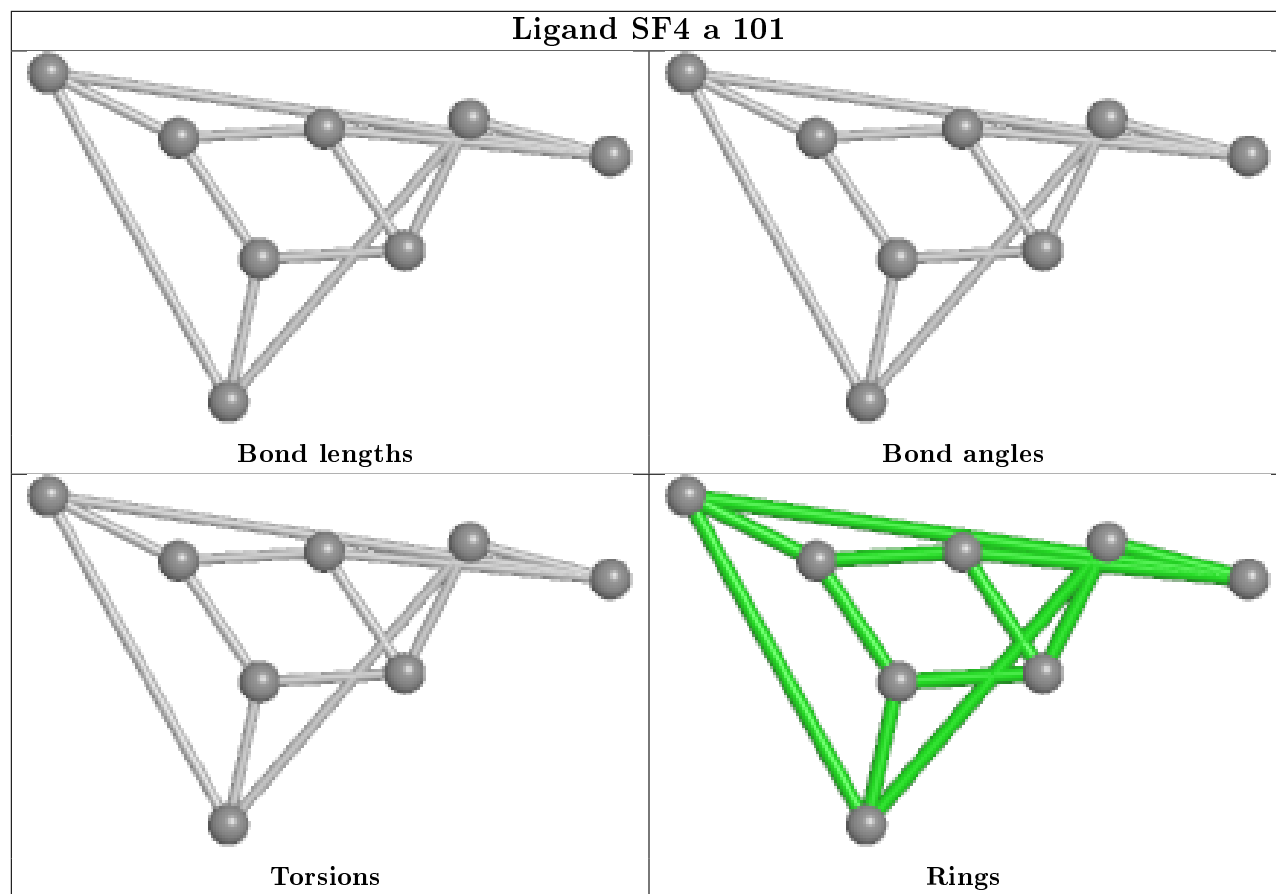
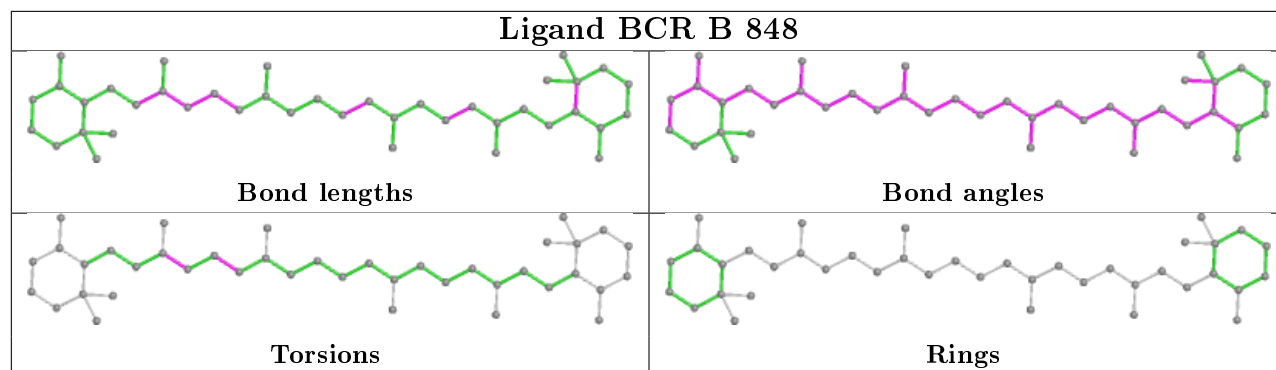


Ligand CLA G 809

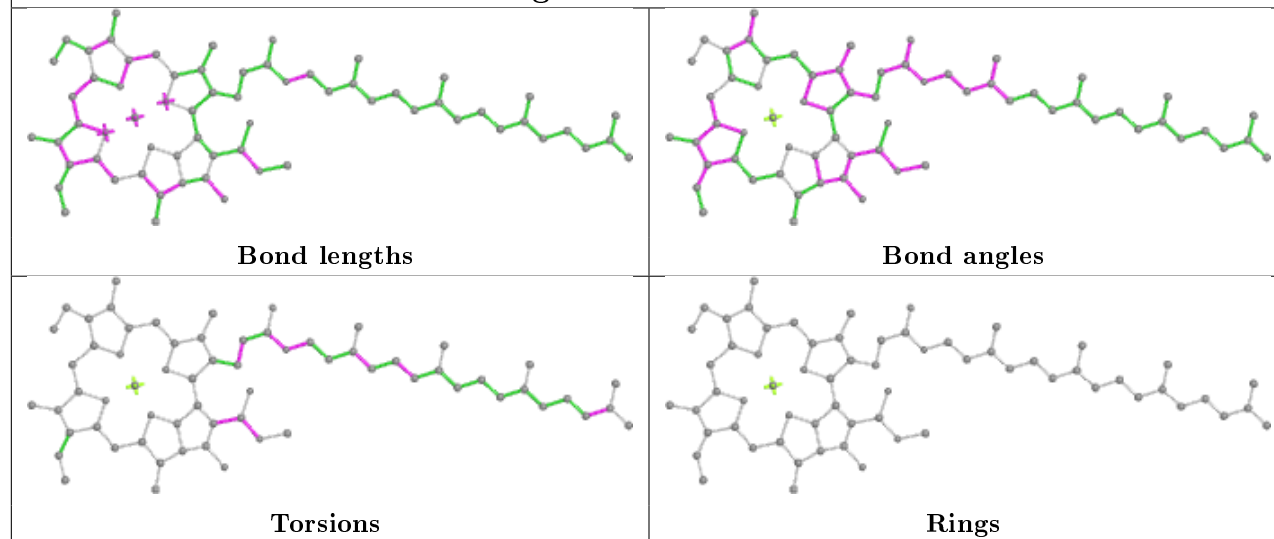


Ligand LHG H 847

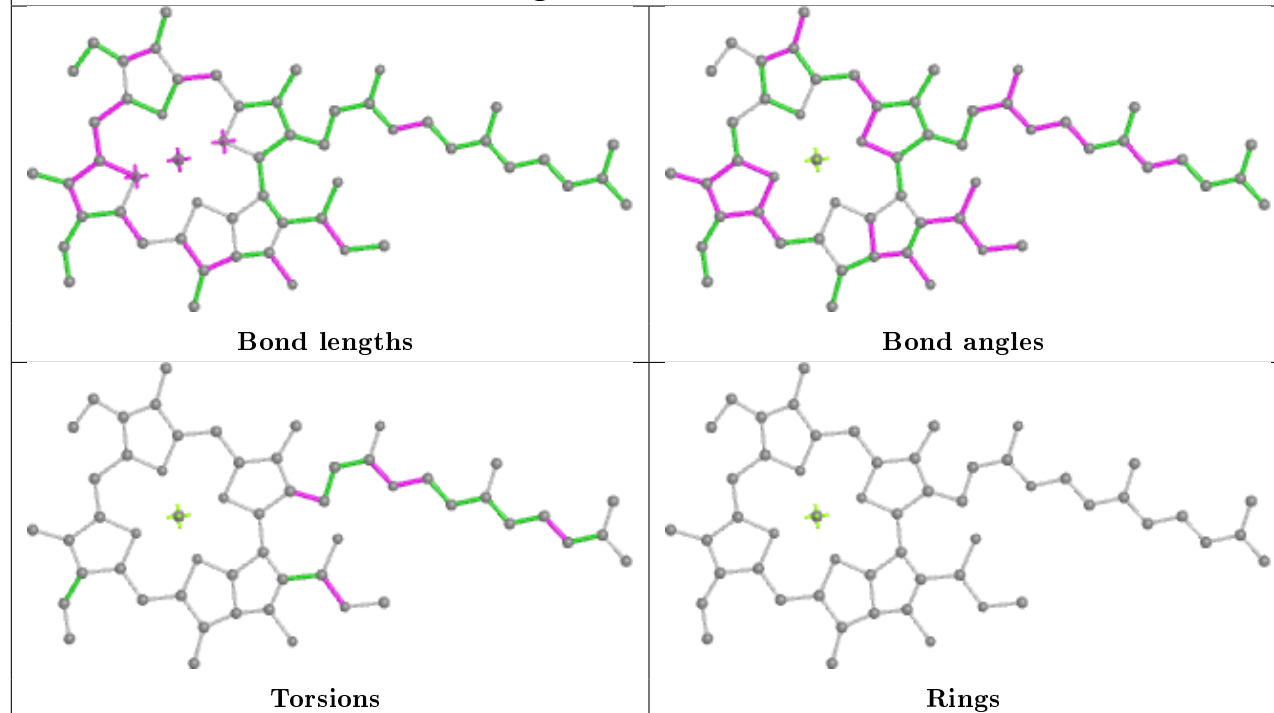


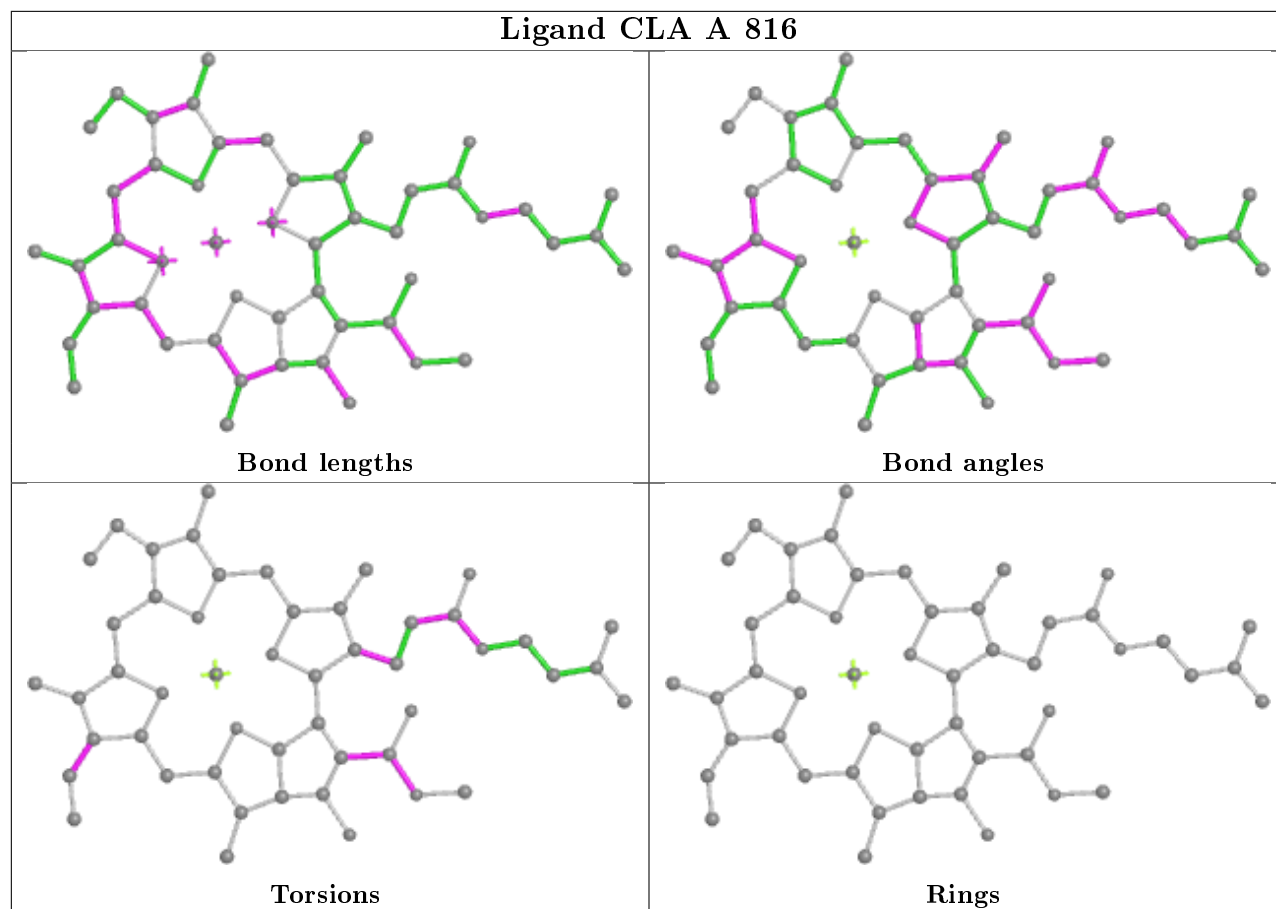


Ligand CLA A 841

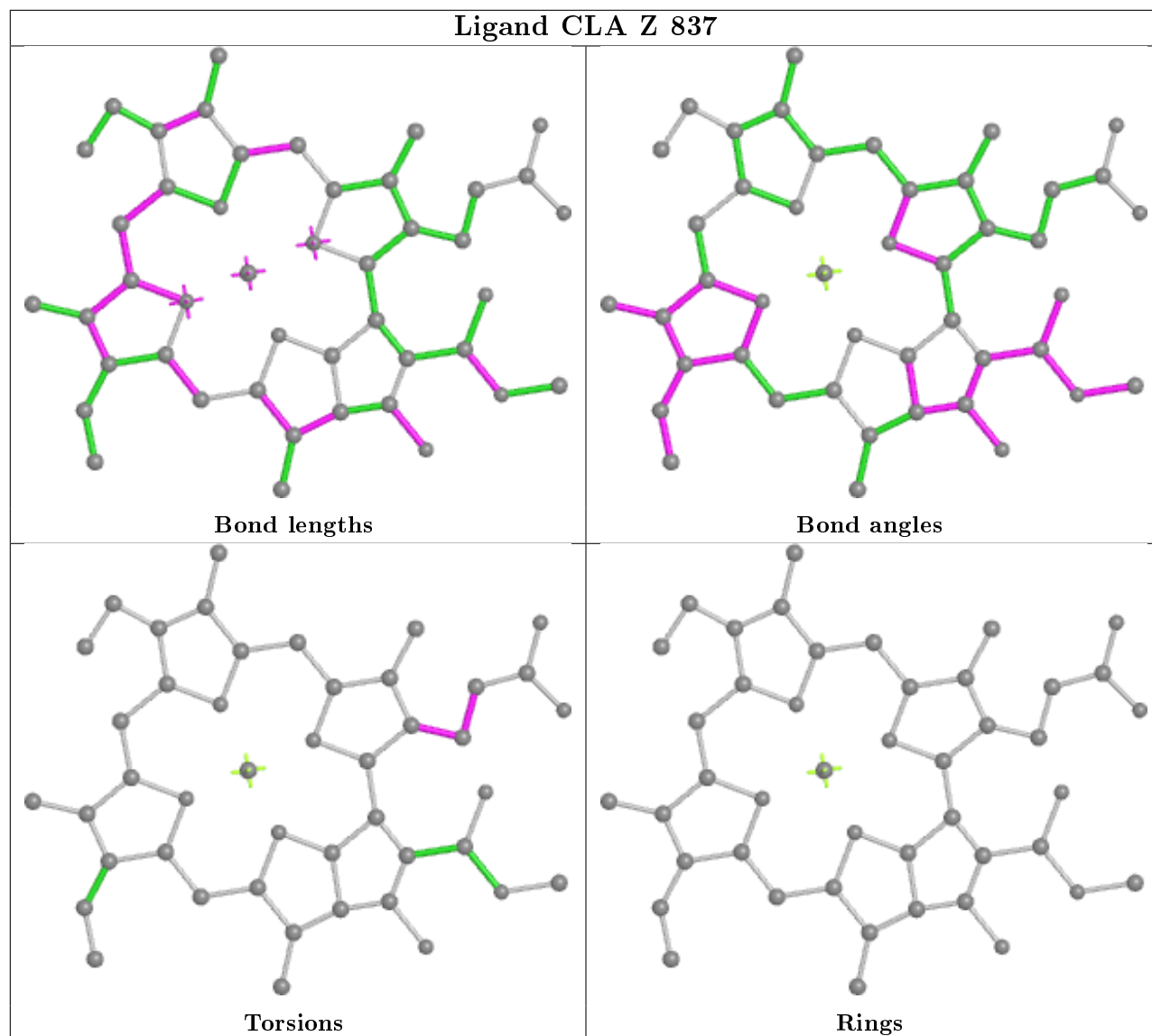


Ligand CLA G 834

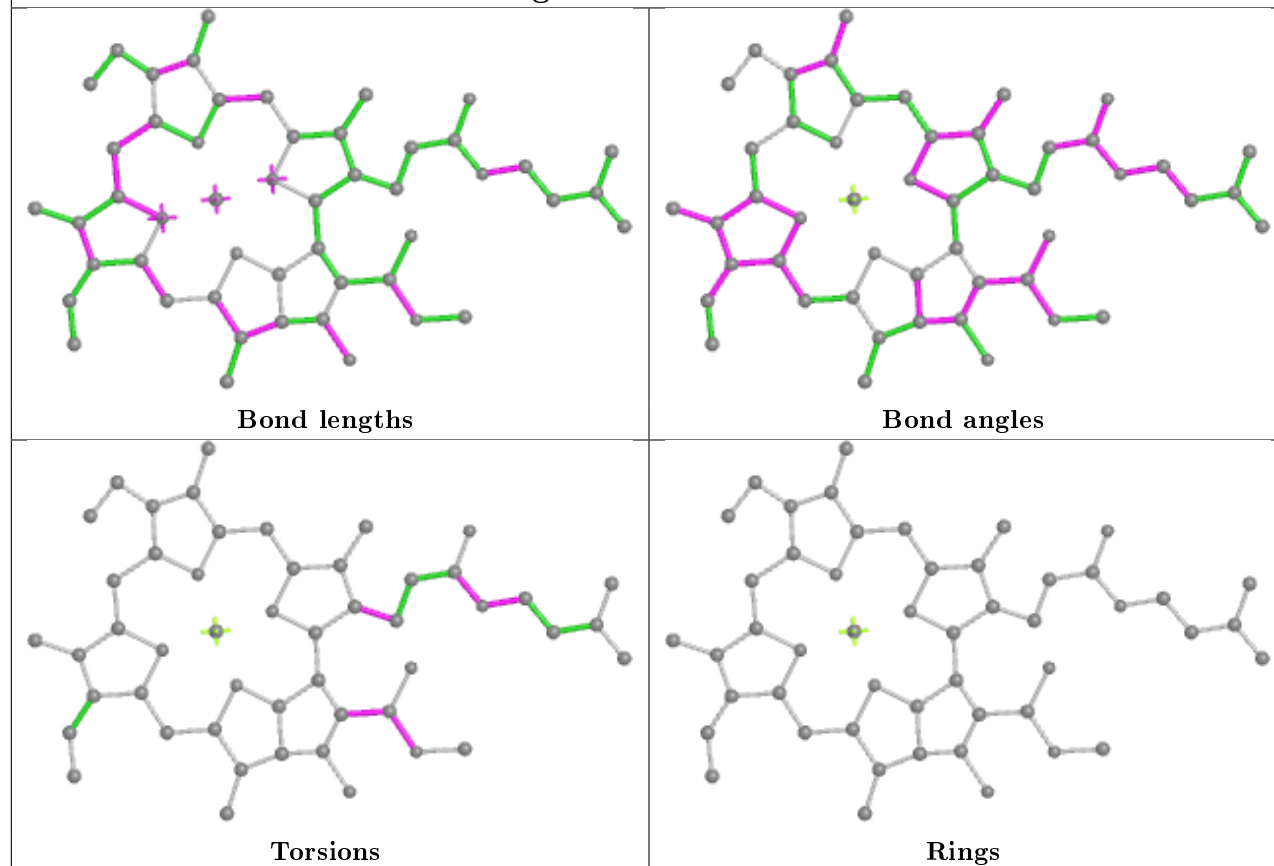




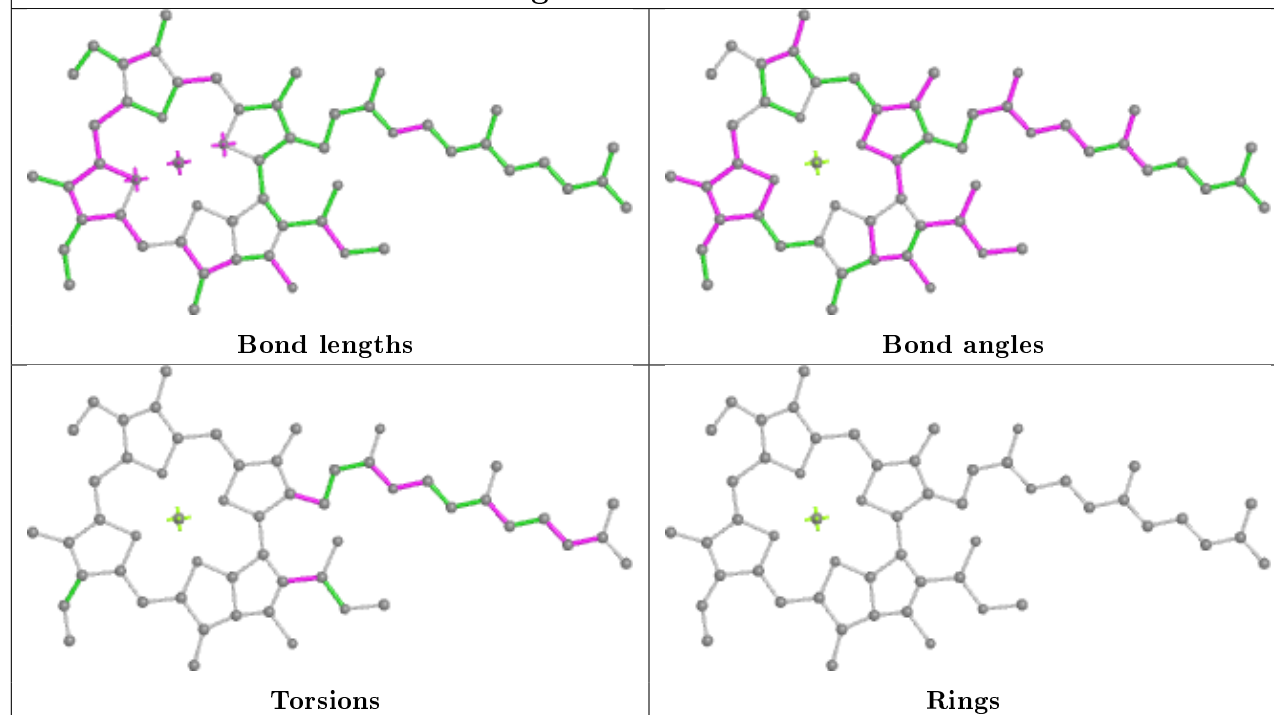
Ligand CLA Z 837

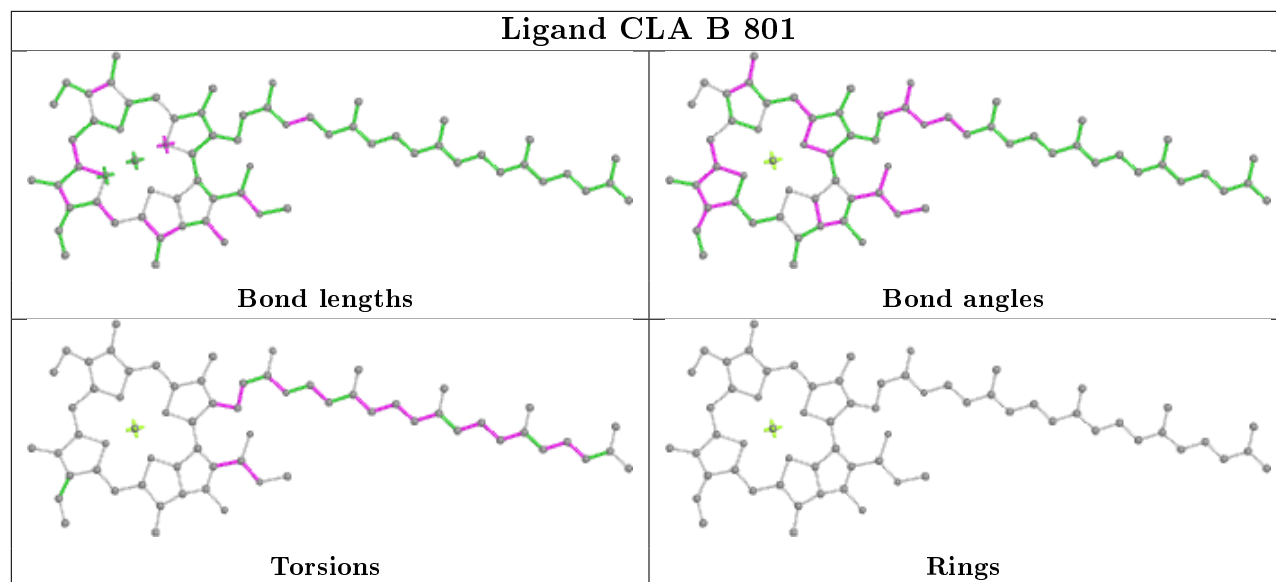
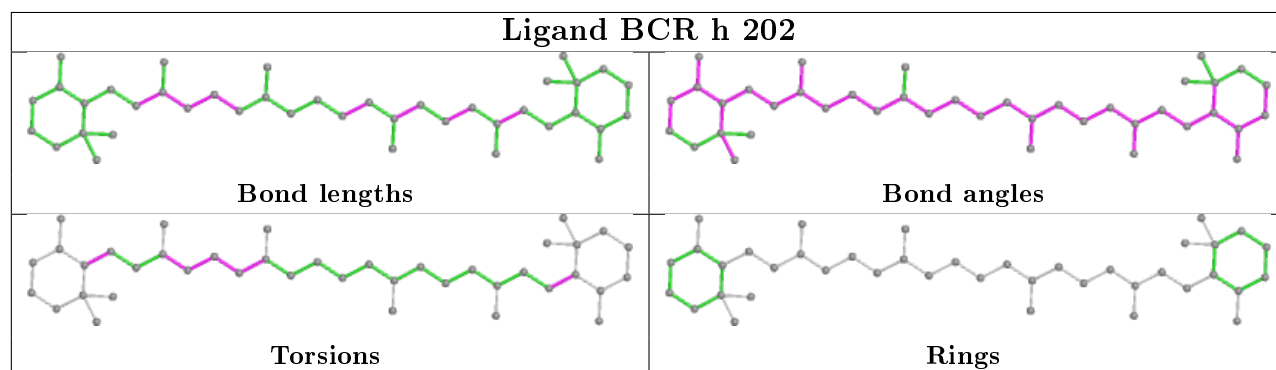
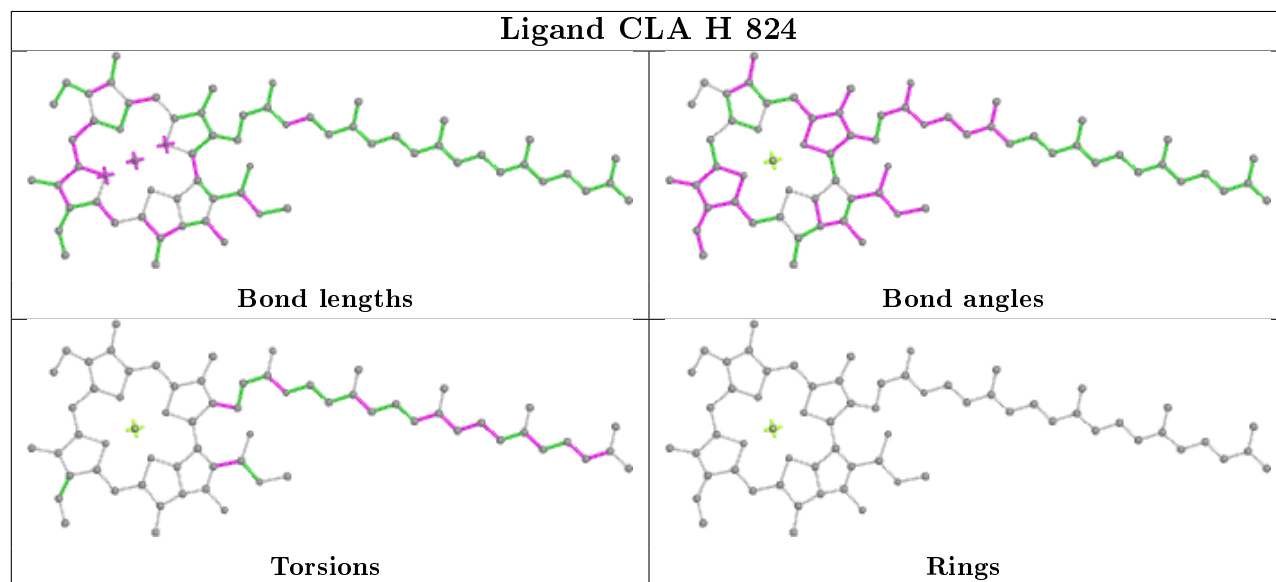


Ligand CLA A 815

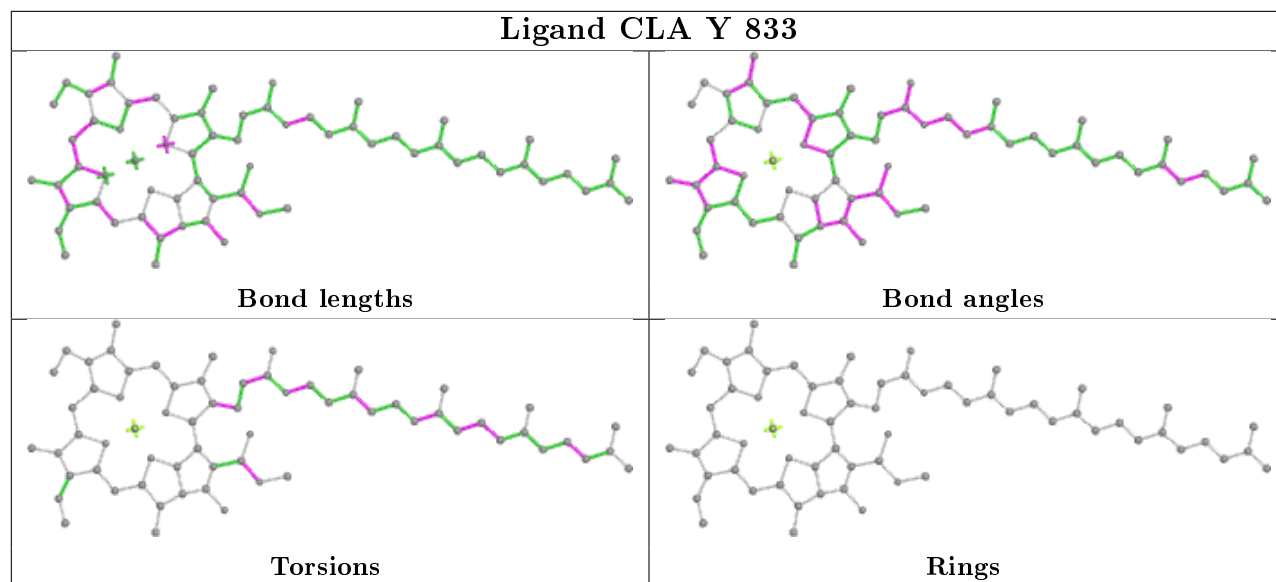


Ligand CLA H 823

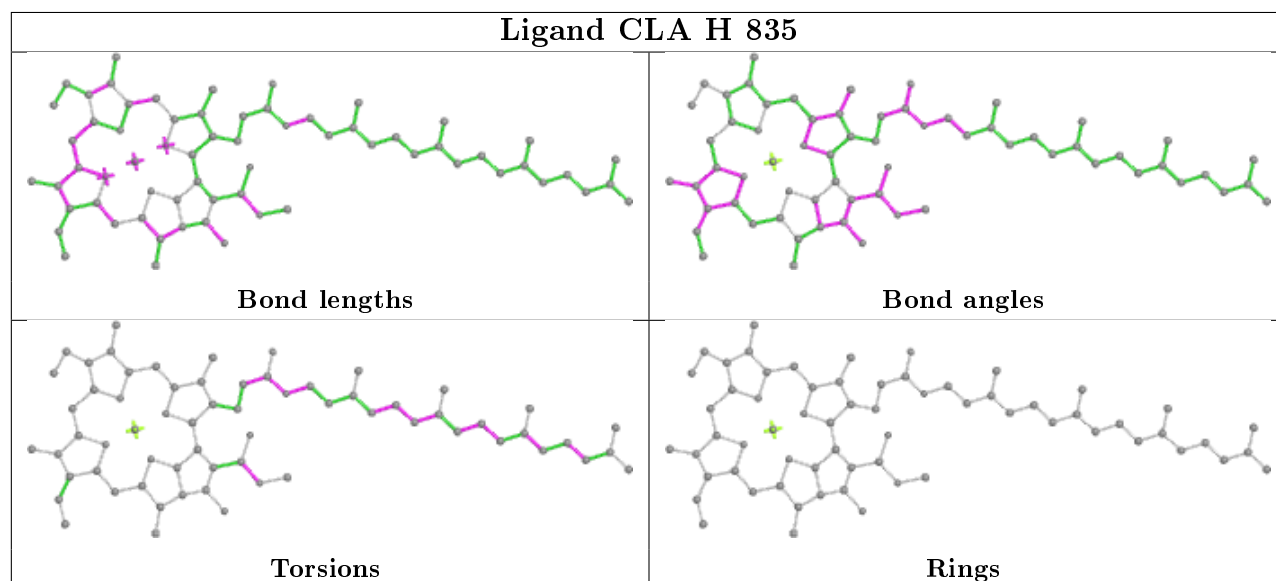


Ligand CLA B 801**Ligand BCR h 202****Ligand CLA H 824**

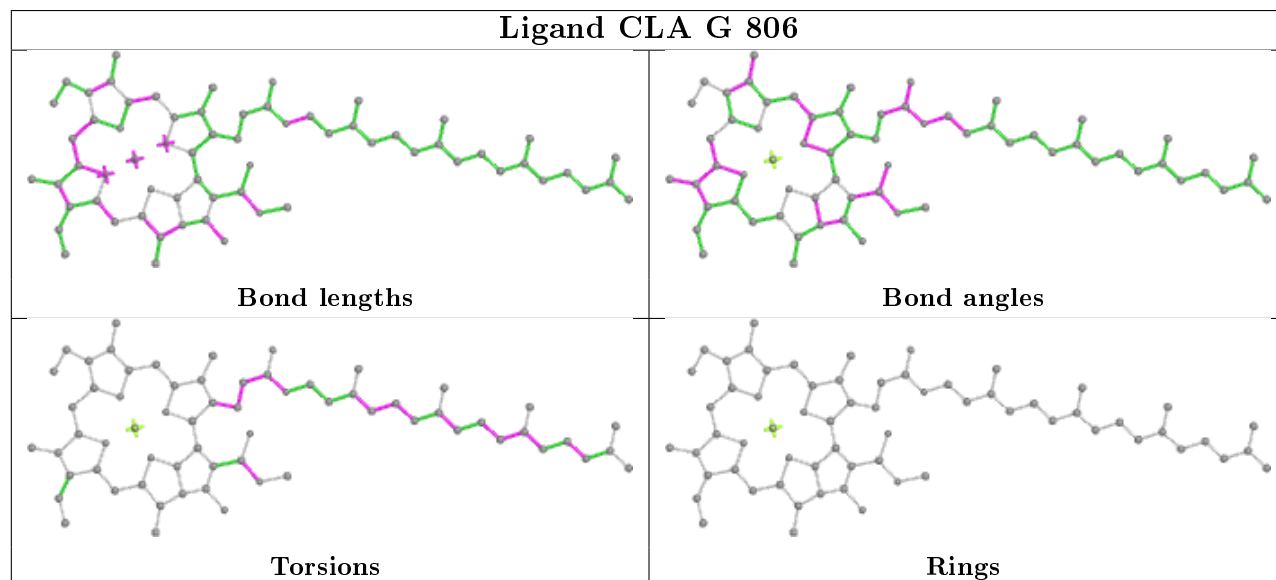
Ligand CLA Y 833



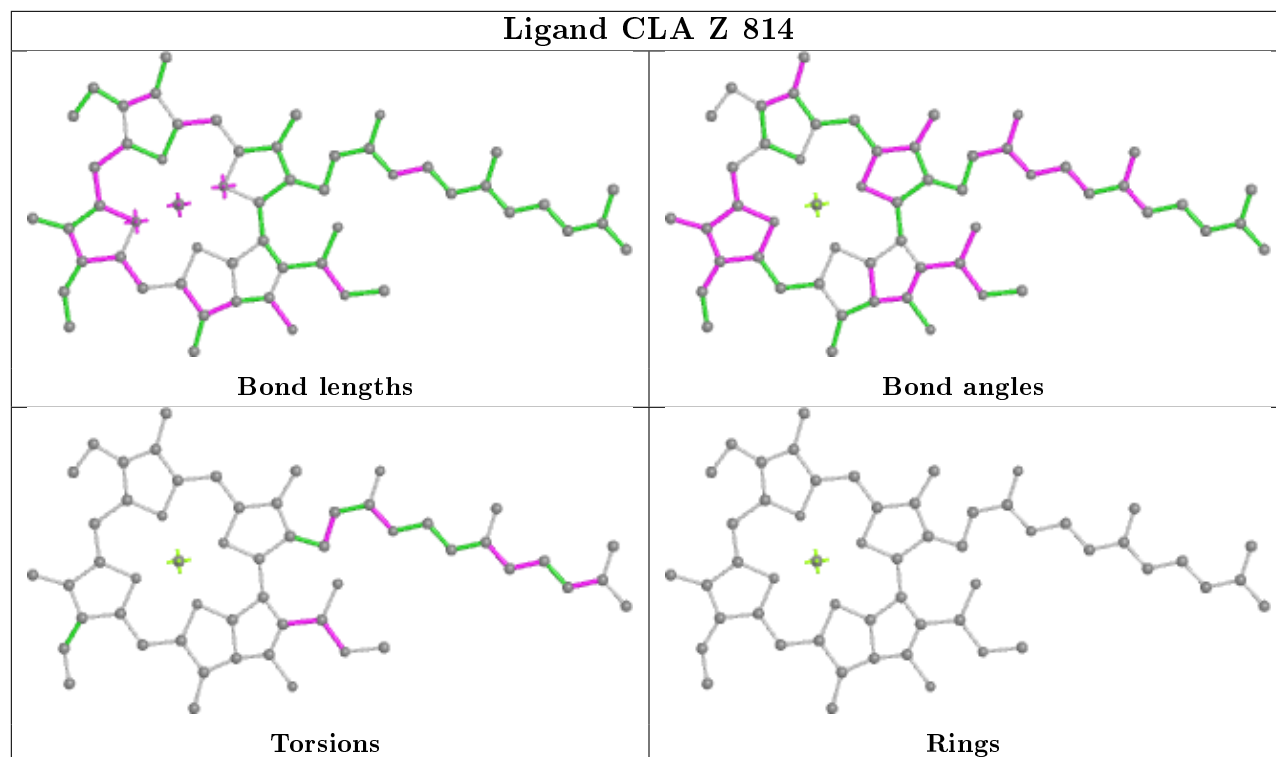
Ligand CLA H 835



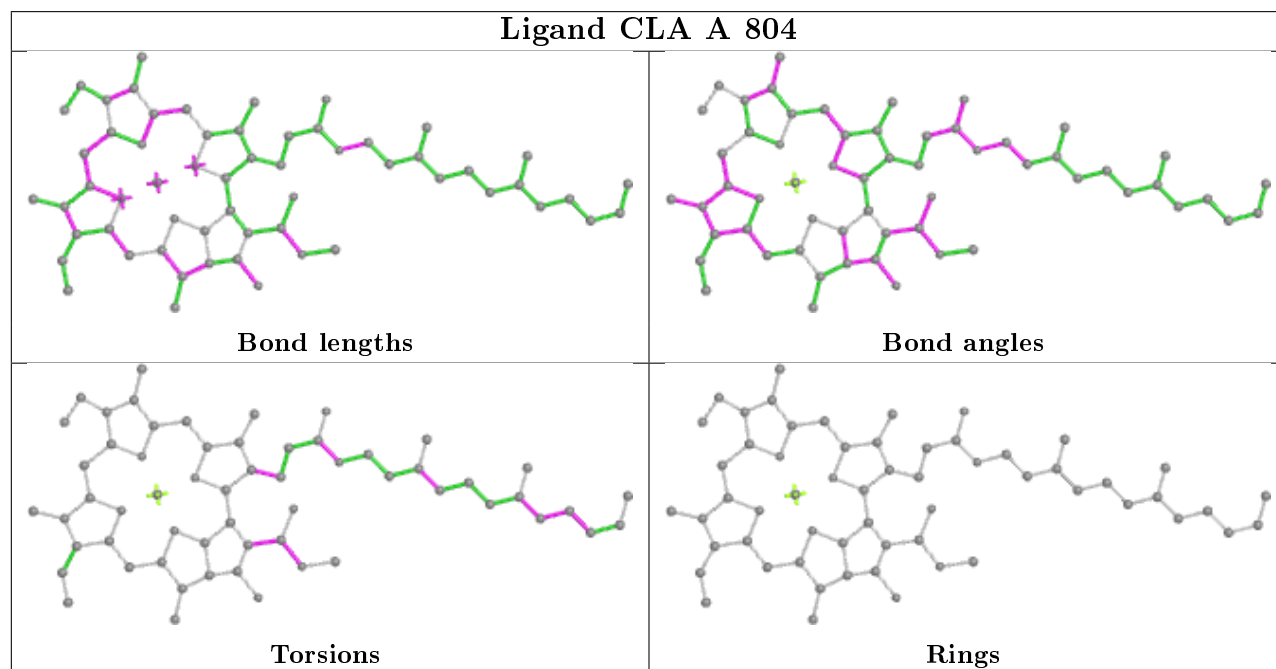
Ligand CLA G 806



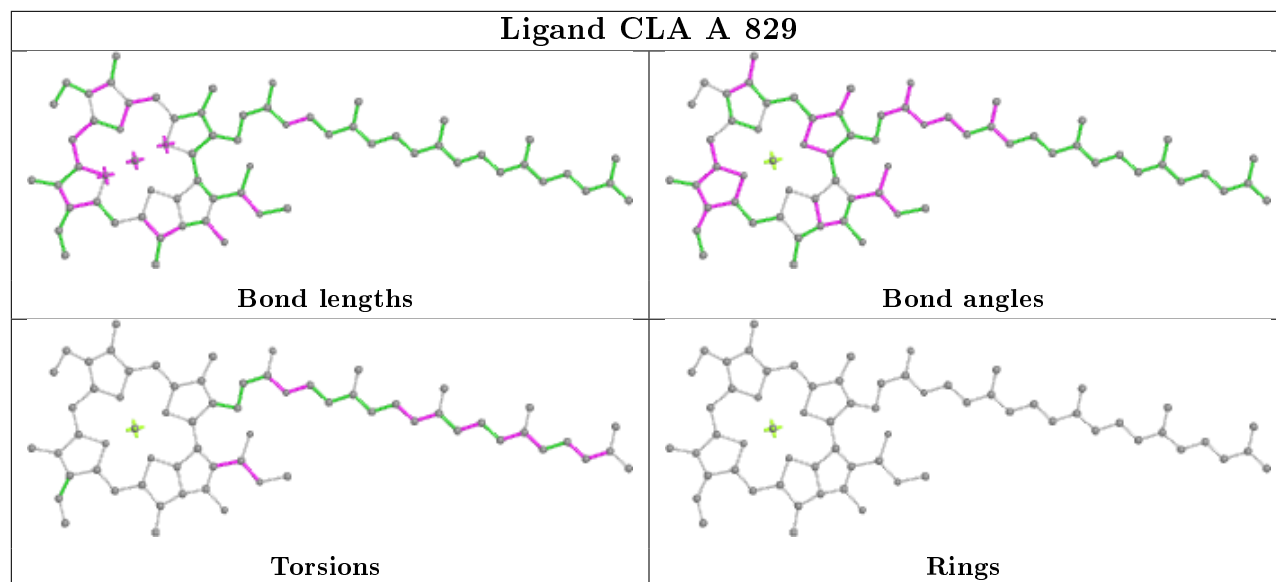
Ligand CLA Z 814



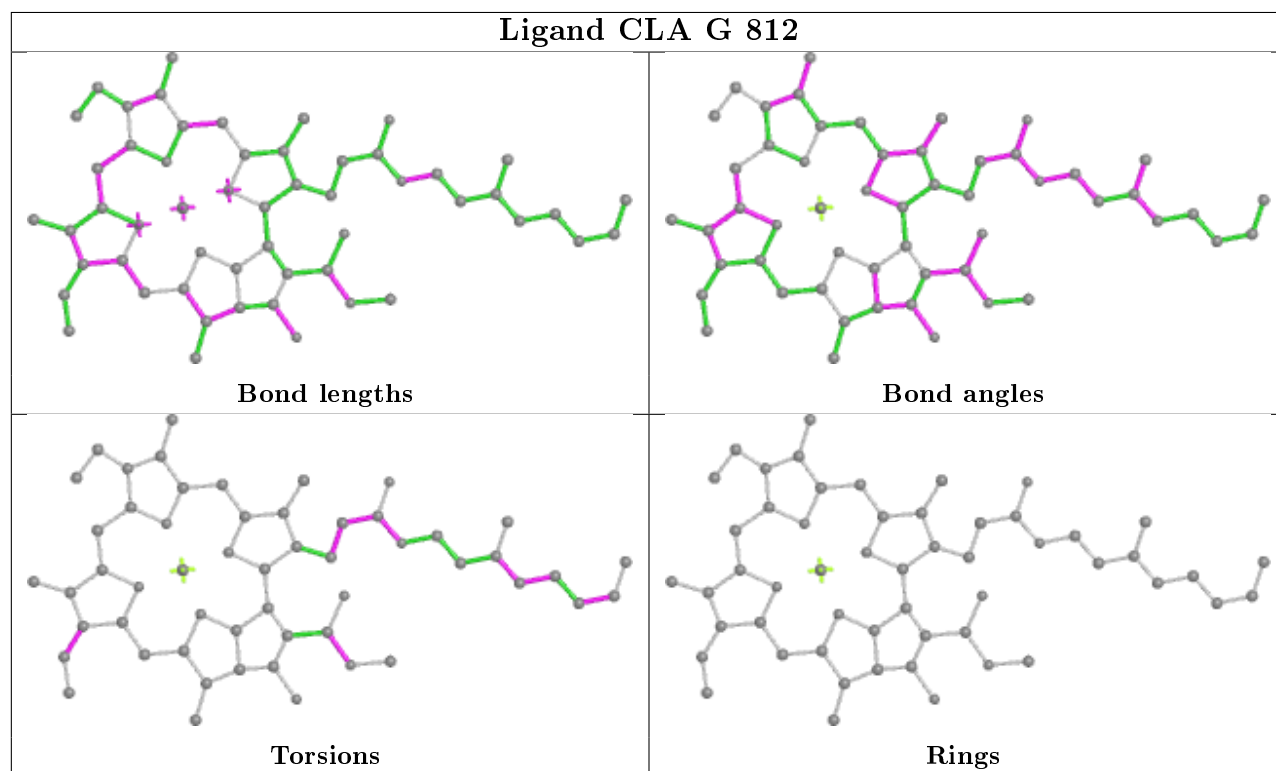
Ligand CLA A 804



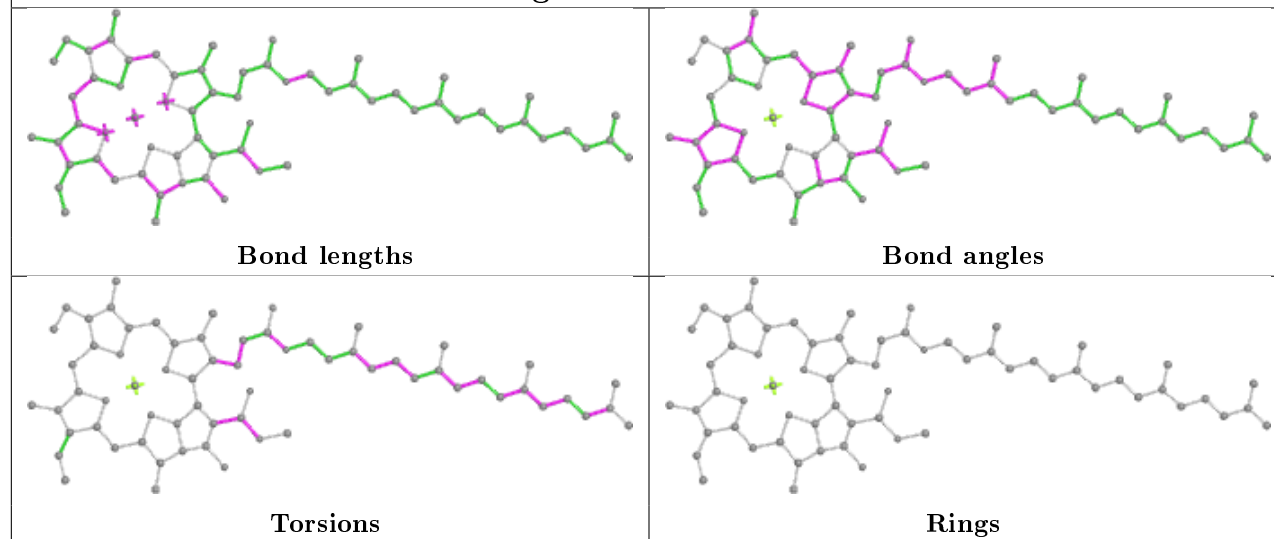
Ligand CLA A 829



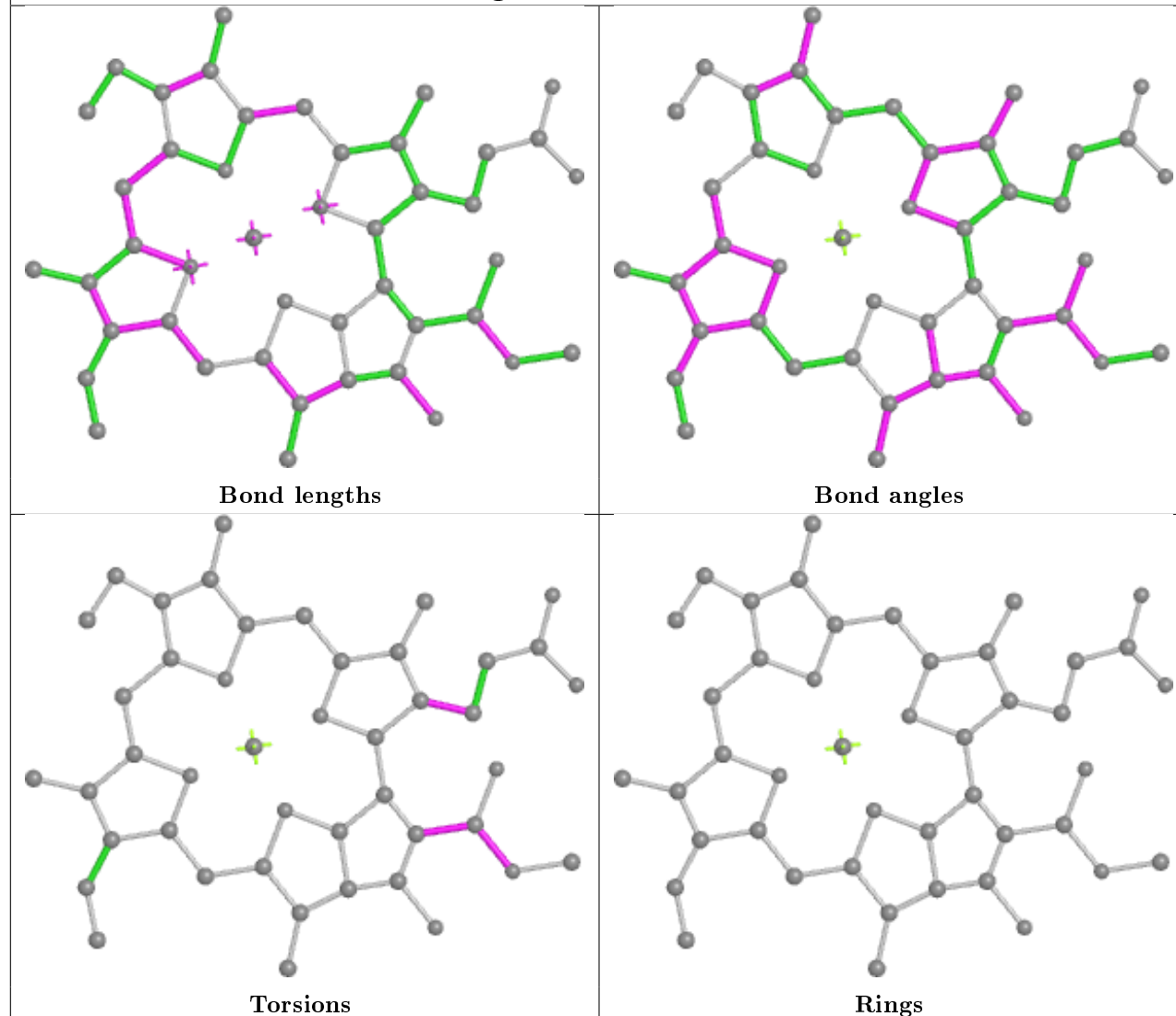
Ligand CLA G 812



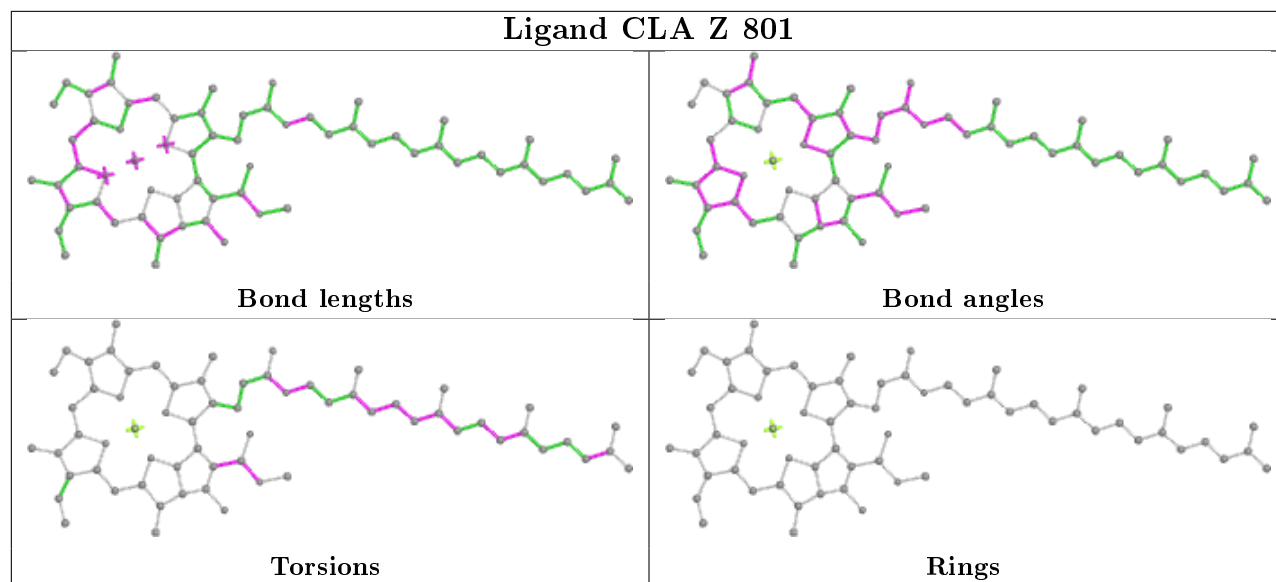
Ligand CLA Y 808



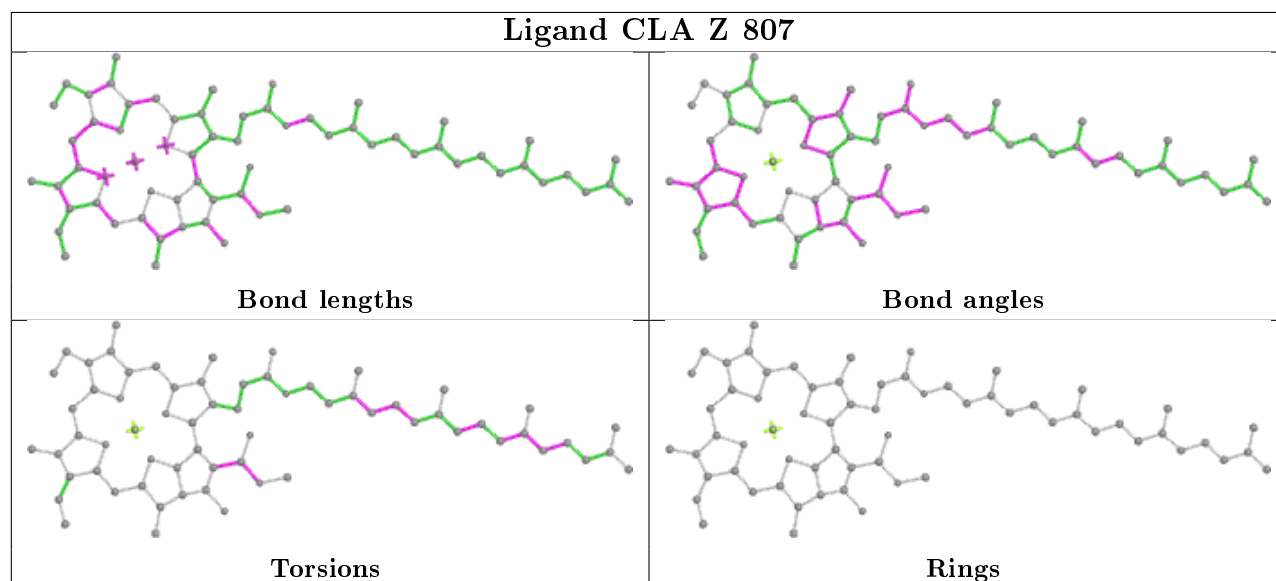
Ligand CLA H 832



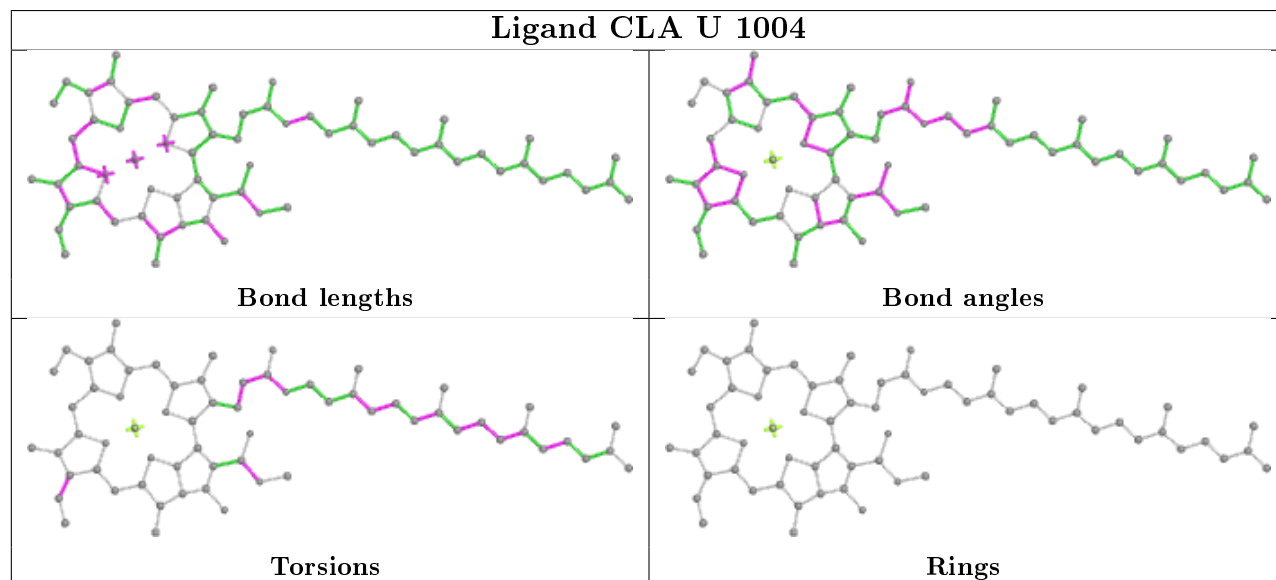
Ligand CLA Z 801

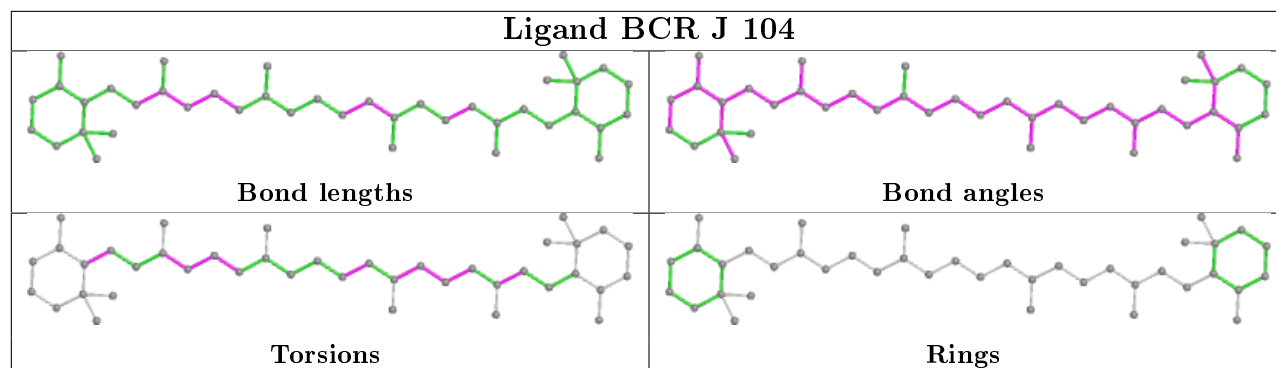
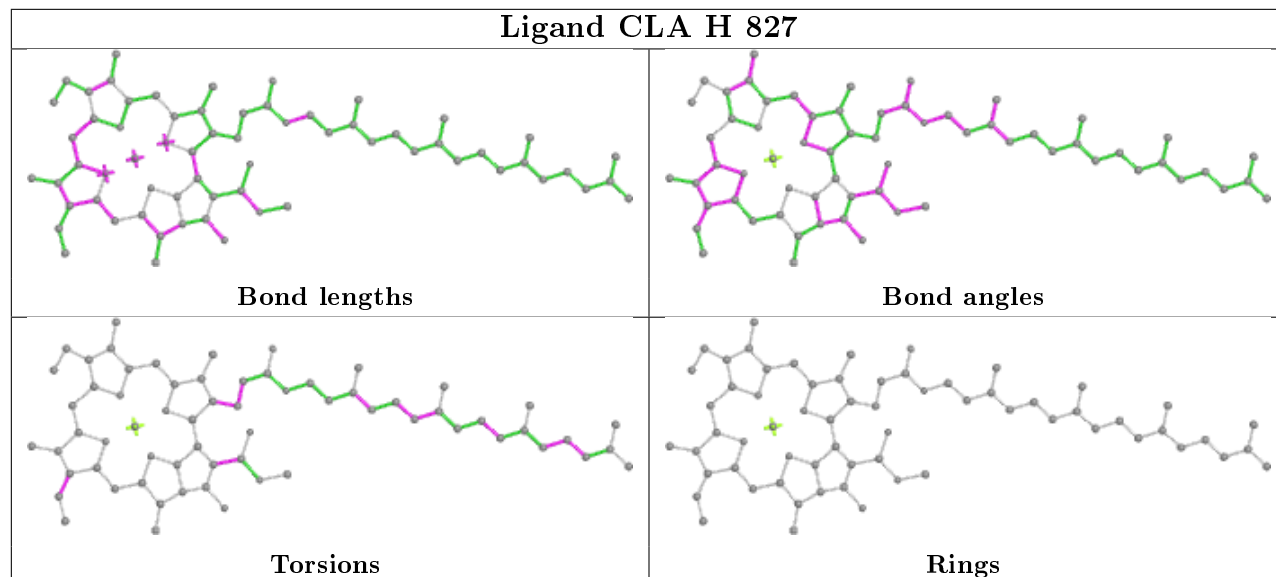
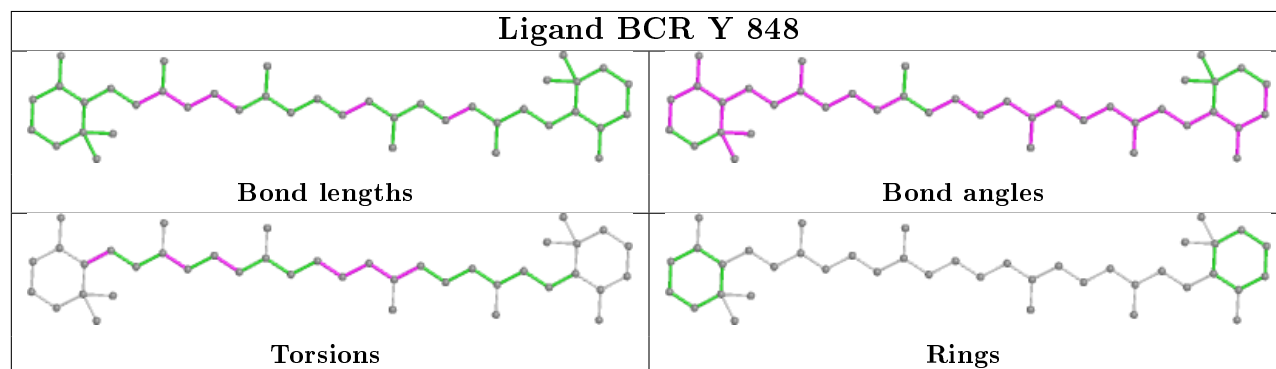


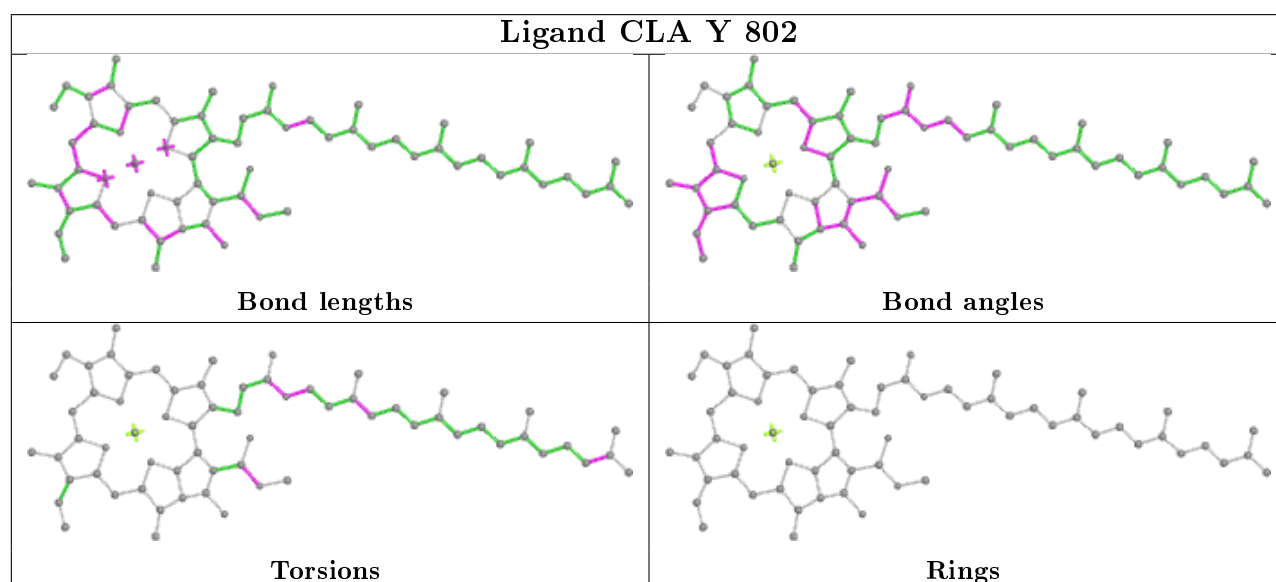
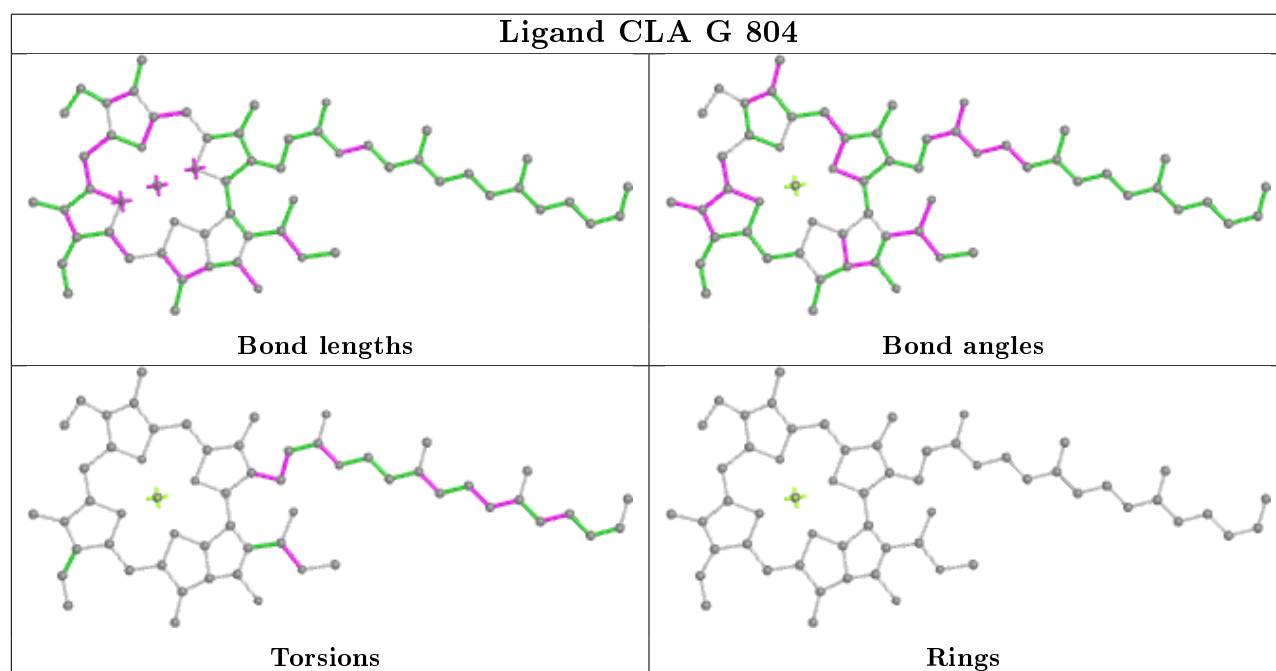
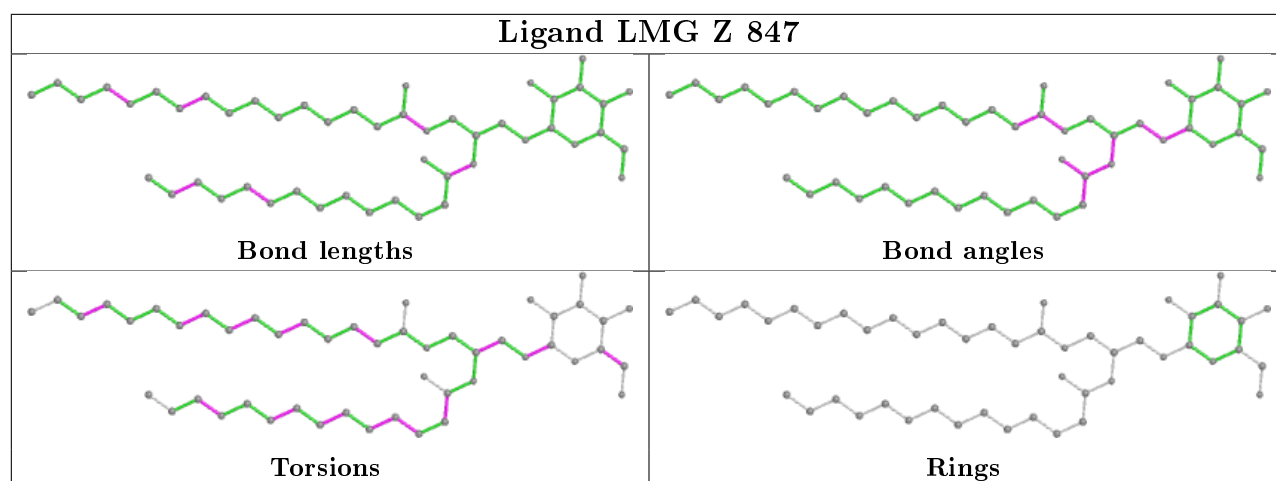
Ligand CLA Z 807



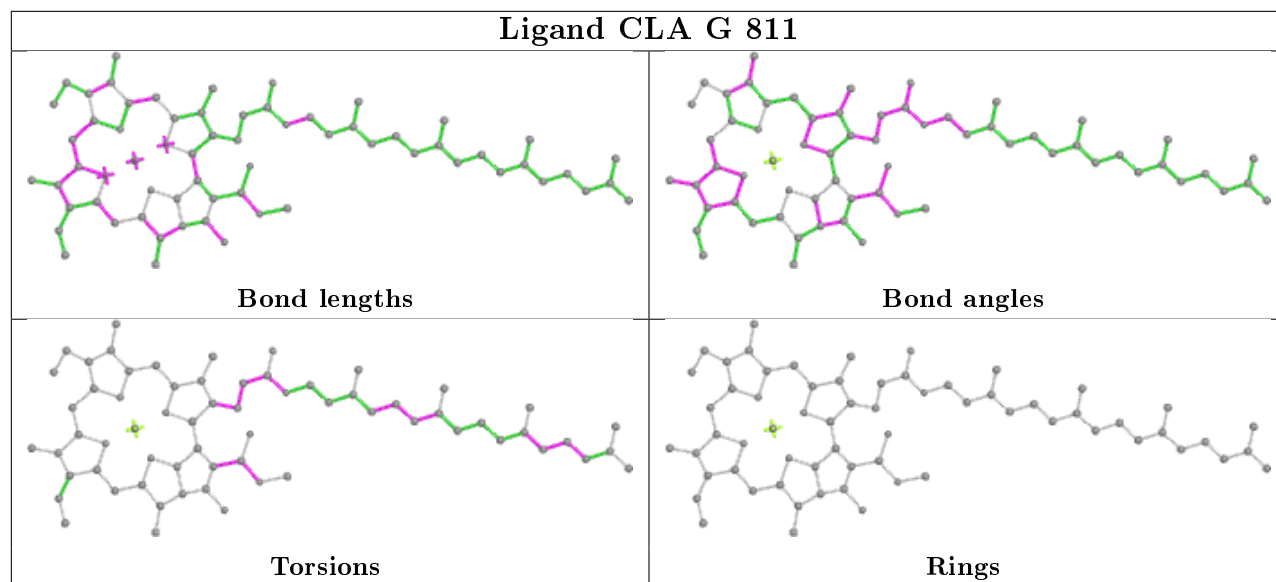
Ligand CLA U 1004



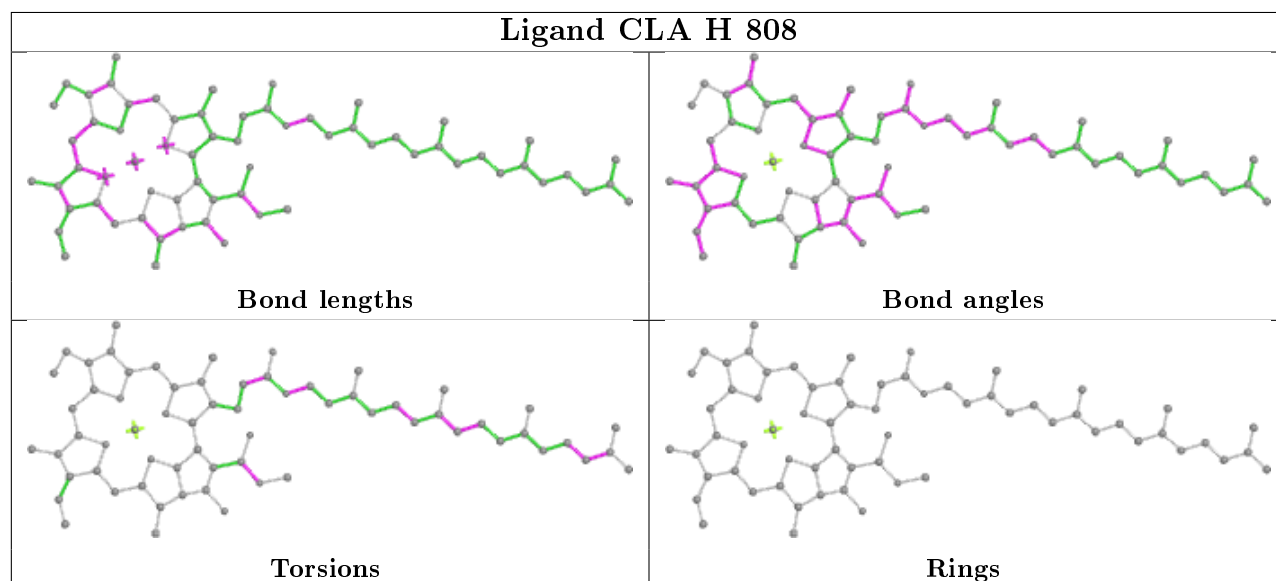
Ligand BCR J 104**Ligand CLA H 827****Ligand BCR Y 848**



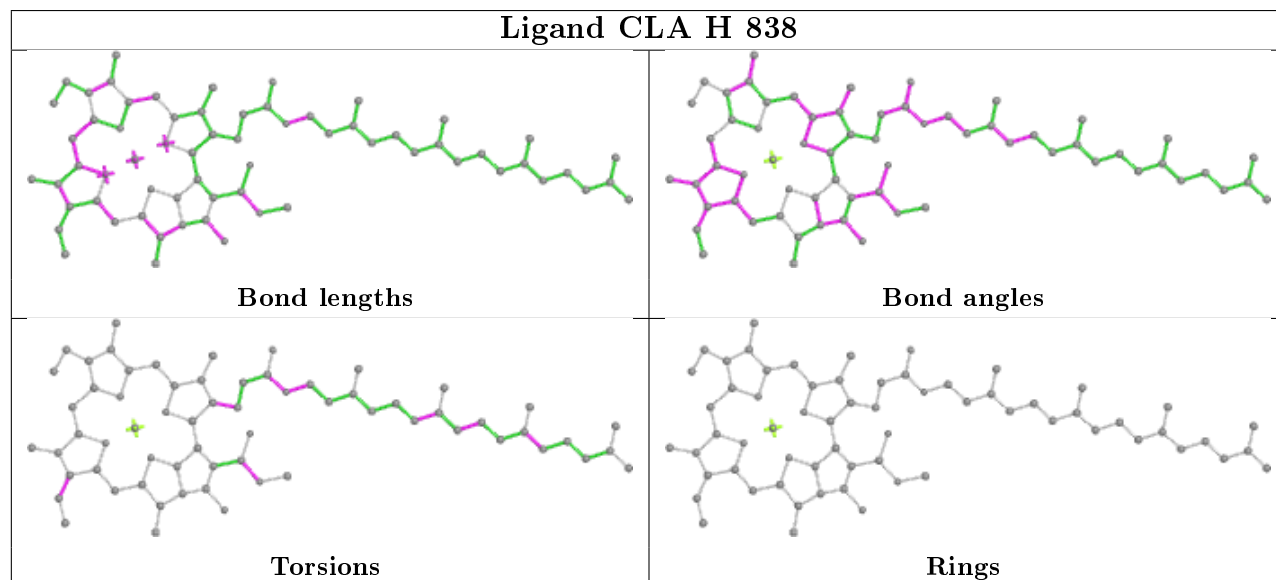
Ligand CLA G 811



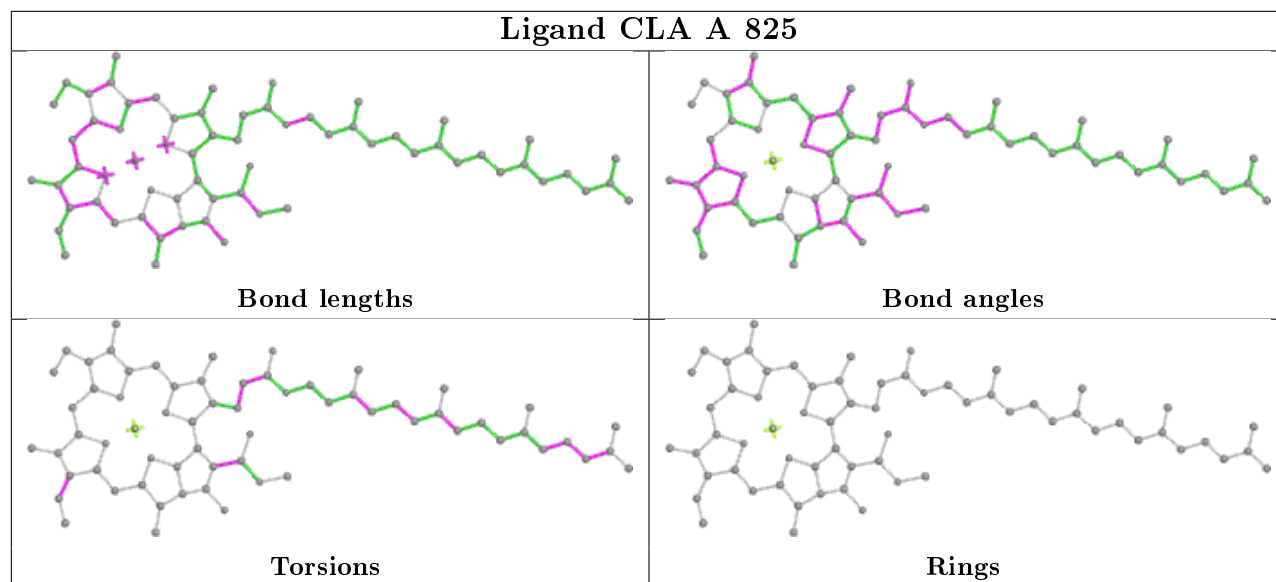
Ligand CLA H 808



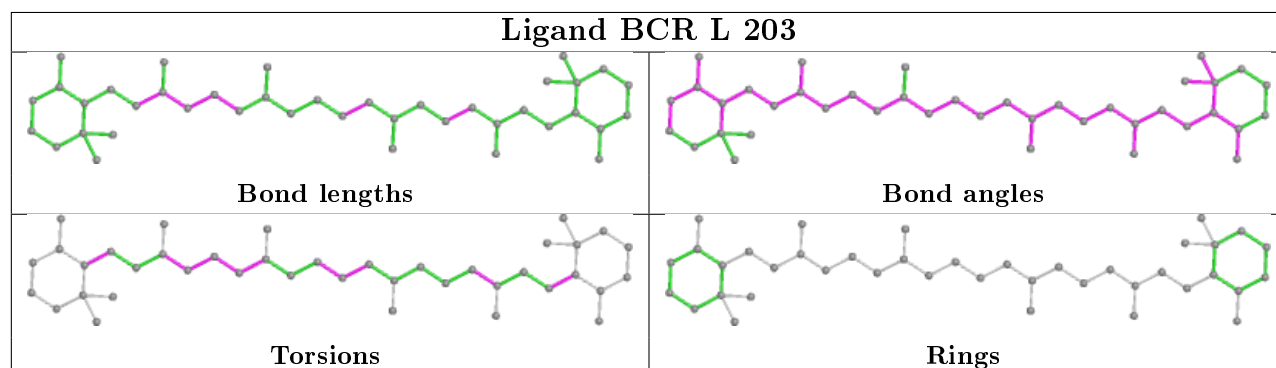
Ligand CLA H 838



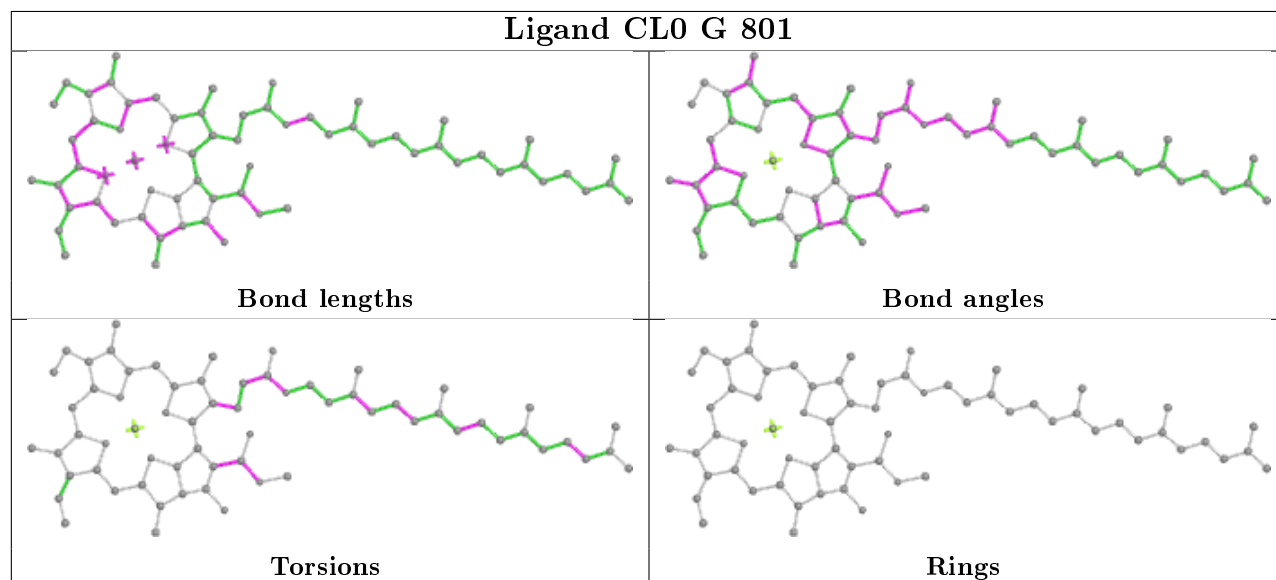
Ligand CLA A 825

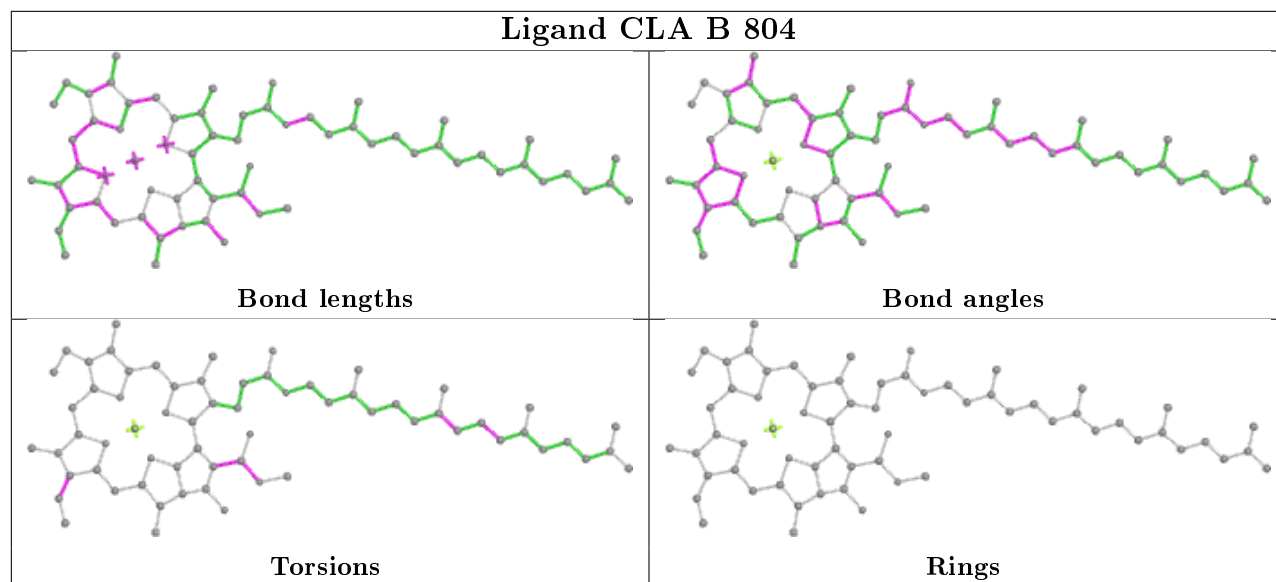
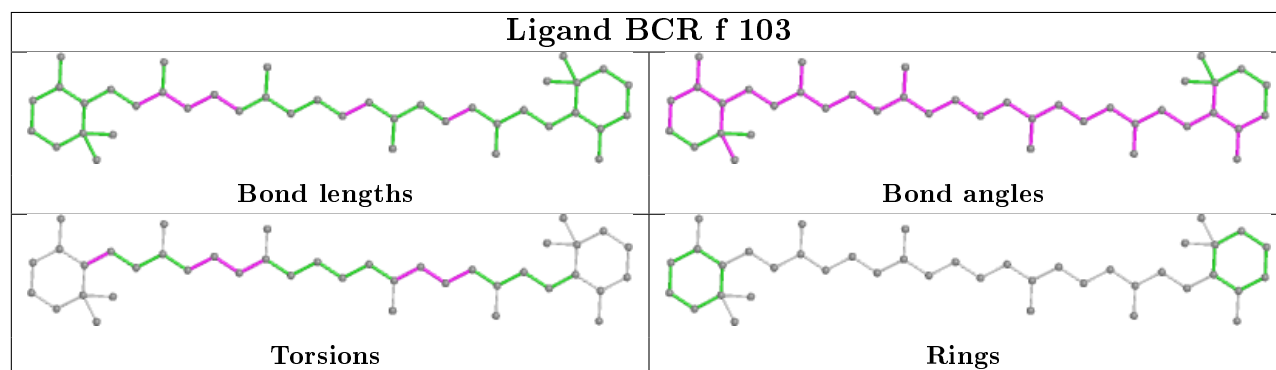
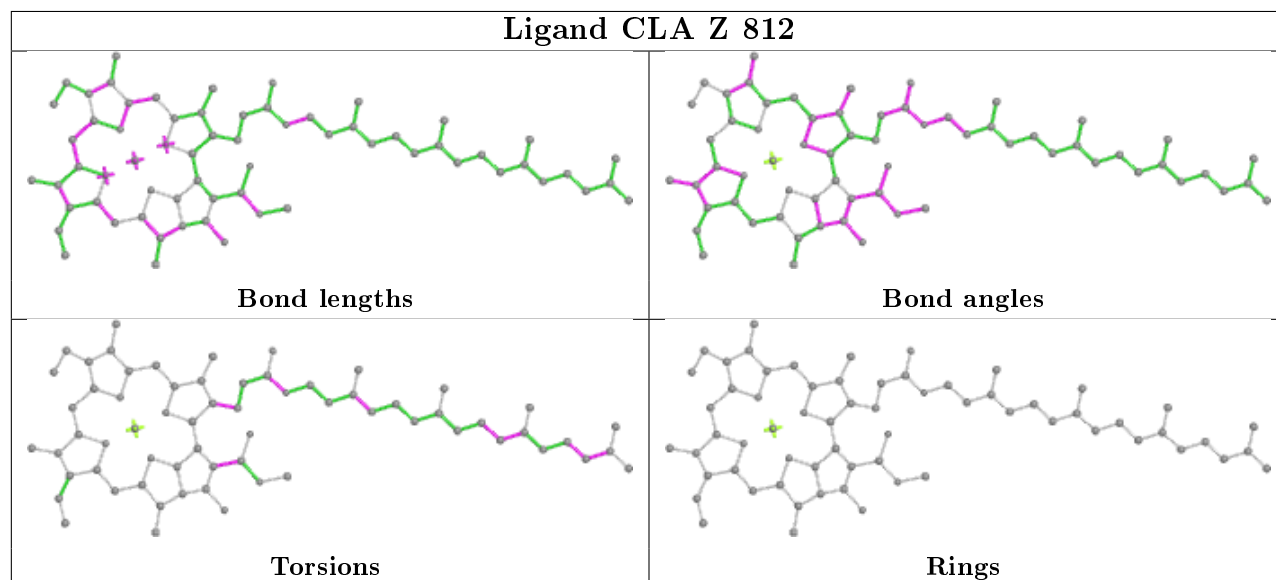


Ligand BCR L 203

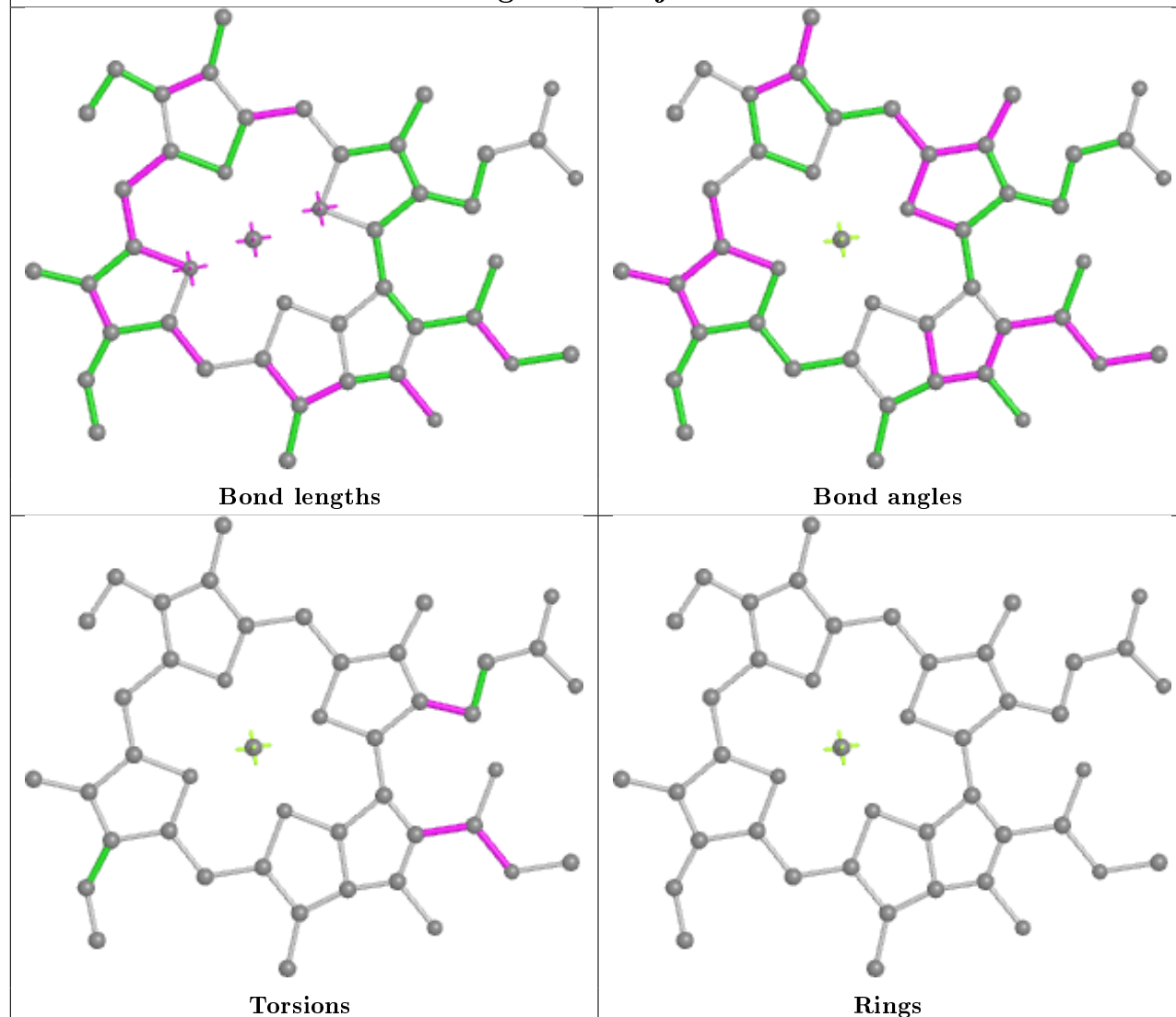


Ligand CL0 G 801

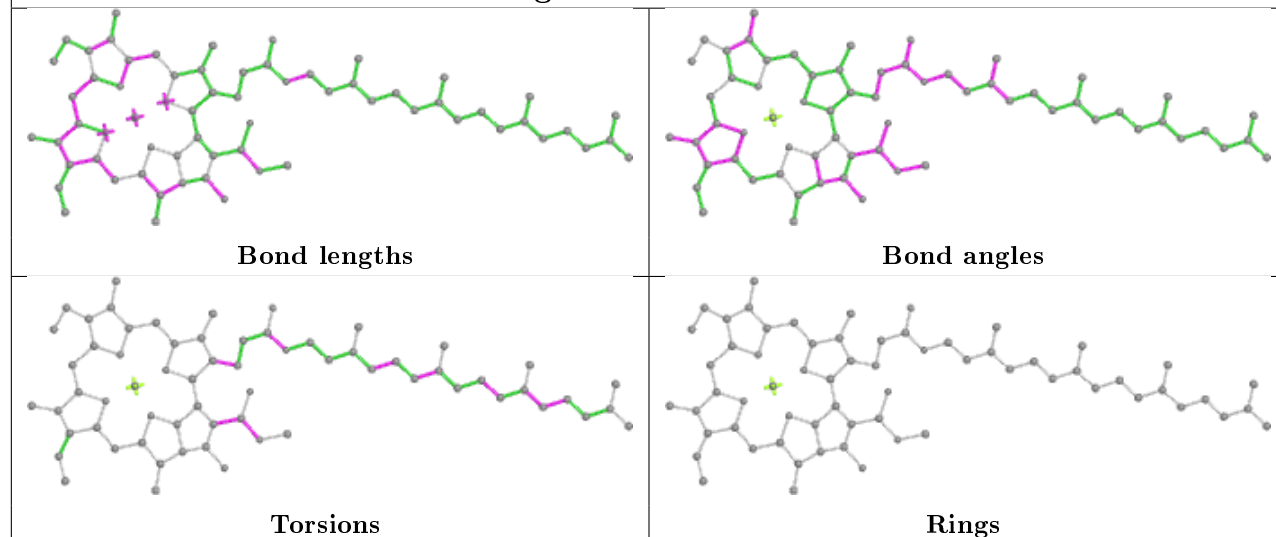


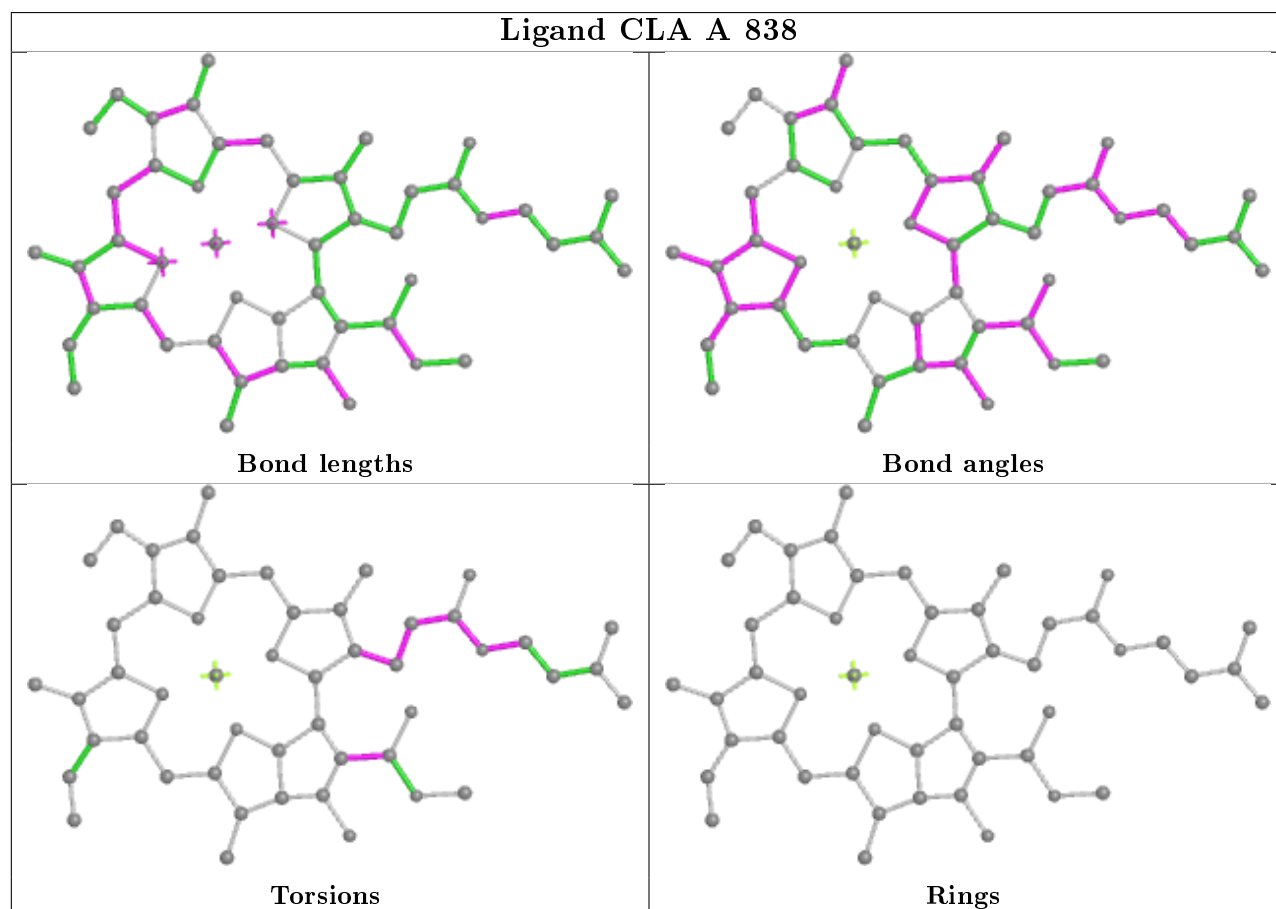
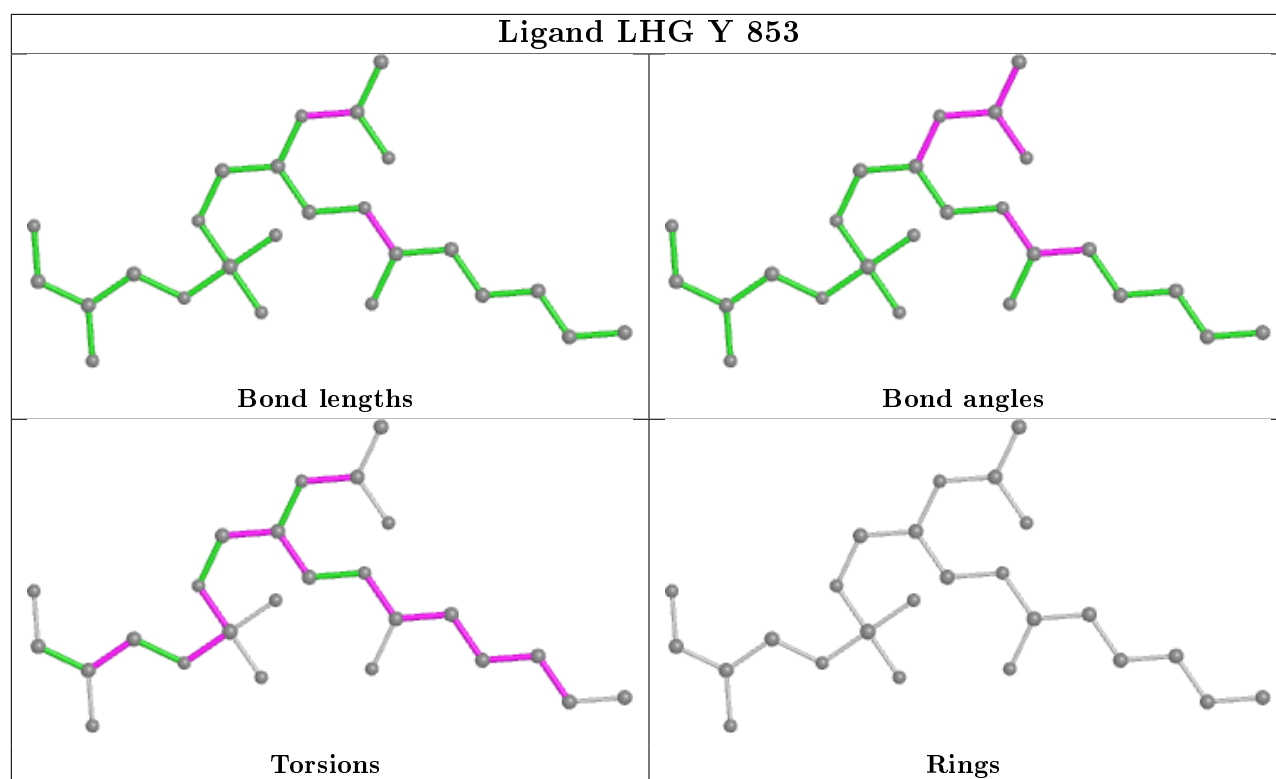
Ligand CLA B 804**Ligand BCR f 103****Ligand CLA Z 812**

Ligand CLA j 102

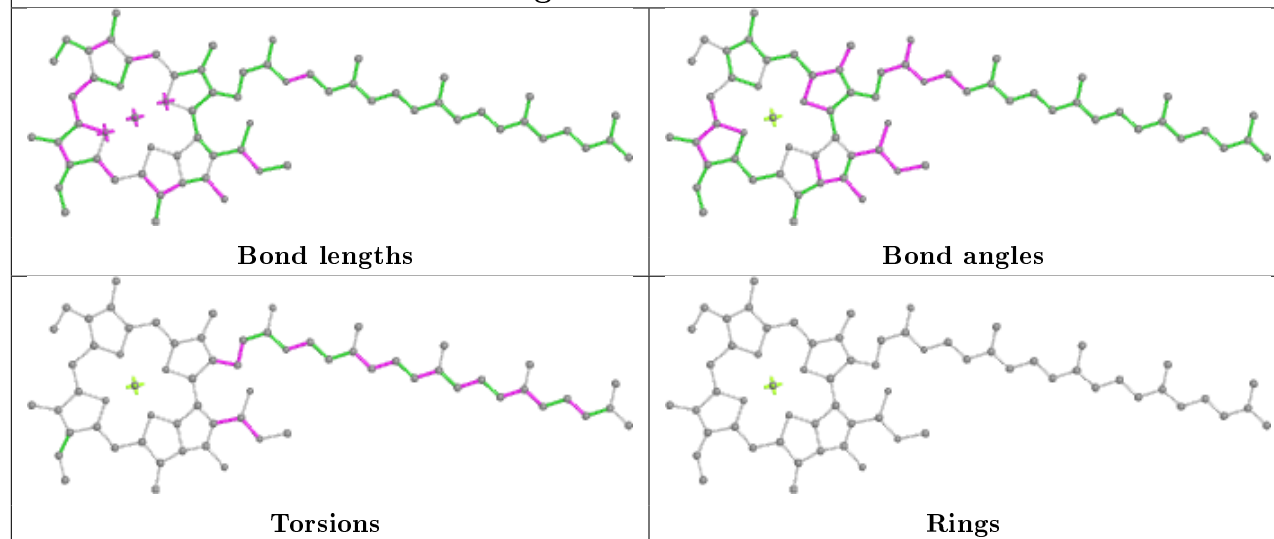


Ligand CLA L 206

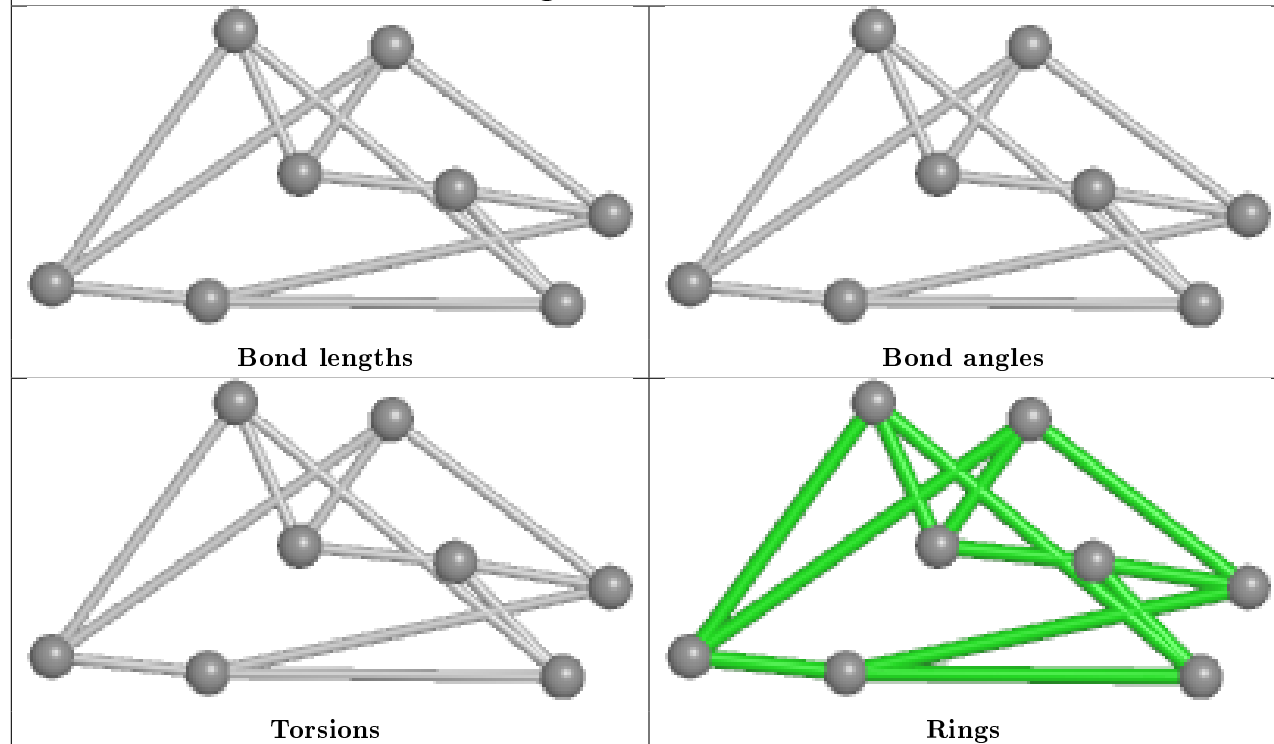


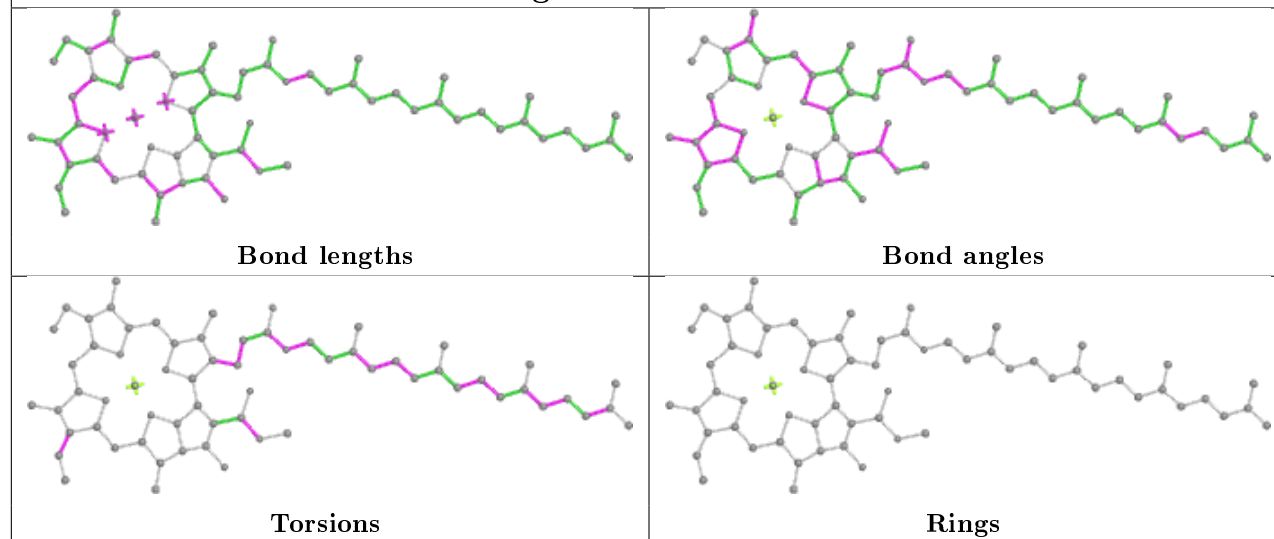
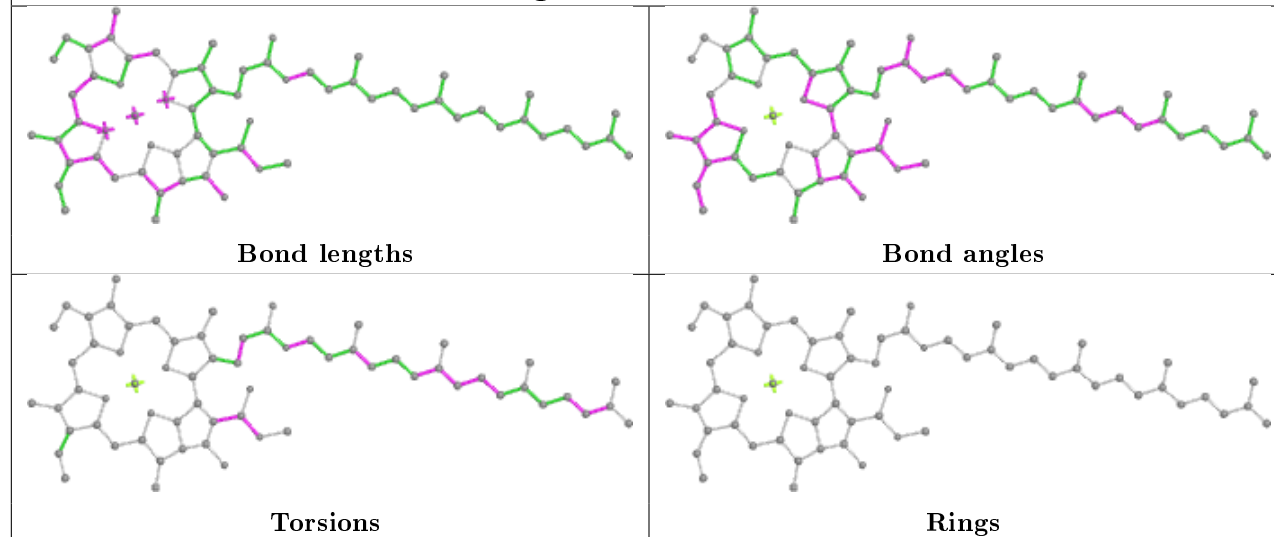


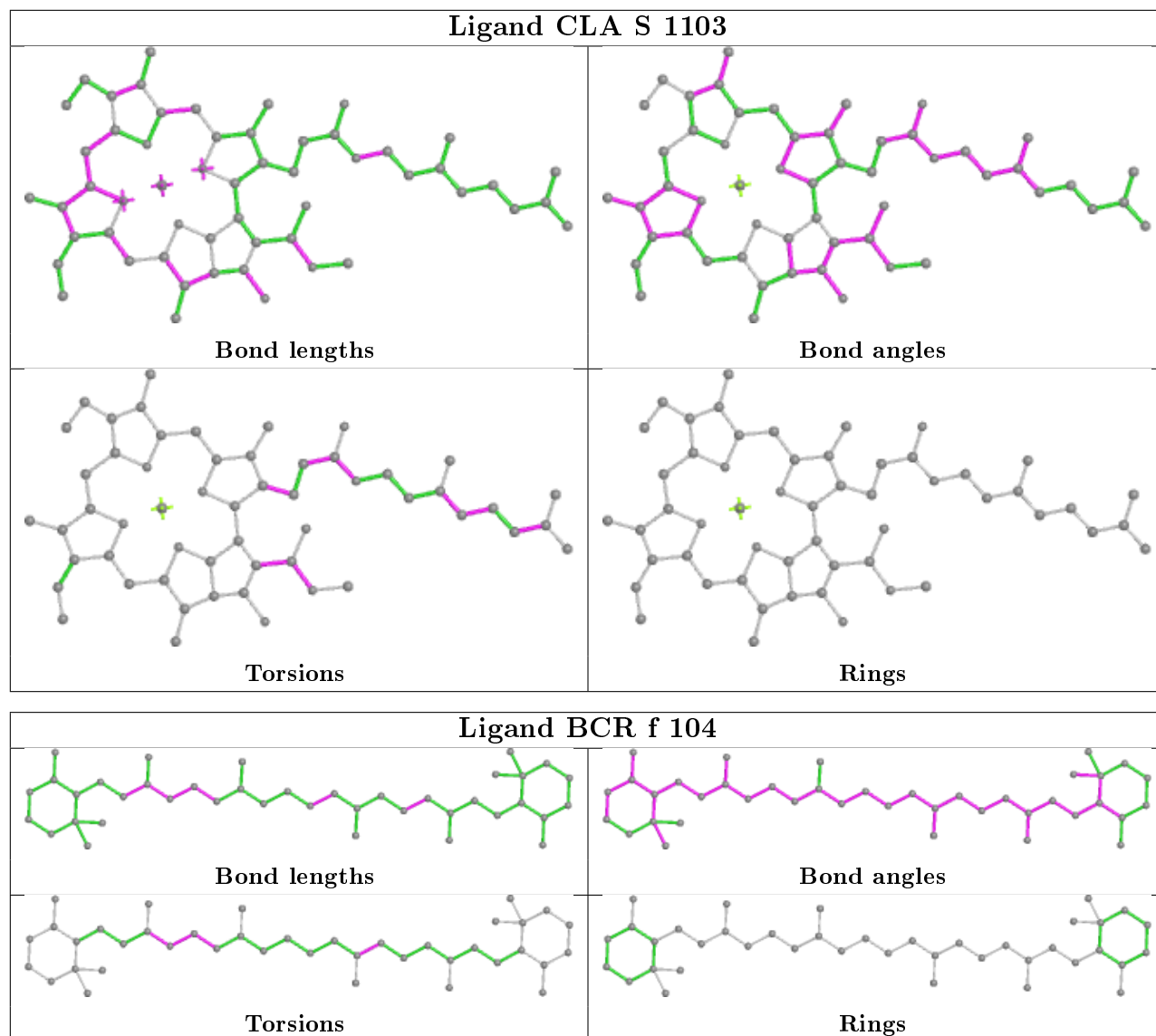
Ligand CLA Z 830



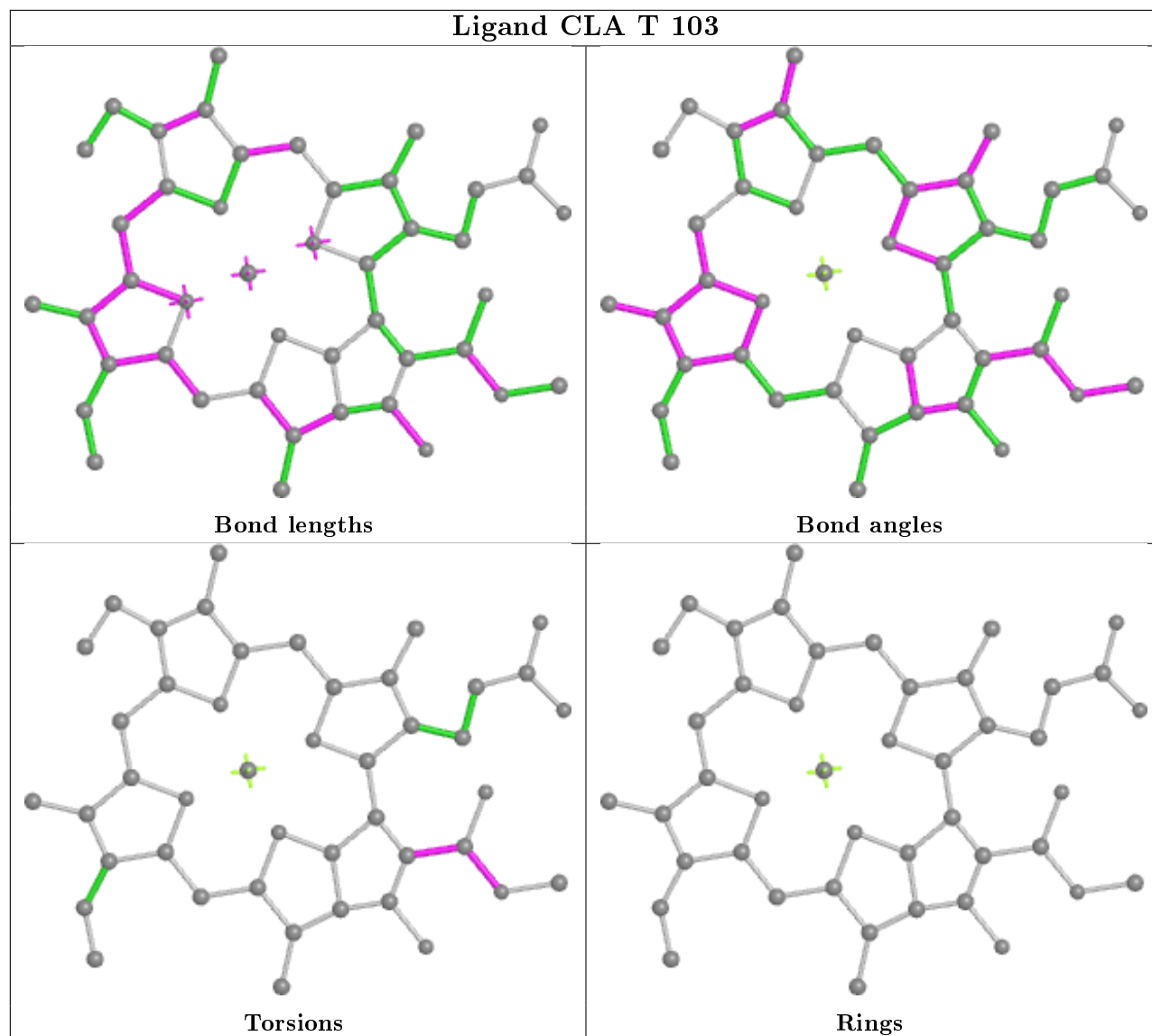
Ligand SF4 N 102



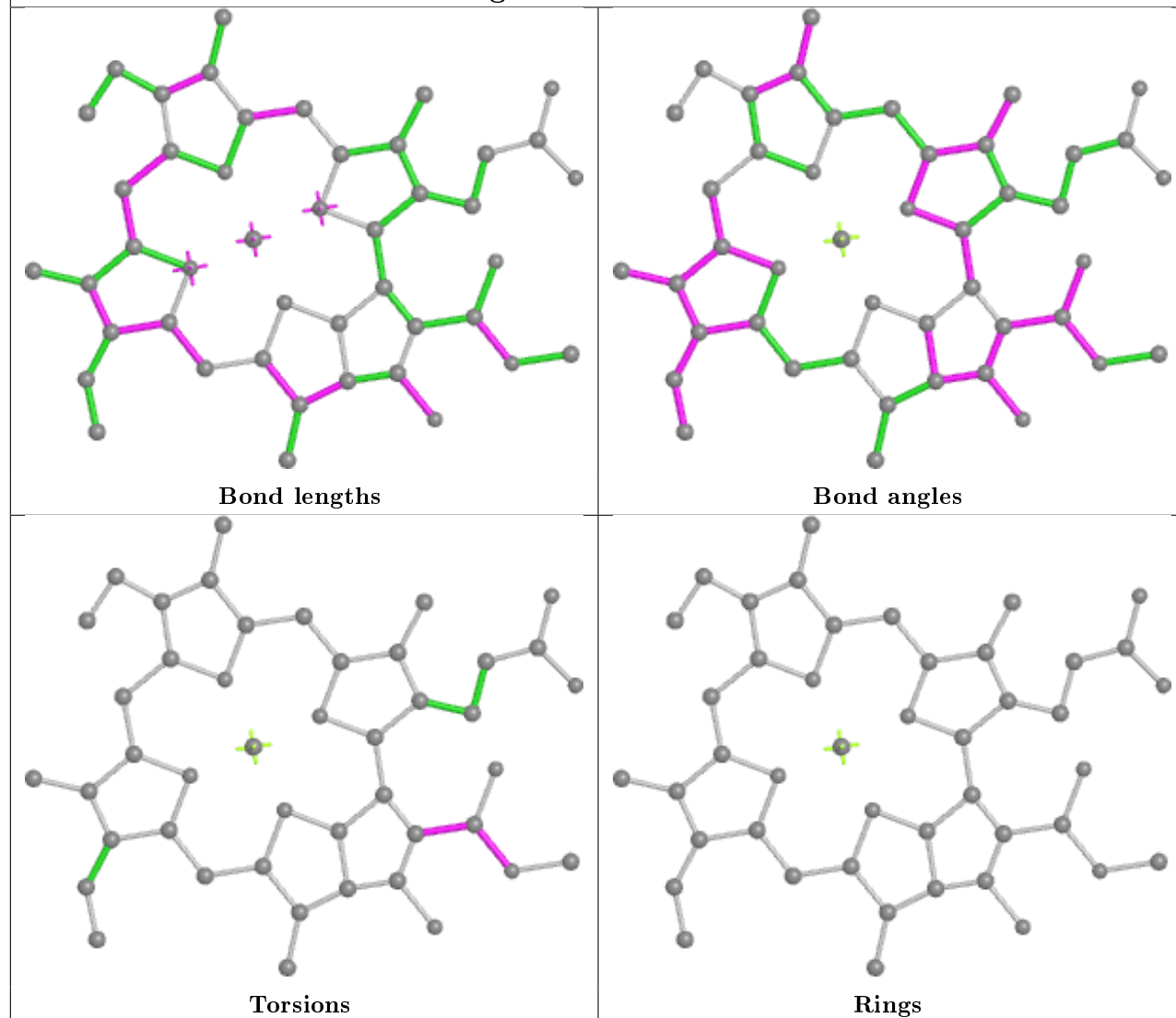
Ligand CLA B 832**Ligand CLA B 810**



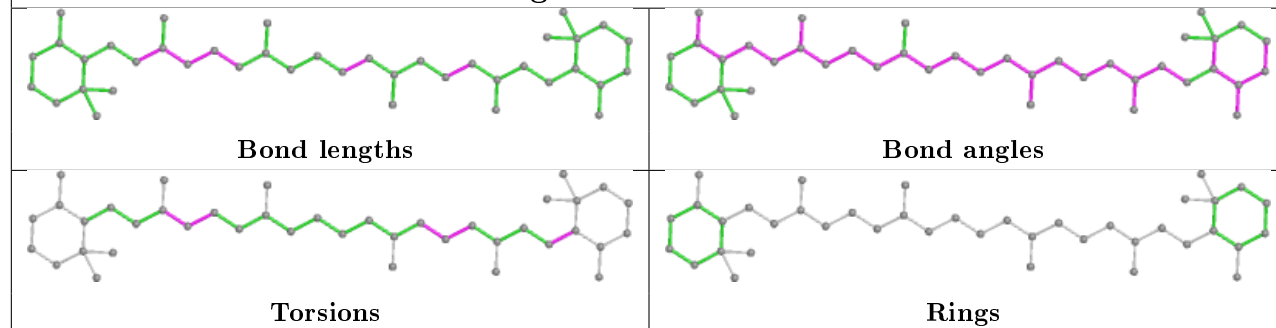
Ligand CLA T 103

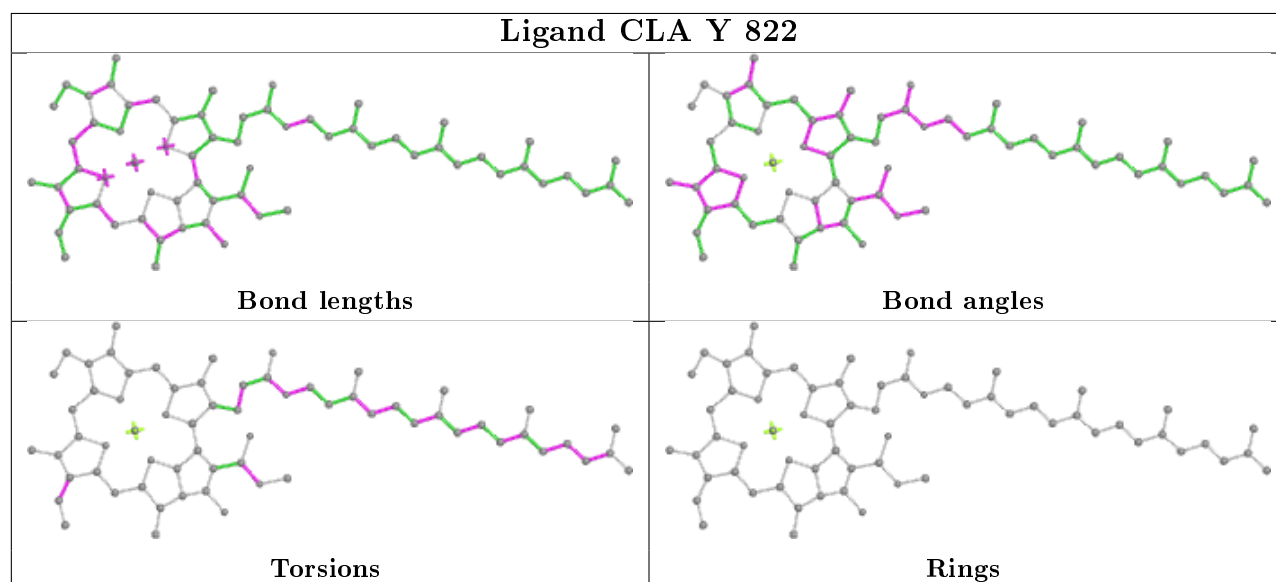
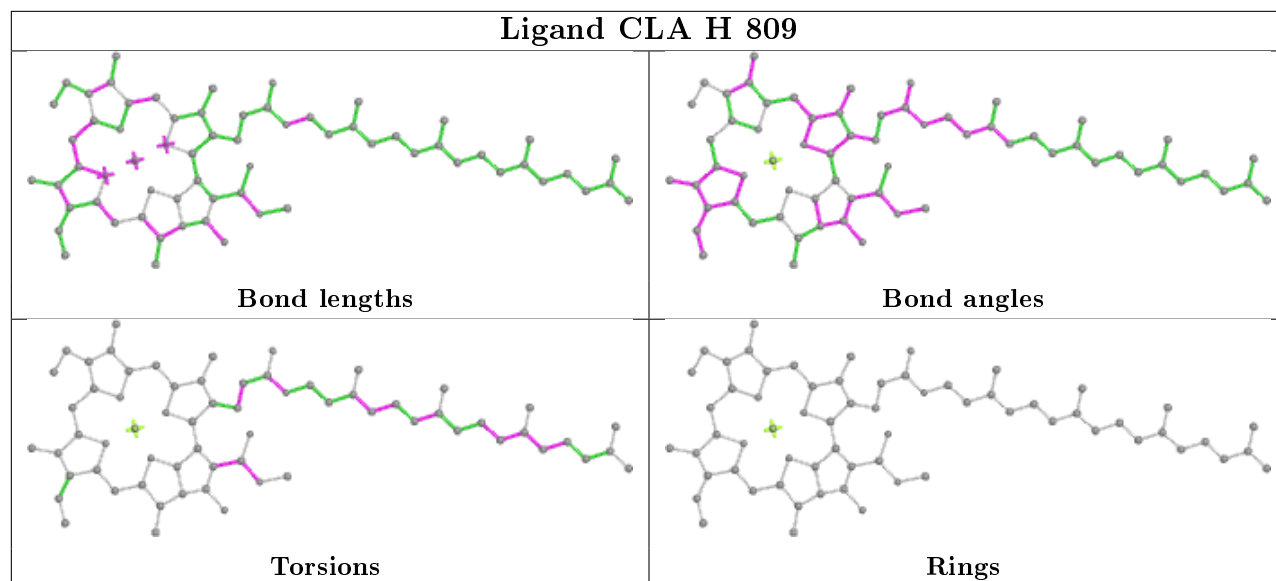
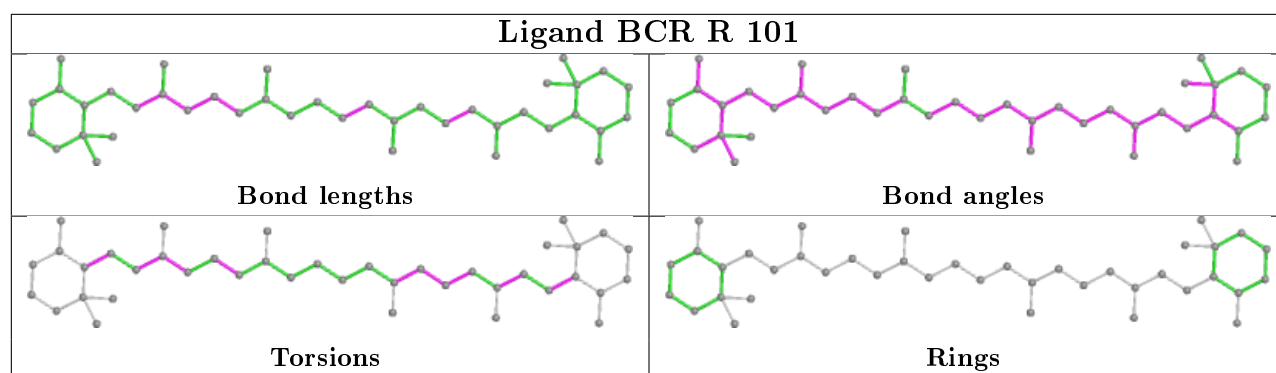


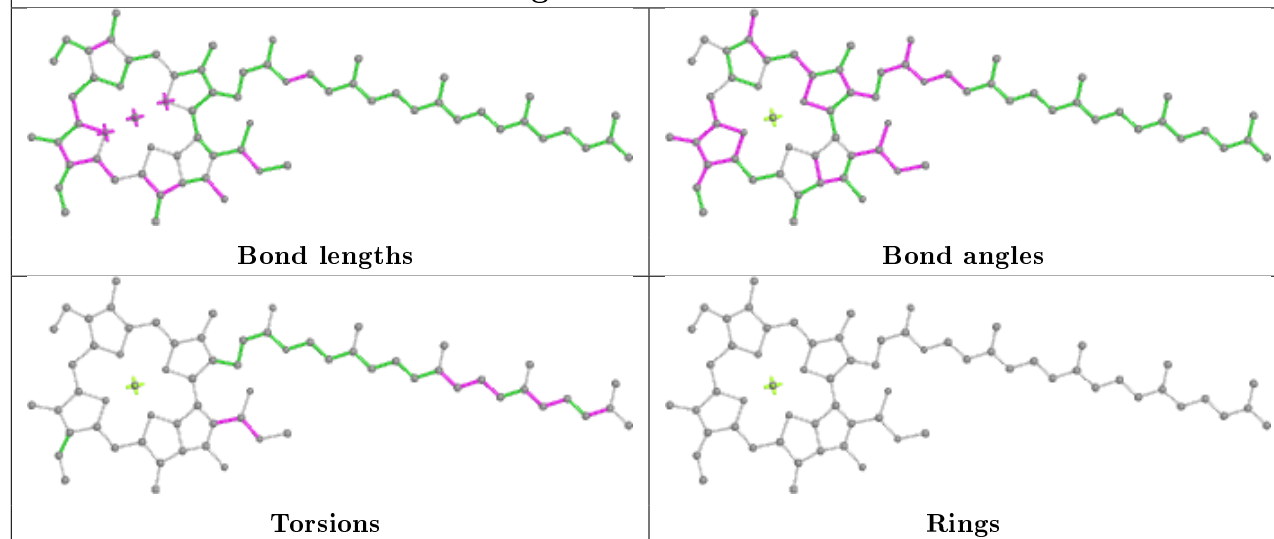
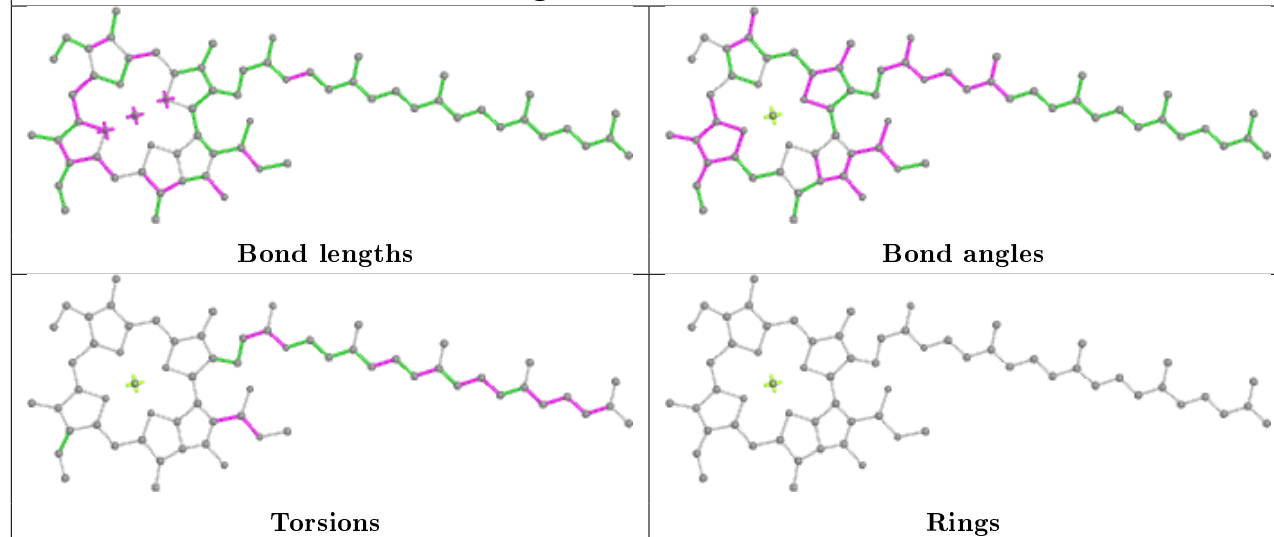
Ligand CLA H 833



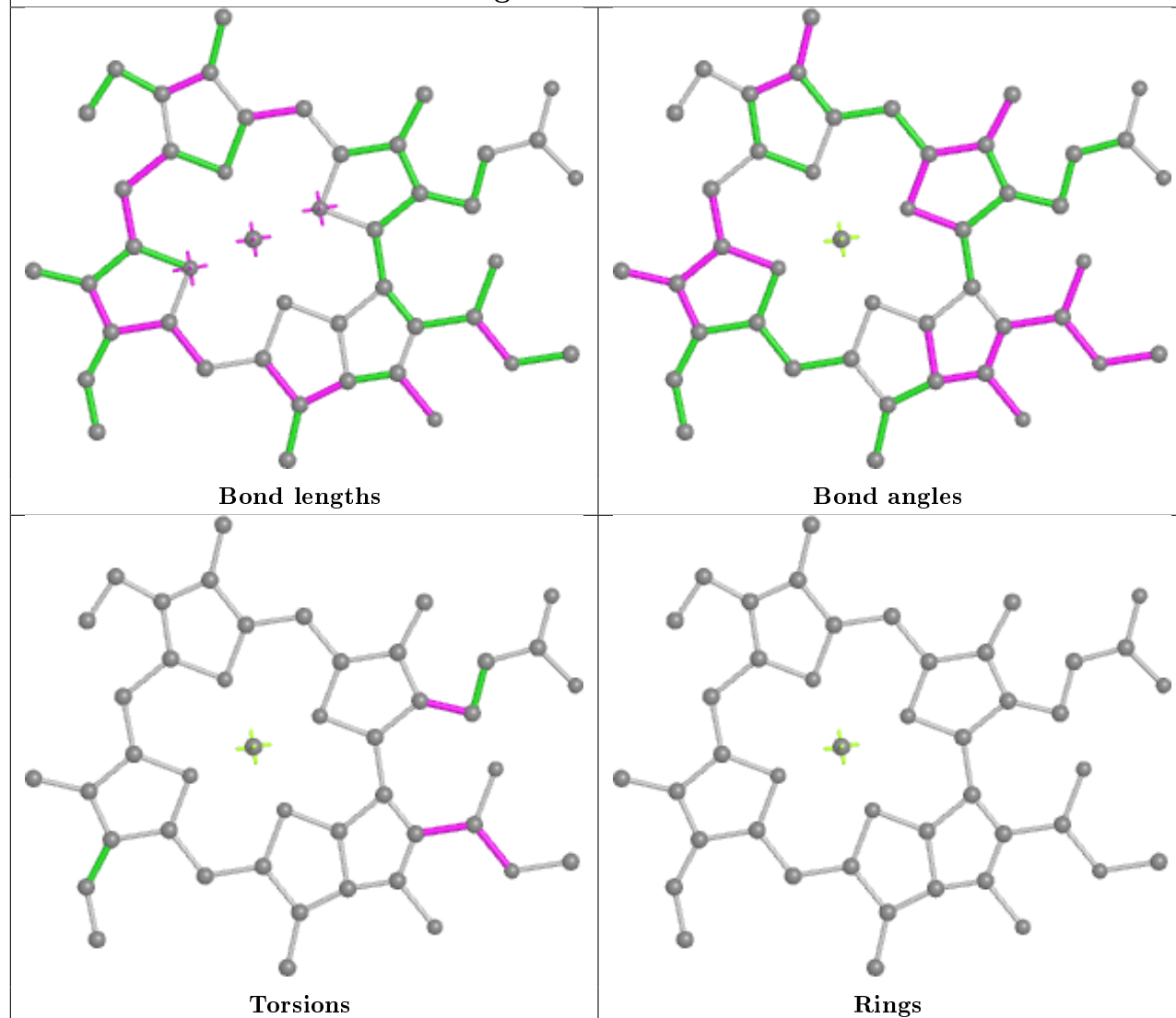
Ligand BCR Y 850



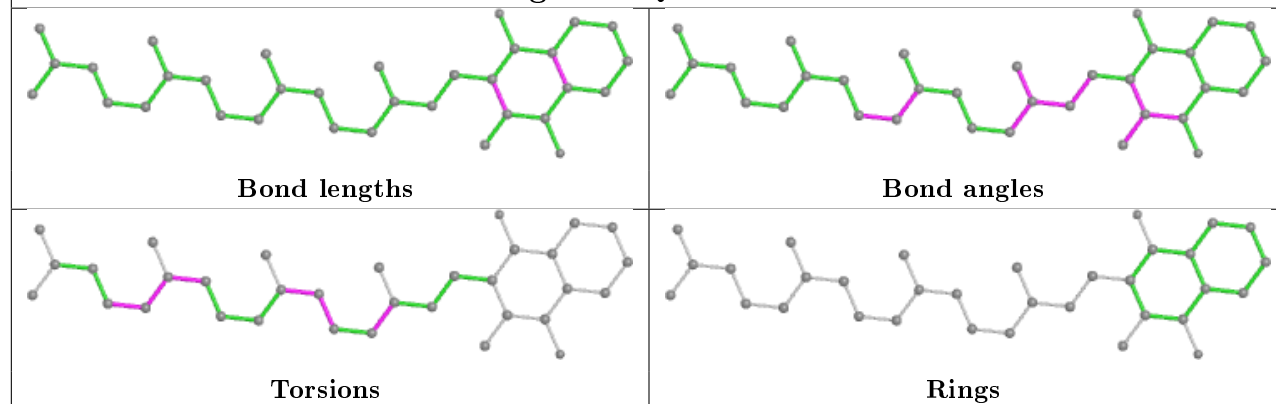


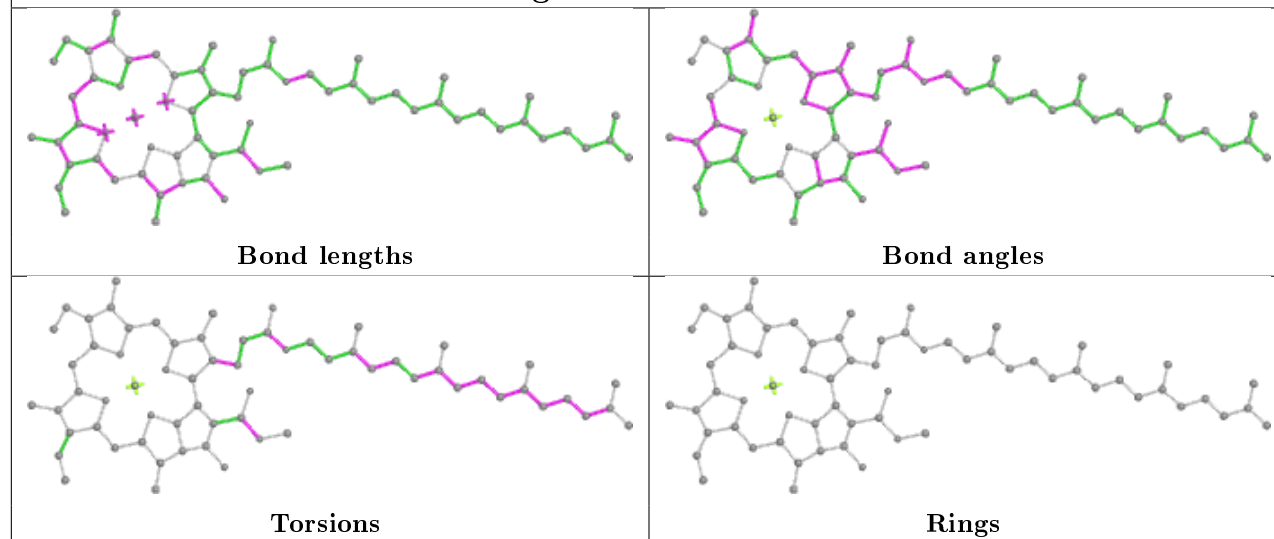
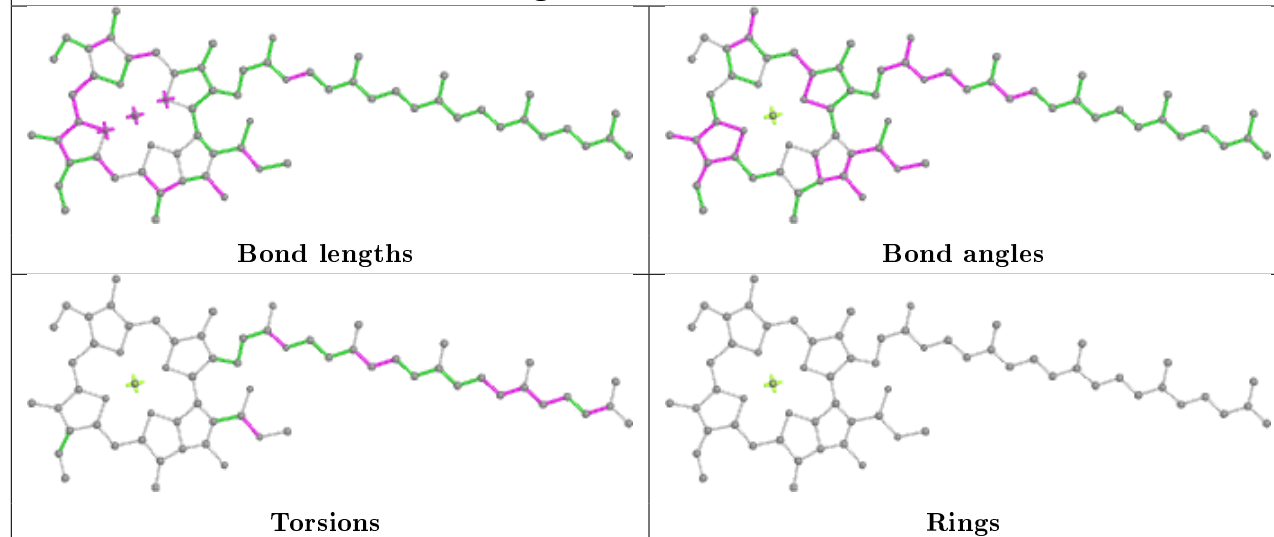
Ligand CLA H 803**Ligand CLA G 837**

Ligand CLA J 101

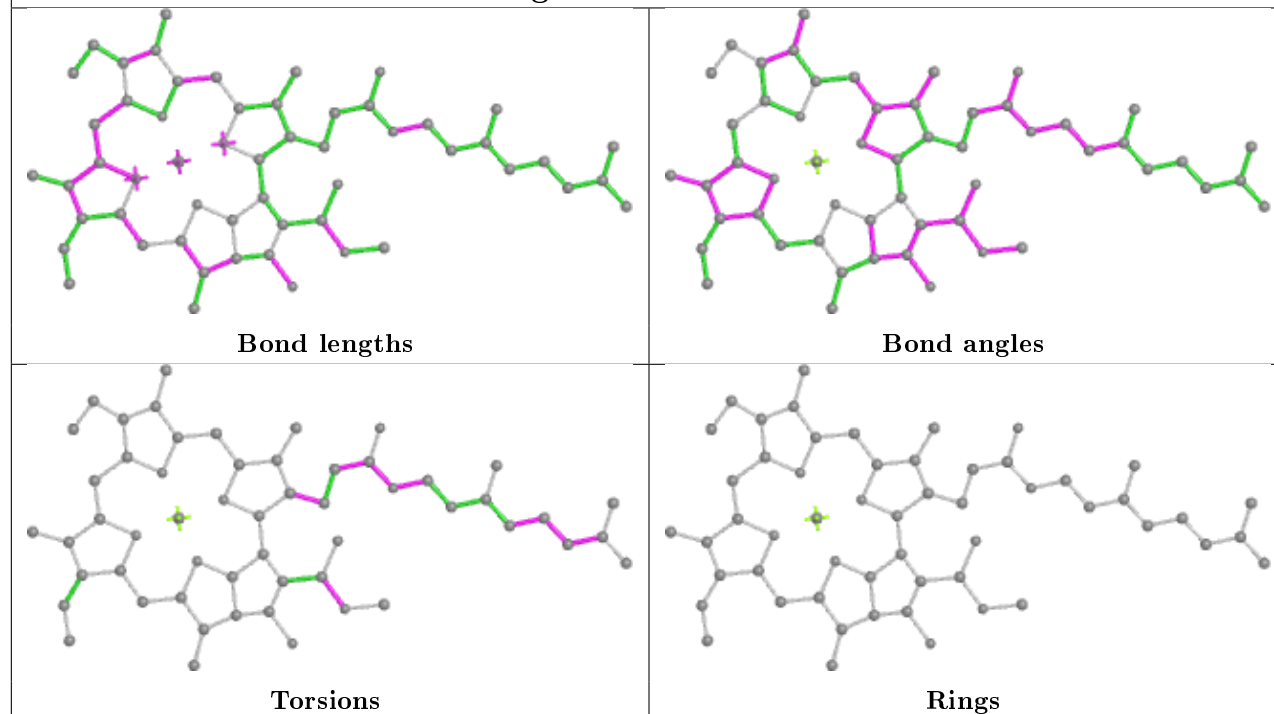


Ligand PQN G 844

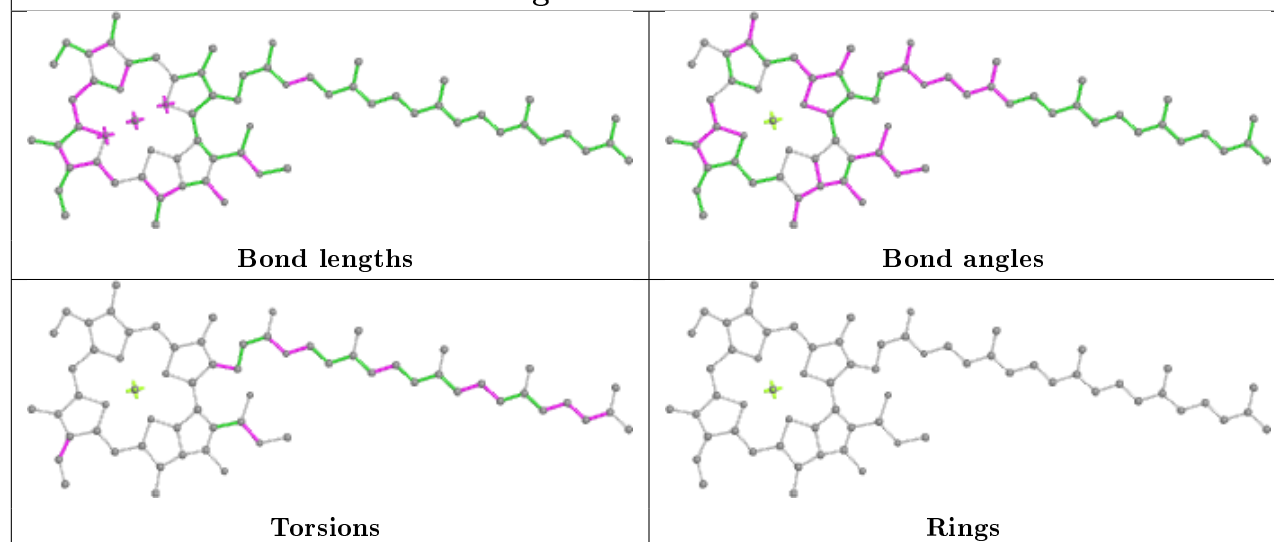


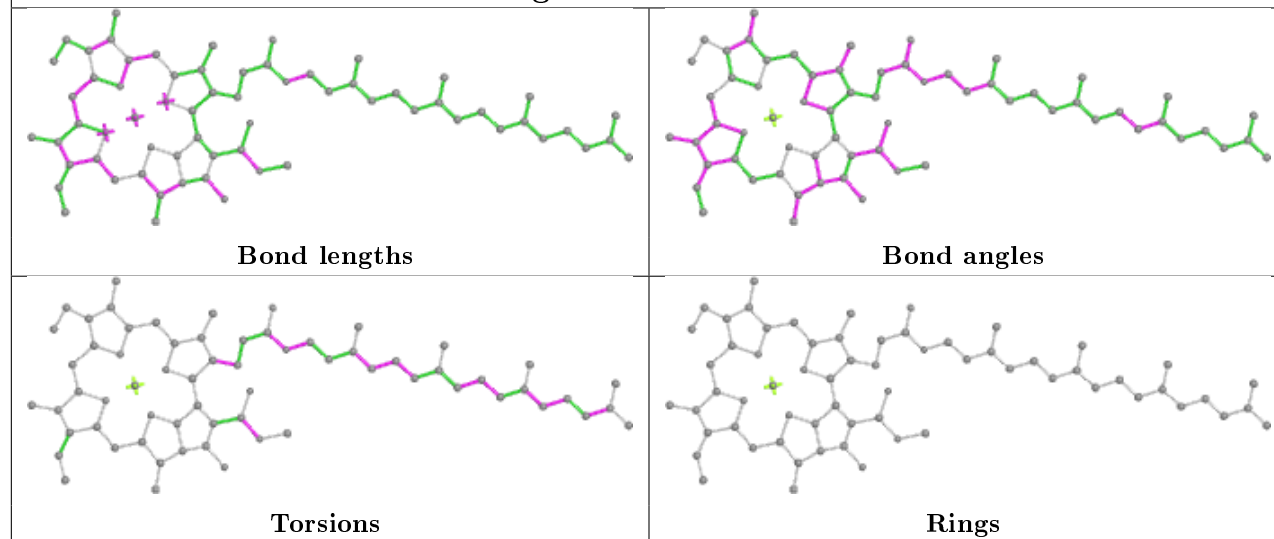
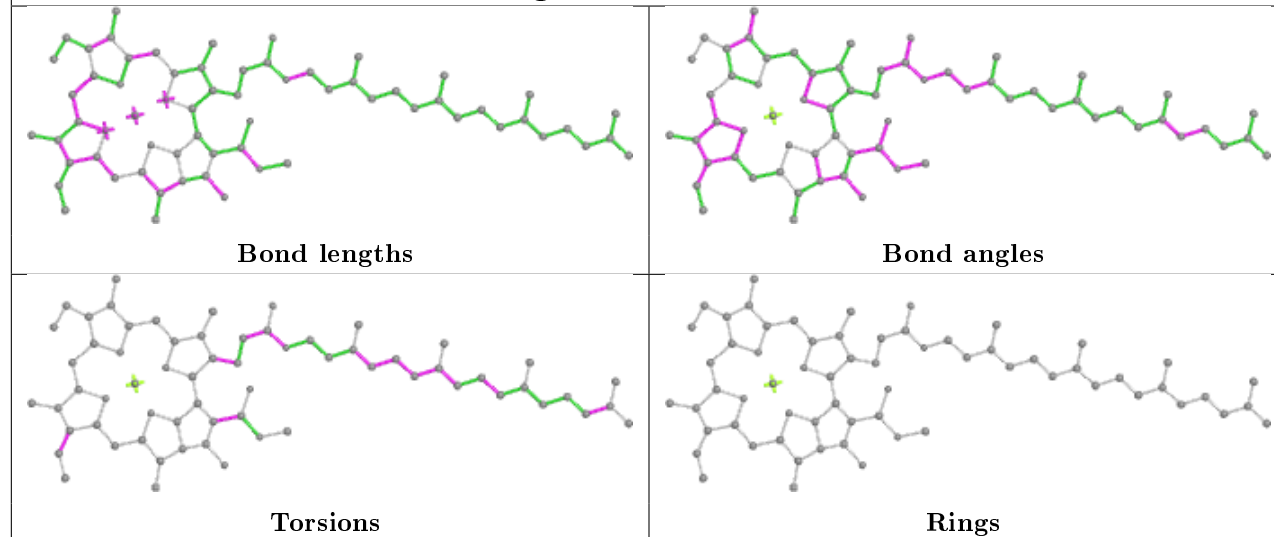
Ligand CLA Y 832**Ligand CLA A 827**

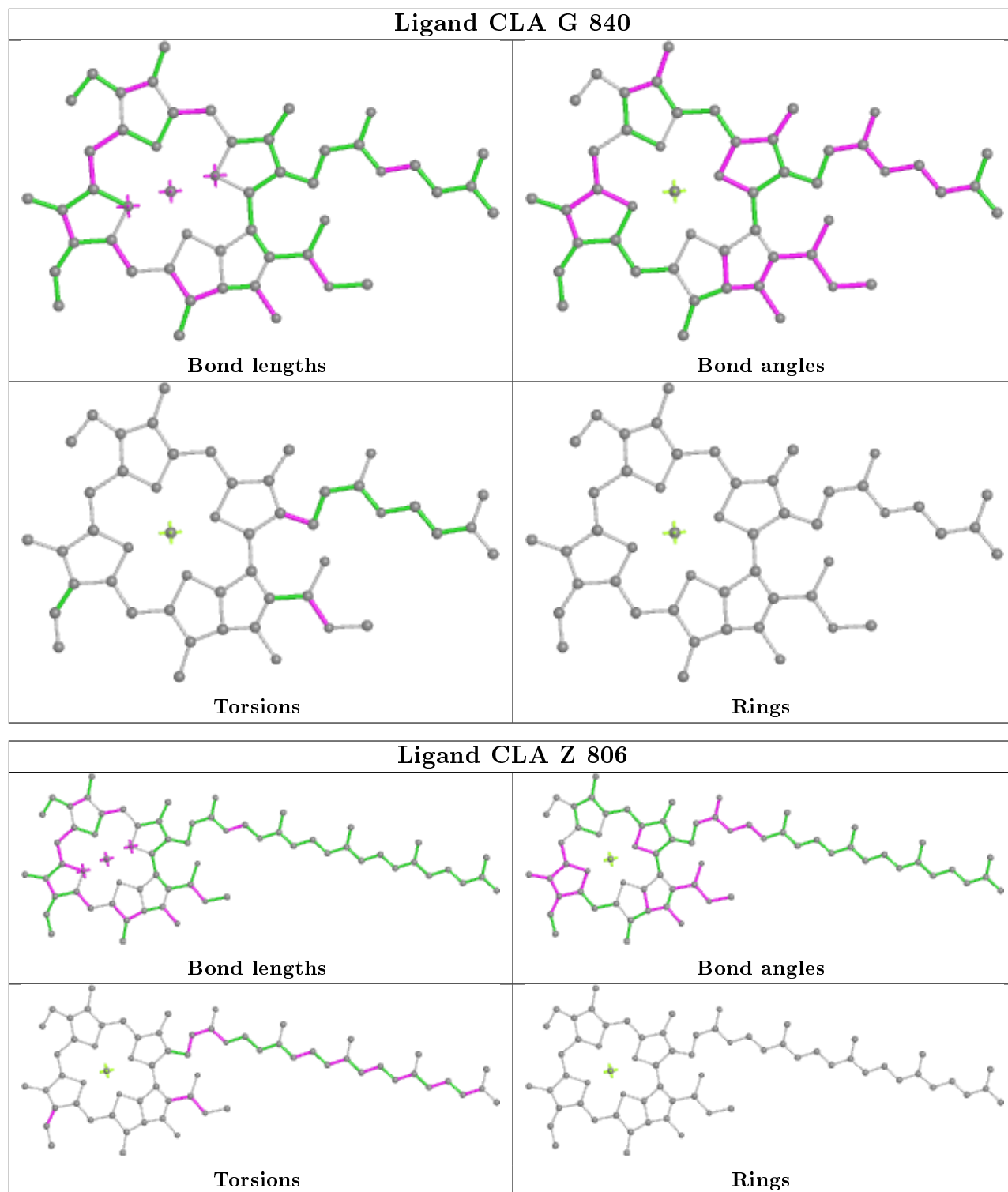
Ligand CLA H 830



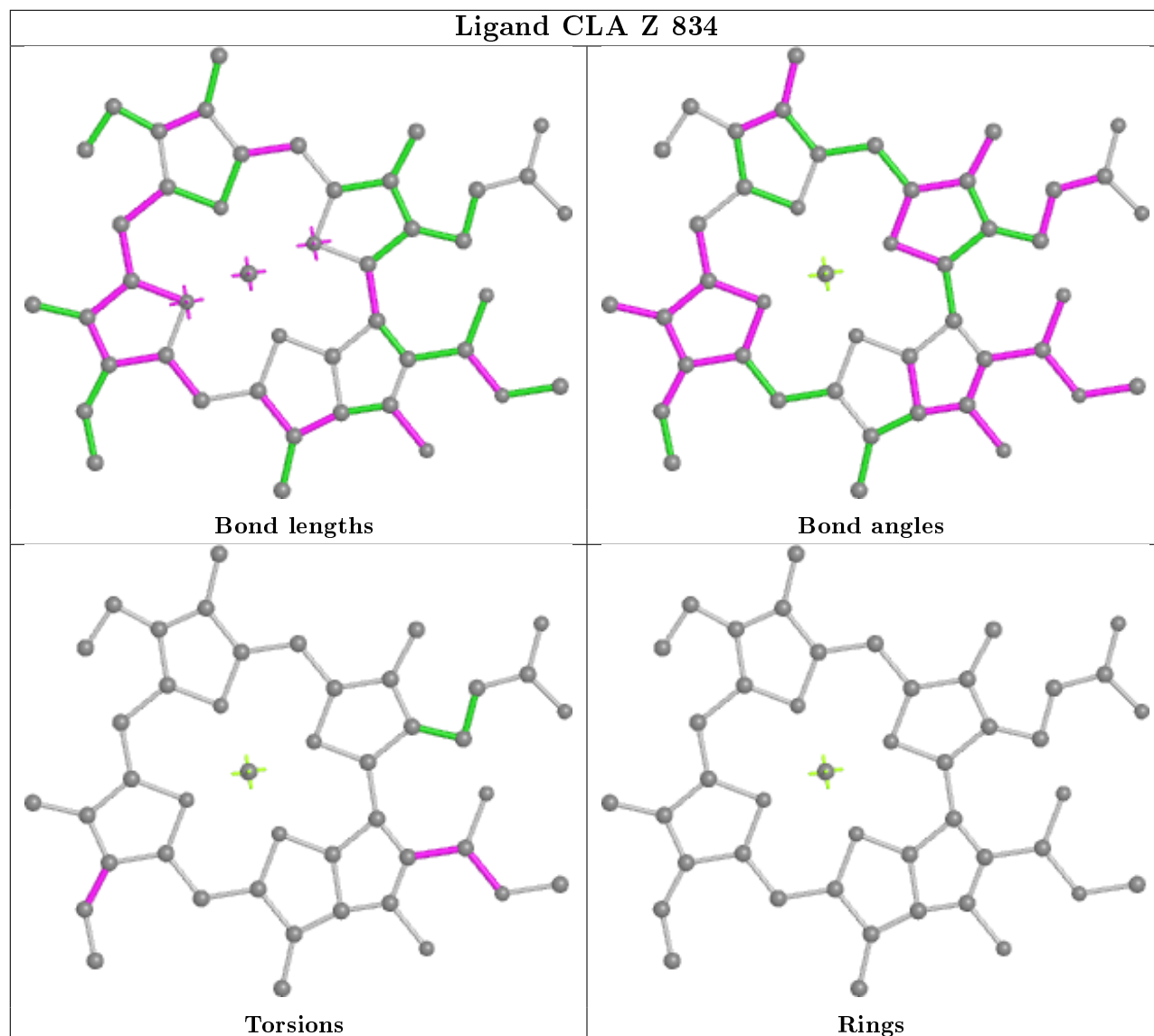
Ligand CLA Y 818



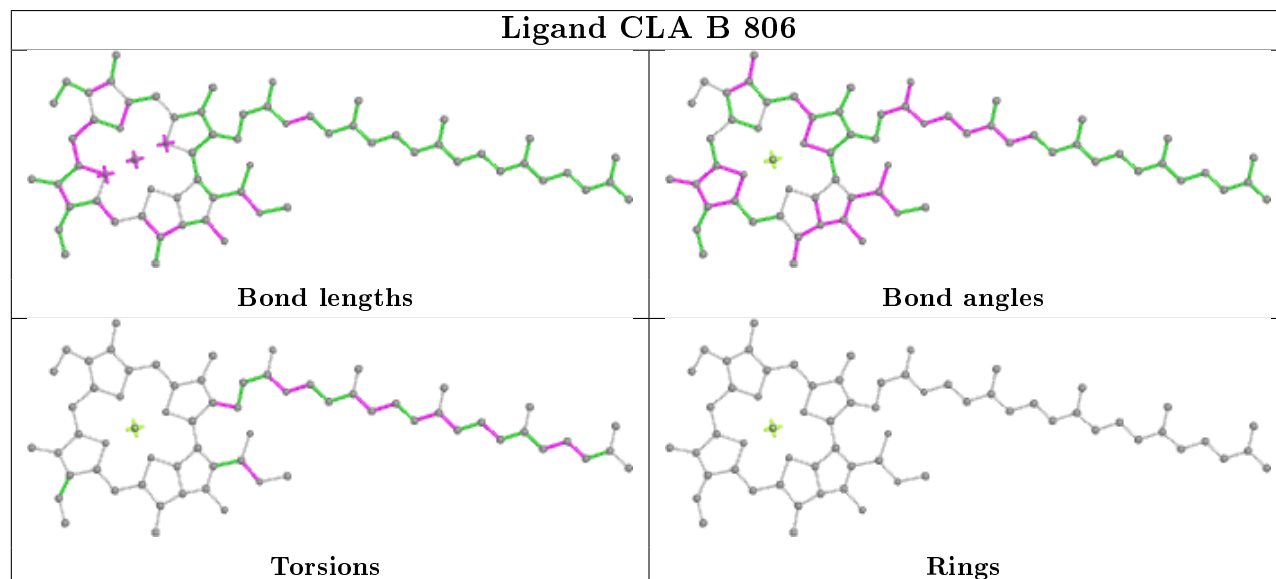
Ligand CLA A 809**Ligand CLA B 813**



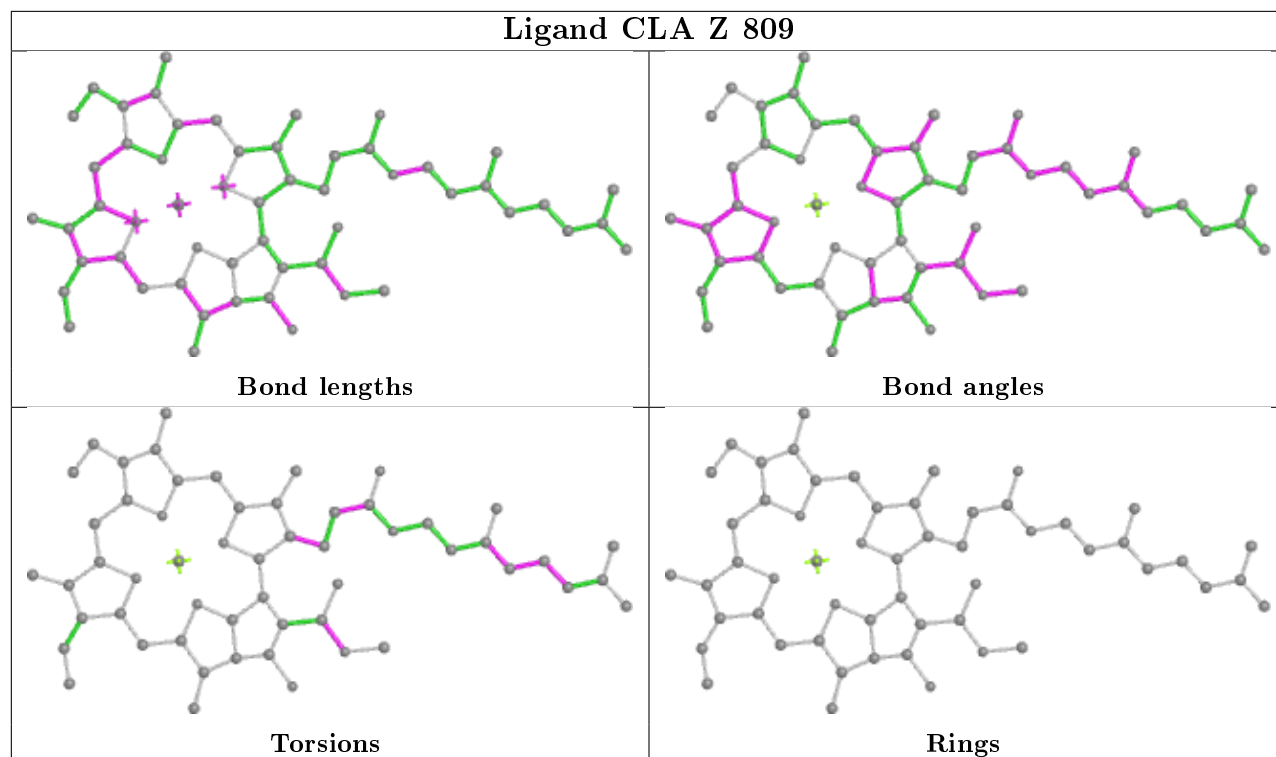
Ligand CLA Z 834



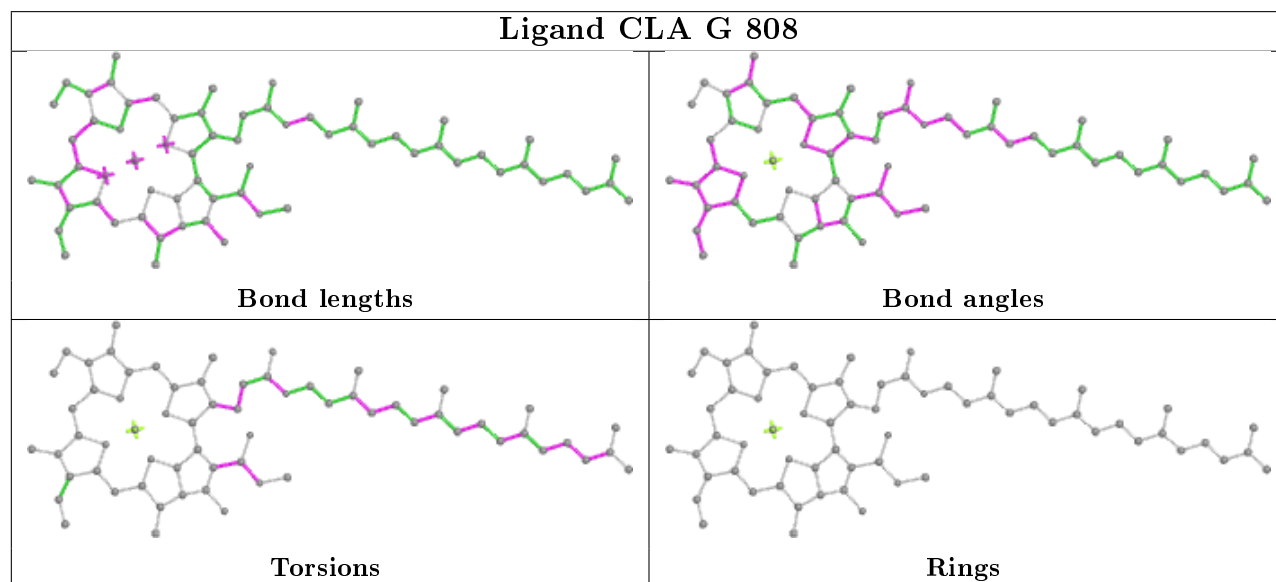
Ligand CLA B 806



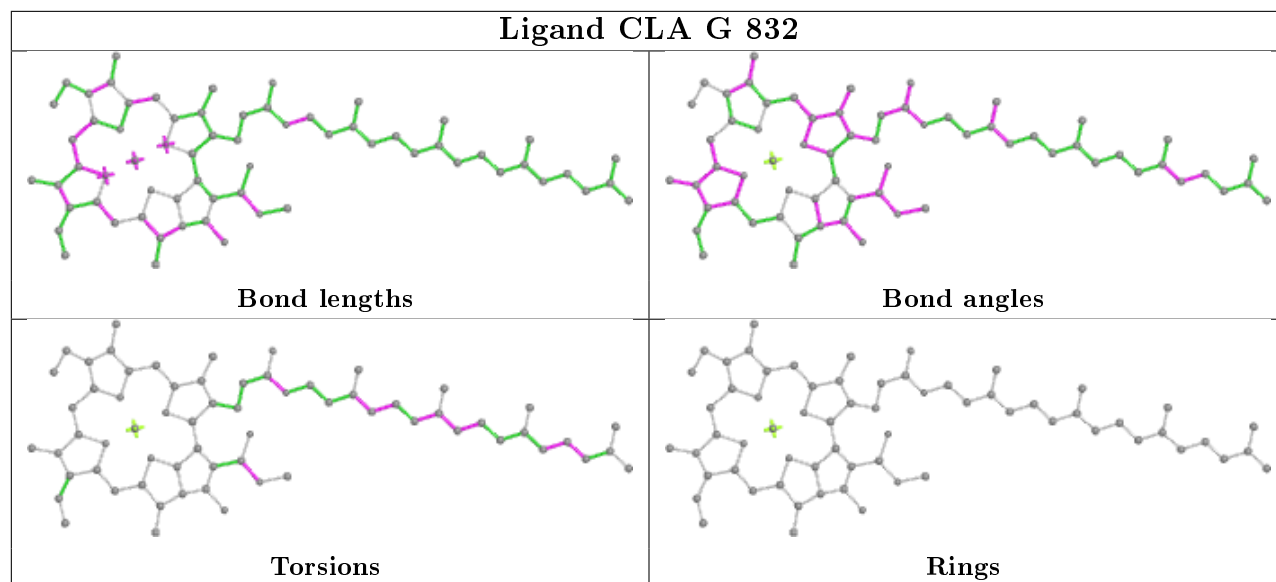
Ligand CLA Z 809



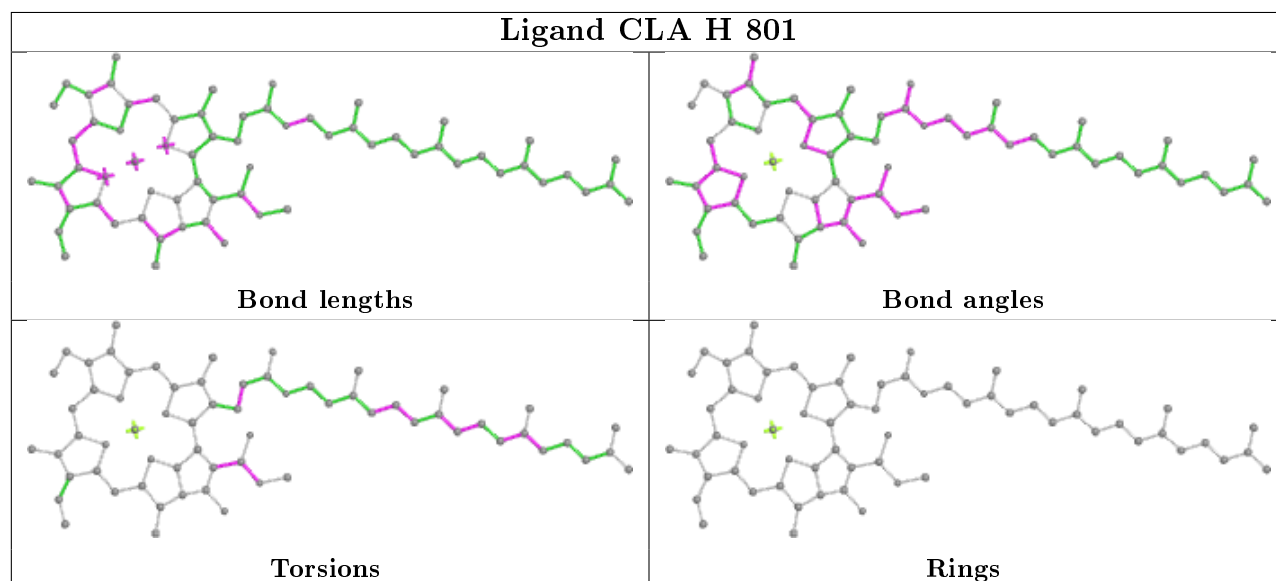
Ligand CLA G 808



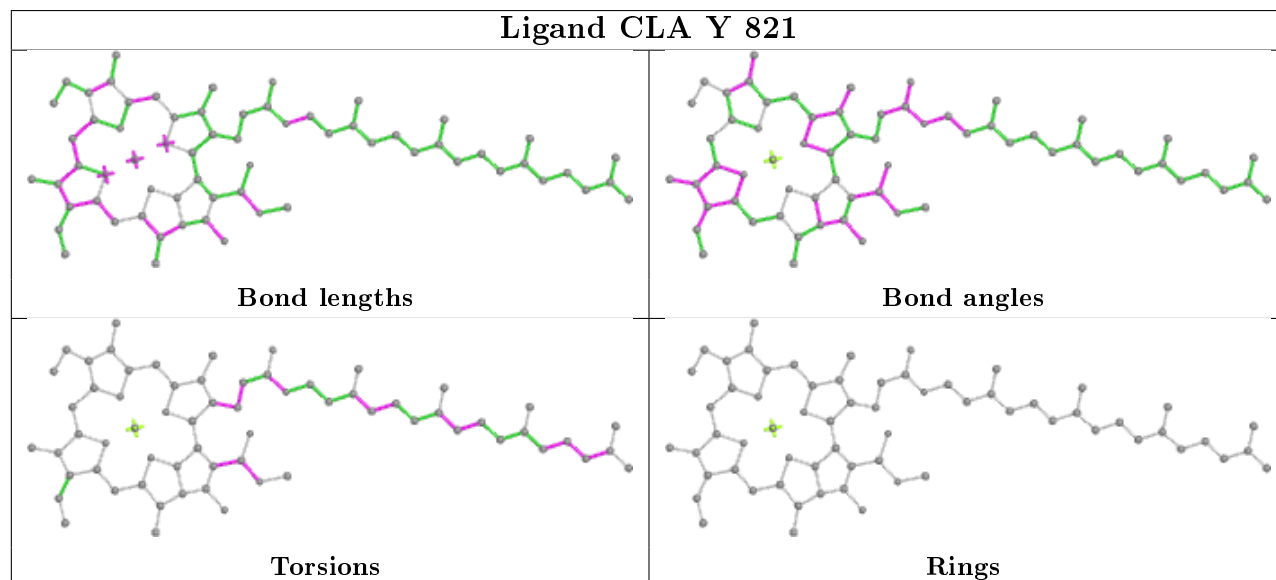
Ligand CLA G 832



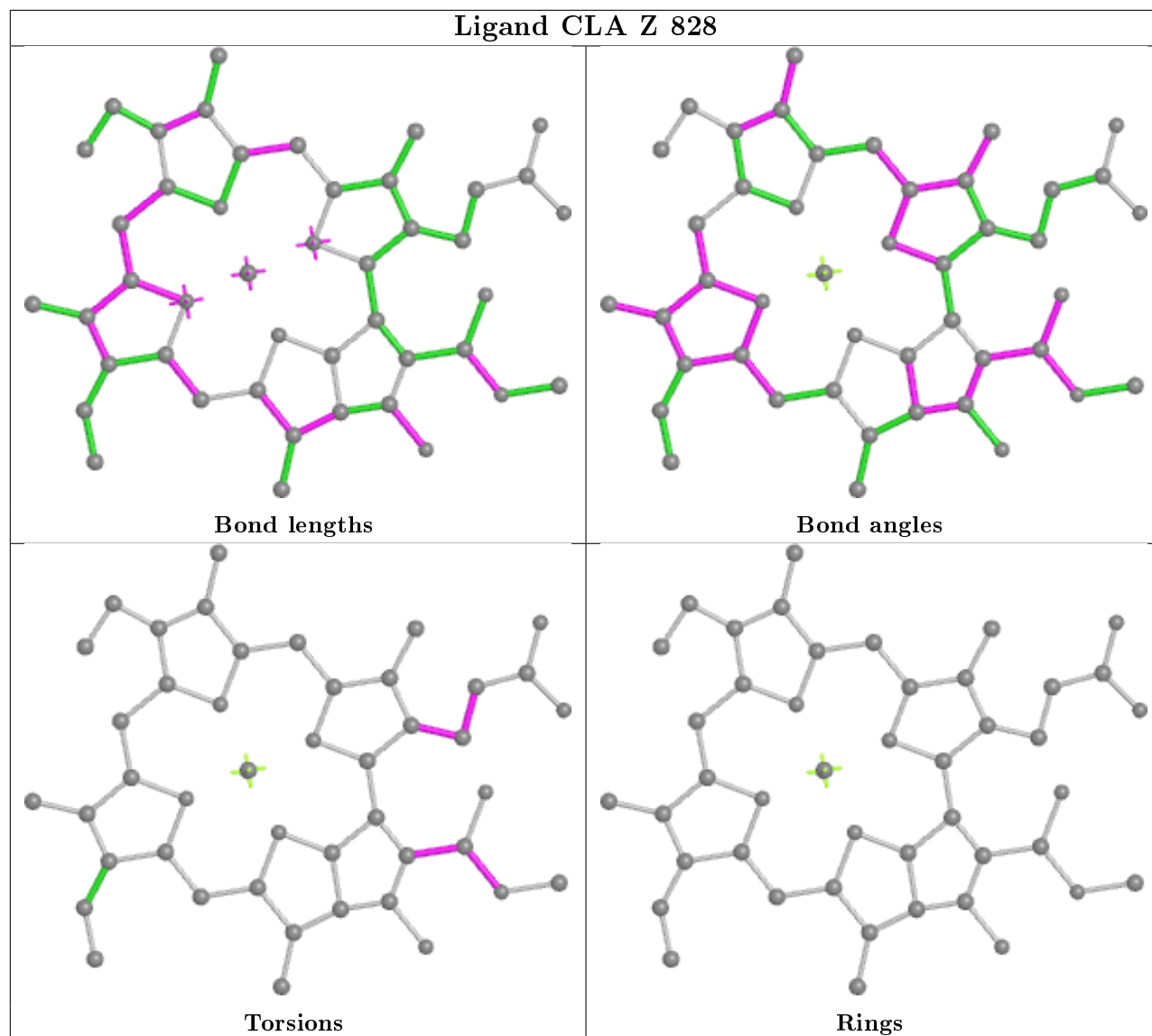
Ligand CLA H 801



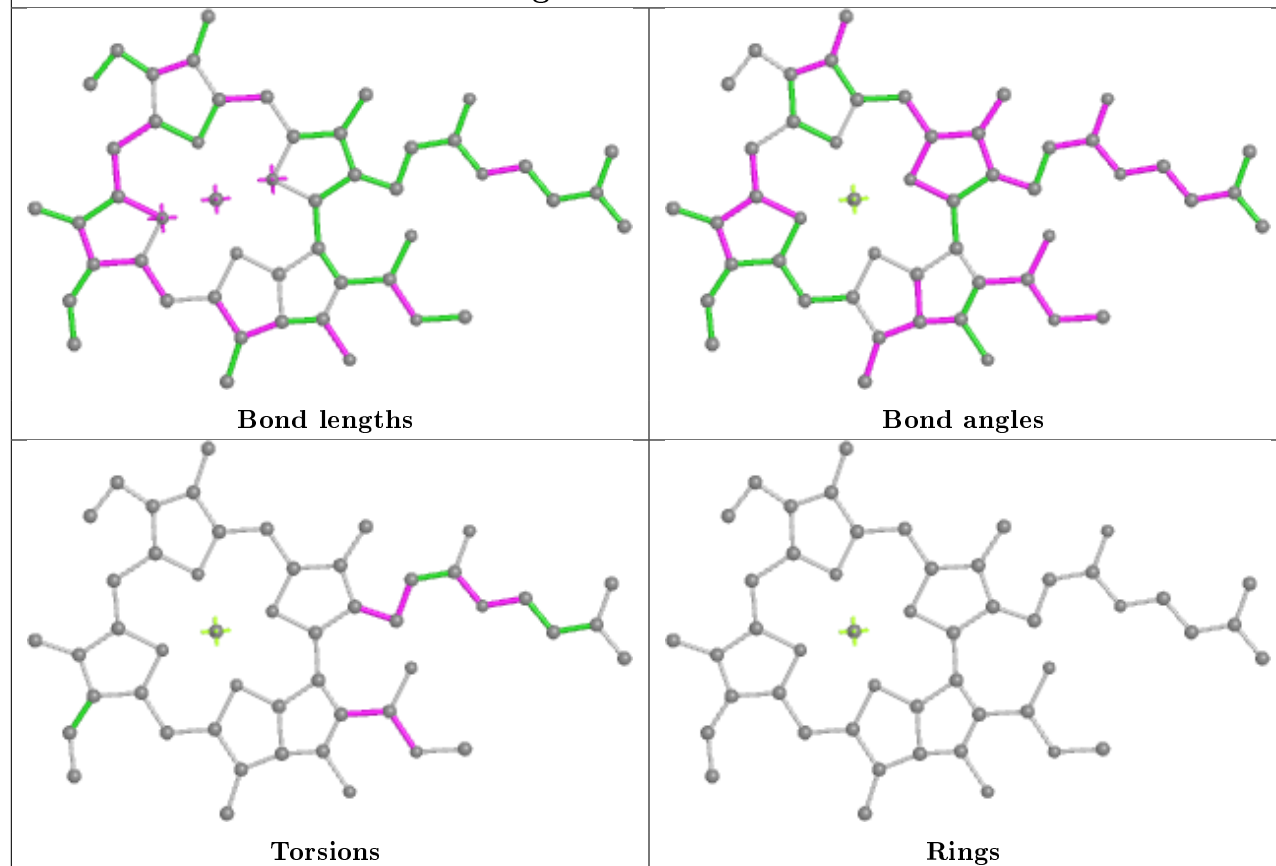
Ligand CLA Y 821



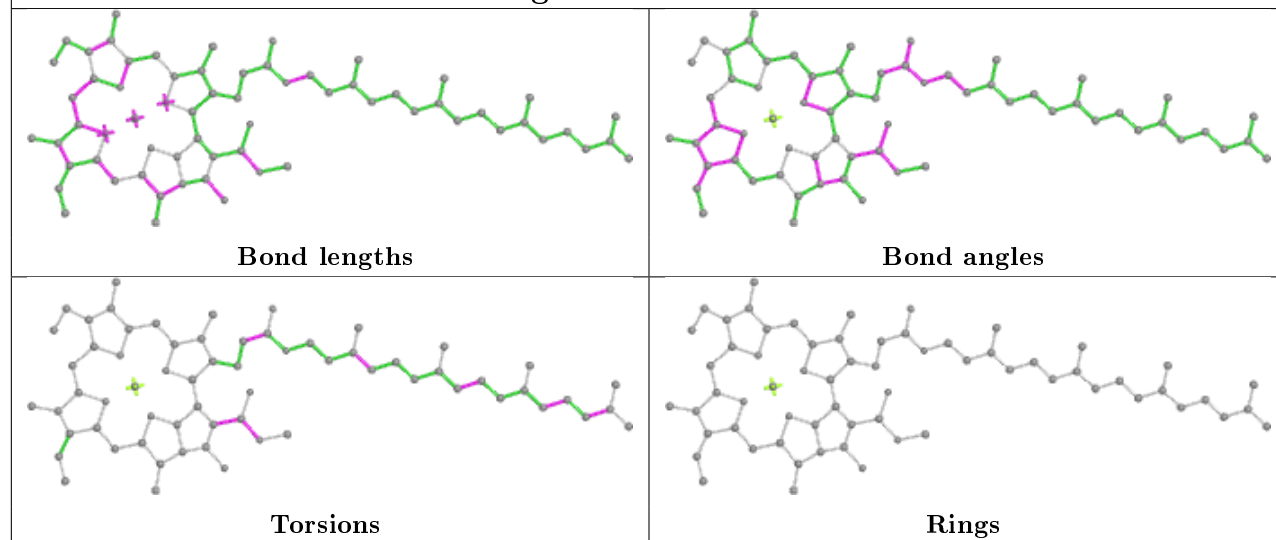
Ligand CLA Z 828



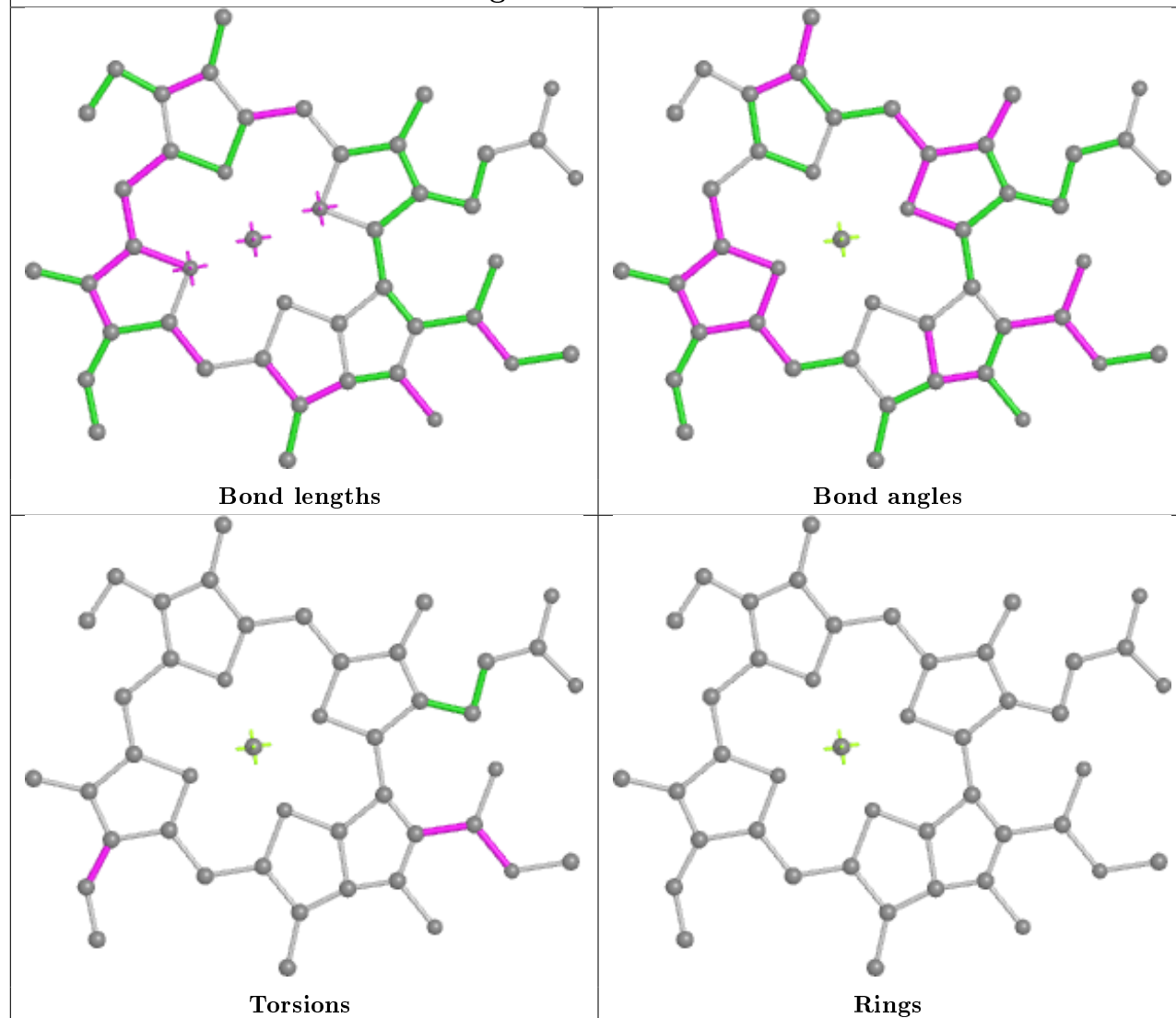
Ligand CLA B 812



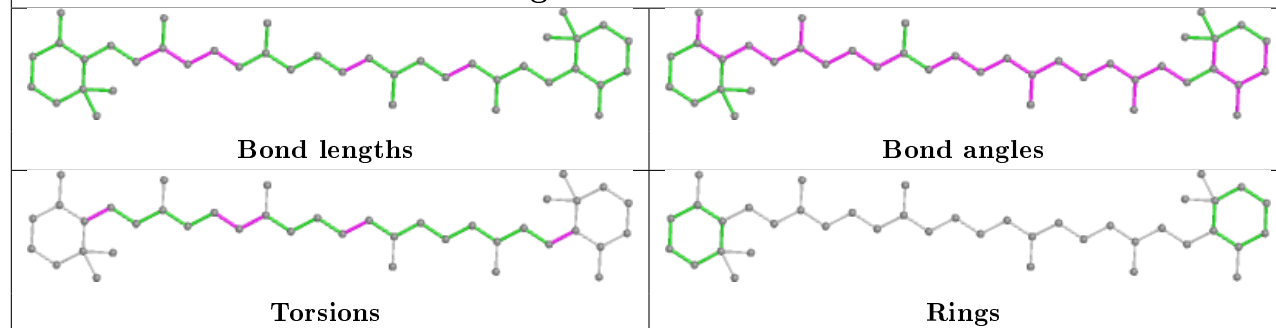
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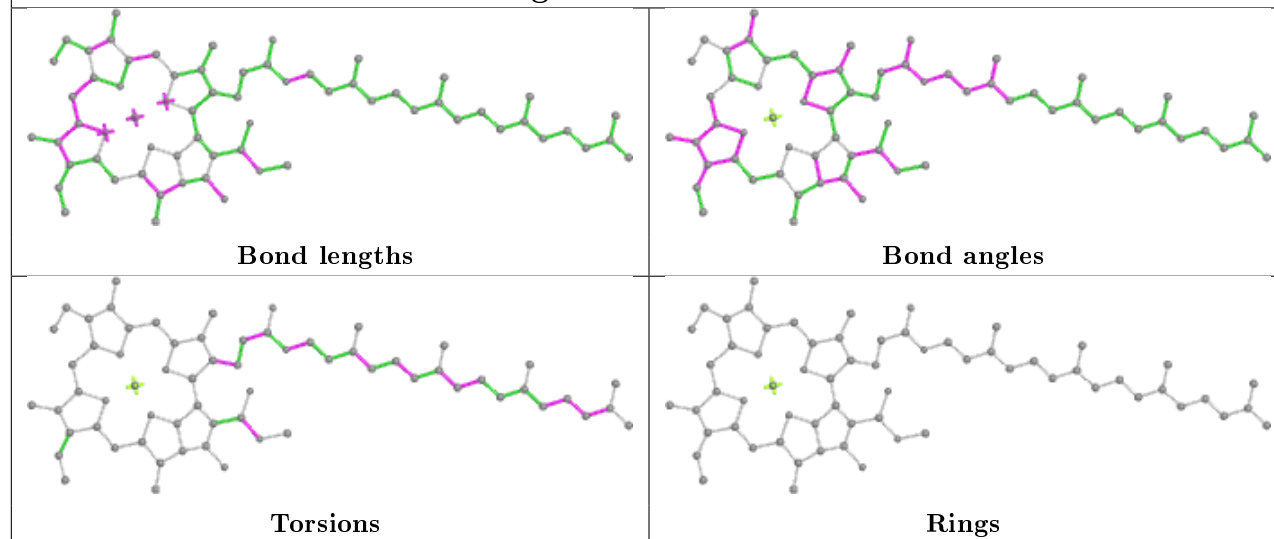
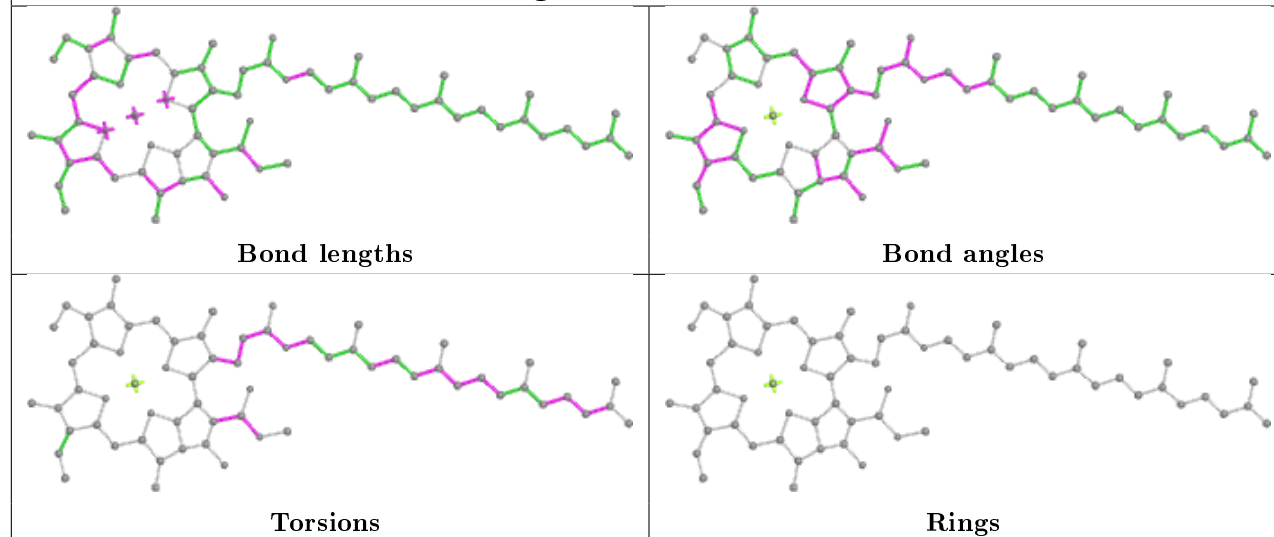


Ligand CLA G 810

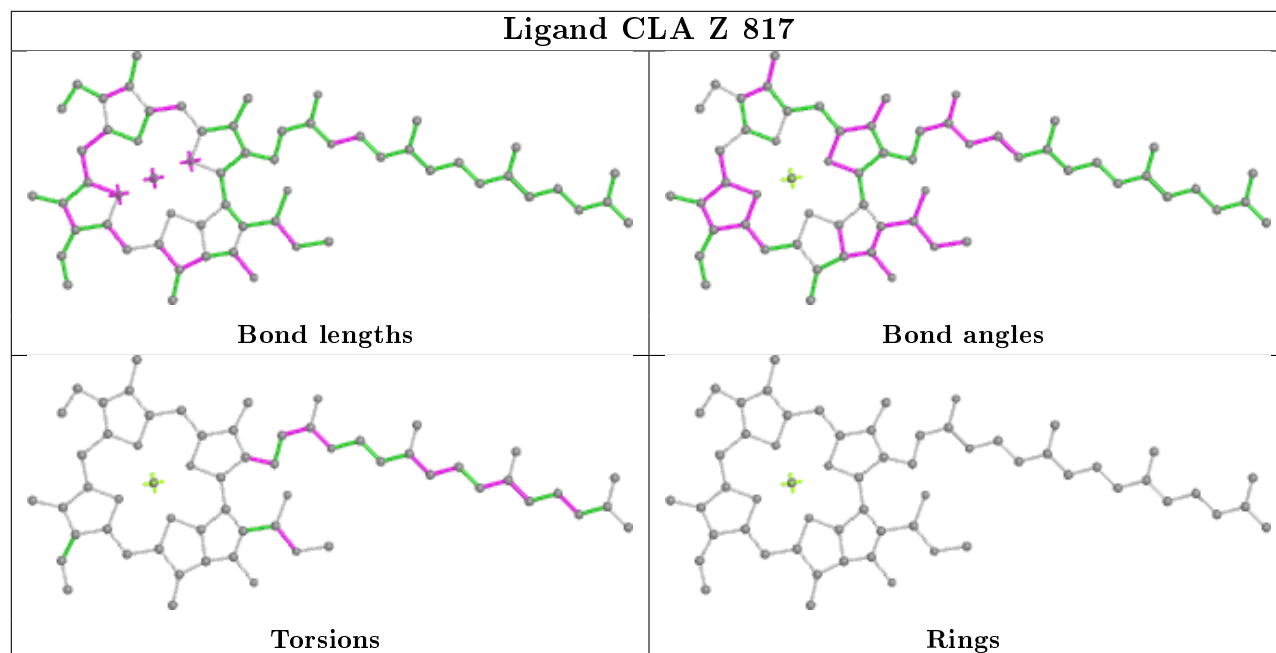


Ligand BCR A 848

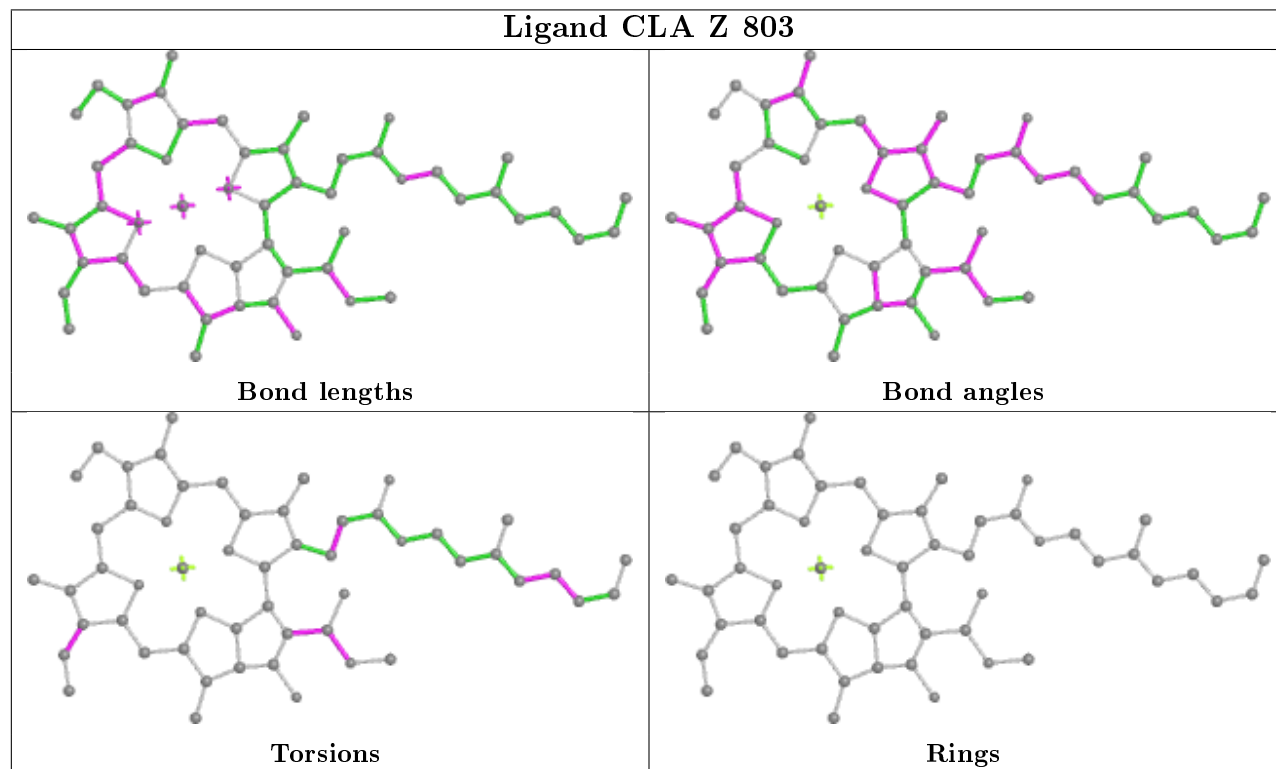


Ligand CLA G 841**Ligand CLA A 805**

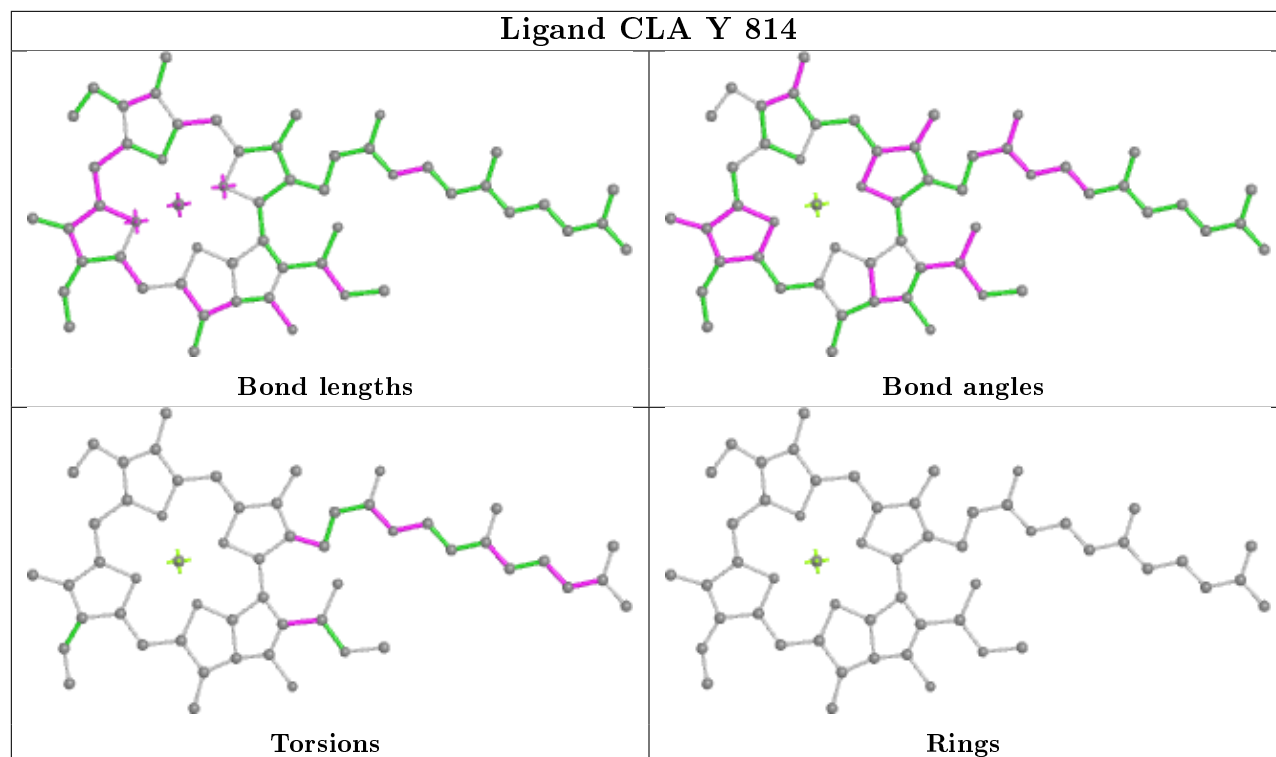
Ligand CLA Z 817



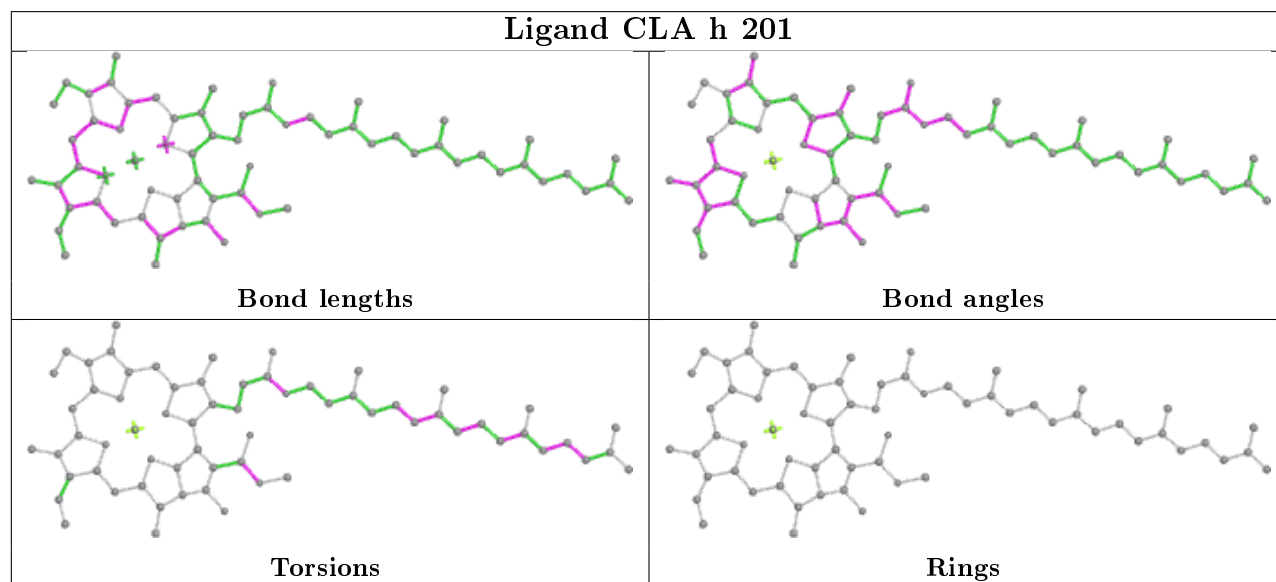
Ligand CLA Z 803



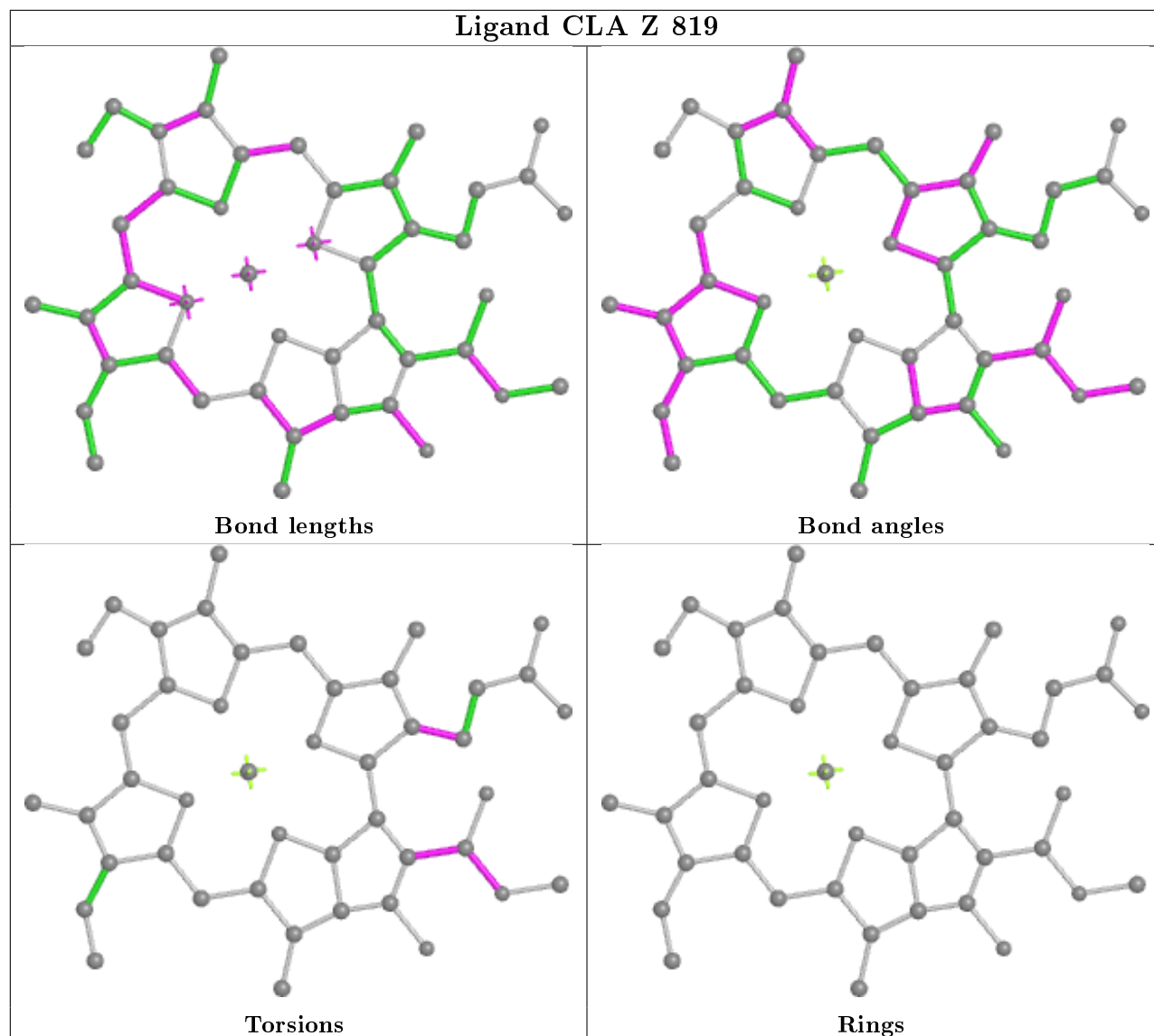
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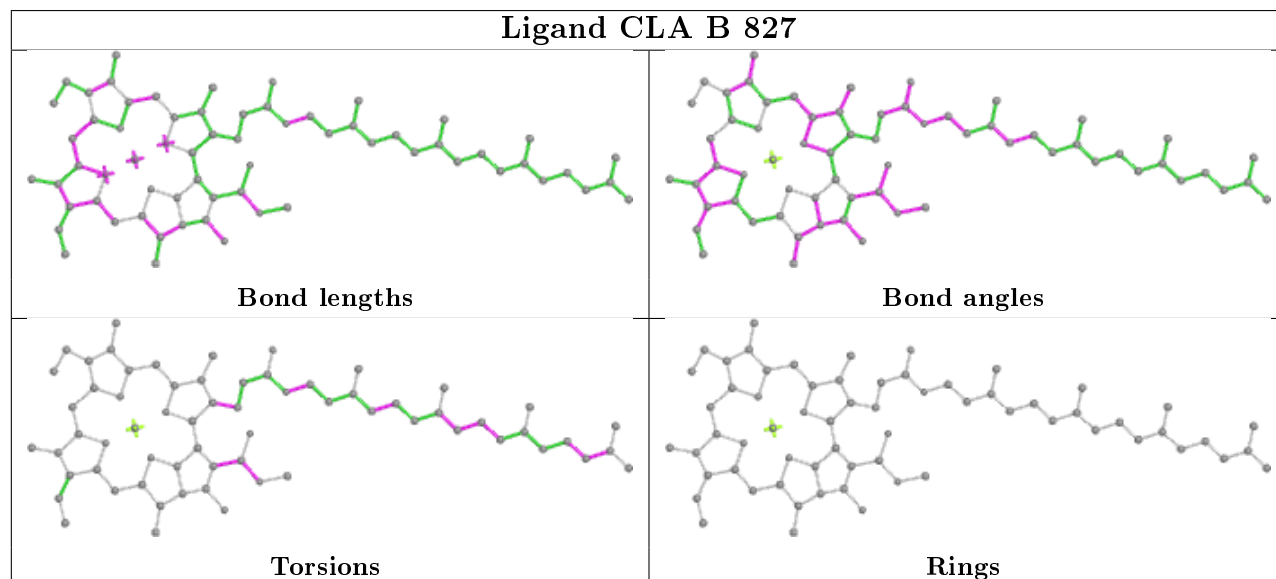
Ligand CLA h 201

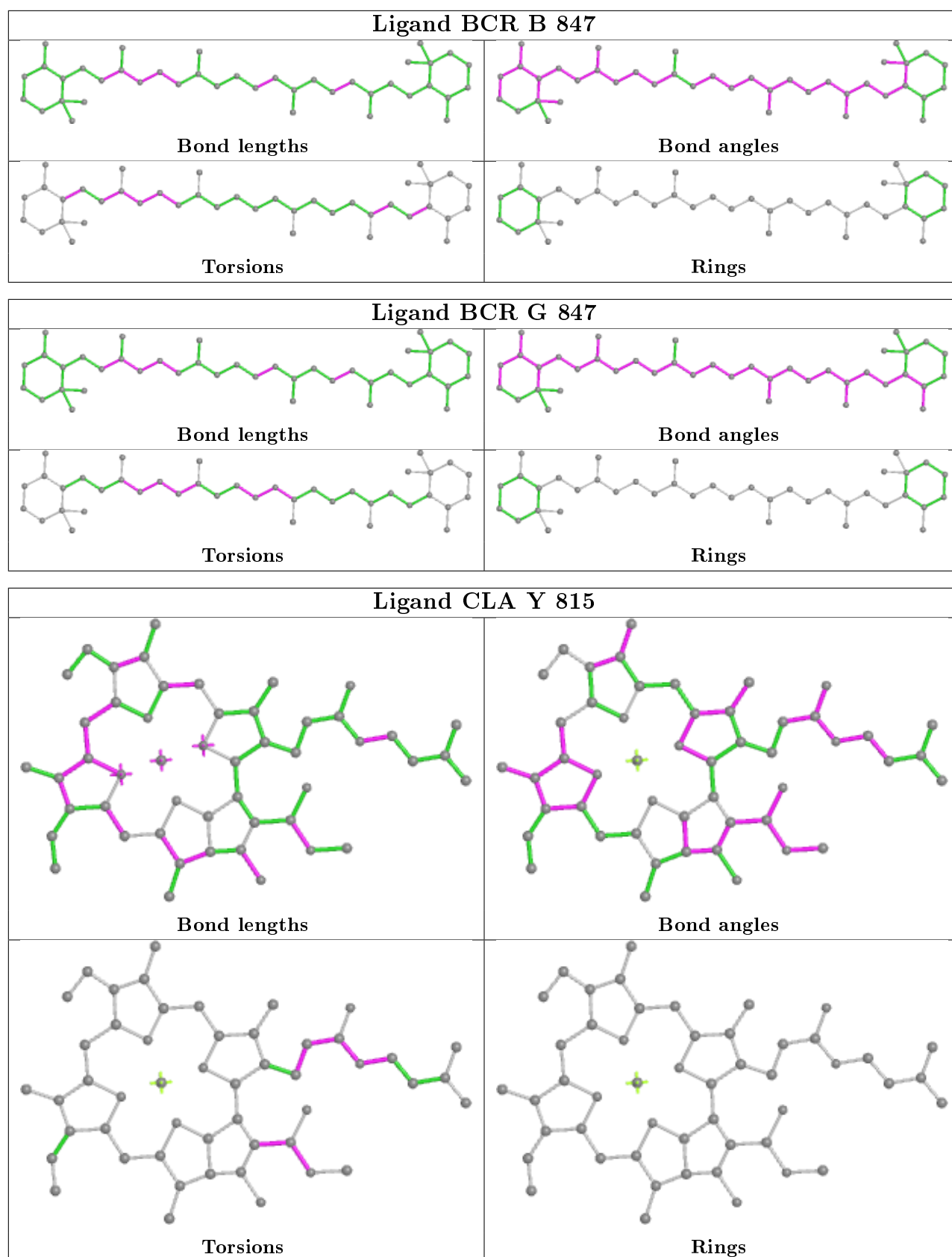


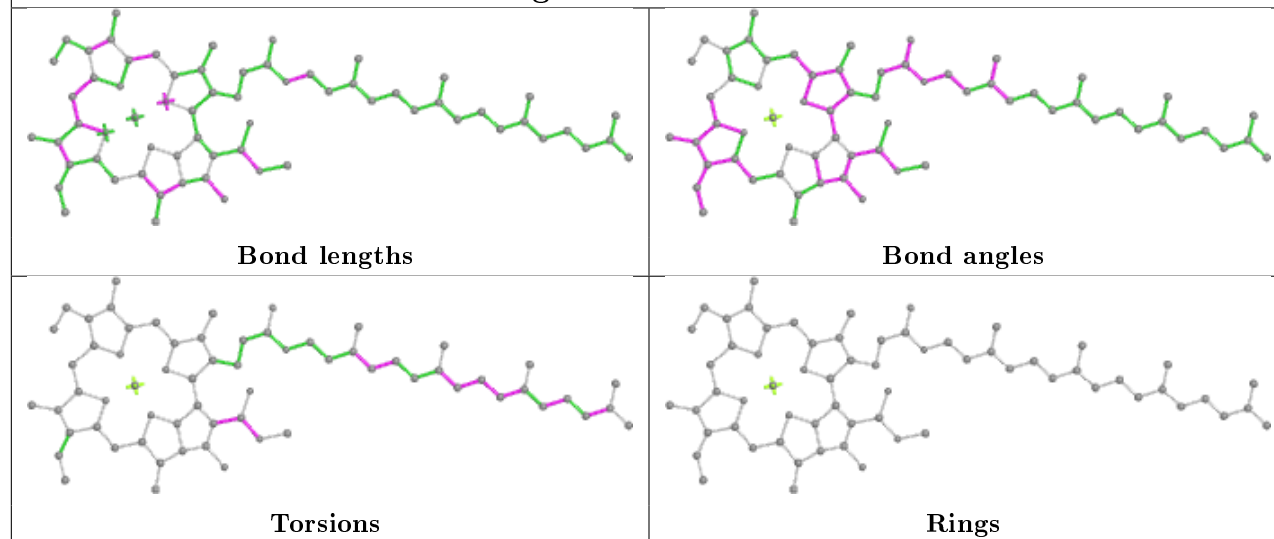
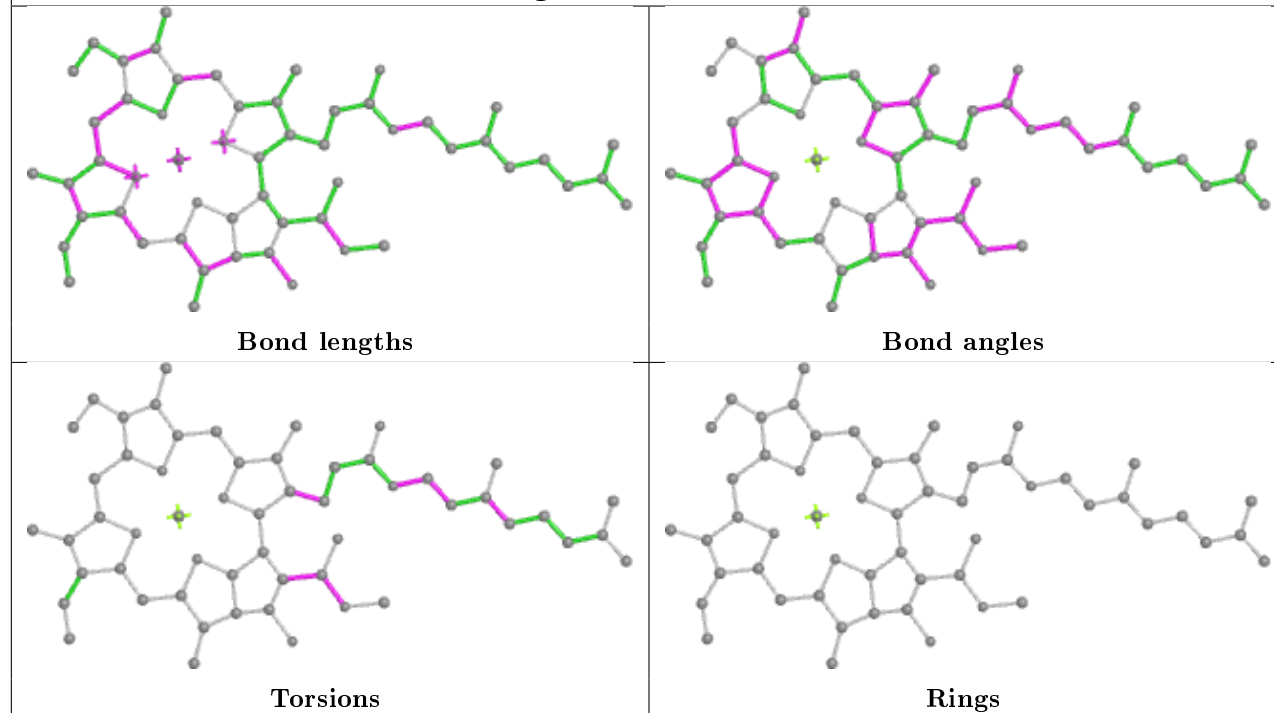
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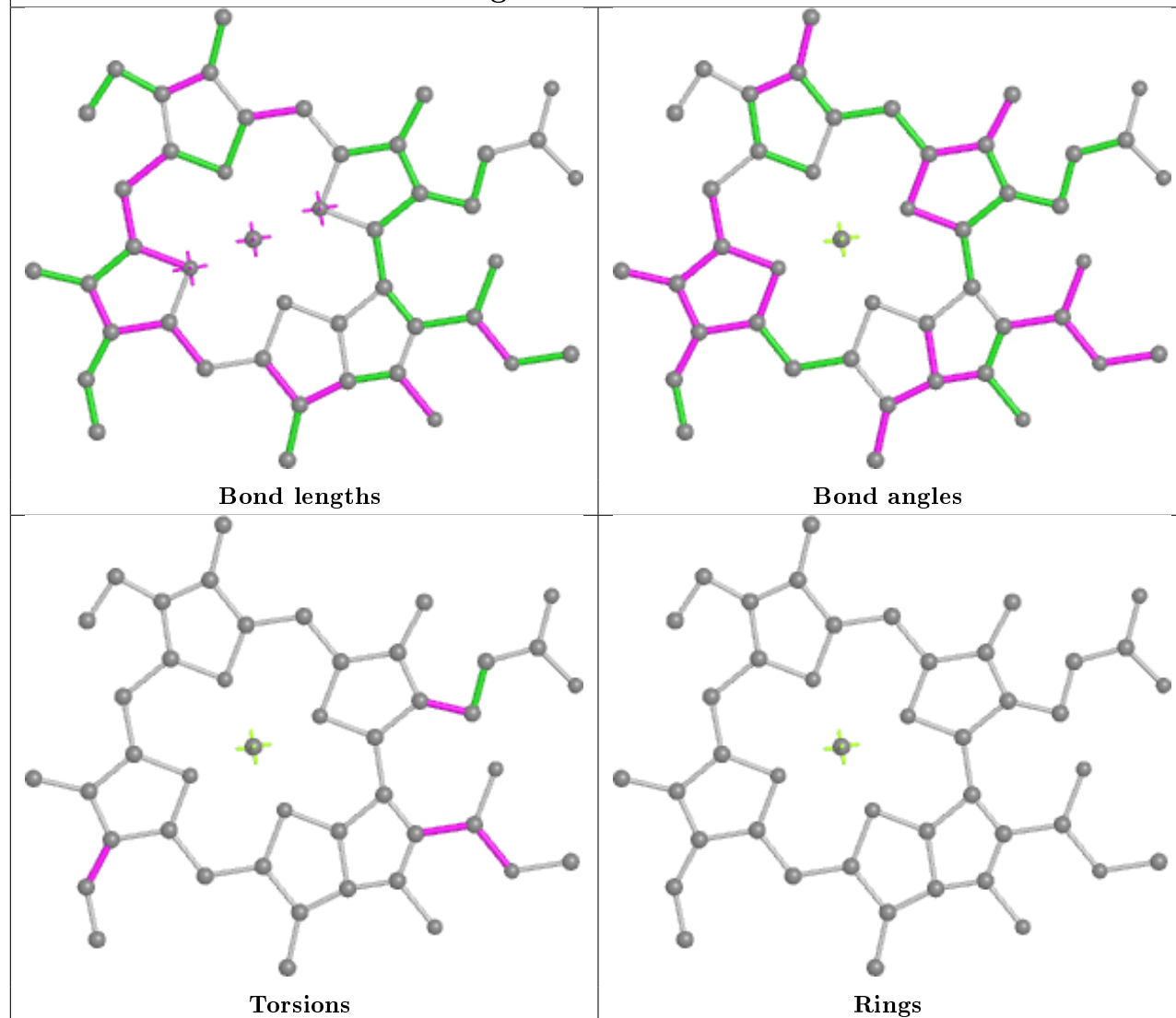
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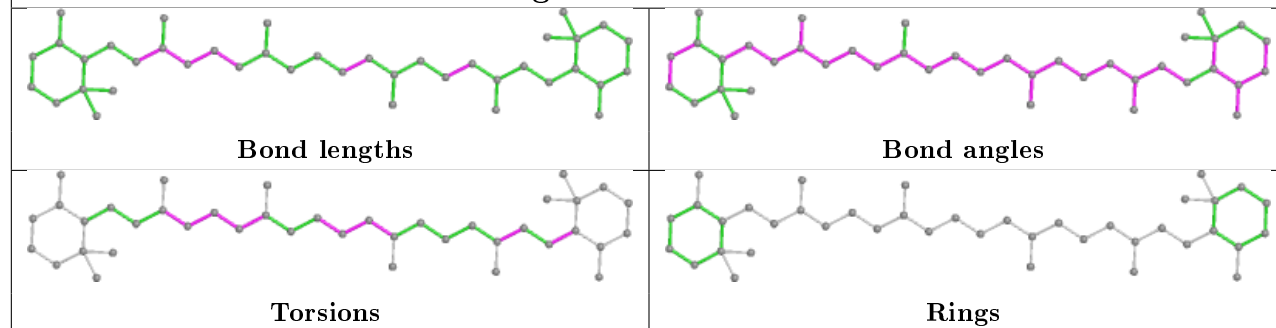


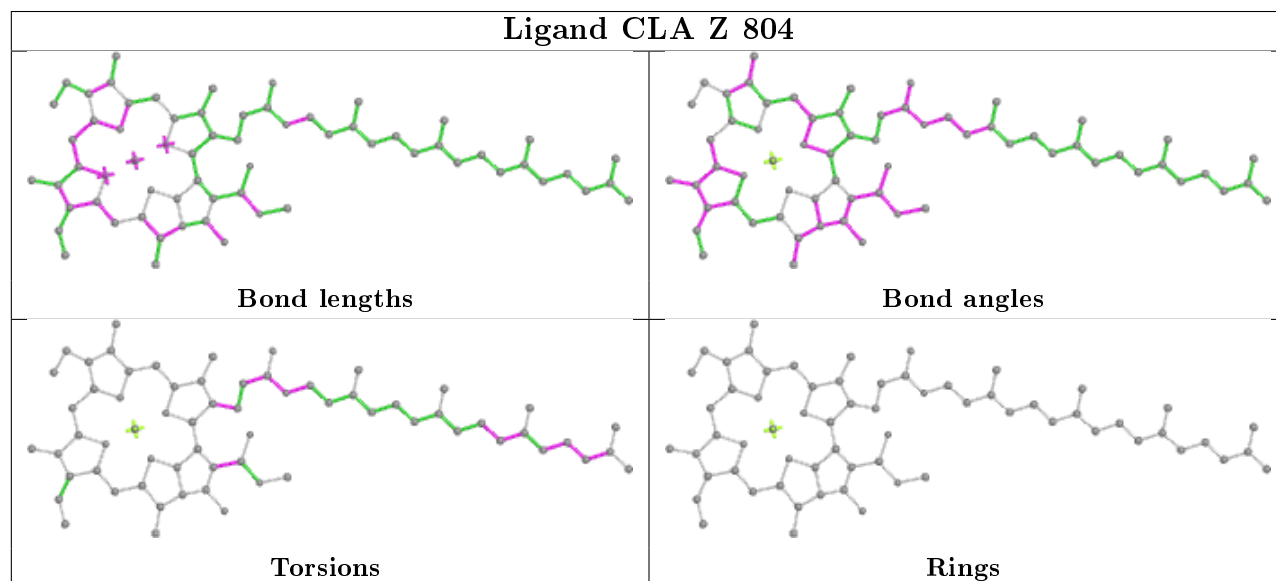
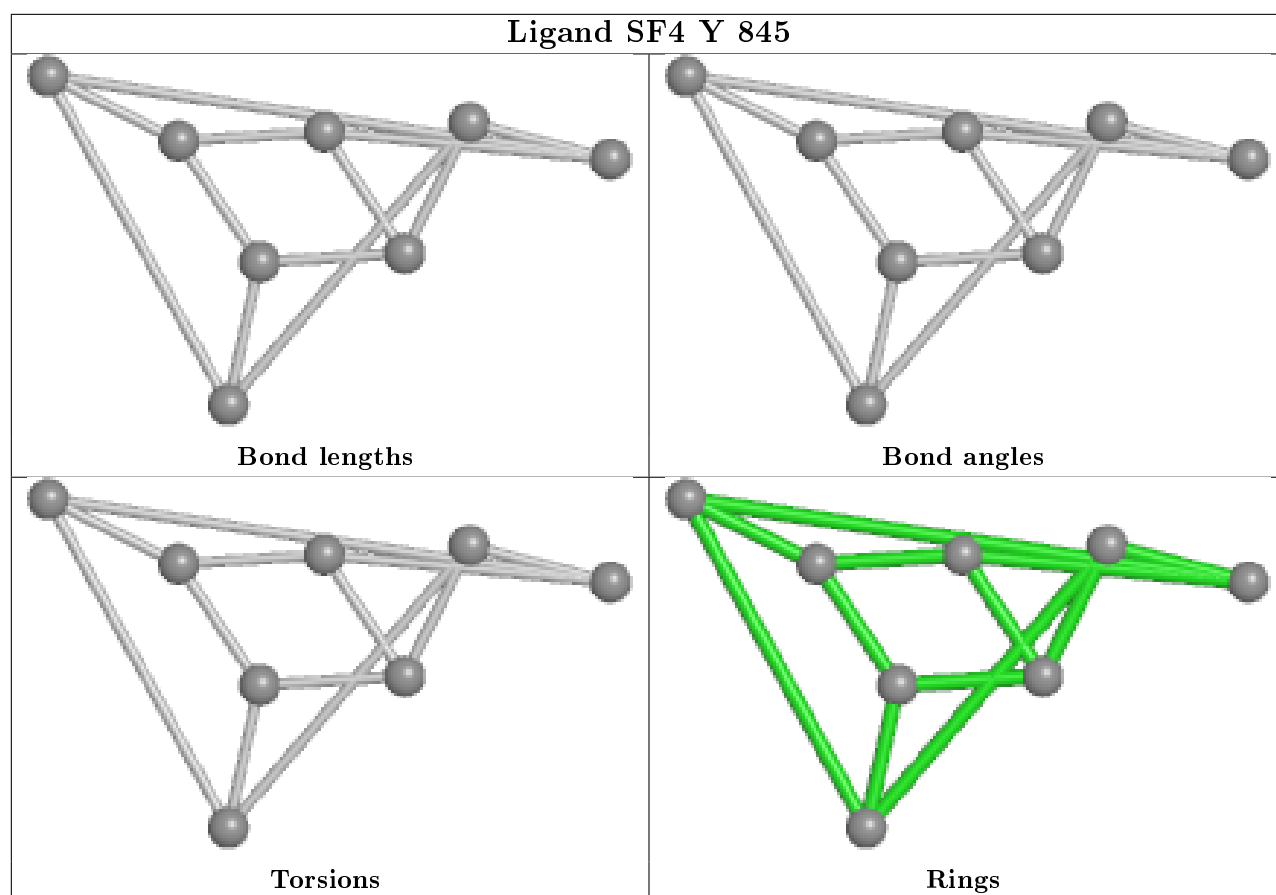
Ligand CLA B 803**Ligand CLA B 824**

Ligand CLA B 821

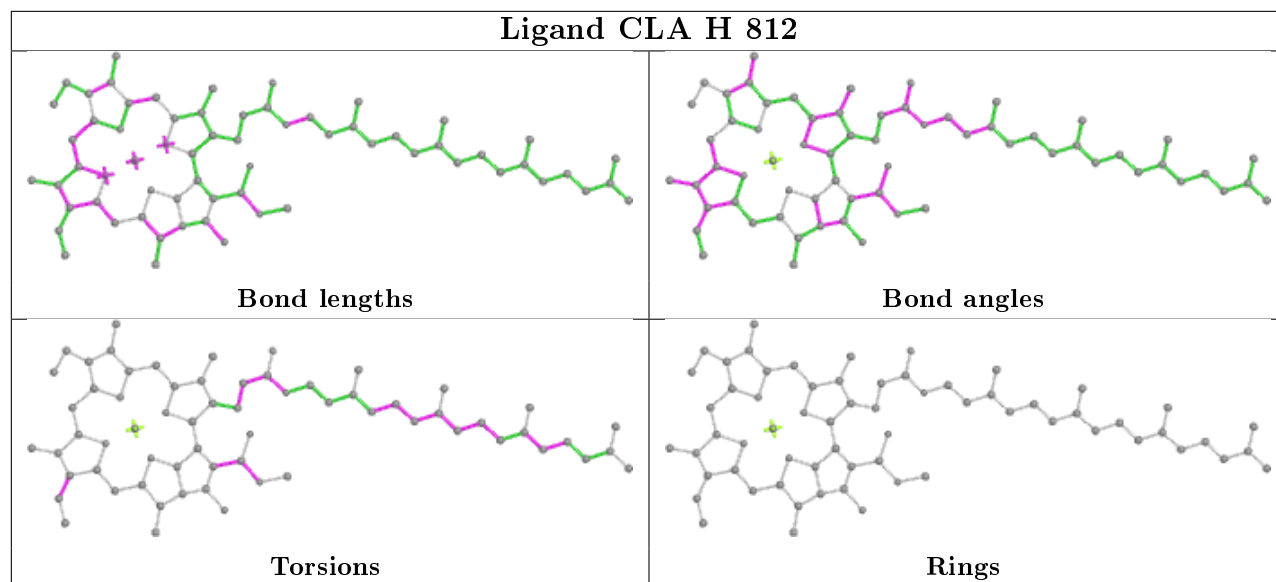


Ligand BCR Z 841

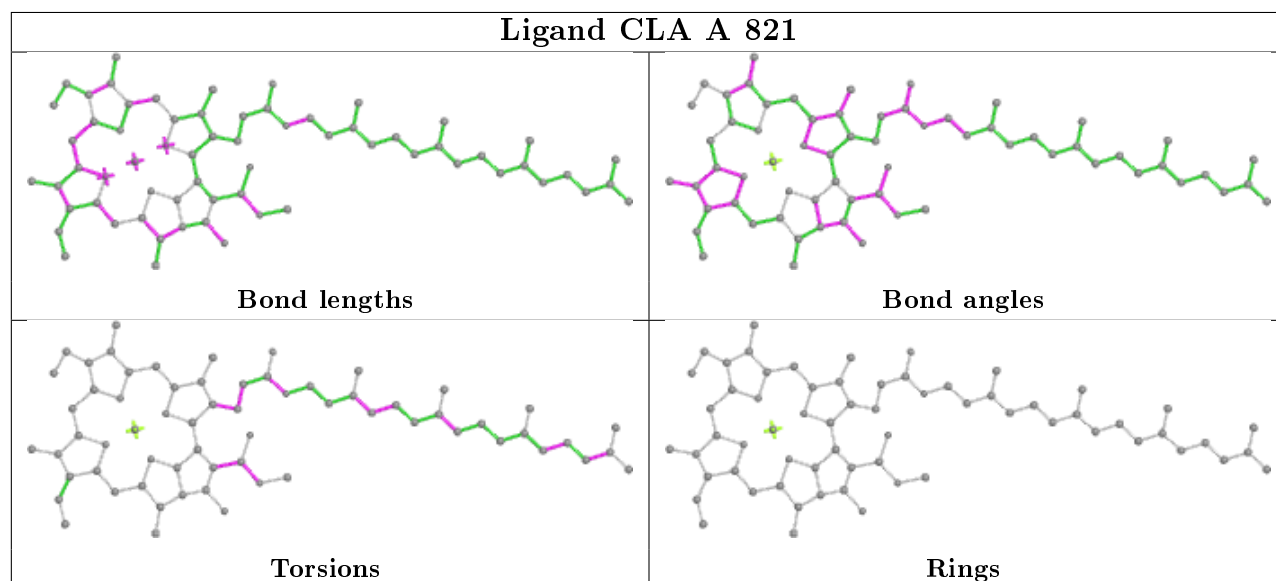




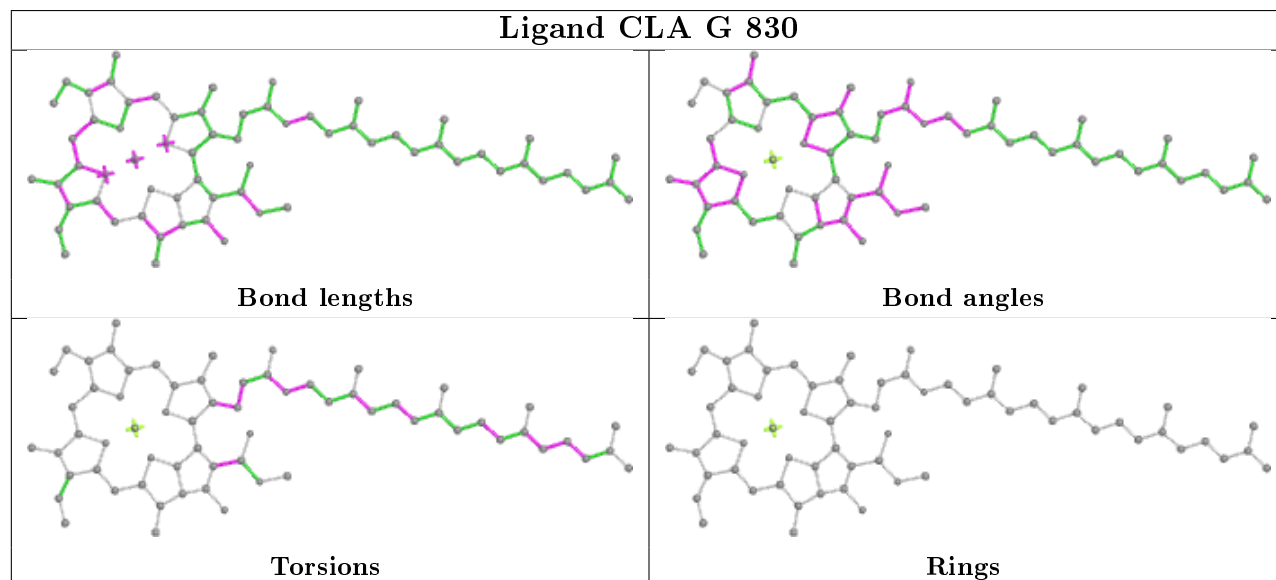
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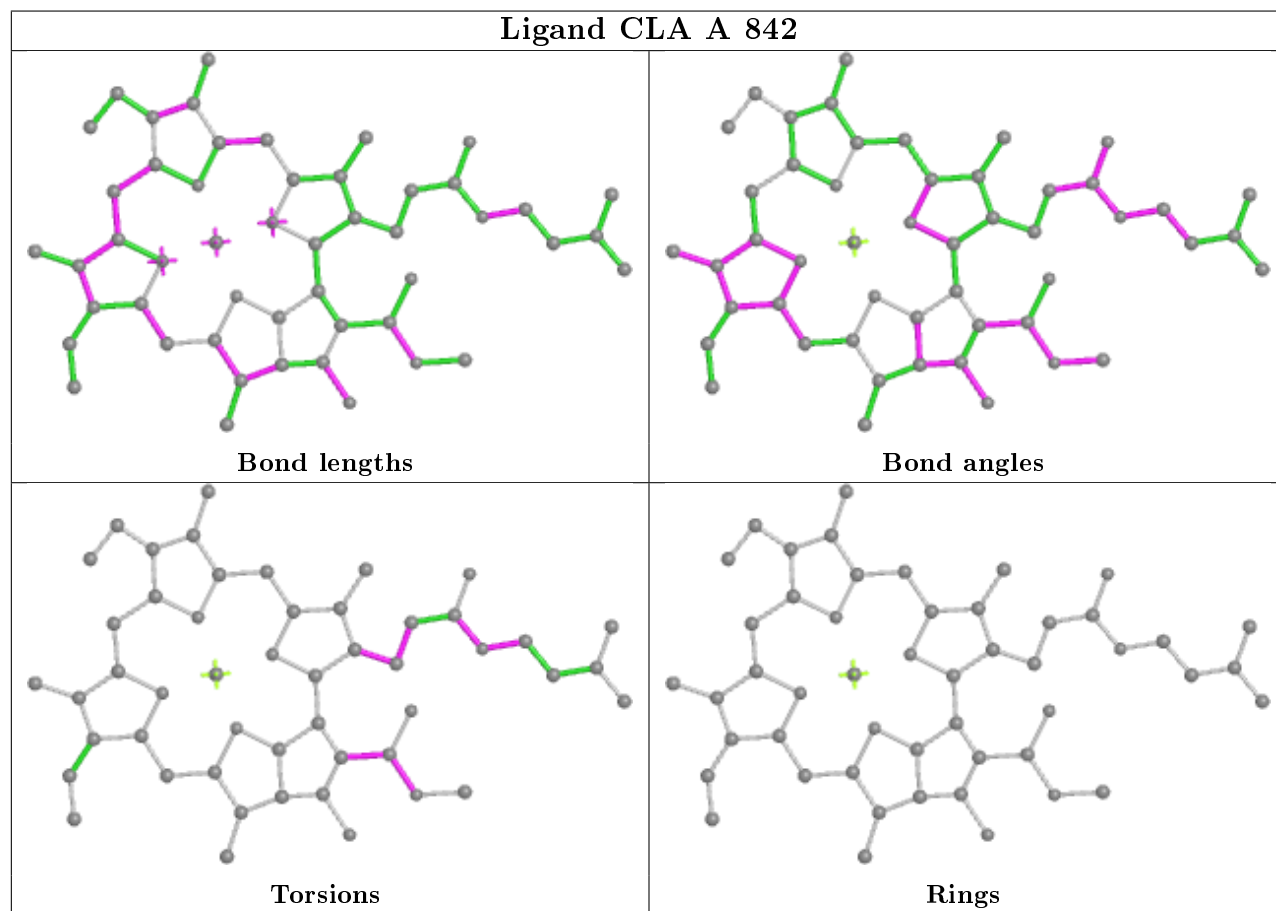
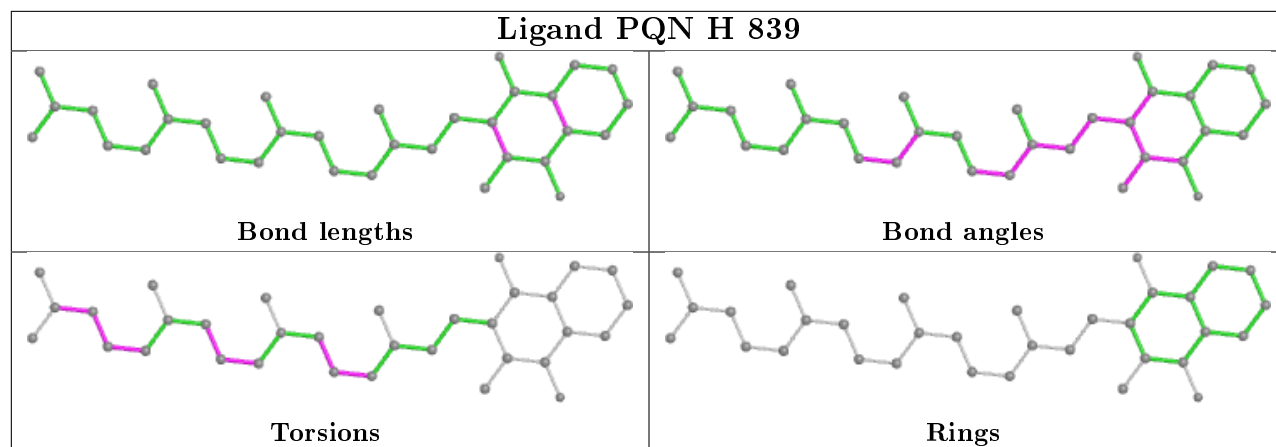


Ligand CLA A 821

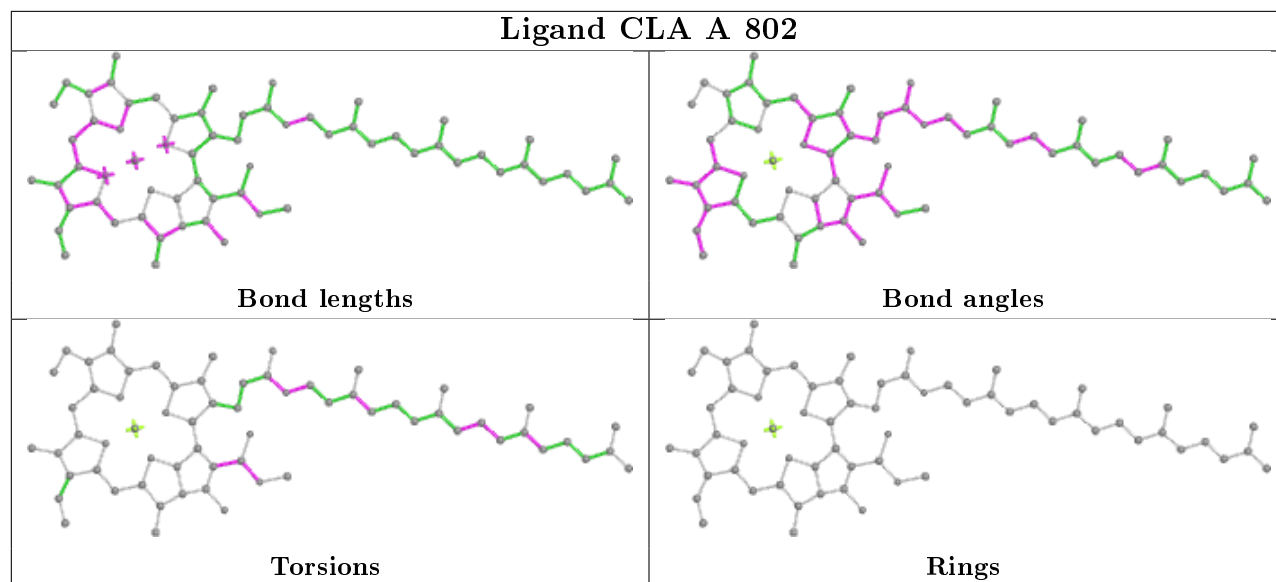


Ligand CLA G 830

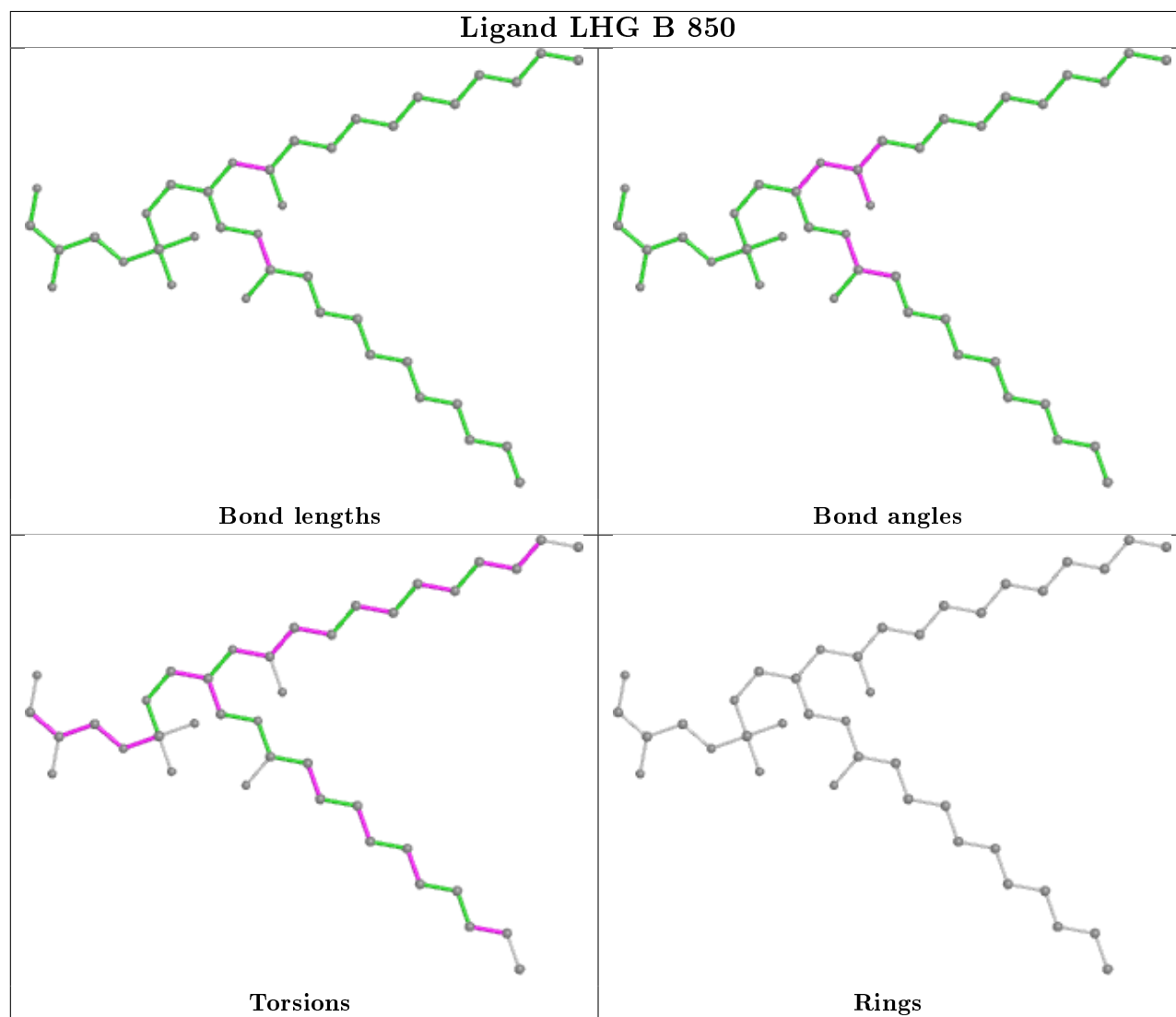




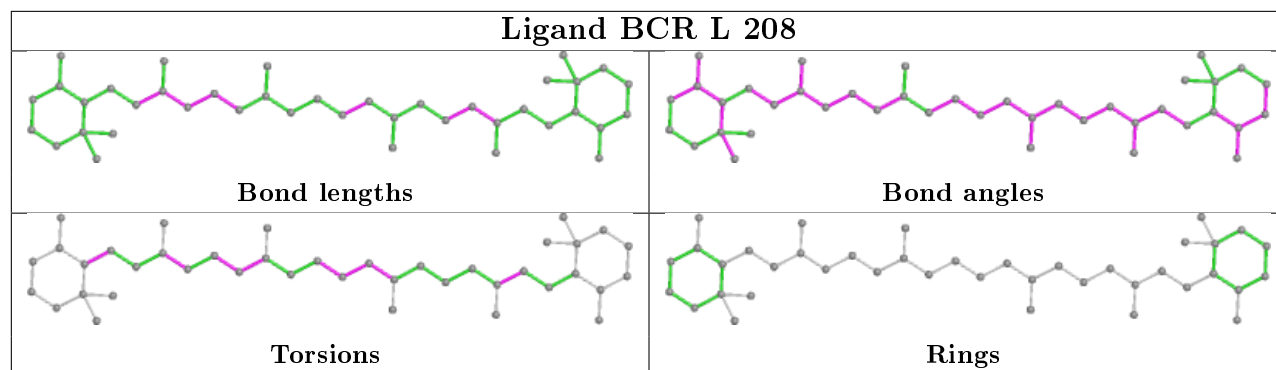
Ligand CLA A 802



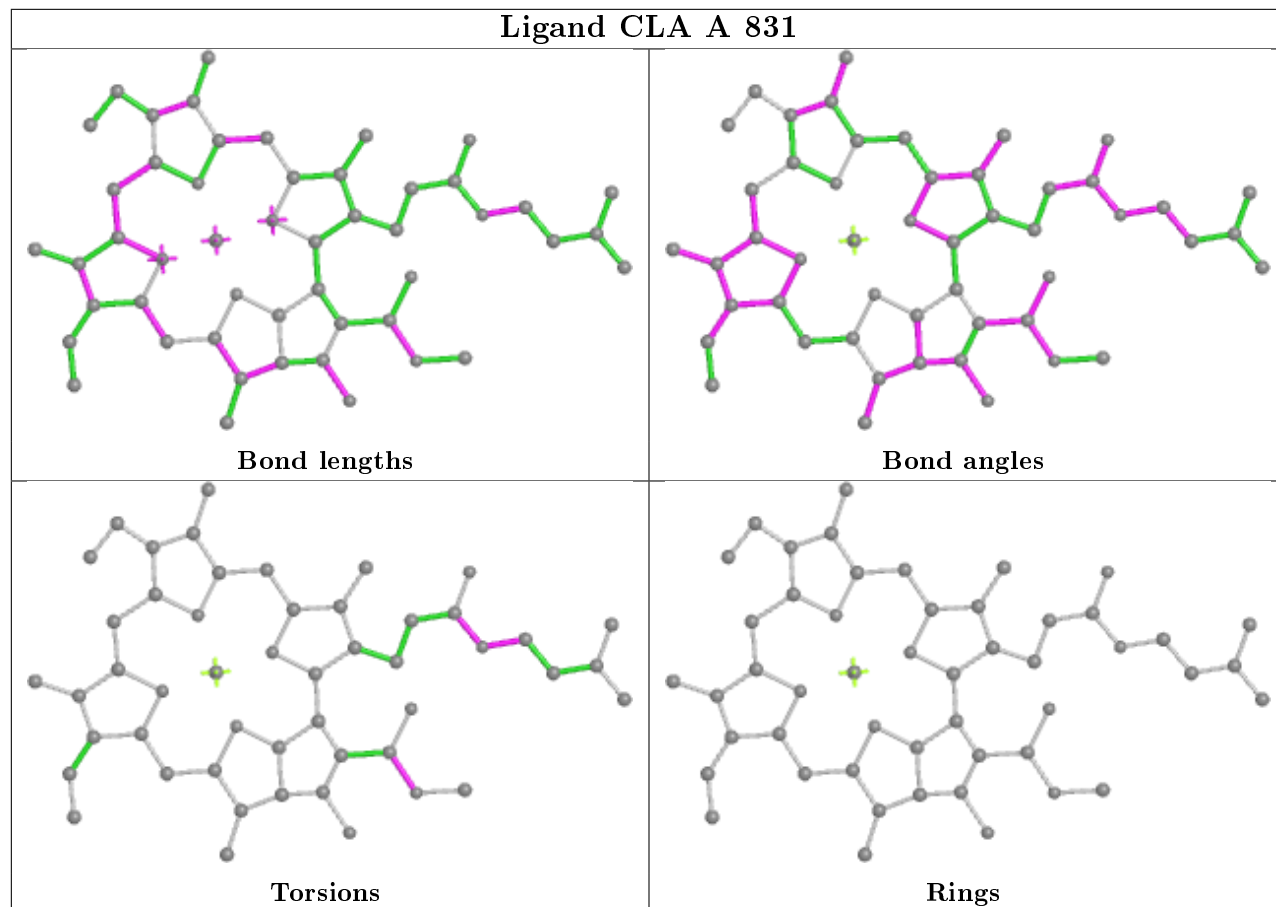
Ligand LHG B 850

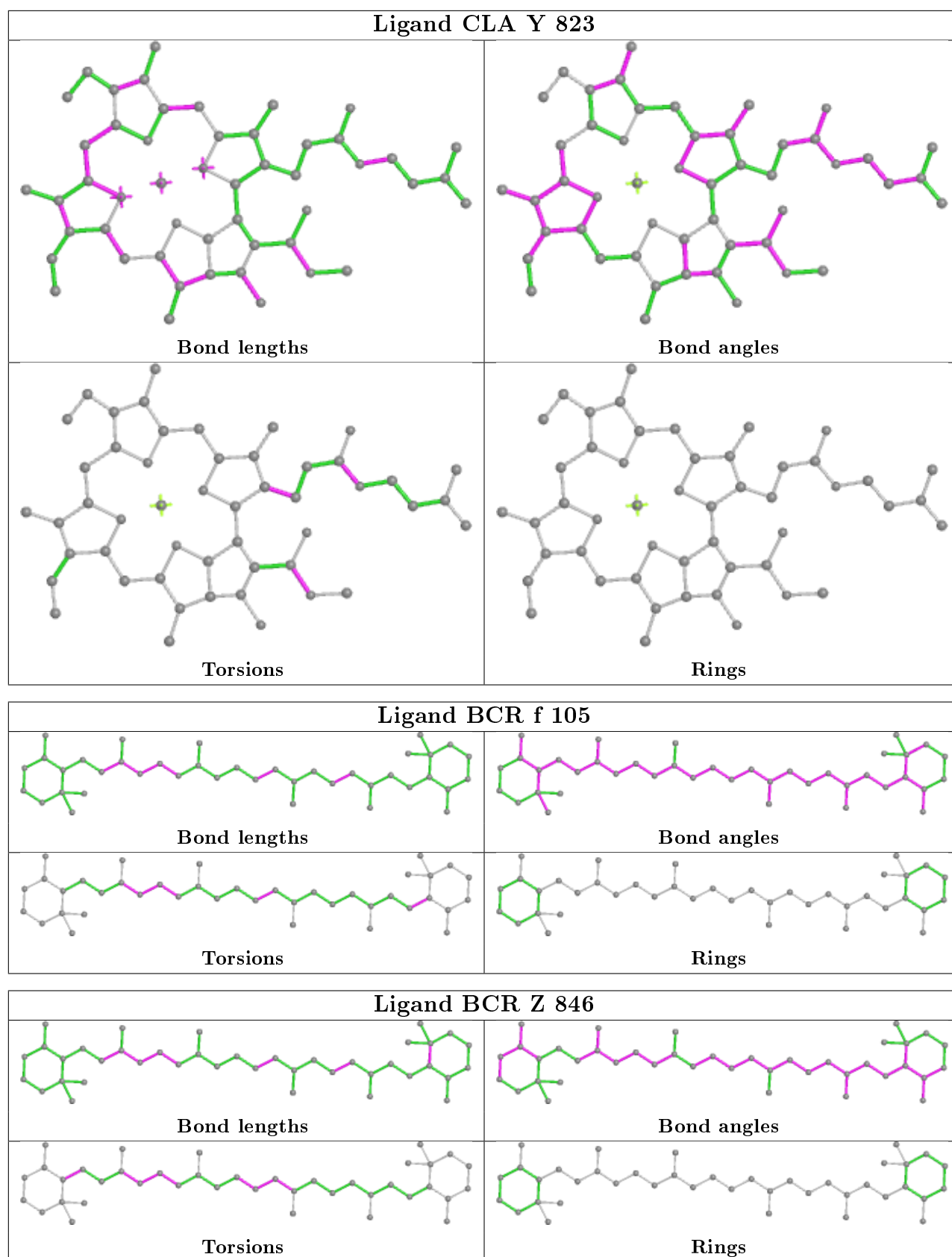


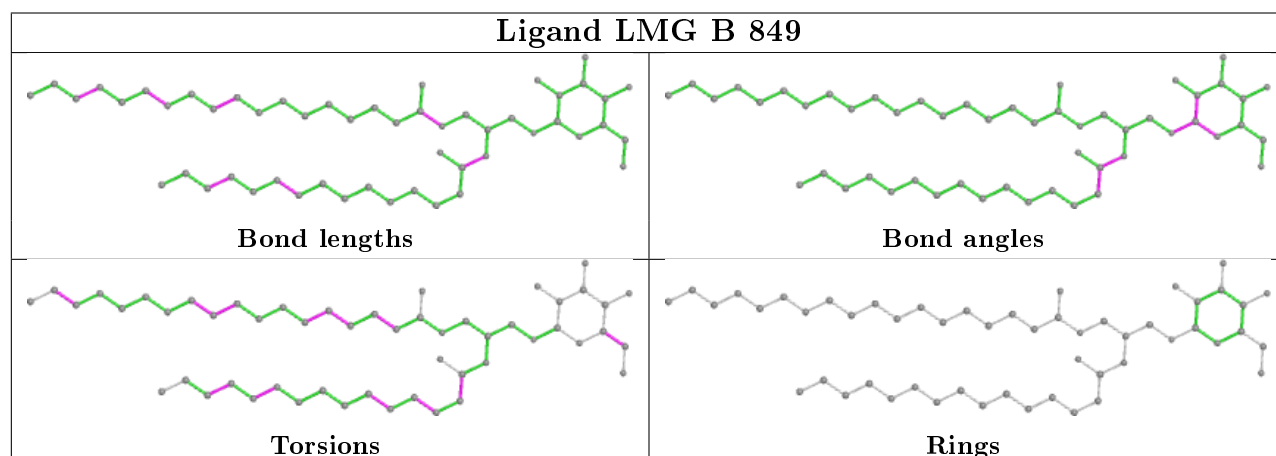
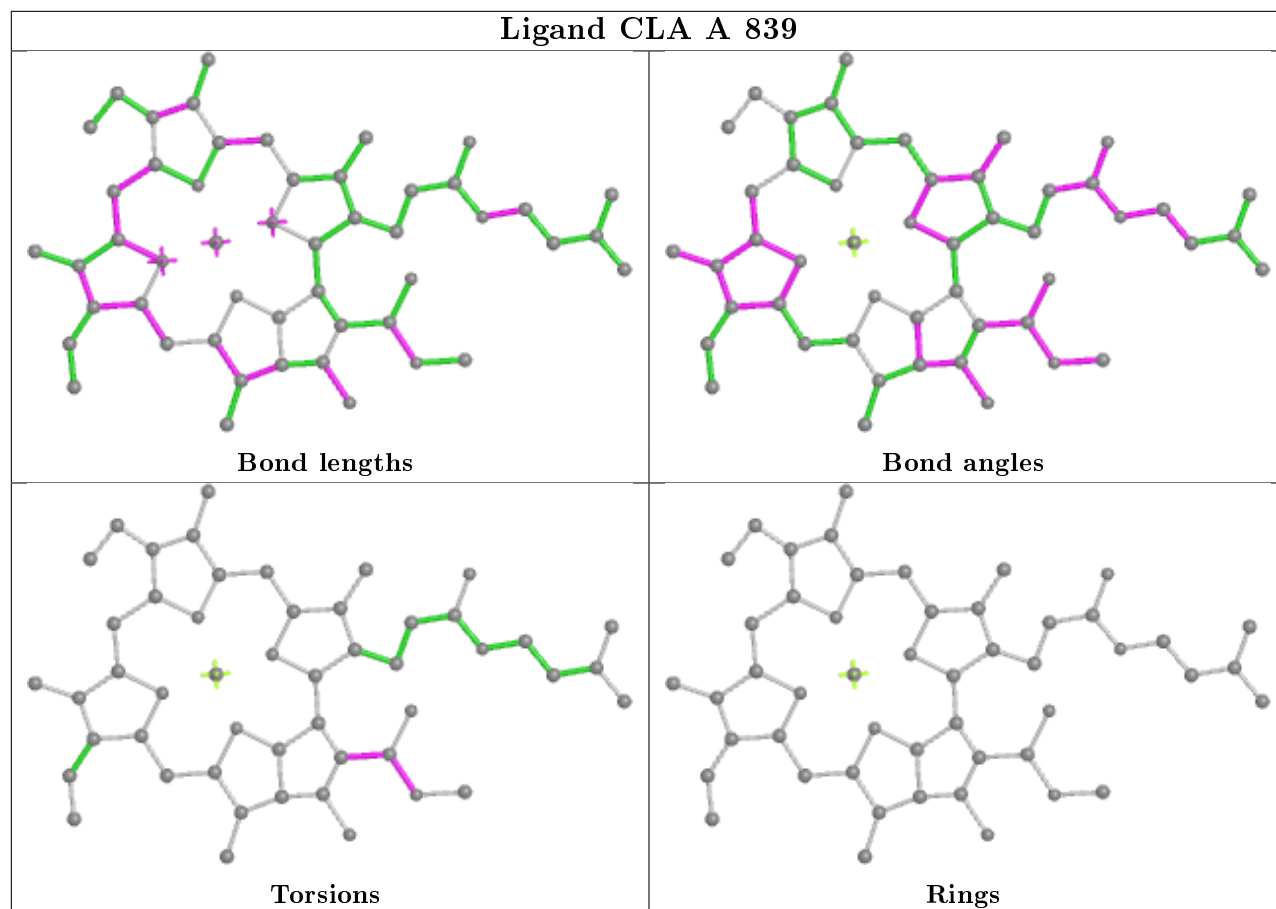
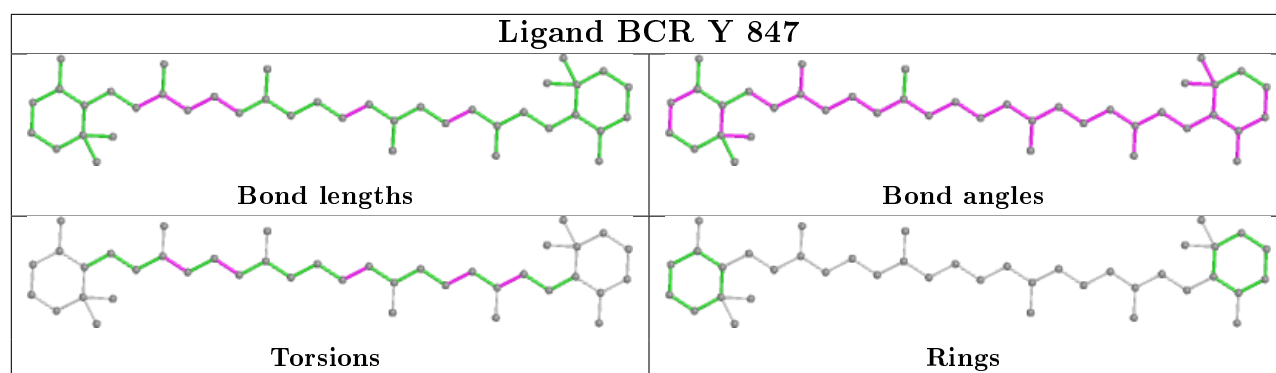
Ligand BCR L 208



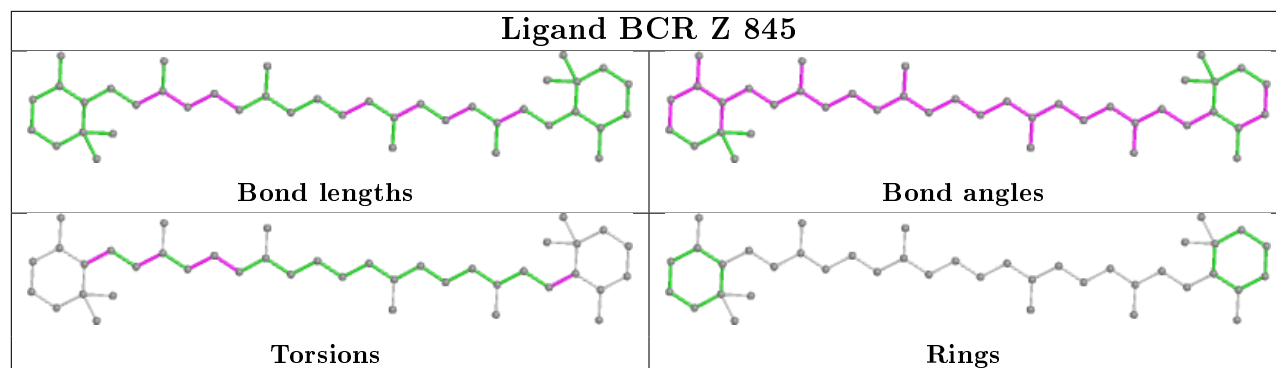
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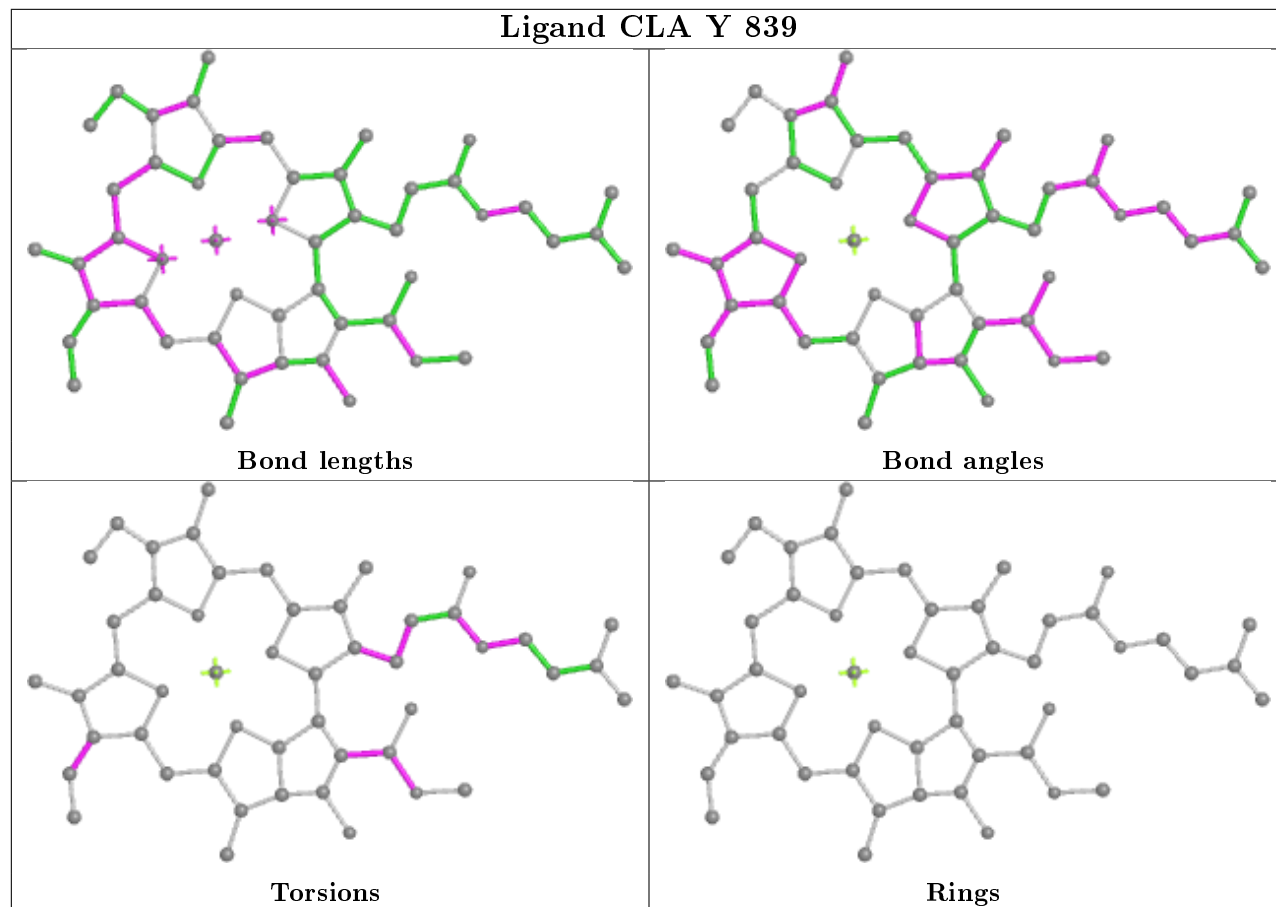




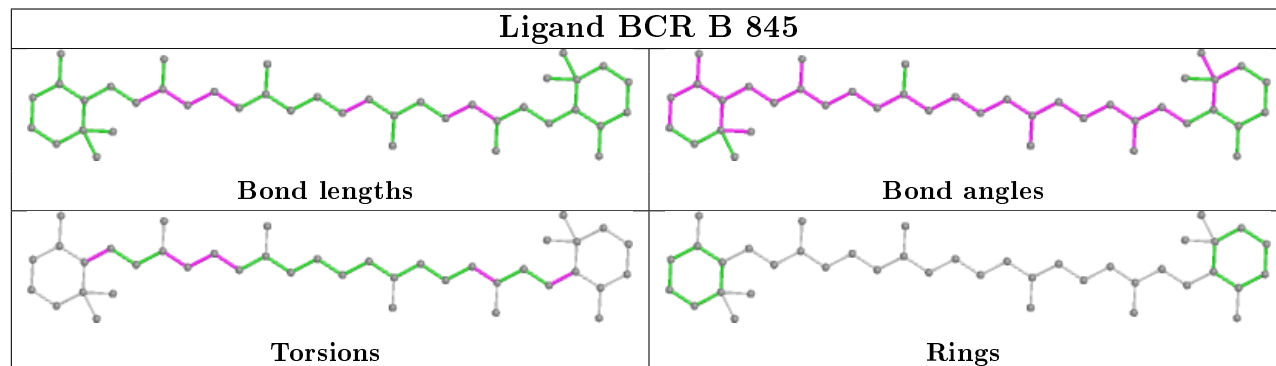
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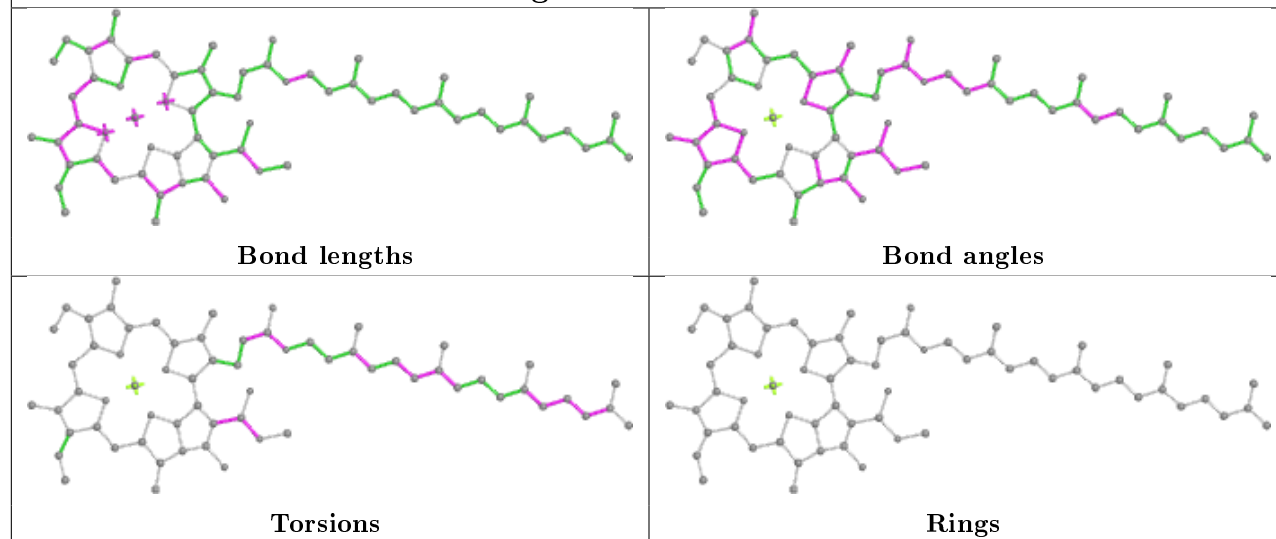
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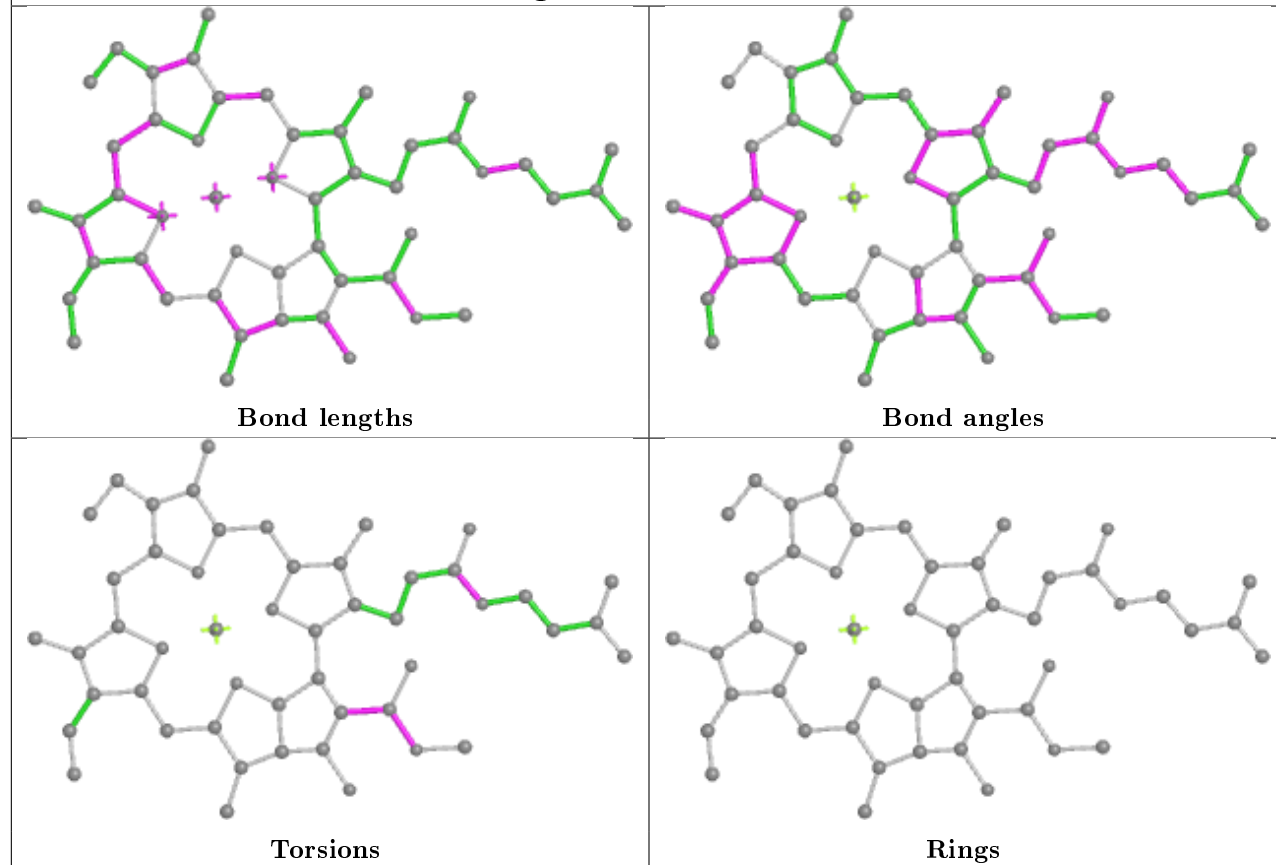
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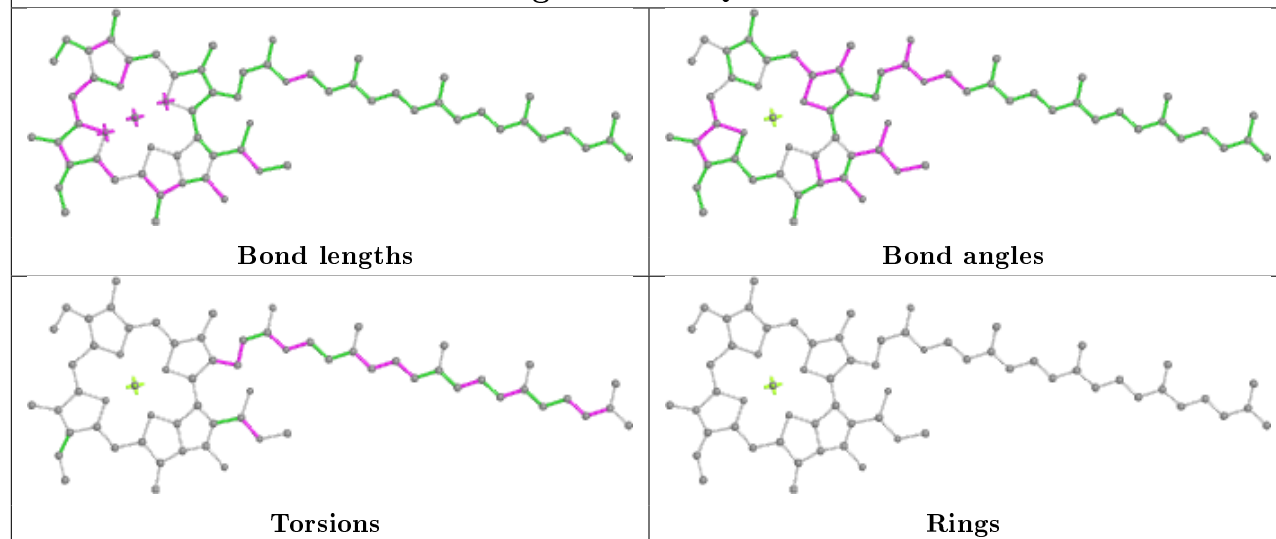
Ligand CLA G 825



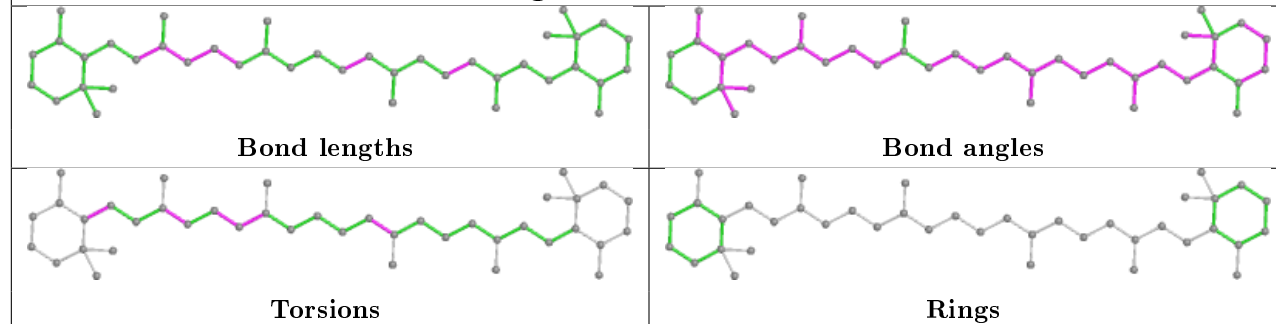
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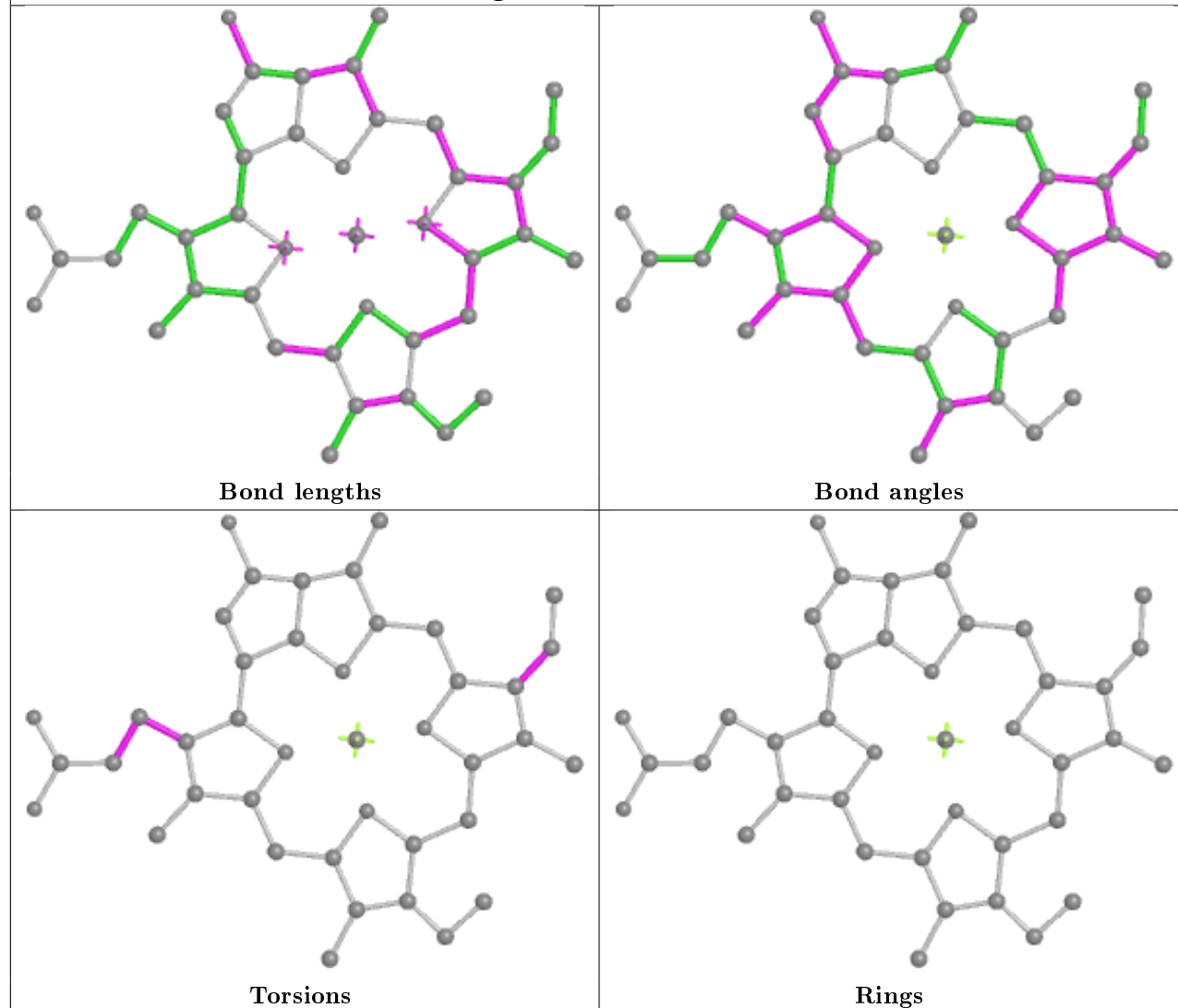
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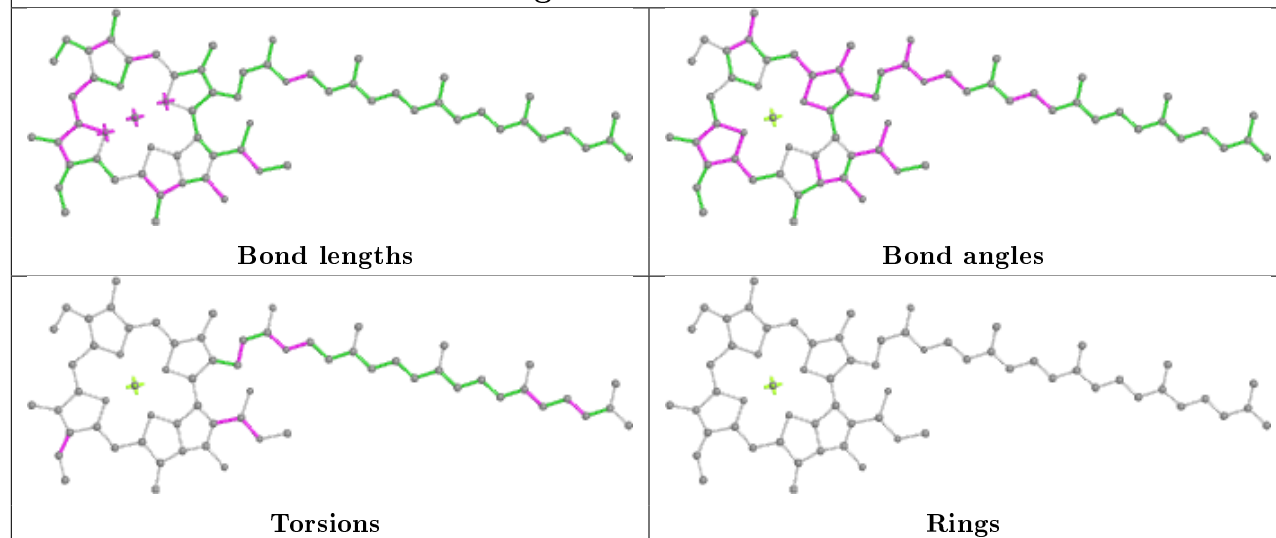
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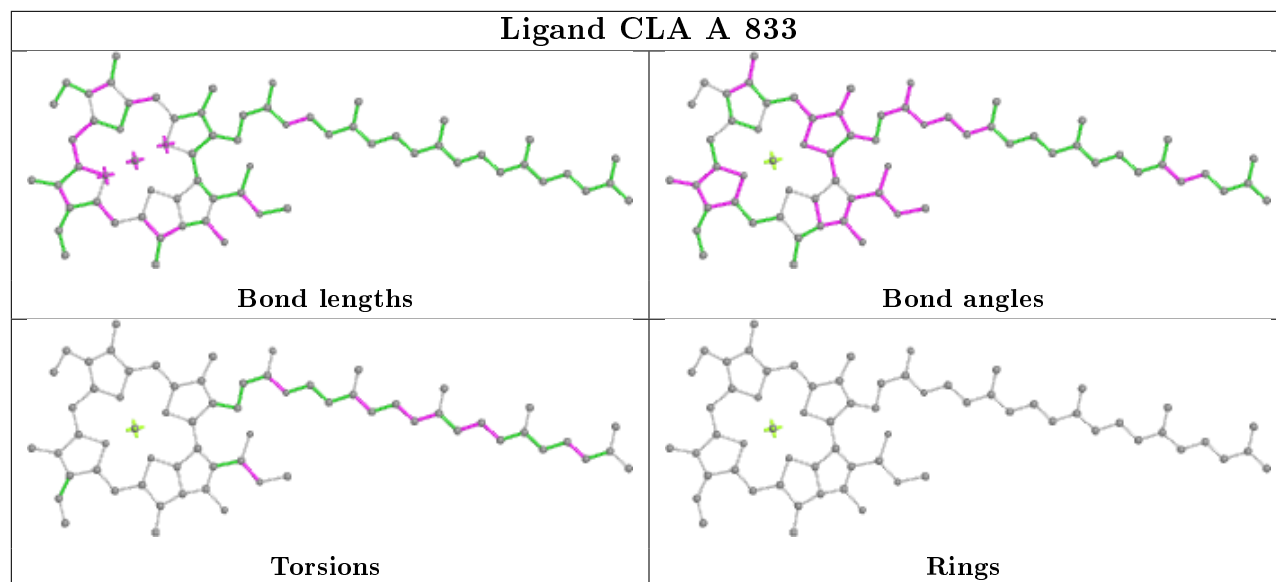
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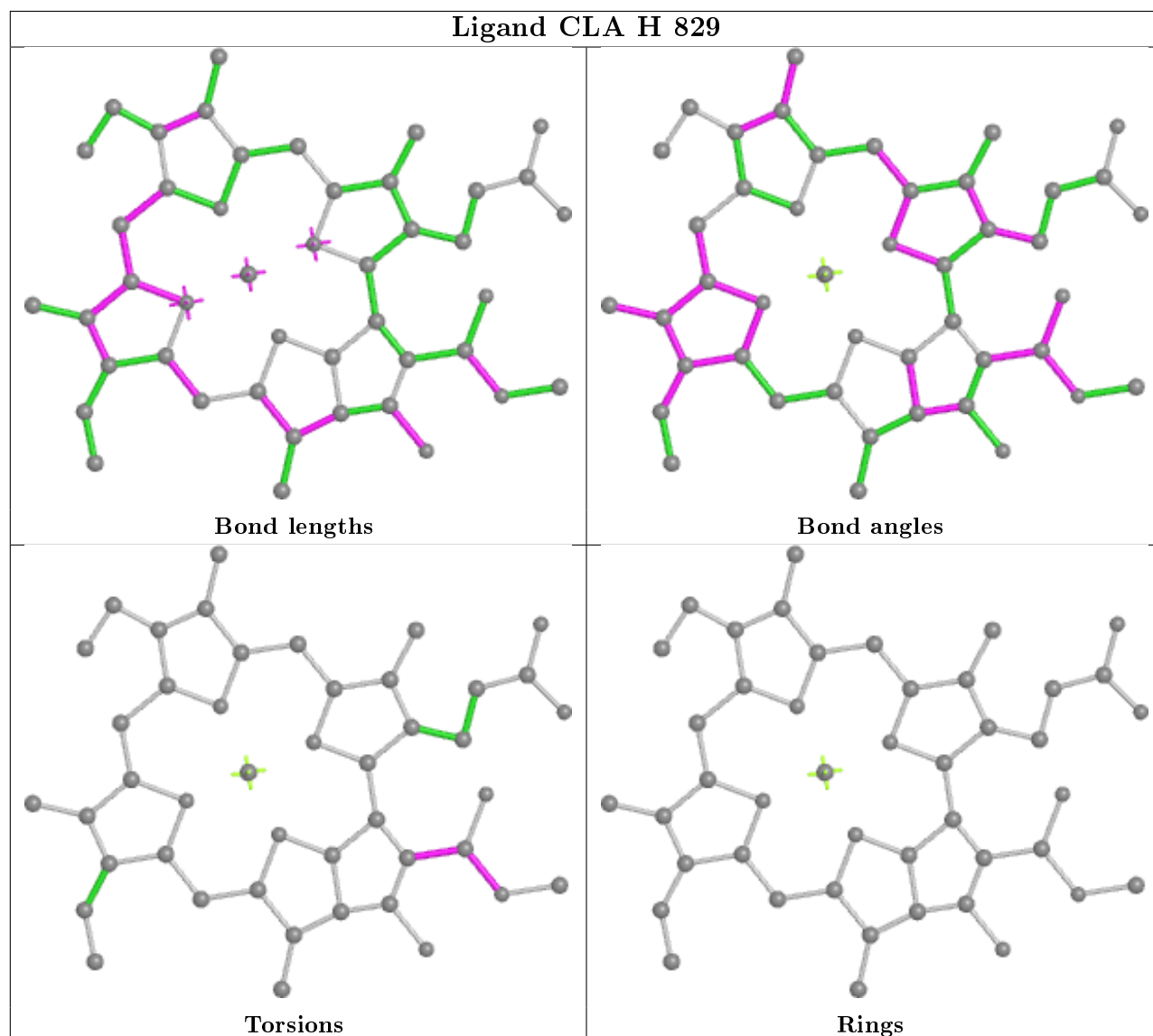
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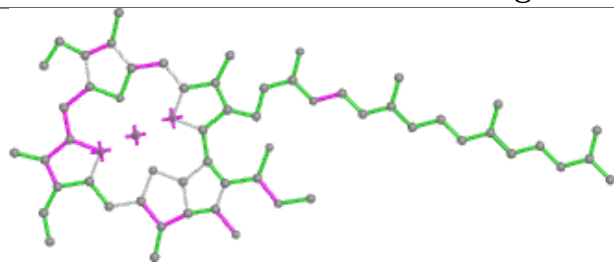
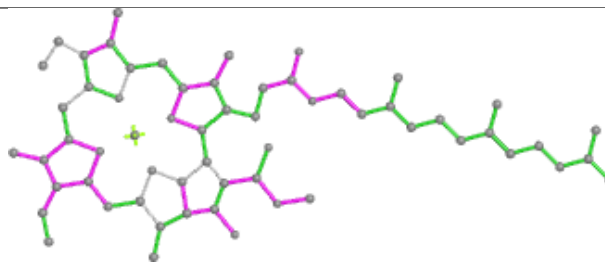
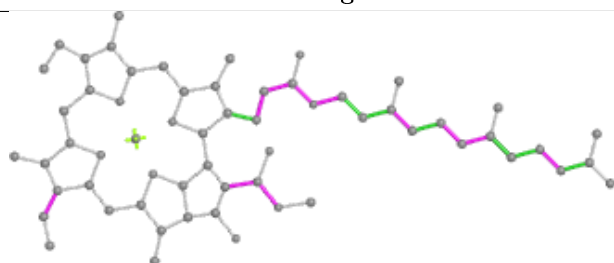
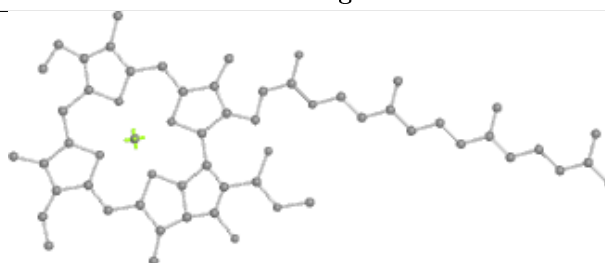
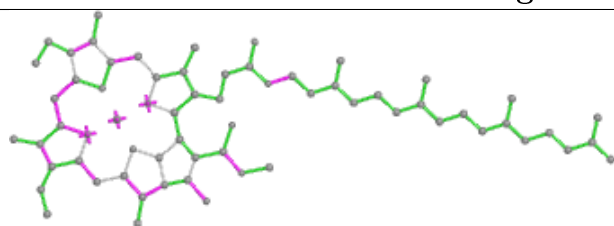
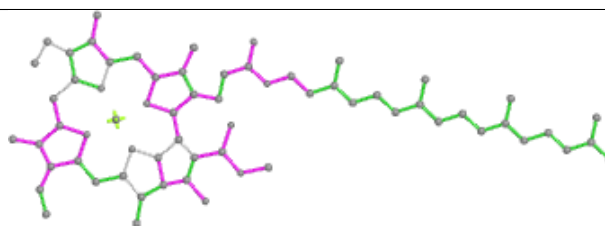
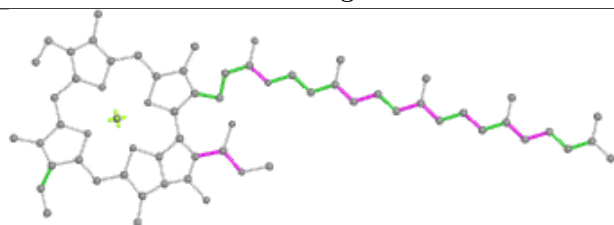
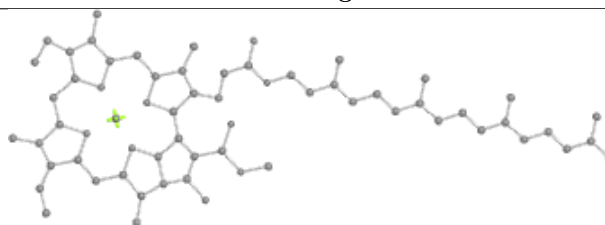


Ligand CLA A 833

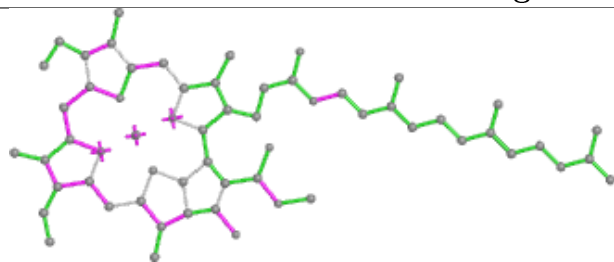


Ligand CLA H 829

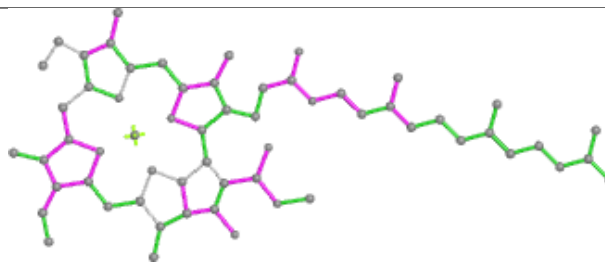


Ligand CLA A 824**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA L 202****Bond lengths****Bond angles****Torsions****Rings**

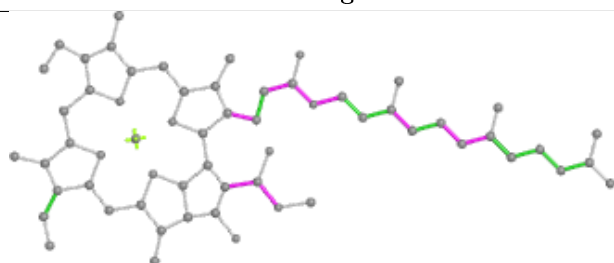
Ligand CLA G 820



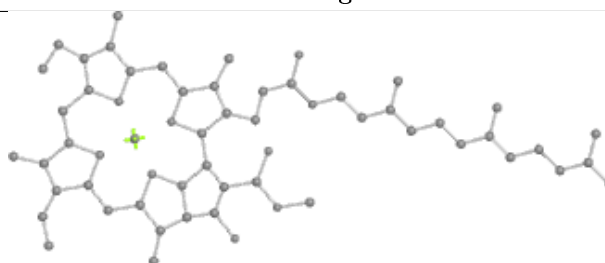
Bond lengths



Bond angles

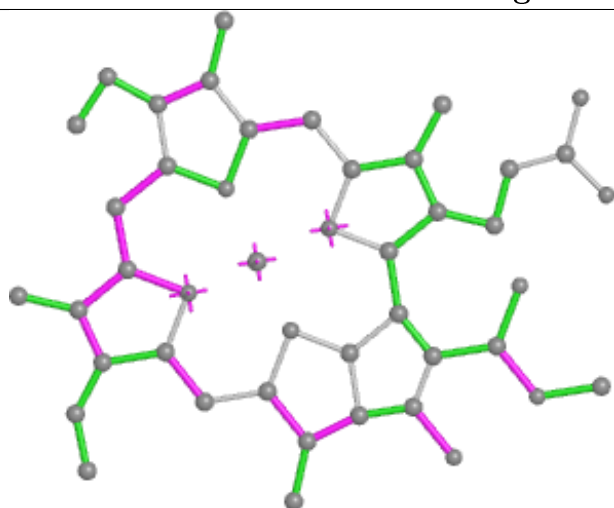


Torsions

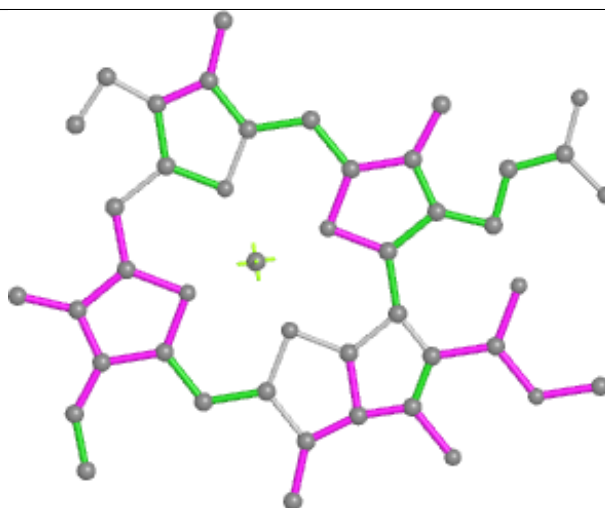


Rings

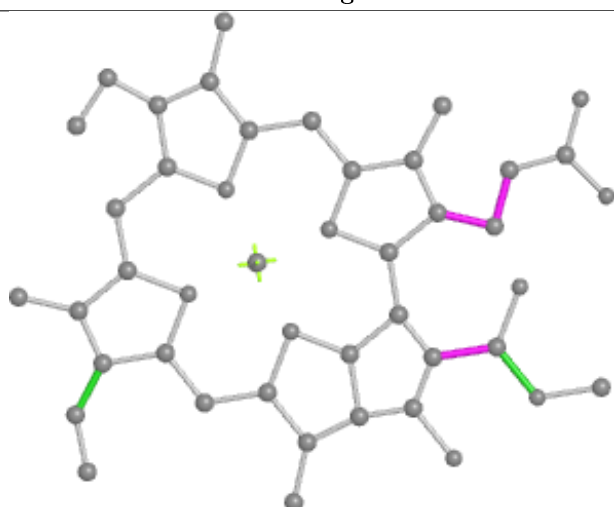
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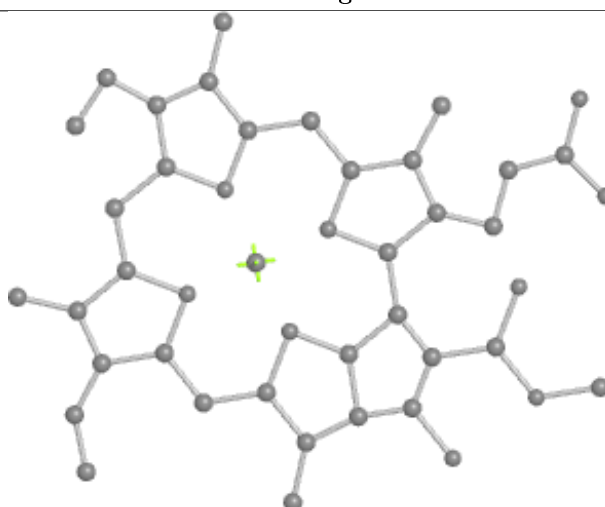
Bond lengths



Bond angles

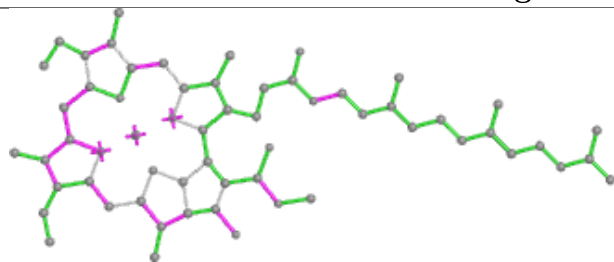


Torsions

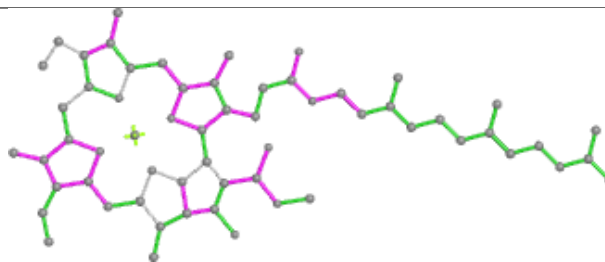


Rings

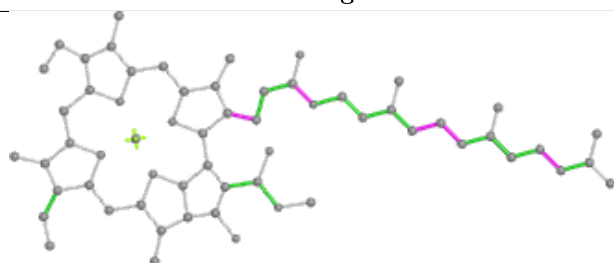
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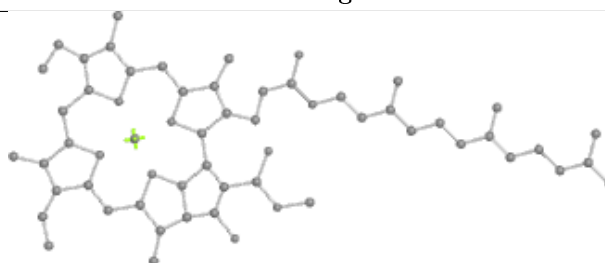
Bond lengths



Bond angles

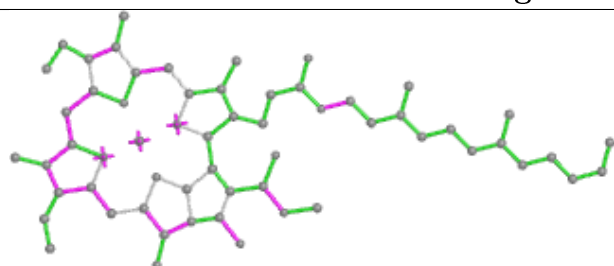


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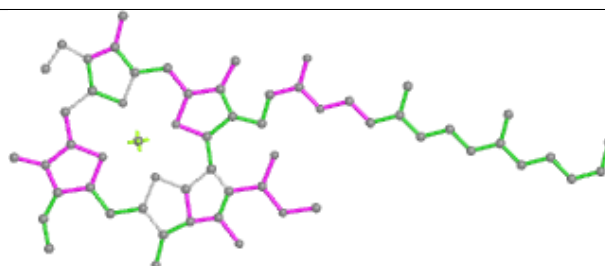


Rings

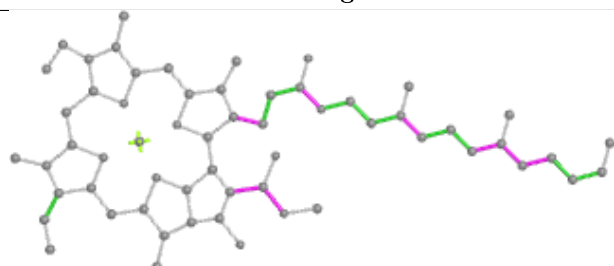
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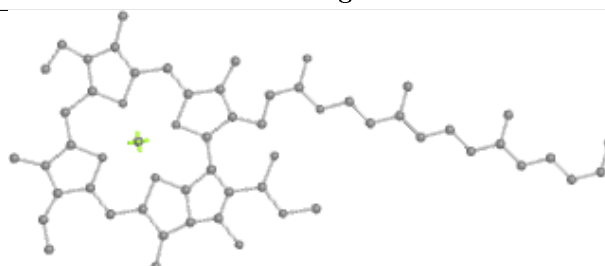
Bond lengths



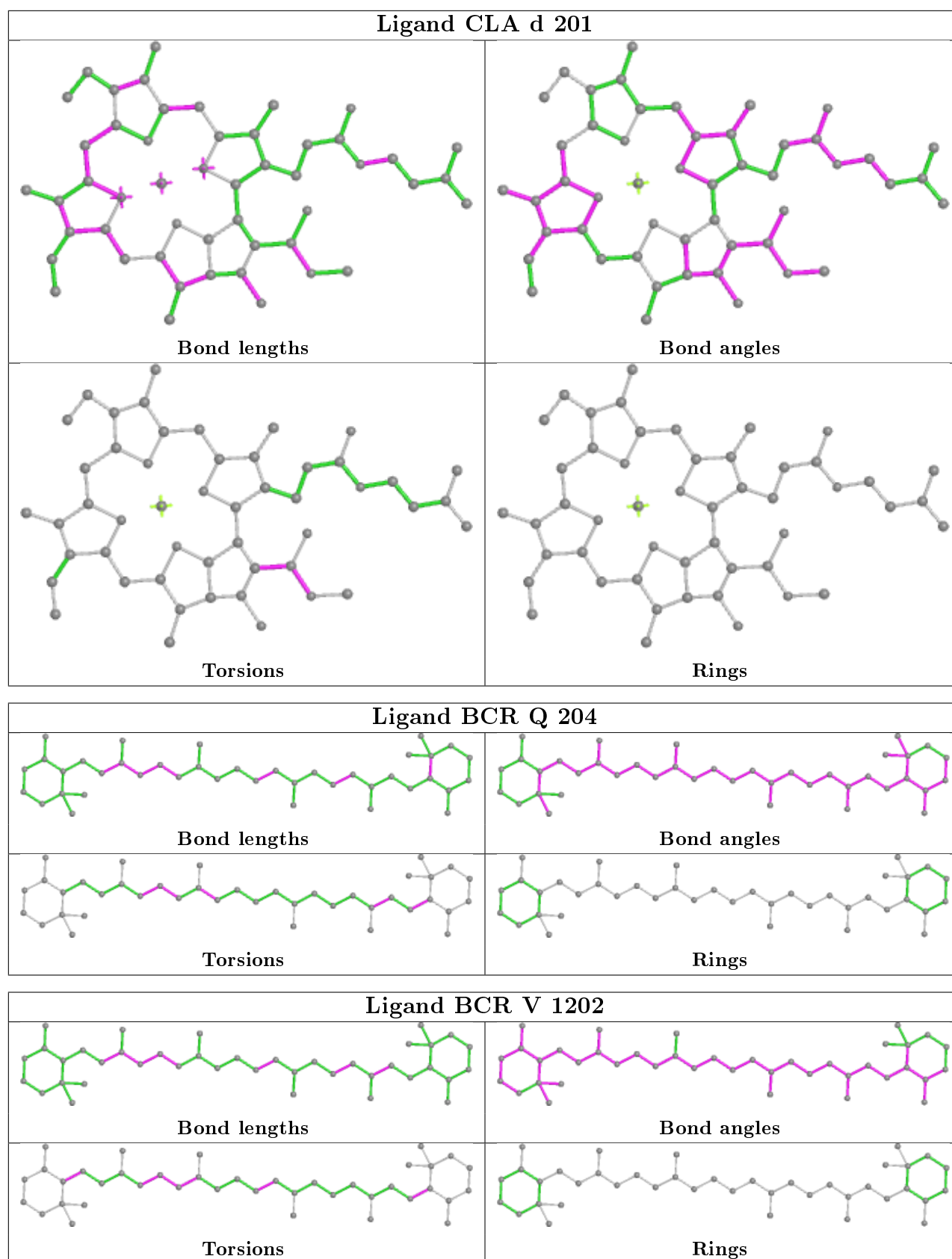
Bond angles



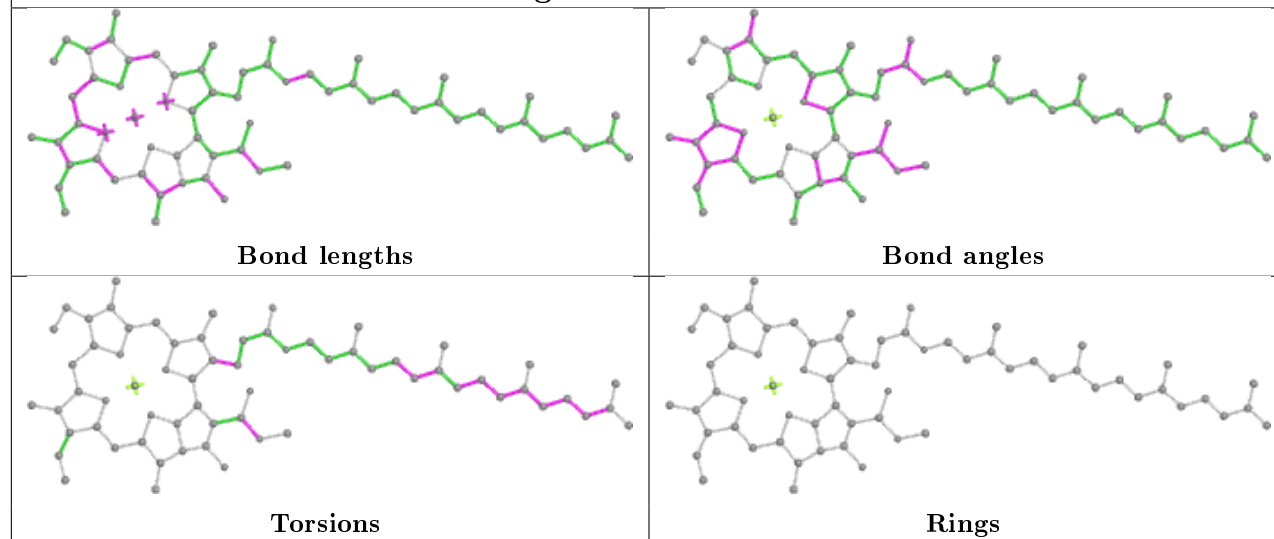
Torsions



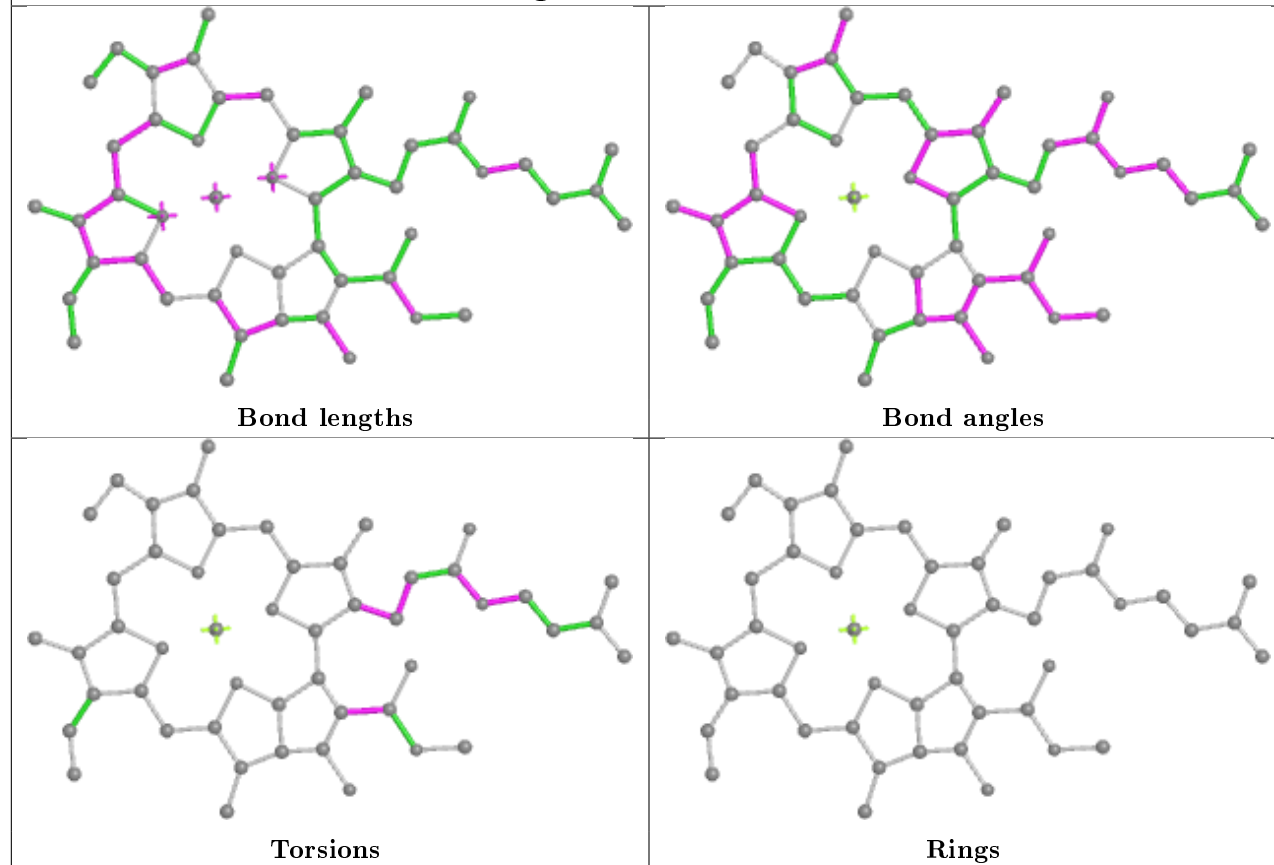
Rings



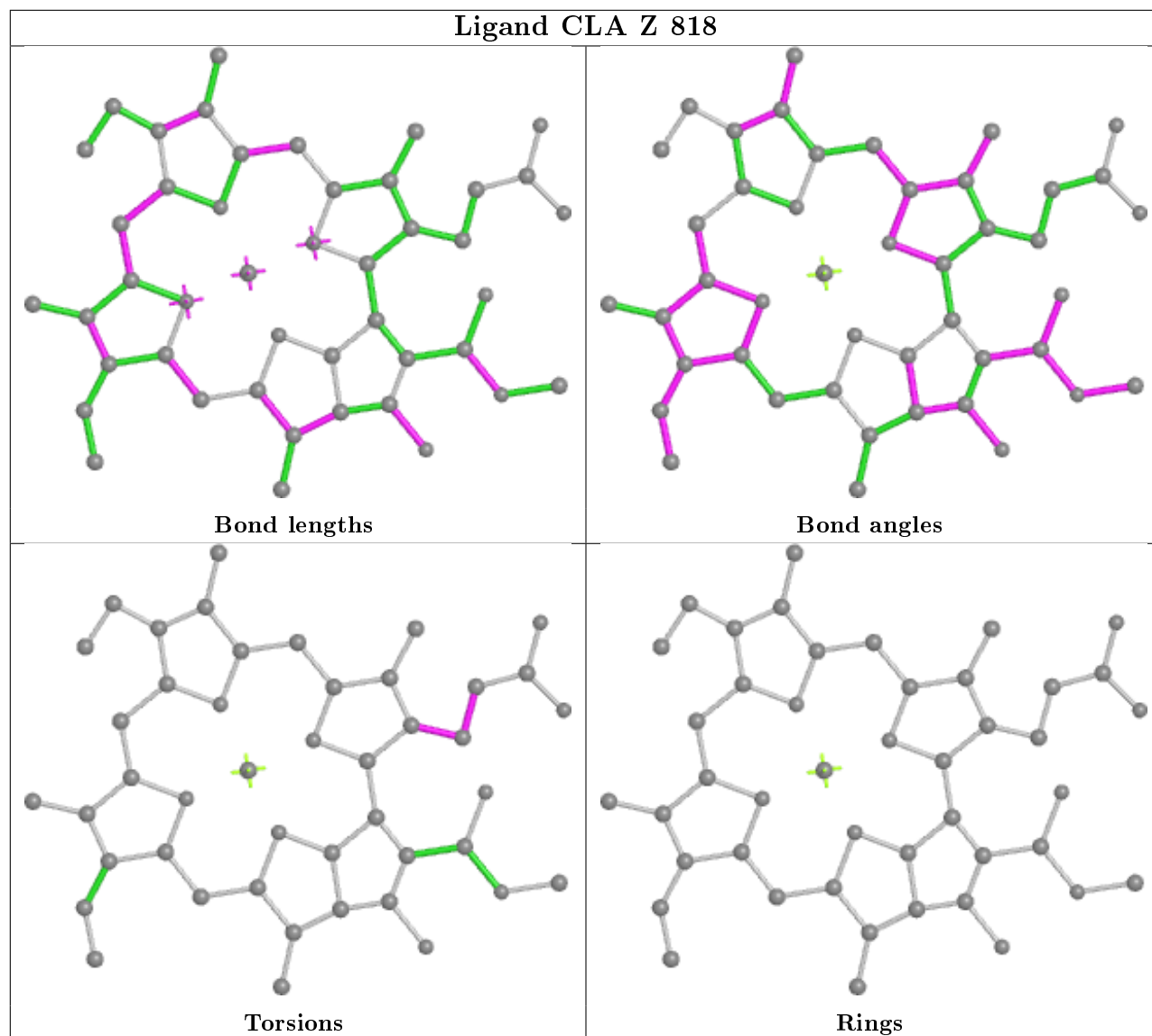
Ligand CLA Z 825

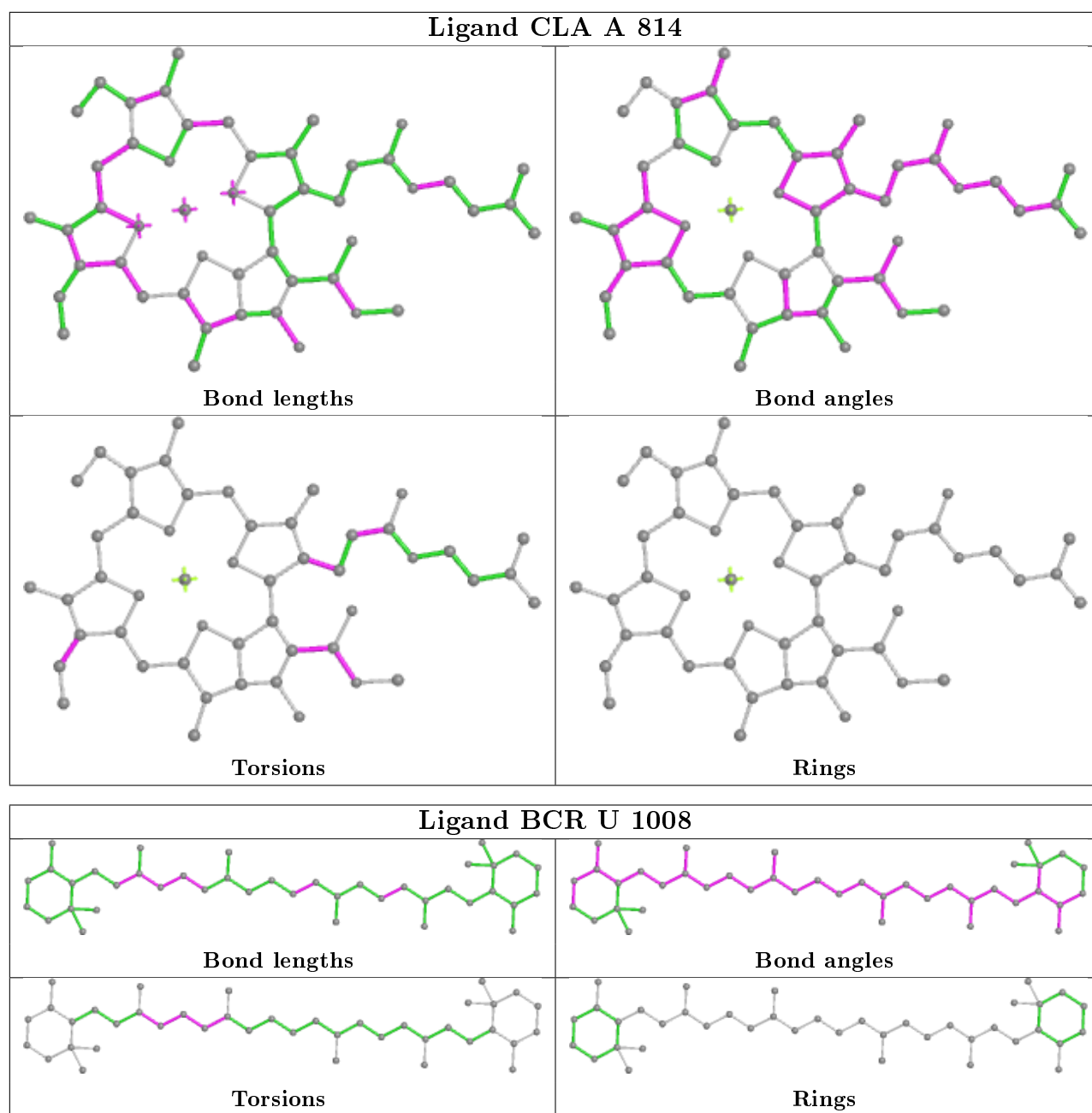


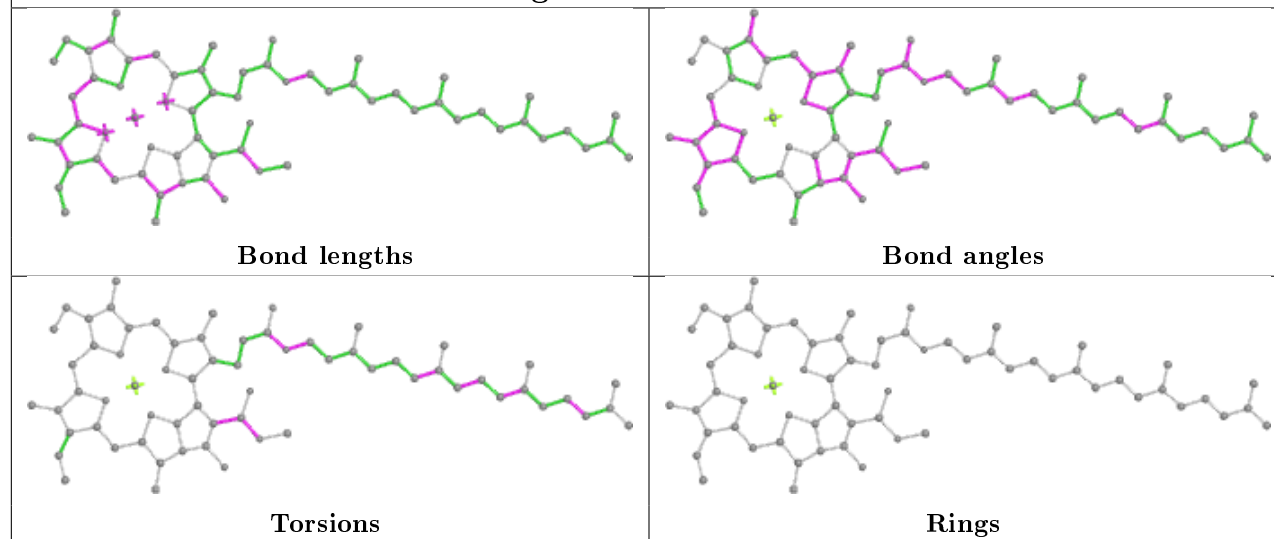
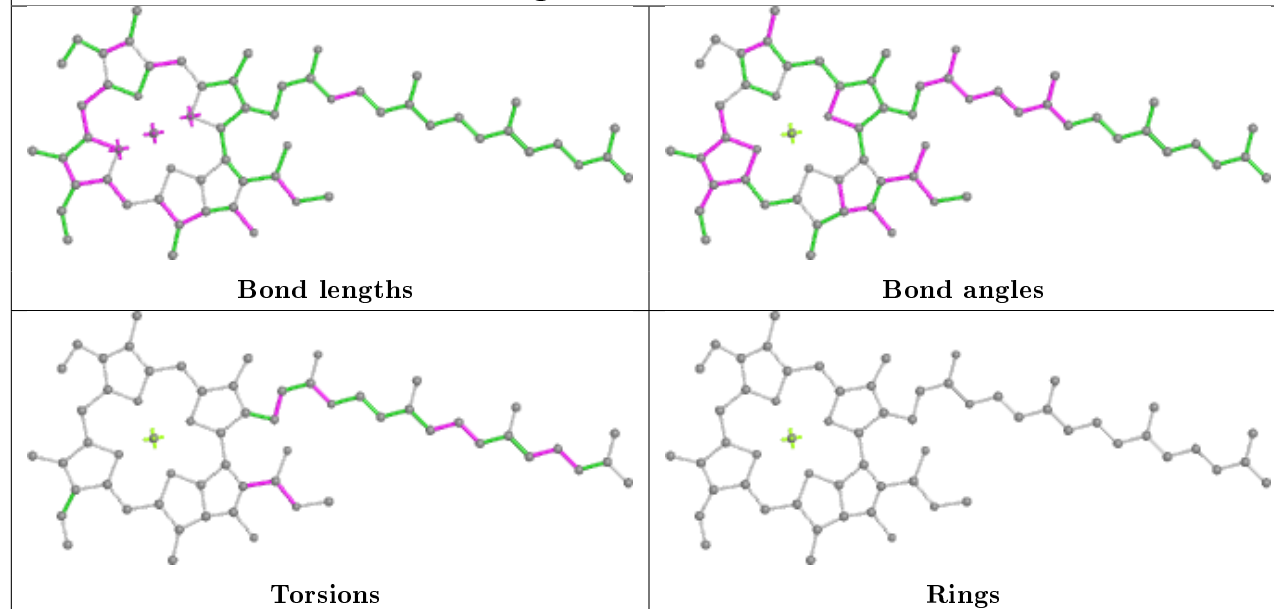
Ligand CLA Y 837

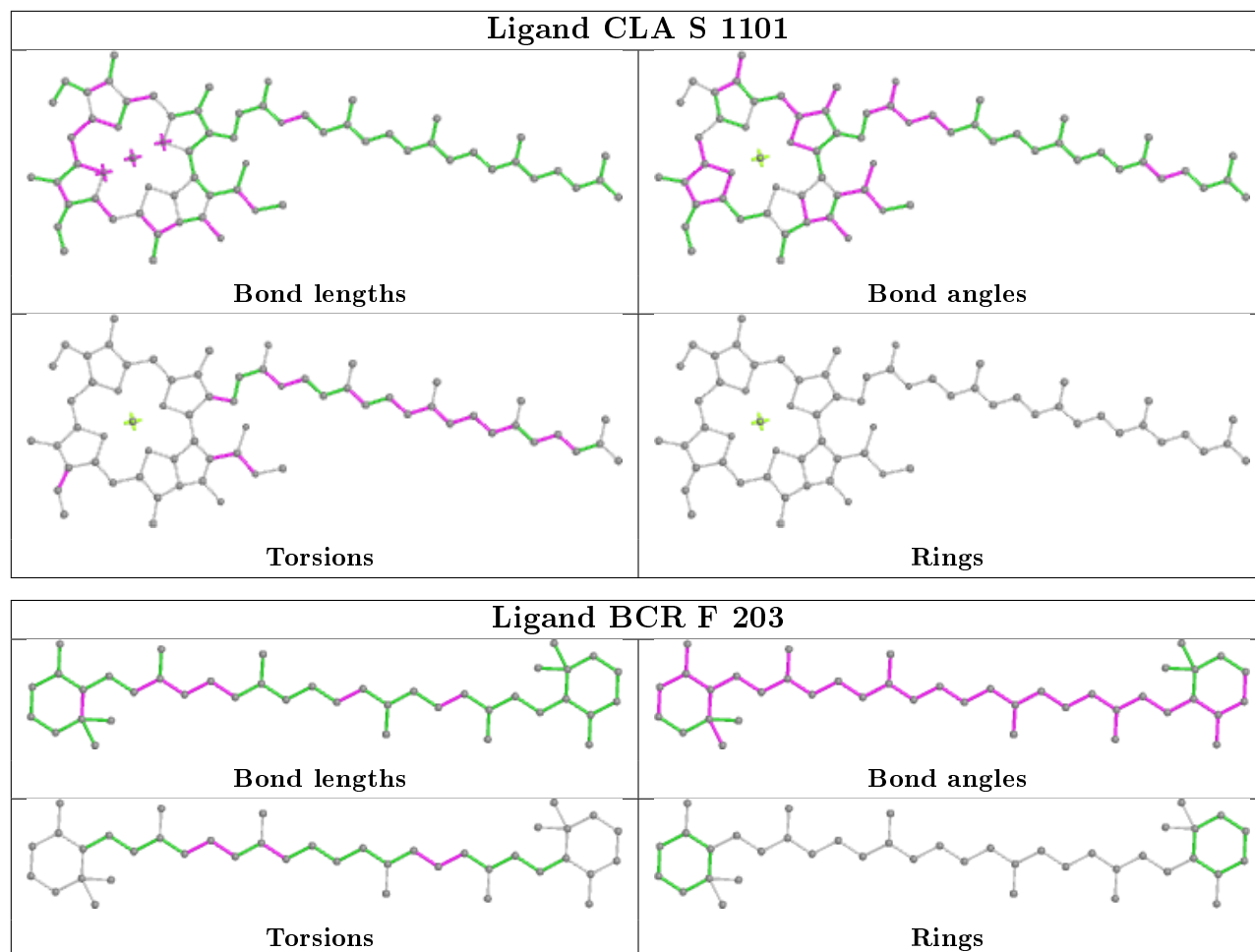


Ligand CLA Z 818

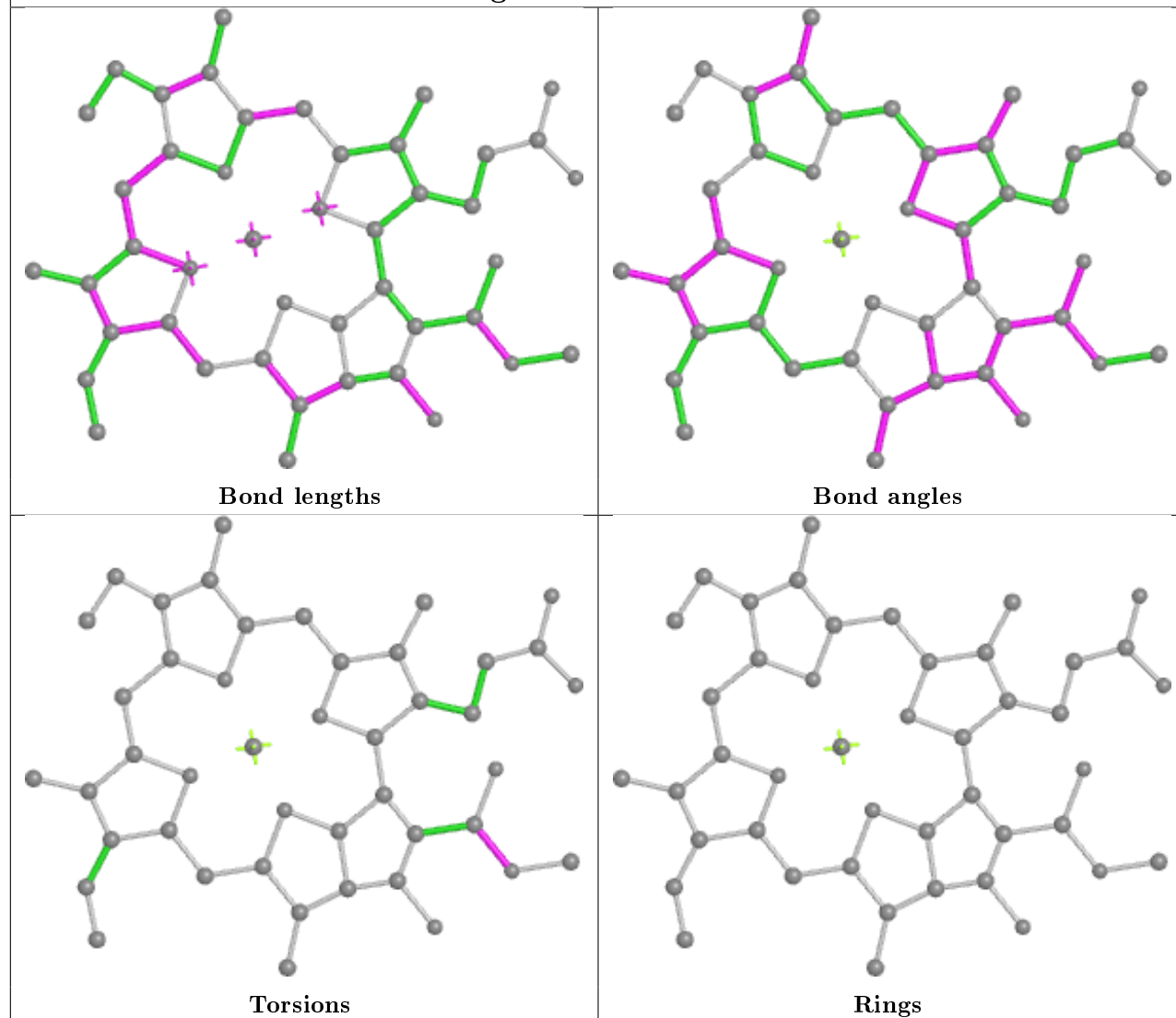




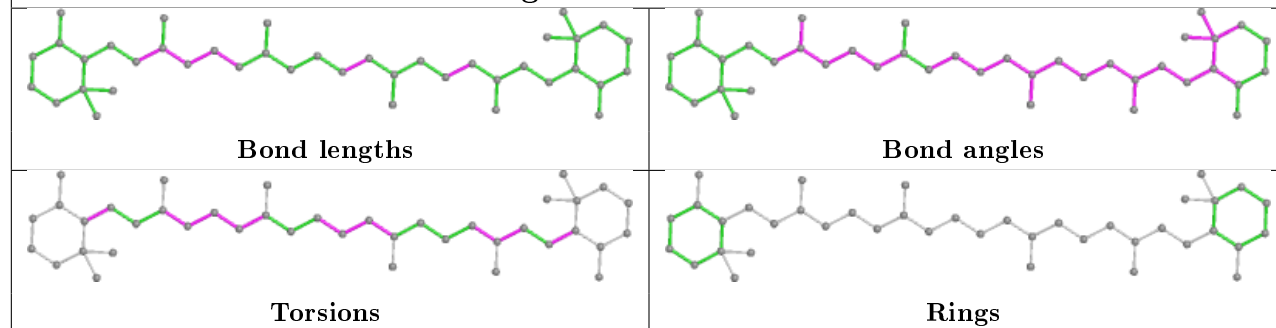
Ligand CLA G 803**Ligand CLA Y 813**

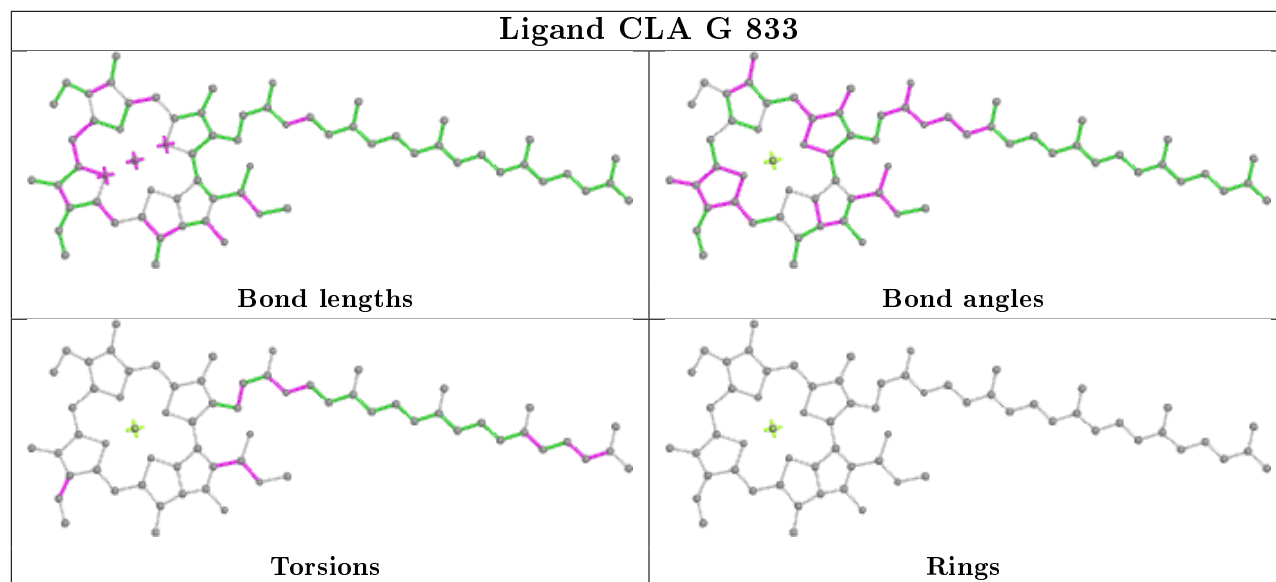
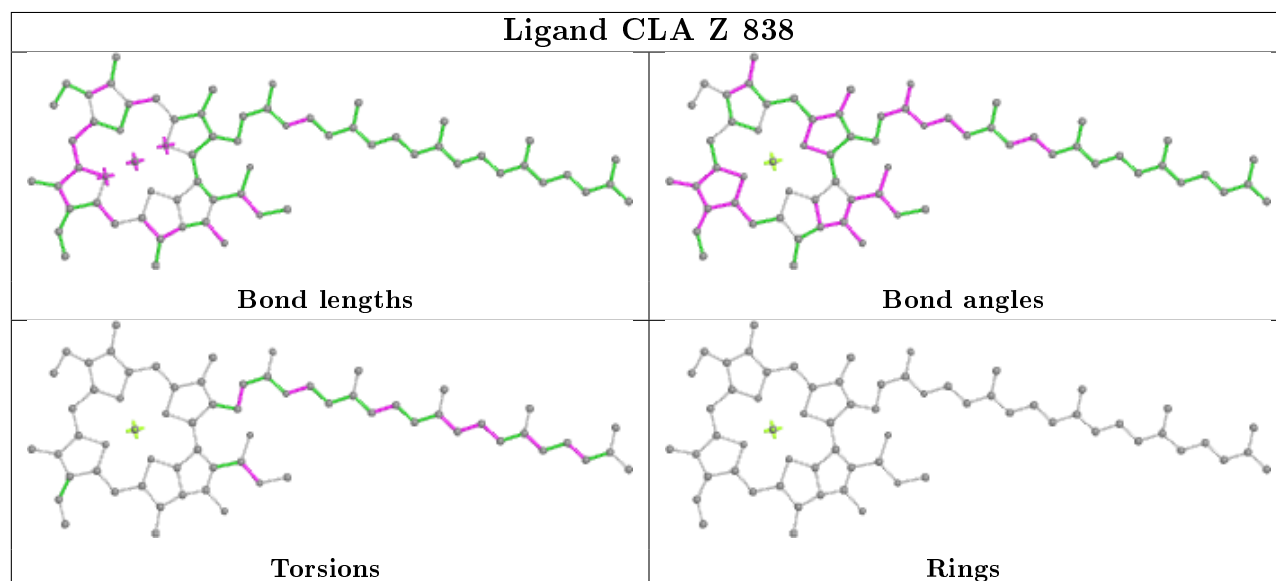
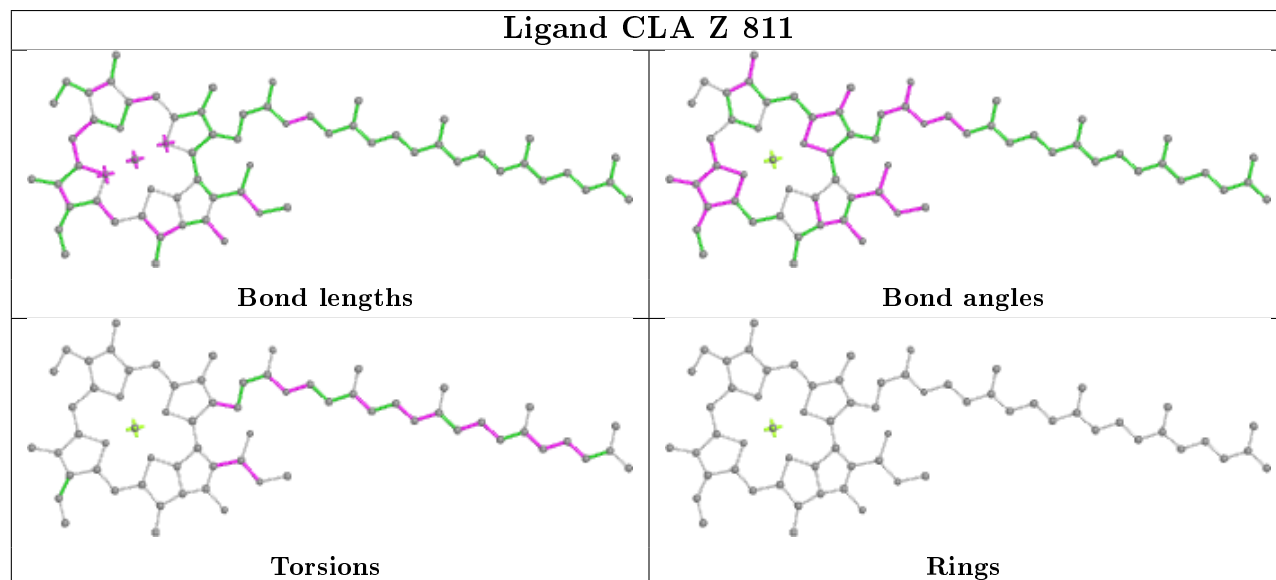


Ligand CLA B 820

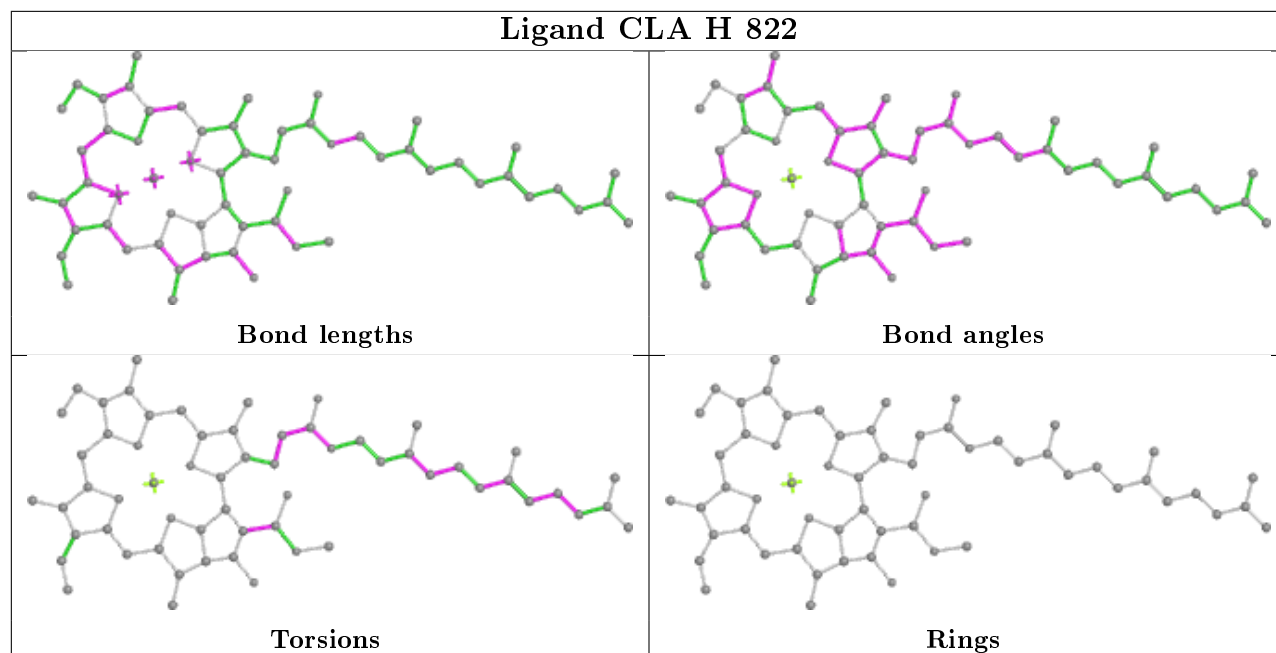


Ligand BCR U 1007

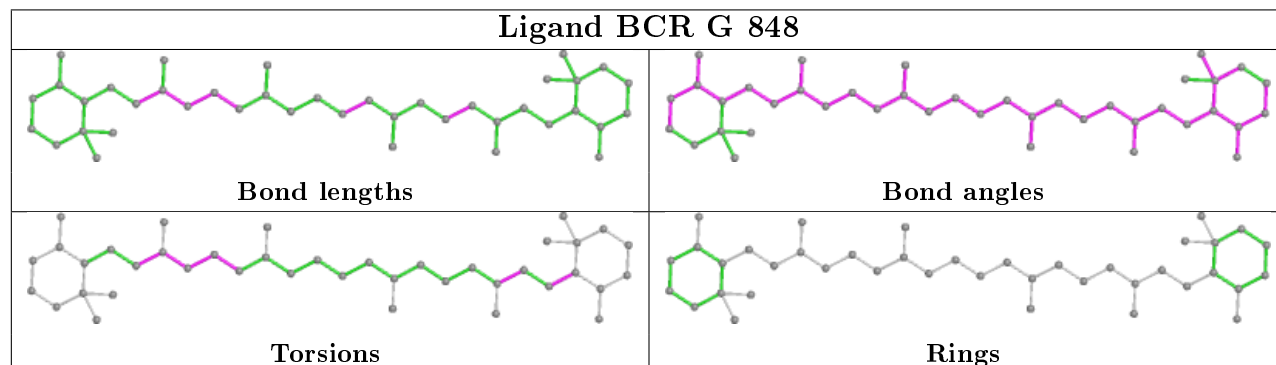


Ligand CLA G 833**Ligand CLA Z 838****Ligand CLA Z 811**

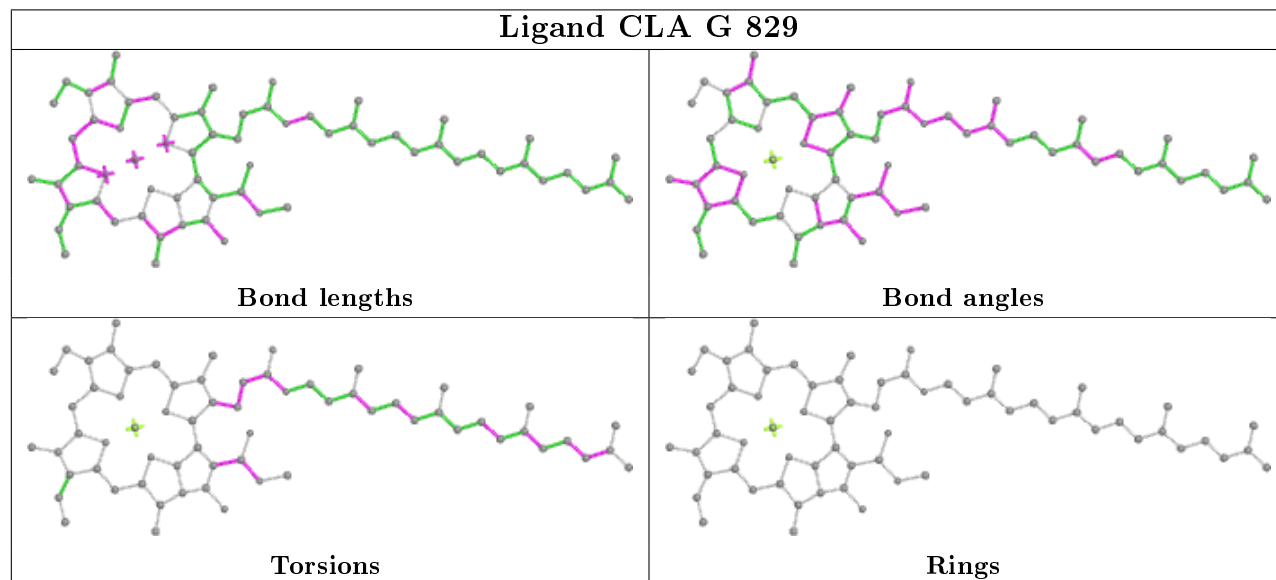
Ligand CLA H 822



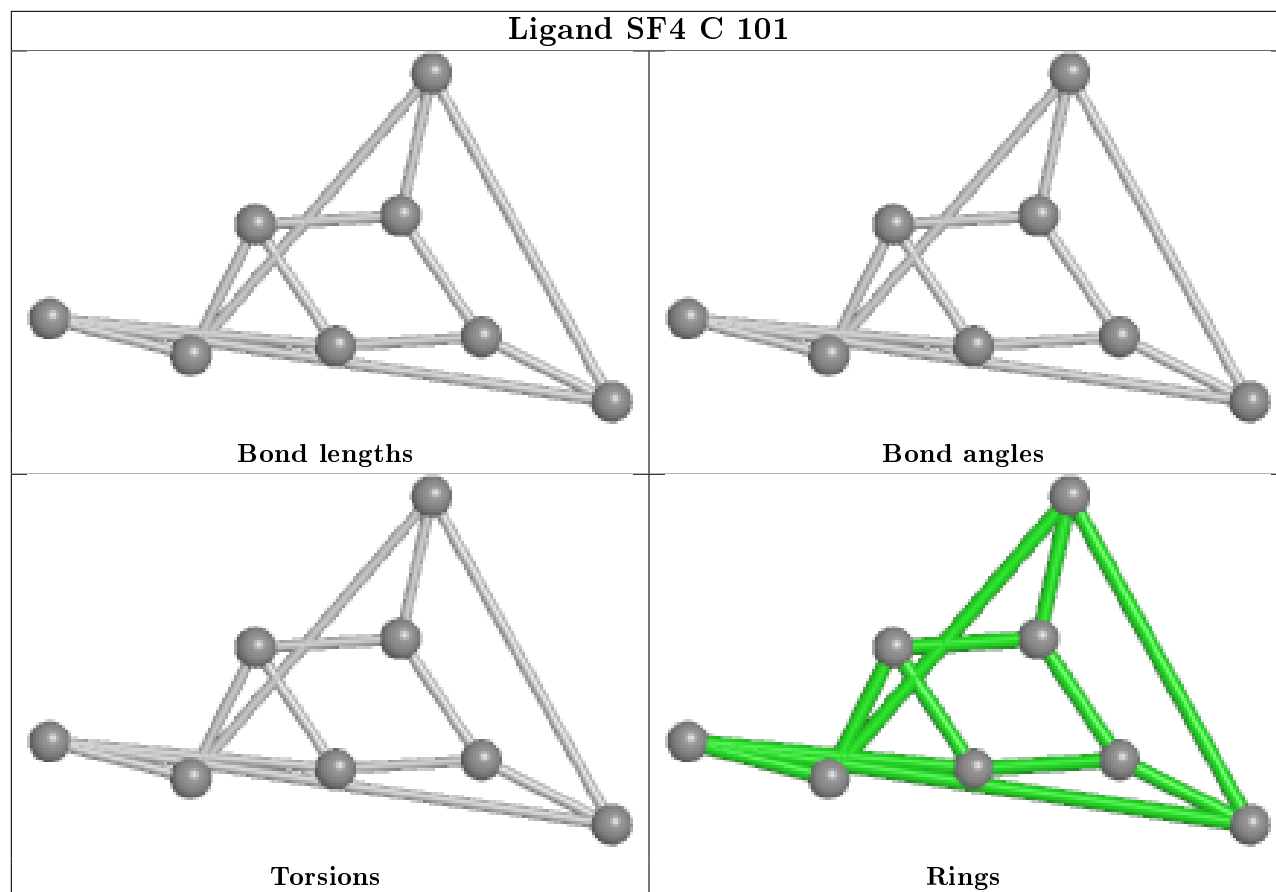
Ligand BCR G 848



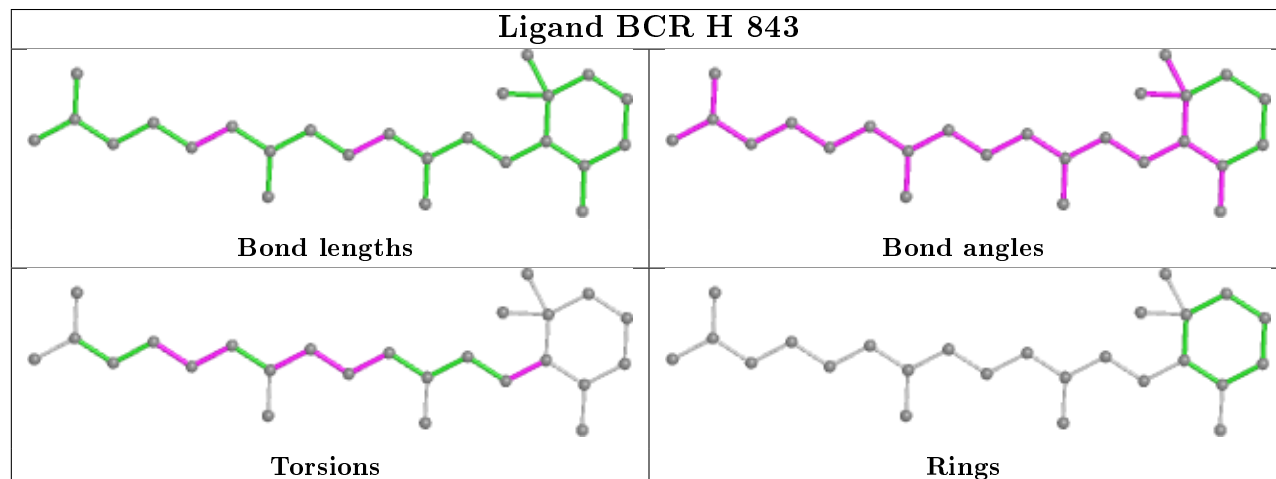
Ligand CLA G 829



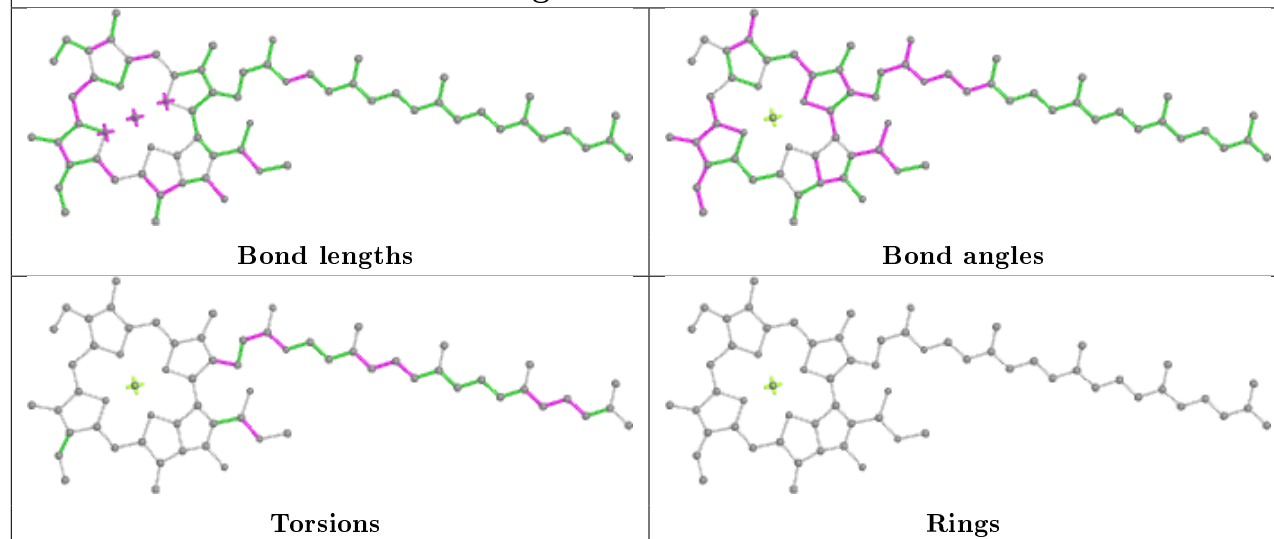
Ligand SF4 C 101



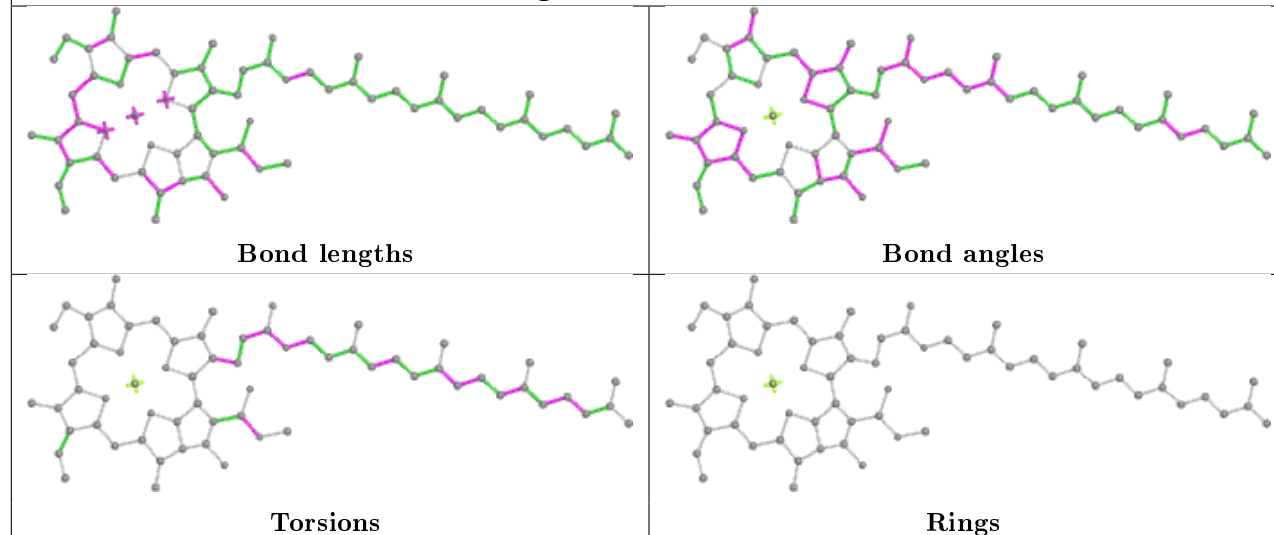
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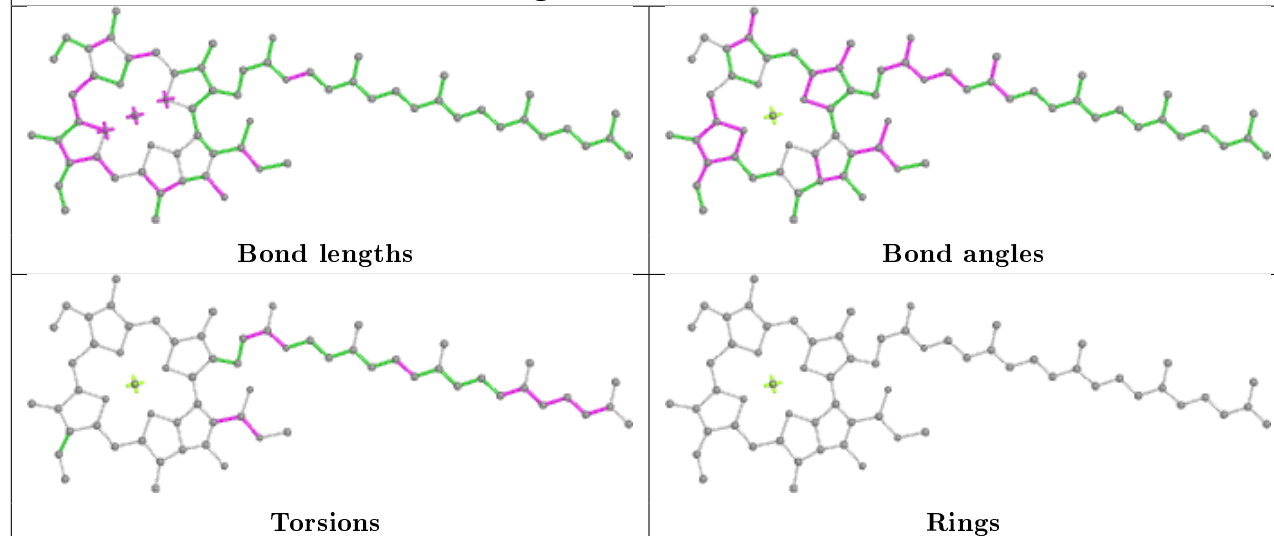
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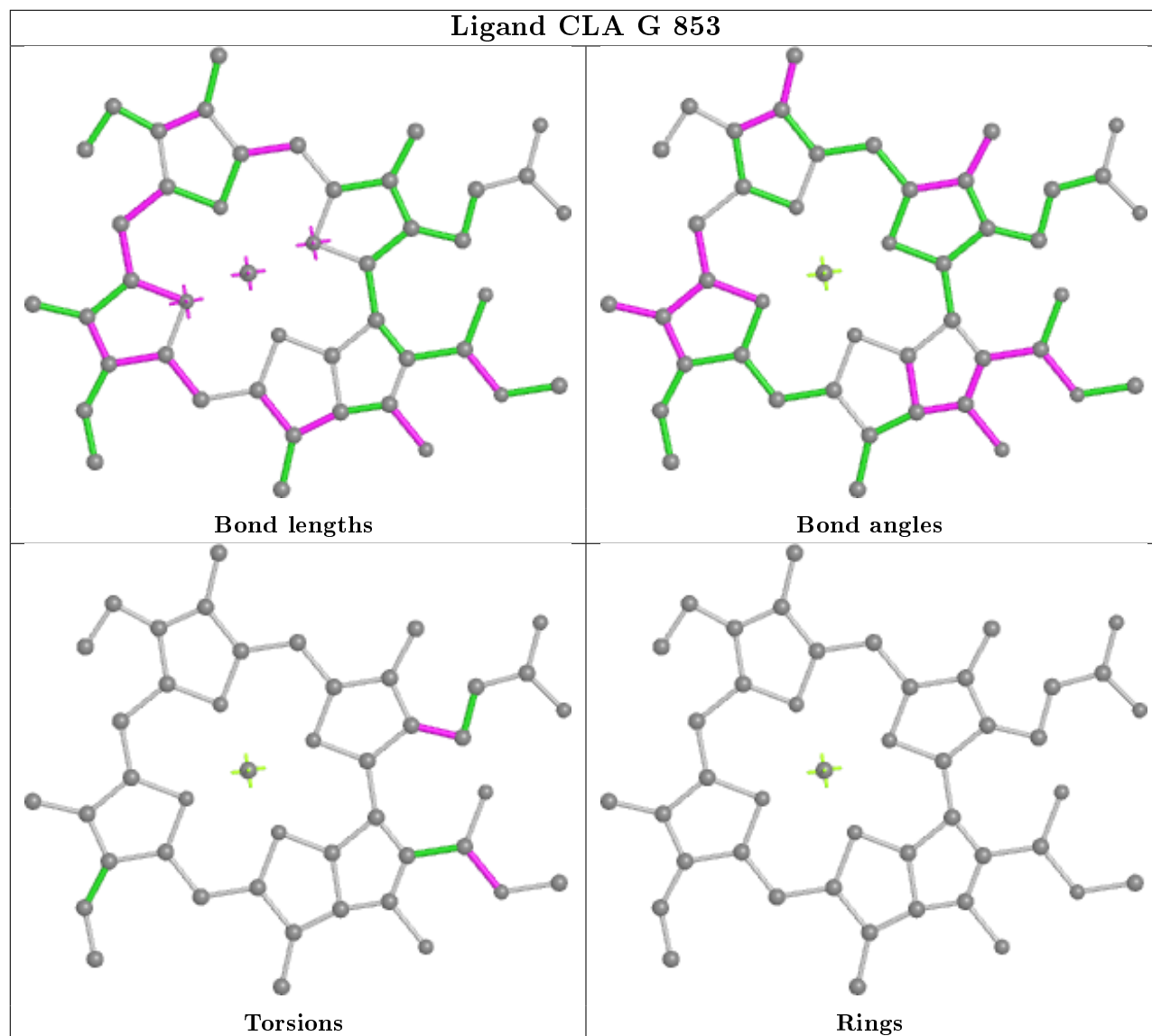
Ligand CLA h 207



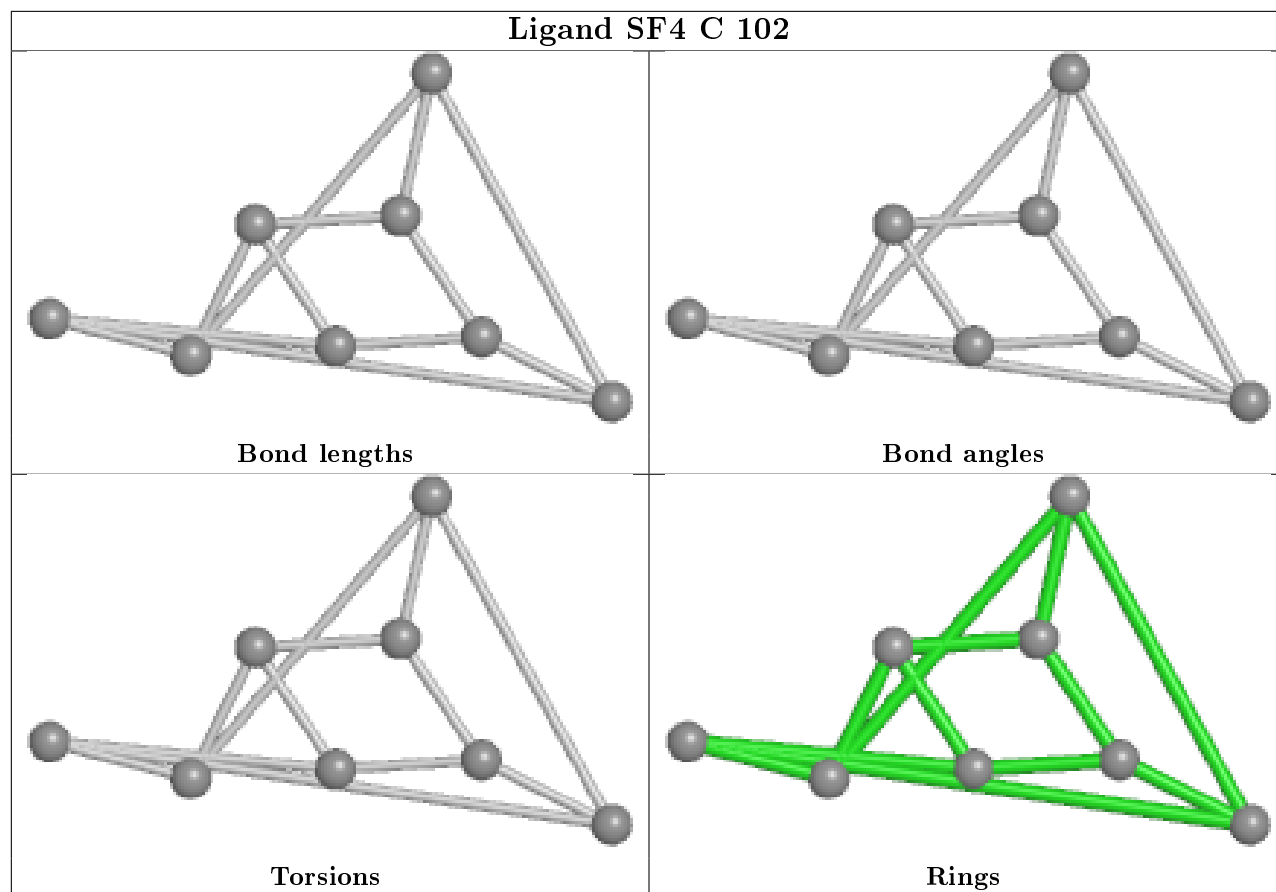
Ligand CLA Y 829



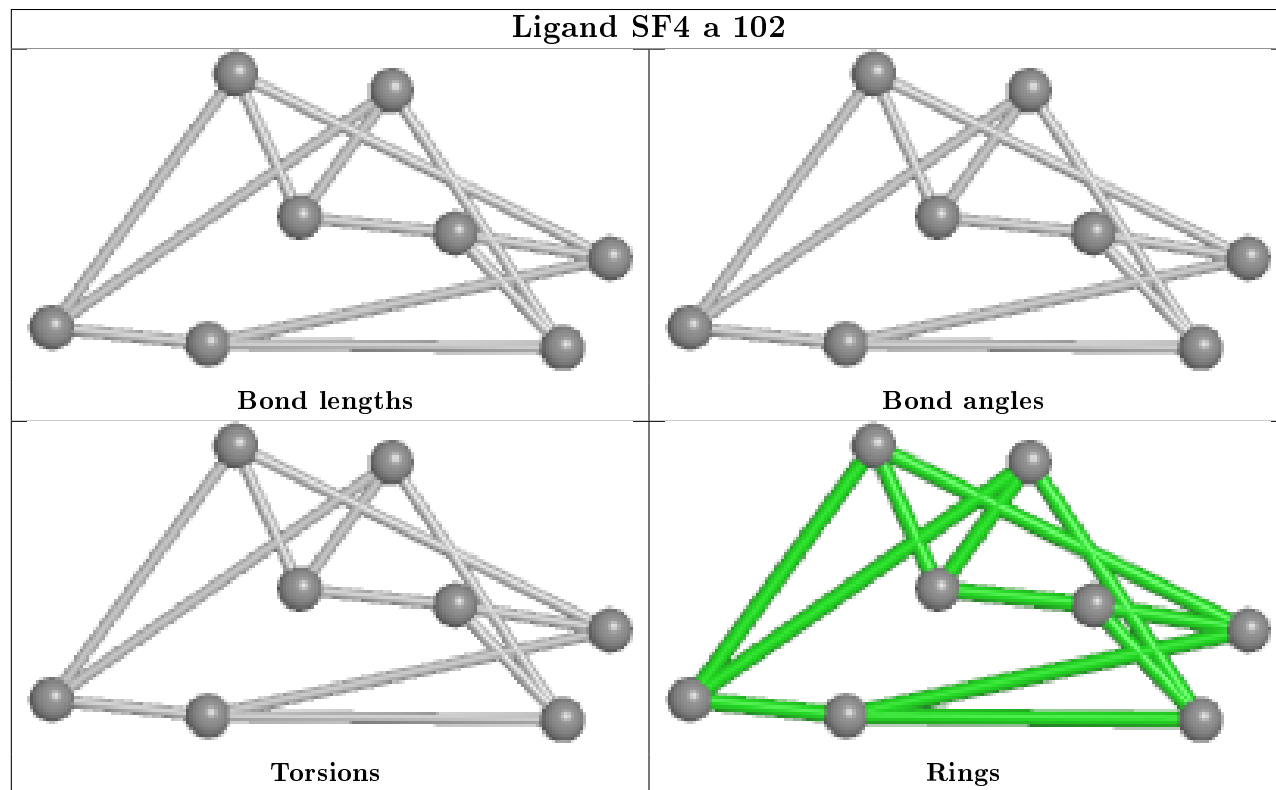
Ligand CLA G 853

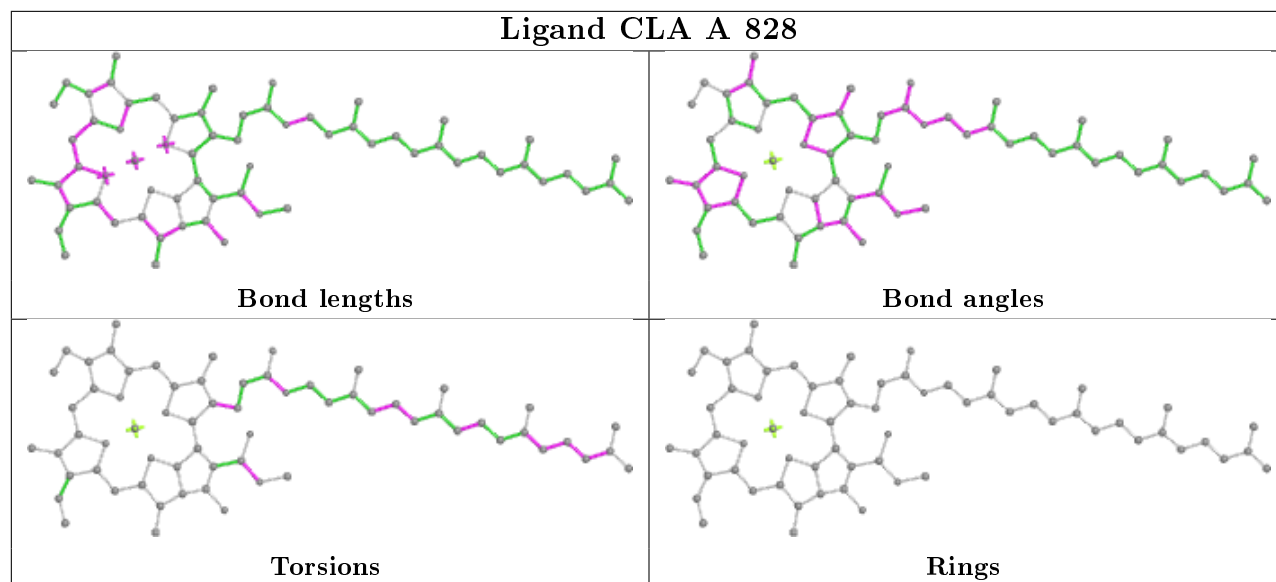
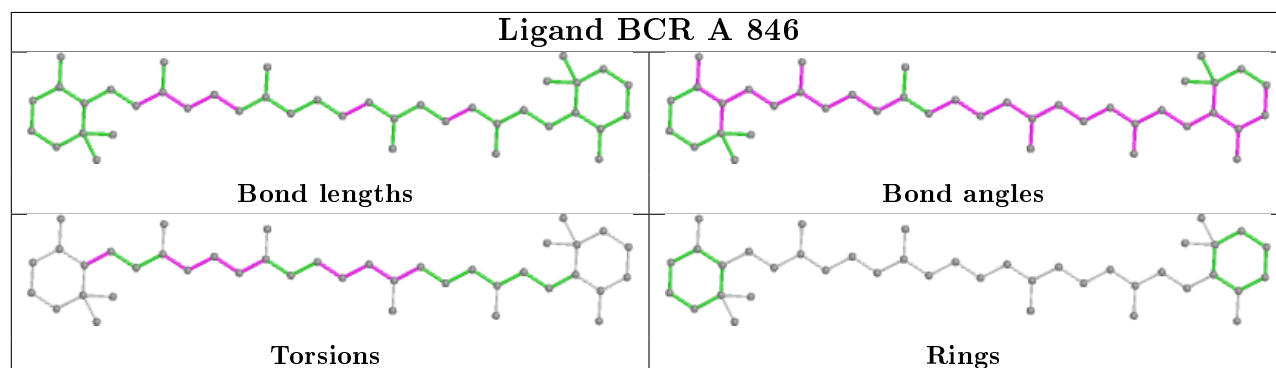
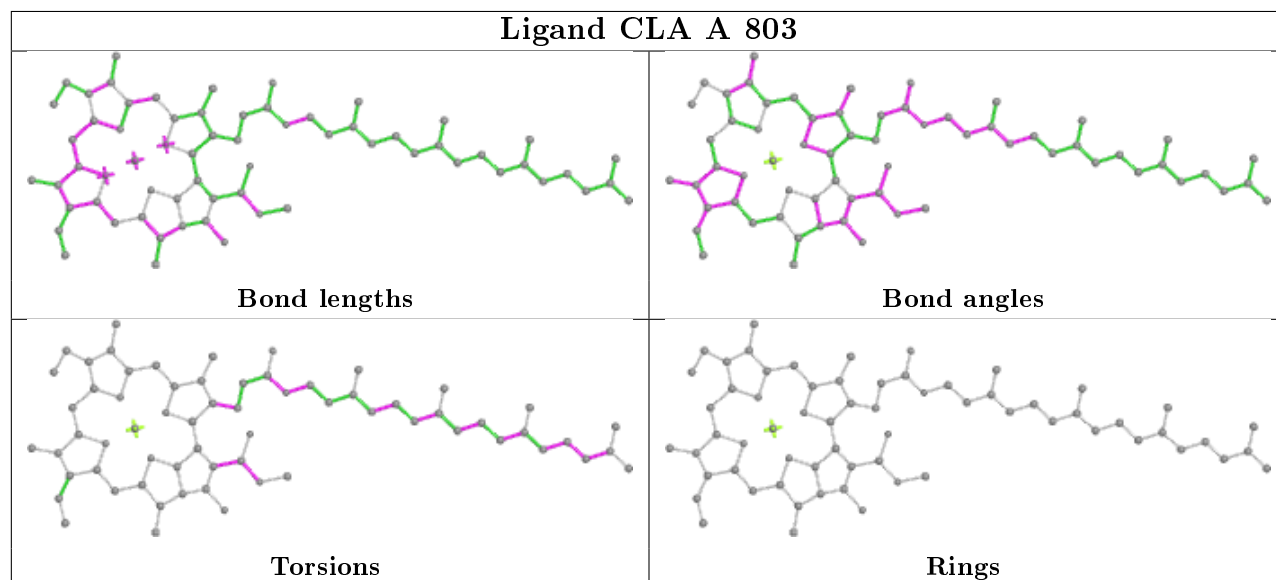


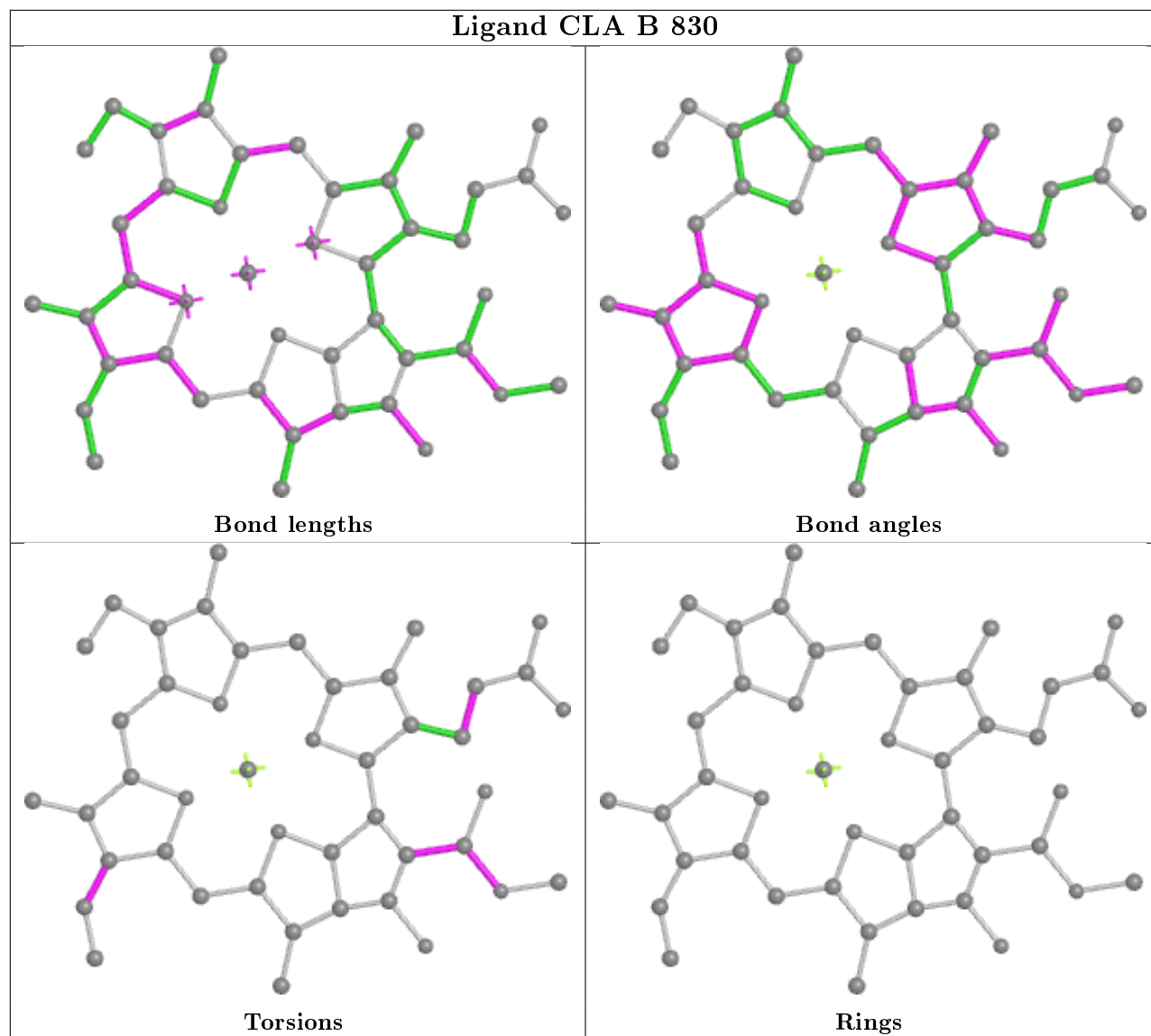
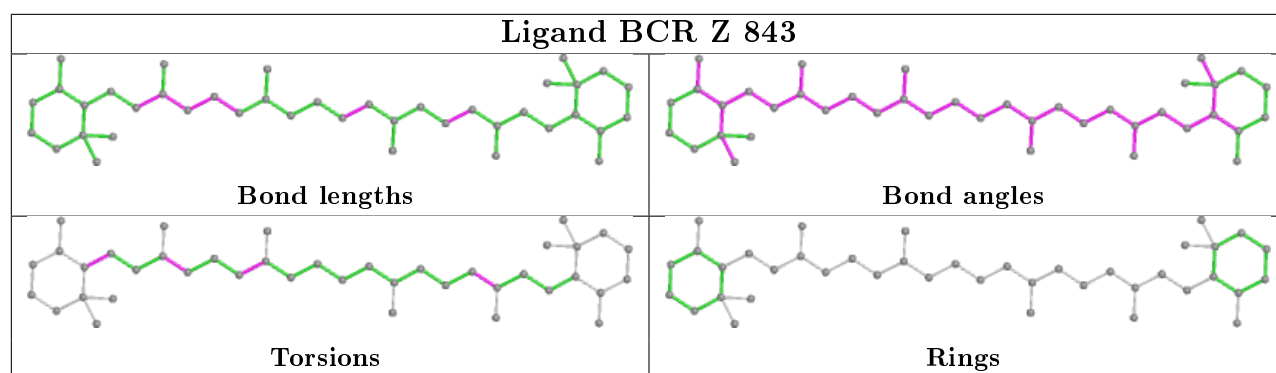
Ligand SF4 C 102



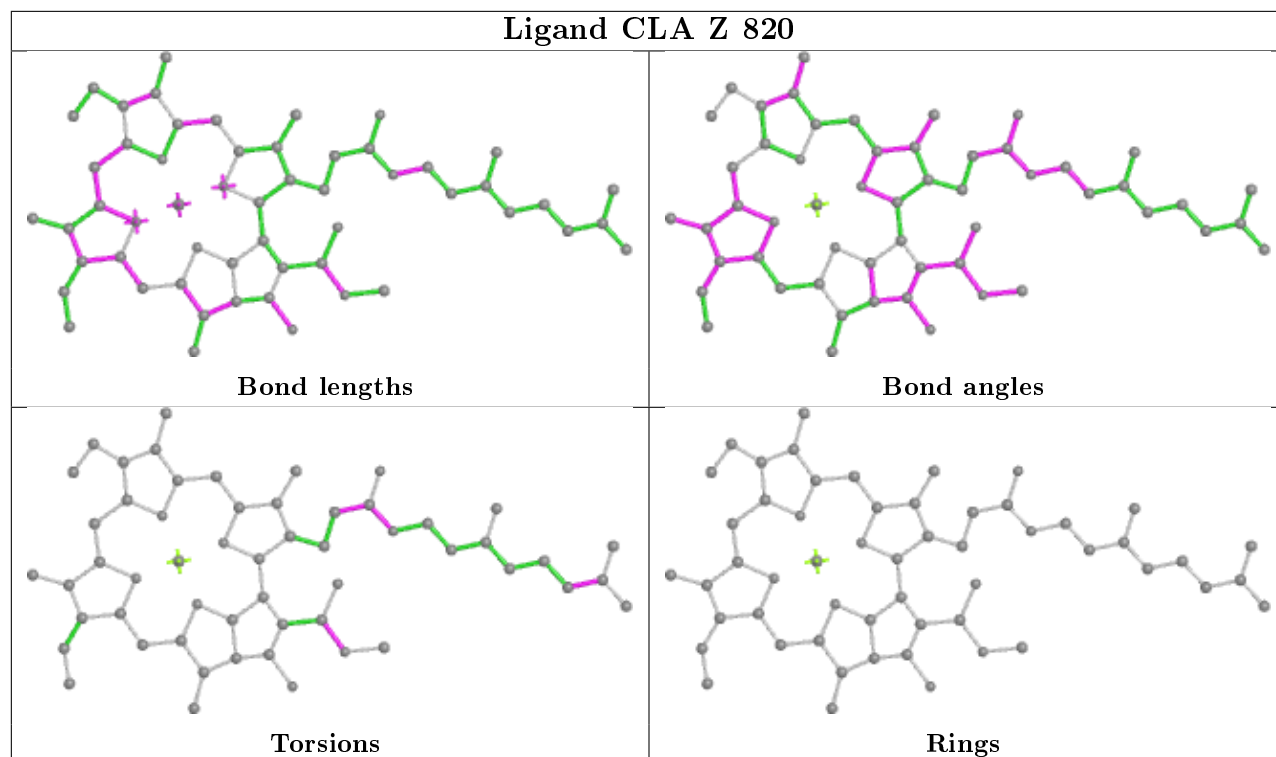
Ligand SF4 a 102



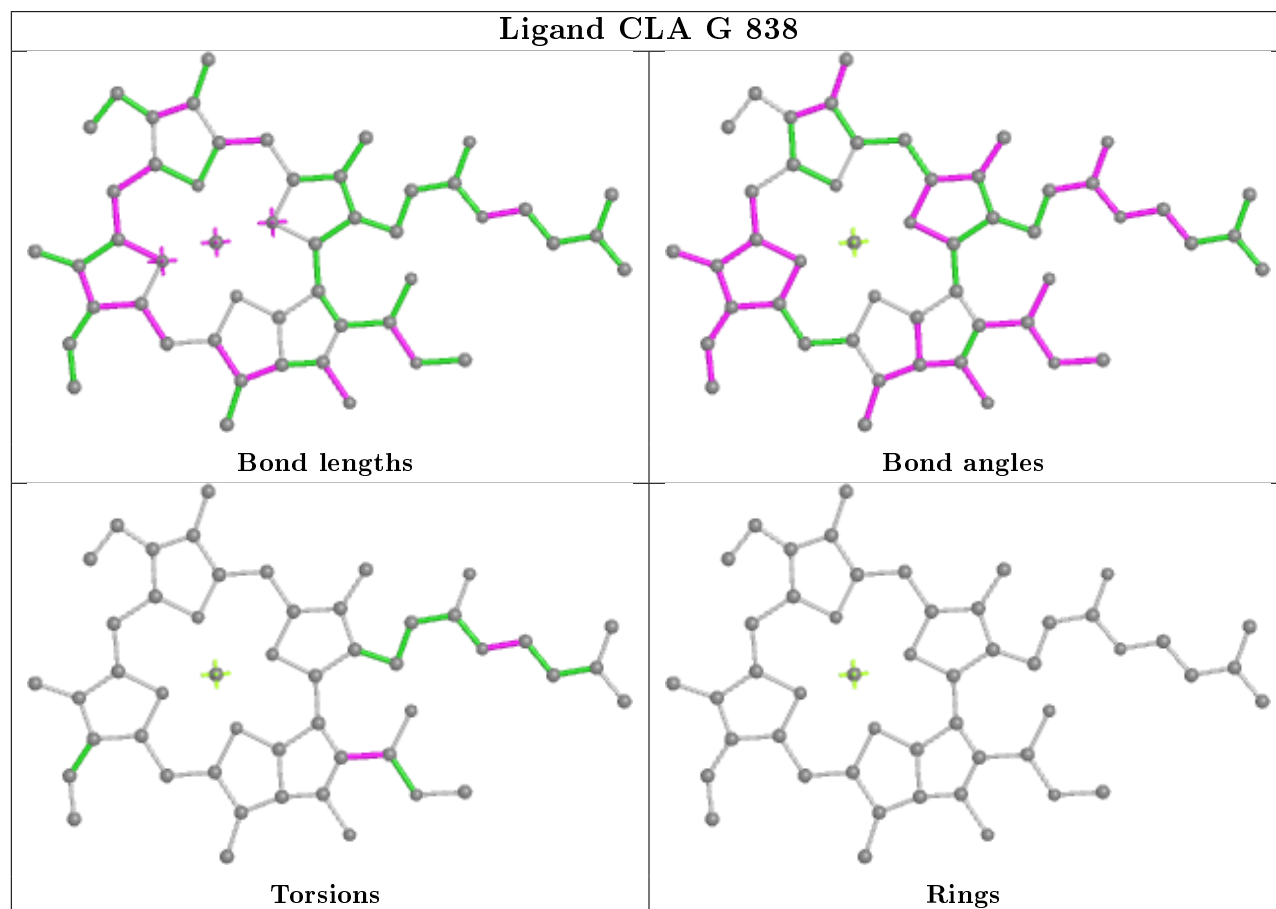
Ligand CLA A 828**Ligand BCR A 846****Ligand CLA A 803**



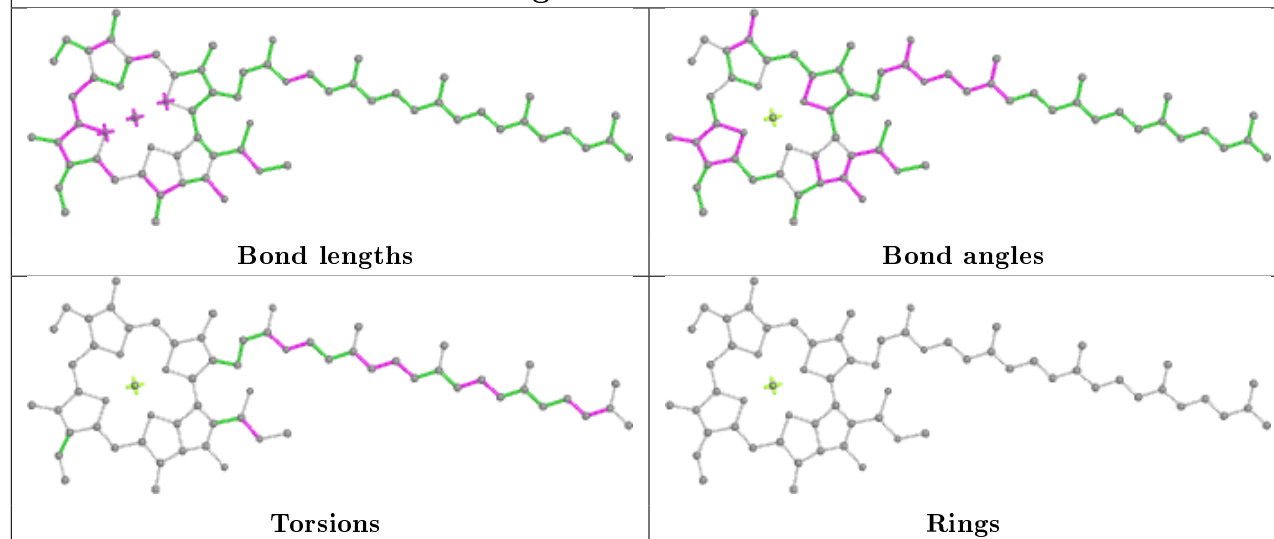
Ligand CLA Z 820



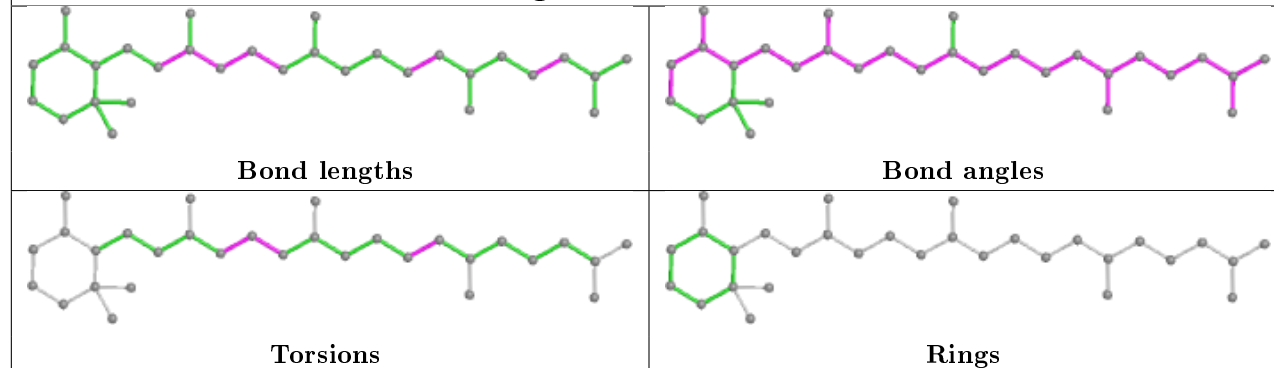
Ligand CLA G 838



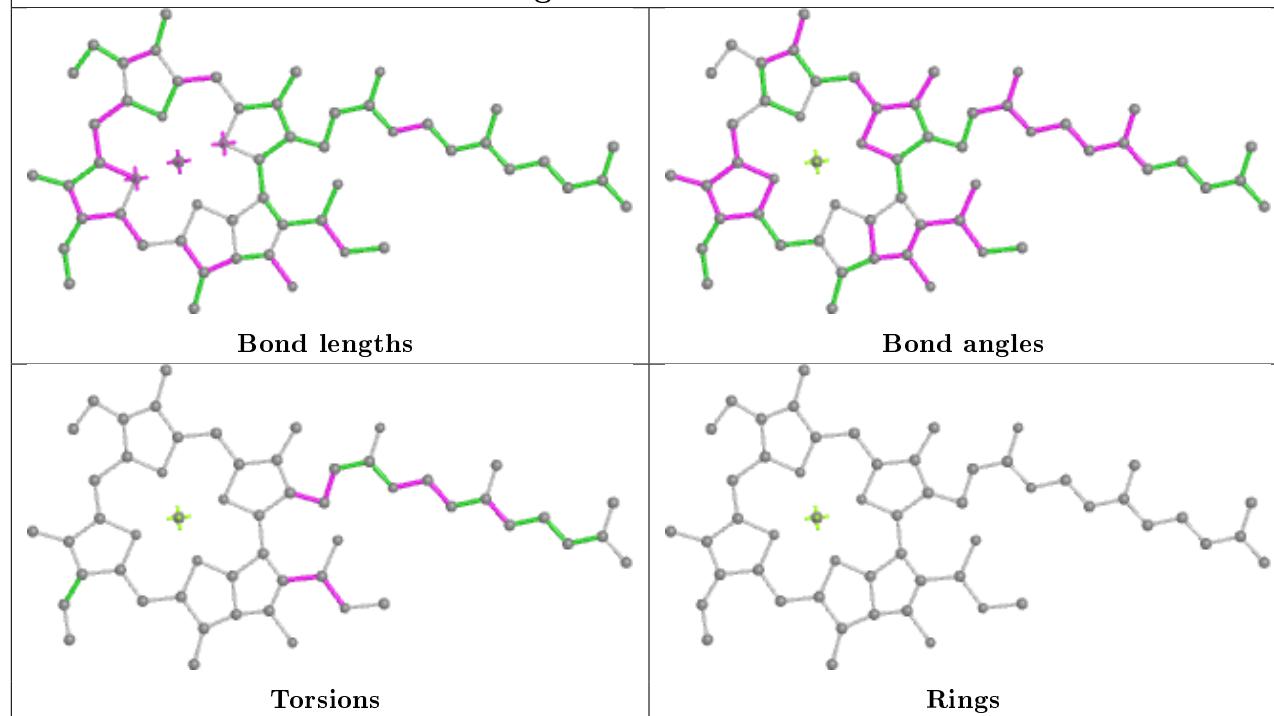
Ligand CLA Y 841

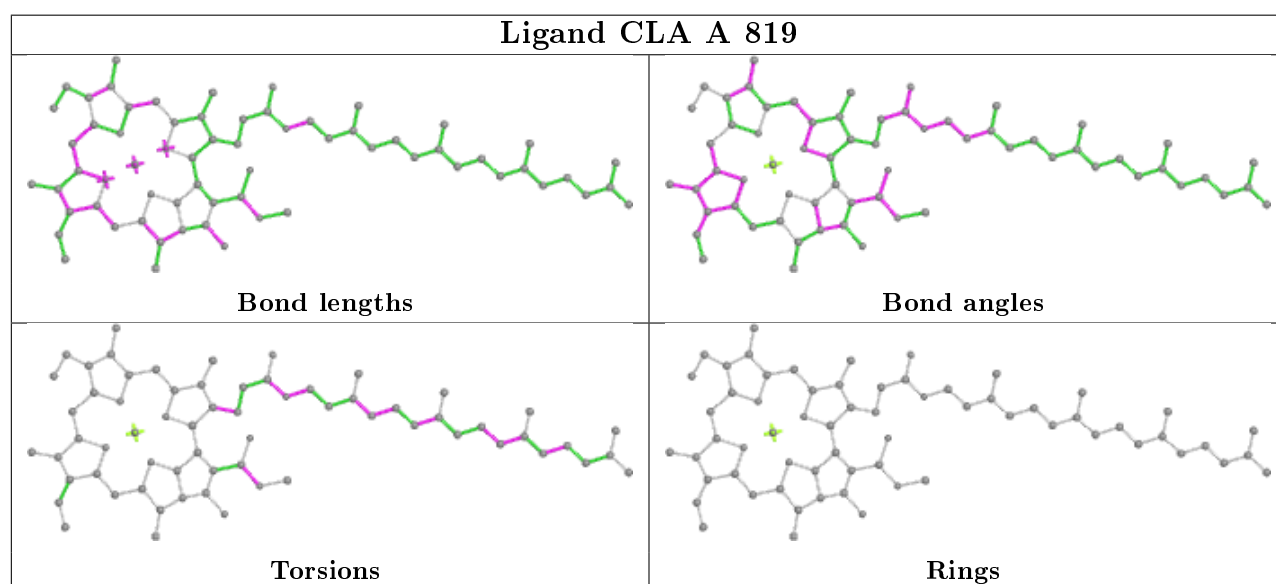
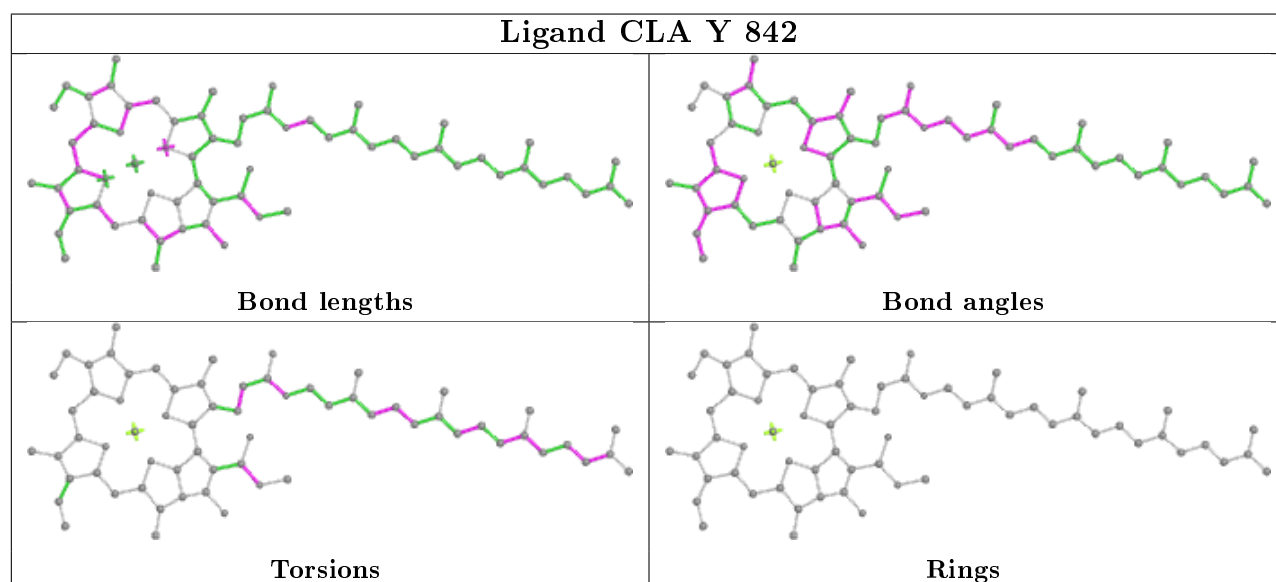
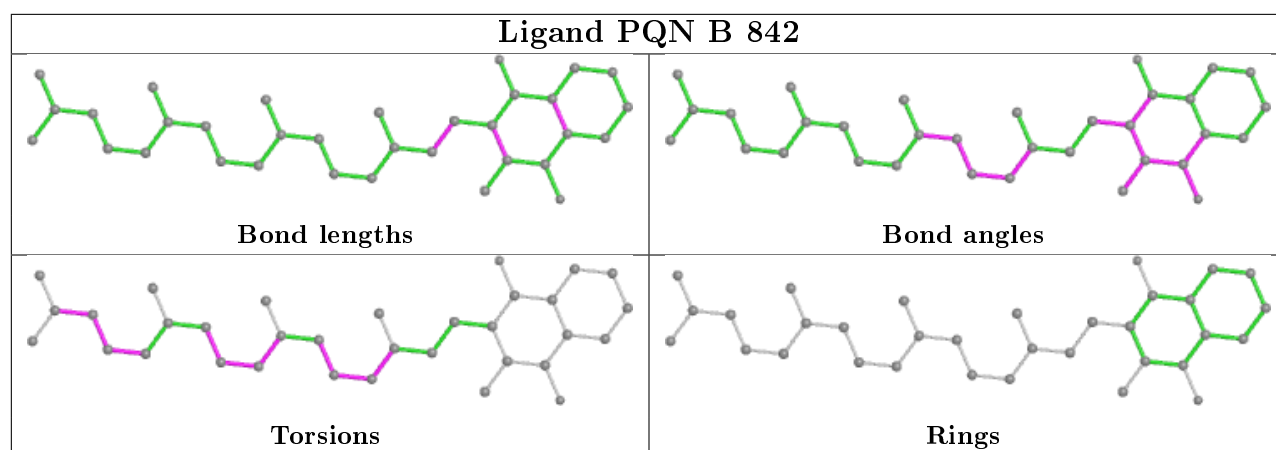


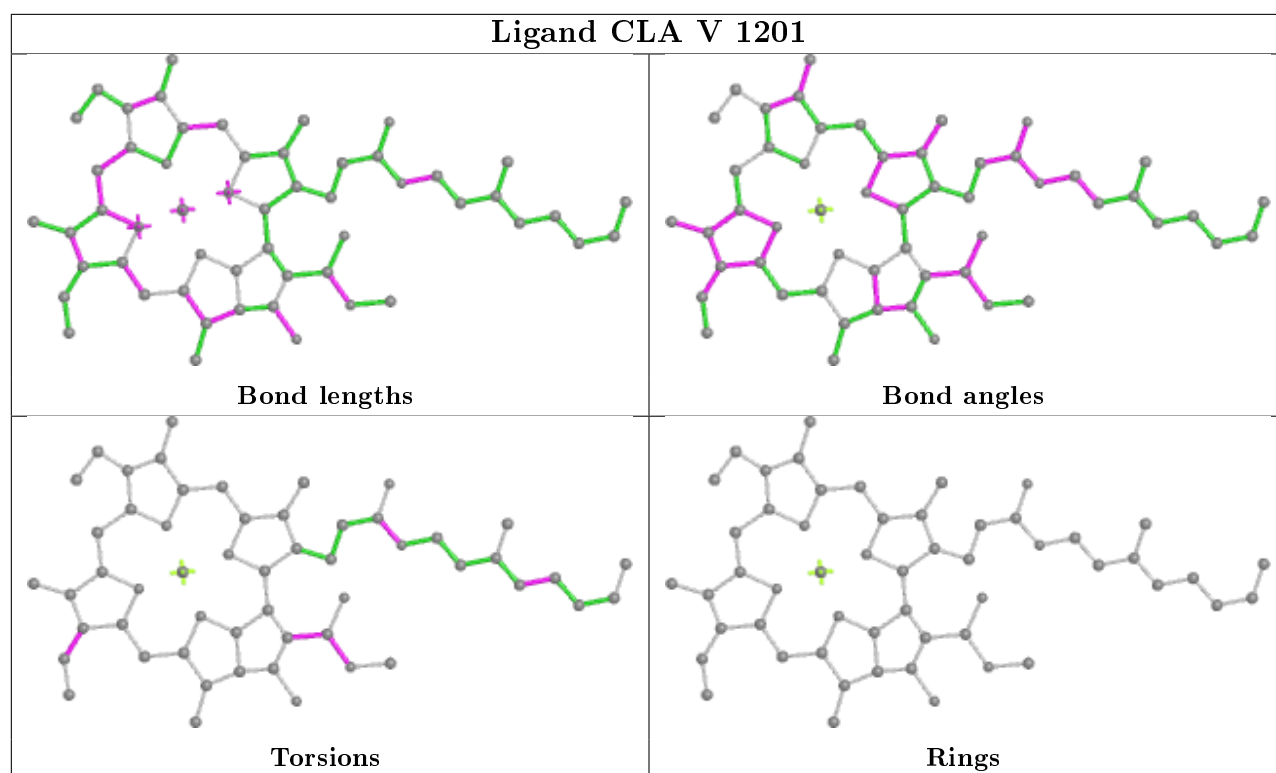
Ligand BCR B 843



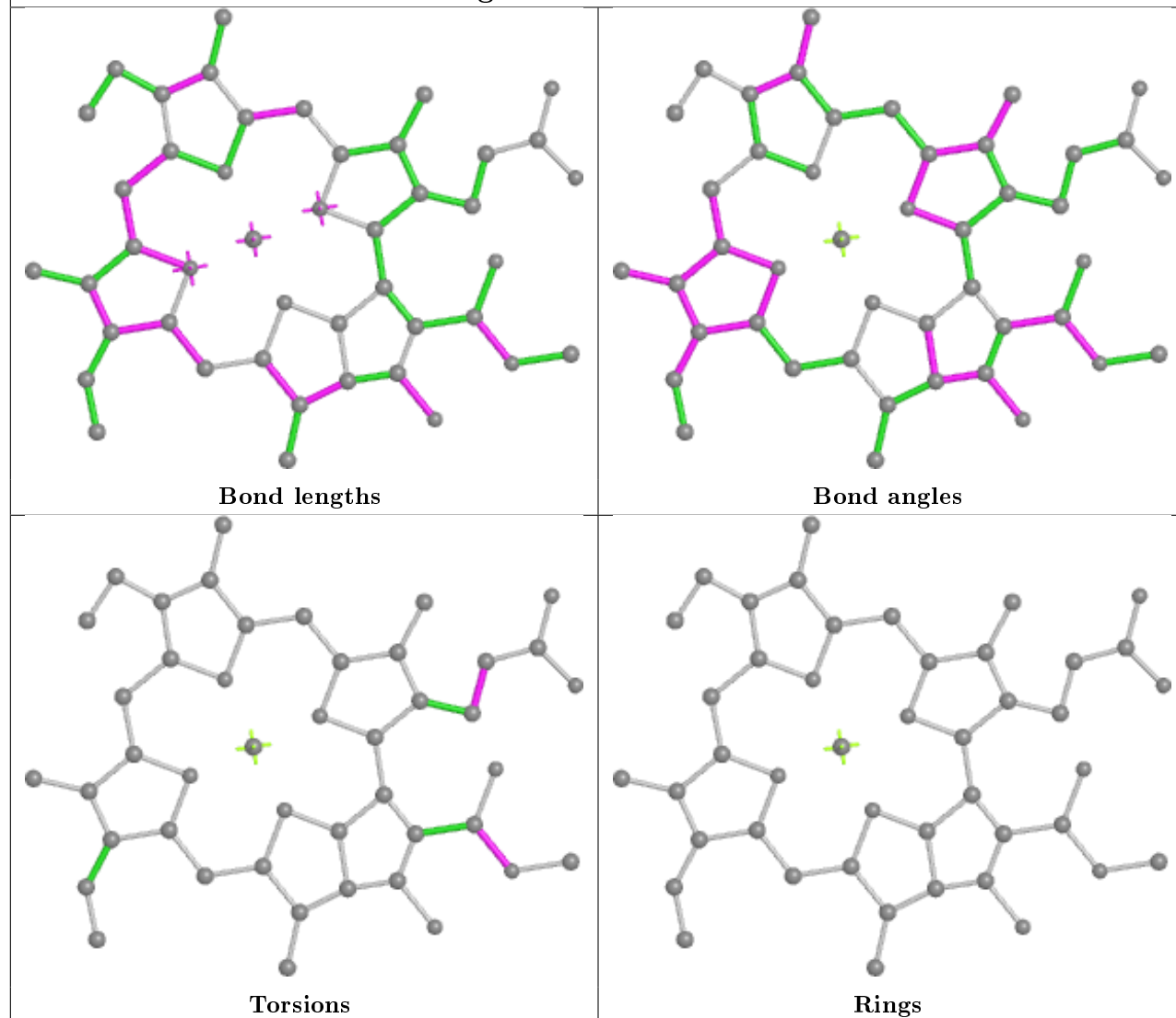
Ligand CLA Z 822



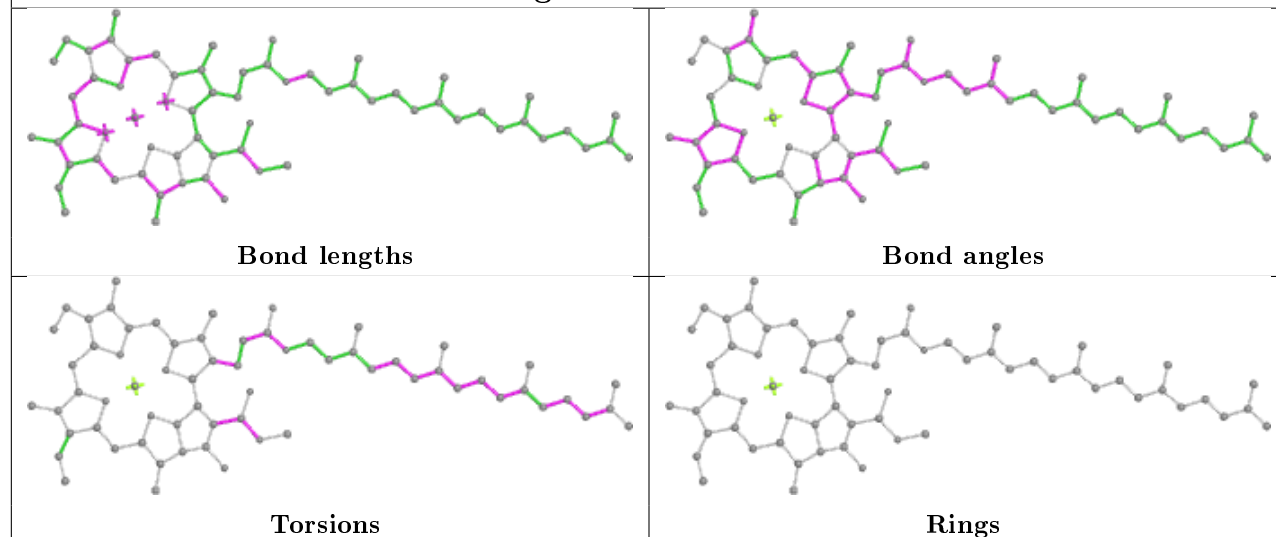




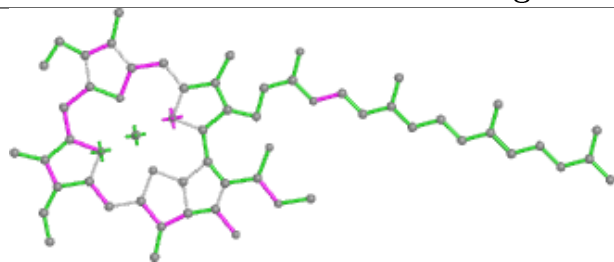
Ligand CLA W 1701



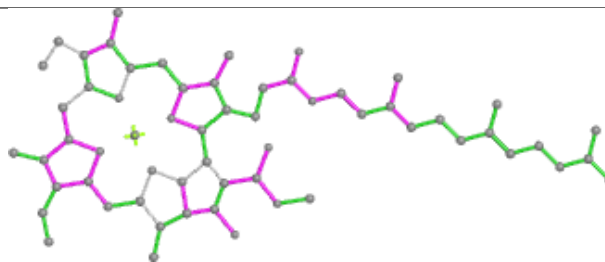
Ligand CLA Z 802



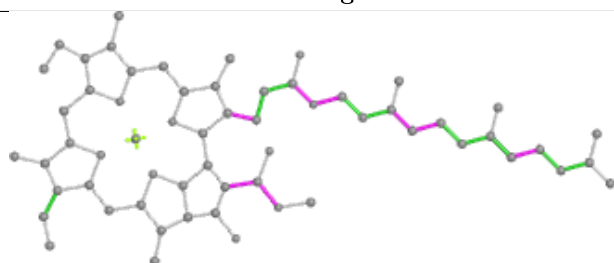
Ligand CLA H 834



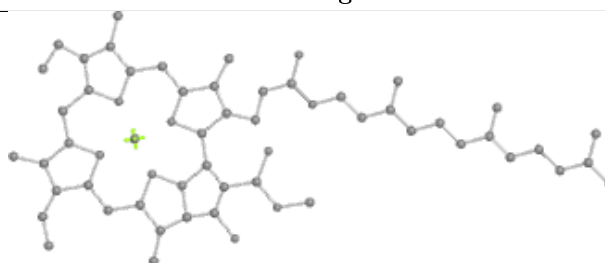
Bond lengths



Bond angles

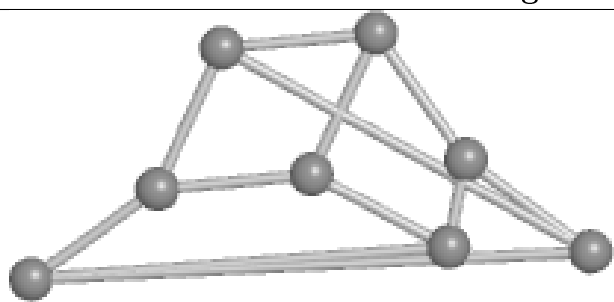


Torsions

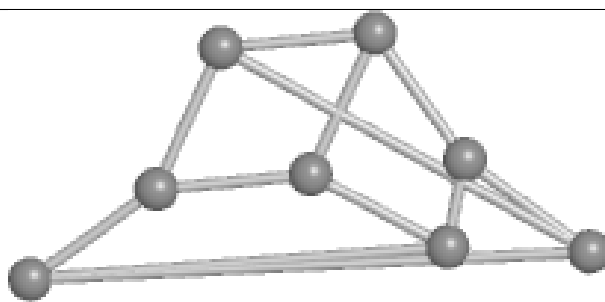


Rings

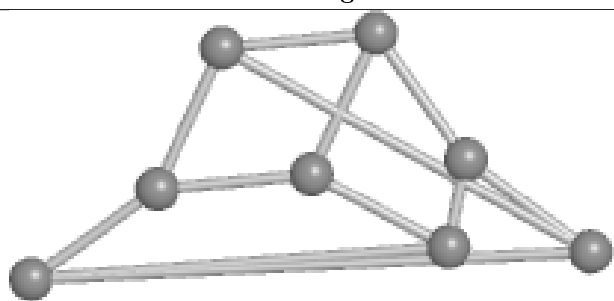
Ligand SF4 A 844



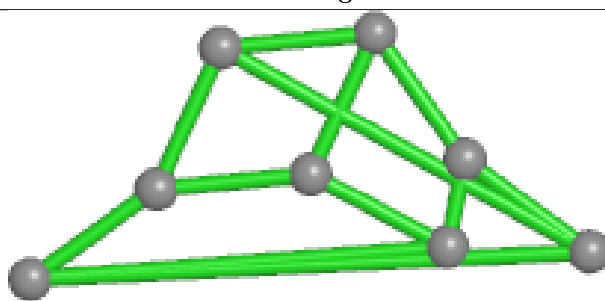
Bond lengths



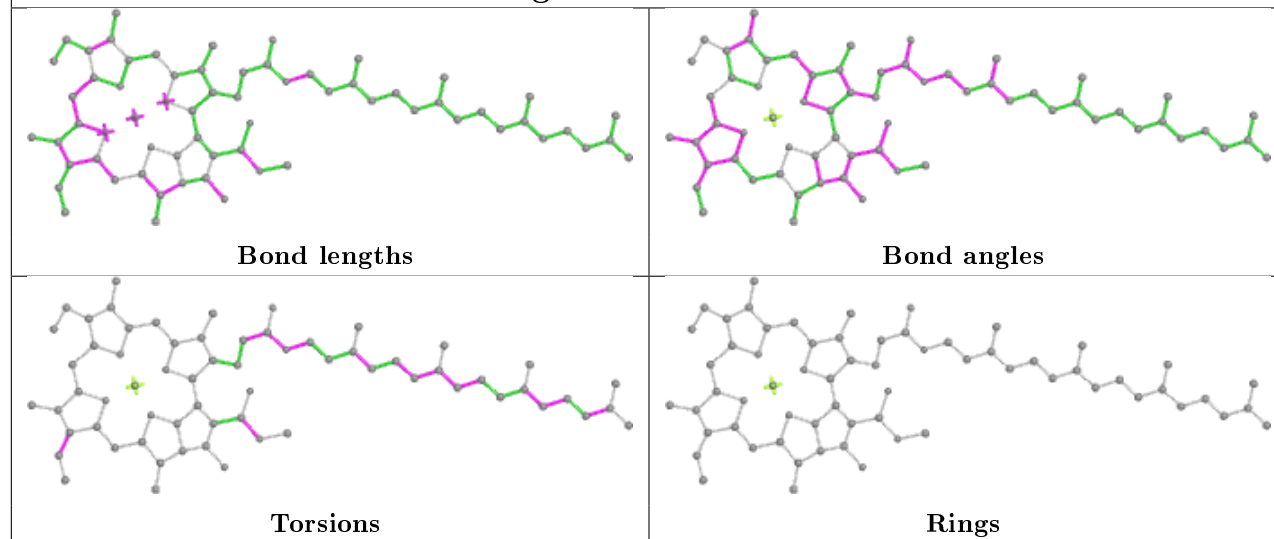
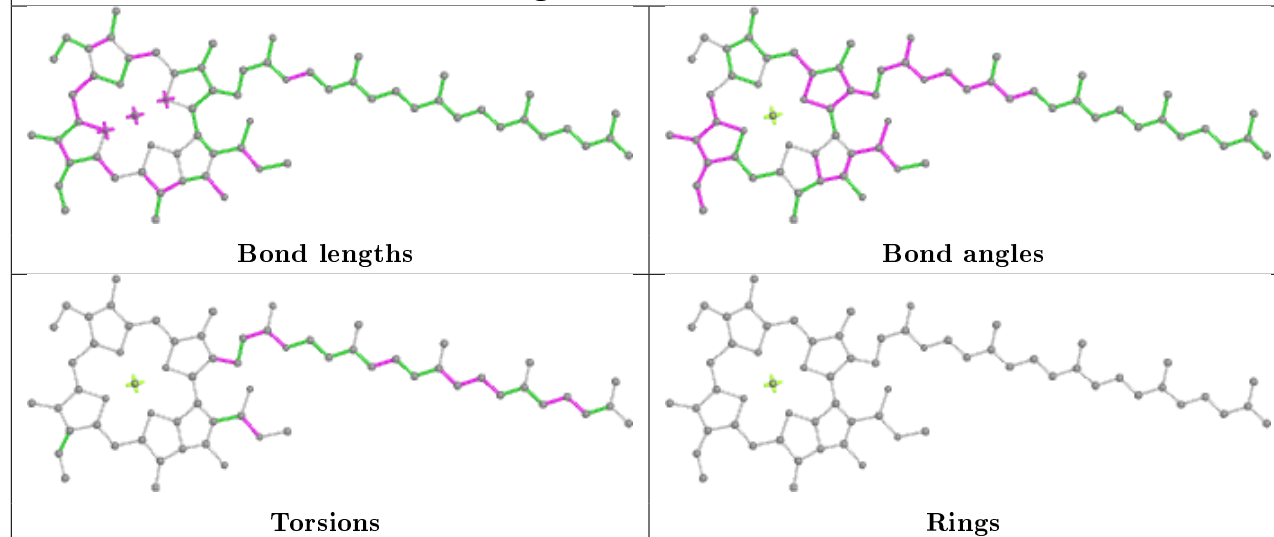
Bond angles



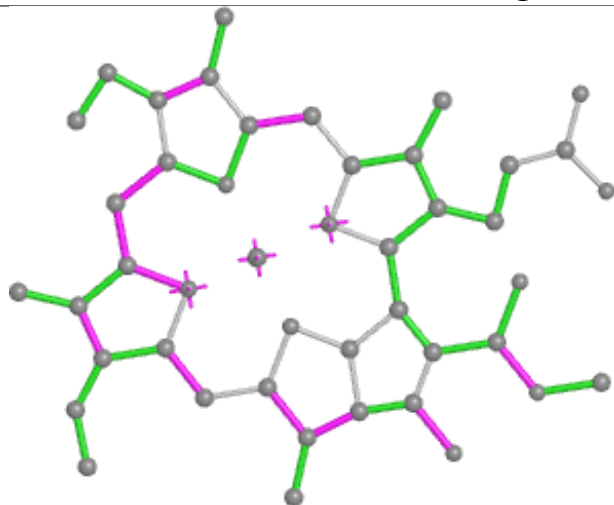
Torsions



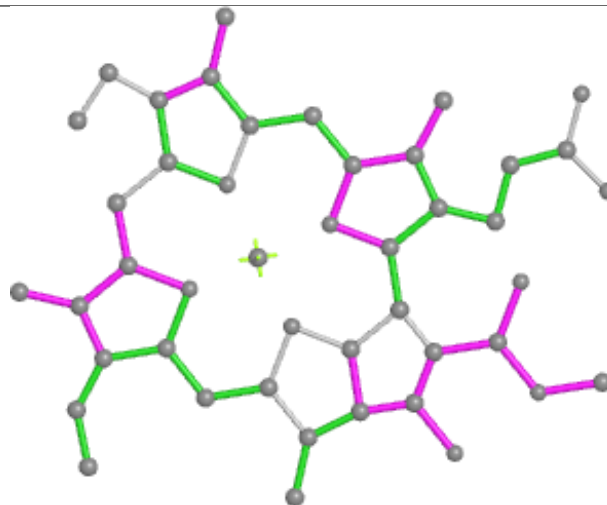
Rings

Ligand CLA B 814**Ligand CLA Y 805**

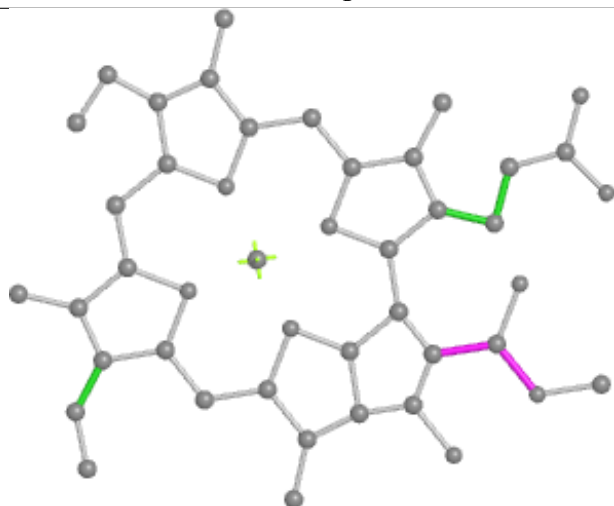
Ligand CLA Q 203



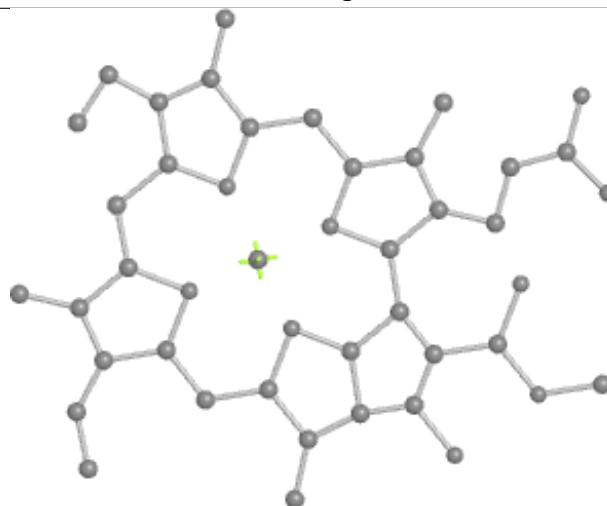
Bond lengths



Bond angles

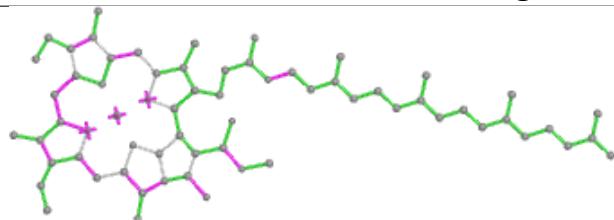


Torsions

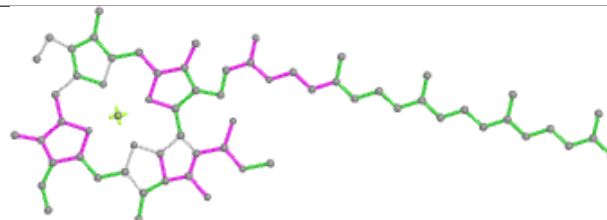


Rings

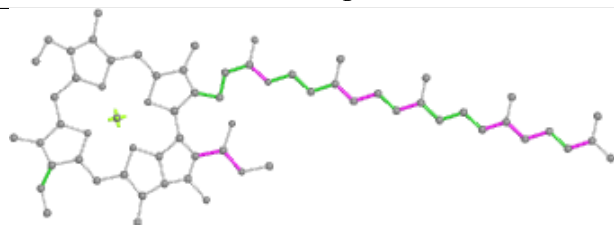
Ligand CLA Y 854



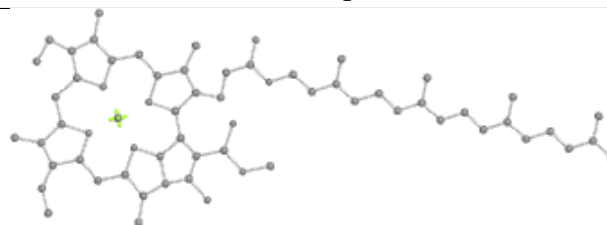
Bond lengths



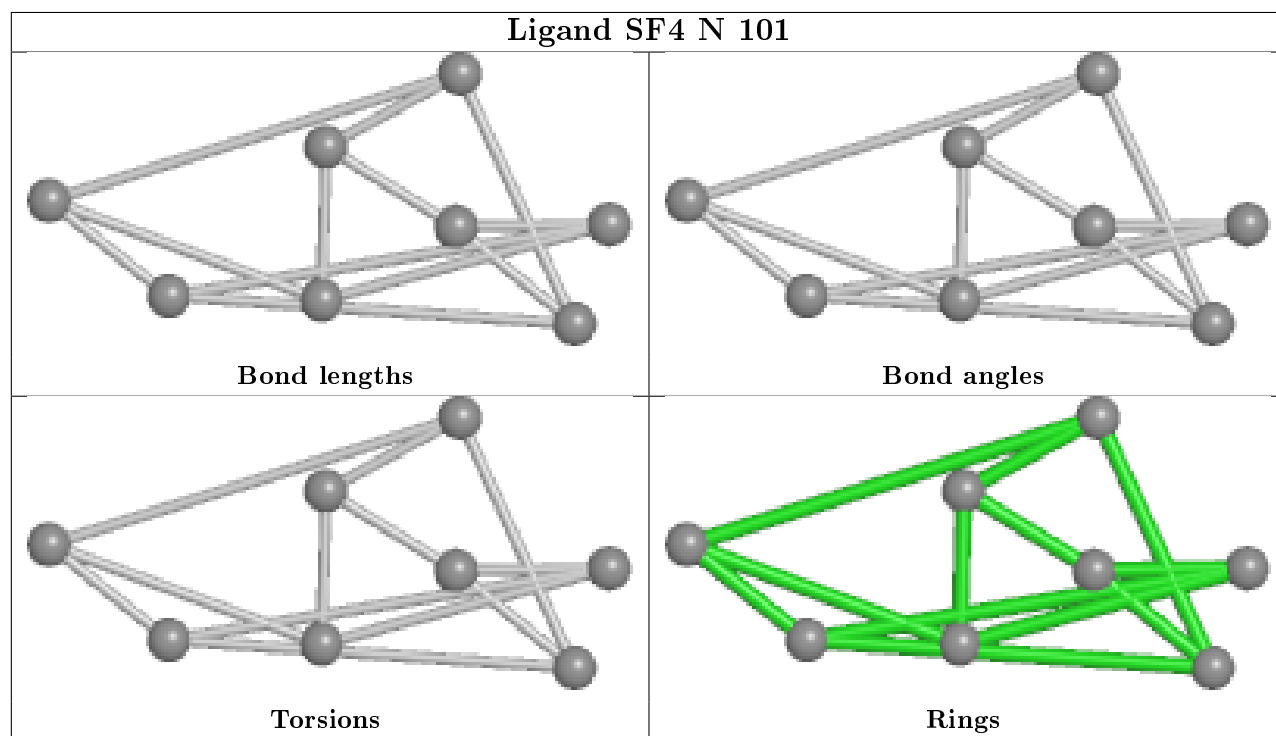
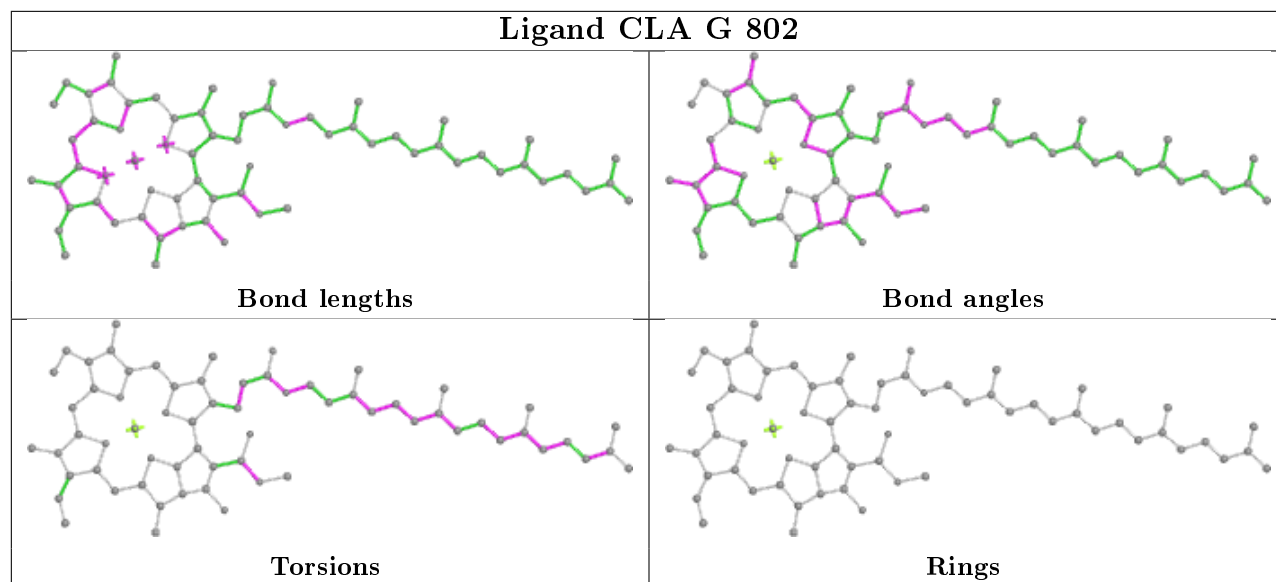
Bond angles

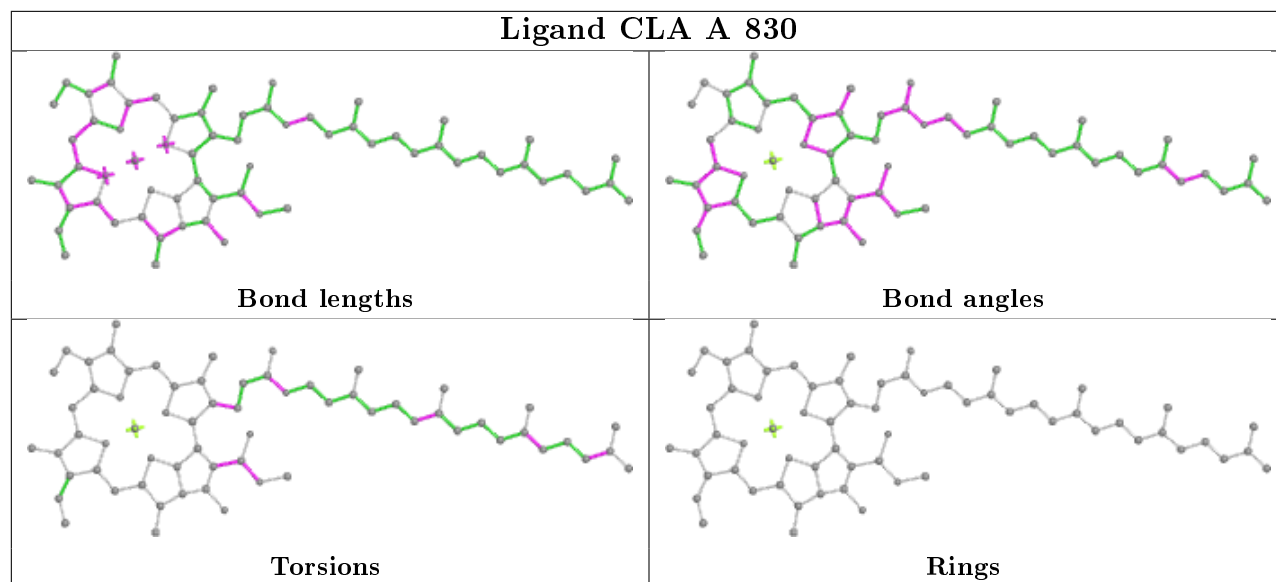
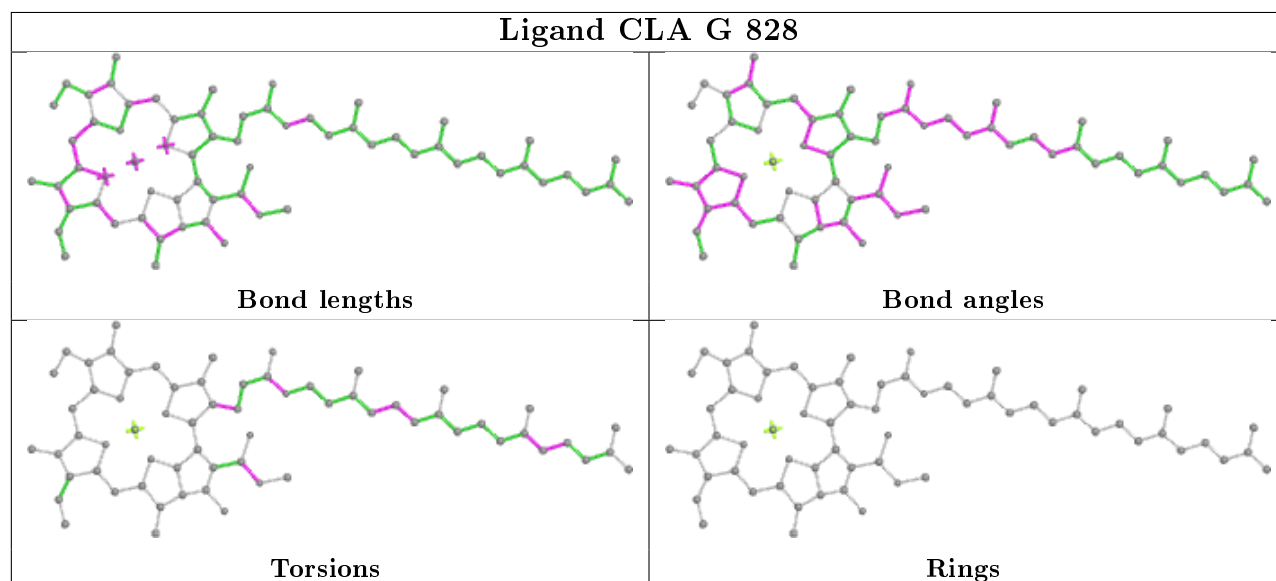


Torsions

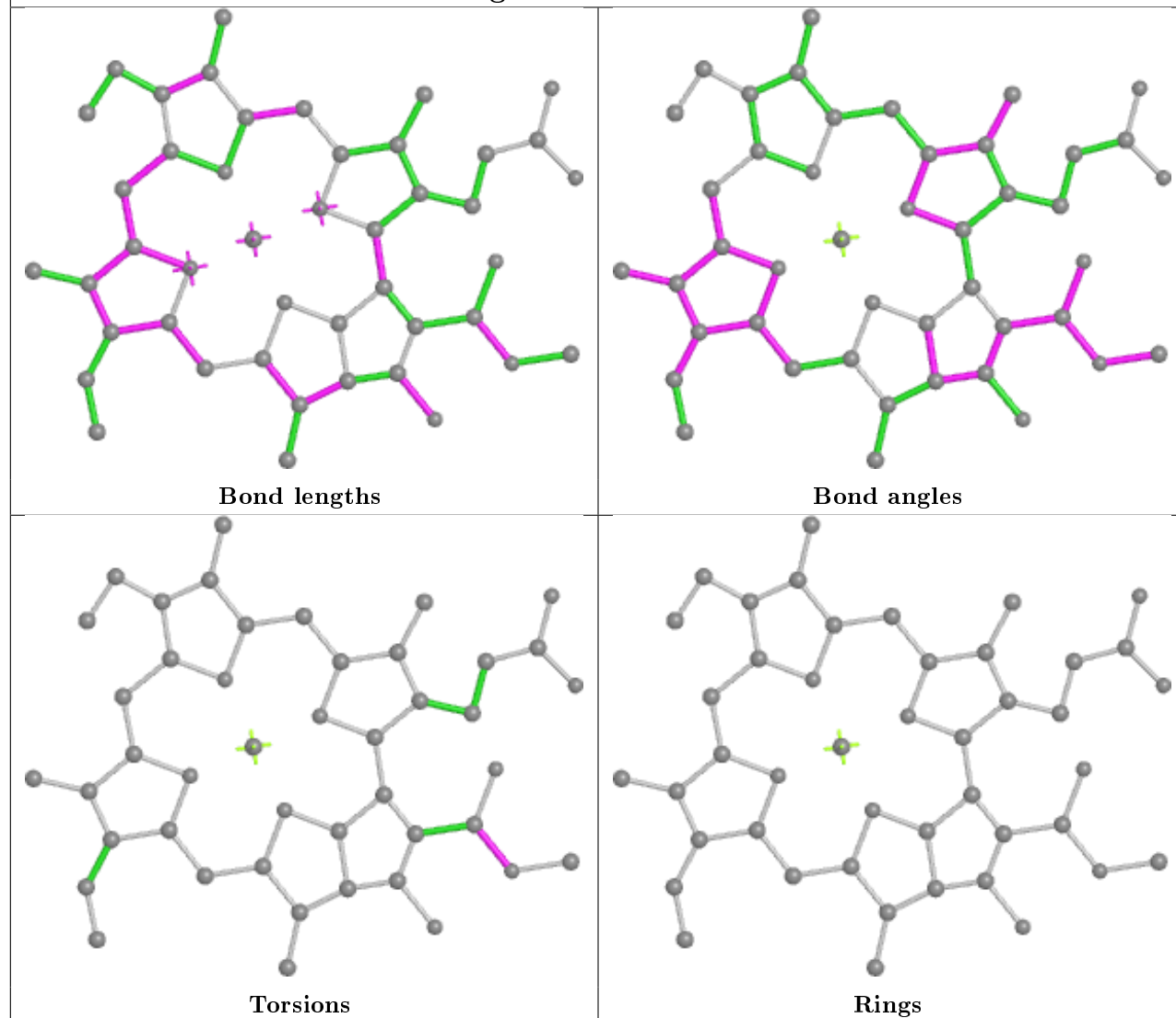


Rings

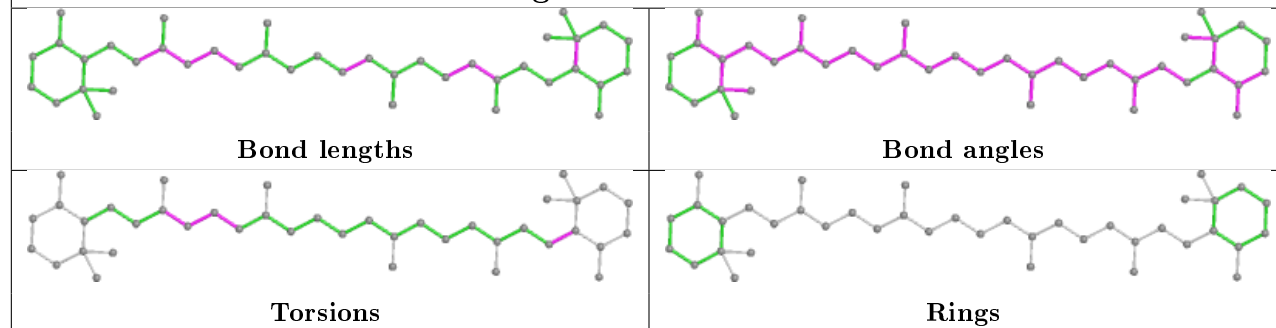


Ligand CLA A 830**Ligand CLA G 828**

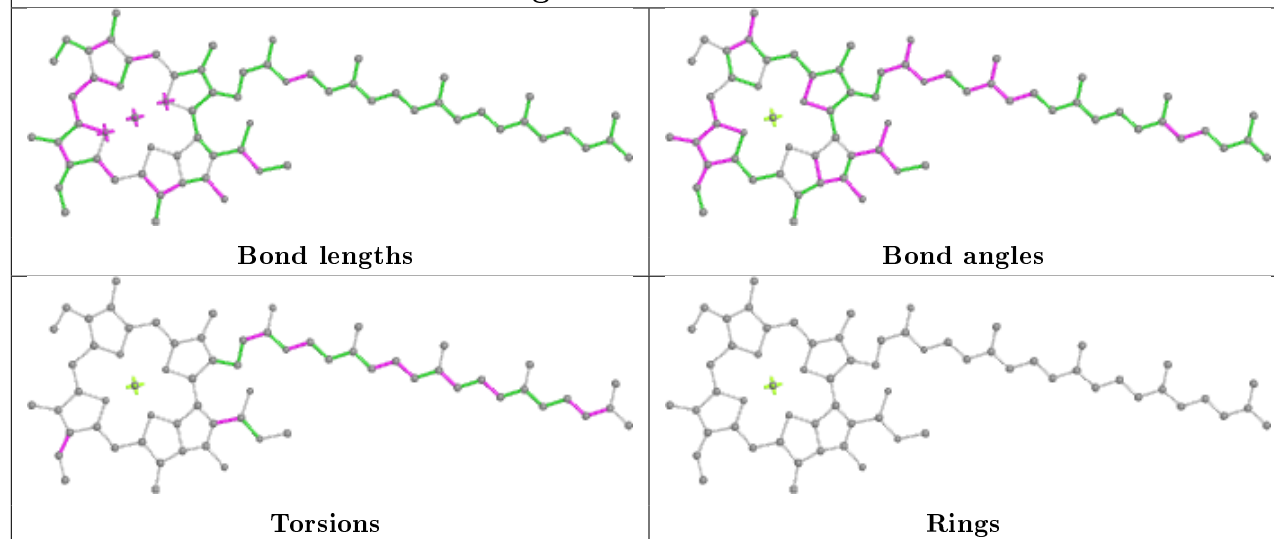
Ligand CLA H 836



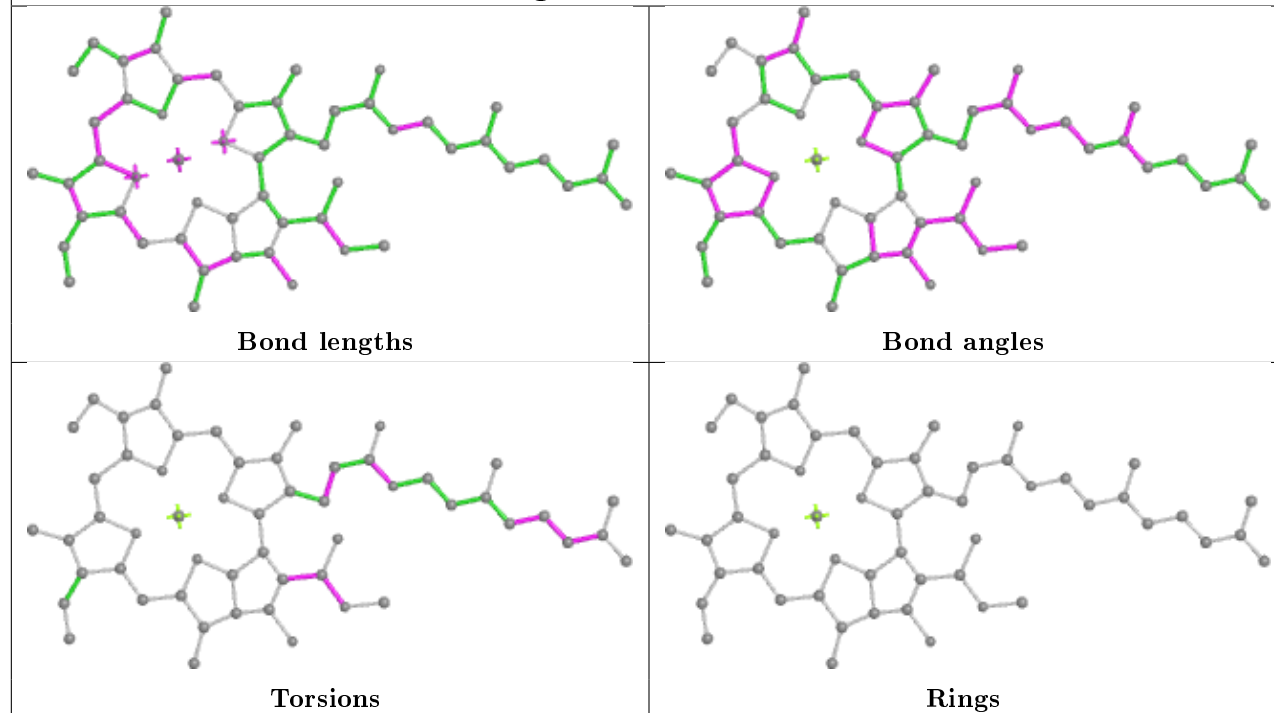
Ligand BCR Z 842



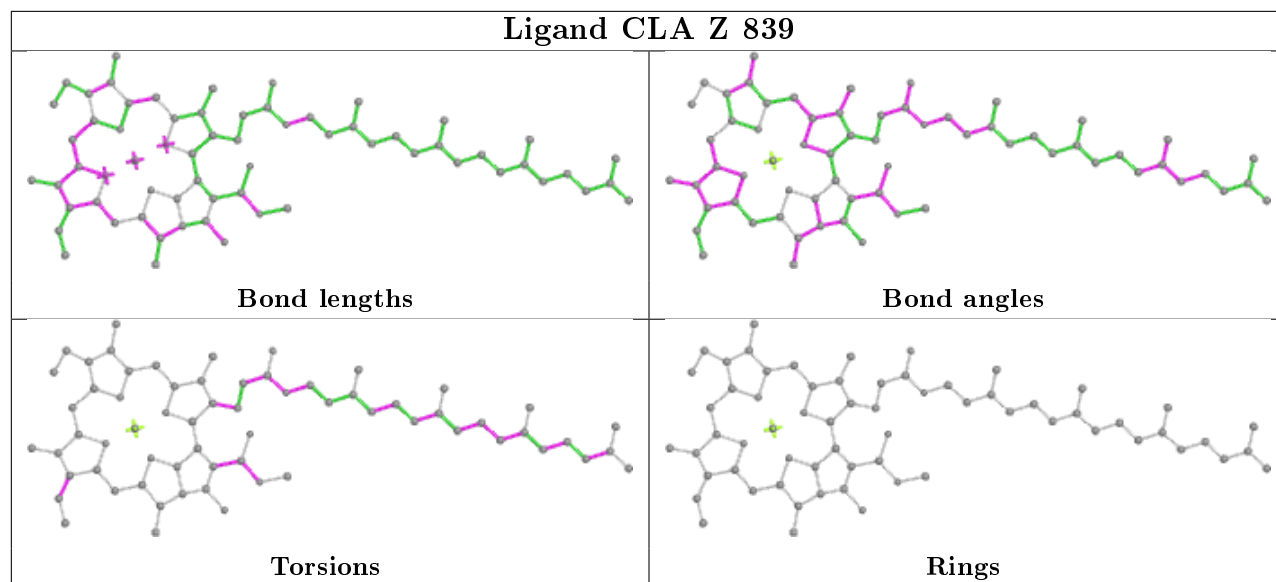
Ligand CLA B 808



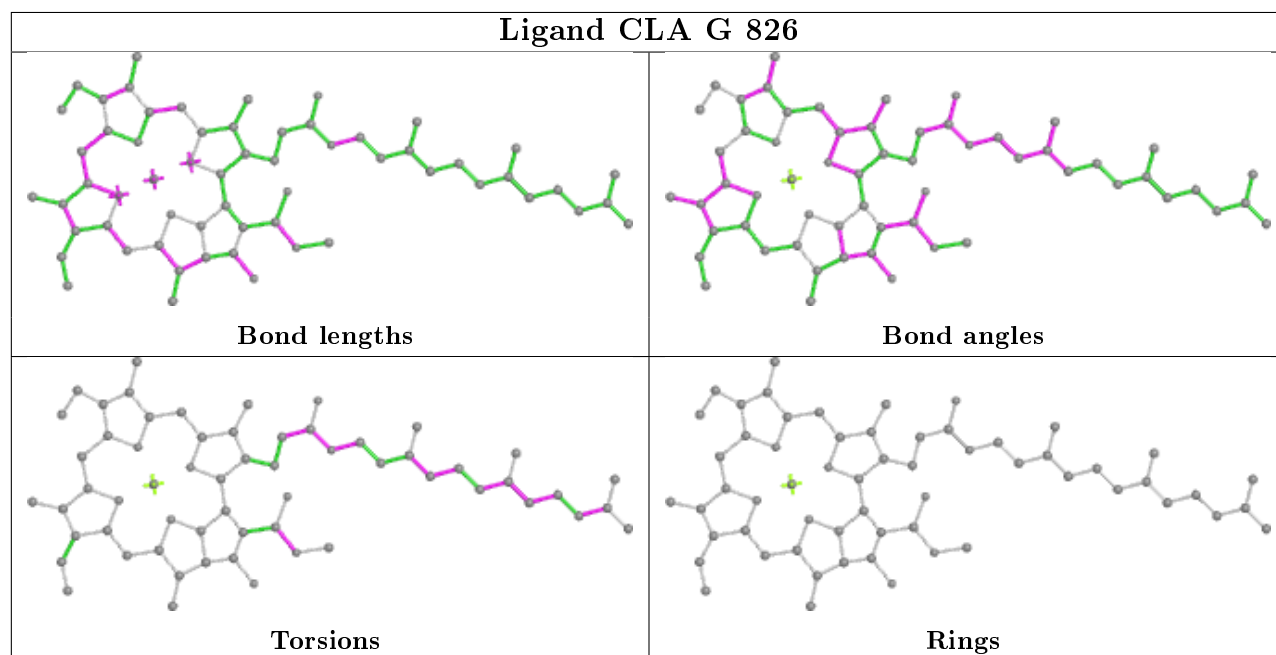
Ligand CLA B 816

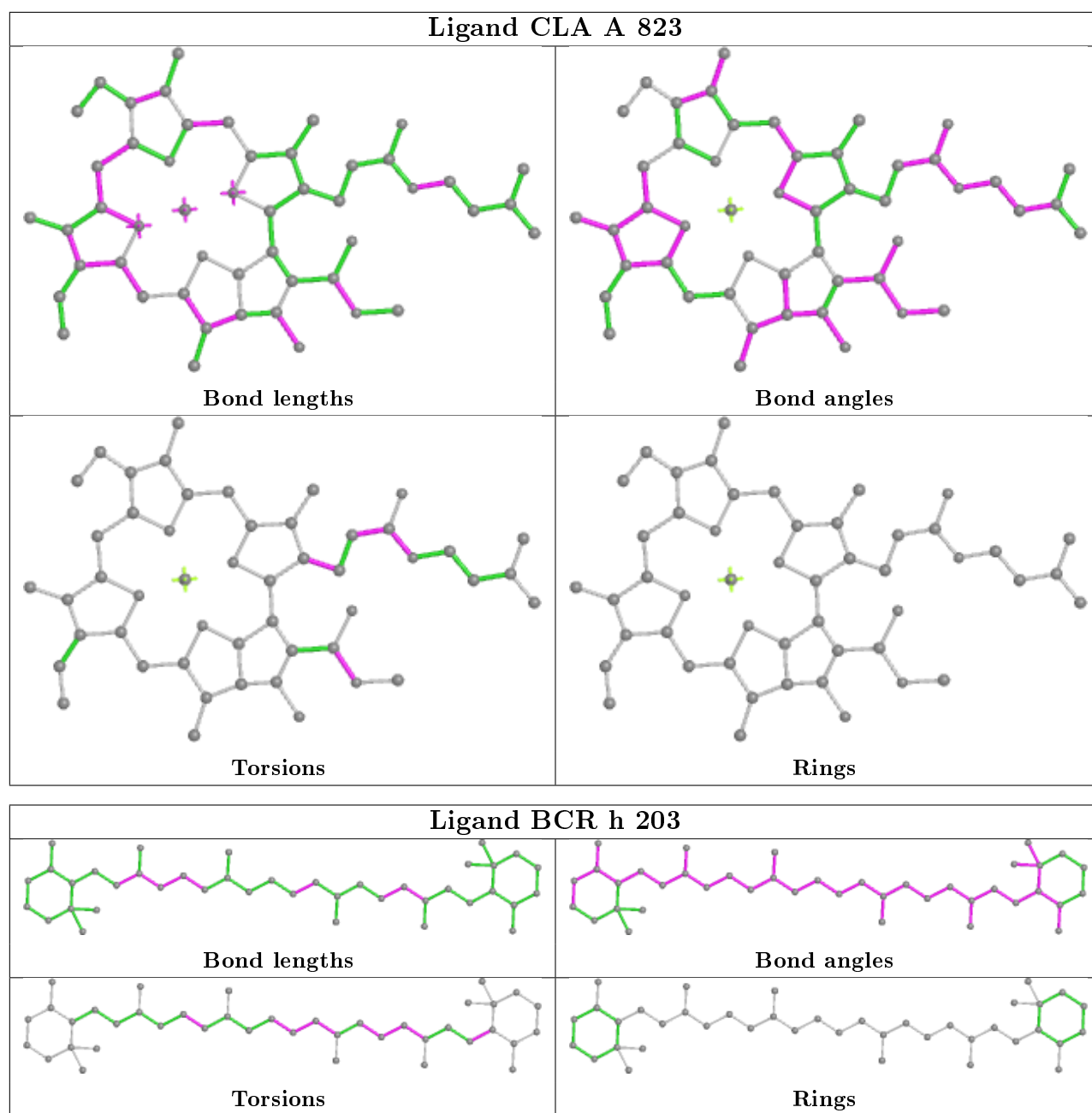


Ligand CLA Z 839

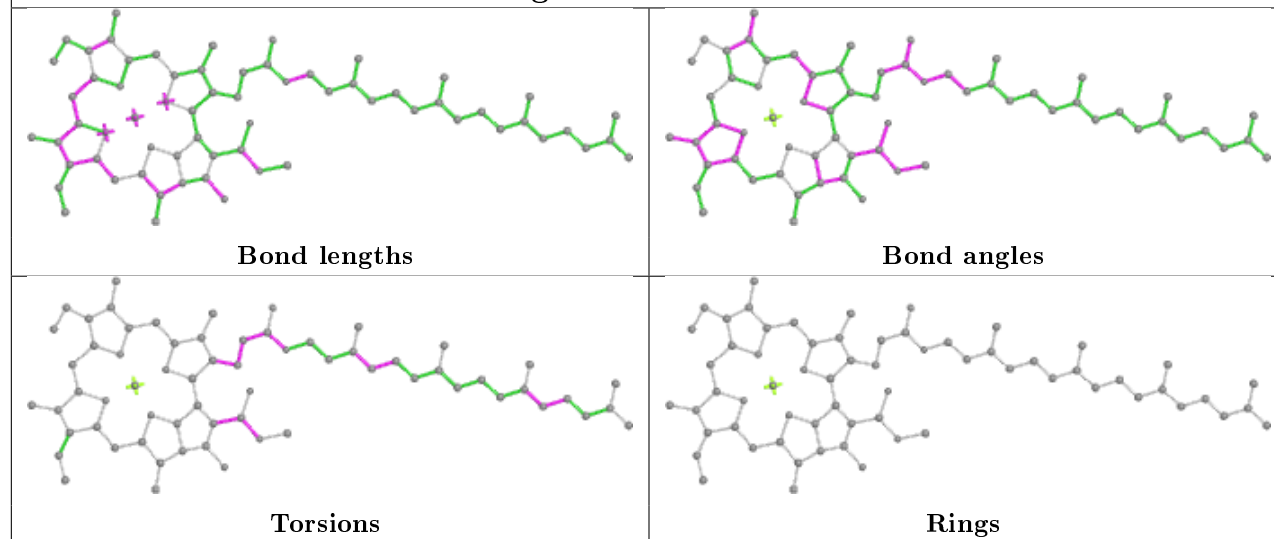


Ligand CLA G 826

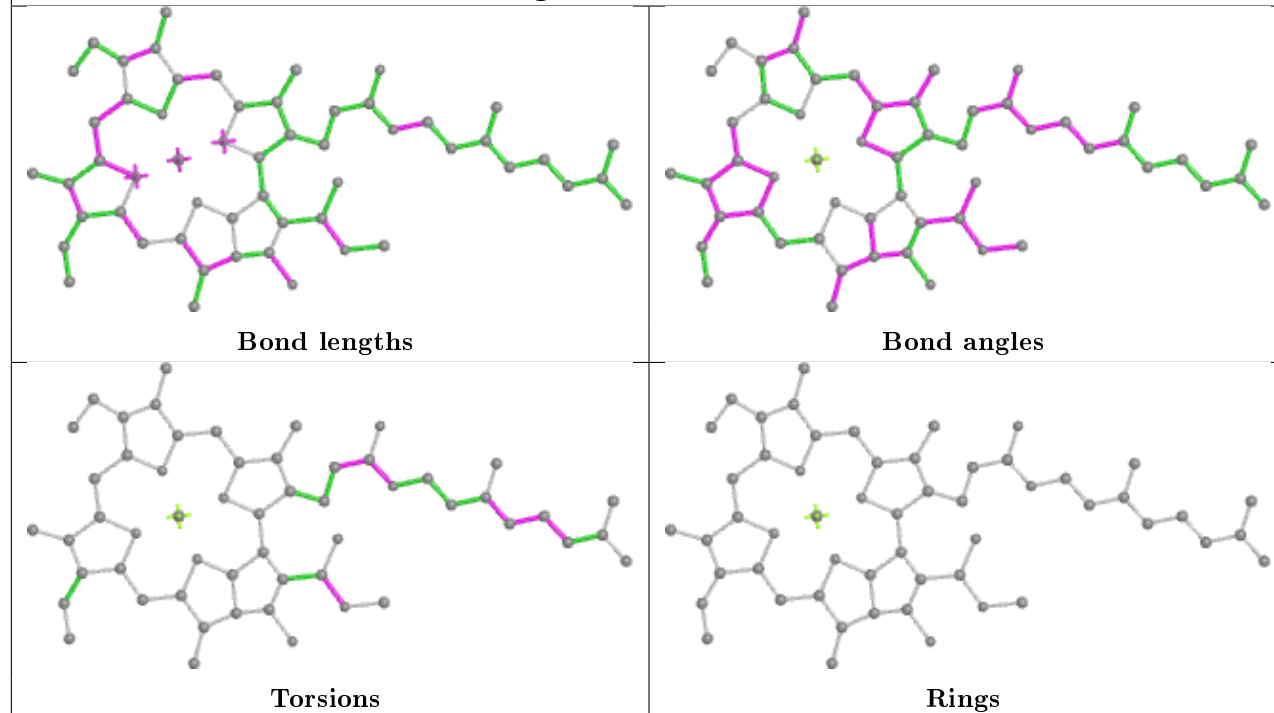


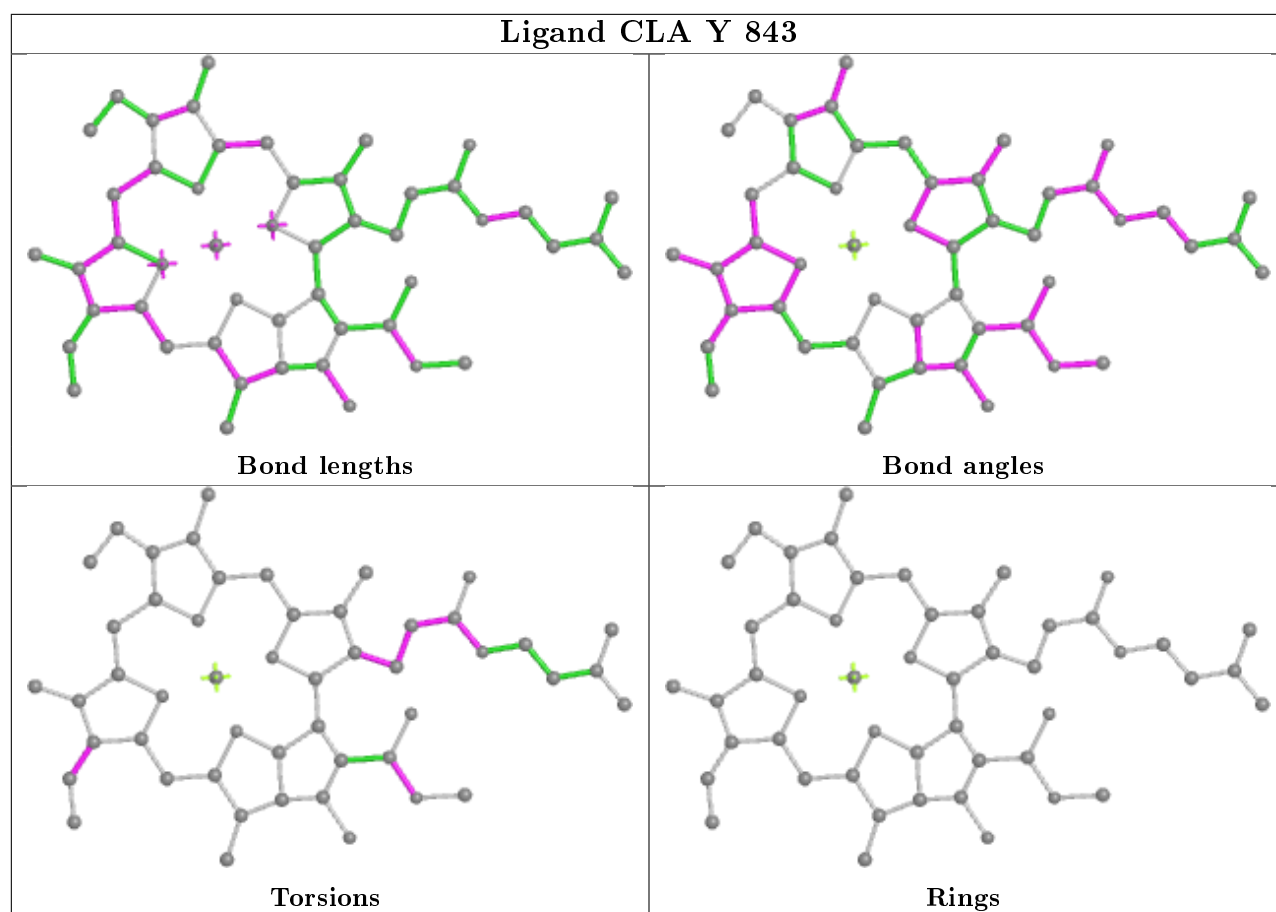


Ligand CLA G 821

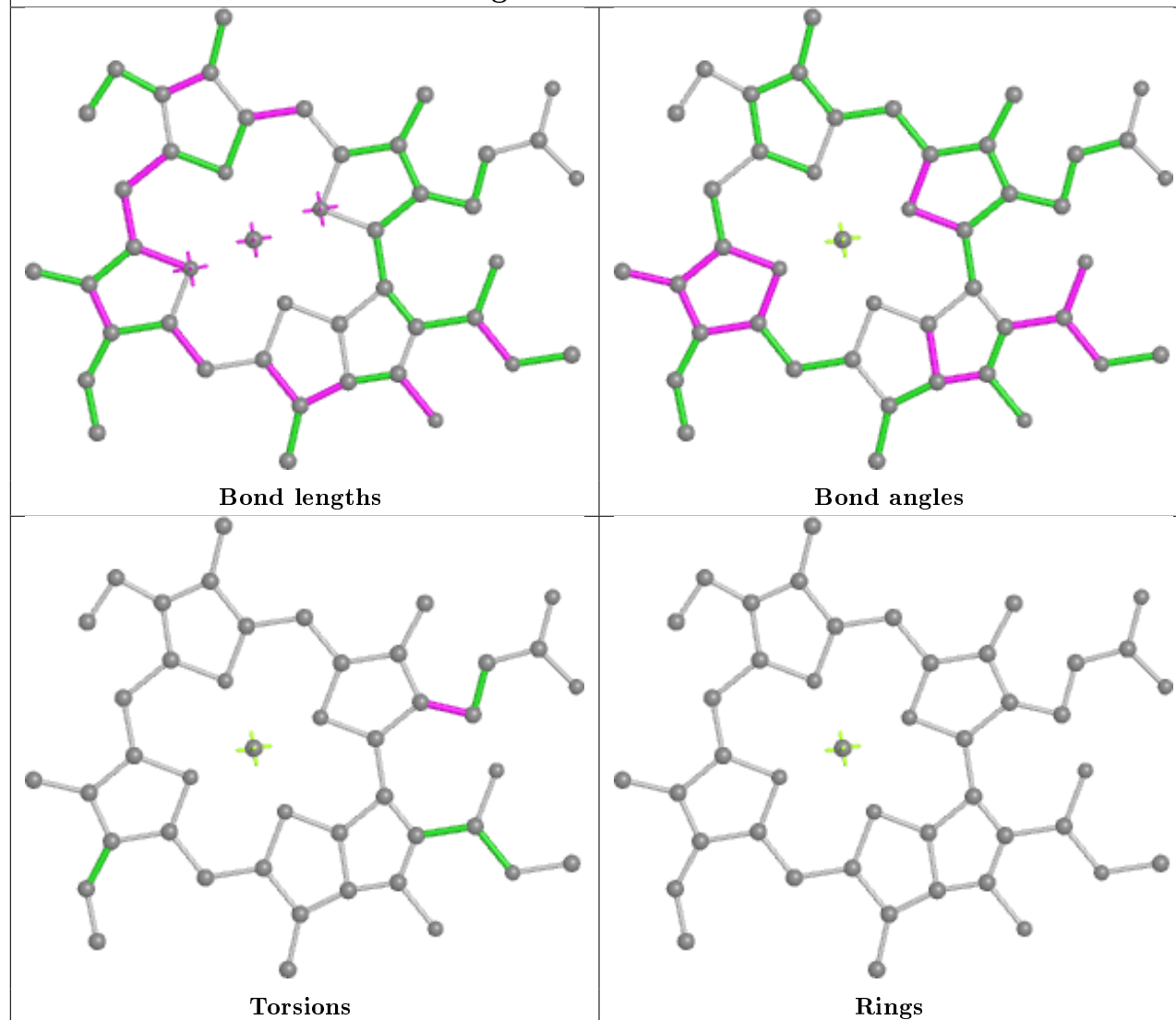


Ligand CLA B 822

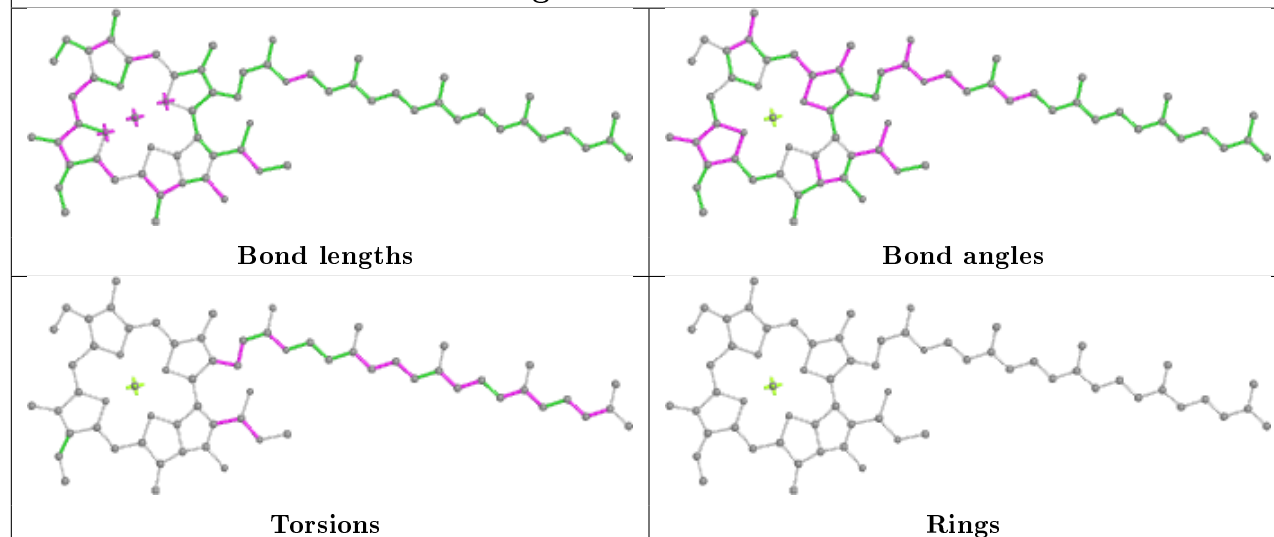




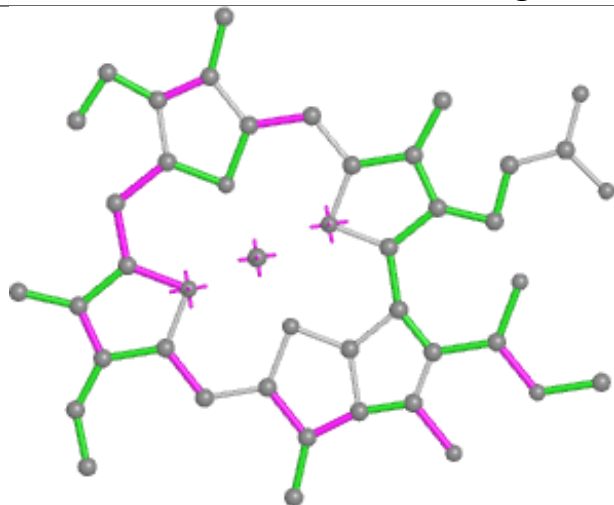
Ligand CLA B 839



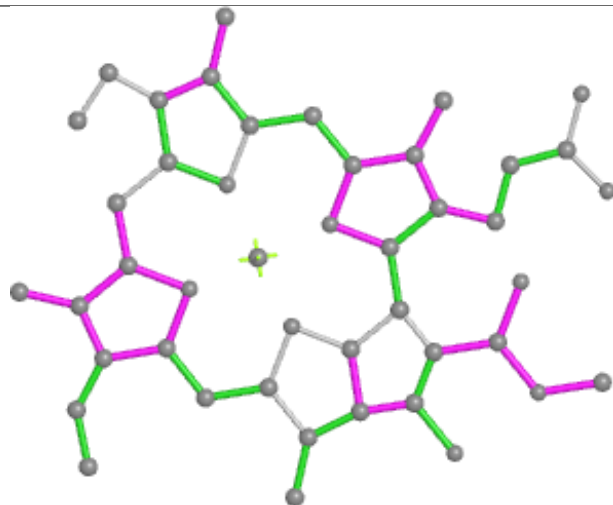
Ligand CLA A 808



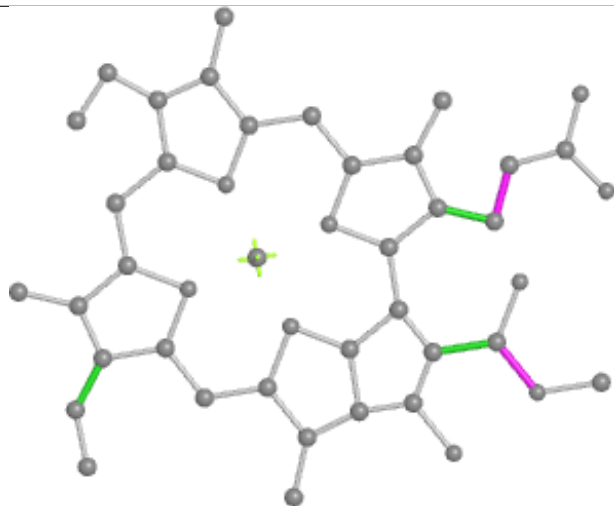
Ligand CLA H 811



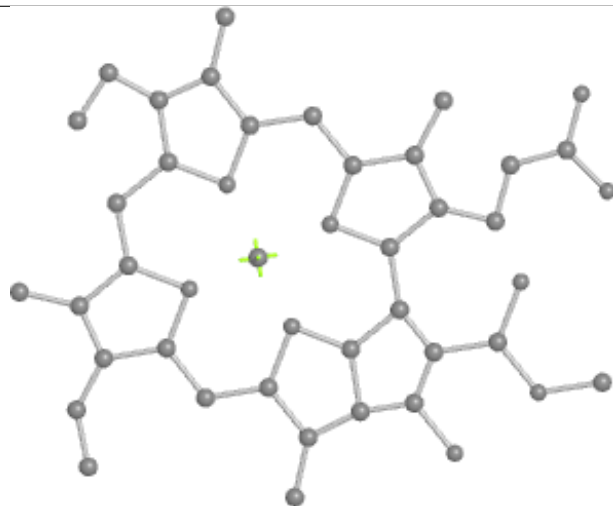
Bond lengths



Bond angles

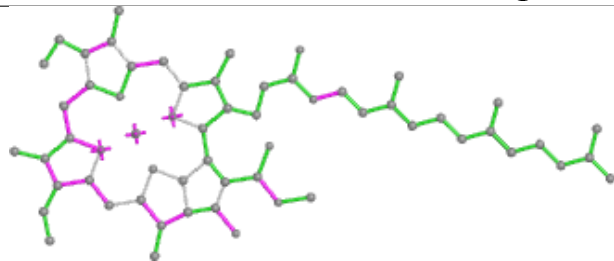


Torsions

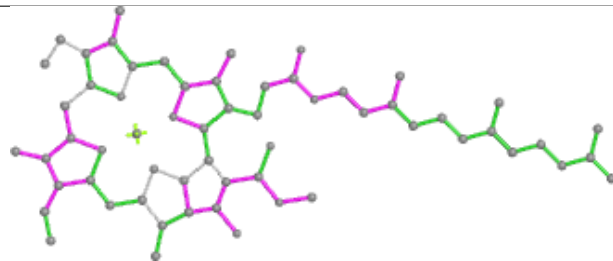


Rings

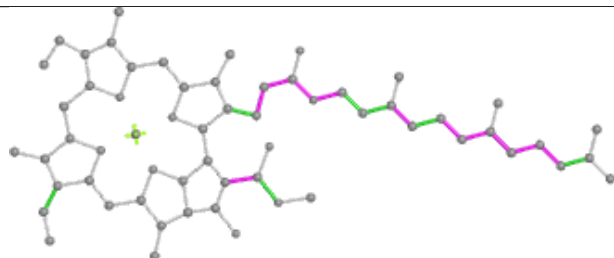
Ligand CLA B 823



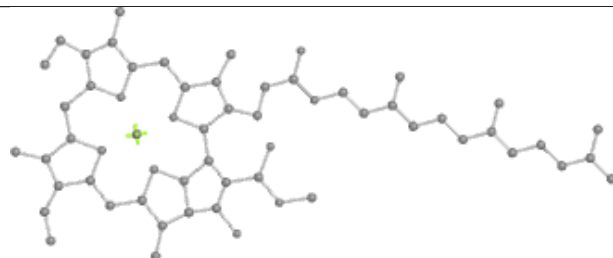
Bond lengths



Bond angles

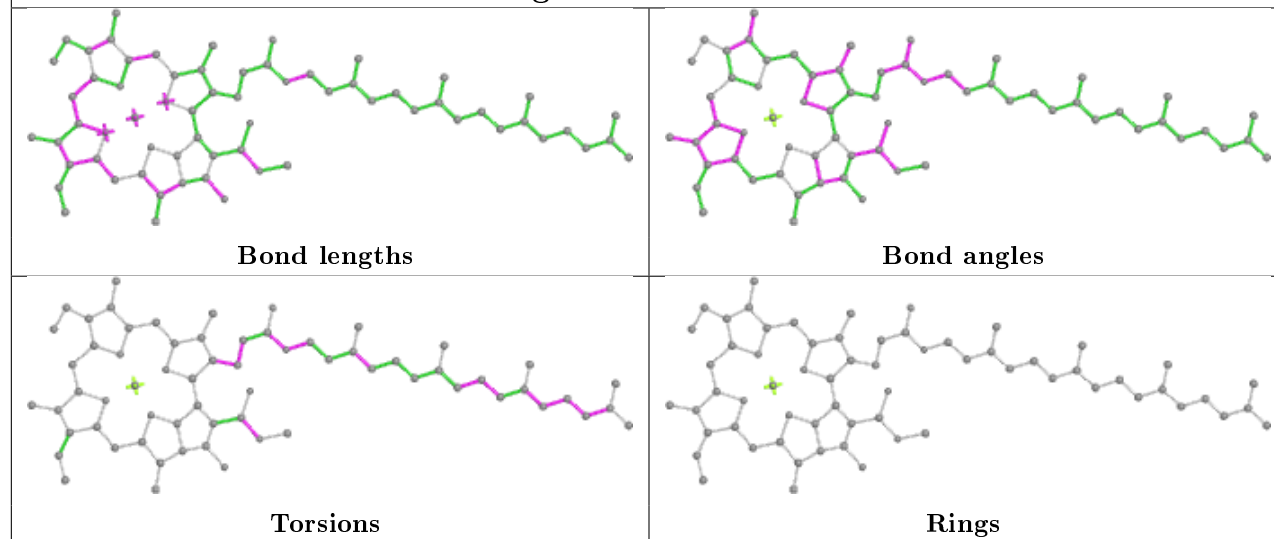


Torsions

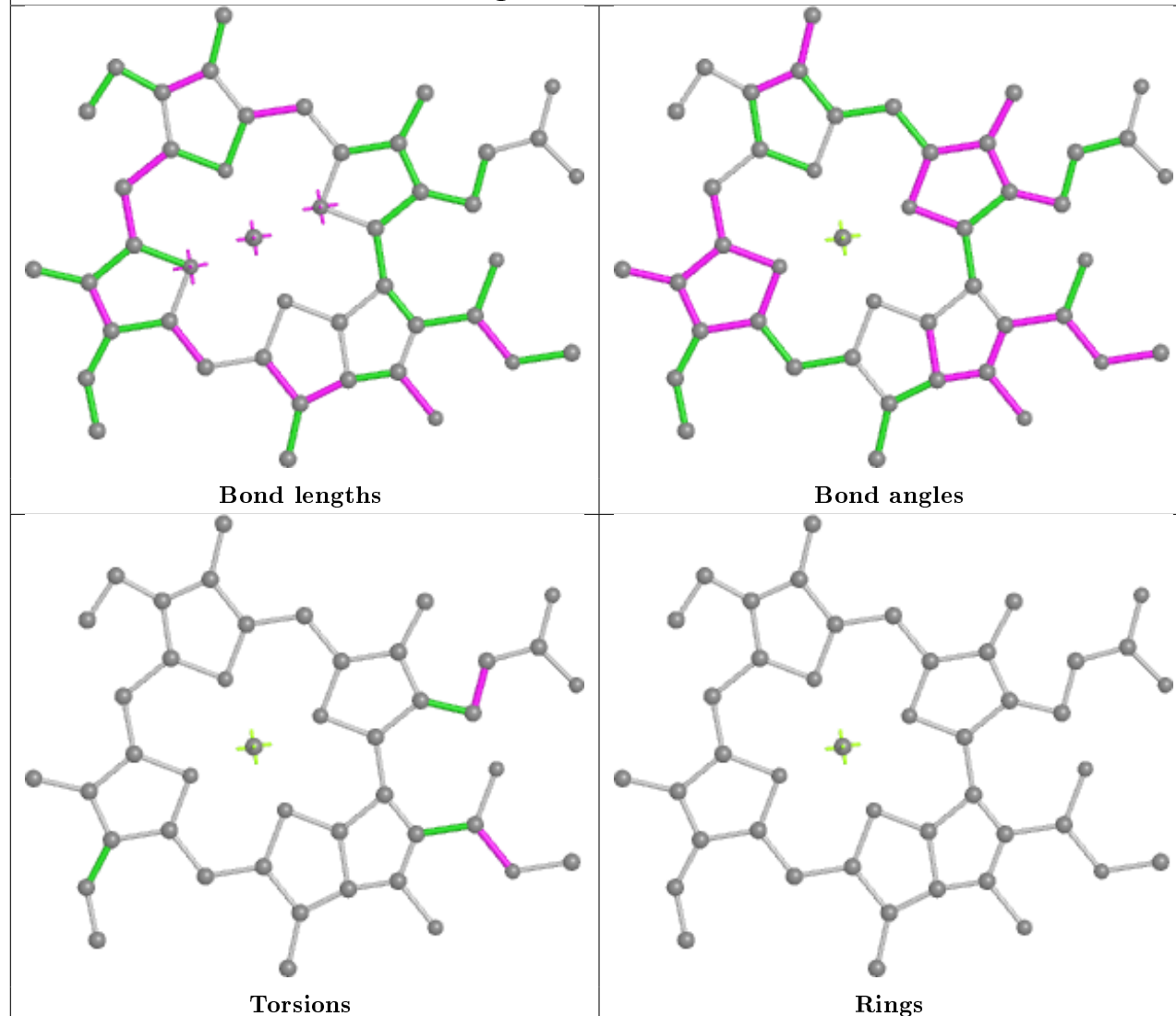


Rings

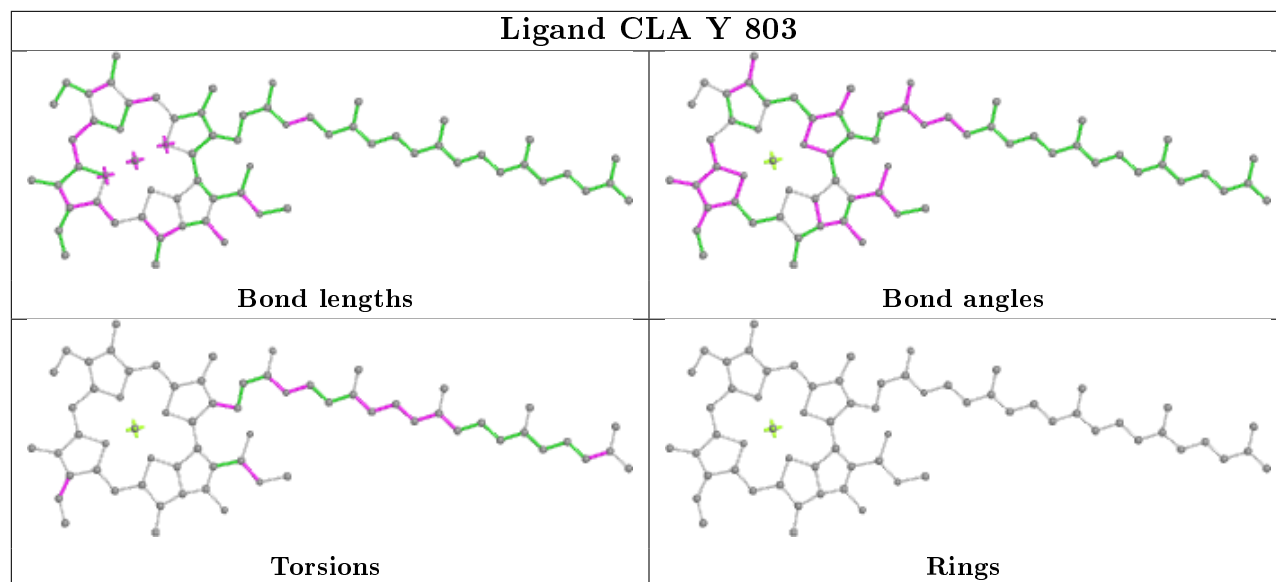
Ligand CLA A 811



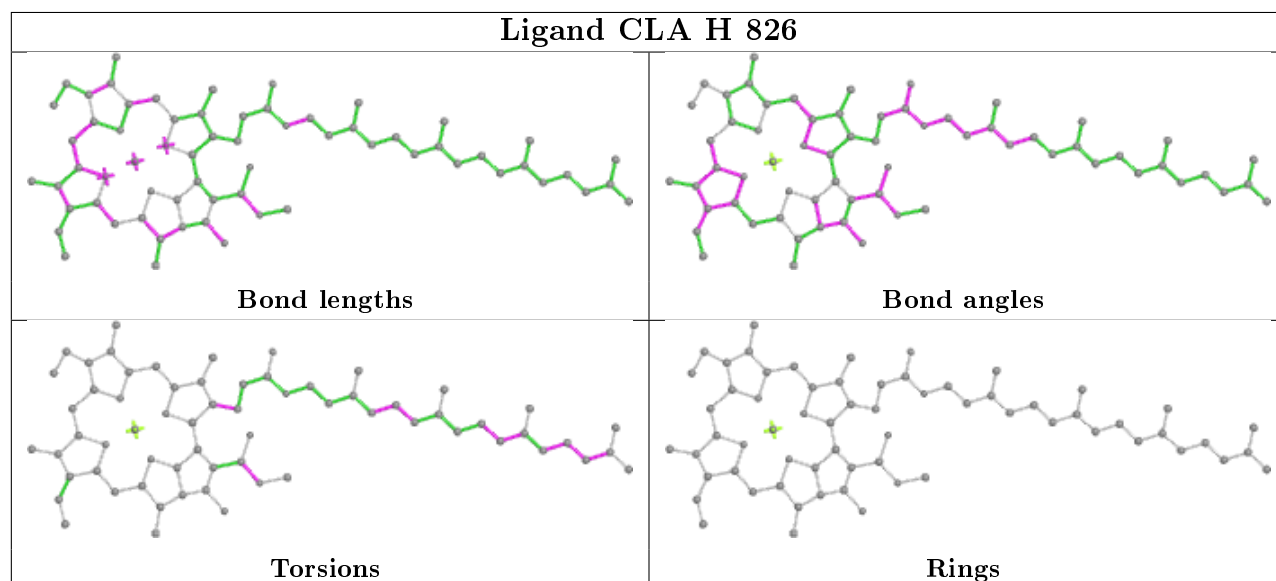
Ligand CLA Z 810



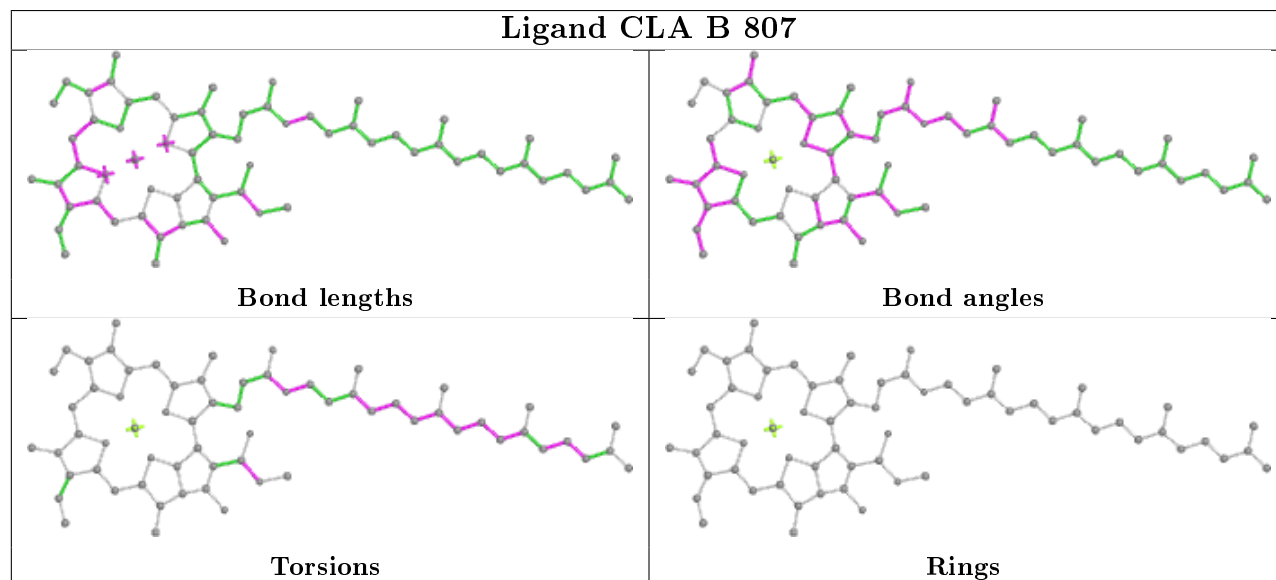
Ligand CLA Y 803

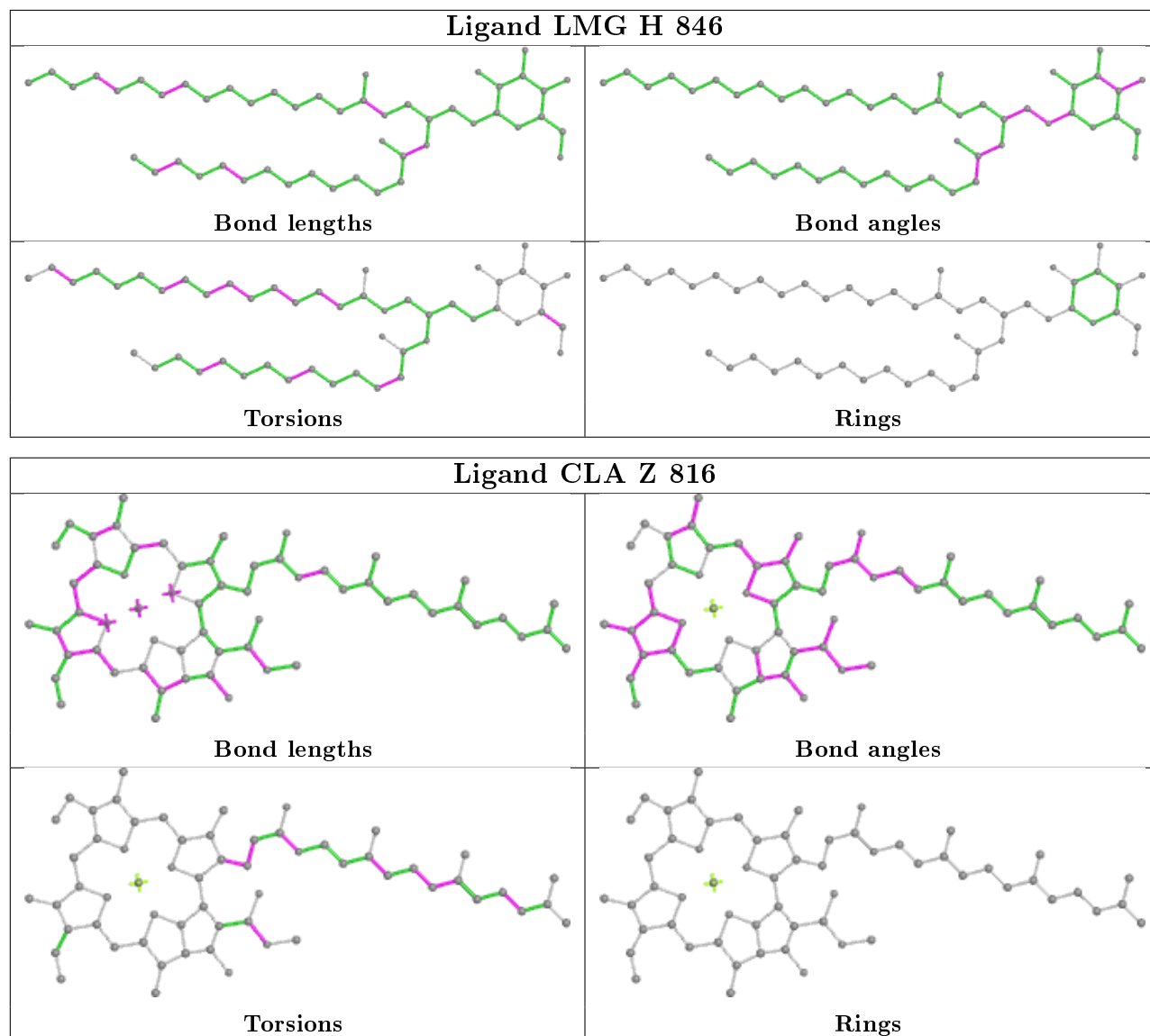


Ligand CLA H 826

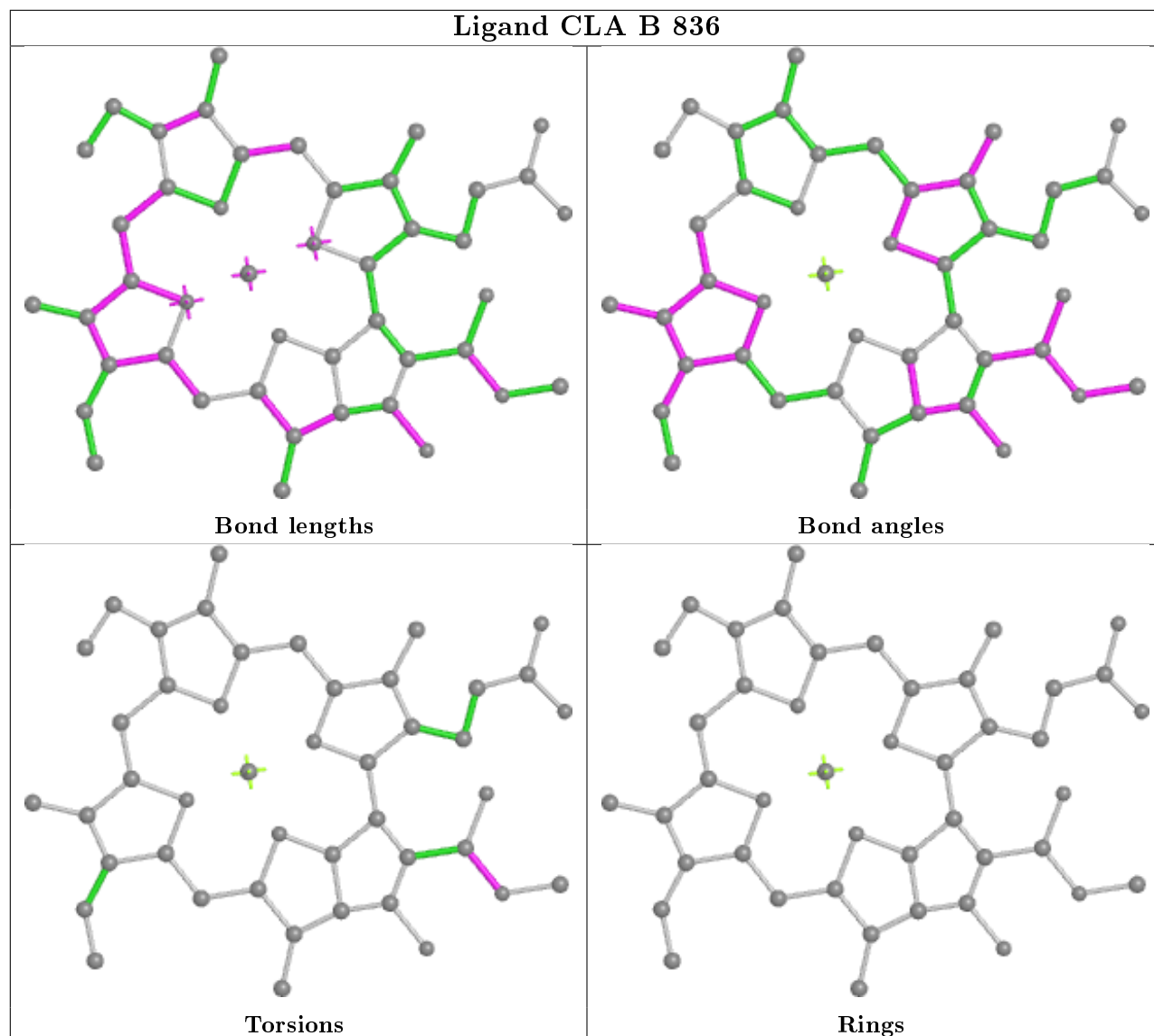


Ligand CLA B 807

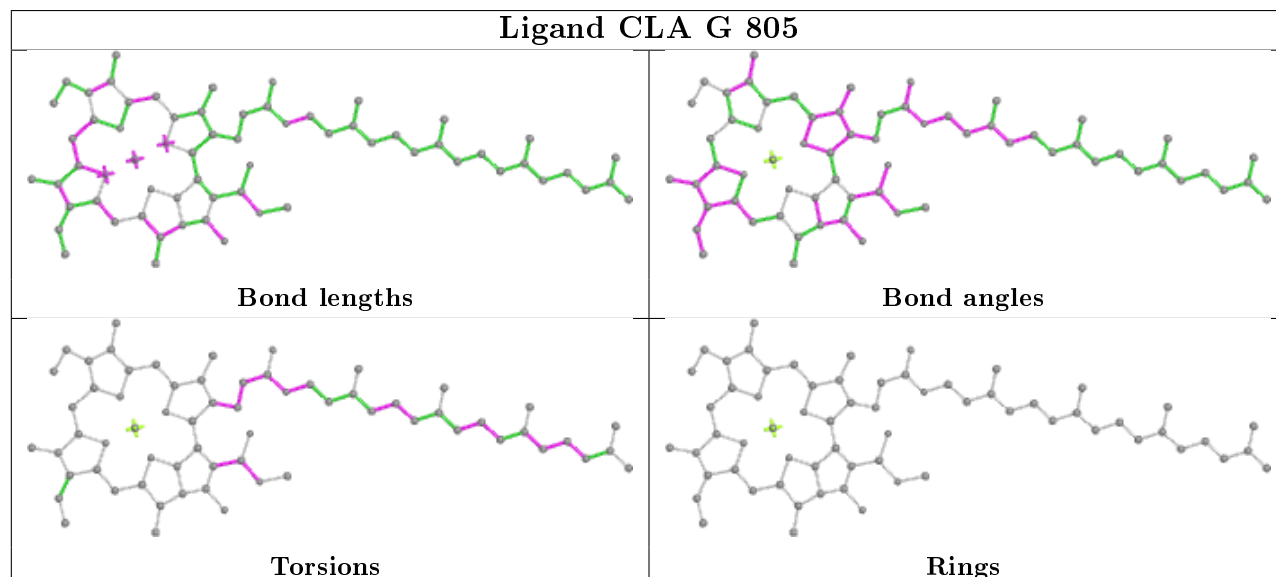


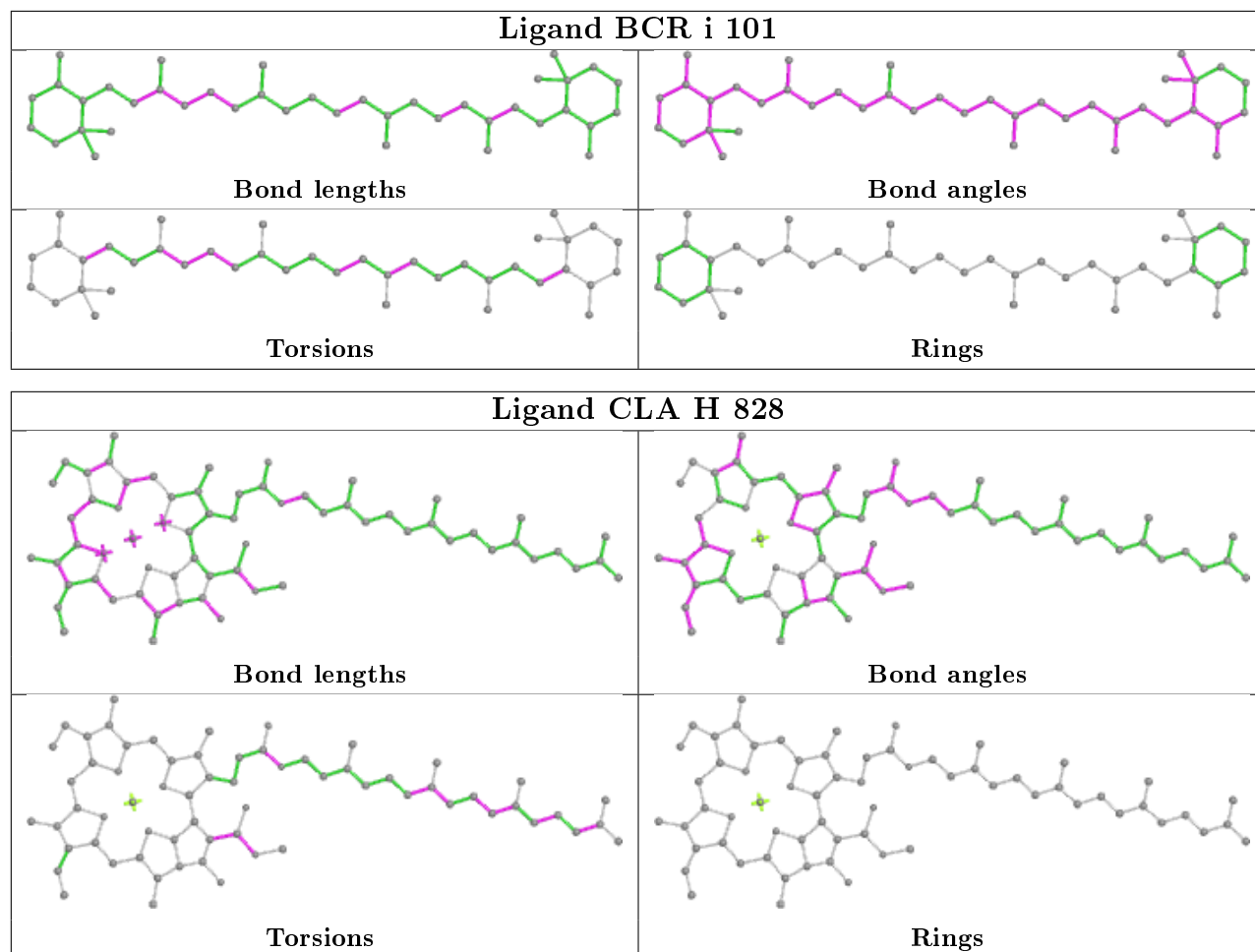


Ligand CLA B 836

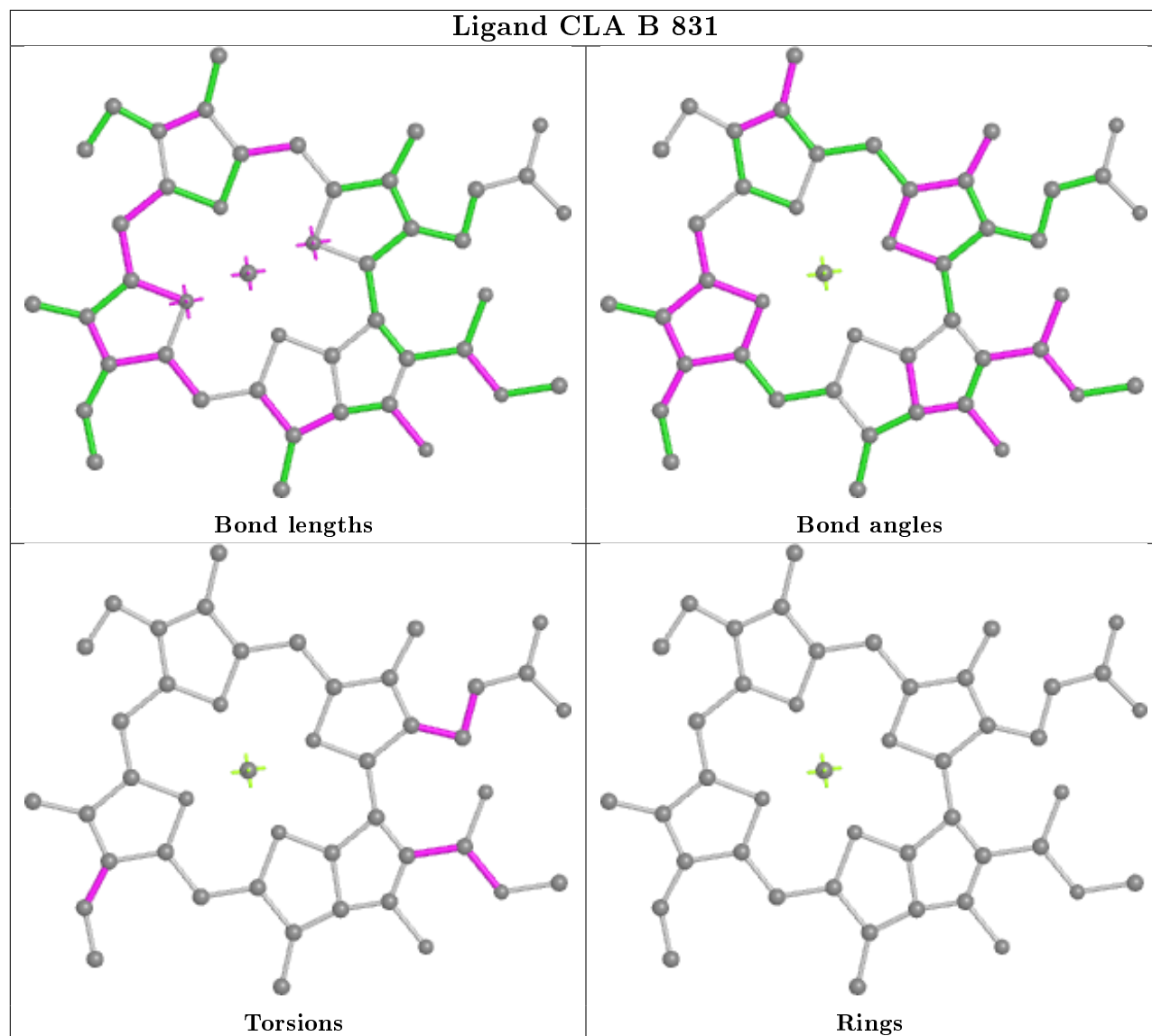


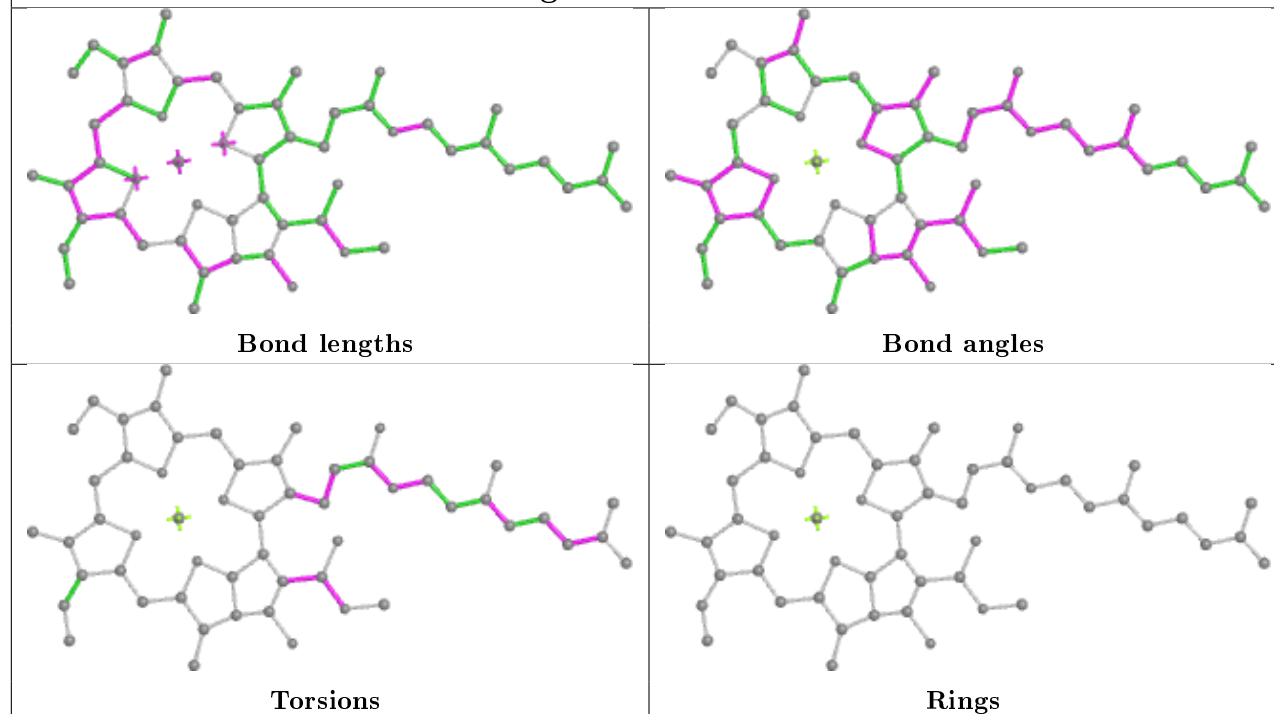
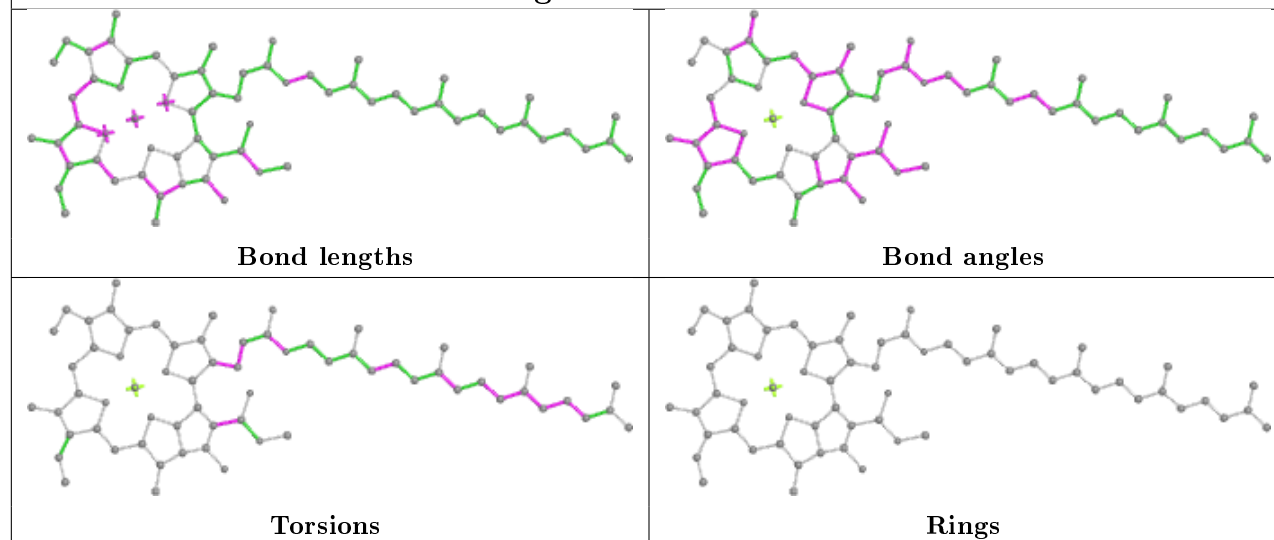
Ligand CLA G 805



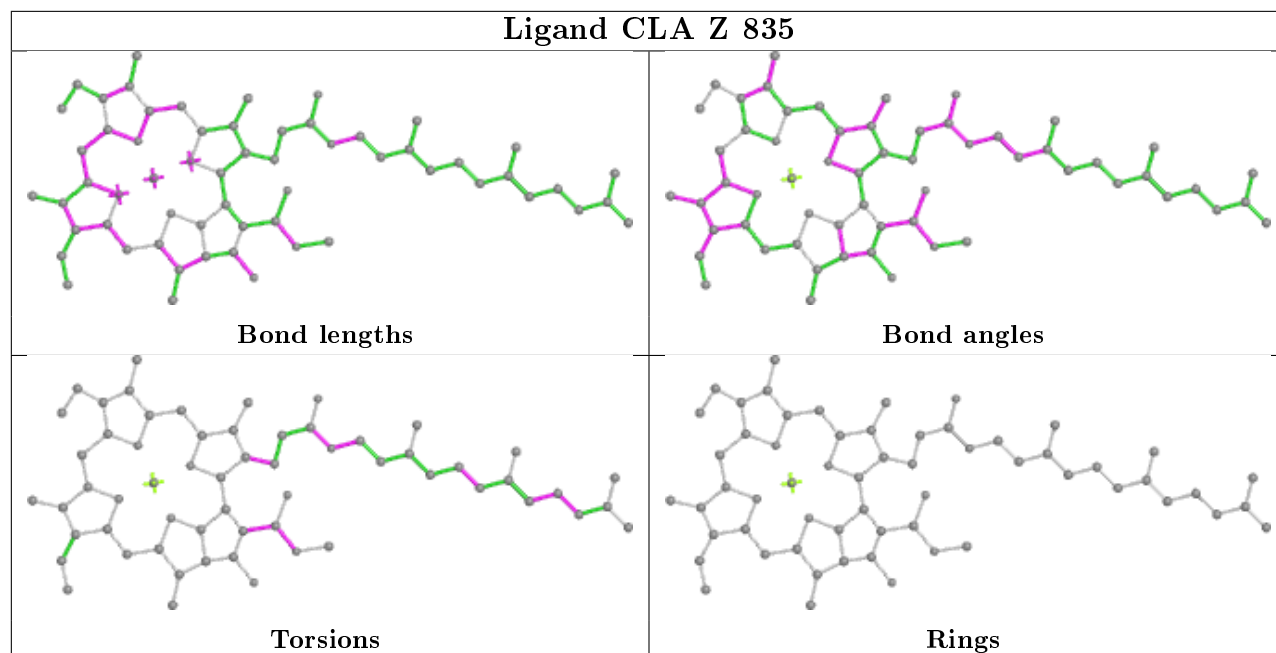


Ligand CLA B 831

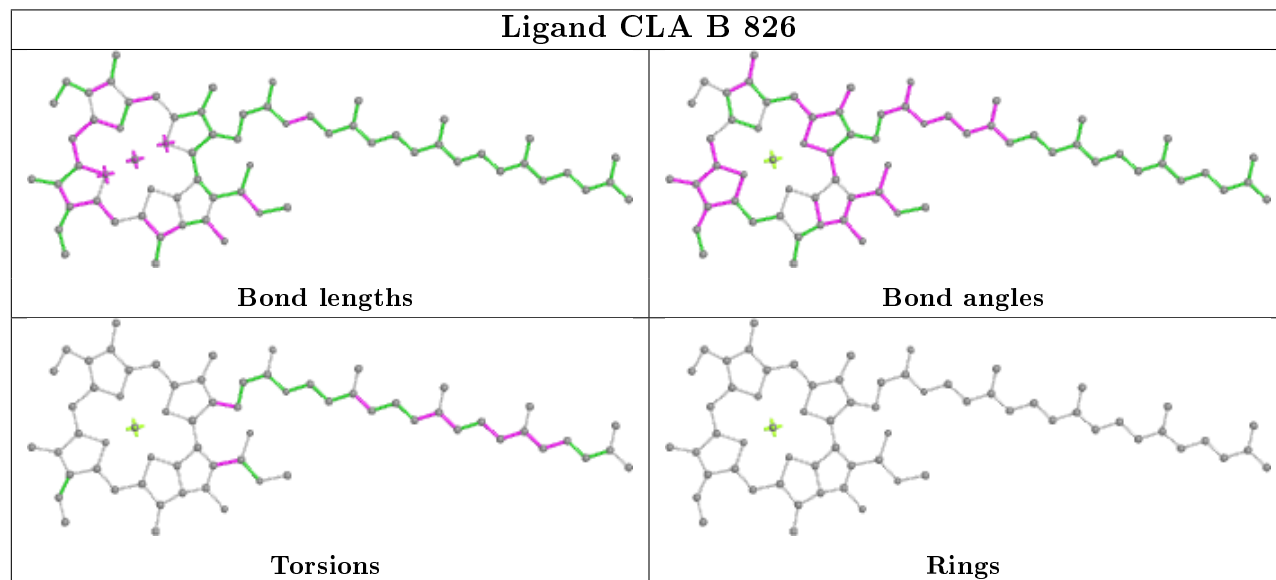


Ligand CLA f 102**Ligand CLA Z 824**

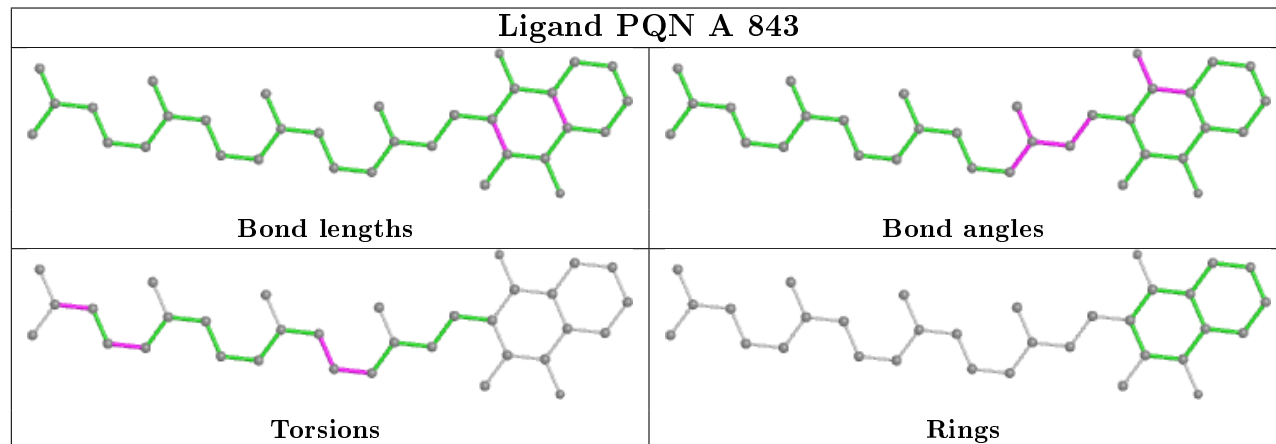
Ligand CLA Z 835



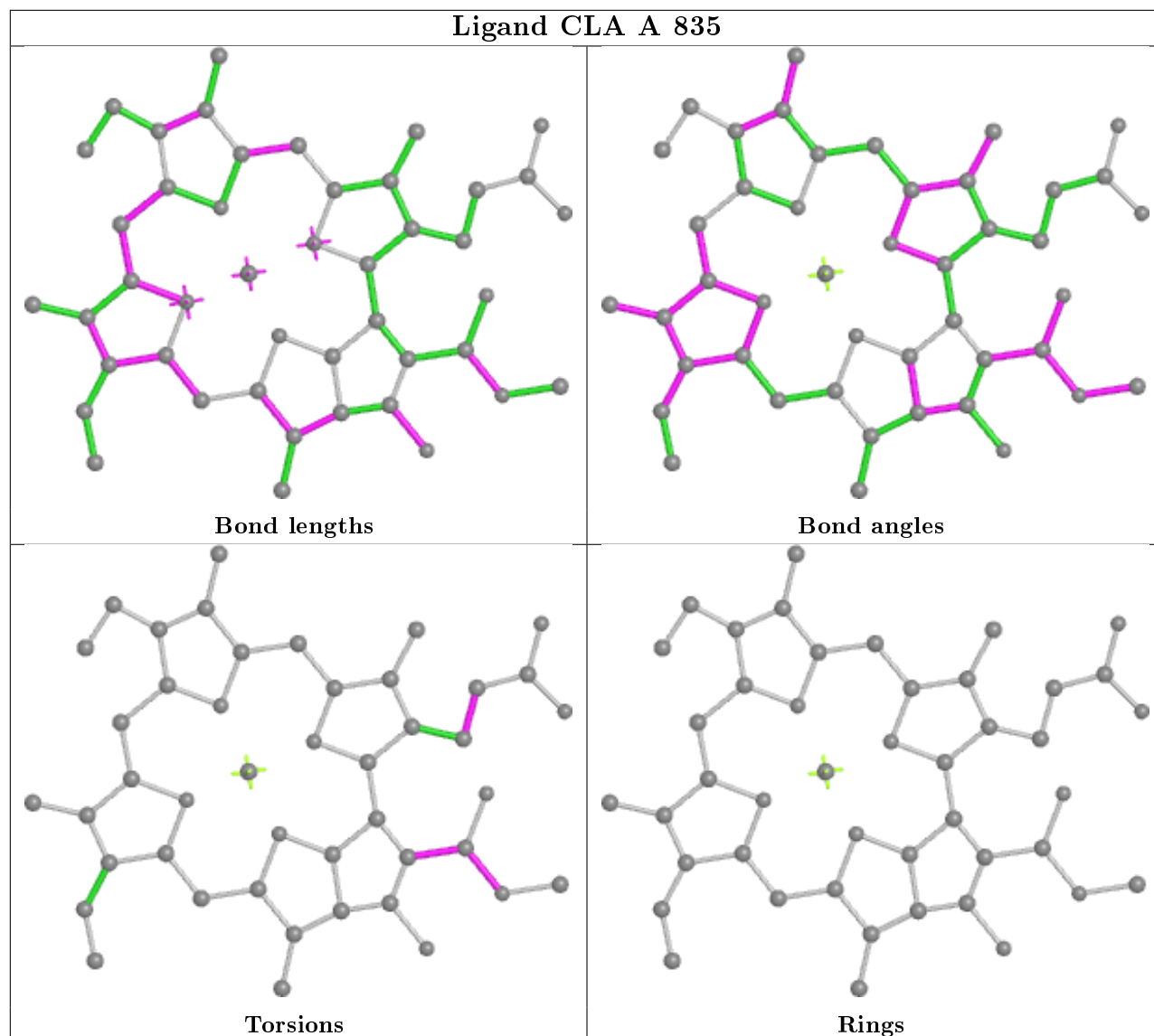
Ligand CLA B 826



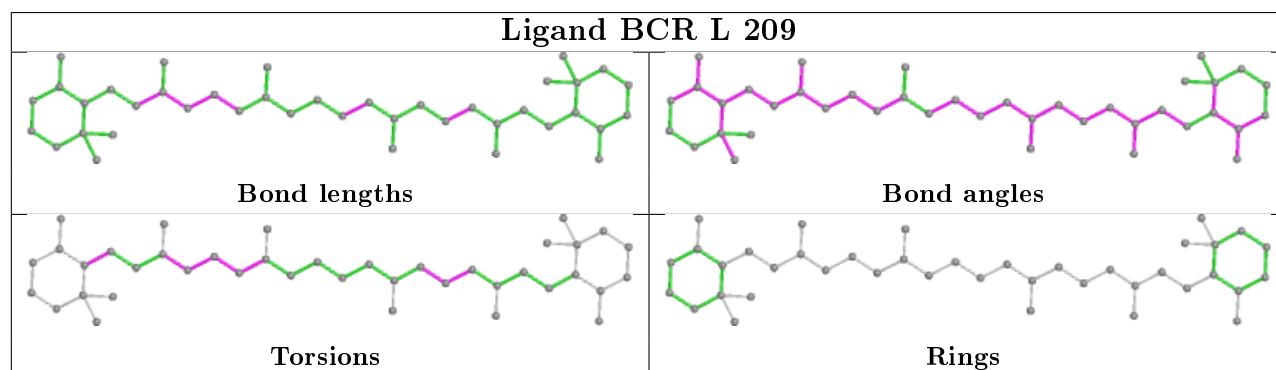
Ligand PQN A 843



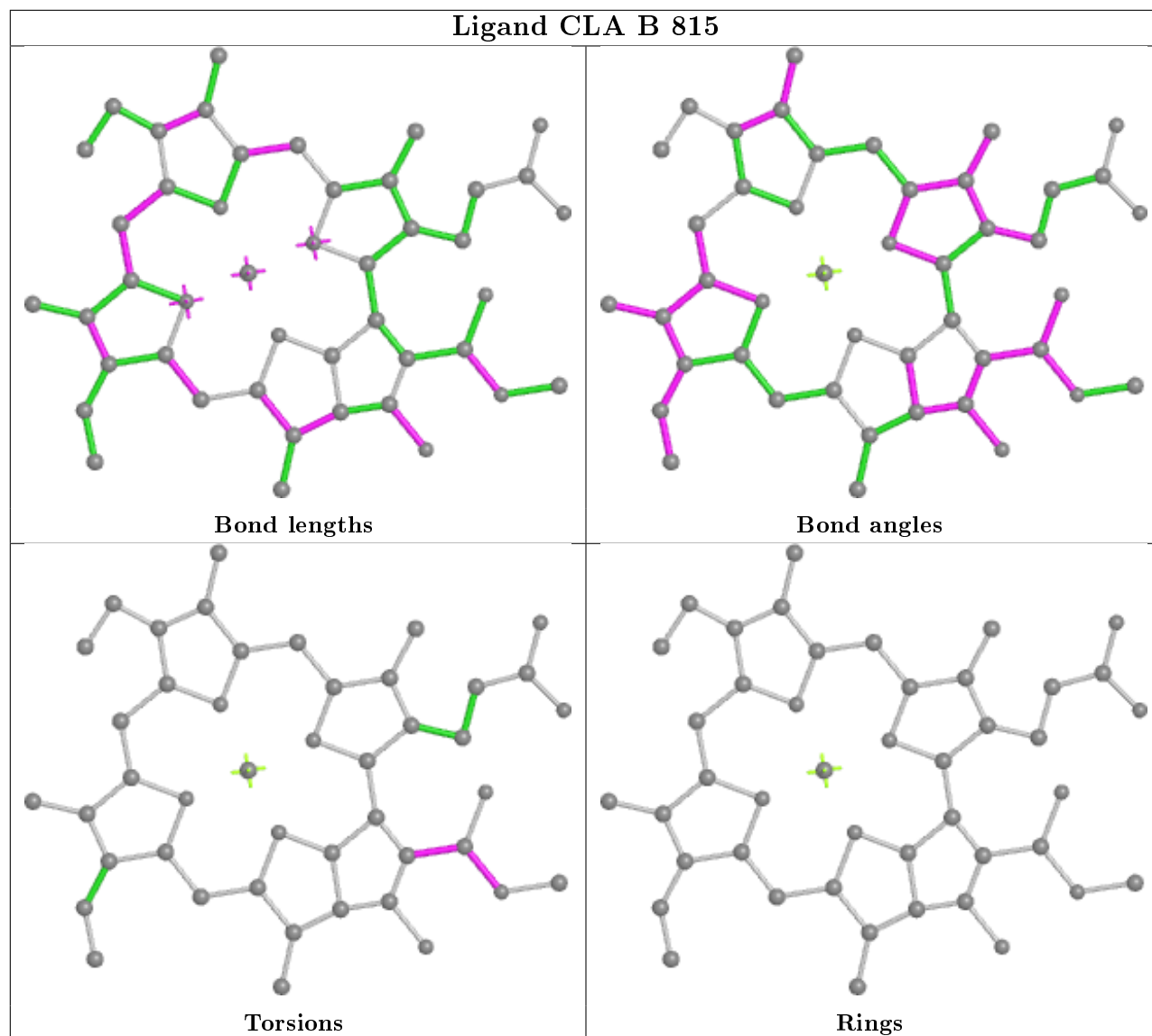
Ligand CLA A 835



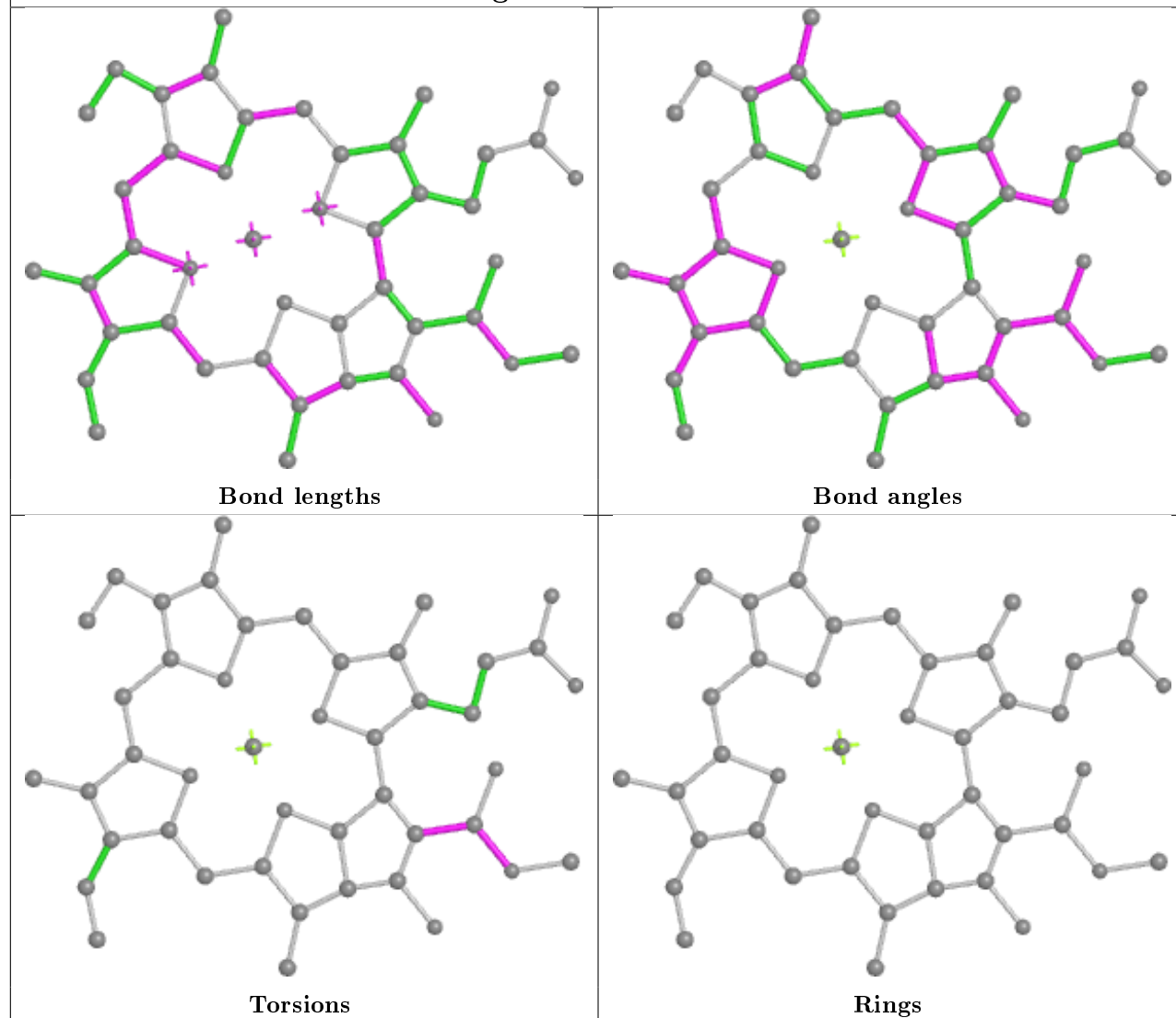
Ligand BCR L 209



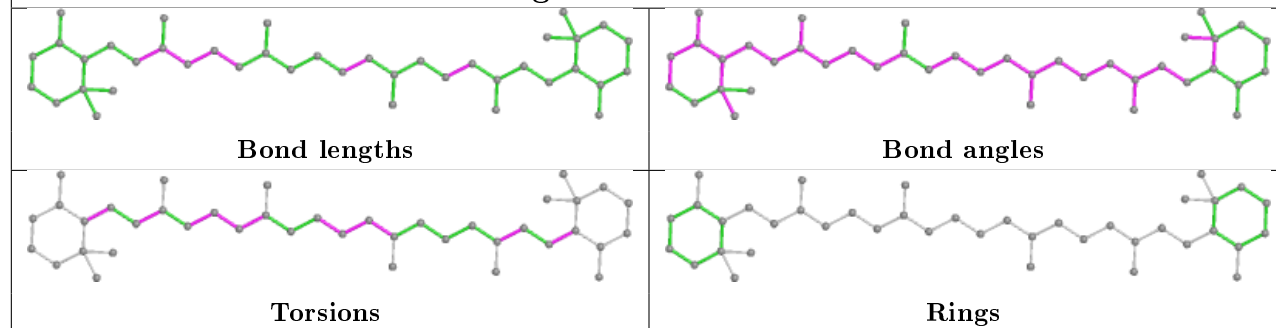
Ligand CLA B 815



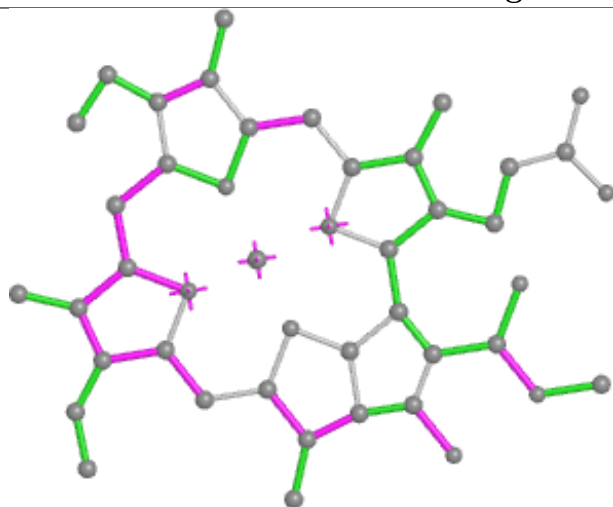
Ligand CLA Z 813



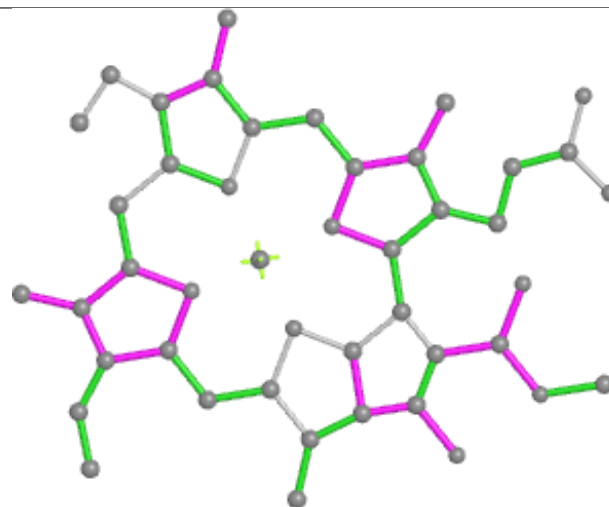
Ligand BCR F 201



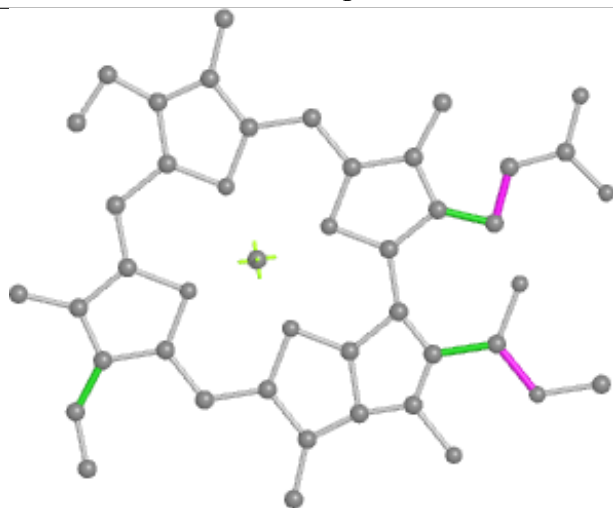
Ligand CLA X 1701



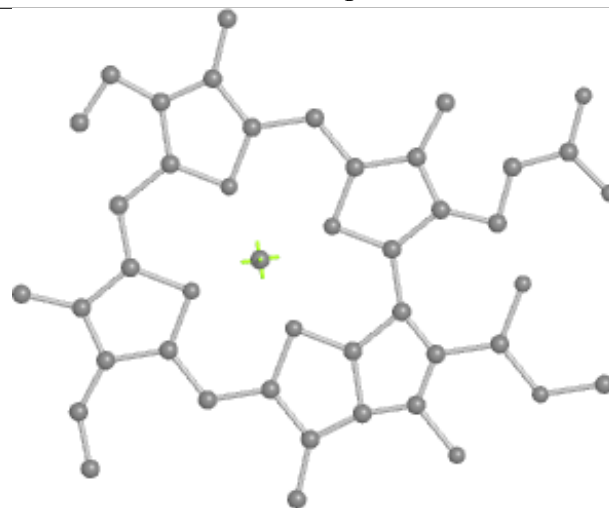
Bond lengths



Bond angles

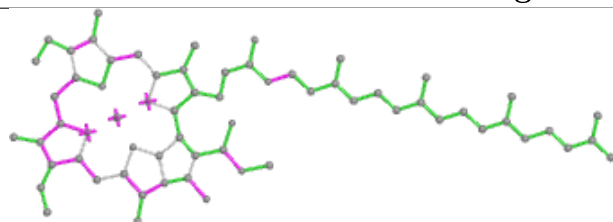


Torsions

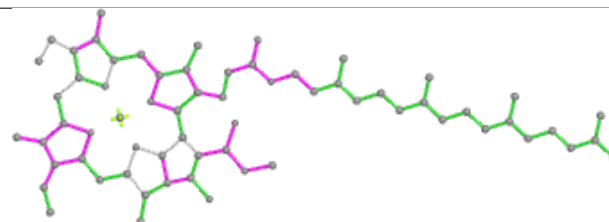


Rings

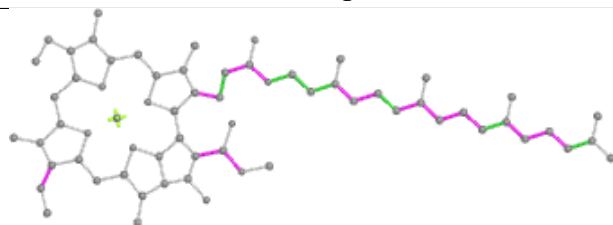
Ligand CLA A 806



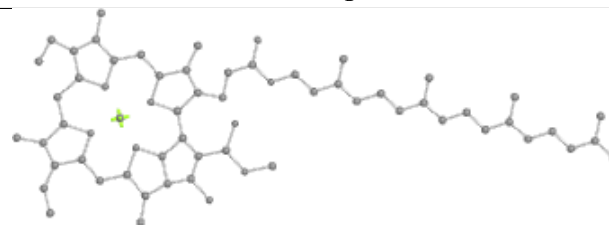
Bond lengths



Bond angles

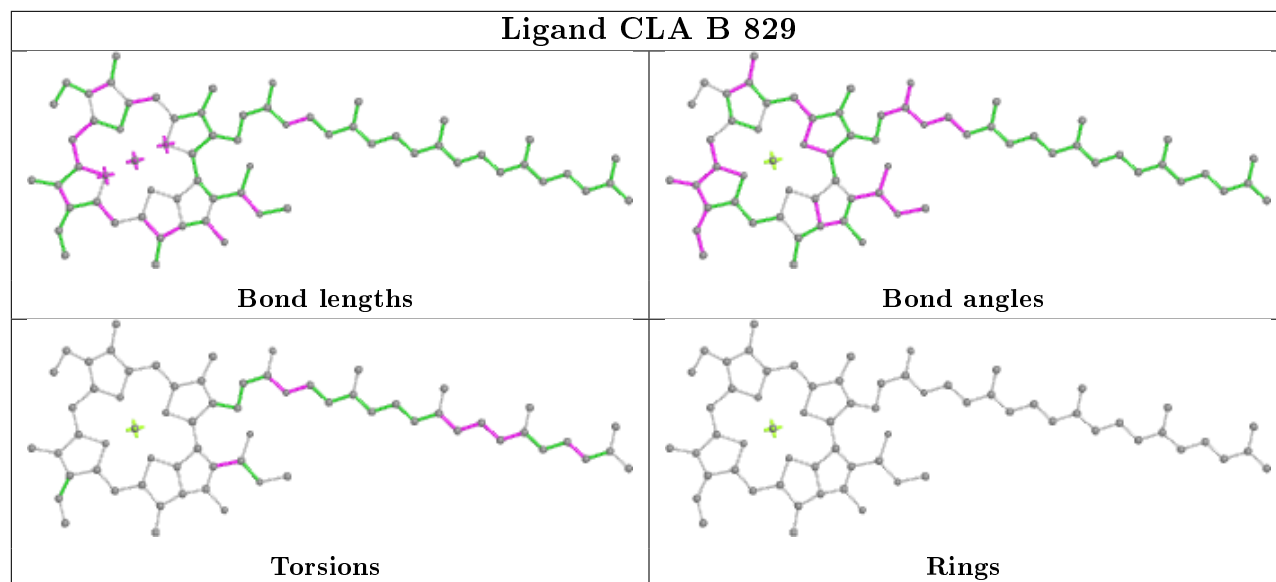


Torsions

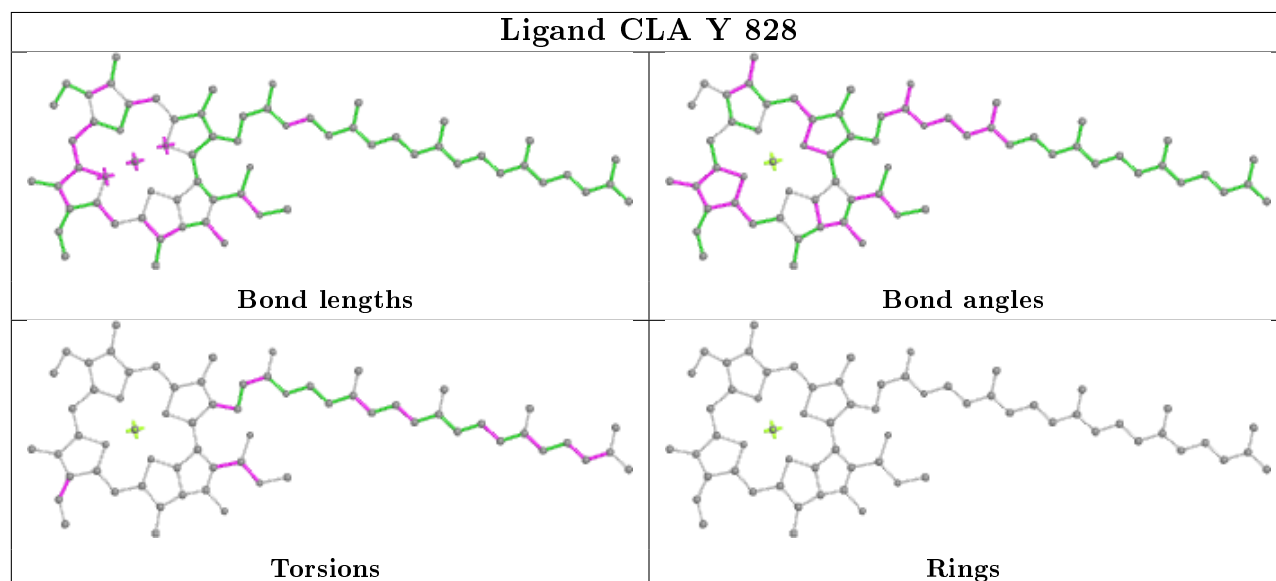


Rings

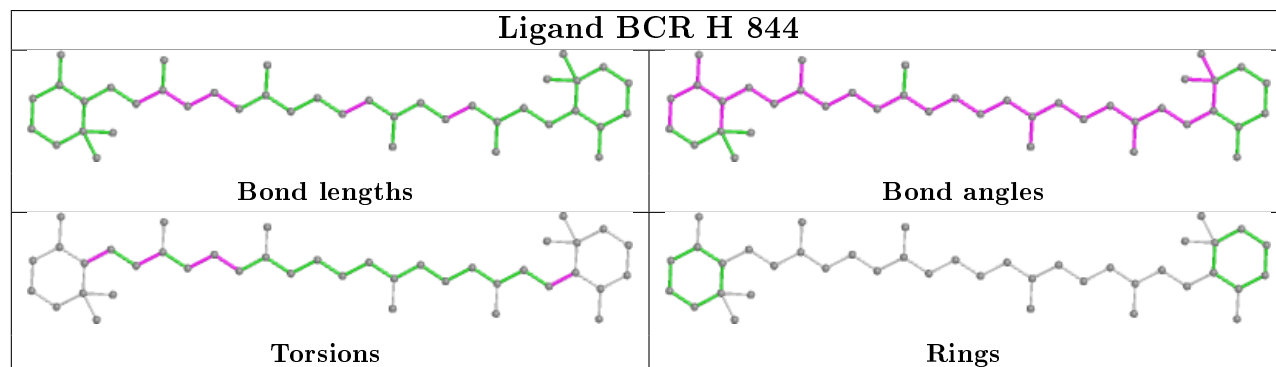
Ligand CLA B 829



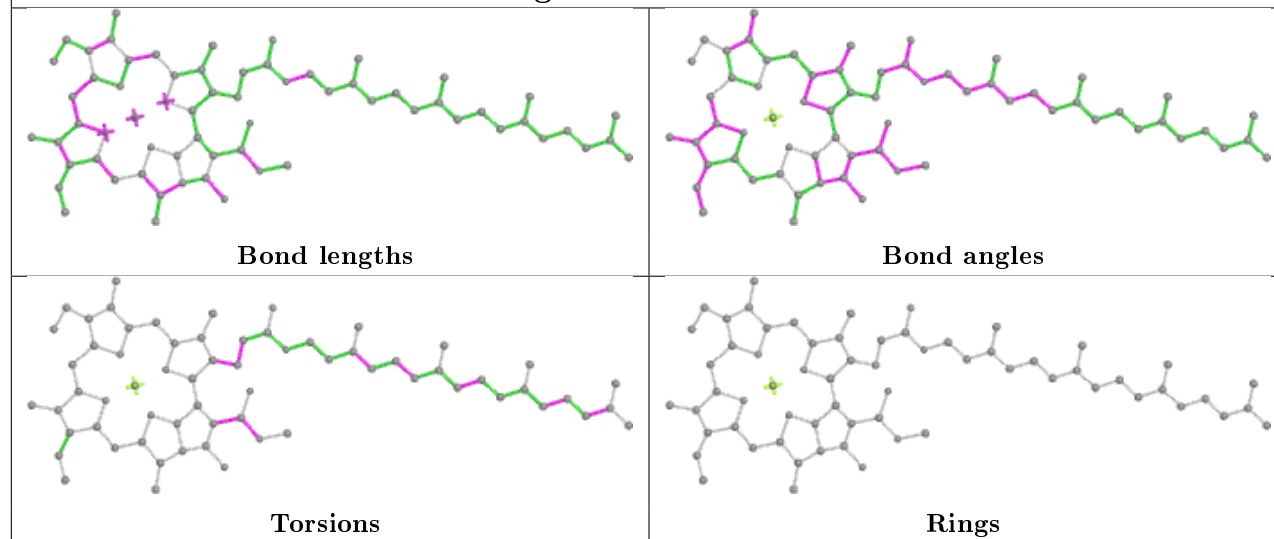
Ligand CLA Y 828



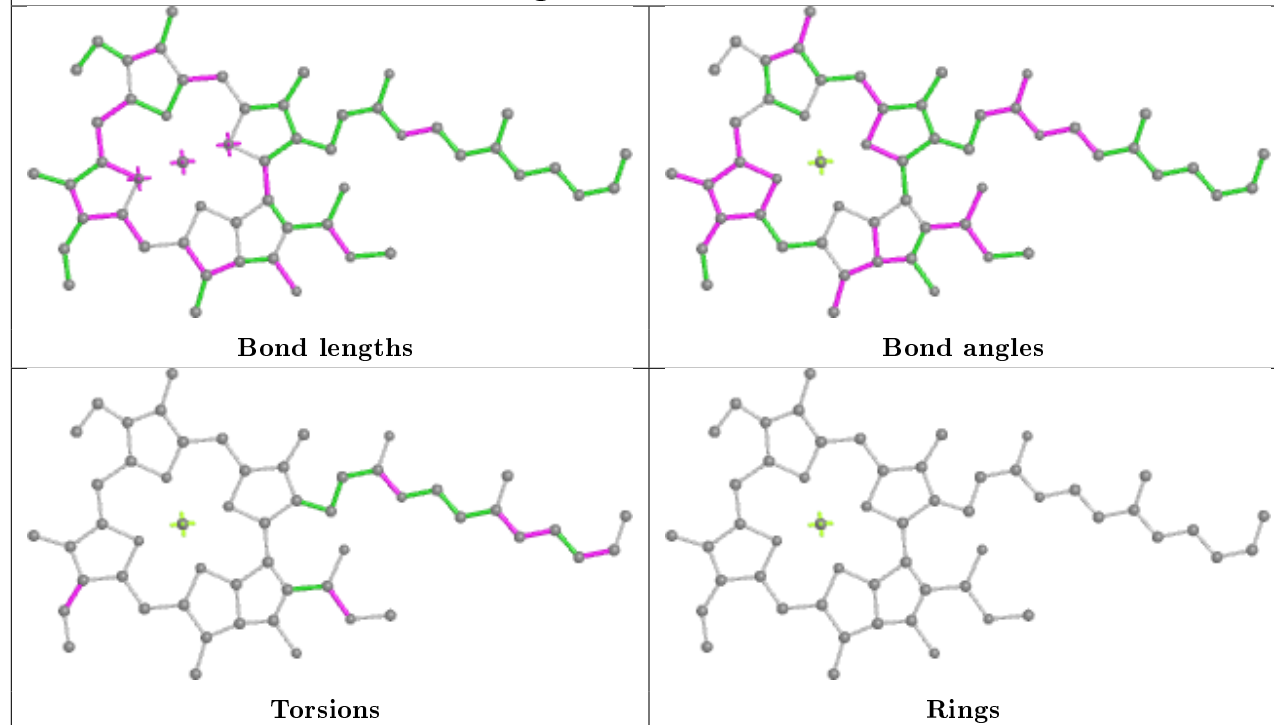
Ligand BCR H 844

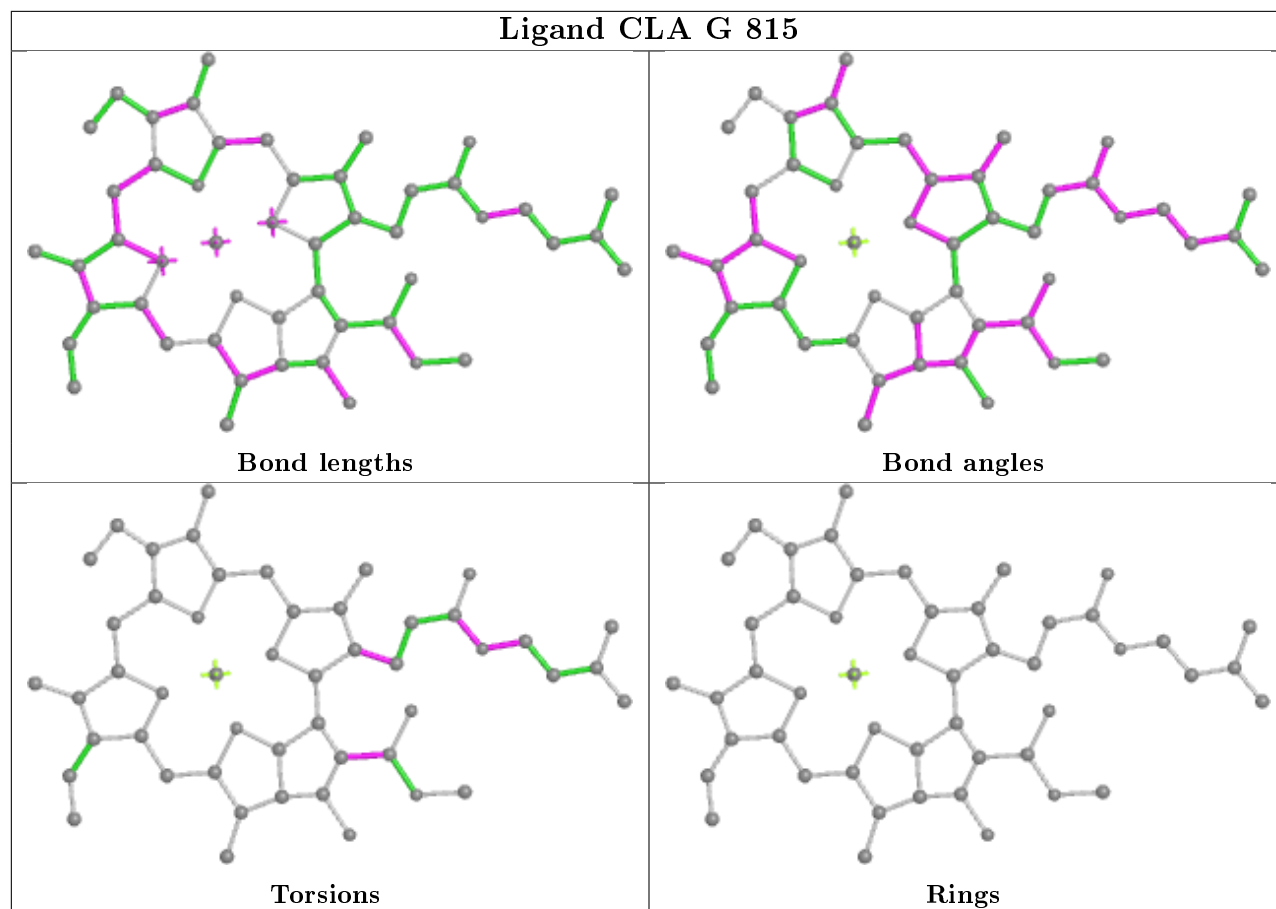


Ligand CLA Z 826

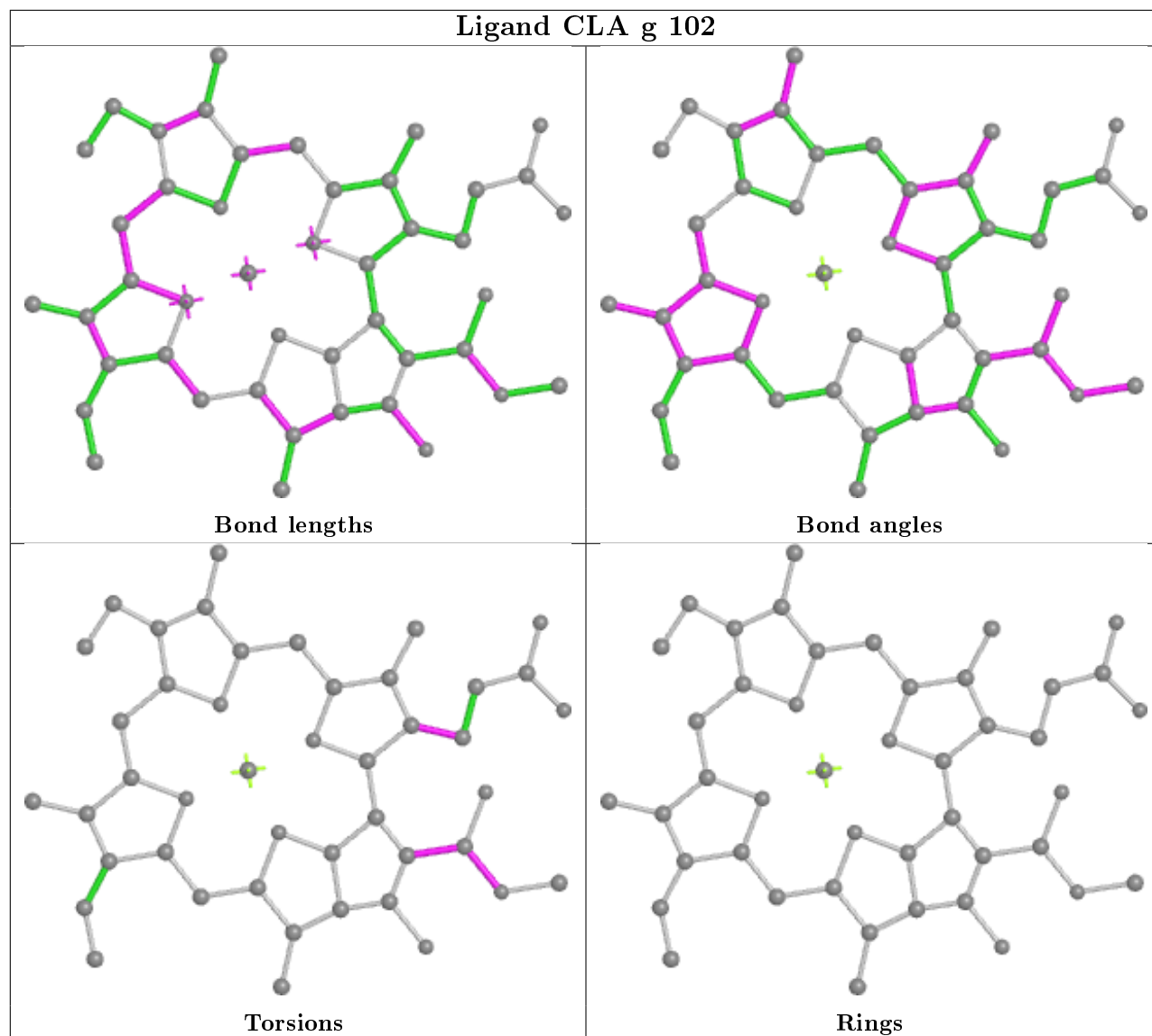


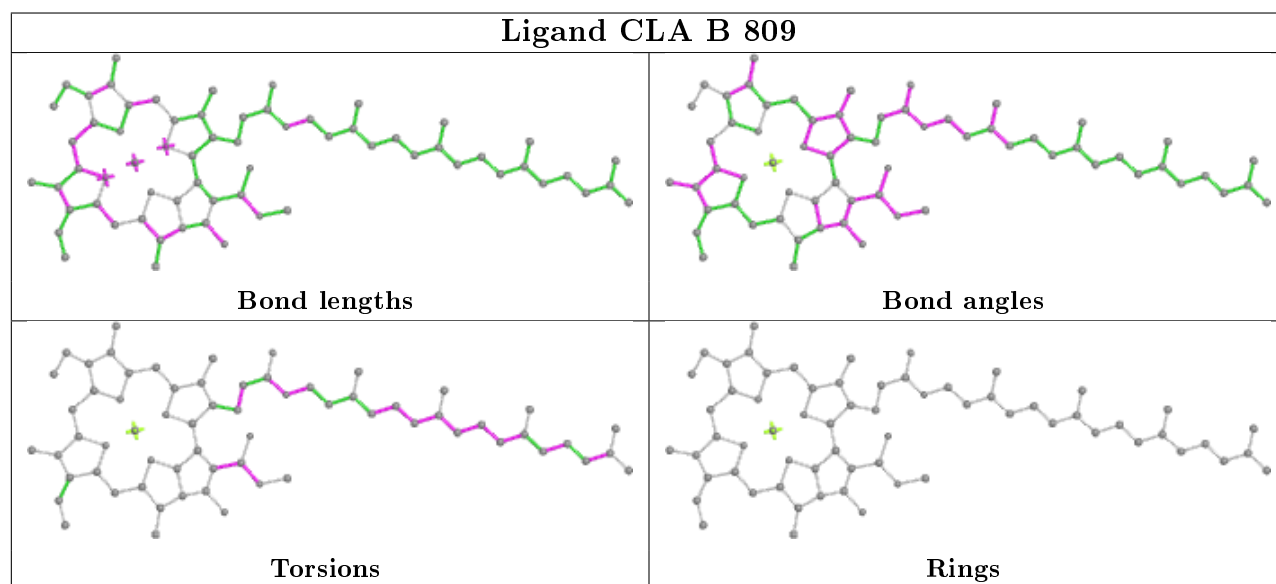
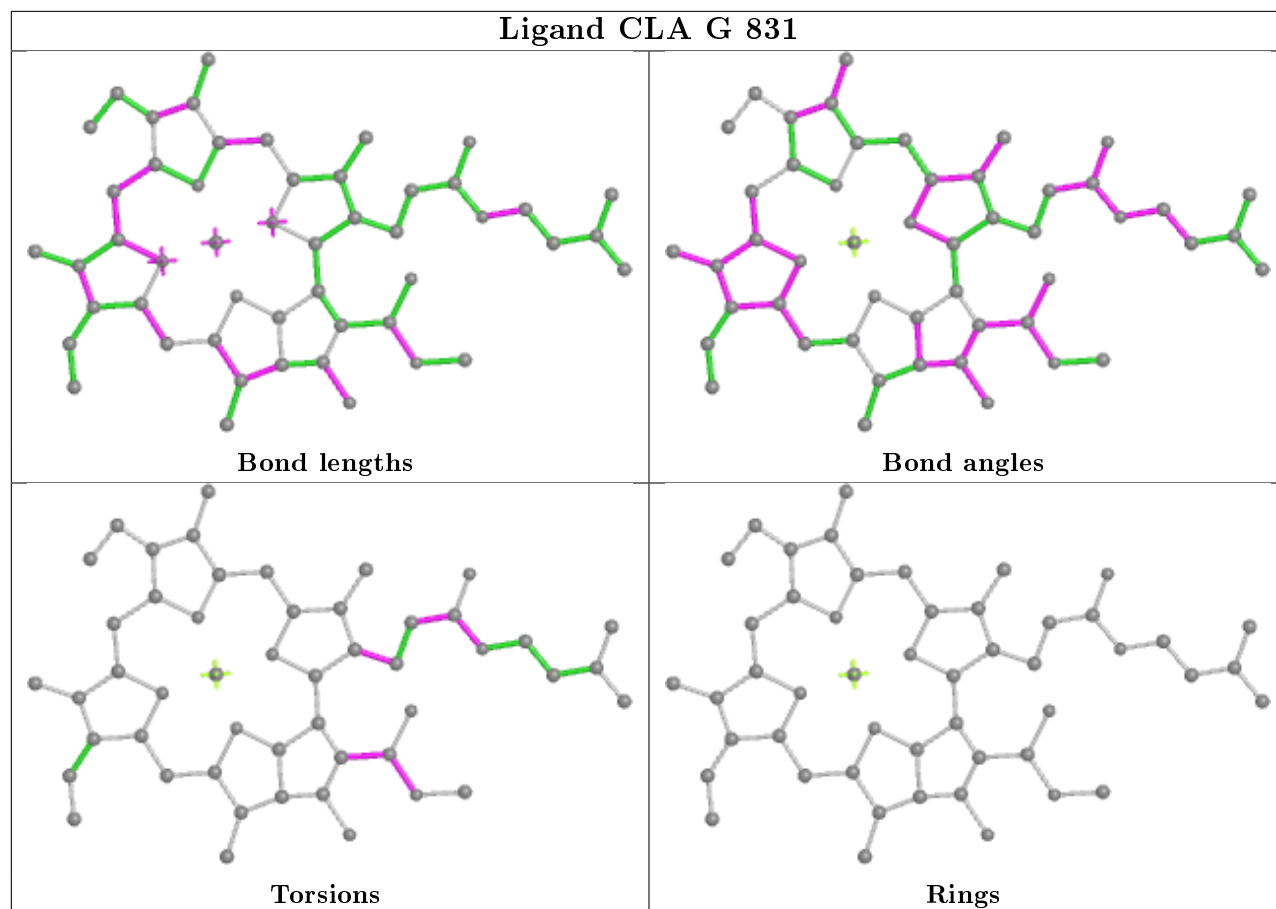
Ligand CLA B 805

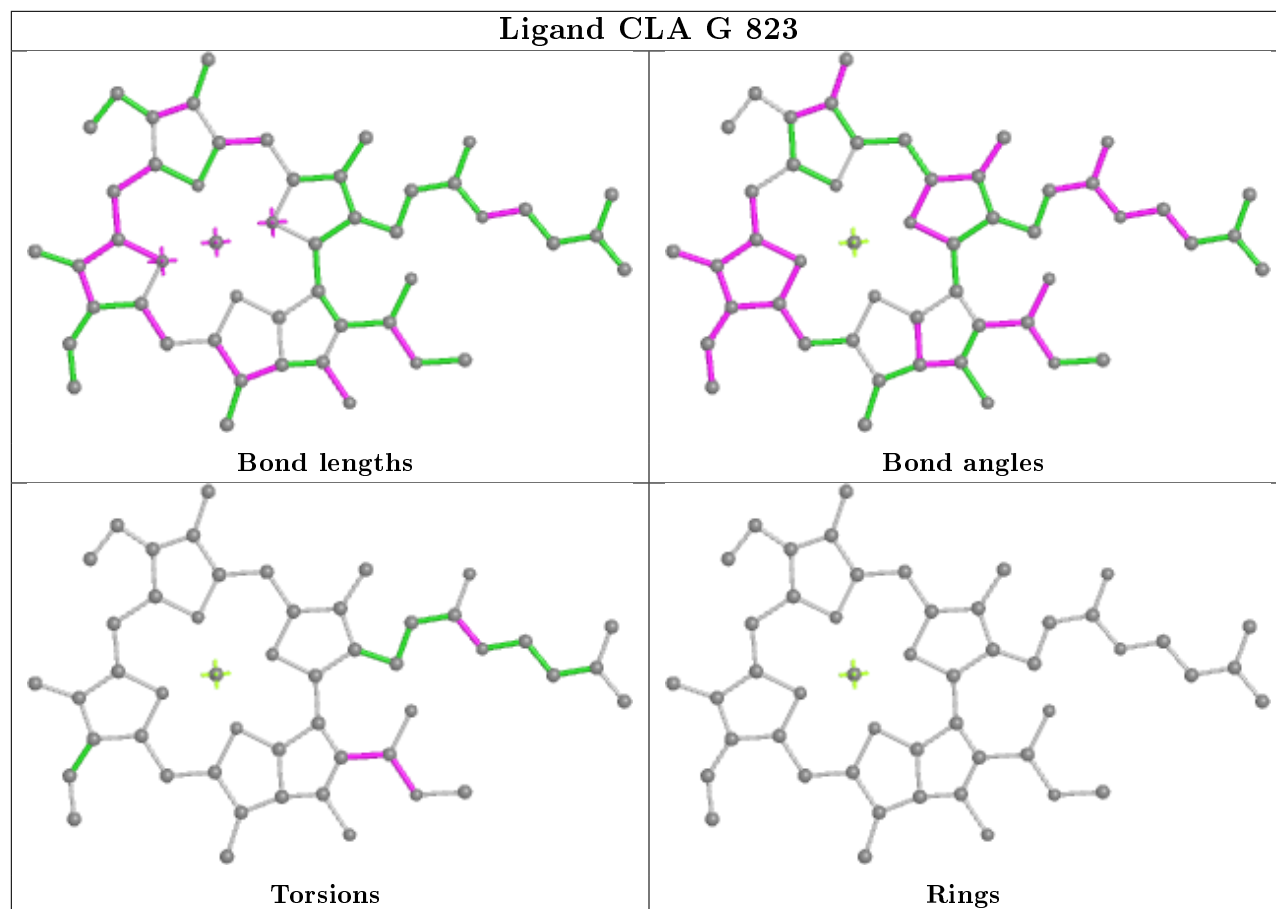
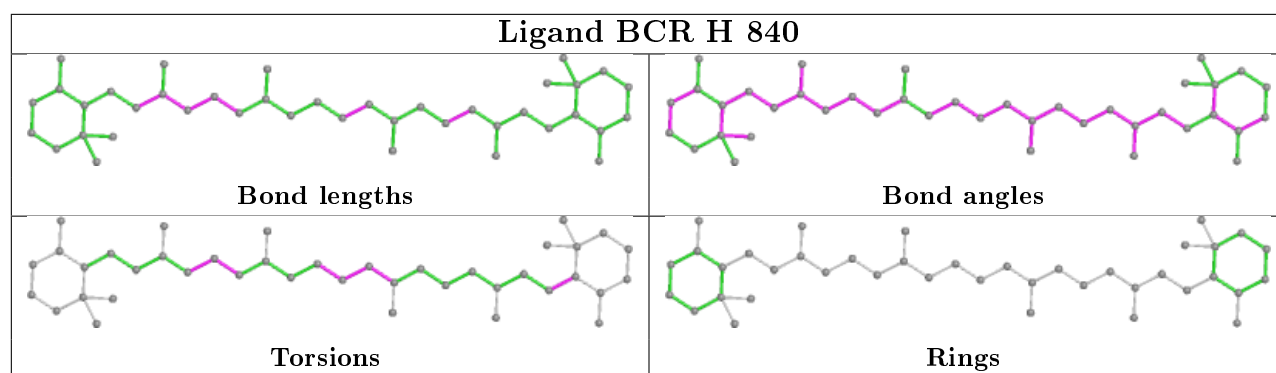




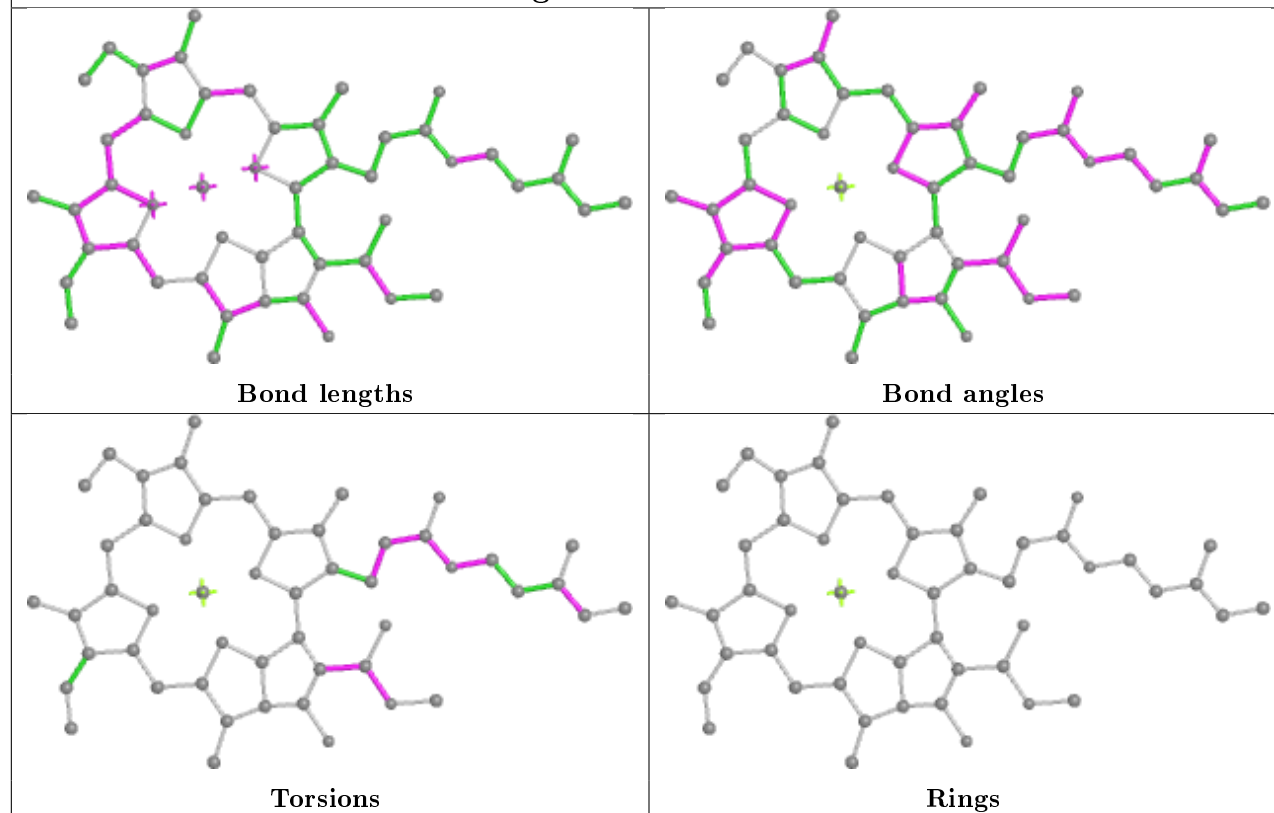
Ligand CLA g 102



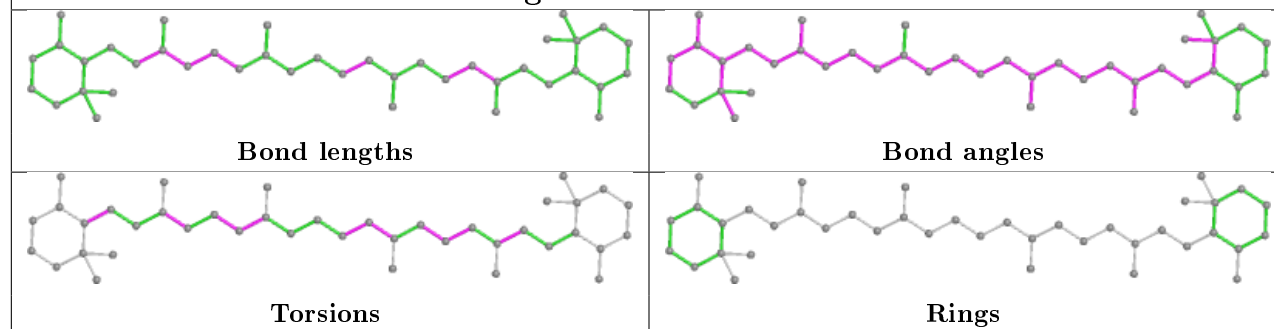




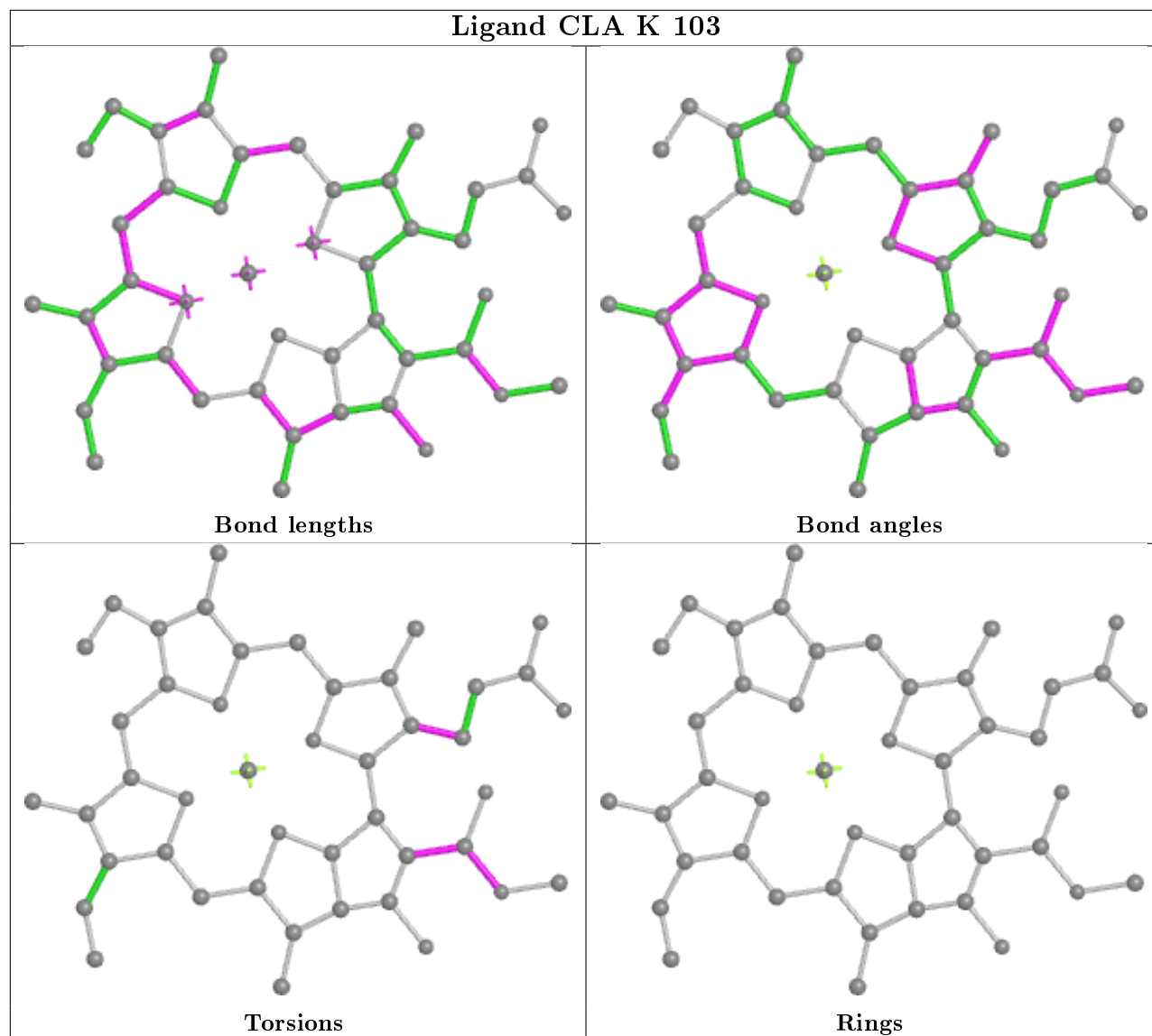
Ligand CLA Y 807



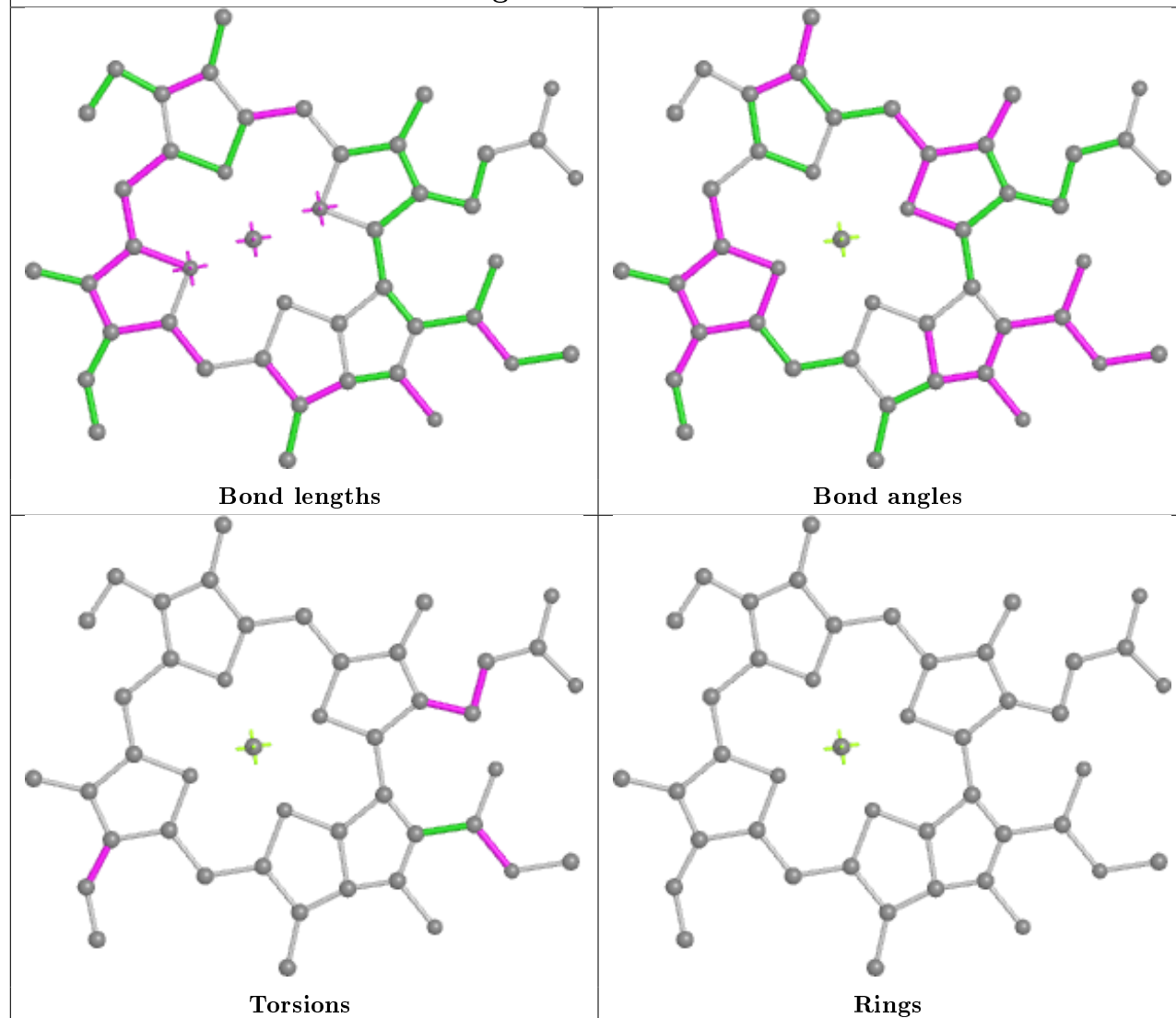
Ligand BCR S 1104



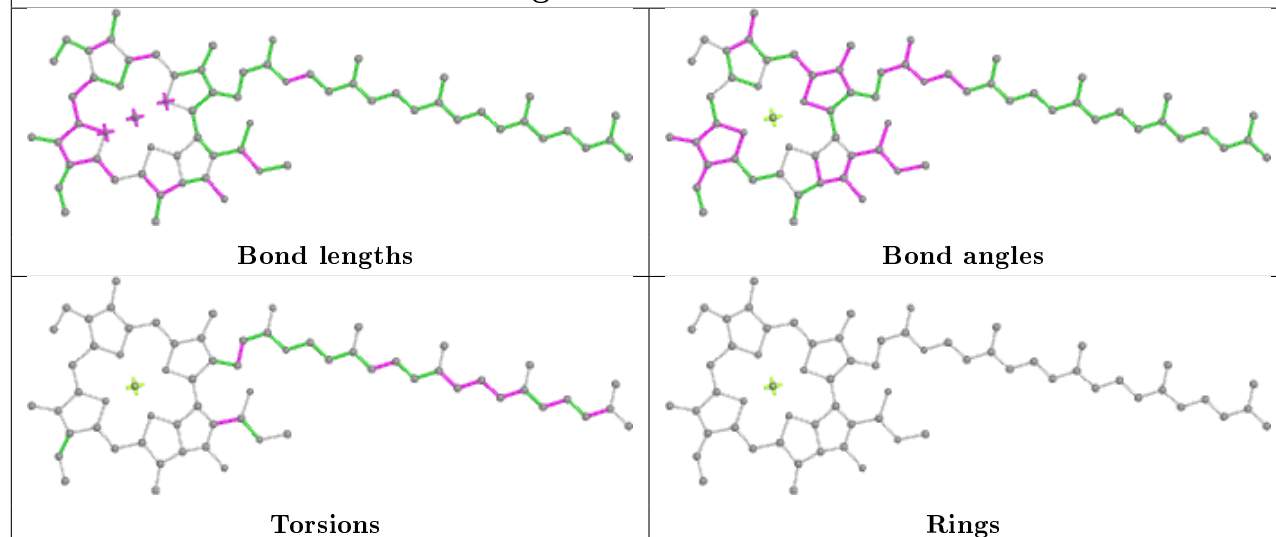
Ligand CLA K 103



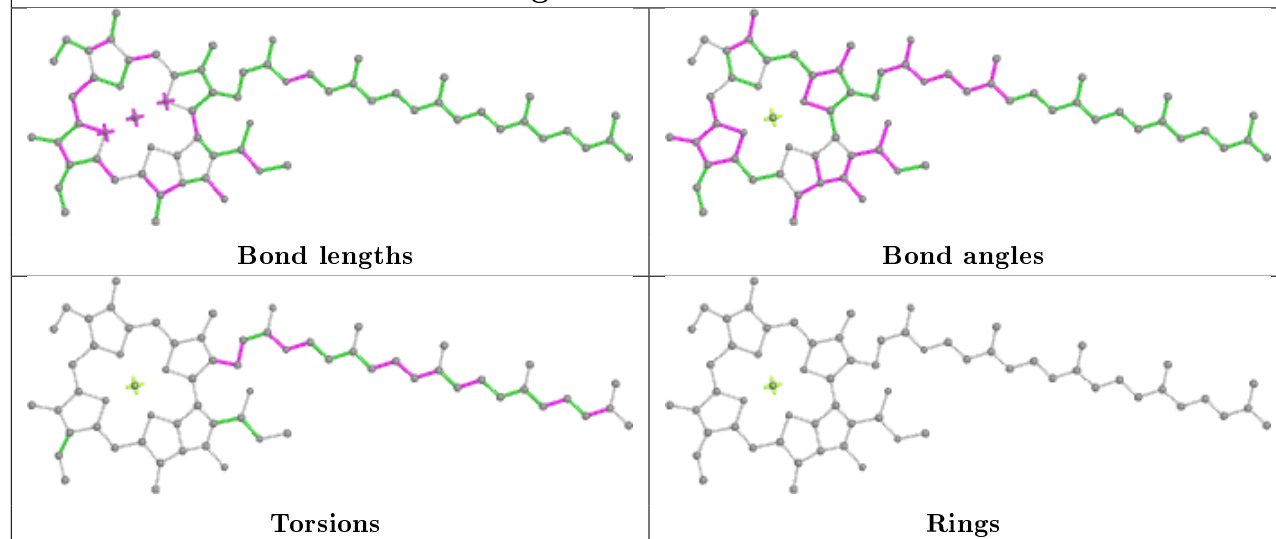
Ligand CLA Z 829



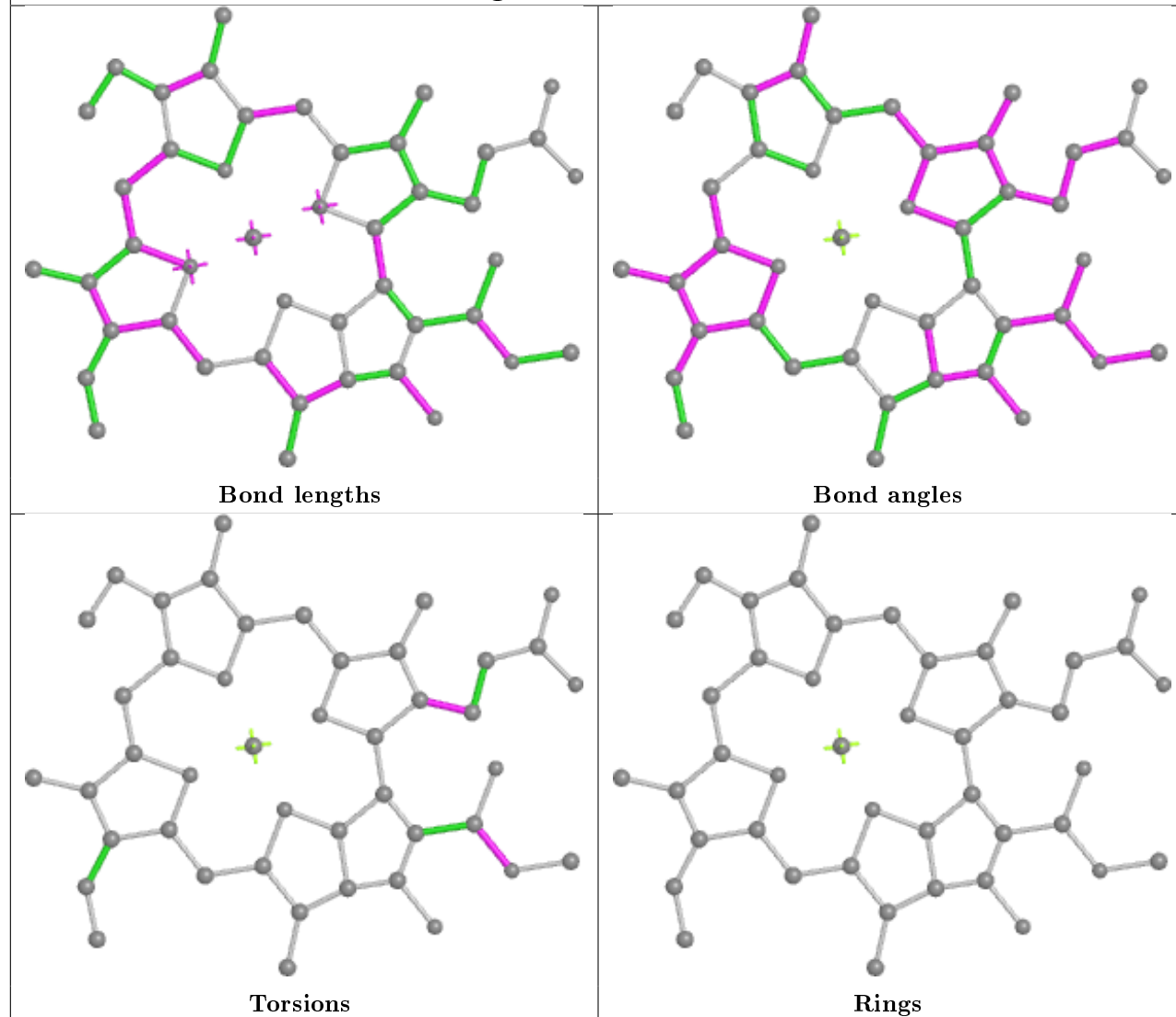
Ligand CLA B 840



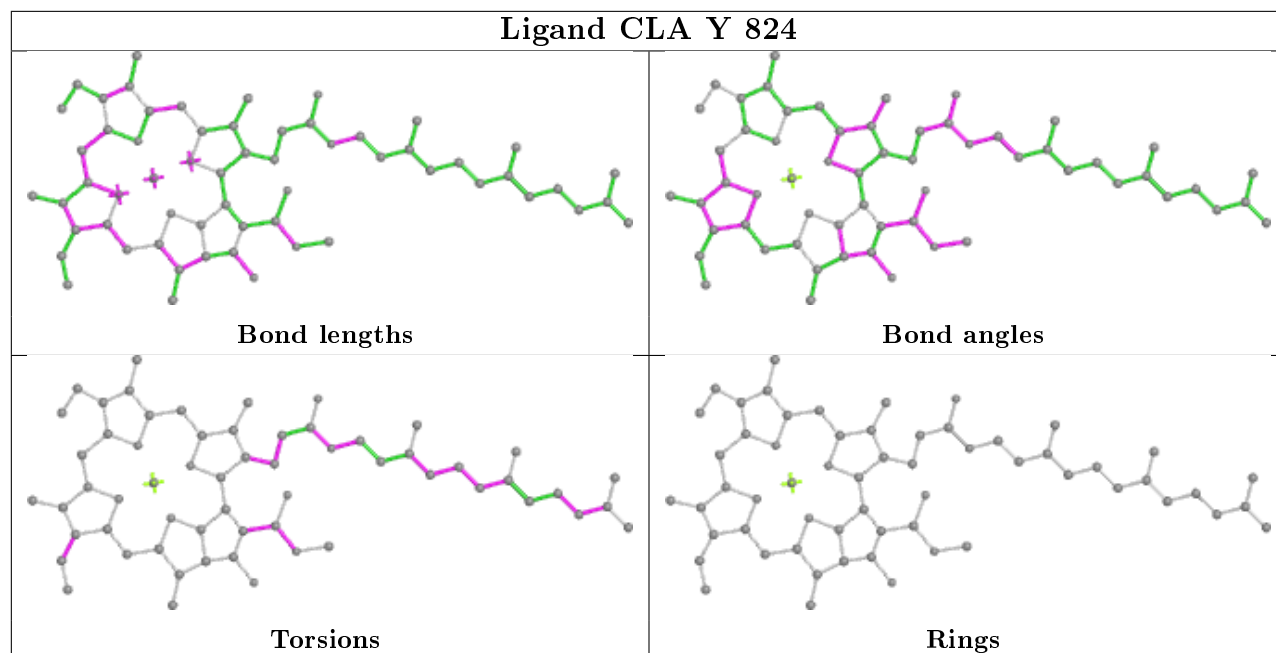
Ligand CLA G 822



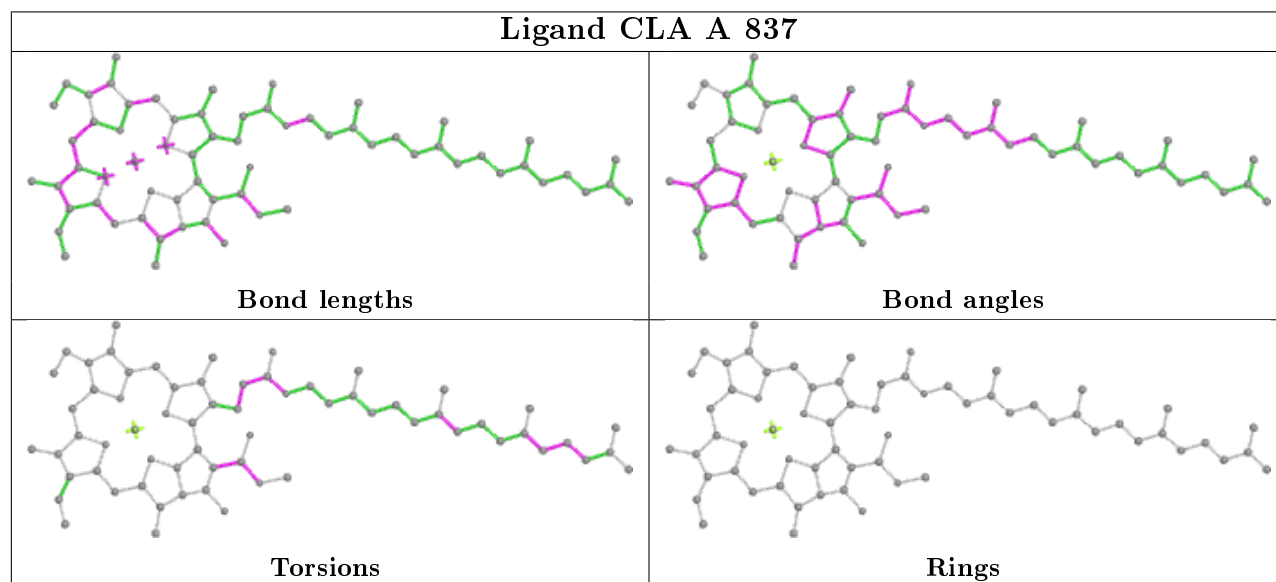
Ligand CLA H 814



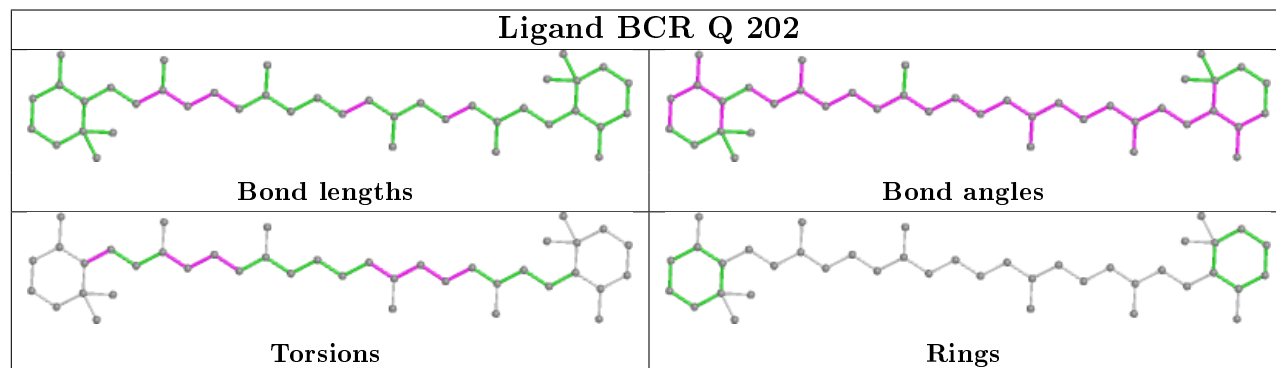
Ligand CLA Y 824



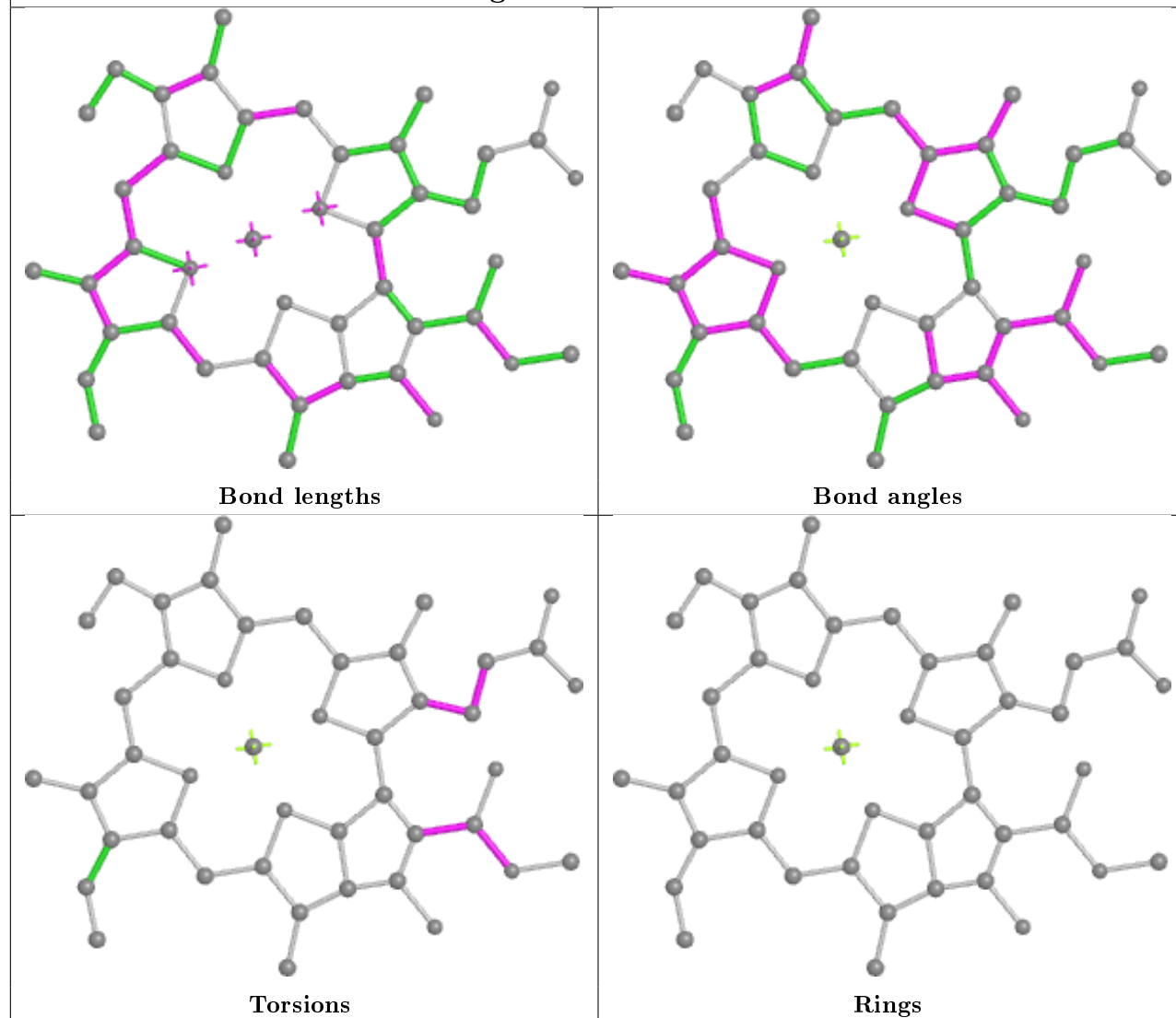
Ligand CLA A 837



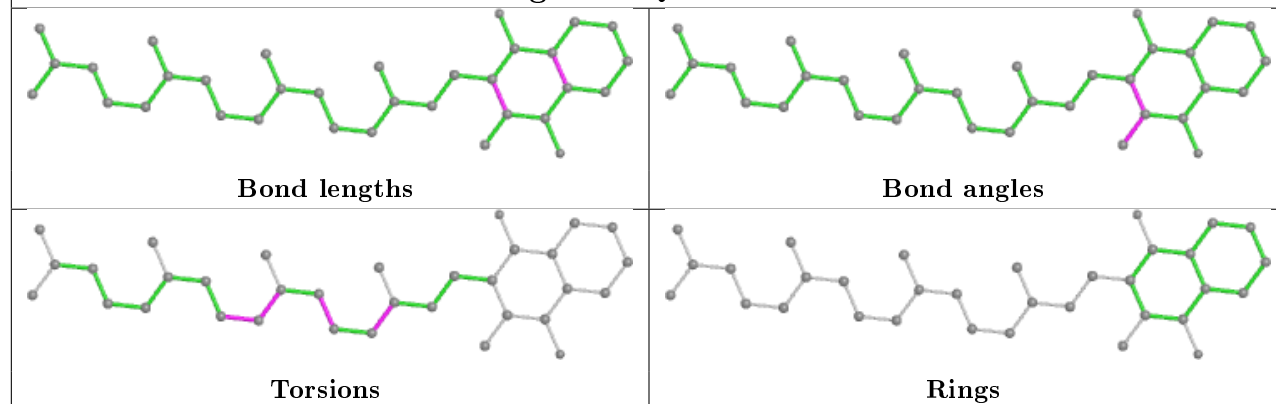
Ligand BCR Q 202



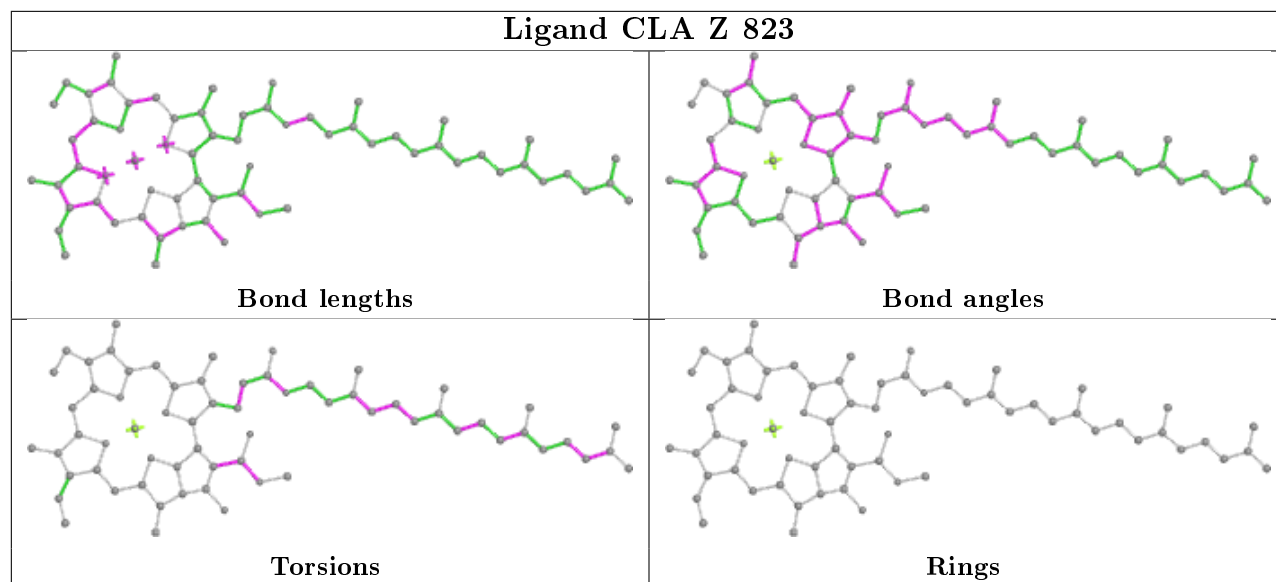
Ligand CLA H 819



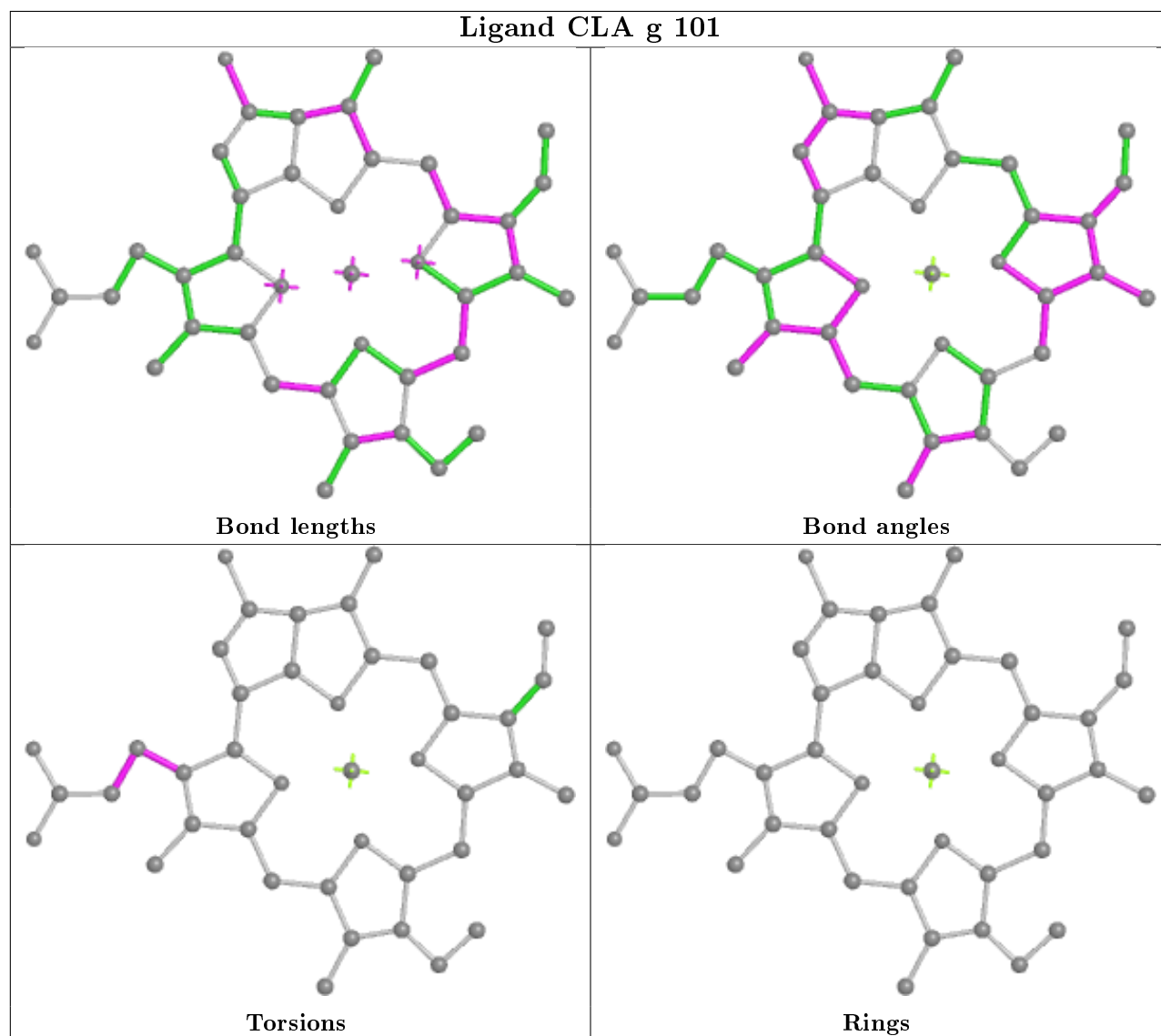
Ligand PQN Y 844



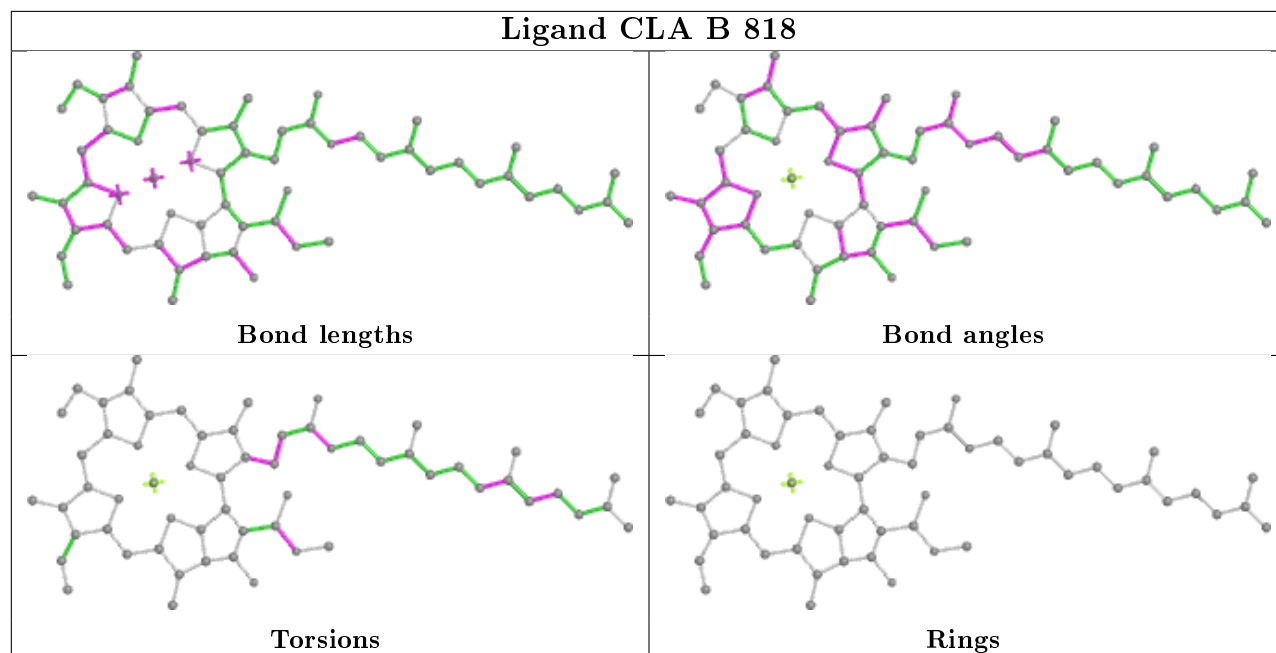
Ligand CLA Z 823



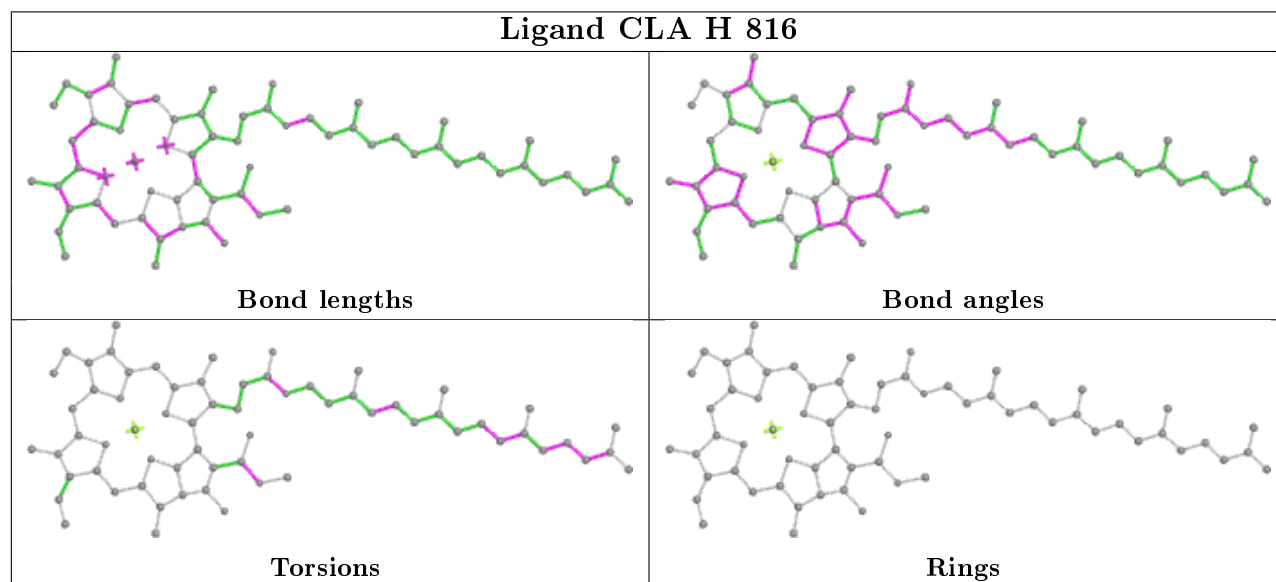
Ligand CLA g 101



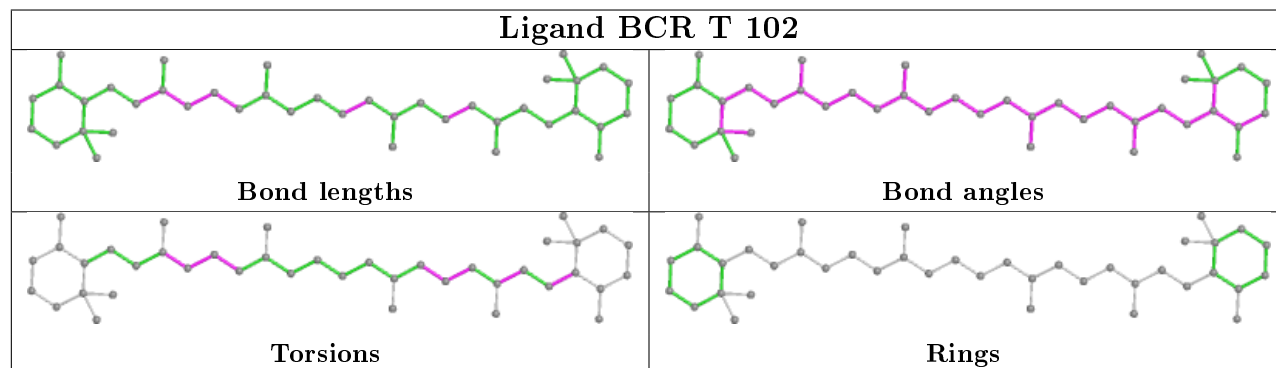
Ligand CLA B 818

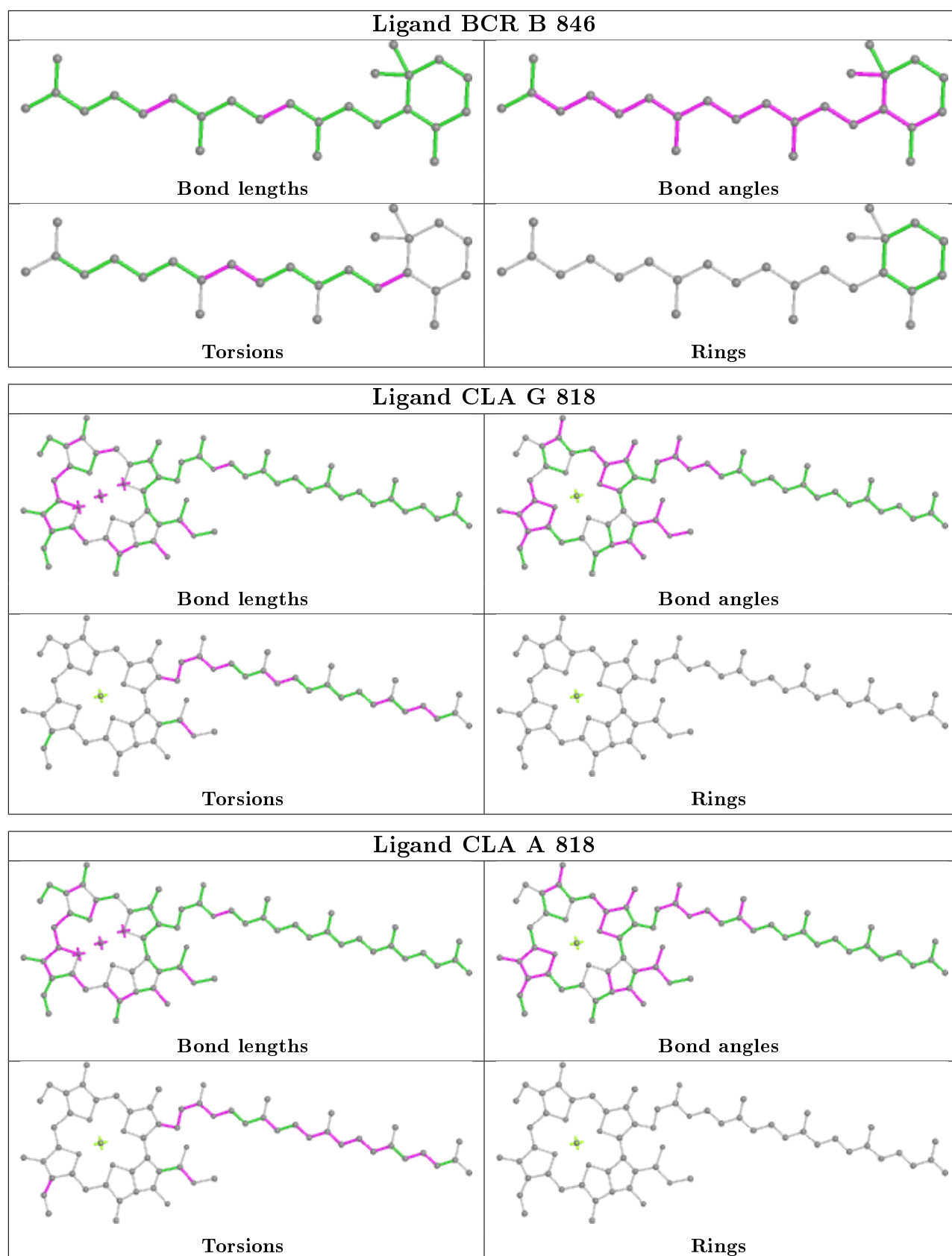


Ligand CLA H 816

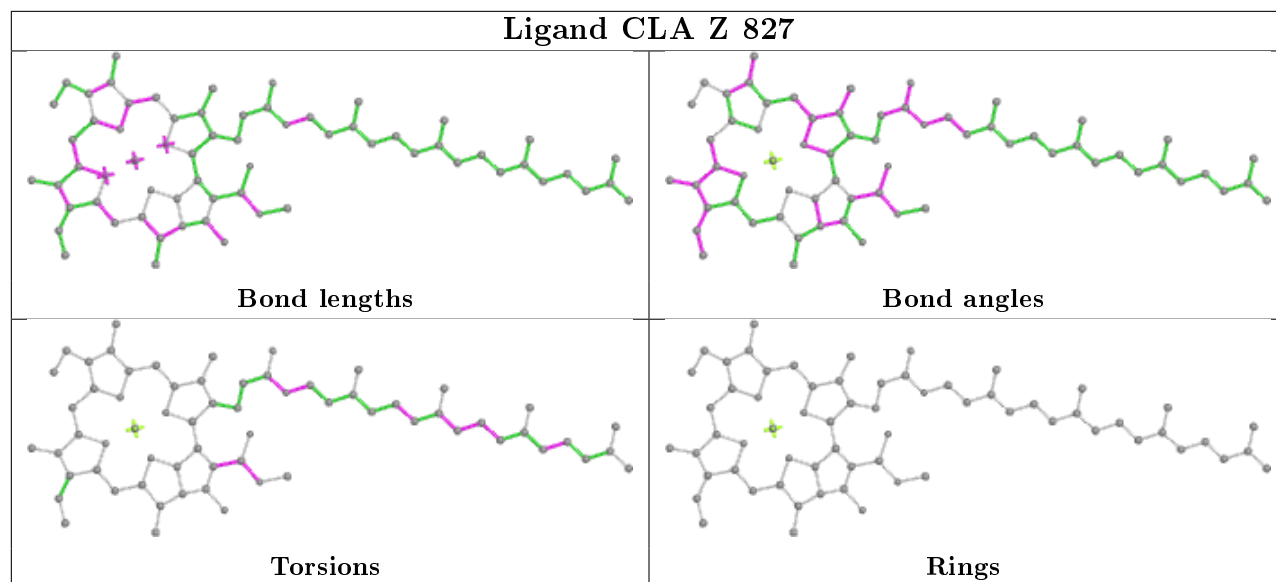


Ligand BCR T 102

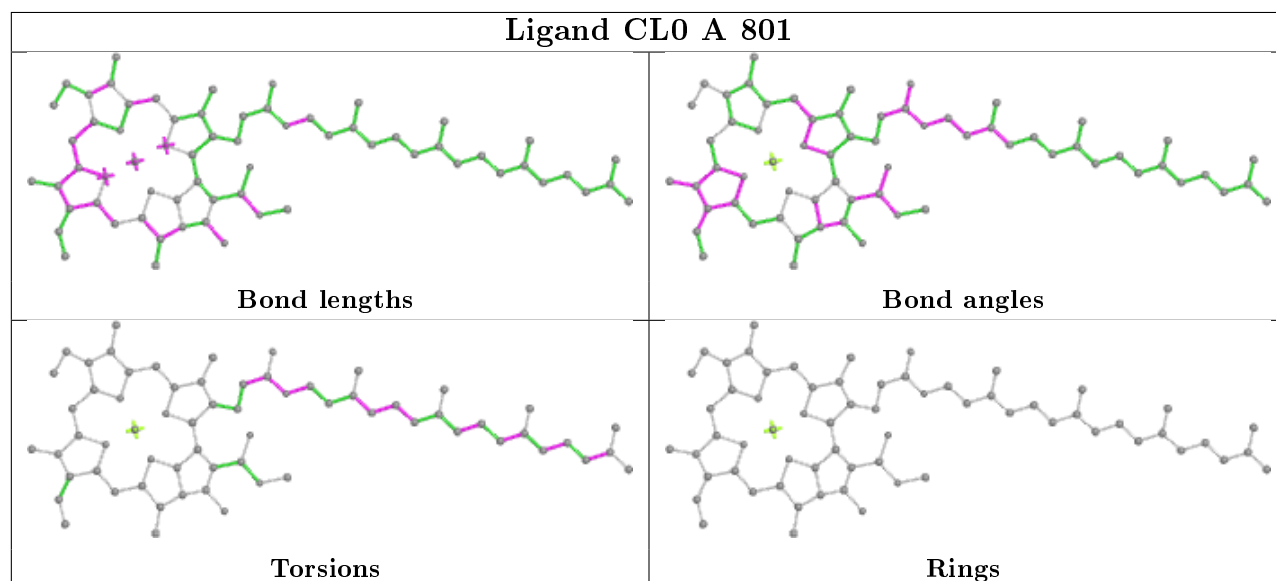




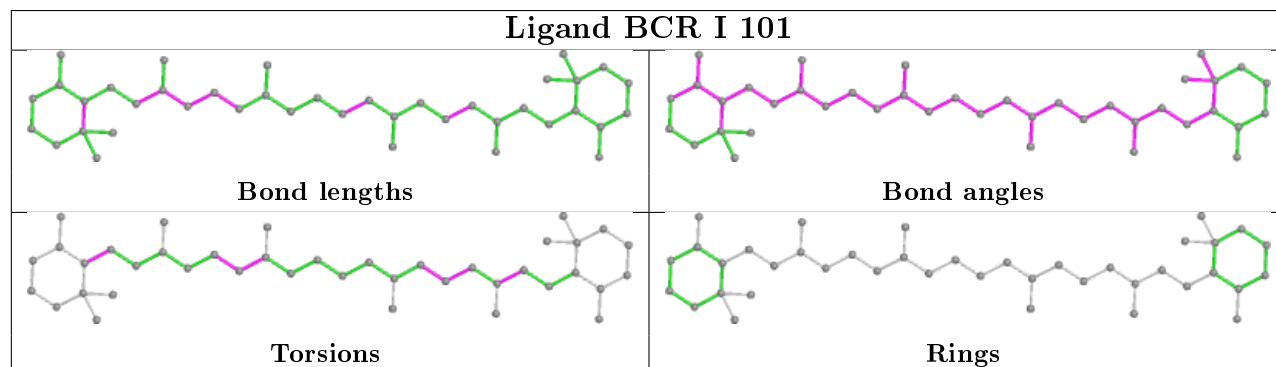
Ligand CLA Z 827



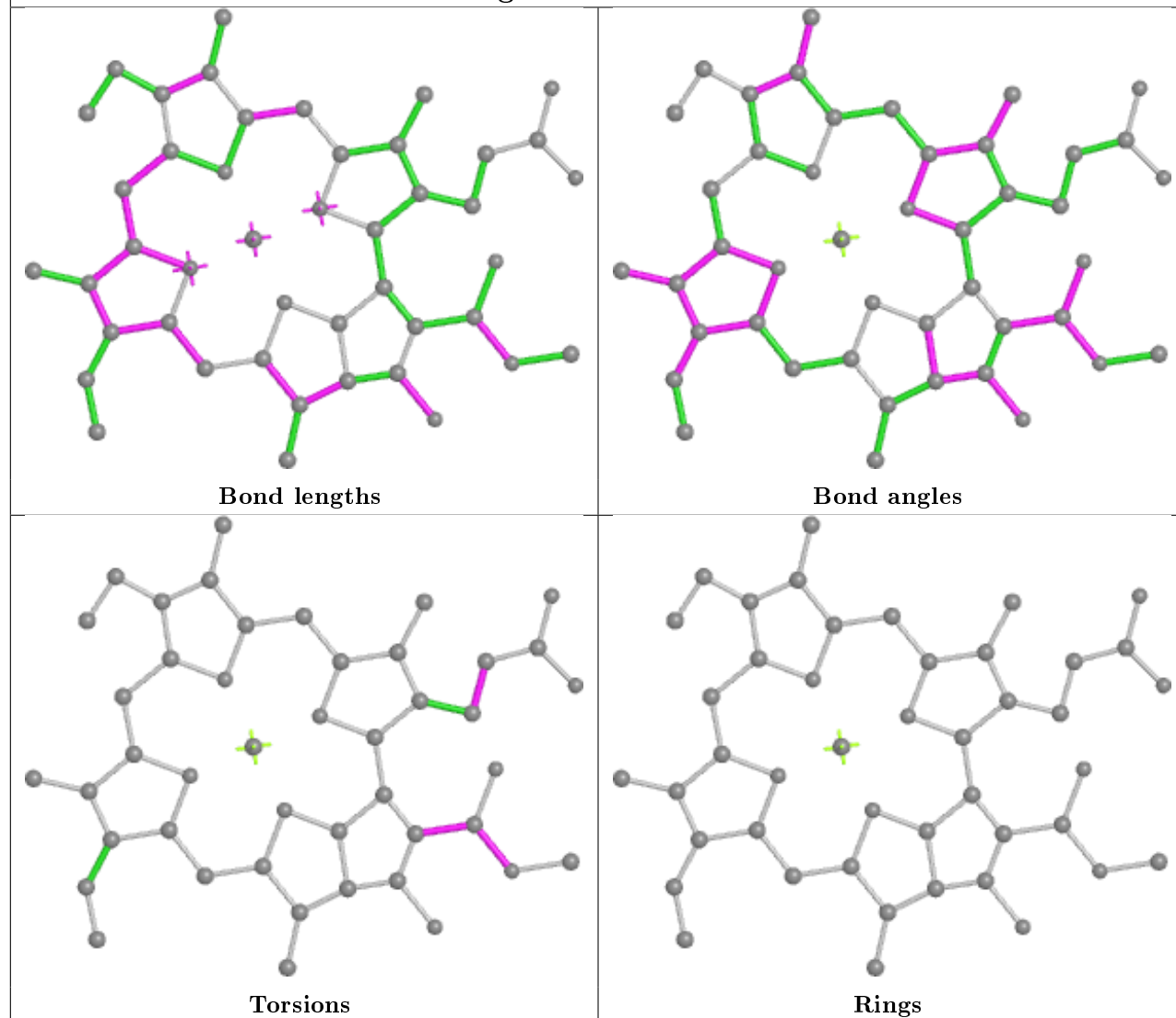
Ligand CL0 A 801



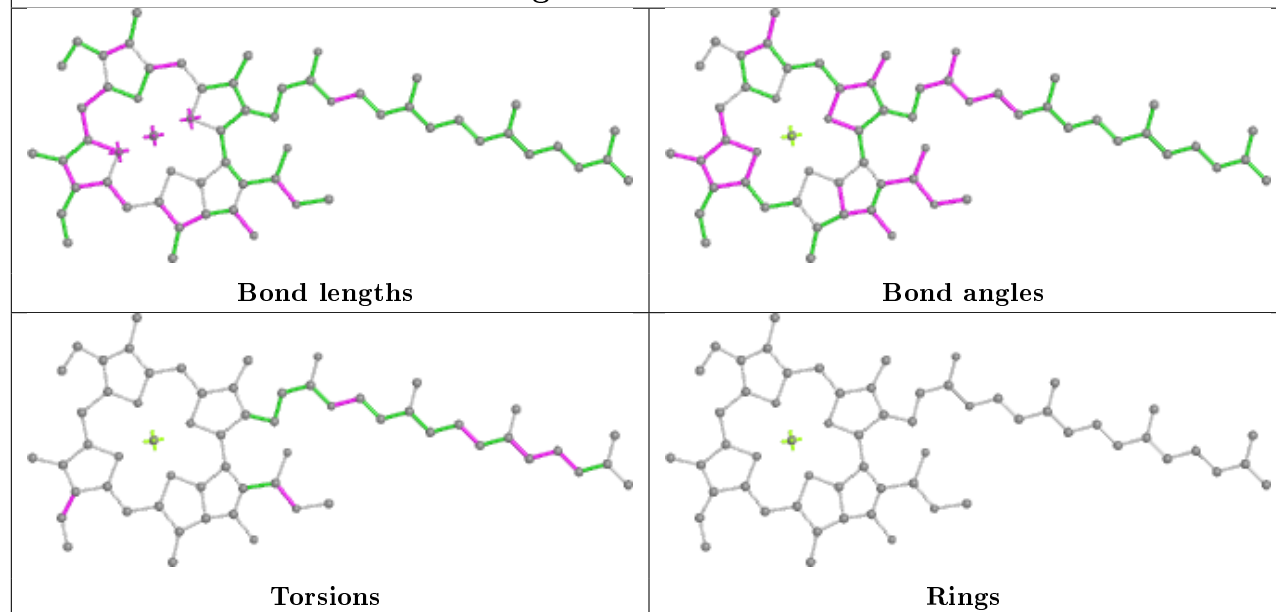
Ligand BCR I 101



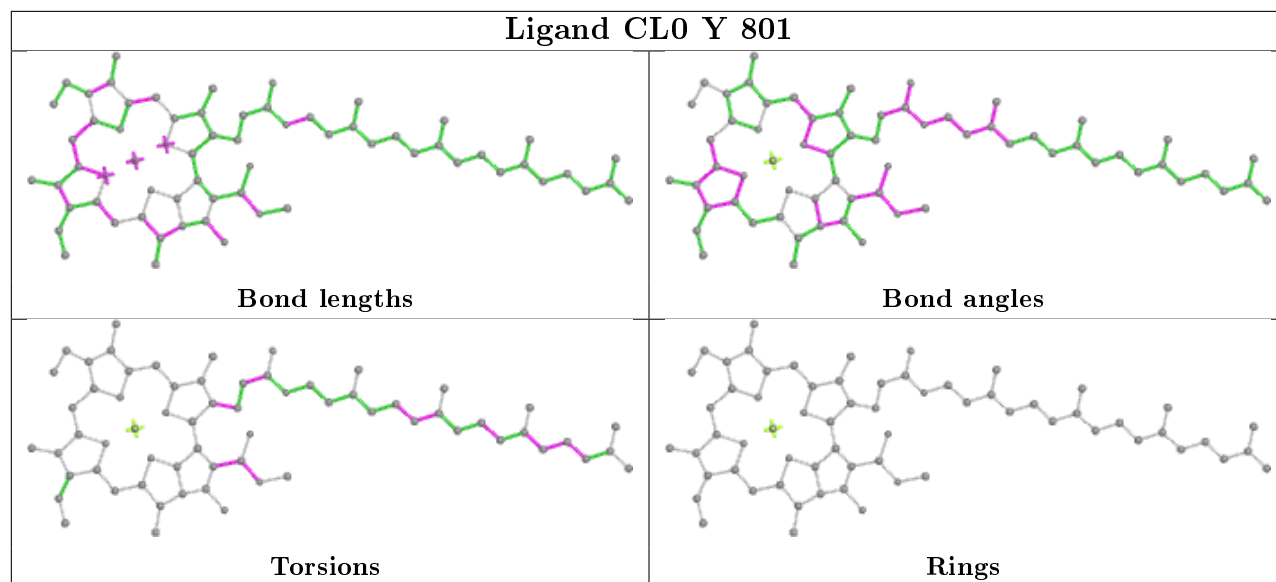
Ligand CLA f 101



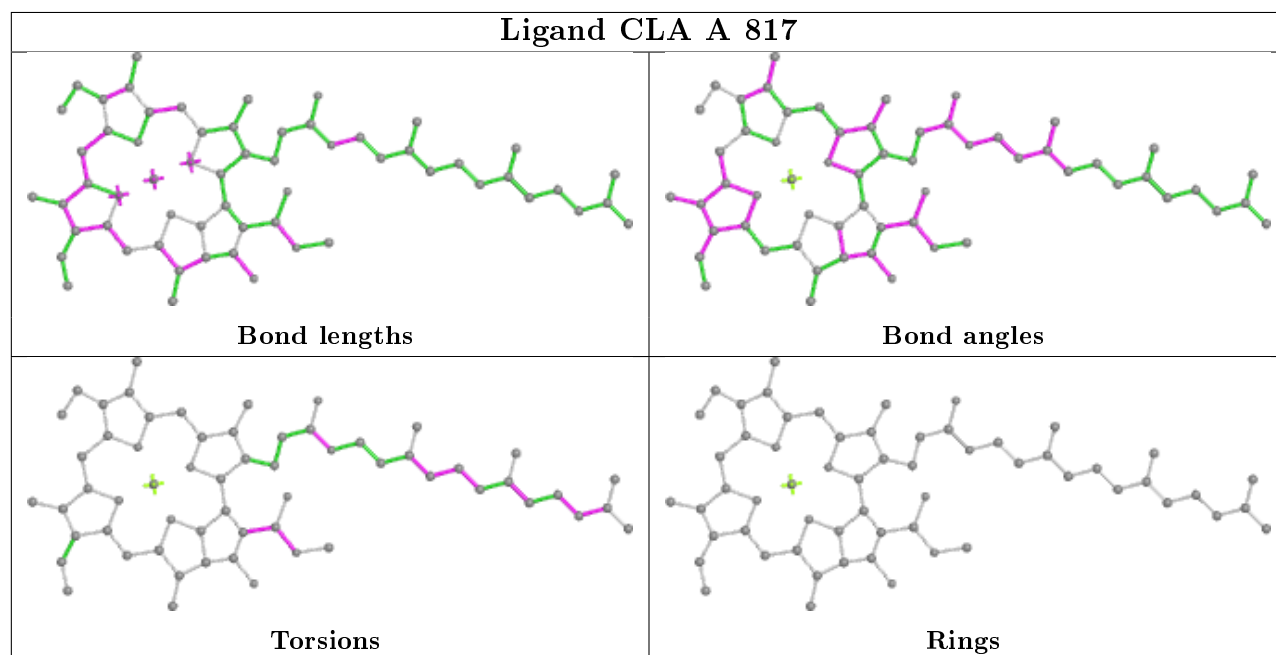
Ligand CLA Y 817



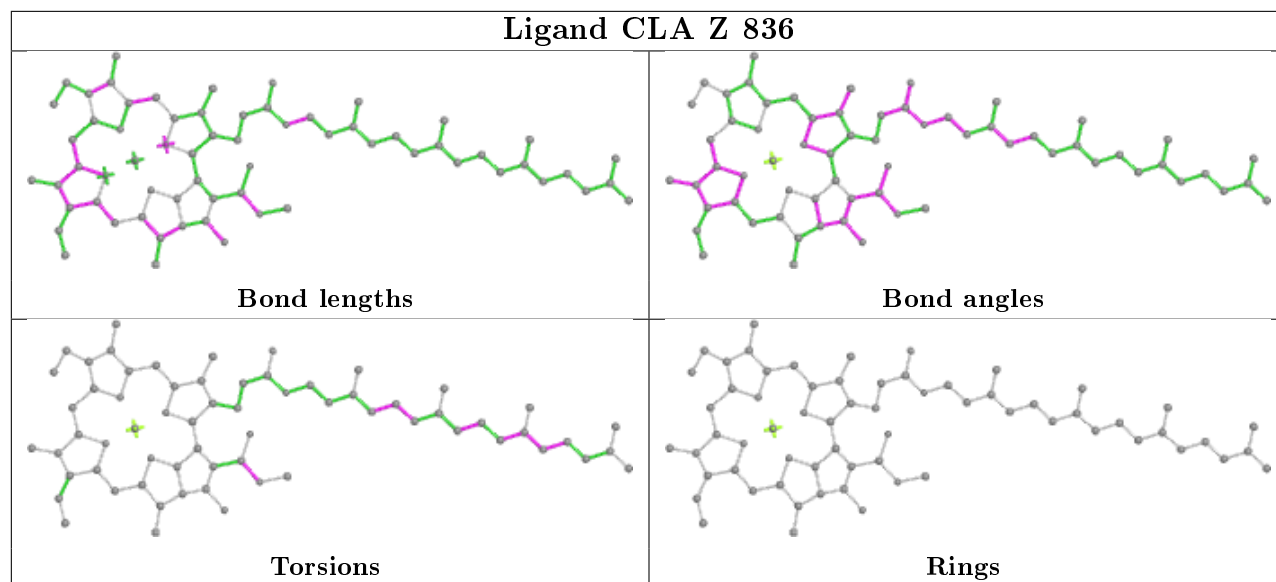
Ligand CL0 Y 801



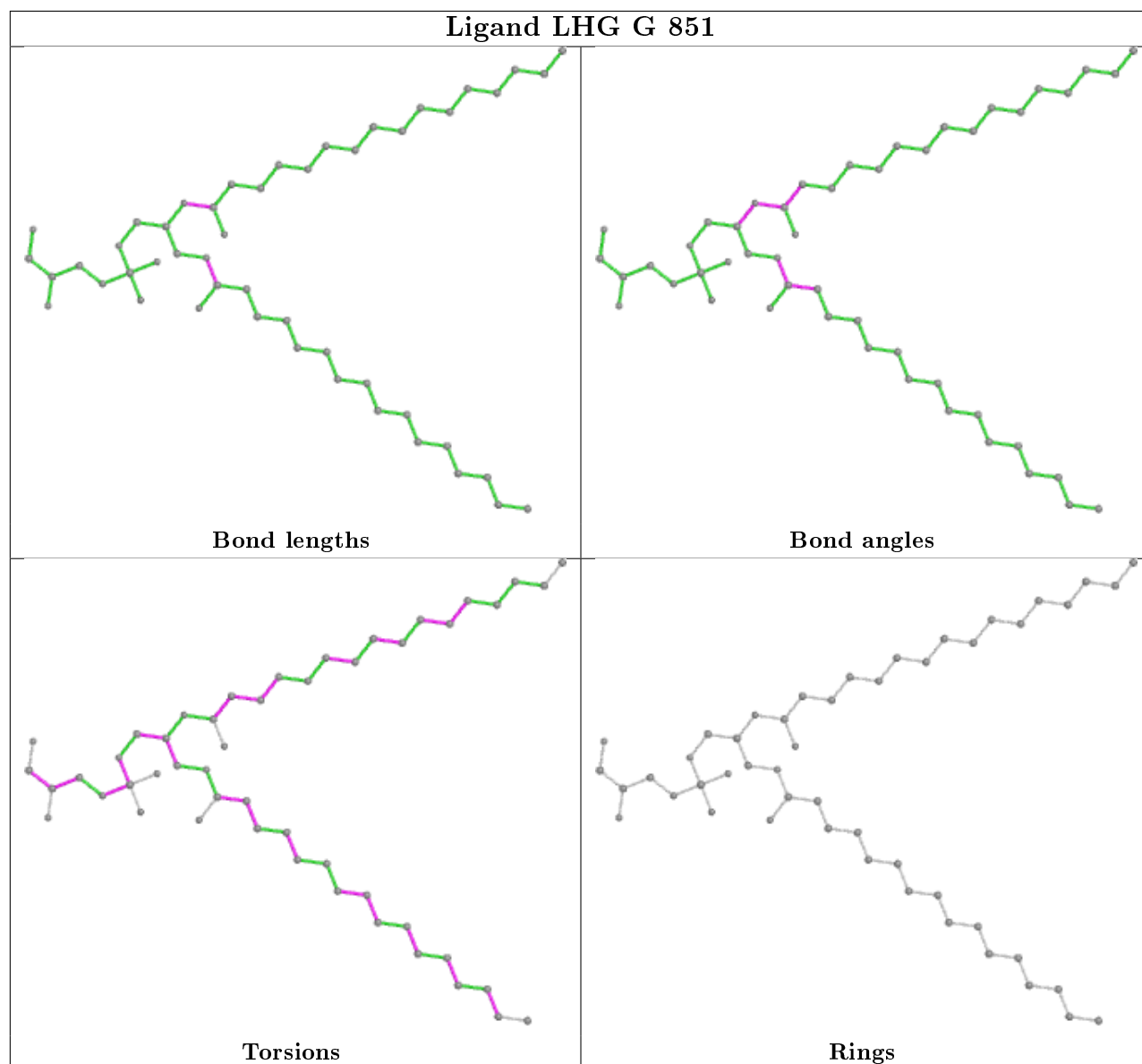
Ligand CLA A 817

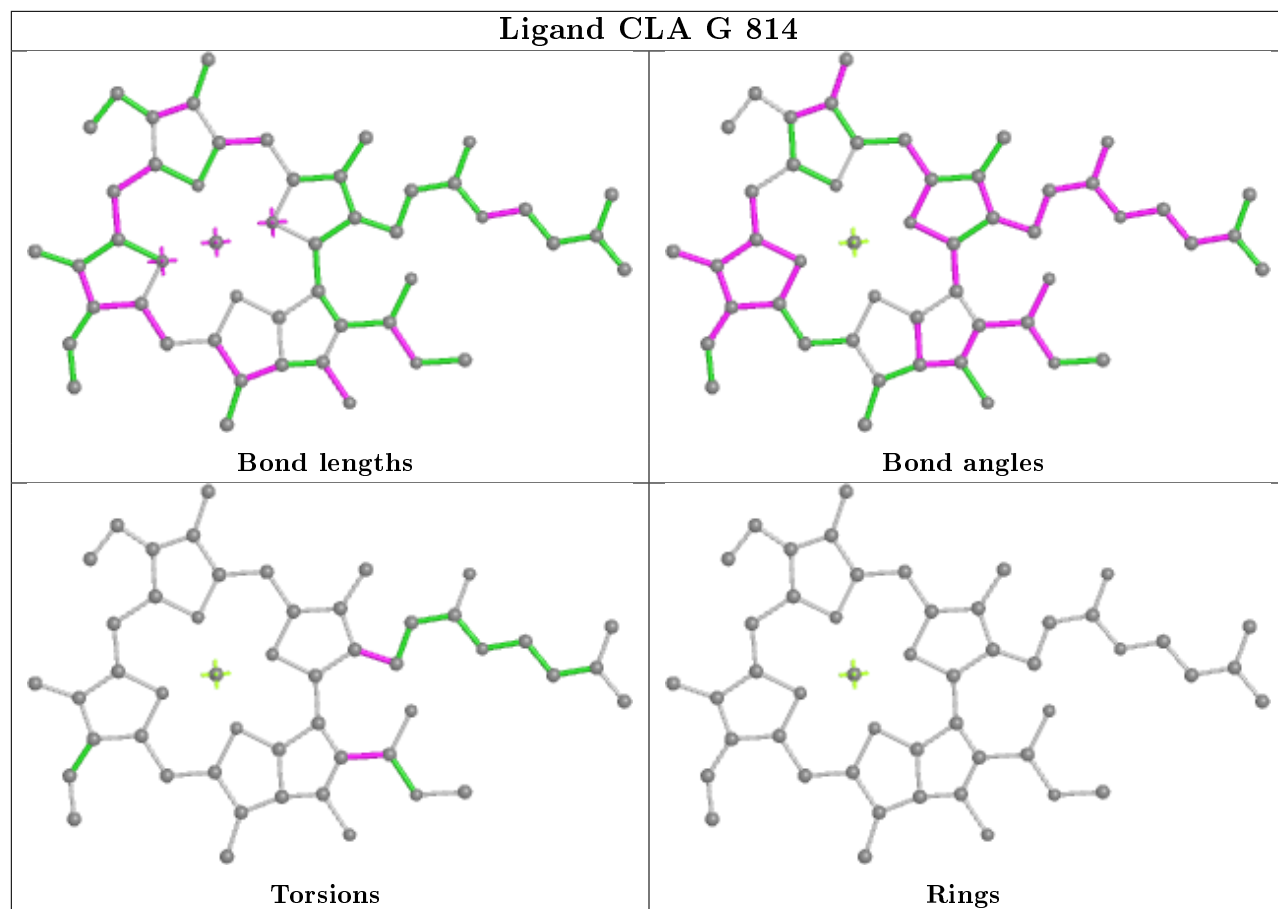


Ligand CLA Z 836

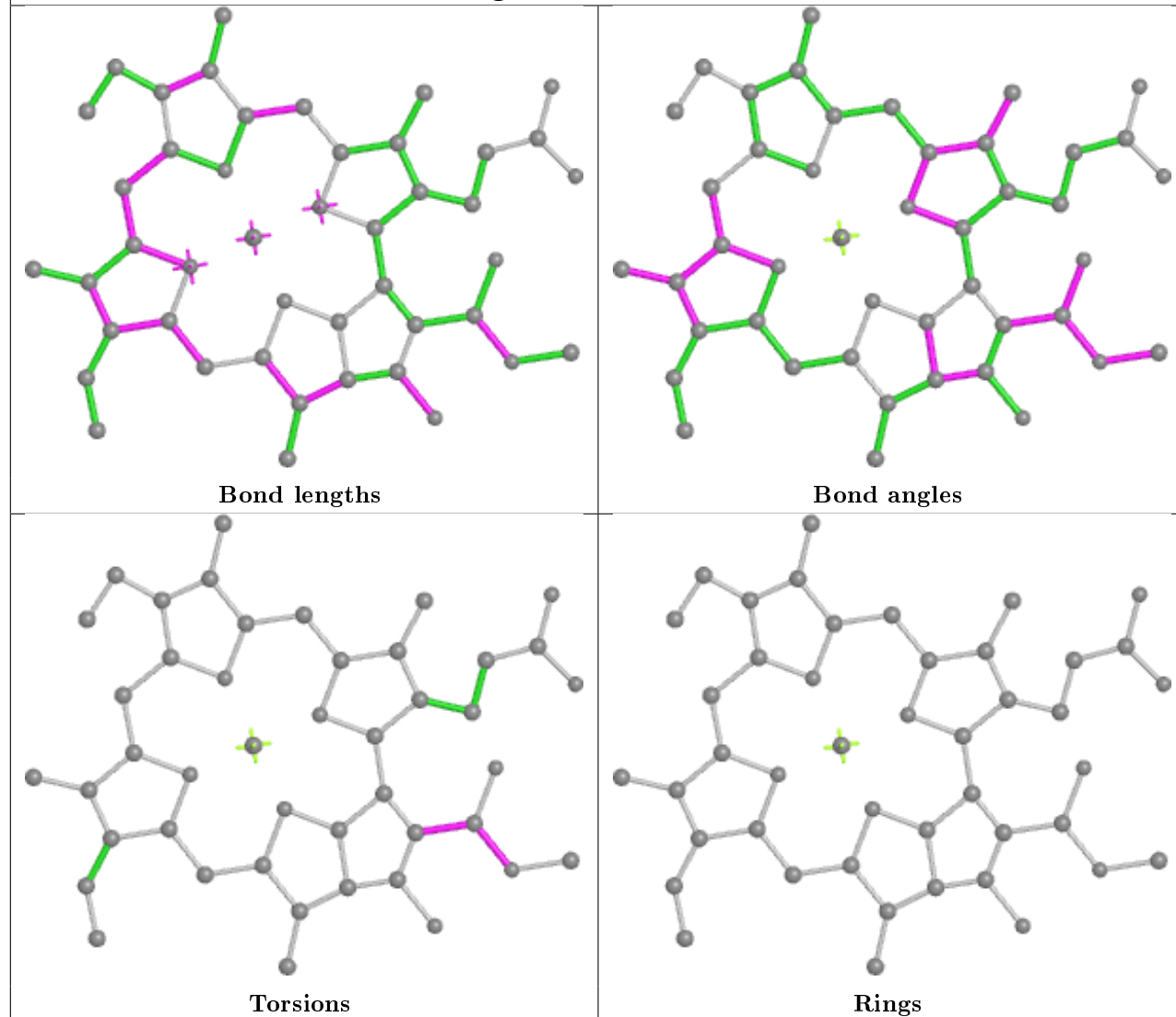


Ligand LHG G 851

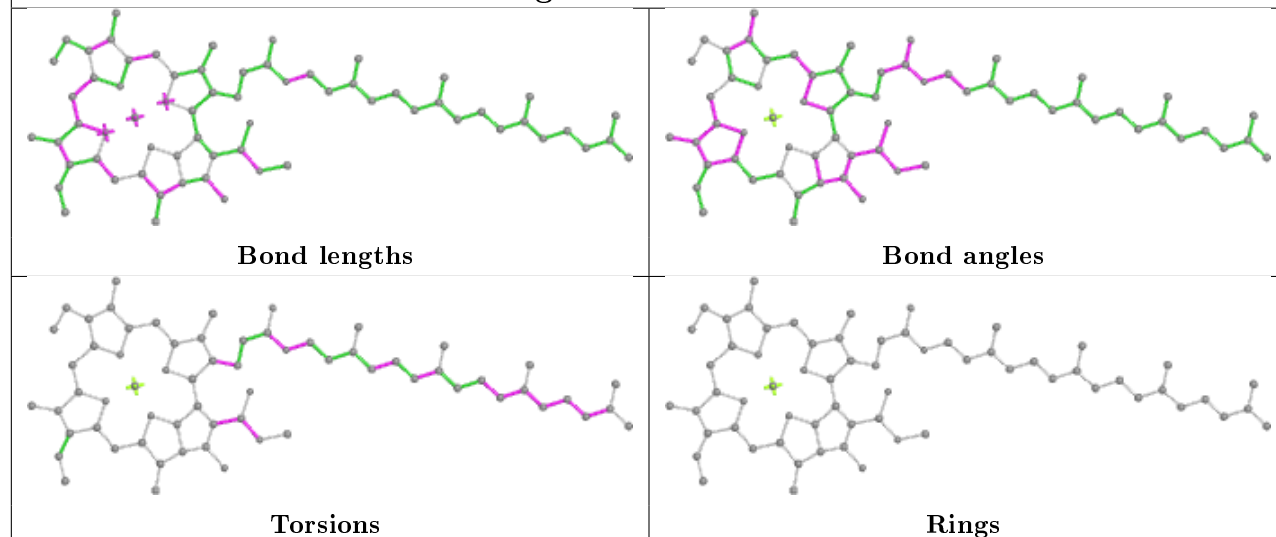




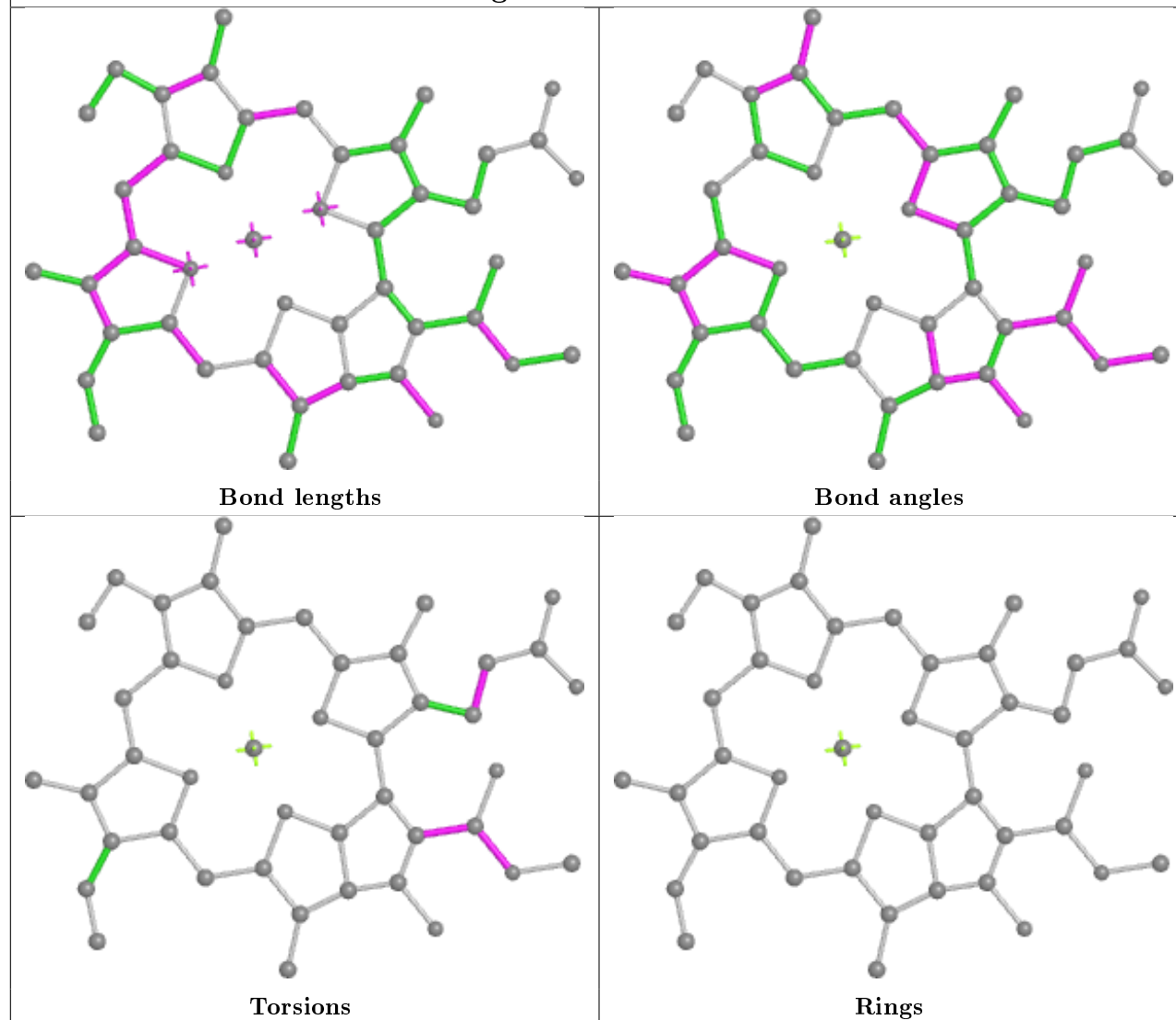
Ligand CLA A 810



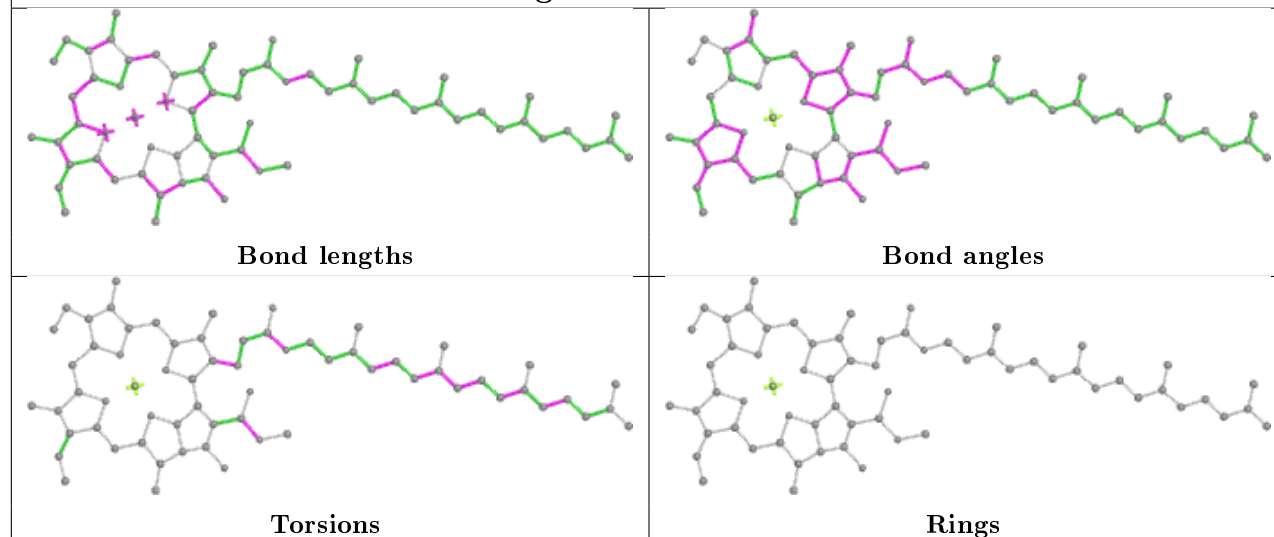
Ligand CLA h 205



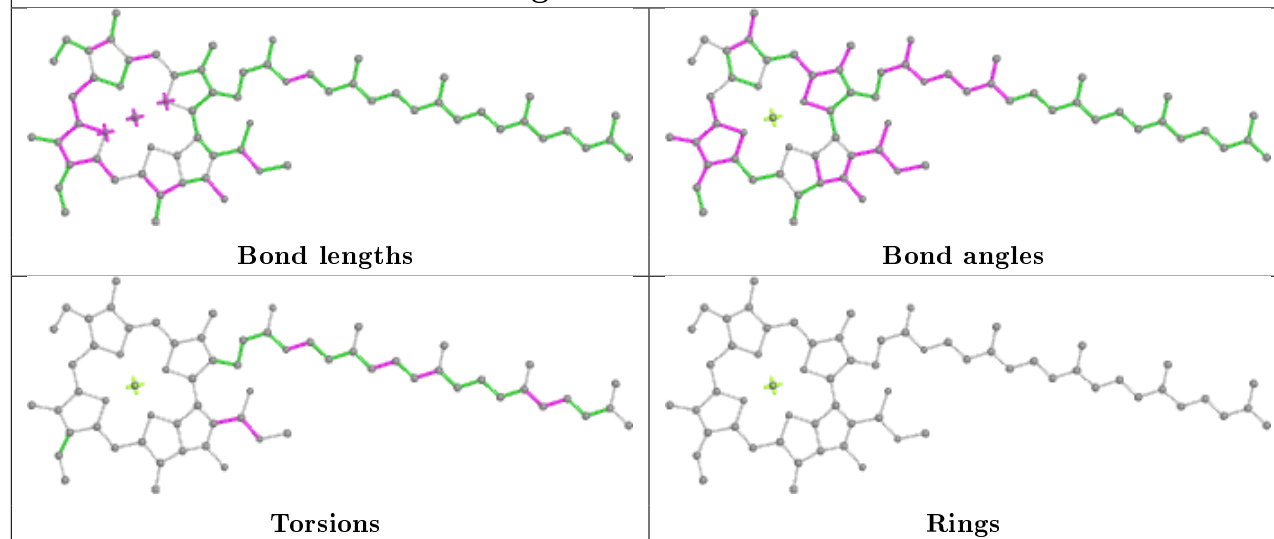
Ligand CLA Y 836



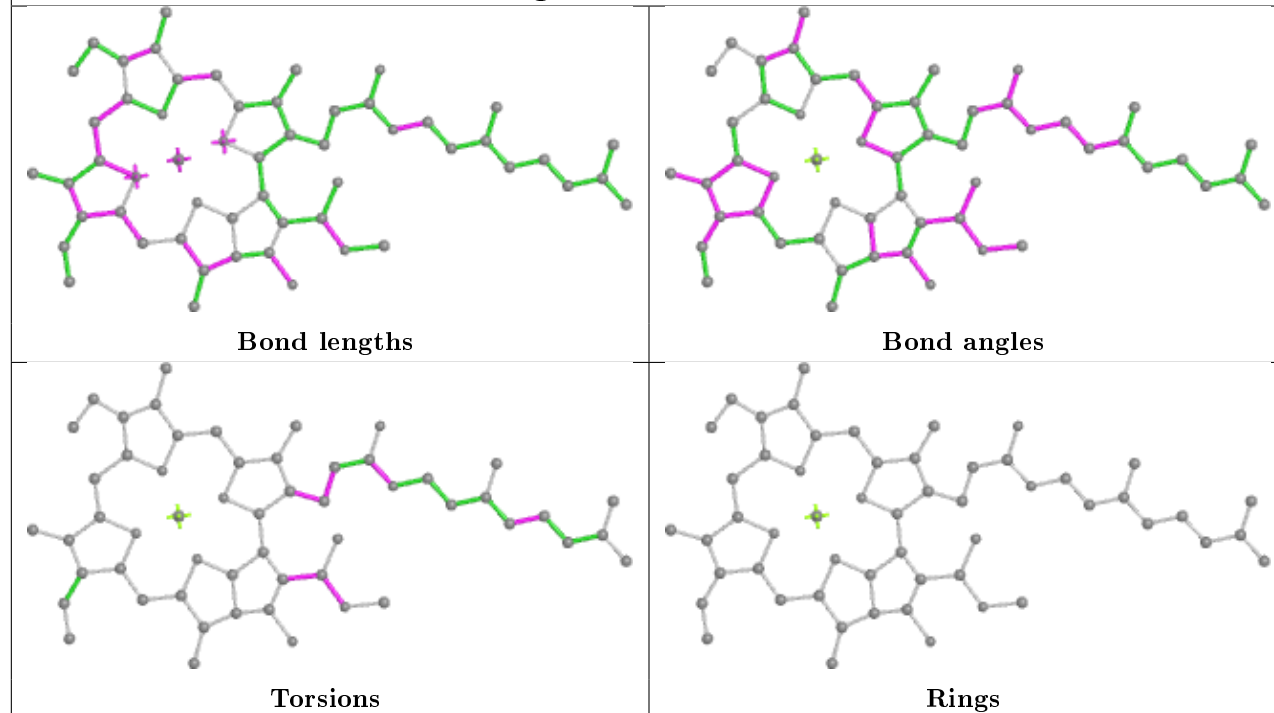
Ligand CLA h 206



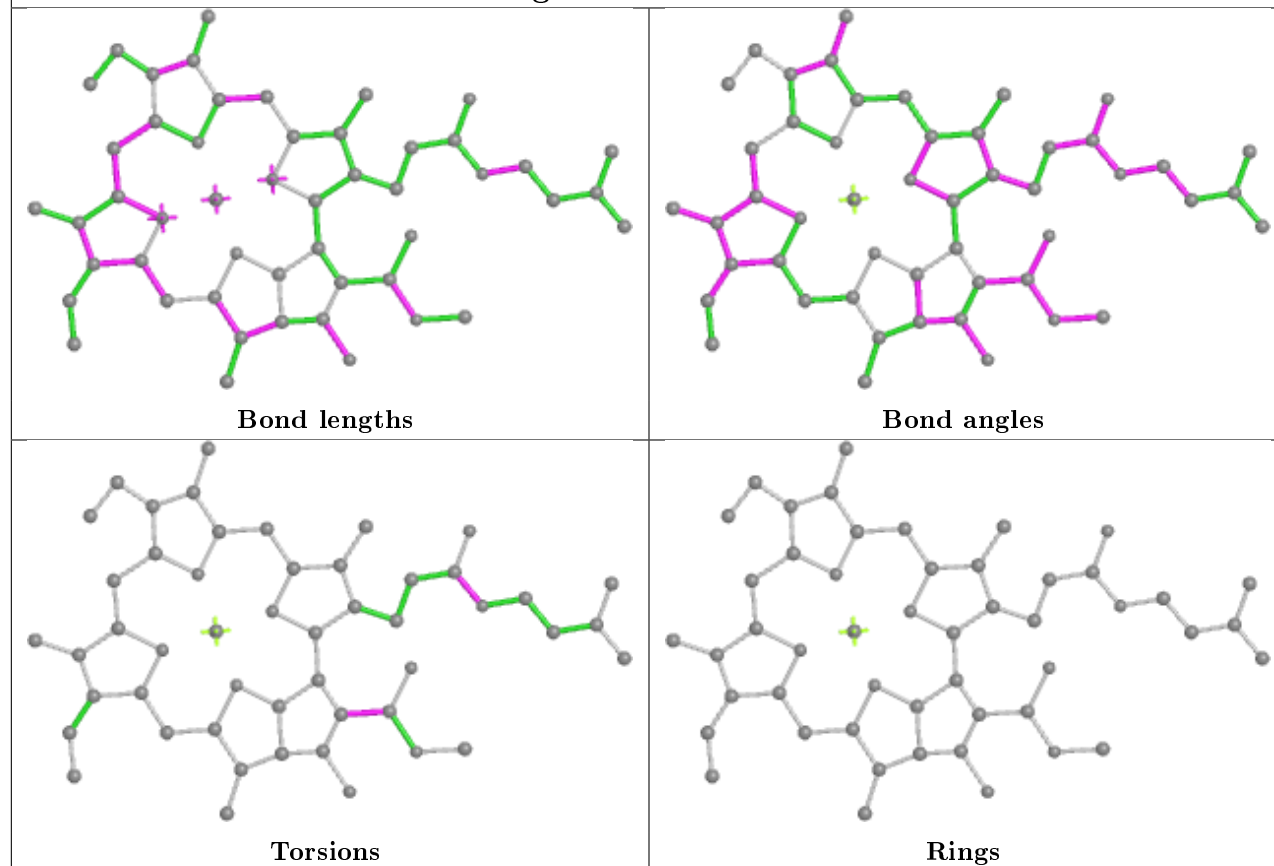
Ligand CLA H 825



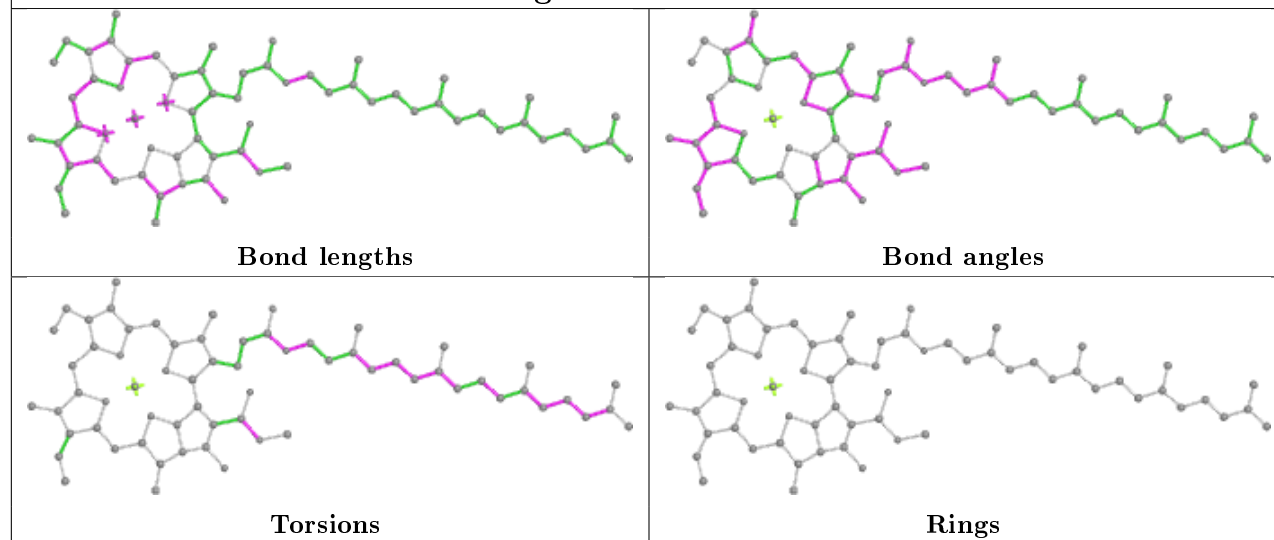
Ligand CLA A 834

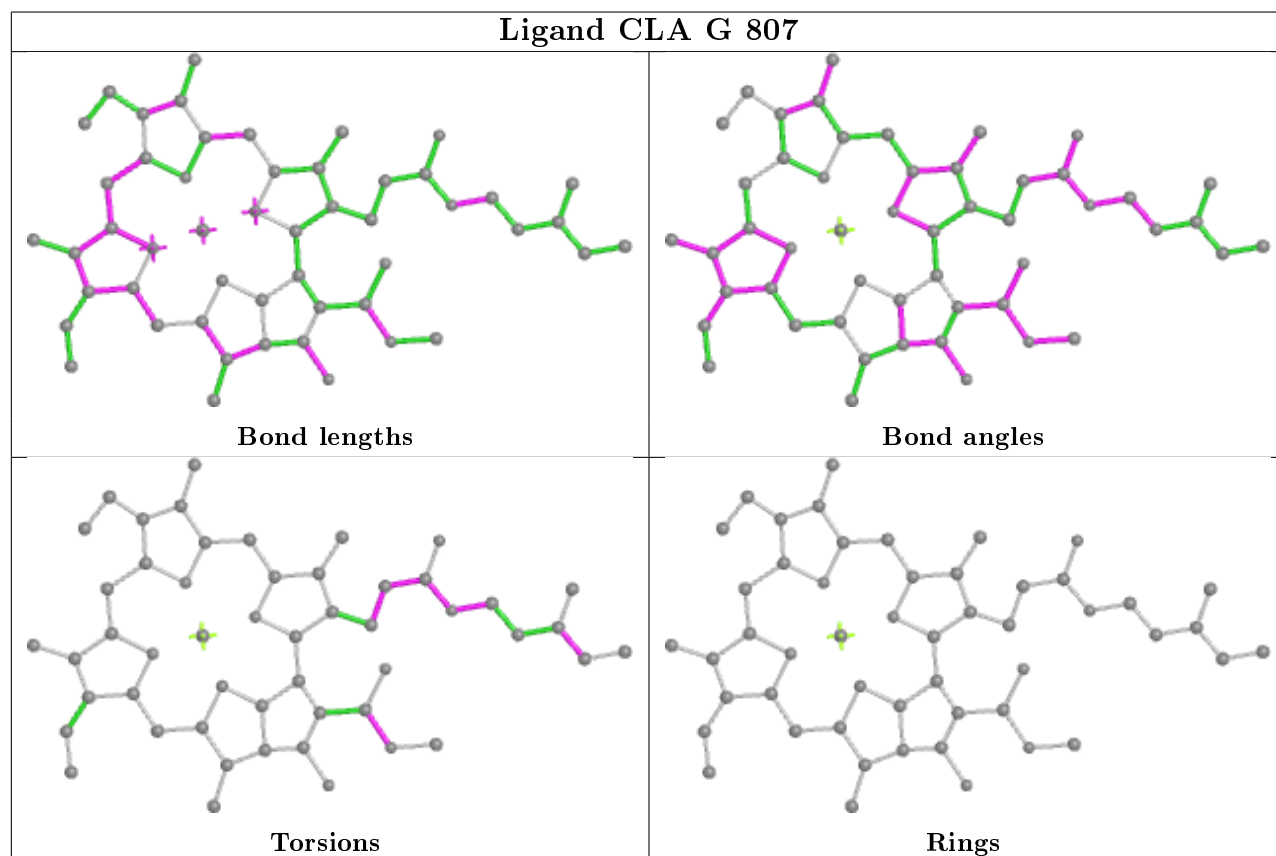
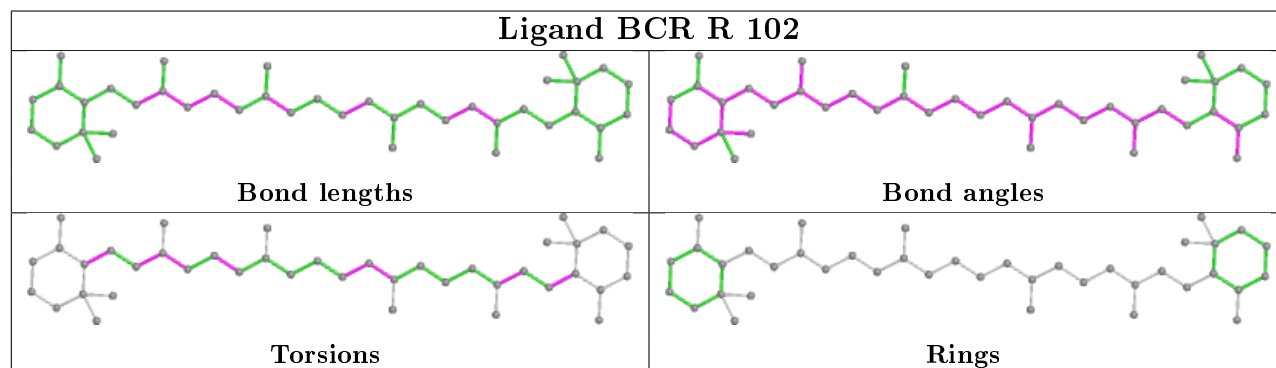
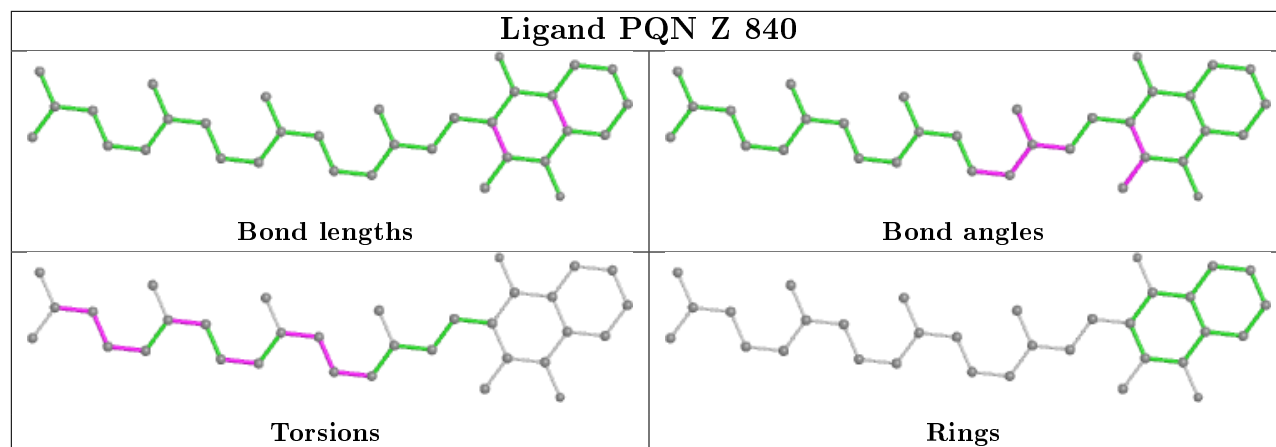


Ligand CLA Y 831

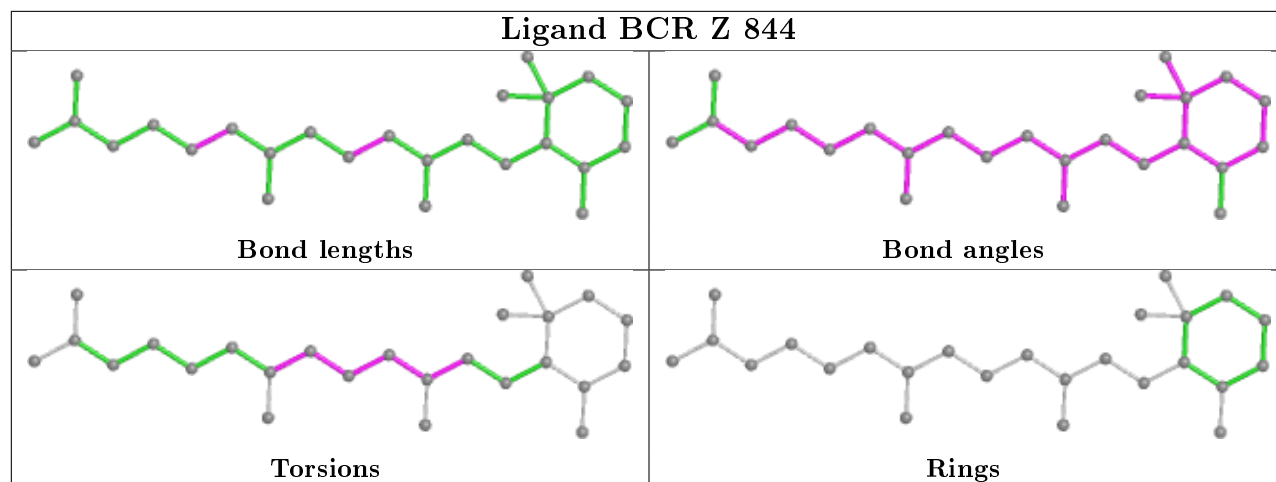


Ligand CLA Z 805

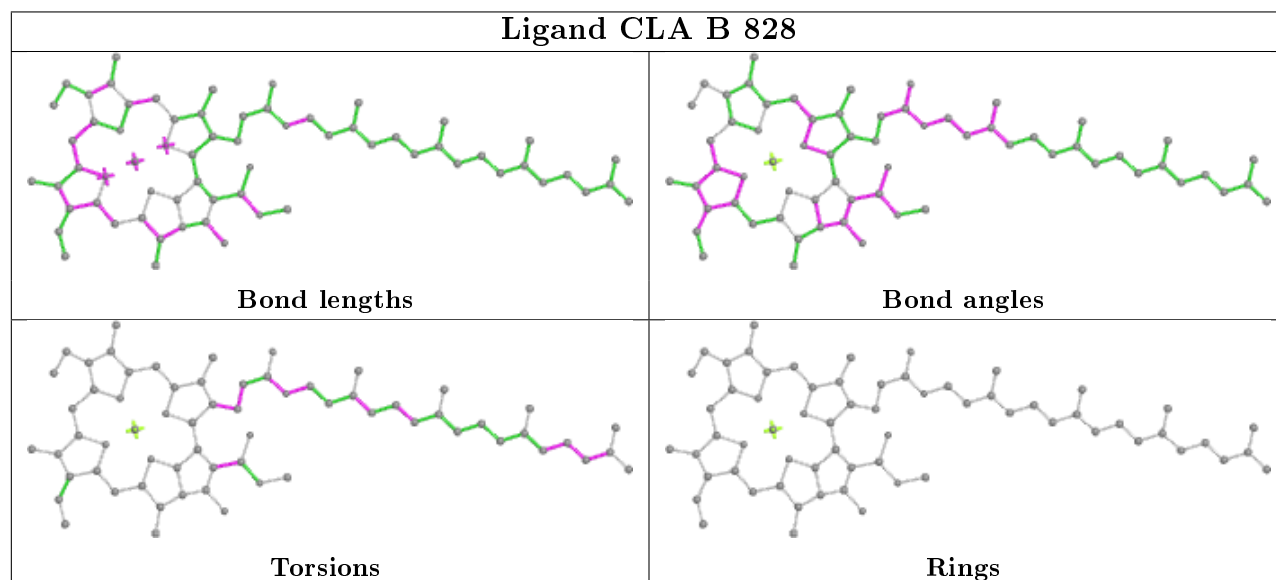




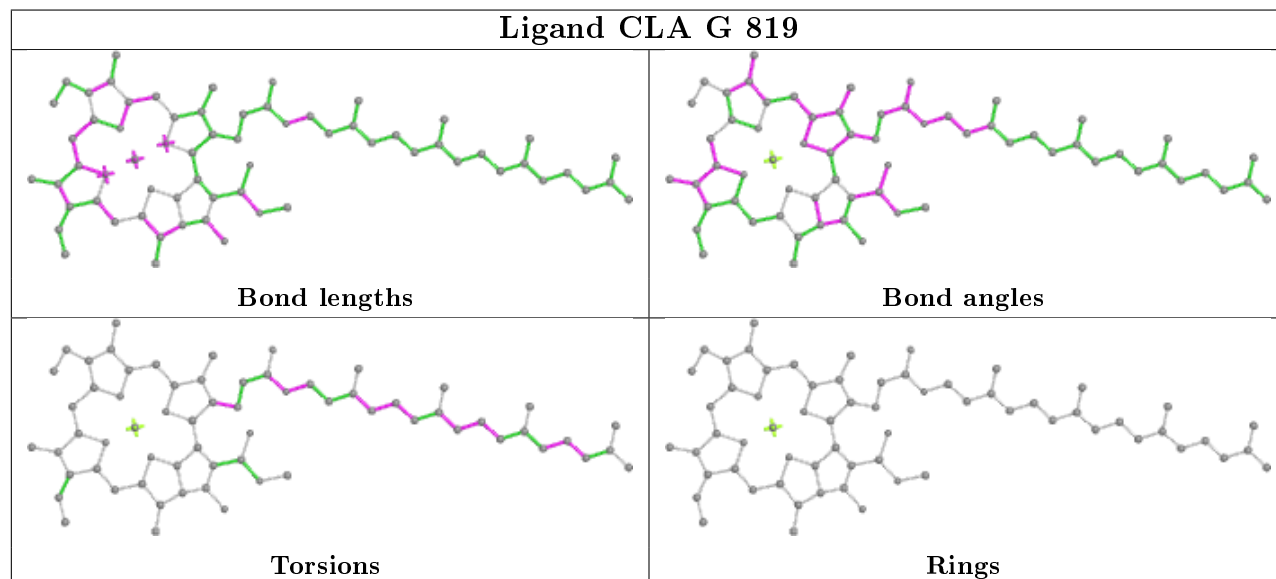
Ligand BCR Z 844



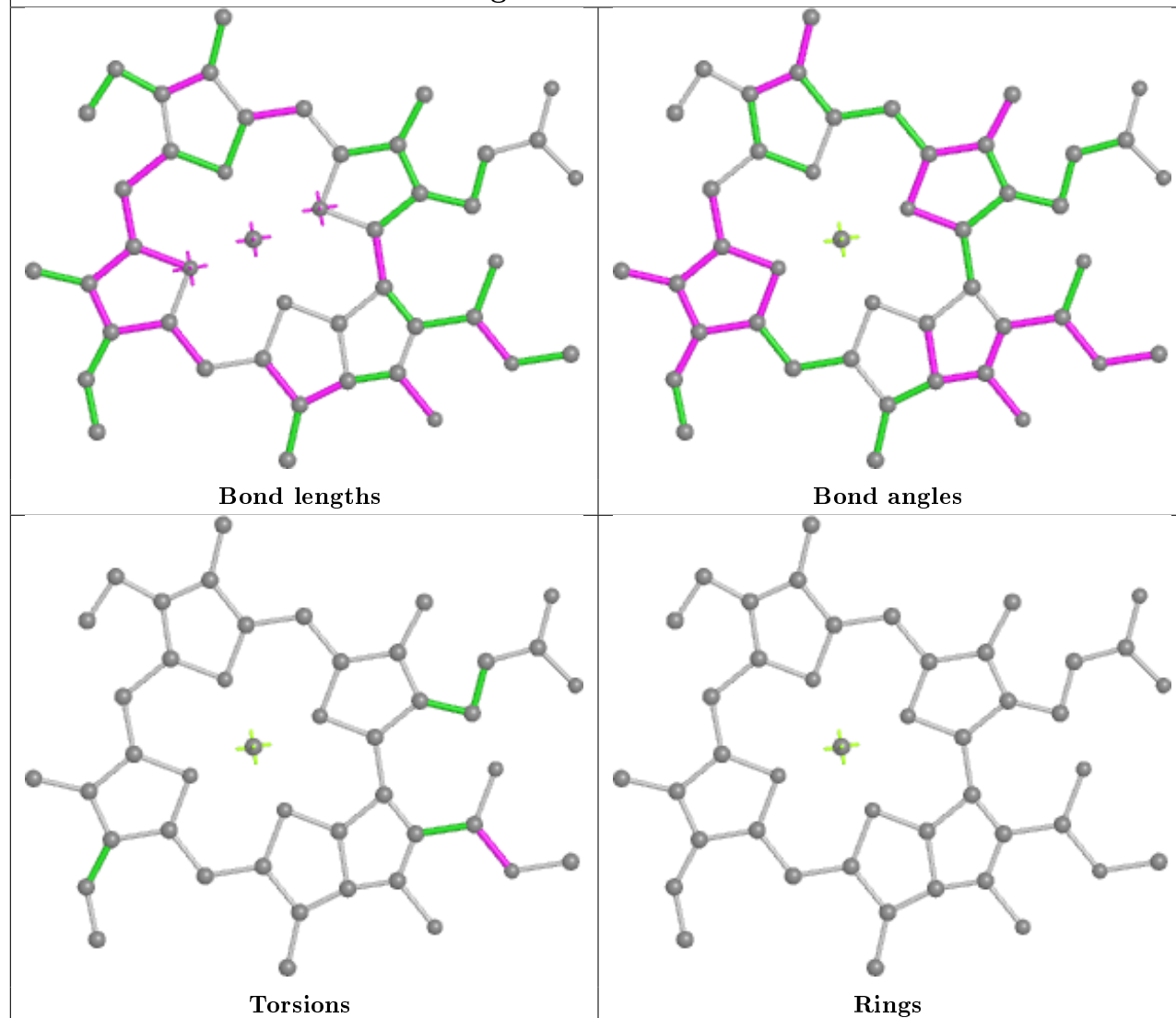
Ligand CLA B 828



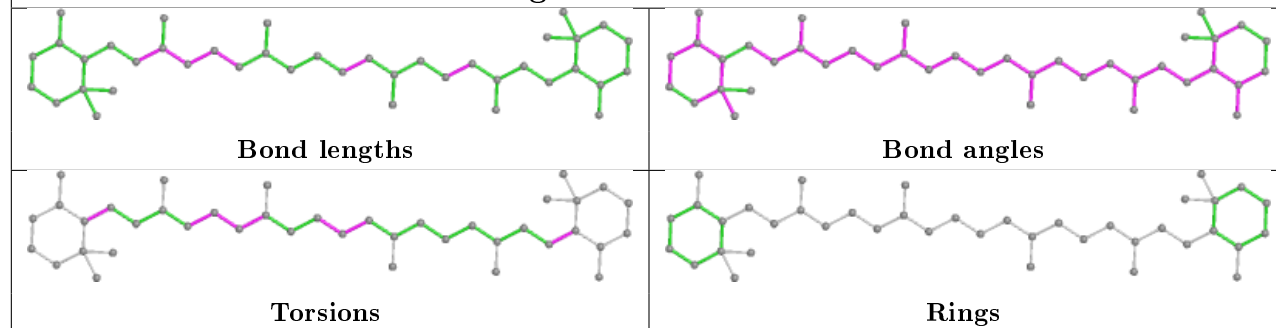
Ligand CLA G 819

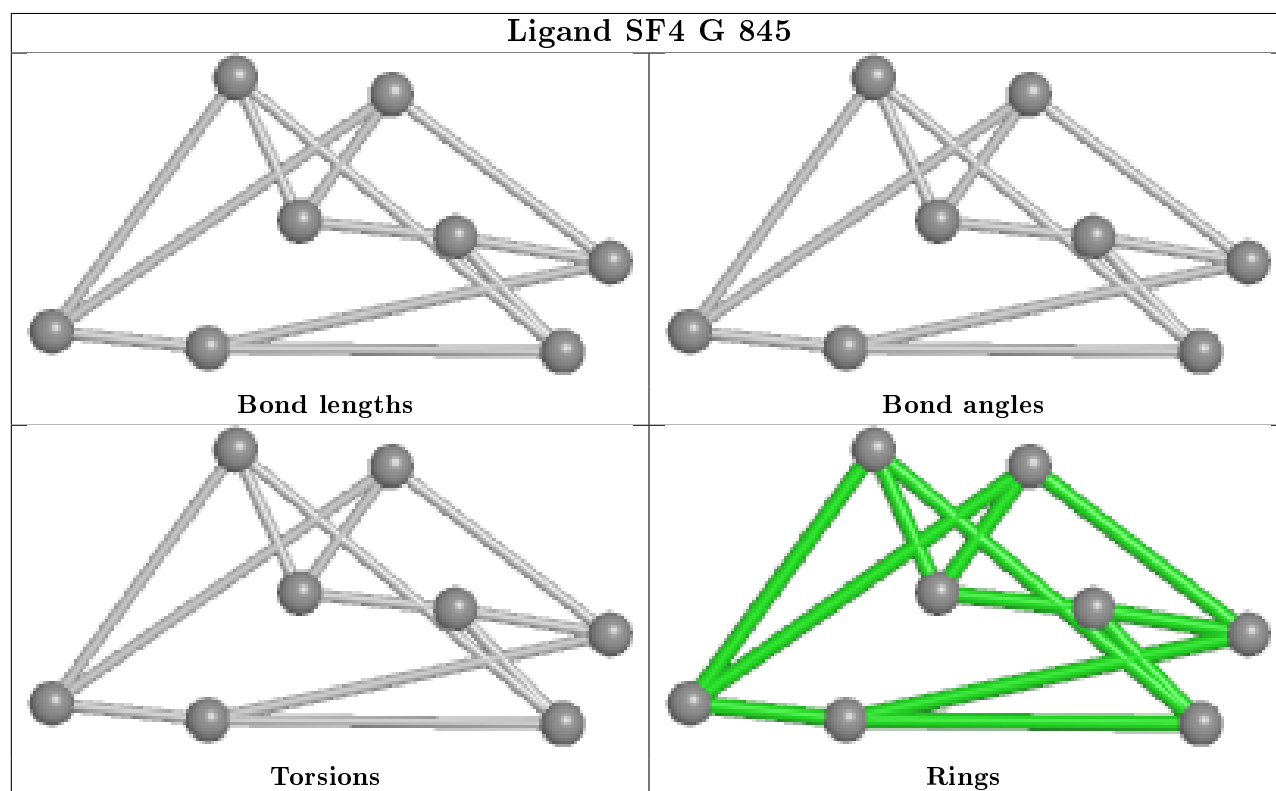
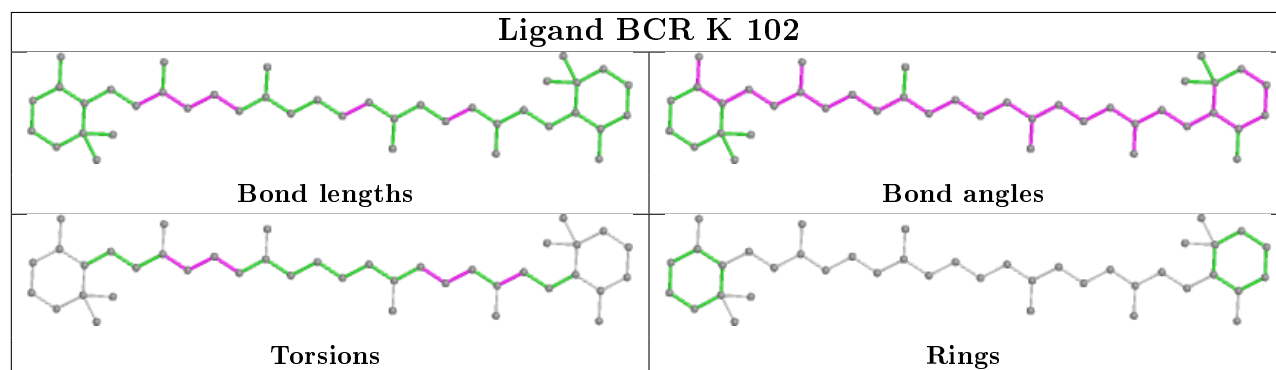
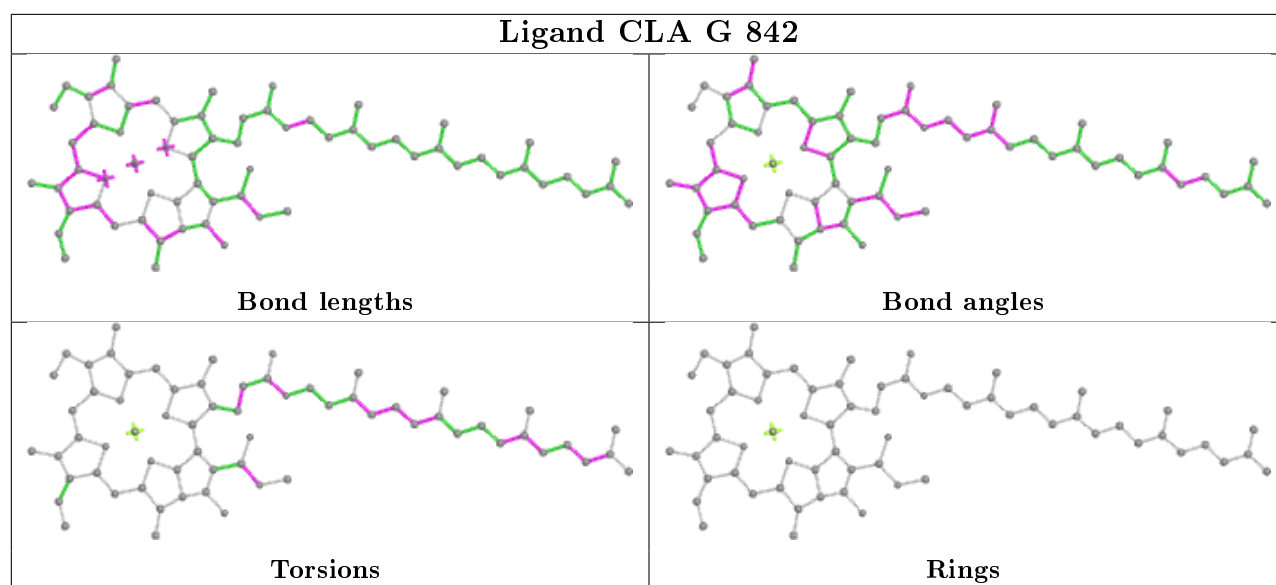


Ligand CLA B 835

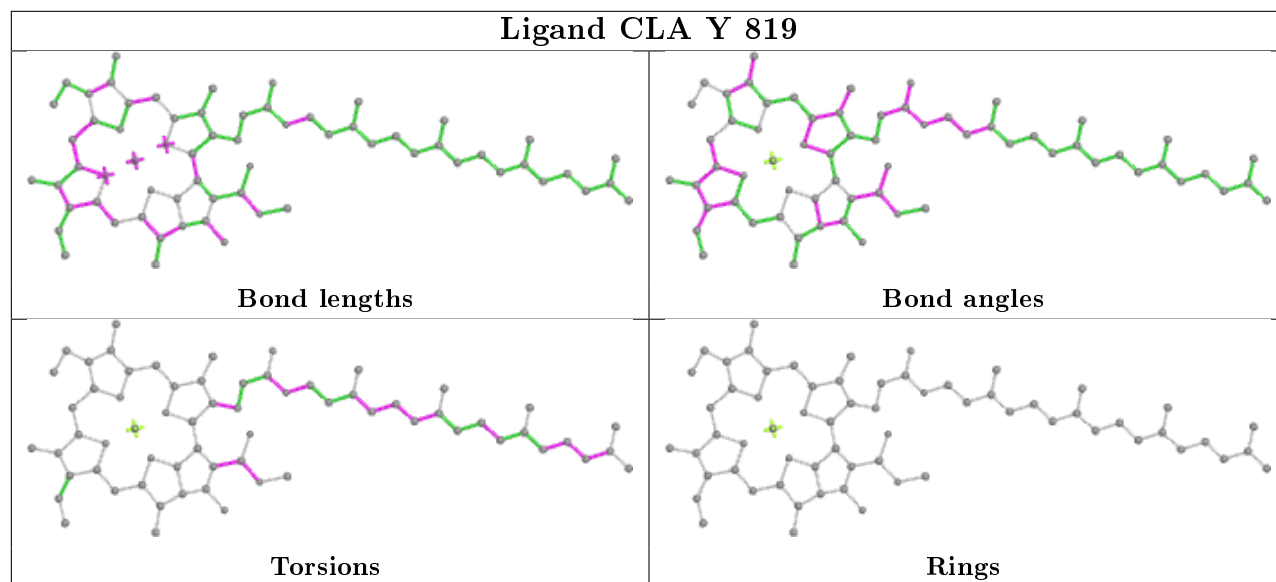


Ligand BCR H 848

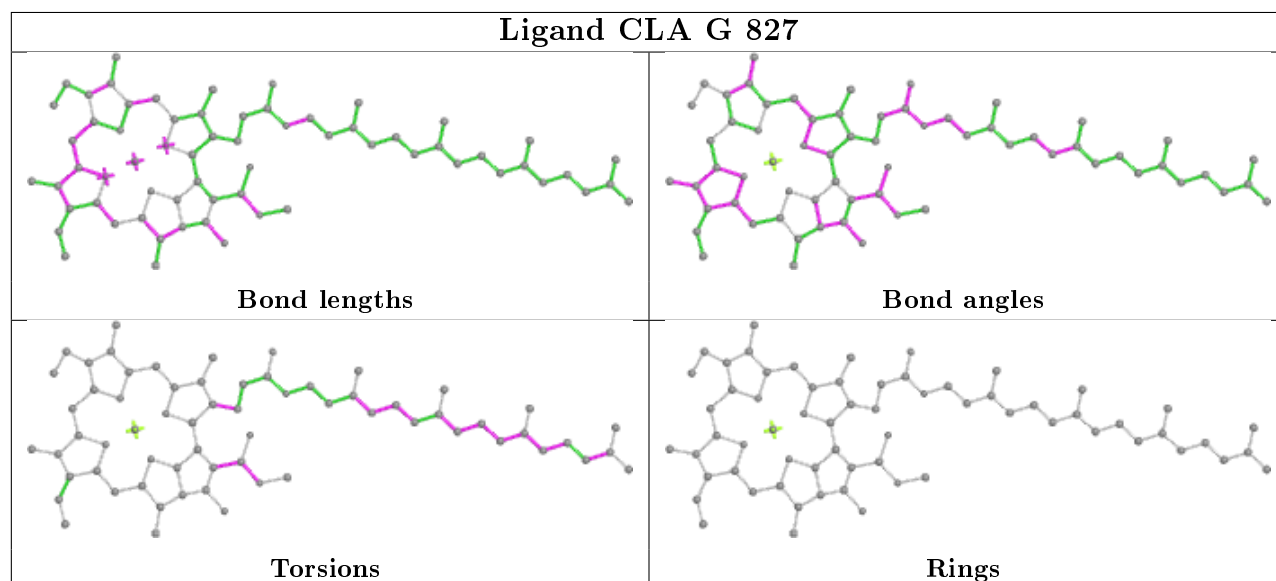


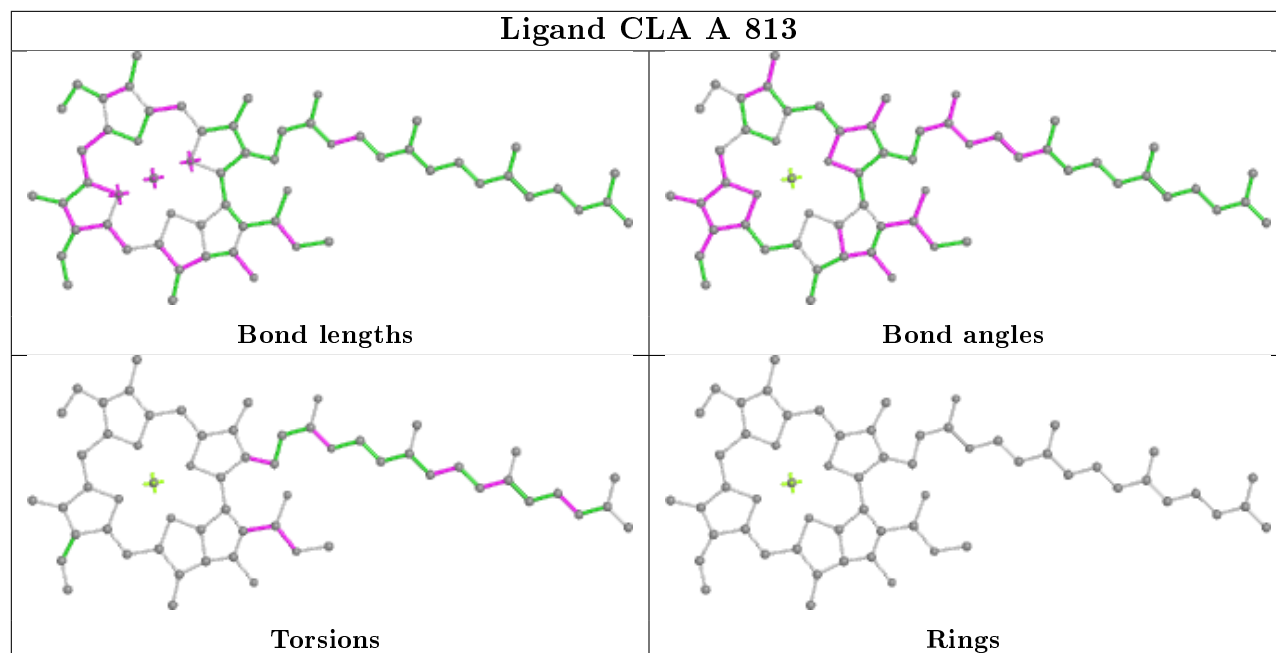
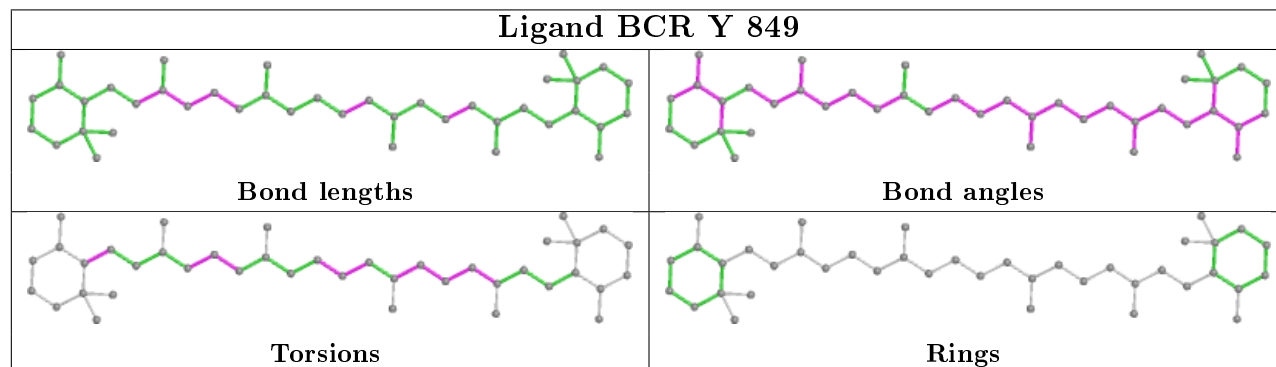


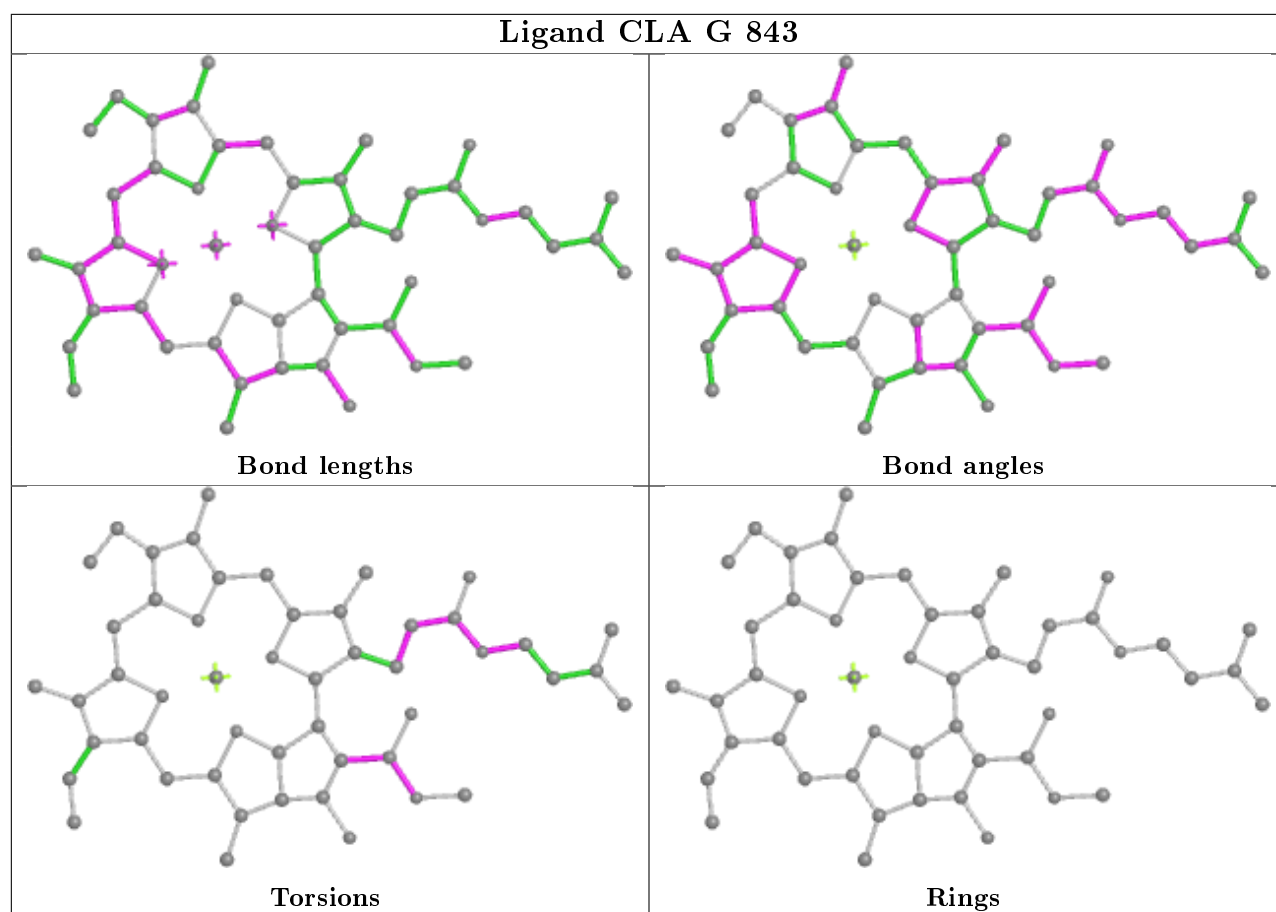
Ligand CLA Y 819



Ligand CLA G 827



Ligand CLA A 813**Ligand BCR Y 849**



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

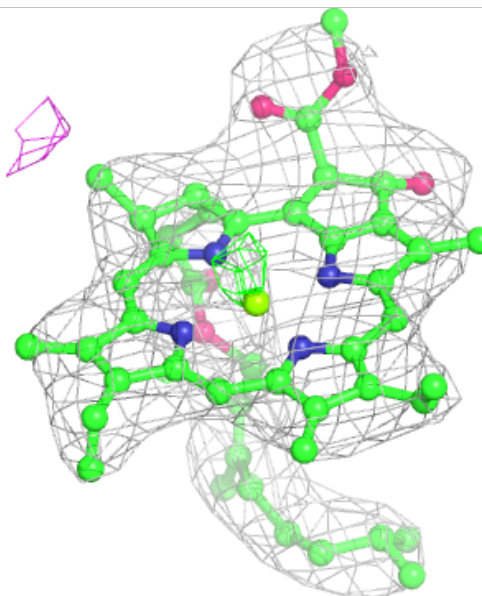
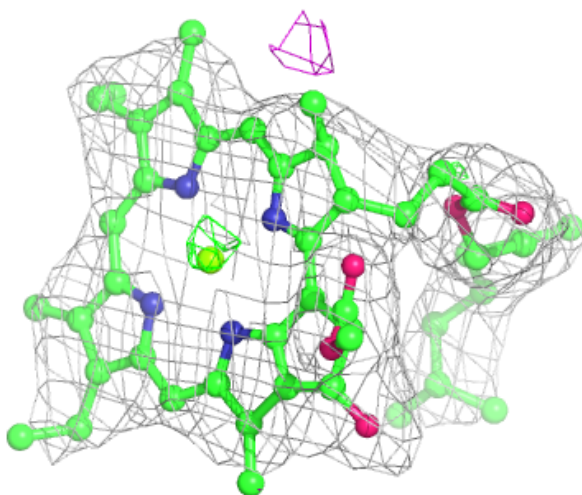
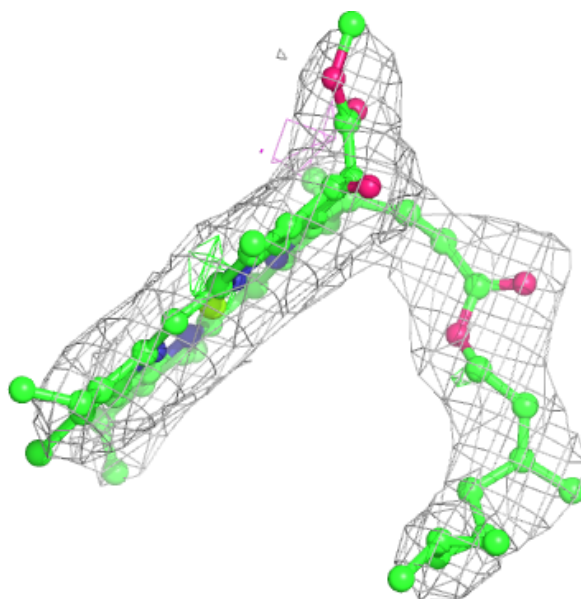
6.4 Ligands

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

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

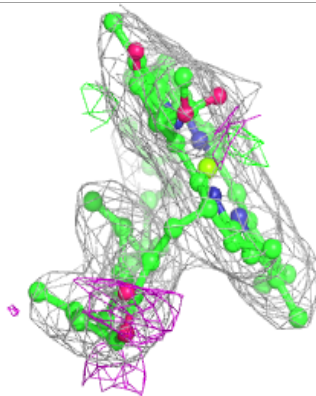
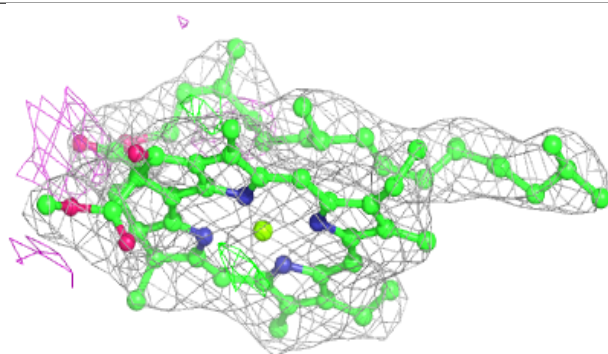
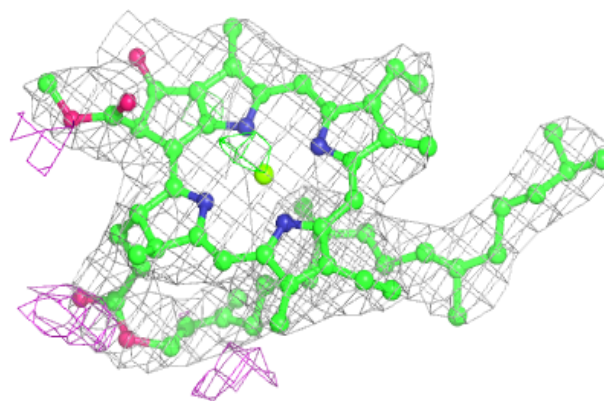
Electron density around CLA B 811:

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

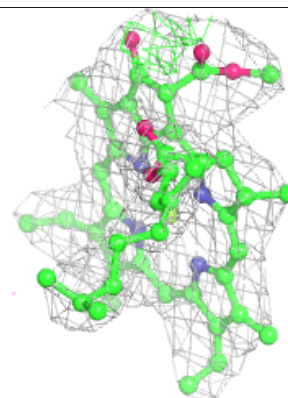
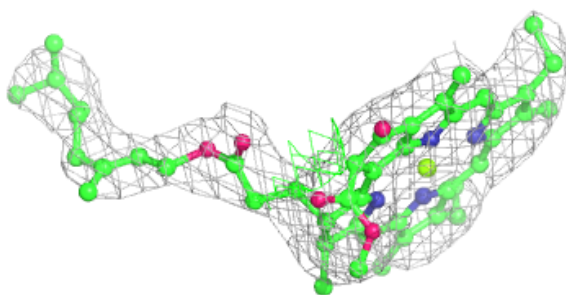
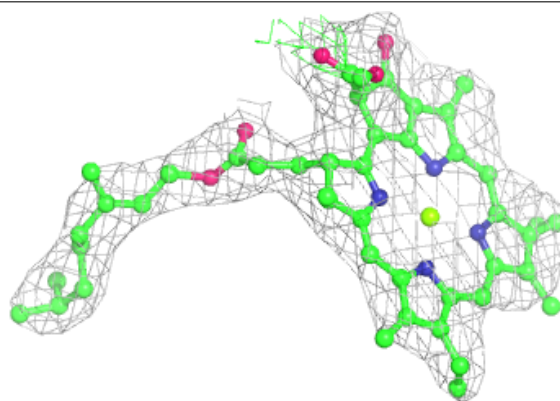


Electron density around CLA B 817:

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

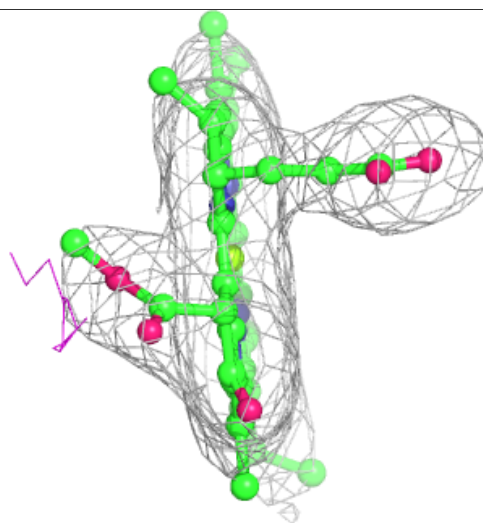
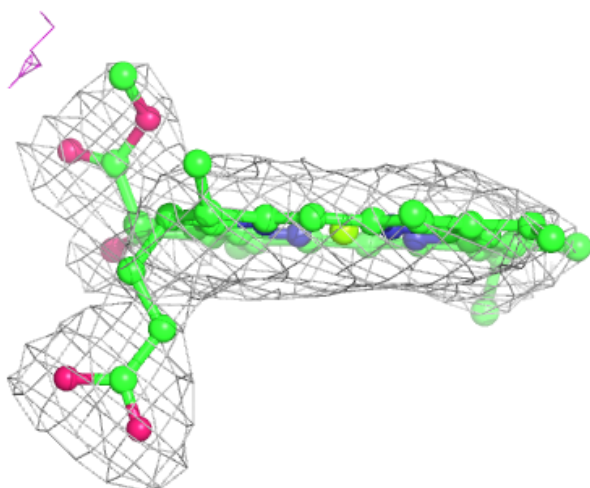
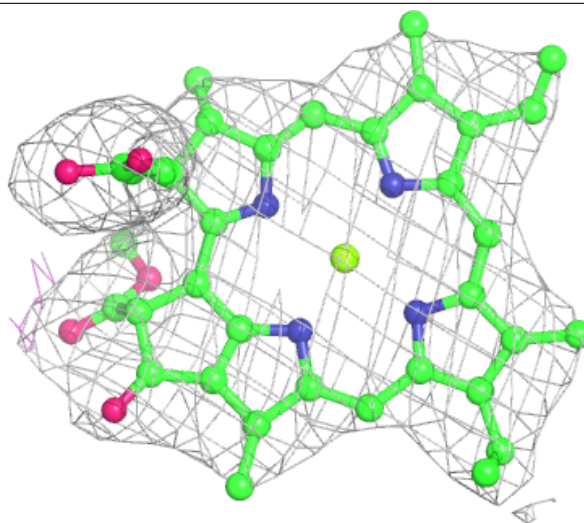
**Electron density around CLA B 833:**

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



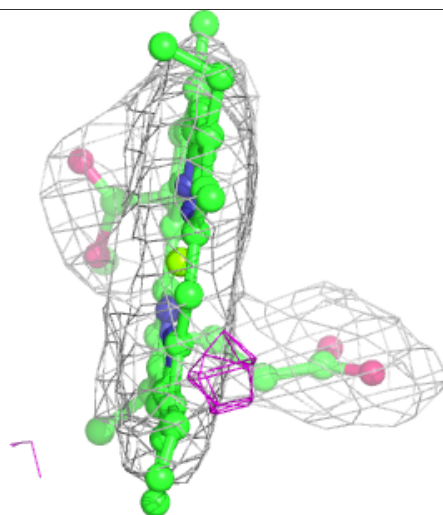
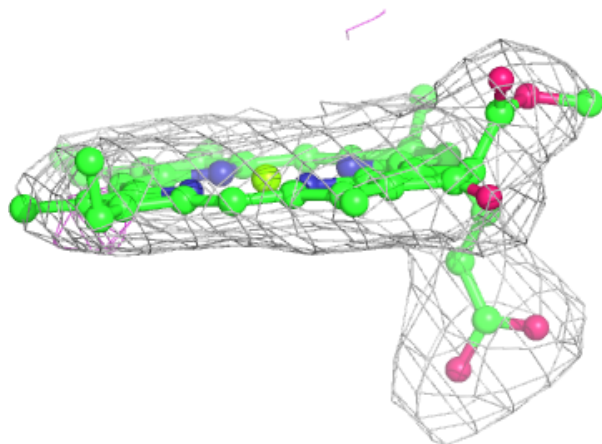
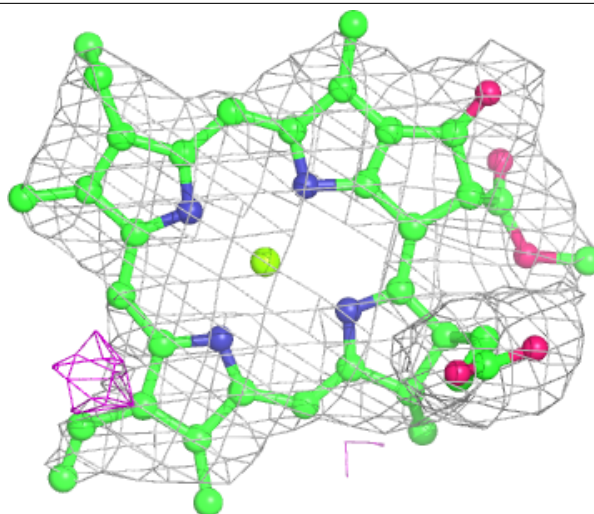
Electron density around CLA H 820:

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



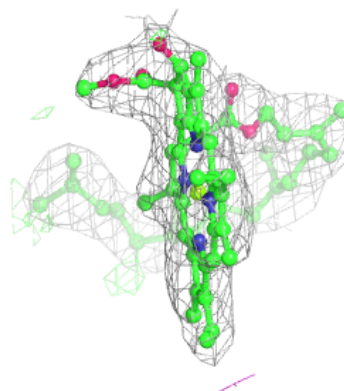
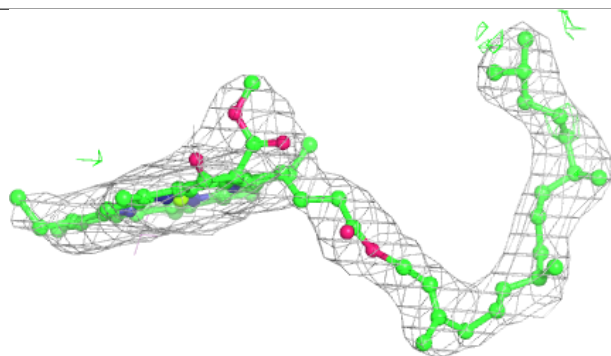
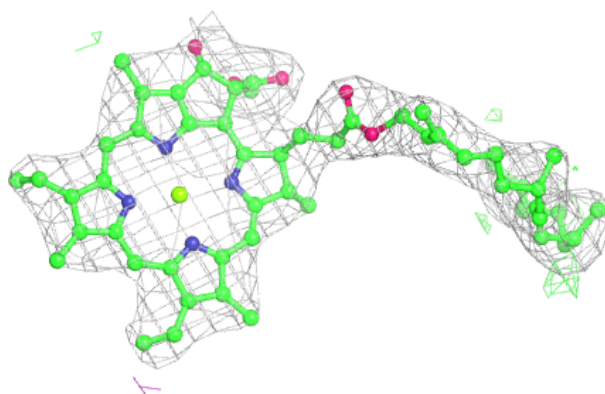
Electron density around CLA Y 810:

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

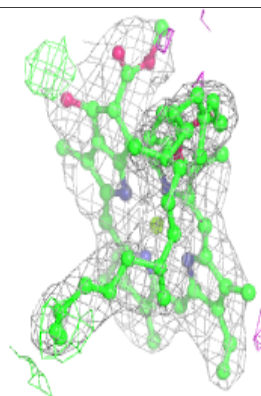
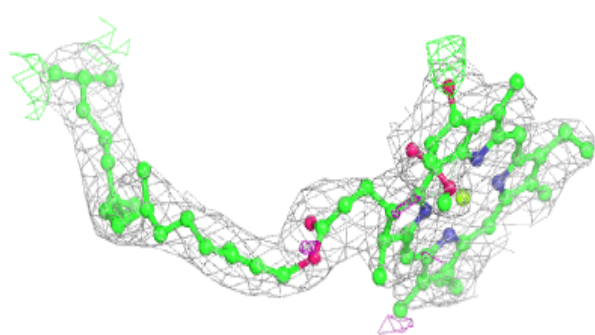
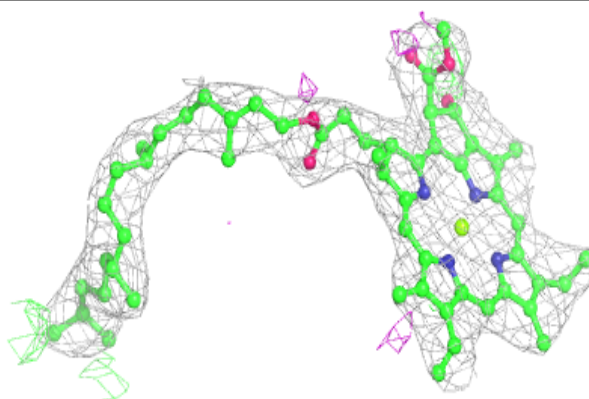


Electron density around CLA Y 827:

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

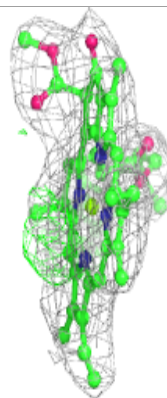
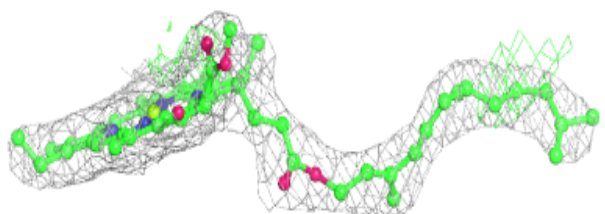
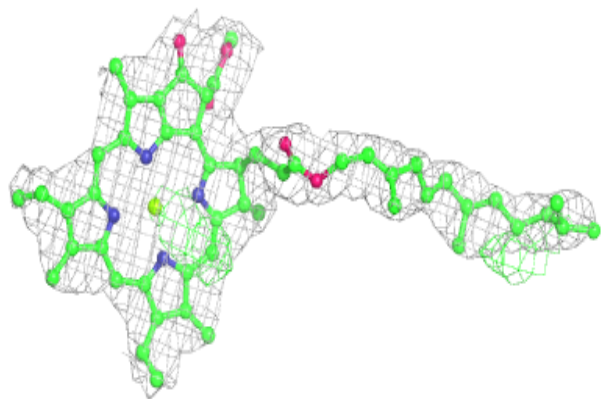
**Electron density around CLA A 852:**

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

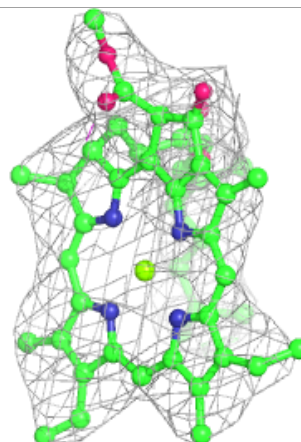
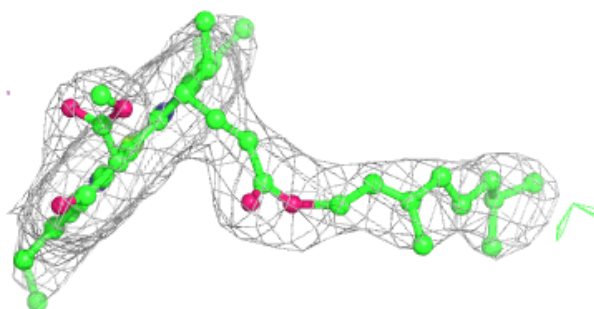
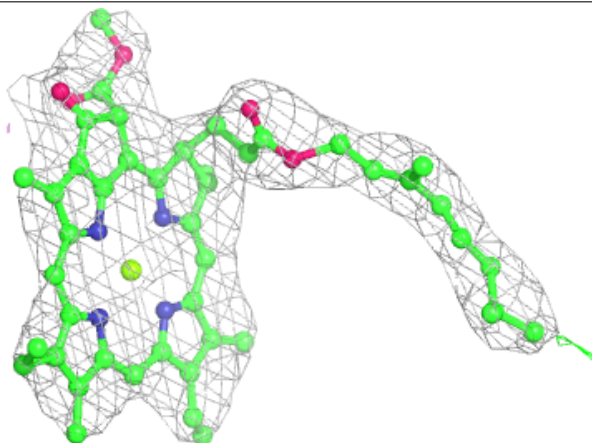


Electron density around CLA A 826:

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

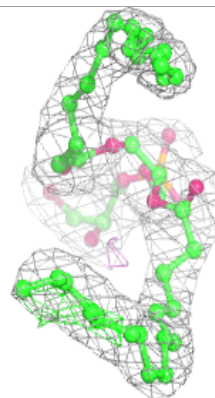
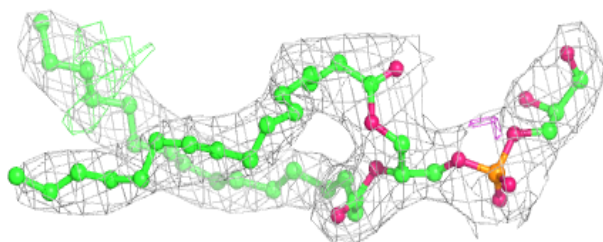
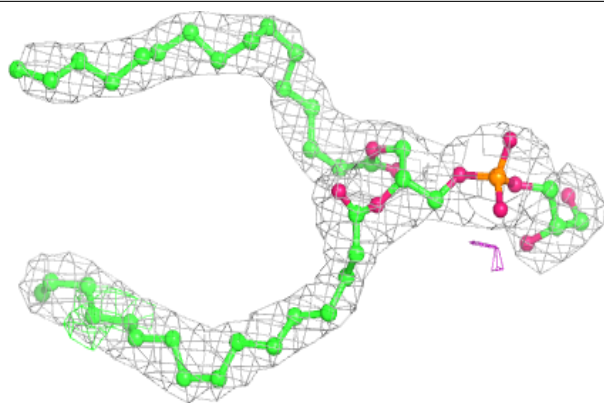
**Electron density around CLA Y 835:**

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

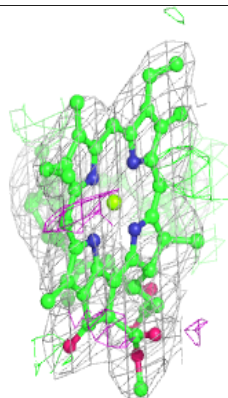
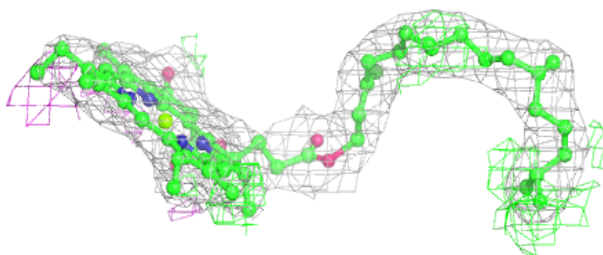
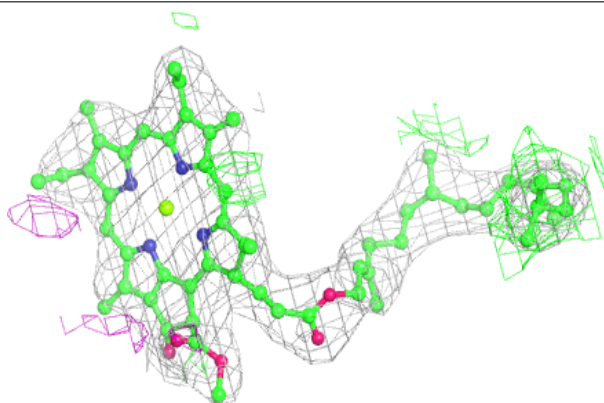


Electron density around LHG Y 852:

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

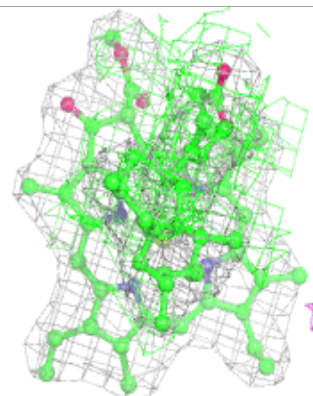
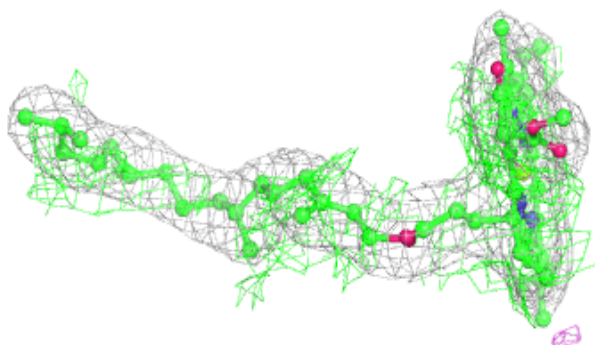
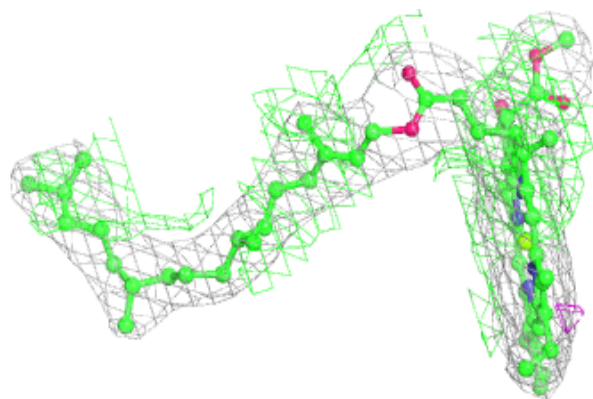
**Electron density around CLA Z 808:**

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

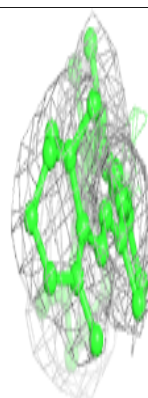
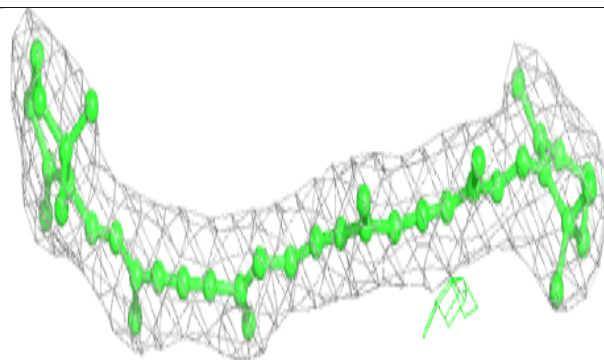
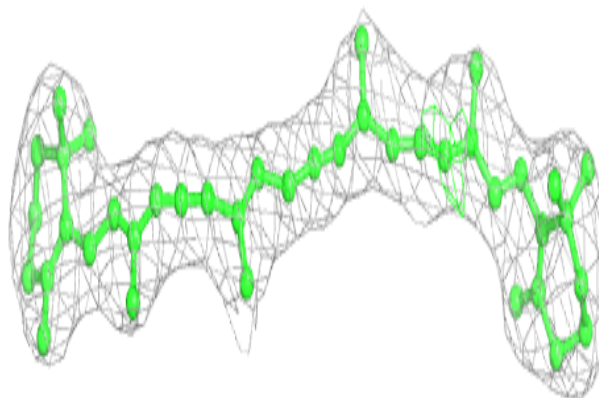


Electron density around CLA B 841:

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

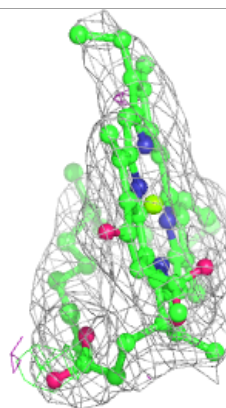
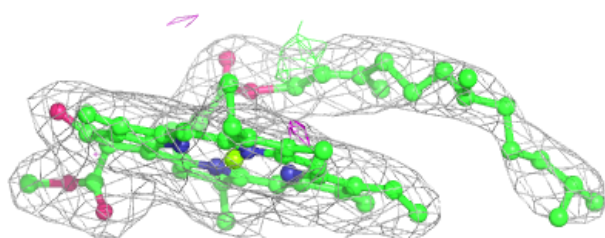
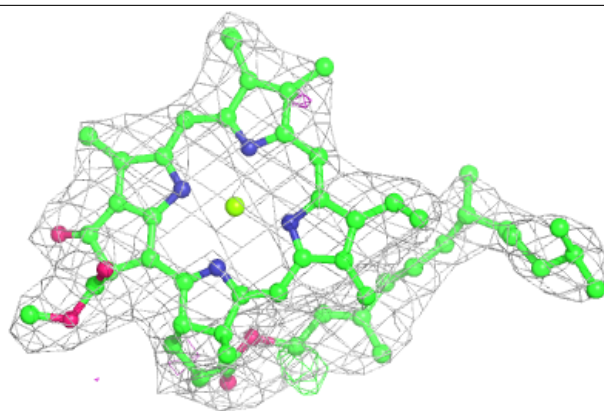
**Electron density around BCR M 101:**

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



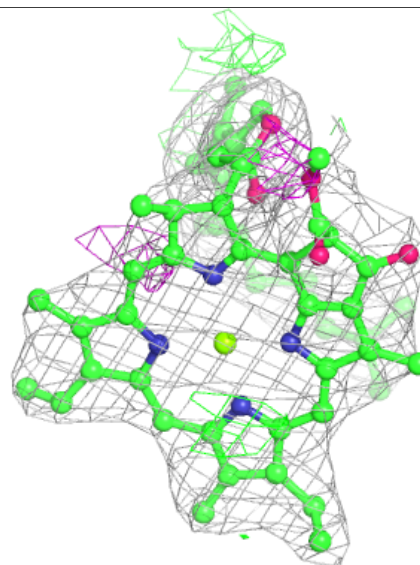
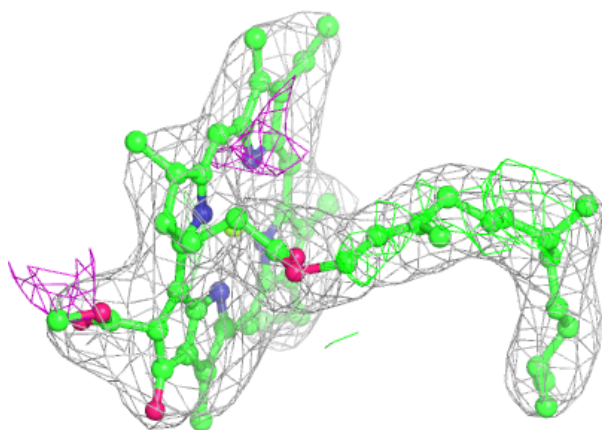
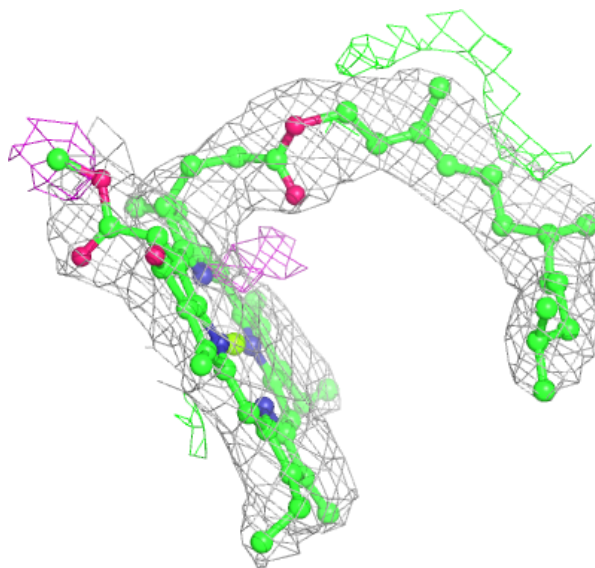
Electron density around CLA H 817:

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



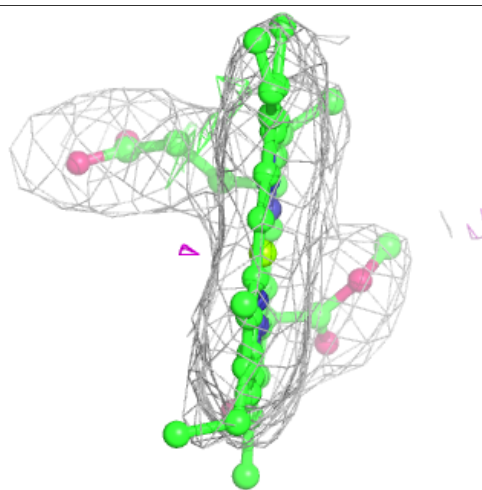
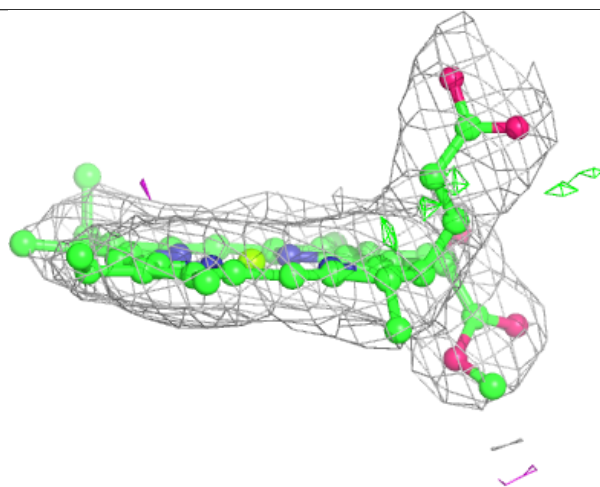
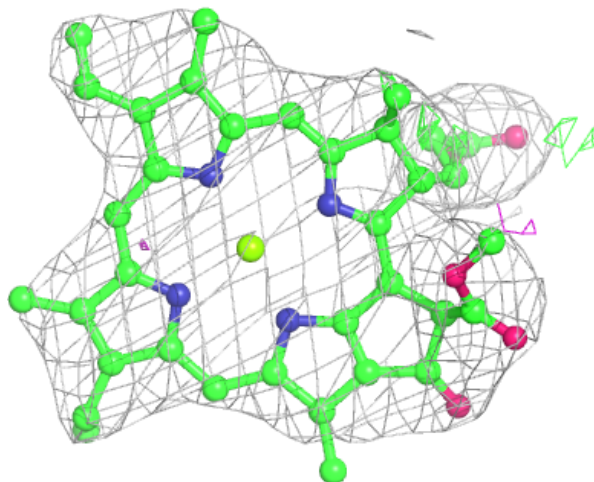
Electron density around CLA H 818:

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



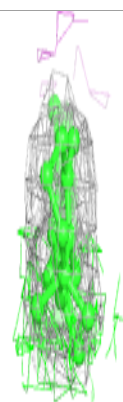
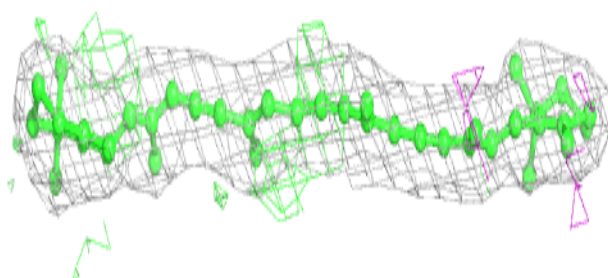
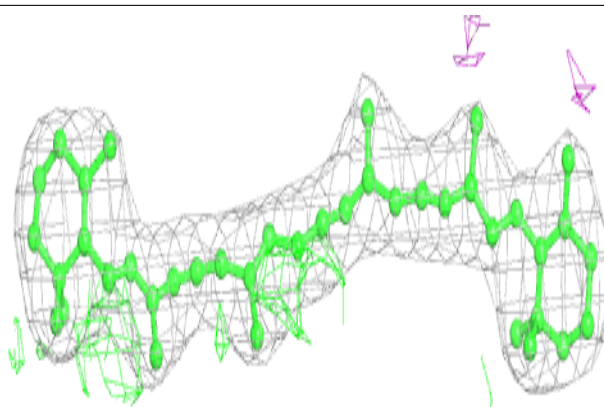
Electron density around CLA H 831:

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

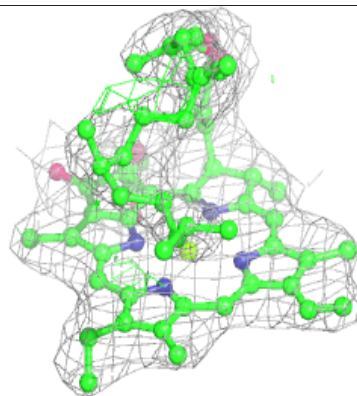
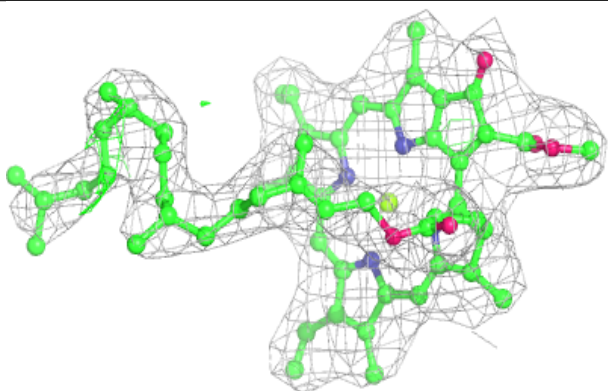
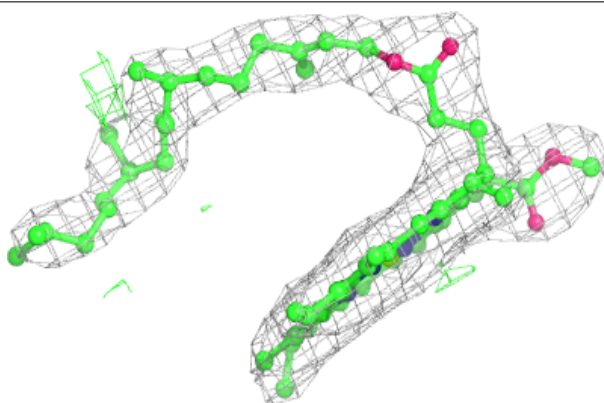


Electron density around BCR U 1005:

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

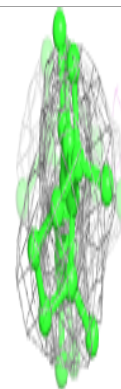
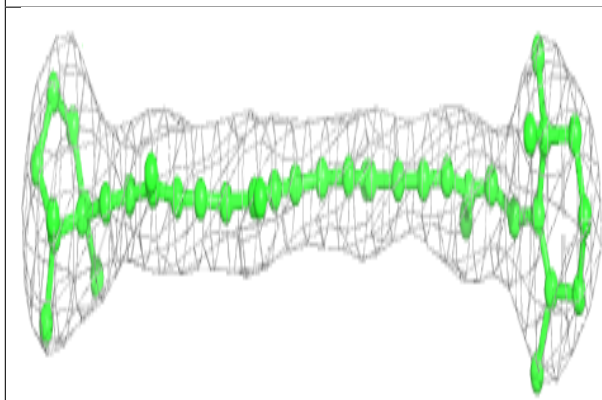
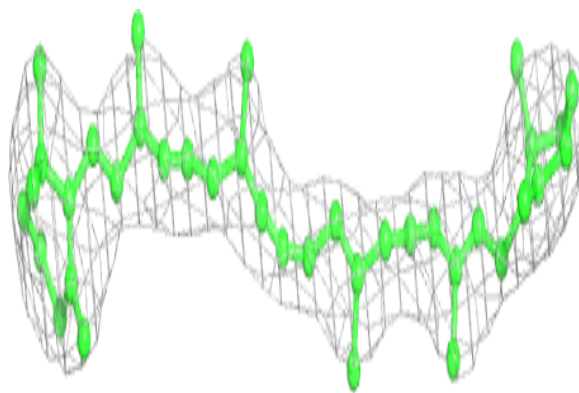
**Electron density around CLA A 832:**

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



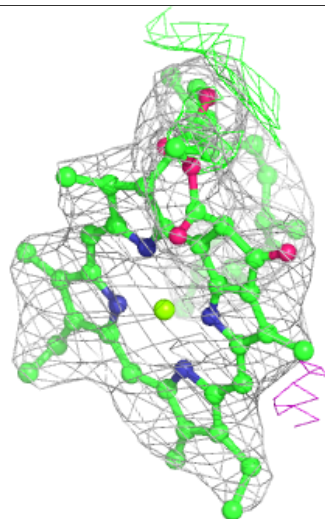
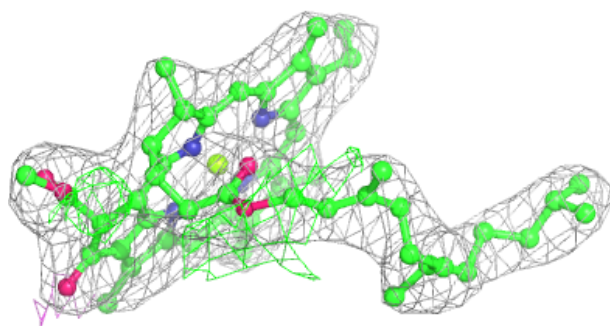
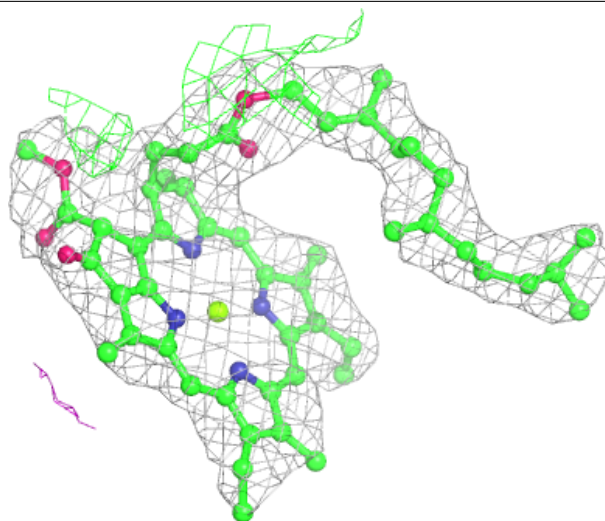
Electron density around BCR G 846:

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



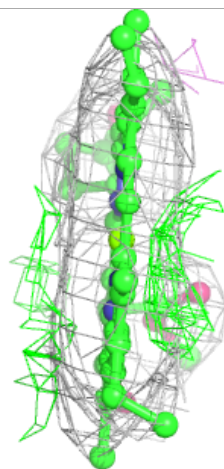
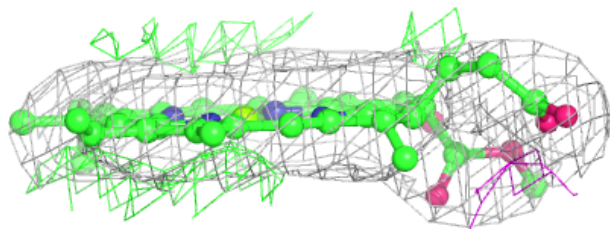
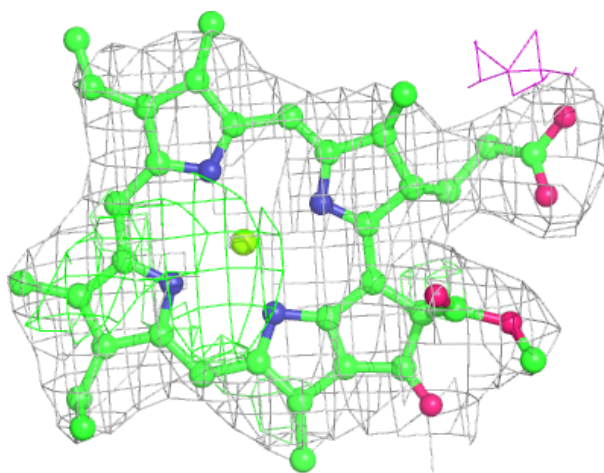
Electron density around CLA G 824:

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



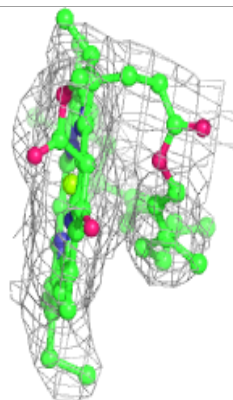
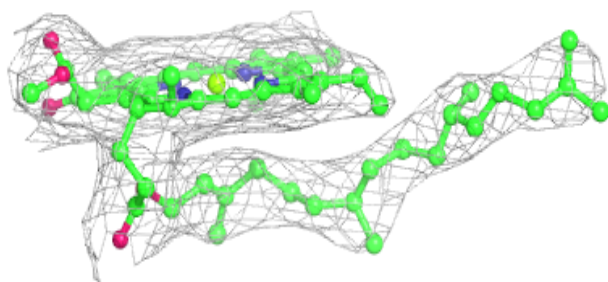
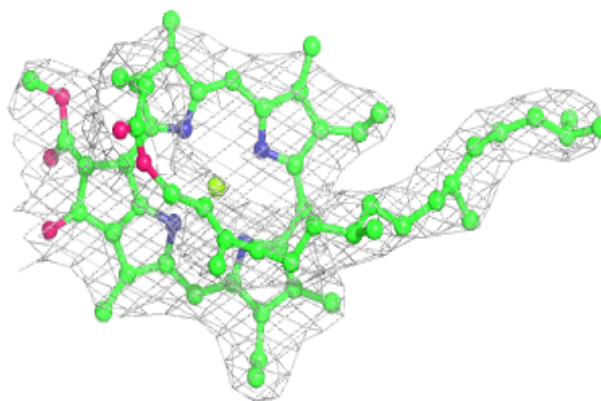
Electron density around CLA d 202:

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

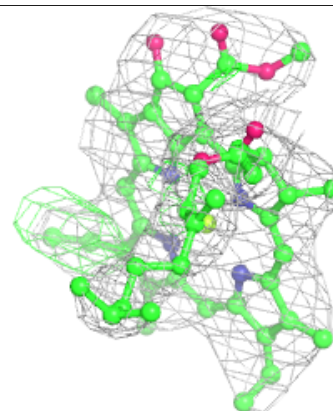
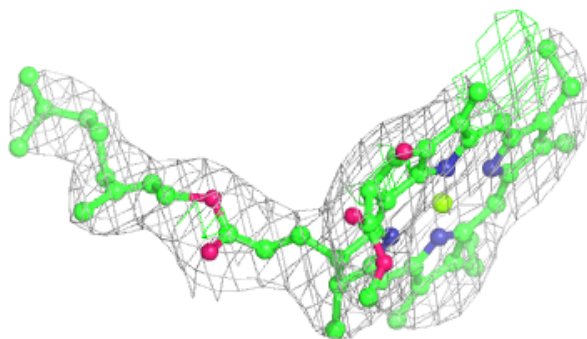
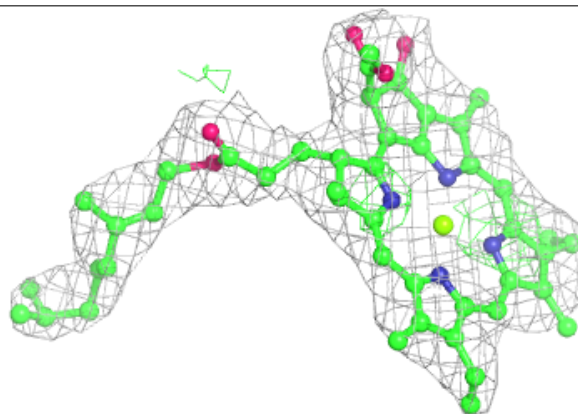


Electron density around CLA B 802:

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

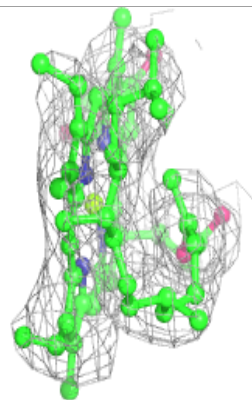
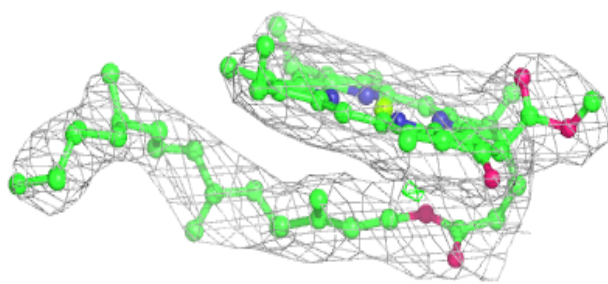
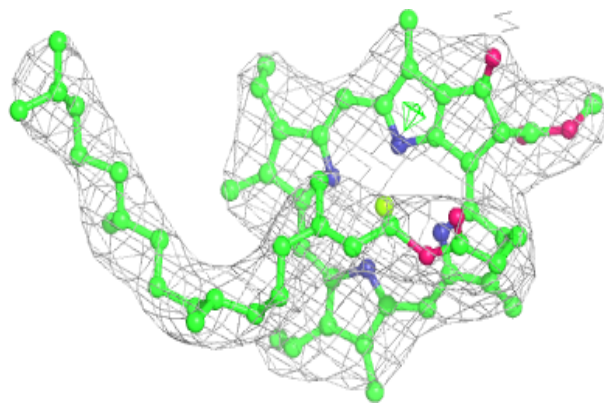
**Electron density around CLA Z 831:**

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

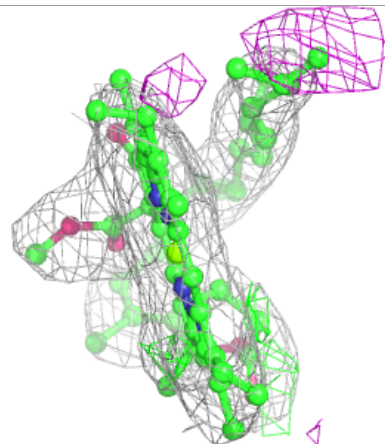
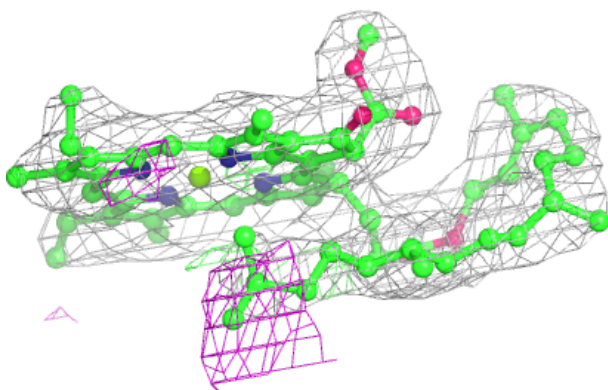
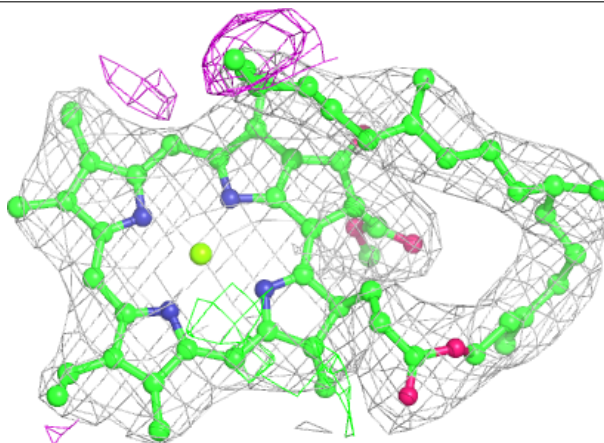


Electron density around CLA B 838:

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

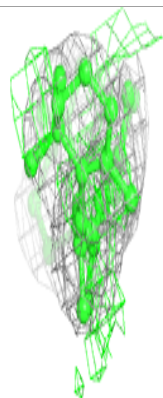
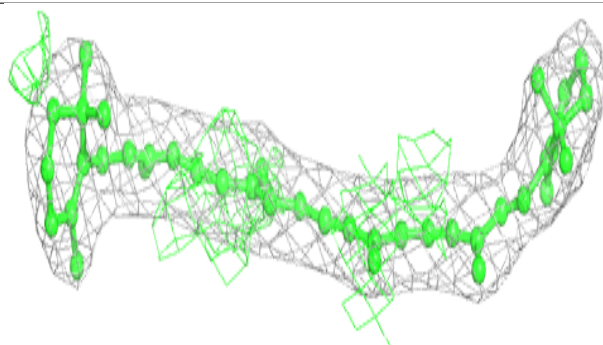
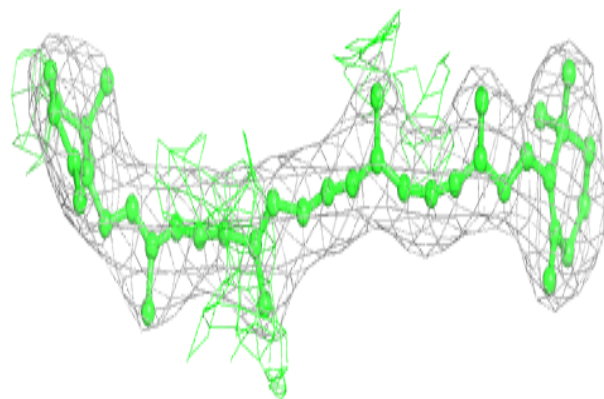
**Electron density around CLA H 804:**

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

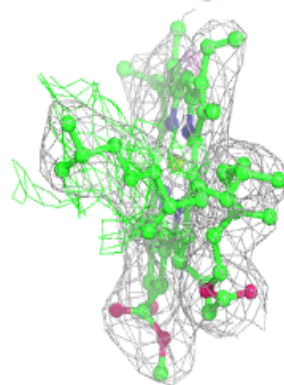
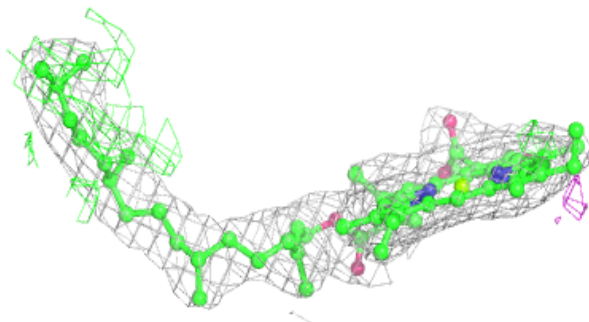
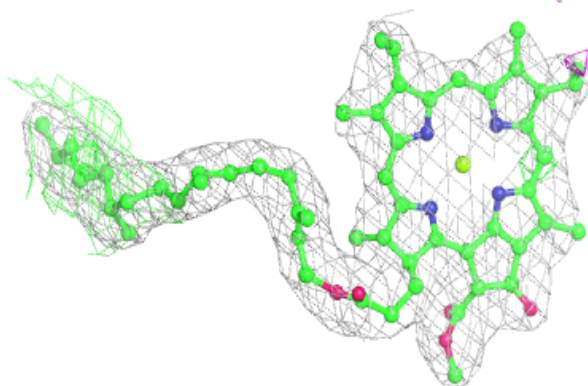


Electron density around BCR e 101:

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

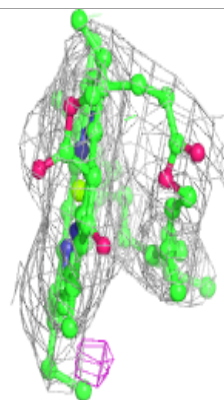
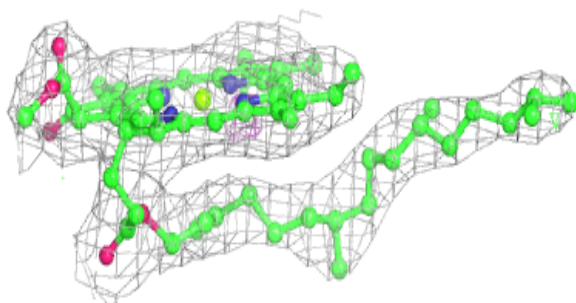
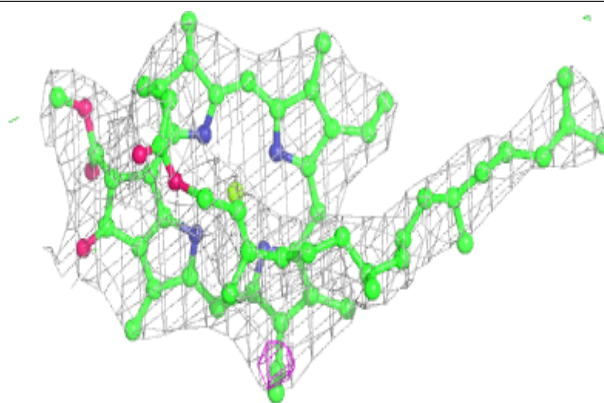
**Electron density around CLA Y 855:**

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

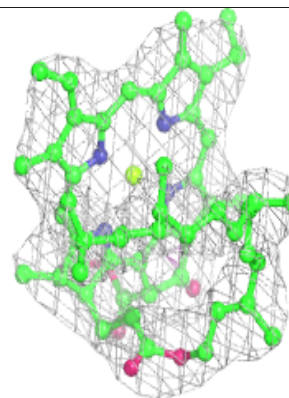
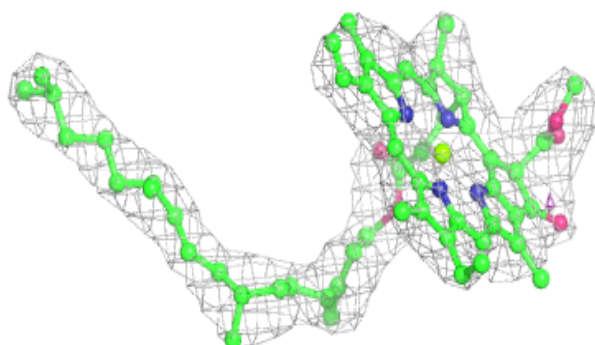
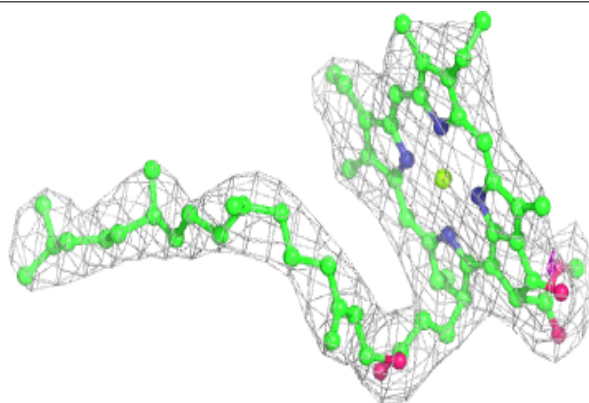


Electron density around CLA G 839:

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

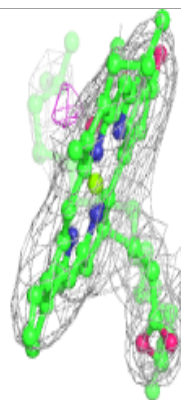
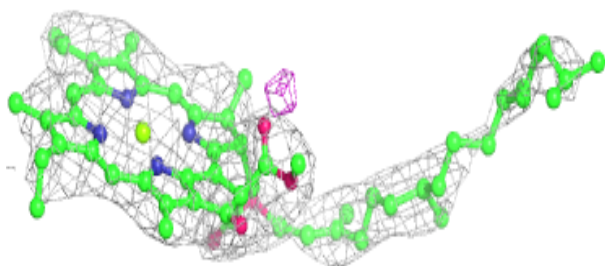
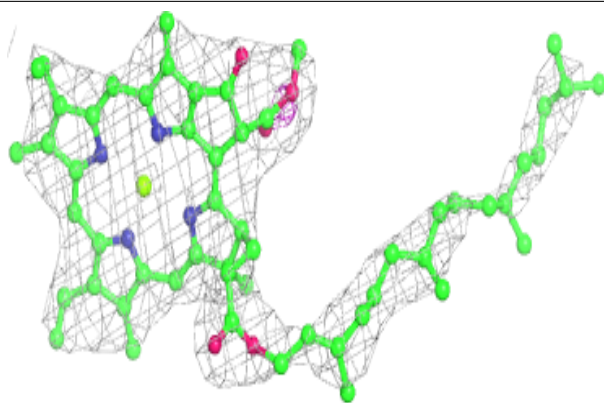
**Electron density around CLA H 813:**

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

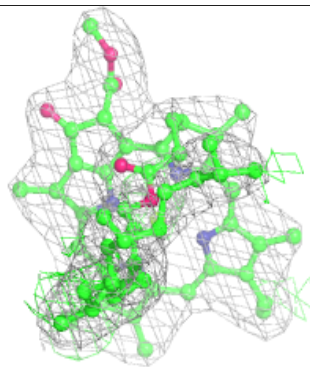
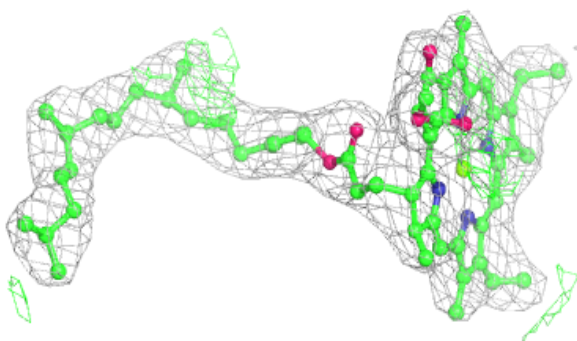


Electron density around CLA A 822:

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

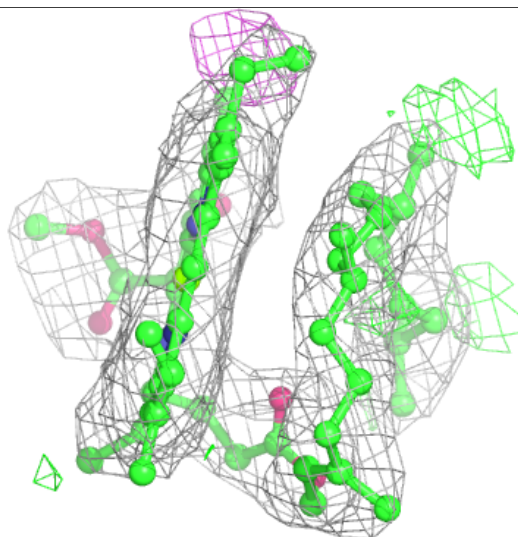
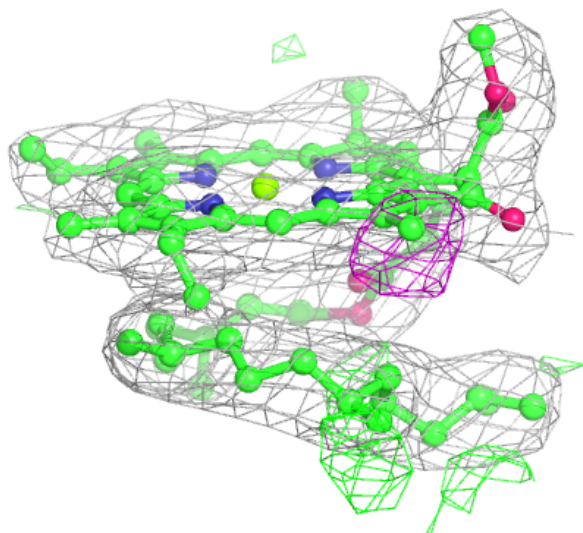
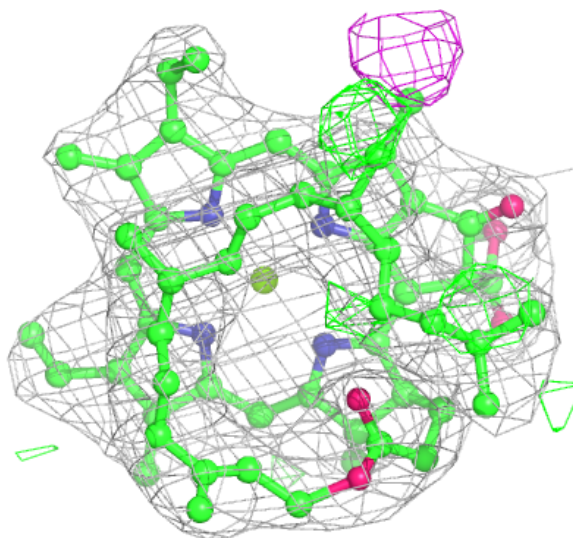
**Electron density around CLA H 837:**

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



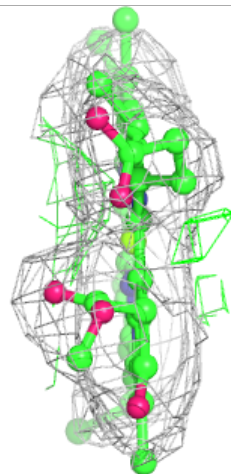
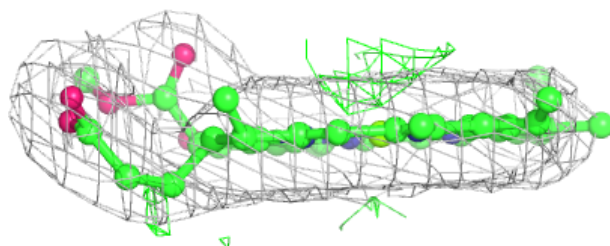
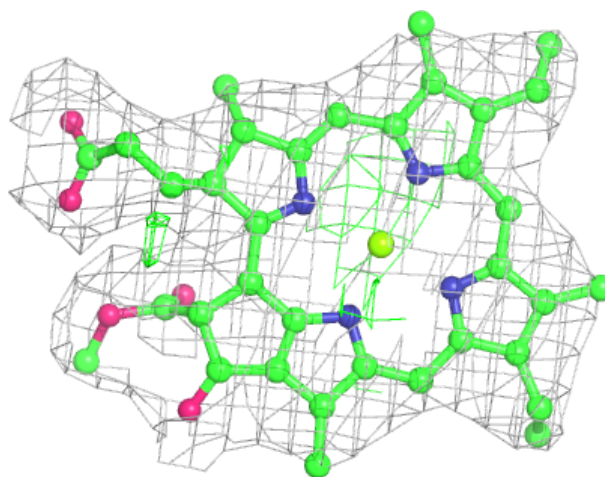
Electron density around CLA L 205:

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



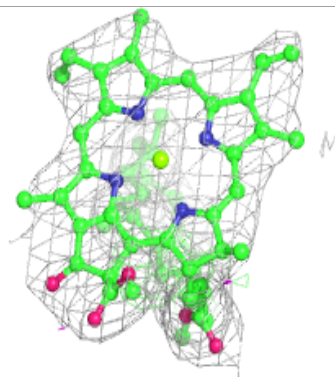
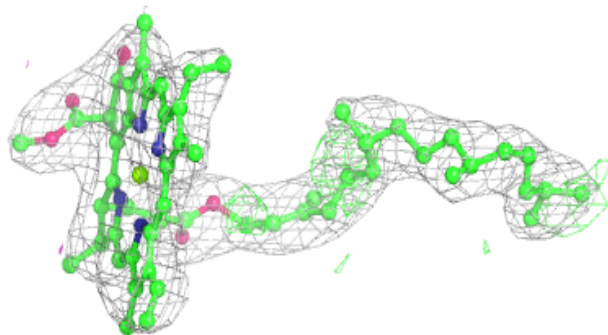
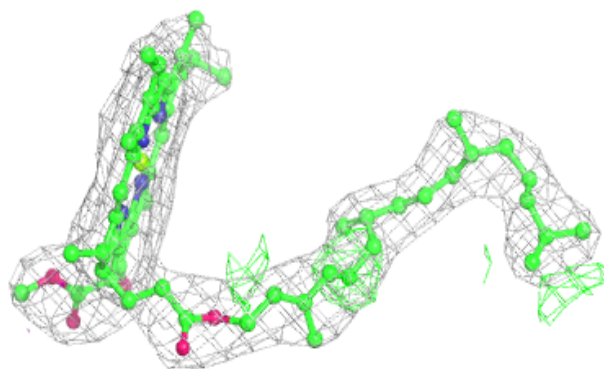
Electron density around CLA F 202:

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



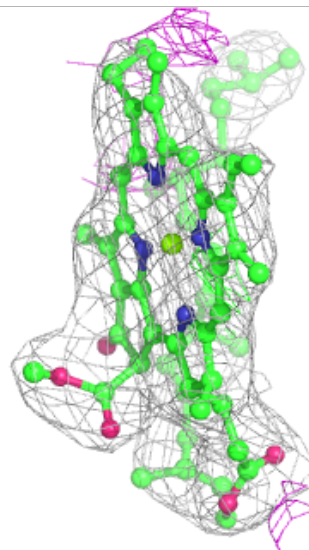
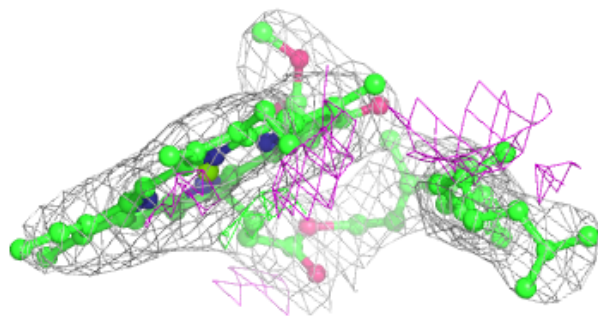
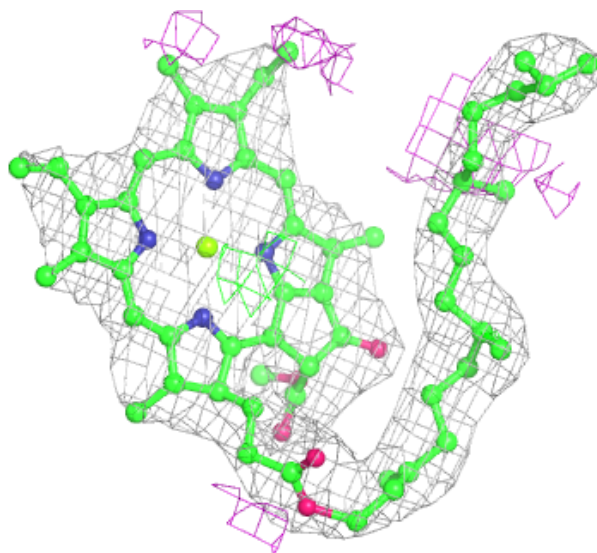
Electron density around CLA Y 830:

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



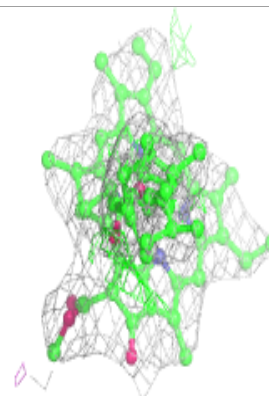
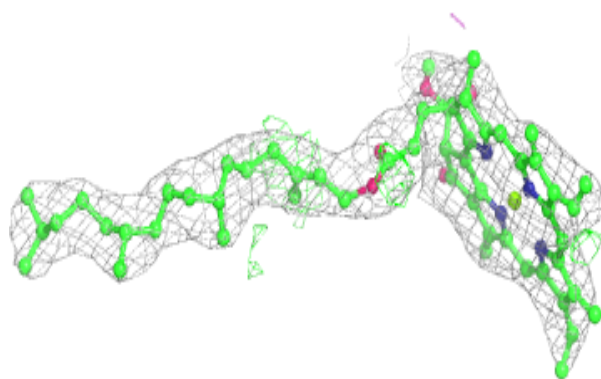
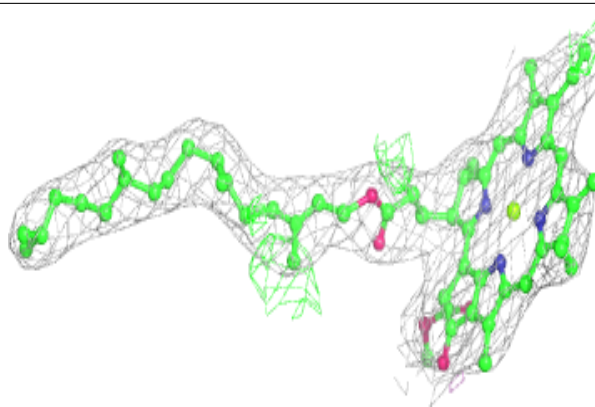
Electron density around CLA Y 825:

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



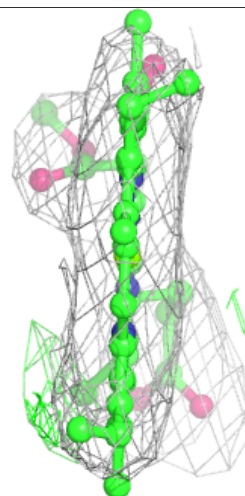
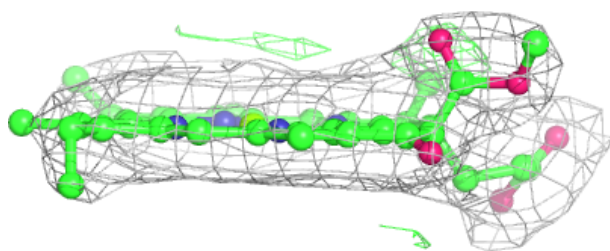
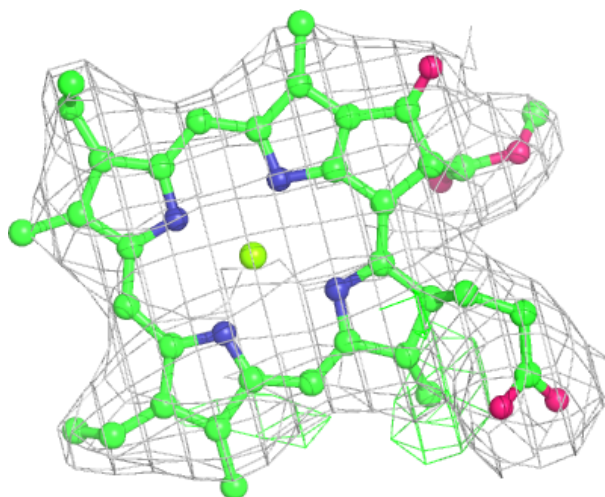
Electron density around CLA Y 809:

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



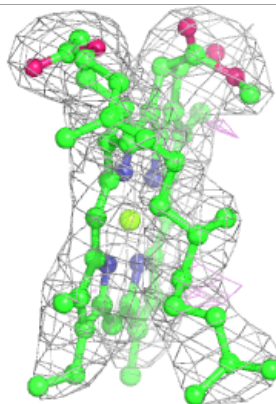
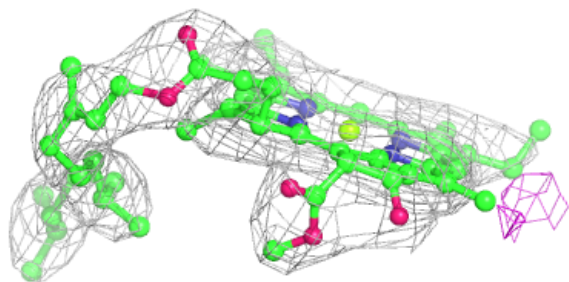
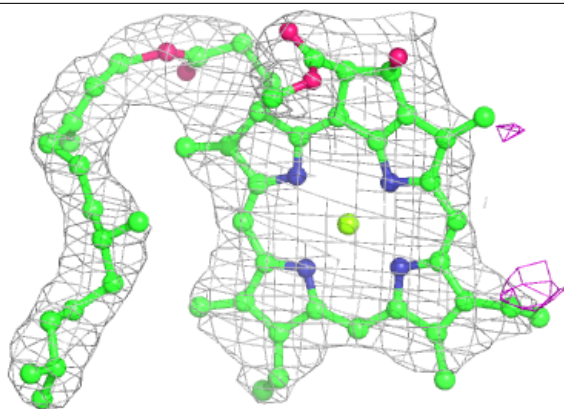
Electron density around CLA W 1701:

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

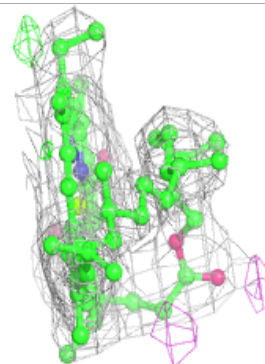
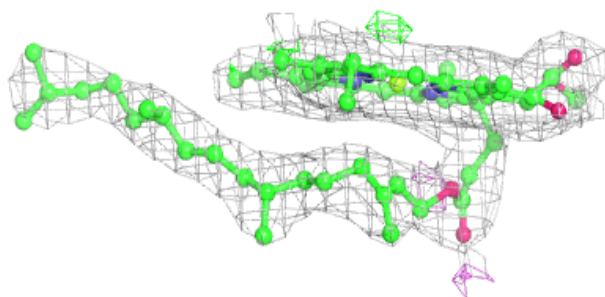
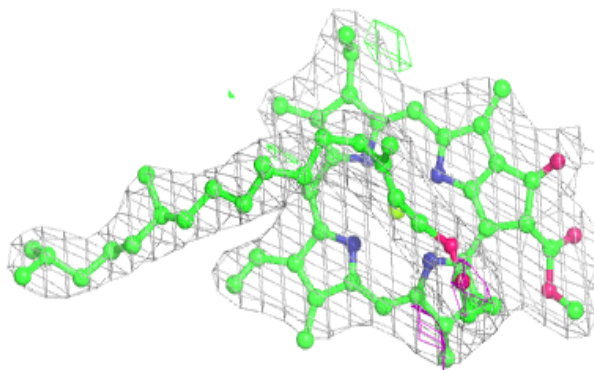


Electron density around CLA G 813:

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

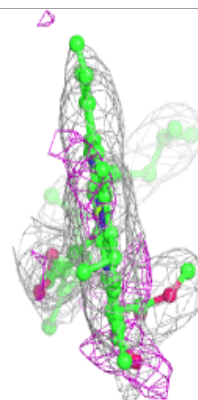
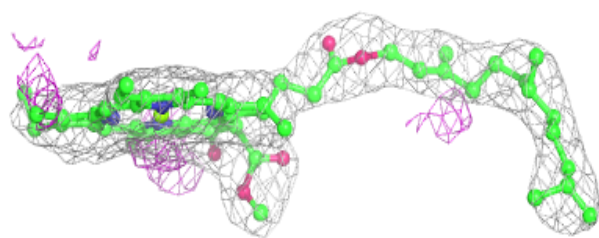
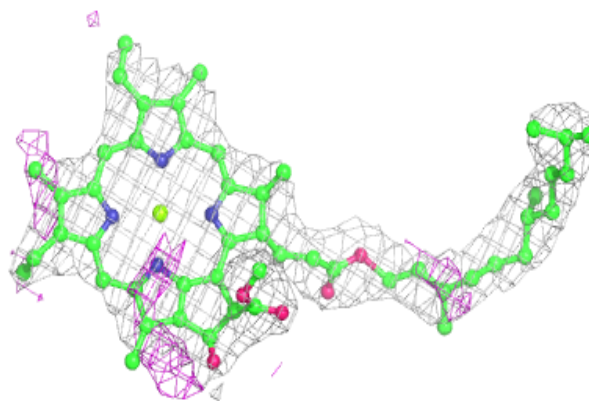
**Electron density around CLA Y 840:**

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

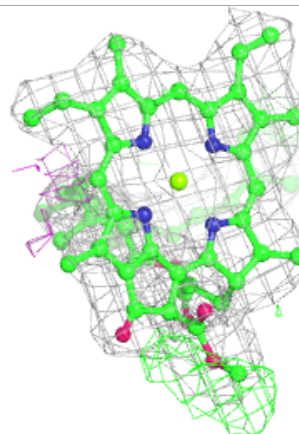
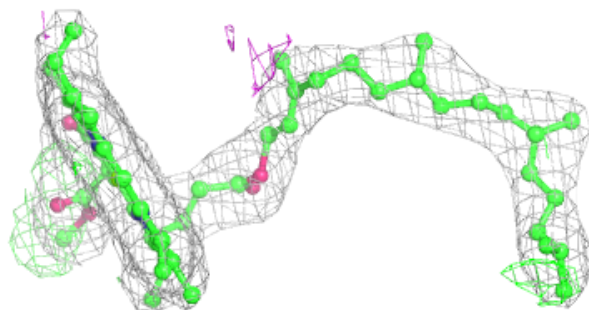
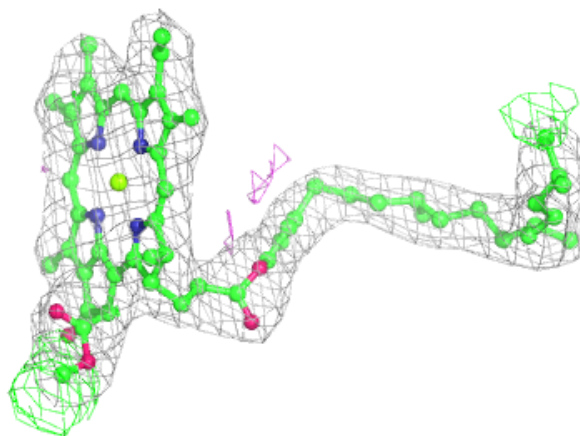


Electron density around CLA B 837:

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

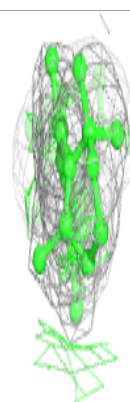
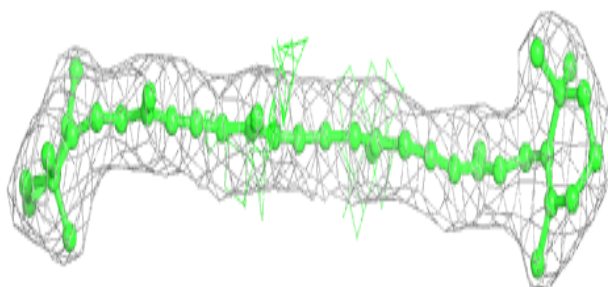
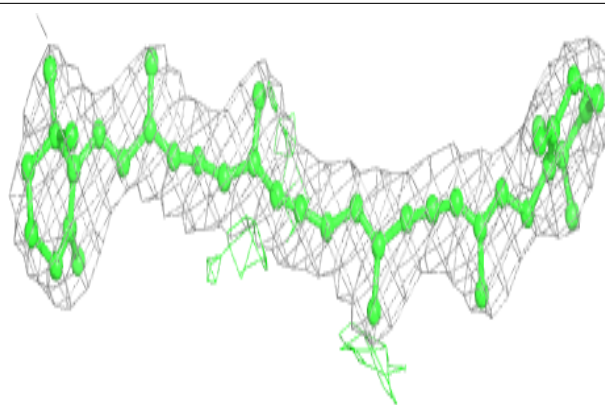
**Electron density around CLA U 1003:**

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



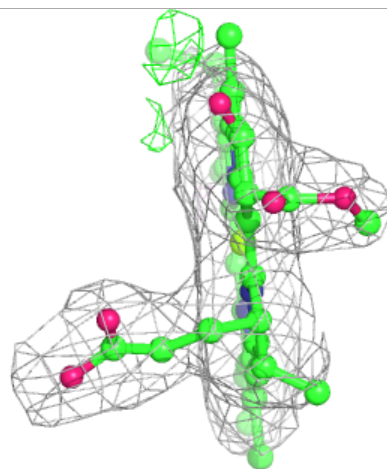
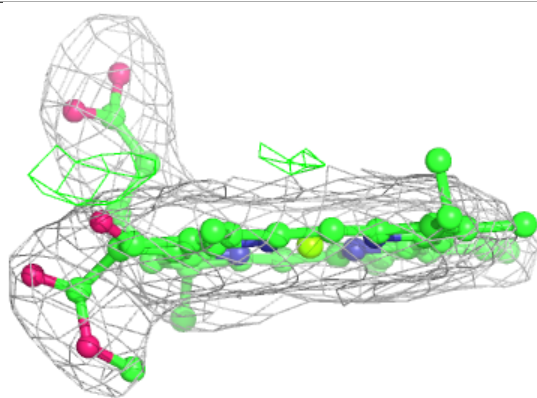
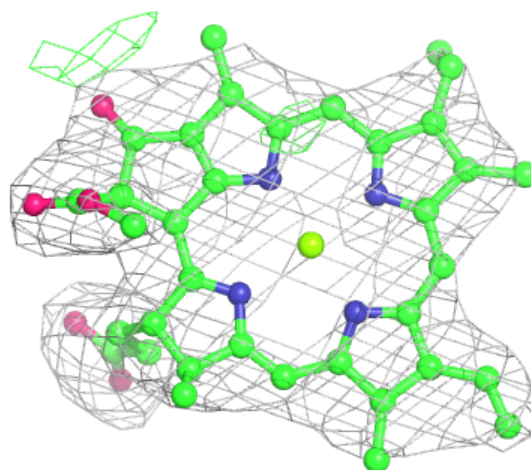
Electron density around BCR H 845:

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



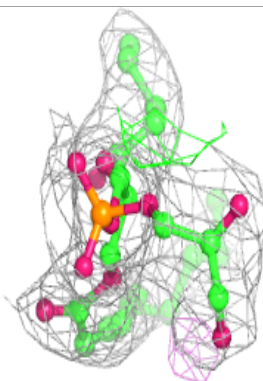
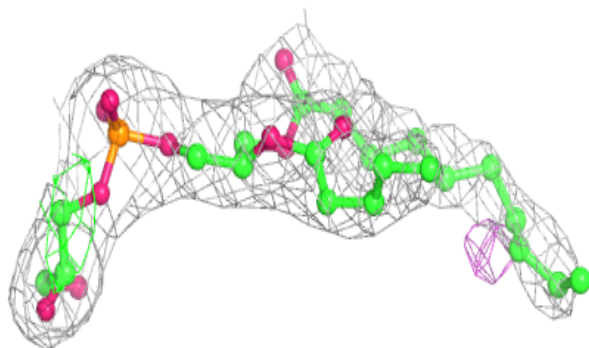
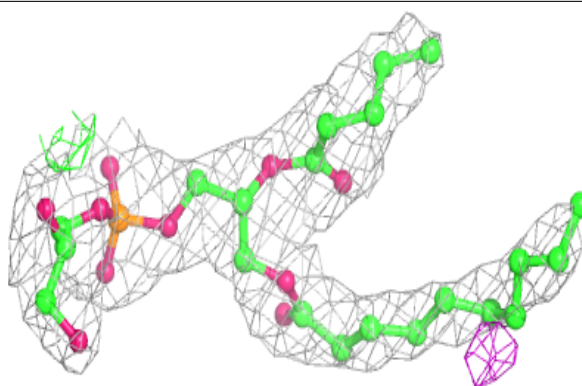
Electron density around CLA B 834:

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

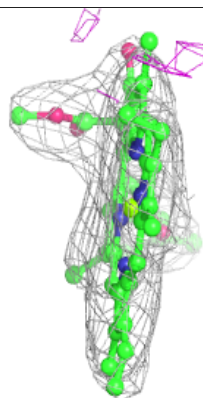
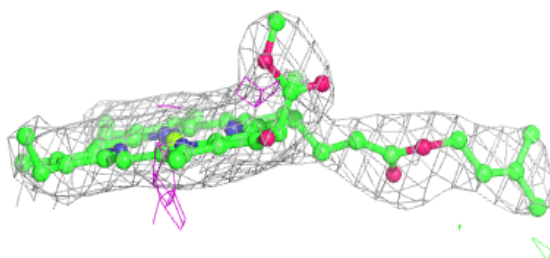
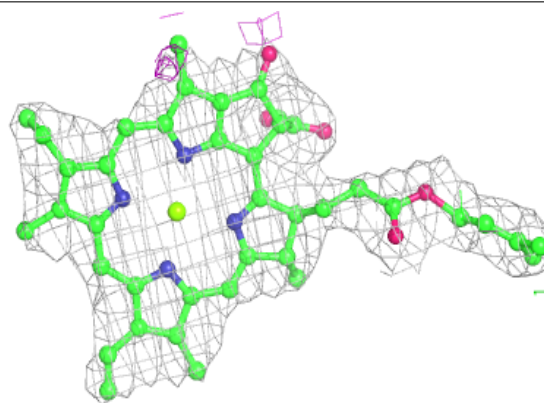


Electron density around LHG G 852:

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

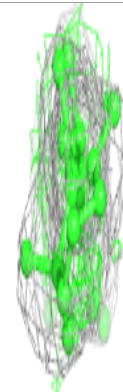
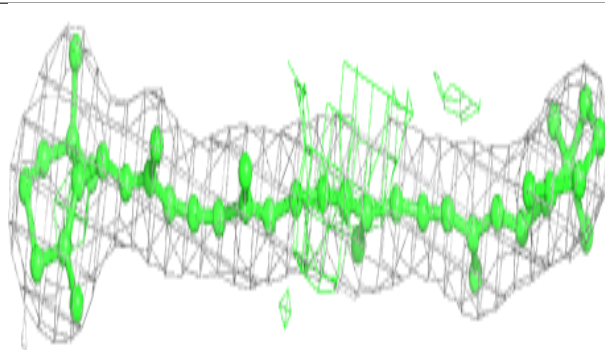
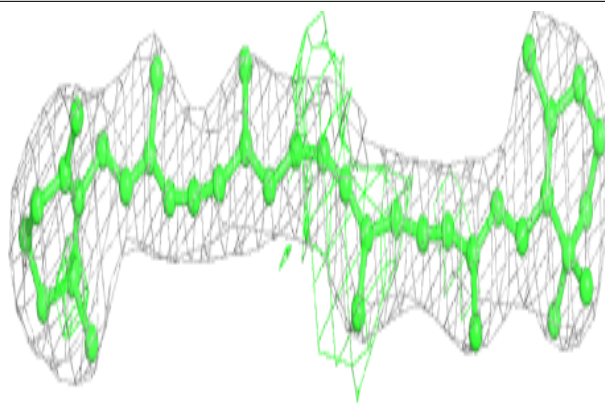
**Electron density around CLA A 836:**

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



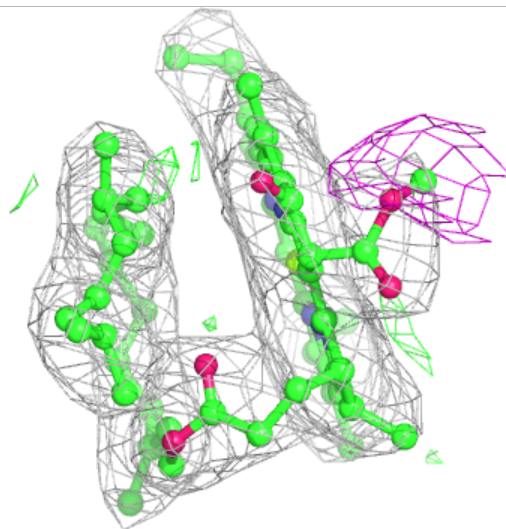
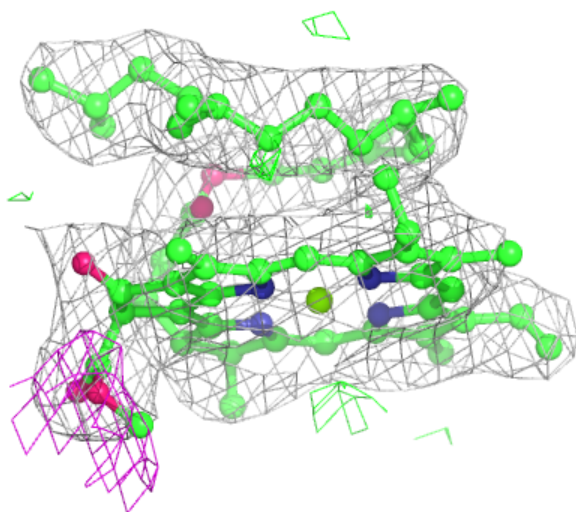
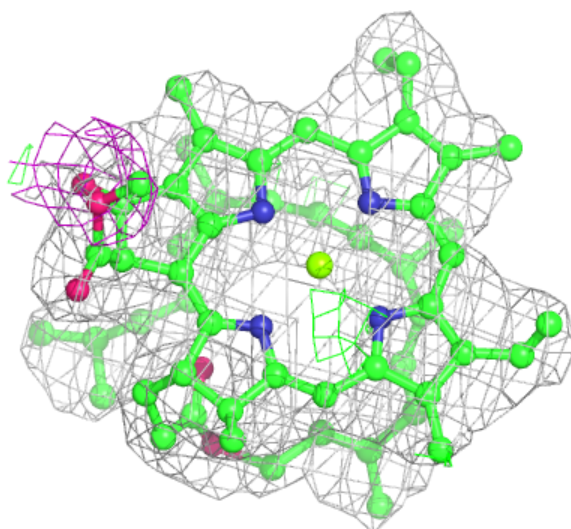
Electron density around BCR J 103:

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



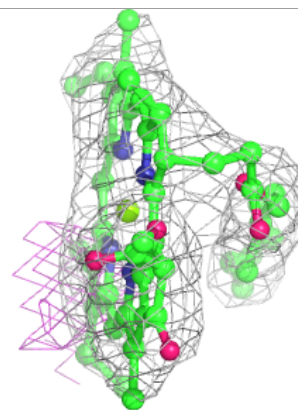
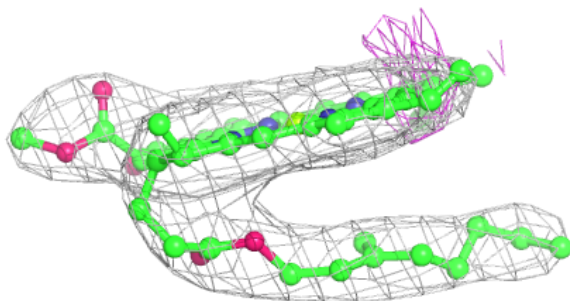
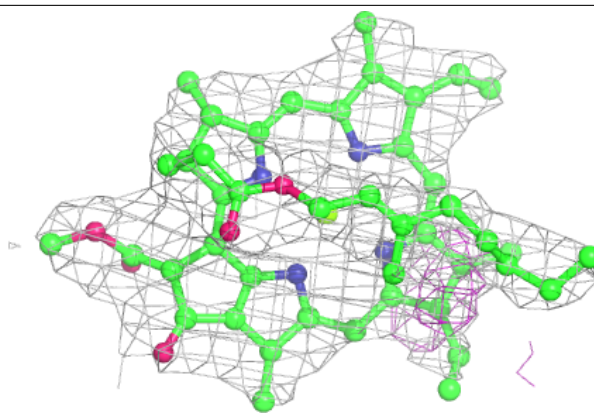
Electron density around CLA U 1002:

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

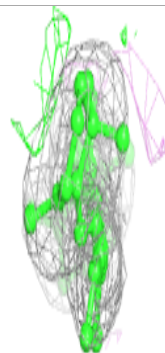
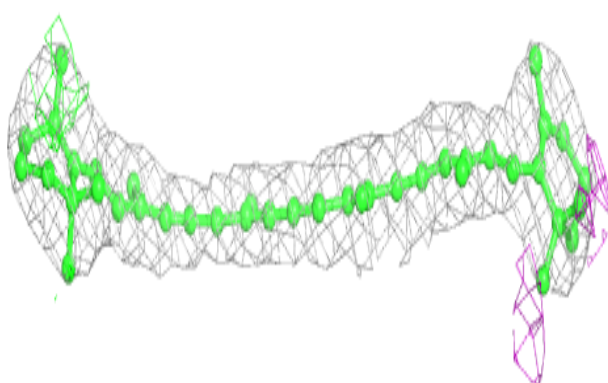
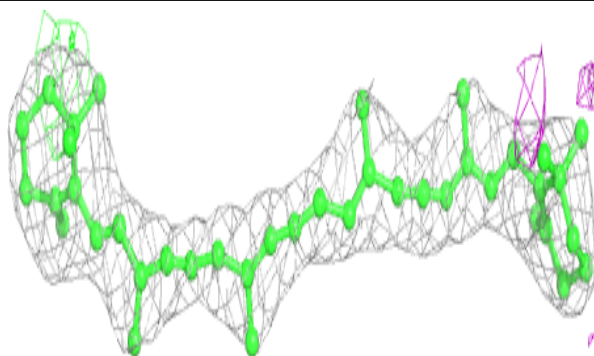


Electron density around CLA A 812:

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

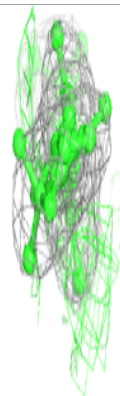
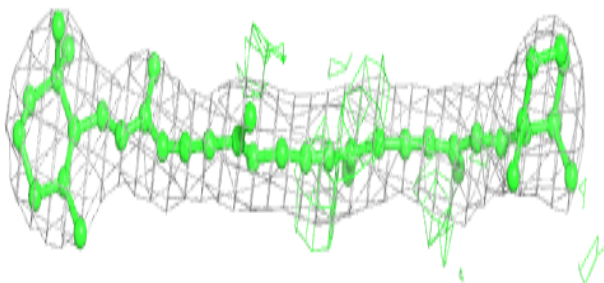
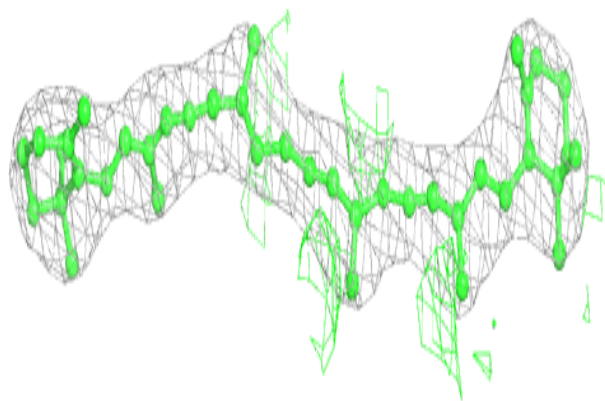
**Electron density around BCR A 847:**

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



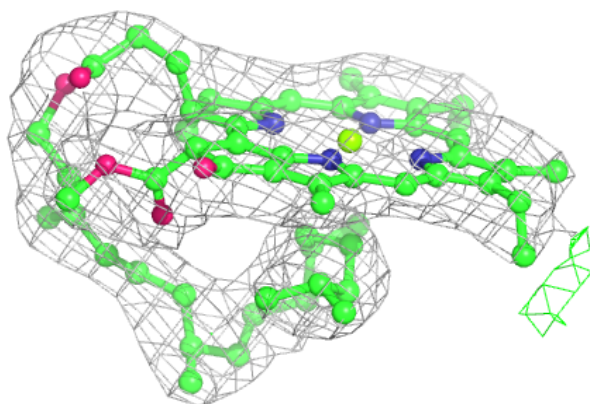
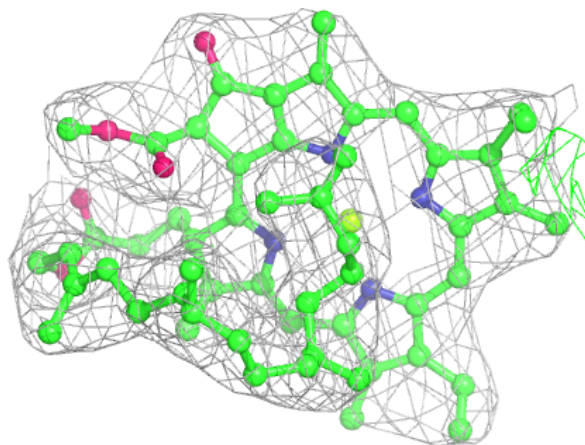
Electron density around BCR G 854:

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



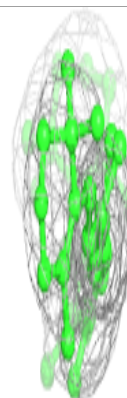
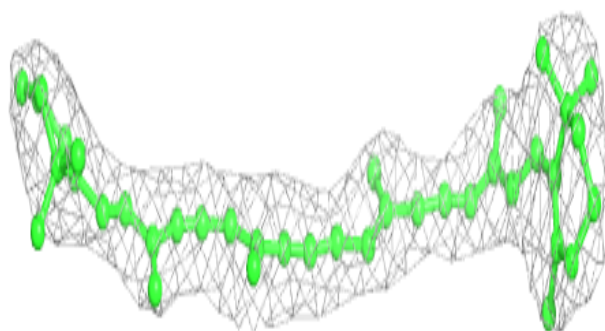
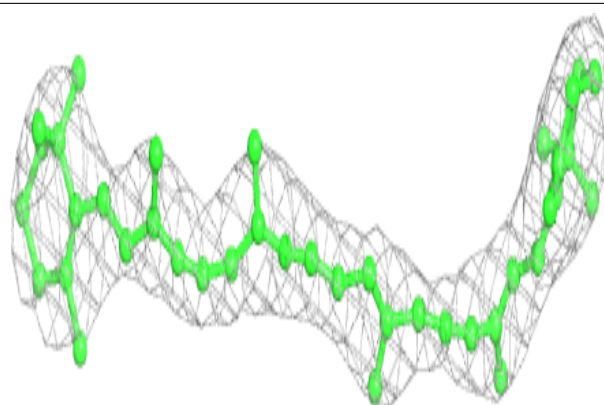
Electron density around CLA H 805:

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

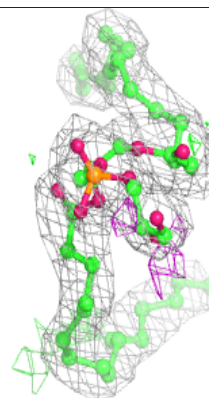
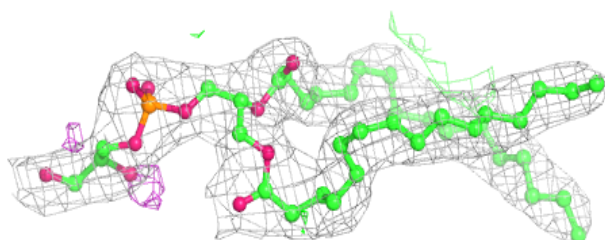
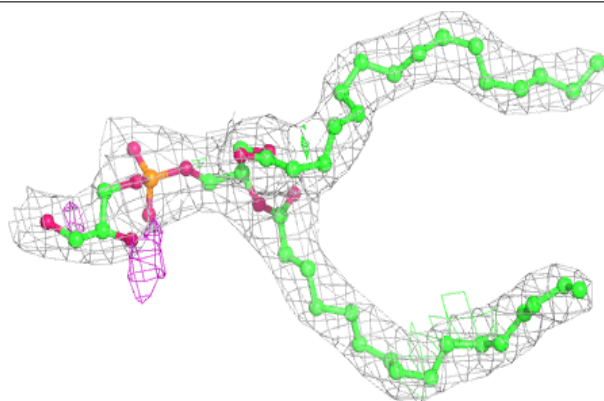


Electron density around BCR Y 846:

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

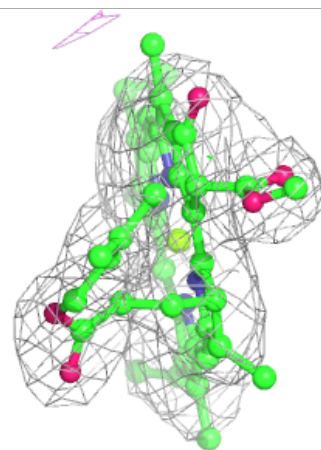
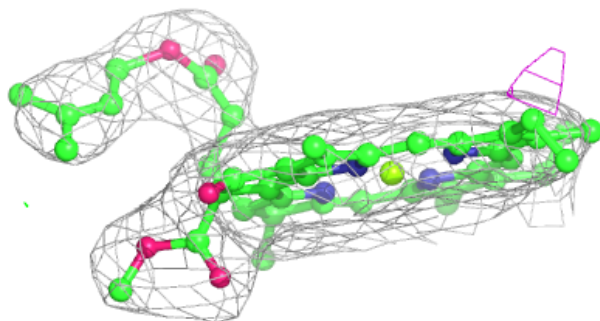
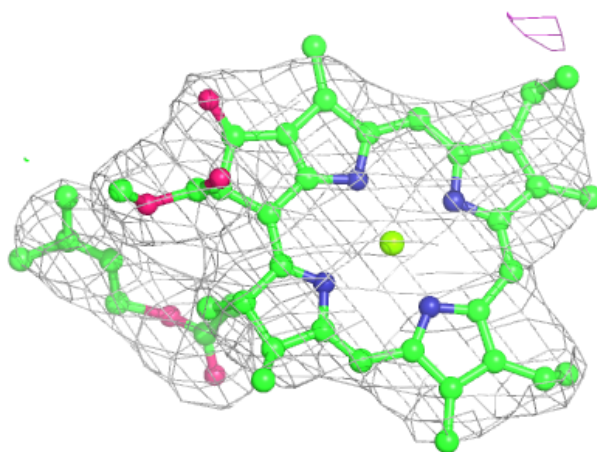
**Electron density around LHG A 850:**

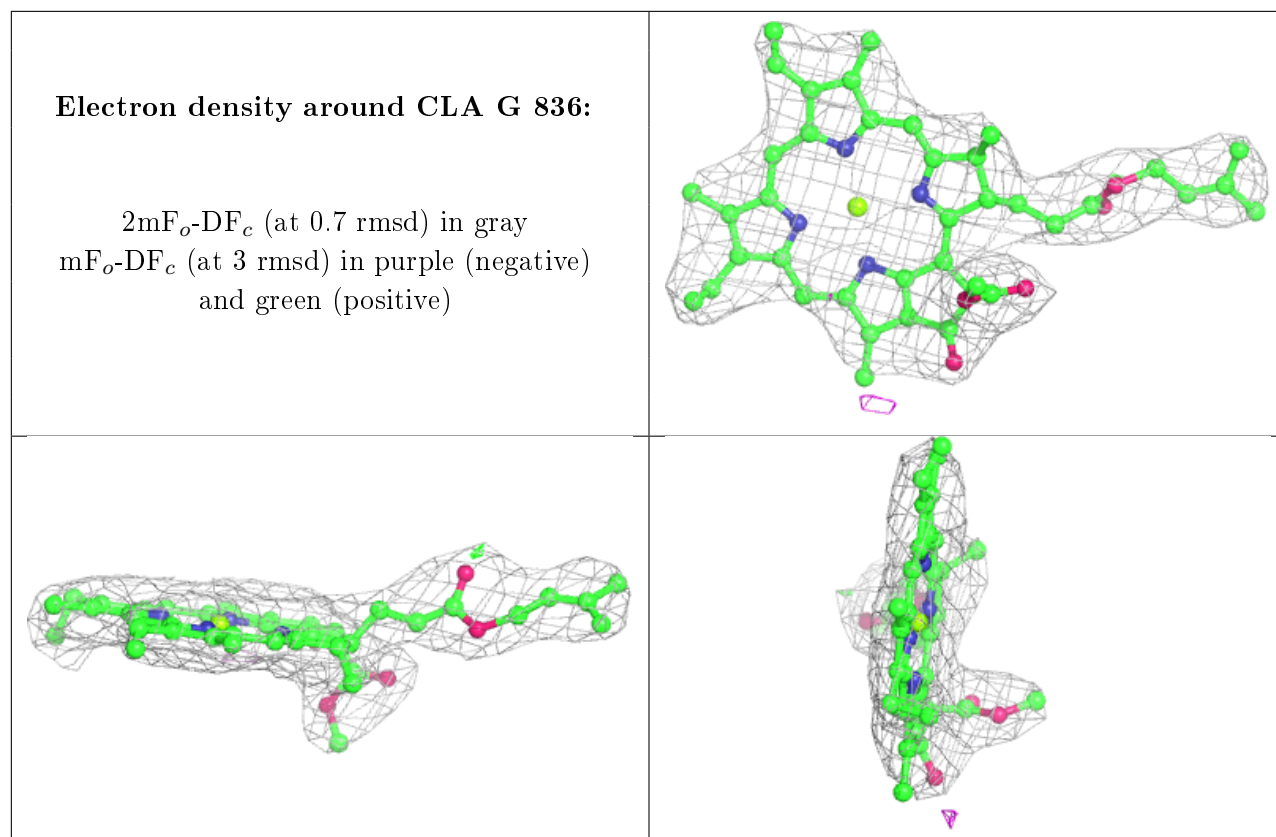
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA G 816:

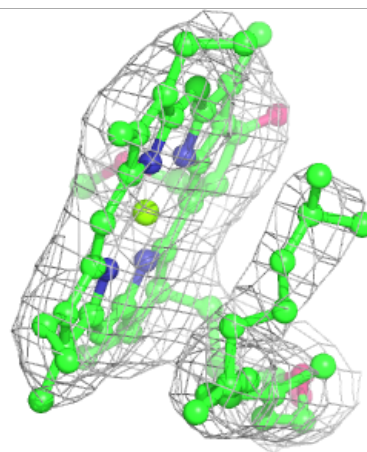
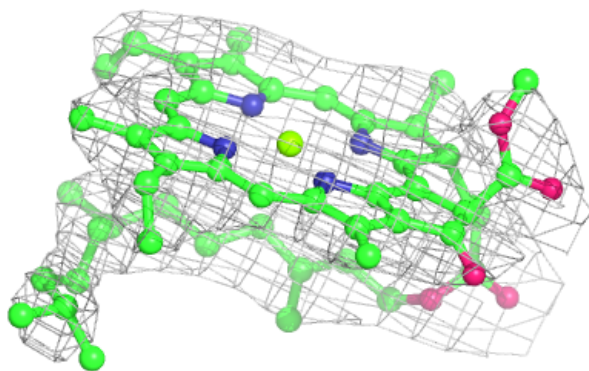
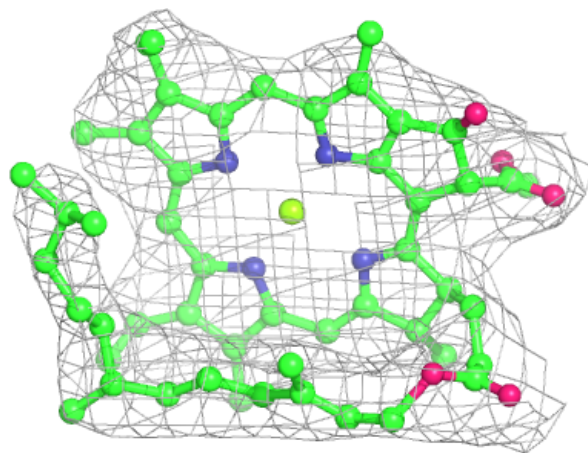
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





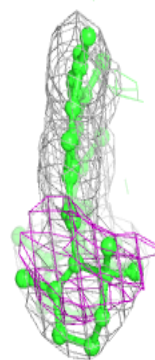
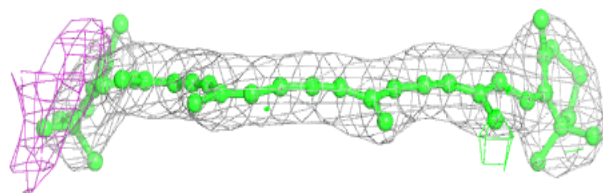
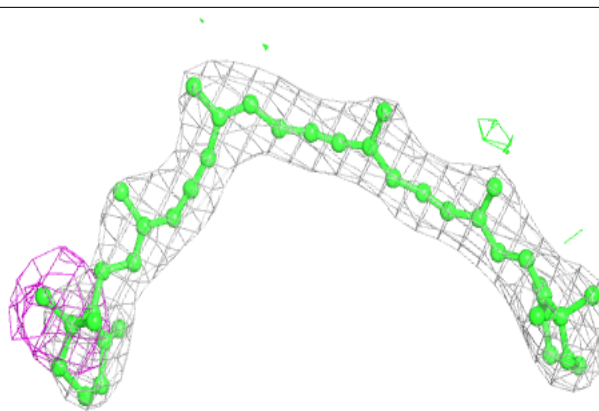
Electron density around CLA A 820:

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

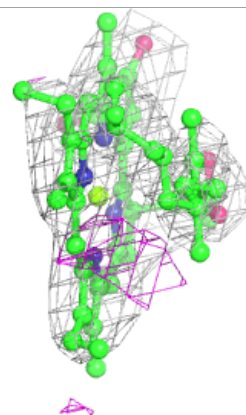
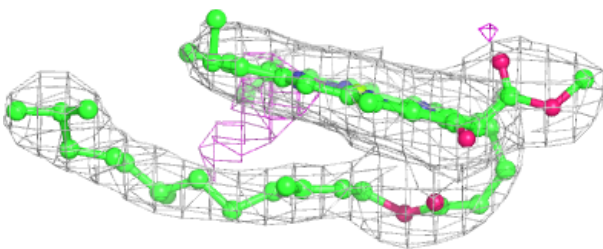
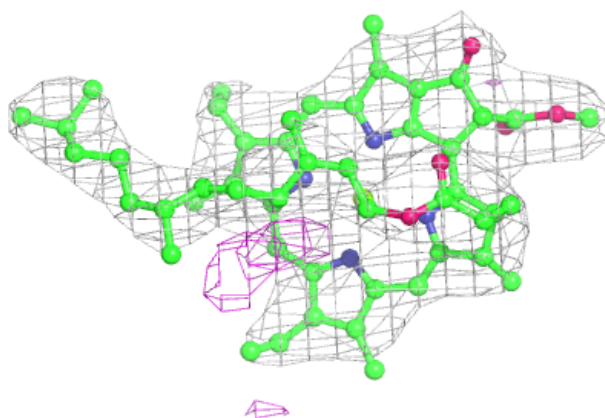


Electron density around BCR d 203:

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

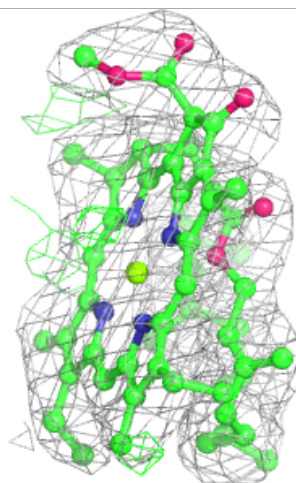
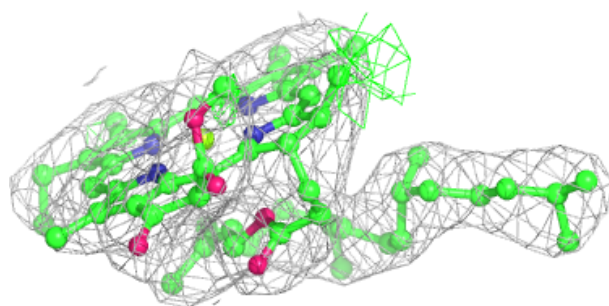
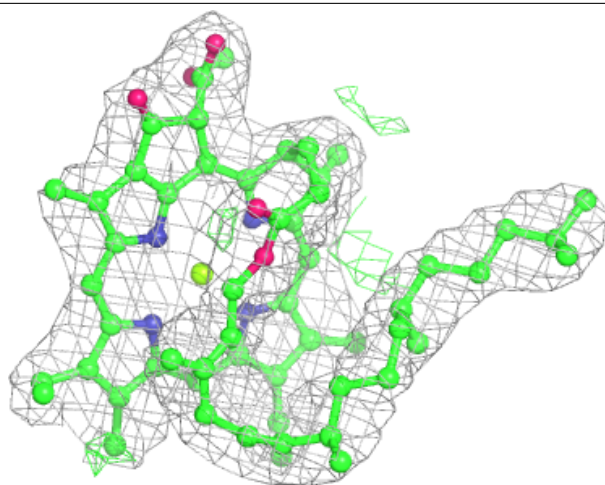
**Electron density around CLA G 817:**

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



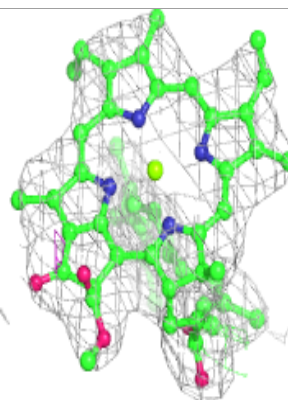
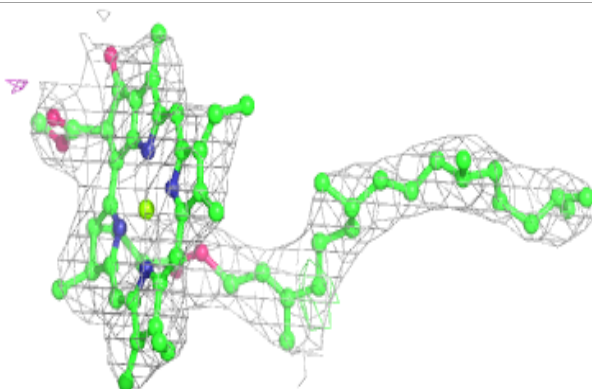
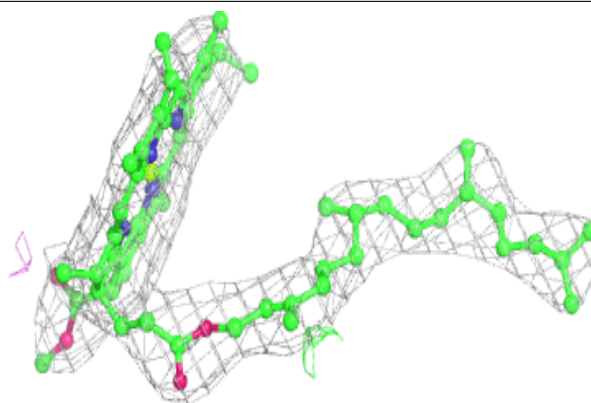
Electron density around CLA H 807:

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

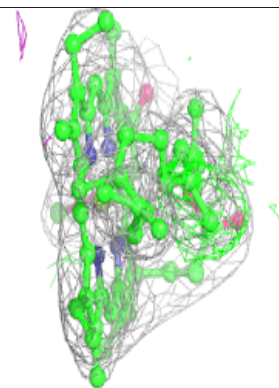
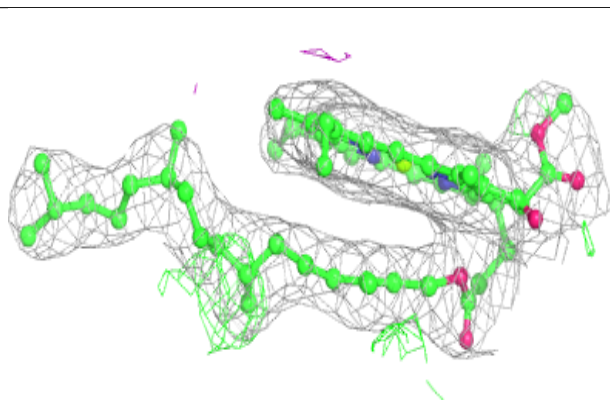
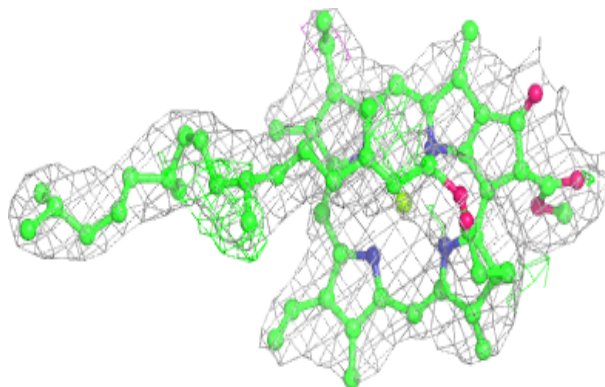


Electron density around CLA Y 811:

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

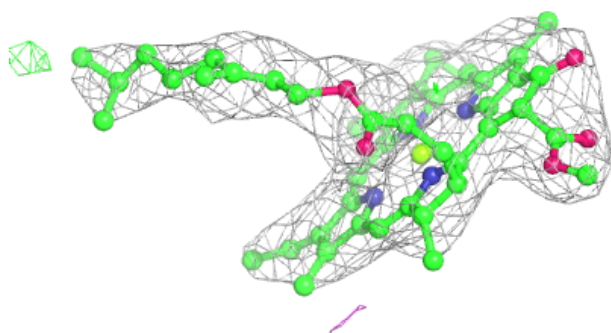
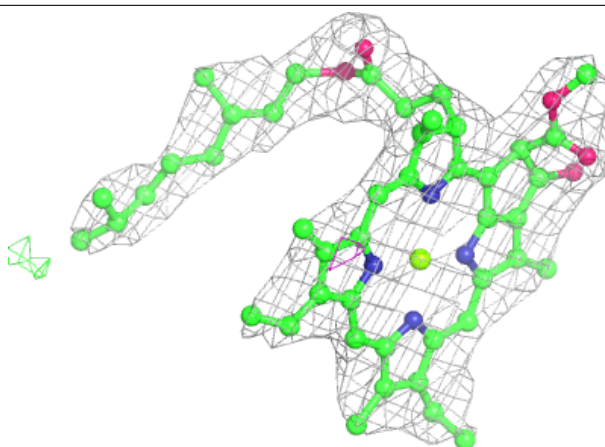
**Electron density around CLA Y 838:**

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

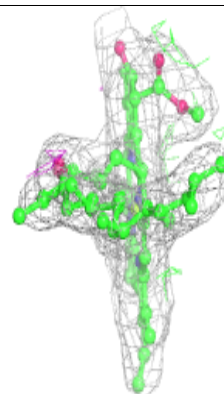
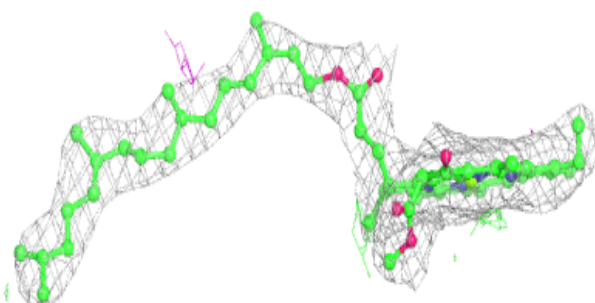
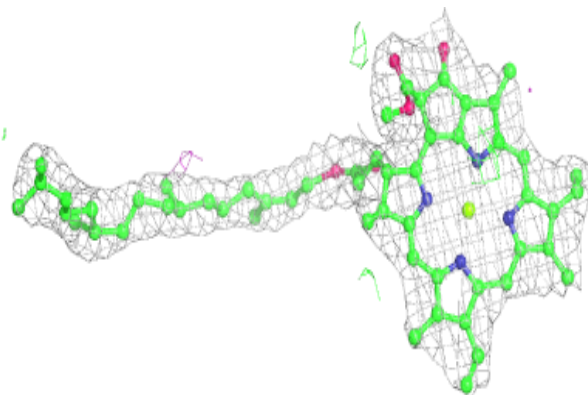


Electron density around CLA H 815:

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

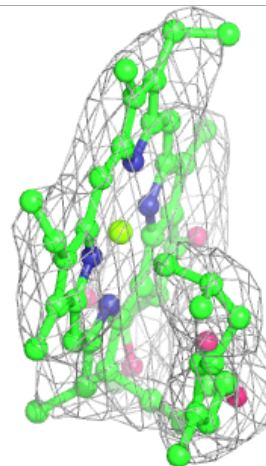
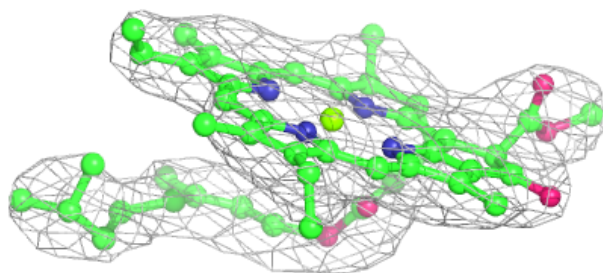
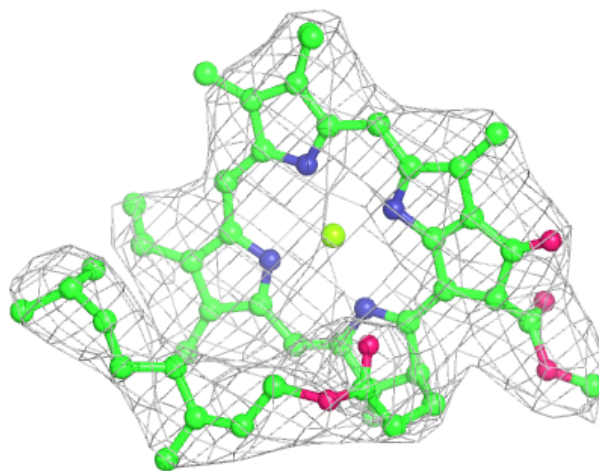
**Electron density around CLA B 825:**

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



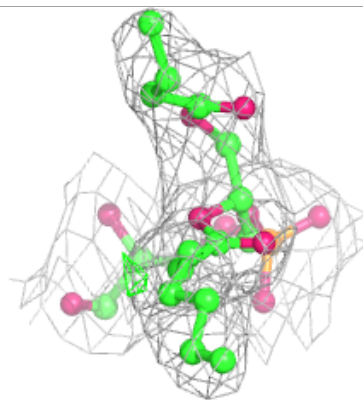
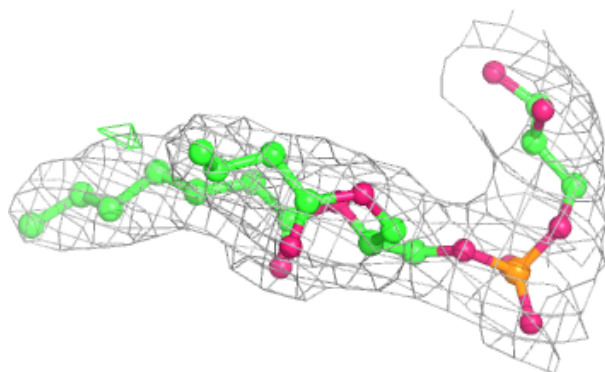
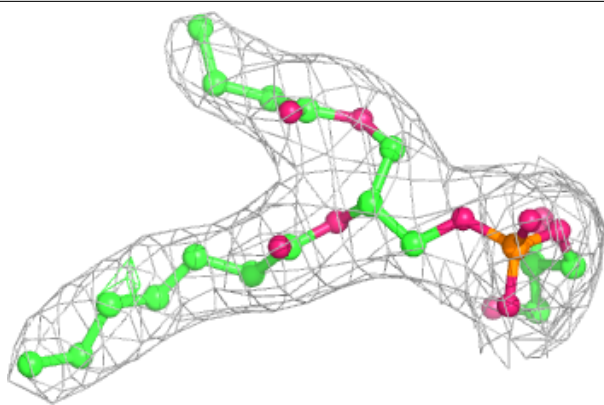
Electron density around CLA Y 812:

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



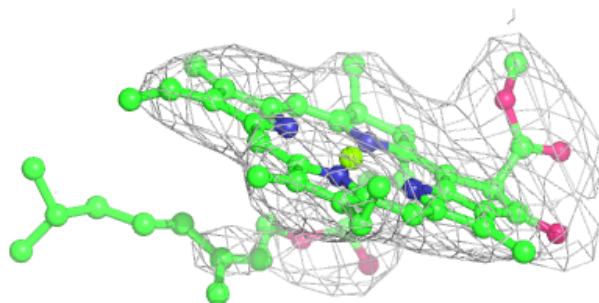
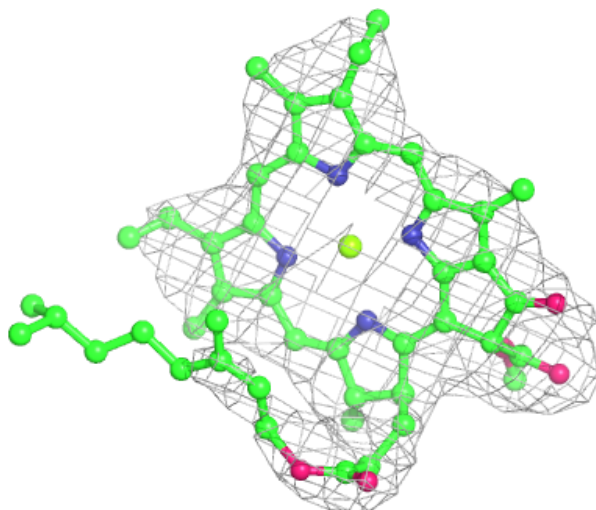
Electron density around LHG j 101:

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



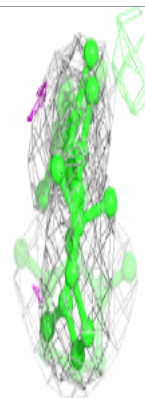
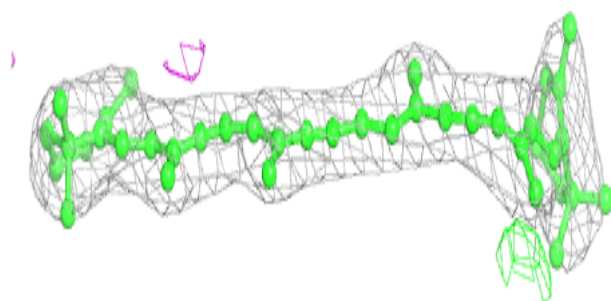
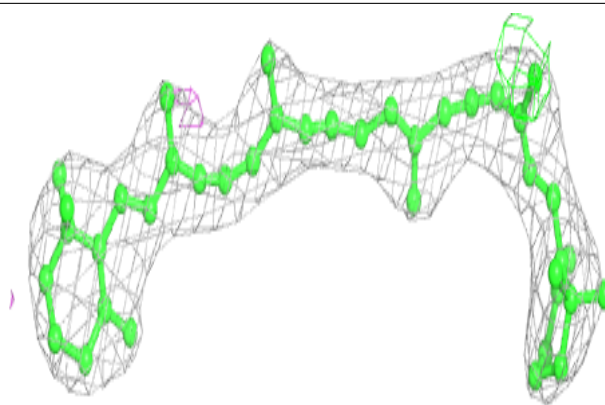
Electron density around CLA J 102:

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



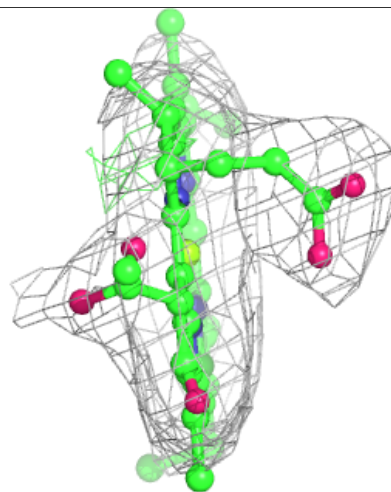
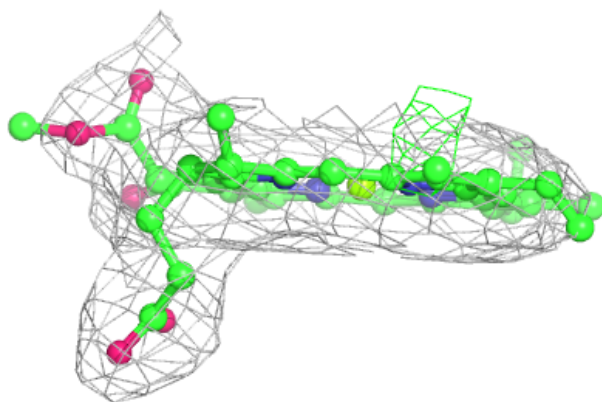
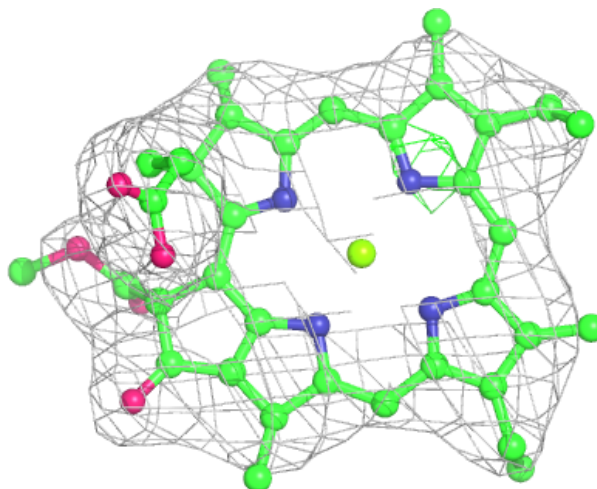
Electron density around BCR B 844:

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



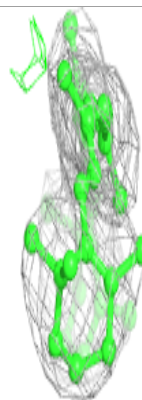
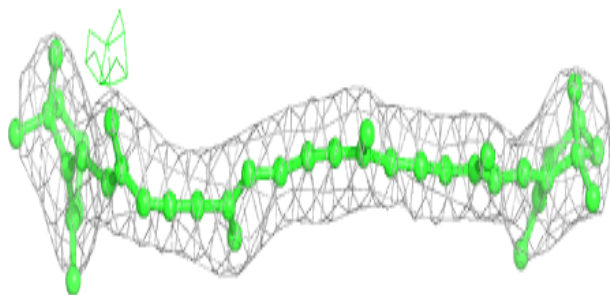
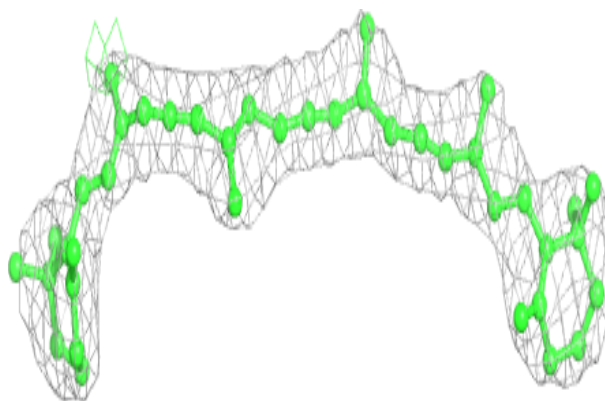
Electron density around CLA S 1102:

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

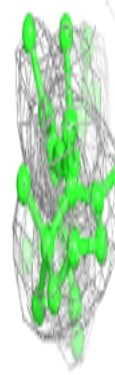
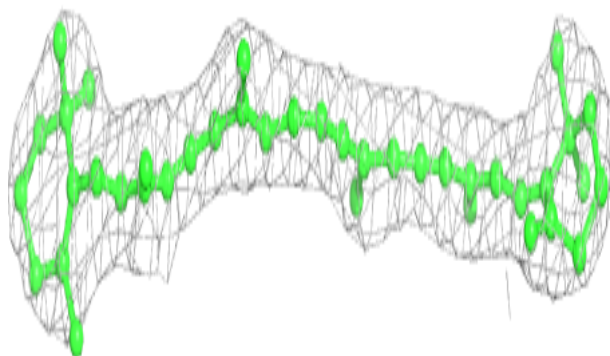
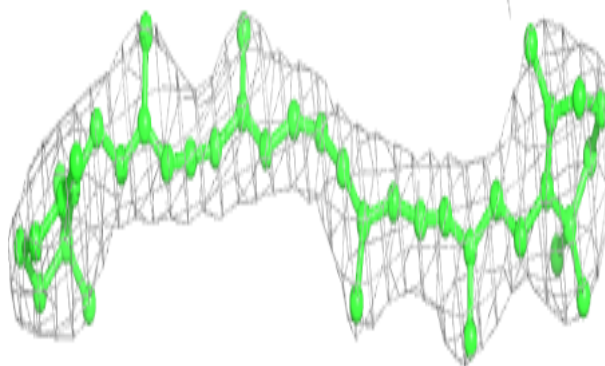


Electron density around BCR H 841:

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

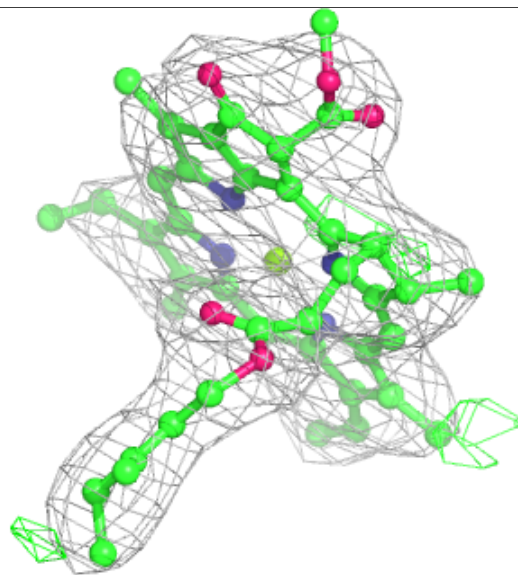
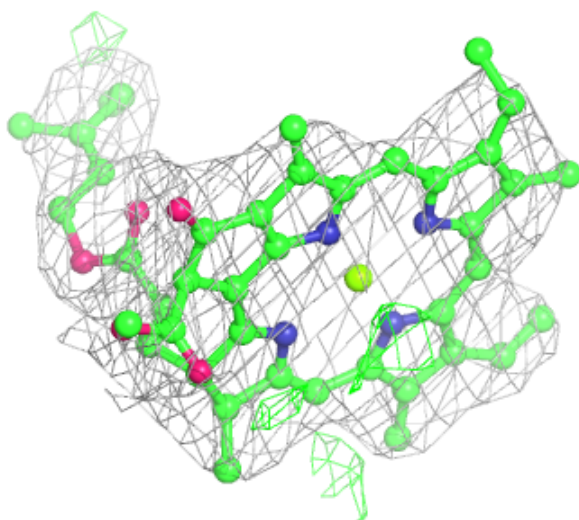
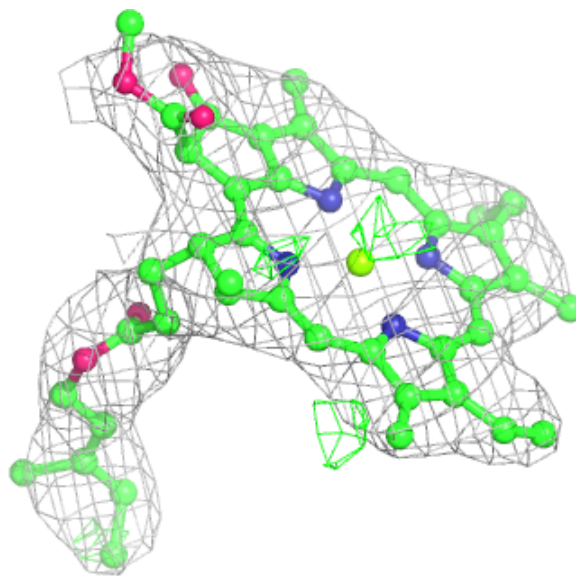
**Electron density around BCR A 845:**

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



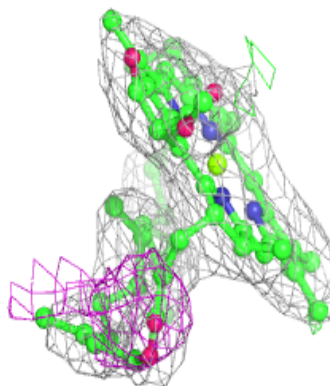
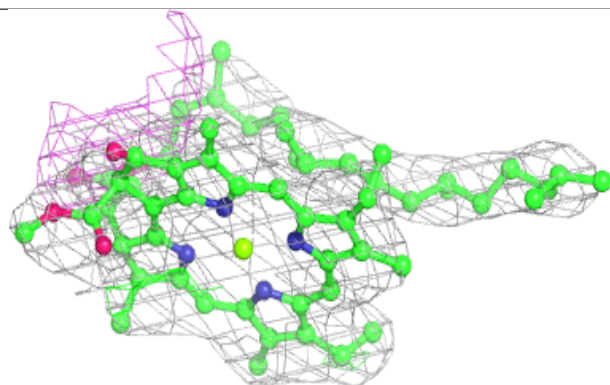
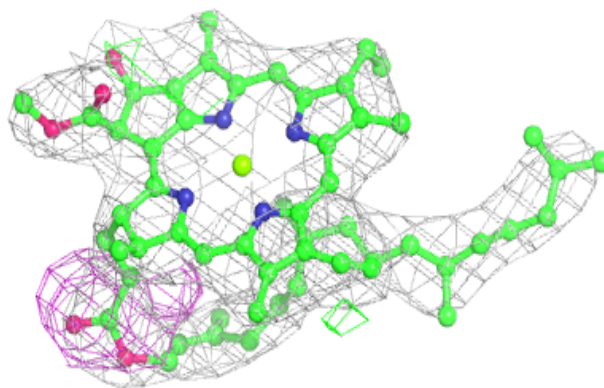
Electron density around CLA A 807:

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



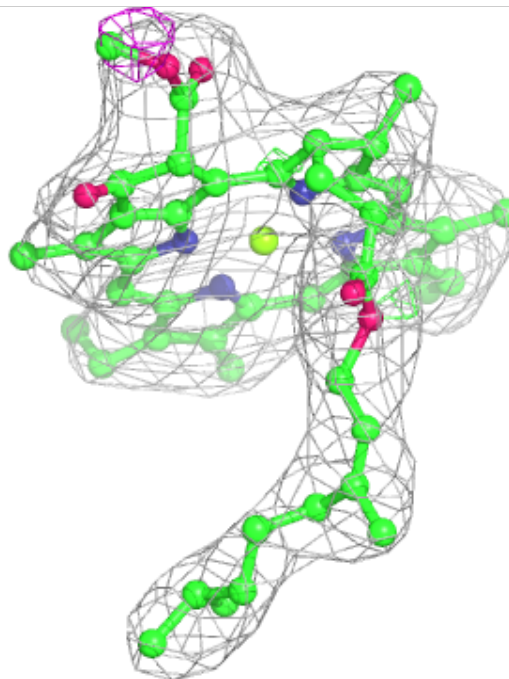
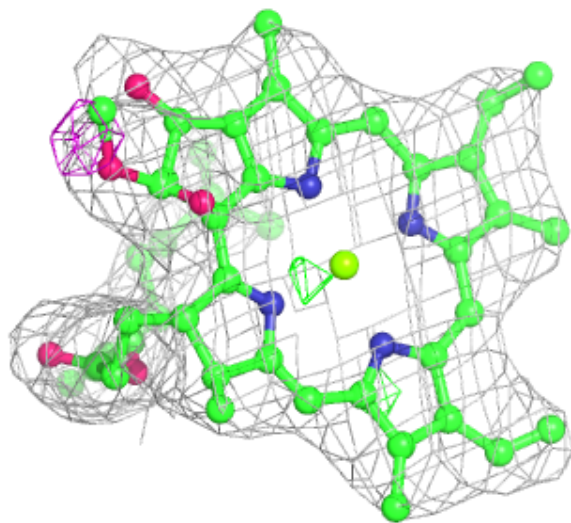
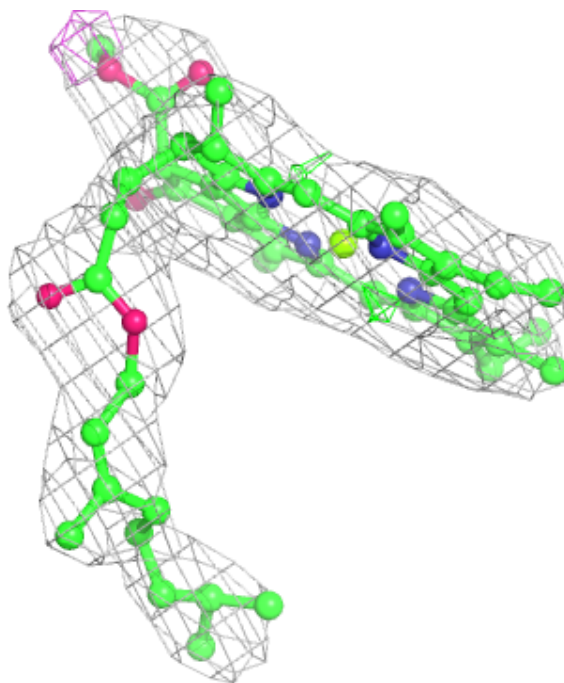
Electron density around CLA Z 815:

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



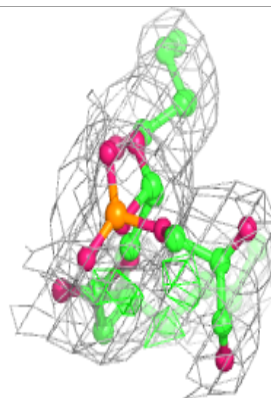
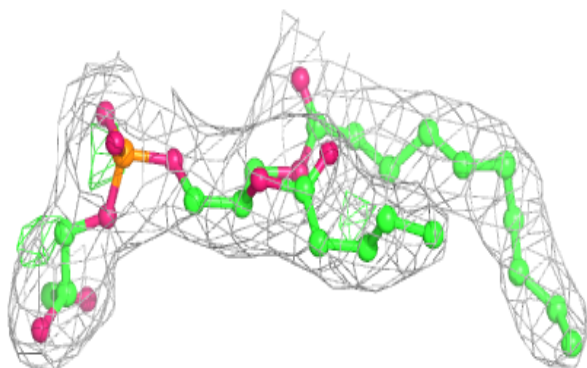
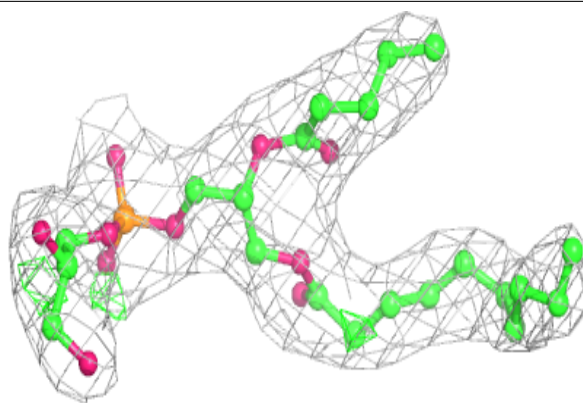
Electron density around CLA H 810:

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

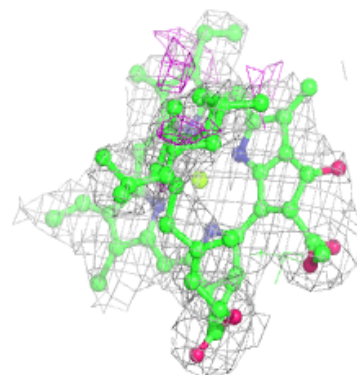
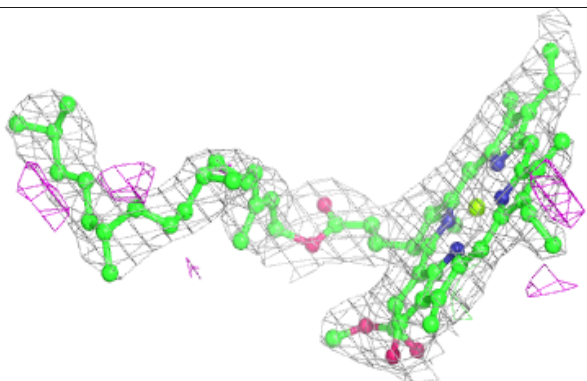
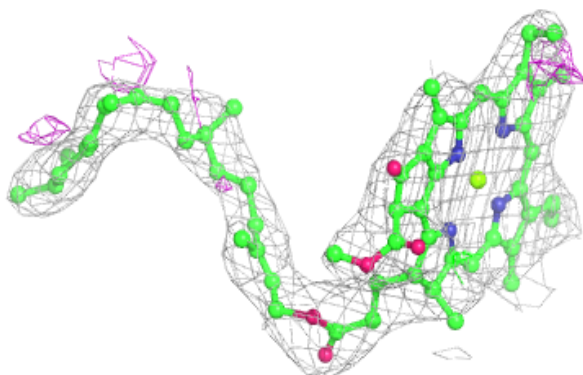


Electron density around LHG A 851:

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

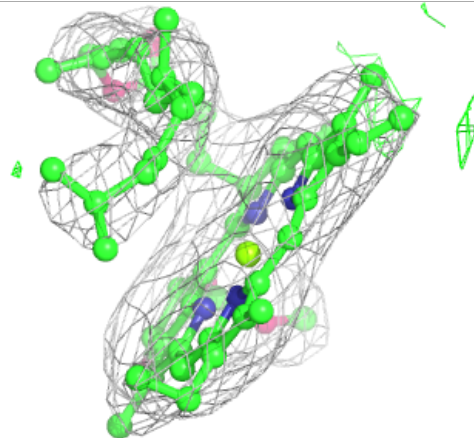
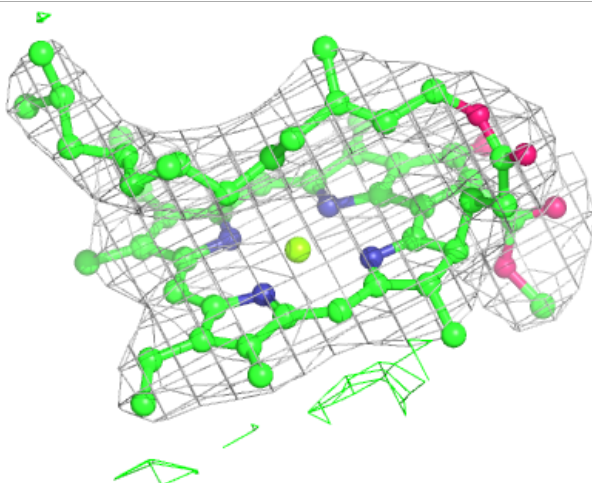
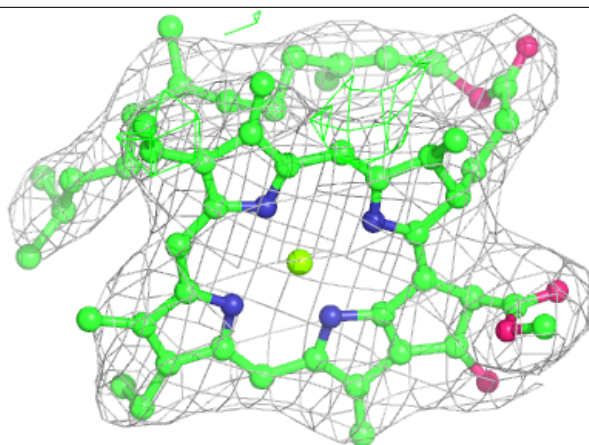
**Electron density around CLA H 802:**

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



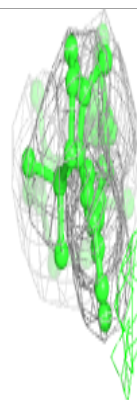
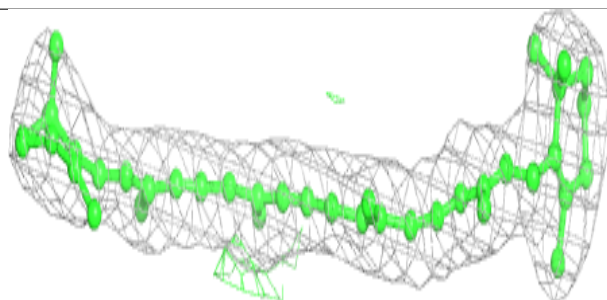
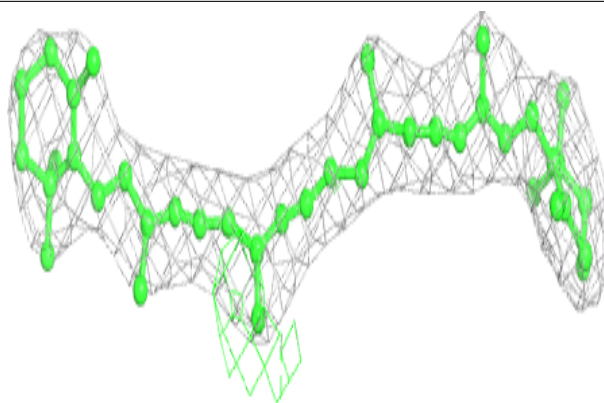
Electron density around CLA Y 820:

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

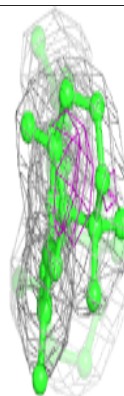
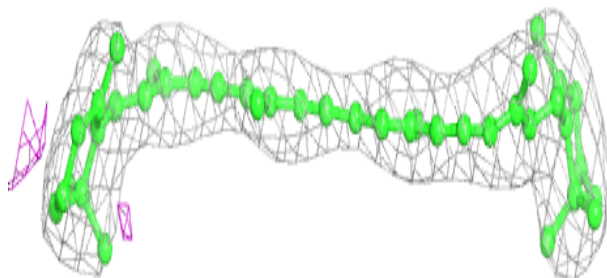
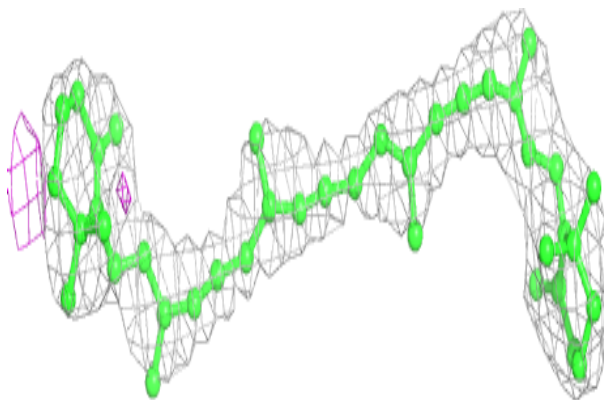


Electron density around BCR G 849:

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

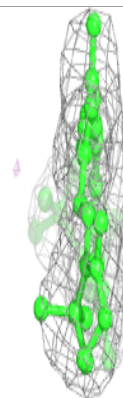
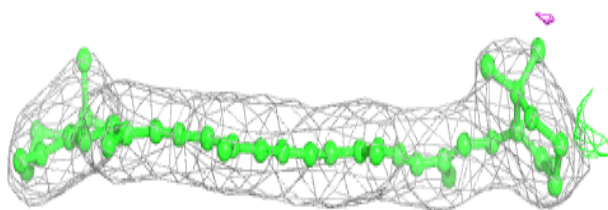
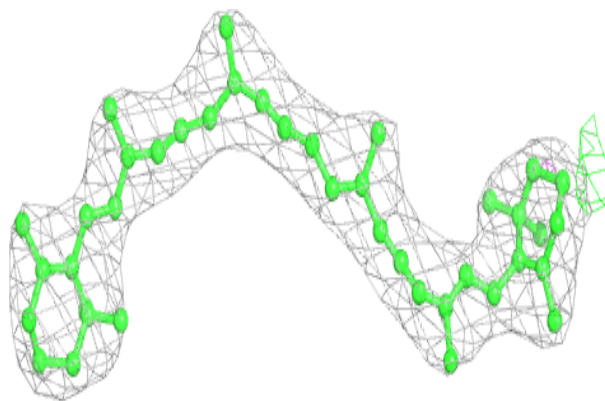
**Electron density around BCR H 842:**

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



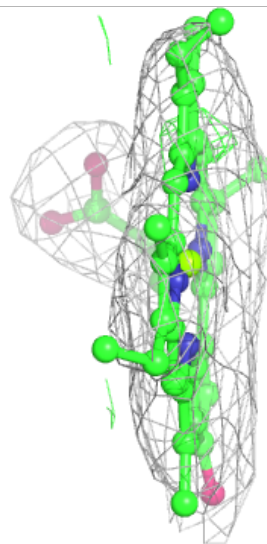
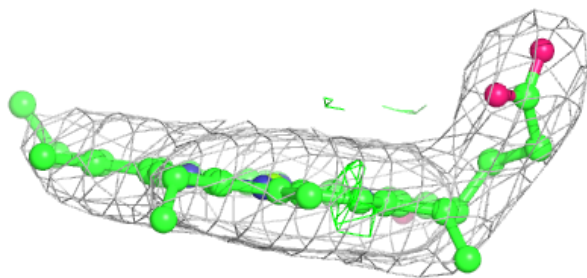
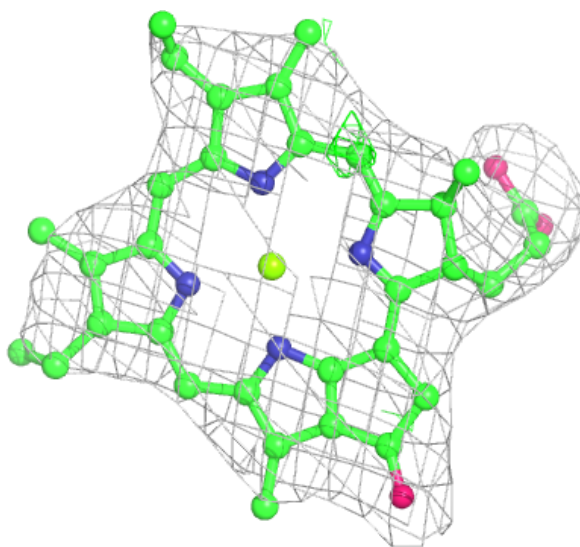
Electron density around BCR Y 851:

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



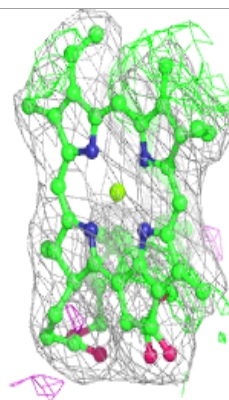
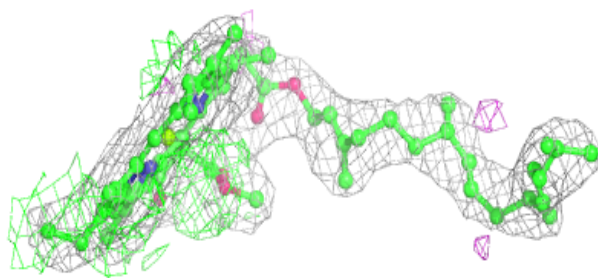
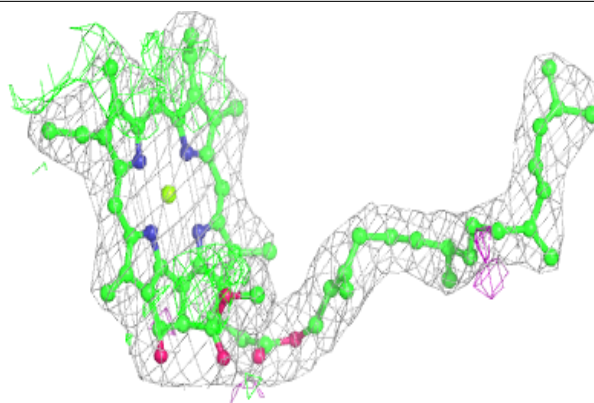
Electron density around CLA T 101:

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

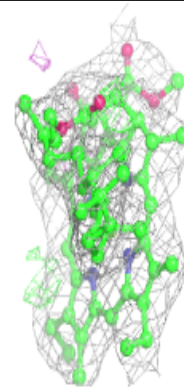
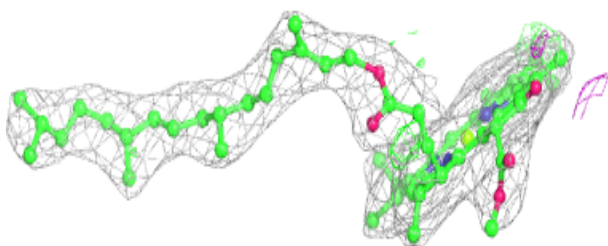
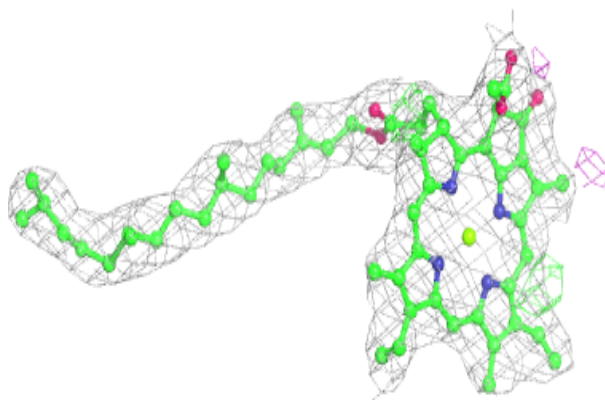


Electron density around CLA U 1006:

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

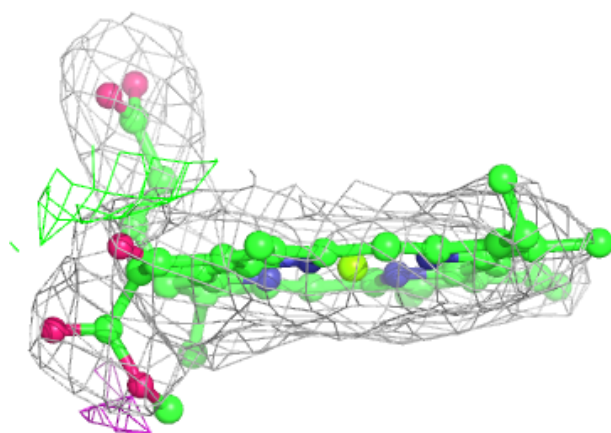
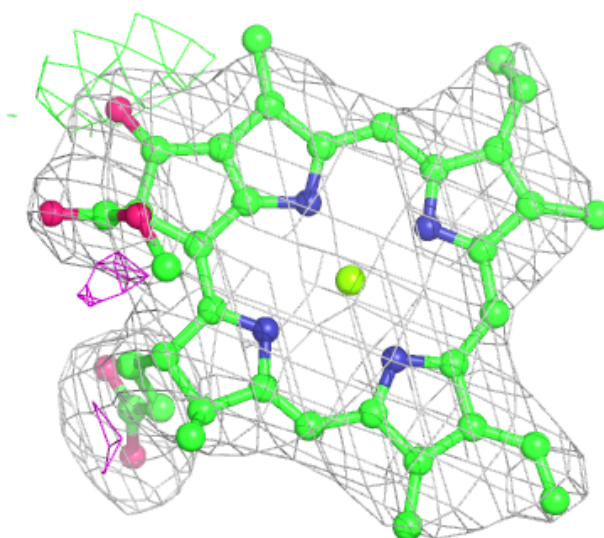
**Electron density around CLA Y 834:**

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



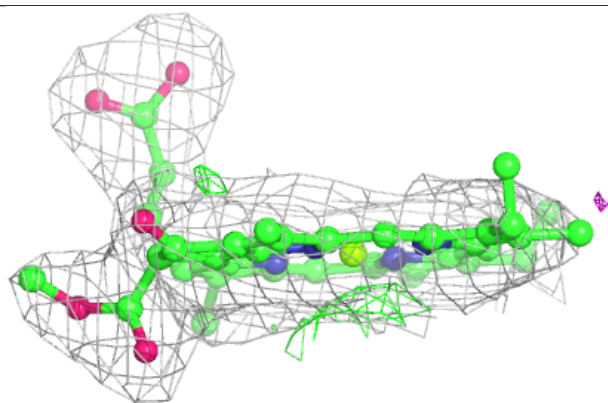
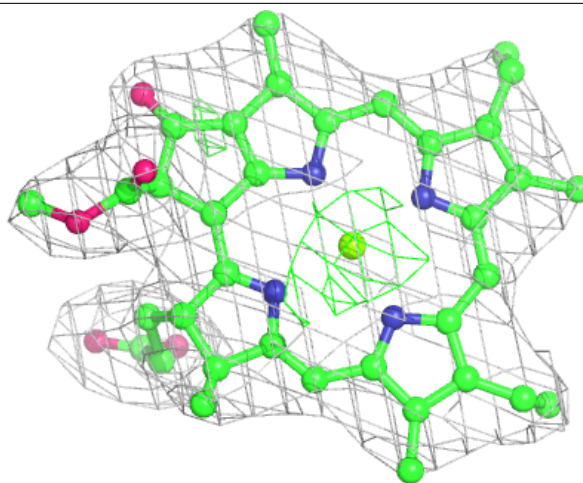
Electron density around CLA Z 832:

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



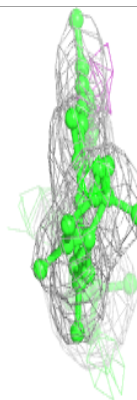
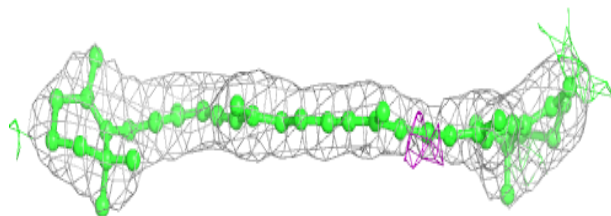
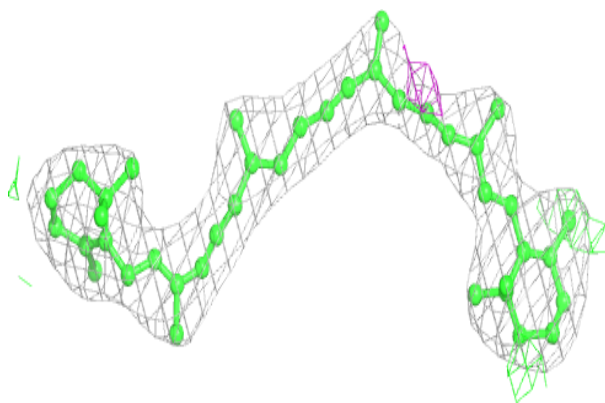
Electron density around CLA Z 833:

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



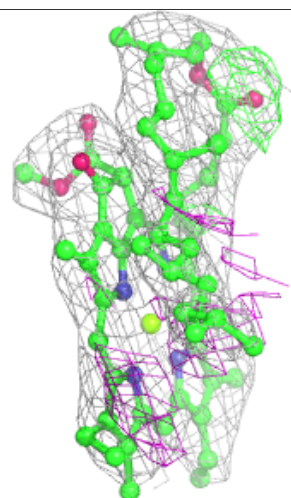
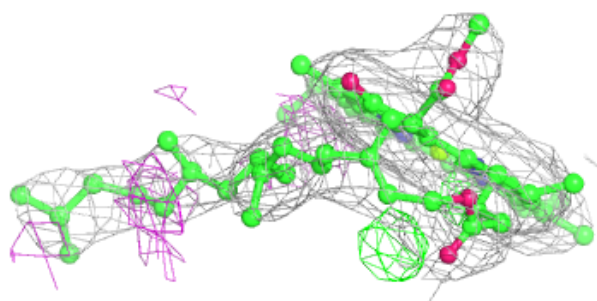
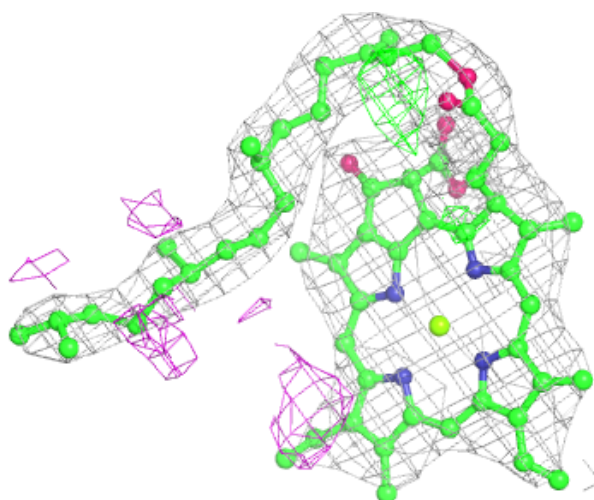
Electron density around BCR A 849:

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



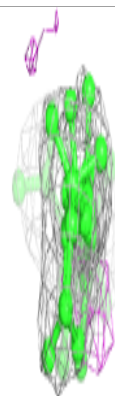
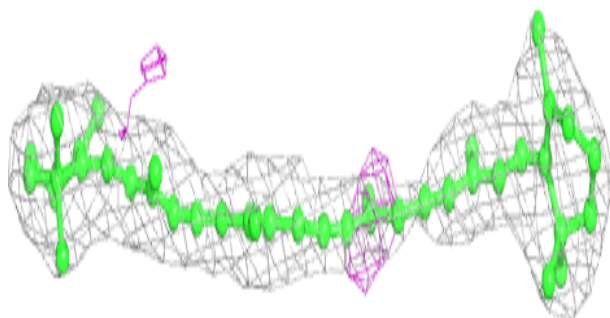
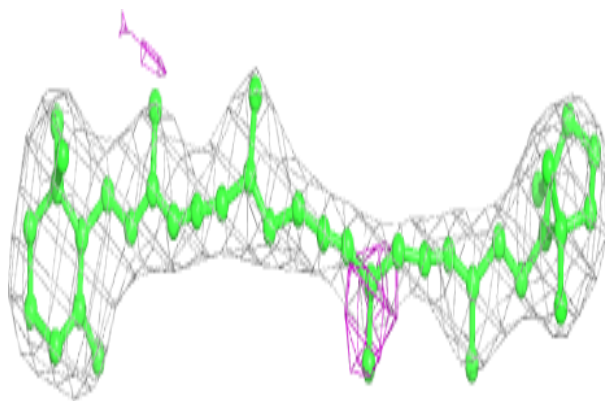
Electron density around CLA A 825:

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

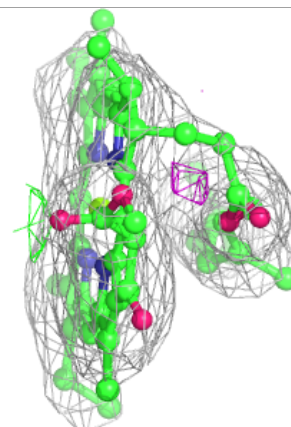
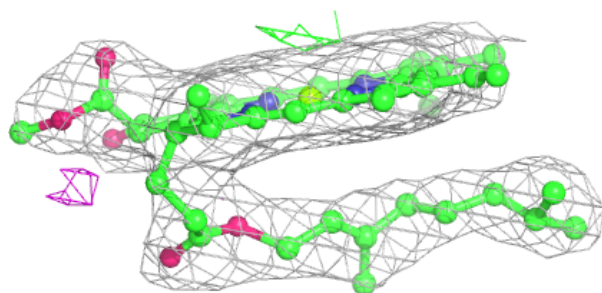
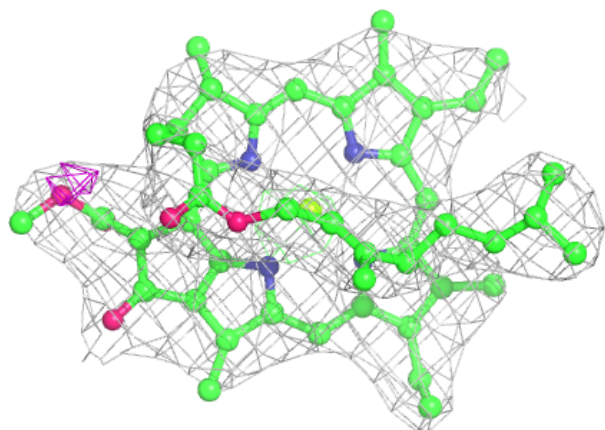


Electron density around BCR B 851:

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

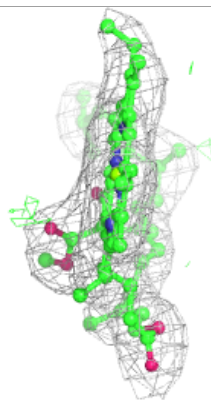
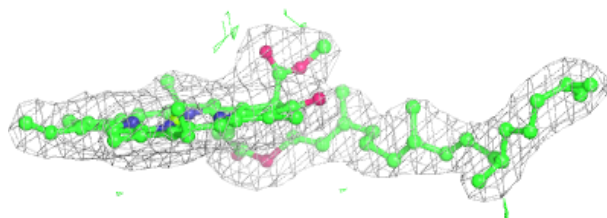
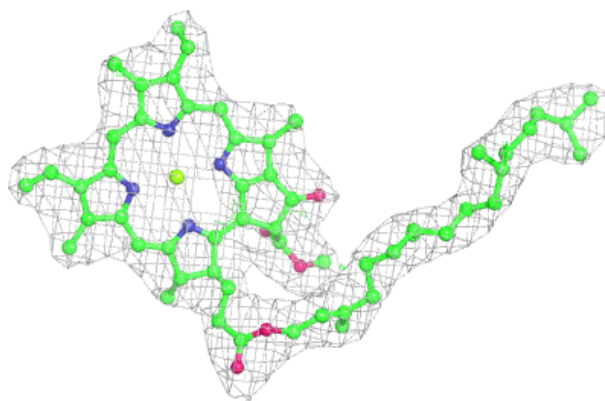
**Electron density around CLA H 821:**

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



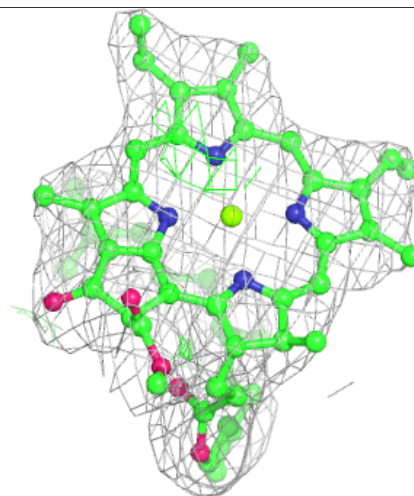
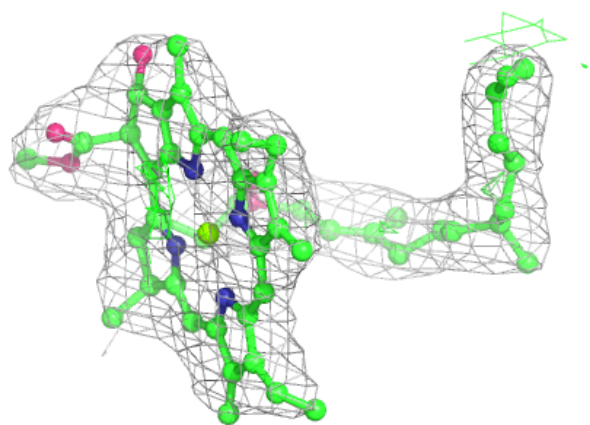
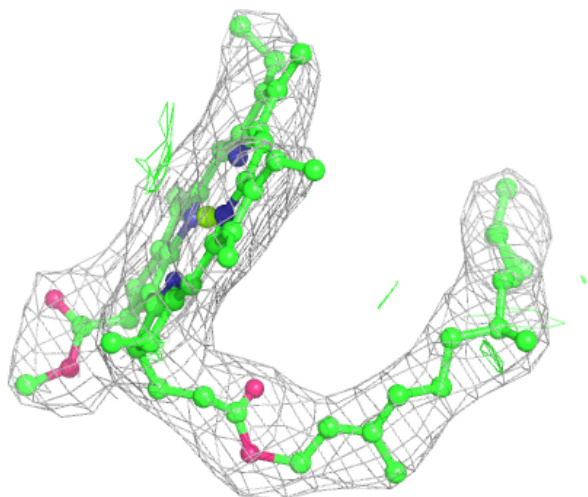
Electron density around CLA L 207:

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



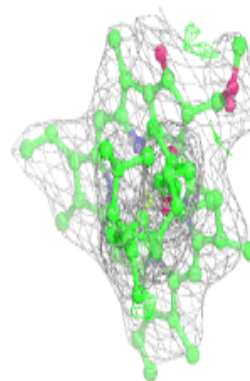
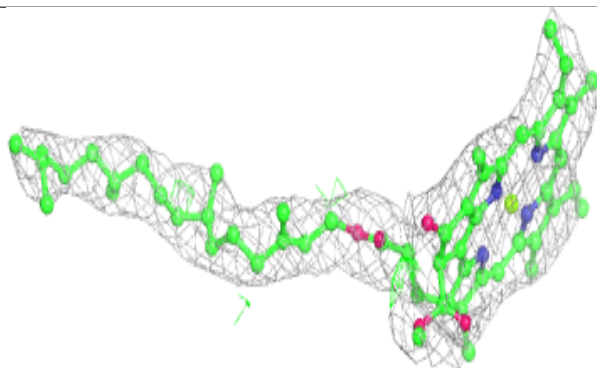
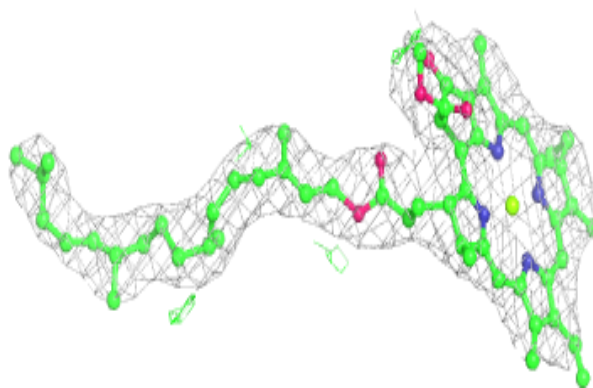
Electron density around CLA B 819:

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

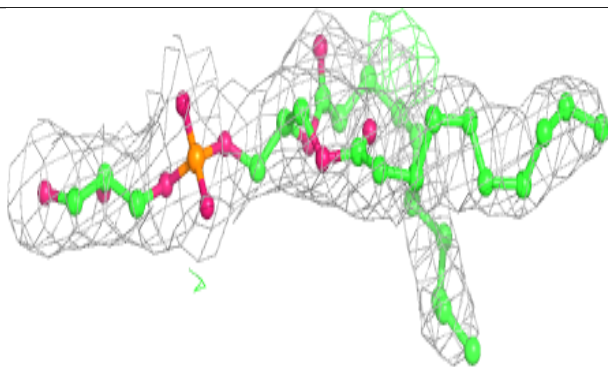
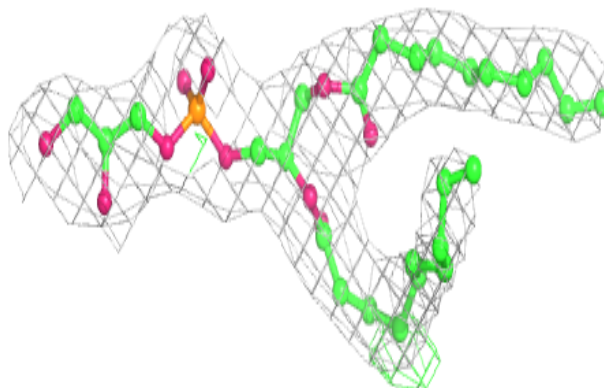


Electron density around CLA G 809:

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

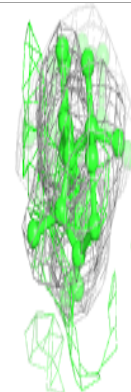
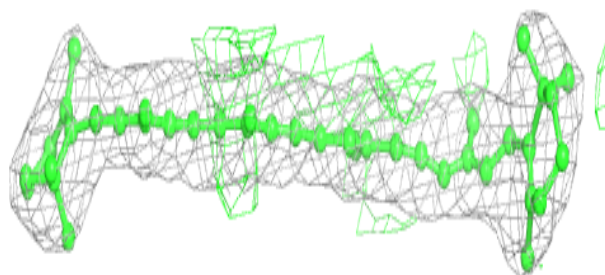
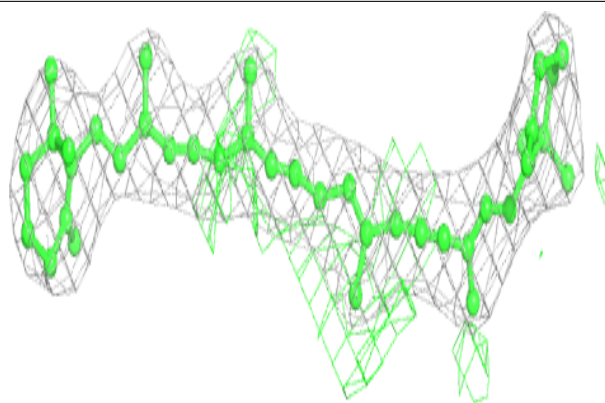
**Electron density around LHG H 847:**

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



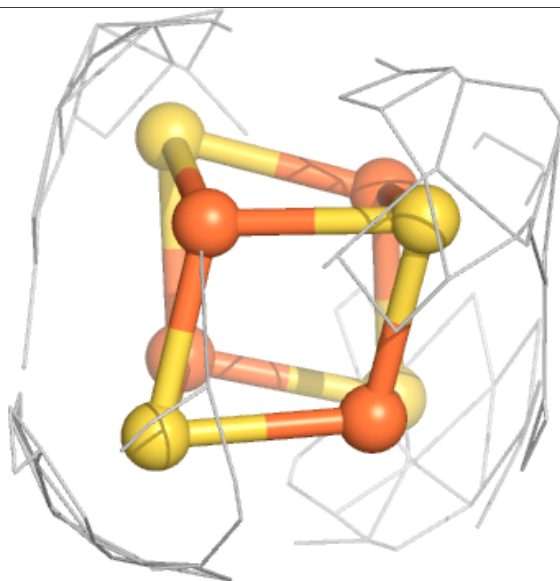
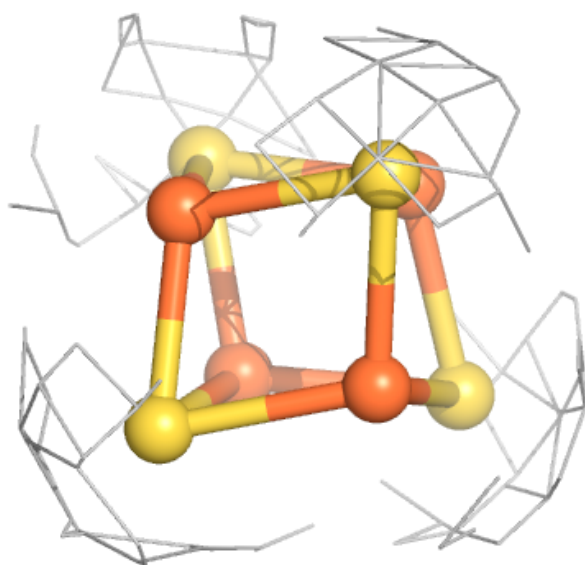
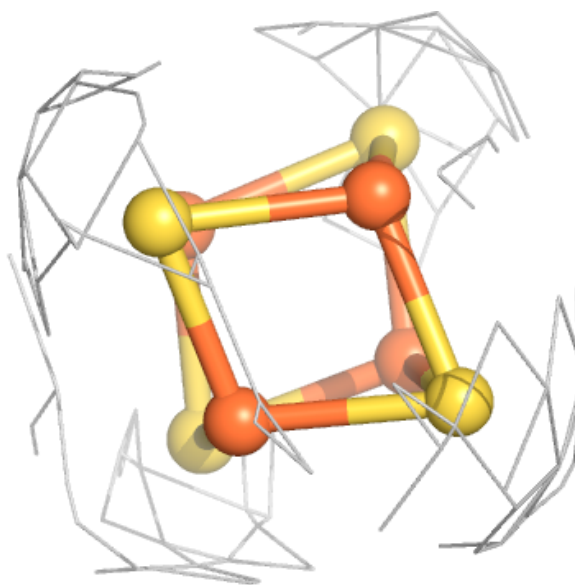
Electron density around BCR B 848:

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



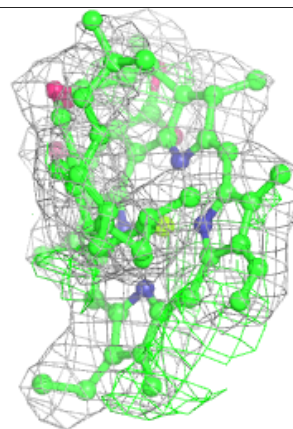
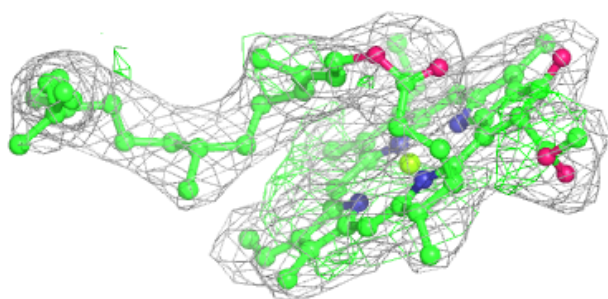
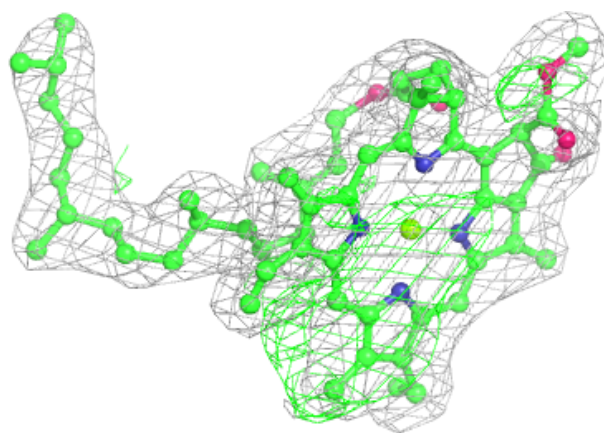
Electron density around SF4 a 101:

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



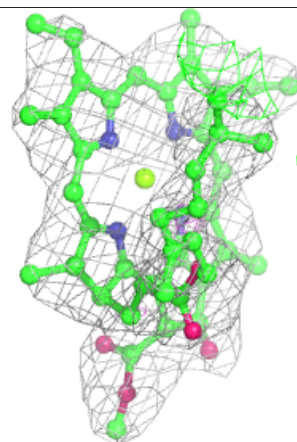
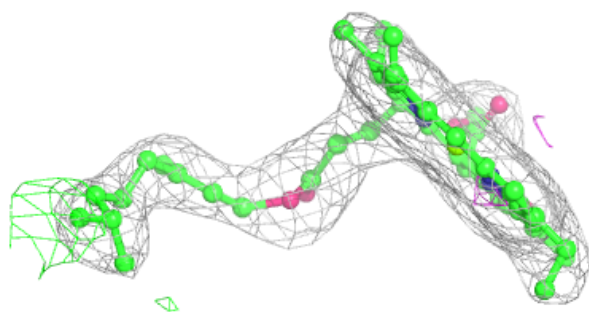
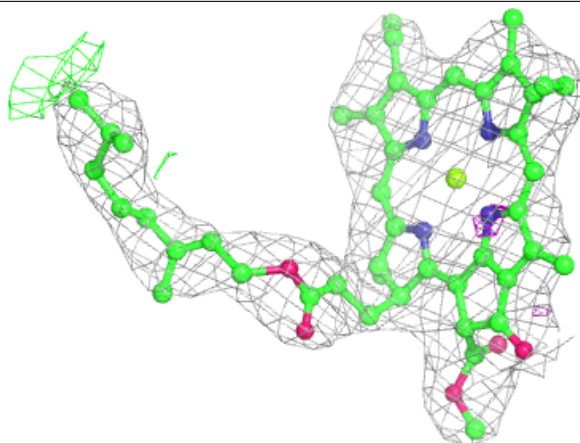
Electron density around CLA A 841:

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

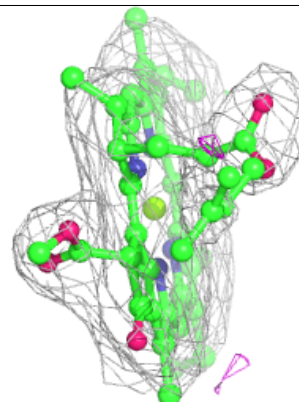
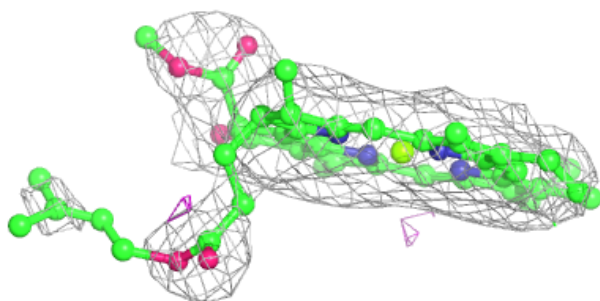
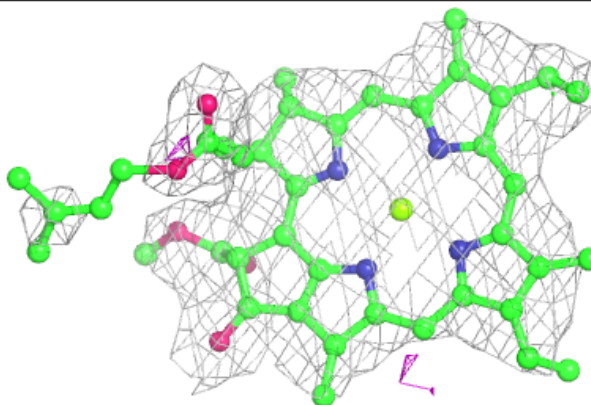


Electron density around CLA G 834:

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

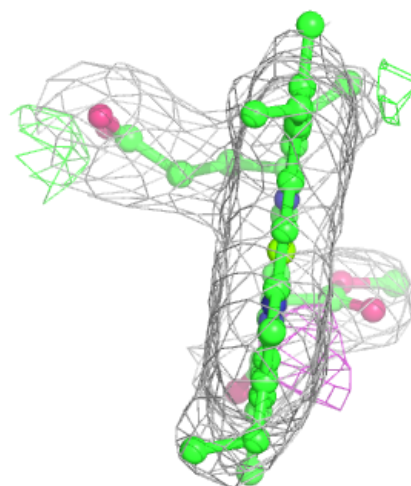
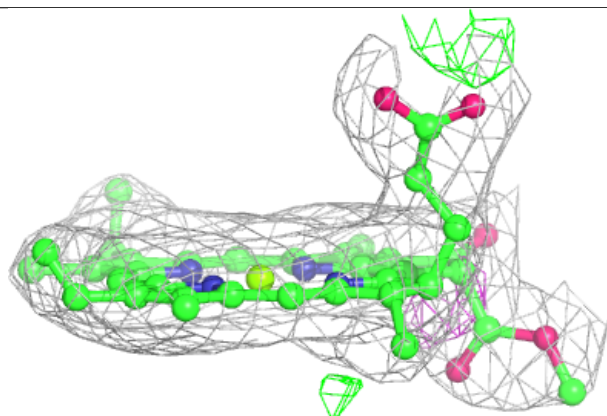
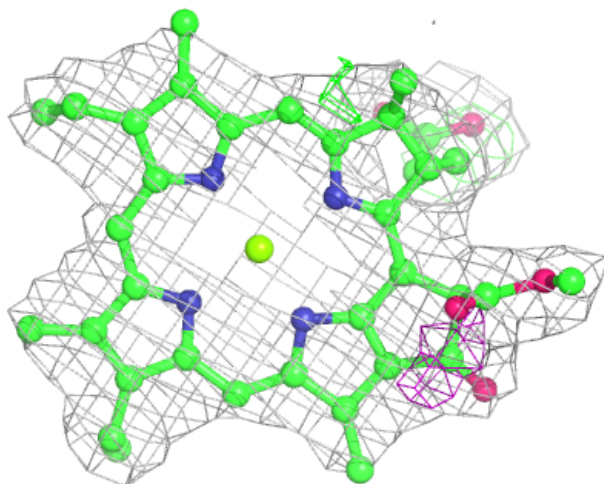
**Electron density around CLA A 816:**

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



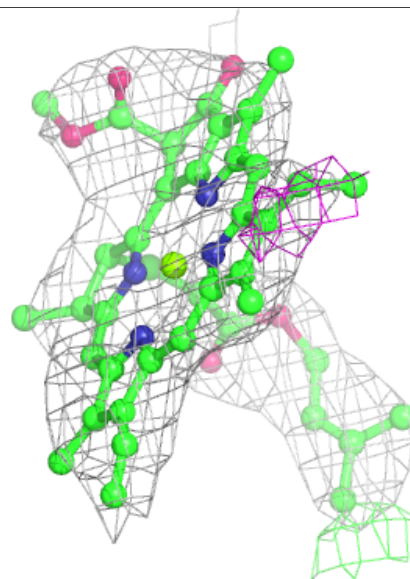
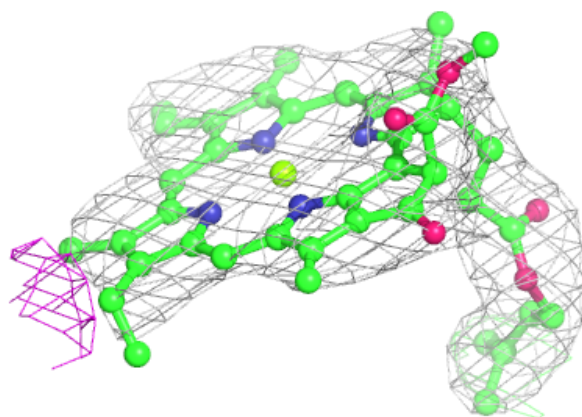
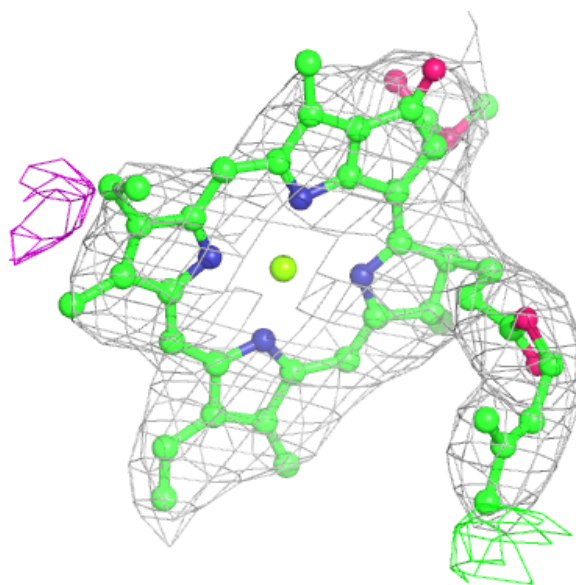
Electron density around CLA Z 837:

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



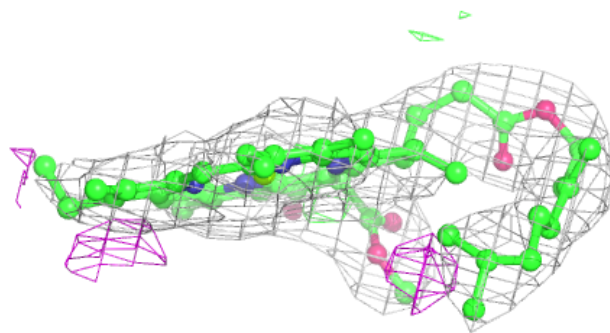
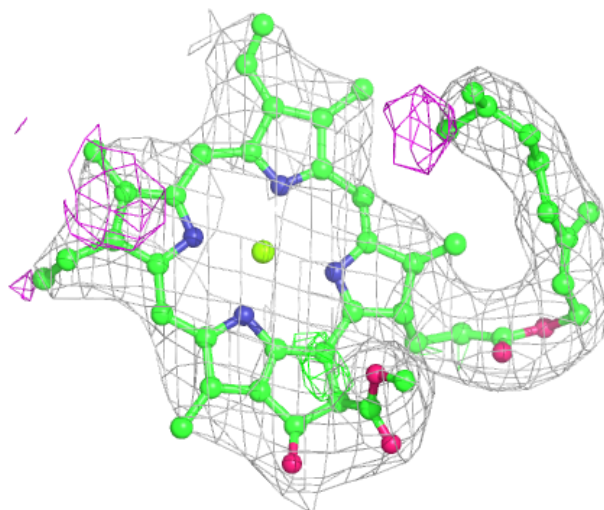
Electron density around CLA A 815:

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



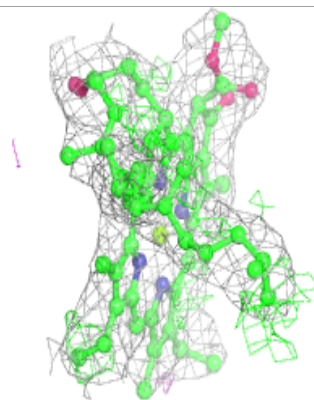
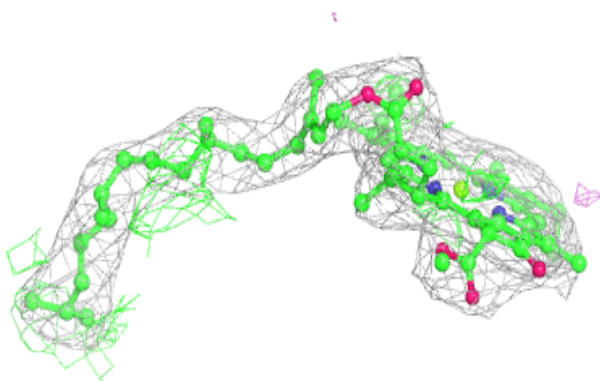
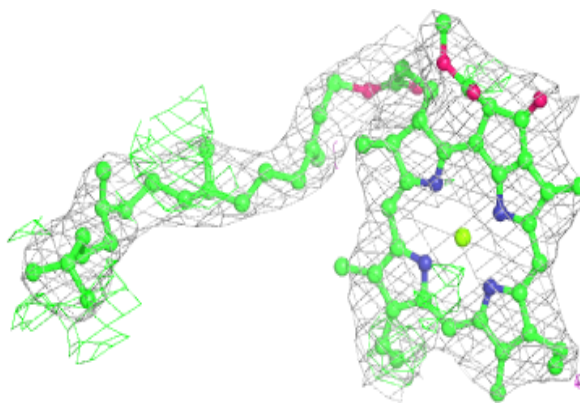
Electron density around CLA H 823:

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

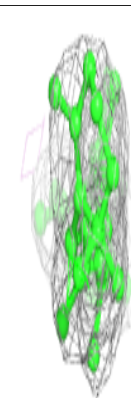
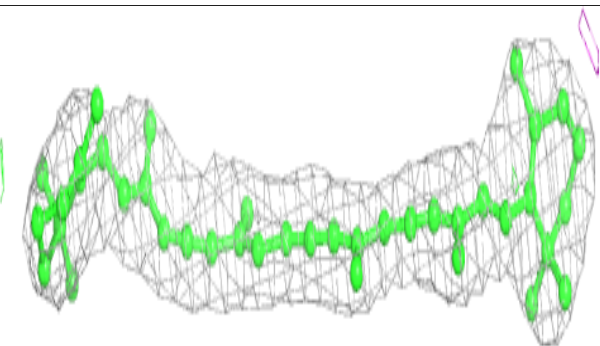
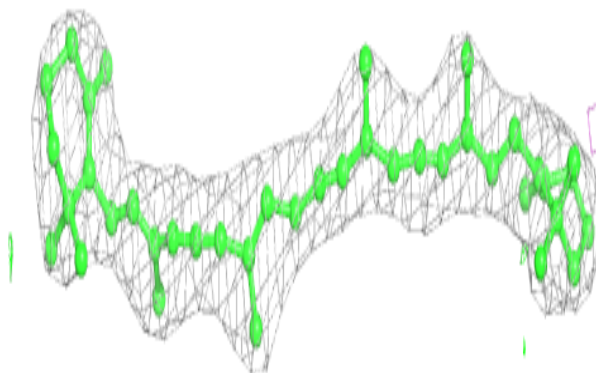


Electron density around CLA B 801:

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

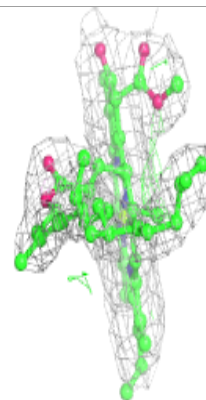
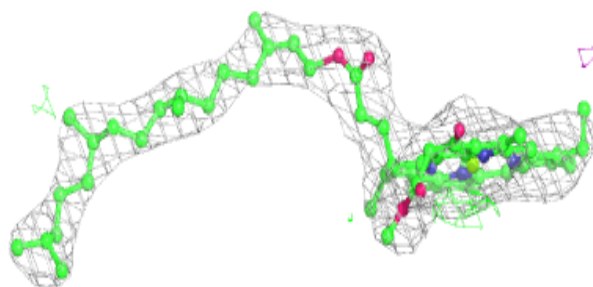
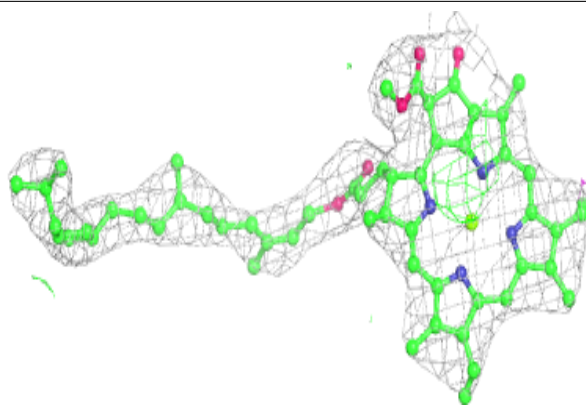
**Electron density around BCR h 202:**

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

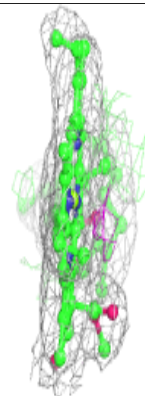
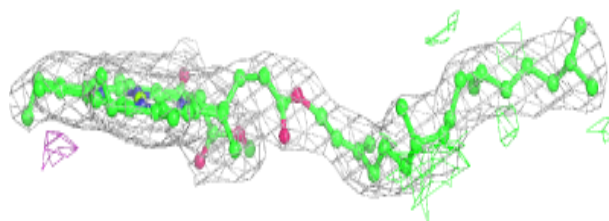
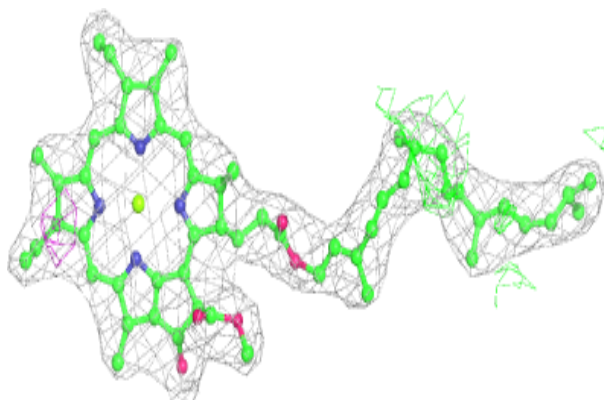


Electron density around CLA H 824:

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

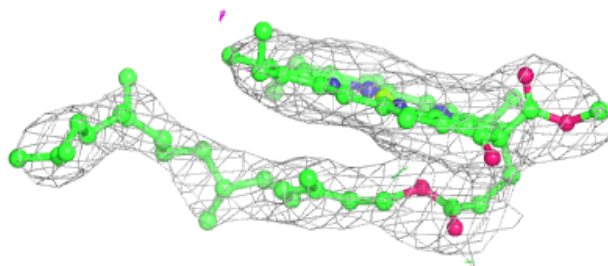
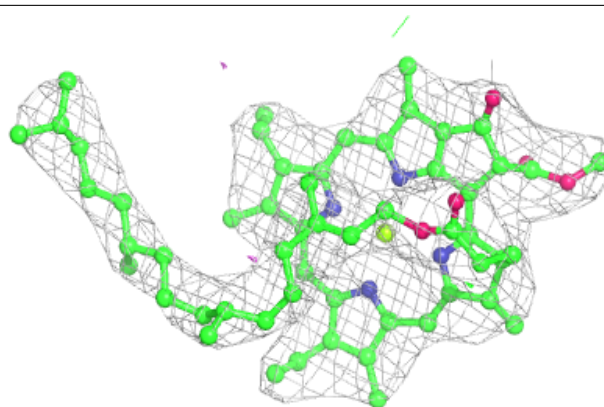
**Electron density around CLA Y 833:**

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

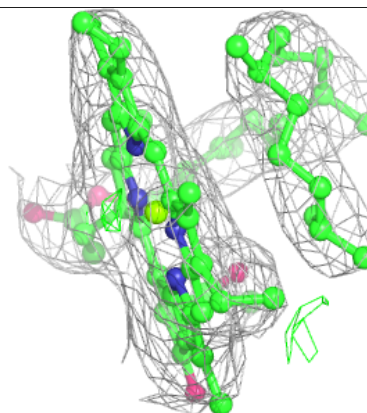
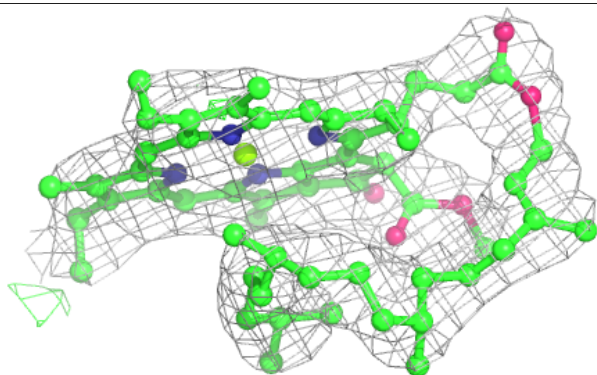
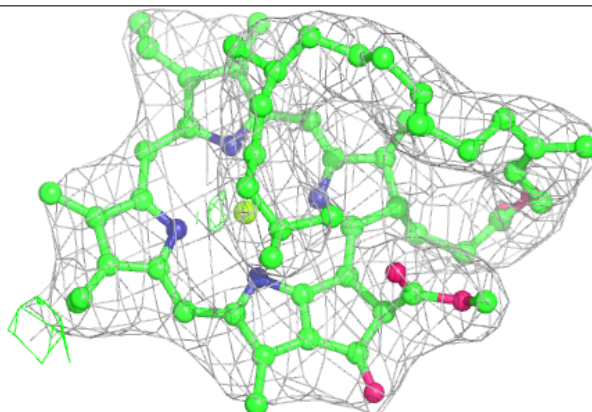


Electron density around CLA H 835:

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

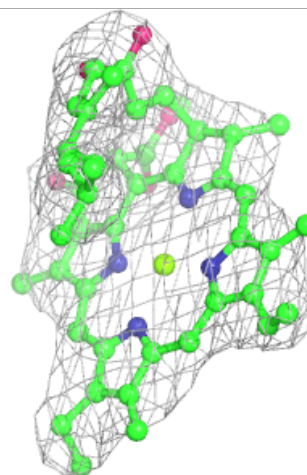
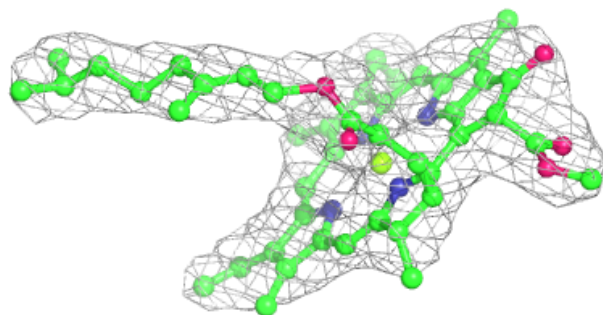
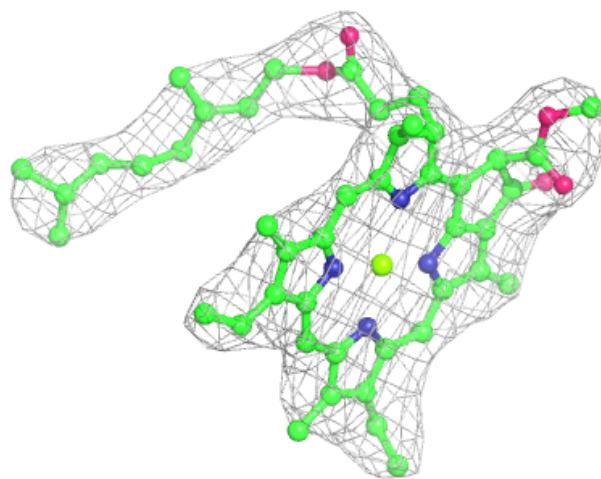
**Electron density around CLA G 806:**

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



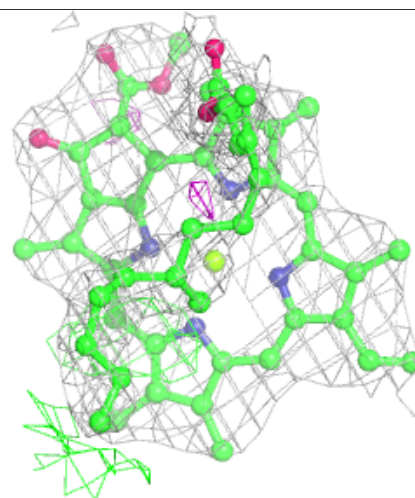
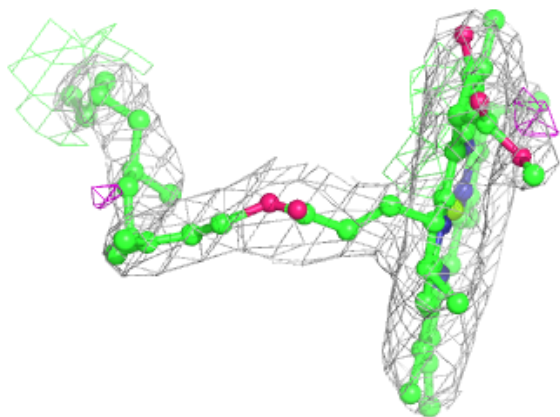
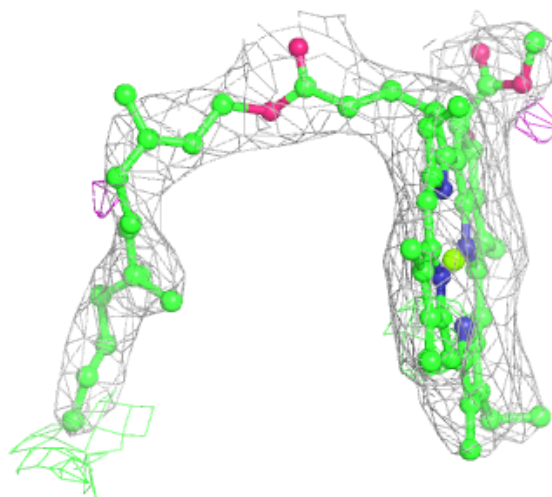
Electron density around CLA Z 814:

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



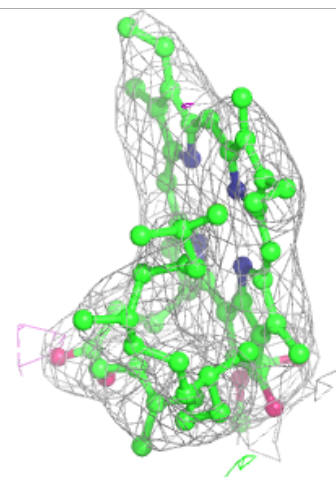
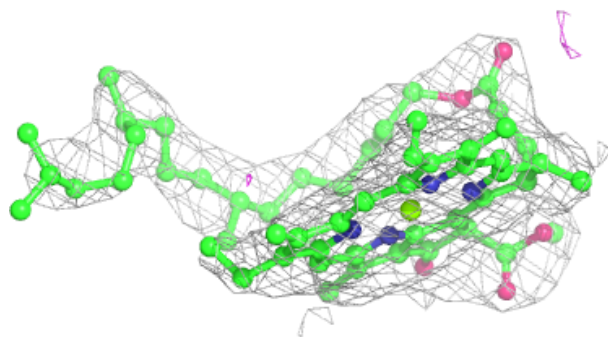
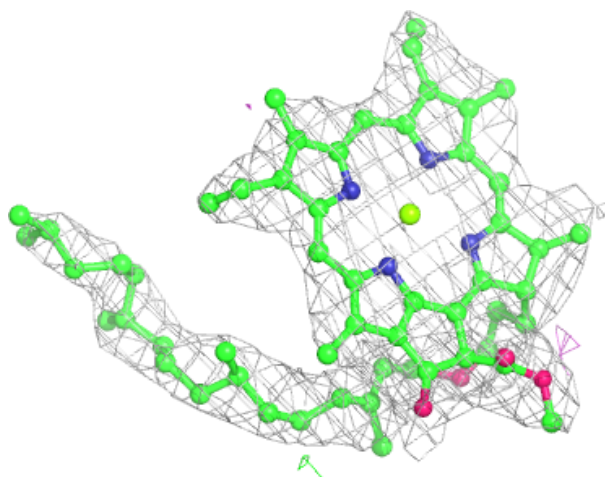
Electron density around CLA A 804:

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



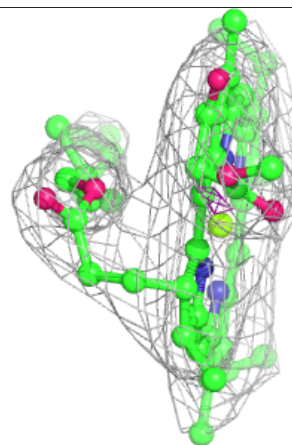
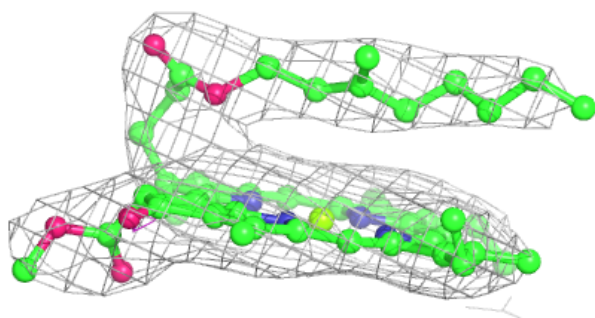
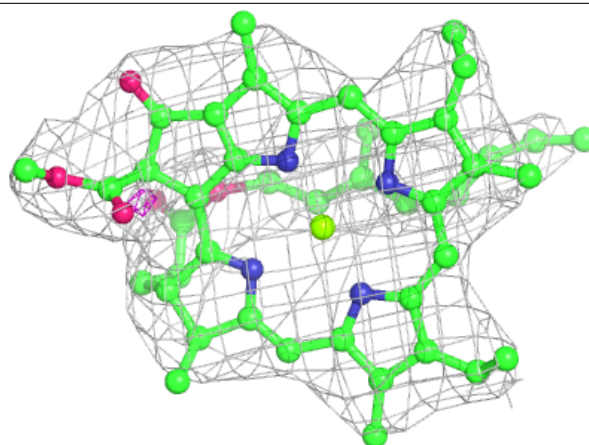
Electron density around CLA A 829:

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

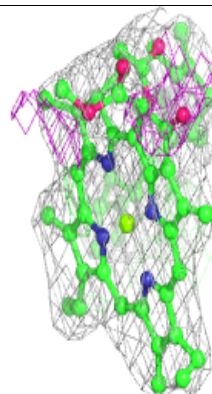
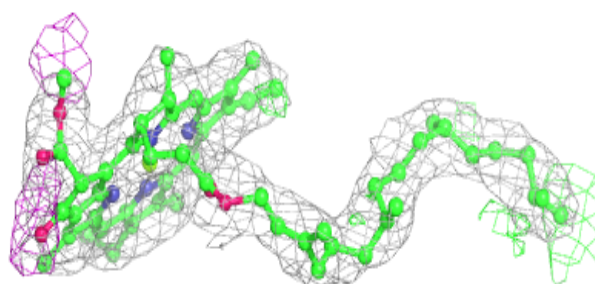
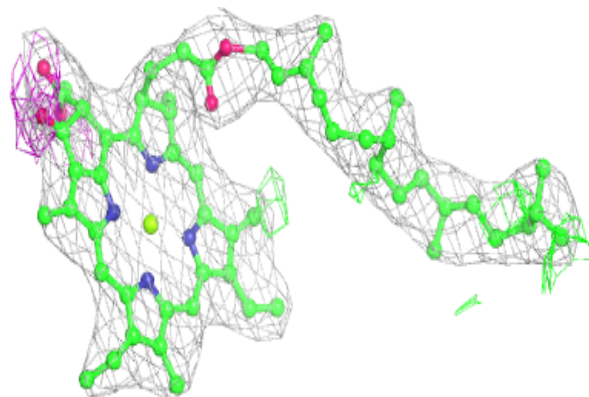


Electron density around CLA G 812:

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

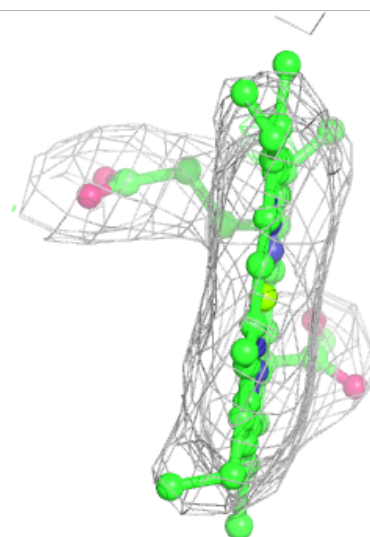
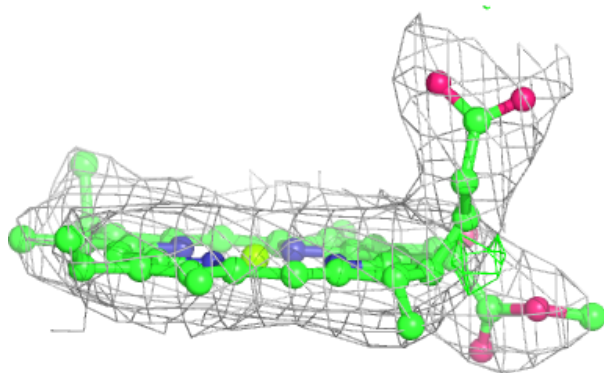
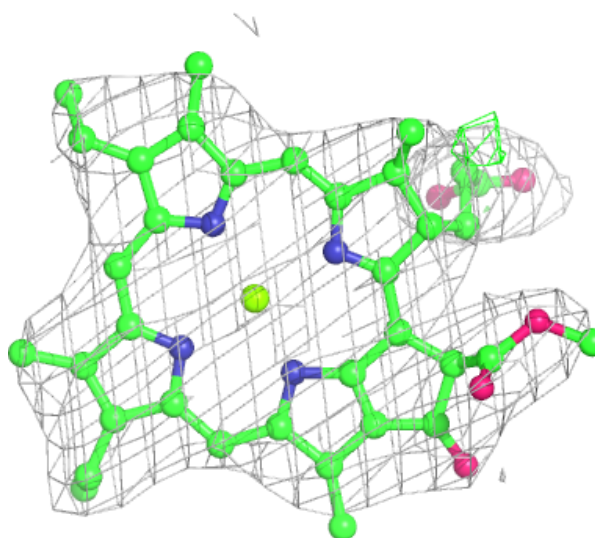
**Electron density around CLA Y 808:**

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



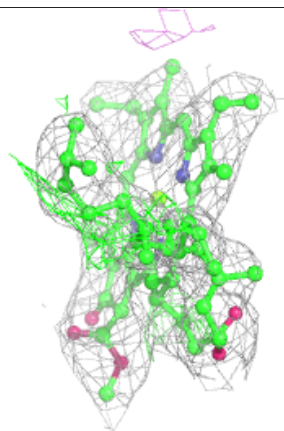
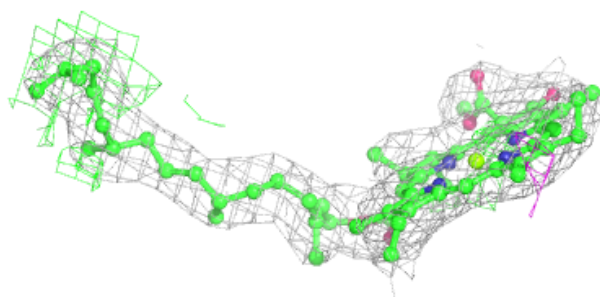
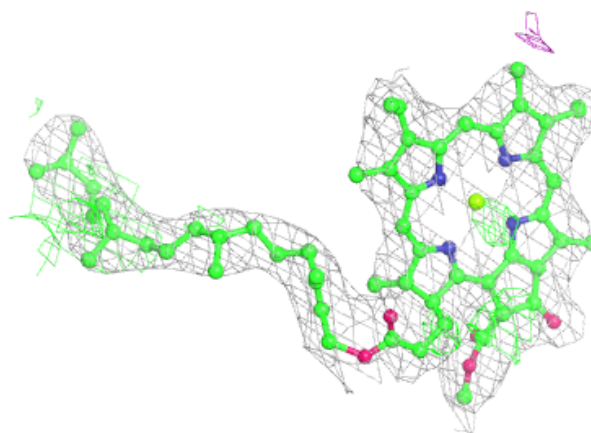
Electron density around CLA H 832:

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



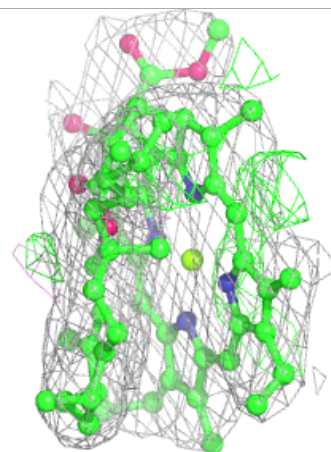
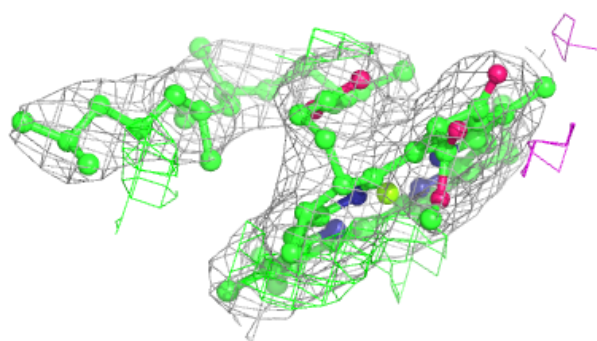
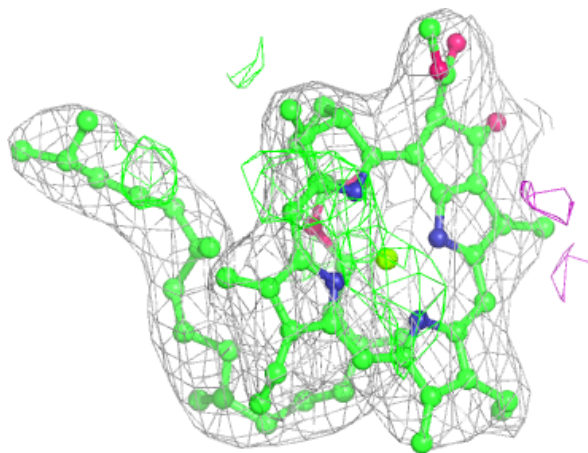
Electron density around CLA Z 801:

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



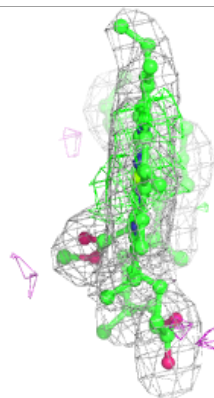
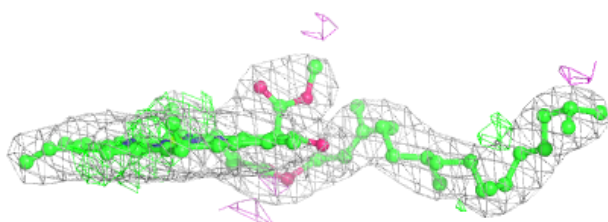
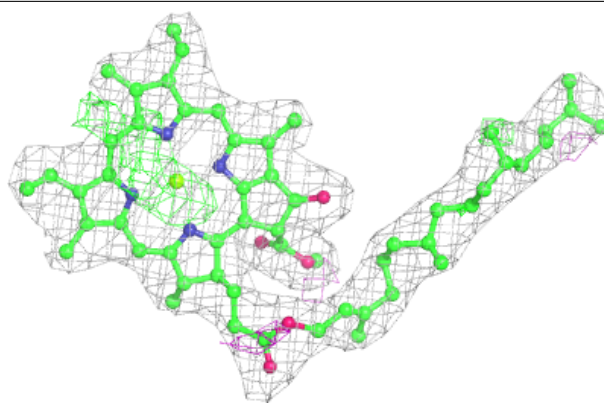
Electron density around CLA Z 807:

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

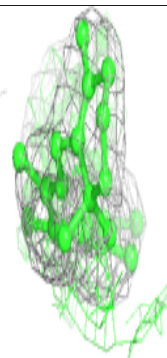
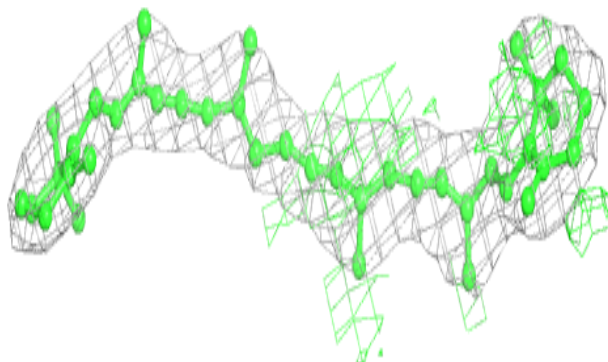
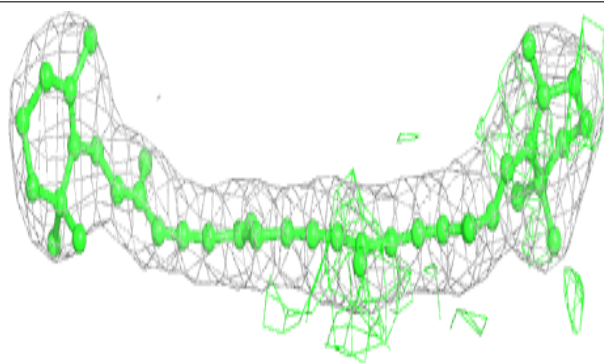


Electron density around CLA U 1004:

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

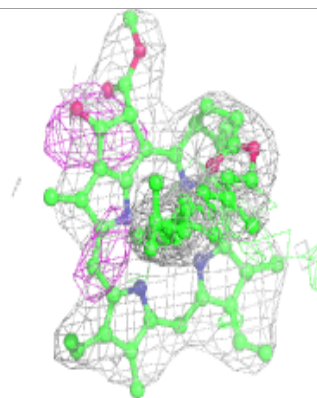
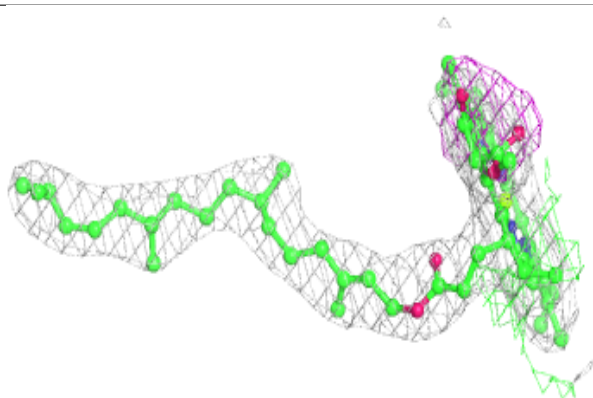
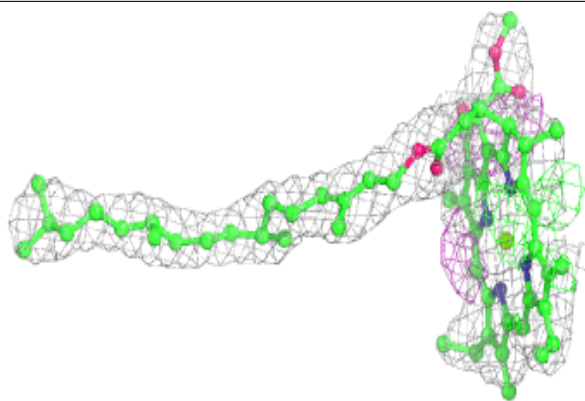
**Electron density around BCR J 104:**

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

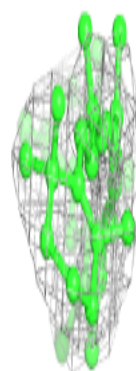
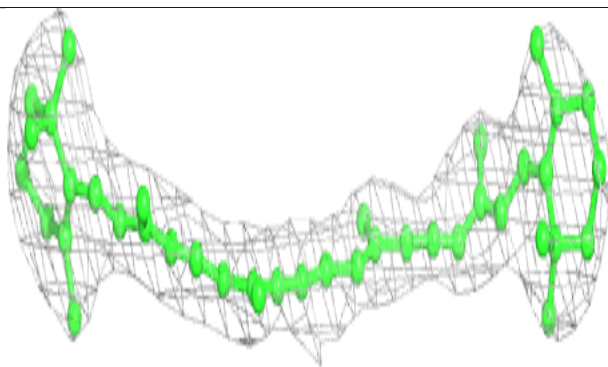
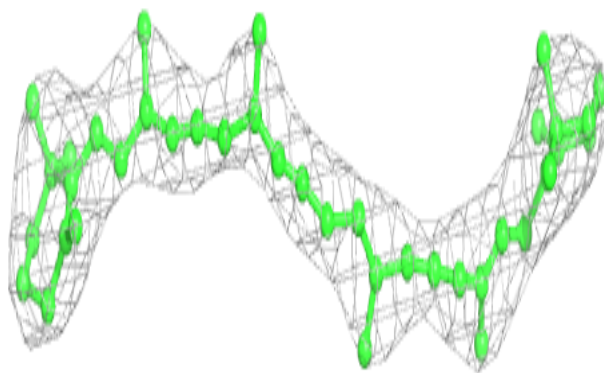


Electron density around CLA H 827:

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

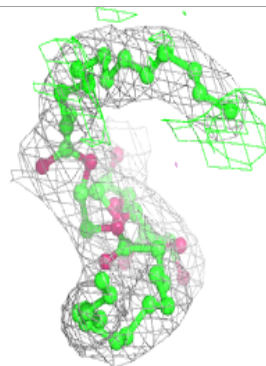
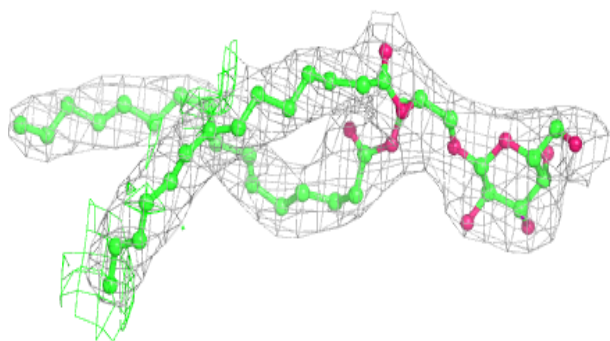
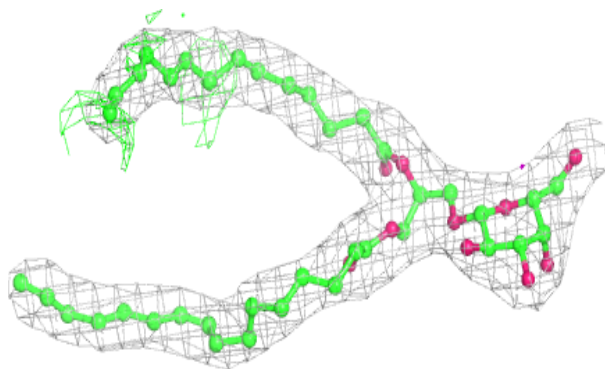
**Electron density around BCR Y 848:**

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

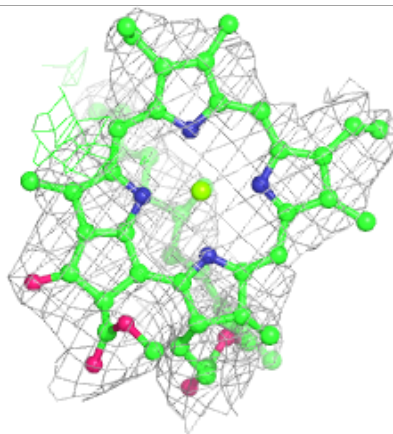
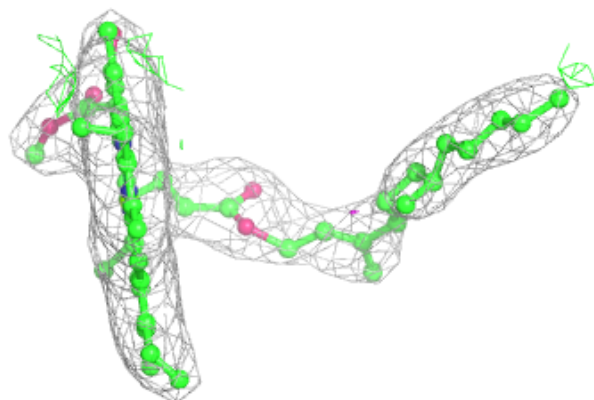
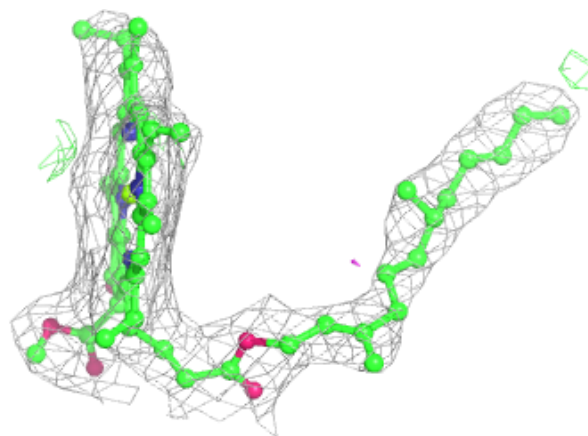


Electron density around LMG Z 847:

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

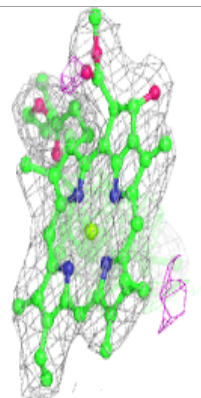
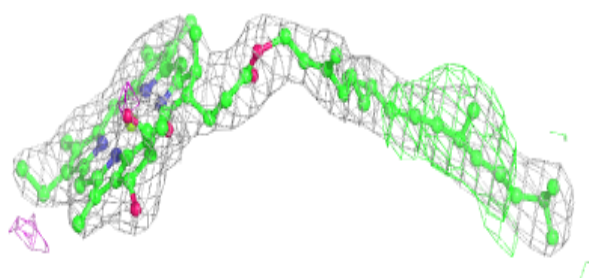
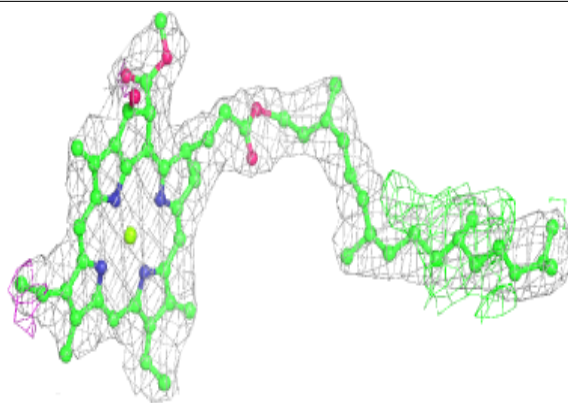
**Electron density around CLA G 804:**

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

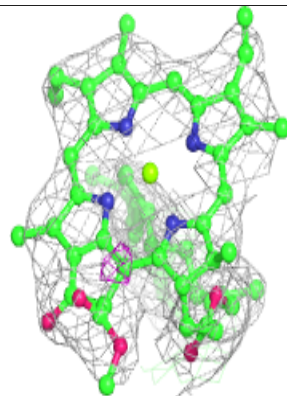
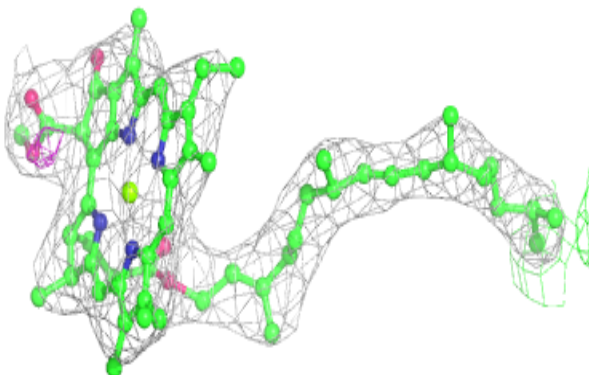
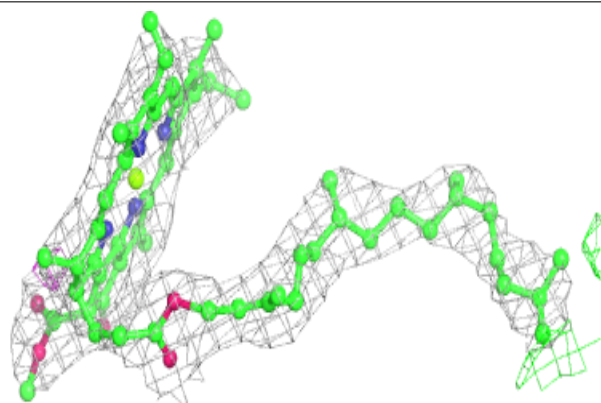


Electron density around CLA Y 802:

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

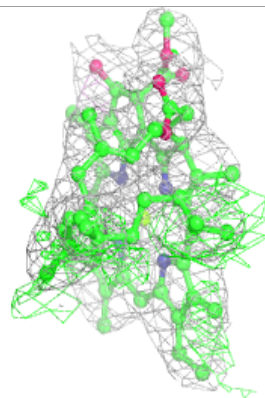
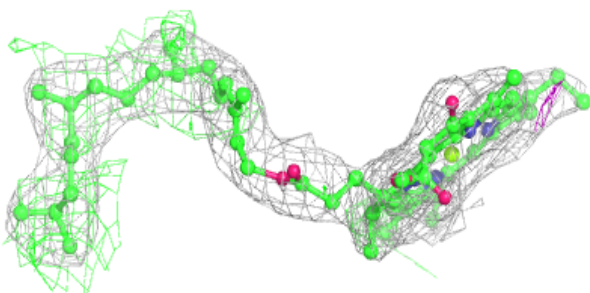
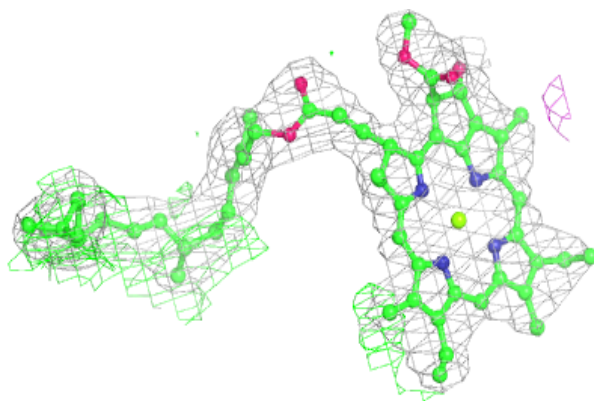
**Electron density around CLA G 811:**

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

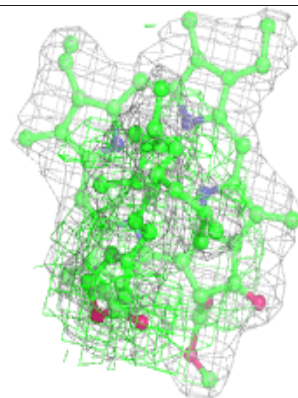
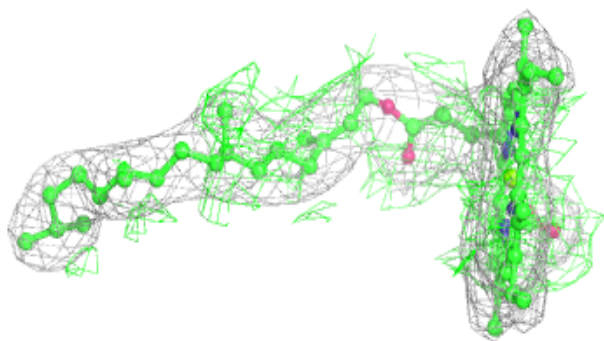
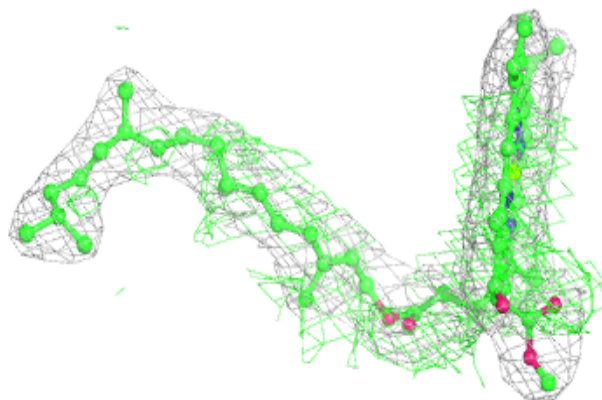


Electron density around CLA H 808:

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

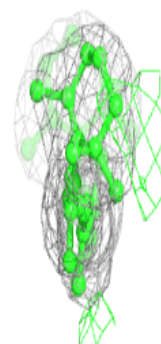
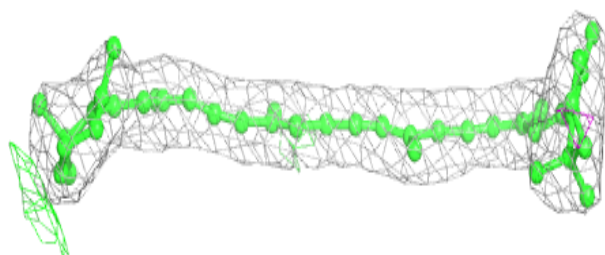
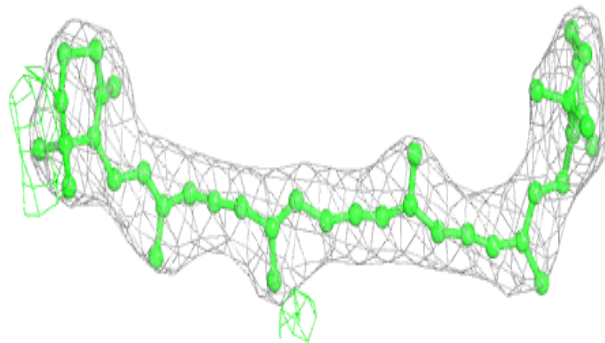
**Electron density around CLA H 838:**

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

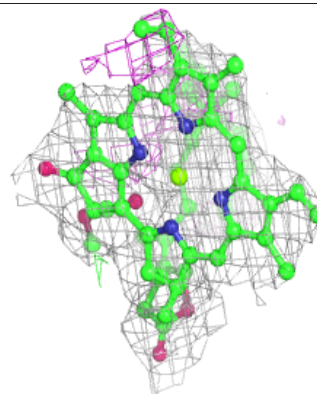
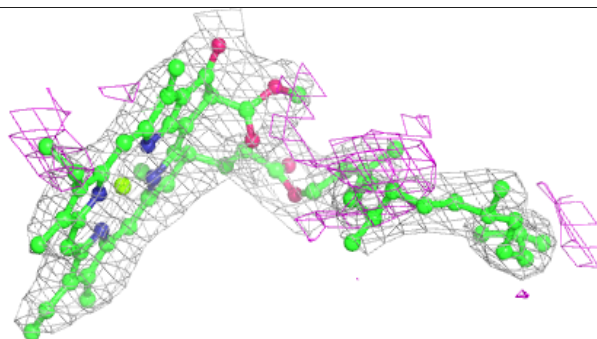
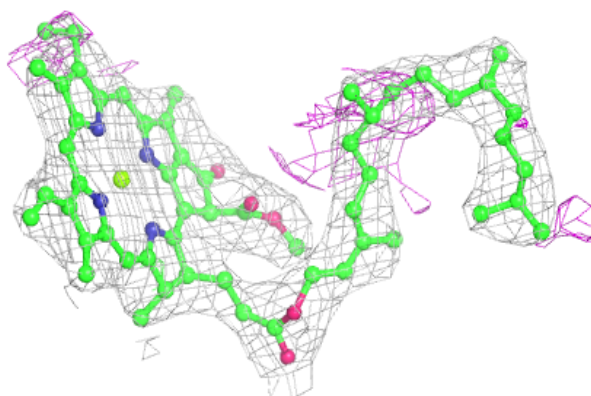


Electron density around BCR L 203:

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

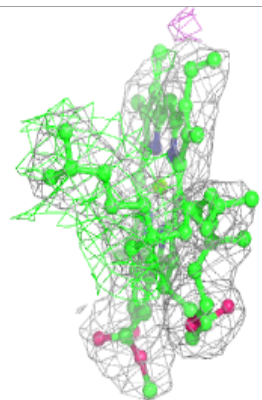
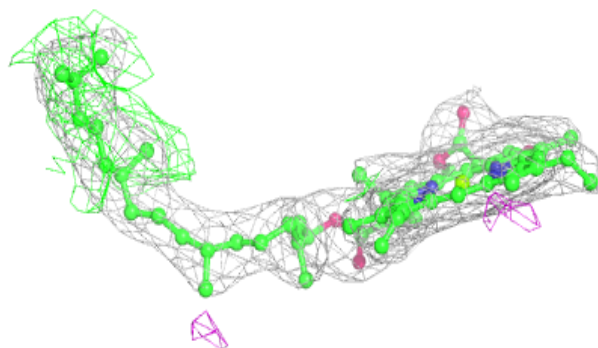
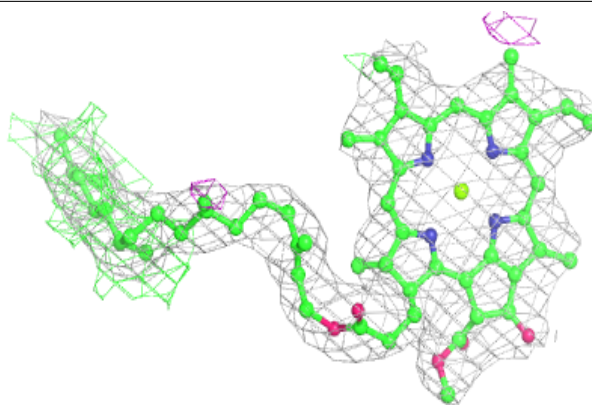
**Electron density around CL0 G 801:**

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

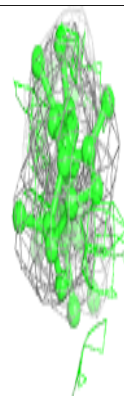
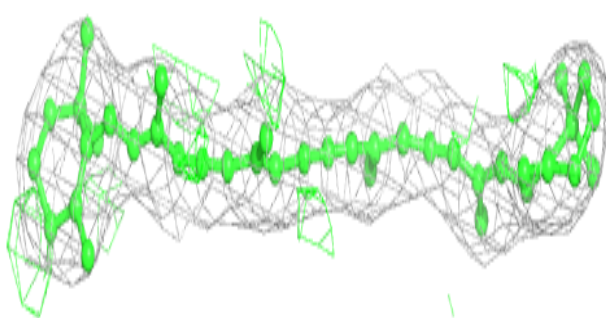
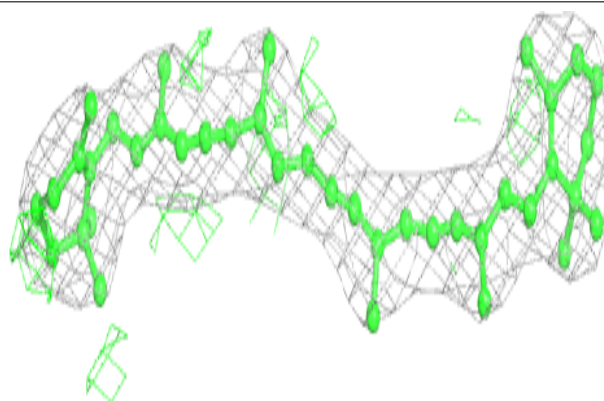


Electron density around CLA B 804:

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

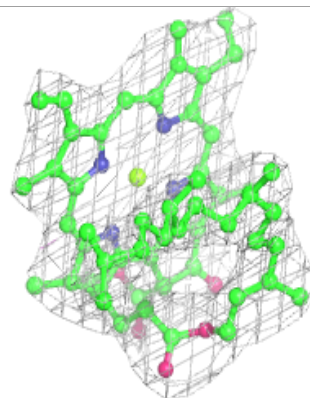
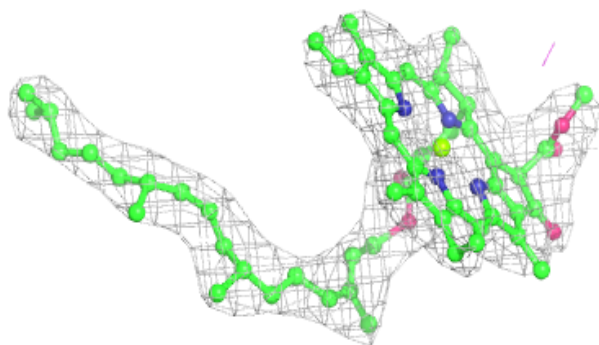
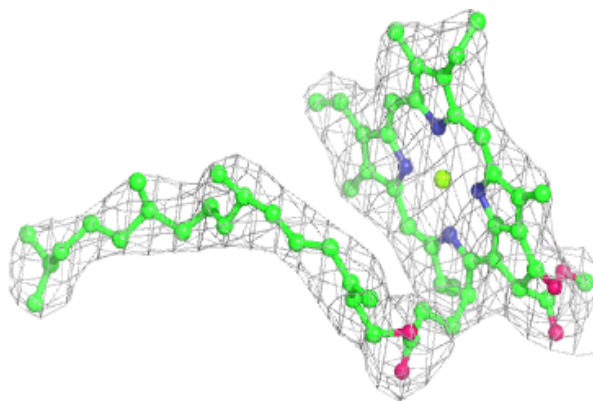
**Electron density around BCR f 103:**

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



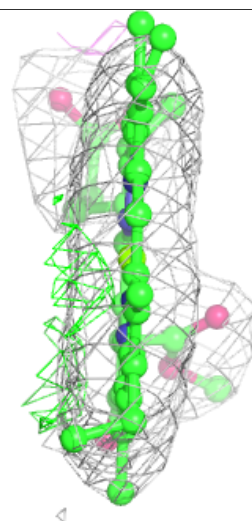
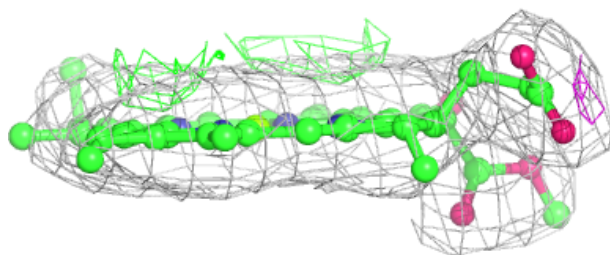
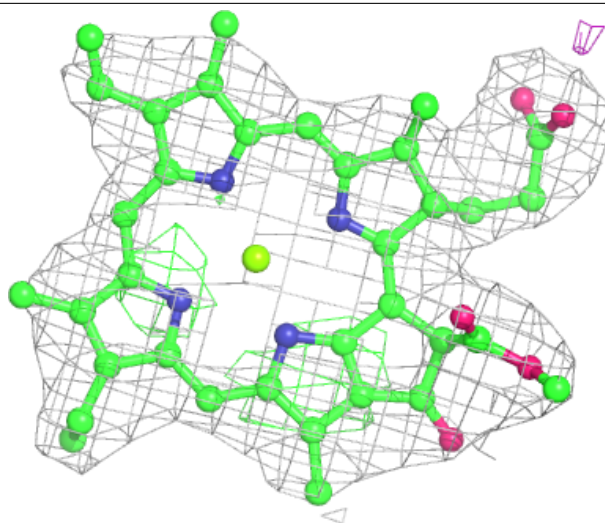
Electron density around CLA Z 812:

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



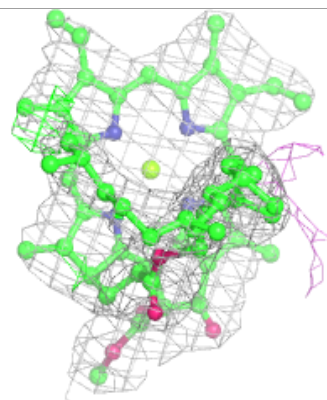
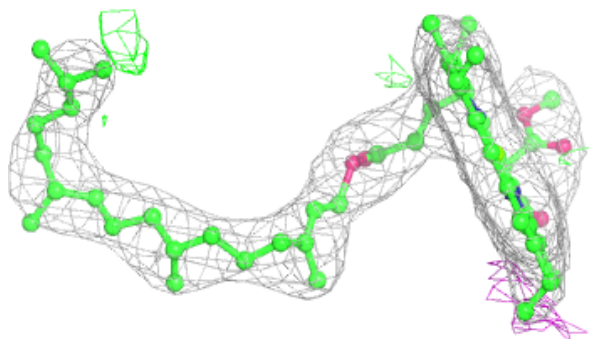
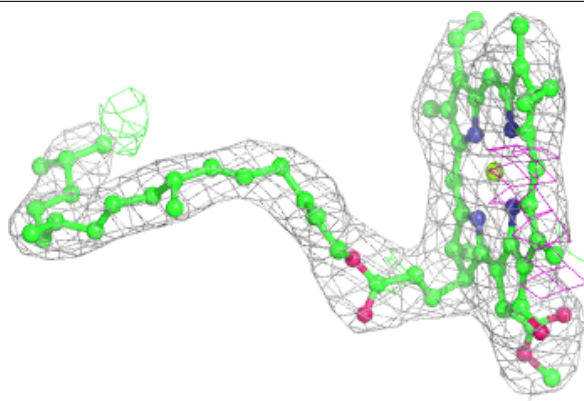
Electron density around CLA j 102:

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

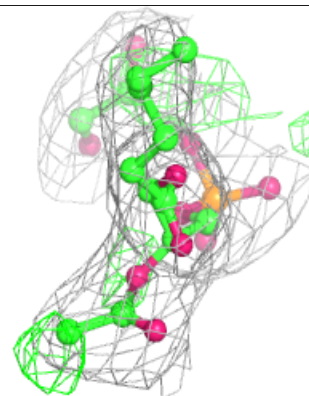
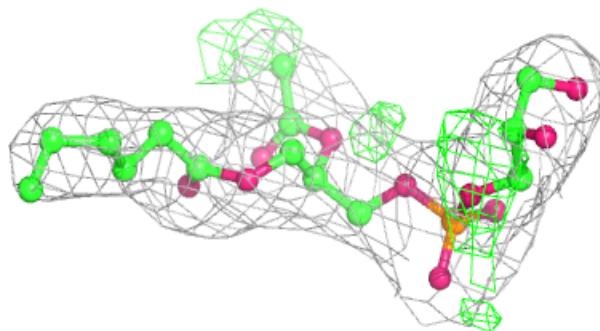
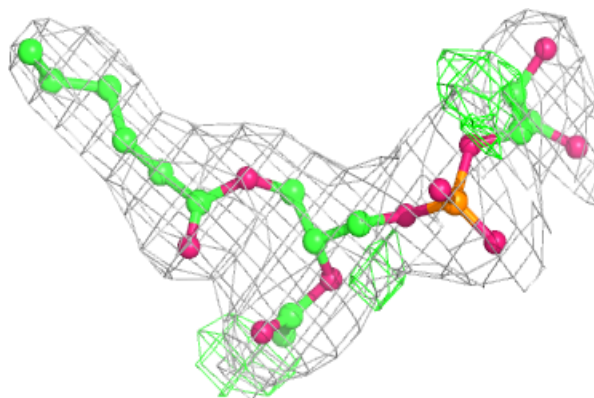


Electron density around CLA L 206:

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

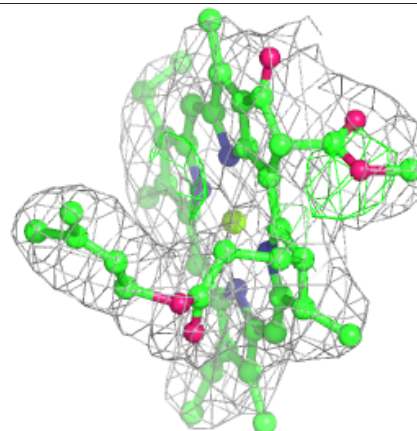
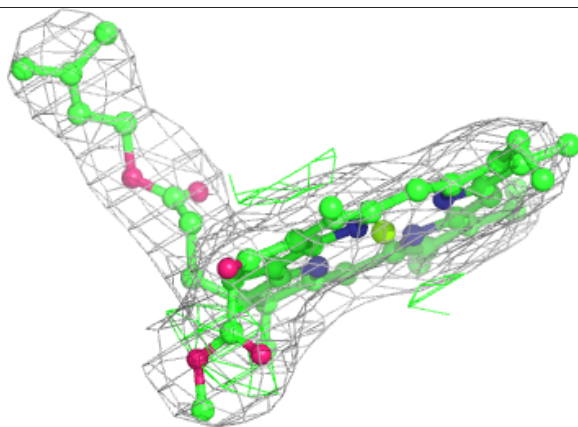
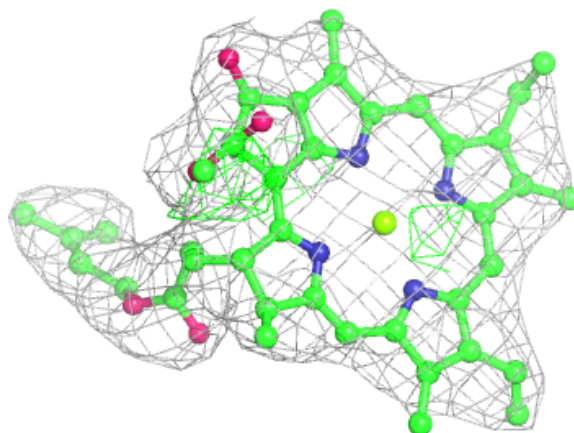
**Electron density around LHG Y 853:**

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



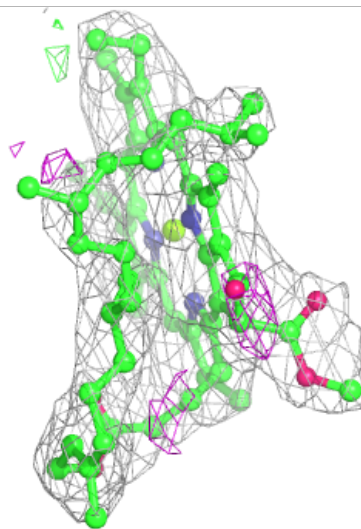
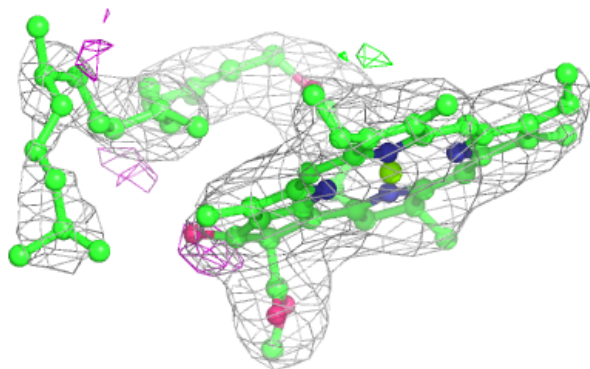
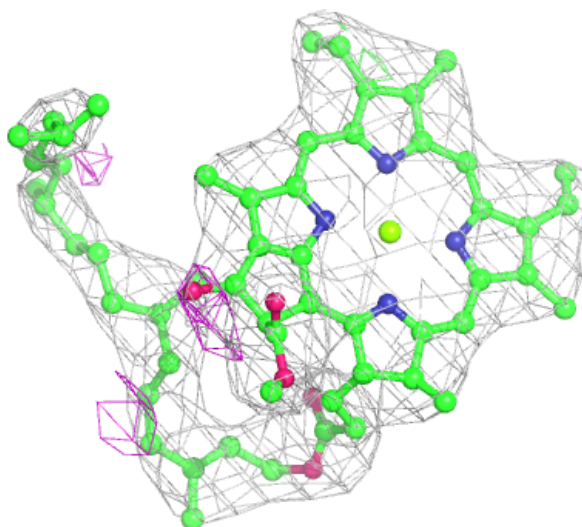
Electron density around CLA A 838:

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



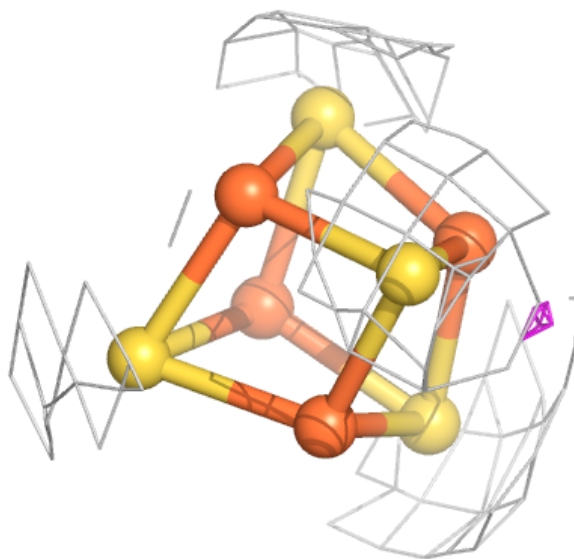
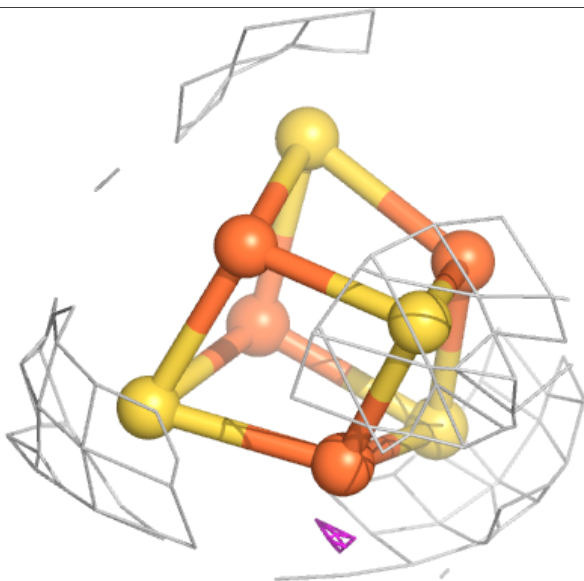
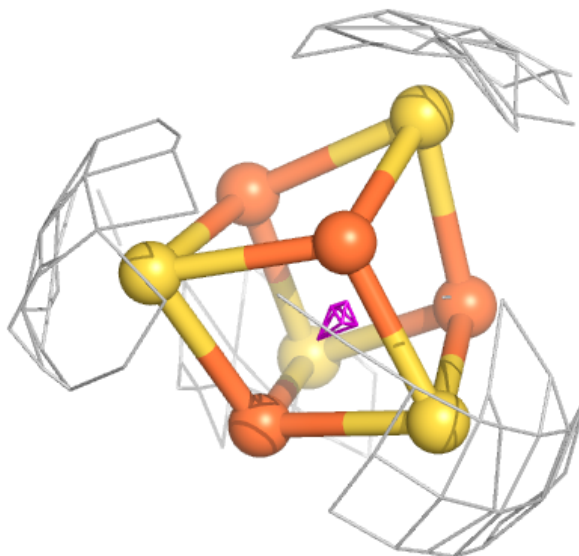
Electron density around CLA Z 830:

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



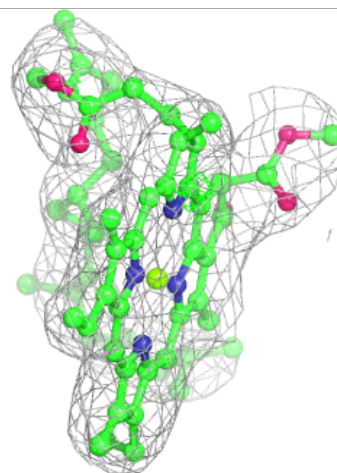
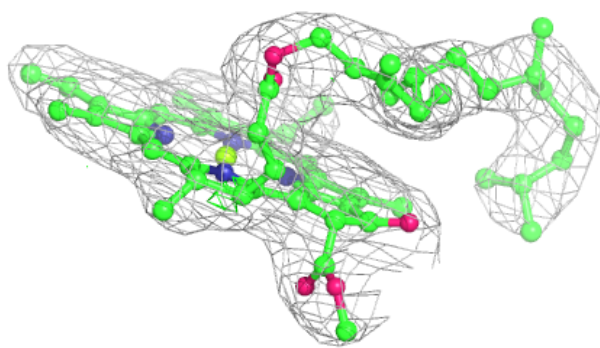
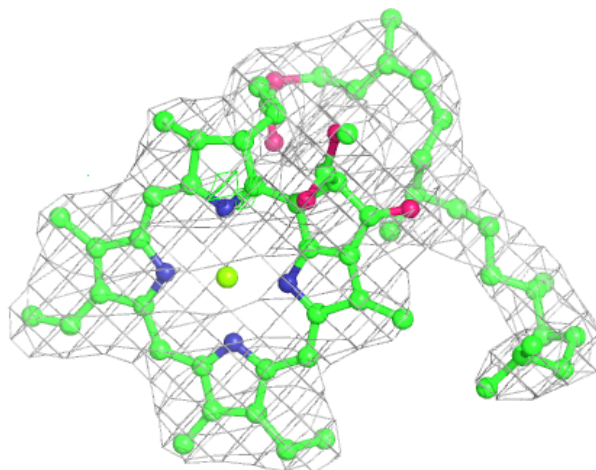
Electron density around SF4 N 102:

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



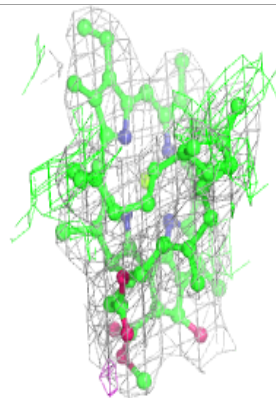
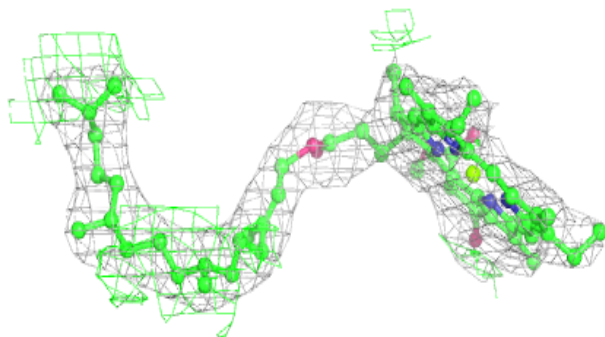
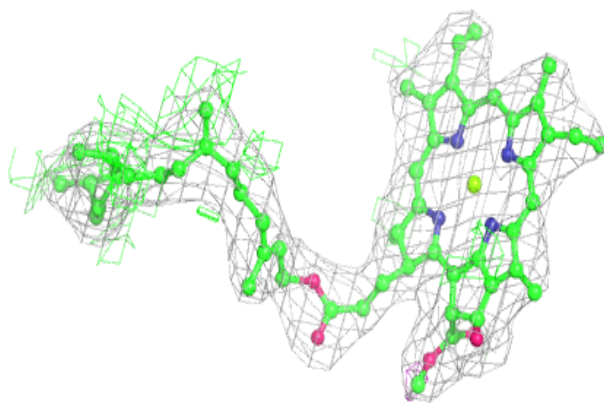
Electron density around CLA B 832:

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



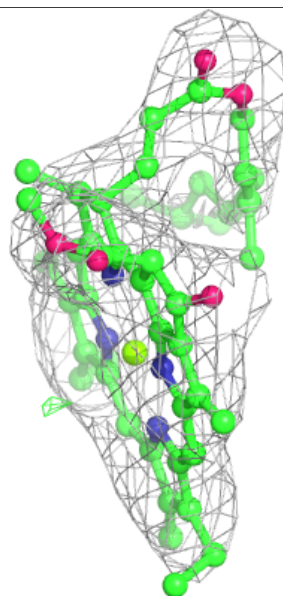
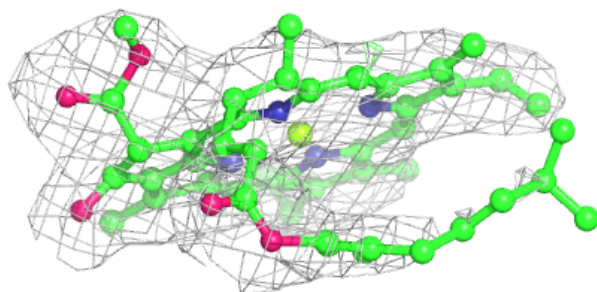
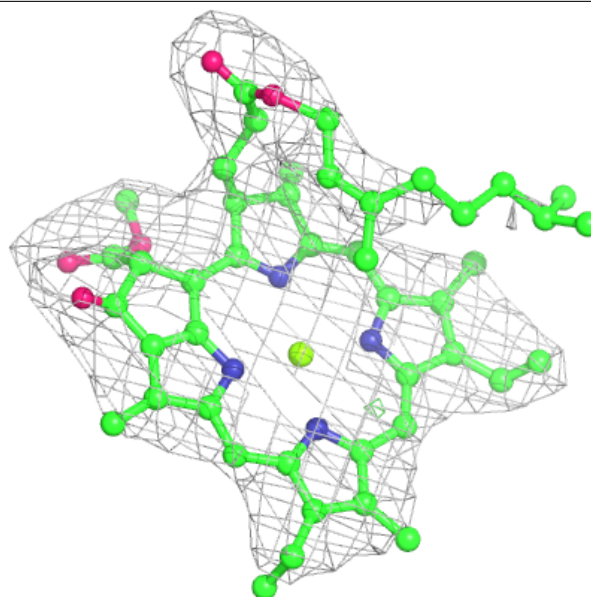
Electron density around CLA B 810:

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



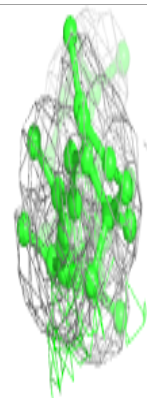
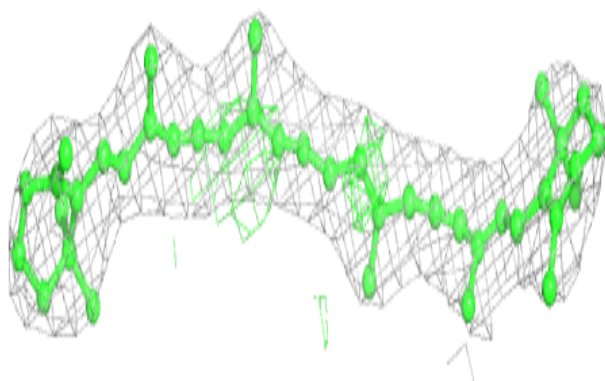
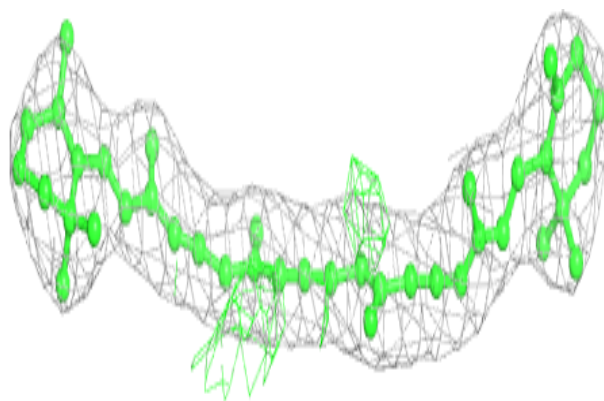
Electron density around CLA S 1103:

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



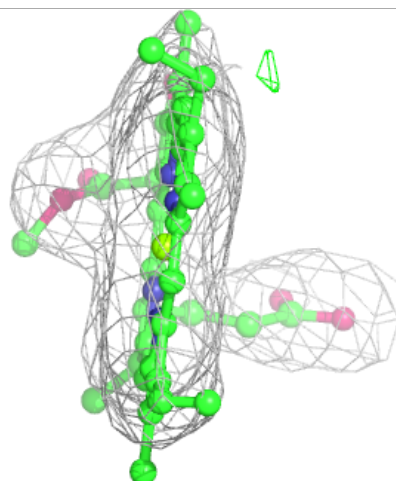
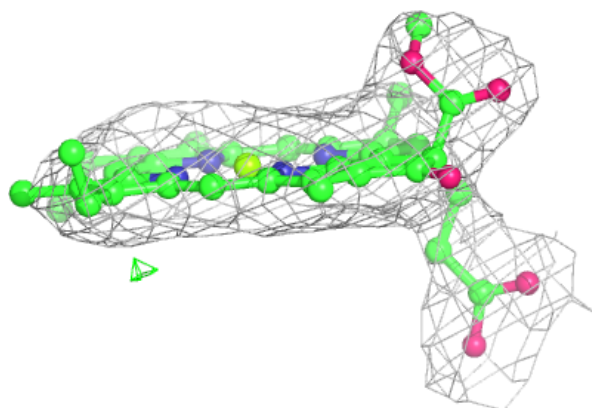
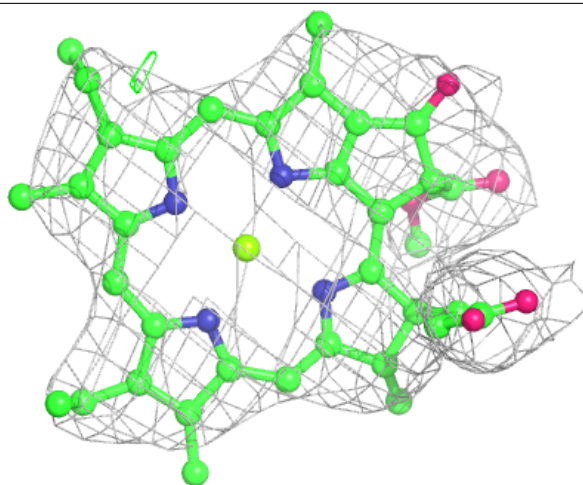
Electron density around BCR f 104:

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



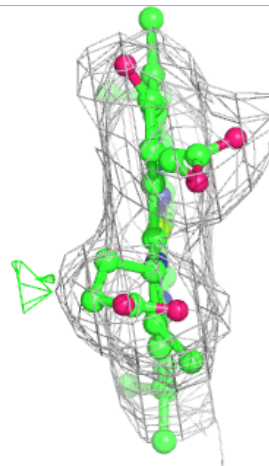
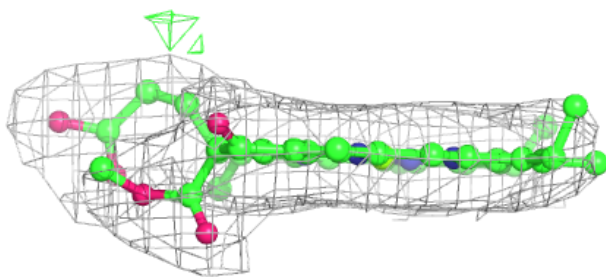
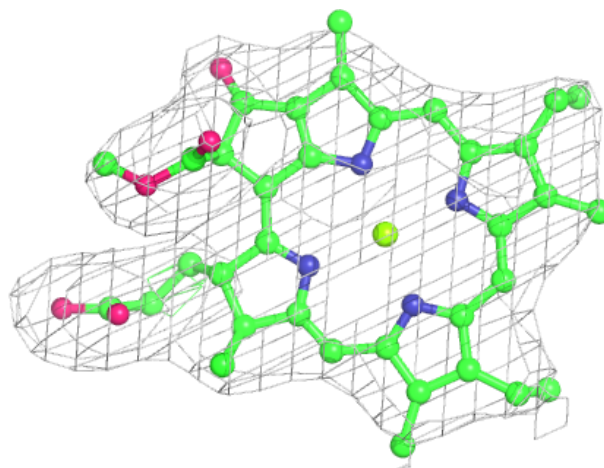
Electron density around CLA T 103:

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



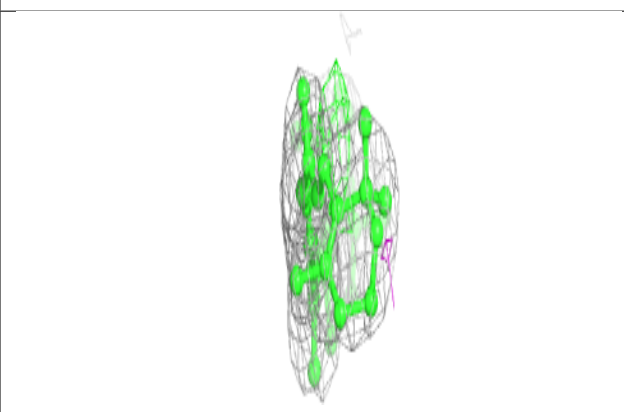
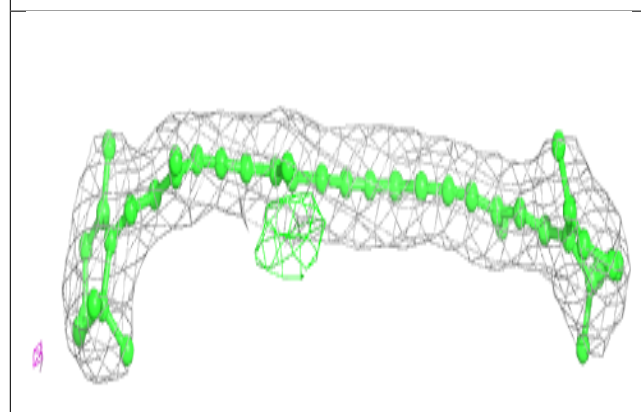
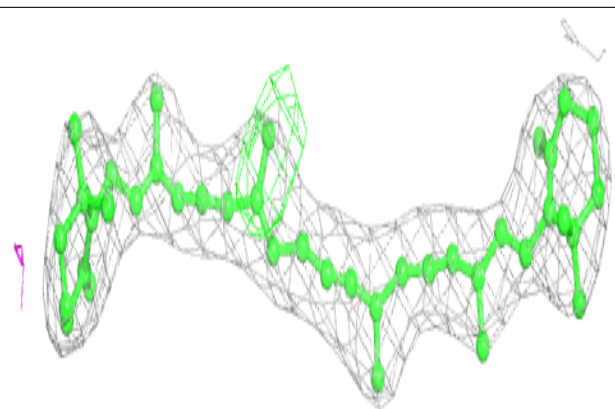
Electron density around CLA H 833:

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

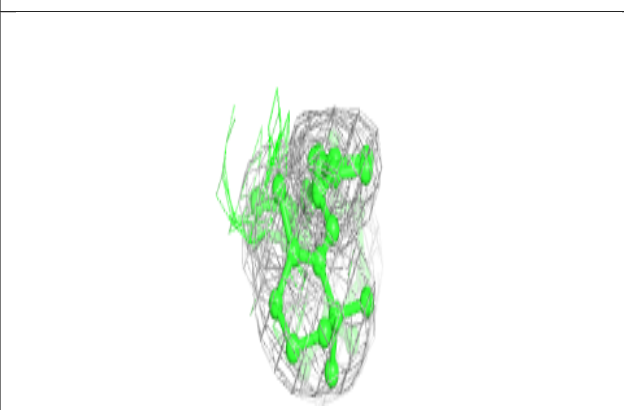
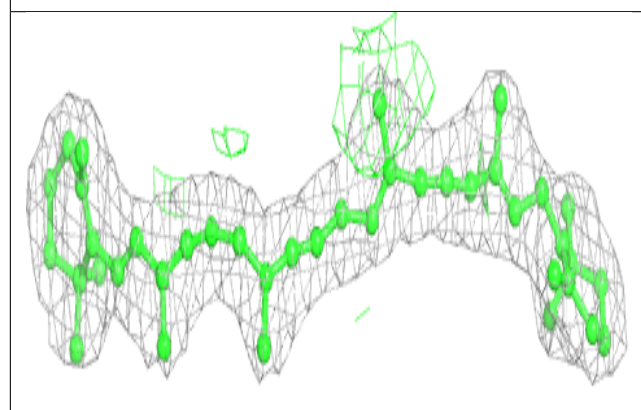
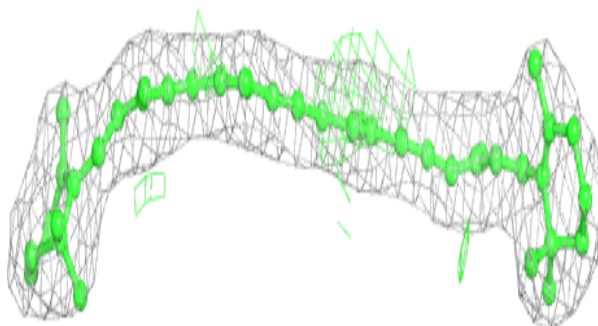


Electron density around BCR Y 850:

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

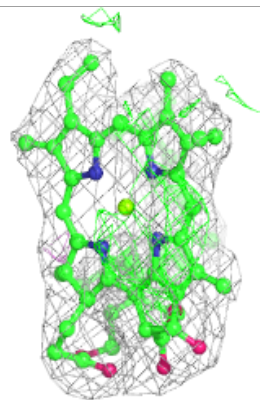
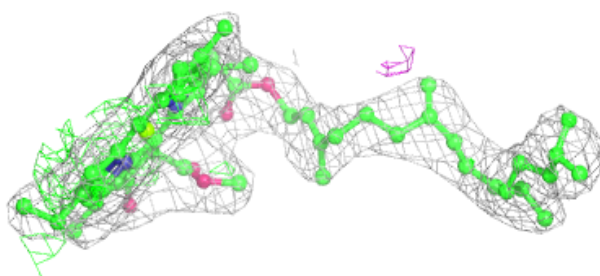
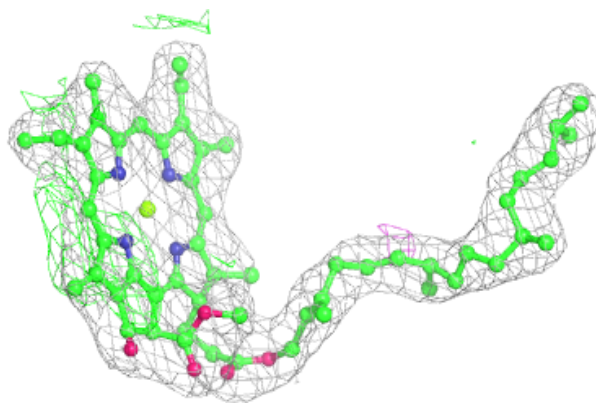
**Electron density around BCR R 101:**

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

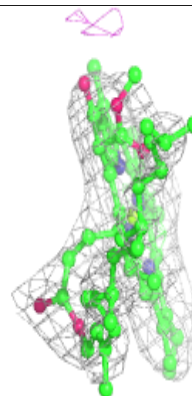
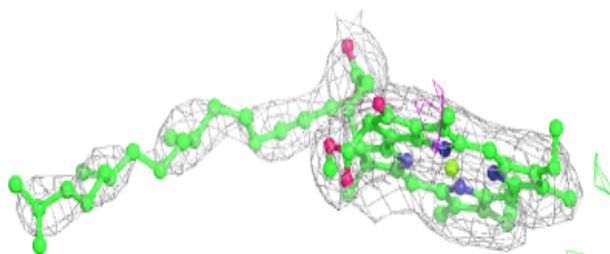
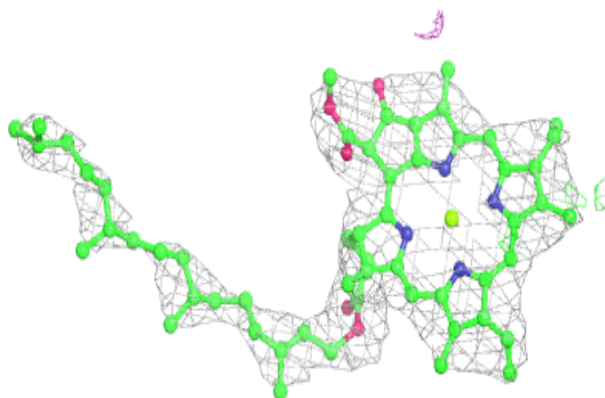


Electron density around CLA H 809:

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

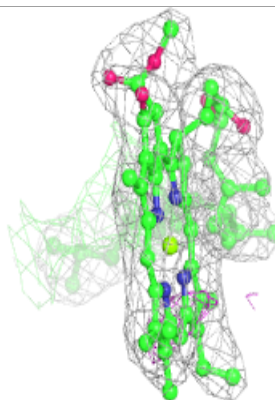
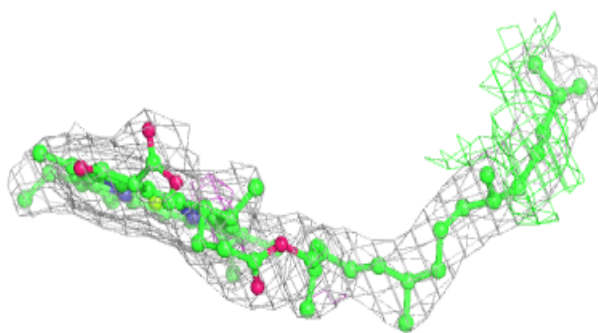
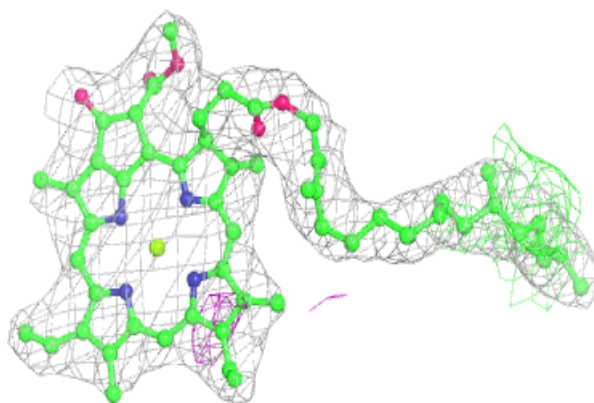
**Electron density around CLA Y 822:**

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

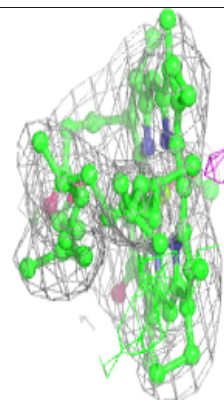
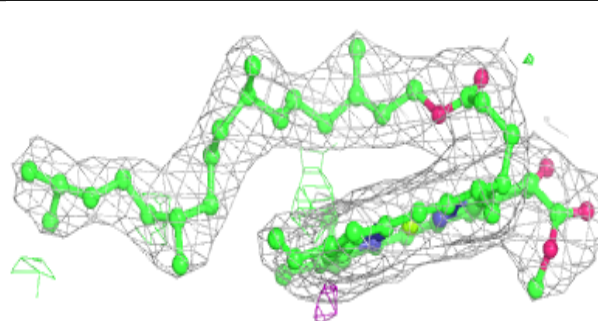
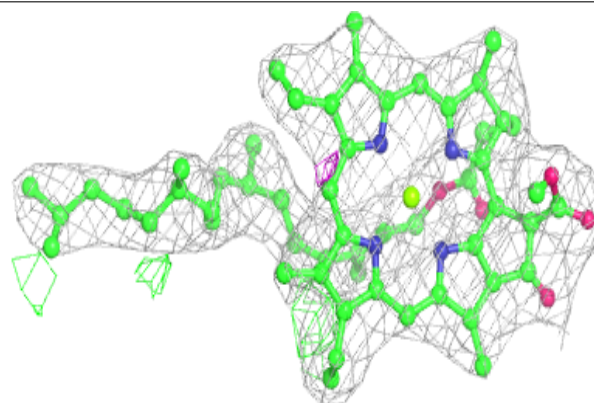


Electron density around CLA H 803:

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

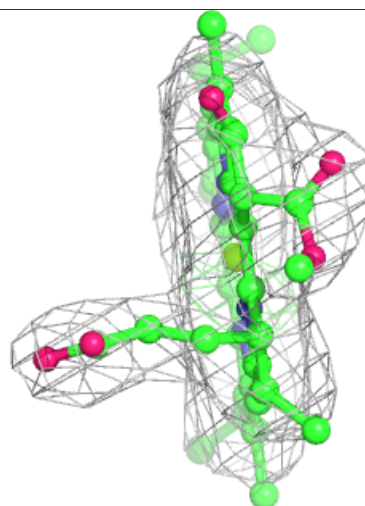
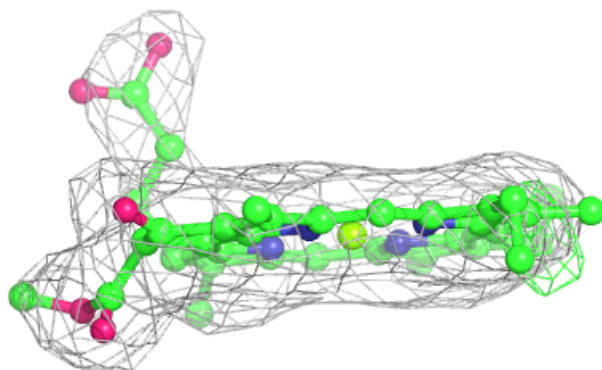
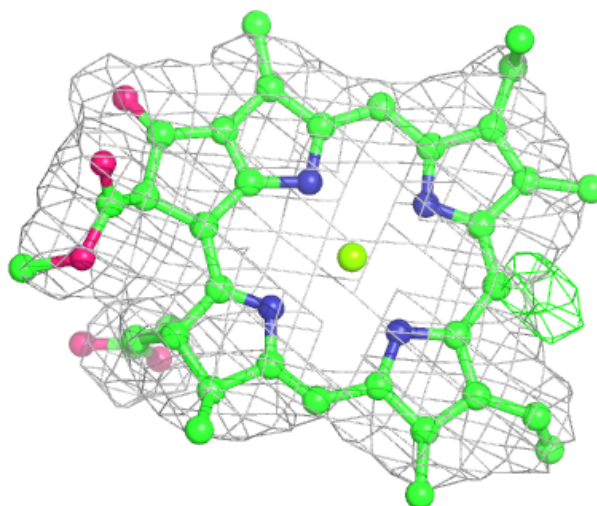
**Electron density around CLA G 837:**

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



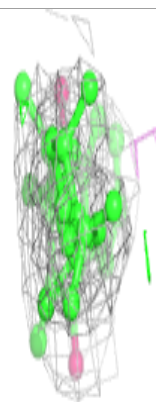
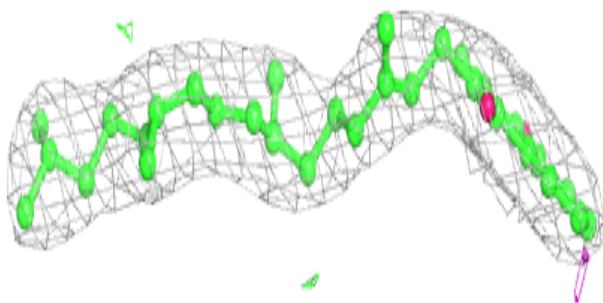
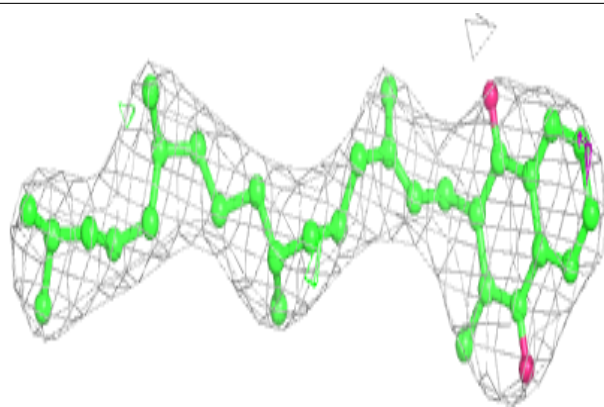
Electron density around CLA J 101:

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

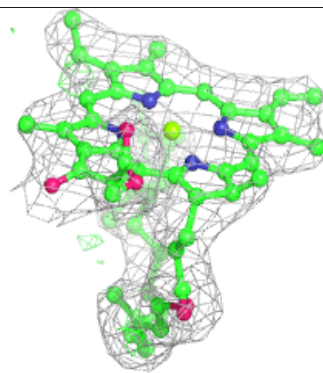
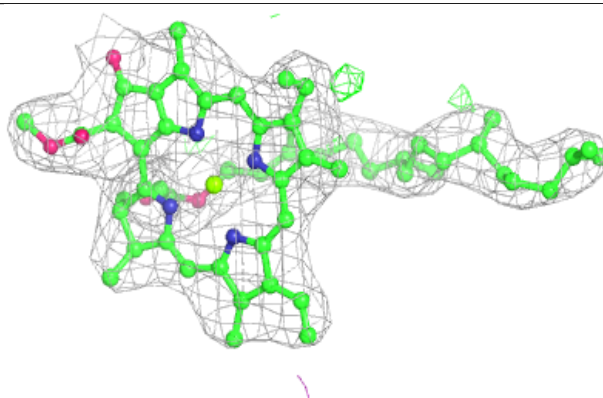
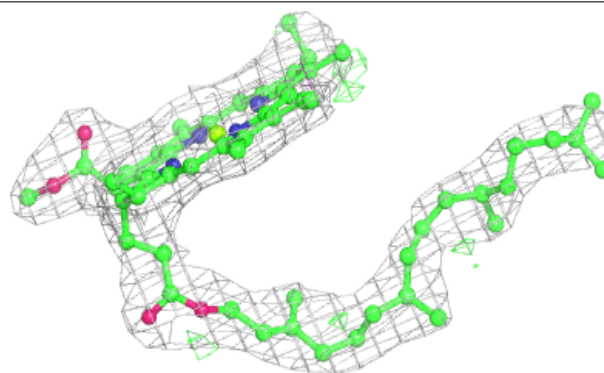


Electron density around PQN G 844:

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

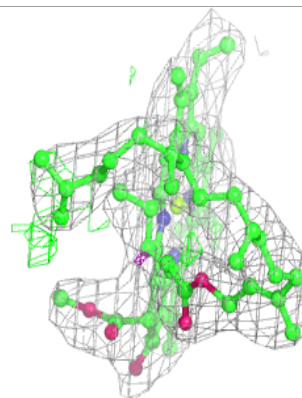
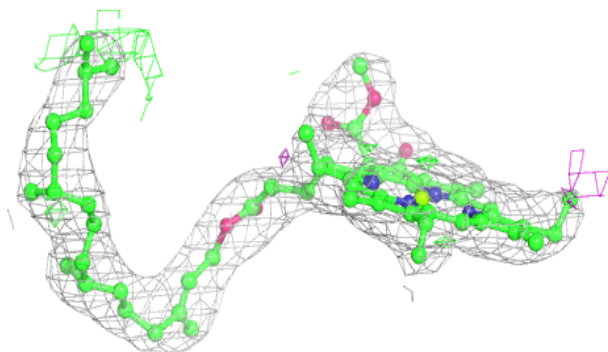
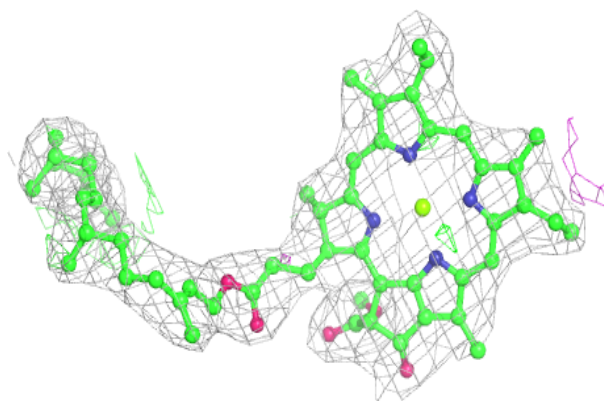
**Electron density around CLA Y 832:**

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

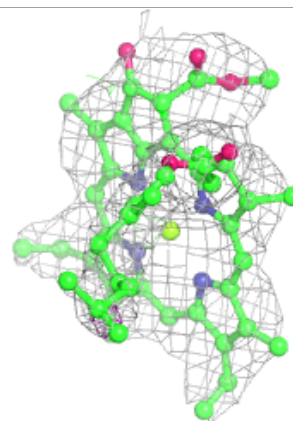
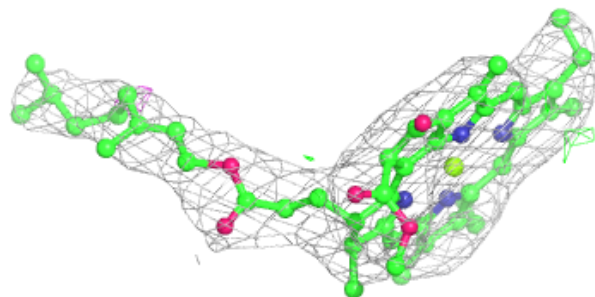
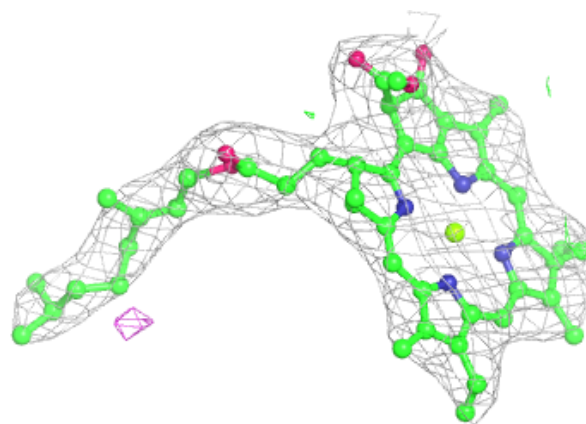


Electron density around CLA A 827:

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

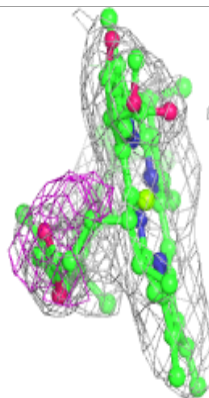
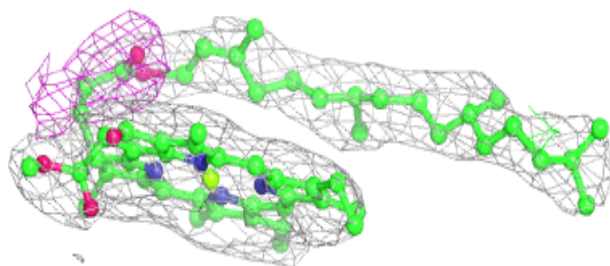
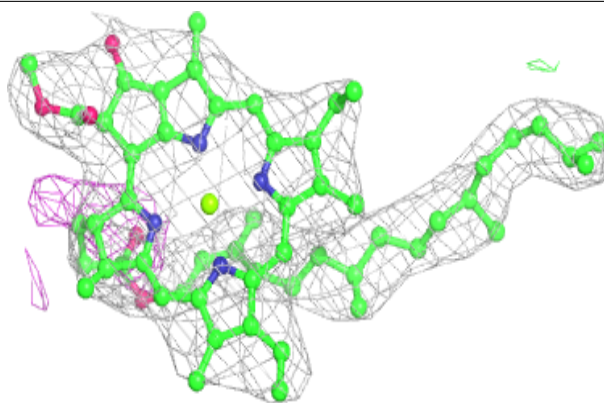
**Electron density around CLA H 830:**

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

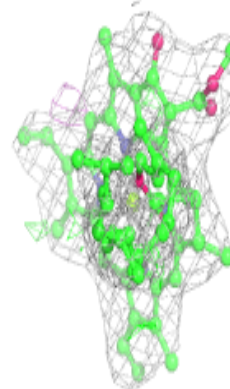
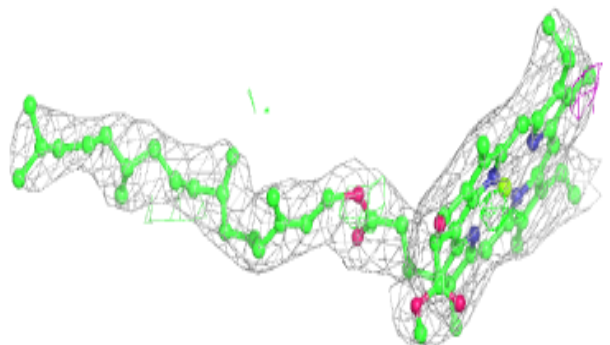
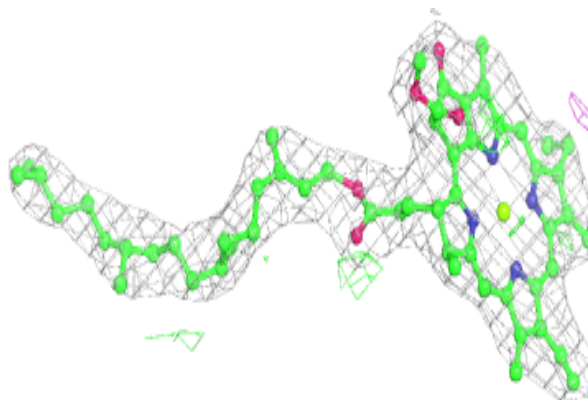


Electron density around CLA Y 818:

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

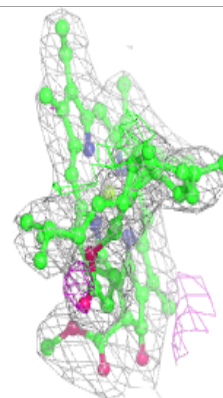
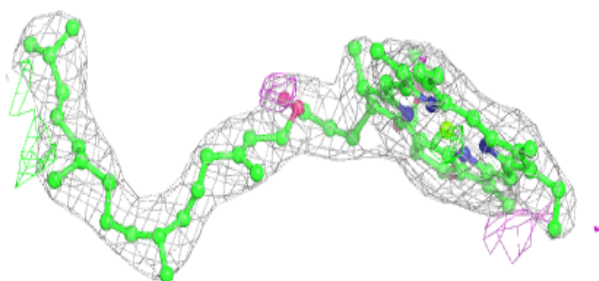
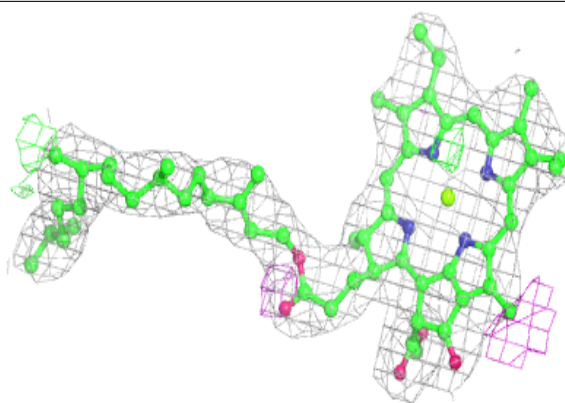
**Electron density around CLA A 809:**

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

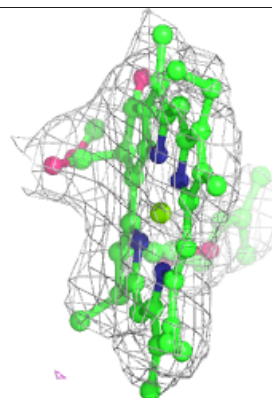
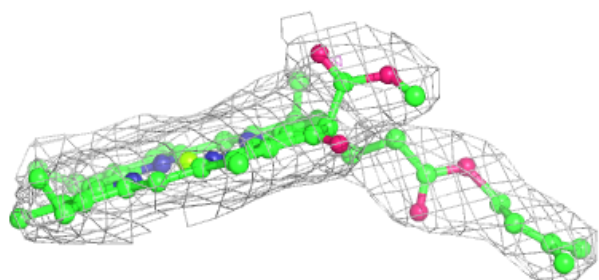
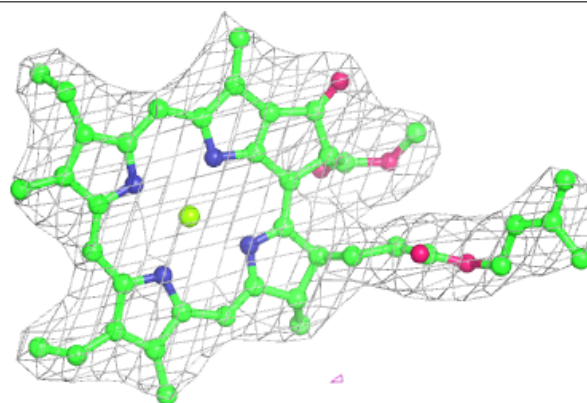


Electron density around CLA B 813:

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

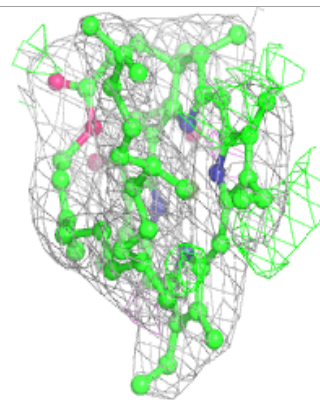
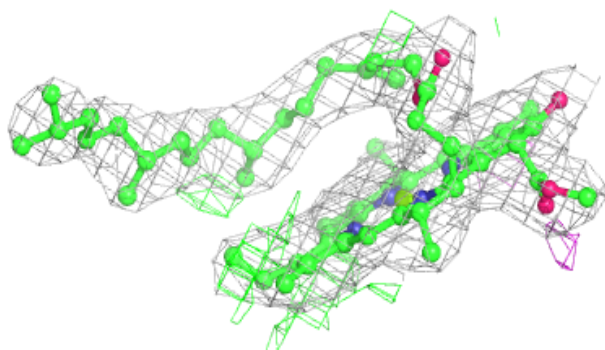
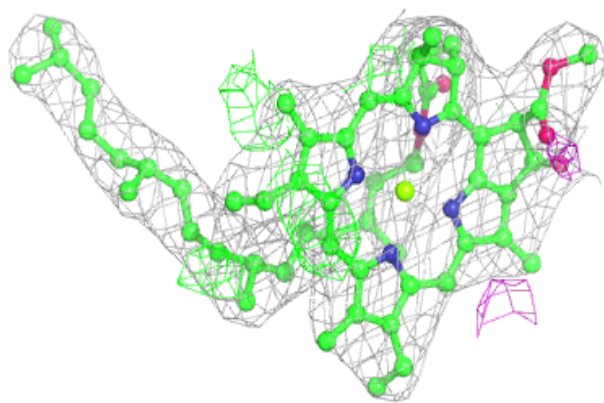
**Electron density around CLA G 840:**

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



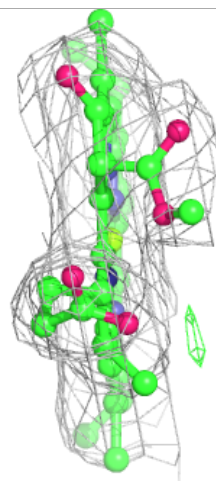
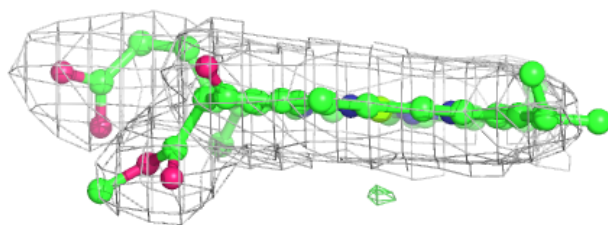
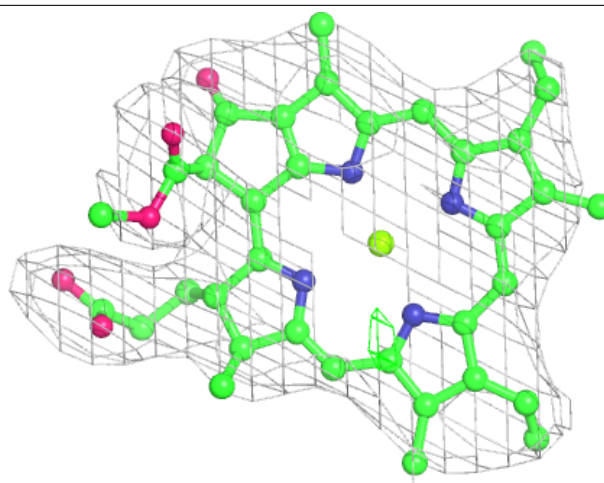
Electron density around CLA Z 806:

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



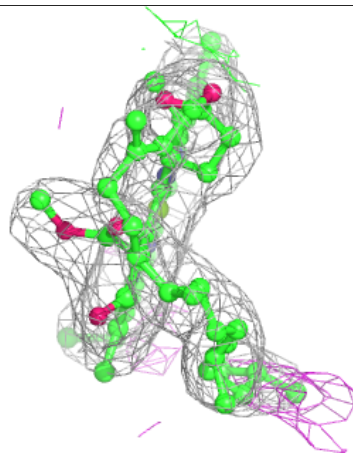
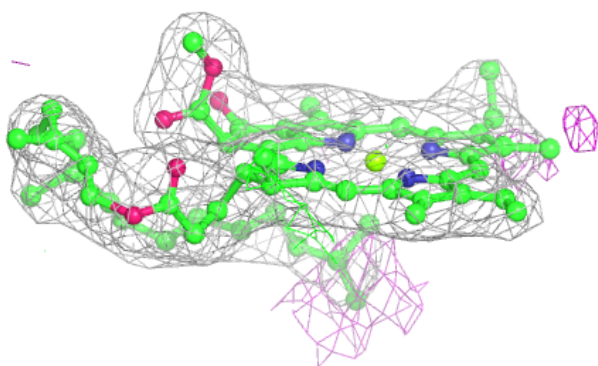
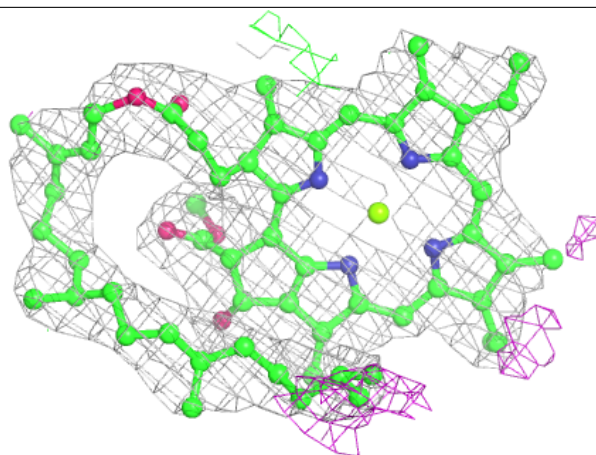
Electron density around CLA Z 834:

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



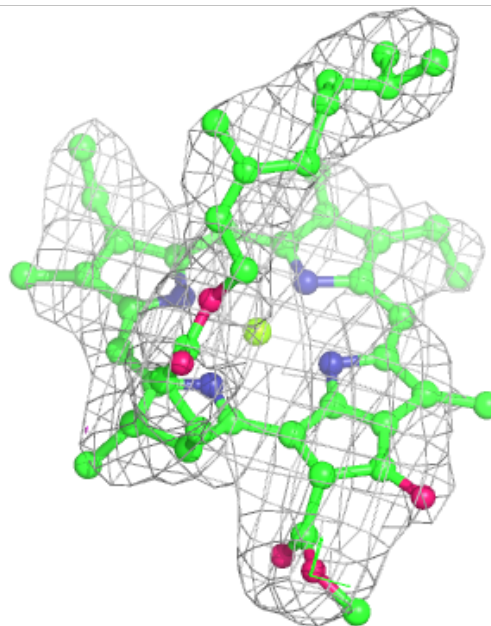
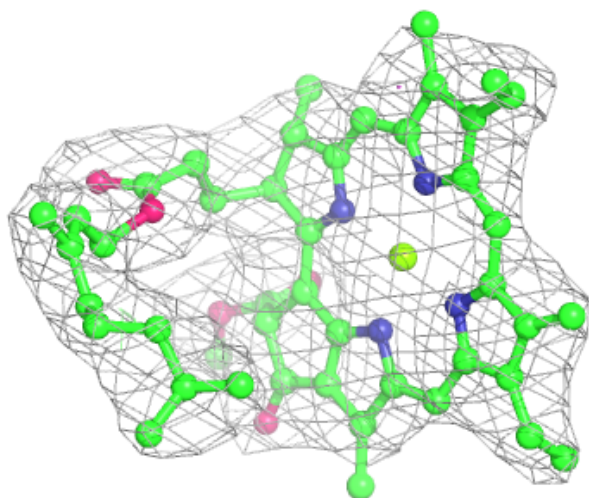
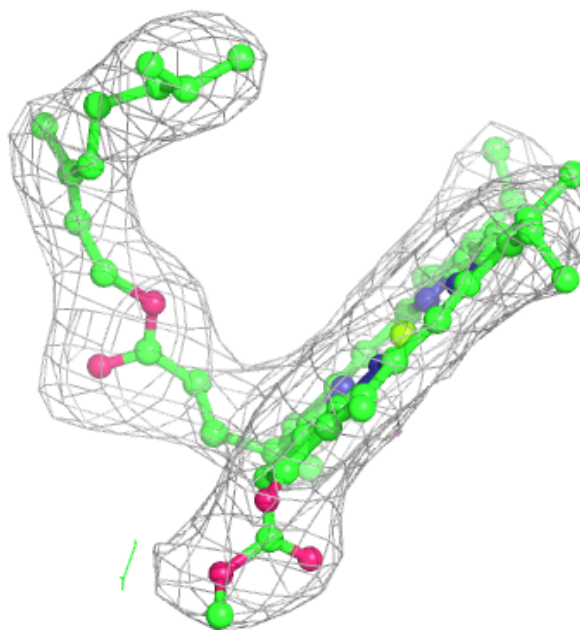
Electron density around CLA B 806:

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



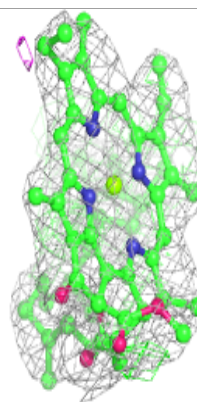
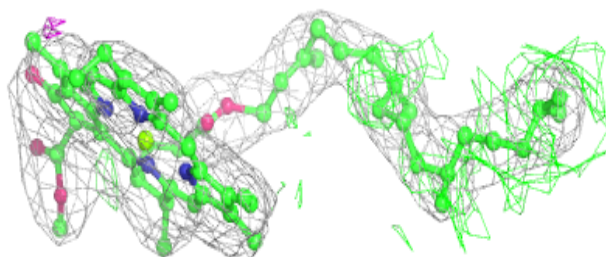
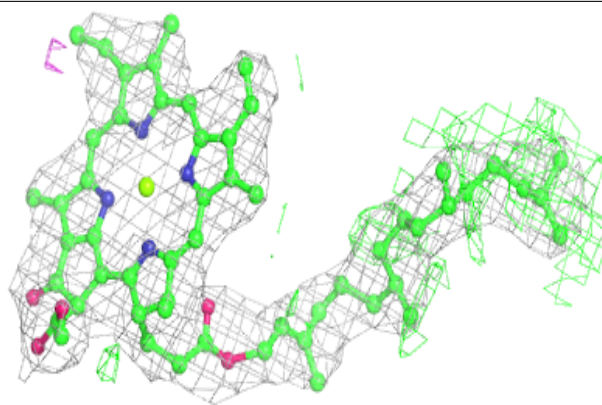
Electron density around CLA Z 809:

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

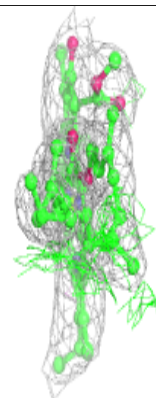
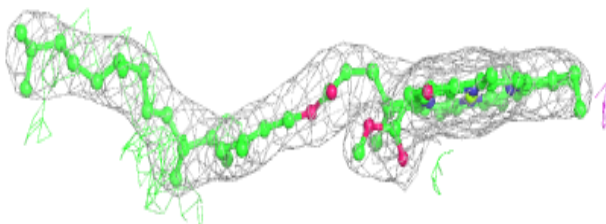
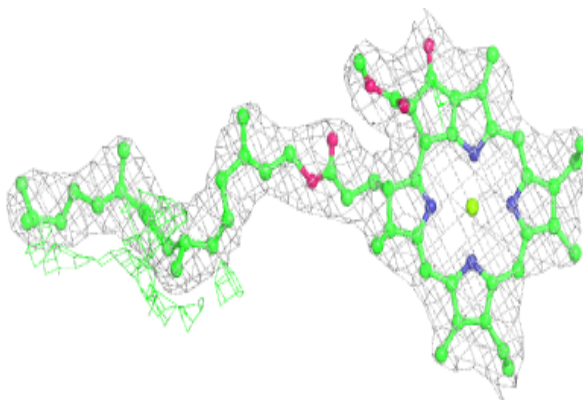


Electron density around CLA G 808:

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

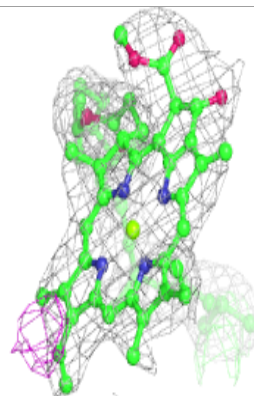
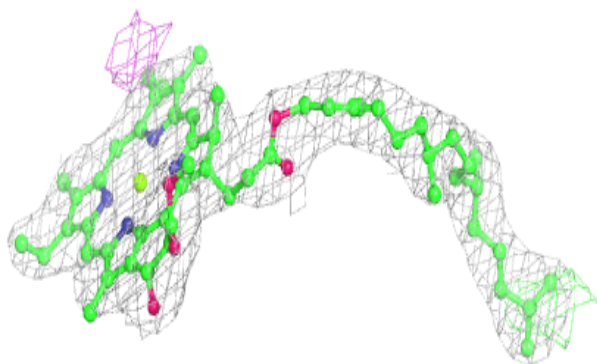
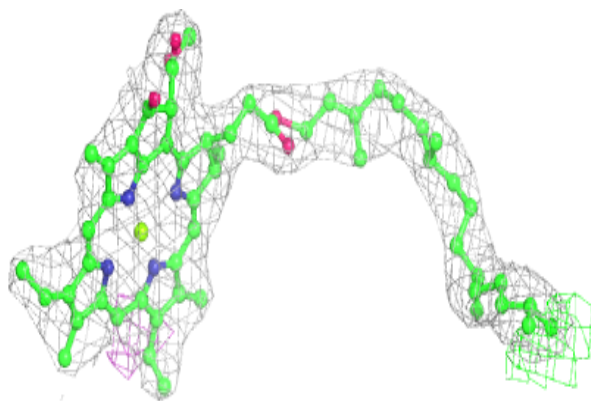
**Electron density around CLA G 832:**

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

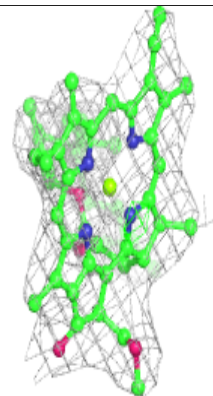
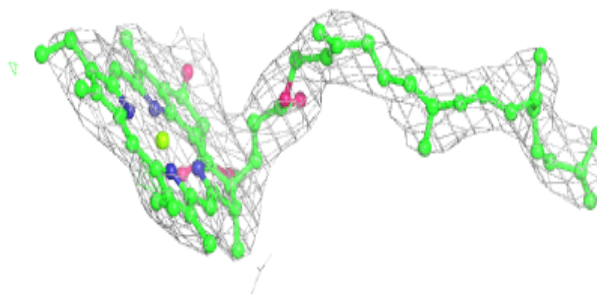
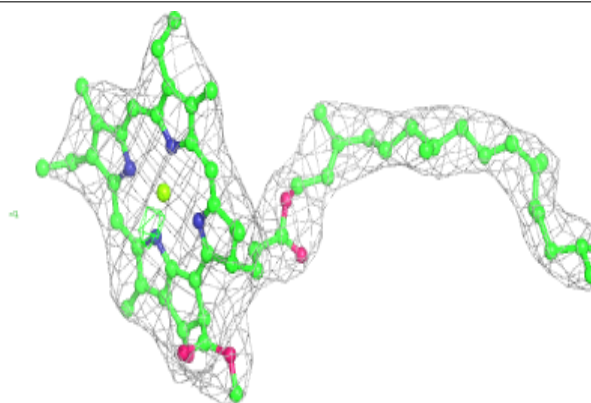


Electron density around CLA H 801:

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

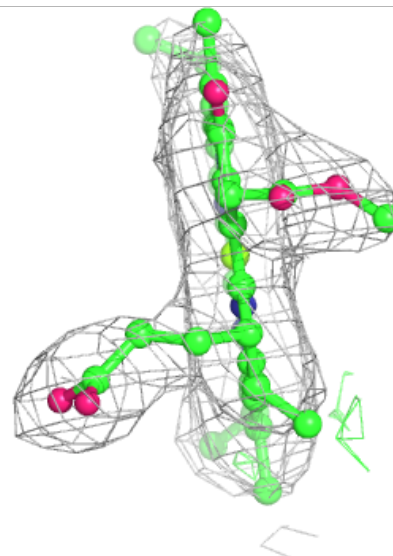
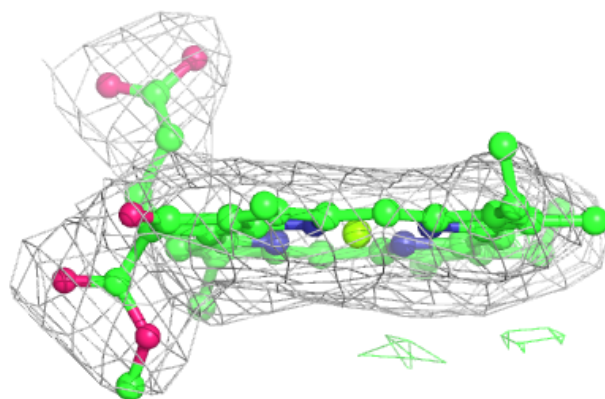
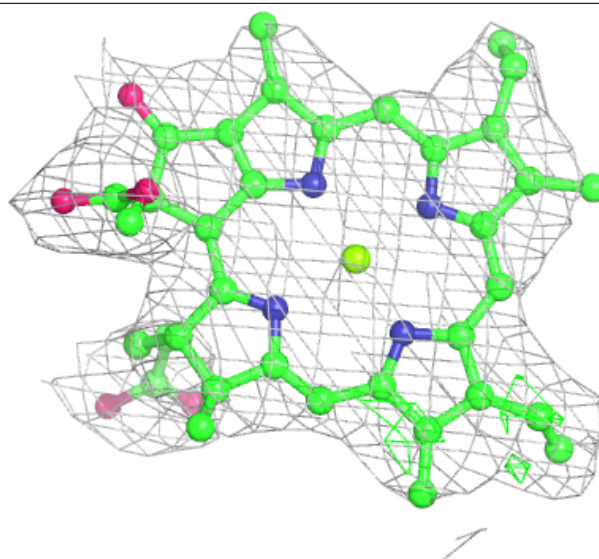
**Electron density around CLA Y 821:**

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



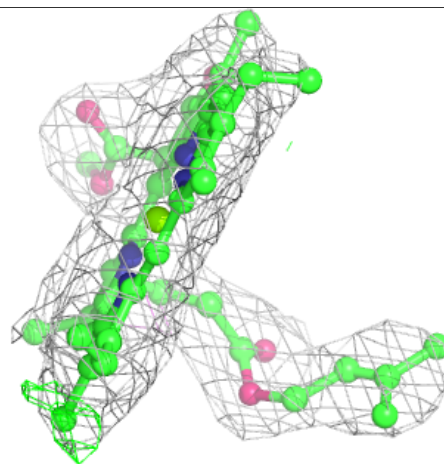
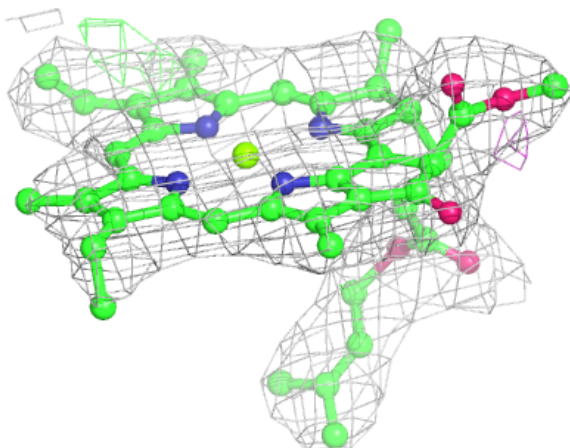
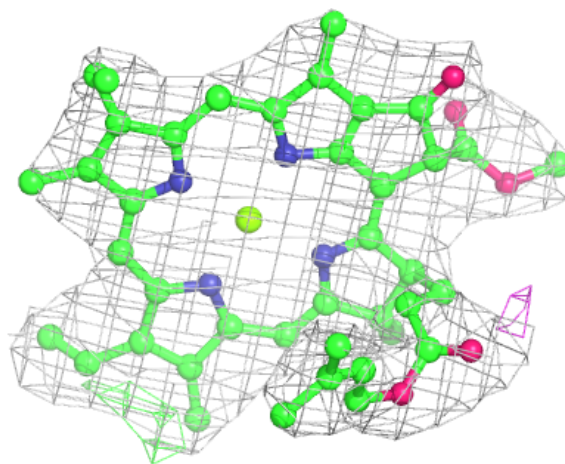
Electron density around CLA Z 828:

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



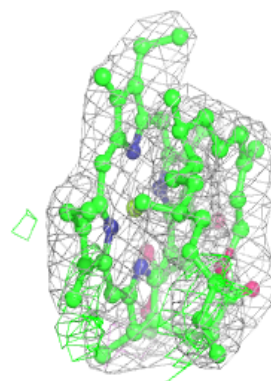
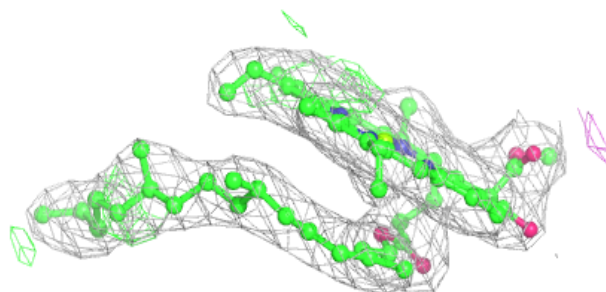
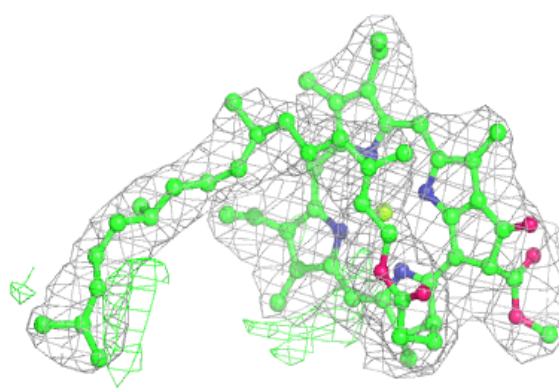
Electron density around CLA B 812:

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



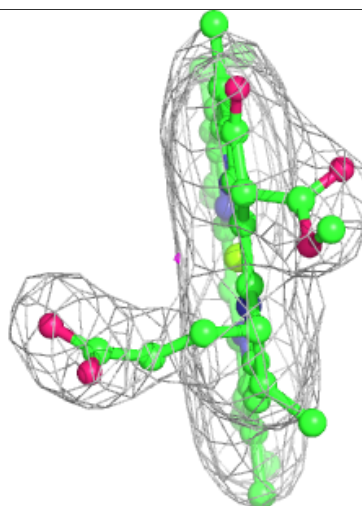
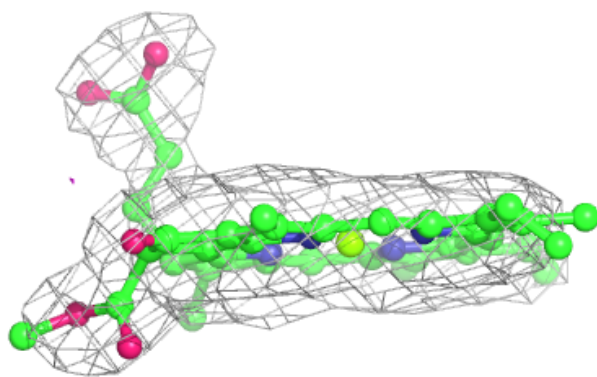
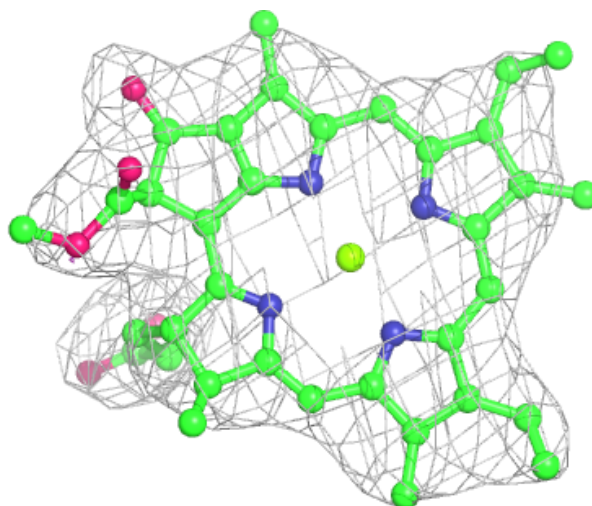
Electron density around CLA H 806:

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



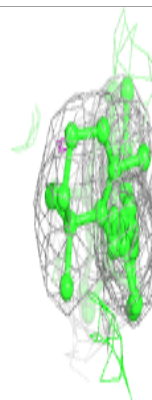
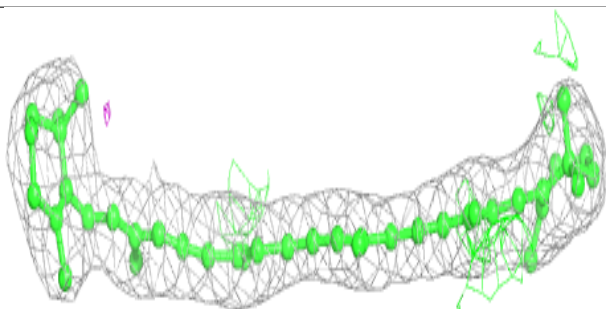
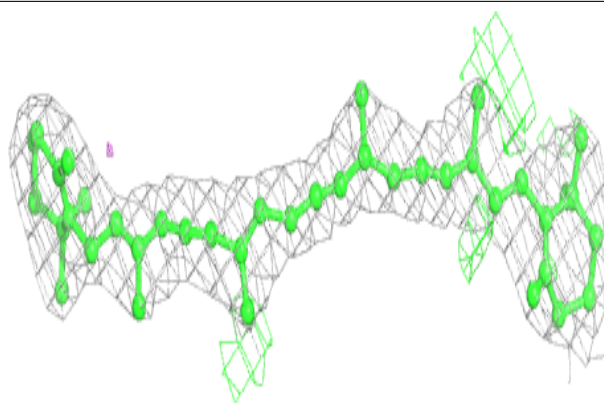
Electron density around CLA G 810:

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

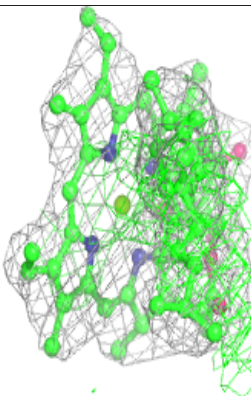
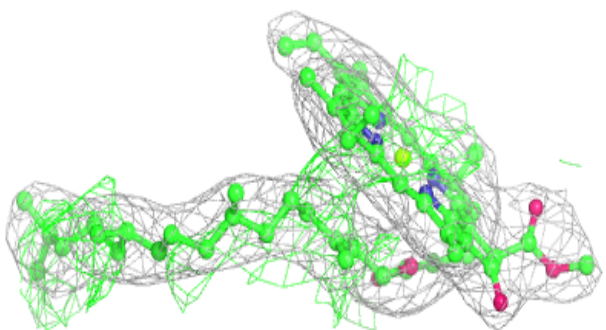
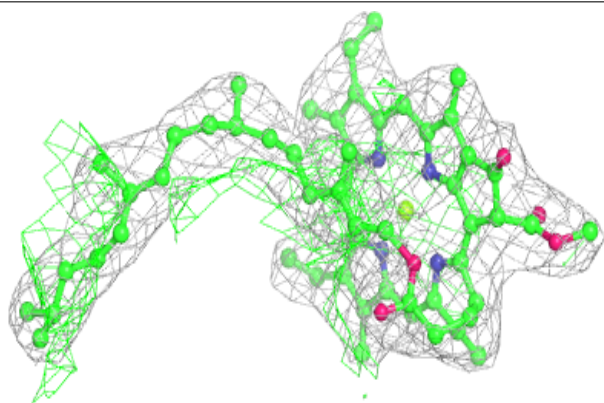


Electron density around BCR A 848:

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

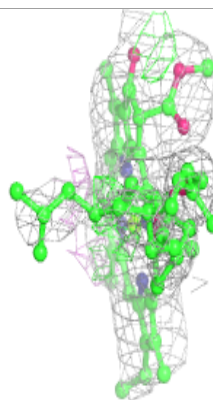
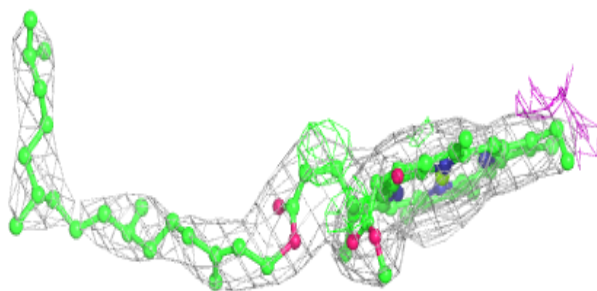
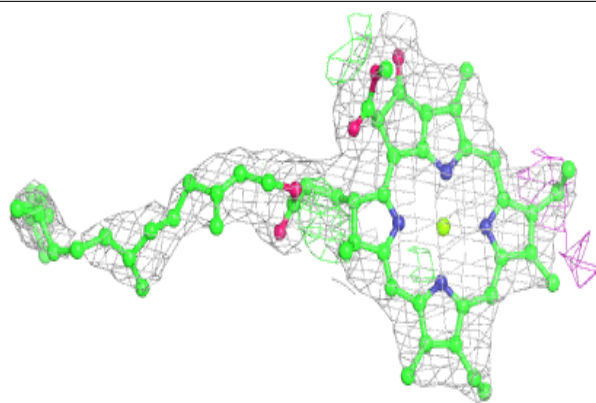
**Electron density around CLA G 841:**

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



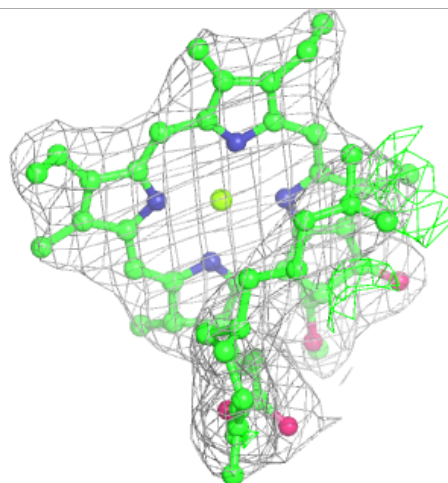
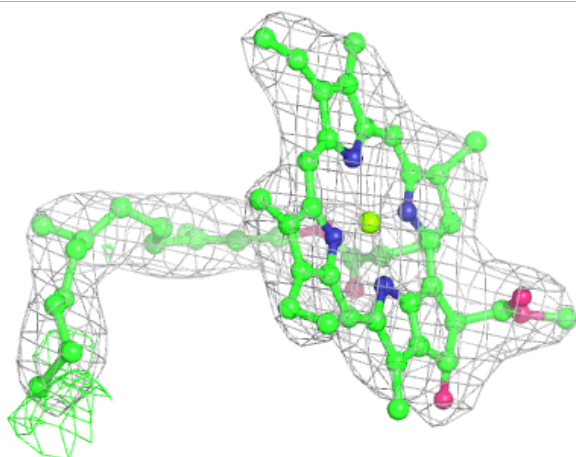
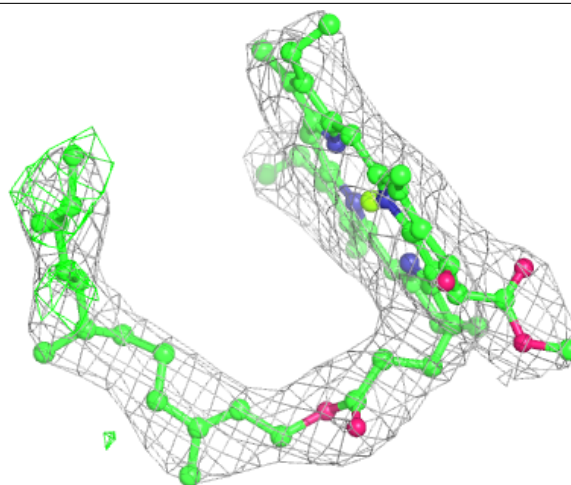
Electron density around CLA A 805:

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



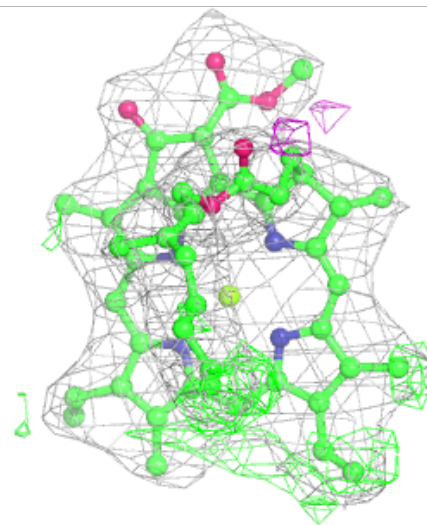
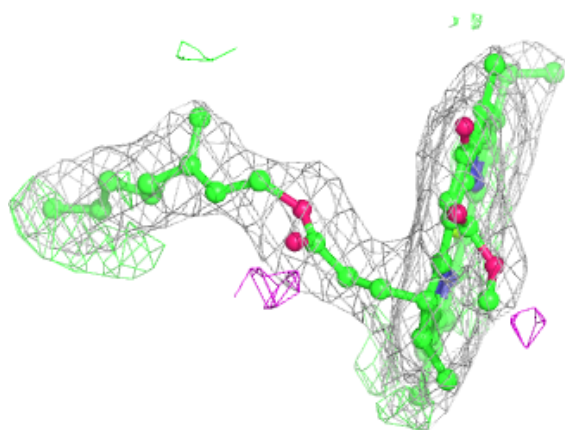
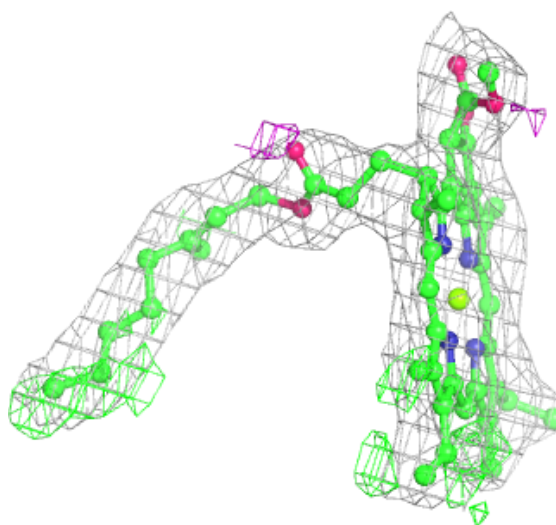
Electron density around CLA Z 817:

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



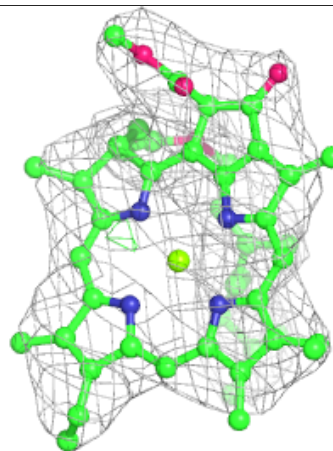
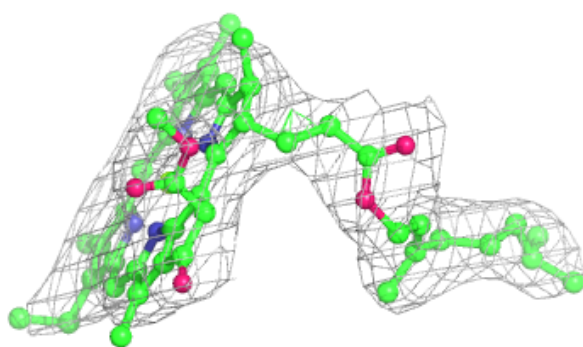
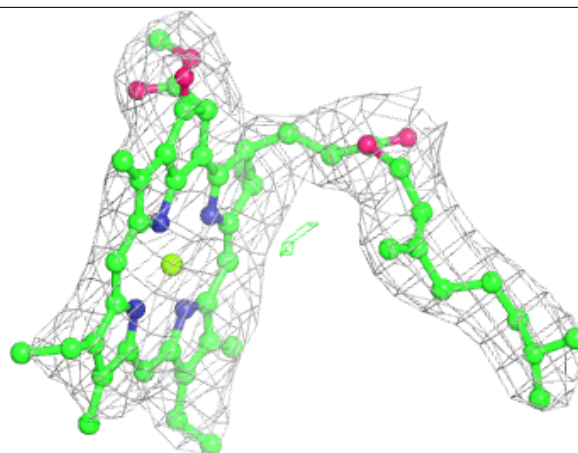
Electron density around CLA Z 803:

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

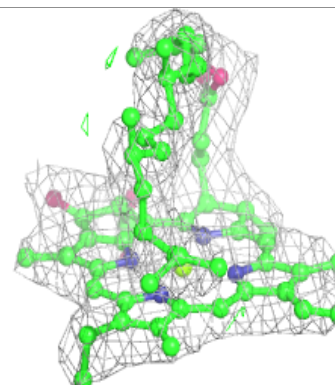
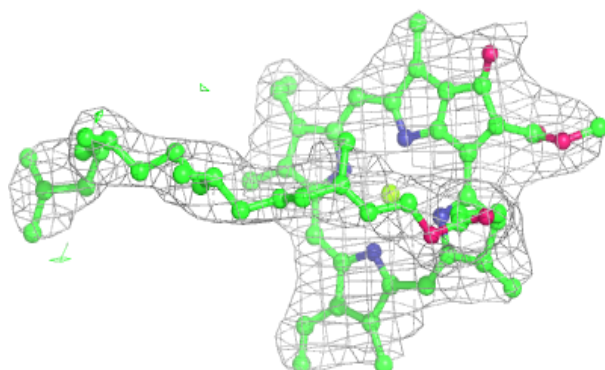
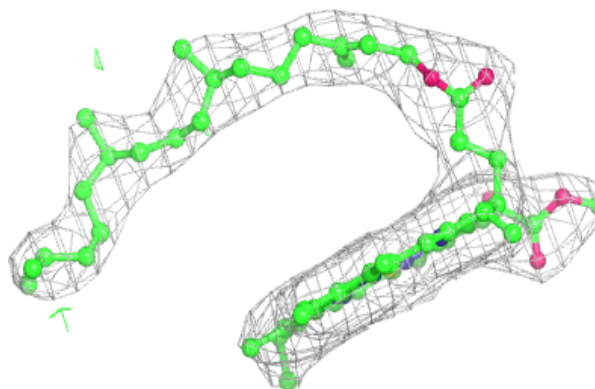


Electron density around CLA Y 814:

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

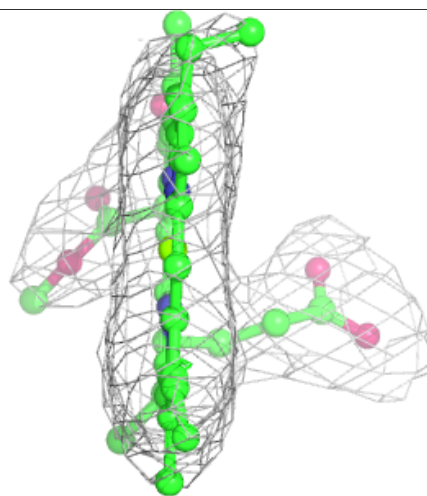
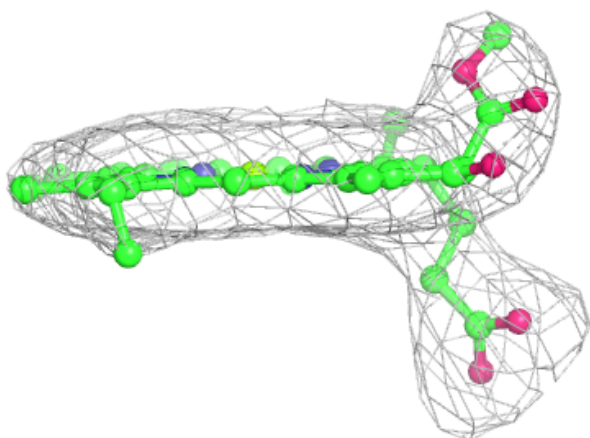
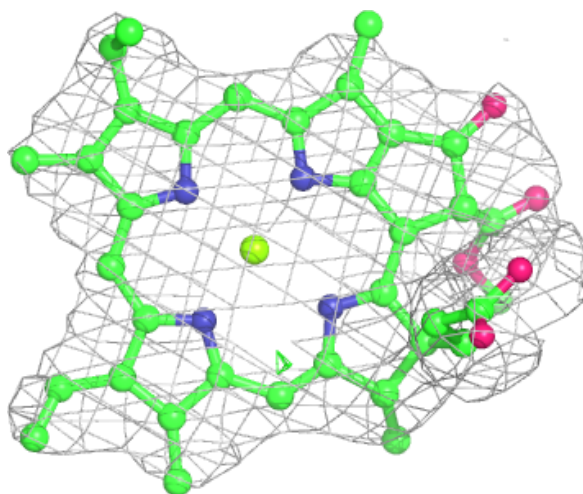
**Electron density around CLA h 201:**

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



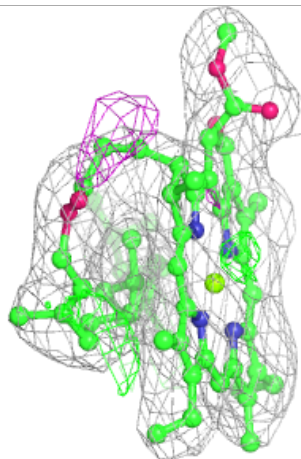
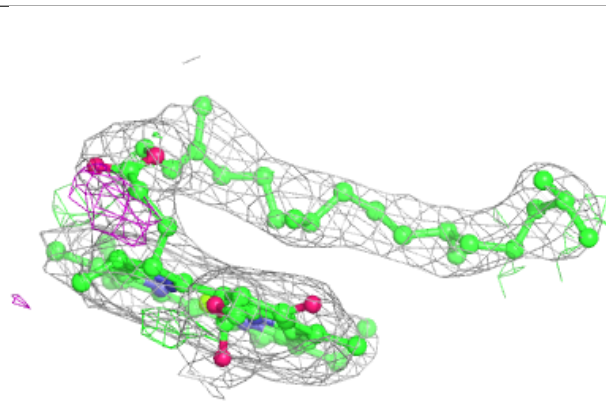
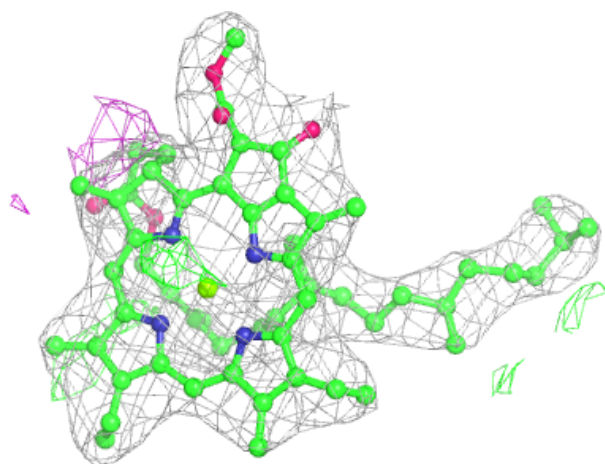
Electron density around CLA Z 819:

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



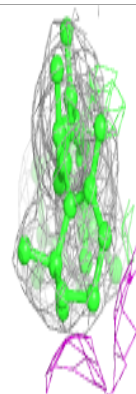
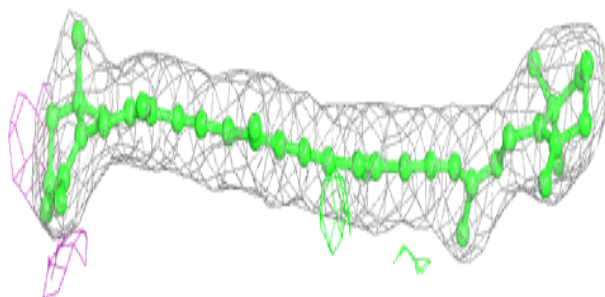
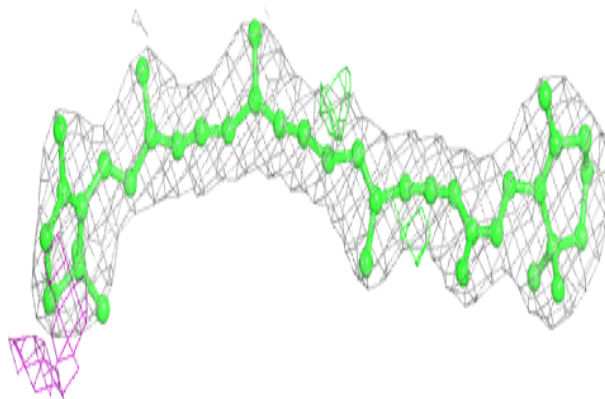
Electron density around CLA B 827:

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

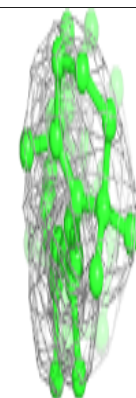
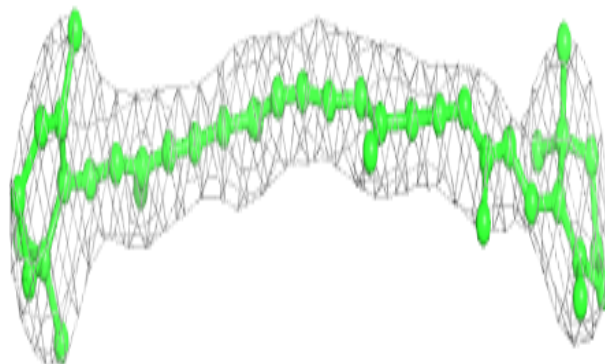
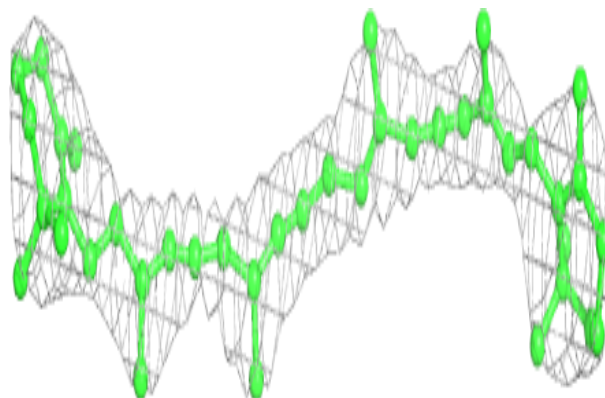


Electron density around BCR B 847:

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

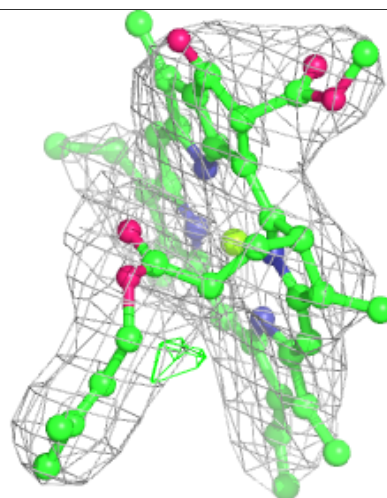
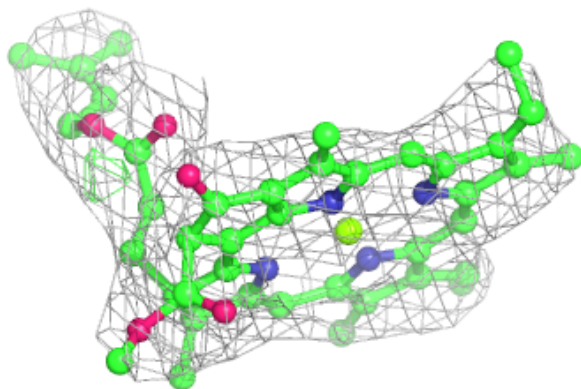
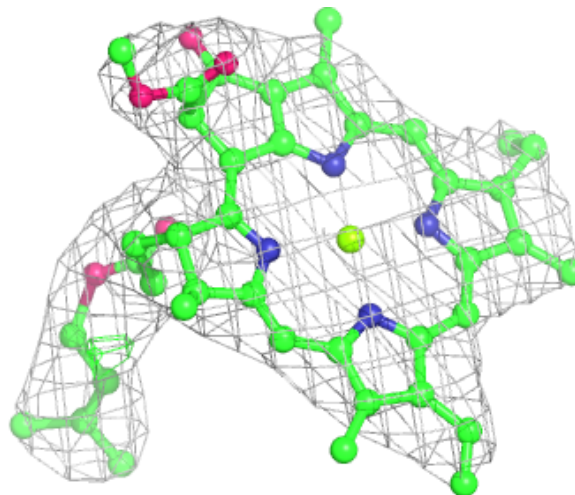
**Electron density around BCR G 847:**

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



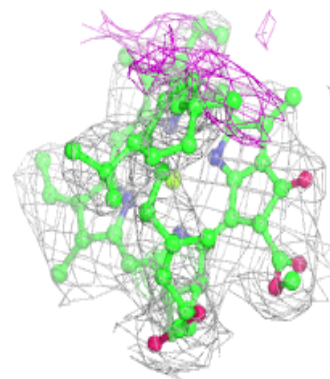
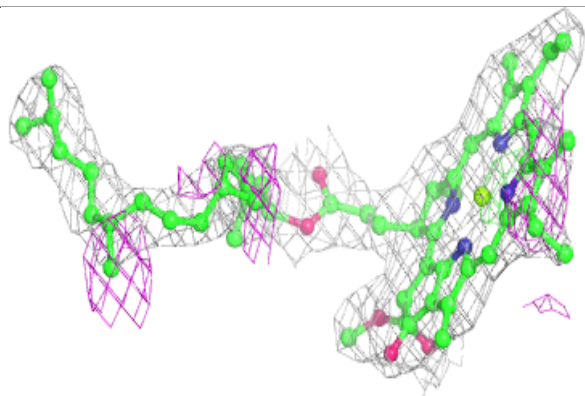
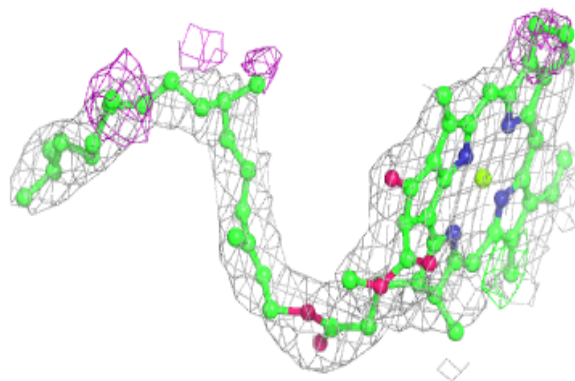
Electron density around CLA Y 815:

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



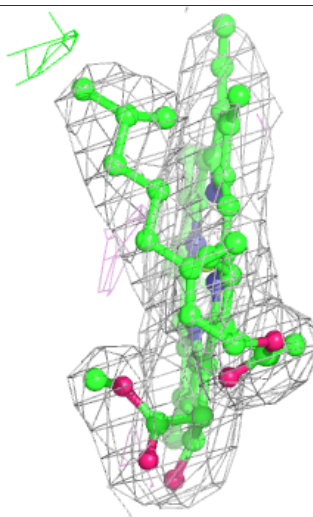
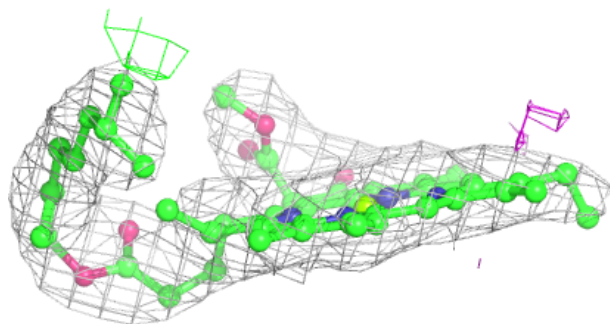
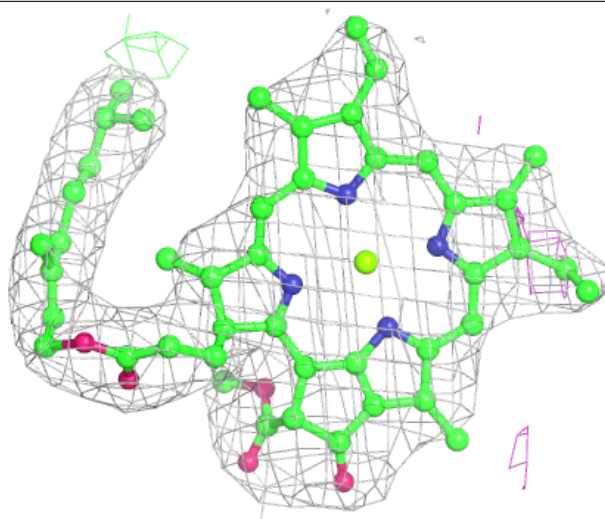
Electron density around CLA B 803:

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



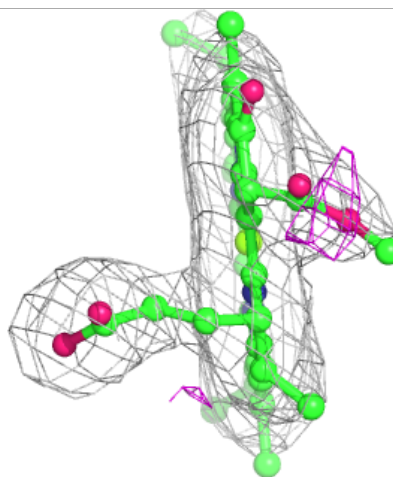
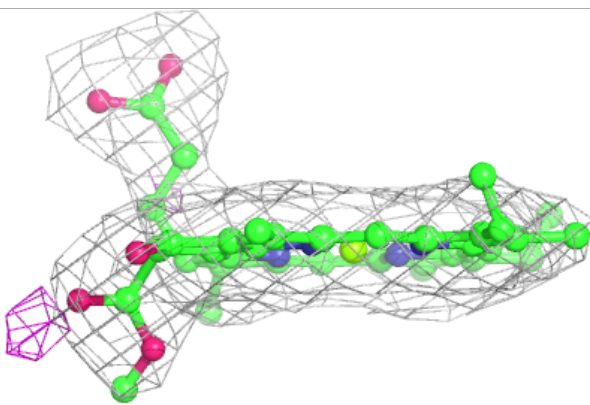
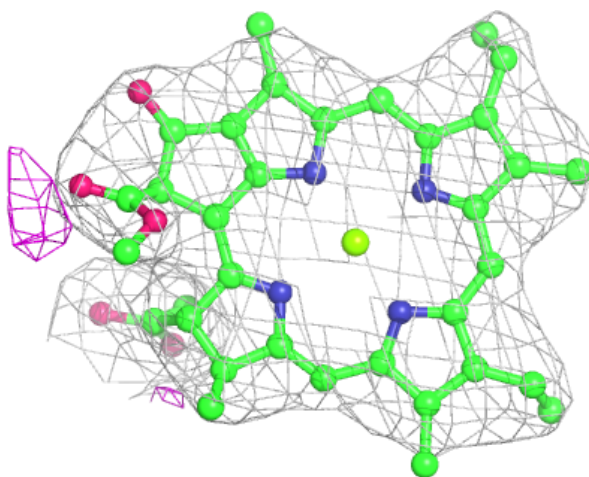
Electron density around CLA B 824:

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



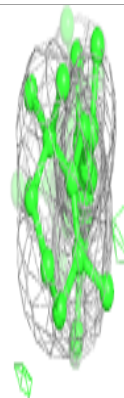
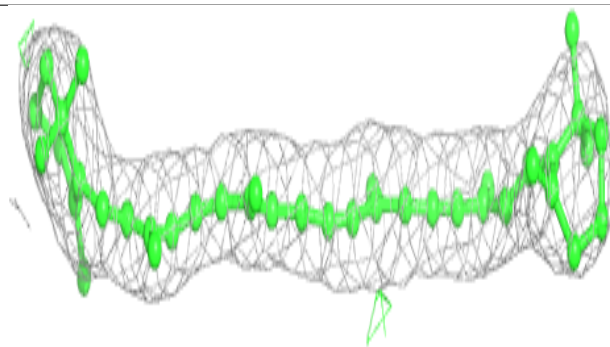
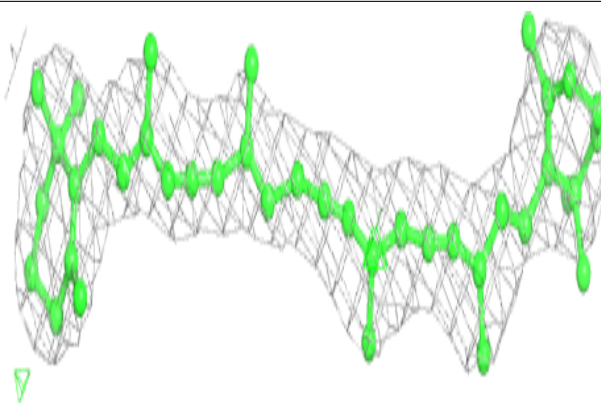
Electron density around CLA B 821:

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



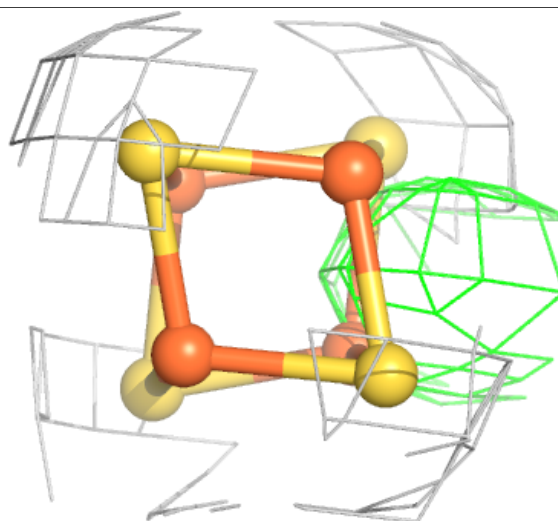
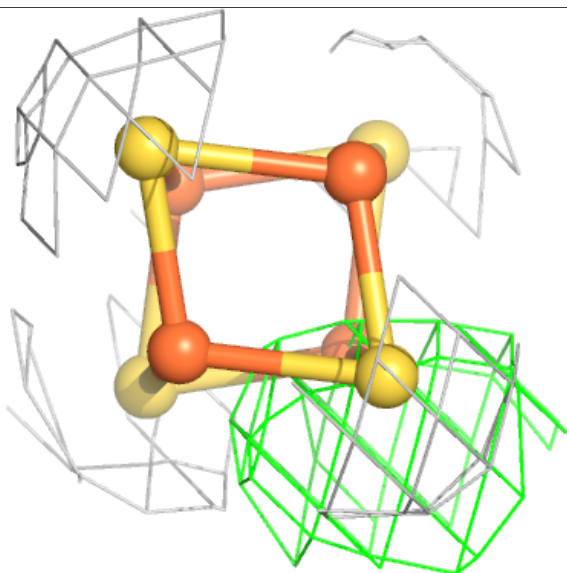
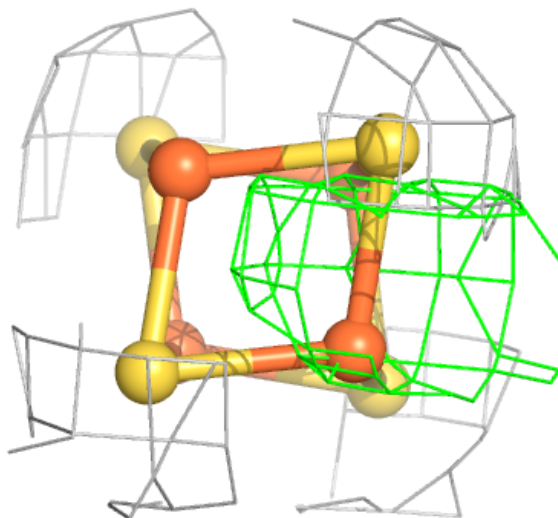
Electron density around BCR Z 841:

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



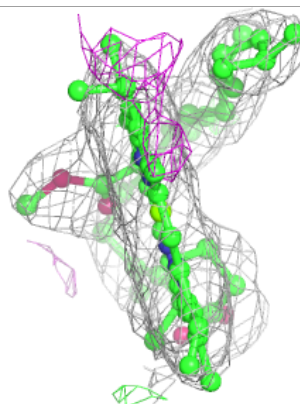
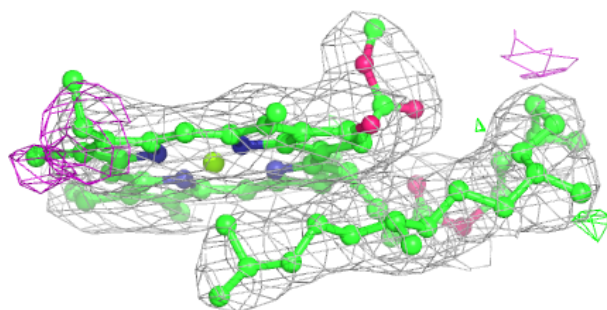
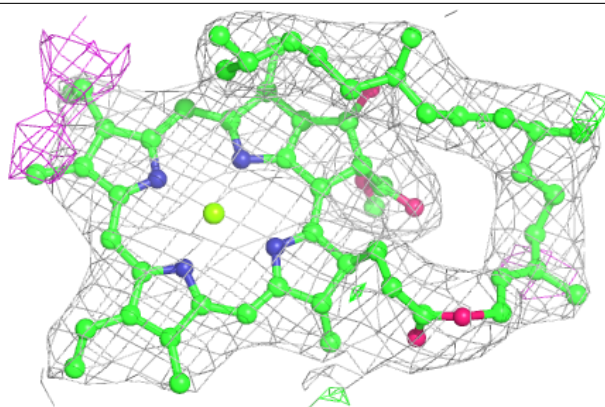
Electron density around SF4 Y 845:

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

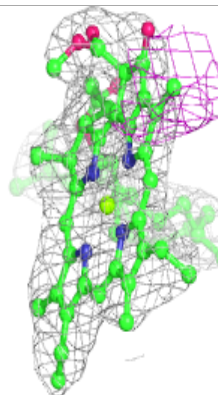
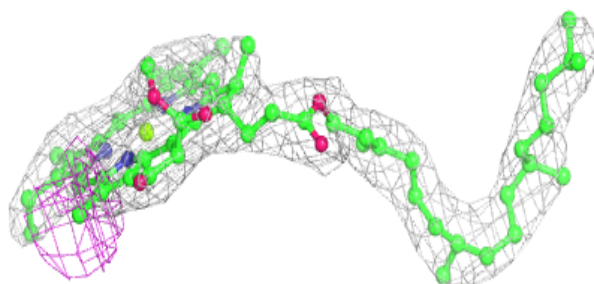
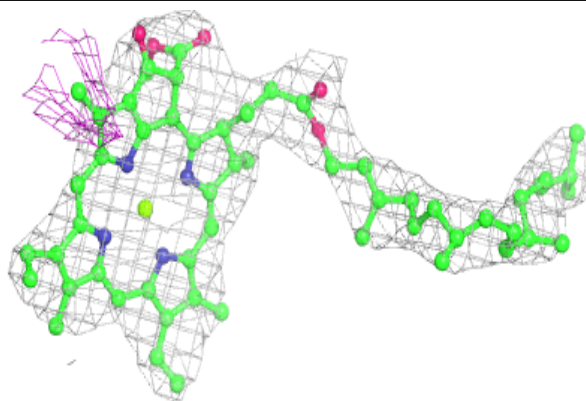


Electron density around CLA Z 804:

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

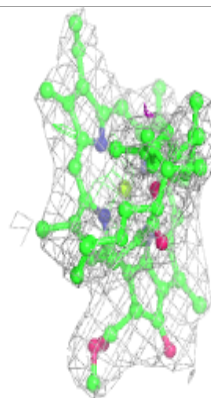
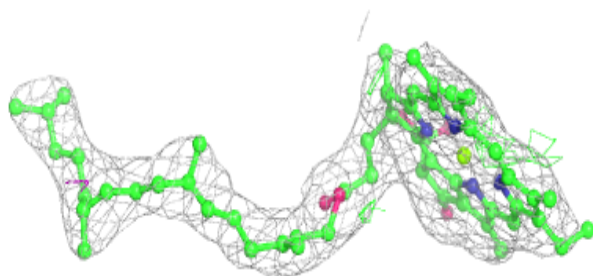
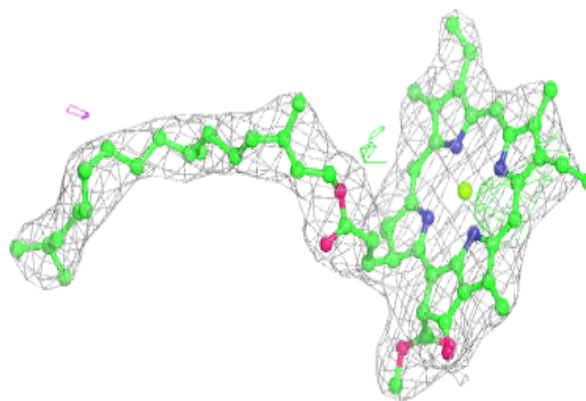
**Electron density around CLA H 812:**

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

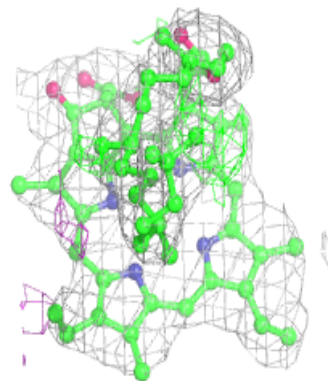
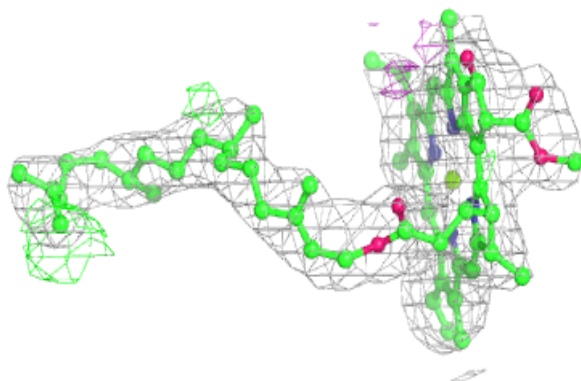
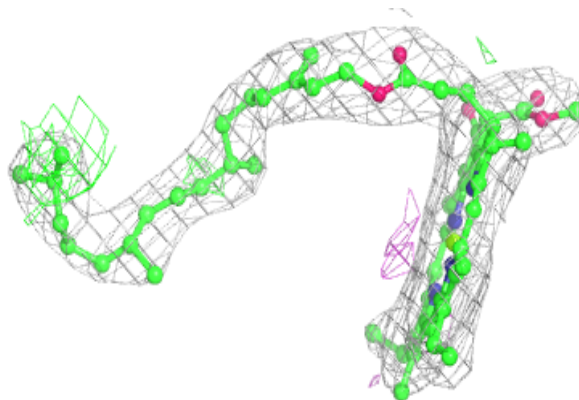


Electron density around CLA A 821:

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

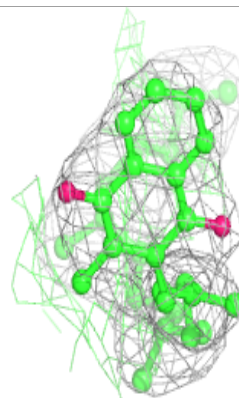
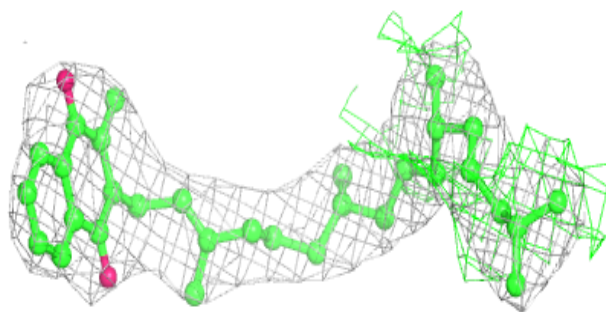
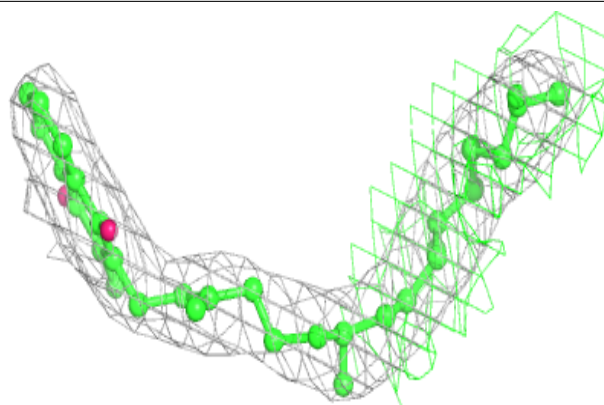
**Electron density around CLA G 830:**

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



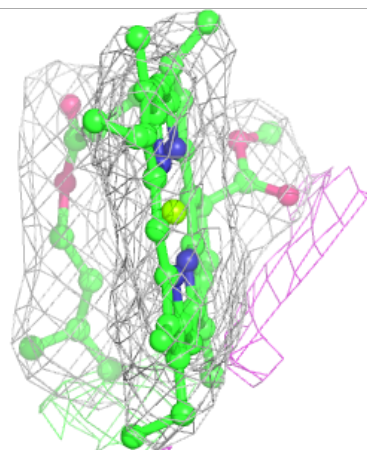
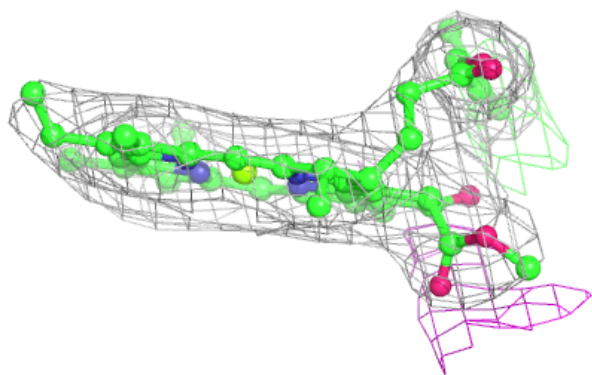
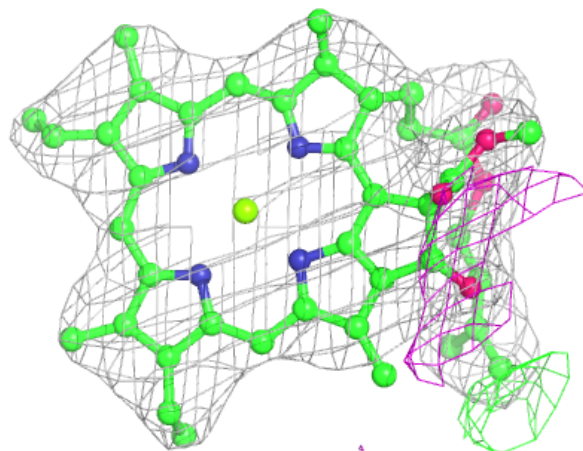
Electron density around PQN H 839:

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

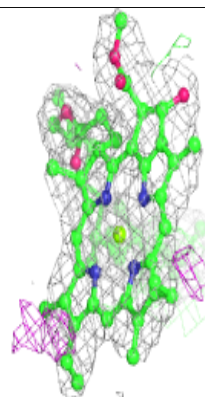
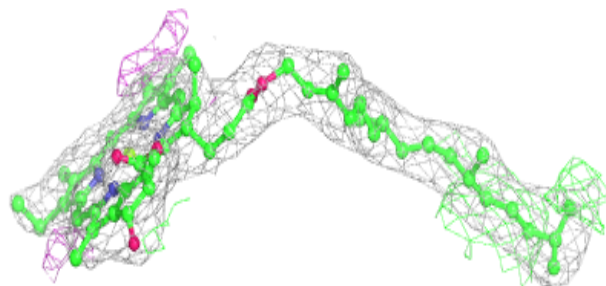
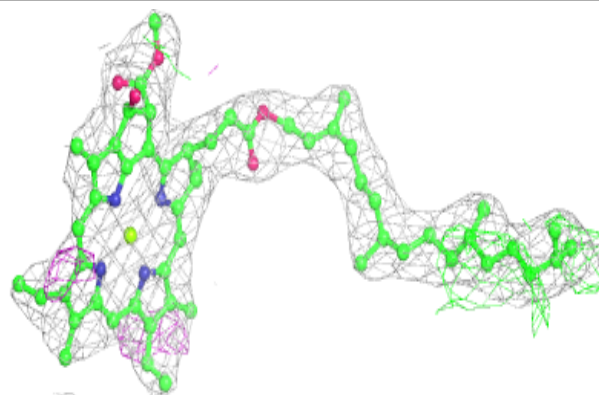


Electron density around CLA A 842:

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

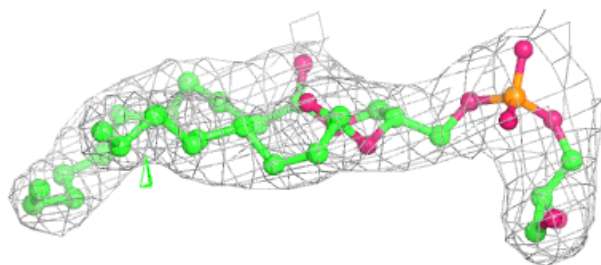
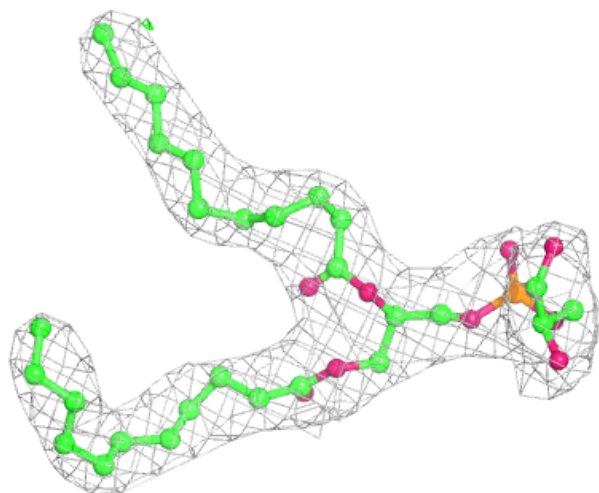
**Electron density around CLA A 802:**

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



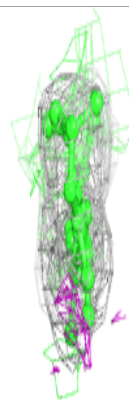
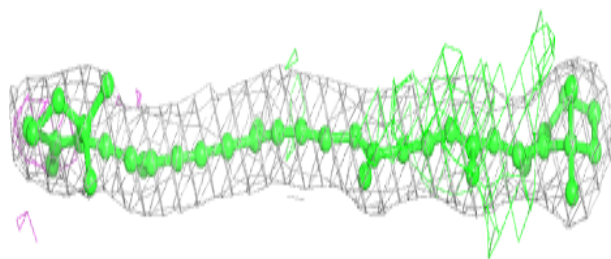
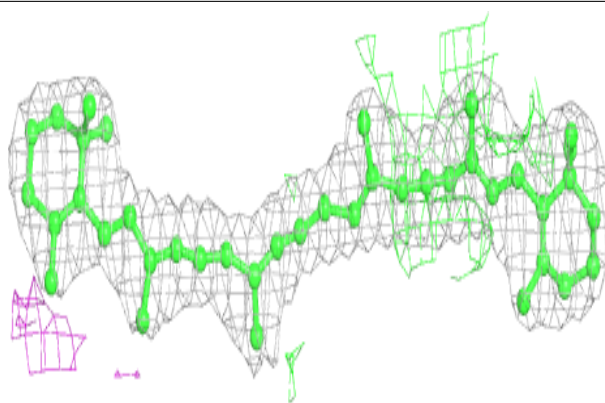
Electron density around LHG B 850:

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



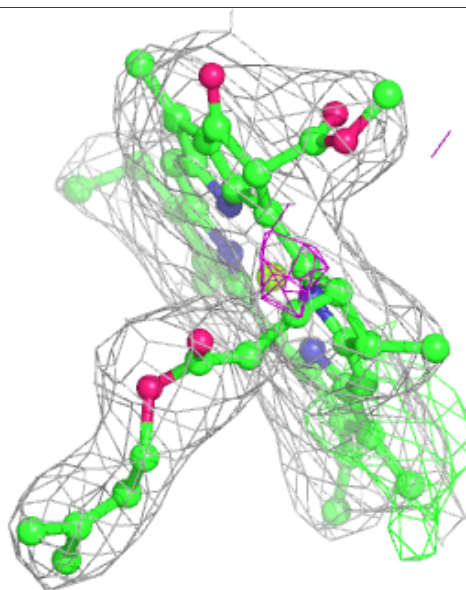
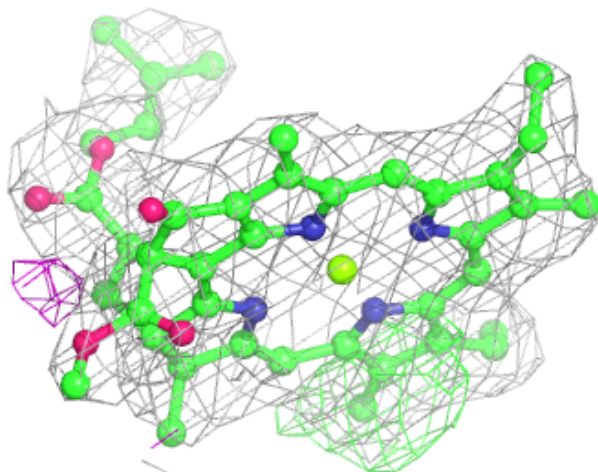
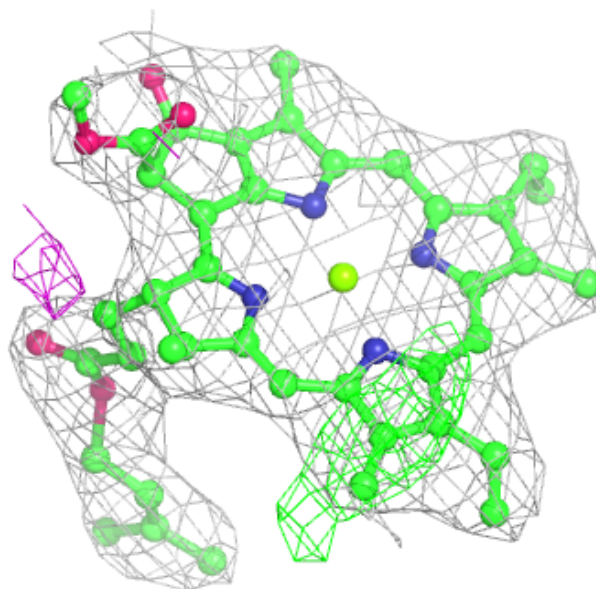
Electron density around BCR L 208:

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



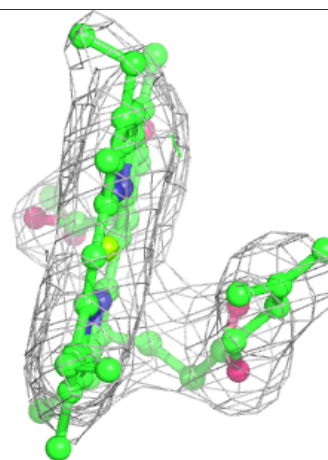
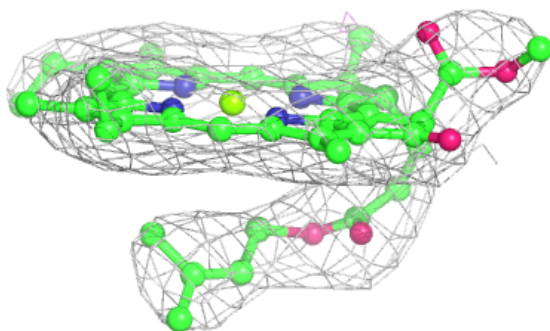
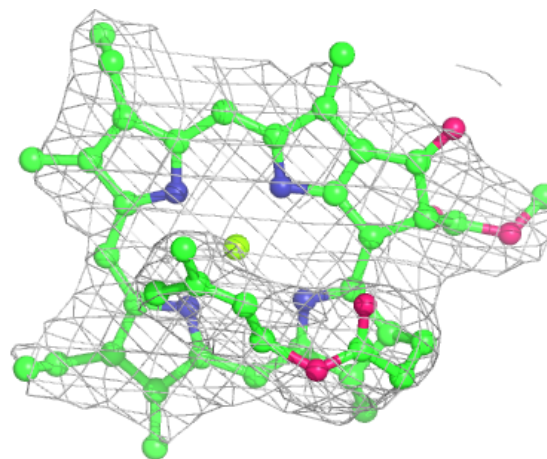
Electron density around CLA A 831:

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



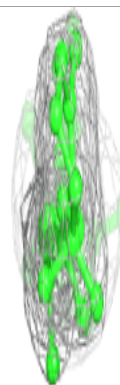
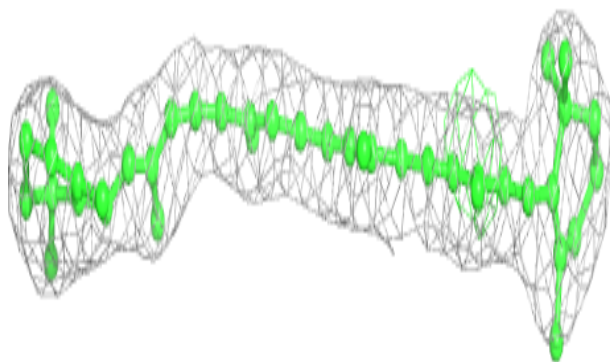
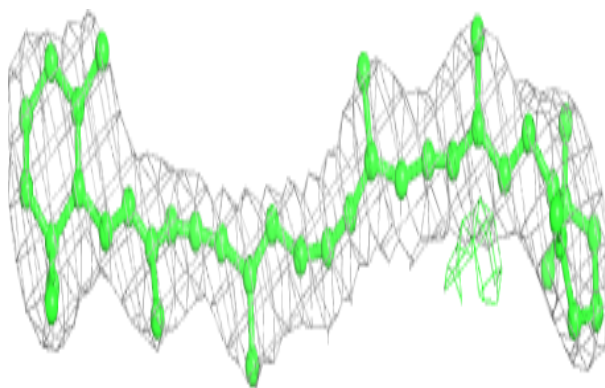
Electron density around CLA Y 823:

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

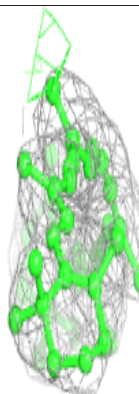
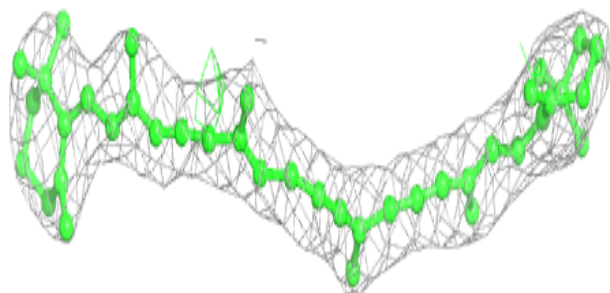
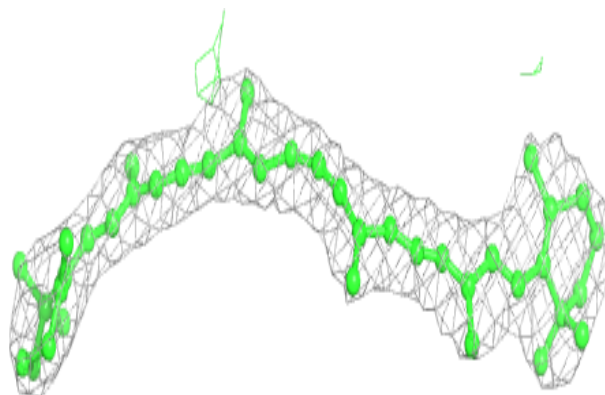


Electron density around BCR f 105:

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

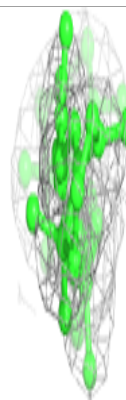
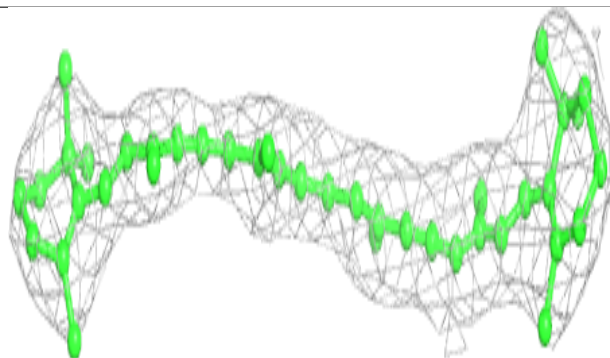
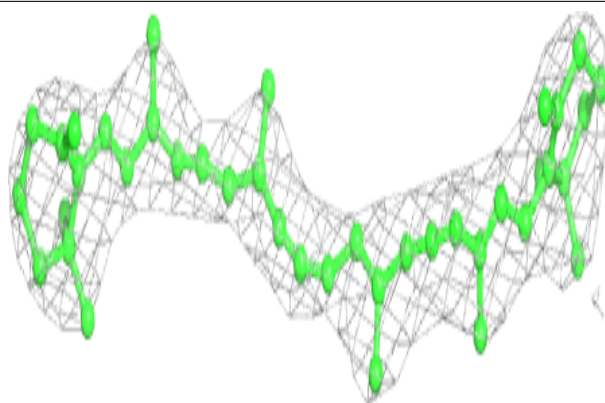
**Electron density around BCR Z 846:**

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

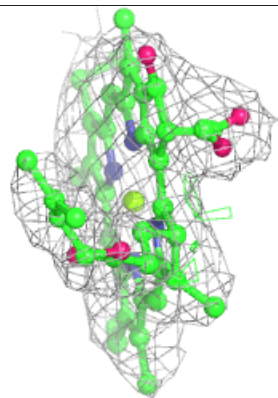
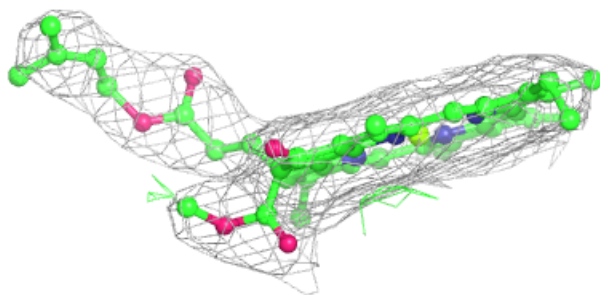
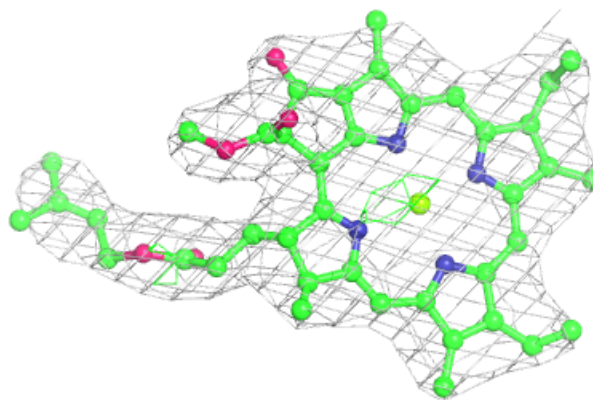


Electron density around BCR Y 847:

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

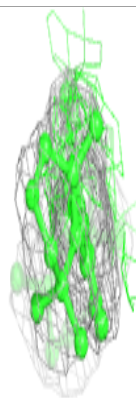
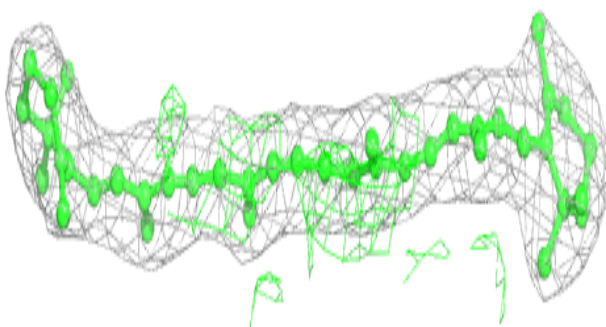
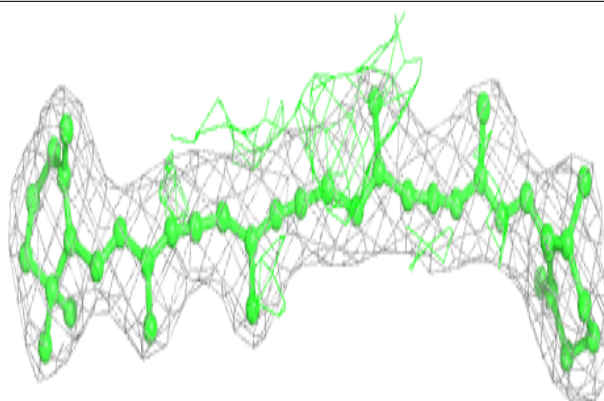
**Electron density around CLA A 839:**

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

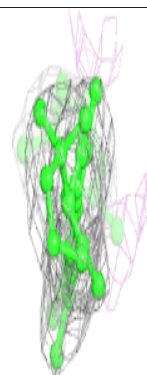
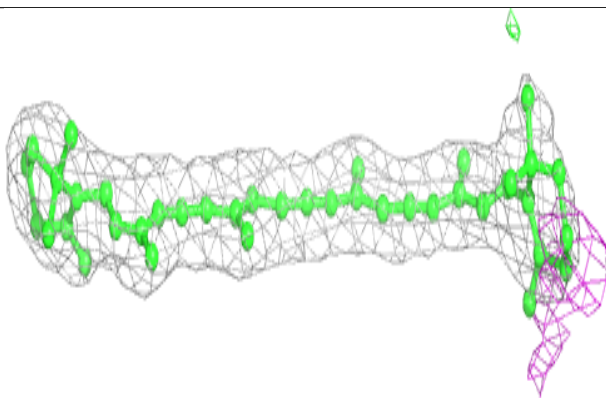
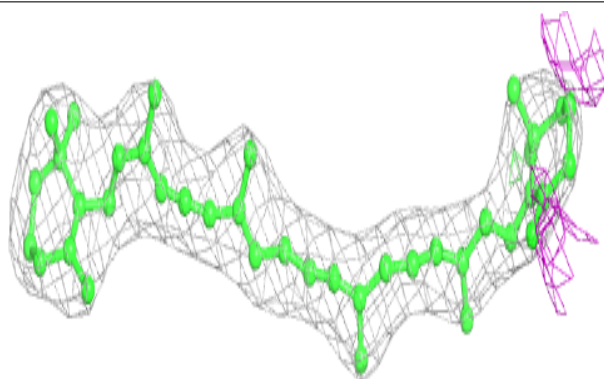


Electron density around BCR Y 856:

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

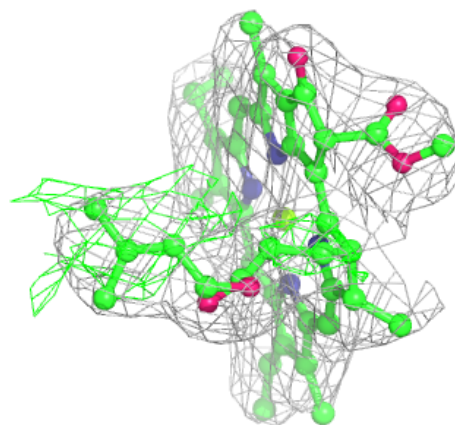
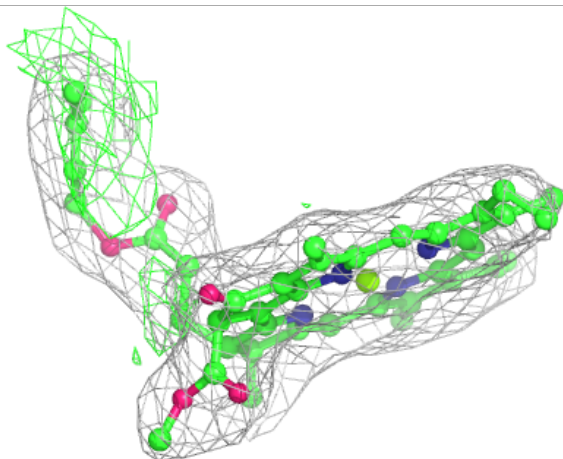
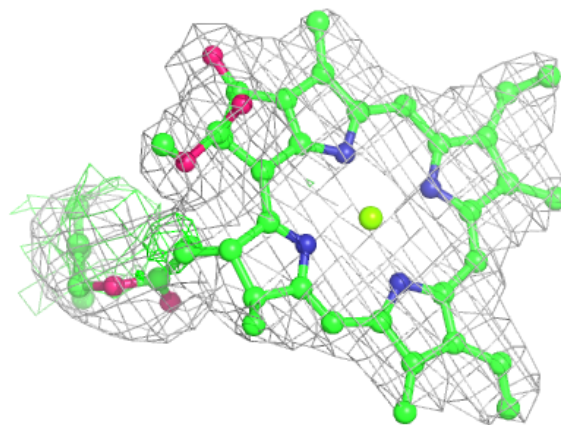
**Electron density around BCR Z 845:**

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



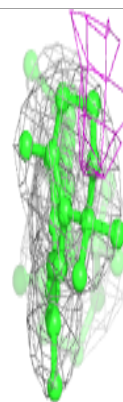
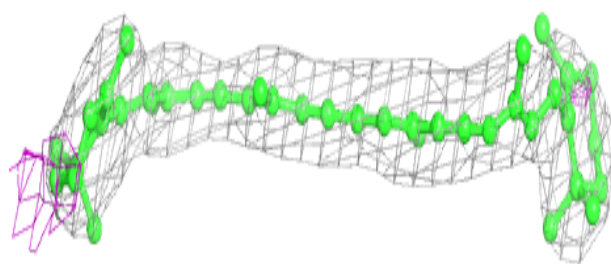
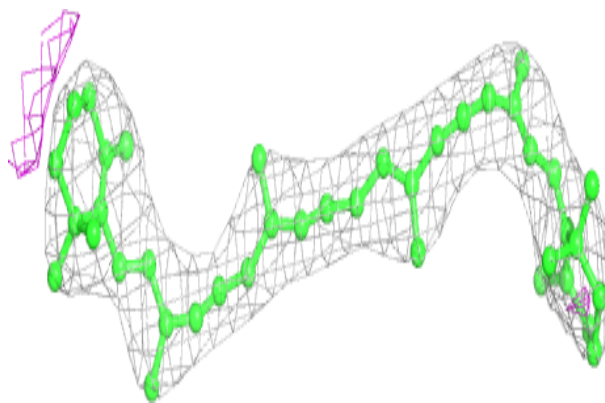
Electron density around CLA Y 839:

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



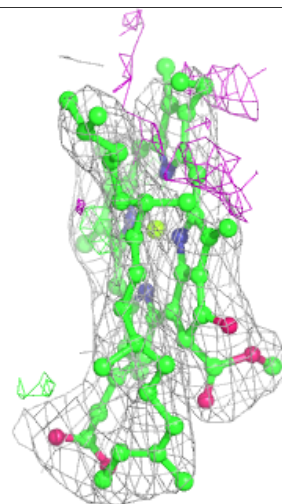
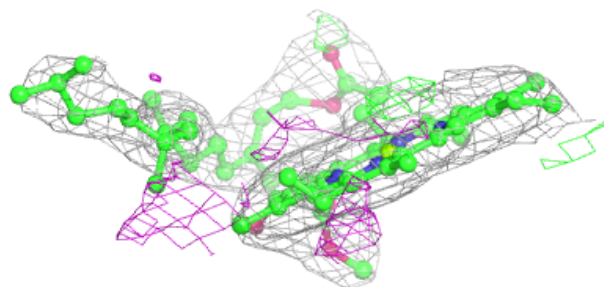
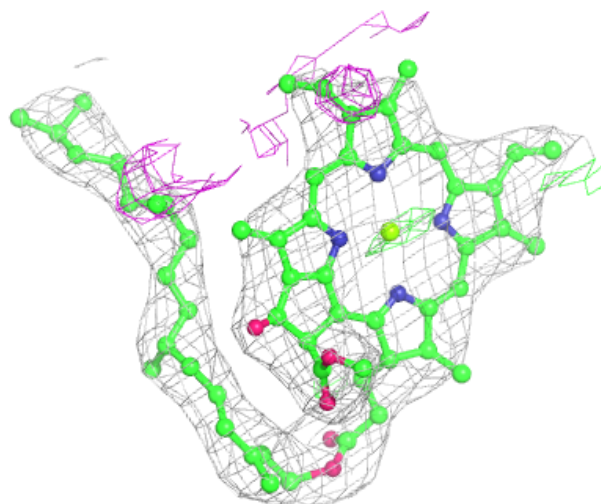
Electron density around BCR B 845:

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



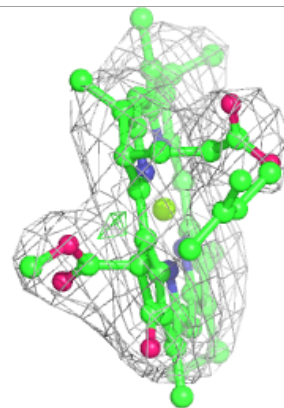
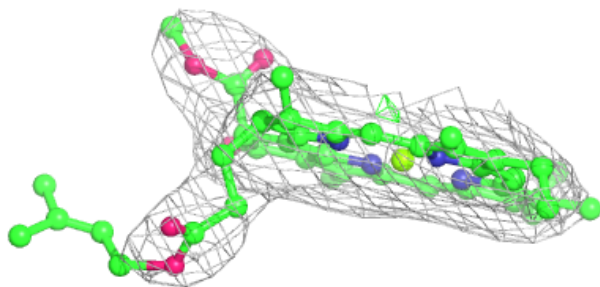
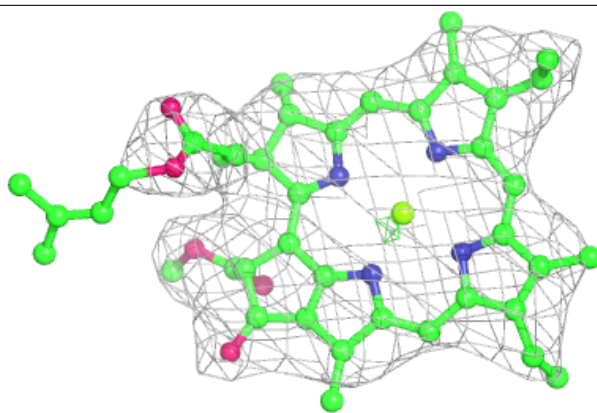
Electron density around CLA G 825:

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



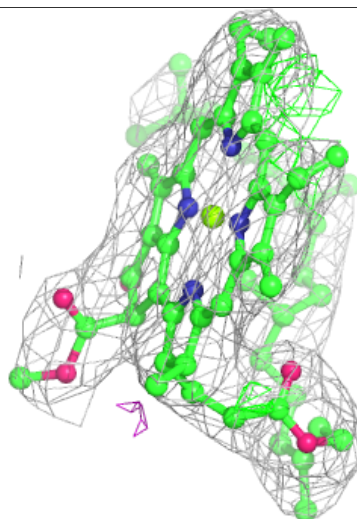
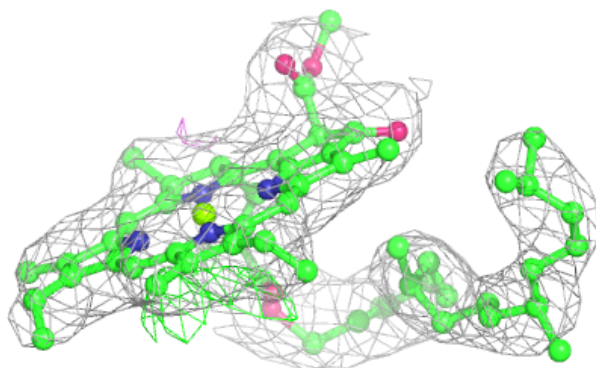
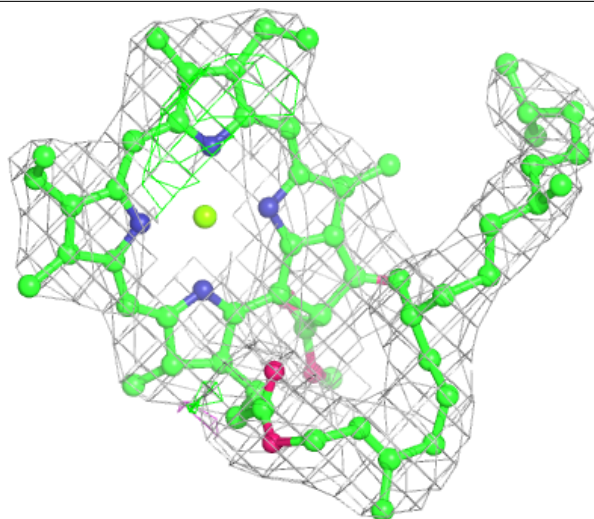
Electron density around CLA Y 816:

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



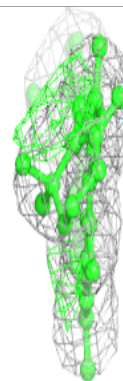
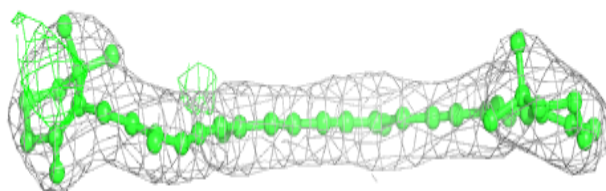
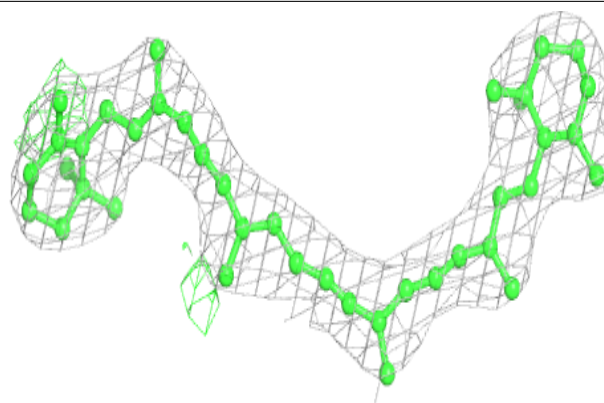
Electron density around CLA Q 201:

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



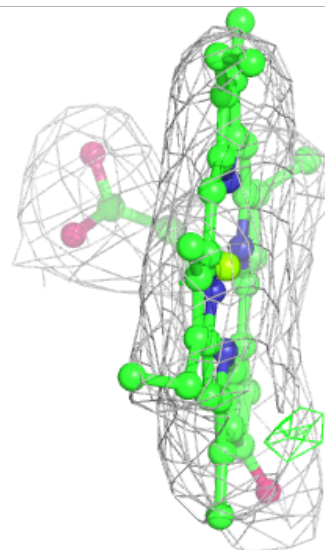
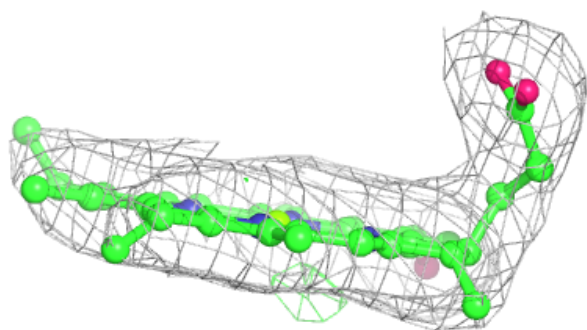
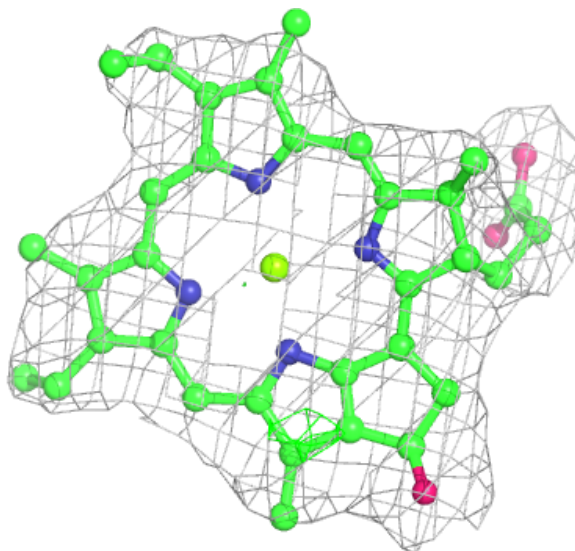
Electron density around BCR G 850:

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



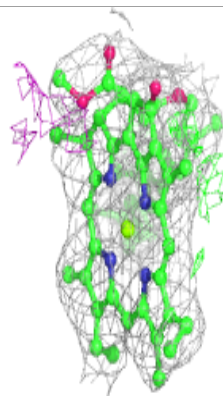
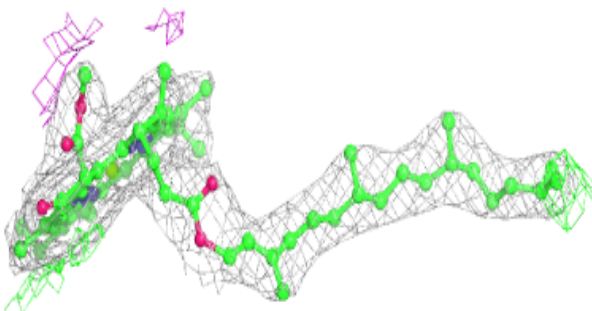
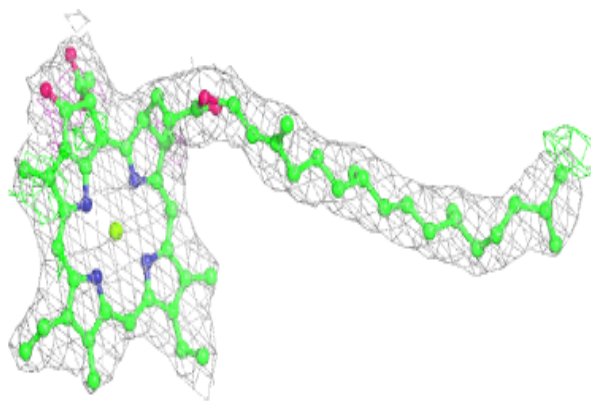
Electron density around CLA K 101:

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

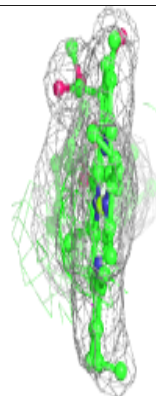
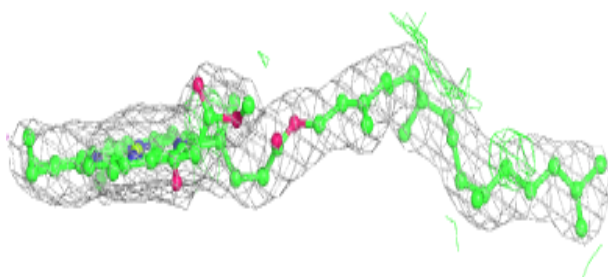
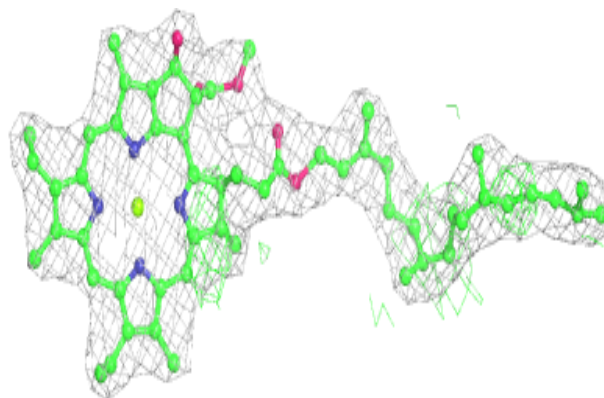


Electron density around CLA L 201:

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

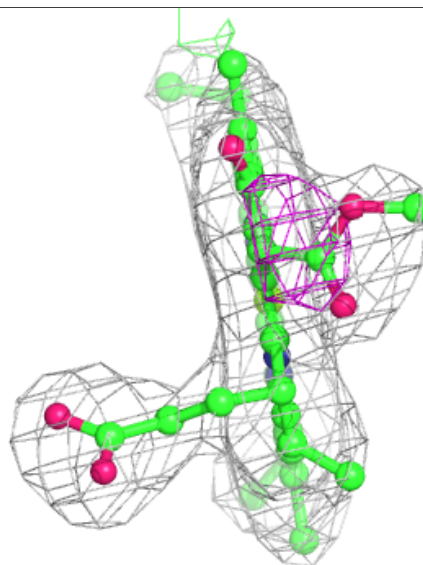
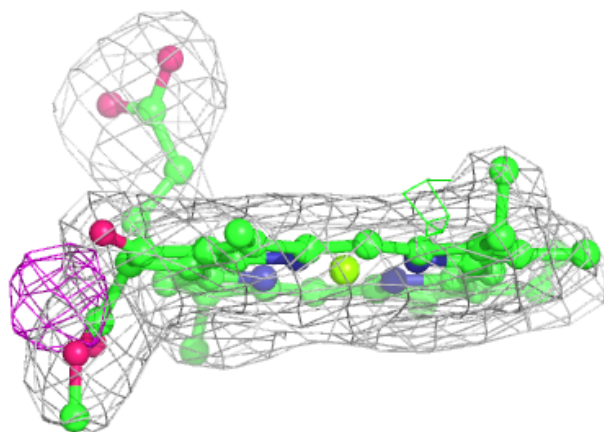
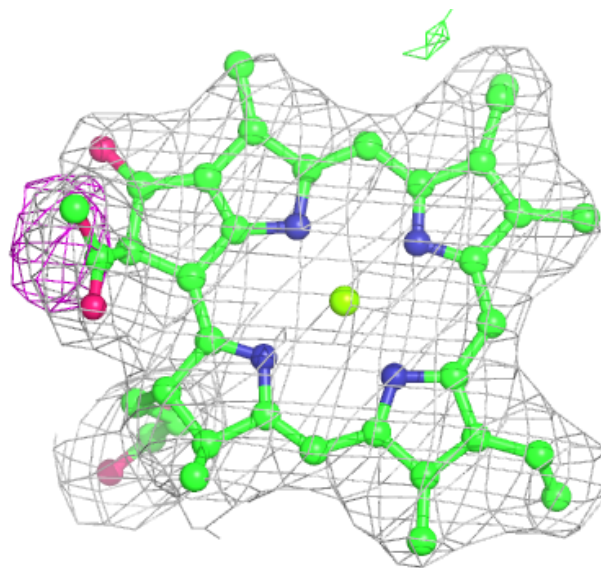
**Electron density around CLA A 833:**

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



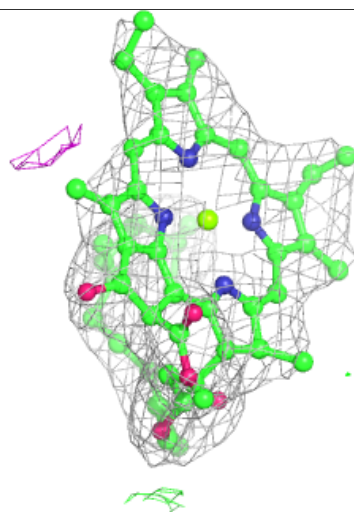
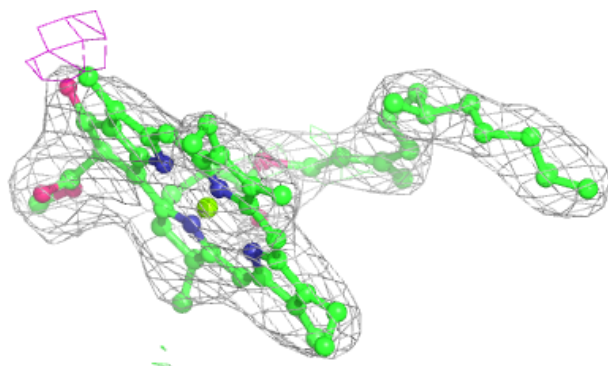
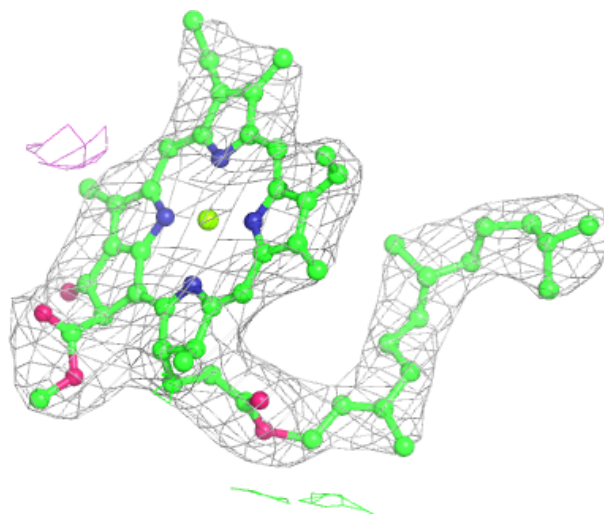
Electron density around CLA H 829:

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



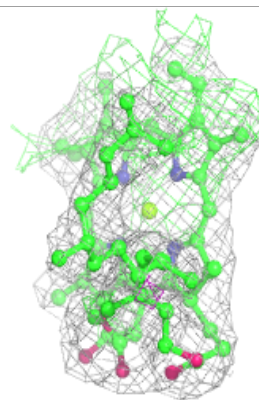
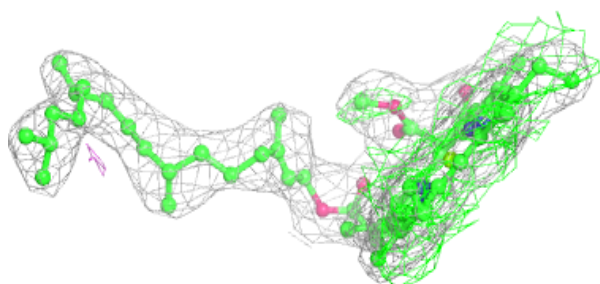
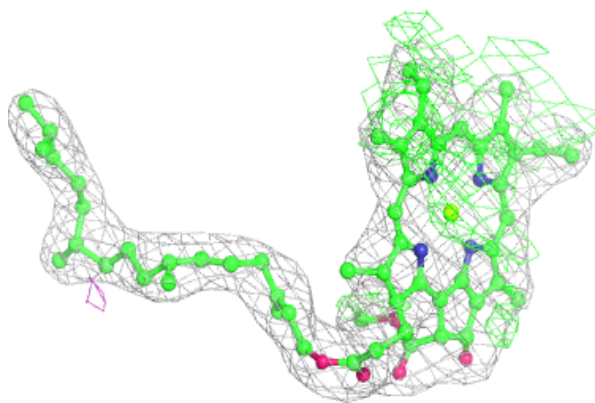
Electron density around CLA A 824:

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

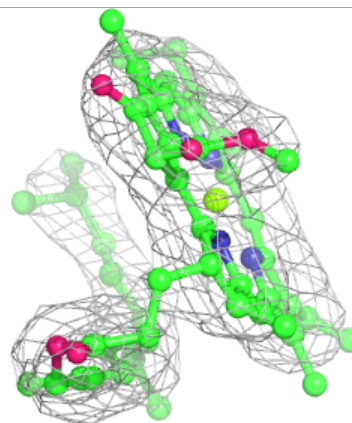
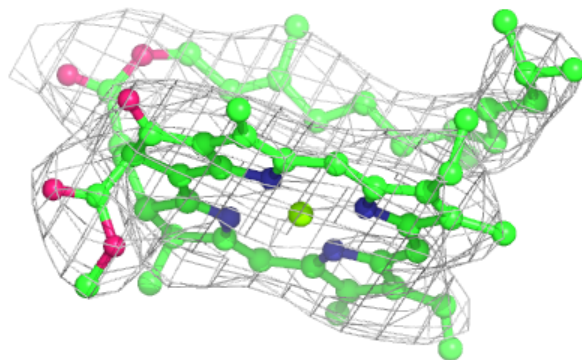
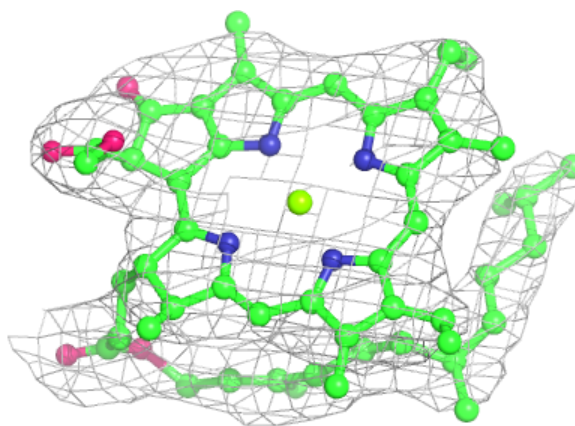


Electron density around CLA L 202:

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

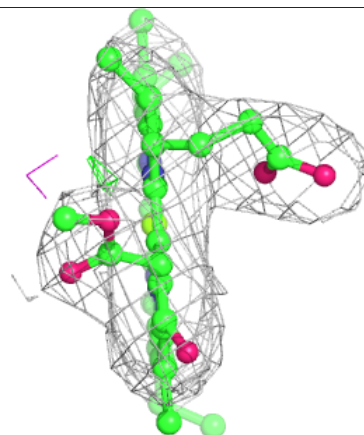
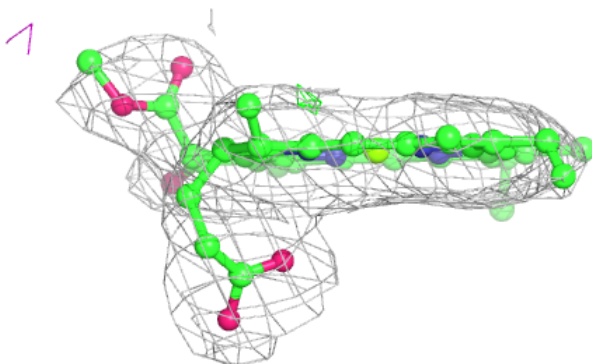
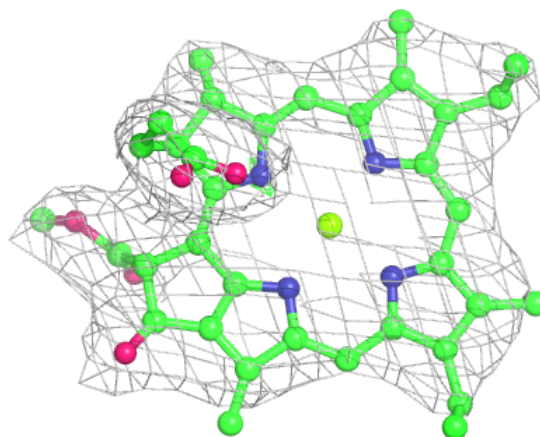
**Electron density around CLA G 820:**

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

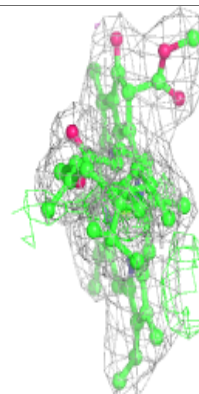
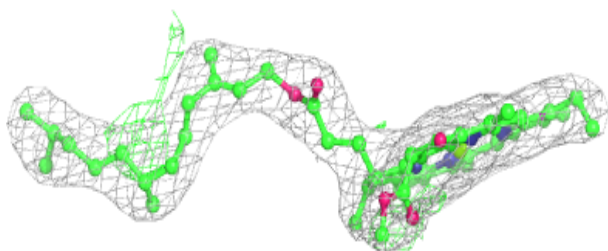
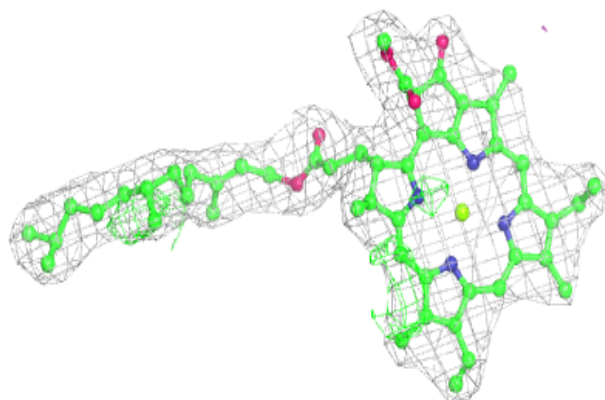


Electron density around CLA G 835:

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

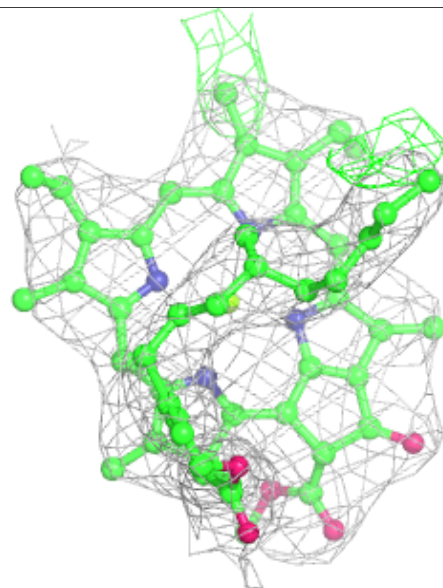
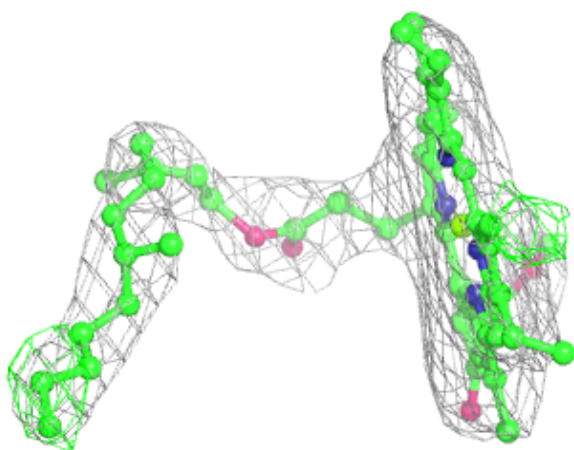
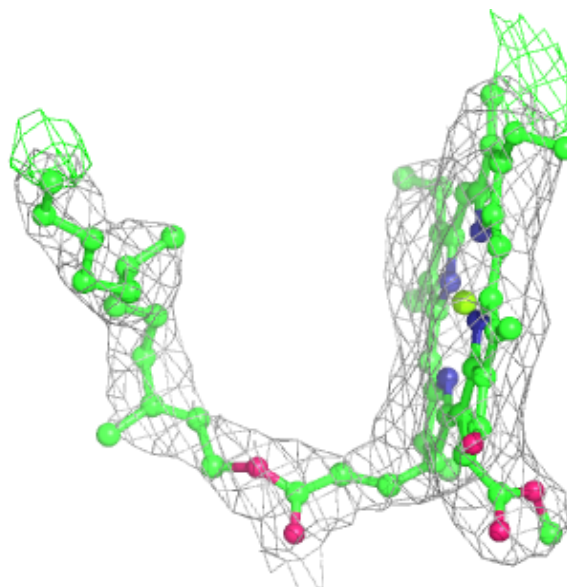
**Electron density around CLA Y 826:**

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



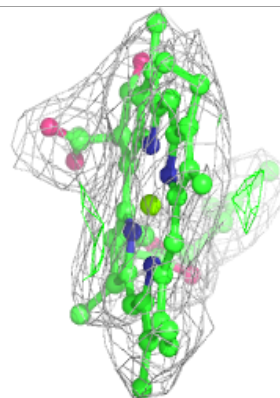
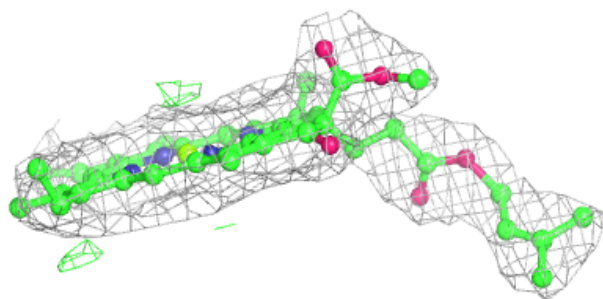
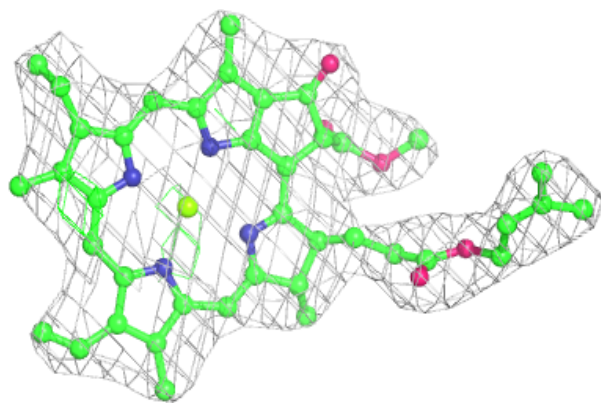
Electron density around CLA Y 804:

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

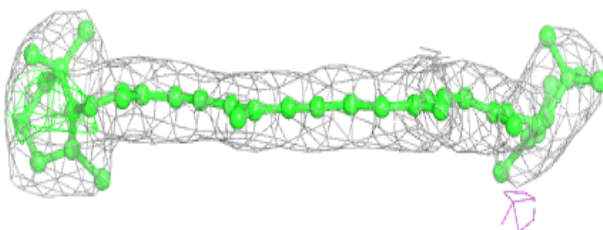
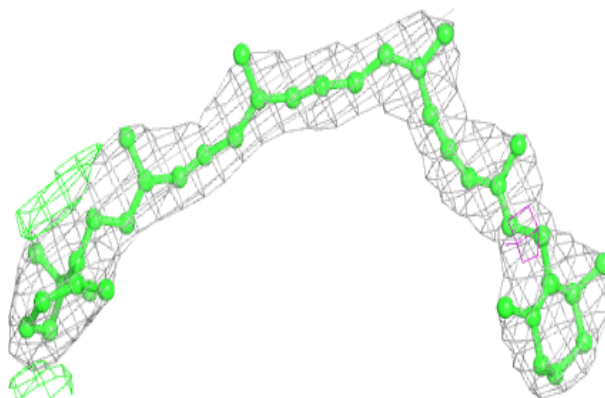


Electron density around CLA d 201:

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

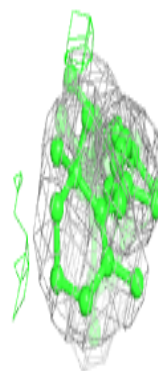
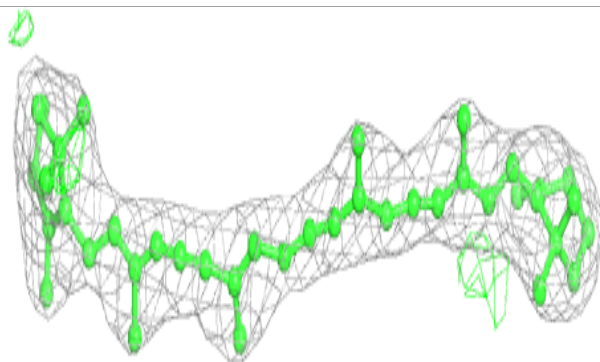
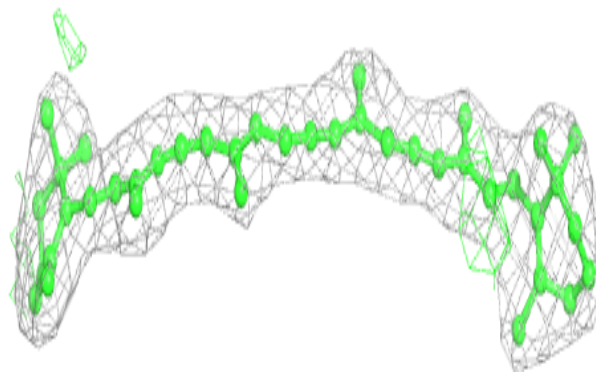
**Electron density around BCR Q 204:**

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



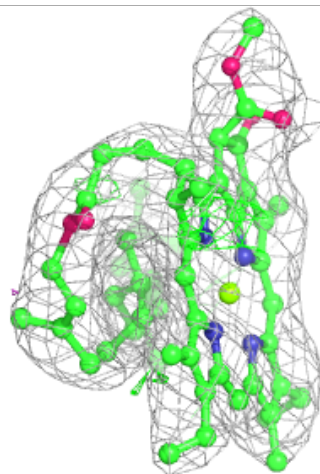
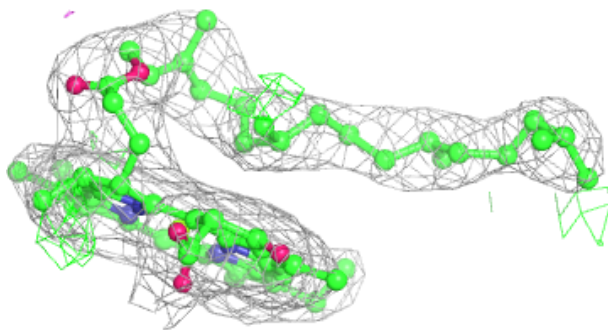
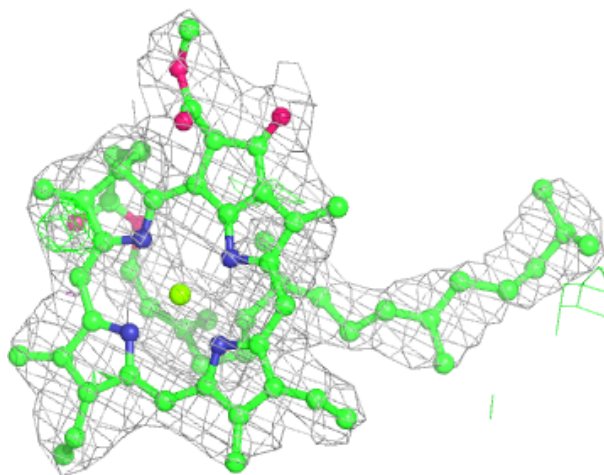
Electron density around BCR V 1202:

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



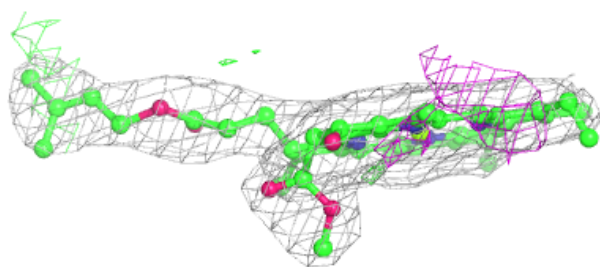
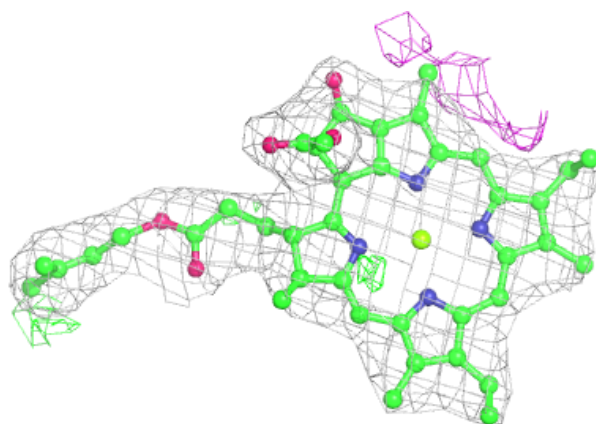
Electron density around CLA Z 825:

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



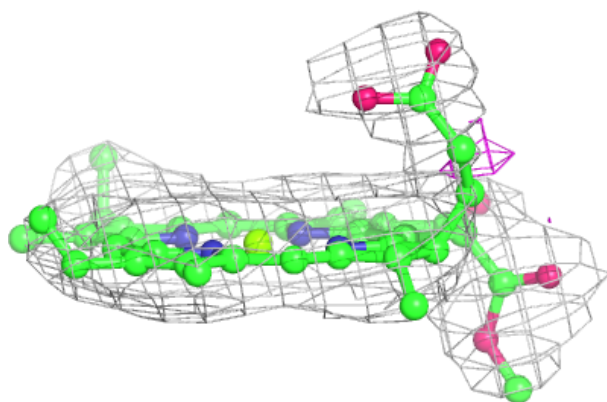
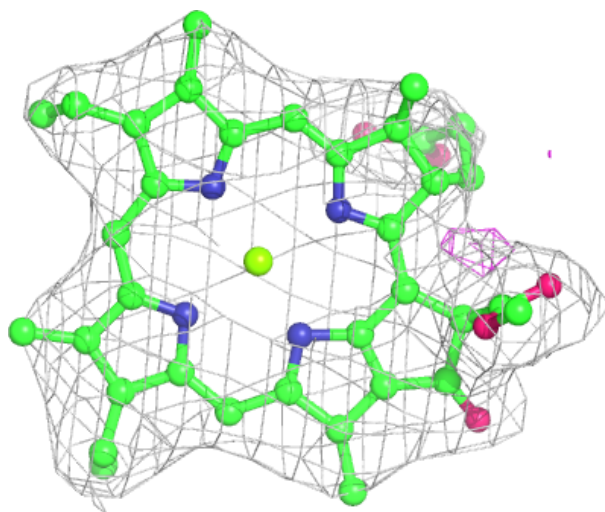
Electron density around CLA Y 837:

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



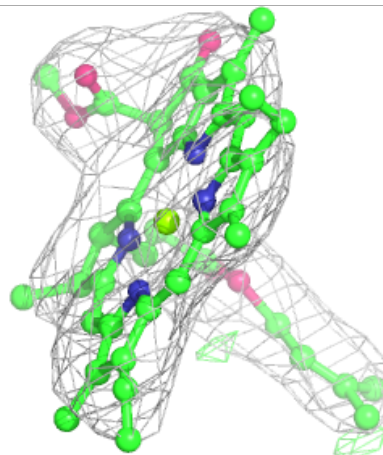
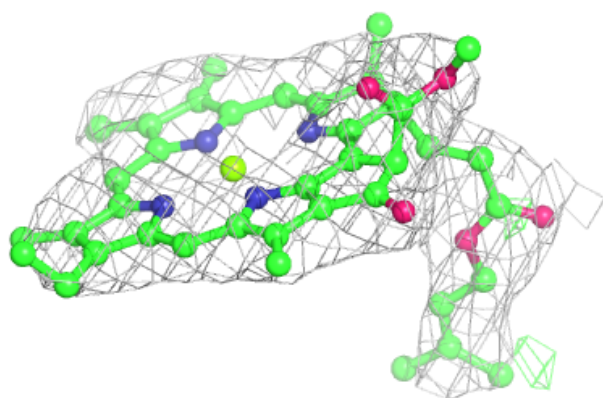
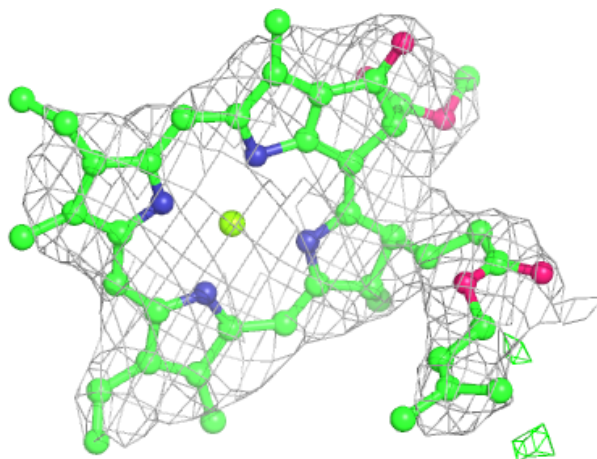
Electron density around CLA Z 818:

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



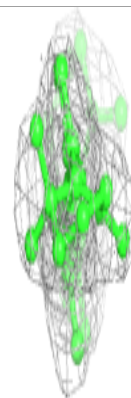
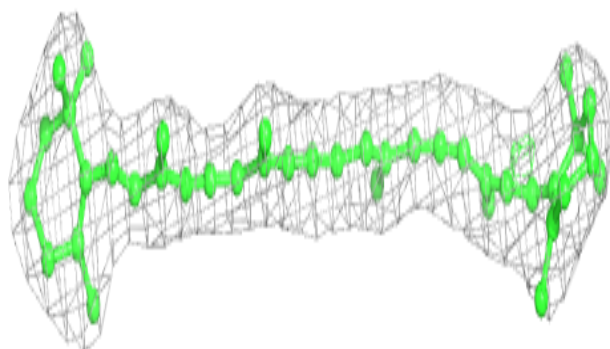
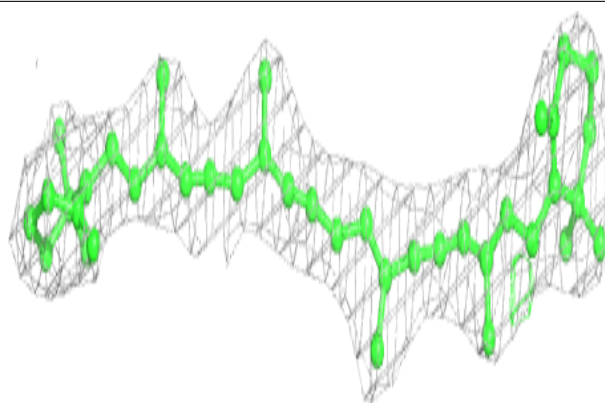
Electron density around CLA A 814:

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

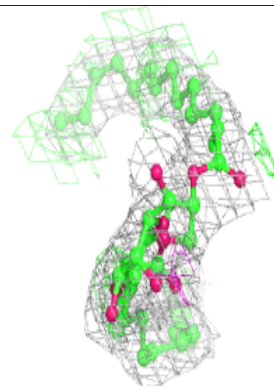
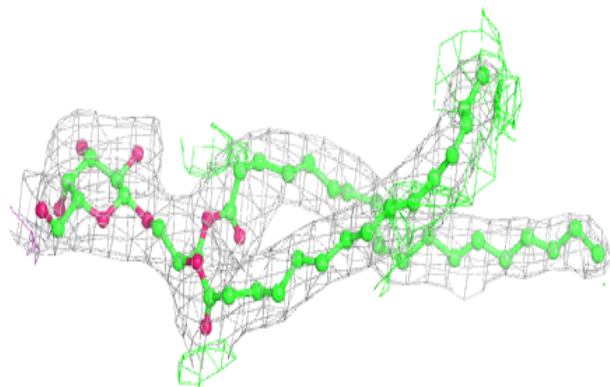
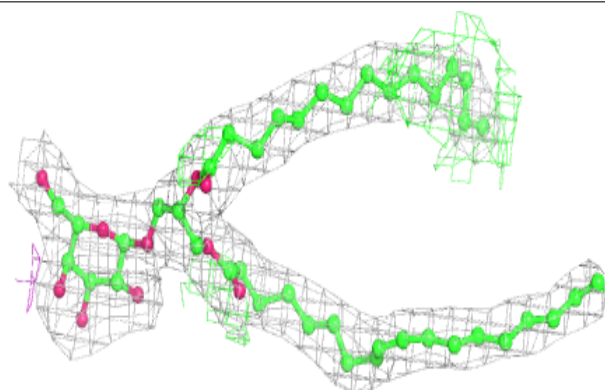


Electron density around BCR U 1008:

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

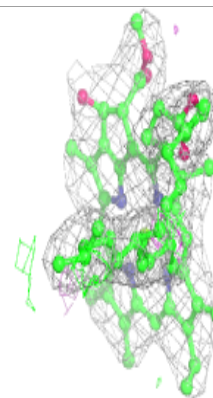
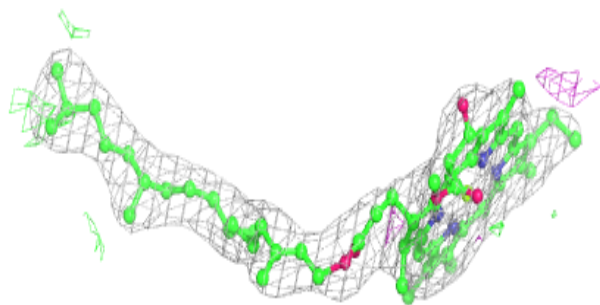
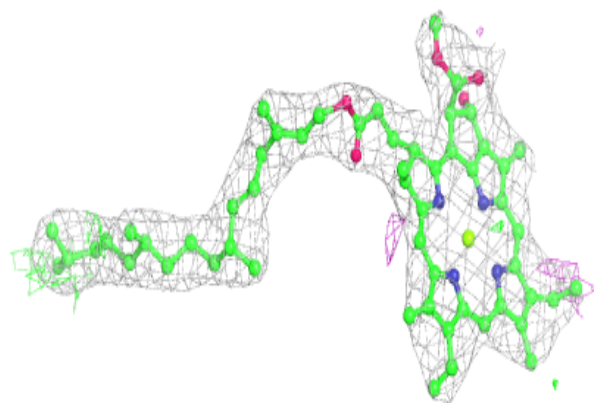
**Electron density around LMG B 849:**

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

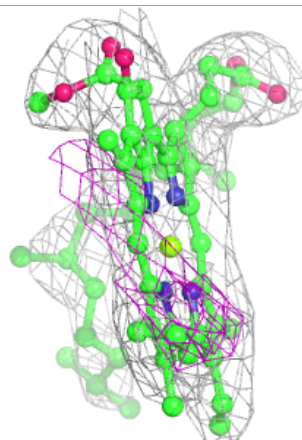
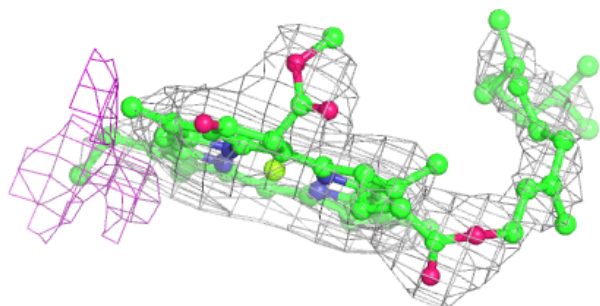
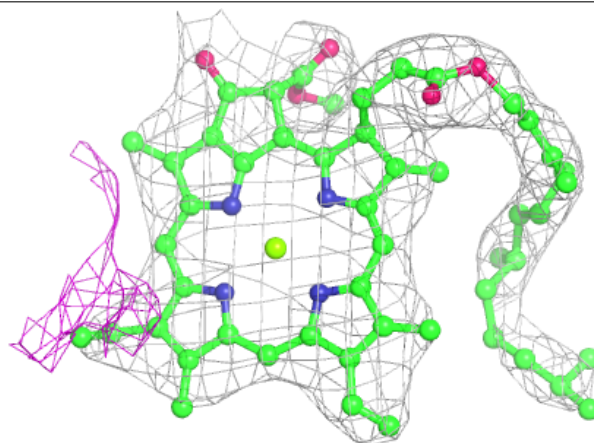


Electron density around CLA G 803:

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

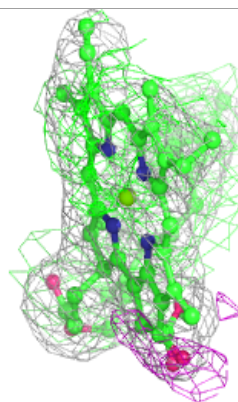
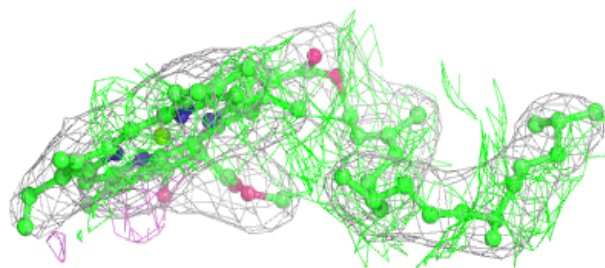
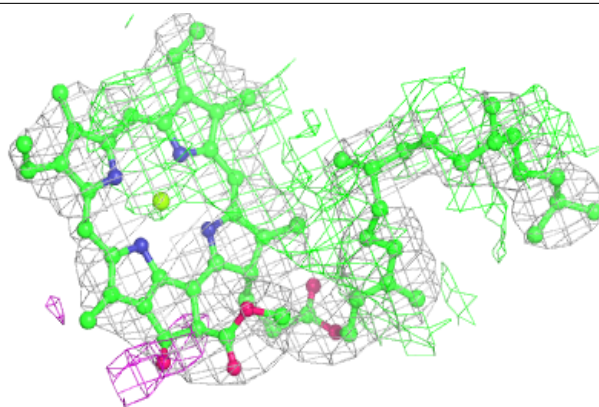
**Electron density around CLA Y 813:**

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

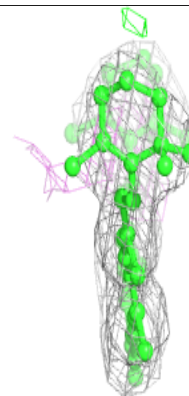
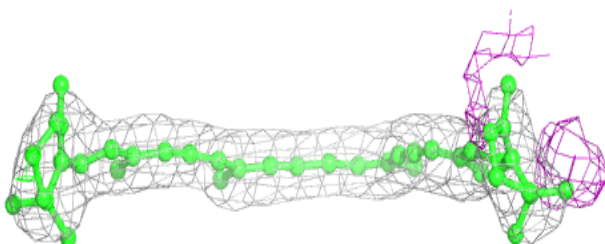
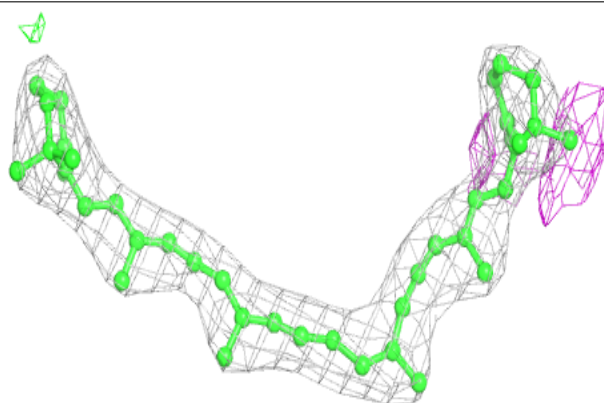


Electron density around CLA S 1101:

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

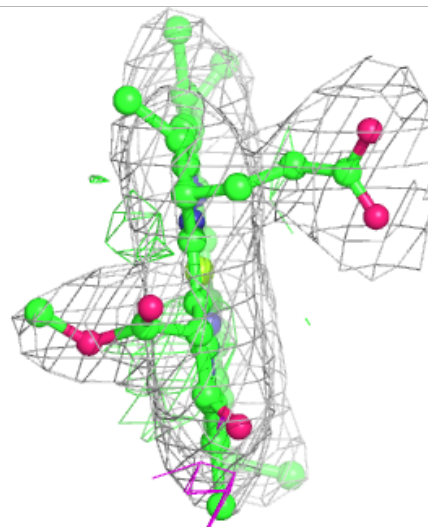
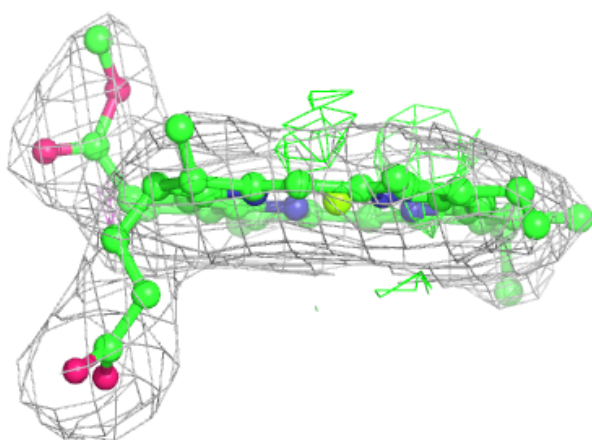
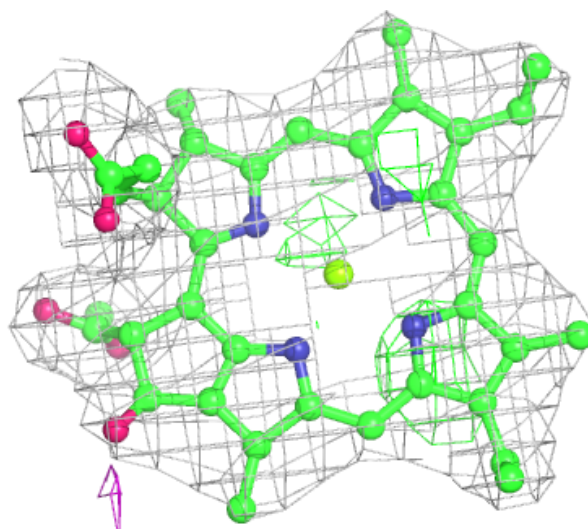
**Electron density around BCR F 203:**

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



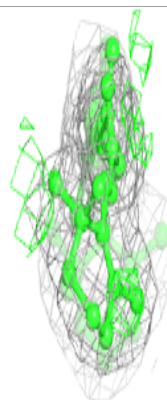
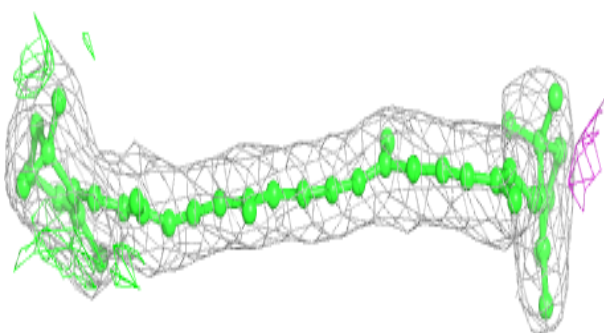
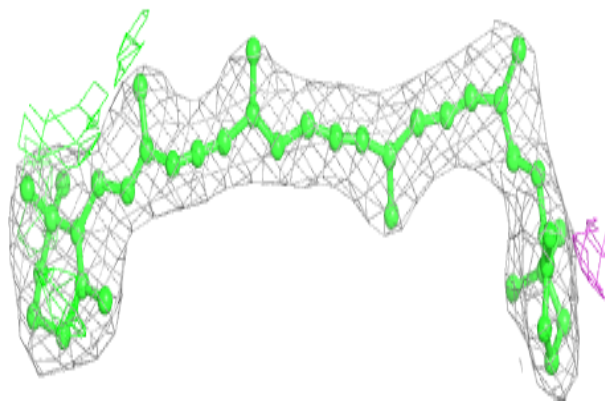
Electron density around CLA B 820:

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

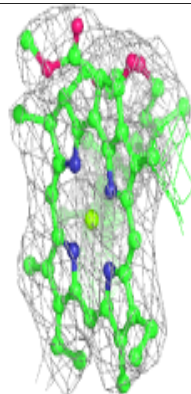
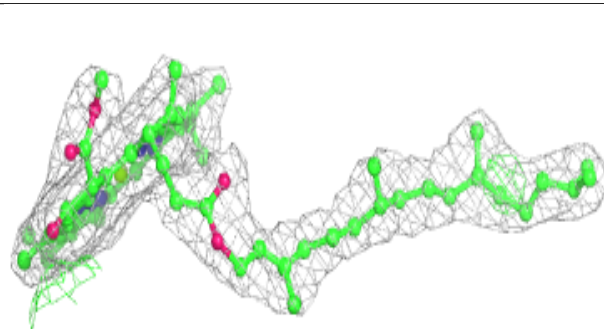
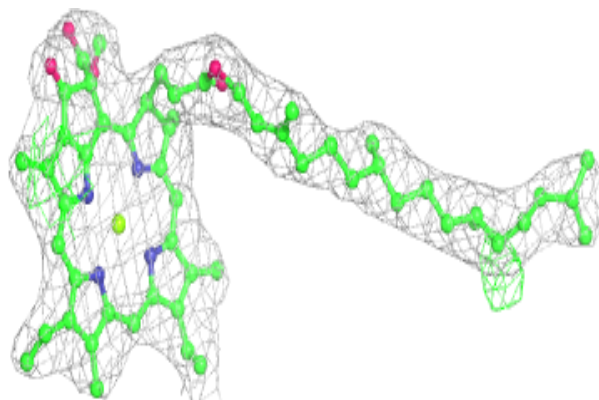


Electron density around BCR U 1007:

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

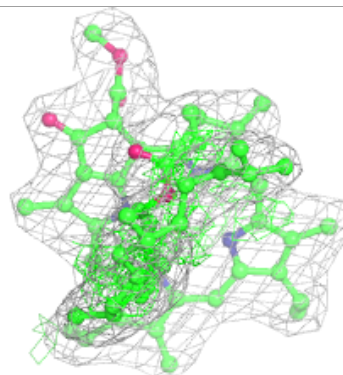
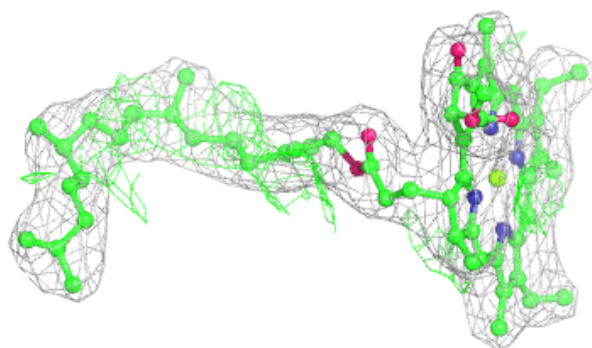
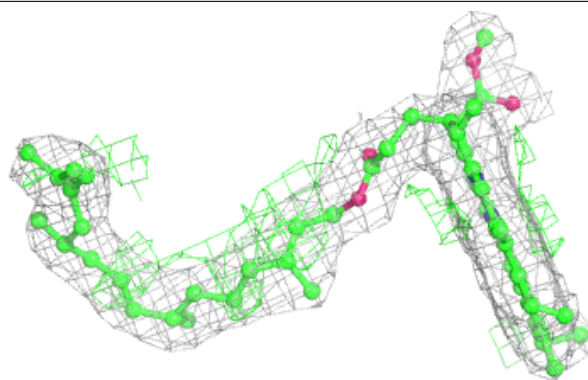
**Electron density around CLA G 833:**

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

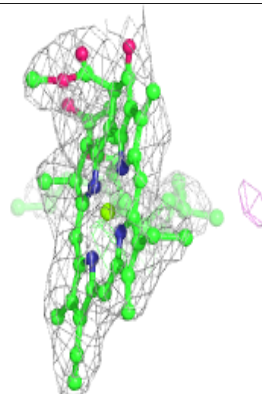
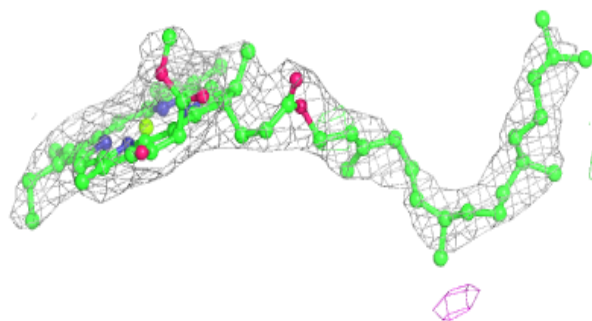
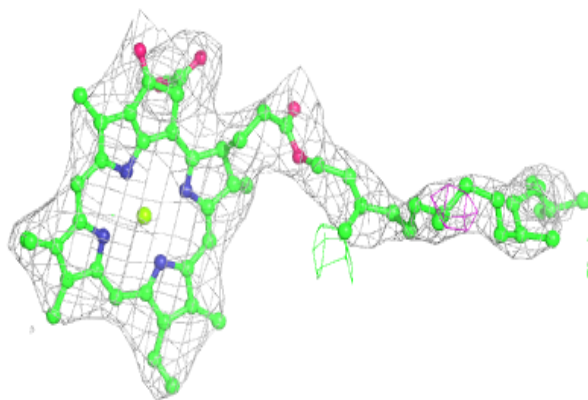


Electron density around CLA Z 838:

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

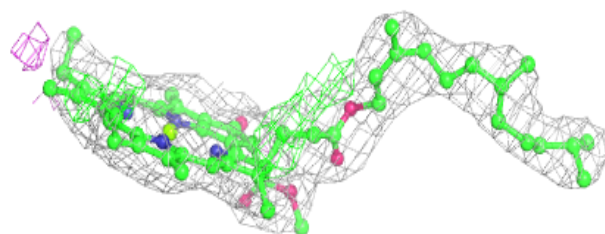
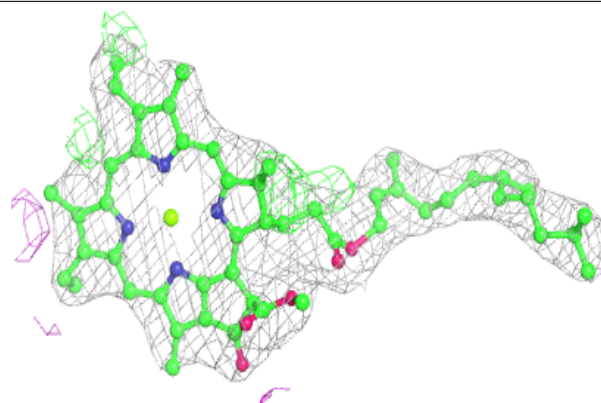
**Electron density around CLA Z 811:**

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

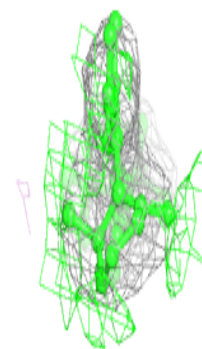
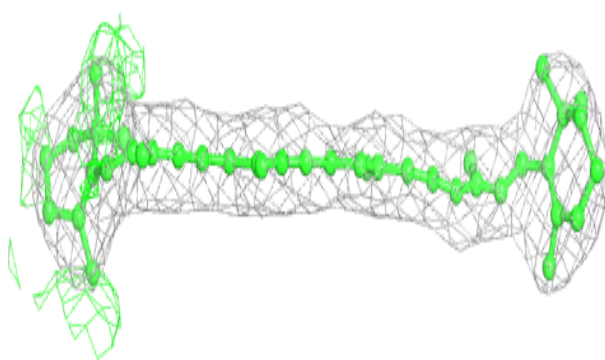
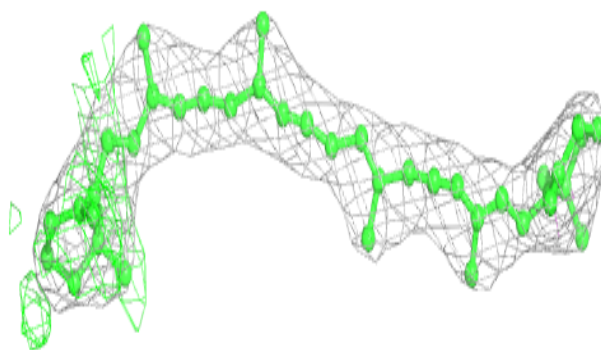


Electron density around CLA H 822:

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

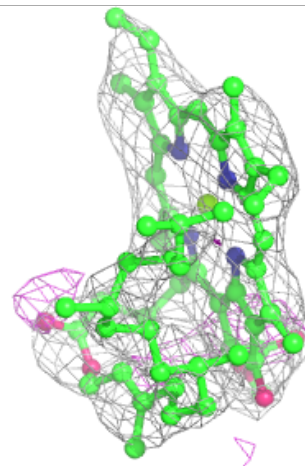
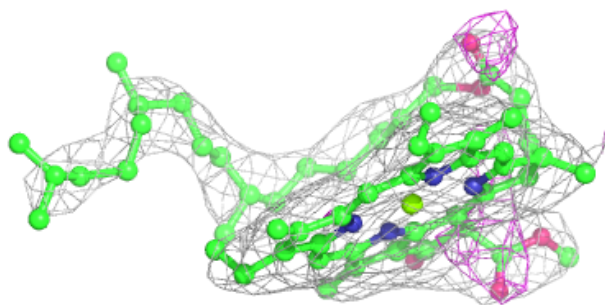
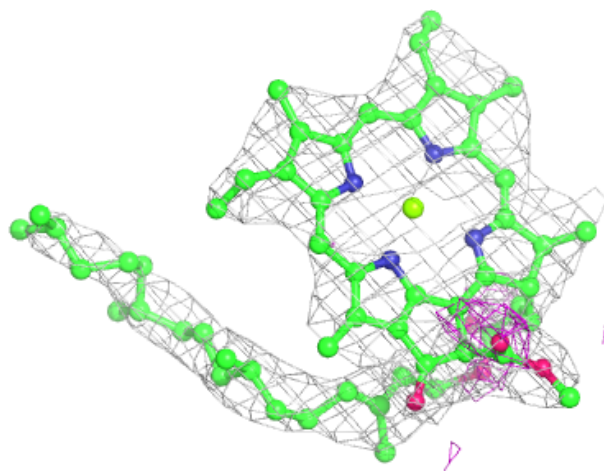
**Electron density around BCR G 848:**

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



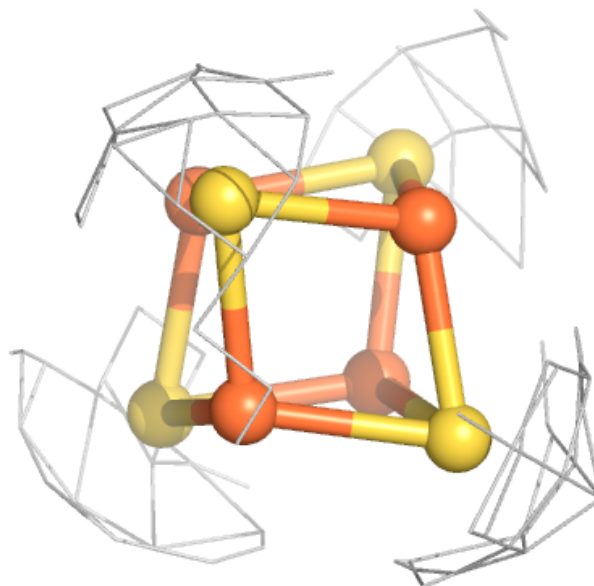
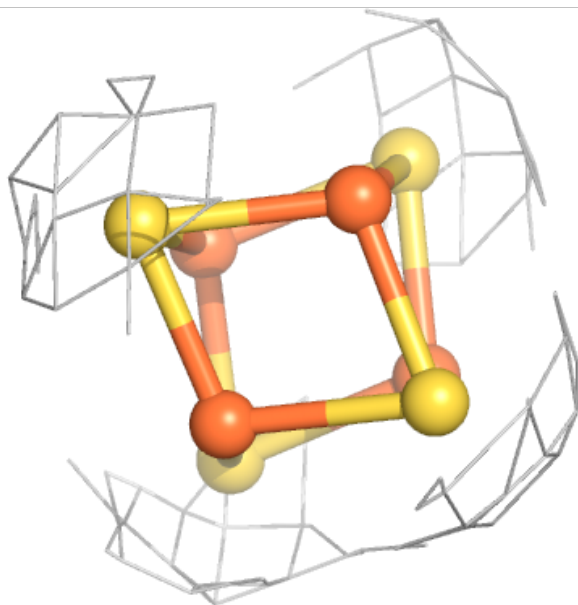
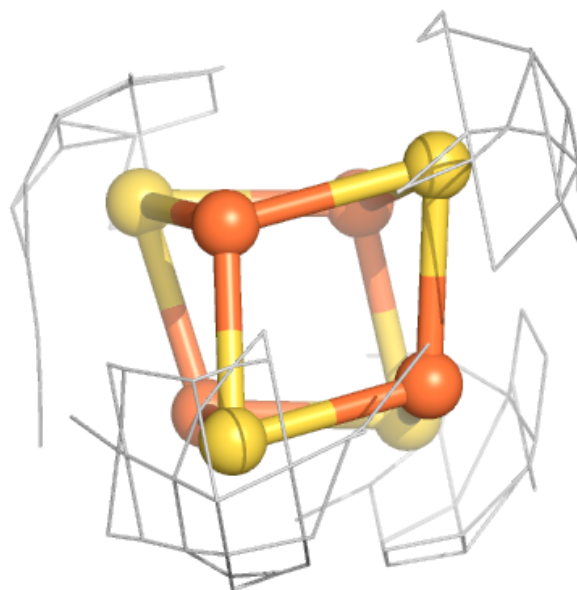
Electron density around CLA G 829:

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



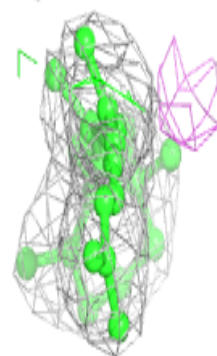
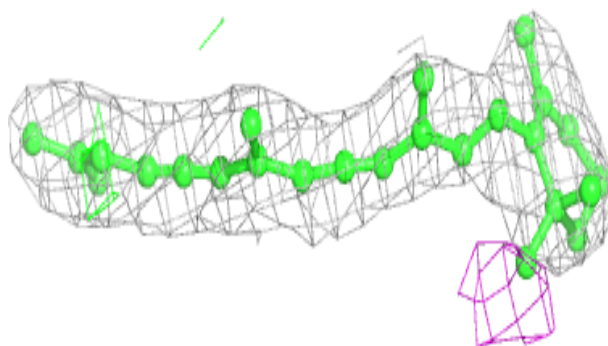
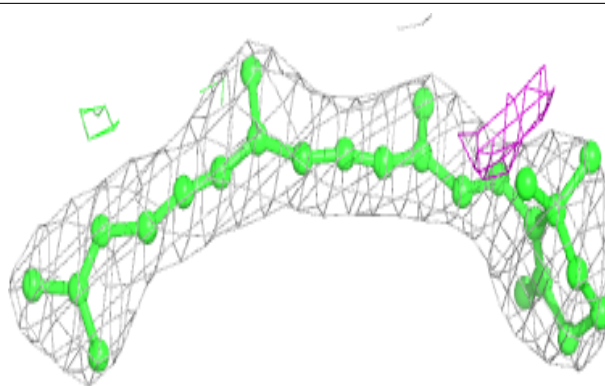
Electron density around SF4 C 101:

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

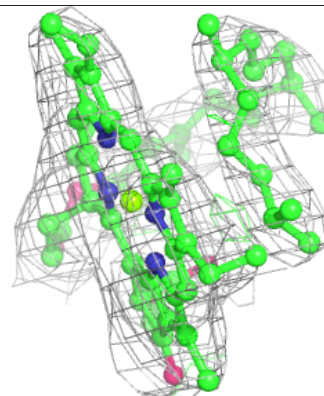
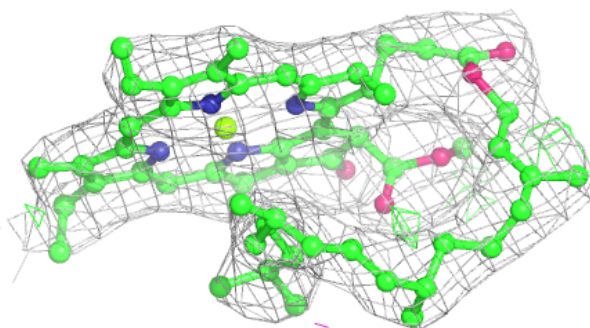
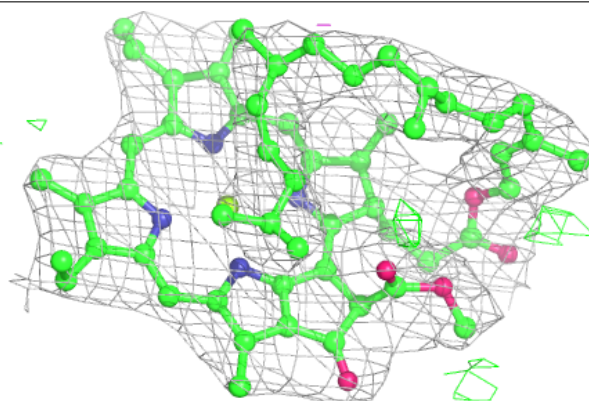


Electron density around BCR H 843:

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

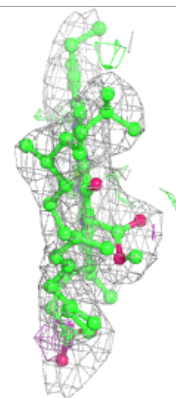
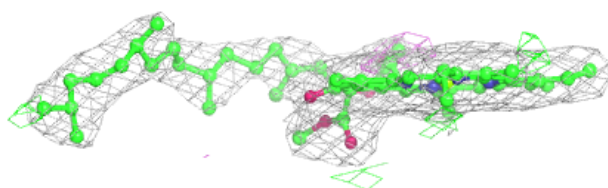
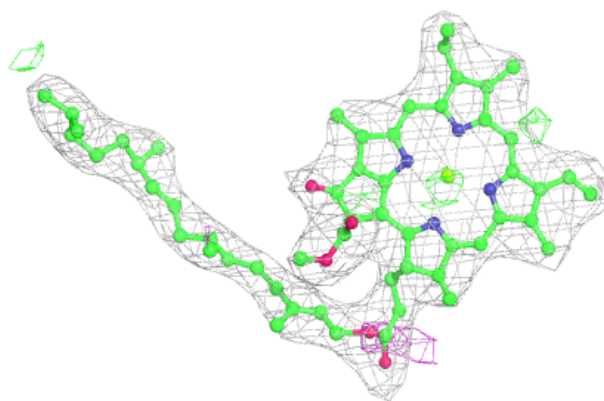
**Electron density around CLA Y 806:**

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

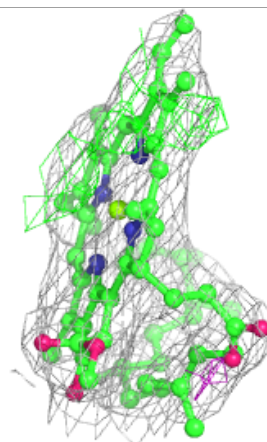
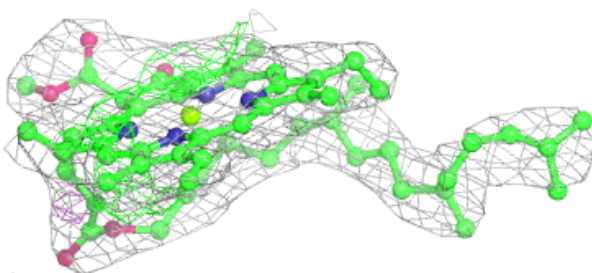
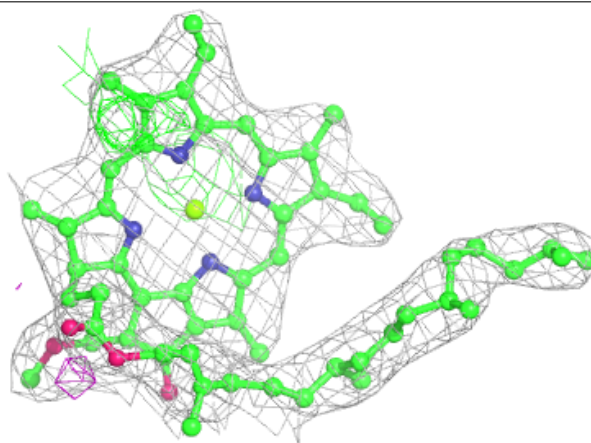


Electron density around CLA h 207:

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

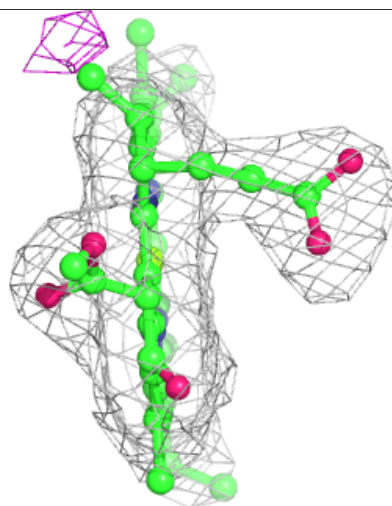
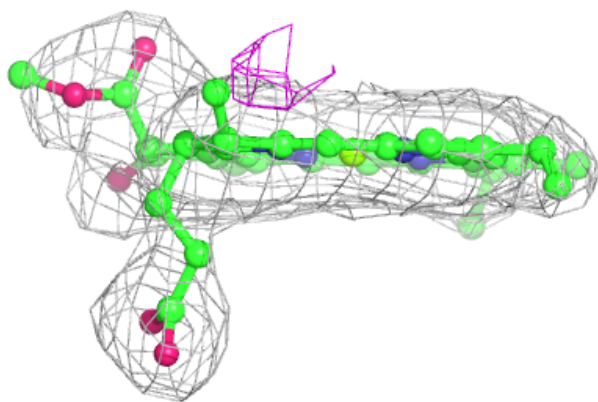
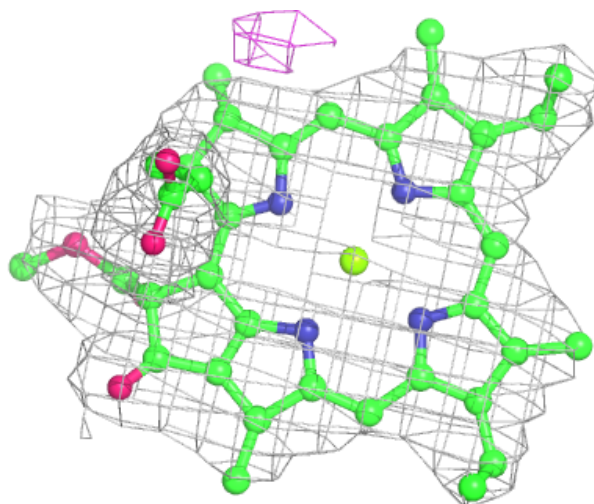
**Electron density around CLA Y 829:**

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



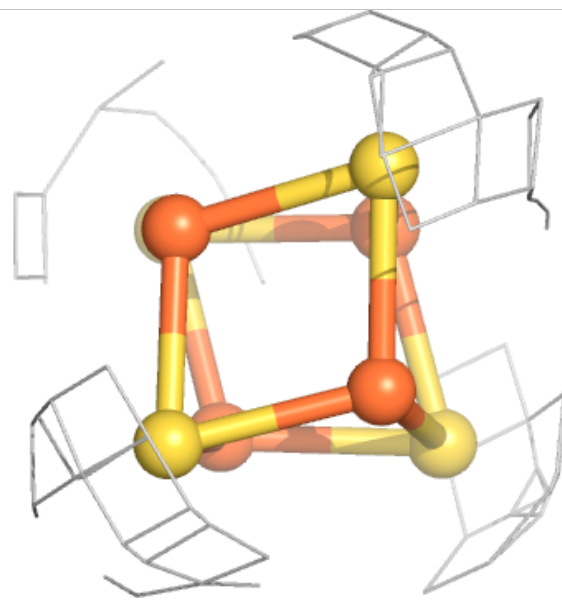
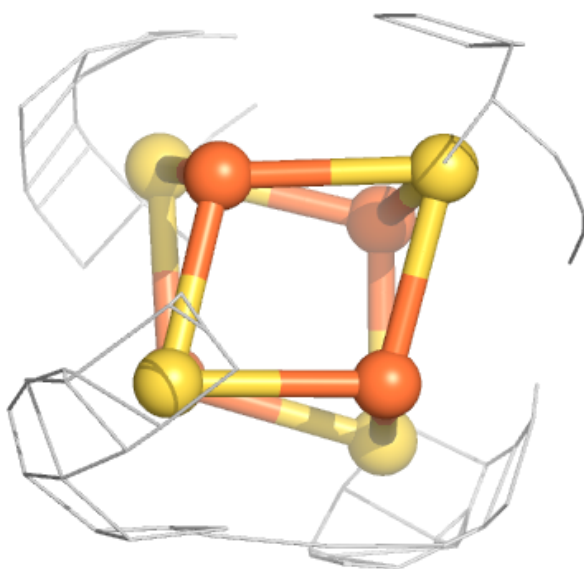
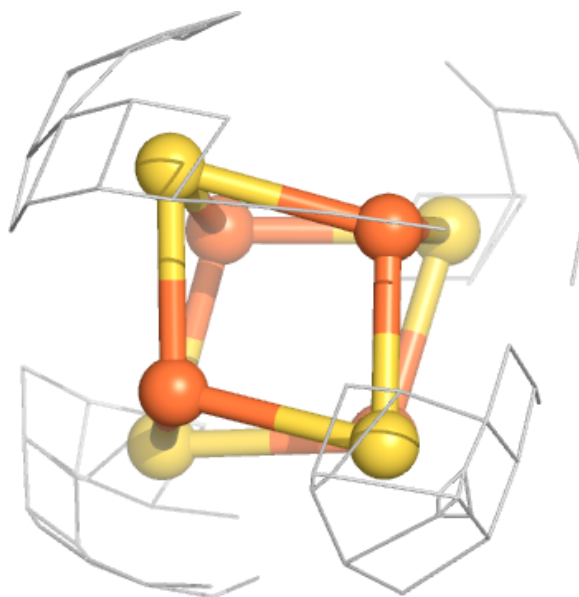
Electron density around CLA G 853:

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



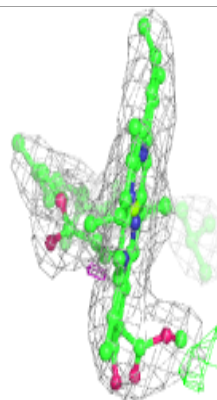
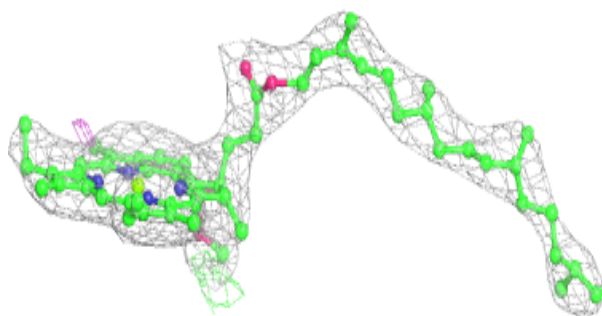
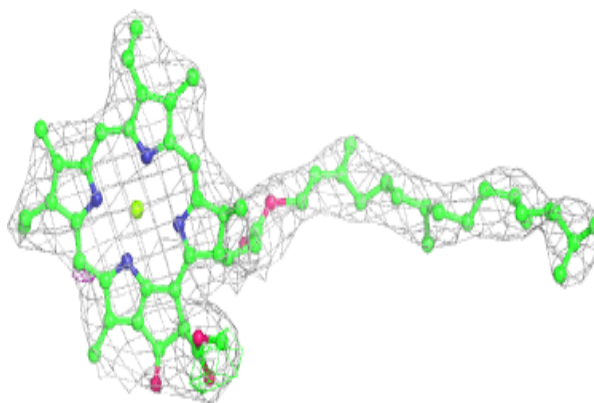
Electron density around SF4 C 102:

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

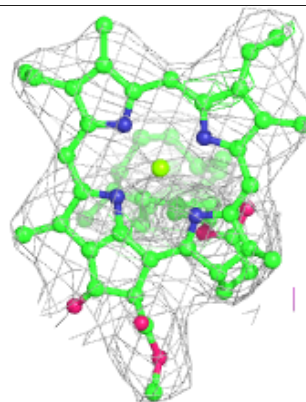
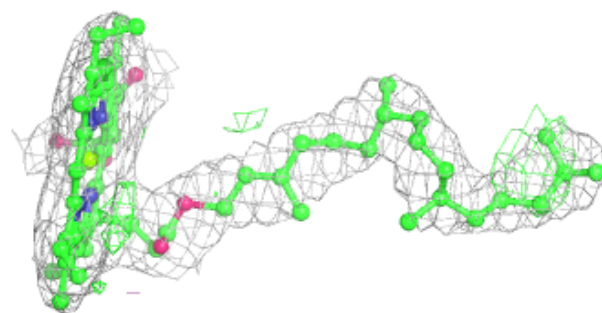
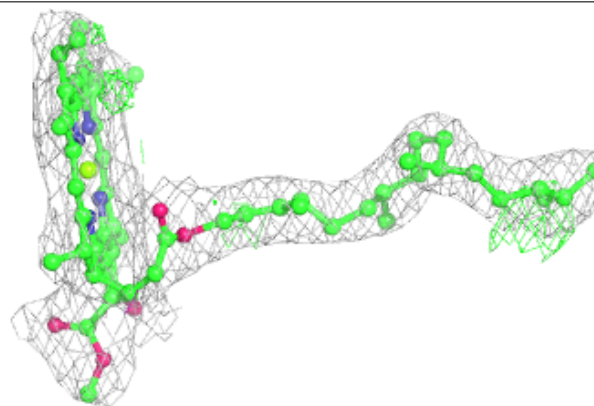


Electron density around CLA Z 823:

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

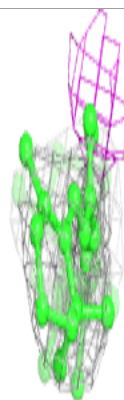
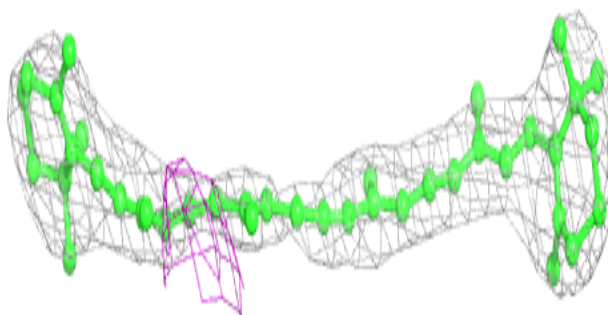
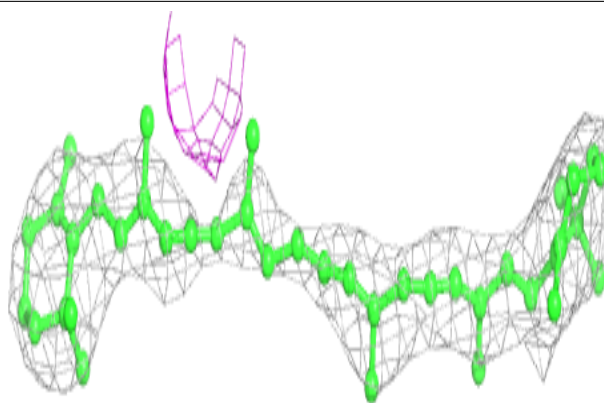
**Electron density around CLA A 828:**

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

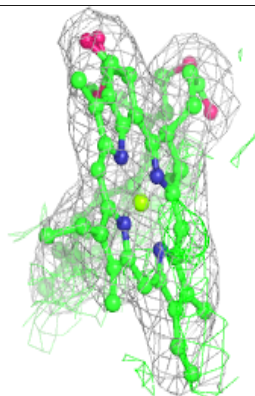
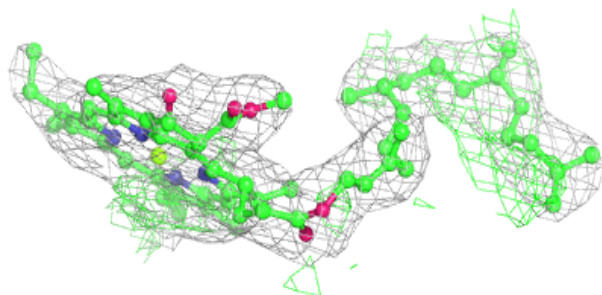
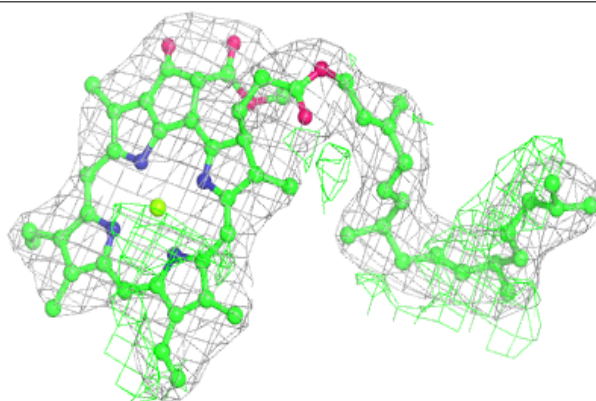


Electron density around BCR A 846:

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

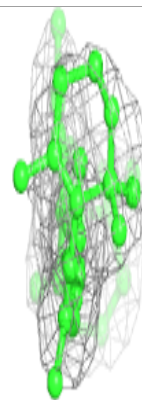
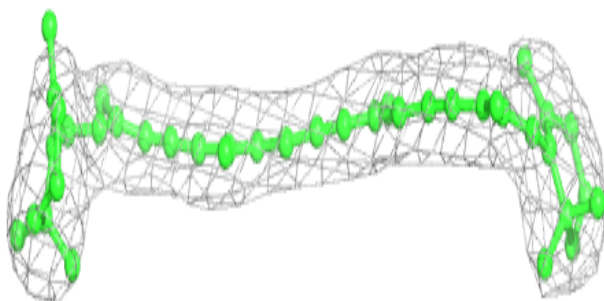
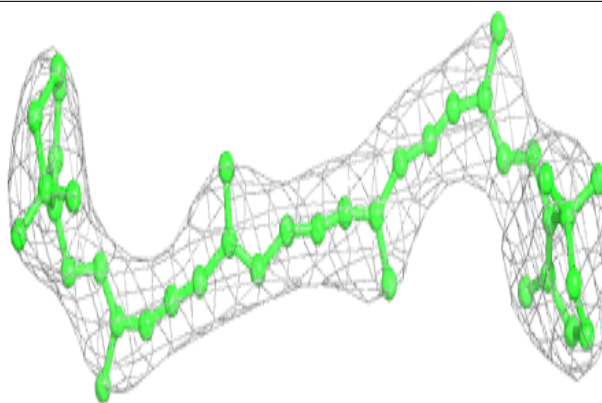
**Electron density around CLA A 803:**

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



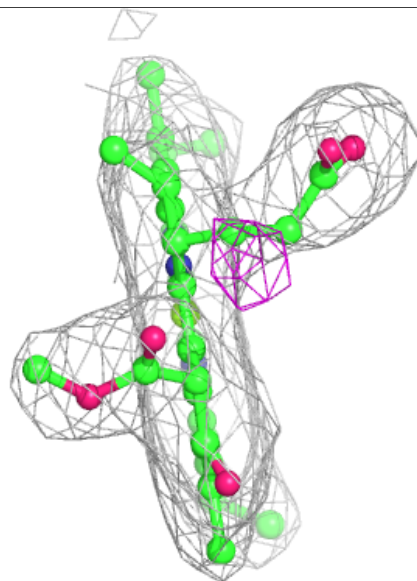
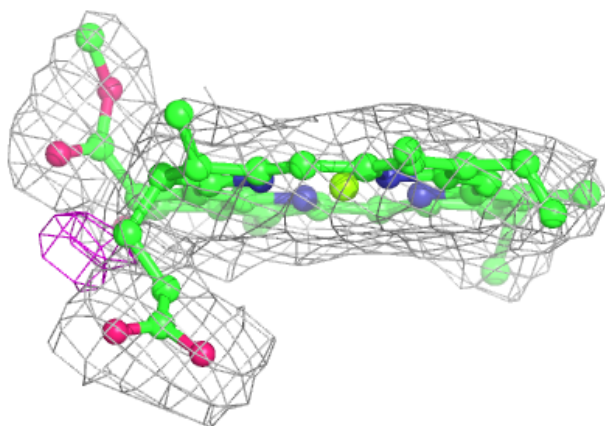
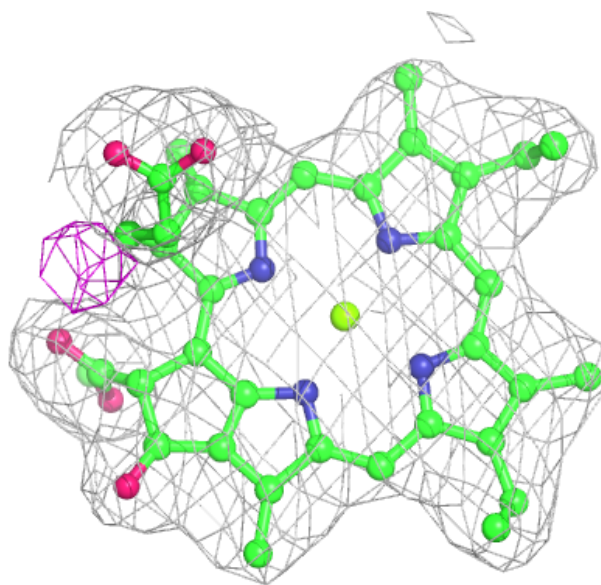
Electron density around BCR Z 843:

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



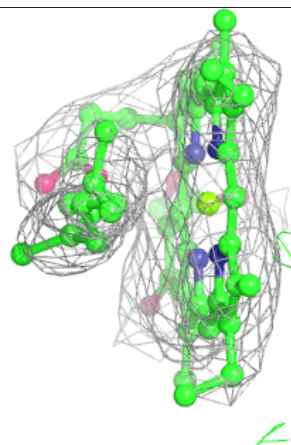
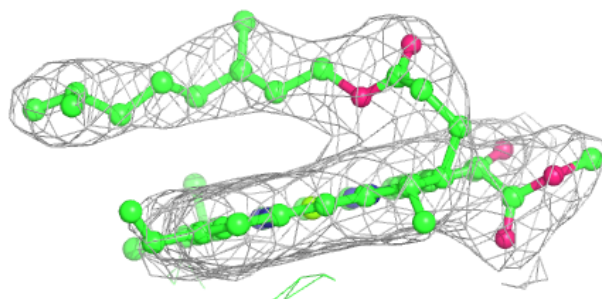
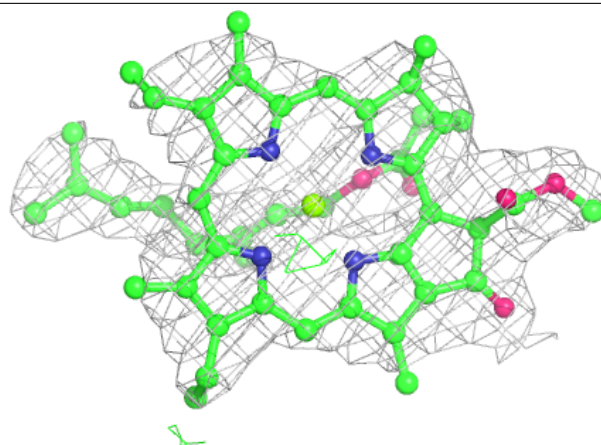
Electron density around CLA B 830:

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



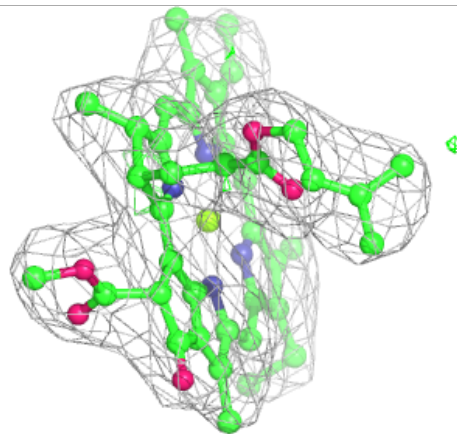
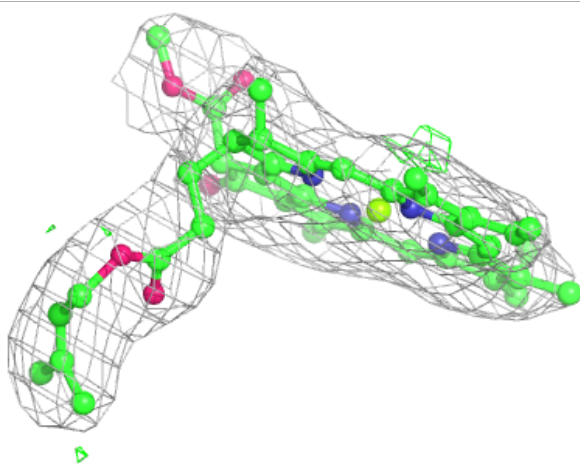
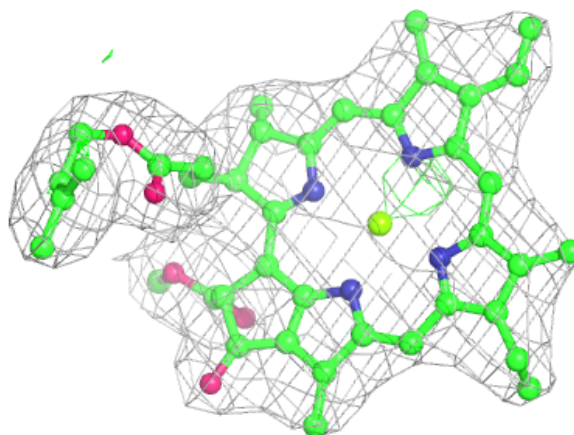
Electron density around CLA Z 820:

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



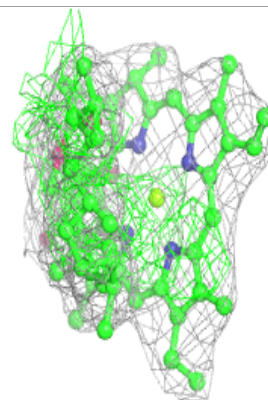
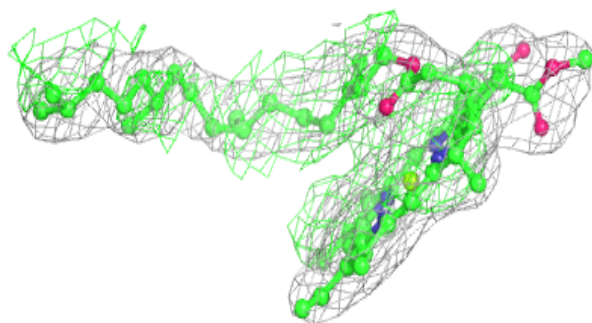
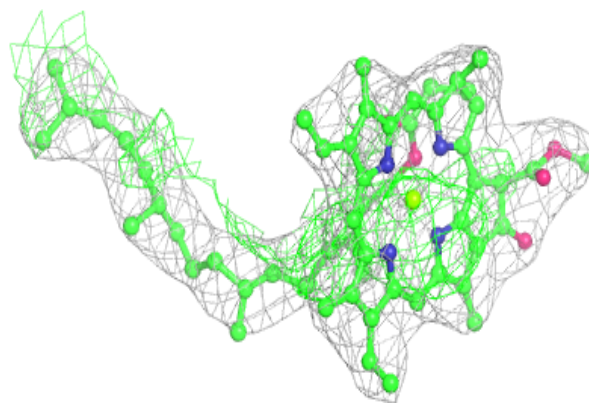
Electron density around CLA G 838:

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

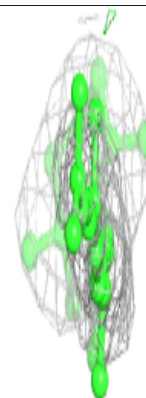
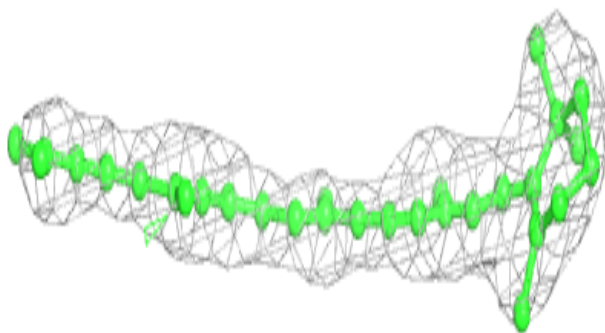
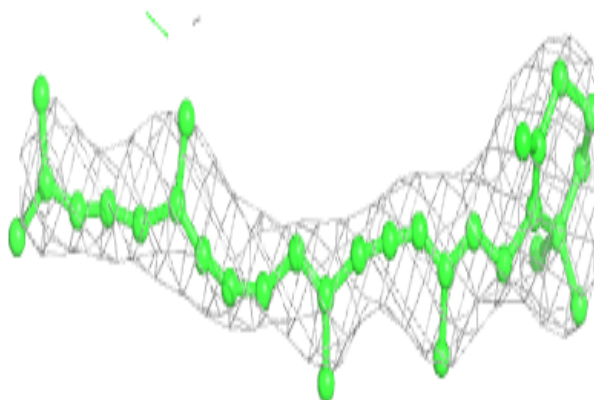


Electron density around CLA Y 841:

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

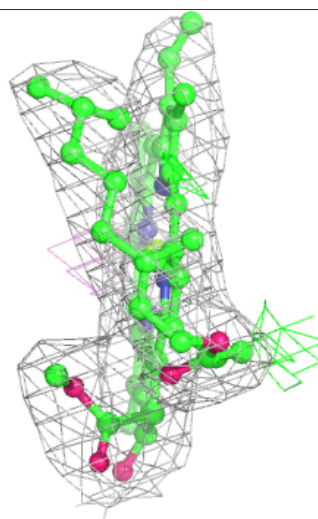
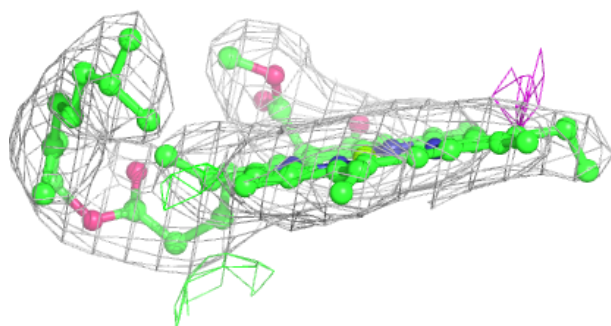
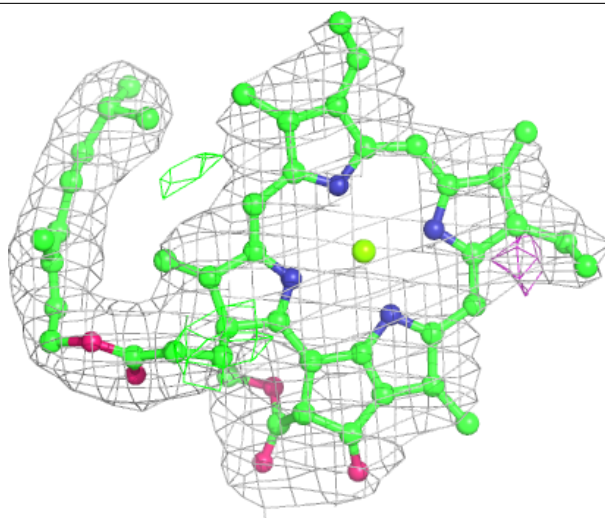
**Electron density around BCR B 843:**

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



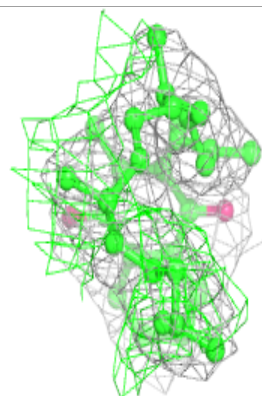
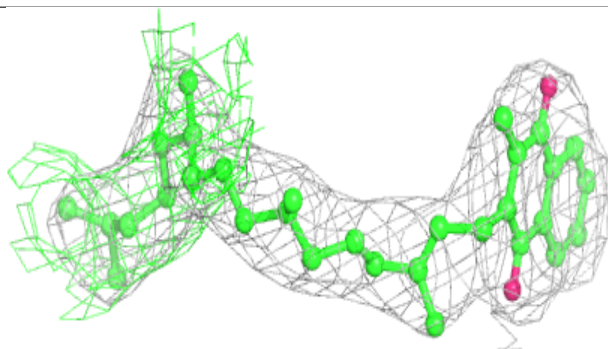
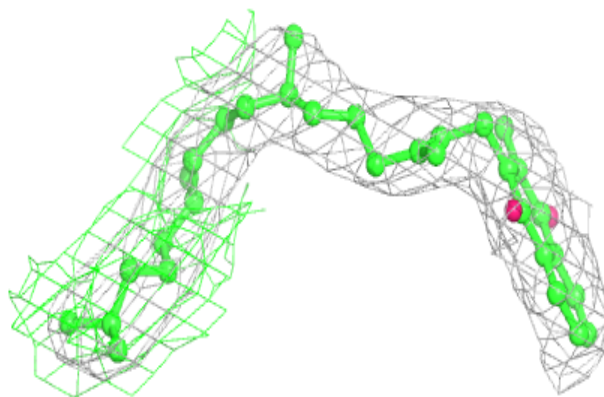
Electron density around CLA Z 822:

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

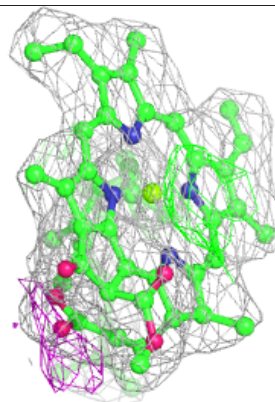
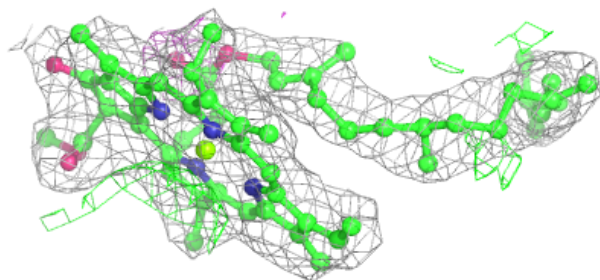
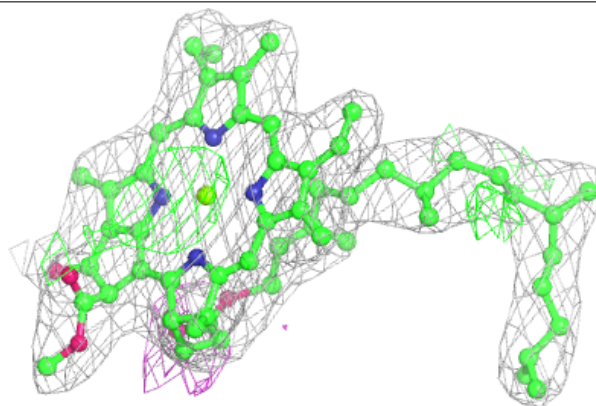


Electron density around PQN B 842:

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

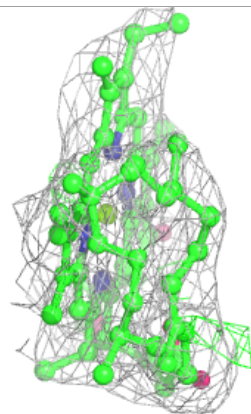
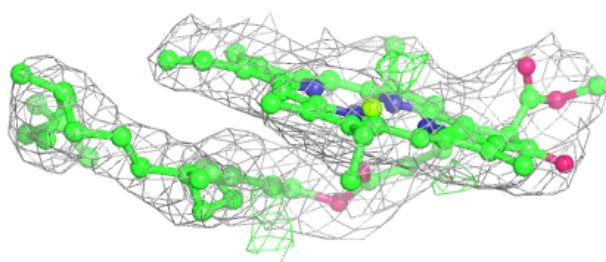
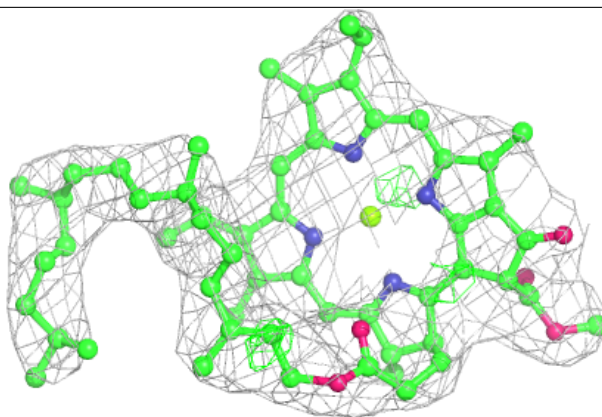
**Electron density around CLA Y 842:**

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



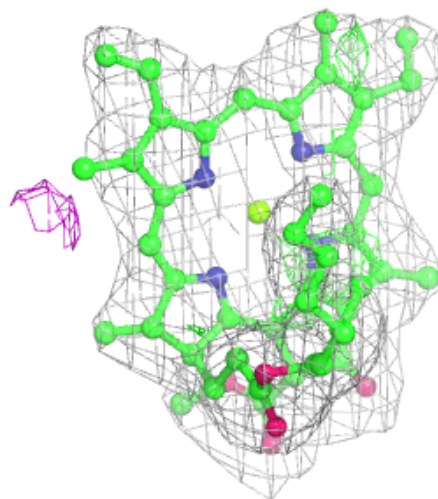
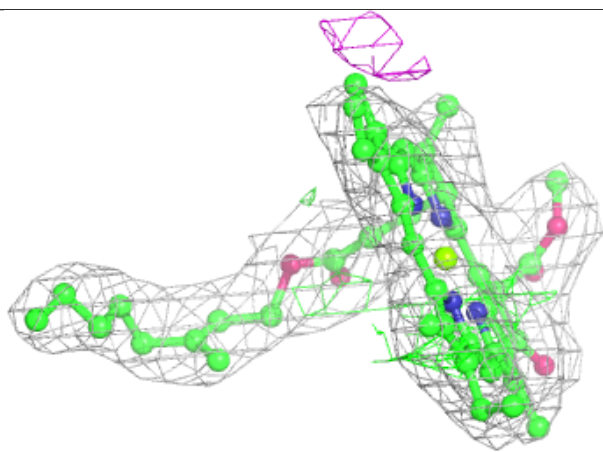
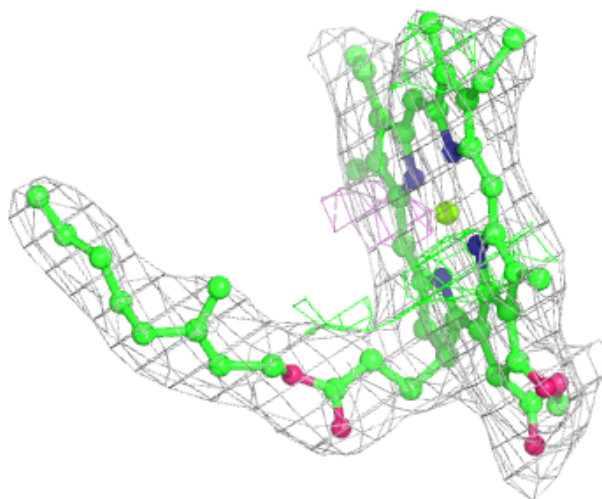
Electron density around CLA A 819:

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



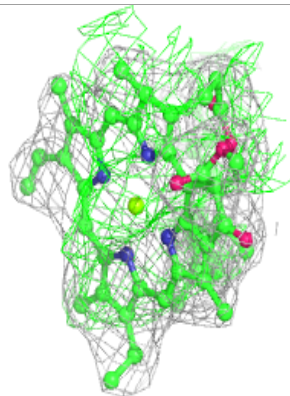
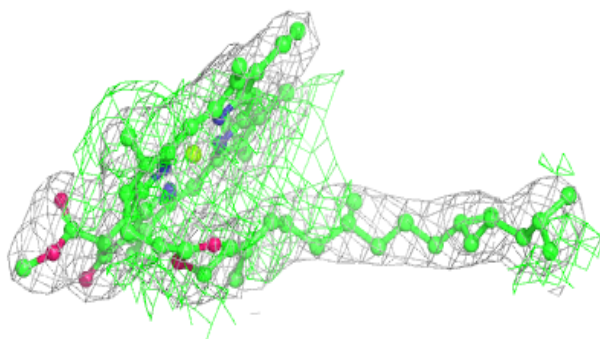
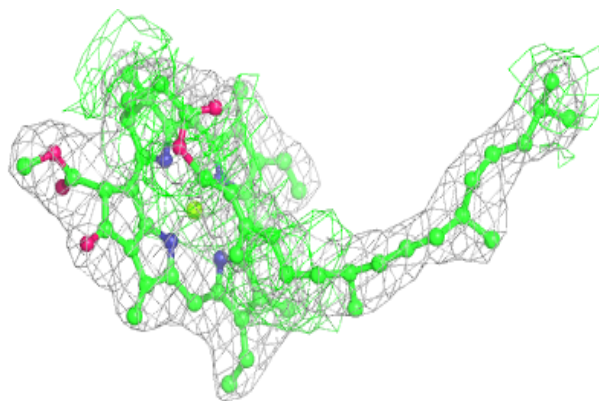
Electron density around CLA V 1201:

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

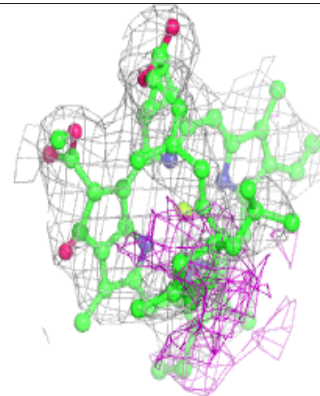
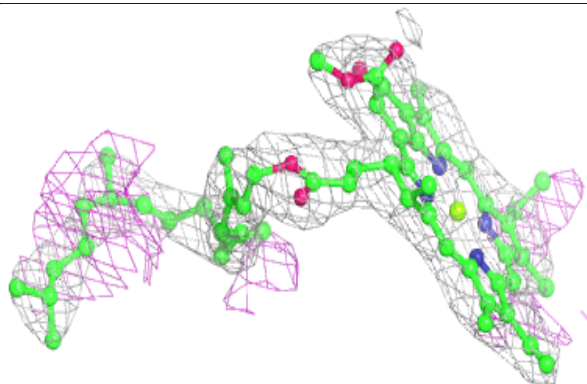
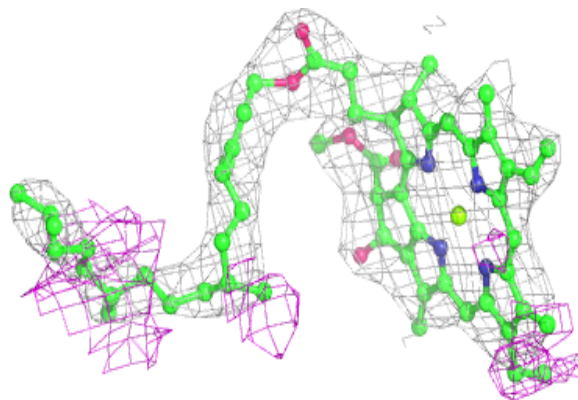


Electron density around CLA A 840:

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

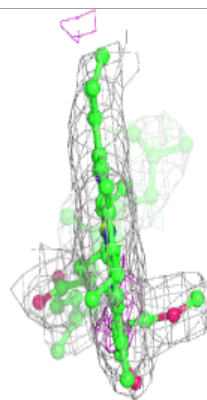
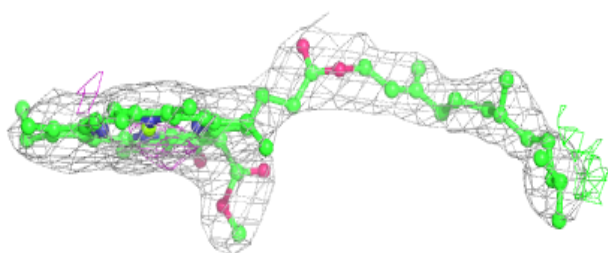
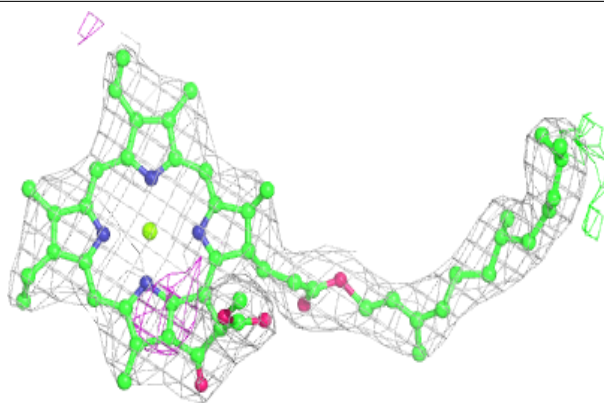
**Electron density around CLA Z 802:**

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

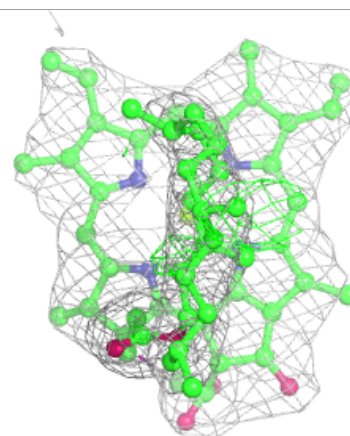
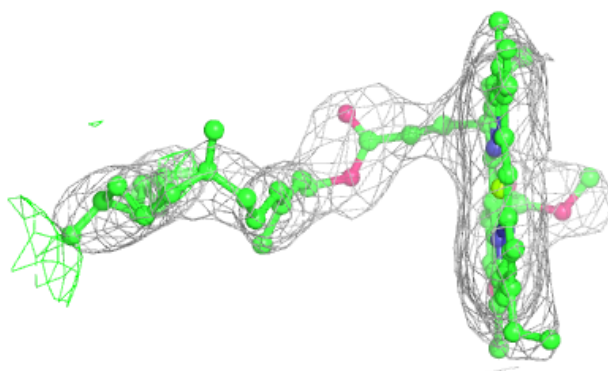
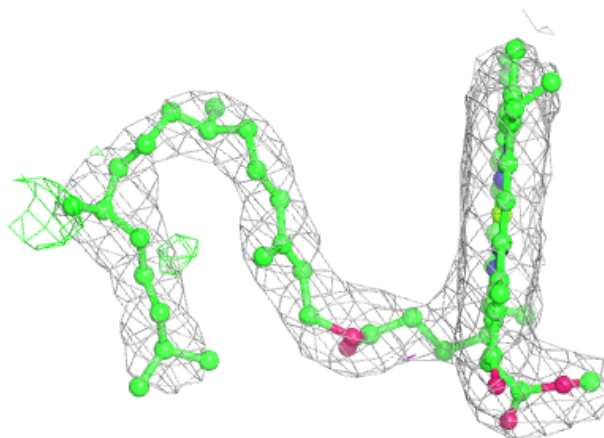


Electron density around CLA H 834:

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

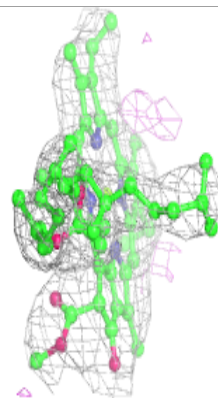
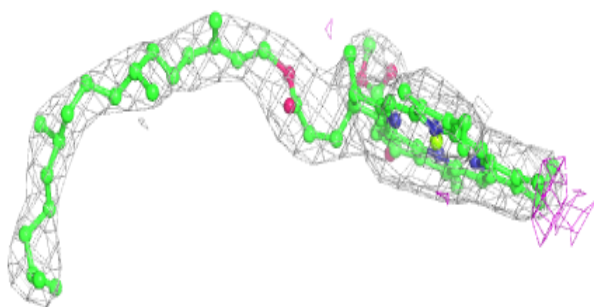
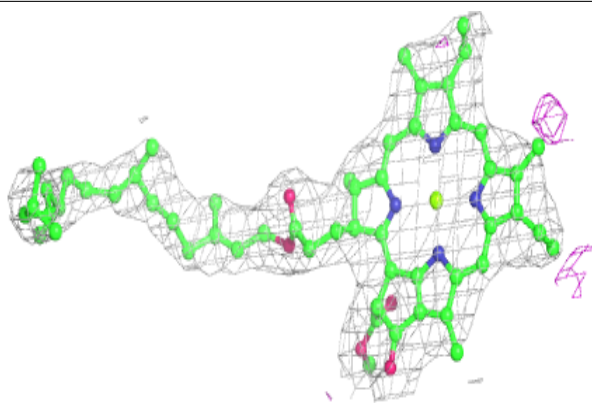
**Electron density around CLA B 814:**

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

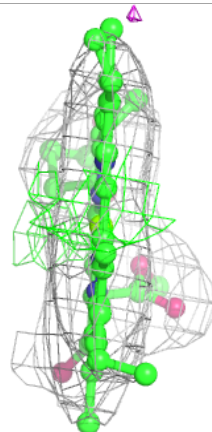
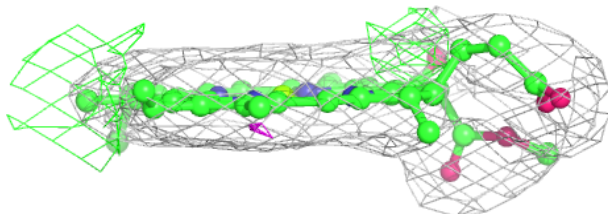
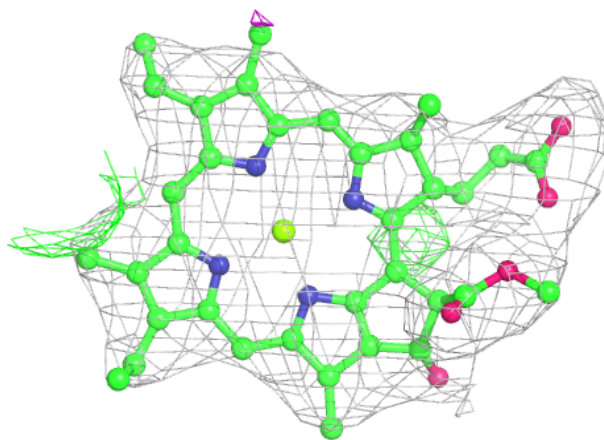


Electron density around CLA Y 805:

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

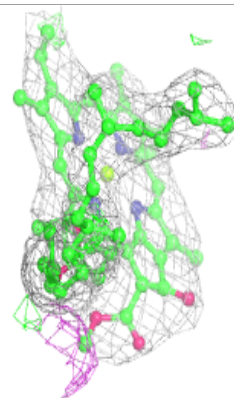
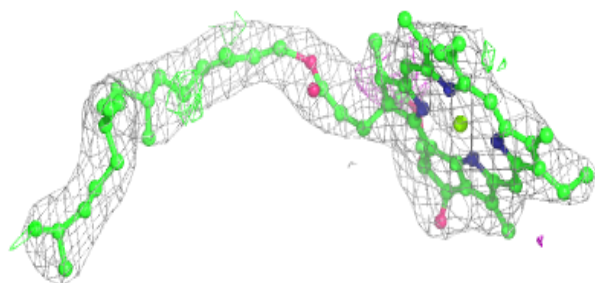
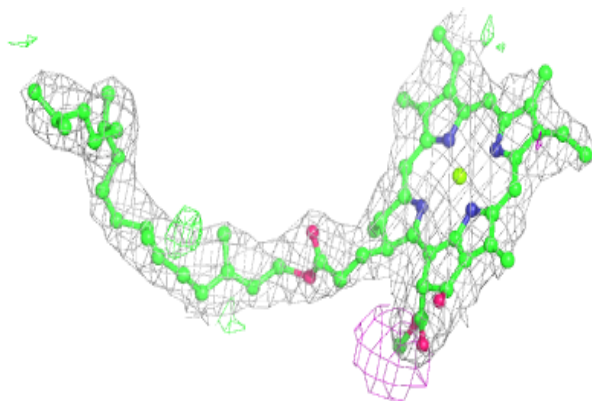
**Electron density around CLA Q 203:**

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



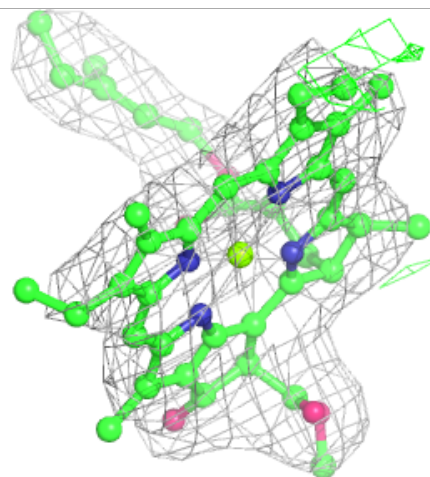
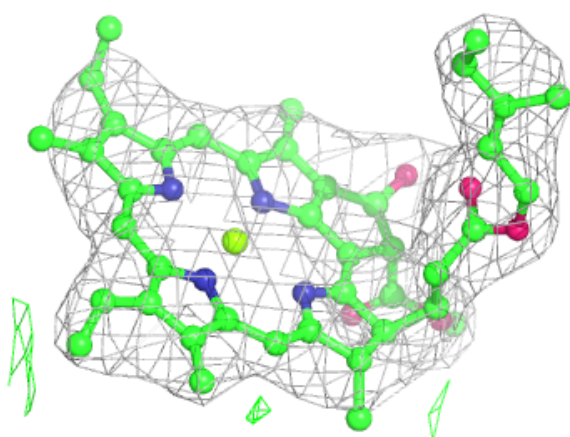
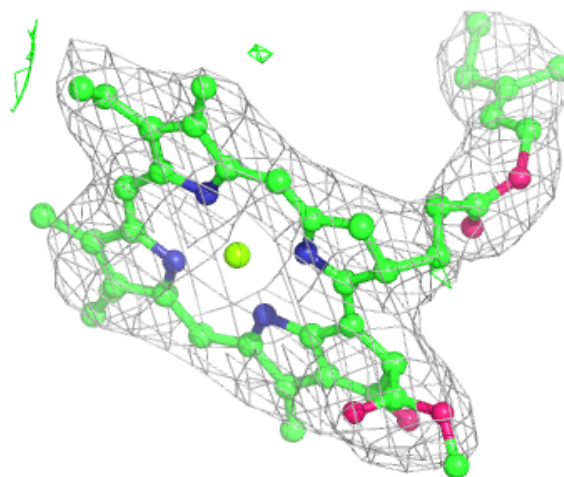
Electron density around CLA Y 854:

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



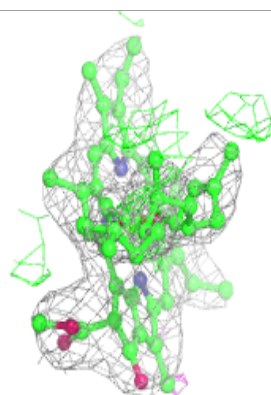
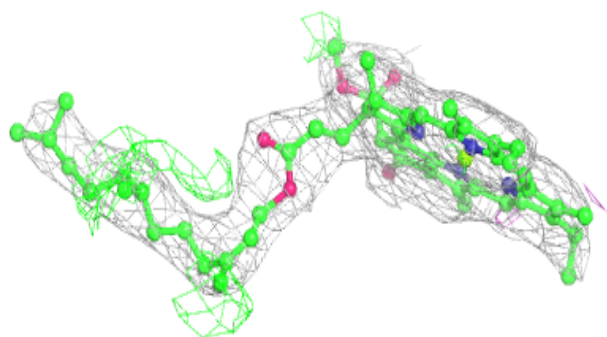
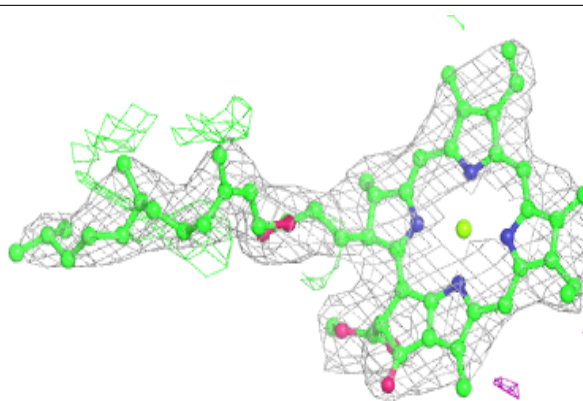
Electron density around CLA G 807:

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



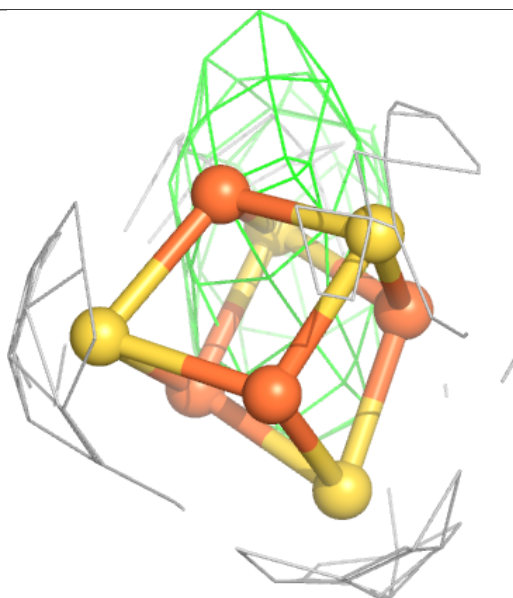
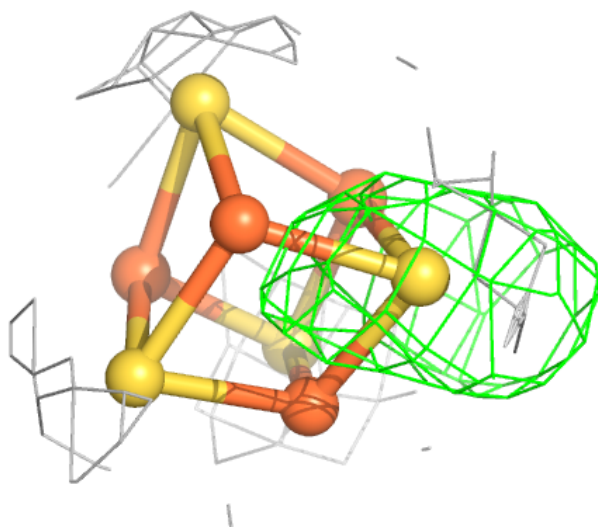
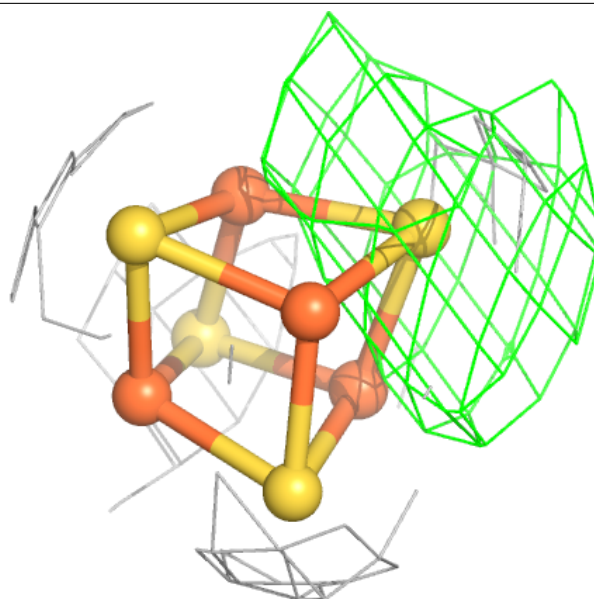
Electron density around CLA Z 821:

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



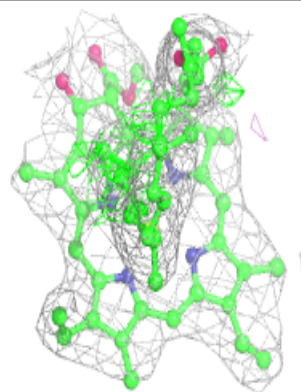
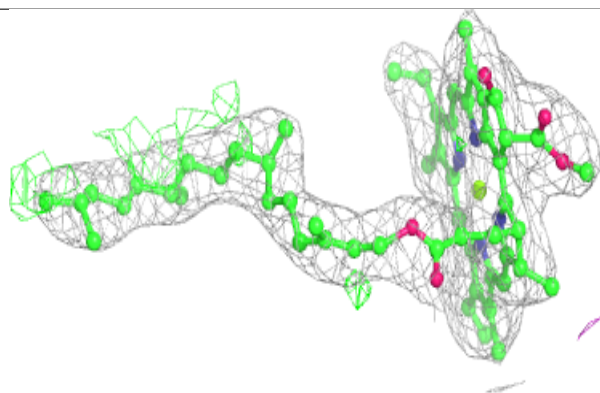
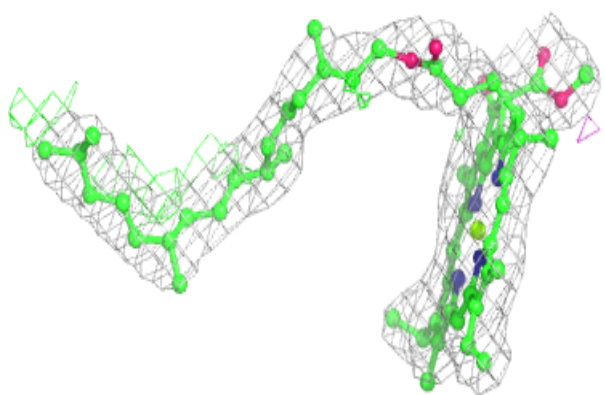
Electron density around SF4 N 101:

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

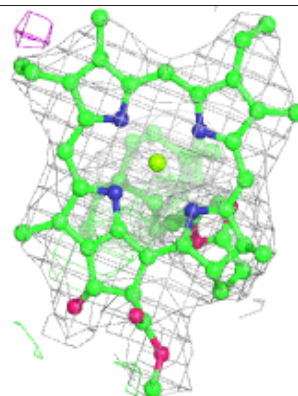
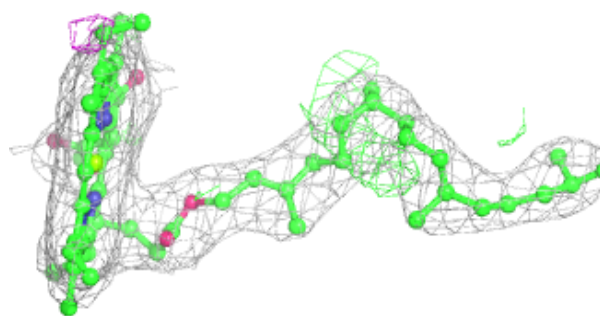
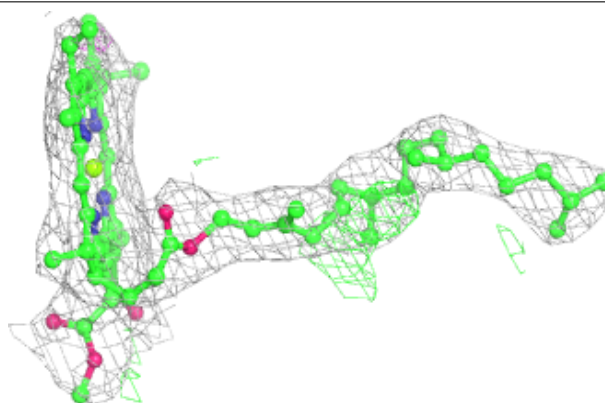


Electron density around CLA A 830:

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

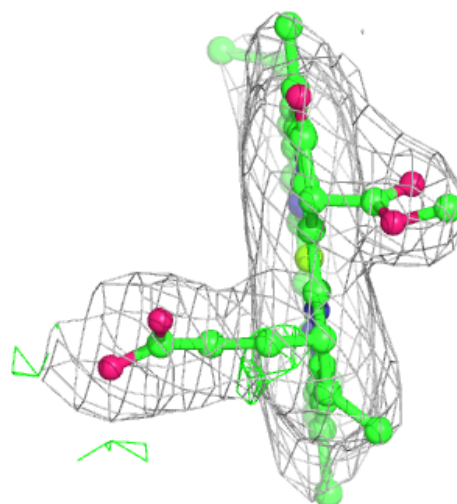
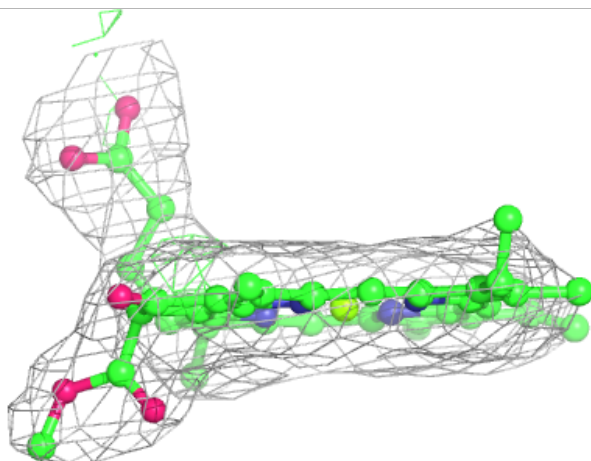
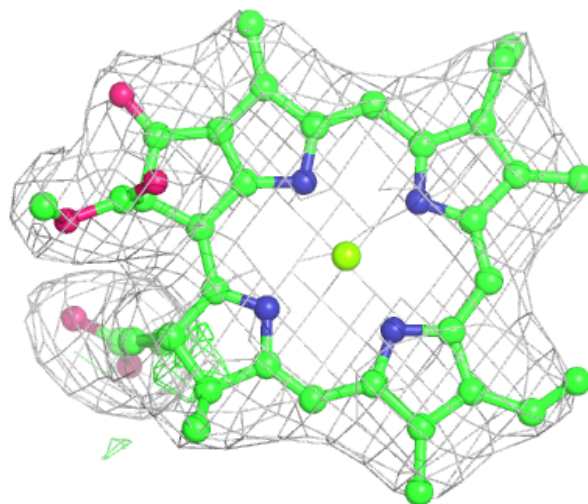
**Electron density around CLA G 828:**

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



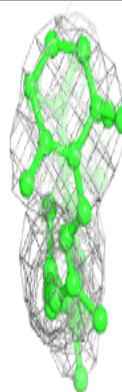
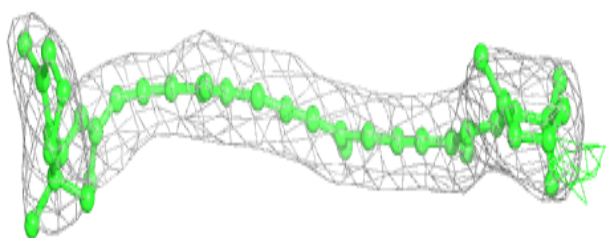
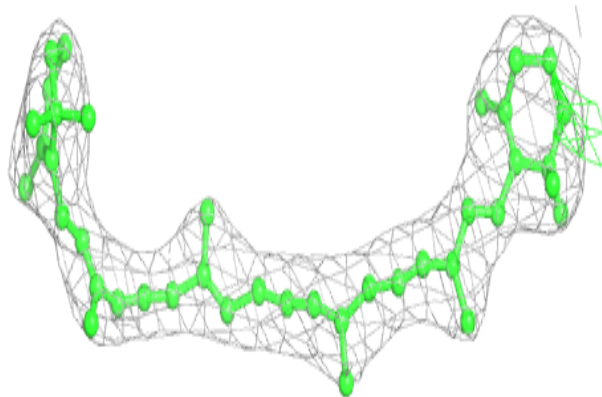
Electron density around CLA H 836:

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

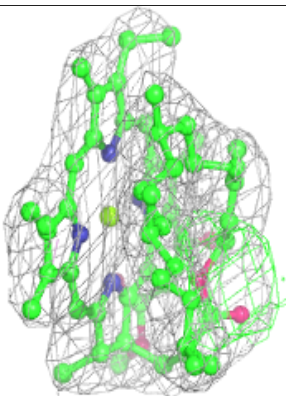
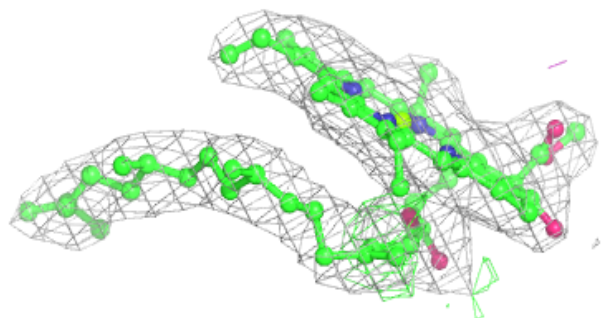
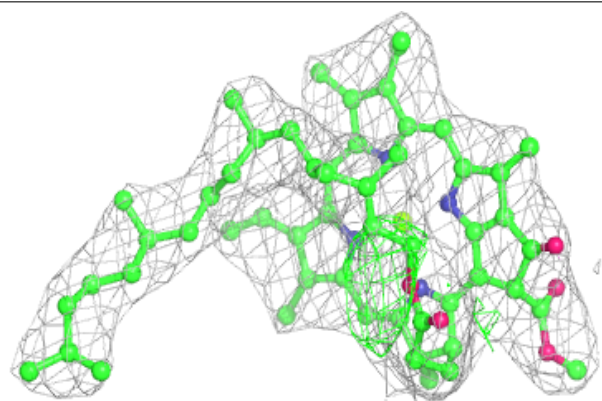


Electron density around BCR Z 842:

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

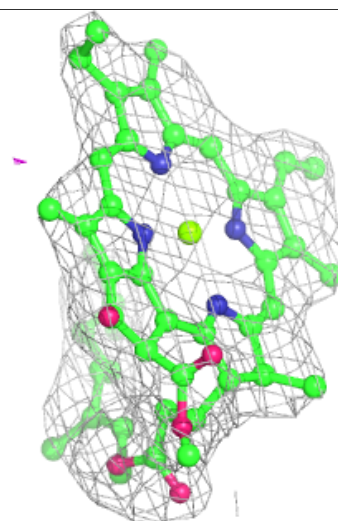
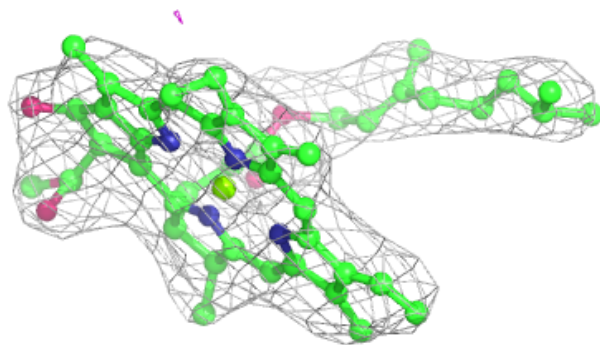
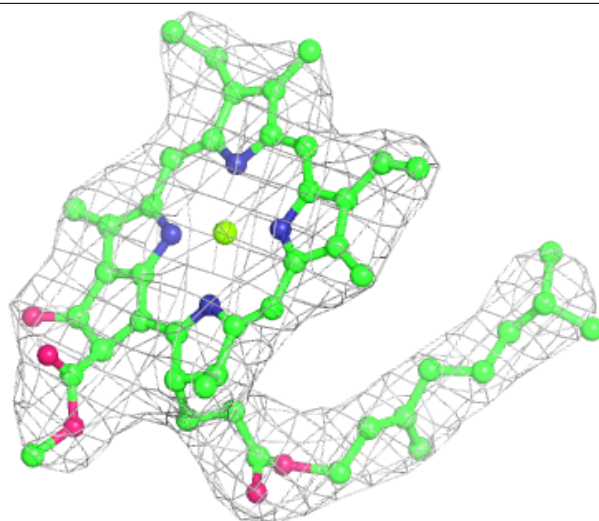
**Electron density around CLA B 808:**

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



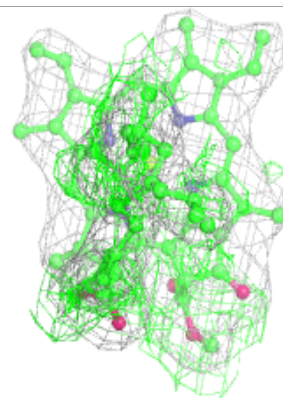
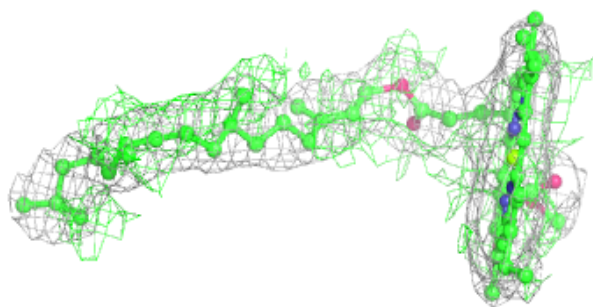
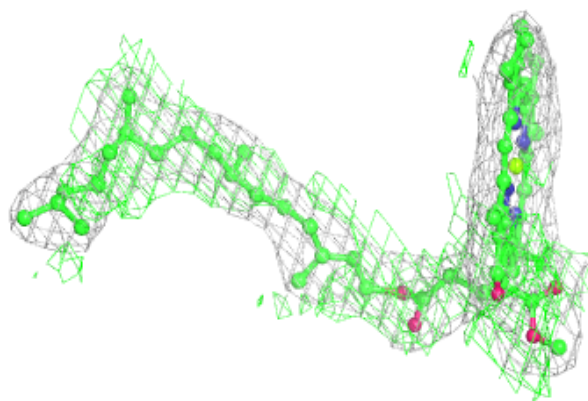
Electron density around CLA B 816:

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

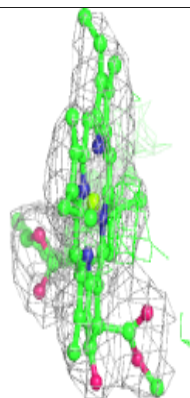
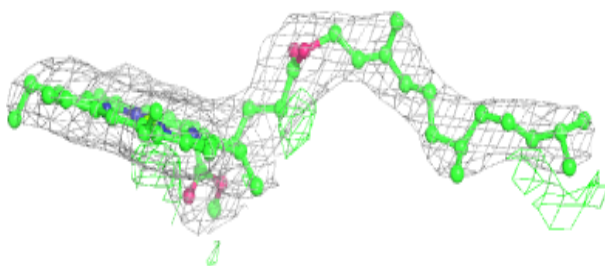
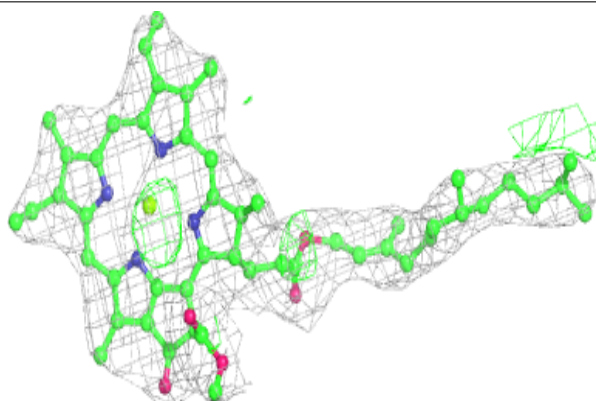


Electron density around CLA Z 839:

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

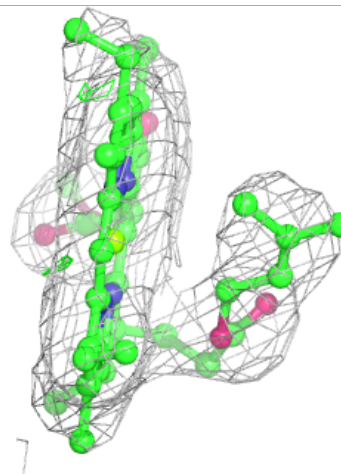
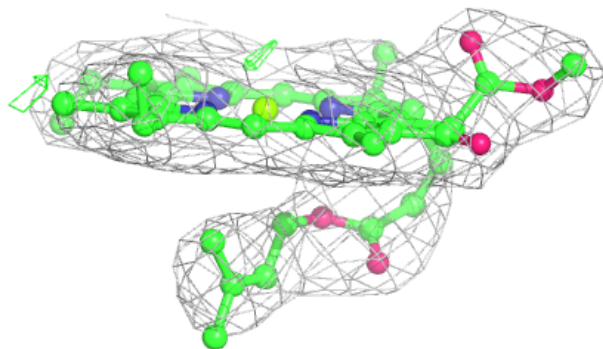
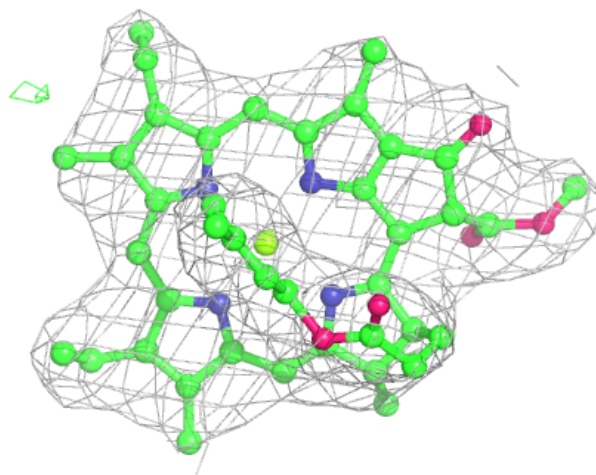
**Electron density around CLA G 826:**

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



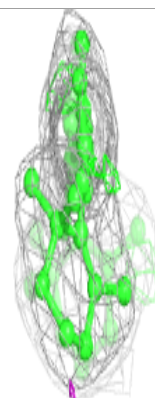
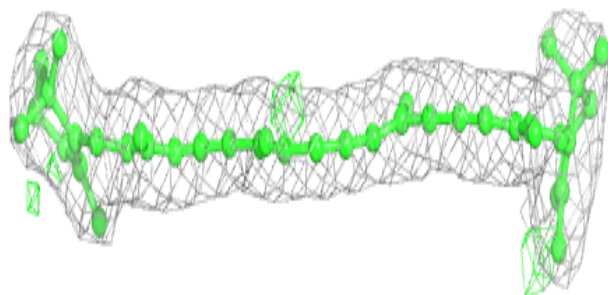
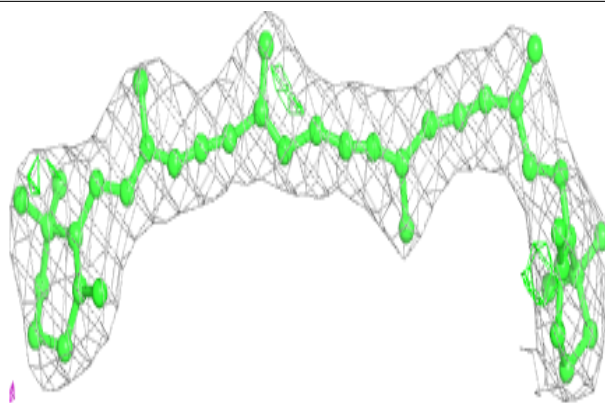
Electron density around CLA A 823:

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

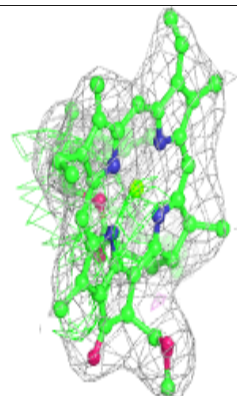
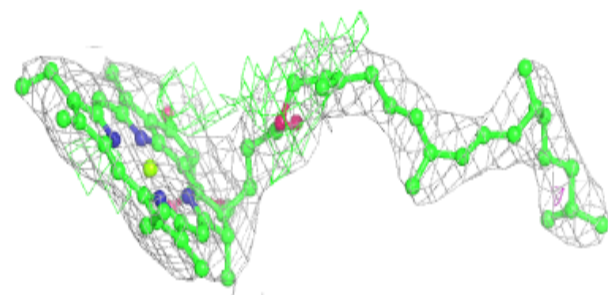
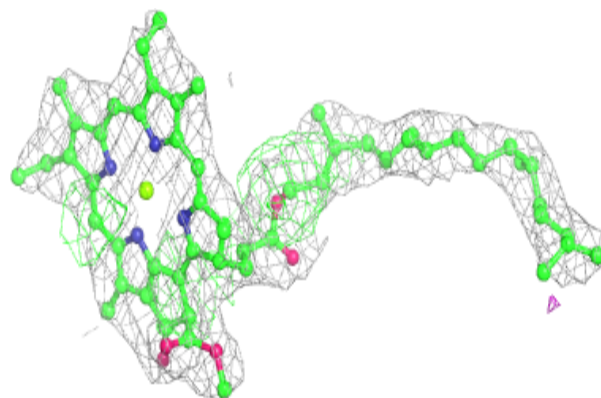


Electron density around BCR h 203:

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

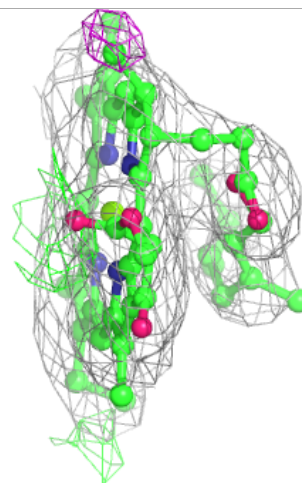
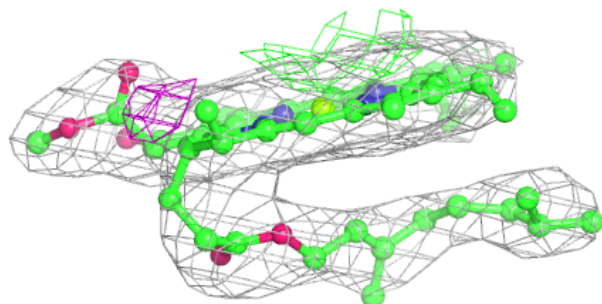
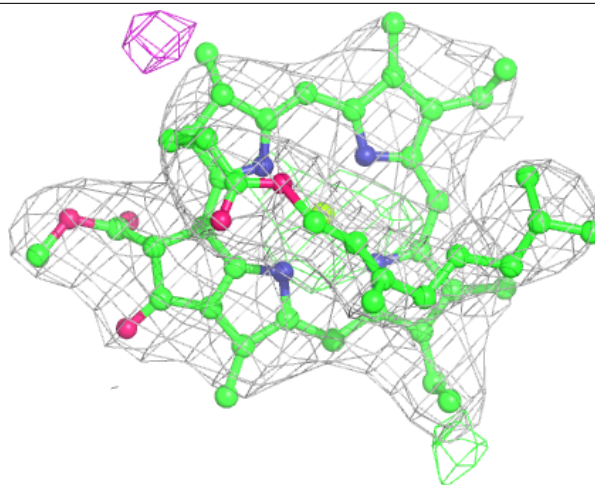
**Electron density around CLA G 821:**

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



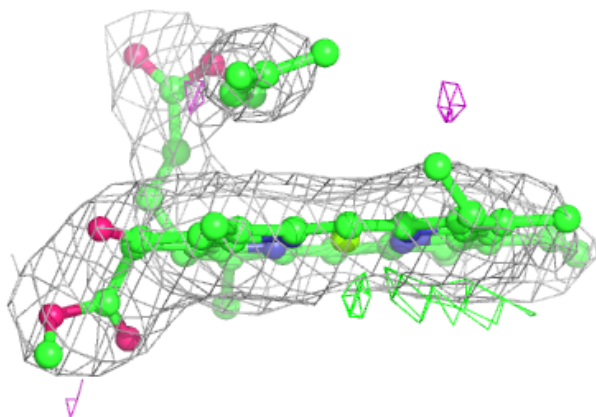
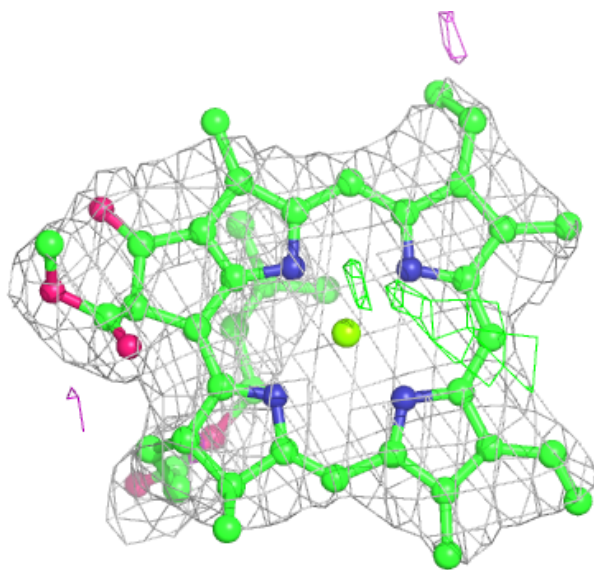
Electron density around CLA B 822:

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



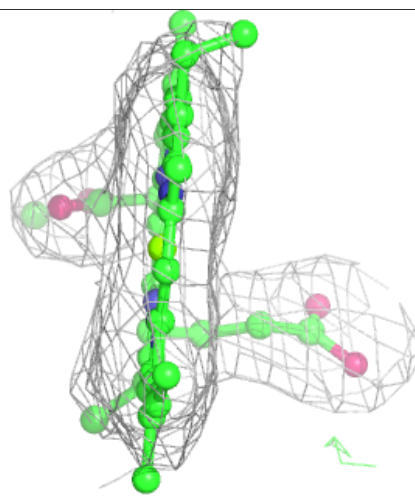
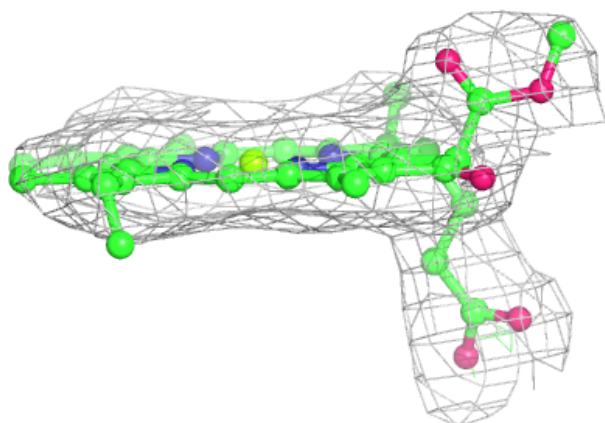
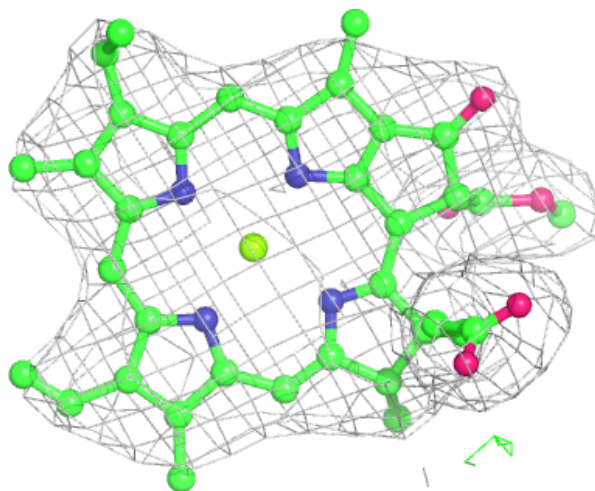
Electron density around CLA Y 843:

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



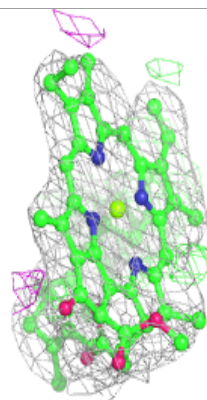
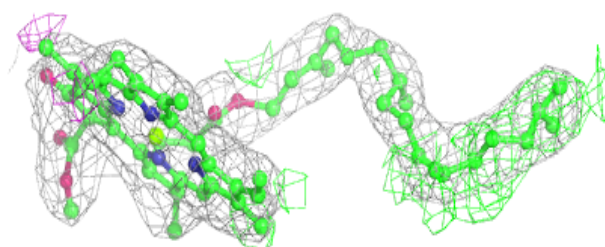
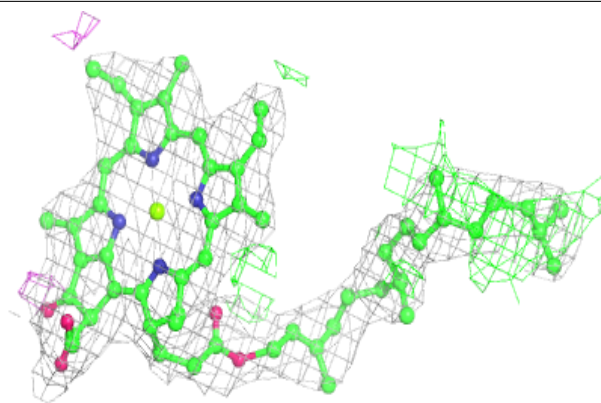
Electron density around CLA B 839:

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



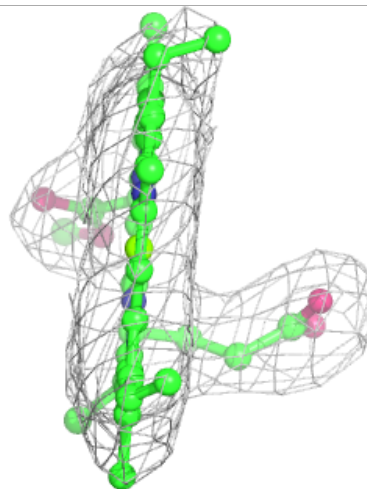
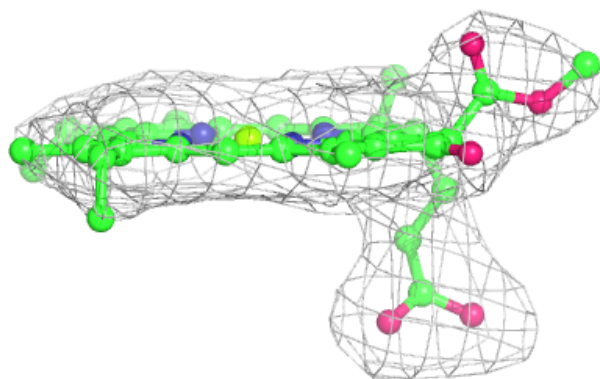
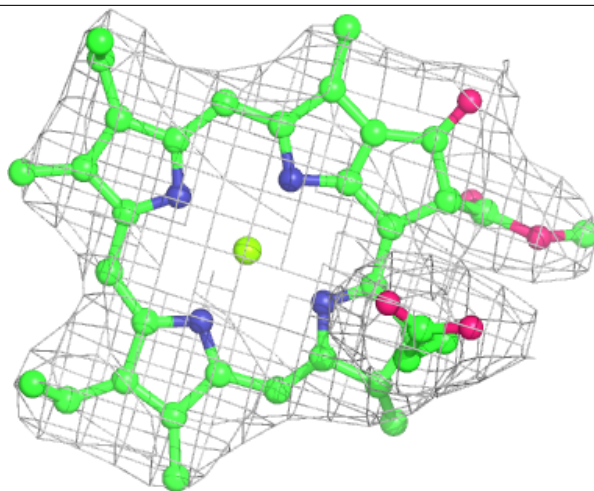
Electron density around CLA A 808:

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



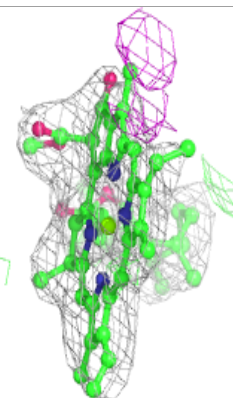
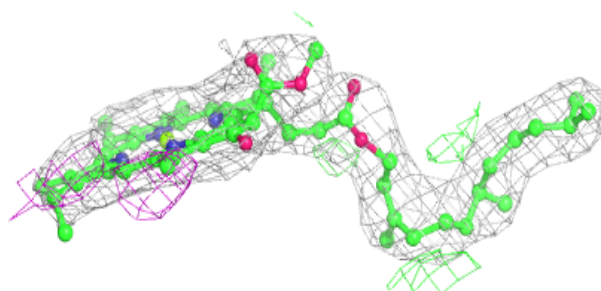
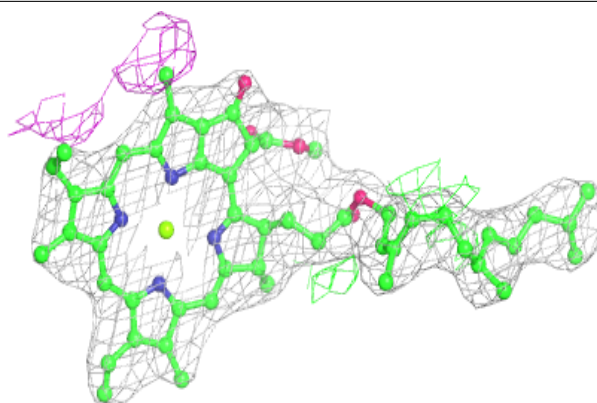
Electron density around CLA H 811:

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

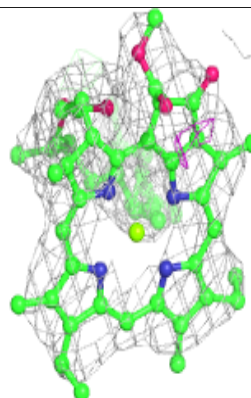
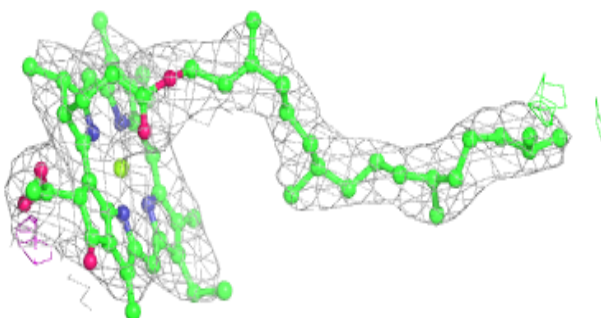
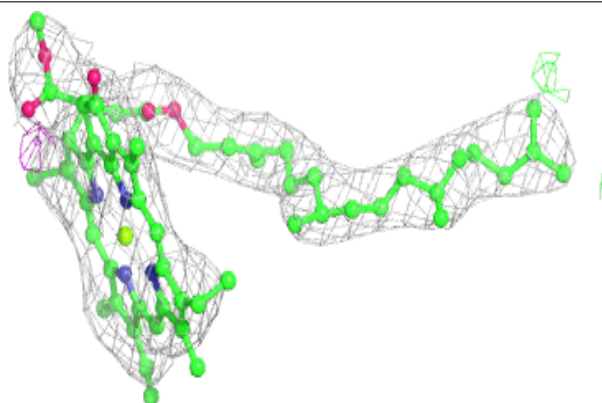


Electron density around CLA B 823:

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

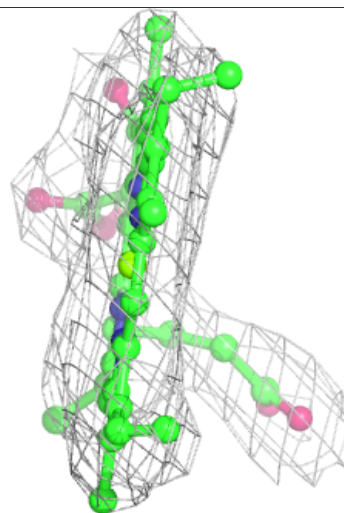
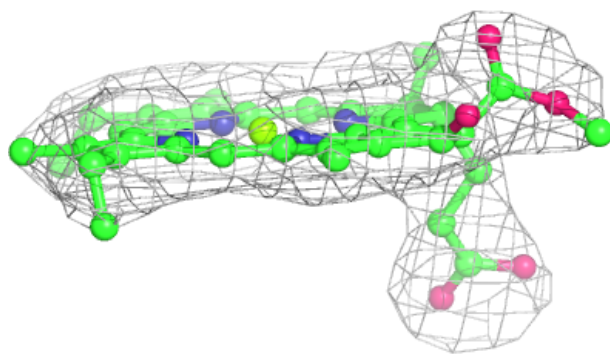
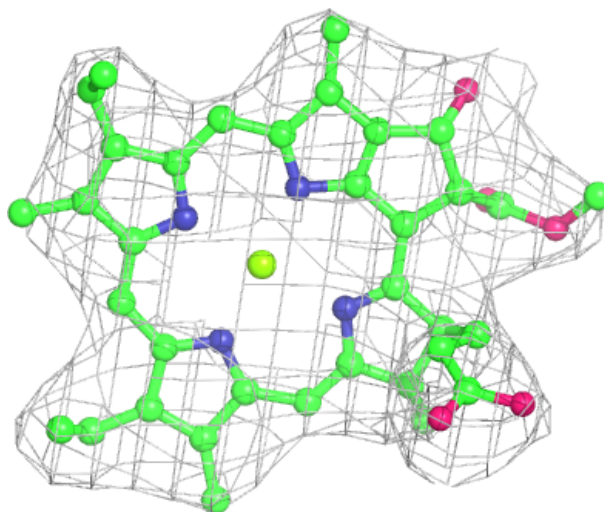
**Electron density around CLA A 811:**

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



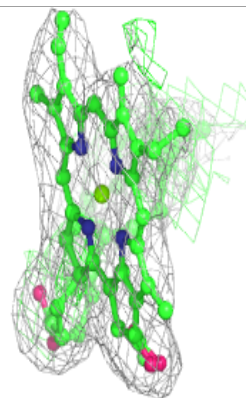
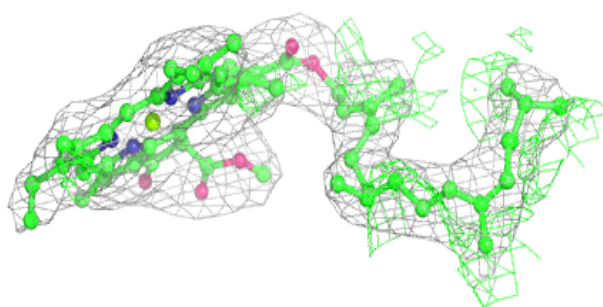
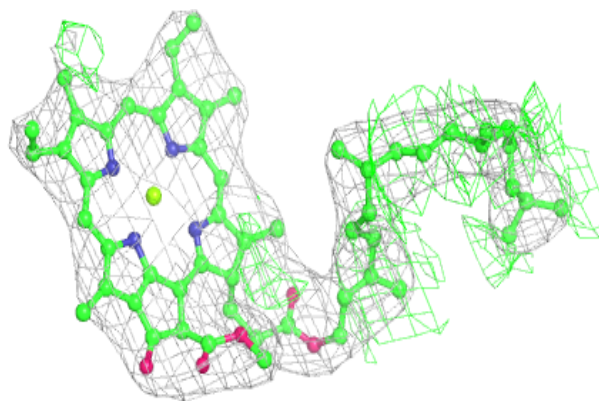
Electron density around CLA Z 810:

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



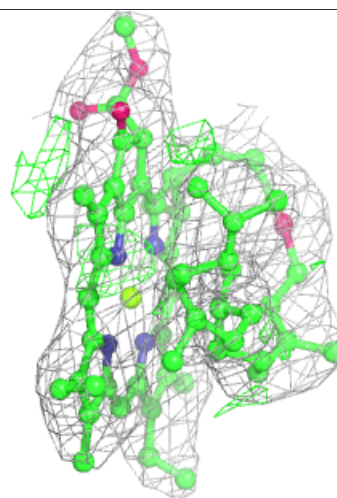
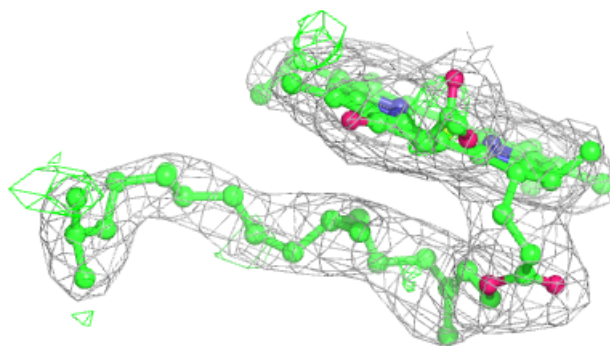
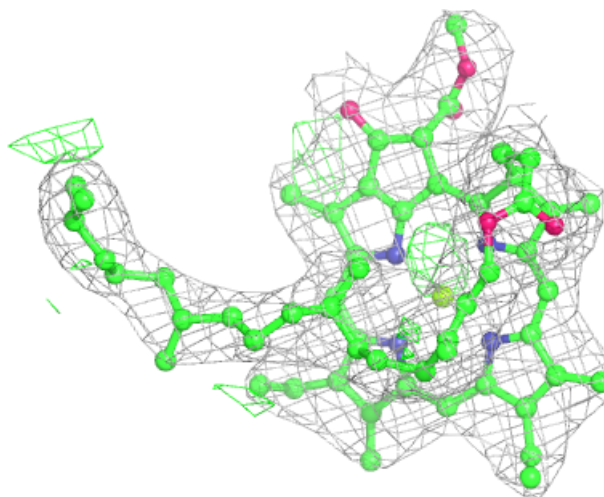
Electron density around CLA Y 803:

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



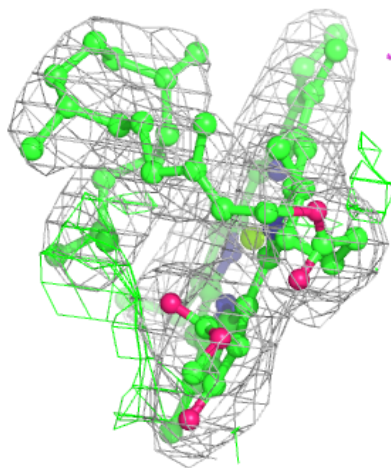
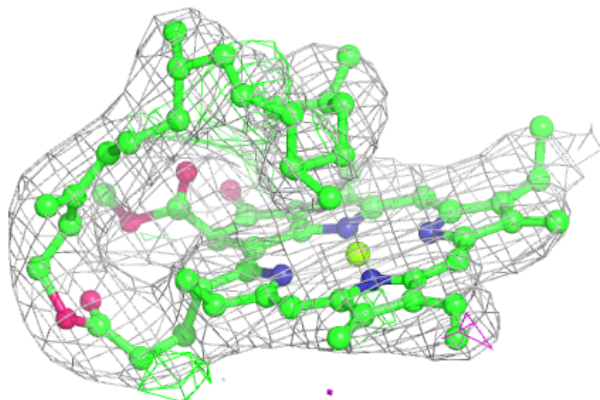
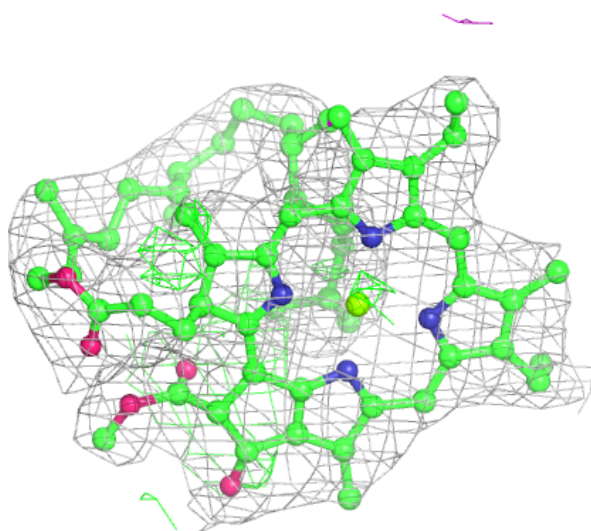
Electron density around CLA H 826:

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



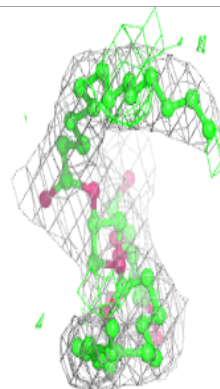
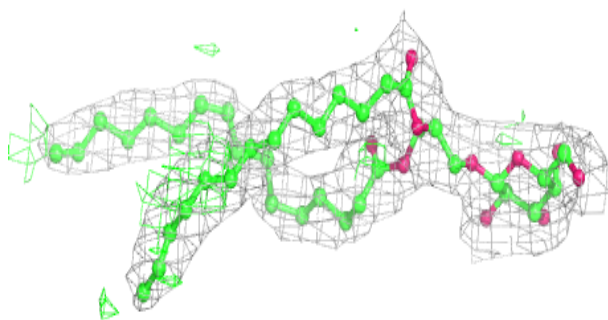
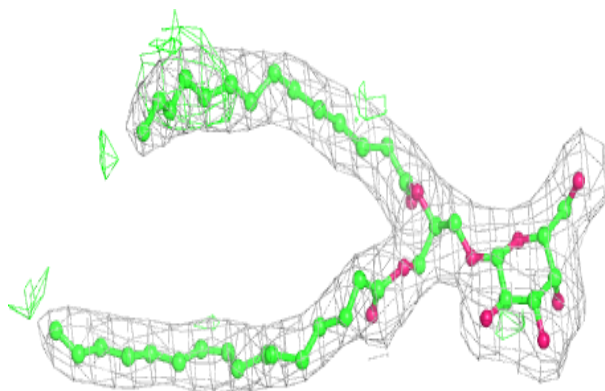
Electron density around CLA B 807:

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

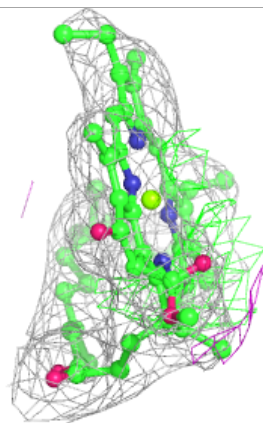
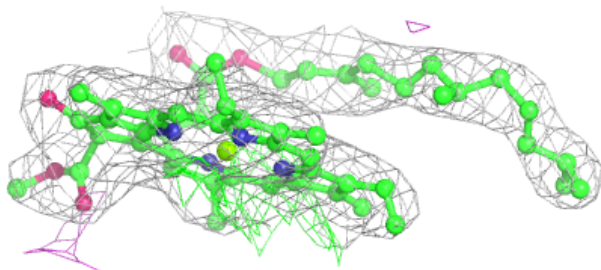
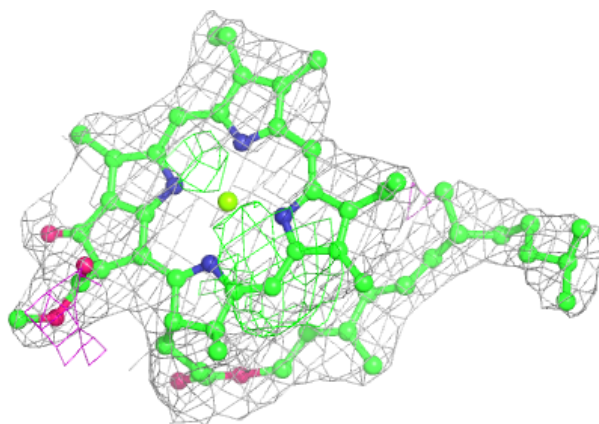


Electron density around LMG H 846:

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

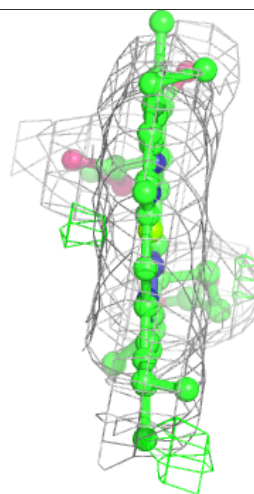
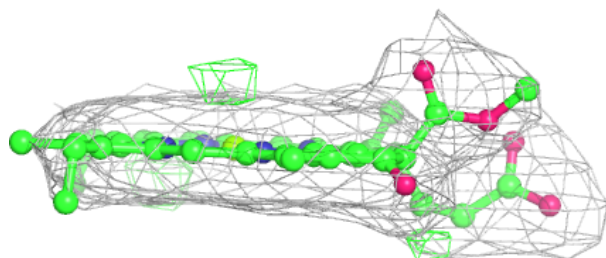
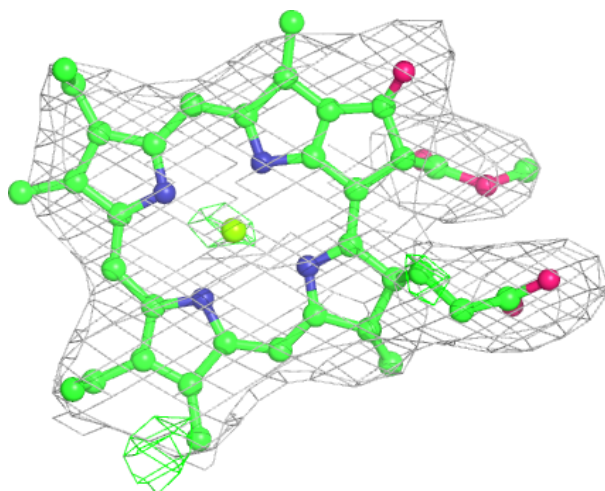
**Electron density around CLA Z 816:**

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



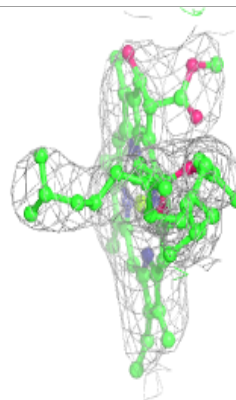
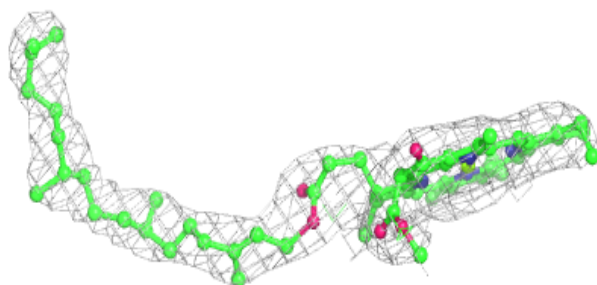
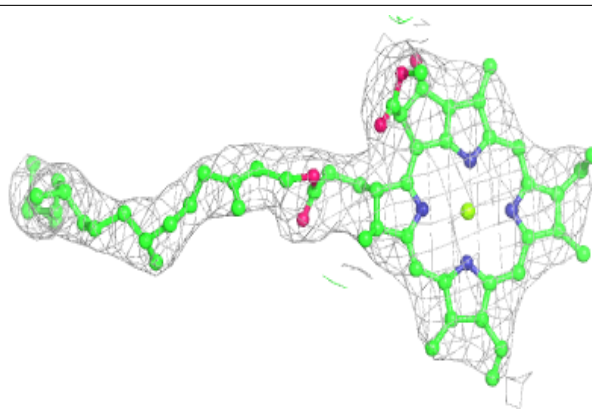
Electron density around CLA B 836:

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

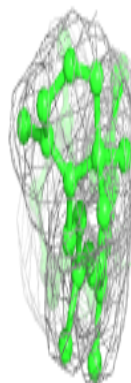
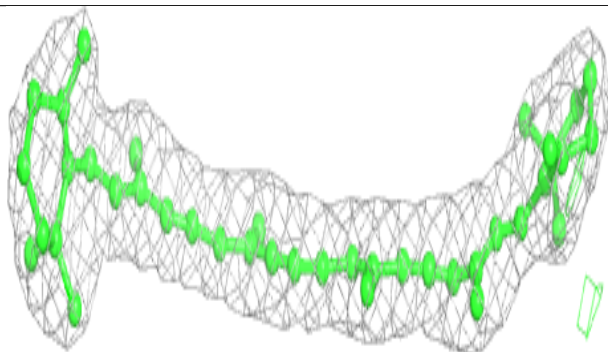
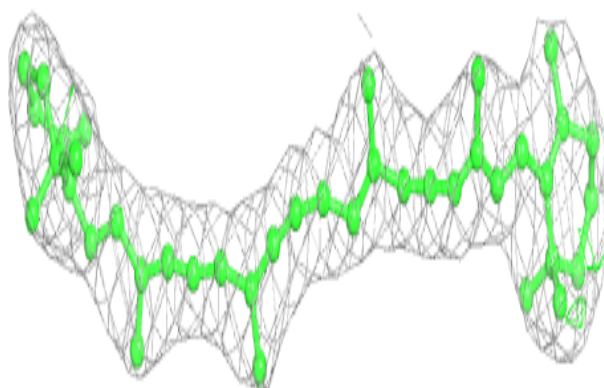


Electron density around CLA G 805:

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

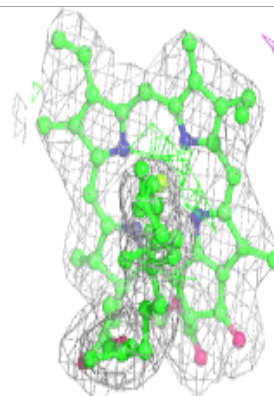
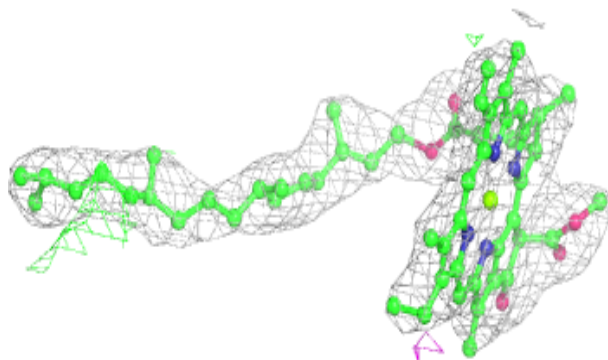
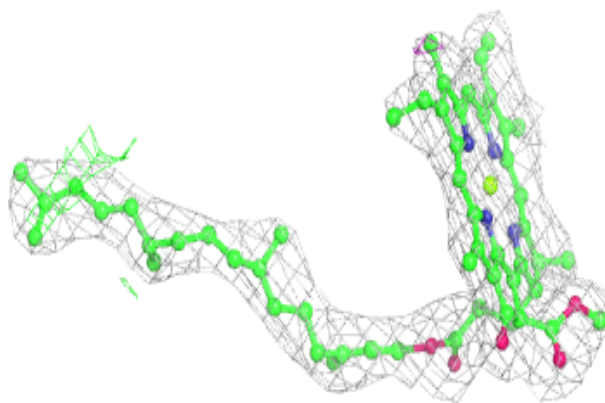
**Electron density around BCR i 101:**

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



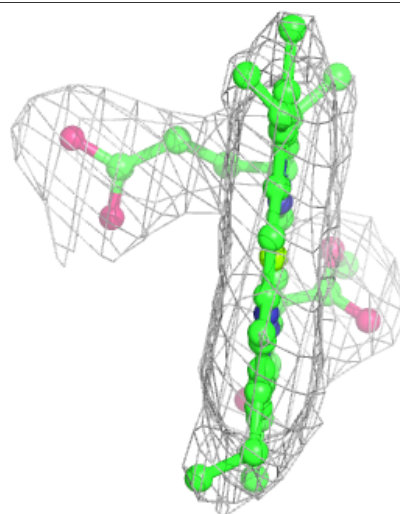
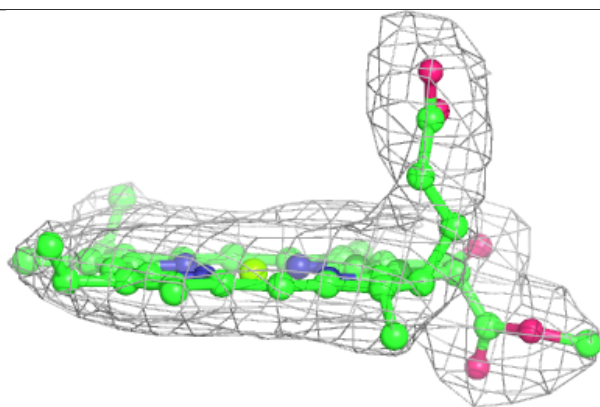
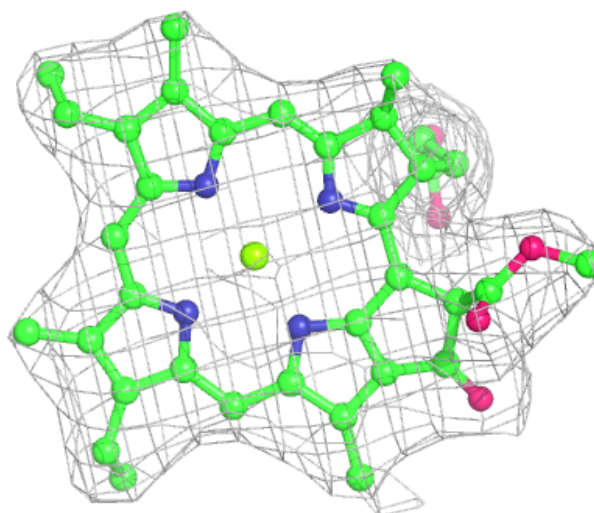
Electron density around CLA H 828:

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



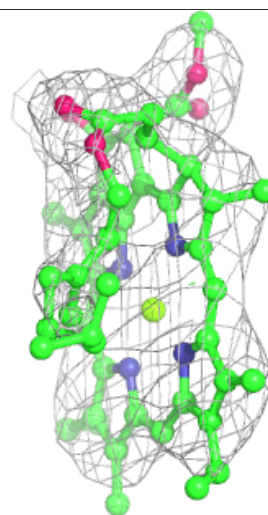
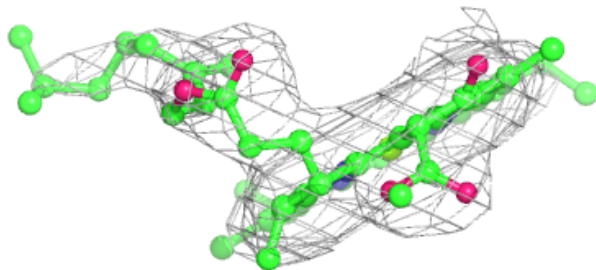
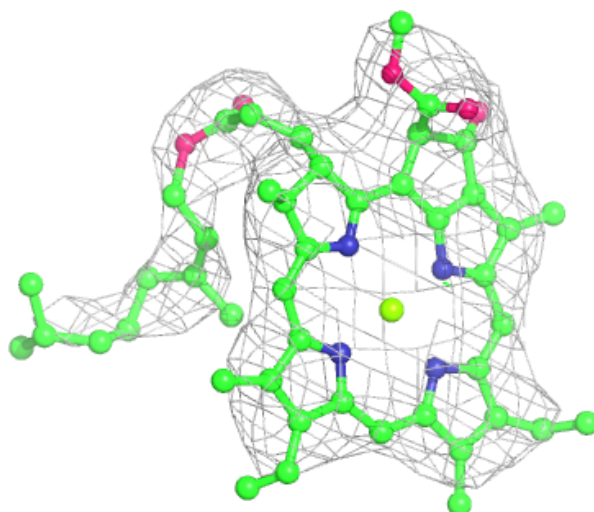
Electron density around CLA B 831:

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



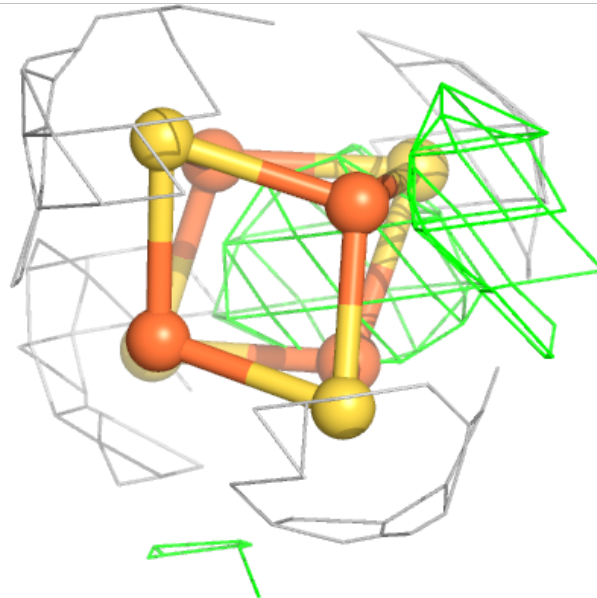
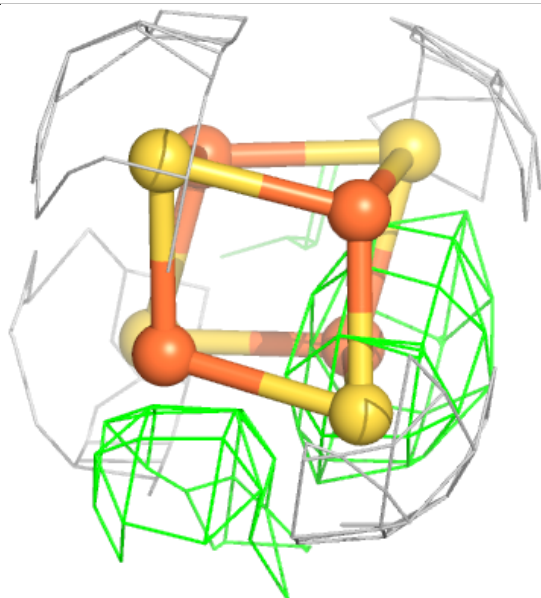
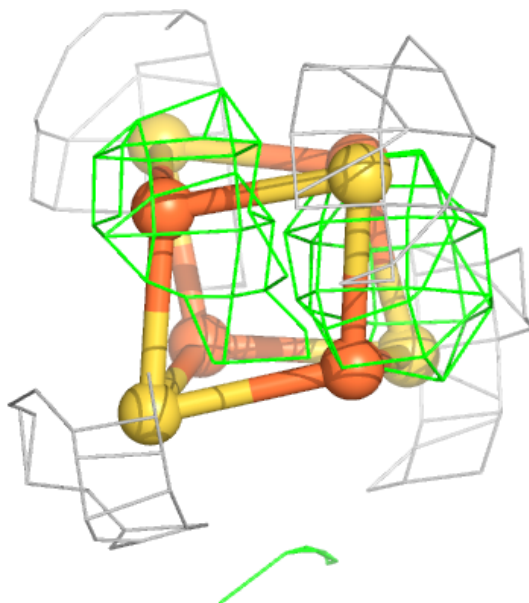
Electron density around CLA f 102:

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



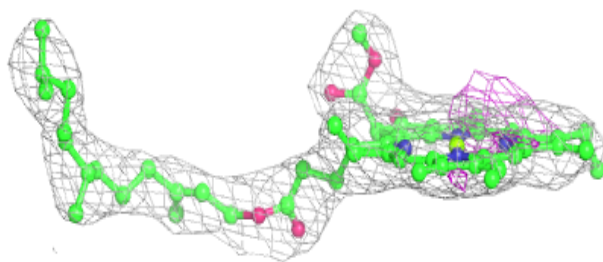
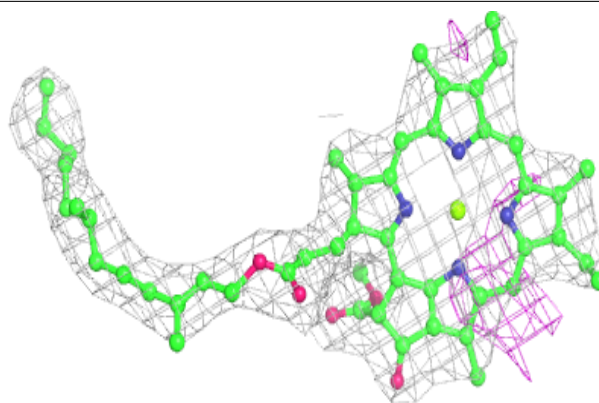
Electron density around SF4 A 844:

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

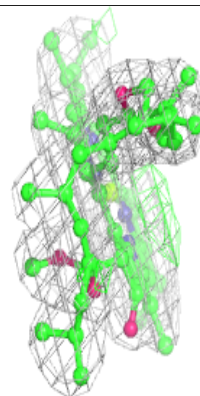
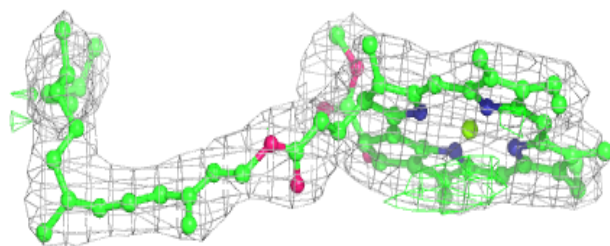
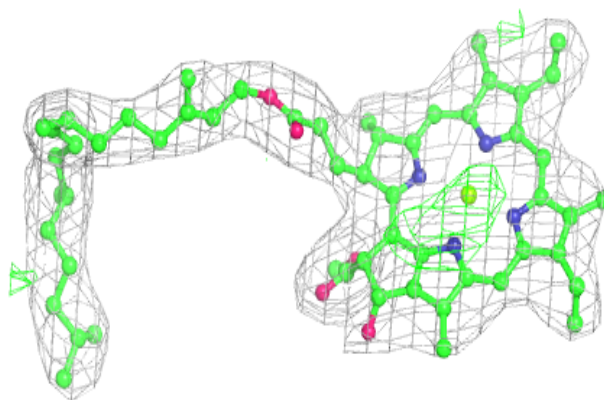


Electron density around CLA Z 835:

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

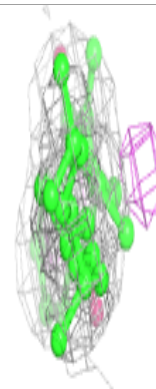
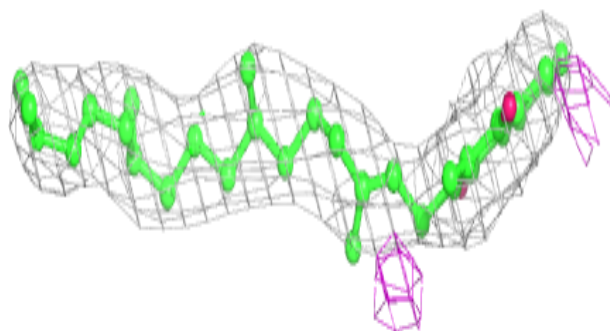
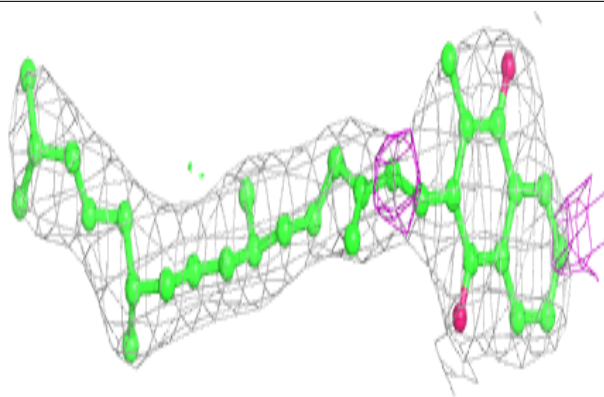
**Electron density around CLA B 826:**

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



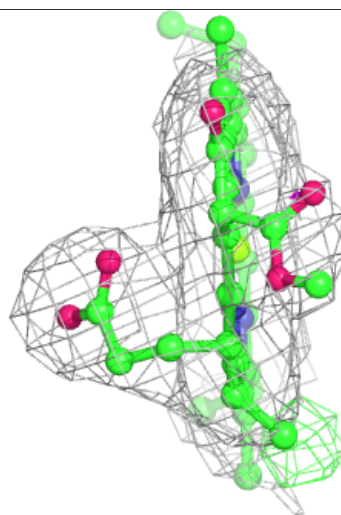
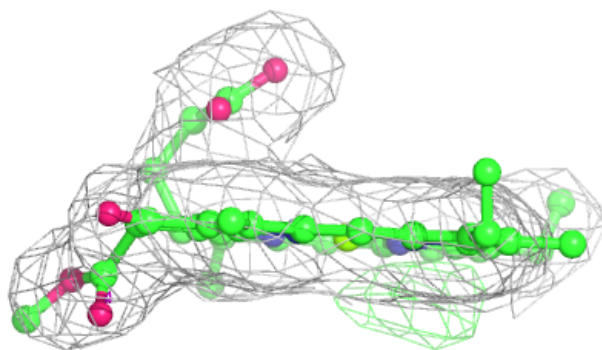
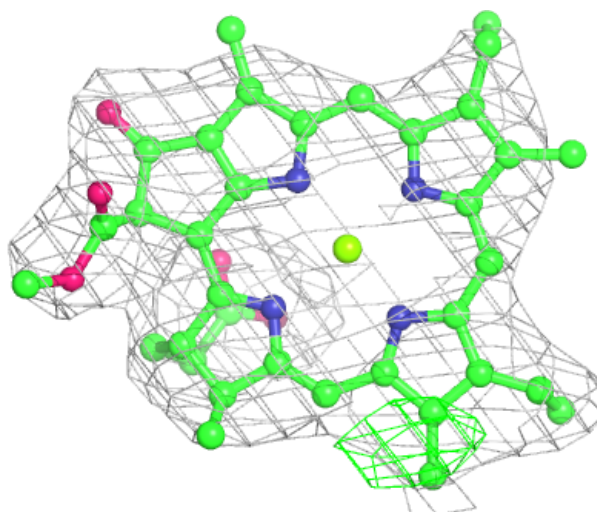
Electron density around PQN A 843:

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



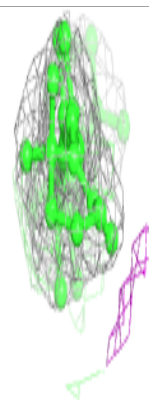
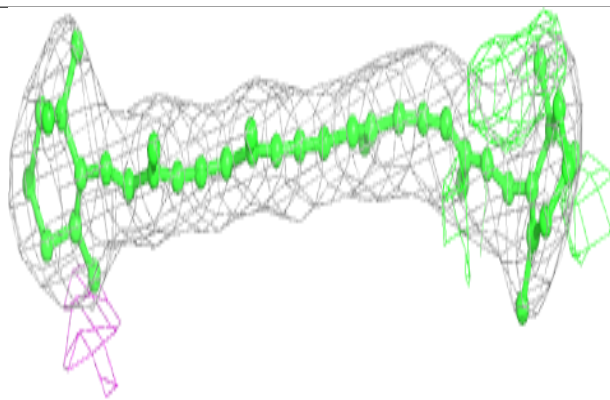
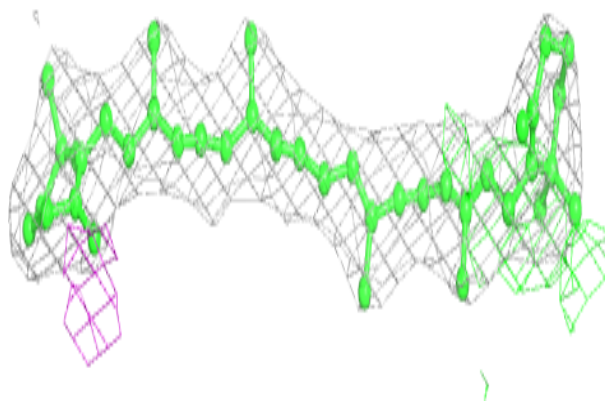
Electron density around CLA A 835:

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



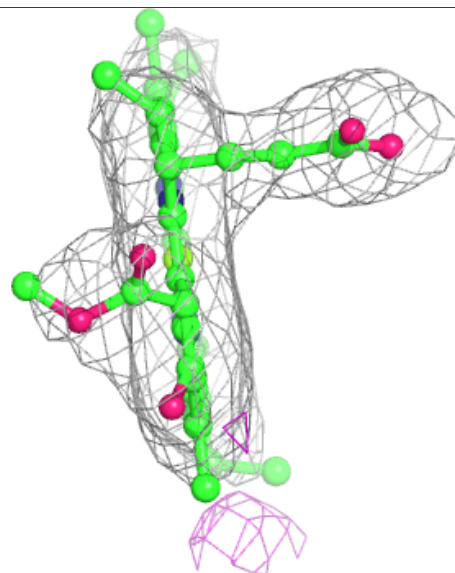
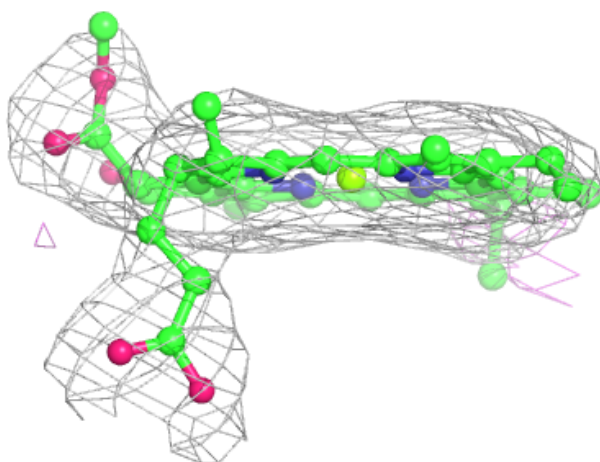
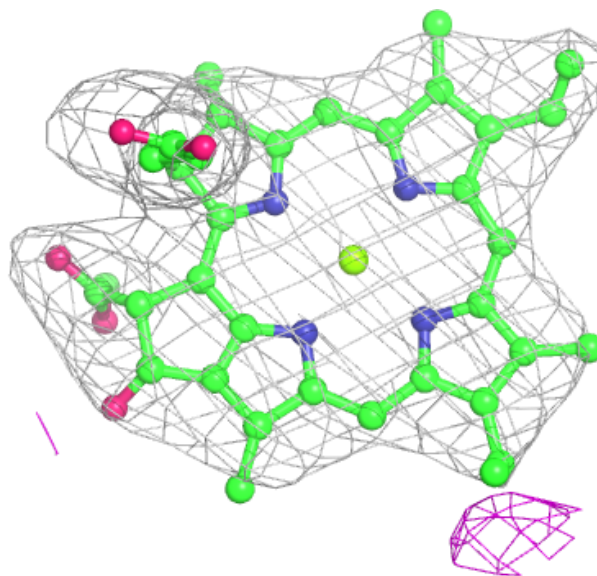
Electron density around BCR L 209:

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



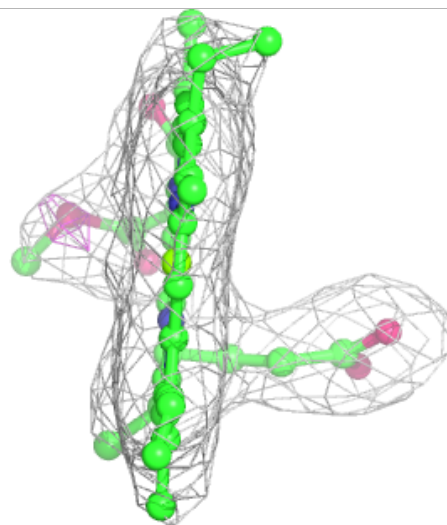
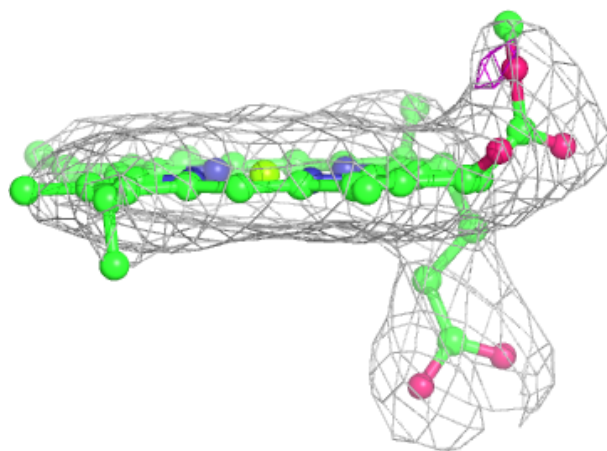
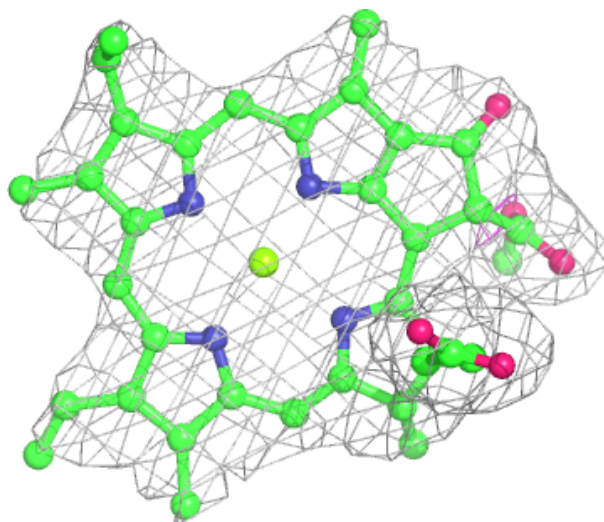
Electron density around CLA B 815:

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



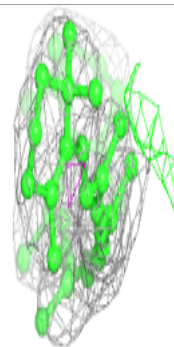
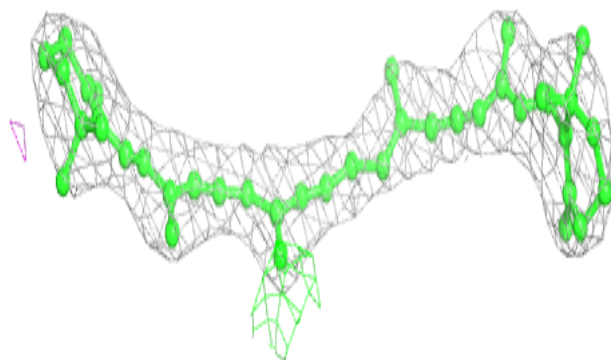
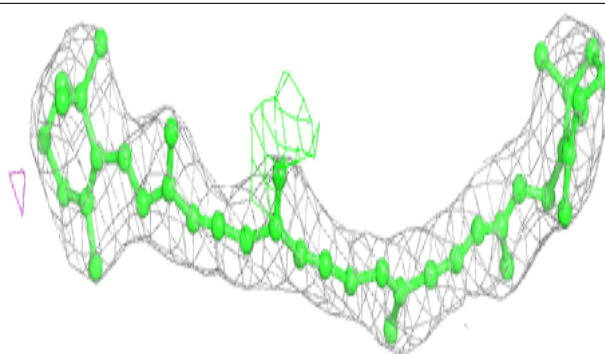
Electron density around CLA Z 813:

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



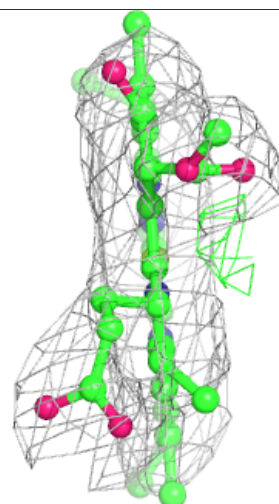
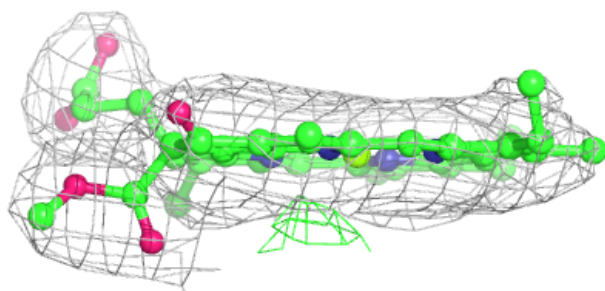
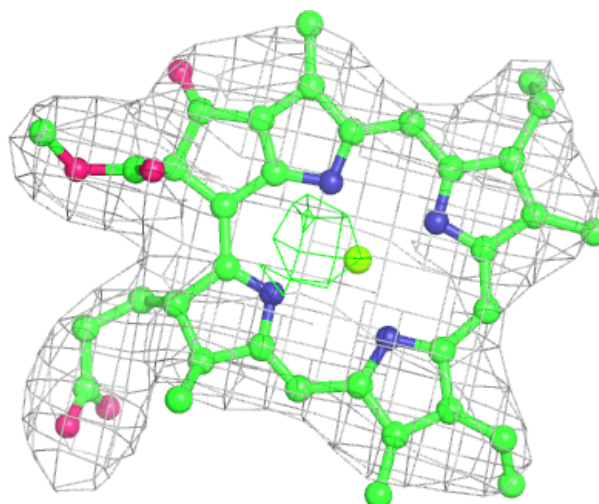
Electron density around BCR F 201:

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



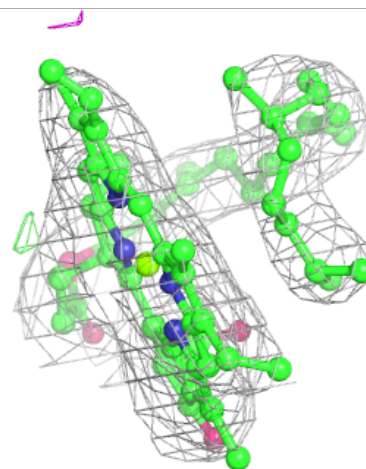
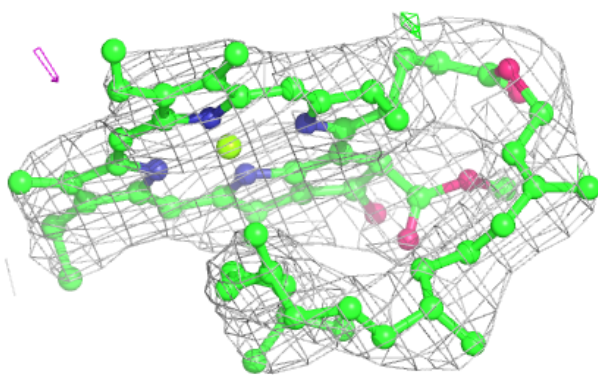
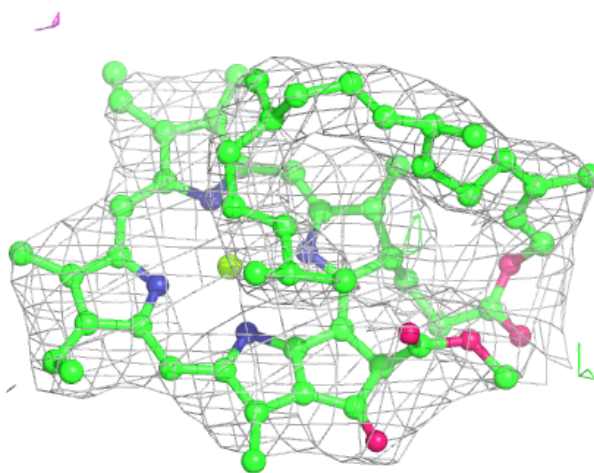
Electron density around CLA X 1701:

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



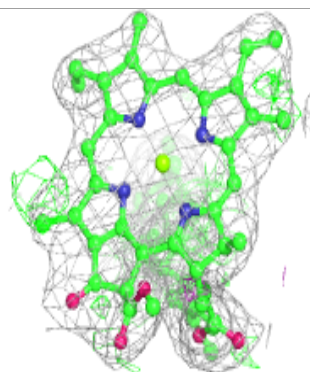
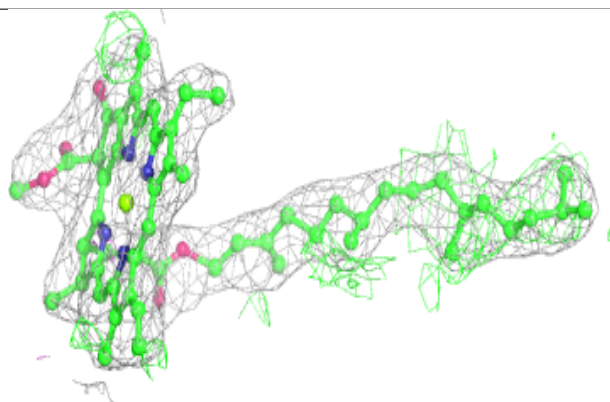
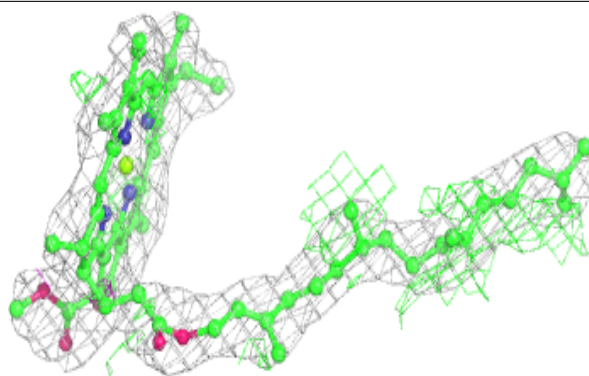
Electron density around CLA A 806:

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

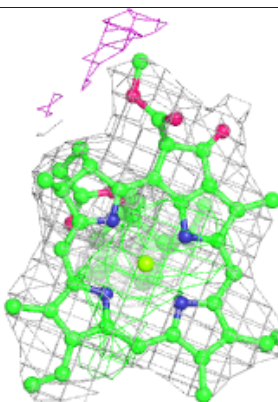
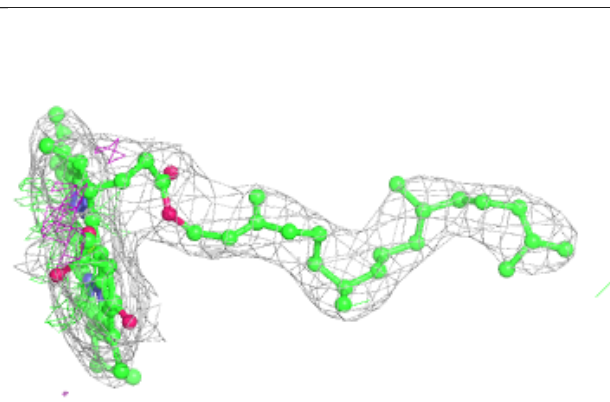
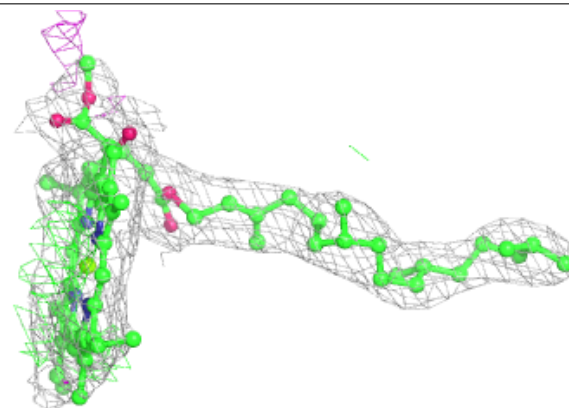


Electron density around CLA B 829:

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

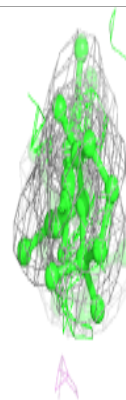
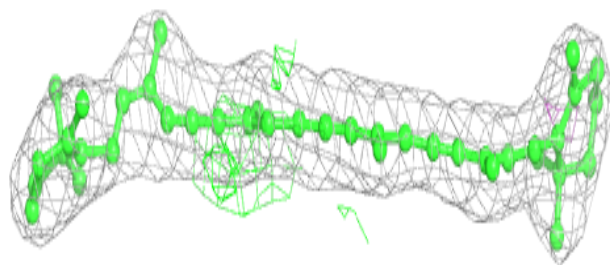
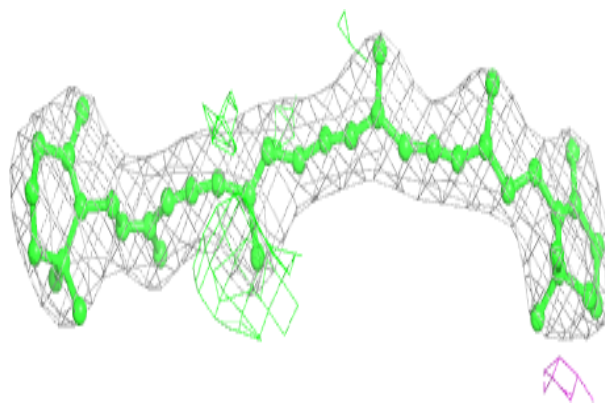
**Electron density around CLA Y 828:**

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

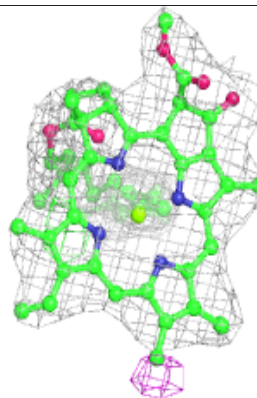
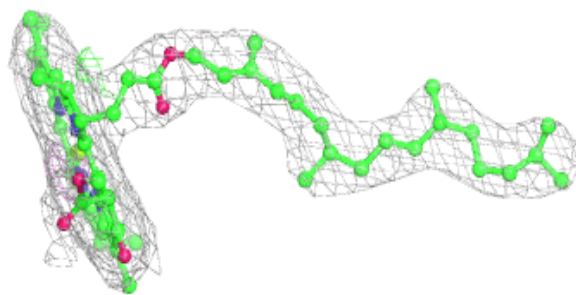
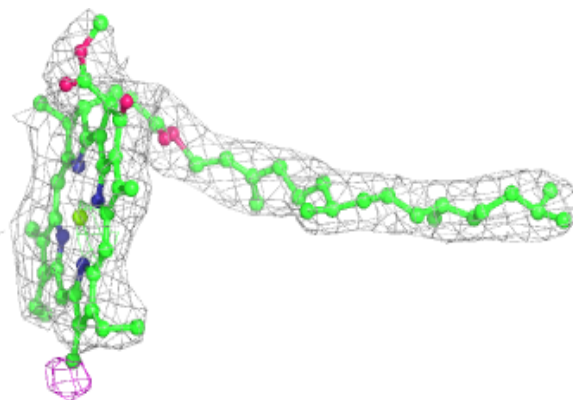


Electron density around BCR H 844:

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

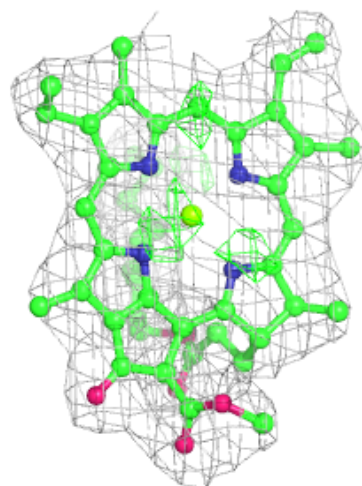
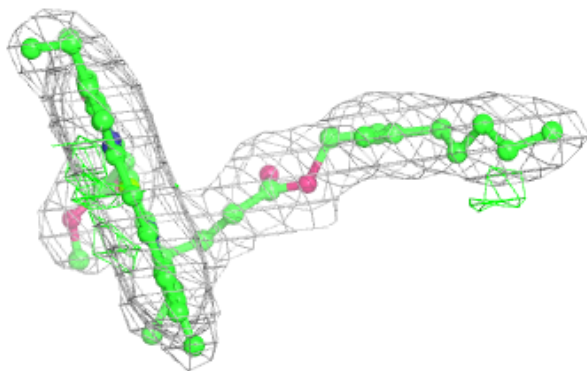
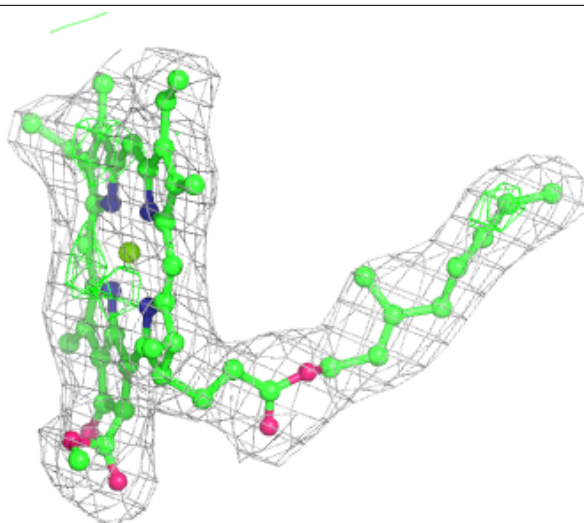
**Electron density around CLA Z 826:**

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



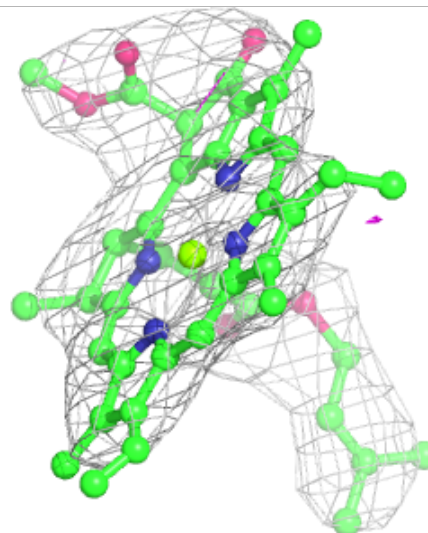
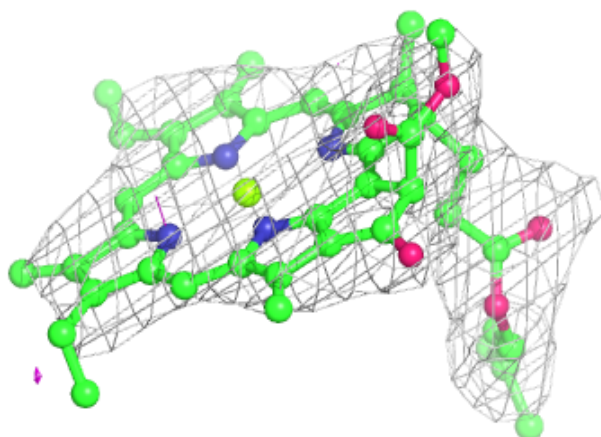
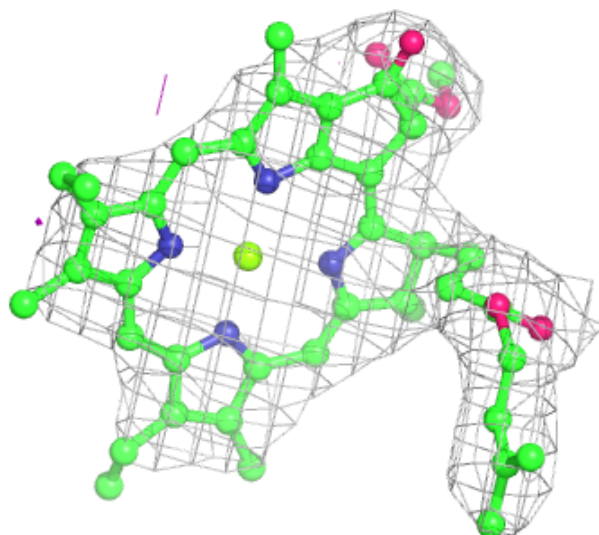
Electron density around CLA B 805:

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



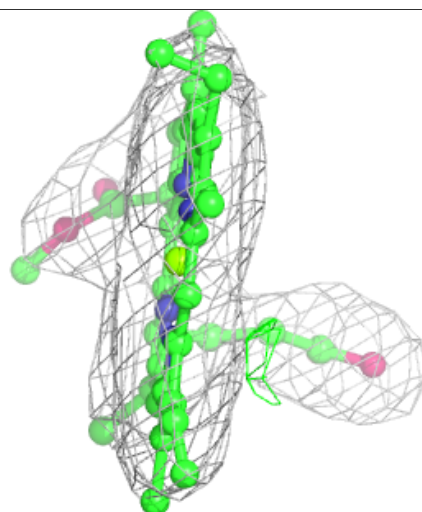
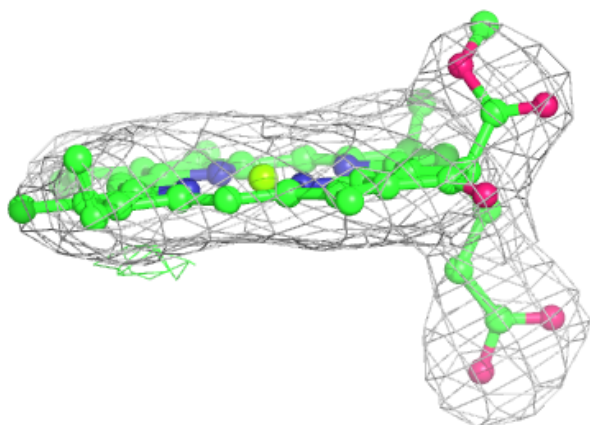
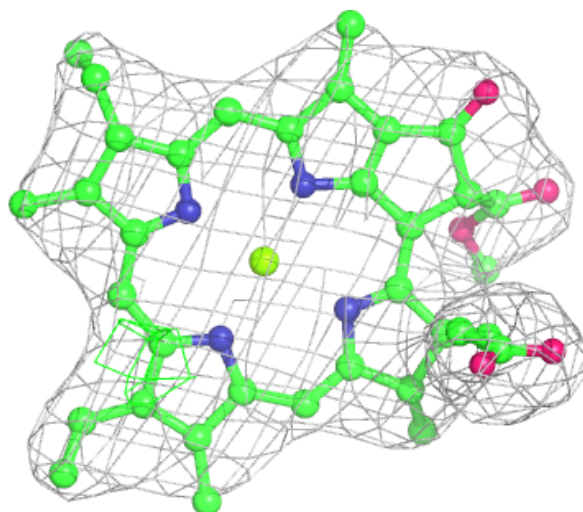
Electron density around CLA G 815:

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



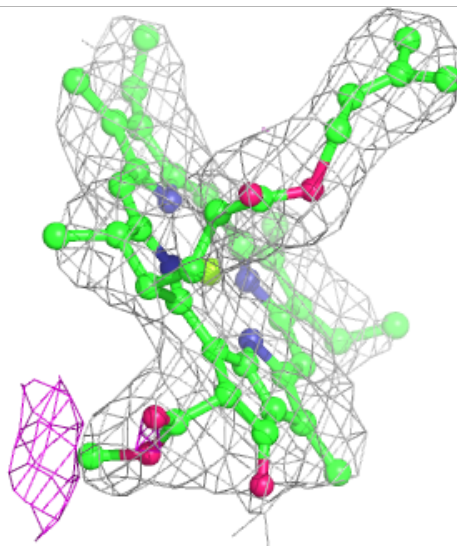
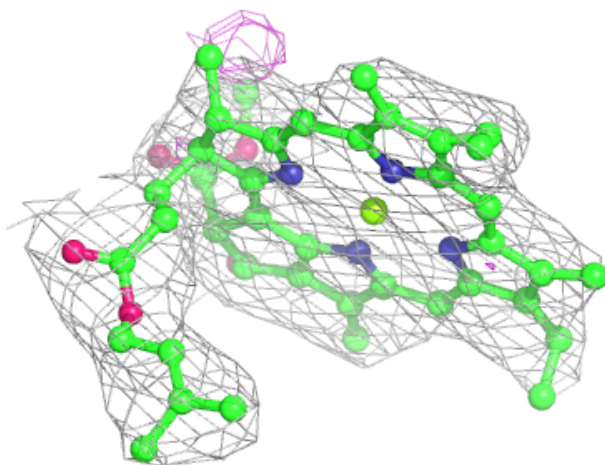
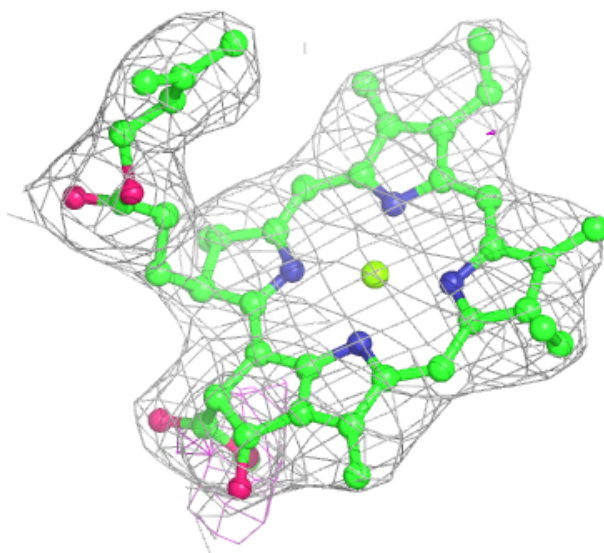
Electron density around CLA g 102:

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



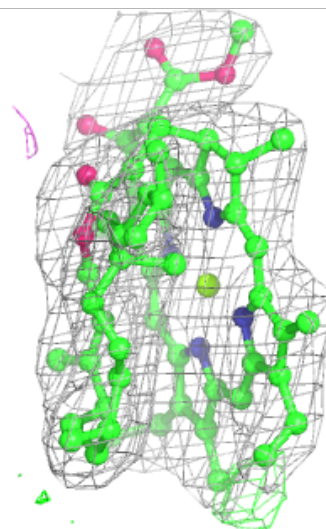
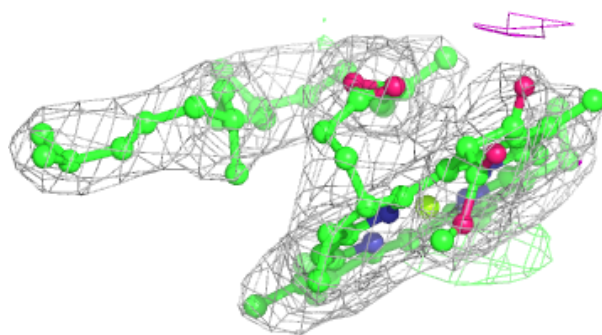
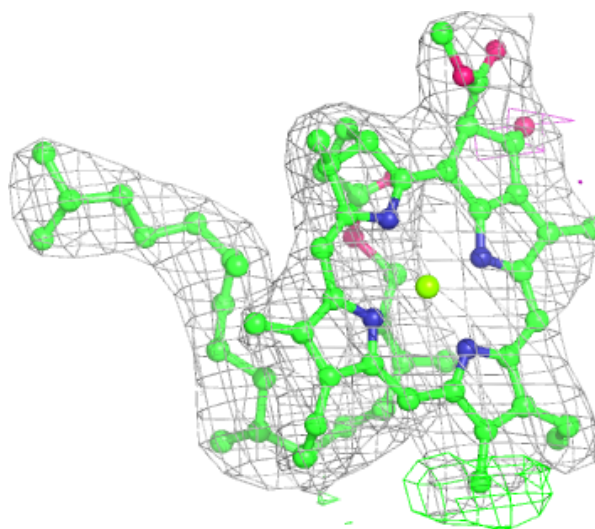
Electron density around CLA G 831:

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



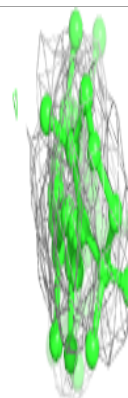
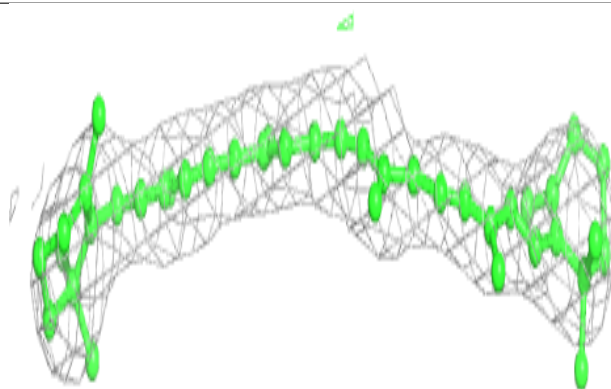
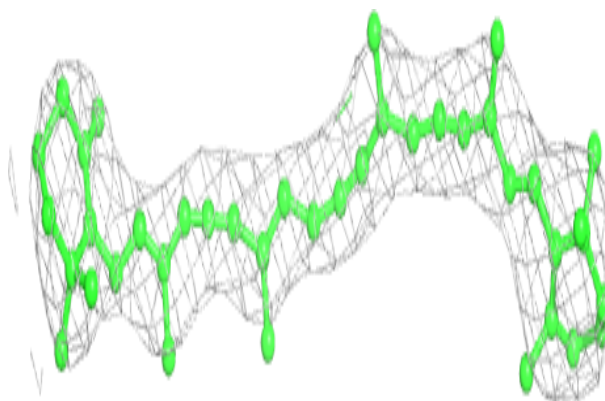
Electron density around CLA B 809:

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



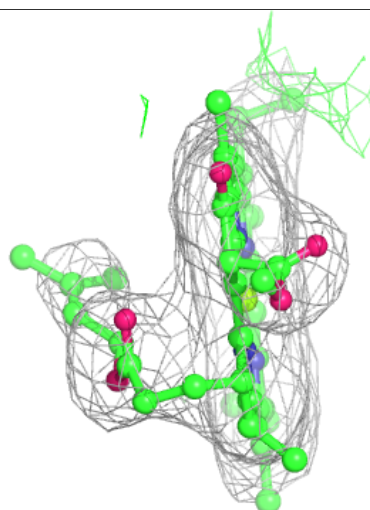
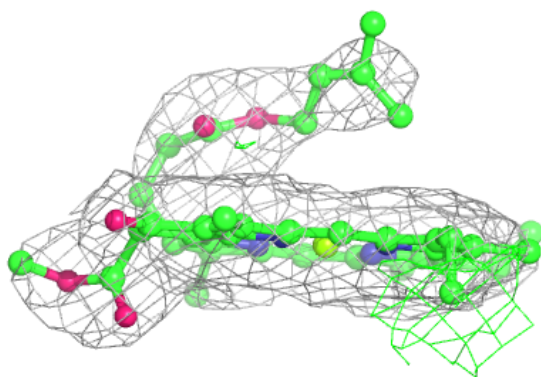
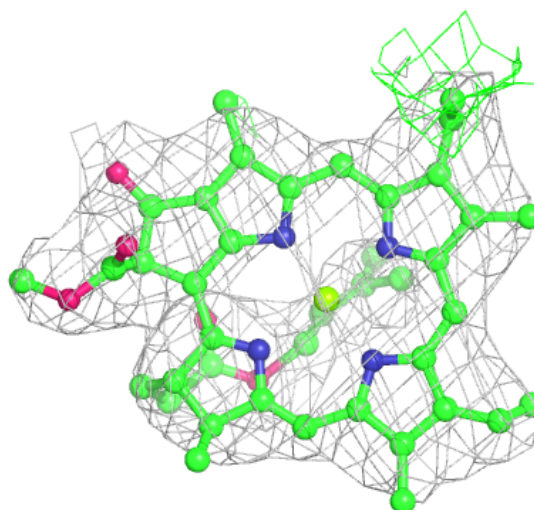
Electron density around BCR H 840:

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



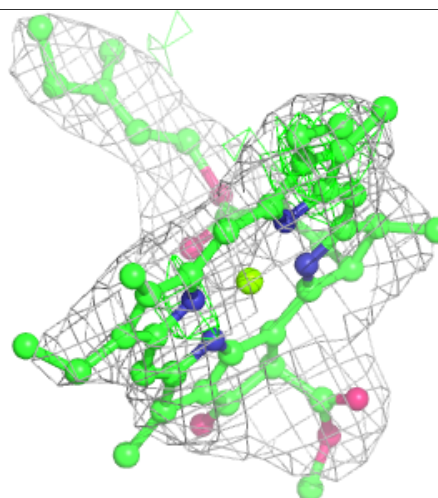
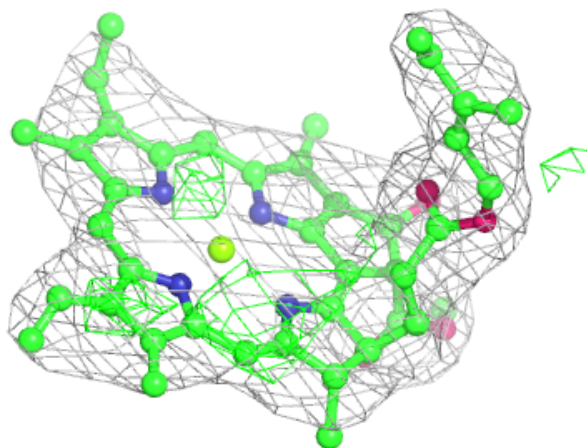
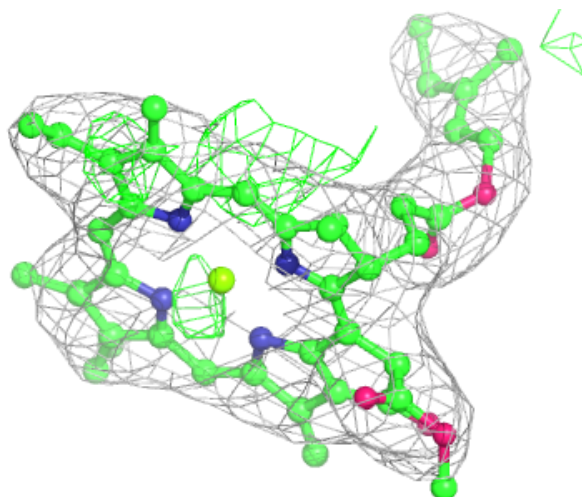
Electron density around CLA G 823:

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



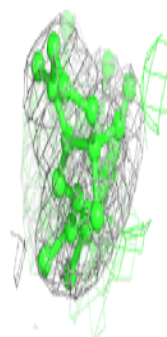
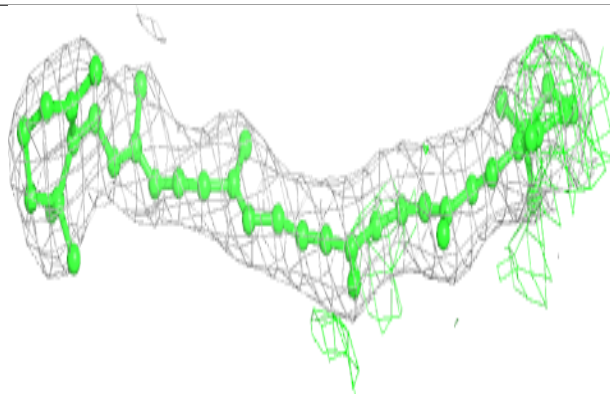
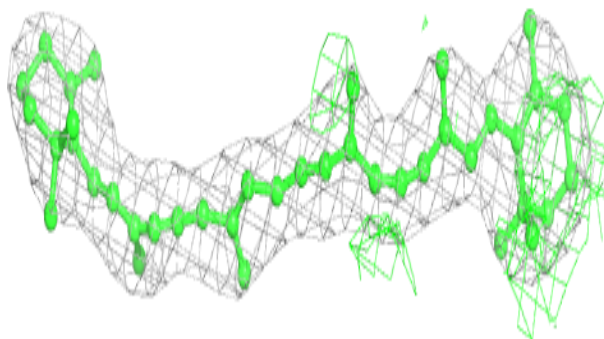
Electron density around CLA Y 807:

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



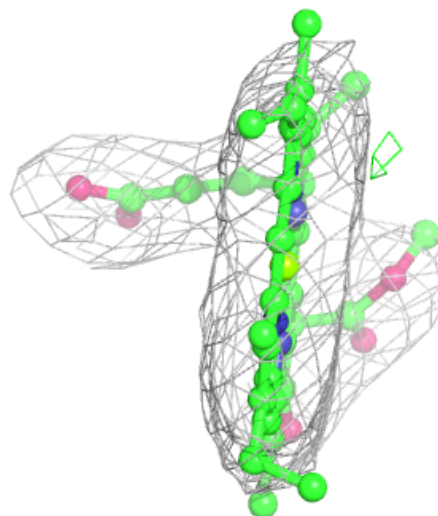
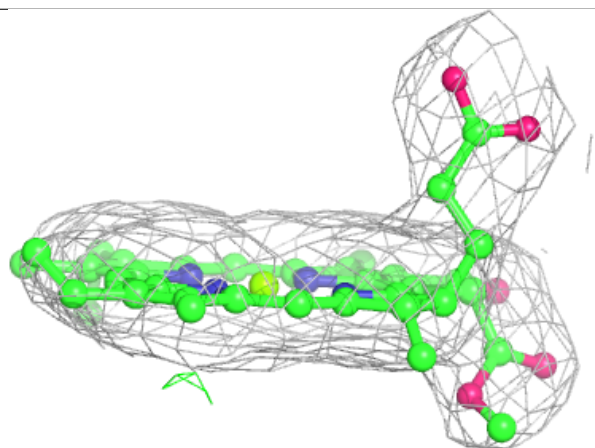
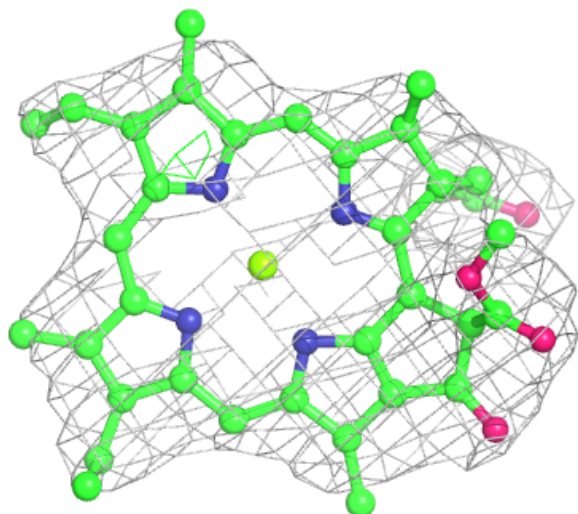
Electron density around BCR S 1104:

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



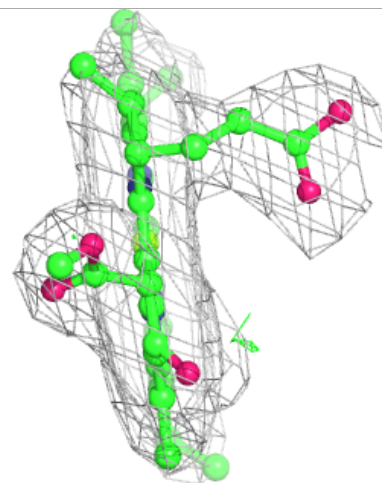
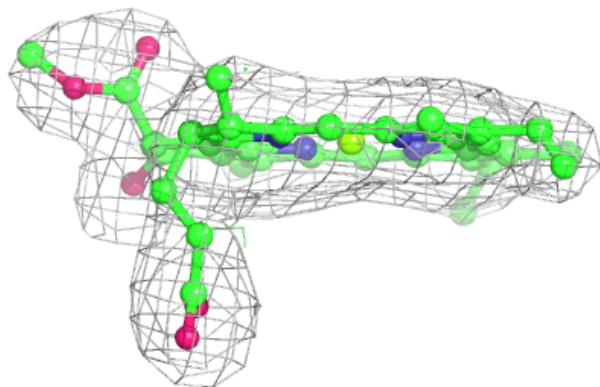
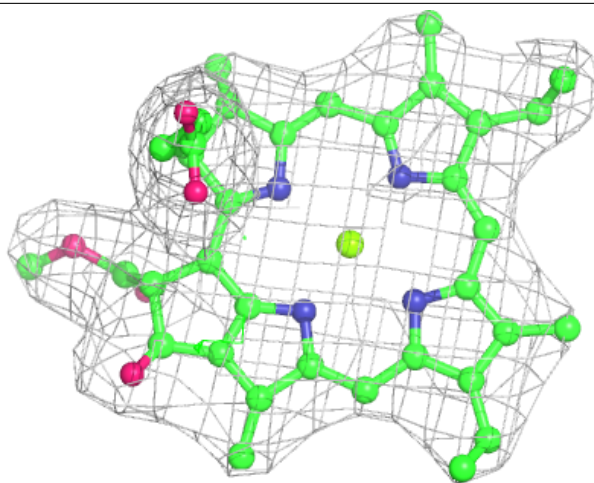
Electron density around CLA K 103:

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



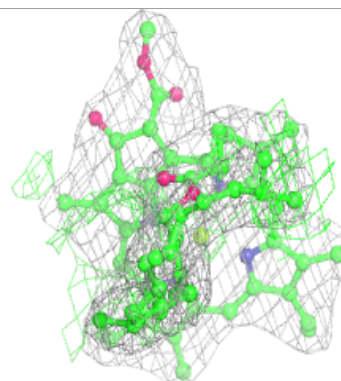
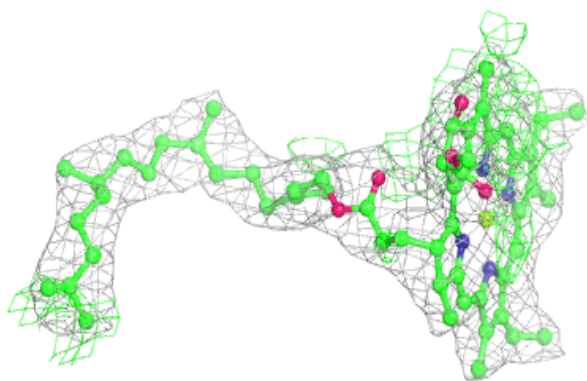
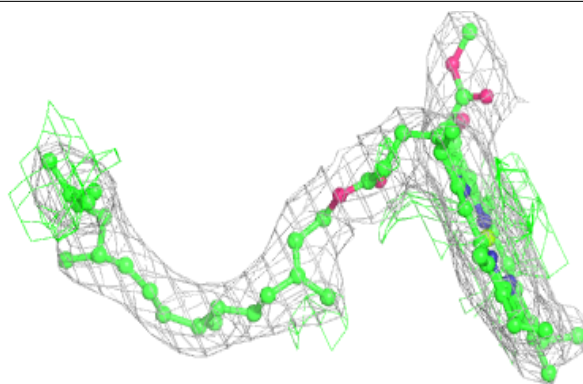
Electron density around CLA Z 829:

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

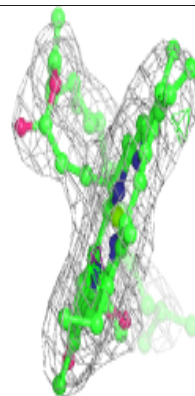
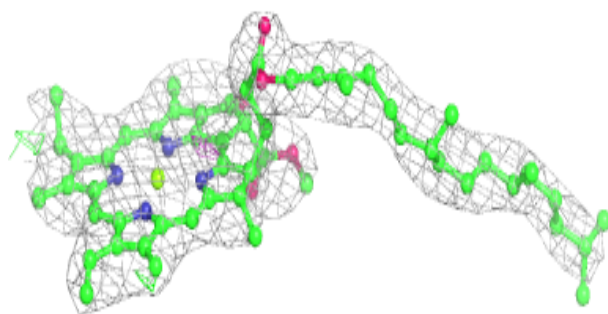
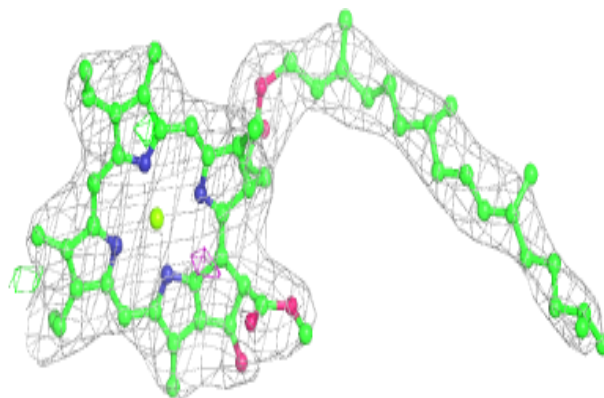


Electron density around CLA B 840:

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

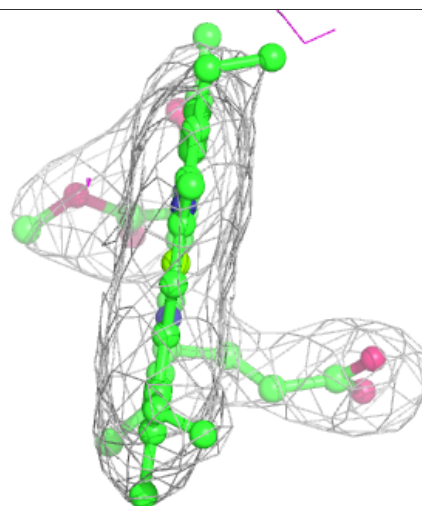
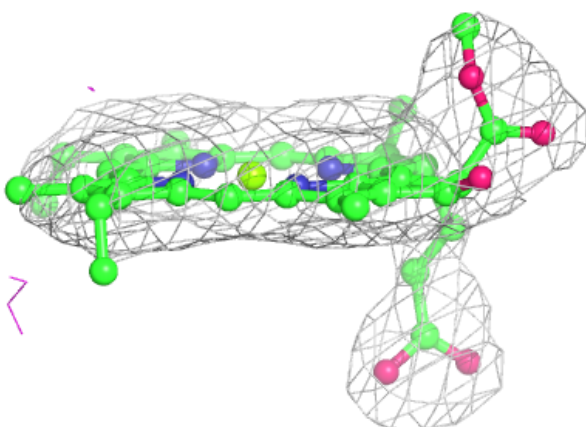
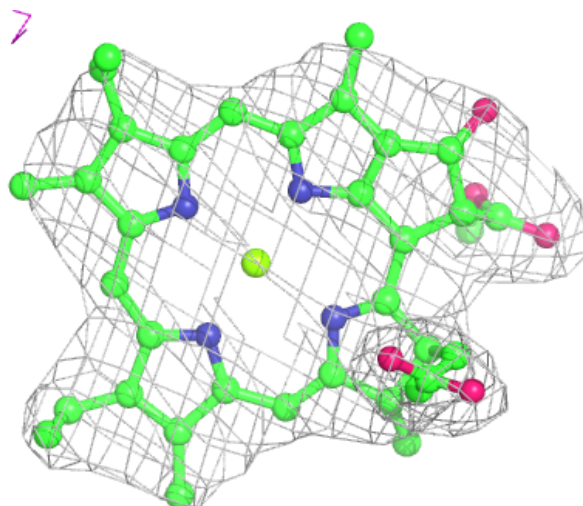
**Electron density around CLA G 822:**

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



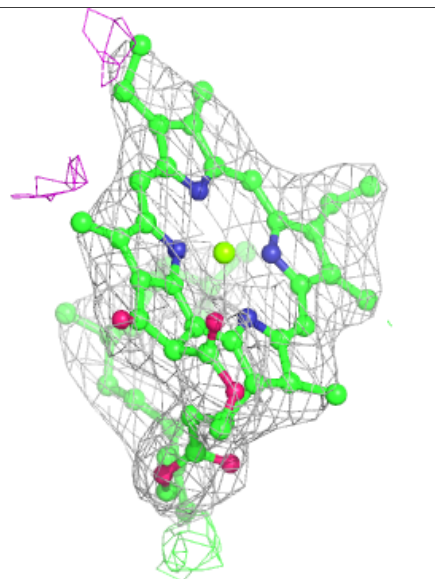
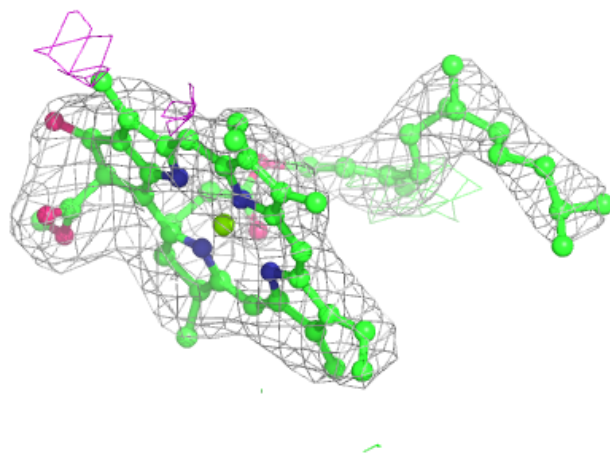
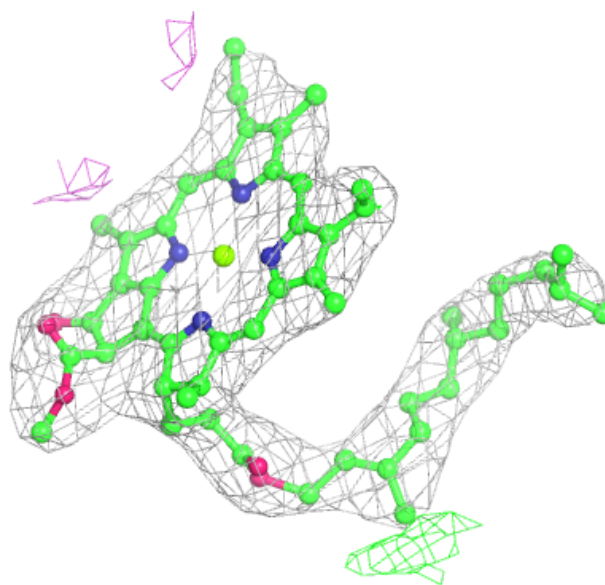
Electron density around CLA H 814:

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



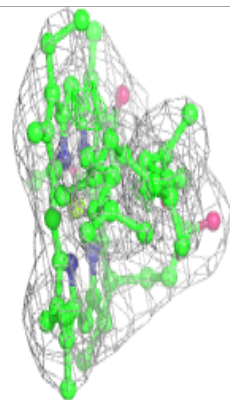
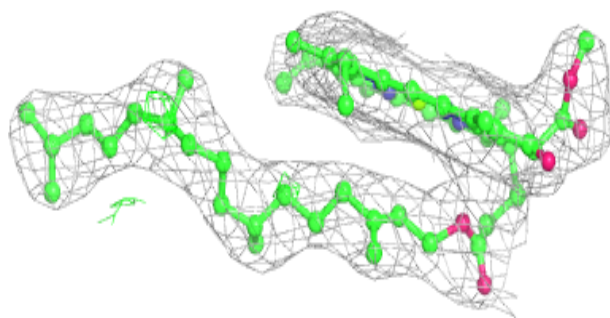
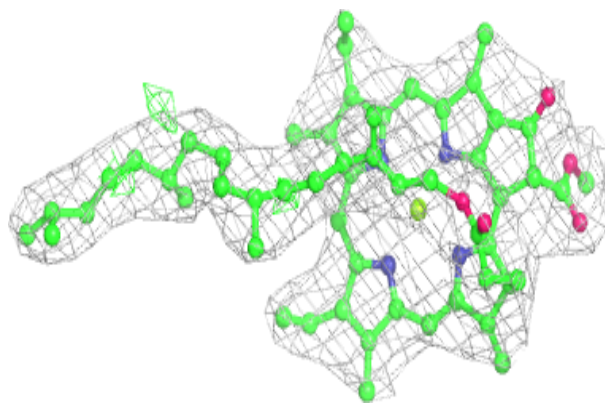
Electron density around CLA Y 824:

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

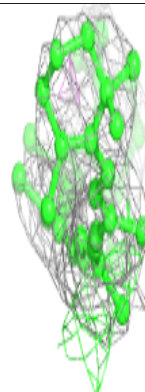
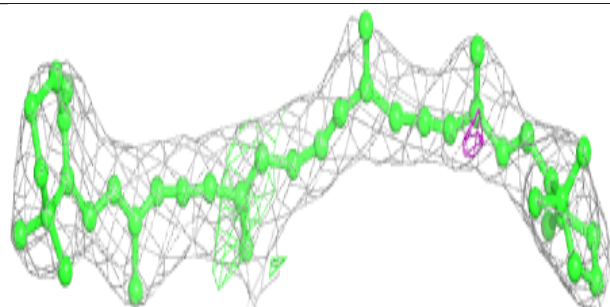
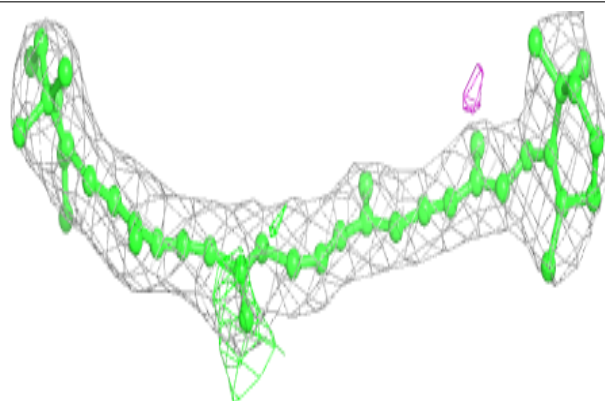


Electron density around CLA A 837:

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

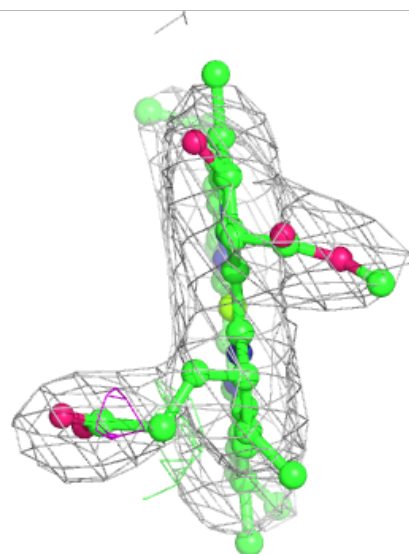
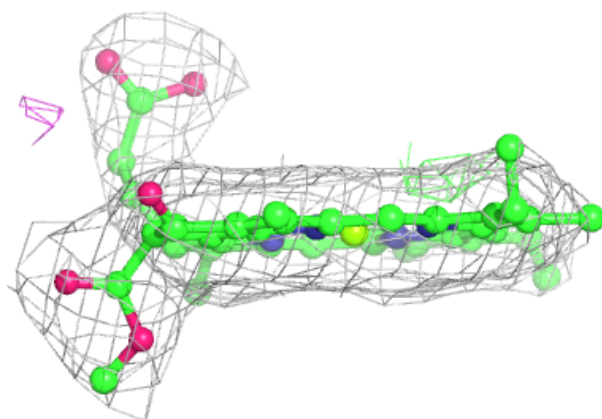
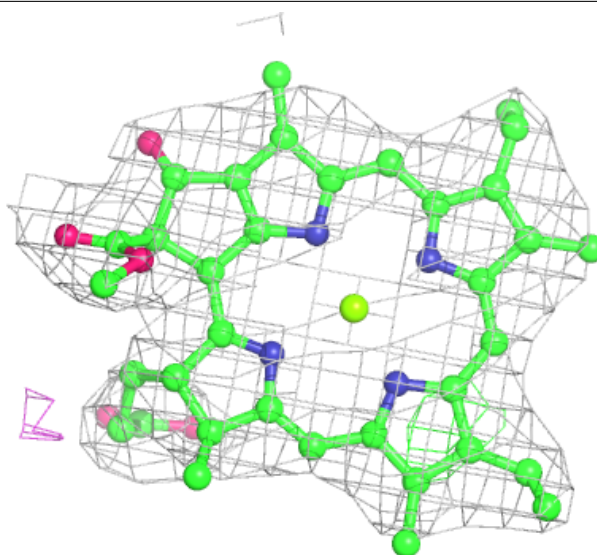
**Electron density around BCR Q 202:**

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



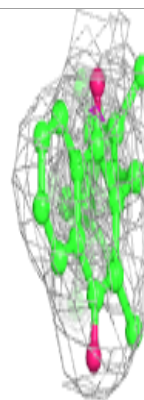
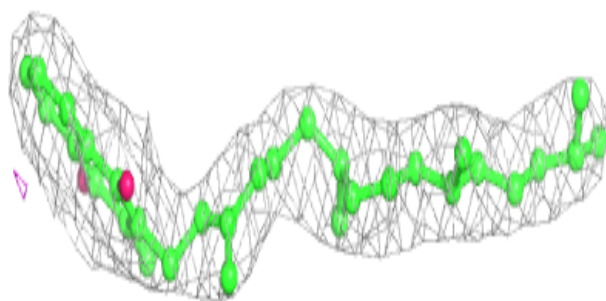
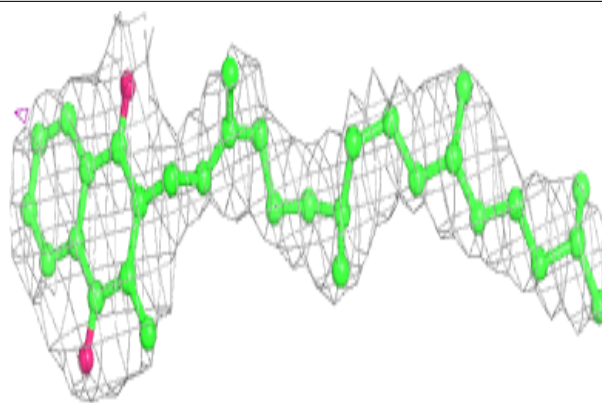
Electron density around CLA H 819:

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



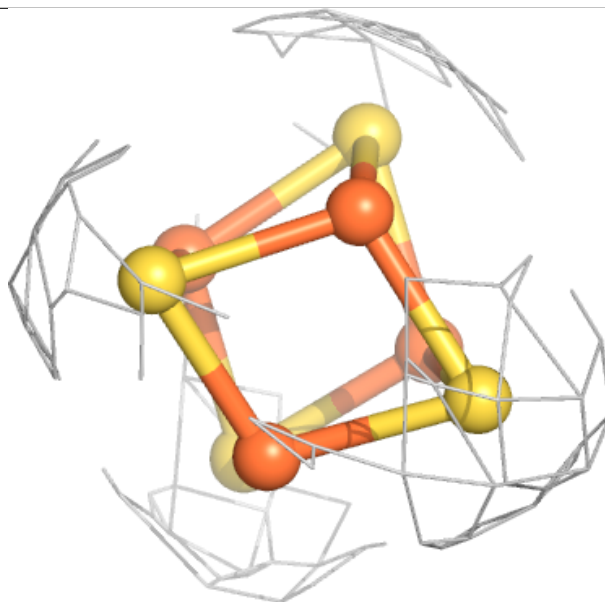
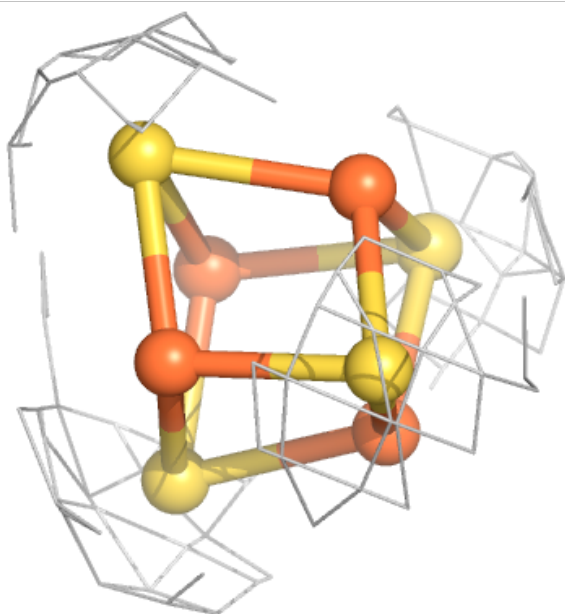
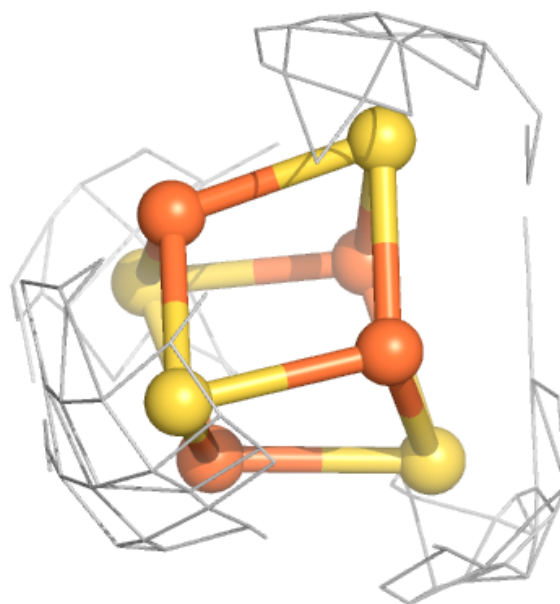
Electron density around PQN Y 844:

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



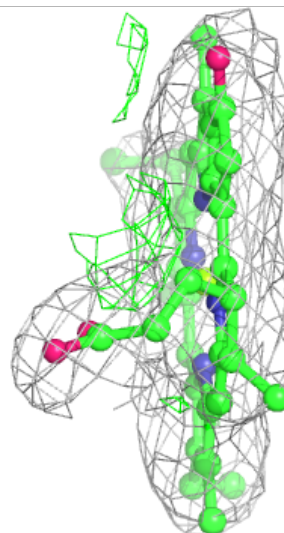
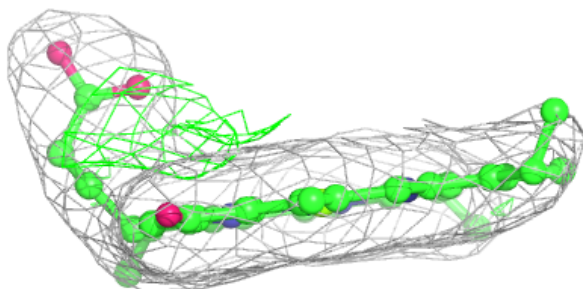
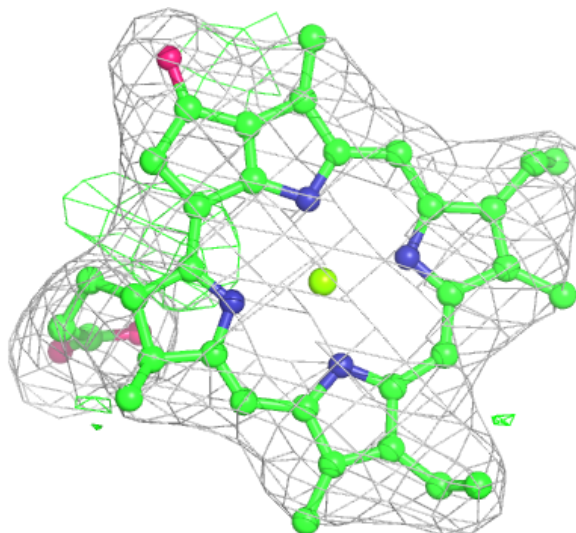
Electron density around SF4 a 102:

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



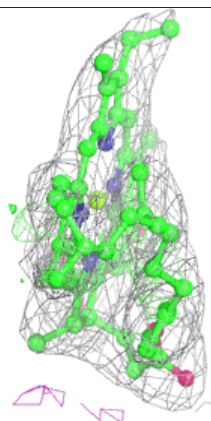
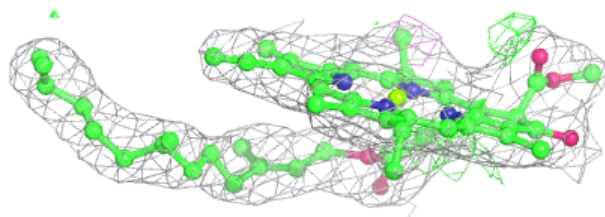
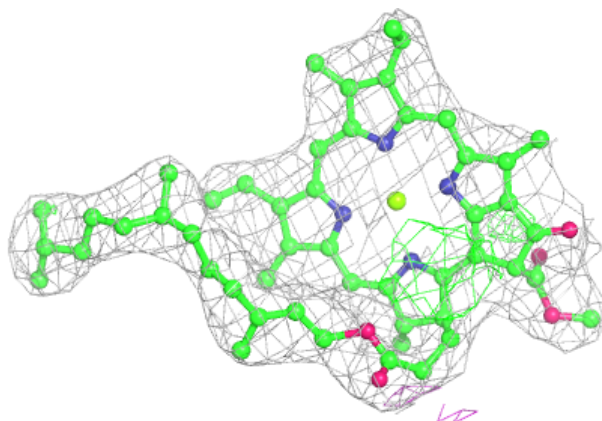
Electron density around CLA g 101:

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

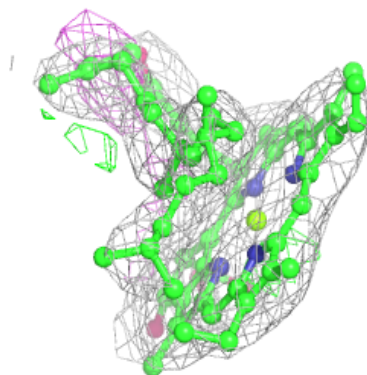
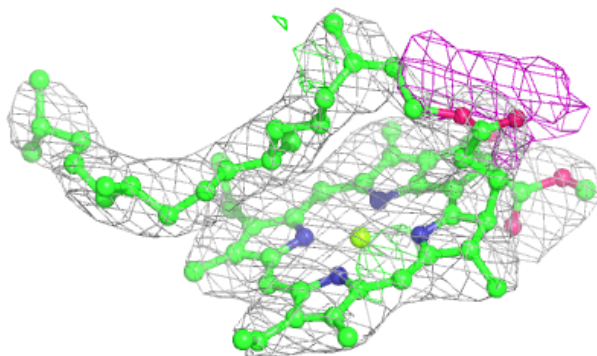
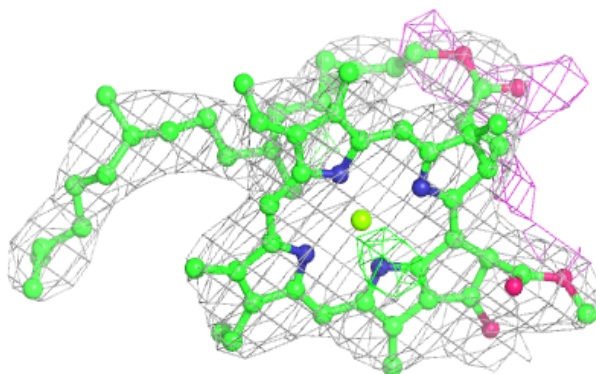


Electron density around CLA B 818:

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

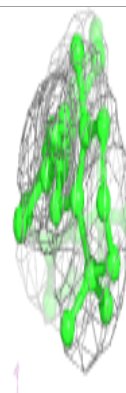
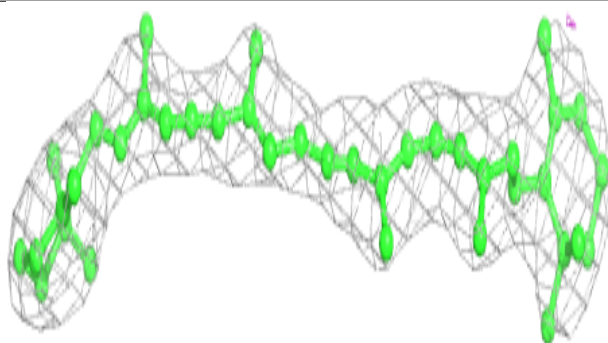
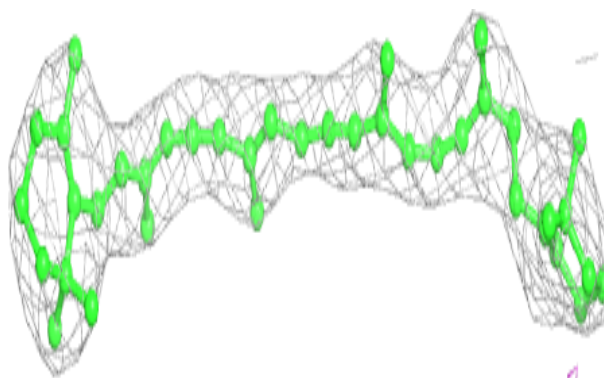
**Electron density around CLA H 816:**

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

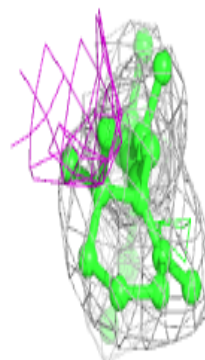
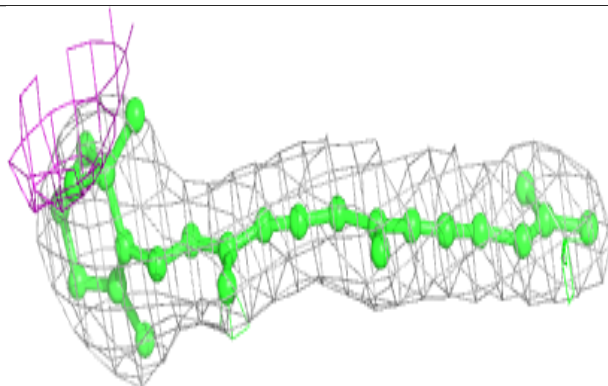
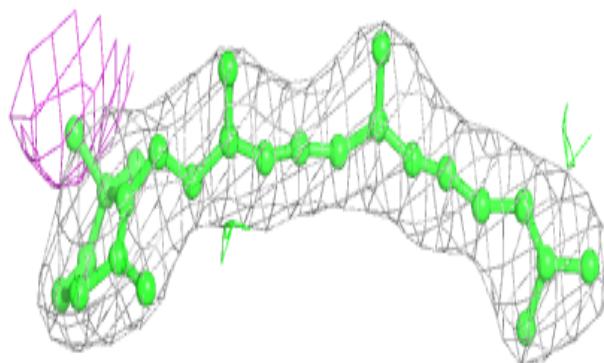


Electron density around BCR T 102:

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

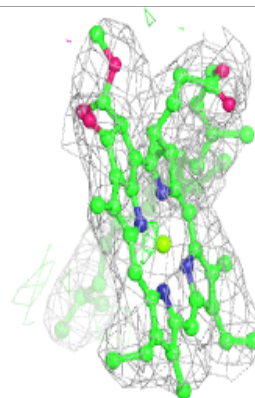
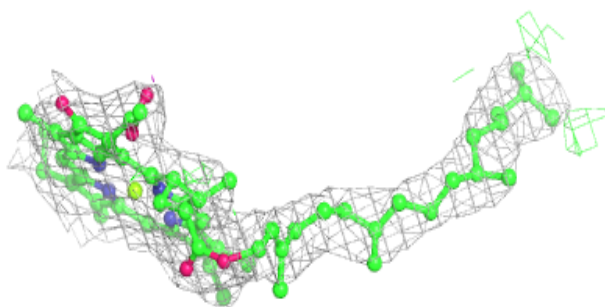
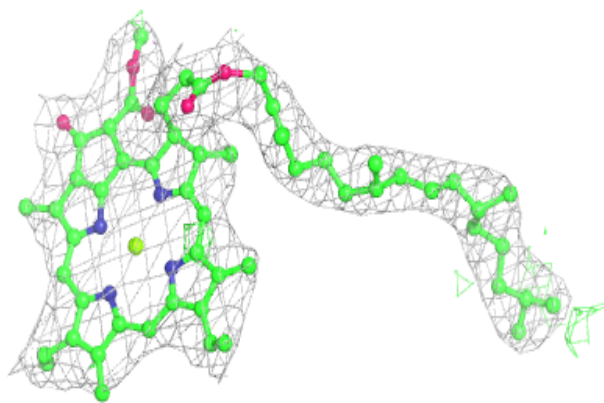
**Electron density around BCR B 846:**

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

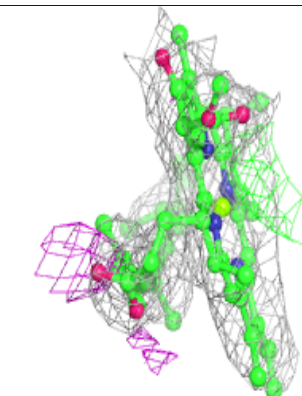
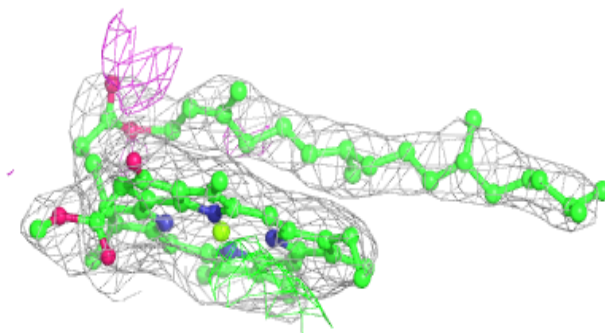
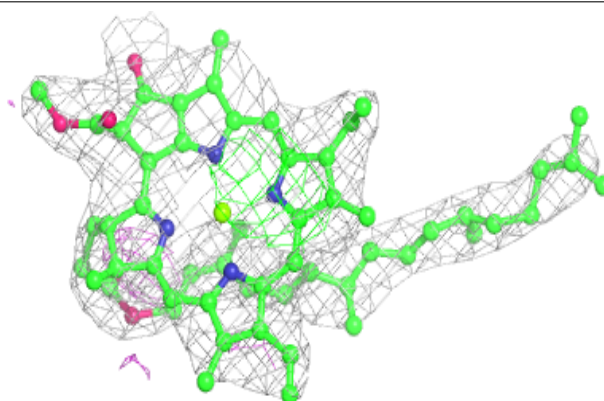


Electron density around CLA G 802:

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

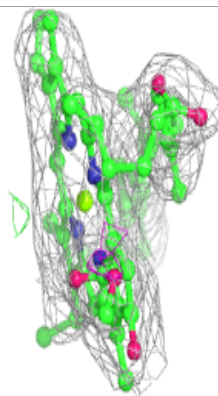
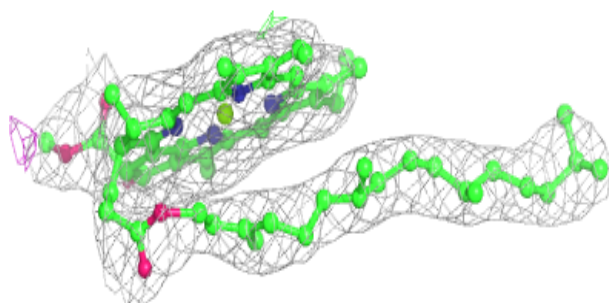
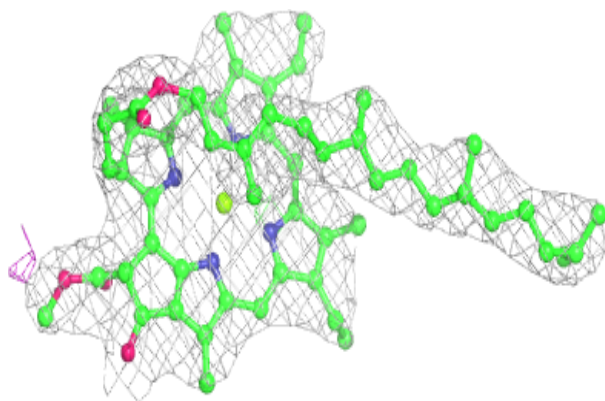
**Electron density around CLA G 818:**

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

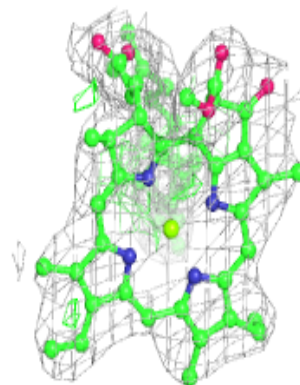
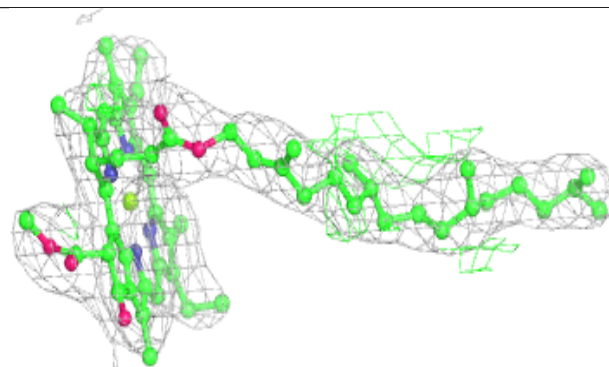
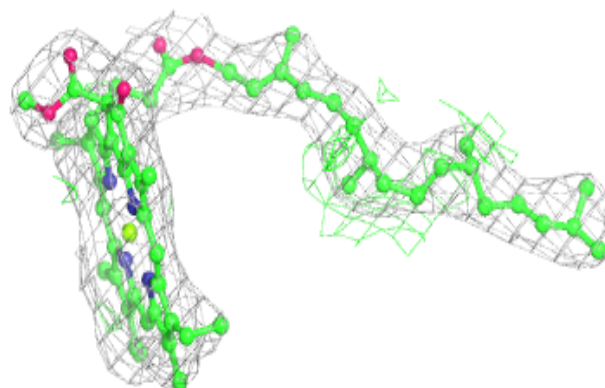


Electron density around CLA A 818:

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

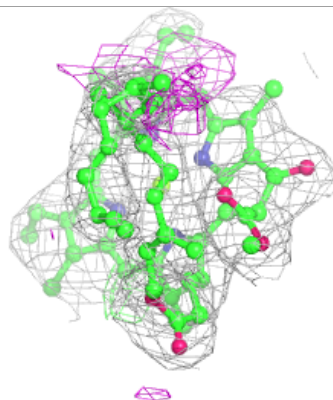
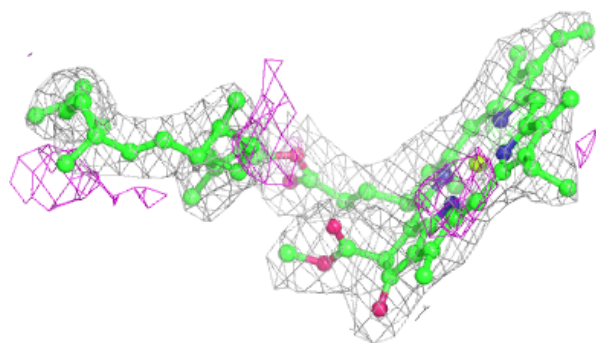
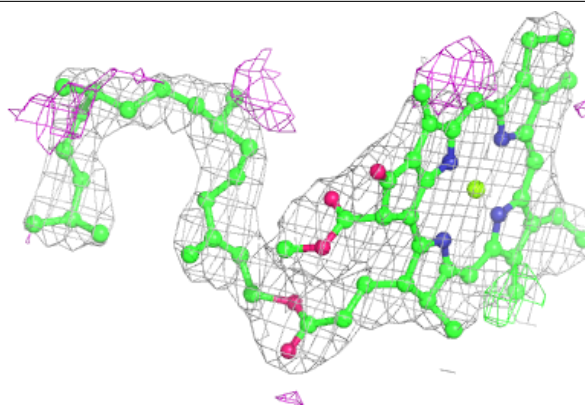
**Electron density around CLA Z 827:**

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

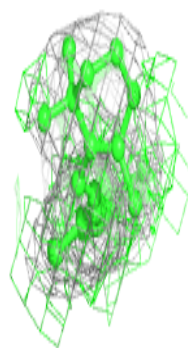
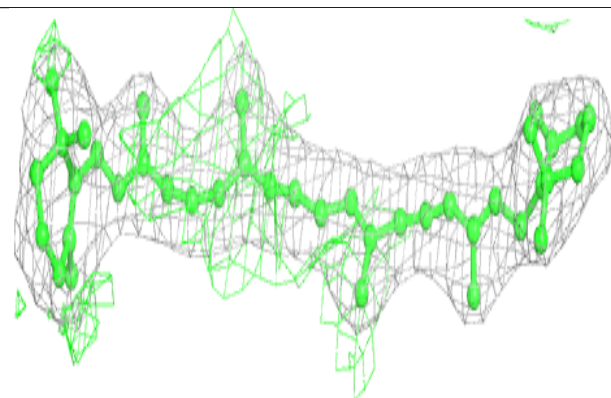
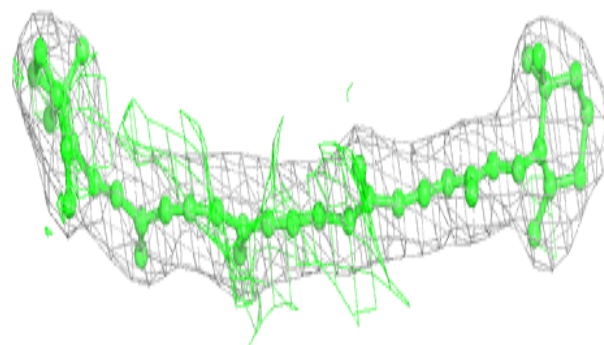


Electron density around CL0 A 801:

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

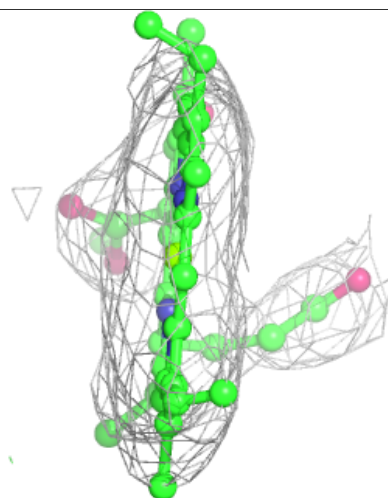
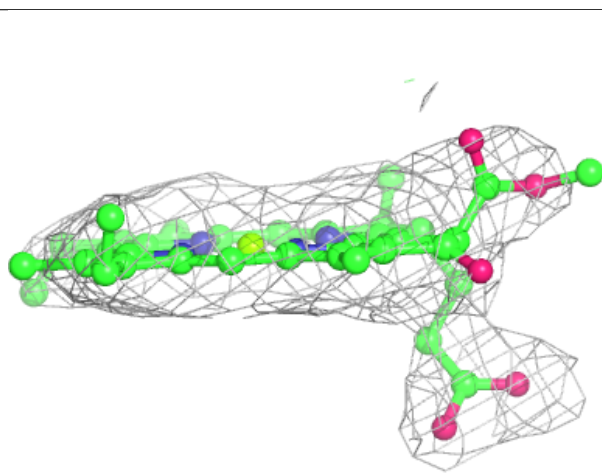
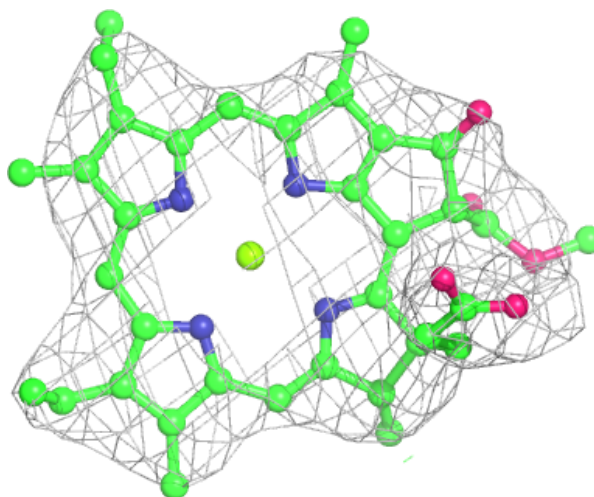
**Electron density around BCR I 101:**

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



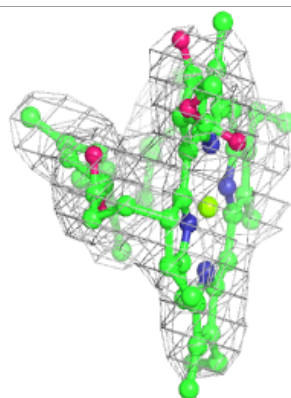
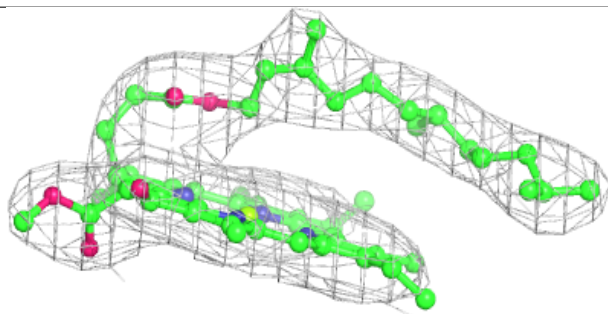
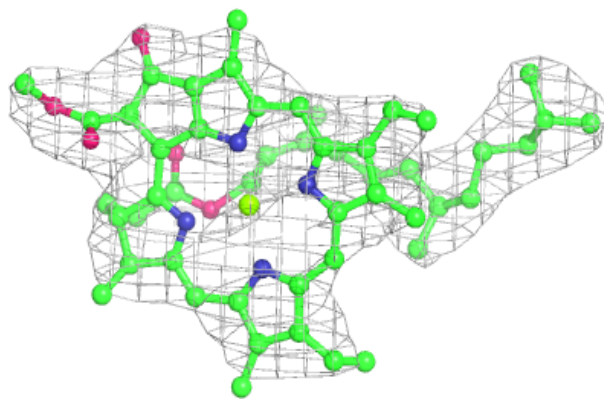
Electron density around CLA f 101:

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

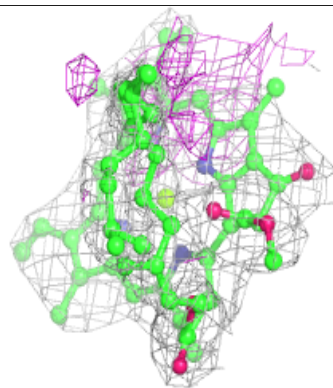
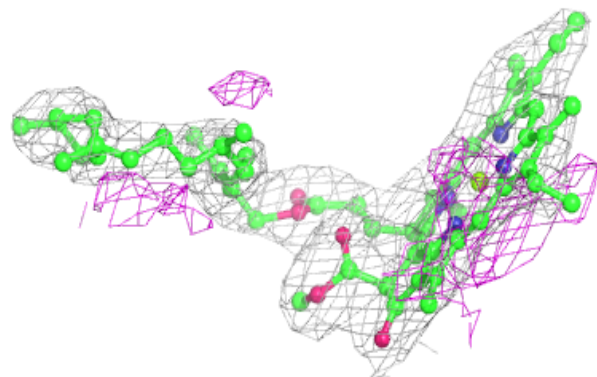
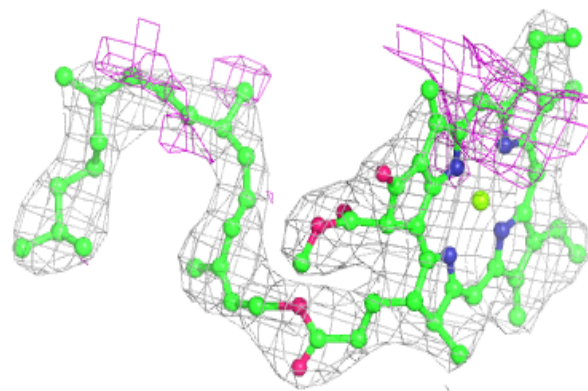


Electron density around CLA Y 817:

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

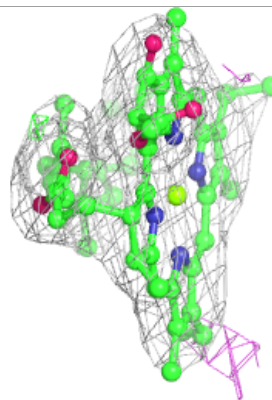
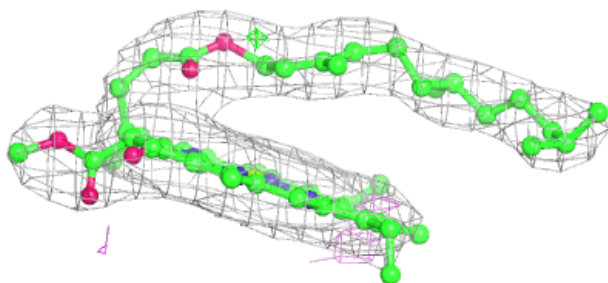
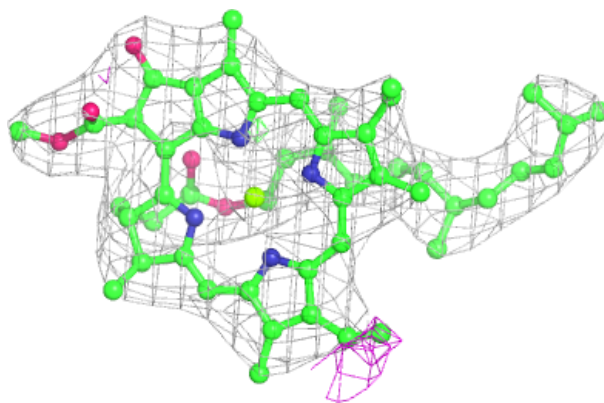
**Electron density around CL0 Y 801:**

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

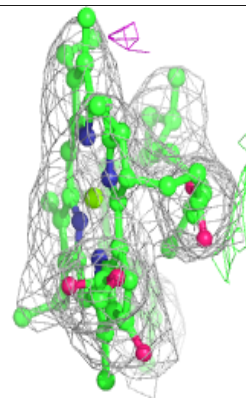
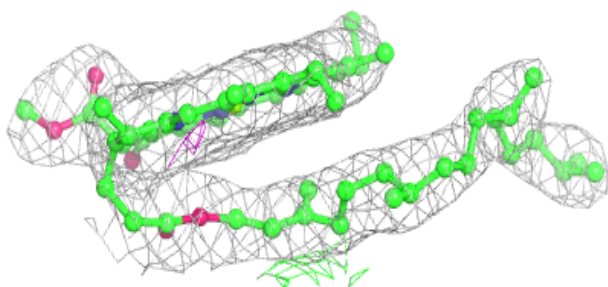
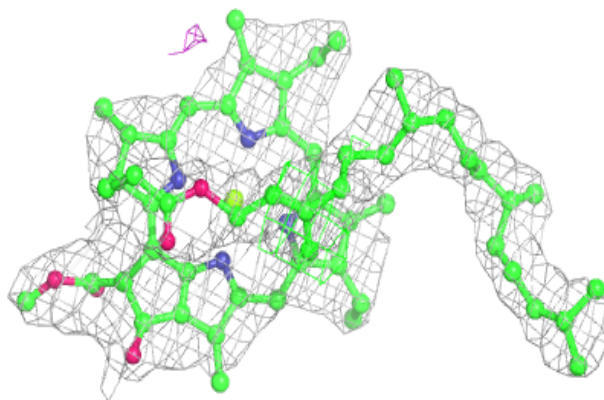


Electron density around CLA A 817:

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

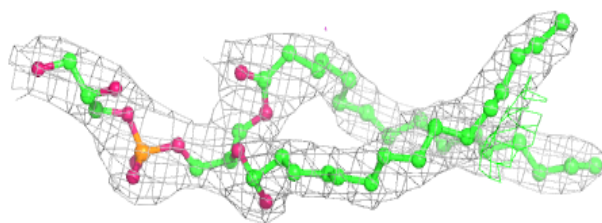
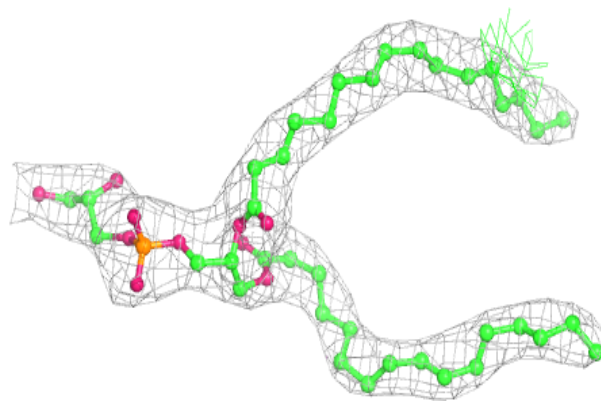
**Electron density around CLA Z 836:**

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



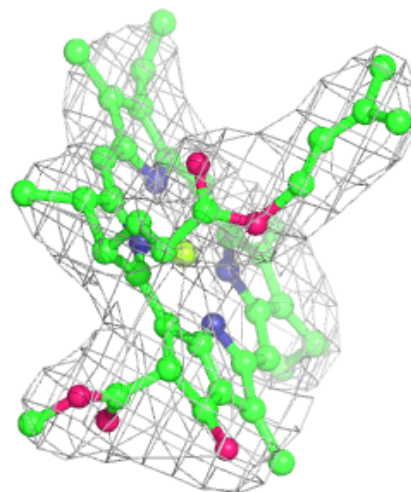
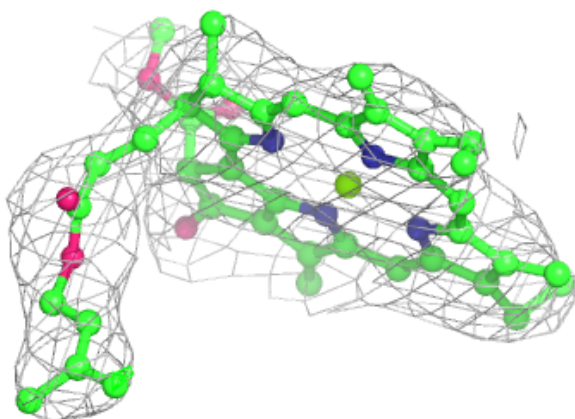
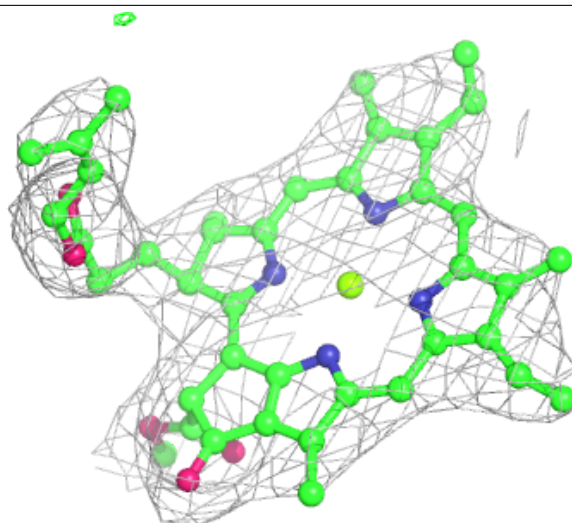
Electron density around LHG G 851:

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



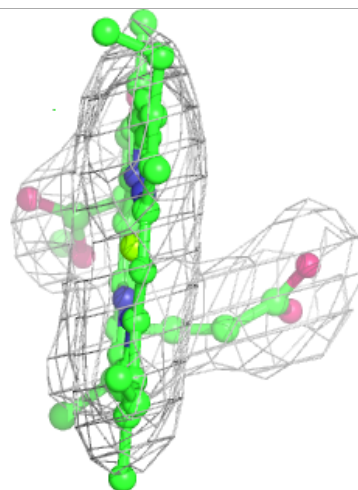
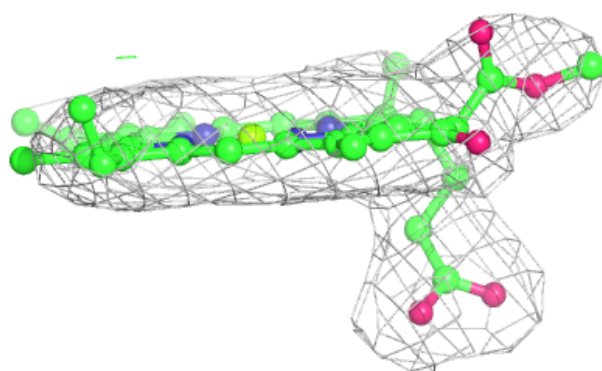
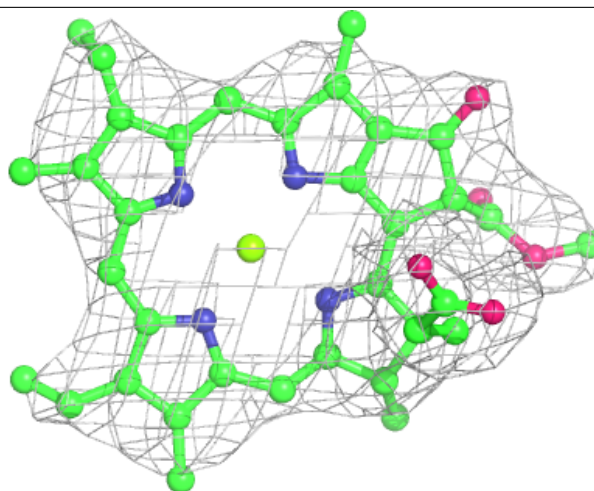
Electron density around CLA G 814:

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



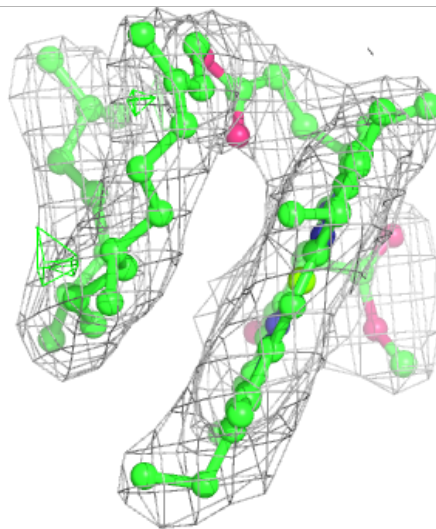
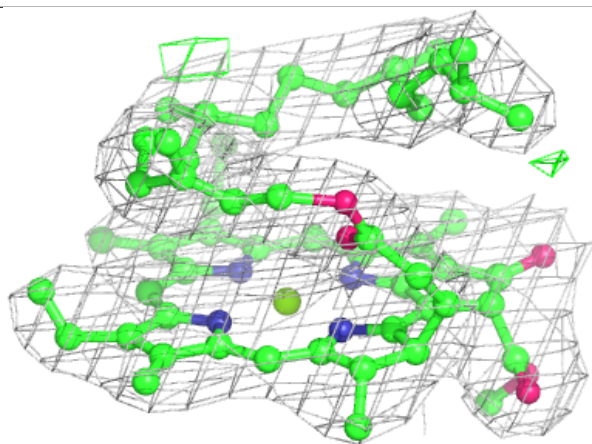
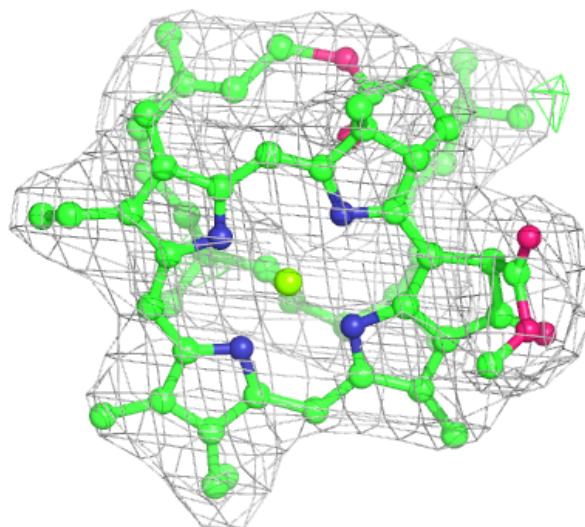
Electron density around CLA A 810:

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



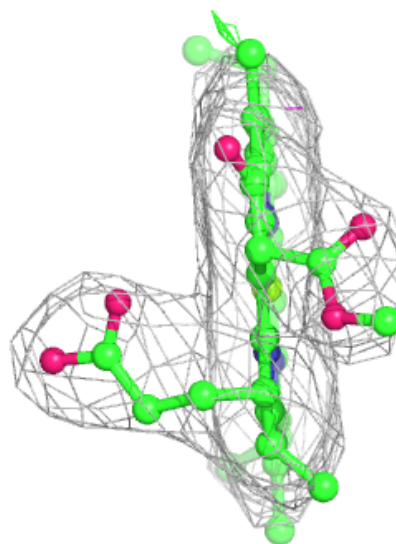
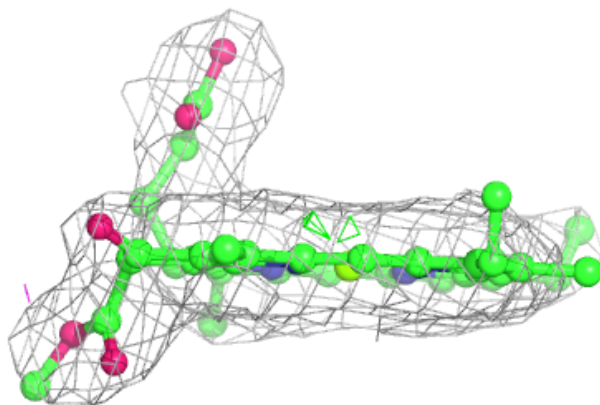
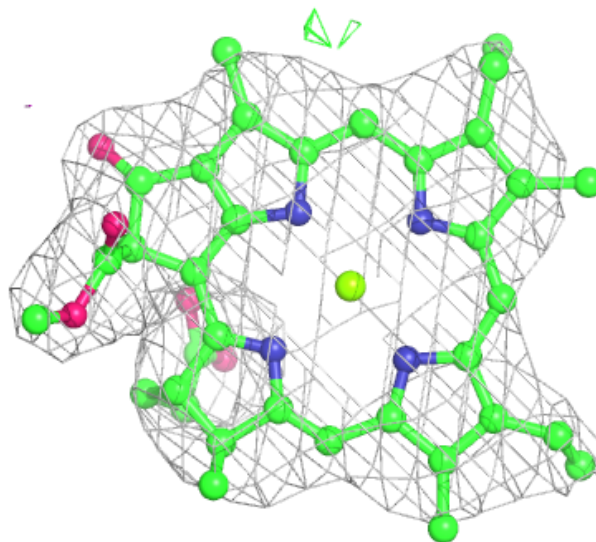
Electron density around CLA h 205:

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



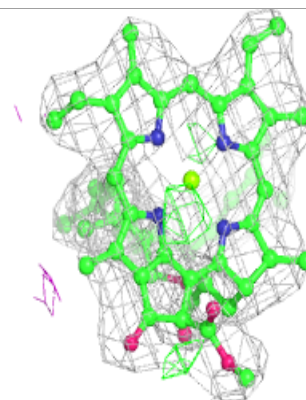
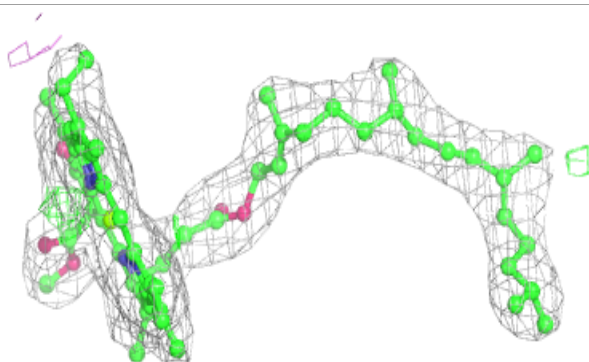
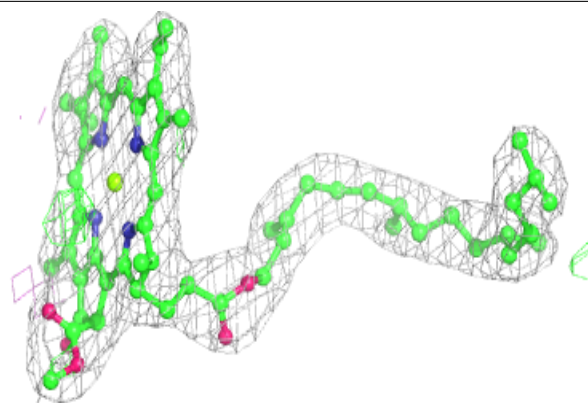
Electron density around CLA Y 836:

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

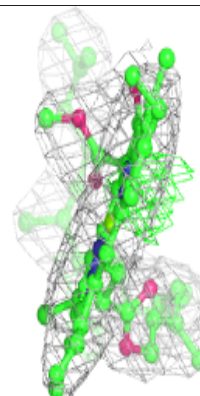
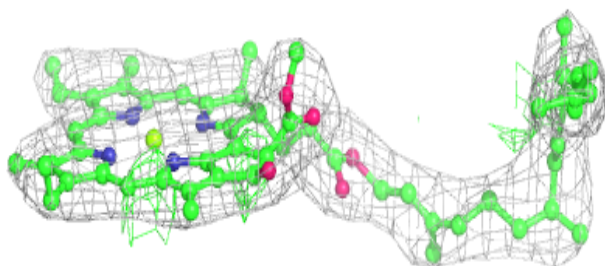
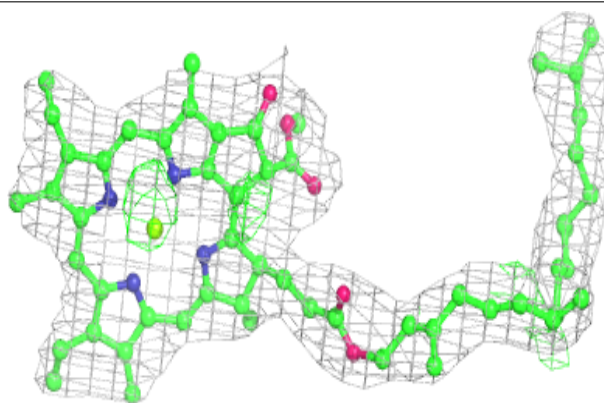


Electron density around CLA h 206:

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

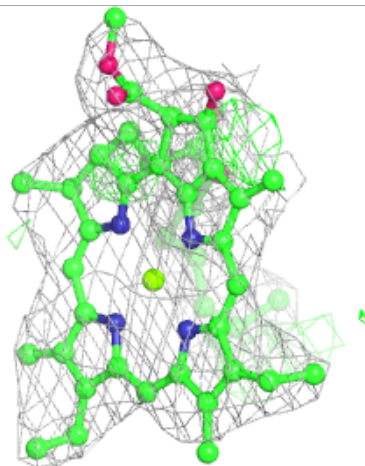
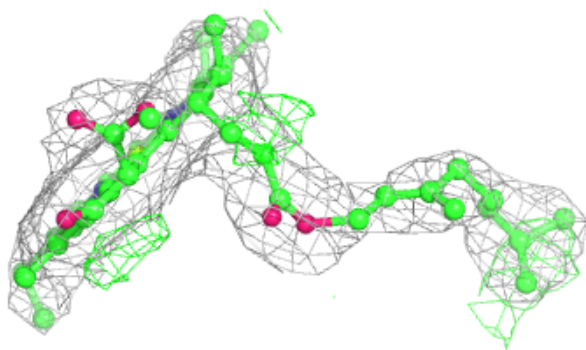
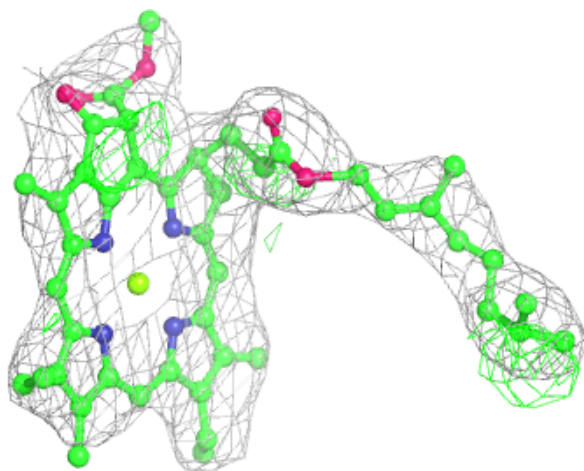
**Electron density around CLA H 825:**

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



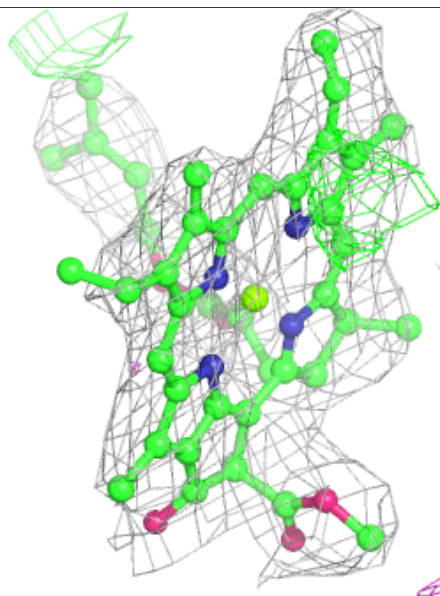
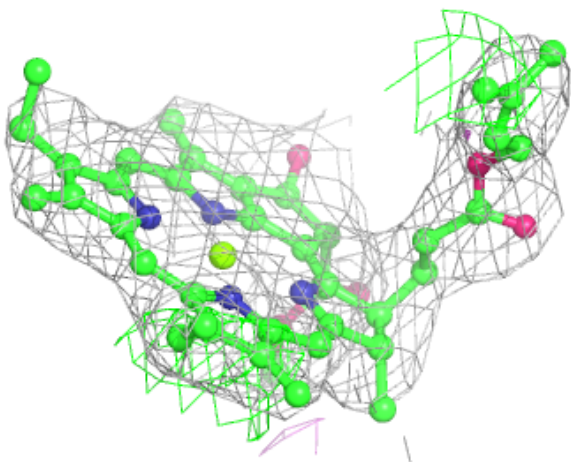
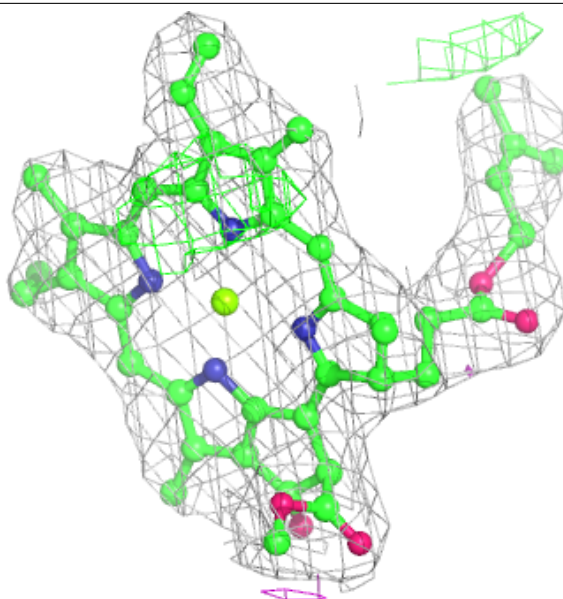
Electron density around CLA A 834:

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



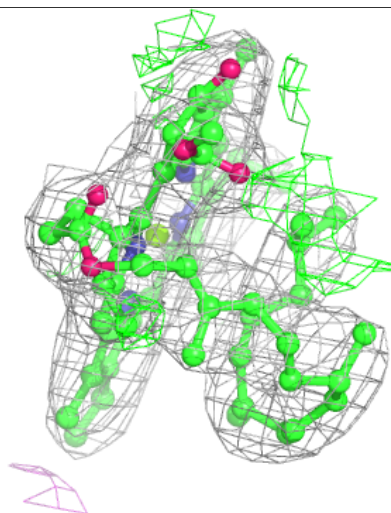
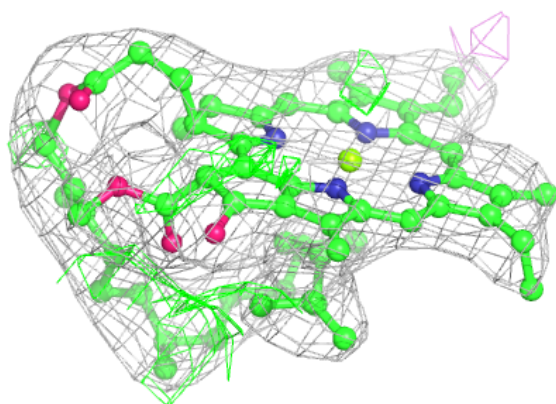
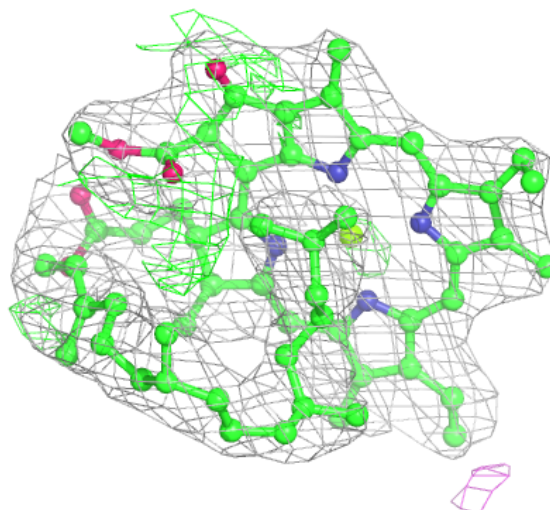
Electron density around CLA Y 831:

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



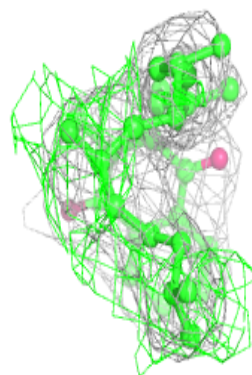
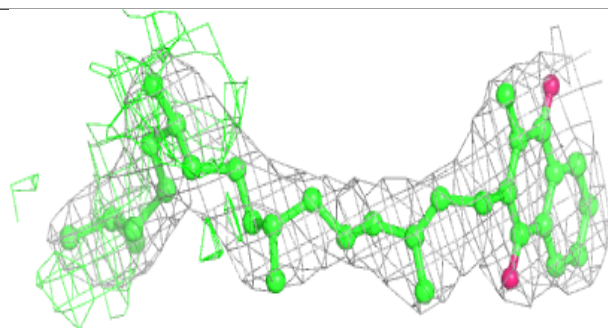
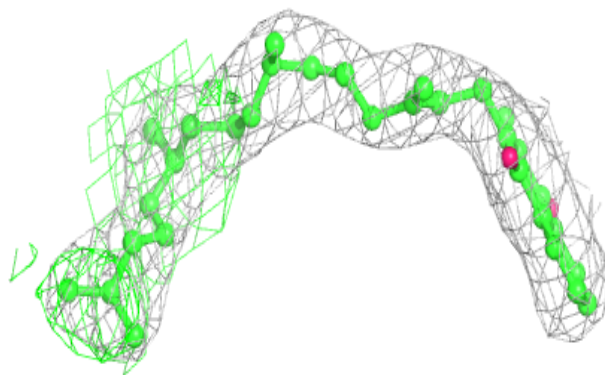
Electron density around CLA Z 805:

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

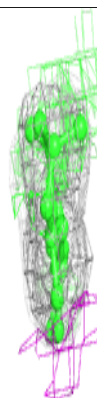
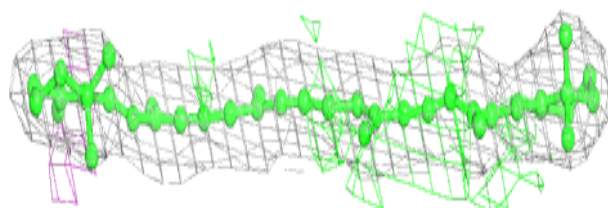
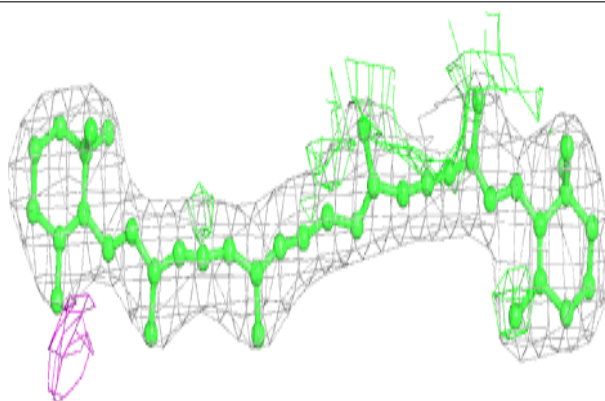


Electron density around PQN Z 840:

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

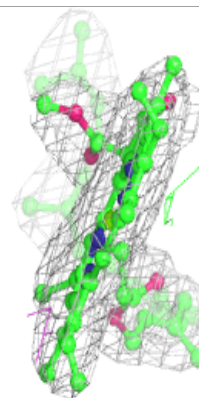
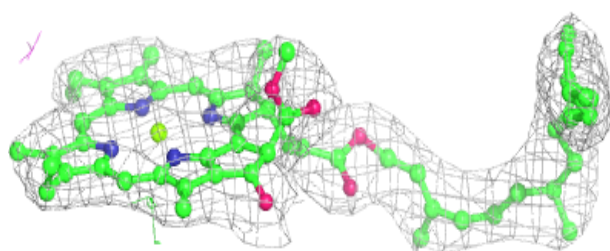
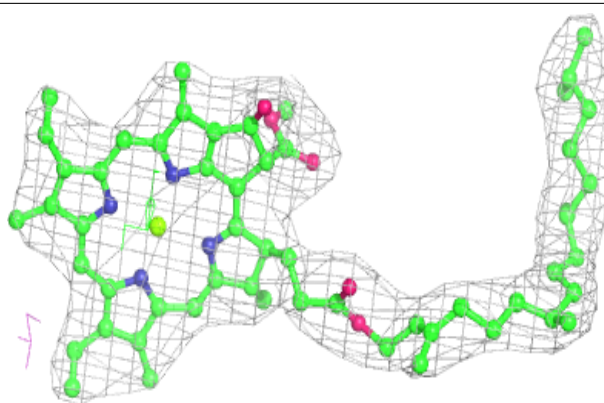
**Electron density around BCR R 102:**

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

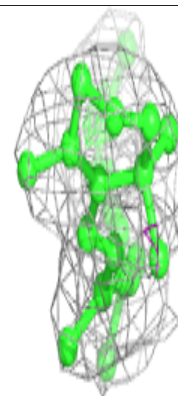
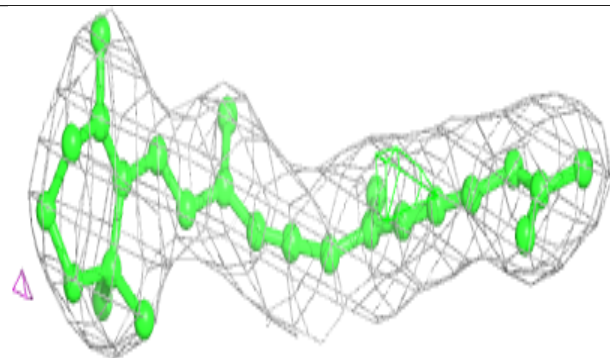
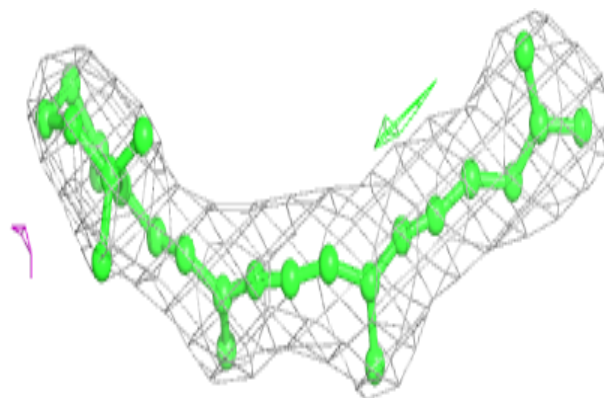


Electron density around CLA Z 824:

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

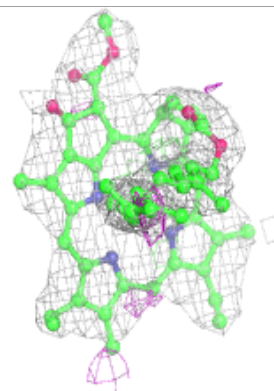
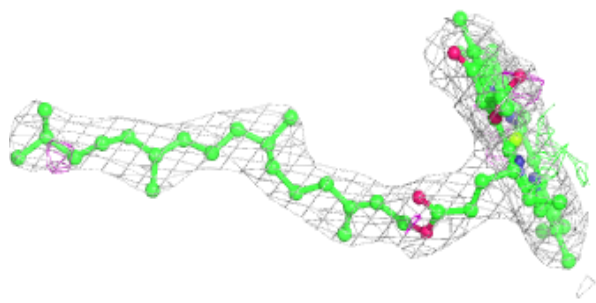
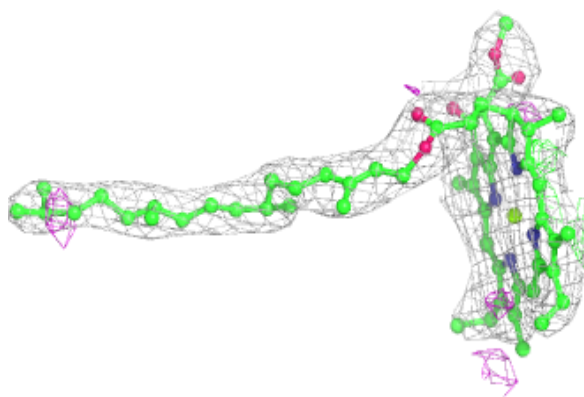
**Electron density around BCR Z 844:**

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

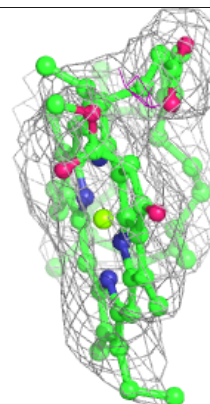
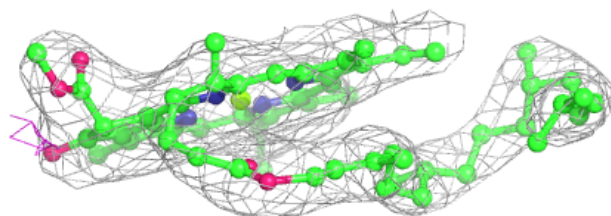
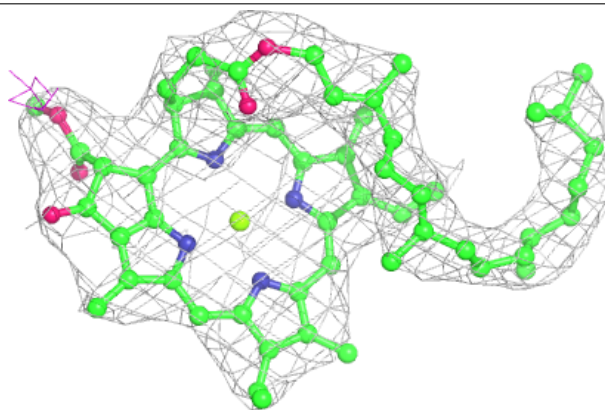


Electron density around CLA B 828:

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

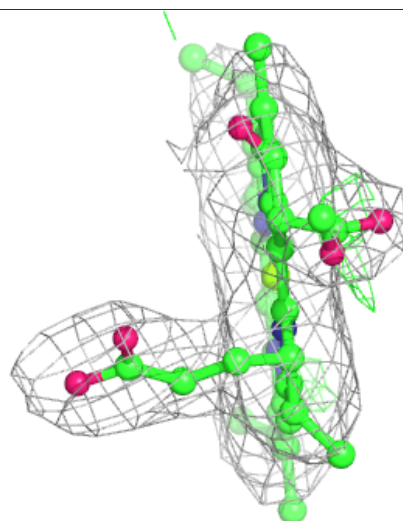
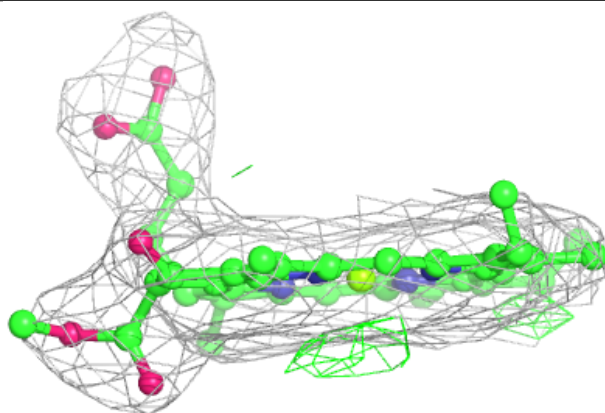
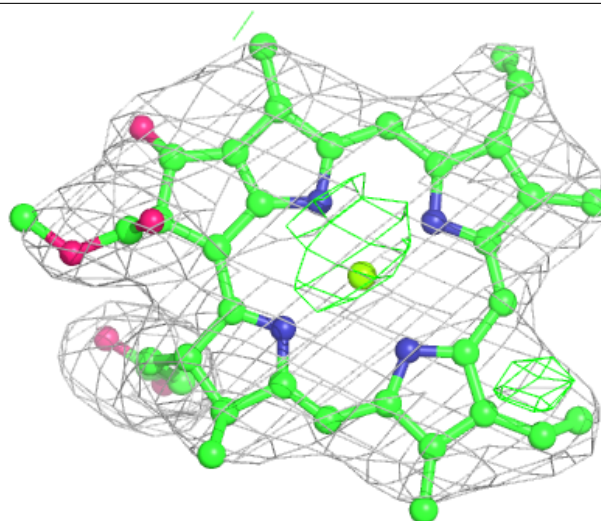
**Electron density around CLA G 819:**

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



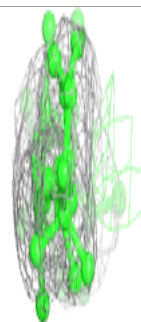
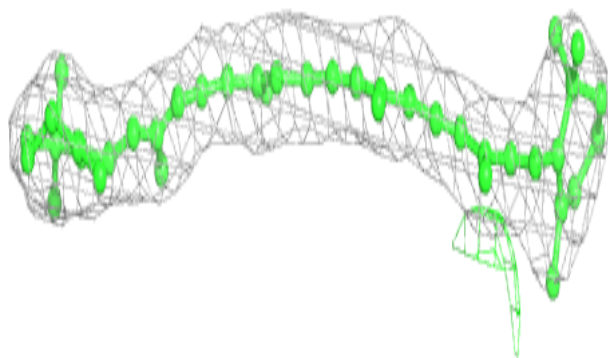
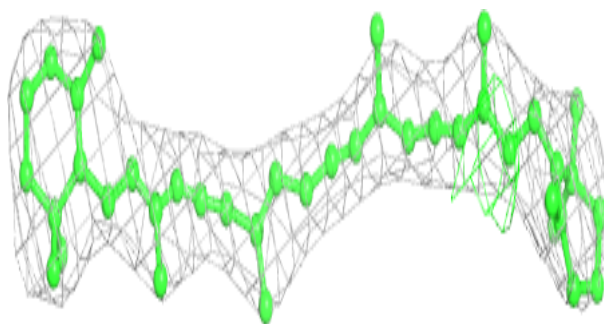
Electron density around CLA B 835:

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

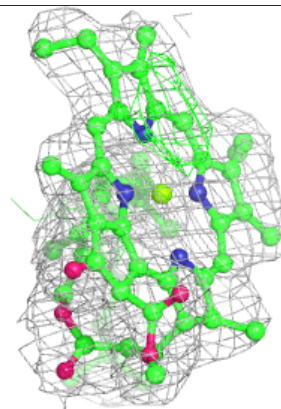
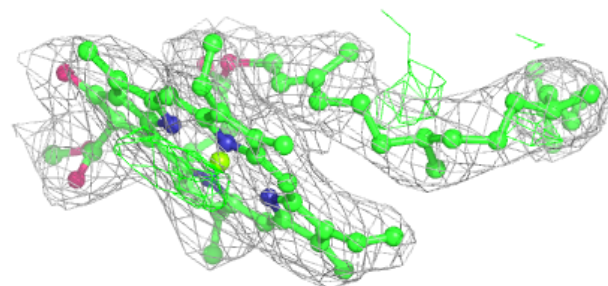
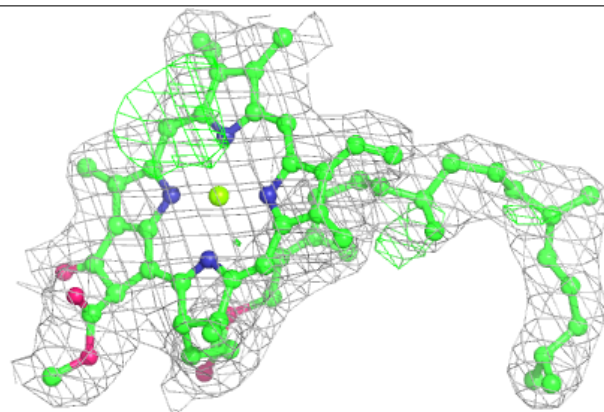


Electron density around BCR H 848:

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

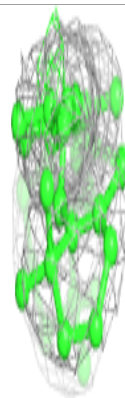
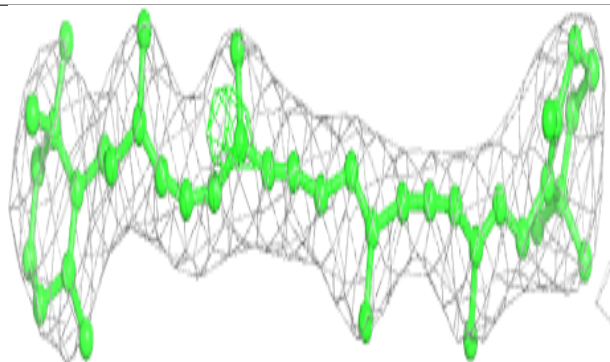
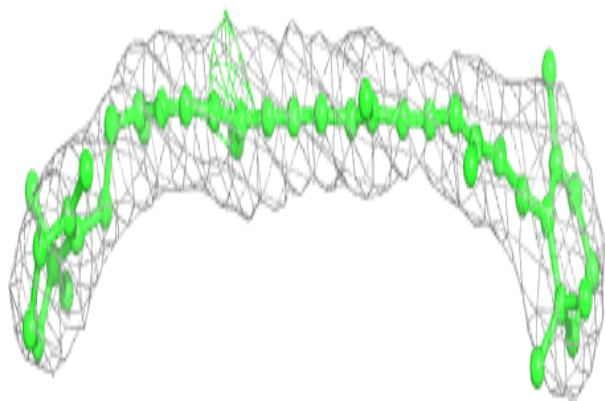
**Electron density around CLA G 842:**

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



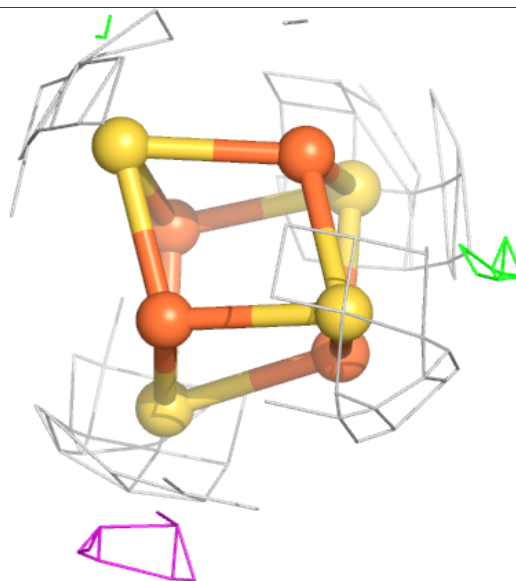
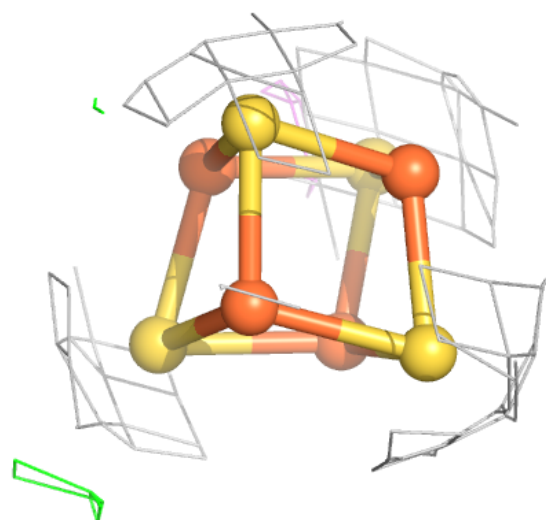
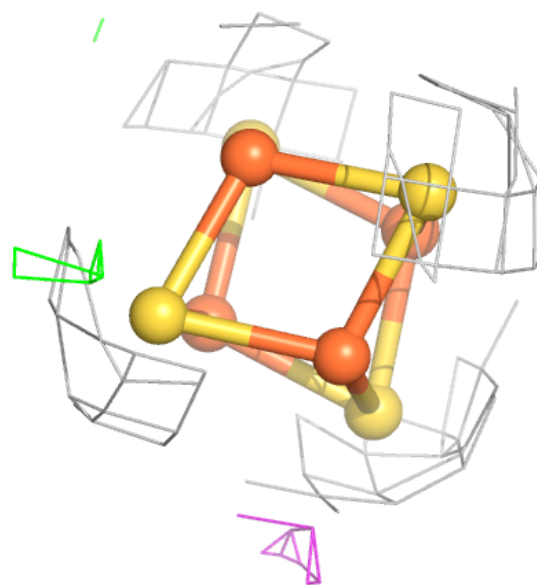
Electron density around BCR K 102:

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



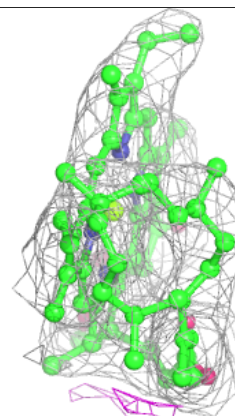
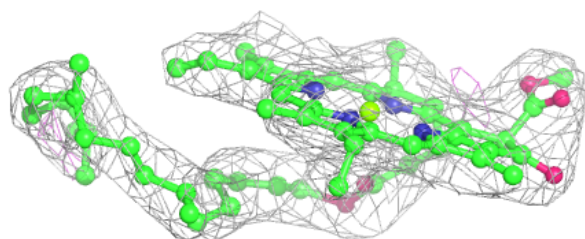
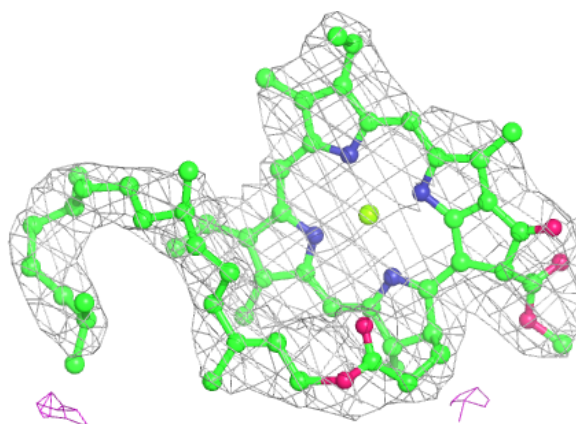
Electron density around SF4 G 845:

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

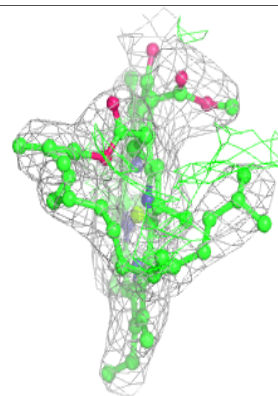
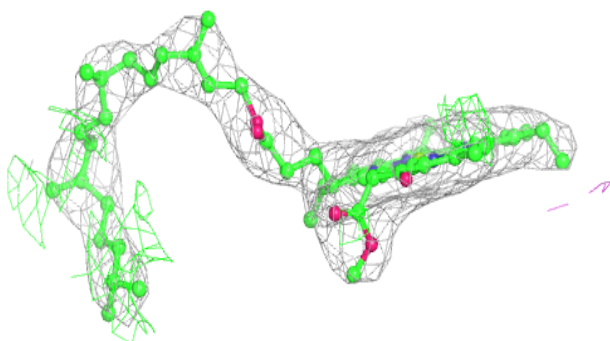
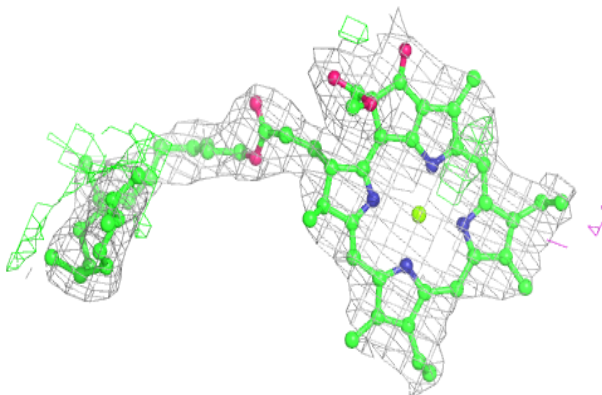


Electron density around CLA Y 819:

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

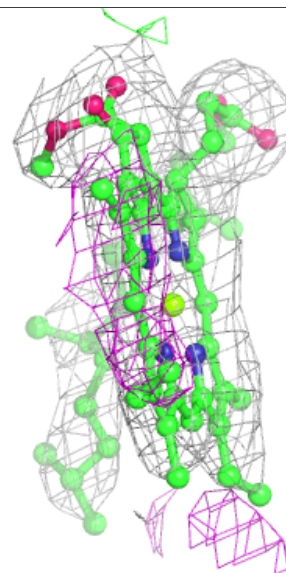
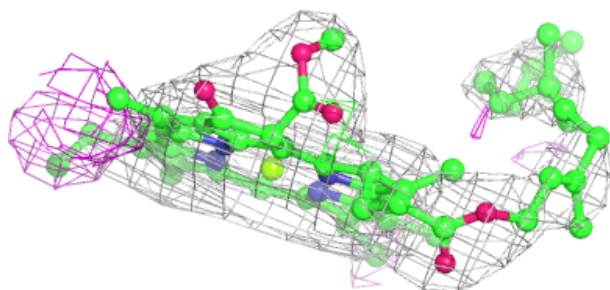
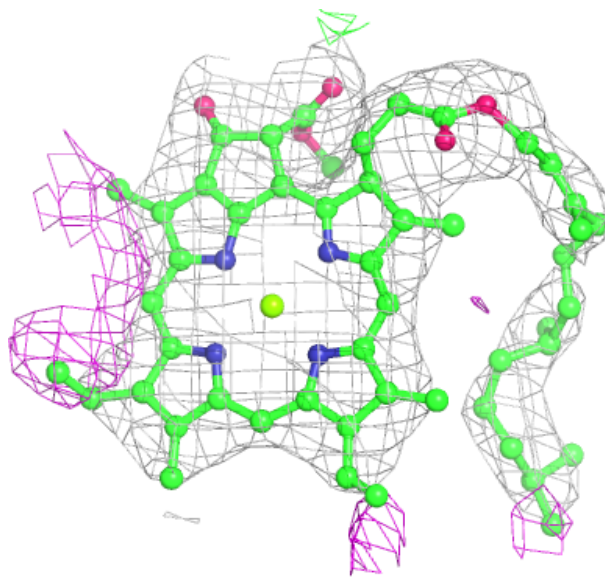
**Electron density around CLA G 827:**

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



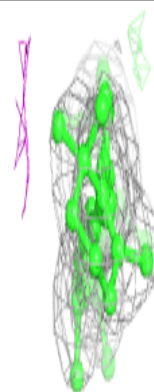
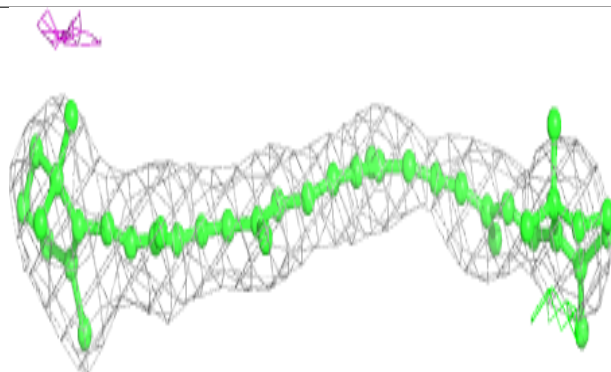
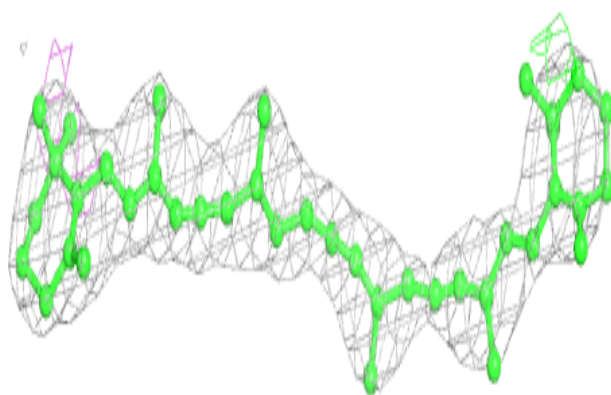
Electron density around CLA A 813:

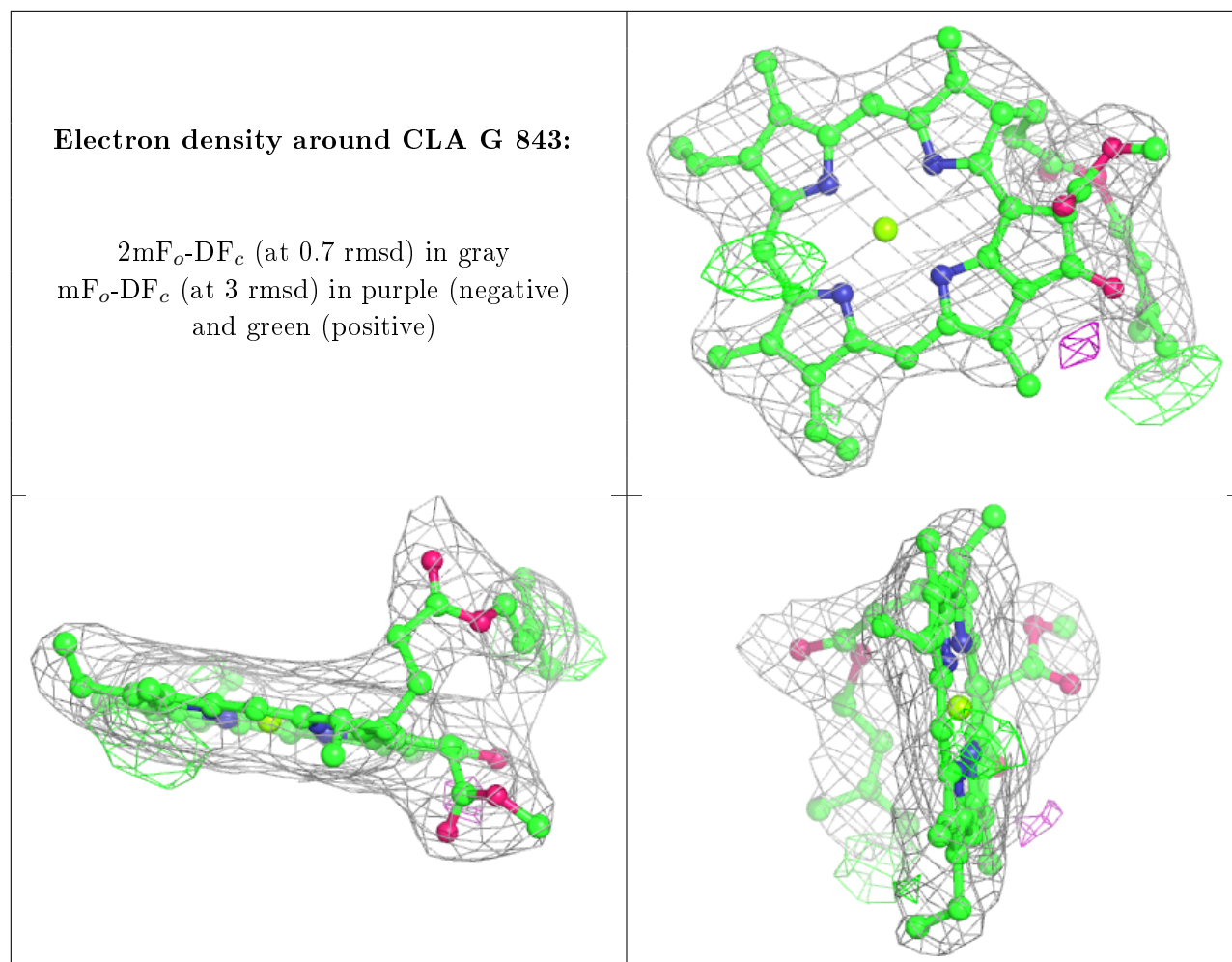
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BCR Y 849:

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





6.5 Other polymers [i](#)

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