



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 05:29 AM BST

PDB ID : 6PFY  
Title : Membrane Protein Megahertz Crystallography at the European XFEL, Photosystem I at synchrotron to 2.9 Å  
Authors : Fromme, R.  
Deposited on : 2019-06-23  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
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) : 2.13

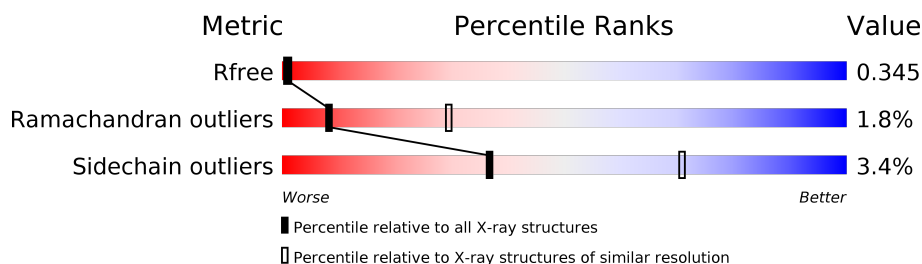
# 1 Overall quality at a glance

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)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

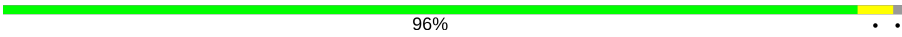
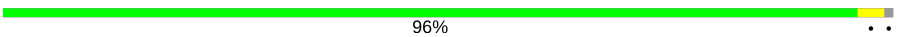








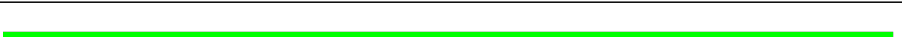


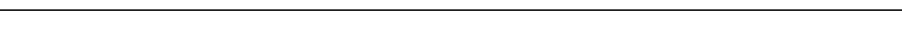

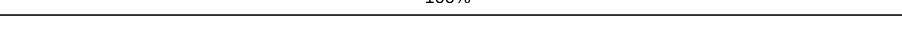
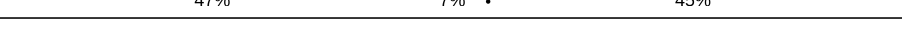

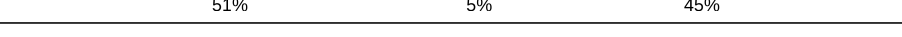
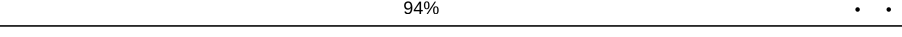
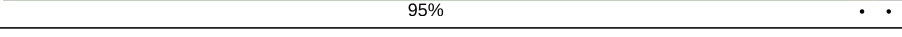
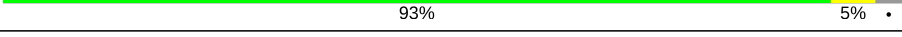
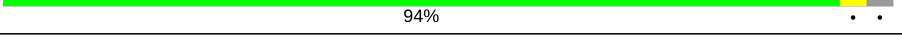
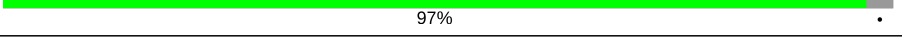
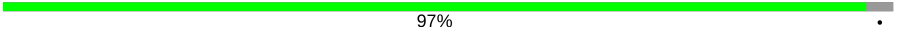
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria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

Mol	Chain	Length	Quality of chain
1	A	755	94% . .
1	G	755	95% . .
1	Y	755	93% 5% .
2	B	741	95% .
2	H	741	96% .
2	Z	741	95% .
3	C	81	96% . .
3	N	81	91% 7% .
3	a	81	93% 6% .

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Mol	Chain	Length	Quality of chain
4	D	139	 96% . .
4	O	139	 96% . .
4	b	139	 91% 8% .
5	E	76	 86% 5% 9%
5	P	76	 83% 8% 9%
5	c	76	 86% 5% 9%
6	F	164	 83% . 14%
6	Q	164	 83% . 14%
6	d	164	 79% 6% . 14%
7	I	38	 95% 5%
7	R	38	 100%
7	e	38	 97% .
8	J	41	 98% .
8	S	41	 98% .
8	f	41	 100%
9	K	83	 47% 7% . 45%
9	T	83	 52% . 45%
9	g	83	 51% 5% 45%
10	L	155	 94% . .
10	U	155	 95% . .
10	h	155	 93% 5% .
11	M	31	 94% . .
11	V	31	 97% .
11	i	31	 97% .
12	W	39	 67% 33%

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Mol	Chain	Length	Quality of chain
12	X	39	
12	j	39	

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	-	-	-
14	CLA	A	829	X	-	-	-
14	CLA	A	830	X	-	-	-
14	CLA	A	831	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	839	X	-	-	-
14	CLA	A	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	842	X	-	-	-
14	CLA	A	843	X	-	-	-
14	CLA	A	854	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	-	-	-
14	CLA	B	828	X	-	-	-
14	CLA	B	829	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	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	-	-	-
14	CLA	G	829	X	-	-	-
14	CLA	G	830	X	-	-	-
14	CLA	G	831	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	852	X	-	-	-
14	CLA	G	853	X	-	-	-
14	CLA	H	801	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	-	-	-
14	CLA	H	827	X	-	-	-
14	CLA	H	828	X	-	-	-
14	CLA	H	829	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	H	839	X	-	-	-
14	CLA	H	840	X	-	-	-
14	CLA	H	851	X	-	-	-
14	CLA	J	101	X	-	-	-
14	CLA	J	102	X	-	-	-
14	CLA	K	101	X	-	-	-
14	CLA	K	102	X	-	-	-
14	CLA	L	201	X	-	-	-
14	CLA	L	202	X	-	-	-
14	CLA	L	204	X	-	-	-
14	CLA	L	205	X	-	-	-
14	CLA	L	206	X	-	-	-
14	CLA	Q	202	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	U	1007	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	-	-	-
14	CLA	Y	809	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	Z	801	X	-	-	-
14	CLA	Z	802	X	-	-	-
14	CLA	Z	803	X	-	-	-
14	CLA	Z	804	X	-	-	-
14	CLA	Z	805	X	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	Z	840	X	-	-	-
14	CLA	Z	841	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	204	X	-	-	-
14	CLA	h	205	X	-	-	-
14	CLA	h	206	X	-	-	-
14	CLA	j	102	X	-	-	-



## 2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 72737 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

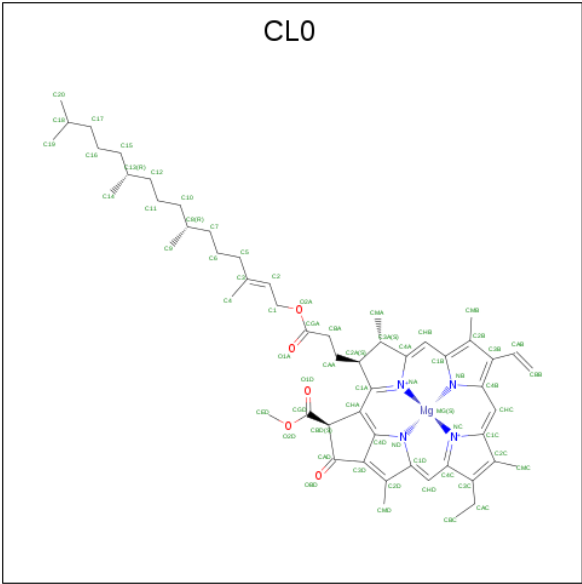
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

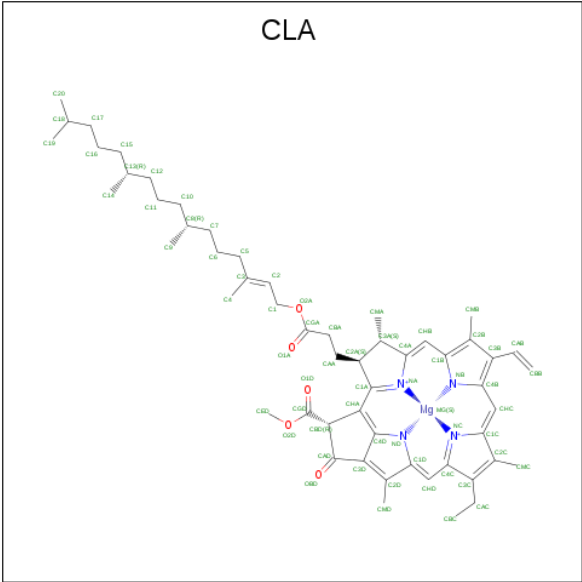
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	M	30	Total	C	N	O	0	0	0
			233	156	35	42			
11	V	30	Total	C	N	O	0	0	0
			233	156	35	42			
11	i	30	Total	C	N	O	0	0	0
			233	156	35	42			

- 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: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (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
			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
			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		

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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
			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
			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
			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 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	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 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 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	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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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
			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
			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 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 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	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 54	C 44	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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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
			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
			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
			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		

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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
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	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	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

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

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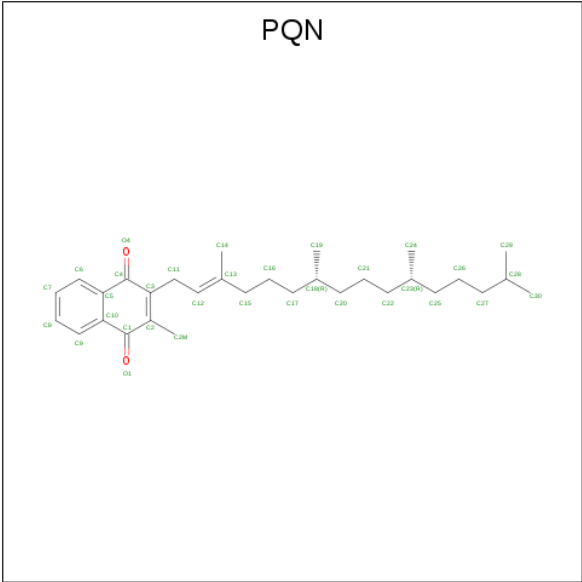
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
14	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
14	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
14	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
14	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
14	Z	1	Total 45	C 35	Mg 1	N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

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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
			65	55	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: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by author).



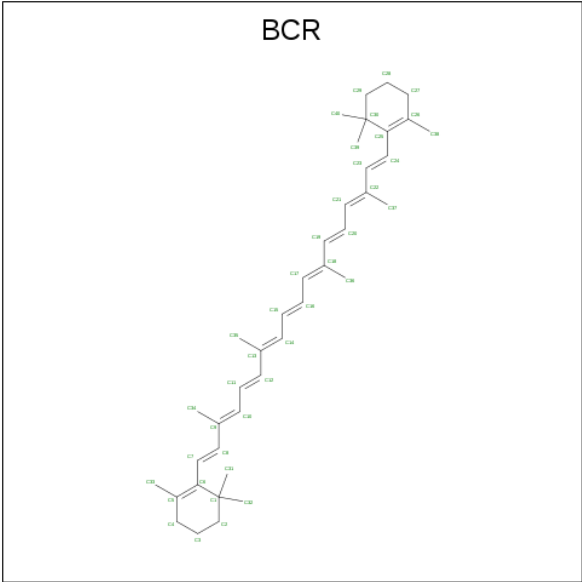
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	A	1	Total	C	O	0	0
			33	31	2		
15	B	1	Total	C	O	0	0
			33	31	2		
15	G	1	Total	C	O	0	0
			33	31	2		
15	H	1	Total	C	O	0	0
			33	31	2		
15	Y	1	Total	C	O	0	0
			33	31	2		
15	Z	1	Total	C	O	0	0
			33	31	2		

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (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: C<sub>40</sub>H<sub>56</sub>) (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	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	F	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	F	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	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	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
17	Q	1	Total C 40 40	0	0

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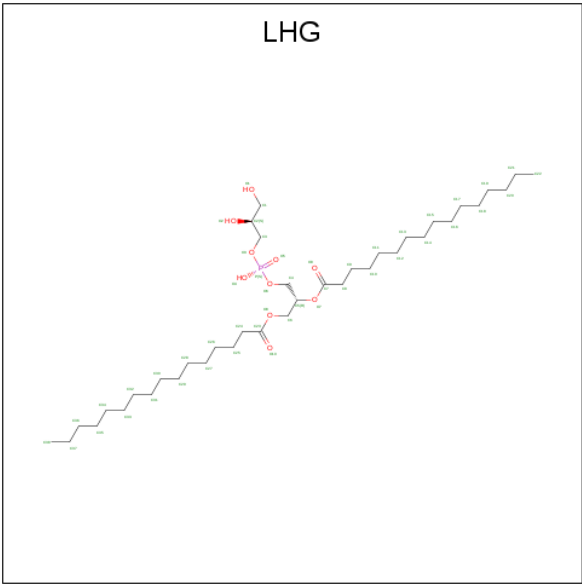
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	Q	1	Total C 40 40	0	0
17	R	1	Total C 40 40	0	0
17	R	1	Total C 40 40	0	0
17	S	1	Total C 40 40	0	0
17	S	1	Total C 40 40	0	0
17	T	1	Total C 40 40	0	0
17	U	1	Total C 40 40	0	0
17	U	1	Total C 40 40	0	0
17	U	1	Total C 40 40	0	0
17	V	1	Total C 40 40	0	0
17	Y	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	Z	1	Total C 25 25	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	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	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: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by author).



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

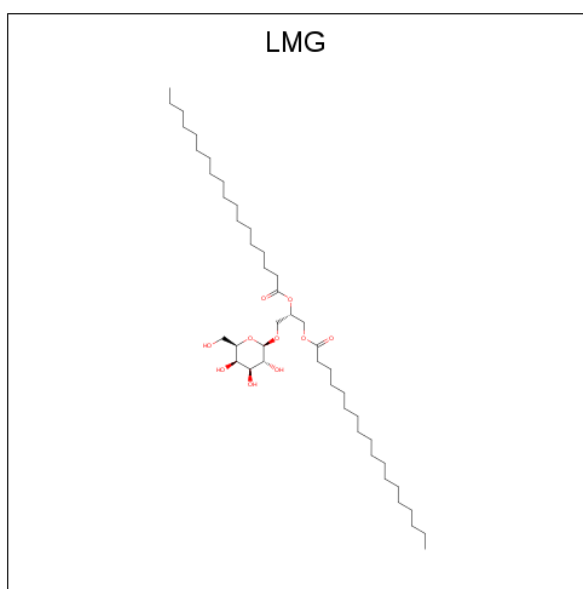
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			32	21	10	1		
18	B	1	Total	C	O	P	0	0
			39	28	10	1		
18	G	1	Total	C	O	P	0	0
			49	38	10	1		
18	G	1	Total	C	O	P	0	0
			32	21	10	1		
18	H	1	Total	C	O	P	0	0
			37	26	10	1		
18	Y	1	Total	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<sub>45</sub>H<sub>86</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by author).



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) (labeled as "Ligand of Interest" by author).

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	23	Total O 23 23	0	0
21	B	20	Total O 20 20	0	0
21	C	7	Total O 7 7	0	0
21	D	15	Total O 15 15	0	0
21	E	6	Total O 6 6	0	0
21	F	7	Total O 7 7	0	0
21	G	32	Total O 32 32	0	0
21	H	38	Total O 38 38	0	0
21	J	3	Total O 3 3	0	0
21	K	2	Total O 2 2	0	0
21	L	4	Total O 4 4	0	0
21	M	1	Total O 1 1	0	0
21	N	2	Total O 2 2	0	0
21	O	7	Total O 7 7	0	0
21	P	3	Total O 3 3	0	0

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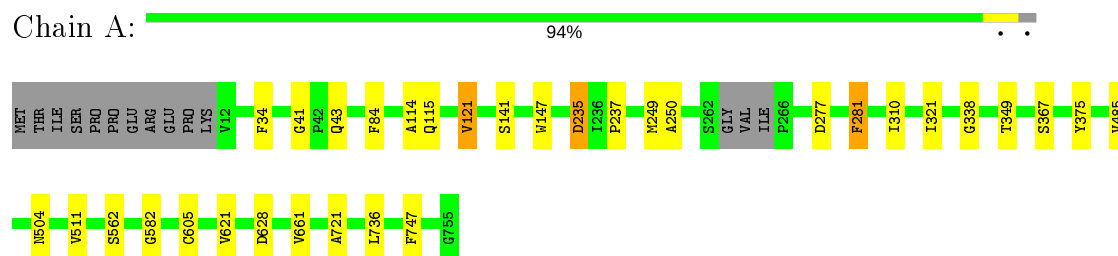
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	Q	7	Total 7	O 7	0	0
21	S	2	Total 2	O 2	0	0
21	T	1	Total 1	O 1	0	0
21	U	9	Total 9	O 9	0	0
21	V	2	Total 2	O 2	0	0
21	W	3	Total 3	O 3	0	0
21	X	2	Total 2	O 2	0	0
21	Y	24	Total 24	O 24	0	0
21	Z	21	Total 21	O 21	0	0
21	a	4	Total 4	O 4	0	0
21	b	6	Total 6	O 6	0	0
21	c	4	Total 4	O 4	0	0
21	d	7	Total 7	O 7	0	0
21	f	5	Total 5	O 5	0	0
21	g	2	Total 2	O 2	0	0
21	h	4	Total 4	O 4	0	0
21	i	1	Total 1	O 1	0	0
21	j	2	Total 2	O 2	0	0

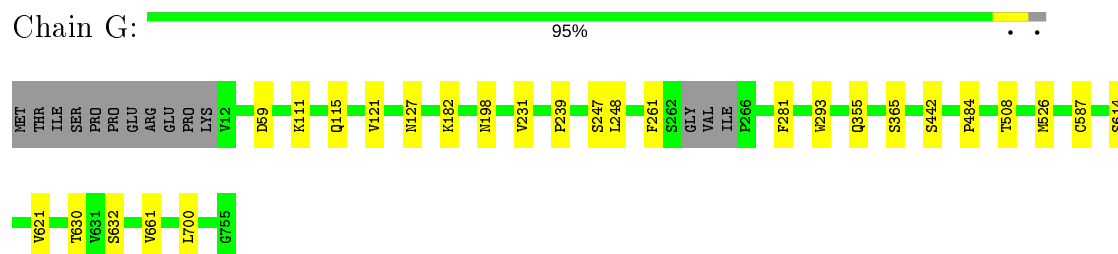
### 3 Residue-property plots

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

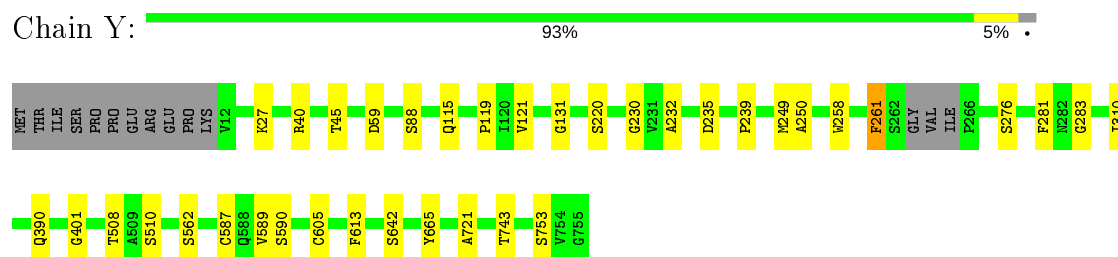
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



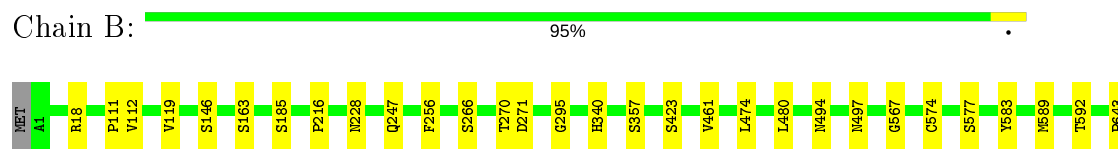
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



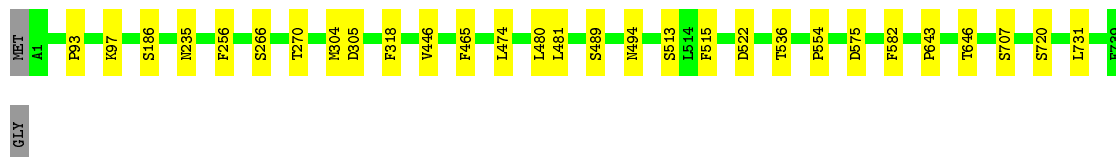
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





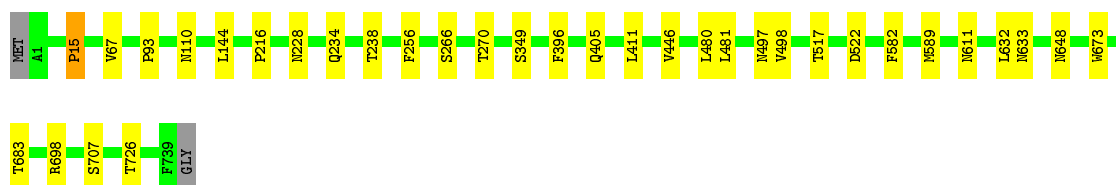
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain H: 96% .



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain Z: 95% .



- Molecule 3: Photosystem I iron-sulfur center

Chain C: 96% ..



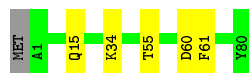
- Molecule 3: Photosystem I iron-sulfur center

Chain N: 91% 7% .



- Molecule 3: Photosystem I iron-sulfur center

Chain a: 93% 6% .



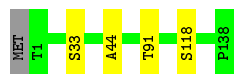
- Molecule 4: Photosystem I reaction center subunit II

Chain D: 96% ..




- Molecule 4: Photosystem I reaction center subunit II

Chain O:  96% ..




- Molecule 4: Photosystem I reaction center subunit II

Chain b:  91% .




- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  86% 5% 9%




- Molecule 5: Photosystem I reaction center subunit IV

Chain P:  83% 8% 9%




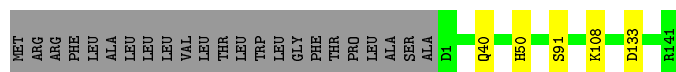
- Molecule 5: Photosystem I reaction center subunit IV

Chain c:  86% 5% 9%




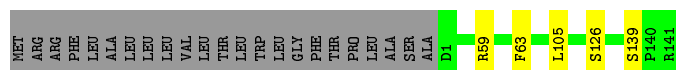
- Molecule 6: Photosystem I reaction center subunit III

Chain F:  83% . 14%




- Molecule 6: Photosystem I reaction center subunit III

Chain Q:  83% . 14%



- Molecule 6: Photosystem I reaction center subunit III

Chain d:  79% 6% • 14%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:  95% 5%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain R:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Photosystem I reaction center subunit VIII

Chain e:  97% •



- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  98% •



- Molecule 8: Photosystem I reaction center subunit IX

Chain S:  98% •



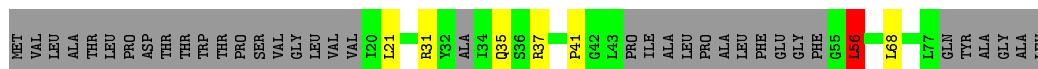
- Molecule 8: Photosystem I reaction center subunit IX

Chain f:  100%

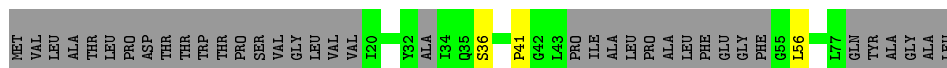
There are no outlier residues recorded for this chain.

- Molecule 9: Photosystem I reaction center subunit PsaK

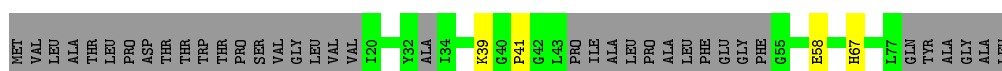
Chain K:  47% 7% • 45%



- Molecule 9: Photosystem I reaction center subunit PsaK



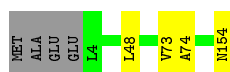
- Molecule 9: Photosystem I reaction center subunit PsaK



- 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



- Molecule 11: Photosystem I reaction center subunit XII







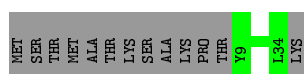
- Molecule 11: Photosystem I reaction center subunit XII

Chain i: 97%



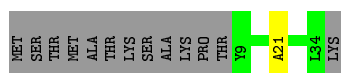
- Molecule 12: Photosystem I 4.8K protein

Chain W: 67% 33%



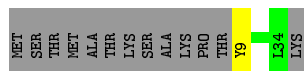
- Molecule 12: Photosystem I 4.8K protein

Chain X: 64% 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, $\alpha$ , $\beta$ , $\gamma$	278.50Å 165.13Å 283.43Å 90.00° 119.42° 90.00°	Depositor
Resolution (Å)	48.87 – 2.90 48.87 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.87-2.90) 93.9 (48.87-2.90)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.303 , 0.343 0.307 , 0.345	Depositor DCC
$R_{free}$ test set	24873 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.7	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 22.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.31$ , $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	0.247 for -h-l,k,h 0.247 for l,k,-h-l 0.177 for h,-k,-h-l 0.176 for -h-l,-k,l 0.176 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	72737	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, 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	0.67	0/5990	0.77	0/8168
1	G	0.68	0/5990	0.76	0/8168
1	Y	0.68	0/5990	0.77	0/8168
2	B	0.66	0/6107	0.78	0/8345
2	H	0.67	0/6107	0.78	0/8345
2	Z	0.66	0/6107	0.74	0/8345
3	C	0.70	0/608	0.84	0/824
3	N	0.72	0/608	0.83	0/824
3	a	0.69	0/608	0.84	0/824
4	D	0.65	0/1101	0.79	0/1492
4	O	0.66	0/1101	0.79	0/1492
4	b	0.66	0/1101	0.82	0/1492
5	E	0.67	0/551	0.81	0/750
5	P	0.70	0/551	0.82	0/750
5	c	0.69	0/551	0.78	0/750
6	F	0.68	0/1087	0.79	0/1476
6	Q	0.69	0/1087	0.80	0/1476
6	d	0.68	0/1087	0.79	0/1476
7	I	0.66	0/312	0.75	0/425
7	R	0.69	0/312	0.77	0/425
7	e	0.66	0/312	0.74	0/425
8	J	0.64	0/350	0.69	0/477
8	S	0.65	0/350	0.70	0/477
8	f	0.67	0/350	0.73	0/477
9	K	0.70	0/331	0.81	0/444
9	T	0.75	0/331	0.84	0/444
9	g	0.73	0/331	0.81	0/444
10	L	0.71	0/1148	0.79	0/1558
10	U	0.71	0/1148	0.78	0/1558
10	h	0.70	0/1148	0.78	0/1558
11	M	0.68	0/236	0.75	0/322
11	V	0.69	0/236	0.80	0/322

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
11	i	0.71	0/236	0.76	0/322
12	W	0.69	0/227	0.71	0/310
12	X	0.66	0/227	0.72	0/310
12	j	0.63	0/227	0.63	0/310
All	All	0.67	0/54144	0.77	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
2	Z	0	1
3	N	0	1
3	a	0	1
5	P	0	1
9	K	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	K	56	LEU	Peptide
3	N	60	ASP	Peptide
5	P	53	SER	Peptide
2	Z	673	TRP	Peptide
3	a	60	ASP	Peptide

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	644 (87%)	74 (10%)	19 (3%)	5	20
1	G	737/755 (98%)	654 (89%)	70 (10%)	13 (2%)	8	29
1	Y	737/755 (98%)	642 (87%)	77 (10%)	18 (2%)	6	22
2	B	737/741 (100%)	633 (86%)	95 (13%)	9 (1%)	13	40
2	H	737/741 (100%)	643 (87%)	87 (12%)	7 (1%)	17	48
2	Z	737/741 (100%)	649 (88%)	79 (11%)	9 (1%)	13	40
3	C	78/81 (96%)	70 (90%)	6 (8%)	2 (3%)	5	20
3	N	78/81 (96%)	67 (86%)	9 (12%)	2 (3%)	5	20
3	a	78/81 (96%)	70 (90%)	7 (9%)	1 (1%)	12	37
4	D	136/139 (98%)	119 (88%)	13 (10%)	4 (3%)	4	18
4	O	136/139 (98%)	123 (90%)	12 (9%)	1 (1%)	22	54
4	b	136/139 (98%)	123 (90%)	9 (7%)	4 (3%)	4	18
5	E	67/76 (88%)	56 (84%)	8 (12%)	3 (4%)	2	9
5	P	67/76 (88%)	56 (84%)	8 (12%)	3 (4%)	2	9
5	c	67/76 (88%)	57 (85%)	7 (10%)	3 (4%)	2	9
6	F	139/164 (85%)	115 (83%)	23 (16%)	1 (1%)	22	54
6	Q	139/164 (85%)	125 (90%)	13 (9%)	1 (1%)	22	54
6	d	139/164 (85%)	113 (81%)	19 (14%)	7 (5%)	2	7
7	I	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	5	19
7	R	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
7	e	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	5	19
8	J	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
8	S	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
8	f	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
9	K	40/83 (48%)	30 (75%)	8 (20%)	2 (5%)	2	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	T	40/83 (48%)	33 (82%)	5 (12%)	2 (5%)	2	7
9	g	40/83 (48%)	31 (78%)	7 (18%)	2 (5%)	2	7
10	L	149/155 (96%)	133 (89%)	16 (11%)	0	100	100
10	U	149/155 (96%)	130 (87%)	17 (11%)	2 (1%)	12	37
10	h	149/155 (96%)	133 (89%)	14 (9%)	2 (1%)	12	37
11	M	28/31 (90%)	25 (89%)	3 (11%)	0	100	100
11	V	28/31 (90%)	28 (100%)	0	0	100	100
11	i	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
12	W	24/39 (62%)	23 (96%)	1 (4%)	0	100	100
12	X	24/39 (62%)	23 (96%)	0	1 (4%)	3	10
12	j	24/39 (62%)	24 (100%)	0	0	100	100
All	All	6630/7029 (94%)	5805 (88%)	705 (11%)	120 (2%)	8	29

5 of 120 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	VAL
1	A	250	ALA
3	C	61	PHE
4	D	95	HIS
5	E	55	VAL

### 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%)	573 (97%)	17 (3%)	42	76
1	G	590/603 (98%)	576 (98%)	14 (2%)	49	79
1	Y	590/603 (98%)	570 (97%)	20 (3%)	37	71
2	B	597/598 (100%)	573 (96%)	24 (4%)	31	65
2	H	597/598 (100%)	575 (96%)	22 (4%)	34	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Z	597/598 (100%)	572 (96%)	25 (4%)	30	63
3	C	67/68 (98%)	67 (100%)	0	100	100
3	N	67/68 (98%)	64 (96%)	3 (4%)	27	61
3	a	67/68 (98%)	64 (96%)	3 (4%)	27	61
4	D	115/116 (99%)	114 (99%)	1 (1%)	78	93
4	O	115/116 (99%)	112 (97%)	3 (3%)	46	77
4	b	115/116 (99%)	108 (94%)	7 (6%)	18	48
5	E	59/65 (91%)	58 (98%)	1 (2%)	60	86
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%)	105 (96%)	4 (4%)	34	68
6	Q	109/128 (85%)	105 (96%)	4 (4%)	34	68
6	d	109/128 (85%)	104 (95%)	5 (5%)	27	60
7	I	32/32 (100%)	31 (97%)	1 (3%)	40	74
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%)	35 (97%)	1 (3%)	43	76
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%)	27 (82%)	6 (18%)	1	5
9	T	33/61 (54%)	32 (97%)	1 (3%)	41	75
9	g	33/61 (54%)	31 (94%)	2 (6%)	18	48
10	L	117/120 (98%)	111 (95%)	6 (5%)	24	56
10	U	117/120 (98%)	115 (98%)	2 (2%)	60	86
10	h	117/120 (98%)	112 (96%)	5 (4%)	29	62
11	M	25/26 (96%)	24 (96%)	1 (4%)	31	65
11	V	25/26 (96%)	25 (100%)	0	100	100
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%)	20 (100%)	0	100	100
12	j	20/31 (64%)	19 (95%)	1 (5%)	24	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5400/5652 (96%)	5216 (97%)	184 (3%)	37 71

5 of 184 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	I	24	THR
4	O	91	THR
6	d	89	ARG
9	K	21	LEU
10	L	41	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	298	HIS
10	L	9	ASN
2	Z	688	HIS
2	H	319	ASN
2	H	604	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 monosaccharides 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	A	827	-	54,68,73	2.18	15 (27%)	61,107,113	2.19	21 (34%)
19	LMG	B	848	-	52,52,55	1.42	7 (13%)	60,60,63	1.36	7 (11%)
14	CLA	A	832	-	44,58,73	2.38	15 (34%)	49,95,113	2.44	17 (34%)
14	CLA	H	825	-	59,73,73	2.18	16 (27%)	67,113,113	2.52	21 (31%)
14	CLA	Z	802	-	59,73,73	2.13	14 (23%)	67,113,113	2.30	17 (25%)
14	CLA	A	820	-	59,73,73	2.27	16 (27%)	67,113,113	2.16	18 (26%)
14	CLA	G	829	-	59,73,73	2.21	14 (23%)	67,113,113	2.01	19 (28%)
14	CLA	H	806	-	59,73,73	2.18	15 (25%)	67,113,113	2.09	18 (26%)
14	CLA	Y	841	-	59,73,73	2.02	13 (22%)	67,113,113	2.16	15 (22%)
14	CLA	H	835	-	36,53,73	2.68	13 (36%)	39,89,113	2.36	13 (33%)
14	CLA	B	803	-	48,62,73	2.37	16 (33%)	53,99,113	2.83	16 (30%)
14	CLA	B	838	-	36,53,73	2.76	13 (36%)	39,89,113	2.34	12 (30%)
14	CLA	L	205	-	59,73,73	2.24	16 (27%)	67,113,113	2.23	18 (26%)
14	CLA	A	815	-	44,58,73	2.60	15 (34%)	49,95,113	2.47	20 (40%)
14	CLA	L	204	-	59,73,73	2.13	15 (25%)	67,113,113	2.15	16 (23%)
14	CLA	W	1701	-	36,53,73	2.71	14 (38%)	39,89,113	2.61	12 (30%)
14	CLA	B	840	-	59,73,73	2.14	12 (20%)	67,113,113	2.24	25 (37%)
14	CLA	B	815	-	49,63,73	2.43	15 (30%)	55,101,113	2.25	13 (23%)
14	CLA	Z	835	-	36,53,73	2.76	14 (38%)	39,89,113	2.28	12 (30%)
17	BCR	M	101	-	41,41,41	2.75	8 (19%)	56,56,56	7.14	28 (50%)
14	CLA	Y	832	-	59,73,73	2.09	14 (23%)	67,113,113	2.35	21 (31%)
14	CLA	G	853	-	36,53,73	2.59	13 (36%)	39,89,113	2.20	13 (33%)
18	LHG	Y	851	14	24,24,48	1.56	2 (8%)	27,30,54	1.44	2 (7%)
14	CLA	H	837	-	59,73,73	2.30	16 (27%)	67,113,113	2.11	18 (26%)
17	BCR	L	208	-	41,41,41	2.65	7 (17%)	56,56,56	7.07	31 (55%)
14	CLA	G	818	-	59,73,73	2.09	14 (23%)	67,113,113	2.48	22 (32%)
14	CLA	Y	810	-	36,53,73	2.72	15 (41%)	39,89,113	2.26	15 (38%)
14	CLA	H	820	-	36,53,73	2.56	12 (33%)	39,89,113	2.66	16 (41%)
14	CLA	L	201	-	59,73,73	2.11	13 (22%)	67,113,113	2.22	20 (29%)
14	CLA	B	806	-	59,73,73	2.09	16 (27%)	67,113,113	2.34	20 (29%)
14	CLA	B	824	-	59,73,73	2.13	14 (23%)	67,113,113	2.29	20 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	A	808	-	45,59,73	2.47	15 (33%)	50,96,113	2.66	15 (30%)
14	CLA	f	101	8	36,53,73	2.75	16 (44%)	39,89,113	2.59	13 (33%)
17	BCR	B	846	-	41,41,41	2.83	7 (17%)	56,56,56	7.13	28 (50%)
14	CLA	Z	819	-	54,68,73	2.24	14 (25%)	61,107,113	2.26	17 (27%)
17	BCR	Y	849	-	41,41,41	3.03	6 (14%)	56,56,56	7.35	29 (51%)
14	CLA	G	826	-	54,68,73	2.28	15 (27%)	61,107,113	2.38	18 (29%)
14	CLA	H	810	2	59,73,73	2.16	13 (22%)	67,113,113	2.49	25 (37%)
14	CLA	A	818	-	54,68,73	2.27	14 (25%)	61,107,113	2.32	19 (31%)
14	CLA	A	814	-	54,68,73	2.27	15 (27%)	61,107,113	2.32	19 (31%)
14	CLA	G	842	18	44,58,73	2.43	15 (34%)	49,95,113	2.63	17 (34%)
17	BCR	R	102	-	41,41,41	2.89	6 (14%)	56,56,56	7.11	25 (44%)
14	CLA	Z	831	-	36,53,73	2.52	15 (41%)	39,89,113	2.51	15 (38%)
17	BCR	Y	845	-	41,41,41	2.73	6 (14%)	56,56,56	7.17	28 (50%)
14	CLA	B	817	-	54,68,73	2.27	16 (29%)	61,107,113	2.13	15 (24%)
14	CLA	Z	832	-	36,53,73	2.51	13 (36%)	39,89,113	2.62	16 (41%)
14	CLA	A	810	-	59,73,73	2.17	14 (23%)	67,113,113	2.13	16 (23%)
17	BCR	I	101	-	41,41,41	2.85	7 (17%)	56,56,56	7.49	22 (39%)
14	CLA	B	826	-	59,73,73	2.06	14 (23%)	67,113,113	1.84	14 (20%)
14	CLA	A	840	-	44,58,73	2.54	16 (36%)	49,95,113	2.55	17 (34%)
14	CLA	B	809	-	59,73,73	2.15	14 (23%)	67,113,113	2.38	21 (31%)
14	CLA	H	809	2	59,73,73	2.05	16 (27%)	67,113,113	2.41	24 (35%)
15	PQN	A	844	-	34,34,34	1.60	2 (5%)	42,45,45	1.18	4 (9%)
14	CLA	Z	805	-	48,62,73	2.21	14 (29%)	53,99,113	2.70	19 (35%)
14	CLA	Z	812	-	49,63,73	2.38	15 (30%)	55,101,113	2.28	18 (32%)
17	BCR	Q	203	-	41,41,41	2.59	6 (14%)	56,56,56	7.18	27 (48%)
14	CLA	A	838	-	44,58,73	2.56	15 (34%)	49,95,113	2.67	22 (44%)
17	BCR	U	1008	-	41,41,41	2.72	6 (14%)	56,56,56	7.03	26 (46%)
14	CLA	Z	817	-	49,63,73	2.36	14 (28%)	55,101,113	2.50	17 (30%)
14	CLA	A	805	14	53,67,73	2.34	16 (30%)	59,105,113	2.37	17 (28%)
14	CLA	A	812	14	59,73,73	2.08	14 (23%)	67,113,113	2.32	18 (26%)
14	CLA	h	201	-	59,73,73	2.14	14 (23%)	67,113,113	2.13	17 (25%)
16	SF4	C	102	3,21	0,12,12	0.00	-	-	-	-
14	CLA	H	807	-	59,73,73	2.09	15 (25%)	67,113,113	2.22	18 (26%)
14	CLA	Y	833	-	49,63,73	2.49	15 (30%)	55,101,113	2.33	17 (30%)
14	CLA	B	836	-	54,68,73	2.28	13 (24%)	61,107,113	2.32	21 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	PQN	H	841	-	34,34,34	1.67	2 (5%)	42,45,45	1.19	4 (9%)
14	CLA	Y	838	-	59,73,73	2.27	14 (23%)	67,113,113	2.28	16 (23%)
14	CLA	G	812	-	48,62,73	2.43	15 (31%)	53,99,113	2.32	19 (35%)
17	BCR	Z	844	-	41,41,41	2.66	6 (14%)	56,56,56	7.02	30 (53%)
14	CLA	J	101	8	36,53,73	2.67	14 (38%)	39,89,113	2.33	13 (33%)
14	CLA	S	1103	-	49,63,73	2.41	15 (30%)	55,101,113	2.56	19 (34%)
14	CLA	Z	824	-	54,68,73	2.36	15 (27%)	61,107,113	2.02	18 (29%)
14	CLA	Z	809	-	59,73,73	2.11	15 (25%)	67,113,113	2.50	24 (35%)
14	CLA	G	819	-	59,73,73	2.19	15 (25%)	67,113,113	2.26	17 (25%)
14	CLA	B	816	-	59,73,73	2.15	15 (25%)	67,113,113	2.20	18 (26%)
14	CLA	Z	826	-	59,73,73	2.14	15 (25%)	67,113,113	2.39	20 (29%)
14	CLA	G	836	-	44,58,73	2.61	15 (34%)	49,95,113	2.64	19 (38%)
17	BCR	G	847	-	41,41,41	2.70	6 (14%)	56,56,56	7.20	29 (51%)
16	SF4	a	101	3	0,12,12	0.00	-	-	-	-
13	CL0	G	801	-	59,73,73	2.42	15 (25%)	67,113,113	2.68	20 (29%)
13	CL0	A	801	-	59,73,73	2.23	14 (23%)	67,113,113	2.51	15 (22%)
17	BCR	F	203	-	41,41,41	2.80	7 (17%)	56,56,56	7.00	28 (50%)
14	CLA	h	205	-	59,73,73	2.24	15 (25%)	67,113,113	2.58	19 (28%)
14	CLA	A	828	-	59,73,73	2.10	15 (25%)	67,113,113	2.02	19 (28%)
13	CL0	Y	801	-	59,73,73	2.32	15 (25%)	67,113,113	2.40	17 (25%)
15	PQN	Y	842	-	34,34,34	1.77	2 (5%)	42,45,45	1.02	3 (7%)
14	CLA	A	843	18	44,58,73	2.54	16 (36%)	49,95,113	2.75	18 (36%)
17	BCR	A	848	-	41,41,41	2.63	6 (14%)	56,56,56	7.17	28 (50%)
14	CLA	B	830	-	36,53,73	2.60	14 (38%)	39,89,113	2.30	12 (30%)
14	CLA	Y	814	-	49,63,73	2.47	16 (32%)	55,101,113	2.29	16 (29%)
17	BCR	B	842	-	30,30,41	3.31	6 (20%)	39,39,56	8.17	20 (51%)
14	CLA	G	834	-	49,63,73	2.41	15 (30%)	55,101,113	2.12	20 (36%)
14	CLA	B	825	-	59,73,73	2.06	14 (23%)	67,113,113	2.32	18 (26%)
14	CLA	B	827	-	59,73,73	2.21	14 (23%)	67,113,113	2.05	15 (22%)
14	CLA	J	102	-	49,63,73	2.45	15 (30%)	55,101,113	2.55	20 (36%)
17	BCR	H	845	-	25,25,41	2.19	2 (8%)	33,33,56	8.00	18 (54%)
18	LHG	G	850	-	48,48,48	0.95	2 (4%)	51,54,54	1.16	5 (9%)
18	LHG	Y	850	-	48,48,48	1.03	2 (4%)	51,54,54	1.30	5 (9%)
14	CLA	H	827	-	59,73,73	2.02	13 (22%)	67,113,113	2.05	17 (25%)
14	CLA	Z	829	-	59,73,73	2.23	17 (28%)	67,113,113	2.21	20 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	G	840	-	59,73,73	2.21	14 (23%)	67,113,113	2.19	18 (26%)
14	CLA	A	813	-	48,62,73	2.43	15 (31%)	53,99,113	2.31	15 (28%)
14	CLA	G	824	-	54,68,73	2.40	15 (27%)	61,107,113	2.13	15 (24%)
14	CLA	Y	828	-	59,73,73	2.19	16 (27%)	67,113,113	2.09	17 (25%)
14	CLA	G	841	-	59,73,73	2.20	15 (25%)	67,113,113	2.13	18 (26%)
14	CLA	A	835	1	36,53,73	2.71	14 (38%)	39,89,113	2.48	13 (33%)
14	CLA	H	815	-	36,53,73	2.75	14 (38%)	39,89,113	2.53	16 (41%)
14	CLA	B	823	2	49,63,73	2.45	14 (28%)	55,101,113	2.34	16 (29%)
17	BCR	B	845	-	25,25,41	2.14	2 (8%)	33,33,56	7.99	14 (42%)
14	CLA	Y	827	-	59,73,73	2.25	16 (27%)	67,113,113	2.03	19 (28%)
14	CLA	Z	827	-	59,73,73	2.07	15 (25%)	67,113,113	2.27	18 (26%)
14	CLA	h	206	-	59,73,73	2.19	16 (27%)	67,113,113	2.25	18 (26%)
17	BCR	h	202	-	41,41,41	2.52	7 (17%)	56,56,56	7.11	29 (51%)
14	CLA	G	814	-	44,58,73	2.51	16 (36%)	49,95,113	2.80	24 (48%)
17	BCR	R	101	-	41,41,41	2.60	7 (17%)	56,56,56	7.50	23 (41%)
14	CLA	H	839	-	59,73,73	2.18	15 (25%)	67,113,113	2.24	19 (28%)
14	CLA	Y	811	14	59,73,73	2.26	14 (23%)	67,113,113	2.07	17 (25%)
14	CLA	G	813	-	54,68,73	2.29	15 (27%)	61,107,113	2.40	19 (31%)
14	CLA	G	804	14	53,67,73	2.30	15 (28%)	59,105,113	2.41	15 (25%)
14	CLA	Z	803	-	59,73,73	2.15	14 (23%)	67,113,113	2.24	20 (29%)
16	SF4	Y	843	1,2	0,12,12	0.00	-	-		
14	CLA	B	835	-	36,53,73	2.63	14 (38%)	39,89,113	2.43	13 (33%)
14	CLA	G	828	-	59,73,73	2.17	15 (25%)	67,113,113	2.15	19 (28%)
14	CLA	Y	806	-	59,73,73	2.24	13 (22%)	67,113,113	2.28	16 (23%)
14	CLA	A	817	-	44,58,73	2.60	15 (34%)	49,95,113	2.57	16 (32%)
17	BCR	A	851	-	41,41,41	2.81	7 (17%)	56,56,56	7.25	28 (50%)
14	CLA	H	831	-	59,73,73	2.09	15 (25%)	67,113,113	2.34	20 (29%)
14	CLA	G	837	-	59,73,73	2.15	15 (25%)	67,113,113	2.29	15 (22%)
14	CLA	g	102	-	36,53,73	2.74	13 (36%)	39,89,113	2.20	11 (28%)
14	CLA	A	833	-	59,73,73	2.04	15 (25%)	67,113,113	2.17	17 (25%)
14	CLA	A	839	-	59,73,73	2.09	15 (25%)	67,113,113	2.13	16 (23%)
17	BCR	S	1105	-	41,41,41	2.88	7 (17%)	56,56,56	7.33	29 (51%)
14	CLA	H	802	-	59,73,73	2.15	14 (23%)	67,113,113	2.41	18 (26%)
17	BCR	U	1009	-	41,41,41	2.46	7 (17%)	56,56,56	7.38	31 (55%)
14	CLA	Y	809	-	59,73,73	2.18	15 (25%)	67,113,113	1.99	18 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	BCR	Q	201	-	41,41,41	2.87	6 (14%)	56,56,56	7.00	27 (48%)
14	CLA	j	102	-	36,53,73	2.73	14 (38%)	39,89,113	2.37	11 (28%)
14	CLA	U	1006	-	59,73,73	2.28	14 (23%)	67,113,113	2.13	17 (25%)
14	CLA	B	808	2	59,73,73	2.05	13 (22%)	67,113,113	2.59	23 (34%)
14	CLA	h	204	10	59,73,73	2.16	14 (23%)	67,113,113	2.05	18 (26%)
14	CLA	Y	825	-	59,73,73	2.12	14 (23%)	67,113,113	2.11	18 (26%)
14	CLA	Y	839	-	44,58,73	2.44	15 (34%)	49,95,113	2.67	19 (38%)
14	CLA	d	202	-	36,53,73	2.68	13 (36%)	39,89,113	2.35	11 (28%)
14	CLA	B	814	-	36,53,73	2.66	13 (36%)	39,89,113	2.67	15 (38%)
14	CLA	Y	829	-	59,73,73	2.23	14 (23%)	67,113,113	2.07	15 (22%)
14	CLA	G	832	-	59,73,73	2.03	14 (23%)	67,113,113	2.19	16 (23%)
17	BCR	H	846	-	41,41,41	2.58	6 (14%)	56,56,56	7.13	27 (48%)
14	CLA	A	826	-	59,73,73	2.14	16 (27%)	67,113,113	2.28	19 (28%)
14	CLA	Z	837	-	54,68,73	2.24	15 (27%)	61,107,113	2.24	20 (32%)
14	CLA	X	1701	-	36,53,73	2.77	14 (38%)	39,89,113	2.34	15 (38%)
14	CLA	G	822	-	59,73,73	2.18	16 (27%)	67,113,113	2.30	17 (25%)
14	CLA	B	804	-	59,73,73	2.04	15 (25%)	67,113,113	2.20	19 (28%)
14	CLA	H	833	-	36,53,73	2.59	15 (41%)	39,89,113	2.51	11 (28%)
14	CLA	Q	202	-	36,53,73	2.62	14 (38%)	39,89,113	2.46	13 (33%)
14	CLA	Y	820	-	54,68,73	2.28	14 (25%)	61,107,113	2.28	17 (27%)
14	CLA	Y	817	-	54,68,73	2.36	16 (29%)	61,107,113	2.05	17 (27%)
15	PQN	B	841	-	34,34,34	1.72	3 (8%)	42,45,45	1.09	4 (9%)
17	BCR	A	850	-	41,41,41	2.75	6 (14%)	56,56,56	7.15	24 (42%)
14	CLA	G	807	-	45,59,73	2.51	14 (31%)	50,96,113	2.31	18 (36%)
14	CLA	A	803	-	59,73,73	2.12	14 (23%)	67,113,113	2.35	22 (32%)
17	BCR	d	203	-	41,41,41	2.70	6 (14%)	56,56,56	6.90	29 (51%)
14	CLA	A	811	-	36,53,73	2.63	14 (38%)	39,89,113	2.66	14 (35%)
14	CLA	Z	813	-	36,53,73	2.73	15 (41%)	39,89,113	2.62	14 (35%)
14	CLA	L	202	-	59,73,73	2.03	14 (23%)	67,113,113	2.30	23 (34%)
14	CLA	H	813	-	59,73,73	2.27	15 (25%)	67,113,113	2.30	19 (28%)
14	CLA	Z	822	-	36,53,73	2.77	13 (36%)	39,89,113	2.49	13 (33%)
17	BCR	h	207	-	41,41,41	2.91	8 (19%)	56,56,56	7.00	18 (32%)
14	CLA	H	814	-	59,73,73	2.24	14 (23%)	67,113,113	2.29	16 (23%)
17	BCR	f	103	-	41,41,41	2.63	6 (14%)	56,56,56	7.10	24 (42%)
14	CLA	A	806	-	59,73,73	2.08	14 (23%)	67,113,113	2.09	16 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	G	827	-	59,73,73	2.18	15 (25%)	67,113,113	1.97	20 (29%)
15	PQN	G	843	-	34,34,34	1.68	2 (5%)	42,45,45	1.17	5 (11%)
14	CLA	Y	816	-	44,58,73	2.51	14 (31%)	49,95,113	2.50	17 (34%)
17	BCR	A	846	-	41,41,41	2.87	6 (14%)	56,56,56	7.35	28 (50%)
14	CLA	H	830	-	36,53,73	2.64	13 (36%)	39,89,113	2.83	15 (38%)
14	CLA	G	821	-	59,73,73	2.23	13 (22%)	67,113,113	2.08	14 (20%)
14	CLA	G	805	-	59,73,73	2.18	15 (25%)	67,113,113	2.17	18 (26%)
14	CLA	Y	808	1	59,73,73	2.14	16 (27%)	67,113,113	2.26	22 (32%)
14	CLA	K	102	-	36,53,73	2.68	13 (36%)	39,89,113	2.40	13 (33%)
14	CLA	G	817	-	54,68,73	2.34	15 (27%)	61,107,113	2.26	18 (29%)
14	CLA	Y	840	-	59,73,73	2.11	14 (23%)	67,113,113	2.02	15 (22%)
17	BCR	e	101	-	41,41,41	2.64	7 (17%)	56,56,56	7.76	32 (57%)
14	CLA	A	804	-	59,73,73	2.27	16 (27%)	67,113,113	2.21	17 (25%)
14	CLA	H	817	-	59,73,73	2.13	14 (23%)	67,113,113	2.53	21 (31%)
14	CLA	H	818	-	54,68,73	2.28	15 (27%)	61,107,113	2.23	20 (32%)
14	CLA	Z	804	-	59,73,73	2.17	14 (23%)	67,113,113	2.06	18 (26%)
14	CLA	G	835	-	36,53,73	2.67	14 (38%)	39,89,113	2.67	13 (33%)
14	CLA	Y	837	-	44,58,73	2.63	16 (36%)	49,95,113	2.47	19 (38%)
17	BCR	J	104	-	41,41,41	2.91	8 (19%)	56,56,56	7.06	27 (48%)
14	CLA	G	811	14	59,73,73	2.20	14 (23%)	67,113,113	2.20	18 (26%)
14	CLA	A	829	-	59,73,73	2.05	15 (25%)	67,113,113	2.37	19 (28%)
14	CLA	Z	825	2	49,63,73	2.50	16 (32%)	55,101,113	2.35	17 (30%)
14	CLA	A	841	-	59,73,73	2.17	13 (22%)	67,113,113	2.11	19 (28%)
14	CLA	Y	819	-	59,73,73	2.26	16 (27%)	67,113,113	2.35	17 (25%)
14	CLA	A	831	-	59,73,73	2.10	14 (23%)	67,113,113	2.20	22 (32%)
14	CLA	B	807	-	59,73,73	2.20	14 (23%)	67,113,113	2.41	17 (25%)
17	BCR	Y	847	-	41,41,41	2.73	6 (14%)	56,56,56	7.17	26 (46%)
14	CLA	H	822	-	49,63,73	2.34	15 (30%)	55,101,113	2.44	16 (29%)
14	CLA	B	832	-	49,63,73	2.40	15 (30%)	55,101,113	2.37	18 (32%)
14	CLA	Z	828	-	59,73,73	2.20	16 (27%)	67,113,113	2.20	18 (26%)
15	PQN	Z	842	-	34,34,34	1.82	2 (5%)	42,45,45	1.28	4 (9%)
14	CLA	G	823	-	44,58,73	2.54	15 (34%)	49,95,113	2.50	17 (34%)
14	CLA	A	836	-	44,58,73	2.58	17 (38%)	49,95,113	2.61	18 (36%)
14	CLA	f	102	-	49,63,73	2.47	15 (30%)	55,101,113	2.47	18 (32%)
14	CLA	U	1004	-	59,73,73	2.20	15 (25%)	67,113,113	2.19	16 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	Y	821	-	59,73,73	2.20	16 (27%)	67,113,113	1.86	18 (26%)
14	CLA	H	836	-	54,68,73	2.25	14 (25%)	61,107,113	2.19	19 (31%)
14	CLA	A	822	-	59,73,73	2.20	17 (28%)	67,113,113	2.01	15 (22%)
14	CLA	Y	822	-	59,73,73	2.20	15 (25%)	67,113,113	2.14	16 (23%)
14	CLA	Y	834	1	36,53,73	2.74	14 (38%)	39,89,113	2.26	12 (30%)
17	BCR	H	844	-	41,41,41	2.96	8 (19%)	56,56,56	7.04	25 (44%)
14	CLA	Y	831	-	44,58,73	2.34	14 (31%)	49,95,113	2.38	14 (28%)
14	CLA	Z	841	-	59,73,73	2.19	15 (25%)	67,113,113	2.30	19 (28%)
17	BCR	G	846	-	41,41,41	2.90	6 (14%)	56,56,56	6.89	27 (48%)
17	BCR	F	201	-	41,41,41	2.78	6 (14%)	56,56,56	7.11	24 (42%)
17	BCR	Y	844	-	41,41,41	2.55	8 (19%)	56,56,56	7.33	23 (41%)
14	CLA	H	829	-	59,73,73	2.17	15 (25%)	67,113,113	2.47	20 (29%)
17	BCR	A	849	-	41,41,41	2.76	7 (17%)	56,56,56	6.98	29 (51%)
14	CLA	H	808	-	59,73,73	2.11	14 (23%)	67,113,113	2.20	21 (31%)
14	CLA	A	824	-	44,58,73	2.61	15 (34%)	49,95,113	2.33	17 (34%)
14	CLA	Z	839	-	36,53,73	2.59	14 (38%)	39,89,113	2.69	15 (38%)
14	CLA	H	826	-	59,73,73	2.19	17 (28%)	67,113,113	2.08	17 (25%)
14	CLA	G	806	-	59,73,73	2.15	15 (25%)	67,113,113	2.24	18 (26%)
14	CLA	A	819	-	59,73,73	2.17	15 (25%)	67,113,113	2.31	20 (29%)
16	SF4	G	844	1,2	0,12,12	0.00	-	-		
14	CLA	Z	815	-	59,73,73	2.24	15 (25%)	67,113,113	2.14	15 (22%)
17	BCR	H	850	-	41,41,41	2.87	6 (14%)	56,56,56	7.05	28 (50%)
14	CLA	Z	810	2	59,73,73	2.06	14 (23%)	67,113,113	2.55	20 (29%)
14	CLA	Y	836	-	59,73,73	2.25	16 (27%)	67,113,113	2.23	20 (29%)
14	CLA	B	805	-	59,73,73	2.12	15 (25%)	67,113,113	2.07	14 (20%)
14	CLA	B	829	-	36,53,73	2.52	14 (38%)	39,89,113	2.45	15 (38%)
14	CLA	Z	801	-	59,73,73	2.09	15 (25%)	67,113,113	2.31	18 (26%)
14	CLA	G	815	-	44,58,73	2.59	14 (31%)	49,95,113	2.79	19 (38%)
17	BCR	Z	845	-	41,41,41	2.55	6 (14%)	56,56,56	7.27	24 (42%)
14	CLA	Z	838	-	59,73,73	2.12	15 (25%)	67,113,113	2.16	15 (22%)
14	CLA	G	816	-	44,58,73	2.54	15 (34%)	49,95,113	2.55	17 (34%)
14	CLA	H	832	-	49,63,73	2.46	14 (28%)	55,101,113	2.31	18 (32%)
14	CLA	U	1002	10	59,73,73	2.17	14 (23%)	67,113,113	2.30	19 (28%)
14	CLA	A	837	-	59,73,73	2.13	13 (22%)	67,113,113	2.01	14 (20%)
14	CLA	H	816	-	49,63,73	2.43	14 (28%)	55,101,113	2.65	20 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	BCR	H	843	-	41,41,41	3.08	6 (14%)	56,56,56	6.96	29 (51%)
17	BCR	Y	852	-	41,41,41	2.63	7 (17%)	56,56,56	7.15	22 (39%)
18	LHG	A	852	-	48,48,48	0.98	2 (4%)	51,54,54	1.23	5 (9%)
14	CLA	A	807	-	59,73,73	2.14	15 (25%)	67,113,113	2.06	20 (29%)
14	CLA	G	820	-	54,68,73	2.25	15 (27%)	61,107,113	2.29	17 (27%)
14	CLA	d	201	-	59,73,73	2.09	14 (23%)	67,113,113	2.02	18 (26%)
14	CLA	Z	834	-	36,53,73	2.65	13 (36%)	39,89,113	2.64	16 (41%)
14	CLA	H	824	2	49,63,73	2.52	15 (30%)	55,101,113	2.61	20 (36%)
17	BCR	H	842	-	41,41,41	2.94	7 (17%)	56,56,56	6.96	22 (39%)
14	CLA	H	819	-	54,68,73	2.31	16 (29%)	61,107,113	2.07	19 (31%)
14	CLA	A	834	-	49,63,73	2.30	14 (28%)	55,101,113	2.25	17 (30%)
14	CLA	B	813	-	59,73,73	2.17	14 (23%)	67,113,113	2.14	18 (26%)
14	CLA	F	202	-	36,53,73	2.61	16 (44%)	39,89,113	2.47	13 (33%)
14	CLA	Y	805	-	59,73,73	2.10	14 (23%)	67,113,113	2.40	21 (31%)
14	CLA	G	830	-	59,73,73	2.11	14 (23%)	67,113,113	2.44	19 (28%)
14	CLA	H	838	-	36,53,73	2.64	15 (41%)	39,89,113	2.63	15 (38%)
17	BCR	Z	847	-	41,41,41	2.60	6 (14%)	56,56,56	7.20	31 (55%)
14	CLA	B	839	-	59,73,73	2.19	16 (27%)	67,113,113	2.13	17 (25%)
14	CLA	H	803	-	59,73,73	2.12	15 (25%)	67,113,113	2.17	19 (28%)
14	CLA	Z	806	-	59,73,73	2.21	16 (27%)	67,113,113	2.24	18 (26%)
19	LMG	Z	849	-	49,49,55	1.28	6 (12%)	57,57,63	1.27	5 (8%)
14	CLA	G	839	-	44,58,73	2.63	15 (34%)	49,95,113	2.72	21 (42%)
14	CLA	A	802	-	59,73,73	2.13	14 (23%)	67,113,113	2.15	15 (22%)
14	CLA	U	1007	-	59,73,73	2.25	14 (23%)	67,113,113	2.17	22 (32%)
14	CLA	Y	802	-	59,73,73	2.17	17 (28%)	67,113,113	2.45	22 (32%)
14	CLA	B	821	-	49,63,73	2.33	14 (28%)	55,101,113	2.14	12 (21%)
14	CLA	A	821	-	54,68,73	2.29	15 (27%)	61,107,113	2.41	19 (31%)
14	CLA	H	804	-	48,62,73	2.37	14 (29%)	53,99,113	2.49	15 (28%)
14	CLA	Z	821	-	36,53,73	2.68	13 (36%)	39,89,113	2.36	16 (41%)
14	CLA	B	819	-	36,53,73	2.60	14 (38%)	39,89,113	2.61	16 (41%)
14	CLA	H	821	-	36,53,73	2.79	14 (38%)	39,89,113	2.37	12 (30%)
14	CLA	A	842	-	59,73,73	2.15	14 (23%)	67,113,113	2.32	19 (28%)
14	CLA	Y	818	-	59,73,73	2.23	14 (23%)	67,113,113	2.27	18 (26%)
17	BCR	U	1005	-	41,41,41	2.86	6 (14%)	56,56,56	7.12	26 (46%)
18	LHG	B	849	-	38,38,48	1.09	2 (5%)	41,44,54	1.24	4 (9%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	L	206	-	59,73,73	2.19	15 (25%)	67,113,113	1.98	18 (26%)
14	CLA	H	812	-	36,53,73	2.60	14 (38%)	39,89,113	2.28	12 (30%)
14	CLA	A	816	-	44,58,73	2.51	15 (34%)	49,95,113	2.53	18 (36%)
14	CLA	H	811	-	49,63,73	2.37	16 (32%)	55,101,113	2.30	23 (41%)
14	CLA	Z	836	-	36,53,73	2.62	14 (38%)	39,89,113	2.85	15 (38%)
14	CLA	Y	803	-	59,73,73	2.21	15 (25%)	67,113,113	2.46	18 (26%)
17	BCR	Z	850	-	41,41,41	2.84	6 (14%)	56,56,56	7.07	24 (42%)
17	BCR	S	1104	-	41,41,41	2.96	6 (14%)	56,56,56	6.95	26 (46%)
14	CLA	B	820	-	36,53,73	2.82	14 (38%)	39,89,113	2.32	13 (33%)
14	CLA	Y	812	-	49,63,73	2.38	15 (30%)	55,101,113	2.22	17 (30%)
14	CLA	B	837	-	59,73,73	2.10	13 (22%)	67,113,113	2.13	19 (28%)
14	CLA	Z	807	-	59,73,73	2.27	13 (22%)	67,113,113	2.12	17 (25%)
14	CLA	Z	818	-	59,73,73	2.25	15 (25%)	67,113,113	2.37	19 (28%)
14	CLA	B	828	-	59,73,73	2.18	13 (22%)	67,113,113	2.35	18 (26%)
14	CLA	U	1003	-	59,73,73	2.20	13 (22%)	67,113,113	2.19	17 (25%)
14	CLA	G	809	-	59,73,73	2.21	15 (25%)	67,113,113	2.13	19 (28%)
14	CLA	g	101	-	32,49,73	2.67	13 (40%)	32,83,113	2.43	11 (34%)
17	BCR	G	848	-	41,41,41	2.64	6 (14%)	56,56,56	7.17	24 (42%)
14	CLA	H	840	-	59,73,73	2.14	13 (22%)	67,113,113	2.50	20 (29%)
14	CLA	Z	808	-	59,73,73	1.98	12 (20%)	67,113,113	2.12	16 (23%)
16	SF4	A	845	1,2	0,12,12	0.00	-	-		
17	BCR	Z	848	-	41,41,41	2.82	7 (17%)	56,56,56	7.30	22 (39%)
19	LMG	H	848	-	49,49,55	1.37	6 (12%)	57,57,63	1.10	4 (7%)
14	CLA	S	1102	8	36,53,73	2.71	14 (38%)	39,89,113	2.29	9 (23%)
14	CLA	A	854	-	59,73,73	2.17	14 (23%)	67,113,113	2.63	18 (26%)
17	BCR	J	103	-	41,41,41	2.70	6 (14%)	56,56,56	6.97	30 (53%)
17	BCR	Y	853	-	41,41,41	2.88	6 (14%)	56,56,56	6.91	29 (51%)
18	LHG	G	851	14	31,31,48	1.27	2 (6%)	34,37,54	1.19	2 (5%)
17	BCR	V	101	-	41,41,41	2.72	6 (14%)	56,56,56	7.26	30 (53%)
17	BCR	Y	848	-	41,41,41	2.56	6 (14%)	56,56,56	7.16	26 (46%)
14	CLA	B	822	-	54,68,73	2.33	14 (25%)	61,107,113	2.12	17 (27%)
14	CLA	G	852	-	59,73,73	2.11	16 (27%)	67,113,113	2.03	20 (29%)
17	BCR	H	847	-	41,41,41	2.51	7 (17%)	56,56,56	7.28	29 (51%)
14	CLA	Z	823	-	49,63,73	2.45	15 (30%)	55,101,113	2.31	16 (29%)
14	CLA	G	833	-	59,73,73	2.20	15 (25%)	67,113,113	2.29	17 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	SF4	N	101	3	0,12,12	0.00	-	-		
14	CLA	G	803	-	59,73,73	2.10	14 (23%)	67,113,113	2.56	21 (31%)
14	CLA	B	833	-	36,53,73	2.64	14 (38%)	39,89,113	2.84	14 (35%)
17	BCR	I	102	-	41,41,41	2.90	6 (14%)	56,56,56	7.00	23 (41%)
18	LHG	A	853	14	31,31,48	1.20	2 (6%)	34,37,54	1.15	2 (5%)
14	CLA	S	1101	-	59,73,73	2.10	15 (25%)	67,113,113	2.18	17 (25%)
14	CLA	Y	824	-	54,68,73	2.35	16 (29%)	61,107,113	2.34	18 (29%)
14	CLA	B	818	-	54,68,73	2.24	15 (27%)	61,107,113	2.25	16 (26%)
18	LHG	H	849	-	36,36,48	1.12	2 (5%)	39,42,54	0.90	2 (5%)
14	CLA	H	805	-	59,73,73	2.21	14 (23%)	67,113,113	2.11	17 (25%)
14	CLA	B	811	-	44,58,73	2.51	15 (34%)	49,95,113	2.38	17 (34%)
17	BCR	B	844	-	41,41,41	2.71	6 (14%)	56,56,56	7.13	27 (48%)
14	CLA	G	810	-	36,53,73	2.79	15 (41%)	39,89,113	2.33	11 (28%)
14	CLA	G	802	-	59,73,73	2.27	16 (27%)	67,113,113	2.16	15 (22%)
14	CLA	Z	820	-	54,68,73	2.25	16 (29%)	61,107,113	2.06	15 (24%)
14	CLA	G	808	1	59,73,73	2.16	14 (23%)	67,113,113	2.07	18 (26%)
17	BCR	A	847	-	41,41,41	2.51	7 (17%)	56,56,56	7.10	25 (44%)
14	CLA	H	851	18	44,58,73	2.55	16 (36%)	49,95,113	2.83	20 (40%)
17	BCR	L	207	-	41,41,41	2.80	7 (17%)	56,56,56	7.07	21 (37%)
16	SF4	a	102	3	0,12,12	0.00	-	-		
14	CLA	B	802	-	59,73,73	2.17	15 (25%)	67,113,113	2.11	18 (26%)
14	CLA	G	838	-	44,58,73	2.54	13 (29%)	49,95,113	2.37	16 (32%)
14	CLA	Y	813	-	54,68,73	2.29	15 (27%)	61,107,113	2.26	17 (27%)
14	CLA	G	825	-	59,73,73	2.17	15 (25%)	67,113,113	2.25	21 (31%)
14	CLA	B	831	-	59,73,73	2.13	14 (23%)	67,113,113	2.35	19 (28%)
17	BCR	G	845	-	41,41,41	2.71	7 (17%)	56,56,56	7.15	27 (48%)
16	SF4	N	102	3	0,12,12	0.00	-	-		
14	CLA	Z	833	-	49,63,73	2.38	14 (28%)	55,101,113	2.41	15 (27%)
17	BCR	B	847	-	41,41,41	2.59	6 (14%)	56,56,56	7.17	26 (46%)
17	BCR	i	101	-	41,41,41	2.80	6 (14%)	56,56,56	7.58	28 (50%)
14	CLA	H	823	-	54,68,73	2.23	15 (27%)	61,107,113	2.25	20 (32%)
14	CLA	Z	811	2	59,73,73	2.12	14 (23%)	67,113,113	2.31	24 (35%)
17	BCR	T	102	-	41,41,41	2.57	6 (14%)	56,56,56	7.29	26 (46%)
14	CLA	G	831	-	44,58,73	2.44	14 (31%)	49,95,113	2.61	18 (36%)
17	BCR	Z	843	-	41,41,41	2.90	7 (17%)	56,56,56	6.88	26 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	Z	830	-	59,73,73	2.01	12 (20%)	67,113,113	2.41	16 (23%)
14	CLA	Z	816	-	36,53,73	2.67	14 (38%)	39,89,113	2.51	12 (30%)
14	CLA	Y	826	-	54,68,73	2.20	14 (25%)	61,107,113	2.22	14 (22%)
14	CLA	Z	814	-	59,73,73	2.18	15 (25%)	67,113,113	2.17	17 (25%)
14	CLA	T	101	-	32,49,73	2.64	13 (40%)	32,83,113	2.43	11 (34%)
14	CLA	B	801	-	59,73,73	2.07	13 (22%)	67,113,113	2.26	16 (23%)
17	BCR	B	843	-	41,41,41	2.72	6 (14%)	56,56,56	7.31	24 (42%)
16	SF4	C	101	3	0,12,12	0.00	-	-		
14	CLA	Y	835	-	44,58,73	2.61	15 (34%)	49,95,113	2.49	18 (36%)
14	CLA	T	103	-	36,53,73	2.70	14 (38%)	39,89,113	2.23	11 (28%)
14	CLA	A	830	-	59,73,73	2.18	16 (27%)	67,113,113	2.05	19 (28%)
14	CLA	B	812	-	59,73,73	2.19	15 (25%)	67,113,113	2.41	20 (29%)
17	BCR	Y	846	-	41,41,41	2.60	6 (14%)	56,56,56	7.42	28 (50%)
14	CLA	K	101	-	32,49,73	2.62	13 (40%)	32,83,113	2.51	11 (34%)
14	CLA	H	834	-	36,53,73	2.63	13 (36%)	39,89,113	2.58	13 (33%)
14	CLA	A	809	1	59,73,73	2.15	15 (25%)	67,113,113	2.04	18 (26%)
17	BCR	G	849	-	41,41,41	2.77	7 (17%)	56,56,56	7.34	30 (53%)
14	CLA	Z	840	-	59,73,73	2.18	14 (23%)	67,113,113	2.09	20 (29%)
14	CLA	H	801	-	59,73,73	2.18	15 (25%)	67,113,113	2.15	20 (29%)
18	LHG	j	101	-	27,27,48	1.28	2 (7%)	30,33,54	1.19	2 (6%)
14	CLA	A	823	-	59,73,73	2.14	16 (27%)	67,113,113	2.40	19 (28%)
14	CLA	H	828	-	59,73,73	2.17	16 (27%)	67,113,113	2.16	20 (29%)
14	CLA	B	834	-	36,53,73	2.65	15 (41%)	39,89,113	2.33	15 (38%)
17	BCR	B	850	-	41,41,41	2.78	6 (14%)	56,56,56	7.08	28 (50%)
14	CLA	A	825	-	54,68,73	2.30	15 (27%)	61,107,113	2.11	15 (24%)
17	BCR	Z	846	-	25,25,41	2.13	2 (8%)	33,33,56	8.00	16 (48%)
14	CLA	Y	807	-	45,59,73	2.53	15 (33%)	50,96,113	2.26	15 (30%)
14	CLA	Y	815	-	44,58,73	2.63	16 (36%)	49,95,113	2.58	14 (28%)
14	CLA	Y	823	-	44,58,73	2.63	14 (31%)	49,95,113	2.50	18 (36%)
14	CLA	Y	804	14	53,67,73	2.31	14 (26%)	59,105,113	2.48	15 (25%)
14	CLA	B	810	-	49,63,73	2.42	15 (30%)	55,101,113	2.39	19 (34%)
14	CLA	Y	830	-	59,73,73	2.21	14 (23%)	67,113,113	2.23	16 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	827	-	3/3/19/25	11/31/129/135	-
19	LMG	B	848	-	-	13/47/67/70	0/1/1/1
14	CLA	A	832	-	3/3/17/25	3/19/117/135	-
14	CLA	H	825	-	3/3/20/25	22/37/135/135	-
14	CLA	Z	802	-	3/3/20/25	19/37/135/135	-
14	CLA	A	820	-	3/3/20/25	18/37/135/135	-
14	CLA	G	829	-	3/3/20/25	16/37/135/135	-
14	CLA	H	806	-	3/3/20/25	17/37/135/135	-
14	CLA	G	803	-	3/3/20/25	12/37/135/135	-
14	CLA	H	835	-	3/3/16/25	2/11/111/135	-
14	CLA	B	803	-	3/3/17/25	7/24/122/135	-
14	CLA	B	838	-	3/3/16/25	0/11/111/135	-
14	CLA	L	205	-	3/3/20/25	16/37/135/135	-
14	CLA	A	815	-	3/3/17/25	9/19/117/135	-
14	CLA	L	204	-	3/3/20/25	20/37/135/135	-
14	CLA	W	1701	-	3/3/16/25	4/11/111/135	-
14	CLA	B	840	-	3/3/20/25	10/37/135/135	-
14	CLA	B	815	-	3/3/18/25	8/25/123/135	-
14	CLA	Z	835	-	3/3/16/25	4/11/111/135	-
17	BCR	M	101	-	-	11/29/63/63	0/2/2/2
14	CLA	Y	832	-	3/3/20/25	20/37/135/135	-
14	CLA	G	853	-	3/3/16/25	4/11/111/135	-
18	LHG	Y	851	14	-	17/28/28/53	-
14	CLA	H	837	-	3/3/20/25	13/37/135/135	-
17	BCR	L	208	-	-	8/29/63/63	0/2/2/2
14	CLA	G	818	-	3/3/20/25	19/37/135/135	-
14	CLA	Y	810	-	3/3/16/25	4/11/111/135	-
14	CLA	H	820	-	3/3/16/25	7/11/111/135	-
14	CLA	L	201	-	3/3/20/25	18/37/135/135	-
14	CLA	B	806	-	3/3/20/25	11/37/135/135	-
14	CLA	B	824	-	3/3/20/25	15/37/135/135	-
14	CLA	A	808	-	3/3/17/25	9/21/119/135	-
14	CLA	f	101	8	3/3/16/25	5/11/111/135	-
17	BCR	B	846	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	Z	819	-	3/3/19/25	14/31/129/135	-
17	BCR	Y	849	-	-	8/29/63/63	0/2/2/2
14	CLA	G	826	-	3/3/19/25	6/31/129/135	-
14	CLA	H	810	2	3/3/20/25	16/37/135/135	-
14	CLA	A	818	-	3/3/19/25	14/31/129/135	-
14	CLA	A	814	-	3/3/19/25	12/31/129/135	-
14	CLA	G	842	18	3/3/17/25	3/19/117/135	-
17	BCR	R	102	-	-	11/29/63/63	0/2/2/2
14	CLA	Z	831	-	3/3/16/25	4/11/111/135	-
17	BCR	Y	845	-	-	4/29/63/63	0/2/2/2
14	CLA	B	817	-	3/3/19/25	9/31/129/135	-
14	CLA	Z	832	-	3/3/16/25	5/11/111/135	-
14	CLA	A	810	-	3/3/20/25	13/37/135/135	-
17	BCR	I	101	-	-	5/29/63/63	0/2/2/2
14	CLA	B	826	-	3/3/20/25	12/37/135/135	-
14	CLA	A	840	-	3/3/17/25	5/19/117/135	-
14	CLA	B	809	-	3/3/20/25	16/37/135/135	-
14	CLA	H	809	2	3/3/20/25	17/37/135/135	-
15	PQN	A	844	-	-	4/23/43/43	0/2/2/2
14	CLA	Z	805	-	3/3/17/25	4/24/122/135	-
14	CLA	Z	812	-	3/3/18/25	13/25/123/135	-
17	BCR	Q	203	-	-	6/29/63/63	0/2/2/2
14	CLA	A	838	-	3/3/17/25	9/19/117/135	-
17	BCR	U	1008	-	-	16/29/63/63	0/2/2/2
14	CLA	Z	817	-	3/3/18/25	10/25/123/135	-
14	CLA	A	805	14	3/3/18/25	15/30/128/135	-
14	CLA	A	812	14	3/3/20/25	12/37/135/135	-
14	CLA	B	812	-	3/3/20/25	23/37/135/135	-
16	SF4	C	102	3,21	-	-	0/6/5/5
14	CLA	H	807	-	3/3/20/25	10/37/135/135	-
14	CLA	Y	833	-	3/3/18/25	11/25/123/135	-
14	CLA	B	836	-	3/3/19/25	8/31/129/135	-
15	PQN	H	841	-	-	5/23/43/43	0/2/2/2
14	CLA	Y	838	-	3/3/20/25	11/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	812	-	3/3/17/25	8/24/122/135	-
17	BCR	Z	844	-	-	8/29/63/63	0/2/2/2
14	CLA	J	101	8	3/3/16/25	5/11/111/135	-
14	CLA	S	1103	-	3/3/18/25	14/25/123/135	-
14	CLA	Z	824	-	3/3/19/25	7/31/129/135	-
14	CLA	Z	809	-	3/3/20/25	15/37/135/135	-
14	CLA	G	819	-	3/3/20/25	19/37/135/135	-
14	CLA	B	816	-	3/3/20/25	8/37/135/135	-
14	CLA	Z	826	-	3/3/20/25	13/37/135/135	-
14	CLA	G	836	-	3/3/17/25	5/19/117/135	-
14	CLA	B	825	-	3/3/20/25	20/37/135/135	-
16	SF4	a	101	3	-	-	0/6/5/5
13	CL0	G	801	-	3/3/20/25	14/37/135/135	-
13	CL0	A	801	-	3/3/20/25	8/37/135/135	-
17	BCR	F	203	-	-	4/29/63/63	0/2/2/2
14	CLA	h	205	-	3/3/20/25	17/37/135/135	-
14	CLA	A	828	-	3/3/20/25	15/37/135/135	-
13	CL0	Y	801	-	3/3/20/25	18/37/135/135	-
15	PQN	Y	842	-	-	7/23/43/43	0/2/2/2
14	CLA	A	843	18	3/3/17/25	9/19/117/135	-
17	BCR	A	848	-	-	11/29/63/63	0/2/2/2
14	CLA	B	830	-	3/3/16/25	5/11/111/135	-
14	CLA	Y	814	-	3/3/18/25	12/25/123/135	-
17	BCR	B	842	-	-	3/24/41/63	0/1/1/2
14	CLA	G	834	-	3/3/18/25	5/25/123/135	-
17	BCR	G	847	-	-	8/29/63/63	0/2/2/2
14	CLA	B	827	-	3/3/20/25	21/37/135/135	-
14	CLA	J	102	-	3/3/18/25	13/25/123/135	-
17	BCR	H	845	-	-	8/18/35/63	0/1/1/2
18	LHG	G	850	-	-	25/53/53/53	-
14	CLA	Z	821	-	3/3/16/25	6/11/111/135	-
14	CLA	H	827	-	3/3/20/25	16/37/135/135	-
14	CLA	Z	829	-	3/3/20/25	15/37/135/135	-
14	CLA	Y	802	-	3/3/20/25	8/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	813	-	3/3/17/25	9/24/122/135	-
14	CLA	G	824	-	3/3/19/25	17/31/129/135	-
14	CLA	Y	828	-	3/3/20/25	15/37/135/135	-
14	CLA	G	841	-	3/3/20/25	15/37/135/135	-
14	CLA	A	835	1	3/3/16/25	4/11/111/135	-
14	CLA	H	815	-	3/3/16/25	5/11/111/135	-
14	CLA	B	823	2	3/3/18/25	12/25/123/135	-
17	BCR	B	845	-	-	4/18/35/63	0/1/1/2
14	CLA	Y	827	-	3/3/20/25	16/37/135/135	-
14	CLA	Z	827	-	3/3/20/25	14/37/135/135	-
14	CLA	h	206	-	3/3/20/25	17/37/135/135	-
17	BCR	h	202	-	-	7/29/63/63	0/2/2/2
14	CLA	G	814	-	3/3/17/25	5/19/117/135	-
17	BCR	A	847	-	-	9/29/63/63	0/2/2/2
14	CLA	H	839	-	3/3/20/25	8/37/135/135	-
14	CLA	Y	811	14	3/3/20/25	18/37/135/135	-
14	CLA	G	813	-	3/3/19/25	12/31/129/135	-
14	CLA	G	804	14	3/3/18/25	11/30/128/135	-
14	CLA	Z	803	-	3/3/20/25	19/37/135/135	-
17	BCR	G	849	-	-	9/29/63/63	0/2/2/2
14	CLA	B	835	-	3/3/16/25	3/11/111/135	-
14	CLA	G	828	-	3/3/20/25	11/37/135/135	-
14	CLA	Y	806	-	3/3/20/25	17/37/135/135	-
14	CLA	A	817	-	3/3/17/25	7/19/117/135	-
17	BCR	A	851	-	-	11/29/63/63	0/2/2/2
14	CLA	H	831	-	3/3/20/25	17/37/135/135	-
14	CLA	G	837	-	3/3/20/25	21/37/135/135	-
14	CLA	g	102	-	3/3/16/25	3/11/111/135	-
14	CLA	A	833	-	3/3/20/25	9/37/135/135	-
14	CLA	A	839	-	3/3/20/25	13/37/135/135	-
17	BCR	S	1105	-	-	12/29/63/63	0/2/2/2
14	CLA	H	802	-	3/3/20/25	19/37/135/135	-
17	BCR	U	1009	-	-	8/29/63/63	0/2/2/2
14	CLA	Y	809	-	3/3/20/25	16/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	Q	201	-	-	11/29/63/63	0/2/2/2
14	CLA	j	102	-	3/3/16/25	4/11/111/135	-
14	CLA	U	1006	-	3/3/20/25	15/37/135/135	-
14	CLA	B	808	2	3/3/20/25	21/37/135/135	-
14	CLA	h	204	10	3/3/20/25	19/37/135/135	-
14	CLA	Y	825	-	3/3/20/25	15/37/135/135	-
14	CLA	Y	839	-	3/3/17/25	5/19/117/135	-
14	CLA	d	202	-	3/3/16/25	3/11/111/135	-
14	CLA	B	814	-	3/3/16/25	3/11/111/135	-
14	CLA	Y	829	-	3/3/20/25	16/37/135/135	-
14	CLA	G	832	-	3/3/20/25	13/37/135/135	-
17	BCR	H	846	-	-	14/29/63/63	0/2/2/2
14	CLA	A	826	-	3/3/20/25	16/37/135/135	-
14	CLA	Z	837	-	3/3/19/25	12/31/129/135	-
14	CLA	X	1701	-	3/3/16/25	3/11/111/135	-
14	CLA	G	822	-	3/3/20/25	12/37/135/135	-
14	CLA	B	804	-	3/3/20/25	14/37/135/135	-
14	CLA	H	833	-	3/3/16/25	6/11/111/135	-
14	CLA	Y	813	-	3/3/19/25	10/31/129/135	-
14	CLA	Y	820	-	3/3/19/25	11/31/129/135	-
14	CLA	Y	817	-	3/3/19/25	7/31/129/135	-
15	PQN	B	841	-	-	8/23/43/43	0/2/2/2
17	BCR	A	850	-	-	6/29/63/63	0/2/2/2
14	CLA	G	807	-	3/3/17/25	7/21/119/135	-
14	CLA	A	803	-	3/3/20/25	7/37/135/135	-
17	BCR	d	203	-	-	5/29/63/63	0/2/2/2
14	CLA	A	811	-	3/3/16/25	4/11/111/135	-
14	CLA	Z	813	-	3/3/16/25	4/11/111/135	-
14	CLA	L	202	-	3/3/20/25	13/37/135/135	-
14	CLA	H	813	-	3/3/20/25	18/37/135/135	-
14	CLA	Z	822	-	3/3/16/25	3/11/111/135	-
17	BCR	h	207	-	-	10/29/63/63	0/2/2/2
14	CLA	H	814	-	3/3/20/25	17/37/135/135	-
17	BCR	f	103	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	806	-	3/3/20/25	22/37/135/135	-
14	CLA	G	827	-	3/3/20/25	15/37/135/135	-
15	PQN	G	843	-	-	11/23/43/43	0/2/2/2
14	CLA	Y	816	-	3/3/17/25	8/19/117/135	-
17	BCR	A	846	-	-	10/29/63/63	0/2/2/2
14	CLA	H	830	-	3/3/16/25	10/11/111/135	-
14	CLA	G	821	-	3/3/20/25	20/37/135/135	-
18	LHG	G	851	14	-	16/36/36/53	-
14	CLA	Y	808	1	3/3/20/25	22/37/135/135	-
14	CLA	K	102	-	3/3/16/25	4/11/111/135	-
14	CLA	G	817	-	3/3/19/25	13/31/129/135	-
14	CLA	Y	840	-	3/3/20/25	13/37/135/135	-
17	BCR	e	101	-	-	18/29/63/63	0/2/2/2
14	CLA	A	804	-	3/3/20/25	16/37/135/135	-
14	CLA	H	817	-	3/3/20/25	14/37/135/135	-
14	CLA	H	818	-	3/3/19/25	15/31/129/135	-
14	CLA	Z	804	-	3/3/20/25	14/37/135/135	-
14	CLA	G	835	-	3/3/16/25	7/11/111/135	-
14	CLA	Y	837	-	3/3/17/25	5/19/117/135	-
17	BCR	J	104	-	-	9/29/63/63	0/2/2/2
14	CLA	G	811	14	3/3/20/25	22/37/135/135	-
14	CLA	A	829	-	3/3/20/25	13/37/135/135	-
14	CLA	Z	825	2	3/3/18/25	10/25/123/135	-
14	CLA	A	841	-	3/3/20/25	16/37/135/135	-
14	CLA	Y	819	-	3/3/20/25	20/37/135/135	-
14	CLA	A	831	-	3/3/20/25	16/37/135/135	-
14	CLA	B	807	-	3/3/20/25	16/37/135/135	-
17	BCR	Y	847	-	-	5/29/63/63	0/2/2/2
14	CLA	H	822	-	3/3/18/25	9/25/123/135	-
14	CLA	B	832	-	3/3/18/25	10/25/123/135	-
14	CLA	Z	828	-	3/3/20/25	17/37/135/135	-
15	PQN	Z	842	-	-	8/23/43/43	0/2/2/2
14	CLA	G	823	-	3/3/17/25	6/19/117/135	-
14	CLA	A	836	-	3/3/17/25	6/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	f	102	-	3/3/18/25	15/25/123/135	-
14	CLA	U	1004	-	3/3/20/25	15/37/135/135	-
14	CLA	Y	821	-	3/3/20/25	19/37/135/135	-
14	CLA	H	836	-	3/3/19/25	17/31/129/135	-
14	CLA	A	822	-	3/3/20/25	16/37/135/135	-
14	CLA	Y	822	-	3/3/20/25	17/37/135/135	-
14	CLA	Y	834	1	3/3/16/25	3/11/111/135	-
17	BCR	H	844	-	-	10/29/63/63	0/2/2/2
14	CLA	Y	831	-	3/3/17/25	6/19/117/135	-
14	CLA	Z	841	-	3/3/20/25	10/37/135/135	-
17	BCR	G	846	-	-	9/29/63/63	0/2/2/2
17	BCR	F	201	-	-	10/29/63/63	0/2/2/2
17	BCR	Y	844	-	-	9/29/63/63	0/2/2/2
14	CLA	H	829	-	3/3/20/25	12/37/135/135	-
17	BCR	A	849	-	-	8/29/63/63	0/2/2/2
14	CLA	H	808	-	3/3/20/25	15/37/135/135	-
14	CLA	Z	839	-	3/3/16/25	1/11/111/135	-
14	CLA	H	826	-	3/3/20/25	9/37/135/135	-
14	CLA	G	806	-	3/3/20/25	22/37/135/135	-
14	CLA	A	819	-	3/3/20/25	20/37/135/135	-
16	SF4	G	844	1,2	-	-	0/6/5/5
14	CLA	Z	815	-	3/3/20/25	9/37/135/135	-
17	BCR	H	850	-	-	8/29/63/63	0/2/2/2
14	CLA	Z	810	2	3/3/20/25	16/37/135/135	-
14	CLA	Y	836	-	3/3/20/25	19/37/135/135	-
14	CLA	B	805	-	3/3/20/25	15/37/135/135	-
14	CLA	B	829	-	3/3/16/25	4/11/111/135	-
14	CLA	Z	801	-	3/3/20/25	17/37/135/135	-
17	BCR	L	207	-	-	11/29/63/63	0/2/2/2
14	CLA	G	815	-	3/3/17/25	7/19/117/135	-
17	BCR	Z	845	-	-	10/29/63/63	0/2/2/2
14	CLA	Z	838	-	3/3/20/25	14/37/135/135	-
14	CLA	G	816	-	3/3/17/25	10/19/117/135	-
14	CLA	H	832	-	3/3/18/25	12/25/123/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	U	1002	10	3/3/20/25	21/37/135/135	-
14	CLA	A	837	-	3/3/20/25	19/37/135/135	-
14	CLA	H	816	-	3/3/18/25	12/25/123/135	-
17	BCR	H	843	-	-	9/29/63/63	0/2/2/2
17	BCR	Y	852	-	-	12/29/63/63	0/2/2/2
18	LHG	A	852	-	-	30/53/53/53	-
14	CLA	A	807	-	3/3/20/25	20/37/135/135	-
14	CLA	G	820	-	3/3/19/25	13/31/129/135	-
14	CLA	d	201	-	3/3/20/25	15/37/135/135	-
14	CLA	Z	834	-	3/3/16/25	5/11/111/135	-
14	CLA	H	824	2	3/3/18/25	13/25/123/135	-
17	BCR	H	842	-	-	10/29/63/63	0/2/2/2
14	CLA	H	819	-	3/3/19/25	14/31/129/135	-
14	CLA	A	834	-	3/3/18/25	10/25/123/135	-
14	CLA	B	813	-	3/3/20/25	19/37/135/135	-
14	CLA	F	202	-	3/3/16/25	2/11/111/135	-
14	CLA	Y	805	-	3/3/20/25	15/37/135/135	-
14	CLA	T	103	-	3/3/16/25	4/11/111/135	-
14	CLA	H	838	-	3/3/16/25	1/11/111/135	-
17	BCR	Z	847	-	-	10/29/63/63	0/2/2/2
14	CLA	B	839	-	3/3/20/25	12/37/135/135	-
14	CLA	H	803	-	3/3/20/25	20/37/135/135	-
14	CLA	Z	806	-	3/3/20/25	13/37/135/135	-
19	LMG	Z	849	-	-	14/44/64/70	0/1/1/1
14	CLA	G	839	-	3/3/17/25	7/19/117/135	-
14	CLA	A	802	-	3/3/20/25	13/37/135/135	-
14	CLA	U	1007	-	3/3/20/25	12/37/135/135	-
14	CLA	G	840	-	3/3/20/25	18/37/135/135	-
14	CLA	B	821	-	3/3/18/25	11/25/123/135	-
14	CLA	A	821	-	3/3/19/25	14/31/129/135	-
14	CLA	H	804	-	3/3/17/25	7/24/122/135	-
18	LHG	Y	850	-	-	32/53/53/53	-
14	CLA	B	819	-	3/3/16/25	2/11/111/135	-
14	CLA	H	821	-	3/3/16/25	3/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	842	-	3/3/20/25	15/37/135/135	-
14	CLA	Y	818	-	3/3/20/25	14/37/135/135	-
17	BCR	U	1005	-	-	6/29/63/63	0/2/2/2
18	LHG	B	849	-	-	28/43/43/53	-
14	CLA	L	206	-	3/3/20/25	9/37/135/135	-
14	CLA	H	812	-	3/3/16/25	4/11/111/135	-
14	CLA	A	816	-	3/3/17/25	8/19/117/135	-
14	CLA	H	811	-	3/3/18/25	9/25/123/135	-
14	CLA	Z	836	-	3/3/16/25	5/11/111/135	-
14	CLA	A	824	-	3/3/17/25	8/19/117/135	-
17	BCR	Z	850	-	-	4/29/63/63	0/2/2/2
17	BCR	S	1104	-	-	9/29/63/63	0/2/2/2
14	CLA	B	820	-	3/3/16/25	6/11/111/135	-
14	CLA	Y	812	-	3/3/18/25	8/25/123/135	-
14	CLA	B	837	-	3/3/20/25	13/37/135/135	-
14	CLA	Z	807	-	3/3/20/25	16/37/135/135	-
14	CLA	Z	818	-	3/3/20/25	13/37/135/135	-
14	CLA	B	828	-	3/3/20/25	9/37/135/135	-
14	CLA	U	1003	-	3/3/20/25	13/37/135/135	-
14	CLA	G	809	-	3/3/20/25	16/37/135/135	-
14	CLA	g	101	-	3/3/14/25	3/5/101/135	-
17	BCR	G	848	-	-	8/29/63/63	0/2/2/2
14	CLA	H	840	-	3/3/20/25	9/37/135/135	-
14	CLA	Z	808	-	3/3/20/25	18/37/135/135	-
16	SF4	A	845	1,2	-	-	0/6/5/5
17	BCR	Z	848	-	-	9/29/63/63	0/2/2/2
19	LMG	H	848	-	-	12/44/64/70	0/1/1/1
14	CLA	S	1102	8	3/3/16/25	6/11/111/135	-
14	CLA	A	854	-	3/3/20/25	14/37/135/135	-
17	BCR	J	103	-	-	6/29/63/63	0/2/2/2
14	CLA	Z	833	-	3/3/18/25	11/25/123/135	-
14	CLA	G	805	-	3/3/20/25	20/37/135/135	-
17	BCR	V	101	-	-	6/29/63/63	0/2/2/2
17	BCR	Y	848	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	822	-	3/3/19/25	14/31/129/135	-
14	CLA	G	852	-	3/3/20/25	11/37/135/135	-
17	BCR	H	847	-	-	8/29/63/63	0/2/2/2
14	CLA	Z	823	-	3/3/18/25	10/25/123/135	-
14	CLA	G	833	-	3/3/20/25	14/37/135/135	-
16	SF4	N	101	3	-	-	0/6/5/5
14	CLA	Y	841	-	3/3/20/25	14/37/135/135	-
14	CLA	B	833	-	3/3/16/25	5/11/111/135	-
17	BCR	I	102	-	-	9/29/63/63	0/2/2/2
18	LHG	A	853	14	-	19/36/36/53	-
14	CLA	S	1101	-	3/3/20/25	19/37/135/135	-
14	CLA	Y	824	-	3/3/19/25	17/31/129/135	-
14	CLA	B	818	-	3/3/19/25	17/31/129/135	-
18	LHG	H	849	-	-	23/41/41/53	-
14	CLA	H	805	-	3/3/20/25	16/37/135/135	-
14	CLA	Y	803	-	3/3/20/25	15/37/135/135	-
14	CLA	B	811	-	3/3/17/25	6/19/117/135	-
17	BCR	B	844	-	-	12/29/63/63	0/2/2/2
14	CLA	G	810	-	3/3/16/25	7/11/111/135	-
14	CLA	G	802	-	3/3/20/25	17/37/135/135	-
14	CLA	Z	820	-	3/3/19/25	12/31/129/135	-
14	CLA	G	808	1	3/3/20/25	16/37/135/135	-
17	BCR	R	101	-	-	8/29/63/63	0/2/2/2
14	CLA	H	851	18	3/3/17/25	12/19/117/135	-
14	CLA	T	101	-	3/3/14/25	3/5/101/135	-
16	SF4	a	102	3	-	-	0/6/5/5
14	CLA	B	802	-	3/3/20/25	10/37/135/135	-
14	CLA	G	838	-	3/3/17/25	4/19/117/135	-
14	CLA	Q	202	-	3/3/16/25	2/11/111/135	-
14	CLA	G	825	-	3/3/20/25	11/37/135/135	-
14	CLA	B	831	-	3/3/20/25	19/37/135/135	-
17	BCR	G	845	-	-	8/29/63/63	0/2/2/2
16	SF4	N	102	3	-	-	0/6/5/5
17	BCR	Y	853	-	-	8/29/63/63	0/2/2/2
17	BCR	B	847	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	i	101	-	-	11/29/63/63	0/2/2/2
14	CLA	H	823	-	3/3/19/25	13/31/129/135	-
14	CLA	Z	811	2	3/3/20/25	18/37/135/135	-
17	BCR	T	102	-	-	10/29/63/63	0/2/2/2
14	CLA	G	831	-	3/3/17/25	10/19/117/135	-
17	BCR	Z	843	-	-	12/29/63/63	0/2/2/2
14	CLA	Z	830	-	3/3/20/25	11/37/135/135	-
14	CLA	Z	816	-	3/3/16/25	5/11/111/135	-
14	CLA	Y	826	-	3/3/19/25	8/31/129/135	-
14	CLA	Z	814	-	3/3/20/25	19/37/135/135	-
14	CLA	B	801	-	3/3/20/25	19/37/135/135	-
17	BCR	B	843	-	-	7/29/63/63	0/2/2/2
16	SF4	C	101	3	-	-	0/6/5/5
14	CLA	Y	835	-	3/3/17/25	8/19/117/135	-
14	CLA	G	830	-	3/3/20/25	13/37/135/135	-
14	CLA	A	830	-	3/3/20/25	17/37/135/135	-
14	CLA	h	201	-	3/3/20/25	12/37/135/135	-
17	BCR	Y	846	-	-	18/29/63/63	0/2/2/2
14	CLA	K	101	-	3/3/14/25	3/5/101/135	-
14	CLA	H	834	-	3/3/16/25	6/11/111/135	-
14	CLA	A	809	1	3/3/20/25	21/37/135/135	-
16	SF4	Y	843	1,2	-	-	0/6/5/5
14	CLA	Z	840	-	3/3/20/25	9/37/135/135	-
14	CLA	H	801	-	3/3/20/25	15/37/135/135	-
18	LHG	j	101	-	-	17/32/32/53	-
14	CLA	A	823	-	3/3/20/25	18/37/135/135	-
14	CLA	H	828	-	3/3/20/25	7/37/135/135	-
14	CLA	B	834	-	3/3/16/25	2/11/111/135	-
17	BCR	B	850	-	-	10/29/63/63	0/2/2/2
14	CLA	A	825	-	3/3/19/25	16/31/129/135	-
17	BCR	Z	846	-	-	8/18/35/63	0/1/1/2
14	CLA	Y	807	-	3/3/17/25	11/21/119/135	-
14	CLA	Y	815	-	3/3/17/25	7/19/117/135	-
14	CLA	Y	823	-	3/3/17/25	8/19/117/135	-

*Continued on next page...*

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	Y	804	14	3/3/18/25	13/30/128/135	-
14	CLA	B	810	-	3/3/18/25	12/25/123/135	-
14	CLA	Y	830	-	3/3/20/25	11/37/135/135	-

The worst 5 of 4615 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	843	BCR	C10-C9	-9.34	1.23	1.35
17	S	1104	BCR	C10-C9	-9.19	1.23	1.35
13	G	801	CL0	MG-NA	9.08	2.27	2.06
13	A	801	CL0	MG-NA	9.06	2.27	2.06
13	Y	801	CL0	MG-NA	8.94	2.27	2.06

The worst 5 of 6696 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Z	848	BCR	C16-C17-C18	33.23	174.73	127.31
17	i	101	BCR	C16-C17-C18	30.09	170.25	127.31
17	Y	846	BCR	C16-C17-C18	29.93	170.03	127.31
17	R	101	BCR	C16-C17-C18	29.41	169.28	127.31
17	Y	849	BCR	C16-C17-C18	28.25	167.63	127.31

5 of 855 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A	827	CLA	NC
14	A	827	CLA	ND
14	A	827	CLA	NA
14	A	832	CLA	NC
14	A	832	CLA	ND

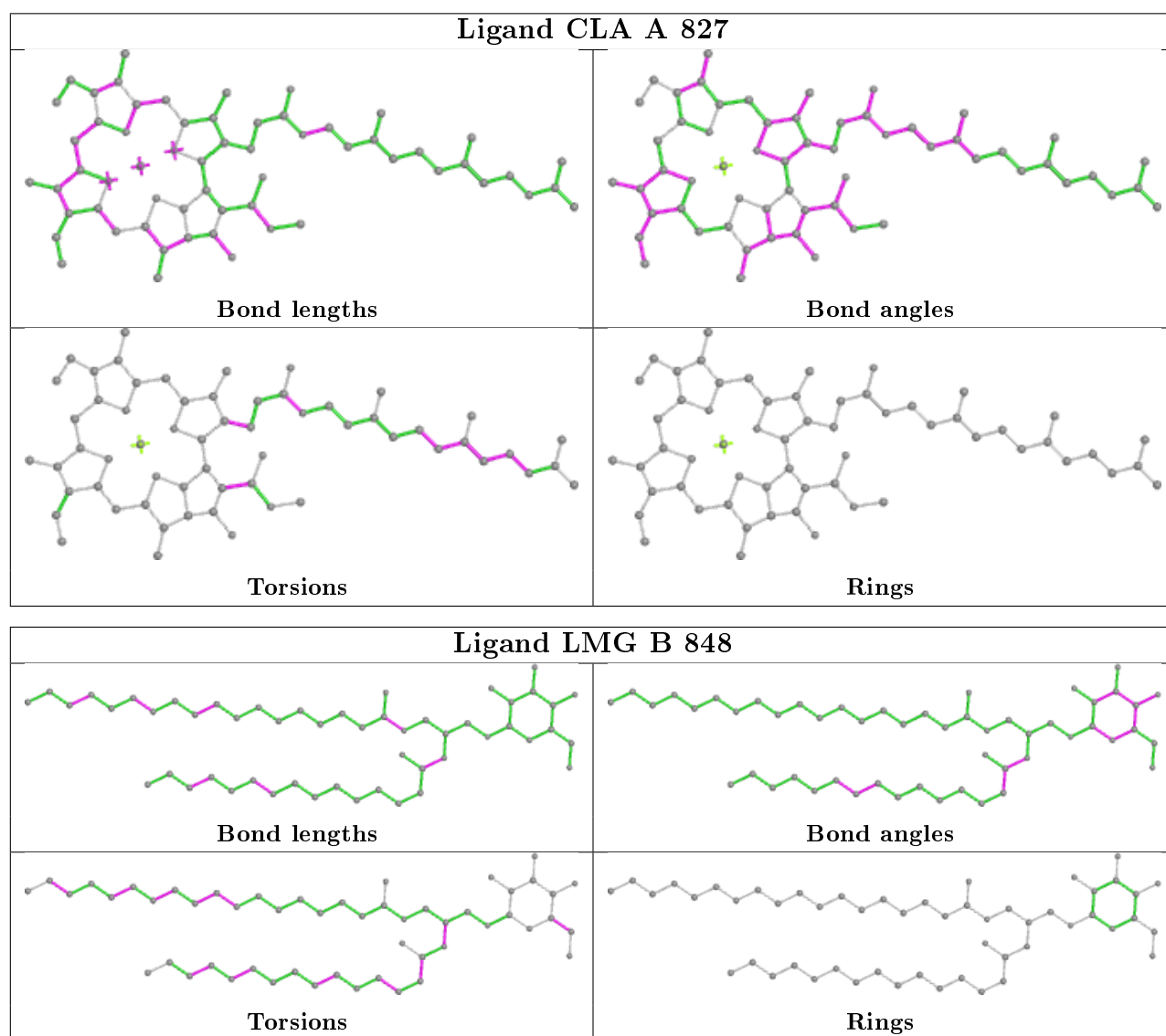
5 of 4192 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	H	825	CLA	CBA-CGA-O2A-C1
14	H	825	CLA	O1A-CGA-O2A-C1
14	H	825	CLA	CHA-CBD-CGD-O1D
14	H	825	CLA	CHA-CBD-CGD-O2D
14	A	820	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

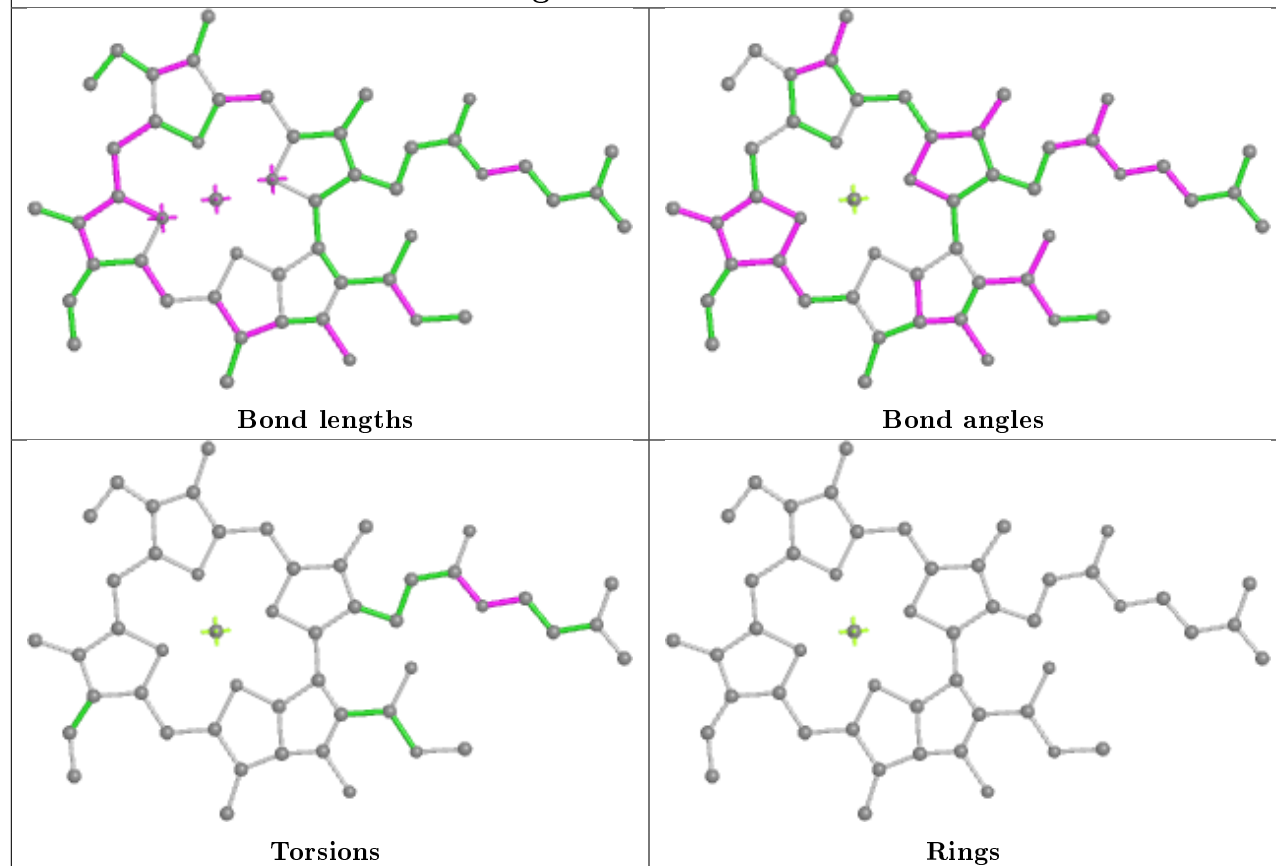
No monomer is involved in short contacts.

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

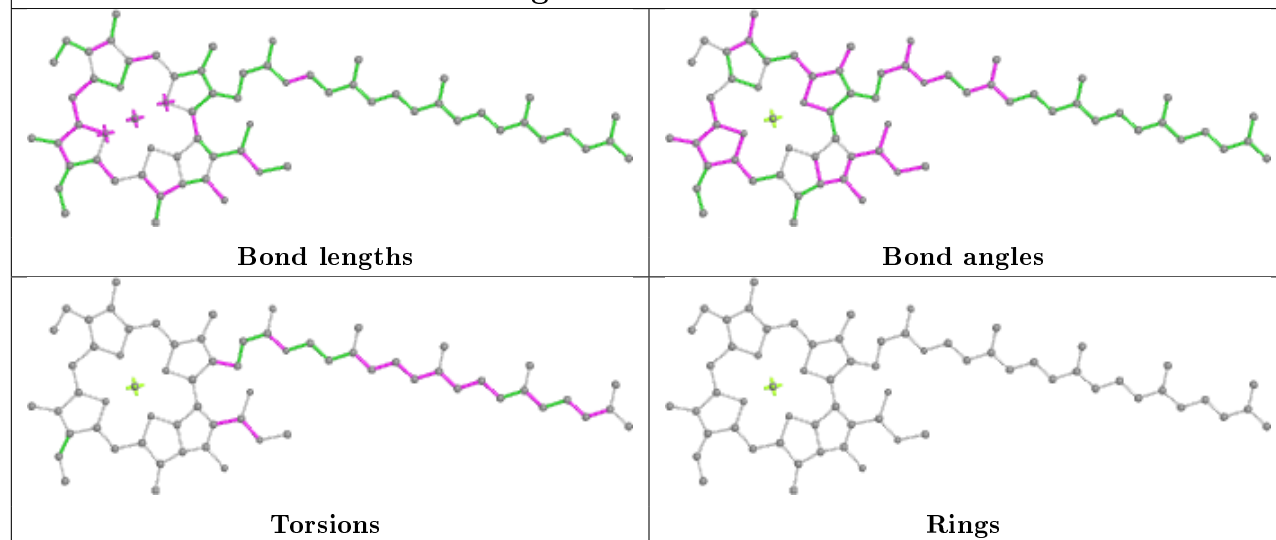




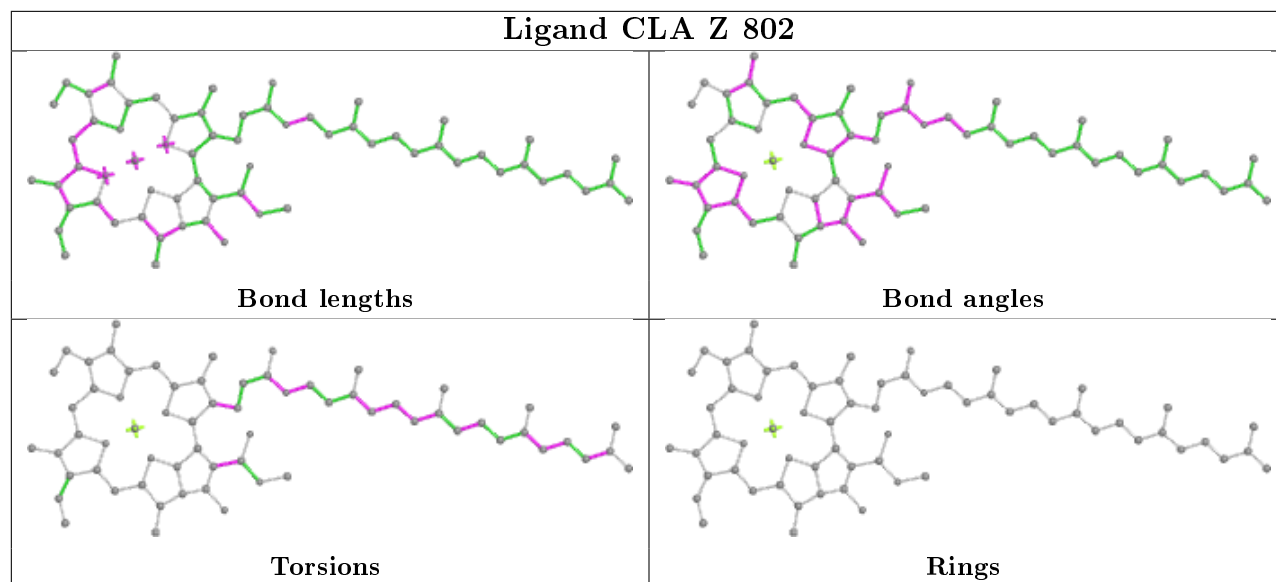
## Ligand CLA A 832



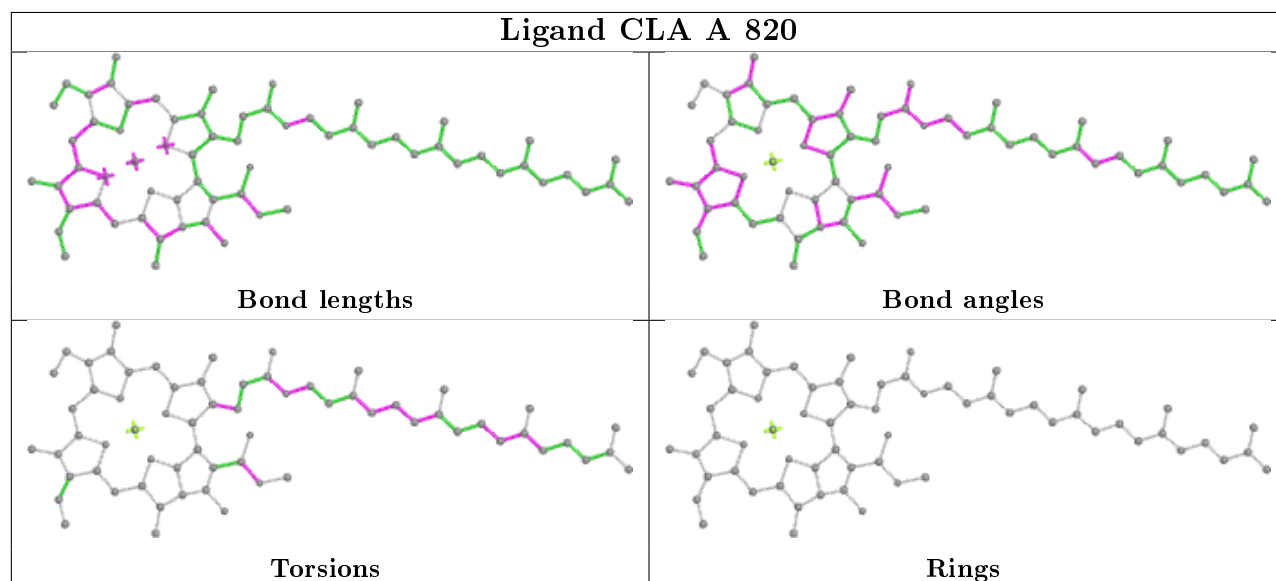
## Ligand CLA H 825



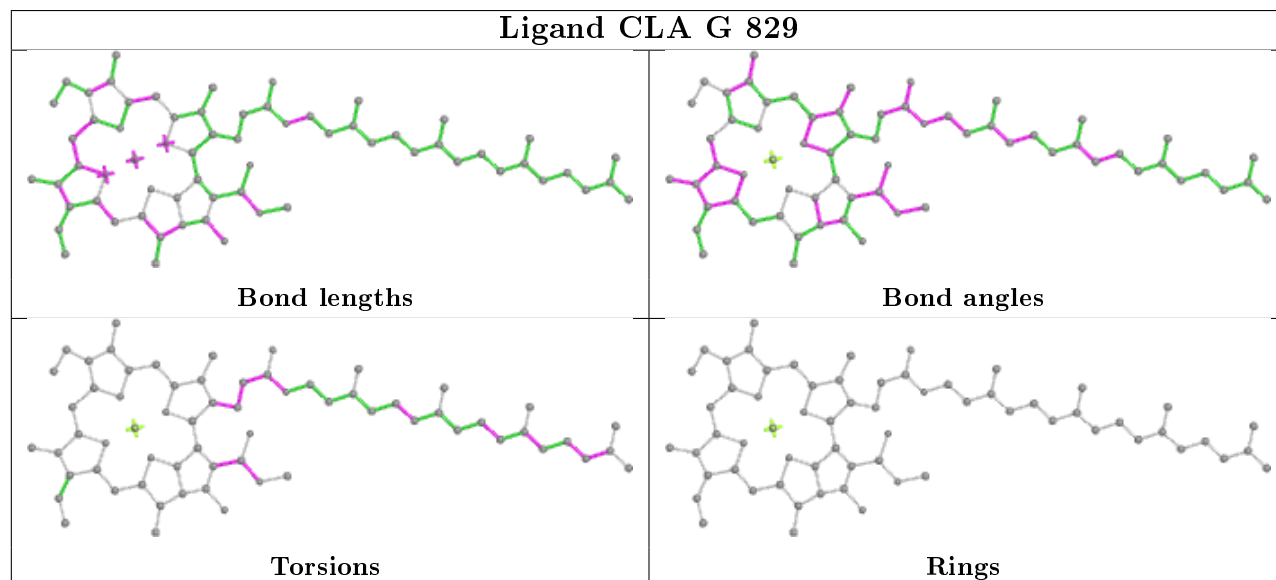
## Ligand CLA Z 802



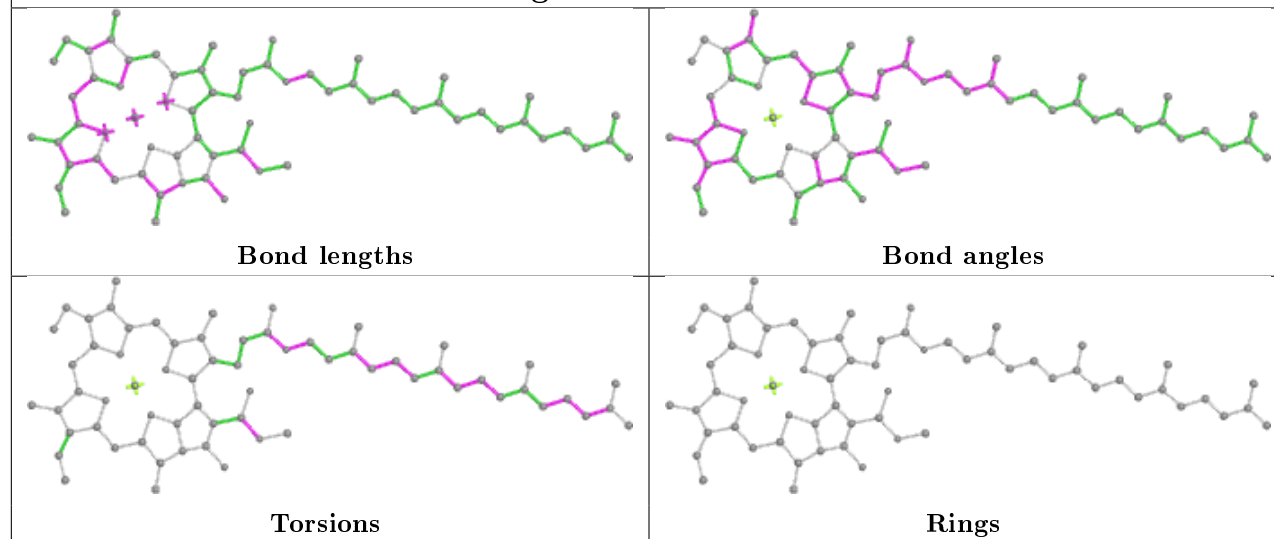
## Ligand CLA A 820



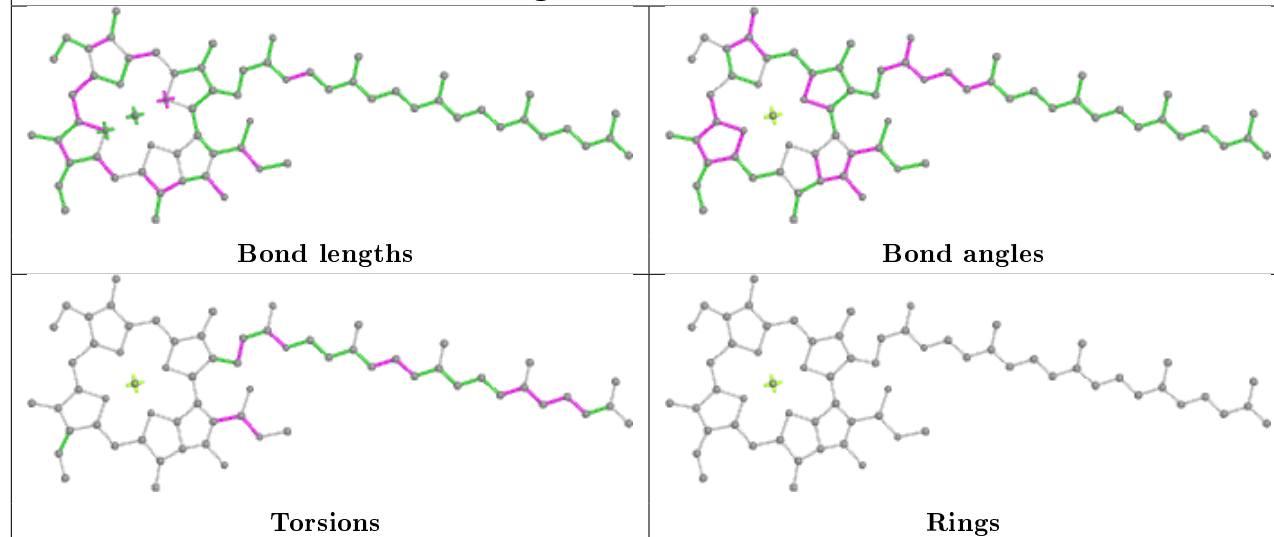
## Ligand CLA G 829



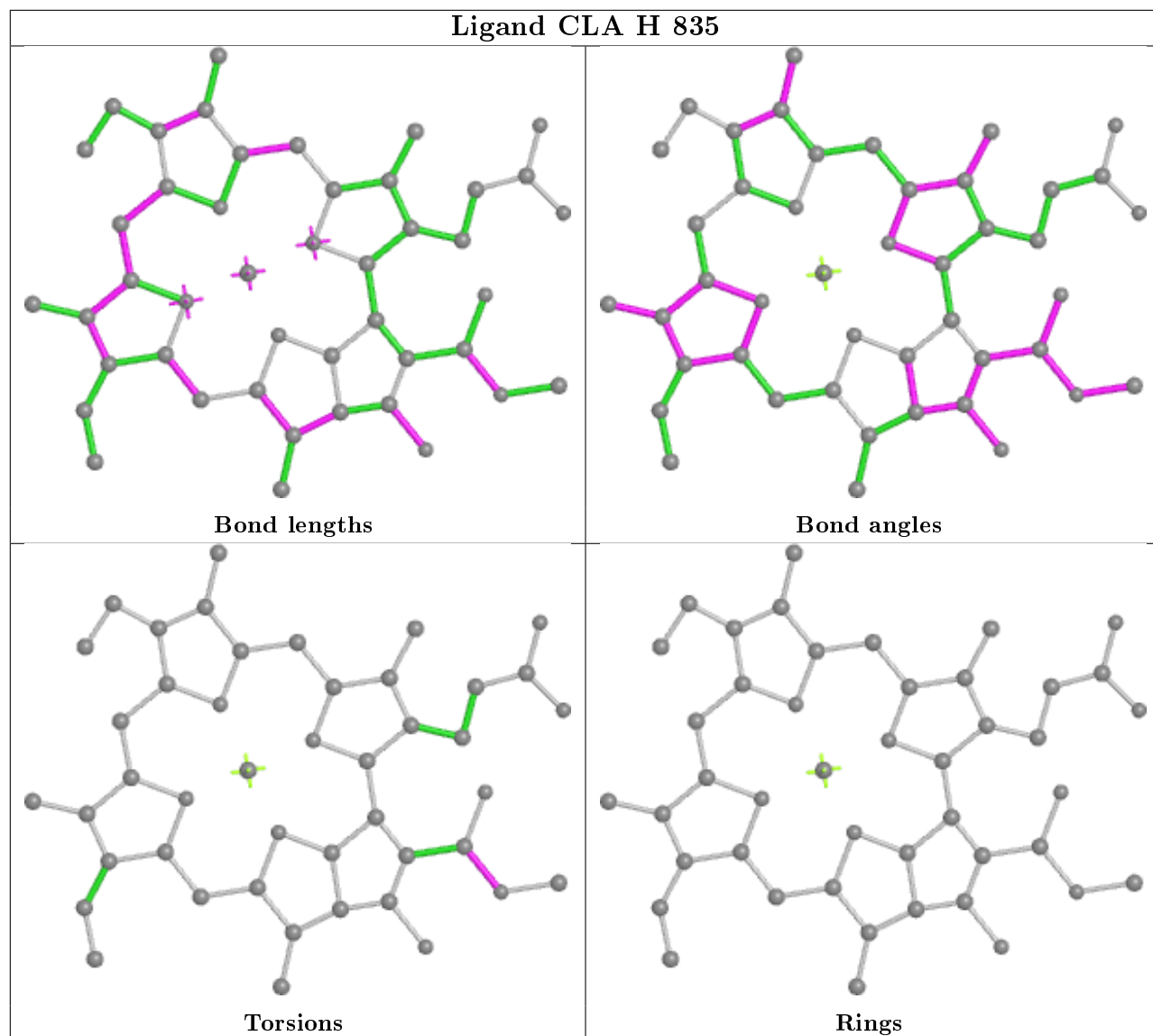
## Ligand CLA H 806

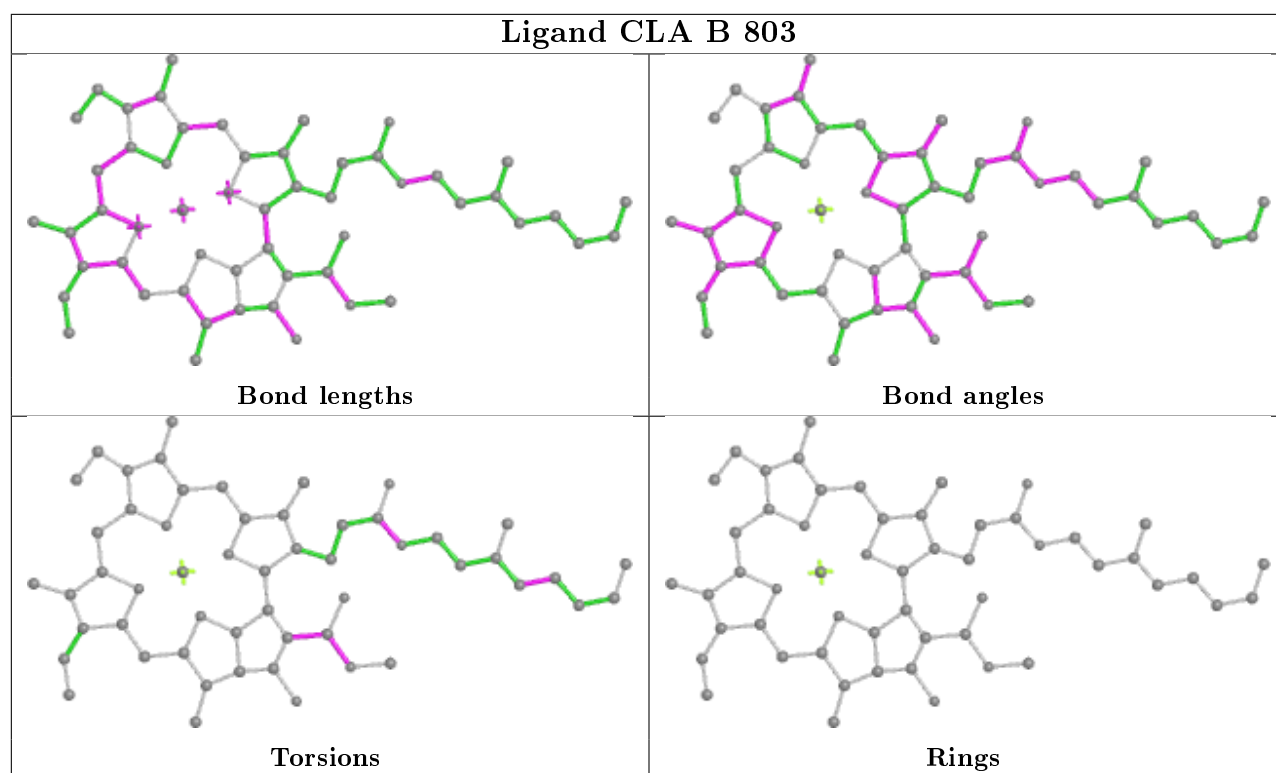


## Ligand CLA Y 841

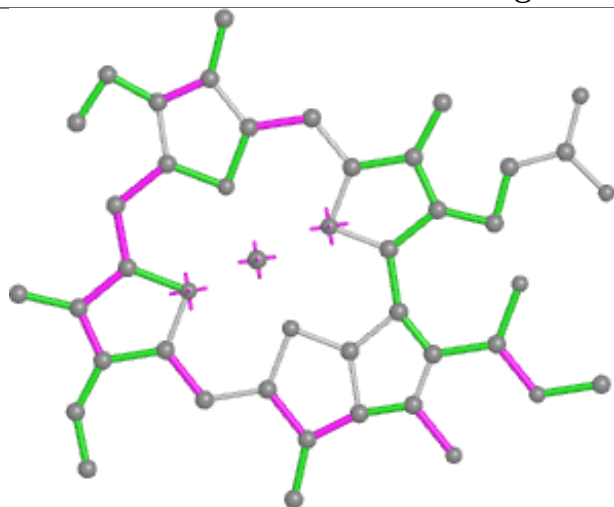


## Ligand CLA H 835

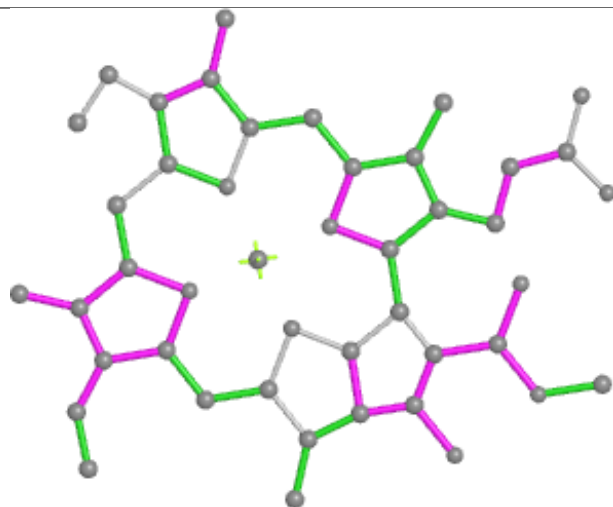




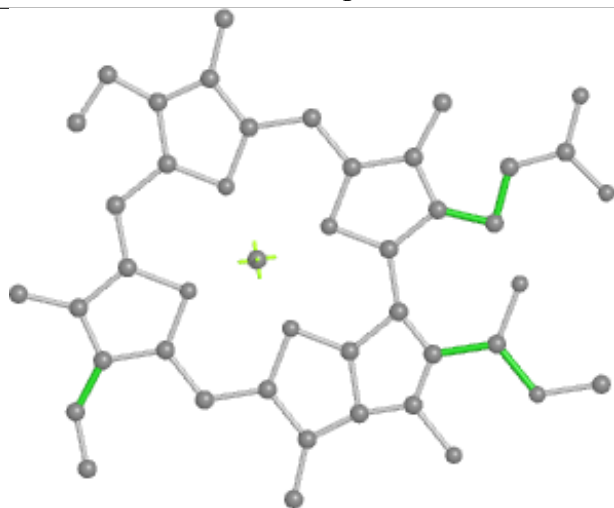
## Ligand CLA B 838



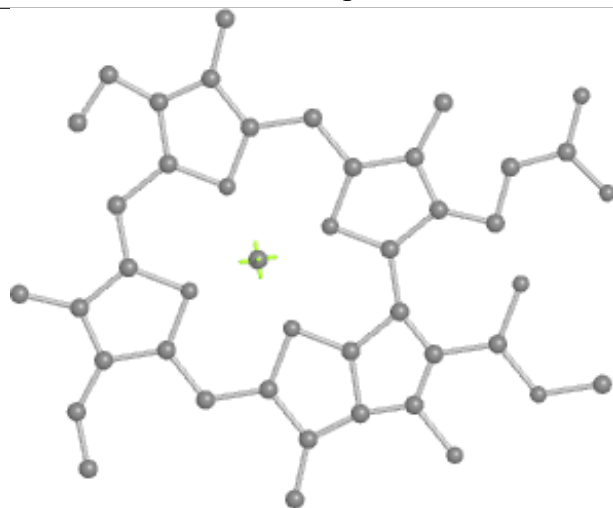
Bond lengths



Bond angles

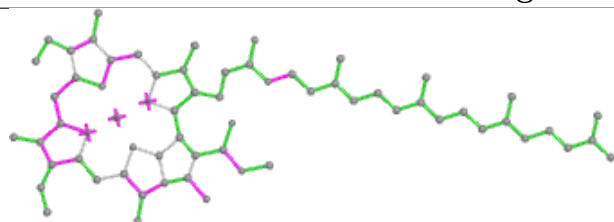


Torsions

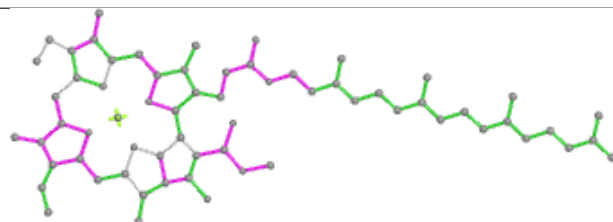


Rings

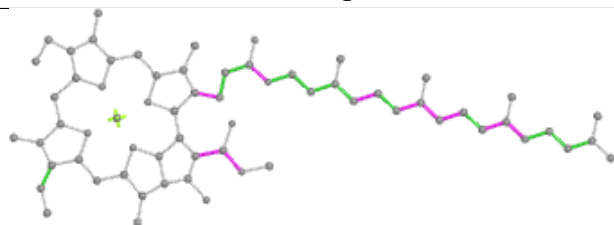
## Ligand CLA L 205



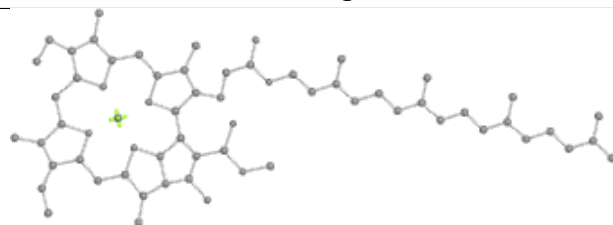
Bond lengths



Bond angles

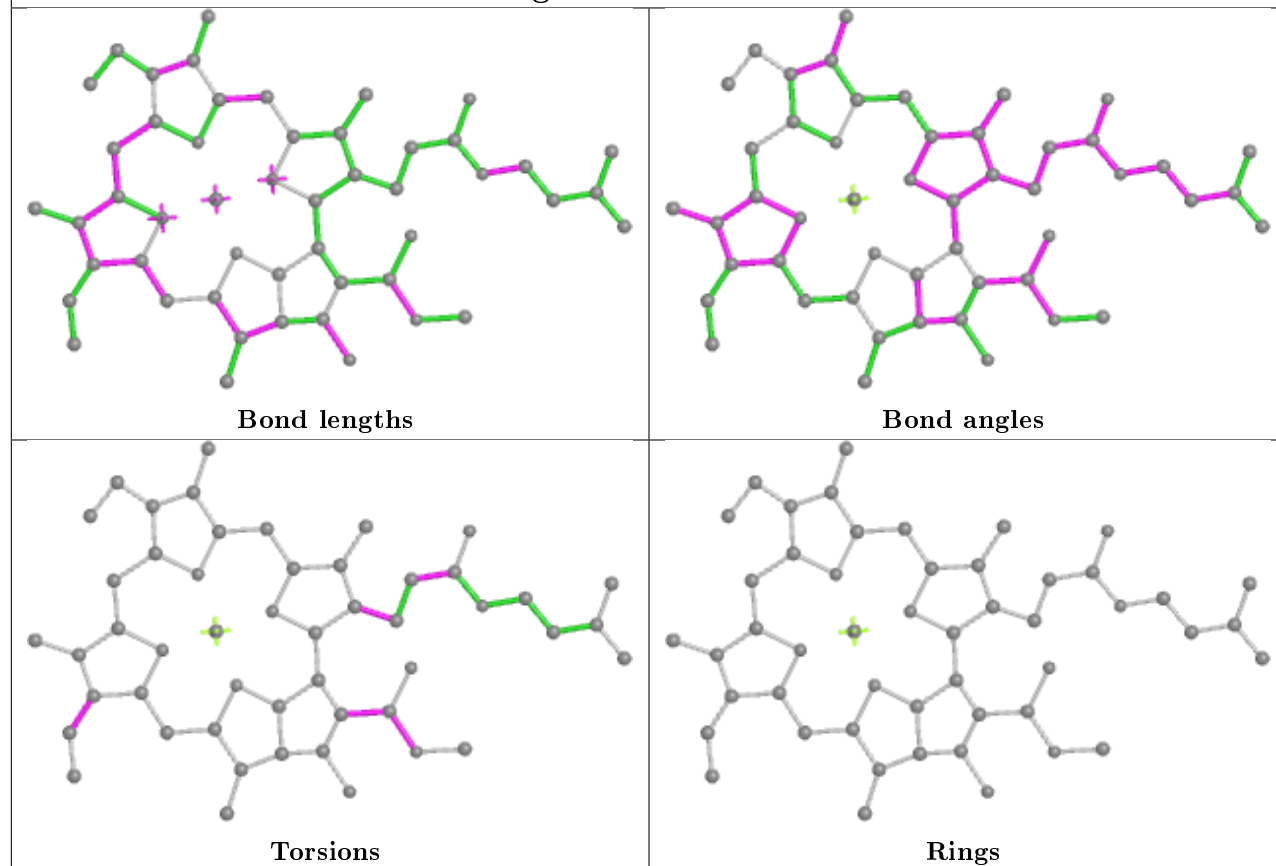


Torsions

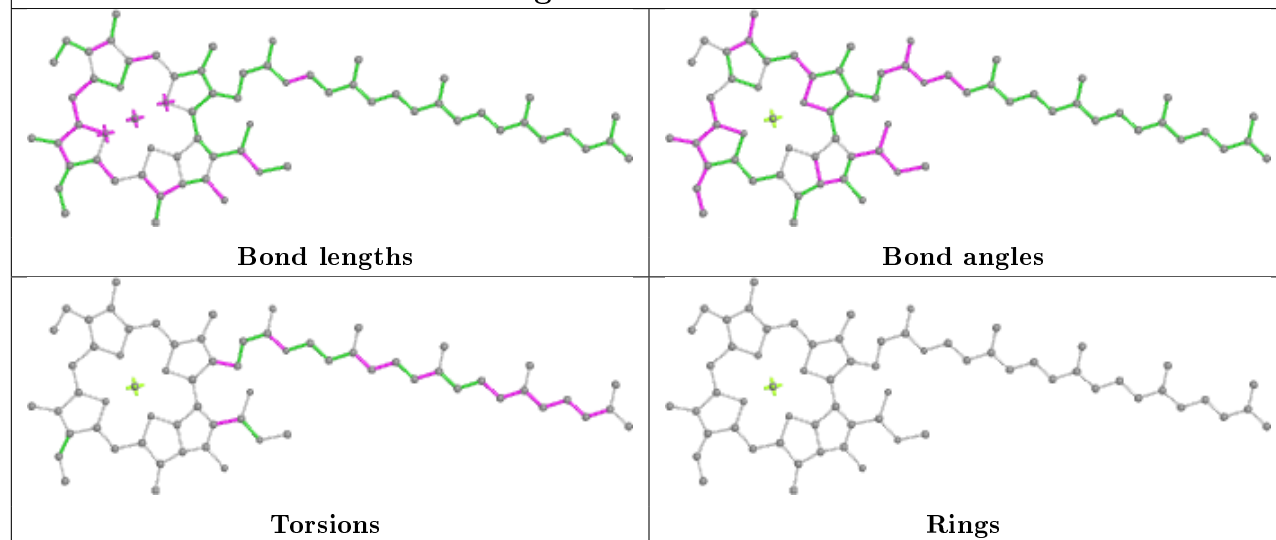


Rings

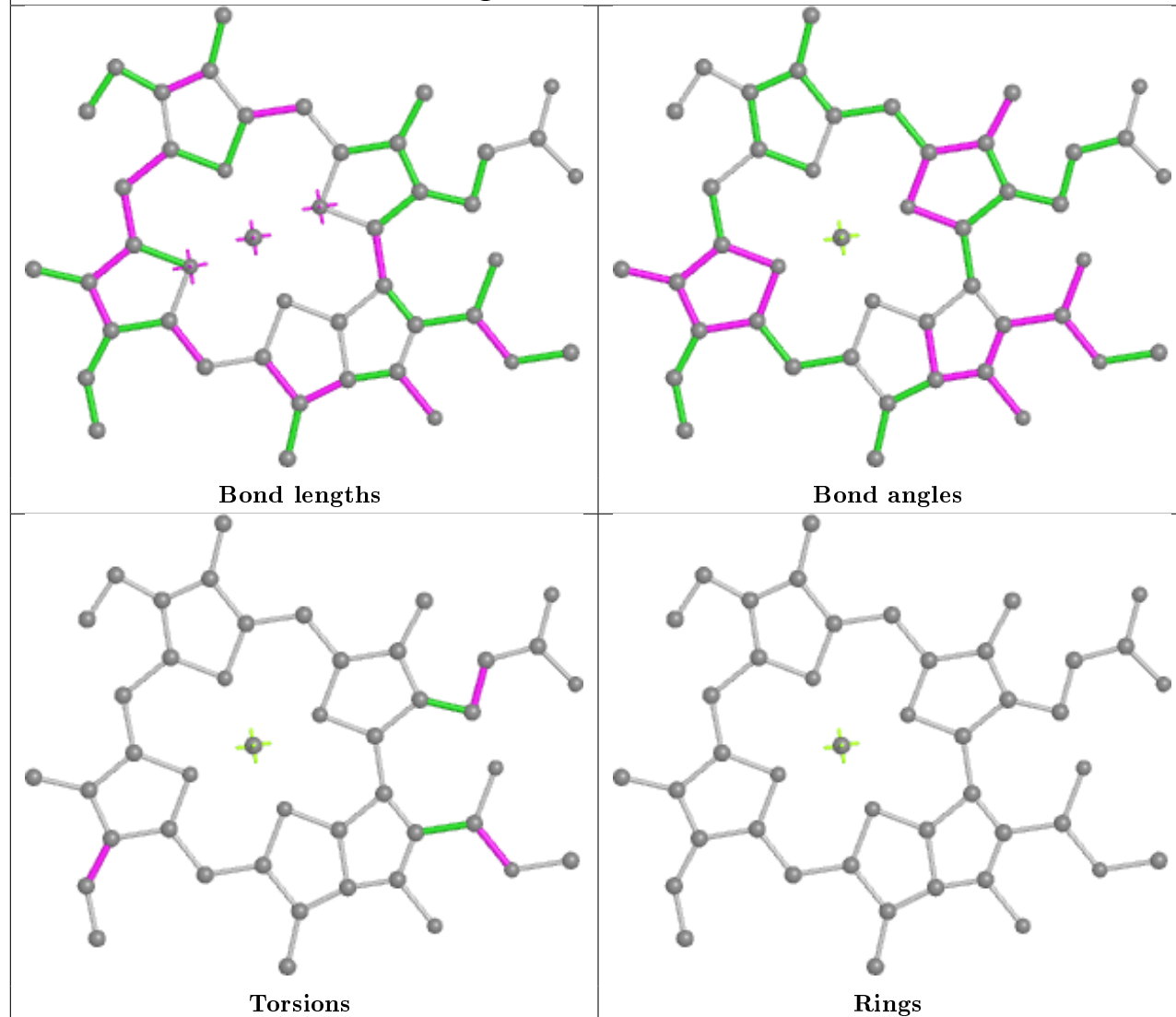
## Ligand CLA A 815



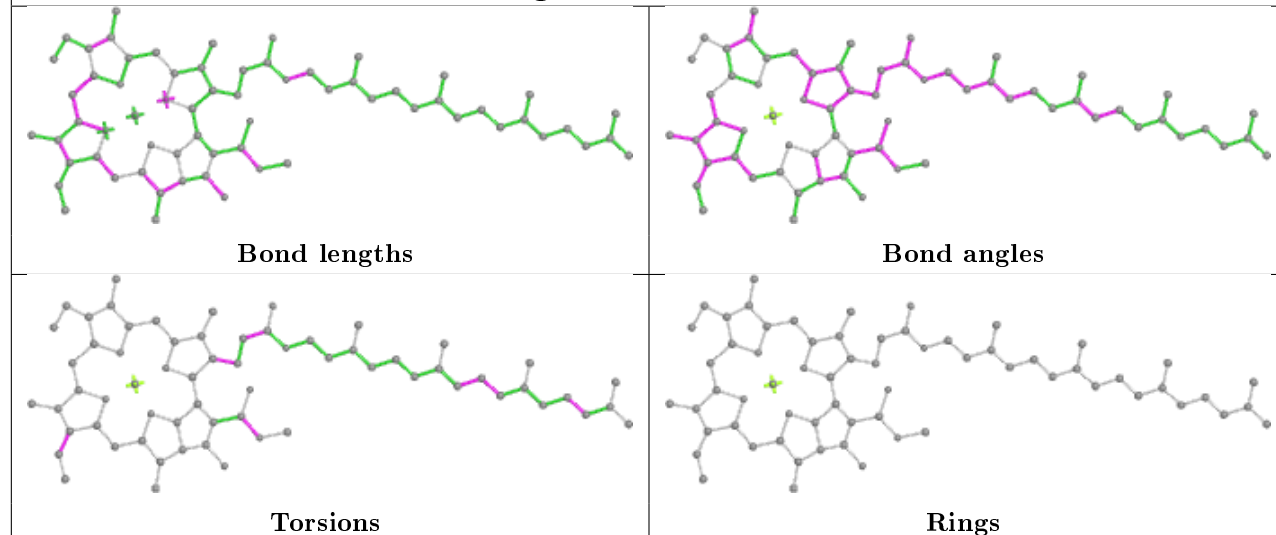
## Ligand CLA L 204



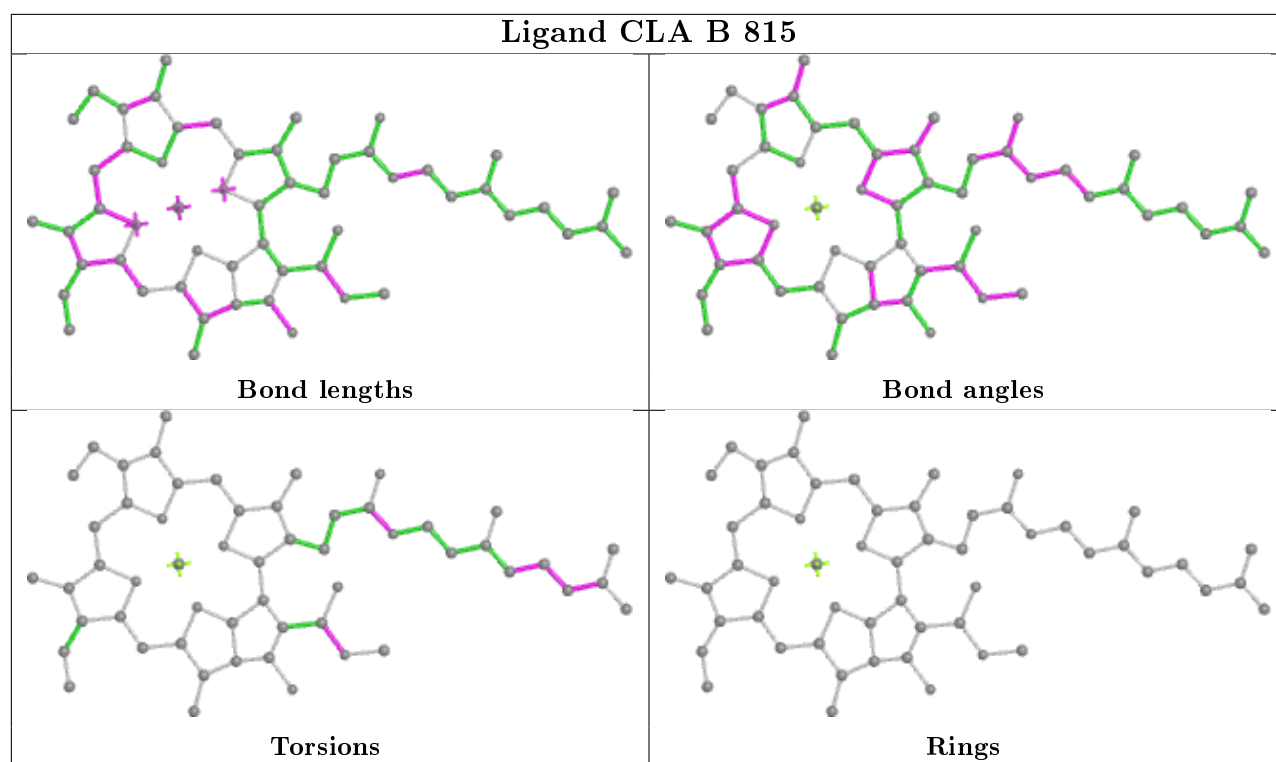
## Ligand CLA W 1701



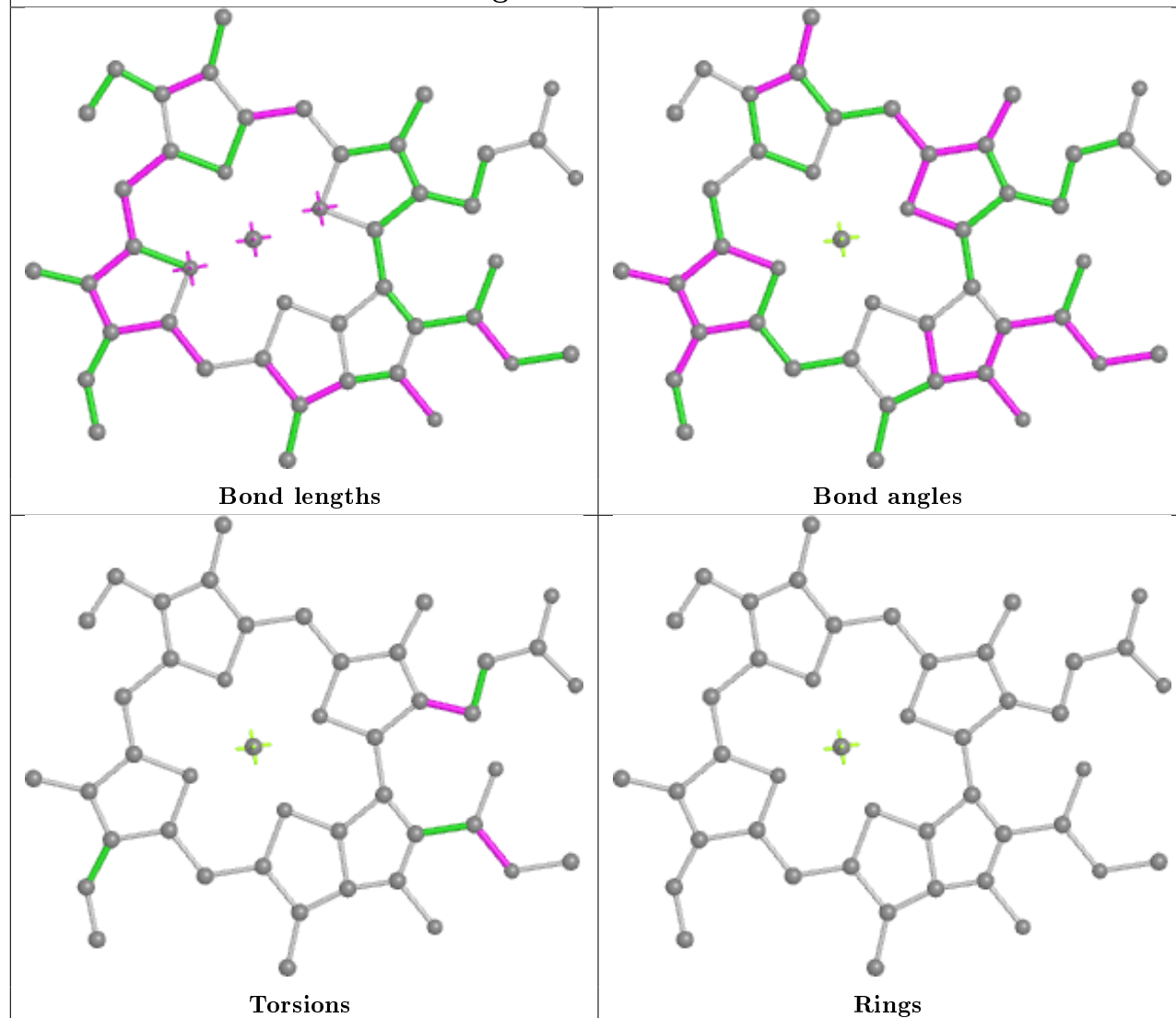
## Ligand CLA B 840



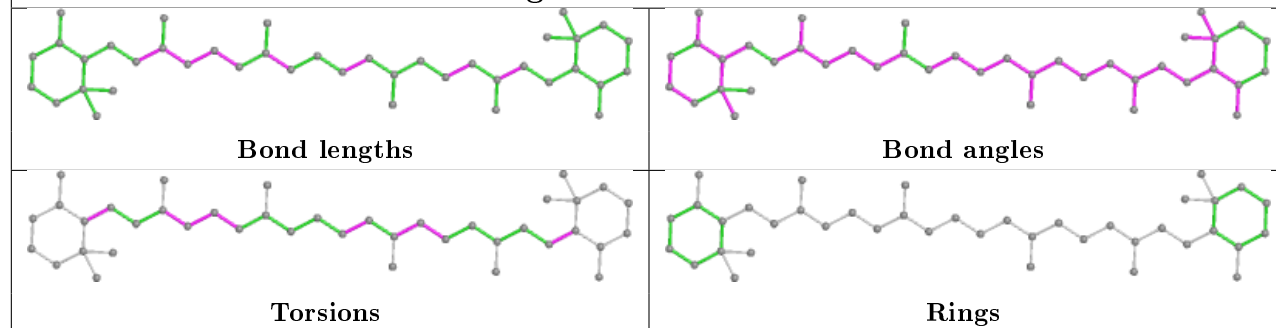




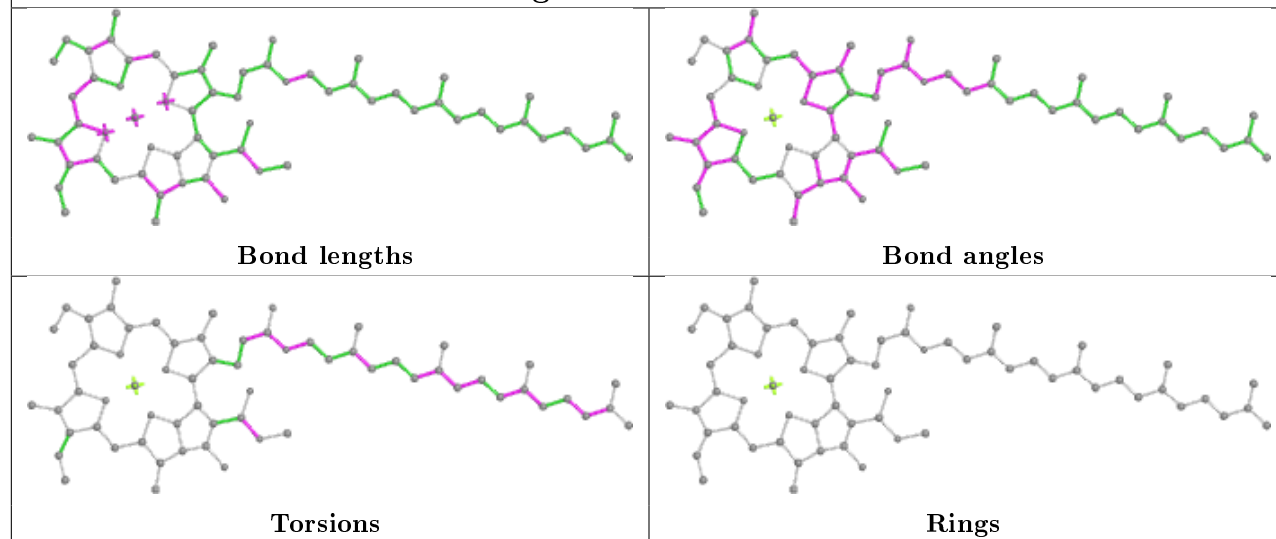
## Ligand CLA Z 835



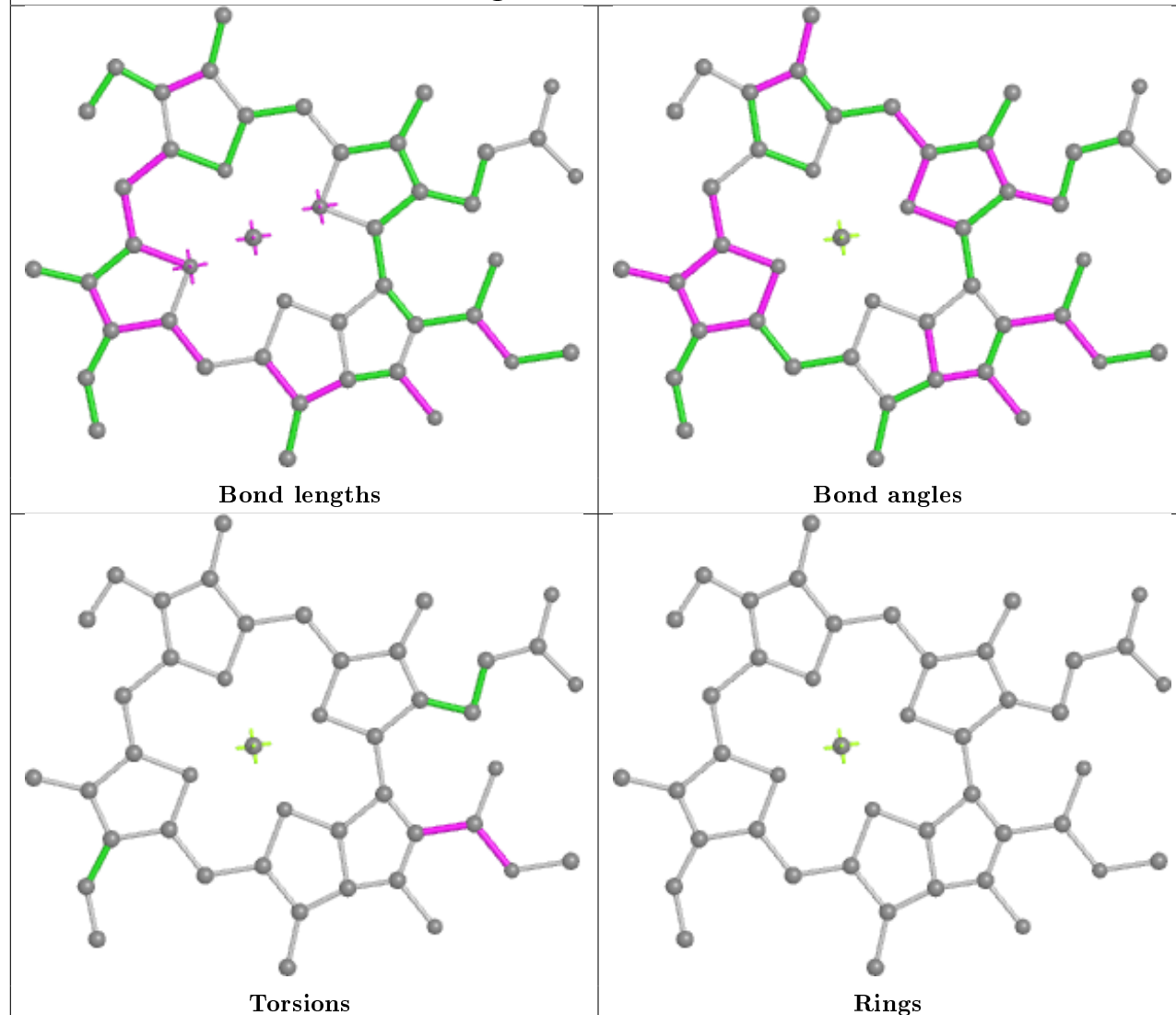
## Ligand BCR M 101

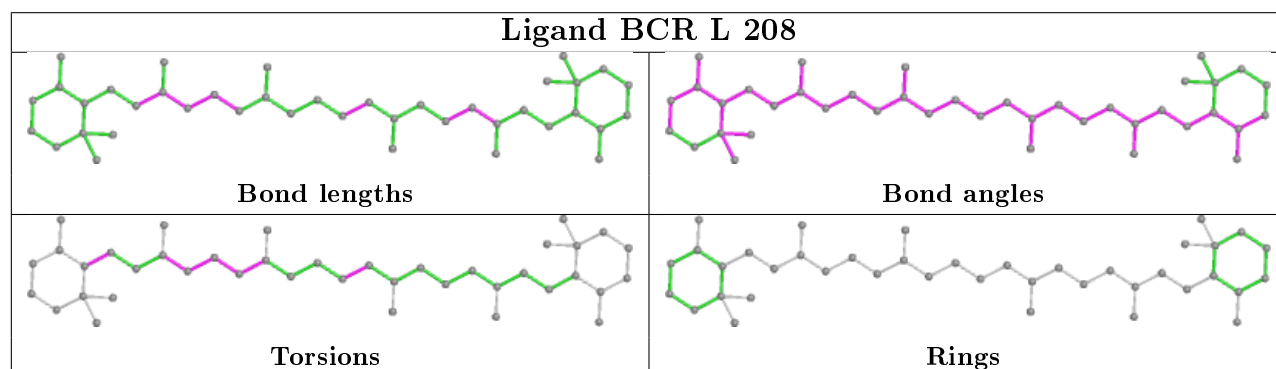
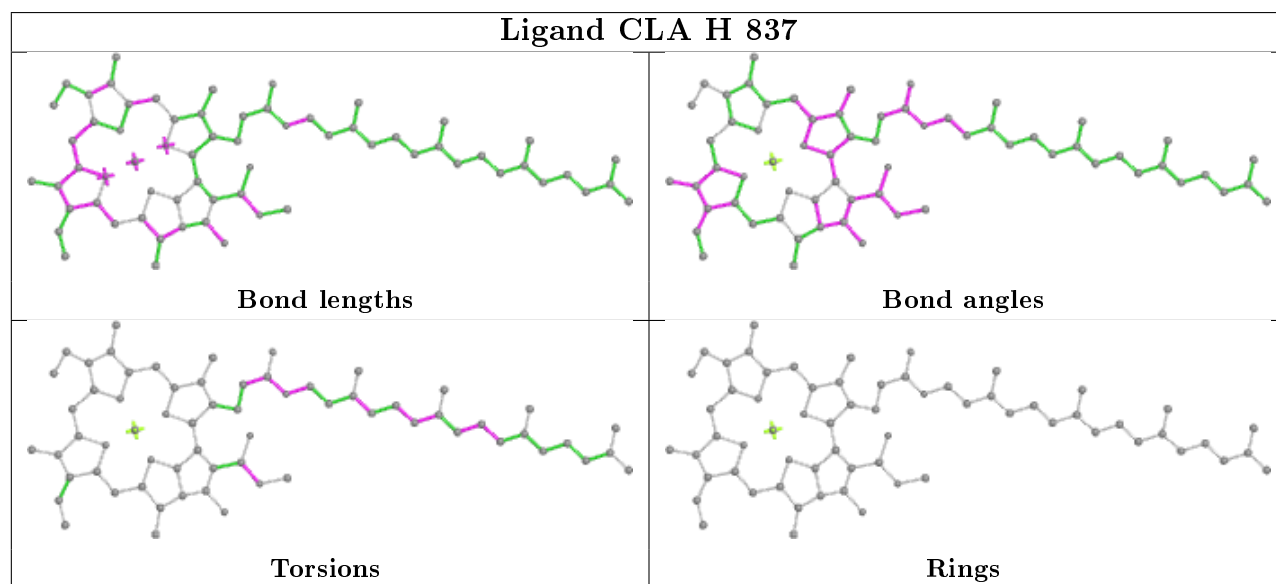
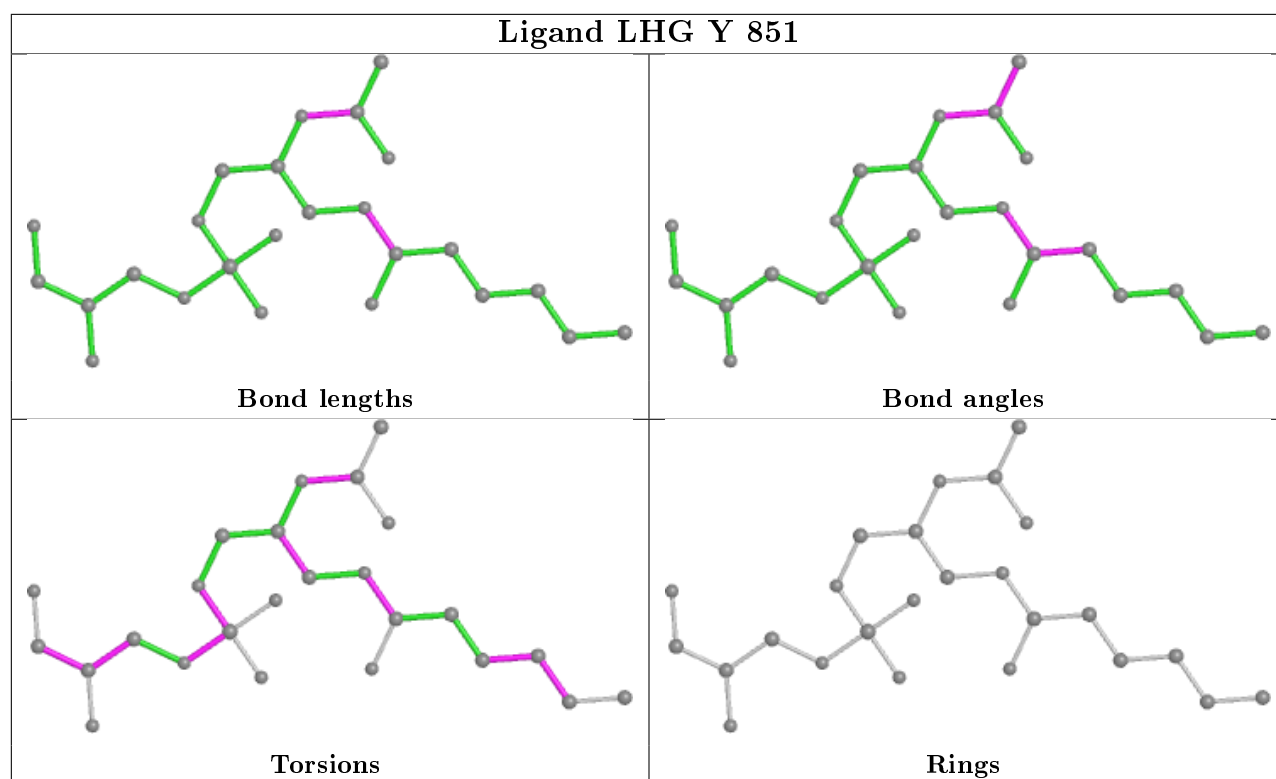


## Ligand CLA Y 832

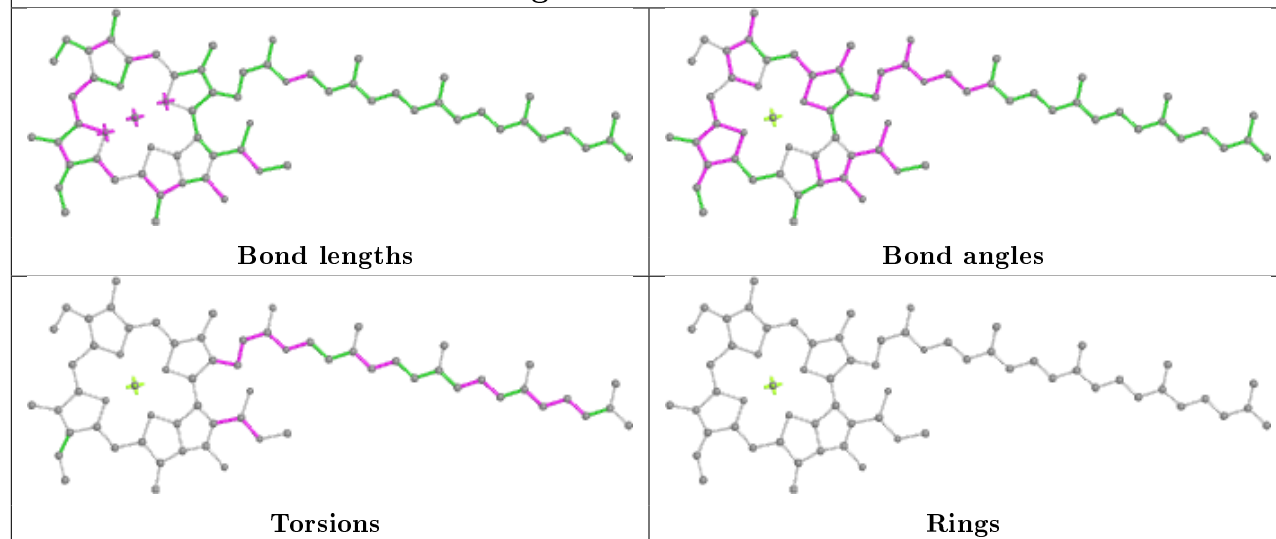


## Ligand CLA G 853

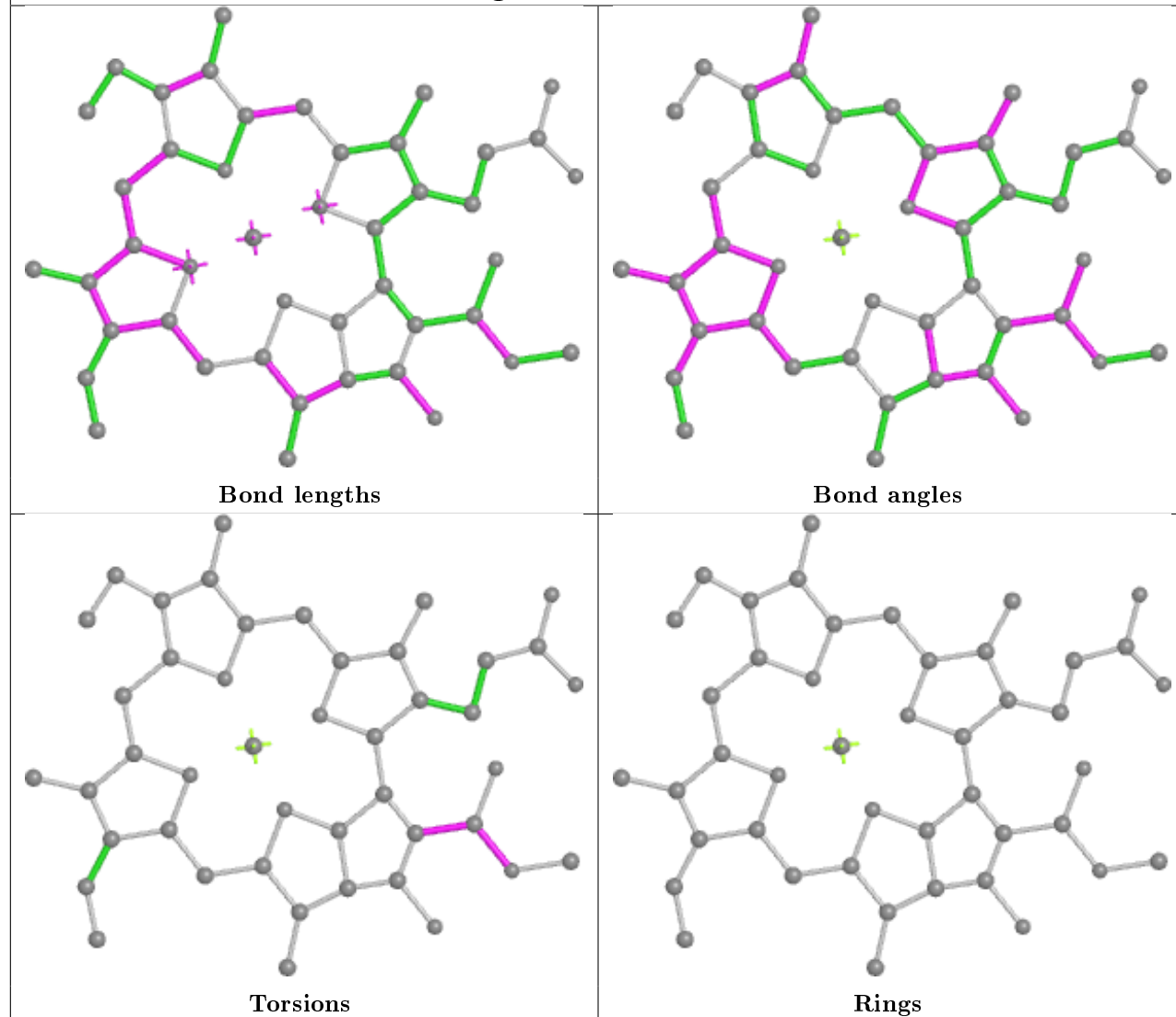




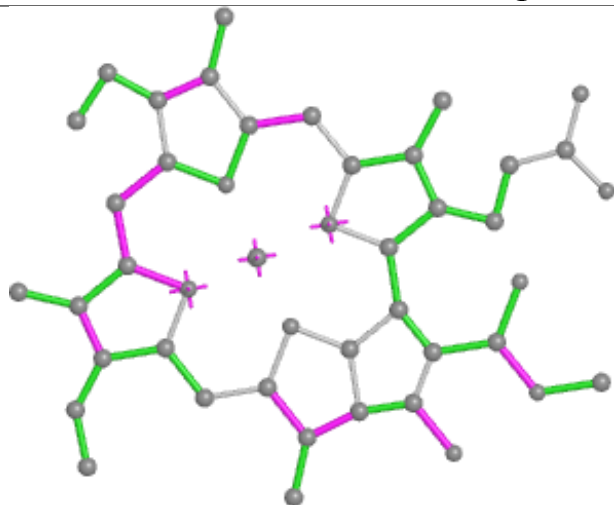
## Ligand CLA G 818



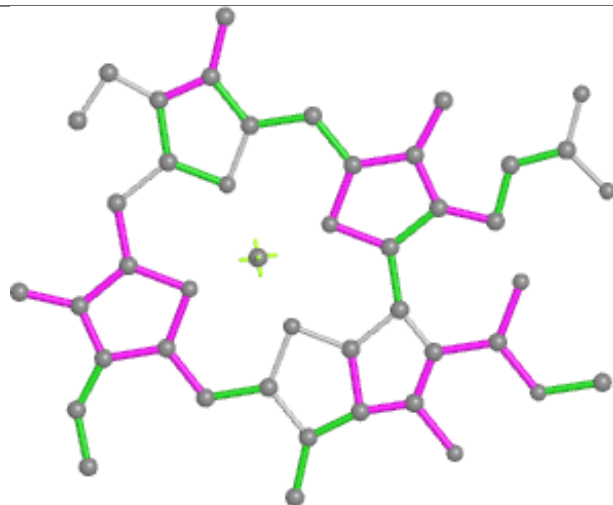
## Ligand CLA Y 810



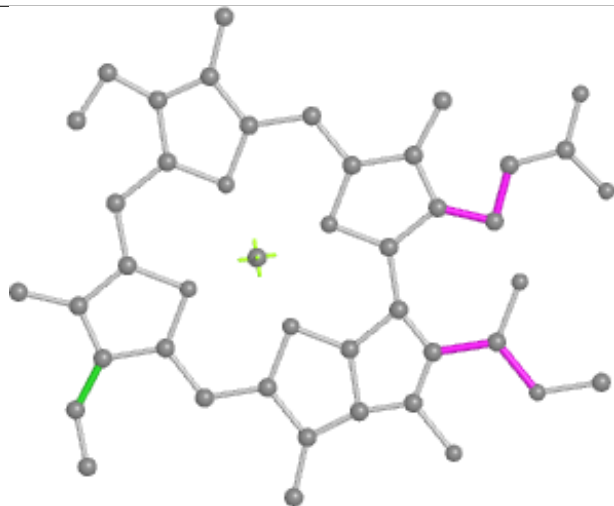
## Ligand CLA H 820



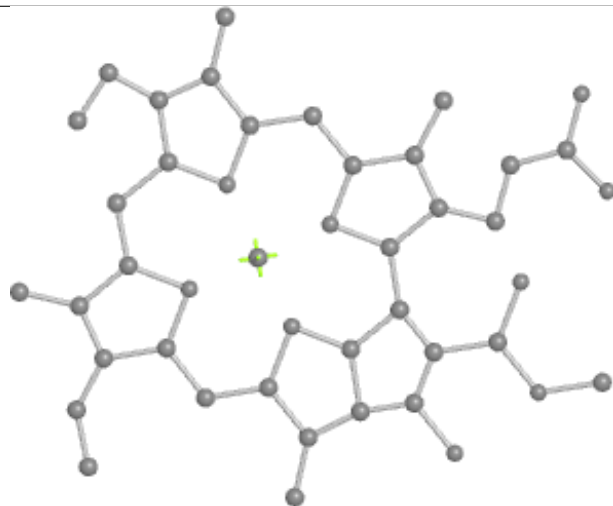
Bond lengths



Bond angles

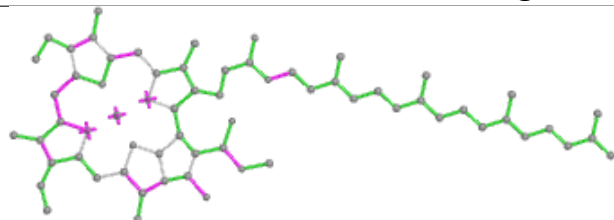


Torsions

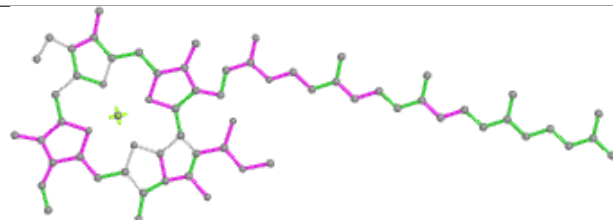


Rings

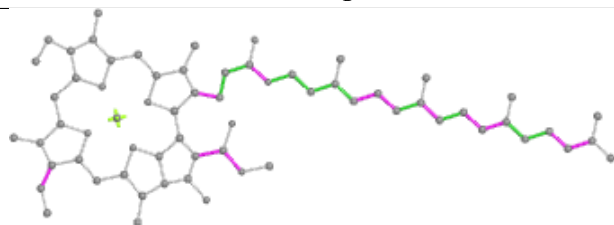
## Ligand CLA L 201



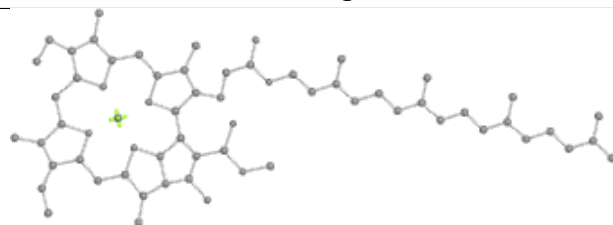
Bond lengths



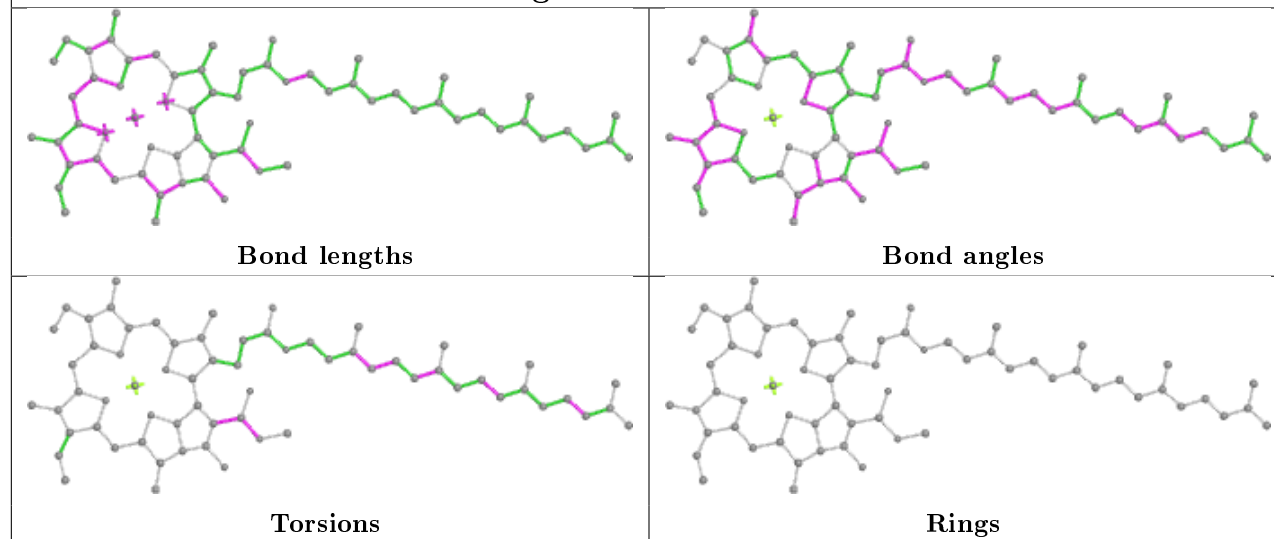
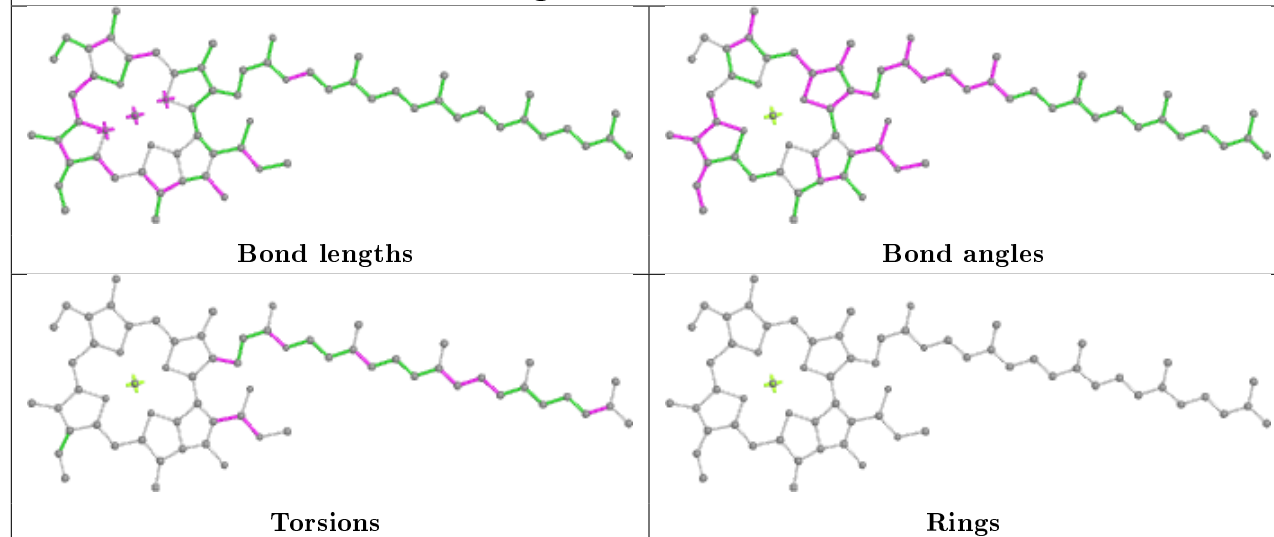
Bond angles

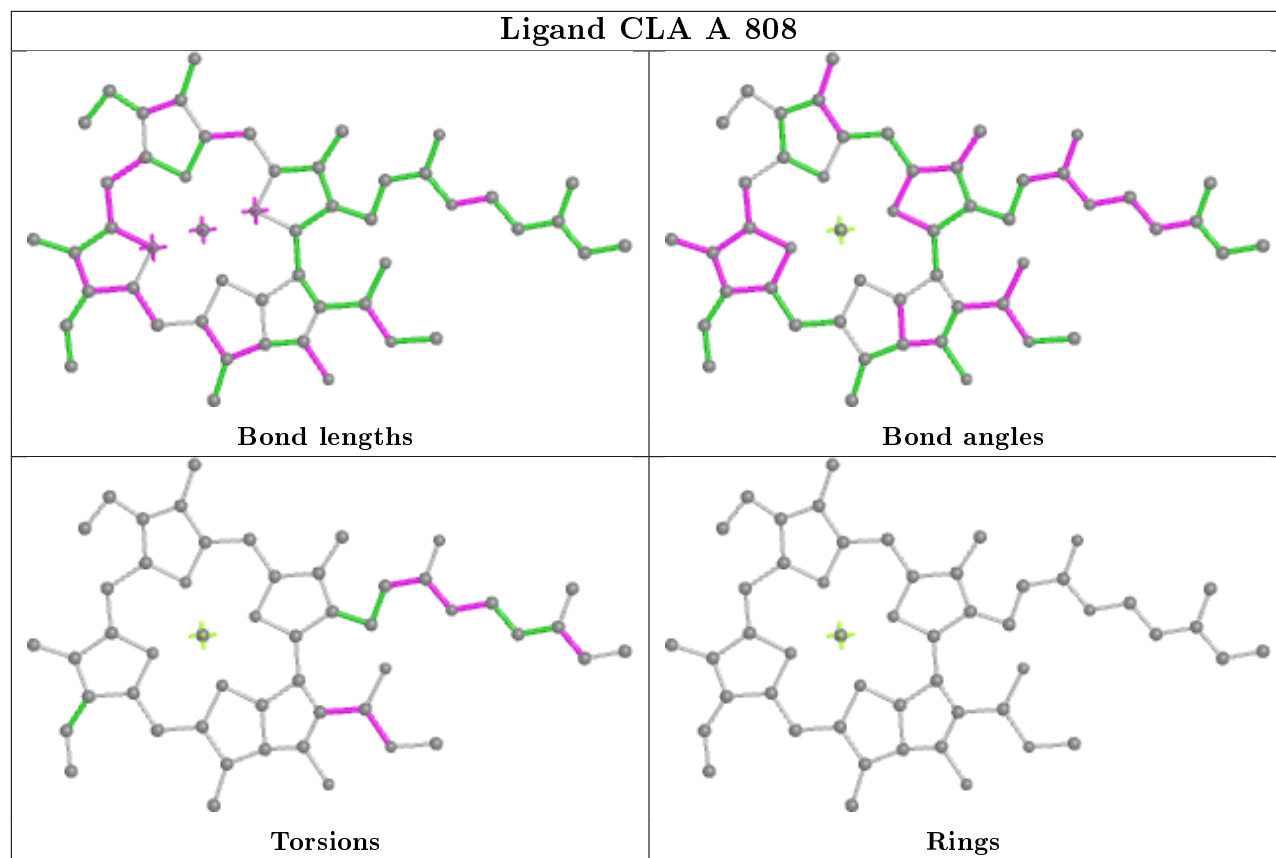


Torsions



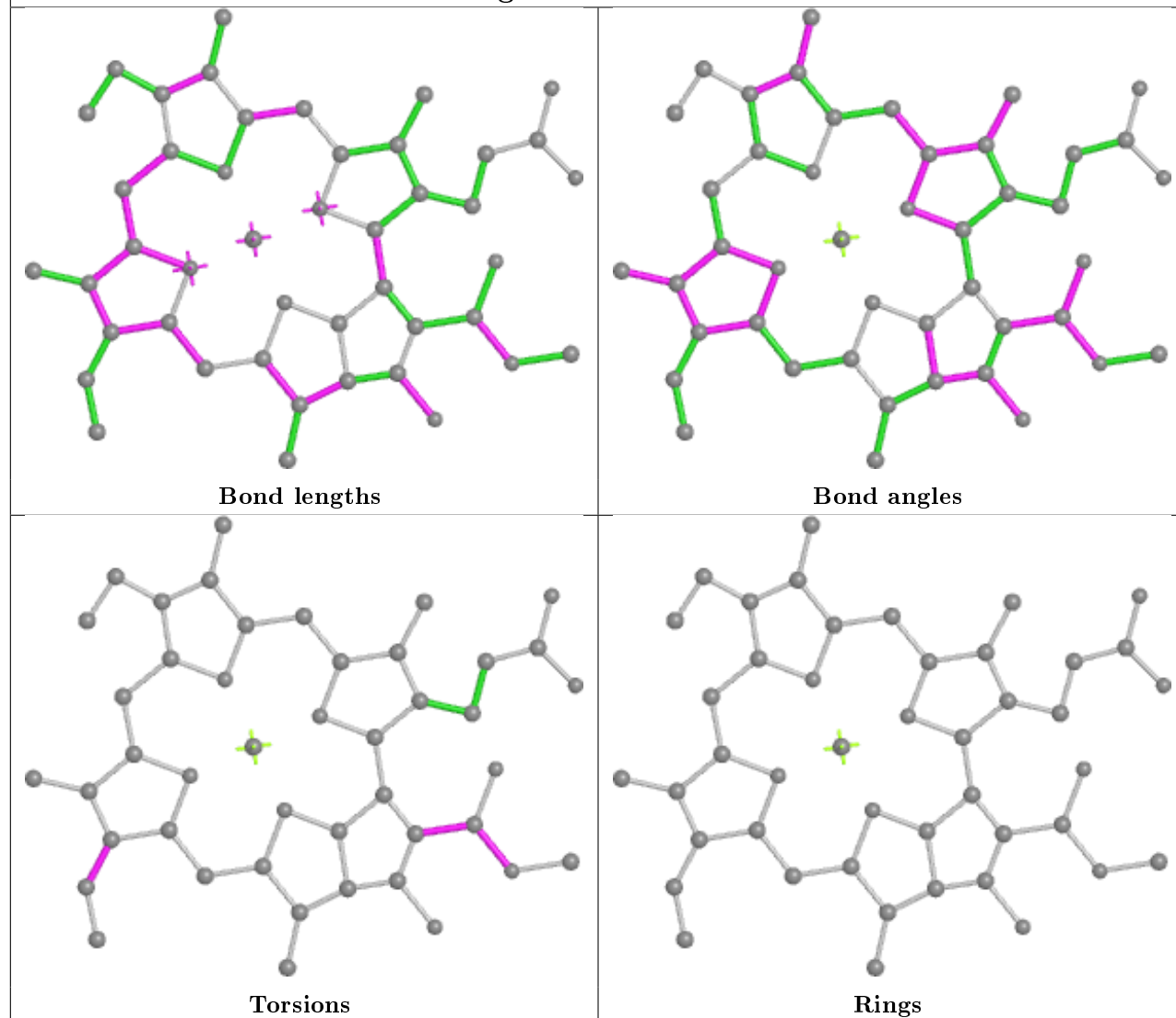
Rings

**Ligand CLA B 806****Ligand CLA B 824**

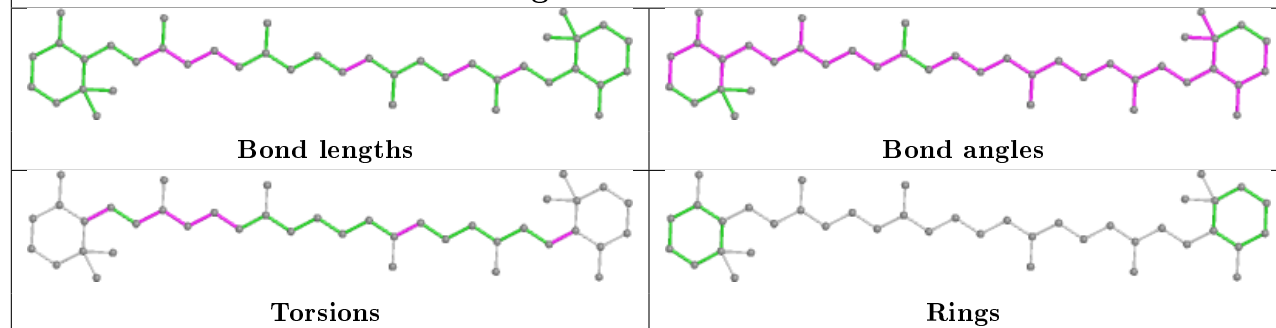




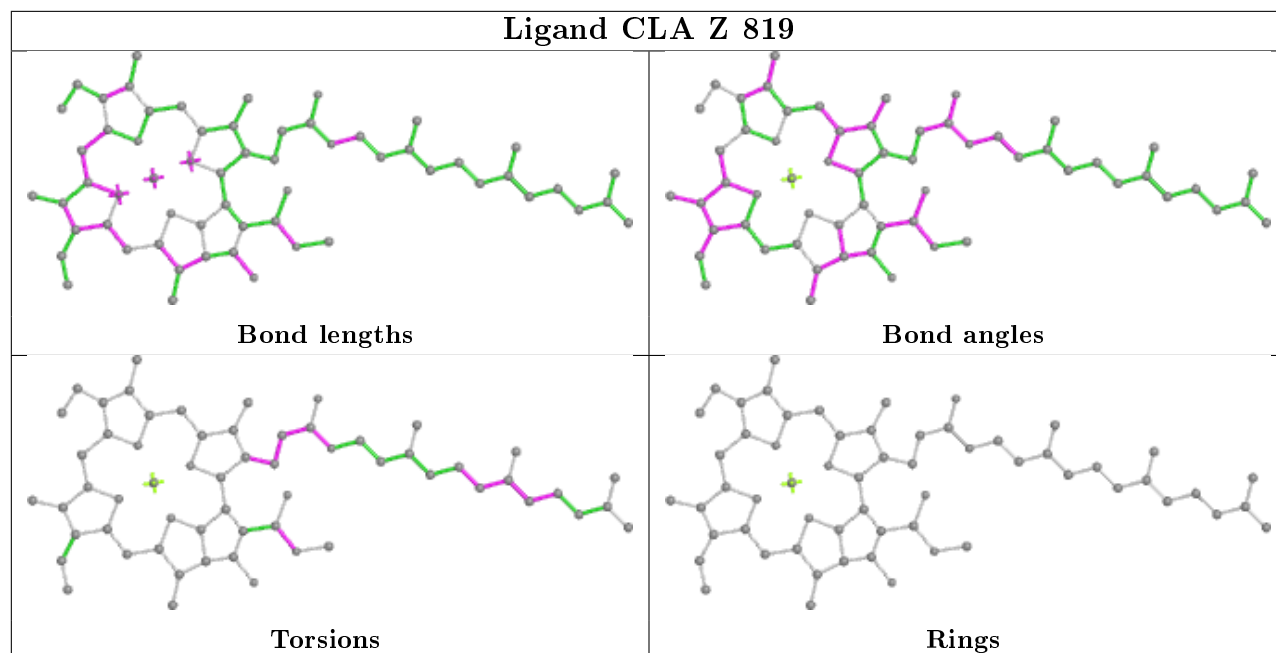
## Ligand CLA f 101



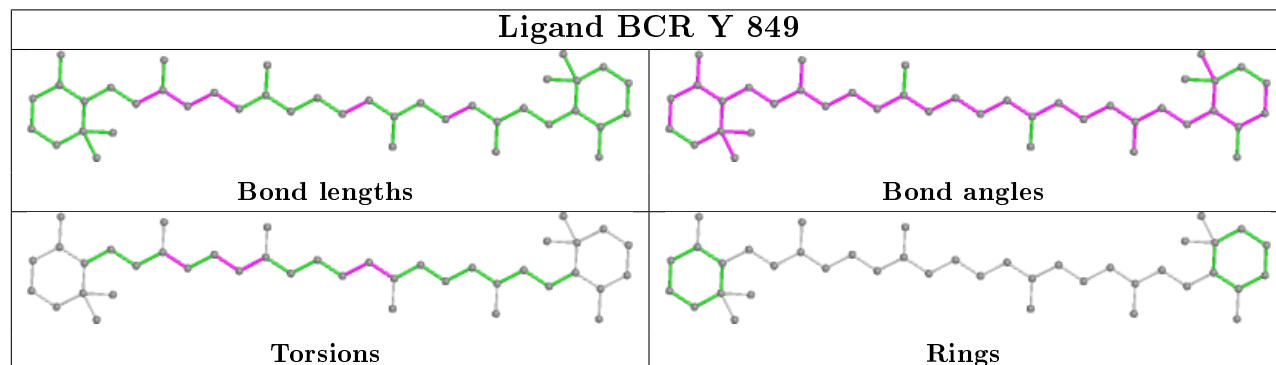
## Ligand BCR B 846



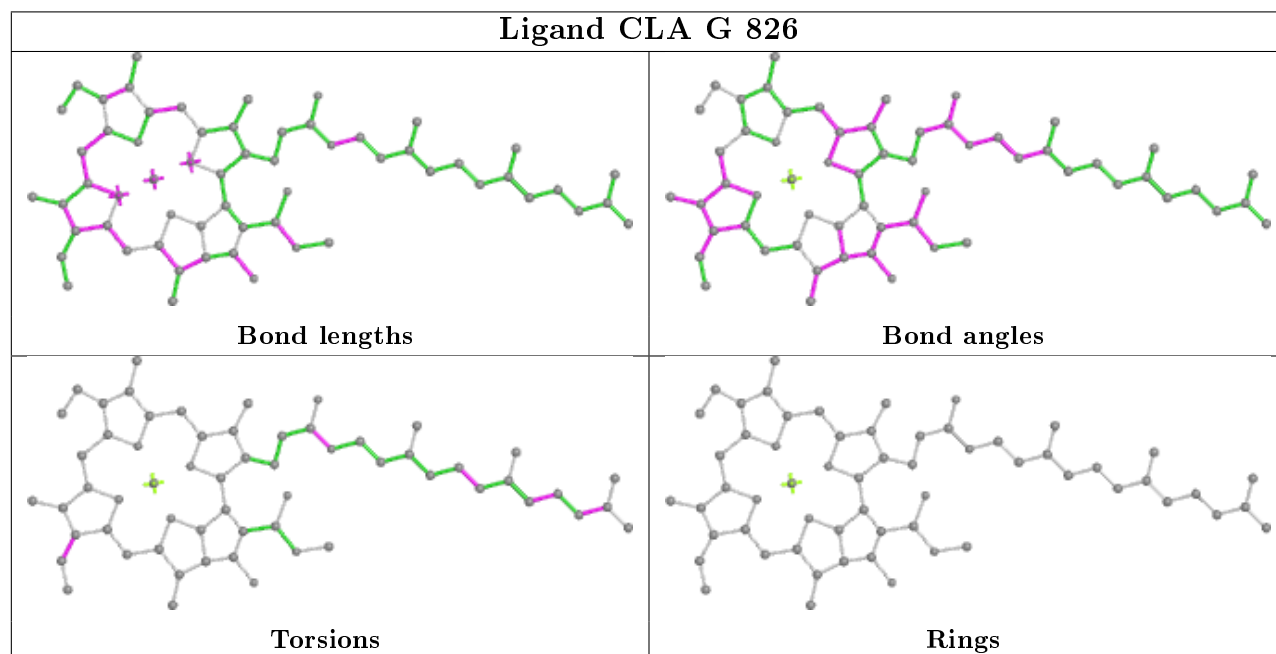
## Ligand CLA Z 819



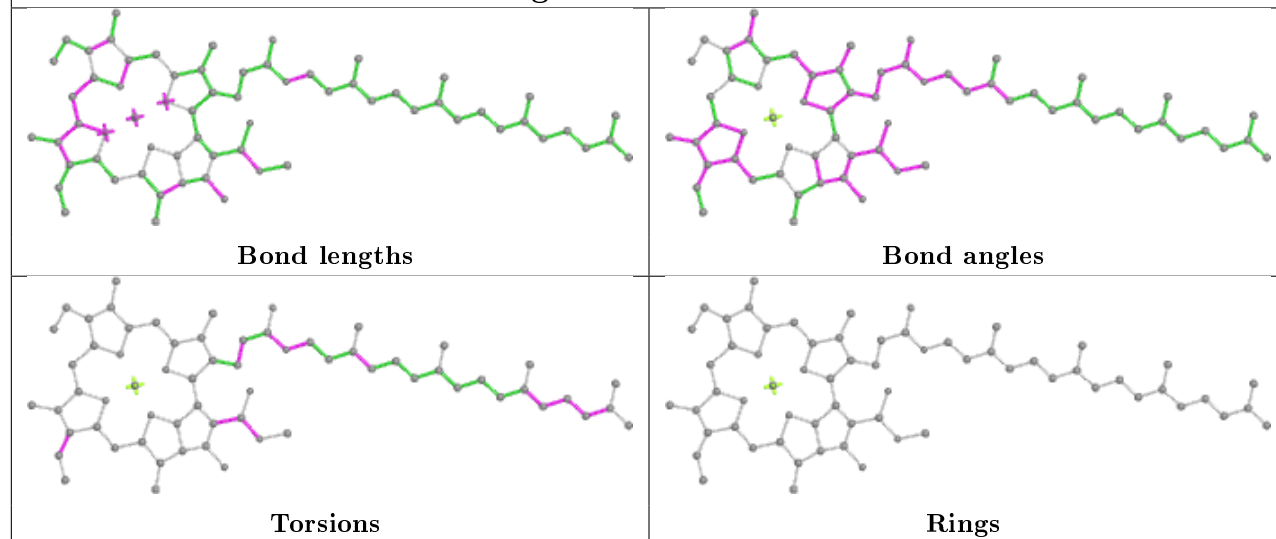
## Ligand BCR Y 849



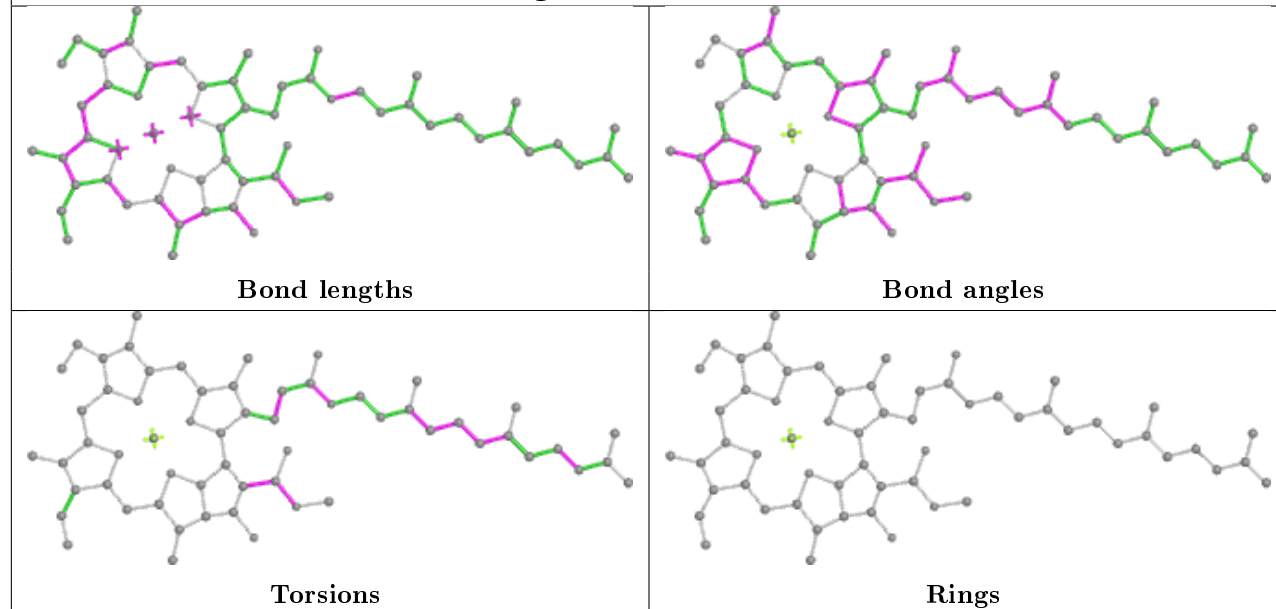
## Ligand CLA G 826



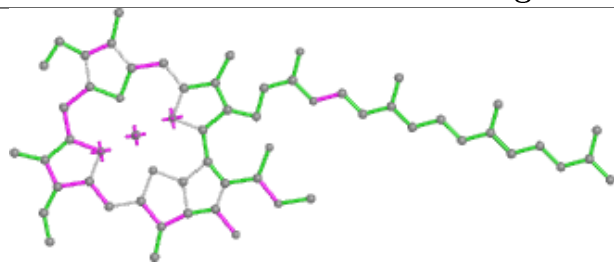
## Ligand CLA H 810



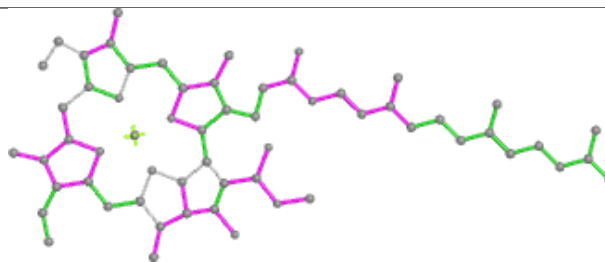
## Ligand CLA A 818



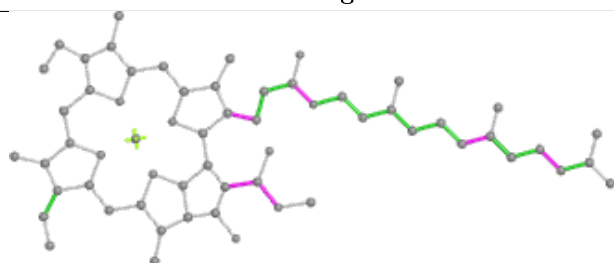
## Ligand CLA A 814



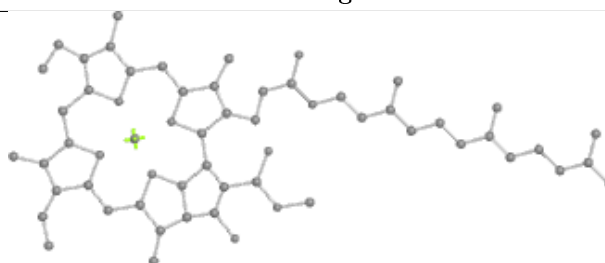
Bond lengths



Bond angles

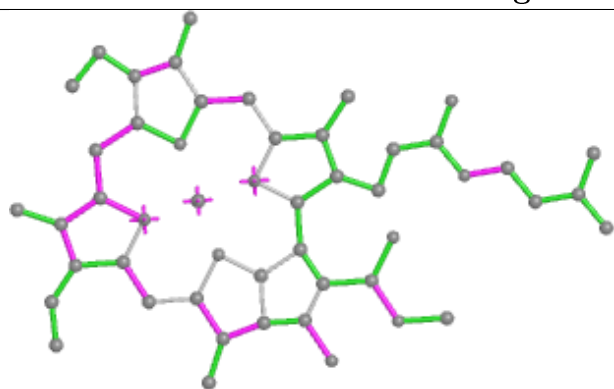


Torsions

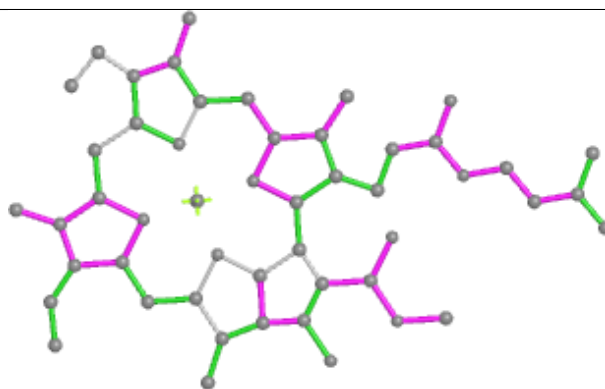


Rings

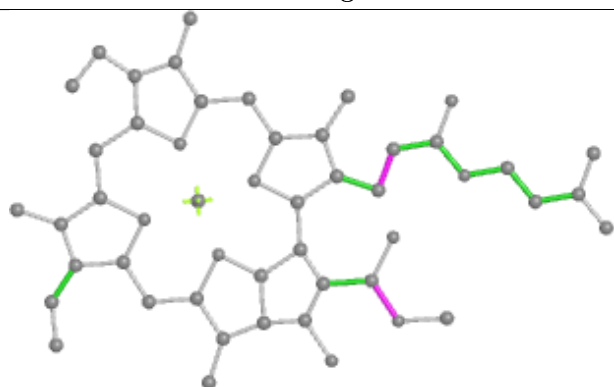
## Ligand CLA G 842



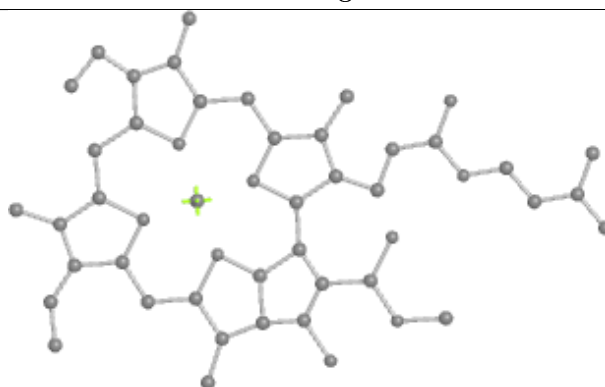
Bond lengths



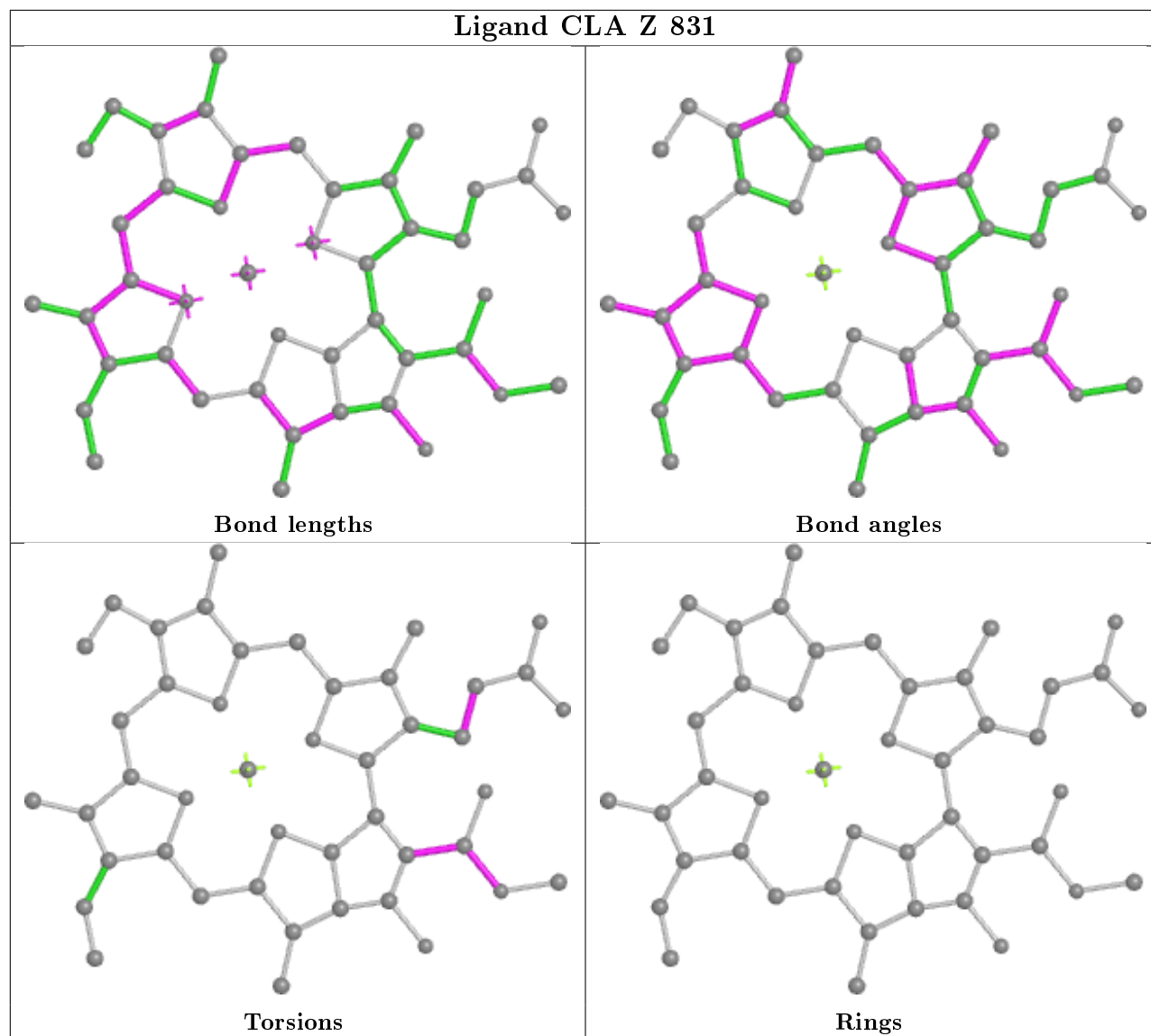
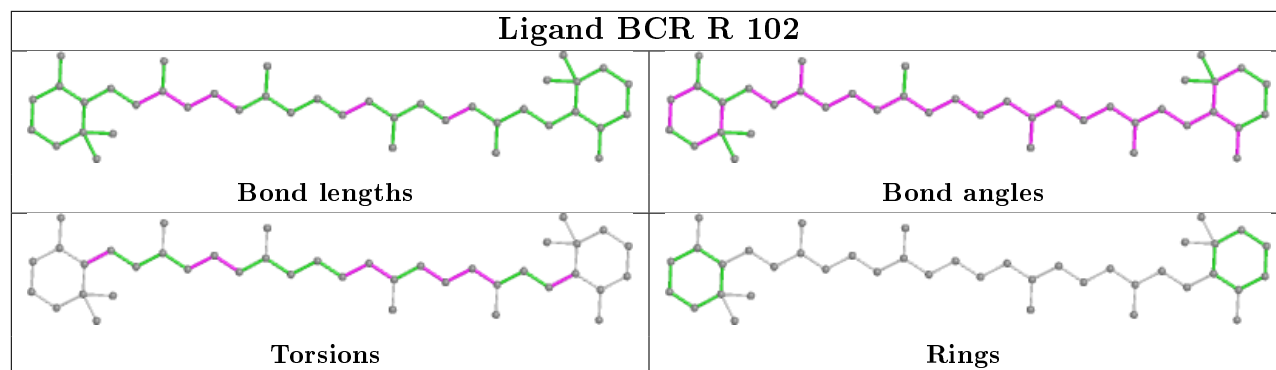
Bond angles

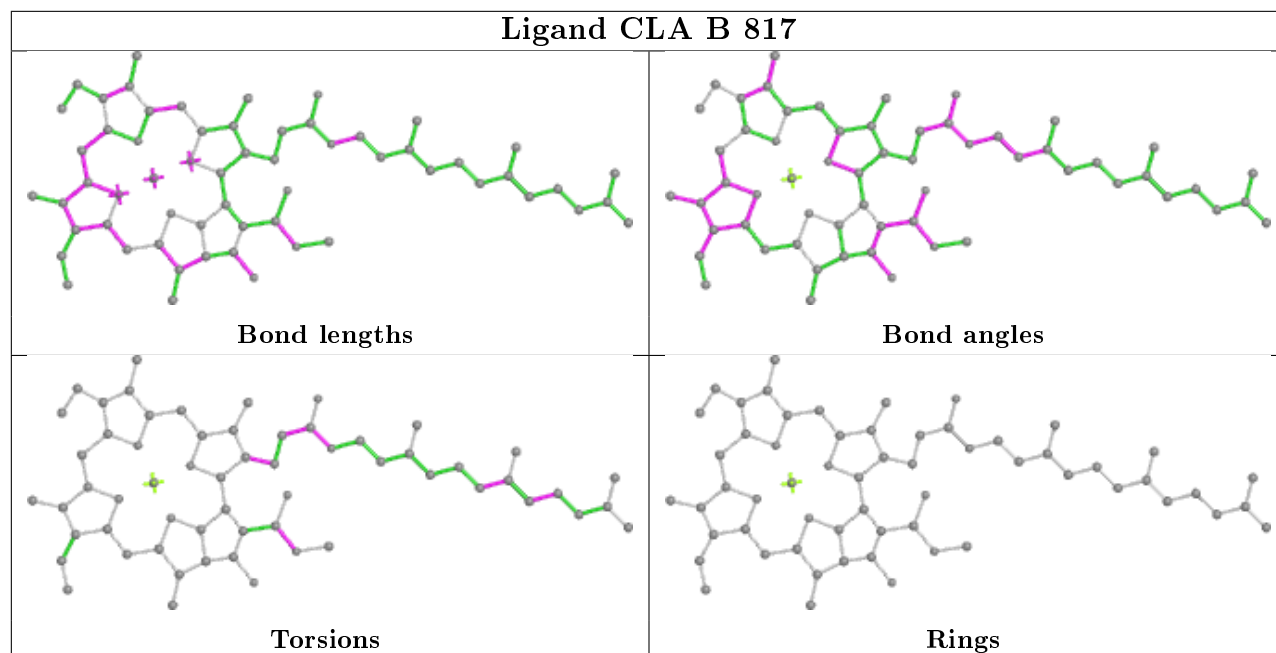
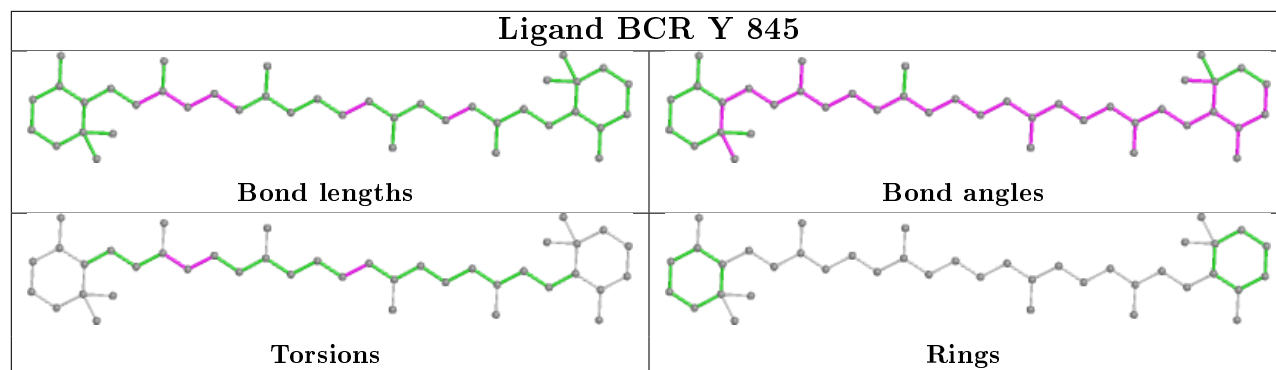


Torsions

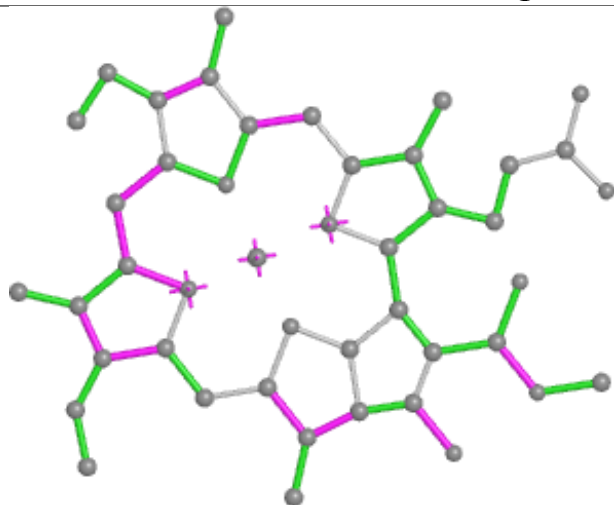


Rings

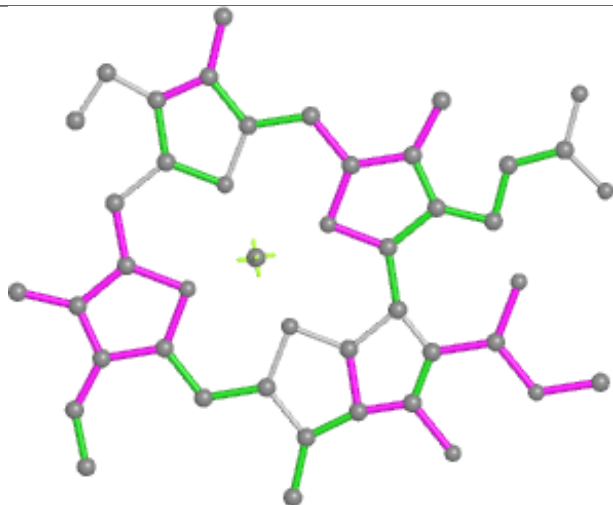




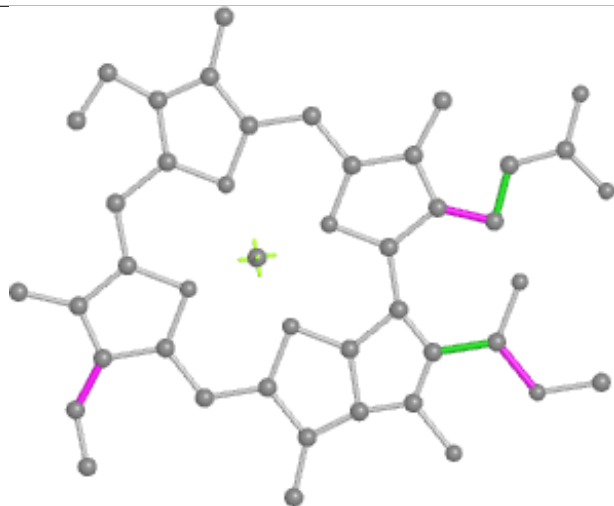
## Ligand CLA Z 832



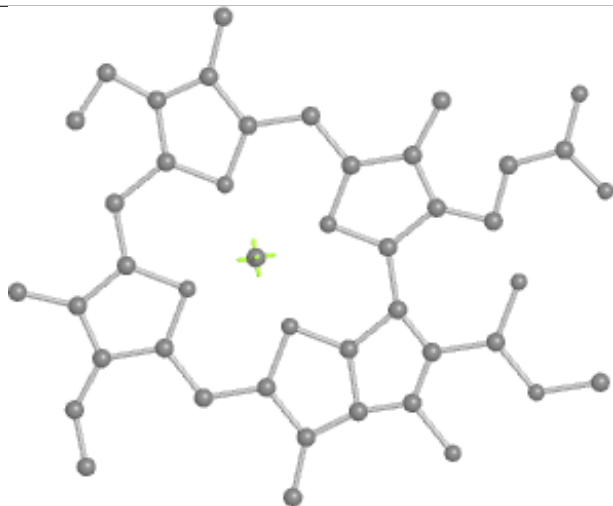
Bond lengths



Bond angles

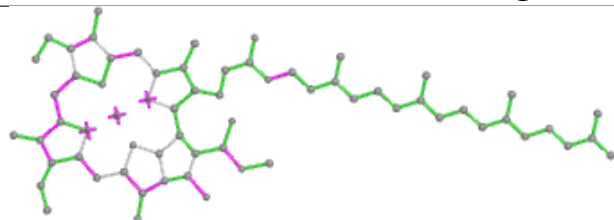


Torsions

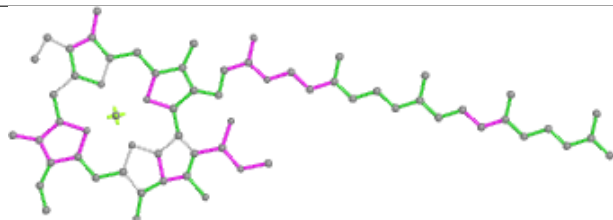


Rings

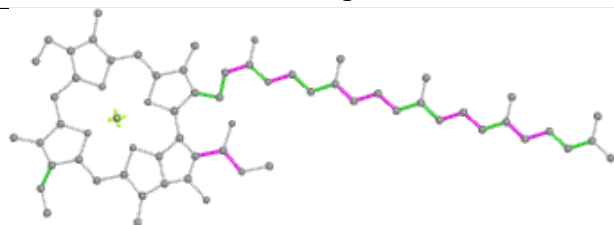
## Ligand CLA A 810



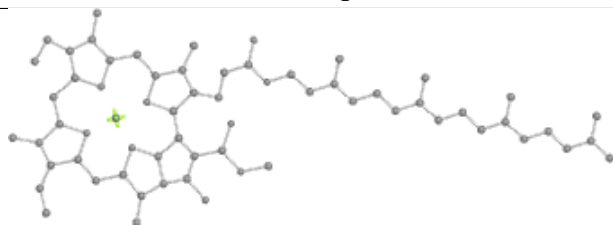
Bond lengths



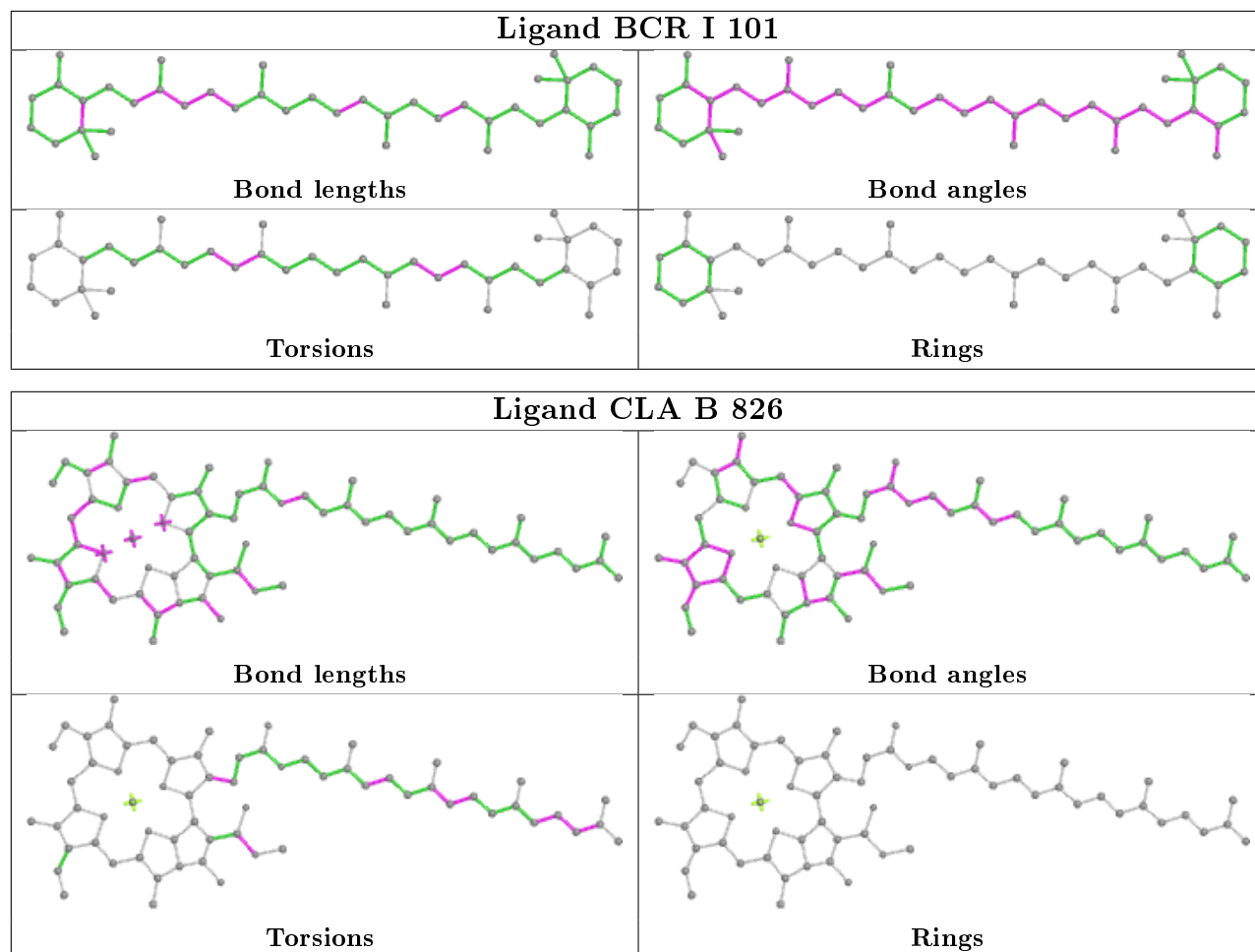
Bond angles



Torsions

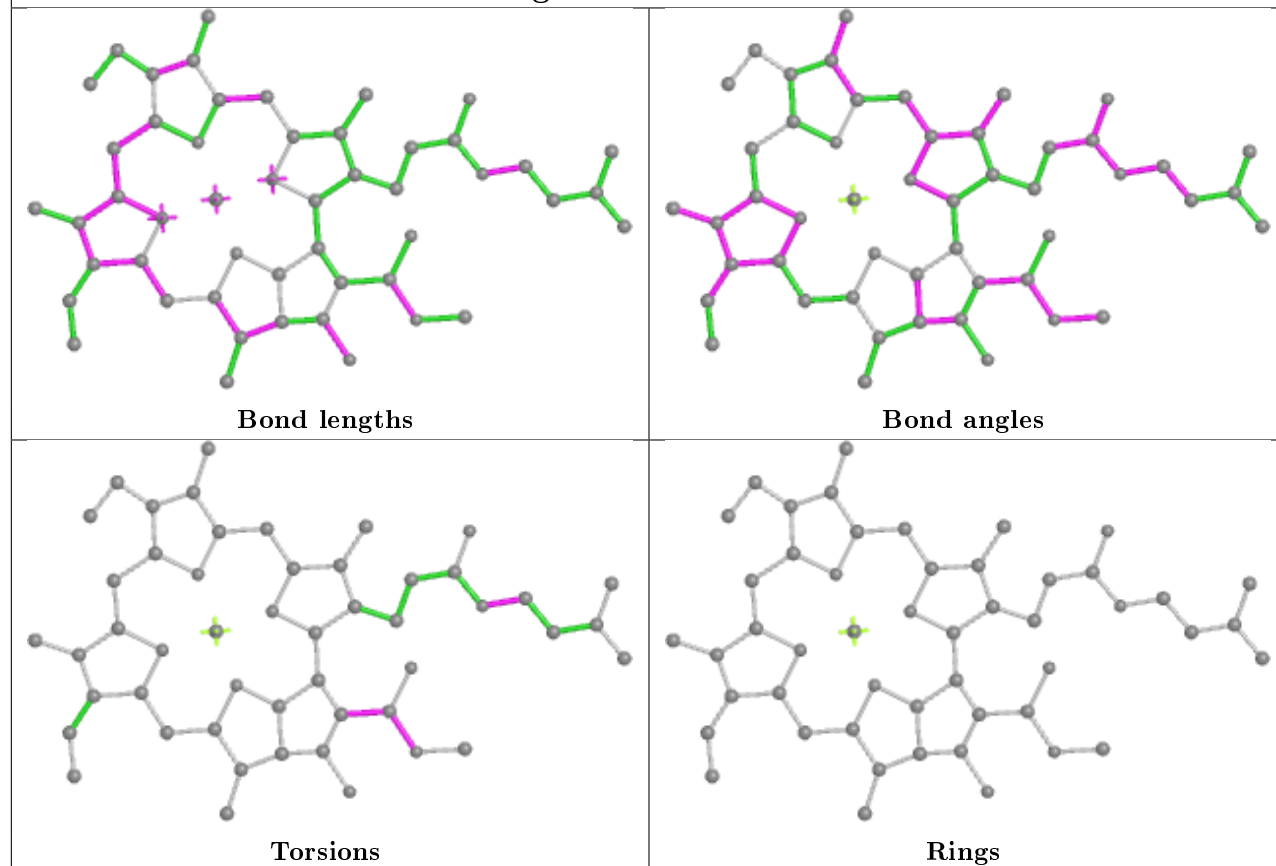


Rings

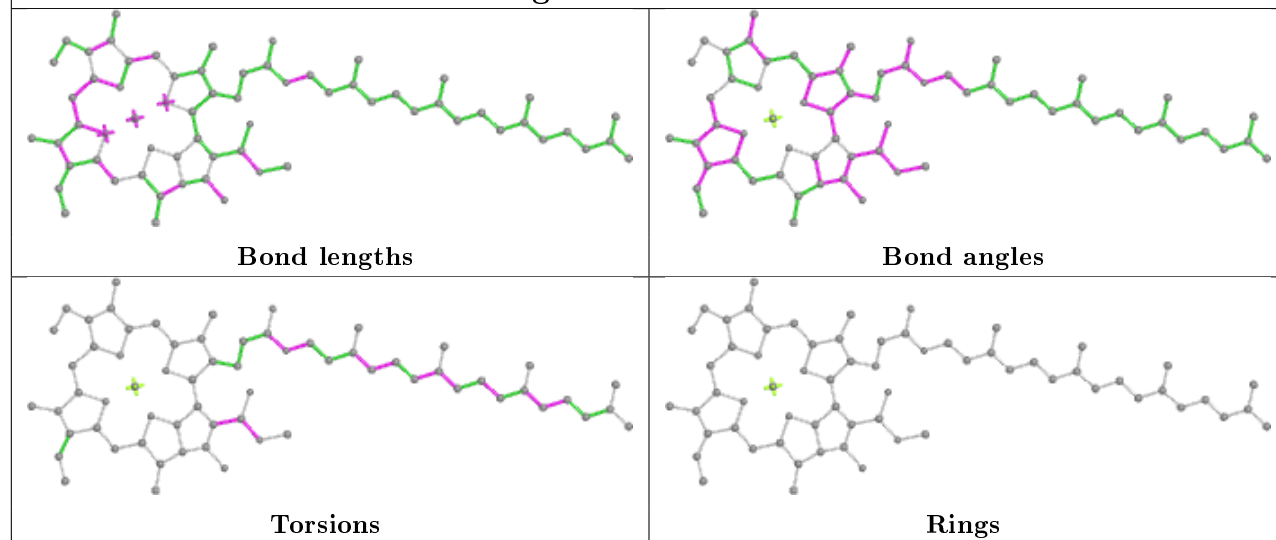


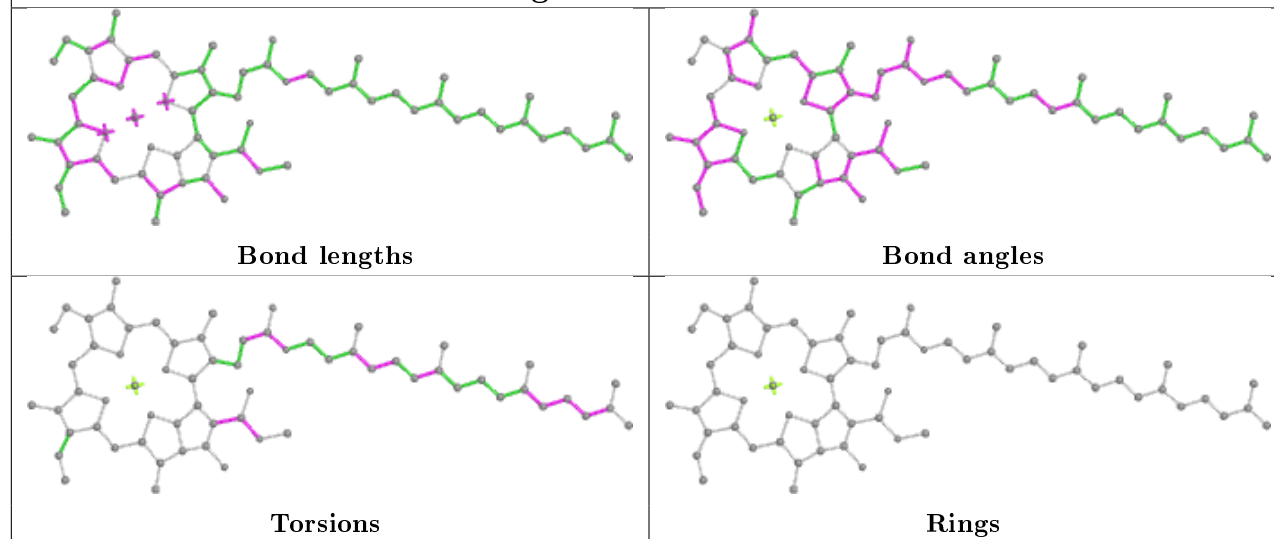
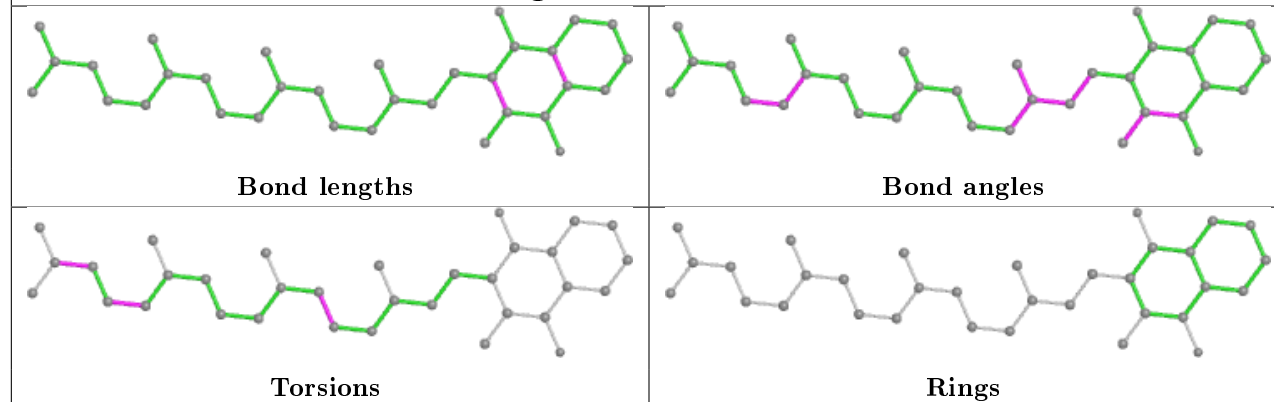


## Ligand CLA A 840

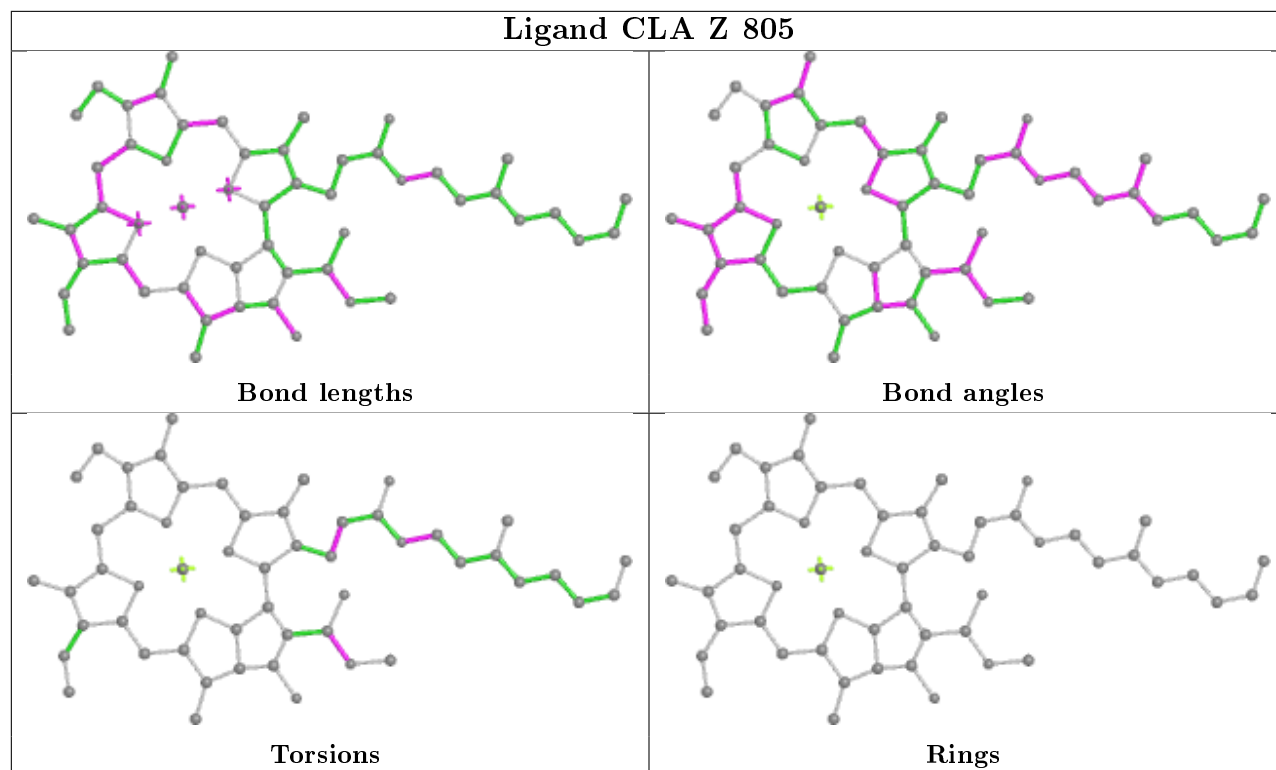


## Ligand CLA B 809

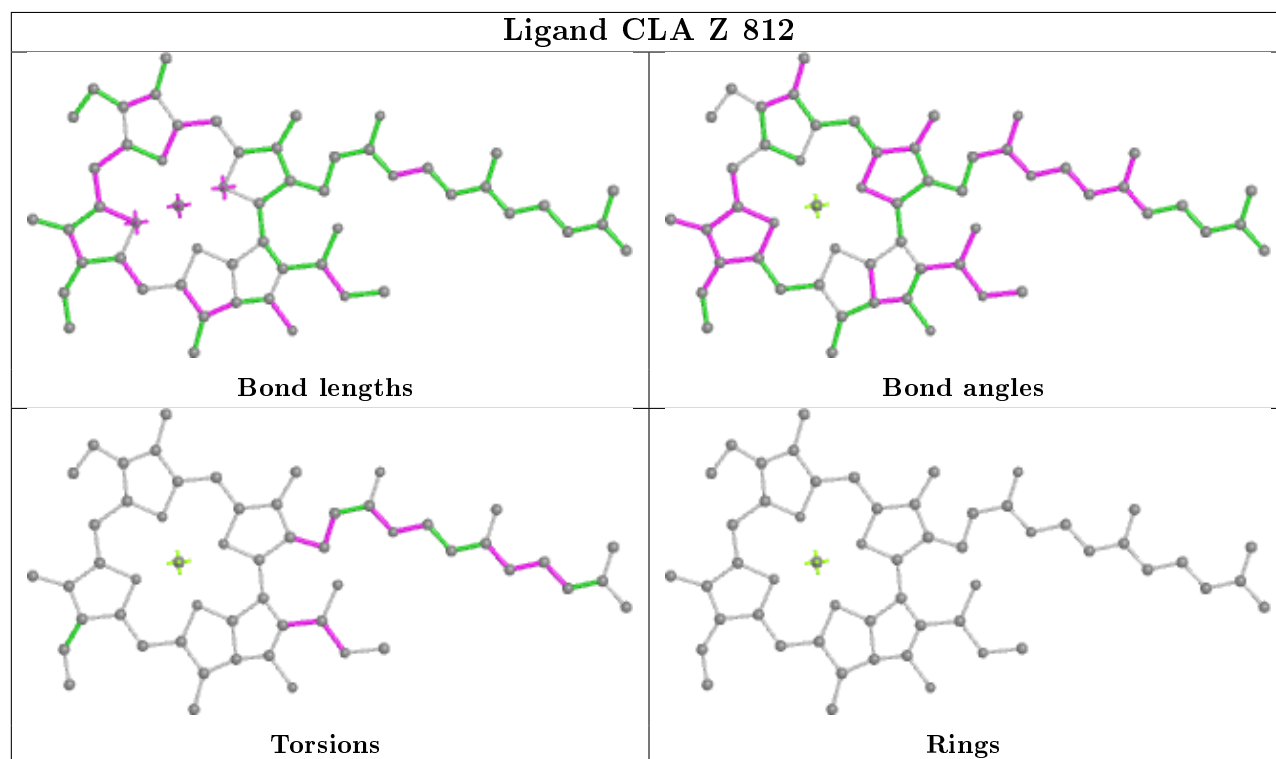


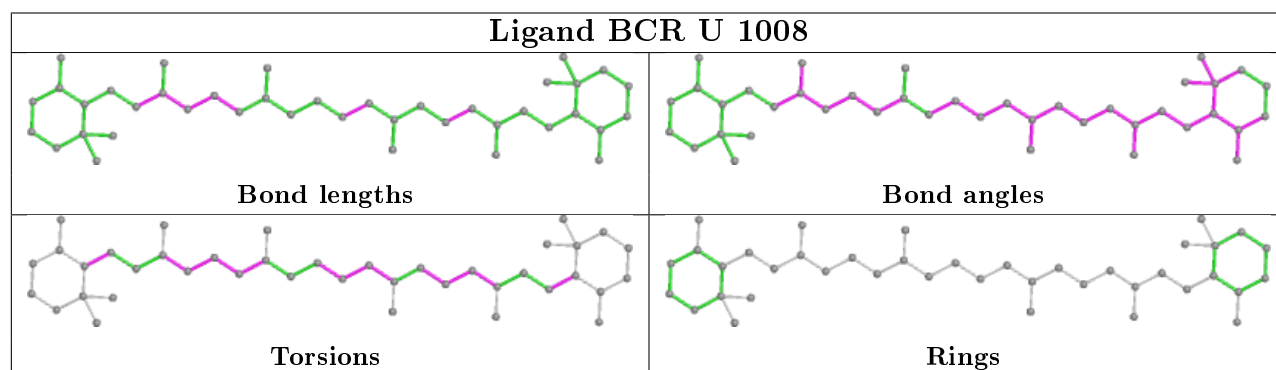
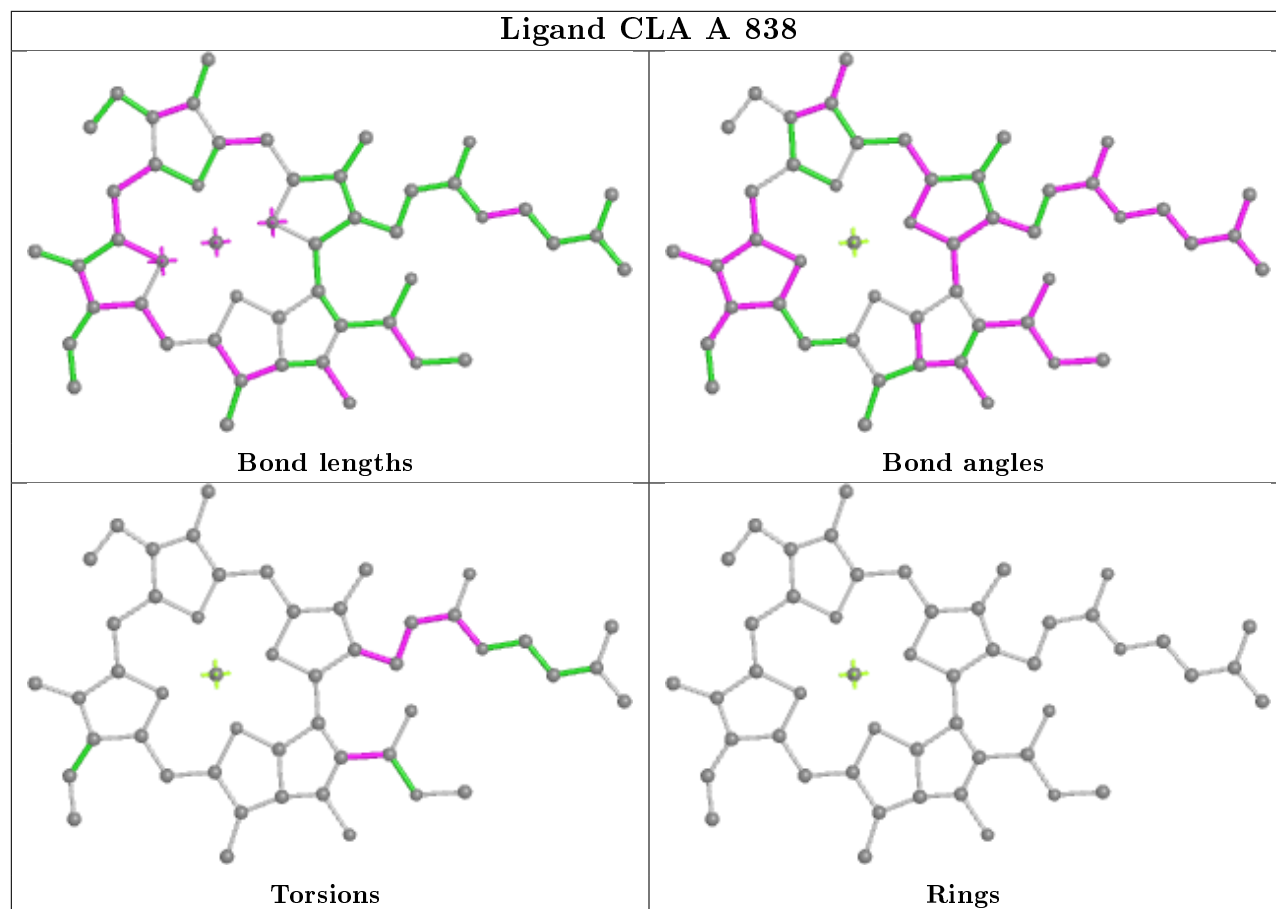
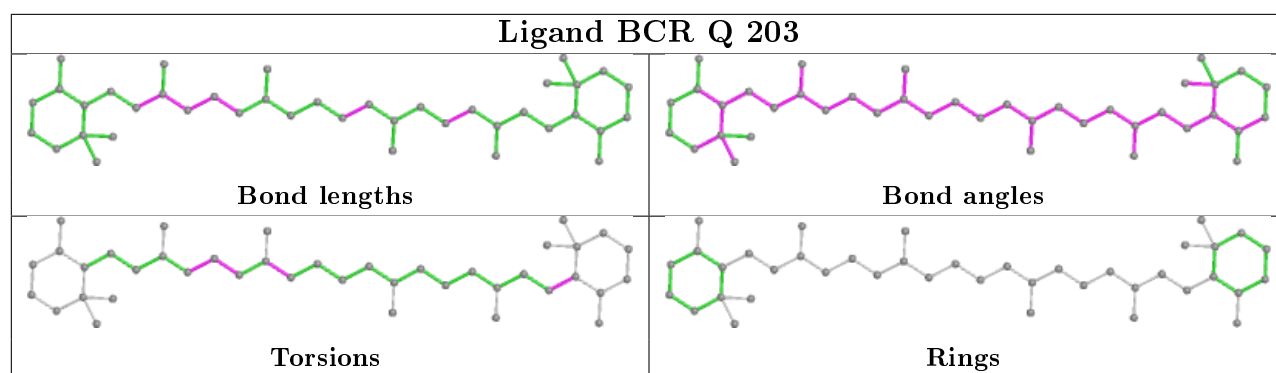
**Ligand CLA H 809****Ligand PQN A 844**

## Ligand CLA Z 805

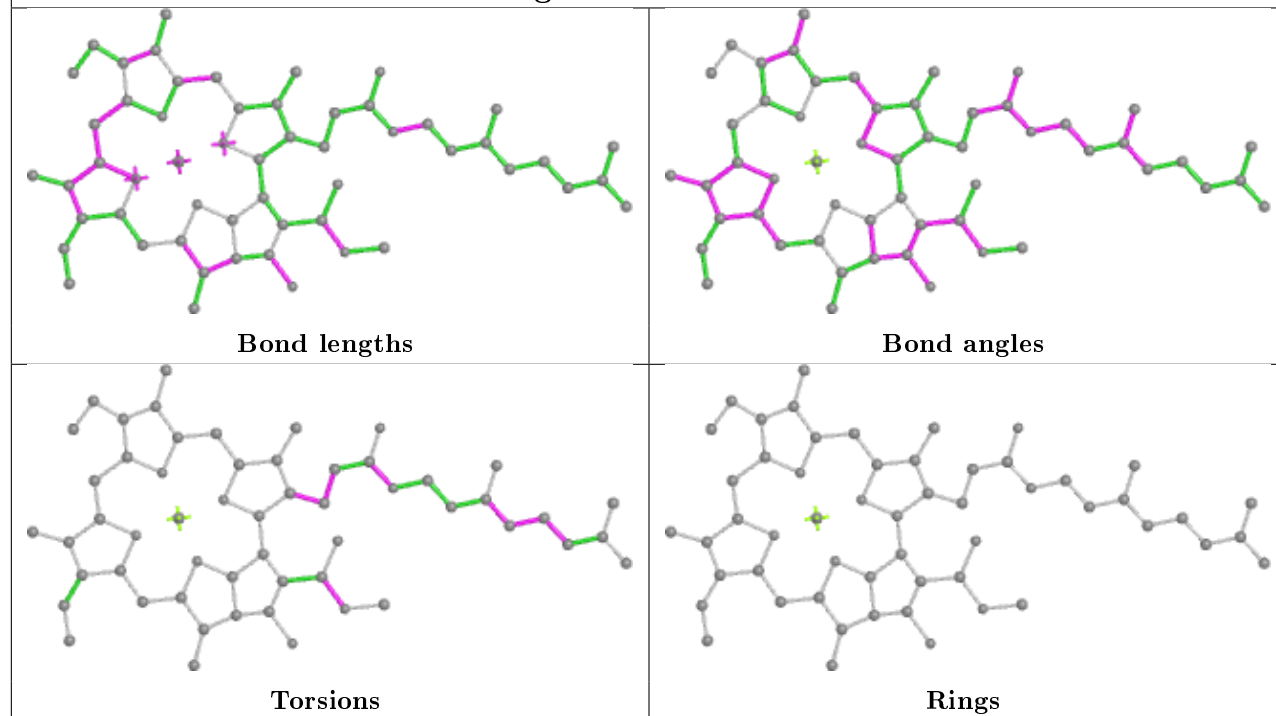


## Ligand CLA Z 812

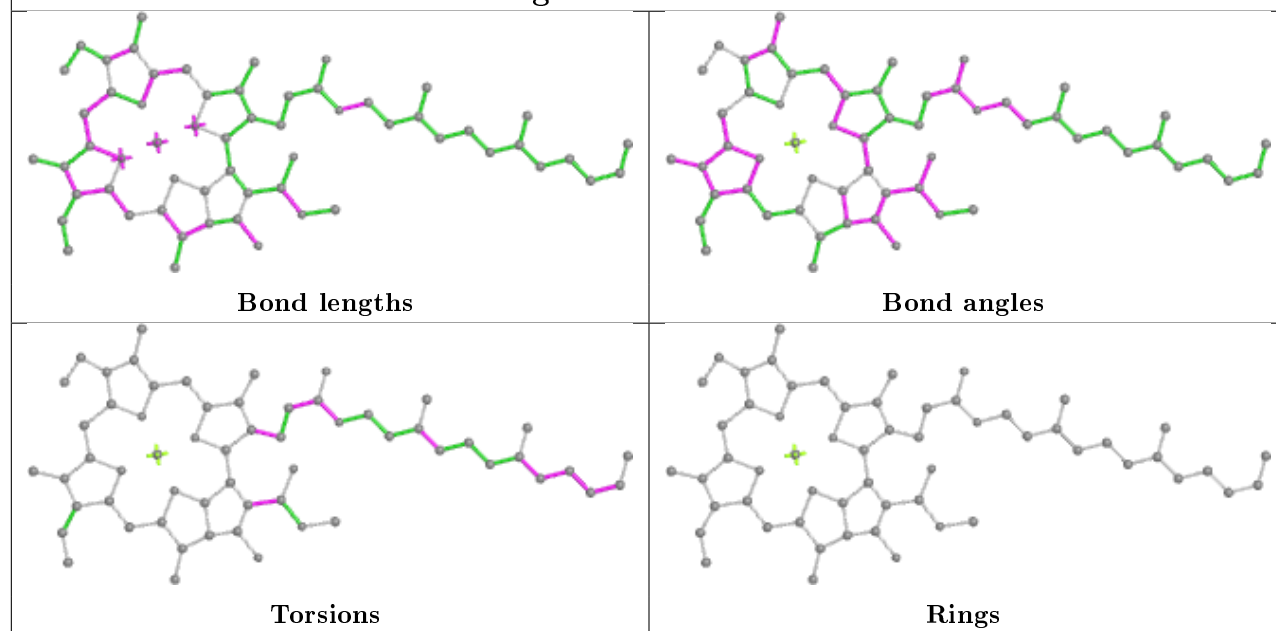


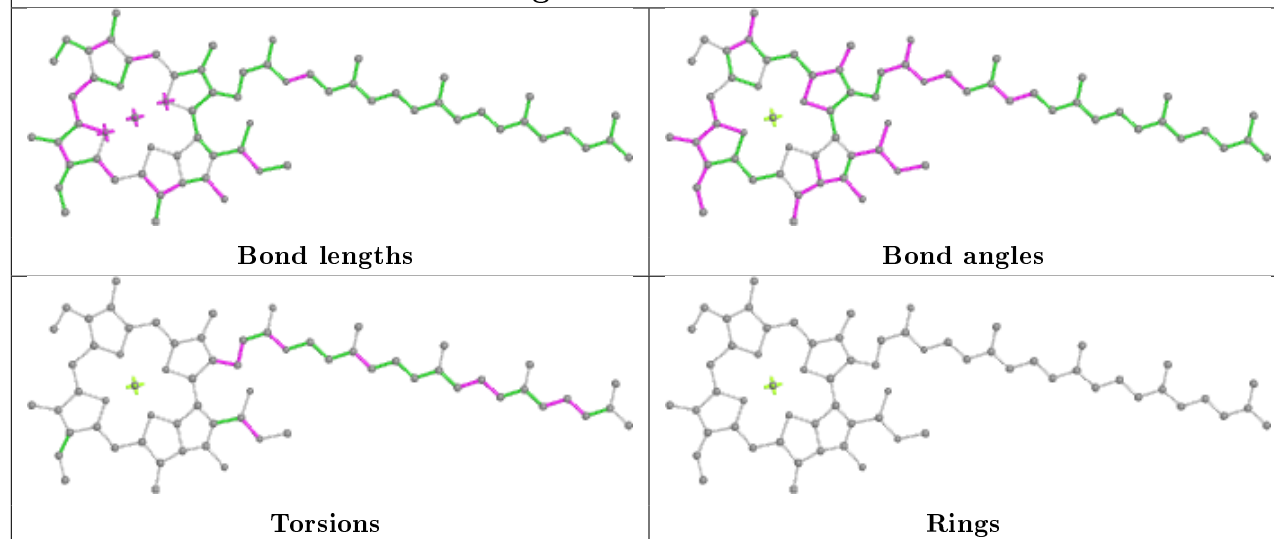
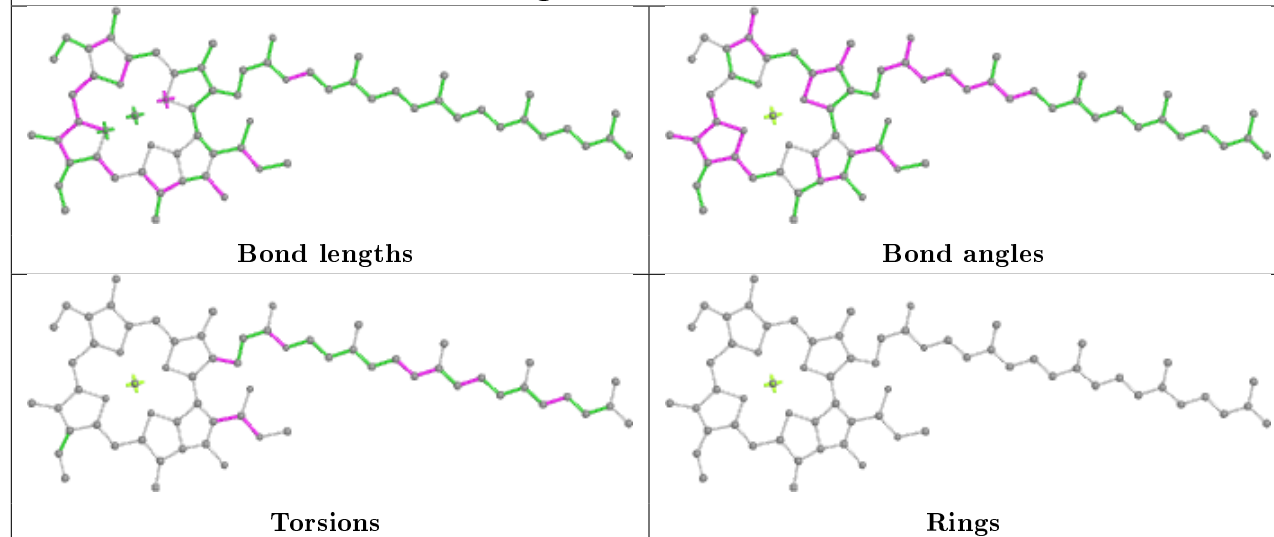


## Ligand CLA Z 817

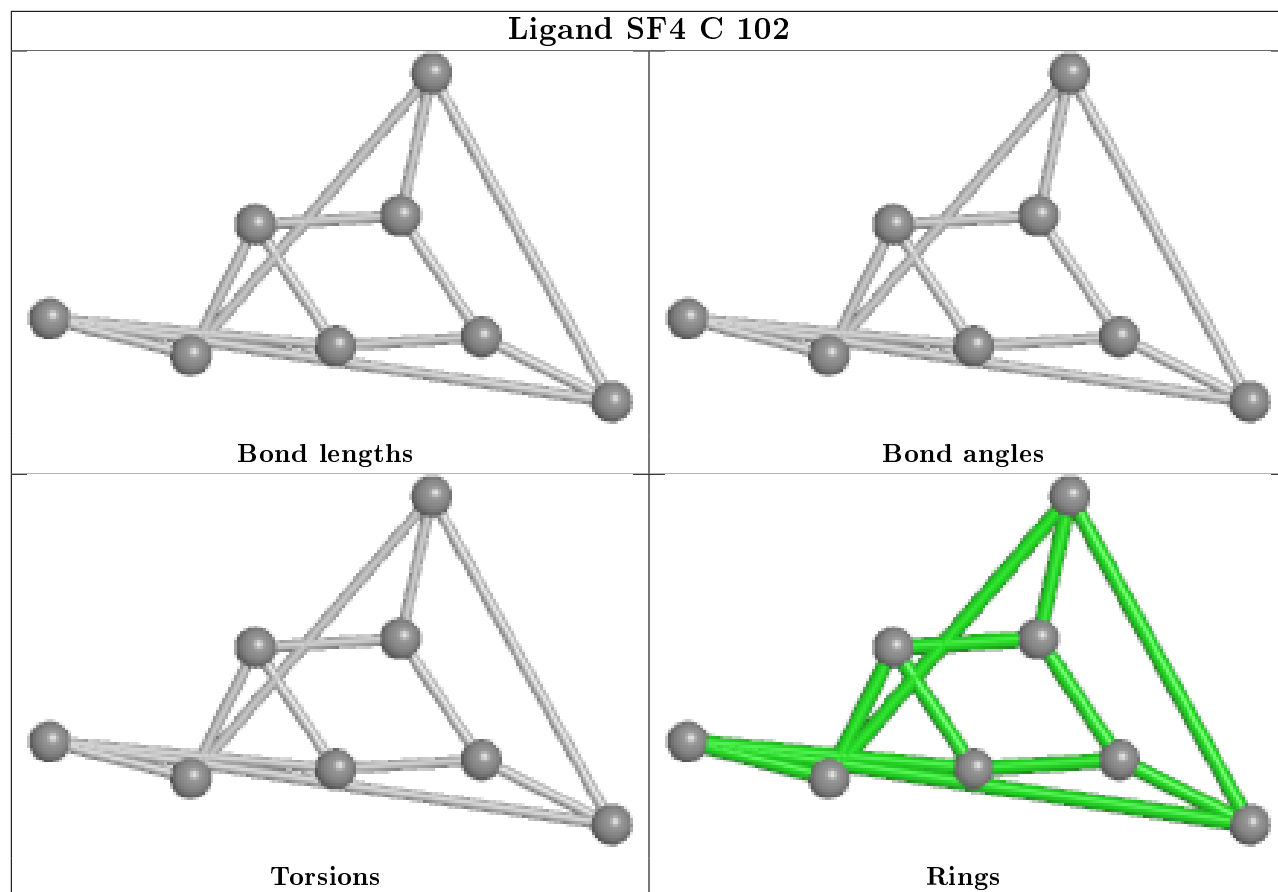


## Ligand CLA A 805

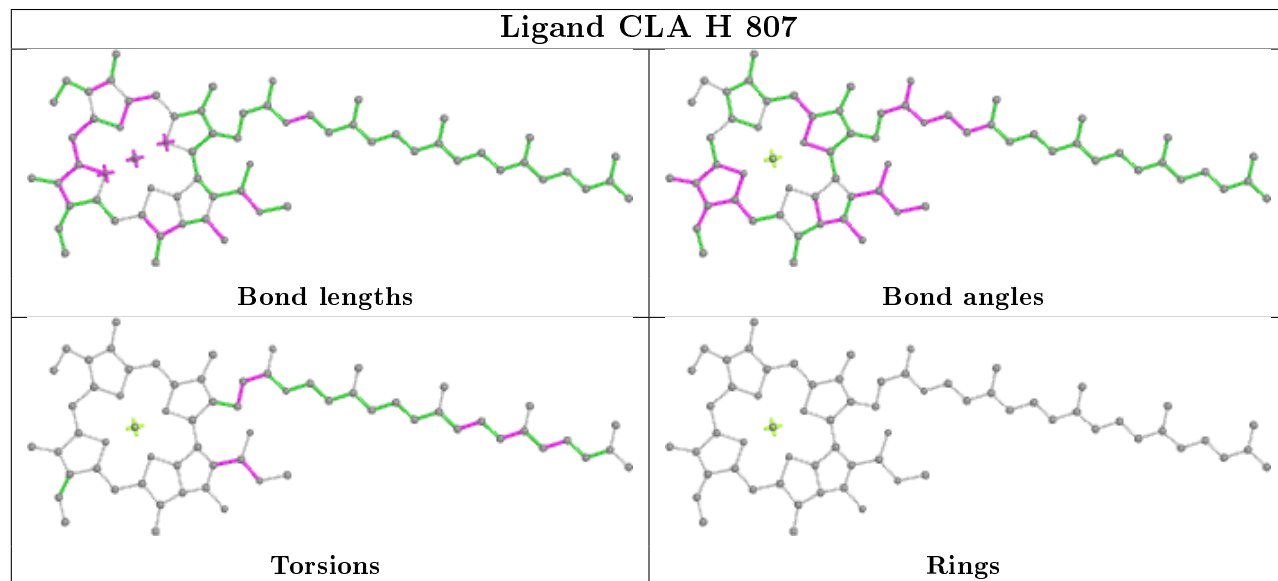


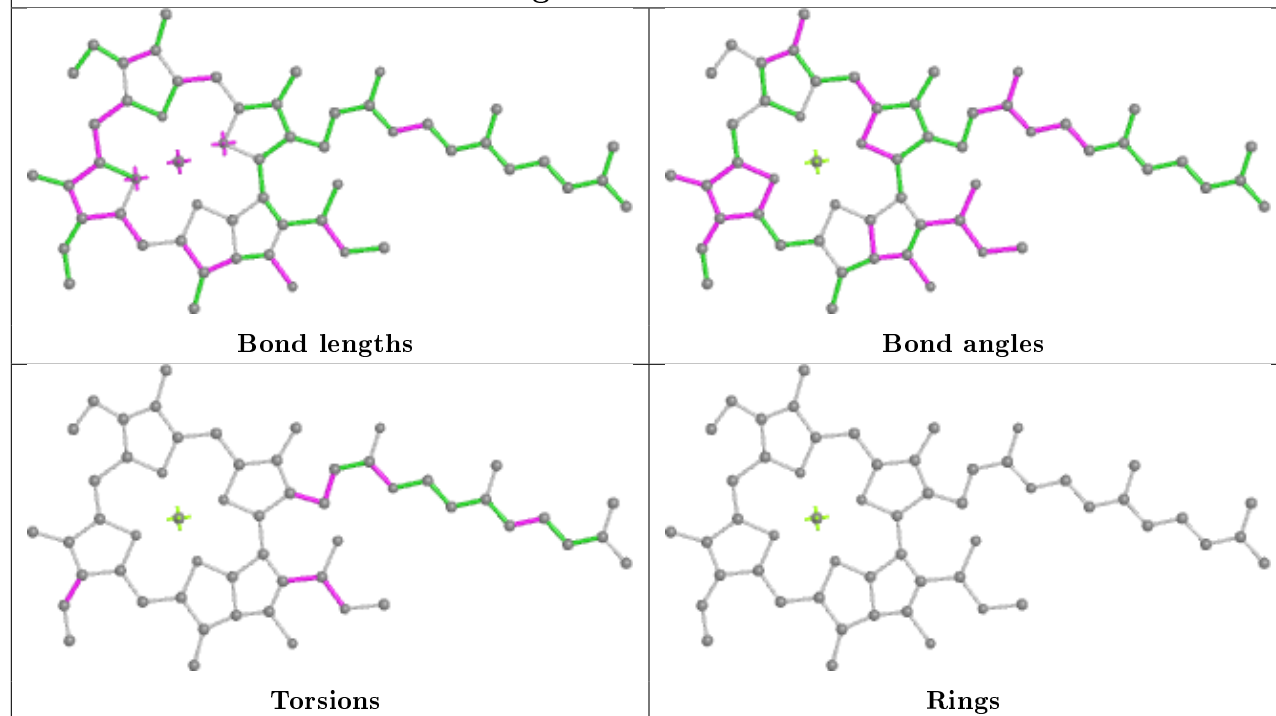
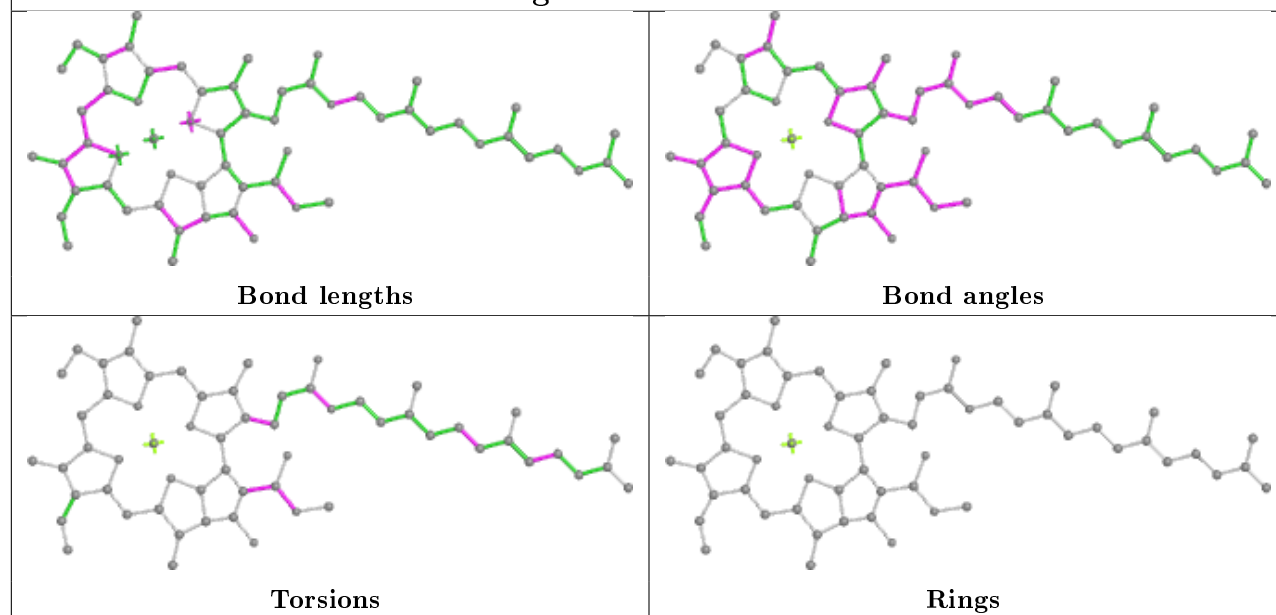
**Ligand CLA A 812****Ligand CLA h 201**

## Ligand SF4 C 102

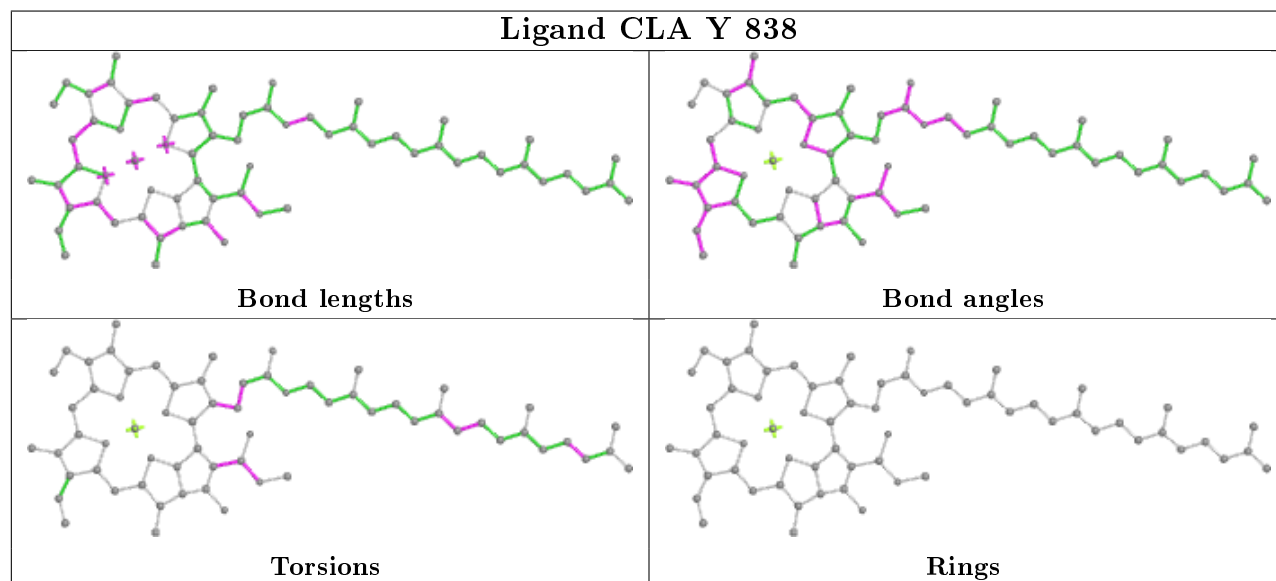
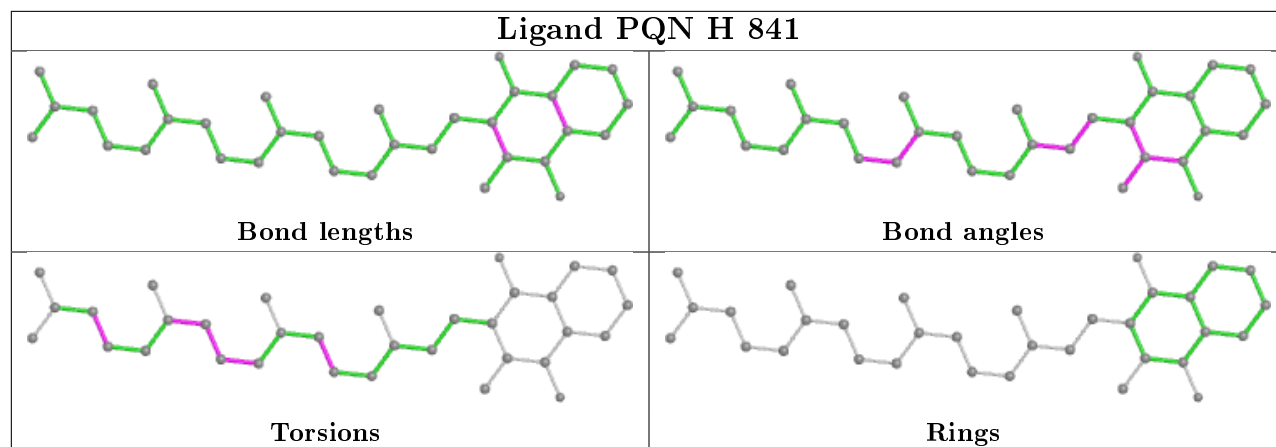


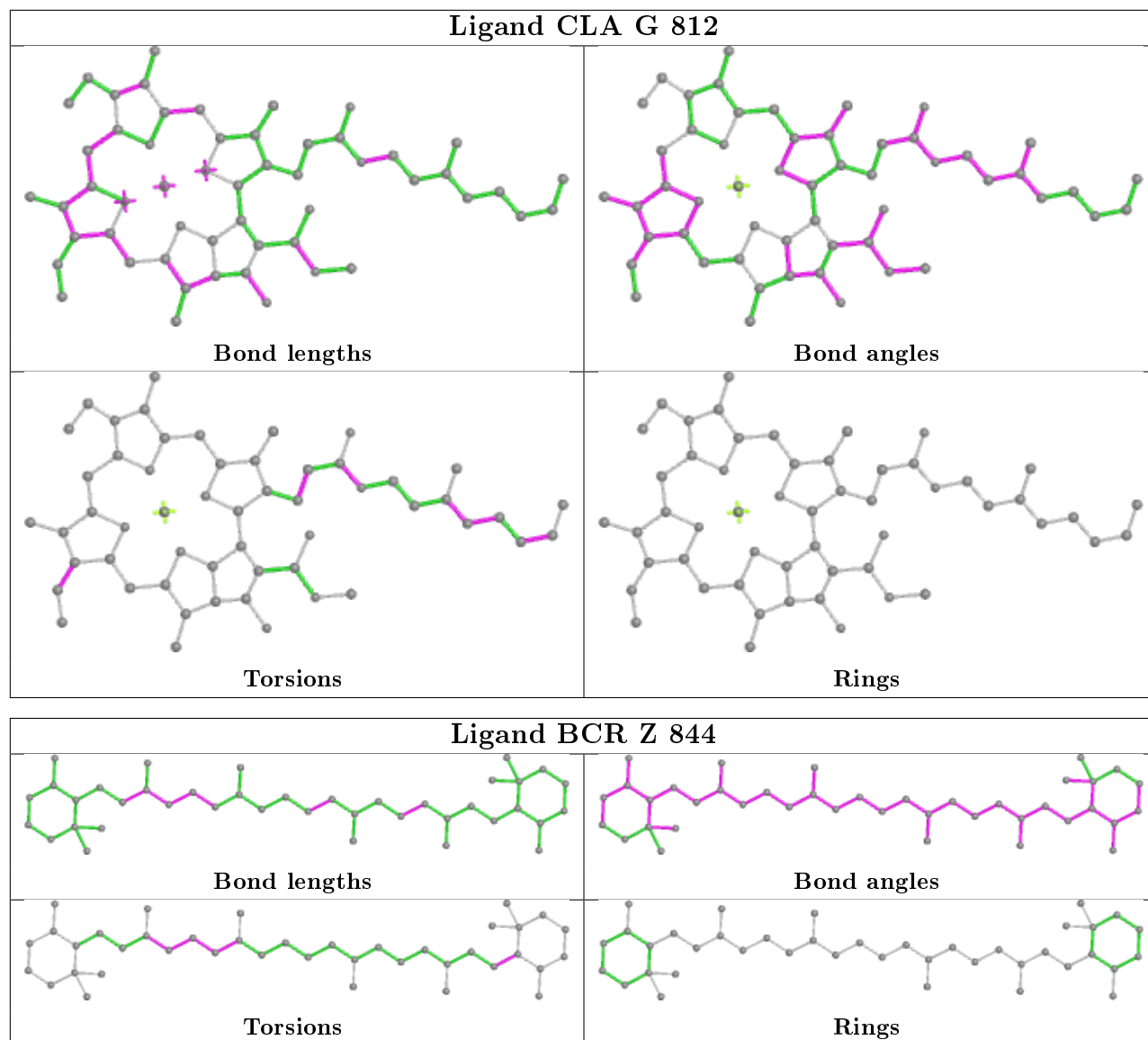
## Ligand CLA H 807



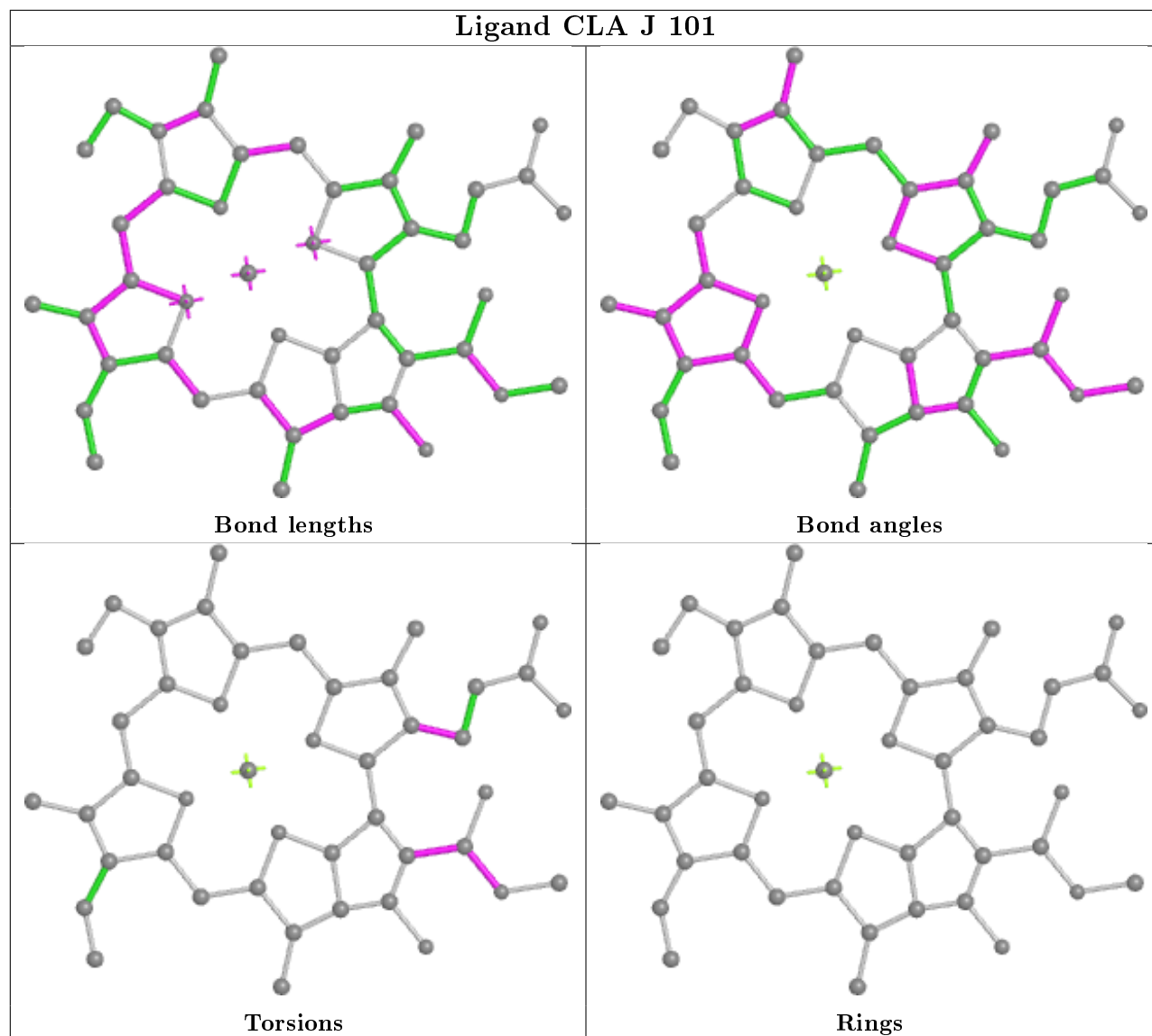
**Ligand CLA Y 833****Ligand CLA B 836**

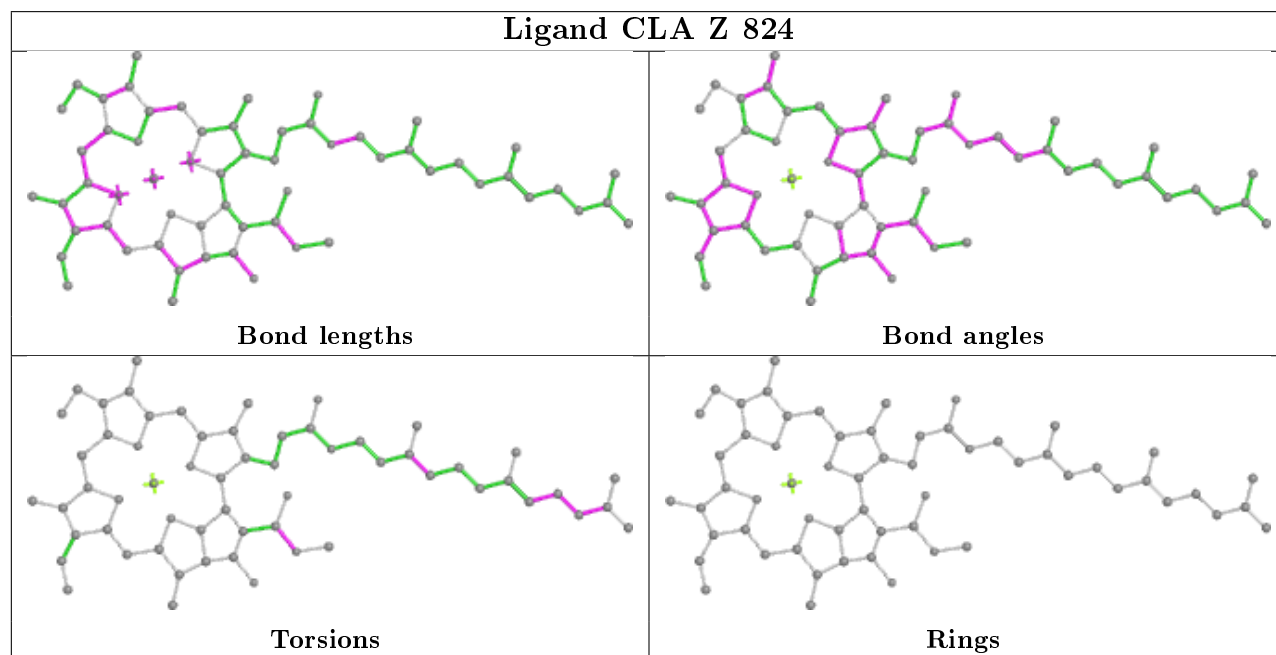
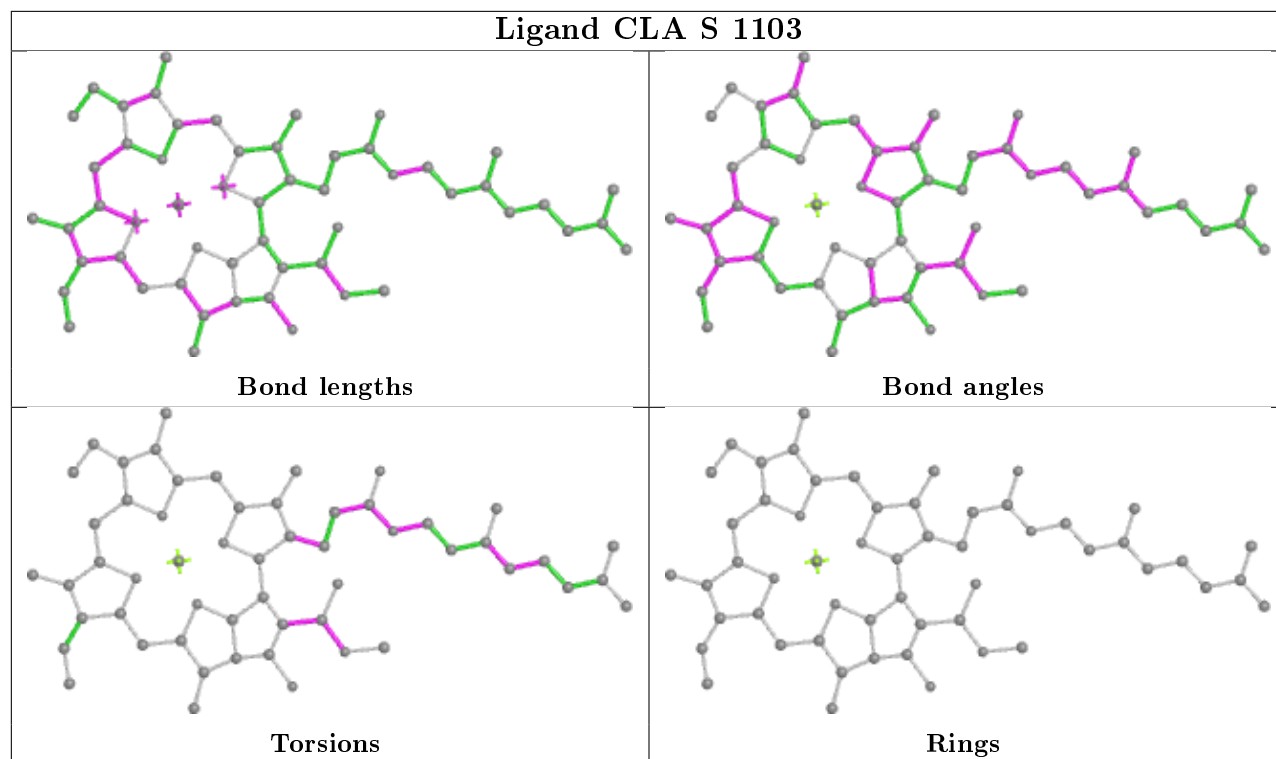




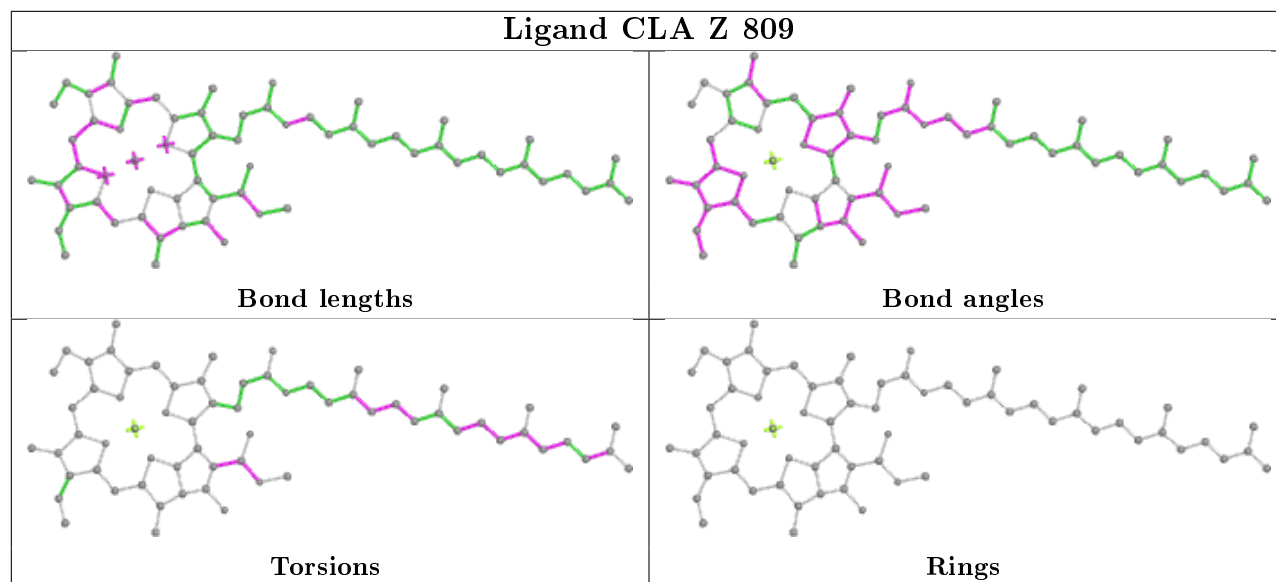


## Ligand CLA J 101

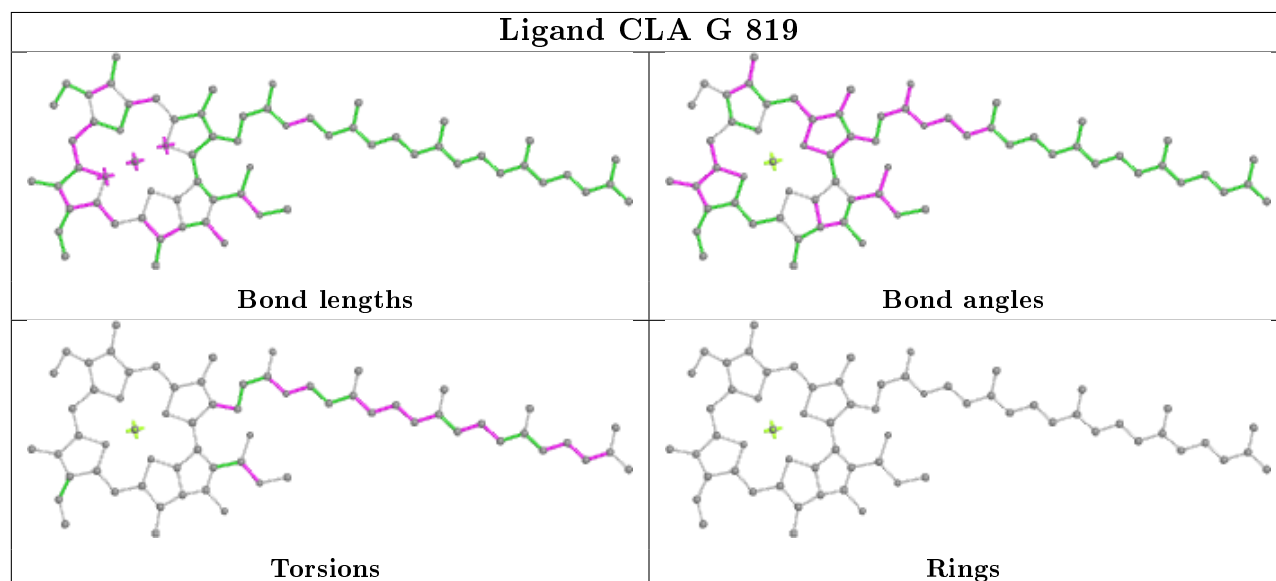




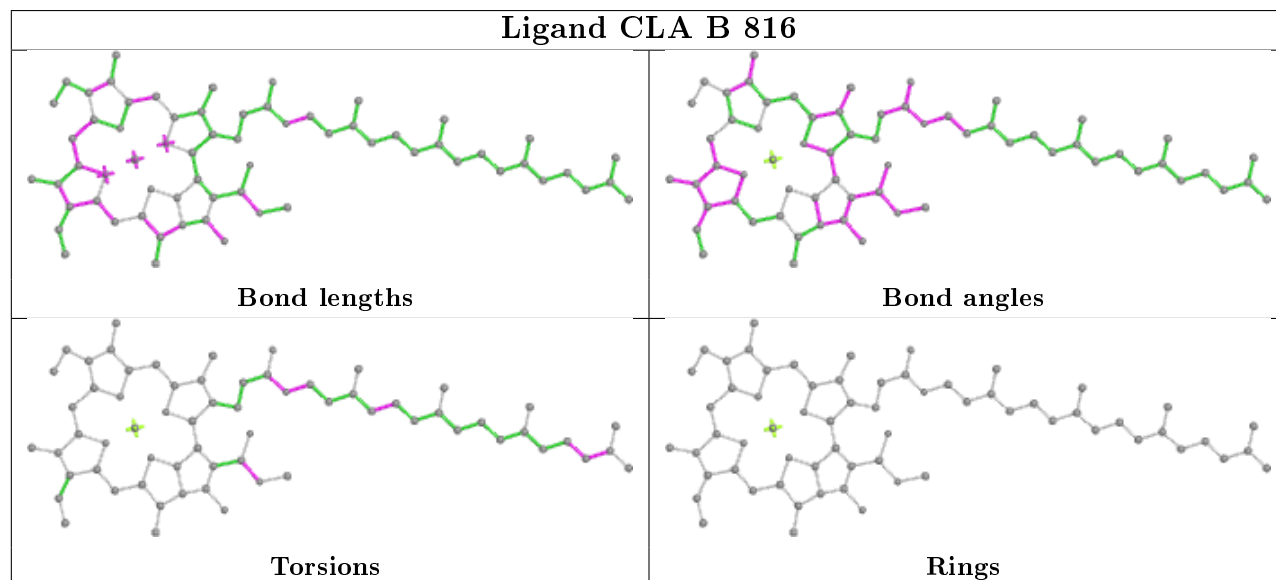
## Ligand CLA Z 809



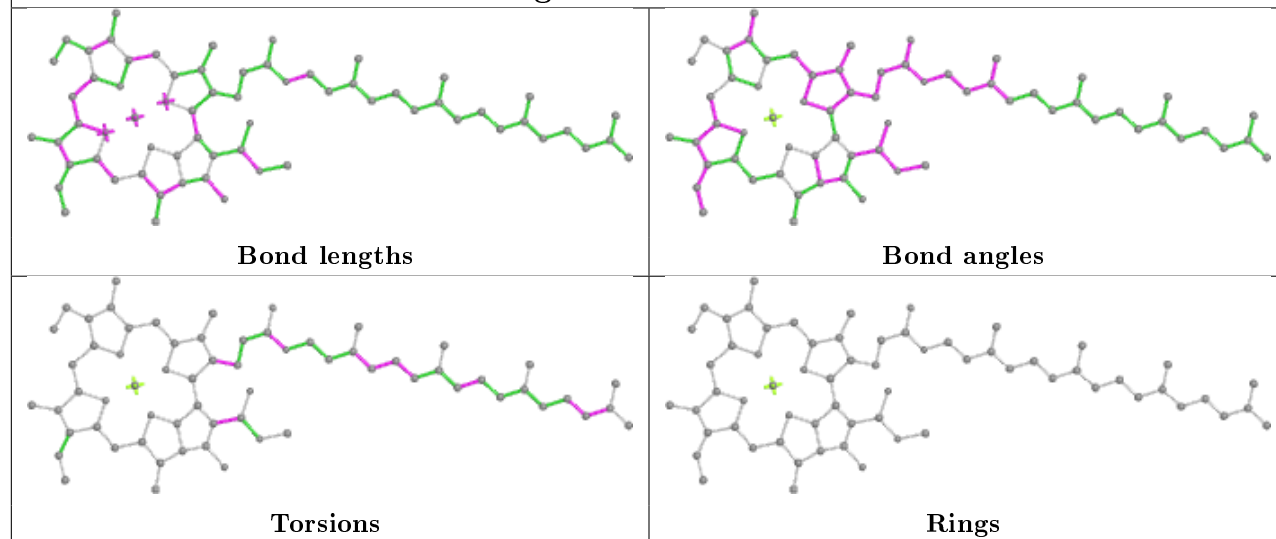
## Ligand CLA G 819



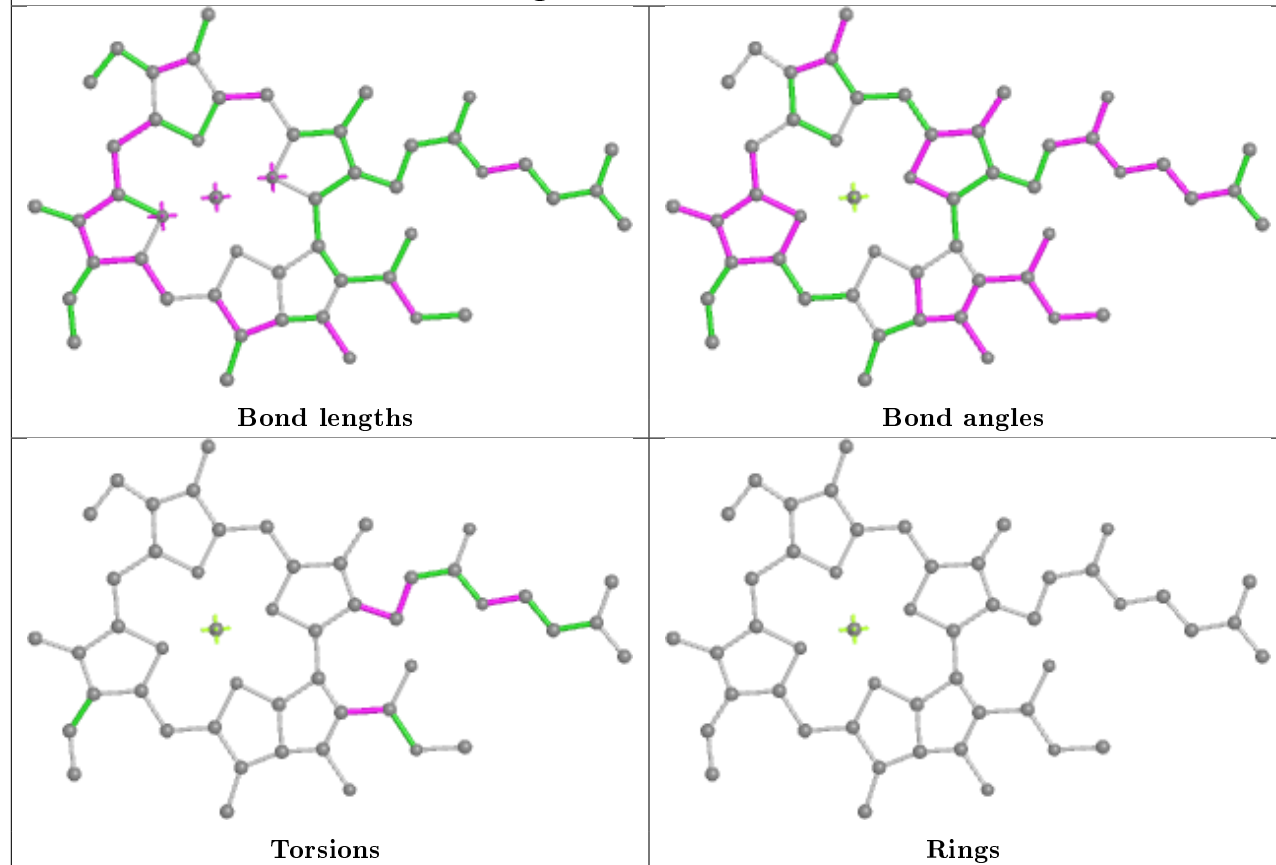
## Ligand CLA B 816

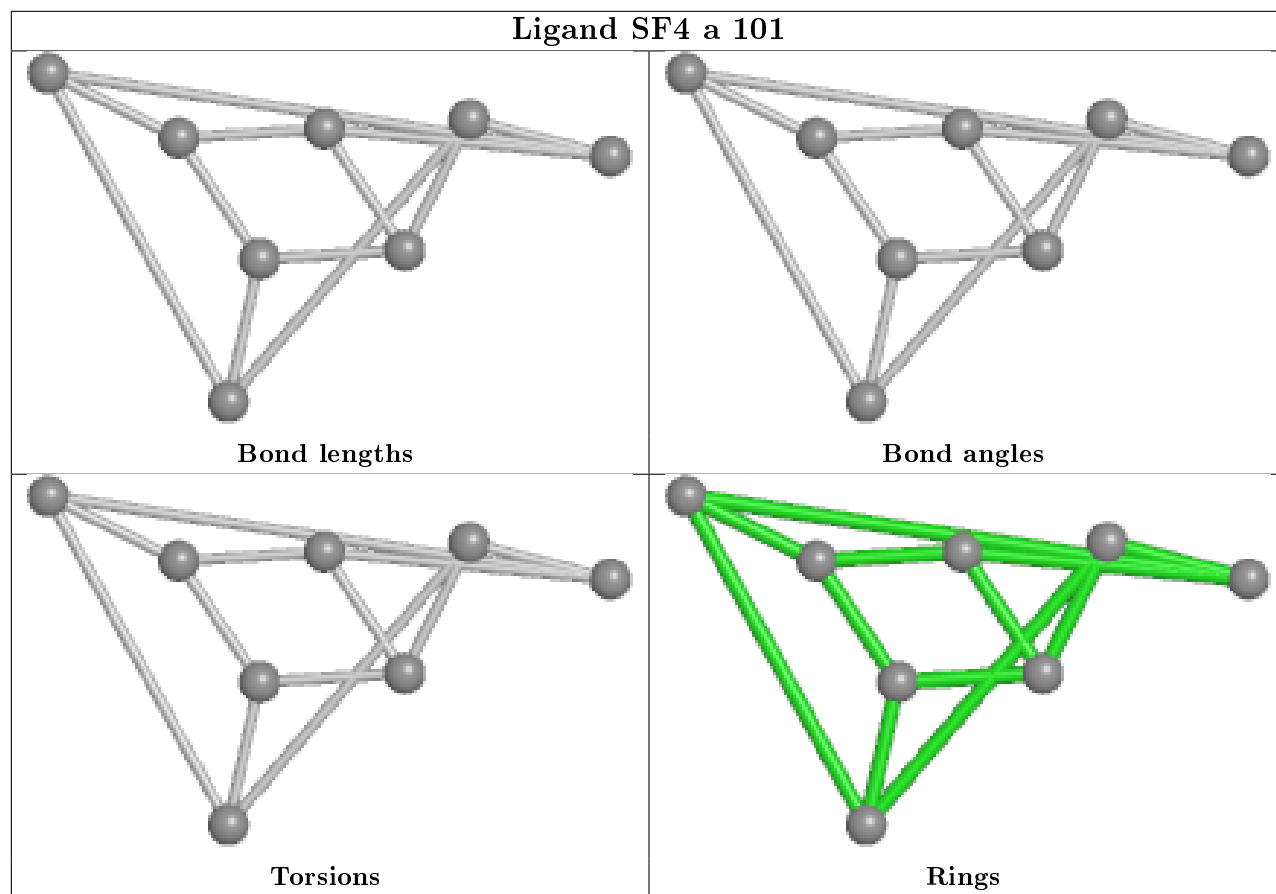
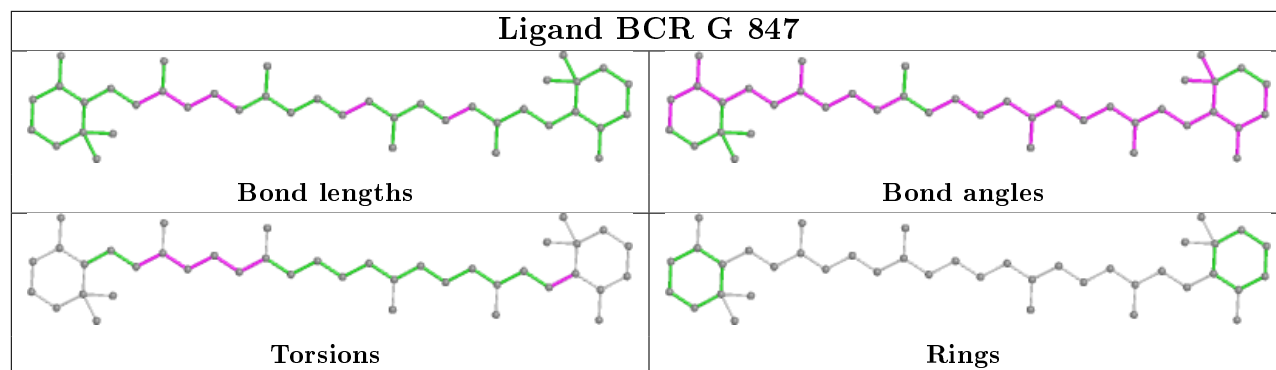


## Ligand CLA Z 826

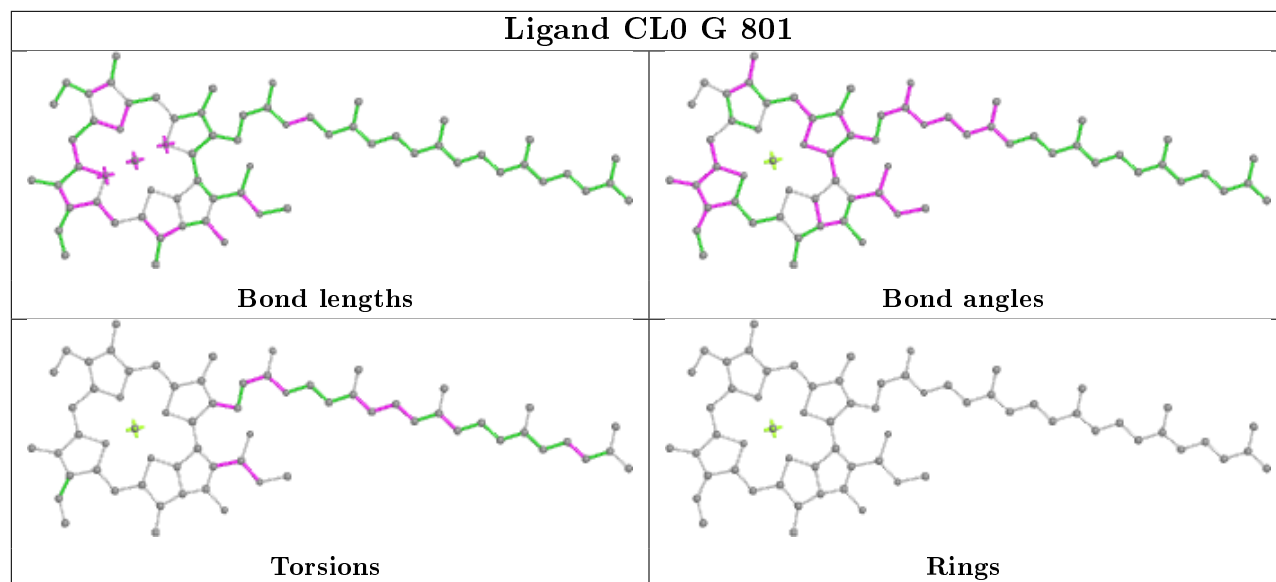


## Ligand CLA G 836

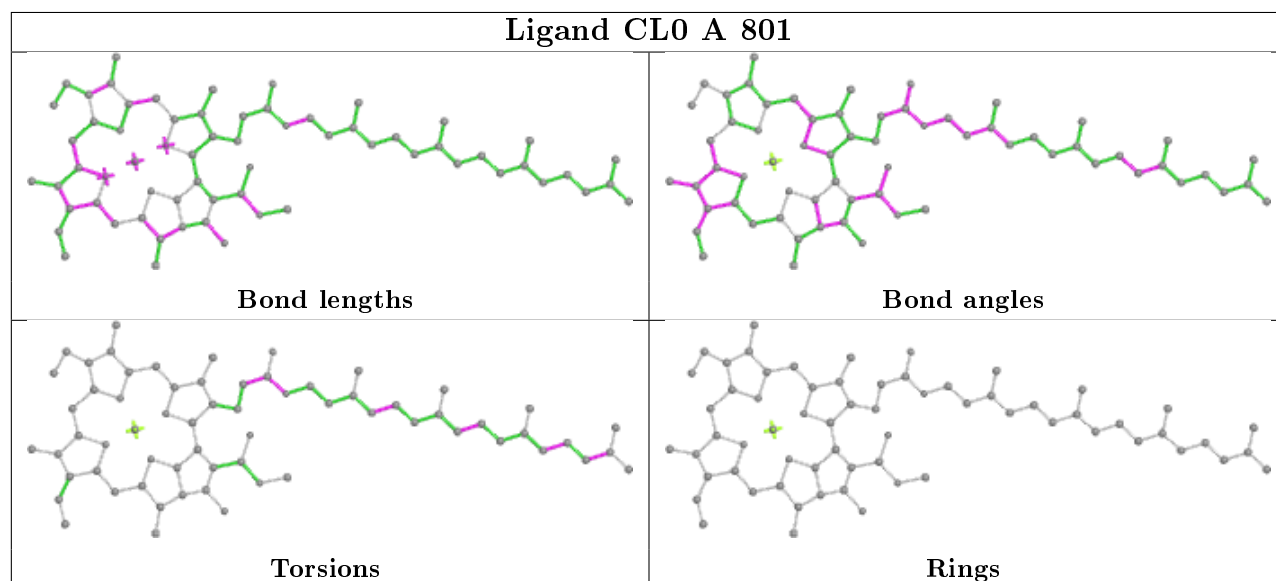




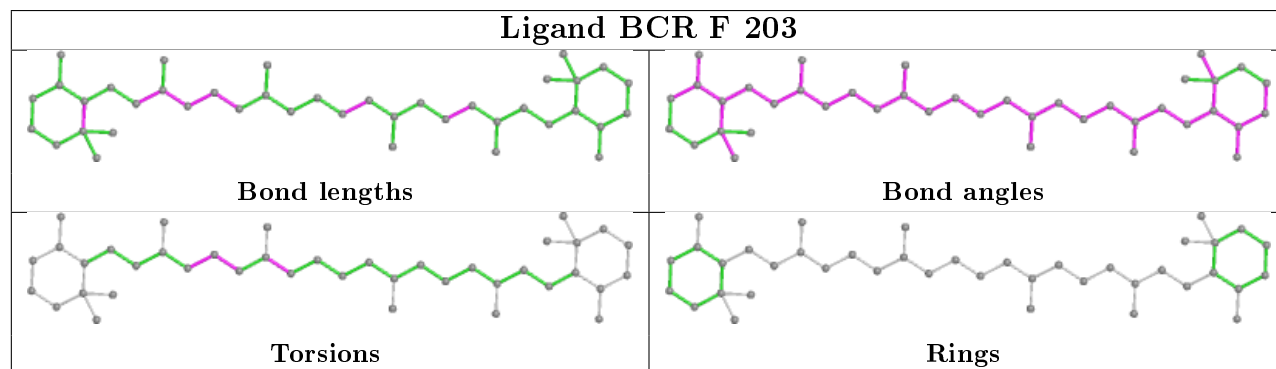
## Ligand CL0 G 801



## Ligand CL0 A 801

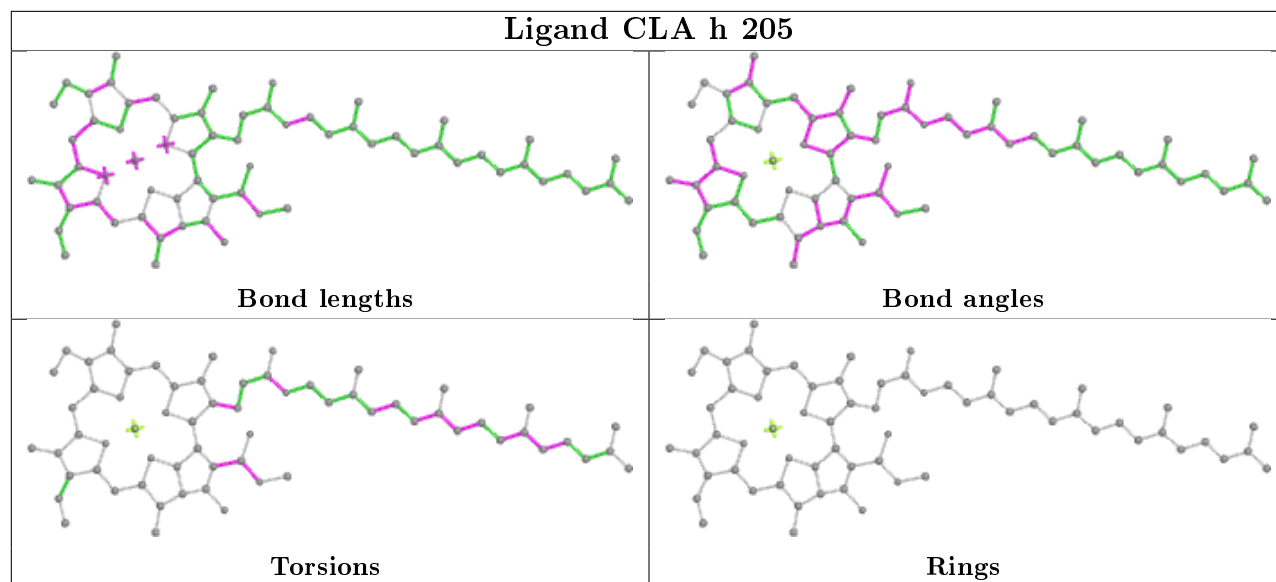


## Ligand BCR F 203

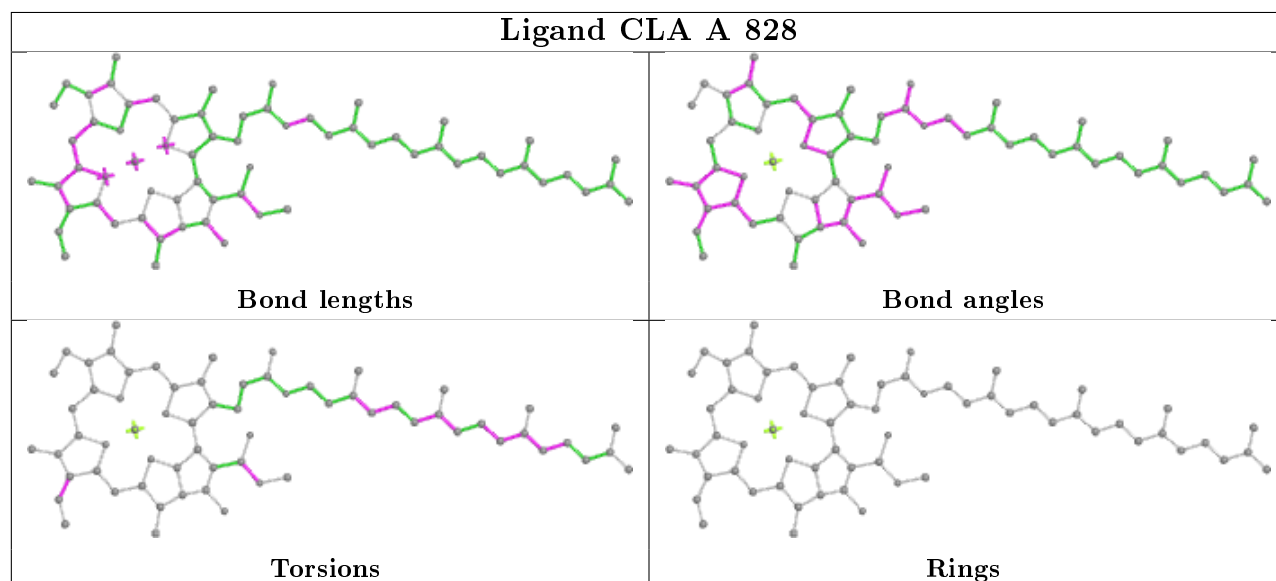




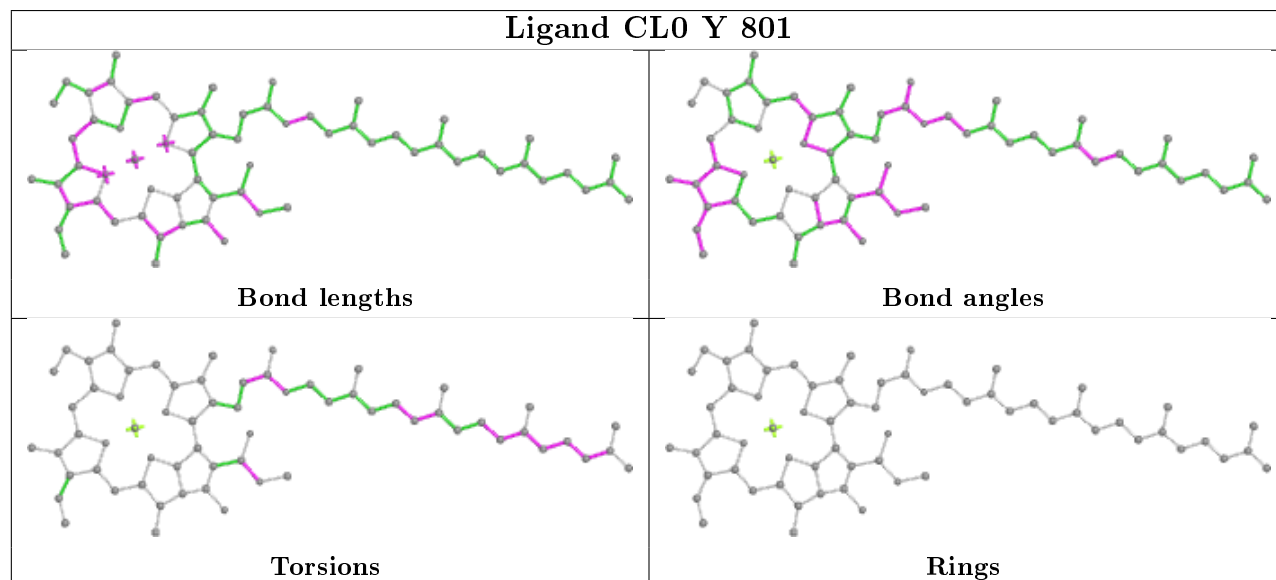
## Ligand CLA h 205

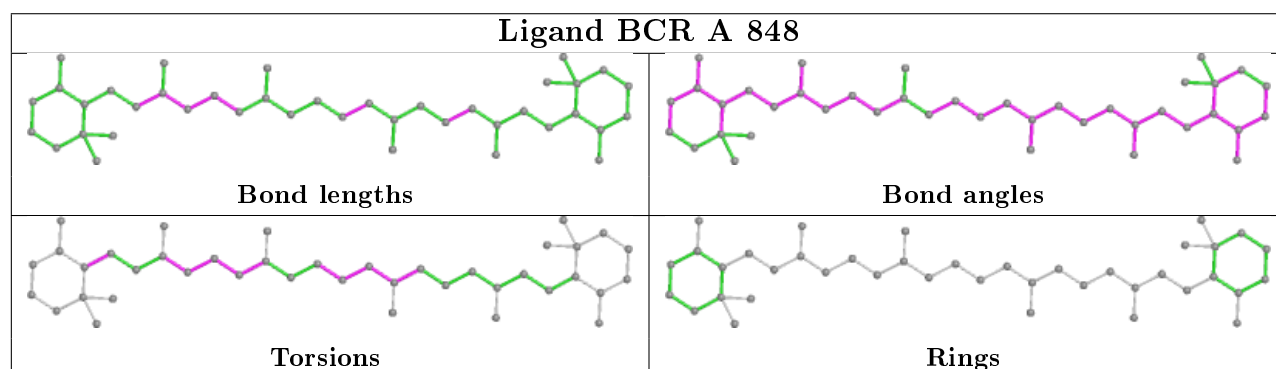
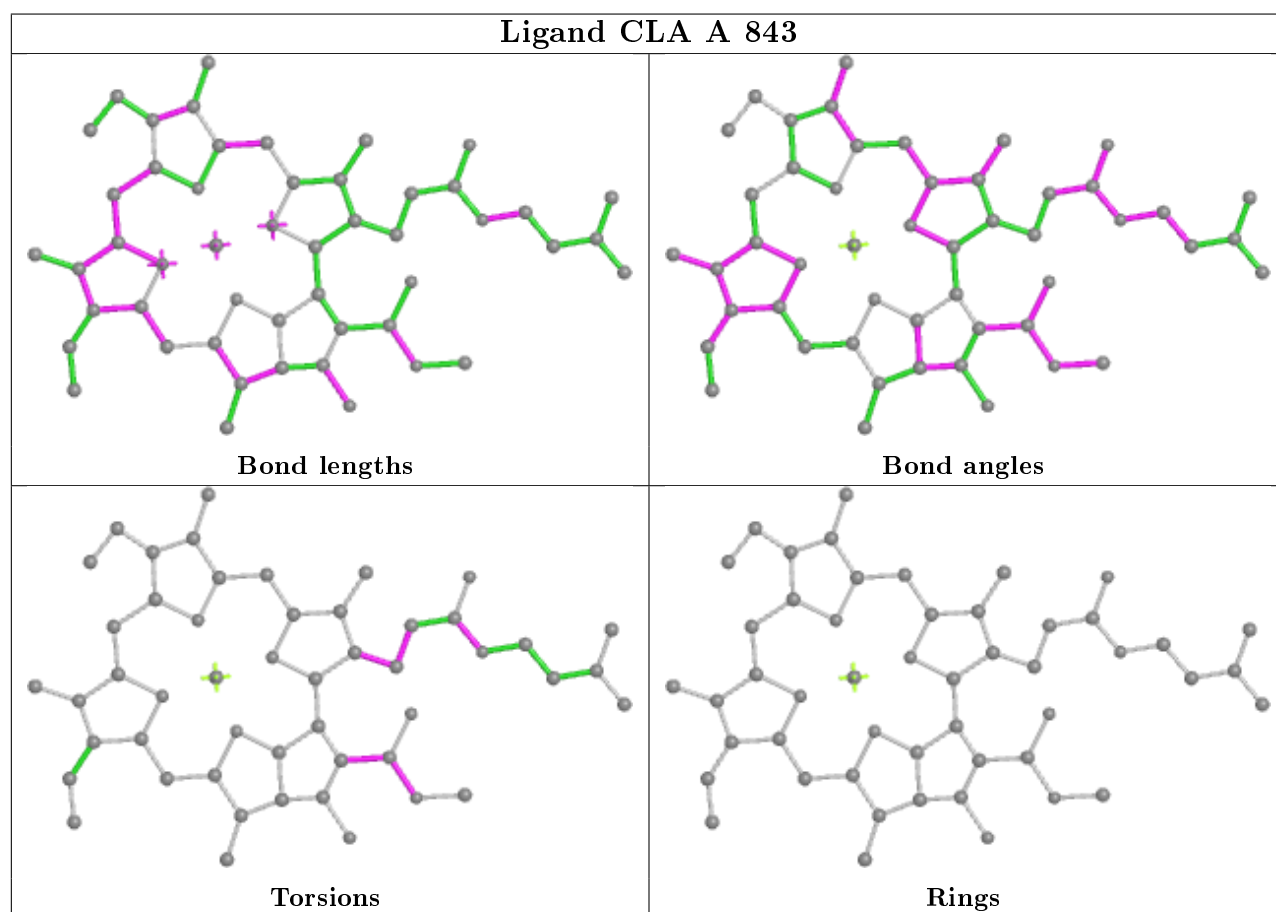
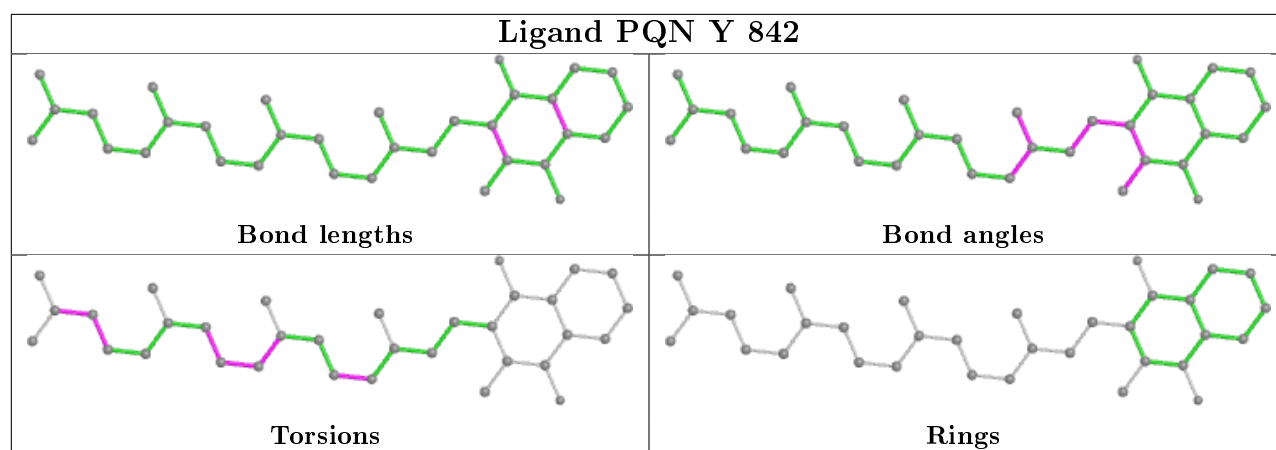


## Ligand CLA A 828

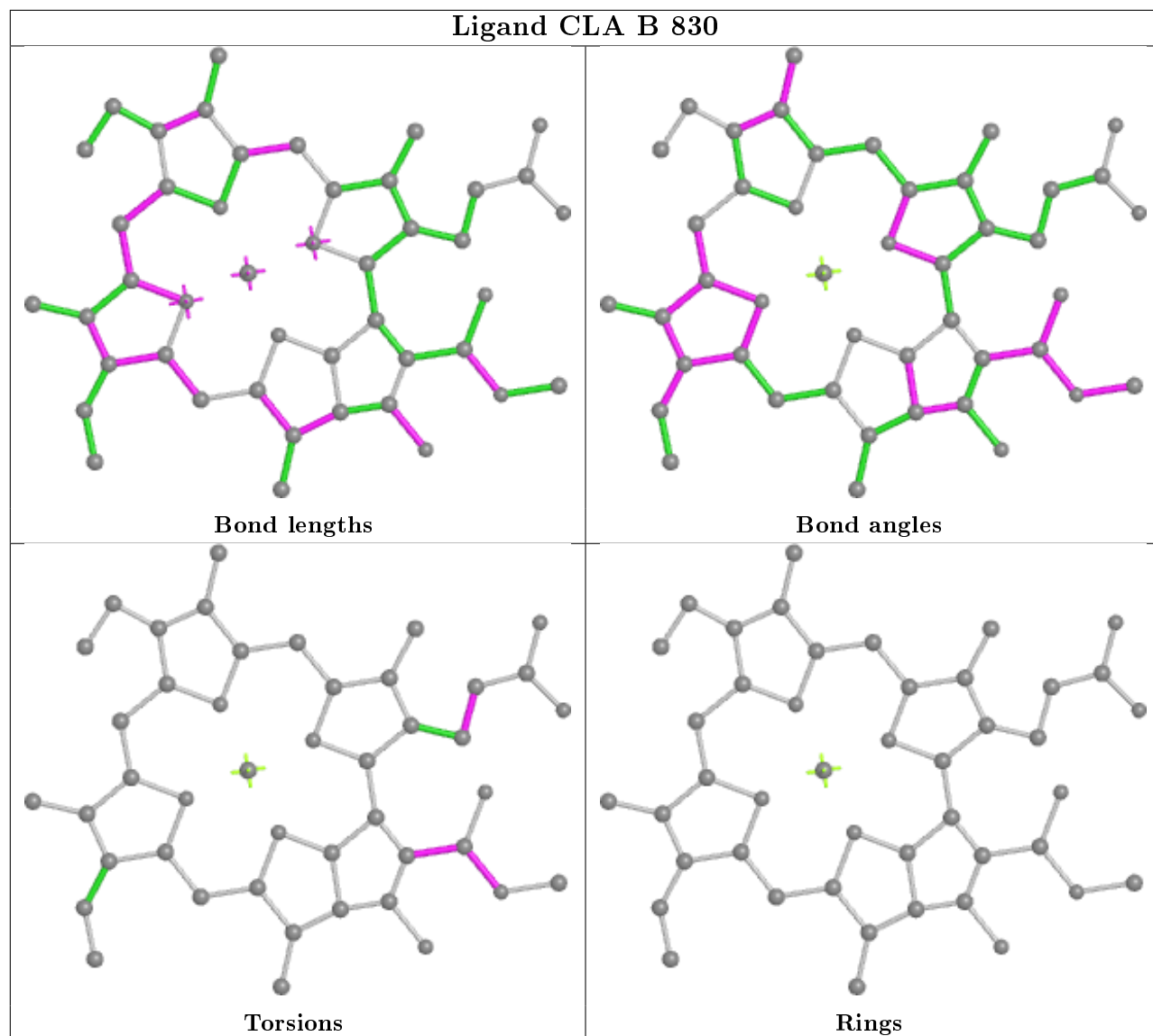


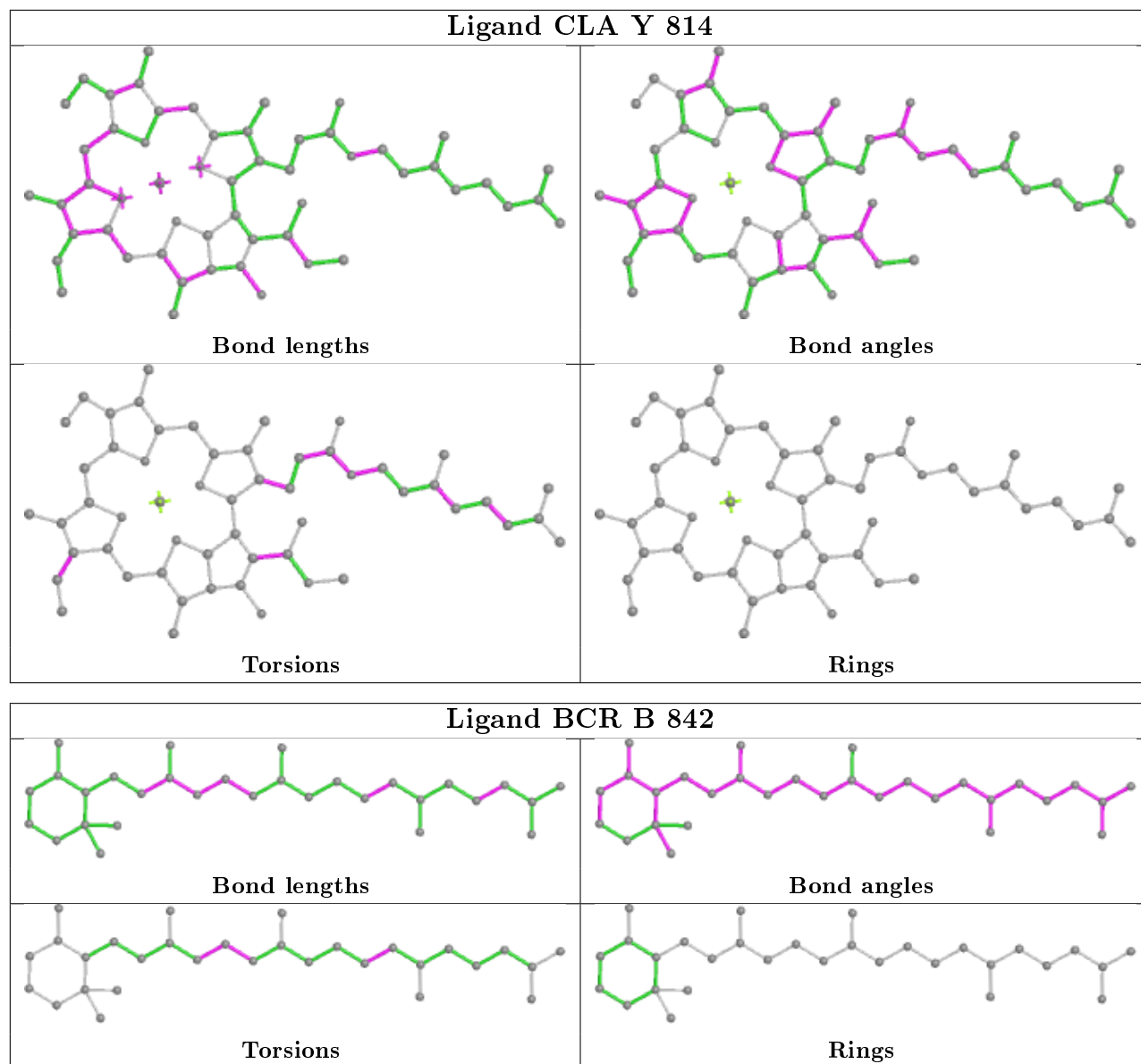
## Ligand CL0 Y 801

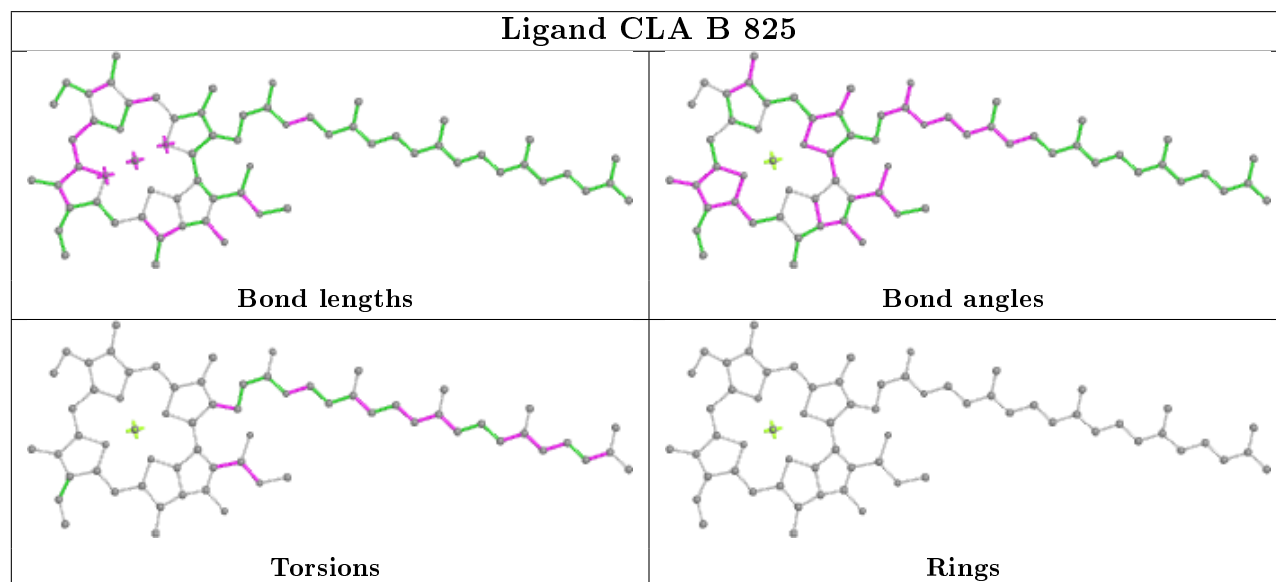
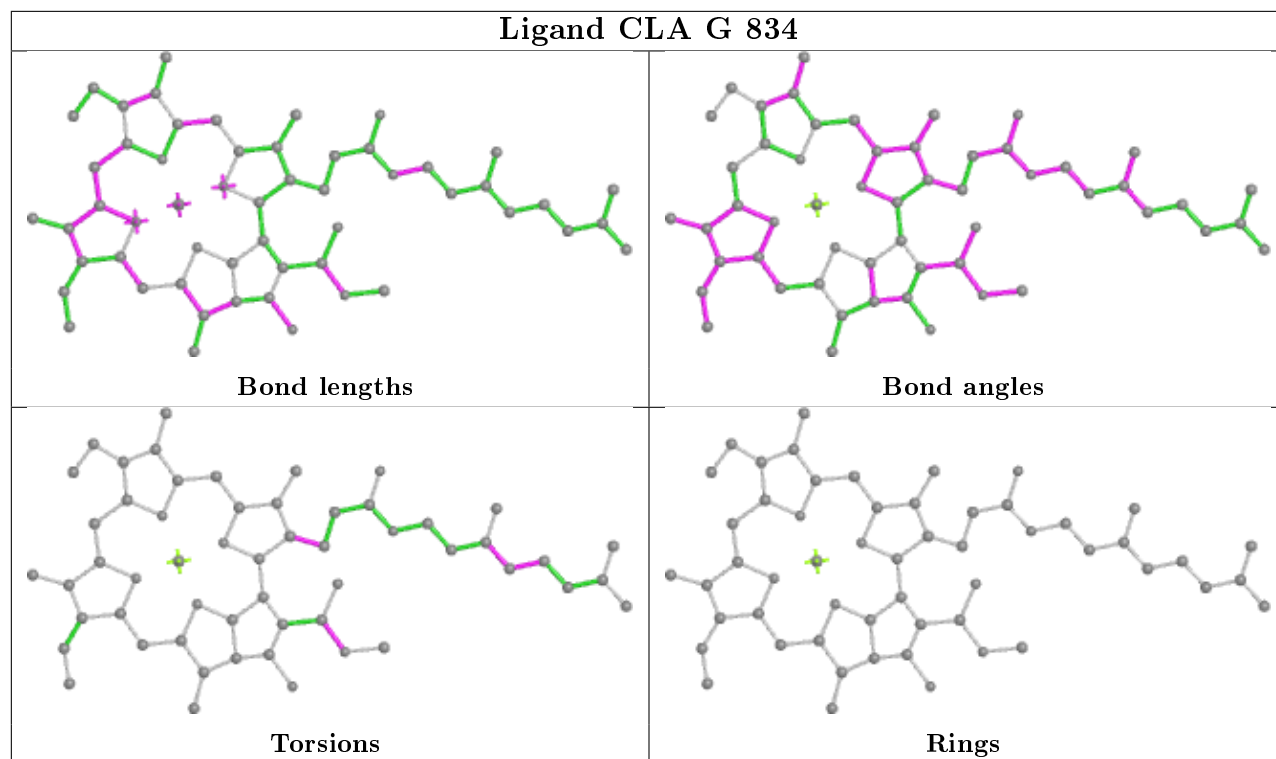




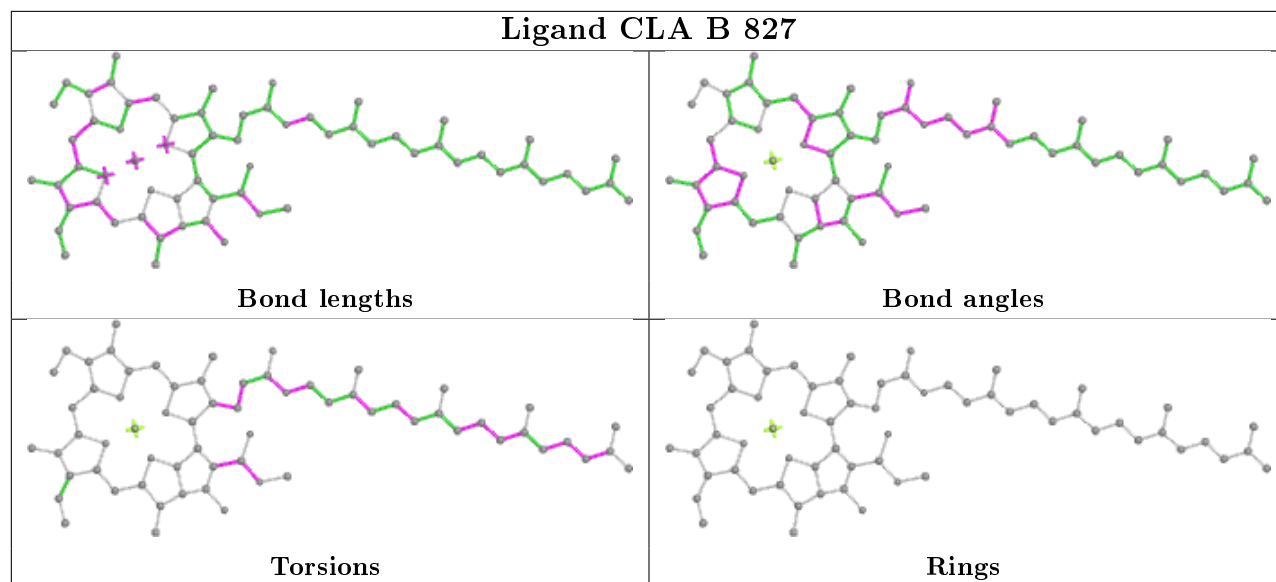
## Ligand CLA B 830



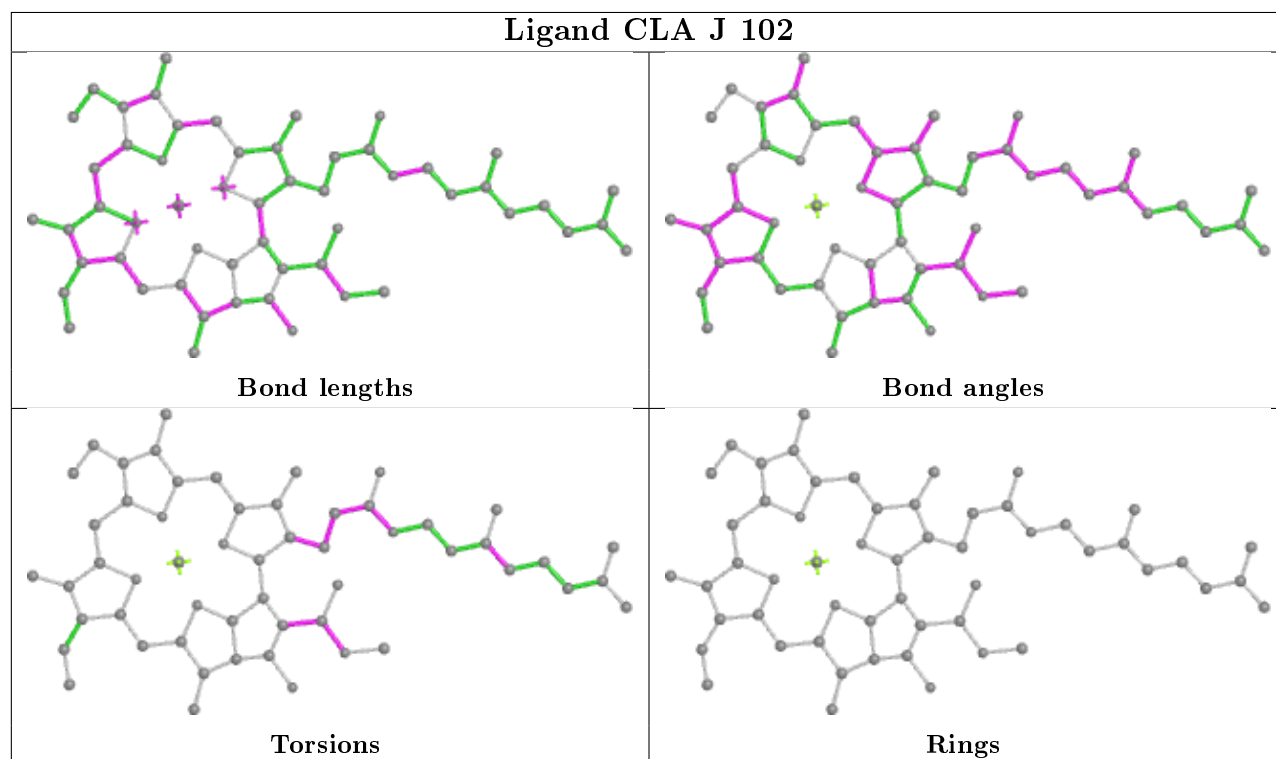


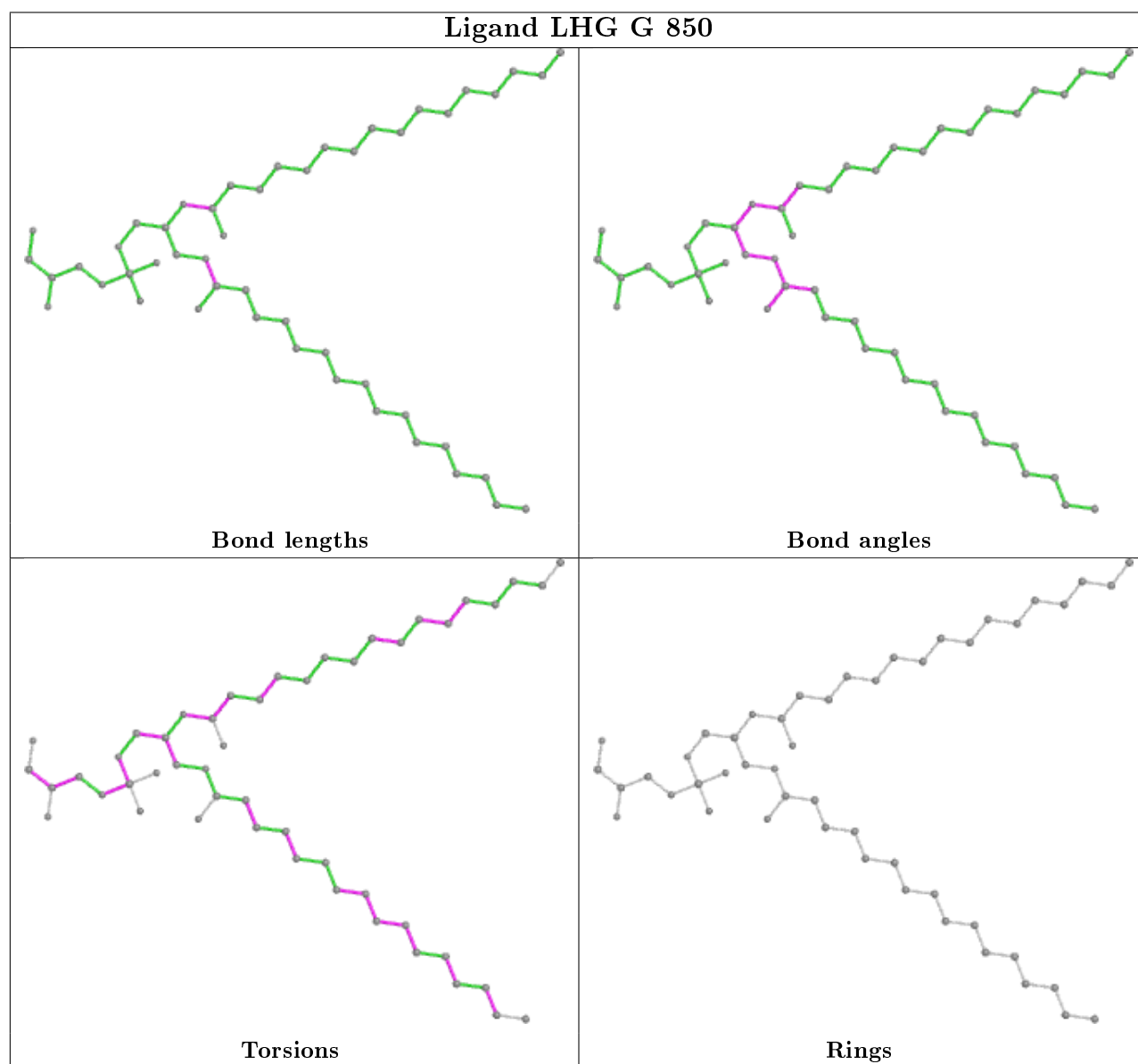
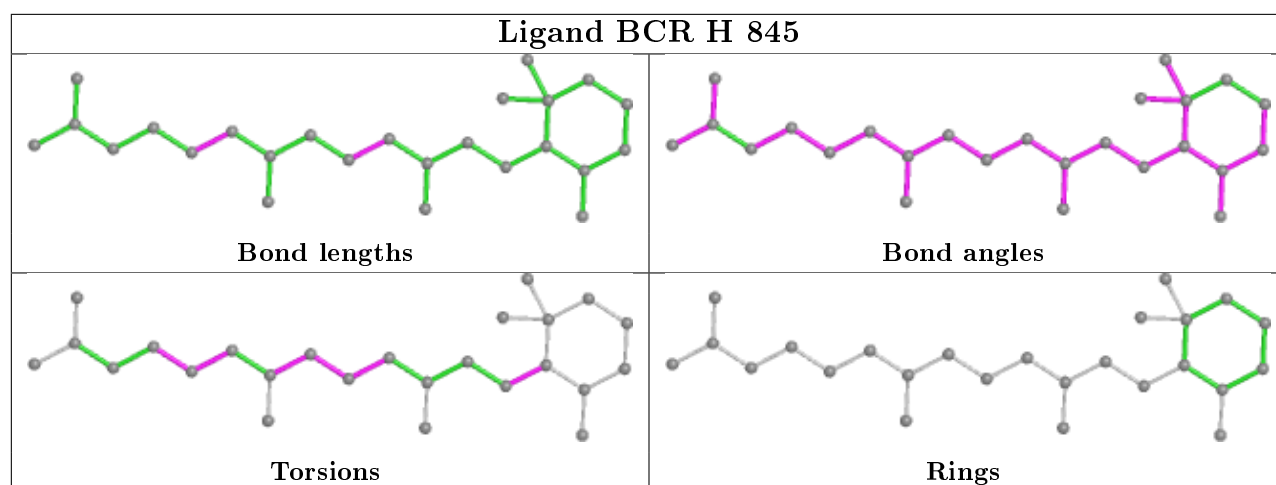


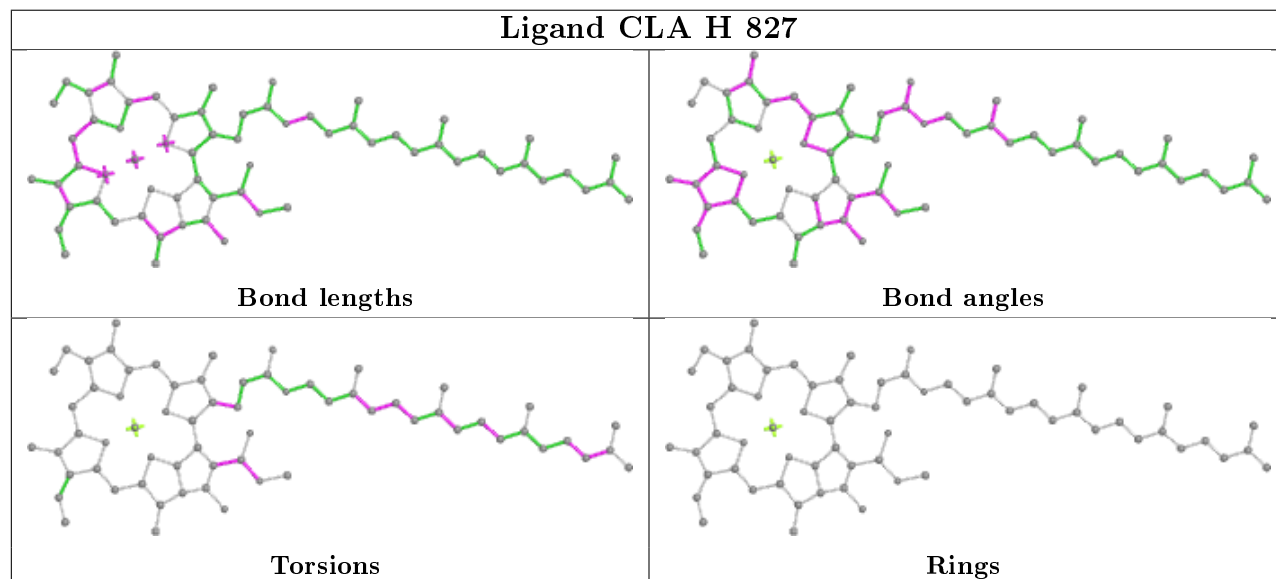
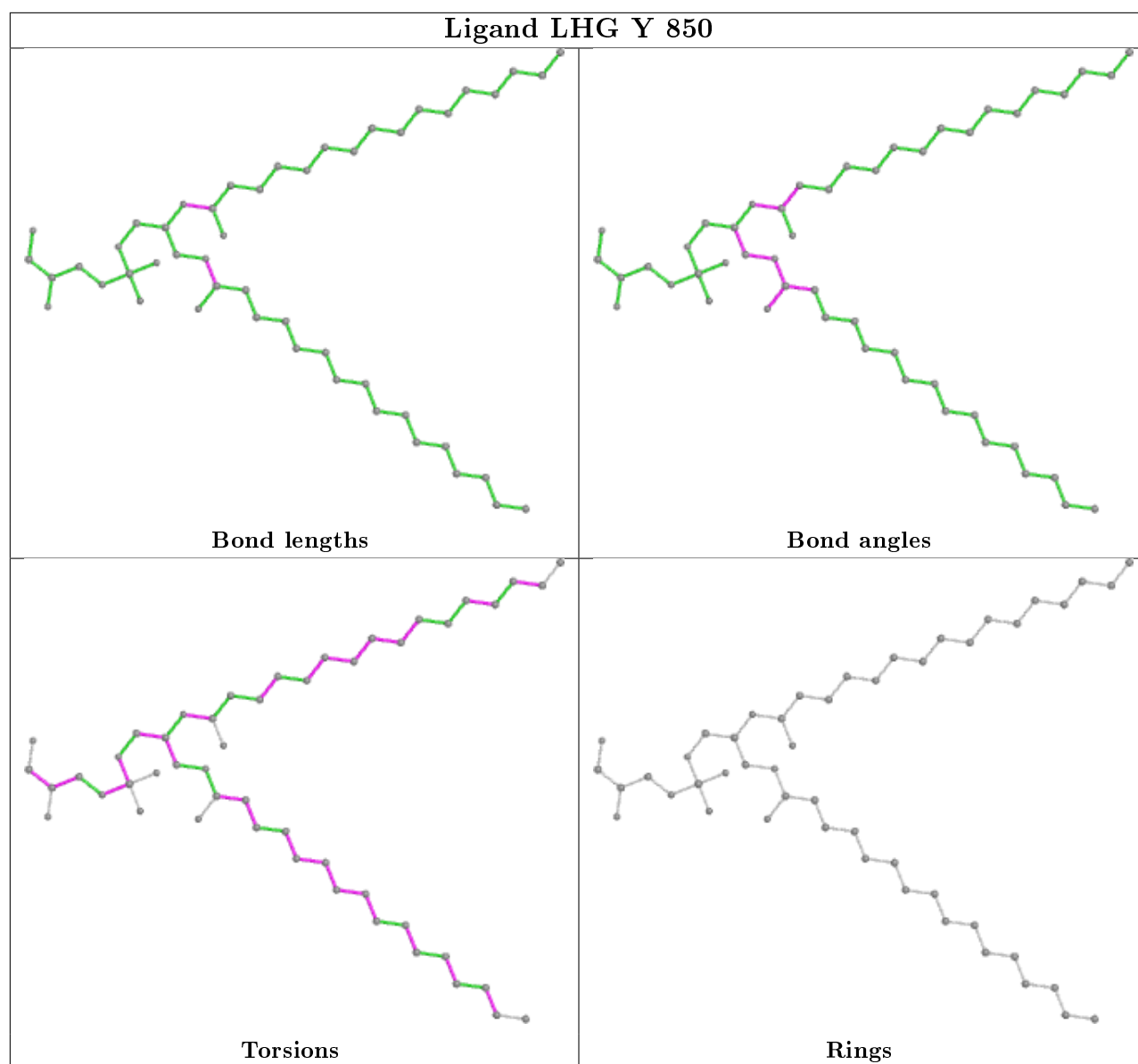
## Ligand CLA B 827



## Ligand CLA J 102

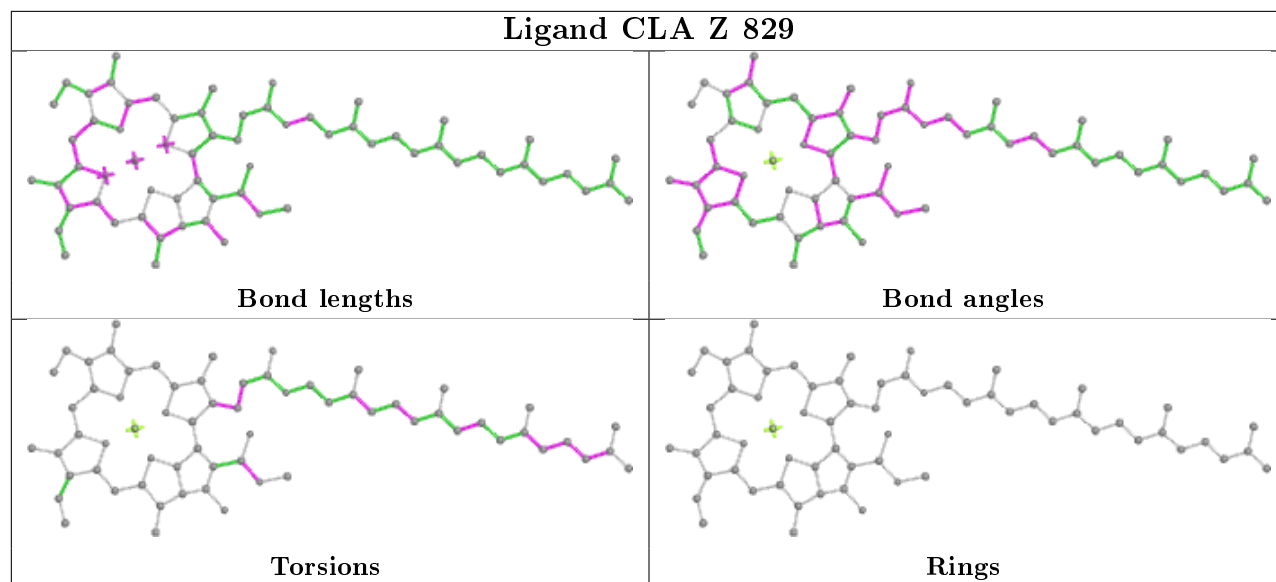




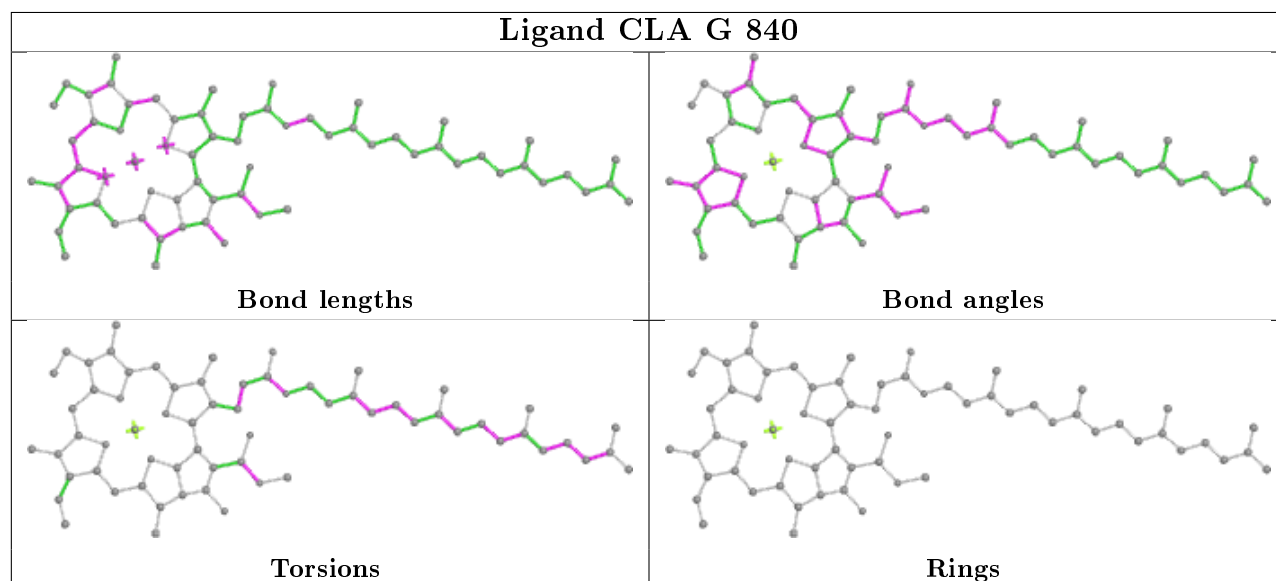




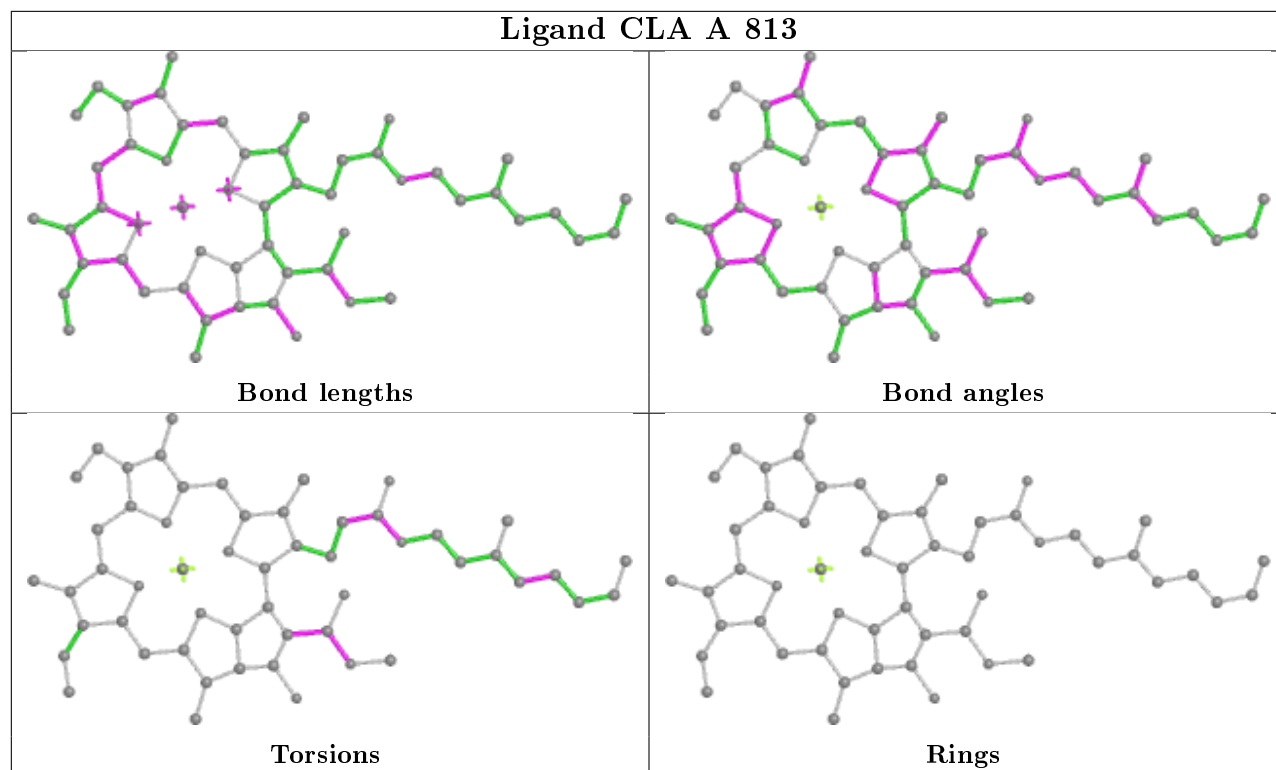
## Ligand CLA Z 829



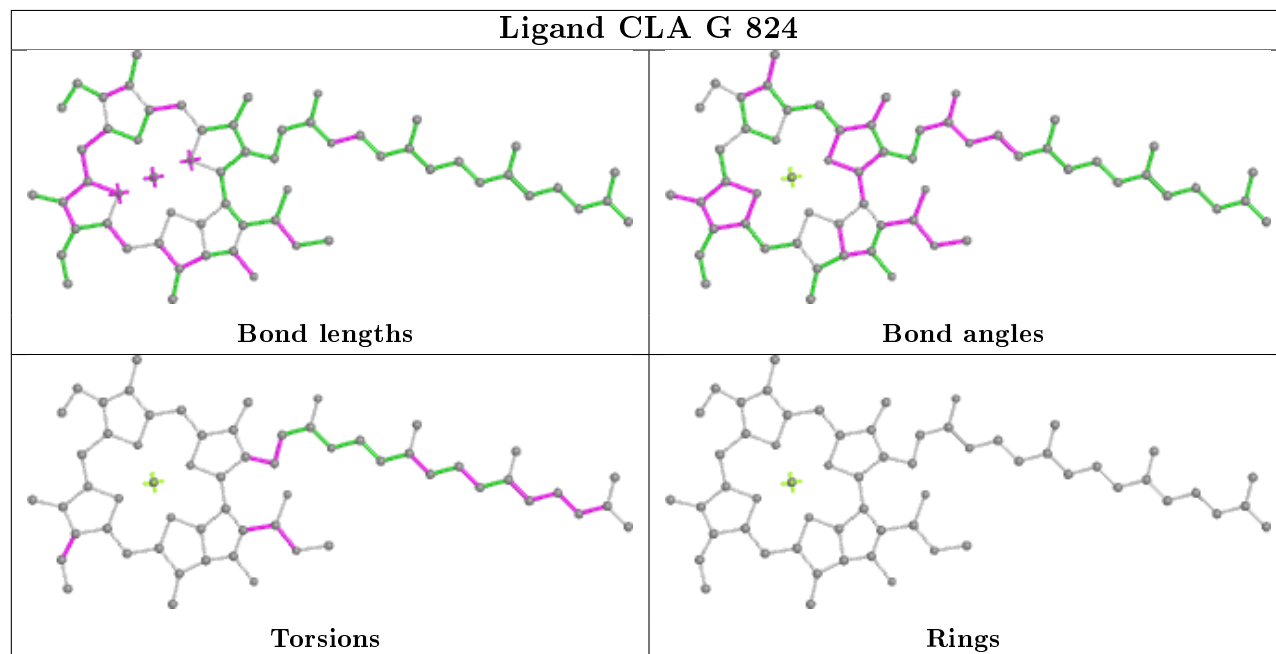
## Ligand CLA G 840



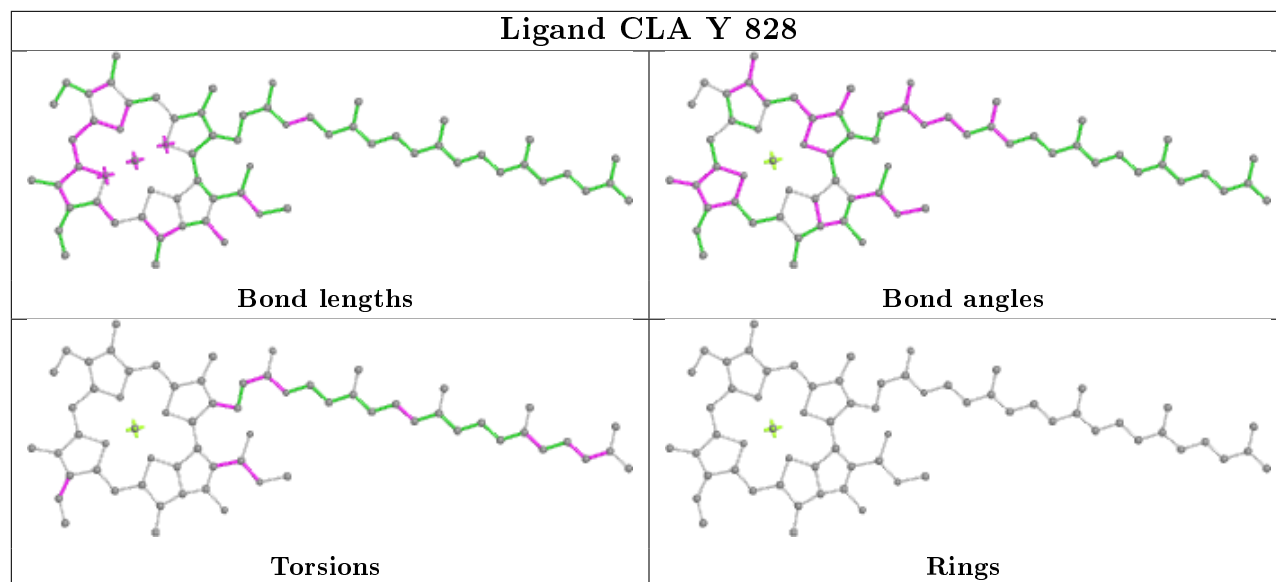
## Ligand CLA A 813



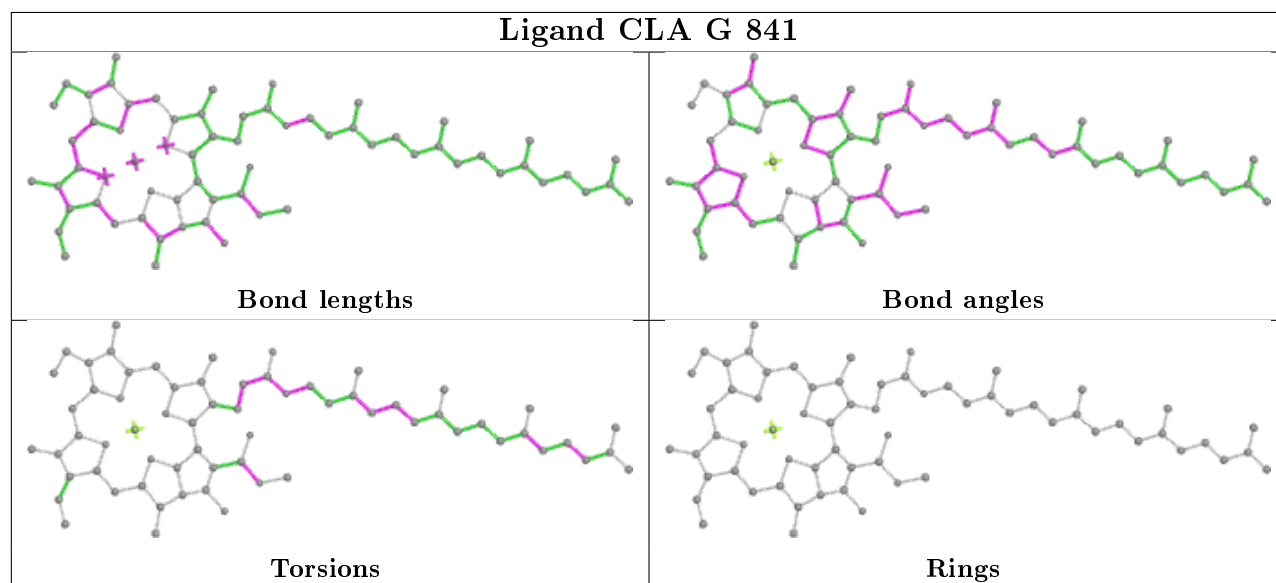
## Ligand CLA G 824



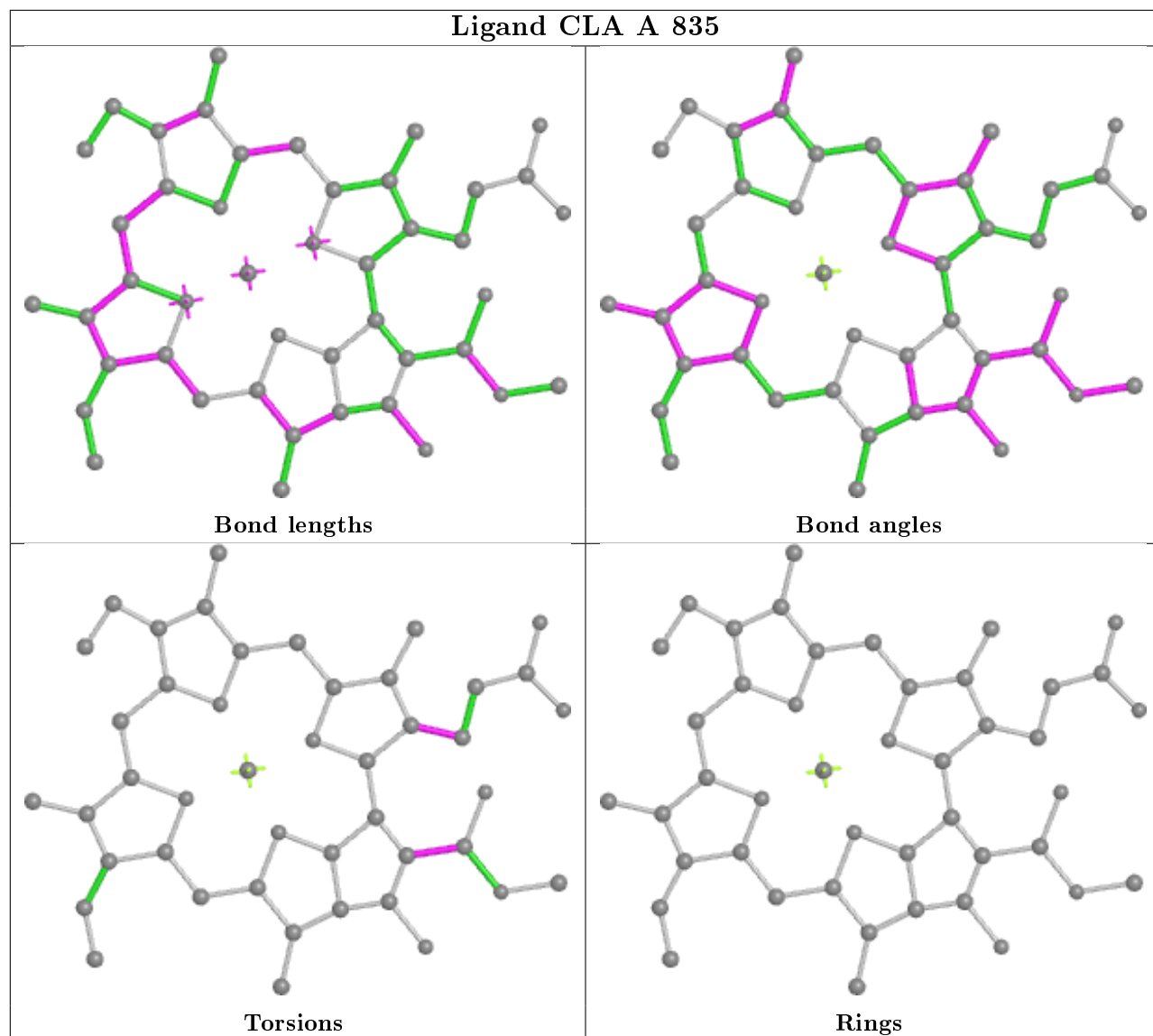
## Ligand CLA Y 828



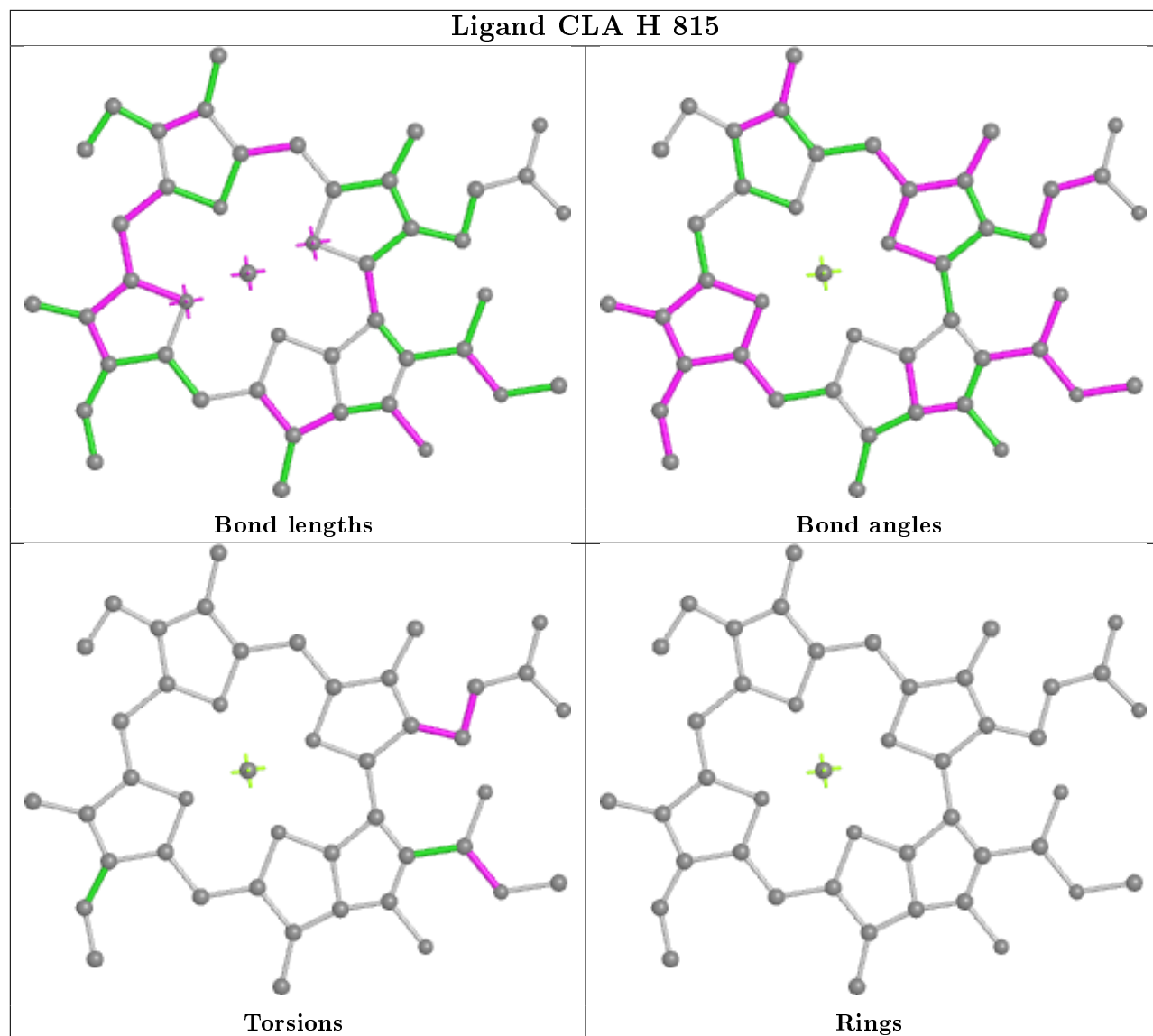
## Ligand CLA G 841



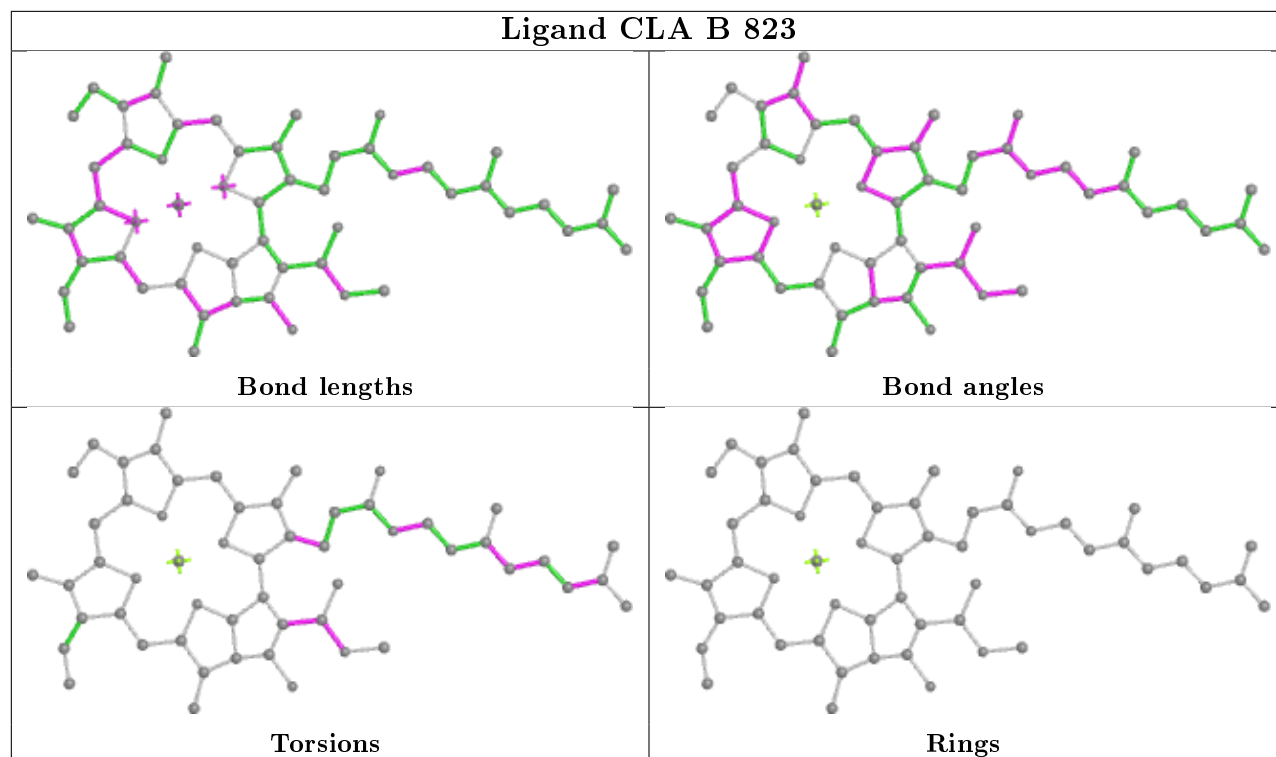
## Ligand CLA A 835



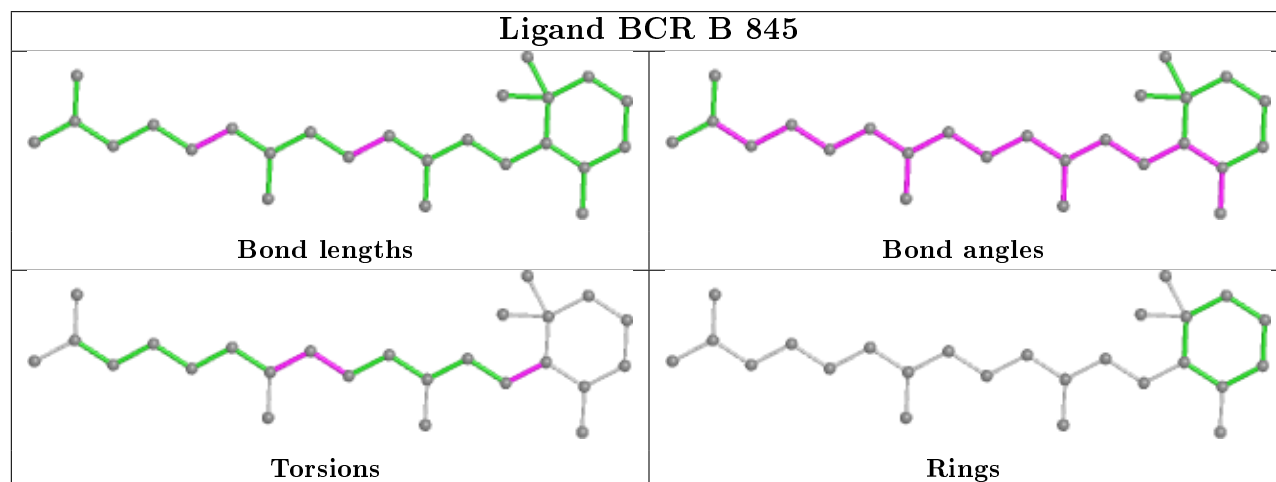
## Ligand CLA H 815



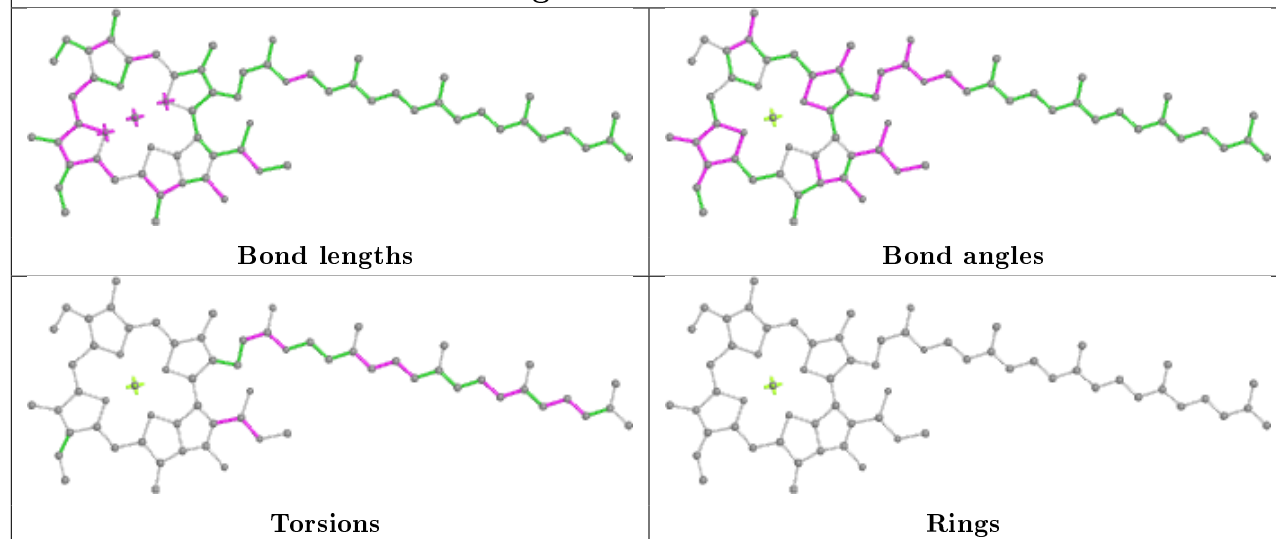
## Ligand CLA B 823



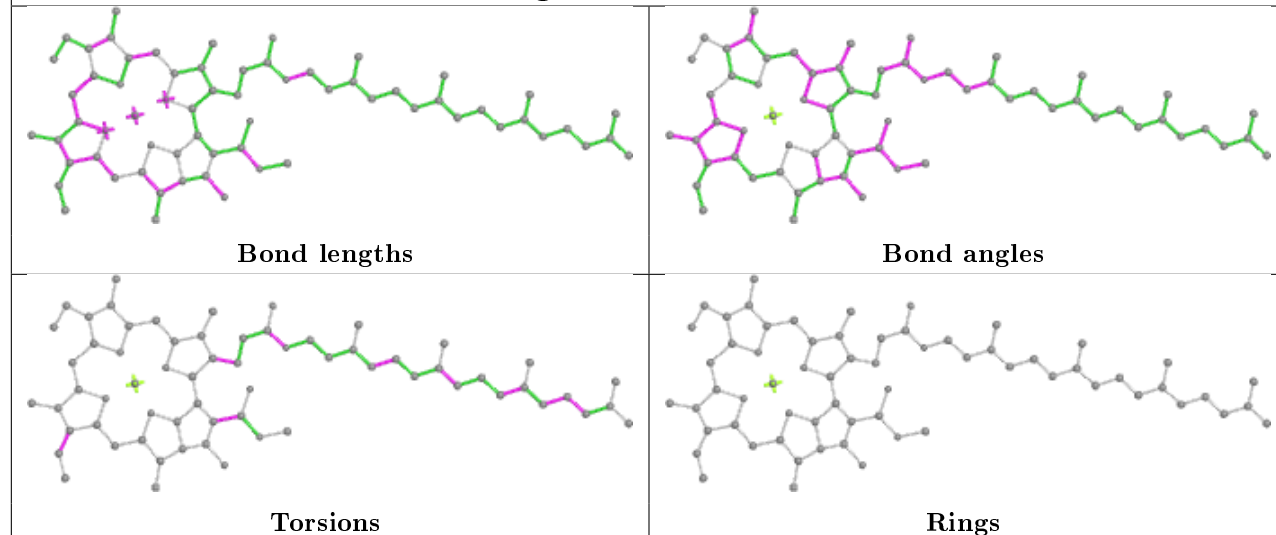
## Ligand BCR B 845



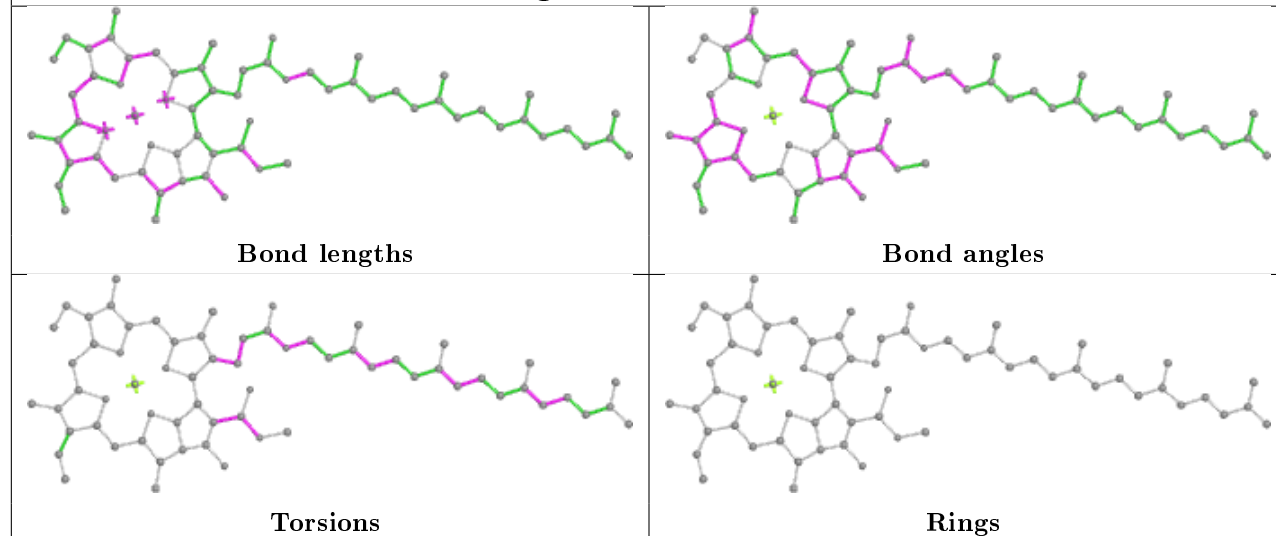
## Ligand CLA Y 827

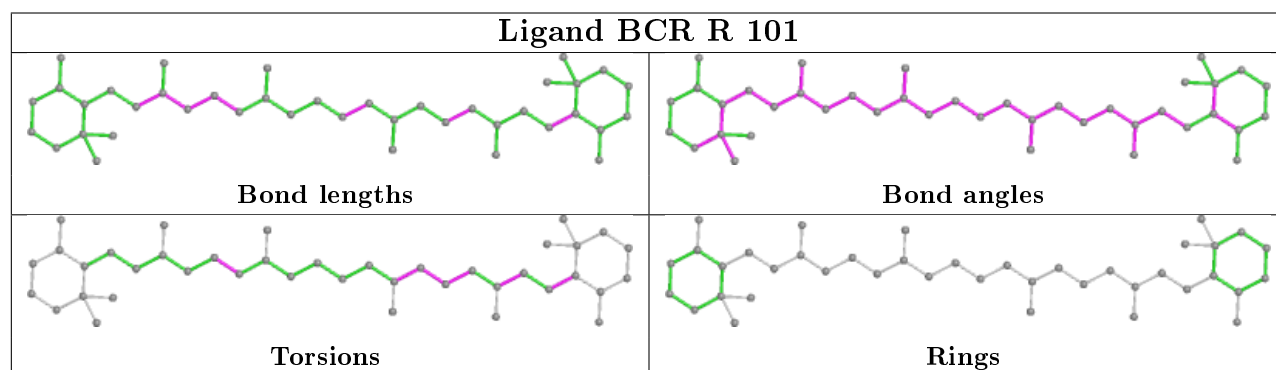
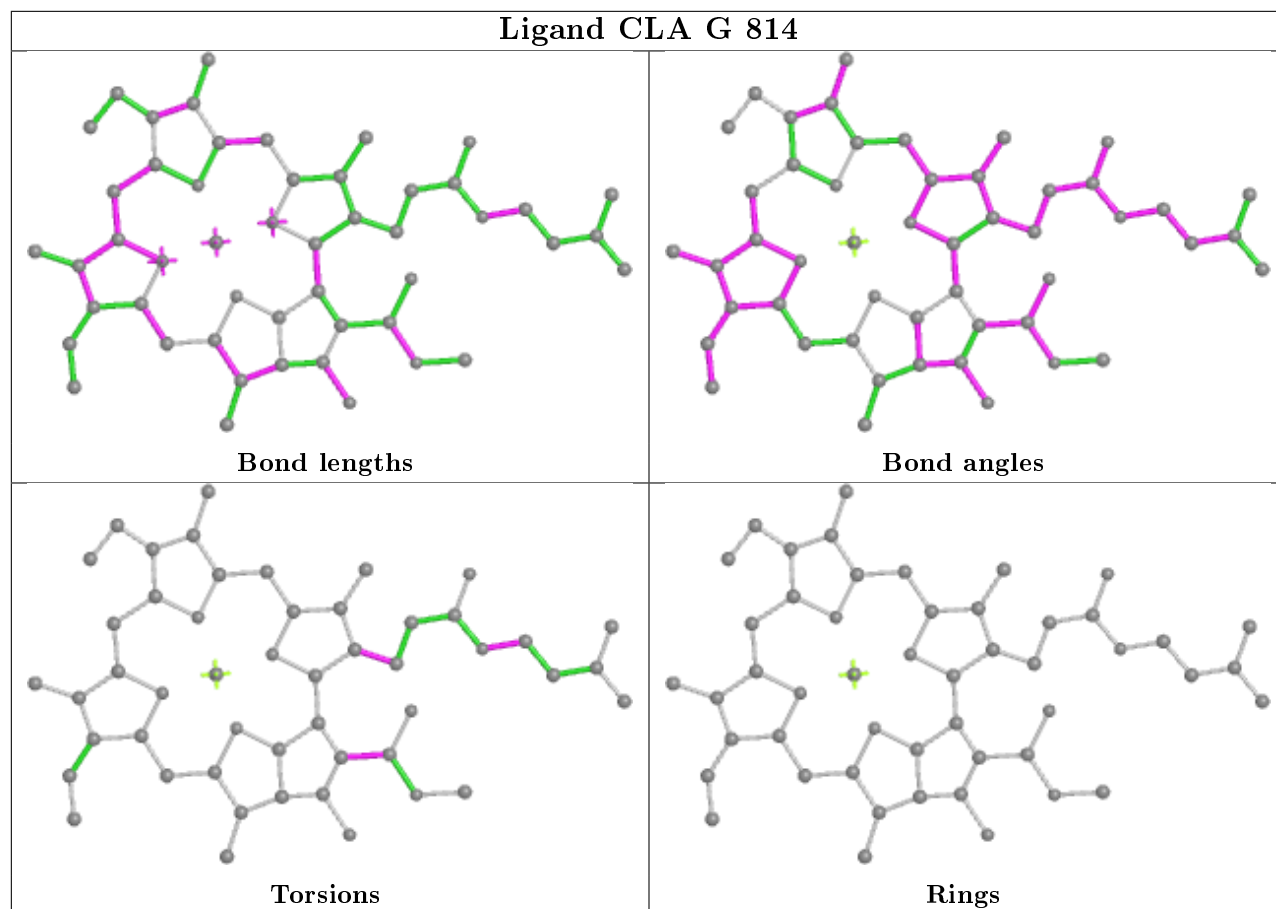
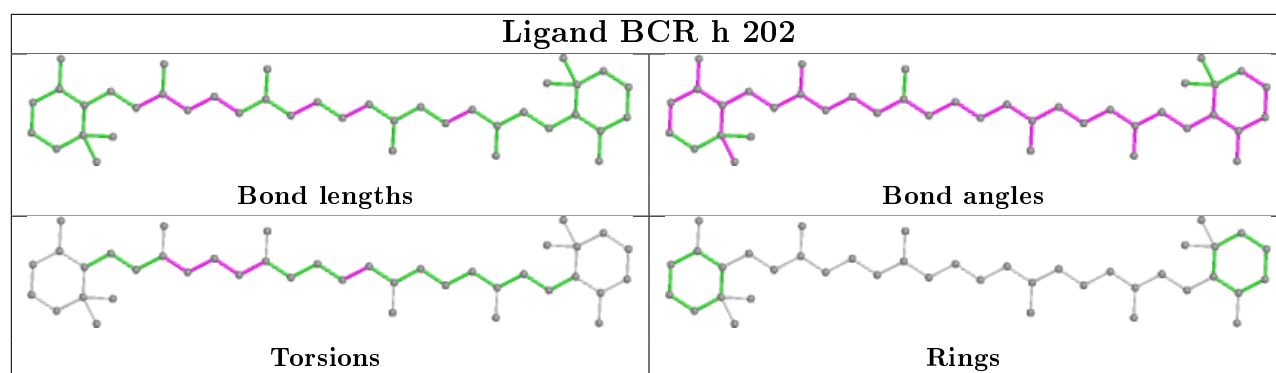


## Ligand CLA Z 827



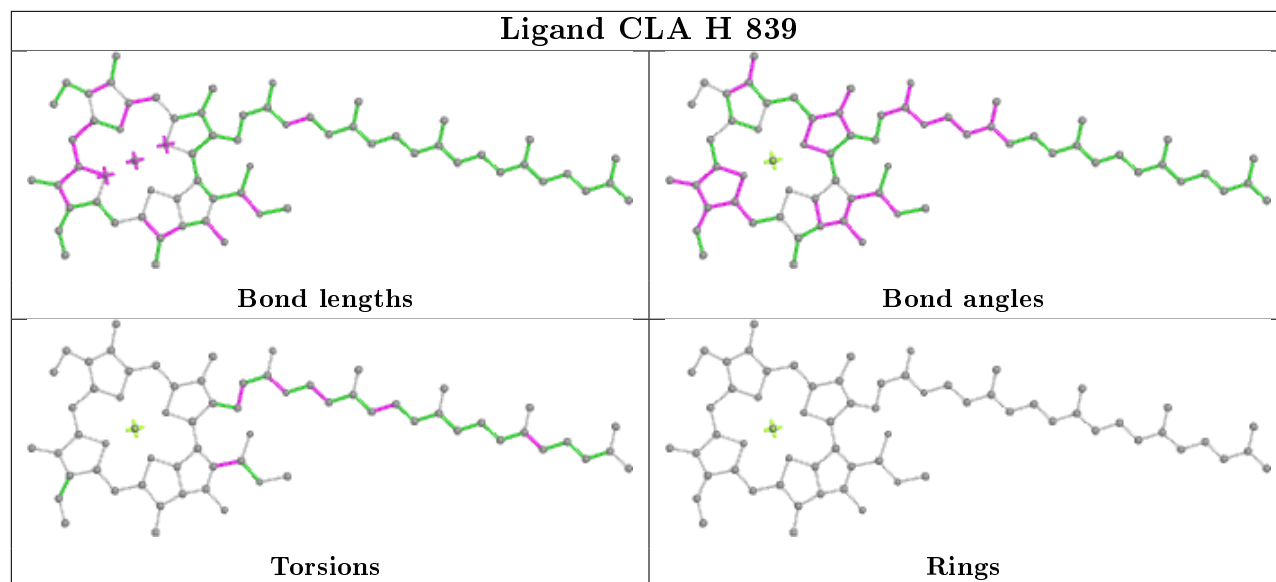
## Ligand CLA h 206



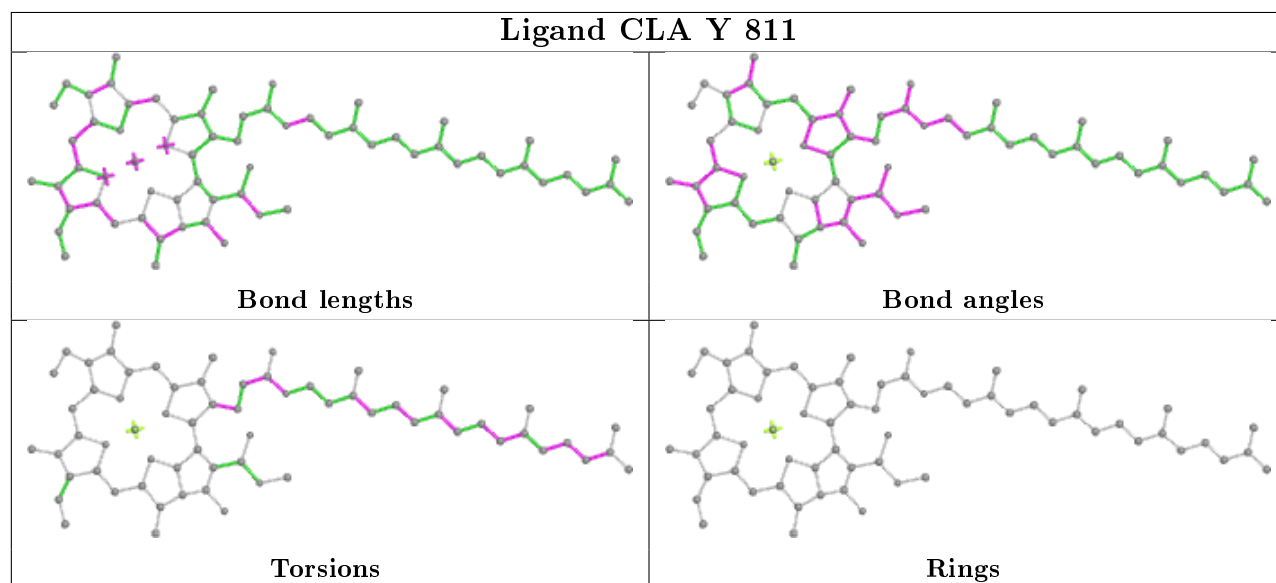


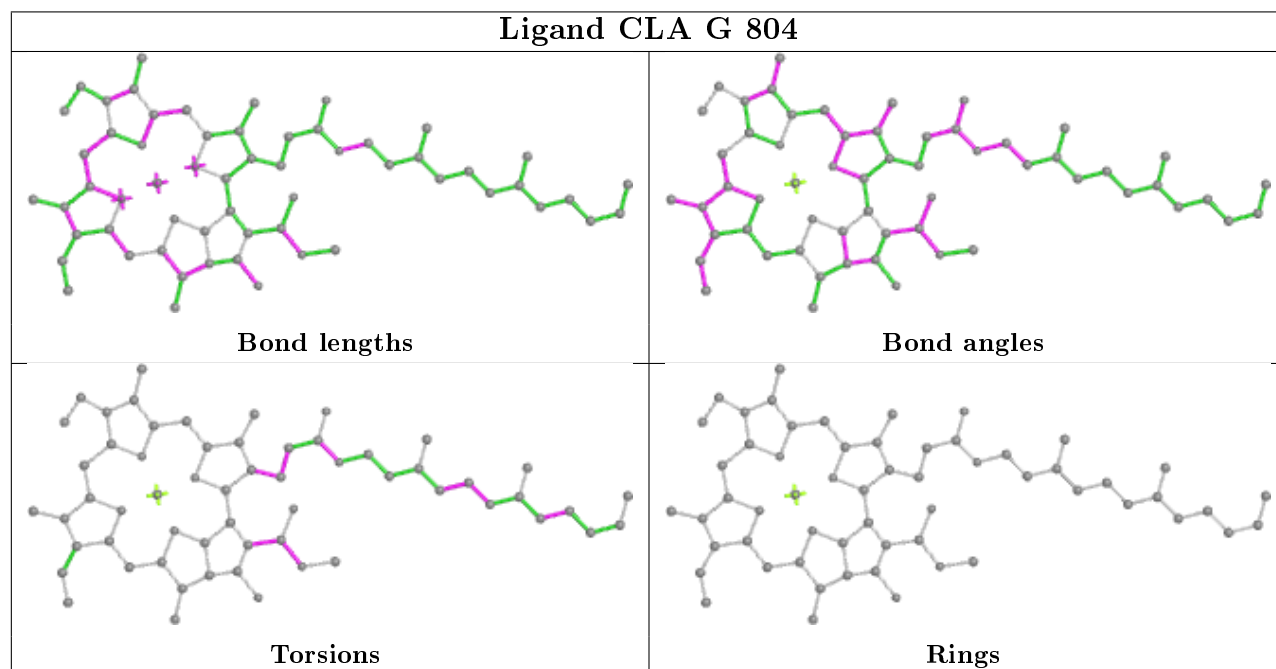
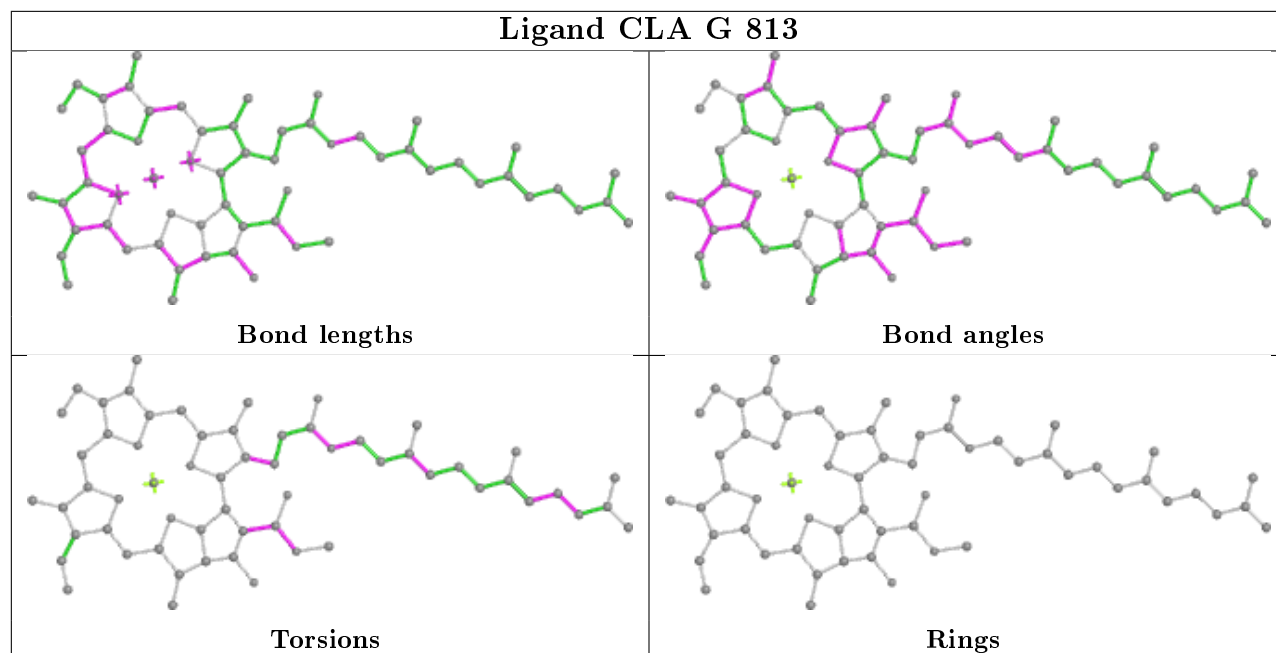


## Ligand CLA H 839

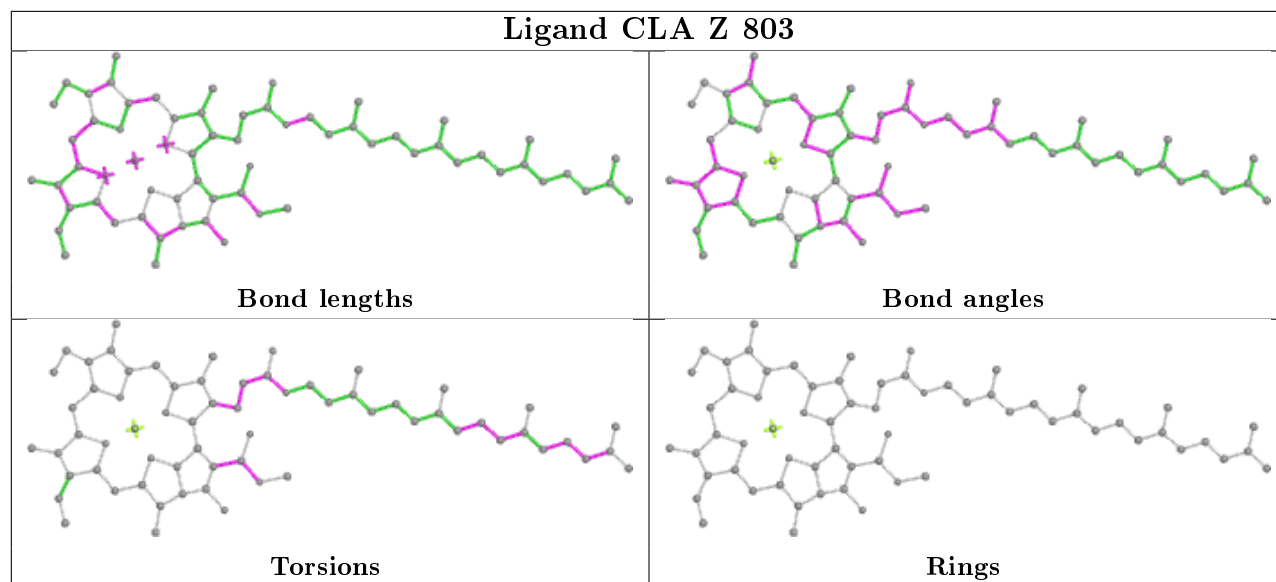


## Ligand CLA Y 811

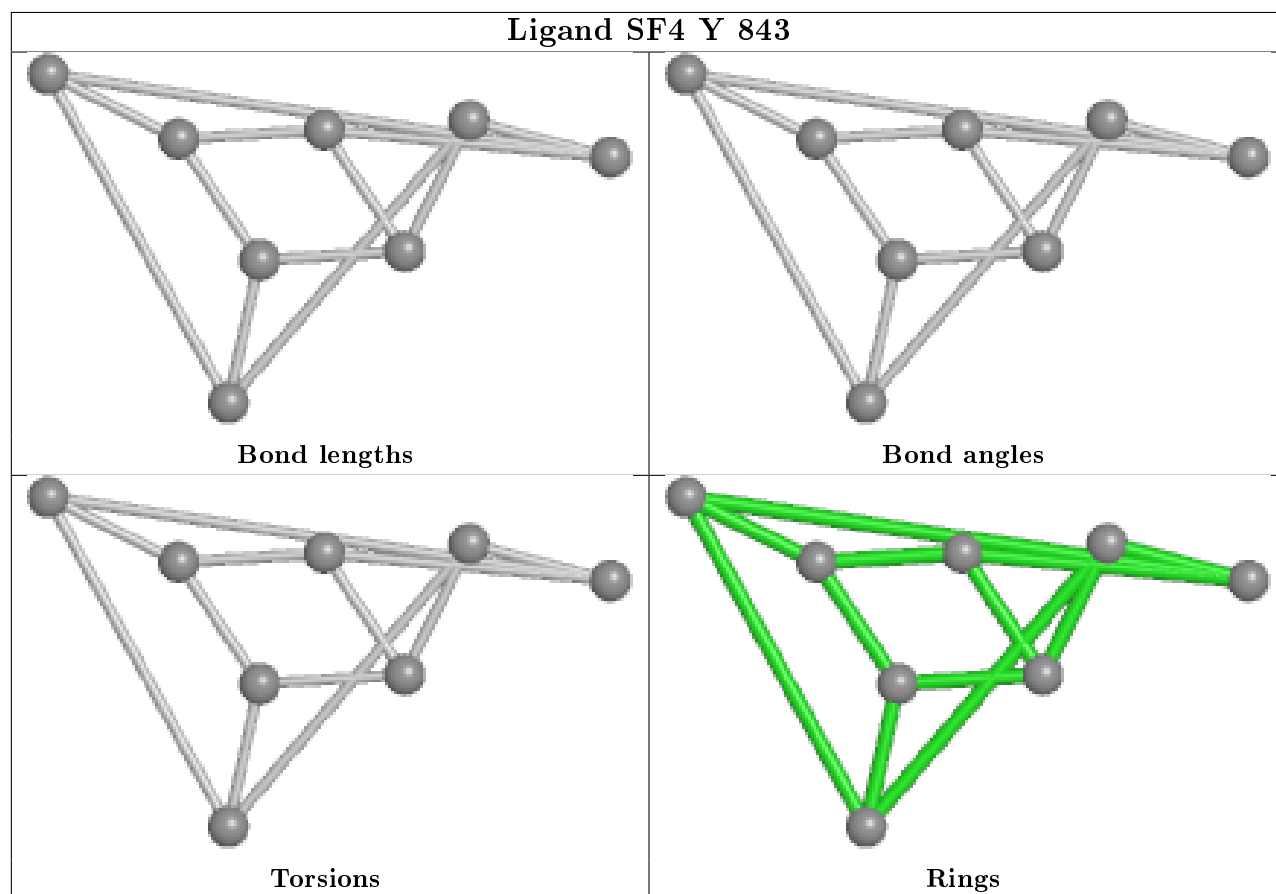




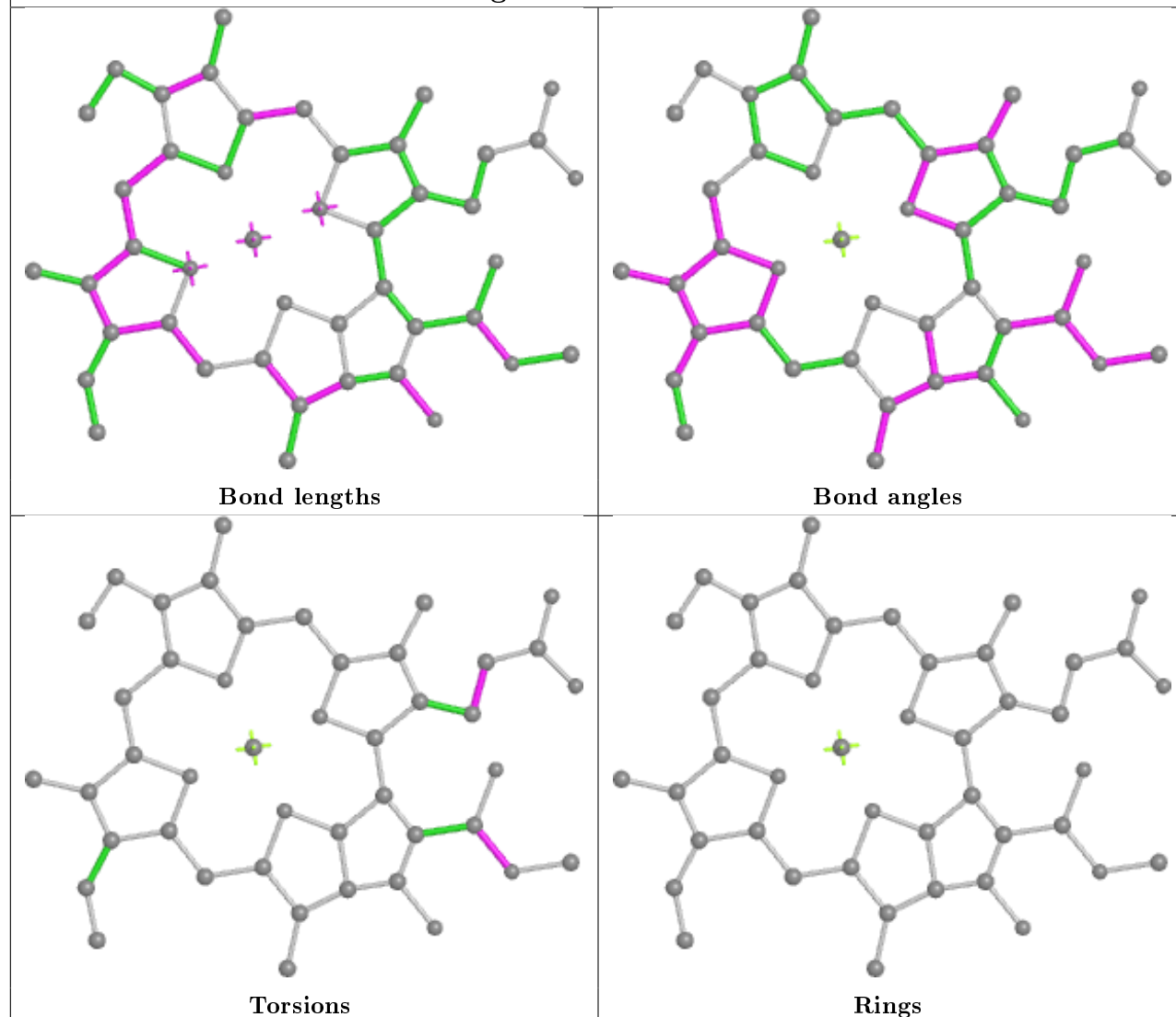
## Ligand CLA Z 803



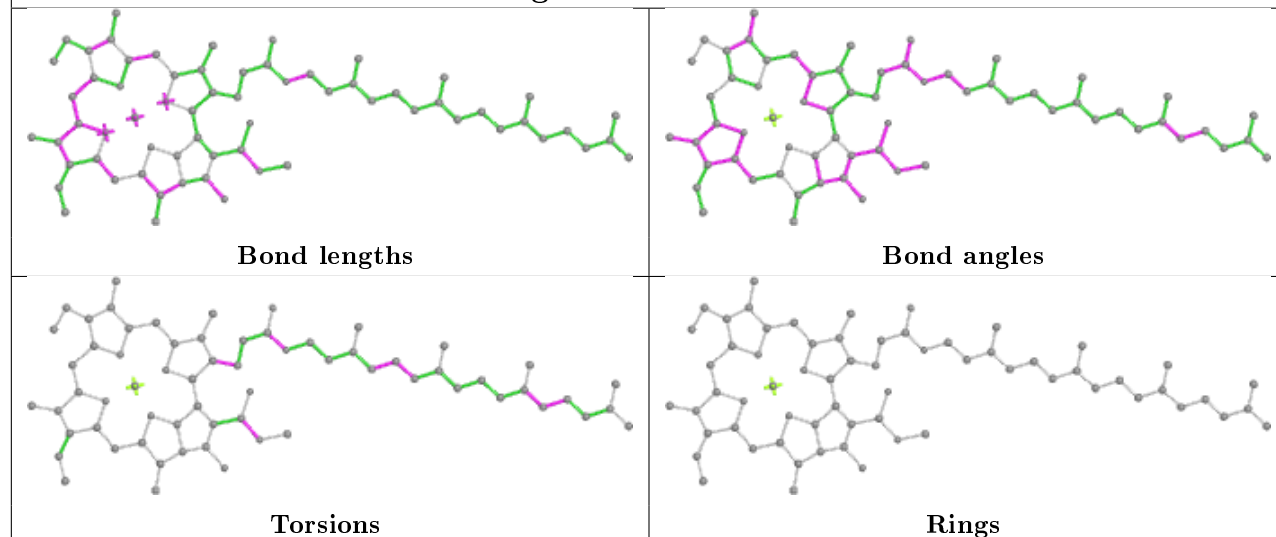
## Ligand SF4 Y 843



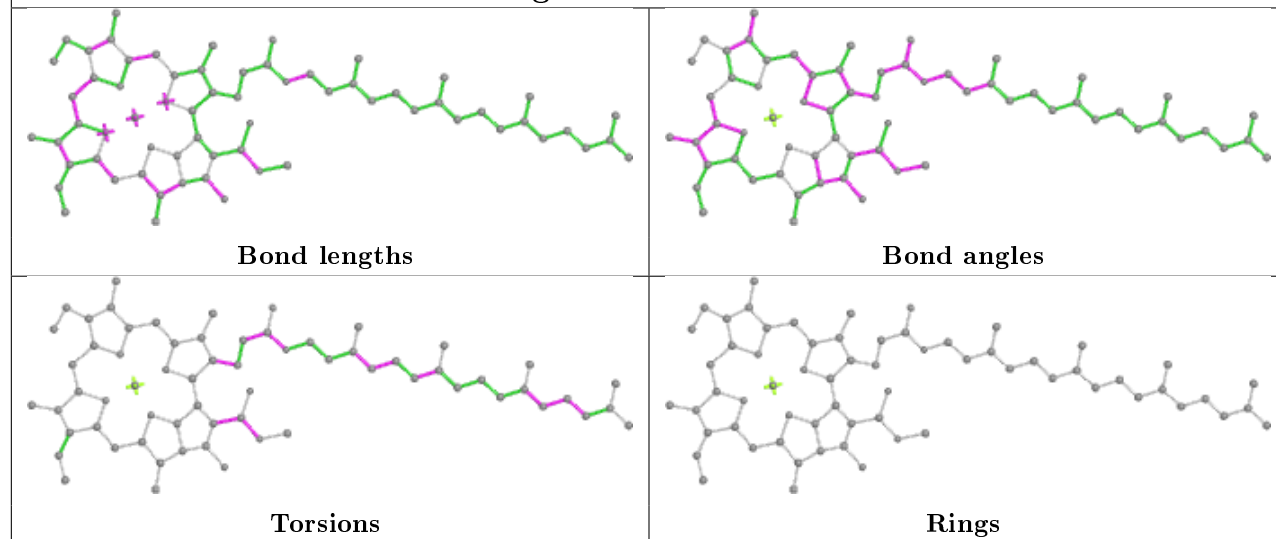
## Ligand CLA B 835



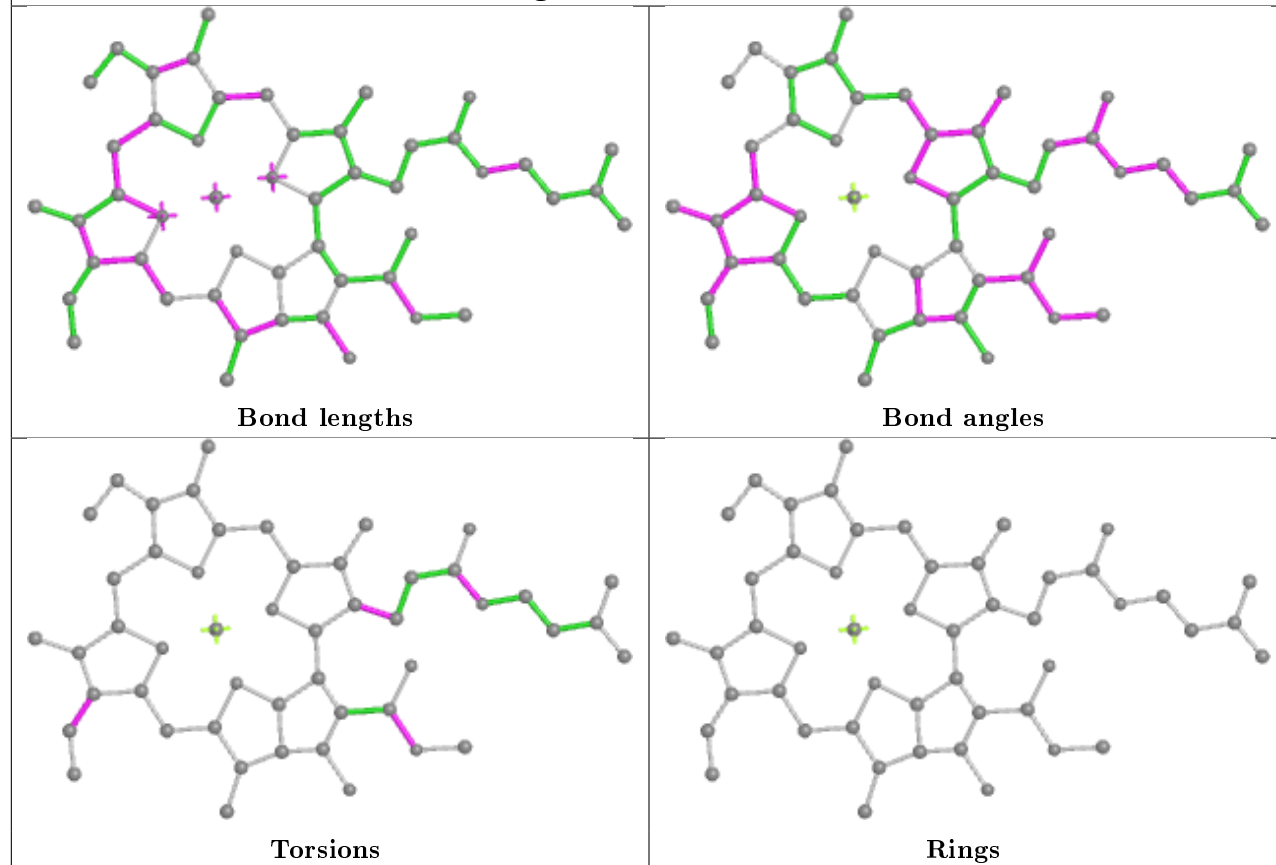
## Ligand CLA G 828

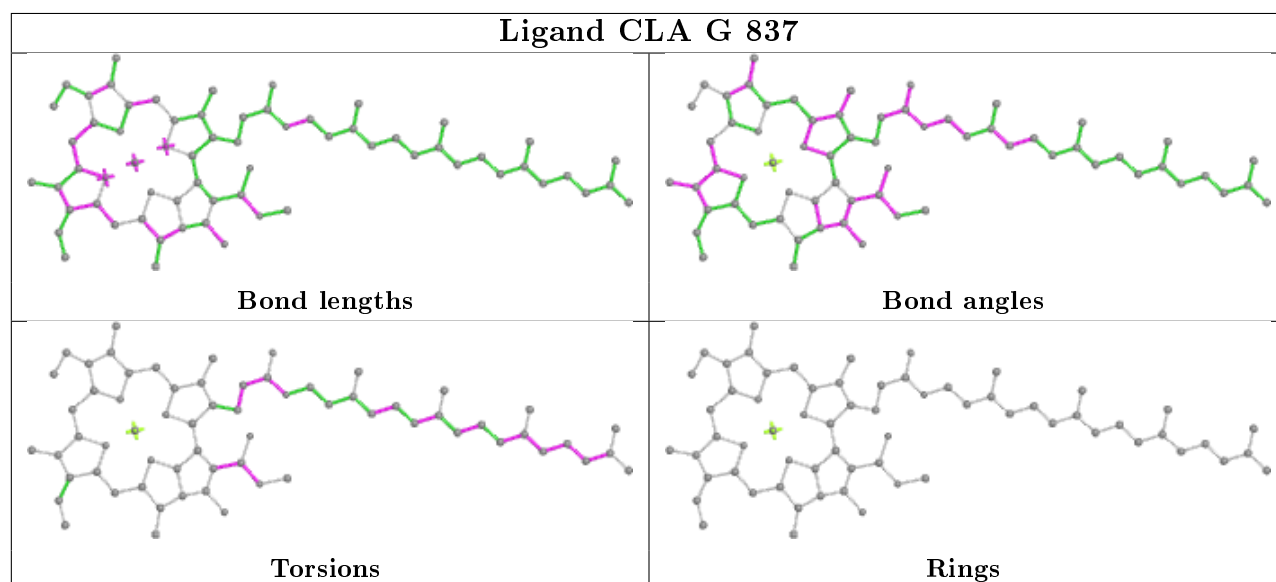
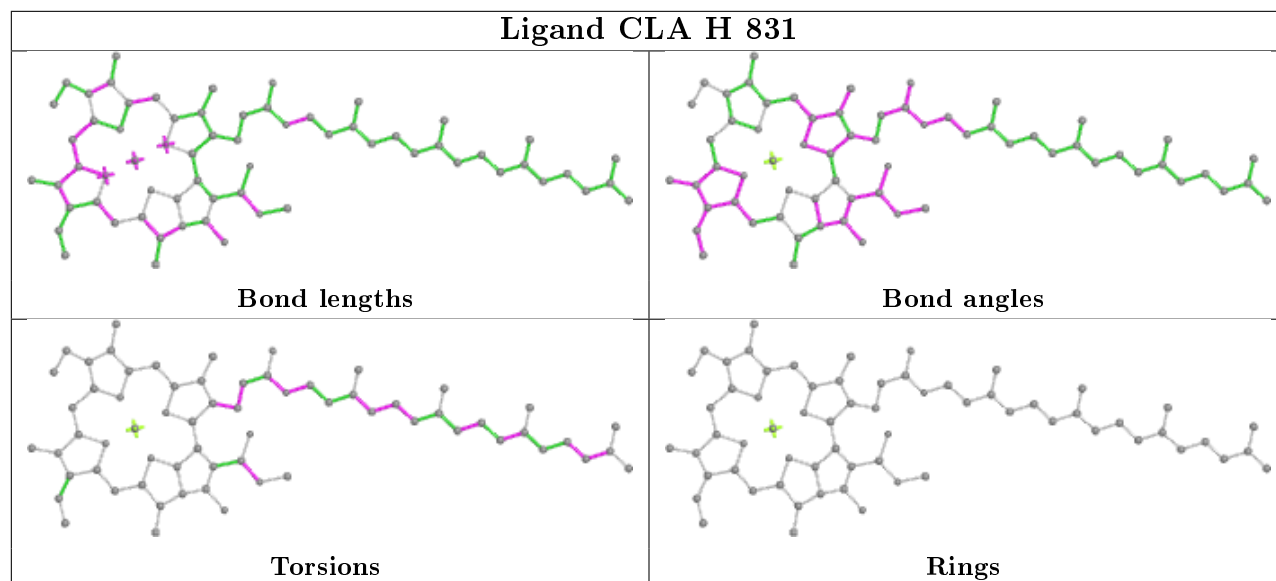
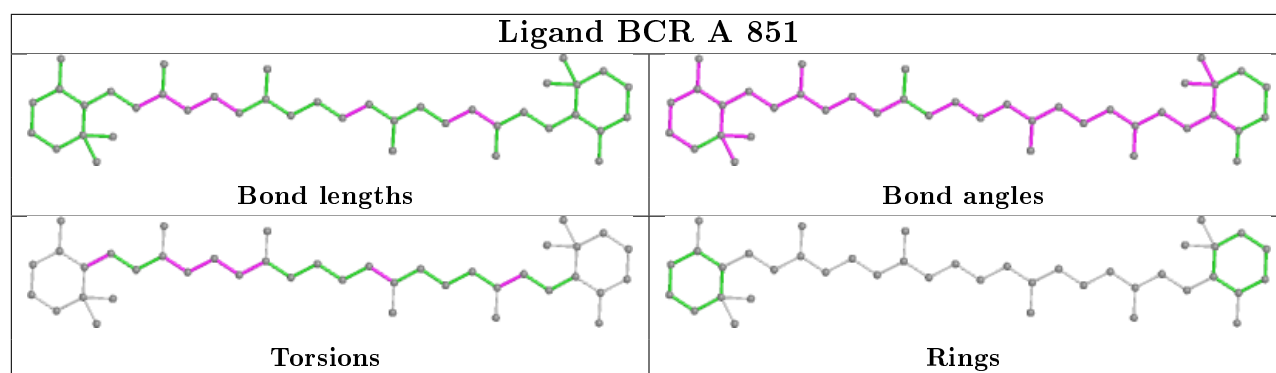


## Ligand CLA Y 806

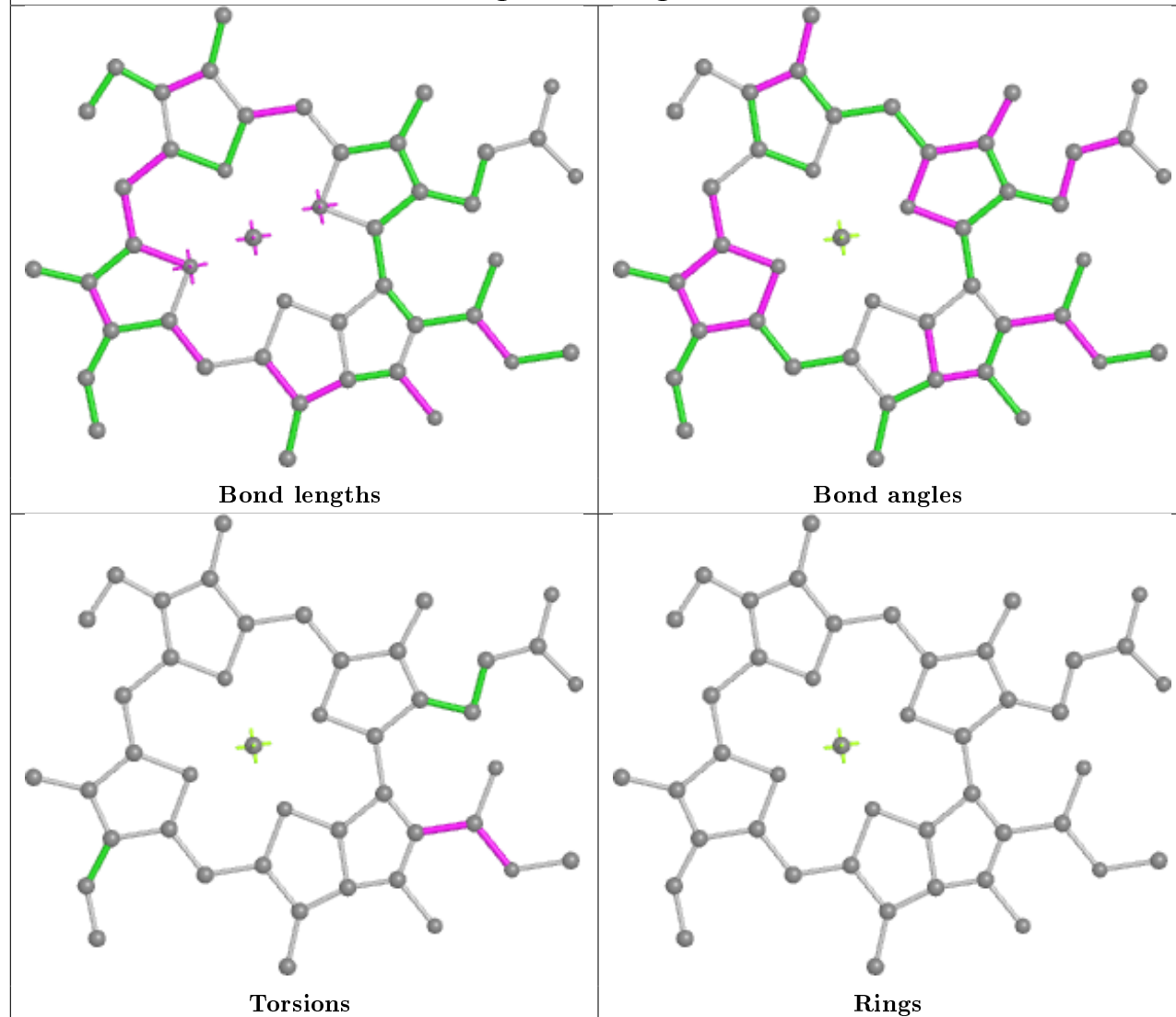


## Ligand CLA A 817

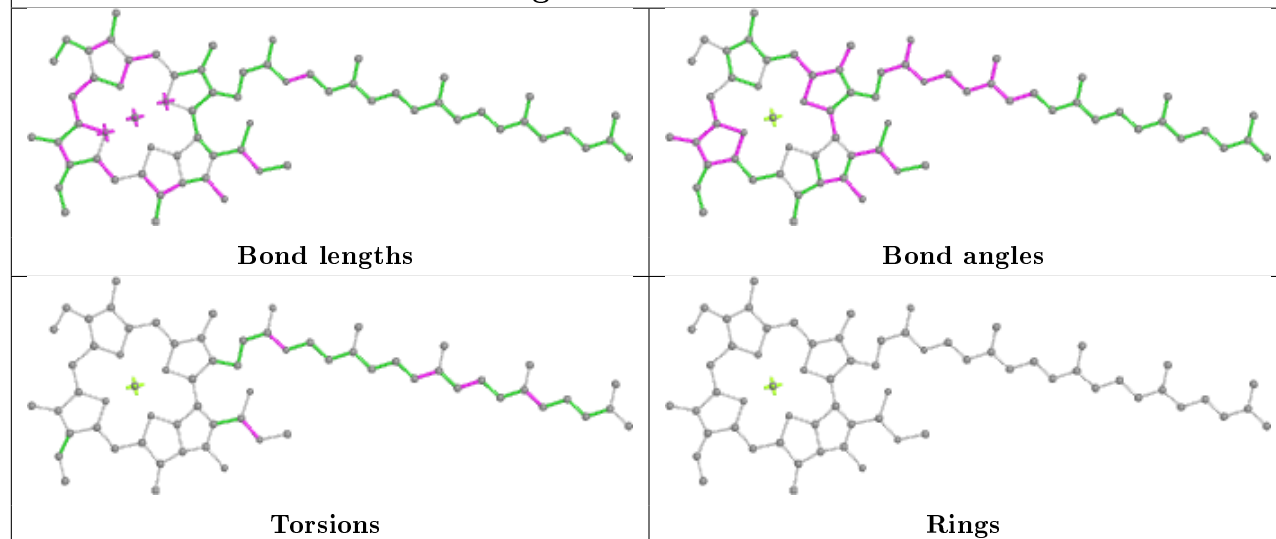




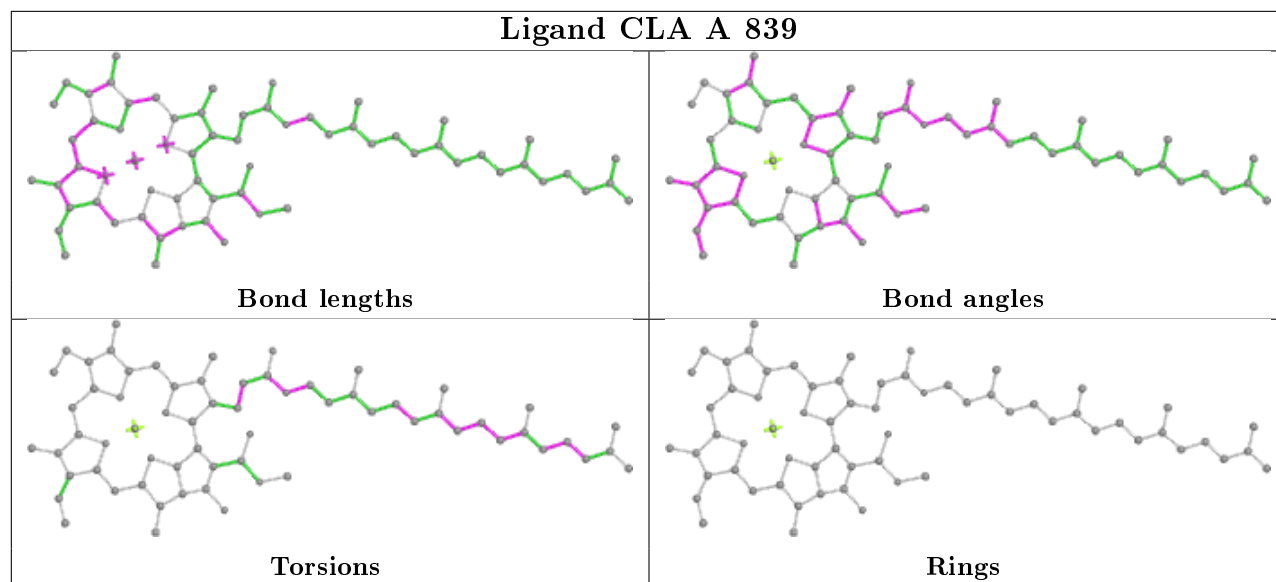
## Ligand CLA g 102



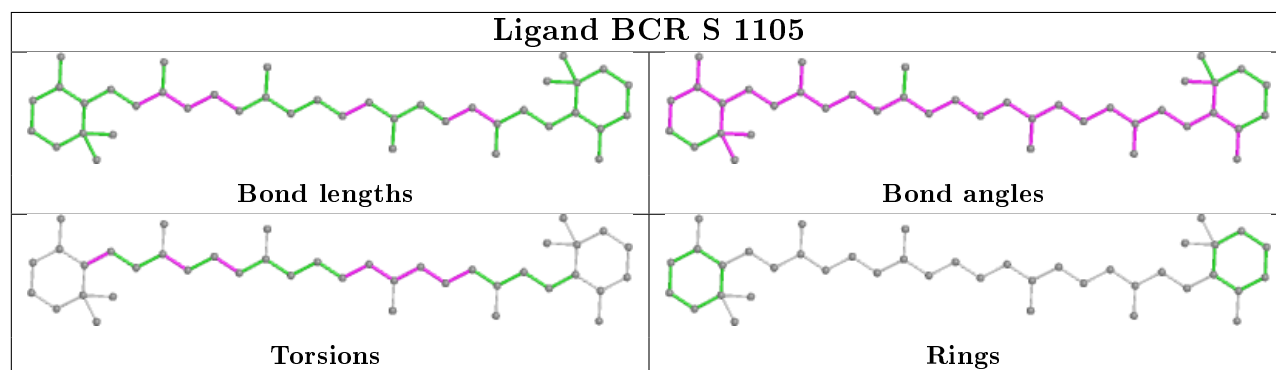
## Ligand CLA A 833



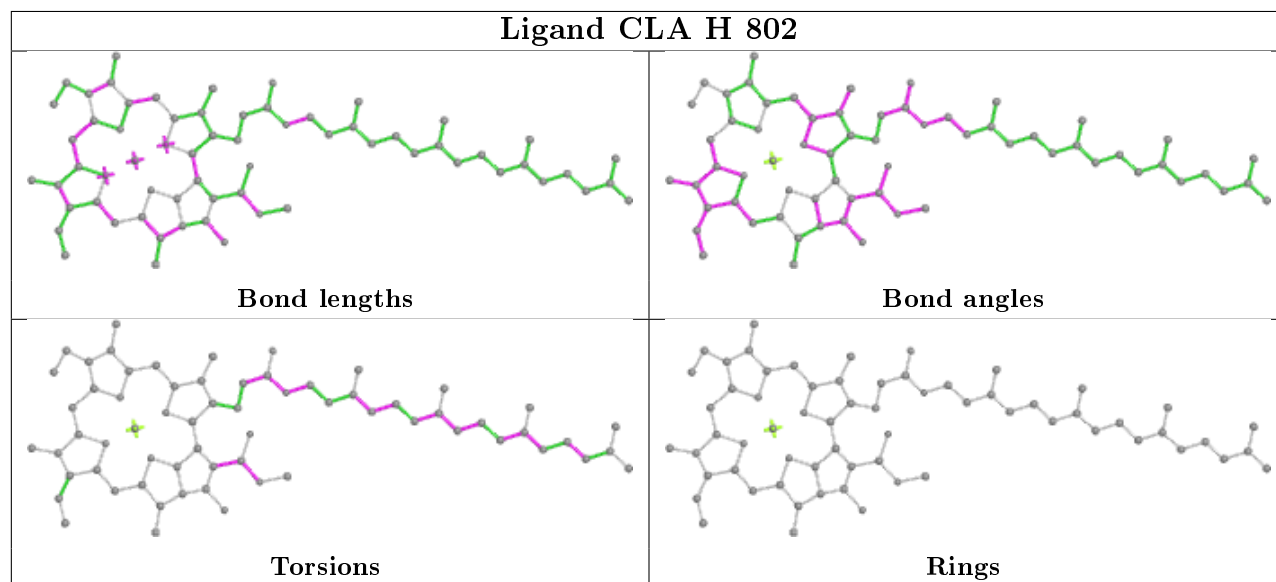
## Ligand CLA A 839



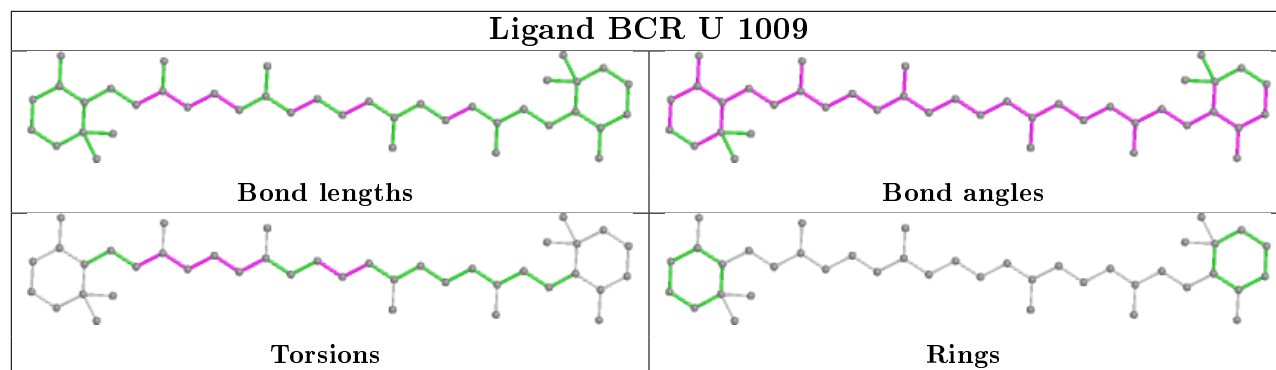
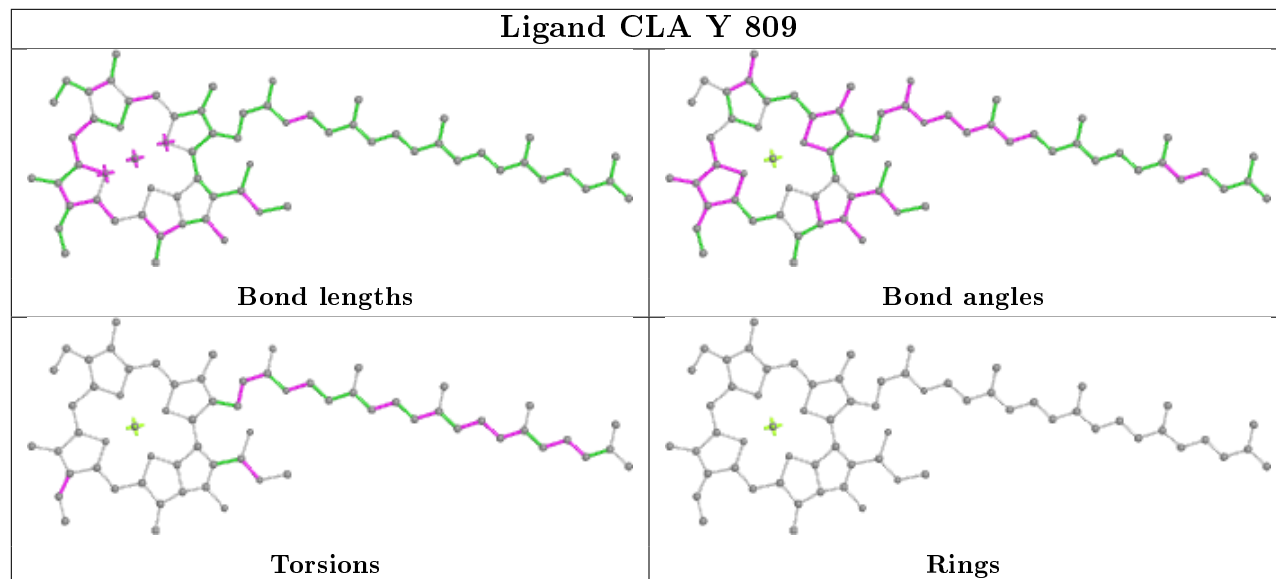
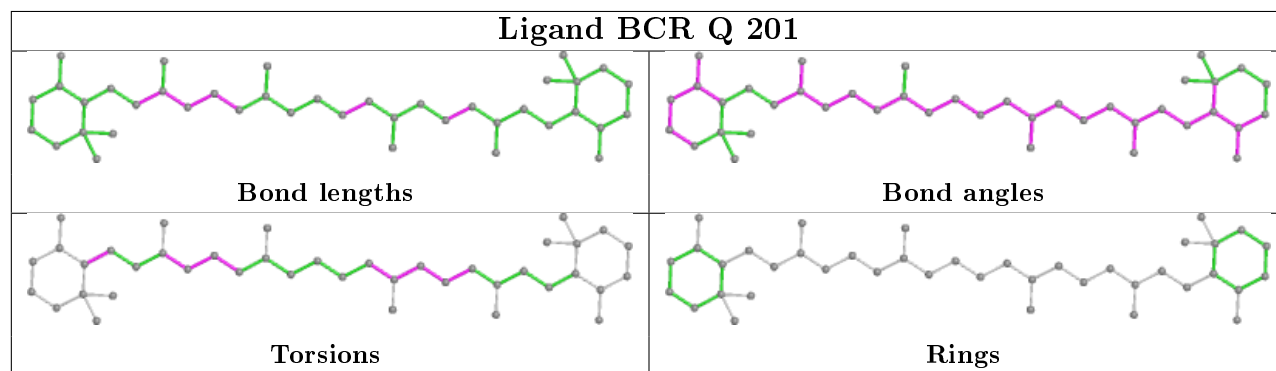
## Ligand BCR S 1105



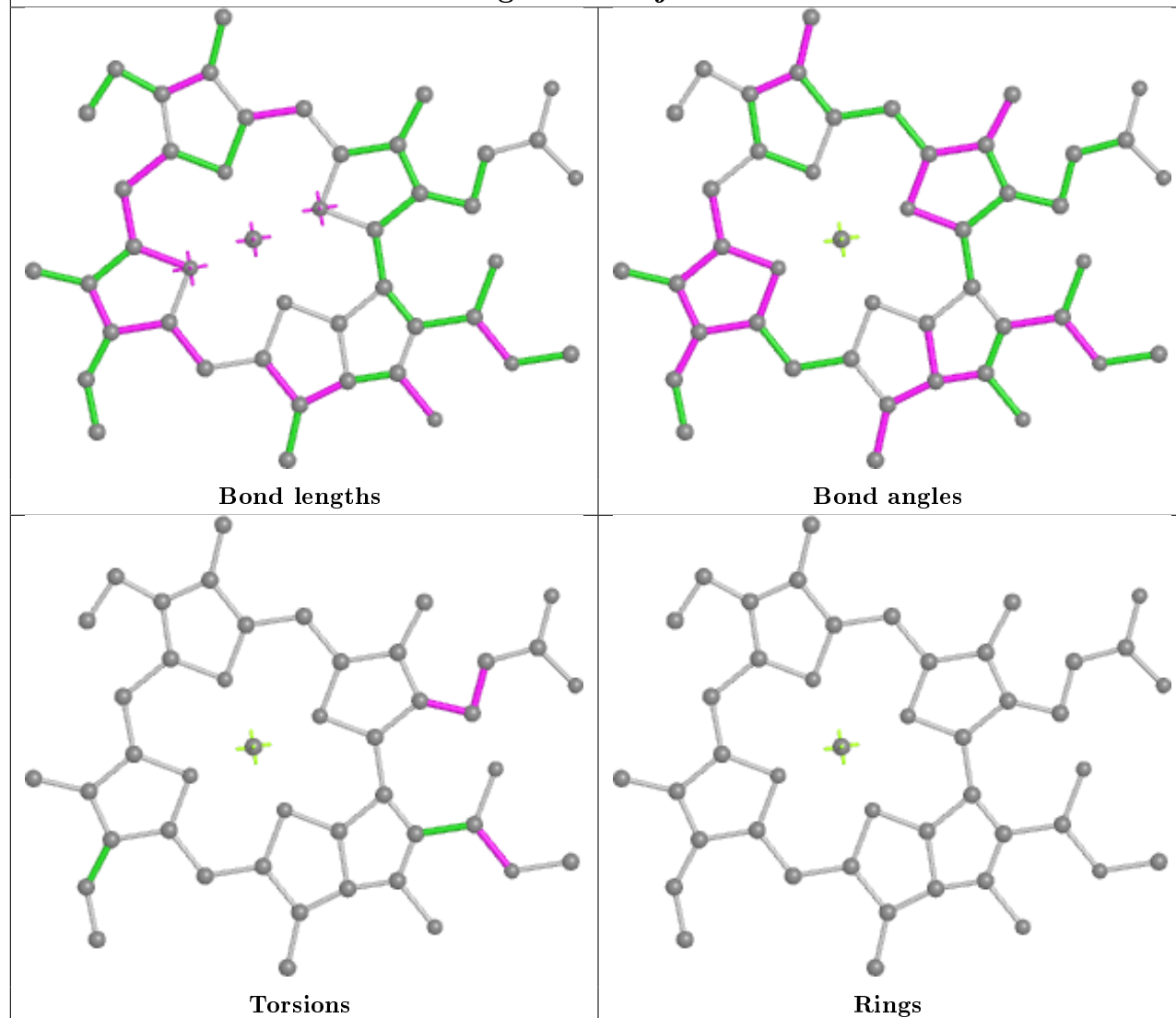
## Ligand CLA H 802



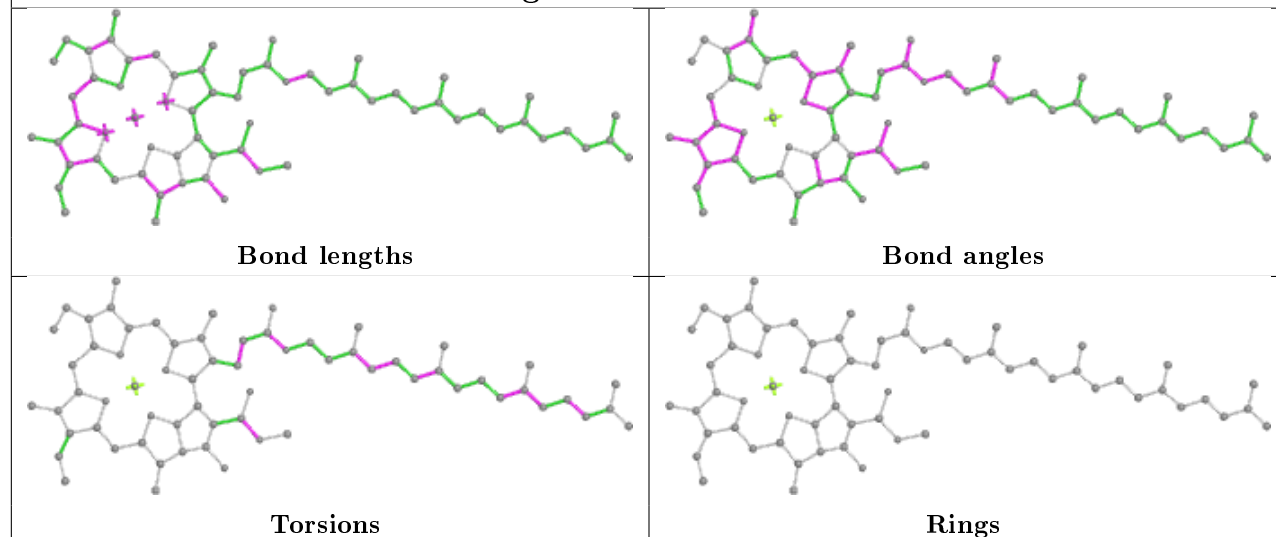


**Ligand BCR U 1009****Ligand CLA Y 809****Ligand BCR Q 201**

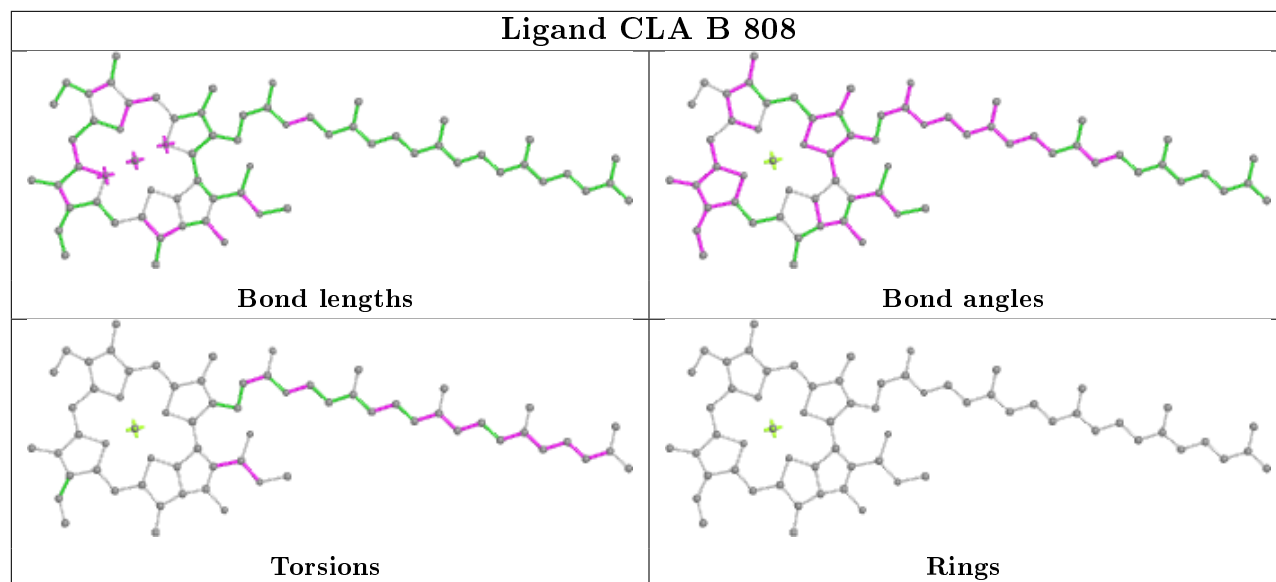
## Ligand CLA j 102



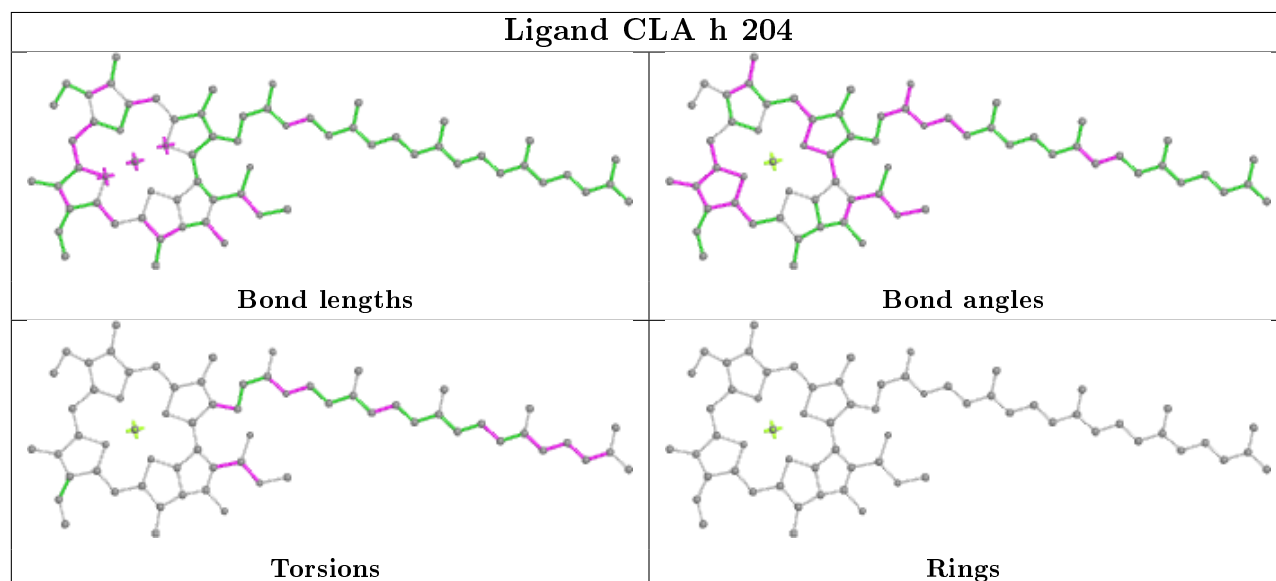
## Ligand CLA U 1006



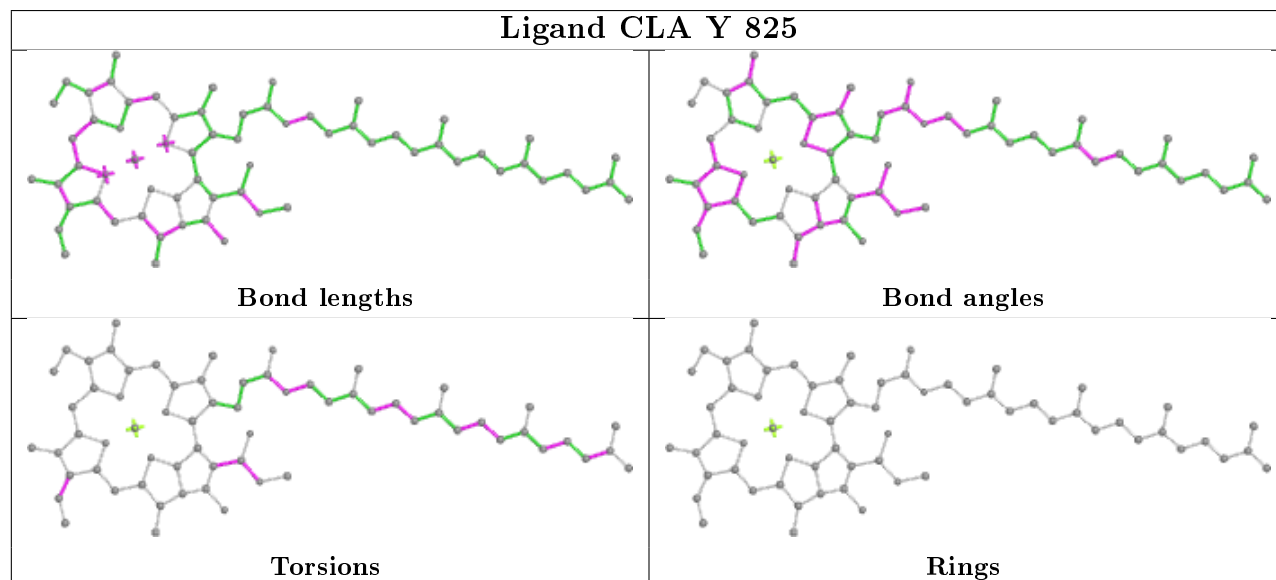
## Ligand CLA B 808

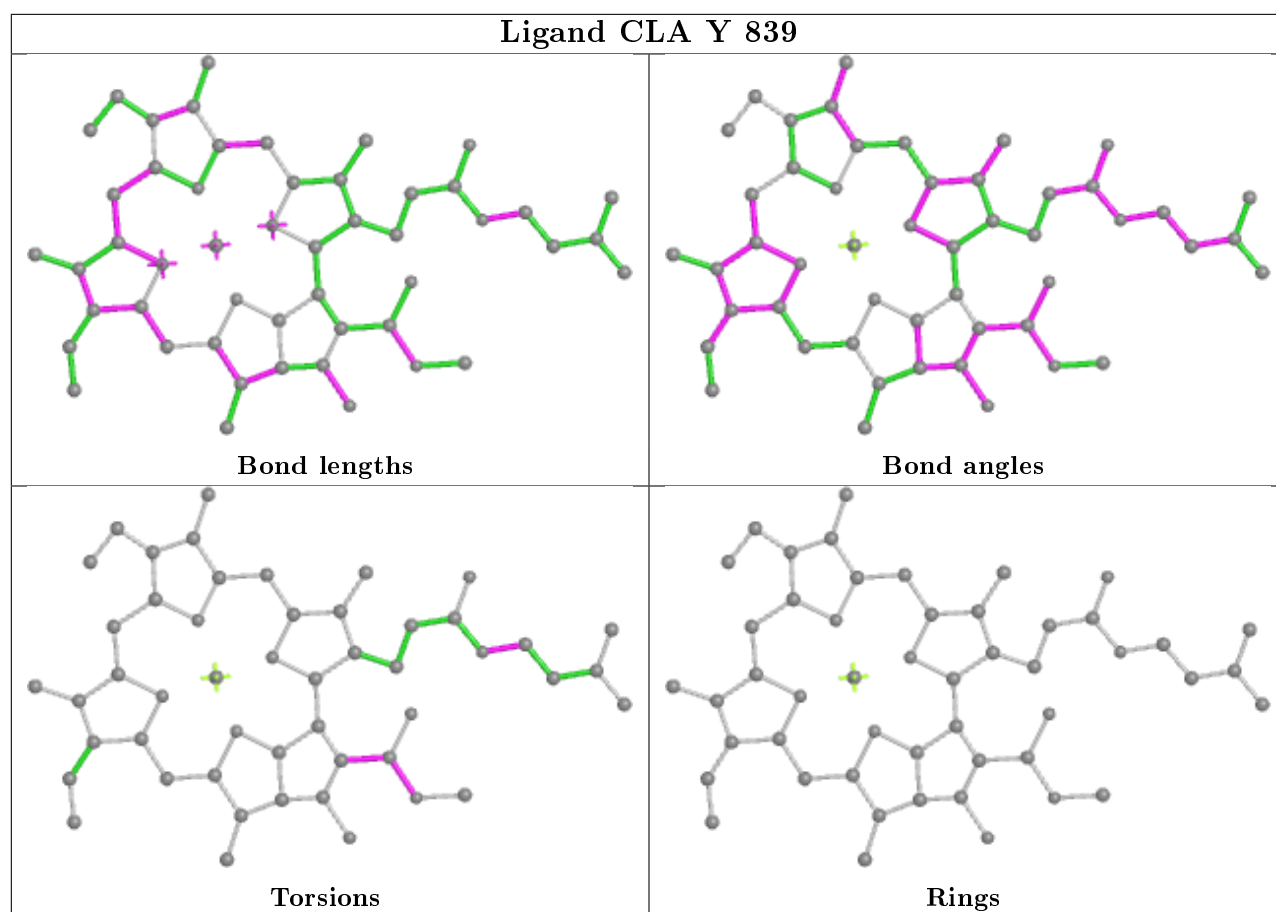


## Ligand CLA h 204

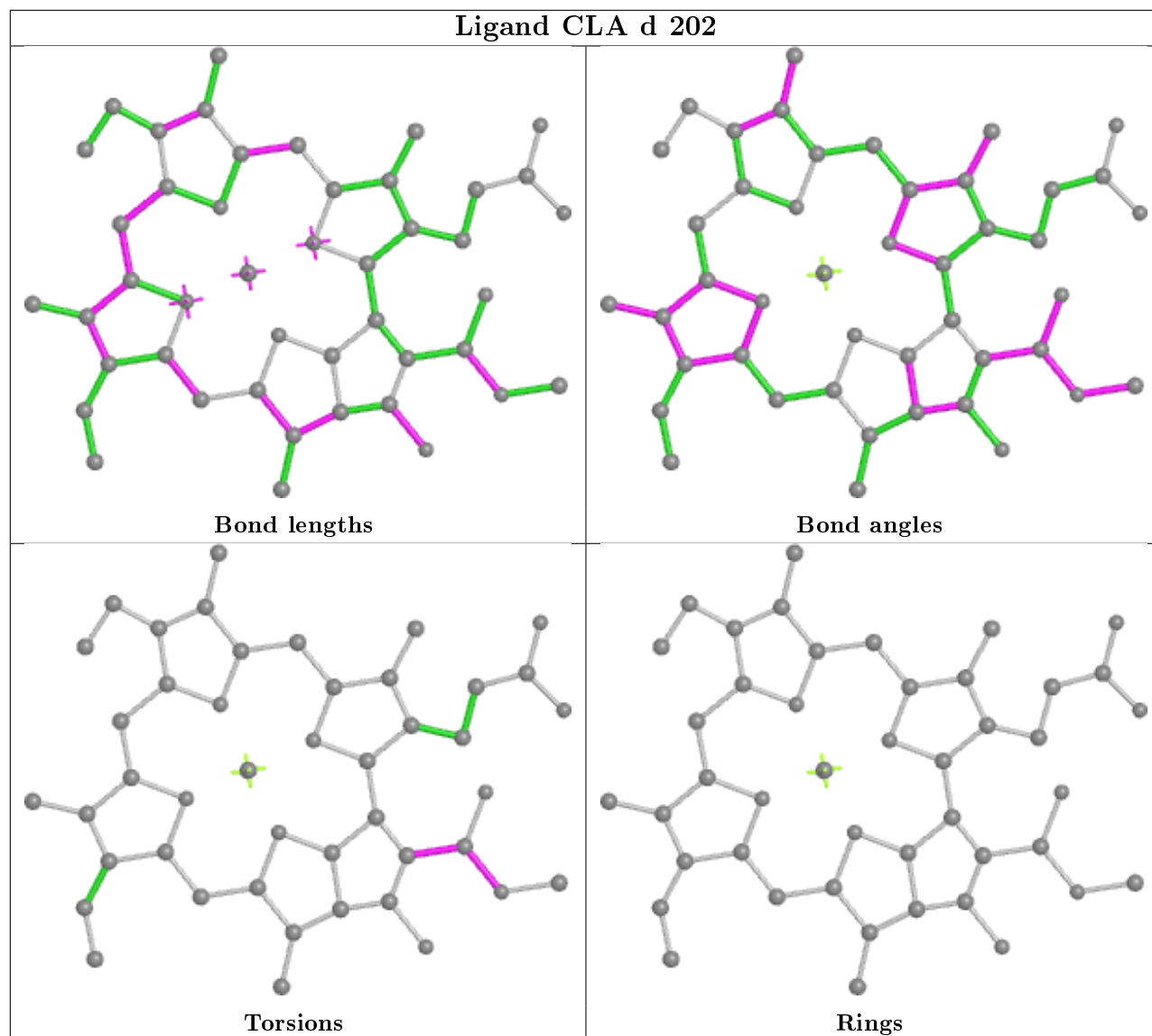


## Ligand CLA Y 825

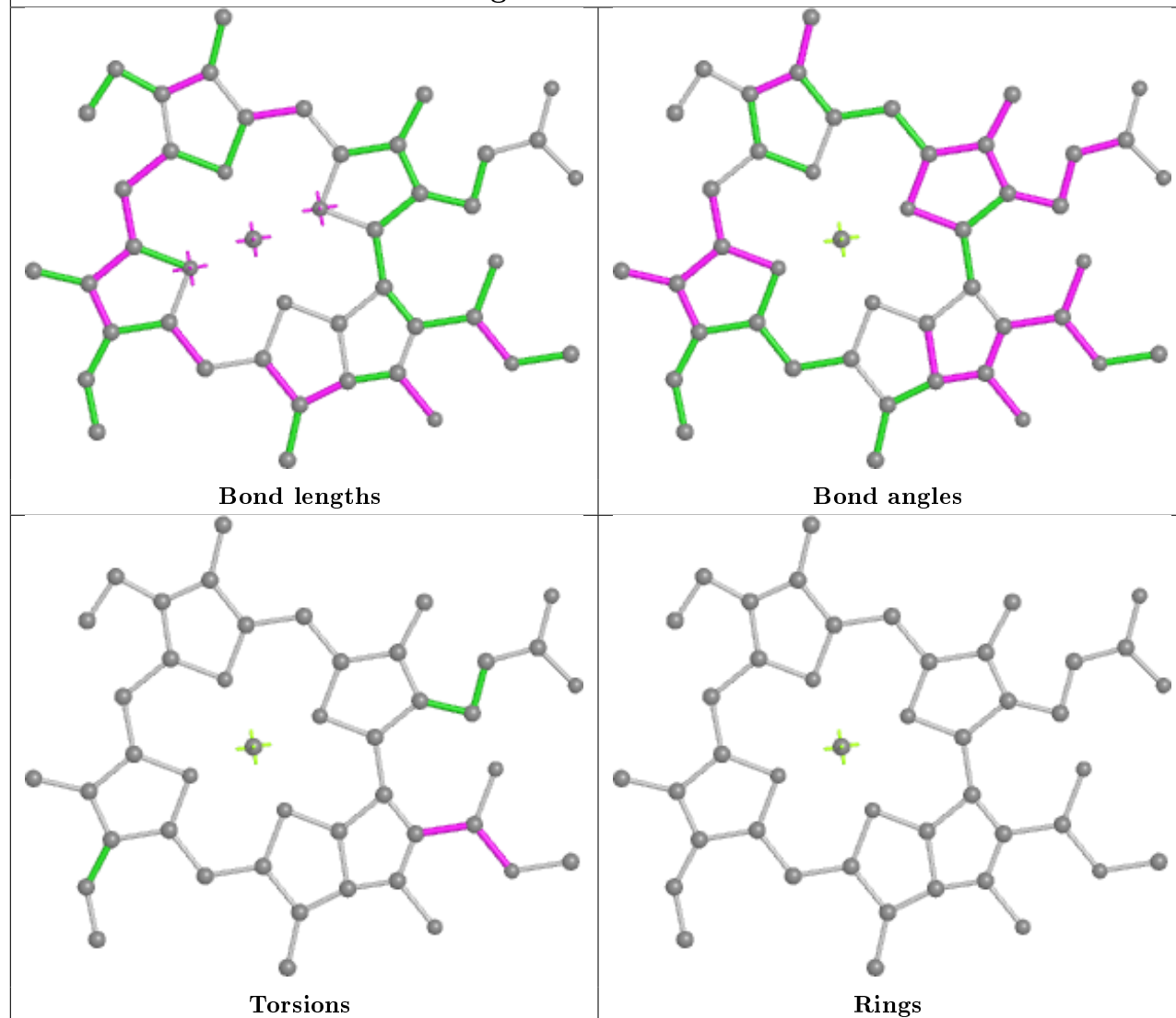




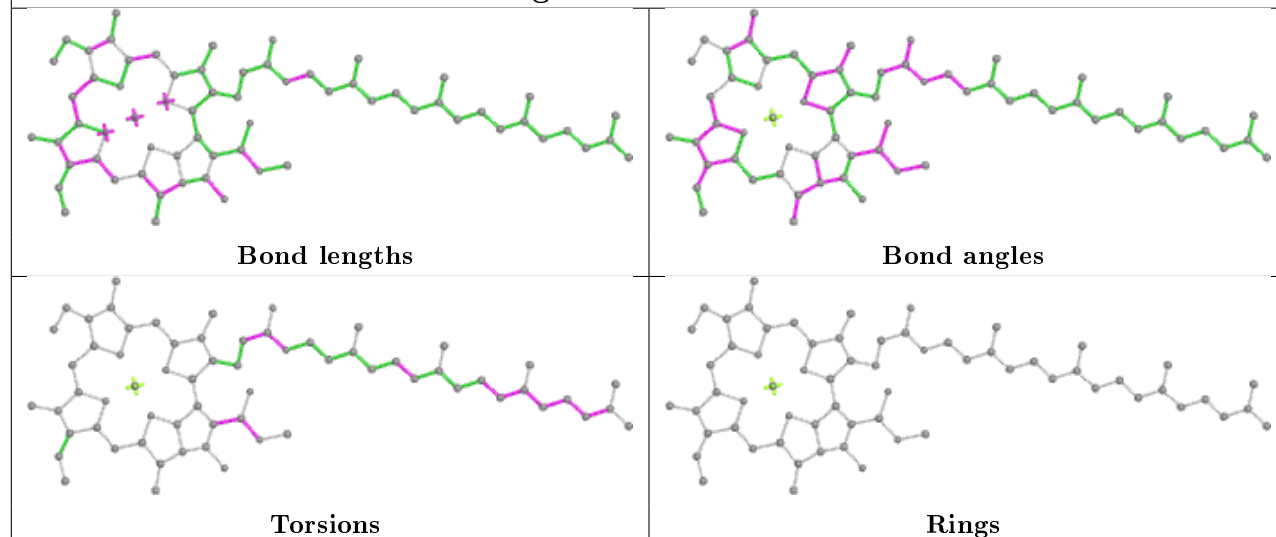
## Ligand CLA d 202

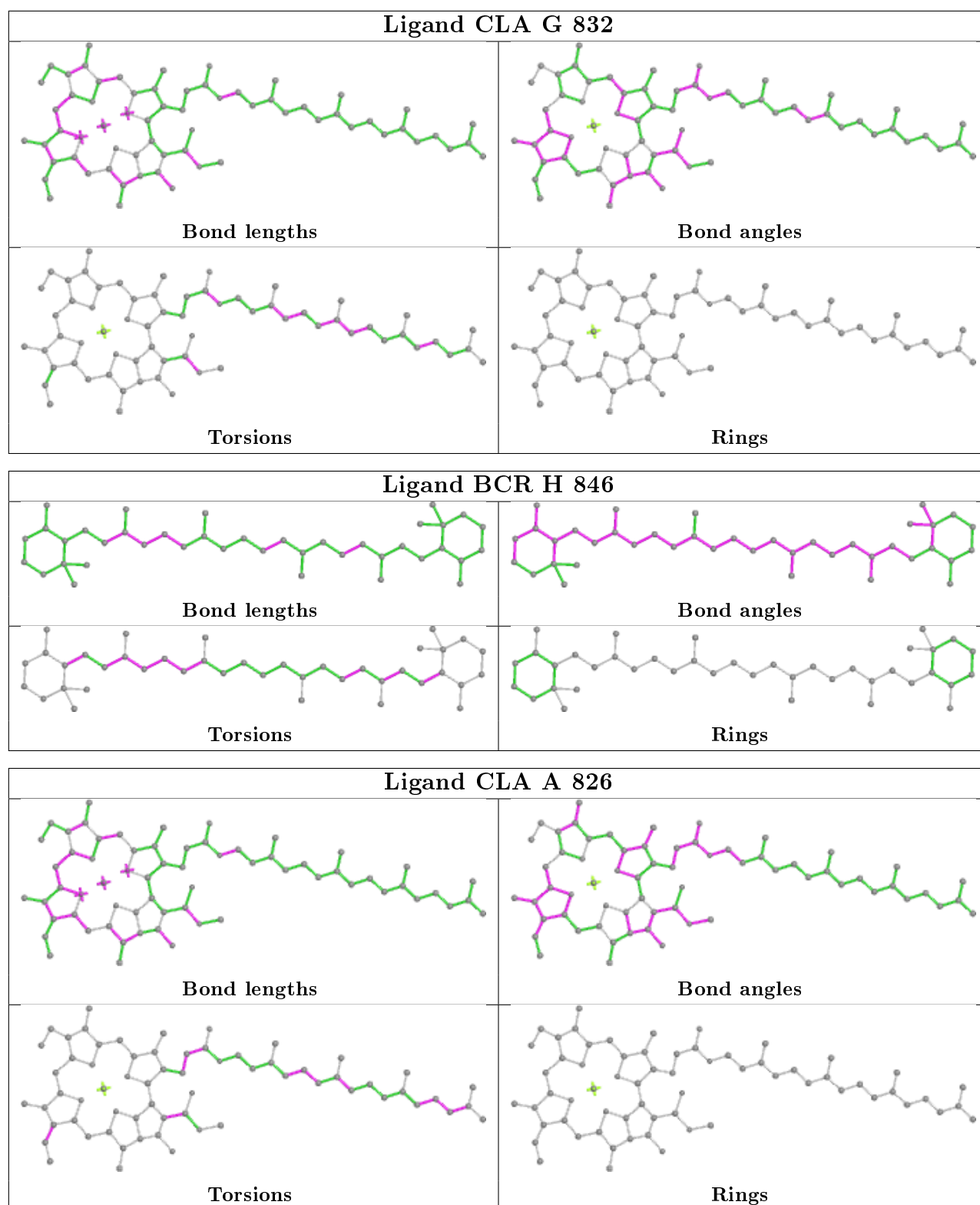


## Ligand CLA B 814

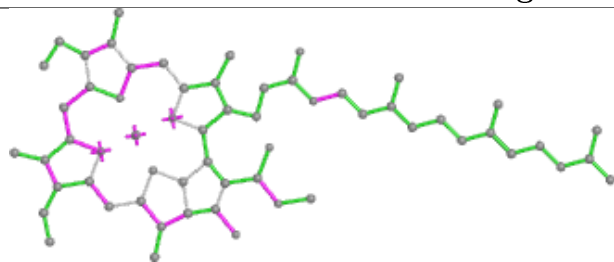


## Ligand CLA Y 829

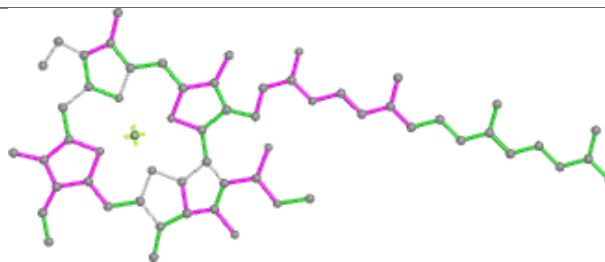




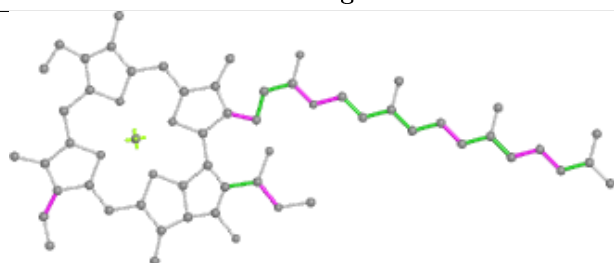
## Ligand CLA Z 837



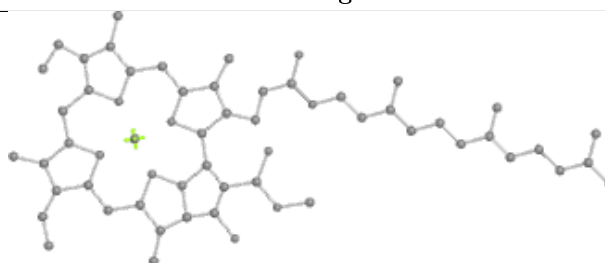
Bond lengths



Bond angles

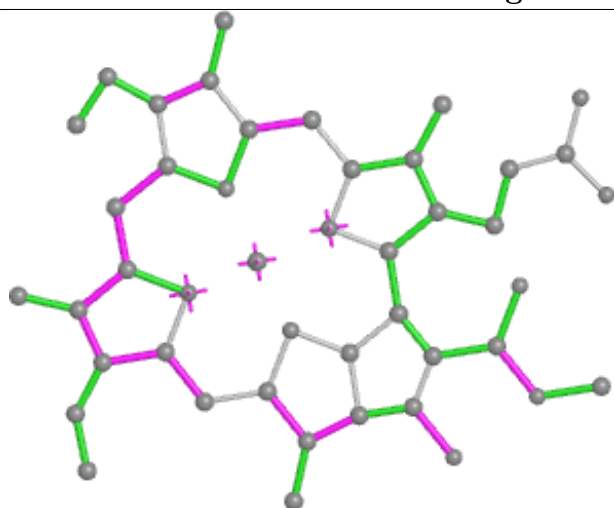


Torsions

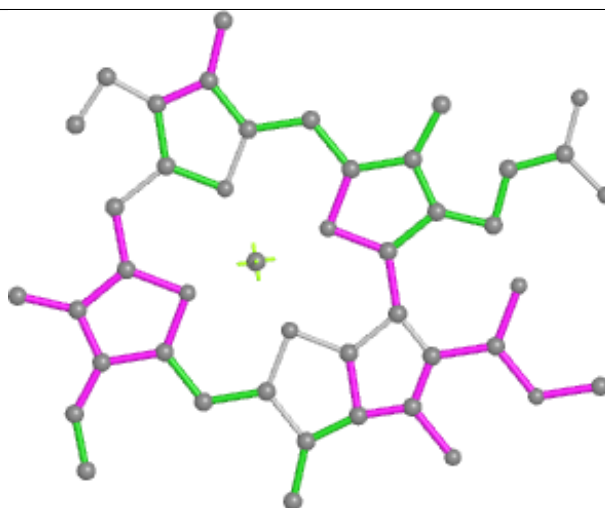


Rings

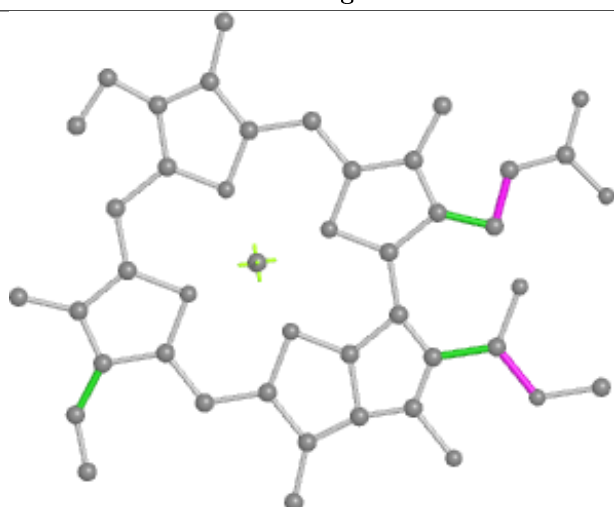
## Ligand CLA X 1701



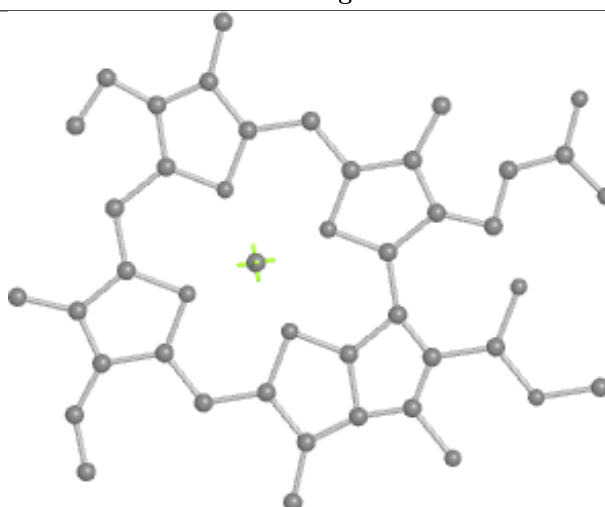
Bond lengths



Bond angles

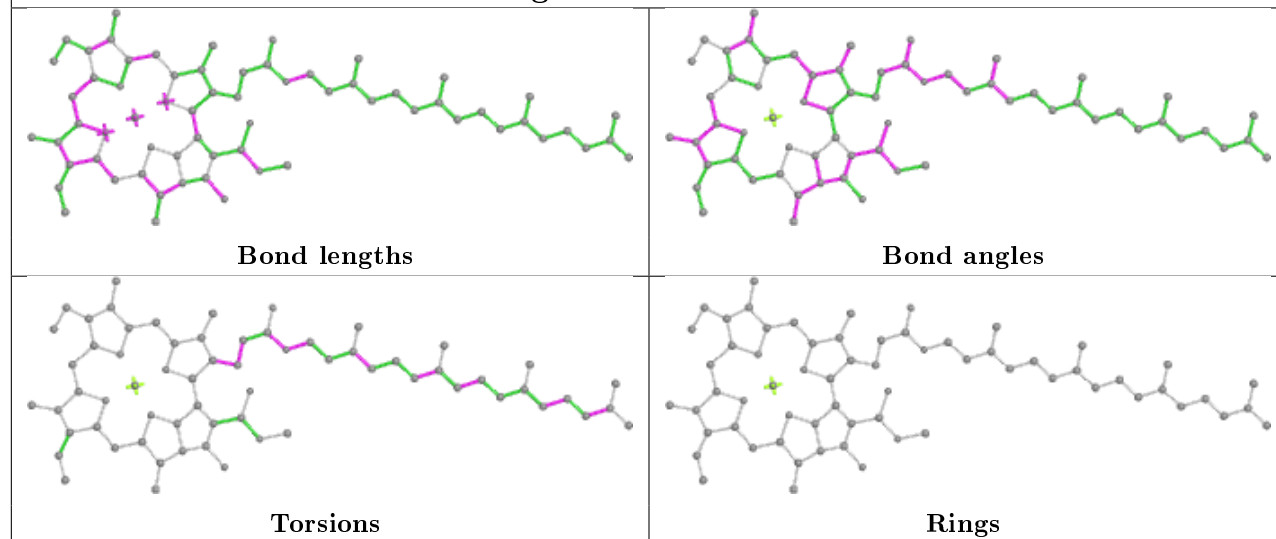
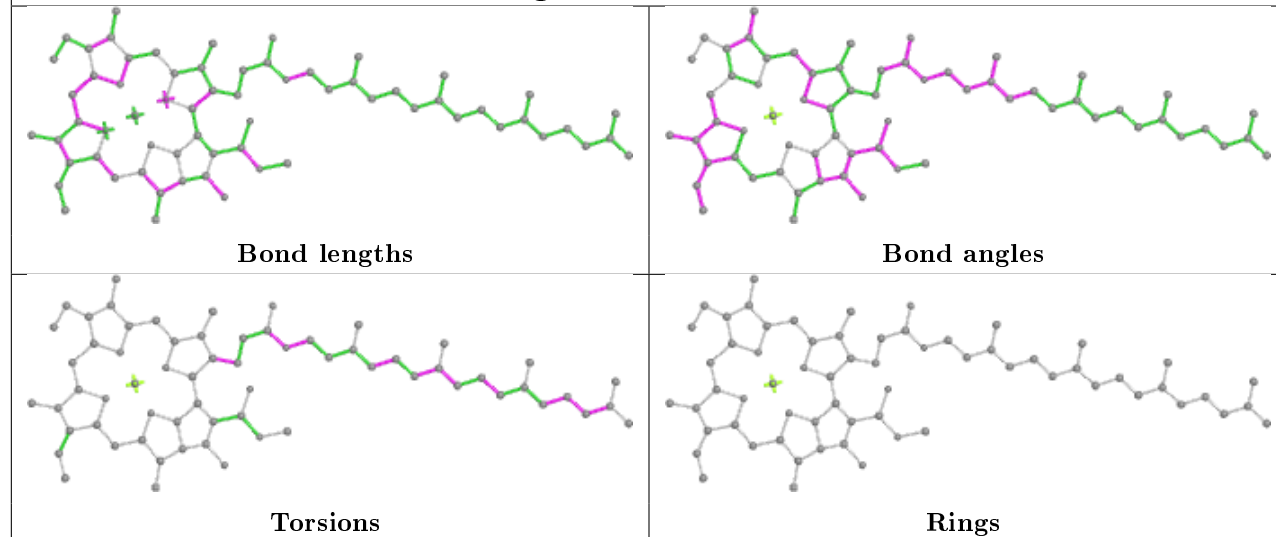


Torsions

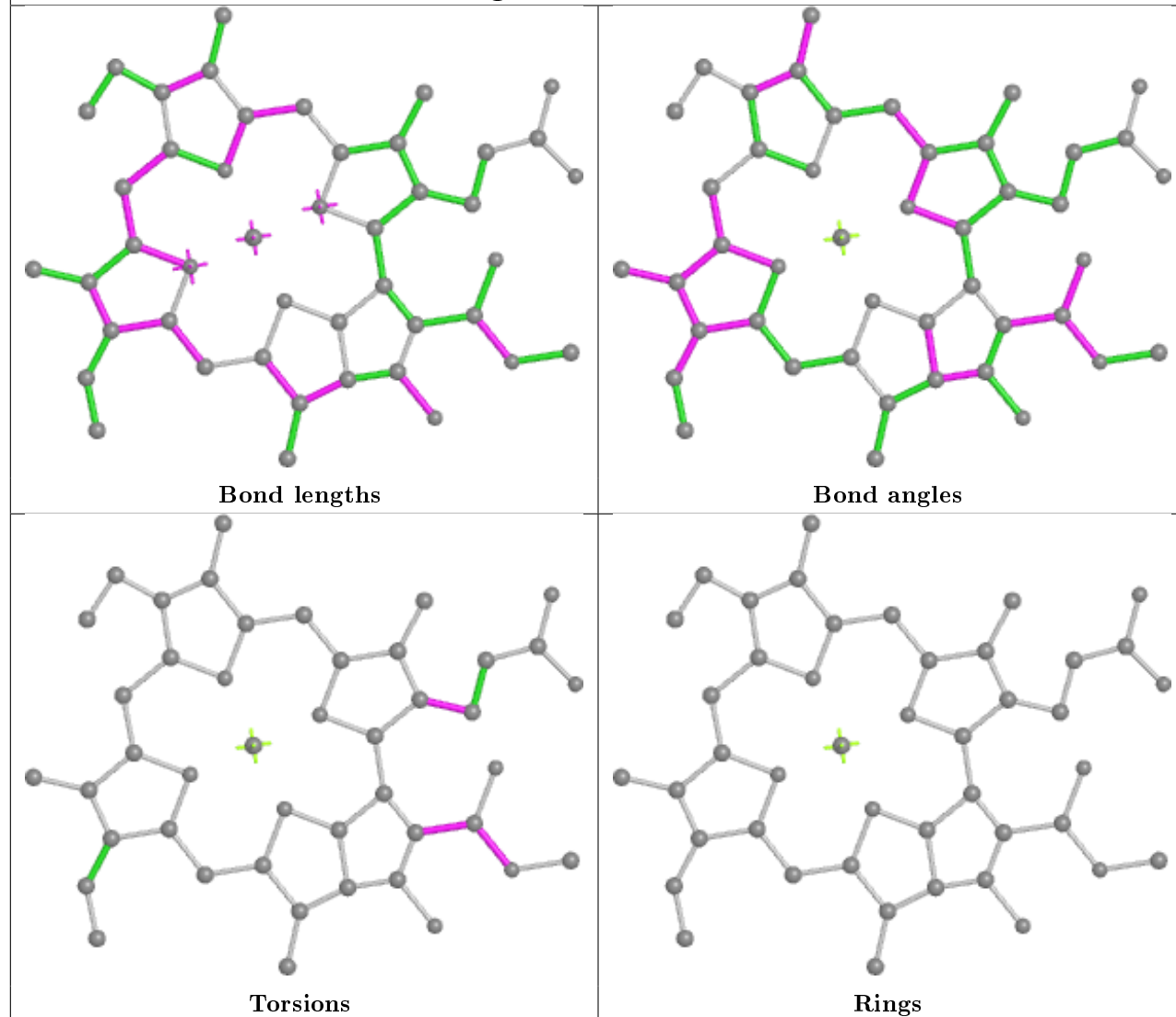


Rings

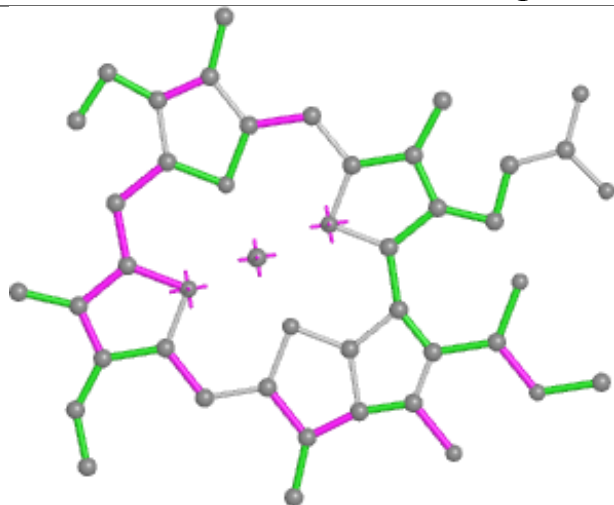


**Ligand CLA G 822****Ligand CLA B 804**

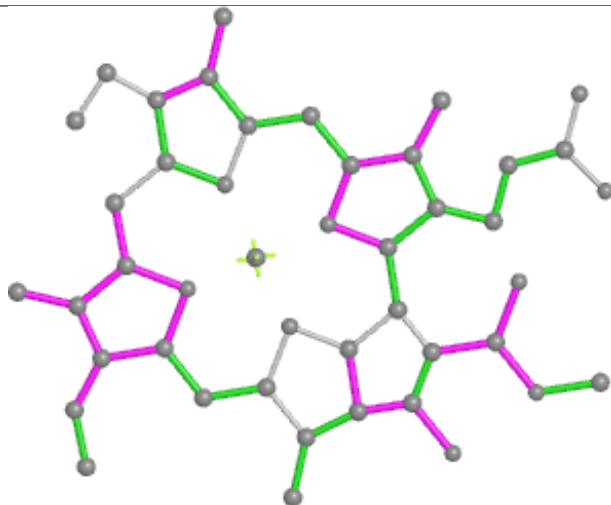
## Ligand CLA H 833



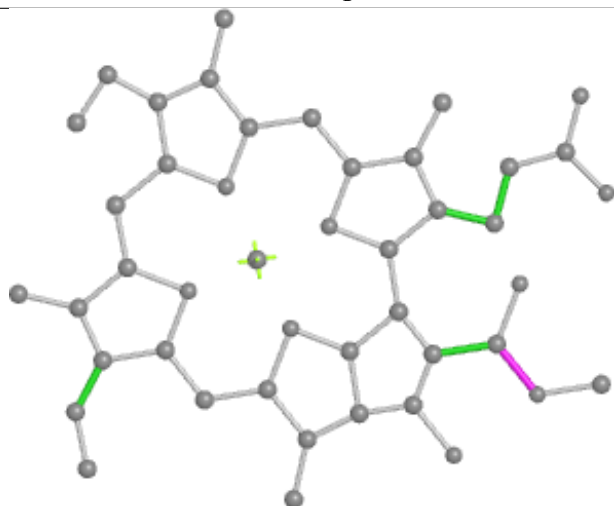
## Ligand CLA Q 202



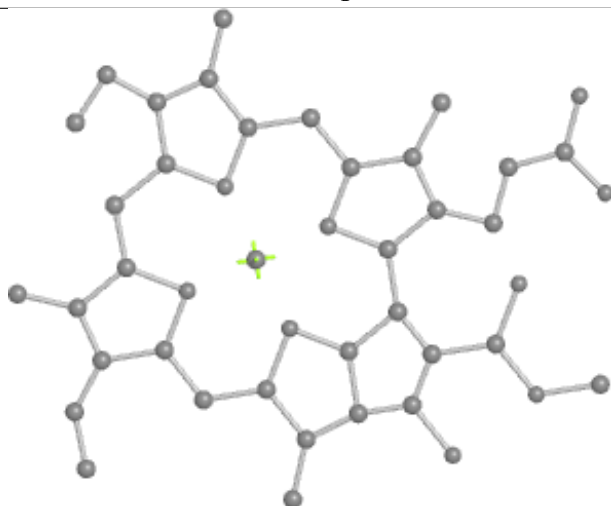
Bond lengths



Bond angles

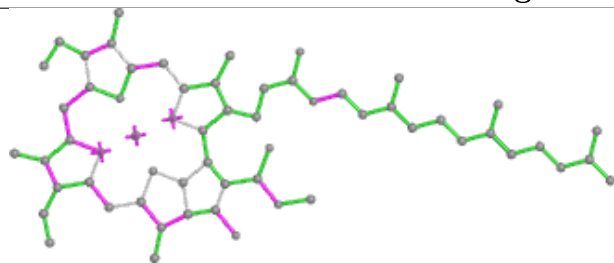


Torsions

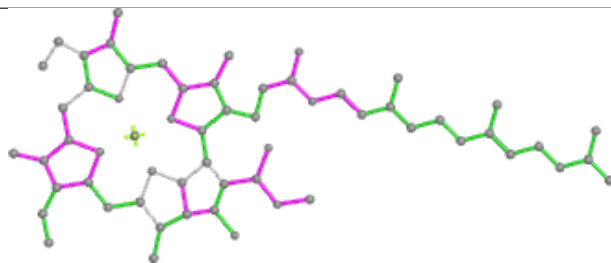


Rings

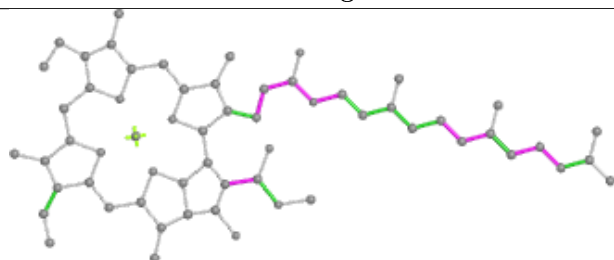
## Ligand CLA Y 820



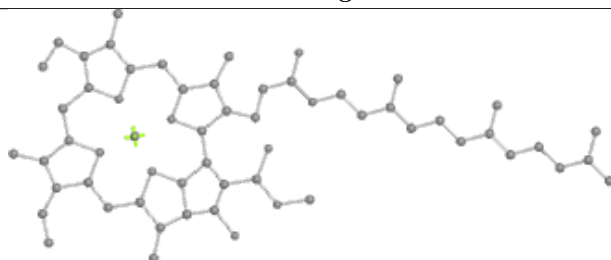
Bond lengths



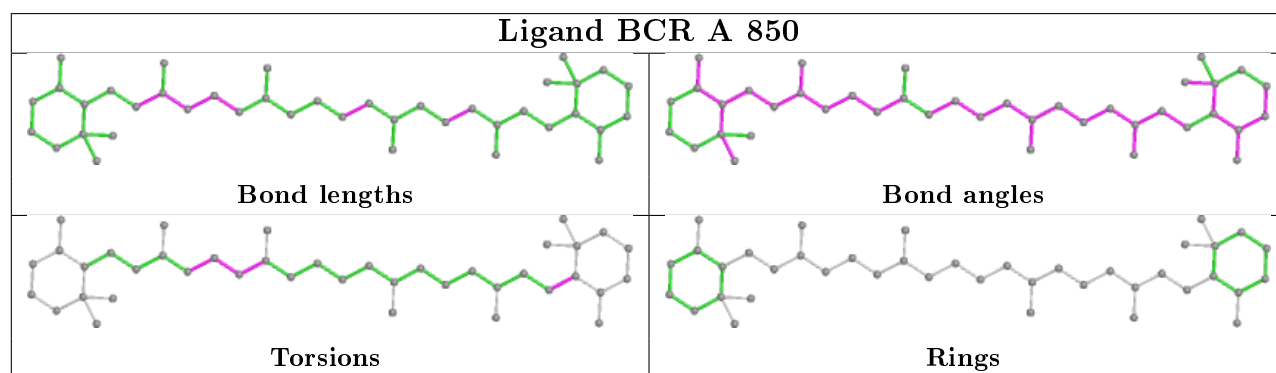
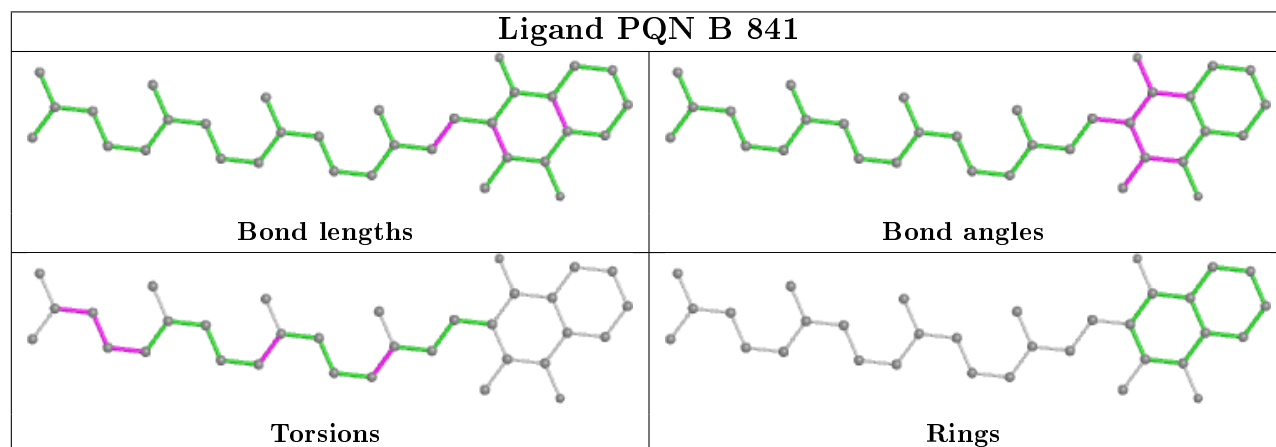
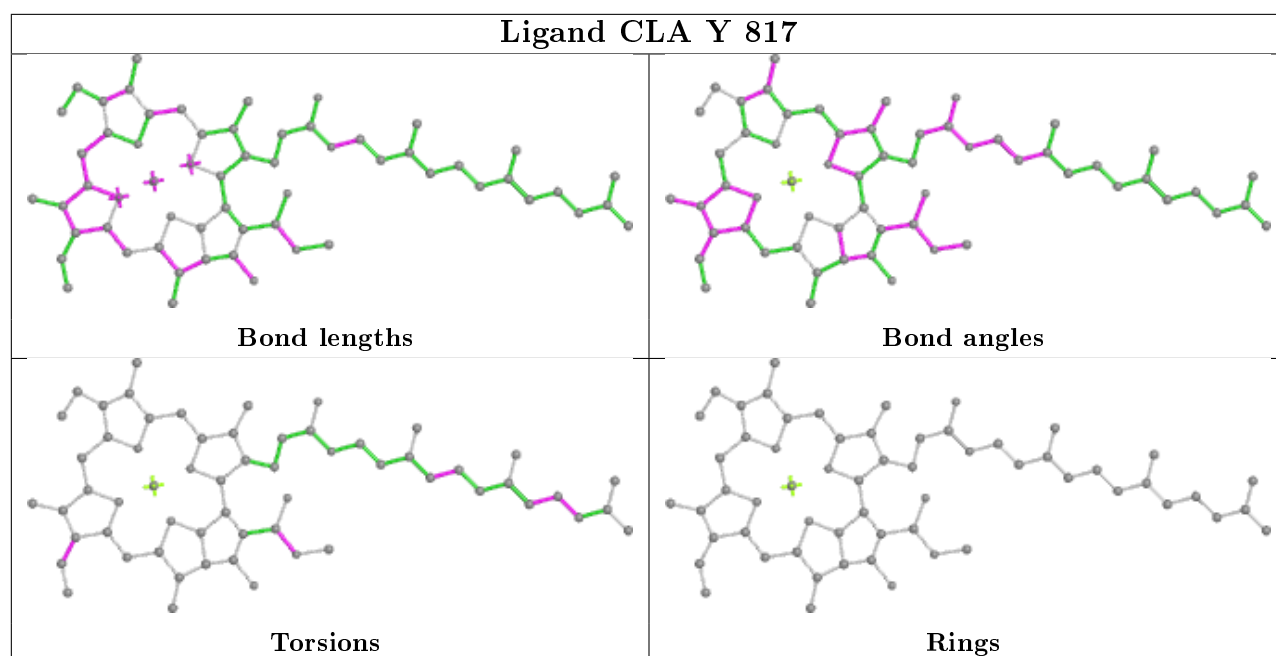
Bond angles

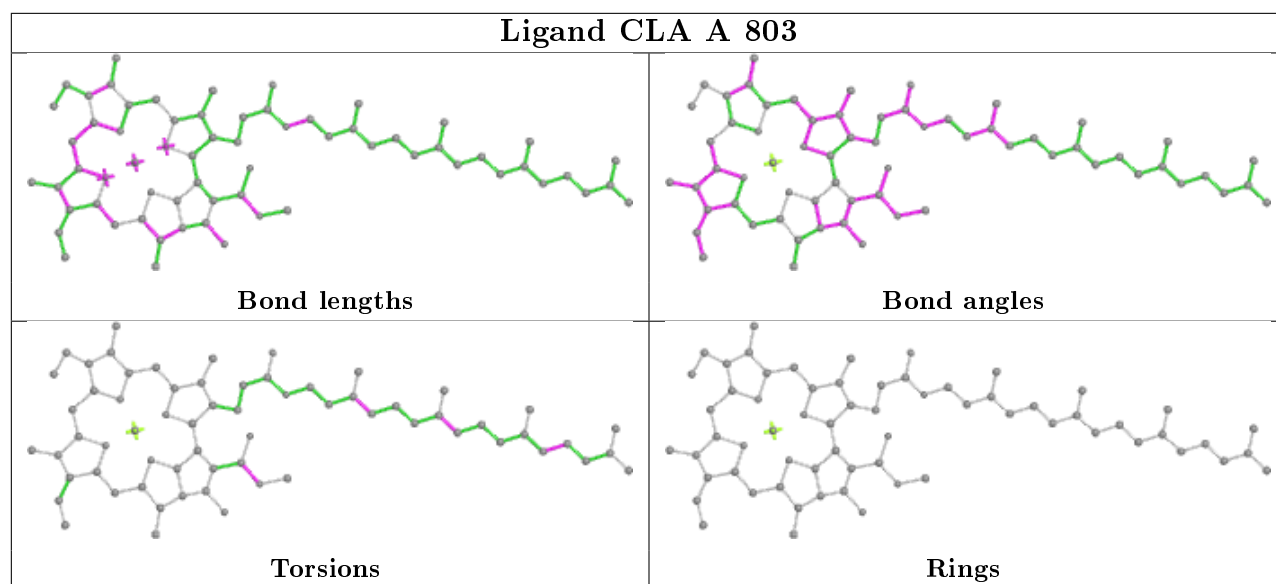
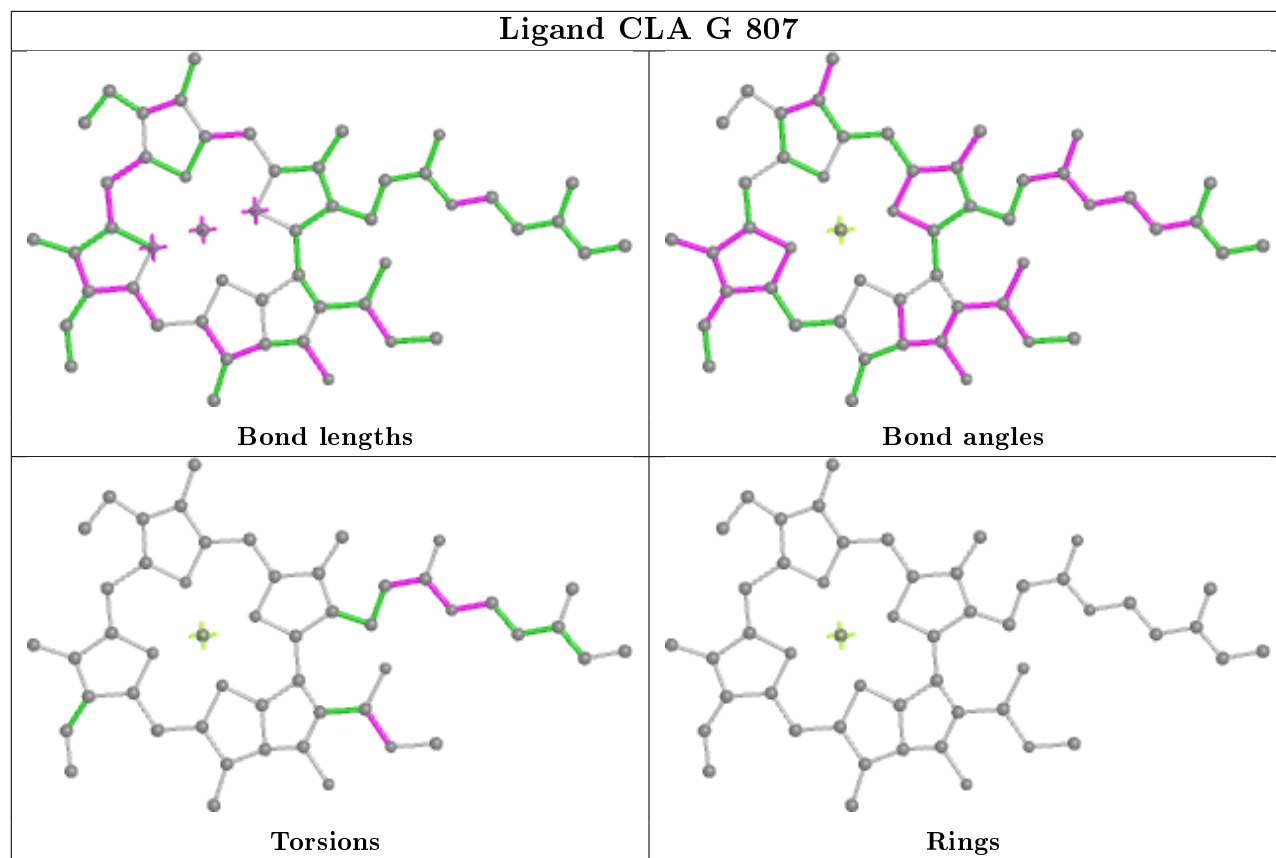


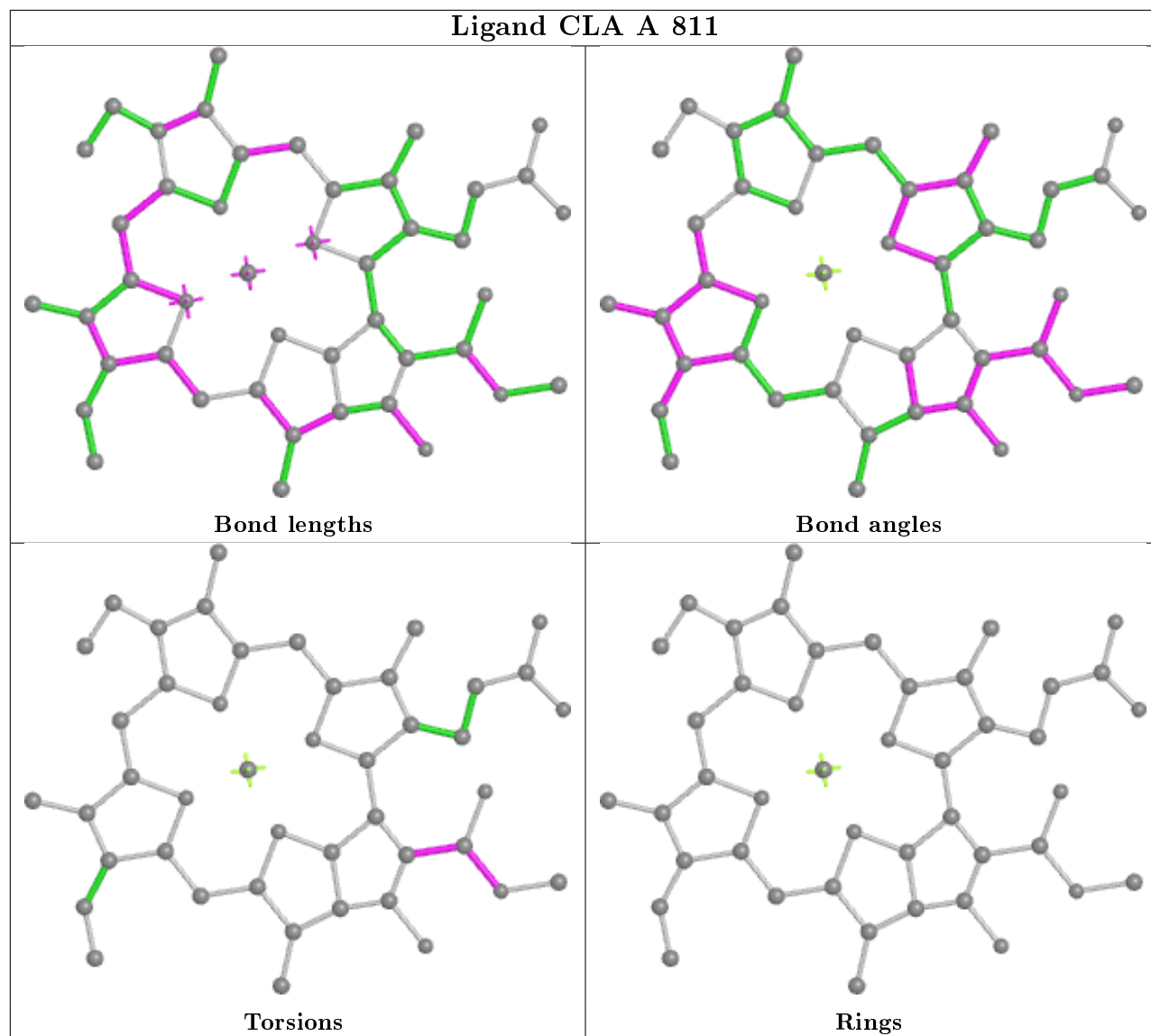
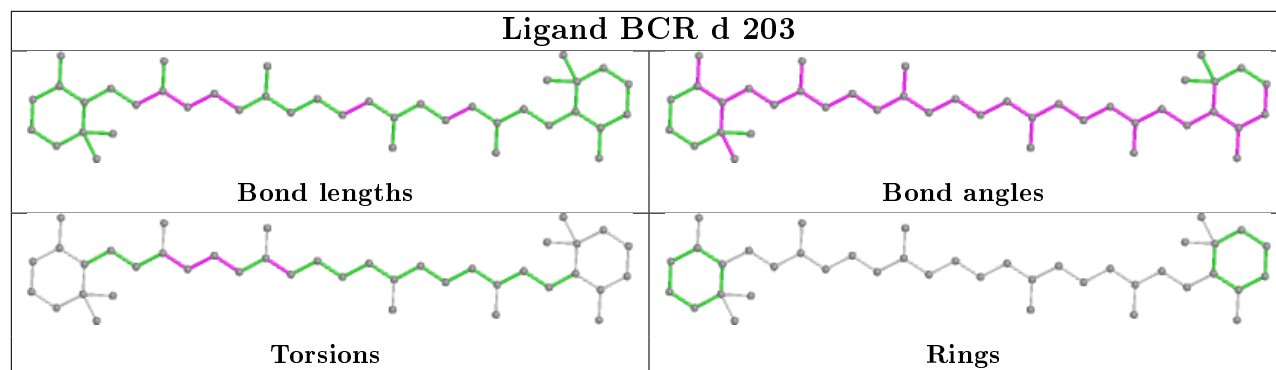
Torsions



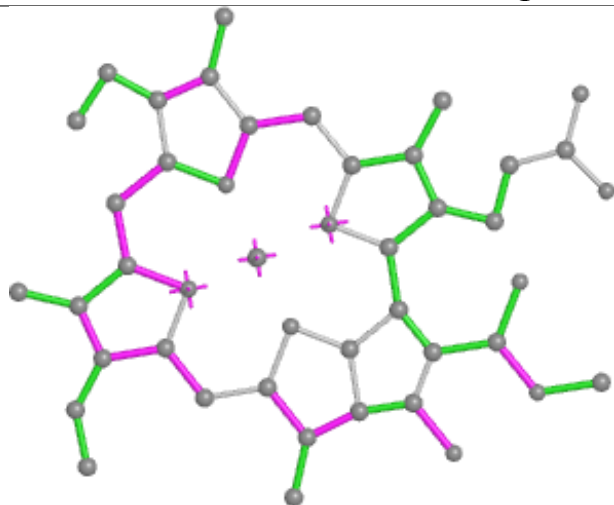
Rings



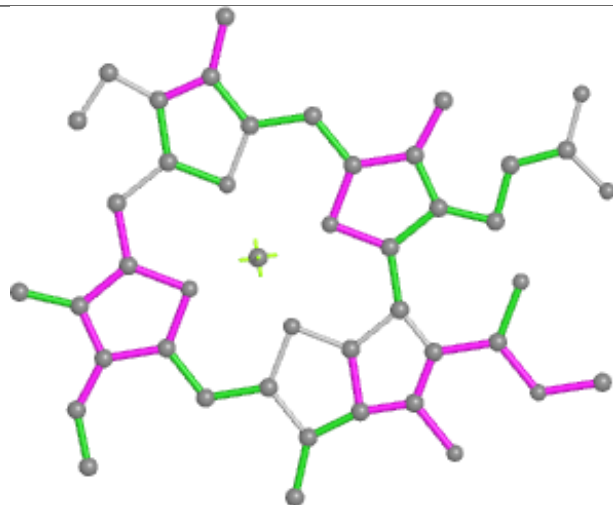




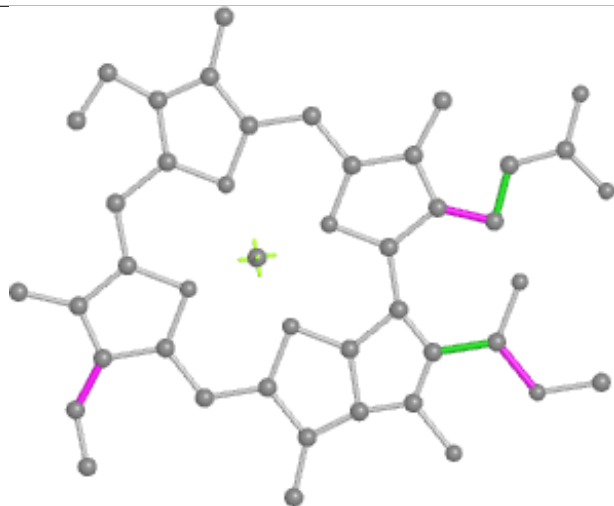
## Ligand CLA Z 813



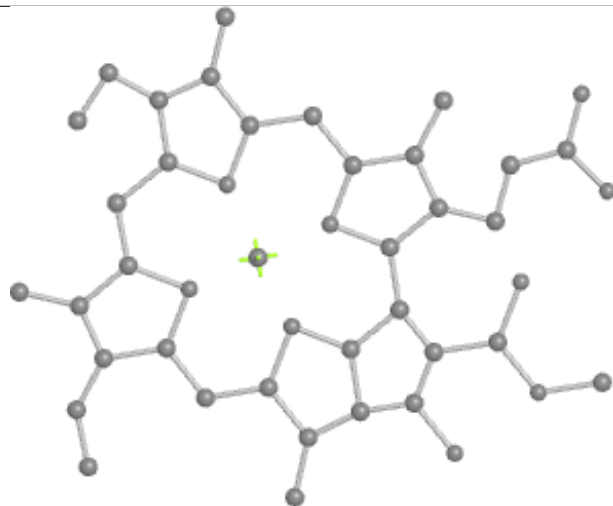
Bond lengths



Bond angles

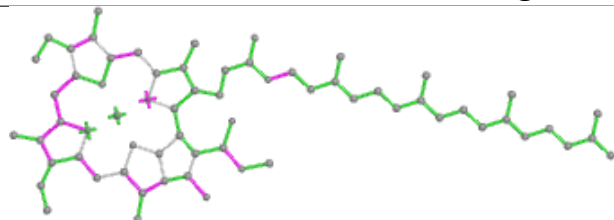


Torsions

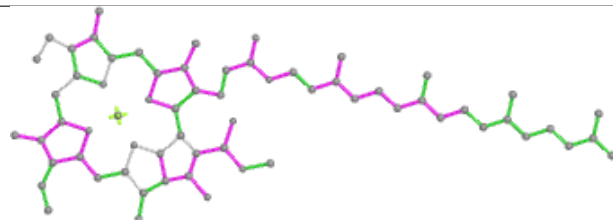


Rings

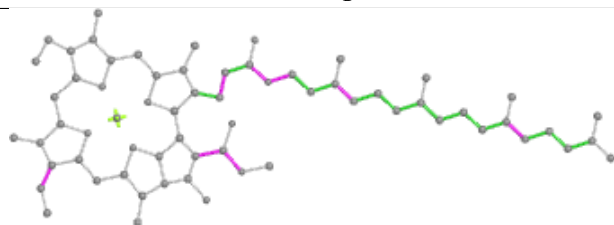
## Ligand CLA L 202



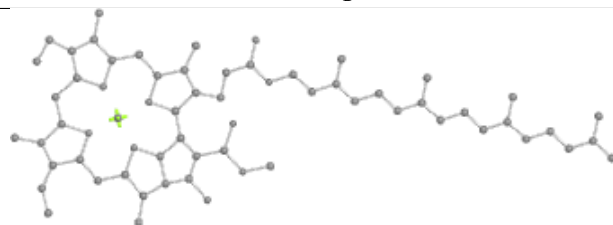
Bond lengths



Bond angles

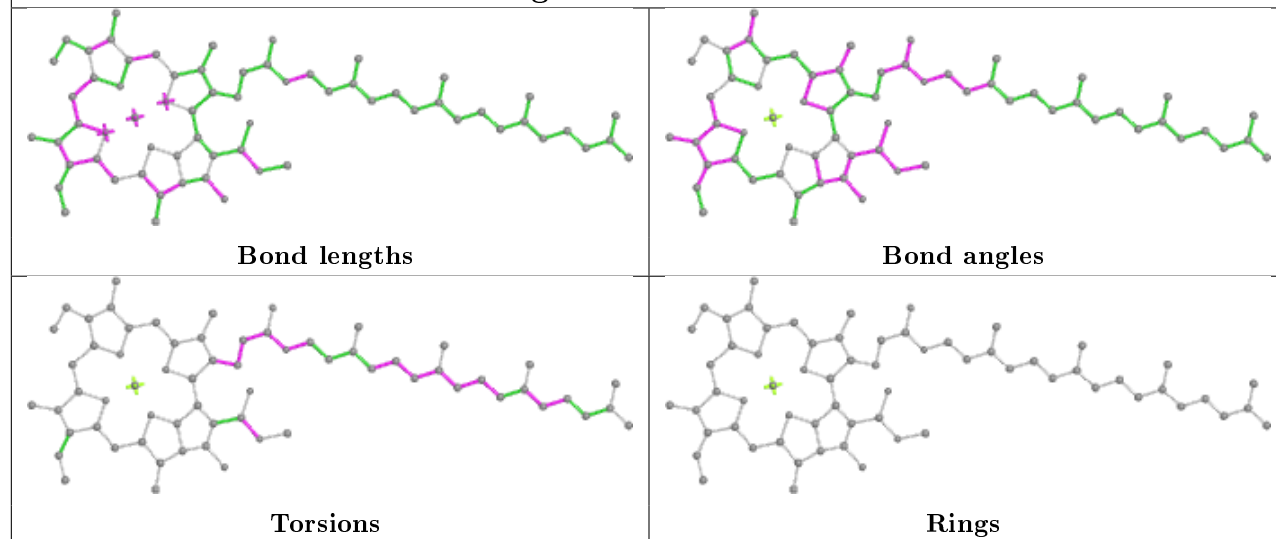


Torsions

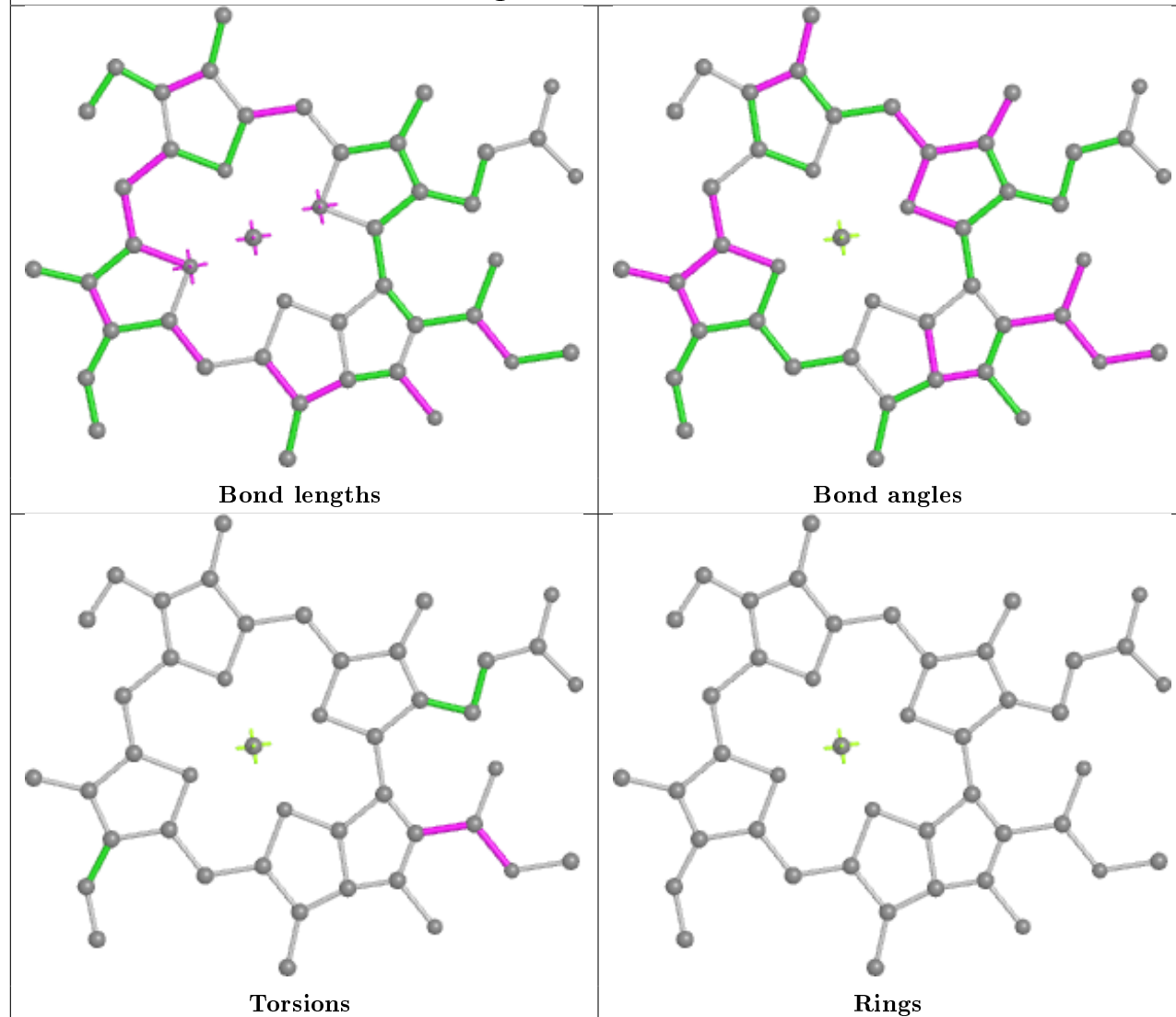


Rings

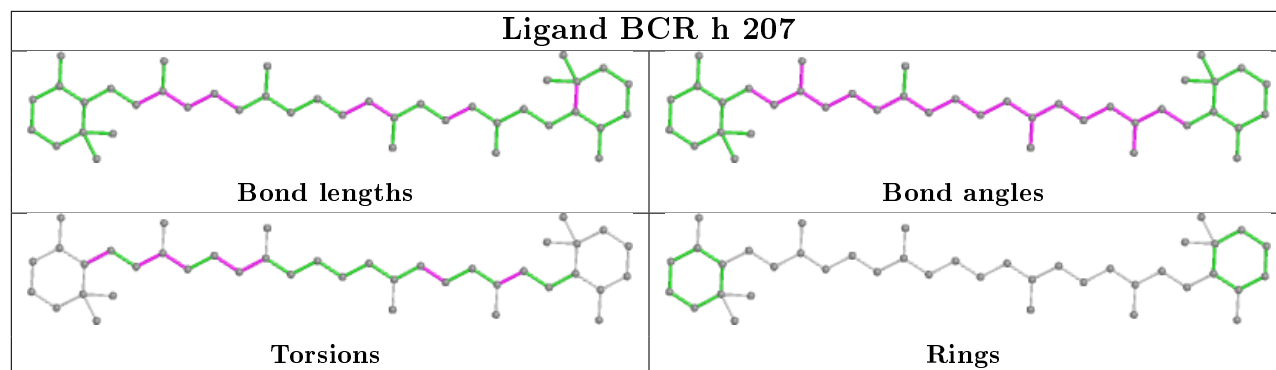
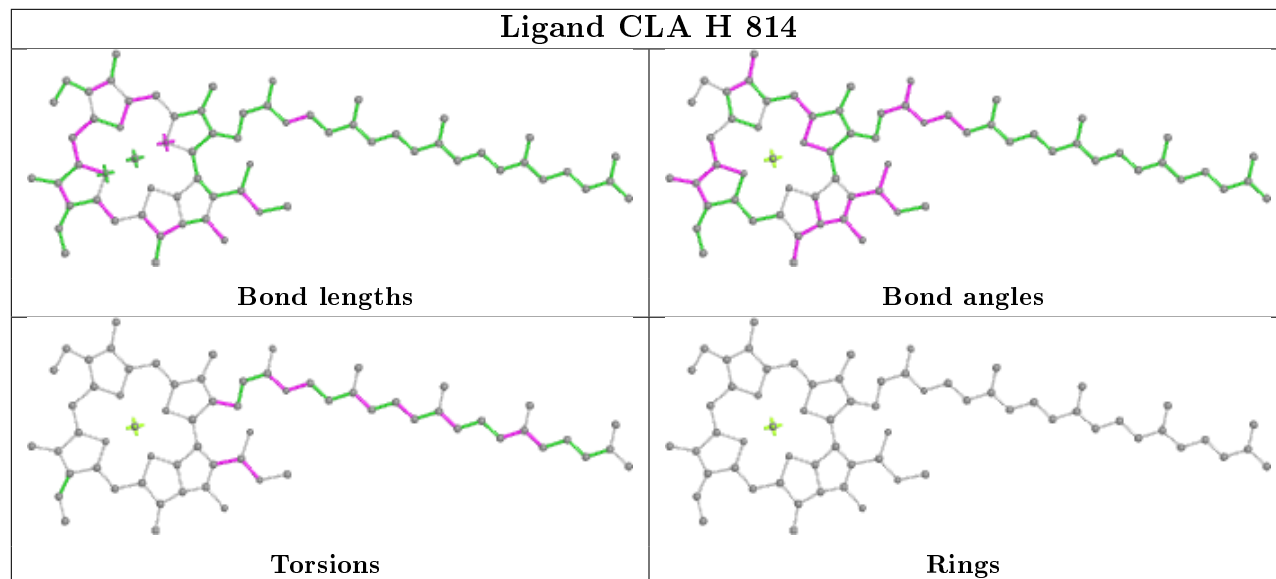
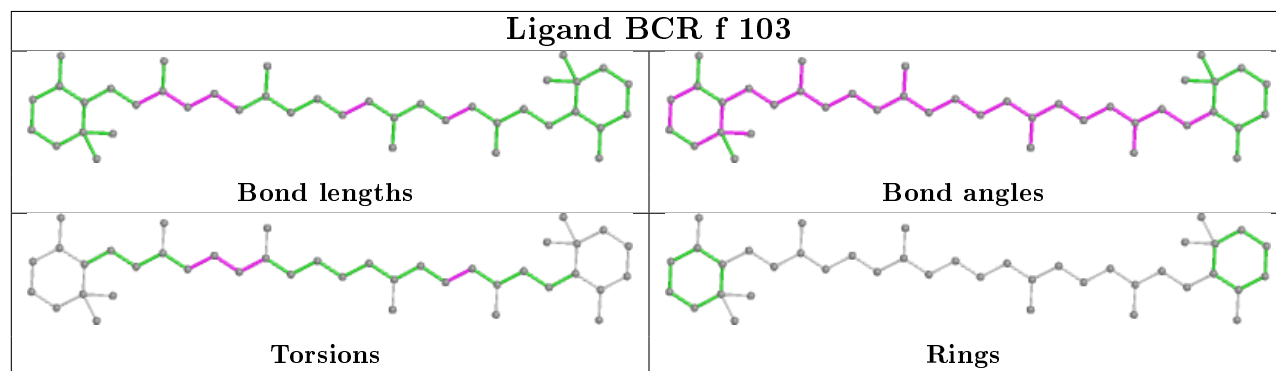
## Ligand CLA H 813



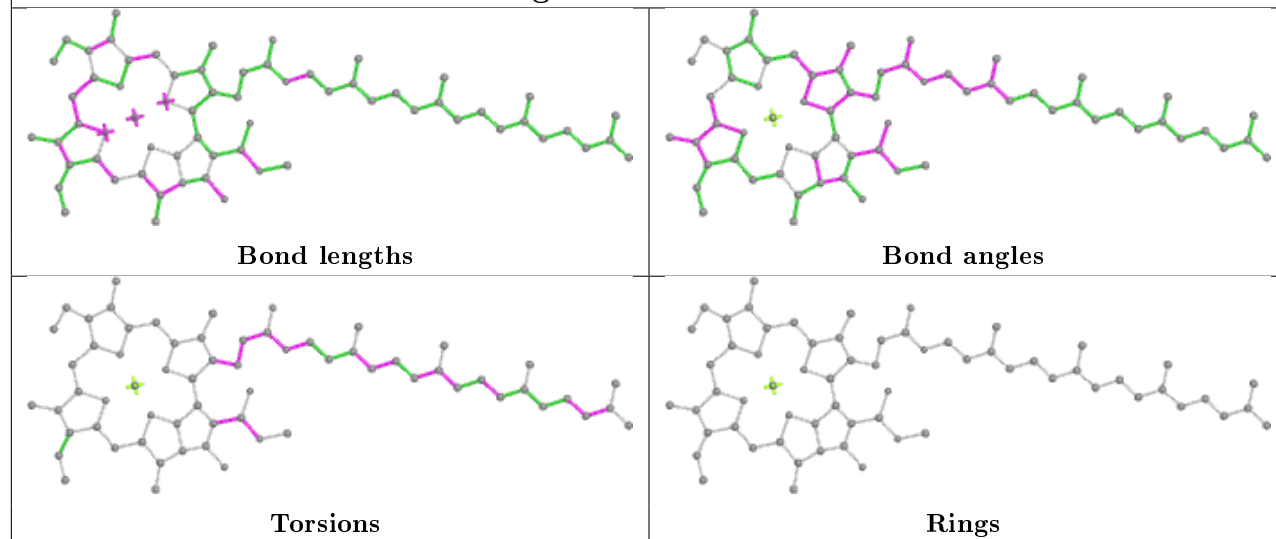
## Ligand CLA Z 822



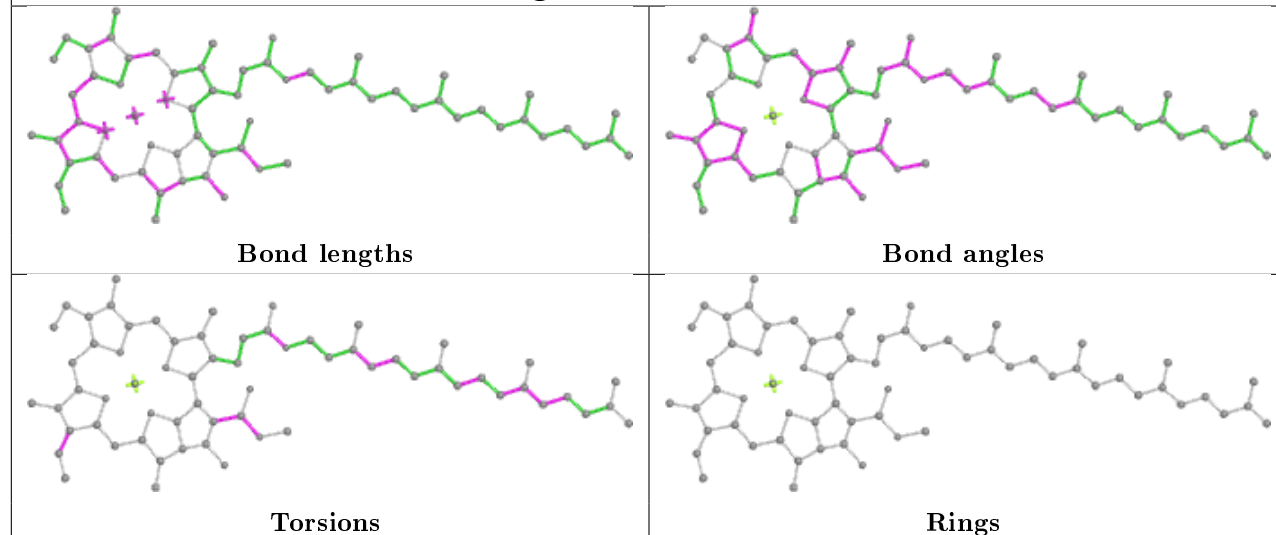


**Ligand BCR h 207****Ligand CLA H 814****Ligand BCR f 103**

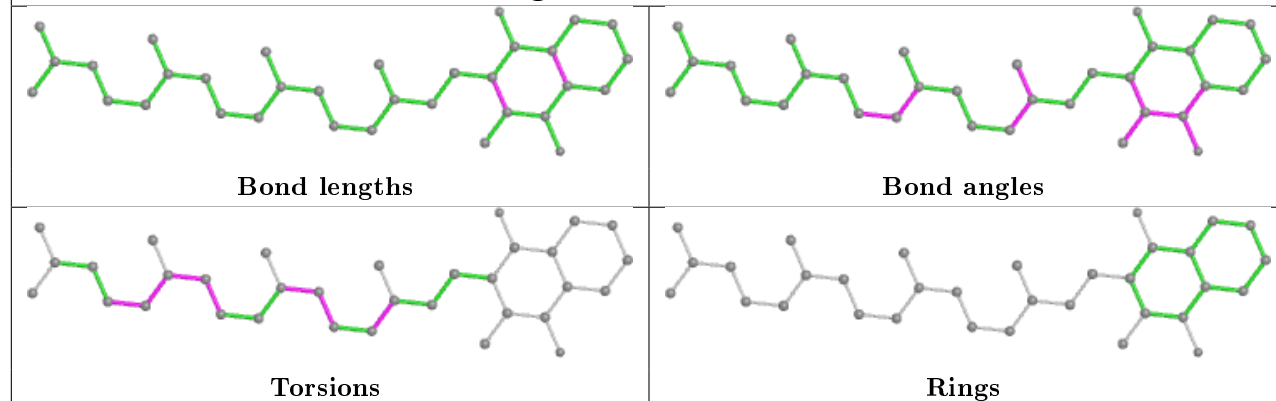
## Ligand CLA A 806

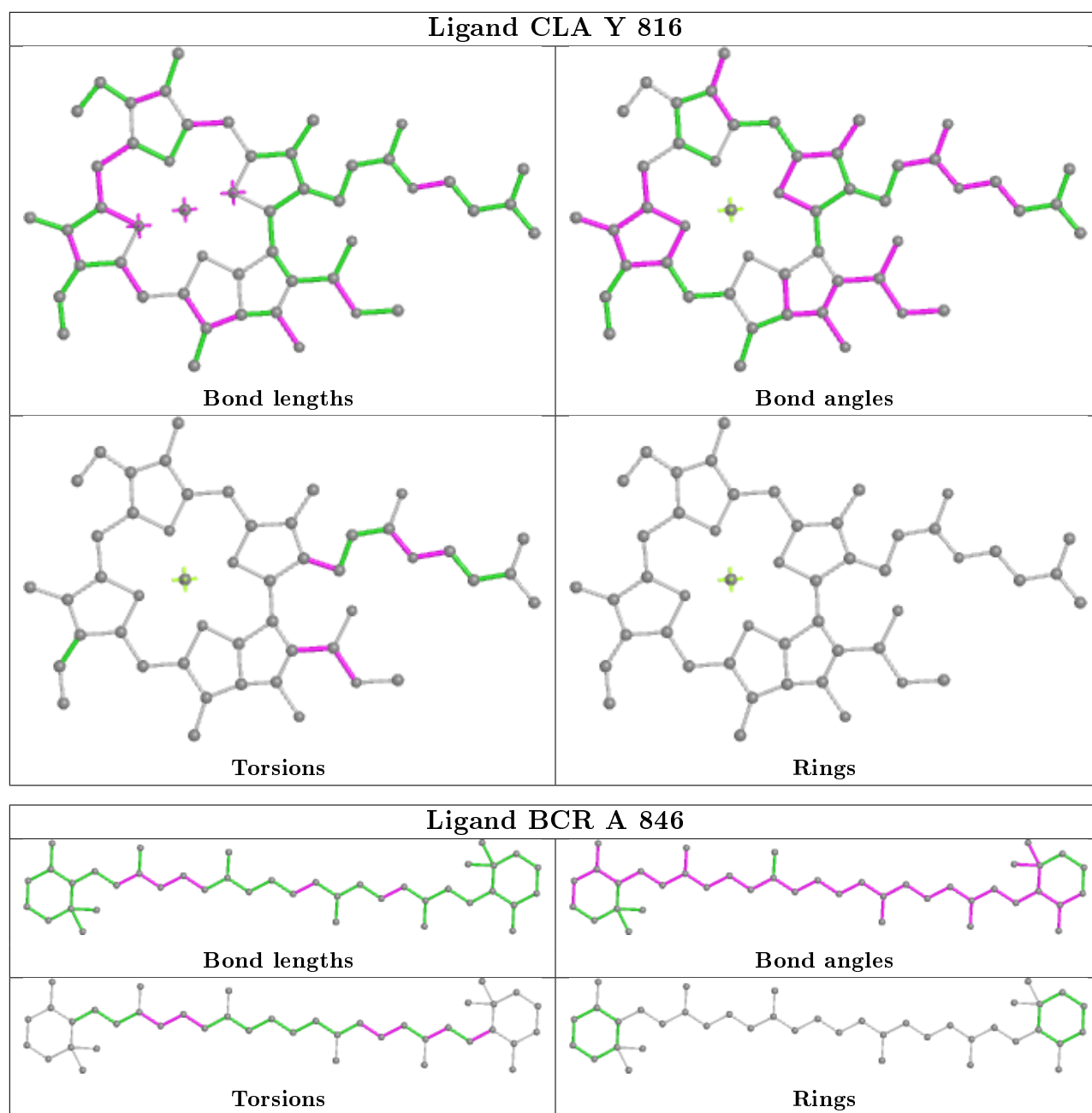


## Ligand CLA G 827

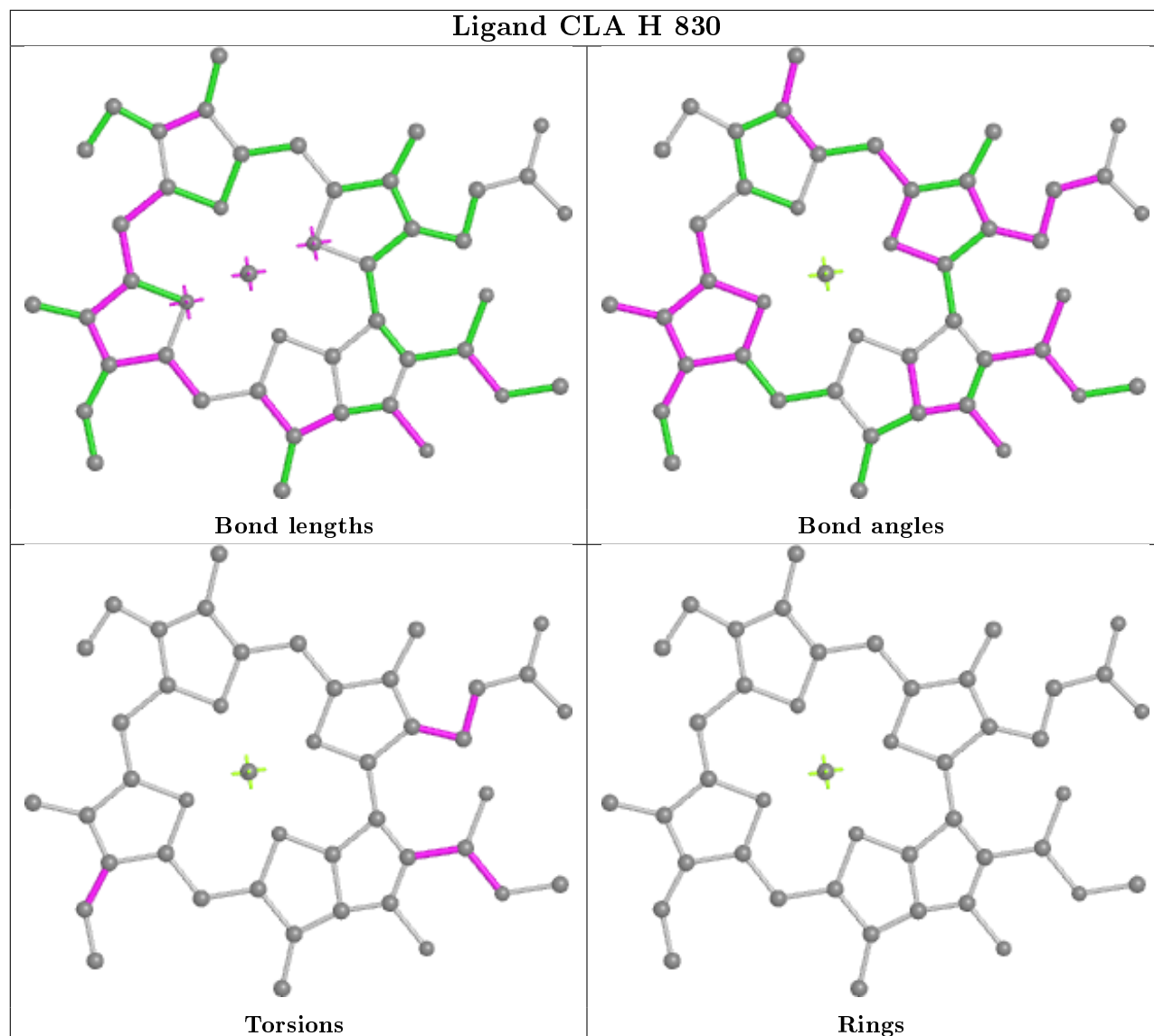


## Ligand PQN G 843

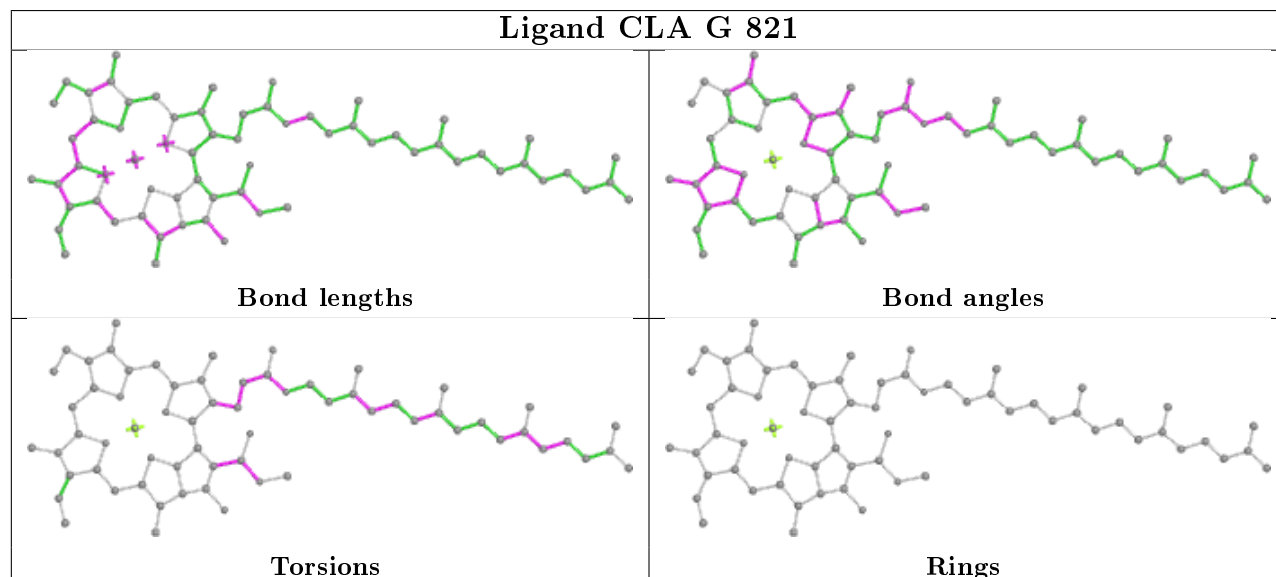


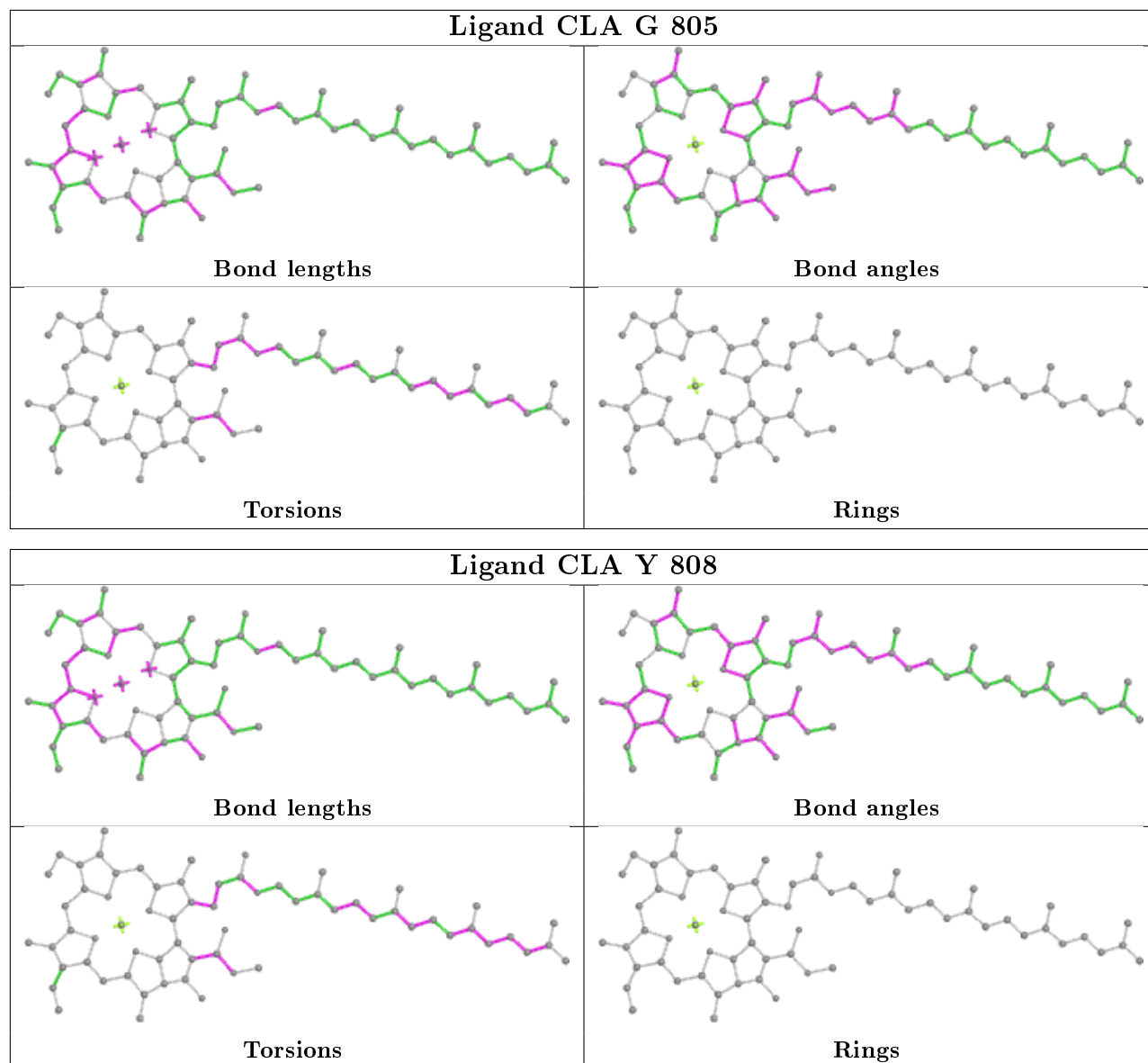


## Ligand CLA H 830

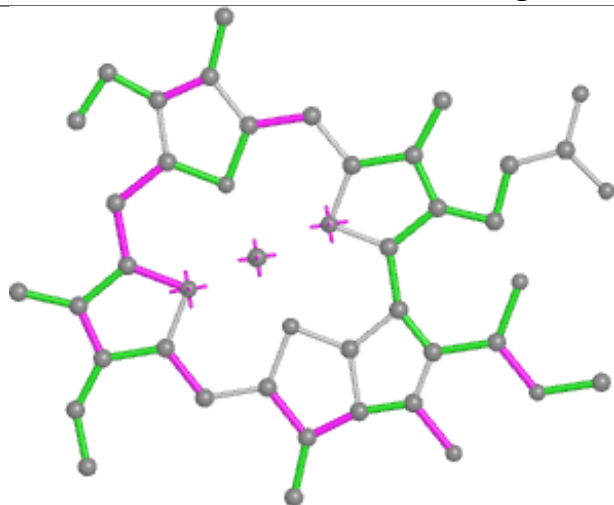


## Ligand CLA G 821

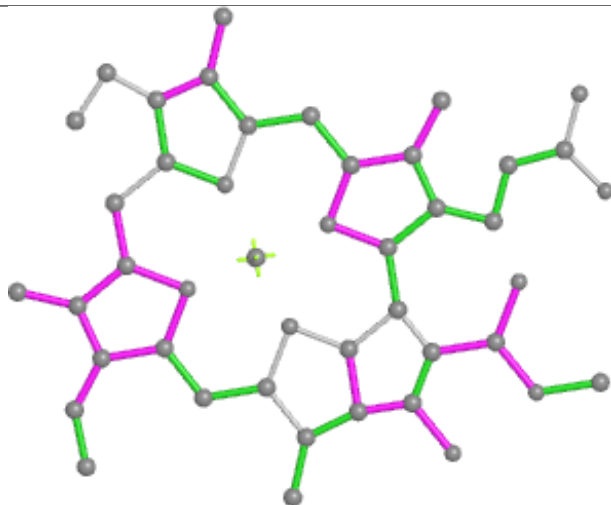




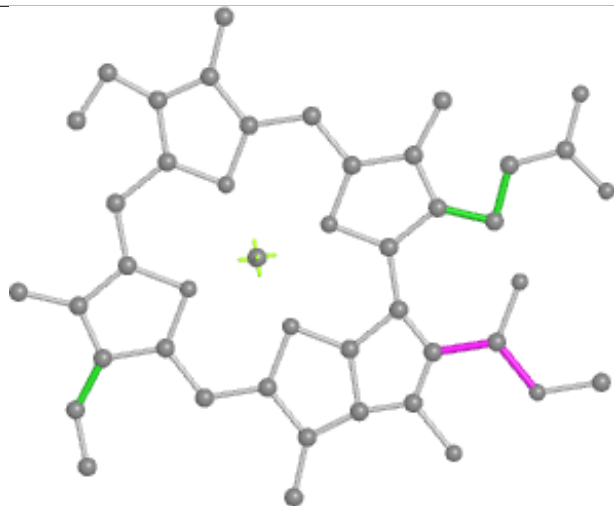
## Ligand CLA K 102



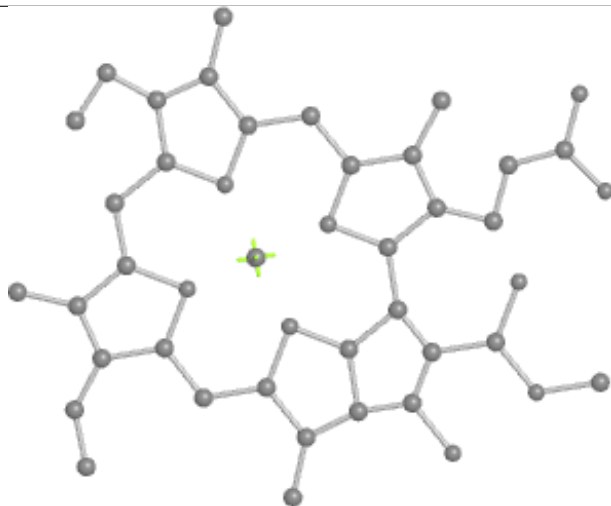
Bond lengths



Bond angles

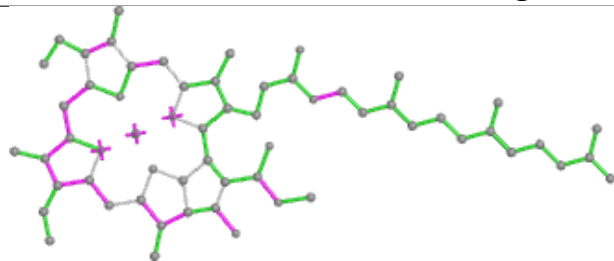


Torsions

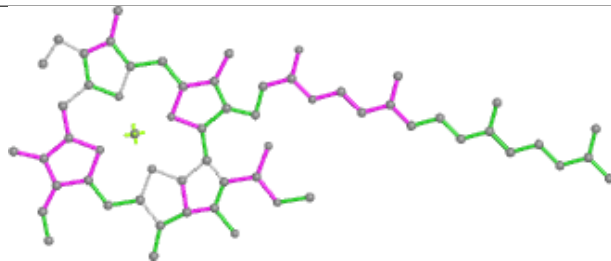


Rings

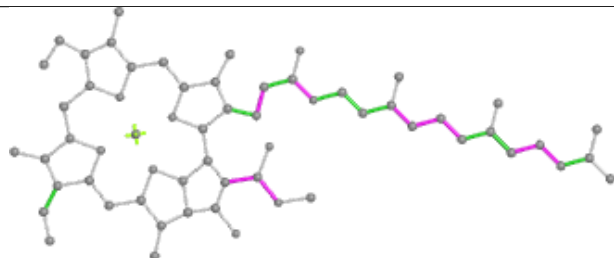
## Ligand CLA G 817



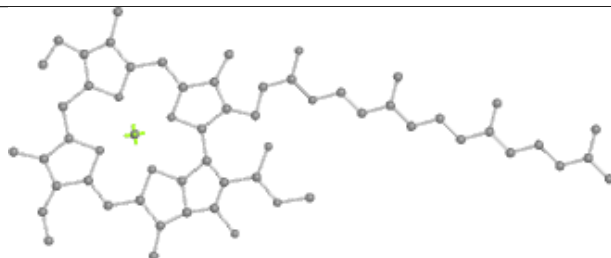
Bond lengths



Bond angles

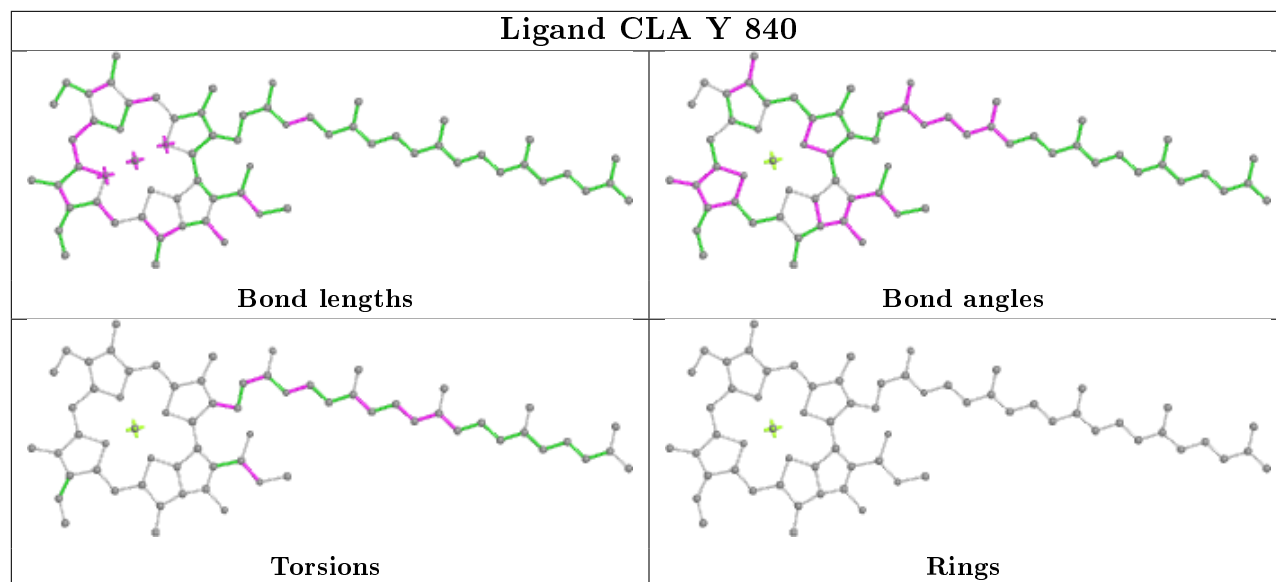


Torsions

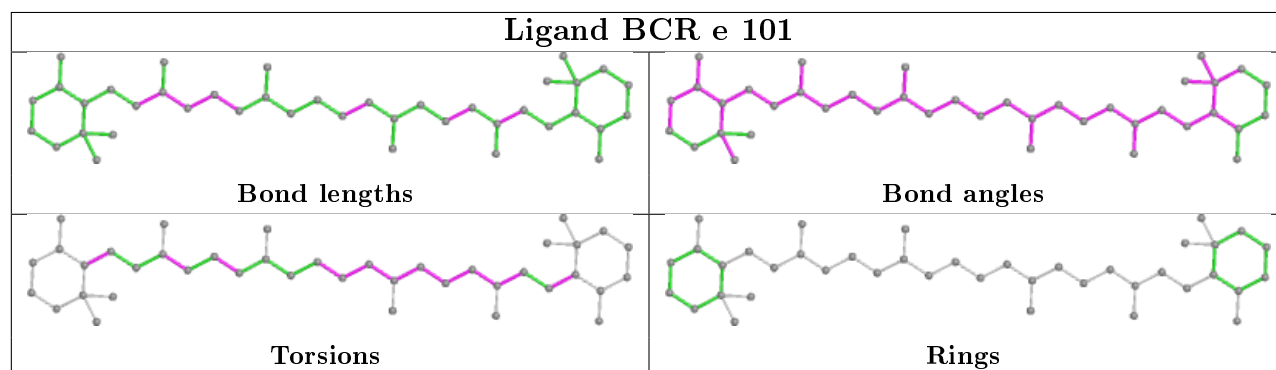


Rings

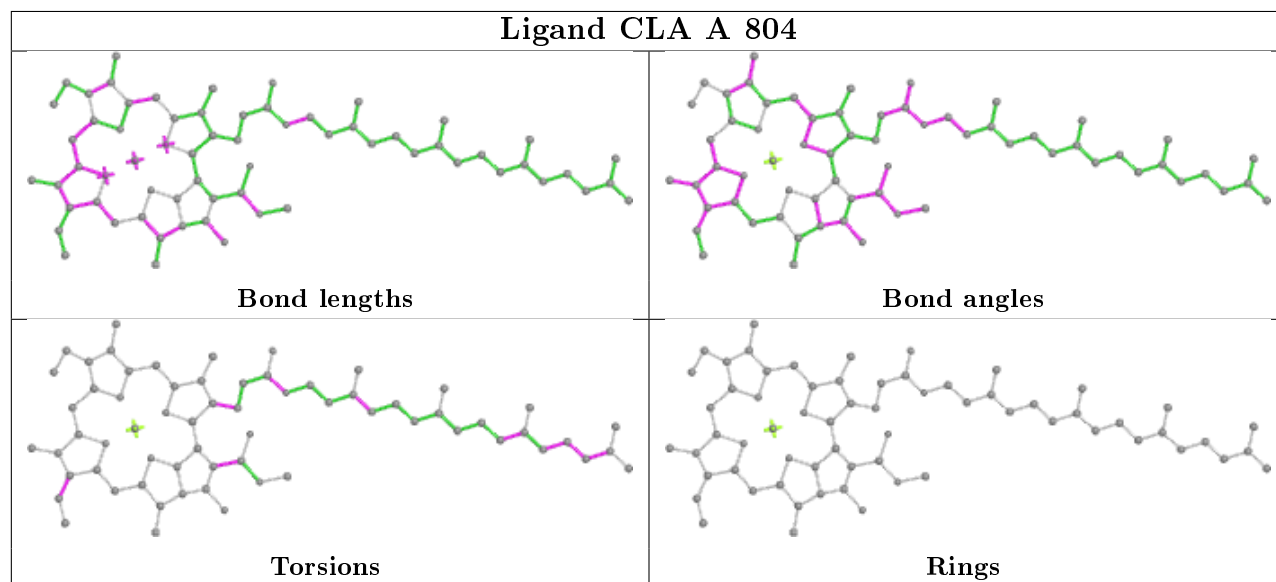
## Ligand CLA Y 840



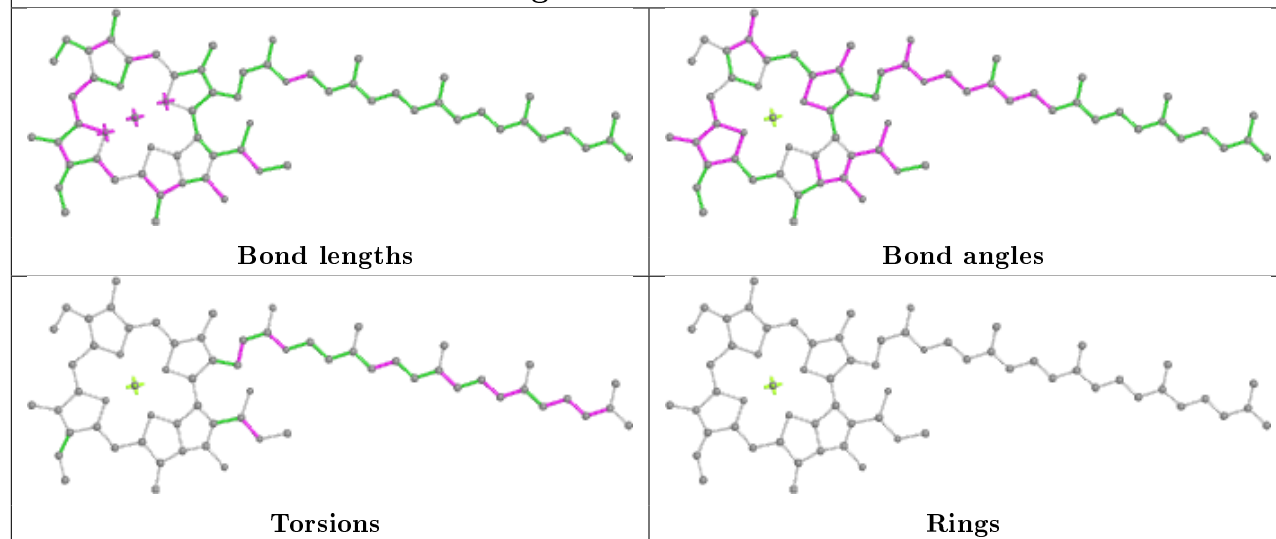
## Ligand BCR e 101



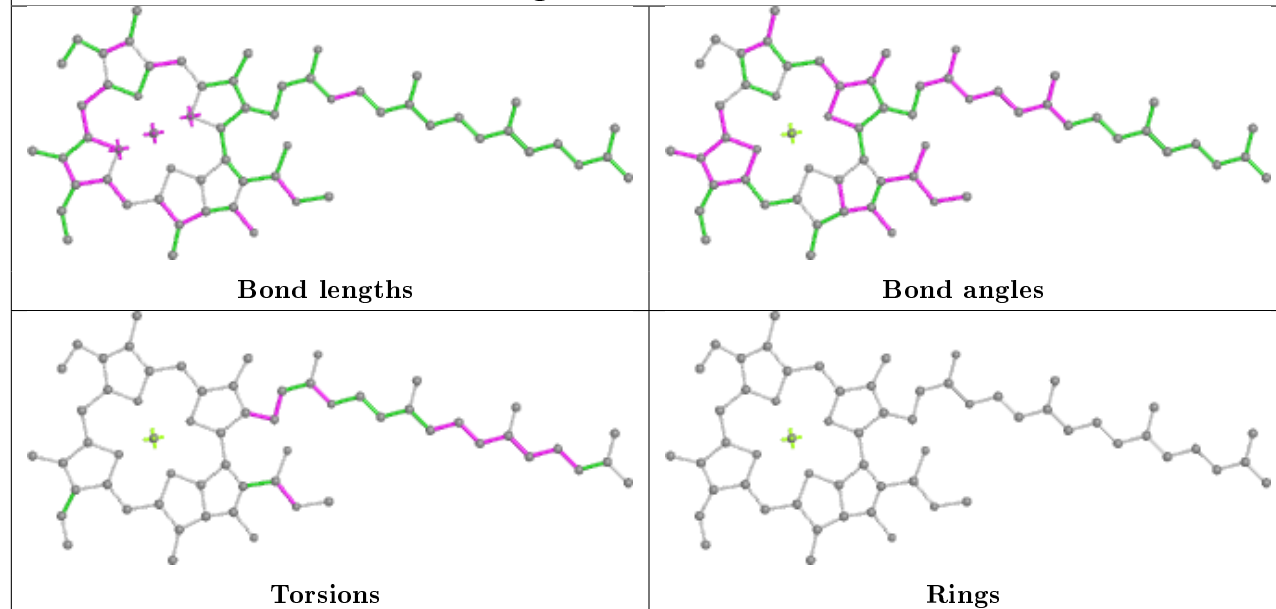
## Ligand CLA A 804



## Ligand CLA H 817

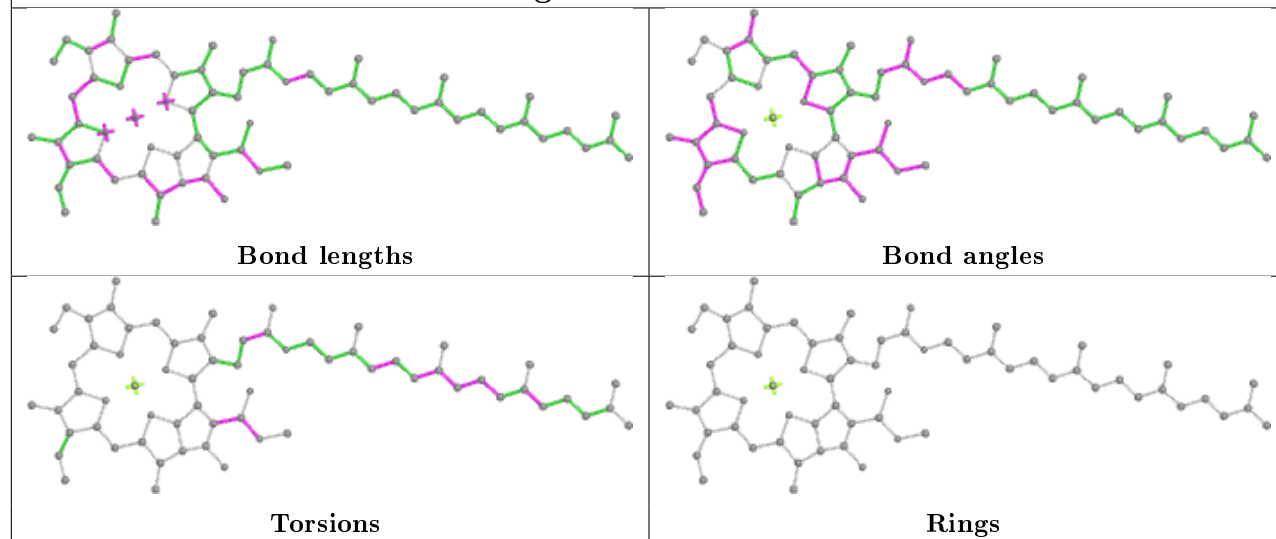


## Ligand CLA H 818

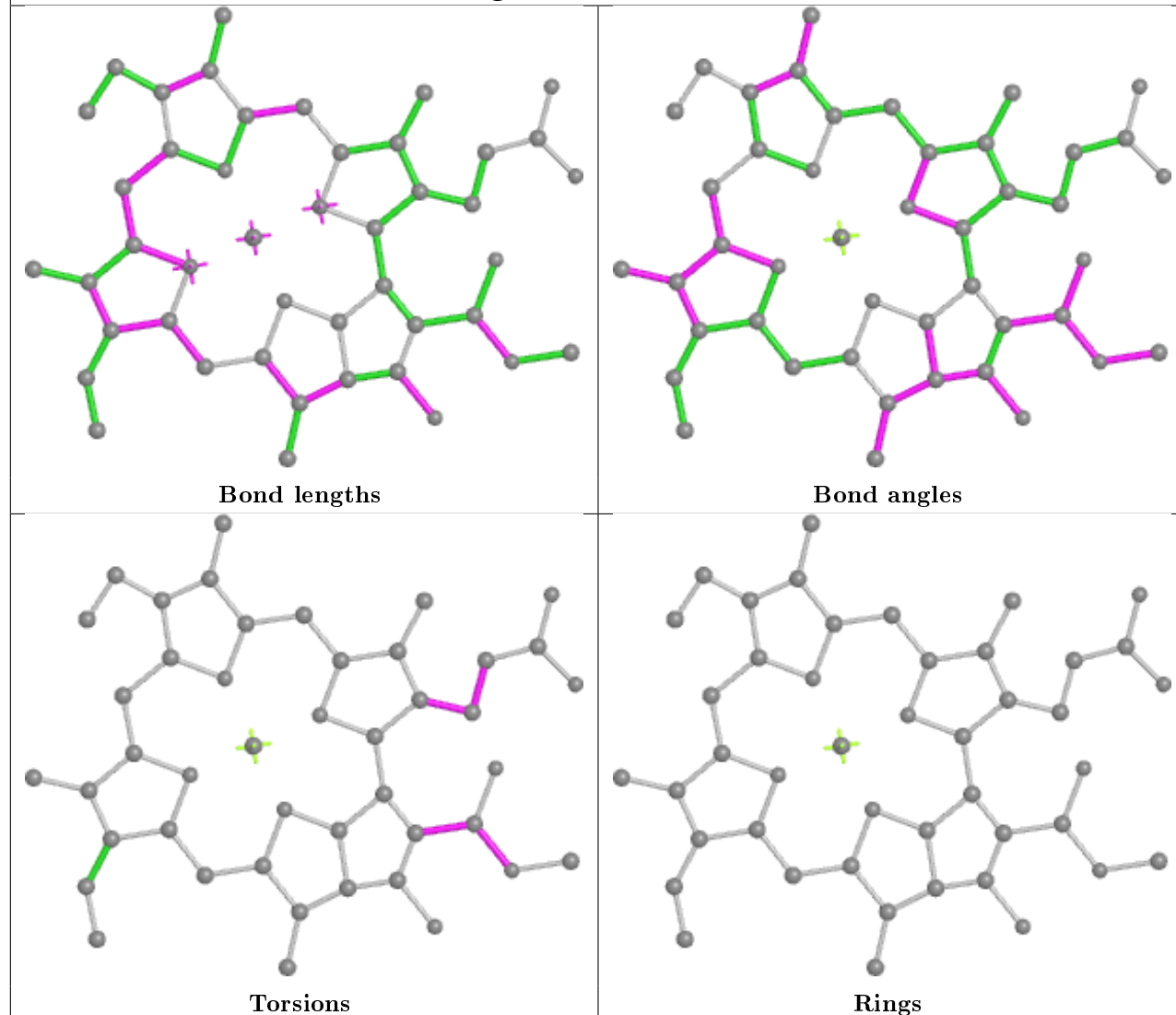


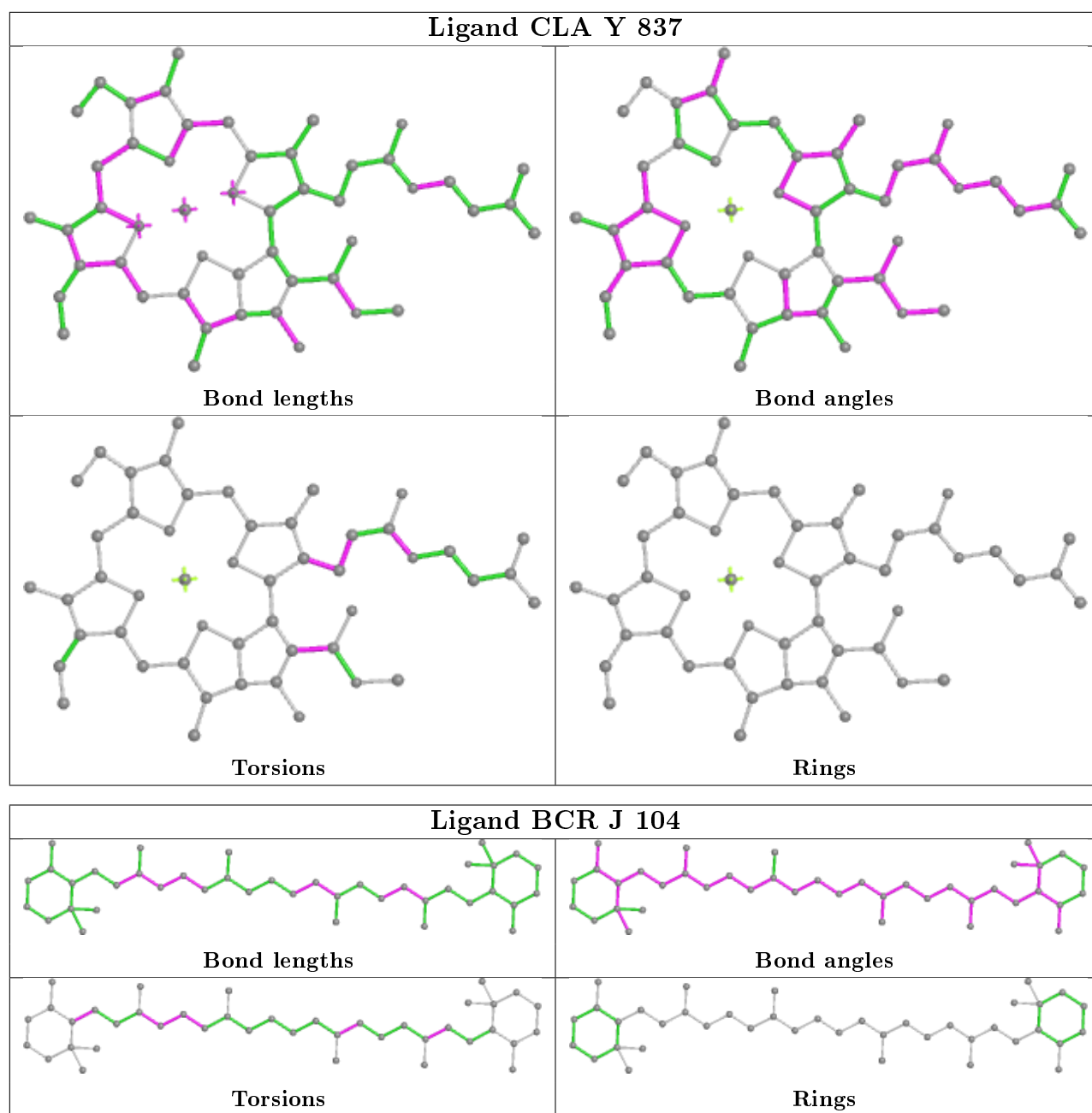


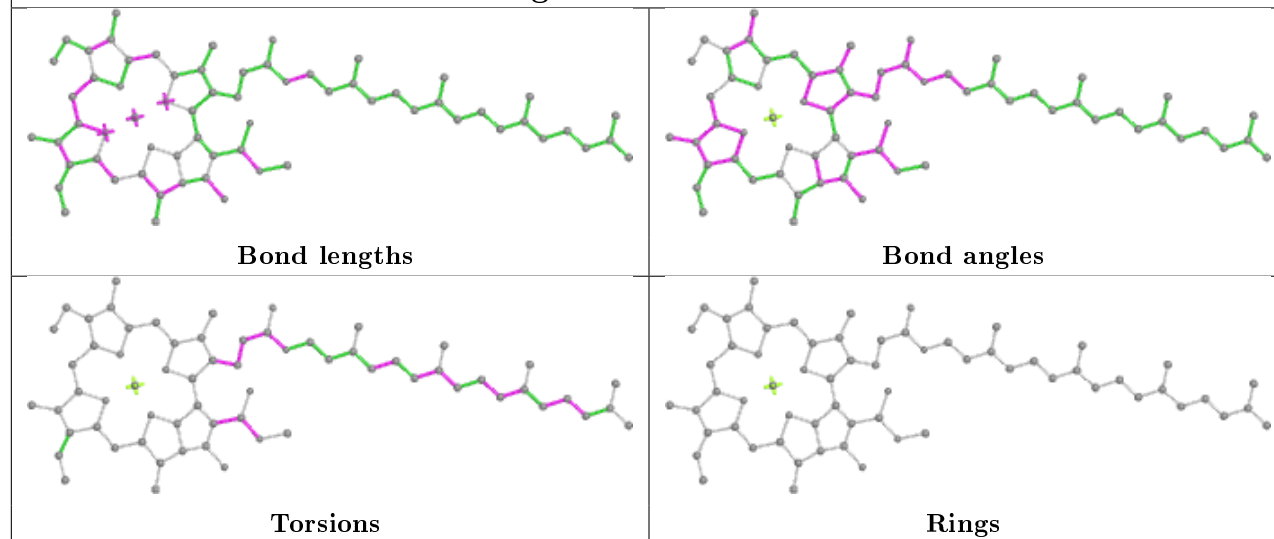
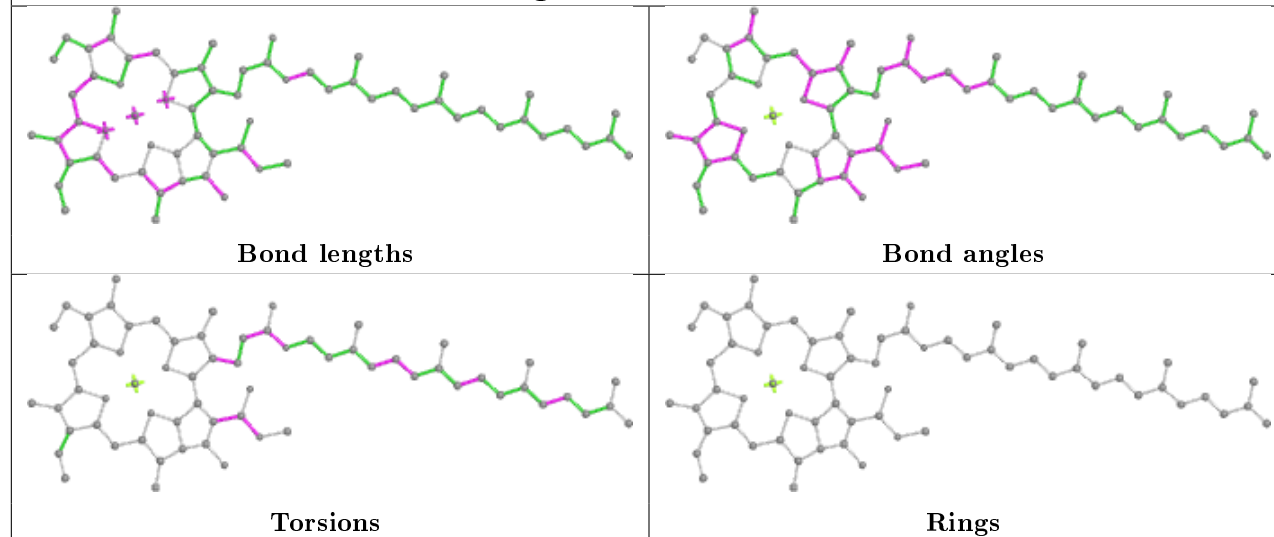
## Ligand CLA Z 804



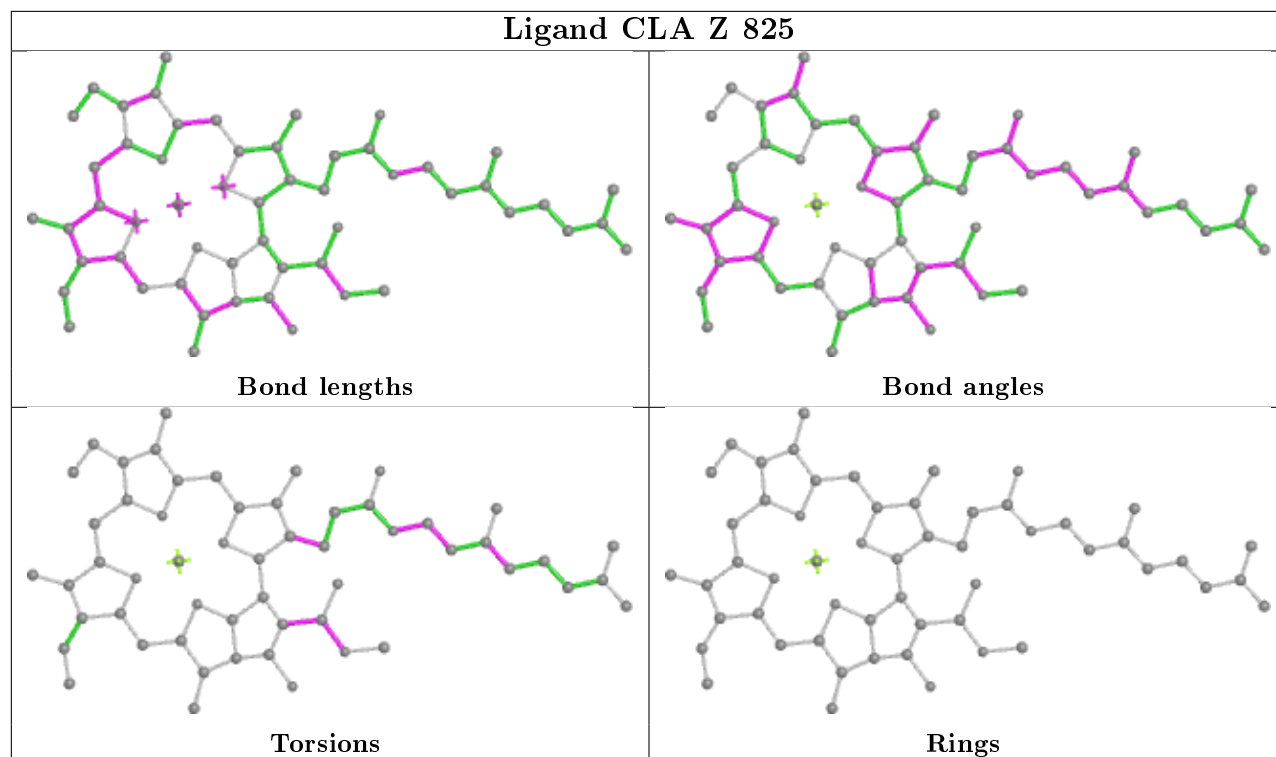
## Ligand CLA G 835



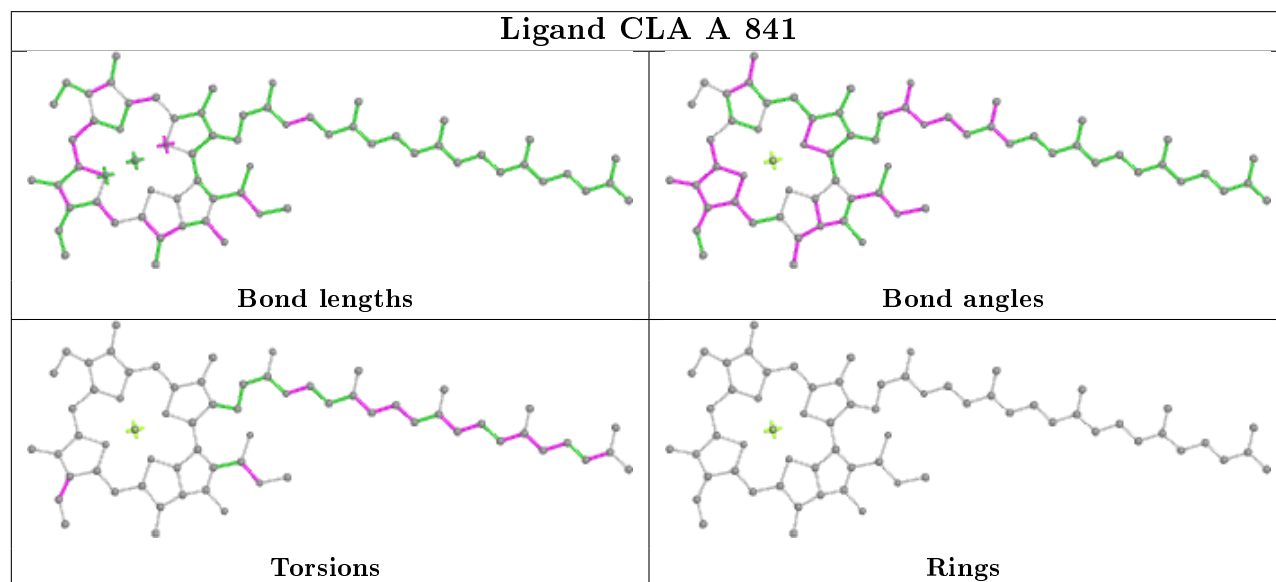


**Ligand CLA G 811****Ligand CLA A 829**

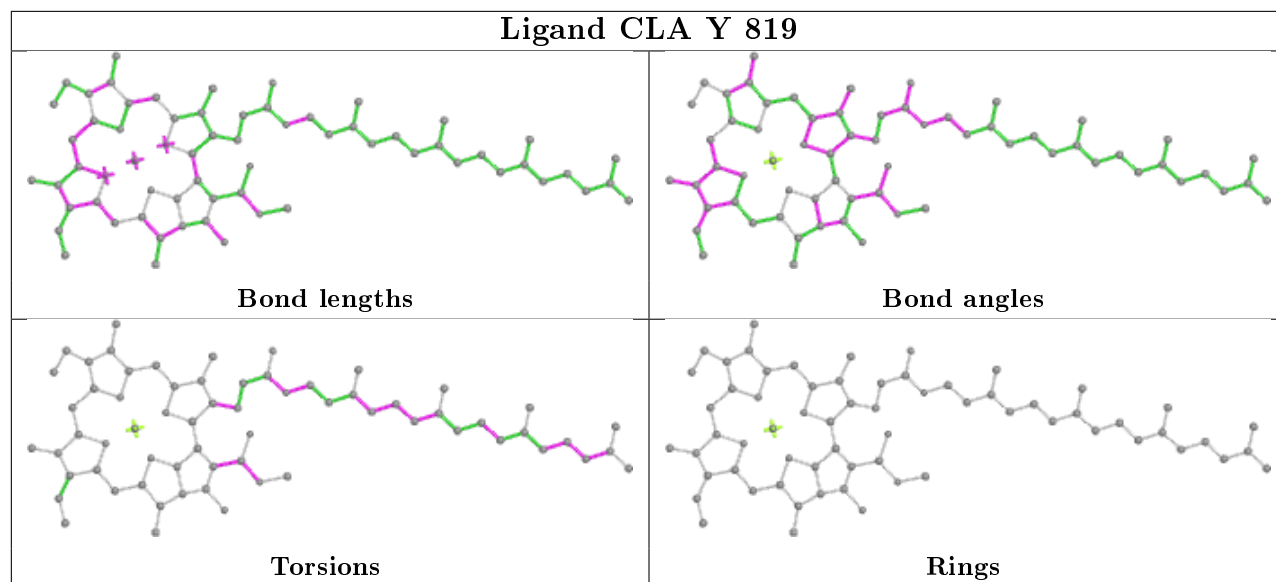
## Ligand CLA Z 825



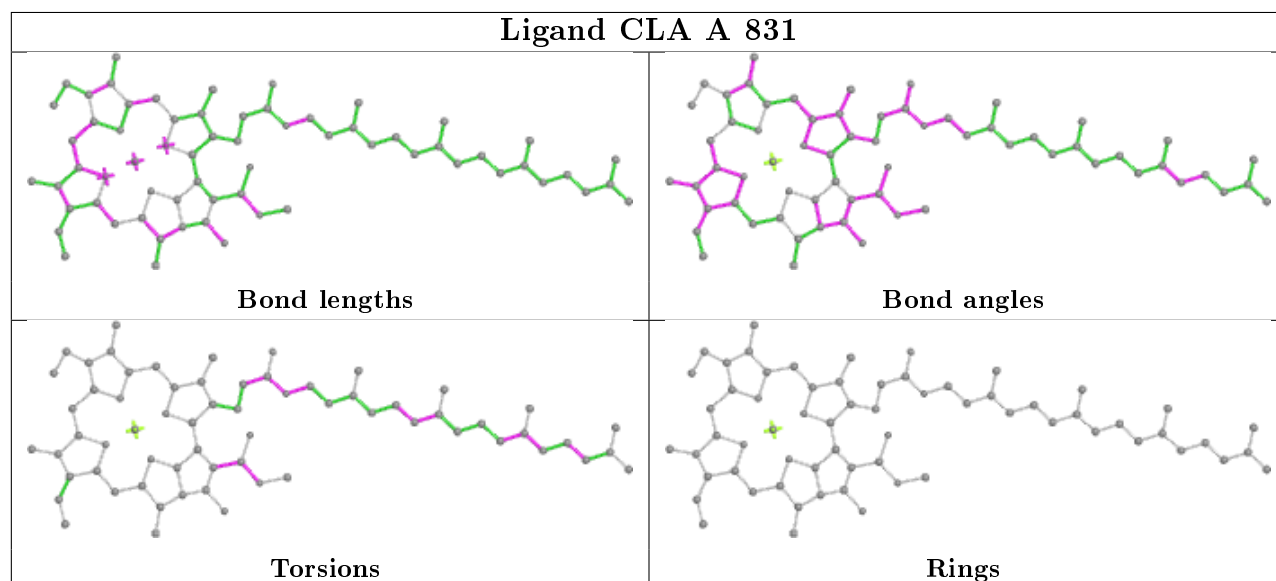
## Ligand CLA A 841



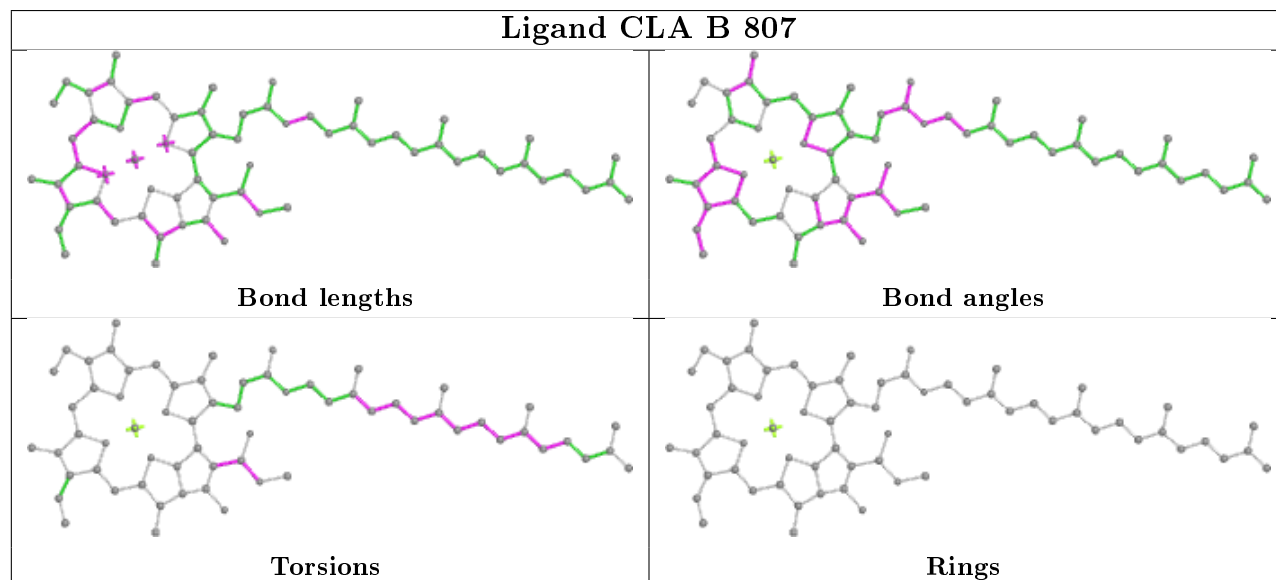
## Ligand CLA Y 819

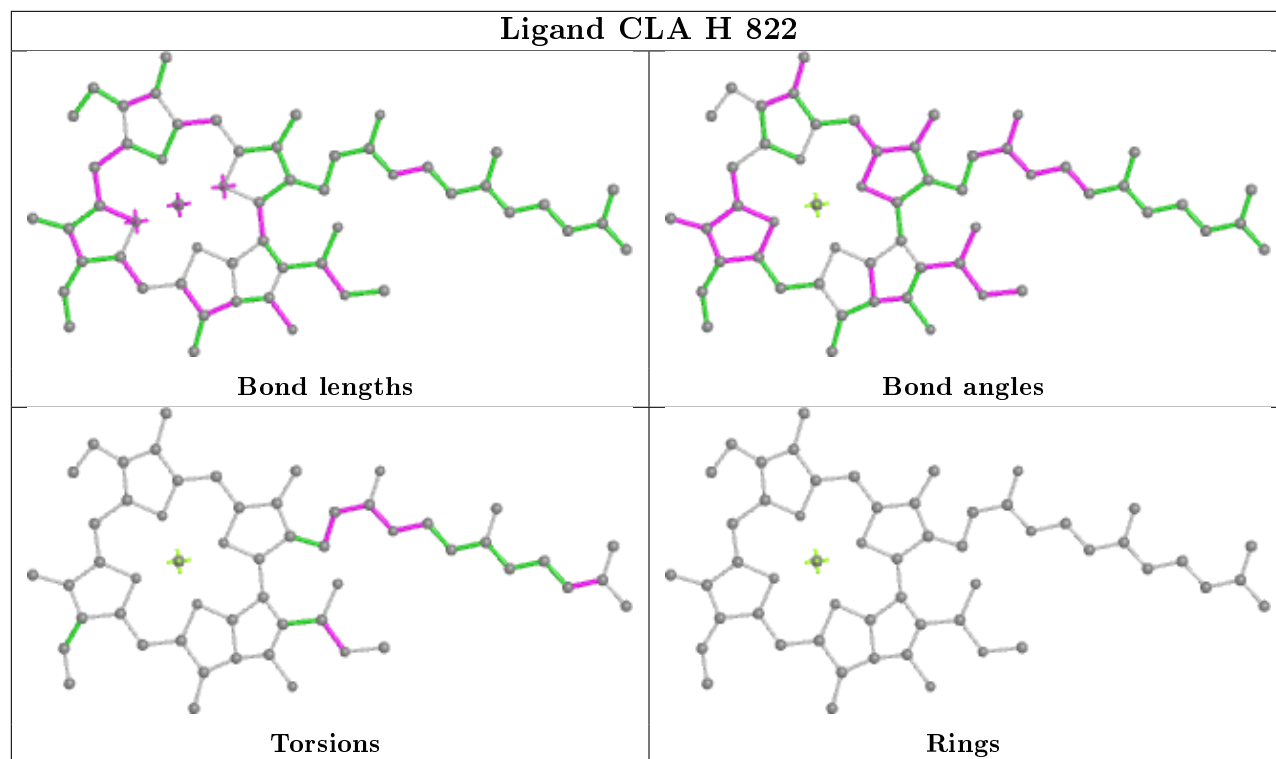
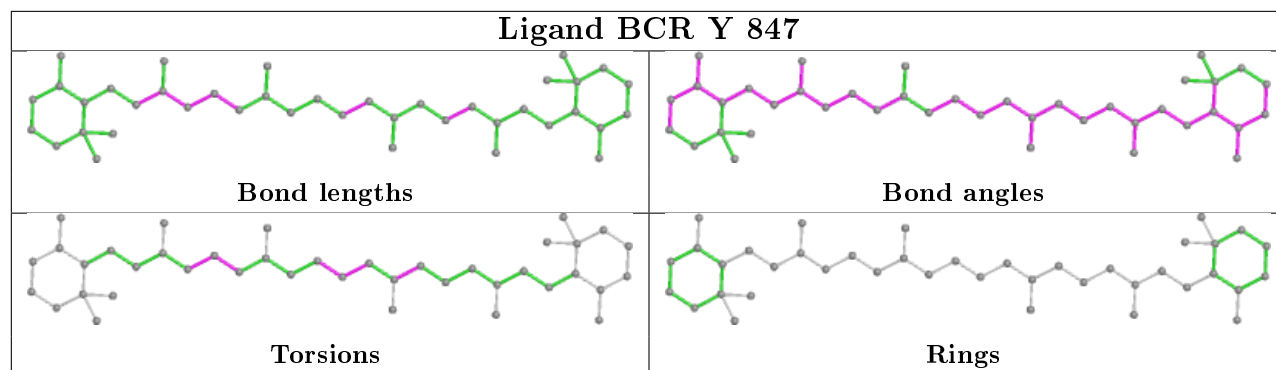


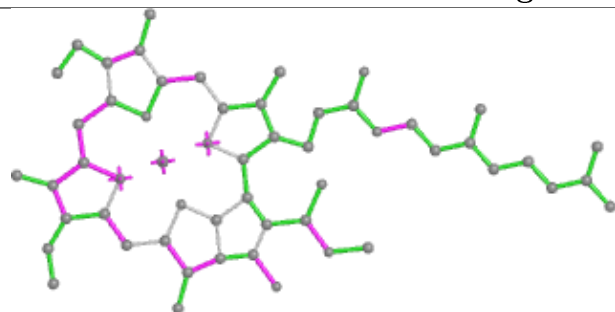
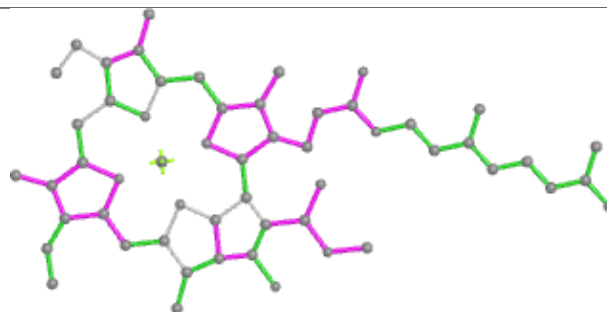
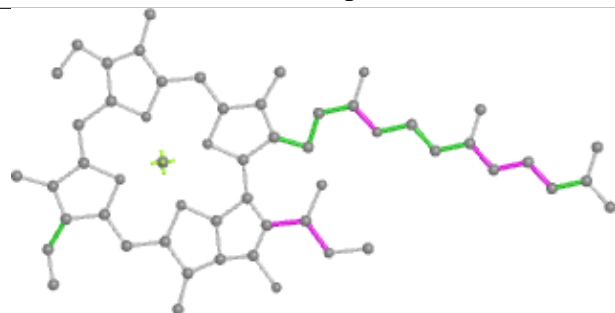
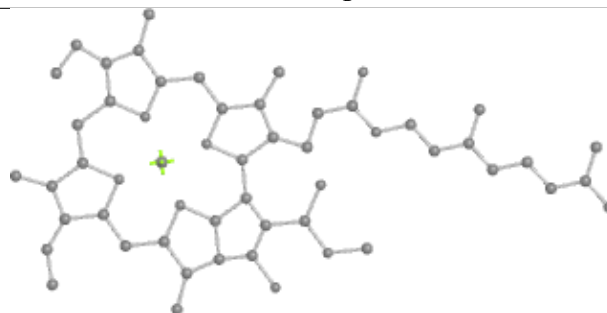
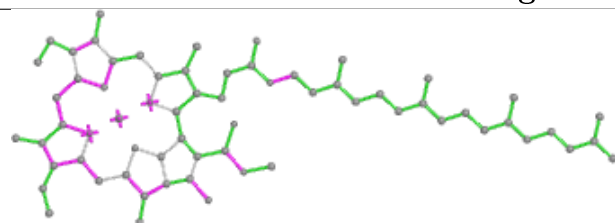
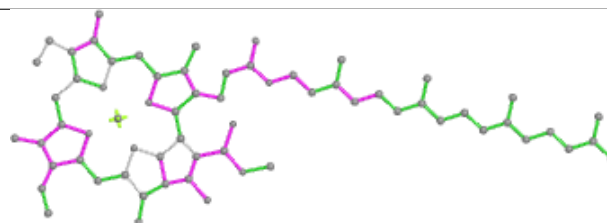
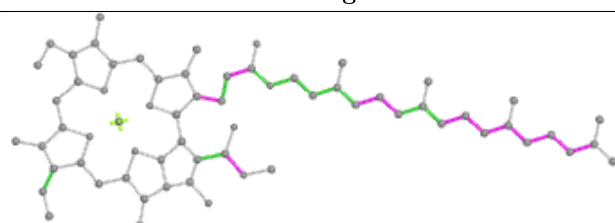
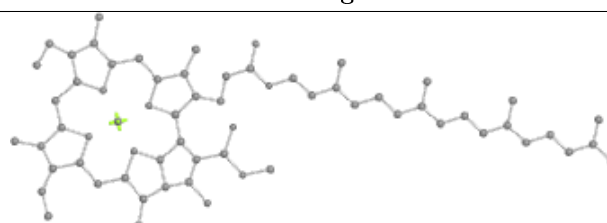
## Ligand CLA A 831

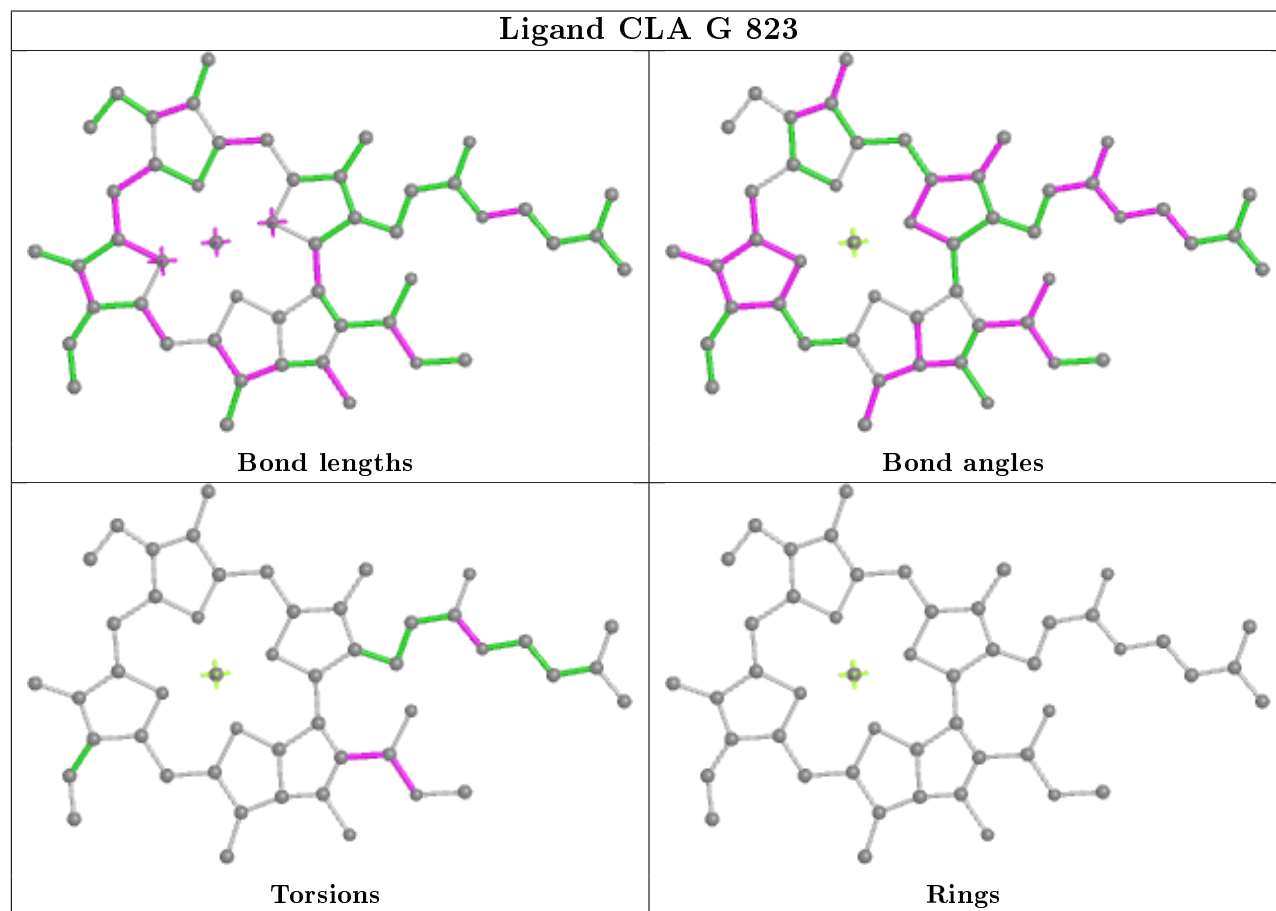
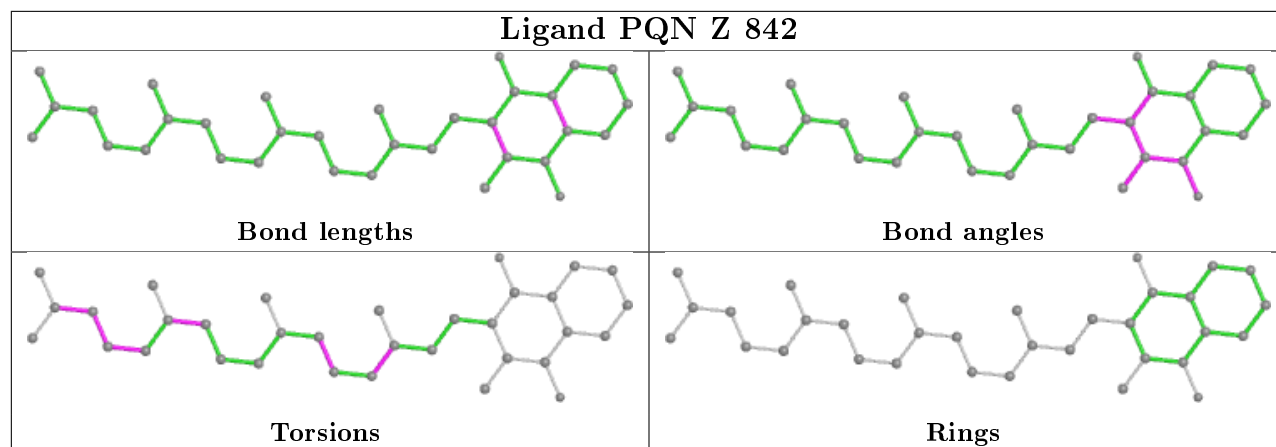


## Ligand CLA B 807



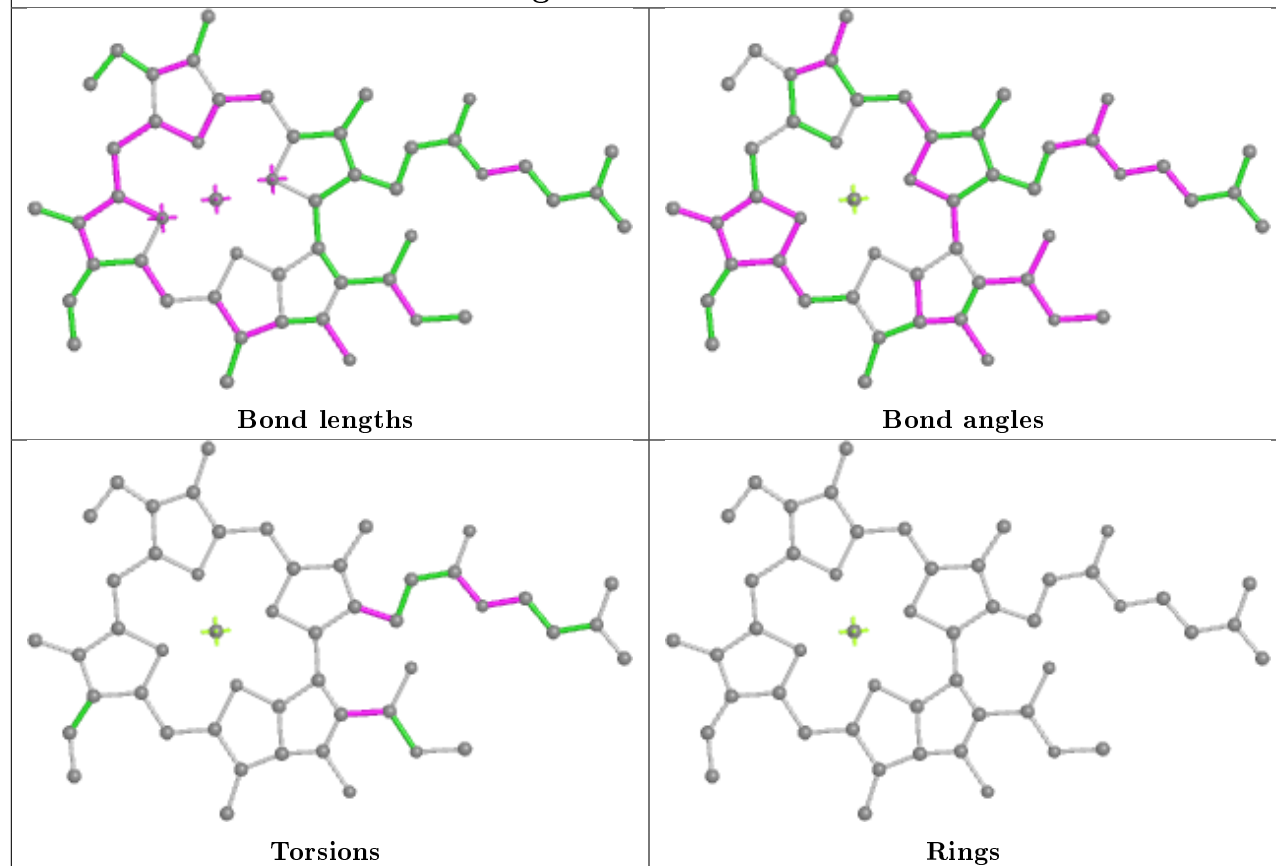


**Ligand CLA B 832****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA Z 828****Bond lengths****Bond angles****Torsions****Rings**

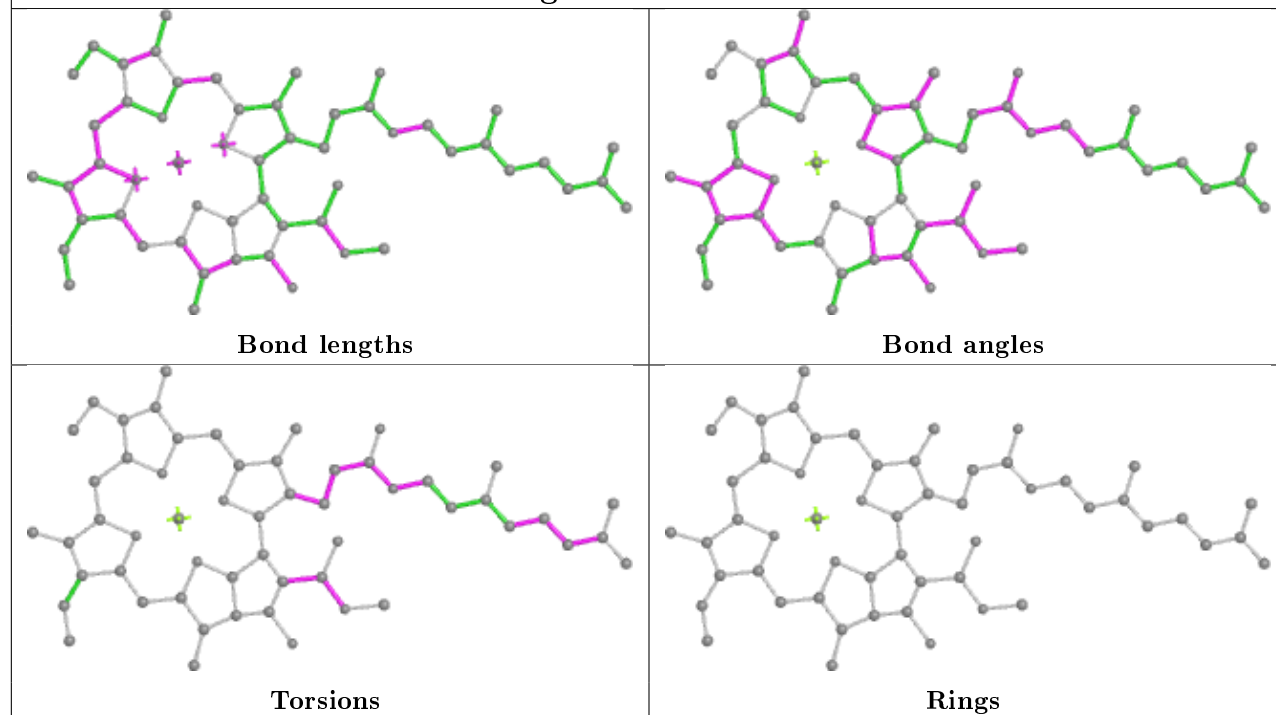


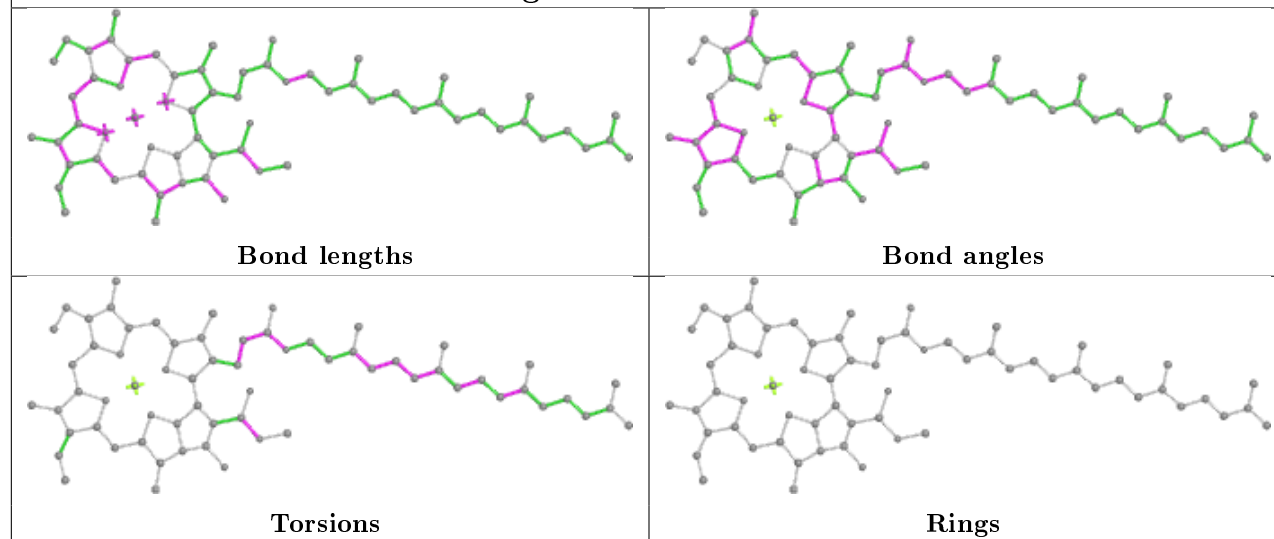
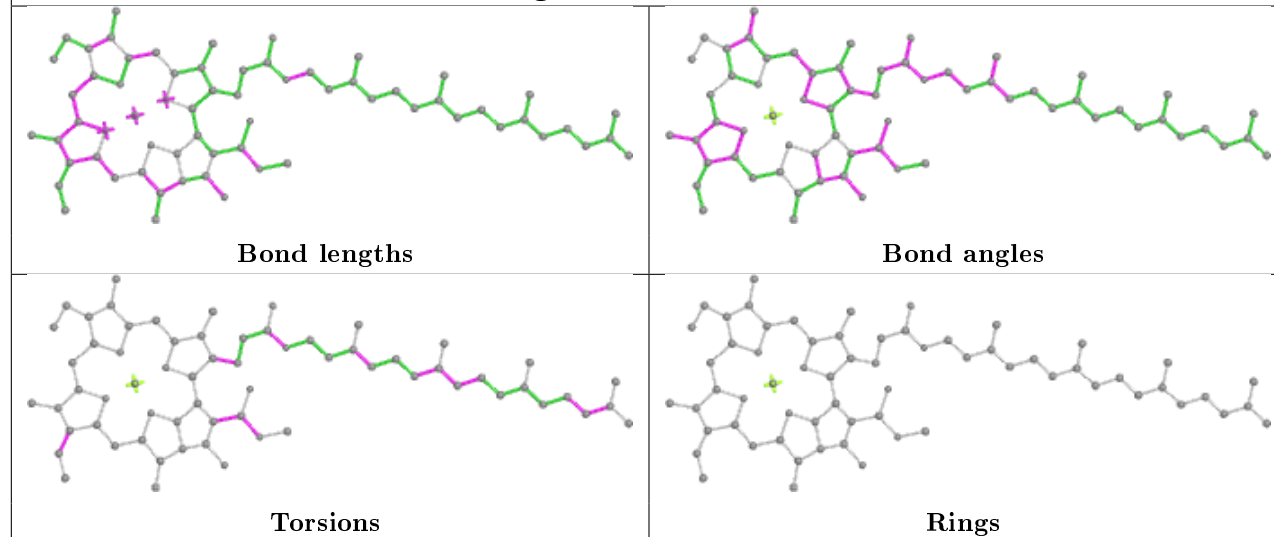


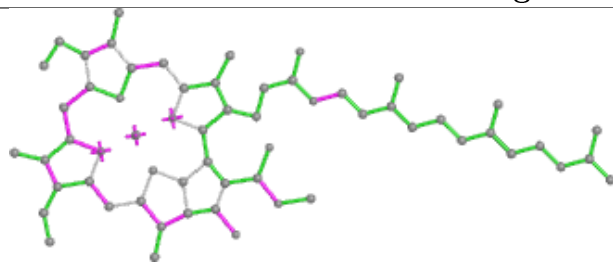
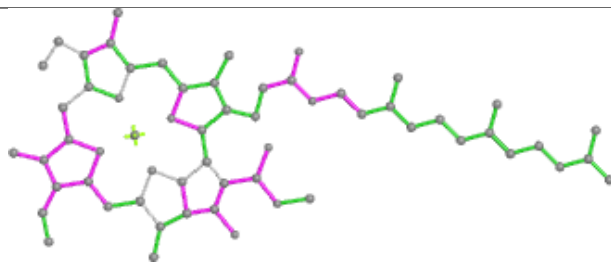
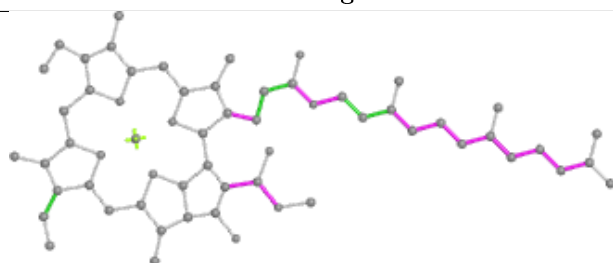
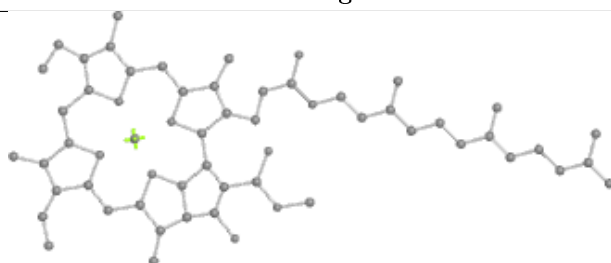
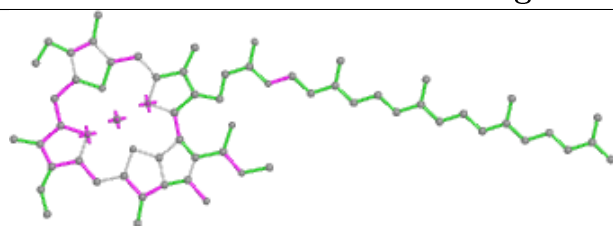
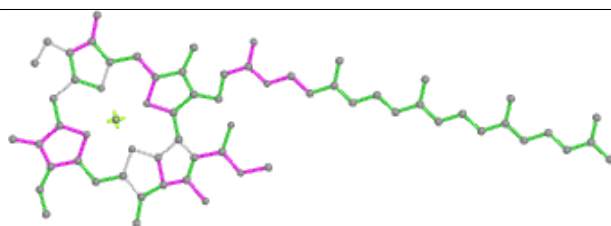
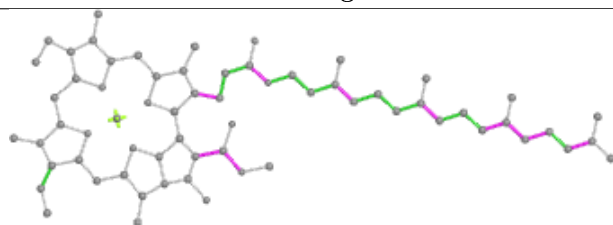
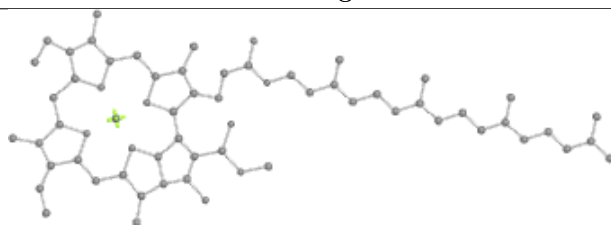
## Ligand CLA A 836



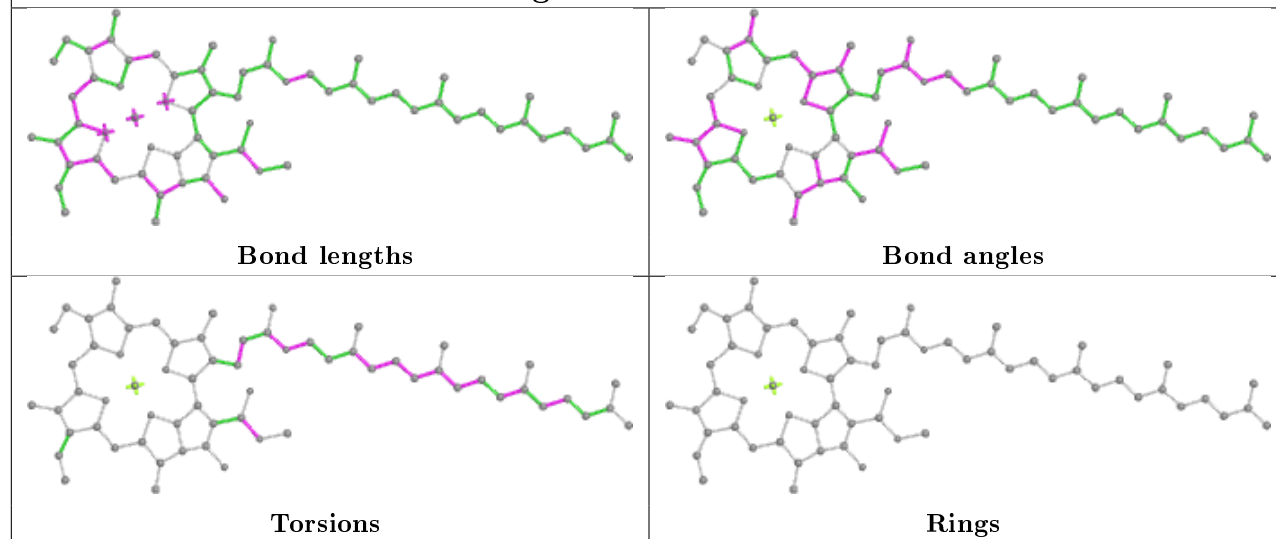
## Ligand CLA f 102



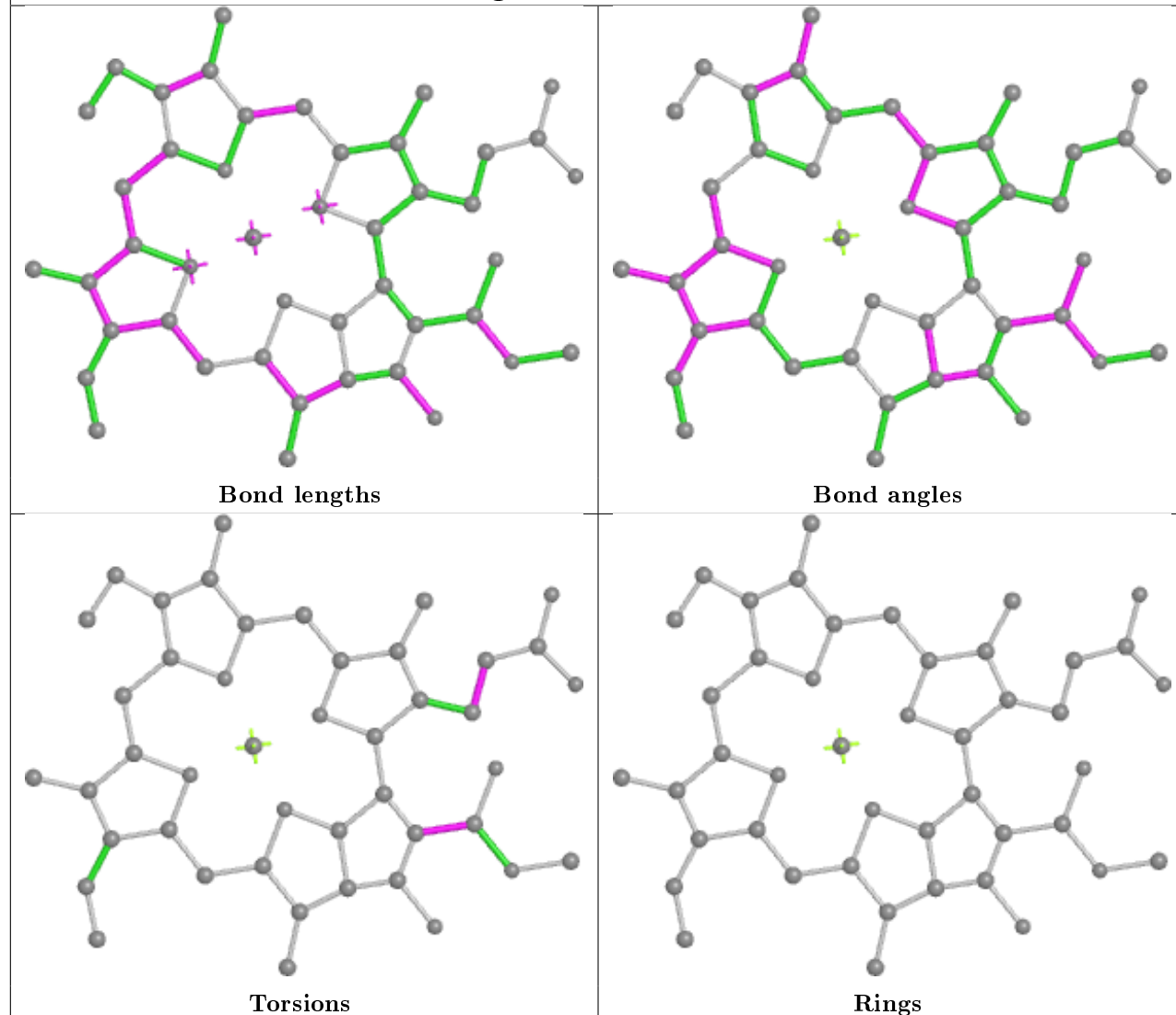
**Ligand CLA U 1004****Ligand CLA Y 821**

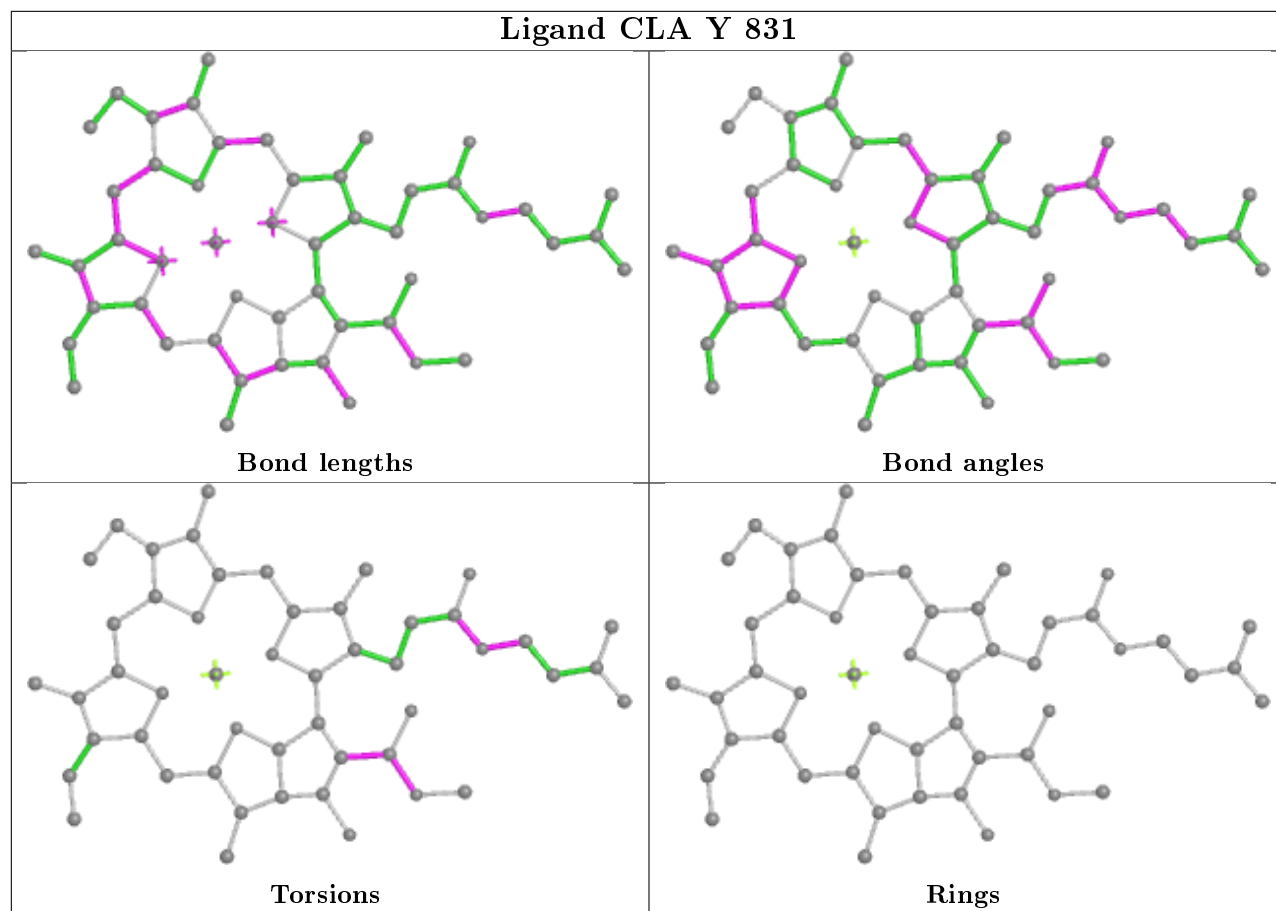
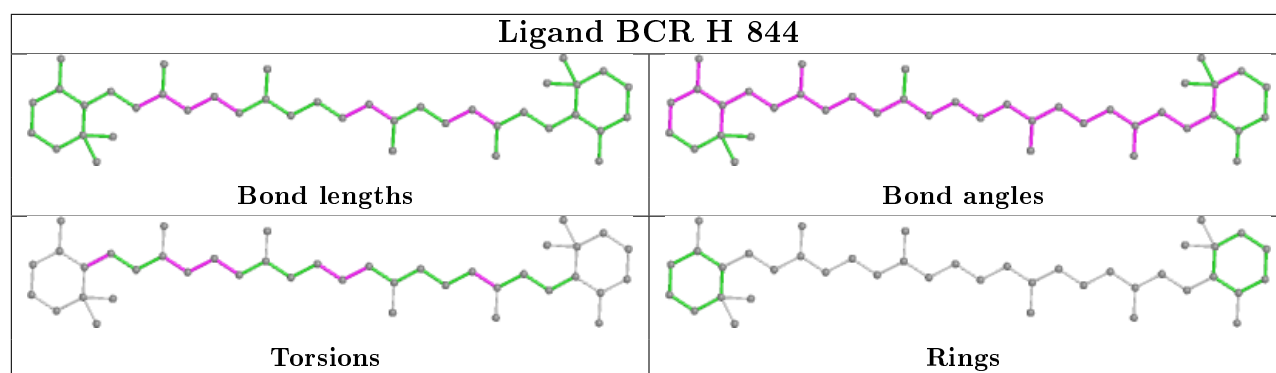
**Ligand CLA H 836****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 822****Bond lengths****Bond angles****Torsions****Rings**

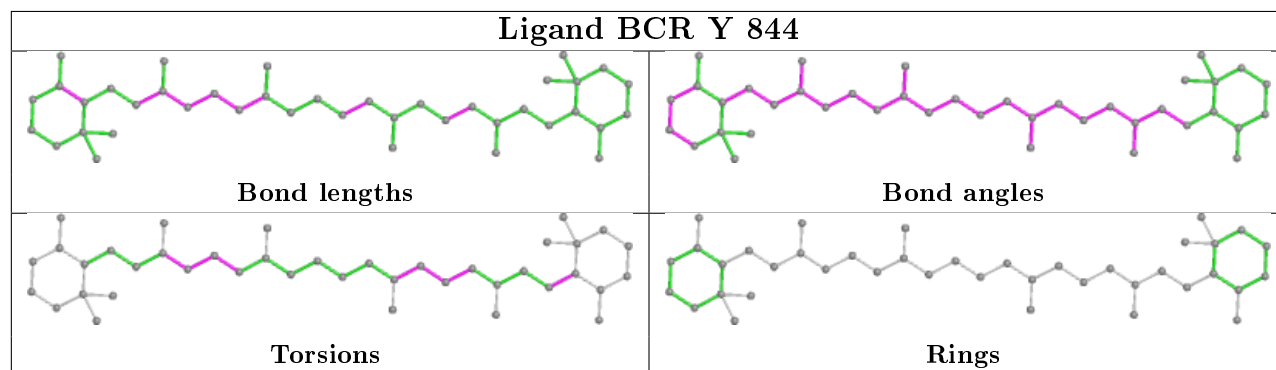
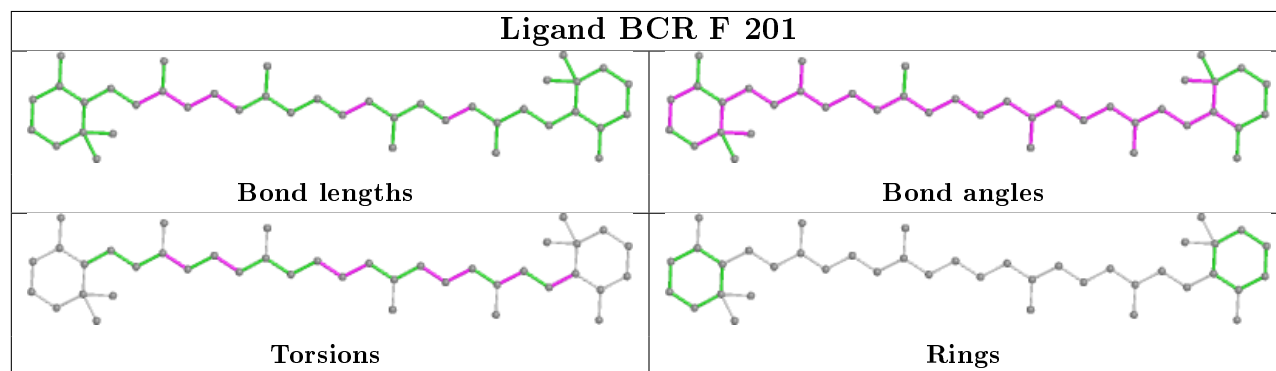
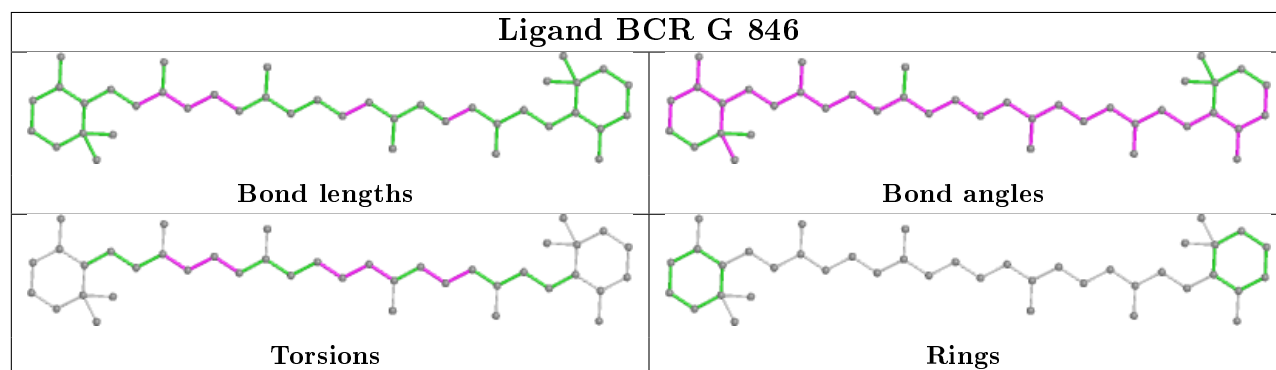
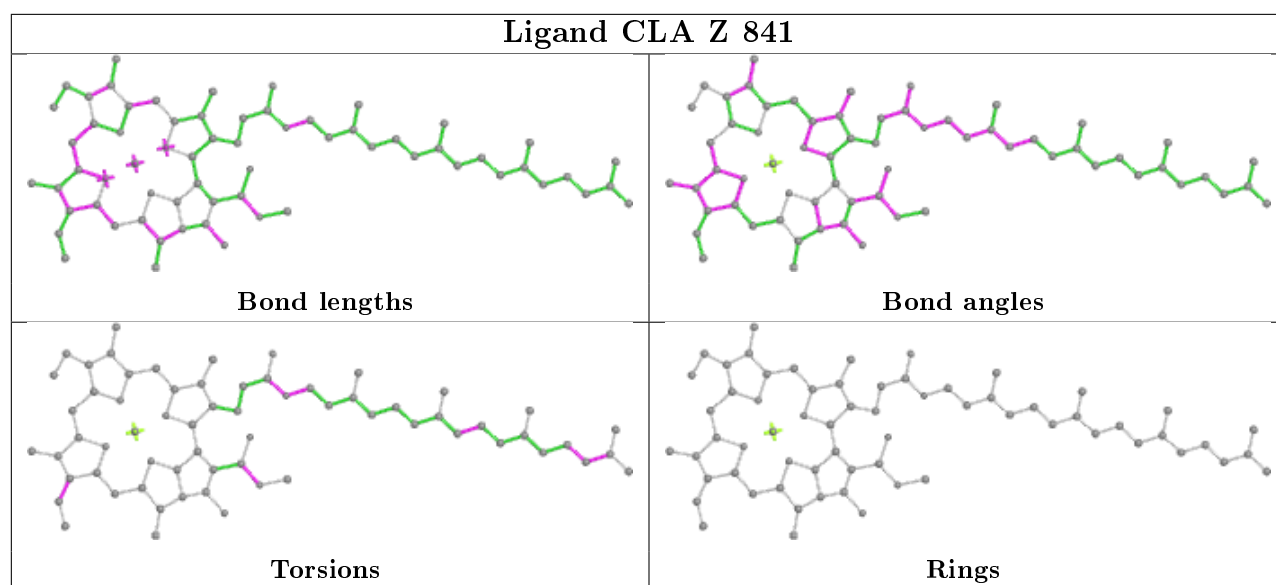
## Ligand CLA Y 822



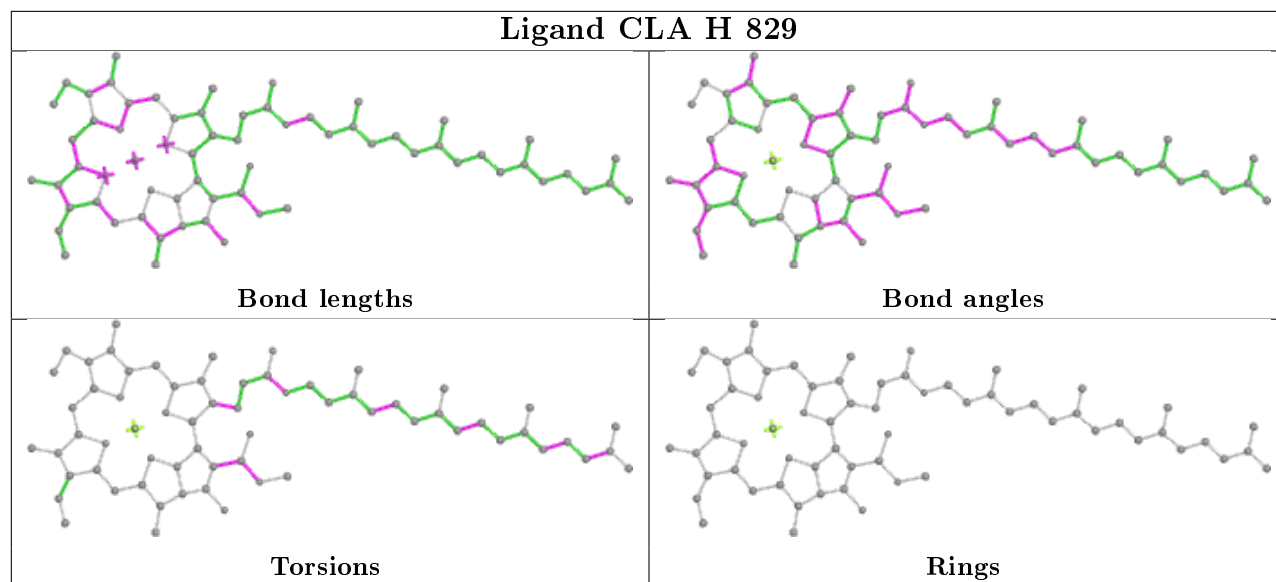
## Ligand CLA Y 834



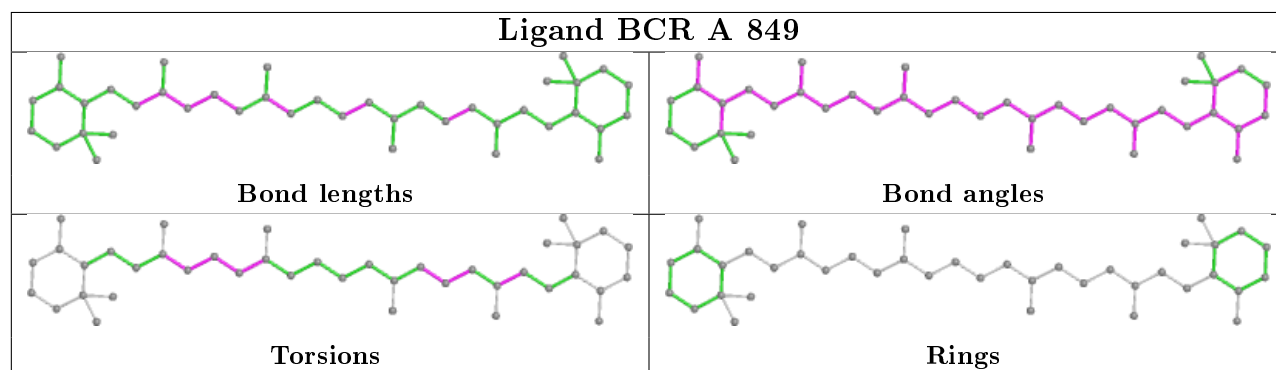




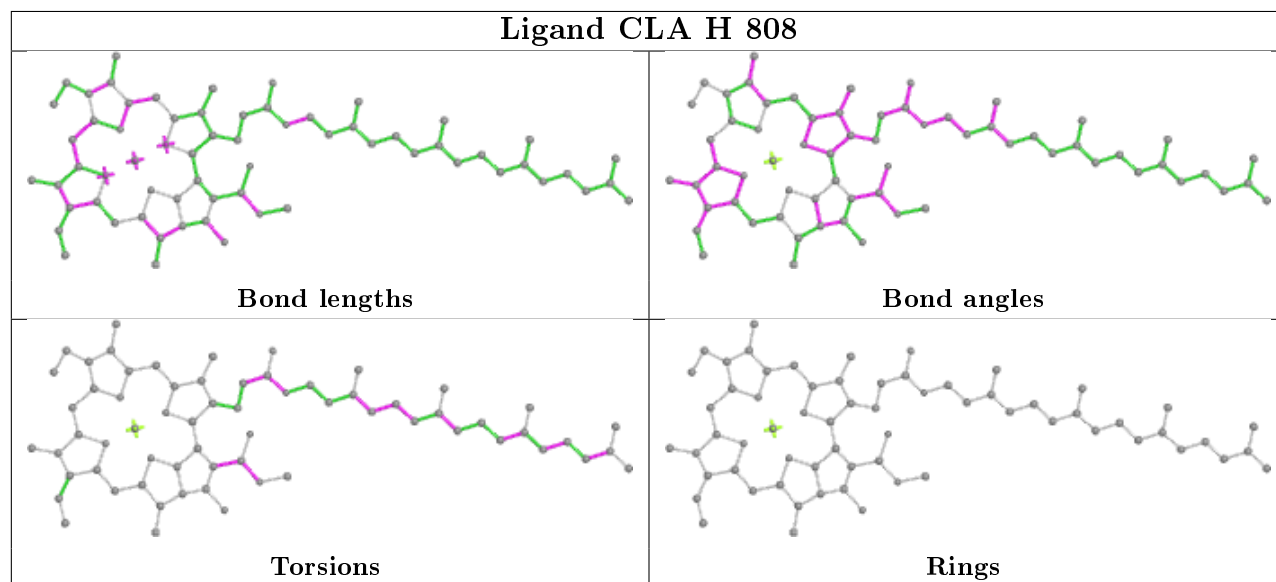
## Ligand CLA H 829

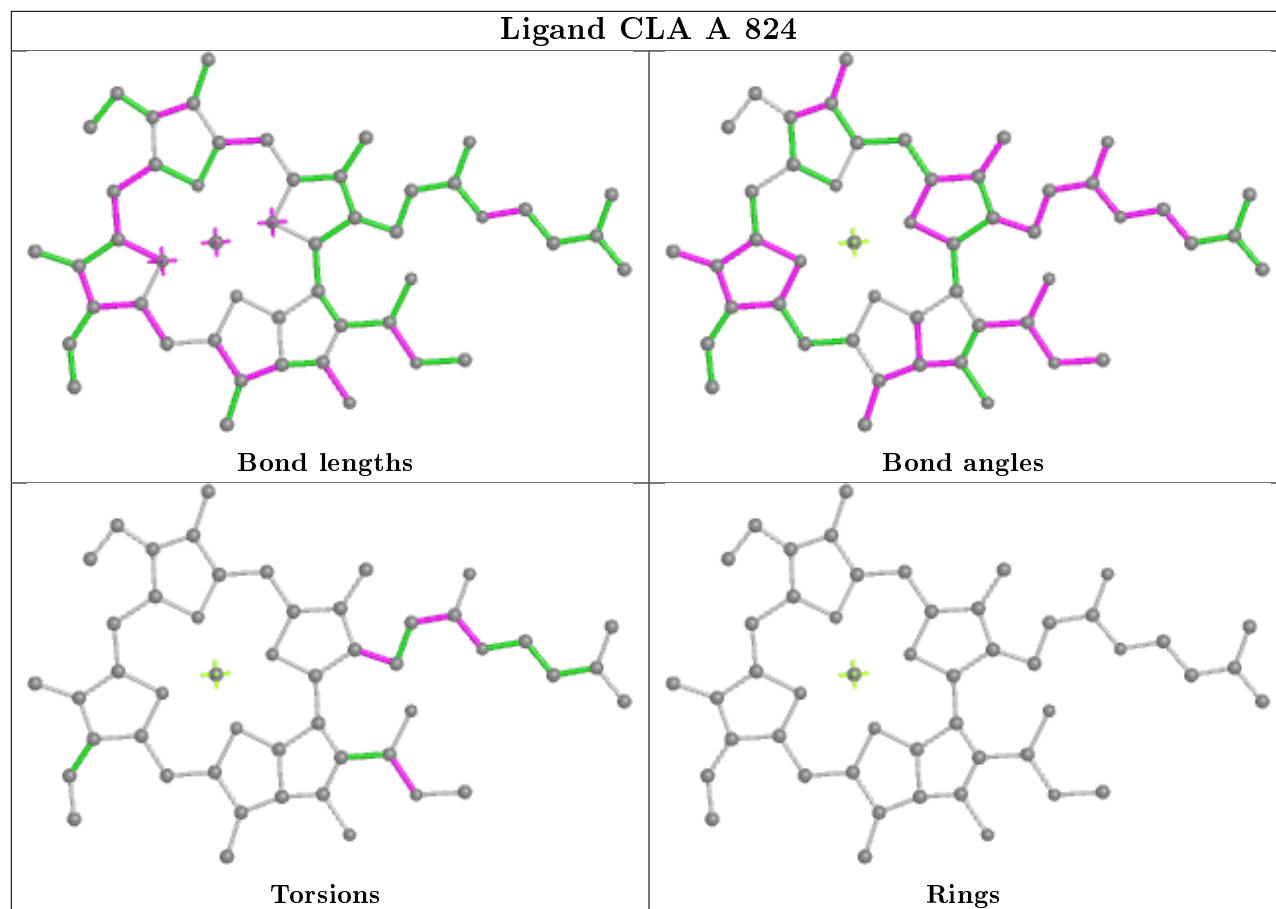


## Ligand BCR A 849



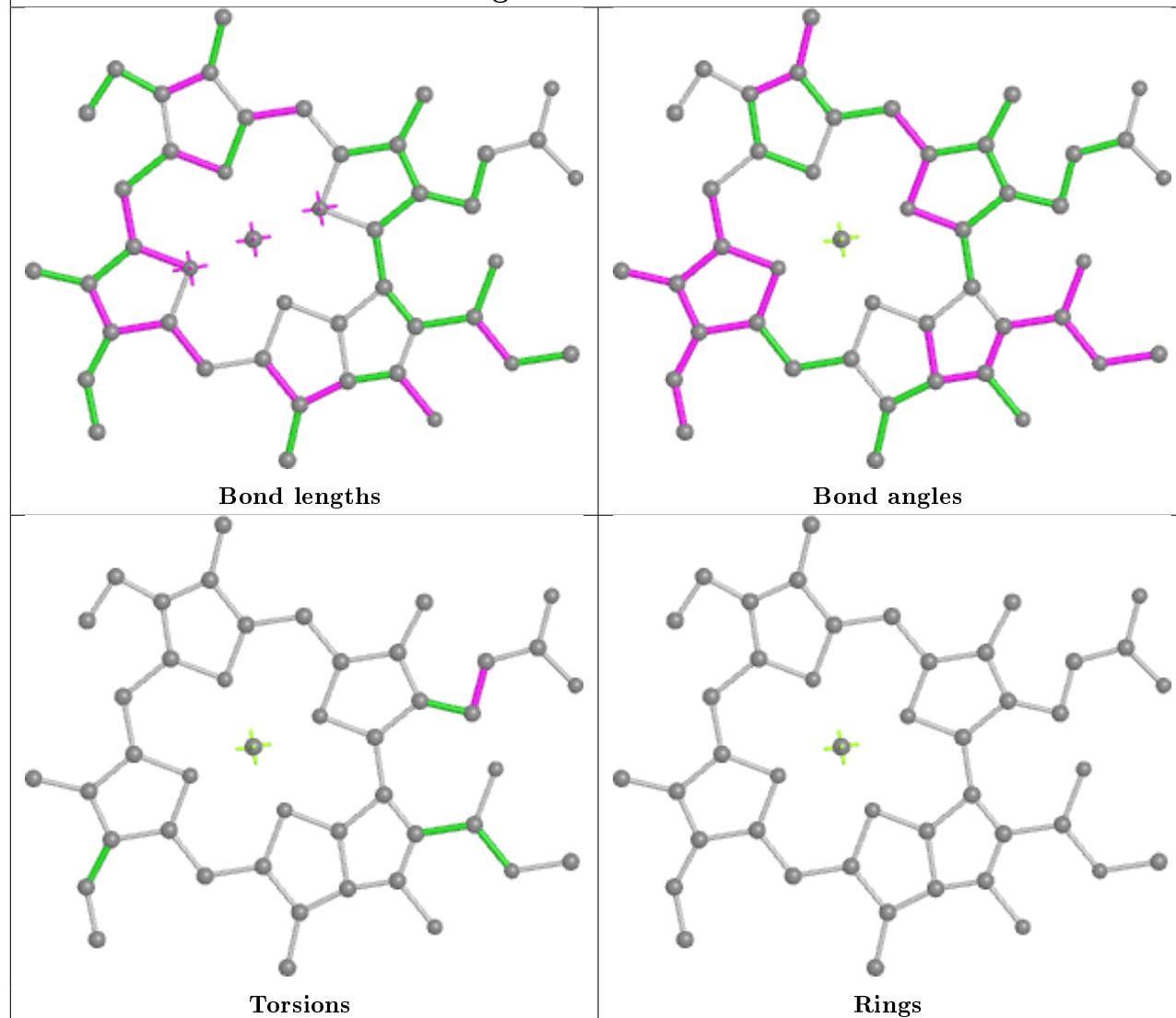
## Ligand CLA H 808



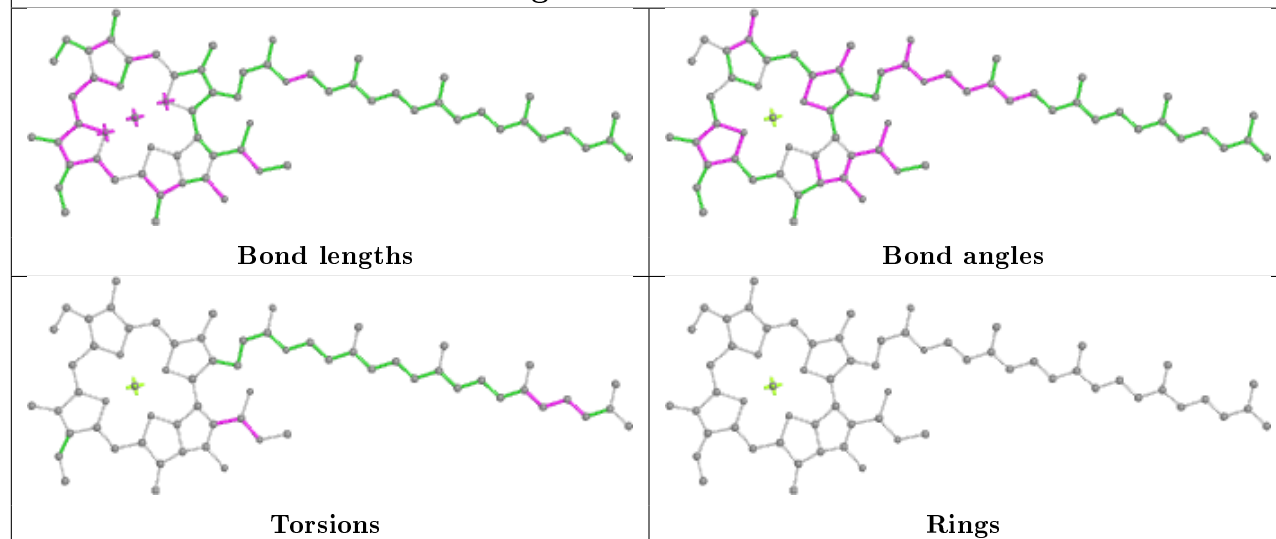


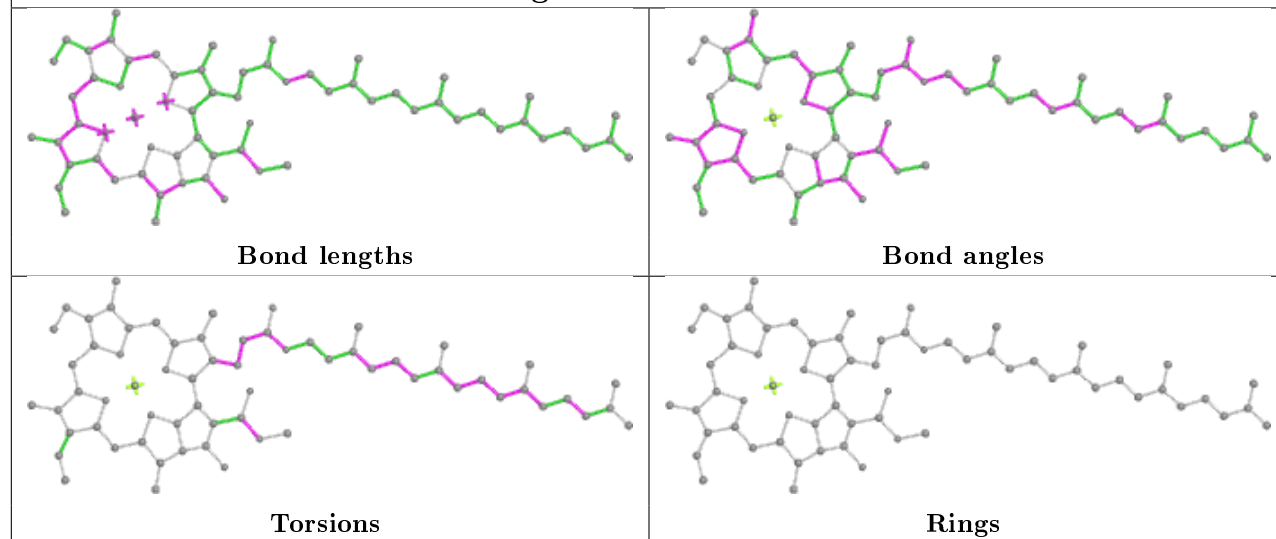
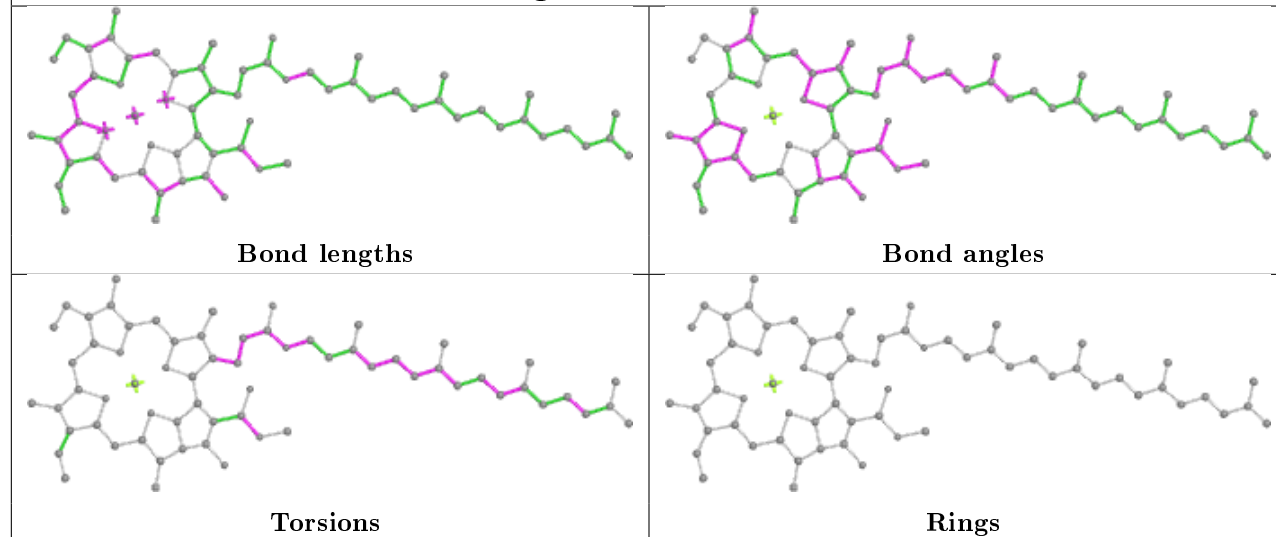


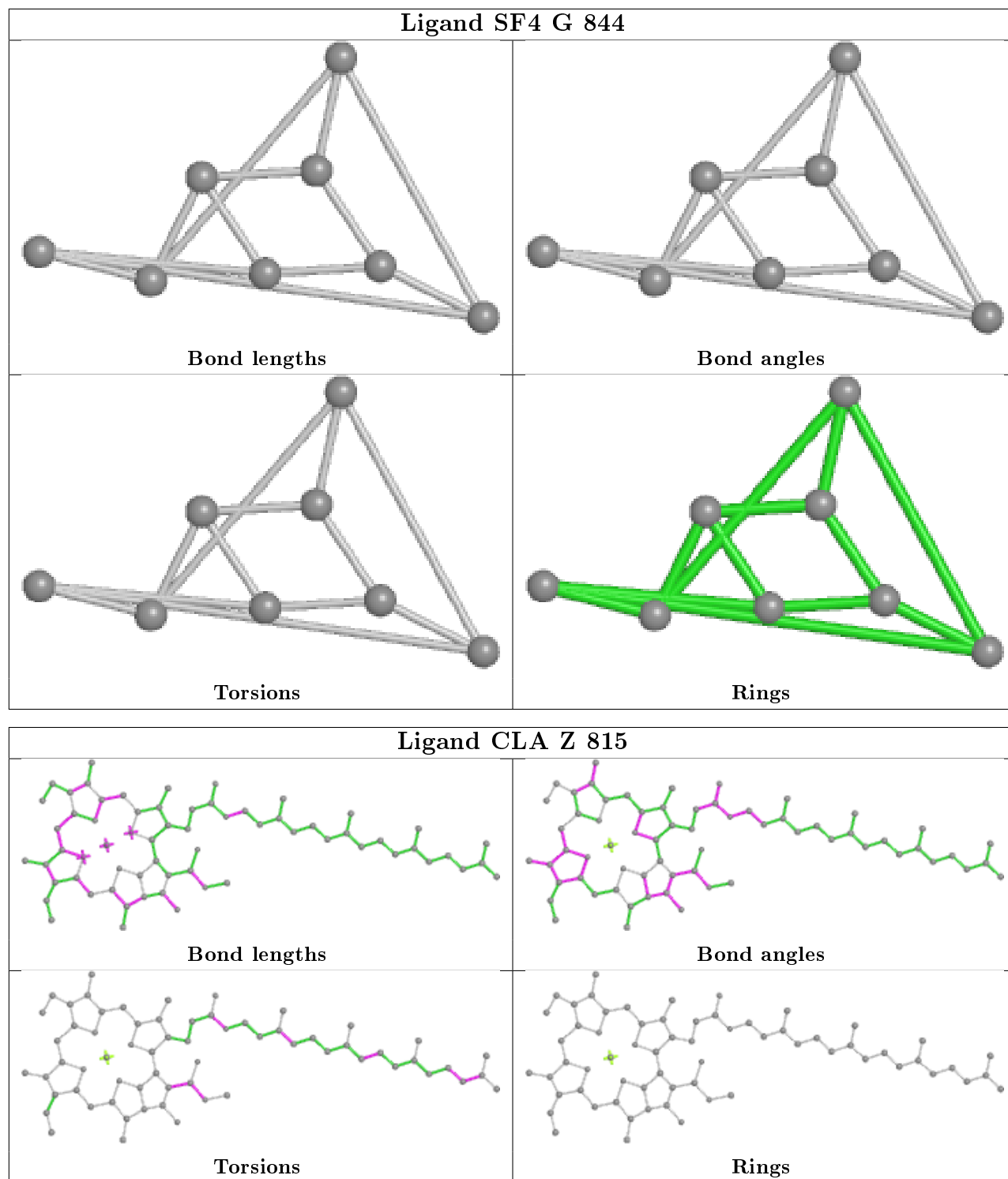
## Ligand CLA Z 839

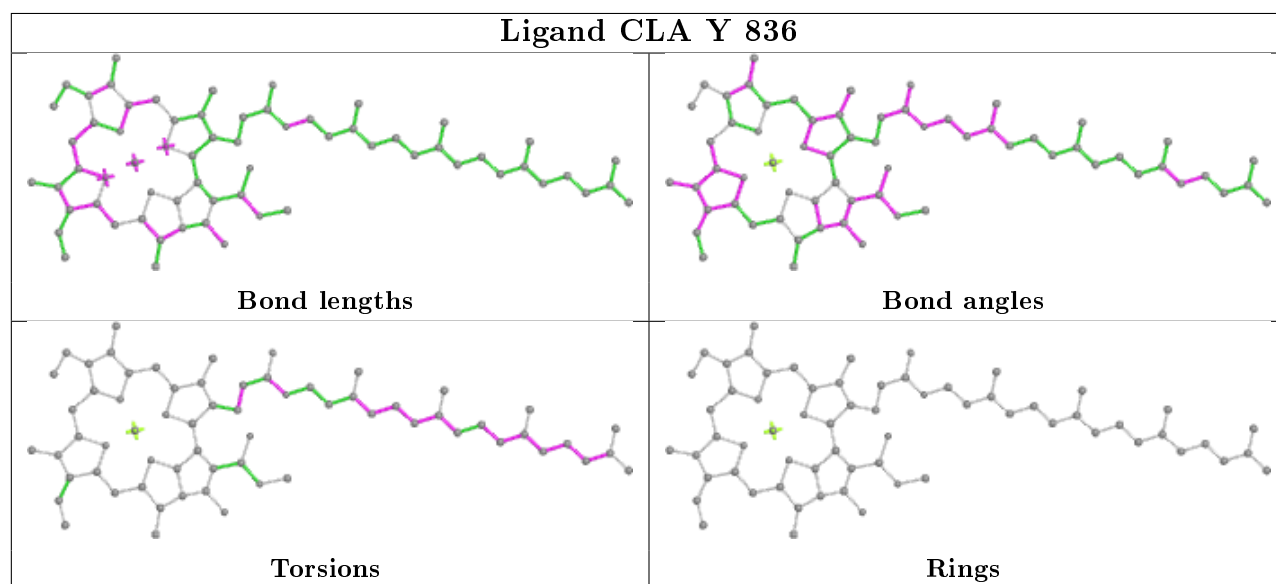
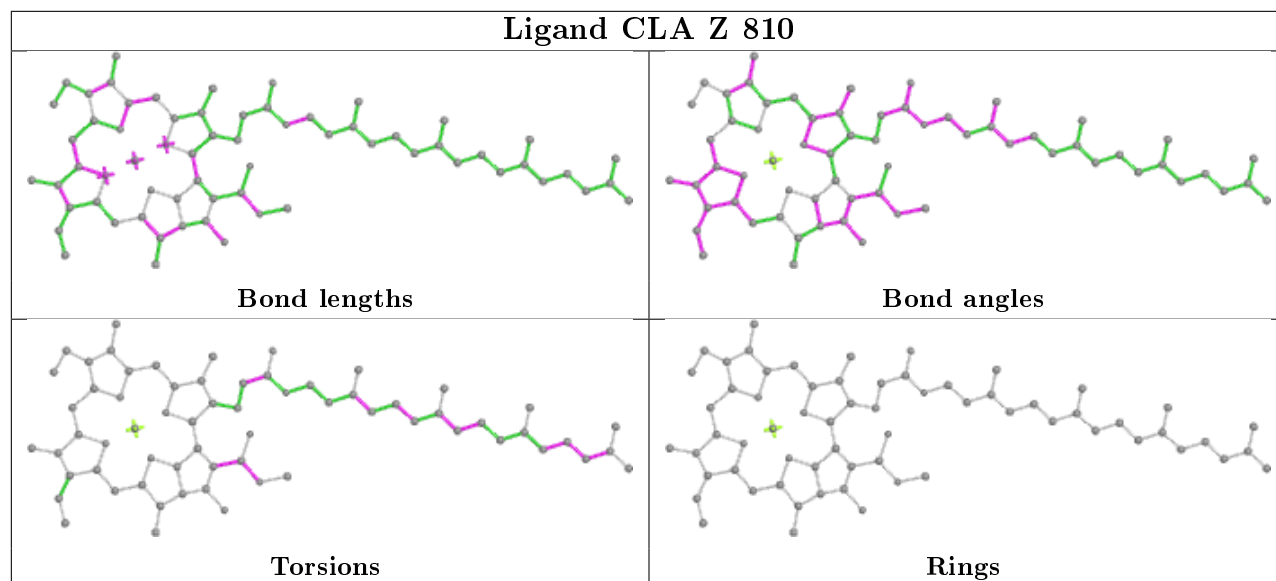
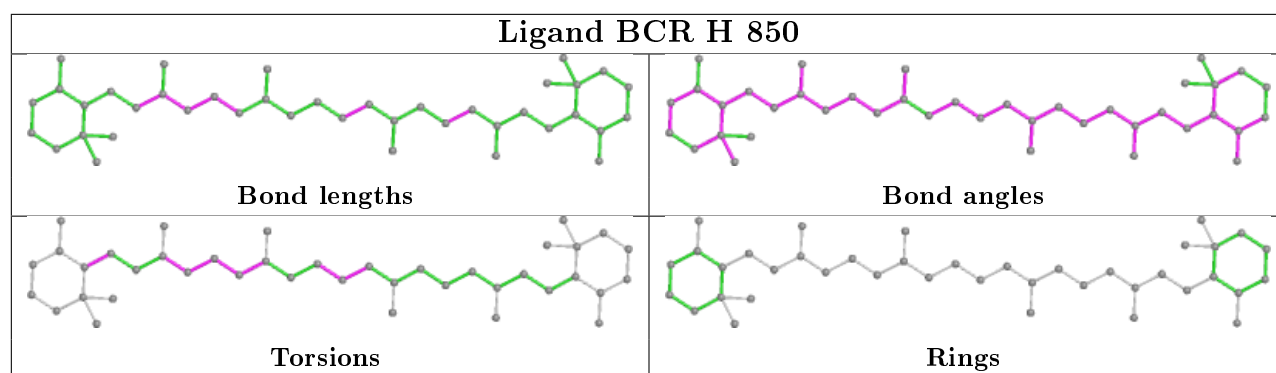


## Ligand CLA H 826

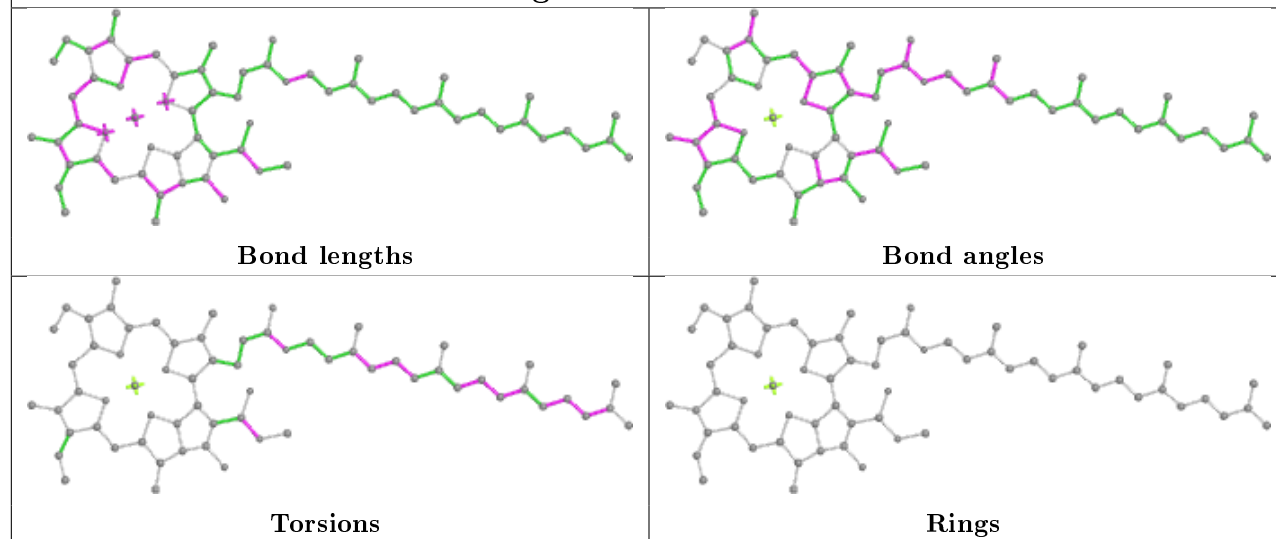


**Ligand CLA G 806****Ligand CLA A 819**

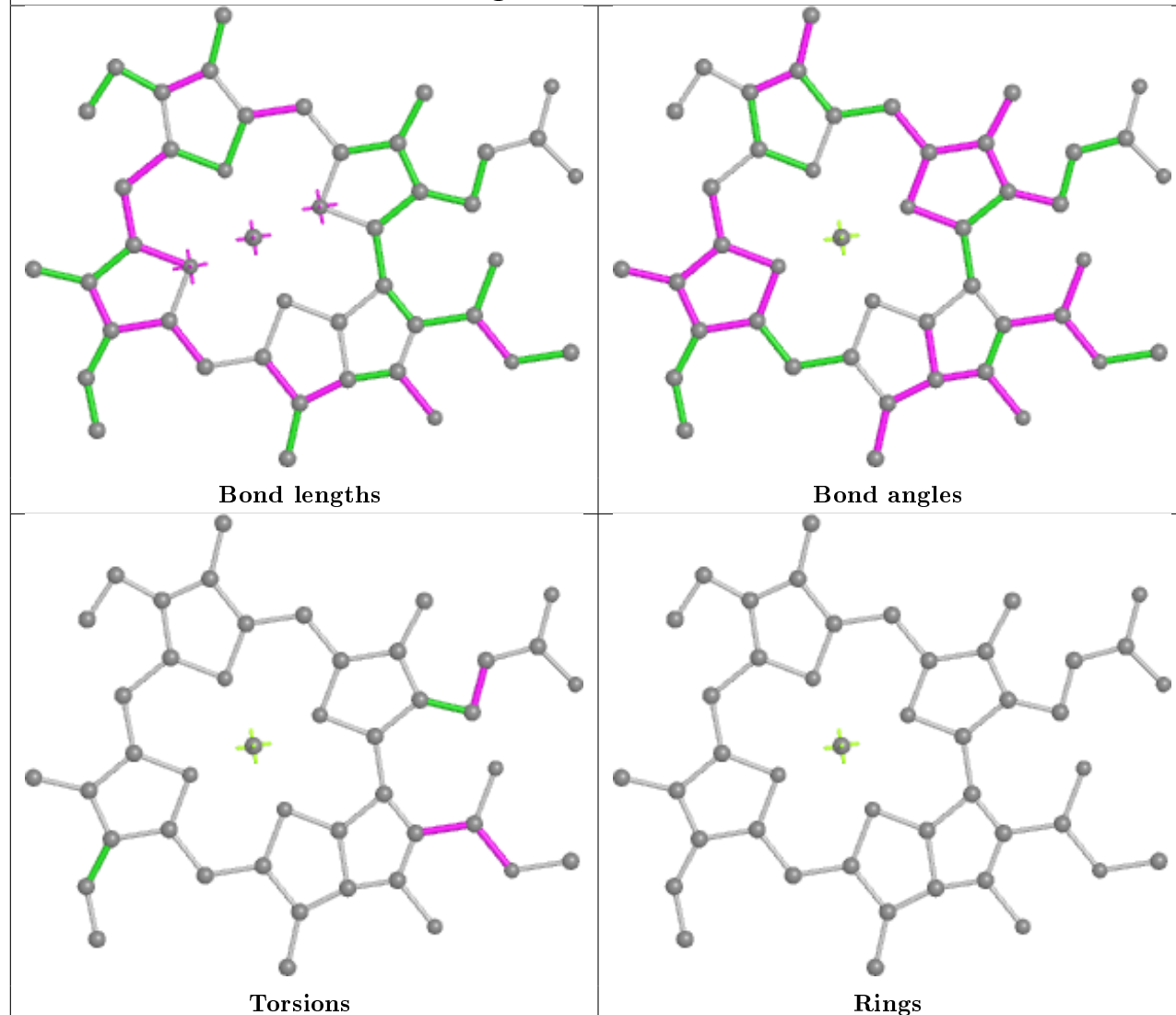




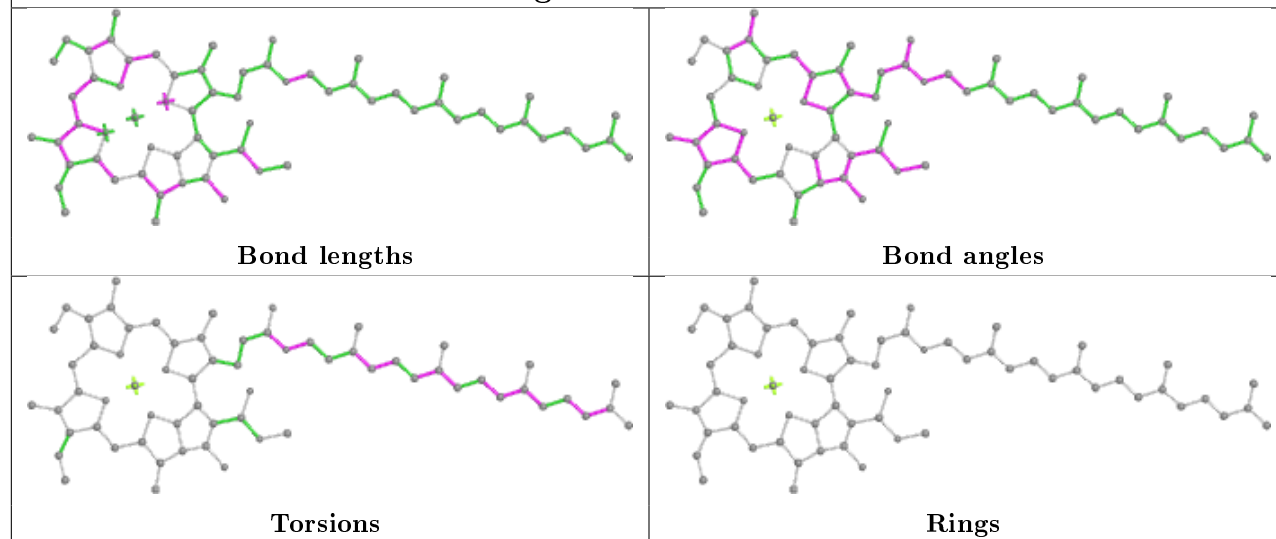
## Ligand CLA B 805



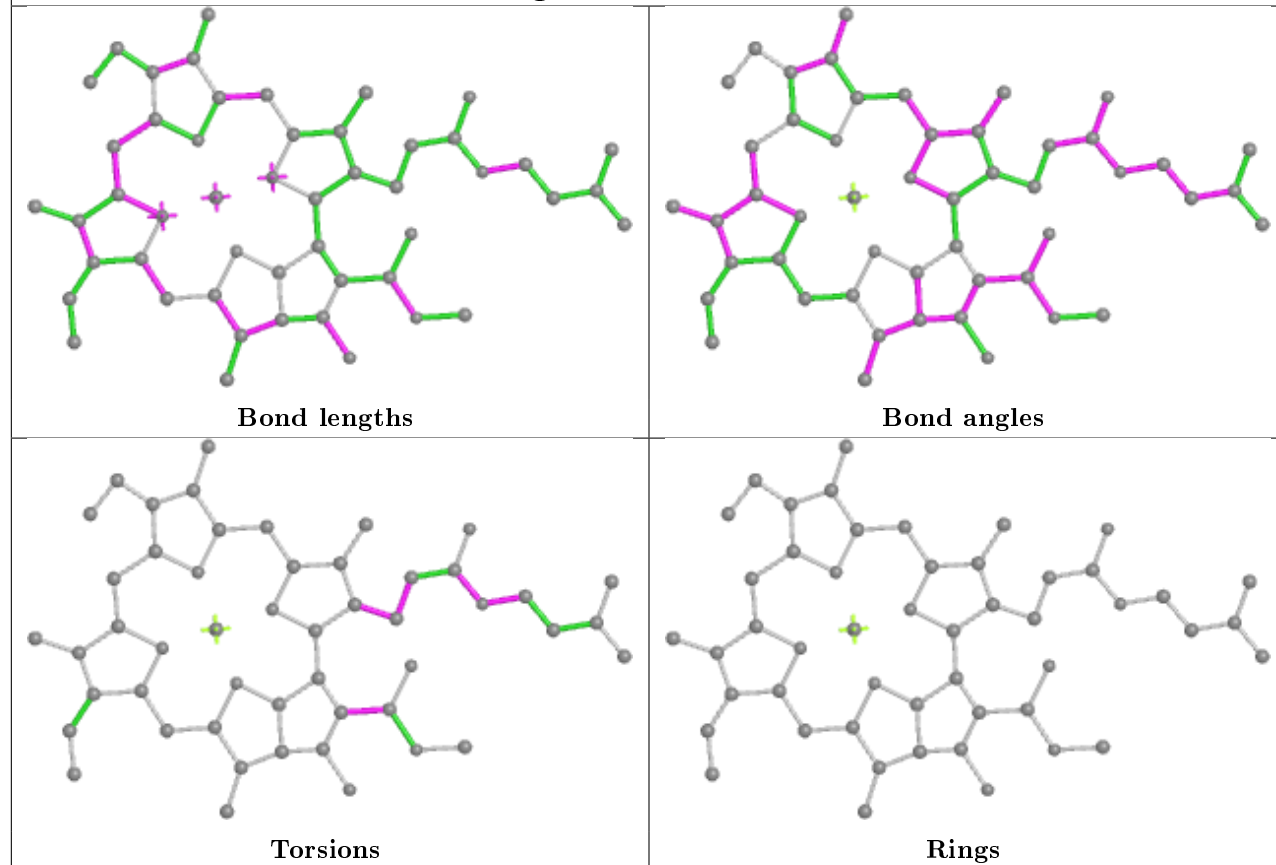
## Ligand CLA B 829

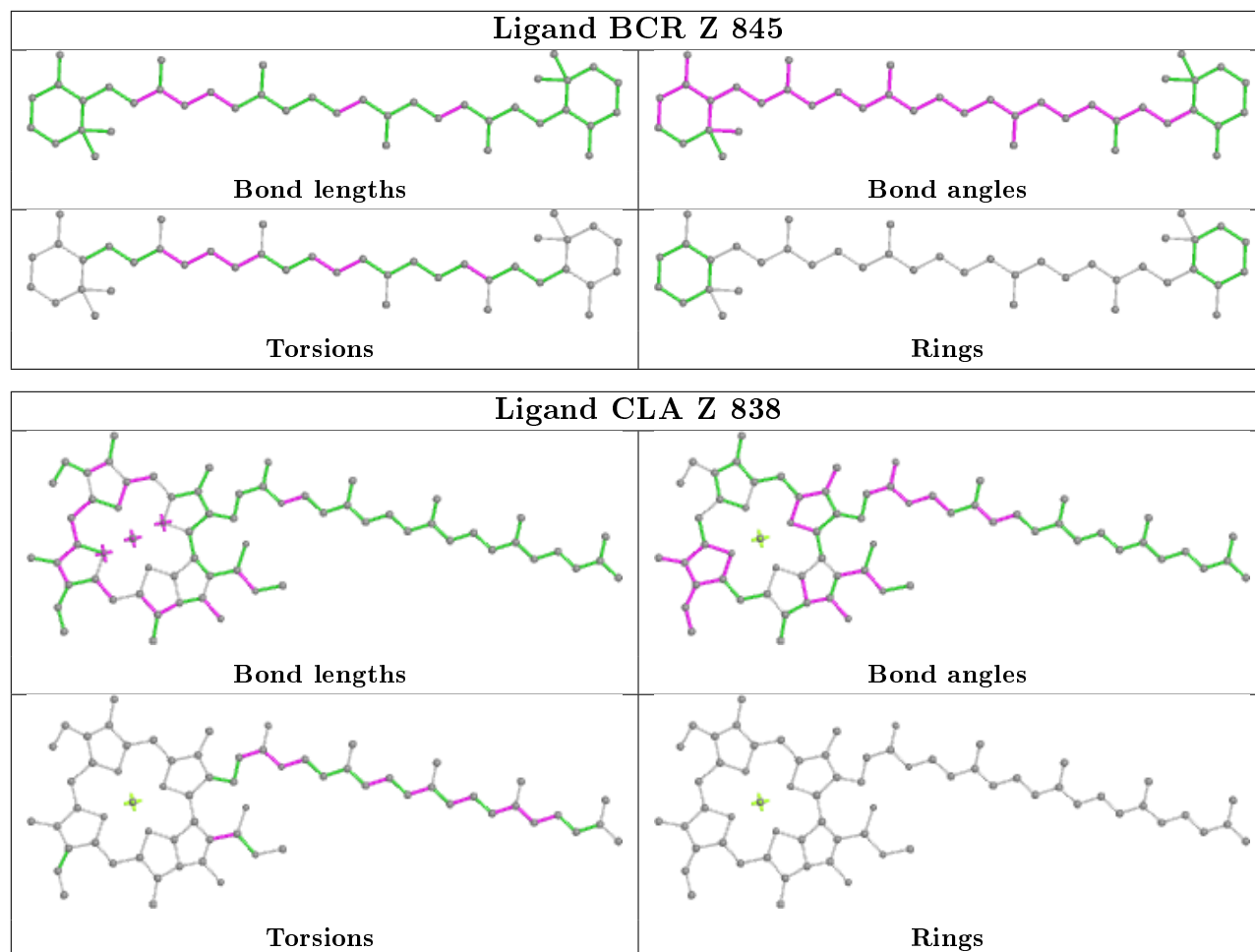


## Ligand CLA Z 801

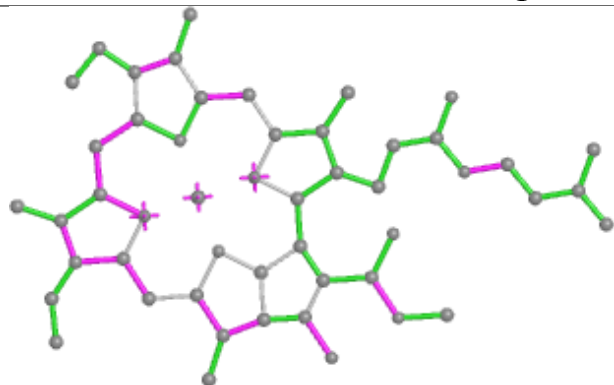


## Ligand CLA G 815

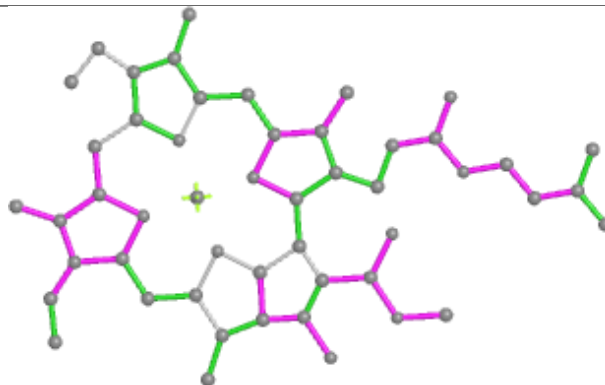




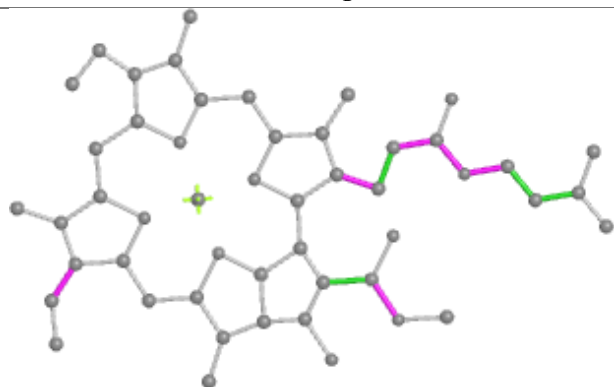
## Ligand CLA G 816



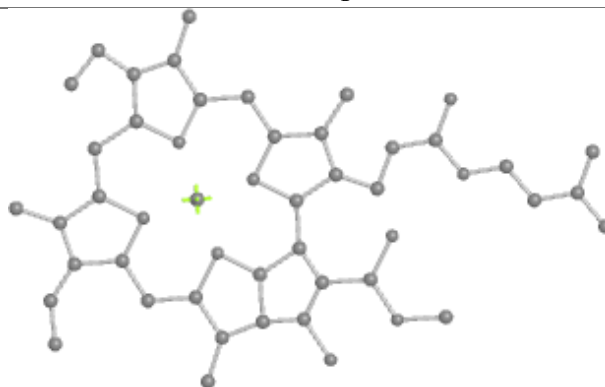
Bond lengths



Bond angles

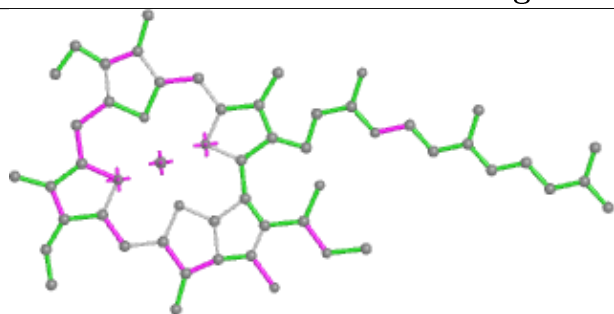


Torsions

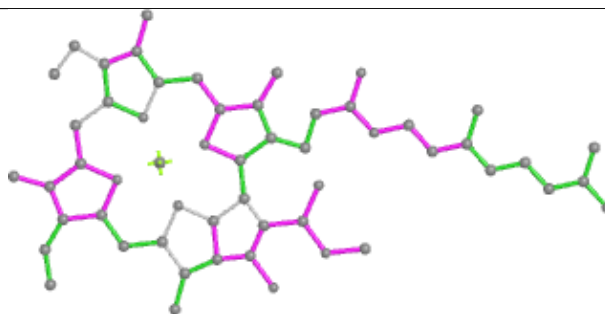


Rings

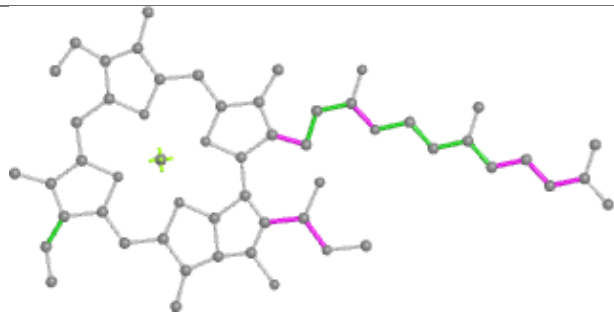
## Ligand CLA H 832



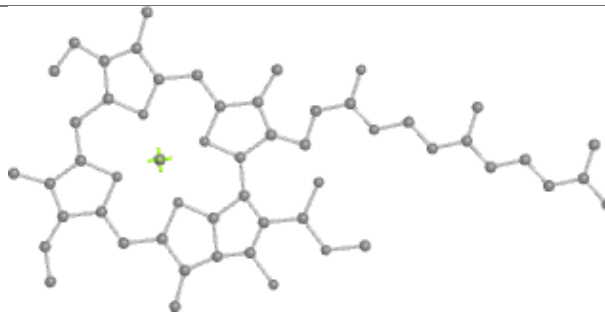
Bond lengths



Bond angles

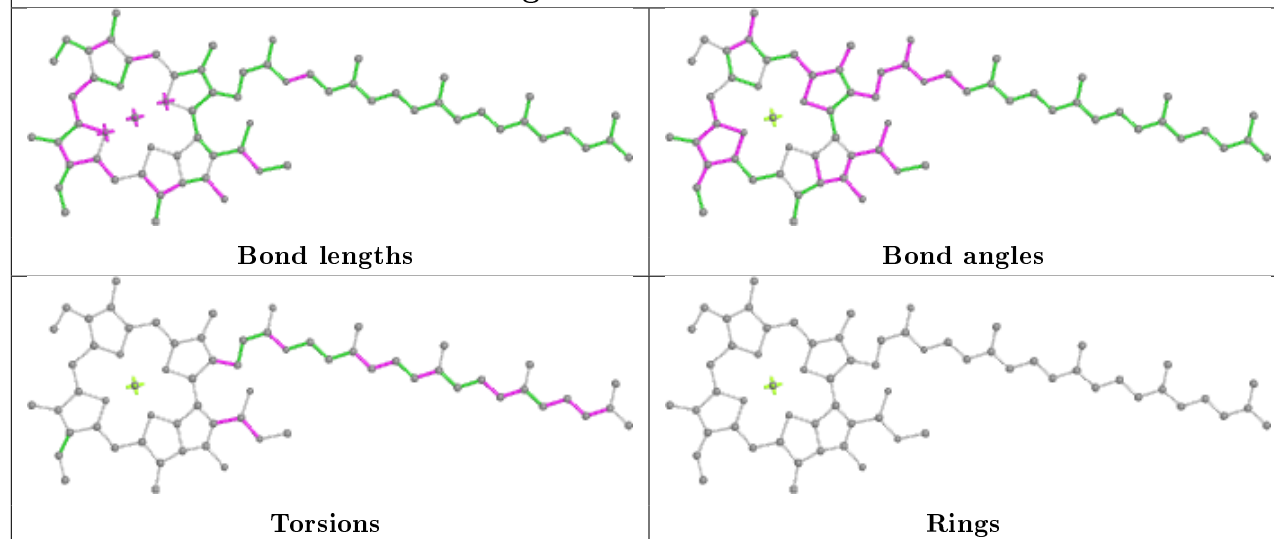
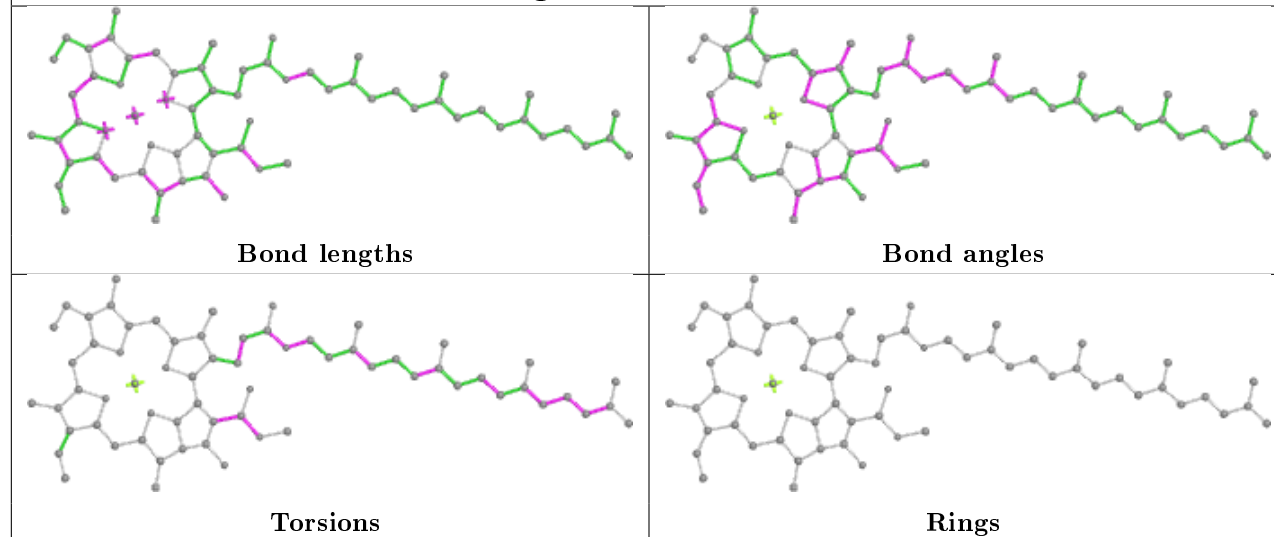


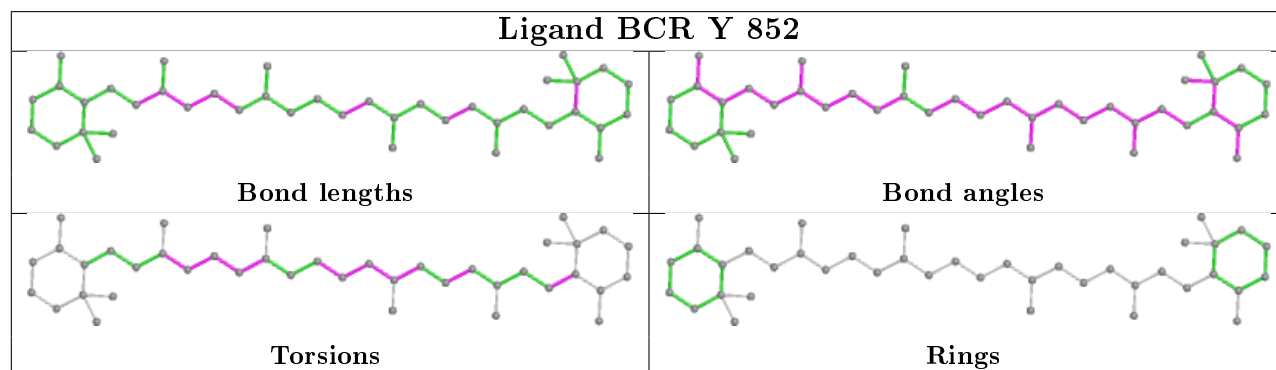
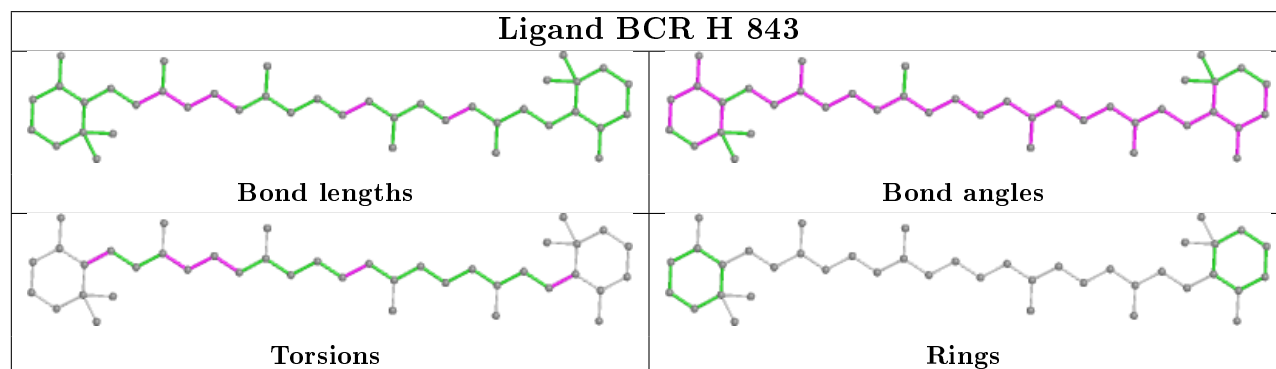
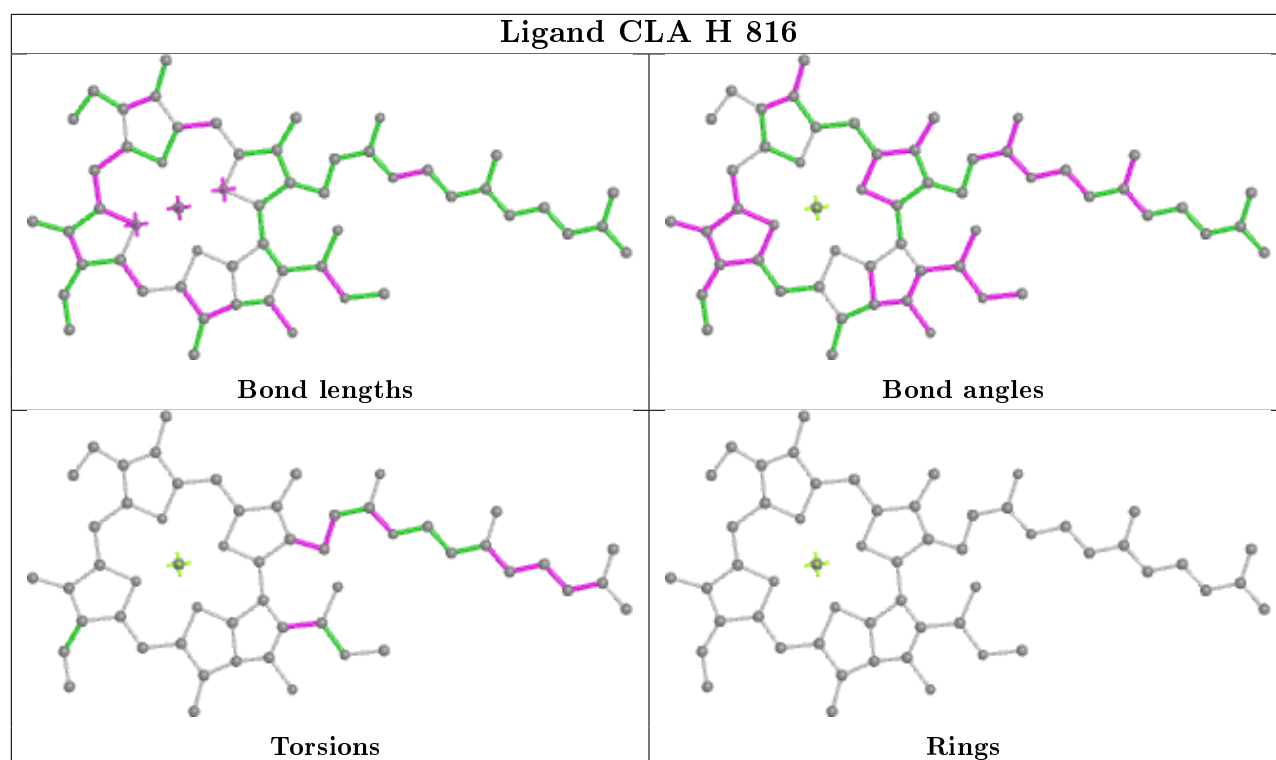
Torsions

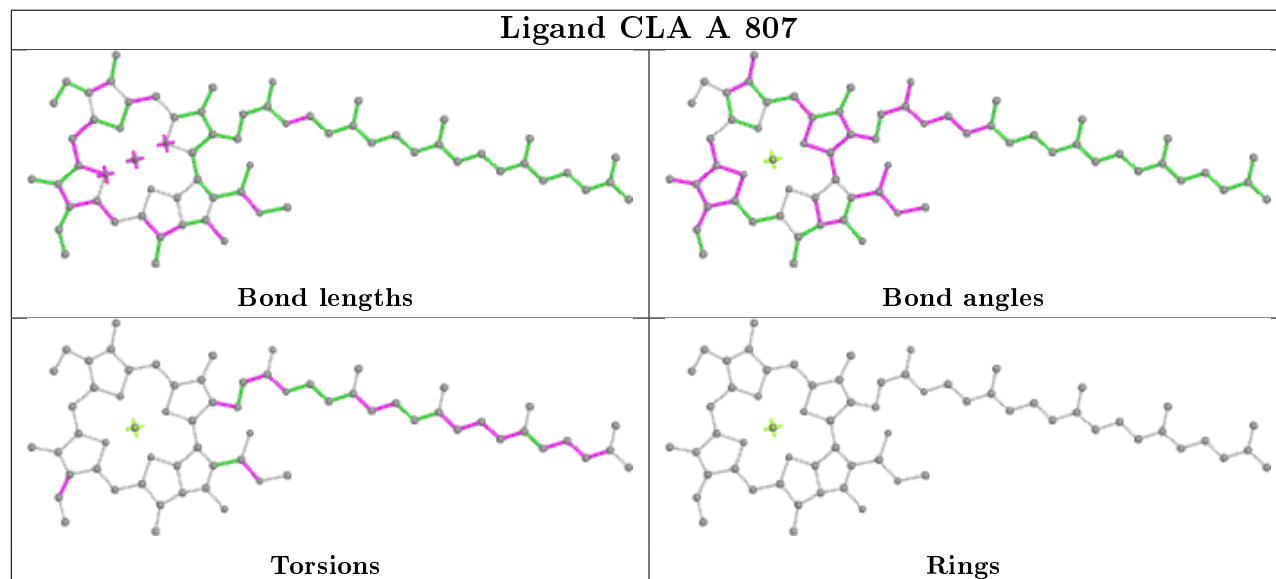
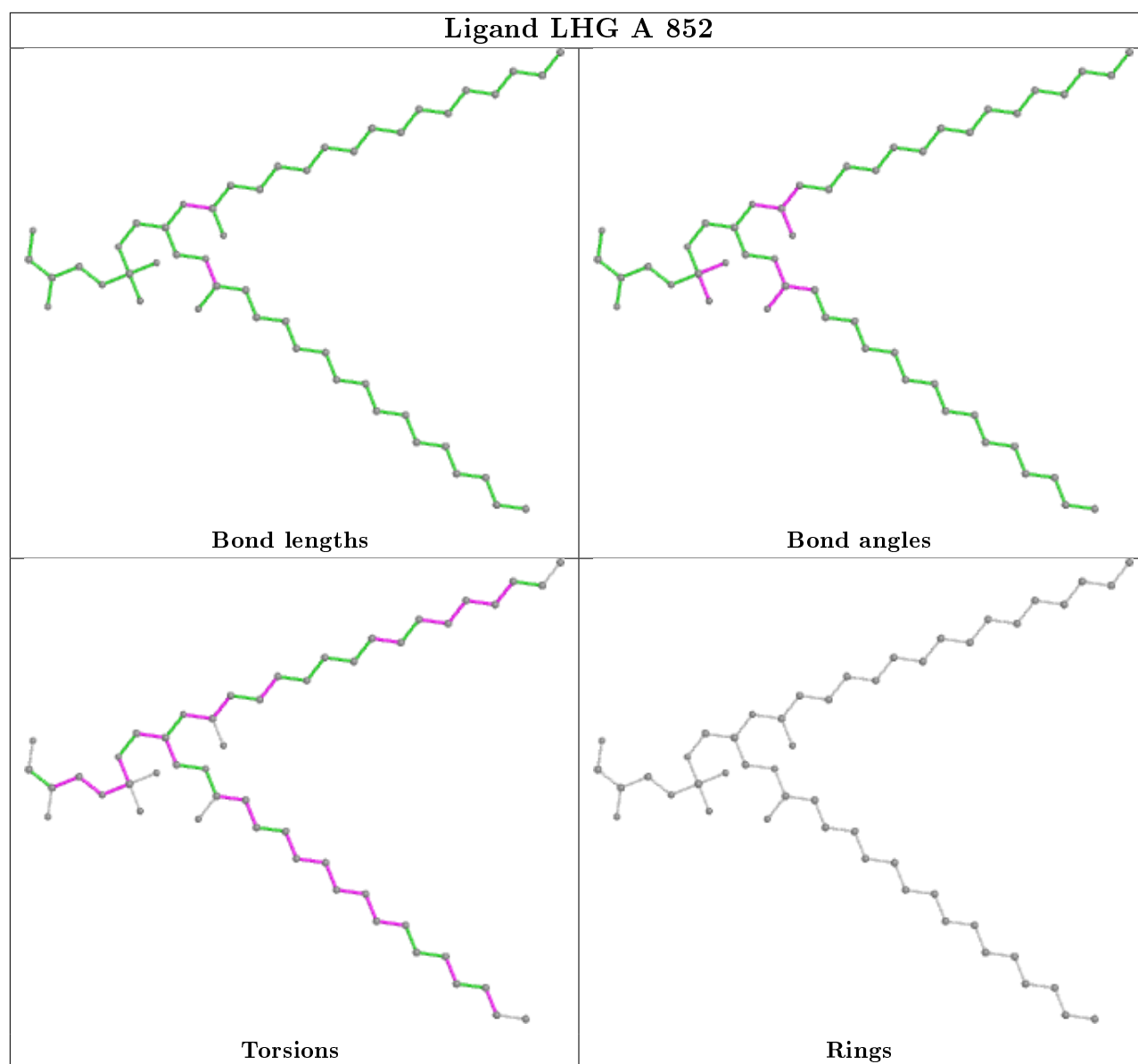


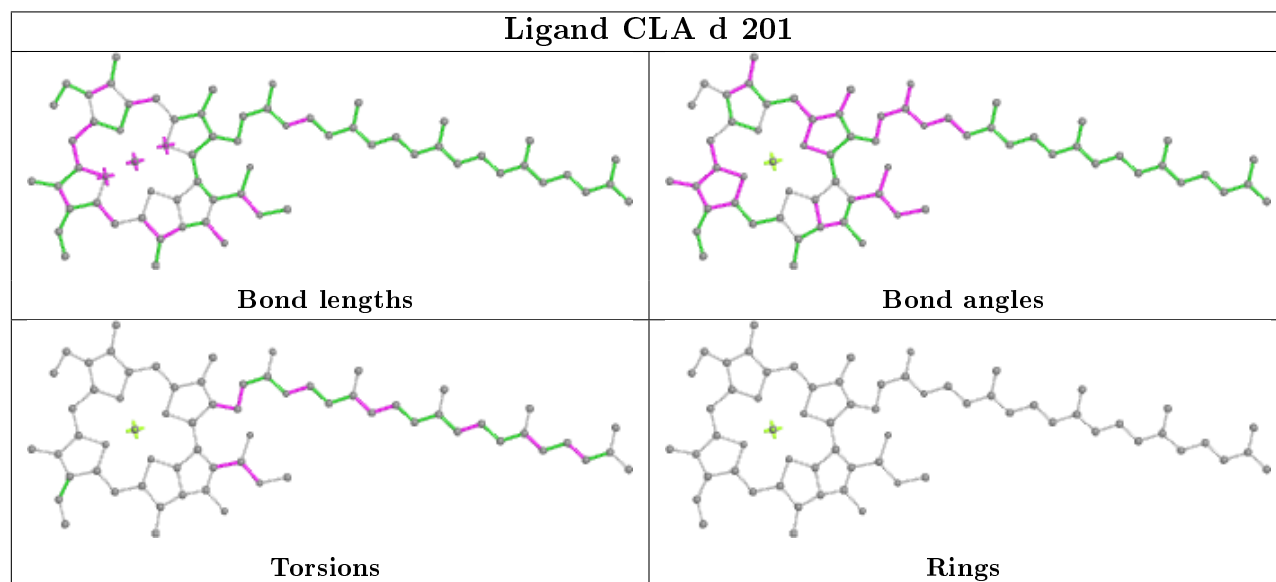
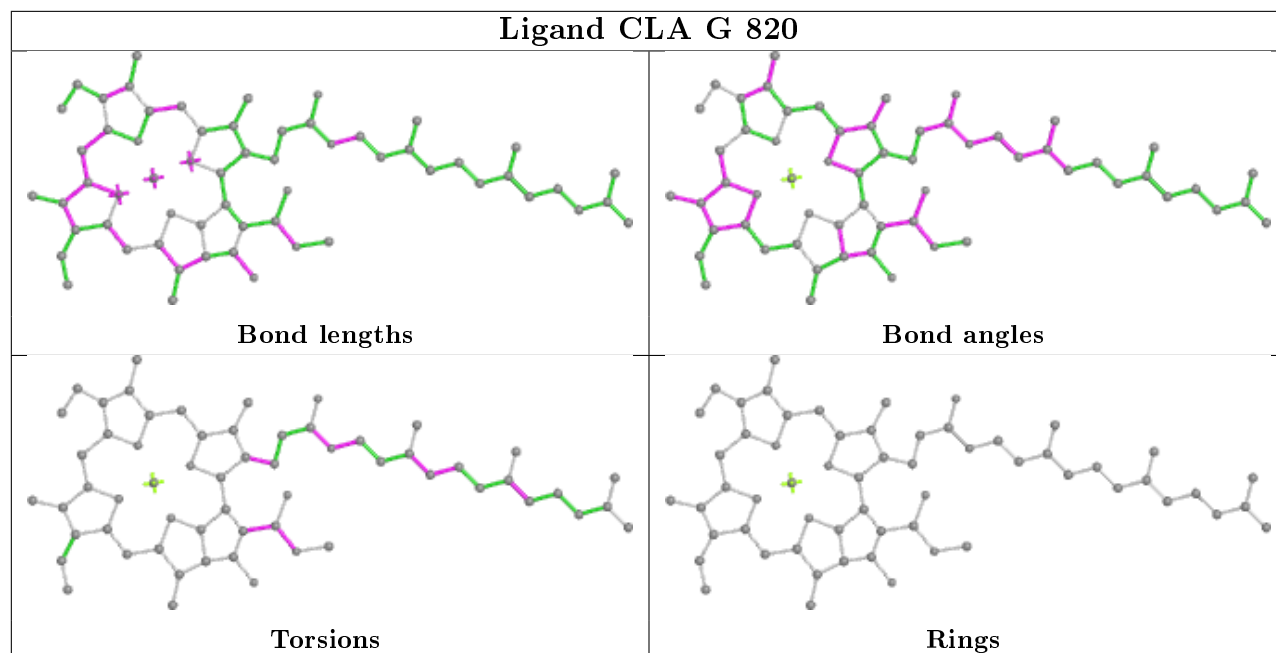
Rings



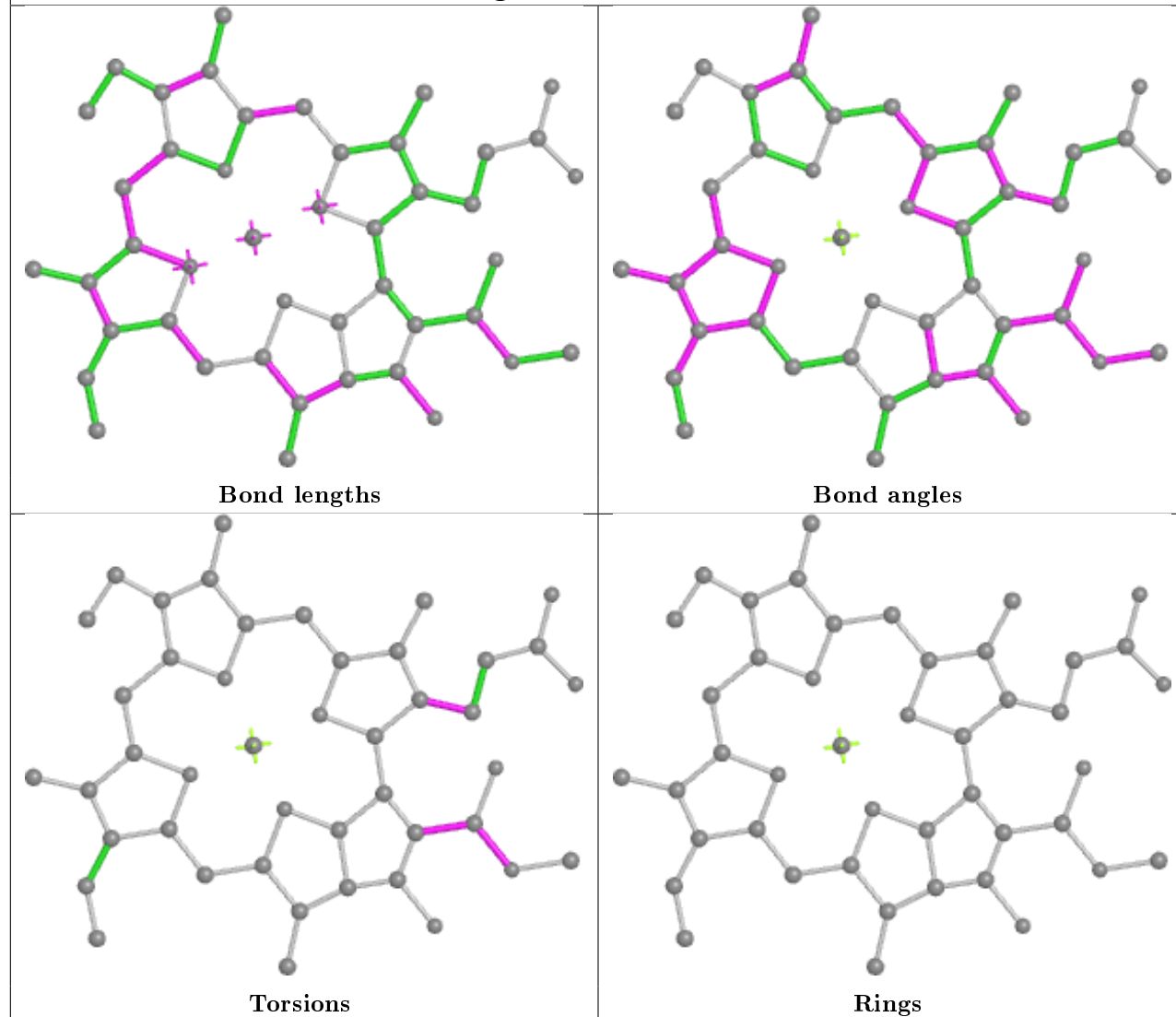
**Ligand CLA U 1002****Ligand CLA A 837**



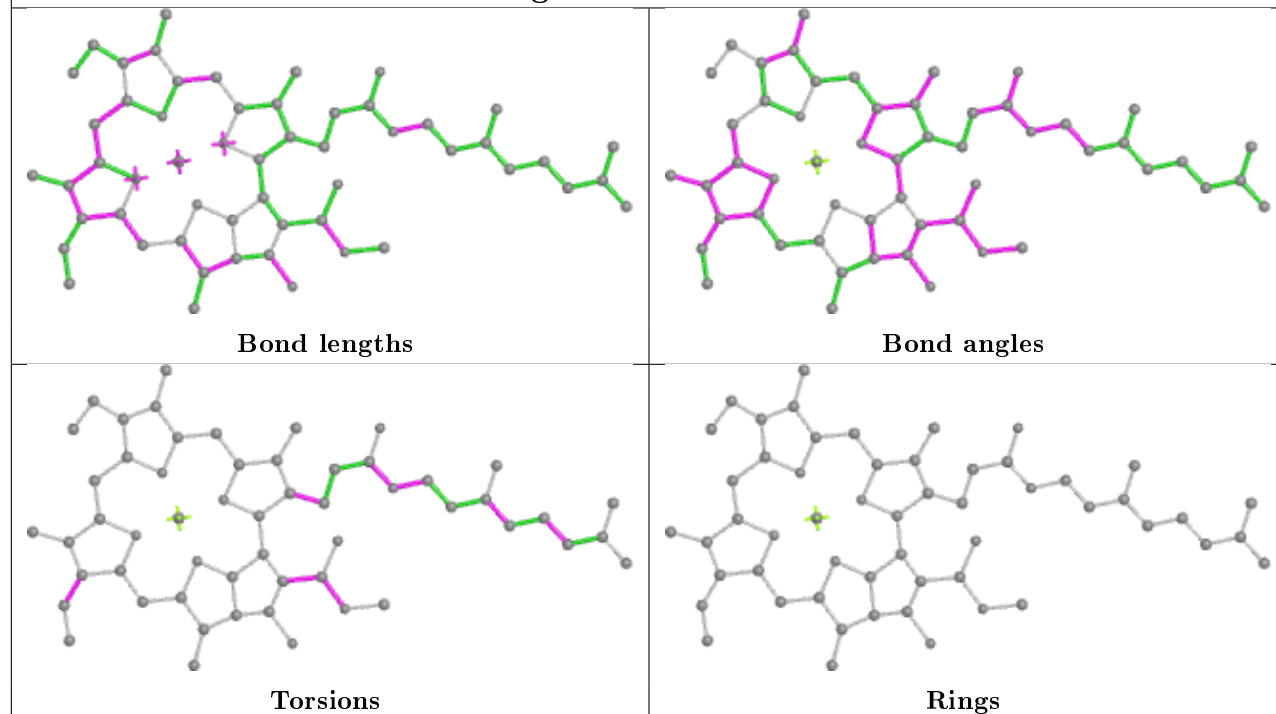




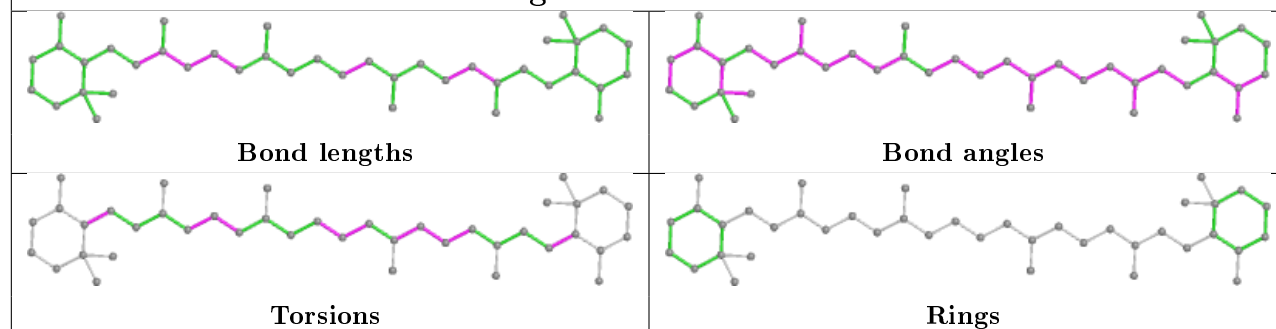
## Ligand CLA Z 834



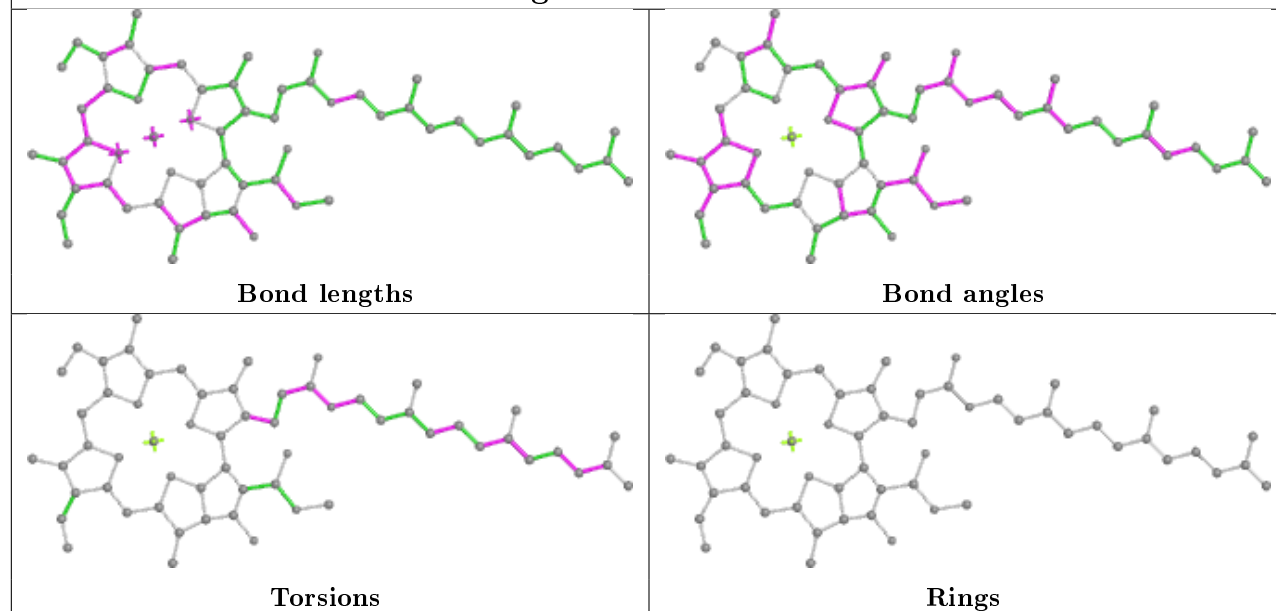
## Ligand CLA H 824



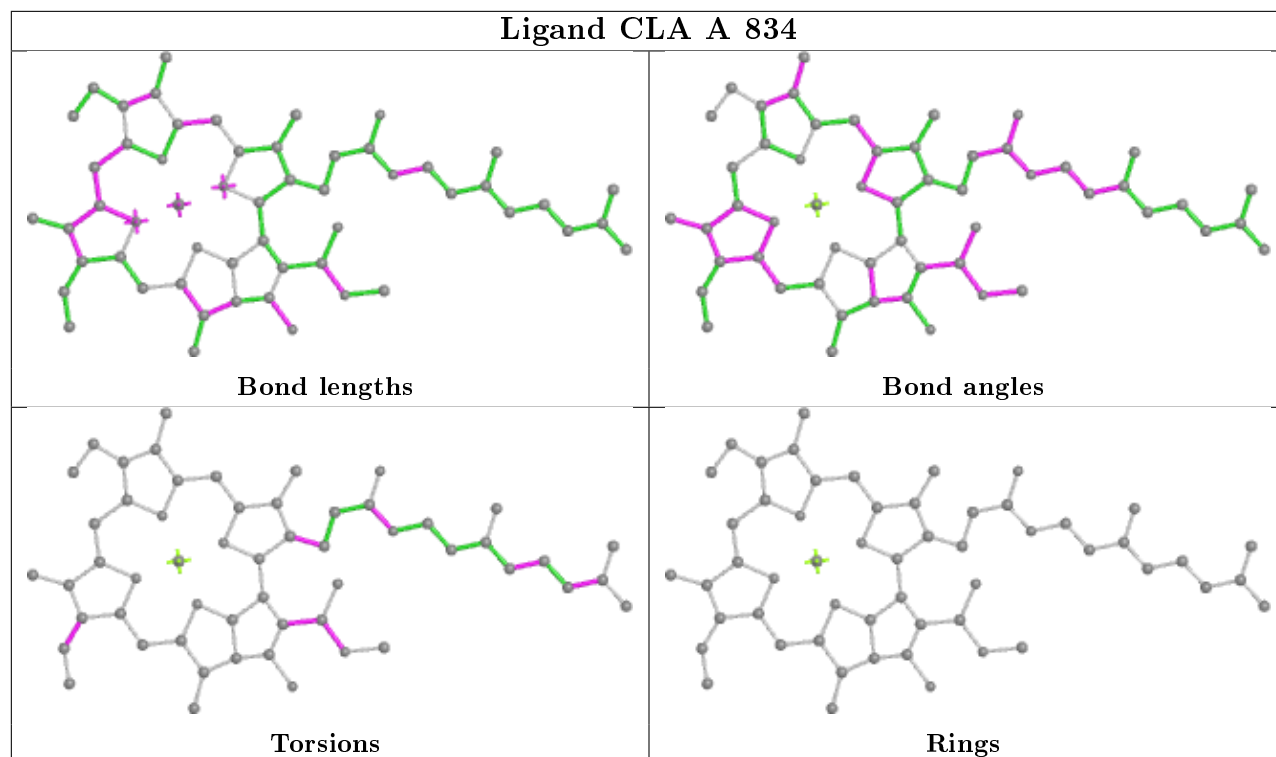
## Ligand BCR H 842



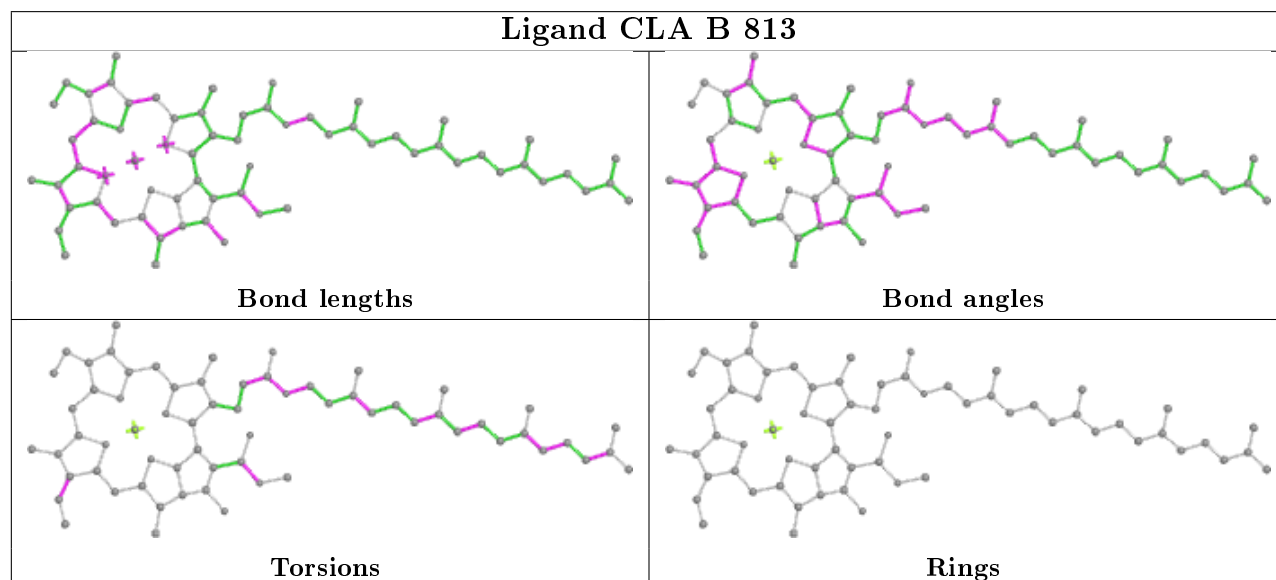
## Ligand CLA H 819



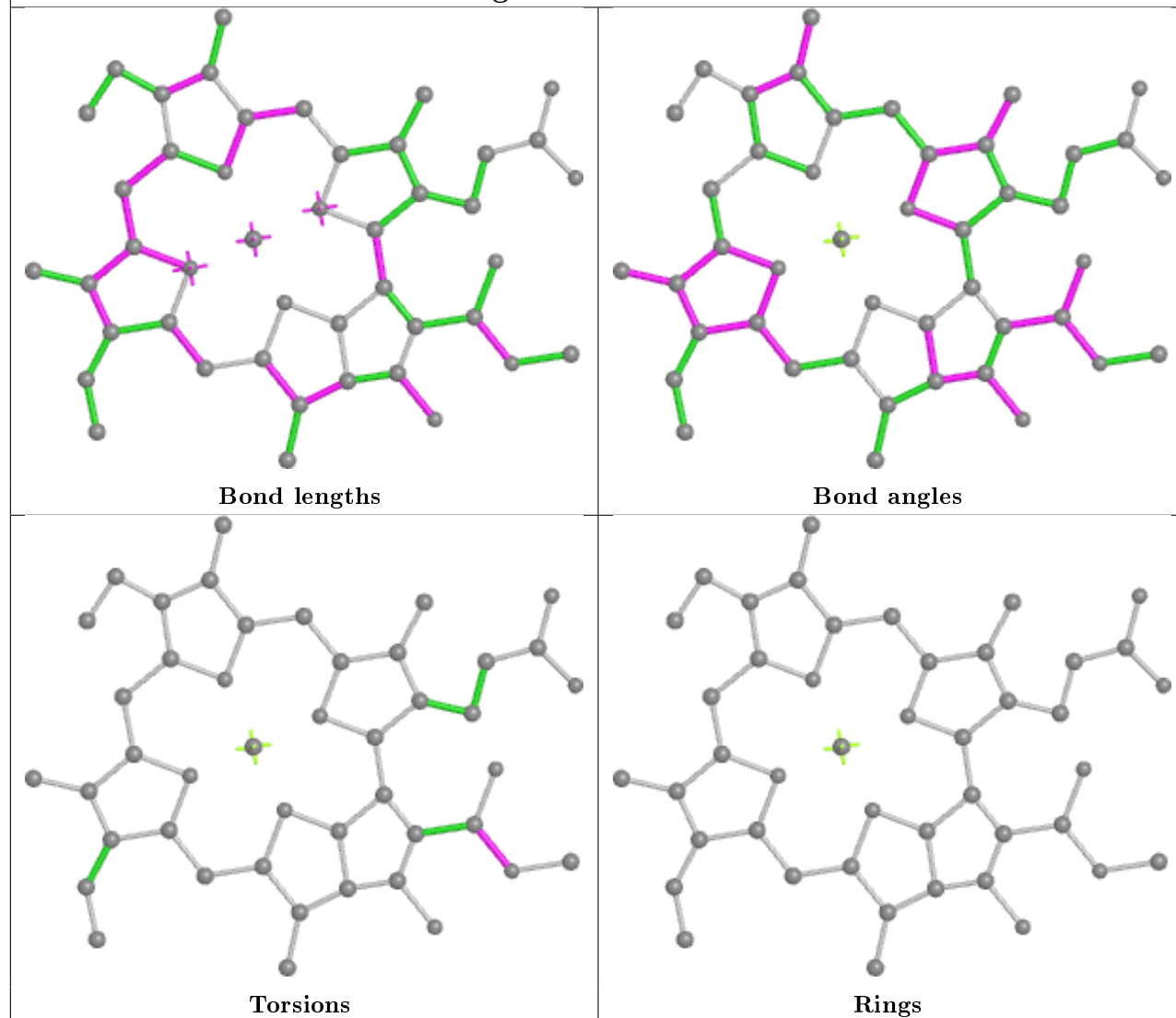
## Ligand CLA A 834



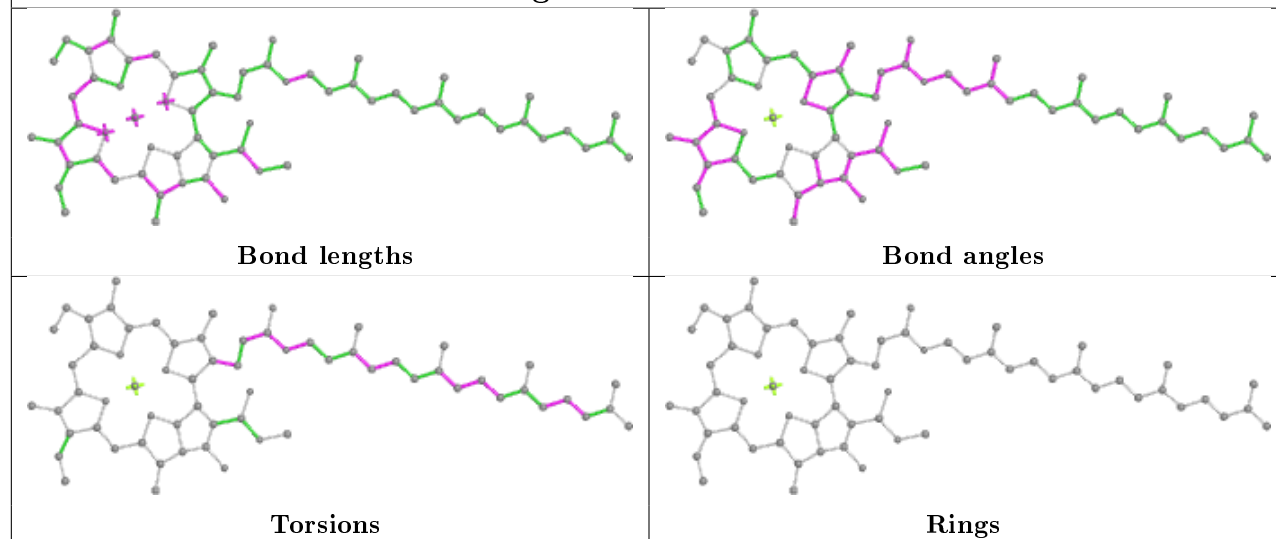
## Ligand CLA B 813



## Ligand CLA F 202

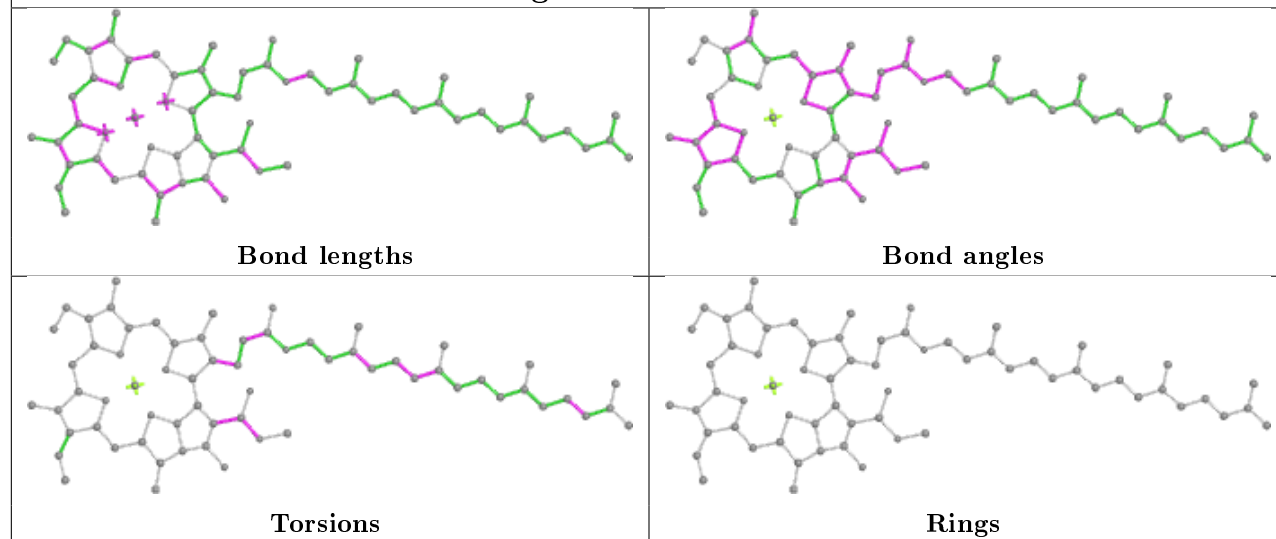


## Ligand CLA Y 805

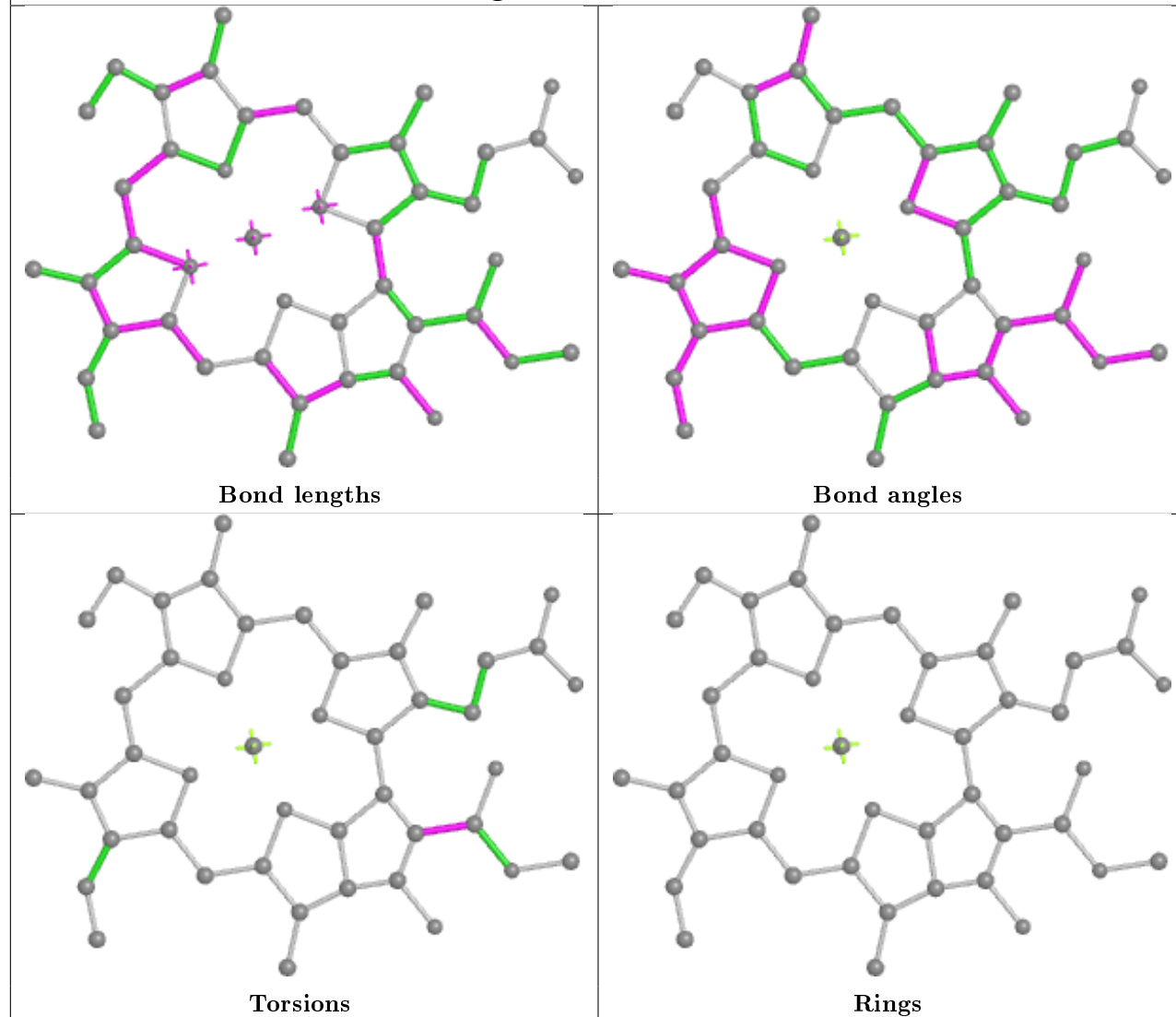


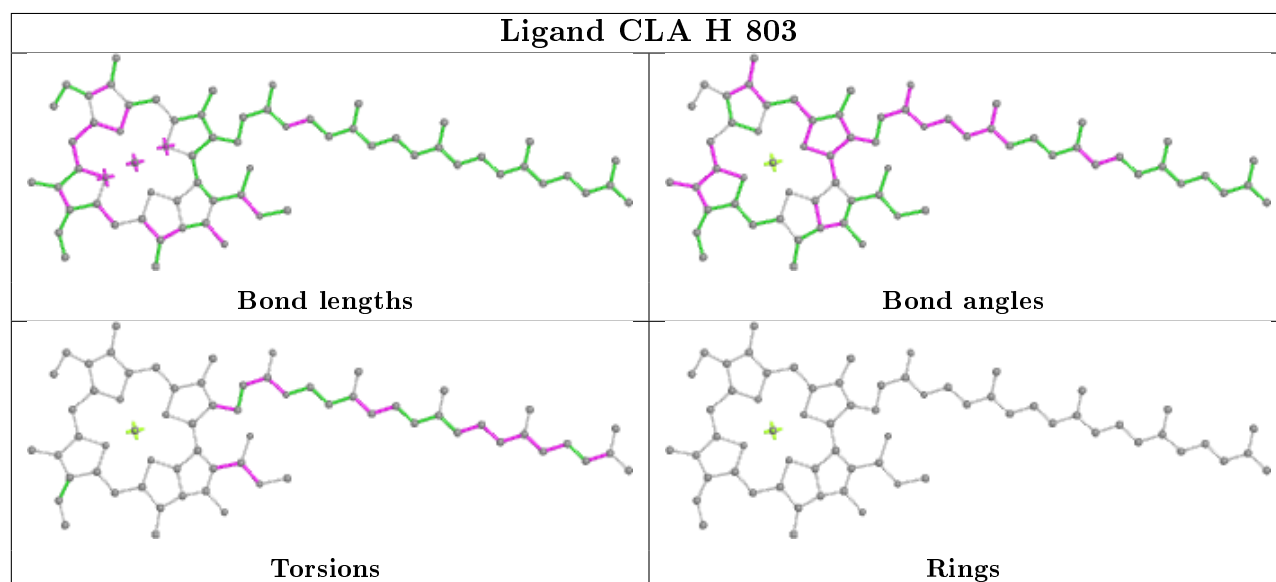
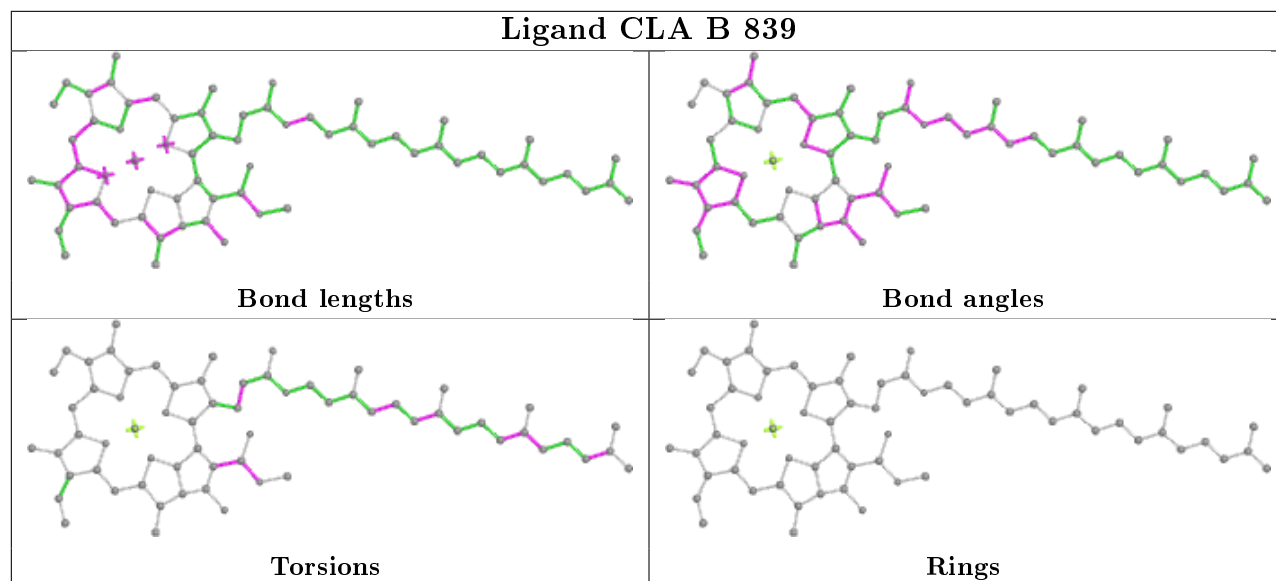
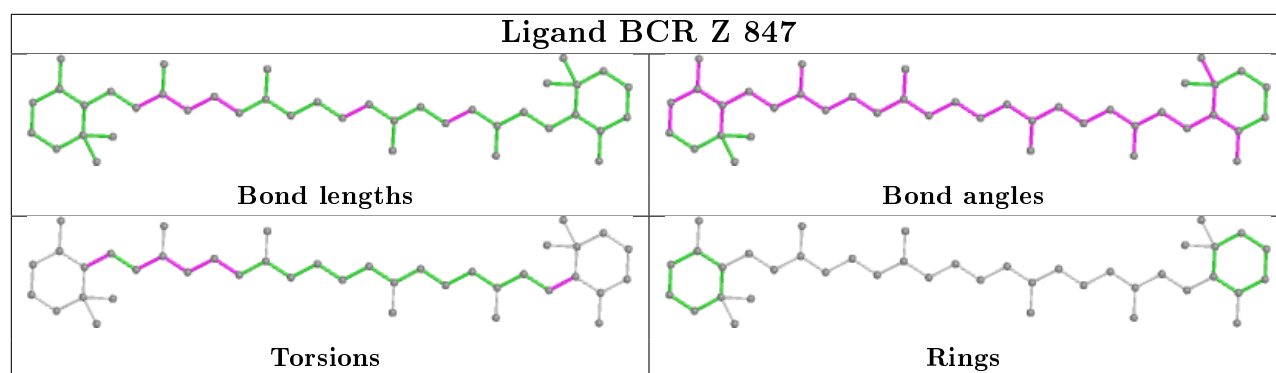


## Ligand CLA G 830

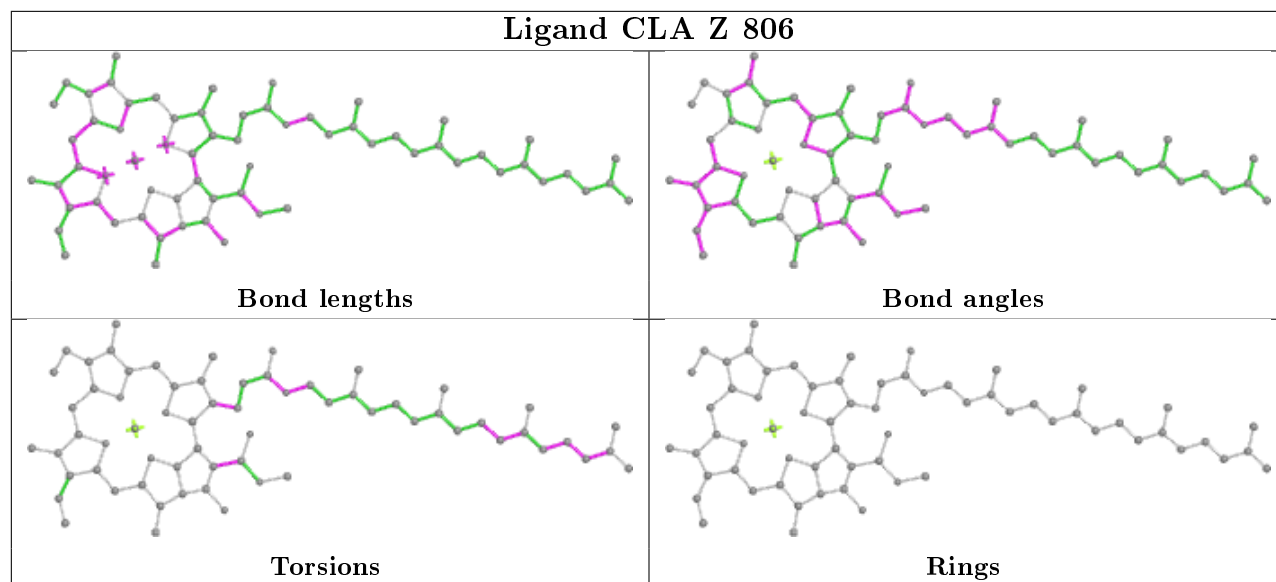


## Ligand CLA H 838

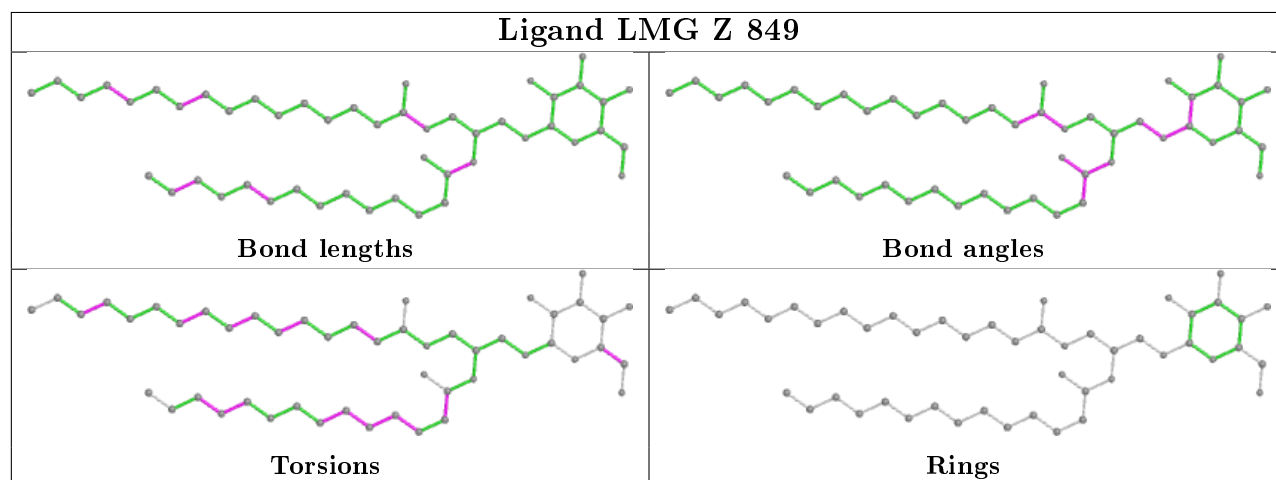


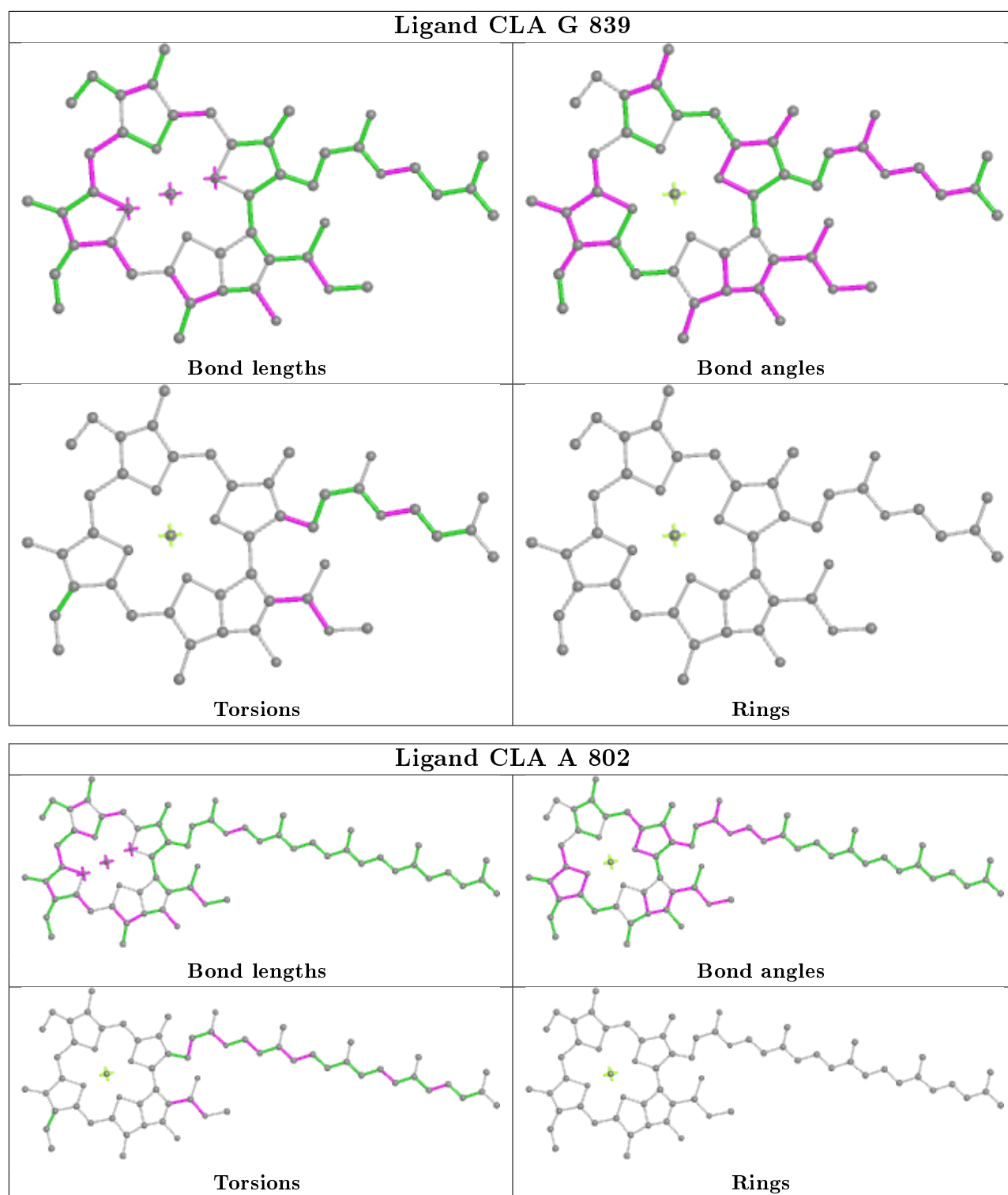


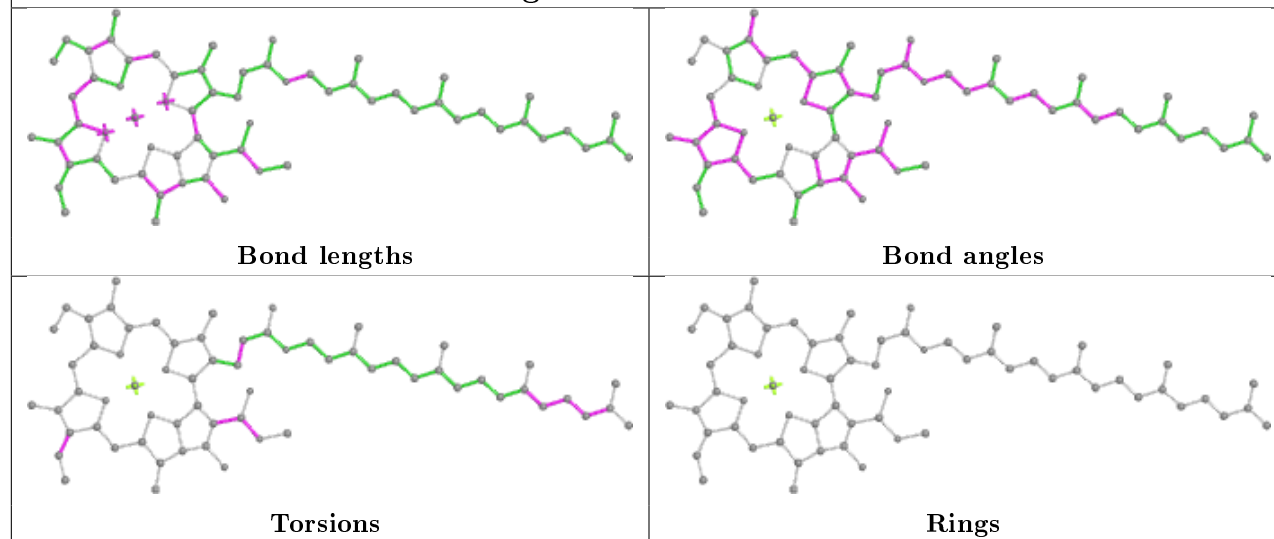
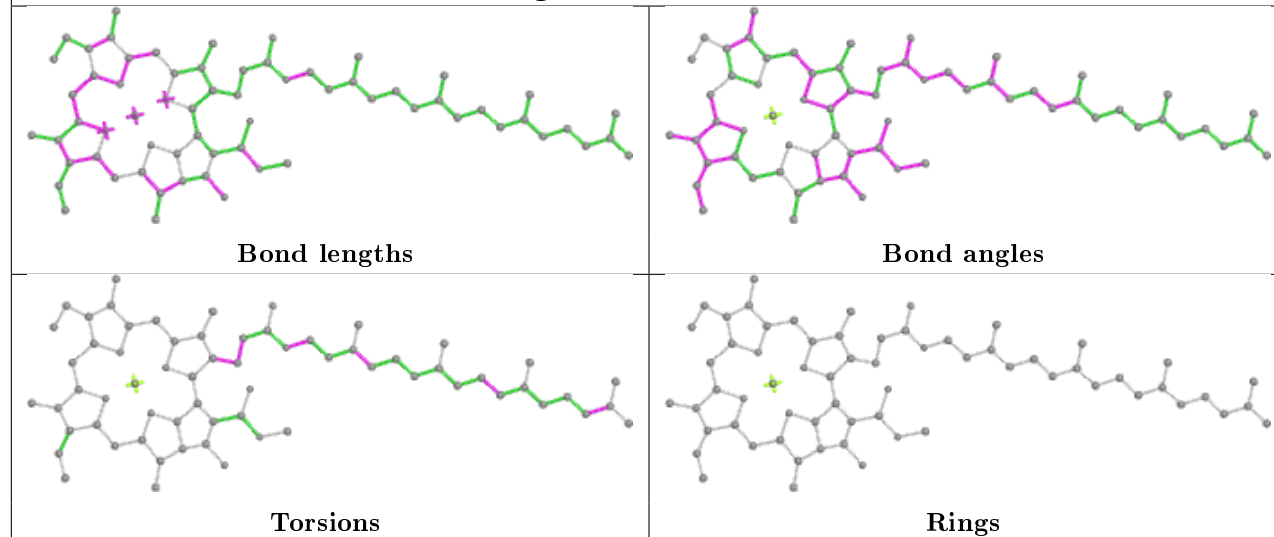
## Ligand CLA Z 806



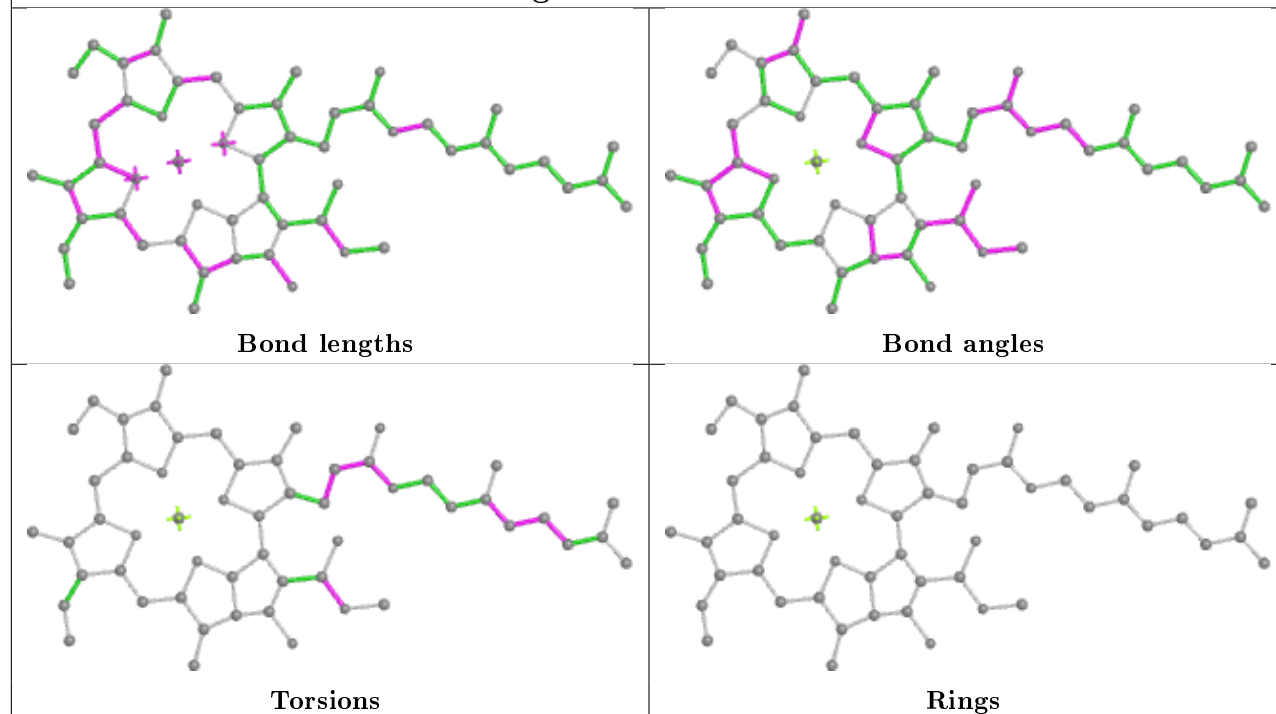
## Ligand LMG Z 849



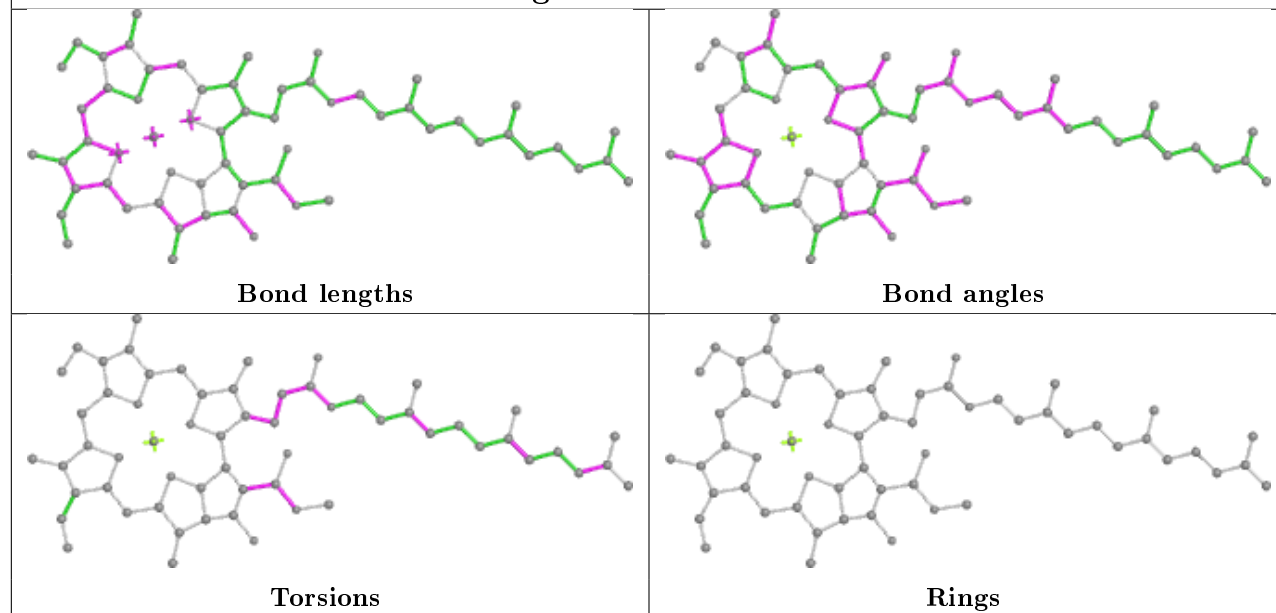


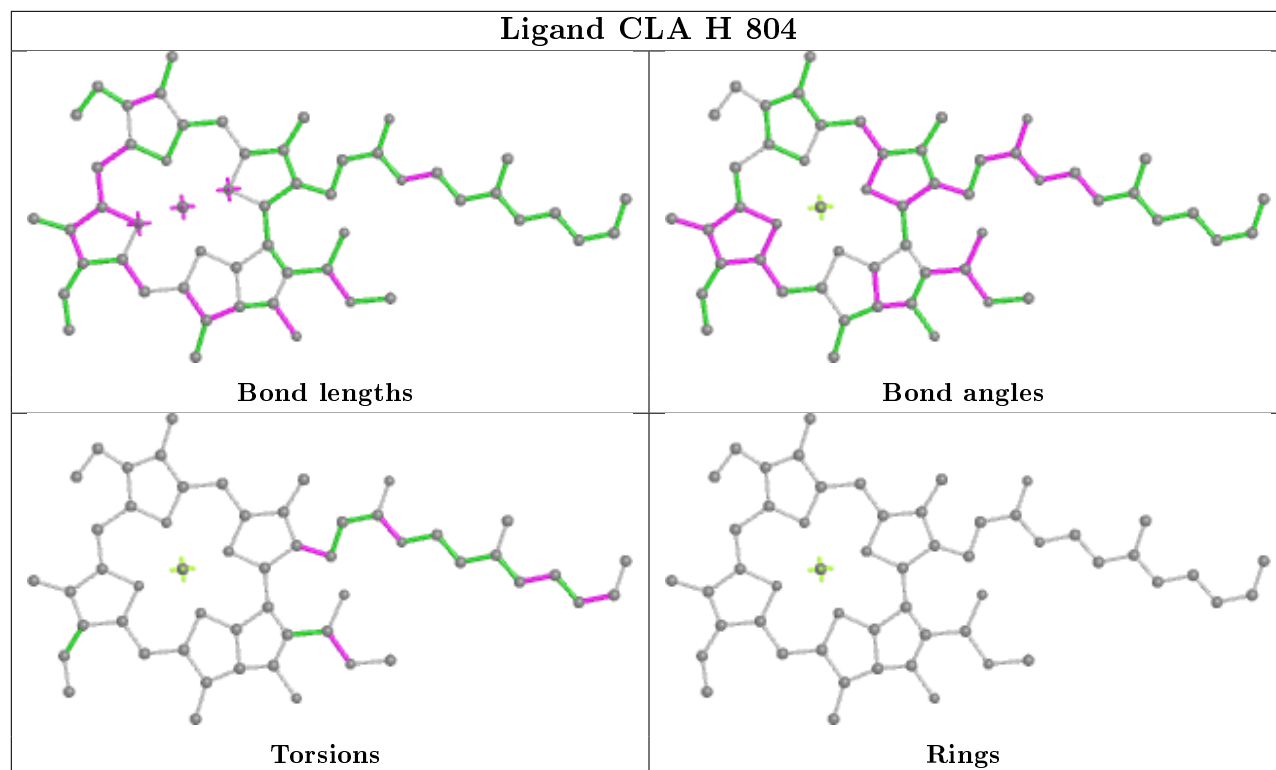
**Ligand CLA U 1007****Ligand CLA Y 802**

## Ligand CLA B 821

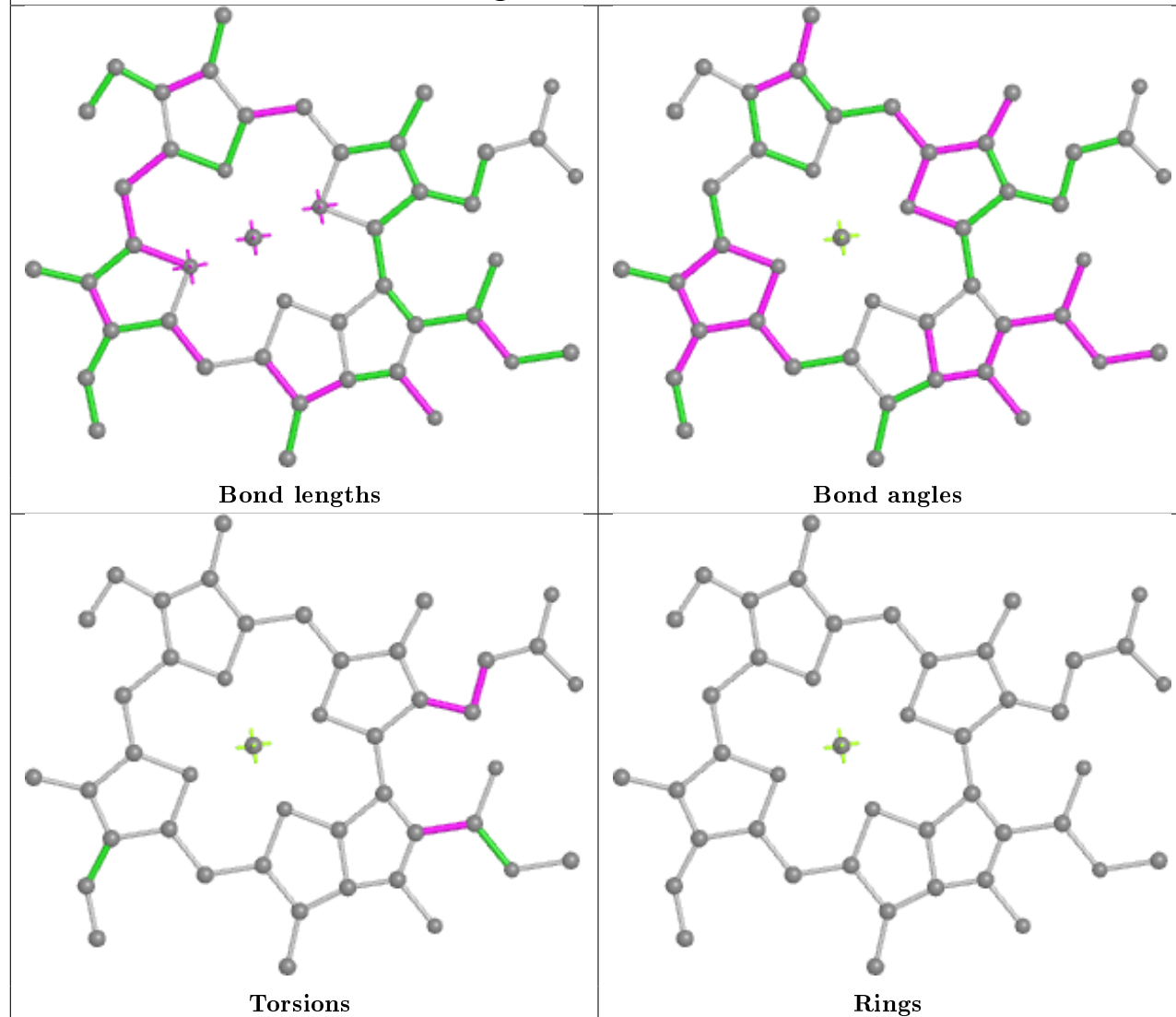


## Ligand CLA A 821



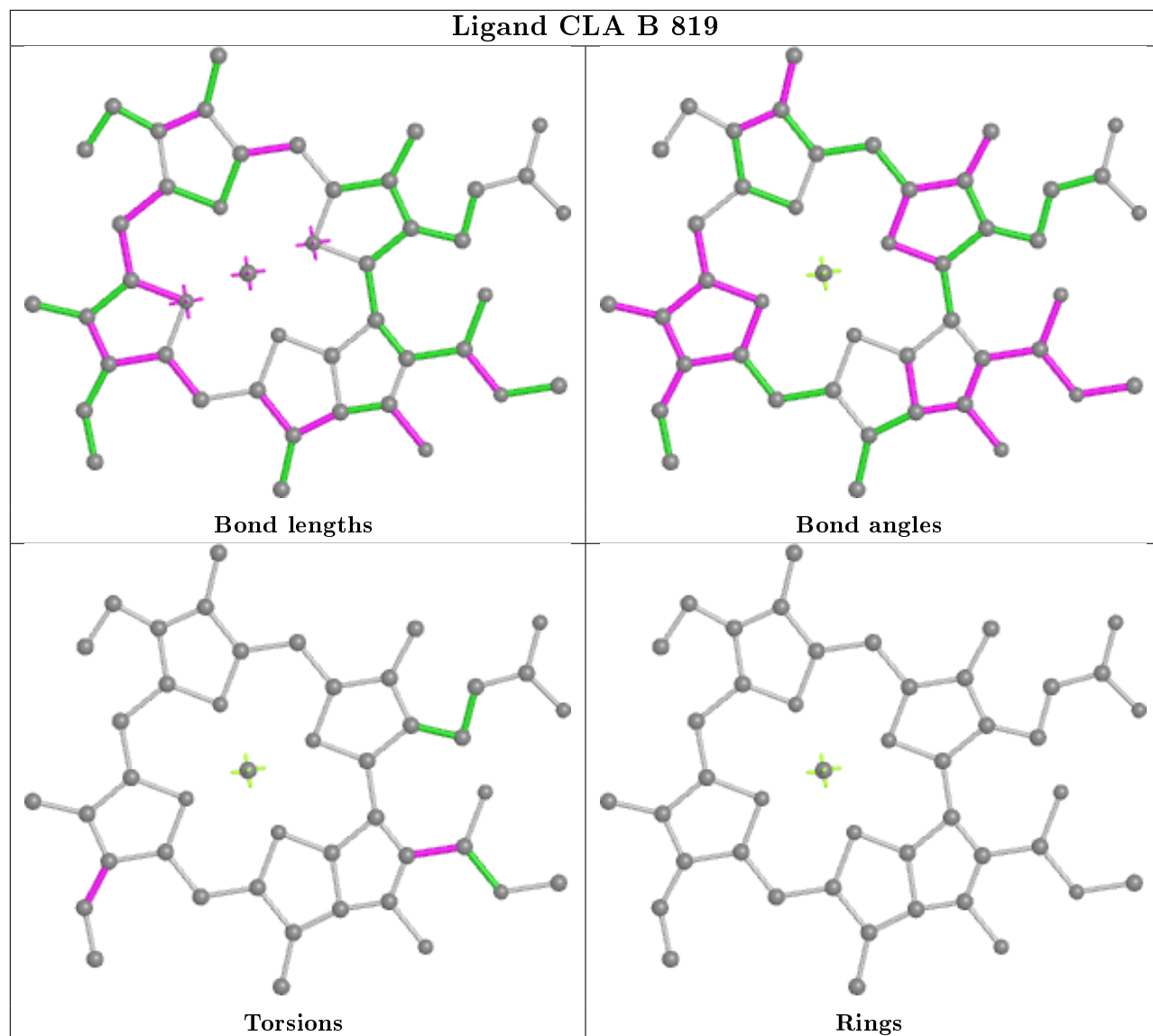


## Ligand CLA Z 821

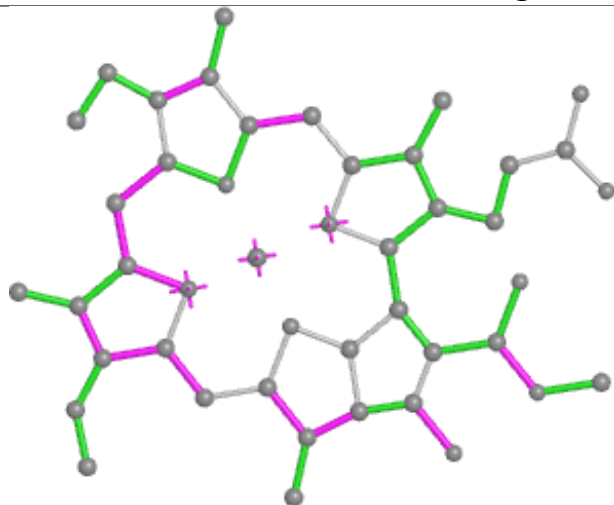




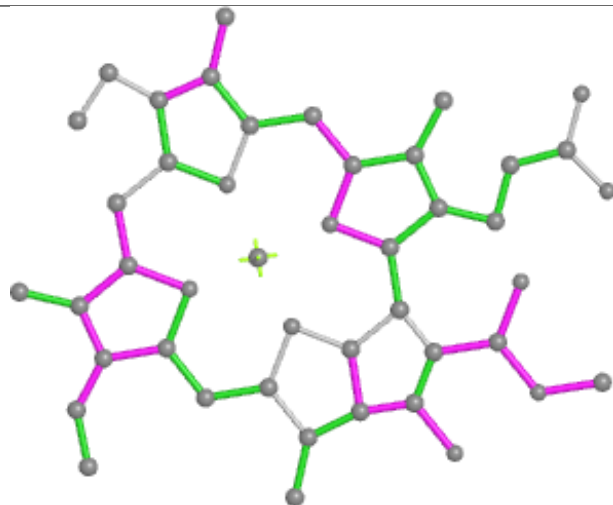
## Ligand CLA B 819



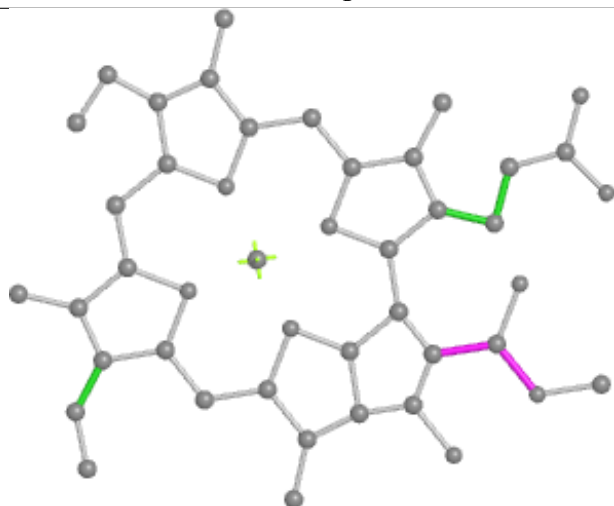
## Ligand CLA H 821



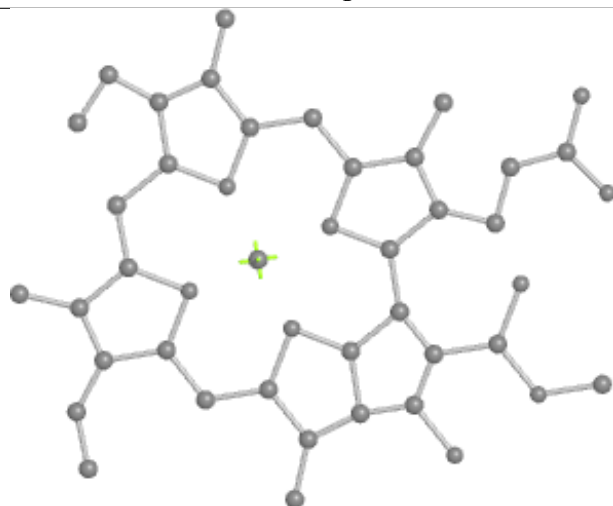
Bond lengths



Bond angles

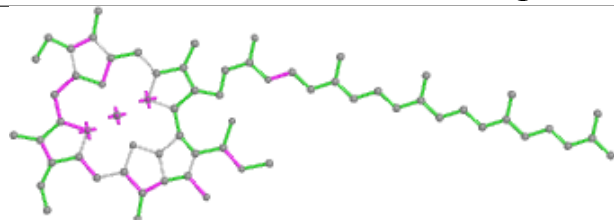


Torsions

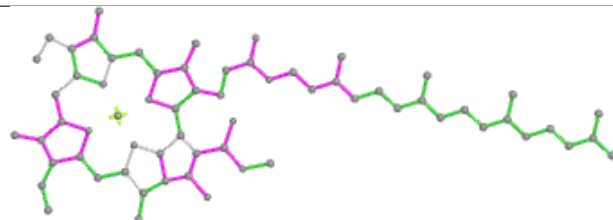


Rings

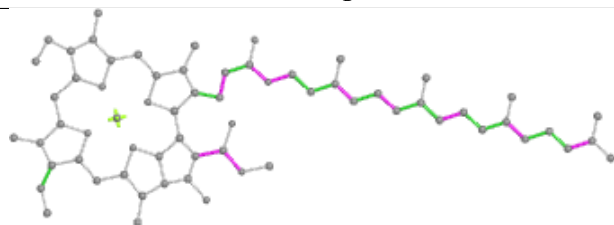
## Ligand CLA A 842



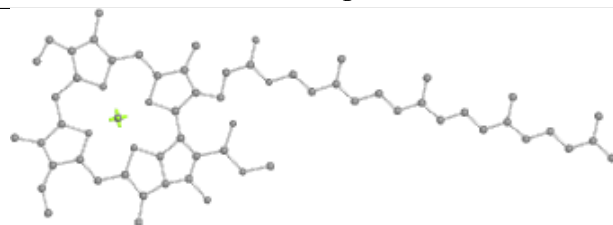
Bond lengths



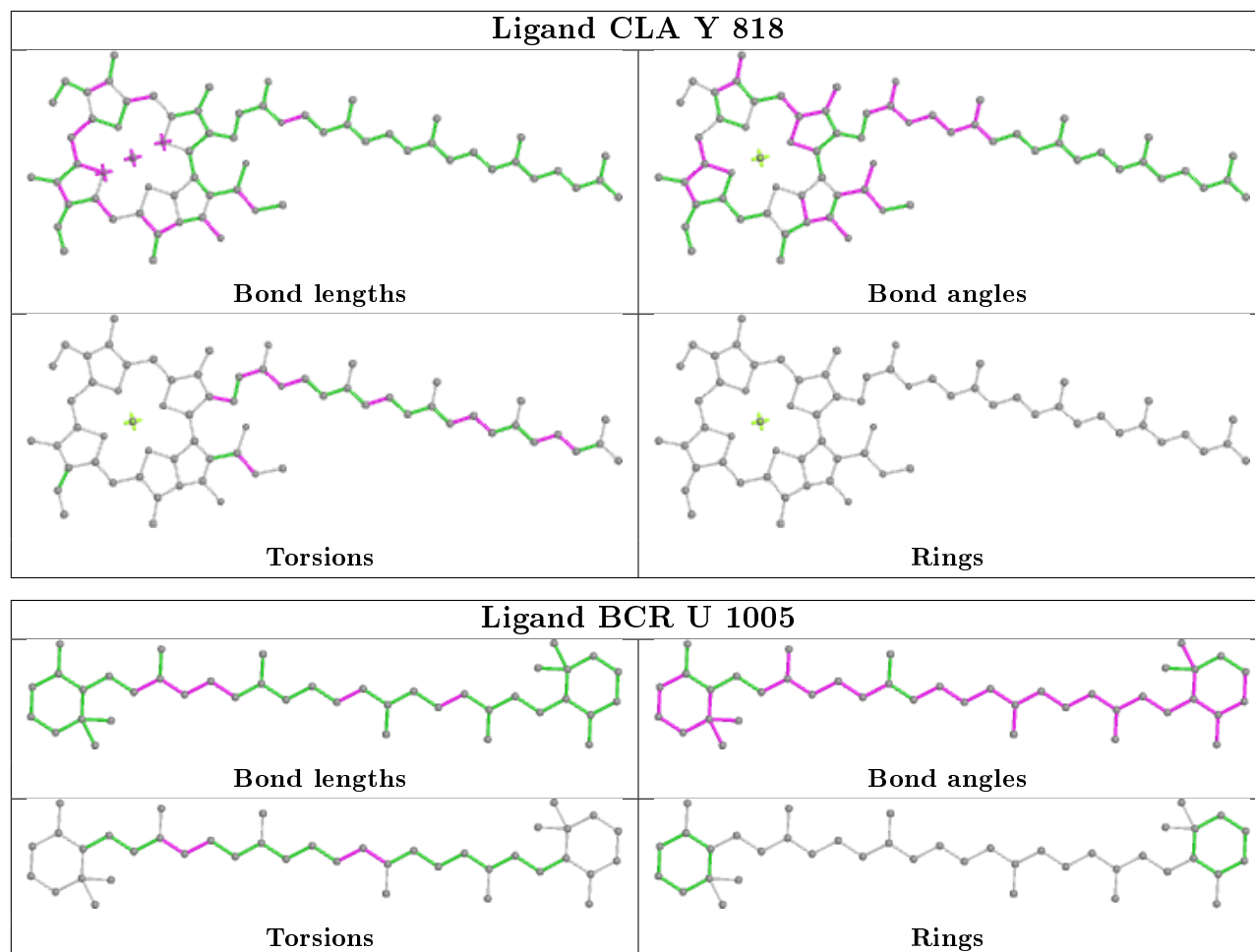
Bond angles

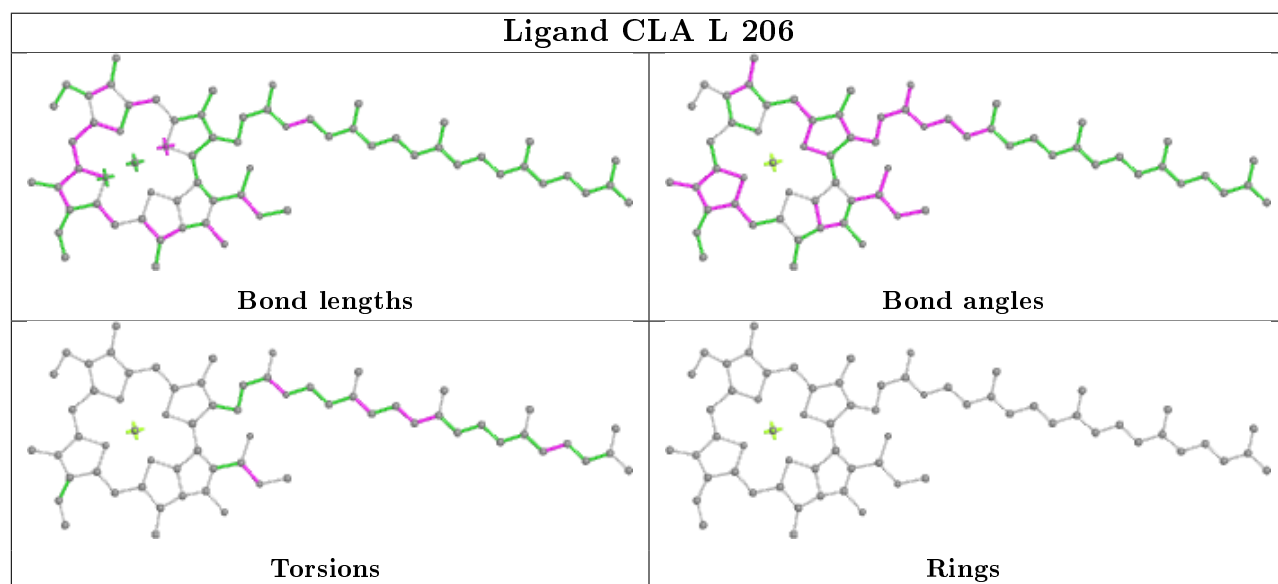
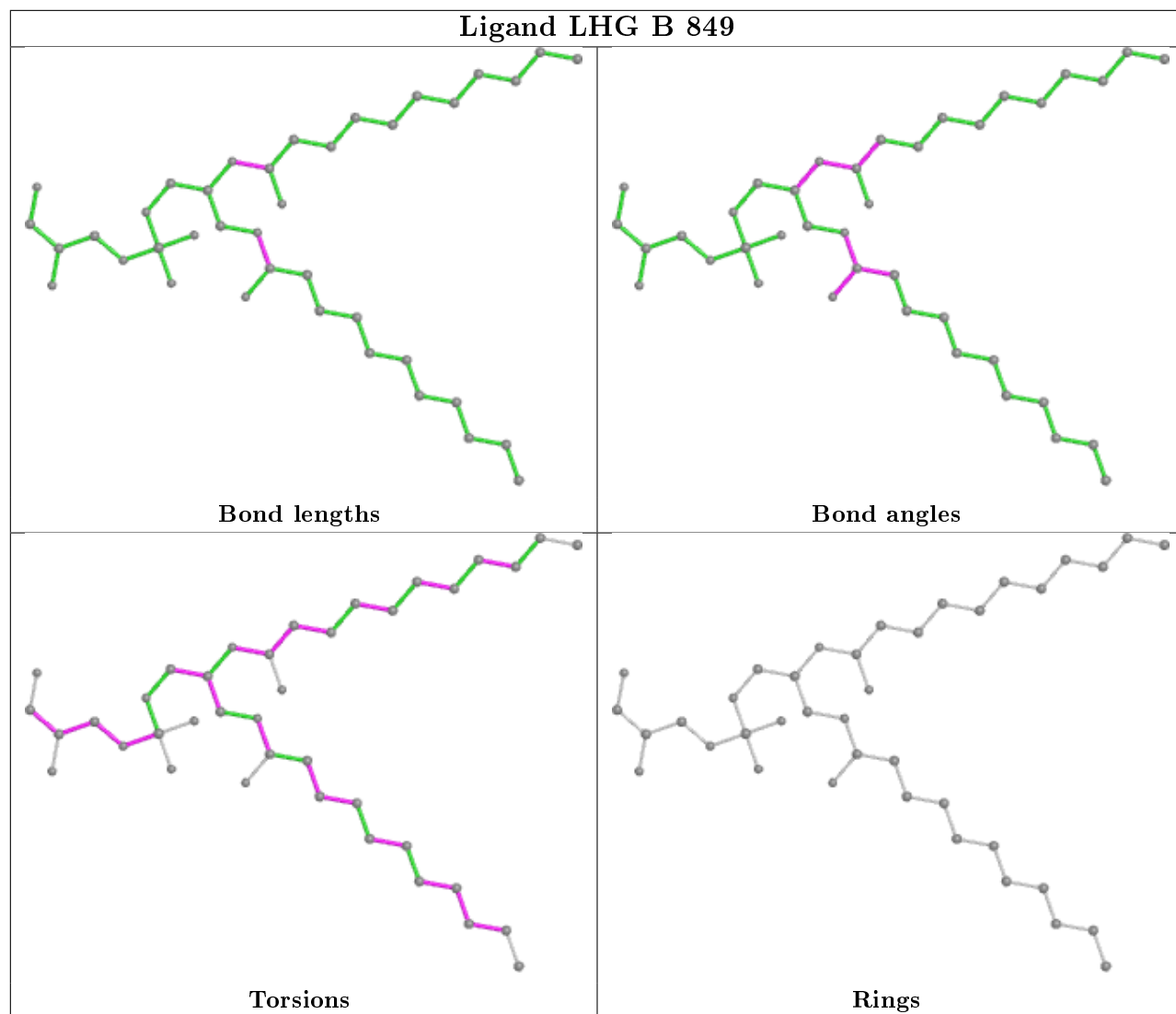


Torsions

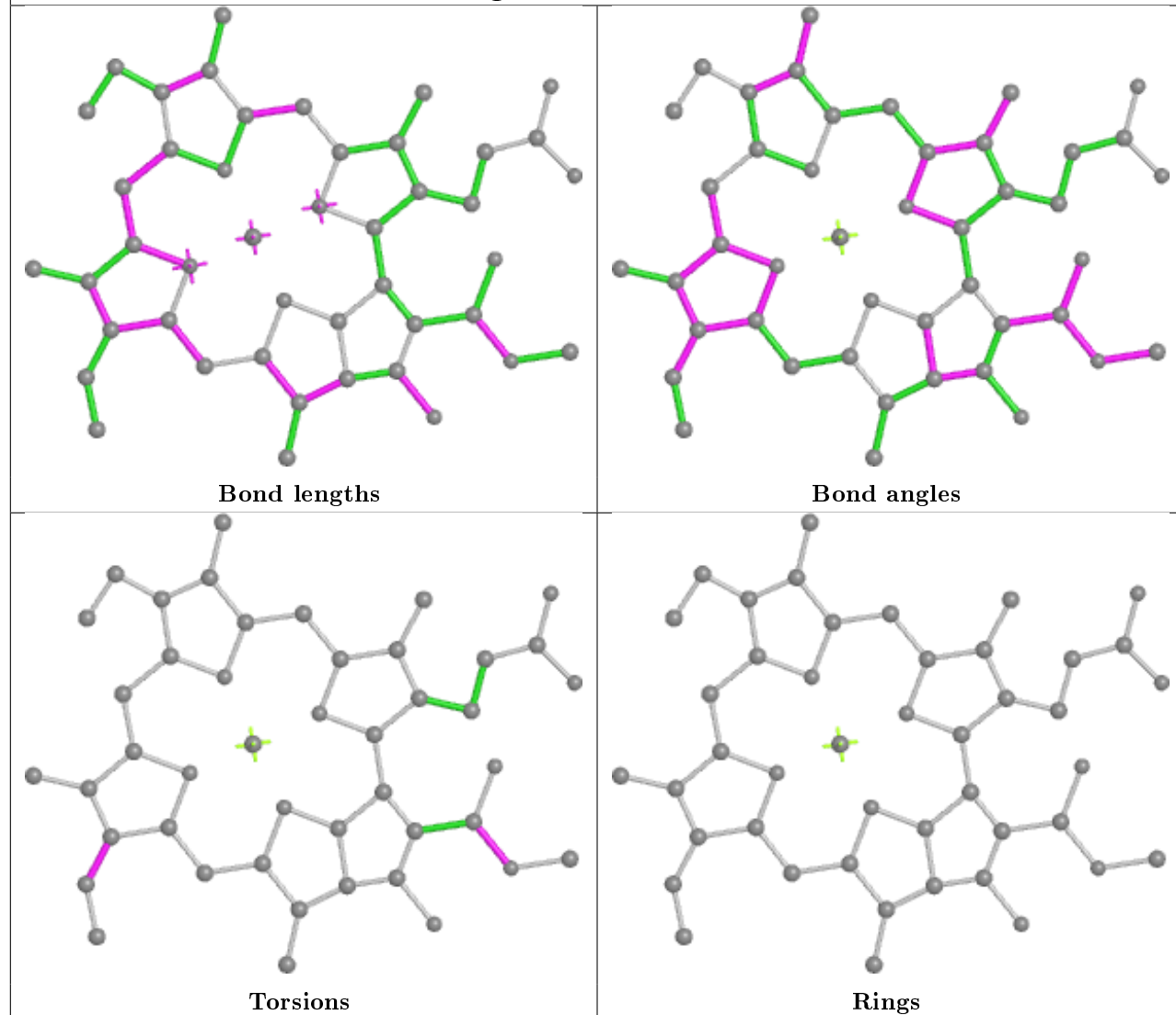


Rings

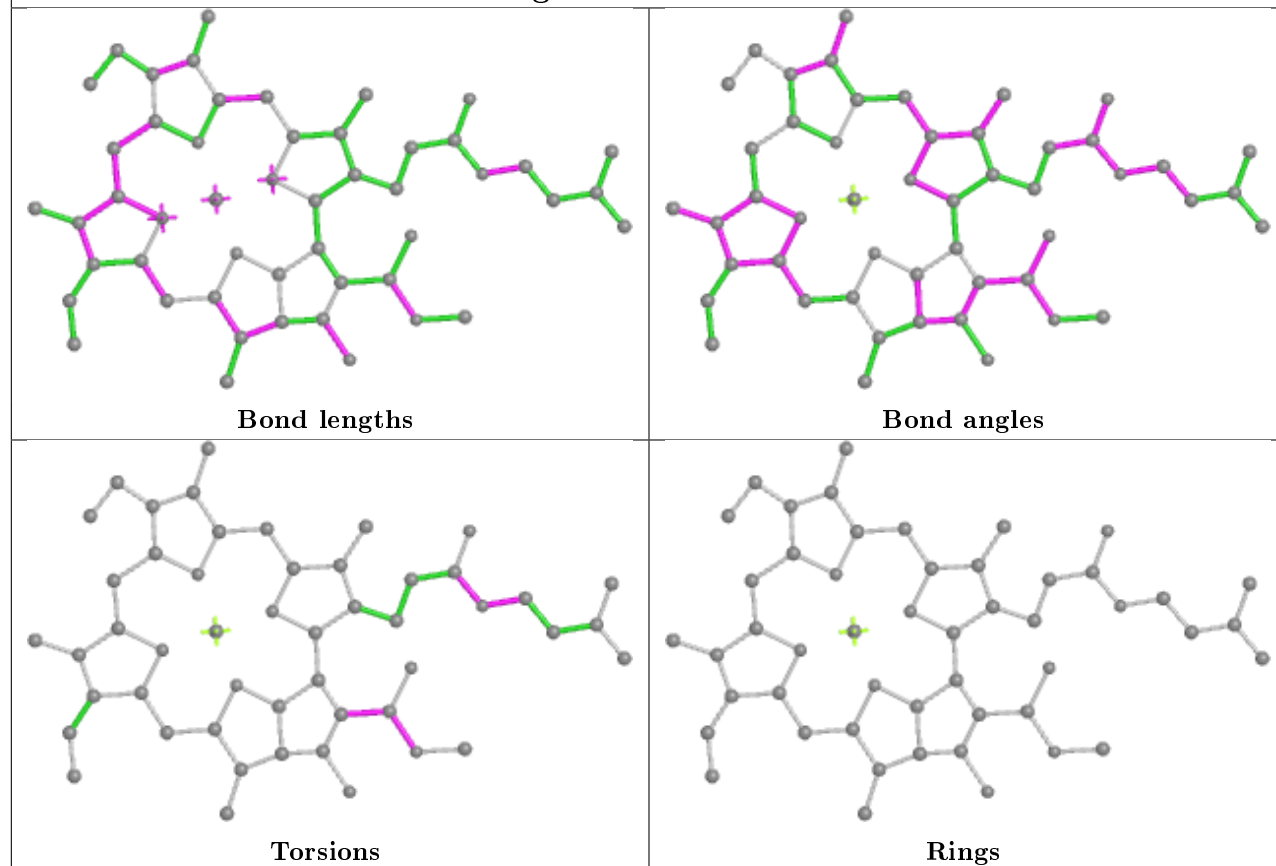




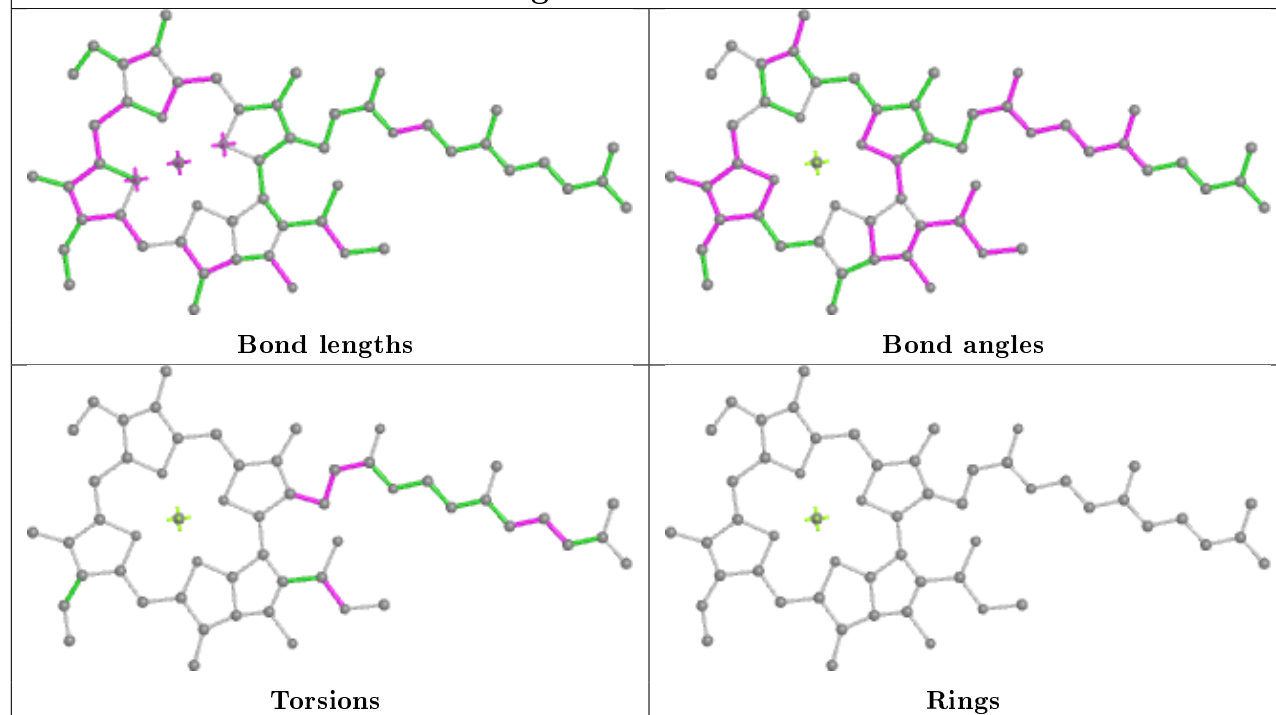
## Ligand CLA H 812



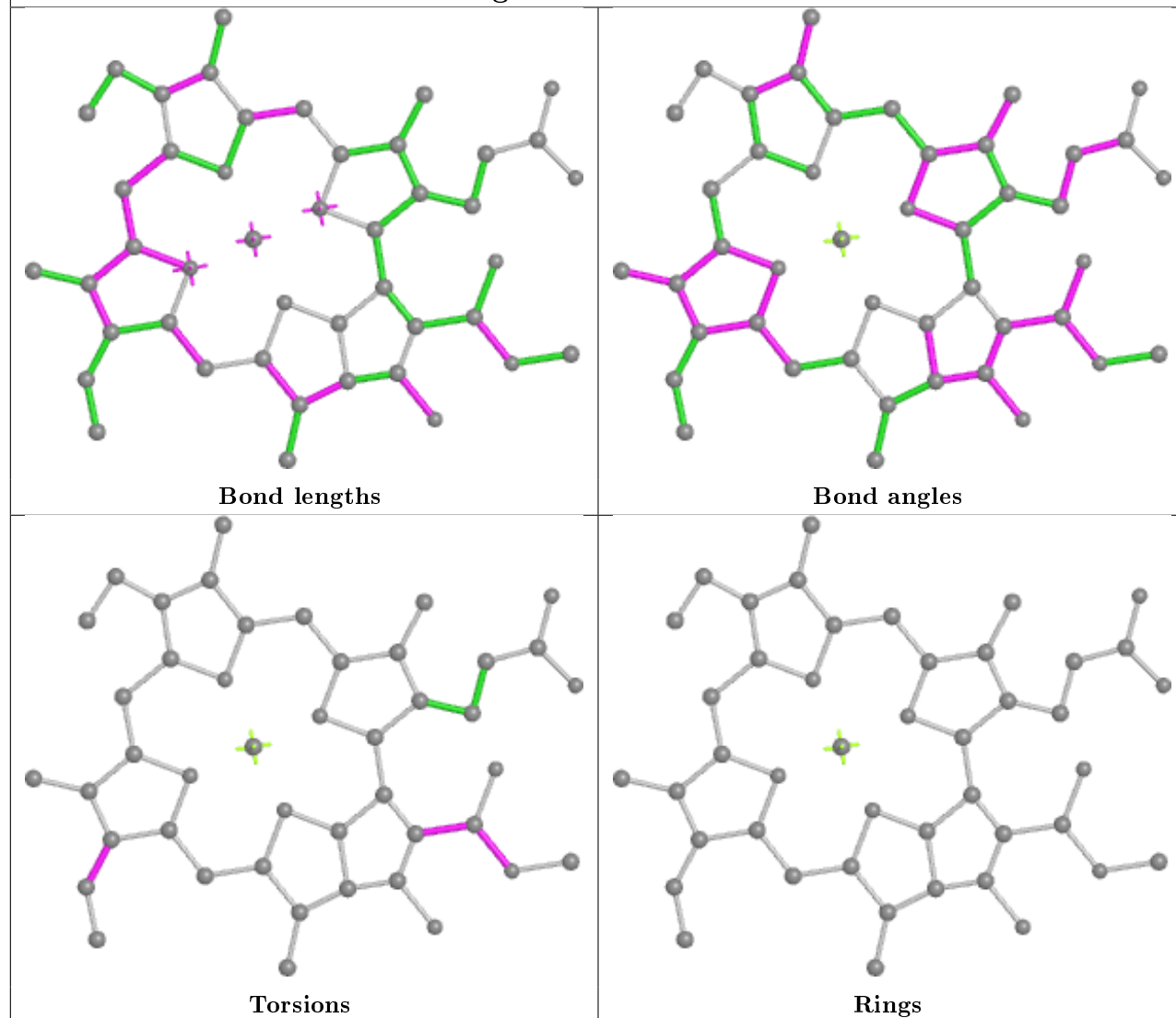
## Ligand CLA A 816



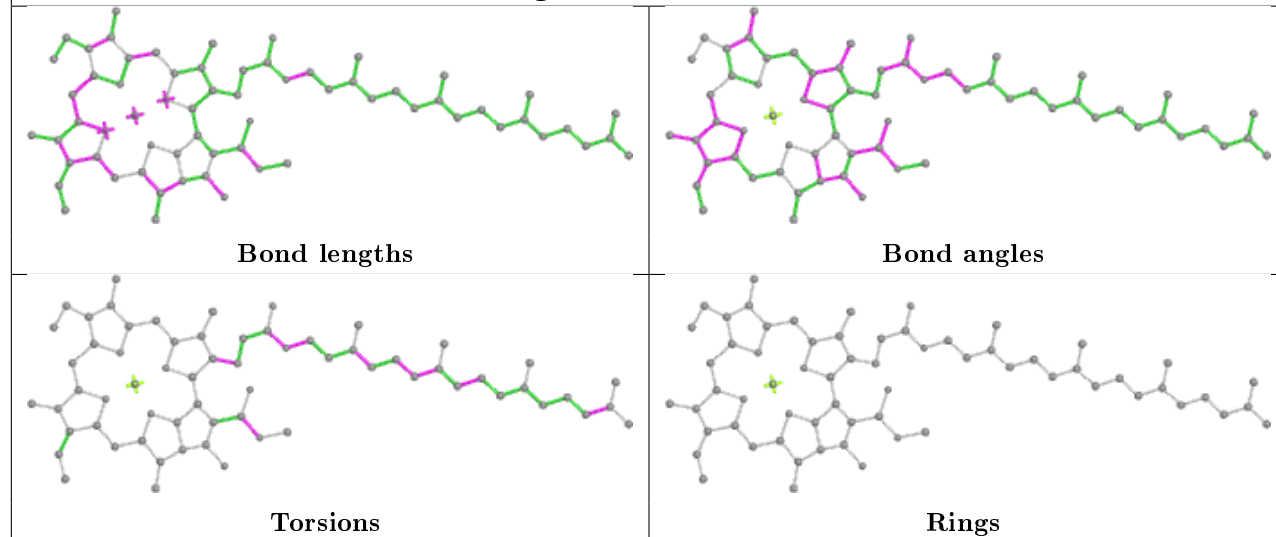
## Ligand CLA H 811

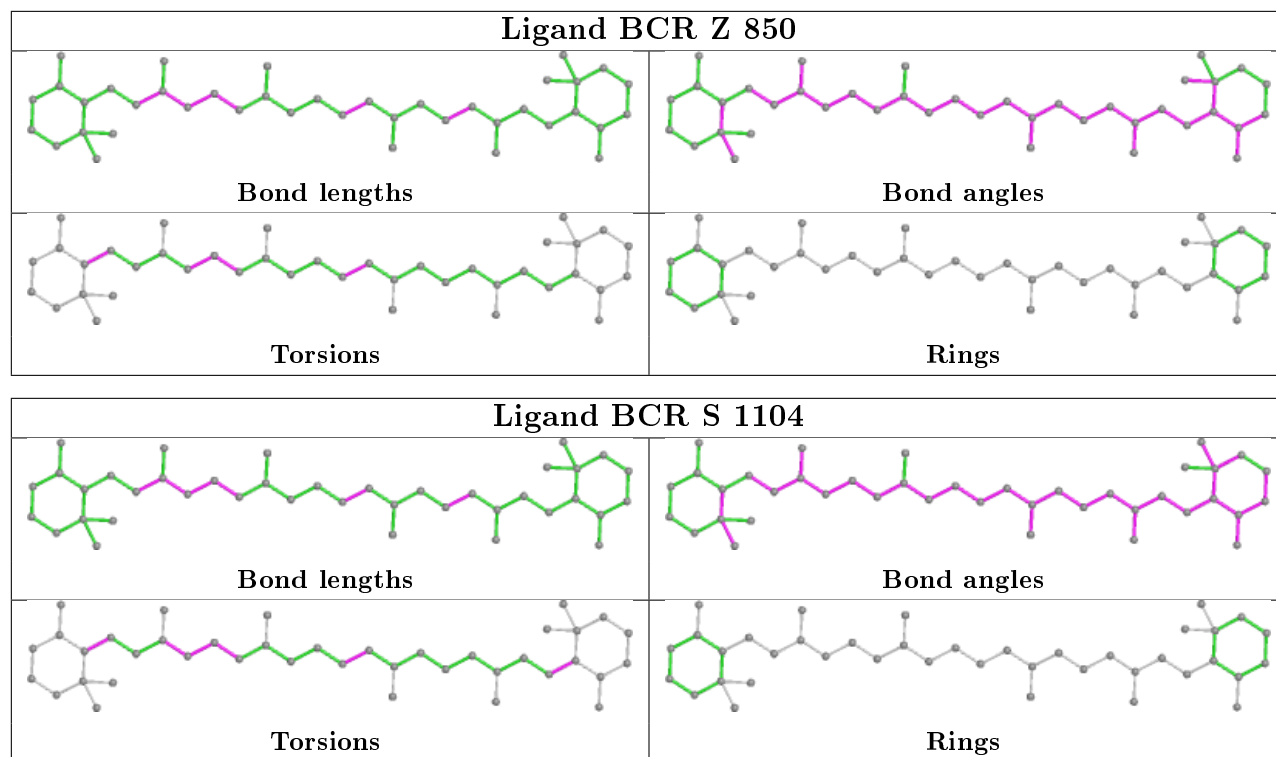


## Ligand CLA Z 836



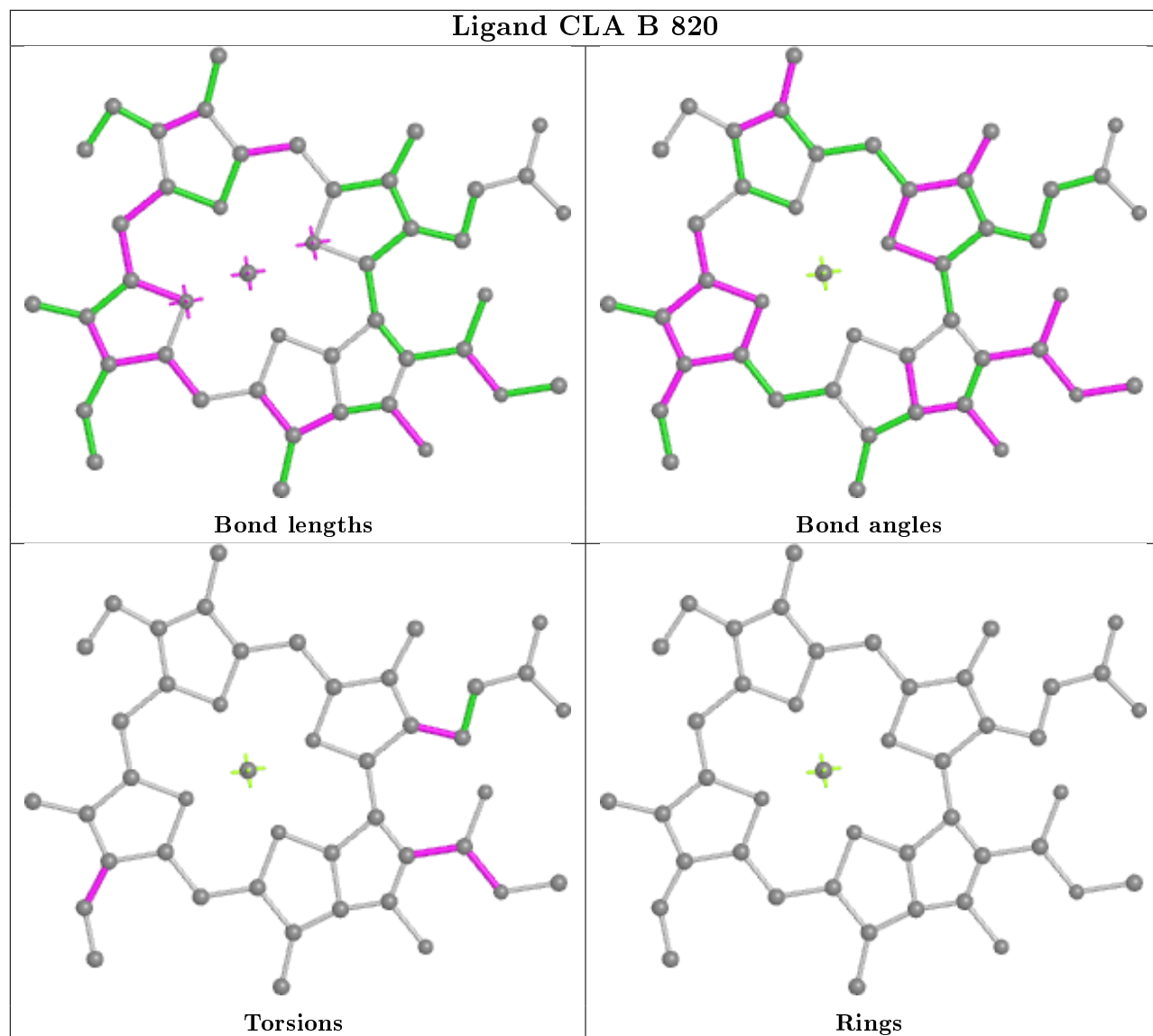
## Ligand CLA Y 803



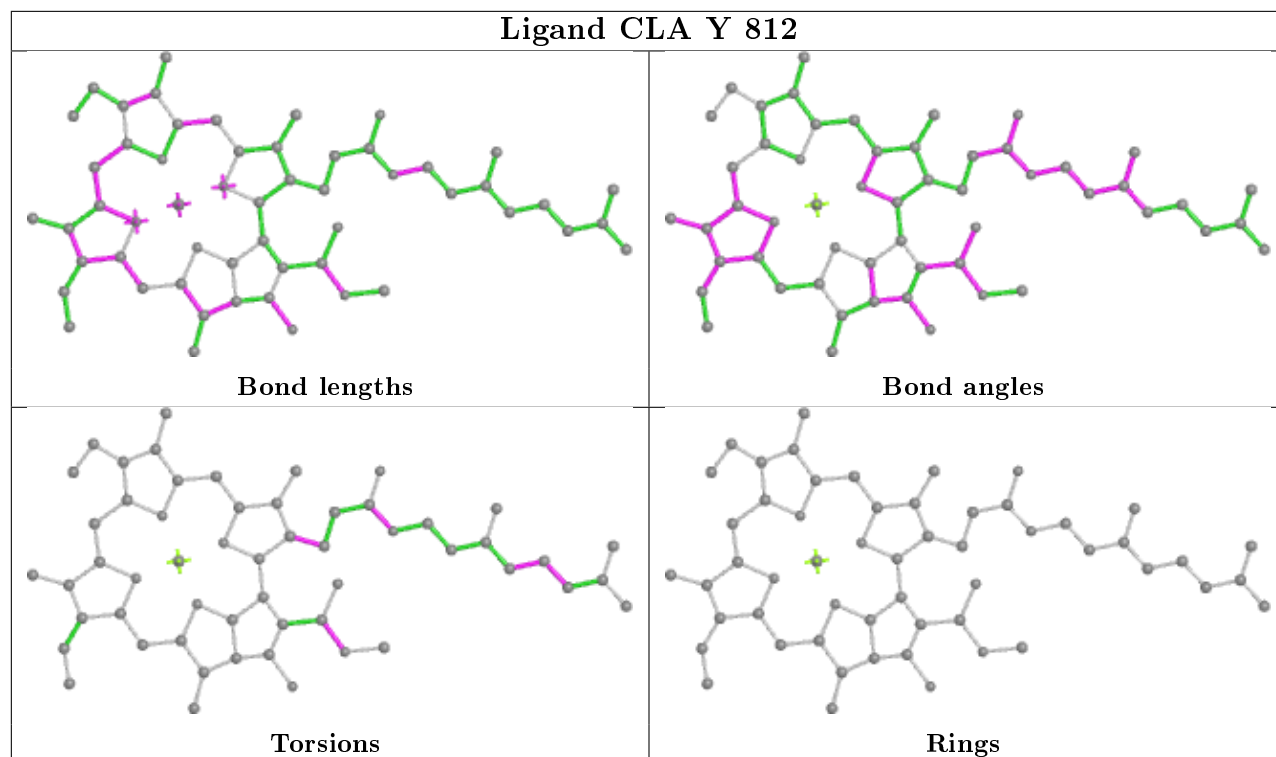




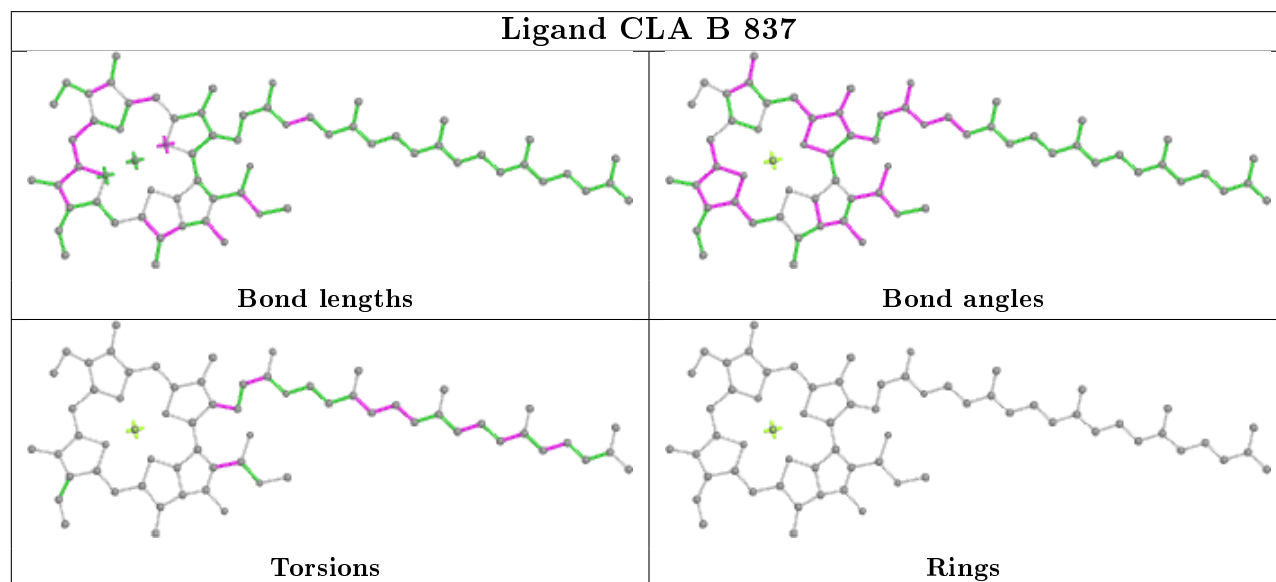
## Ligand CLA B 820



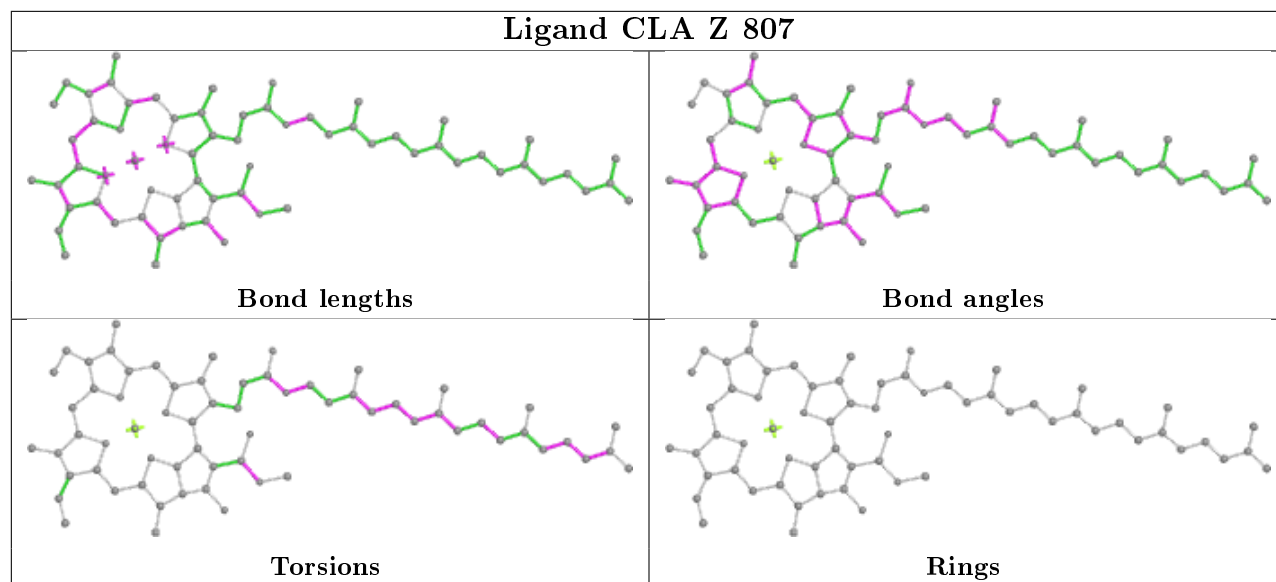
## Ligand CLA Y 812



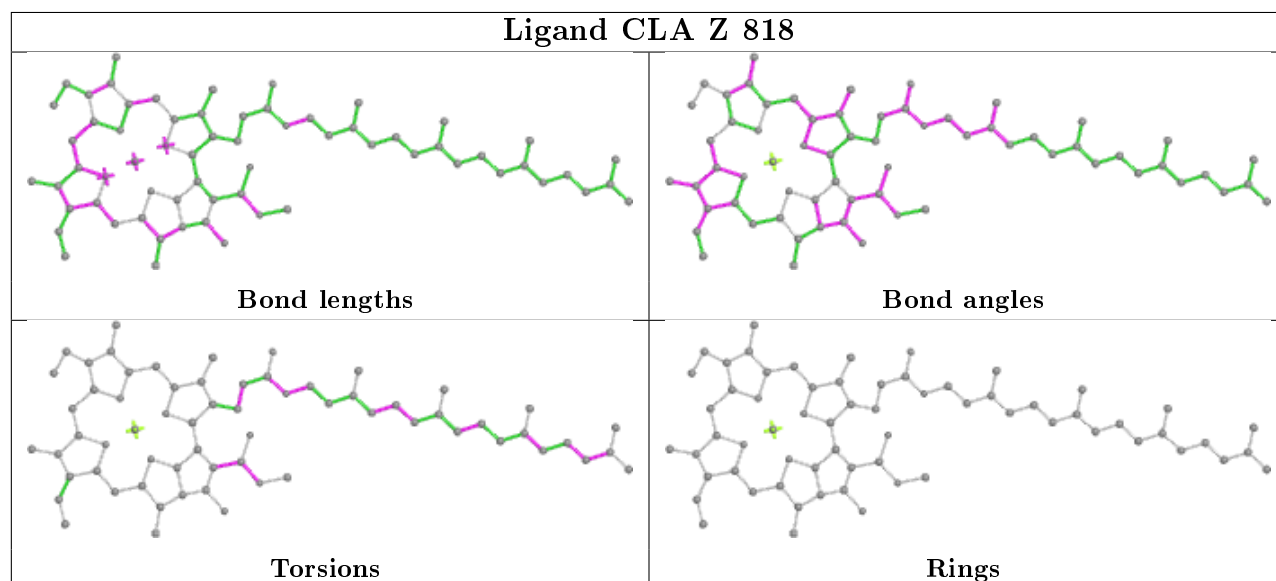
## Ligand CLA B 837



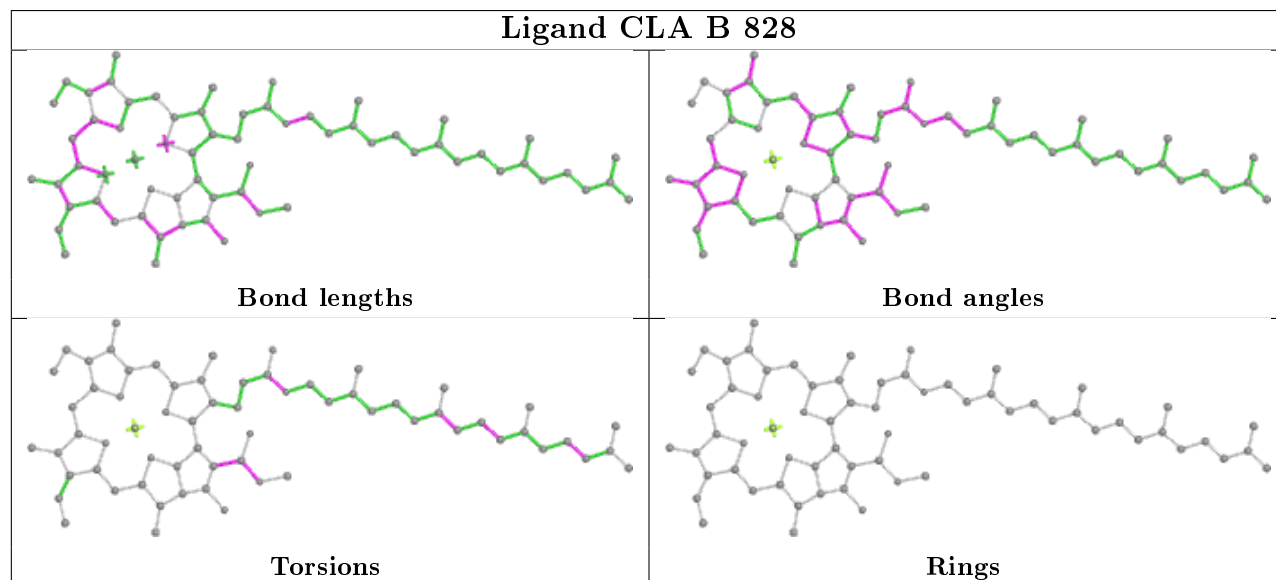
## Ligand CLA Z 807

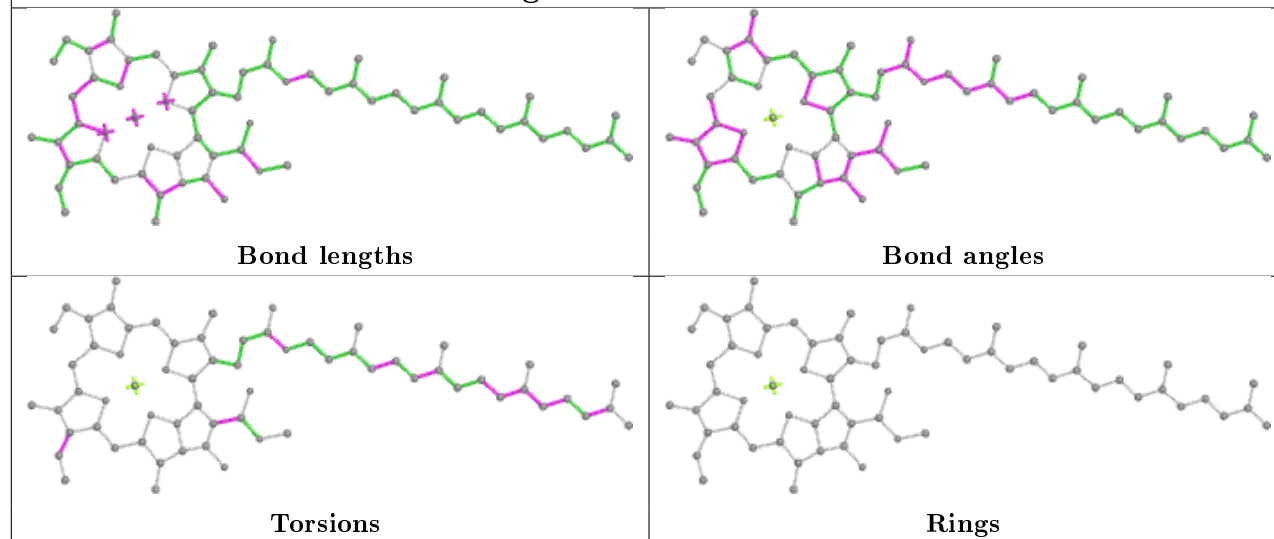
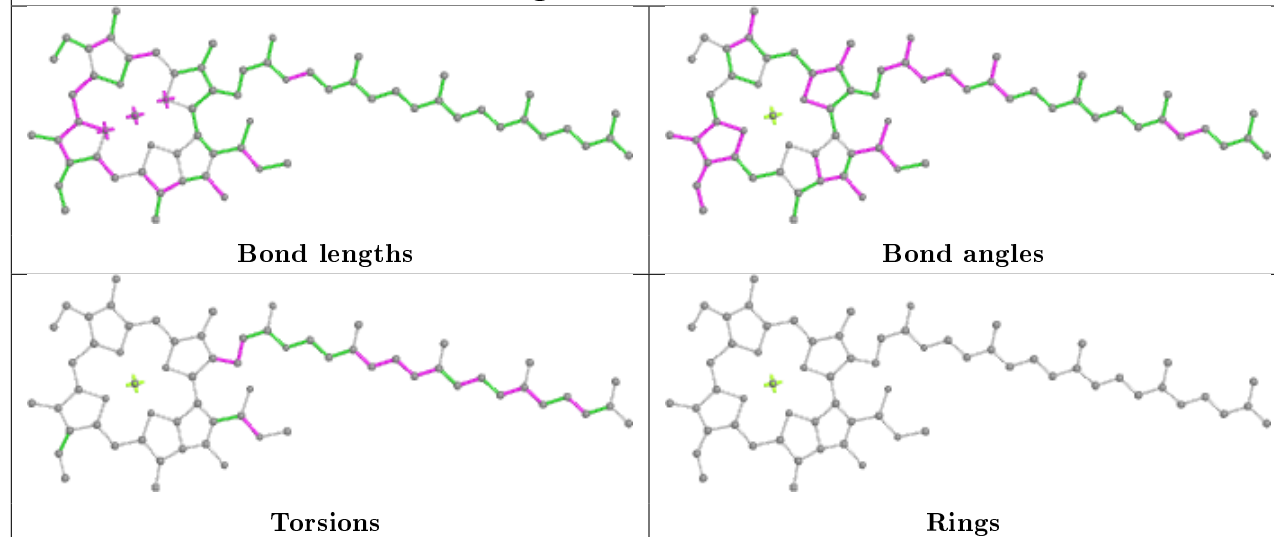


## Ligand CLA Z 818

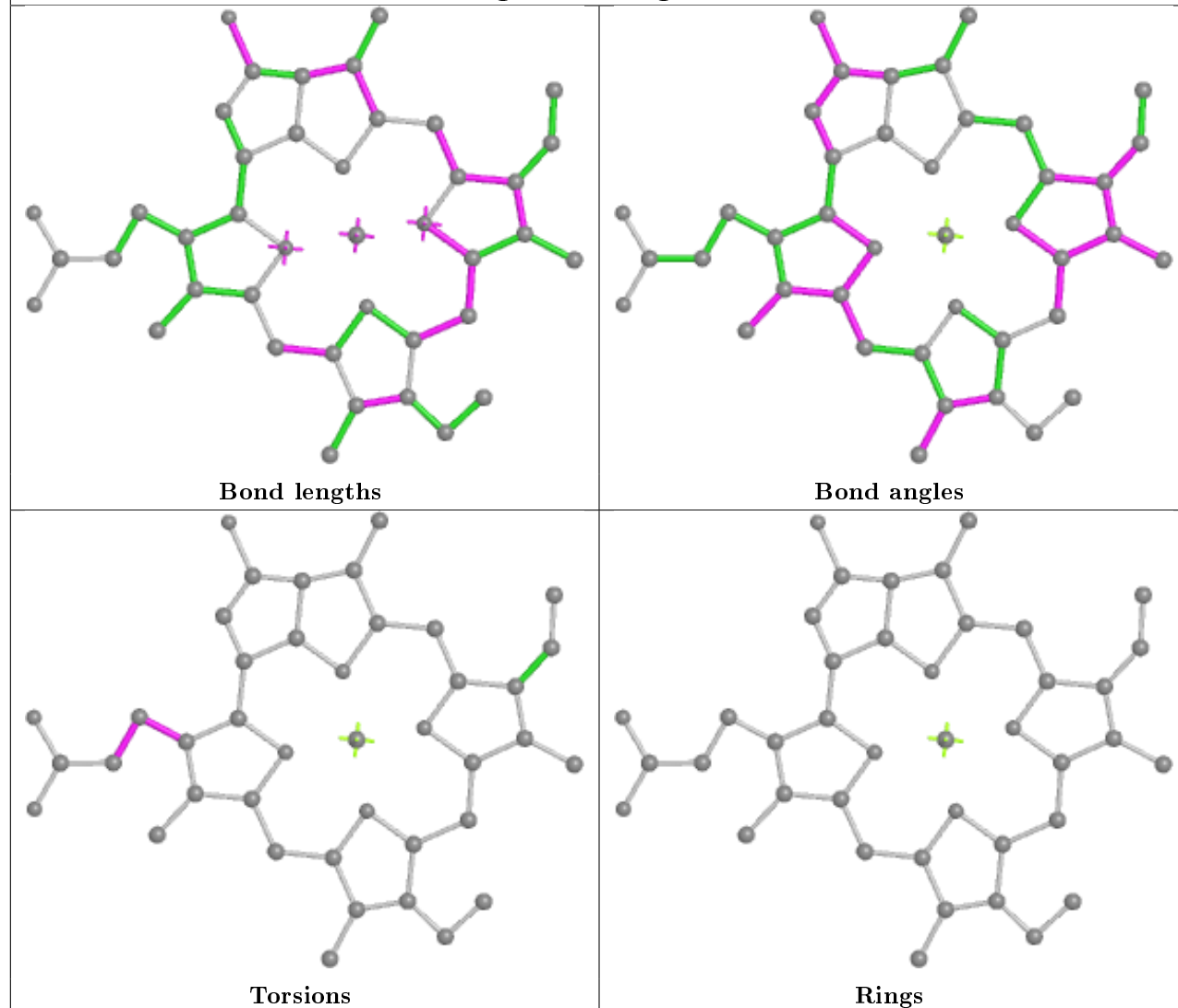


## Ligand CLA B 828

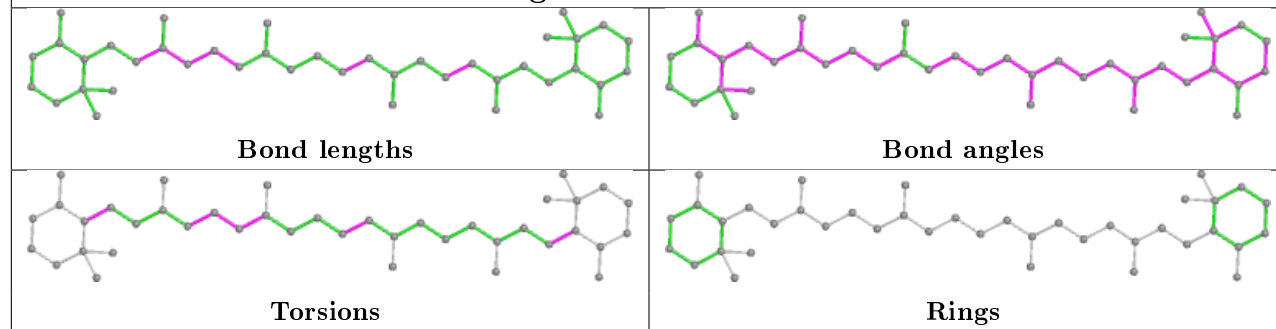


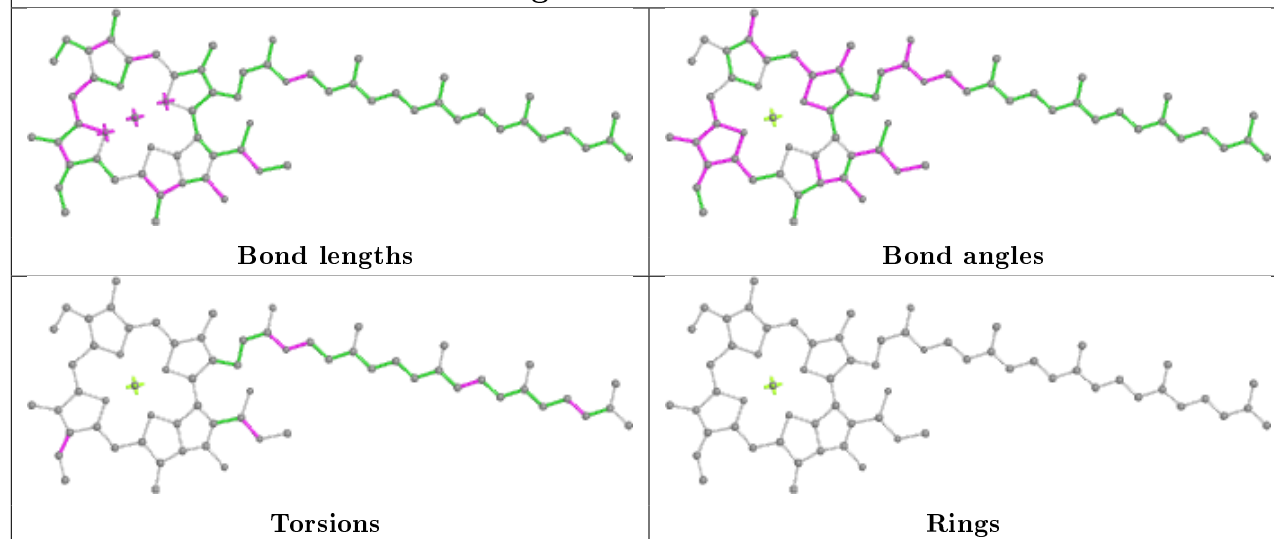
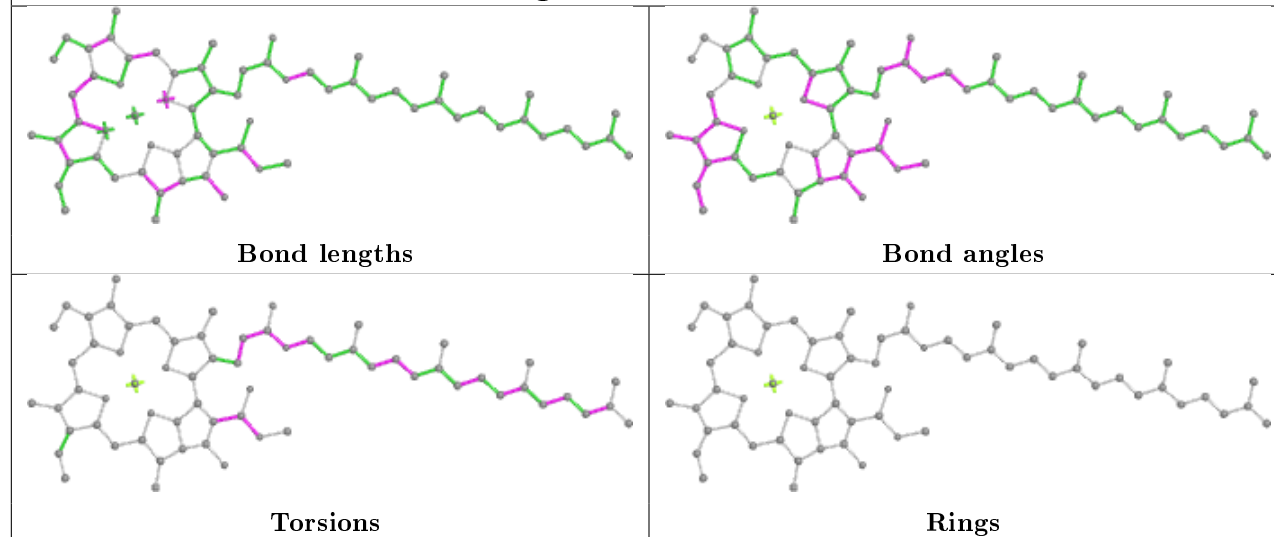
**Ligand CLA U 1003****Ligand CLA G 809**

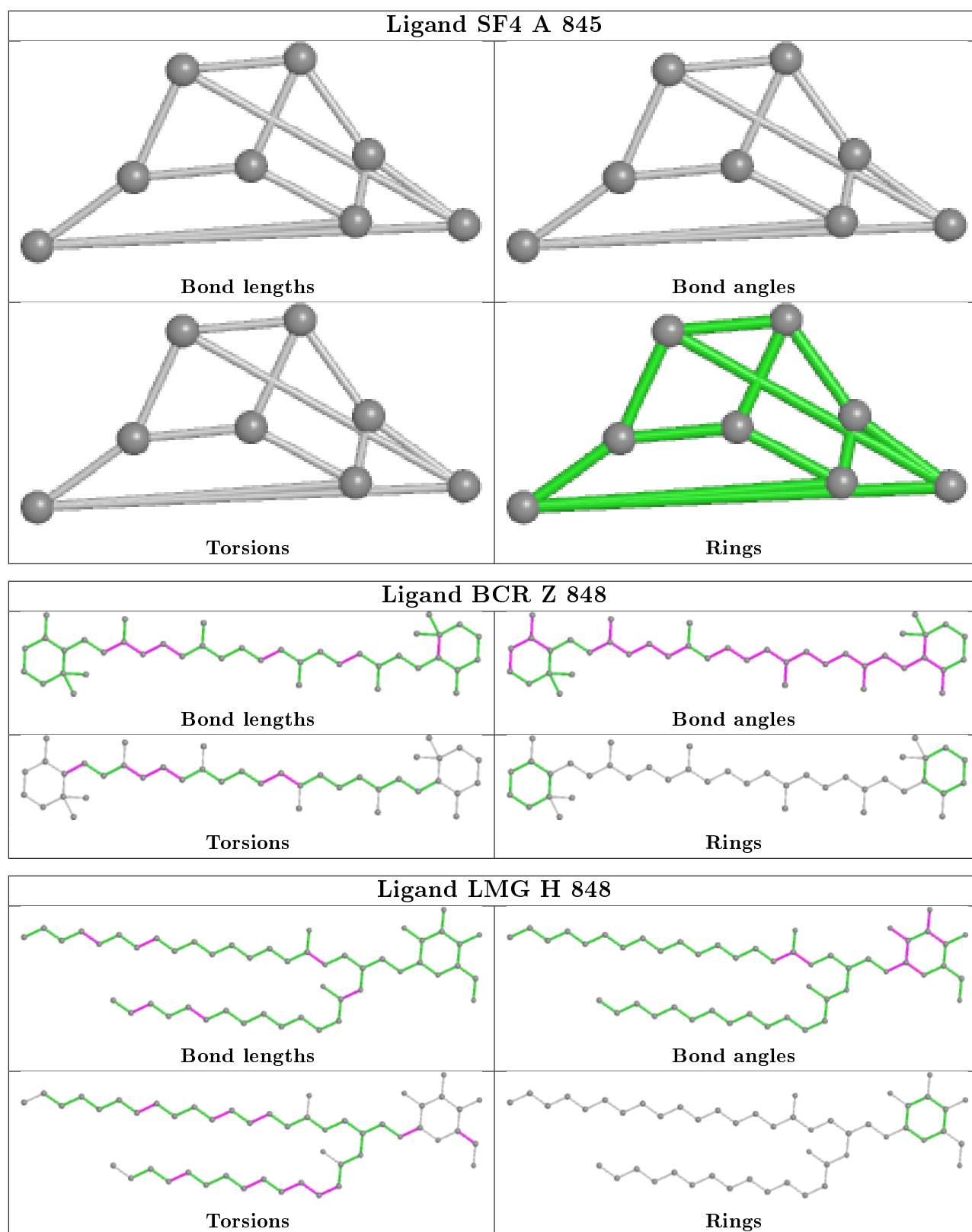
## Ligand CLA g 101

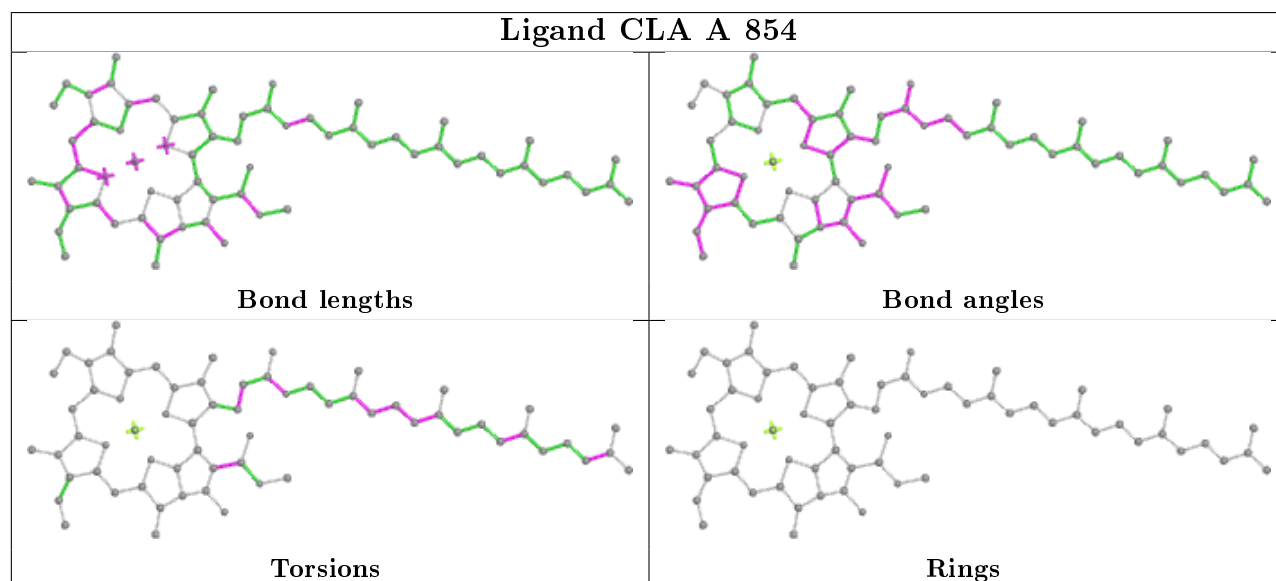
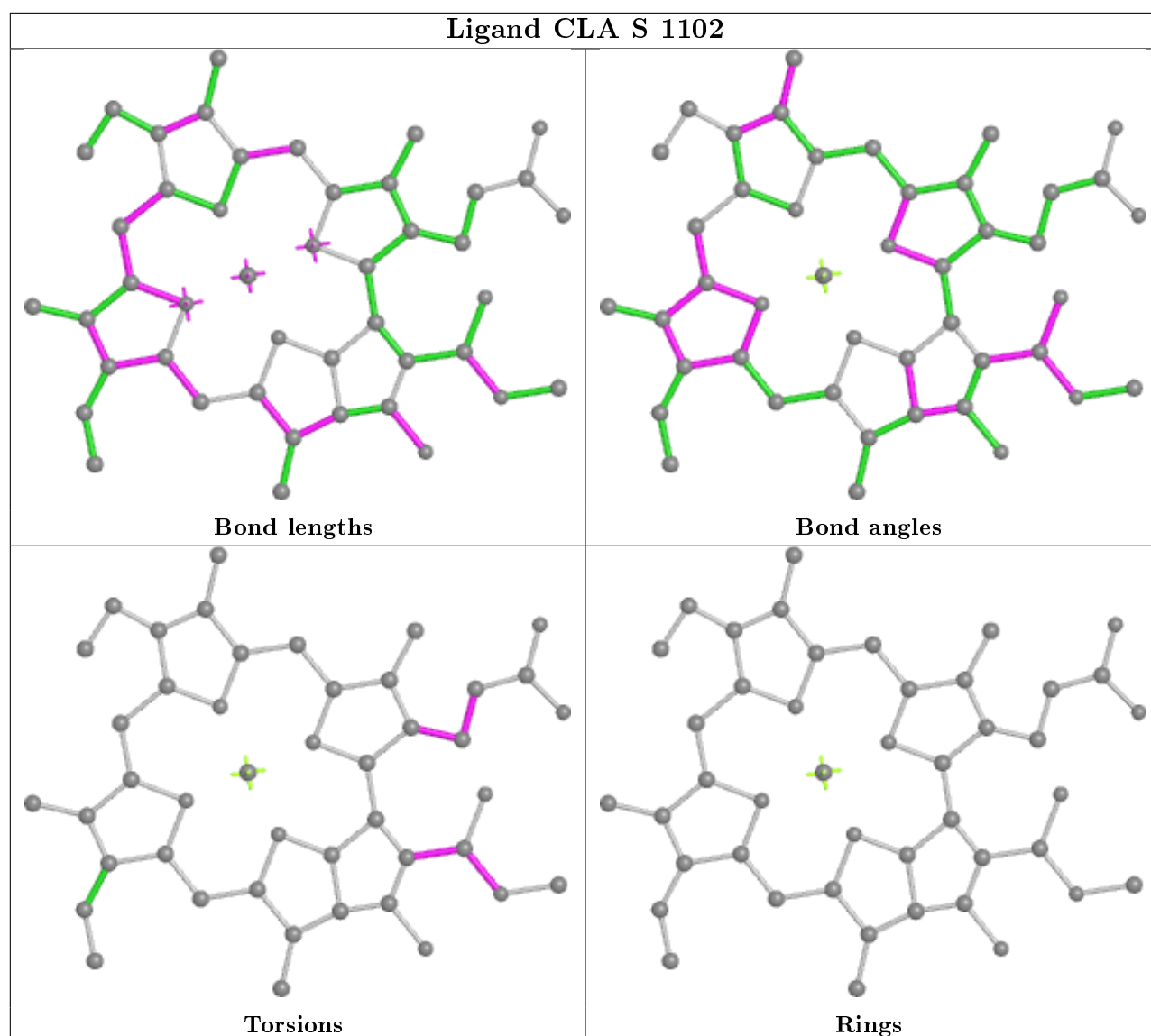


## Ligand BCR G 848

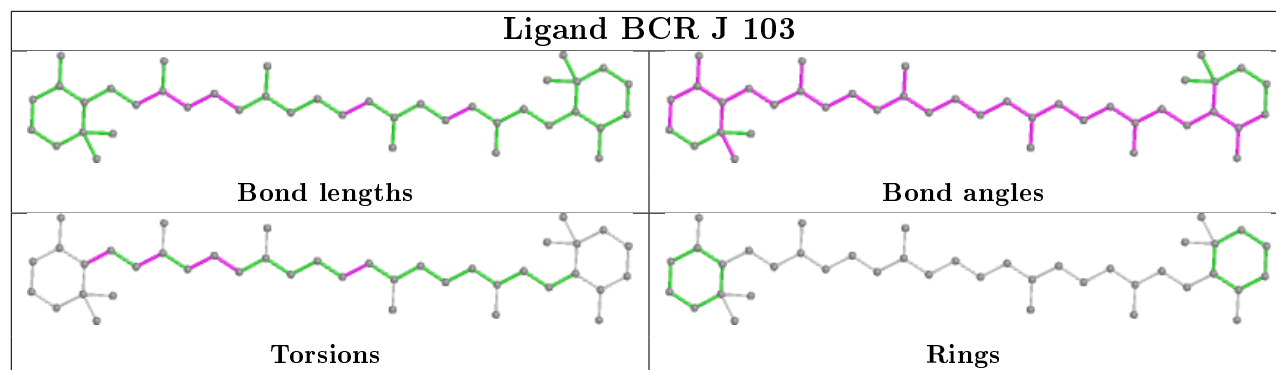
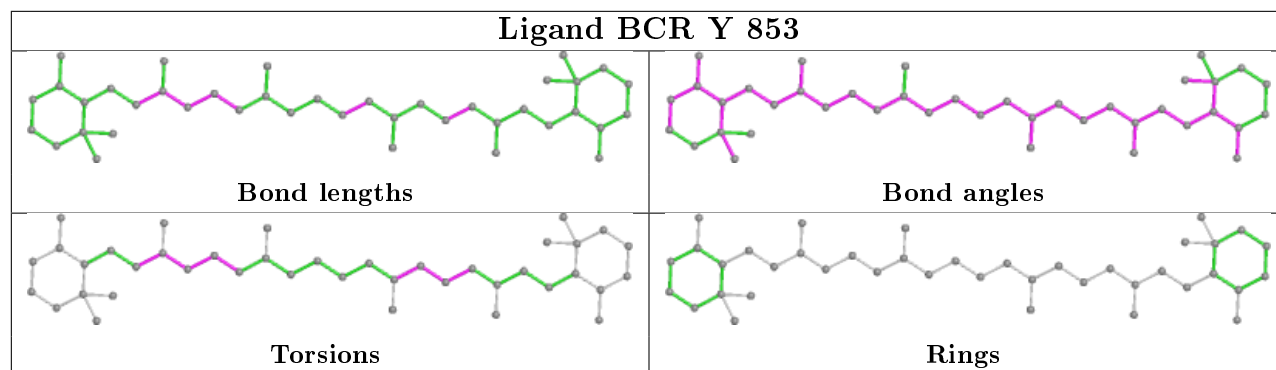
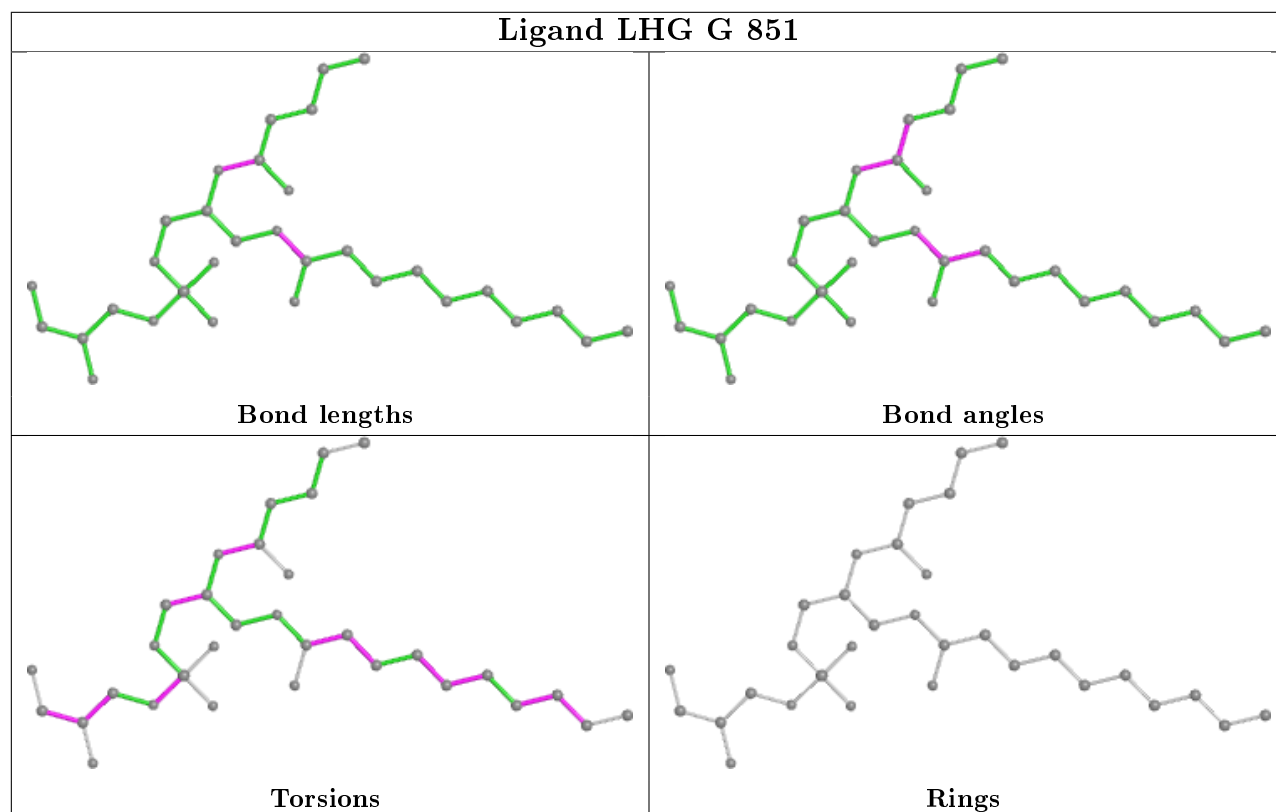


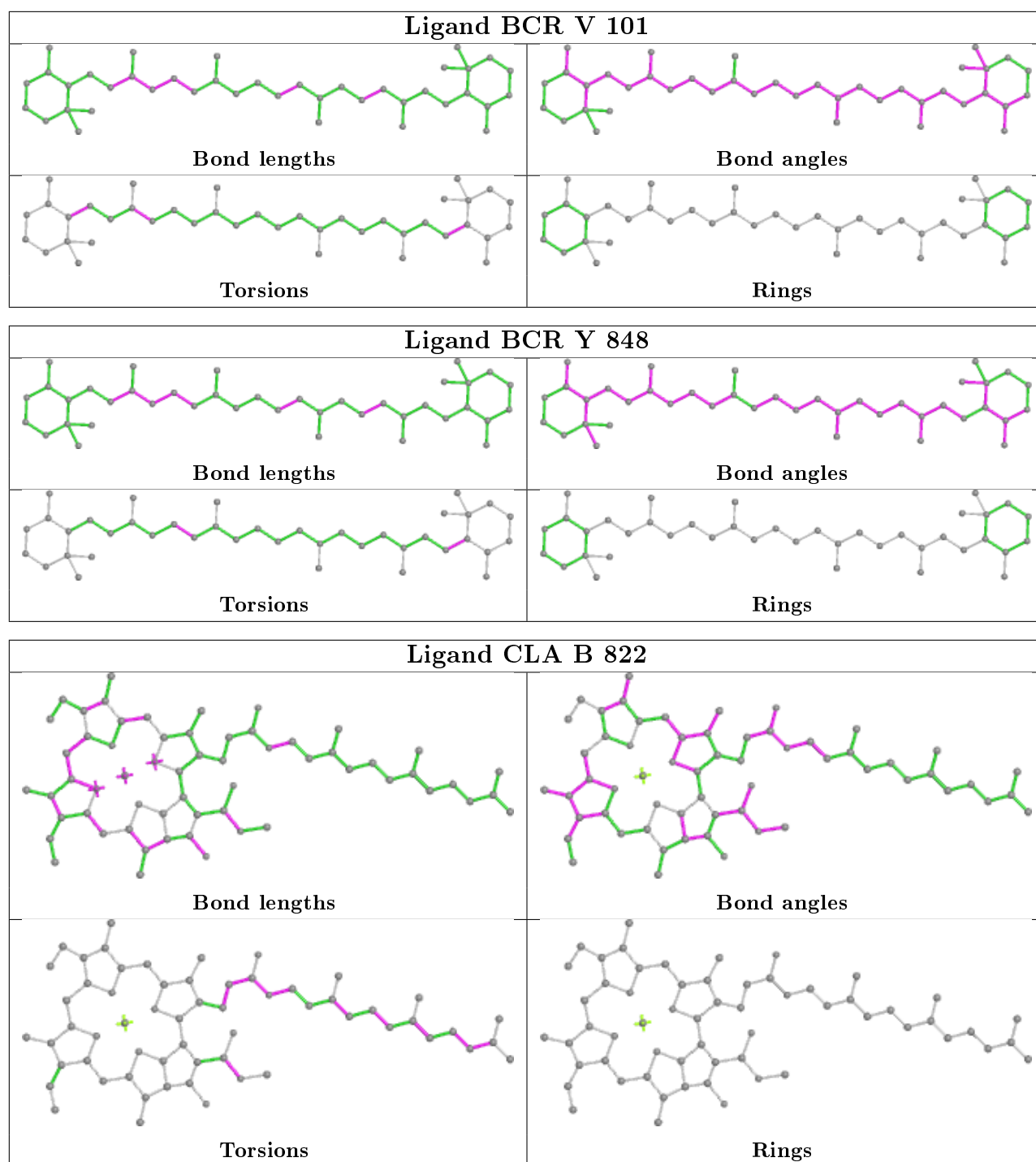
**Ligand CLA H 840****Ligand CLA Z 808**



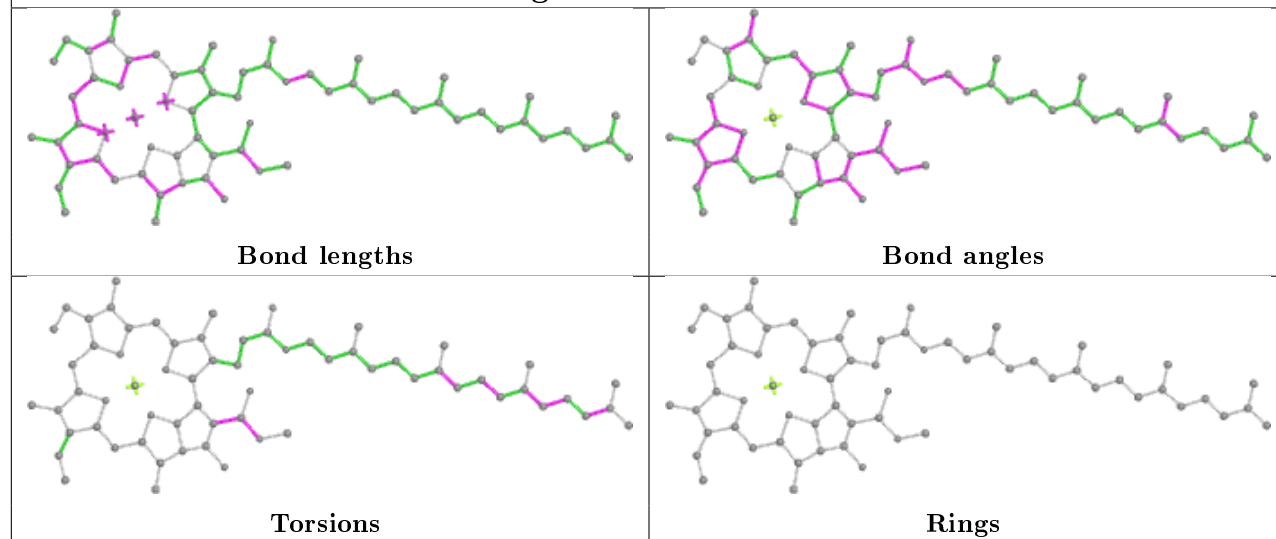




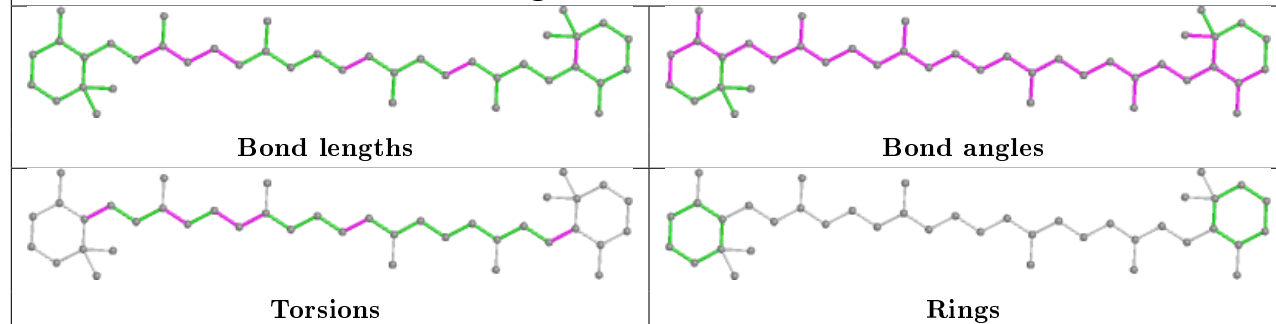
**Ligand BCR J 103****Ligand BCR Y 853****Ligand LHG G 851**



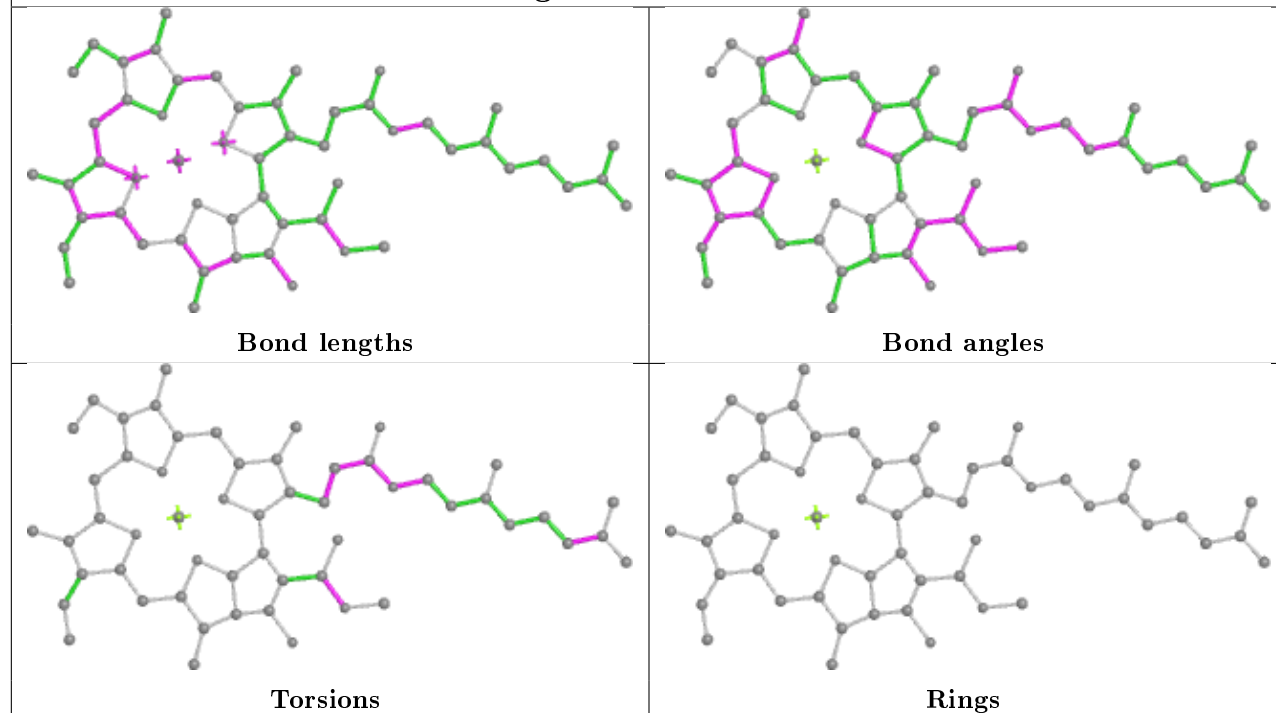
## Ligand CLA G 852

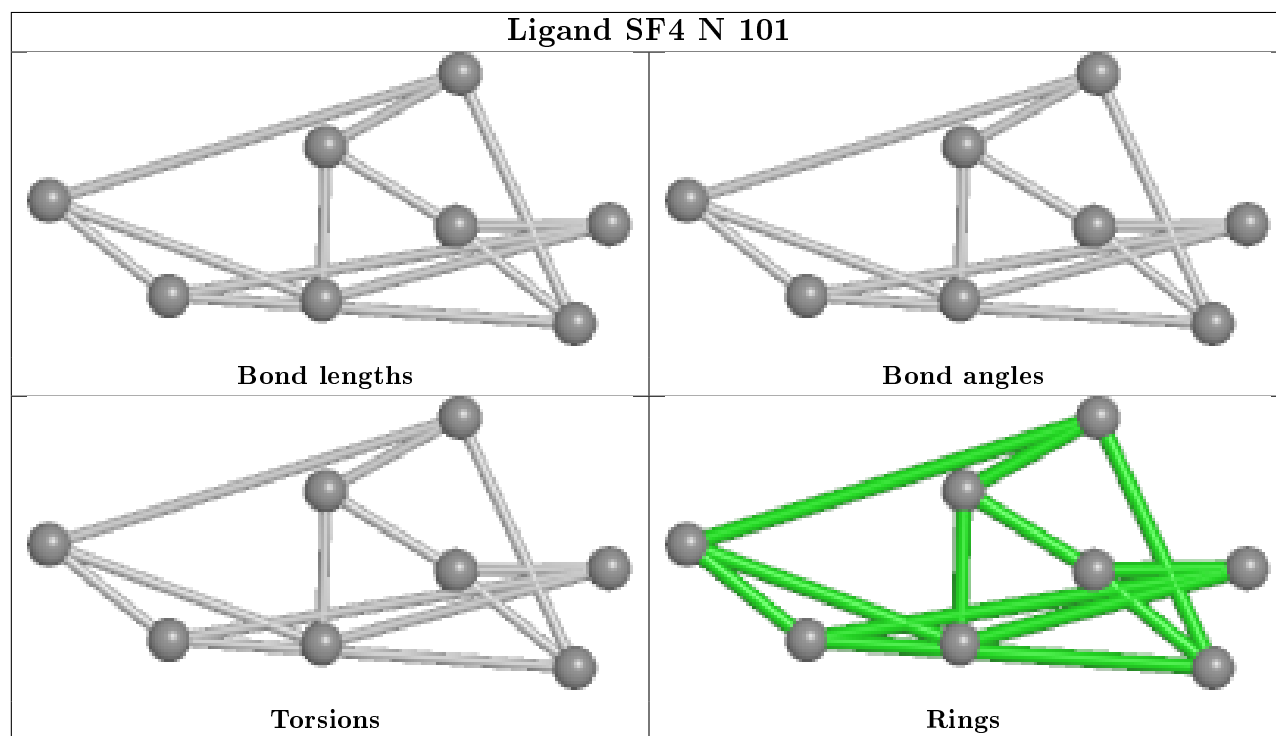
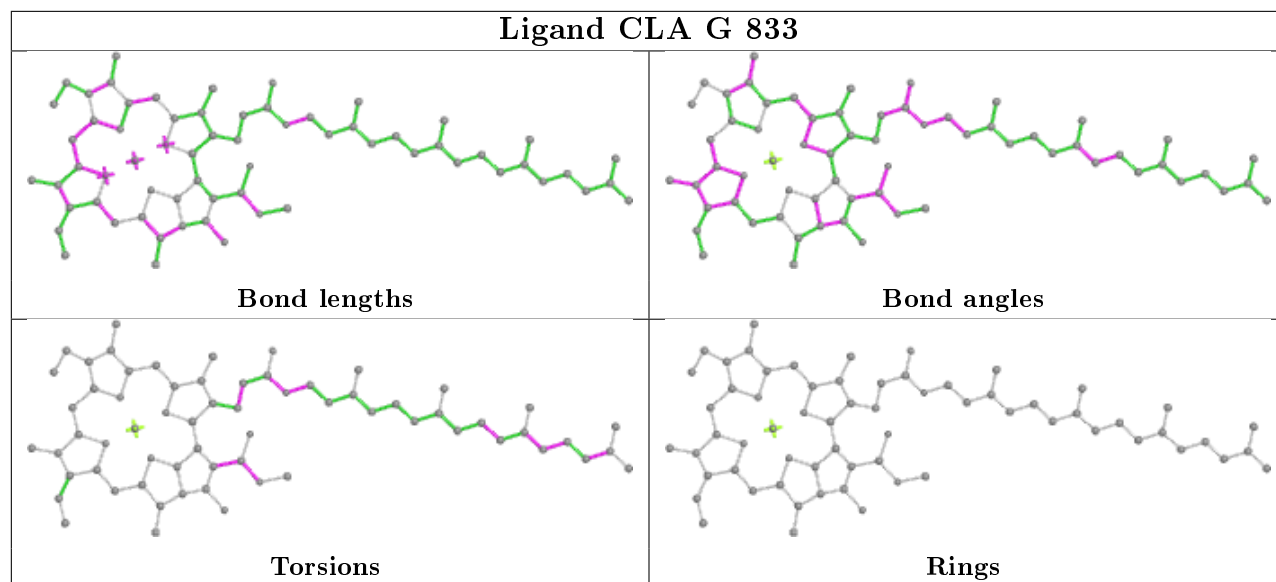


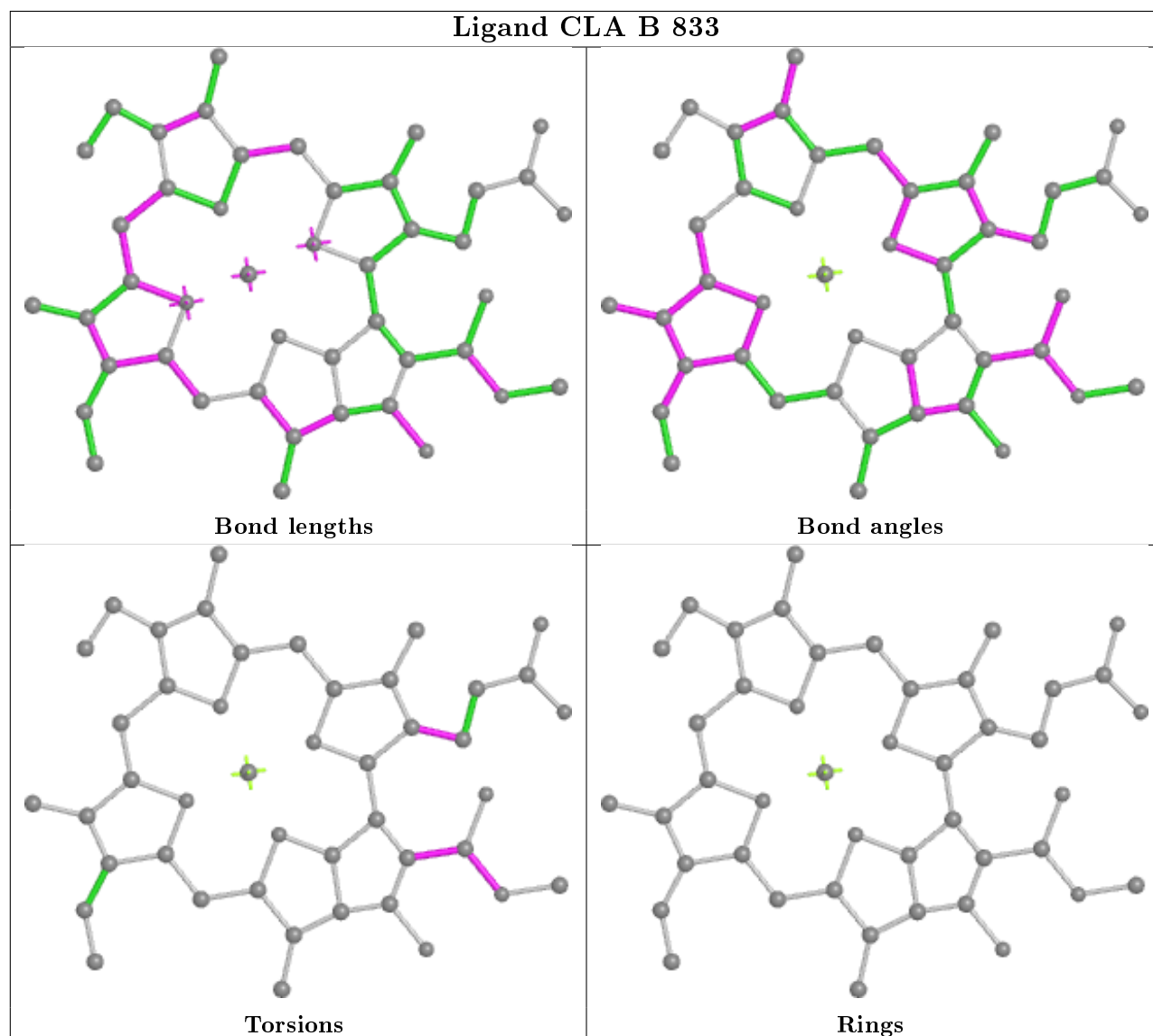
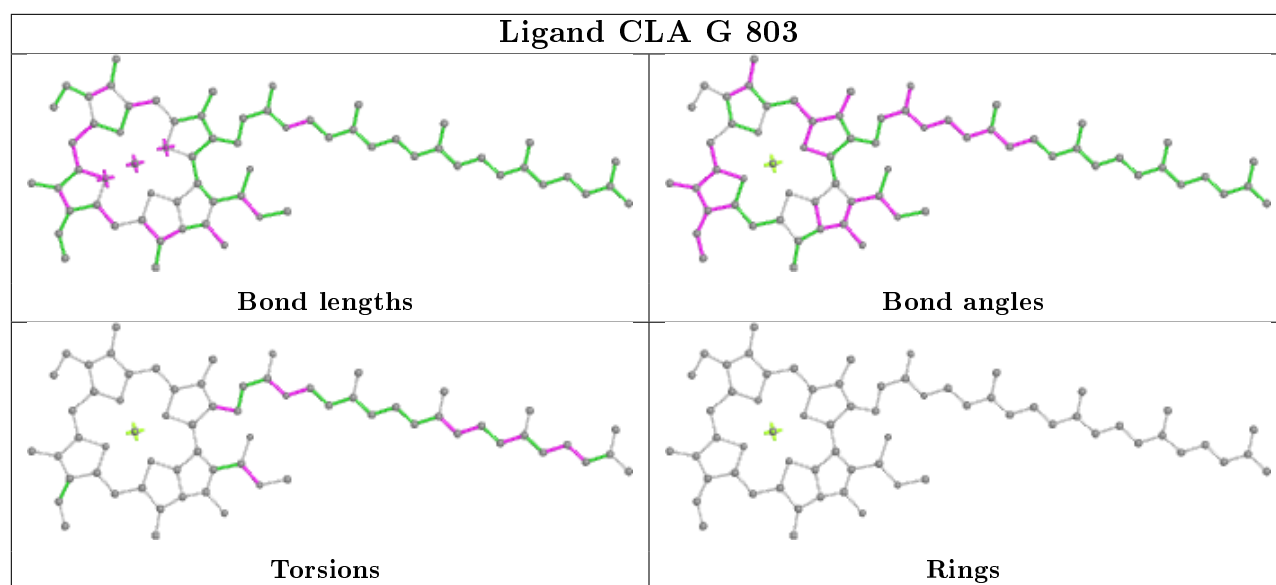
## Ligand BCR H 847

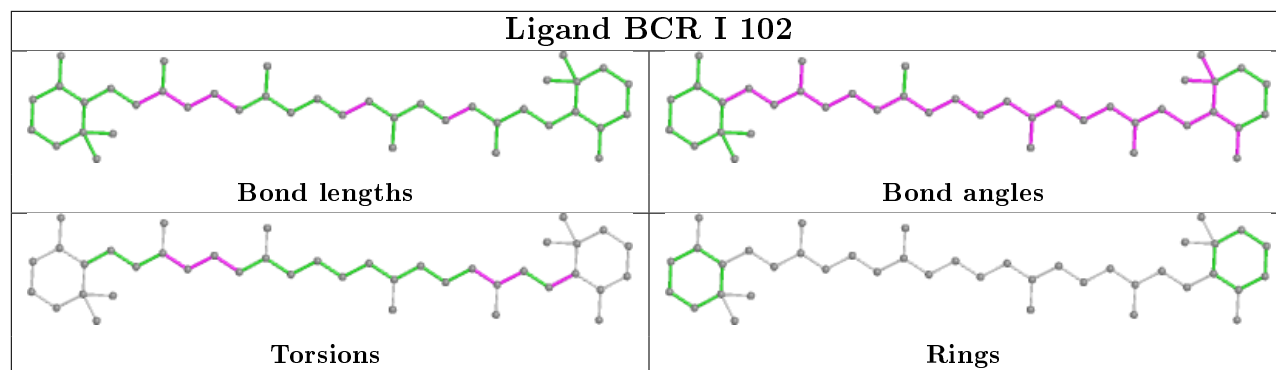
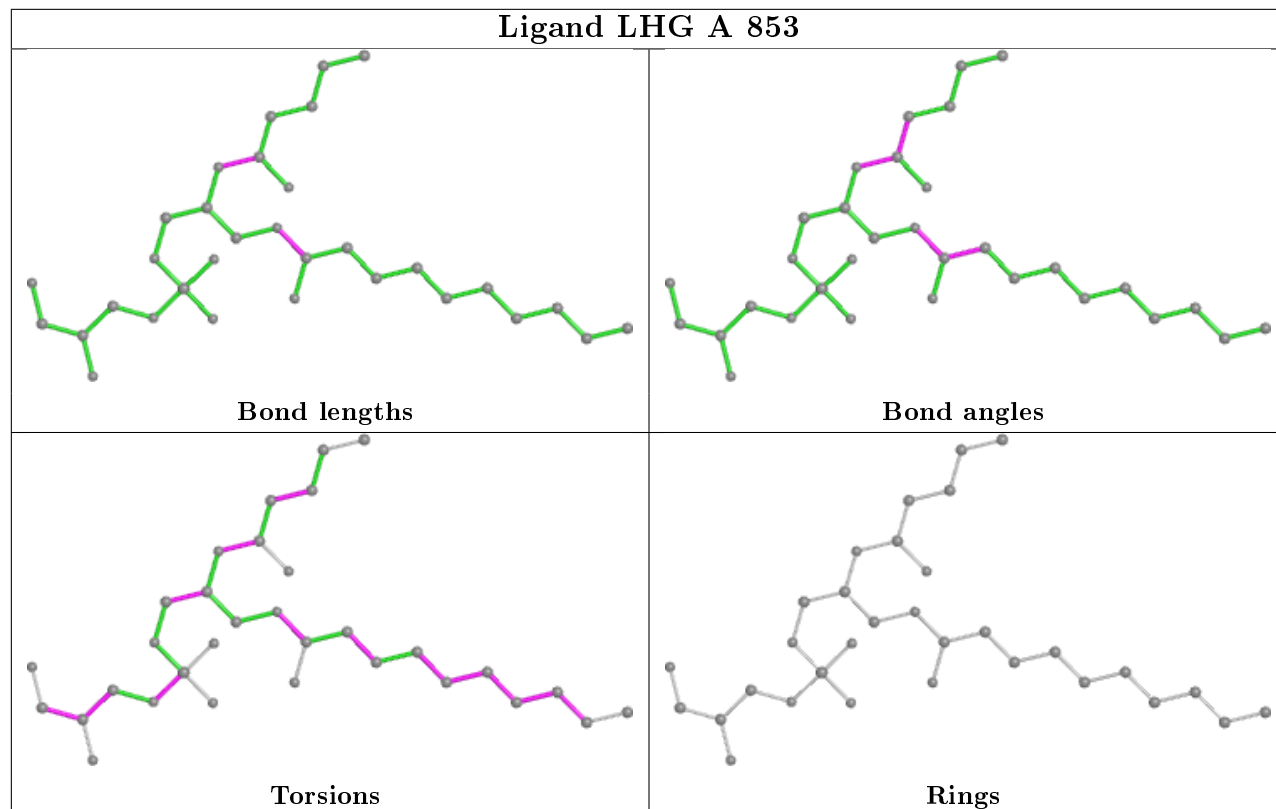
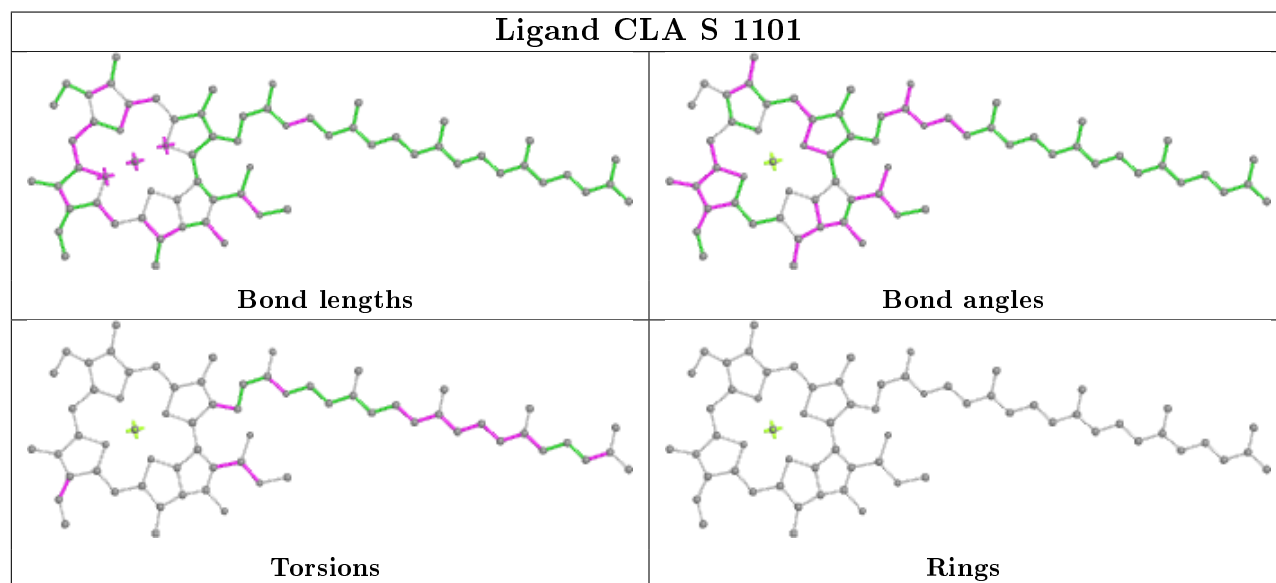


## Ligand CLA Z 823

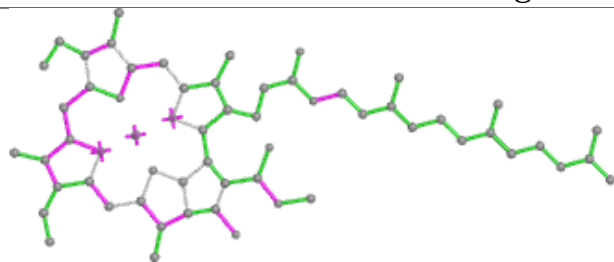




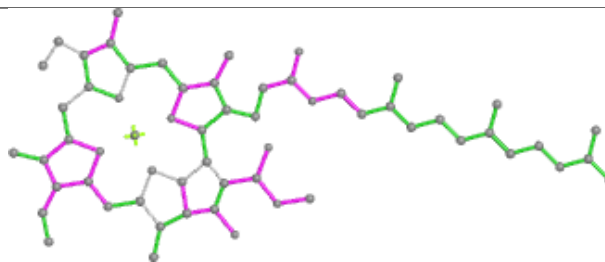


**Ligand BCR I 102****Ligand LHG A 853****Ligand CLA S 1101**

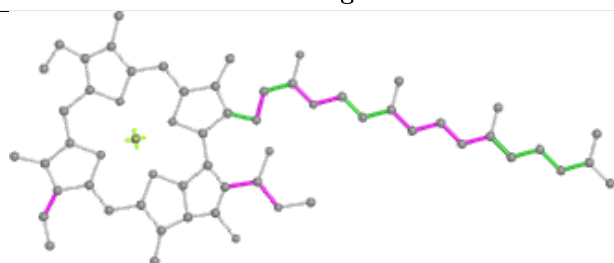
## Ligand CLA Y 824



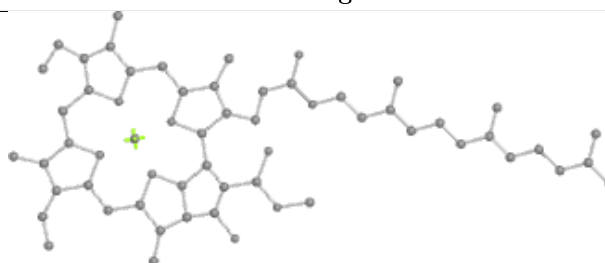
Bond lengths



Bond angles

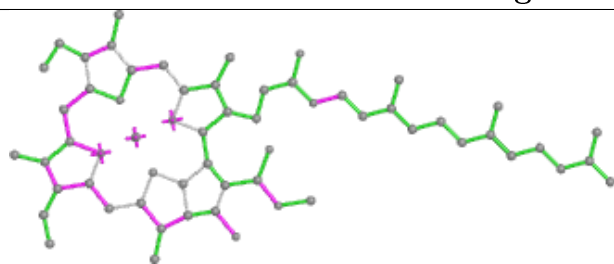


Torsions

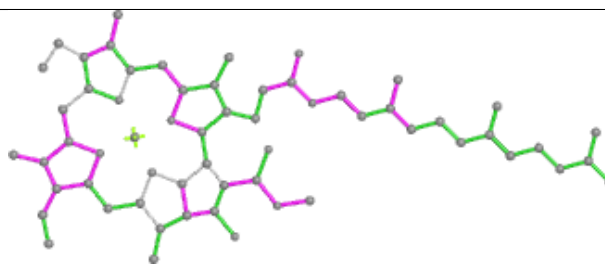


Rings

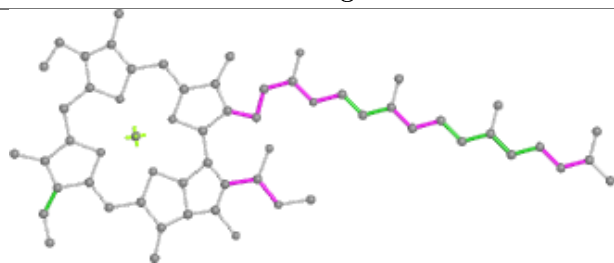
## Ligand CLA B 818



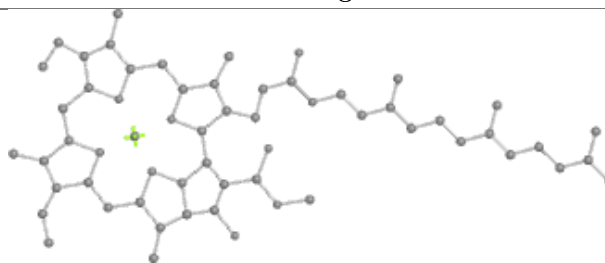
Bond lengths



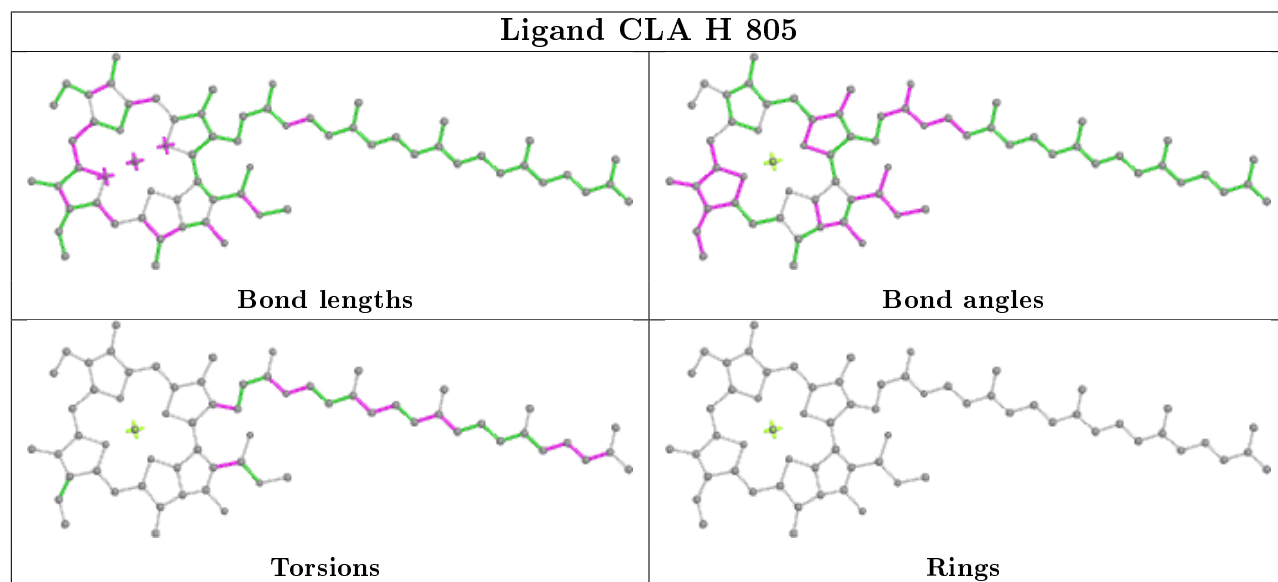
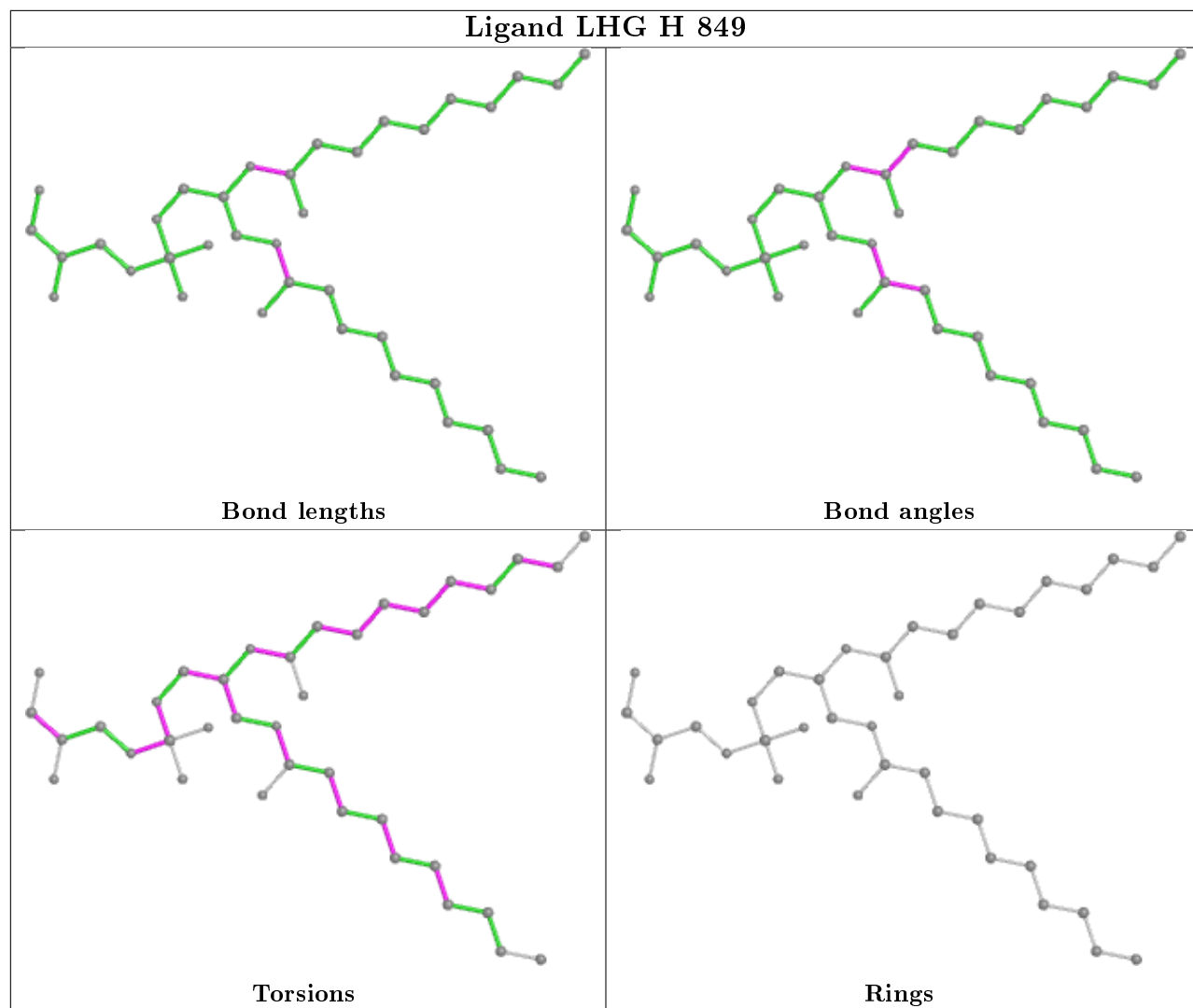
Bond angles



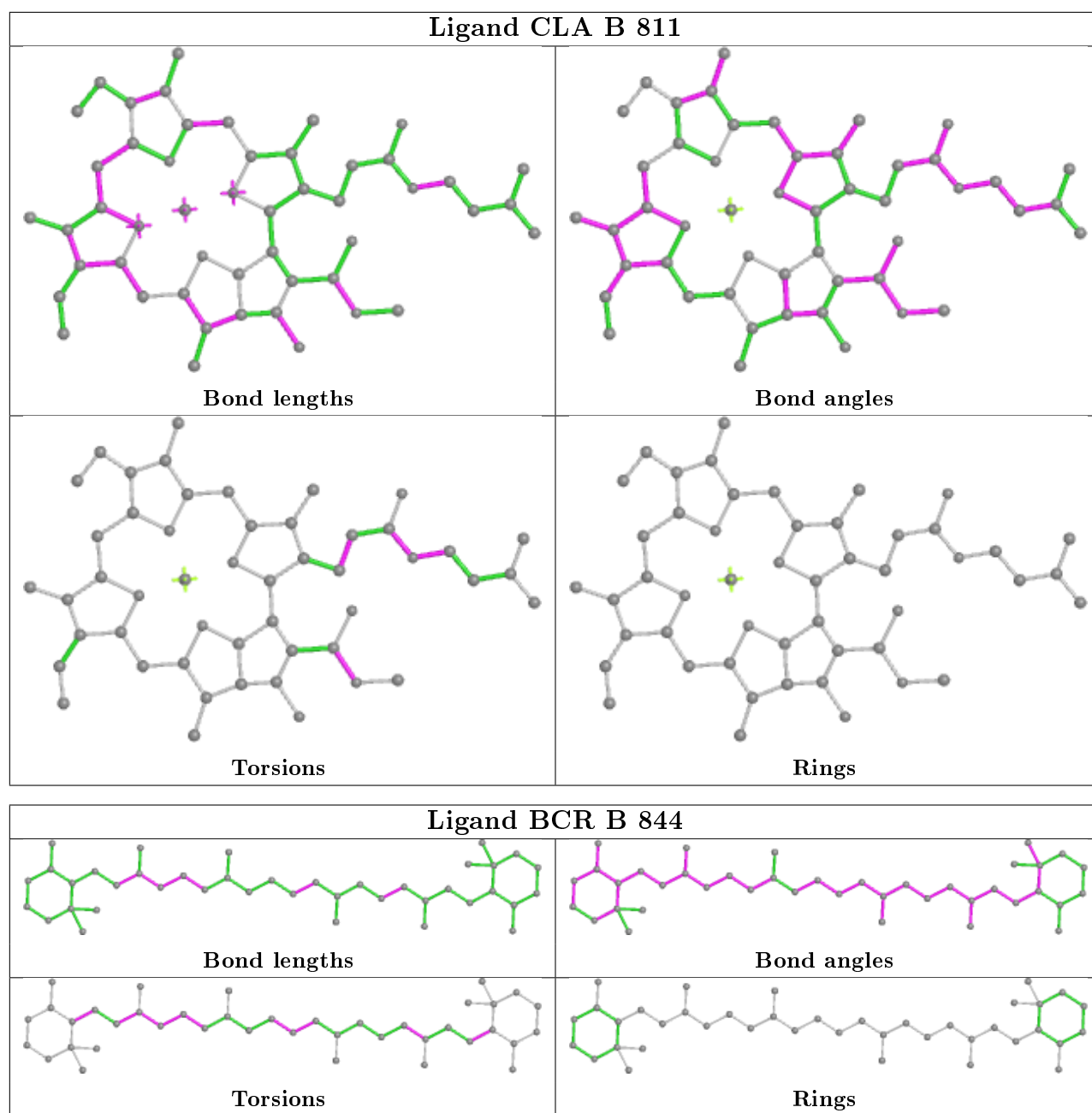
Torsions



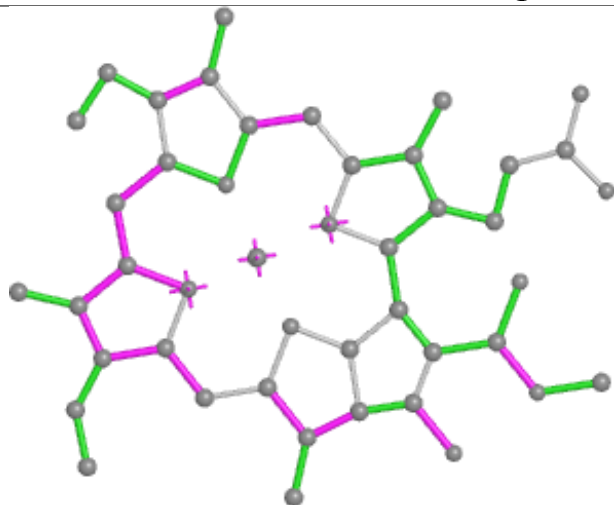
Rings



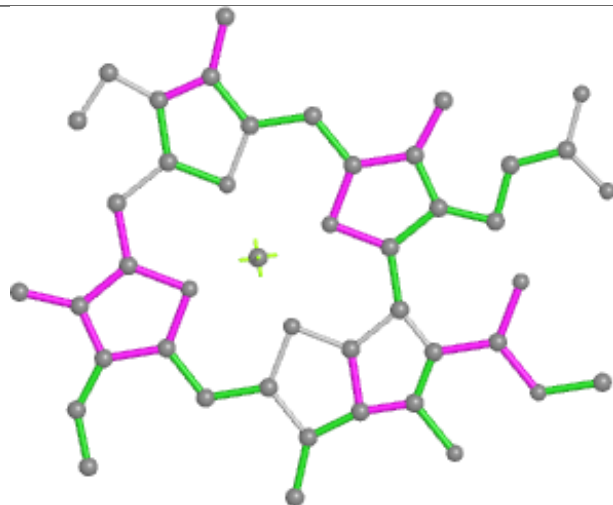




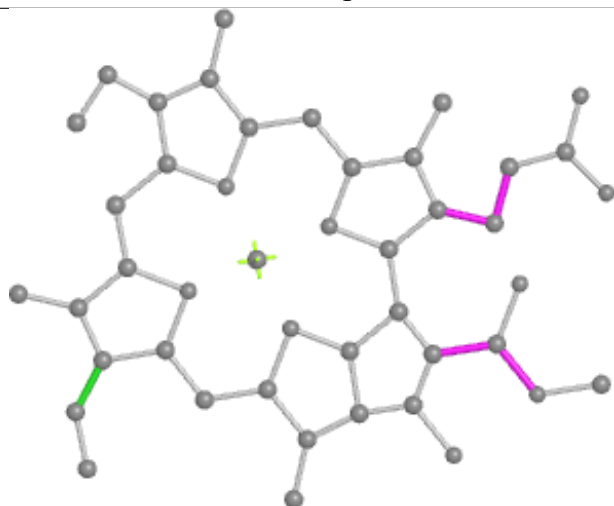
## Ligand CLA G 810



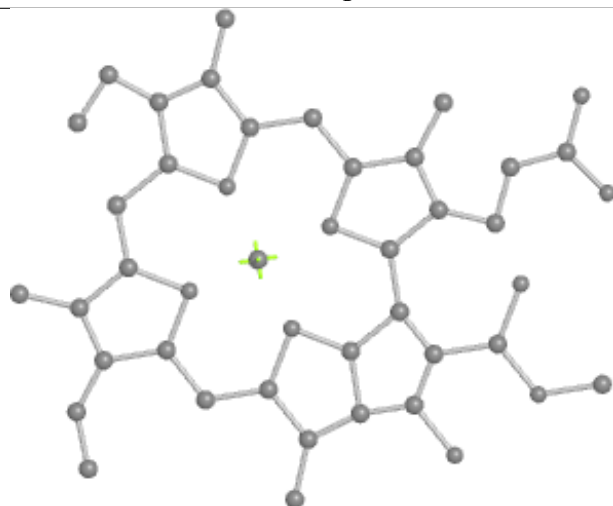
Bond lengths



Bond angles

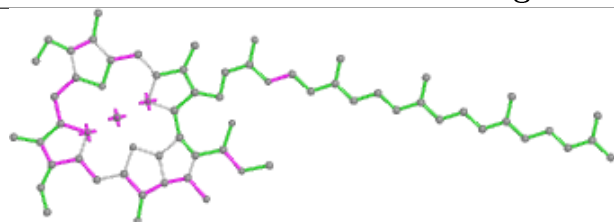


Torsions

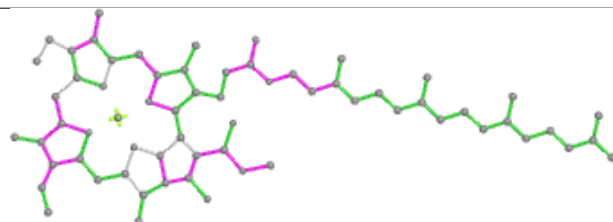


Rings

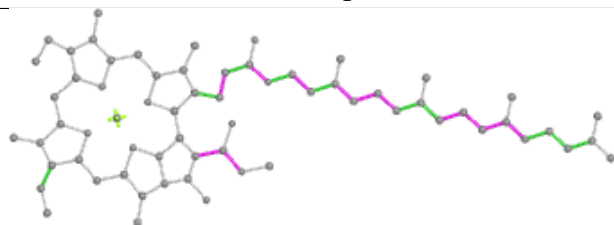
## Ligand CLA G 802



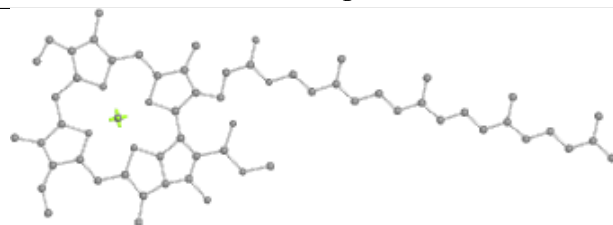
Bond lengths



Bond angles

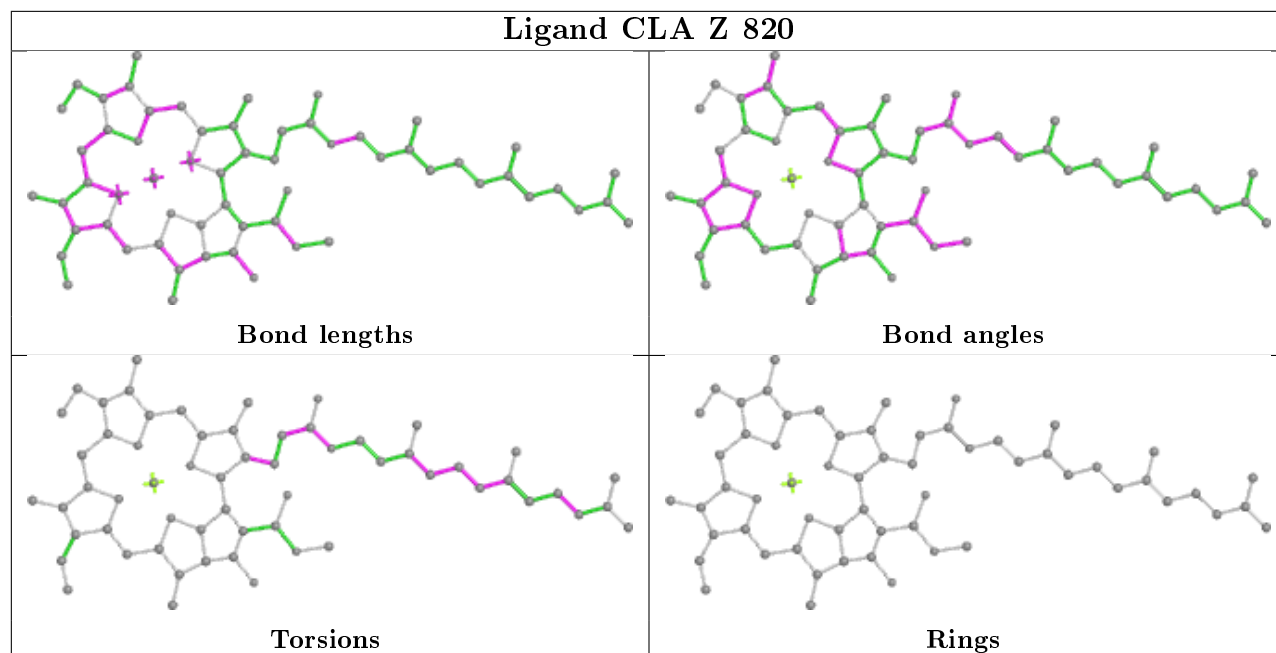


Torsions

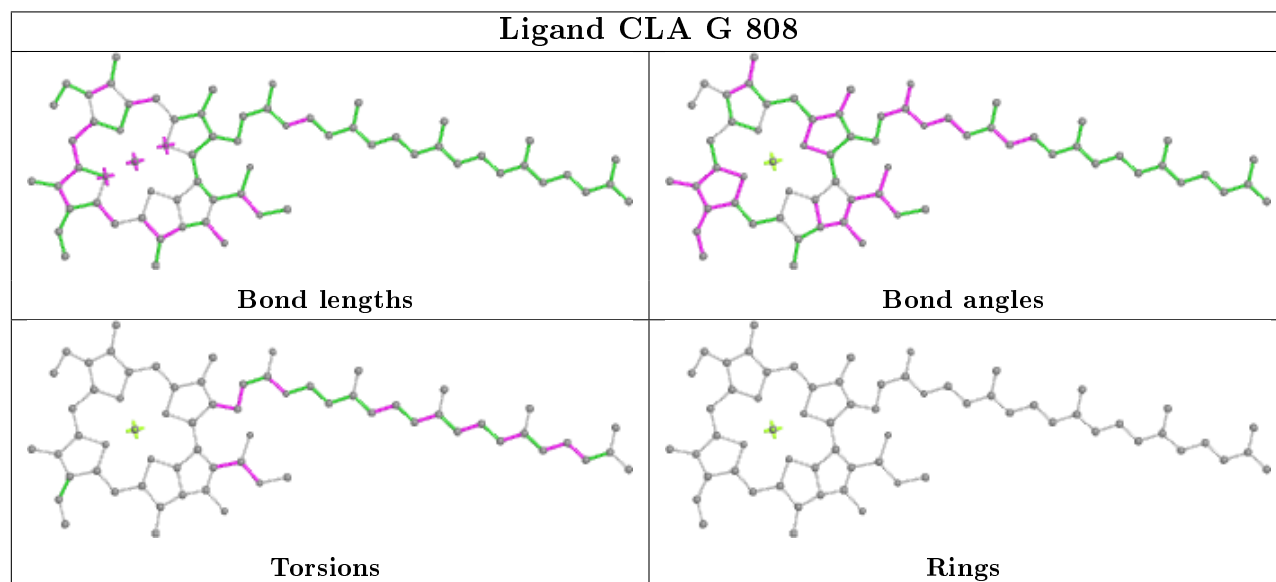


Rings

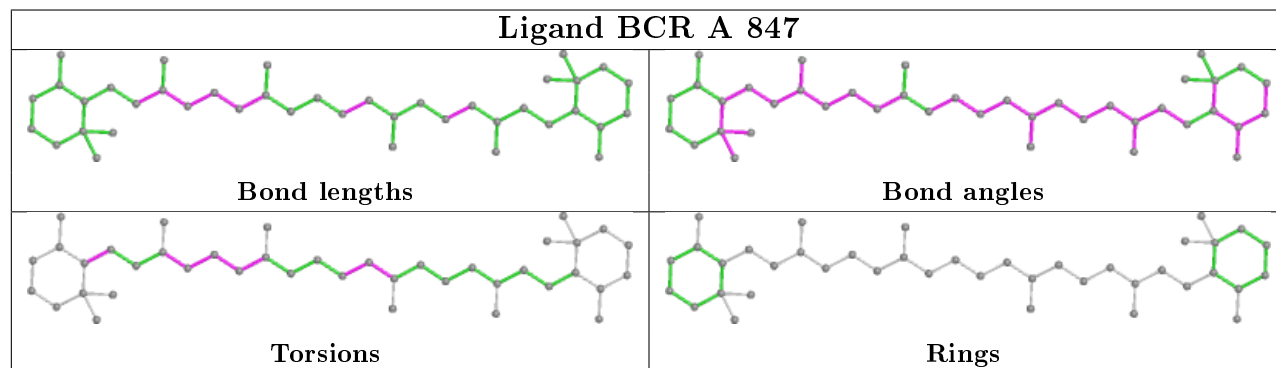
## Ligand CLA Z 820

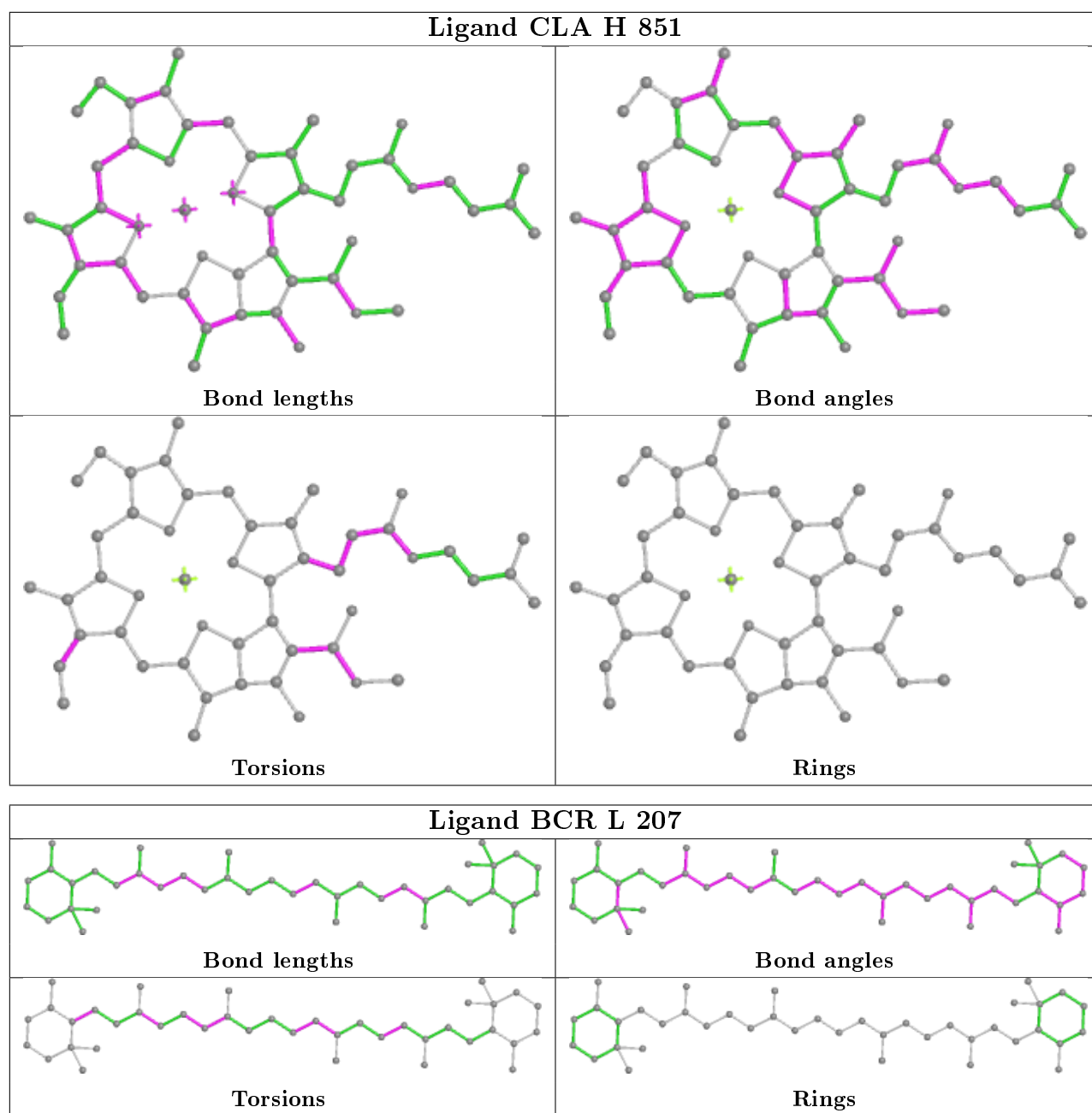


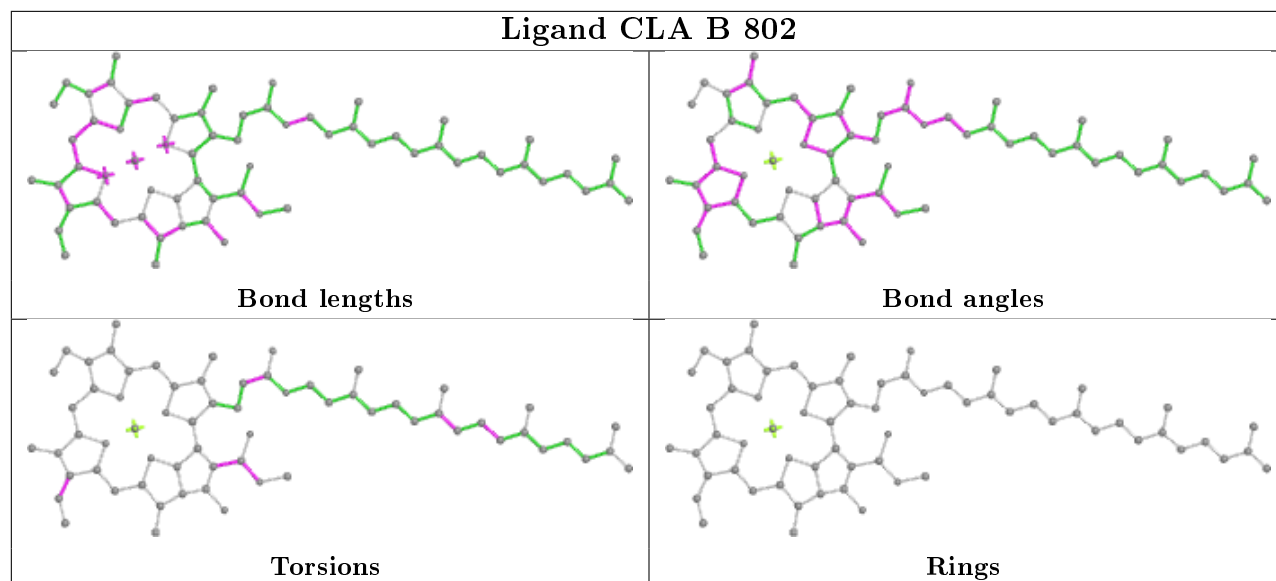
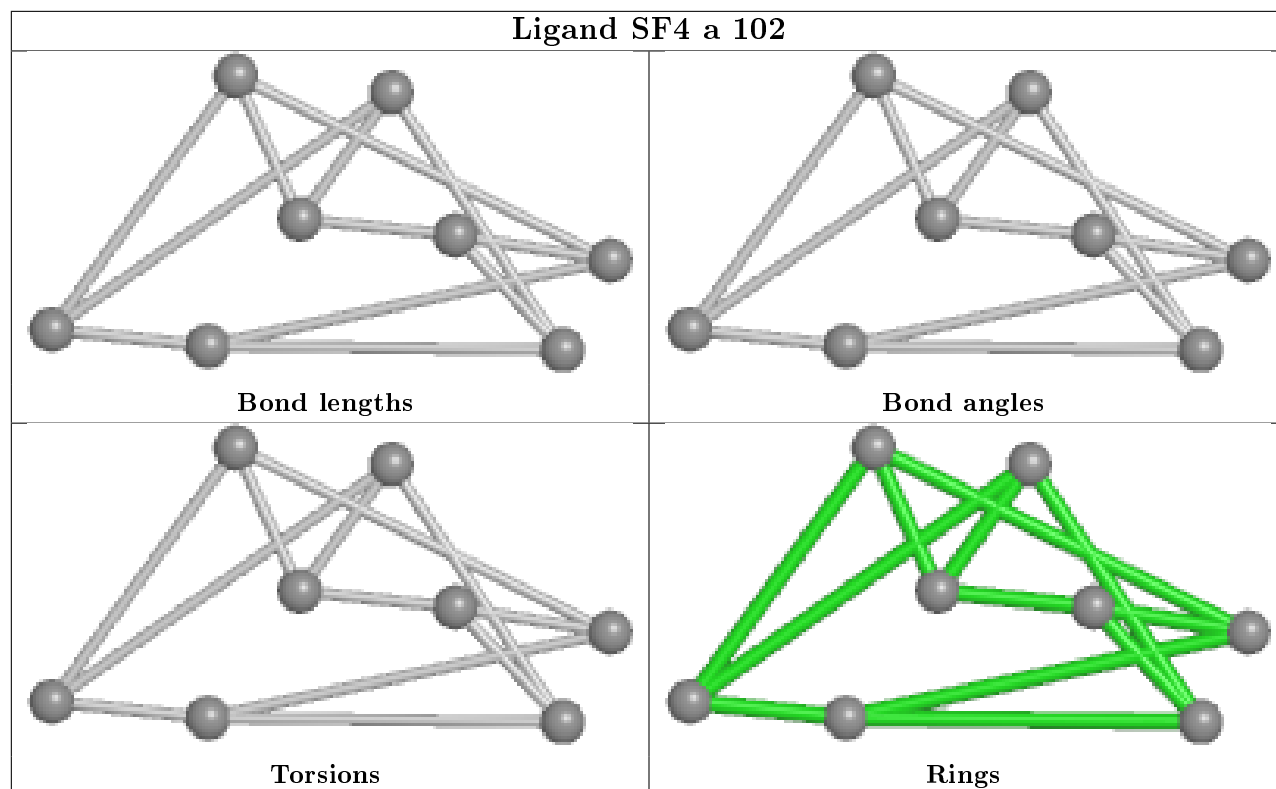
## Ligand CLA G 808

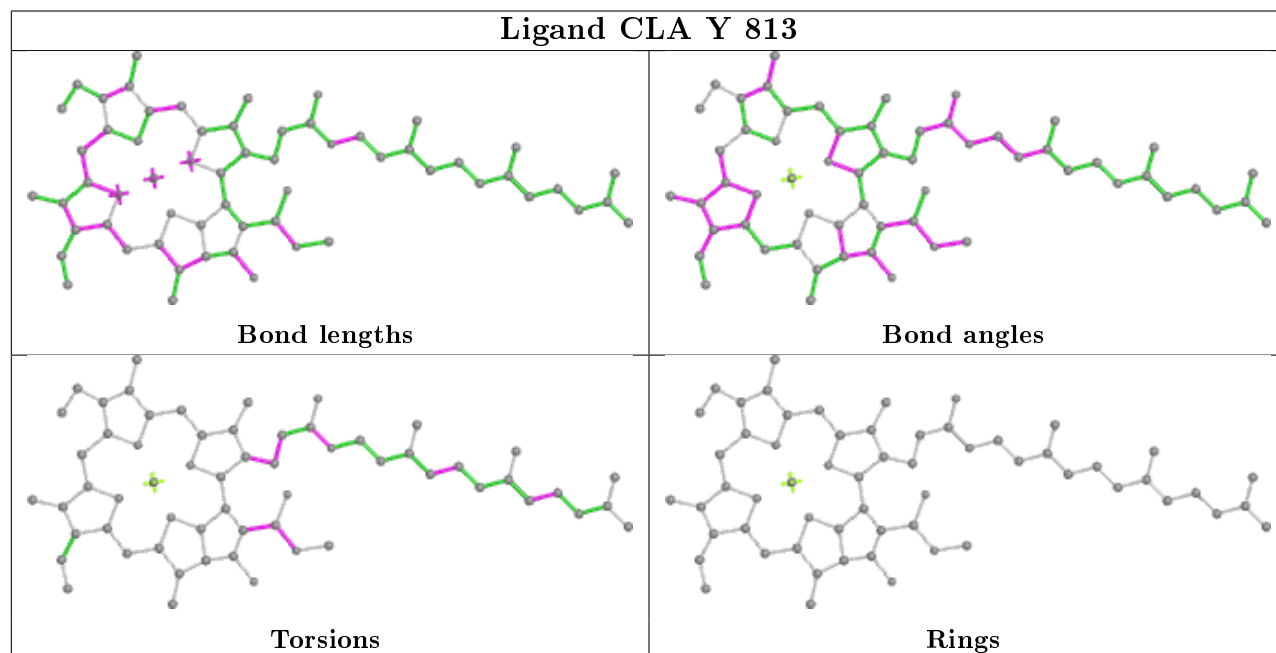
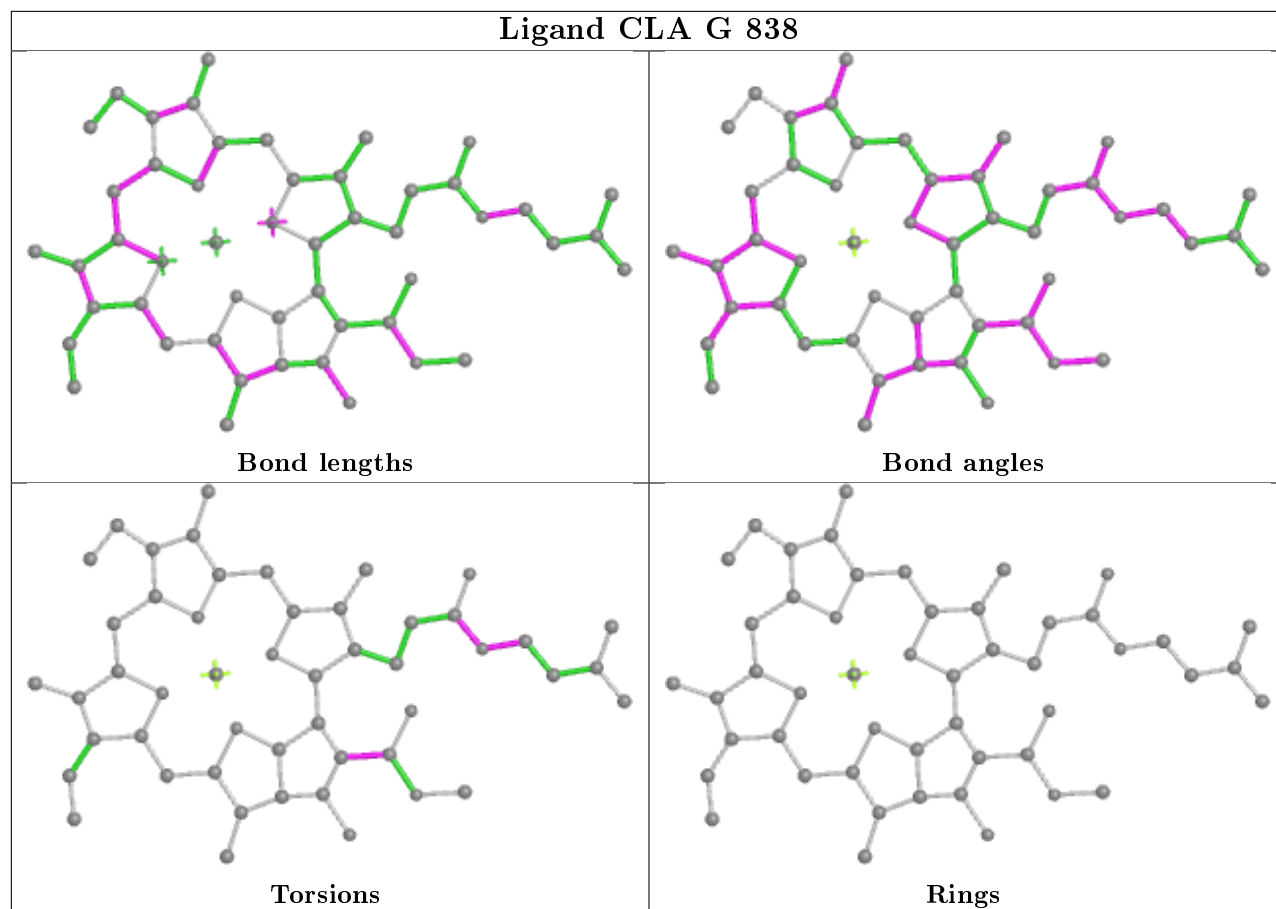


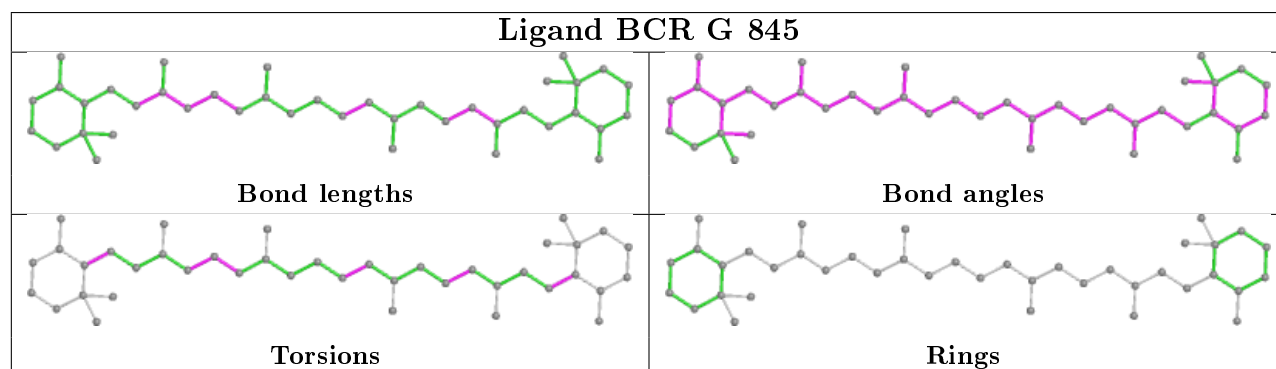
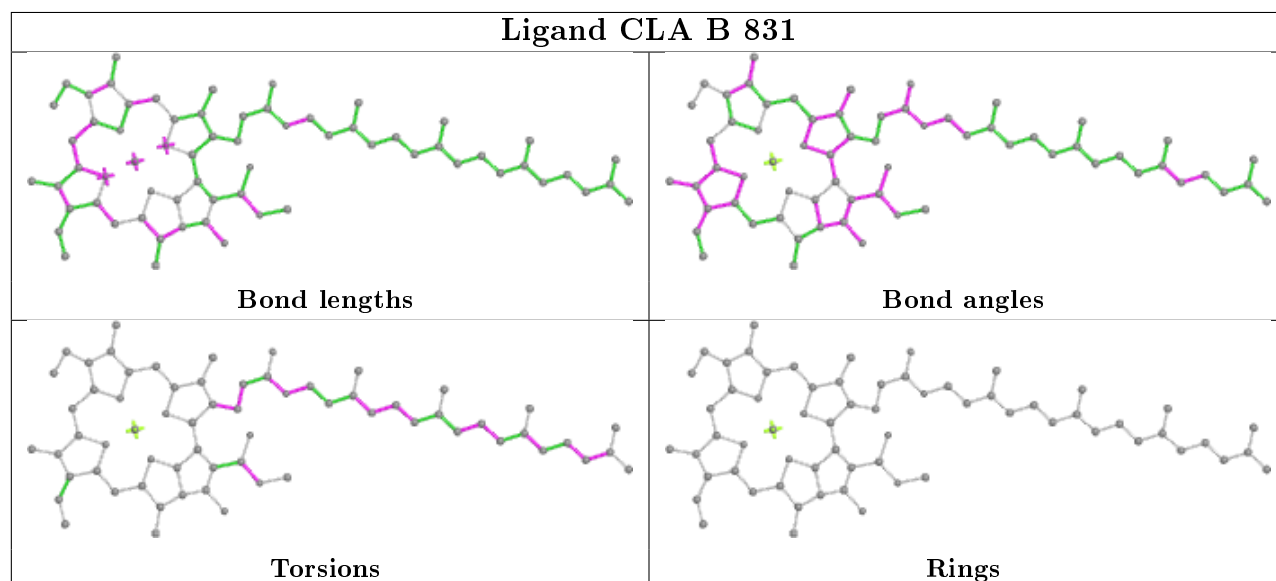
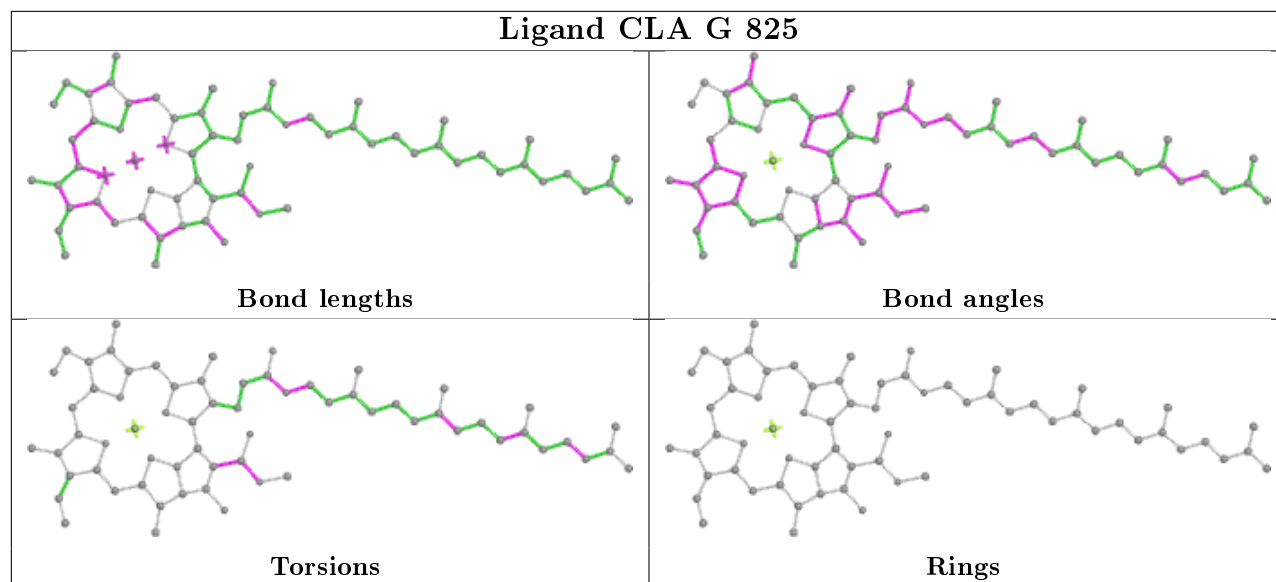
## Ligand BCR A 847

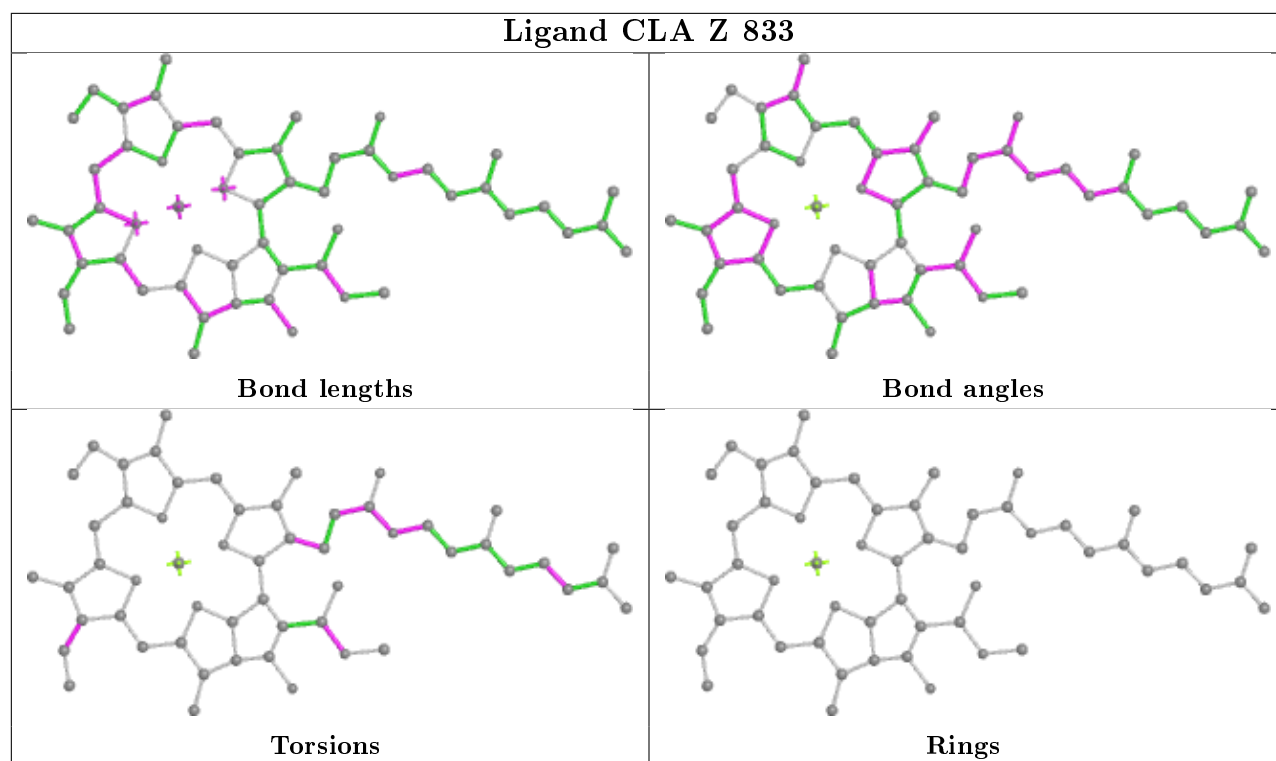
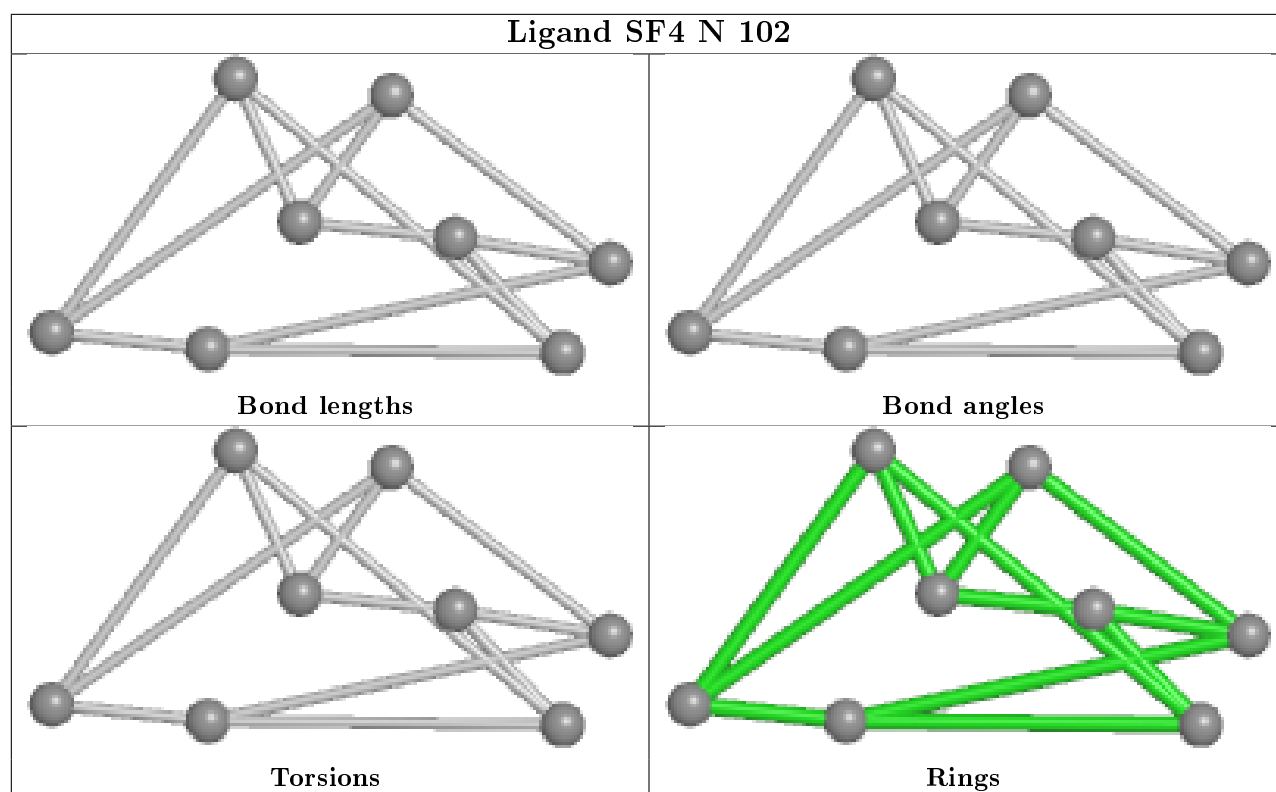




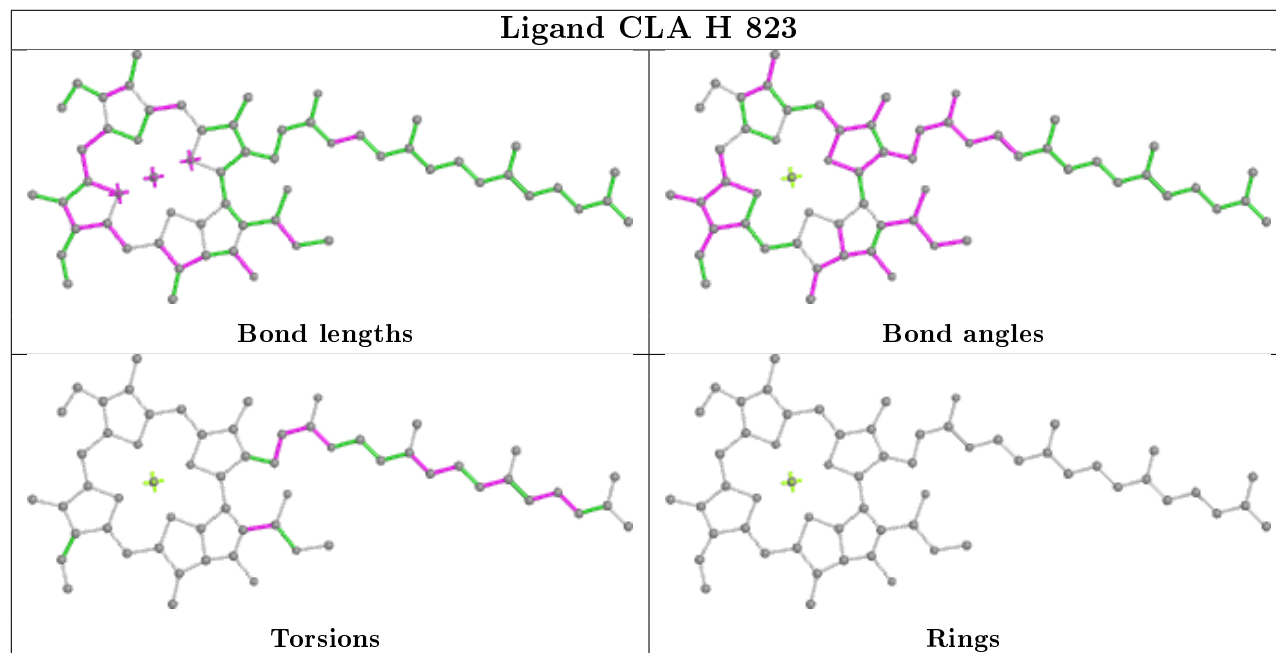
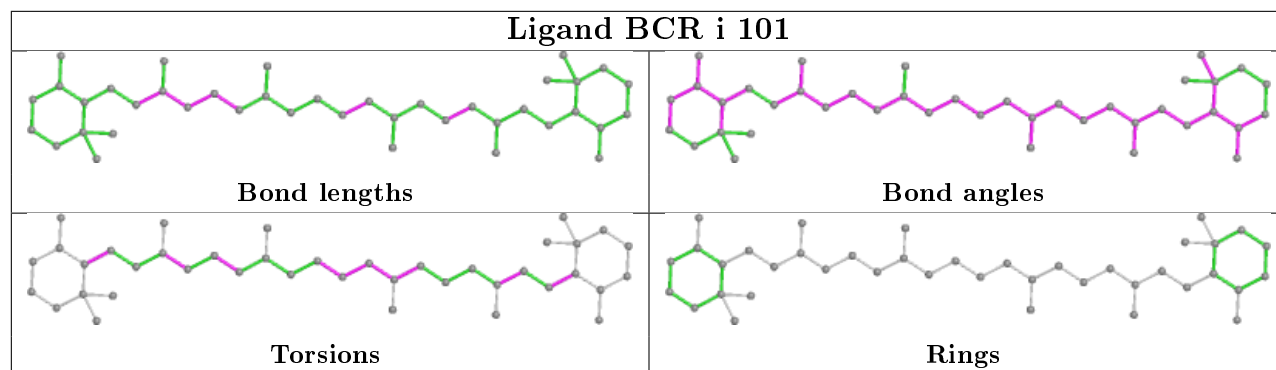
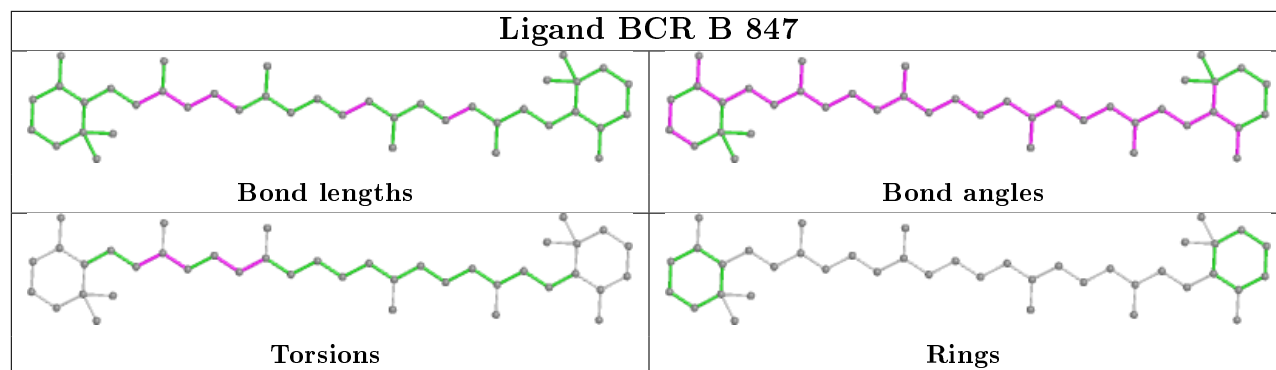


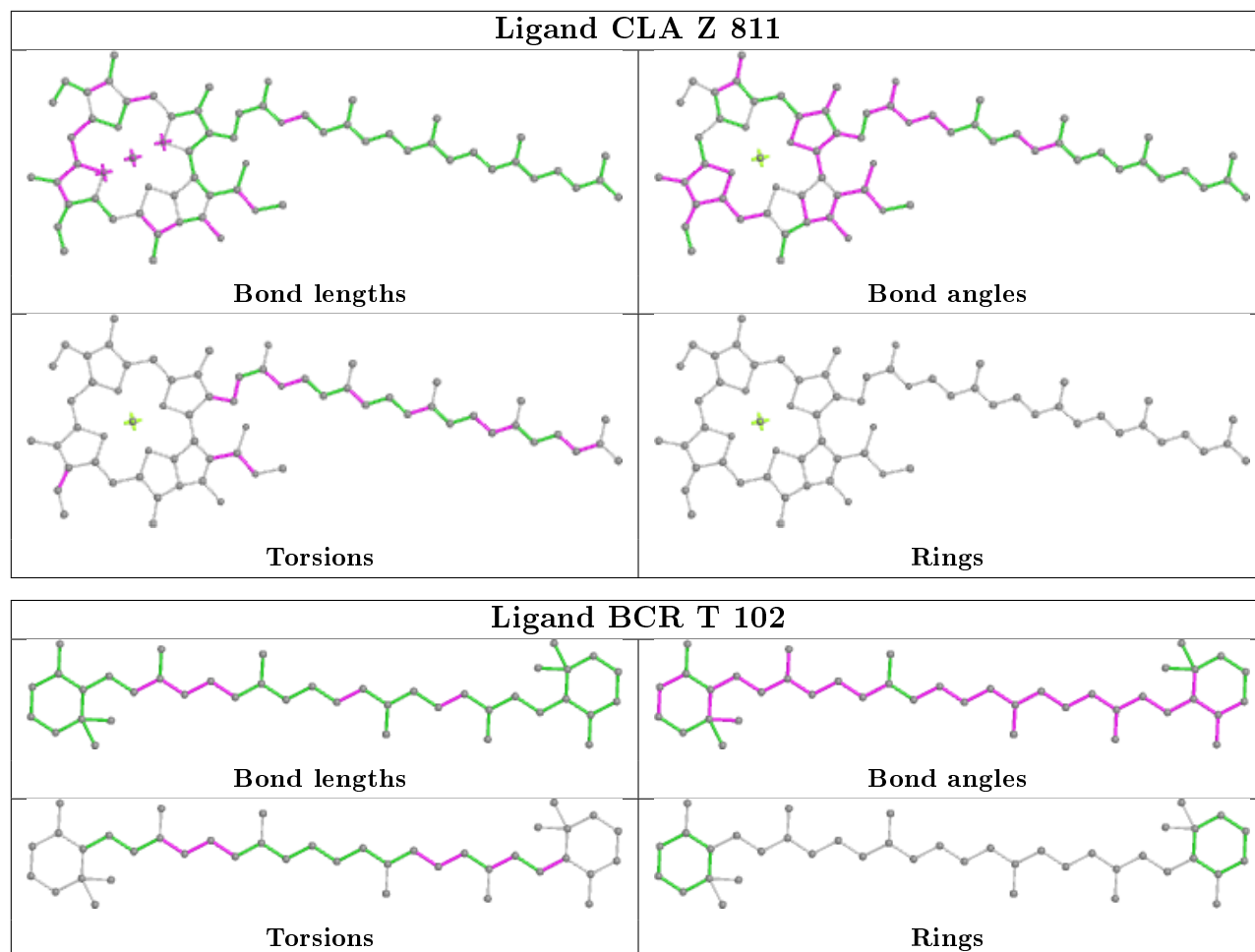


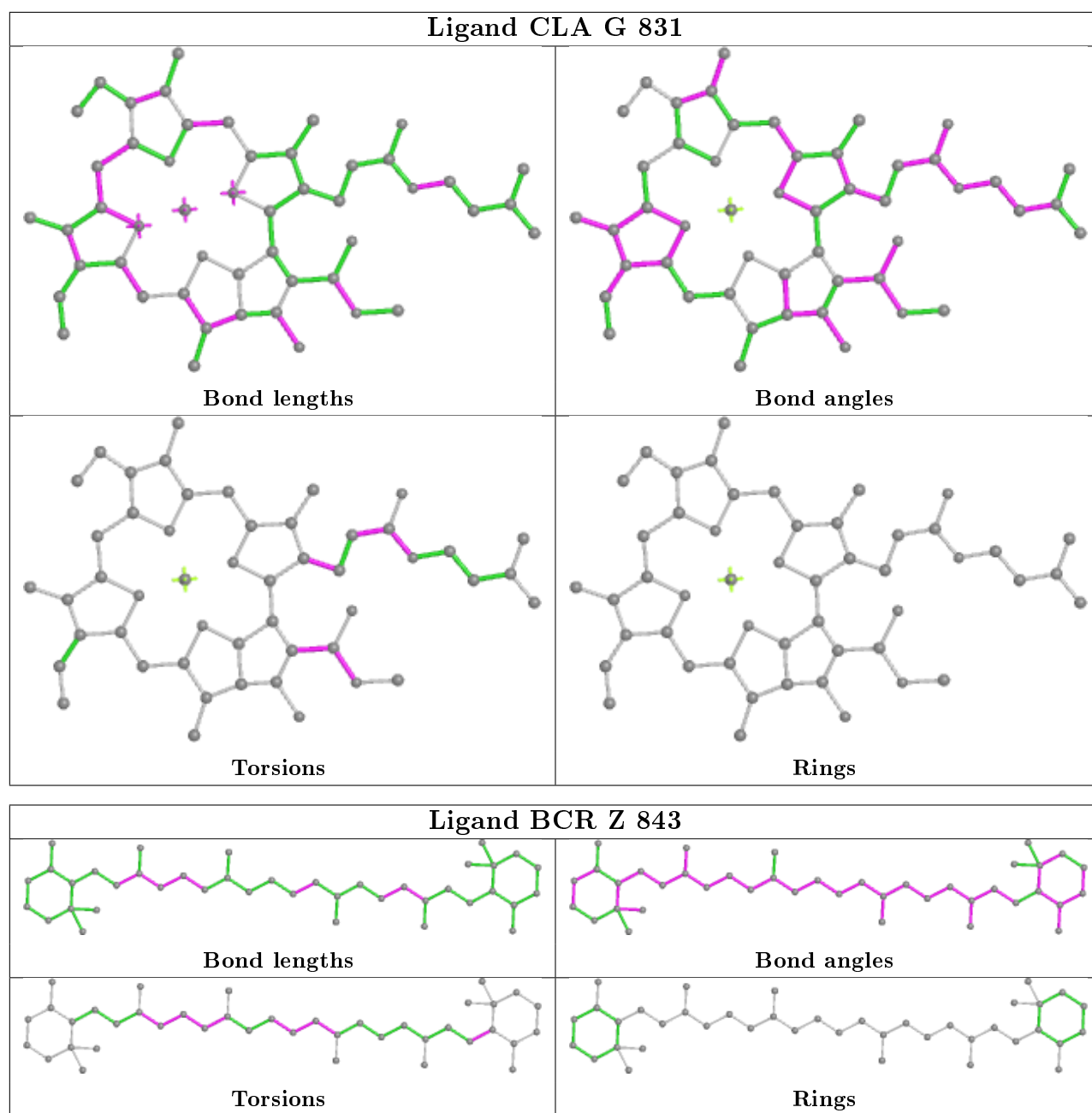




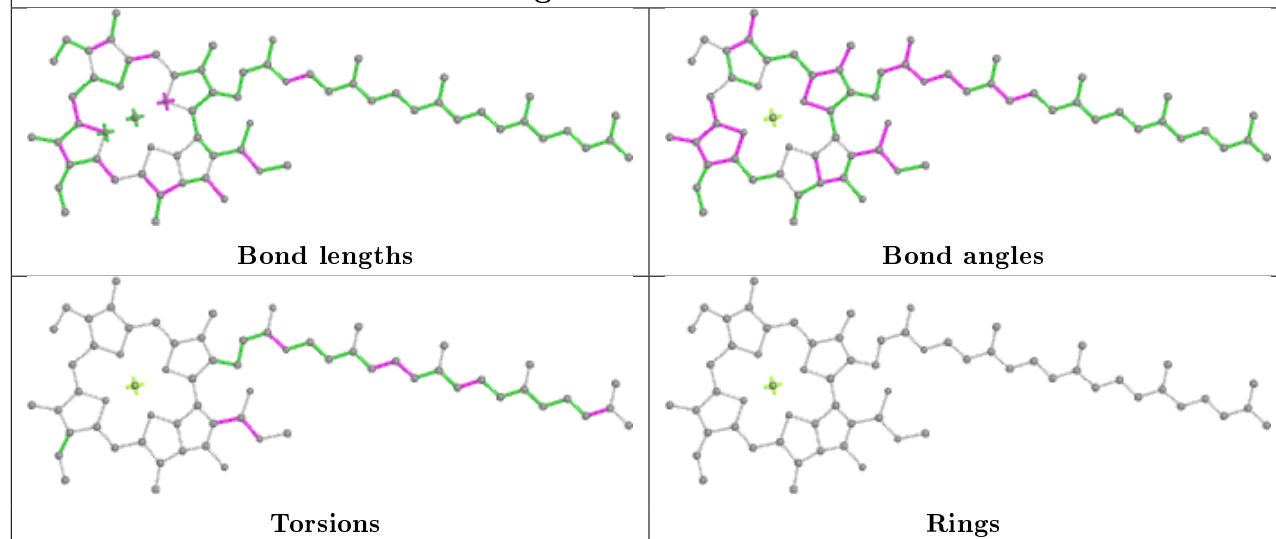




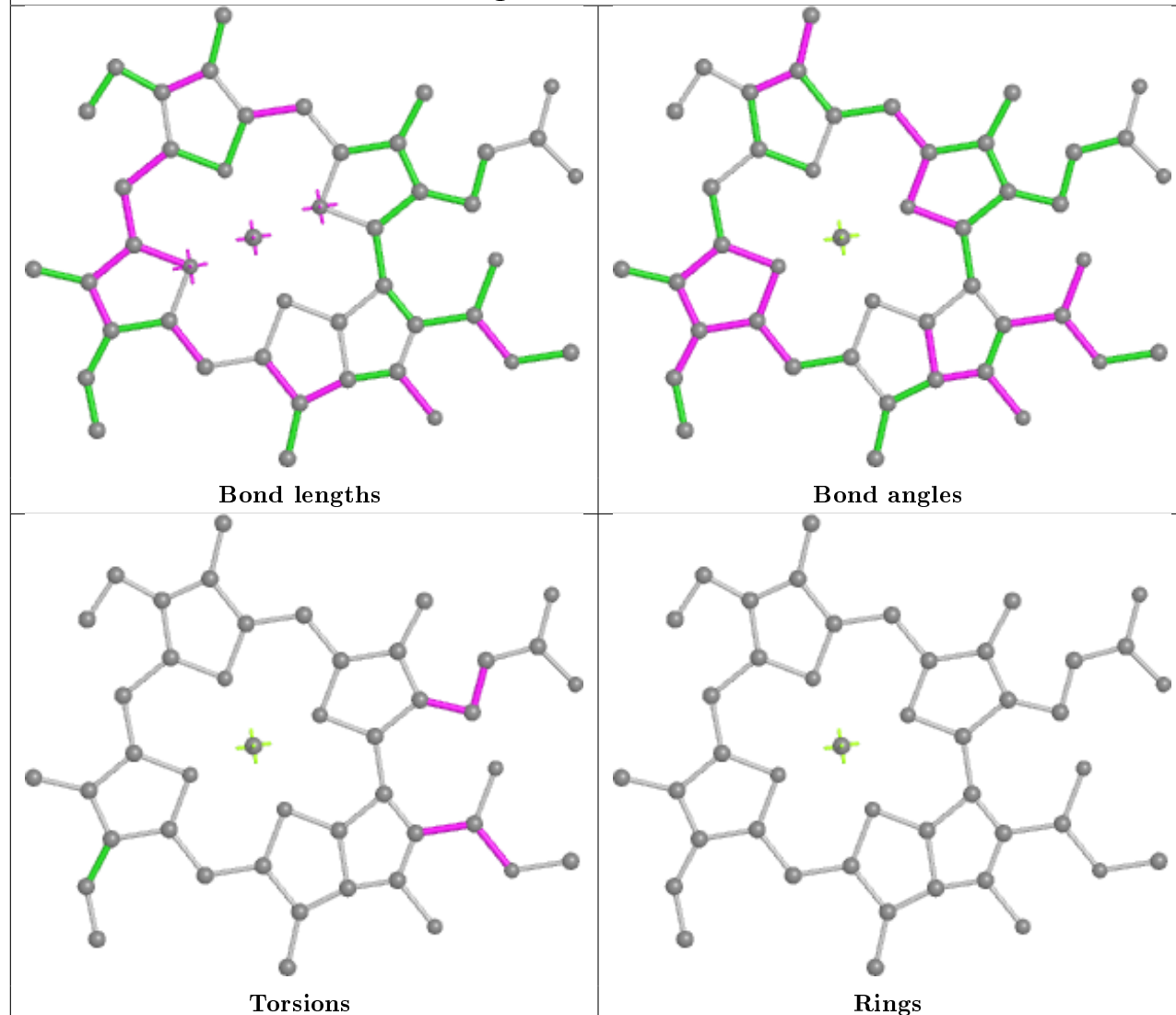




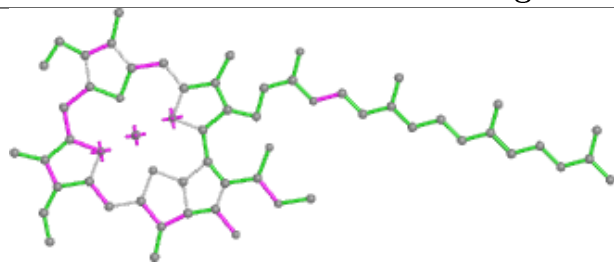
## Ligand CLA Z 830



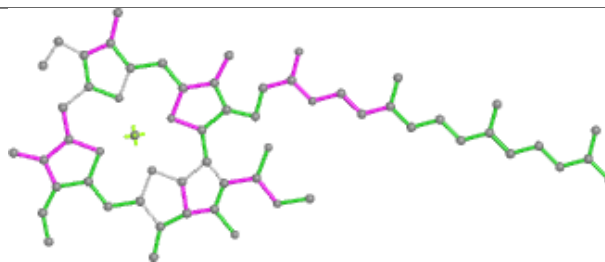
## Ligand CLA Z 816



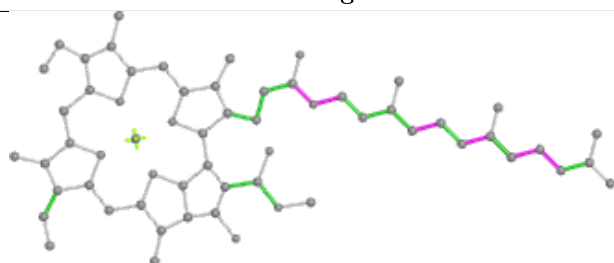
## Ligand CLA Y 826



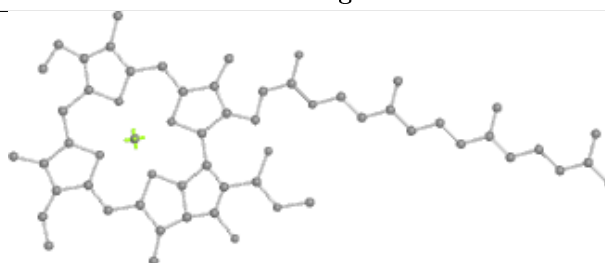
Bond lengths



Bond angles

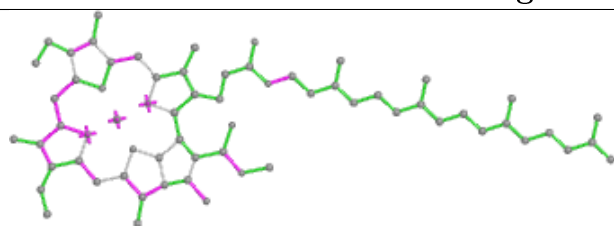


Torsions

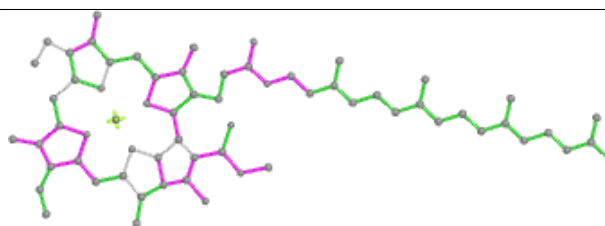


Rings

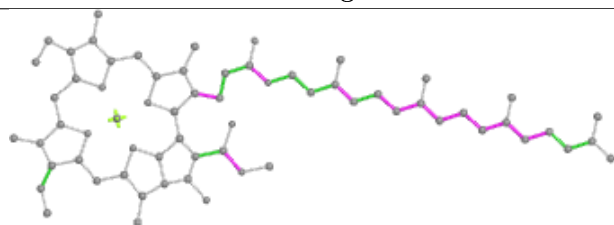
## Ligand CLA Z 814



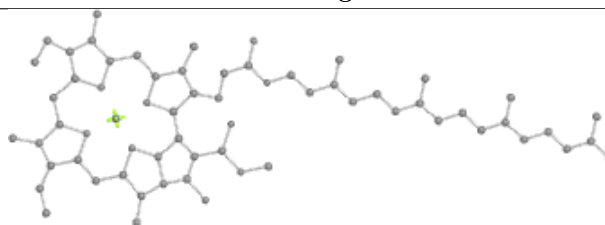
Bond lengths



Bond angles

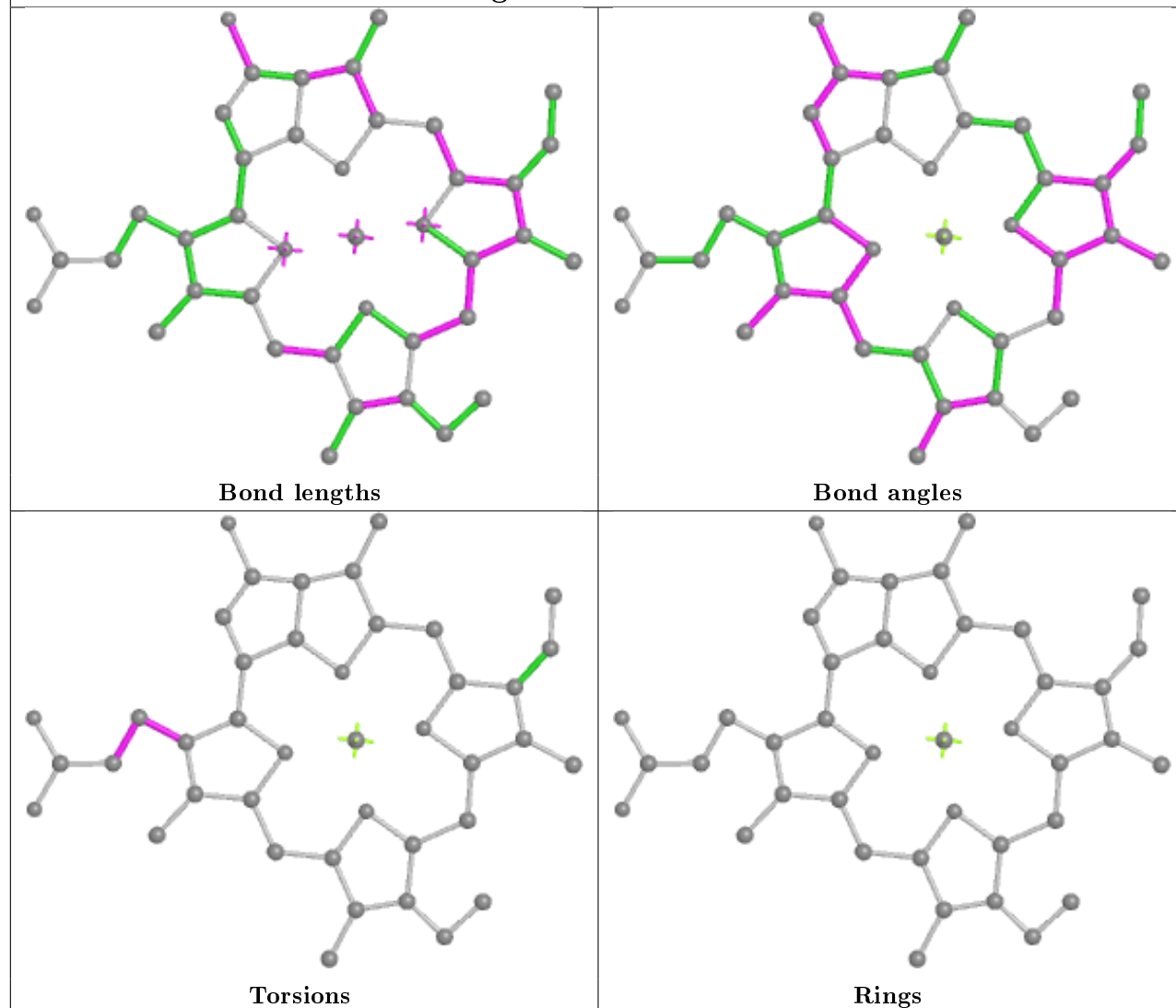


Torsions

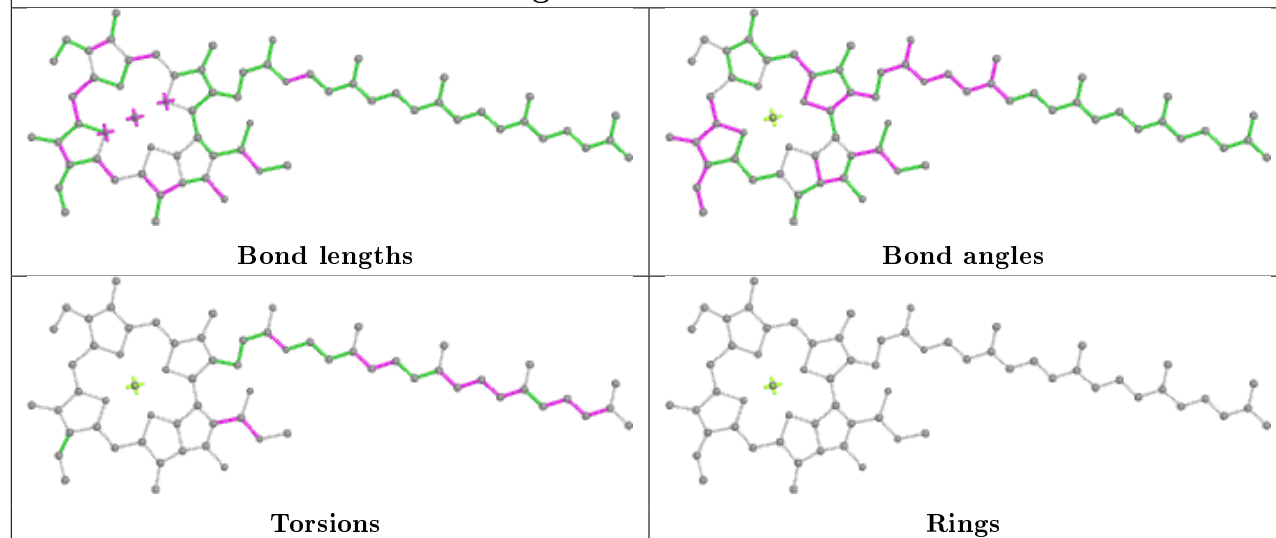


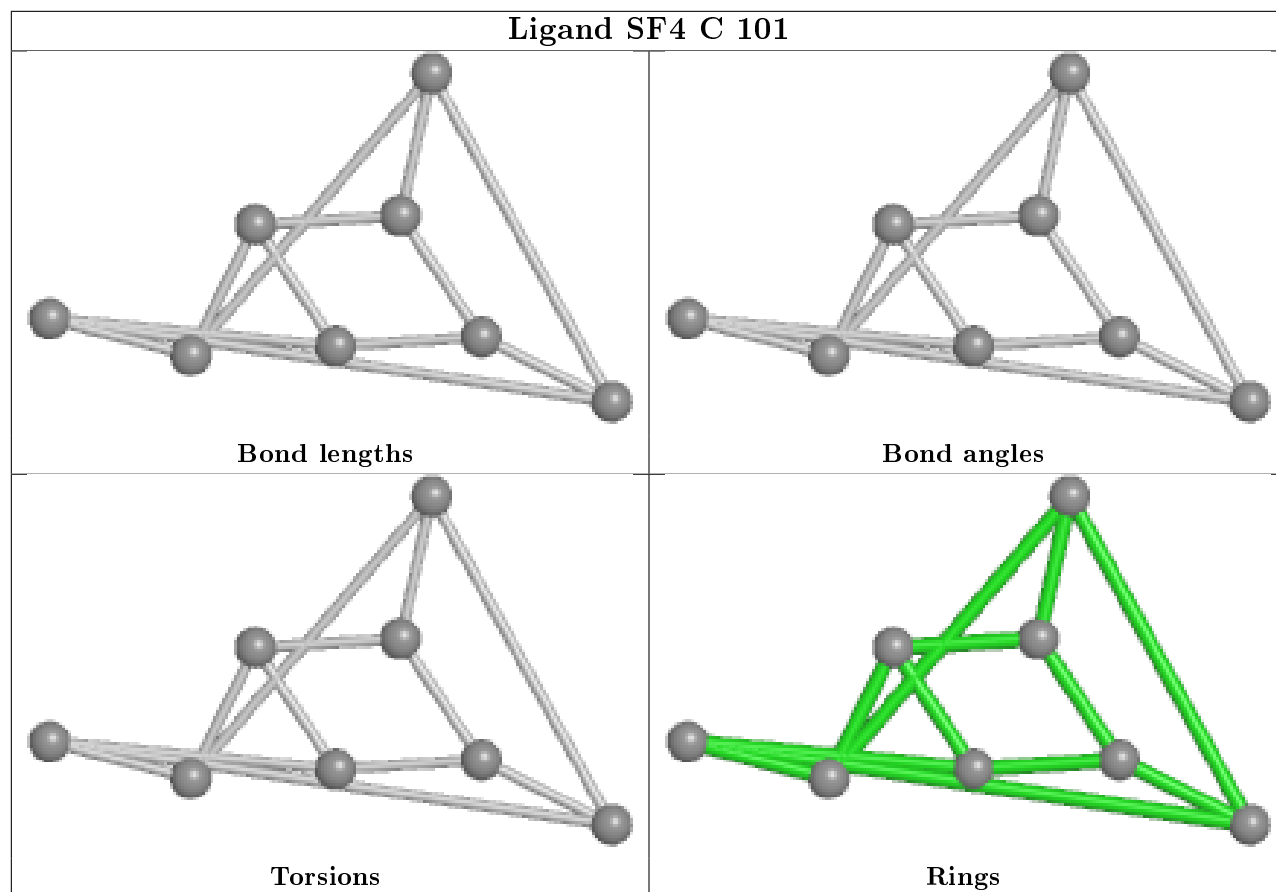
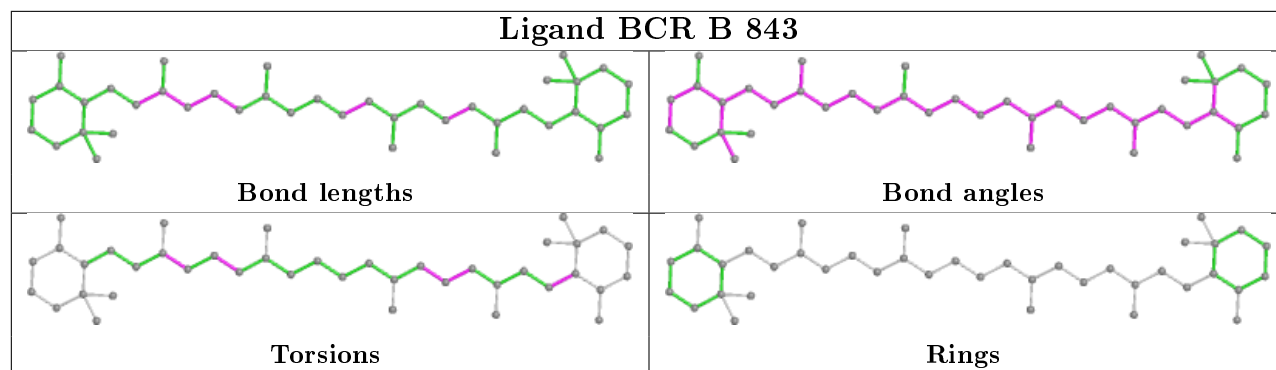
Rings

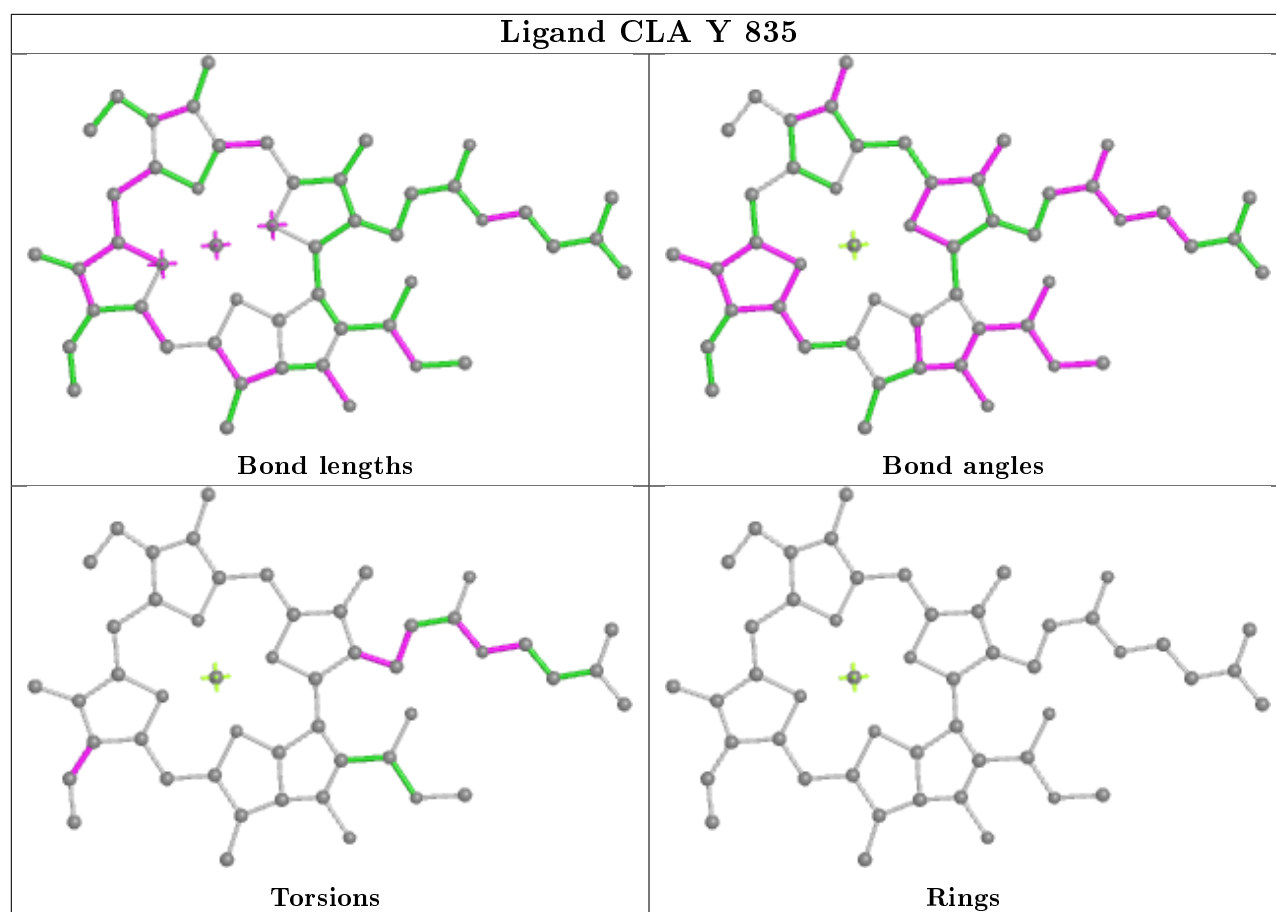
## Ligand CLA T 101



## Ligand CLA B 801

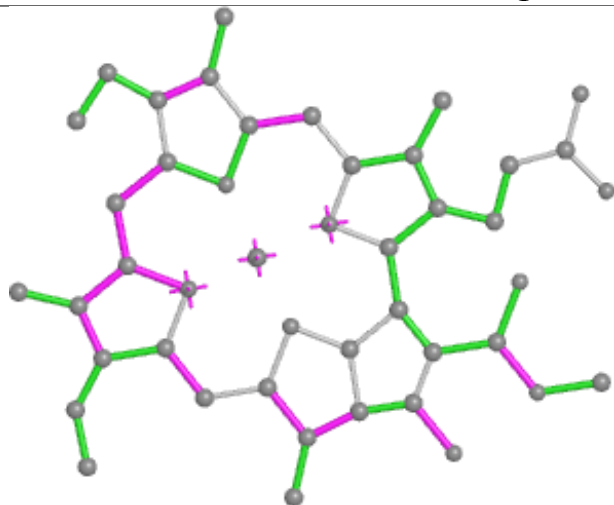




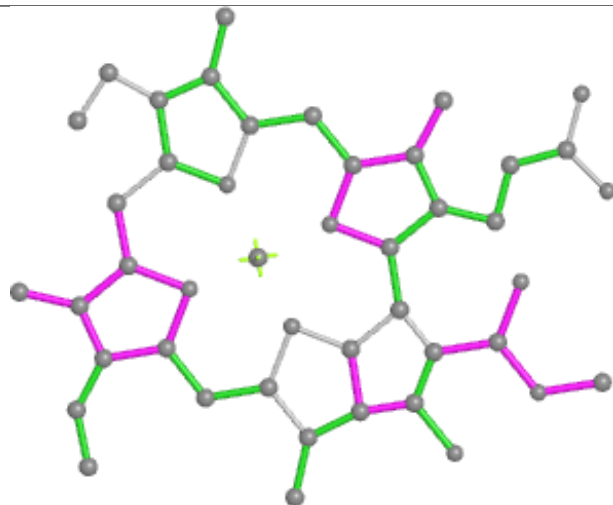




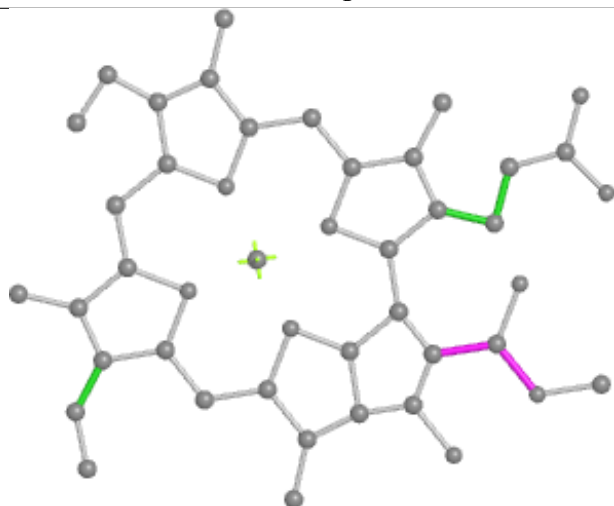
## Ligand CLA T 103



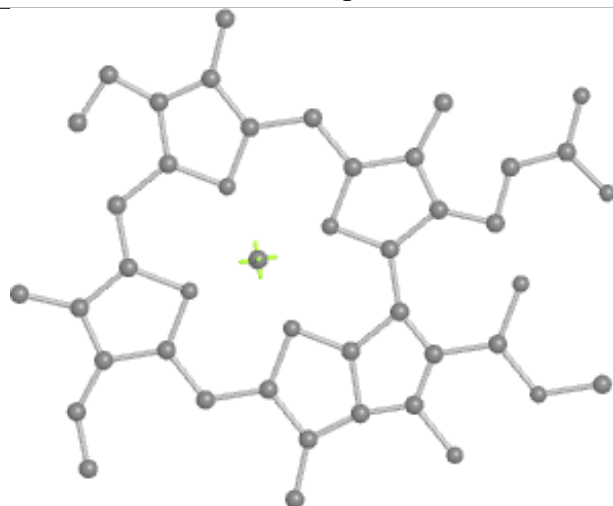
Bond lengths



Bond angles

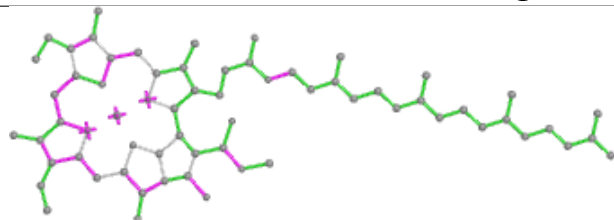


Torsions

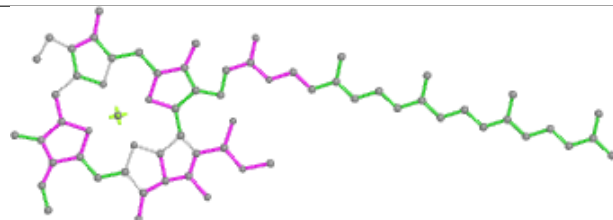


Rings

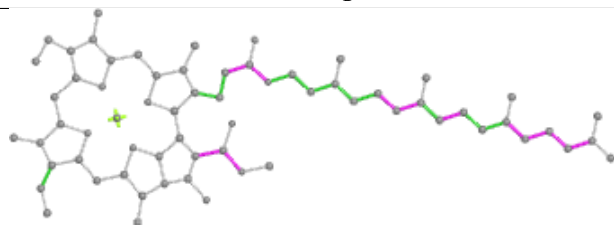
## Ligand CLA A 830



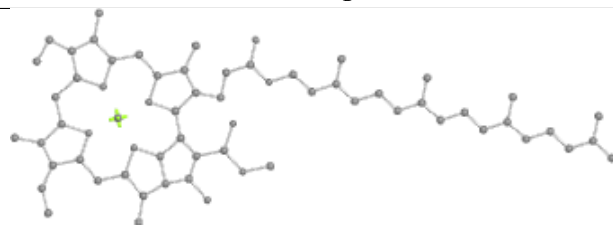
Bond lengths



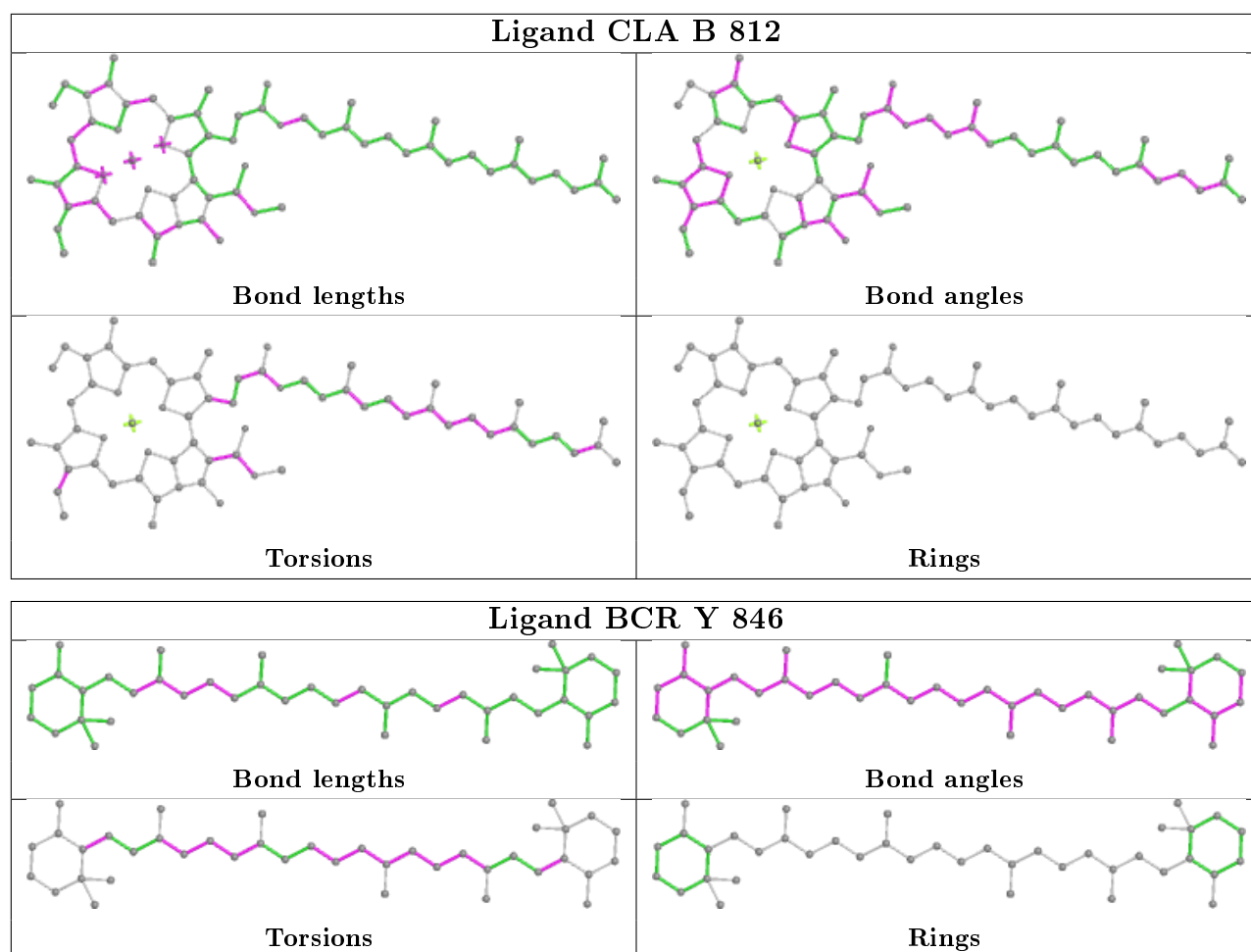
Bond angles



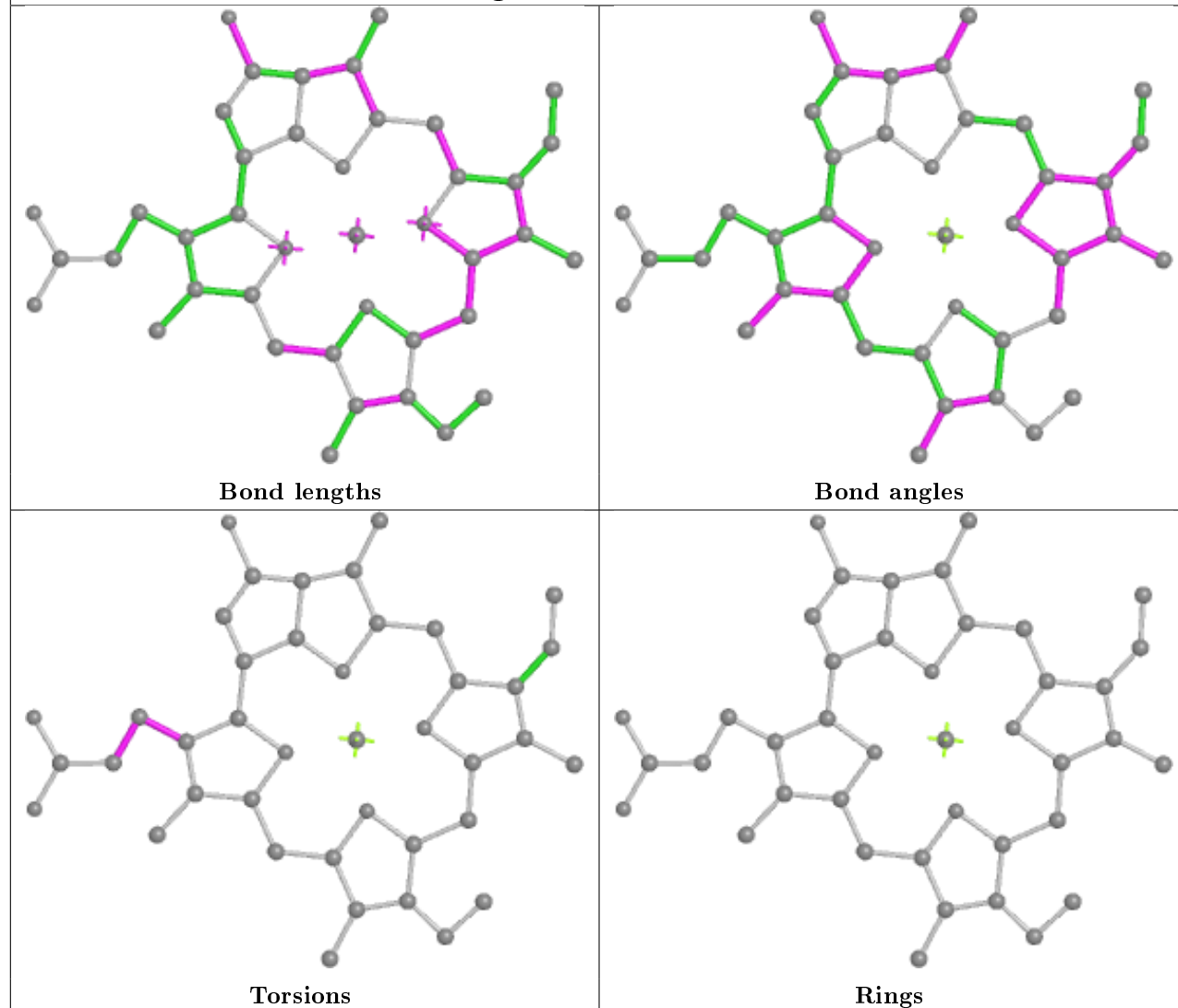
Torsions



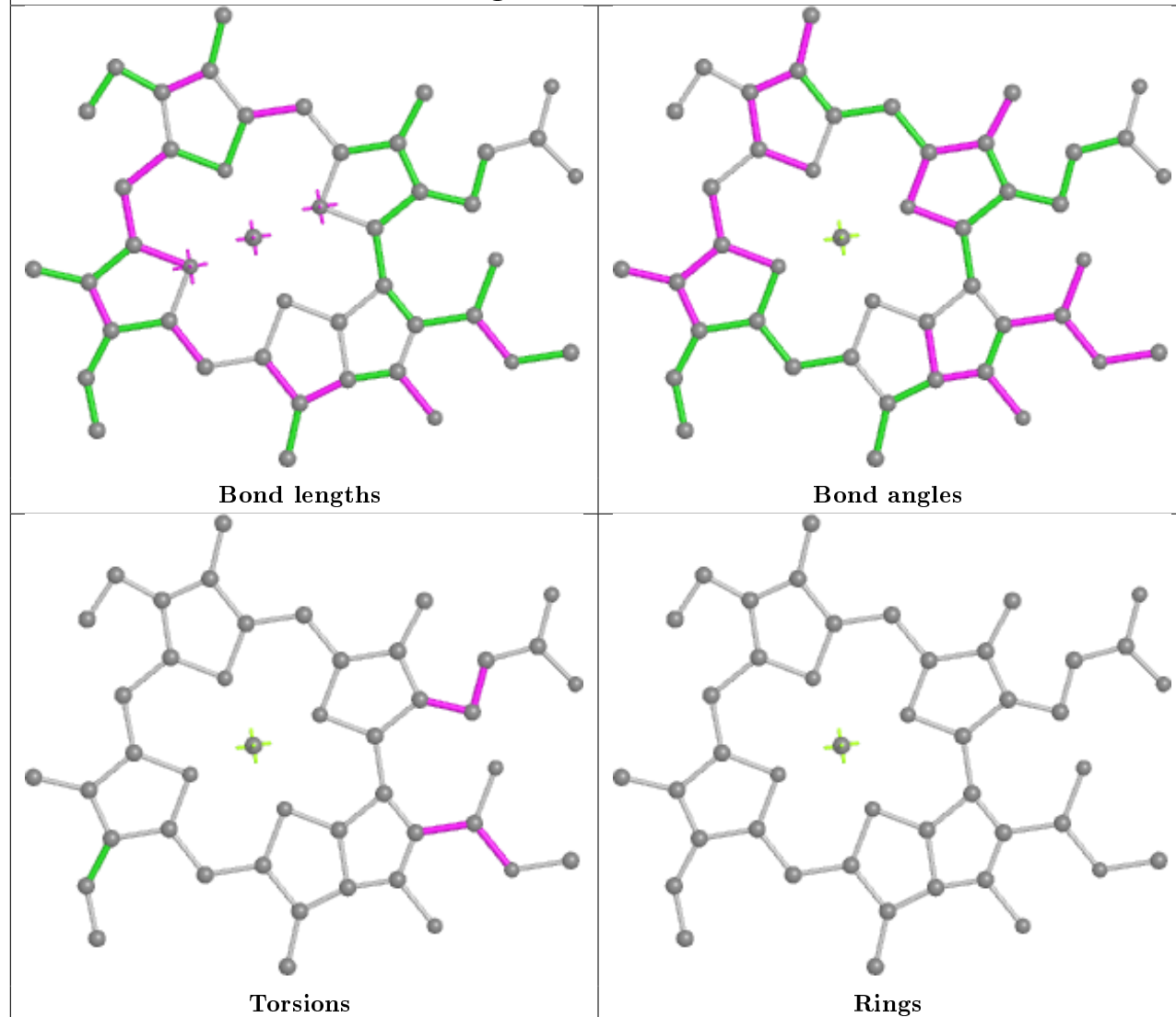
Rings



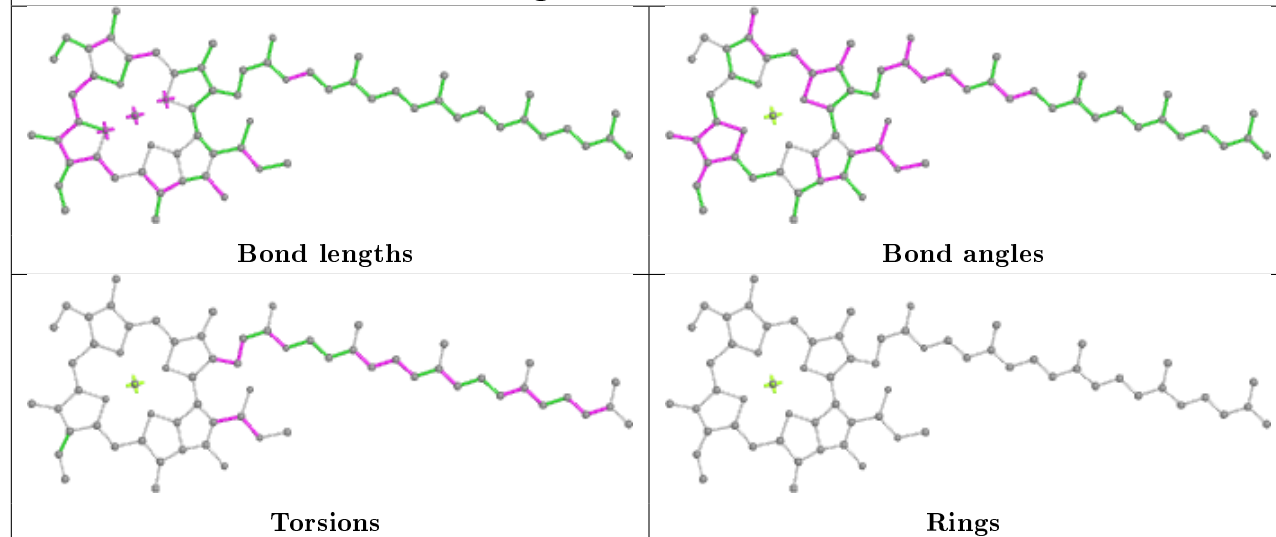
## Ligand CLA K 101

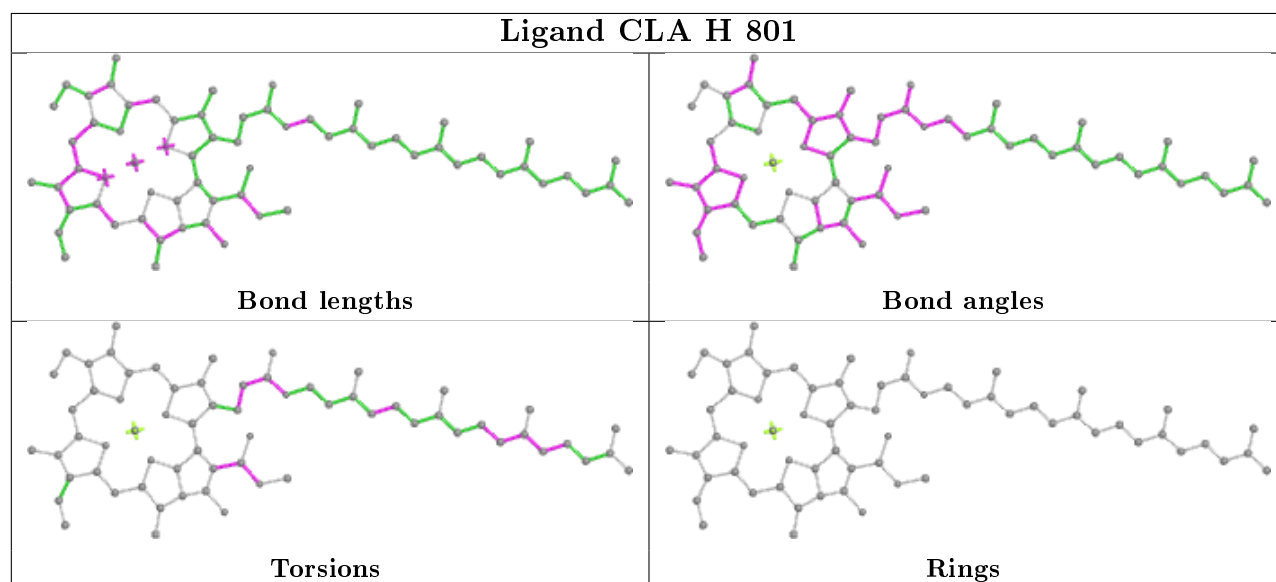
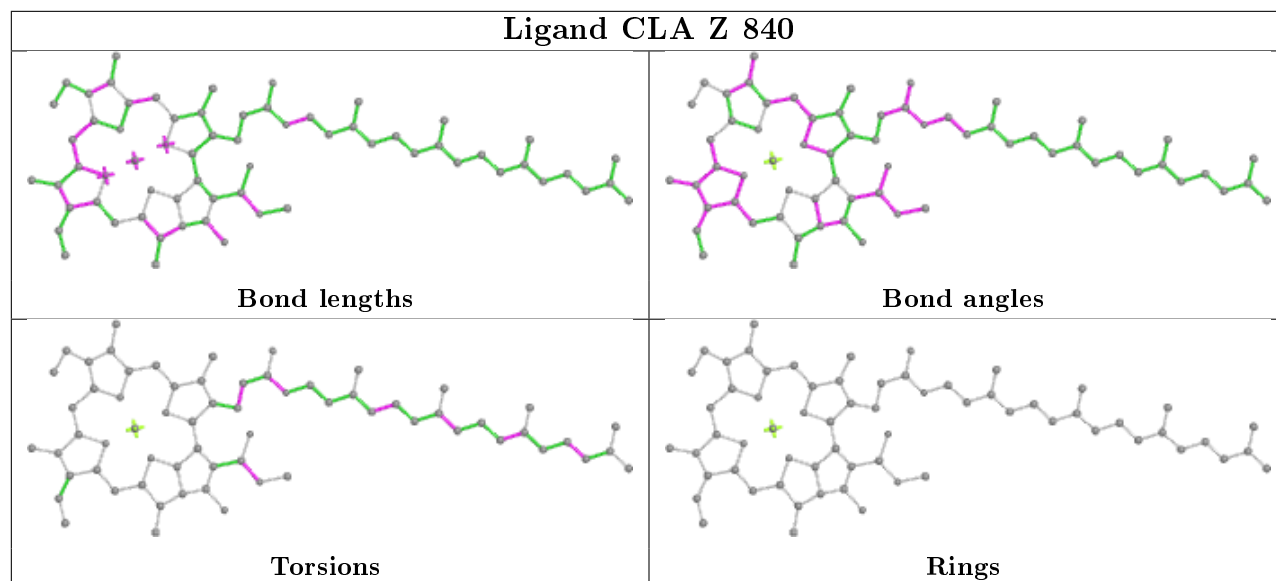
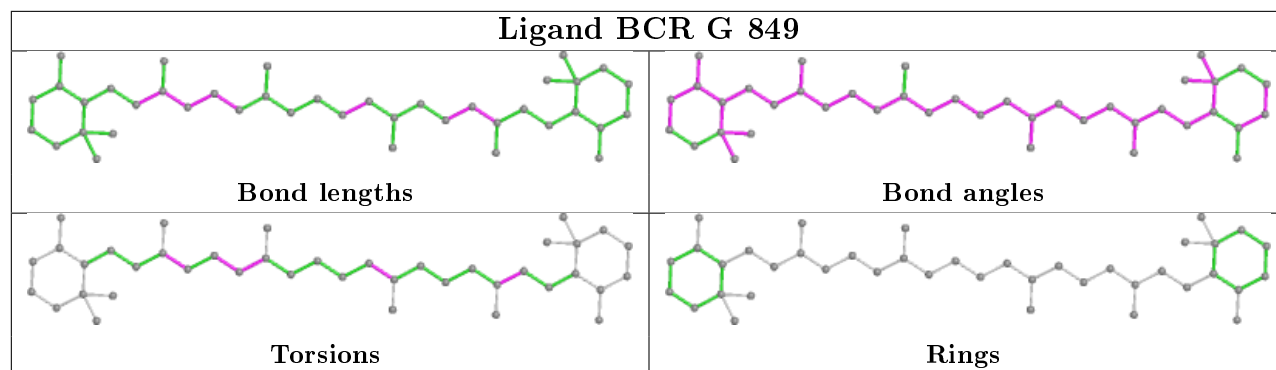


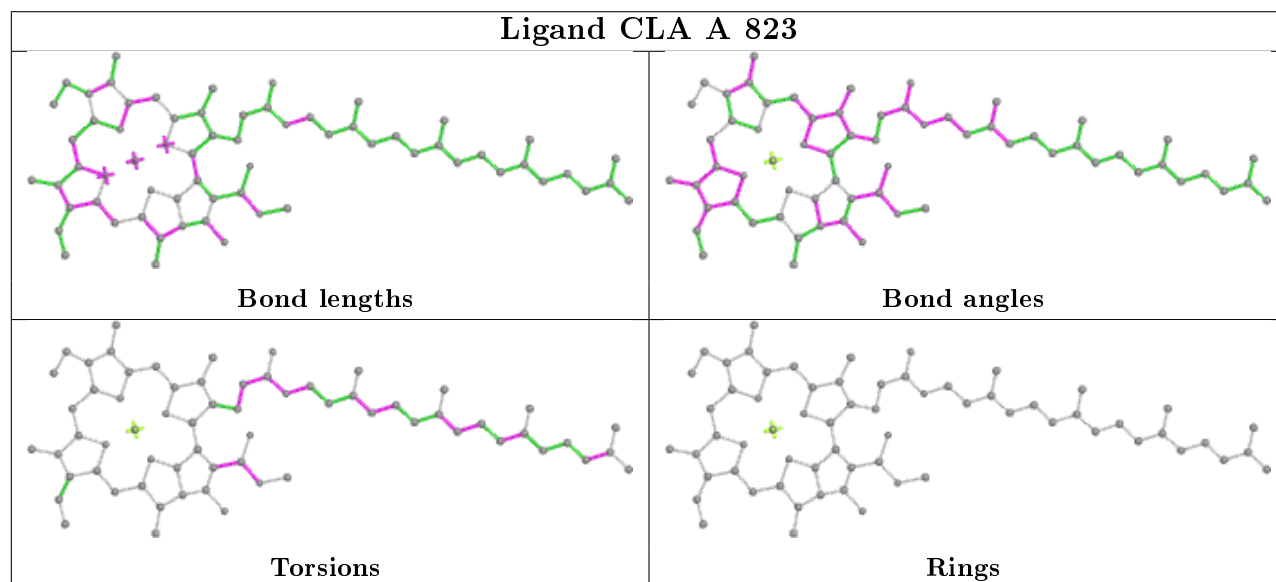
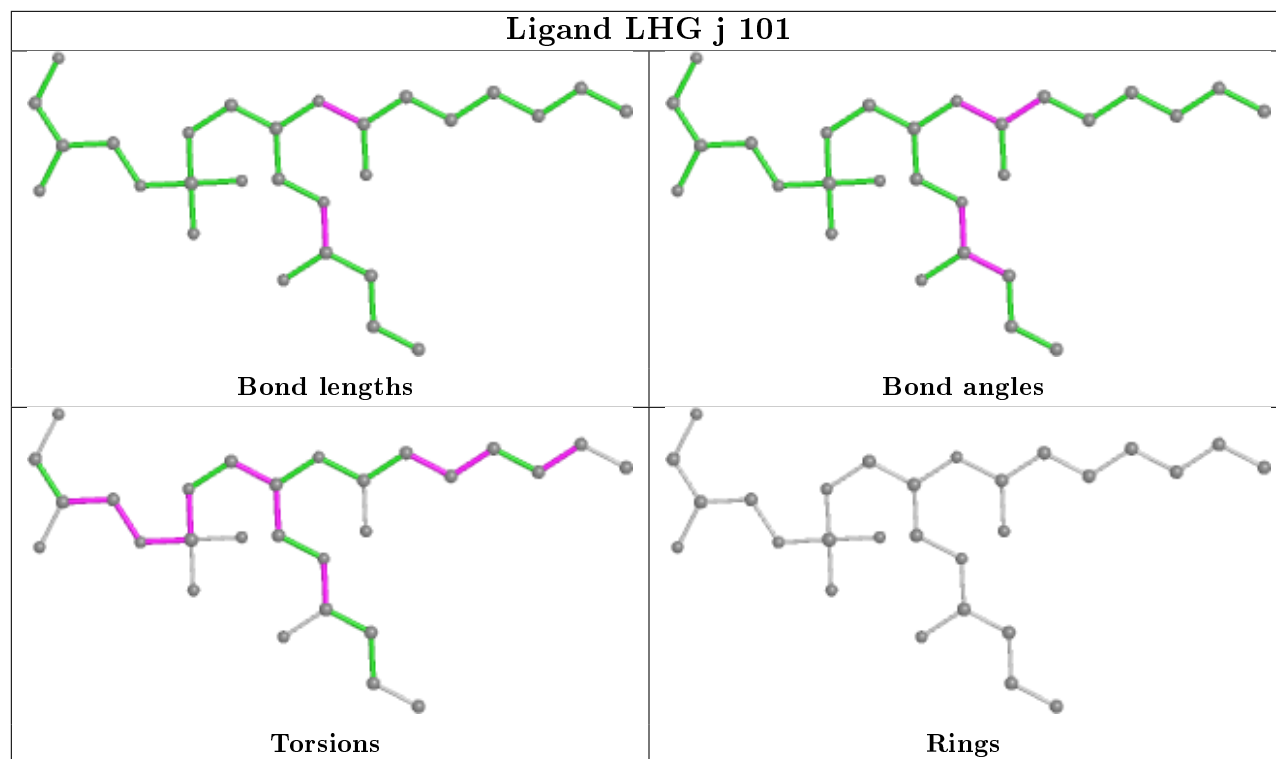
## Ligand CLA H 834



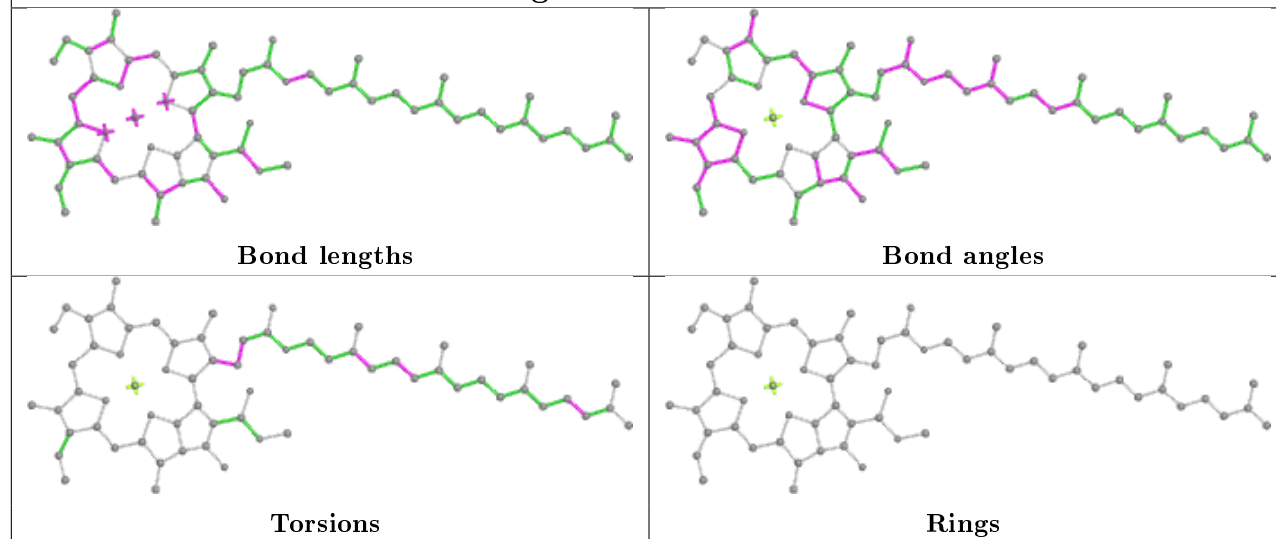
## Ligand CLA A 809



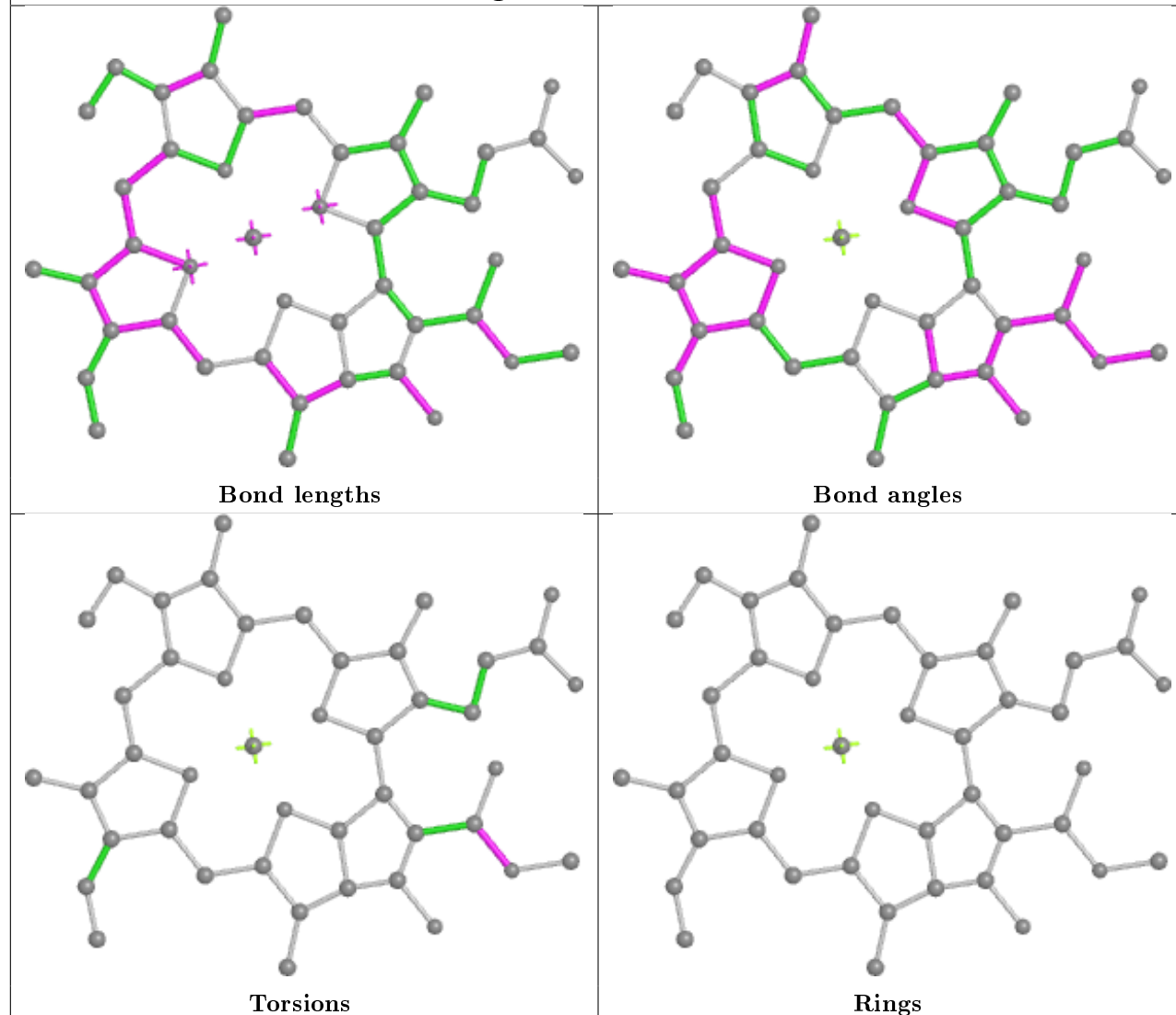


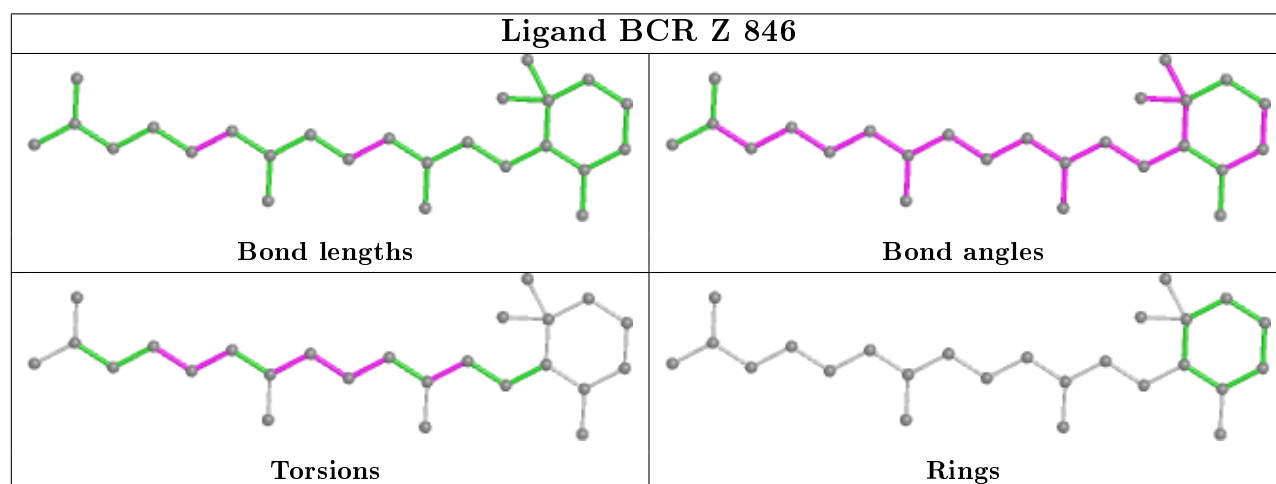
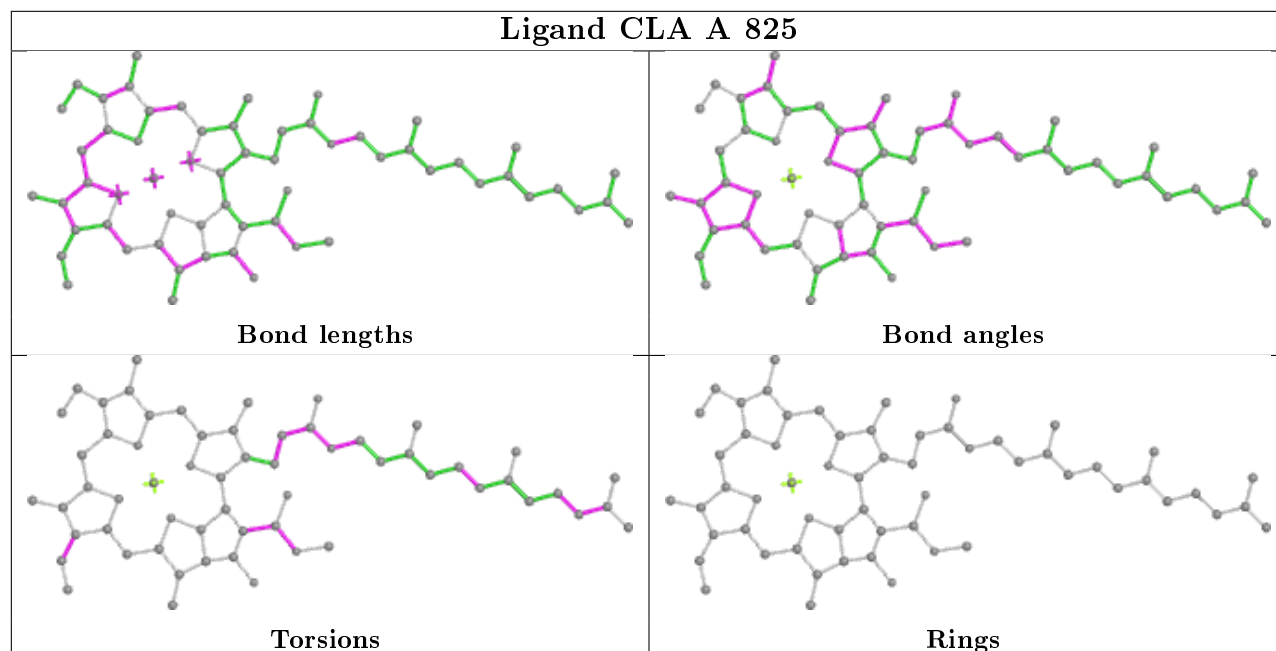
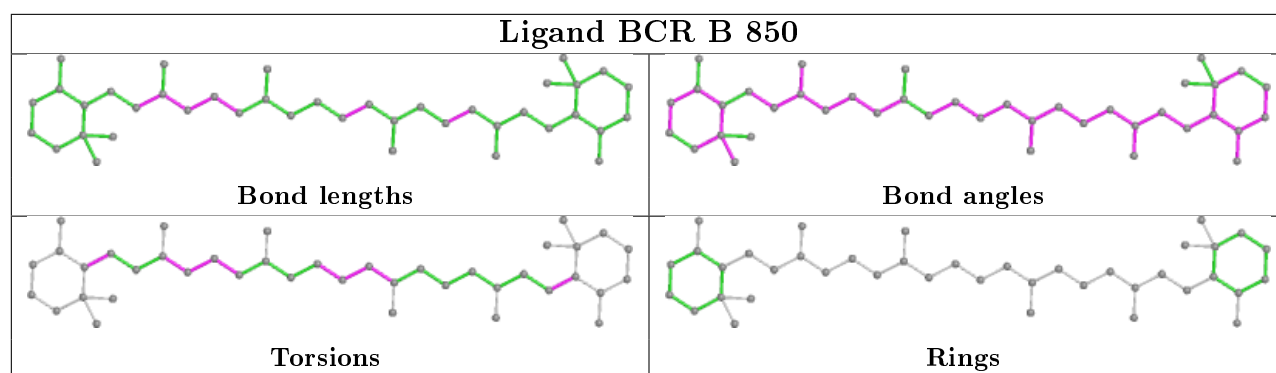


## Ligand CLA H 828



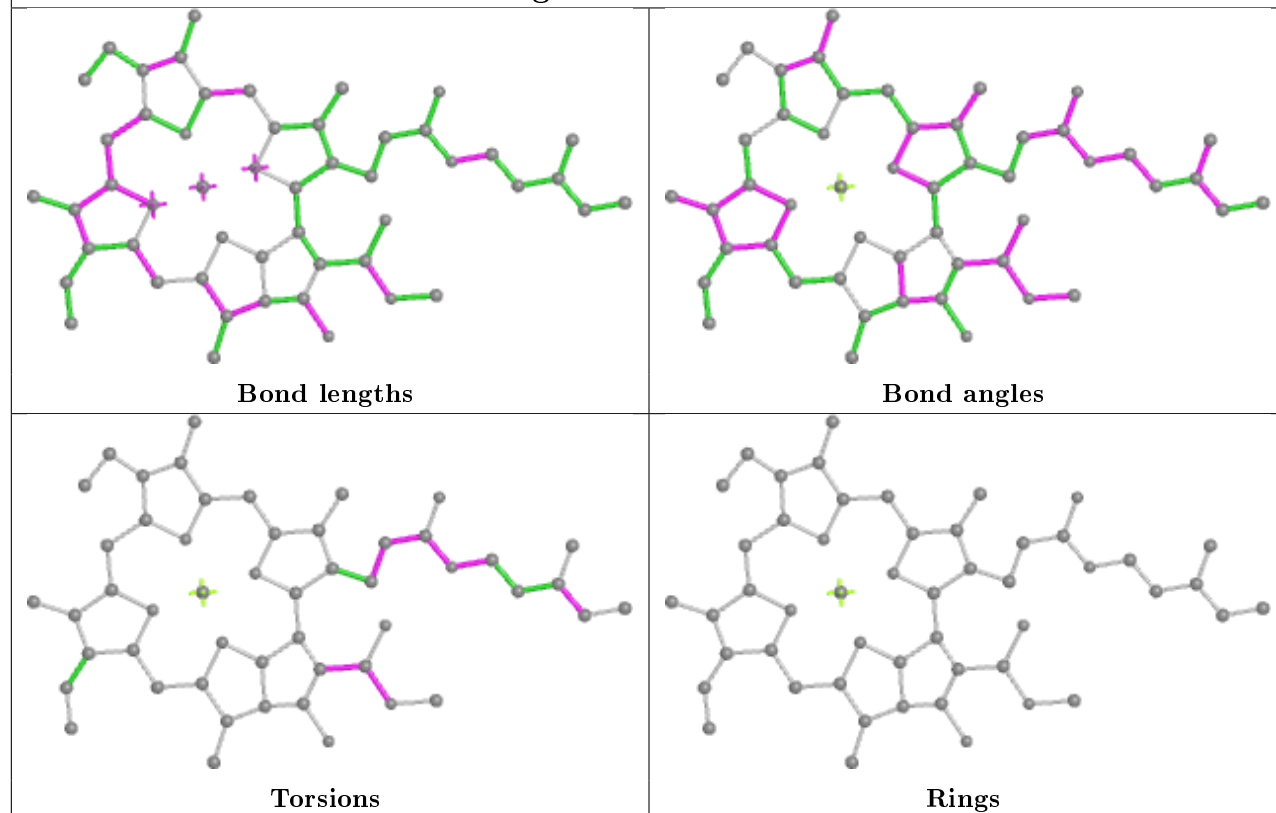
## Ligand CLA B 834



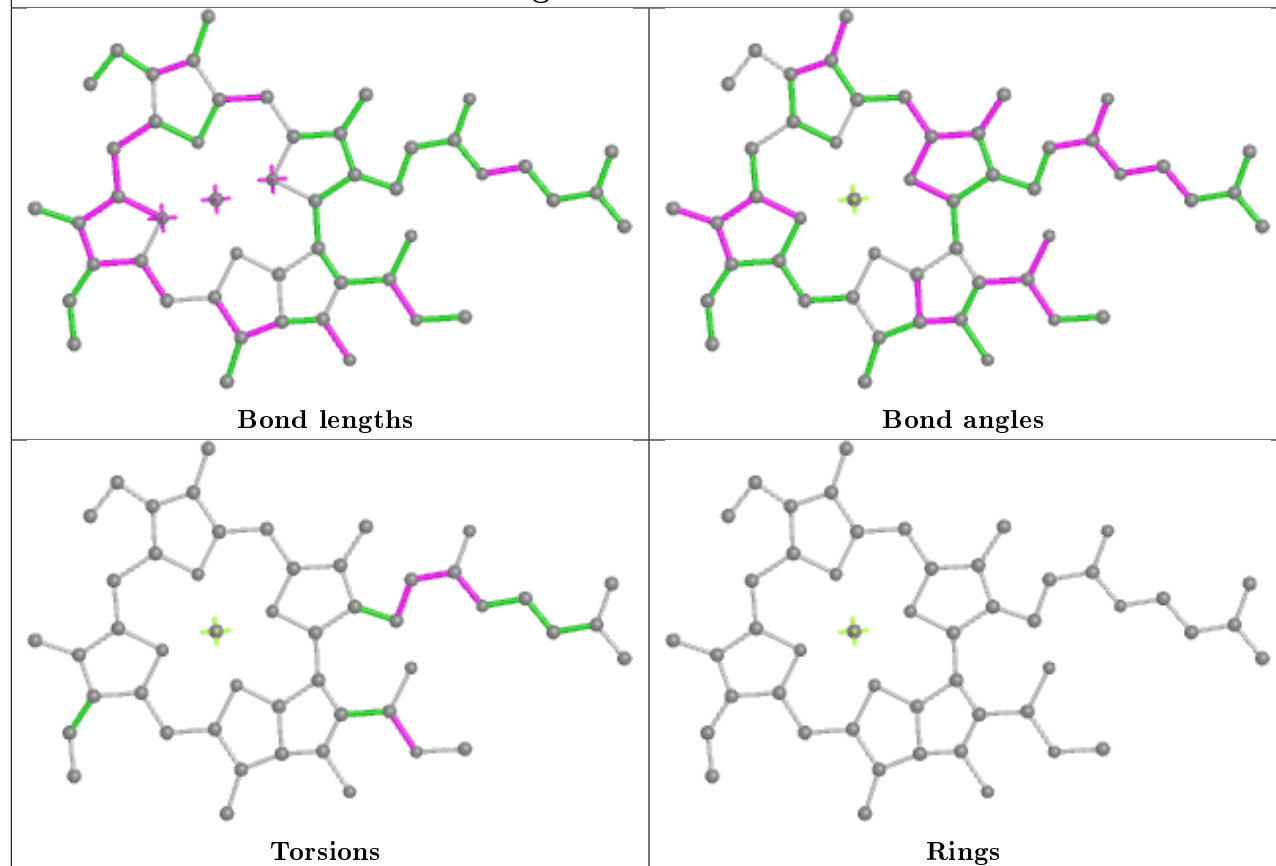




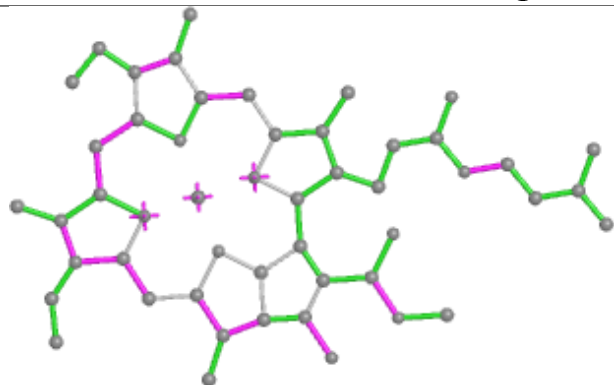
## Ligand CLA Y 807



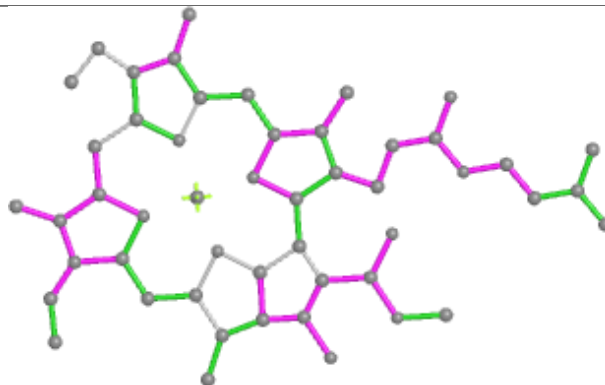
## Ligand CLA Y 815



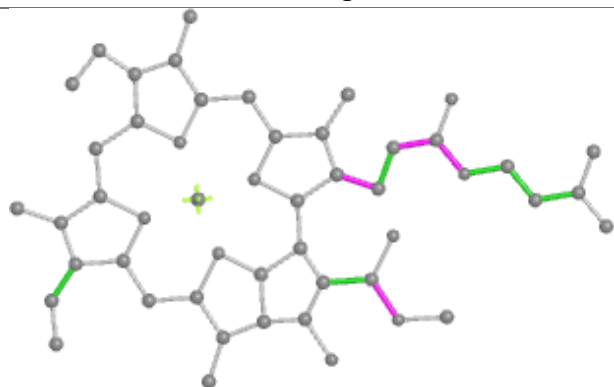
## Ligand CLA Y 823



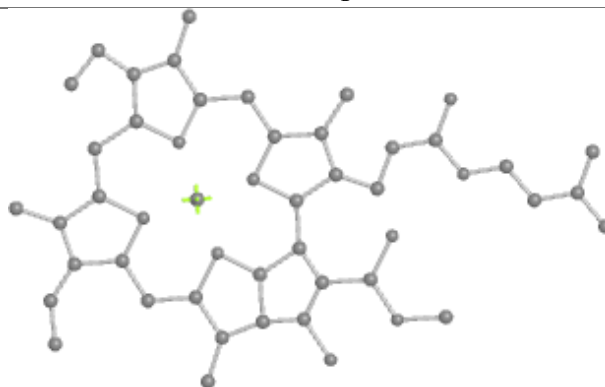
Bond lengths



Bond angles

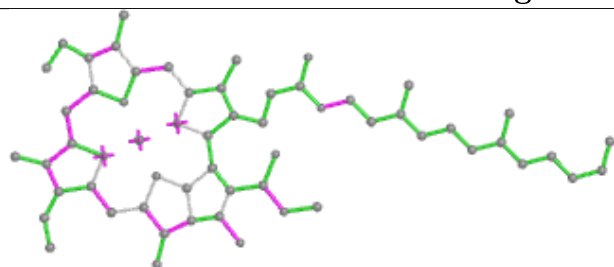


Torsions

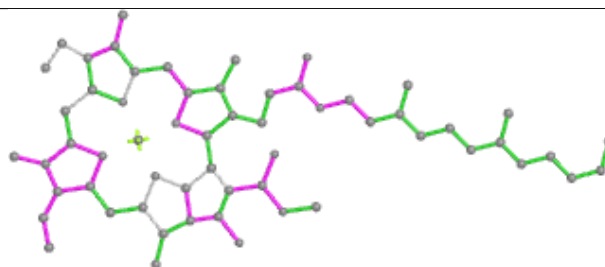


Rings

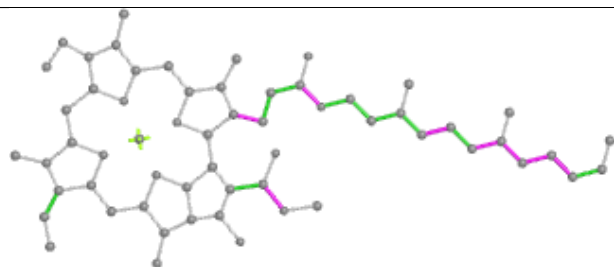
## Ligand CLA Y 804



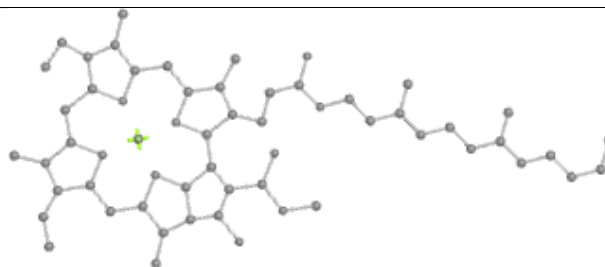
Bond lengths



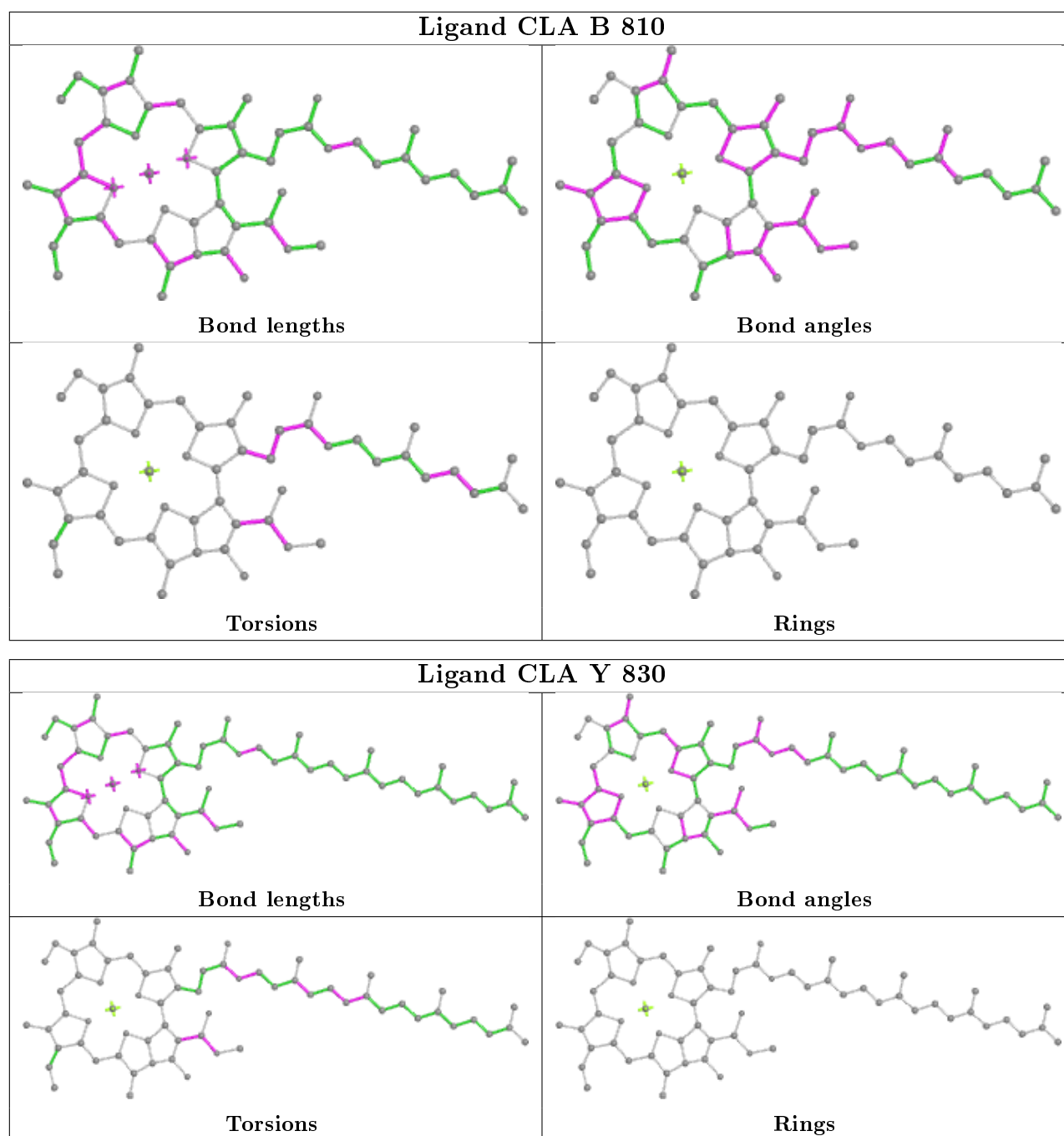
Bond angles



Torsions



Rings



## 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.

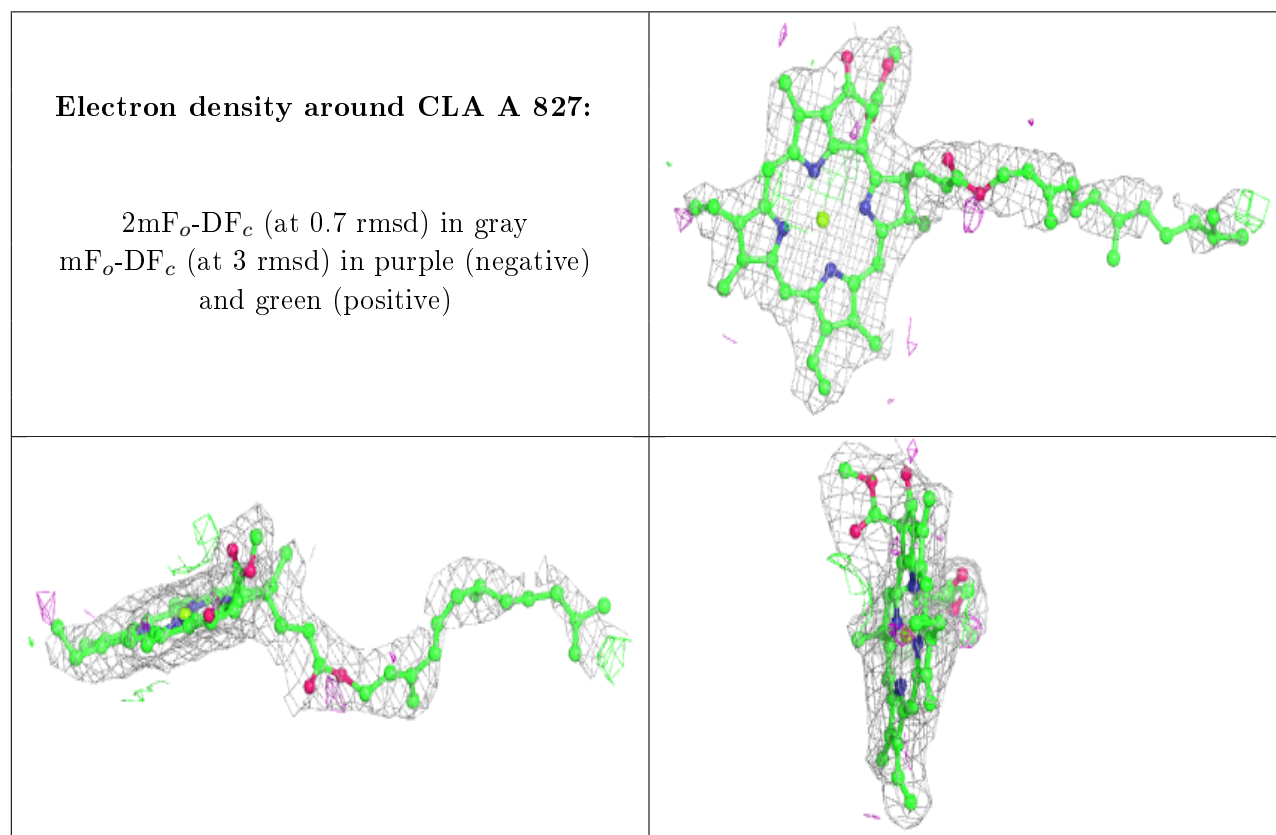
### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

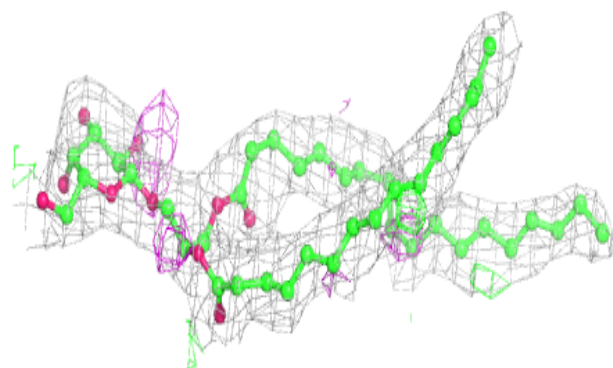
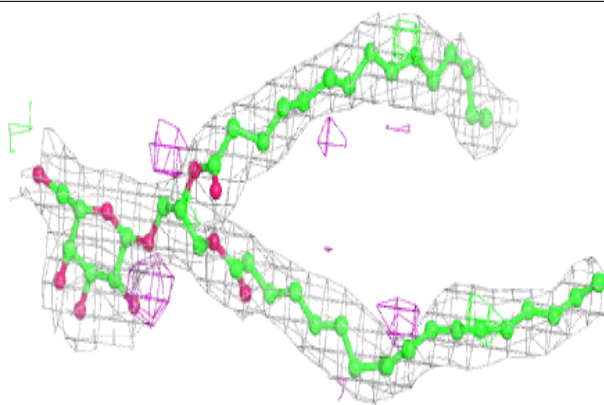
Unable to reproduce the depositors R factor - this section is therefore empty.

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.



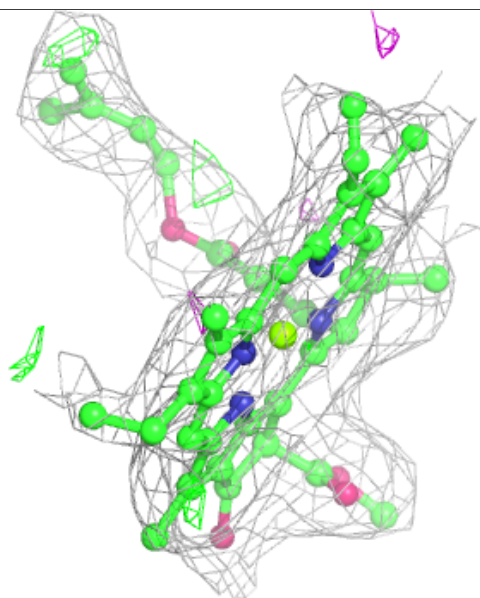
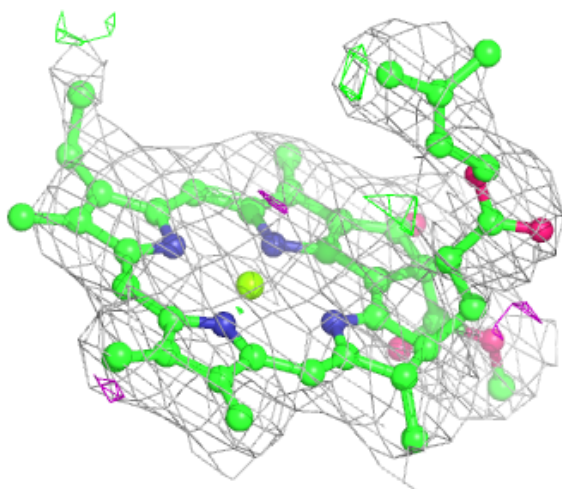
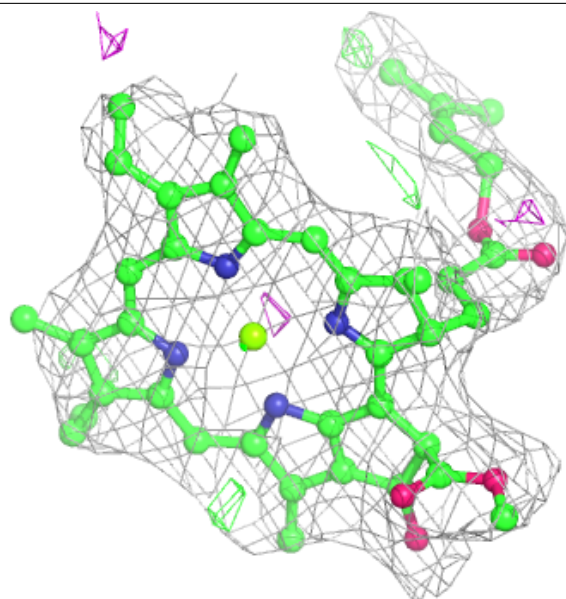
**Electron density around LMG B 848:**

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



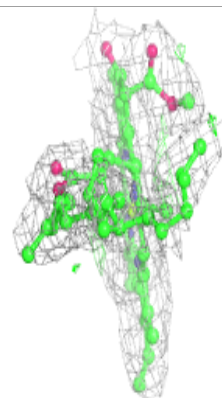
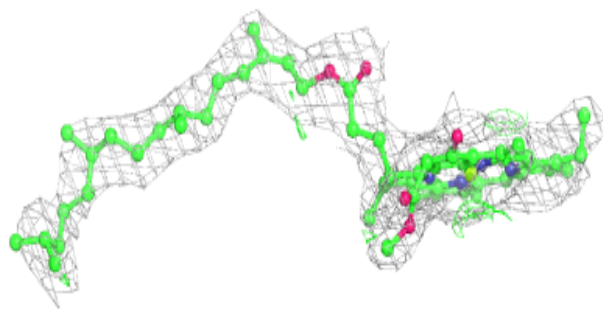
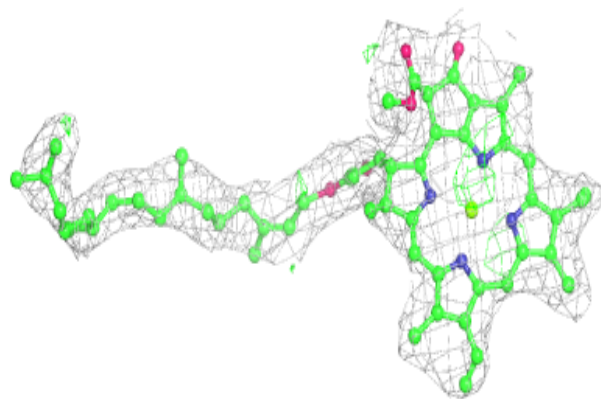
**Electron density around CLA A 832:**

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

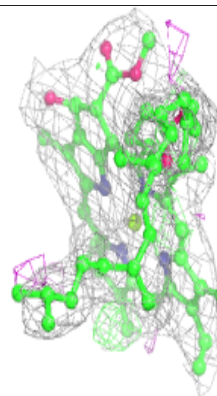
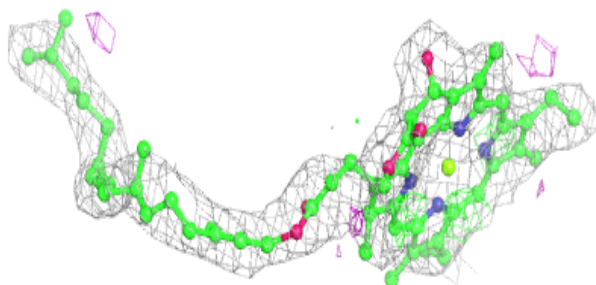
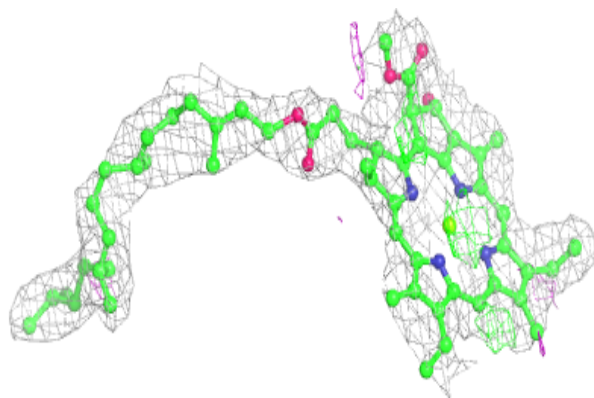


**Electron density around CLA H 825:**

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

**Electron density around CLA Z 802:**

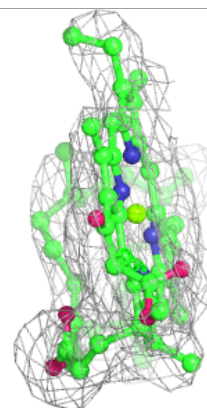
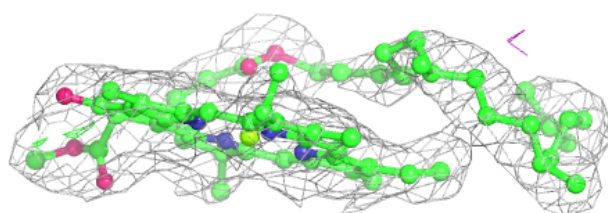
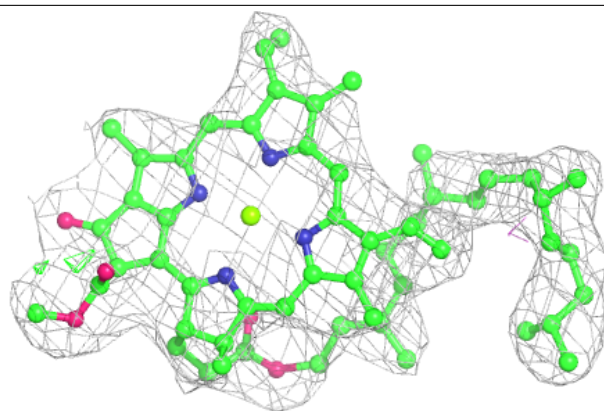
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA A 820:**

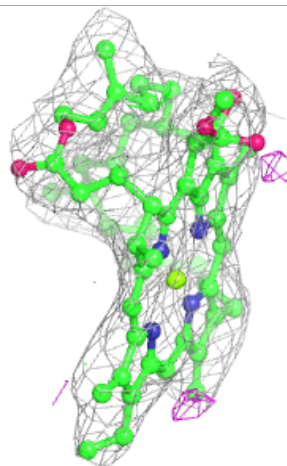
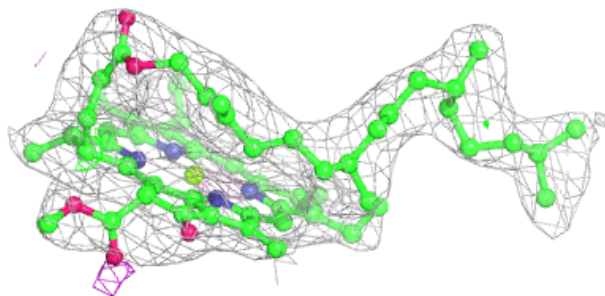
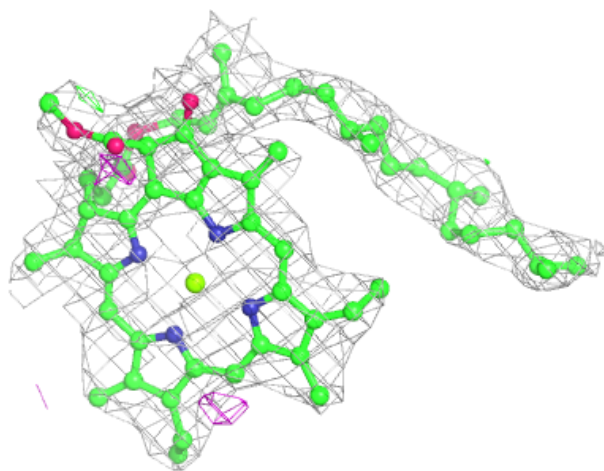
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





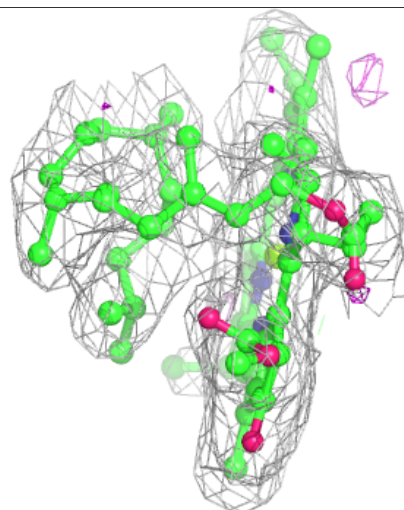
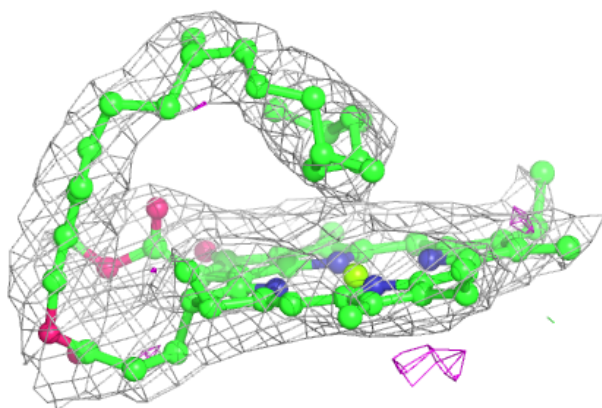
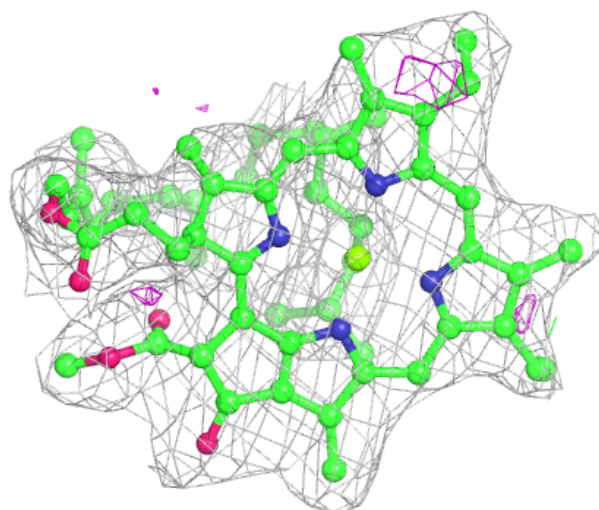
**Electron density around CLA G 829:**

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



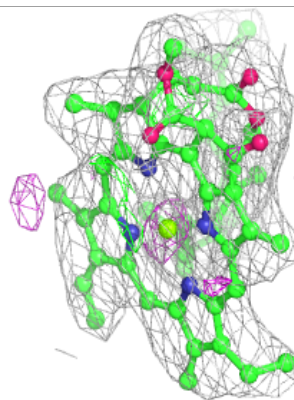
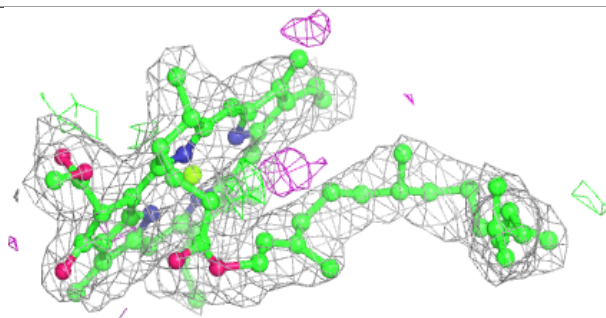
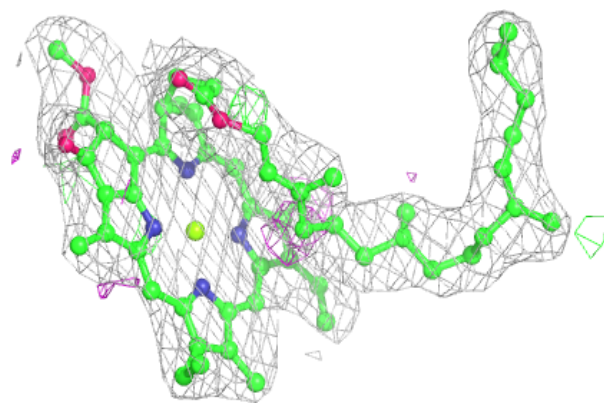
**Electron density around CLA H 806:**

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



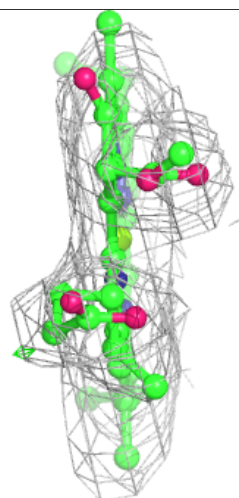
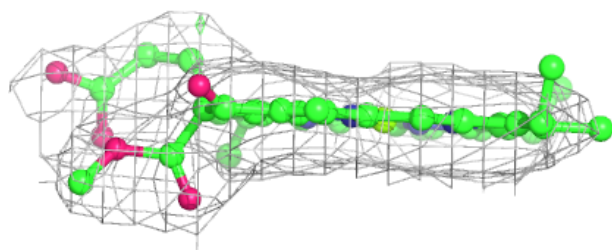
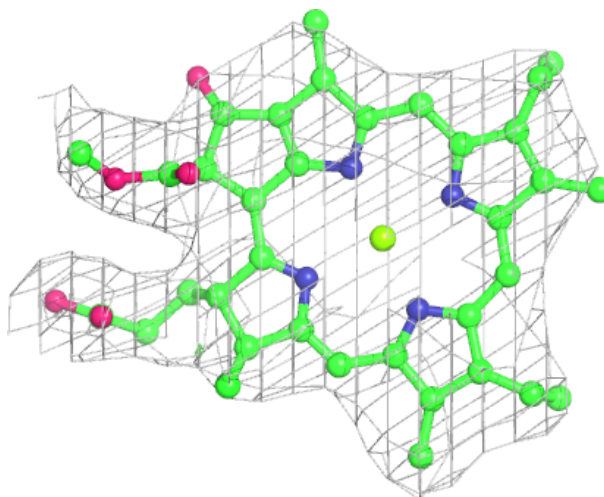
**Electron density around CLA Y 841:**

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



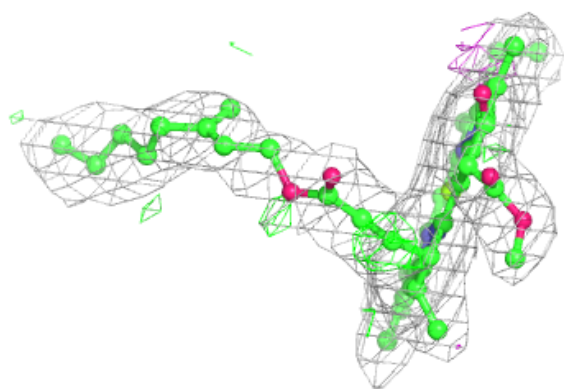
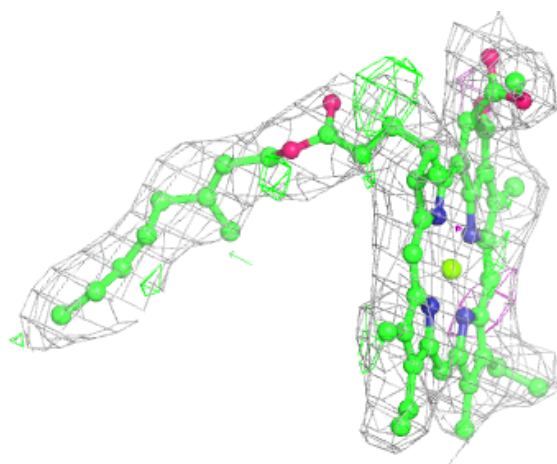
**Electron density around CLA H 835:**

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



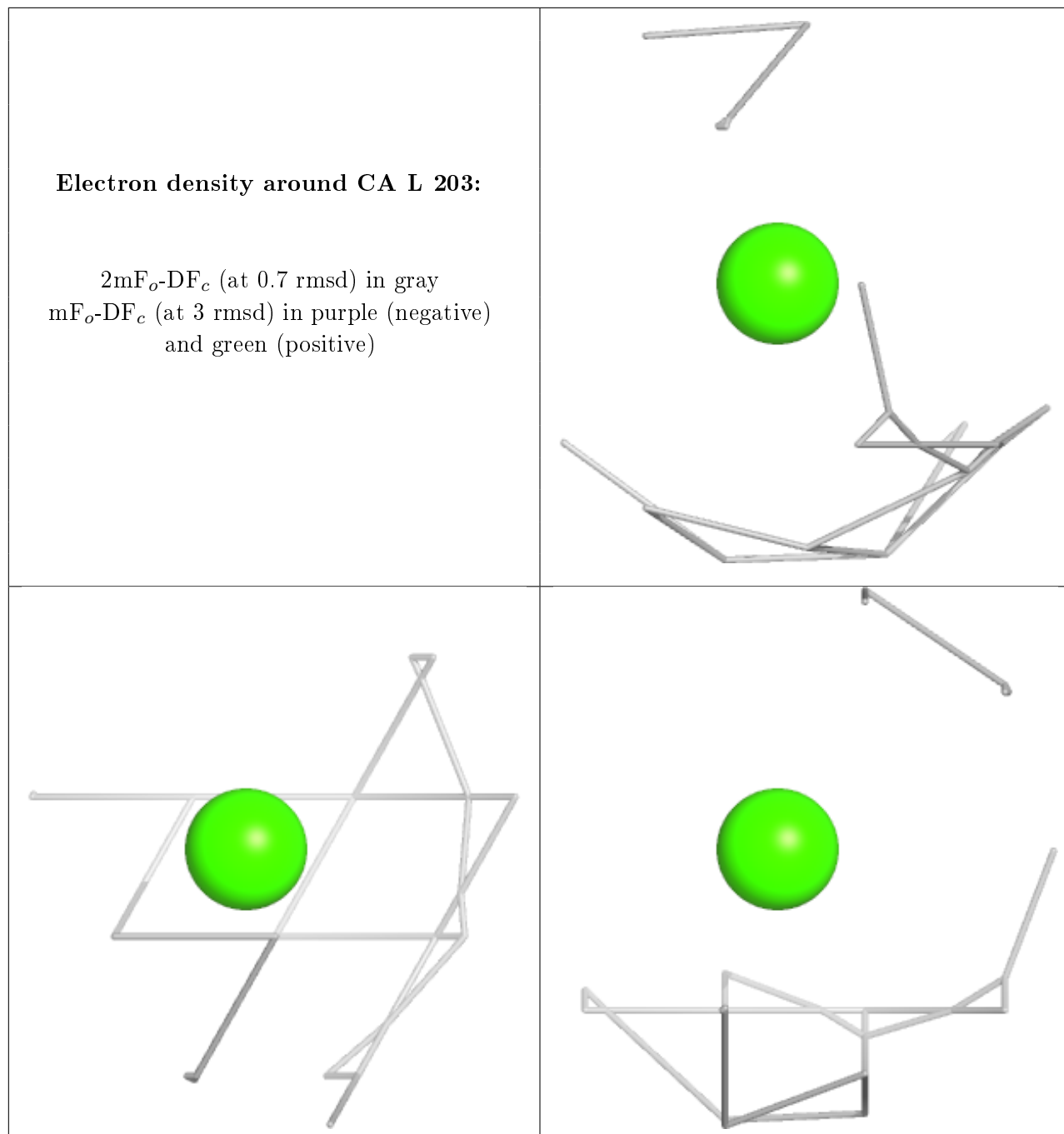
**Electron density around CLA B 803:**

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



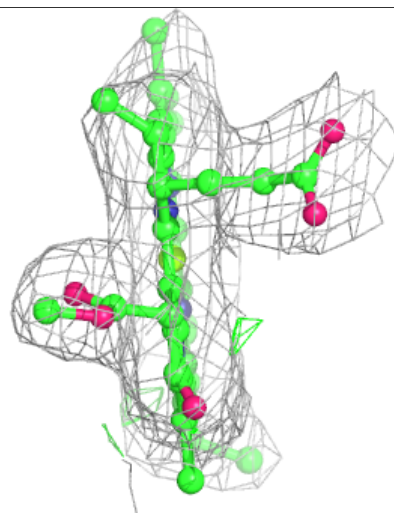
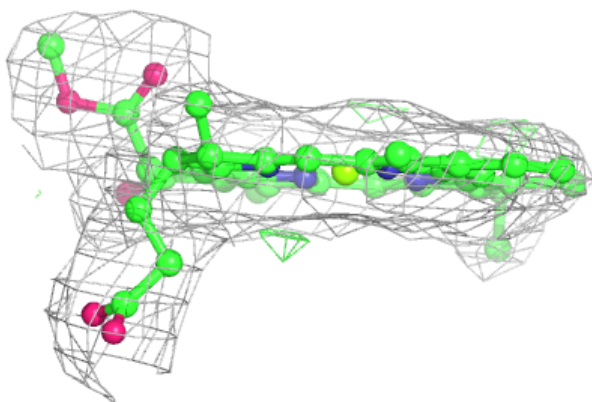
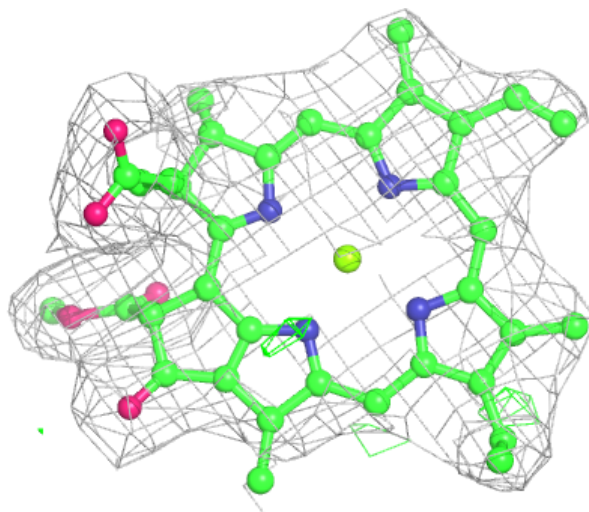
**Electron density around CA L 203:**

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



**Electron density around CLA B 838:**

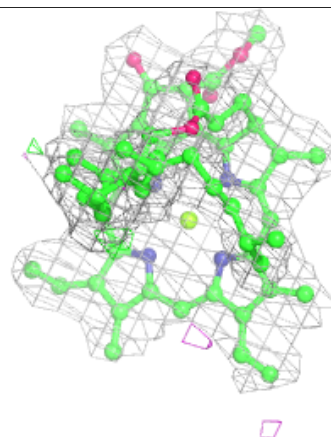
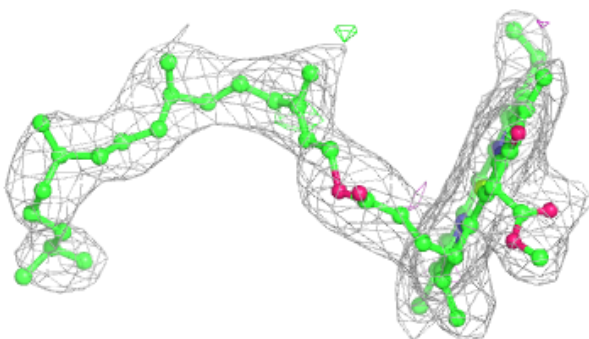
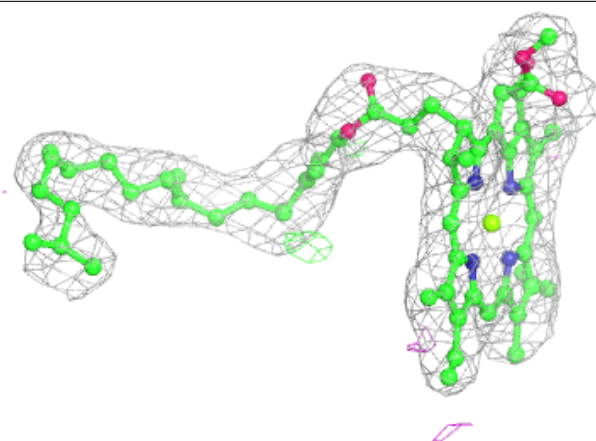
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA L 205:**

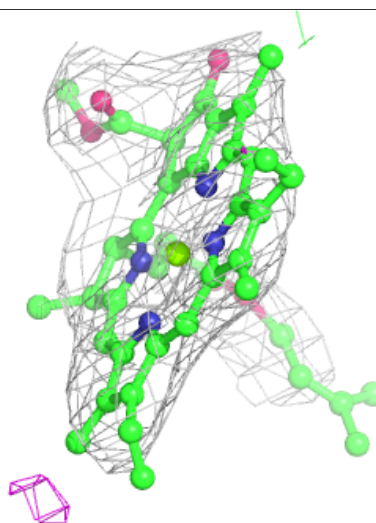
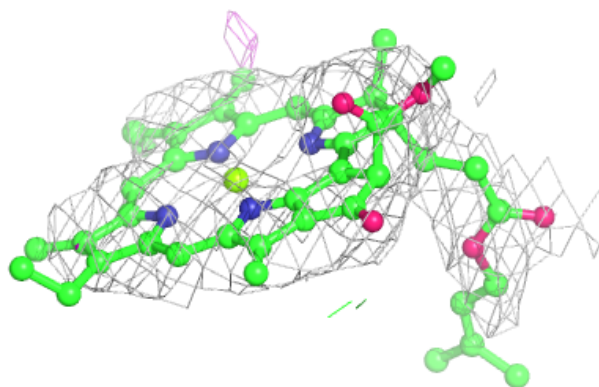
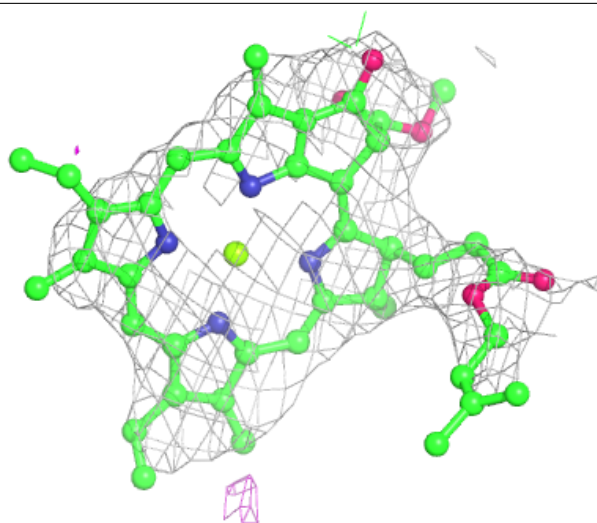
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





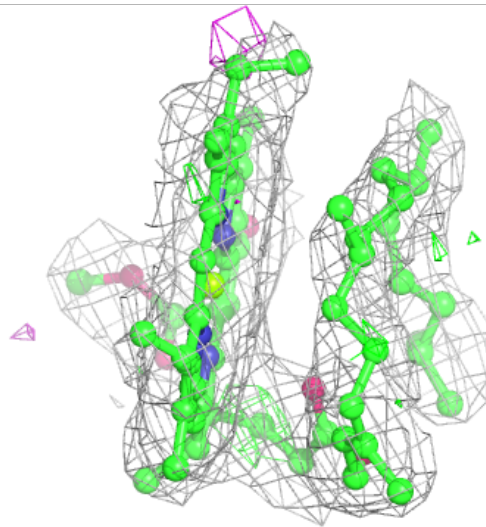
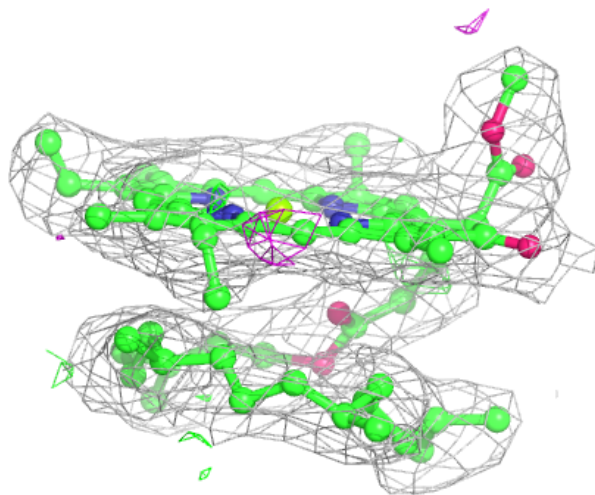
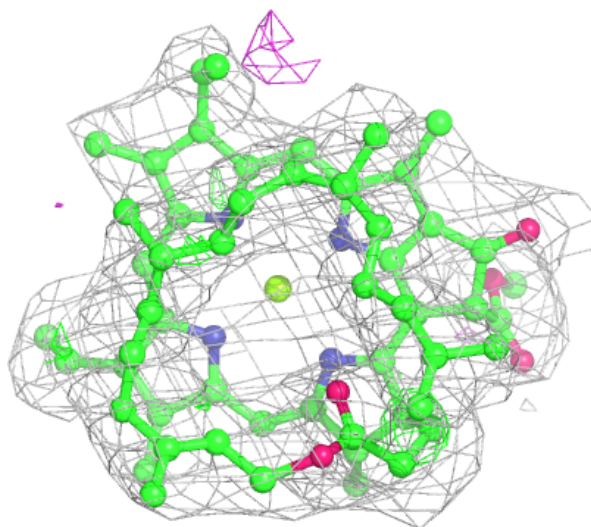
**Electron density around CLA A 815:**

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



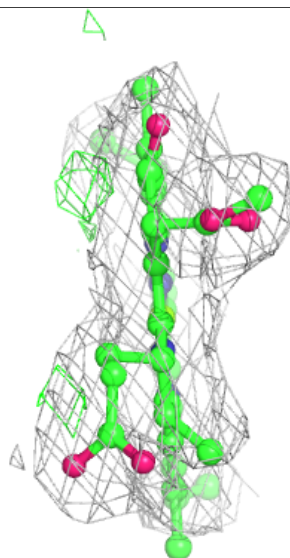
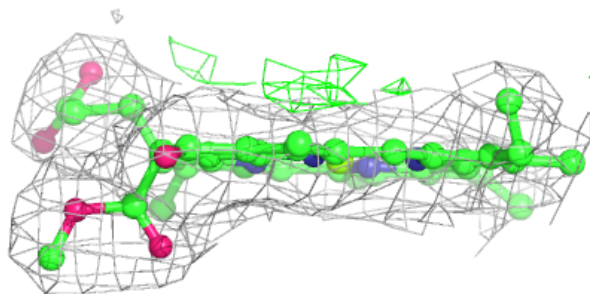
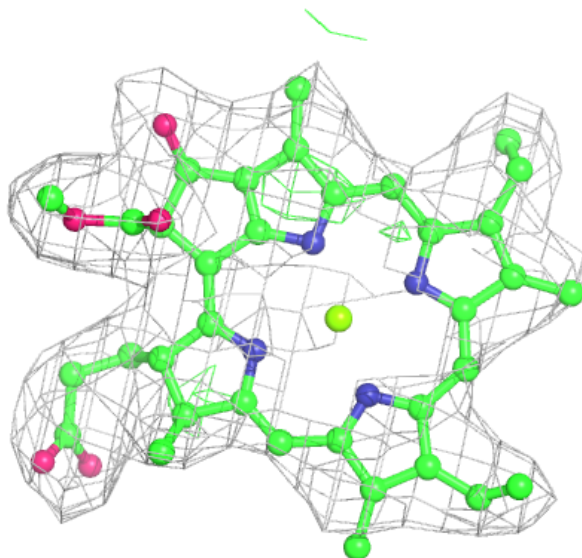
**Electron density around CLA L 204:**

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



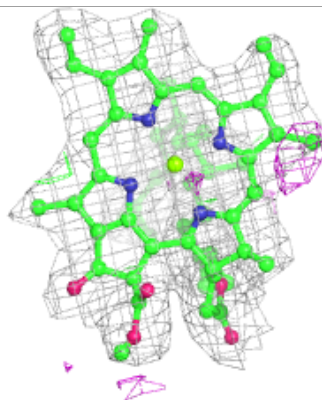
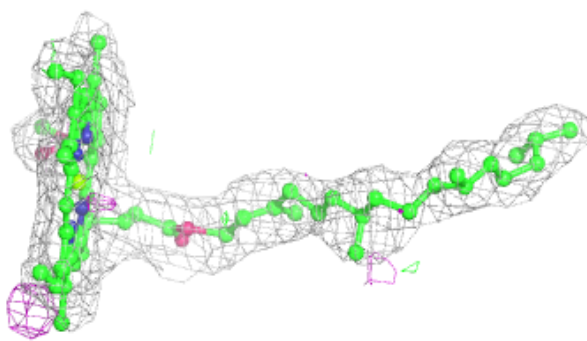
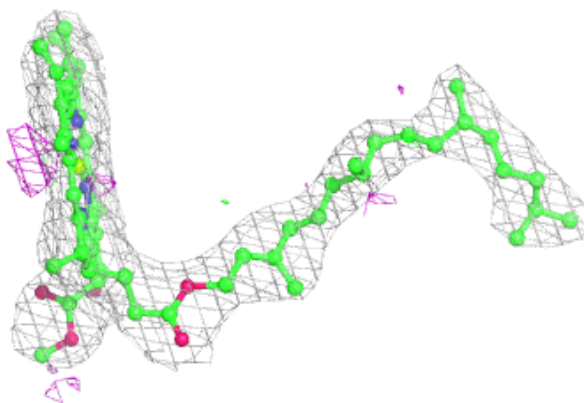
**Electron density around CLA W 1701:**

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



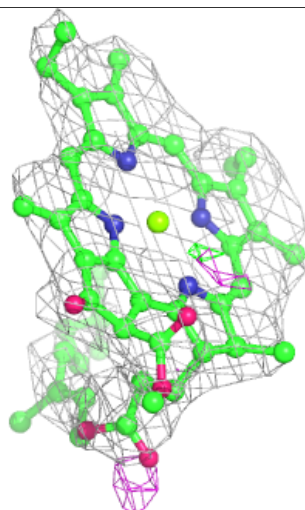
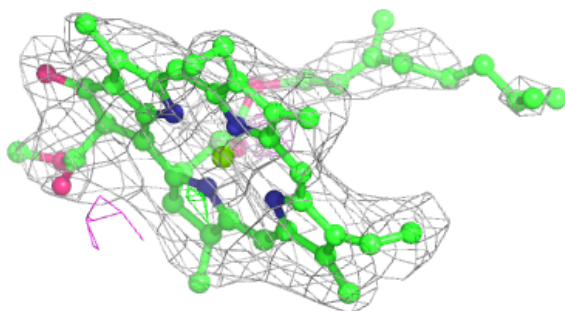
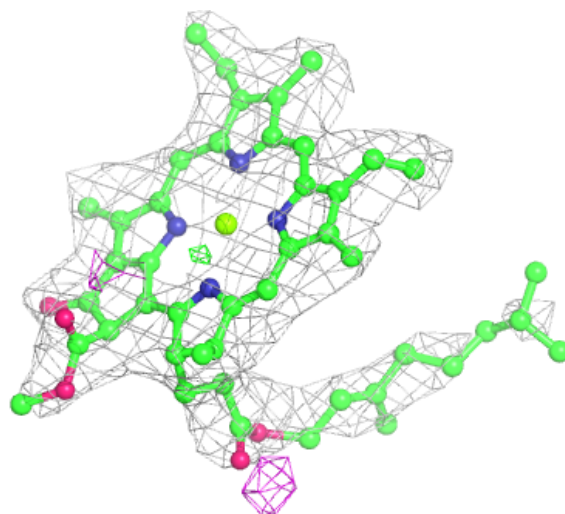
**Electron density around CLA B 840:**

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



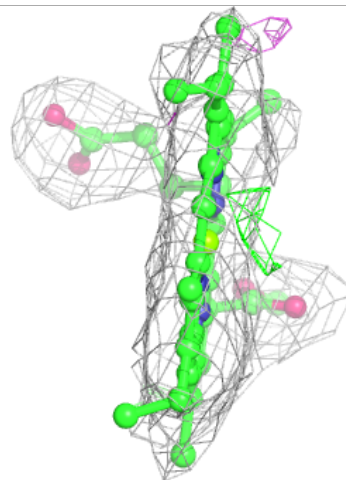
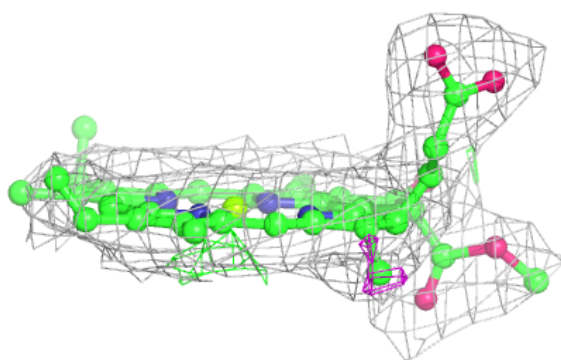
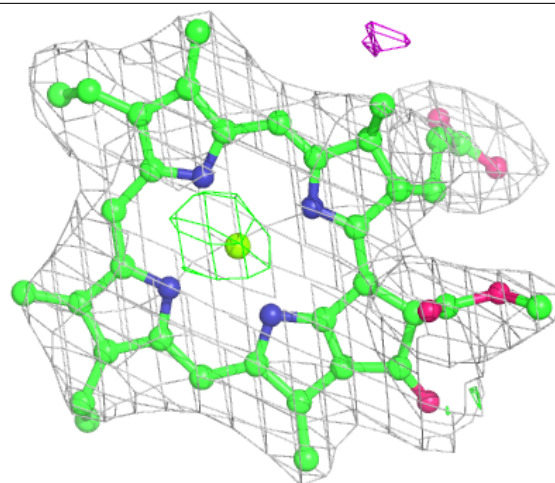
**Electron density around CLA B 815:**

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



**Electron density around CLA Z 835:**

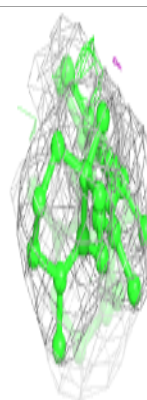
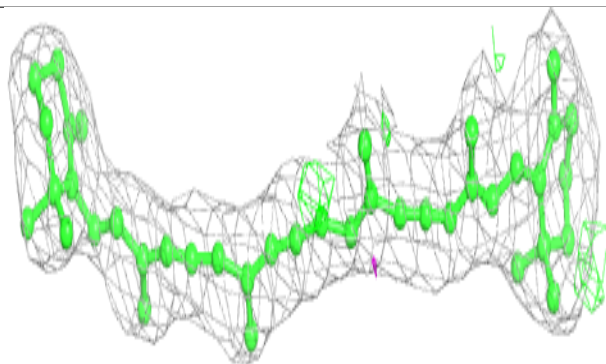
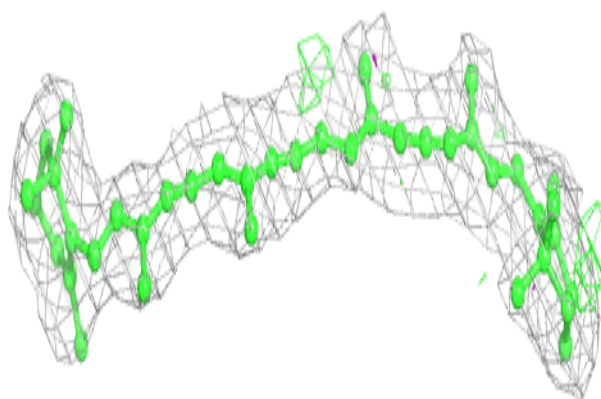
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



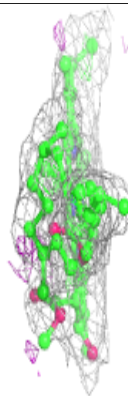
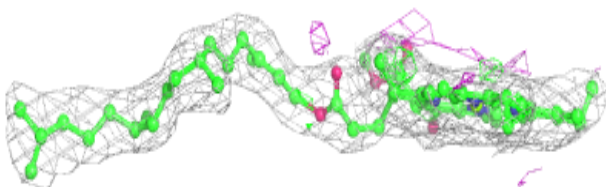
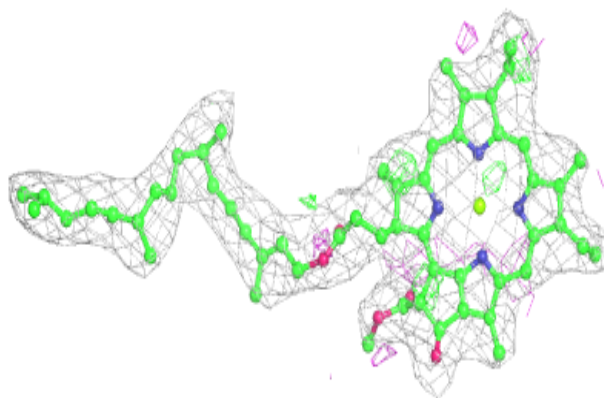


**Electron density around BCR M 101:**

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

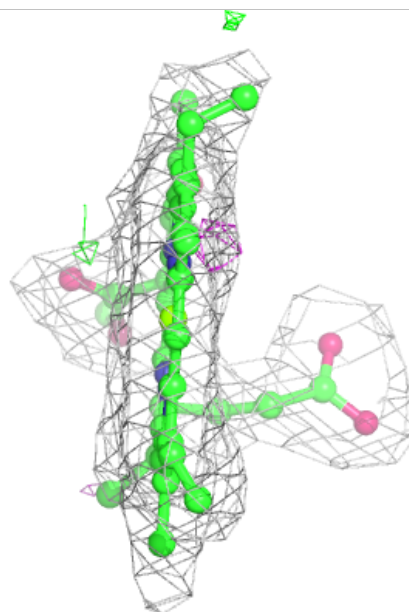
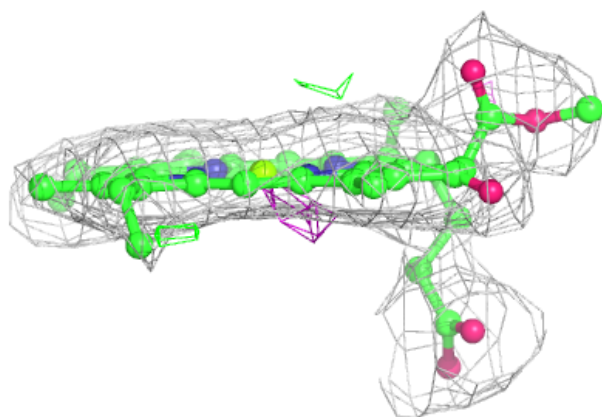
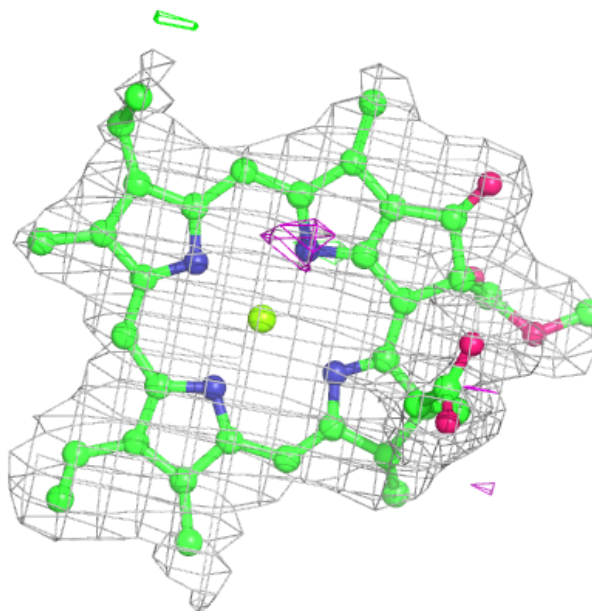
**Electron density around CLA Y 832:**

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



**Electron density around CLA G 853:**

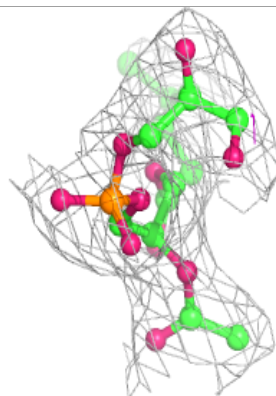
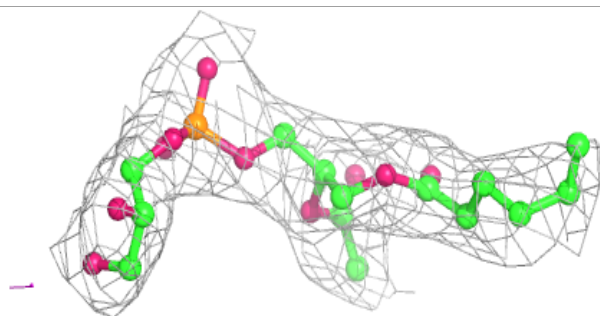
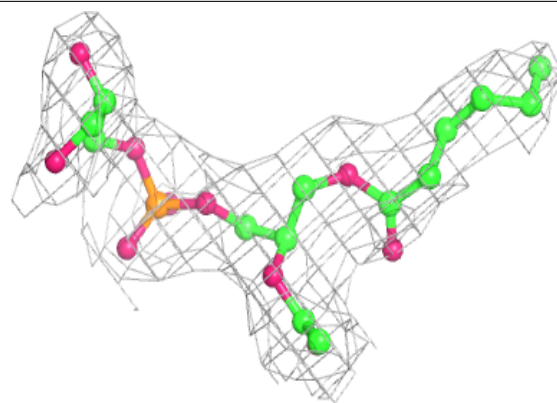
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



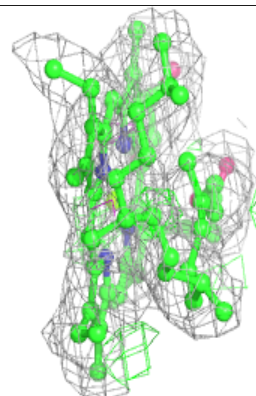
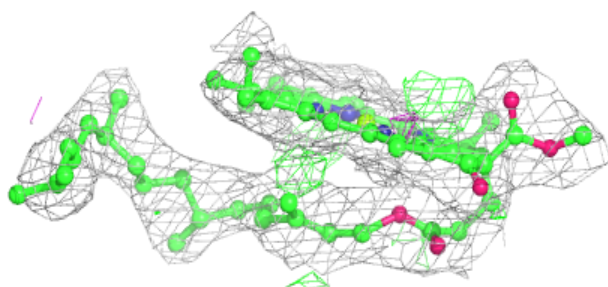
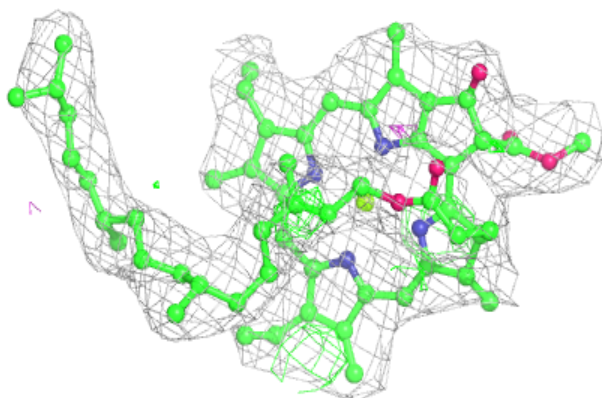


**Electron density around LHG Y 851:**

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

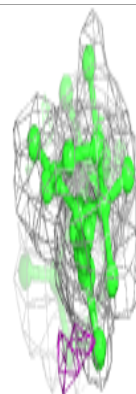
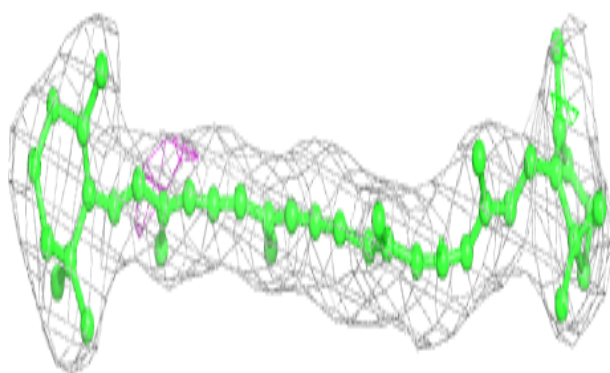
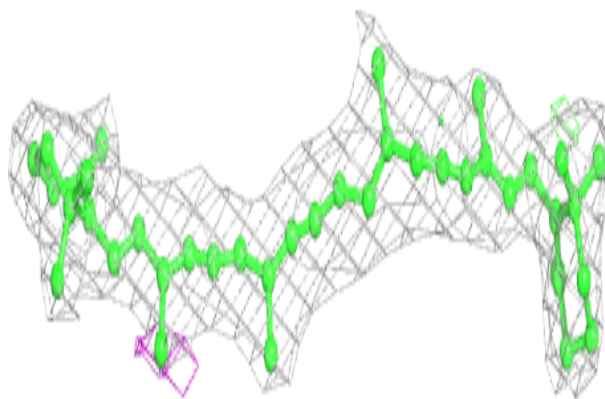
**Electron density around CLA H 837:**

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

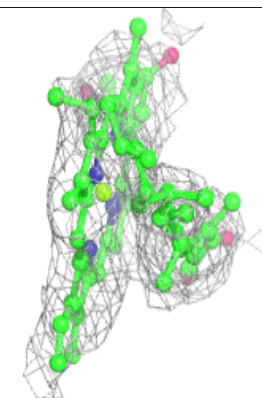
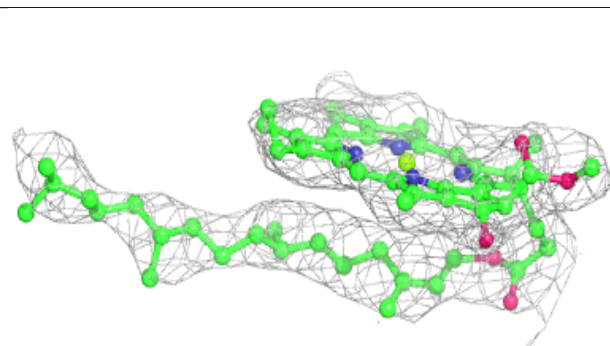
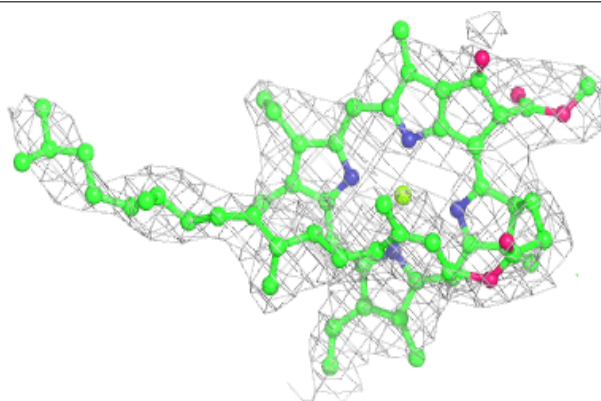


**Electron density around BCR L 208:**

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

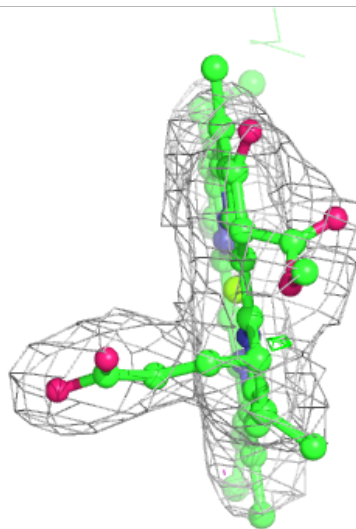
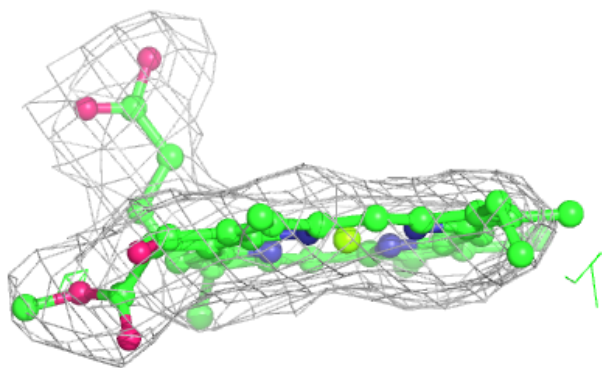
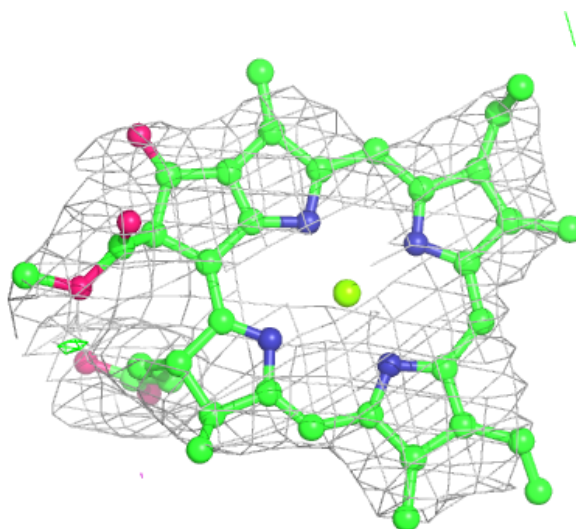
**Electron density around CLA G 818:**

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



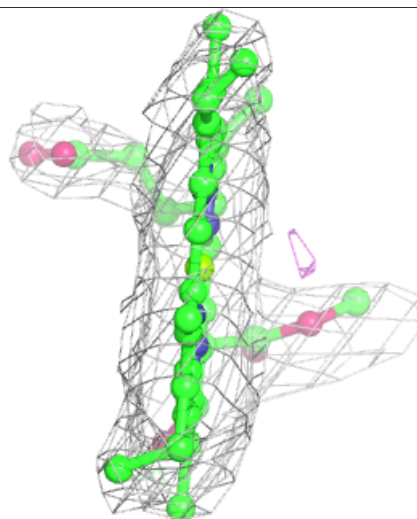
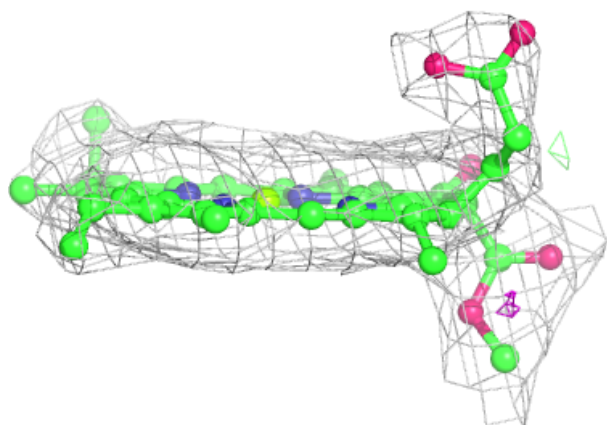
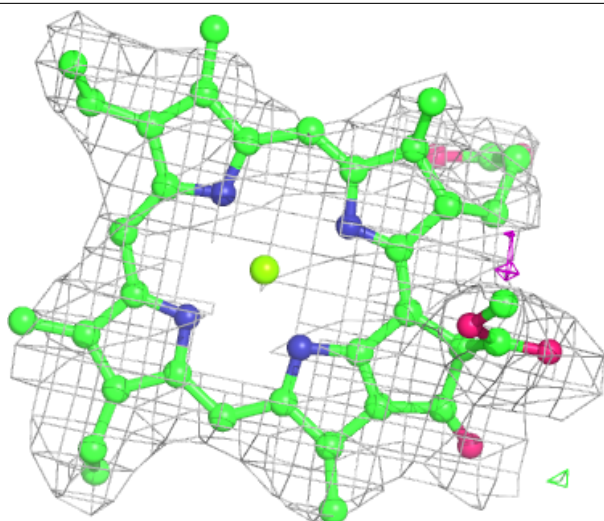
**Electron density around CLA Y 810:**

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



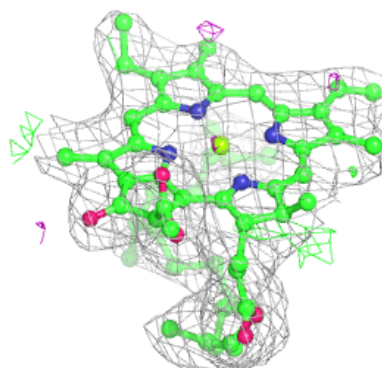
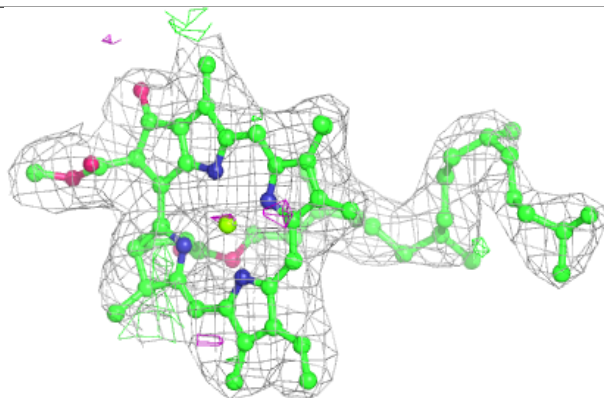
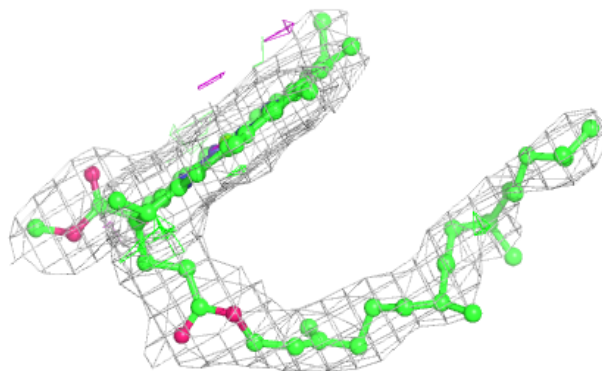
**Electron density around CLA H 820:**

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

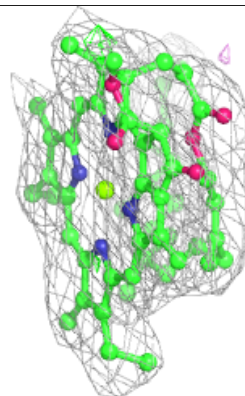
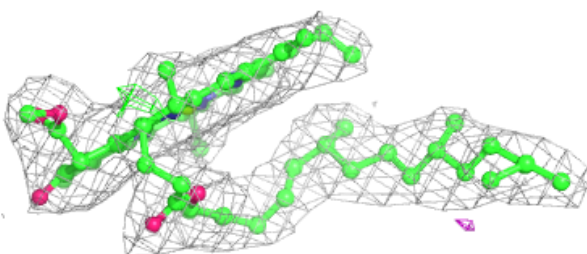
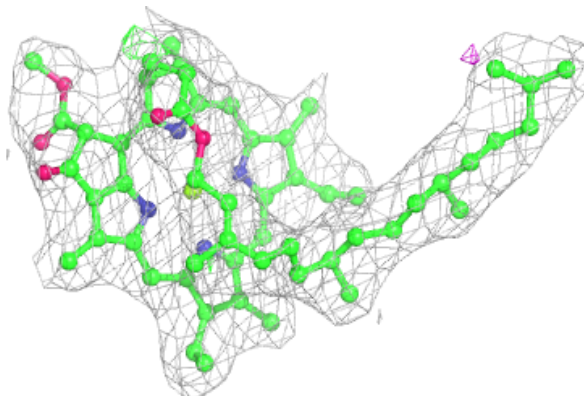


**Electron density around CLA L 201:**

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

**Electron density around CLA B 806:**

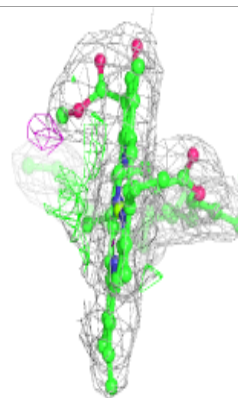
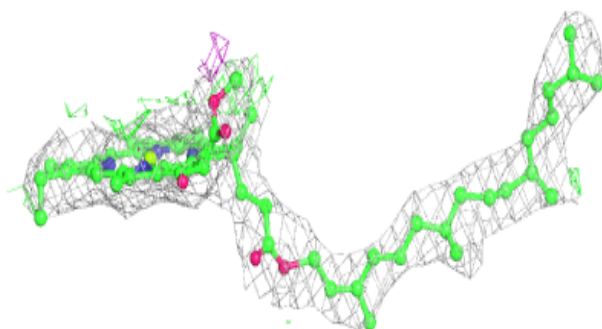
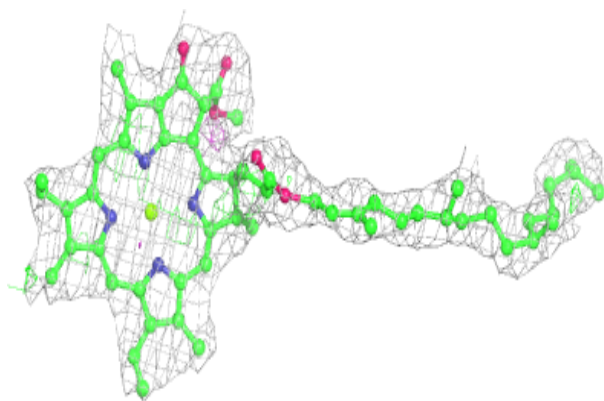
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





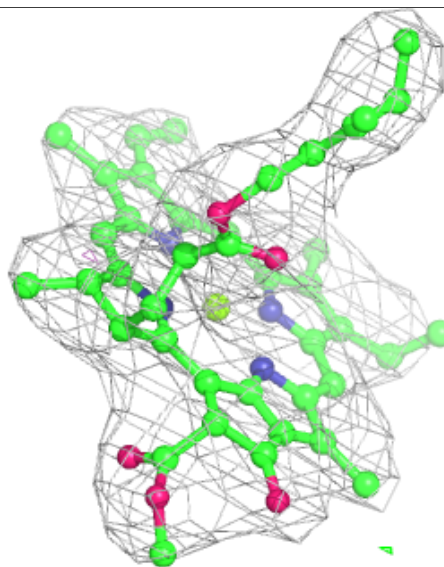
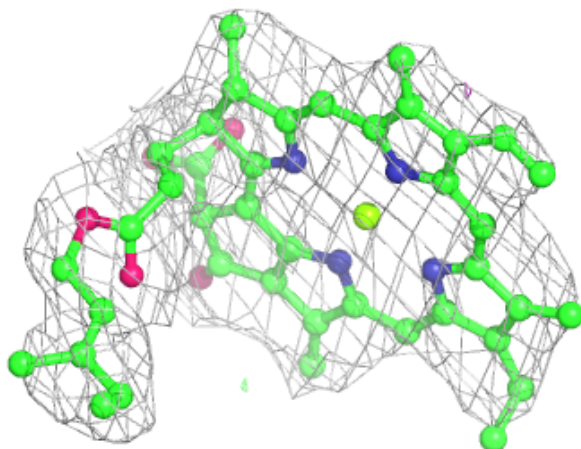
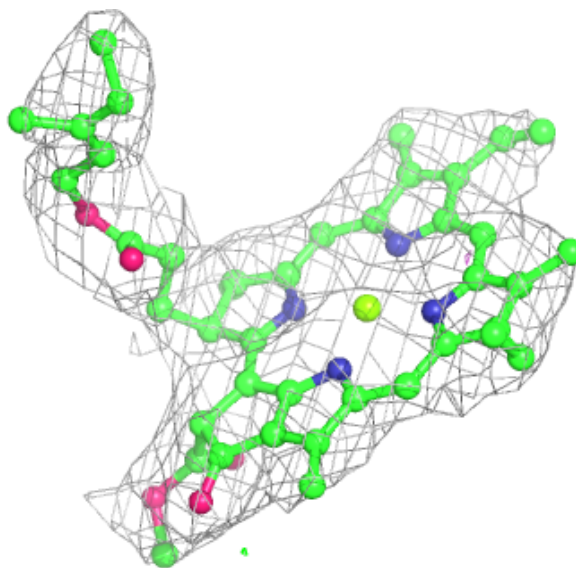
**Electron density around CLA B 824:**

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



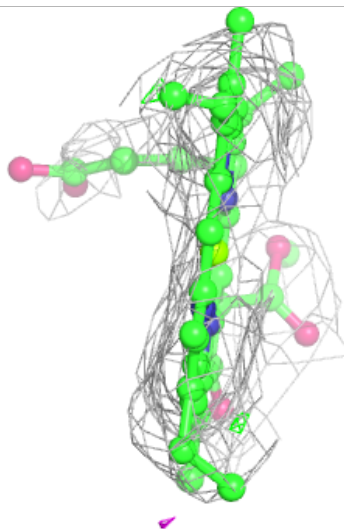
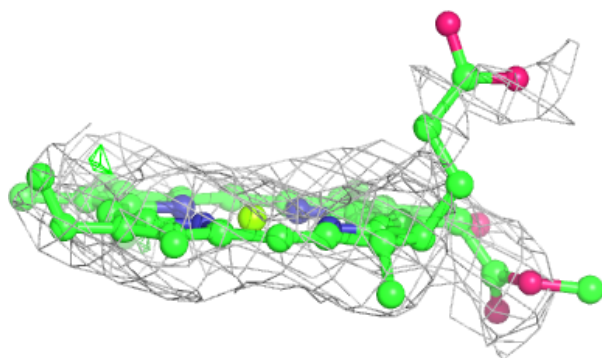
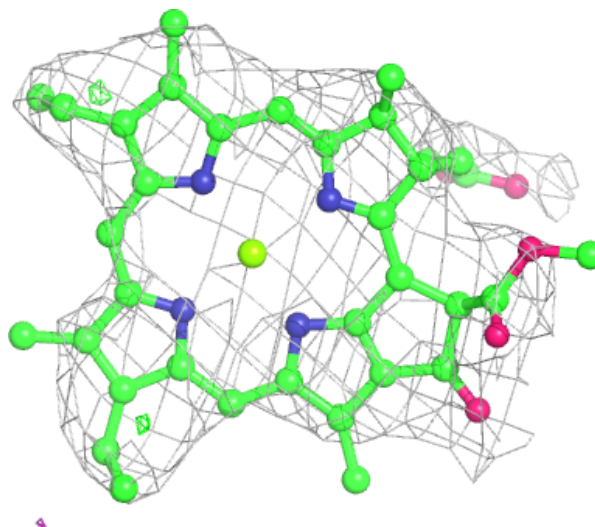
**Electron density around CLA A 808:**

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



**Electron density around CLA f 101:**

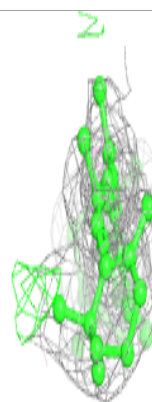
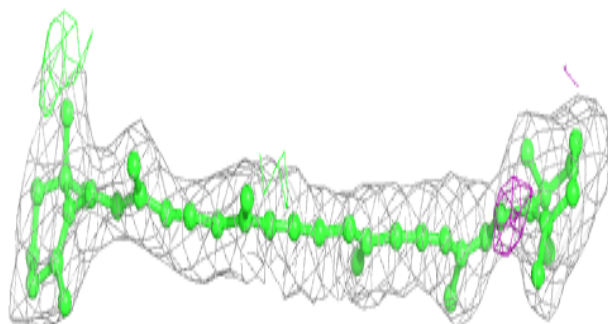
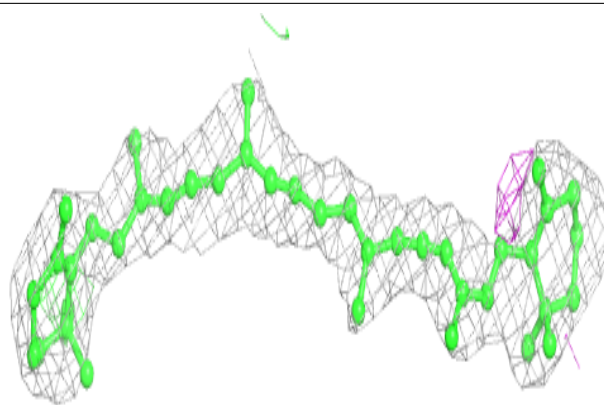
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



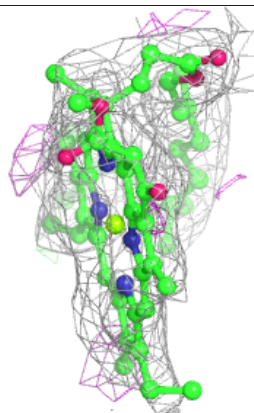
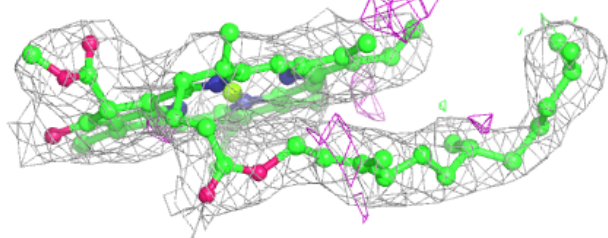
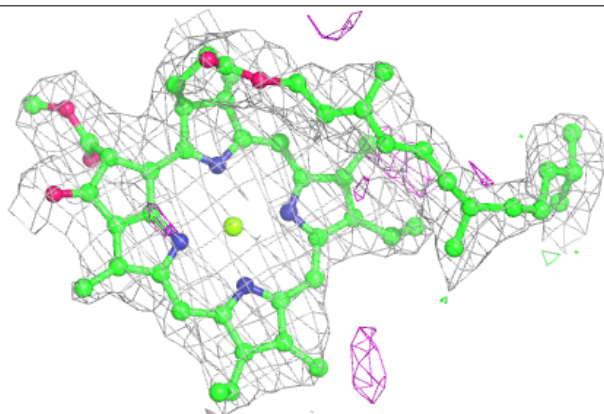


**Electron density around BCR B 846:**

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

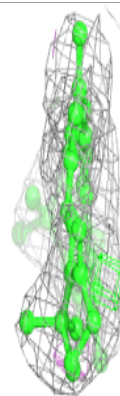
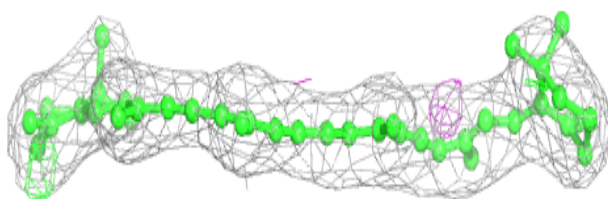
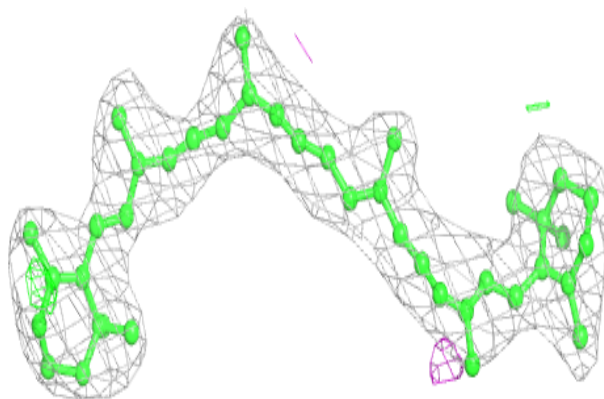
**Electron density around CLA Z 819:**

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

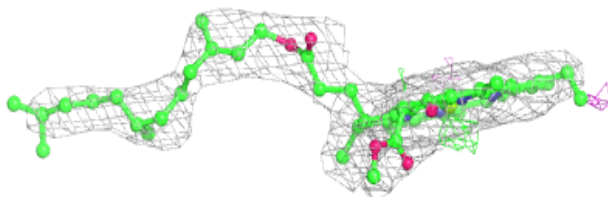
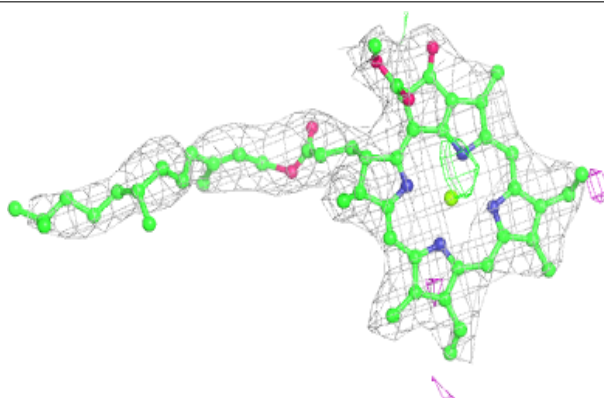


**Electron density around BCR Y 849:**

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

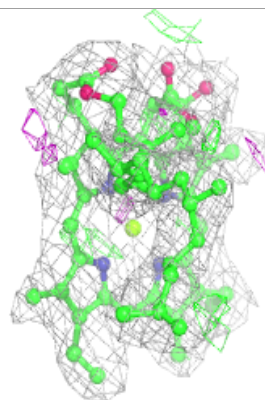
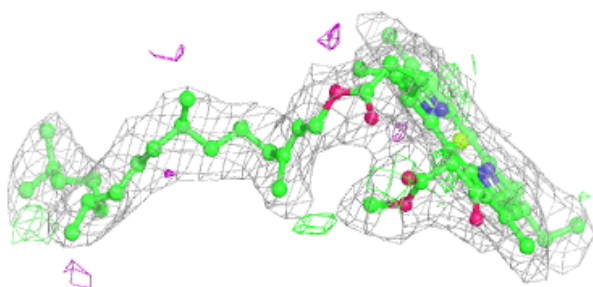
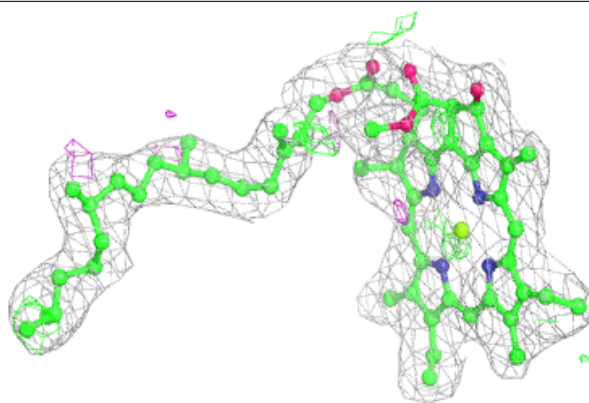
**Electron density around CLA G 826:**

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

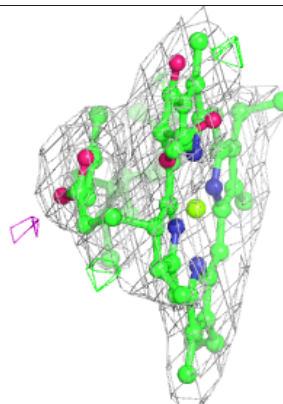
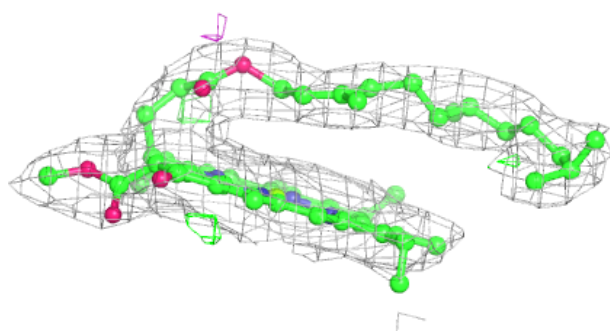
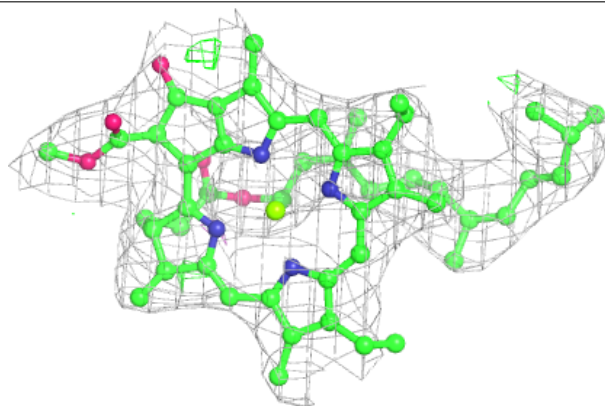


**Electron density around CLA H 810:**

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

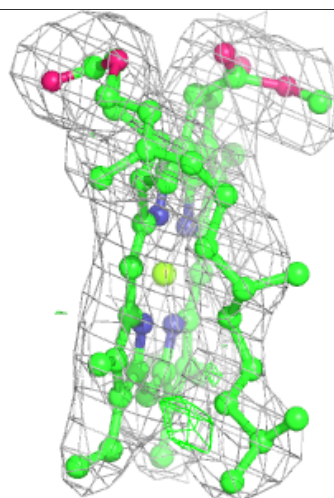
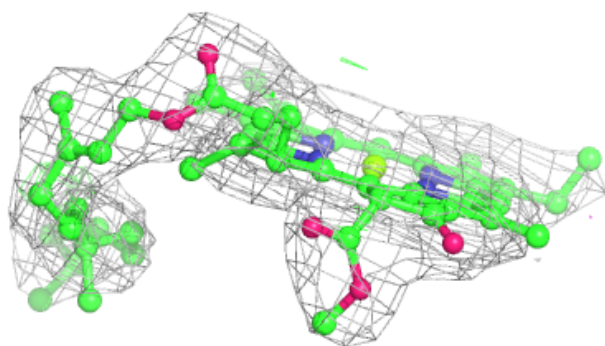
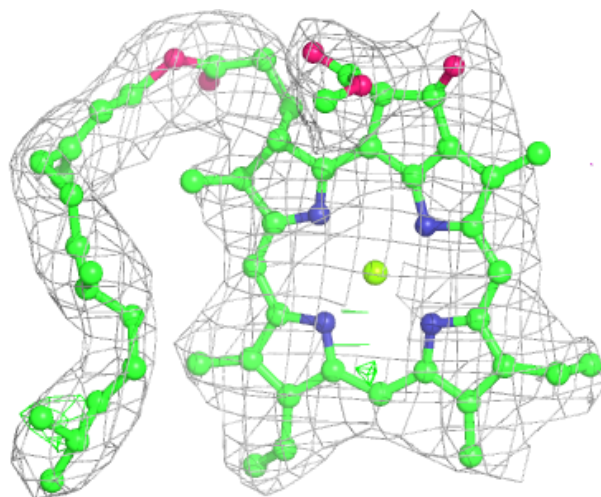
**Electron density around CLA A 818:**

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



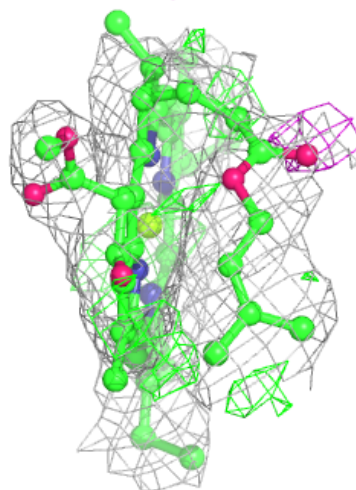
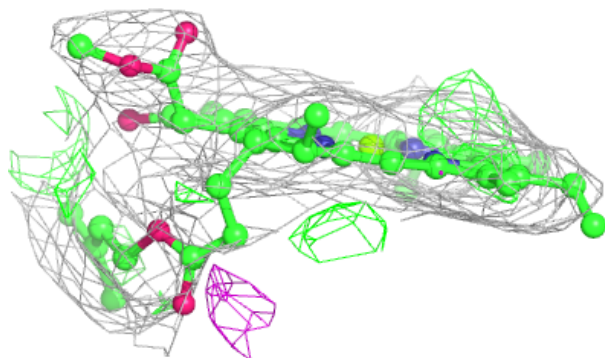
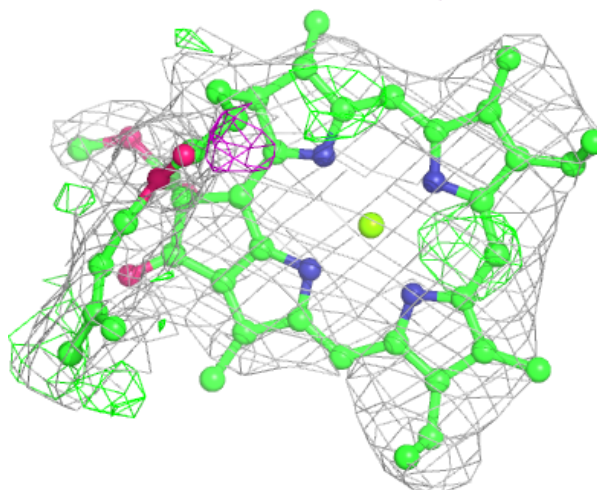
**Electron density around CLA A 814:**

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



**Electron density around CLA G 842:**

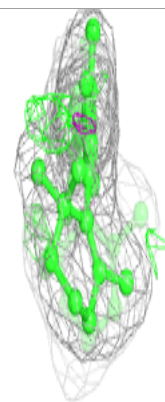
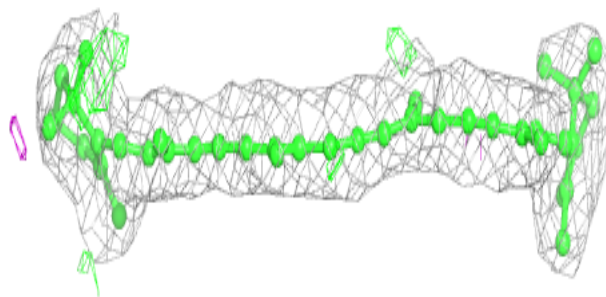
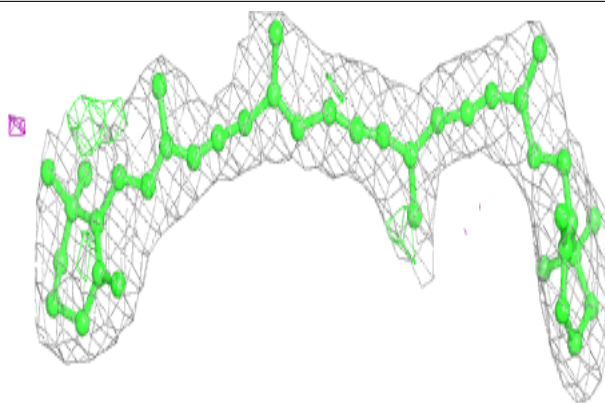
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





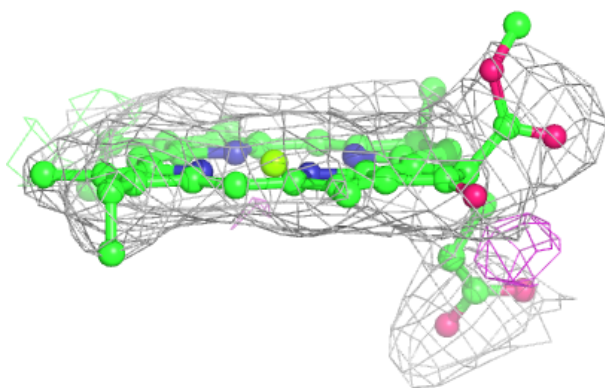
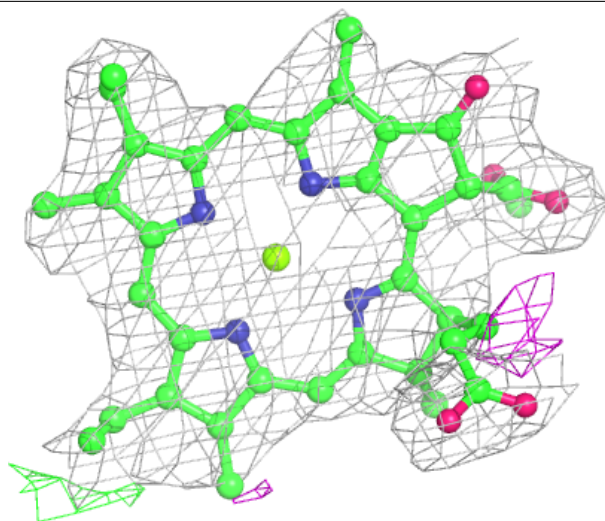
**Electron density around BCR R 102:**

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



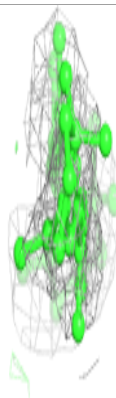
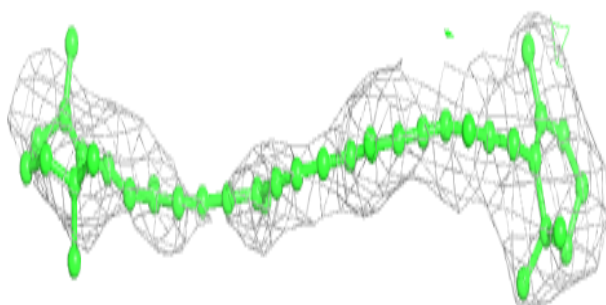
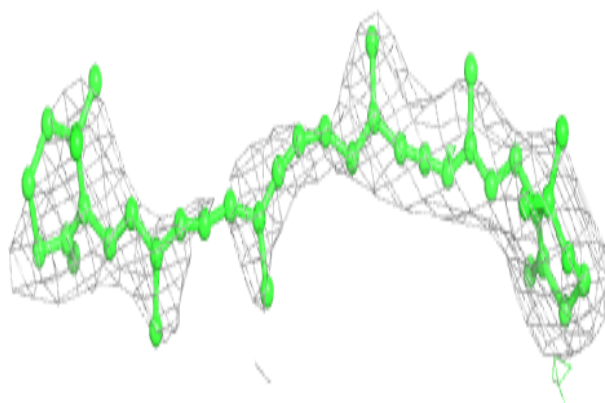
**Electron density around CLA Z 831:**

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

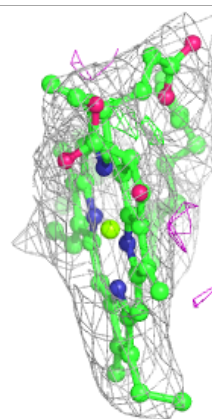
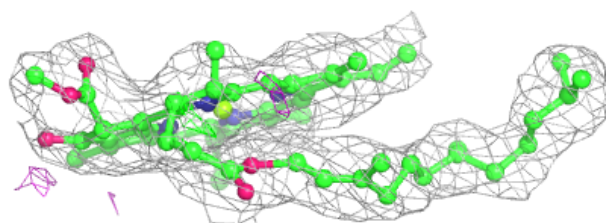
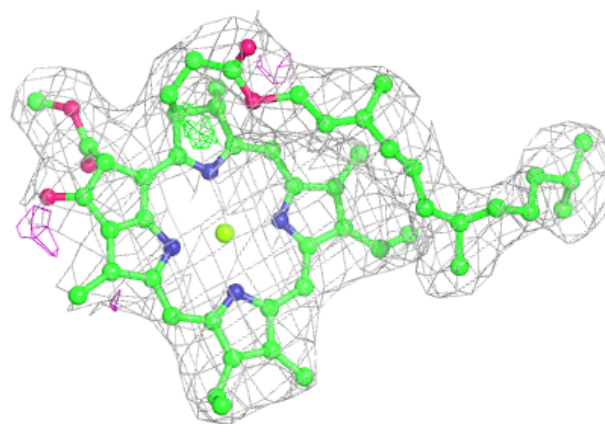


**Electron density around BCR Y 845:**

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

**Electron density around CLA B 817:**

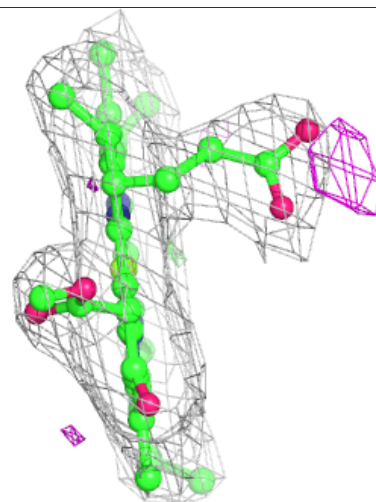
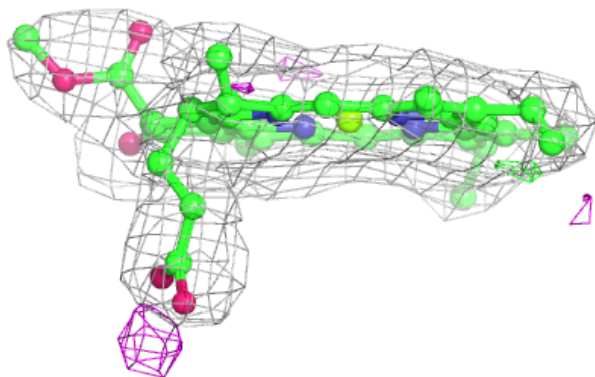
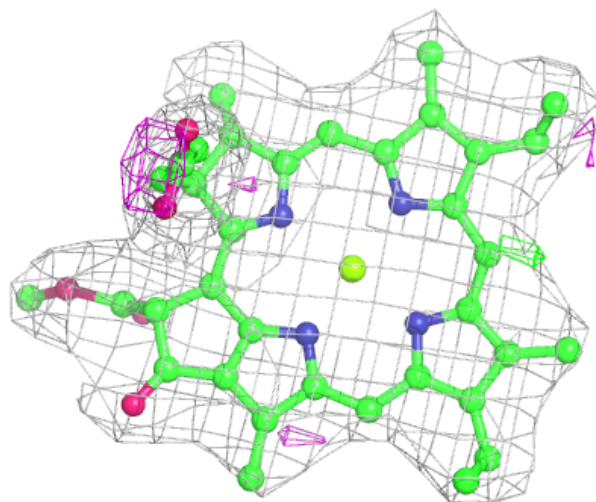
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





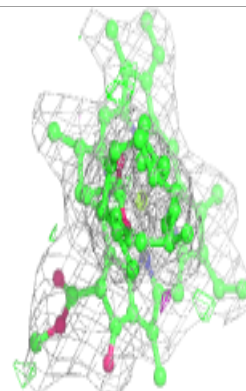
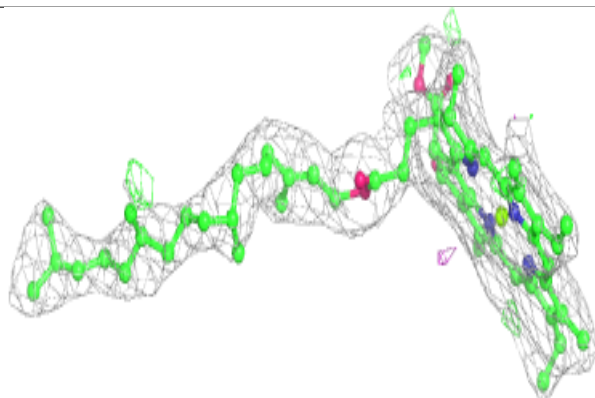
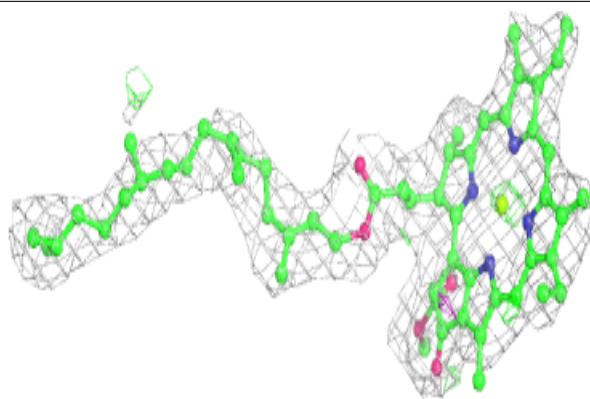
**Electron density around CLA Z 832:**

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

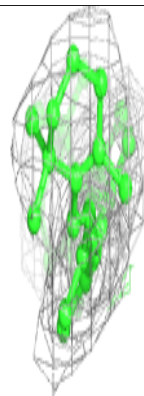
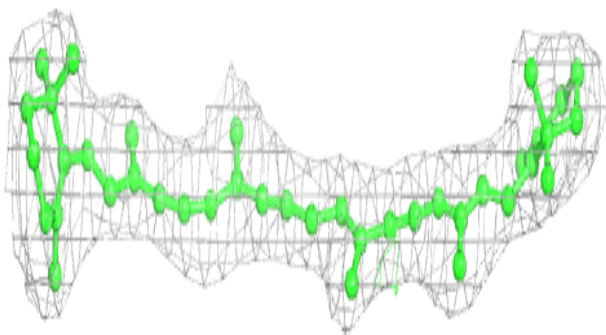
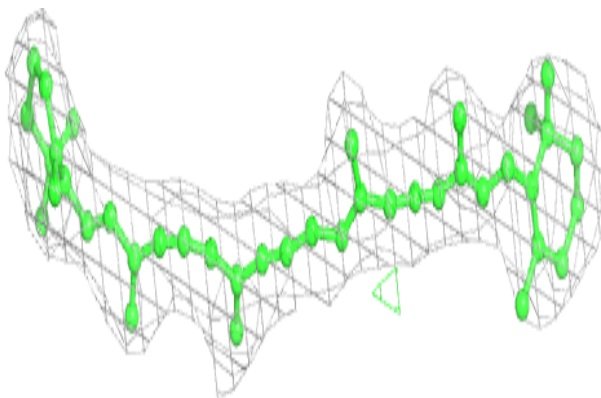


**Electron density around CLA A 810:**

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

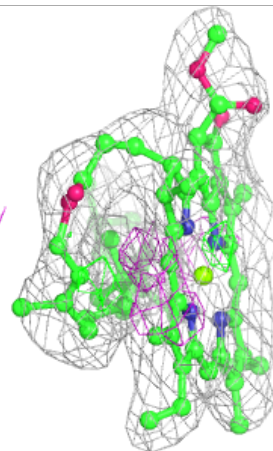
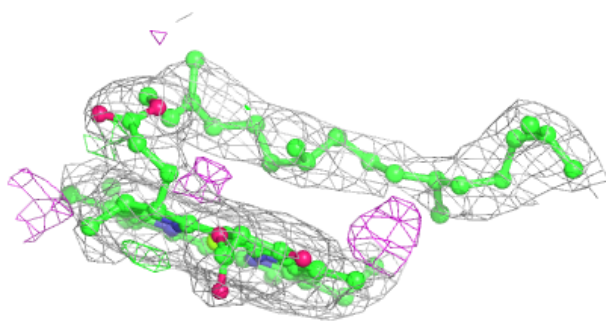
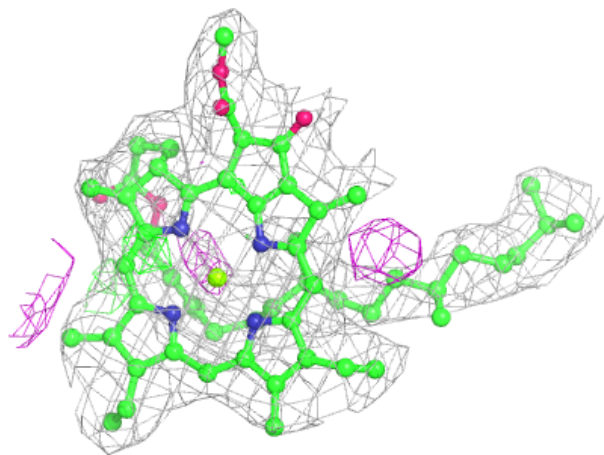
**Electron density around BCR I 101:**

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



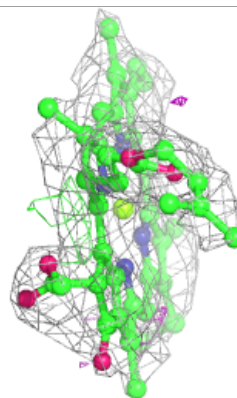
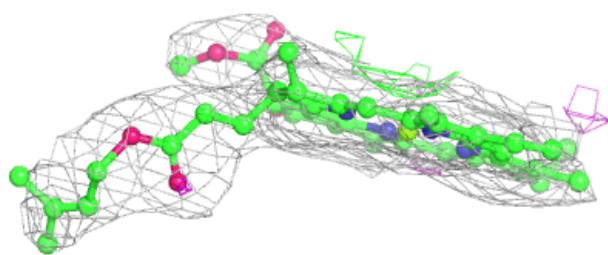
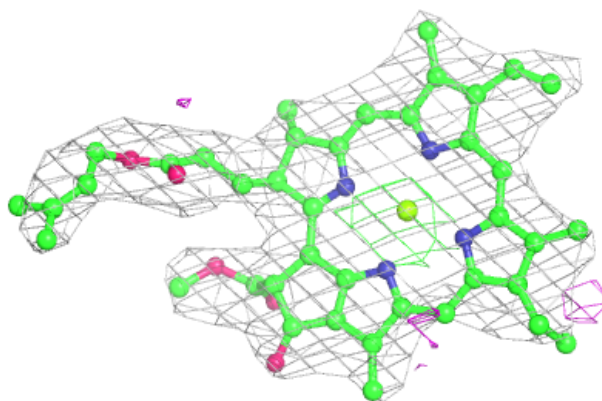
**Electron density around CLA B 826:**

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

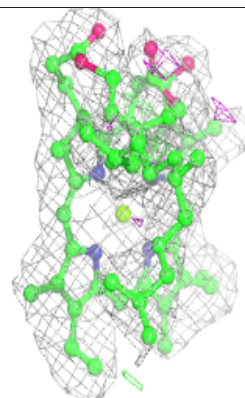
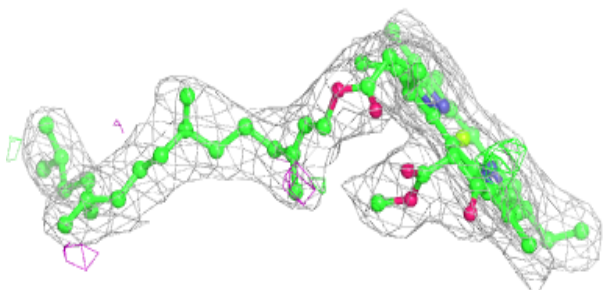
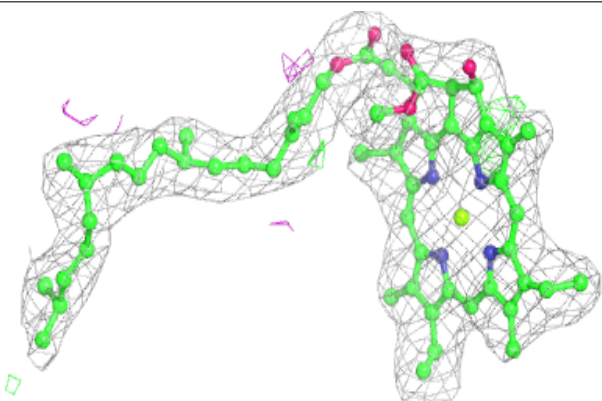


**Electron density around CLA A 840:**

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

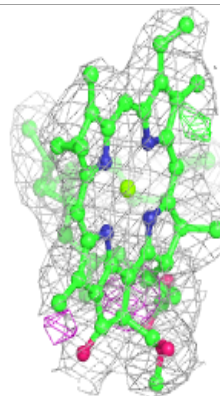
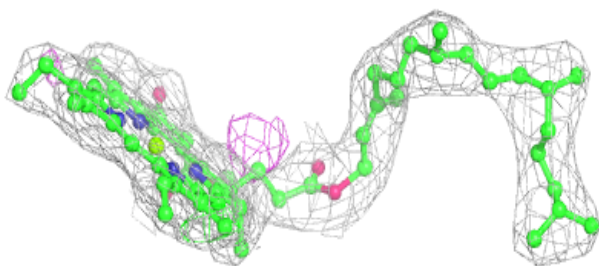
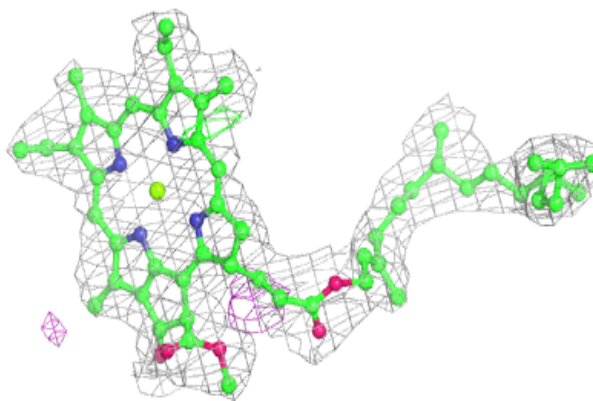
**Electron density around CLA B 809:**

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

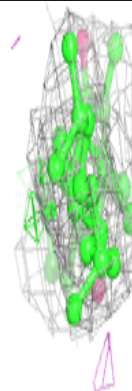
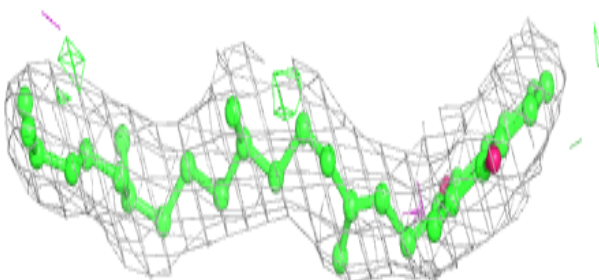
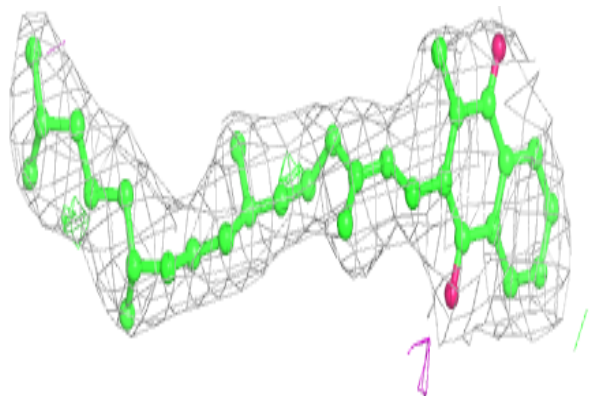


**Electron density around CLA H 809:**

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

**Electron density around PQN A 844:**

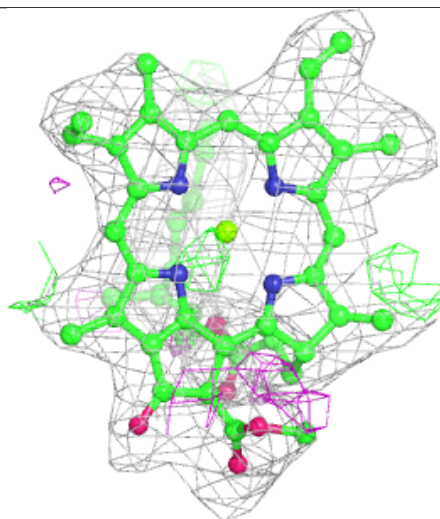
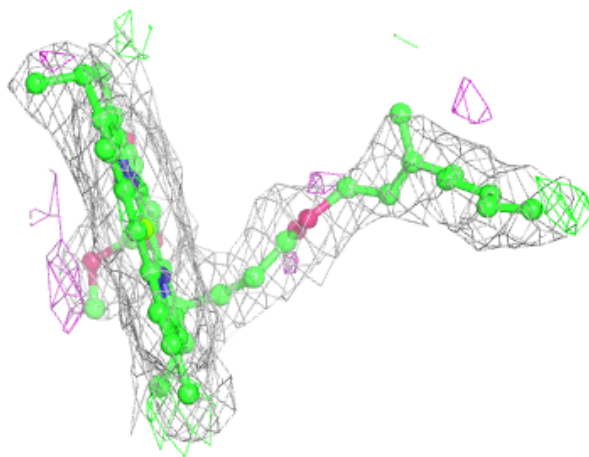
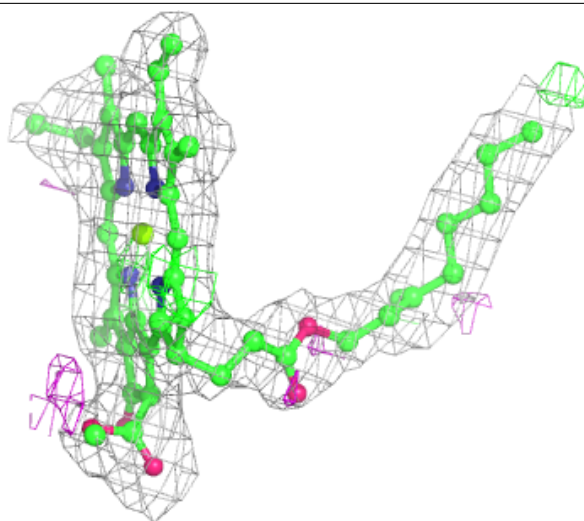
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





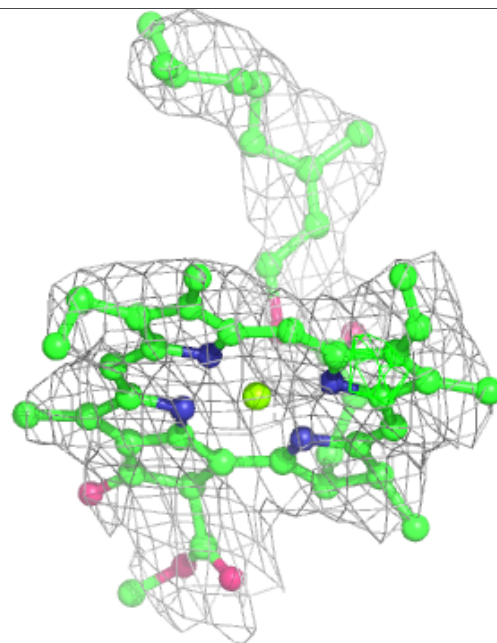
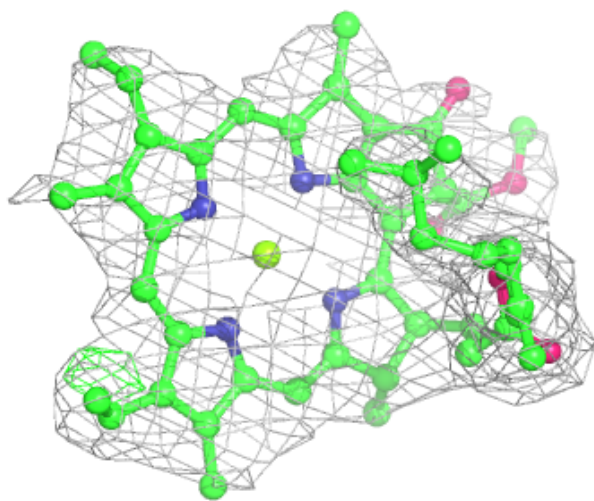
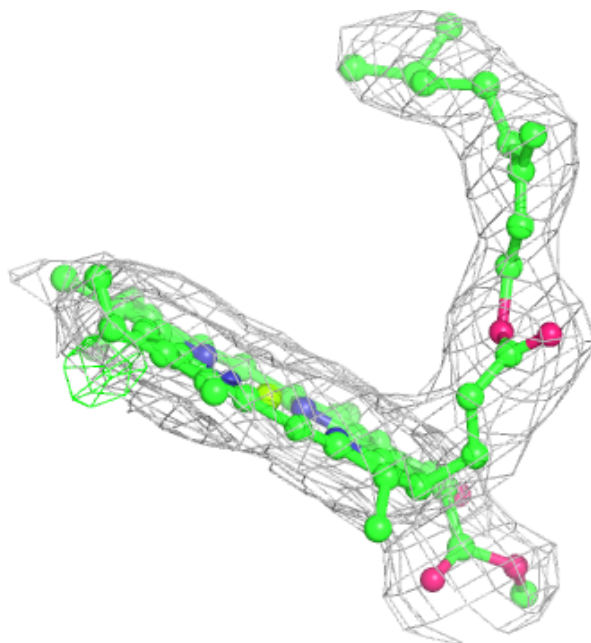
**Electron density around CLA Z 805:**

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



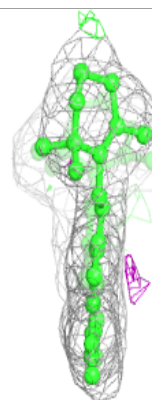
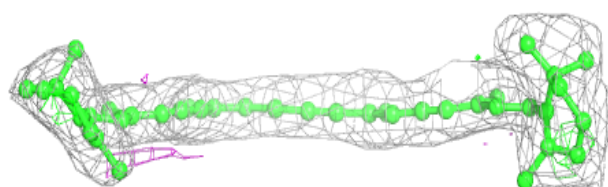
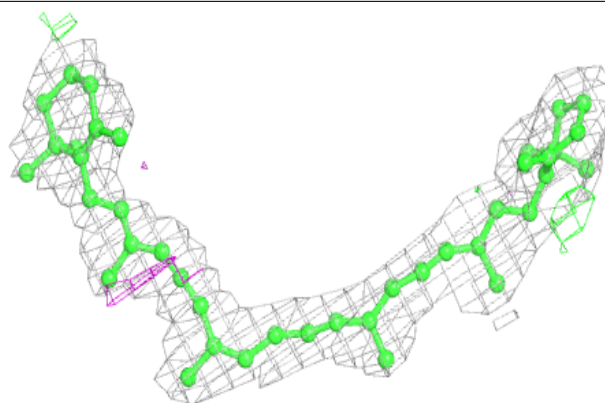
**Electron density around CLA Z 812:**

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

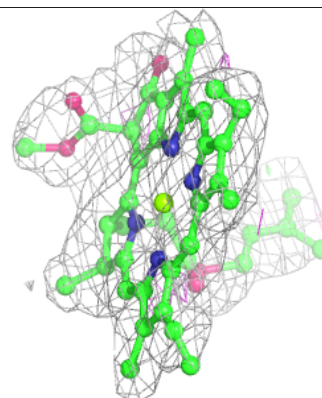
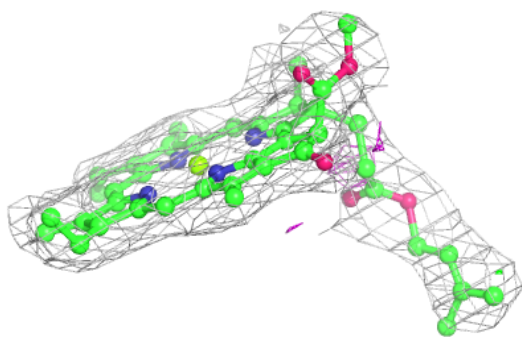
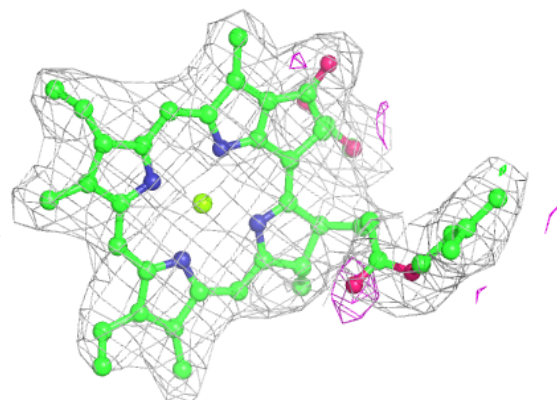


**Electron density around BCR Q 203:**

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

**Electron density around CLA A 838:**

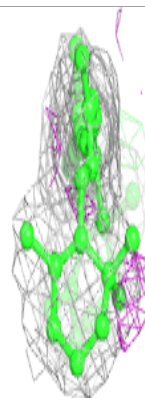
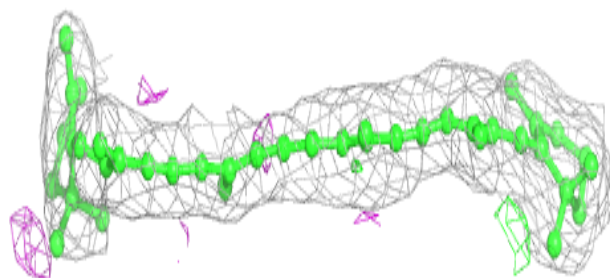
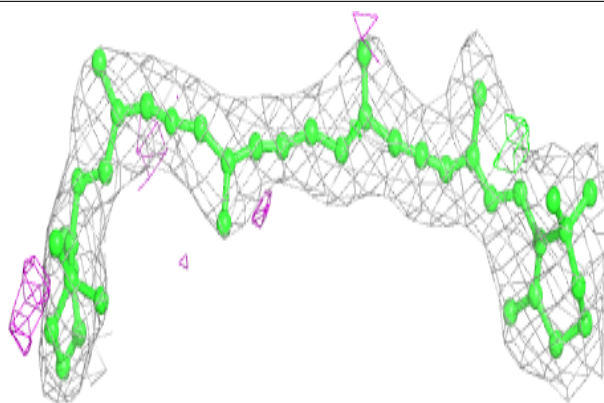
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





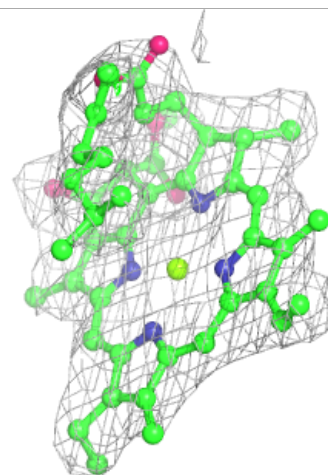
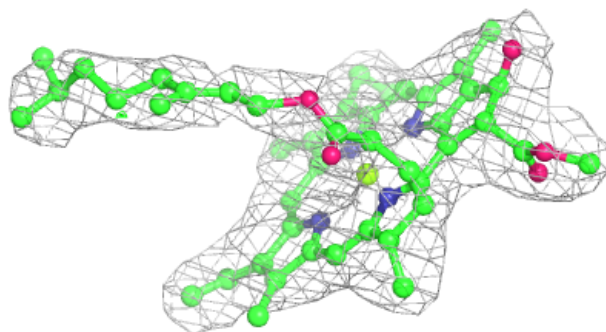
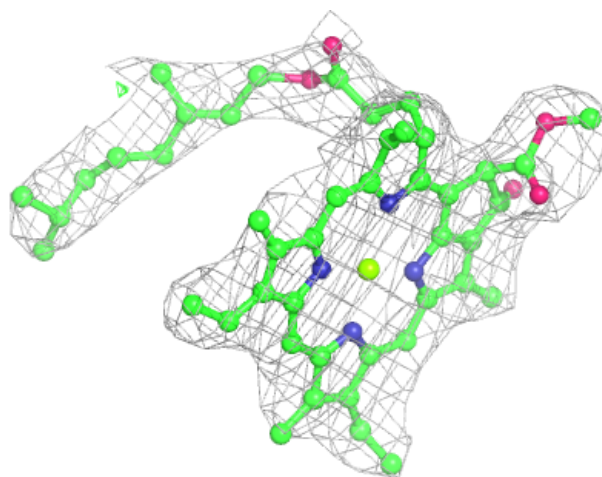
**Electron density around BCR U 1008:**

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



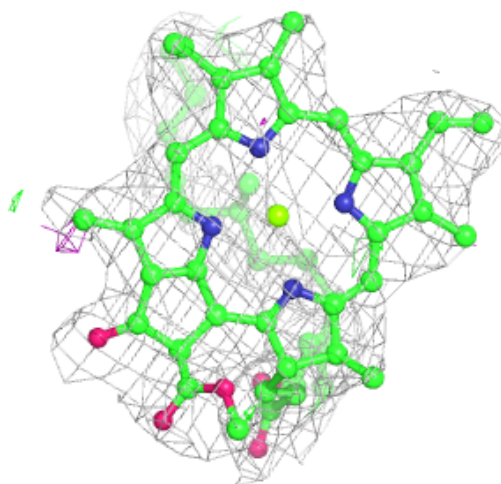
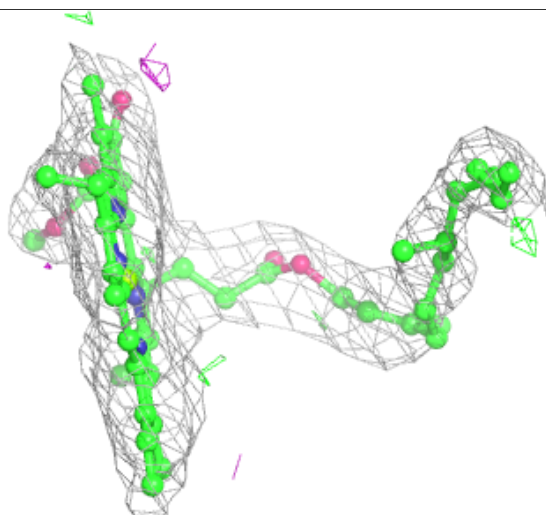
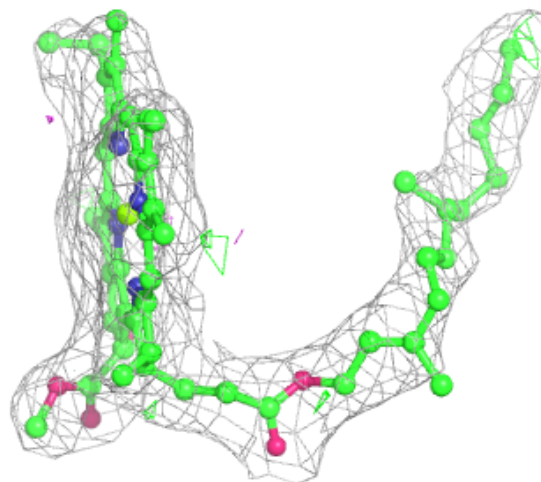
**Electron density around CLA Z 817:**

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



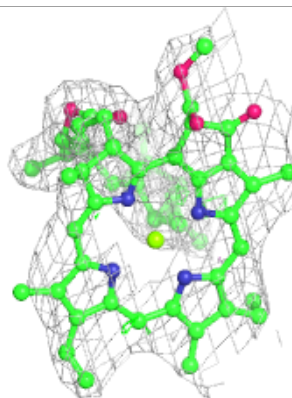
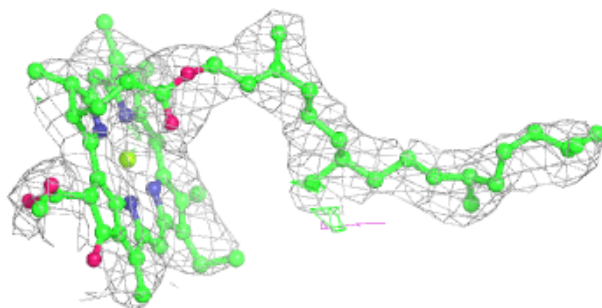
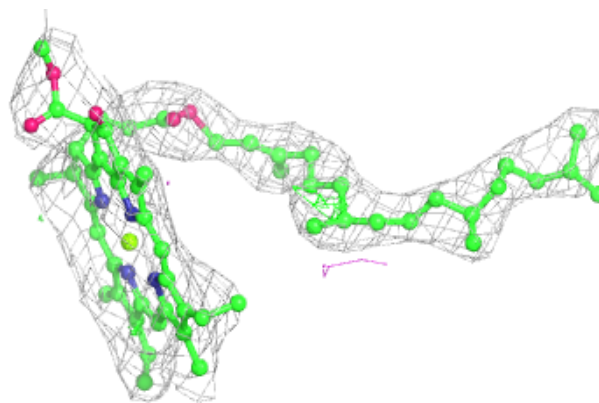
**Electron density around CLA A 805:**

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

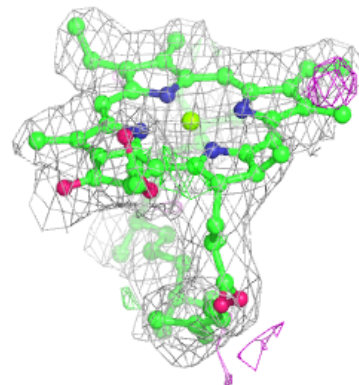
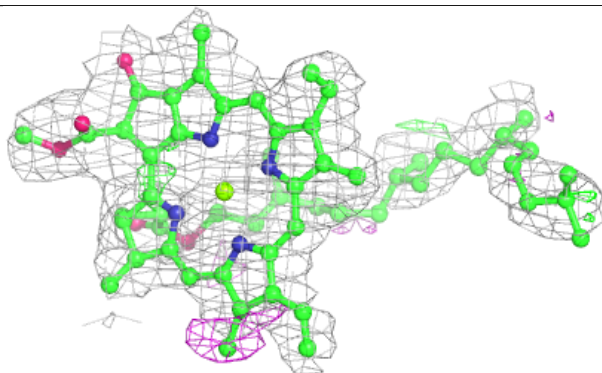
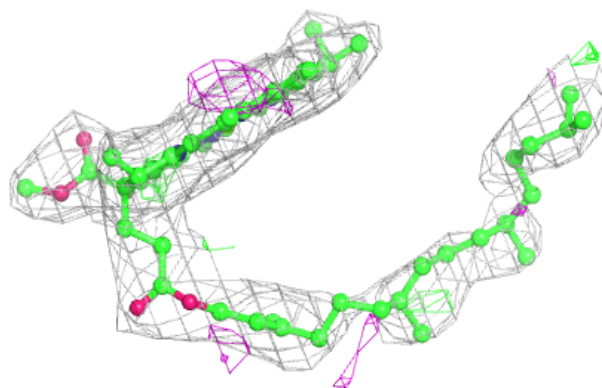


**Electron density around CLA A 812:**

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

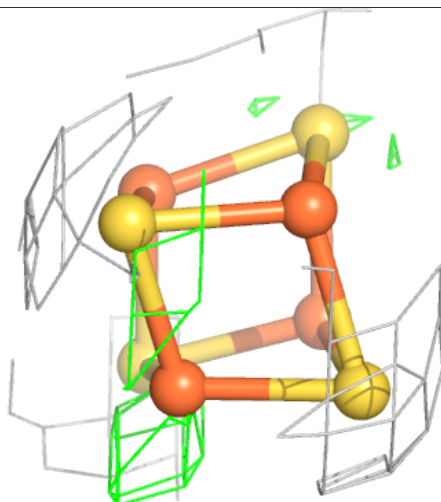
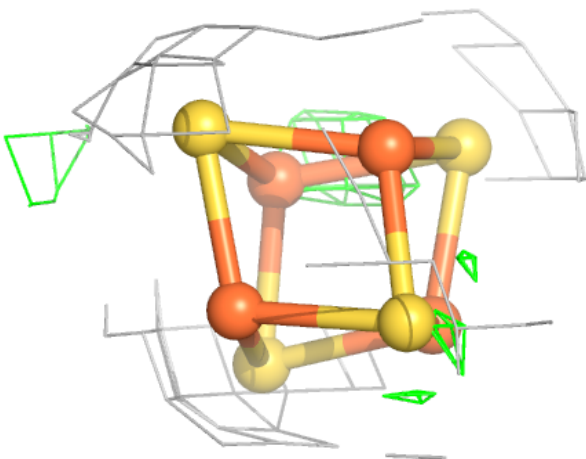
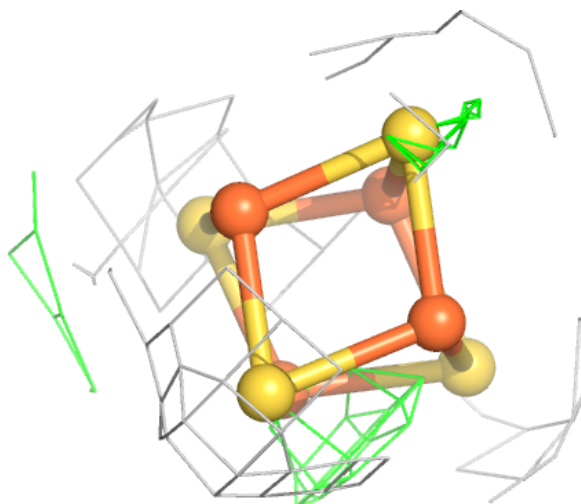
**Electron density around CLA h 201:**

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



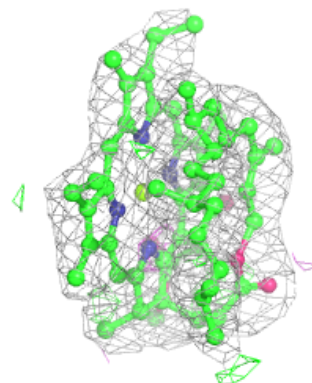
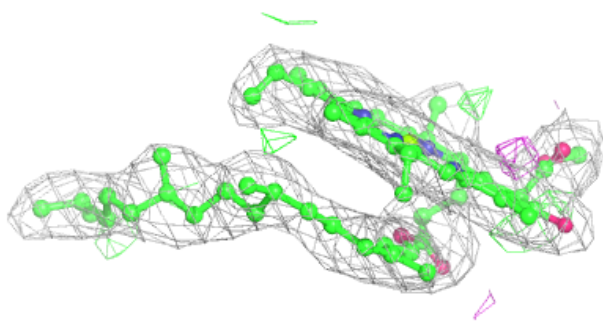
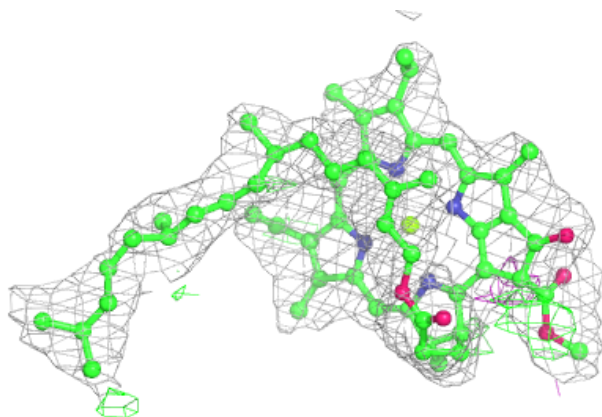
**Electron density around SF4 C 102:**

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



**Electron density around CLA H 807:**

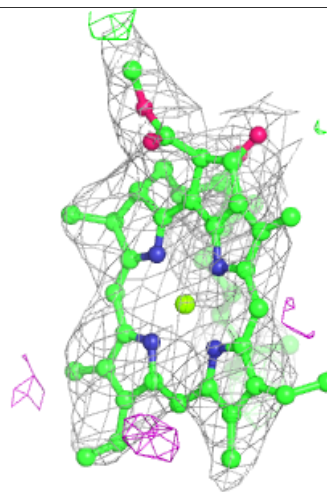
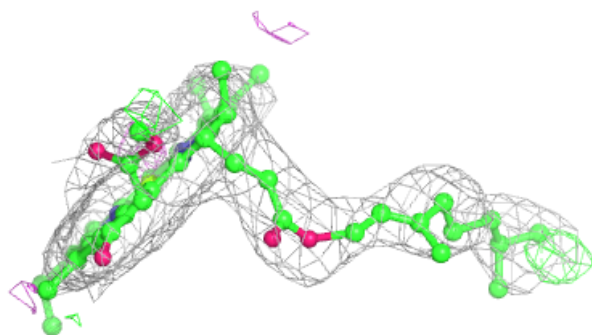
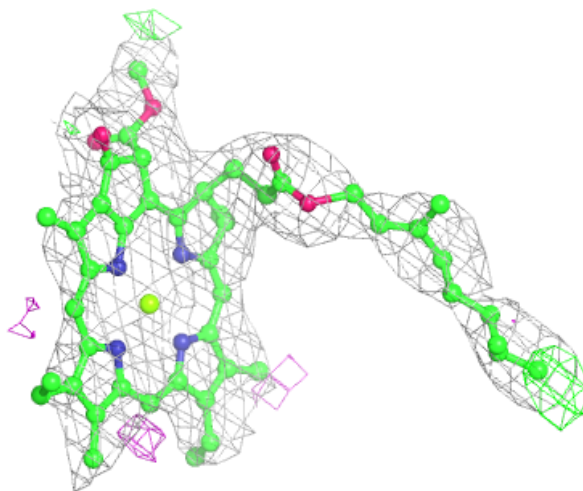
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





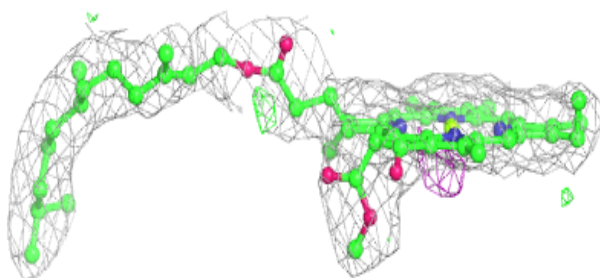
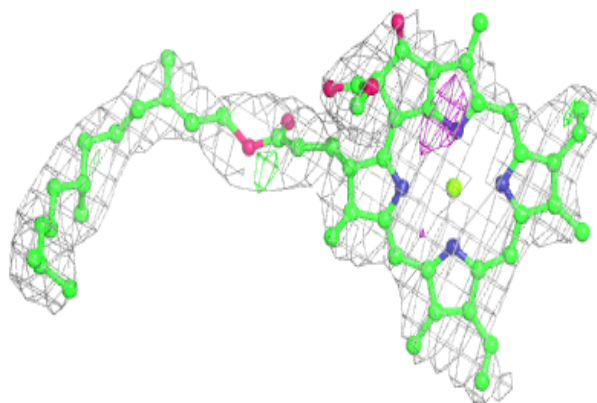
**Electron density around CLA Y 833:**

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

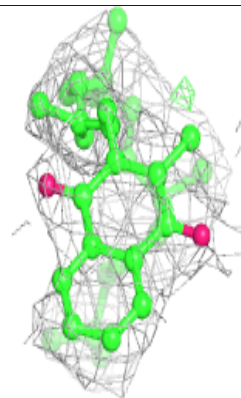
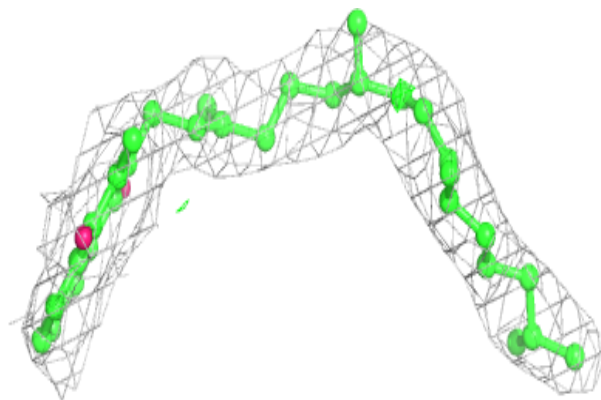


**Electron density around CLA B 836:**

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

**Electron density around PQN H 841:**

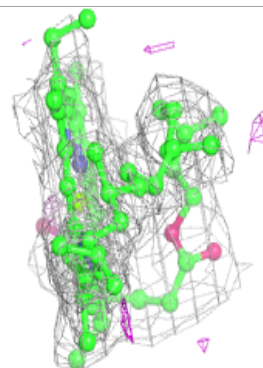
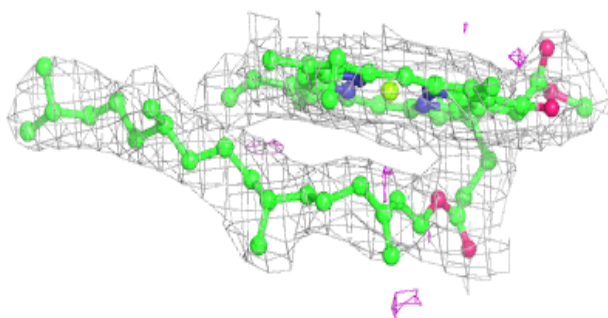
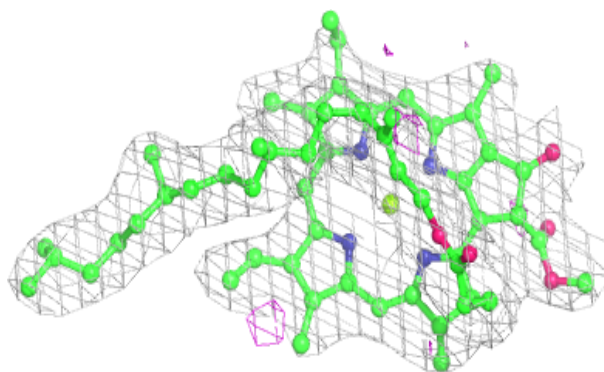
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



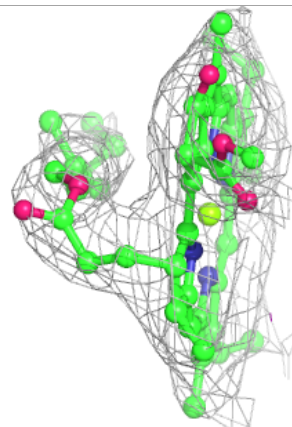
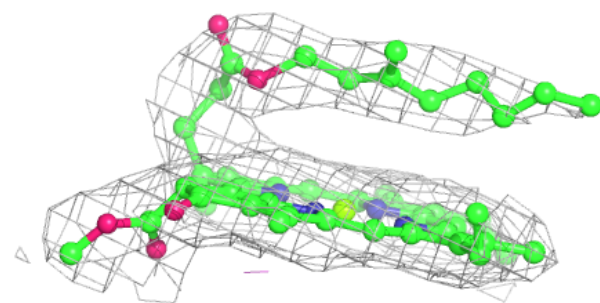
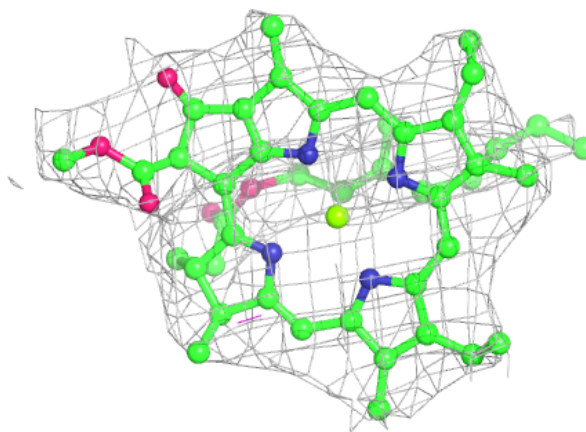


**Electron density around CLA Y 838:**

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

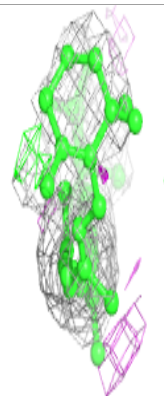
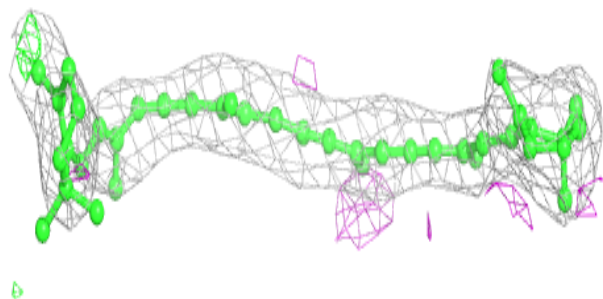
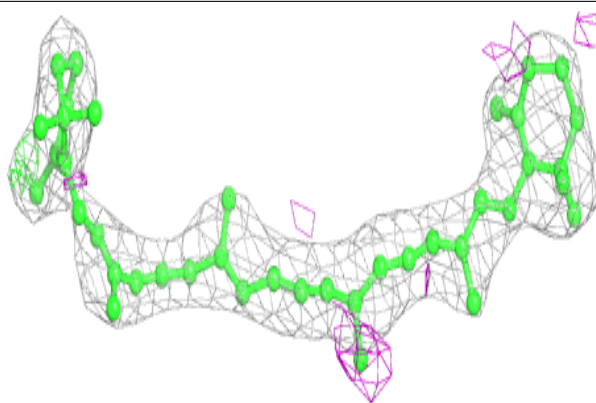
**Electron density around CLA G 812:**

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



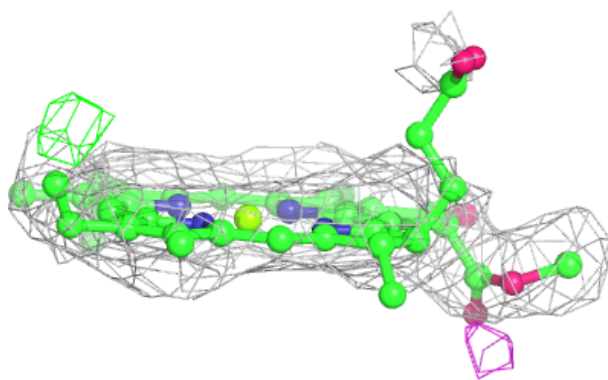
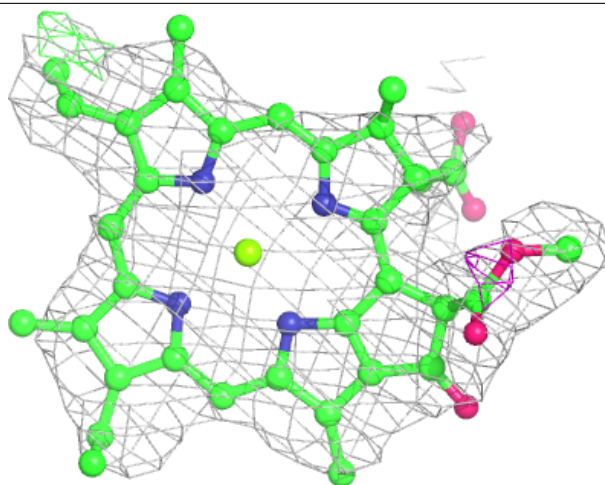
**Electron density around BCR Z 844:**

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



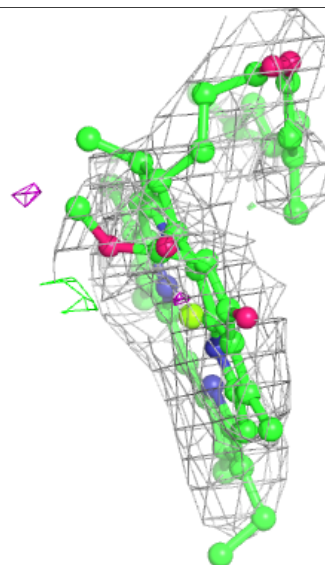
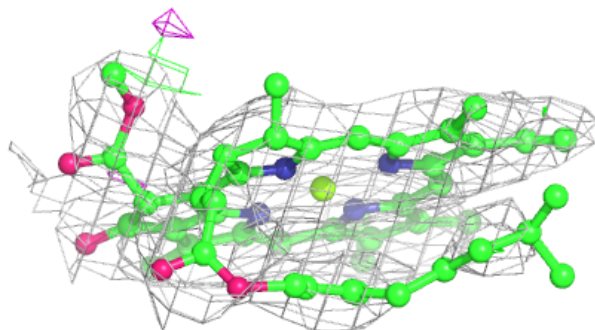
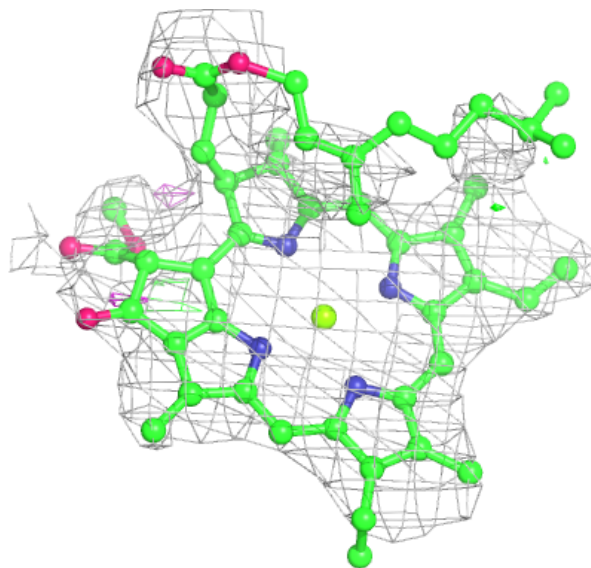
**Electron density around CLA J 101:**

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



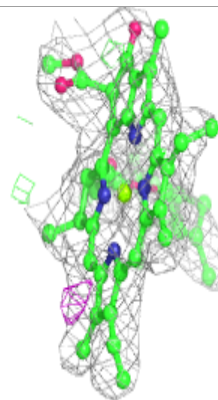
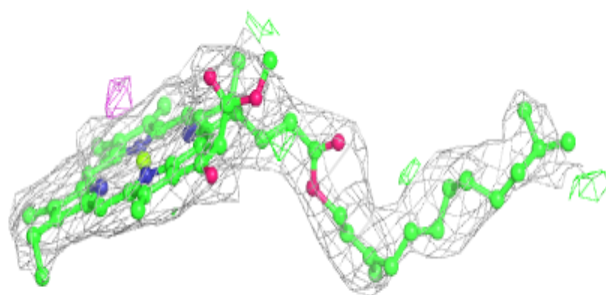
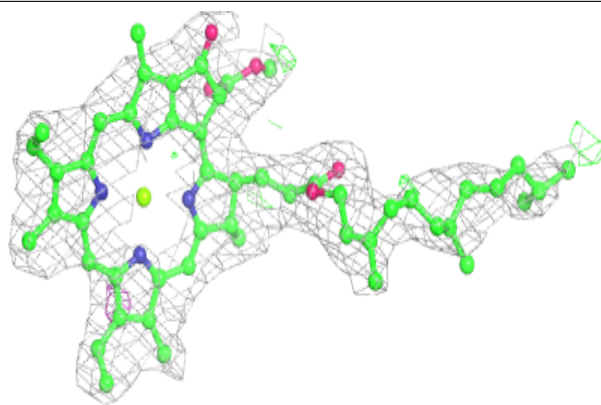
**Electron density around CLA S 1103:**

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



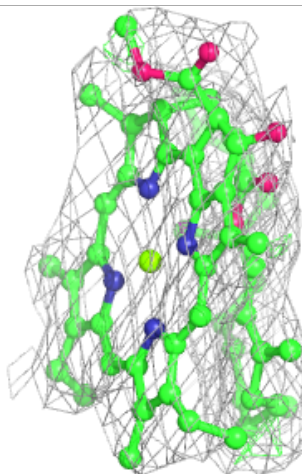
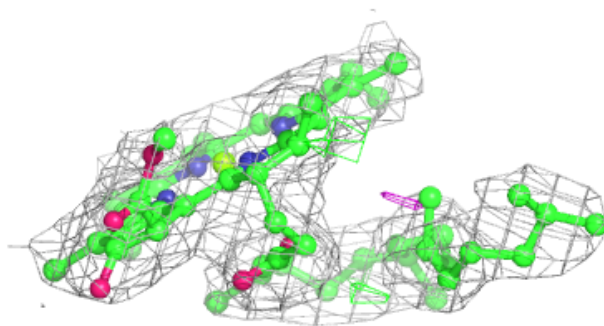
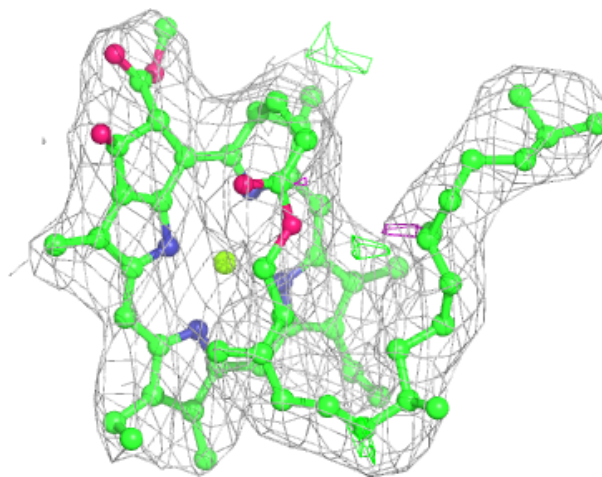
**Electron density around CLA Z 824:**

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



**Electron density around CLA Z 809:**

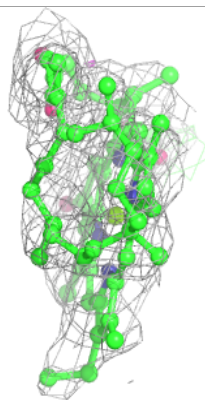
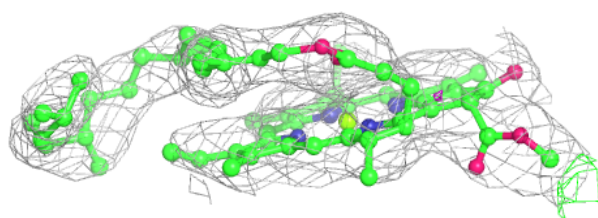
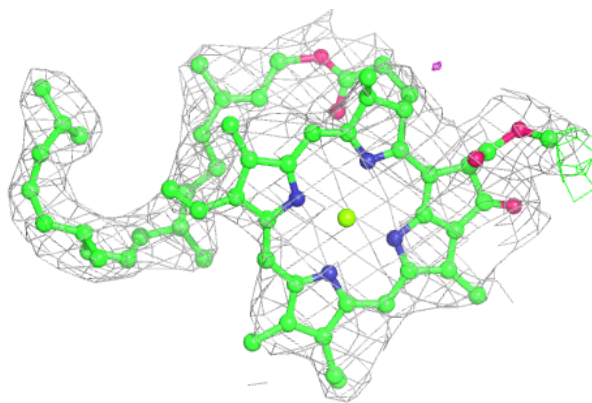
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

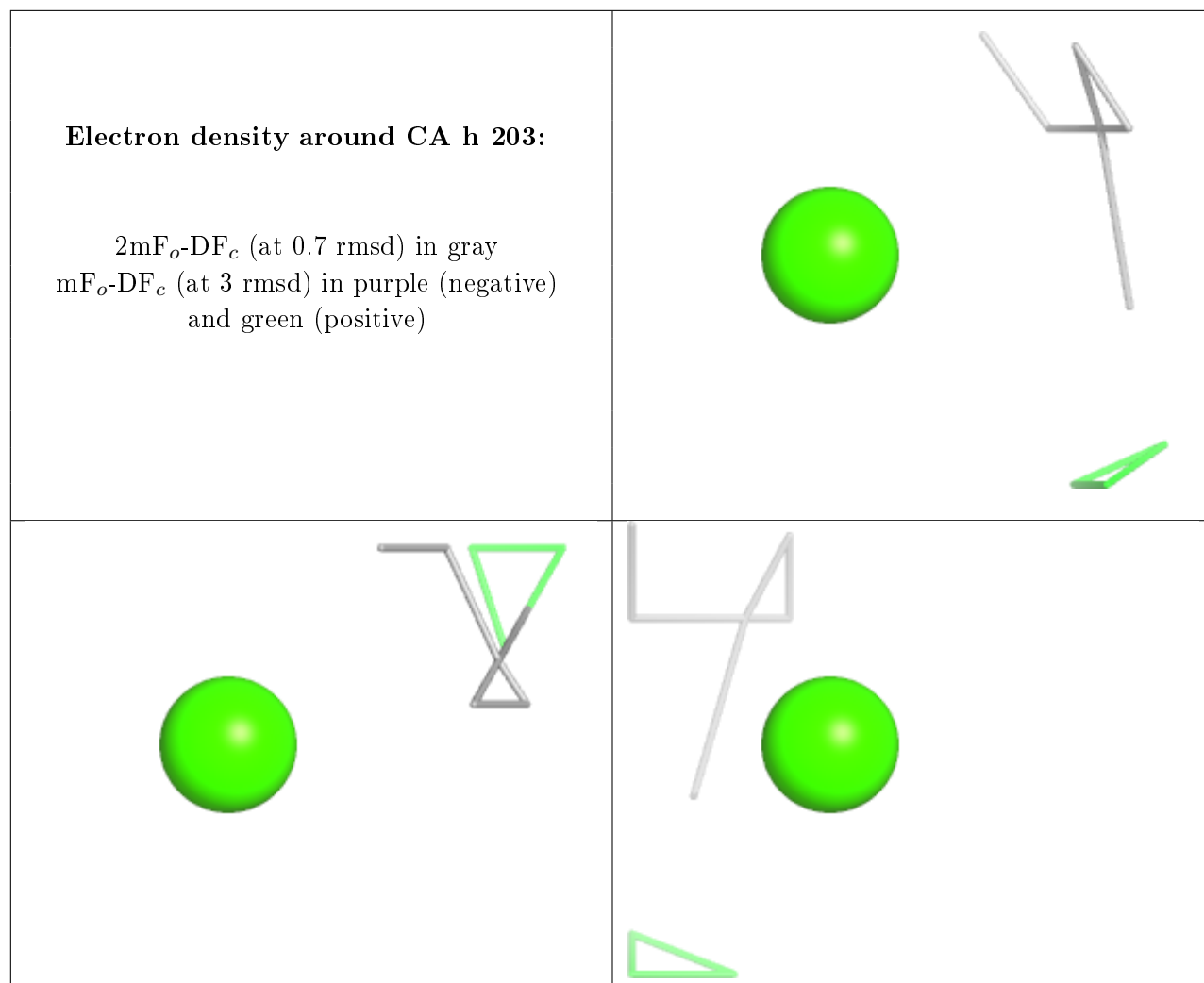




**Electron density around CLA G 819:**

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

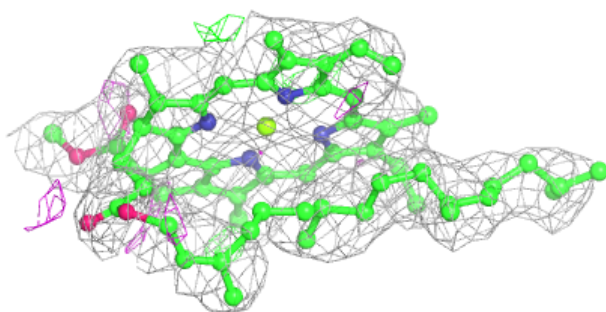
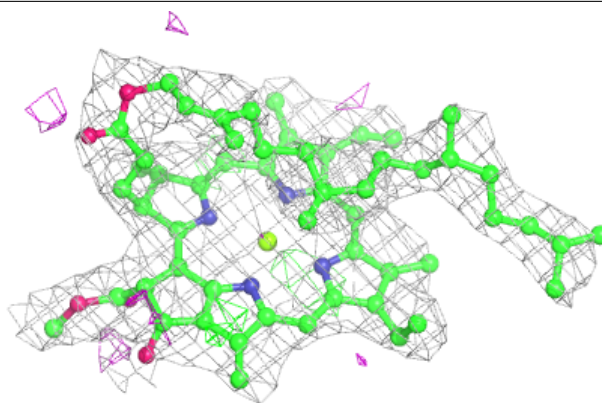




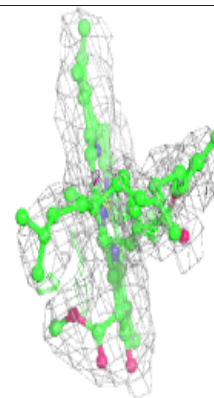
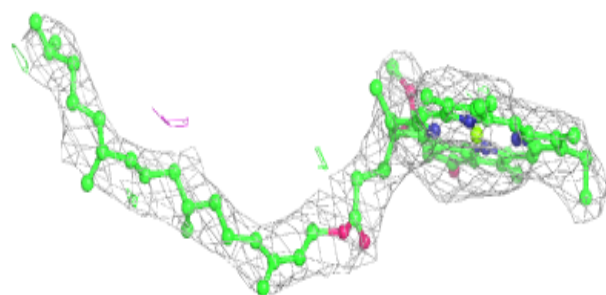
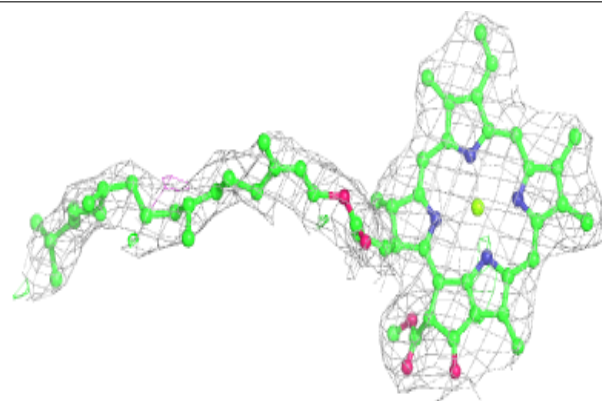


**Electron density around CLA B 816:**

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

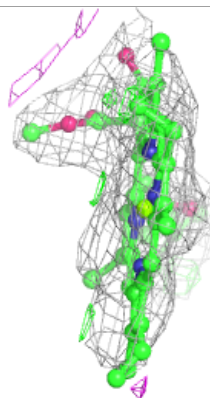
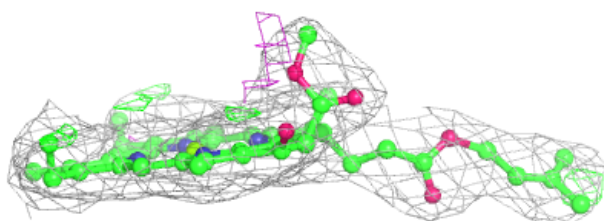
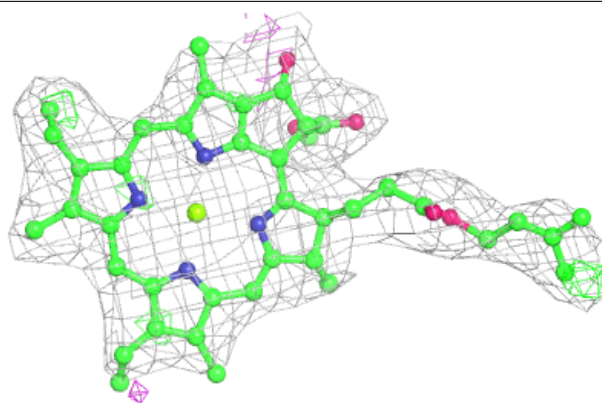
**Electron density around CLA Z 826:**

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

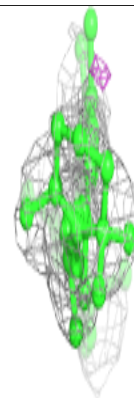
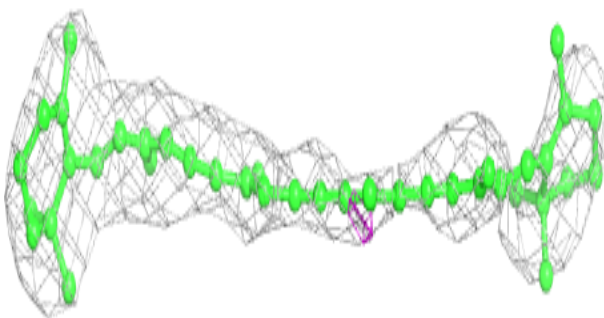
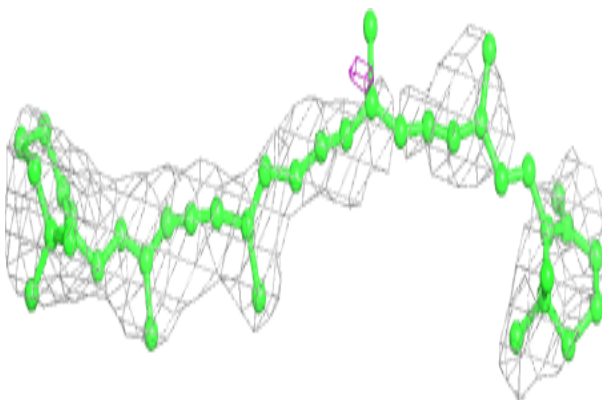


**Electron density around CLA G 836:**

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

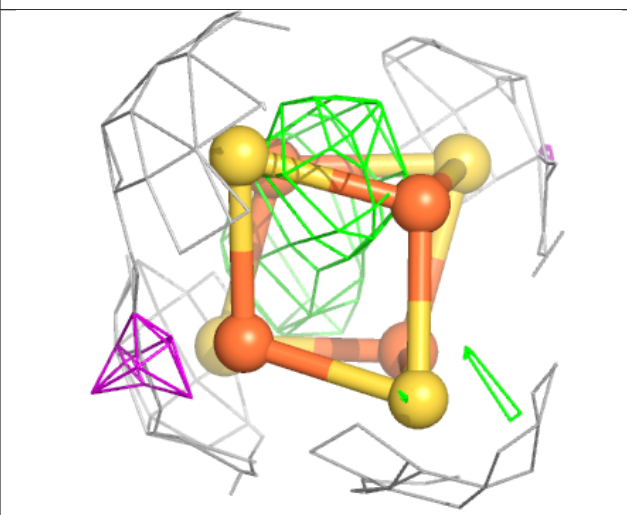
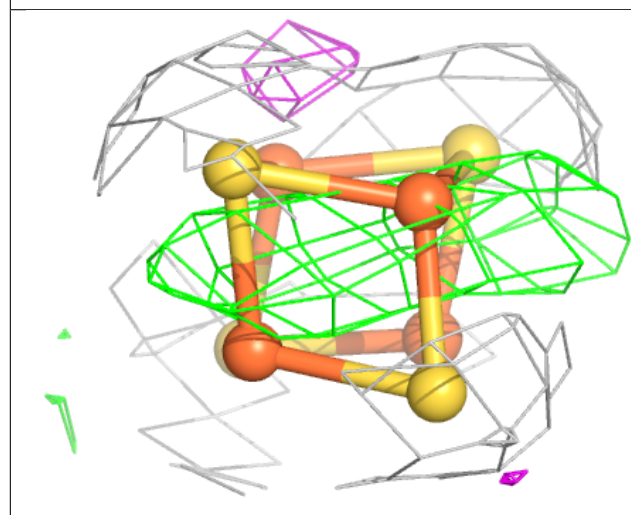
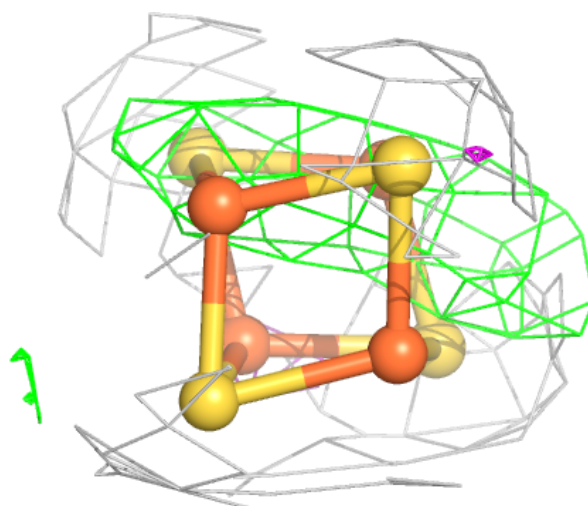
**Electron density around BCR G 847:**

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



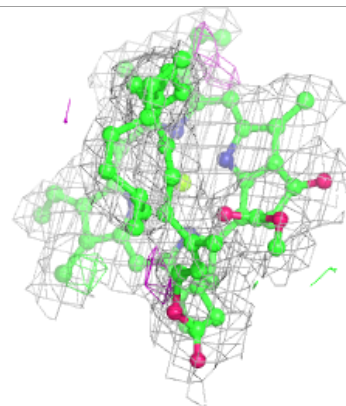
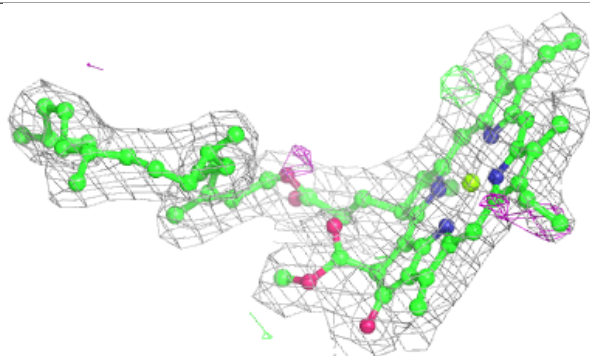
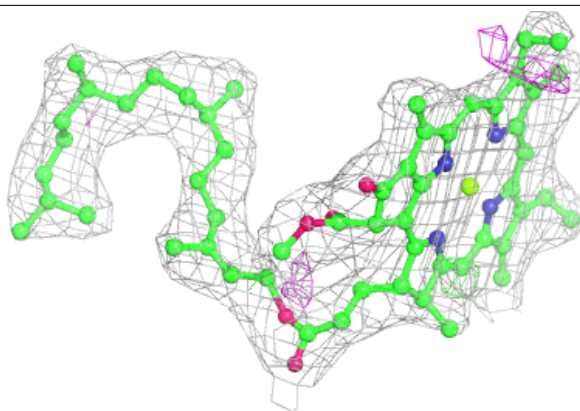
**Electron density around SF4 a 101:**

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

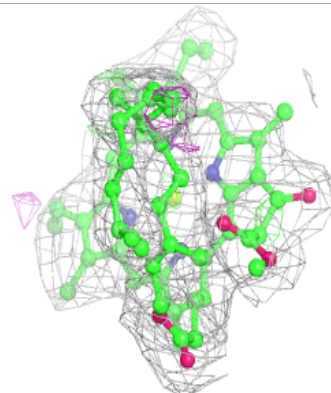
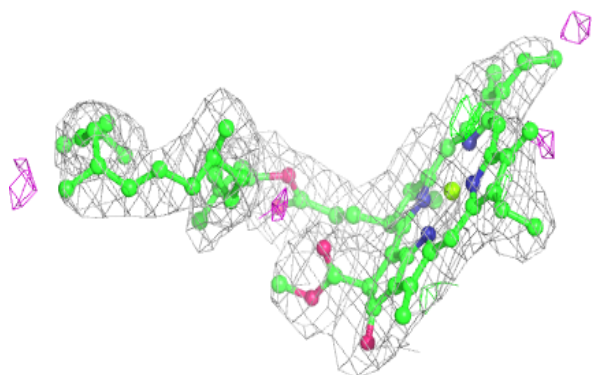
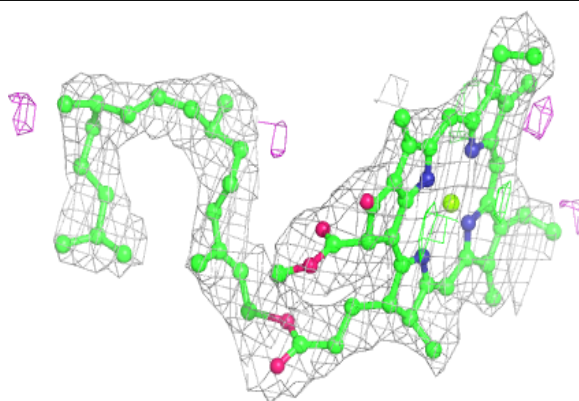


**Electron density around CL0 G 801:**

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

**Electron density around CL0 A 801:**

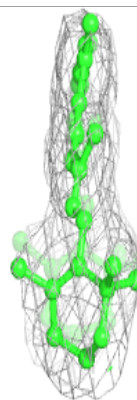
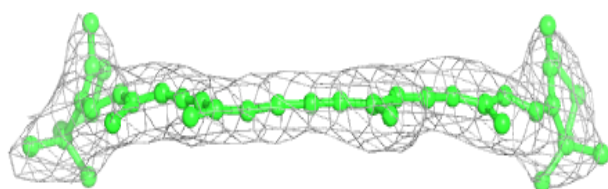
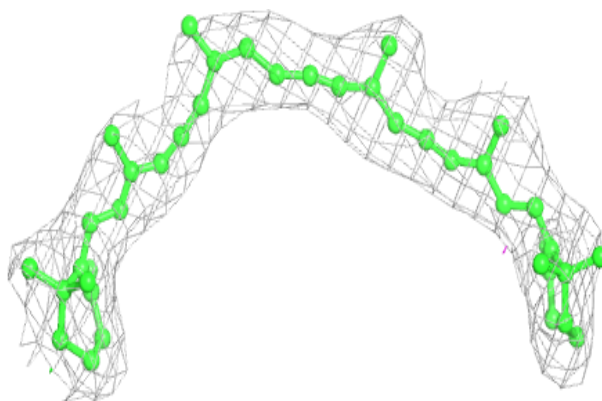
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



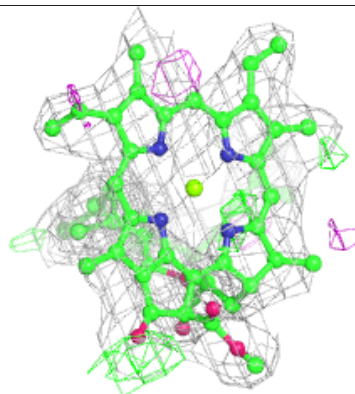
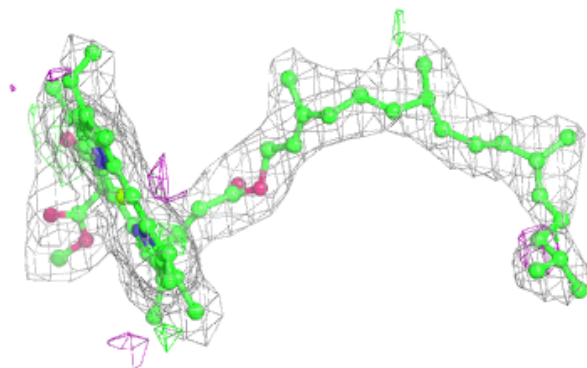
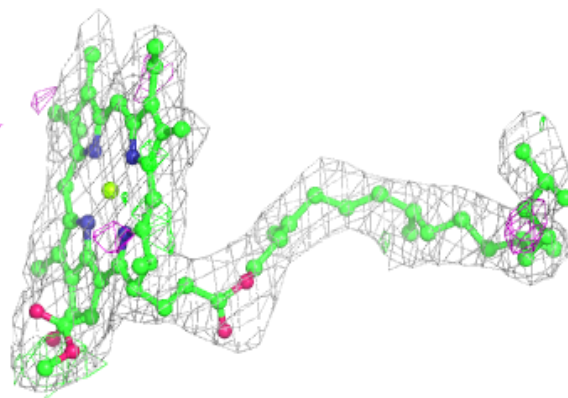


**Electron density around BCR F 203:**

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

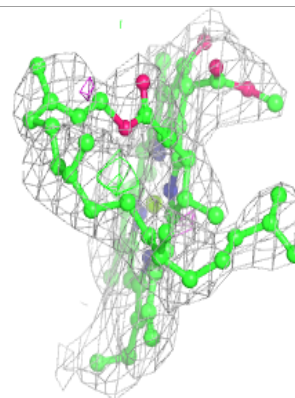
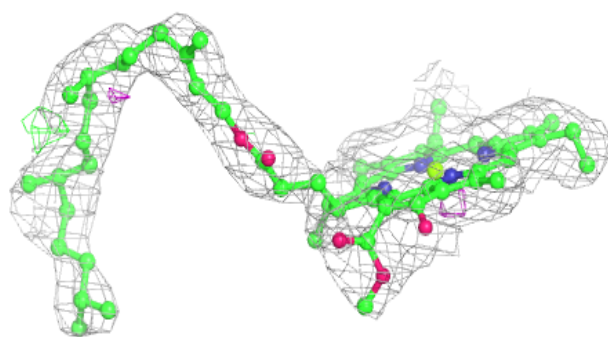
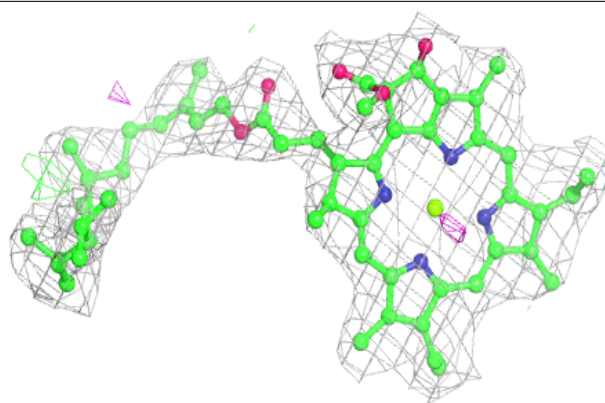
**Electron density around CLA h 205:**

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

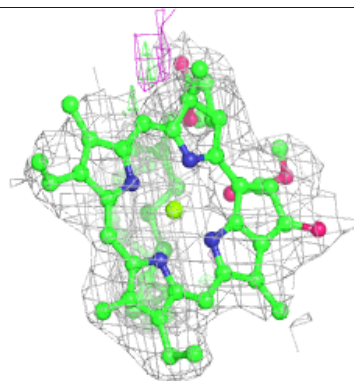
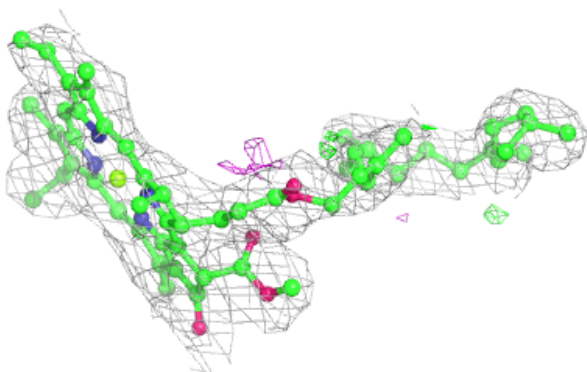
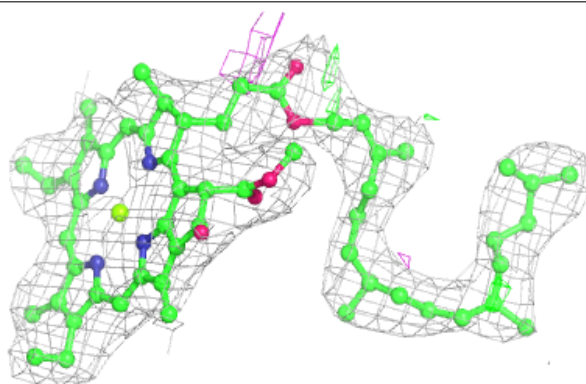


**Electron density around CLA A 828:**

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

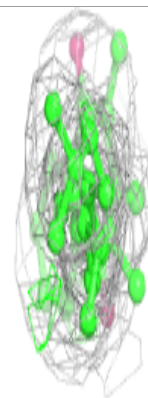
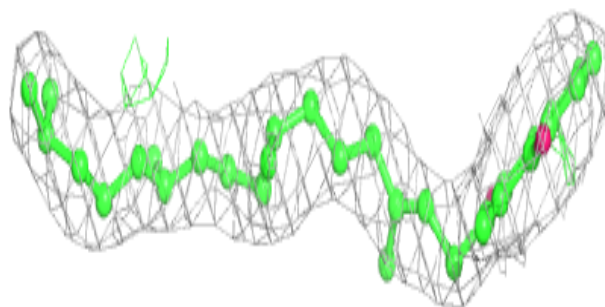
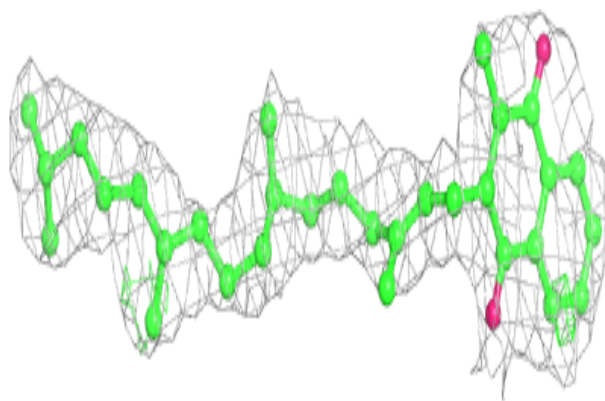
**Electron density around CL0 Y 801:**

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



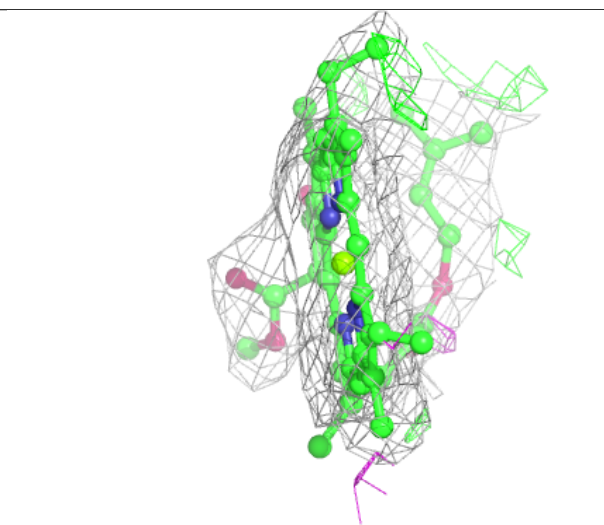
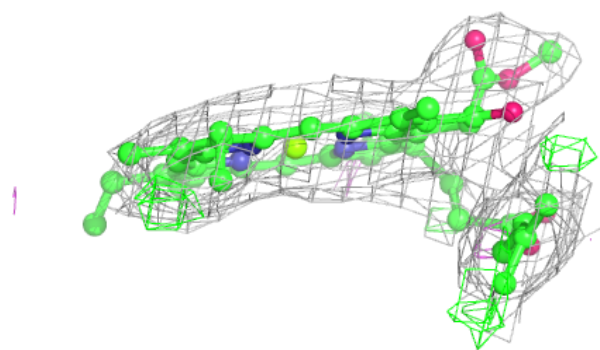
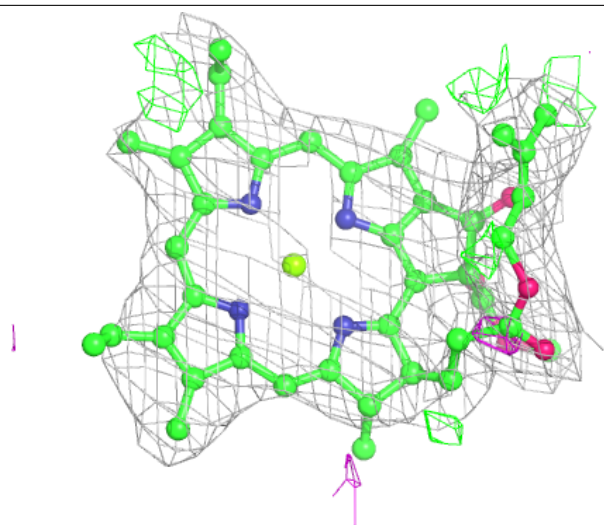
**Electron density around PQN Y 842:**

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



**Electron density around CLA A 843:**

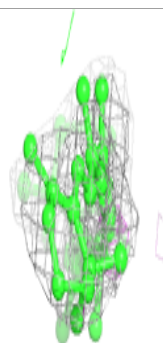
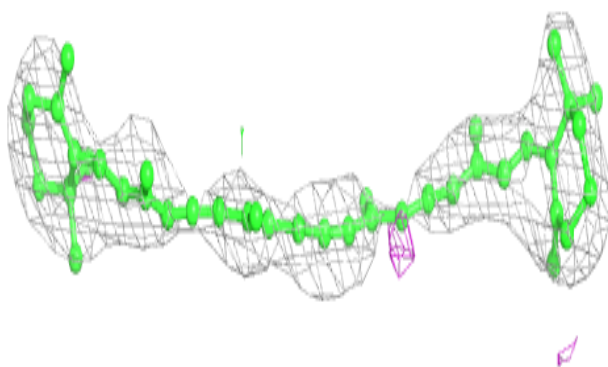
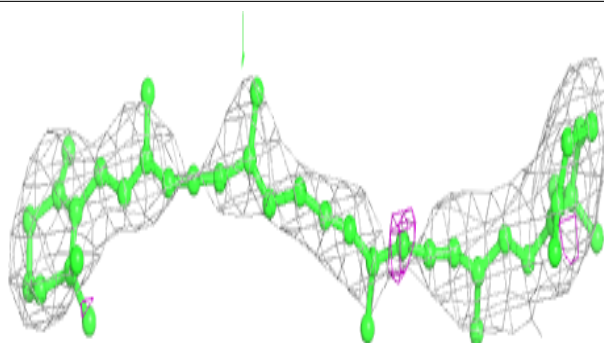
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





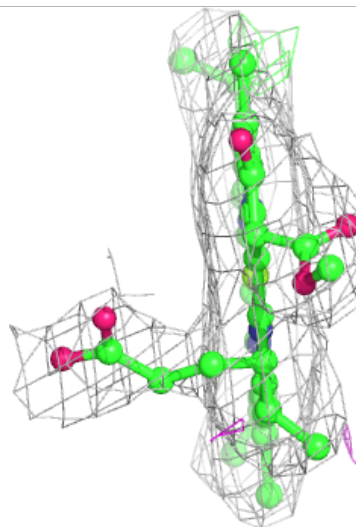
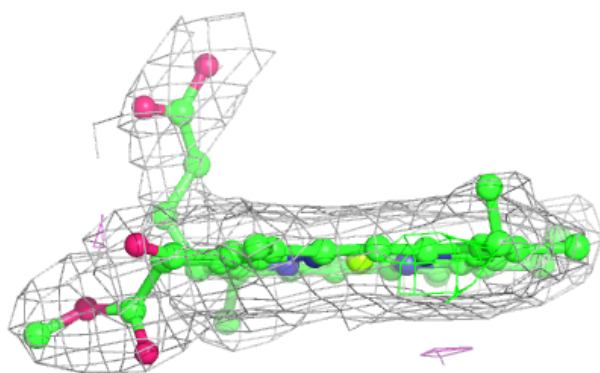
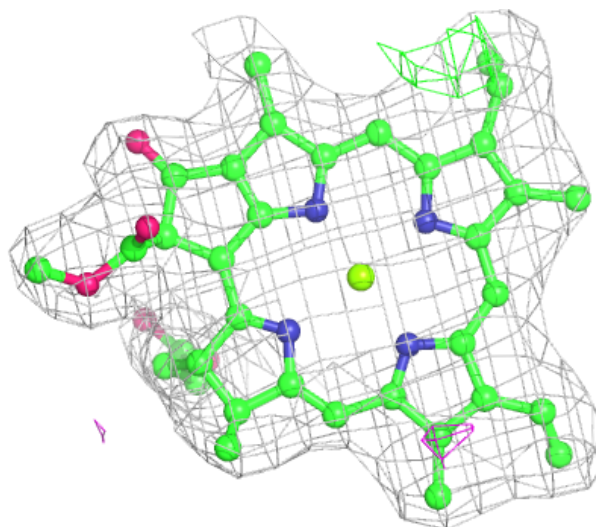
**Electron density around BCR A 848:**

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



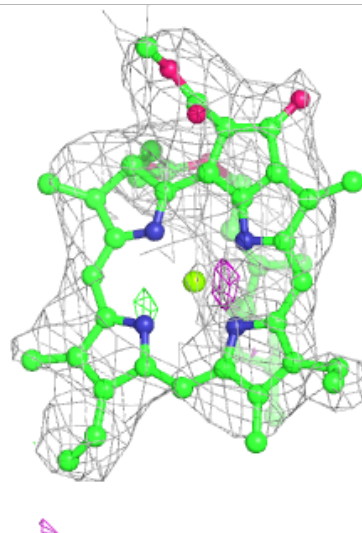
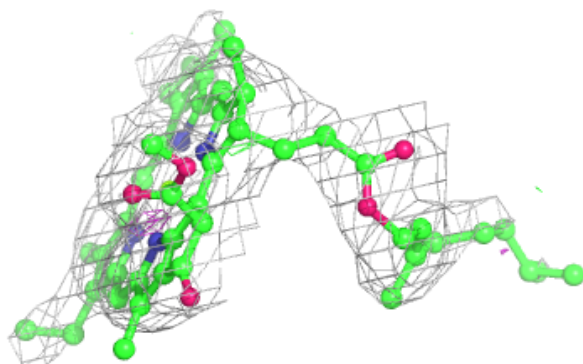
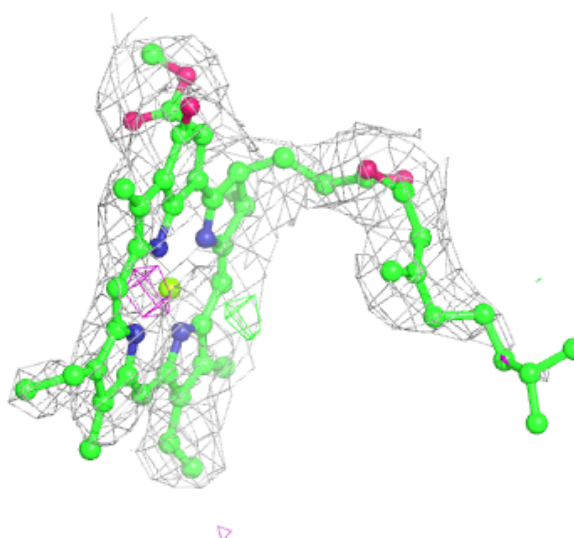
**Electron density around CLA B 830:**

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



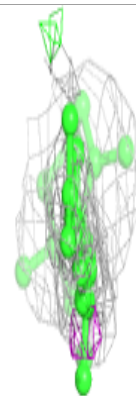
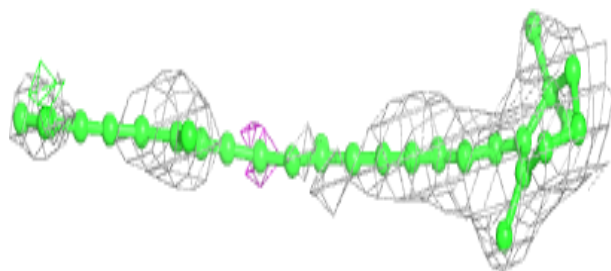
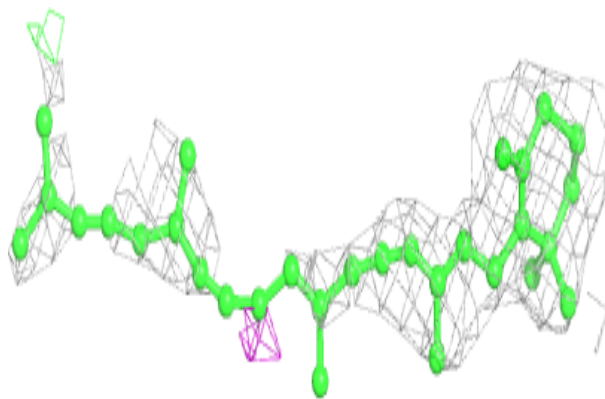
**Electron density around CLA Y 814:**

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



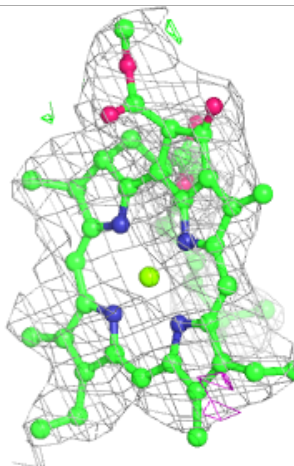
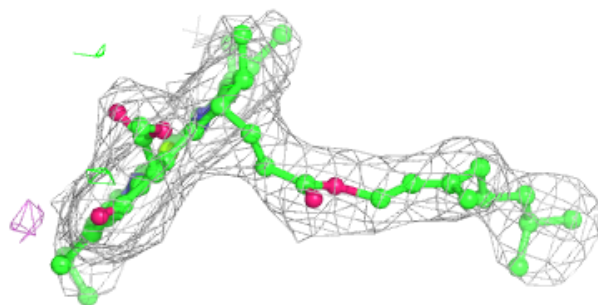
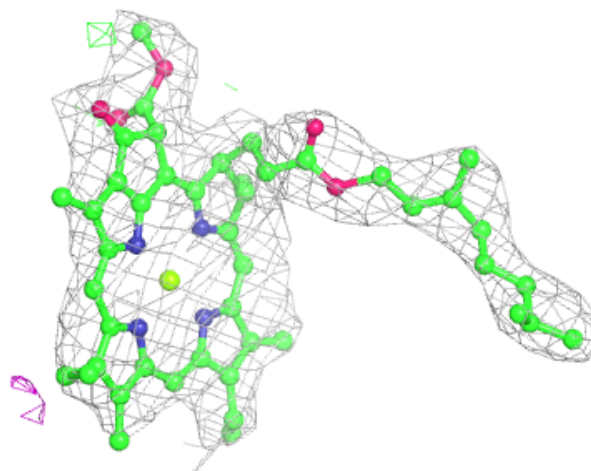
**Electron density around BCR B 842:**

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



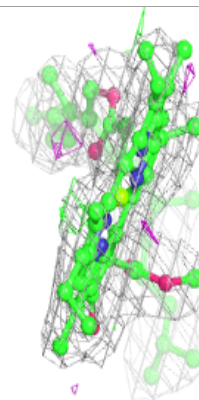
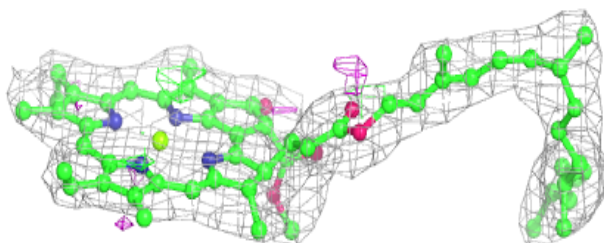
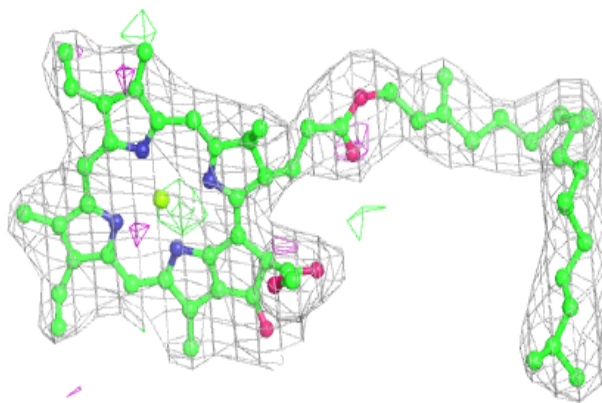
**Electron density around CLA G 834:**

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

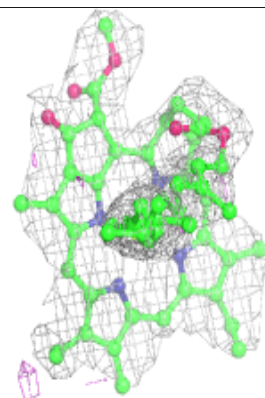
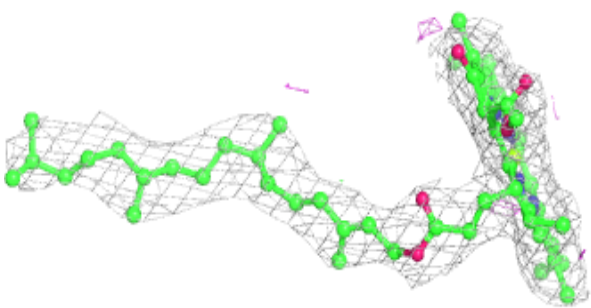
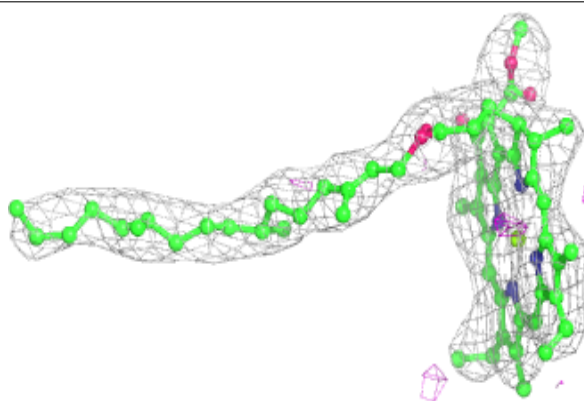


**Electron density around CLA B 825:**

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

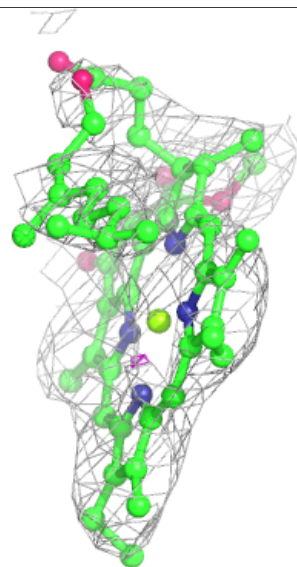
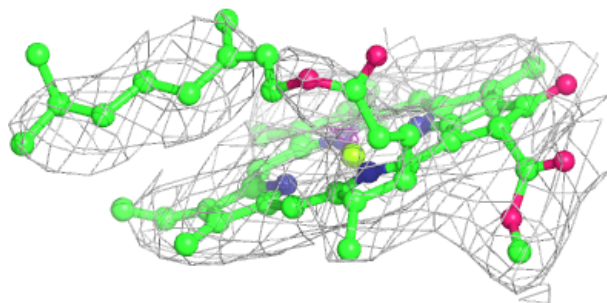
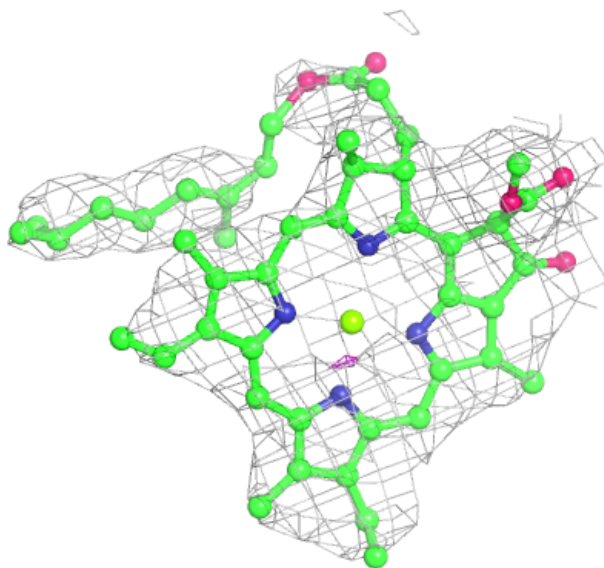
**Electron density around CLA B 827:**

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



**Electron density around CLA J 102:**

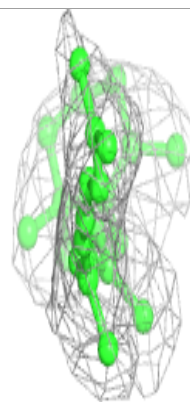
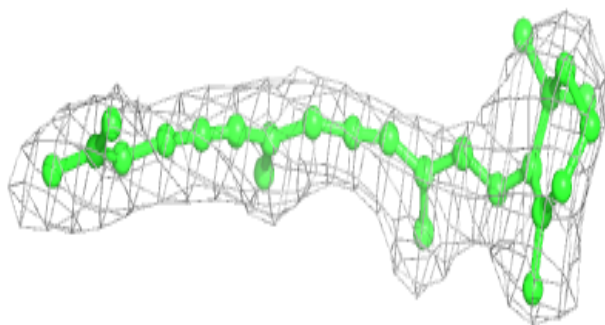
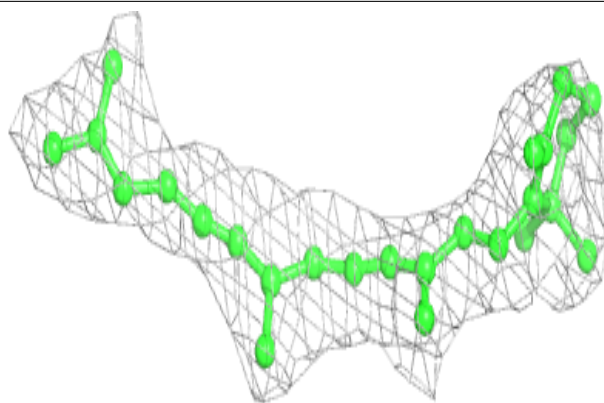
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



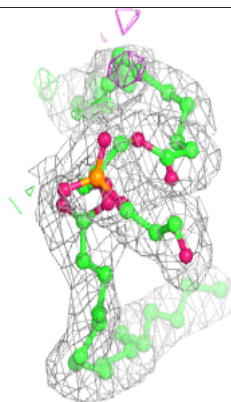
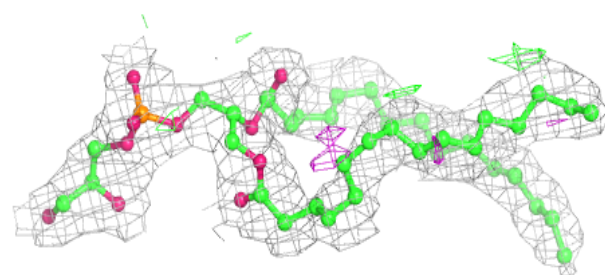
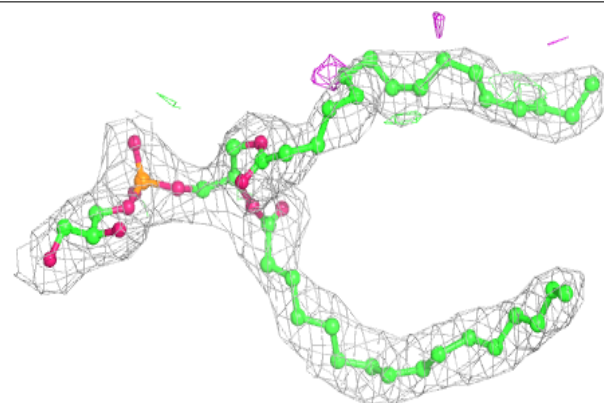


**Electron density around BCR H 845:**

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

**Electron density around LHG G 850:**

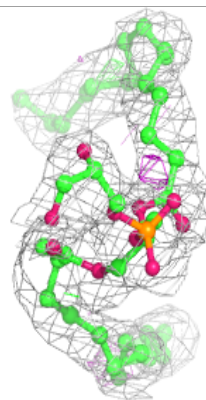
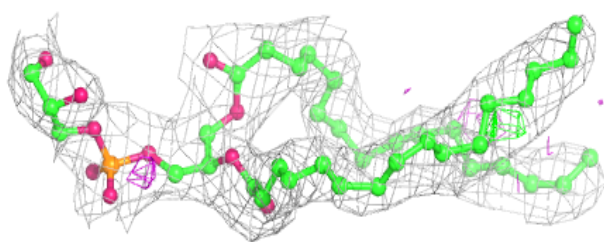
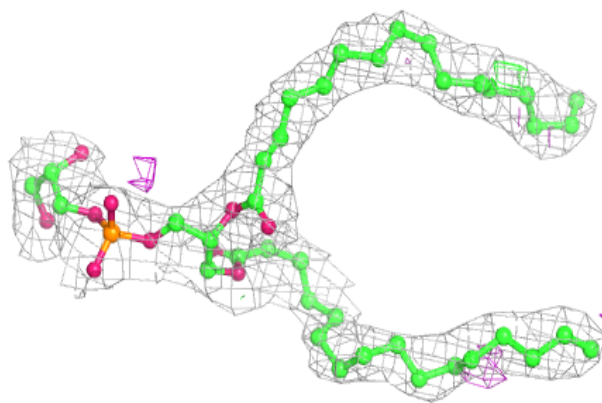
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





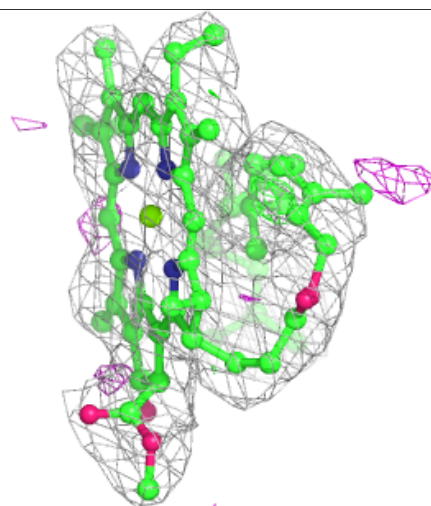
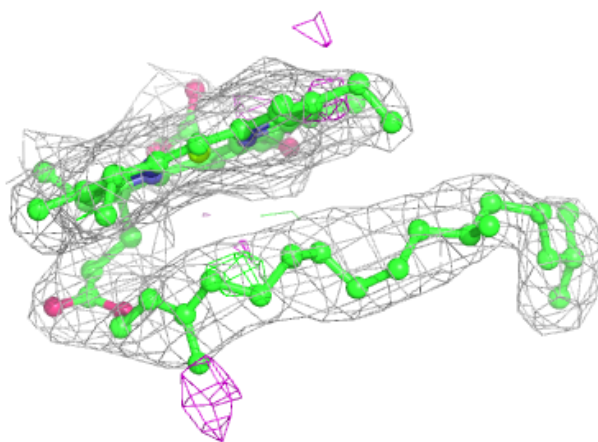
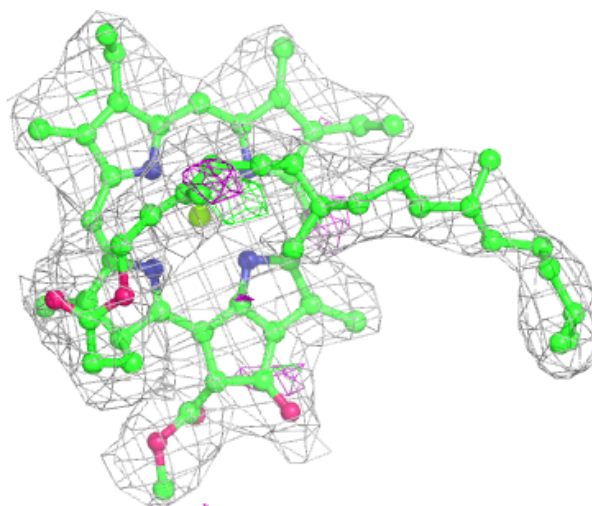
**Electron density around LHG Y 850:**

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



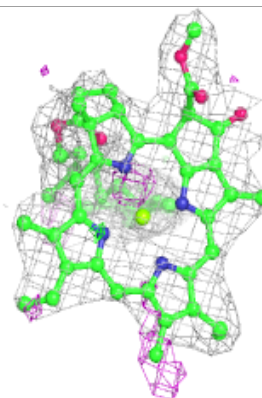
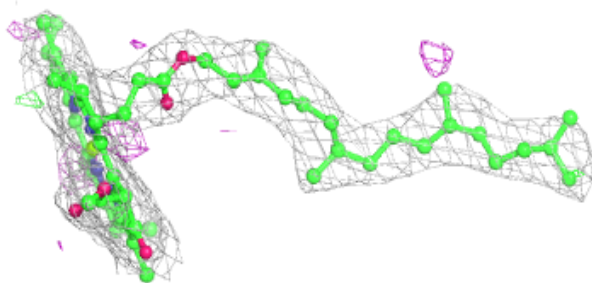
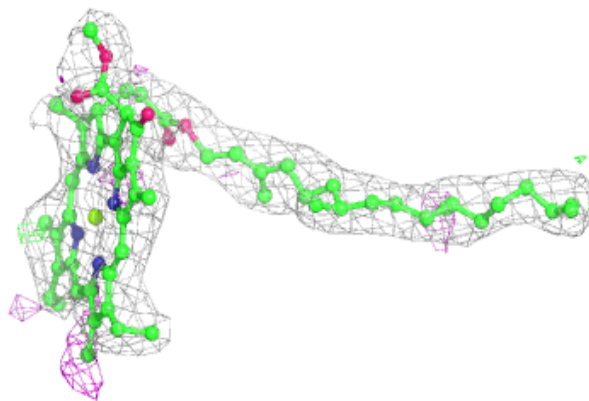
**Electron density around CLA H 827:**

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

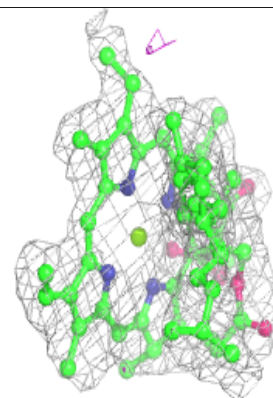
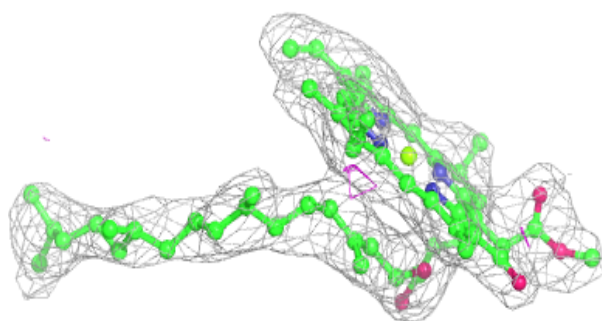
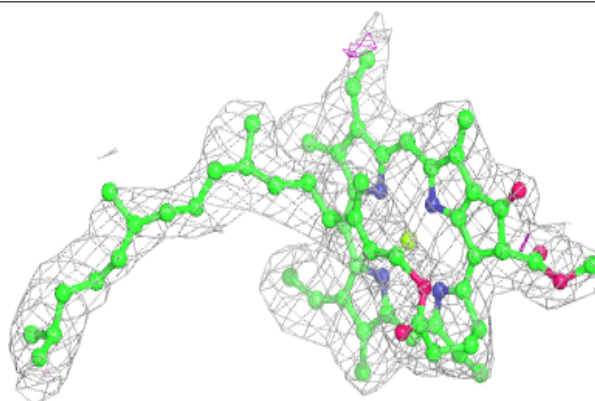


**Electron density around CLA Z 829:**

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

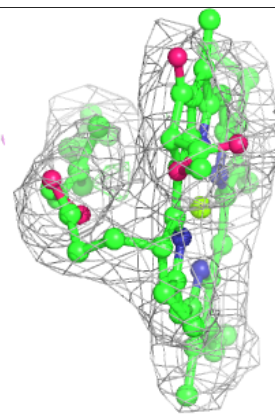
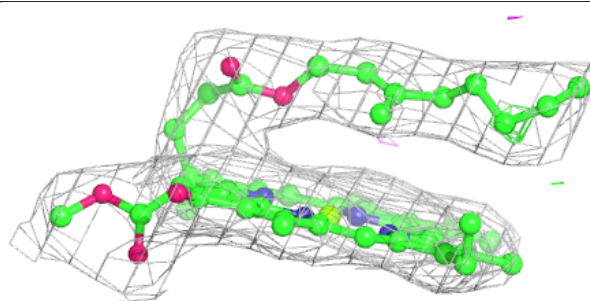
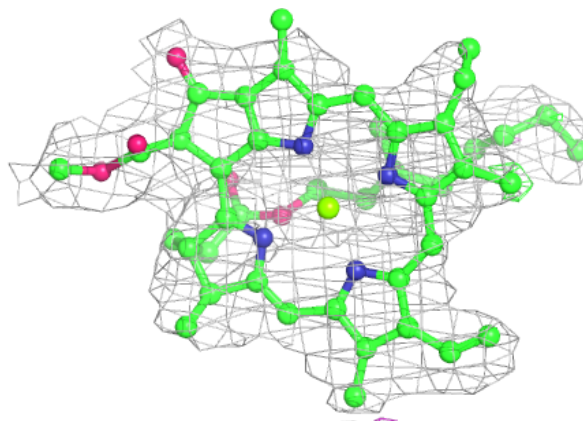
**Electron density around CLA G 840:**

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



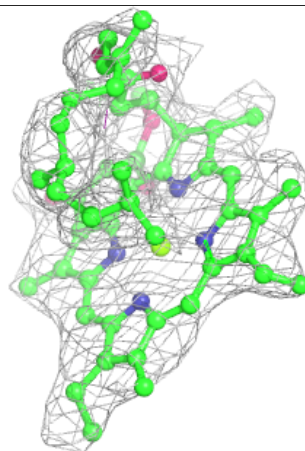
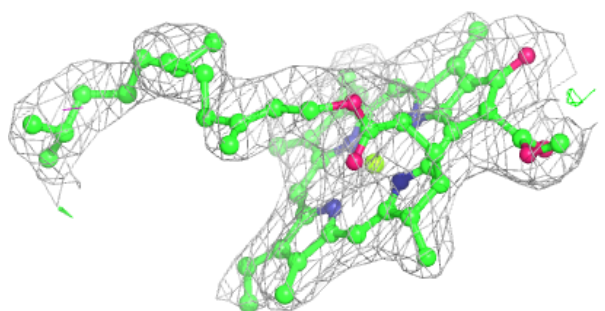
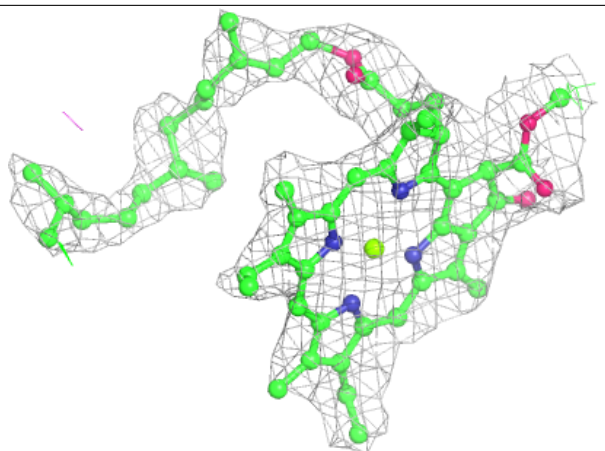
**Electron density around CLA A 813:**

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

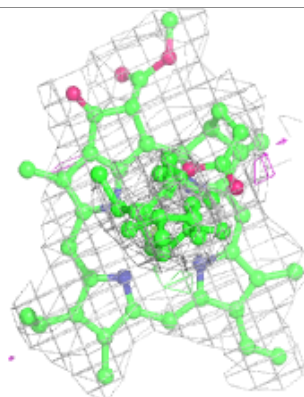
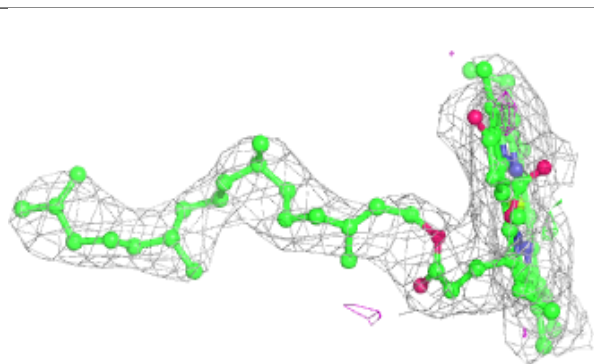
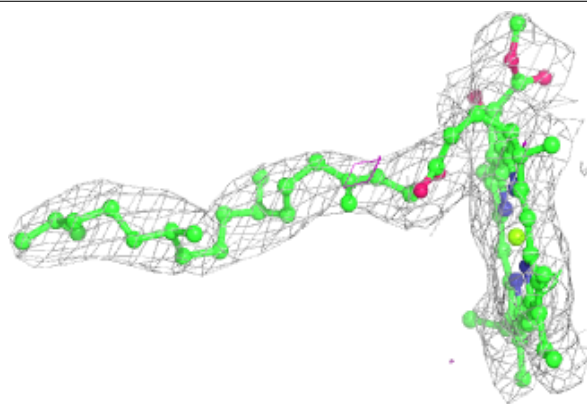


**Electron density around CLA G 824:**

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

**Electron density around CLA Y 828:**

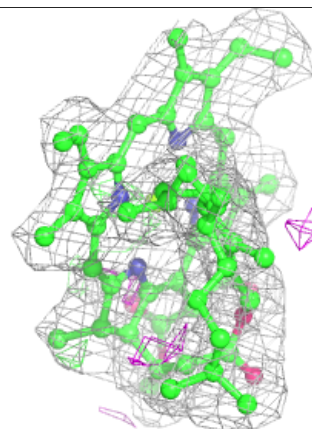
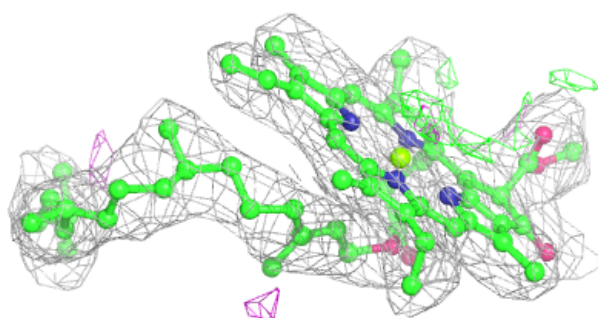
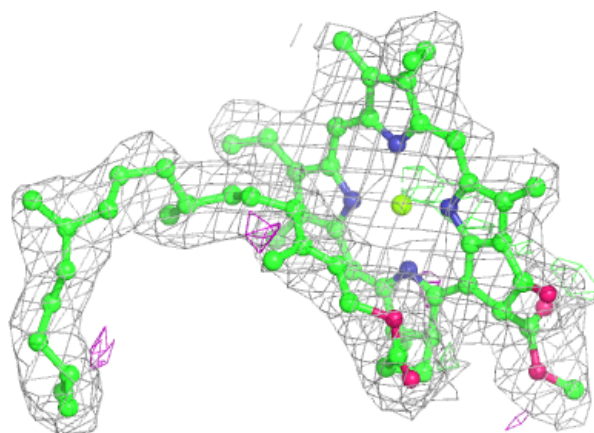
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





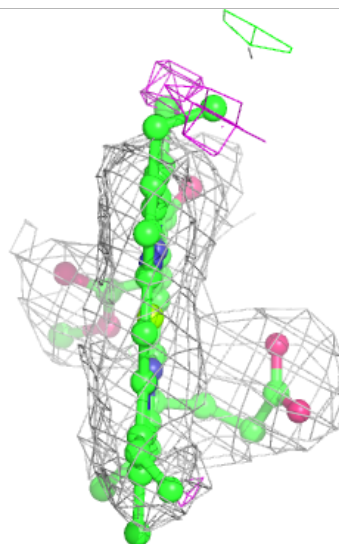
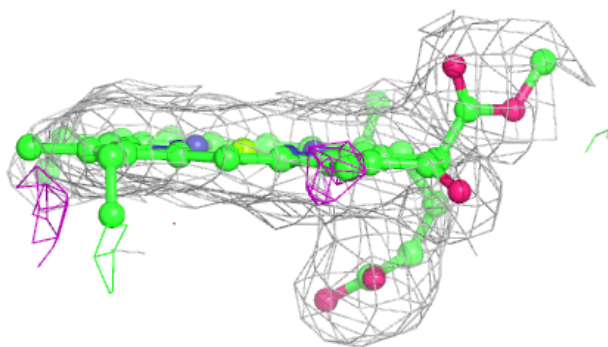
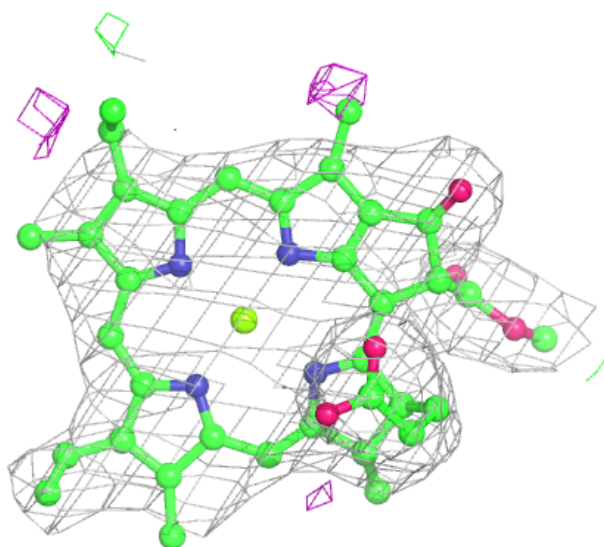
**Electron density around CLA G 841:**

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



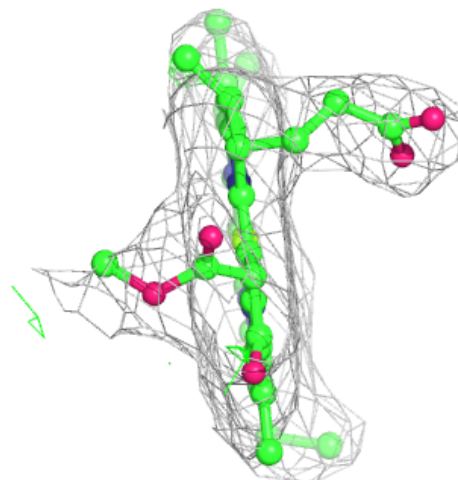
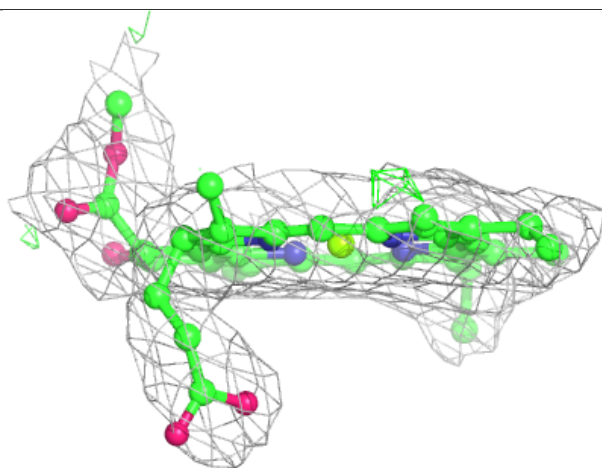
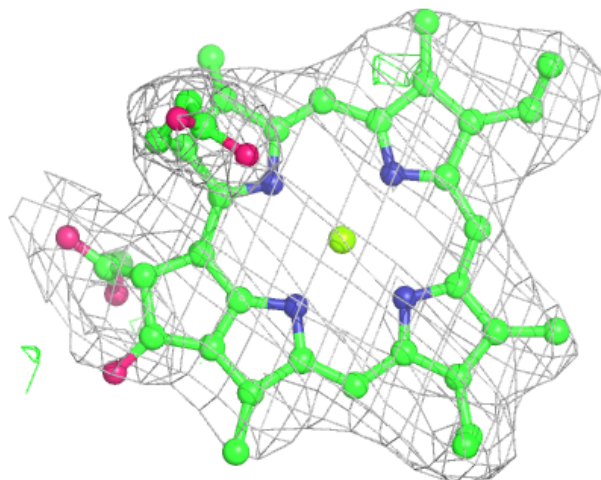
**Electron density around CLA A 835:**

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



**Electron density around CLA H 815:**

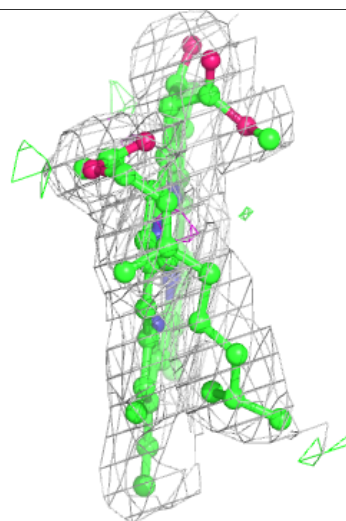
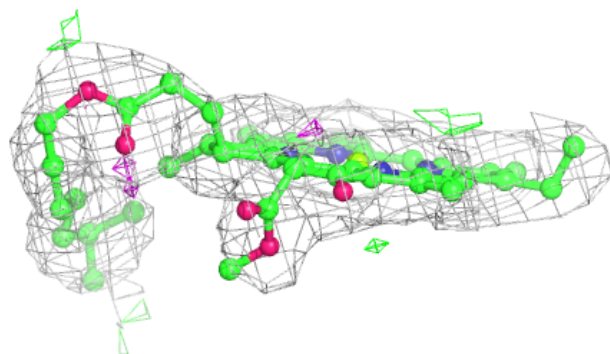
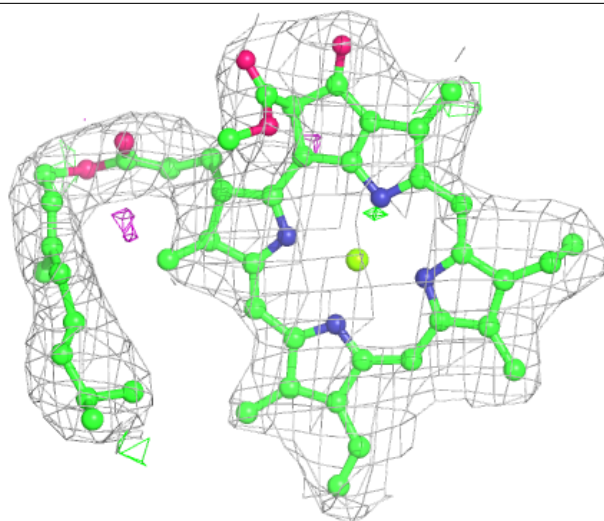
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





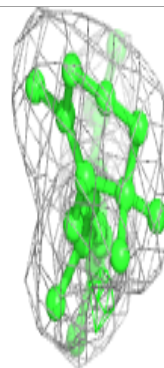
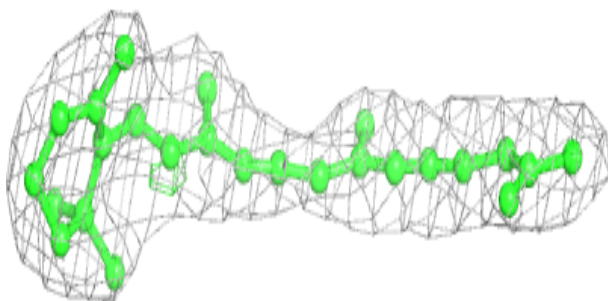
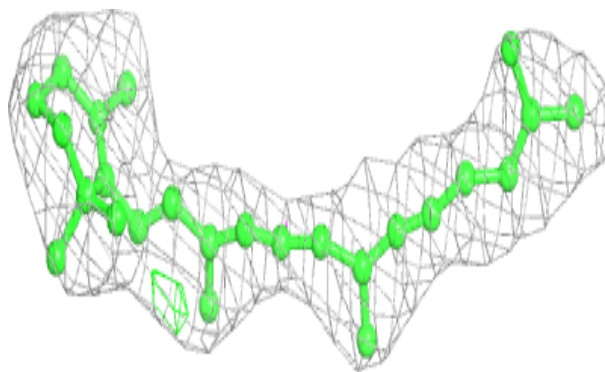
**Electron density around CLA B 823:**

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

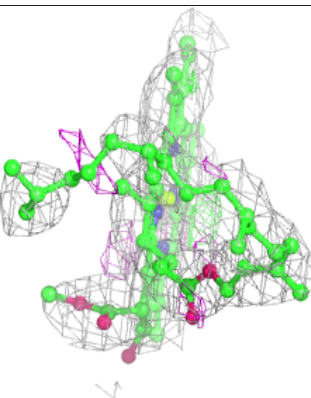
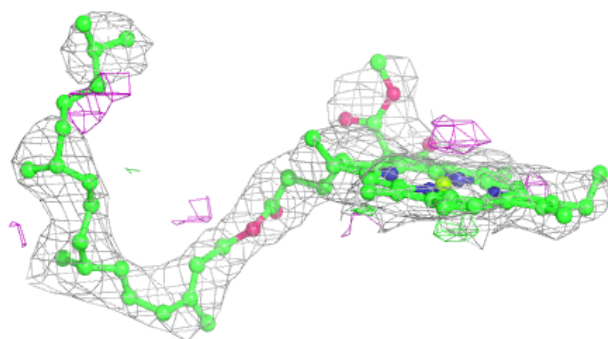
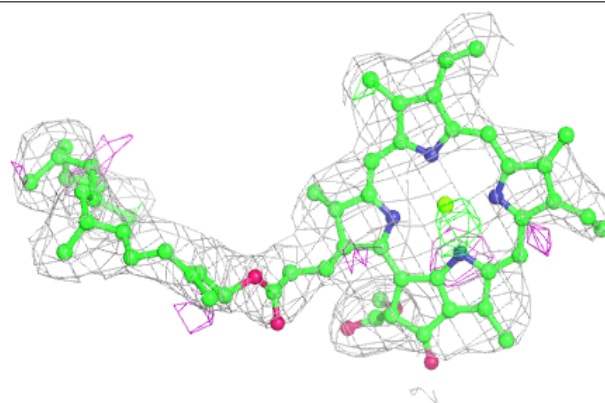


**Electron density around BCR B 845:**

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

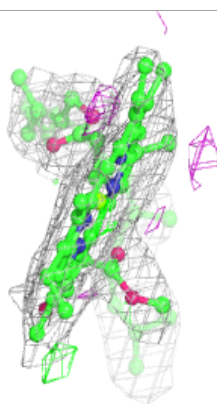
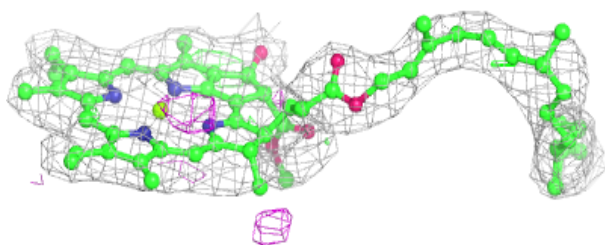
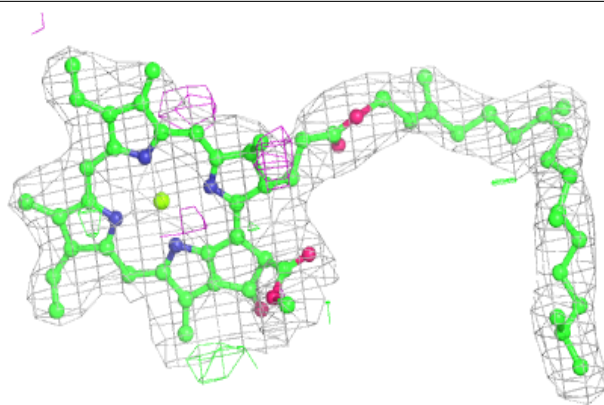
**Electron density around CLA Y 827:**

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

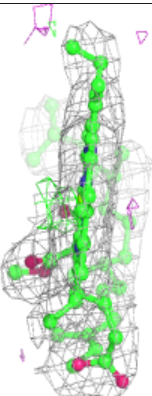
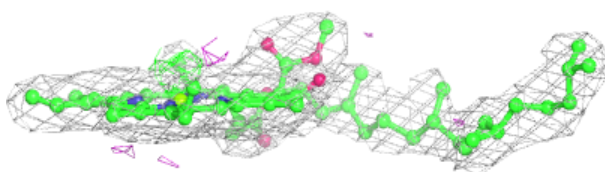
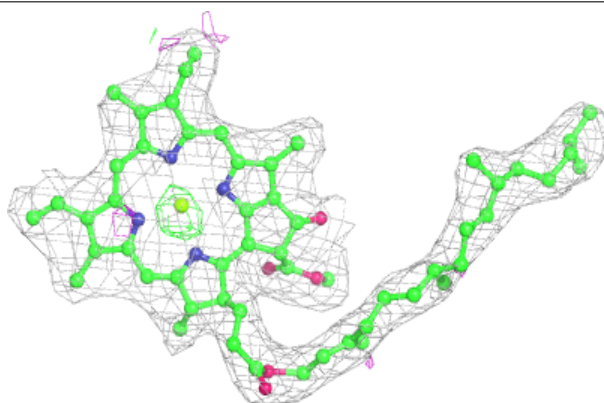


**Electron density around CLA Z 827:**

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

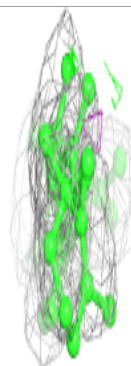
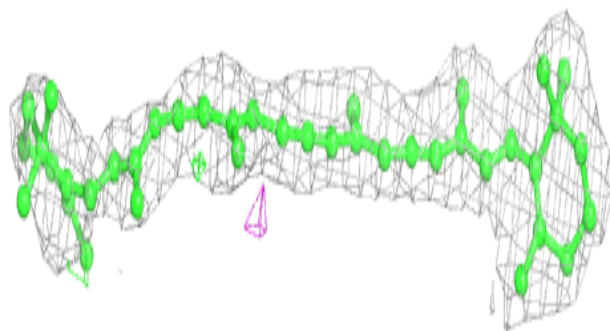
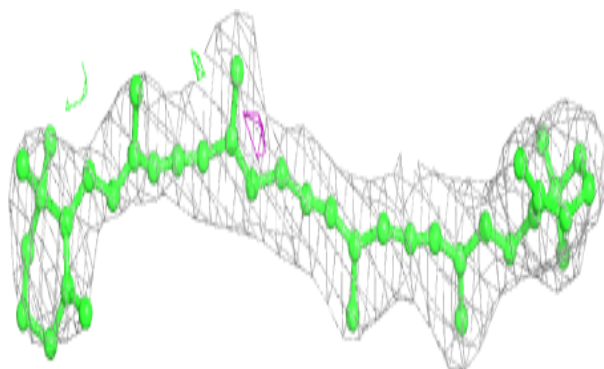
**Electron density around CLA h 206:**

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



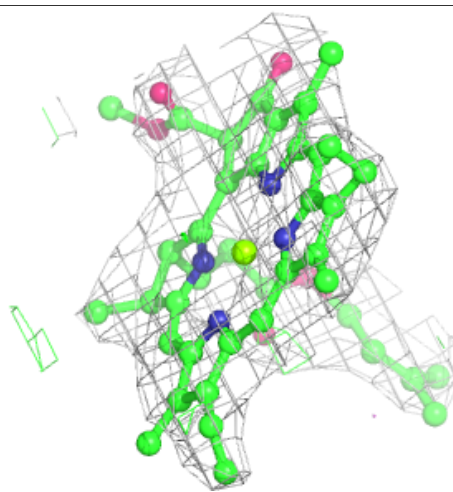
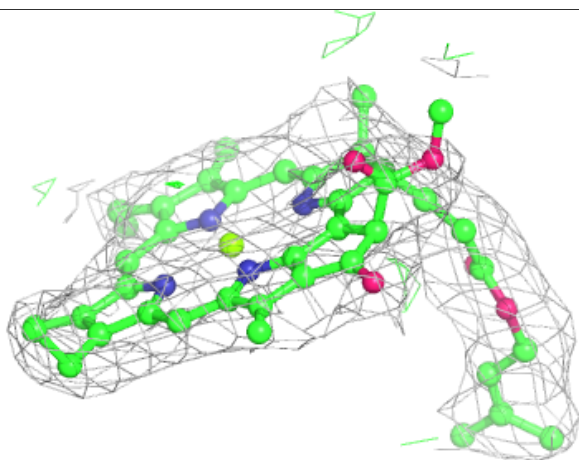
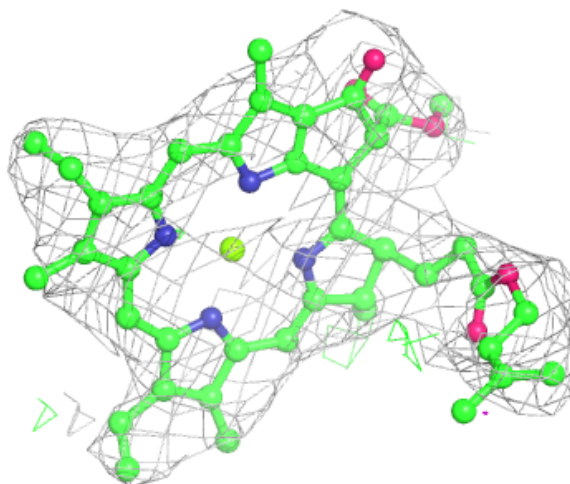
**Electron density around BCR h 202:**

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



**Electron density around CLA G 814:**

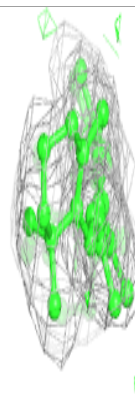
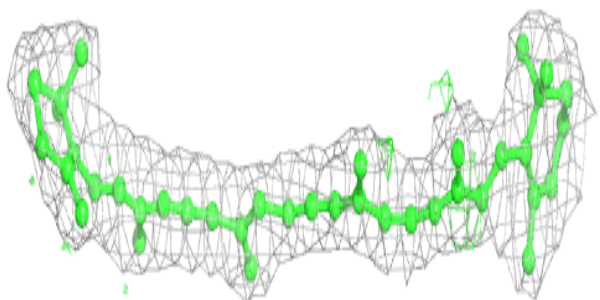
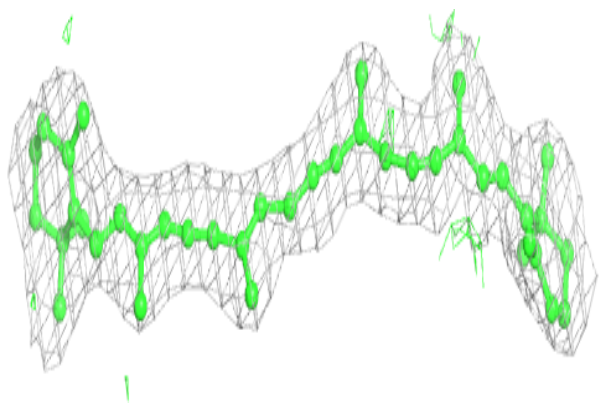
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



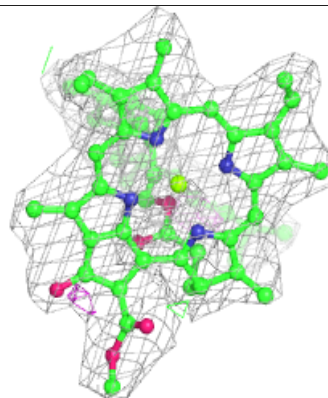
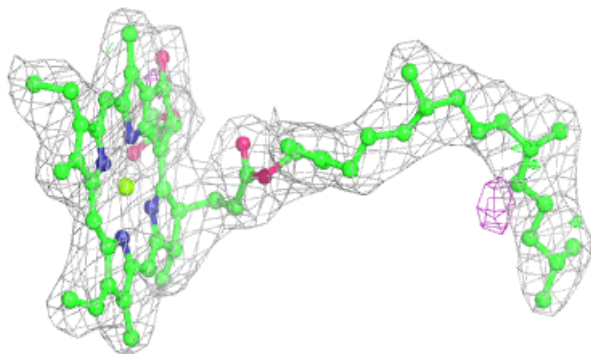
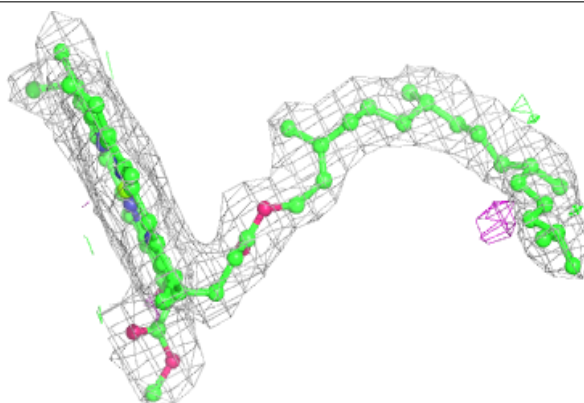


**Electron density around BCR R 101:**

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

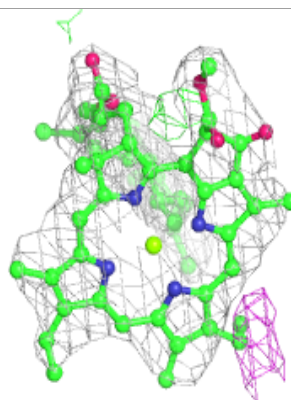
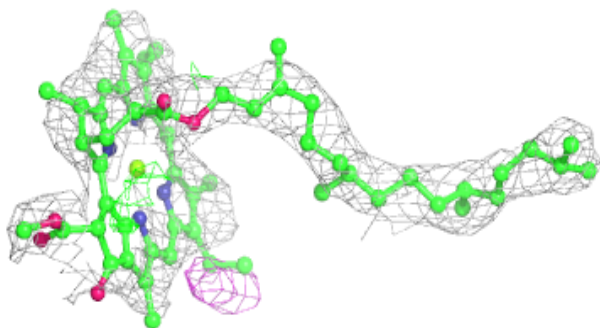
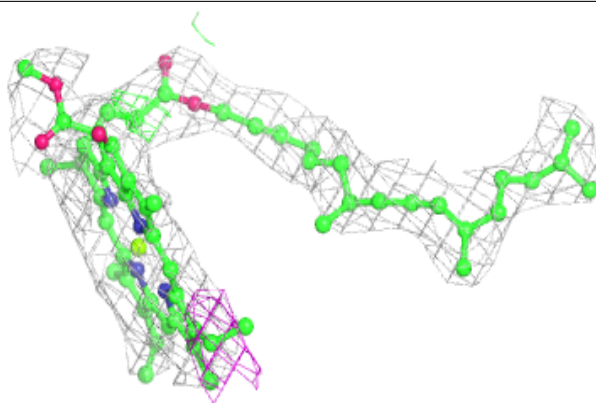
**Electron density around CLA H 839:**

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



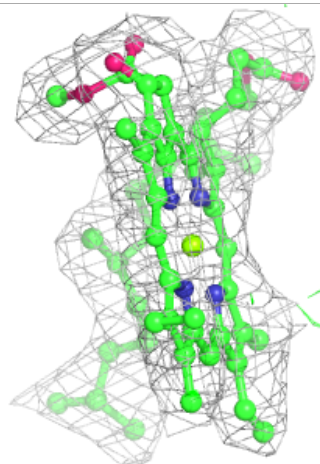
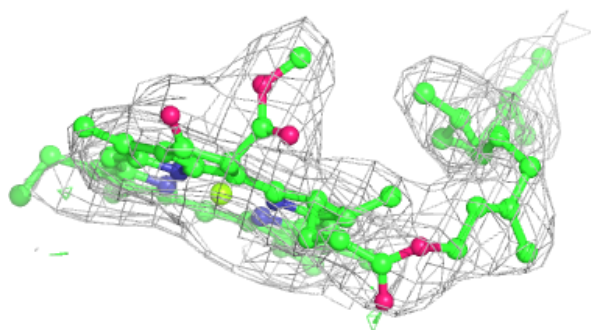
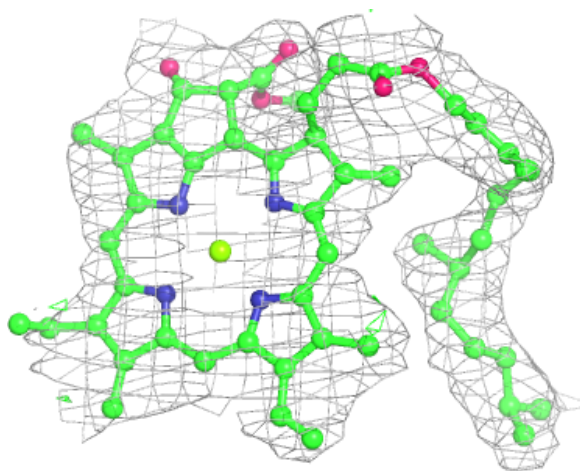
**Electron density around CLA Y 811:**

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



**Electron density around CLA G 813:**

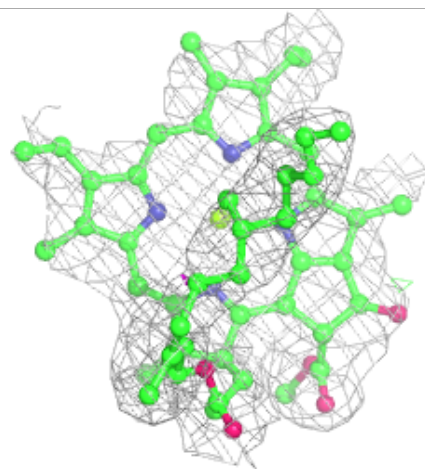
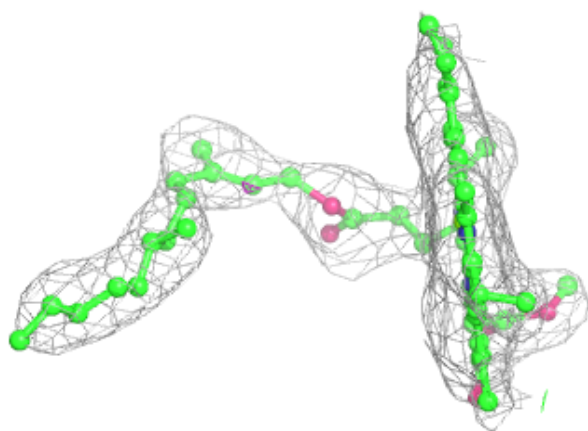
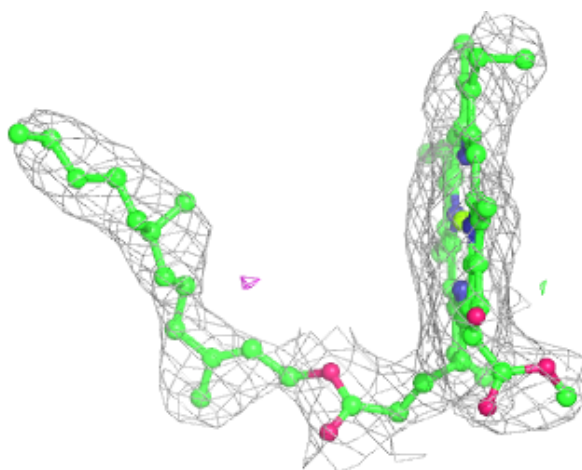
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





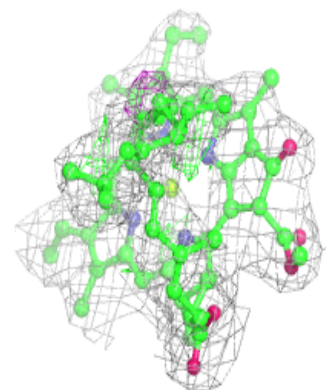
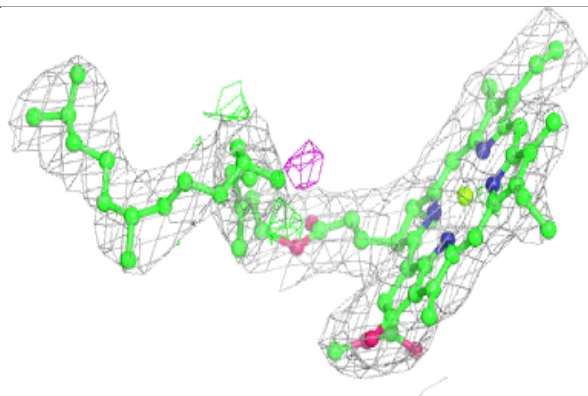
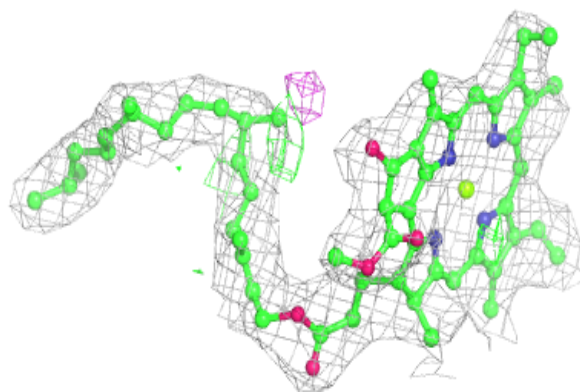
**Electron density around CLA G 804:**

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



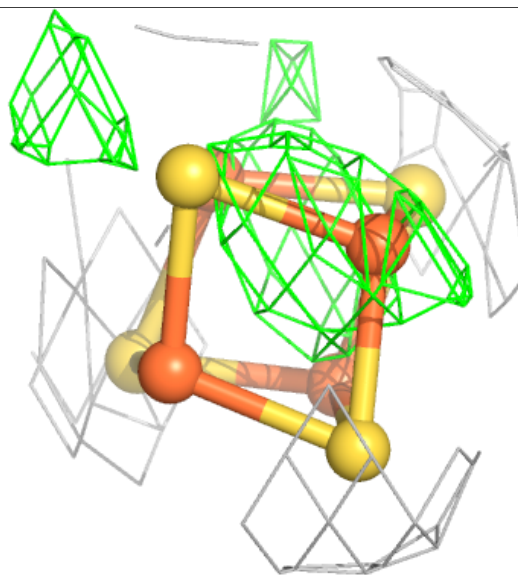
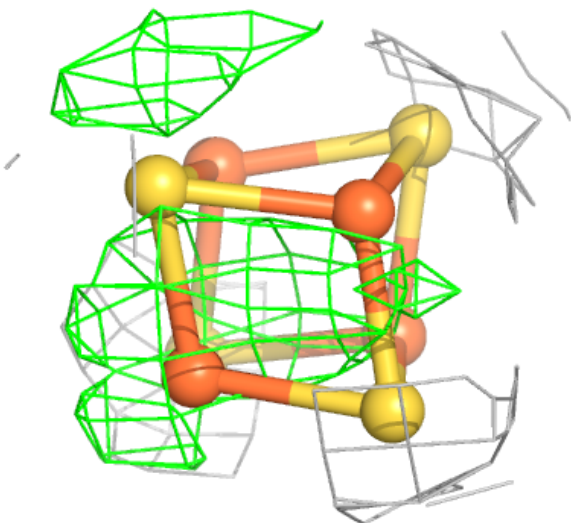
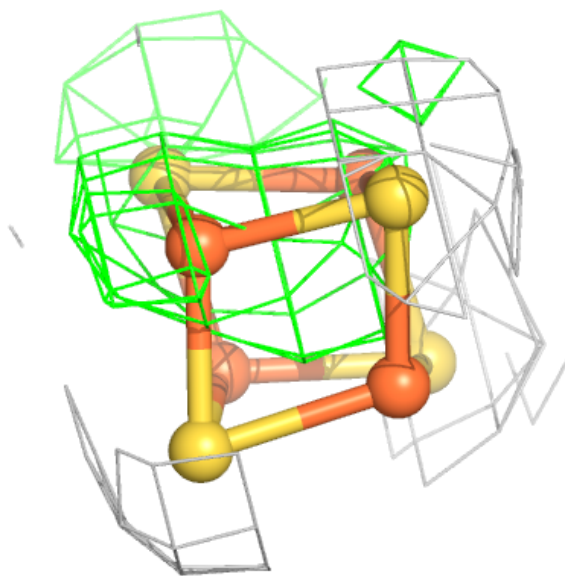
**Electron density around CLA Z 803:**

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



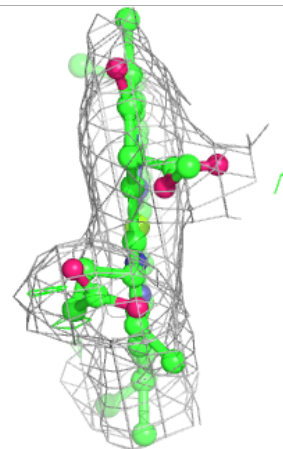
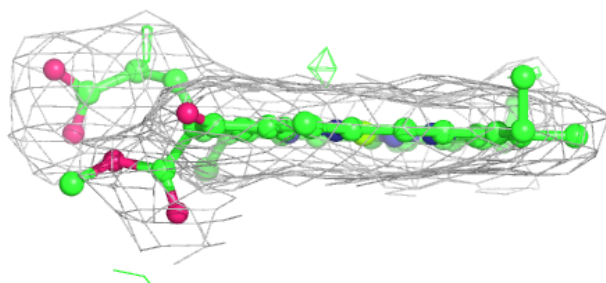
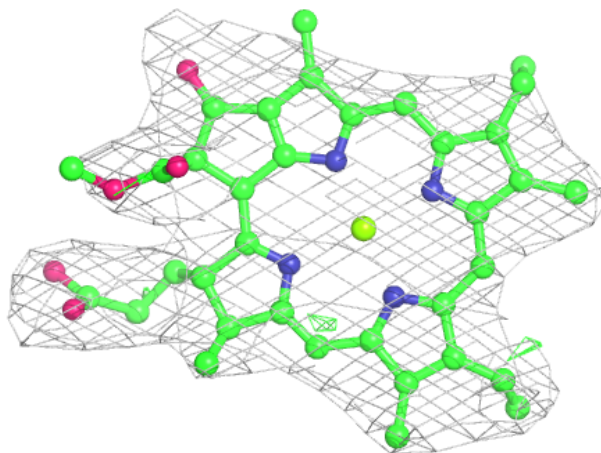
**Electron density around SF4 Y 843:**

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



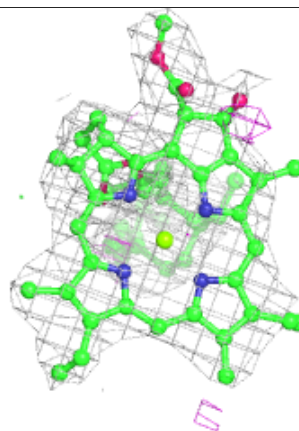
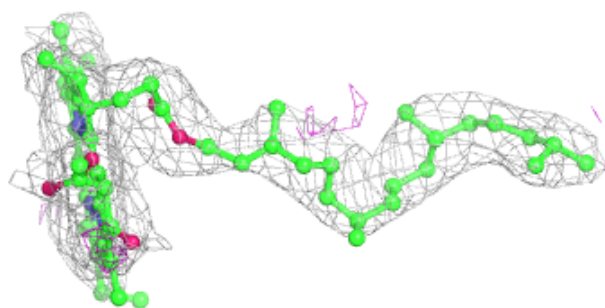
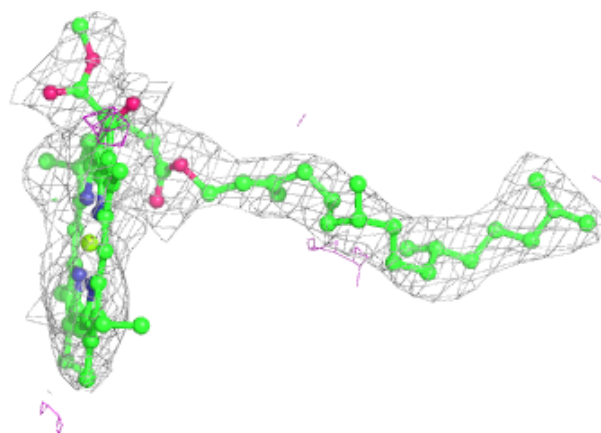
**Electron density around CLA B 835:**

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



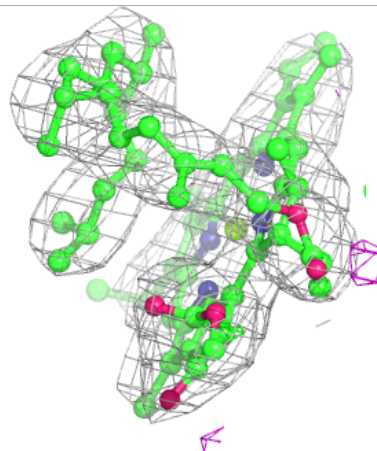
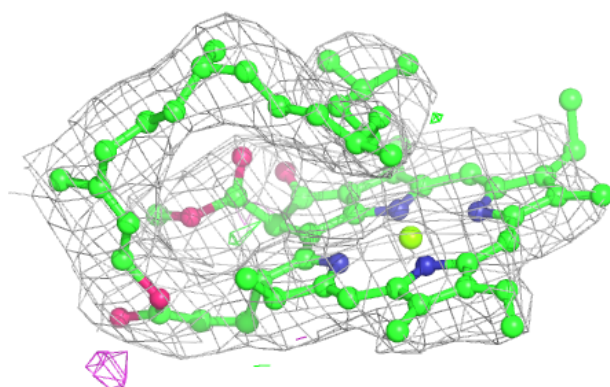
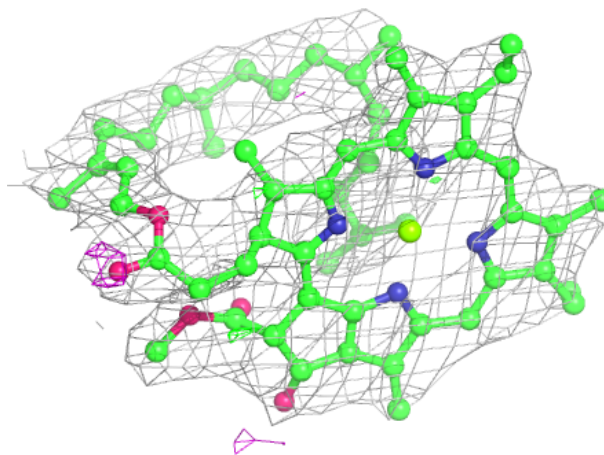
**Electron density around CLA G 828:**

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



**Electron density around CLA Y 806:**

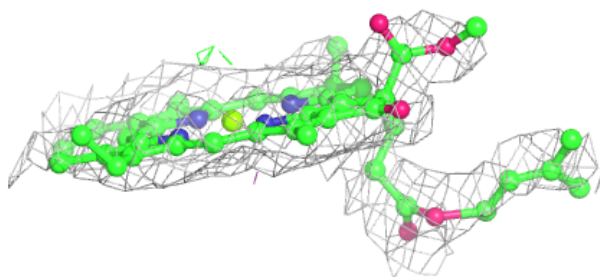
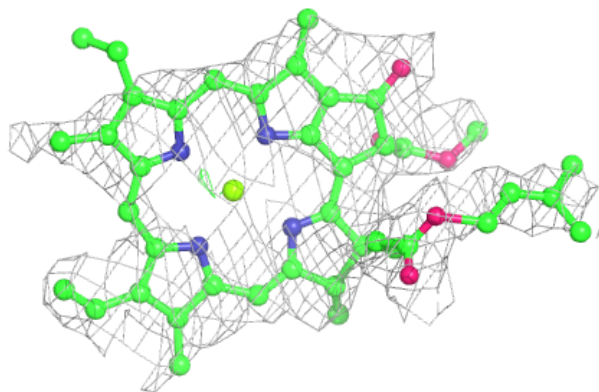
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



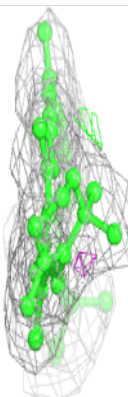
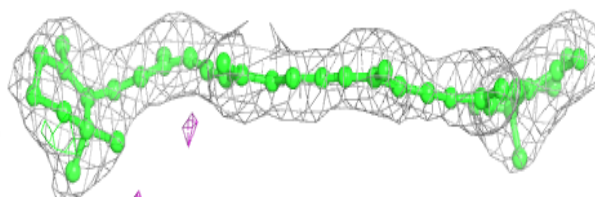
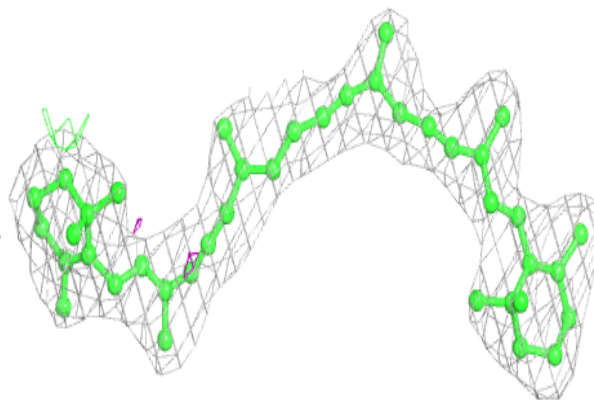


**Electron density around CLA A 817:**

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

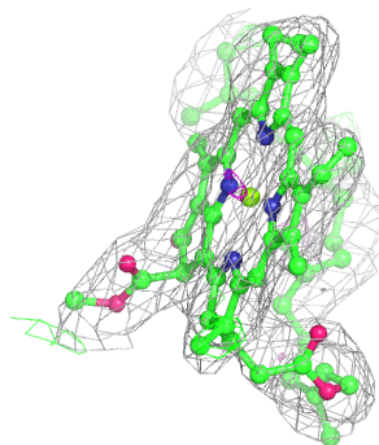
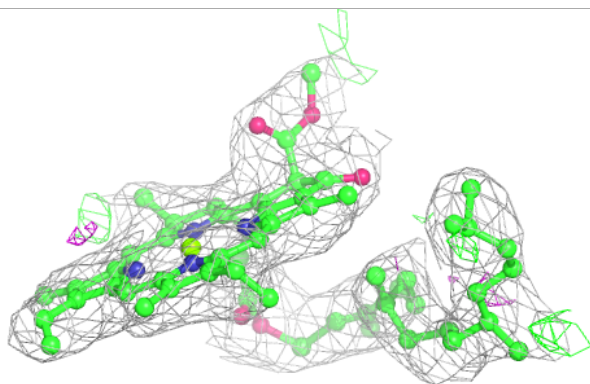
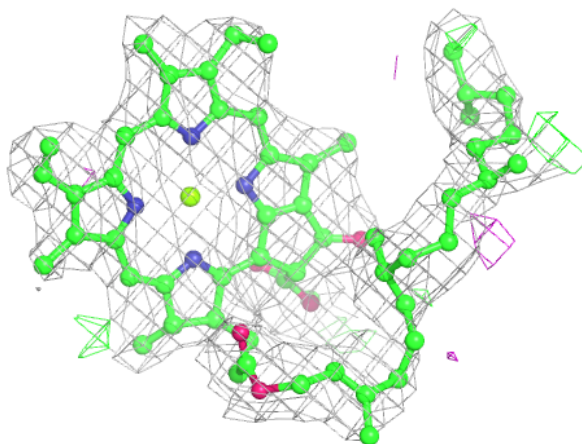
**Electron density around BCR A 851:**

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



**Electron density around CLA H 831:**

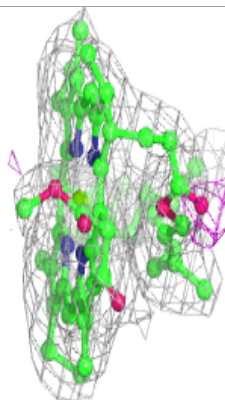
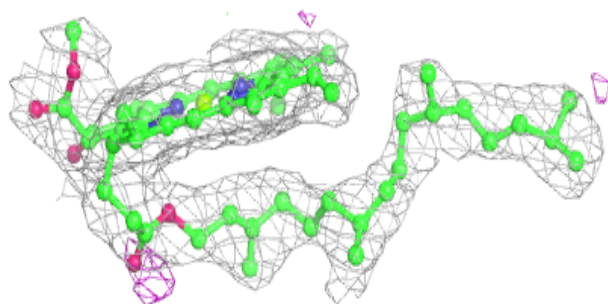
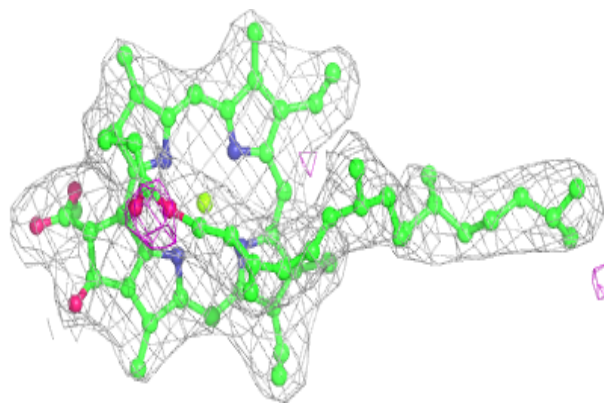
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





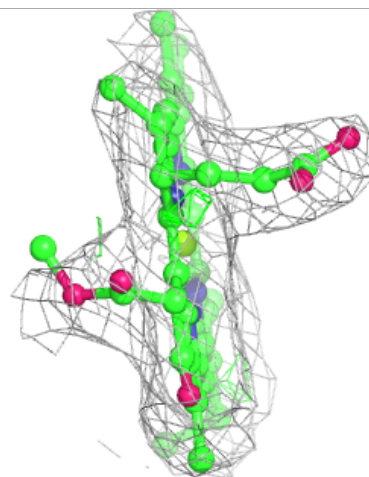
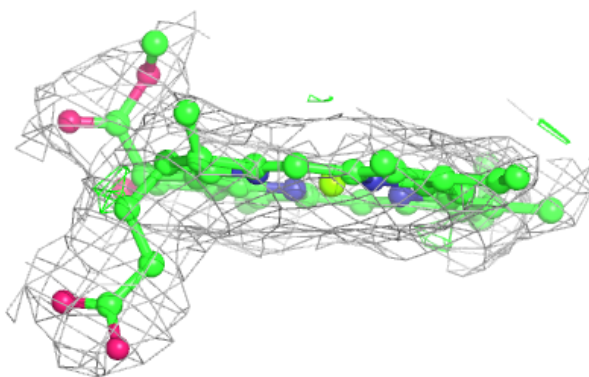
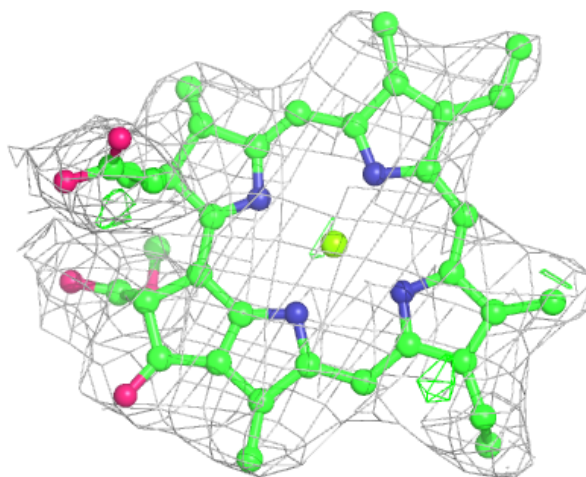
**Electron density around CLA G 837:**

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



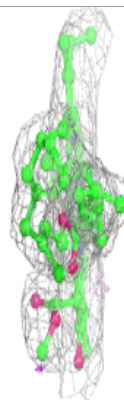
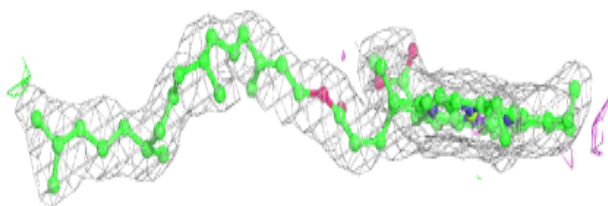
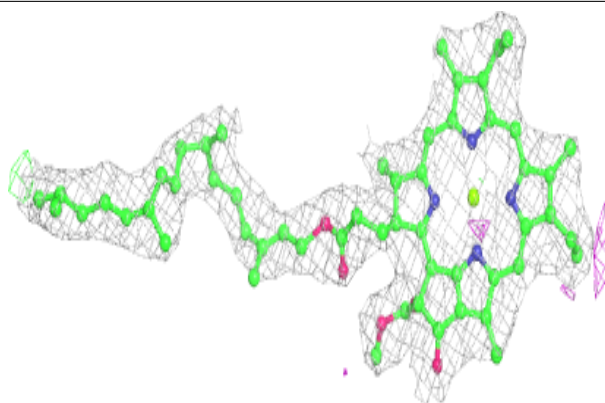
**Electron density around CLA g 102:**

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

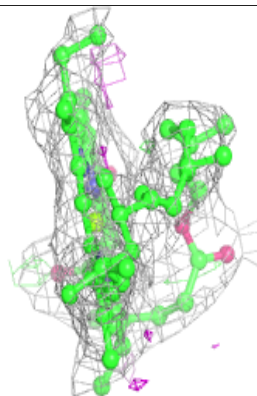
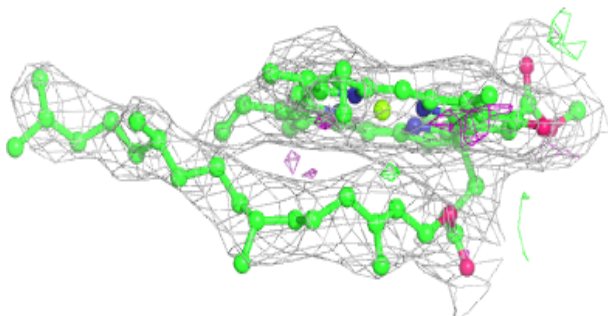
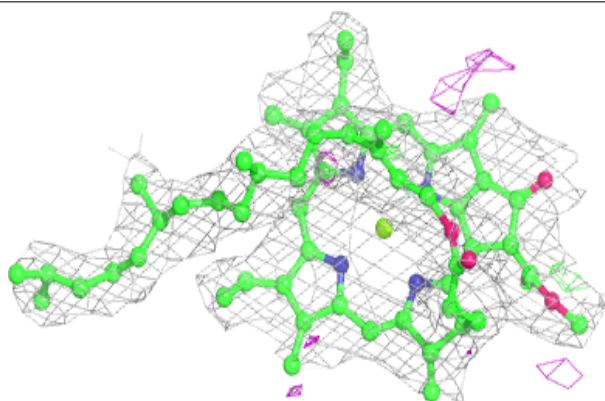


**Electron density around CLA A 833:**

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

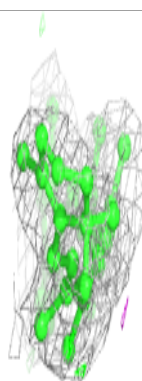
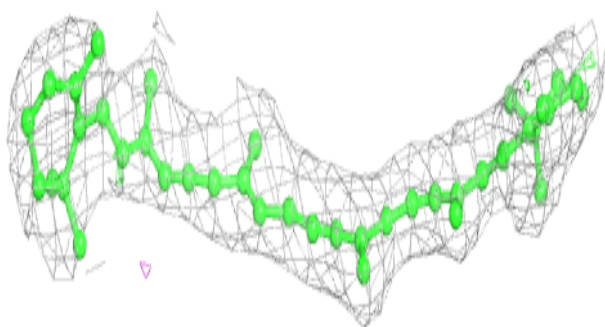
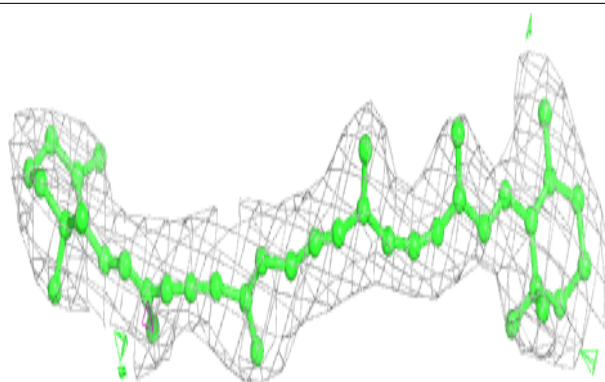
**Electron density around CLA A 839:**

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

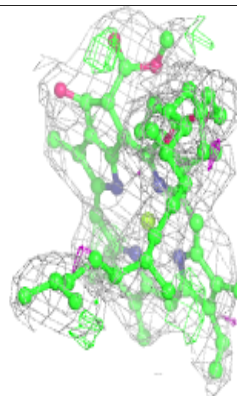
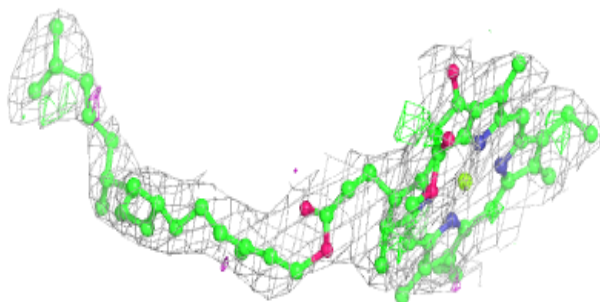
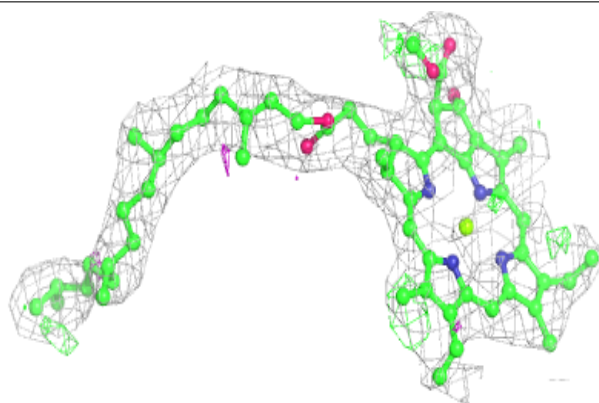


**Electron density around BCR S 1105:**

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

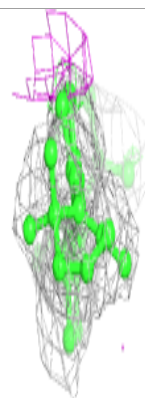
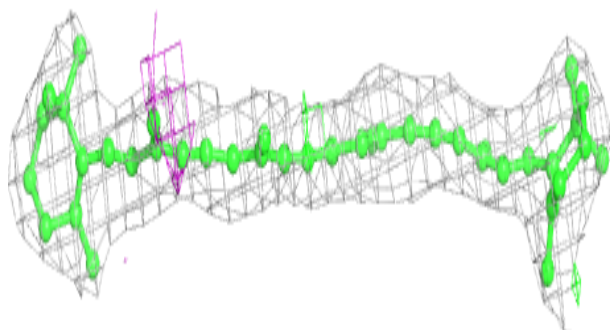
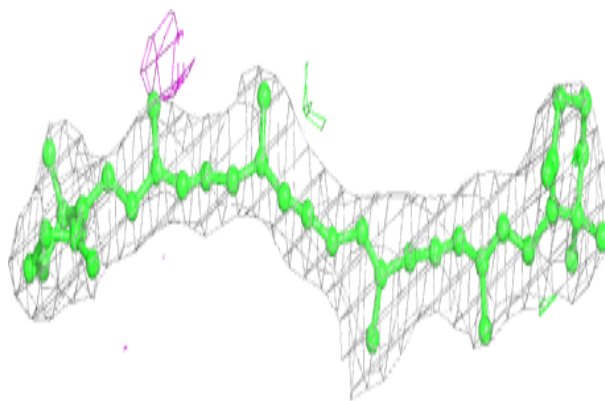
**Electron density around CLA H 802:**

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

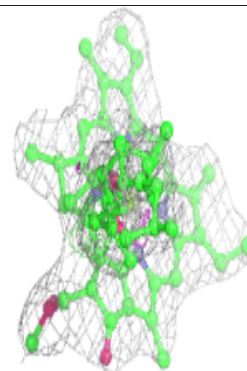
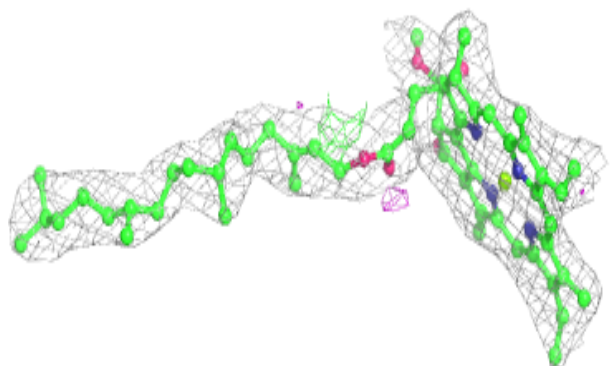
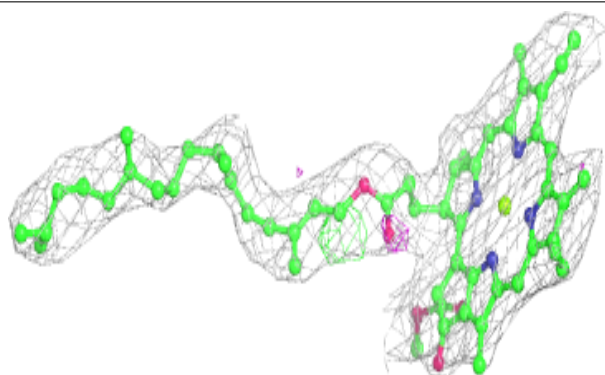


**Electron density around BCR U 1009:**

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

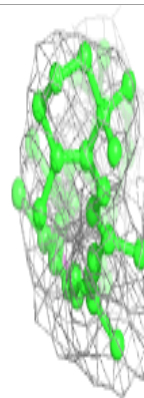
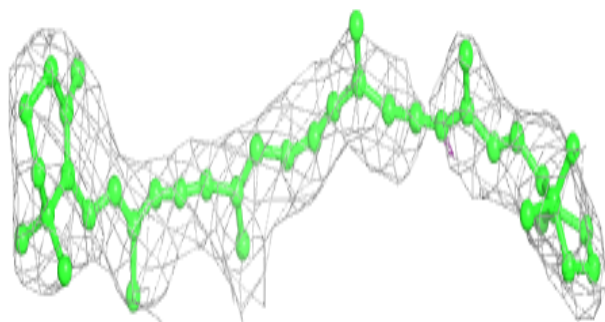
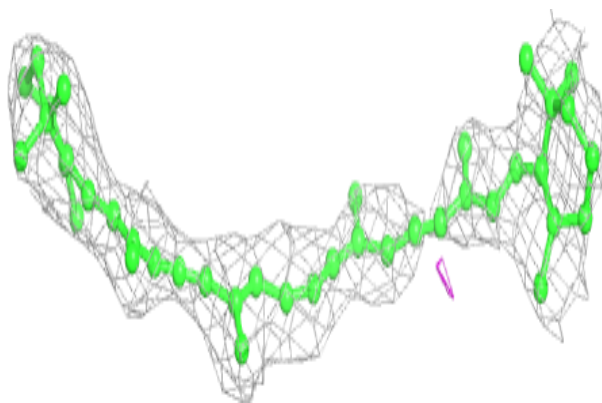
**Electron density around CLA Y 809:**

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



**Electron density around BCR Q 201:**

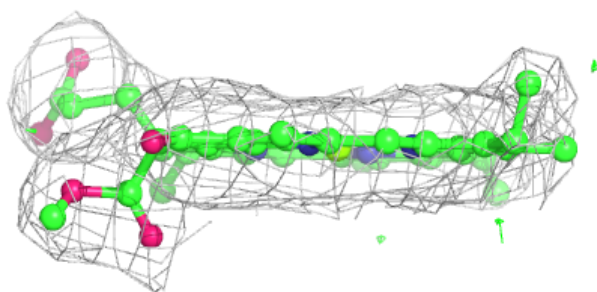
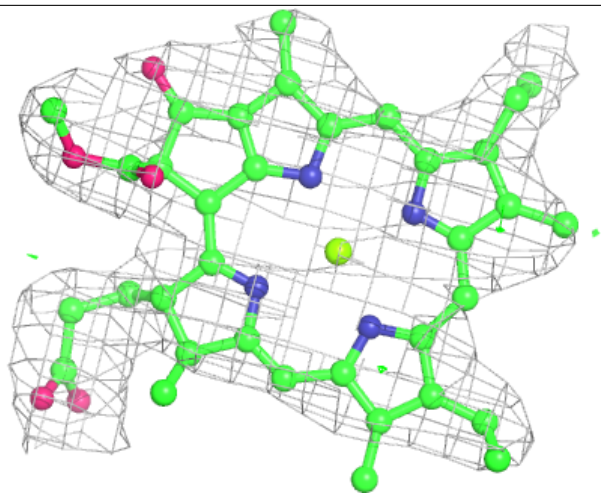
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





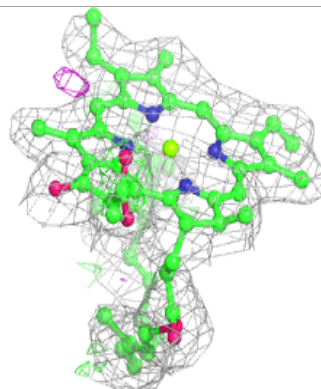
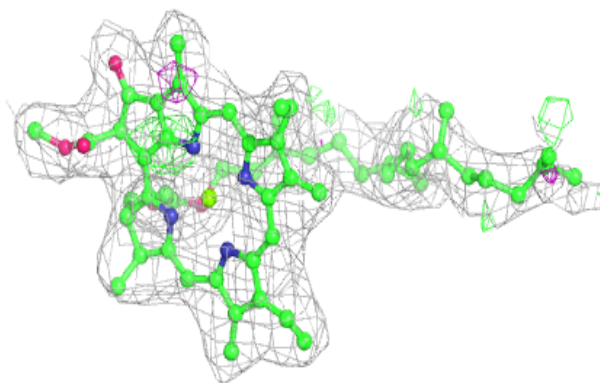
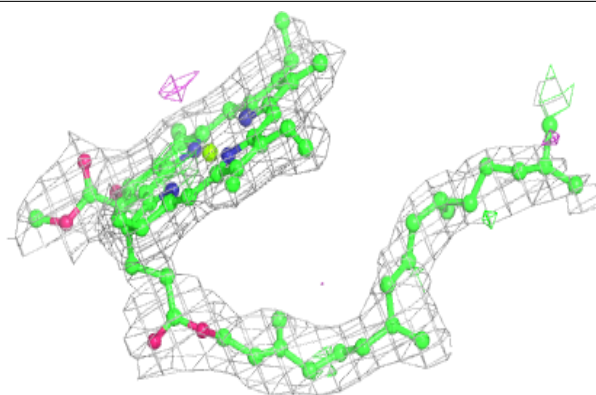
**Electron density around CLA j 102:**

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

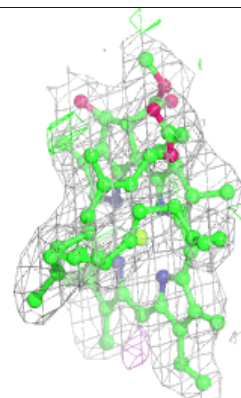
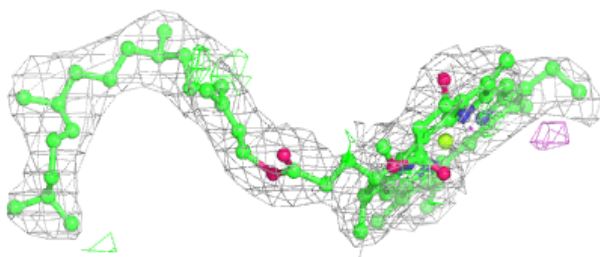
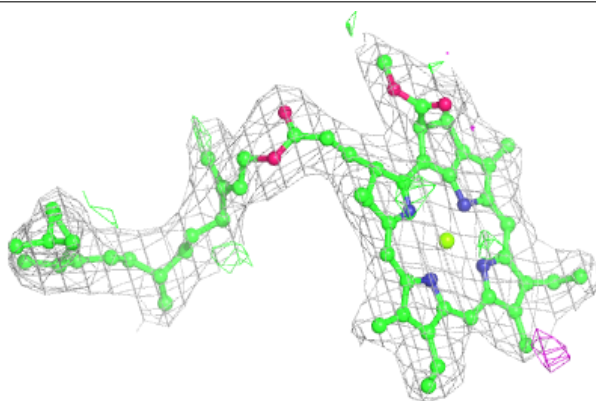


**Electron density around CLA U 1006:**

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

**Electron density around CLA B 808:**

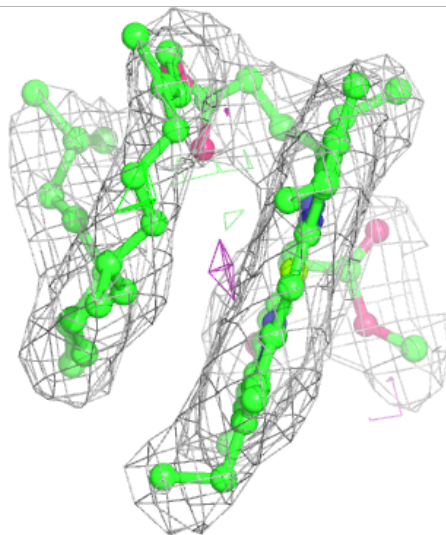
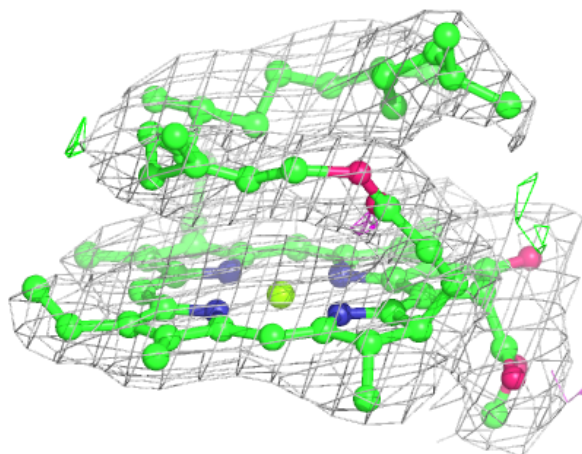
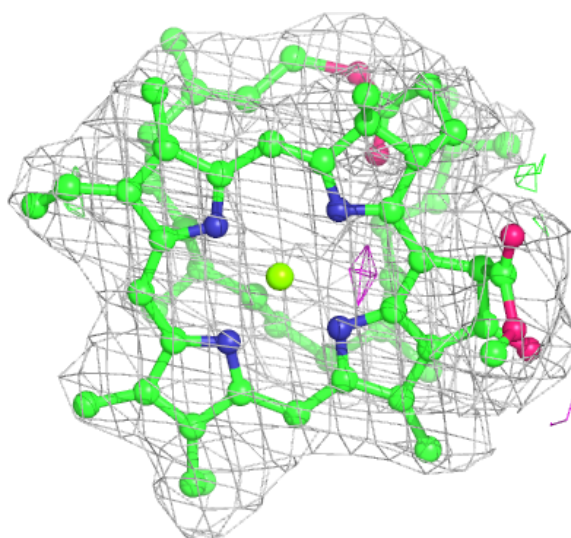
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





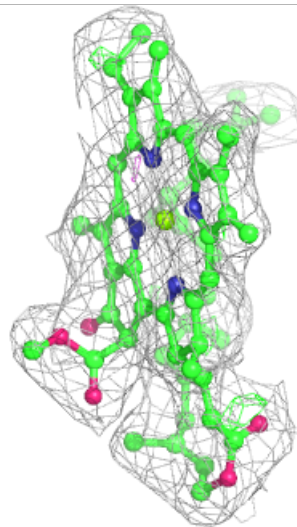
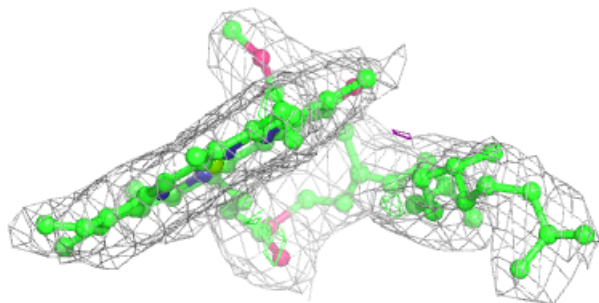
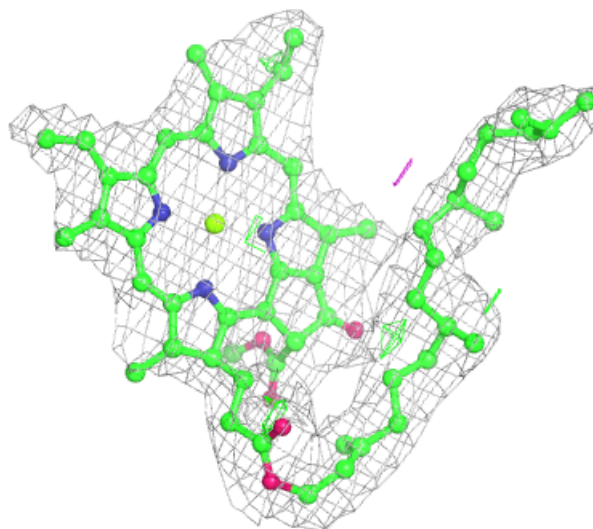
**Electron density around CLA h 204:**

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



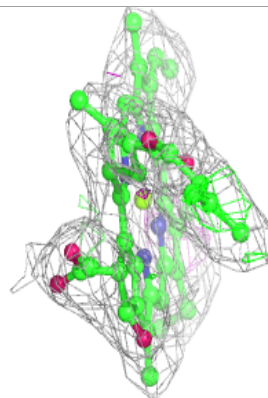
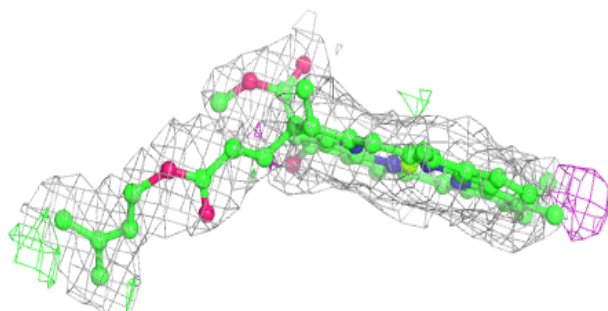
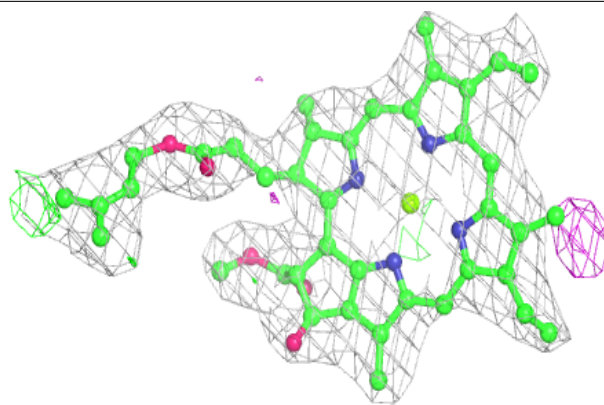
**Electron density around CLA Y 825:**

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



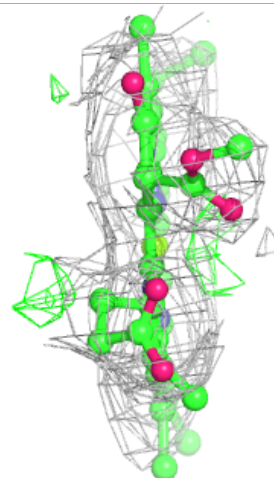
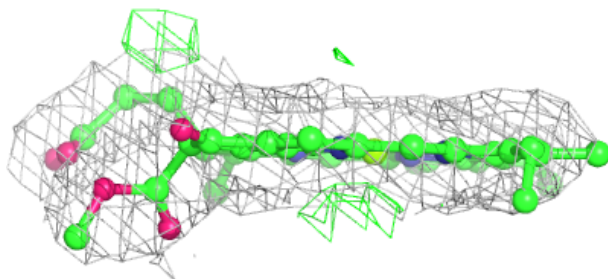
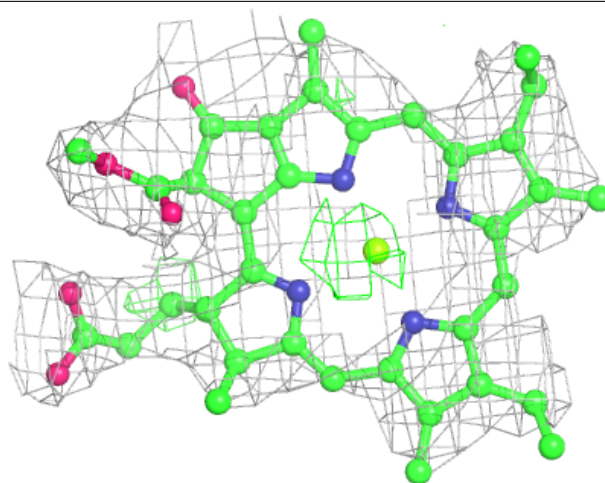
**Electron density around CLA Y 839:**

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



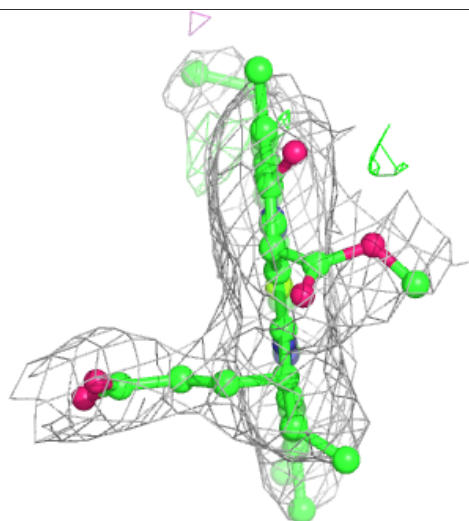
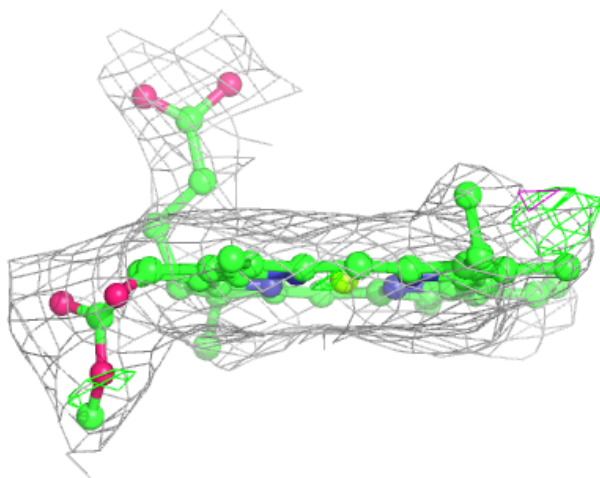
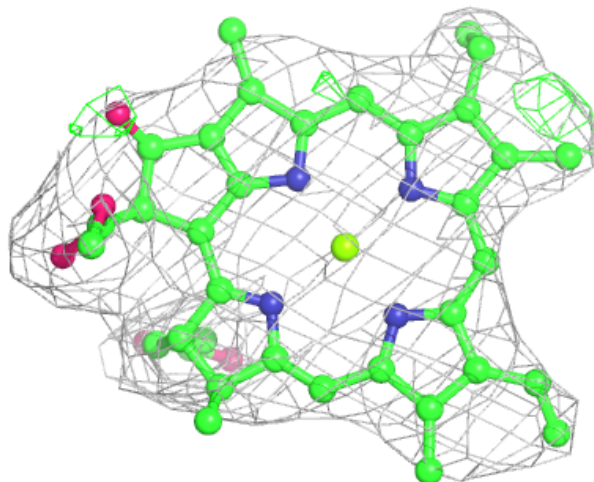
**Electron density around CLA d 202:**

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



**Electron density around CLA B 814:**

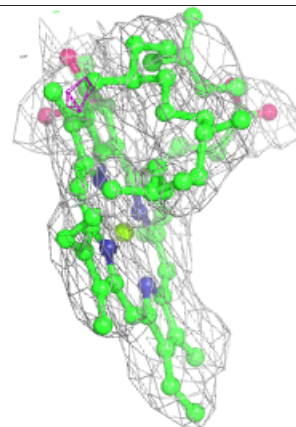
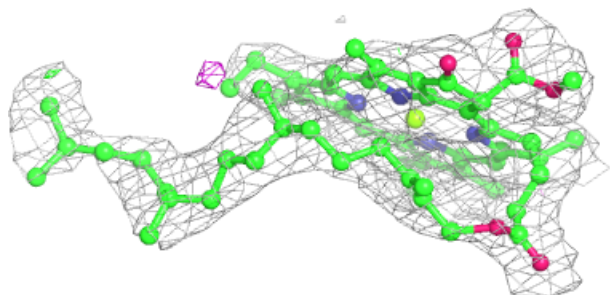
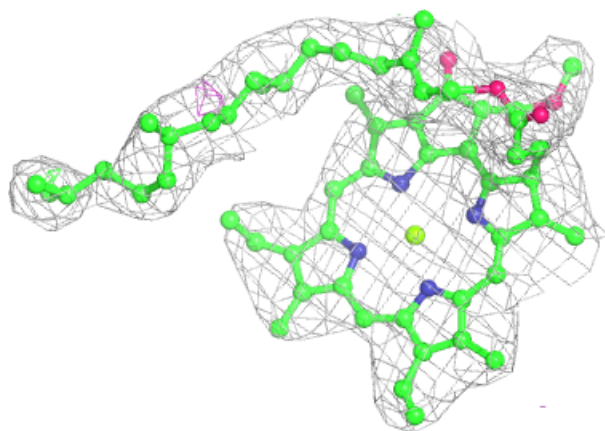
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



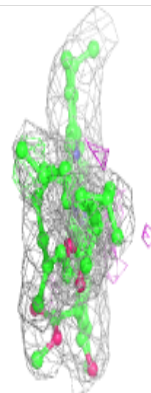
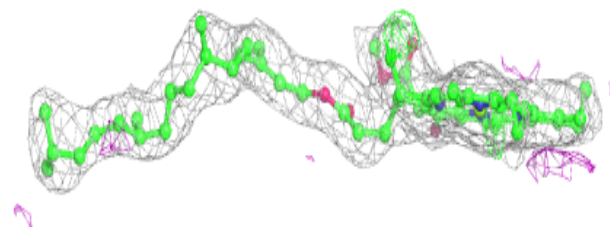
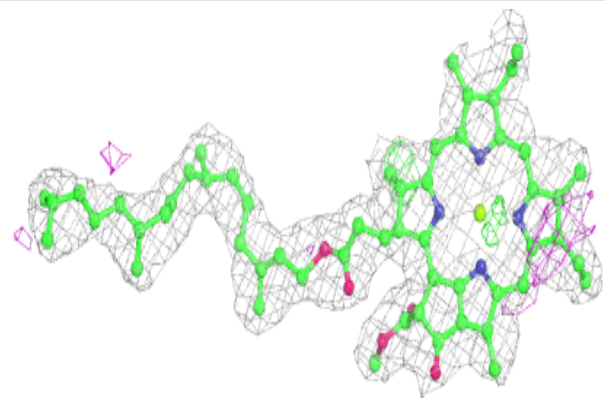


**Electron density around CLA Y 829:**

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

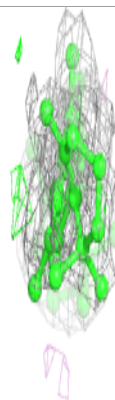
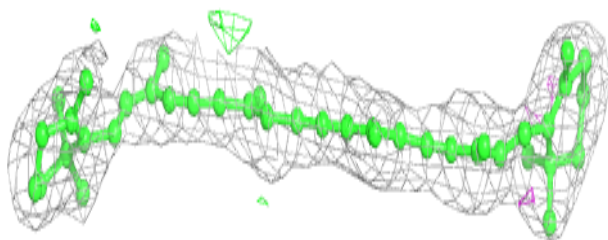
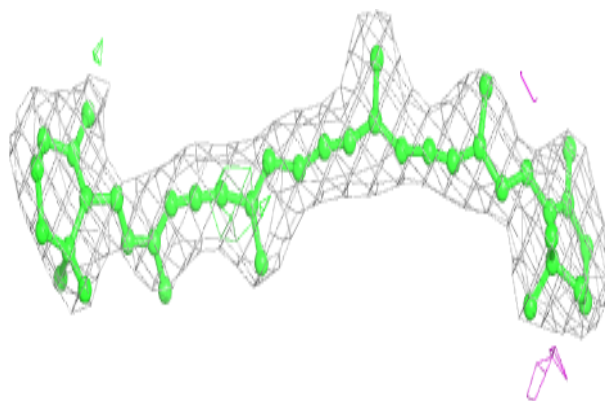
**Electron density around CLA G 832:**

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



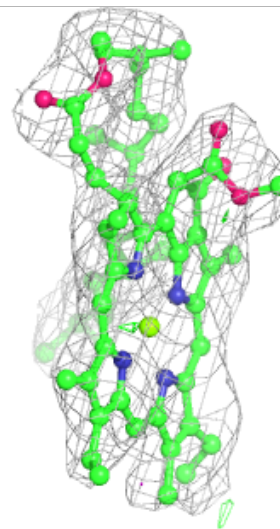
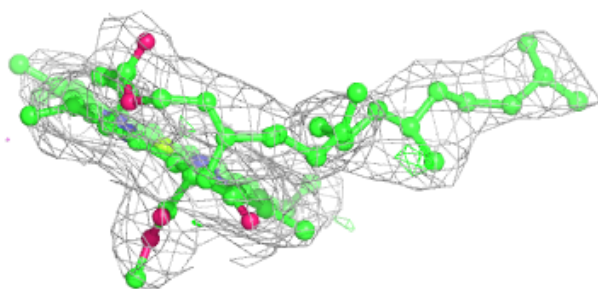
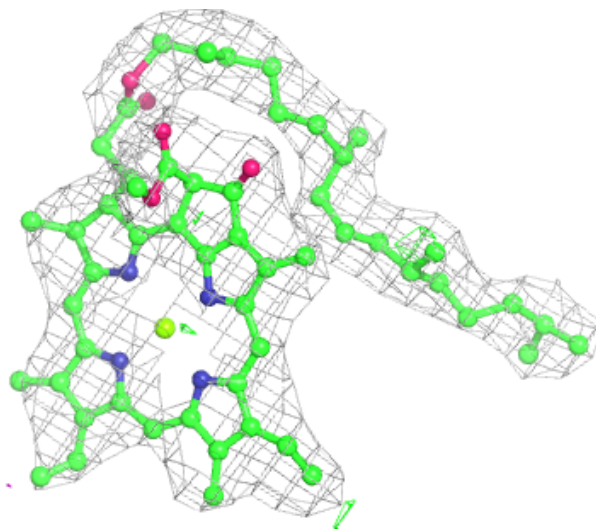
**Electron density around BCR H 846:**

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



**Electron density around CLA A 826:**

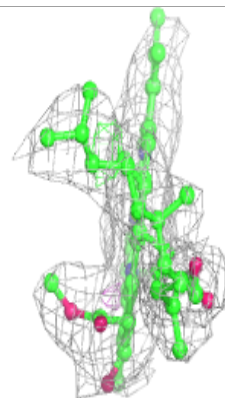
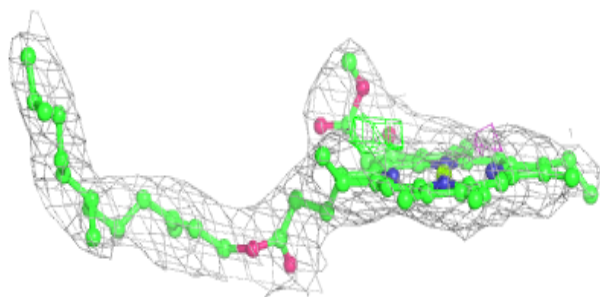
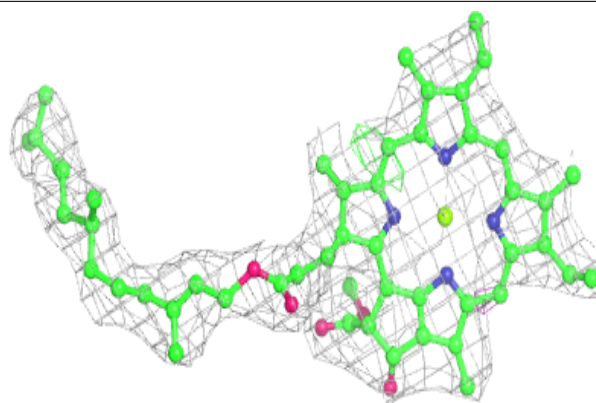
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





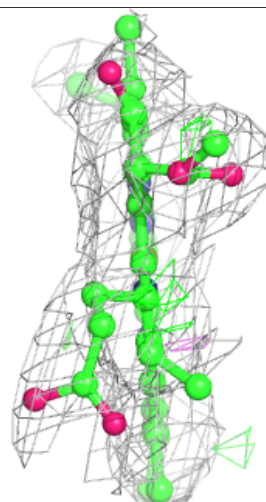
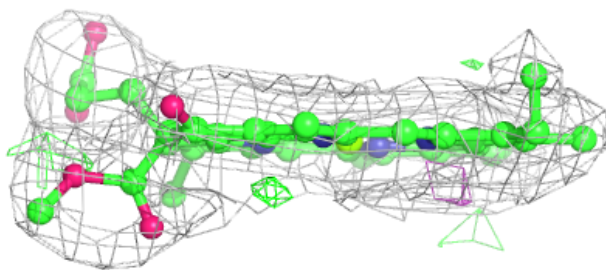
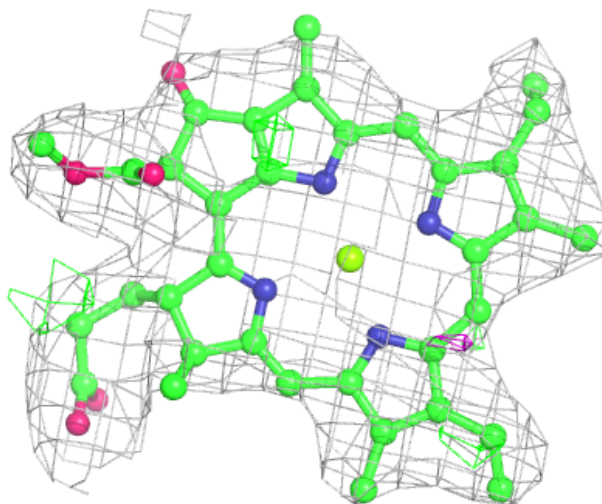
**Electron density around CLA Z 837:**

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



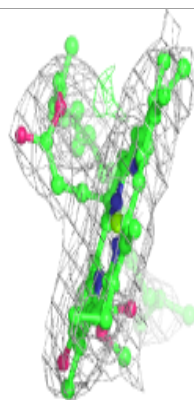
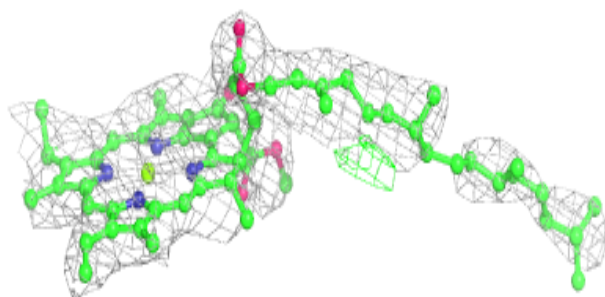
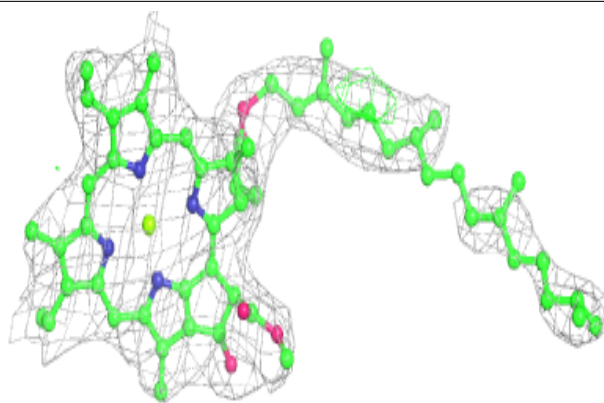
**Electron density around CLA X 1701:**

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



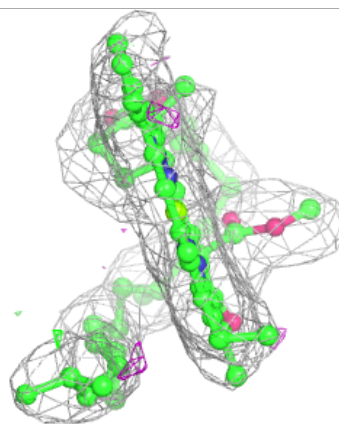
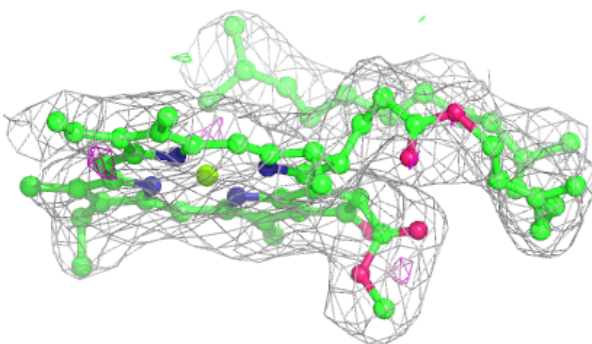
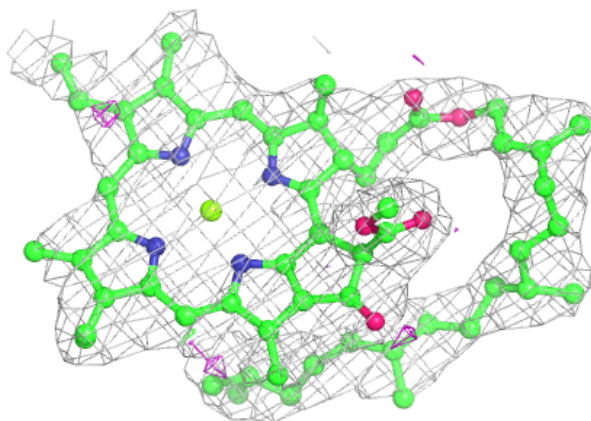
**Electron density around CLA G 822:**

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



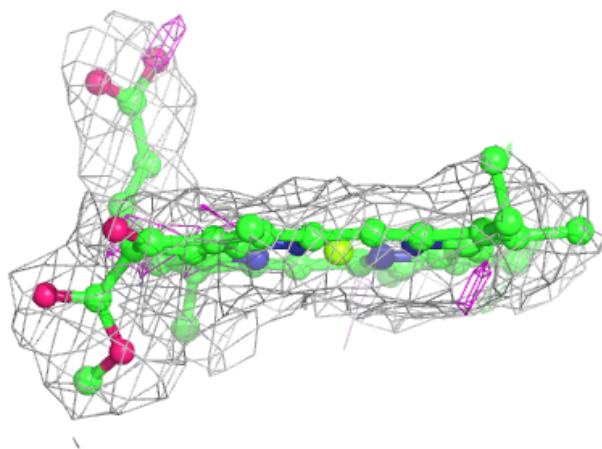
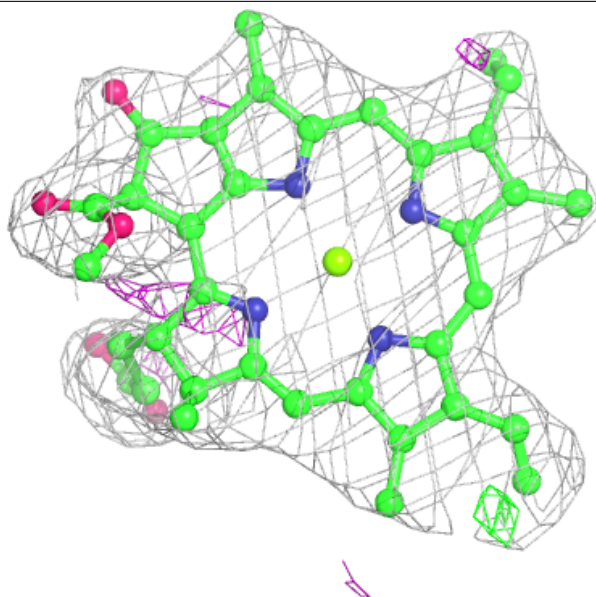
**Electron density around CLA B 804:**

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



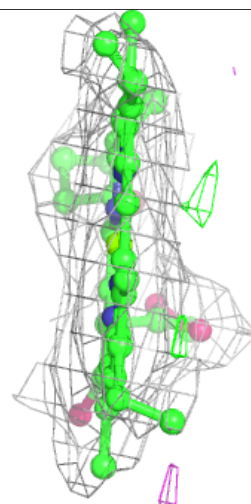
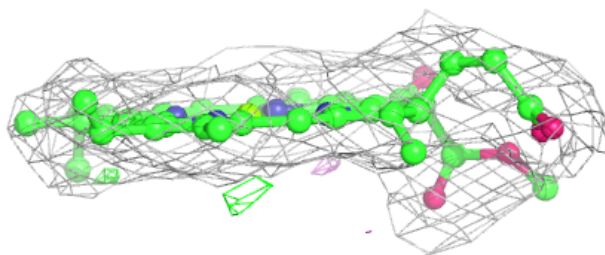
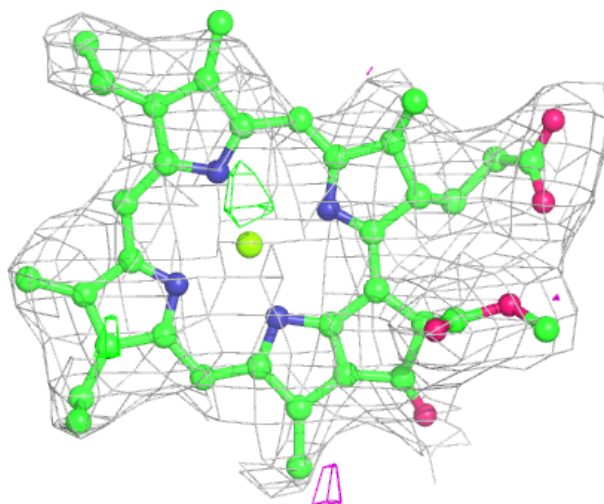
**Electron density around CLA H 833:**

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



**Electron density around CLA Q 202:**

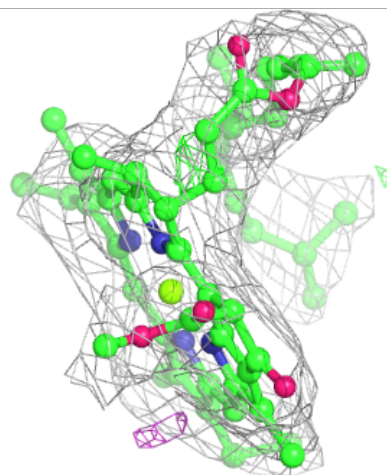
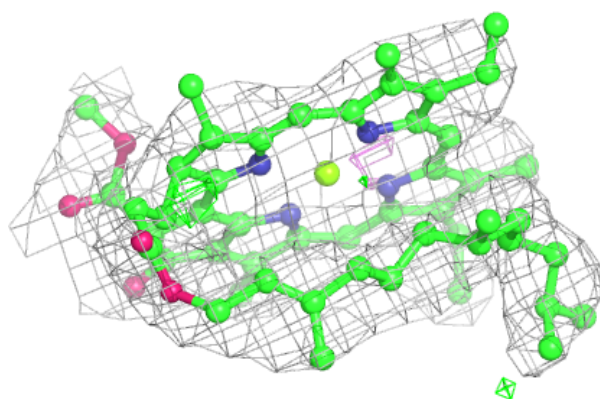
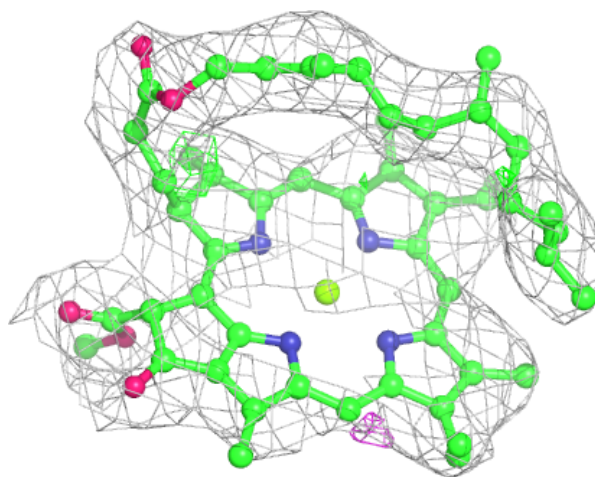
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





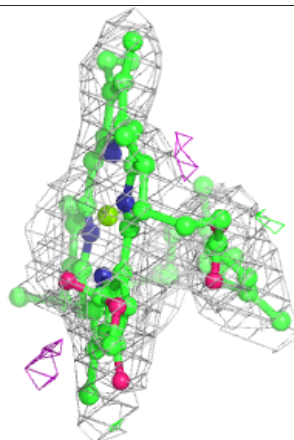
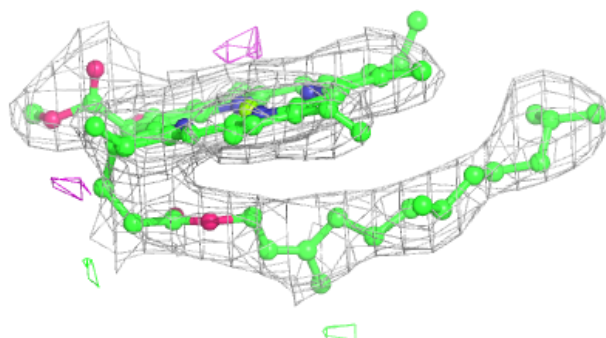
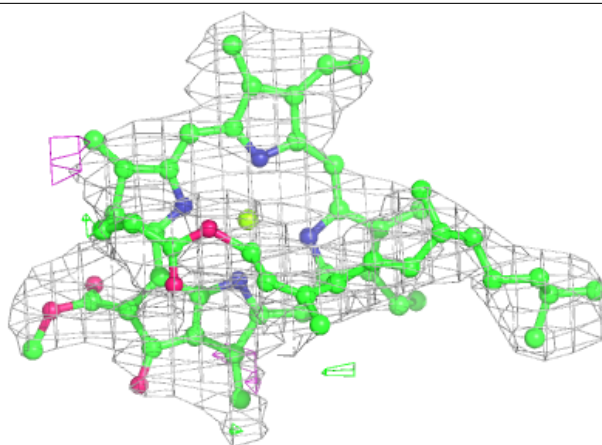
**Electron density around CLA Y 820:**

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

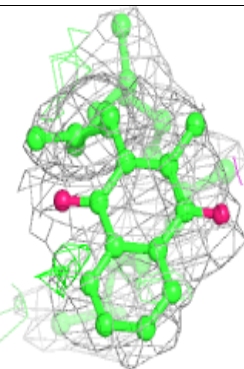
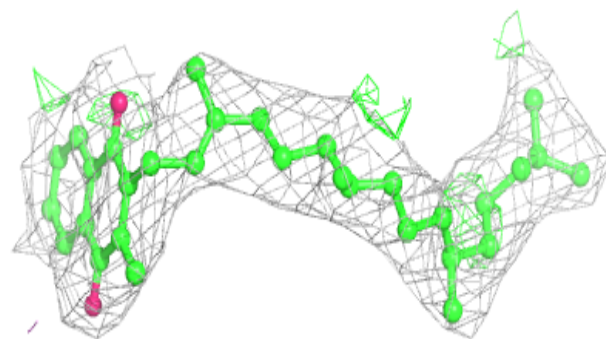
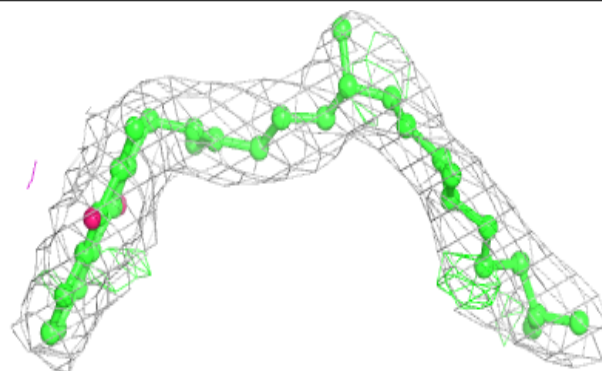


**Electron density around CLA Y 817:**

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

**Electron density around PQN B 841:**

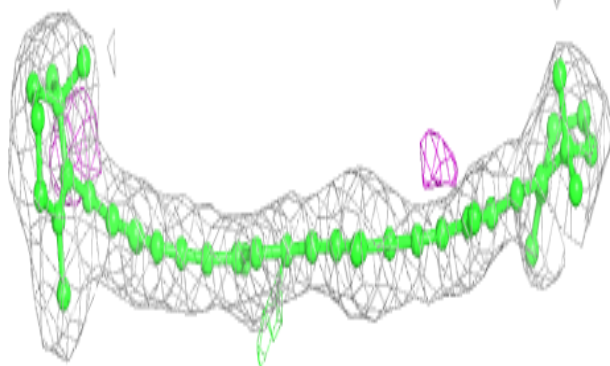
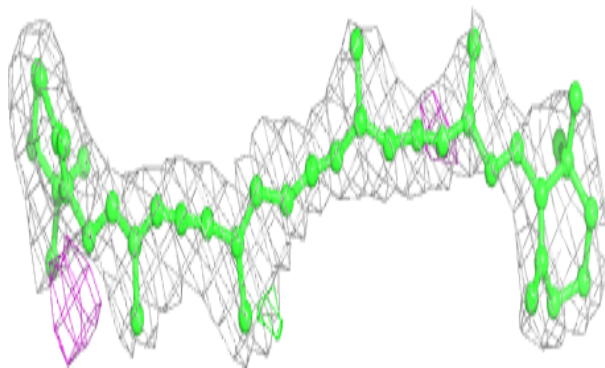
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





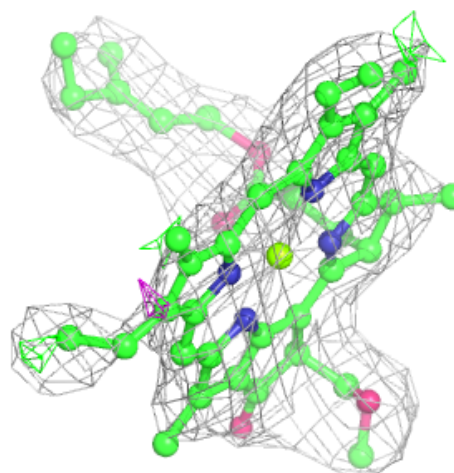
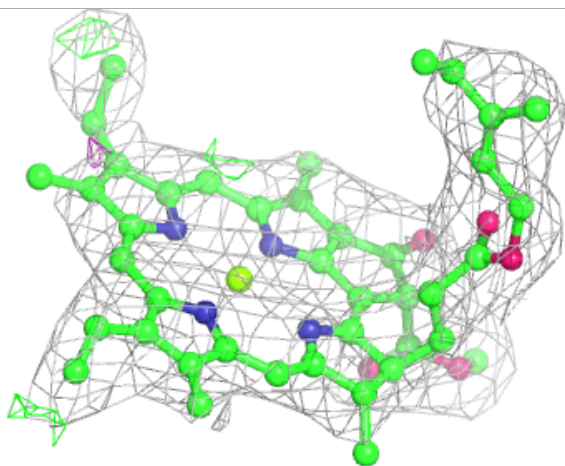
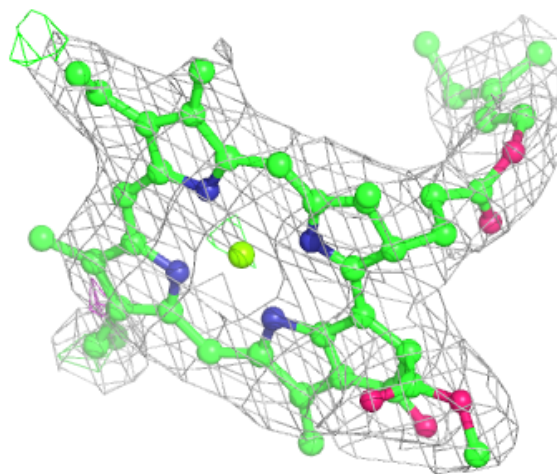
**Electron density around BCR A 850:**

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



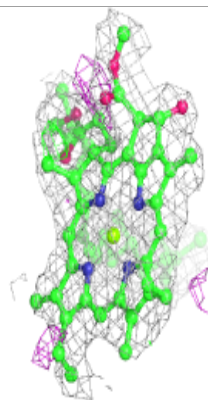
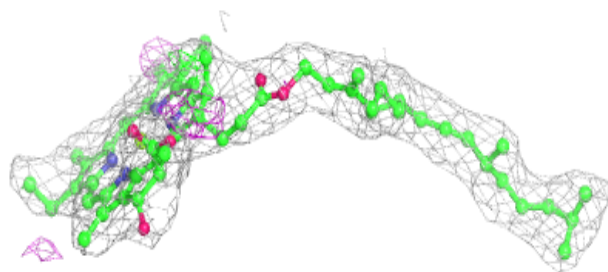
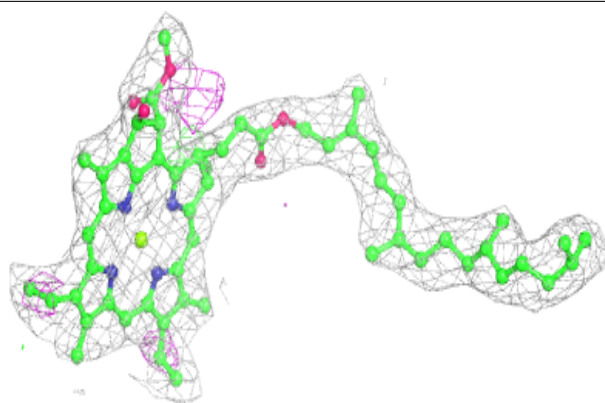
**Electron density around CLA G 807:**

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

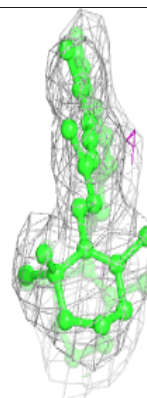
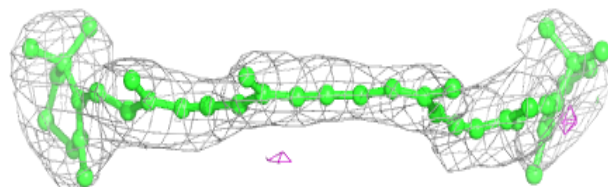
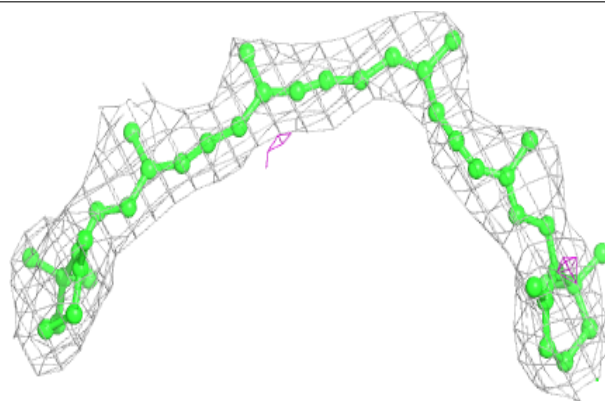


**Electron density around CLA A 803:**

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

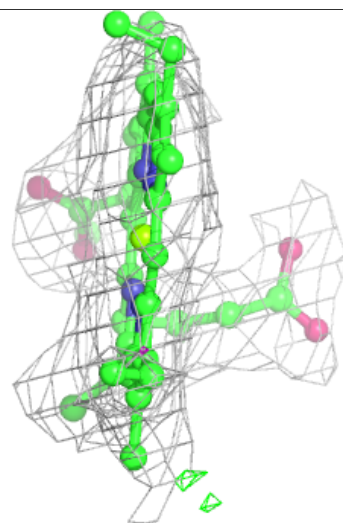
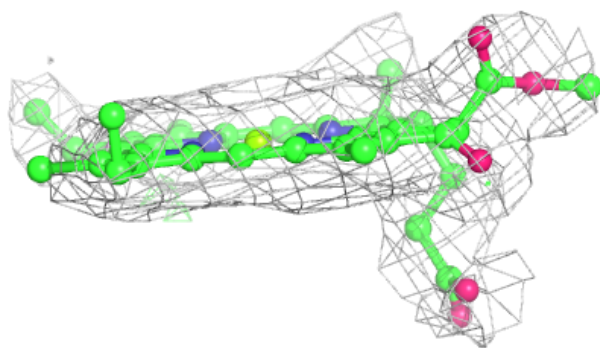
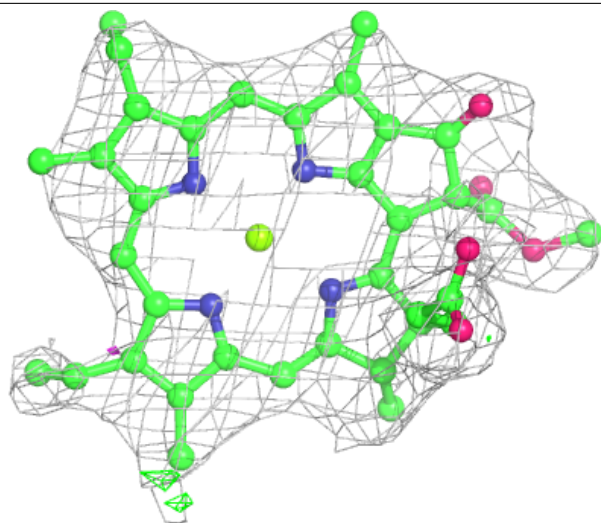
**Electron density around BCR d 203:**

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



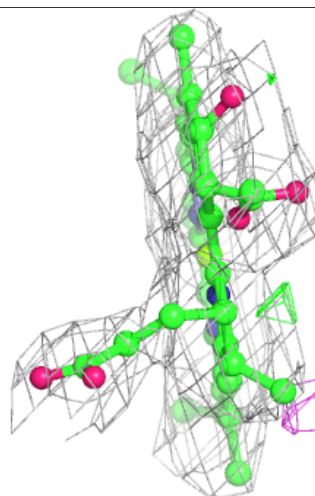
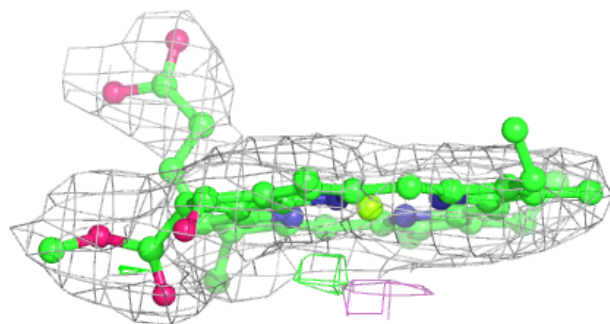
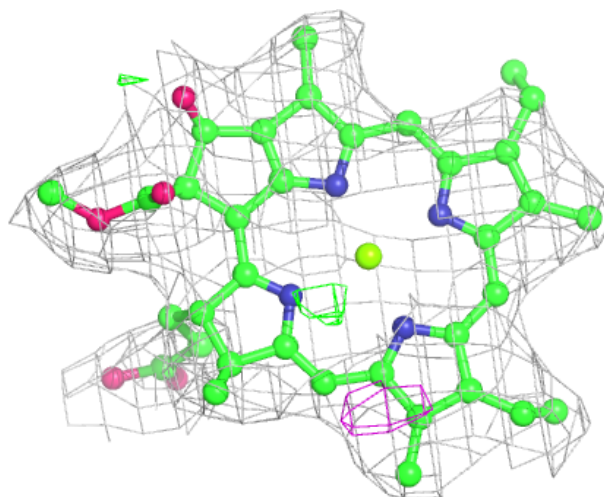
**Electron density around CLA A 811:**

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



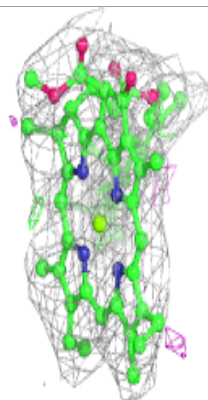
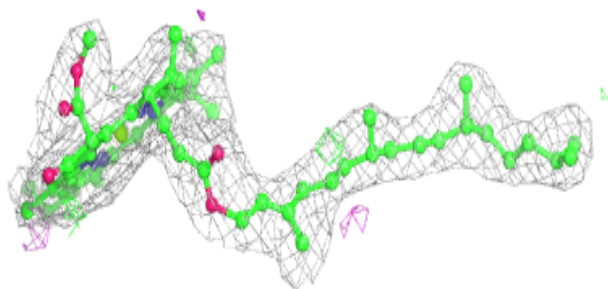
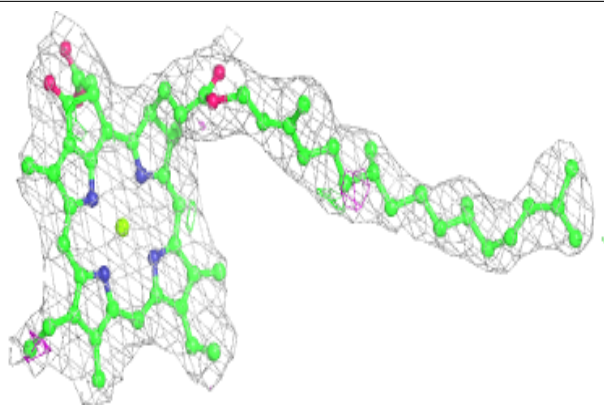
**Electron density around CLA Z 813:**

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

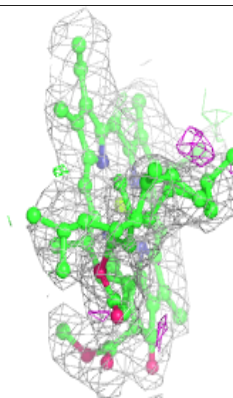
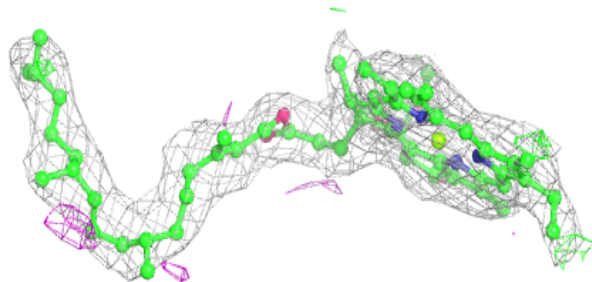
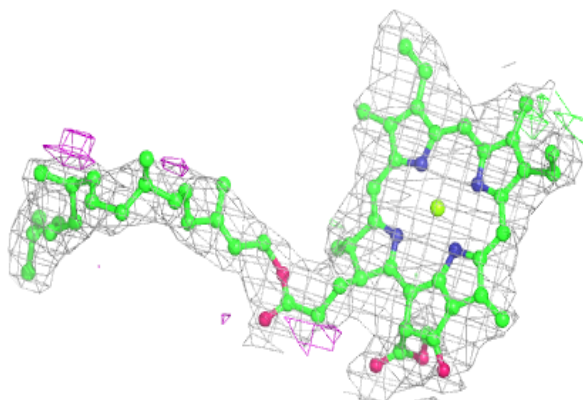


**Electron density around CLA L 202:**

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

**Electron density around CLA H 813:**

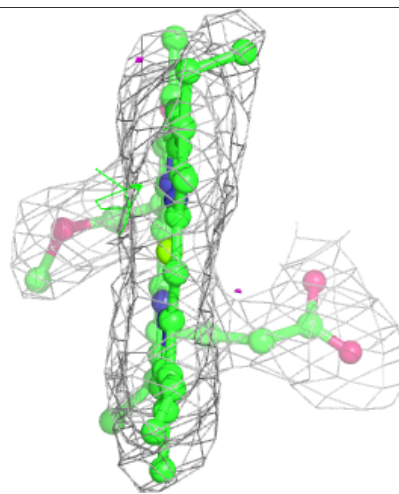
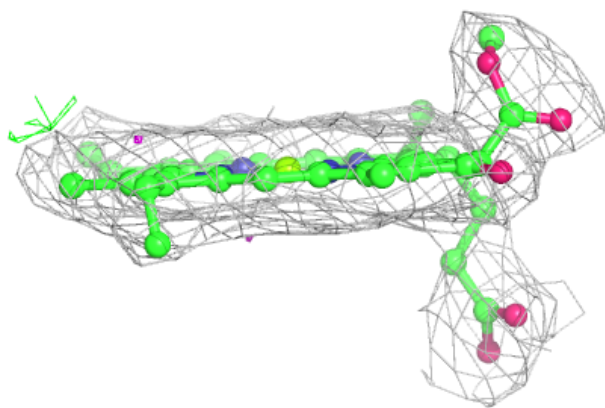
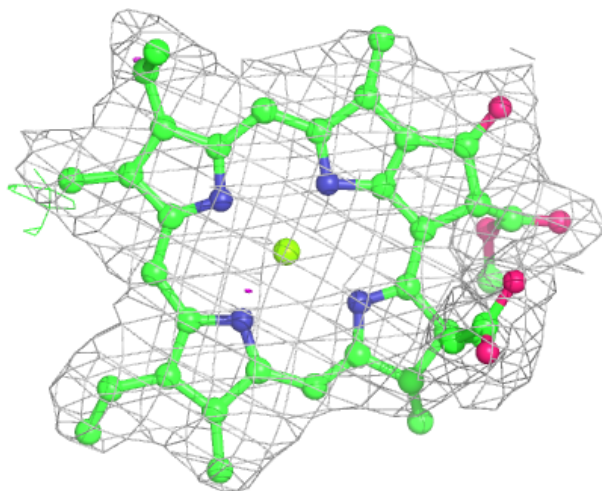
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





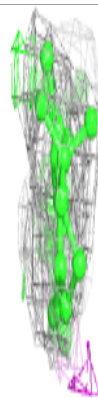
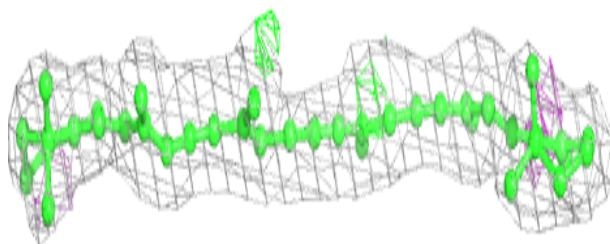
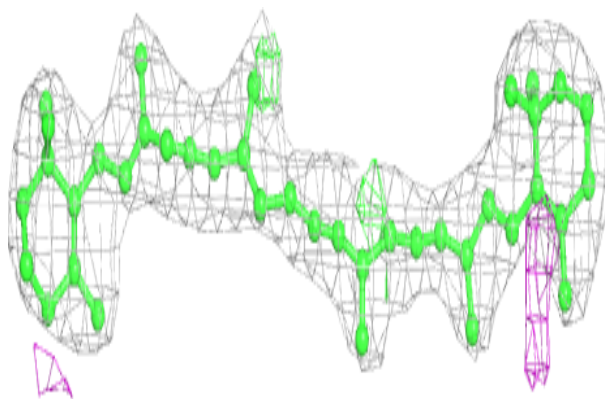
**Electron density around CLA Z 822:**

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

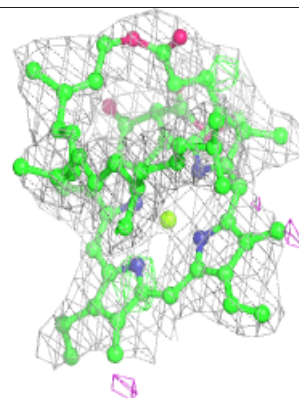
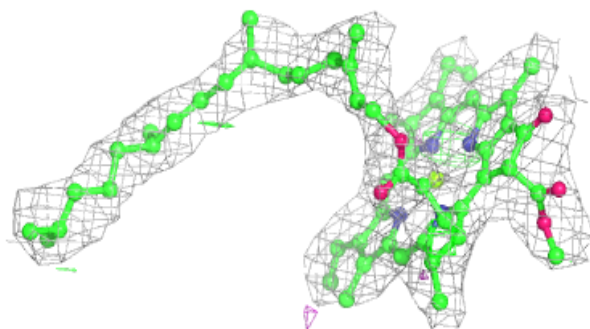
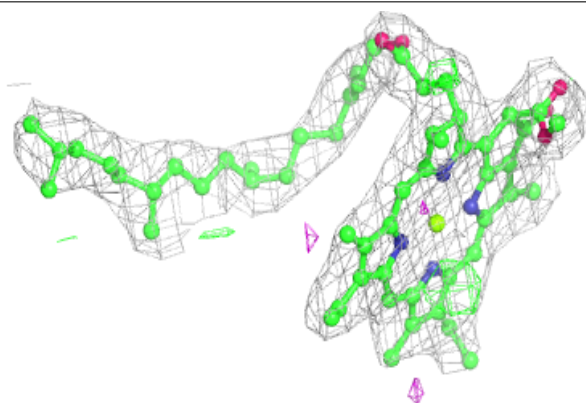


**Electron density around BCR h 207:**

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

**Electron density around CLA H 814:**

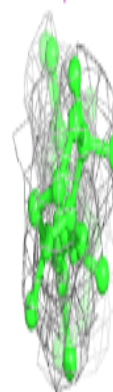
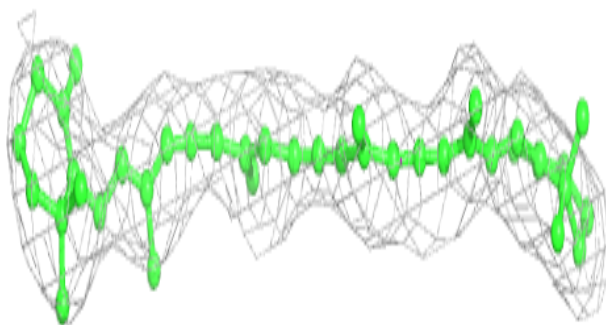
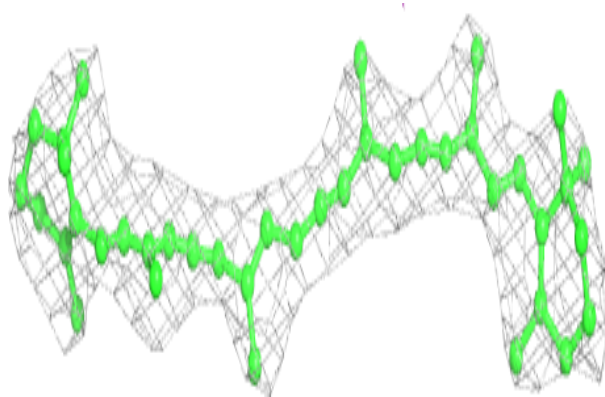
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



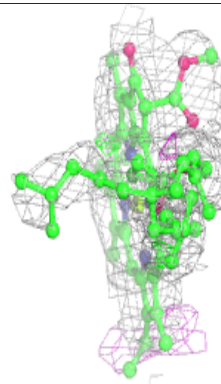
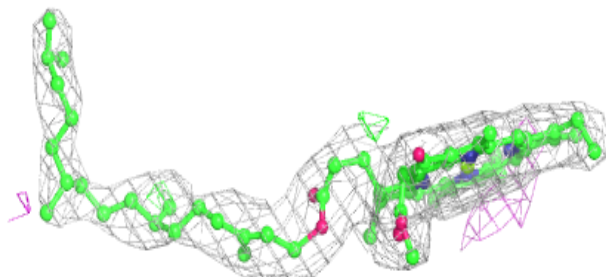
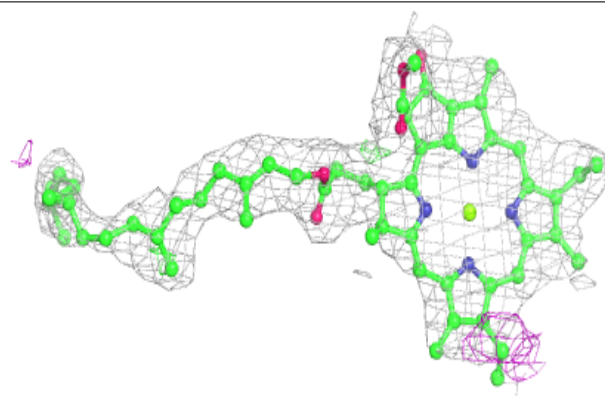


**Electron density around BCR f 103:**

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

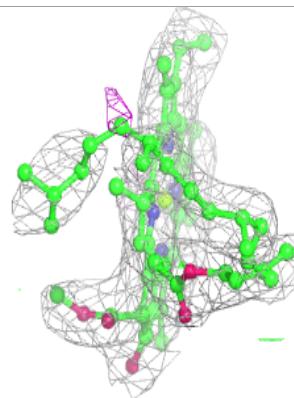
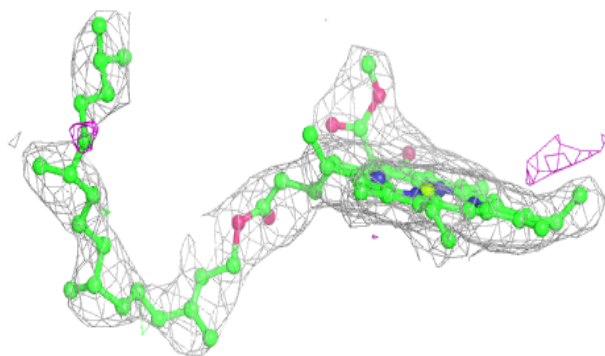
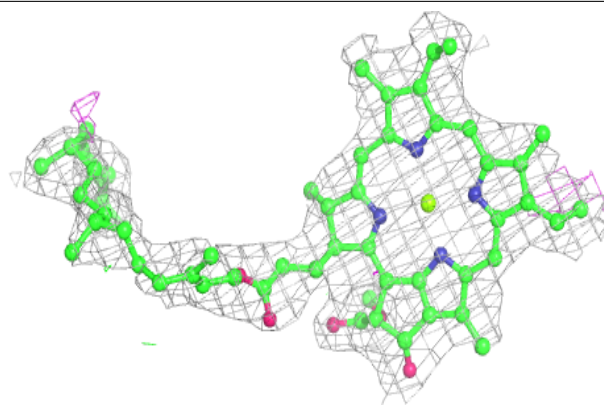
**Electron density around CLA A 806:**

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

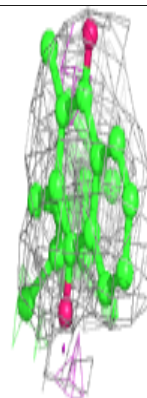
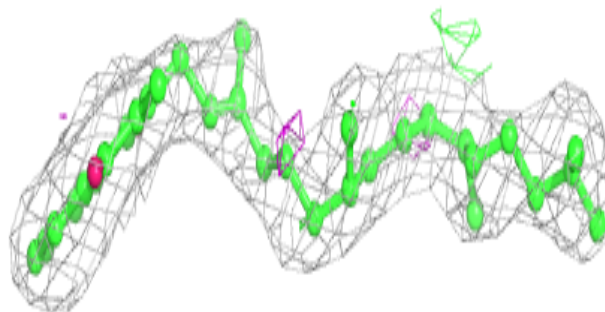
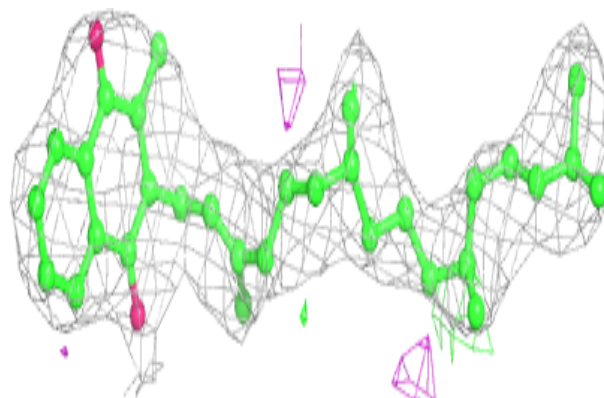


**Electron density around CLA G 827:**

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

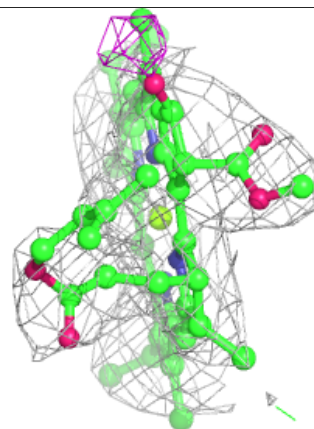
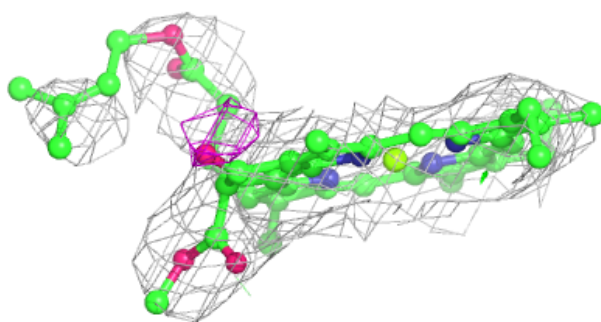
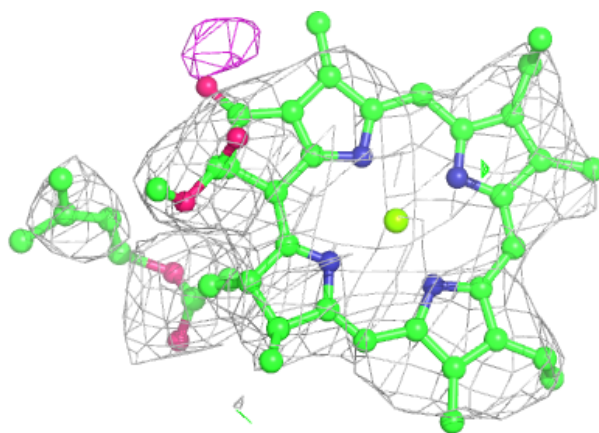
**Electron density around PQN G 843:**

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

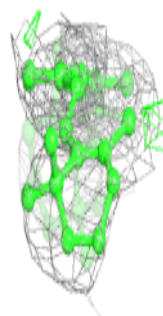
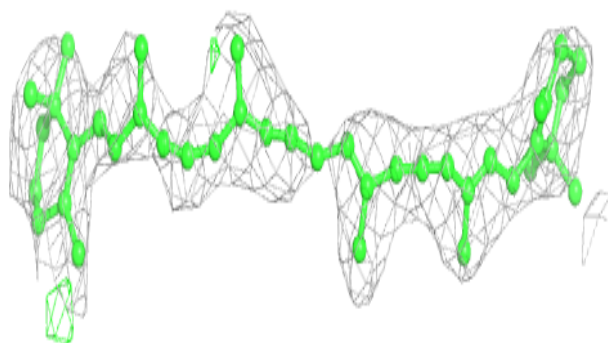
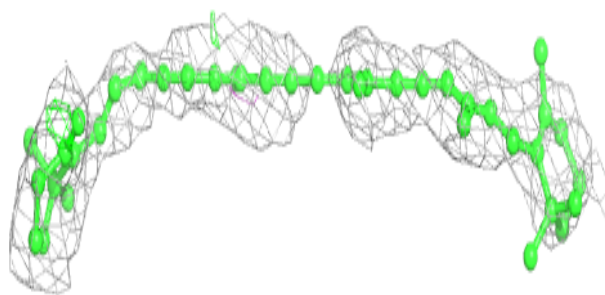


**Electron density around CLA Y 816:**

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

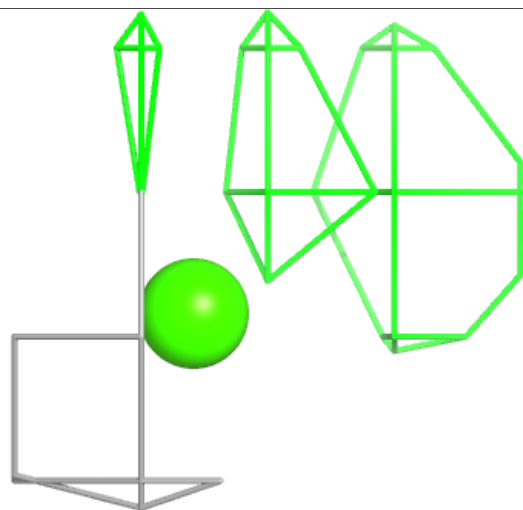
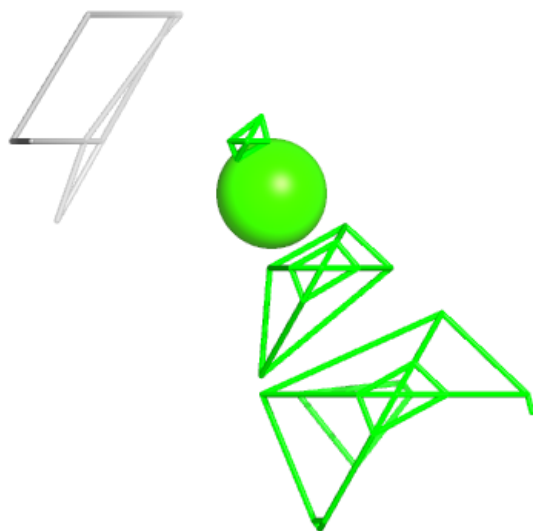
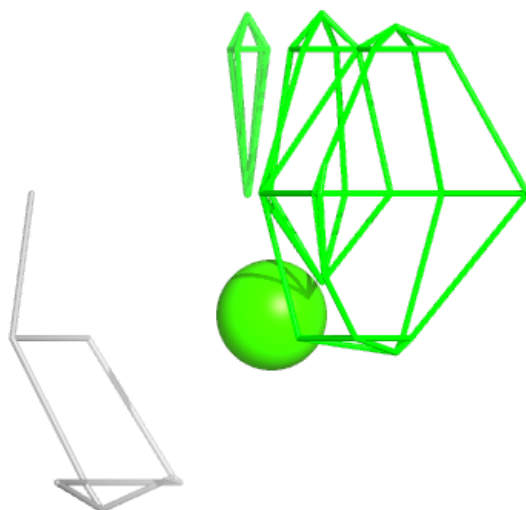
**Electron density around BCR A 846:**

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



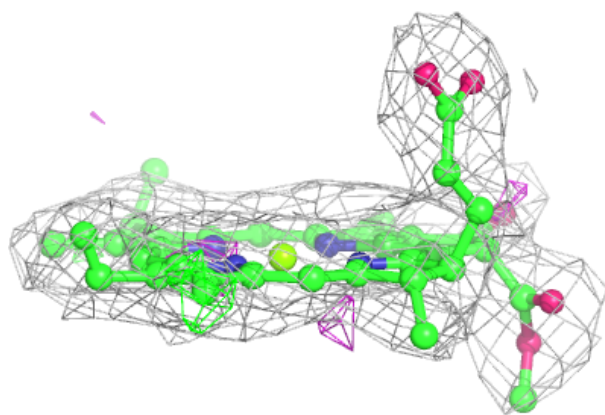
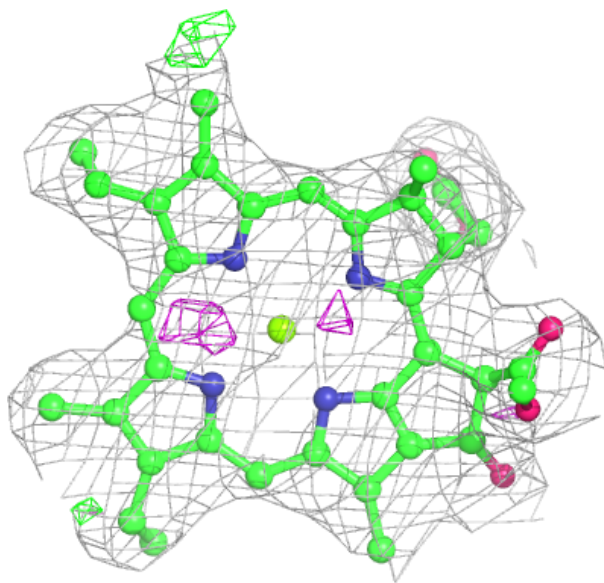
**Electron density around CA U 1001:**

$2mF_o-DF_c$  (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:**

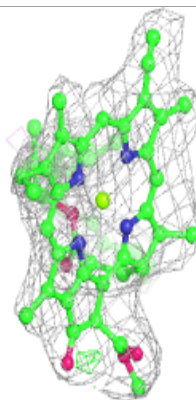
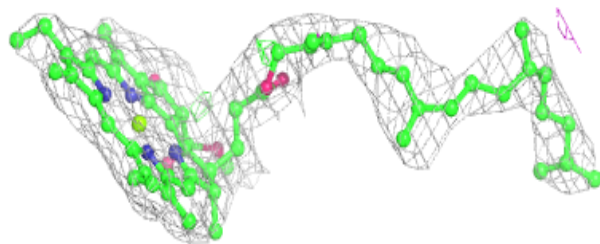
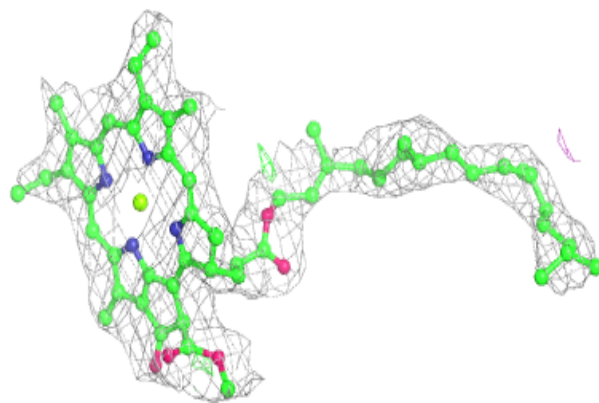
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



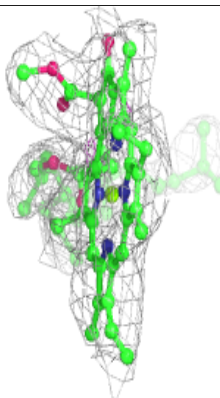
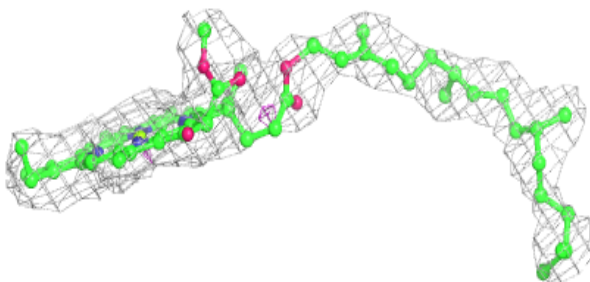
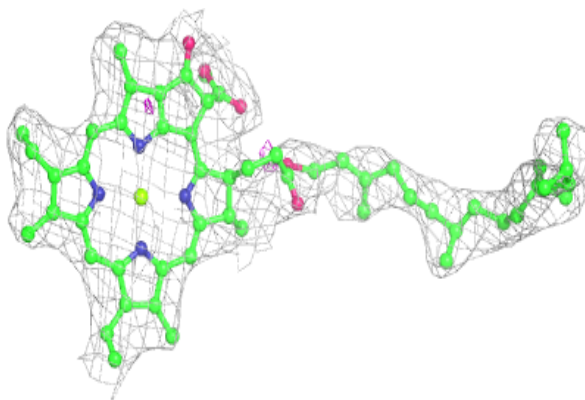


**Electron density around CLA G 821:**

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

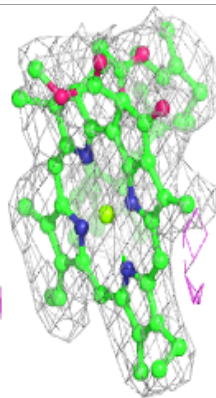
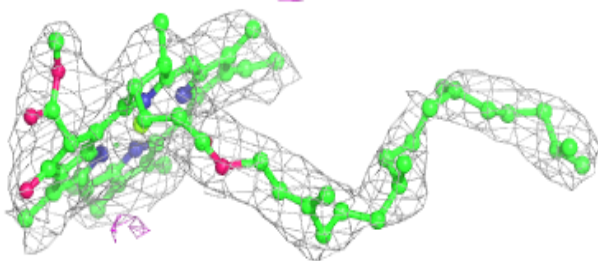
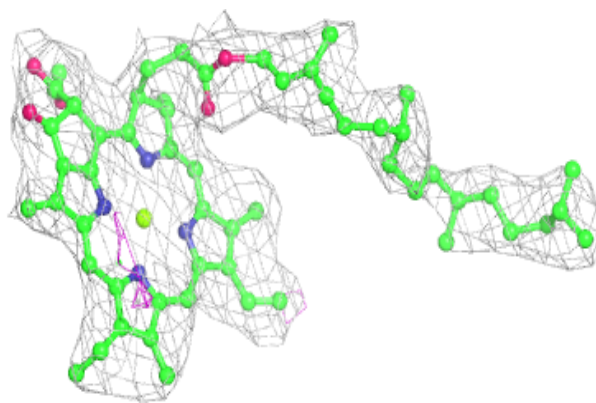
**Electron density around CLA G 805:**

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



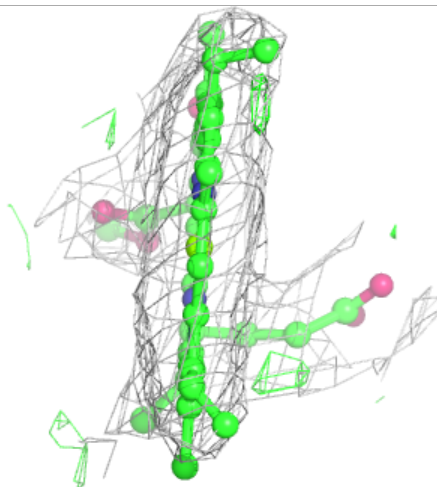
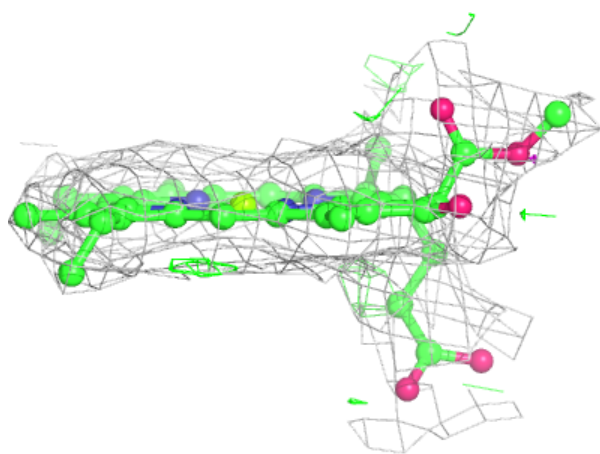
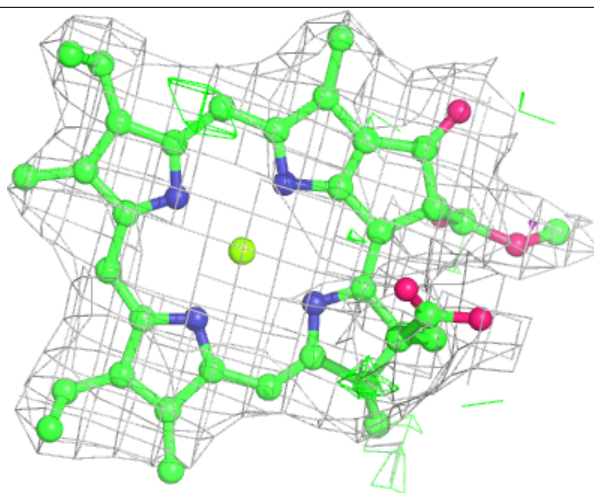
**Electron density around CLA Y 808:**

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



**Electron density around CLA H 812:**

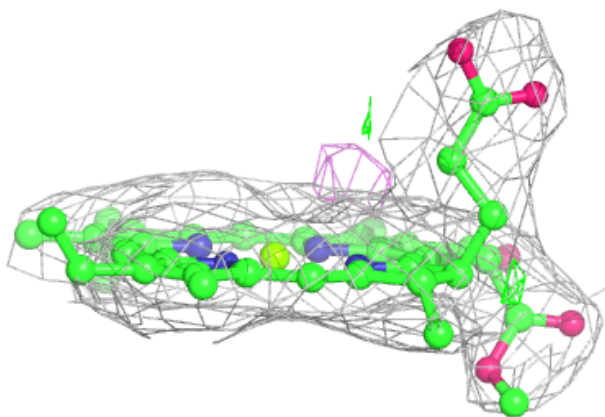
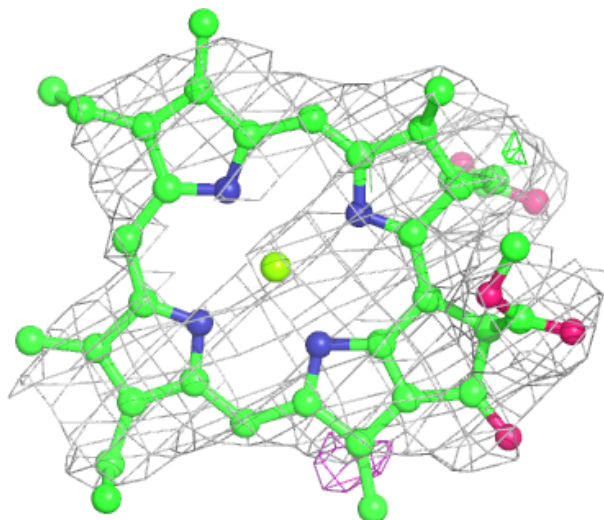
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





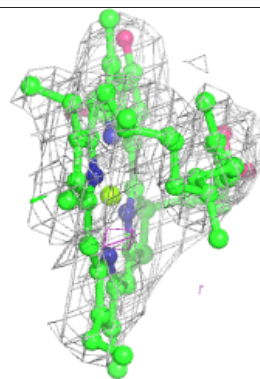
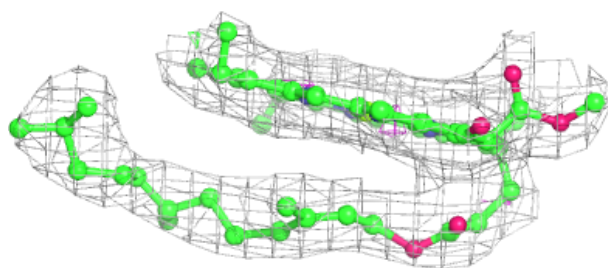
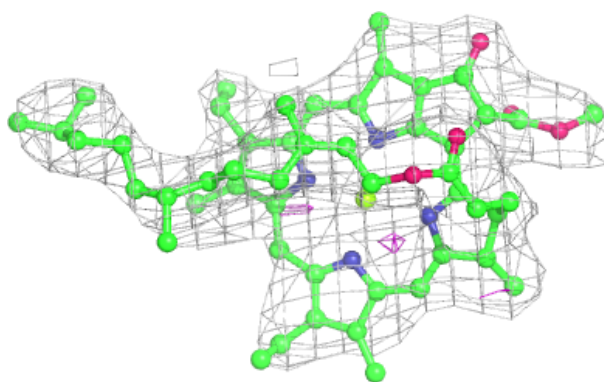
**Electron density around CLA K 102:**

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

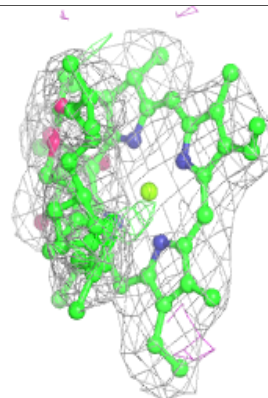
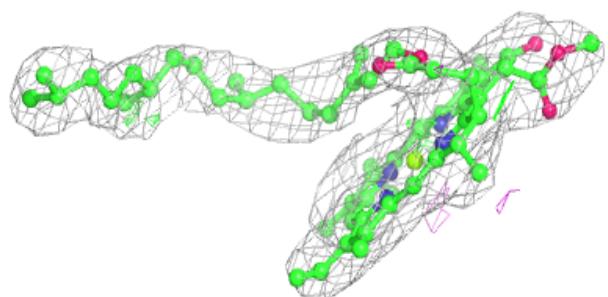
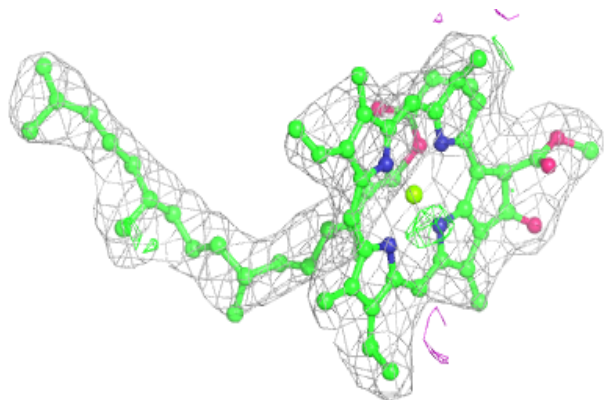


**Electron density around CLA G 817:**

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

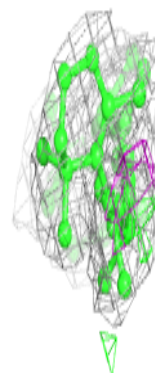
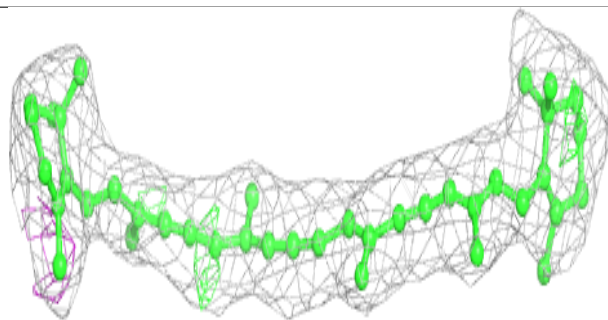
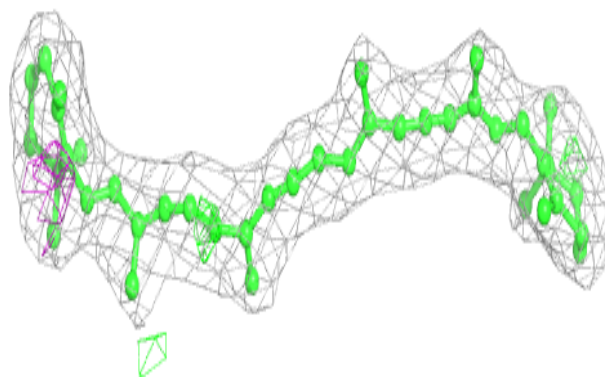
**Electron density around CLA Y 840:**

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

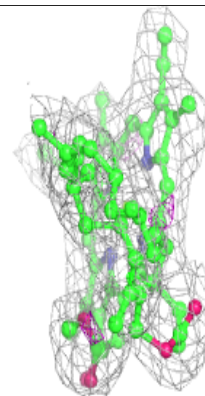
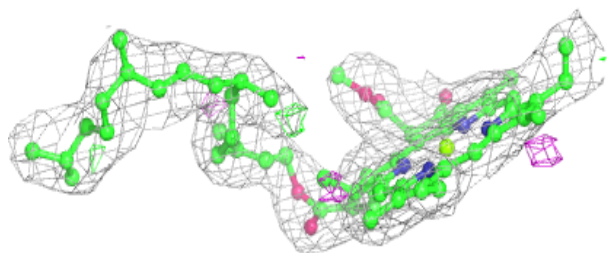
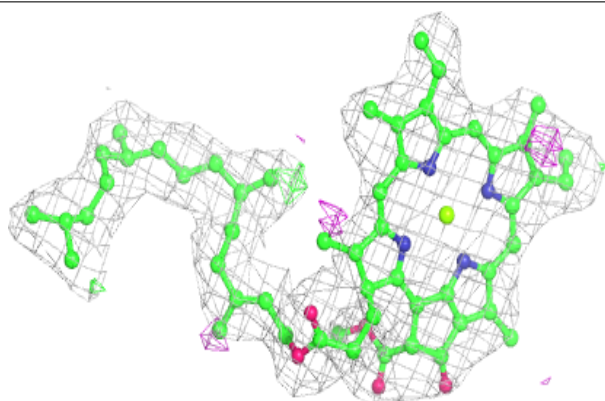


**Electron density around BCR e 101:**

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

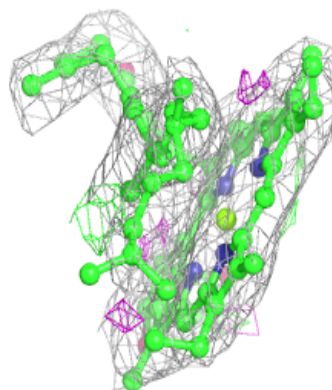
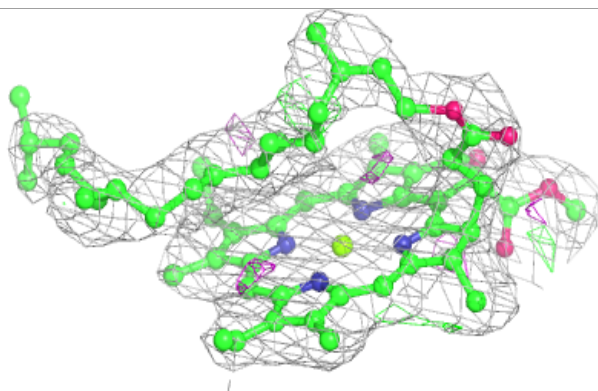
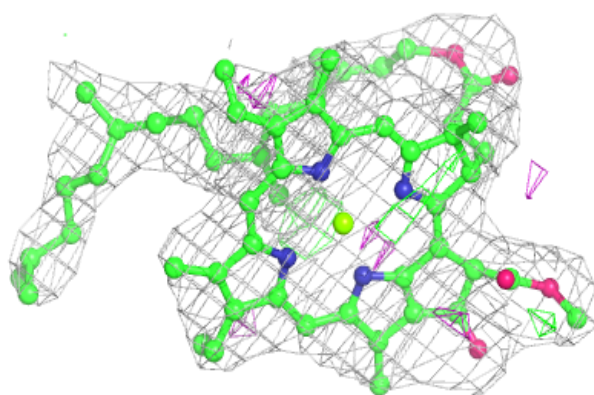
**Electron density around CLA A 804:**

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

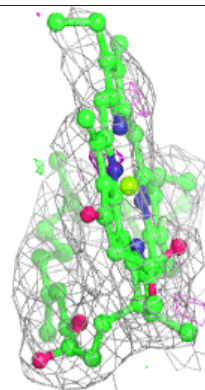
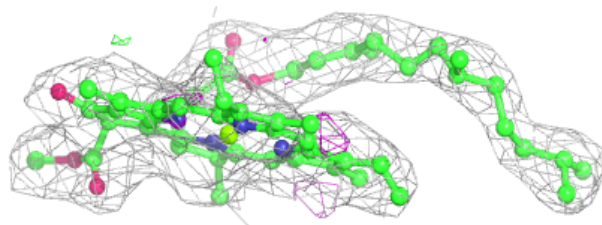
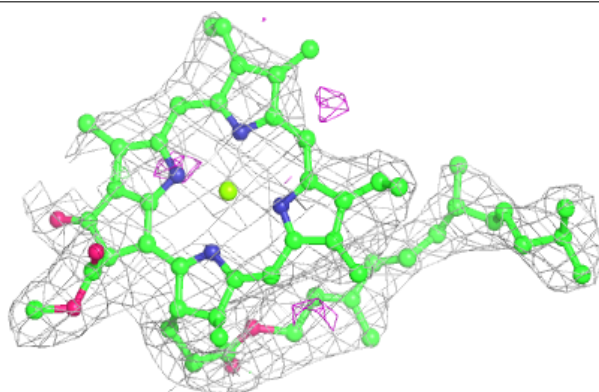


**Electron density around CLA H 817:**

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

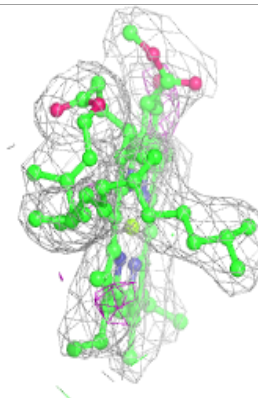
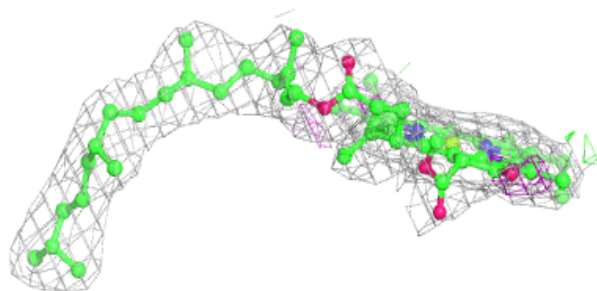
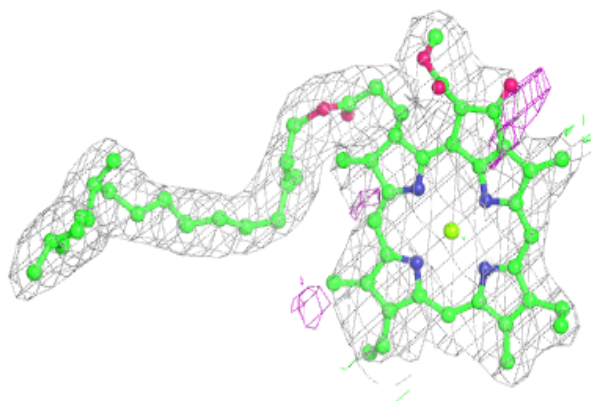
**Electron density around CLA H 818:**

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



**Electron density around CLA Z 804:**

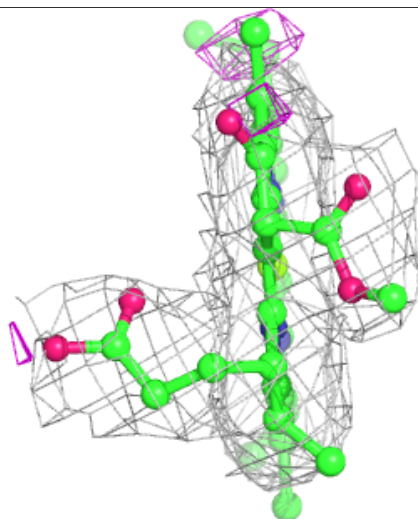
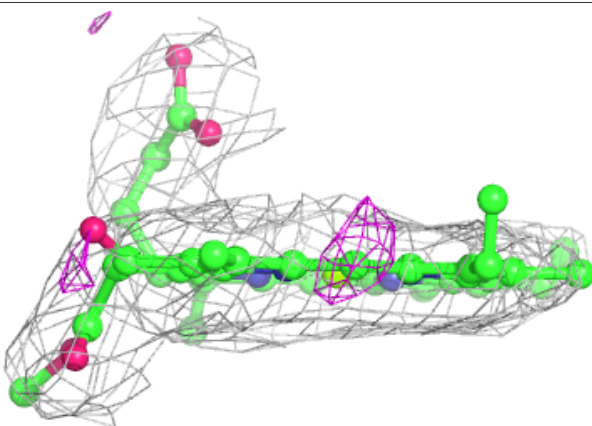
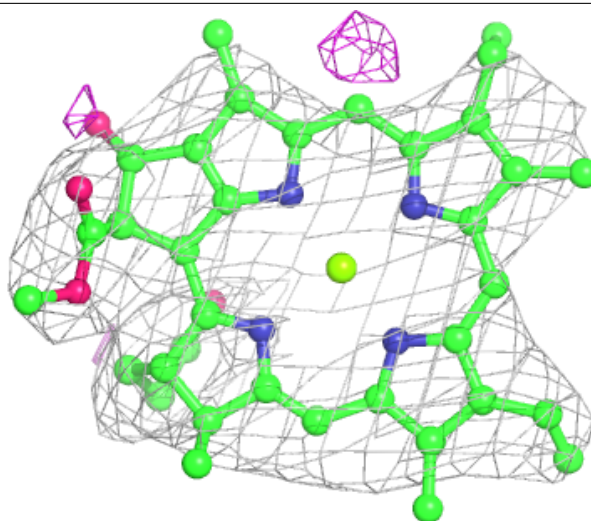
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





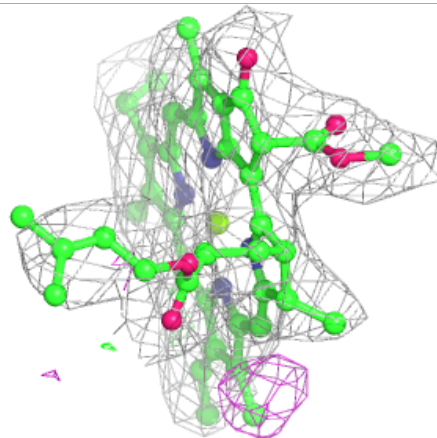
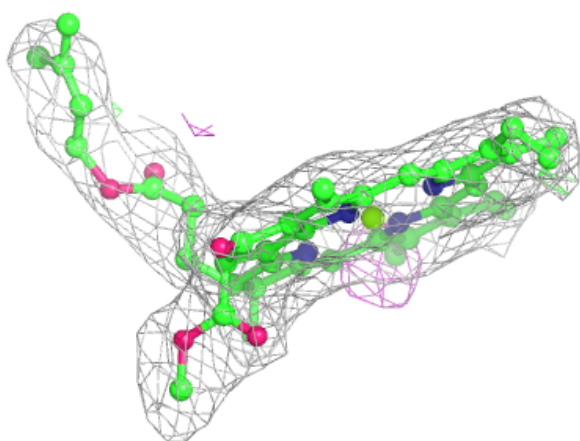
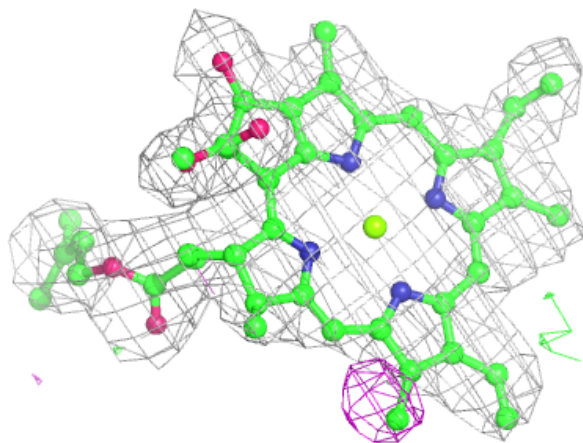
**Electron density around CLA G 835:**

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



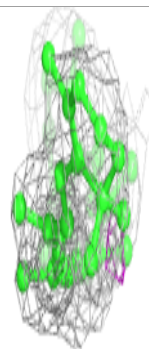
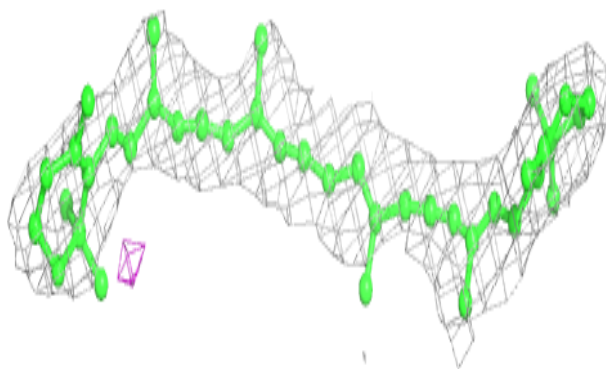
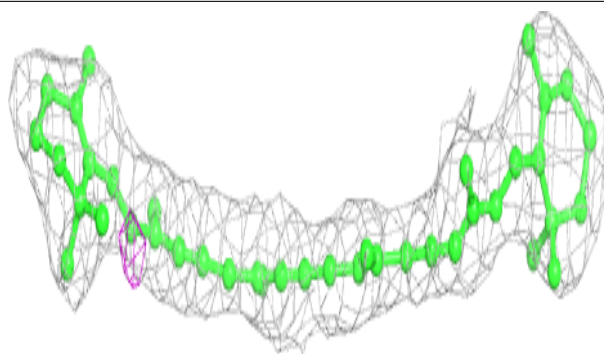
**Electron density around CLA Y 837:**

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

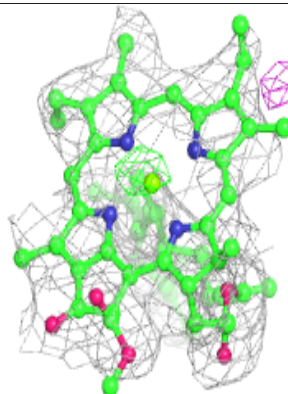
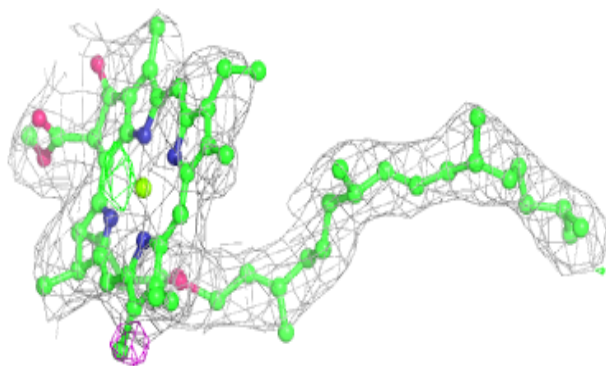
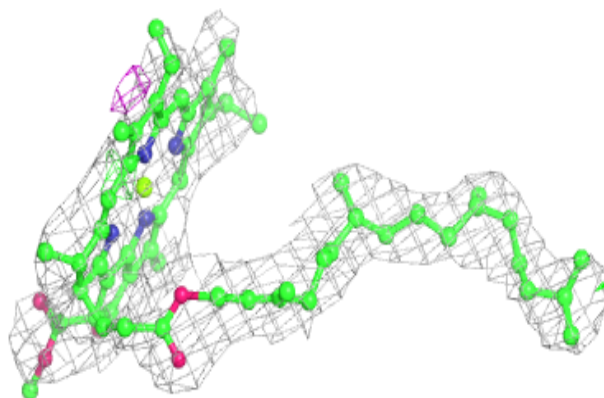


**Electron density around BCR J 104:**

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

**Electron density around CLA G 811:**

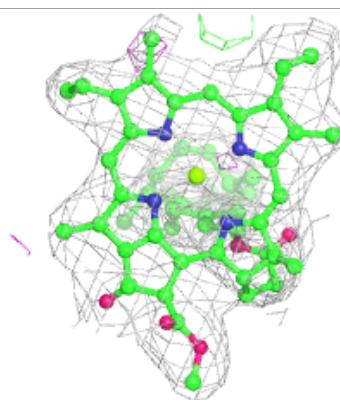
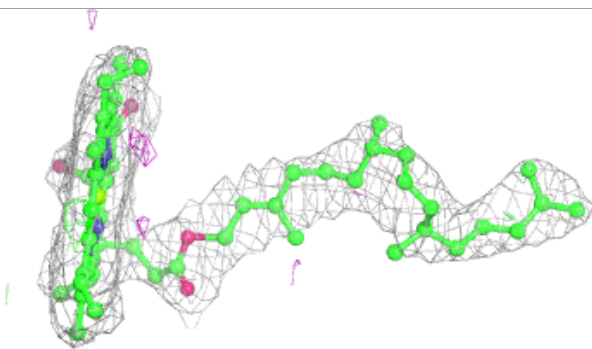
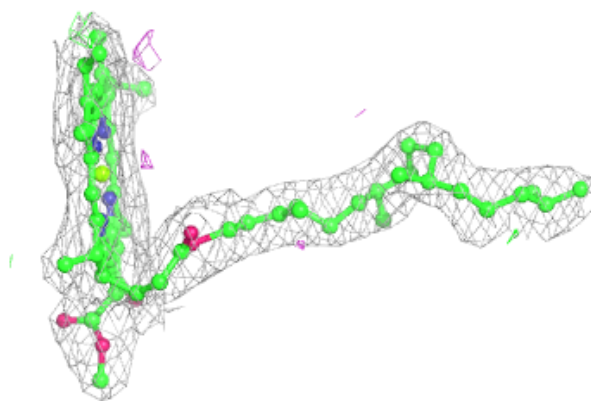
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





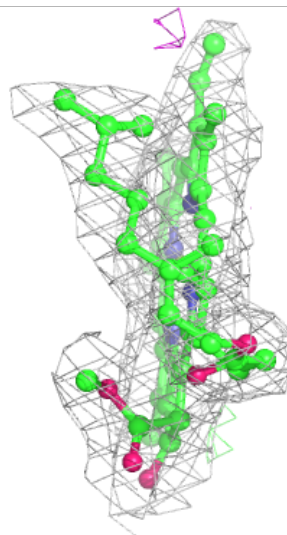
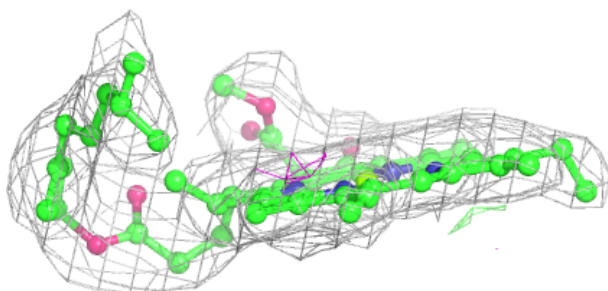
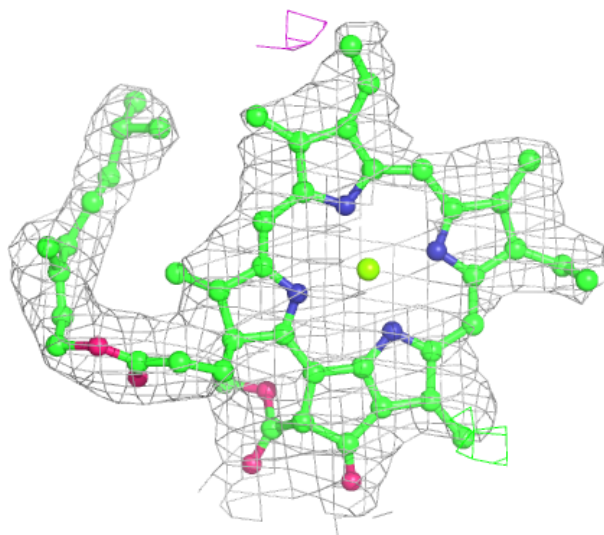
**Electron density around CLA A 829:**

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



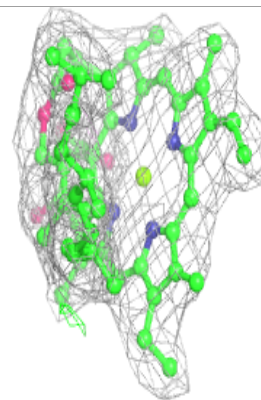
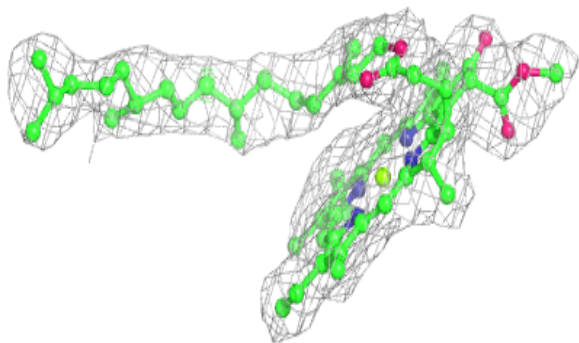
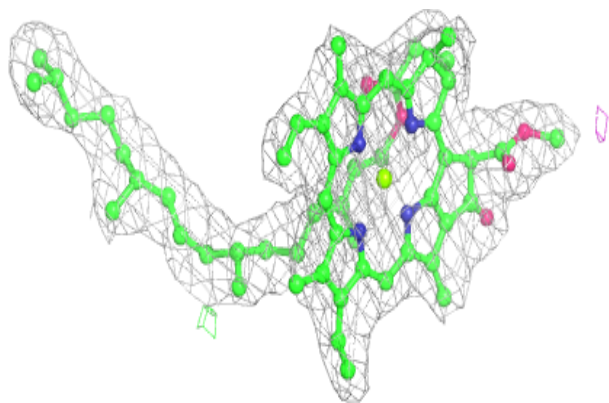
**Electron density around CLA Z 825:**

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

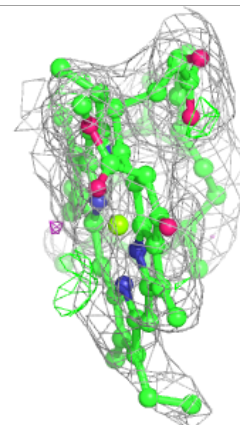
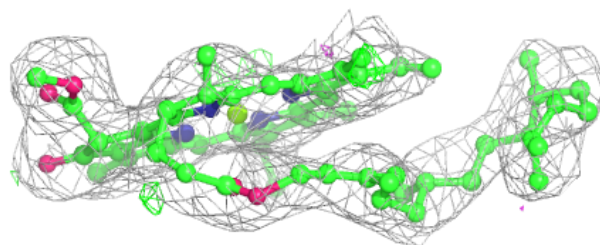
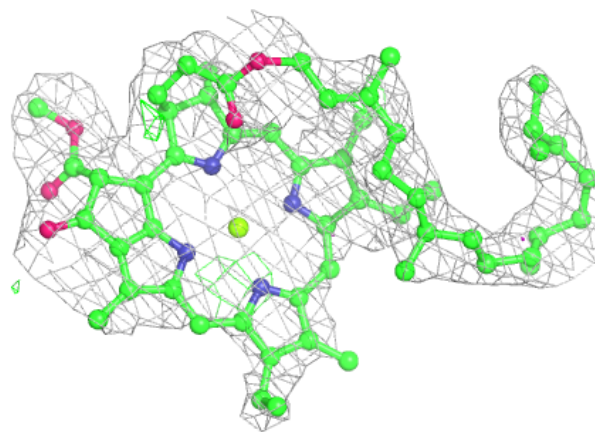


**Electron density around CLA A 841:**

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

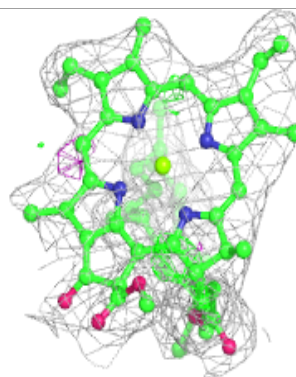
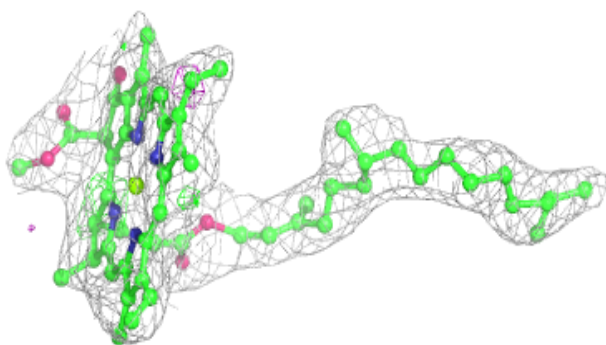
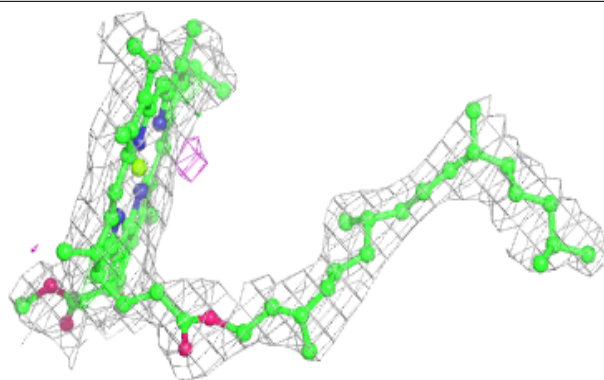
**Electron density around CLA Y 819:**

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



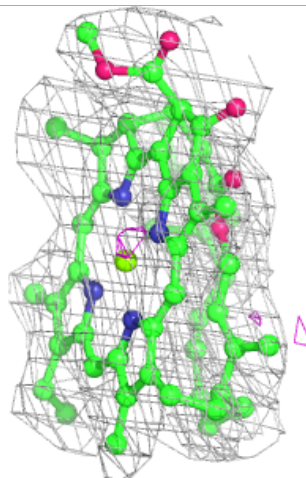
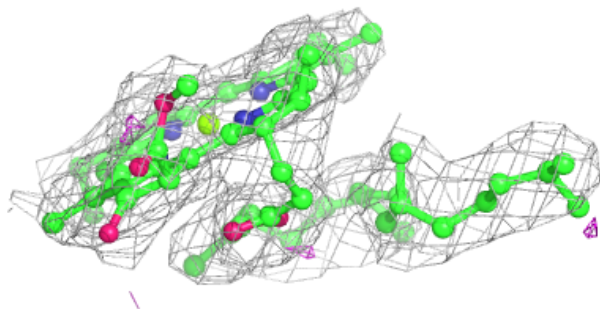
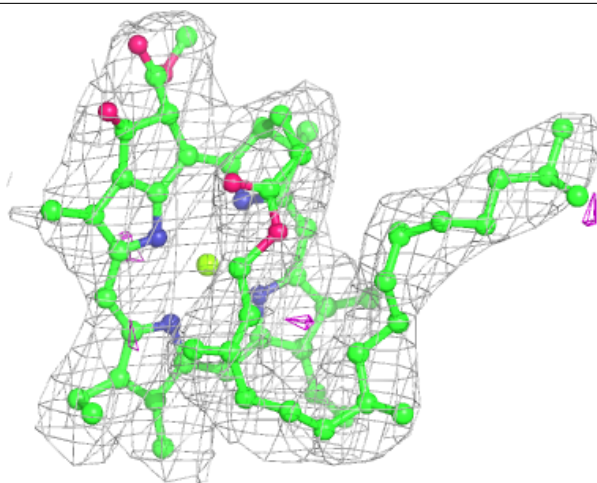
**Electron density around CLA A 831:**

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



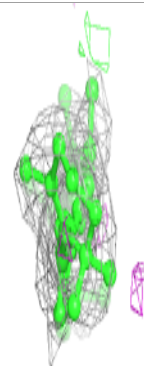
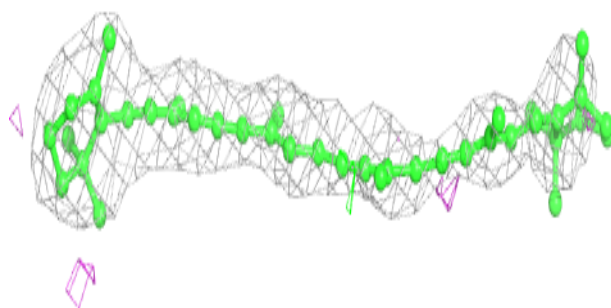
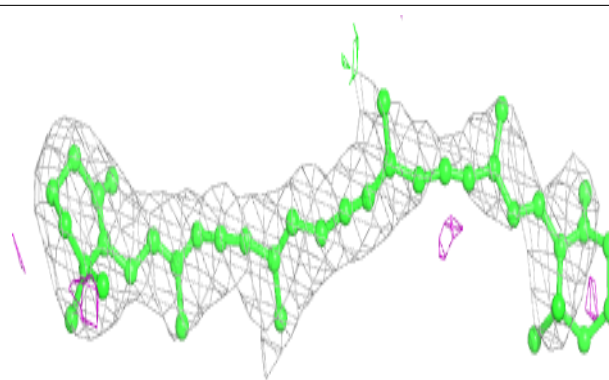
**Electron density around CLA B 807:**

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



**Electron density around BCR Y 847:**

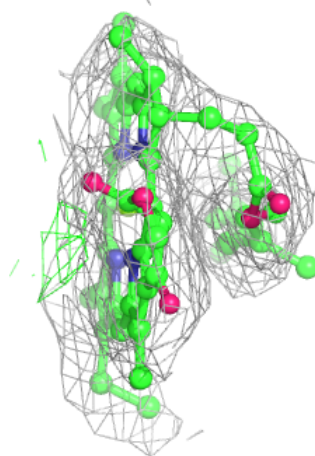
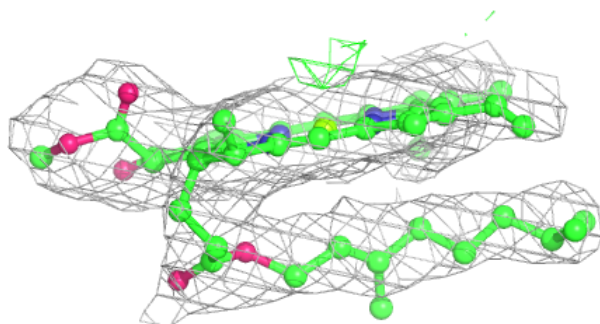
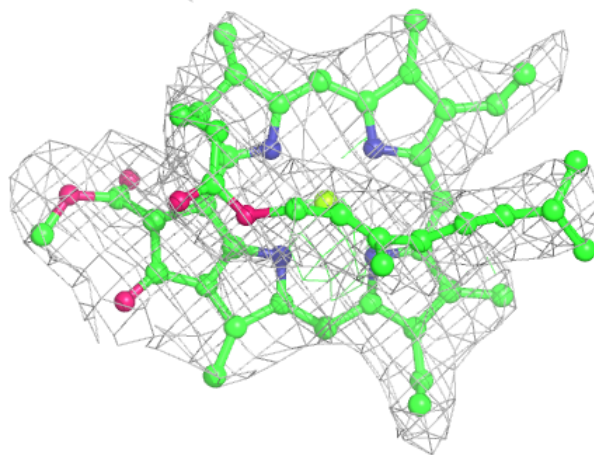
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





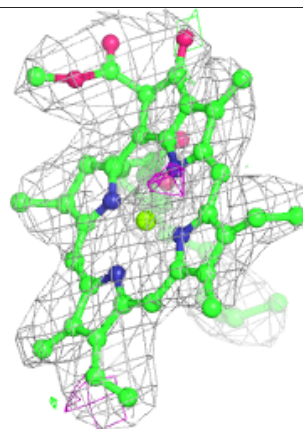
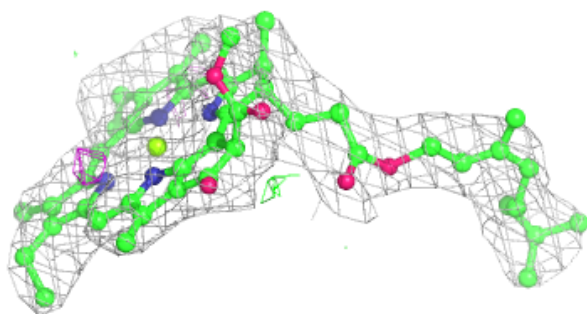
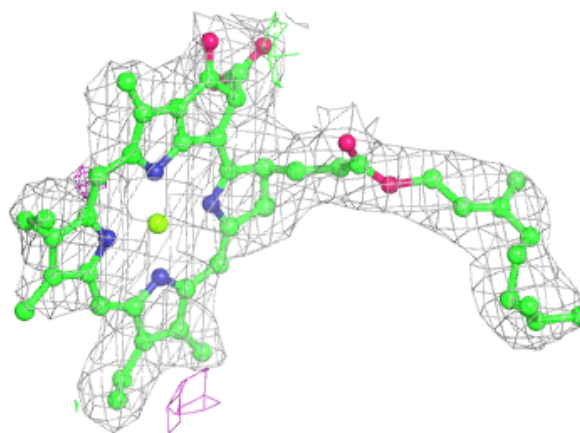
**Electron density around CLA H 822:**

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



**Electron density around CLA B 832:**

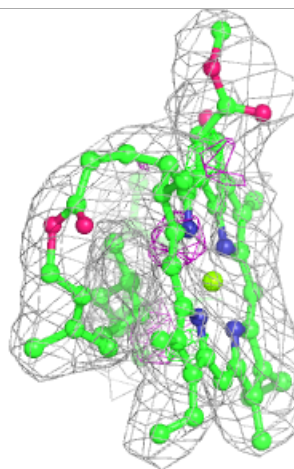
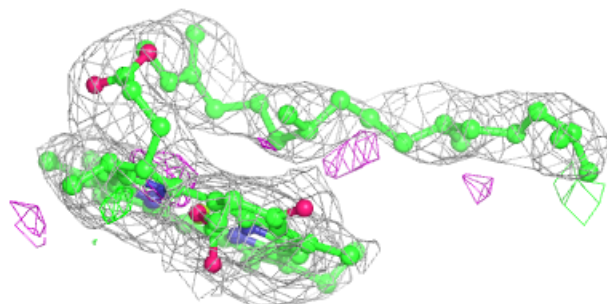
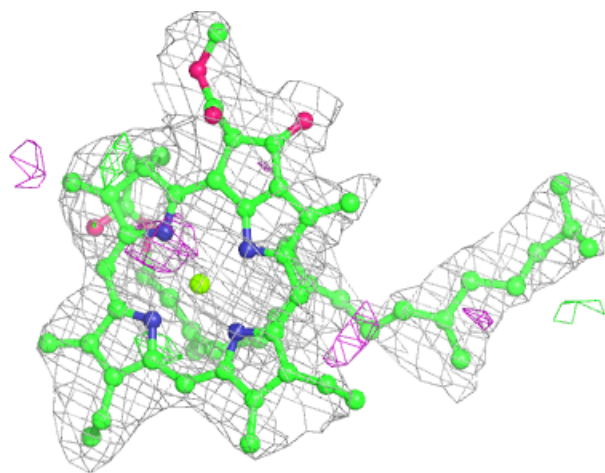
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





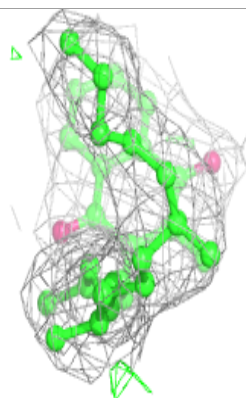
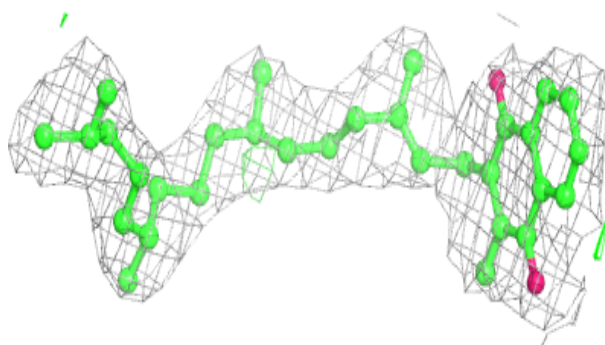
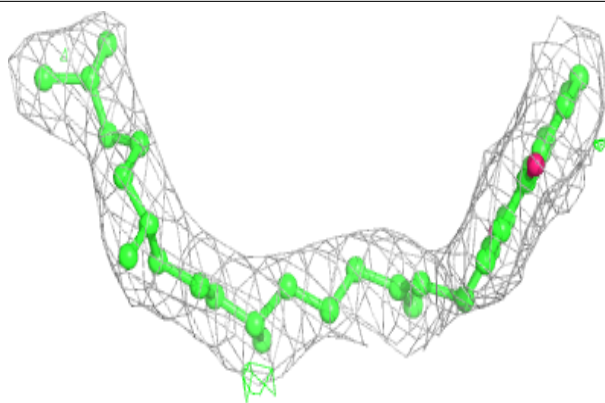
**Electron density around CLA Z 828:**

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



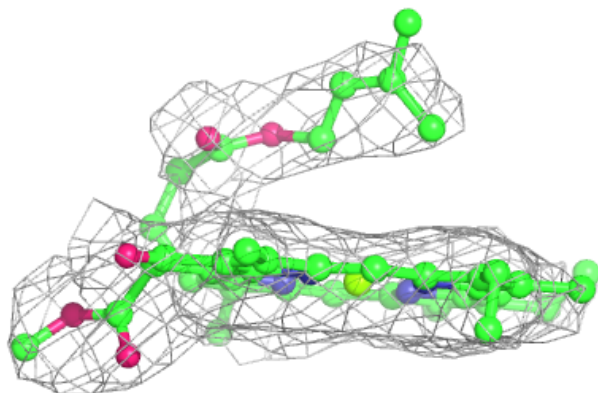
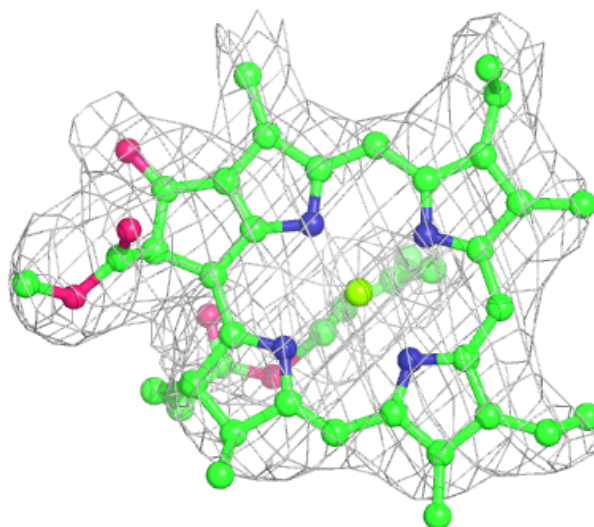
**Electron density around PQN Z 842:**

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



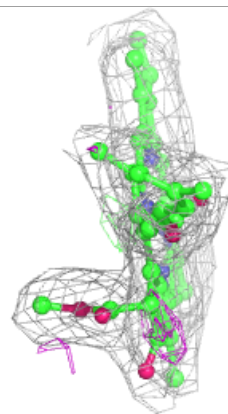
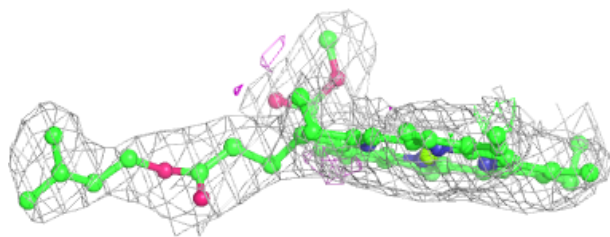
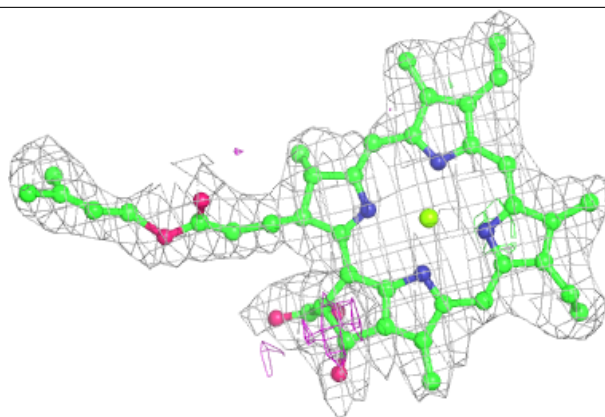
**Electron density around CLA G 823:**

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



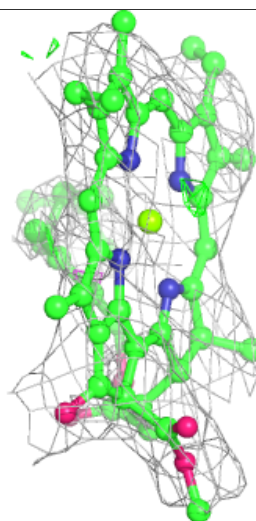
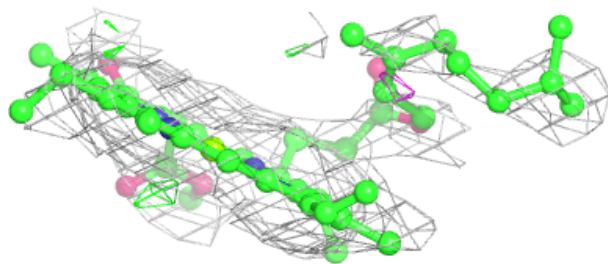
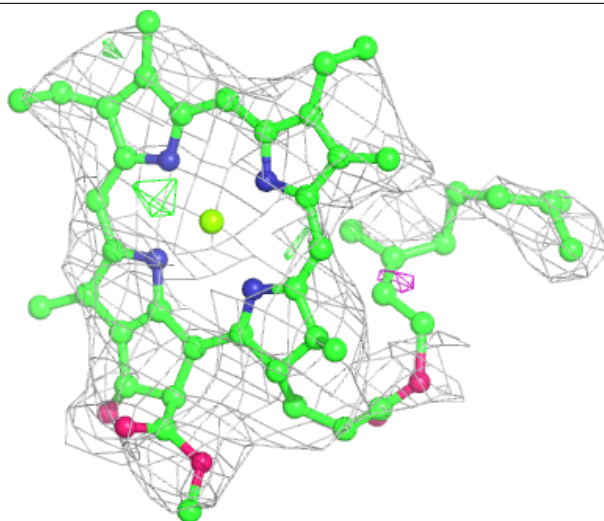
**Electron density around CLA A 836:**

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



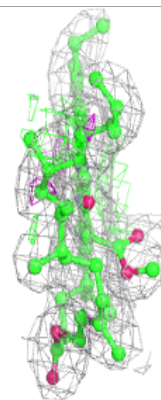
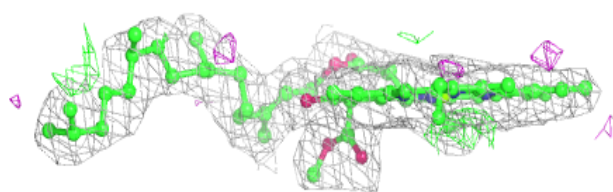
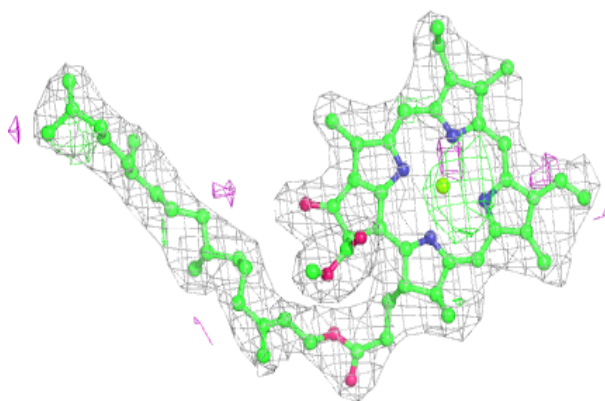
**Electron density around CLA f 102:**

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

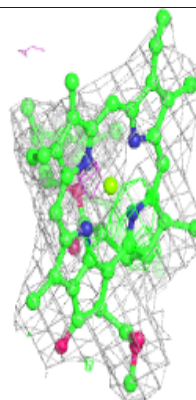
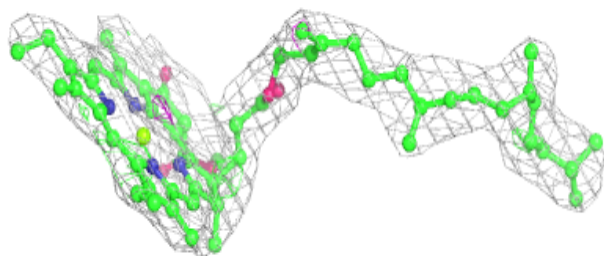
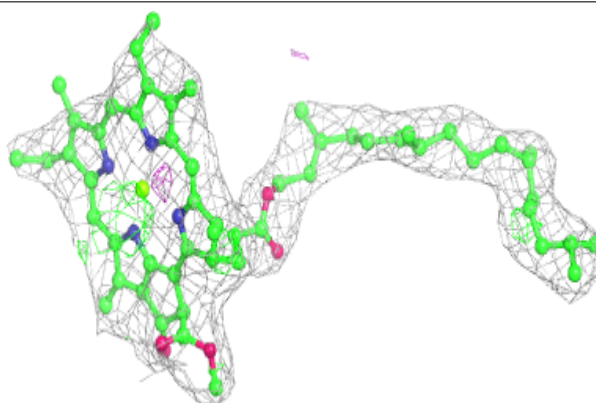


**Electron density around CLA U 1004:**

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

**Electron density around CLA Y 821:**

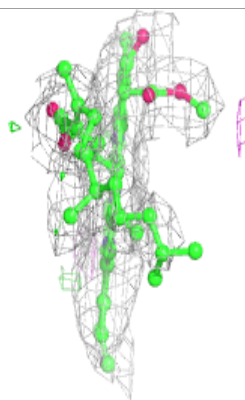
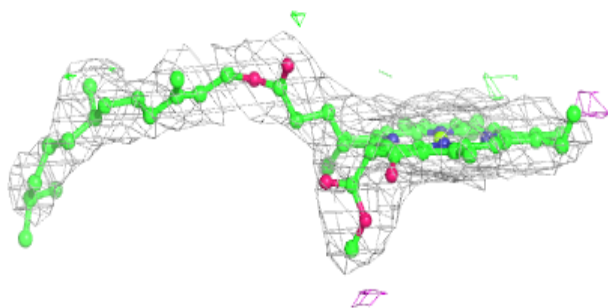
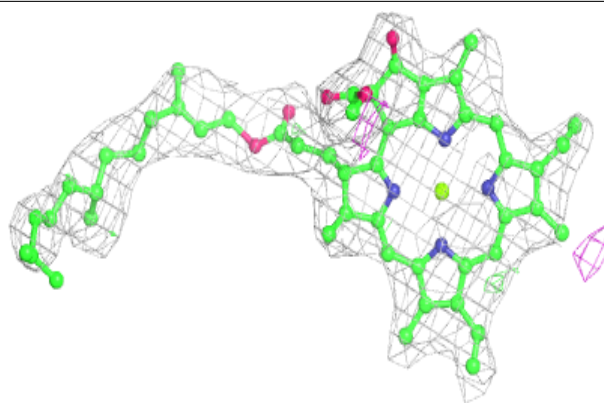
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



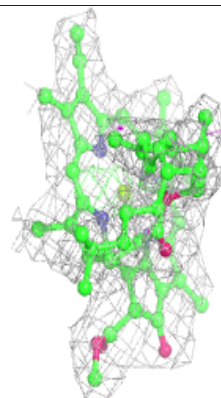
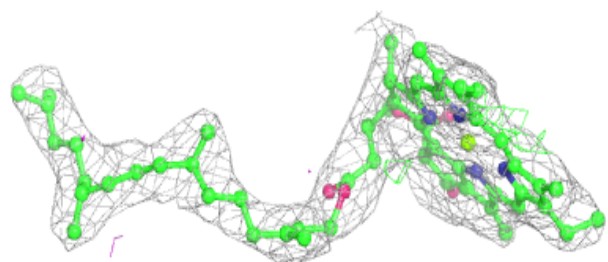
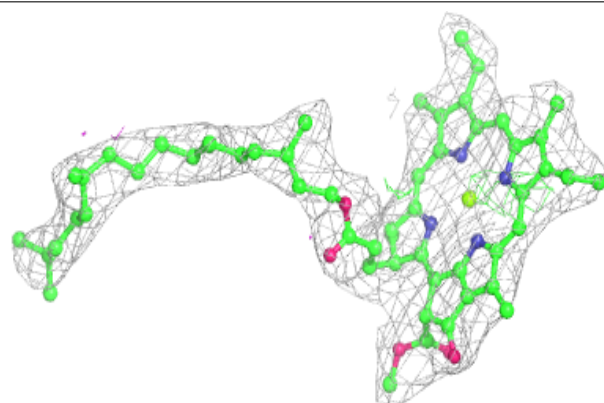


**Electron density around CLA H 836:**

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

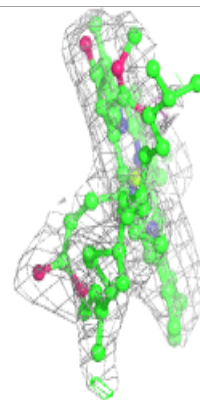
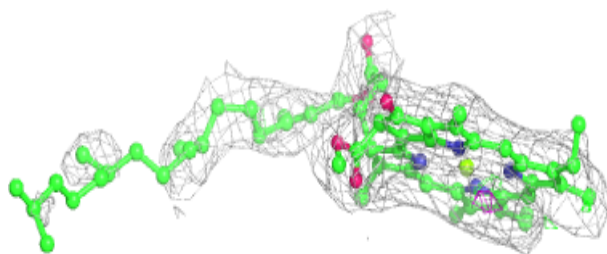
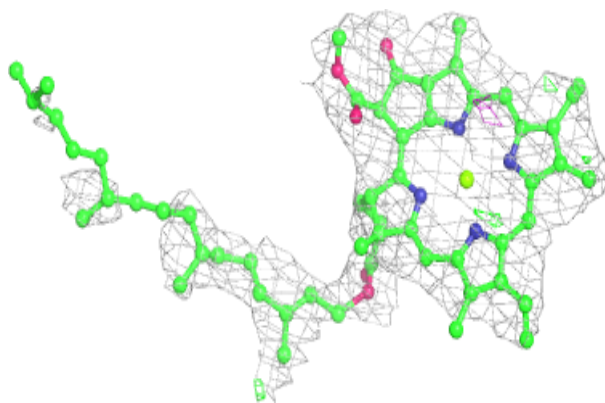
**Electron density around CLA A 822:**

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



**Electron density around CLA Y 822:**

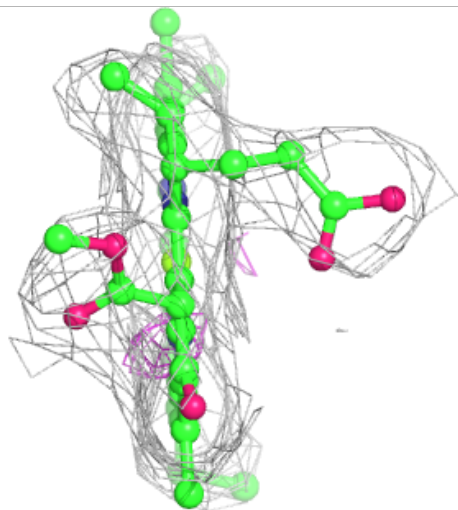
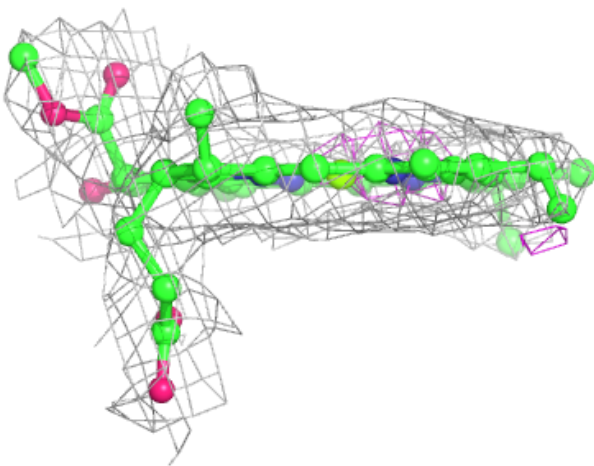
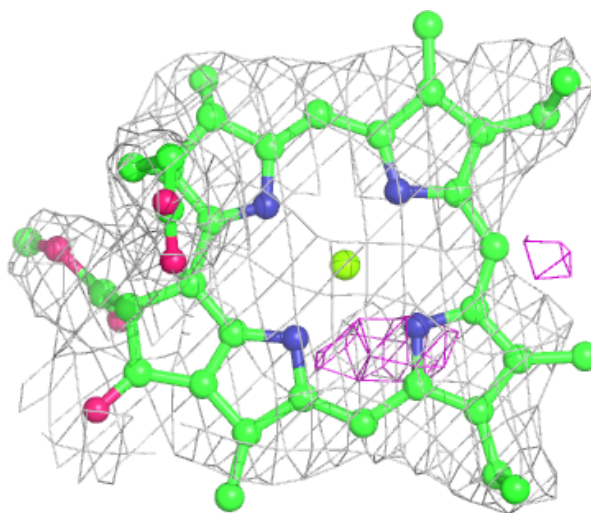
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





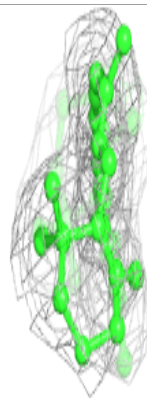
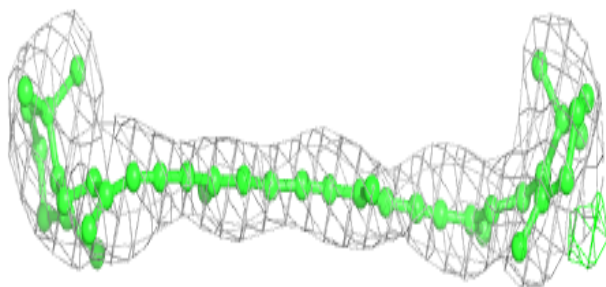
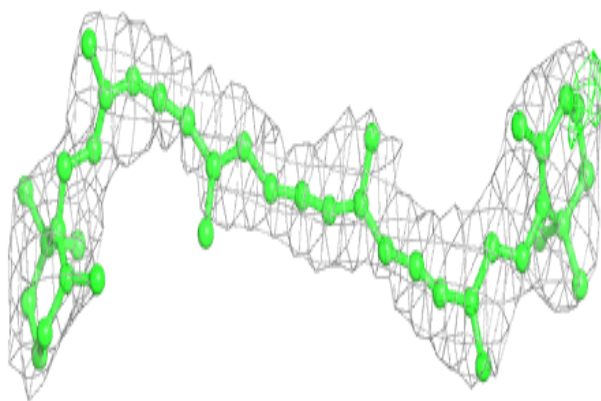
**Electron density around CLA Y 834:**

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



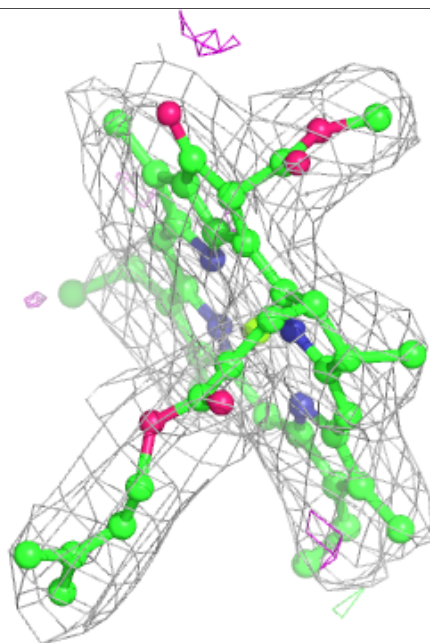
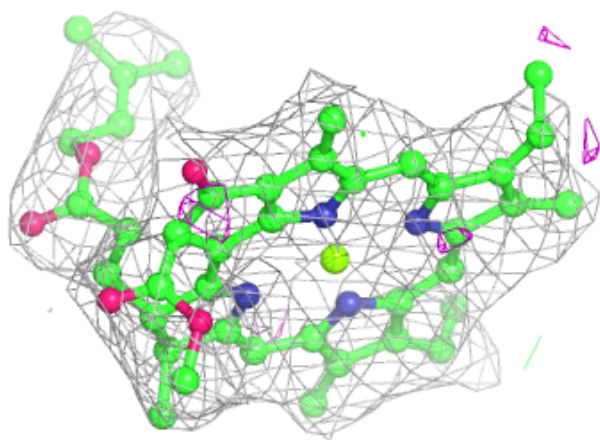
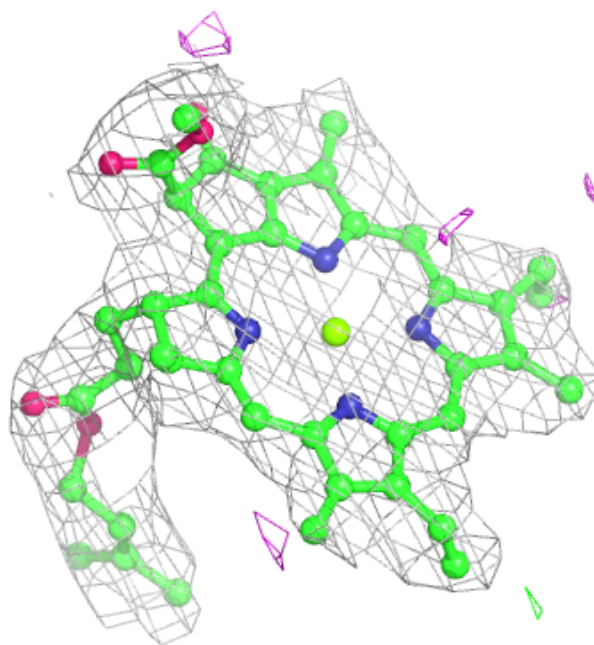
**Electron density around BCR H 844:**

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



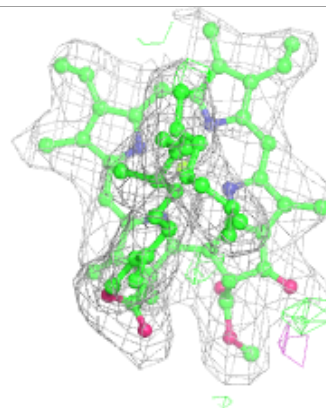
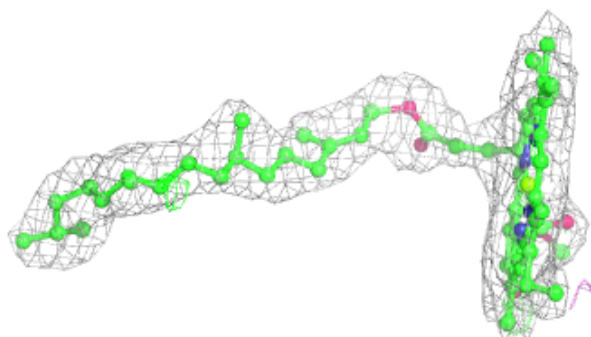
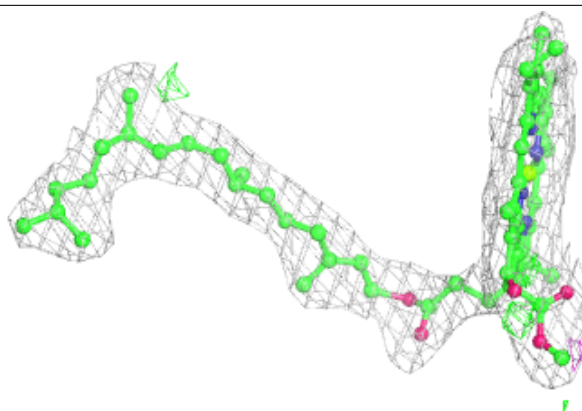
**Electron density around CLA Y 831:**

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

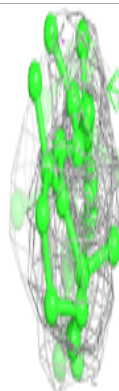
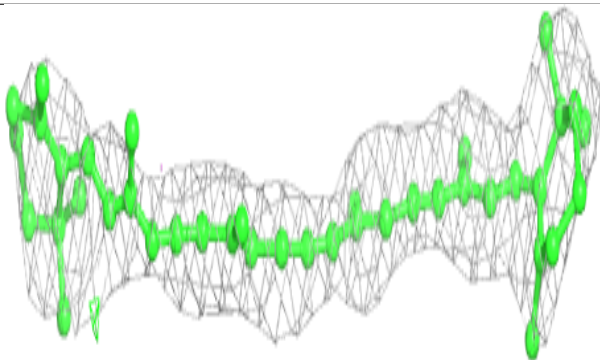
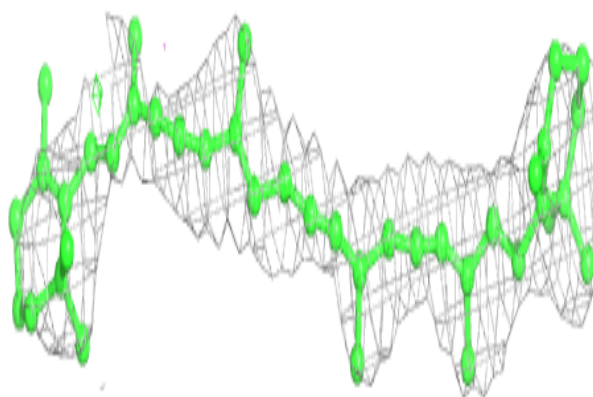


**Electron density around CLA Z 841:**

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

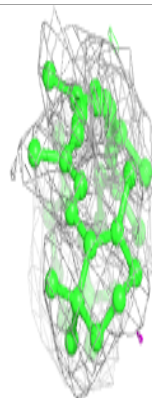
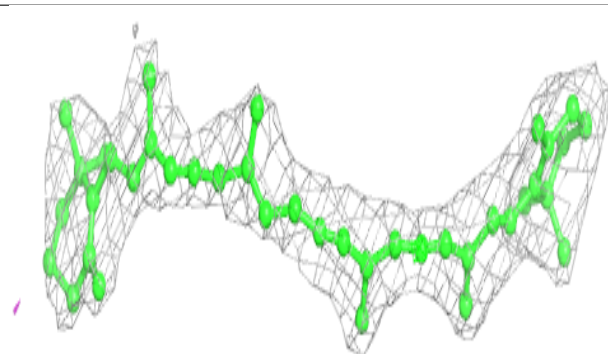
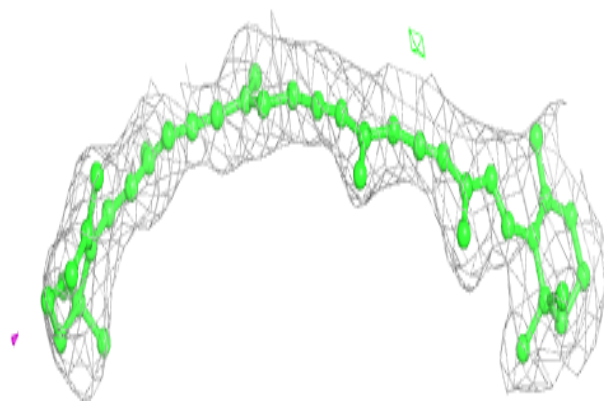
**Electron density around BCR G 846:**

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

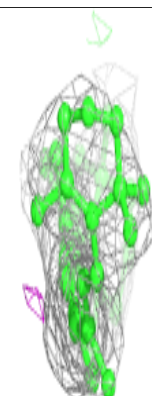
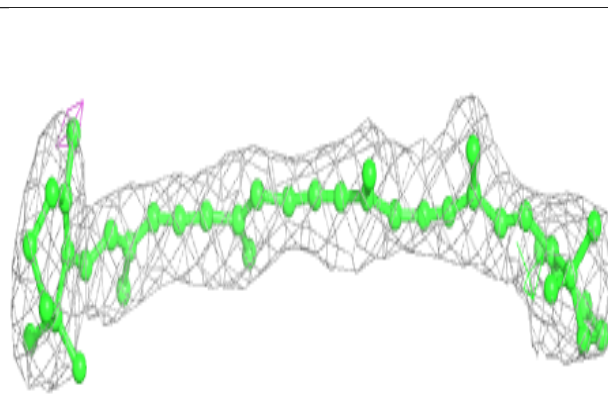
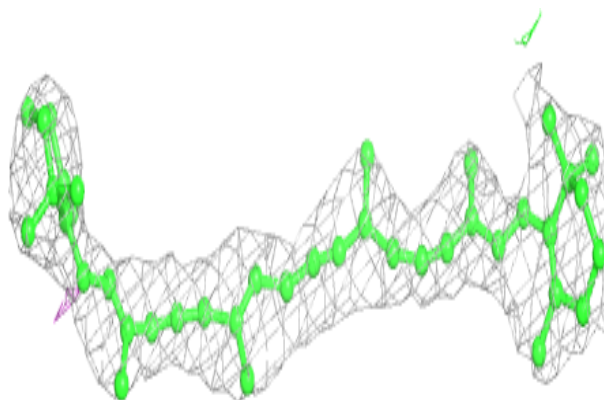


**Electron density around BCR F 201:**

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

**Electron density around BCR Y 844:**

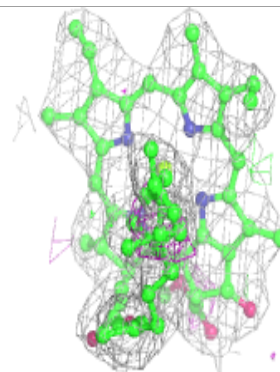
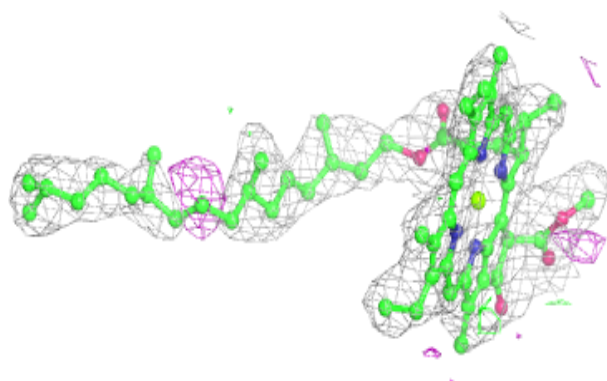
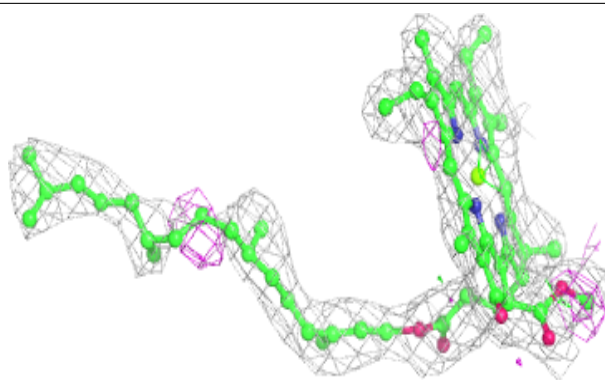
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



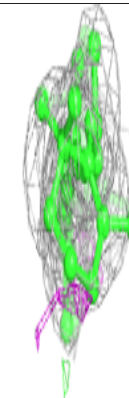
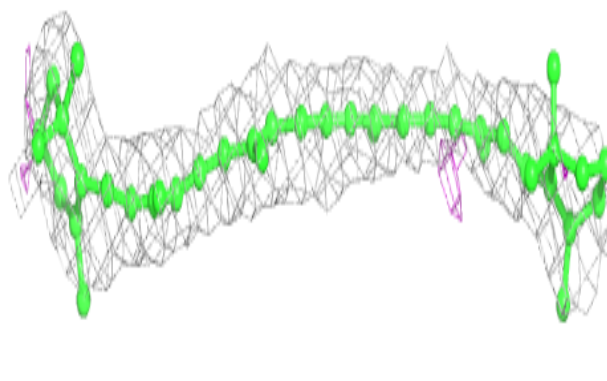
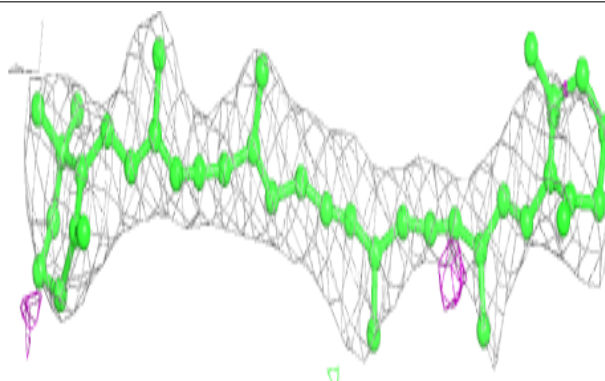


**Electron density around CLA H 829:**

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

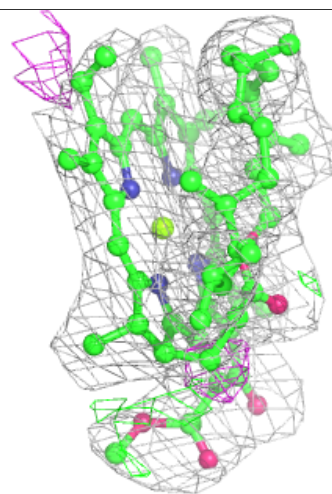
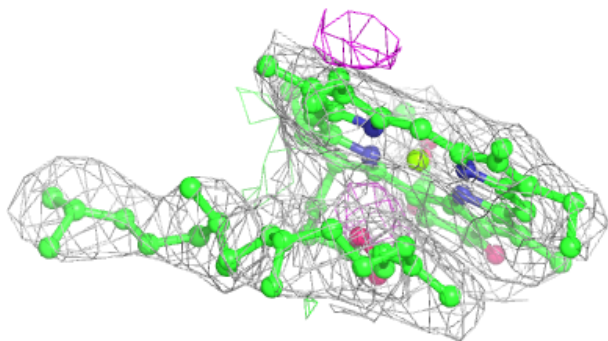
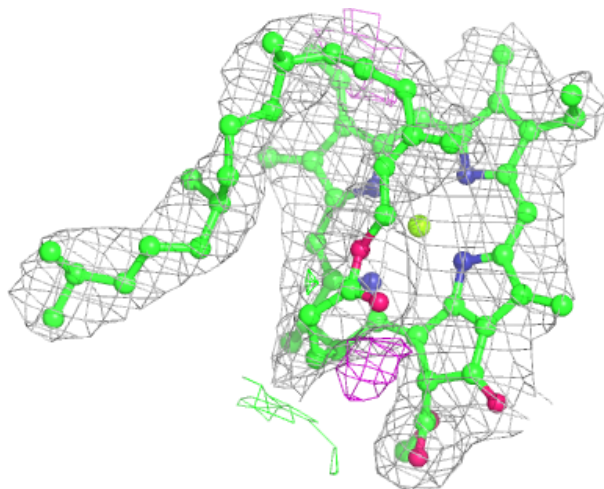
**Electron density around BCR A 849:**

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



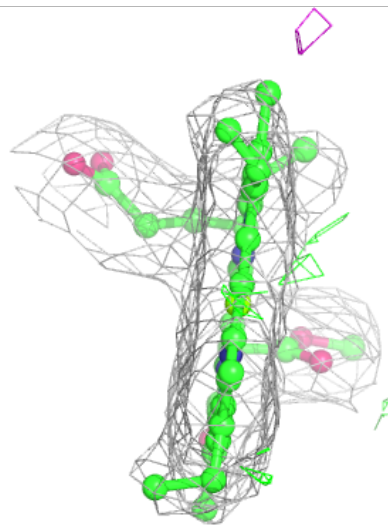
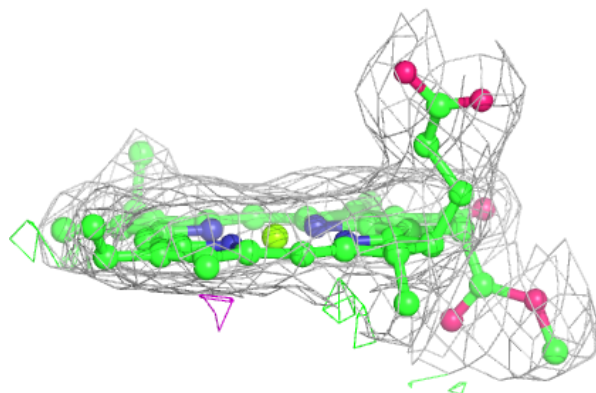
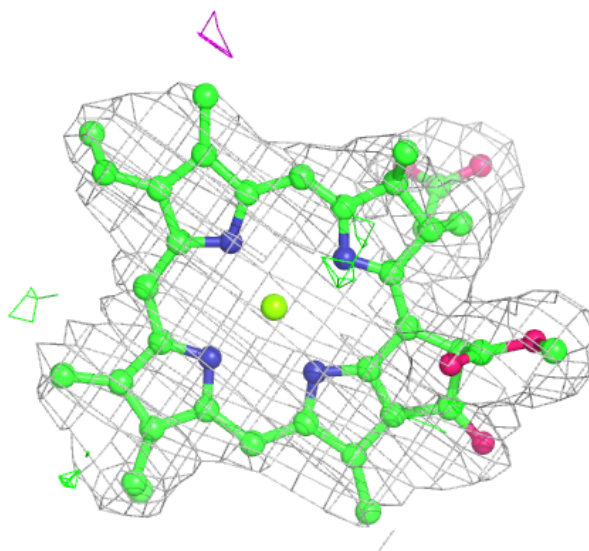
**Electron density around CLA H 808:**

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



**Electron density around CLA Z 839:**

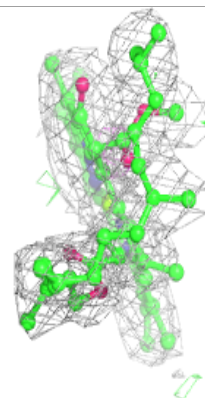
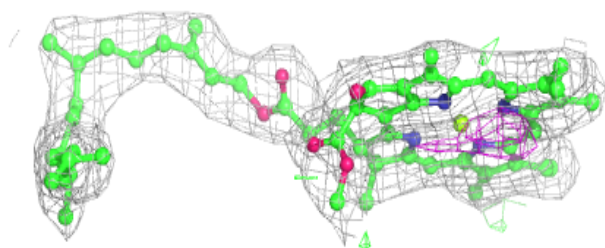
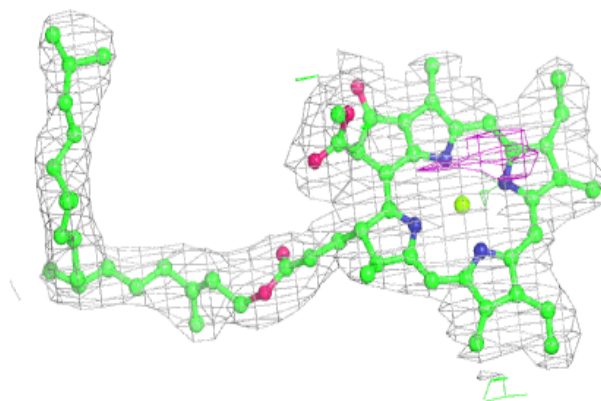
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



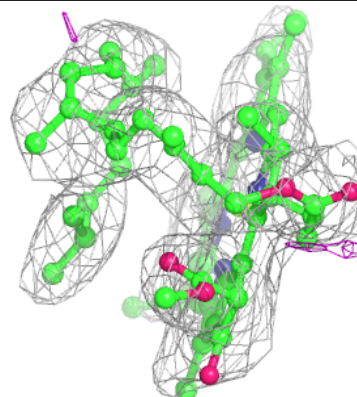
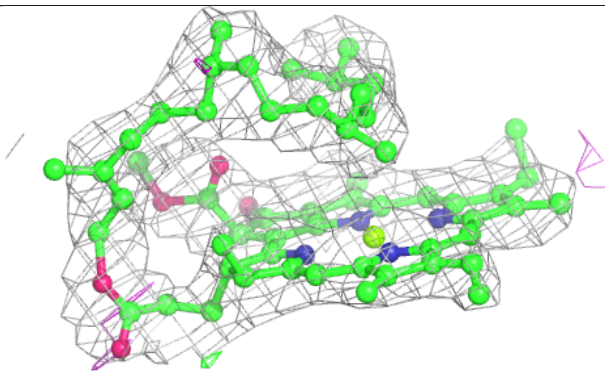
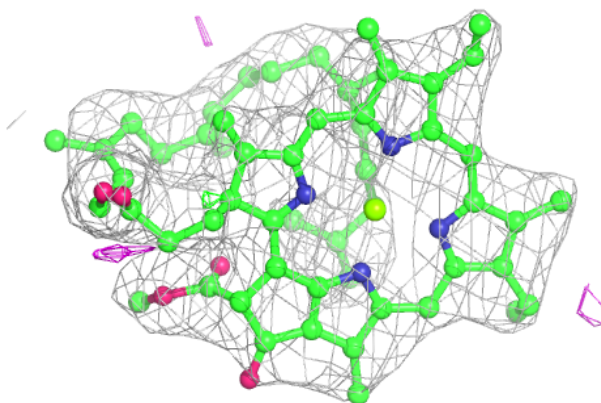


**Electron density around CLA H 826:**

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

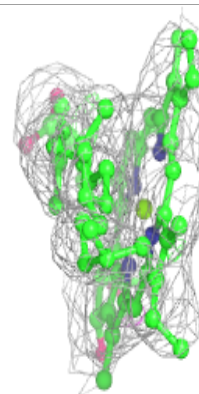
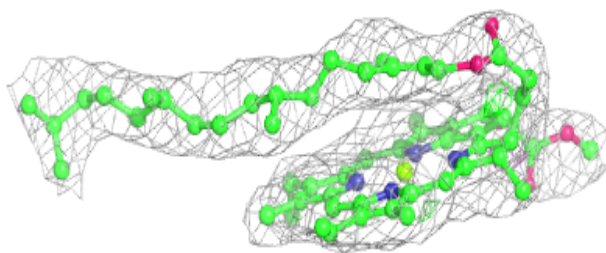
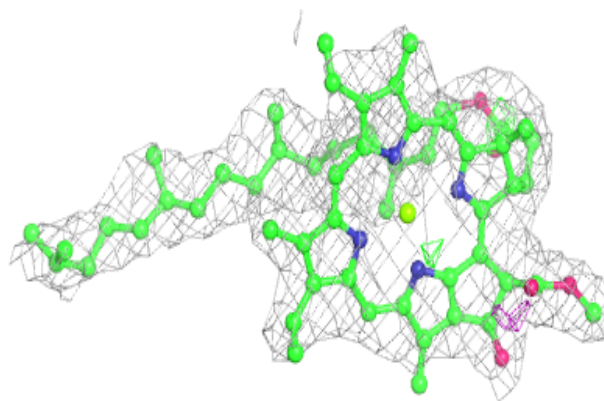
**Electron density around CLA G 806:**

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



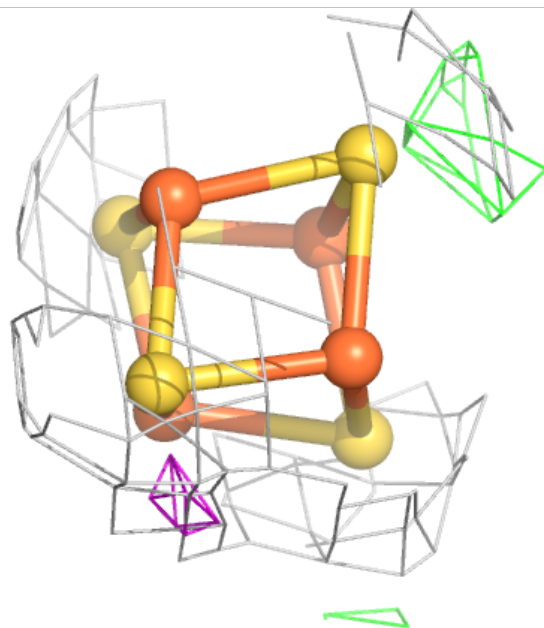
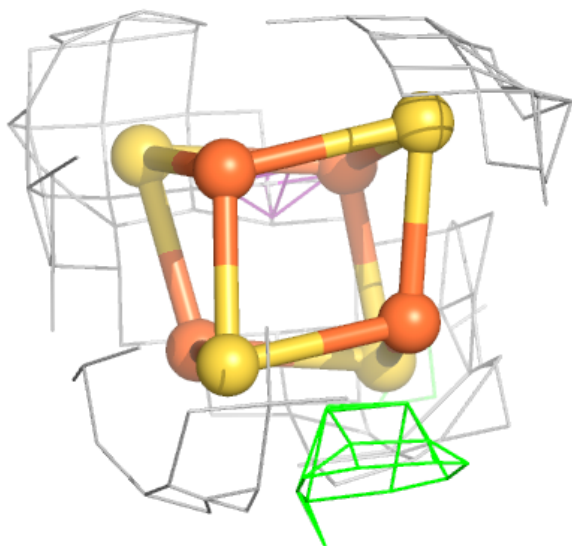
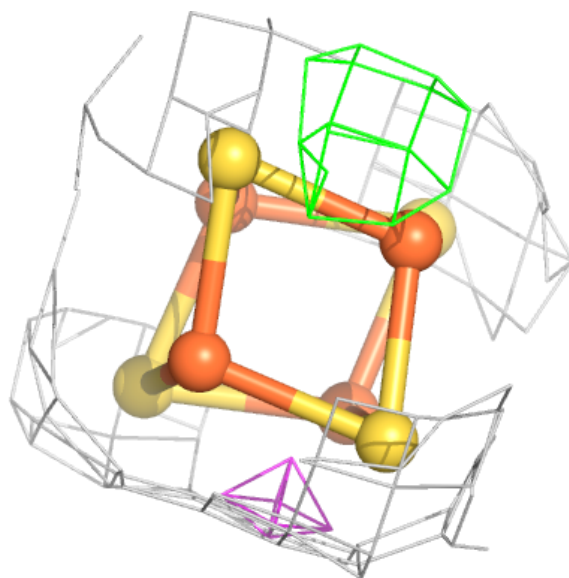
**Electron density around CLA A 819:**

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



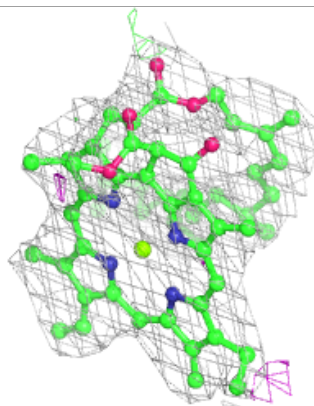
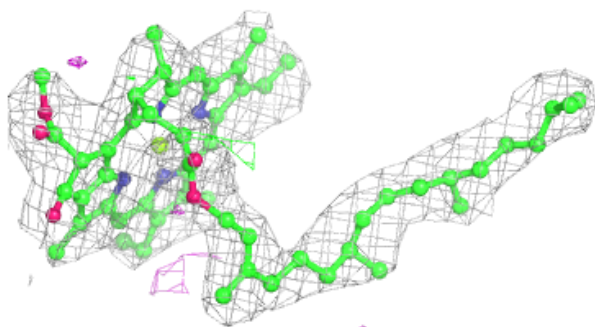
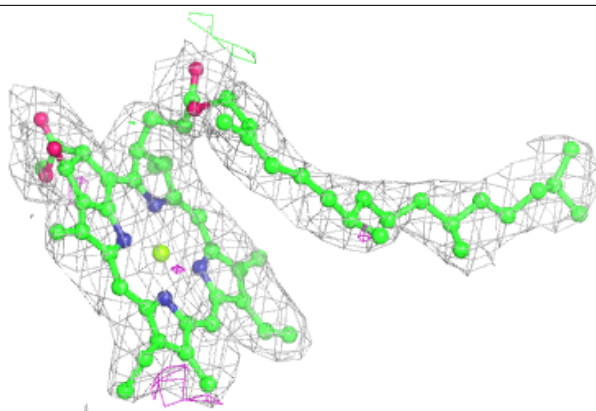
**Electron density around SF4 G 844:**

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

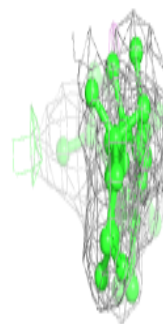
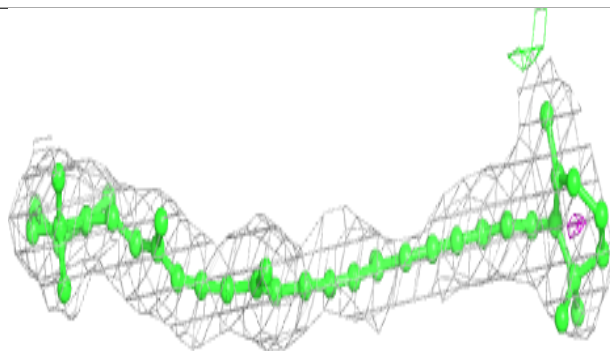
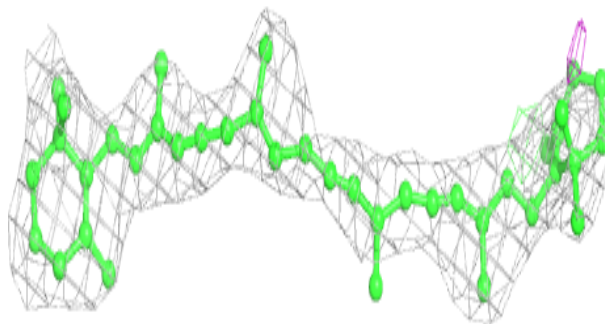


**Electron density around CLA Z 815:**

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

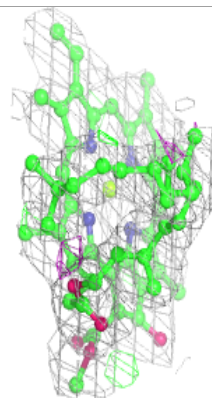
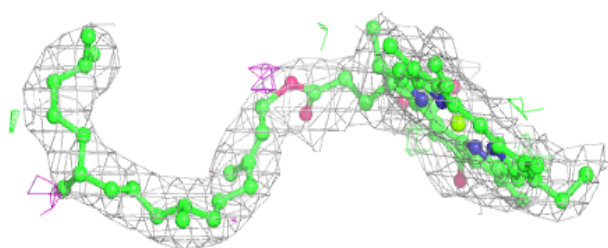
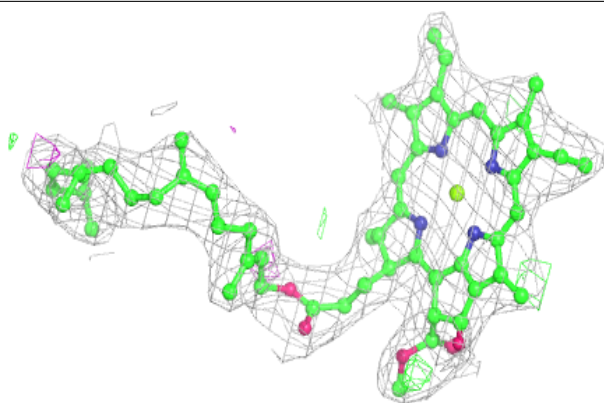
**Electron density around BCR H 850:**

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

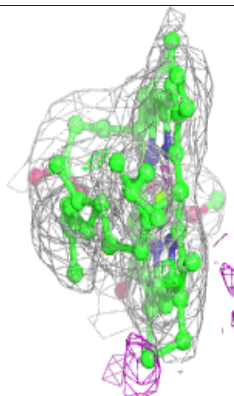
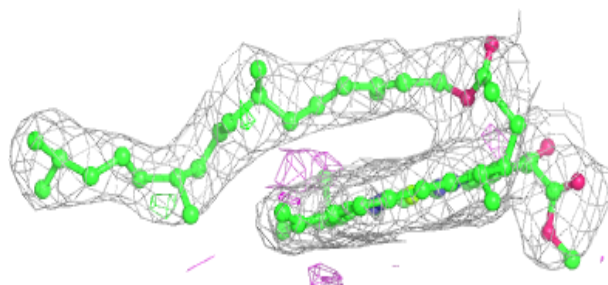
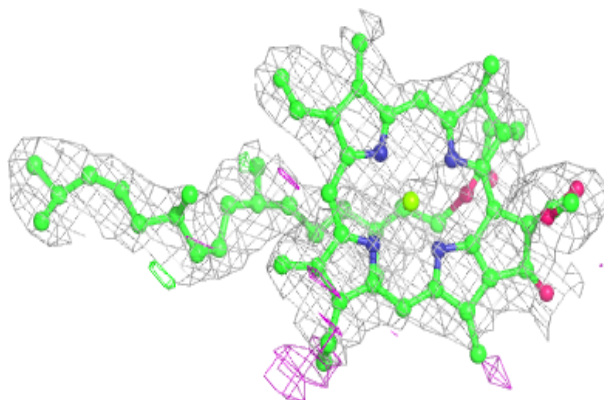


**Electron density around CLA Z 810:**

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

**Electron density around CLA Y 836:**

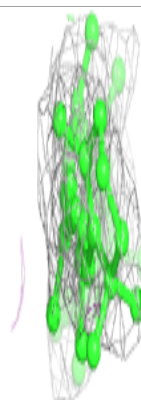
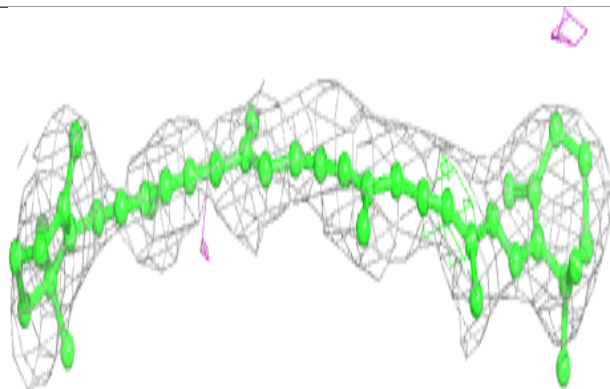
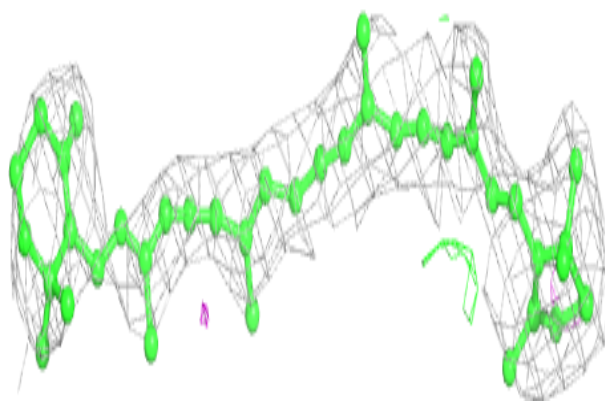
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





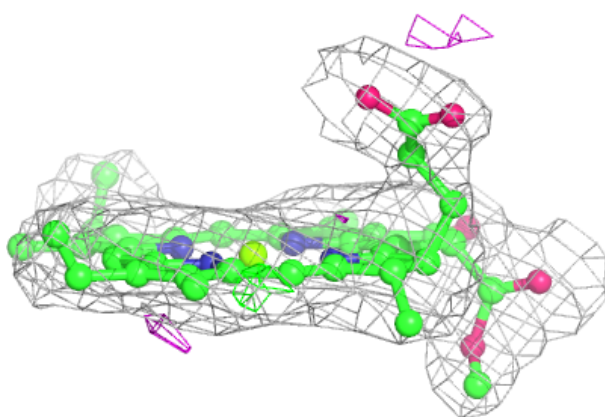
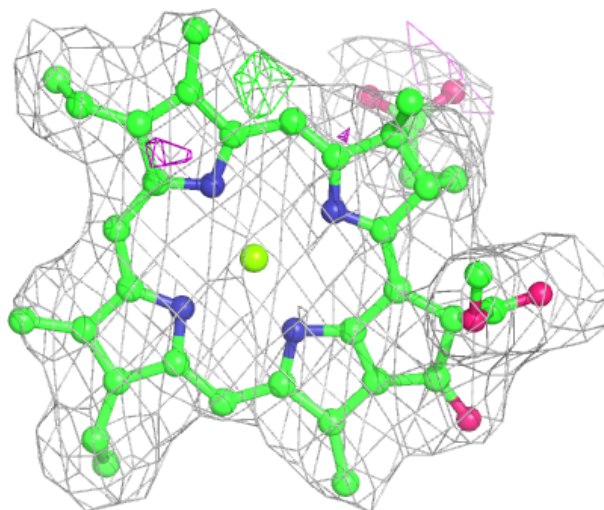
**Electron density around BCR H 842:**

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



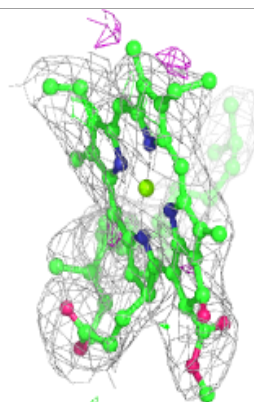
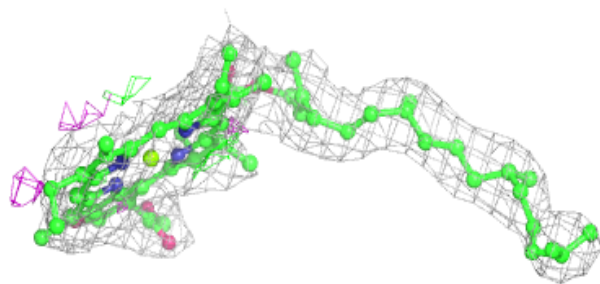
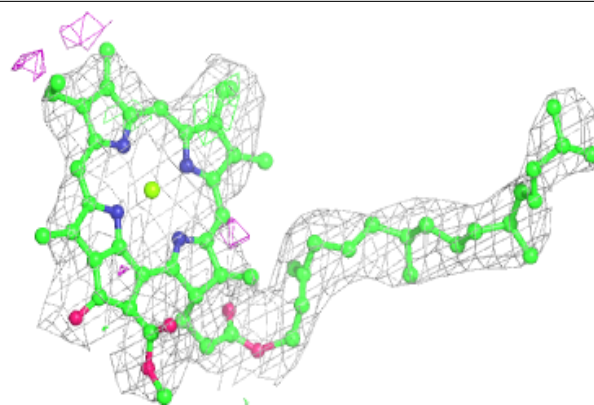
**Electron density around CLA B 829:**

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



**Electron density around CLA Z 801:**

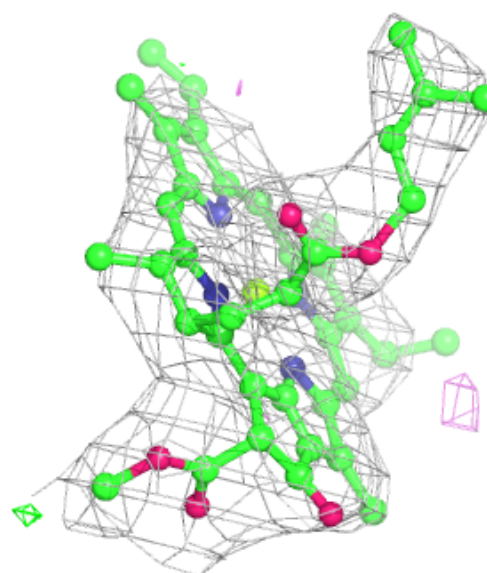
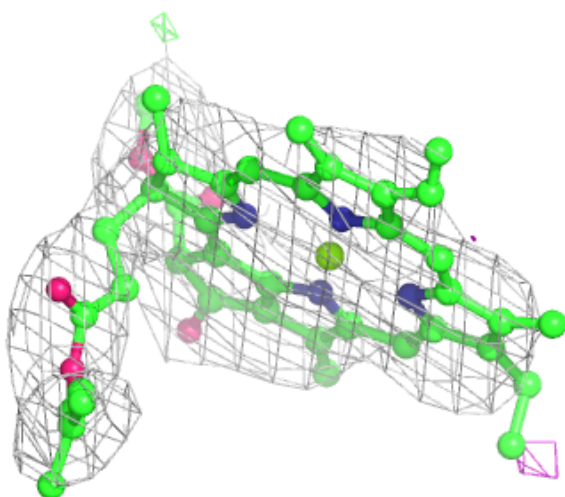
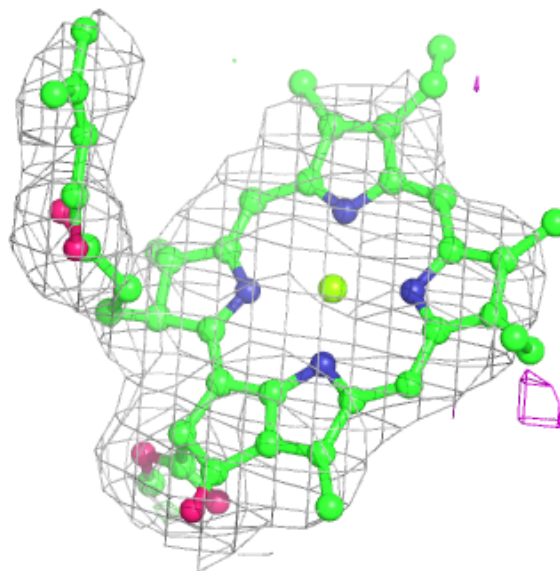
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





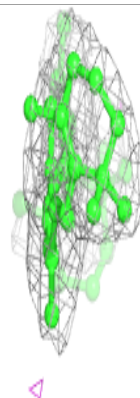
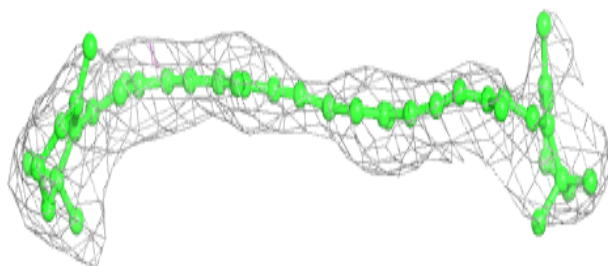
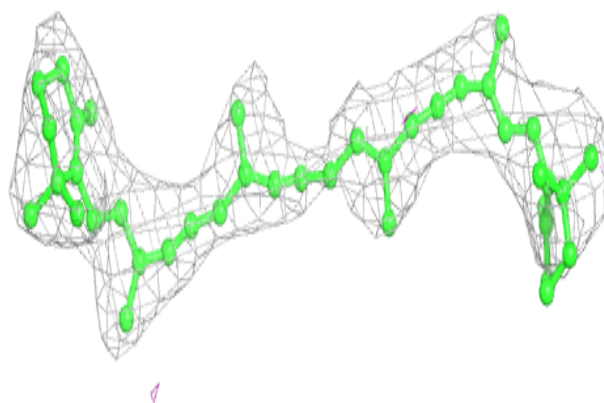
**Electron density around CLA G 815:**

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

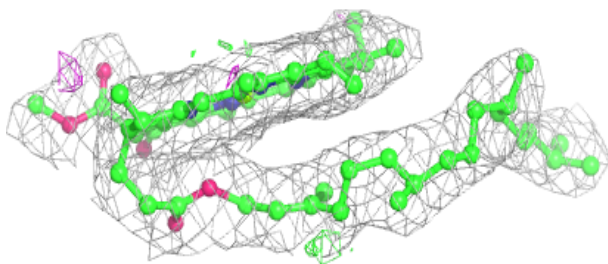
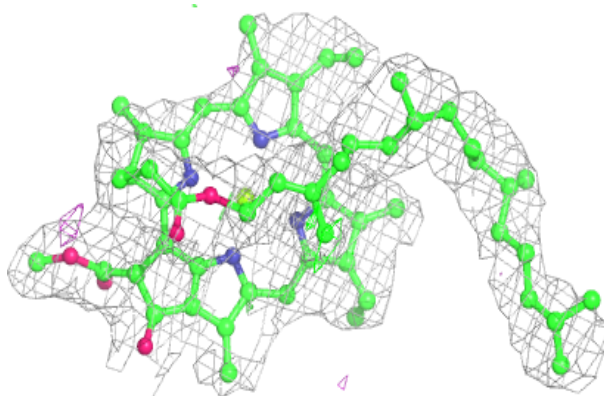


**Electron density around BCR Z 845:**

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

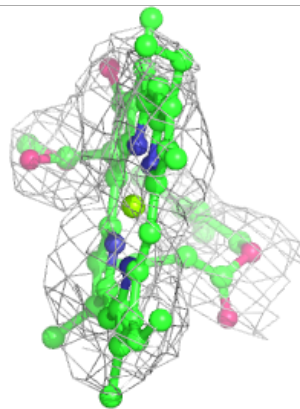
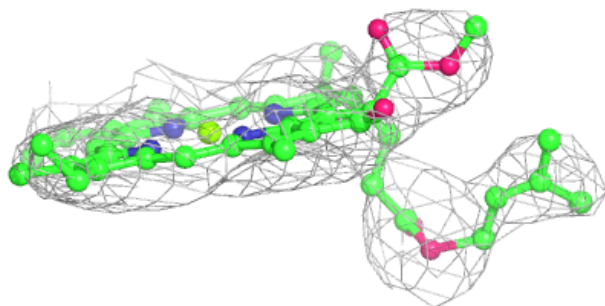
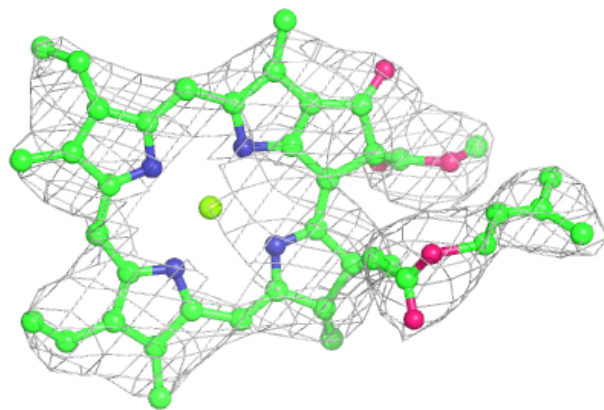
**Electron density around CLA Z 838:**

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



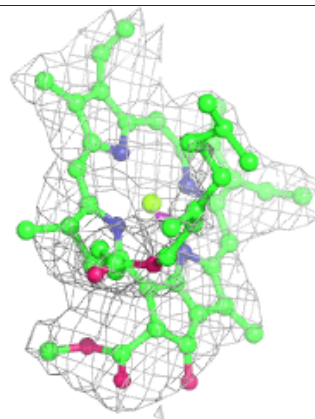
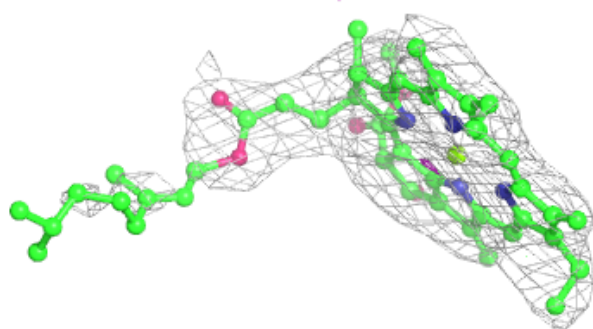
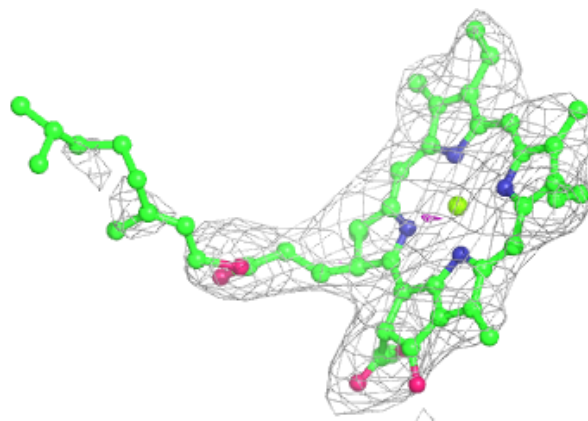
**Electron density around CLA G 816:**

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



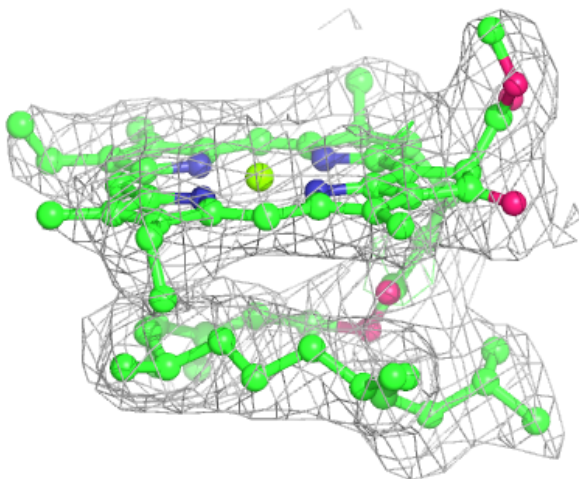
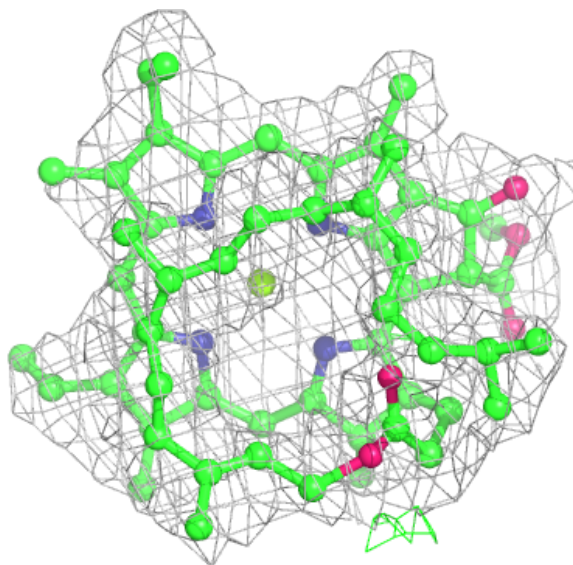
**Electron density around CLA H 832:**

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



**Electron density around CLA U 1002:**

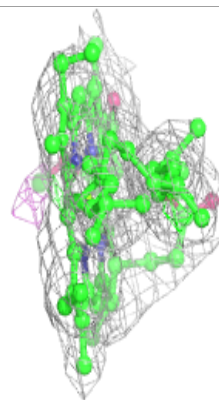
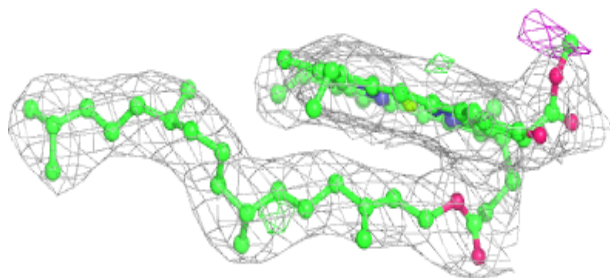
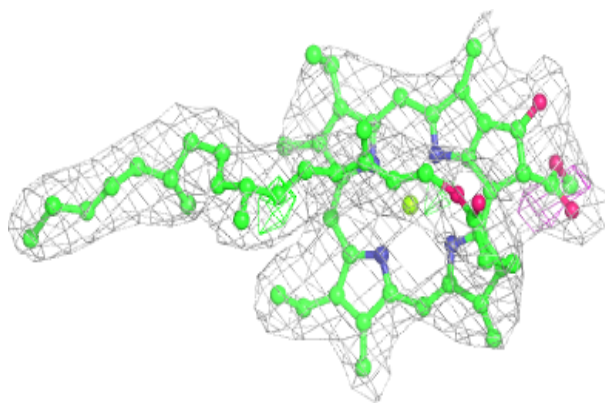
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



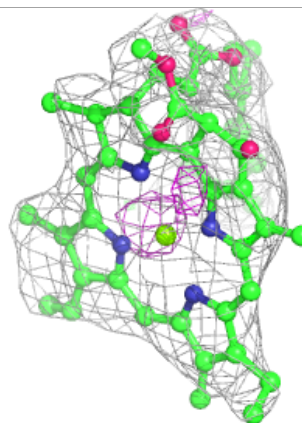
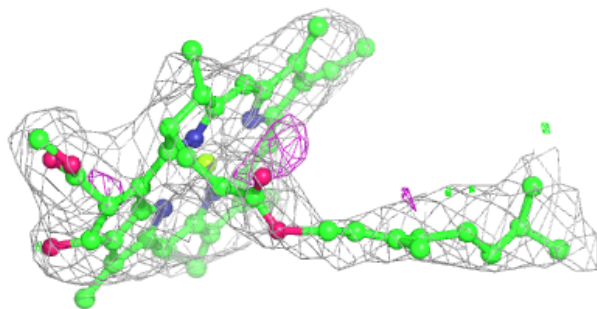
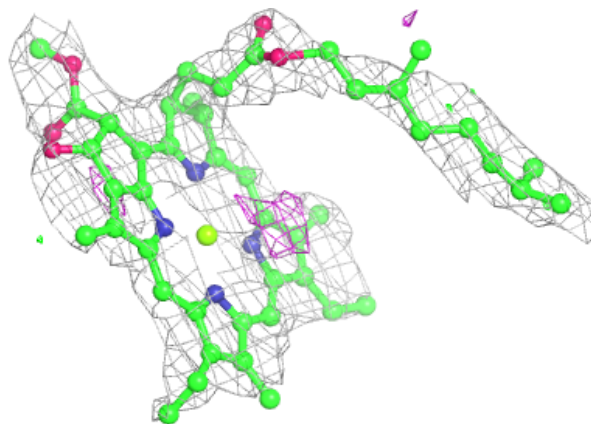


**Electron density around CLA A 837:**

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

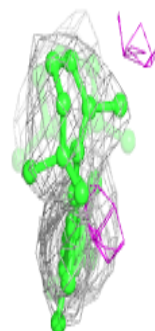
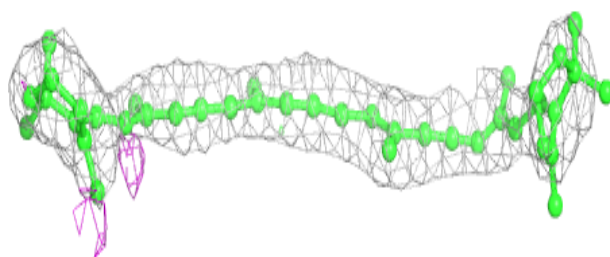
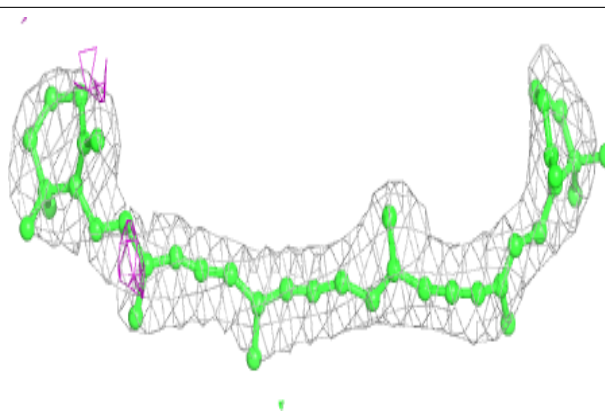
**Electron density around CLA H 816:**

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

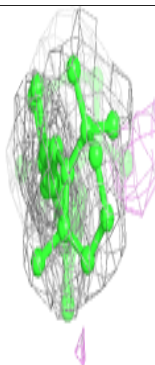
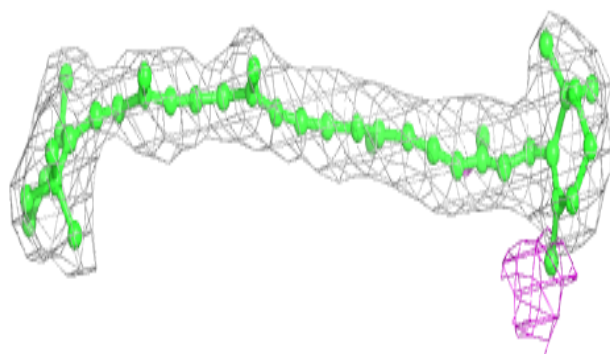
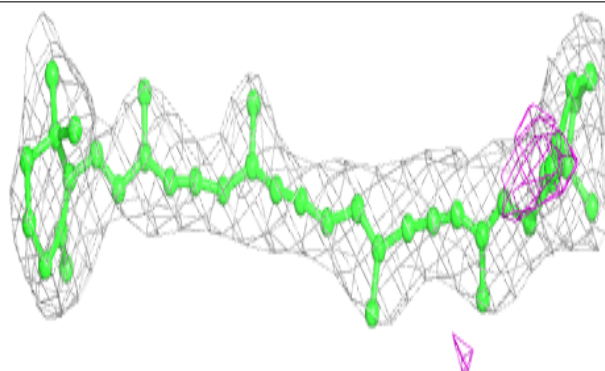


**Electron density around BCR H 843:**

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

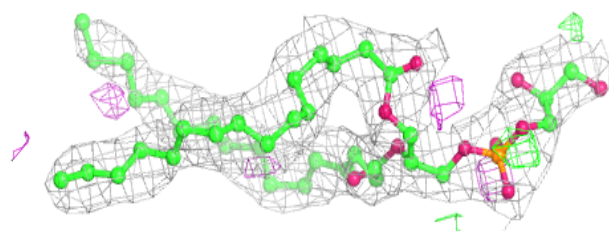
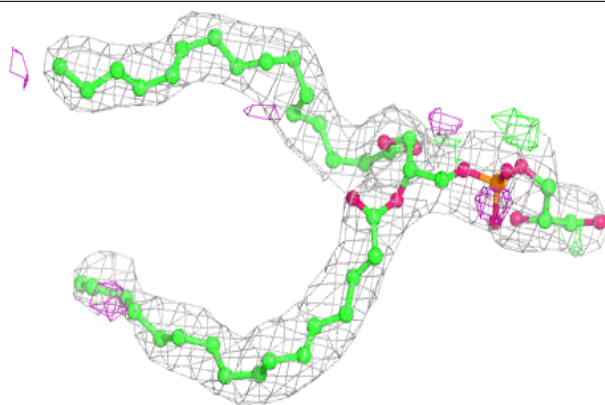
**Electron density around BCR Y 852:**

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

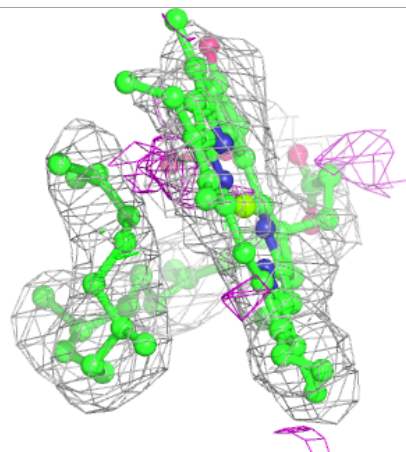
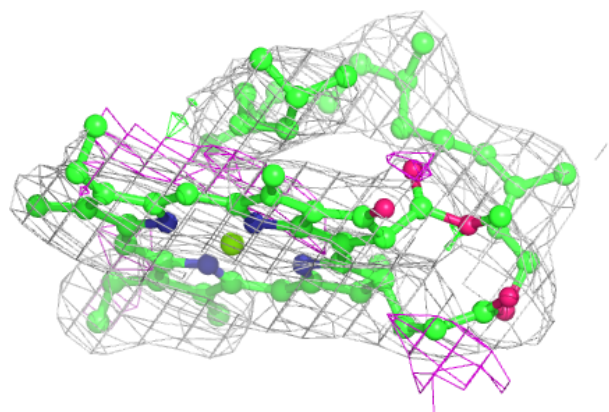
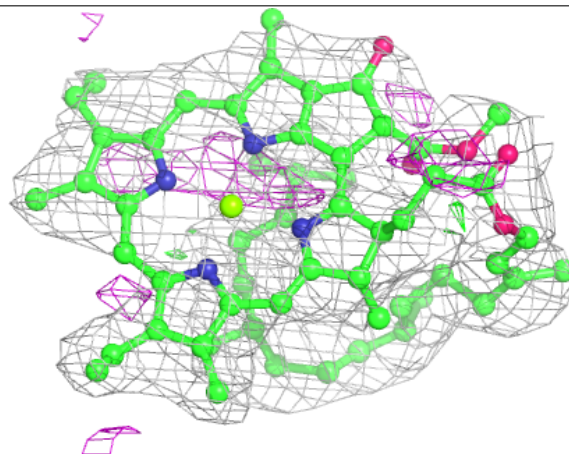


**Electron density around LHG A 852:**

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

**Electron density around CLA A 807:**

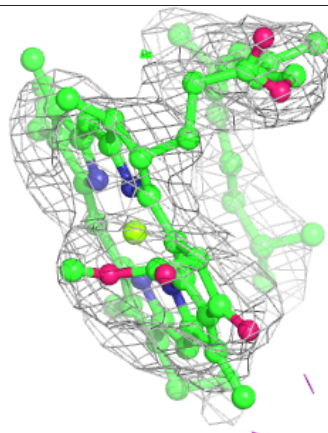
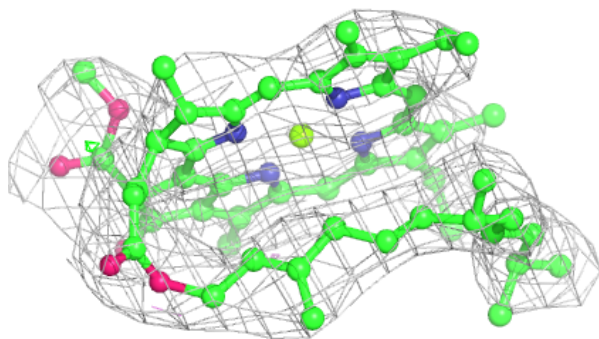
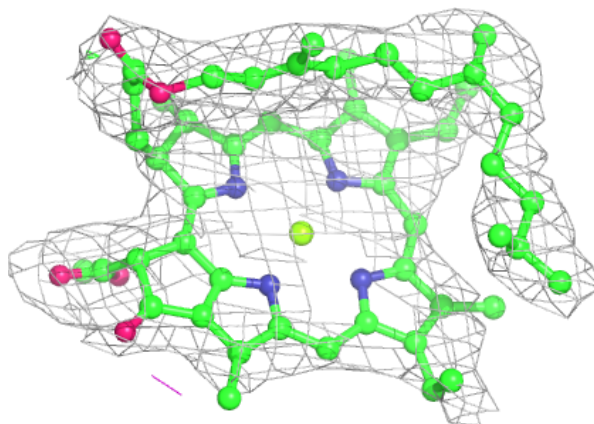
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





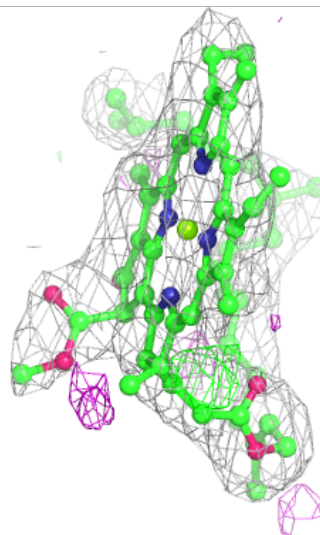
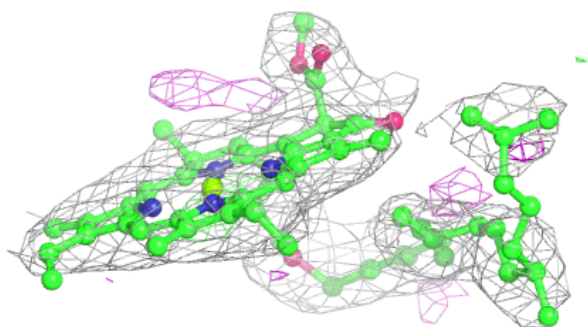
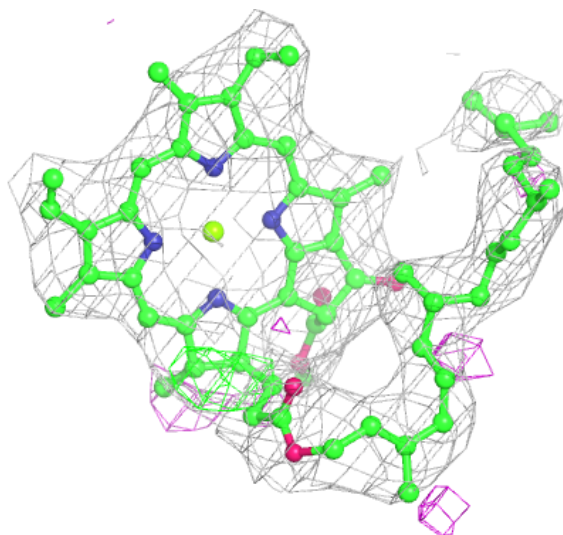
**Electron density around CLA G 820:**

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



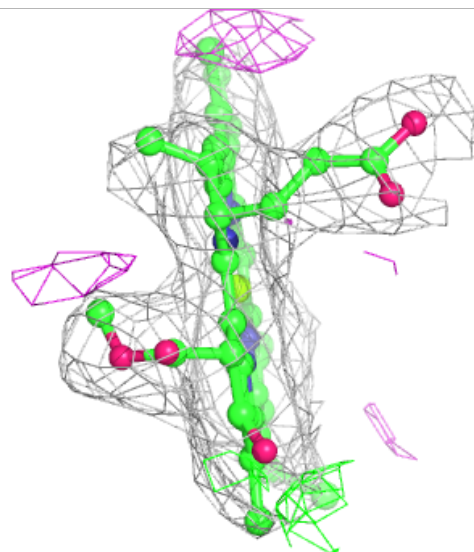
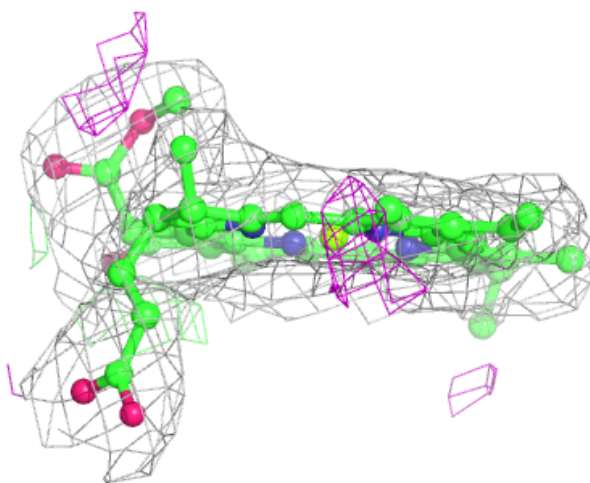
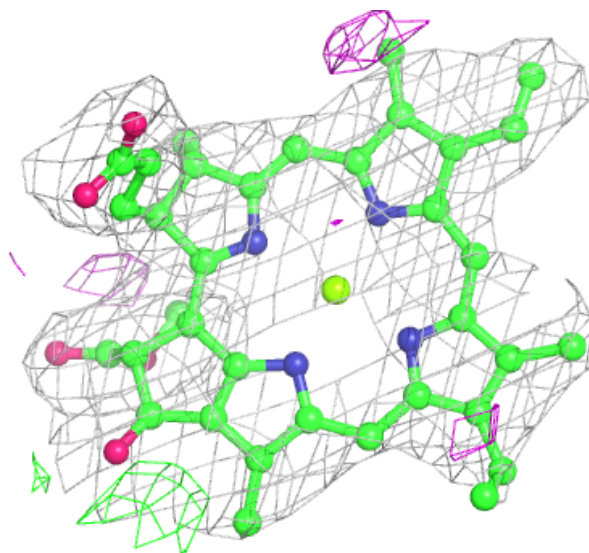
**Electron density around CLA d 201:**

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



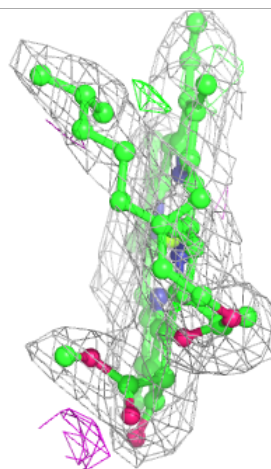
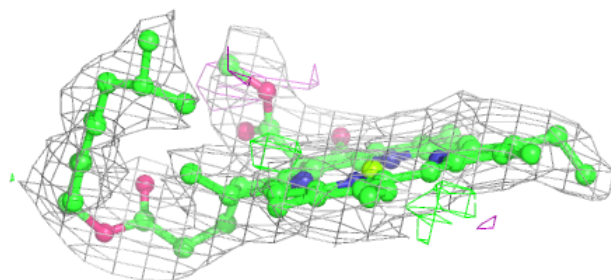
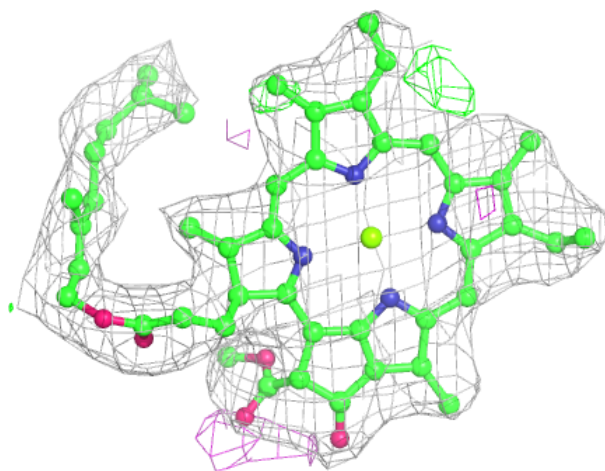
**Electron density around CLA Z 834:**

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



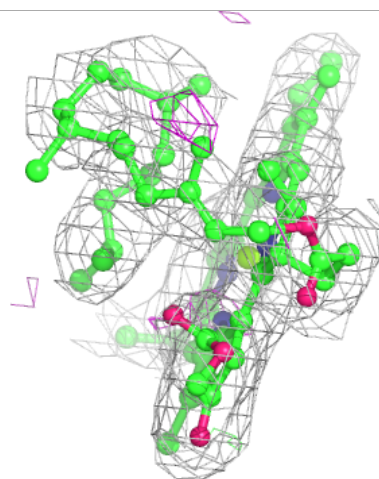
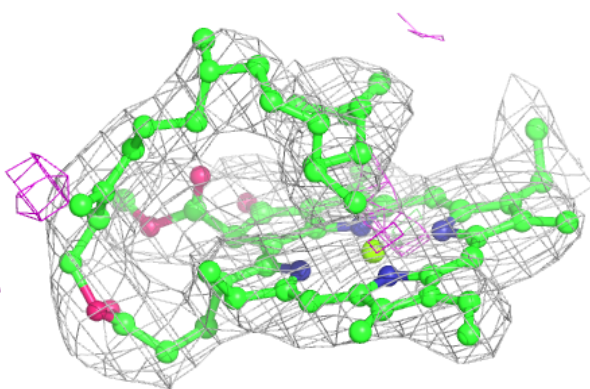
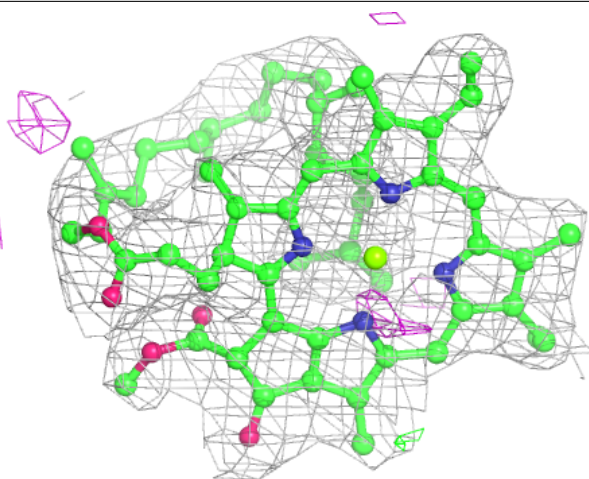
**Electron density around CLA H 824:**

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



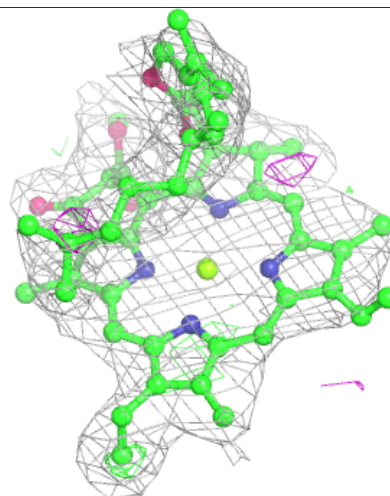
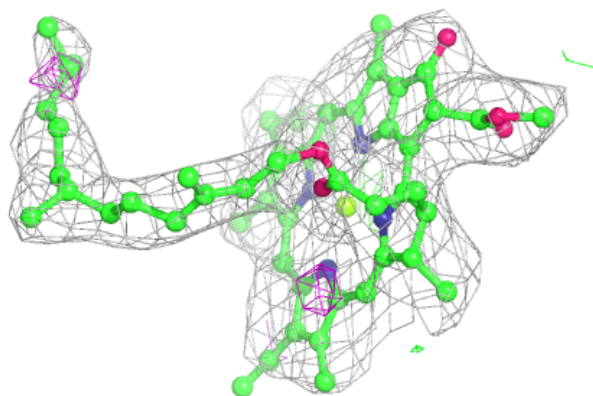
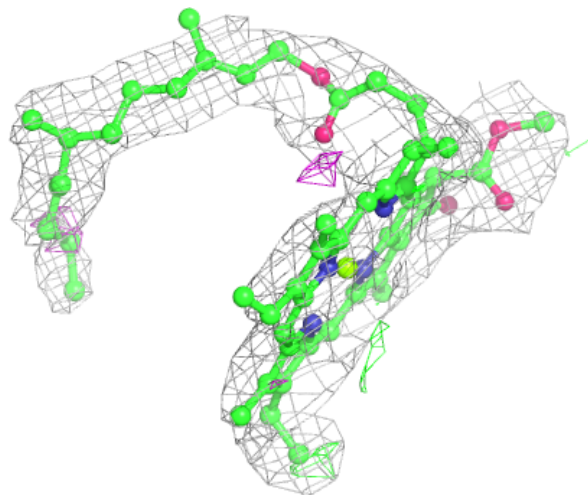
**Electron density around CLA B 805:**

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



**Electron density around CLA H 819:**

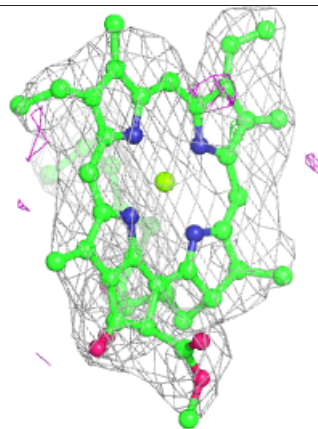
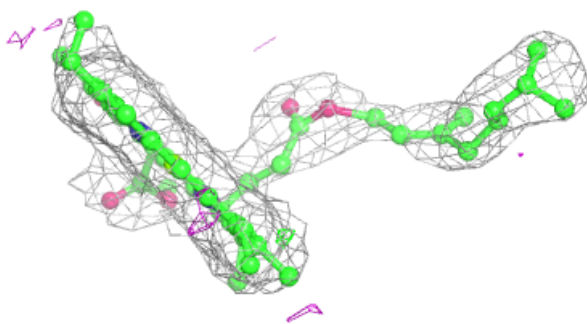
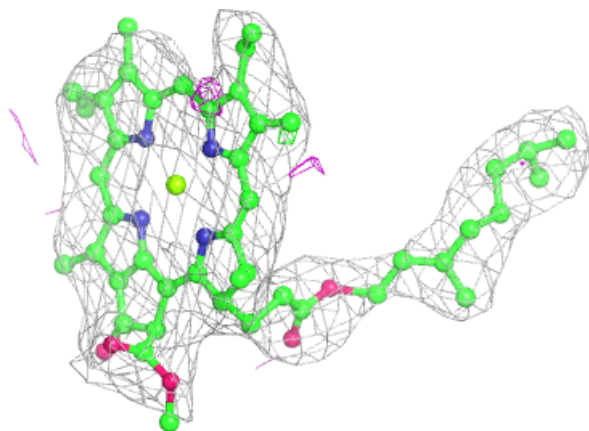
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





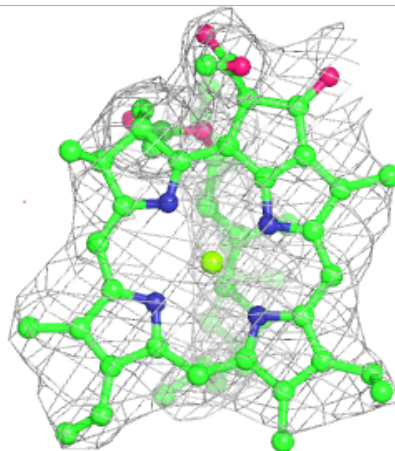
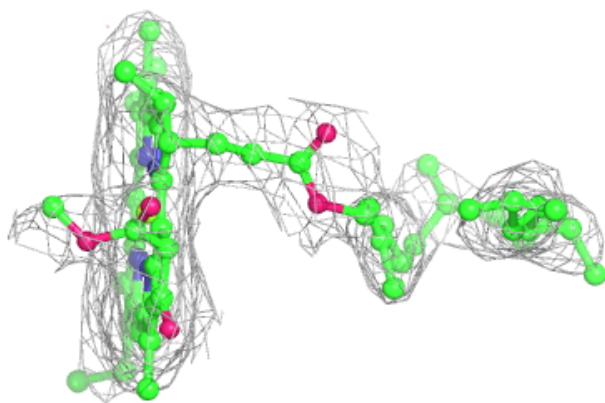
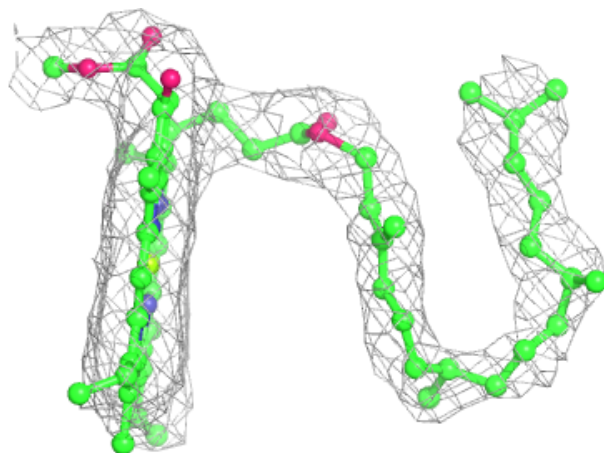
**Electron density around CLA A 834:**

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



**Electron density around CLA B 813:**

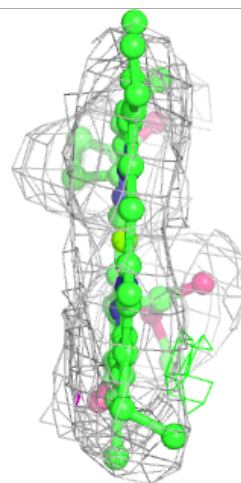
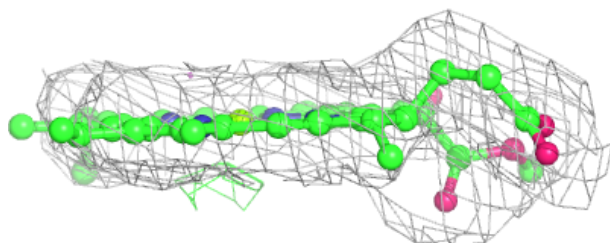
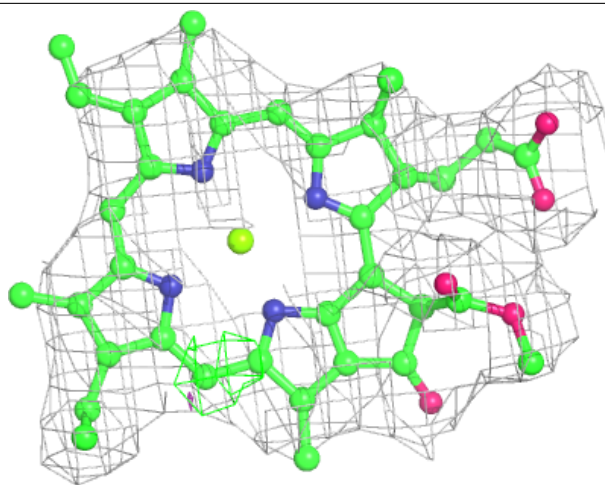
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





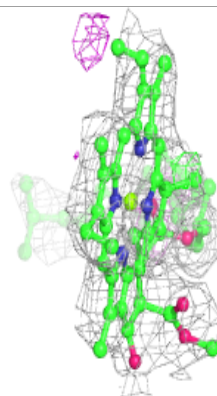
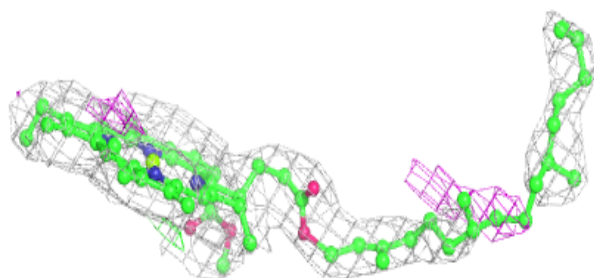
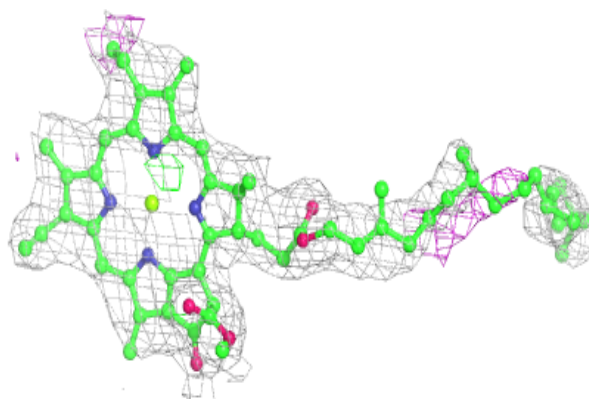
**Electron density around CLA F 202:**

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

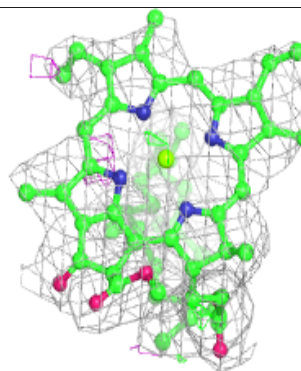
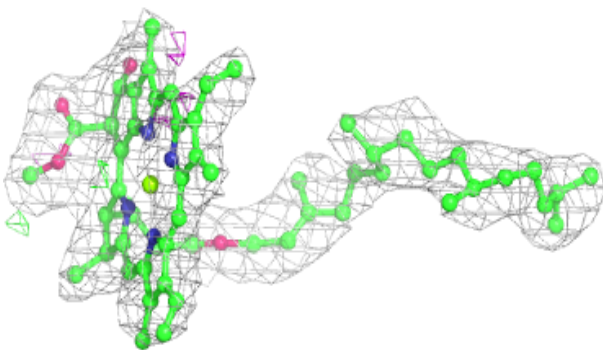
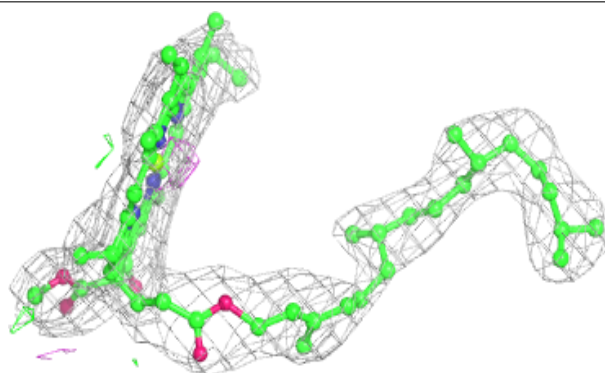


**Electron density around CLA Y 805:**

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

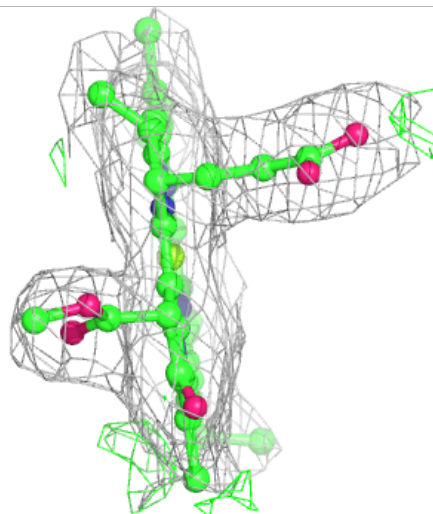
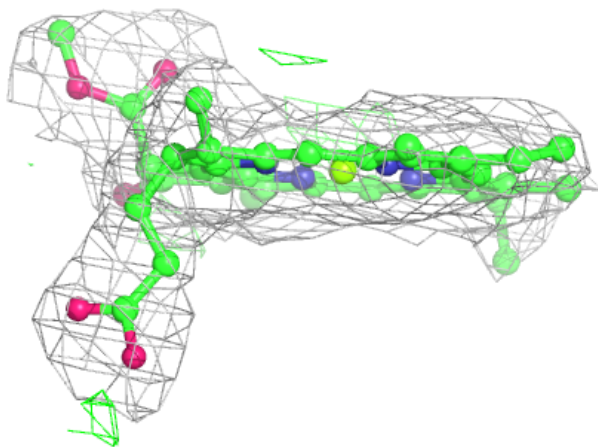
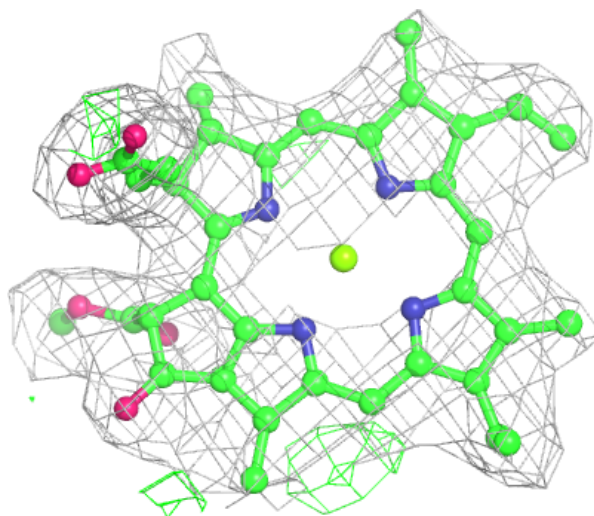
**Electron density around CLA G 830:**

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



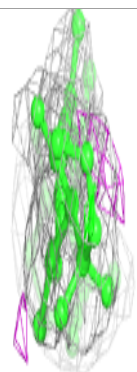
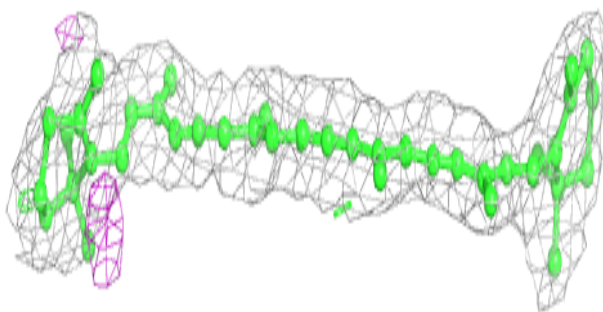
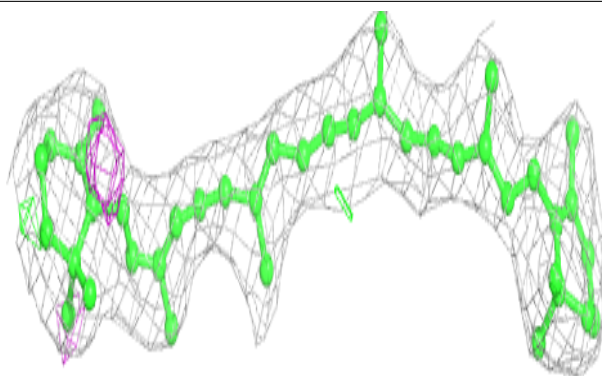
**Electron density around CLA H 838:**

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

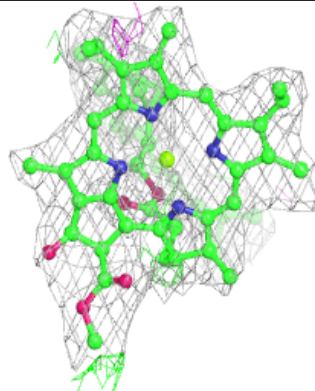
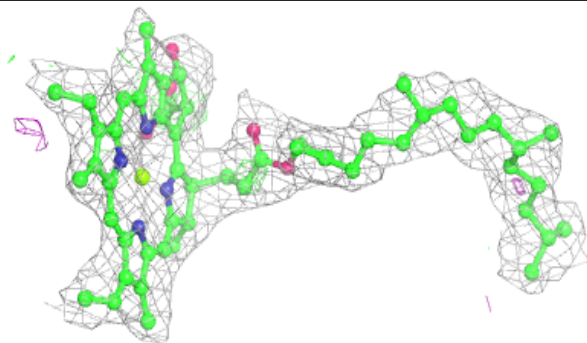
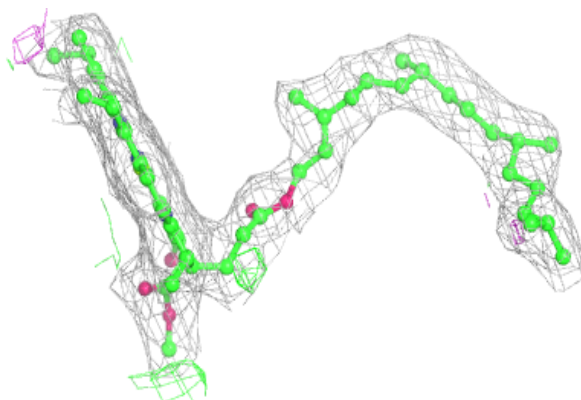


**Electron density around BCR Z 847:**

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

**Electron density around CLA B 839:**

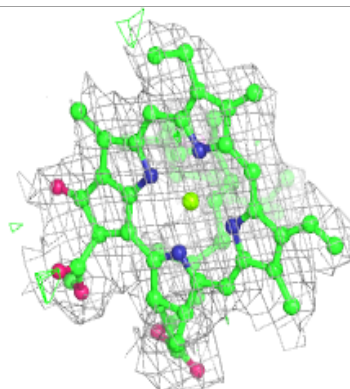
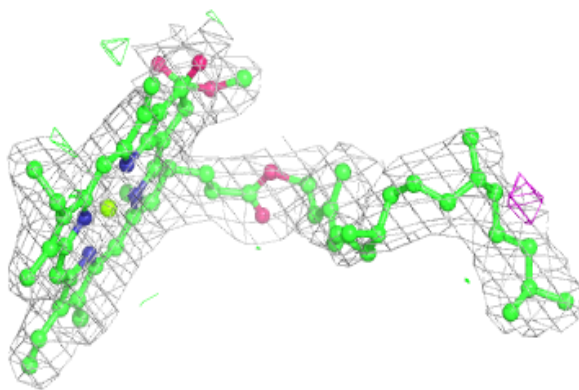
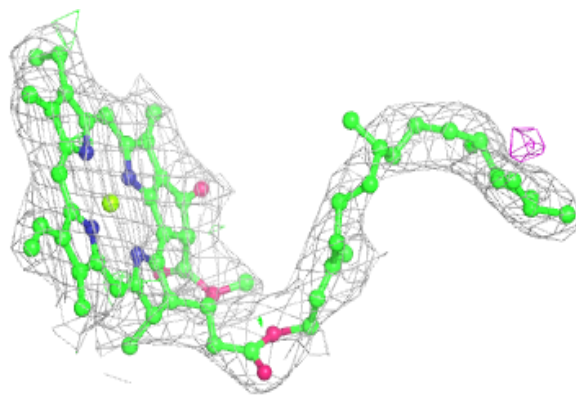
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



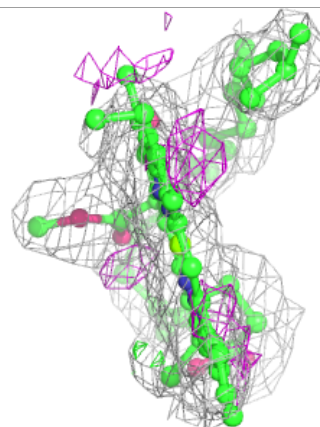
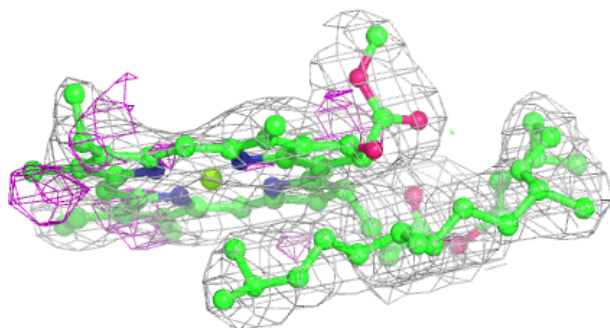
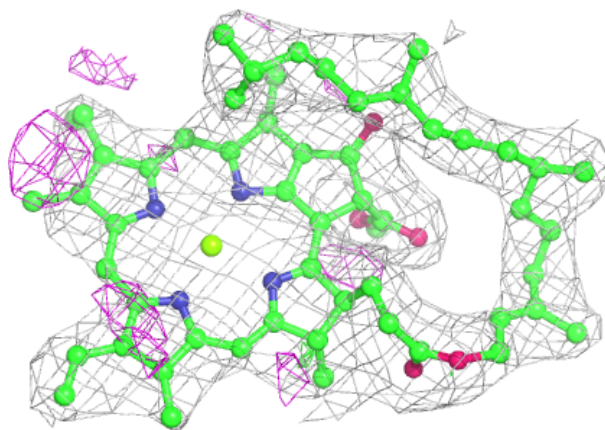


**Electron density around CLA H 803:**

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

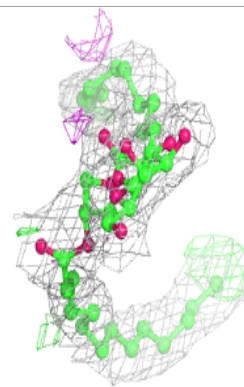
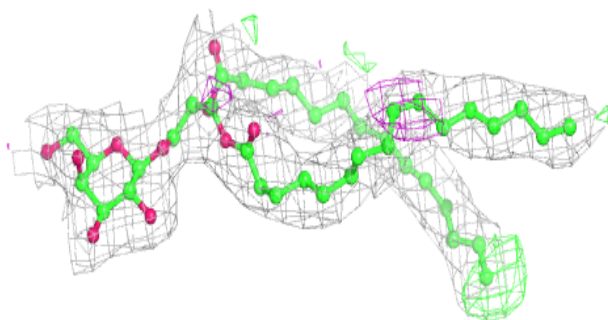
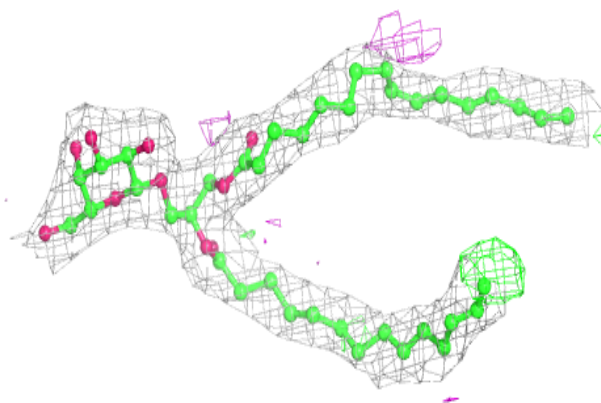
**Electron density around CLA Z 806:**

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

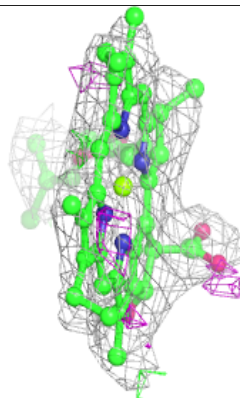
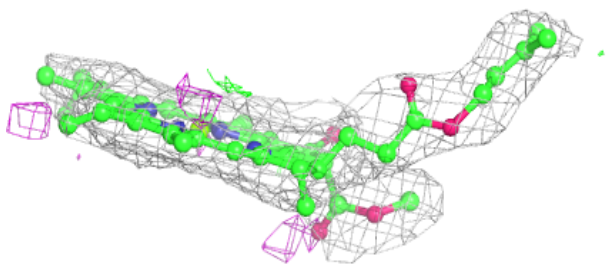
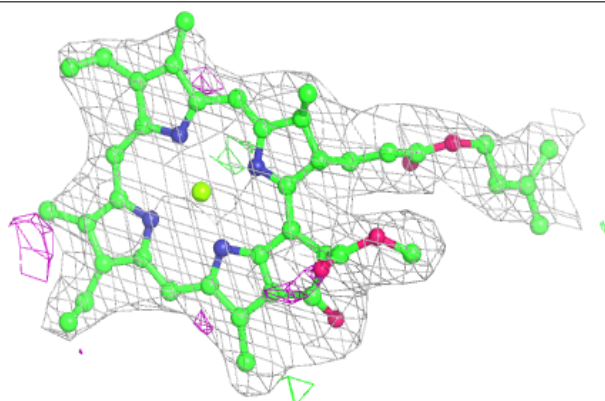


**Electron density around LMG Z 849:**

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

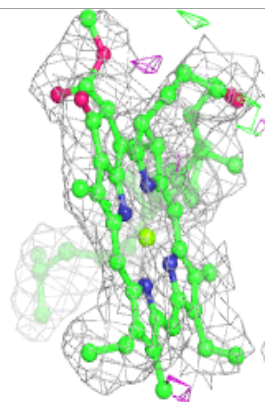
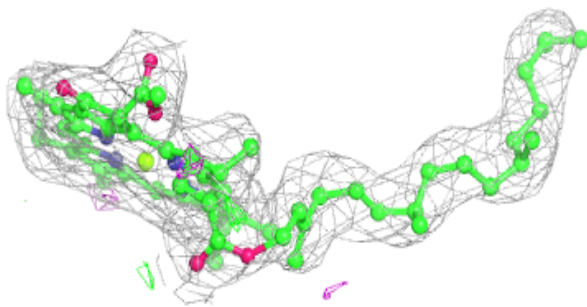
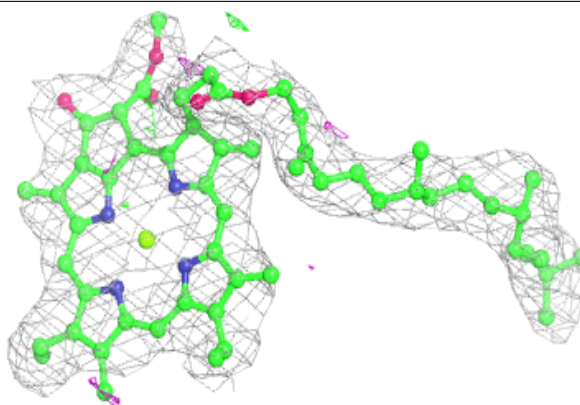
**Electron density around CLA G 839:**

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

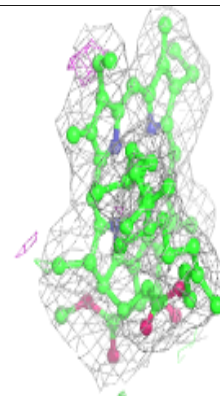
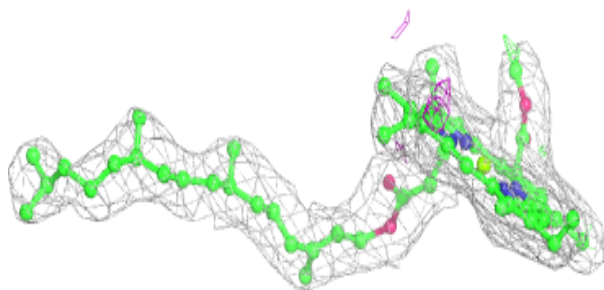
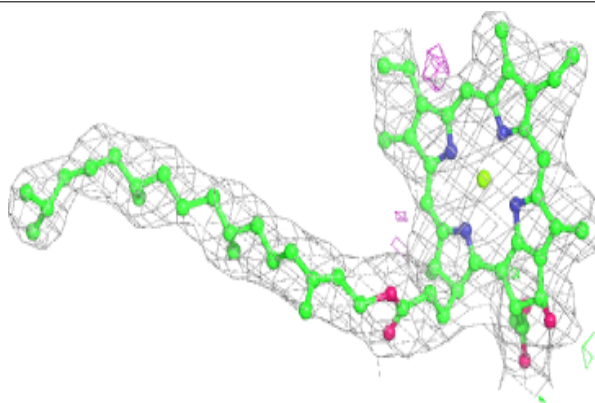


**Electron density around CLA A 802:**

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

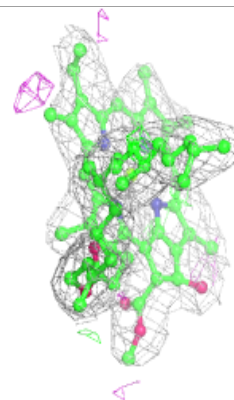
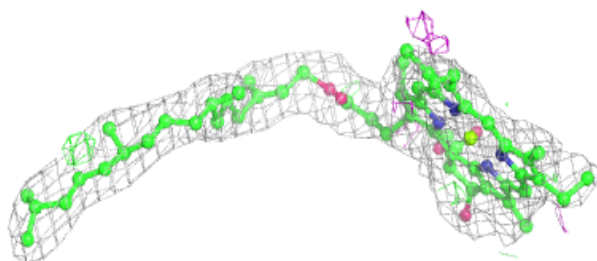
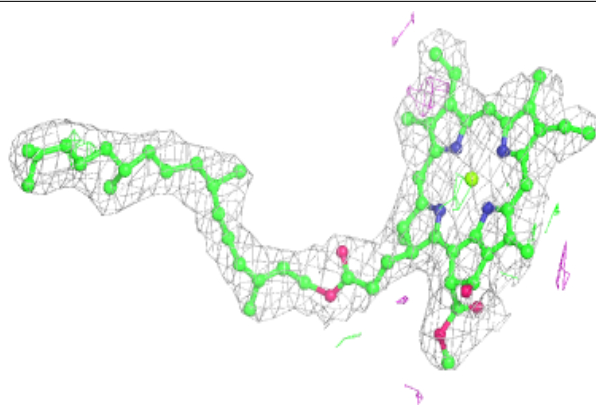
**Electron density around CLA U 1007:**

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



**Electron density around CLA Y 802:**

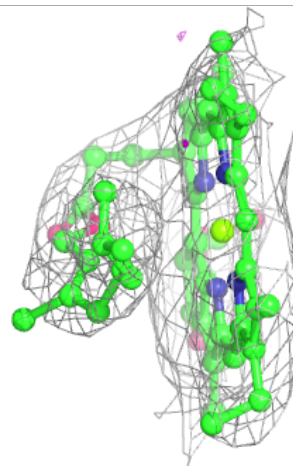
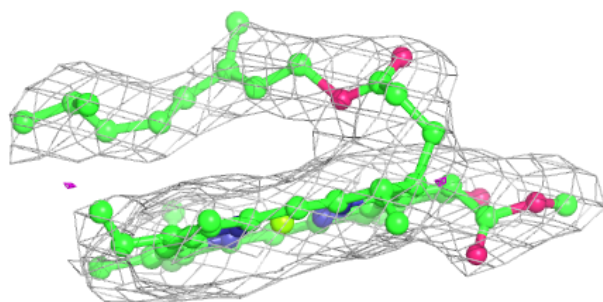
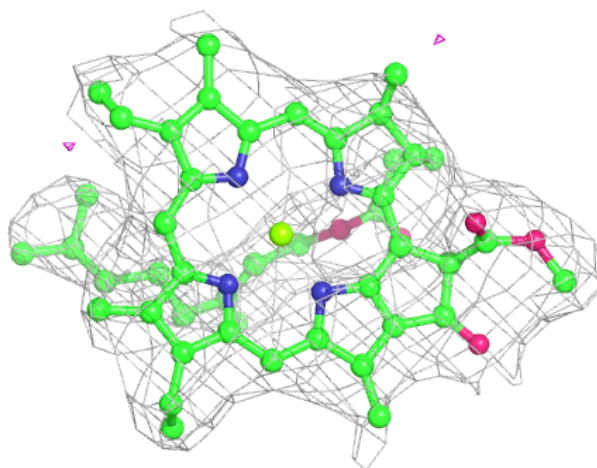
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





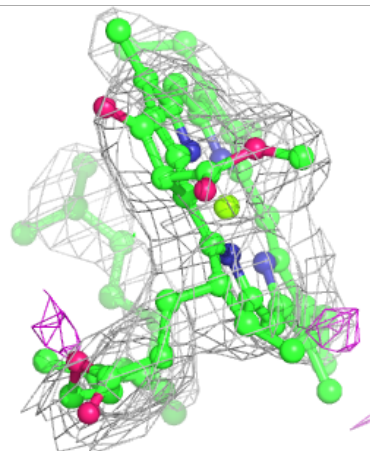
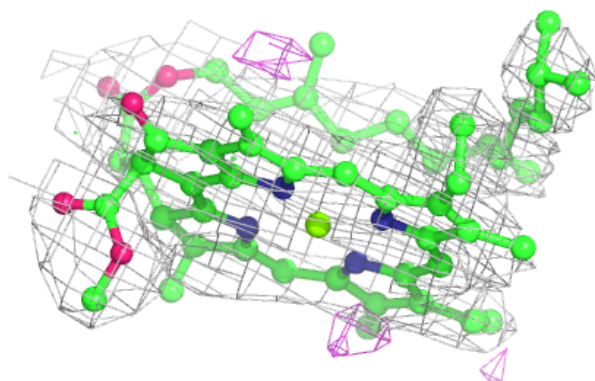
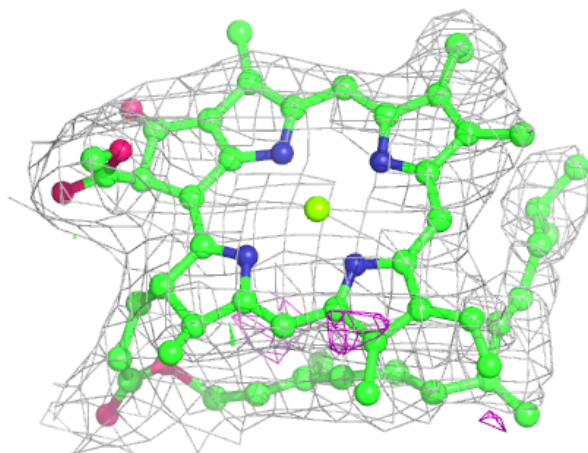
**Electron density around CLA B 821:**

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



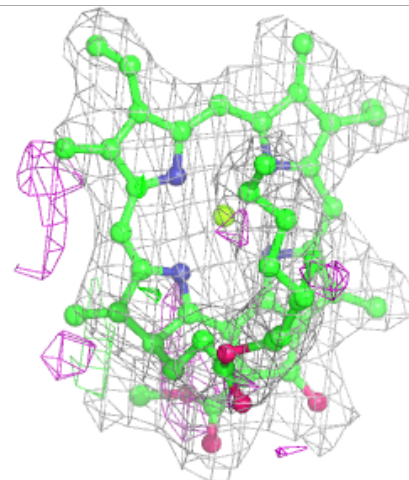
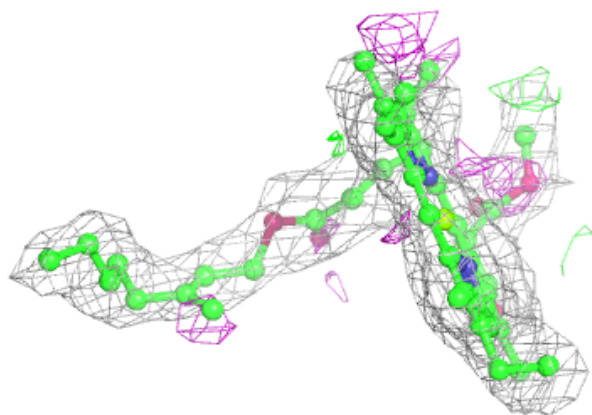
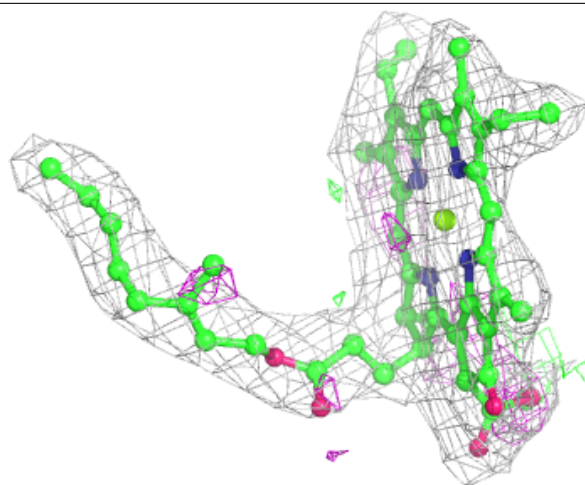
**Electron density around CLA A 821:**

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



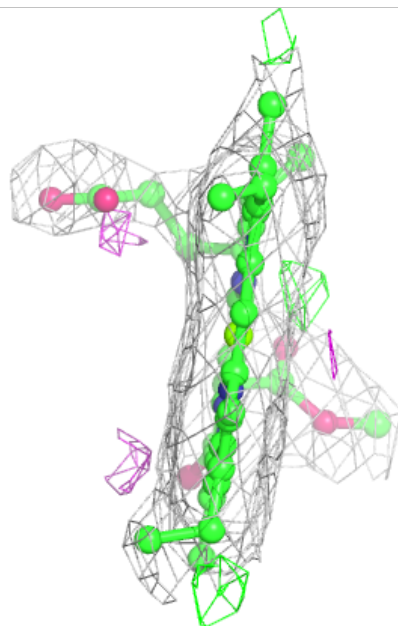
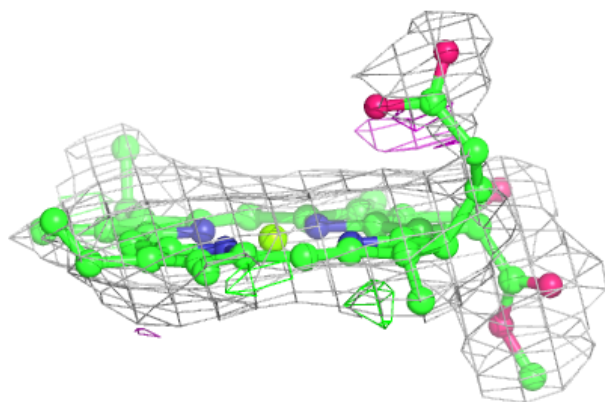
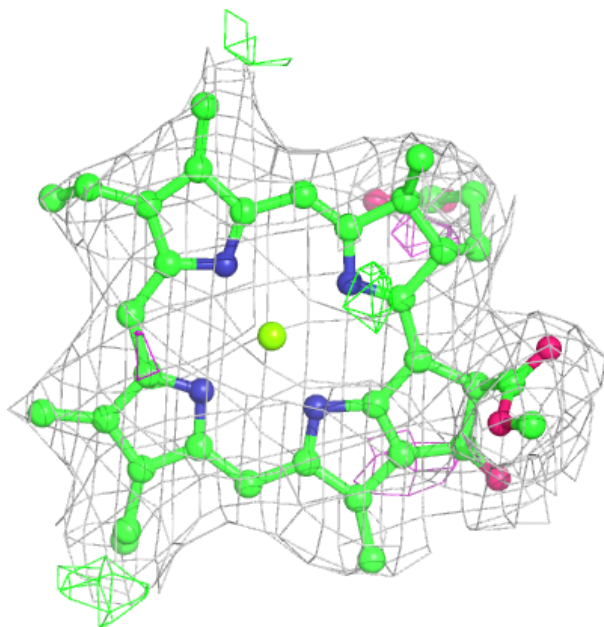
**Electron density around CLA H 804:**

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



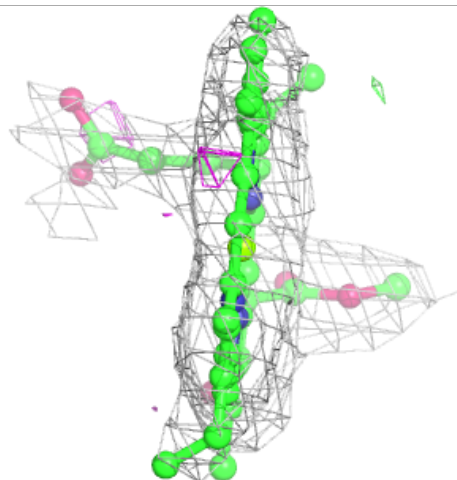
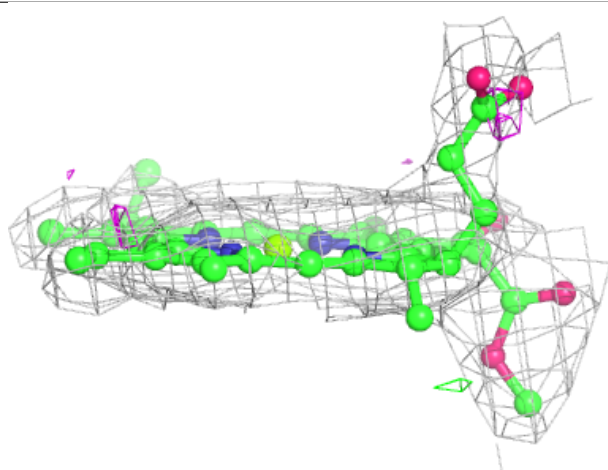
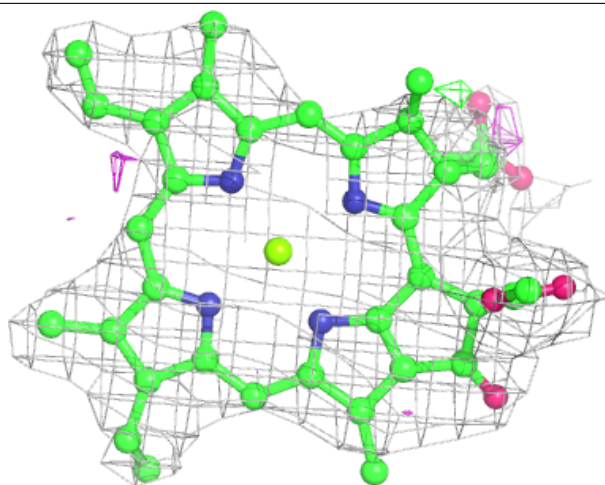
**Electron density around CLA Z 821:**

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



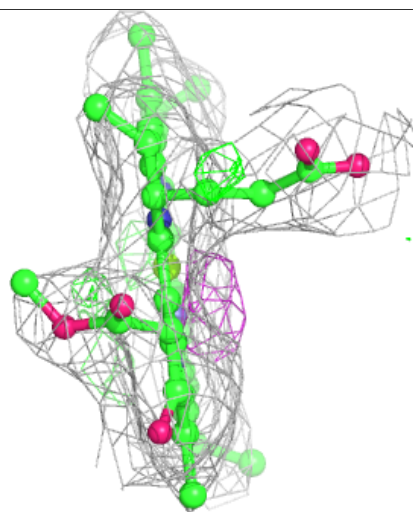
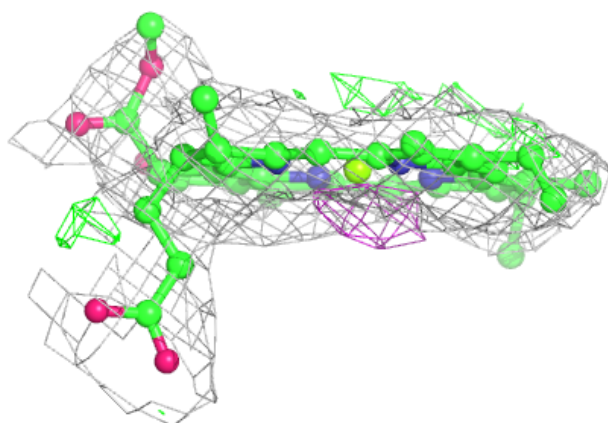
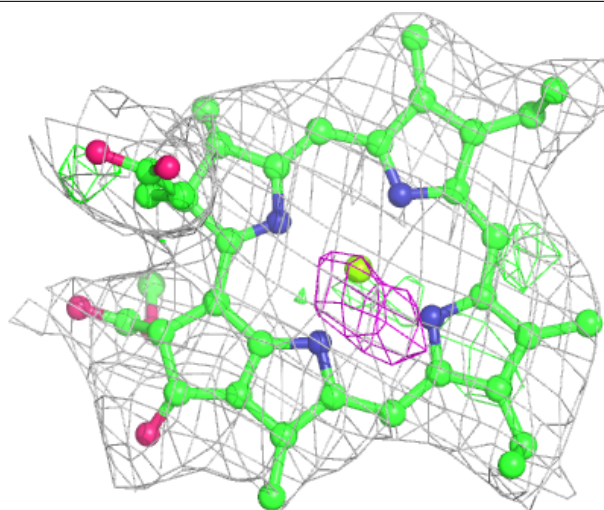
**Electron density around CLA B 819:**

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



**Electron density around CLA H 821:**

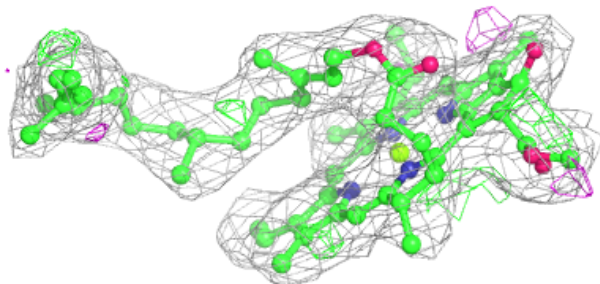
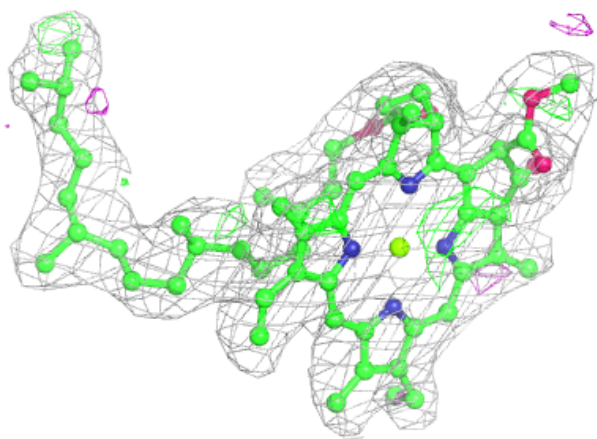
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



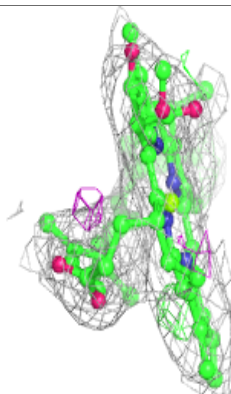
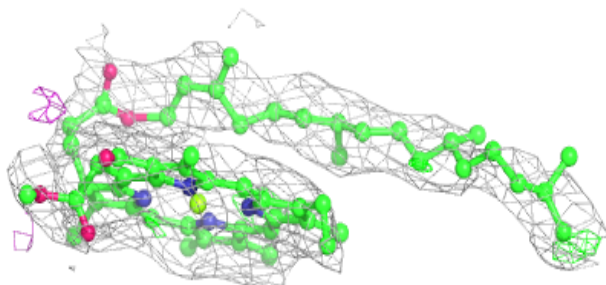
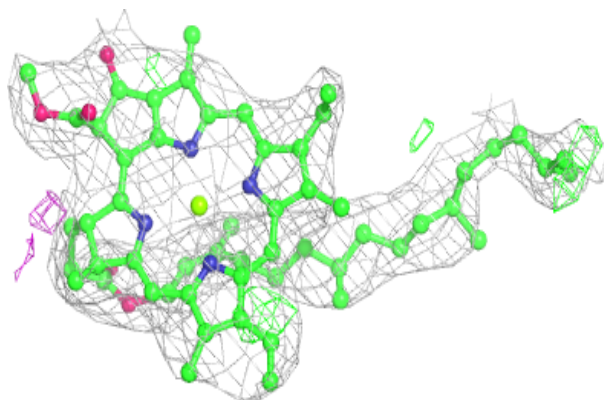


**Electron density around CLA A 842:**

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

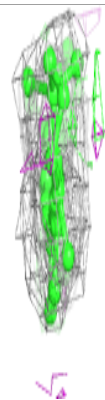
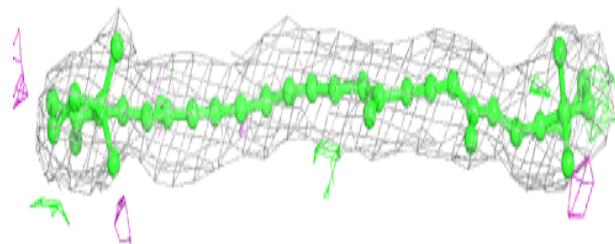
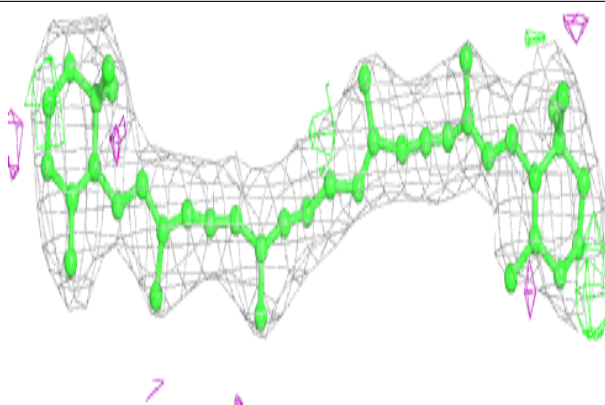
**Electron density around CLA Y 818:**

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



**Electron density around BCR U 1005:**

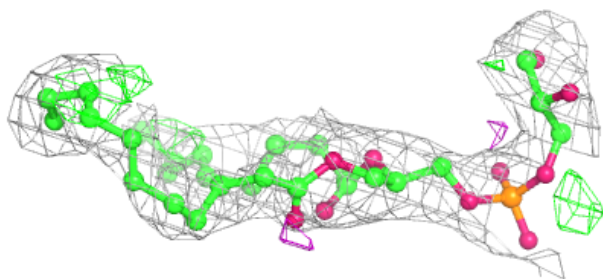
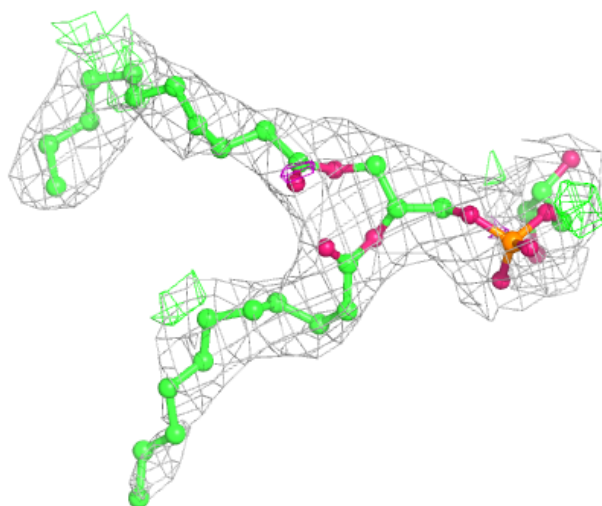
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





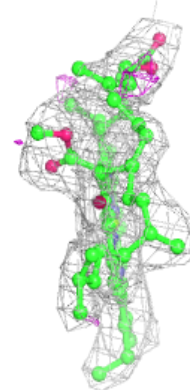
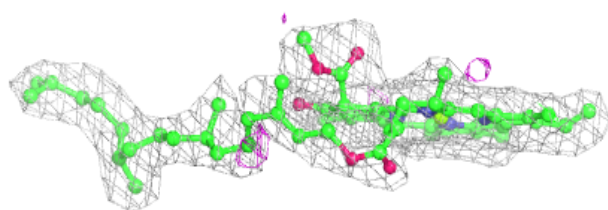
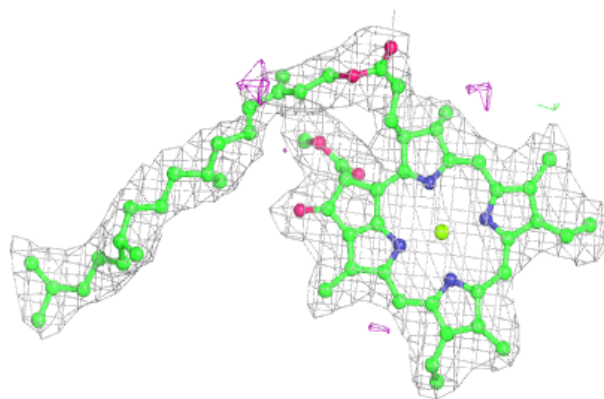
**Electron density around LHG B 849:**

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



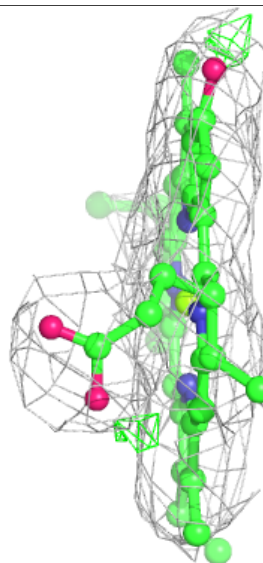
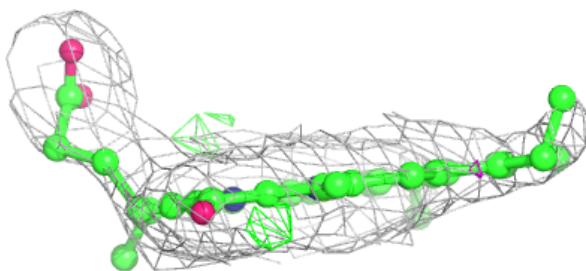
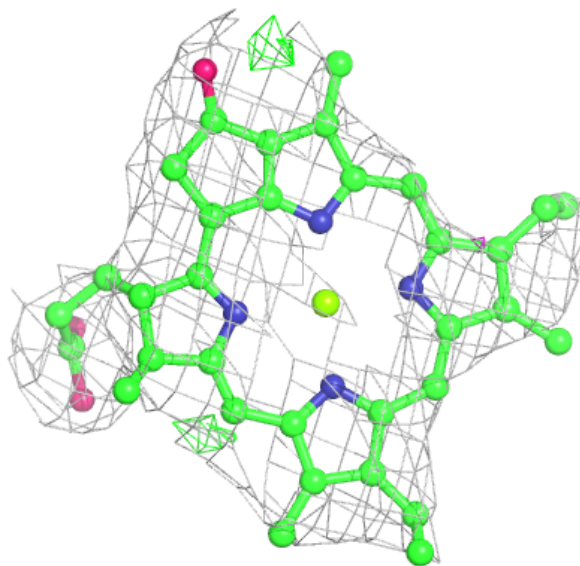
**Electron density around CLA L 206:**

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



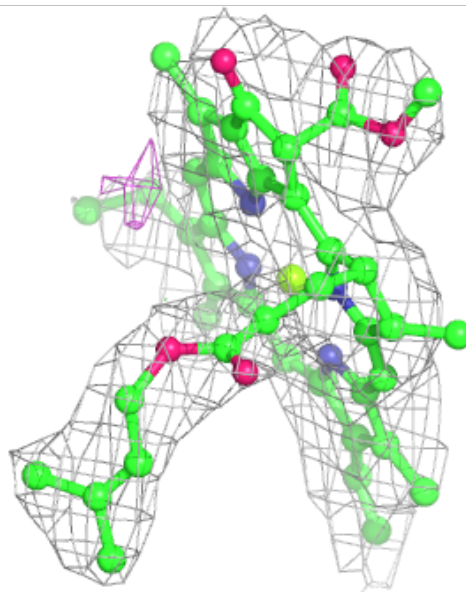
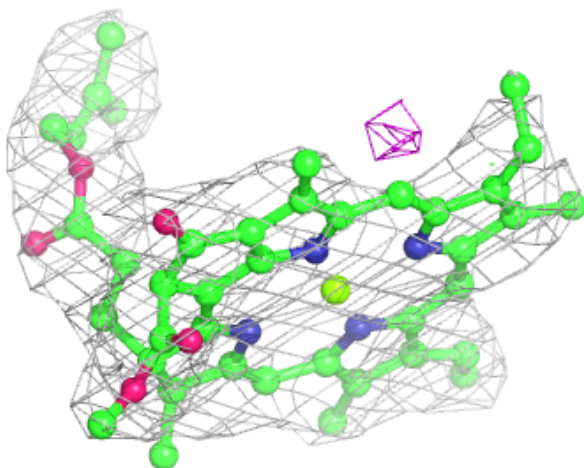
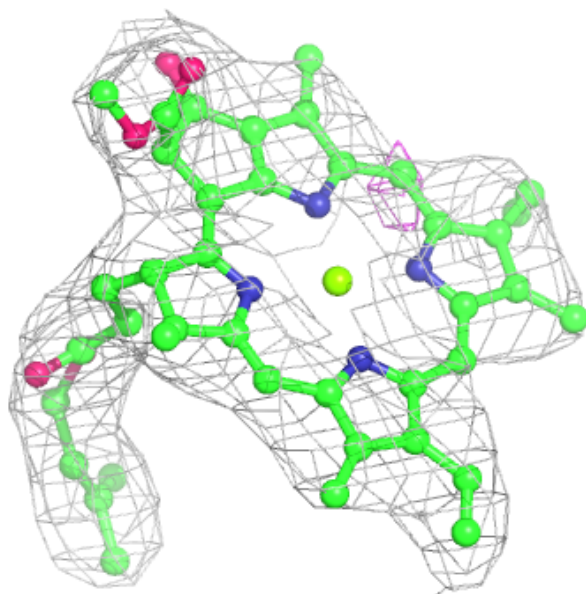
**Electron density around CLA T 101:**

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



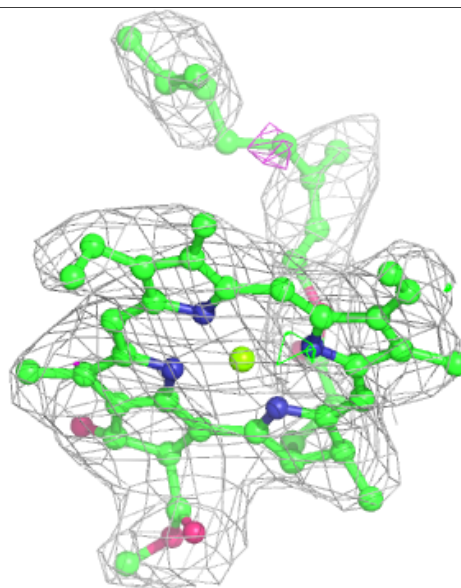
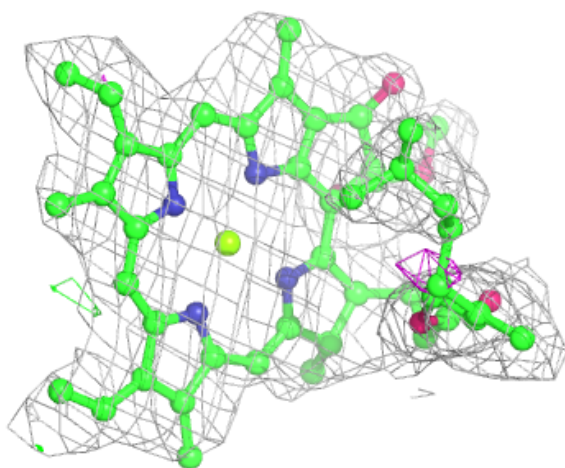
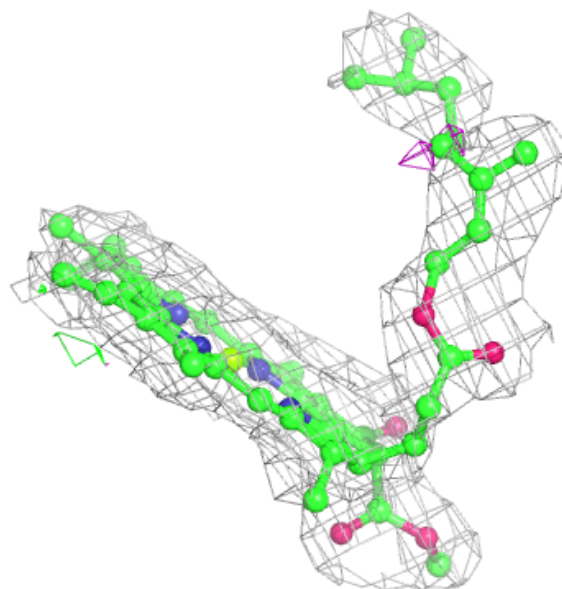
**Electron density around CLA A 816:**

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



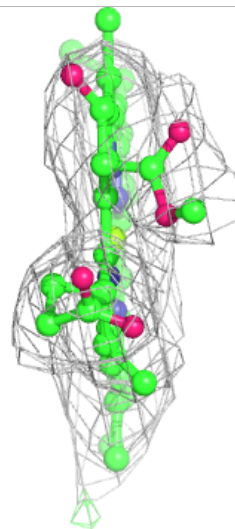
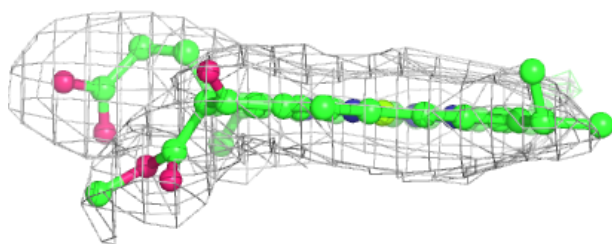
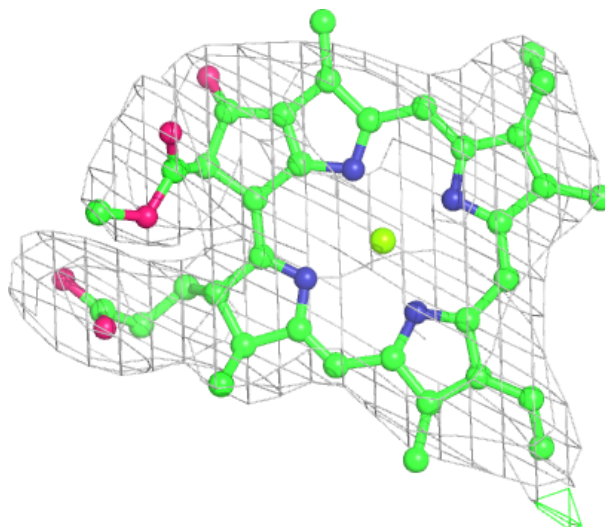
**Electron density around CLA H 811:**

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



**Electron density around CLA Z 836:**

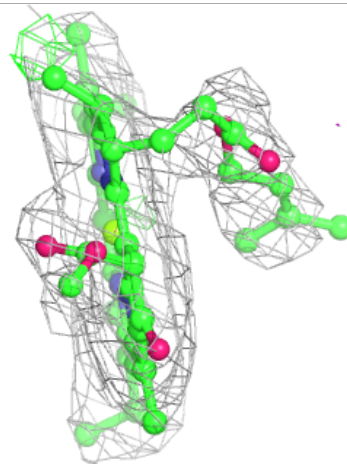
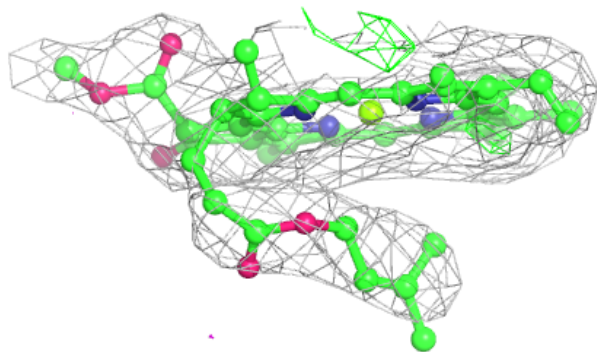
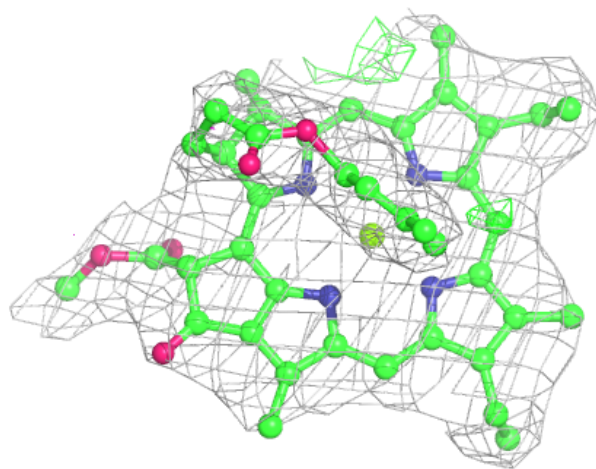
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





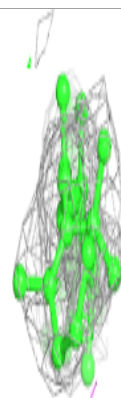
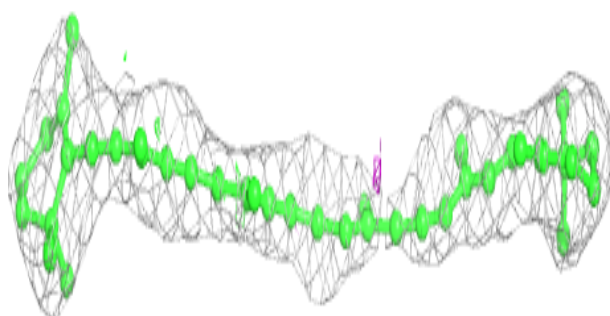
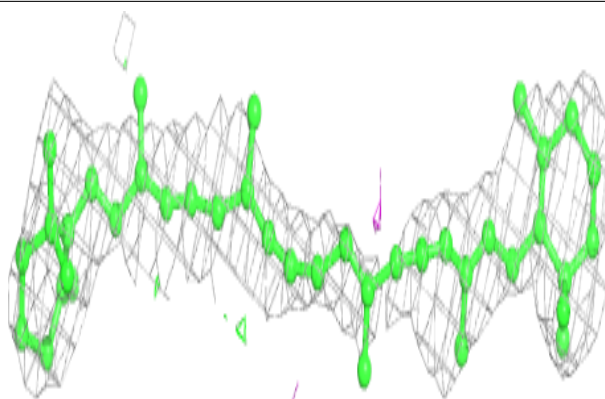
**Electron density around CLA A 824:**

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

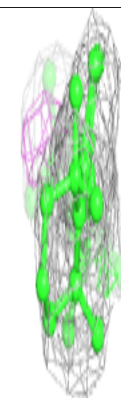
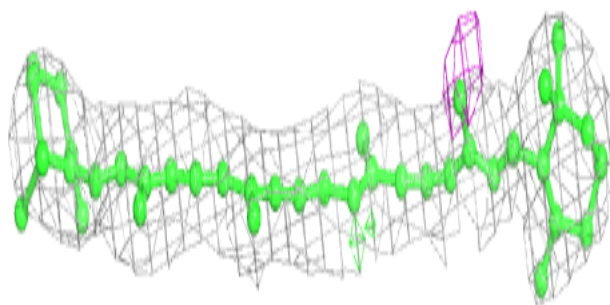
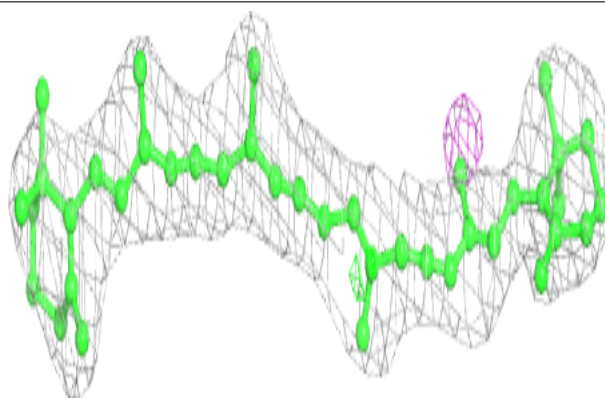


**Electron density around BCR Z 850:**

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

**Electron density around BCR S 1104:**

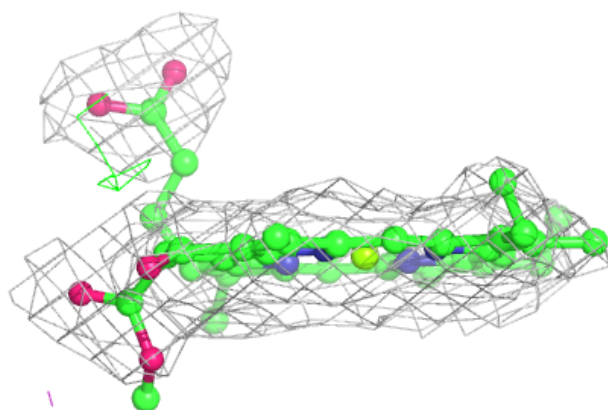
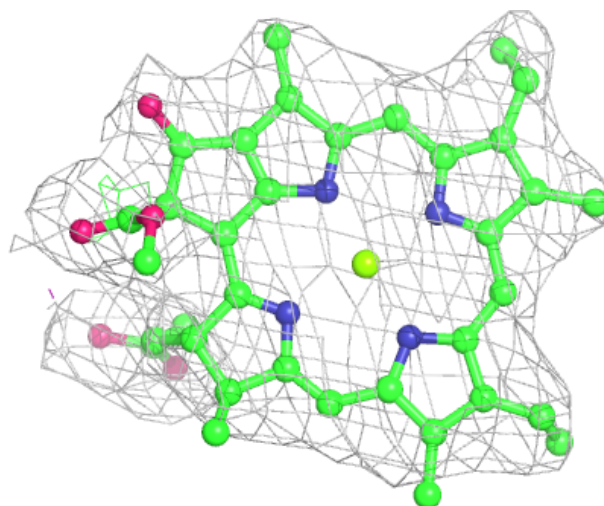
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





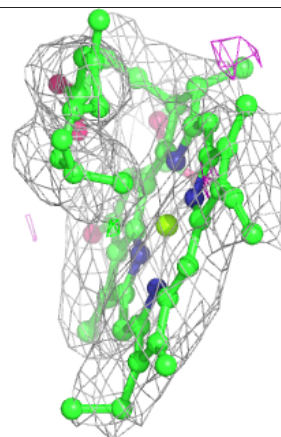
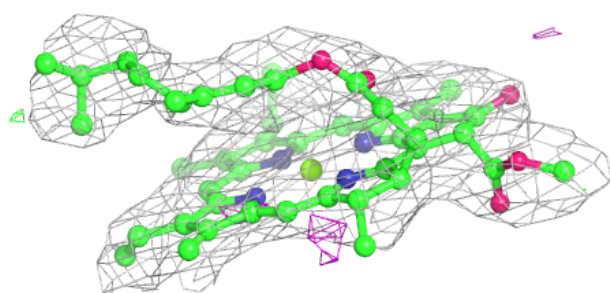
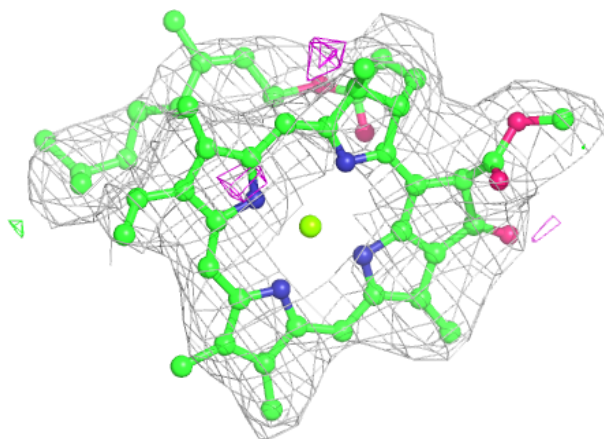
**Electron density around CLA B 820:**

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

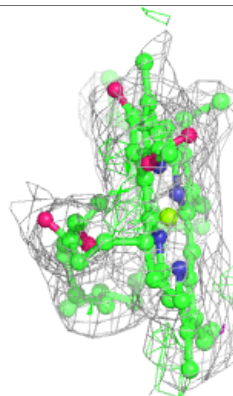
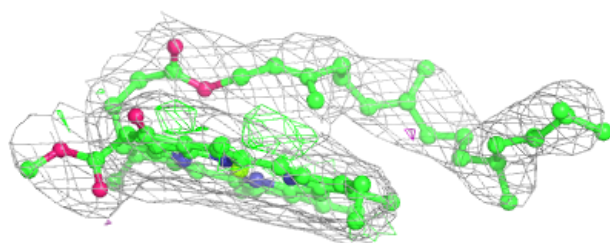
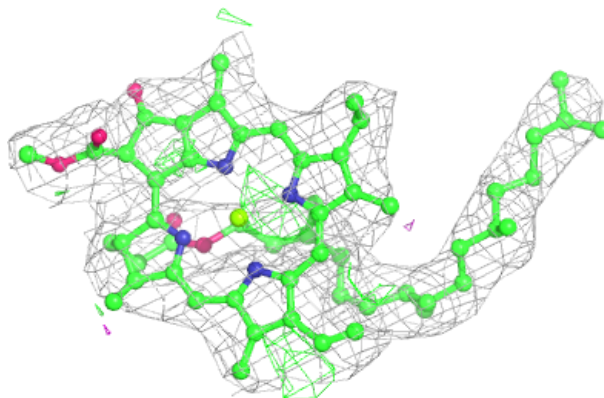


**Electron density around CLA Y 812:**

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

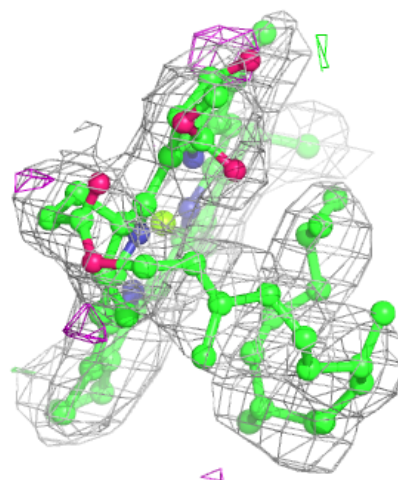
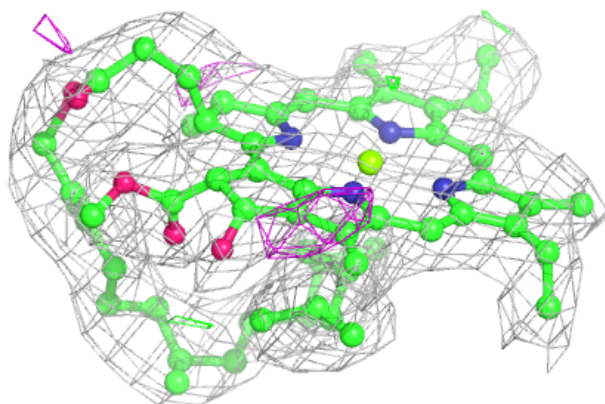
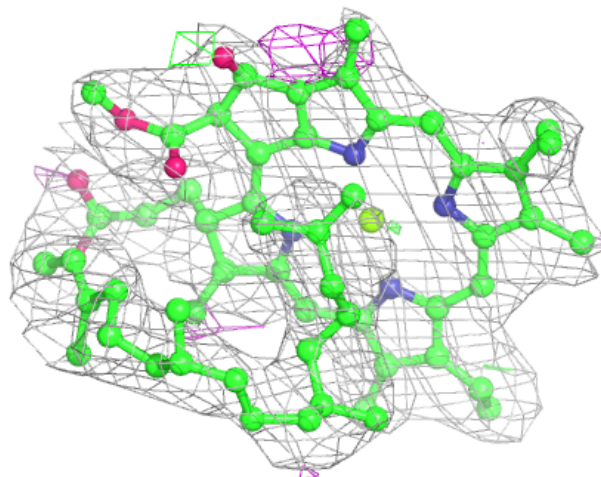
**Electron density around CLA B 837:**

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



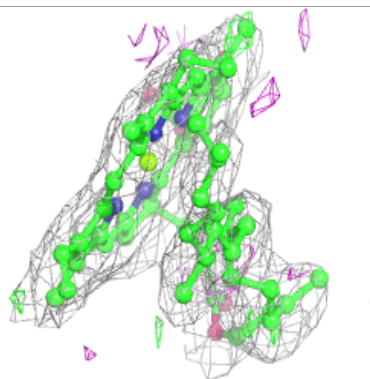
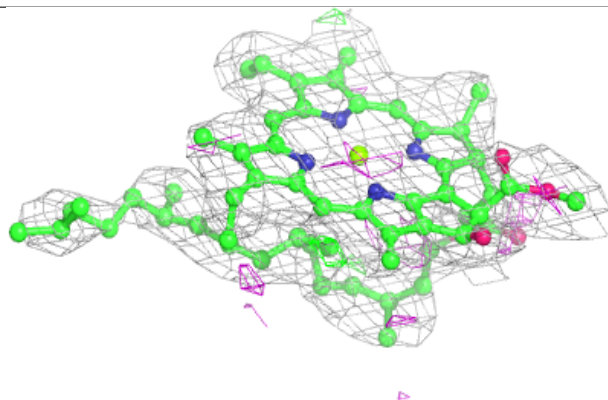
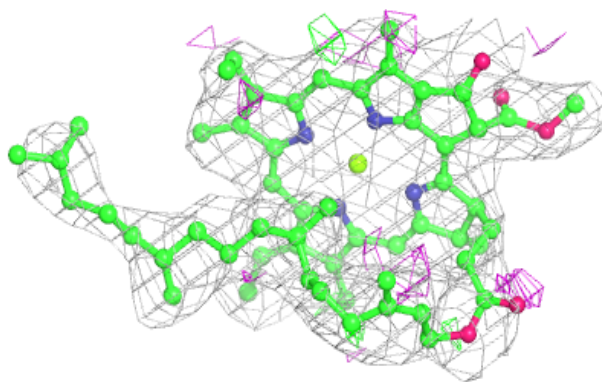
**Electron density around CLA Z 807:**

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

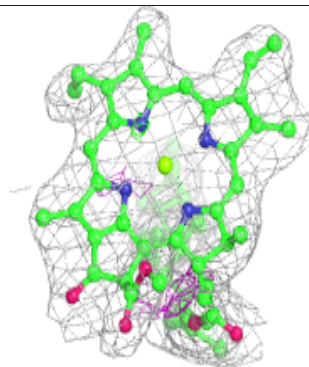
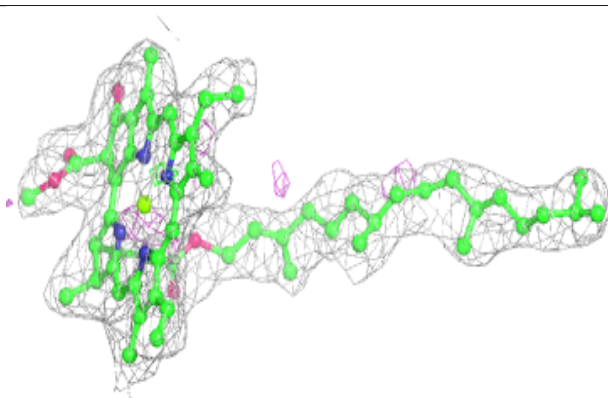
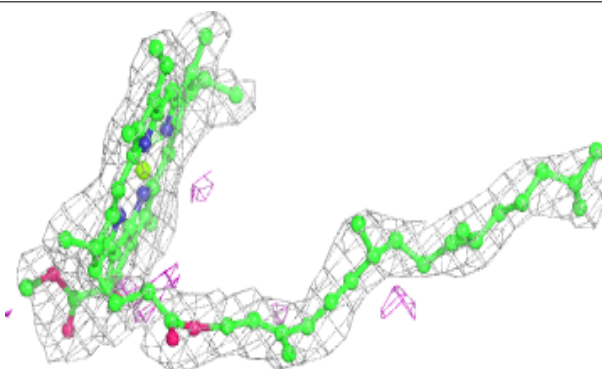


**Electron density around CLA Z 818:**

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

**Electron density around CLA B 828:**

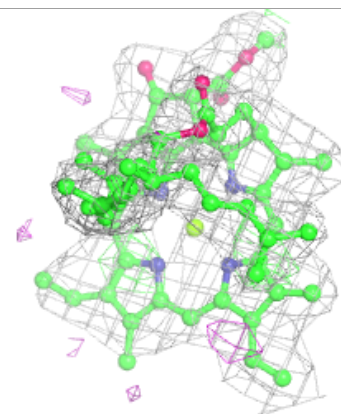
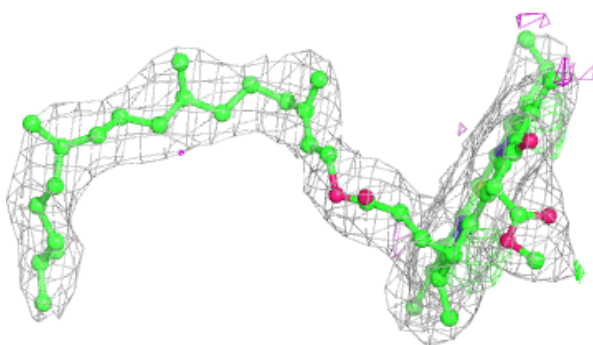
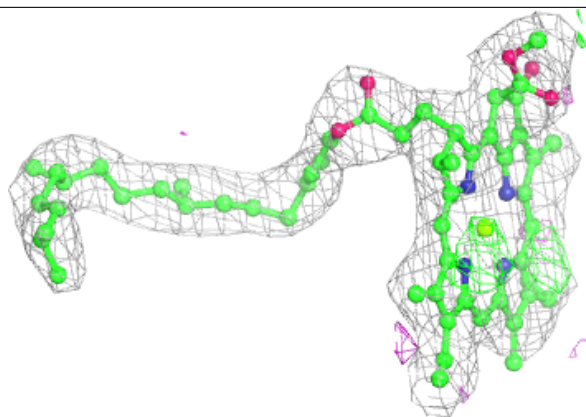
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



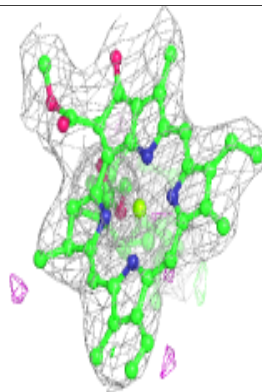
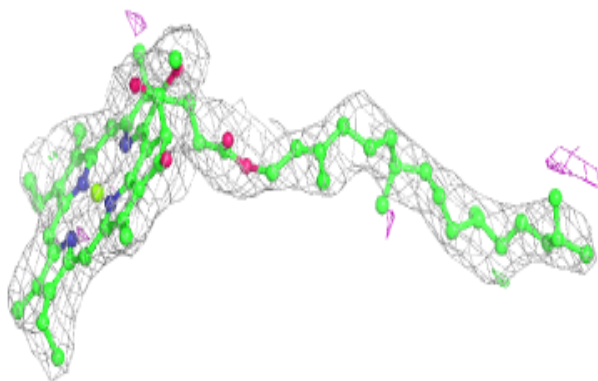
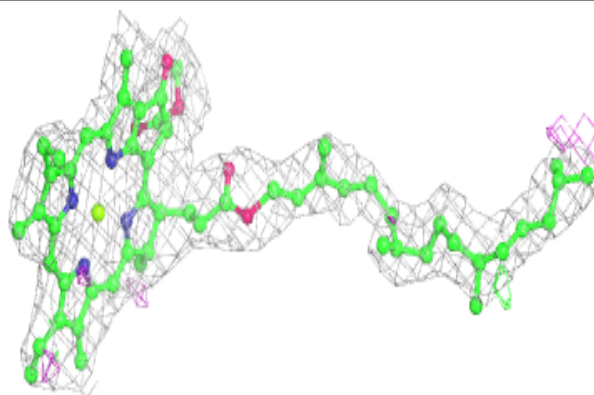


**Electron density around CLA U 1003:**

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

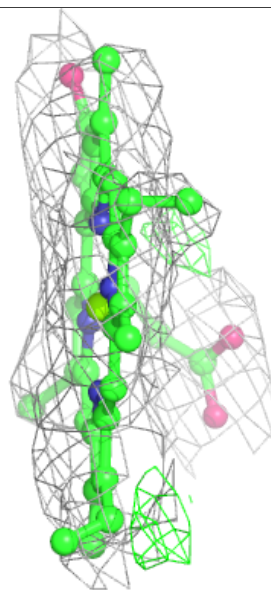
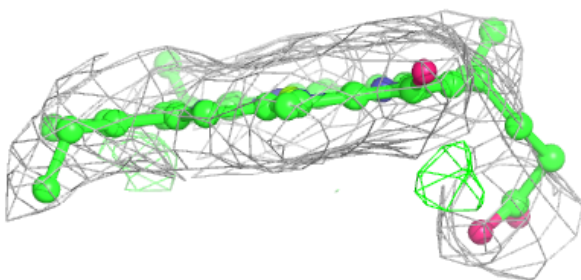
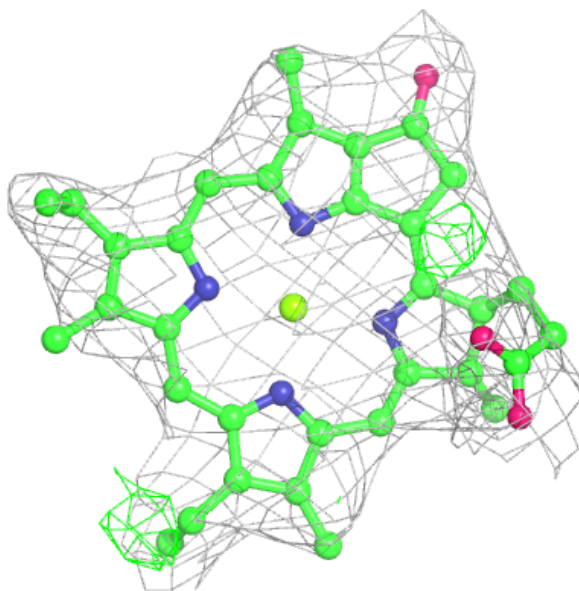
**Electron density around CLA G 809:**

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



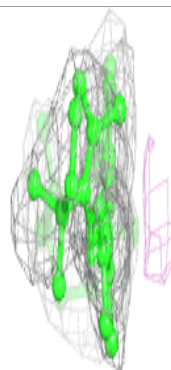
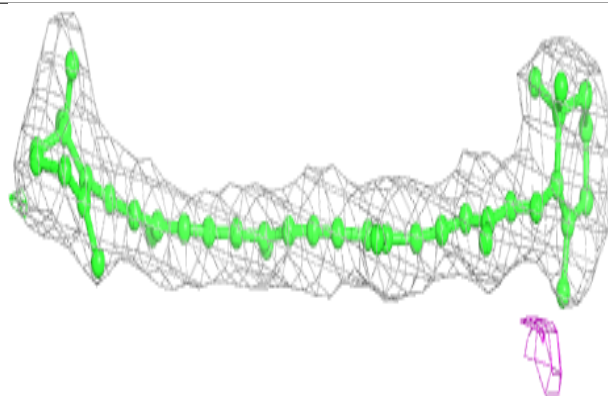
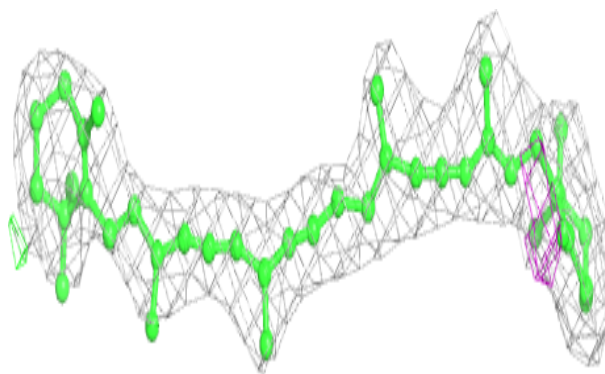
**Electron density around CLA g 101:**

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

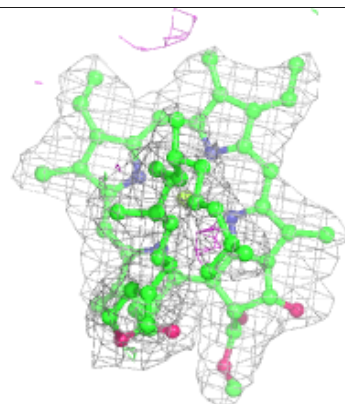
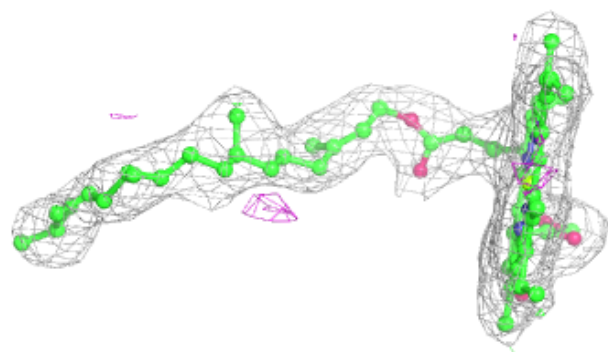
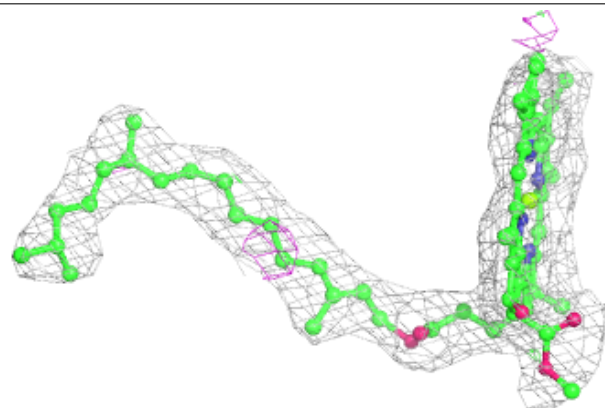


**Electron density around BCR G 848:**

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

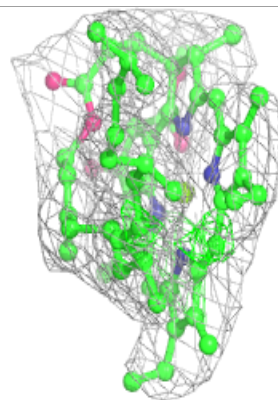
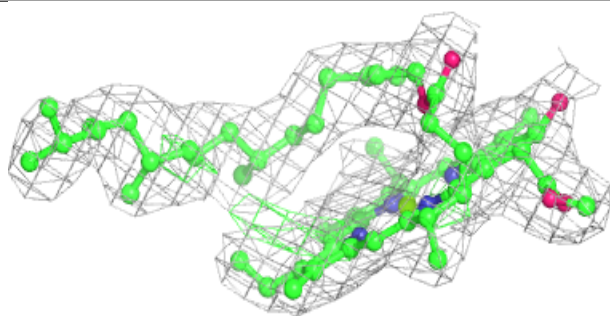
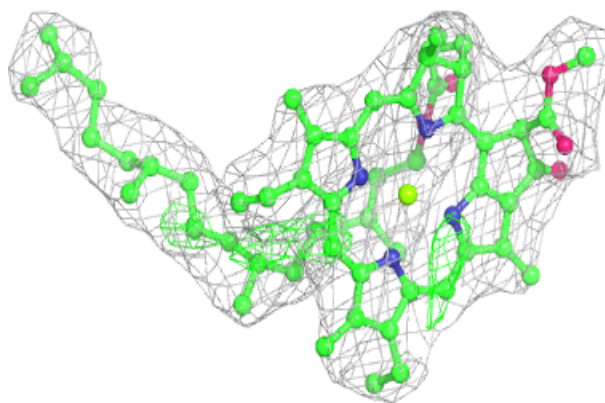
**Electron density around CLA H 840:**

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



**Electron density around CLA Z 808:**

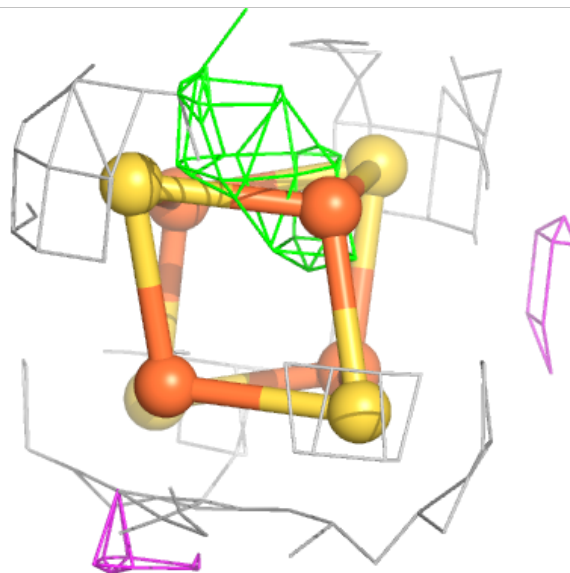
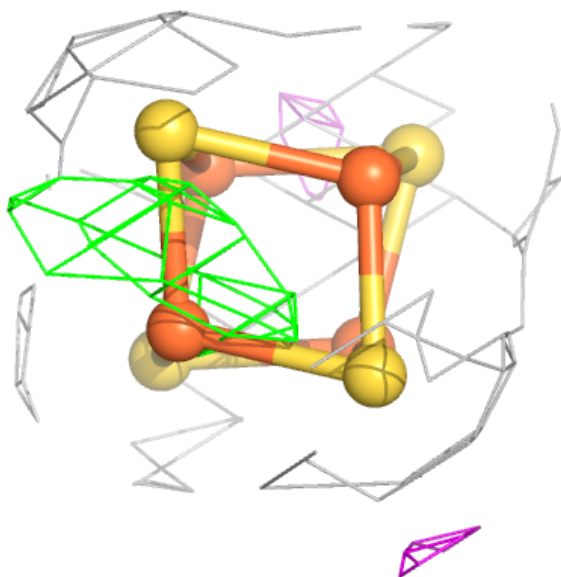
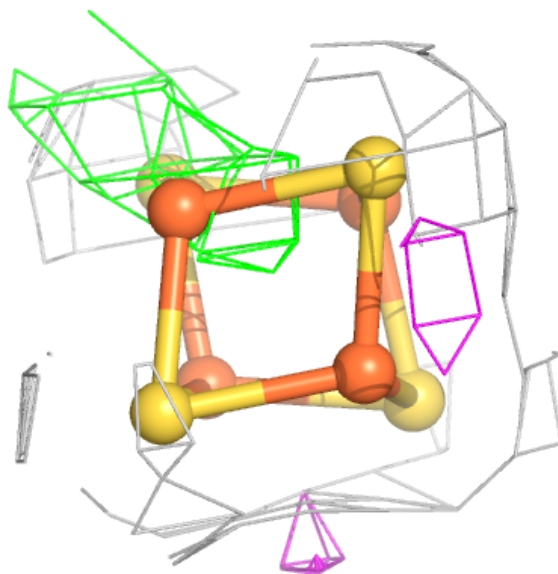
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





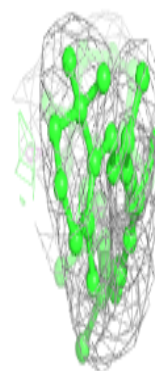
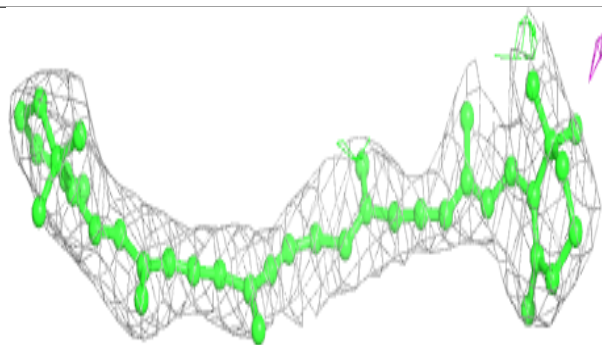
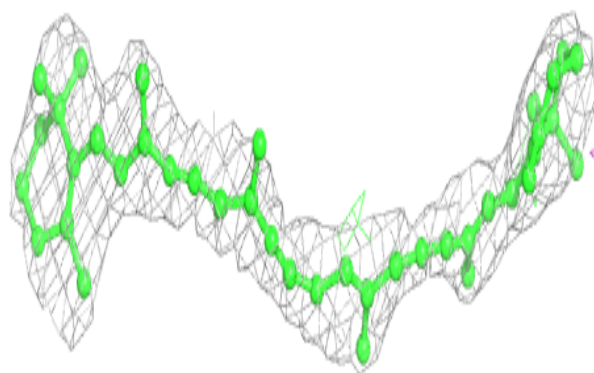
**Electron density around SF4 A 845:**

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

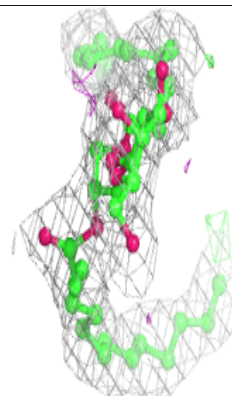
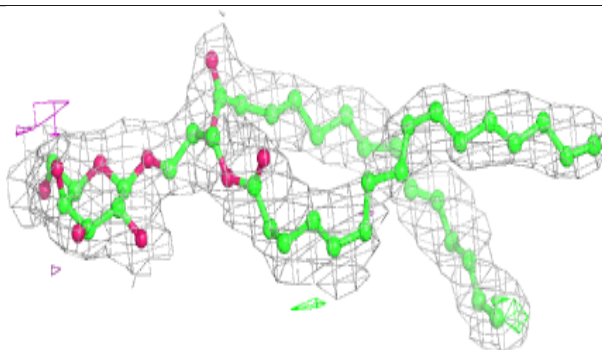
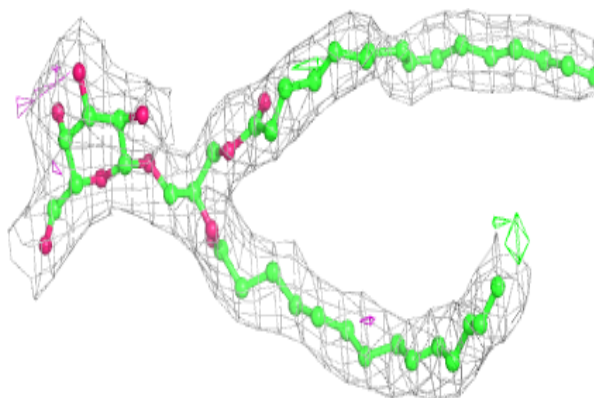


**Electron density around BCR Z 848:**

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

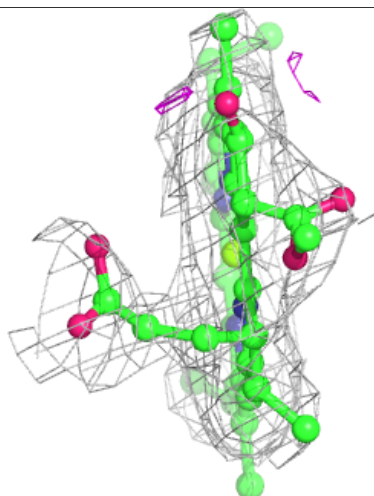
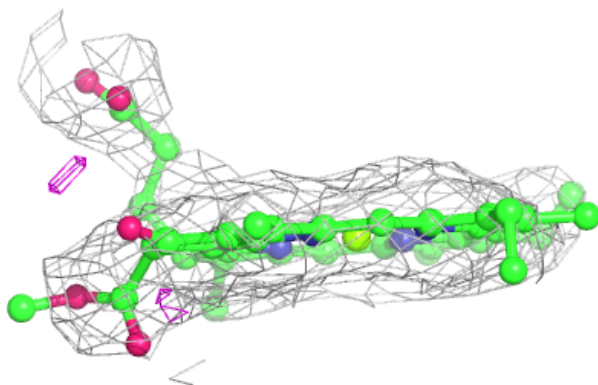
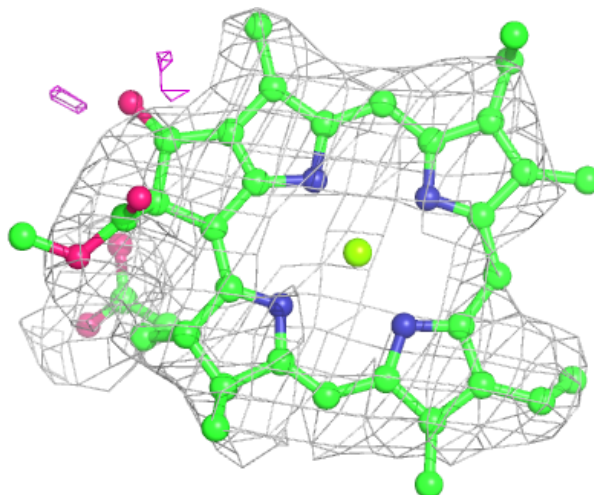
**Electron density around LMG H 848:**

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



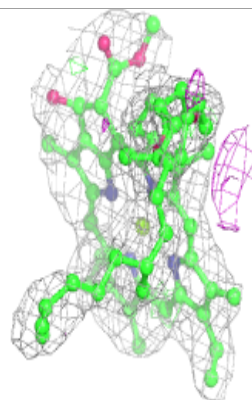
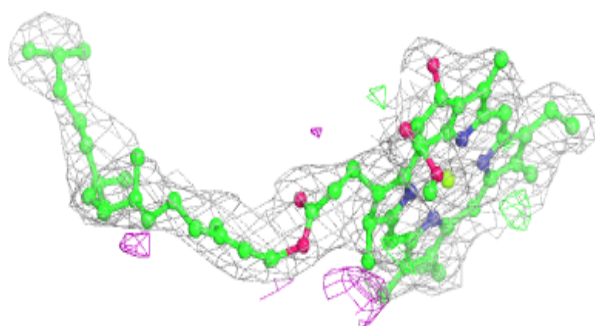
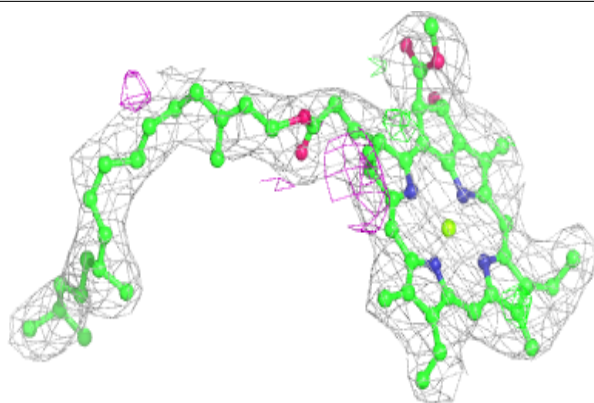
**Electron density around CLA S 1102:**

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

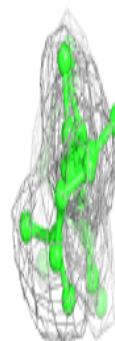
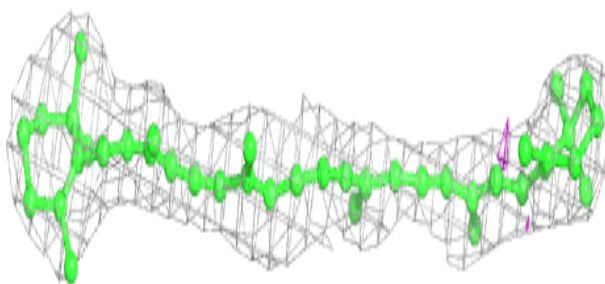
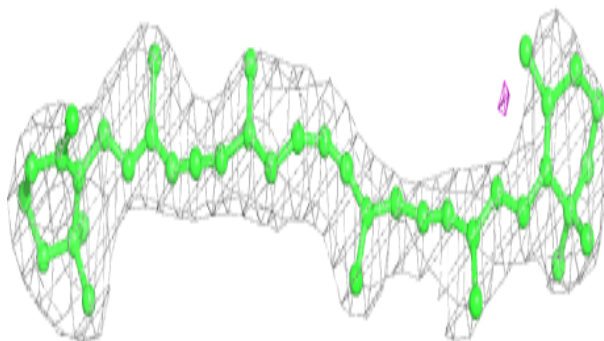


**Electron density around CLA A 854:**

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

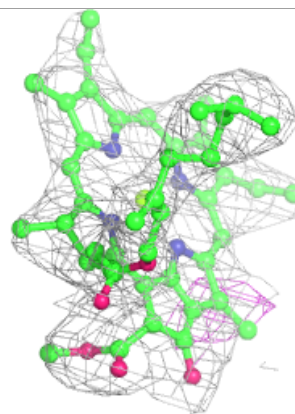
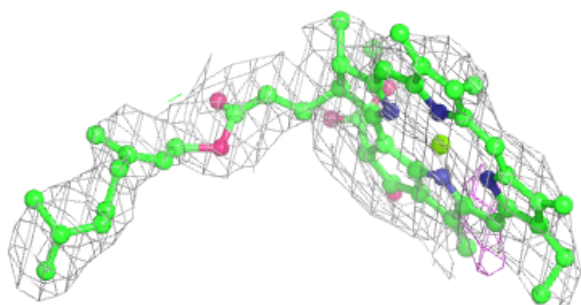
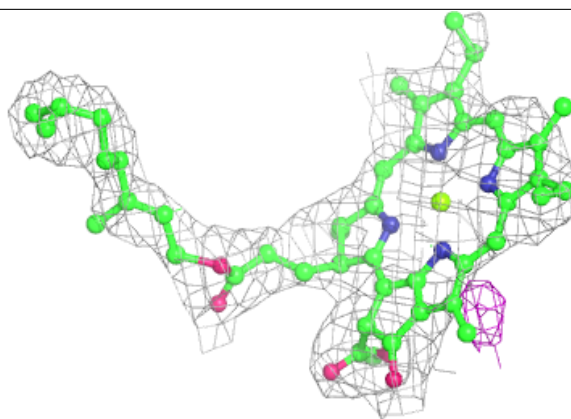
**Electron density around BCR J 103:**

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

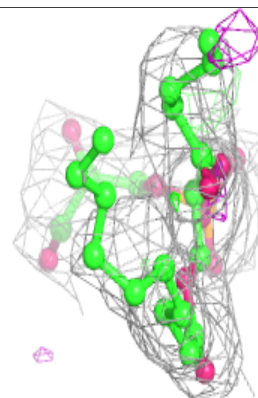
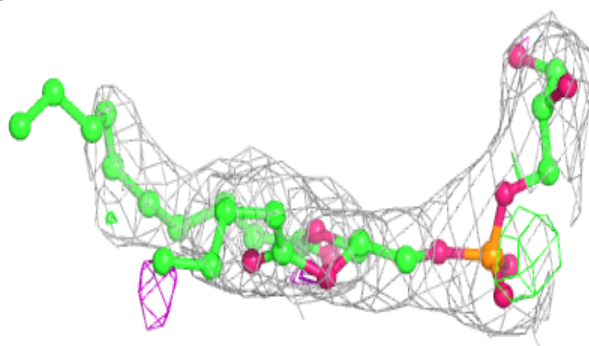
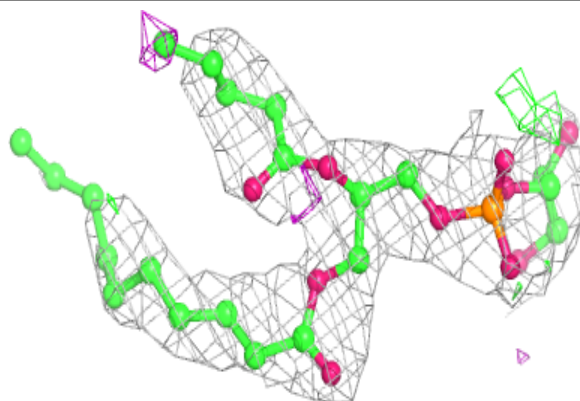


**Electron density around CLA Z 833:**

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

**Electron density around LHG G 851:**

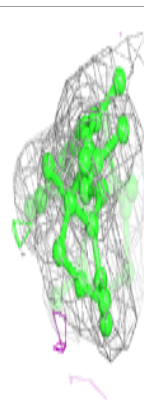
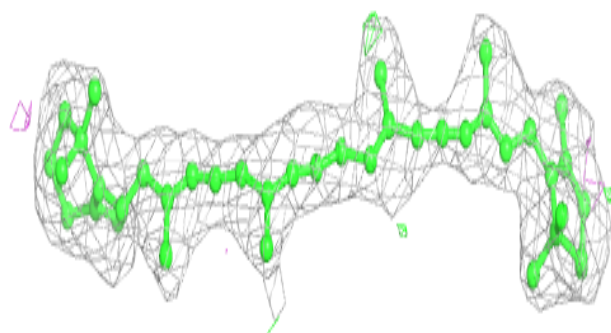
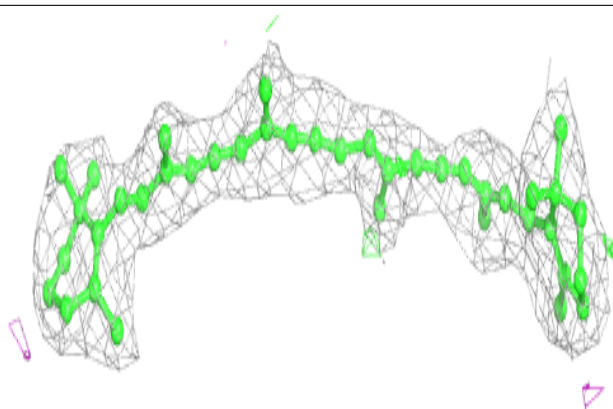
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



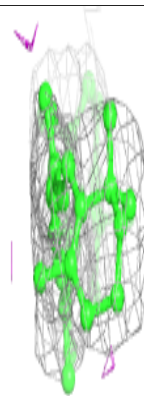
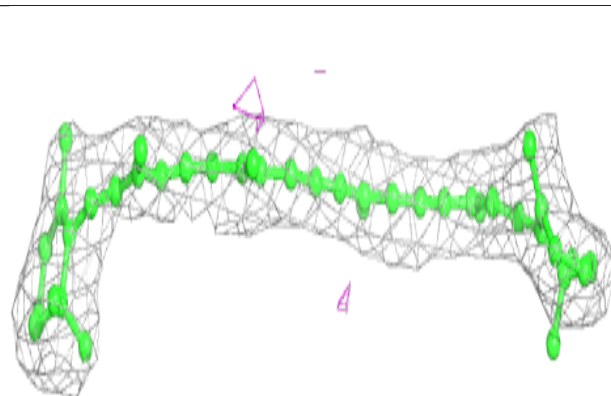
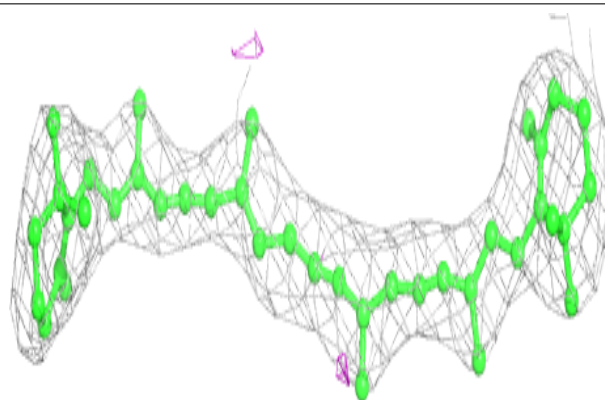


**Electron density around BCR V 101:**

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

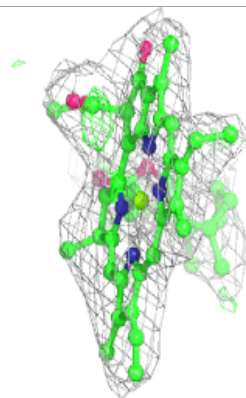
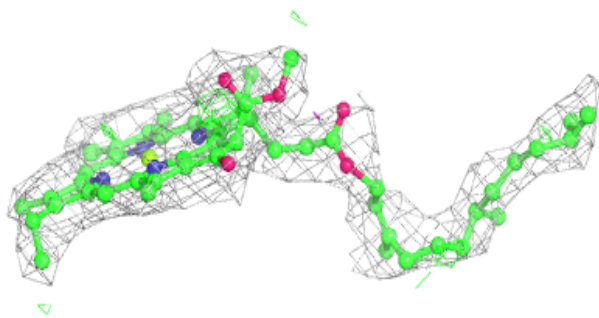
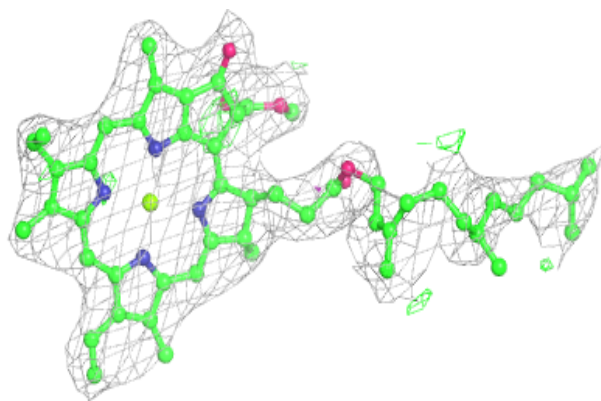
**Electron density around BCR Y 848:**

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

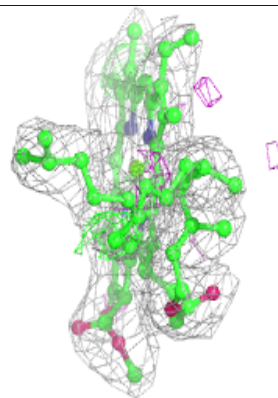
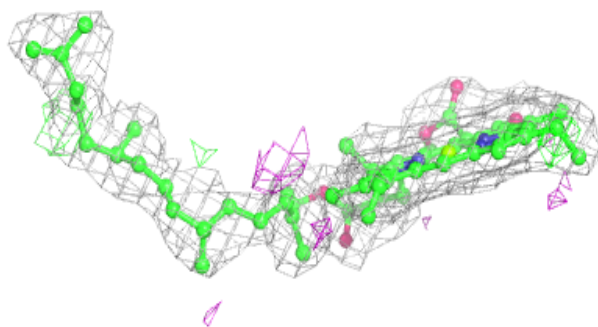
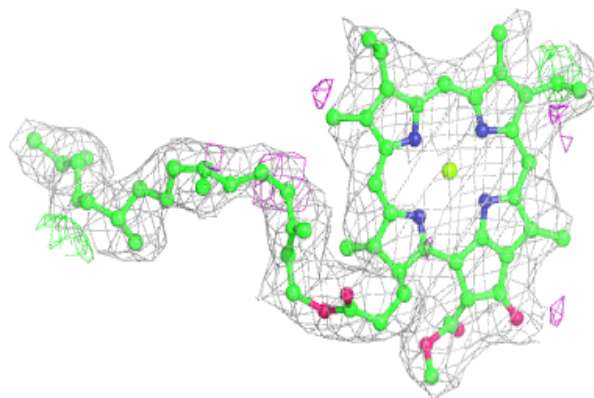


**Electron density around CLA B 822:**

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

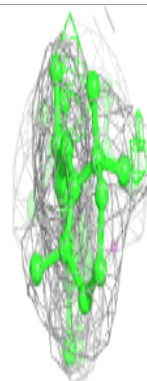
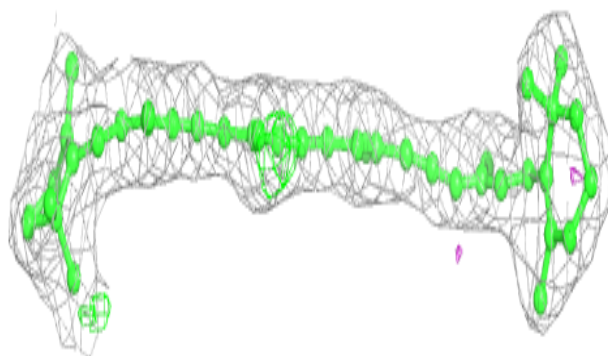
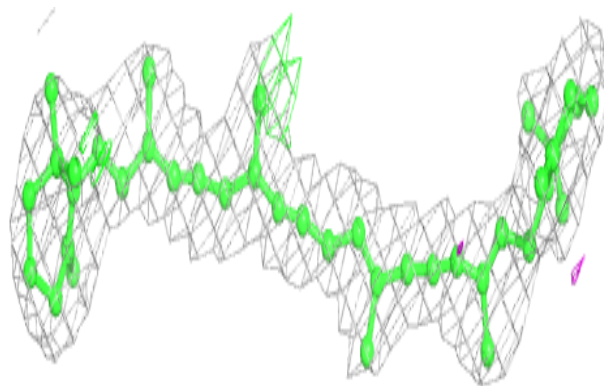
**Electron density around CLA G 852:**

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

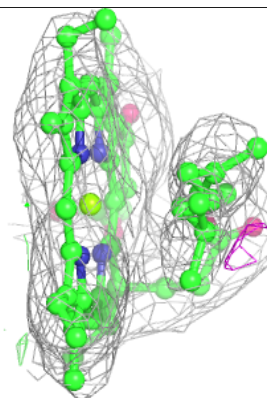
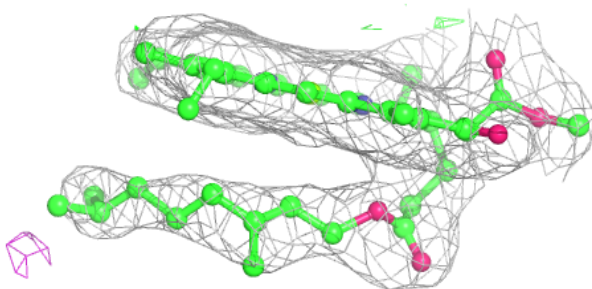
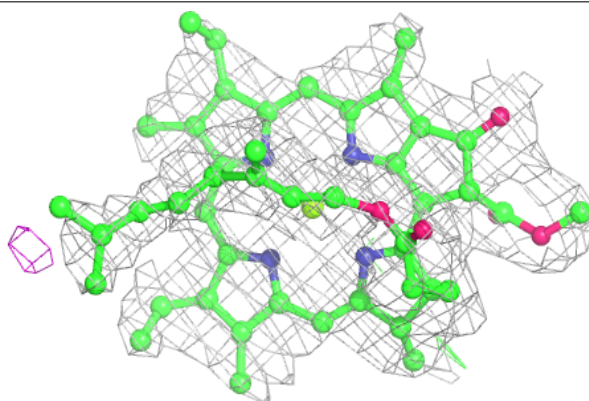


**Electron density around BCR H 847:**

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

**Electron density around CLA Z 823:**

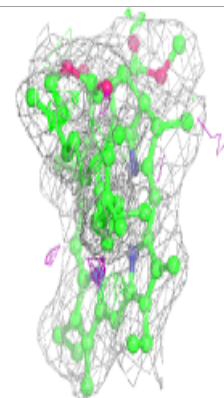
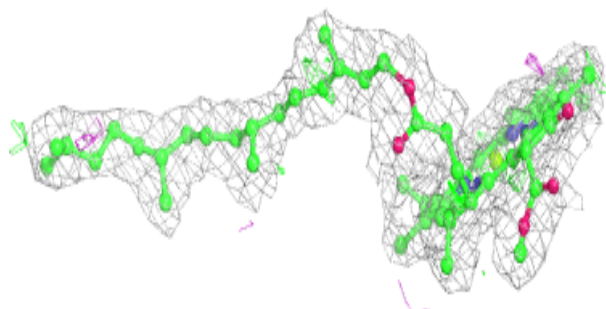
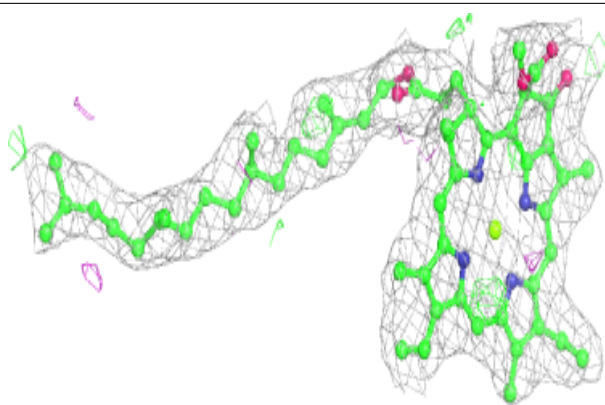
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





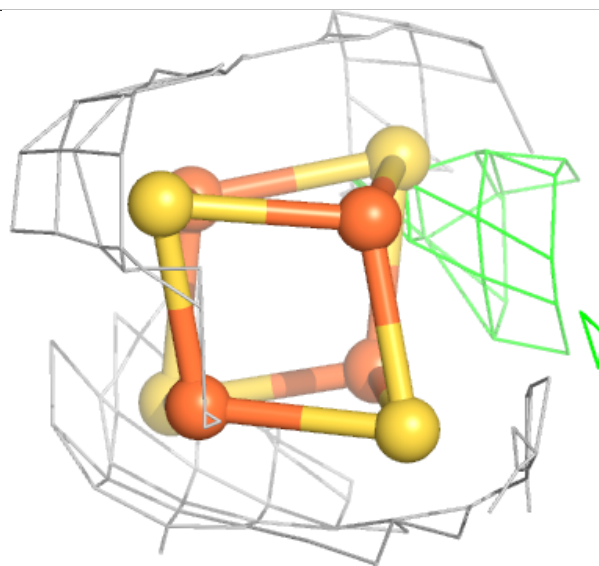
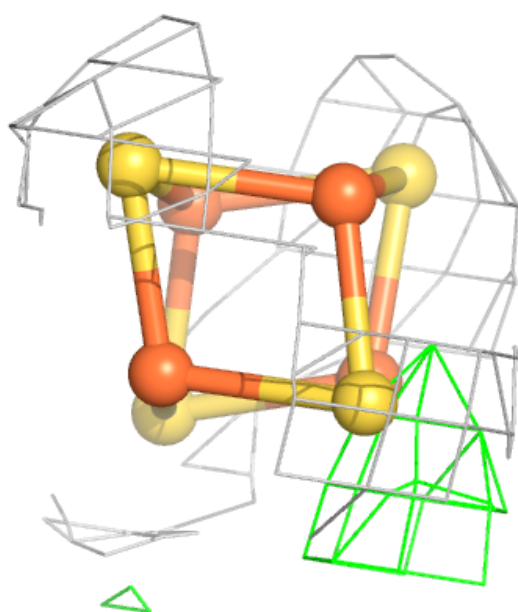
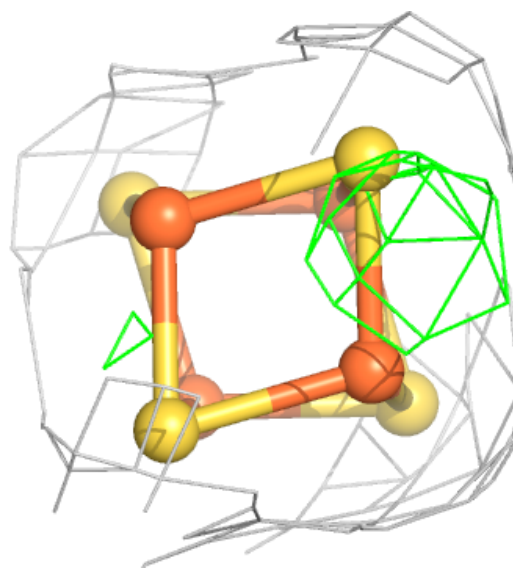
**Electron density around CLA G 833:**

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



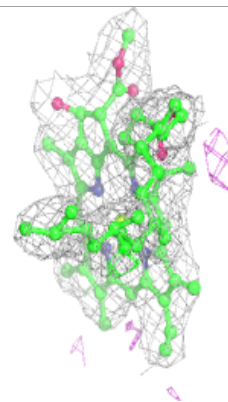
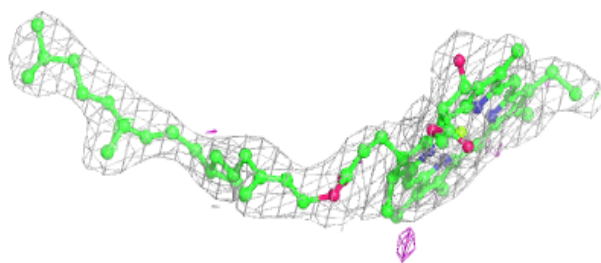
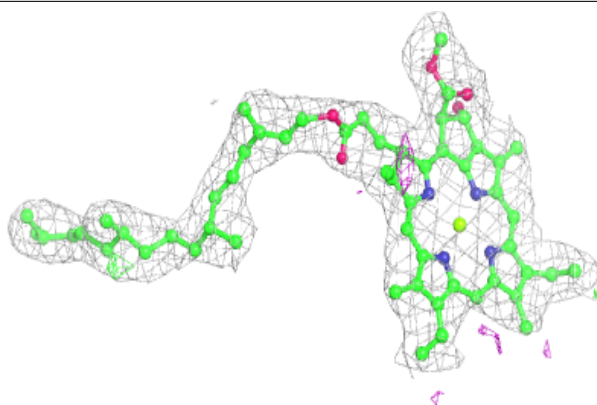
**Electron density around SF4 N 101:**

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



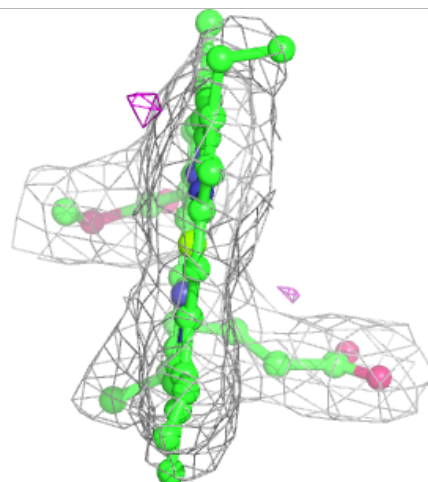
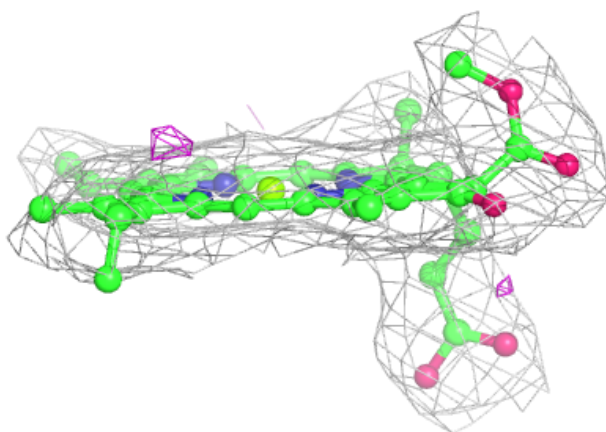
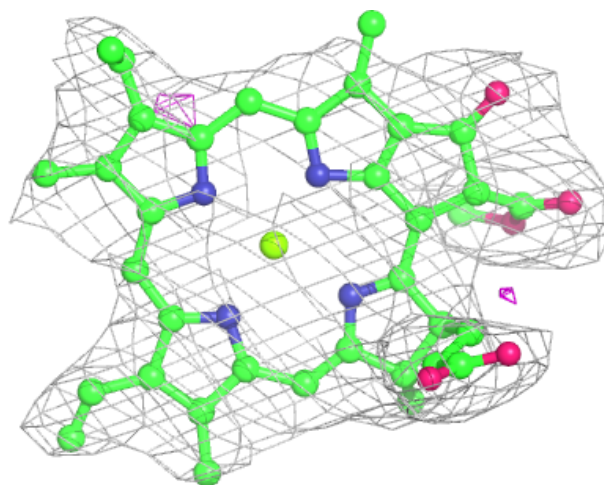
**Electron density around CLA G 803:**

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



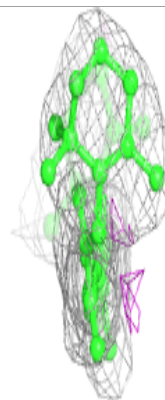
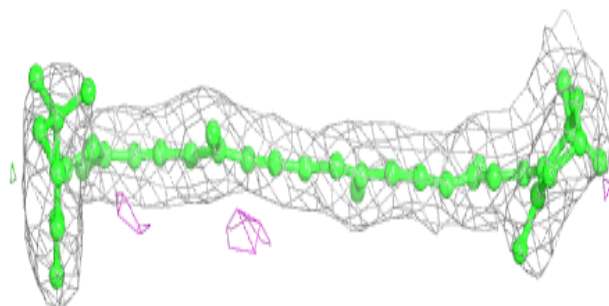
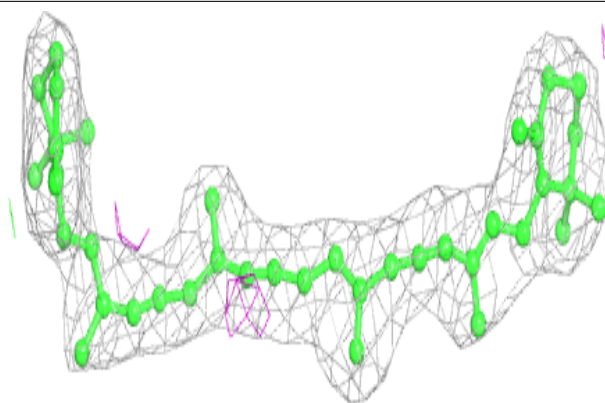
**Electron density around CLA B 833:**

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

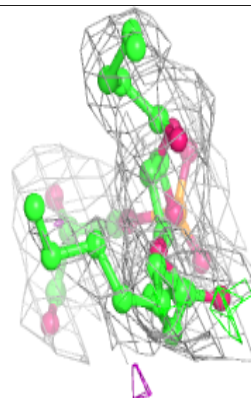
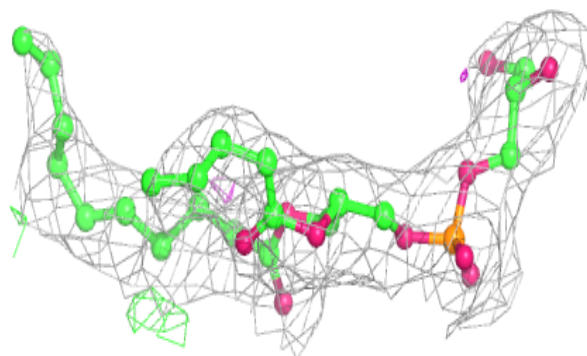
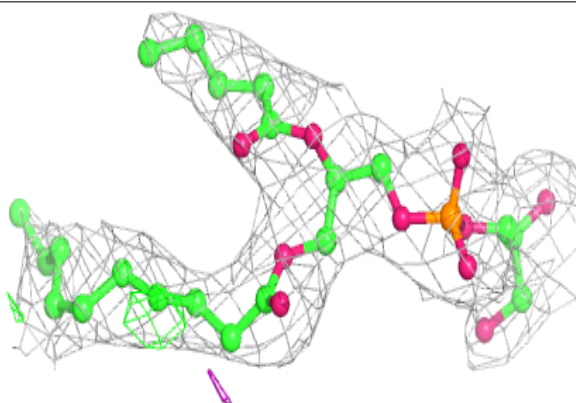


**Electron density around BCR I 102:**

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

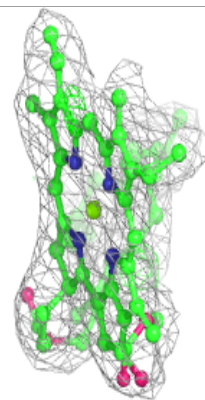
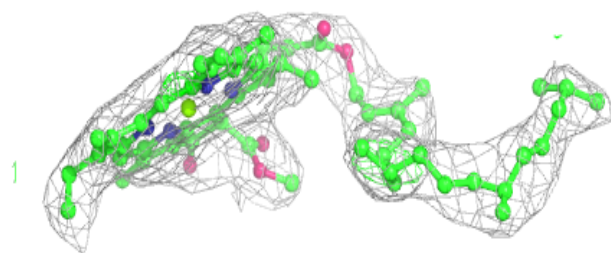
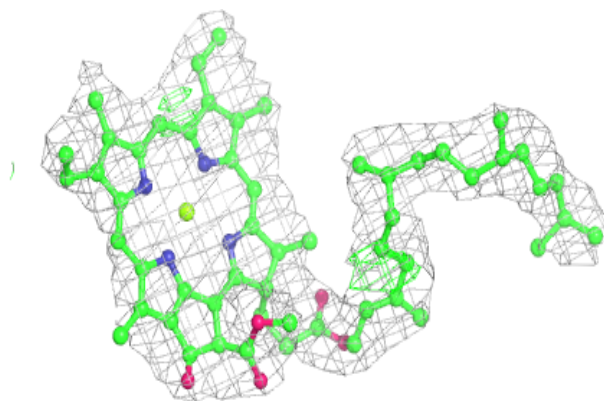
**Electron density around LHG A 853:**

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

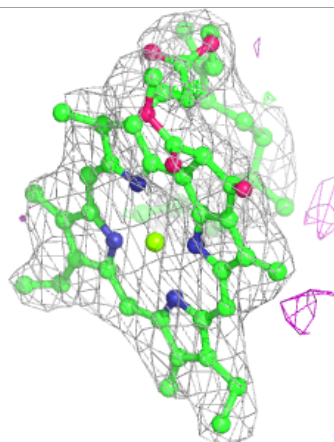
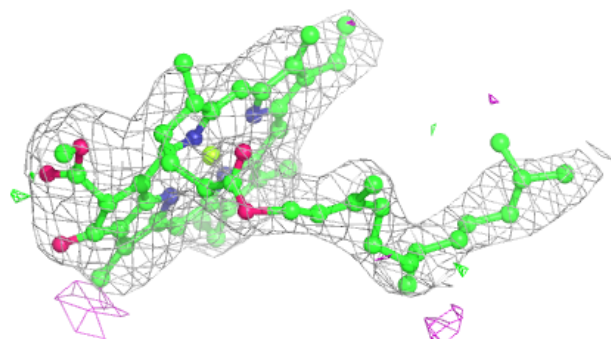
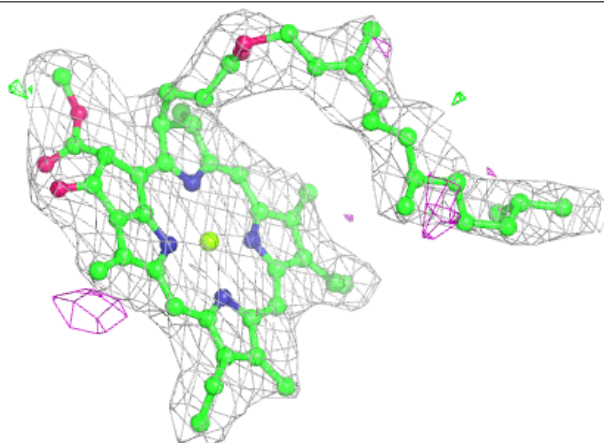


**Electron density around CLA S 1101:**

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

**Electron density around CLA Y 824:**

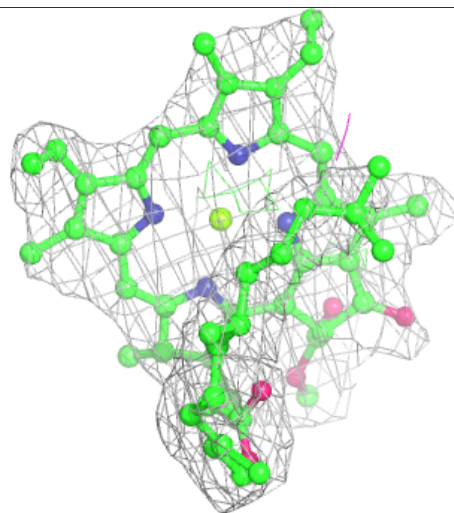
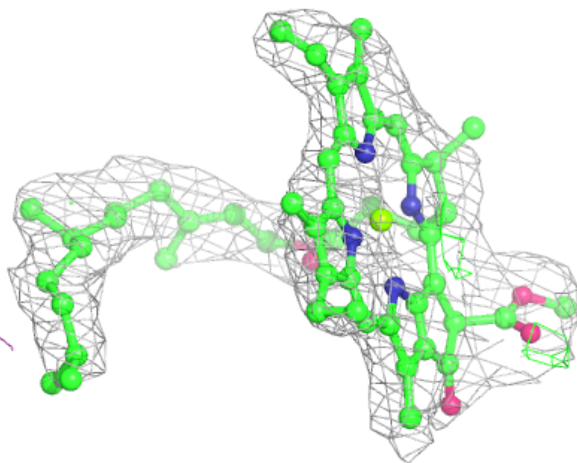
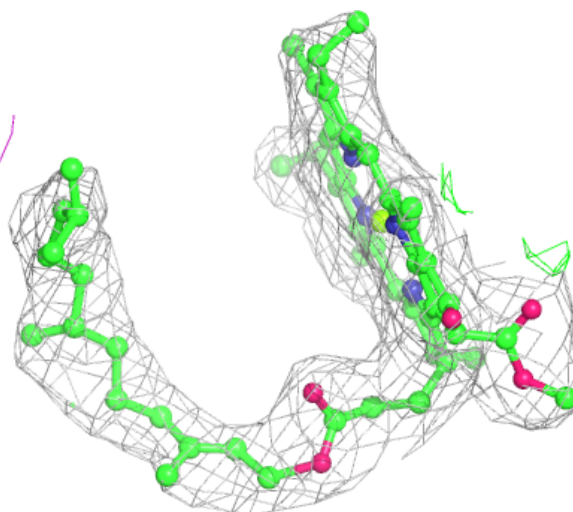
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





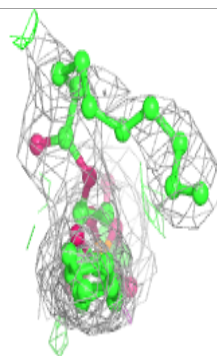
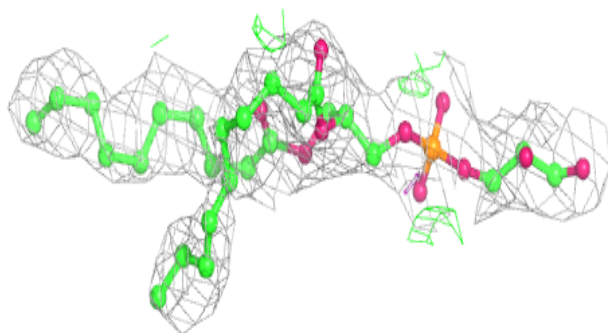
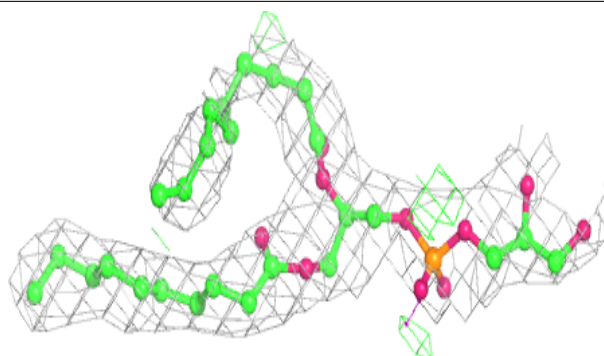
**Electron density around CLA B 818:**

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

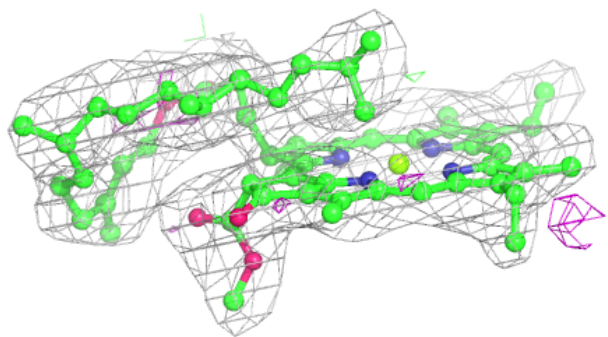
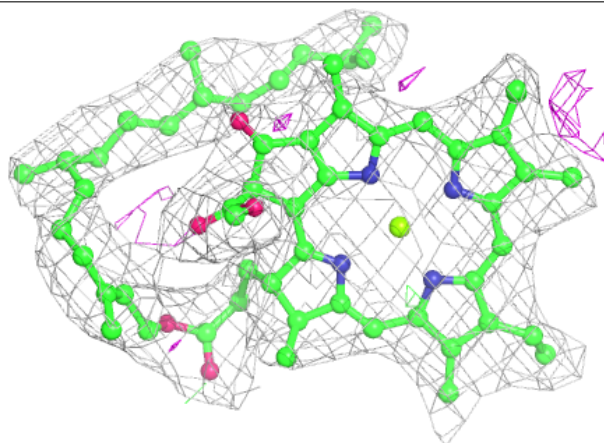


**Electron density around LHG H 849:**

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

**Electron density around CLA H 805:**

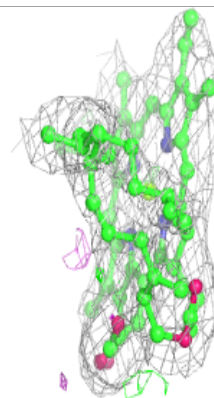
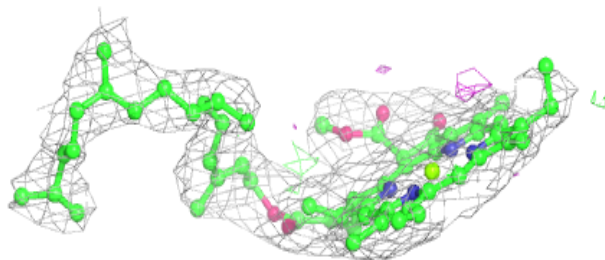
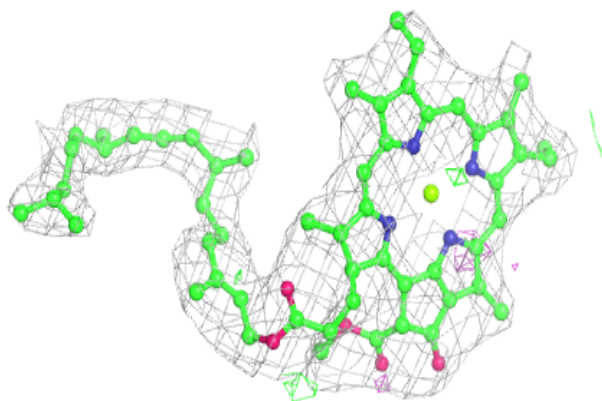
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





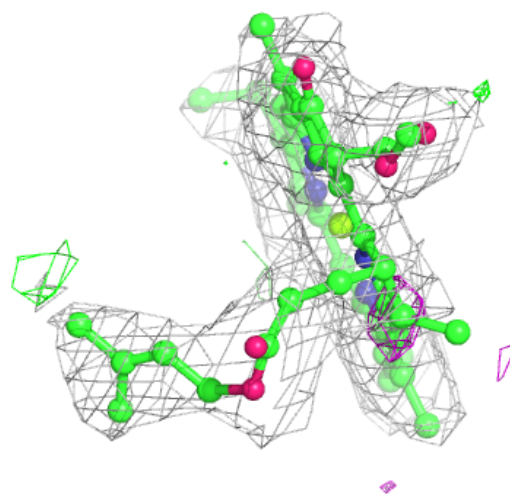
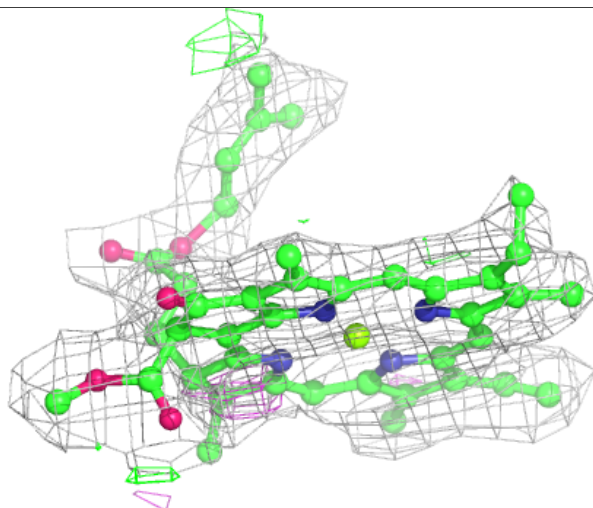
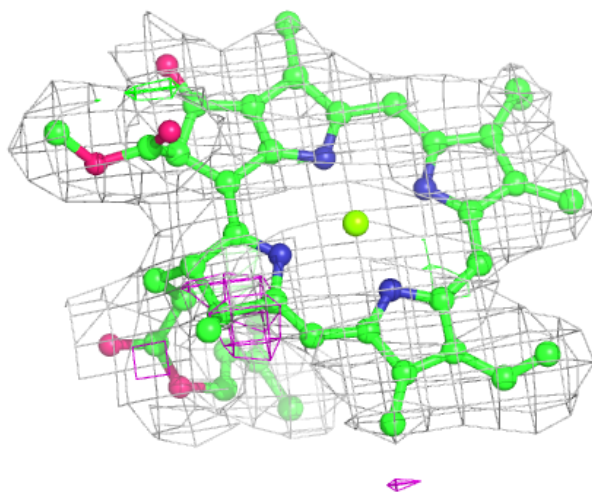
**Electron density around CLA Y 803:**

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



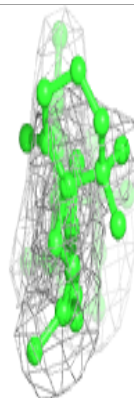
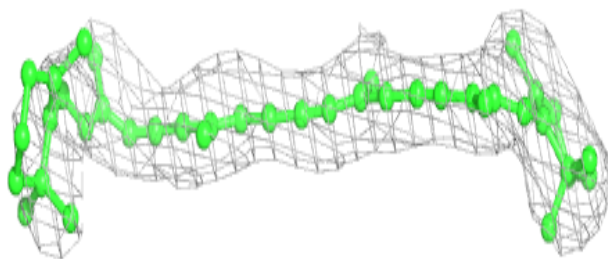
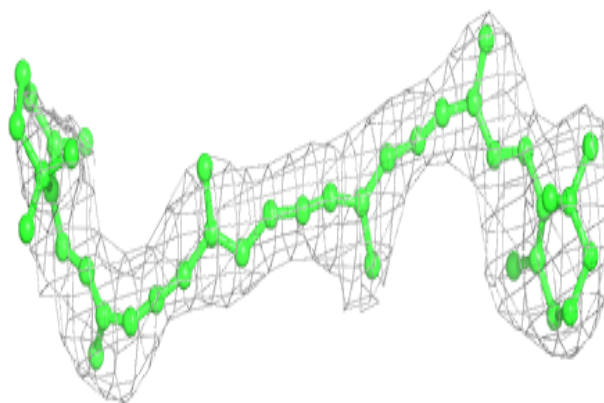
**Electron density around CLA B 811:**

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



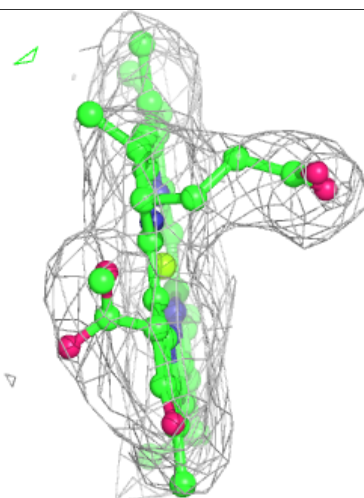
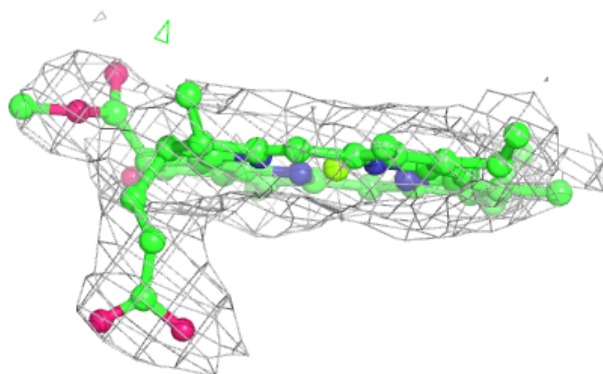
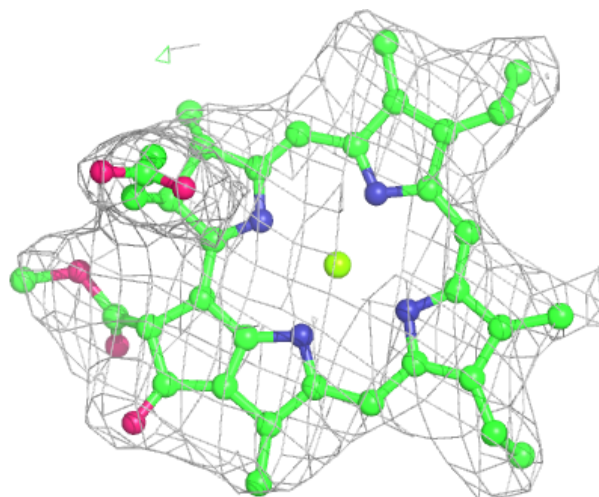
**Electron density around BCR B 844:**

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



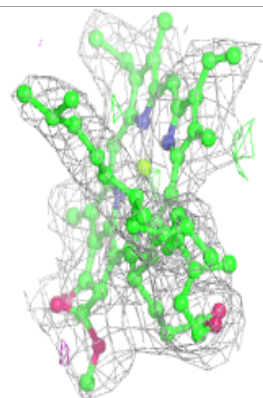
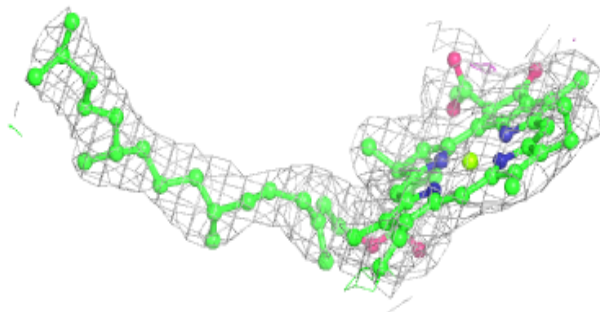
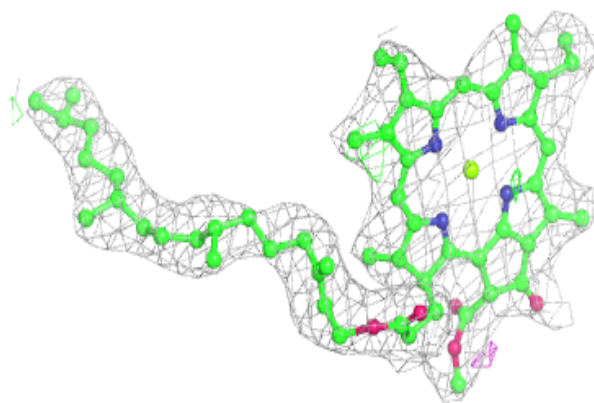
**Electron density around CLA G 810:**

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



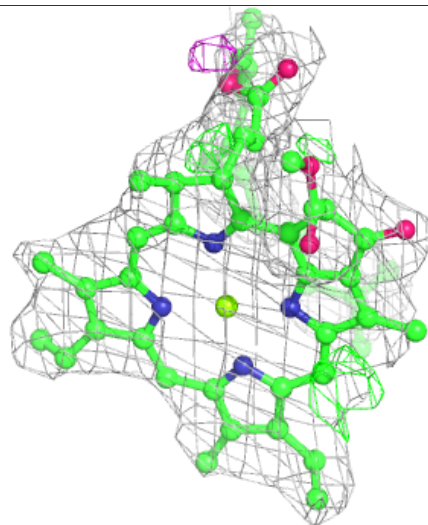
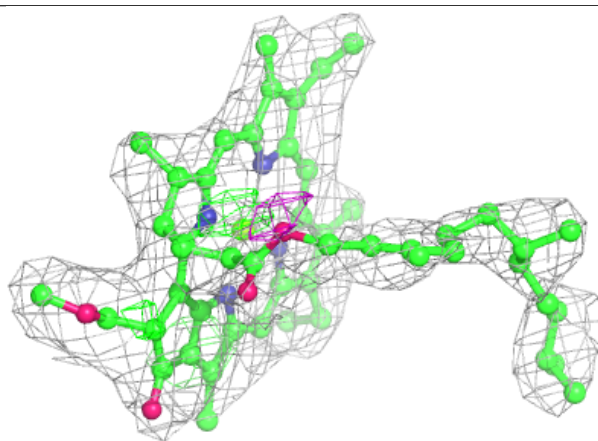
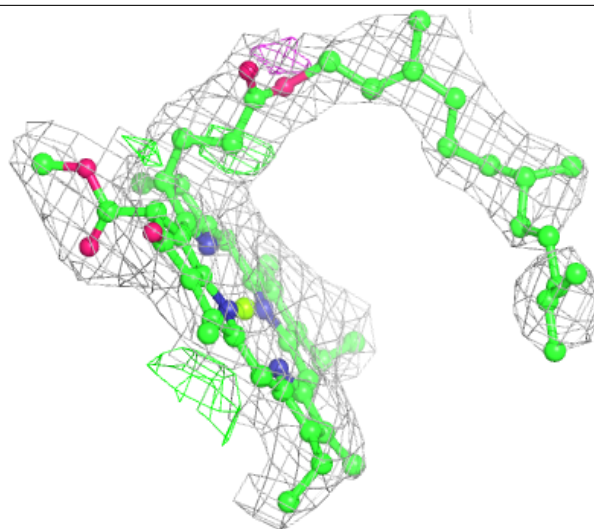
**Electron density around CLA G 802:**

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



**Electron density around CLA Z 820:**

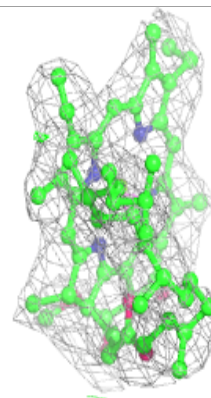
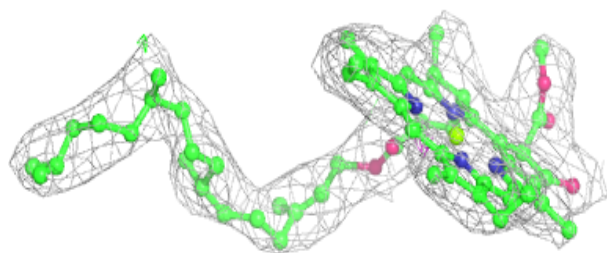
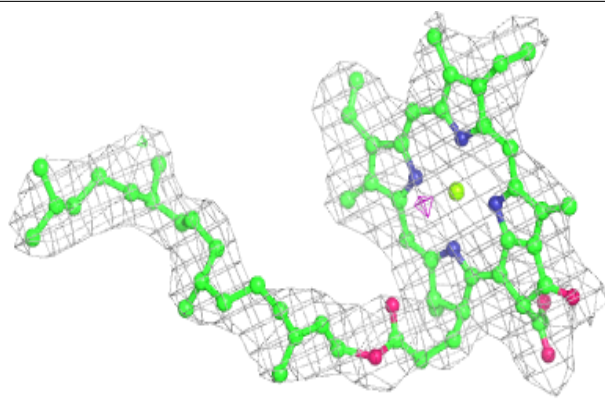
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



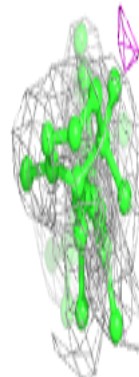
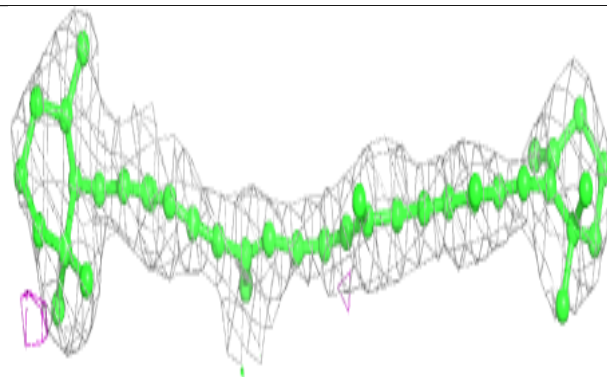
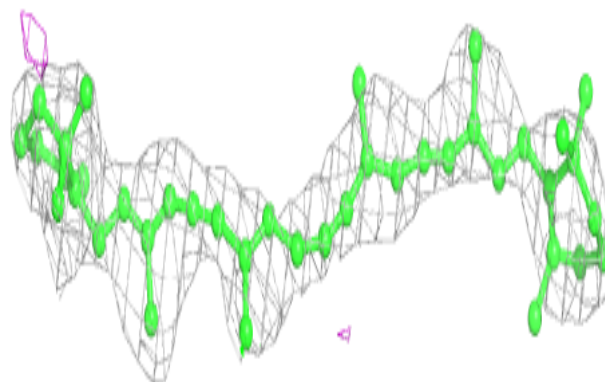


**Electron density around CLA G 808:**

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

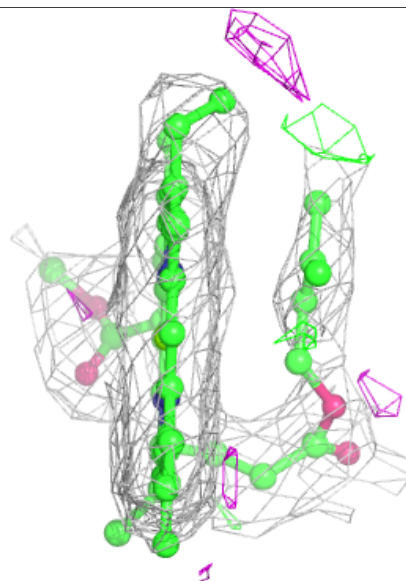
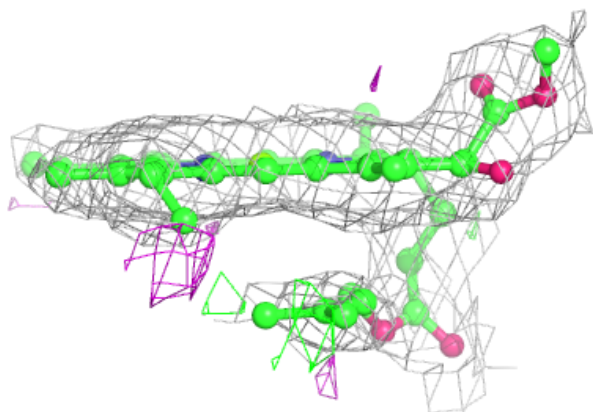
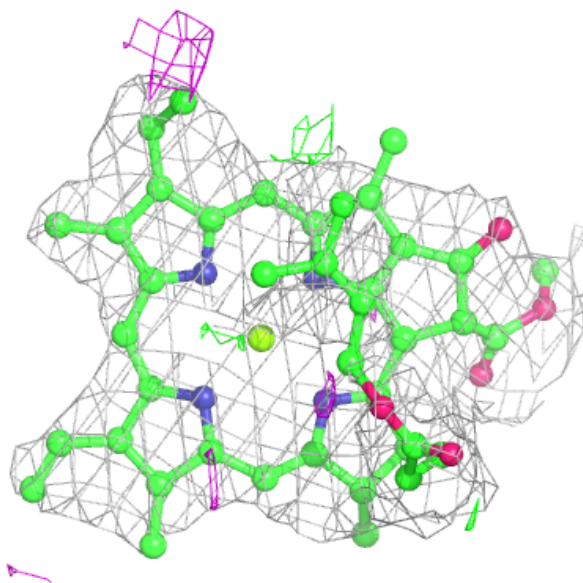
**Electron density around BCR A 847:**

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



**Electron density around CLA H 851:**

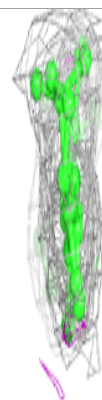
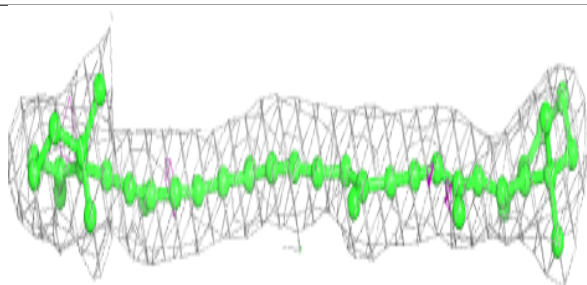
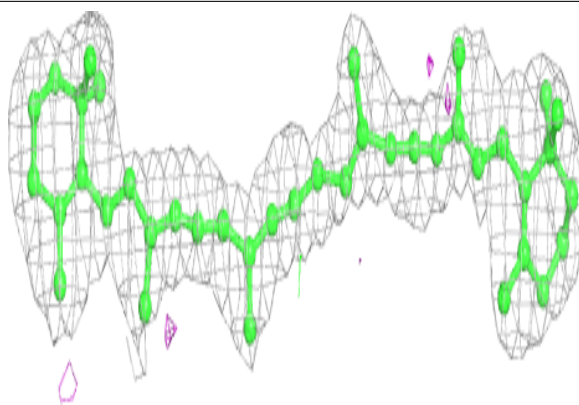
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





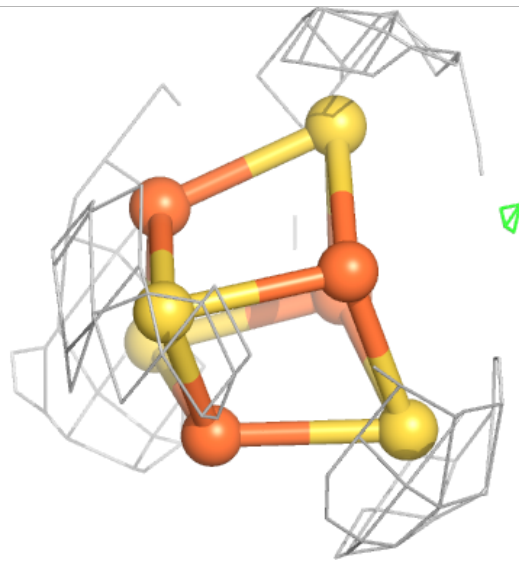
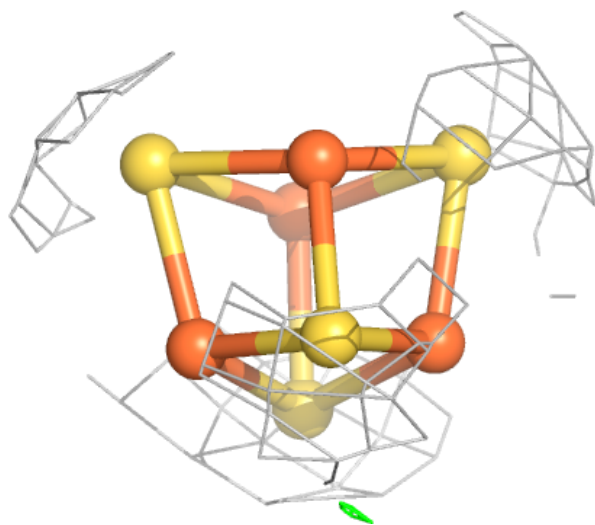
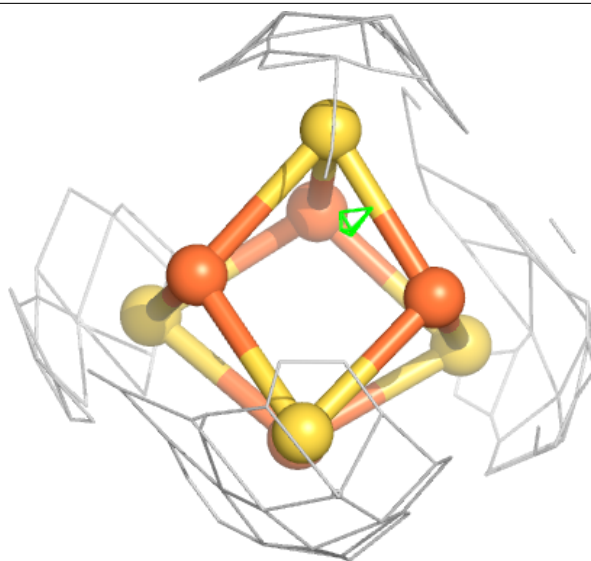
**Electron density around BCR L 207:**

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



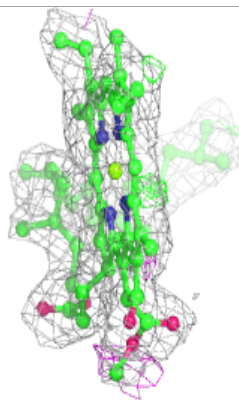
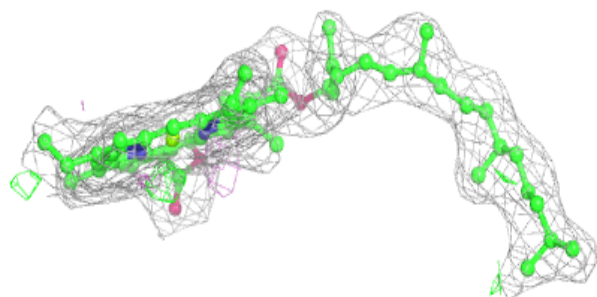
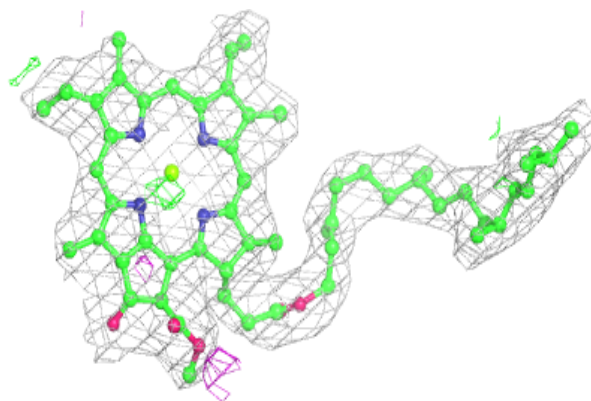
**Electron density around SF4 a 102:**

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



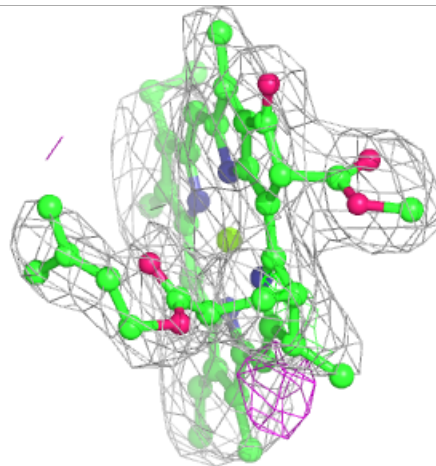
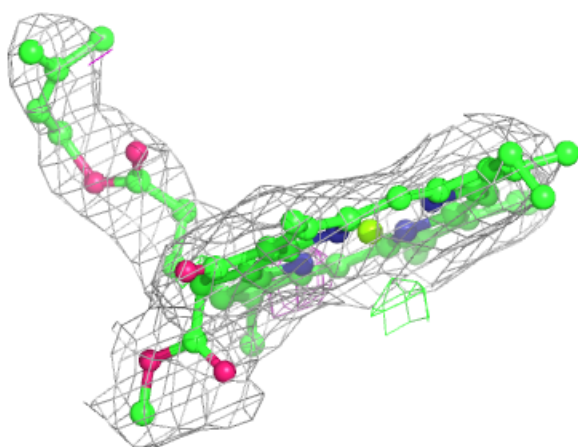
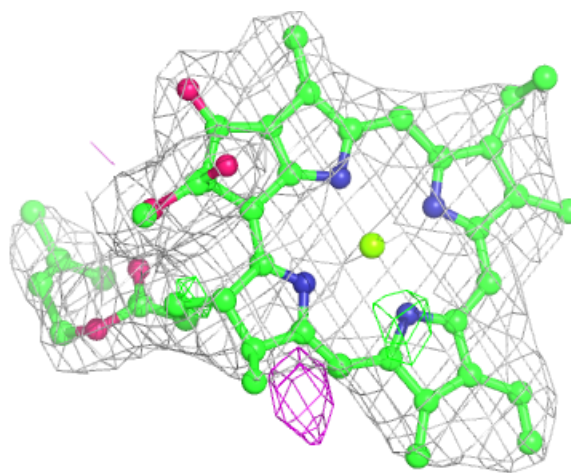
**Electron density around CLA B 802:**

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



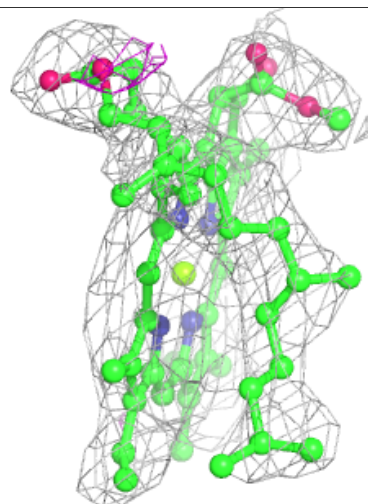
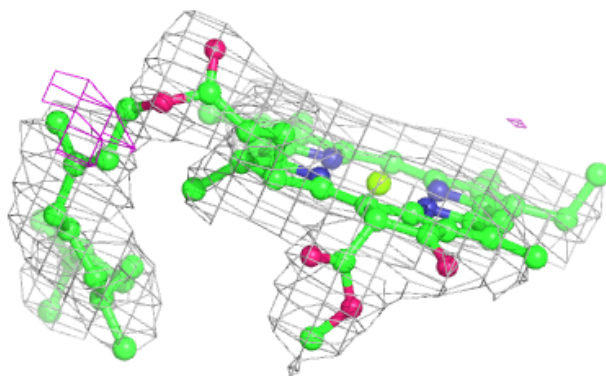
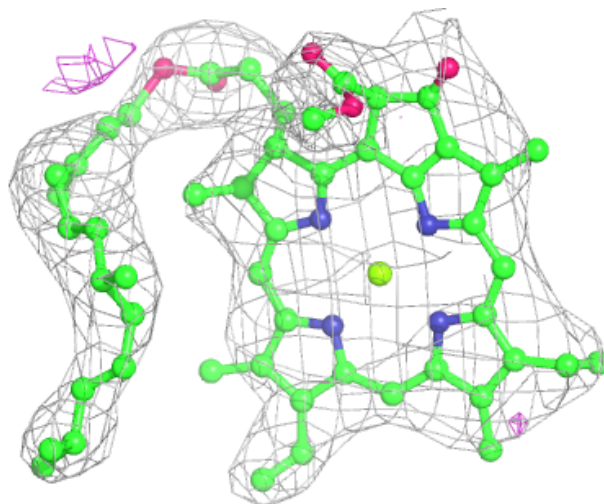
**Electron density around CLA G 838:**

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



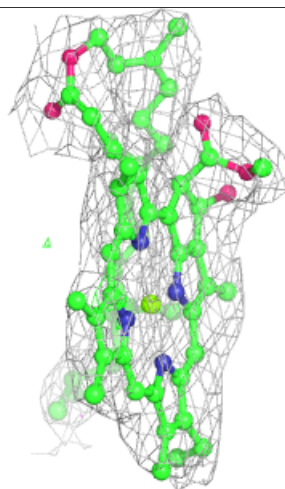
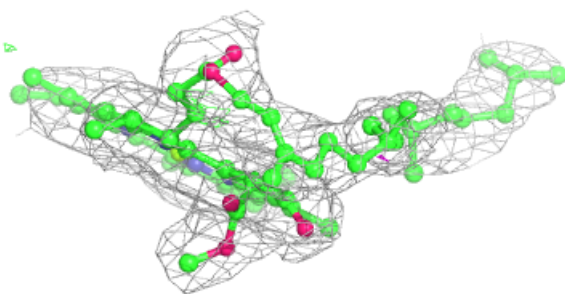
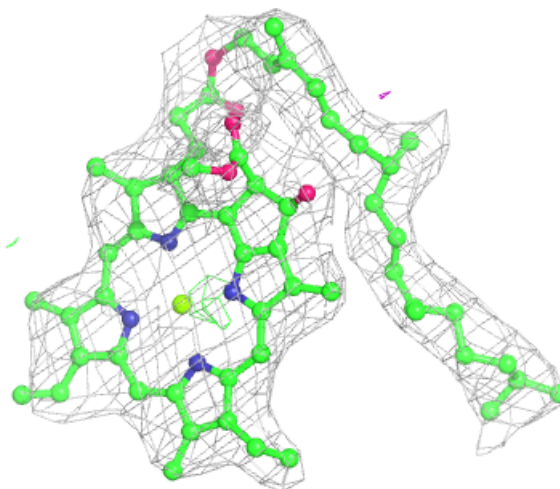
**Electron density around CLA Y 813:**

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



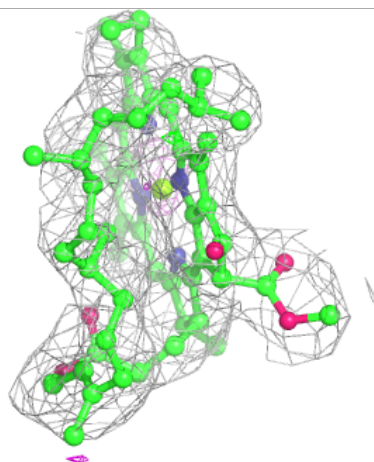
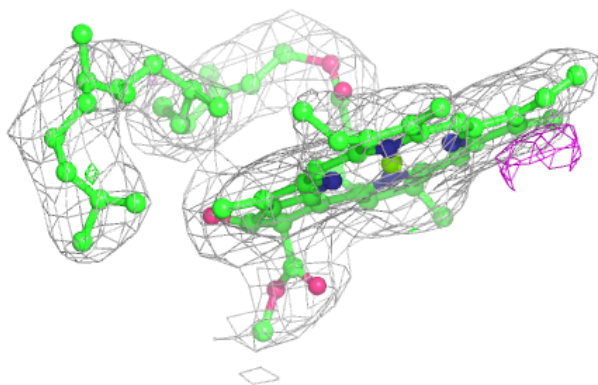
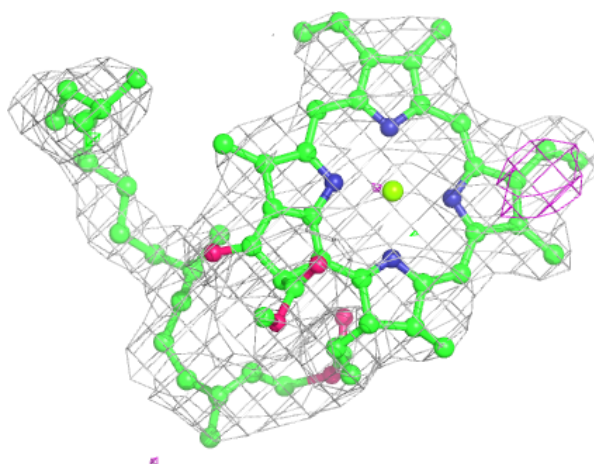
**Electron density around CLA G 825:**

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



**Electron density around CLA B 831:**

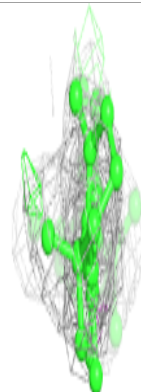
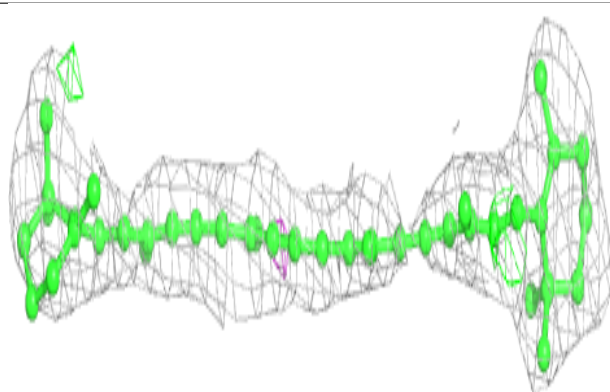
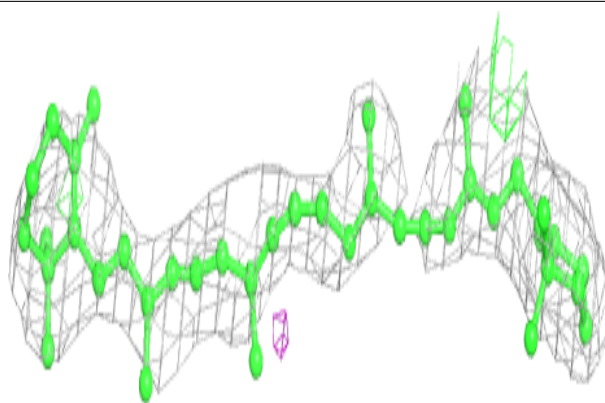
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around BCR G 845:**

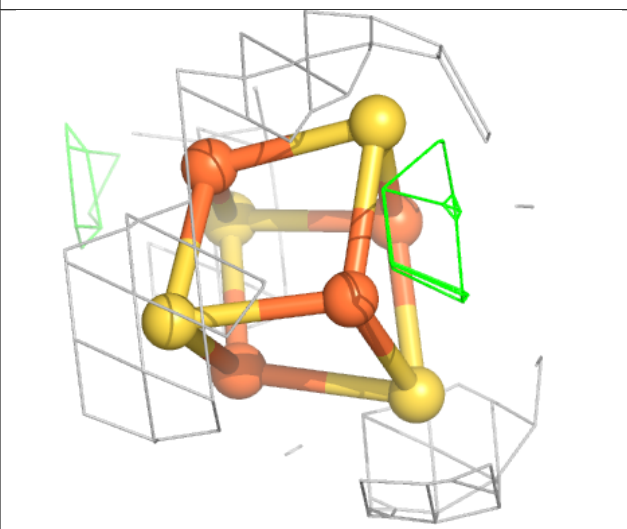
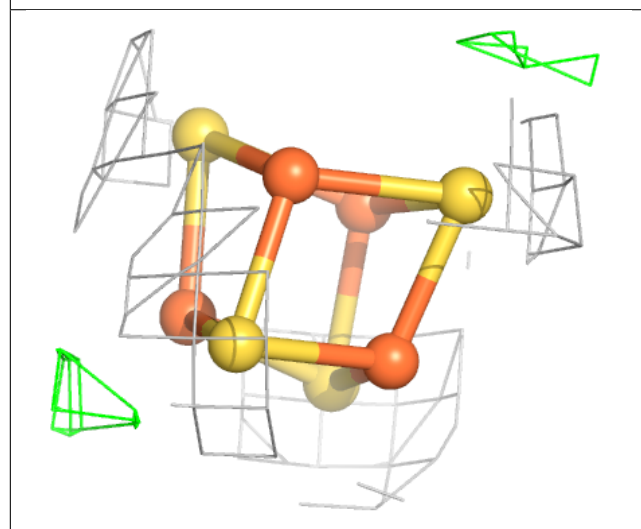
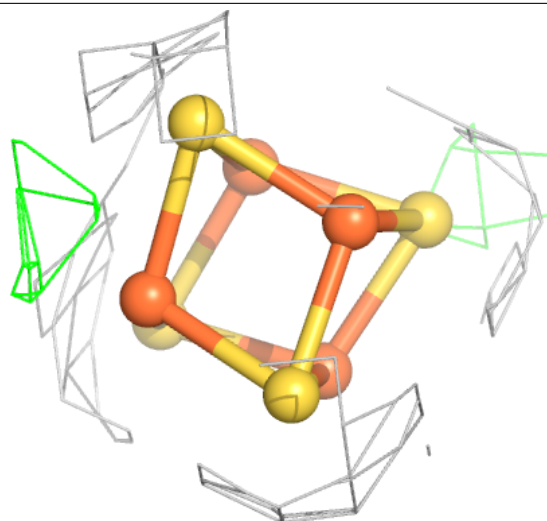
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





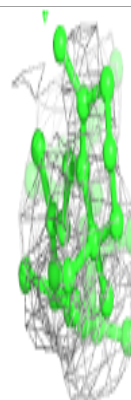
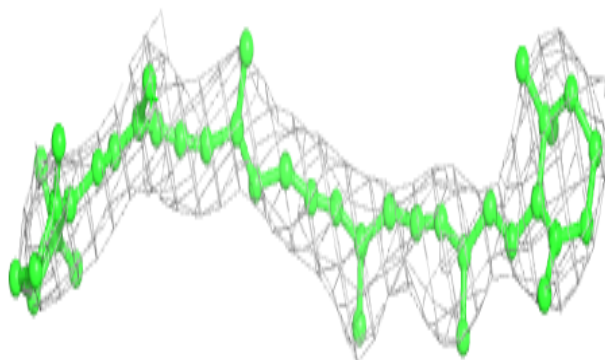
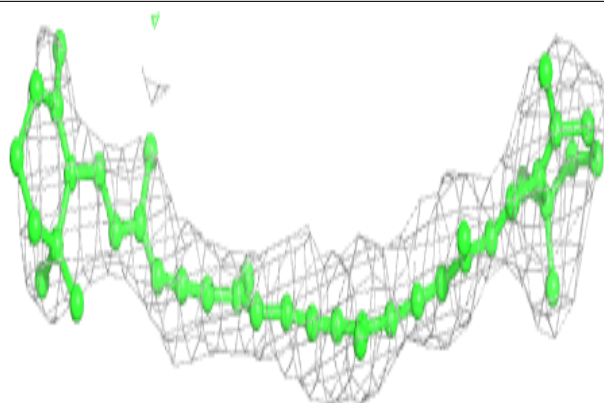
**Electron density around SF4 N 102:**

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

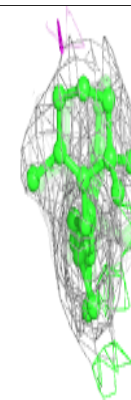
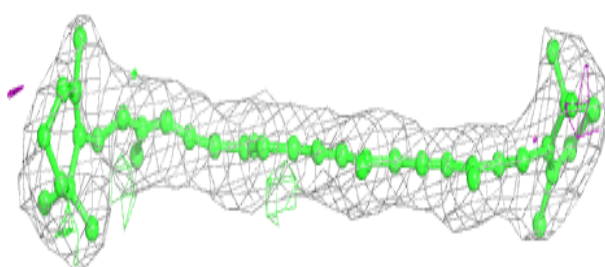
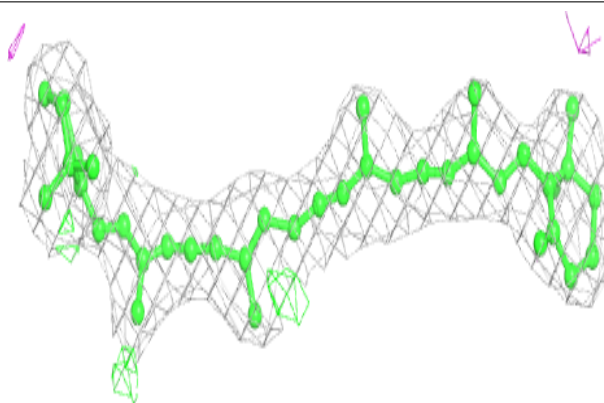


**Electron density around BCR Y 853:**

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

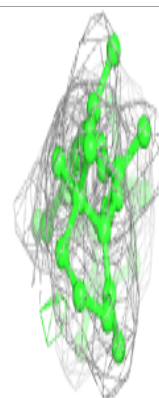
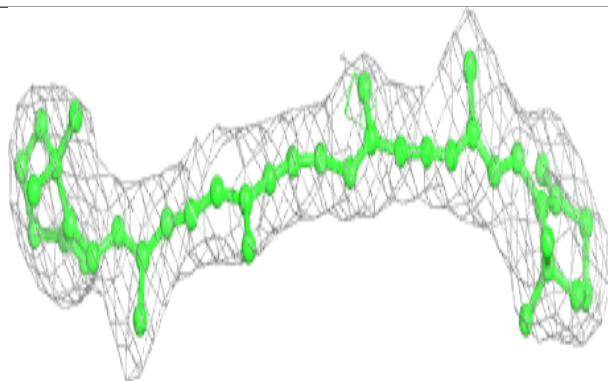
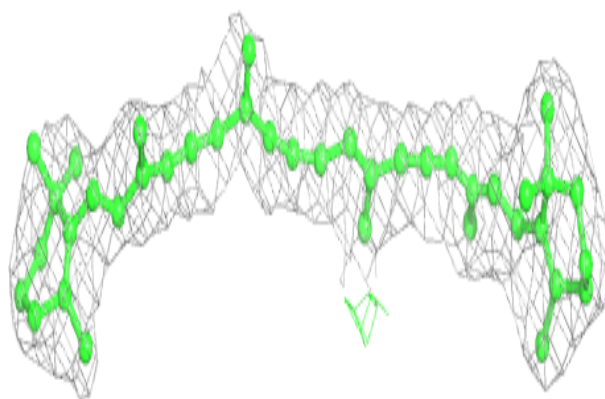
**Electron density around BCR B 847:**

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

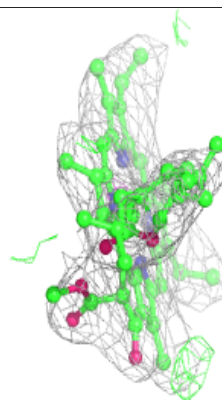
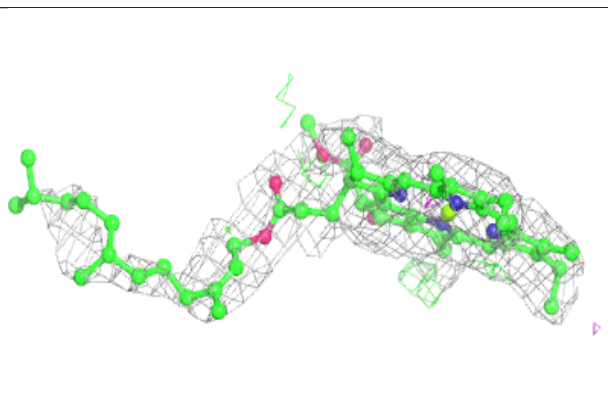
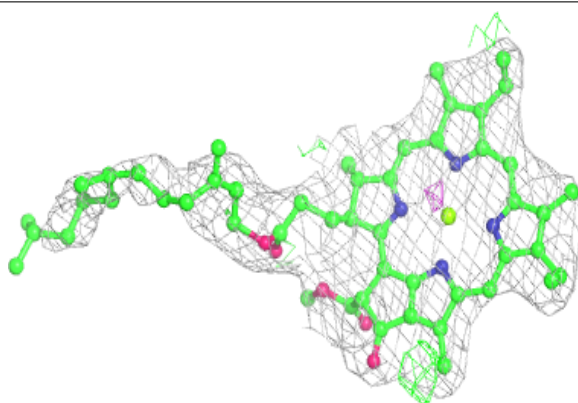


**Electron density around BCR i 101:**

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

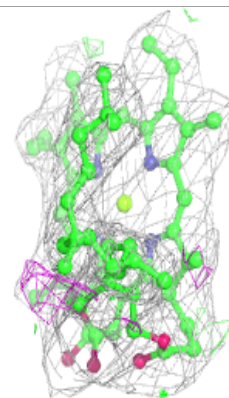
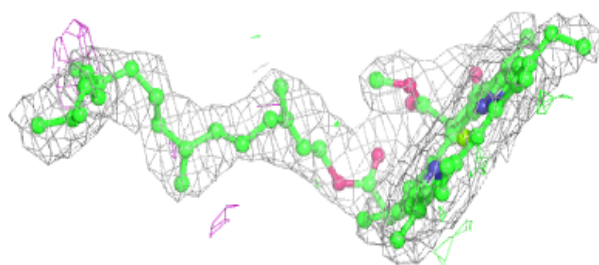
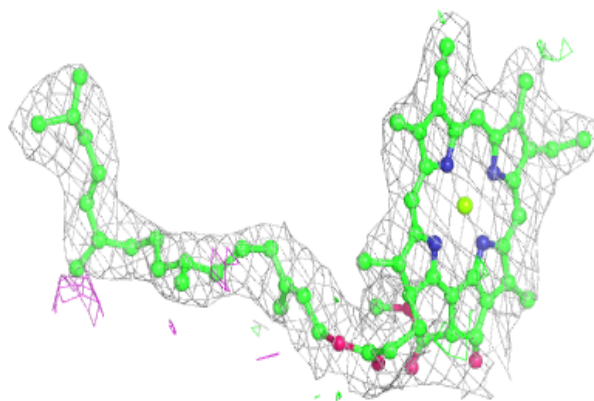
**Electron density around CLA H 823:**

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

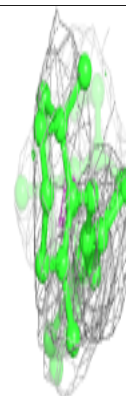
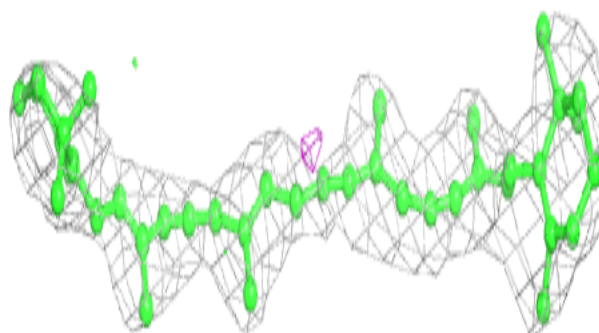
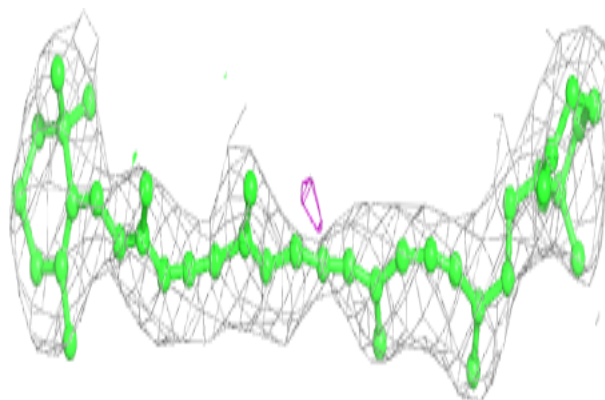


**Electron density around CLA Z 811:**

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

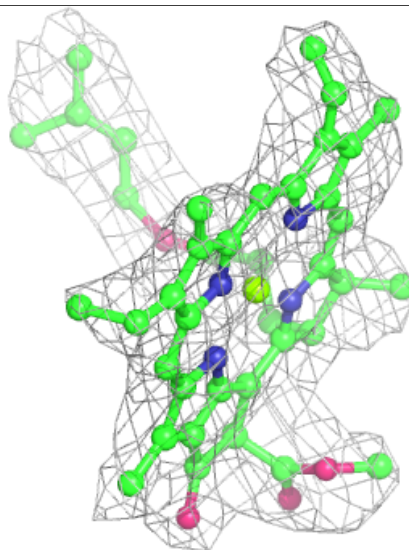
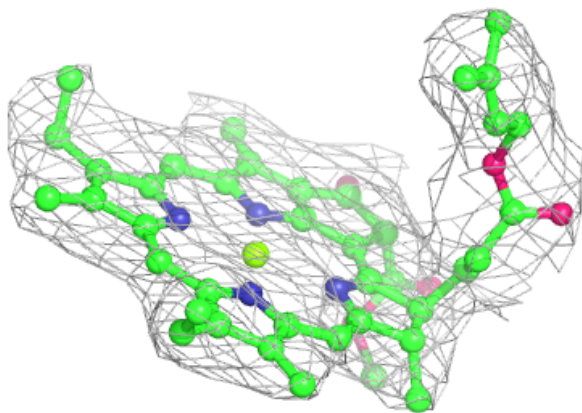
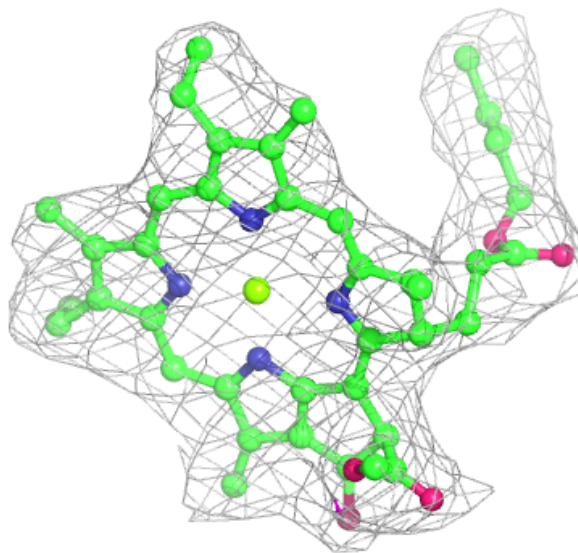
**Electron density around BCR T 102:**

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



**Electron density around CLA G 831:**

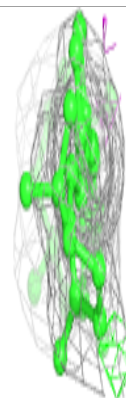
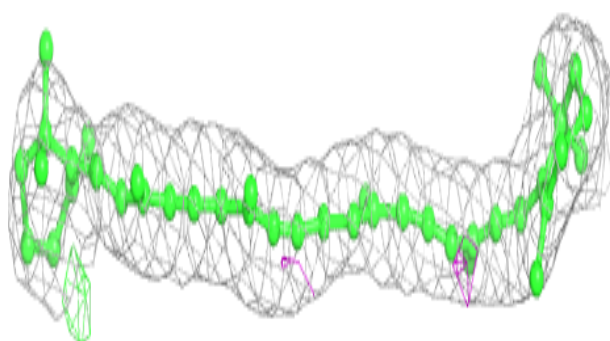
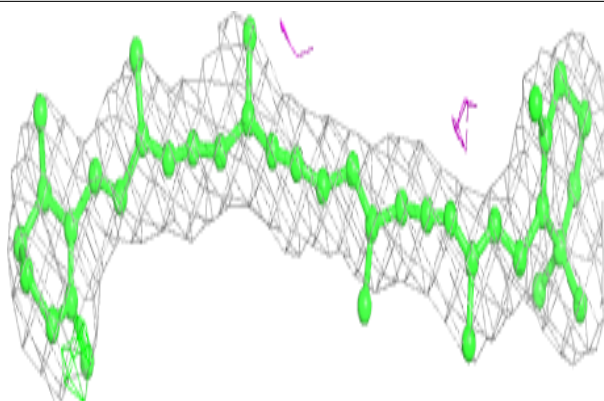
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



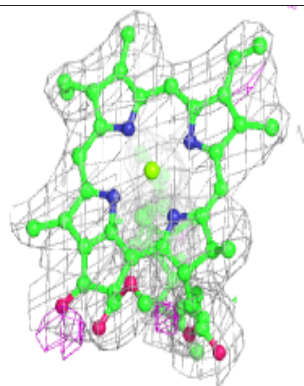
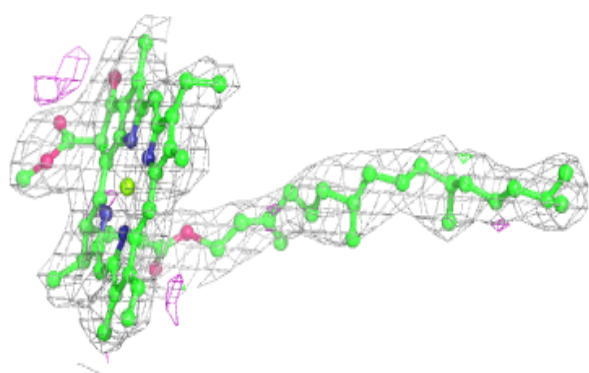
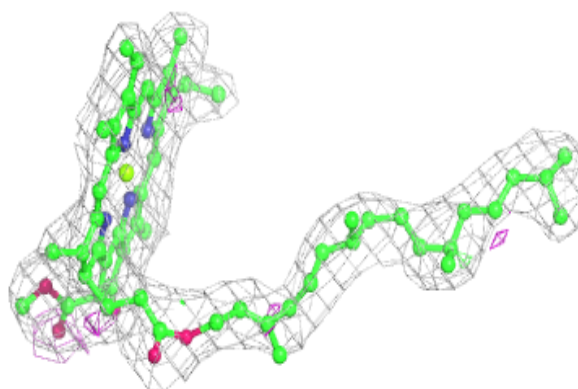


**Electron density around BCR Z 843:**

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

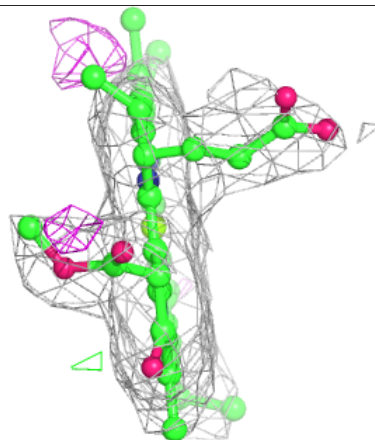
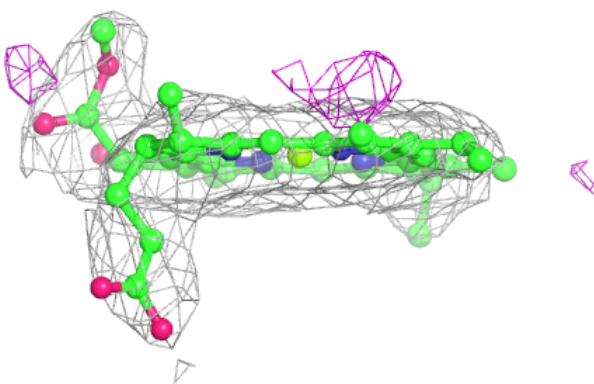
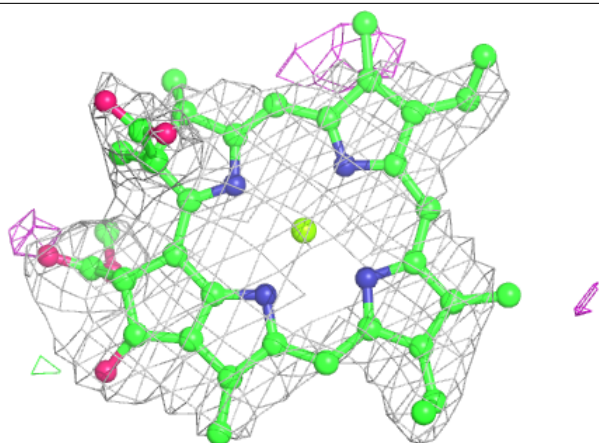
**Electron density around CLA Z 830:**

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

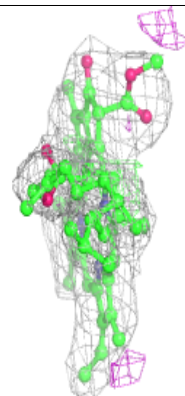
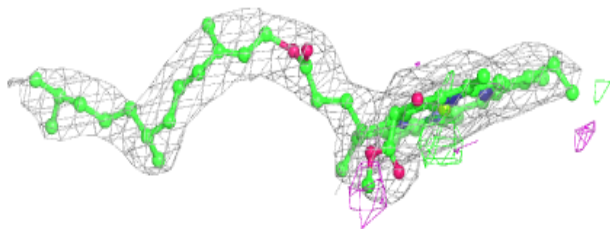
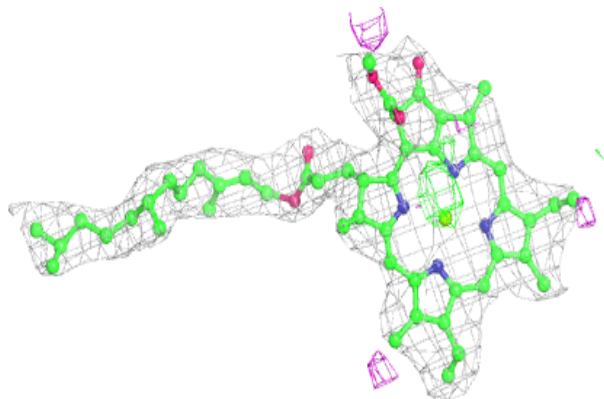


**Electron density around CLA Z 816:**

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

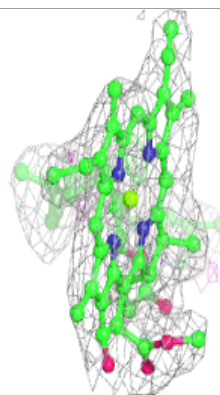
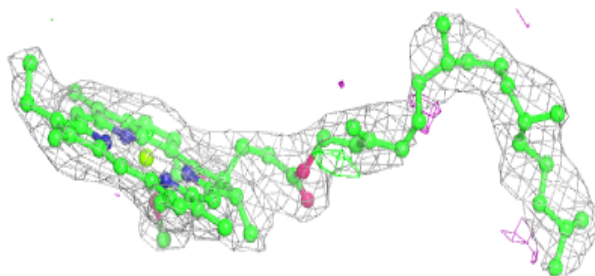
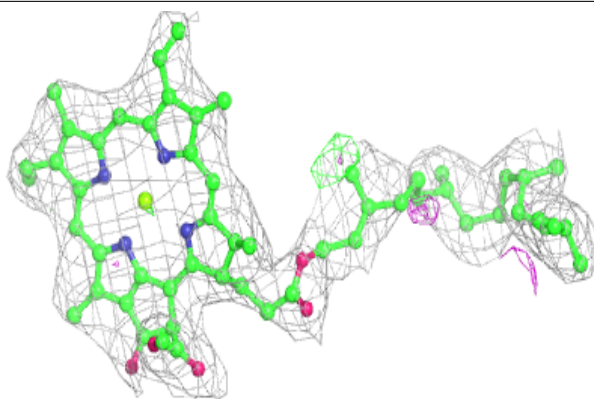
**Electron density around CLA Y 826:**

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

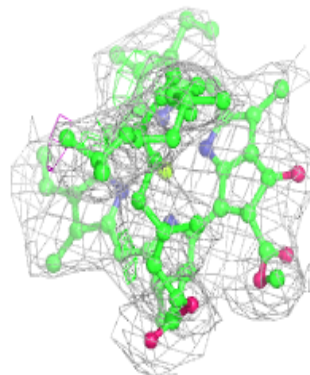
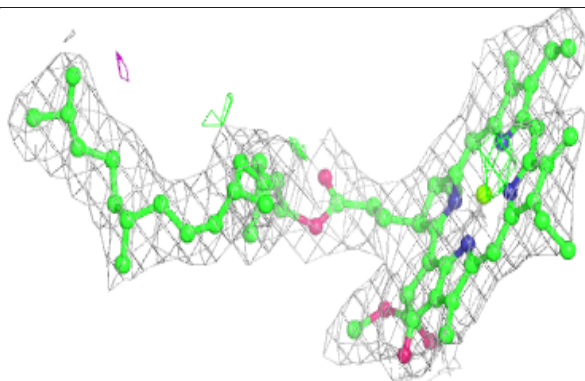
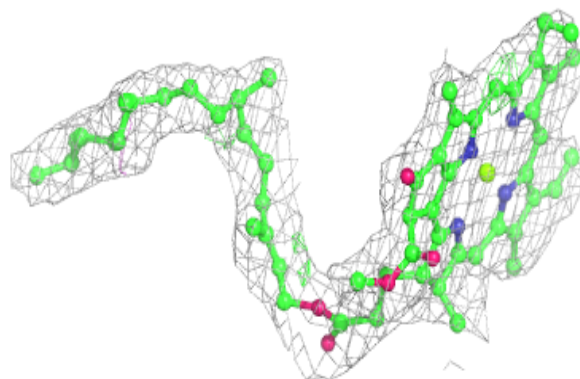


**Electron density around CLA Z 814:**

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

**Electron density around CLA B 801:**

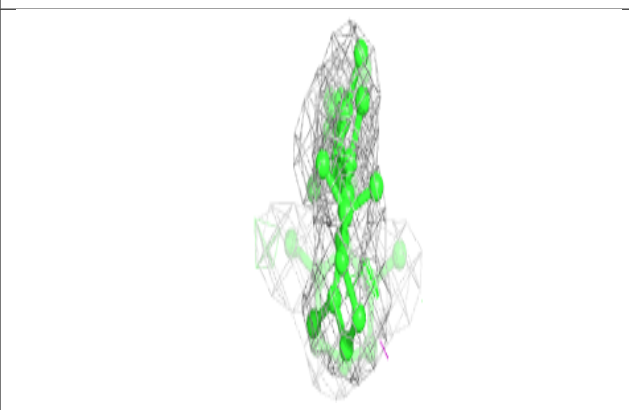
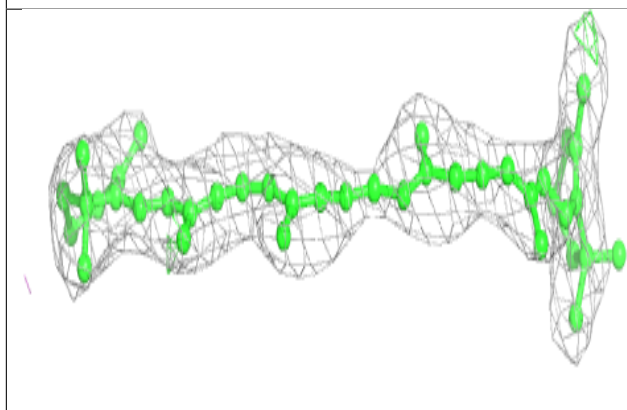
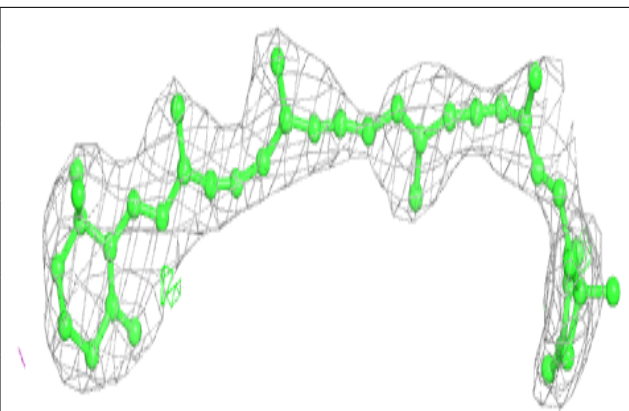
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





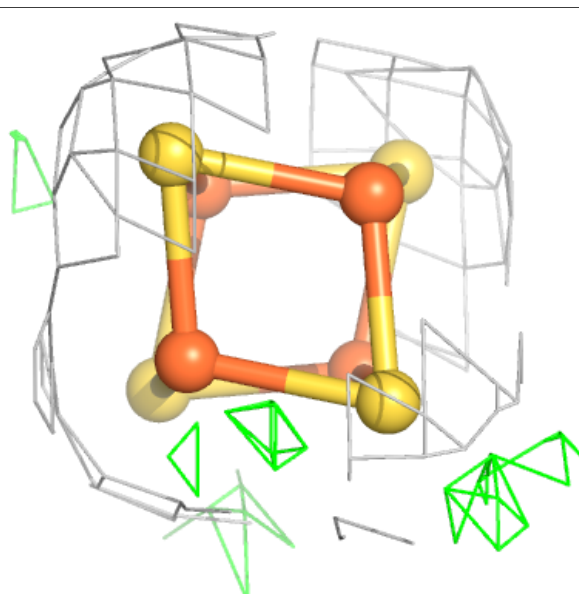
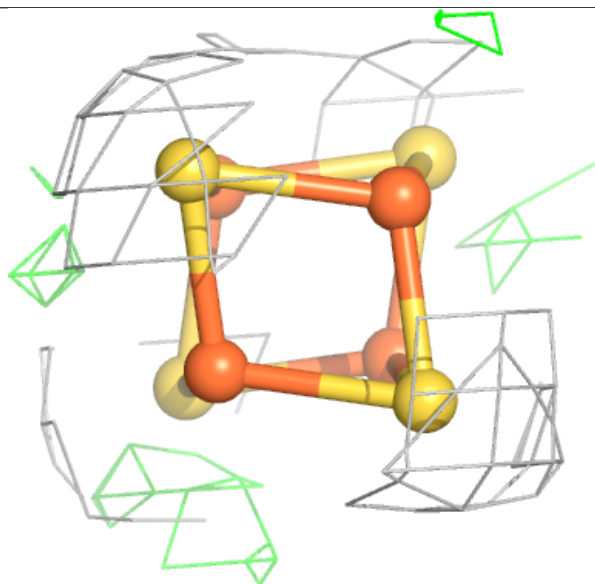
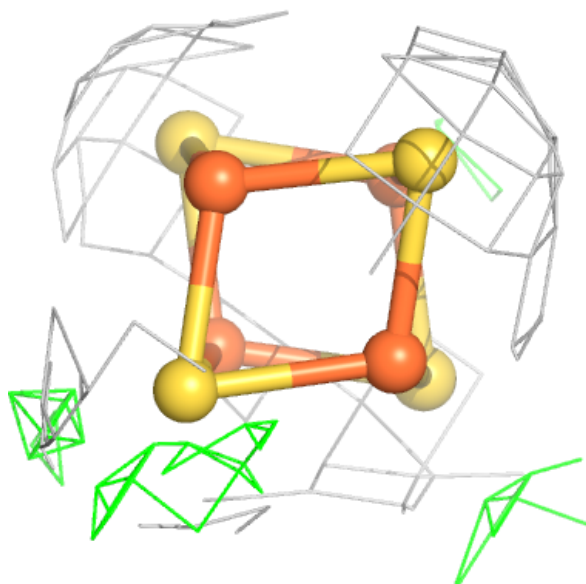
**Electron density around BCR B 843:**

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



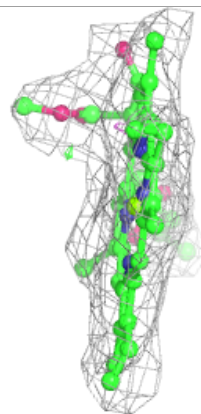
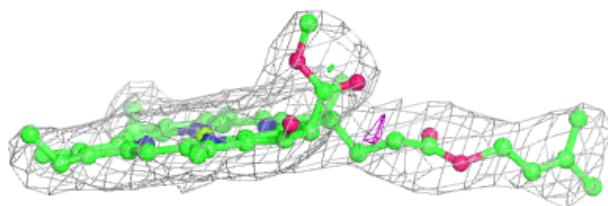
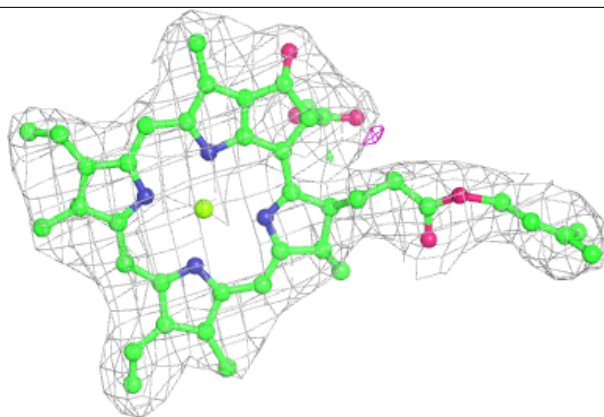
**Electron density around SF4 C 101:**

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



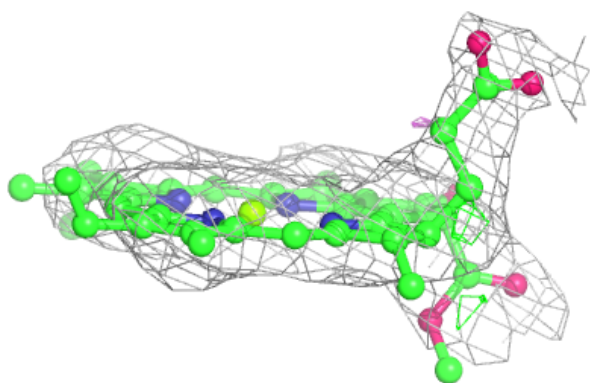
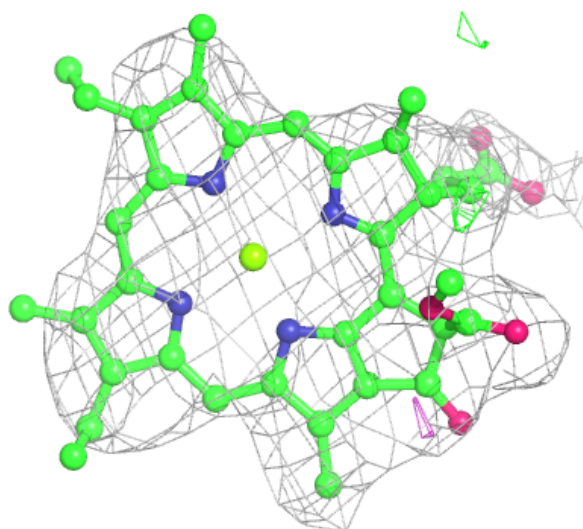
**Electron density around CLA Y 835:**

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



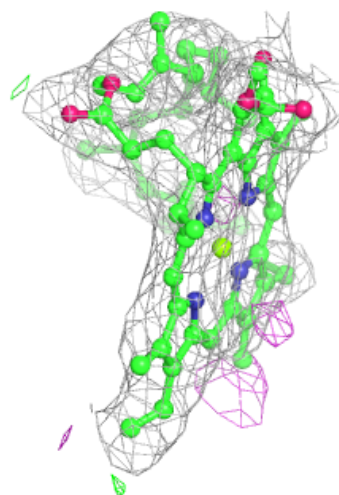
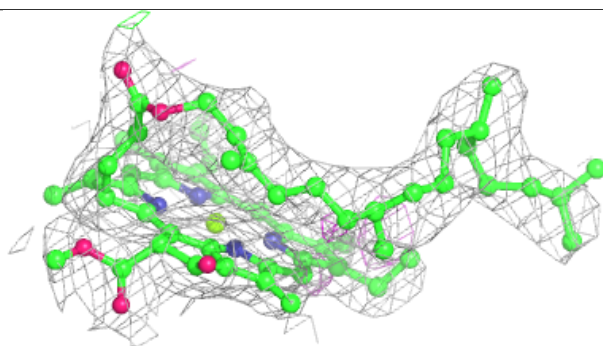
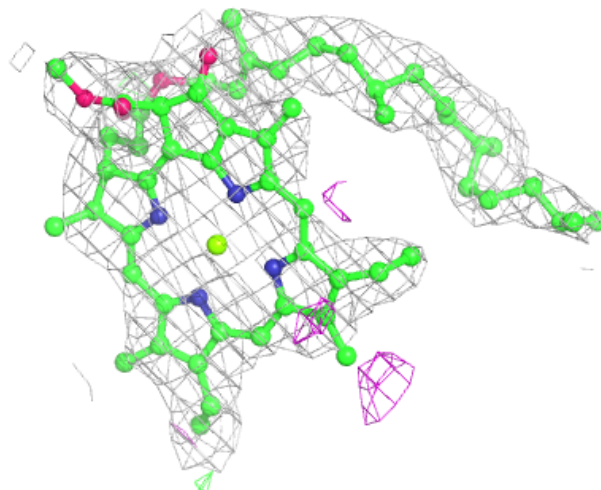
**Electron density around CLA T 103:**

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



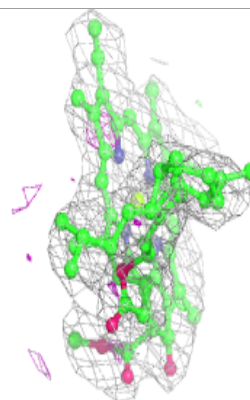
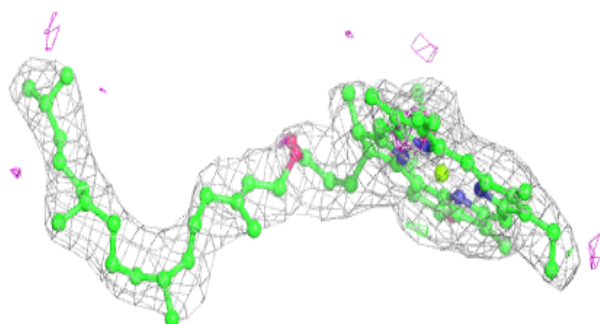
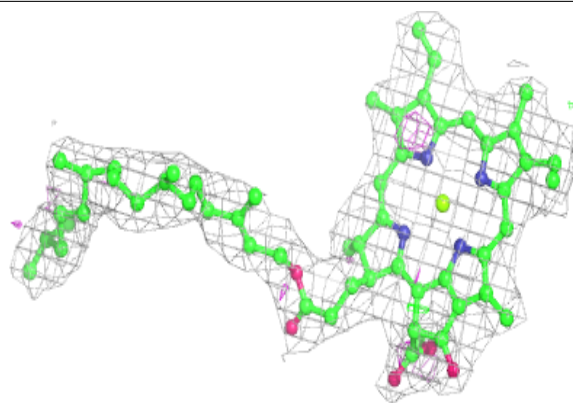
**Electron density around CLA A 830:**

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

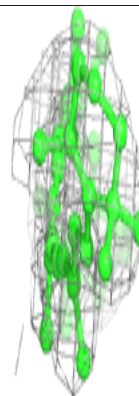
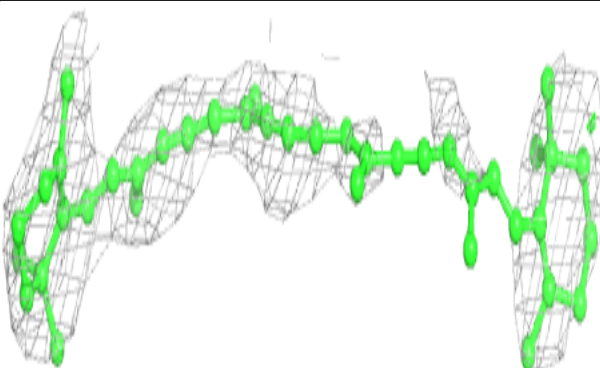
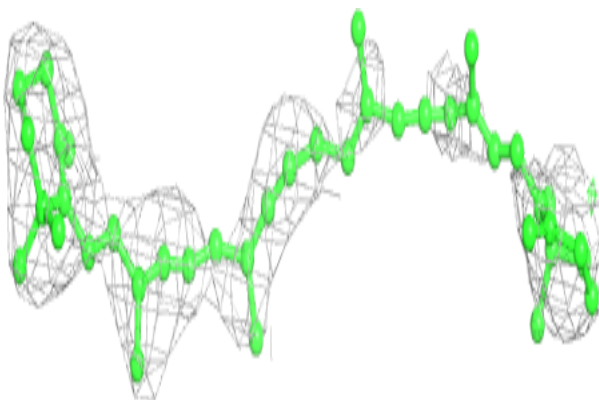


**Electron density around CLA B 812:**

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

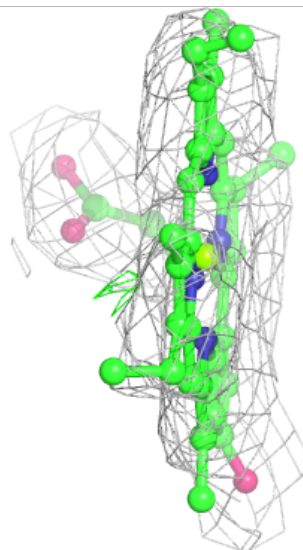
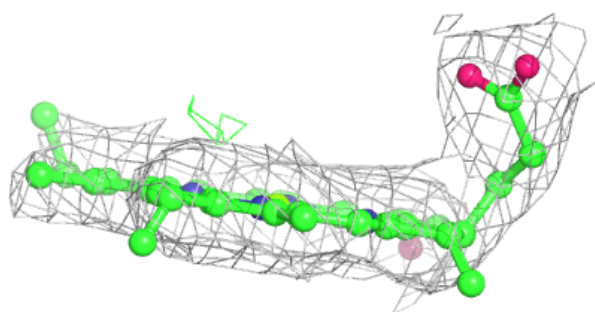
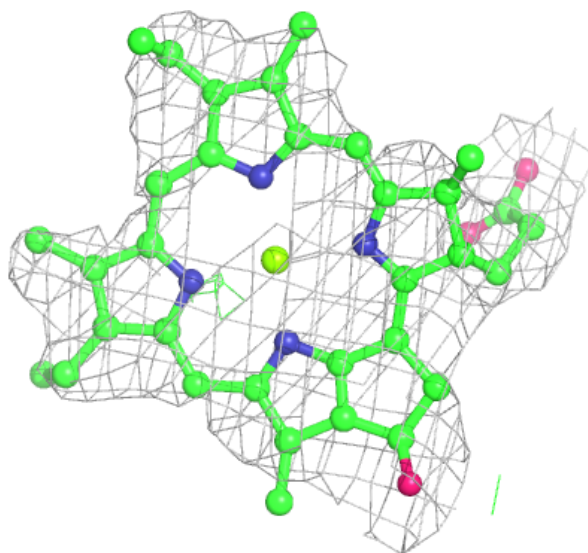
**Electron density around BCR Y 846:**

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



**Electron density around CLA K 101:**

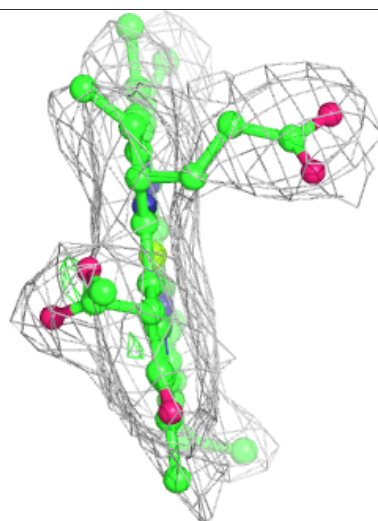
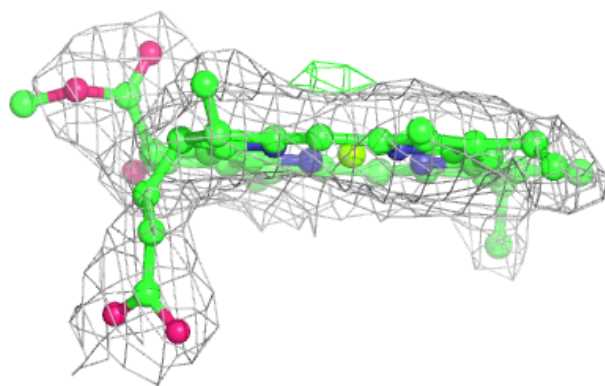
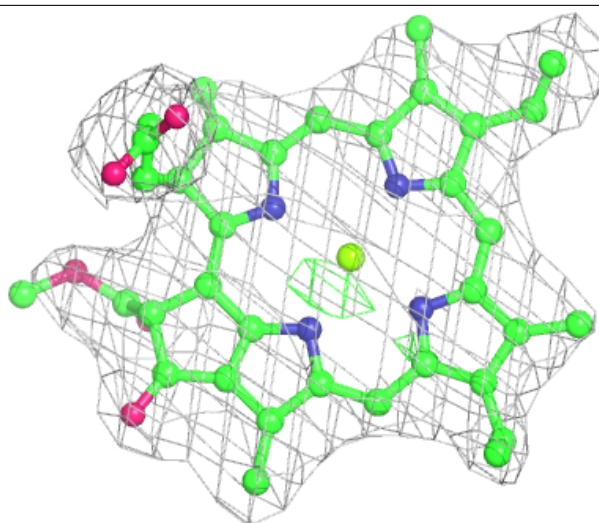
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA H 834:**

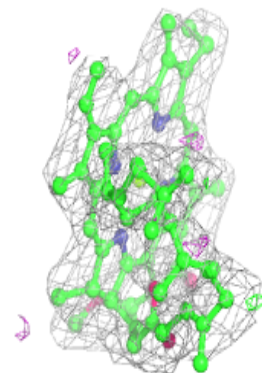
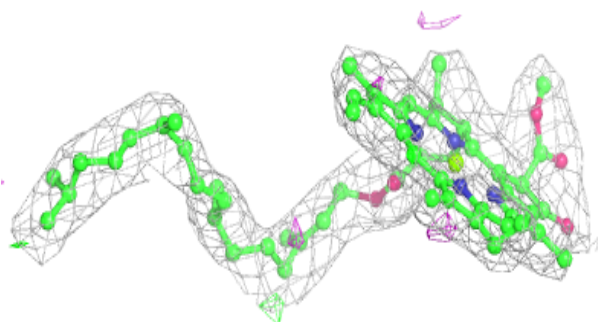
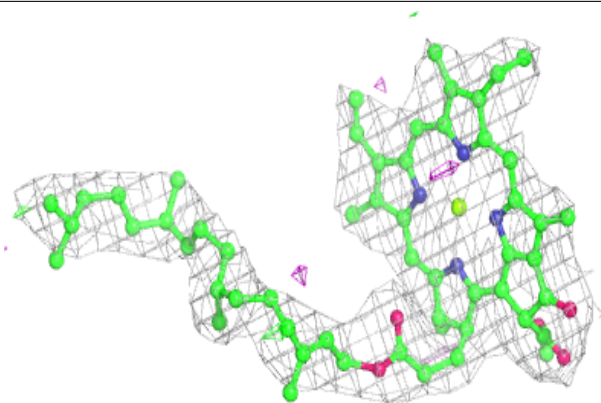
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



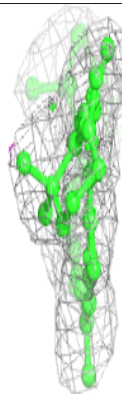
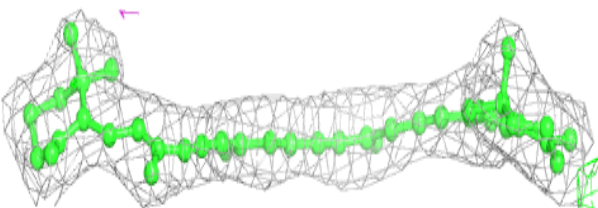
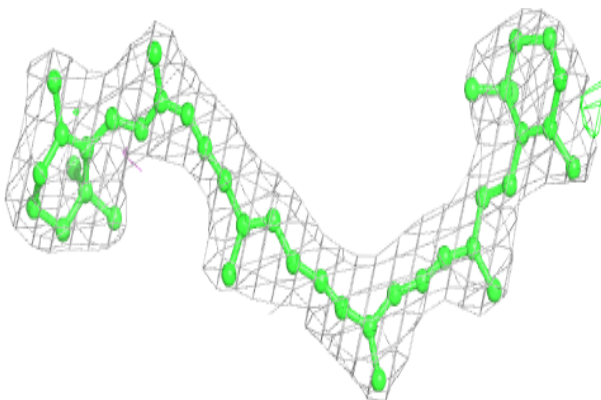


**Electron density around CLA A 809:**

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

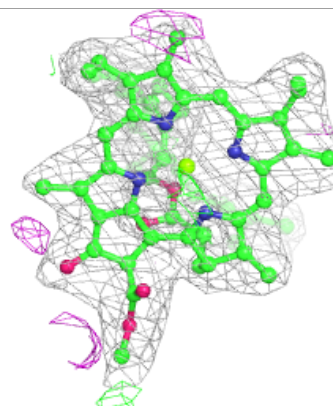
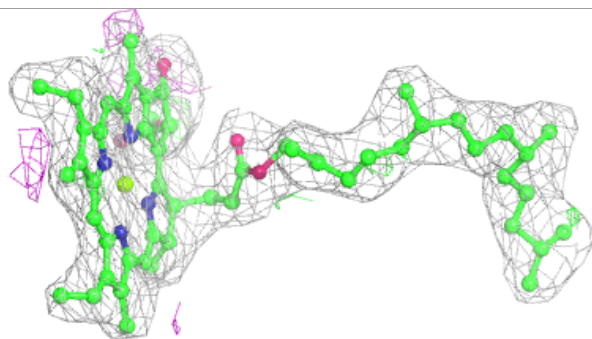
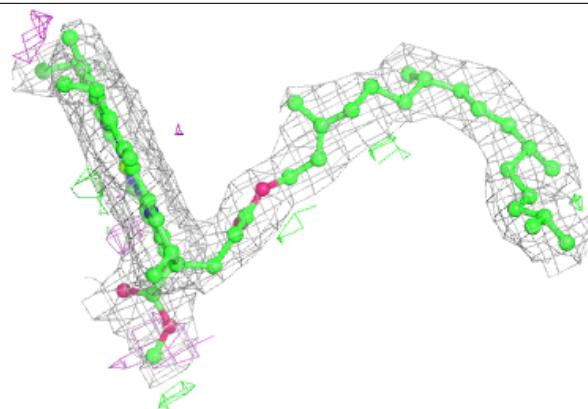
**Electron density around BCR G 849:**

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

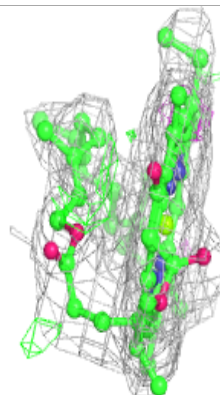
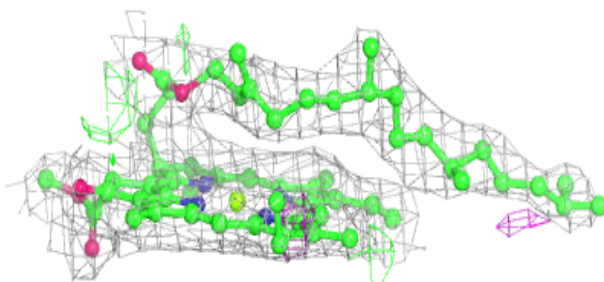
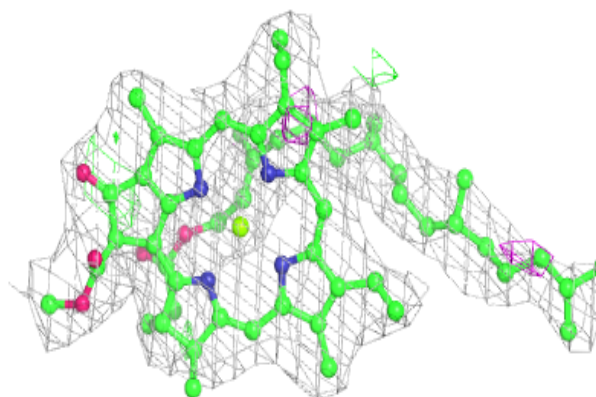


**Electron density around CLA Z 840:**

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

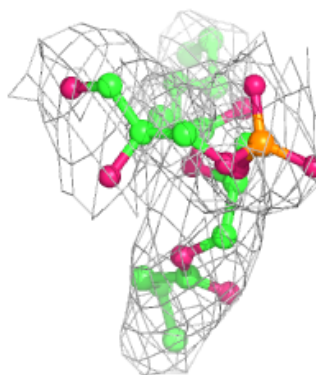
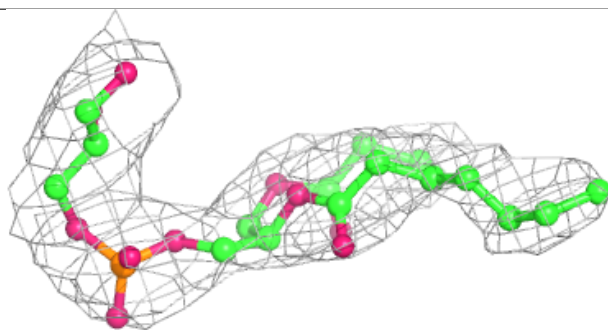
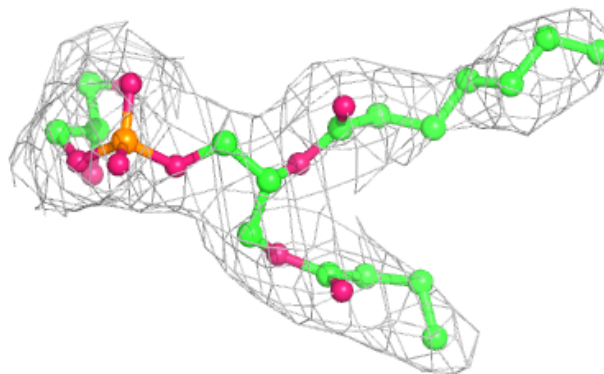
**Electron density around CLA H 801:**

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

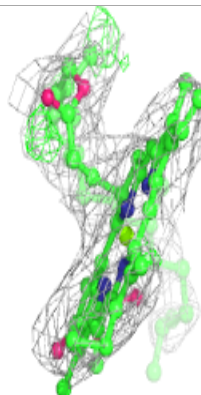
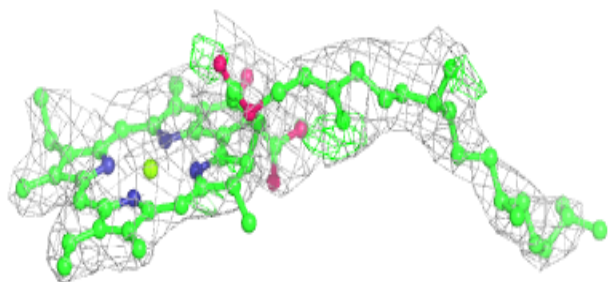
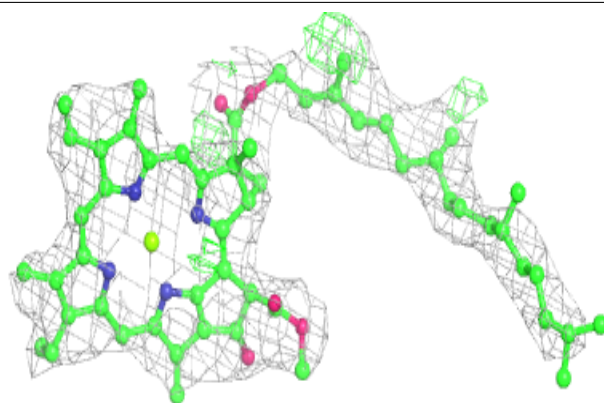


**Electron density around LHG j 101:**

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

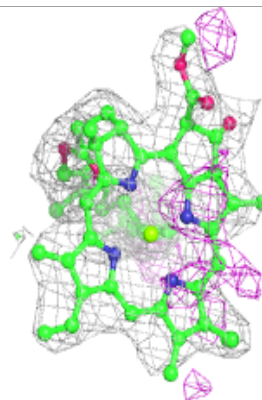
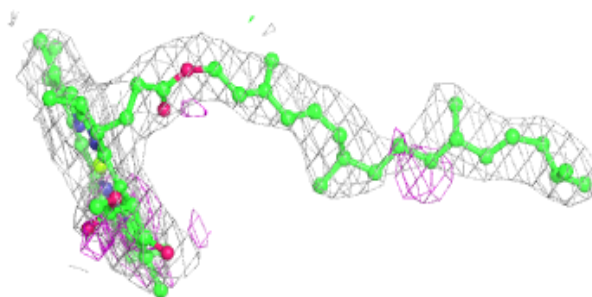
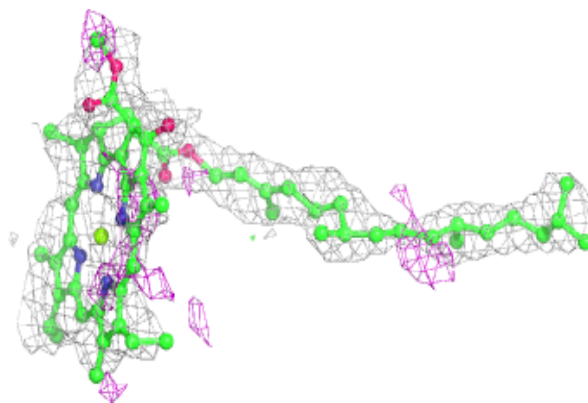
**Electron density around CLA A 823:**

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



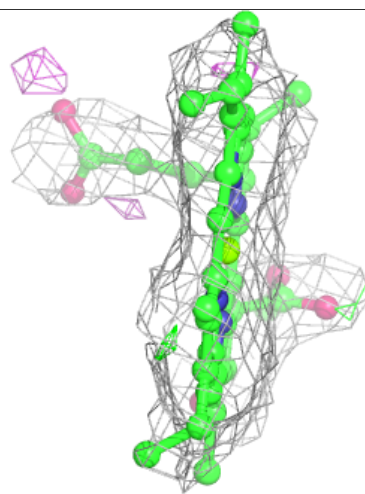
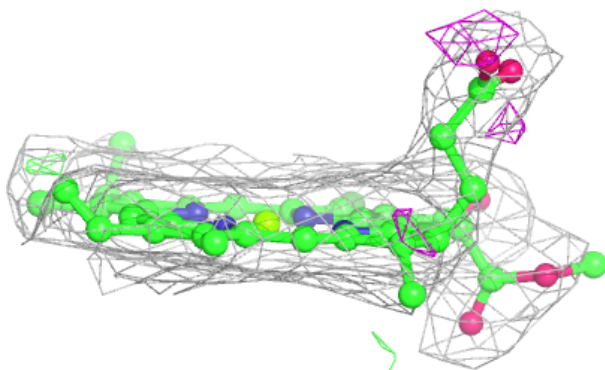
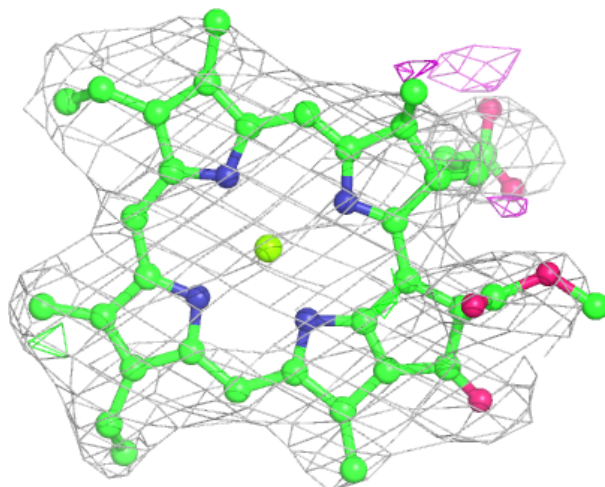
**Electron density around CLA H 828:**

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



**Electron density around CLA B 834:**

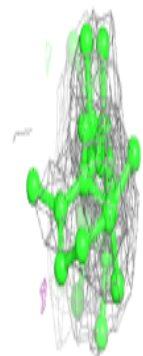
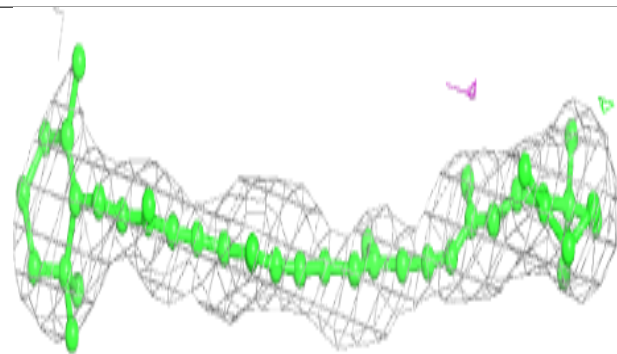
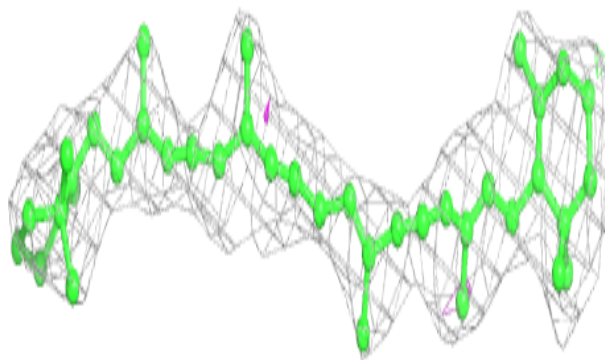
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





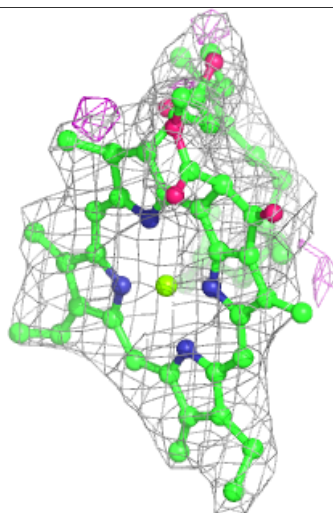
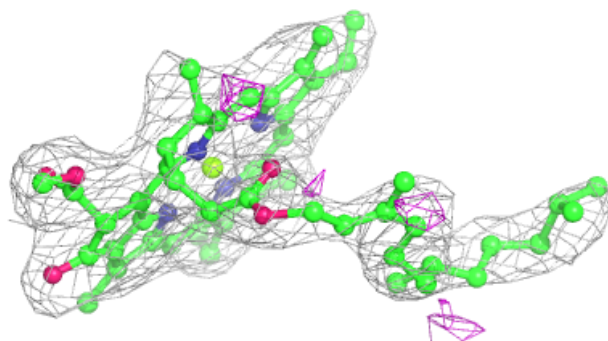
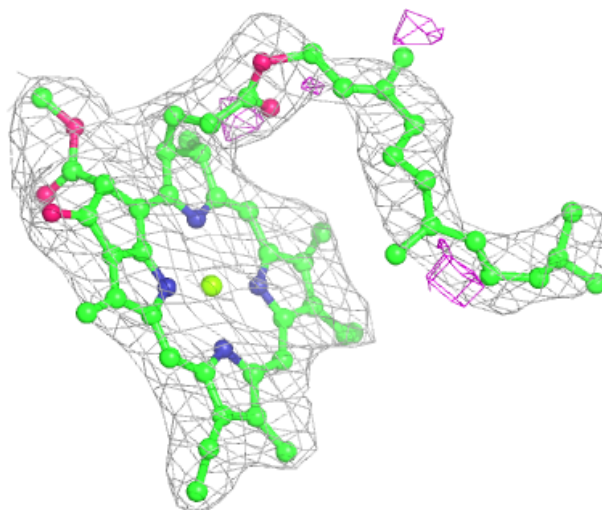
**Electron density around BCR B 850:**

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



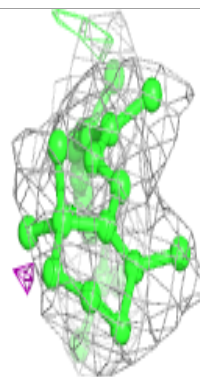
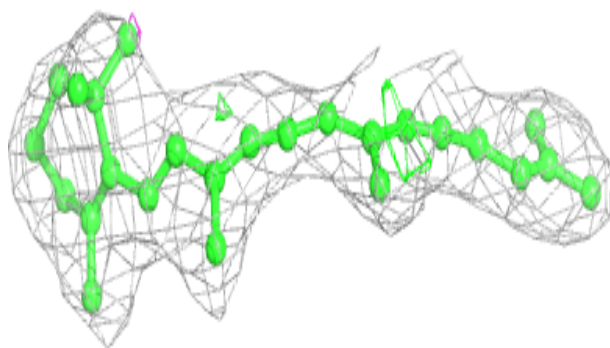
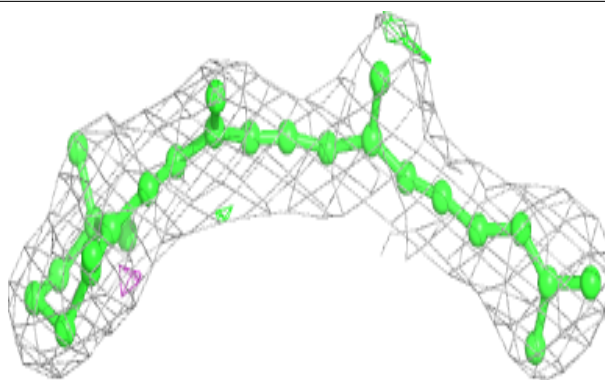
**Electron density around CLA A 825:**

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



**Electron density around BCR Z 846:**

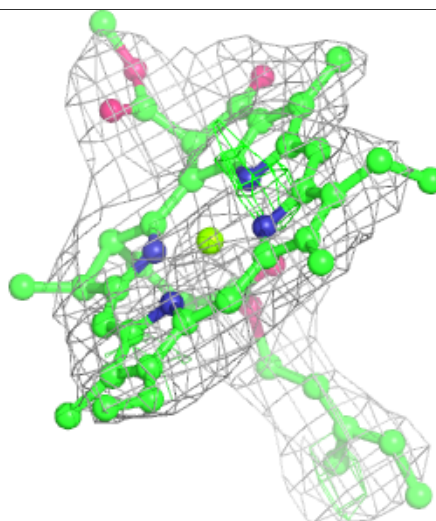
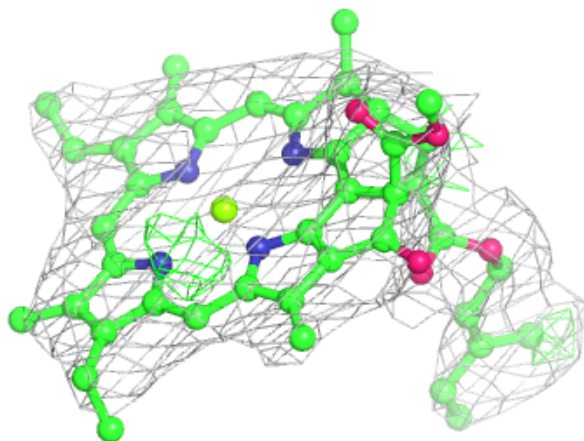
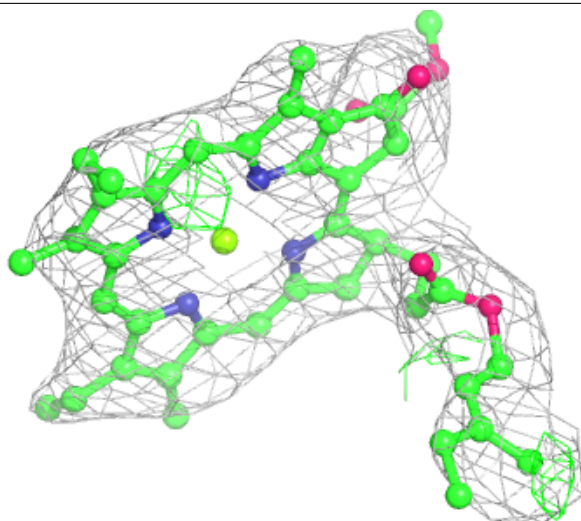
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





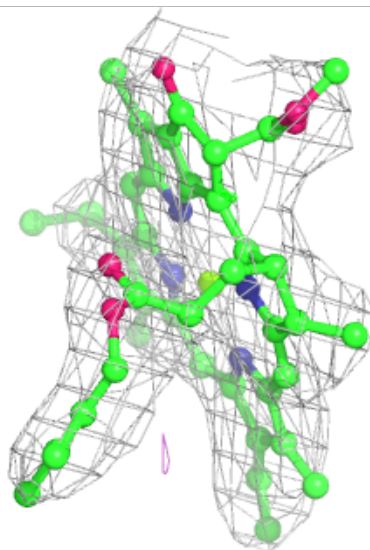
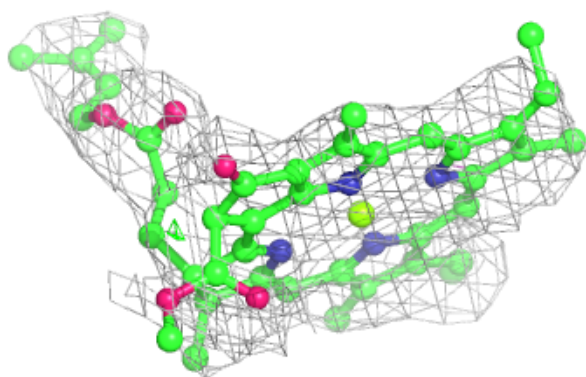
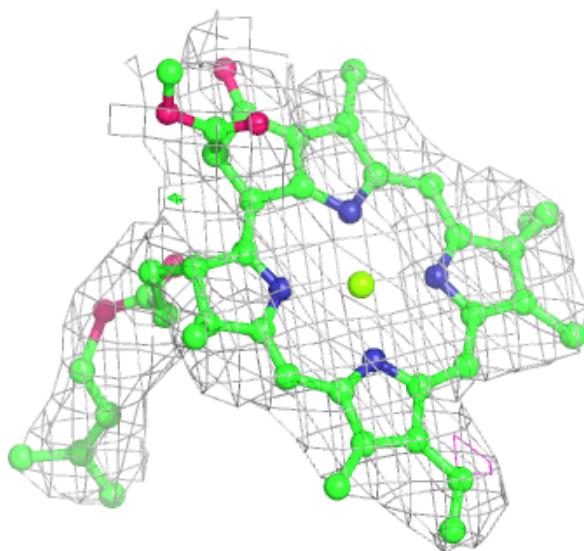
**Electron density around CLA Y 807:**

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



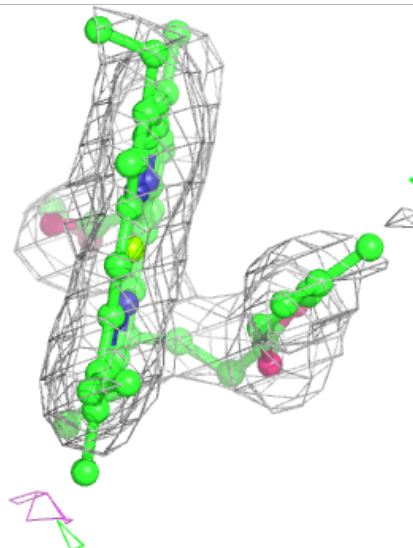
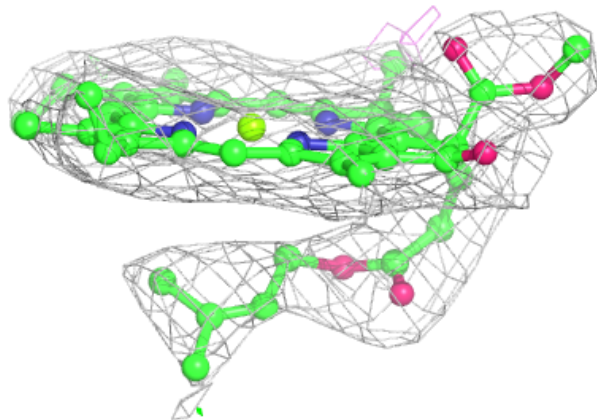
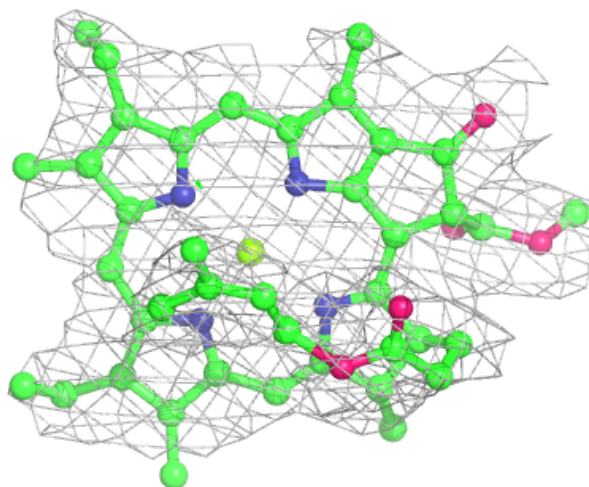
**Electron density around CLA Y 815:**

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



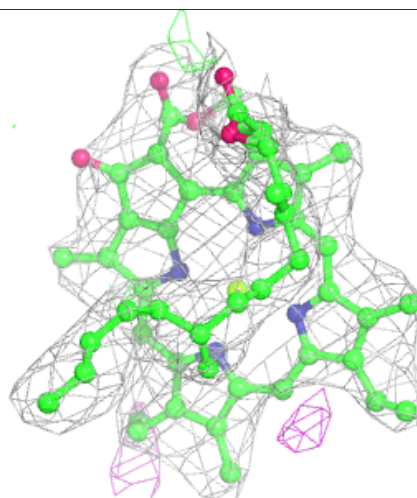
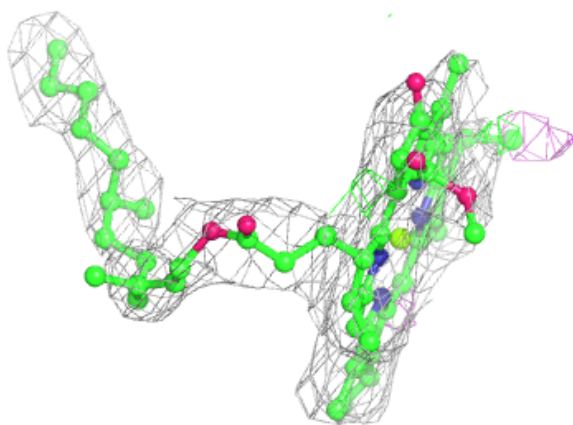
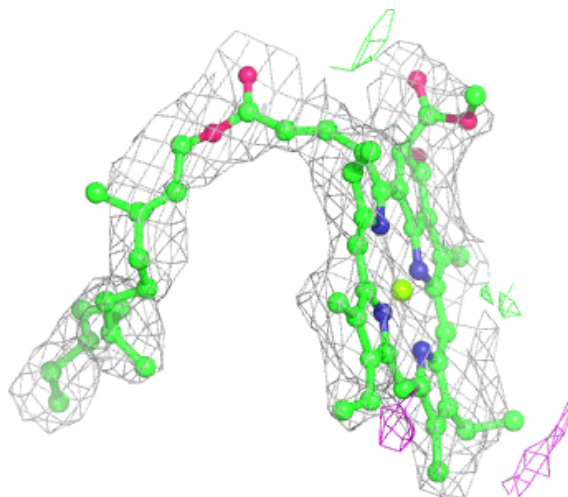
**Electron density around CLA Y 823:**

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



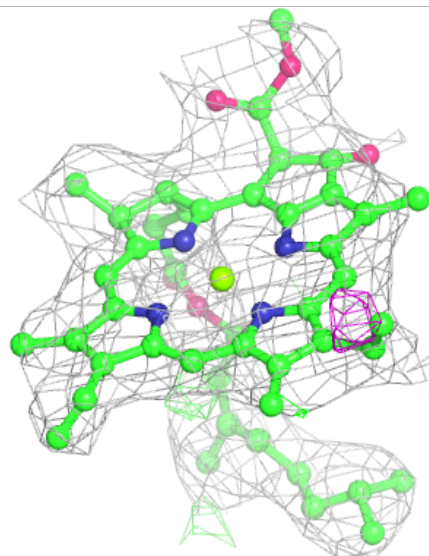
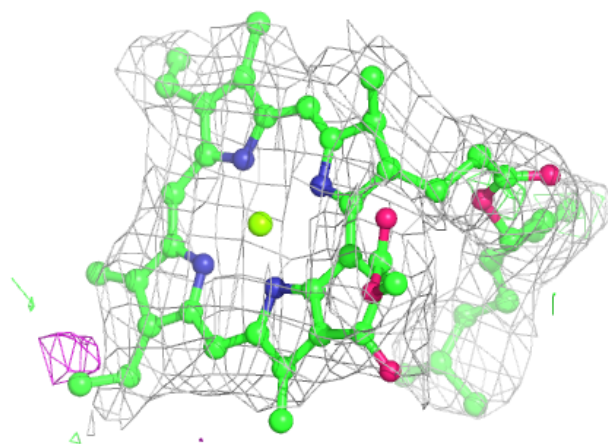
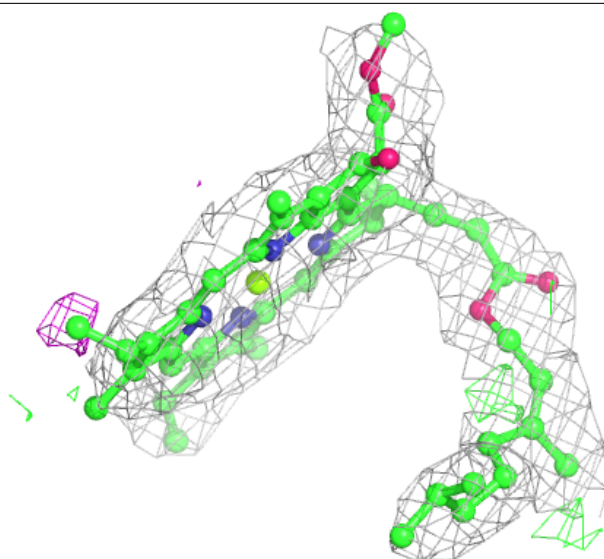
**Electron density around CLA Y 804:**

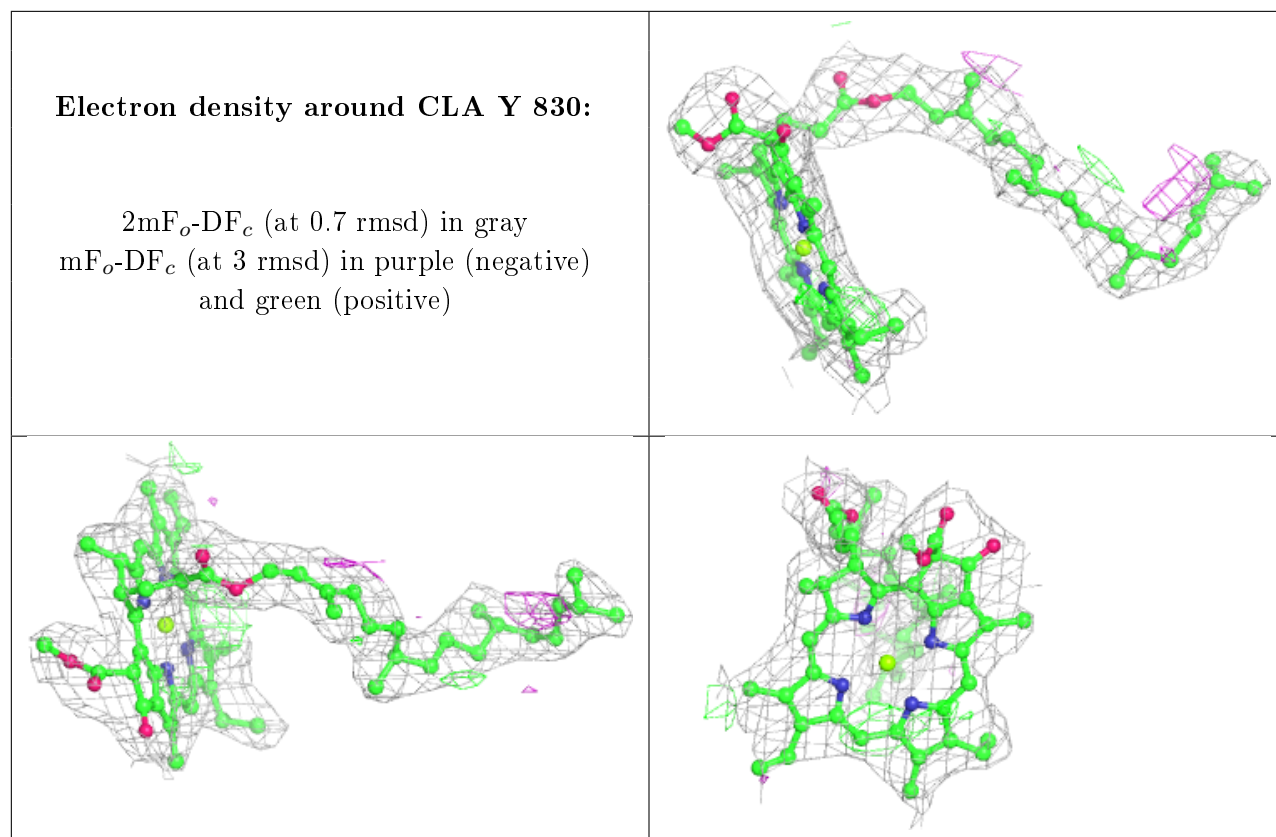
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 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)





## 6.5 Other polymers [i](#)

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