



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 11:35 AM UTC

PDB ID : 6PFY / pdb_00006pfy
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

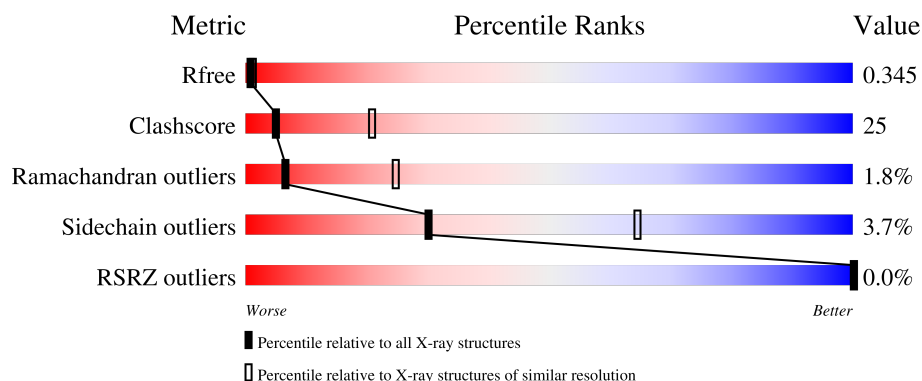
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



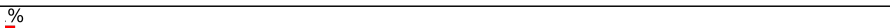
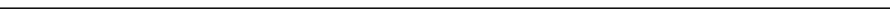
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	755	
1	G	755	
1	Y	755	
2	B	741	
2	H	741	

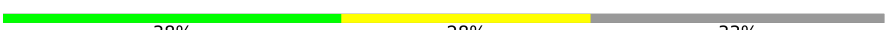
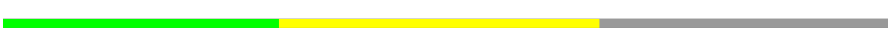
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Mol	Chain	Length	Quality of chain
2	Z	741	
3	C	81	
3	N	81	
3	a	81	
4	D	139	
4	O	139	
4	b	139	
5	E	76	
5	P	76	
5	c	76	
6	F	164	
6	Q	164	
6	d	164	
7	I	38	
7	R	38	
7	e	38	
8	J	41	
8	S	41	
8	f	41	
9	K	83	
9	T	83	
9	g	83	
10	L	155	
10	U	155	
10	h	155	

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Mol	Chain	Length	Quality of chain
11	M	31	
11	V	31	
11	i	31	
12	W	39	
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	826	X	-	-	-
14	CLA	A	827	X	-	-	-
14	CLA	A	828	X	-	-	-
14	CLA	A	829	X	-	X	-
14	CLA	A	830	X	-	-	-
14	CLA	A	831	X	-	-	-
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	839	X	-	-	-
14	CLA	A	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	842	X	-	-	-
14	CLA	A	843	X	-	-	-
14	CLA	A	854	X	-	-	-
14	CLA	B	801	X	-	X	-
14	CLA	B	802	X	-	-	-
14	CLA	B	803	X	-	-	-
14	CLA	B	804	X	-	-	-
14	CLA	B	805	X	-	-	-
14	CLA	B	806	X	-	-	-
14	CLA	B	807	X	-	-	-
14	CLA	B	808	X	-	-	-
14	CLA	B	809	X	-	-	-
14	CLA	B	810	X	-	-	-
14	CLA	B	811	X	-	-	-
14	CLA	B	812	X	-	-	-
14	CLA	B	813	X	-	-	-
14	CLA	B	814	X	-	-	-
14	CLA	B	815	X	-	-	-
14	CLA	B	816	X	-	-	-
14	CLA	B	817	X	-	-	-
14	CLA	B	818	X	-	-	-
14	CLA	B	819	X	-	-	-
14	CLA	B	820	X	-	-	-
14	CLA	B	821	X	-	-	-
14	CLA	B	822	X	-	-	-
14	CLA	B	823	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	824	X	-	-	-
14	CLA	B	825	X	-	-	-
14	CLA	B	826	X	-	-	-
14	CLA	B	827	X	-	-	-
14	CLA	B	828	X	-	-	-
14	CLA	B	829	X	-	-	-
14	CLA	B	830	X	-	-	-
14	CLA	B	831	X	-	-	-
14	CLA	B	832	X	-	-	-
14	CLA	B	833	X	-	-	-
14	CLA	B	834	X	-	-	-
14	CLA	B	835	X	-	-	-
14	CLA	B	836	X	-	-	-
14	CLA	B	837	X	-	-	-
14	CLA	B	838	X	-	-	-
14	CLA	B	839	X	-	-	-
14	CLA	B	840	X	-	-	-
14	CLA	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
16	SF4	A	845	-	-	X	-
16	SF4	N	101	-	-	X	-
16	SF4	N	102	-	-	X	-
16	SF4	Y	843	-	-	X	-

2 Entry composition

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

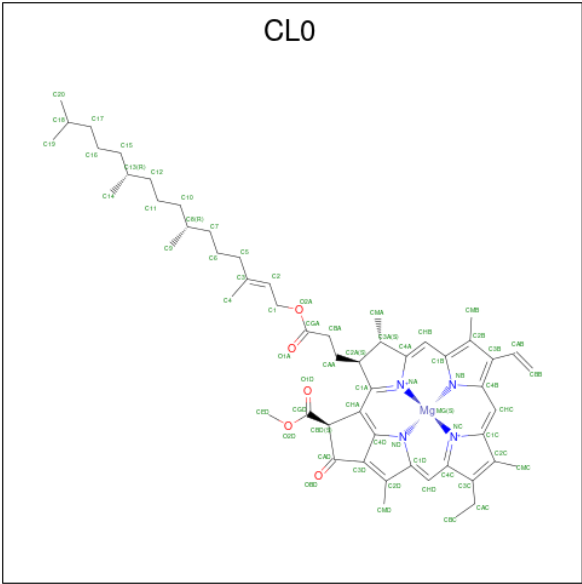
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

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 (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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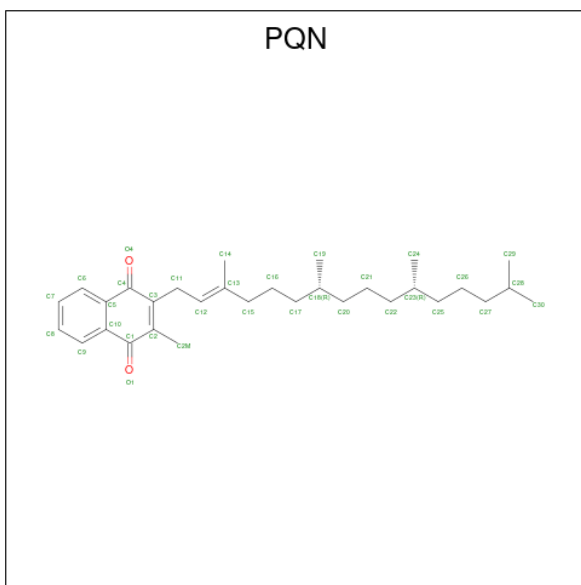
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	Z	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5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

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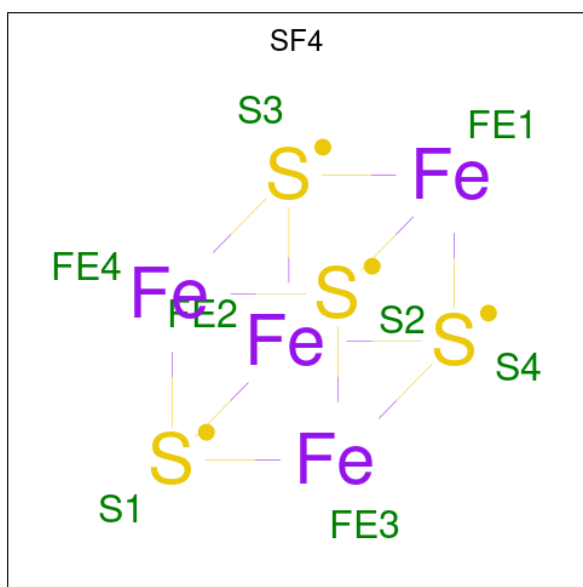
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	Z	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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 (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



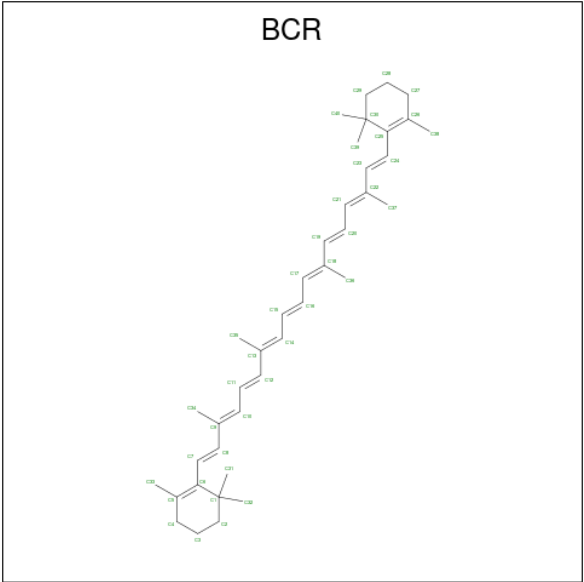
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	A	1	Total 33	C 31	O 2	0	0
15	B	1	Total 33	C 31	O 2	0	0
15	G	1	Total 33	C 31	O 2	0	0
15	H	1	Total 33	C 31	O 2	0	0
15	Y	1	Total 33	C 31	O 2	0	0
15	Z	1	Total 33	C 31	O 2	0	0

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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 (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



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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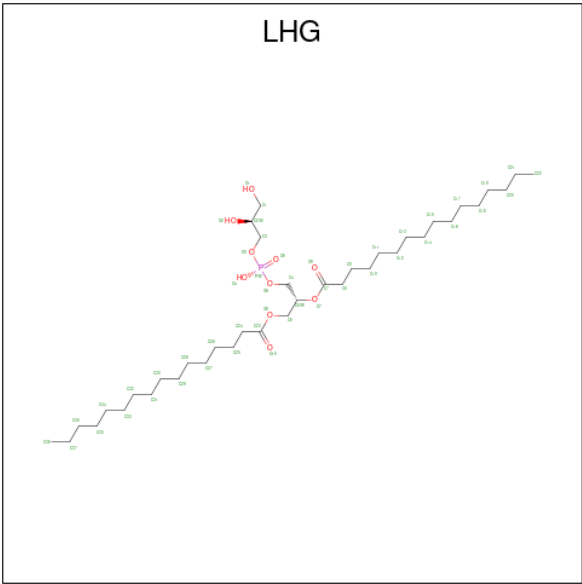
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	Q	1	Total C 40 40	0	0
17	R	1	Total C 40 40	0	0
17	R	1	Total C 40 40	0	0
17	S	1	Total C 40 40	0	0
17	S	1	Total C 40 40	0	0
17	T	1	Total C 40 40	0	0
17	U	1	Total C 40 40	0	0
17	U	1	Total C 40 40	0	0
17	U	1	Total C 40 40	0	0
17	V	1	Total C 40 40	0	0
17	Y	1	Total 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 (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



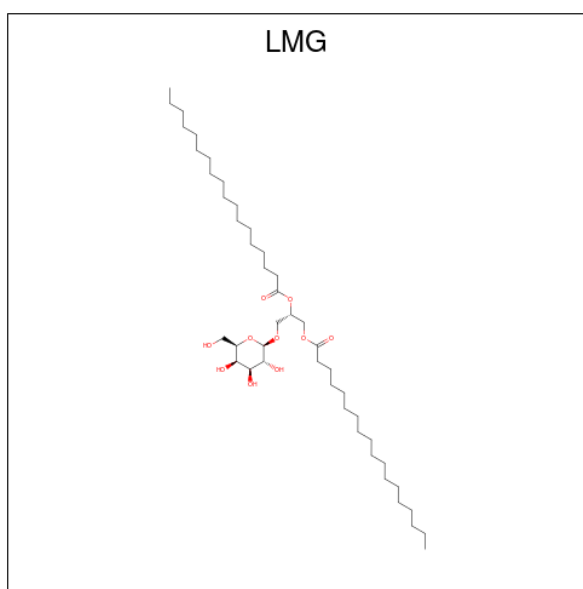
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O P 49 38 10 1	0	0

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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 (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



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 (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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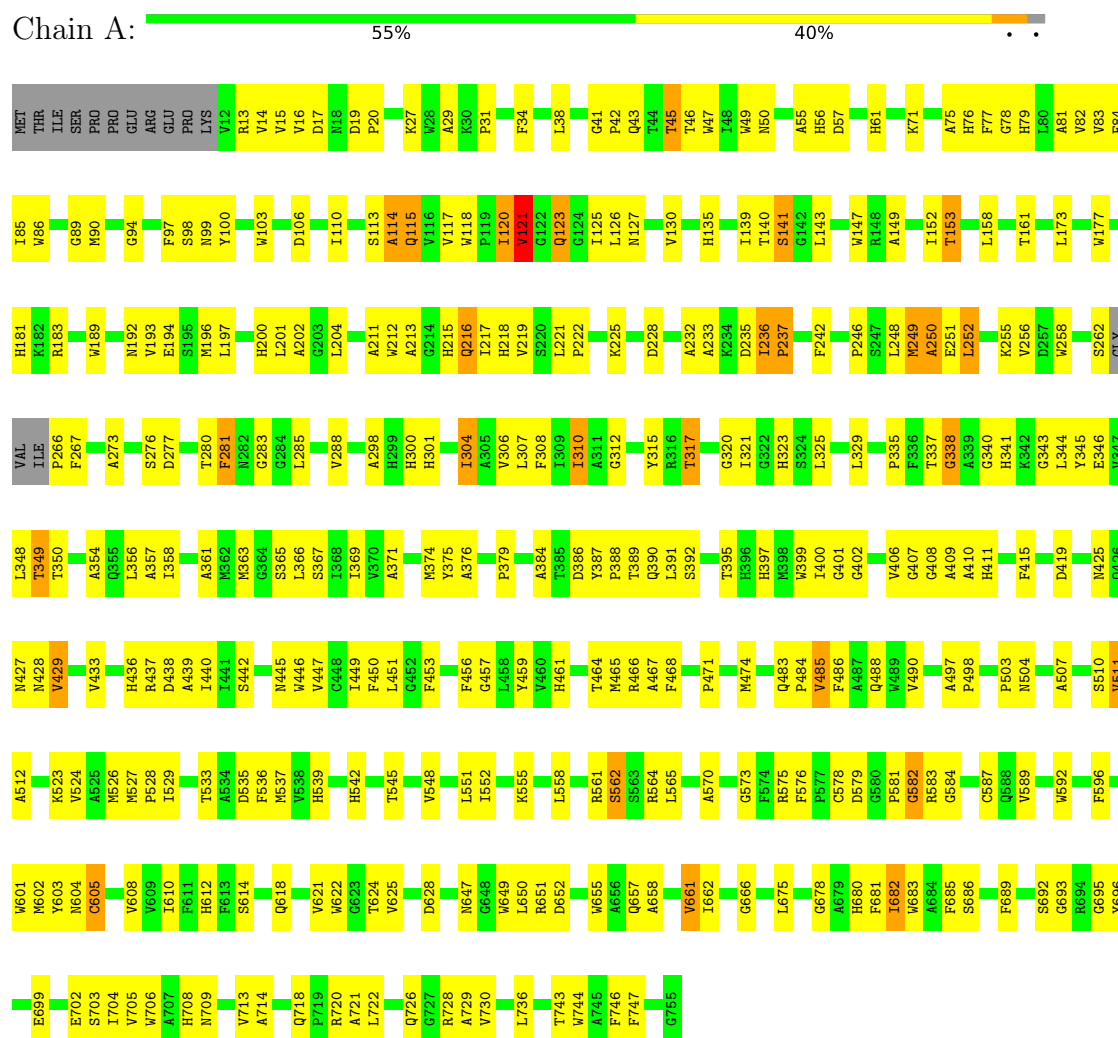
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	Q	7	Total O 7 7	0	0
21	S	2	Total O 2 2	0	0
21	T	1	Total O 1 1	0	0
21	U	9	Total O 9 9	0	0
21	V	2	Total O 2 2	0	0
21	W	3	Total O 3 3	0	0
21	X	2	Total O 2 2	0	0
21	Y	24	Total O 24 24	0	0
21	Z	21	Total O 21 21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

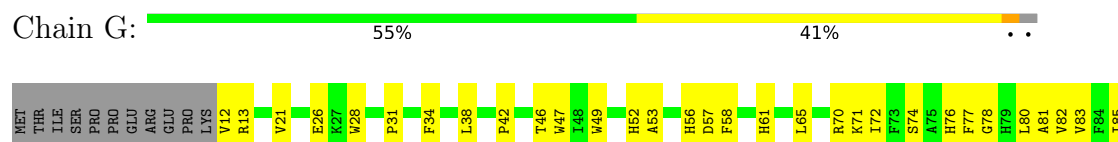
3 Residue-property plots

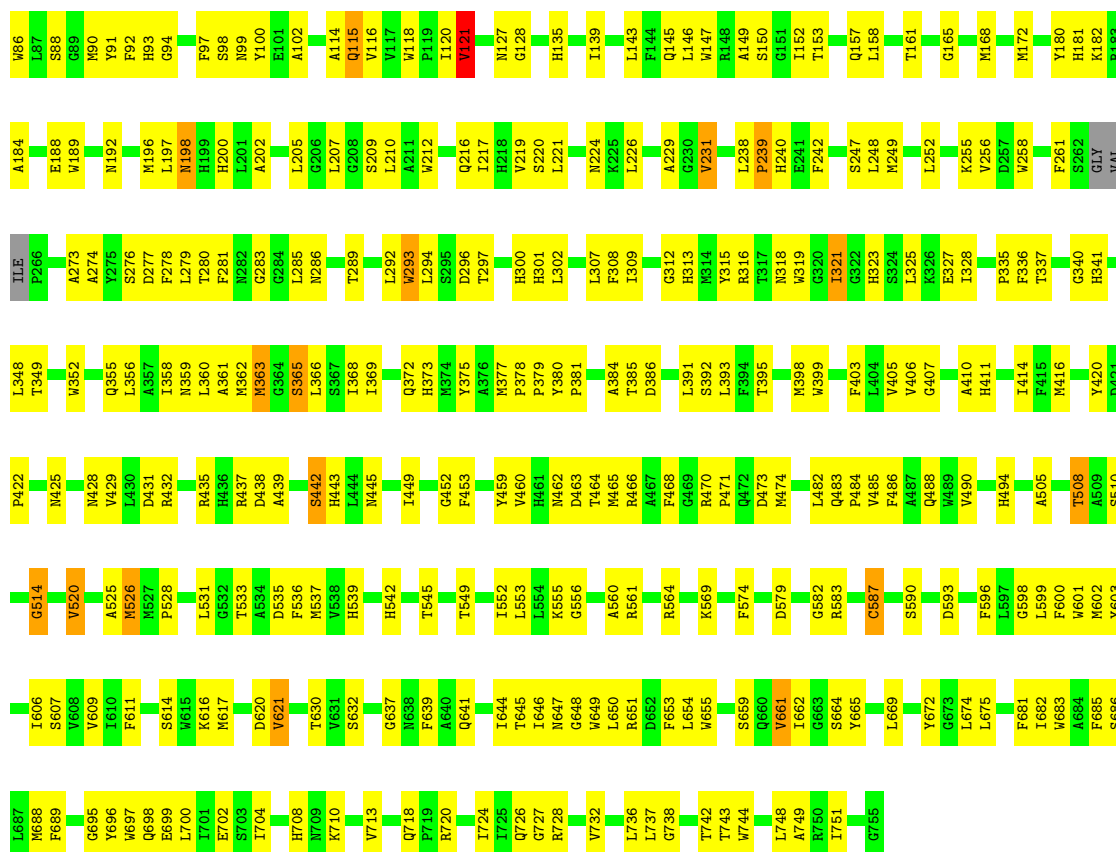
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



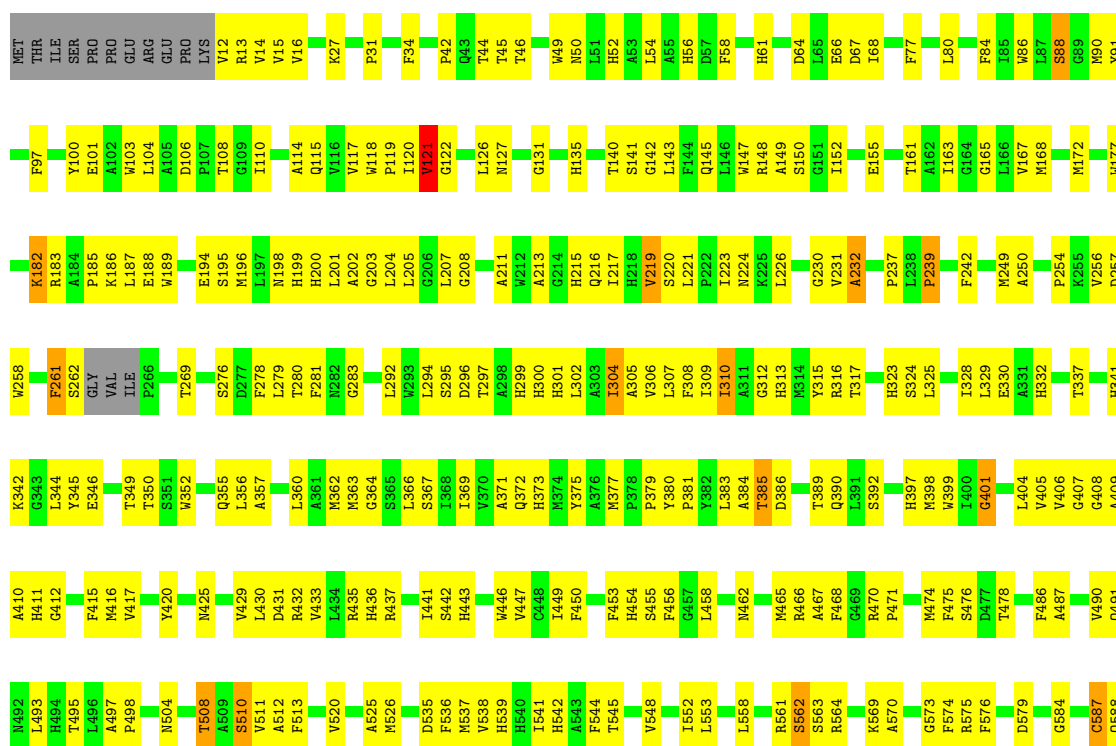
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

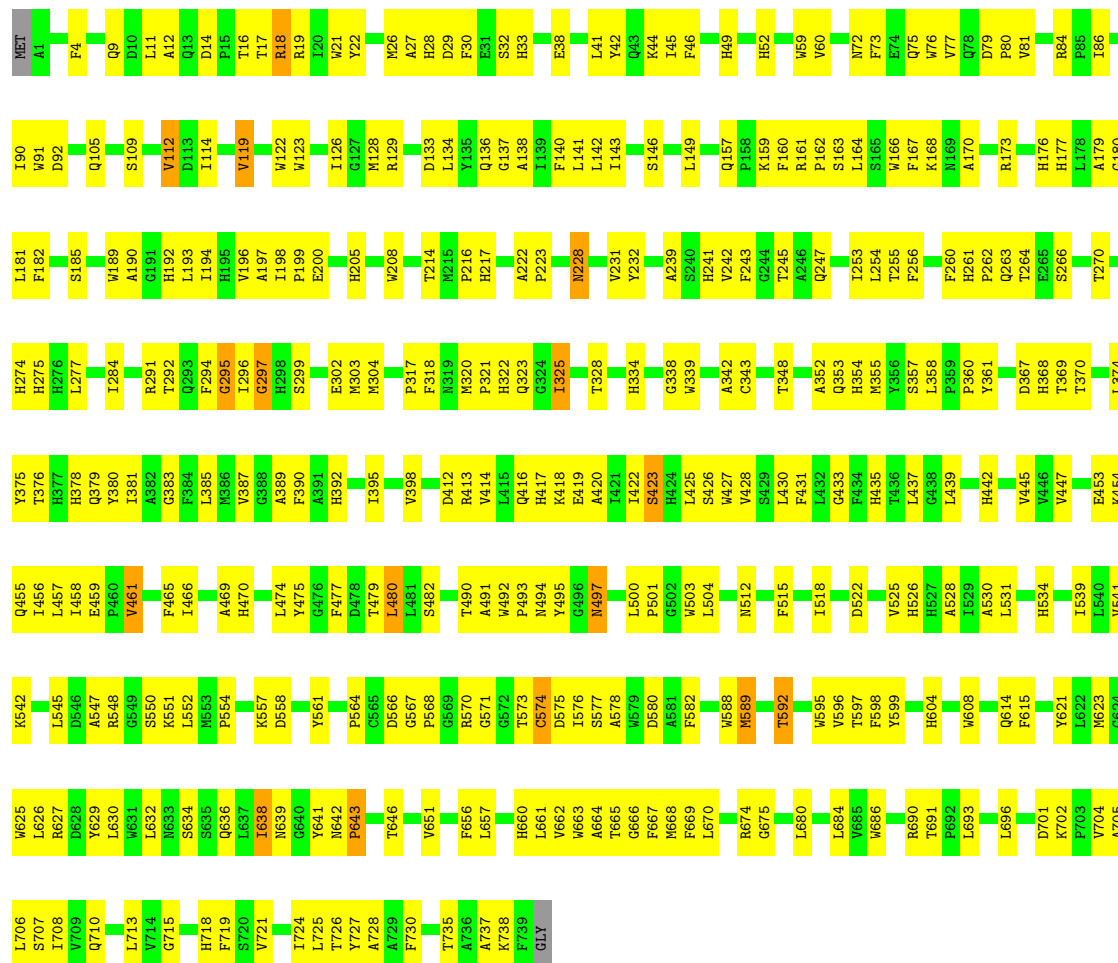
Chain Y: 52% 43%





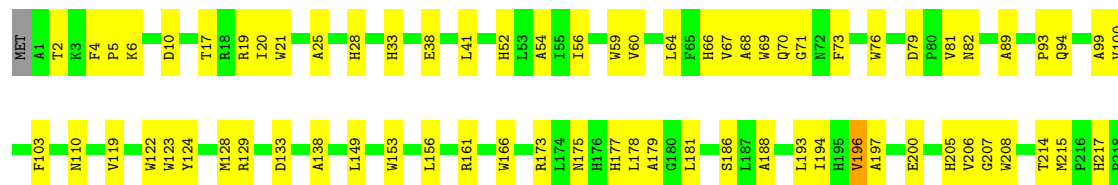
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

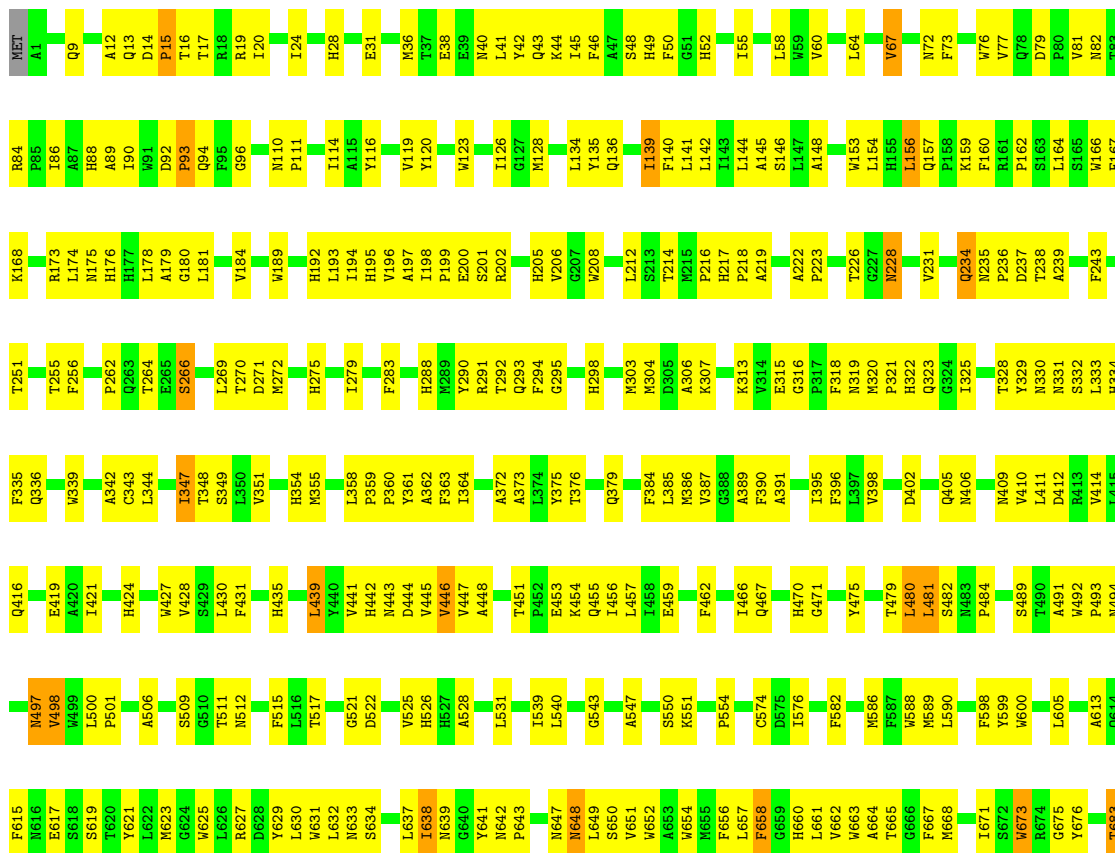
Chain B: 55% 43%



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain H: 57% 41%



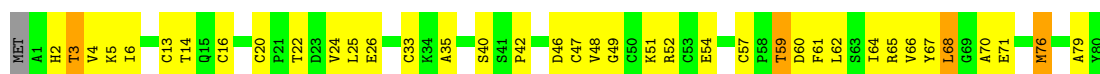




- Molecule 3: Photosystem I iron-sulfur center



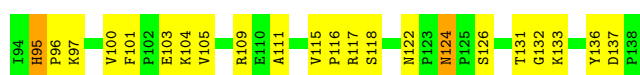
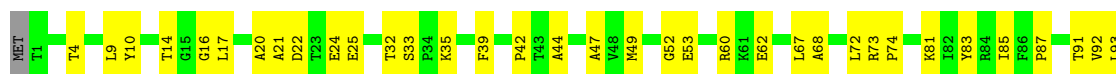
- Molecule 3: Photosystem I iron-sulfur center



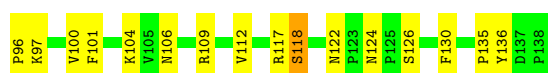
- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Photosystem I reaction center subunit II

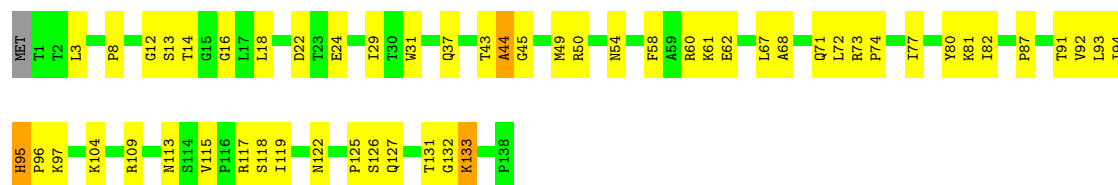


- Molecule 4: Photosystem I reaction center subunit II



- Molecule 4: Photosystem I reaction center subunit II





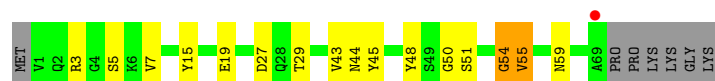
• Molecule 5: Photosystem I reaction center subunit IV



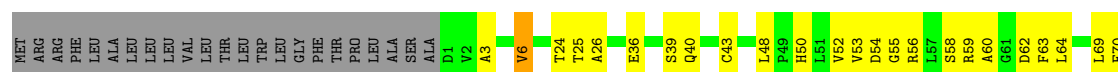
• Molecule 5: Photosystem I reaction center subunit IV



• Molecule 5: Photosystem I reaction center subunit IV



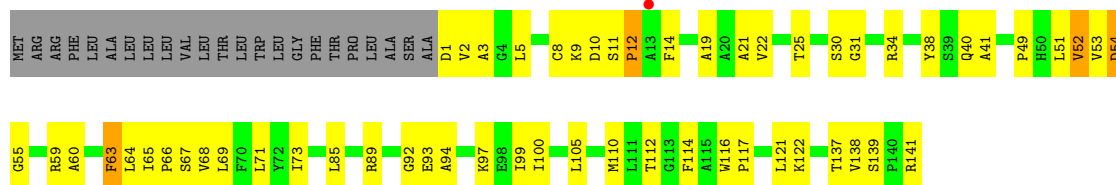
• Molecule 6: Photosystem I reaction center subunit III



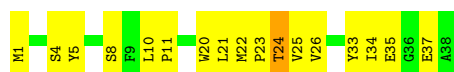
• Molecule 6: Photosystem I reaction center subunit III



• Molecule 6: Photosystem I reaction center subunit III



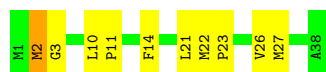
- Molecule 7: Photosystem I reaction center subunit VIII



- Molecule 7: Photosystem I reaction center subunit VIII



- Molecule 7: Photosystem I reaction center subunit VIII



- Molecule 8: Photosystem I reaction center subunit IX



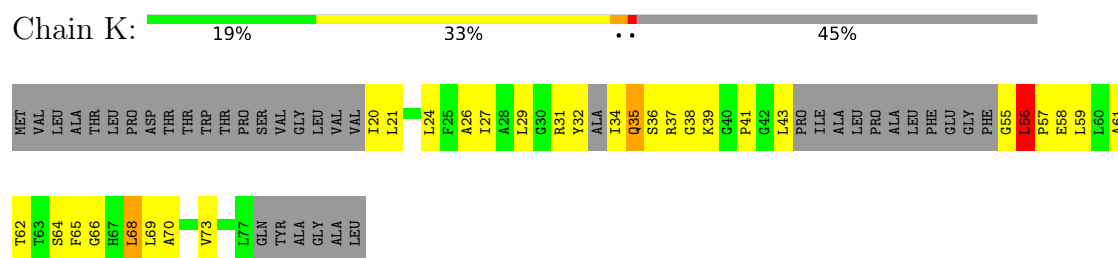
- Molecule 8: Photosystem I reaction center subunit IX



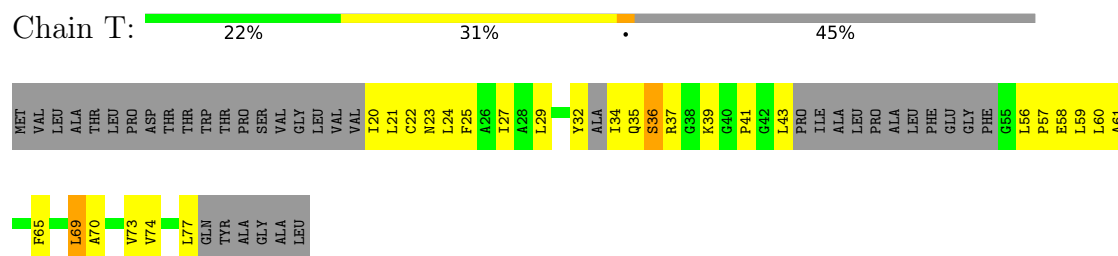
- Molecule 8: Photosystem I reaction center subunit IX



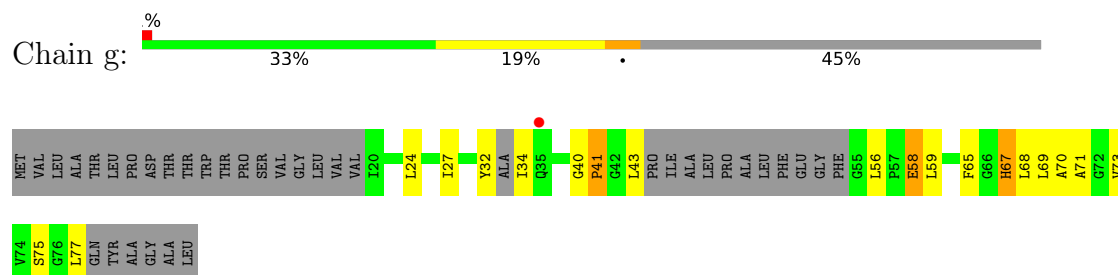
- Molecule 9: Photosystem I reaction center subunit PsaK



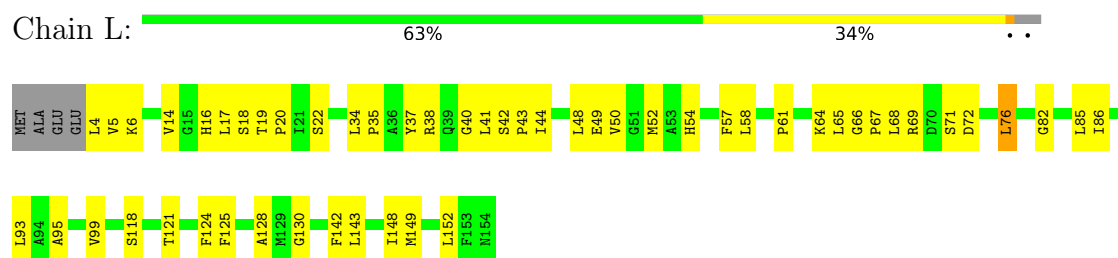
- Molecule 9: Photosystem I reaction center subunit PsaK



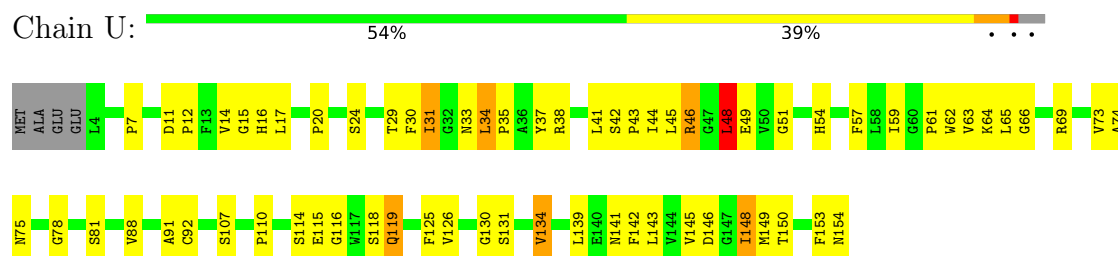
- Molecule 9: Photosystem I reaction center subunit PsaK



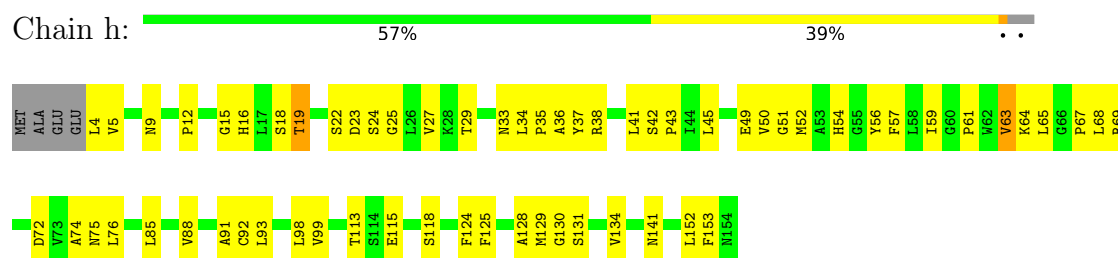
- Molecule 10: Photosystem I reaction center subunit XI



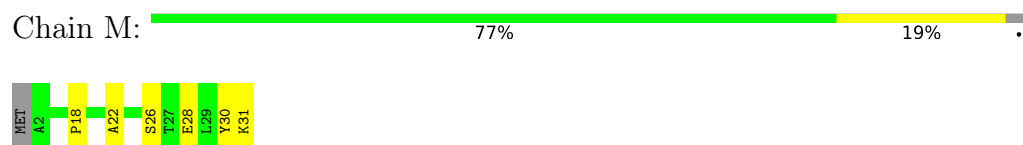
- Molecule 10: Photosystem I reaction center subunit XI



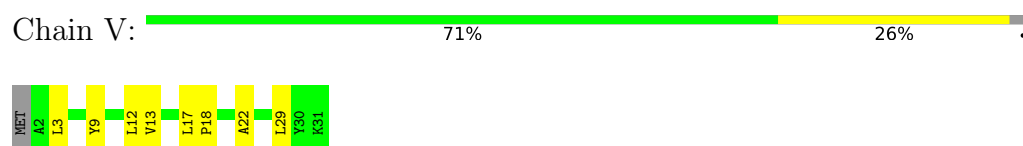
- Molecule 10: Photosystem I reaction center subunit XI



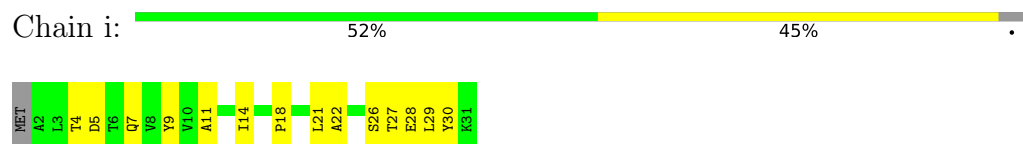
- Molecule 11: Photosystem I reaction center subunit XII



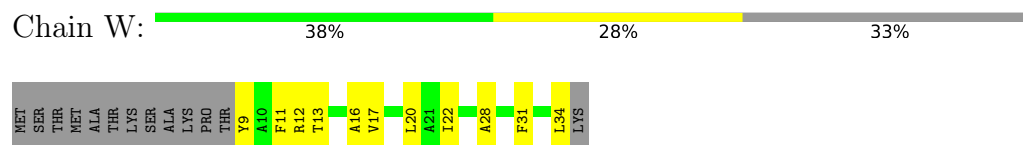
- Molecule 11: Photosystem I reaction center subunit XII



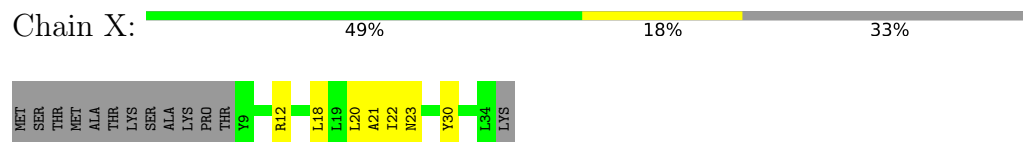
- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 12: Photosystem I 4.8K protein



- Molecule 12: Photosystem I 4.8K protein



- Molecule 12: Photosystem I 4.8K protein



MET	SER	THR	MET	ALA	THR	LYS	SER	ALA	LYS	PRO	THR	Y9	A10	F11	R12	L18	L19	L20	A21	I22	N23	F24	L25	V26	A27	A28	Y29	Y30	L34	LYS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.14$	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	0.87	EDS
Total number of atoms	72737	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.02	0/5990	1.46	2/8168 (0.0%)
1	G	1.03	0/5990	1.46	3/8168 (0.0%)
1	Y	1.03	0/5990	1.47	8/8168 (0.1%)
2	B	1.00	0/6107	1.46	5/8345 (0.1%)
2	H	1.01	0/6107	1.47	0/8345
2	Z	1.00	0/6107	1.45	4/8345 (0.0%)
3	C	1.05	0/608	1.39	0/824
3	N	1.09	0/608	1.35	0/824
3	a	1.06	0/608	1.42	0/824
4	D	1.00	0/1101	1.32	0/1492
4	O	1.00	0/1101	1.32	0/1492
4	b	1.01	0/1101	1.36	5/1492 (0.3%)
5	E	1.03	0/551	1.31	0/750
5	P	1.06	0/551	1.29	0/750
5	c	1.06	0/551	1.30	0/750
6	F	1.04	0/1087	1.51	0/1476
6	Q	1.04	0/1087	1.45	0/1476
6	d	1.01	0/1087	1.47	2/1476 (0.1%)
7	I	1.01	0/312	1.36	0/425
7	R	1.03	0/312	1.45	2/425 (0.5%)
7	e	0.96	0/312	1.35	0/425
8	J	0.97	0/350	1.41	0/477
8	S	0.97	0/350	1.52	0/477
8	f	0.99	0/350	1.40	0/477
9	K	1.02	0/331	1.48	0/444
9	T	1.08	0/331	1.55	0/444
9	g	1.07	0/331	1.57	0/444
10	L	1.04	0/1148	1.50	0/1558
10	U	1.05	0/1148	1.53	7/1558 (0.4%)
10	h	1.04	0/1148	1.47	0/1558
11	M	1.03	0/236	1.42	0/322
11	V	1.06	0/236	1.61	0/322

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	i	1.06	0/236	1.51	0/322
12	W	1.00	0/227	1.51	2/310 (0.6%)
12	X	0.93	0/227	1.42	0/310
12	j	0.92	0/227	1.30	0/310
All	All	1.02	0/54144	1.45	40/73773 (0.1%)

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.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	U	51	GLY	CA-C-N	6.33	129.62	120.38
10	U	51	GLY	C-N-CA	6.33	129.62	120.38
2	B	568	PRO	CA-C-N	6.05	125.84	120.10
2	B	568	PRO	C-N-CA	6.05	125.84	120.10
1	A	589	VAL	N-CA-C	-5.89	107.76	113.53

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 ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5791	0	5649	315	0
1	G	5791	0	5649	331	0
1	Y	5791	0	5648	335	0
2	B	5889	0	5650	359	0
2	H	5889	0	5650	341	0
2	Z	5889	0	5651	364	0
3	C	598	0	581	38	0
3	N	598	0	582	41	0
3	a	598	0	581	19	0
4	D	1075	0	1077	47	0
4	O	1075	0	1077	35	0
4	b	1075	0	1077	37	0
5	E	539	0	528	22	0
5	P	539	0	528	9	0
5	c	539	0	528	9	0
6	F	1065	0	1077	47	0
6	Q	1065	0	1077	46	0
6	d	1065	0	1077	48	0
7	I	301	0	306	18	0
7	R	301	0	306	21	0
7	e	301	0	306	9	0
8	J	338	0	347	20	0
8	S	338	0	347	30	0
8	f	338	0	347	21	0
9	K	328	0	348	35	0
9	T	328	0	348	29	0
9	g	328	0	348	19	0
10	L	1119	0	1125	51	0
10	U	1119	0	1125	58	0
10	h	1119	0	1125	61	0
11	M	233	0	252	8	0
11	V	233	0	252	7	0
11	i	233	0	252	14	0
12	W	219	0	221	8	0
12	X	219	0	221	6	0
12	j	219	0	221	11	0
13	A	65	0	72	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	G	65	0	72	8	0
13	Y	65	0	72	8	0
14	A	2554	0	2558	237	0
14	B	2324	0	2304	245	0
14	F	45	0	32	2	0
14	G	2534	0	2523	245	0
14	H	2389	0	2372	232	0
14	J	100	0	81	0	0
14	K	86	0	62	2	0
14	L	325	0	360	21	0
14	Q	45	0	32	4	0
14	S	165	0	154	6	0
14	T	86	0	61	1	0
14	U	325	0	360	39	0
14	W	45	0	33	2	0
14	X	45	0	33	4	0
14	Y	2380	0	2388	195	0
14	Z	2384	0	2365	256	0
14	d	110	0	105	11	0
14	f	100	0	82	3	0
14	g	86	0	62	3	0
14	h	260	0	288	26	0
14	j	45	0	32	0	0
15	A	33	0	46	9	0
15	B	33	0	46	4	0
15	G	33	0	46	4	0
15	H	33	0	46	5	0
15	Y	33	0	46	10	0
15	Z	33	0	46	4	0
16	A	8	0	0	4	0
16	C	16	0	0	1	0
16	G	8	0	0	1	0
16	N	16	0	0	4	0
16	Y	8	0	0	3	0
16	a	16	0	0	2	0
17	A	240	0	291	43	0
17	B	255	0	302	42	0
17	F	80	0	98	9	0
17	G	200	0	240	42	0
17	H	265	0	318	47	0
17	I	80	0	97	12	0
17	J	80	0	97	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	L	80	0	96	13	0
17	M	40	0	49	6	0
17	Q	80	0	98	20	0
17	R	80	0	96	6	0
17	S	80	0	97	23	0
17	T	40	0	48	6	0
17	U	120	0	144	33	0
17	V	40	0	49	6	0
17	Y	320	0	386	75	0
17	Z	265	0	317	46	0
17	d	40	0	49	9	0
17	e	40	0	48	7	0
17	f	40	0	48	8	0
17	h	80	0	97	19	0
17	i	40	0	48	3	0
18	A	81	0	108	6	0
18	B	39	0	48	1	0
18	G	81	0	108	8	0
18	H	37	0	44	3	0
18	Y	74	0	94	8	0
18	j	28	0	26	4	0
19	B	52	0	77	8	0
19	H	49	0	68	4	0
19	Z	49	0	68	4	0
20	L	1	0	0	0	0
20	U	1	0	0	0	0
20	h	1	0	0	0	0
21	A	23	0	0	2	0
21	B	20	0	0	1	0
21	C	7	0	0	3	0
21	D	15	0	0	2	0
21	E	6	0	0	1	0
21	F	7	0	0	1	0
21	G	32	0	0	10	0
21	H	38	0	0	7	0
21	J	3	0	0	0	0
21	K	2	0	0	0	0
21	L	4	0	0	0	0
21	M	1	0	0	0	0
21	N	2	0	0	1	0
21	O	7	0	0	0	0
21	P	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	Q	7	0	0	0	0
21	S	2	0	0	0	0
21	T	1	0	0	0	0
21	U	9	0	0	1	0
21	V	2	0	0	0	0
21	W	3	0	0	0	0
21	X	2	0	0	0	0
21	Y	24	0	0	11	0
21	Z	21	0	0	3	0
21	a	4	0	0	0	0
21	b	6	0	0	0	0
21	c	4	0	0	3	0
21	d	7	0	0	1	0
21	f	5	0	0	0	0
21	g	2	0	0	7	0
21	h	4	0	0	0	0
21	i	1	0	0	0	0
21	j	2	0	0	0	0
All	All	72737	0	72017	3615	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

The worst 5 of 3615 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:814:CLA:O2A	14:H:814:CLA:C1	1.63	1.43
14:h:204:CLA:O2A	14:h:204:CLA:C1	1.63	1.43
1:G:399:TRP:CD1	14:G:828:CLA:HAB	1.78	1.19
2:H:318:PHE:CD1	14:H:822:CLA:HAB	1.77	1.19
1:G:639:PHE:CD2	21:G:906:HOH:O	1.98	1.16

There are no symmetry-related clashes.

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%)	4	17
1	G	737/755 (98%)	654 (89%)	70 (10%)	13 (2%)	6	25
1	Y	737/755 (98%)	642 (87%)	77 (10%)	18 (2%)	4	18
2	B	737/741 (100%)	633 (86%)	95 (13%)	9 (1%)	10	34
2	H	737/741 (100%)	643 (87%)	87 (12%)	7 (1%)	14	41
2	Z	737/741 (100%)	649 (88%)	79 (11%)	9 (1%)	10	34
3	C	78/81 (96%)	70 (90%)	6 (8%)	2 (3%)	4	17
3	N	78/81 (96%)	67 (86%)	9 (12%)	2 (3%)	4	17
3	a	78/81 (96%)	70 (90%)	7 (9%)	1 (1%)	9	32
4	D	136/139 (98%)	119 (88%)	13 (10%)	4 (3%)	3	15
4	O	136/139 (98%)	123 (90%)	12 (9%)	1 (1%)	18	48
4	b	136/139 (98%)	123 (90%)	9 (7%)	4 (3%)	3	15
5	E	67/76 (88%)	56 (84%)	8 (12%)	3 (4%)	2	8
5	P	67/76 (88%)	56 (84%)	8 (12%)	3 (4%)	2	8
5	c	67/76 (88%)	57 (85%)	7 (10%)	3 (4%)	2	8
6	F	139/164 (85%)	115 (83%)	23 (16%)	1 (1%)	18	48
6	Q	139/164 (85%)	125 (90%)	13 (9%)	1 (1%)	18	48
6	d	139/164 (85%)	113 (81%)	19 (14%)	7 (5%)	1	6
7	I	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	4	15
7	R	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
7	e	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	4	15
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%)	1	6
9	T	40/83 (48%)	33 (82%)	5 (12%)	2 (5%)	1	6
9	g	40/83 (48%)	31 (78%)	7 (18%)	2 (5%)	1	6
10	L	149/155 (96%)	133 (89%)	16 (11%)	0	100	100
10	U	149/155 (96%)	130 (87%)	17 (11%)	2 (1%)	9	32
10	h	149/155 (96%)	133 (89%)	14 (9%)	2 (1%)	9	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	2	9
12	j	24/39 (62%)	24 (100%)	0	0	100	100
All	All	6630/7029 (94%)	5805 (88%)	705 (11%)	120 (2%)	6	25

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%)	566 (96%)	24 (4%)	27	61
1	G	590/603 (98%)	574 (97%)	16 (3%)	39	73
1	Y	590/603 (98%)	566 (96%)	24 (4%)	27	61
2	B	597/598 (100%)	574 (96%)	23 (4%)	28	63
2	H	597/598 (100%)	578 (97%)	19 (3%)	34	68
2	Z	597/598 (100%)	573 (96%)	24 (4%)	28	62
3	C	67/68 (98%)	62 (92%)	5 (8%)	12	37
3	N	67/68 (98%)	64 (96%)	3 (4%)	24	58
3	a	67/68 (98%)	65 (97%)	2 (3%)	36	70
4	D	115/116 (99%)	112 (97%)	3 (3%)	40	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	O	115/116 (99%)	110 (96%)	5 (4%)	26	60
4	b	115/116 (99%)	110 (96%)	5 (4%)	26	60
5	E	59/65 (91%)	57 (97%)	2 (3%)	32	66
5	P	59/65 (91%)	57 (97%)	2 (3%)	32	66
5	c	59/65 (91%)	58 (98%)	1 (2%)	53	82
6	F	109/128 (85%)	107 (98%)	2 (2%)	51	80
6	Q	109/128 (85%)	105 (96%)	4 (4%)	30	64
6	d	109/128 (85%)	105 (96%)	4 (4%)	30	64
7	I	32/32 (100%)	31 (97%)	1 (3%)	35	69
7	R	32/32 (100%)	31 (97%)	1 (3%)	35	69
7	e	32/32 (100%)	31 (97%)	1 (3%)	35	69
8	J	36/36 (100%)	35 (97%)	1 (3%)	38	72
8	S	36/36 (100%)	34 (94%)	2 (6%)	19	50
8	f	36/36 (100%)	35 (97%)	1 (3%)	38	72
9	K	33/61 (54%)	28 (85%)	5 (15%)	3	9
9	T	33/61 (54%)	32 (97%)	1 (3%)	36	70
9	g	33/61 (54%)	32 (97%)	1 (3%)	36	70
10	L	117/120 (98%)	112 (96%)	5 (4%)	26	60
10	U	117/120 (98%)	110 (94%)	7 (6%)	17	47
10	h	117/120 (98%)	110 (94%)	7 (6%)	17	47
11	M	25/26 (96%)	25 (100%)	0	100	100
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%)	19 (95%)	1 (5%)	22	53
12	X	20/31 (64%)	20 (100%)	0	100	100
12	j	20/31 (64%)	20 (100%)	0	100	100
All	All	5400/5652 (96%)	5198 (96%)	202 (4%)	30	64

5 of 202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	P	62	LEU
1	Y	304	ILE

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Mol	Chain	Res	Type
10	h	72	ASP
6	Q	139	SER
10	U	148	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 158 such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	200	HIS
2	Z	688	HIS
1	Y	390	GLN
2	Z	136	GLN
4	b	121	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	Z	806	-	69,73,73	2.27	24 (34%)	82,113,113	2.44	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	Z	801	-	69,73,73	2.20	21 (30%)	82,113,113	2.52	26 (31%)
14	CLA	G	821	-	69,73,73	2.30	21 (30%)	82,113,113	2.46	24 (29%)
18	LHG	A	853	14	31,31,48	1.20	2 (6%)	34,37,54	1.17	2 (5%)
14	CLA	A	837	-	69,73,73	2.22	19 (27%)	82,113,113	2.43	24 (29%)
17	BCR	G	848	-	41,41,41	2.48	6 (14%)	56,56,56	7.32	24 (42%)
17	BCR	F	201	-	41,41,41	2.59	6 (14%)	56,56,56	7.26	24 (42%)
14	CLA	A	807	-	69,73,73	2.26	23 (33%)	82,113,113	2.45	29 (35%)
14	CLA	G	820	-	64,68,73	2.33	23 (35%)	76,107,113	2.54	27 (35%)
14	CLA	Y	820	-	64,68,73	2.32	22 (34%)	76,107,113	2.63	26 (34%)
14	CLA	G	840	-	69,73,73	2.26	23 (33%)	82,113,113	2.44	26 (31%)
14	CLA	B	817	-	64,68,73	2.34	23 (35%)	76,107,113	2.32	21 (27%)
14	CLA	A	804	-	69,73,73	2.33	23 (33%)	82,113,113	2.43	26 (31%)
14	CLA	A	833	-	69,73,73	2.20	20 (28%)	82,113,113	2.45	27 (32%)
14	CLA	G	831	-	54,58,73	2.50	19 (35%)	64,95,113	2.79	30 (46%)
14	CLA	Z	814	-	69,73,73	2.28	23 (33%)	82,113,113	2.37	25 (30%)
14	CLA	G	823	-	54,58,73	2.56	23 (42%)	64,95,113	2.77	25 (39%)
14	CLA	U	1002	10	69,73,73	2.25	22 (31%)	82,113,113	2.55	26 (31%)
14	CLA	Y	830	-	69,73,73	2.28	20 (28%)	82,113,113	2.38	24 (29%)
15	PQN	Y	842	-	34,34,34	1.80	2 (5%)	43,45,45	1.05	3 (6%)
15	PQN	Z	842	-	34,34,34	1.85	2 (5%)	43,45,45	1.27	3 (6%)
14	CLA	Y	839	-	54,58,73	2.51	23 (42%)	64,95,113	2.85	27 (42%)
14	CLA	G	853	-	49,53,73	2.47	23 (46%)	58,89,113	2.58	25 (43%)
14	CLA	Z	830	-	69,73,73	2.17	19 (27%)	82,113,113	2.57	22 (26%)
14	CLA	B	801	-	69,73,73	2.19	20 (28%)	82,113,113	2.44	26 (31%)
17	BCR	L	208	-	41,41,41	2.49	6 (14%)	56,56,56	7.19	30 (53%)
14	CLA	H	801	-	69,73,73	2.25	22 (31%)	82,113,113	2.48	26 (31%)
17	BCR	B	843	-	41,41,41	2.56	7 (17%)	56,56,56	7.46	24 (42%)
14	CLA	Z	818	-	69,73,73	2.31	22 (31%)	82,113,113	2.50	25 (30%)
14	CLA	Y	816	-	54,58,73	2.56	23 (42%)	64,95,113	2.81	26 (40%)
17	BCR	H	846	-	41,41,41	2.44	6 (14%)	56,56,56	7.28	27 (48%)
14	CLA	Z	816	-	49,53,73	2.53	20 (40%)	58,89,113	2.87	22 (37%)
14	CLA	A	817	-	54,58,73	2.60	21 (38%)	64,95,113	2.80	26 (40%)
14	CLA	Y	806	-	69,73,73	2.26	21 (30%)	82,113,113	2.48	27 (32%)
17	BCR	G	845	-	41,41,41	2.55	6 (14%)	56,56,56	7.32	29 (51%)
14	CLA	B	810	-	59,63,73	2.41	22 (37%)	70,101,113	2.61	29 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	803	-	58,62,73	2.47	23 (39%)	68,99,113	3.07	25 (36%)
13	CL0	A	801	-	58,73,73	3.09	18 (31%)	60,113,113	2.71	16 (26%)
14	CLA	A	854	-	69,73,73	2.24	19 (27%)	82,113,113	2.57	27 (32%)
14	CLA	A	824	-	54,58,73	2.62	23 (42%)	64,95,113	2.61	26 (40%)
14	CLA	H	809	2	69,73,73	2.13	21 (30%)	82,113,113	2.56	32 (39%)
17	BCR	V	101	-	41,41,41	2.54	6 (14%)	56,56,56	7.40	30 (53%)
14	CLA	Z	803	-	69,73,73	2.22	21 (30%)	82,113,113	2.45	28 (34%)
14	CLA	X	1701	-	49,53,73	2.65	22 (44%)	58,89,113	2.56	24 (41%)
17	BCR	Y	845	-	41,41,41	2.53	6 (14%)	56,56,56	7.32	29 (51%)
15	PQN	G	843	-	34,34,34	1.71	2 (5%)	43,45,45	1.21	6 (13%)
17	BCR	B	844	-	41,41,41	2.52	6 (14%)	56,56,56	7.28	28 (50%)
17	BCR	M	101	-	41,41,41	2.55	7 (17%)	56,56,56	7.29	28 (50%)
14	CLA	B	826	-	69,73,73	2.23	22 (31%)	82,113,113	2.32	24 (29%)
14	CLA	B	807	-	69,73,73	2.28	21 (30%)	82,113,113	2.51	23 (28%)
14	CLA	A	802	-	69,73,73	2.21	19 (27%)	82,113,113	2.42	25 (30%)
13	CL0	G	801	-	58,73,73	3.07	17 (29%)	60,113,113	2.90	20 (33%)
16	SF4	N	102	3	0,12,12	-	-	-	-	-
14	CLA	B	834	-	49,53,73	2.58	21 (42%)	58,89,113	2.65	25 (43%)
14	CLA	H	820	-	49,53,73	2.49	19 (38%)	58,89,113	2.86	24 (41%)
14	CLA	Y	804	14	63,67,73	2.35	22 (34%)	74,105,113	2.75	23 (31%)
14	CLA	Z	826	-	69,73,73	2.21	20 (28%)	82,113,113	2.67	29 (35%)
17	BCR	I	101	-	41,41,41	2.63	7 (17%)	56,56,56	7.64	22 (39%)
14	CLA	H	832	-	59,63,73	2.48	19 (32%)	70,101,113	2.49	26 (37%)
14	CLA	h	201	-	69,73,73	2.20	20 (28%)	82,113,113	2.37	27 (32%)
17	BCR	A	848	-	41,41,41	2.48	6 (14%)	56,56,56	7.31	28 (50%)
17	BCR	U	1009	-	41,41,41	2.35	7 (17%)	56,56,56	7.51	31 (55%)
14	CLA	L	202	-	69,73,73	2.24	20 (28%)	82,113,113	2.53	32 (39%)
14	CLA	Y	823	-	54,58,73	2.64	20 (37%)	64,95,113	2.75	26 (40%)
17	BCR	R	101	-	41,41,41	2.44	7 (17%)	56,56,56	7.66	24 (42%)
17	BCR	A	851	-	41,41,41	2.56	6 (14%)	56,56,56	7.42	27 (48%)
14	CLA	B	825	-	69,73,73	2.16	21 (30%)	82,113,113	2.52	25 (30%)
17	BCR	Z	844	-	41,41,41	2.51	6 (14%)	56,56,56	7.17	30 (53%)
14	CLA	T	101	-	45,49,73	2.54	19 (42%)	54,83,113	2.87	23 (42%)
14	CLA	B	812	-	69,73,73	2.25	22 (31%)	82,113,113	2.56	29 (35%)
14	CLA	A	811	-	49,53,73	2.55	22 (44%)	58,89,113	2.79	25 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	H	827	-	69,73,73	2.18	19 (27%)	82,113,113	2.40	26 (31%)
14	CLA	Y	803	-	69,73,73	2.25	22 (31%)	82,113,113	2.65	25 (30%)
14	CLA	A	805	14	63,67,73	2.36	21 (33%)	74,105,113	2.58	26 (35%)
17	BCR	Z	846	-	25,25,41	2.11	2 (8%)	33,33,56	8.10	18 (54%)
14	CLA	G	838	-	54,58,73	2.58	20 (37%)	64,95,113	2.72	24 (37%)
14	CLA	Y	841	-	69,73,73	2.16	19 (27%)	82,113,113	2.39	22 (26%)
14	CLA	B	811	-	54,58,73	2.57	22 (40%)	64,95,113	2.65	26 (40%)
14	CLA	Y	833	-	59,63,73	2.54	23 (38%)	70,101,113	2.54	25 (35%)
14	CLA	A	815	-	54,58,73	2.60	22 (40%)	64,95,113	2.87	31 (48%)
14	CLA	H	835	-	49,53,73	2.56	19 (38%)	58,89,113	2.80	23 (39%)
17	BCR	i	101	-	41,41,41	2.59	6 (14%)	56,56,56	7.74	31 (55%)
14	CLA	G	830	-	69,73,73	2.23	20 (28%)	82,113,113	2.41	25 (30%)
14	CLA	Z	834	-	49,53,73	2.58	21 (42%)	58,89,113	2.90	25 (43%)
14	CLA	A	843	18	54,58,73	2.54	23 (42%)	64,95,113	3.03	27 (42%)
14	CLA	B	808	2	69,73,73	2.15	21 (30%)	82,113,113	2.60	32 (39%)
14	CLA	B	821	-	59,63,73	2.42	22 (37%)	70,101,113	2.47	22 (31%)
14	CLA	G	827	-	69,73,73	2.27	20 (28%)	82,113,113	2.31	28 (34%)
14	CLA	A	838	-	54,58,73	2.56	22 (40%)	64,95,113	2.87	30 (46%)
14	CLA	S	1102	8	49,53,73	2.58	22 (44%)	58,89,113	2.73	21 (36%)
17	BCR	h	202	-	41,41,41	2.40	7 (17%)	56,56,56	7.25	29 (51%)
14	CLA	G	816	-	54,58,73	2.58	22 (40%)	64,95,113	2.74	25 (39%)
18	LHG	B	849	-	38,38,48	1.09	2 (5%)	41,44,54	1.26	4 (9%)
14	CLA	H	804	-	58,62,73	2.44	20 (34%)	68,99,113	2.86	25 (36%)
14	CLA	H	833	-	49,53,73	2.49	22 (44%)	58,89,113	2.83	24 (41%)
14	CLA	B	819	-	49,53,73	2.57	23 (46%)	58,89,113	2.79	27 (46%)
17	BCR	Z	845	-	41,41,41	2.44	6 (14%)	56,56,56	7.41	24 (42%)
14	CLA	B	836	-	64,68,73	2.34	22 (34%)	76,107,113	2.56	27 (35%)
19	LMG	H	848	-	49,49,55	1.46	8 (16%)	57,57,63	1.12	5 (8%)
14	CLA	H	807	-	69,73,73	2.19	21 (30%)	82,113,113	2.63	27 (32%)
14	CLA	A	825	-	64,68,73	2.34	21 (32%)	76,107,113	2.46	26 (34%)
14	CLA	Y	835	-	54,58,73	2.55	21 (38%)	64,95,113	2.72	26 (40%)
14	CLA	B	839	-	69,73,73	2.30	22 (31%)	82,113,113	2.42	26 (31%)
14	CLA	Z	841	-	69,73,73	2.28	21 (30%)	82,113,113	2.59	28 (34%)
14	CLA	H	825	-	69,73,73	2.25	23 (33%)	82,113,113	2.72	30 (36%)
17	BCR	Y	844	-	41,41,41	2.43	8 (19%)	56,56,56	7.48	24 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	G	837	-	69,73,73	2.20	22 (31%)	82,113,113	2.52	23 (28%)
14	CLA	H	814	-	69,73,73	2.31	20 (28%)	82,113,113	2.55	24 (29%)
14	CLA	Z	807	-	69,73,73	2.33	18 (26%)	82,113,113	2.18	23 (28%)
14	CLA	A	808	-	55,59,73	2.51	23 (41%)	64,96,113	2.94	23 (35%)
17	BCR	G	846	-	41,41,41	2.68	6 (14%)	56,56,56	7.04	27 (48%)
14	CLA	A	821	-	64,68,73	2.38	23 (35%)	76,107,113	2.55	25 (32%)
17	BCR	Y	846	-	41,41,41	2.43	6 (14%)	56,56,56	7.57	28 (50%)
14	CLA	A	816	-	54,58,73	2.51	23 (42%)	64,95,113	2.96	29 (45%)
17	BCR	S	1105	-	41,41,41	2.65	6 (14%)	56,56,56	7.49	29 (51%)
14	CLA	B	805	-	69,73,73	2.21	21 (30%)	82,113,113	2.38	25 (30%)
14	CLA	H	817	-	69,73,73	2.18	20 (28%)	82,113,113	2.67	29 (35%)
14	CLA	H	831	-	69,73,73	2.18	21 (30%)	82,113,113	2.73	30 (36%)
17	BCR	Y	847	-	41,41,41	2.54	6 (14%)	56,56,56	7.31	26 (46%)
14	CLA	Z	808	-	69,73,73	2.11	20 (28%)	82,113,113	2.46	25 (30%)
14	CLA	B	815	-	59,63,73	2.45	22 (37%)	70,101,113	2.52	21 (30%)
14	CLA	B	802	-	69,73,73	2.26	23 (33%)	82,113,113	2.23	27 (32%)
14	CLA	g	101	-	45,49,73	2.56	18 (40%)	54,83,113	2.73	21 (38%)
14	CLA	Y	826	-	64,68,73	2.30	20 (31%)	76,107,113	2.46	23 (30%)
17	BCR	A	850	-	41,41,41	2.55	7 (17%)	56,56,56	7.29	24 (42%)
14	CLA	d	201	-	69,73,73	2.17	21 (30%)	82,113,113	2.43	27 (32%)
17	BCR	R	102	-	41,41,41	2.67	6 (14%)	56,56,56	7.28	25 (44%)
17	BCR	S	1104	-	41,41,41	2.69	6 (14%)	56,56,56	7.08	26 (46%)
14	CLA	A	819	-	69,73,73	2.24	20 (28%)	82,113,113	2.49	29 (35%)
14	CLA	Z	819	-	64,68,73	2.32	21 (32%)	76,107,113	2.62	24 (31%)
14	CLA	Z	828	-	69,73,73	2.30	21 (30%)	82,113,113	2.43	27 (32%)
14	CLA	A	836	-	54,58,73	2.61	22 (40%)	64,95,113	2.83	28 (43%)
17	BCR	Y	848	-	41,41,41	2.40	6 (14%)	56,56,56	7.29	25 (44%)
17	BCR	H	843	-	41,41,41	2.80	6 (14%)	56,56,56	7.11	29 (51%)
17	BCR	G	847	-	41,41,41	2.51	6 (14%)	56,56,56	7.35	30 (53%)
14	CLA	H	802	-	69,73,73	2.24	21 (30%)	82,113,113	2.55	27 (32%)
17	BCR	Z	848	-	41,41,41	2.62	7 (17%)	56,56,56	7.48	23 (41%)
16	SF4	N	101	3	0,12,12	-	-	-	-	-
14	CLA	G	822	-	69,73,73	2.24	22 (31%)	82,113,113	2.60	26 (31%)
14	CLA	Z	838	-	69,73,73	2.24	21 (30%)	82,113,113	2.48	24 (29%)
14	CLA	G	841	-	69,73,73	2.24	21 (30%)	82,113,113	2.32	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	H	829	-	69,73,73	2.27	21 (30%)	82,113,113	2.58	28 (34%)
14	CLA	T	103	-	49,53,73	2.60	22 (44%)	58,89,113	2.68	21 (36%)
14	CLA	Z	836	-	49,53,73	2.55	22 (44%)	58,89,113	2.96	24 (41%)
14	CLA	B	813	-	69,73,73	2.21	20 (28%)	82,113,113	2.44	26 (31%)
14	CLA	B	824	-	69,73,73	2.27	22 (31%)	82,113,113	2.59	29 (35%)
14	CLA	G	802	-	69,73,73	2.30	23 (33%)	82,113,113	2.44	23 (28%)
17	BCR	A	849	-	41,41,41	2.57	6 (14%)	56,56,56	7.13	29 (51%)
18	LHG	Y	850	-	48,48,48	1.03	2 (4%)	51,54,54	1.31	5 (9%)
14	CLA	Y	807	-	55,59,73	2.55	24 (43%)	64,96,113	2.74	25 (39%)
17	BCR	B	850	-	41,41,41	2.56	6 (14%)	56,56,56	7.23	28 (50%)
14	CLA	Z	831	-	49,53,73	2.48	21 (42%)	58,89,113	2.93	25 (43%)
14	CLA	f	102	-	59,63,73	2.50	22 (37%)	70,101,113	2.71	26 (37%)
14	CLA	A	835	1	49,53,73	2.56	21 (42%)	58,89,113	2.74	23 (39%)
17	BCR	H	844	-	41,41,41	2.72	7 (17%)	56,56,56	7.18	25 (44%)
14	CLA	Y	812	-	59,63,73	2.42	22 (37%)	70,101,113	2.57	25 (35%)
14	CLA	H	815	-	49,53,73	2.56	21 (42%)	58,89,113	2.90	27 (46%)
14	CLA	B	816	-	69,73,73	2.28	22 (31%)	82,113,113	2.42	26 (31%)
14	CLA	h	206	-	69,73,73	2.24	21 (30%)	82,113,113	2.58	25 (30%)
17	BCR	J	104	-	41,41,41	2.69	6 (14%)	56,56,56	7.20	27 (48%)
14	CLA	Z	811	2	69,73,73	2.19	21 (30%)	82,113,113	2.63	34 (41%)
14	CLA	H	834	-	49,53,73	2.53	21 (42%)	58,89,113	2.91	23 (39%)
14	CLA	B	840	-	69,73,73	2.17	19 (27%)	82,113,113	2.59	33 (40%)
14	CLA	Y	813	-	64,68,73	2.33	22 (34%)	76,107,113	2.54	27 (35%)
16	SF4	a	102	3	0,12,12	-	-	-	-	-
14	CLA	B	831	-	69,73,73	2.22	21 (30%)	82,113,113	2.57	29 (35%)
14	CLA	Y	828	-	69,73,73	2.30	22 (31%)	82,113,113	2.37	26 (31%)
14	CLA	H	818	-	64,68,73	2.33	20 (31%)	76,107,113	2.53	28 (36%)
14	CLA	B	832	-	59,63,73	2.42	23 (38%)	70,101,113	2.70	25 (35%)
14	CLA	G	835	-	49,53,73	2.57	21 (42%)	58,89,113	2.95	23 (39%)
14	CLA	B	809	-	69,73,73	2.30	20 (28%)	82,113,113	2.51	30 (36%)
14	CLA	Z	817	-	59,63,73	2.41	23 (38%)	70,101,113	2.67	27 (38%)
14	CLA	A	840	-	54,58,73	2.61	22 (40%)	64,95,113	2.75	25 (39%)
14	CLA	A	813	-	58,62,73	2.46	21 (36%)	68,99,113	2.46	22 (32%)
14	CLA	B	823	2	59,63,73	2.45	23 (38%)	70,101,113	2.47	23 (32%)
14	CLA	Z	824	-	64,68,73	2.41	22 (34%)	76,107,113	2.36	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	G	804	14	63,67,73	2.35	21 (33%)	74,105,113	2.69	22 (29%)
17	BCR	Y	852	-	41,41,41	2.50	7 (17%)	56,56,56	7.30	23 (41%)
14	CLA	A	823	-	69,73,73	2.20	23 (33%)	82,113,113	2.65	27 (32%)
14	CLA	G	806	-	69,73,73	2.22	23 (33%)	82,113,113	2.52	26 (31%)
14	CLA	Y	836	-	69,73,73	2.32	22 (31%)	82,113,113	2.40	29 (35%)
18	LHG	A	852	-	48,48,48	0.98	2 (4%)	51,54,54	1.24	5 (9%)
14	CLA	S	1103	-	59,63,73	2.46	21 (35%)	70,101,113	2.79	28 (40%)
14	CLA	B	838	-	49,53,73	2.67	20 (40%)	58,89,113	2.50	23 (39%)
17	BCR	Z	843	-	41,41,41	2.70	6 (14%)	56,56,56	7.02	26 (46%)
14	CLA	L	204	-	69,73,73	2.21	21 (30%)	82,113,113	2.48	26 (31%)
14	CLA	G	832	-	69,73,73	2.19	19 (27%)	82,113,113	2.50	24 (29%)
17	BCR	J	103	-	41,41,41	2.54	6 (14%)	56,56,56	7.11	30 (53%)
17	BCR	A	847	-	41,41,41	2.37	7 (17%)	56,56,56	7.26	26 (46%)
14	CLA	Z	810	2	69,73,73	2.13	21 (30%)	82,113,113	2.60	26 (31%)
14	CLA	d	202	-	49,53,73	2.59	19 (38%)	58,89,113	2.61	20 (34%)
14	CLA	H	808	-	69,73,73	2.22	20 (28%)	82,113,113	2.44	30 (36%)
14	CLA	Y	819	-	69,73,73	2.30	22 (31%)	82,113,113	2.63	26 (31%)
14	CLA	H	811	-	59,63,73	2.40	22 (37%)	70,101,113	2.59	32 (45%)
14	CLA	A	832	-	54,58,73	2.40	20 (37%)	64,95,113	2.65	28 (43%)
14	CLA	L	201	-	69,73,73	2.19	21 (30%)	82,113,113	2.45	28 (34%)
14	CLA	Y	814	-	59,63,73	2.49	24 (40%)	70,101,113	2.54	27 (38%)
14	CLA	A	809	1	69,73,73	2.24	22 (31%)	82,113,113	2.40	25 (30%)
17	BCR	B	842	-	30,30,41	3.10	6 (20%)	39,39,56	8.24	20 (51%)
17	BCR	B	845	-	25,25,41	2.10	2 (8%)	33,33,56	8.07	14 (42%)
18	LHG	Y	851	14	24,24,48	1.58	2 (8%)	27,30,54	1.48	2 (7%)
17	BCR	h	207	-	41,41,41	2.69	7 (17%)	56,56,56	7.14	19 (33%)
16	SF4	A	845	2,1	0,12,12	-	-	-	-	-
14	CLA	Y	817	-	64,68,73	2.39	22 (34%)	76,107,113	2.50	27 (35%)
14	CLA	Y	831	-	54,58,73	2.43	21 (38%)	64,95,113	2.79	22 (34%)
17	BCR	T	102	-	41,41,41	2.42	6 (14%)	56,56,56	7.43	27 (48%)
14	CLA	G	818	-	69,73,73	2.21	20 (28%)	82,113,113	2.55	27 (32%)
14	CLA	H	828	-	69,73,73	2.20	22 (31%)	82,113,113	2.43	26 (31%)
14	CLA	J	101	8	49,53,73	2.55	19 (38%)	58,89,113	2.77	24 (41%)
14	CLA	Y	824	-	64,68,73	2.37	22 (34%)	76,107,113	2.58	28 (36%)
17	BCR	f	103	-	41,41,41	2.47	6 (14%)	56,56,56	7.24	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	g	102	-	49,53,73	2.61	21 (42%)	58,89,113	2.59	22 (37%)
14	CLA	L	206	-	69,73,73	2.23	22 (31%)	82,113,113	2.44	27 (32%)
16	SF4	G	844	2,1	0,12,12	-	-	-		
14	CLA	H	839	-	69,73,73	2.24	22 (31%)	82,113,113	2.51	28 (34%)
17	BCR	Y	853	-	41,41,41	2.68	6 (14%)	56,56,56	7.05	29 (51%)
14	CLA	Y	810	-	49,53,73	2.57	23 (46%)	58,89,113	2.64	26 (44%)
14	CLA	H	819	-	64,68,73	2.34	23 (35%)	76,107,113	2.37	29 (38%)
14	CLA	A	827	-	64,68,73	2.29	20 (31%)	76,107,113	2.57	28 (36%)
17	BCR	I	102	-	41,41,41	2.70	6 (14%)	56,56,56	7.17	23 (41%)
14	CLA	U	1006	-	69,73,73	2.31	21 (30%)	82,113,113	2.41	26 (31%)
14	CLA	G	839	-	54,58,73	2.65	20 (37%)	64,95,113	2.78	29 (45%)
14	CLA	H	851	18	54,58,73	2.56	23 (42%)	64,95,113	3.00	28 (43%)
14	CLA	G	833	-	69,73,73	2.28	21 (30%)	82,113,113	2.61	30 (36%)
14	CLA	A	814	-	64,68,73	2.34	23 (35%)	76,107,113	2.58	27 (35%)
14	CLA	H	805	-	69,73,73	2.30	21 (30%)	82,113,113	2.42	26 (31%)
17	BCR	e	101	-	41,41,41	2.50	7 (17%)	56,56,56	7.87	32 (57%)
16	SF4	a	101	3	0,12,12	-	-	-		
14	CLA	H	822	-	59,63,73	2.38	23 (38%)	70,101,113	2.72	25 (35%)
17	BCR	A	846	-	41,41,41	2.66	6 (14%)	56,56,56	7.51	27 (48%)
14	CLA	A	826	-	69,73,73	2.28	22 (31%)	82,113,113	2.46	28 (34%)
16	SF4	C	101	3	0,12,12	-	-	-		
17	BCR	H	850	-	41,41,41	2.66	6 (14%)	56,56,56	7.20	28 (50%)
15	PQN	B	841	-	34,34,34	1.76	3 (8%)	43,45,45	1.16	5 (11%)
14	CLA	G	803	-	69,73,73	2.19	20 (28%)	82,113,113	2.53	29 (35%)
14	CLA	A	803	-	69,73,73	2.21	21 (30%)	82,113,113	2.40	32 (39%)
14	CLA	G	829	-	69,73,73	2.26	20 (28%)	82,113,113	2.25	29 (35%)
14	CLA	L	205	-	69,73,73	2.26	23 (33%)	82,113,113	2.51	28 (34%)
14	CLA	G	824	-	64,68,73	2.42	19 (29%)	76,107,113	2.48	24 (31%)
14	CLA	A	812	14	69,73,73	2.16	20 (28%)	82,113,113	2.55	26 (31%)
14	CLA	Z	812	-	59,63,73	2.44	22 (37%)	70,101,113	2.50	26 (37%)
14	CLA	Z	823	-	59,63,73	2.48	22 (37%)	70,101,113	2.43	24 (34%)
14	CLA	A	806	-	69,73,73	2.15	19 (27%)	82,113,113	2.42	28 (34%)
14	CLA	B	804	-	69,73,73	2.18	20 (28%)	82,113,113	2.54	27 (32%)
18	LHG	H	849	-	36,36,48	1.13	2 (5%)	39,42,54	0.91	2 (5%)
14	CLA	B	830	-	49,53,73	2.58	21 (42%)	58,89,113	2.57	23 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	829	-	69,73,73	2.18	20 (28%)	82,113,113	2.56	28 (34%)
17	BCR	F	203	-	41,41,41	2.61	7 (17%)	56,56,56	7.13	28 (50%)
14	CLA	G	826	-	64,68,73	2.33	22 (34%)	76,107,113	2.58	27 (35%)
14	CLA	Y	832	-	69,73,73	2.22	22 (31%)	82,113,113	2.38	26 (31%)
14	CLA	Z	827	-	69,73,73	2.17	22 (31%)	82,113,113	2.46	25 (30%)
17	BCR	U	1005	-	41,41,41	2.62	6 (14%)	56,56,56	7.27	25 (44%)
14	CLA	Y	834	1	49,53,73	2.61	19 (38%)	58,89,113	2.65	23 (39%)
14	CLA	Y	805	-	69,73,73	2.20	21 (30%)	82,113,113	2.60	30 (36%)
14	CLA	G	814	-	54,58,73	2.52	22 (40%)	64,95,113	3.01	34 (53%)
14	CLA	H	824	2	59,63,73	2.52	23 (38%)	70,101,113	2.68	28 (40%)
14	CLA	A	822	-	69,73,73	2.32	23 (33%)	82,113,113	2.39	22 (26%)
14	CLA	A	841	-	69,73,73	2.25	21 (30%)	82,113,113	2.49	29 (35%)
14	CLA	Z	825	2	59,63,73	2.49	23 (38%)	70,101,113	2.57	25 (35%)
14	CLA	G	810	-	49,53,73	2.64	23 (46%)	58,89,113	2.71	23 (39%)
17	BCR	Q	203	-	41,41,41	2.46	6 (14%)	56,56,56	7.31	28 (50%)
14	CLA	A	834	-	59,63,73	2.37	22 (37%)	70,101,113	2.67	25 (35%)
14	CLA	A	842	-	69,73,73	2.20	19 (27%)	82,113,113	2.41	27 (32%)
14	CLA	H	816	-	59,63,73	2.51	22 (37%)	70,101,113	2.79	27 (38%)
14	CLA	Y	838	-	69,73,73	2.32	21 (30%)	82,113,113	2.43	25 (30%)
14	CLA	G	807	-	55,59,73	2.57	22 (40%)	64,96,113	2.68	27 (42%)
14	CLA	Z	804	-	69,73,73	2.29	20 (28%)	82,113,113	2.21	27 (32%)
14	CLA	B	829	-	49,53,73	2.50	21 (42%)	58,89,113	2.90	24 (41%)
14	CLA	Z	833	-	59,63,73	2.44	22 (37%)	70,101,113	2.56	24 (34%)
14	CLA	Y	815	-	54,58,73	2.60	21 (38%)	64,95,113	2.85	26 (40%)
14	CLA	G	812	-	58,62,73	2.48	20 (34%)	68,99,113	2.64	29 (42%)
14	CLA	U	1004	-	69,73,73	2.21	21 (30%)	82,113,113	2.53	24 (29%)
14	CLA	U	1007	-	69,73,73	2.31	23 (33%)	82,113,113	2.45	32 (39%)
17	BCR	Z	847	-	41,41,41	2.46	6 (14%)	56,56,56	7.33	32 (57%)
14	CLA	K	102	-	49,53,73	2.55	20 (40%)	58,89,113	2.73	22 (37%)
14	CLA	H	813	-	69,73,73	2.34	22 (31%)	82,113,113	2.44	27 (32%)
14	CLA	A	810	-	69,73,73	2.24	21 (30%)	82,113,113	2.34	25 (30%)
15	PQN	A	844	-	34,34,34	1.63	2 (5%)	43,45,45	1.19	3 (6%)
14	CLA	Z	815	-	69,73,73	2.29	21 (30%)	82,113,113	2.32	20 (24%)
19	LMG	Z	849	-	49,49,55	1.37	7 (14%)	57,57,63	1.27	6 (10%)
14	CLA	Y	837	-	54,58,73	2.63	22 (40%)	64,95,113	2.67	29 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	Y	827	-	69,73,73	2.31	22 (31%)	82,113,113	2.38	30 (36%)
14	CLA	Y	808	1	69,73,73	2.22	22 (31%)	82,113,113	2.53	28 (34%)
14	CLA	G	852	-	69,73,73	2.23	22 (31%)	82,113,113	2.20	25 (30%)
14	CLA	Y	821	-	69,73,73	2.25	24 (34%)	82,113,113	2.30	26 (31%)
14	CLA	F	202	-	49,53,73	2.47	21 (42%)	58,89,113	2.81	25 (43%)
14	CLA	Y	829	-	69,73,73	2.33	21 (30%)	82,113,113	2.27	24 (29%)
14	CLA	j	102	-	49,53,73	2.62	21 (42%)	58,89,113	2.73	20 (34%)
14	CLA	G	842	18	54,58,73	2.52	22 (40%)	64,95,113	2.88	26 (40%)
14	CLA	Y	825	-	69,73,73	2.23	22 (31%)	82,113,113	2.41	27 (32%)
14	CLA	B	837	-	69,73,73	2.19	19 (27%)	82,113,113	2.48	29 (35%)
17	BCR	B	846	-	41,41,41	2.63	7 (17%)	56,56,56	7.25	26 (46%)
14	CLA	H	838	-	49,53,73	2.56	23 (46%)	58,89,113	2.94	24 (41%)
14	CLA	B	822	-	64,68,73	2.38	19 (29%)	76,107,113	2.41	26 (34%)
14	CLA	Z	837	-	64,68,73	2.32	22 (34%)	76,107,113	2.58	30 (39%)
17	BCR	Y	849	-	41,41,41	2.78	6 (14%)	56,56,56	7.53	30 (53%)
14	CLA	Y	811	14	69,73,73	2.30	20 (28%)	82,113,113	2.33	24 (29%)
14	CLA	h	204	10	69,73,73	2.28	20 (28%)	82,113,113	2.26	27 (32%)
14	CLA	B	818	-	64,68,73	2.30	23 (35%)	76,107,113	2.49	25 (32%)
14	CLA	J	102	-	59,63,73	2.48	23 (38%)	70,101,113	2.73	29 (41%)
14	CLA	U	1003	-	69,73,73	2.23	20 (28%)	82,113,113	2.39	23 (28%)
14	CLA	H	823	-	64,68,73	2.35	20 (31%)	76,107,113	2.59	30 (39%)
14	CLA	Q	202	-	49,53,73	2.53	20 (40%)	58,89,113	2.68	21 (36%)
14	CLA	Y	809	-	69,73,73	2.25	23 (33%)	82,113,113	2.33	26 (31%)
17	BCR	U	1008	-	41,41,41	2.54	7 (17%)	56,56,56	7.18	25 (44%)
17	BCR	H	845	-	25,25,41	2.16	2 (8%)	33,33,56	8.11	18 (54%)
14	CLA	Z	813	-	49,53,73	2.60	21 (42%)	58,89,113	2.67	22 (37%)
14	CLA	H	810	2	69,73,73	2.25	22 (31%)	82,113,113	2.73	33 (40%)
17	BCR	H	842	-	41,41,41	2.73	6 (14%)	56,56,56	7.12	23 (41%)
14	CLA	Z	802	-	69,73,73	2.19	21 (30%)	82,113,113	2.52	29 (35%)
14	CLA	G	828	-	69,73,73	2.25	23 (33%)	82,113,113	2.43	26 (31%)
14	CLA	Z	821	-	49,53,73	2.56	20 (40%)	58,89,113	2.76	27 (46%)
14	CLA	Y	822	-	69,73,73	2.27	23 (33%)	82,113,113	2.53	26 (31%)
14	CLA	G	815	-	54,58,73	2.58	22 (40%)	64,95,113	2.97	27 (42%)
14	CLA	Z	829	-	69,73,73	2.29	22 (31%)	82,113,113	2.45	29 (35%)
14	CLA	G	825	-	69,73,73	2.27	22 (31%)	82,113,113	2.35	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	820	-	49,53,73	2.63	21 (42%)	58,89,113	2.62	23 (39%)
14	CLA	Y	802	-	69,73,73	2.28	21 (30%)	82,113,113	2.42	32 (39%)
14	CLA	H	812	-	49,53,73	2.59	22 (44%)	58,89,113	2.67	24 (41%)
14	CLA	A	818	-	64,68,73	2.35	22 (34%)	76,107,113	2.65	28 (36%)
14	CLA	H	806	-	69,73,73	2.29	21 (30%)	82,113,113	2.43	28 (34%)
14	CLA	H	837	-	69,73,73	2.38	22 (31%)	82,113,113	2.40	27 (32%)
14	CLA	G	834	-	59,63,73	2.43	22 (37%)	70,101,113	2.49	29 (41%)
14	CLA	A	830	-	69,73,73	2.30	23 (33%)	82,113,113	2.18	28 (34%)
14	CLA	G	836	-	54,58,73	2.67	21 (38%)	64,95,113	2.68	27 (42%)
14	CLA	Z	840	-	69,73,73	2.22	21 (30%)	82,113,113	2.35	22 (26%)
14	CLA	W	1701	-	49,53,73	2.60	20 (40%)	58,89,113	2.86	23 (39%)
14	CLA	B	827	-	69,73,73	2.30	21 (30%)	82,113,113	2.35	27 (32%)
14	CLA	H	821	-	49,53,73	2.66	19 (38%)	58,89,113	2.67	22 (37%)
14	CLA	H	826	-	69,73,73	2.27	23 (33%)	82,113,113	2.32	25 (30%)
14	CLA	Z	809	-	69,73,73	2.20	20 (28%)	82,113,113	2.67	33 (40%)
17	BCR	d	203	-	41,41,41	2.54	6 (14%)	56,56,56	7.02	29 (51%)
15	PQN	H	841	-	34,34,34	1.70	2 (5%)	43,45,45	1.26	4 (9%)
14	CLA	B	806	-	69,73,73	2.23	22 (31%)	82,113,113	2.63	30 (36%)
17	BCR	Z	850	-	41,41,41	2.64	6 (14%)	56,56,56	7.22	23 (41%)
14	CLA	H	803	-	69,73,73	2.24	20 (28%)	82,113,113	2.35	29 (35%)
14	CLA	K	101	-	45,49,73	2.49	21 (46%)	54,83,113	2.89	22 (40%)
14	CLA	G	808	1	69,73,73	2.27	22 (31%)	82,113,113	2.48	25 (30%)
14	CLA	Z	822	-	49,53,73	2.58	21 (42%)	58,89,113	2.79	25 (43%)
14	CLA	Y	818	-	69,73,73	2.26	19 (27%)	82,113,113	2.55	27 (32%)
14	CLA	G	811	14	69,73,73	2.27	21 (30%)	82,113,113	2.42	25 (30%)
14	CLA	G	813	-	64,68,73	2.35	22 (34%)	76,107,113	2.61	28 (36%)
17	BCR	L	207	-	41,41,41	2.63	6 (14%)	56,56,56	7.23	21 (37%)
14	CLA	G	805	-	69,73,73	2.20	23 (33%)	82,113,113	2.55	24 (29%)
18	LHG	j	101	-	27,27,48	1.29	2 (7%)	30,33,54	1.22	3 (10%)
16	SF4	C	102	3,21	0,12,12	-	-	-	-	-
19	LMG	B	848	-	52,52,55	1.51	7 (13%)	60,60,63	1.37	7 (11%)
14	CLA	B	828	-	69,73,73	2.24	20 (28%)	82,113,113	2.52	29 (35%)
18	LHG	G	851	14	31,31,48	1.27	2 (6%)	34,37,54	1.20	2 (5%)
16	SF4	Y	843	2,1	0,12,12	-	-	-	-	-
14	CLA	A	839	-	69,73,73	2.23	21 (30%)	82,113,113	2.38	23 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	820	-	69,73,73	2.32	23 (33%)	82,113,113	2.40	27 (32%)
14	CLA	Z	820	-	64,68,73	2.32	22 (34%)	76,107,113	2.37	24 (31%)
14	CLA	B	835	-	49,53,73	2.59	21 (42%)	58,89,113	2.79	24 (41%)
18	LHG	G	850	-	48,48,48	0.94	2 (4%)	51,54,54	1.18	5 (9%)
14	CLA	G	817	-	64,68,73	2.39	22 (34%)	76,107,113	2.53	29 (38%)
14	CLA	H	840	-	69,73,73	2.23	20 (28%)	82,113,113	2.70	28 (34%)
14	CLA	S	1101	-	69,73,73	2.23	20 (28%)	82,113,113	2.48	24 (29%)
17	BCR	H	847	-	41,41,41	2.39	7 (17%)	56,56,56	7.41	29 (51%)
14	CLA	H	830	-	49,53,73	2.55	20 (40%)	58,89,113	3.06	28 (48%)
14	CLA	Z	832	-	49,53,73	2.45	21 (42%)	58,89,113	2.81	26 (44%)
14	CLA	h	205	-	69,73,73	2.28	22 (31%)	82,113,113	2.75	25 (30%)
14	CLA	B	833	-	49,53,73	2.56	22 (44%)	58,89,113	2.97	24 (41%)
14	CLA	B	814	-	49,53,73	2.57	21 (42%)	58,89,113	2.85	24 (41%)
17	BCR	G	849	-	41,41,41	2.56	6 (14%)	56,56,56	7.51	32 (57%)
14	CLA	Z	835	-	49,53,73	2.62	19 (38%)	58,89,113	2.64	23 (39%)
14	CLA	Y	840	-	69,73,73	2.25	22 (31%)	82,113,113	2.35	22 (26%)
14	CLA	Z	839	-	49,53,73	2.53	21 (42%)	58,89,113	2.95	26 (44%)
14	CLA	A	831	-	69,73,73	2.23	22 (31%)	82,113,113	2.32	27 (32%)
17	BCR	B	847	-	41,41,41	2.46	6 (14%)	56,56,56	7.29	26 (46%)
14	CLA	G	809	-	69,73,73	2.27	21 (30%)	82,113,113	2.54	32 (39%)
17	BCR	Q	201	-	41,41,41	2.65	6 (14%)	56,56,56	7.16	27 (48%)
13	CL0	Y	801	-	58,73,73	3.19	18 (31%)	60,113,113	2.54	16 (26%)
14	CLA	G	819	-	69,73,73	2.27	22 (31%)	82,113,113	2.50	26 (31%)
14	CLA	f	101	8	49,53,73	2.59	19 (38%)	58,89,113	2.94	24 (41%)
14	CLA	A	828	-	69,73,73	2.21	20 (28%)	82,113,113	2.30	28 (34%)
14	CLA	Z	805	-	58,62,73	2.30	22 (37%)	68,99,113	2.93	27 (39%)
14	CLA	H	836	-	64,68,73	2.31	21 (32%)	76,107,113	2.42	27 (35%)

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	Z	806	-	1/1/15/20	12/39/115/115	-
14	CLA	Z	801	-	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	821	-	1/1/15/20	17/39/115/115	-
18	LHG	A	853	14	-	18/36/36/53	-
14	CLA	A	837	-	1/1/15/20	20/39/115/115	-
17	BCR	G	848	-	-	8/29/63/63	0/2/2/2
17	BCR	F	201	-	-	10/29/63/63	0/2/2/2
14	CLA	A	807	-	1/1/15/20	22/39/115/115	-
14	CLA	G	820	-	1/1/14/20	12/33/109/115	-
14	CLA	Y	820	-	1/1/14/20	12/33/109/115	-
14	CLA	G	840	-	1/1/15/20	17/39/115/115	-
14	CLA	B	817	-	1/1/14/20	8/33/109/115	-
14	CLA	A	804	-	1/1/15/20	16/39/115/115	-
14	CLA	A	833	-	1/1/15/20	11/39/115/115	-
14	CLA	G	831	-	1/1/12/20	12/21/97/115	-
14	CLA	Z	814	-	1/1/15/20	18/39/115/115	-
14	CLA	G	823	-	1/1/12/20	6/21/97/115	-
14	CLA	U	1002	10	1/1/15/20	21/39/115/115	-
14	CLA	Y	830	-	1/1/15/20	11/39/115/115	-
15	PQN	Y	842	-	-	7/23/43/43	0/2/2/2
15	PQN	Z	842	-	-	8/23/43/43	0/2/2/2
14	CLA	Y	839	-	1/1/12/20	3/21/97/115	-
14	CLA	G	853	-	1/1/11/20	4/15/91/115	-
14	CLA	Z	830	-	1/1/15/20	10/39/115/115	-
14	CLA	B	801	-	1/1/15/20	17/39/115/115	-
17	BCR	L	208	-	-	8/29/63/63	0/2/2/2
14	CLA	H	801	-	1/1/15/20	13/39/115/115	-
17	BCR	B	843	-	-	7/29/63/63	0/2/2/2
14	CLA	Z	818	-	1/1/15/20	14/39/115/115	-
14	CLA	Y	816	-	1/1/12/20	8/21/97/115	-
17	BCR	H	846	-	-	14/29/63/63	0/2/2/2
14	CLA	Z	816	-	1/1/11/20	4/15/91/115	-
14	CLA	A	817	-	1/1/12/20	7/21/97/115	-
14	CLA	Y	806	-	1/1/15/20	16/39/115/115	-
17	BCR	G	845	-	-	8/29/63/63	0/2/2/2
14	CLA	B	810	-	1/1/13/20	12/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	803	-	1/1/12/20	7/26/102/115	-
13	CL0	A	801	-	3/3/20/25	8/37/135/135	-
14	CLA	A	854	-	1/1/15/20	16/39/115/115	-
14	CLA	A	824	-	1/1/12/20	10/21/97/115	-
14	CLA	H	809	2	1/1/15/20	14/39/115/115	-
17	BCR	V	101	-	-	6/29/63/63	0/2/2/2
14	CLA	Z	803	-	1/1/15/20	15/39/115/115	-
14	CLA	X	1701	-	1/1/11/20	5/15/91/115	-
17	BCR	Y	845	-	-	4/29/63/63	0/2/2/2
15	PQN	G	843	-	-	10/23/43/43	0/2/2/2
17	BCR	B	844	-	-	12/29/63/63	0/2/2/2
17	BCR	M	101	-	-	11/29/63/63	0/2/2/2
14	CLA	B	826	-	1/1/15/20	14/39/115/115	-
14	CLA	B	807	-	1/1/15/20	18/39/115/115	-
14	CLA	A	802	-	1/1/15/20	13/39/115/115	-
13	CL0	G	801	-	3/3/20/25	13/37/135/135	-
16	SF4	N	102	3	-	-	0/6/5/5
14	CLA	B	834	-	1/1/11/20	6/15/91/115	-
14	CLA	H	820	-	1/1/11/20	9/15/91/115	-
14	CLA	Y	804	14	1/1/13/20	13/32/108/115	-
14	CLA	Z	826	-	1/1/15/20	12/39/115/115	-
17	BCR	I	101	-	-	5/29/63/63	0/2/2/2
14	CLA	H	832	-	1/1/13/20	14/27/103/115	-
14	CLA	h	201	-	1/1/15/20	10/39/115/115	-
17	BCR	A	848	-	-	10/29/63/63	0/2/2/2
17	BCR	U	1009	-	-	8/29/63/63	0/2/2/2
14	CLA	L	202	-	1/1/15/20	15/39/115/115	-
14	CLA	Y	823	-	1/1/12/20	9/21/97/115	-
17	BCR	R	101	-	-	8/29/63/63	0/2/2/2
17	BCR	A	851	-	-	11/29/63/63	0/2/2/2
14	CLA	B	825	-	1/1/15/20	21/39/115/115	-
17	BCR	Z	844	-	-	8/29/63/63	0/2/2/2
14	CLA	T	101	-	1/1/9/20	7/9/81/115	-
14	CLA	B	812	-	1/1/15/20	21/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	811	-	1/1/11/20	6/15/91/115	-
14	CLA	H	827	-	1/1/15/20	14/39/115/115	-
14	CLA	Y	803	-	1/1/15/20	15/39/115/115	-
14	CLA	A	805	14	1/1/13/20	15/32/108/115	-
17	BCR	Z	846	-	-	9/18/35/63	0/1/1/2
14	CLA	G	838	-	1/1/12/20	3/21/97/115	-
14	CLA	Y	841	-	1/1/15/20	13/39/115/115	-
14	CLA	B	811	-	1/1/12/20	6/21/97/115	-
14	CLA	Y	833	-	1/1/13/20	10/27/103/115	-
14	CLA	A	815	-	1/1/12/20	9/21/97/115	-
14	CLA	H	835	-	1/1/11/20	6/15/91/115	-
17	BCR	i	101	-	-	11/29/63/63	0/2/2/2
14	CLA	G	830	-	1/1/15/20	13/39/115/115	-
14	CLA	Z	834	-	1/1/11/20	5/15/91/115	-
14	CLA	A	843	18	1/1/12/20	9/21/97/115	-
14	CLA	B	808	2	1/1/15/20	16/39/115/115	-
14	CLA	B	821	-	1/1/13/20	13/27/103/115	-
14	CLA	G	827	-	1/1/15/20	16/39/115/115	-
14	CLA	A	838	-	1/1/12/20	7/21/97/115	-
14	CLA	S	1102	8	1/1/11/20	7/15/91/115	-
17	BCR	h	202	-	-	7/29/63/63	0/2/2/2
14	CLA	G	816	-	1/1/12/20	8/21/97/115	-
18	LHG	B	849	-	-	28/43/43/53	-
14	CLA	H	804	-	1/1/12/20	9/26/102/115	-
14	CLA	H	833	-	1/1/11/20	6/15/91/115	-
14	CLA	B	819	-	1/1/11/20	4/15/91/115	-
17	BCR	Z	845	-	-	10/29/63/63	0/2/2/2
14	CLA	B	836	-	1/1/14/20	7/33/109/115	-
19	LMG	H	848	-	-	12/44/64/70	0/1/1/1
14	CLA	H	807	-	1/1/15/20	8/39/115/115	-
14	CLA	A	825	-	1/1/14/20	14/33/109/115	-
14	CLA	Y	835	-	1/1/12/20	8/21/97/115	-
14	CLA	B	839	-	1/1/15/20	12/39/115/115	-
14	CLA	Z	841	-	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	825	-	1/1/15/20	22/39/115/115	-
17	BCR	Y	844	-	-	8/29/63/63	0/2/2/2
14	CLA	G	837	-	1/1/15/20	20/39/115/115	-
14	CLA	H	814	-	1/1/15/20	17/39/115/115	-
14	CLA	Z	807	-	1/1/15/20	16/39/115/115	-
14	CLA	A	808	-	1/1/12/20	8/23/99/115	-
17	BCR	G	846	-	-	9/29/63/63	0/2/2/2
14	CLA	A	821	-	1/1/14/20	13/33/109/115	-
17	BCR	Y	846	-	-	18/29/63/63	0/2/2/2
14	CLA	A	816	-	1/1/12/20	5/21/97/115	-
17	BCR	S	1105	-	-	12/29/63/63	0/2/2/2
14	CLA	B	805	-	1/1/15/20	14/39/115/115	-
14	CLA	H	817	-	1/1/15/20	15/39/115/115	-
14	CLA	H	831	-	1/1/15/20	17/39/115/115	-
17	BCR	Y	847	-	-	6/29/63/63	0/2/2/2
14	CLA	Z	808	-	1/1/15/20	17/39/115/115	-
14	CLA	B	815	-	1/1/13/20	10/27/103/115	-
14	CLA	B	802	-	1/1/15/20	10/39/115/115	-
14	CLA	g	101	-	1/1/9/20	4/9/81/115	-
14	CLA	Y	826	-	1/1/14/20	10/33/109/115	-
17	BCR	A	850	-	-	6/29/63/63	0/2/2/2
14	CLA	d	201	-	1/1/15/20	13/39/115/115	-
17	BCR	R	102	-	-	11/29/63/63	0/2/2/2
17	BCR	S	1104	-	-	9/29/63/63	0/2/2/2
14	CLA	A	819	-	1/1/15/20	20/39/115/115	-
14	CLA	Z	819	-	1/1/14/20	14/33/109/115	-
14	CLA	Z	828	-	1/1/15/20	19/39/115/115	-
14	CLA	A	836	-	1/1/12/20	5/21/97/115	-
17	BCR	Y	848	-	-	2/29/63/63	0/2/2/2
17	BCR	H	843	-	-	9/29/63/63	0/2/2/2
17	BCR	G	847	-	-	7/29/63/63	0/2/2/2
14	CLA	H	802	-	1/1/15/20	21/39/115/115	-
17	BCR	Z	848	-	-	9/29/63/63	0/2/2/2
16	SF4	N	101	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	822	-	1/1/15/20	12/39/115/115	-
14	CLA	Z	838	-	1/1/15/20	13/39/115/115	-
14	CLA	G	841	-	1/1/15/20	14/39/115/115	-
14	CLA	H	829	-	1/1/15/20	12/39/115/115	-
14	CLA	T	103	-	1/1/11/20	6/15/91/115	-
14	CLA	Z	836	-	1/1/11/20	6/15/91/115	-
14	CLA	B	813	-	1/1/15/20	19/39/115/115	-
14	CLA	B	824	-	1/1/15/20	15/39/115/115	-
14	CLA	G	802	-	1/1/15/20	15/39/115/115	-
17	BCR	A	849	-	-	8/29/63/63	0/2/2/2
18	LHG	Y	850	-	-	31/53/53/53	-
14	CLA	Y	807	-	1/1/12/20	10/23/99/115	-
17	BCR	B	850	-	-	9/29/63/63	0/2/2/2
14	CLA	Z	831	-	1/1/11/20	5/15/91/115	-
14	CLA	f	102	-	1/1/13/20	14/27/103/115	-
14	CLA	A	835	1	1/1/11/20	2/15/91/115	-
17	BCR	H	844	-	-	10/29/63/63	0/2/2/2
14	CLA	Y	812	-	1/1/13/20	8/27/103/115	-
14	CLA	H	815	-	1/1/11/20	7/15/91/115	-
14	CLA	B	816	-	1/1/15/20	8/39/115/115	-
14	CLA	h	206	-	1/1/15/20	15/39/115/115	-
17	BCR	J	104	-	-	9/29/63/63	0/2/2/2
14	CLA	Z	811	2	1/1/15/20	18/39/115/115	-
14	CLA	H	834	-	1/1/11/20	5/15/91/115	-
14	CLA	B	840	-	1/1/15/20	10/39/115/115	-
14	CLA	Y	813	-	1/1/14/20	9/33/109/115	-
16	SF4	a	102	3	-	-	0/6/5/5
14	CLA	B	831	-	1/1/15/20	19/39/115/115	-
14	CLA	Y	828	-	1/1/15/20	13/39/115/115	-
14	CLA	H	818	-	1/1/14/20	16/33/109/115	-
14	CLA	B	832	-	1/1/13/20	12/27/103/115	-
14	CLA	G	835	-	1/1/11/20	5/15/91/115	-
14	CLA	B	809	-	1/1/15/20	17/39/115/115	-
14	CLA	Z	817	-	1/1/13/20	11/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	840	-	1/1/12/20	3/21/97/115	-
14	CLA	A	813	-	1/1/12/20	6/26/102/115	-
14	CLA	B	823	2	1/1/13/20	12/27/103/115	-
14	CLA	Z	824	-	1/1/14/20	8/33/109/115	-
14	CLA	G	804	14	1/1/13/20	10/32/108/115	-
17	BCR	Y	852	-	-	13/29/63/63	0/2/2/2
14	CLA	A	823	-	1/1/15/20	17/39/115/115	-
14	CLA	G	806	-	1/1/15/20	20/39/115/115	-
14	CLA	Y	836	-	1/1/15/20	18/39/115/115	-
18	LHG	A	852	-	-	29/53/53/53	-
14	CLA	S	1103	-	1/1/13/20	14/27/103/115	-
14	CLA	B	838	-	1/1/11/20	2/15/91/115	-
17	BCR	Z	843	-	-	12/29/63/63	0/2/2/2
14	CLA	L	204	-	1/1/15/20	20/39/115/115	-
14	CLA	G	832	-	1/1/15/20	15/39/115/115	-
17	BCR	J	103	-	-	6/29/63/63	0/2/2/2
17	BCR	A	847	-	-	9/29/63/63	0/2/2/2
14	CLA	Z	810	2	1/1/15/20	13/39/115/115	-
14	CLA	d	202	-	1/1/11/20	2/15/91/115	-
14	CLA	H	808	-	1/1/15/20	17/39/115/115	-
14	CLA	Y	819	-	1/1/15/20	18/39/115/115	-
14	CLA	H	811	-	1/1/13/20	9/27/103/115	-
14	CLA	A	832	-	1/1/12/20	3/21/97/115	-
14	CLA	L	201	-	1/1/15/20	17/39/115/115	-
14	CLA	Y	814	-	1/1/13/20	11/27/103/115	-
14	CLA	A	809	1	1/1/15/20	20/39/115/115	-
17	BCR	B	842	-	-	3/24/41/63	0/1/1/2
17	BCR	B	845	-	-	4/18/35/63	0/1/1/2
18	LHG	Y	851	14	-	17/28/28/53	-
17	BCR	h	207	-	-	10/29/63/63	0/2/2/2
16	SF4	A	845	2,1	-	-	0/6/5/5
14	CLA	Y	817	-	1/1/14/20	10/33/109/115	-
14	CLA	Y	831	-	1/1/12/20	6/21/97/115	-
17	BCR	T	102	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	818	-	1/1/15/20	18/39/115/115	-
14	CLA	H	828	-	1/1/15/20	7/39/115/115	-
14	CLA	J	101	8	1/1/11/20	7/15/91/115	-
14	CLA	Y	824	-	1/1/14/20	14/33/109/115	-
17	BCR	f	103	-	-	5/29/63/63	0/2/2/2
14	CLA	g	102	-	1/1/11/20	3/15/91/115	-
14	CLA	L	206	-	1/1/15/20	9/39/115/115	-
16	SF4	G	844	2,1	-	-	0/6/5/5
14	CLA	H	839	-	1/1/15/20	6/39/115/115	-
17	BCR	Y	853	-	-	6/29/63/63	0/2/2/2
14	CLA	Y	810	-	1/1/11/20	2/15/91/115	-
14	CLA	H	819	-	1/1/14/20	14/33/109/115	-
14	CLA	A	827	-	1/1/14/20	10/33/109/115	-
17	BCR	I	102	-	-	9/29/63/63	0/2/2/2
14	CLA	U	1006	-	1/1/15/20	15/39/115/115	-
14	CLA	G	839	-	1/1/12/20	5/21/97/115	-
14	CLA	H	851	18	1/1/12/20	13/21/97/115	-
14	CLA	G	833	-	1/1/15/20	16/39/115/115	-
14	CLA	A	814	-	1/1/14/20	11/33/109/115	-
14	CLA	H	805	-	1/1/15/20	16/39/115/115	-
17	BCR	e	101	-	-	18/29/63/63	0/2/2/2
17	BCR	A	846	-	-	10/29/63/63	0/2/2/2
14	CLA	H	822	-	1/1/13/20	9/27/103/115	-
16	SF4	a	101	3	-	-	0/6/5/5
14	CLA	A	826	-	1/1/15/20	16/39/115/115	-
16	SF4	C	101	3	-	-	0/6/5/5
17	BCR	H	850	-	-	8/29/63/63	0/2/2/2
15	PQN	B	841	-	-	9/23/43/43	0/2/2/2
14	CLA	G	803	-	1/1/15/20	12/39/115/115	-
14	CLA	A	803	-	1/1/15/20	9/39/115/115	-
14	CLA	G	829	-	1/1/15/20	14/39/115/115	-
14	CLA	L	205	-	1/1/15/20	15/39/115/115	-
14	CLA	G	824	-	1/1/14/20	17/33/109/115	-
14	CLA	A	812	14	1/1/15/20	12/39/115/115	-
14	CLA	Z	812	-	1/1/13/20	12/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	Z	823	-	1/1/13/20	10/27/103/115	-
14	CLA	A	806	-	1/1/15/20	24/39/115/115	-
14	CLA	B	804	-	1/1/15/20	14/39/115/115	-
18	LHG	H	849	-	-	21/41/41/53	-
14	CLA	B	830	-	1/1/11/20	3/15/91/115	-
14	CLA	A	829	-	1/1/15/20	11/39/115/115	-
17	BCR	F	203	-	-	4/29/63/63	0/2/2/2
14	CLA	G	826	-	1/1/14/20	7/33/109/115	-
14	CLA	Y	832	-	1/1/15/20	21/39/115/115	-
14	CLA	Z	827	-	1/1/15/20	13/39/115/115	-
17	BCR	U	1005	-	-	6/29/63/63	0/2/2/2
14	CLA	Y	834	1	1/1/11/20	3/15/91/115	-
14	CLA	Y	805	-	1/1/15/20	16/39/115/115	-
14	CLA	G	814	-	1/1/12/20	4/21/97/115	-
14	CLA	H	824	2	1/1/13/20	13/27/103/115	-
14	CLA	A	822	-	1/1/15/20	13/39/115/115	-
14	CLA	A	841	-	1/1/15/20	16/39/115/115	-
14	CLA	Z	825	2	1/1/13/20	9/27/103/115	-
14	CLA	G	810	-	1/1/11/20	7/15/91/115	-
17	BCR	Q	203	-	-	5/29/63/63	0/2/2/2
14	CLA	A	834	-	1/1/13/20	8/27/103/115	-
14	CLA	A	842	-	1/1/15/20	12/39/115/115	-
14	CLA	H	816	-	1/1/13/20	10/27/103/115	-
14	CLA	Y	838	-	1/1/15/20	9/39/115/115	-
14	CLA	G	807	-	1/1/12/20	7/23/99/115	-
14	CLA	Z	804	-	1/1/15/20	13/39/115/115	-
14	CLA	B	829	-	1/1/11/20	5/15/91/115	-
14	CLA	Z	833	-	1/1/13/20	12/27/103/115	-
14	CLA	Y	815	-	1/1/12/20	7/21/97/115	-
14	CLA	G	812	-	1/1/12/20	8/26/102/115	-
14	CLA	U	1004	-	1/1/15/20	15/39/115/115	-
14	CLA	U	1007	-	1/1/15/20	14/39/115/115	-
17	BCR	Z	847	-	-	10/29/63/63	0/2/2/2
14	CLA	K	102	-	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	813	-	1/1/15/20	18/39/115/115	-
14	CLA	A	810	-	1/1/15/20	12/39/115/115	-
15	PQN	A	844	-	-	4/23/43/43	0/2/2/2
14	CLA	Z	815	-	1/1/15/20	10/39/115/115	-
19	LMG	Z	849	-	-	14/44/64/70	0/1/1/1
14	CLA	Y	837	-	1/1/12/20	5/21/97/115	-
14	CLA	Y	827	-	1/1/15/20	15/39/115/115	-
14	CLA	Y	808	1	1/1/15/20	20/39/115/115	-
14	CLA	G	852	-	1/1/15/20	11/39/115/115	-
14	CLA	Y	821	-	1/1/15/20	16/39/115/115	-
14	CLA	F	202	-	1/1/11/20	4/15/91/115	-
14	CLA	Y	829	-	1/1/15/20	13/39/115/115	-
14	CLA	j	102	-	1/1/11/20	6/15/91/115	-
14	CLA	G	842	18	1/1/12/20	5/21/97/115	-
14	CLA	Y	825	-	1/1/15/20	14/39/115/115	-
14	CLA	B	837	-	1/1/15/20	11/39/115/115	-
17	BCR	B	846	-	-	11/29/63/63	0/2/2/2
14	CLA	H	838	-	1/1/11/20	0/15/91/115	-
14	CLA	B	822	-	1/1/14/20	13/33/109/115	-
14	CLA	Z	837	-	1/1/14/20	12/33/109/115	-
17	BCR	Y	849	-	-	8/29/63/63	0/2/2/2
14	CLA	Y	811	14	1/1/15/20	17/39/115/115	-
14	CLA	h	204	10	1/1/15/20	18/39/115/115	-
14	CLA	B	818	-	1/1/14/20	17/33/109/115	-
14	CLA	J	102	-	1/1/13/20	13/27/103/115	-
14	CLA	U	1003	-	1/1/15/20	12/39/115/115	-
14	CLA	H	823	-	1/1/14/20	13/33/109/115	-
14	CLA	Q	202	-	1/1/11/20	2/15/91/115	-
14	CLA	Y	809	-	1/1/15/20	15/39/115/115	-
17	BCR	U	1008	-	-	16/29/63/63	0/2/2/2
17	BCR	H	845	-	-	8/18/35/63	0/1/1/2
14	CLA	Z	813	-	1/1/11/20	6/15/91/115	-
14	CLA	H	810	2	1/1/15/20	16/39/115/115	-
17	BCR	H	842	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	Z	802	-	1/1/15/20	18/39/115/115	-
14	CLA	G	828	-	1/1/15/20	12/39/115/115	-
14	CLA	Z	821	-	1/1/11/20	9/15/91/115	-
14	CLA	Y	822	-	1/1/15/20	17/39/115/115	-
14	CLA	G	815	-	1/1/12/20	5/21/97/115	-
14	CLA	Z	829	-	1/1/15/20	13/39/115/115	-
14	CLA	G	825	-	1/1/15/20	10/39/115/115	-
14	CLA	B	820	-	1/1/11/20	9/15/91/115	-
14	CLA	Y	802	-	1/1/15/20	10/39/115/115	-
14	CLA	H	812	-	1/1/11/20	6/15/91/115	-
14	CLA	A	818	-	1/1/14/20	14/33/109/115	-
14	CLA	H	806	-	1/1/15/20	16/39/115/115	-
14	CLA	H	837	-	1/1/15/20	14/39/115/115	-
14	CLA	G	834	-	1/1/13/20	7/27/103/115	-
14	CLA	A	830	-	1/1/15/20	15/39/115/115	-
14	CLA	G	836	-	1/1/12/20	4/21/97/115	-
14	CLA	Z	840	-	1/1/15/20	11/39/115/115	-
14	CLA	W	1701	-	1/1/11/20	6/15/91/115	-
14	CLA	B	827	-	1/1/15/20	20/39/115/115	-
14	CLA	H	821	-	1/1/11/20	6/15/91/115	-
14	CLA	H	826	-	1/1/15/20	8/39/115/115	-
14	CLA	Z	809	-	1/1/15/20	17/39/115/115	-
17	BCR	d	203	-	-	6/29/63/63	0/2/2/2
15	PQN	H	841	-	-	5/23/43/43	0/2/2/2
14	CLA	B	806	-	1/1/15/20	10/39/115/115	-
17	BCR	Z	850	-	-	4/29/63/63	0/2/2/2
14	CLA	H	803	-	1/1/15/20	17/39/115/115	-
14	CLA	K	101	-	1/1/9/20	6/9/81/115	-
14	CLA	G	808	1	1/1/15/20	18/39/115/115	-
14	CLA	Z	822	-	1/1/11/20	6/15/91/115	-
14	CLA	Y	818	-	1/1/15/20	14/39/115/115	-
14	CLA	G	811	14	1/1/15/20	21/39/115/115	-
14	CLA	G	813	-	1/1/14/20	11/33/109/115	-
17	BCR	L	207	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	805	-	1/1/15/20	20/39/115/115	-
18	LHG	j	101	-	-	16/32/32/53	-
16	SF4	C	102	3,21	-	-	0/6/5/5
19	LMG	B	848	-	-	12/47/67/70	0/1/1/1
14	CLA	B	828	-	1/1/15/20	9/39/115/115	-
18	LHG	G	851	14	-	15/36/36/53	-
16	SF4	Y	843	2,1	-	-	0/6/5/5
14	CLA	A	839	-	1/1/15/20	13/39/115/115	-
14	CLA	A	820	-	1/1/15/20	16/39/115/115	-
14	CLA	Z	820	-	1/1/14/20	10/33/109/115	-
14	CLA	B	835	-	1/1/11/20	6/15/91/115	-
18	LHG	G	850	-	-	26/53/53/53	-
14	CLA	G	817	-	1/1/14/20	13/33/109/115	-
14	CLA	H	840	-	1/1/15/20	9/39/115/115	-
14	CLA	S	1101	-	1/1/15/20	18/39/115/115	-
17	BCR	H	847	-	-	8/29/63/63	0/2/2/2
14	CLA	H	830	-	1/1/11/20	10/15/91/115	-
14	CLA	Z	832	-	1/1/11/20	6/15/91/115	-
14	CLA	h	205	-	1/1/15/20	15/39/115/115	-
14	CLA	B	833	-	1/1/11/20	6/15/91/115	-
14	CLA	B	814	-	1/1/11/20	2/15/91/115	-
17	BCR	G	849	-	-	9/29/63/63	0/2/2/2
14	CLA	Z	835	-	1/1/11/20	8/15/91/115	-
14	CLA	Y	840	-	1/1/15/20	12/39/115/115	-
14	CLA	Z	839	-	1/1/11/20	2/15/91/115	-
14	CLA	A	831	-	1/1/15/20	14/39/115/115	-
17	BCR	B	847	-	-	6/29/63/63	0/2/2/2
14	CLA	G	809	-	1/1/15/20	16/39/115/115	-
17	BCR	Q	201	-	-	11/29/63/63	0/2/2/2
13	CL0	Y	801	-	3/3/20/25	17/37/135/135	-
14	CLA	G	819	-	1/1/15/20	19/39/115/115	-
14	CLA	f	101	8	1/1/11/20	5/15/91/115	-
14	CLA	A	828	-	1/1/15/20	17/39/115/115	-
14	CLA	Z	805	-	1/1/12/20	4/26/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	836	-	1/1/14/20	18/33/109/115	-

The worst 5 of 6514 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	801	CL0	C1D-C2D	10.15	1.51	1.39
13	Y	801	CL0	C1A-CHA	9.64	1.51	1.40
13	A	801	CL0	C1A-CHA	9.53	1.50	1.40
13	A	801	CL0	C1B-C2B	9.36	1.50	1.39
13	Y	801	CL0	C1D-C2D	9.06	1.49	1.39

The worst 5 of 9226 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Z	848	BCR	C16-C17-C18	33.83	174.73	127.28
17	i	101	BCR	C16-C17-C18	30.64	170.25	127.28
17	Y	846	BCR	C16-C17-C18	30.48	170.03	127.28
17	R	101	BCR	C16-C17-C18	29.95	169.28	127.28
17	Y	849	BCR	C16-C17-C18	28.77	167.63	127.28

5 of 291 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	801	CL0	ND
13	A	801	CL0	NA
13	A	801	CL0	NC
13	G	801	CL0	ND
13	G	801	CL0	NA

5 of 4154 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	G	801	CL0	C3A-C2A-CAA-CBA
13	G	801	CL0	CBD-CGD-O2D-CED
13	G	801	CL0	C4-C3-C5-C6
13	Y	801	CL0	CBD-CGD-O2D-CED
14	A	802	CLA	CBA-CGA-O2A-C1

There are no ring outliers.

366 monomers are involved in 1911 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	Z	806	CLA	11	0
14	Z	801	CLA	11	0
14	G	821	CLA	13	0
18	A	853	LHG	1	0
14	A	837	CLA	4	0
17	G	848	BCR	11	0
17	F	201	BCR	7	0
14	A	807	CLA	19	0
14	G	820	CLA	6	0
14	Y	820	CLA	2	0
14	G	840	CLA	10	0
14	B	817	CLA	6	0
14	A	804	CLA	5	0
14	A	833	CLA	6	0
14	G	831	CLA	4	0
14	Z	814	CLA	15	0
14	U	1002	CLA	11	0
14	Y	830	CLA	8	0
15	Y	842	PQN	10	0
15	Z	842	PQN	4	0
14	Y	839	CLA	4	0
14	G	853	CLA	3	0
14	Z	830	CLA	1	0
14	B	801	CLA	21	0
17	L	208	BCR	5	0
14	H	801	CLA	7	0
17	B	843	BCR	2	0
14	Z	818	CLA	4	0
14	Y	816	CLA	5	0
17	H	846	BCR	9	0
14	Z	816	CLA	5	0
14	A	817	CLA	1	0
14	Y	806	CLA	5	0
17	G	845	BCR	6	0
14	B	810	CLA	5	0
14	B	803	CLA	7	0
13	A	801	CL0	9	0
14	A	854	CLA	10	0
14	A	824	CLA	1	0
14	H	809	CLA	16	0
17	V	101	BCR	6	0
14	Z	803	CLA	13	0
14	X	1701	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Y	845	BCR	7	0
15	G	843	PQN	4	0
17	B	844	BCR	6	0
17	M	101	BCR	6	0
14	B	826	CLA	13	0
14	B	807	CLA	7	0
14	A	802	CLA	12	0
13	G	801	CL0	8	0
16	N	102	SF4	2	0
14	B	834	CLA	4	0
14	H	820	CLA	2	0
14	Y	804	CLA	6	0
14	Z	826	CLA	10	0
17	I	101	BCR	5	0
14	H	832	CLA	9	0
14	h	201	CLA	6	0
17	A	848	BCR	8	0
17	U	1009	BCR	10	0
14	L	202	CLA	8	0
14	Y	823	CLA	2	0
17	R	101	BCR	6	0
17	A	851	BCR	10	0
14	B	825	CLA	6	0
17	Z	844	BCR	8	0
14	B	812	CLA	13	0
14	A	811	CLA	3	0
14	H	827	CLA	7	0
14	Y	803	CLA	5	0
14	A	805	CLA	4	0
17	Z	846	BCR	4	0
14	G	838	CLA	2	0
14	Y	841	CLA	9	0
14	B	811	CLA	2	0
14	Y	833	CLA	5	0
14	A	815	CLA	2	0
14	H	835	CLA	2	0
17	i	101	BCR	3	0
14	G	830	CLA	7	0
14	Z	834	CLA	9	0
14	A	843	CLA	2	0
14	B	808	CLA	13	0
14	B	821	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	G	827	CLA	5	0
14	A	838	CLA	2	0
14	S	1102	CLA	1	0
17	h	202	BCR	11	0
14	G	816	CLA	1	0
18	B	849	LHG	1	0
14	H	804	CLA	7	0
14	H	833	CLA	7	0
14	B	819	CLA	6	0
17	Z	845	BCR	6	0
14	B	836	CLA	7	0
19	H	848	LMG	4	0
14	H	807	CLA	7	0
14	A	825	CLA	3	0
14	Y	835	CLA	2	0
14	B	839	CLA	8	0
14	Z	841	CLA	7	0
14	H	825	CLA	7	0
17	Y	844	BCR	10	0
14	G	837	CLA	5	0
14	H	814	CLA	5	0
14	Z	807	CLA	7	0
14	A	808	CLA	3	0
17	G	846	BCR	5	0
14	A	821	CLA	7	0
17	Y	846	BCR	6	0
14	A	816	CLA	1	0
17	S	1105	BCR	11	0
14	B	805	CLA	12	0
14	H	817	CLA	9	0
14	H	831	CLA	6	0
17	Y	847	BCR	3	0
14	Z	808	CLA	10	0
14	B	802	CLA	19	0
14	g	101	CLA	1	0
14	Y	826	CLA	6	0
17	A	850	BCR	9	0
14	d	201	CLA	6	0
17	S	1104	BCR	13	0
14	A	819	CLA	9	0
14	Z	819	CLA	11	0
14	Z	828	CLA	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	836	CLA	2	0
17	Y	848	BCR	7	0
17	H	843	BCR	5	0
17	G	847	BCR	5	0
14	H	802	CLA	15	0
17	Z	848	BCR	9	0
16	N	101	SF4	2	0
14	G	822	CLA	2	0
14	Z	838	CLA	5	0
14	G	841	CLA	9	0
14	H	829	CLA	11	0
14	T	103	CLA	1	0
14	Z	836	CLA	1	0
14	B	813	CLA	3	0
14	B	824	CLA	5	0
14	G	802	CLA	19	0
17	A	849	BCR	6	0
18	Y	850	LHG	3	0
14	Y	807	CLA	1	0
17	B	850	BCR	7	0
14	Z	831	CLA	4	0
14	f	102	CLA	1	0
14	A	835	CLA	3	0
17	H	844	BCR	7	0
14	Y	812	CLA	1	0
14	H	815	CLA	5	0
14	B	816	CLA	7	0
14	h	206	CLA	7	0
17	J	104	BCR	12	0
14	Z	811	CLA	12	0
14	H	834	CLA	2	0
14	B	840	CLA	2	0
14	Y	813	CLA	6	0
16	a	102	SF4	1	0
14	B	831	CLA	10	0
14	Y	828	CLA	13	0
14	H	818	CLA	7	0
14	B	832	CLA	9	0
14	B	809	CLA	7	0
14	Z	817	CLA	2	0
14	A	840	CLA	8	0
14	A	813	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	823	CLA	5	0
14	Z	824	CLA	3	0
14	G	804	CLA	7	0
17	Y	852	BCR	11	0
14	A	823	CLA	6	0
14	G	806	CLA	10	0
14	Y	836	CLA	8	0
18	A	852	LHG	5	0
14	S	1103	CLA	2	0
14	B	838	CLA	7	0
17	Z	843	BCR	2	0
14	L	204	CLA	6	0
14	G	832	CLA	5	0
17	J	103	BCR	8	0
17	A	847	BCR	3	0
14	Z	810	CLA	15	0
14	d	202	CLA	5	0
14	H	808	CLA	10	0
14	Y	819	CLA	7	0
14	H	811	CLA	2	0
14	A	832	CLA	3	0
14	L	201	CLA	2	0
14	Y	814	CLA	7	0
14	A	809	CLA	13	0
17	B	842	BCR	4	0
17	B	845	BCR	7	0
18	Y	851	LHG	5	0
17	h	207	BCR	8	0
16	A	845	SF4	4	0
14	Y	817	CLA	7	0
14	Y	831	CLA	4	0
17	T	102	BCR	6	0
14	G	818	CLA	8	0
14	H	828	CLA	11	0
14	Y	824	CLA	3	0
17	f	103	BCR	8	0
14	g	102	CLA	2	0
14	L	206	CLA	4	0
16	G	844	SF4	1	0
14	H	839	CLA	6	0
17	Y	853	BCR	19	0
14	H	819	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	827	CLA	10	0
17	I	102	BCR	7	0
14	U	1006	CLA	4	0
14	G	839	CLA	3	0
14	H	851	CLA	5	0
14	G	833	CLA	7	0
14	A	814	CLA	9	0
14	H	805	CLA	2	0
17	e	101	BCR	7	0
16	a	101	SF4	1	0
14	H	822	CLA	10	0
17	A	846	BCR	8	0
14	A	826	CLA	7	0
17	H	850	BCR	8	0
15	B	841	PQN	4	0
14	G	803	CLA	15	0
14	A	803	CLA	11	0
14	G	829	CLA	7	0
14	L	205	CLA	2	0
14	G	824	CLA	6	0
14	A	812	CLA	8	0
14	Z	812	CLA	2	0
14	Z	823	CLA	3	0
14	A	806	CLA	5	0
14	B	804	CLA	8	0
18	H	849	LHG	3	0
14	B	830	CLA	3	0
14	A	829	CLA	21	0
17	F	203	BCR	2	0
14	G	826	CLA	12	0
14	Y	832	CLA	5	0
14	Z	827	CLA	8	0
17	U	1005	BCR	12	0
14	Y	834	CLA	3	0
14	Y	805	CLA	6	0
14	G	814	CLA	3	0
14	H	824	CLA	9	0
14	A	822	CLA	10	0
14	A	841	CLA	10	0
14	Z	825	CLA	6	0
17	Q	203	BCR	4	0
14	A	834	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	842	CLA	8	0
14	H	816	CLA	1	0
14	Y	838	CLA	9	0
14	G	807	CLA	6	0
14	Z	804	CLA	25	0
14	B	829	CLA	4	0
14	Z	833	CLA	8	0
14	Y	815	CLA	2	0
14	G	812	CLA	1	0
14	U	1004	CLA	8	0
14	U	1007	CLA	11	0
17	Z	847	BCR	12	0
14	K	102	CLA	1	0
14	H	813	CLA	9	0
14	A	810	CLA	2	0
15	A	844	PQN	9	0
14	Z	815	CLA	4	0
19	Z	849	LMG	4	0
14	Y	837	CLA	1	0
14	Y	827	CLA	7	0
14	Y	808	CLA	11	0
14	G	852	CLA	17	0
14	Y	821	CLA	10	0
14	F	202	CLA	2	0
14	Y	829	CLA	7	0
14	G	842	CLA	1	0
14	Y	825	CLA	7	0
14	B	837	CLA	7	0
17	B	846	BCR	9	0
14	H	838	CLA	7	0
14	B	822	CLA	3	0
14	Z	837	CLA	7	0
17	Y	849	BCR	12	0
14	Y	811	CLA	5	0
14	h	204	CLA	10	0
14	B	818	CLA	3	0
14	U	1003	CLA	10	0
14	H	823	CLA	4	0
14	Q	202	CLA	4	0
14	Y	809	CLA	2	0
17	U	1008	BCR	11	0
17	H	845	BCR	5	0

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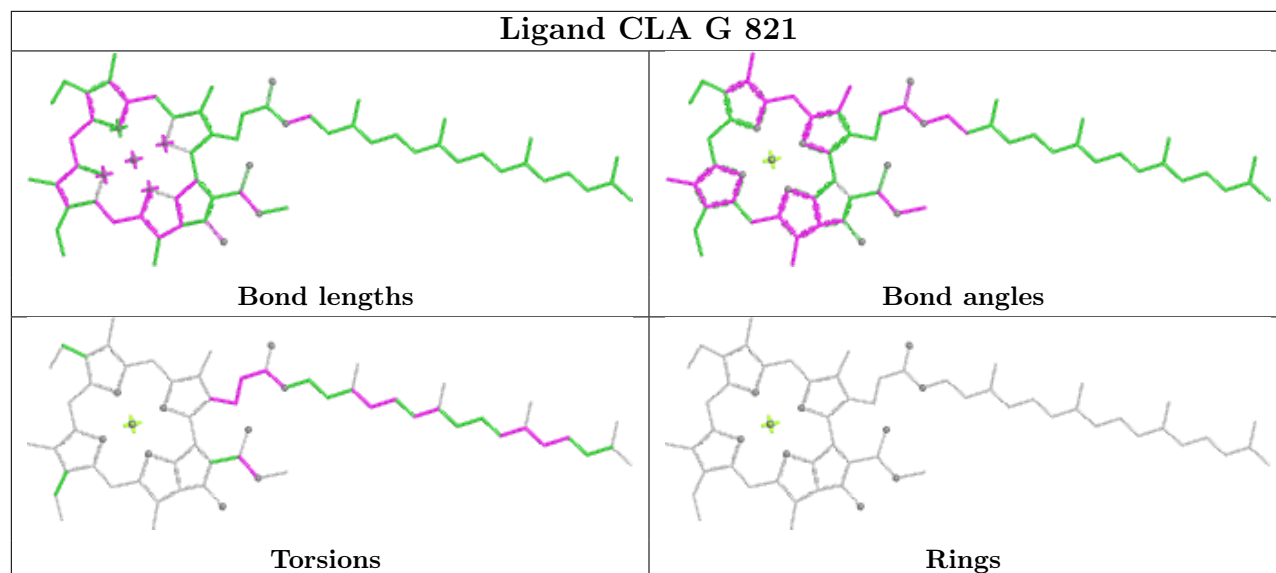
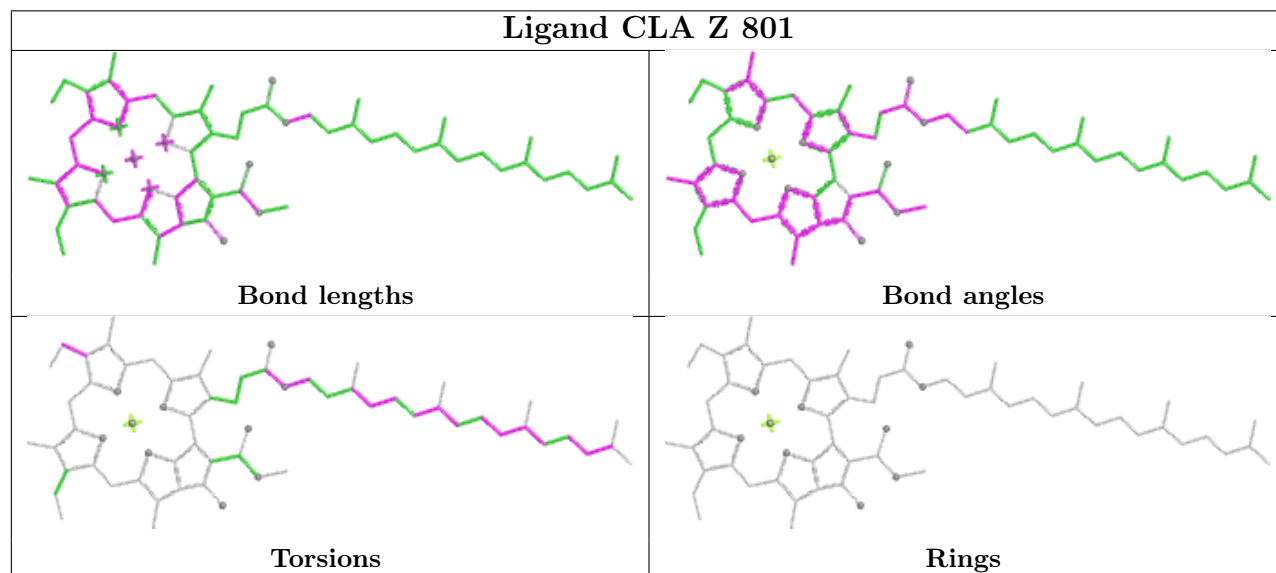
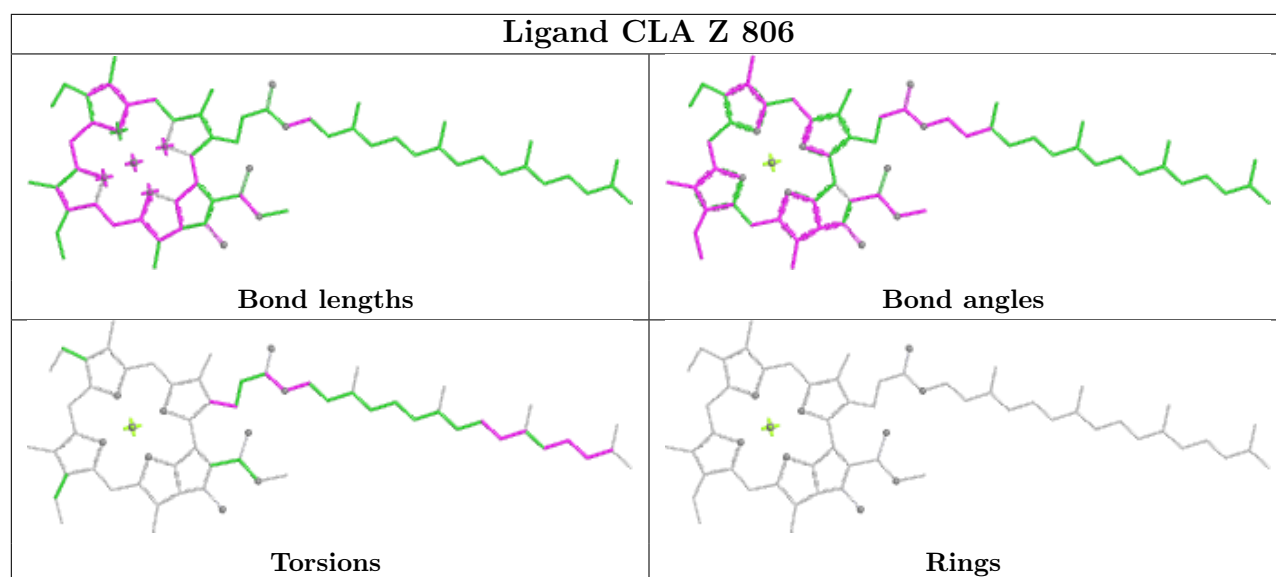
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	Z	813	CLA	3	0
14	H	810	CLA	9	0
17	H	842	BCR	4	0
14	Z	802	CLA	12	0
14	G	828	CLA	11	0
14	Z	821	CLA	6	0
14	Y	822	CLA	4	0
14	G	815	CLA	7	0
14	Z	829	CLA	7	0
14	G	825	CLA	15	0
14	B	820	CLA	1	0
14	Y	802	CLA	9	0
14	H	812	CLA	2	0
14	A	818	CLA	3	0
14	H	806	CLA	10	0
14	H	837	CLA	14	0
14	G	834	CLA	2	0
14	A	830	CLA	10	0
14	G	836	CLA	3	0
14	Z	840	CLA	8	0
14	W	1701	CLA	2	0
14	B	827	CLA	11	0
14	H	821	CLA	1	0
14	H	826	CLA	5	0
14	Z	809	CLA	10	0
17	d	203	BCR	9	0
15	H	841	PQN	5	0
14	B	806	CLA	5	0
17	Z	850	BCR	5	0
14	H	803	CLA	14	0
14	K	101	CLA	1	0
14	G	808	CLA	5	0
14	Z	822	CLA	1	0
14	Y	818	CLA	8	0
14	G	811	CLA	7	0
14	G	813	CLA	6	0
17	L	207	BCR	8	0
14	G	805	CLA	9	0
18	j	101	LHG	4	0
16	C	102	SF4	1	0
19	B	848	LMG	8	0
14	B	828	CLA	10	0

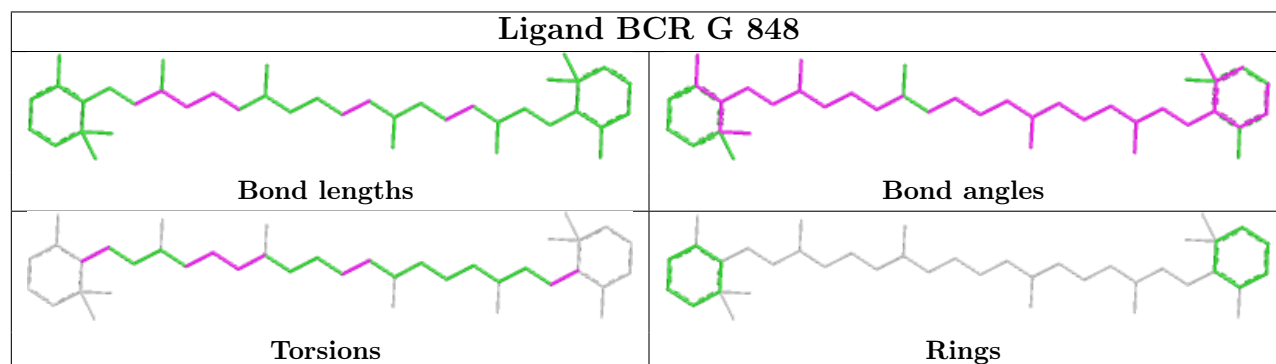
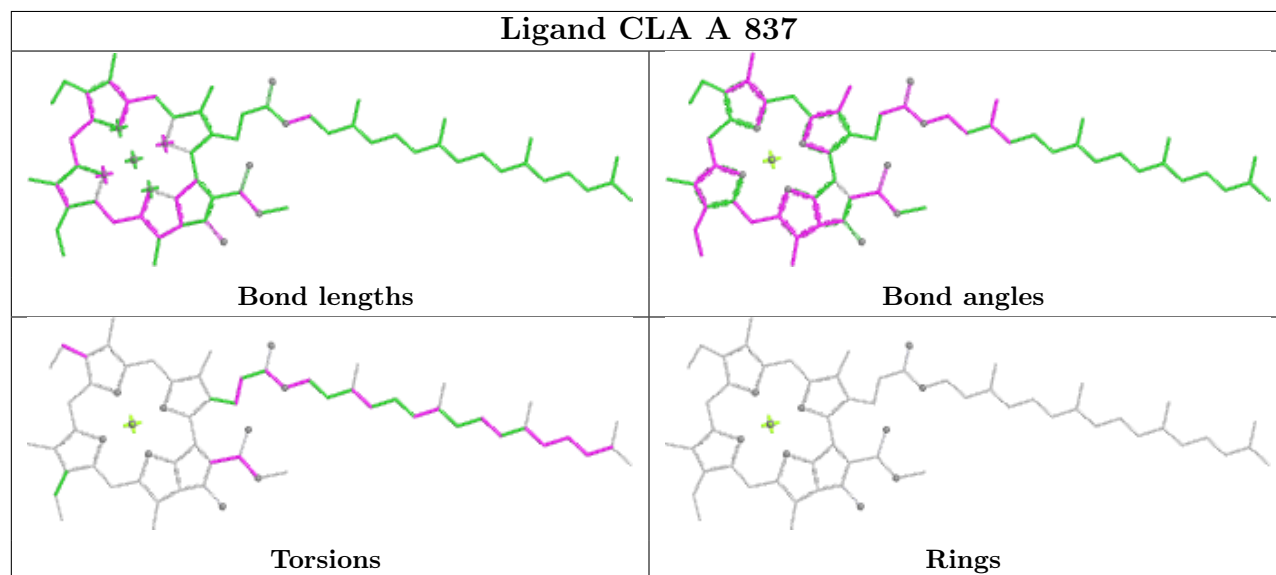
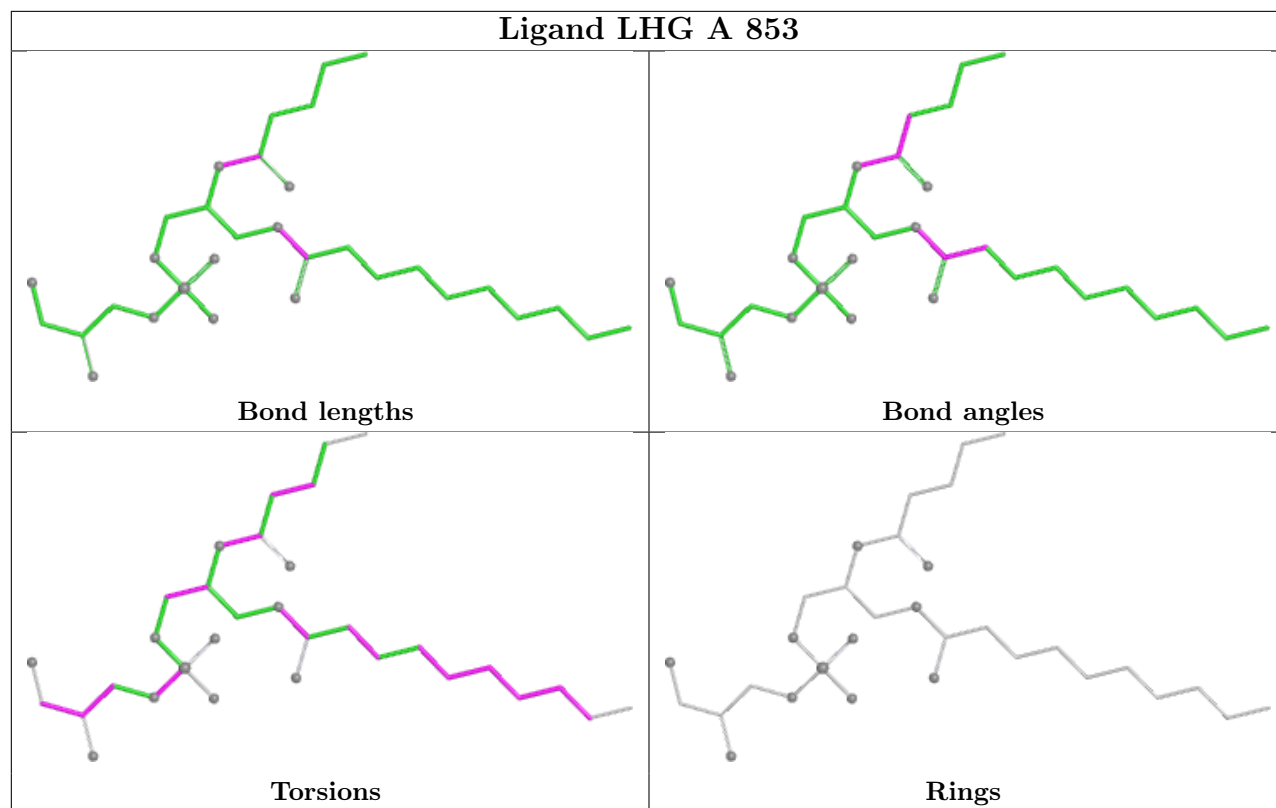
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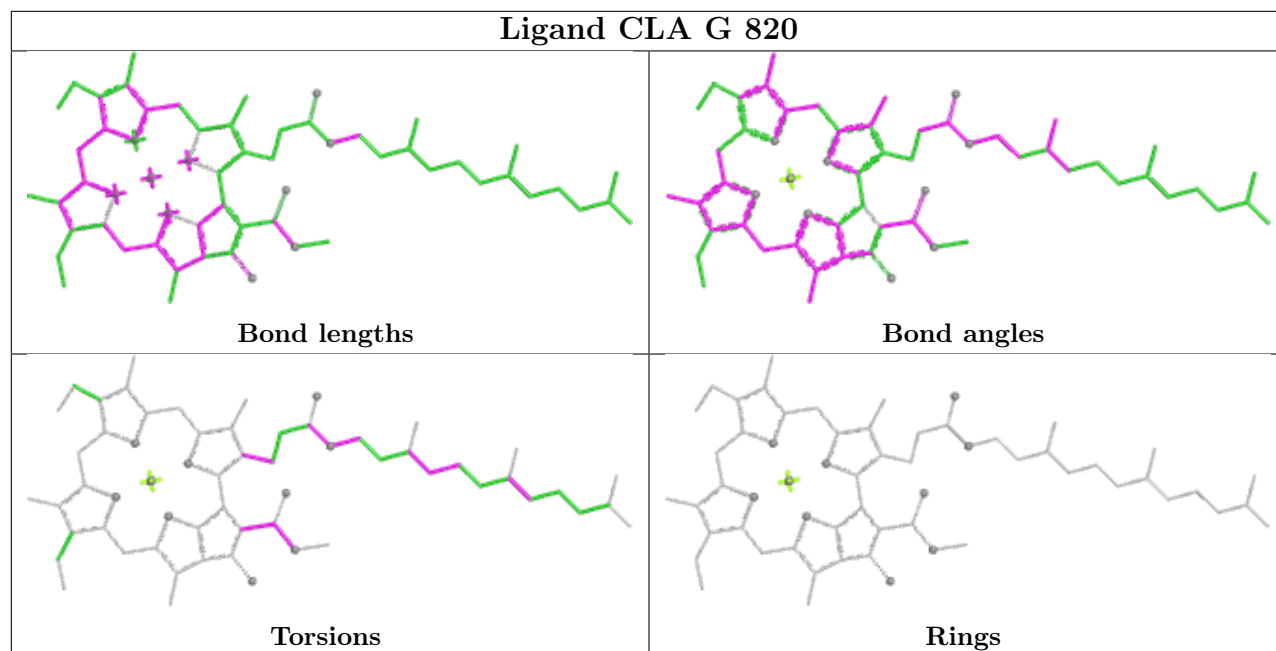
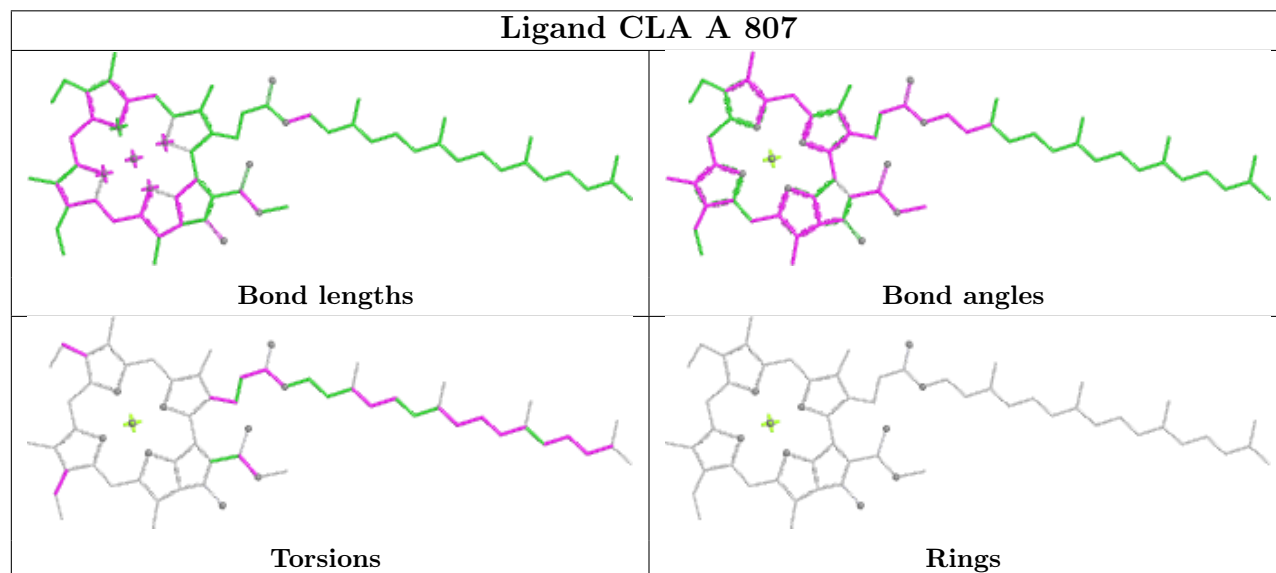
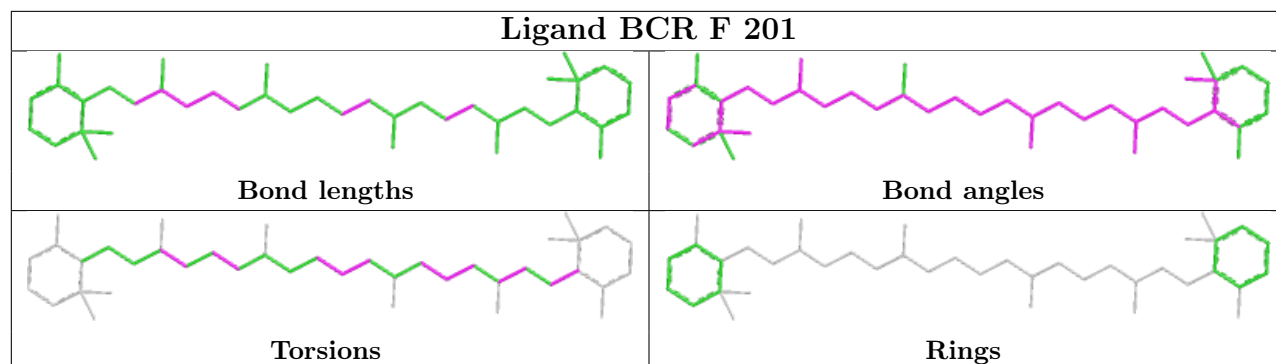
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	G	851	LHG	3	0
16	Y	843	SF4	3	0
14	A	839	CLA	5	0
14	A	820	CLA	10	0
14	Z	820	CLA	4	0
14	B	835	CLA	3	0
18	G	850	LHG	5	0
14	G	817	CLA	5	0
14	H	840	CLA	2	0
14	S	1101	CLA	3	0
17	H	847	BCR	11	0
14	H	830	CLA	4	0
14	Z	832	CLA	4	0
14	h	205	CLA	4	0
14	B	833	CLA	6	0
14	B	814	CLA	7	0
17	G	849	BCR	15	0
14	Z	835	CLA	4	0
14	Y	840	CLA	8	0
14	Z	839	CLA	3	0
14	A	831	CLA	8	0
17	B	847	BCR	7	0
14	G	809	CLA	8	0
17	Q	201	BCR	16	0
13	Y	801	CL0	8	0
14	G	819	CLA	10	0
14	f	101	CLA	2	0
14	A	828	CLA	2	0
14	Z	805	CLA	3	0

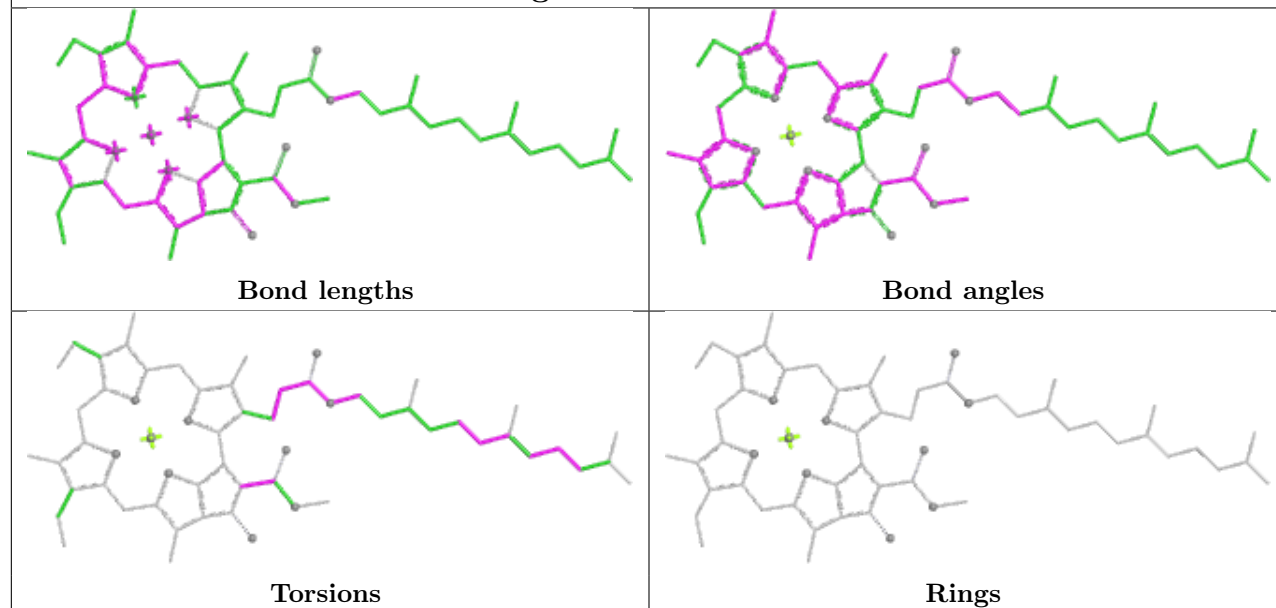
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



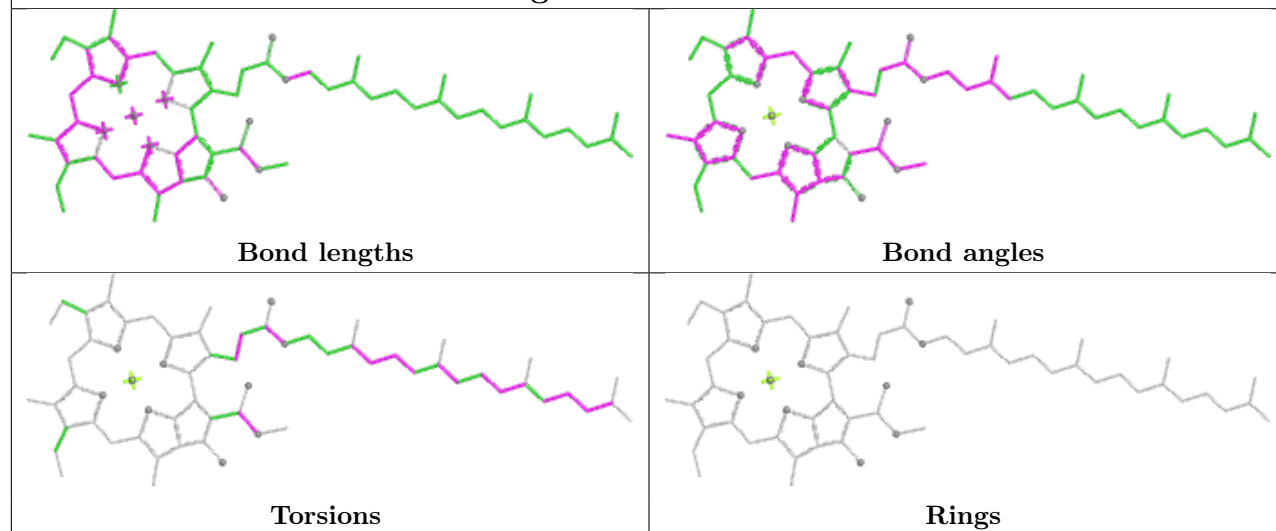




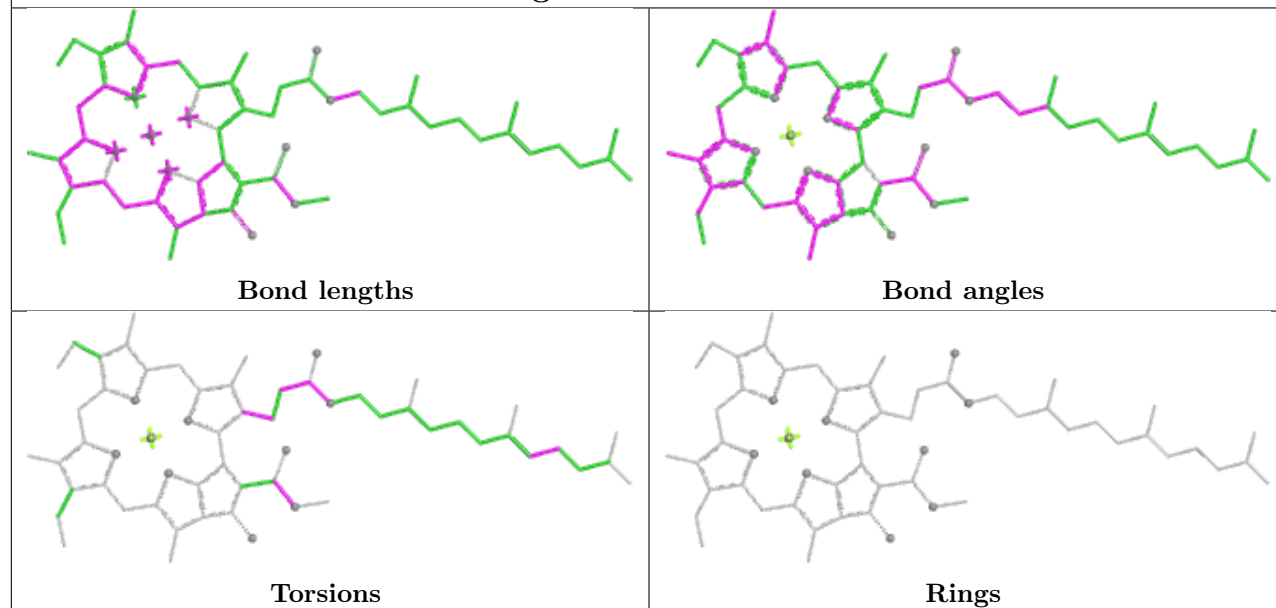
Ligand CLA Y 820



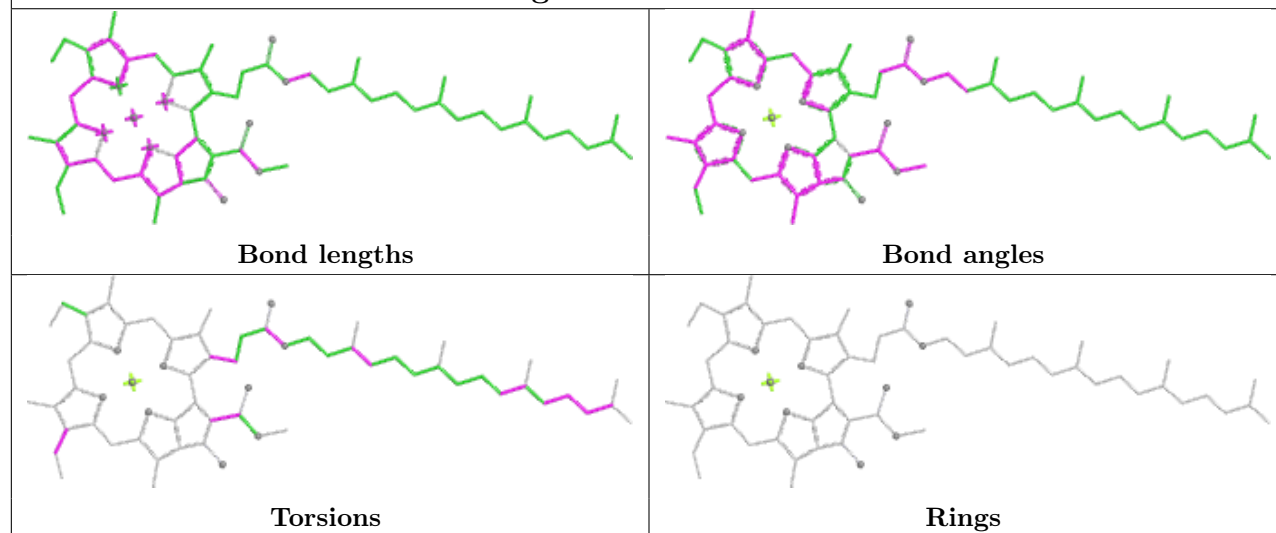
Ligand CLA G 840



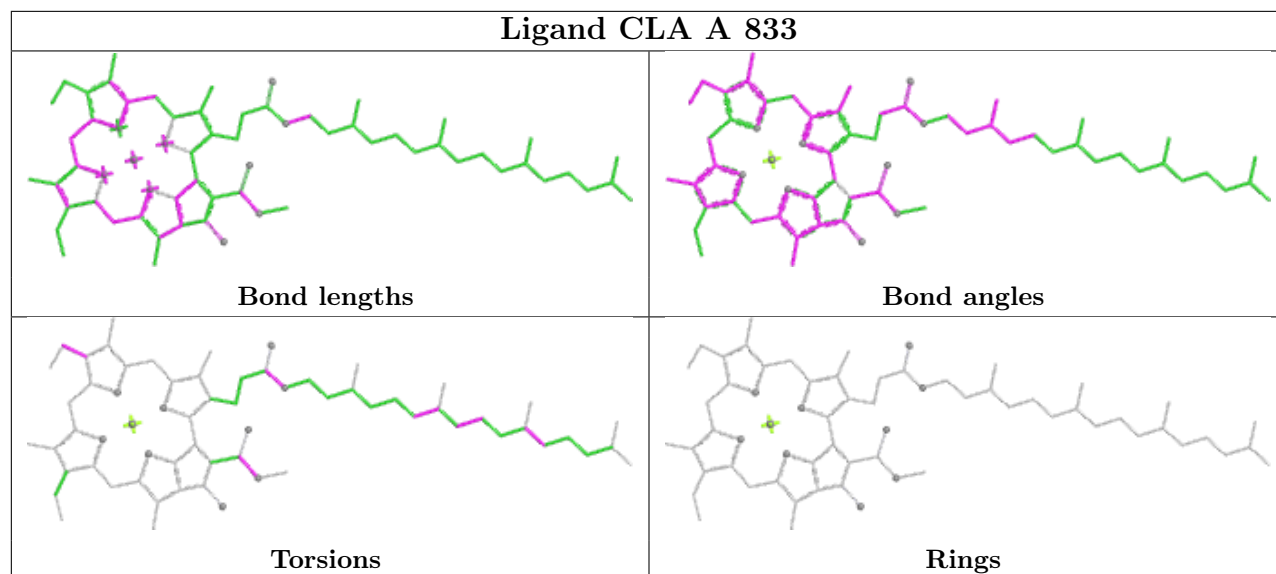
Ligand CLA B 817



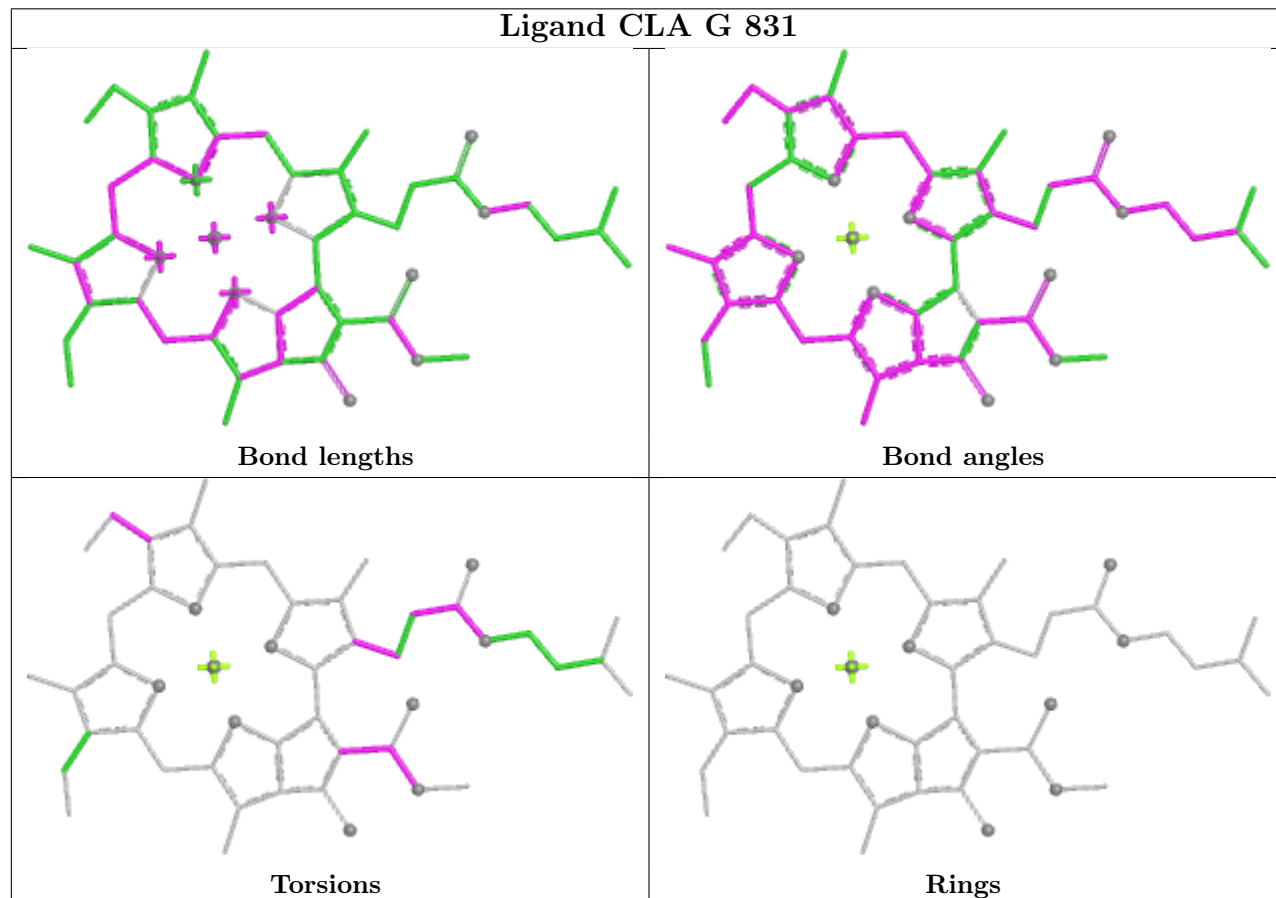
Ligand CLA A 804



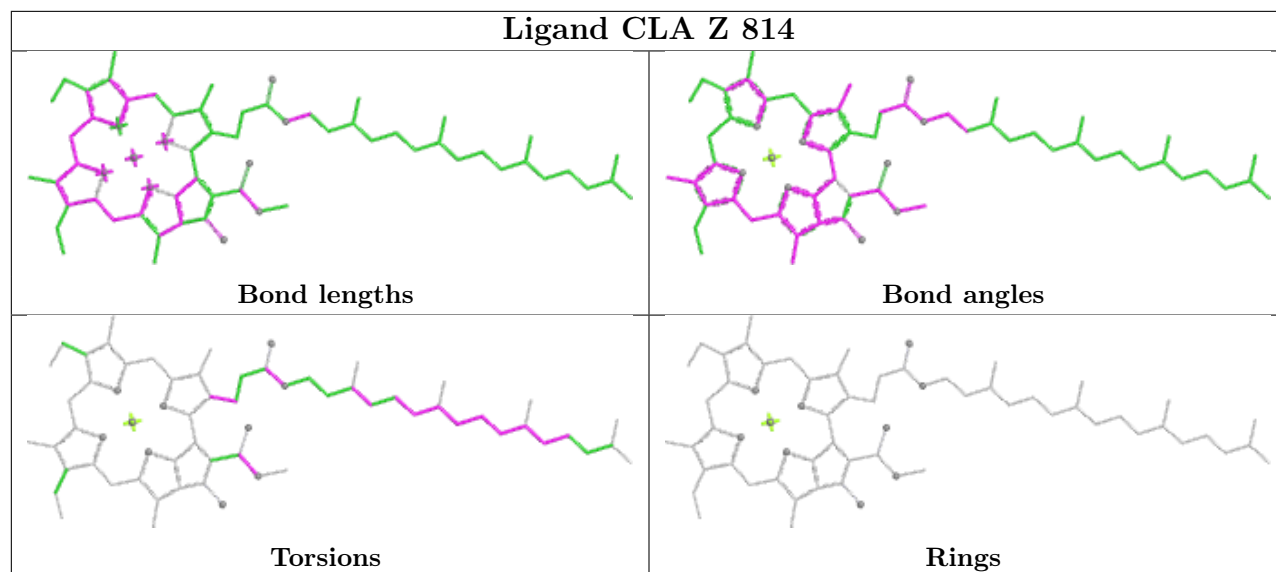
Ligand CLA A 833



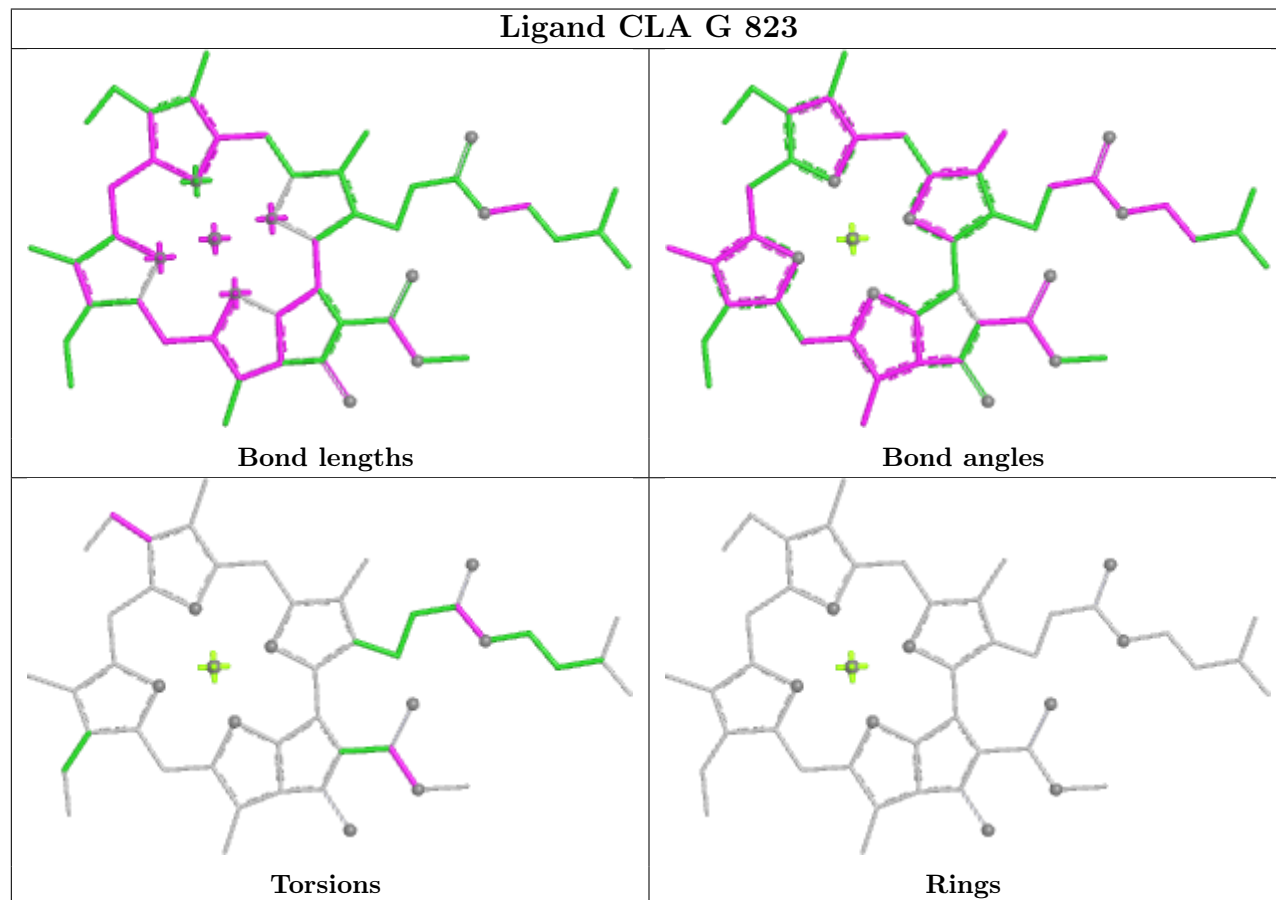
Ligand CLA G 831

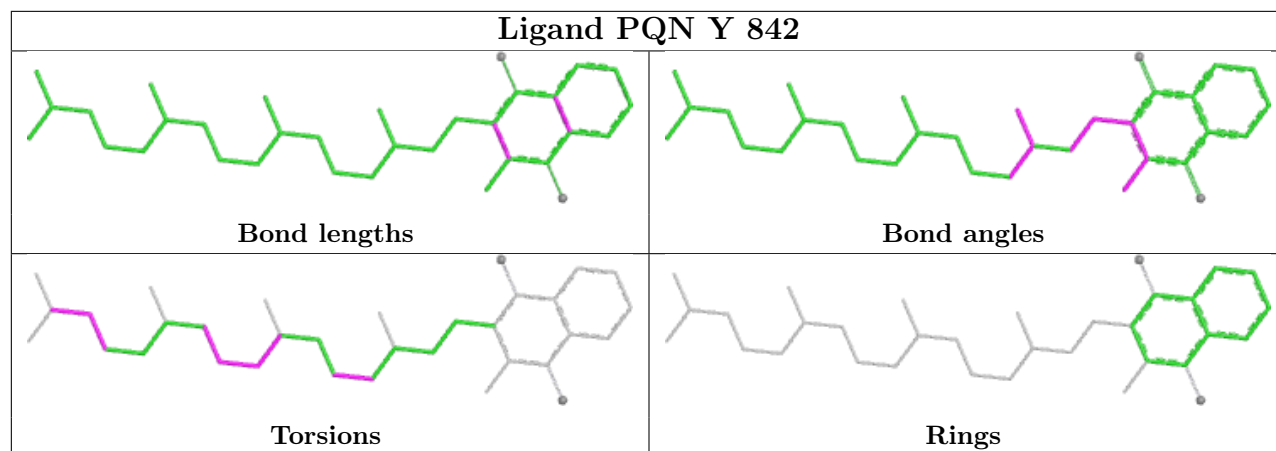
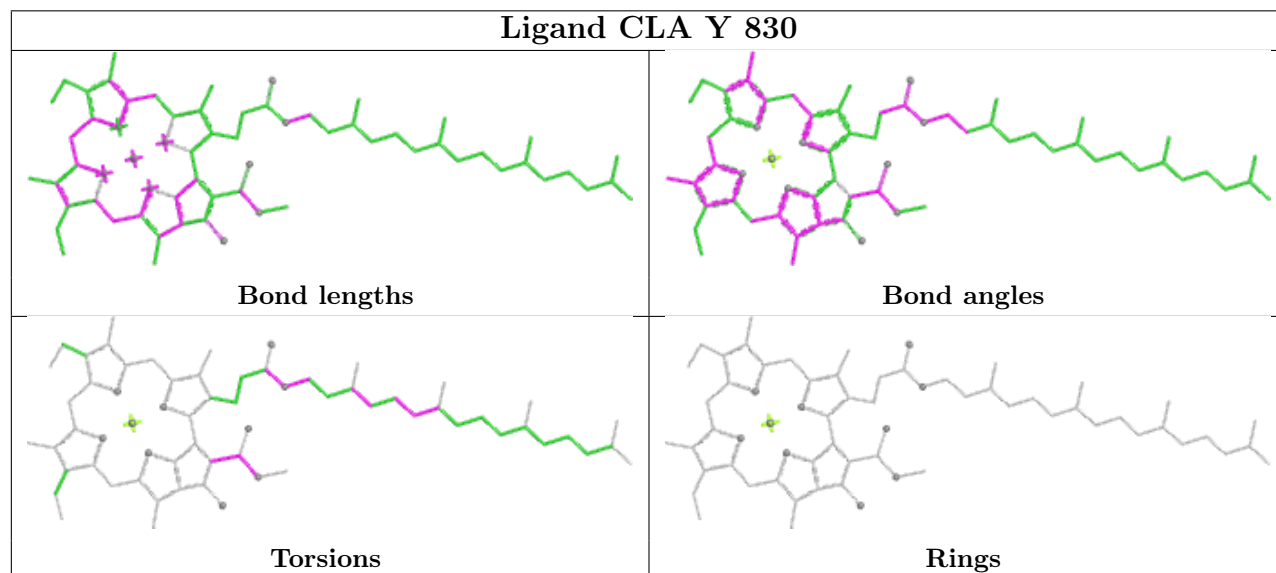
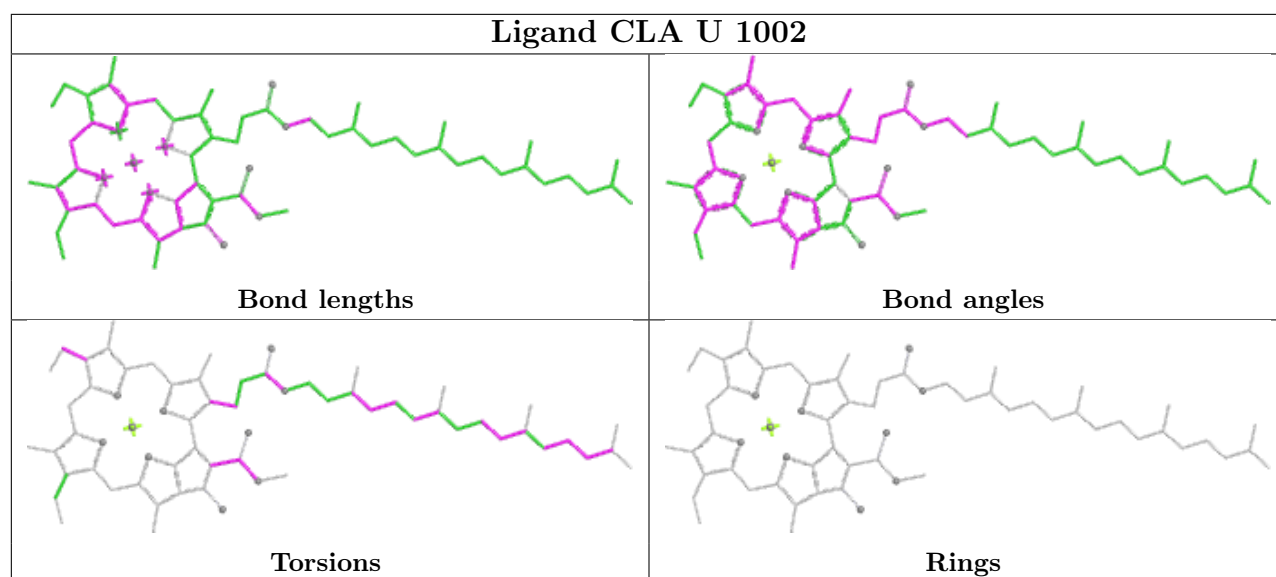


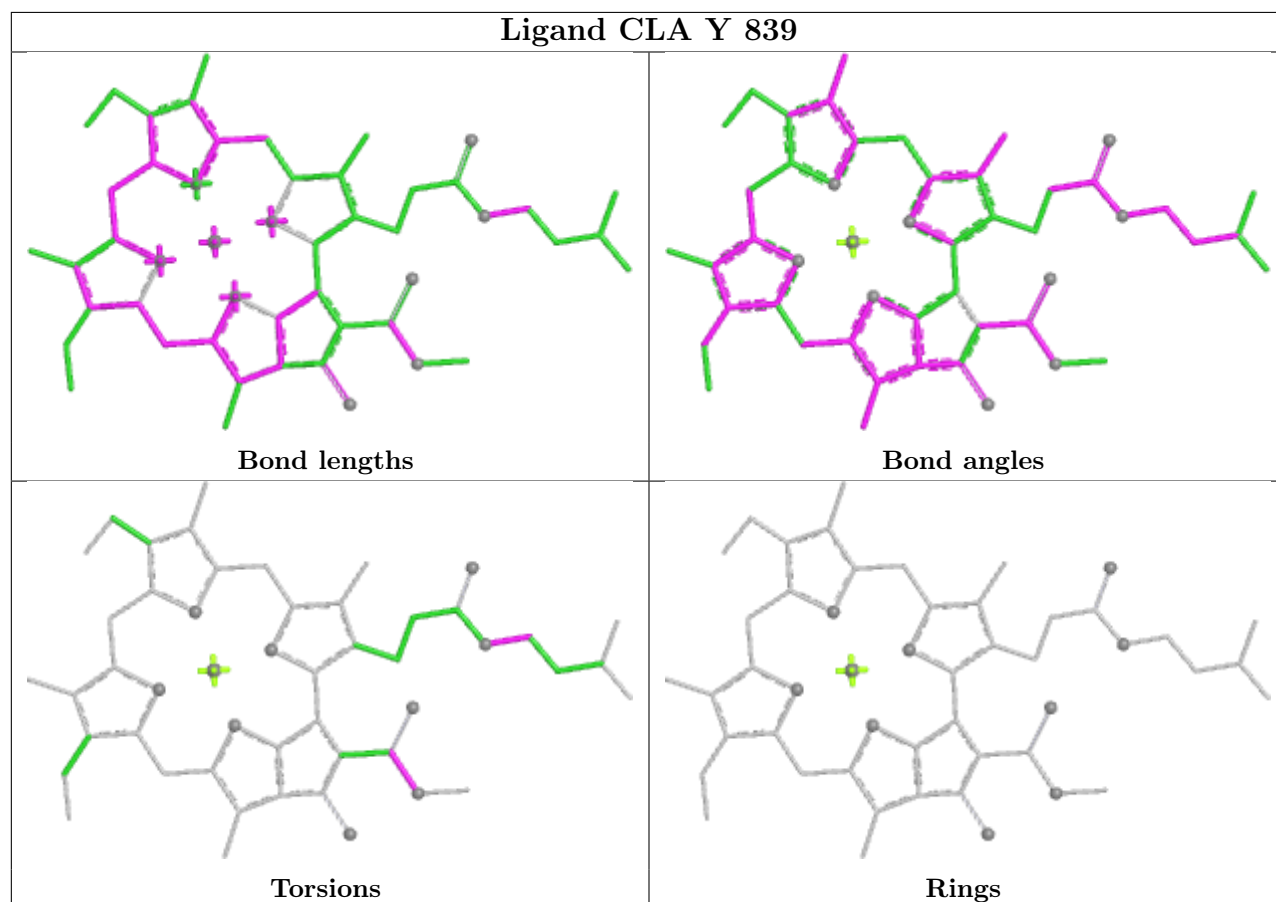
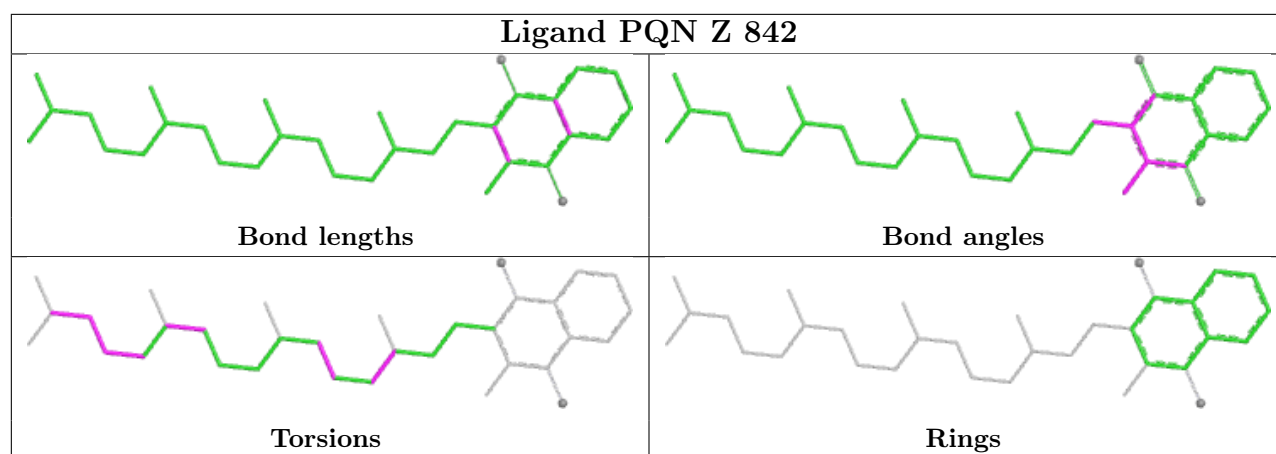
Ligand CLA Z 814



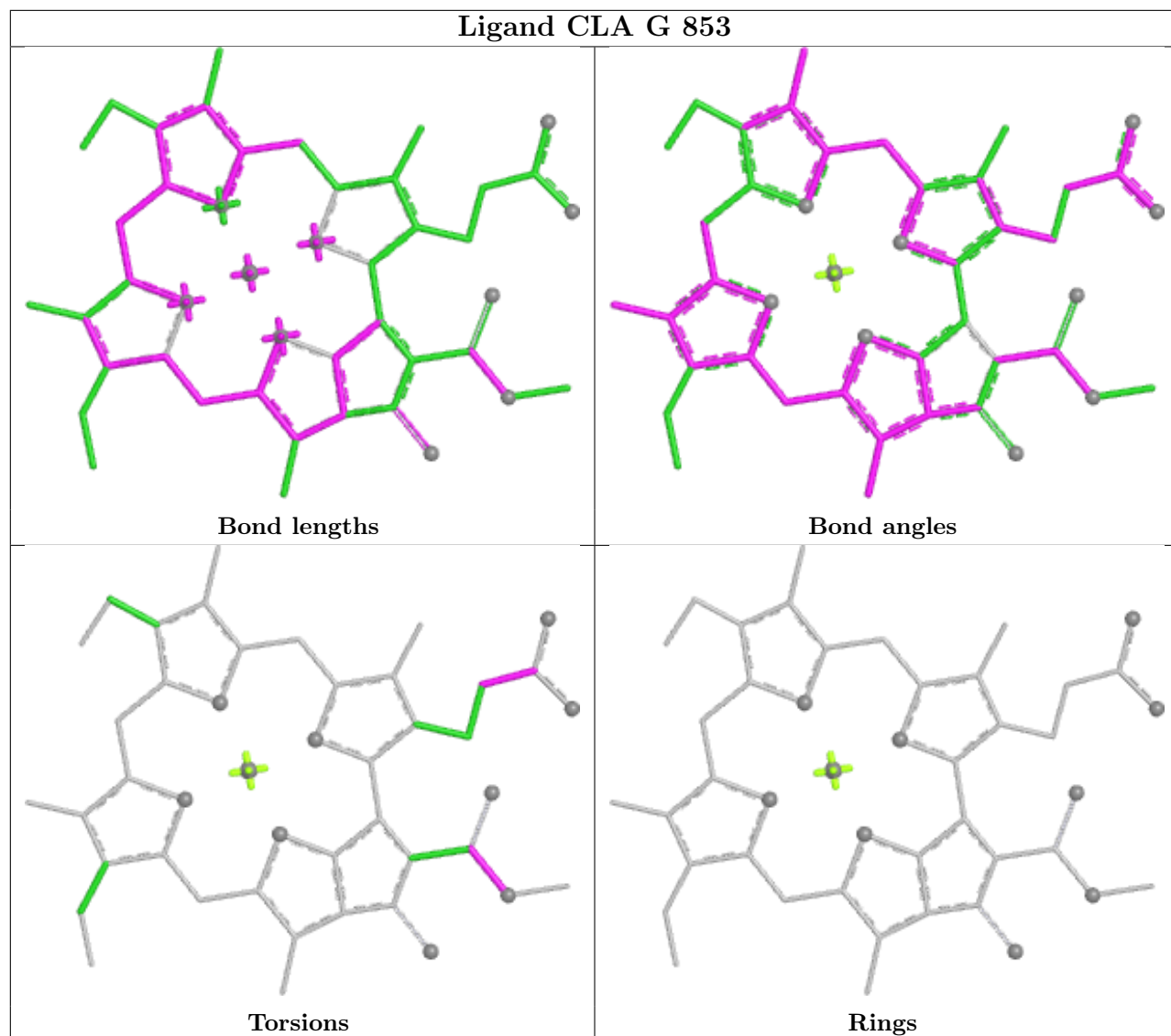
Ligand CLA G 823



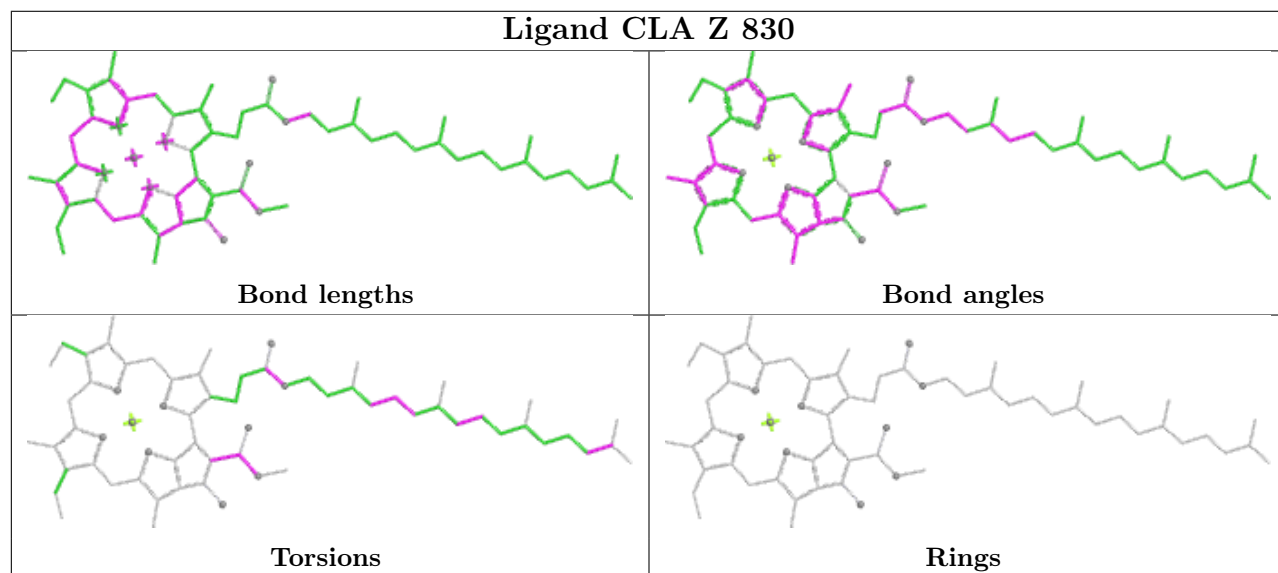


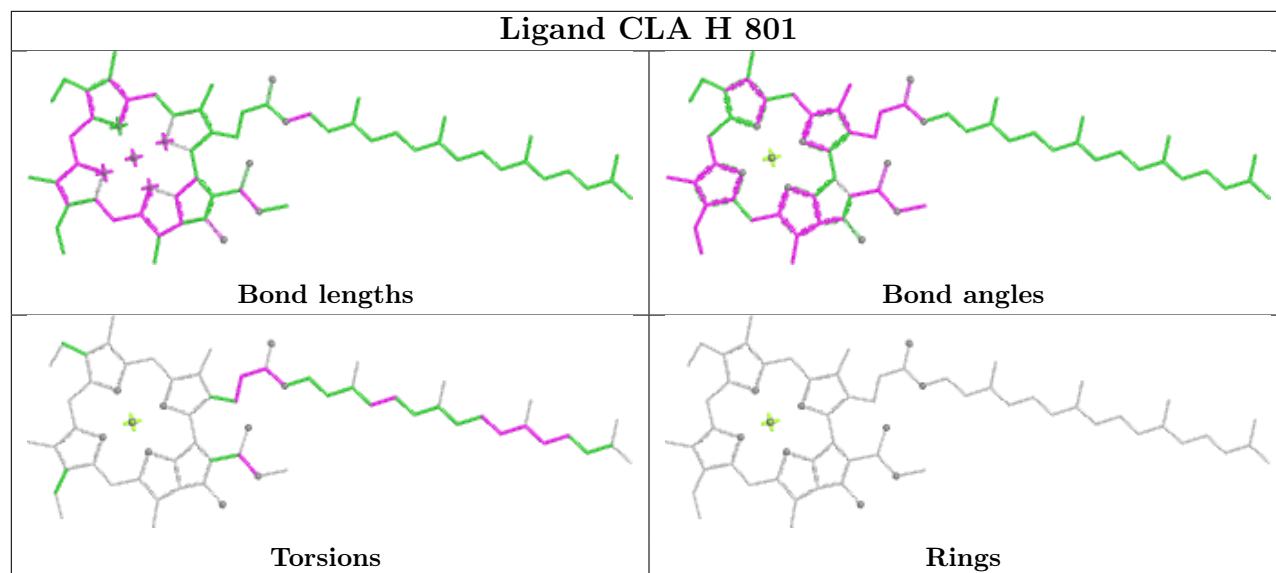
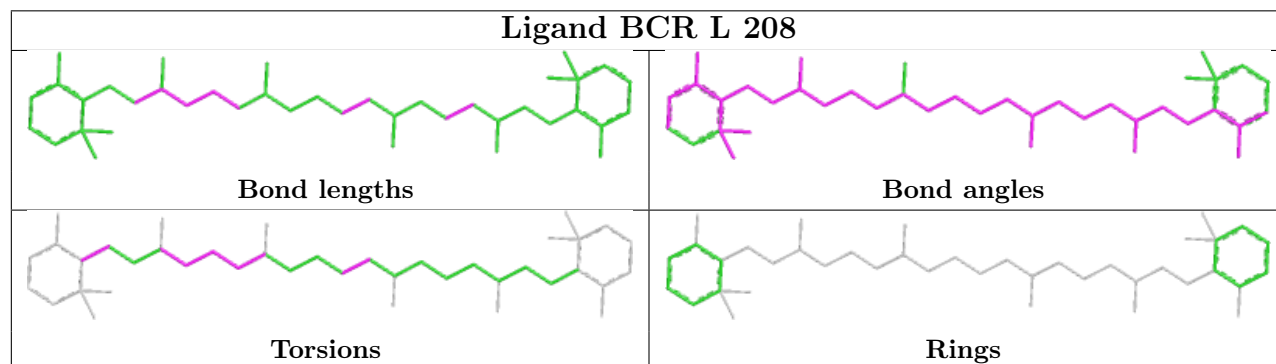
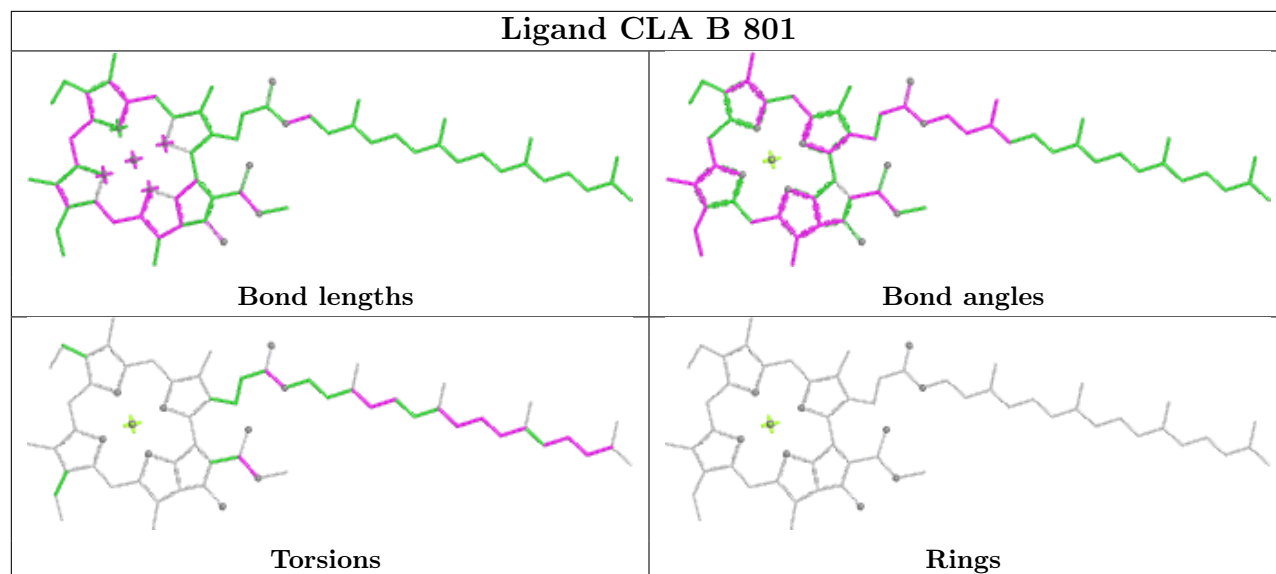


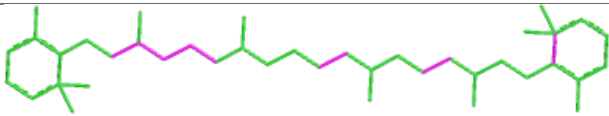
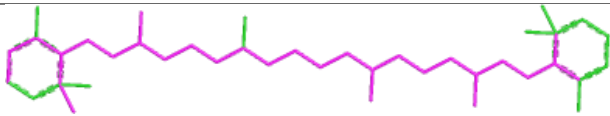
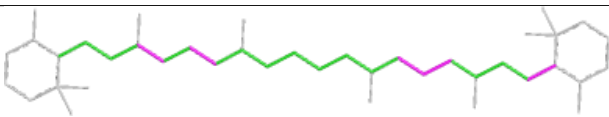
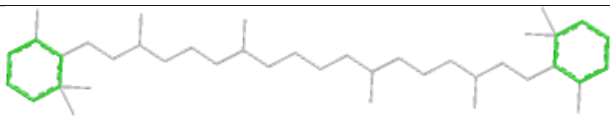
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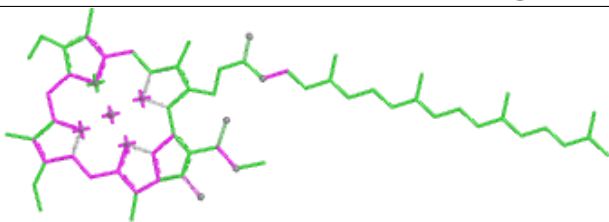
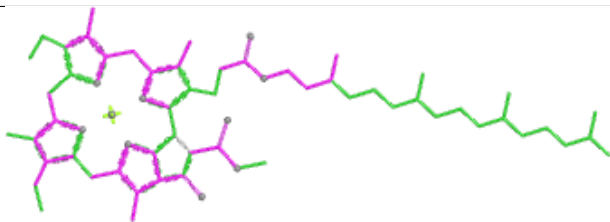
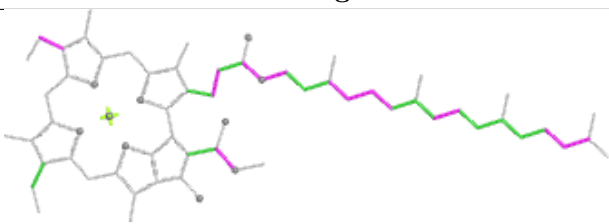
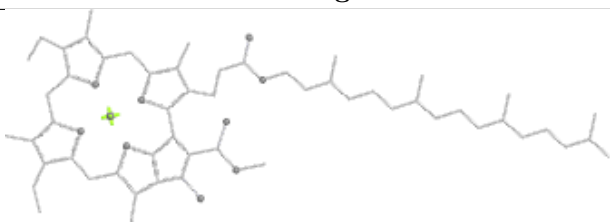


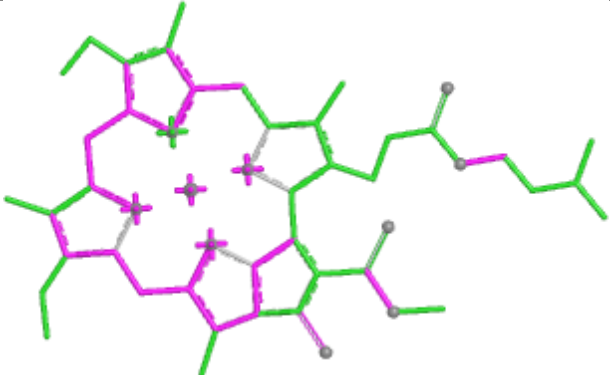
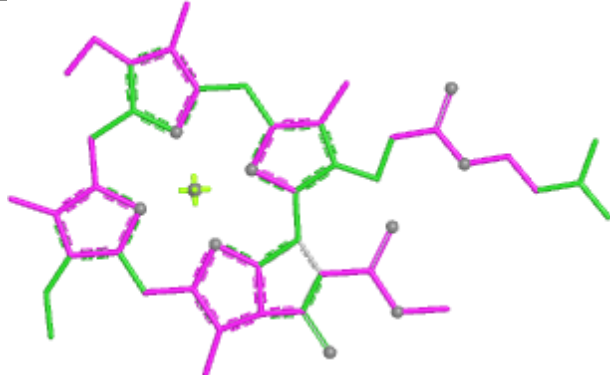
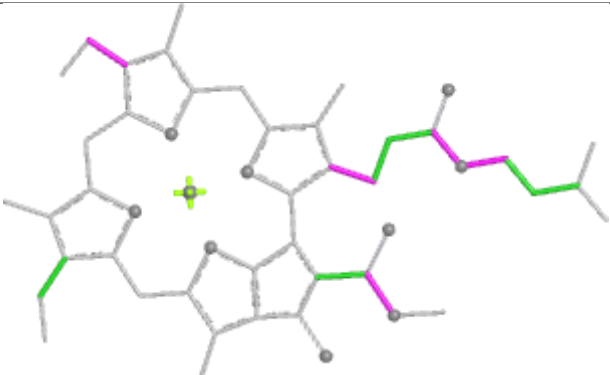
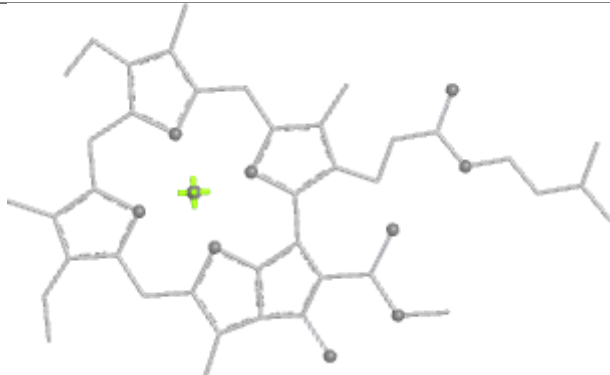
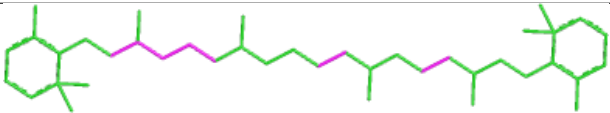
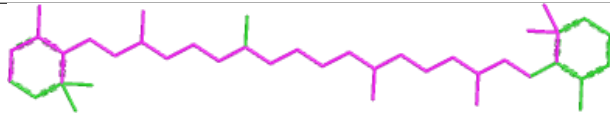
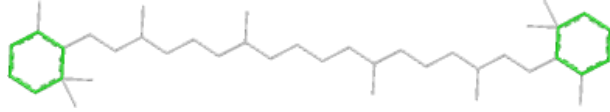
Ligand CLA Z 830



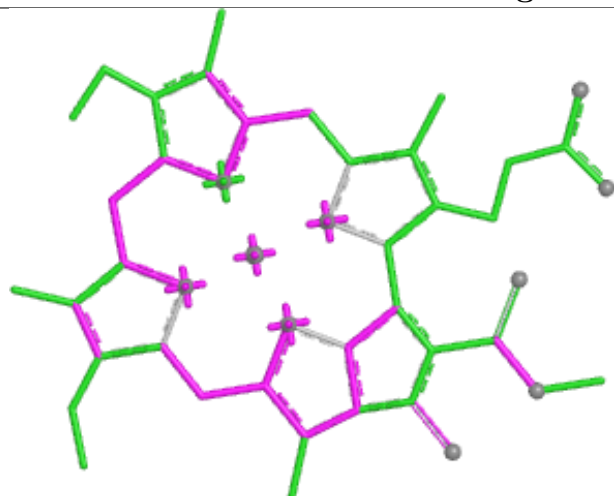


Ligand BCR B 843	
	
Bond lengths	Bond angles
	
Torsions	Rings

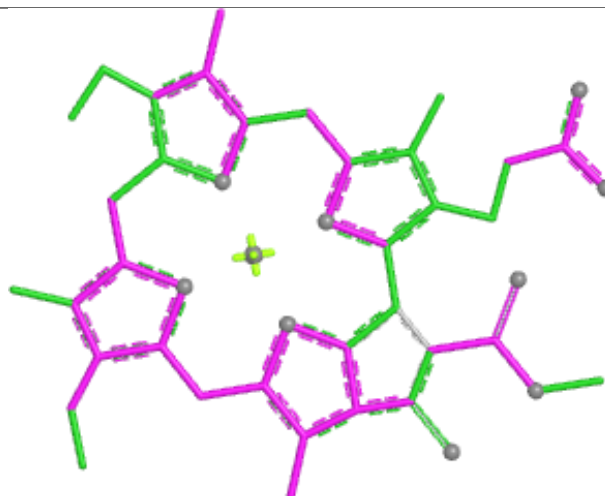
Ligand CLA Z 818	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Y 816	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR H 846	
 Bond lengths	 Bond angles
 Torsions	 Rings

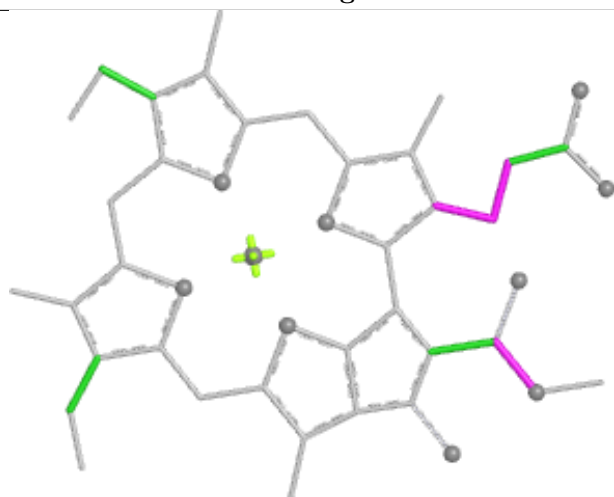
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Bond lengths



Bond angles

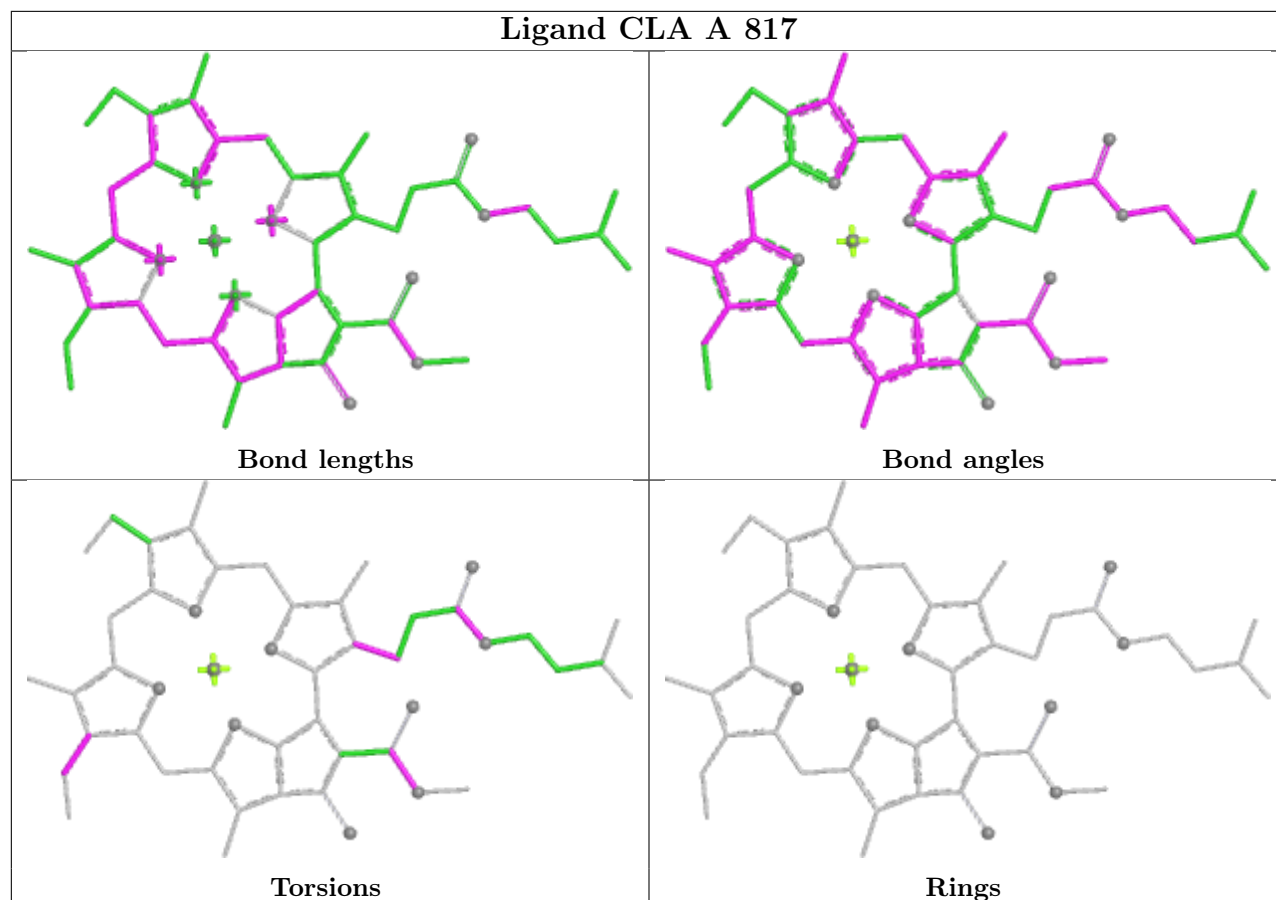


Torsions

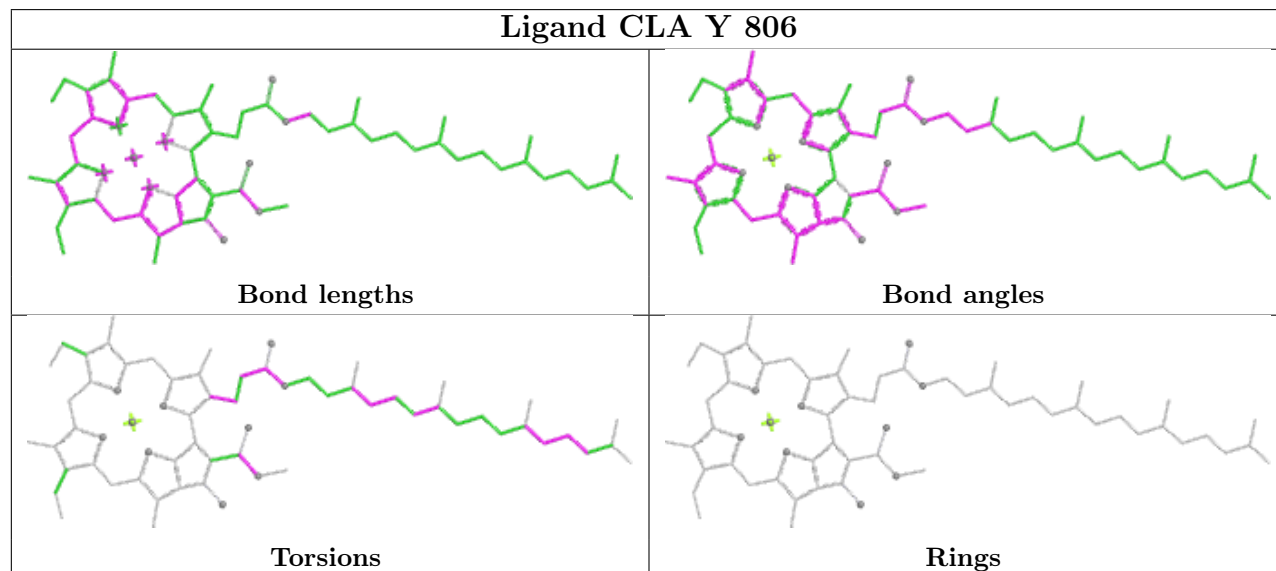


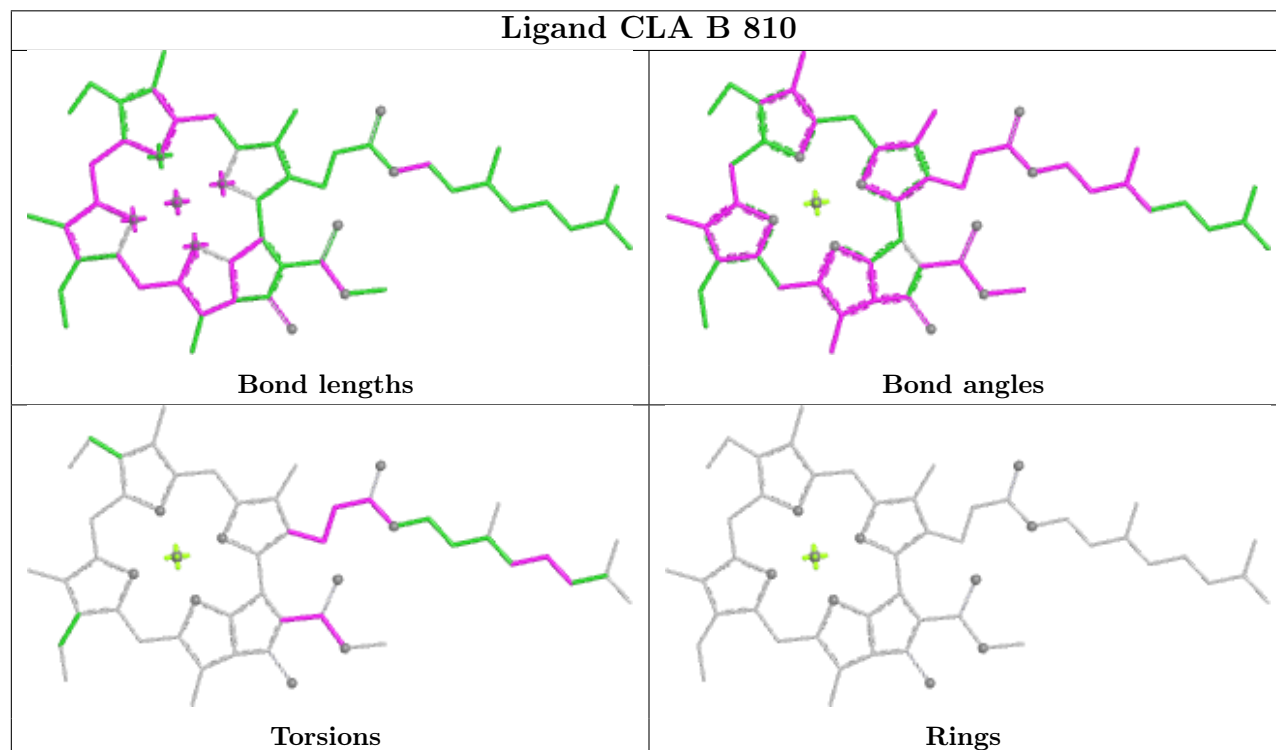
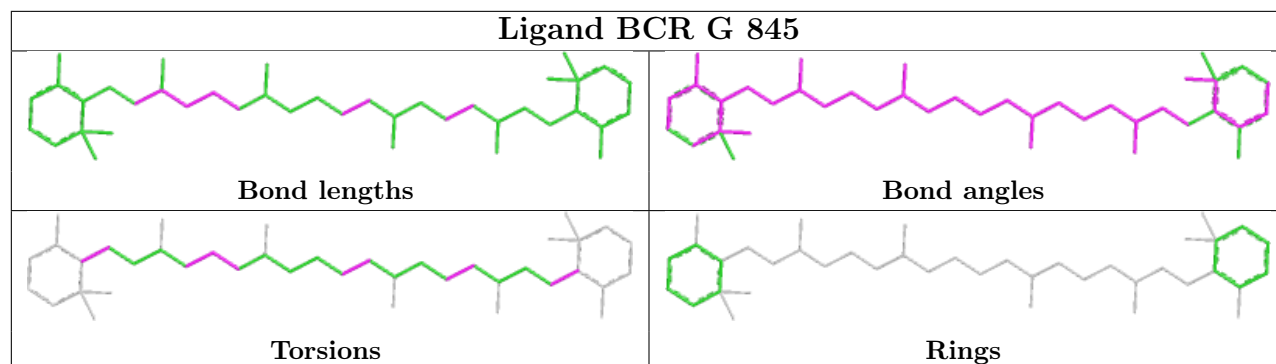
Rings

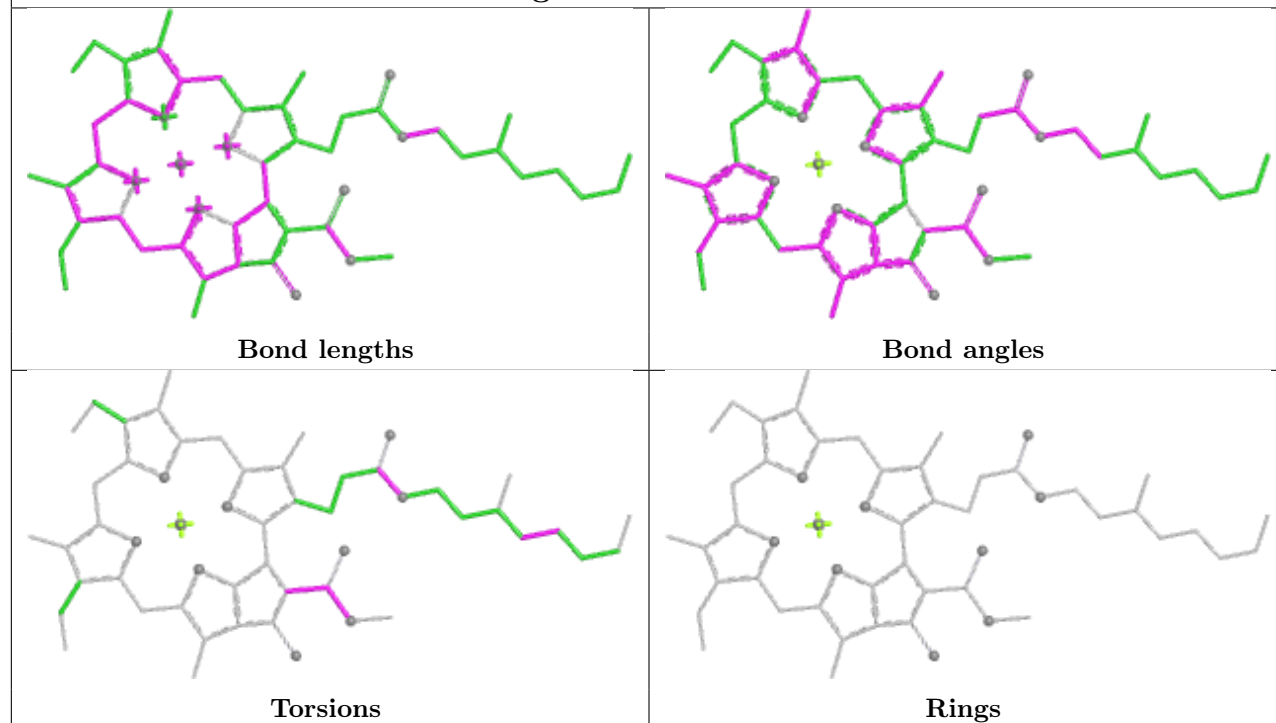
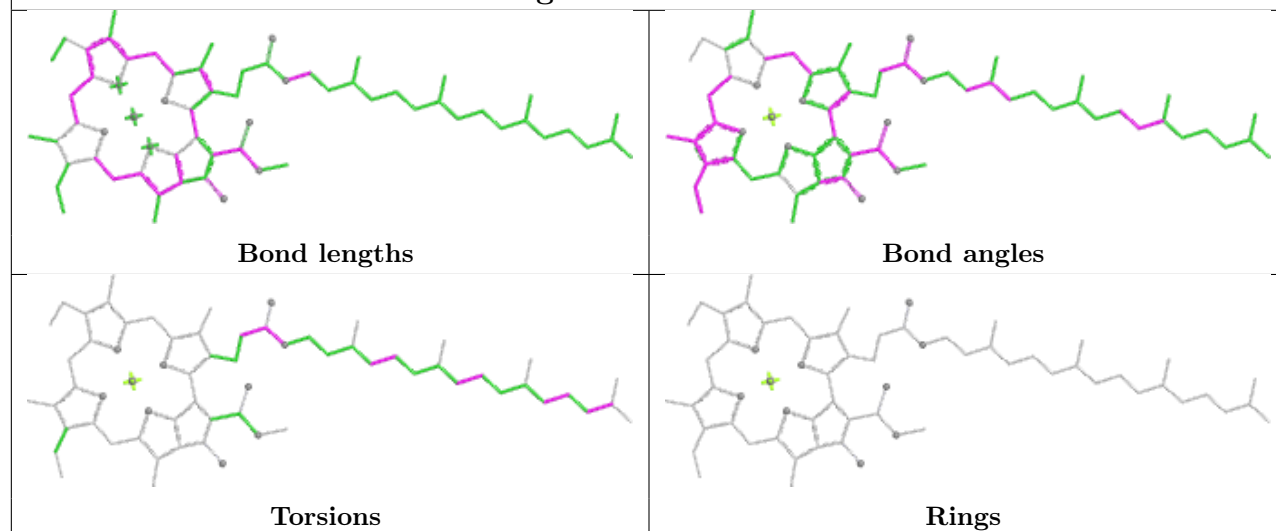
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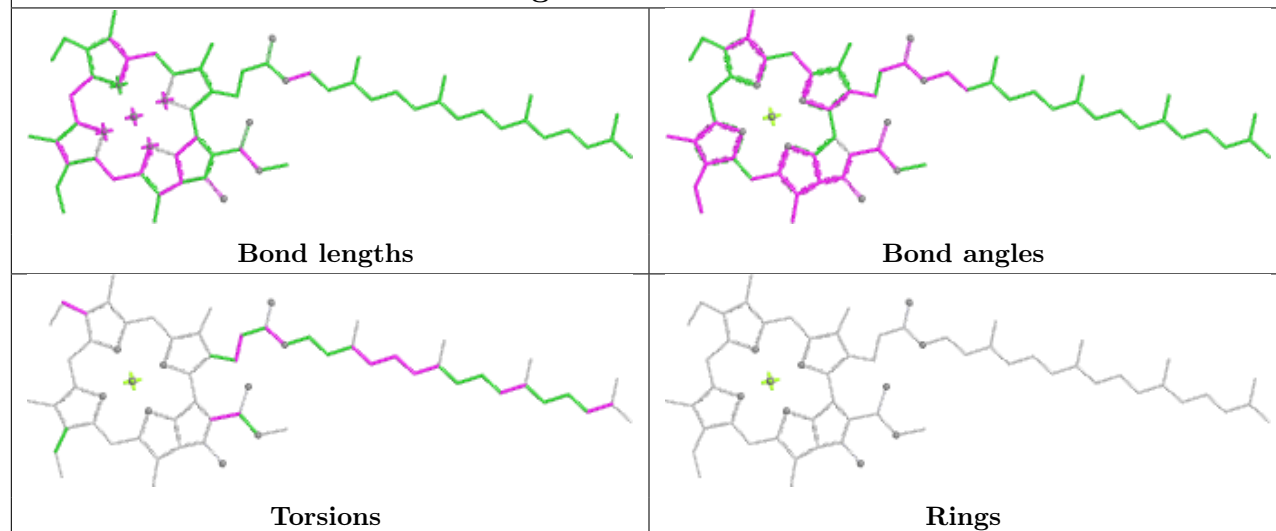
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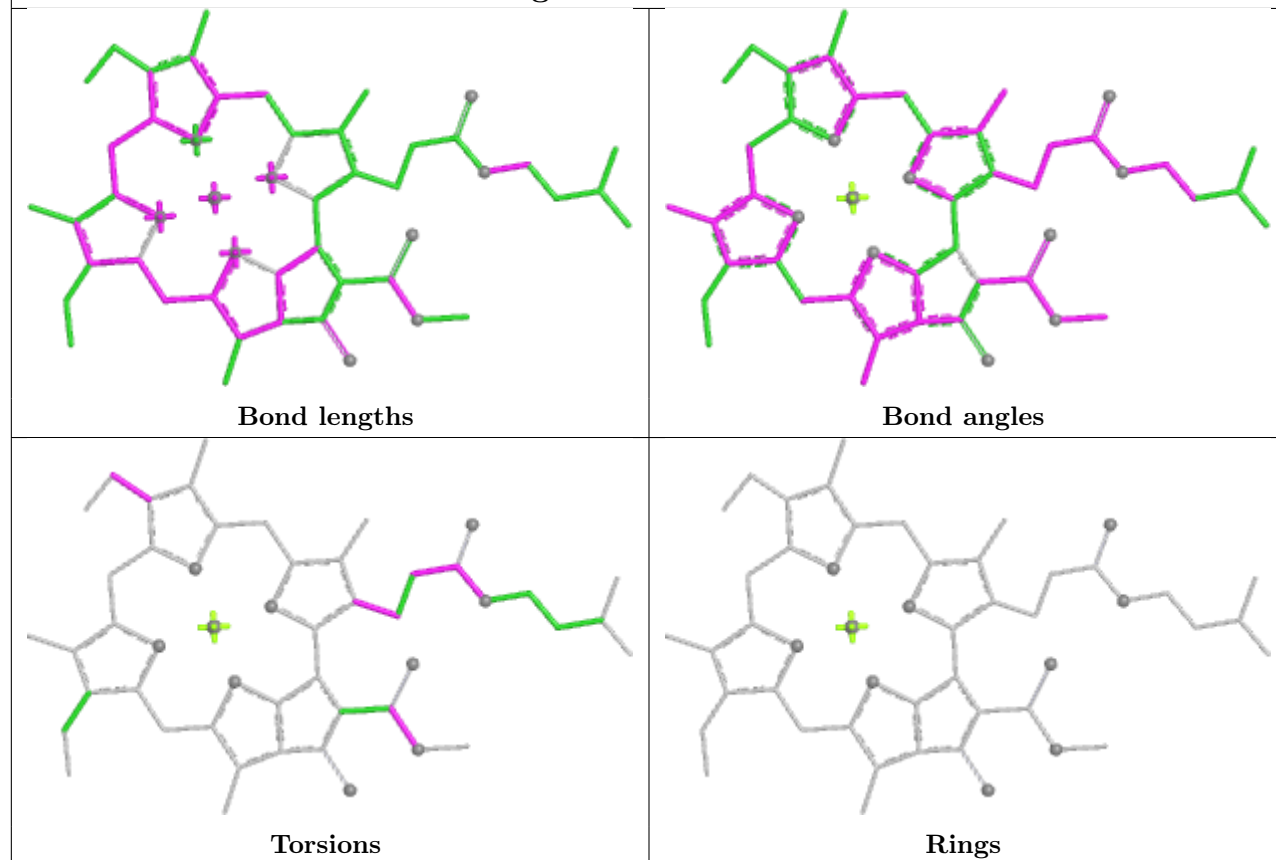


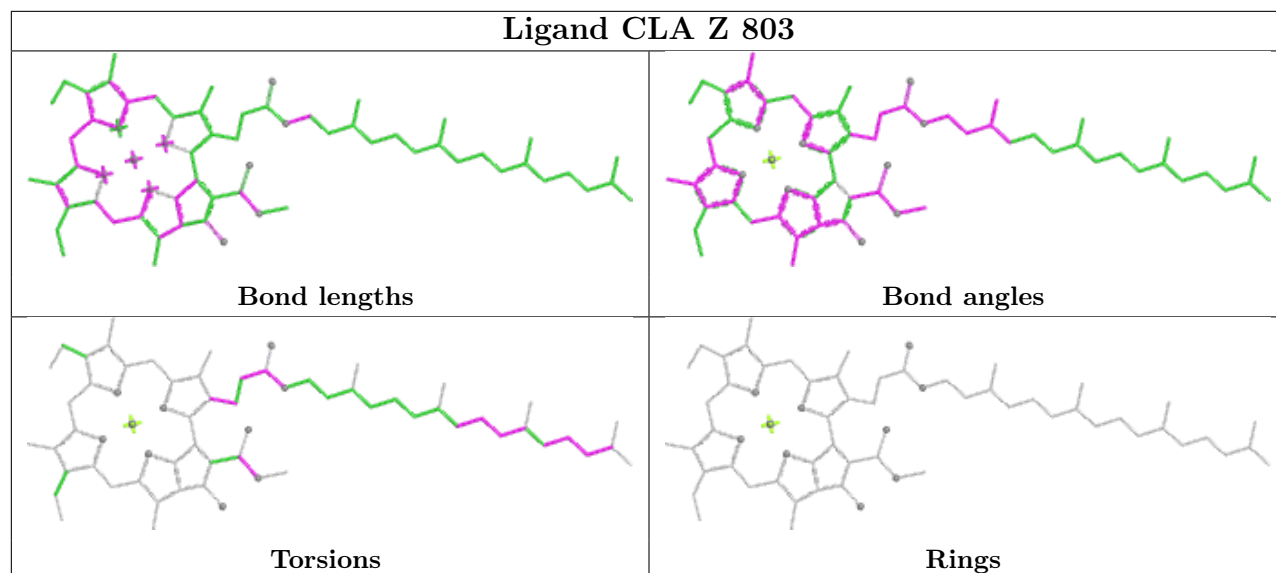
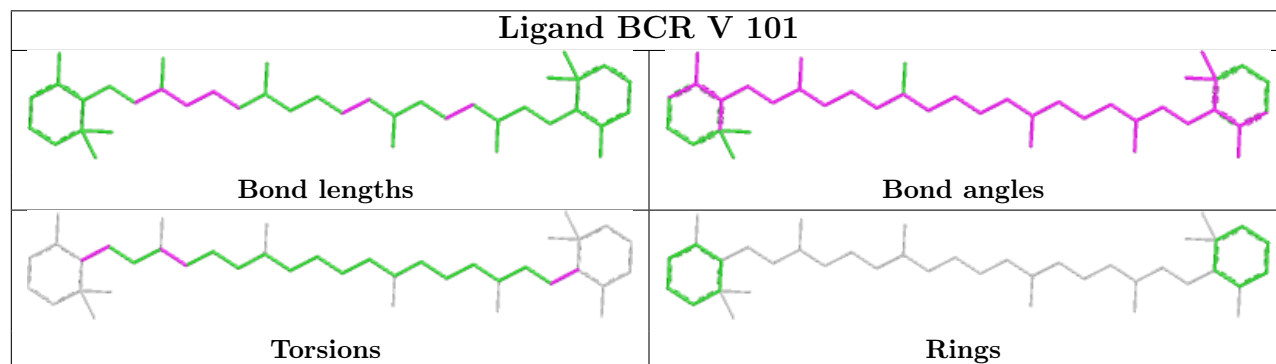
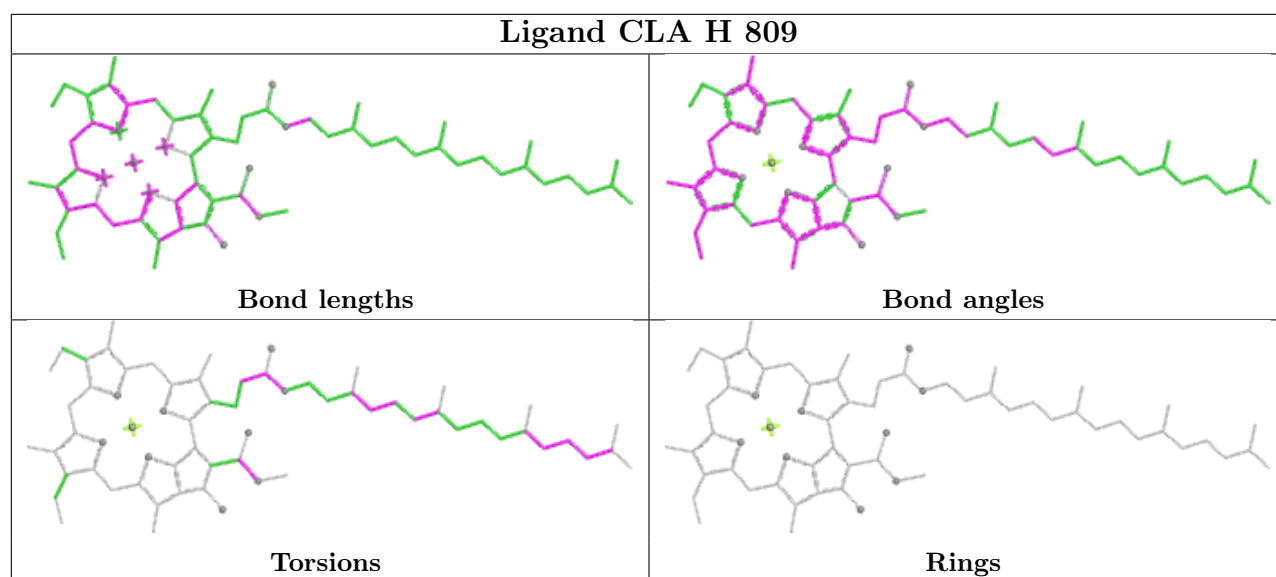
Ligand CLA B 803**Ligand CL0 A 801**

Ligand CLA A 854

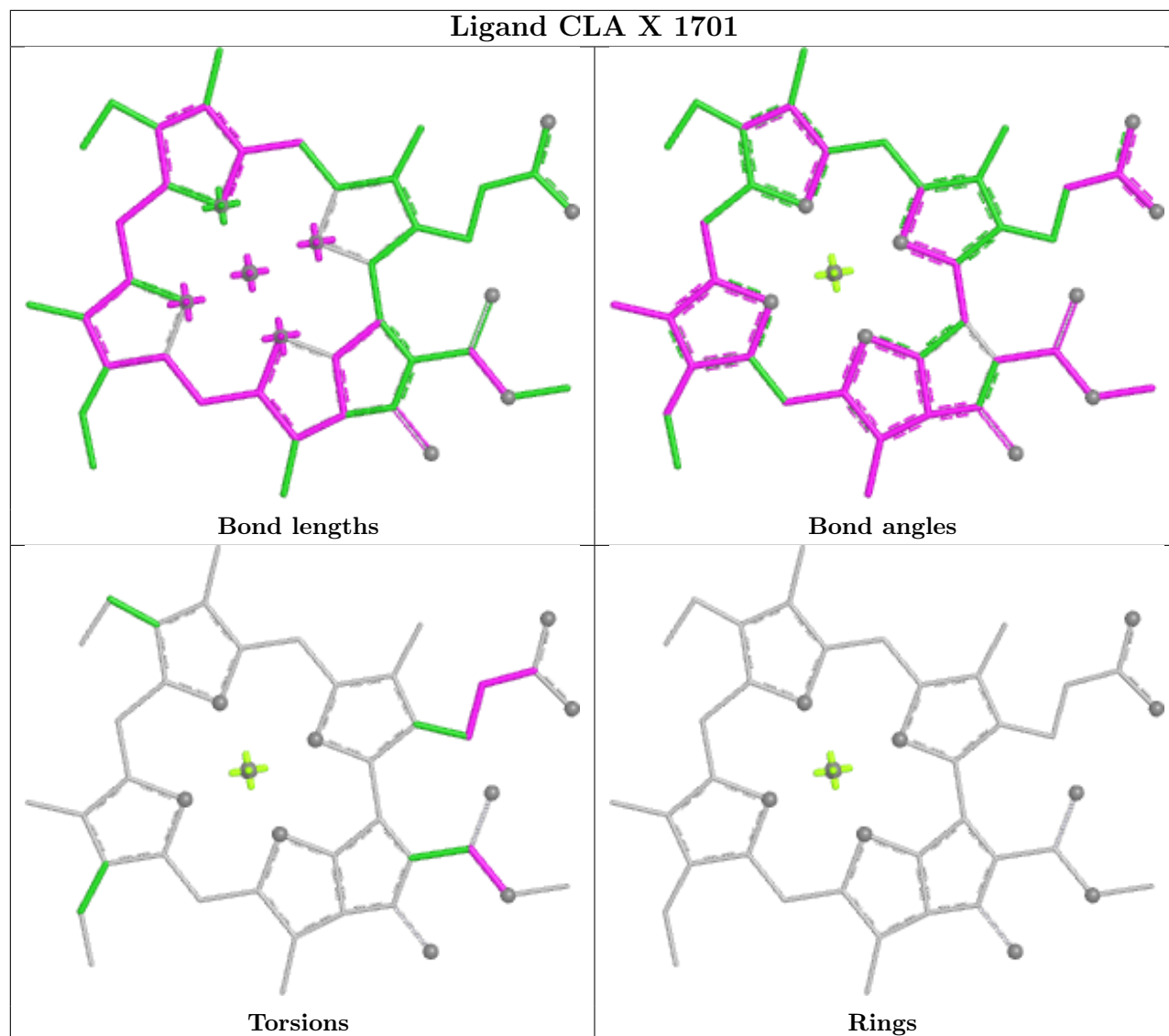


Ligand CLA A 824

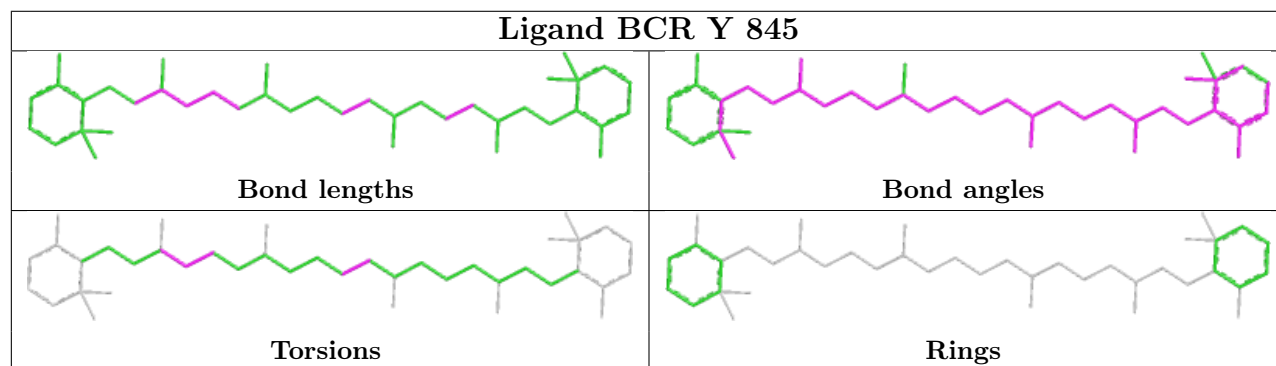


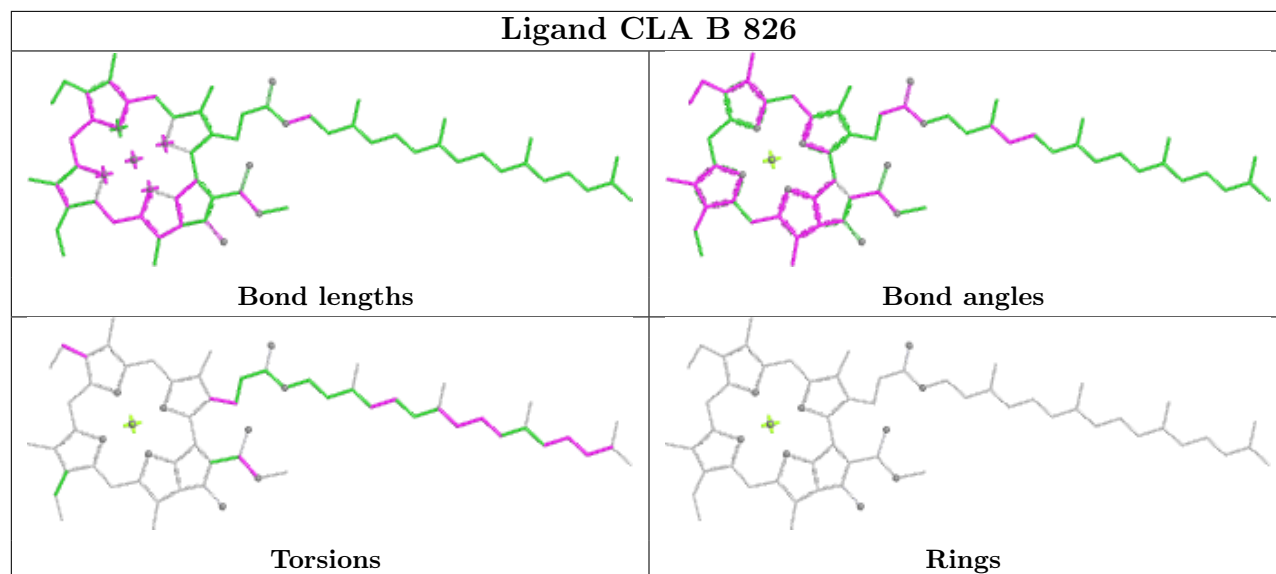
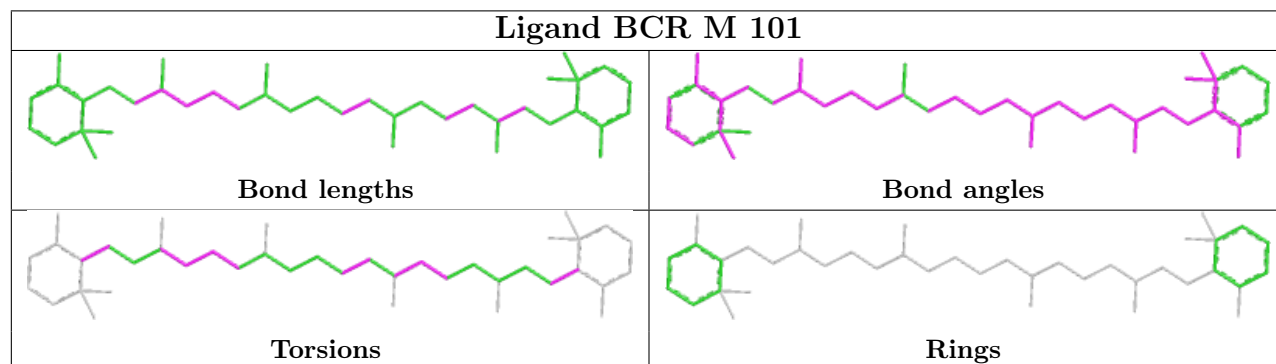
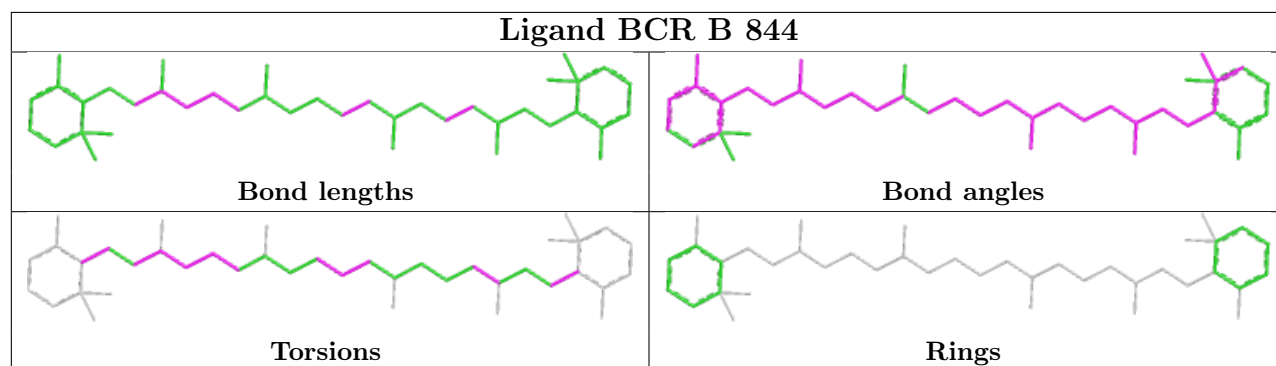
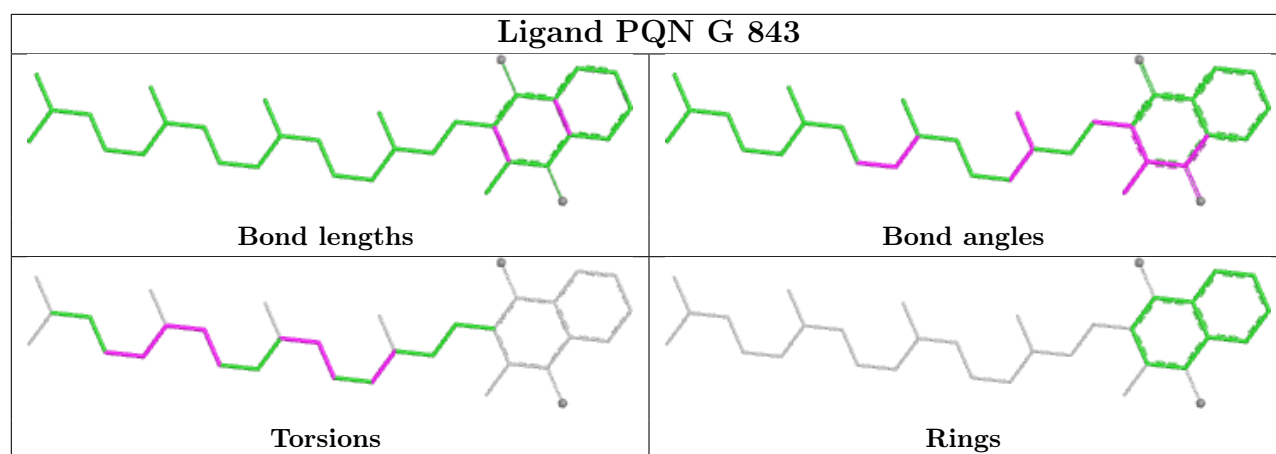


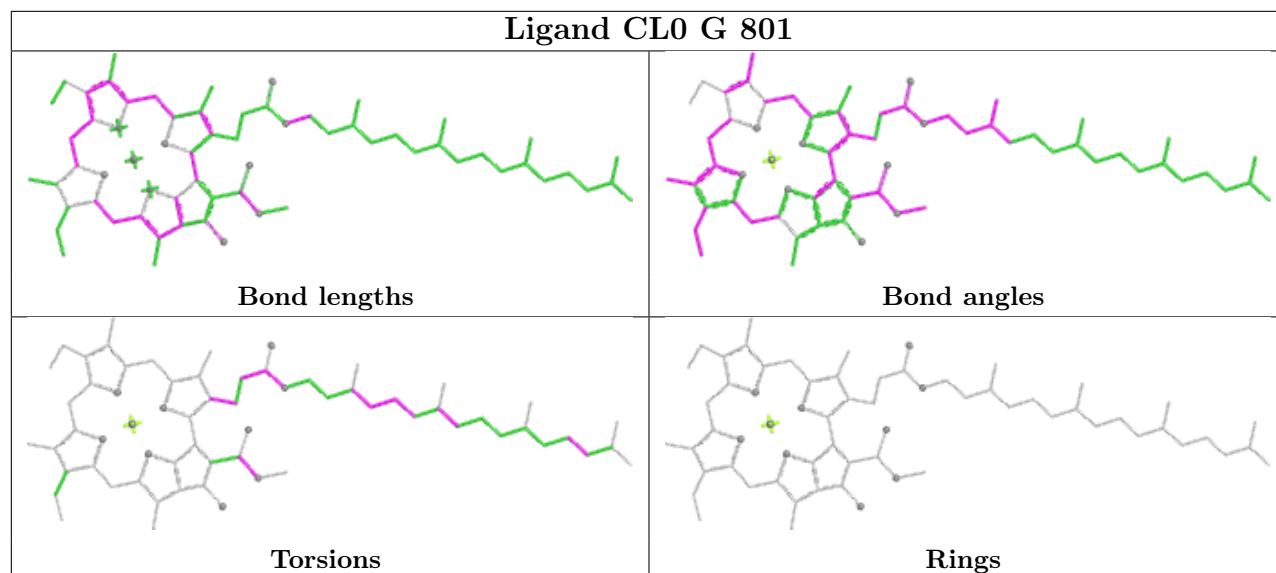
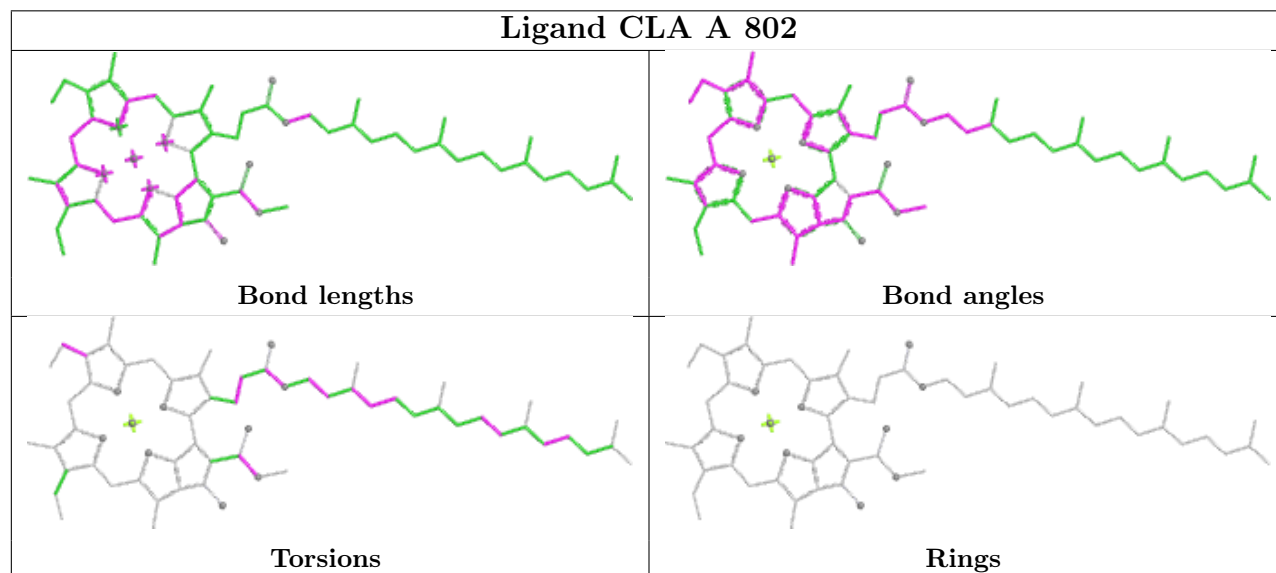
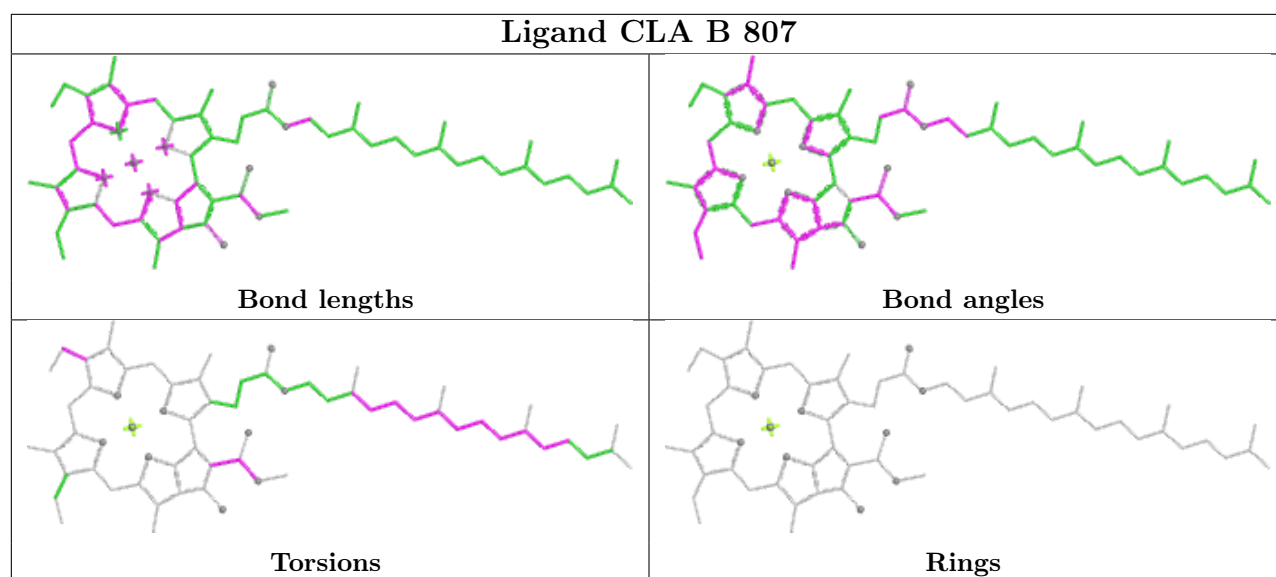
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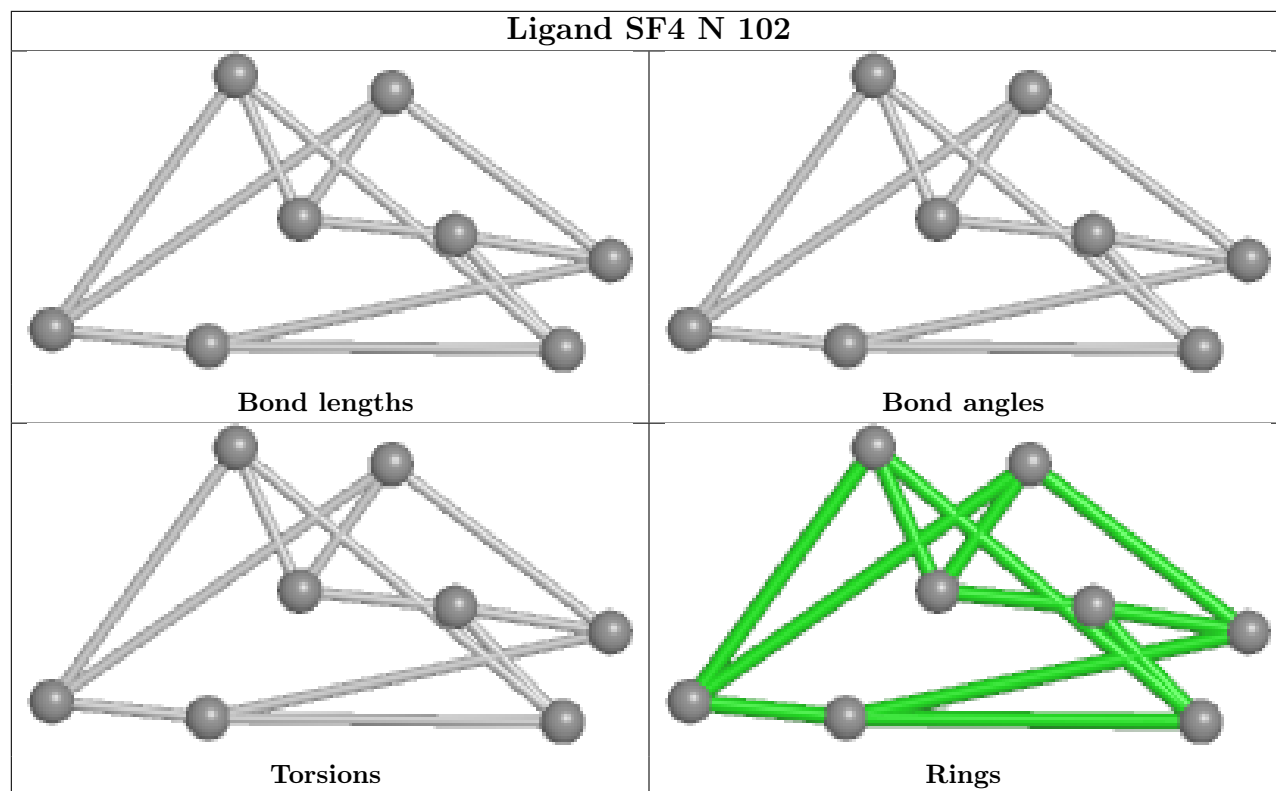


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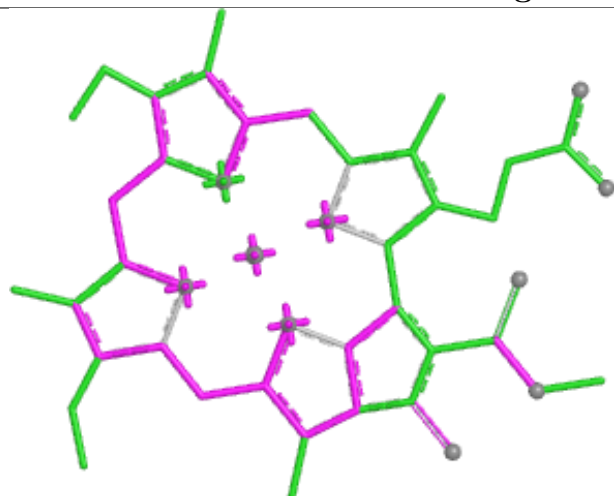




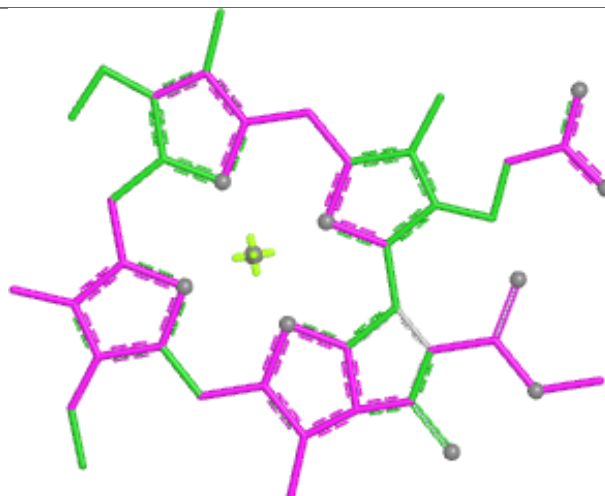




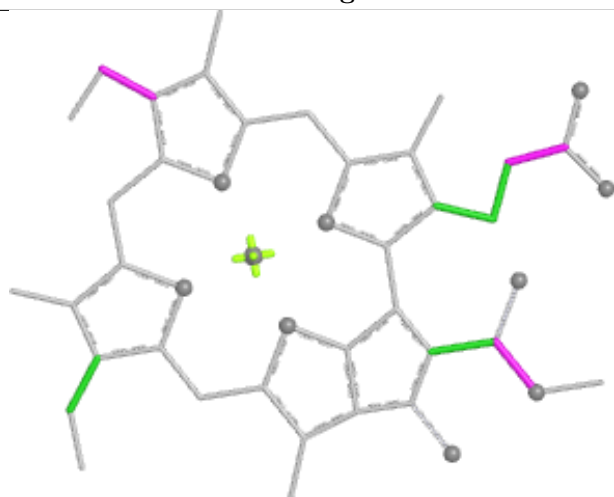
Ligand CLA B 834



Bond lengths



Bond angles

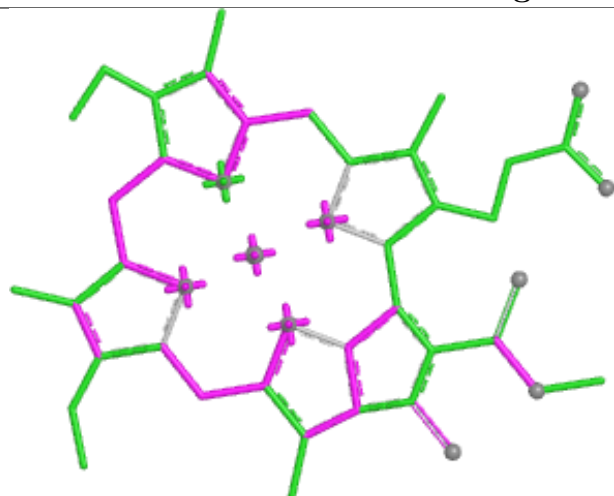


Torsions

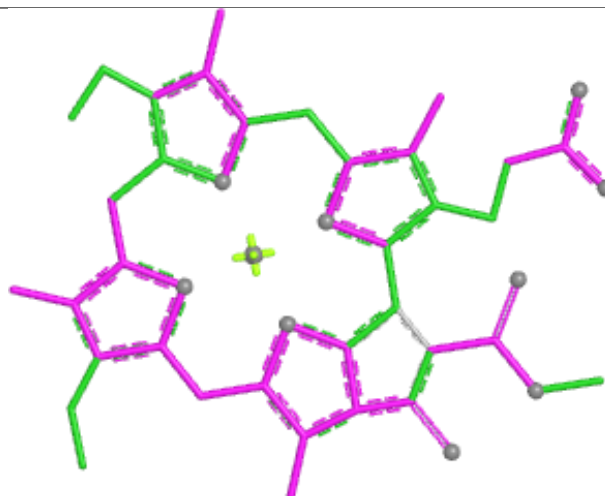


Rings

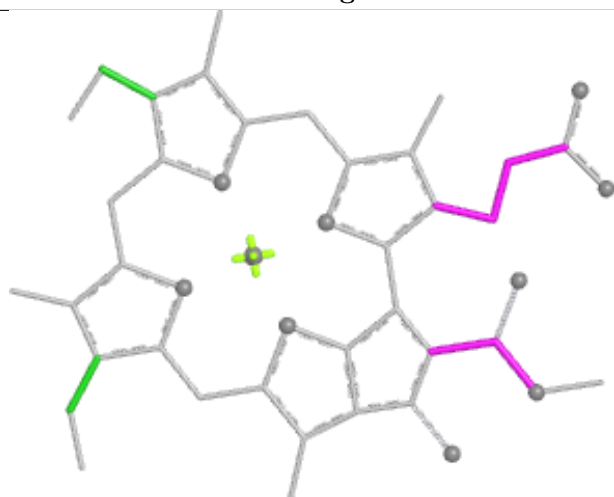
Ligand CLA H 820



Bond lengths



Bond angles

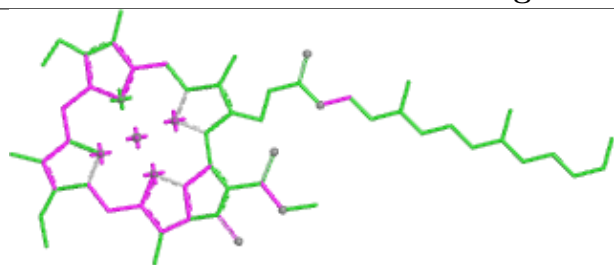


Torsions

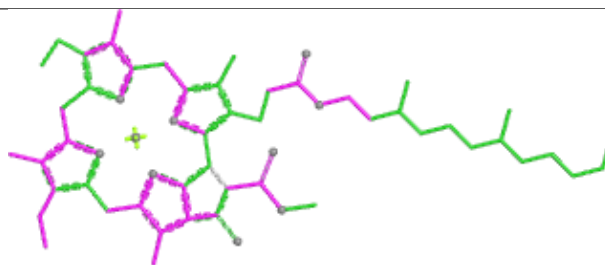


Rings

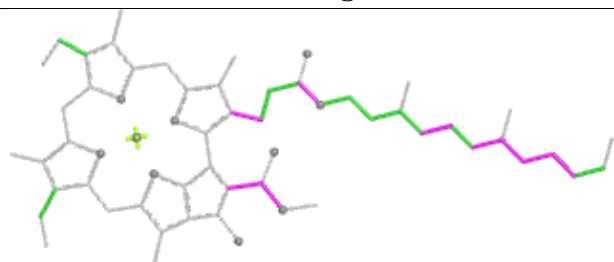
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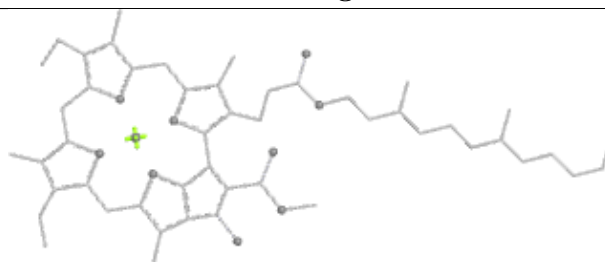
Bond lengths



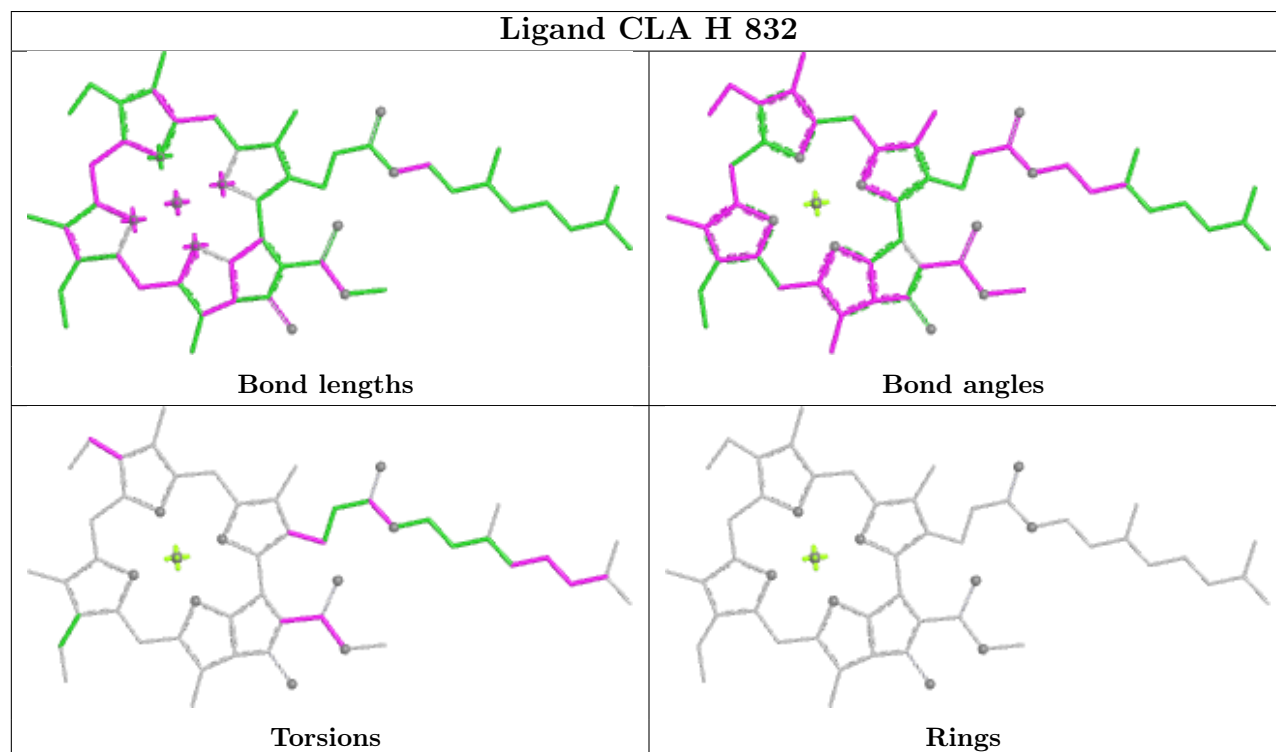
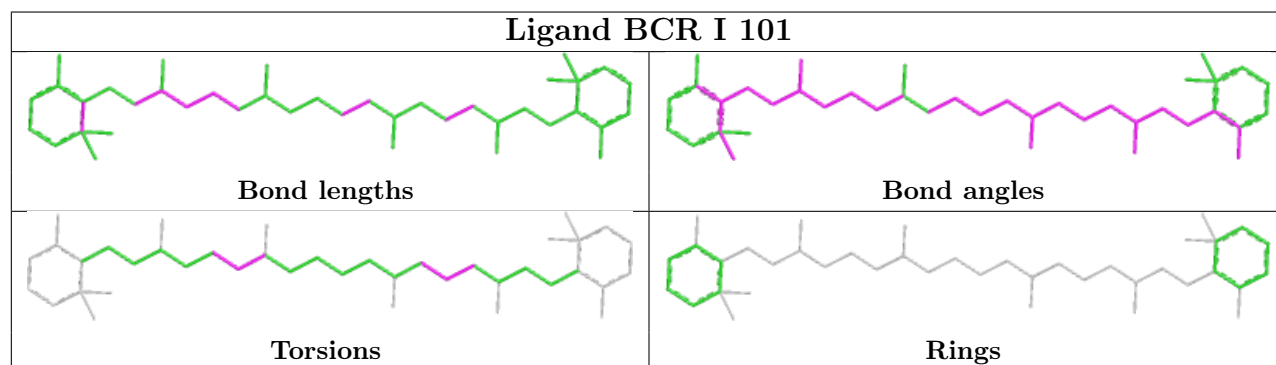
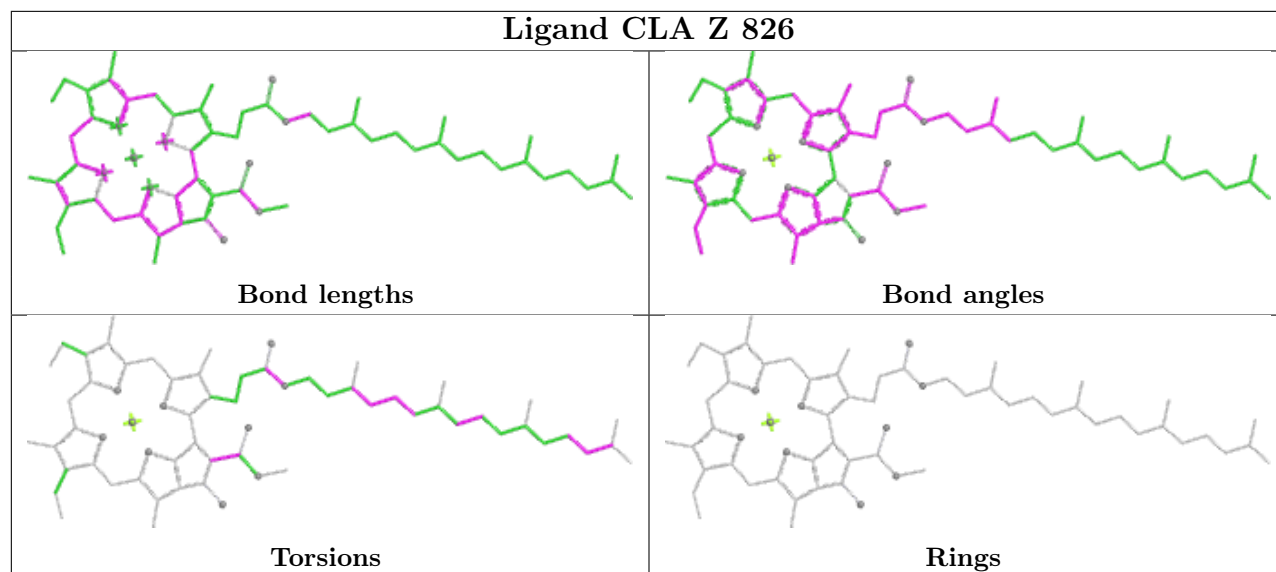
Bond angles

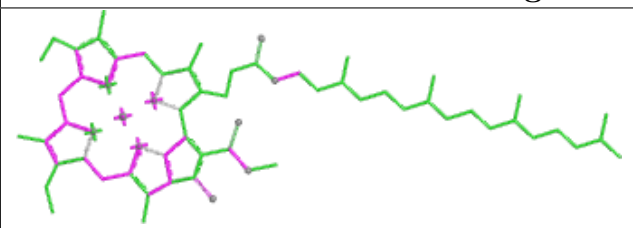
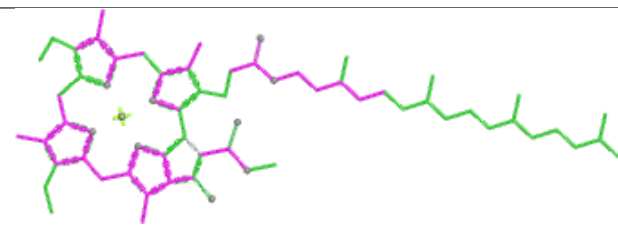
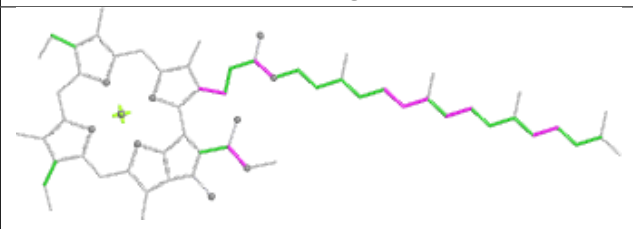
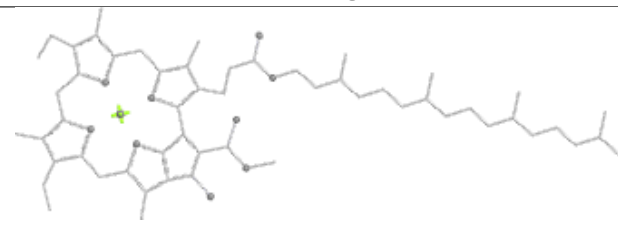


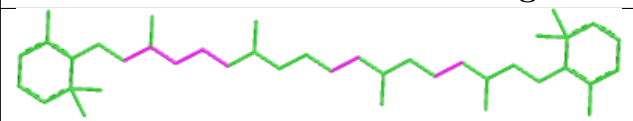
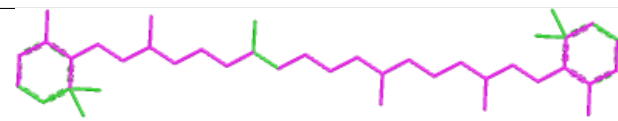
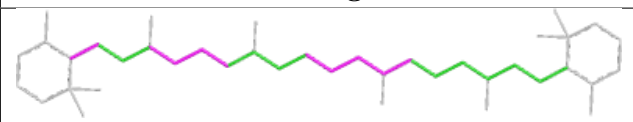
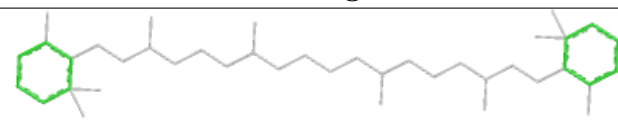
Torsions

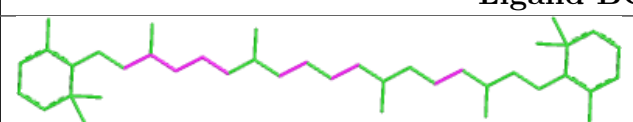
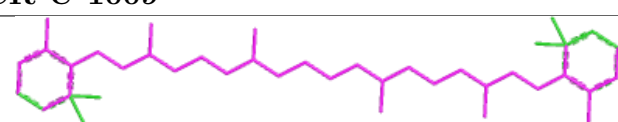
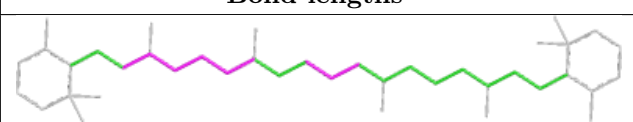
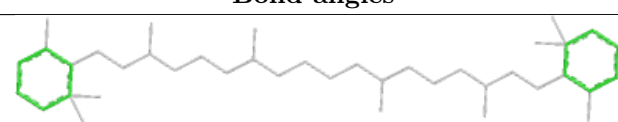


Rings

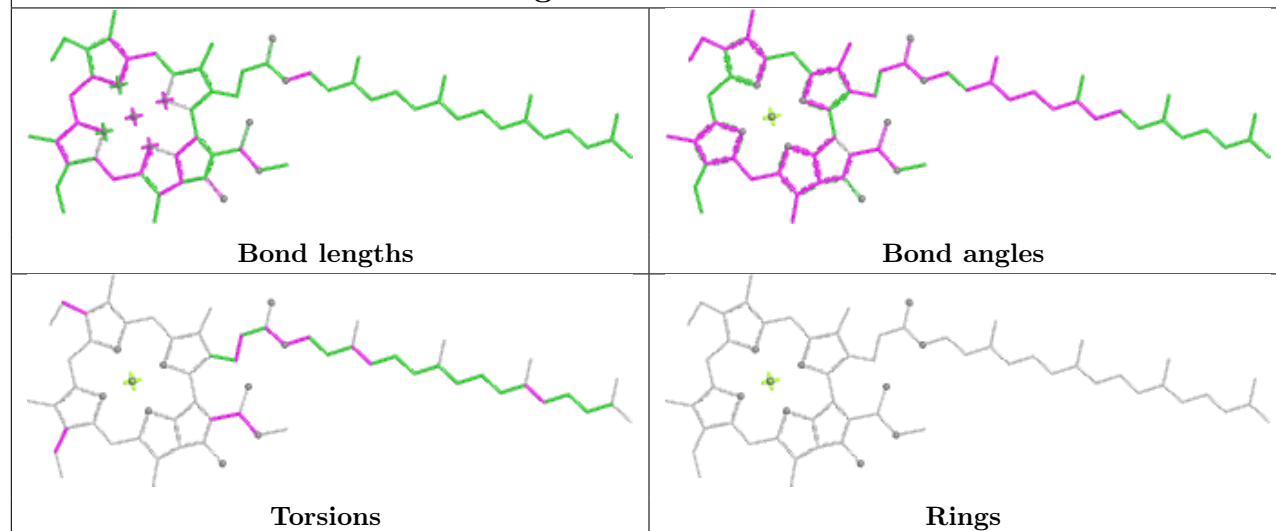


Ligand CLA h 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

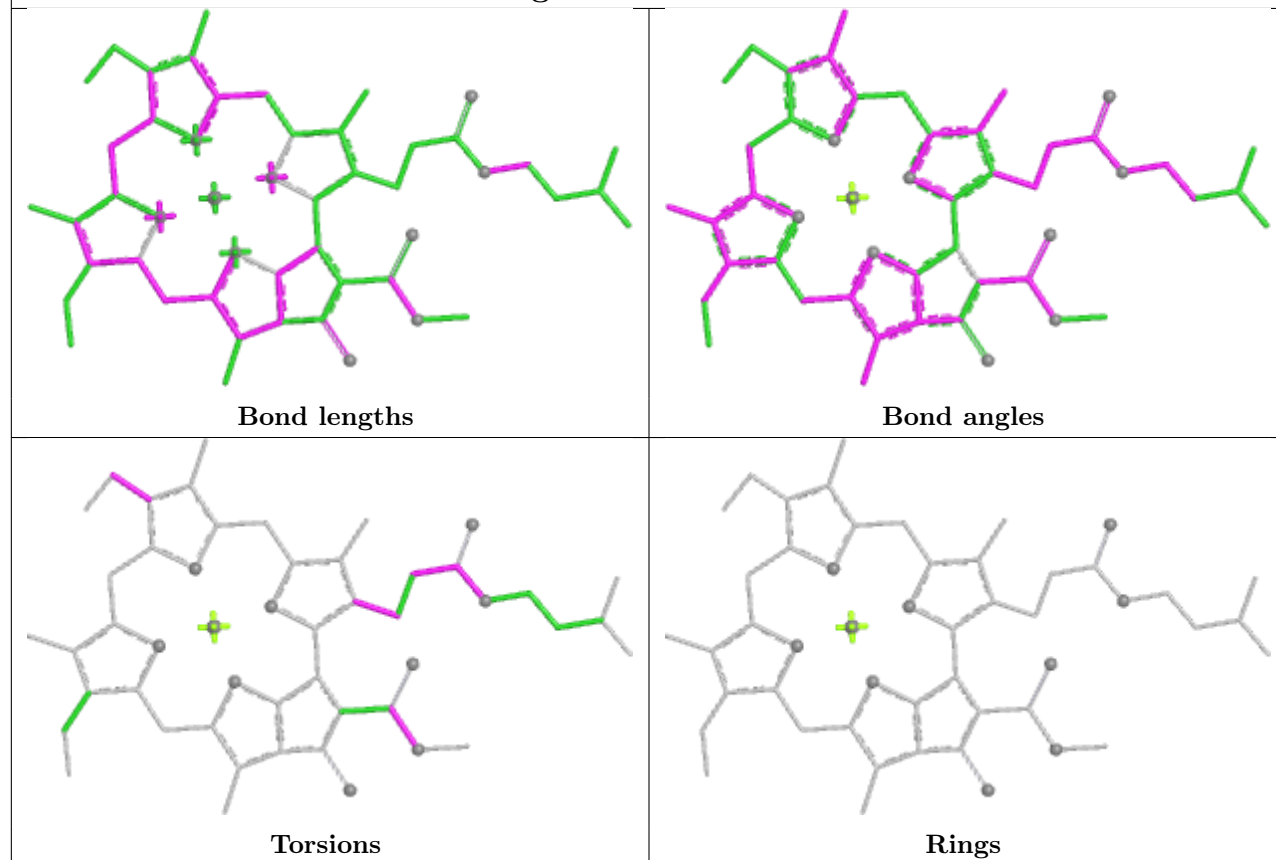
Ligand BCR A 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

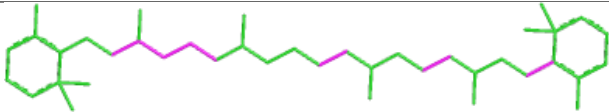
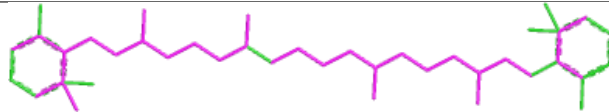
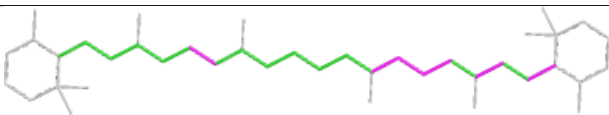
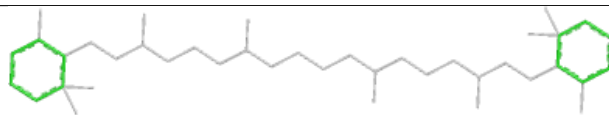
Ligand BCR U 1009	
	
Bond lengths	Bond angles
	
Torsions	Rings

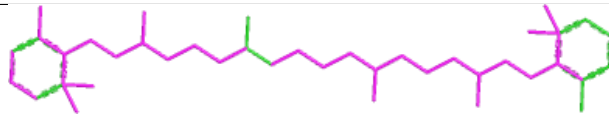
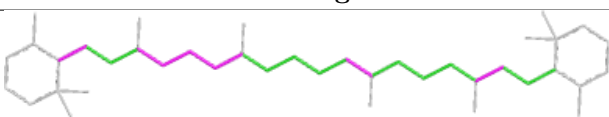
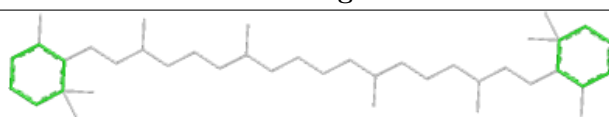
Ligand CLA L 202

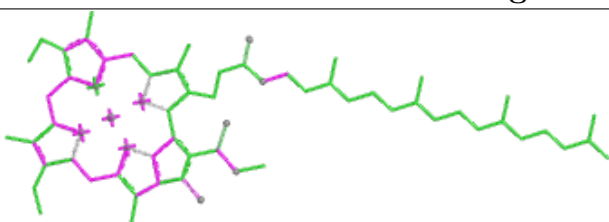
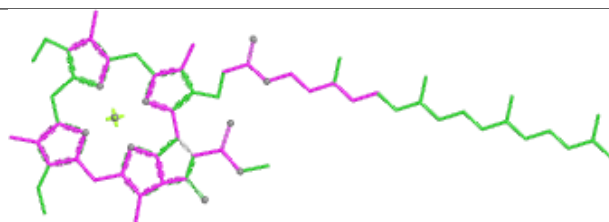
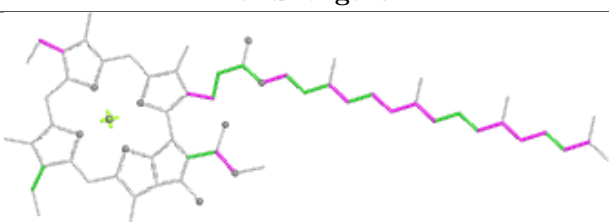
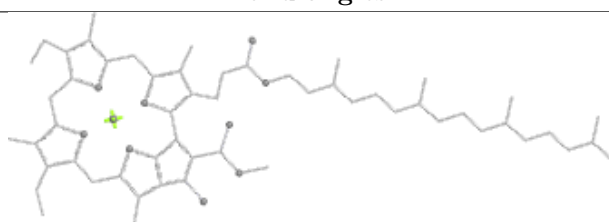


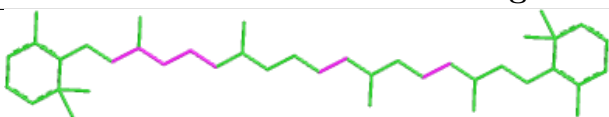
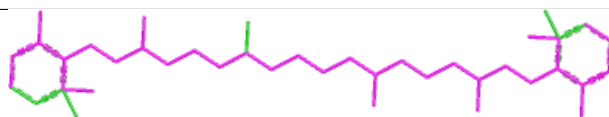
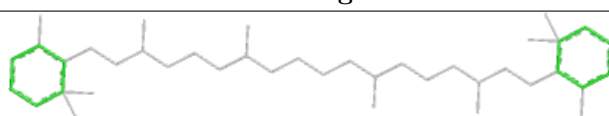
Ligand CLA Y 823

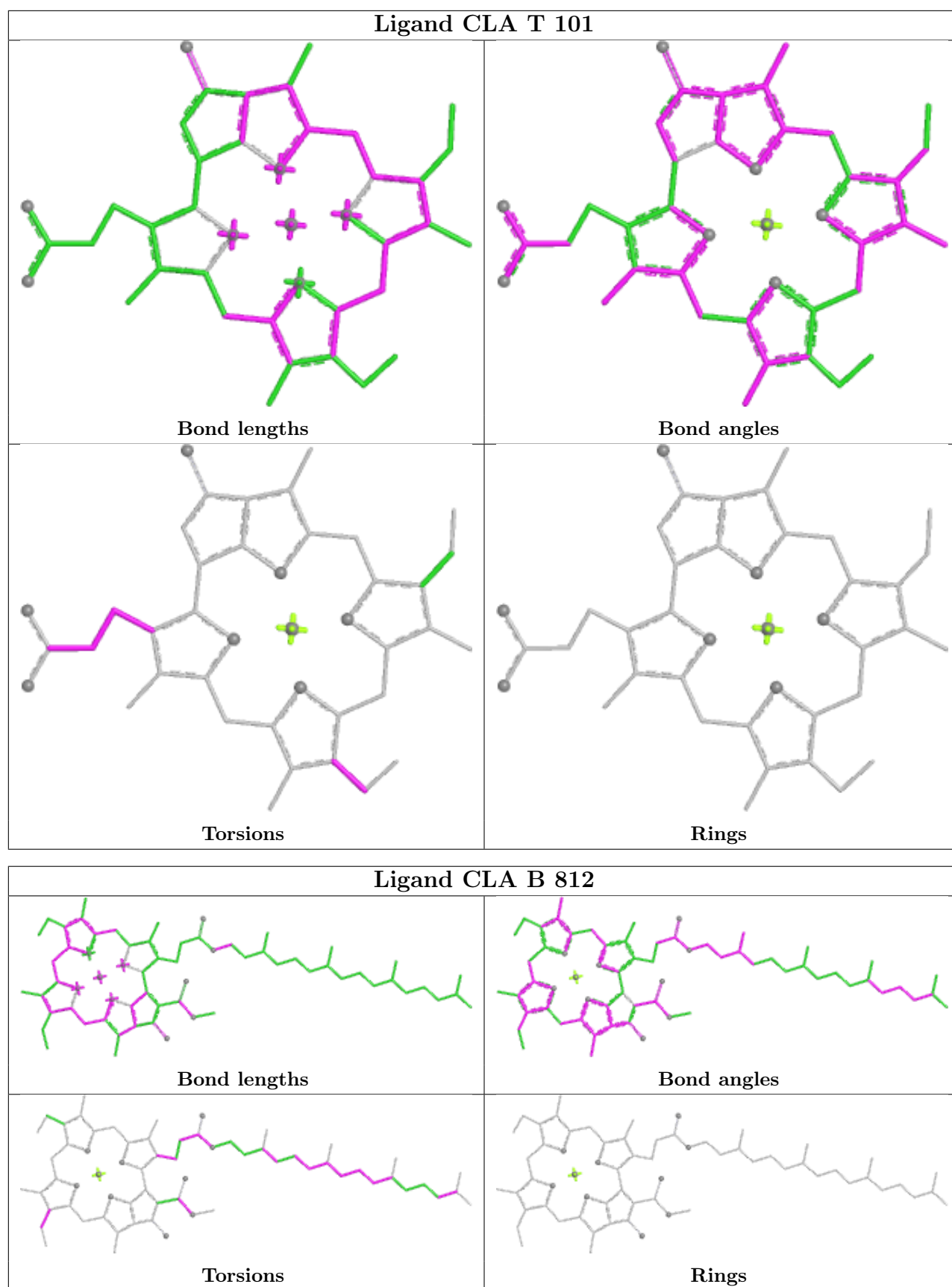


Ligand BCR R 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

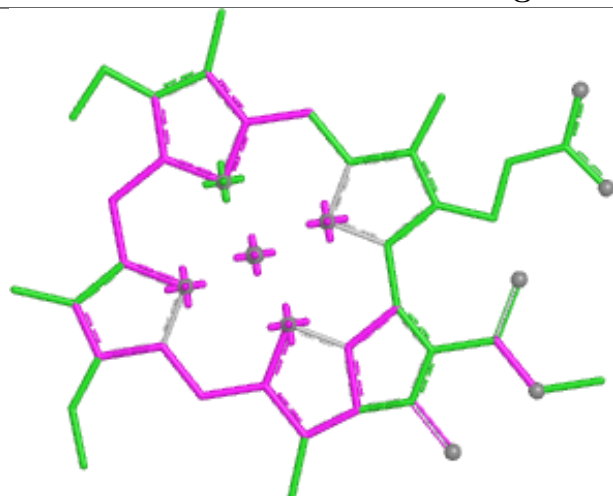
Ligand BCR A 851	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

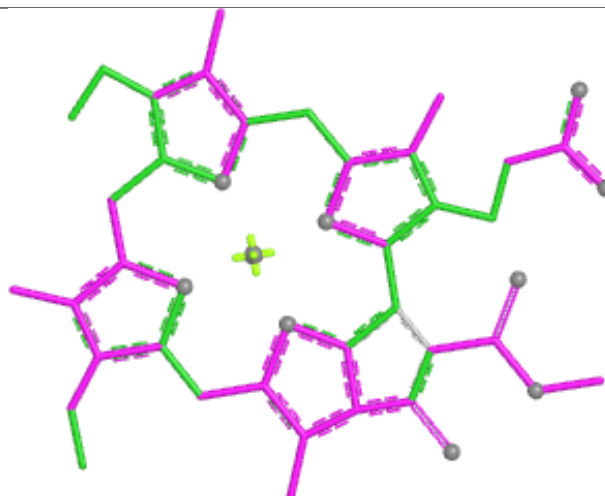
Ligand BCR Z 844	
	
Bond lengths	Bond angles
	
Torsions	Rings



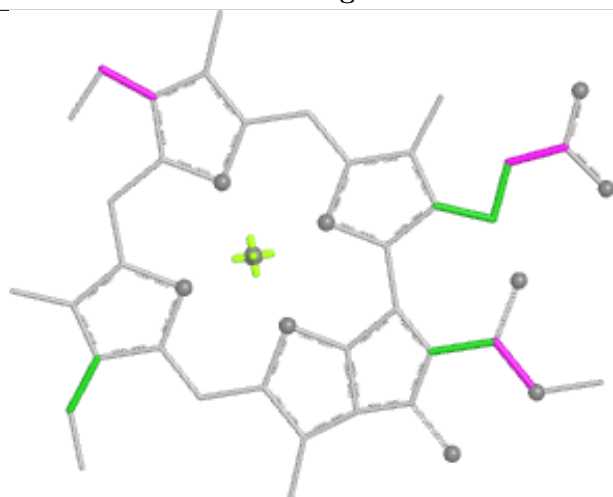
Ligand CLA A 811



Bond lengths



Bond angles

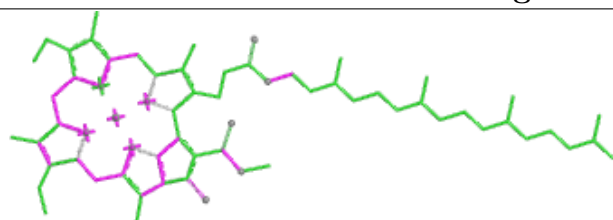


Torsions

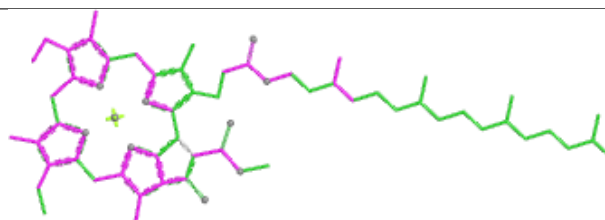


Rings

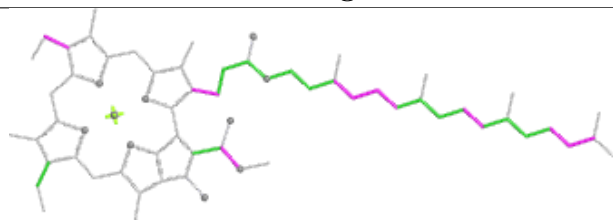
Ligand CLA H 827



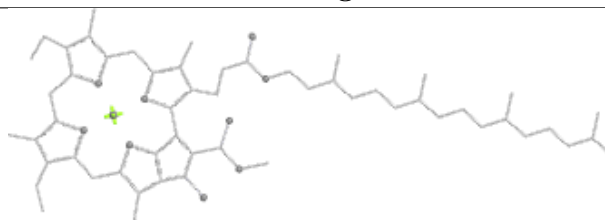
Bond lengths



Bond angles

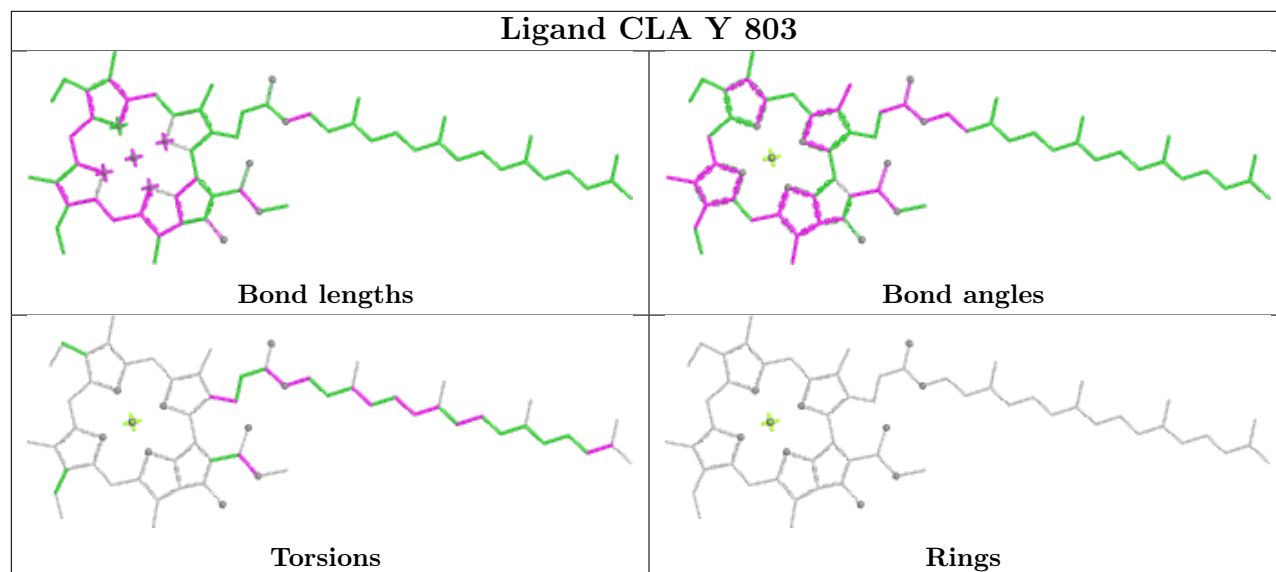


Torsions

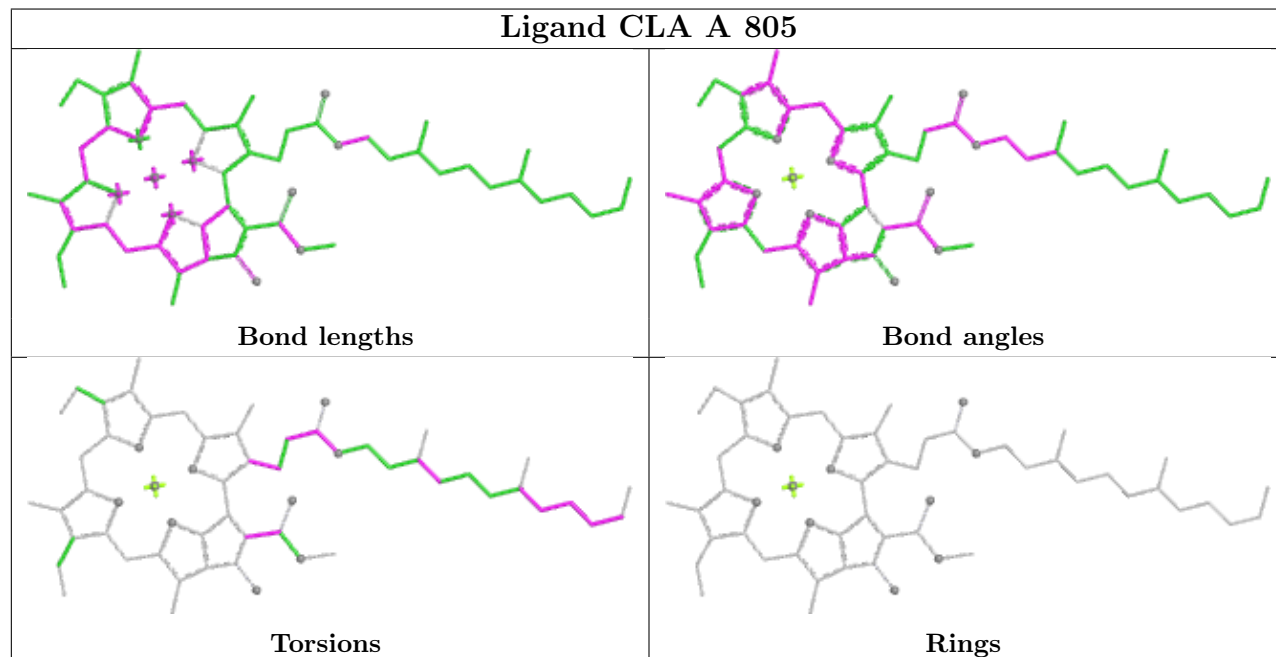


Rings

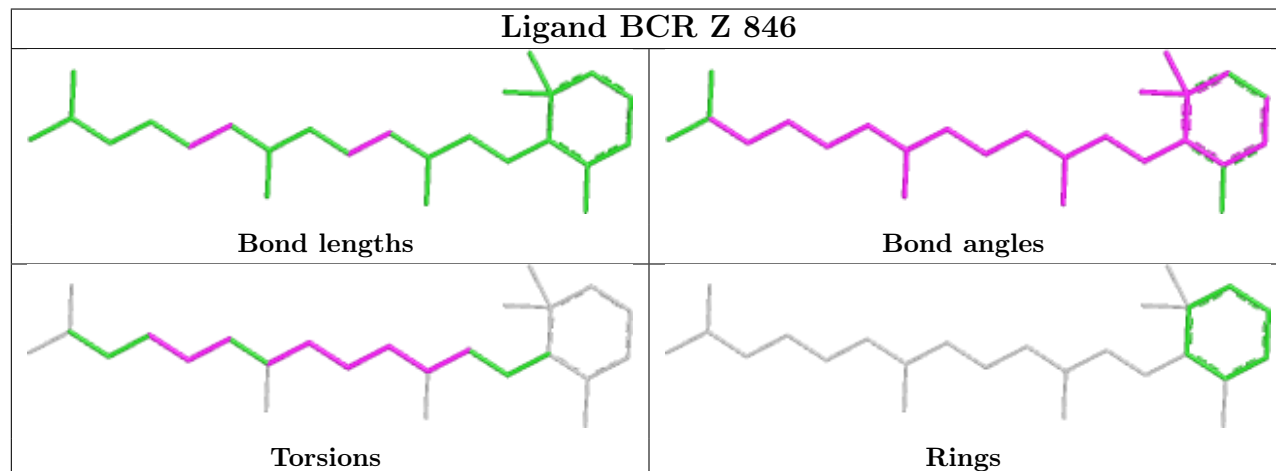
Ligand CLA Y 803



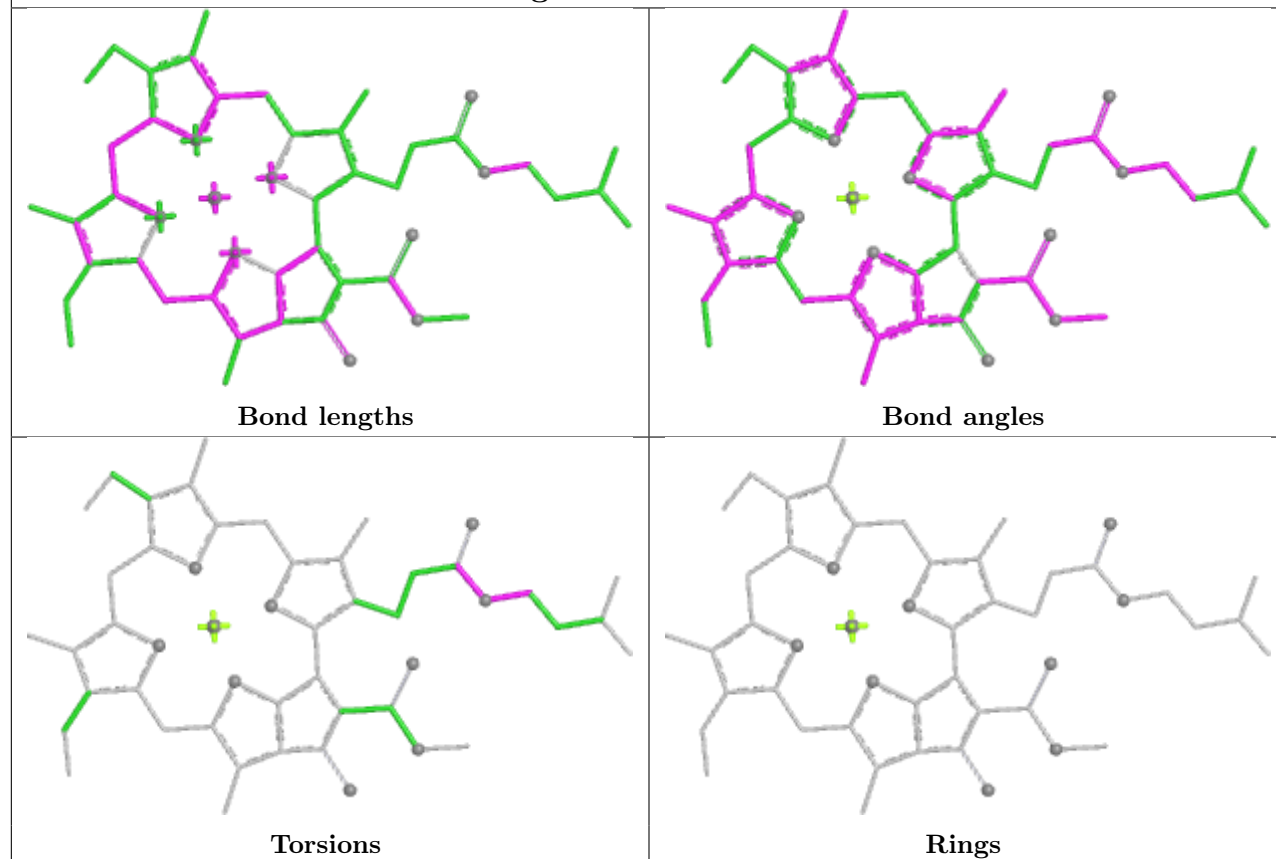
Ligand CLA A 805



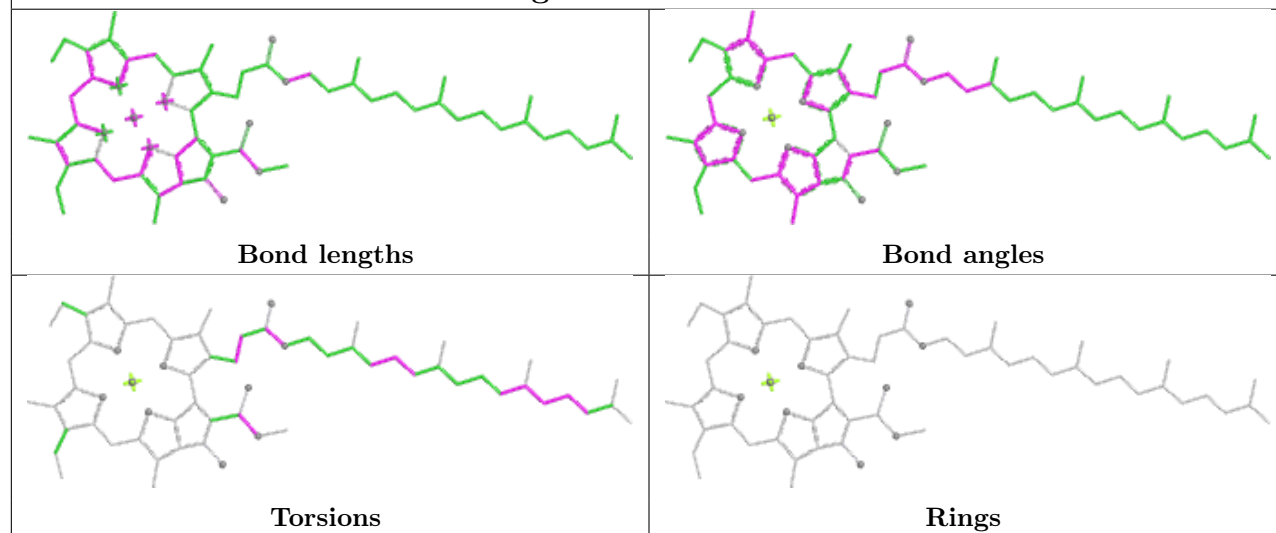
Ligand BCR Z 846



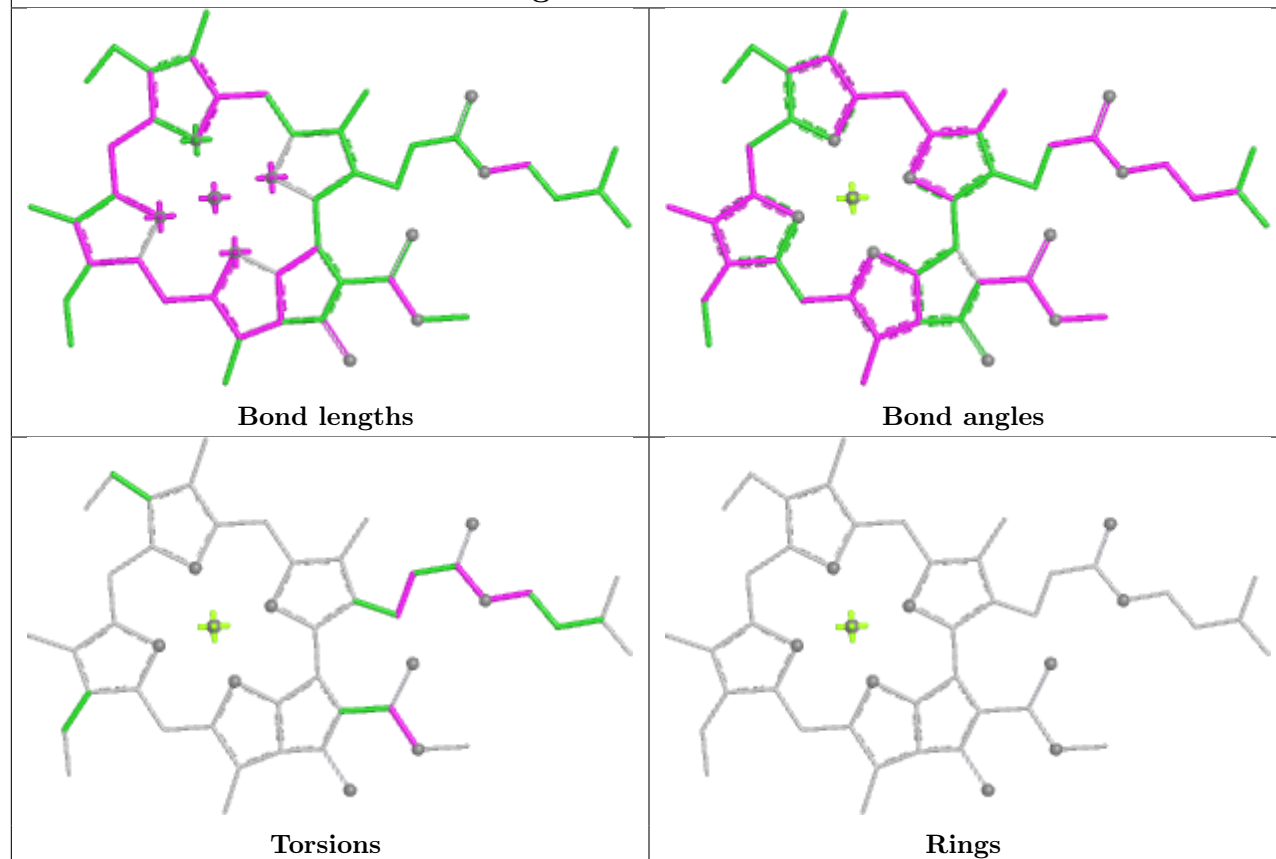
Ligand CLA G 838



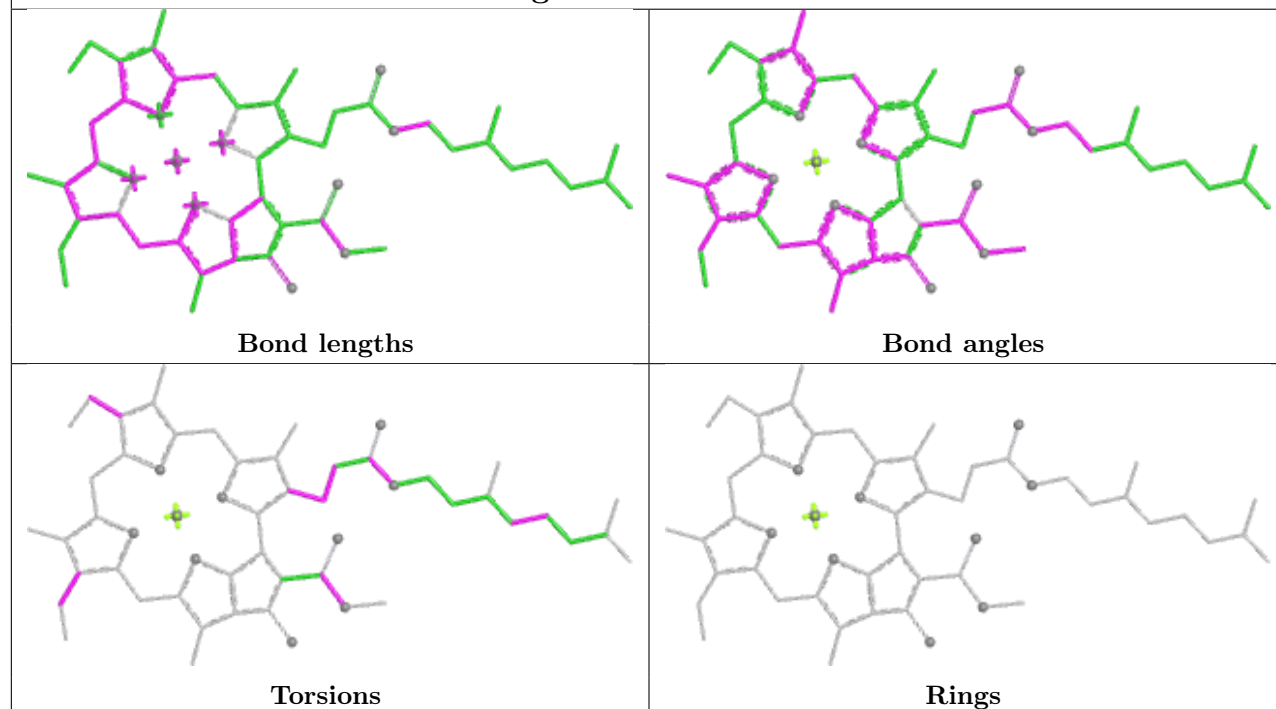
Ligand CLA Y 841



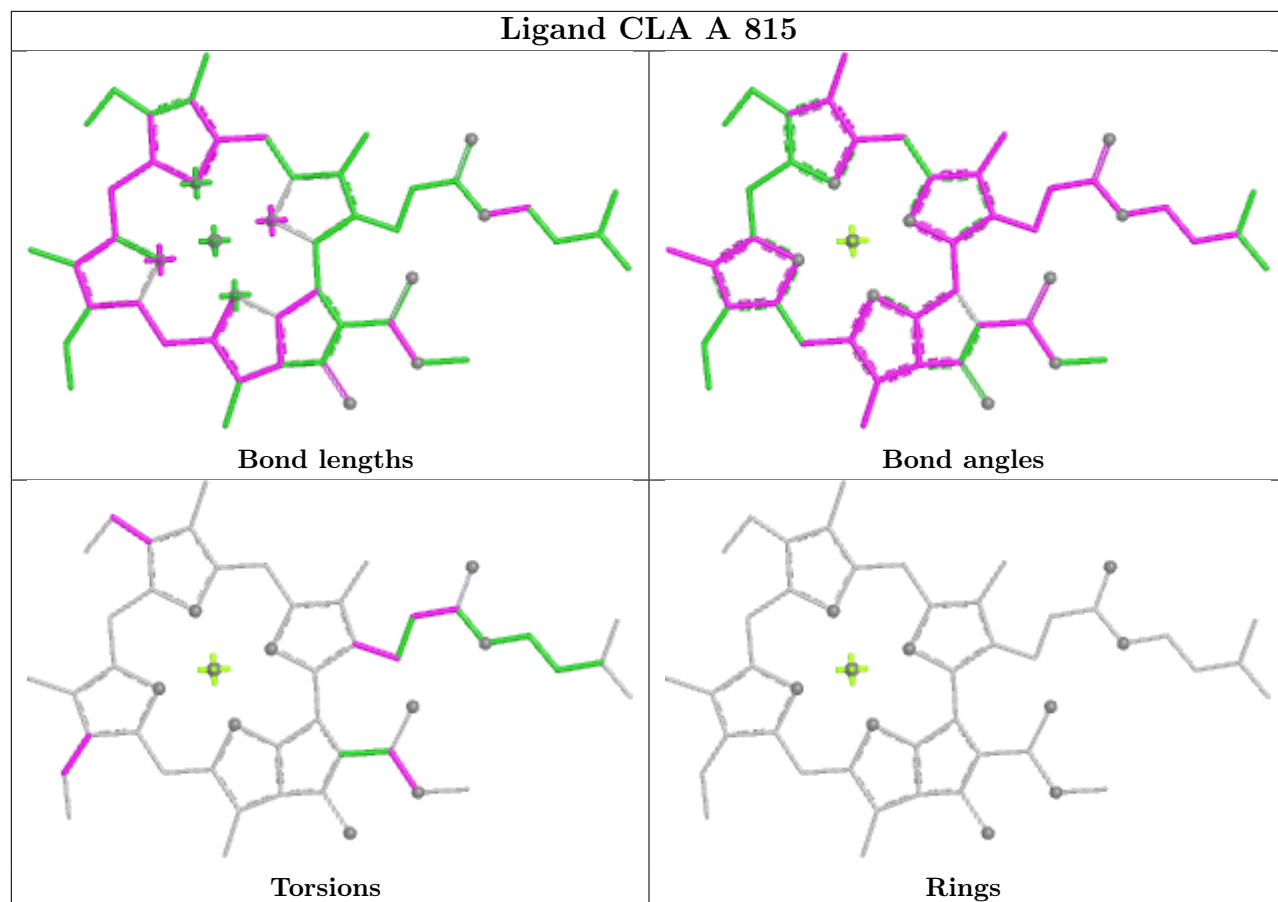
Ligand CLA B 811



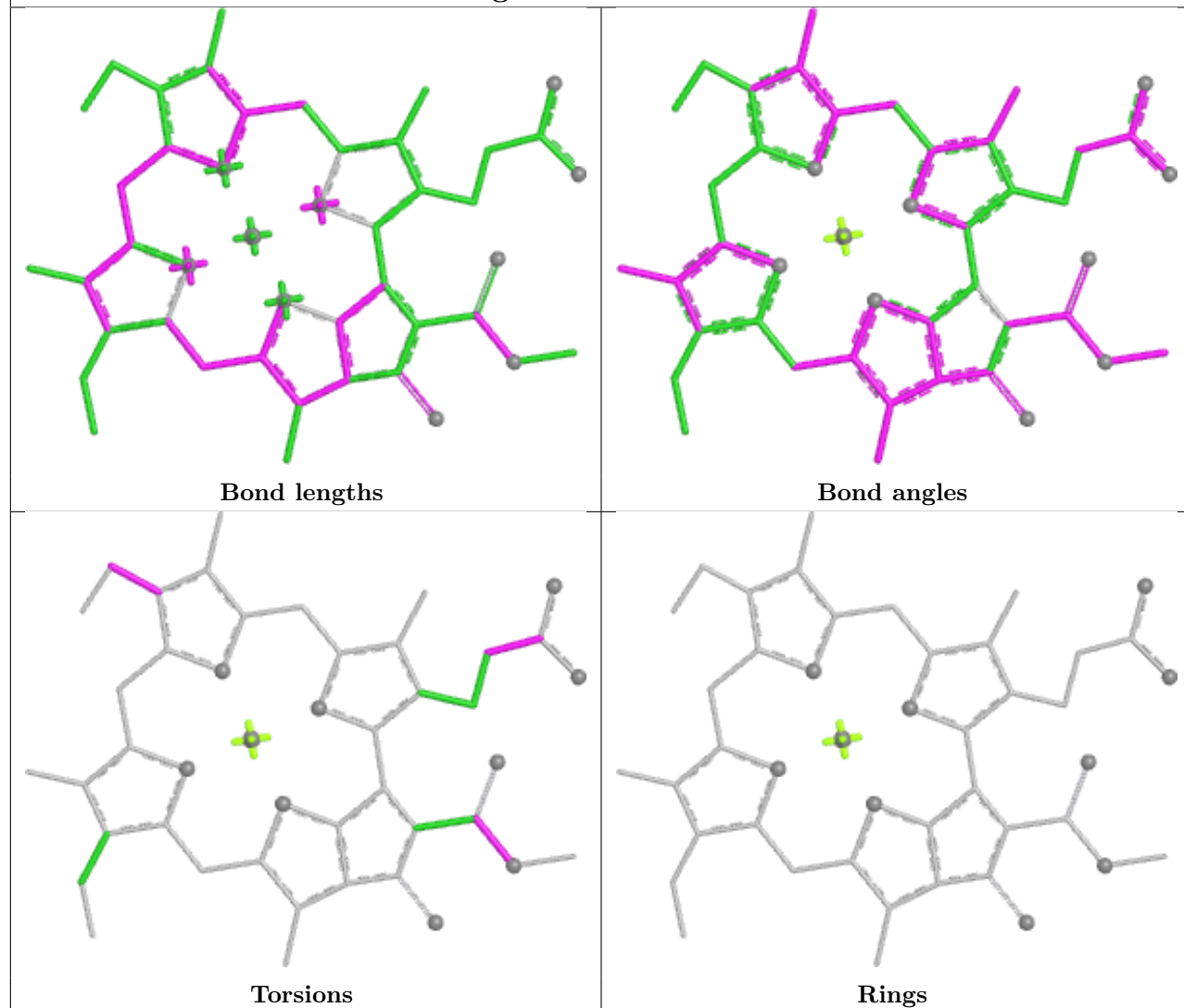
Ligand CLA Y 833



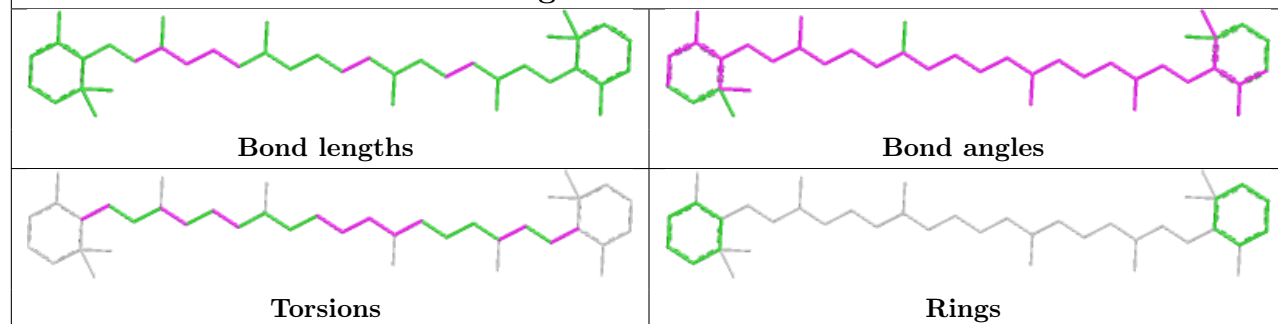
Ligand CLA A 815



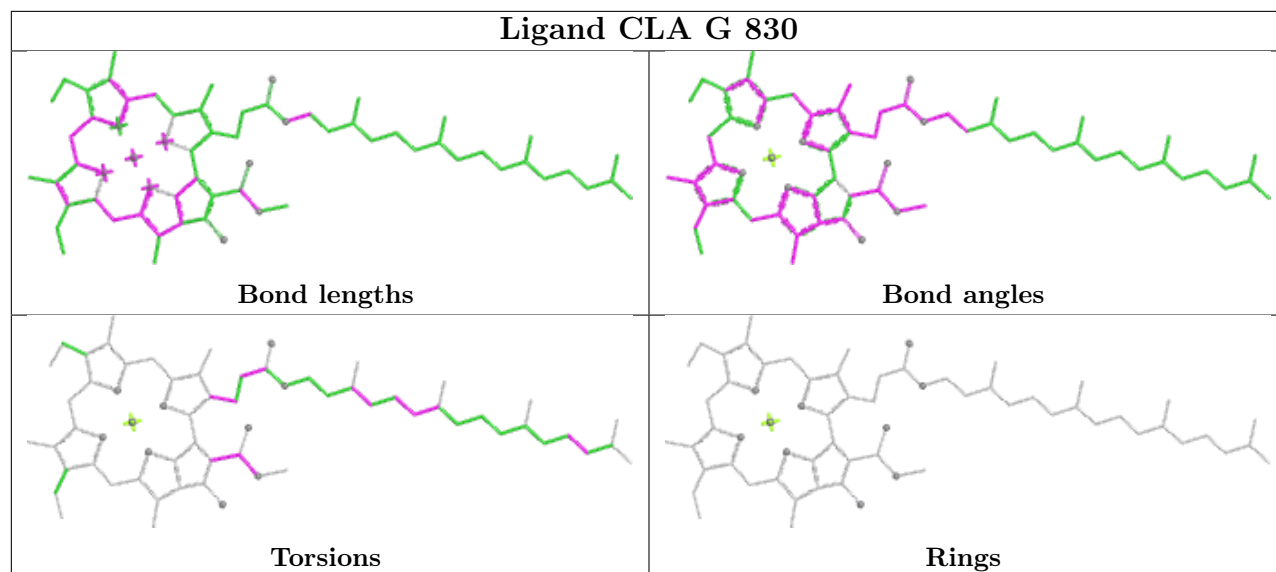
Ligand CLA H 835



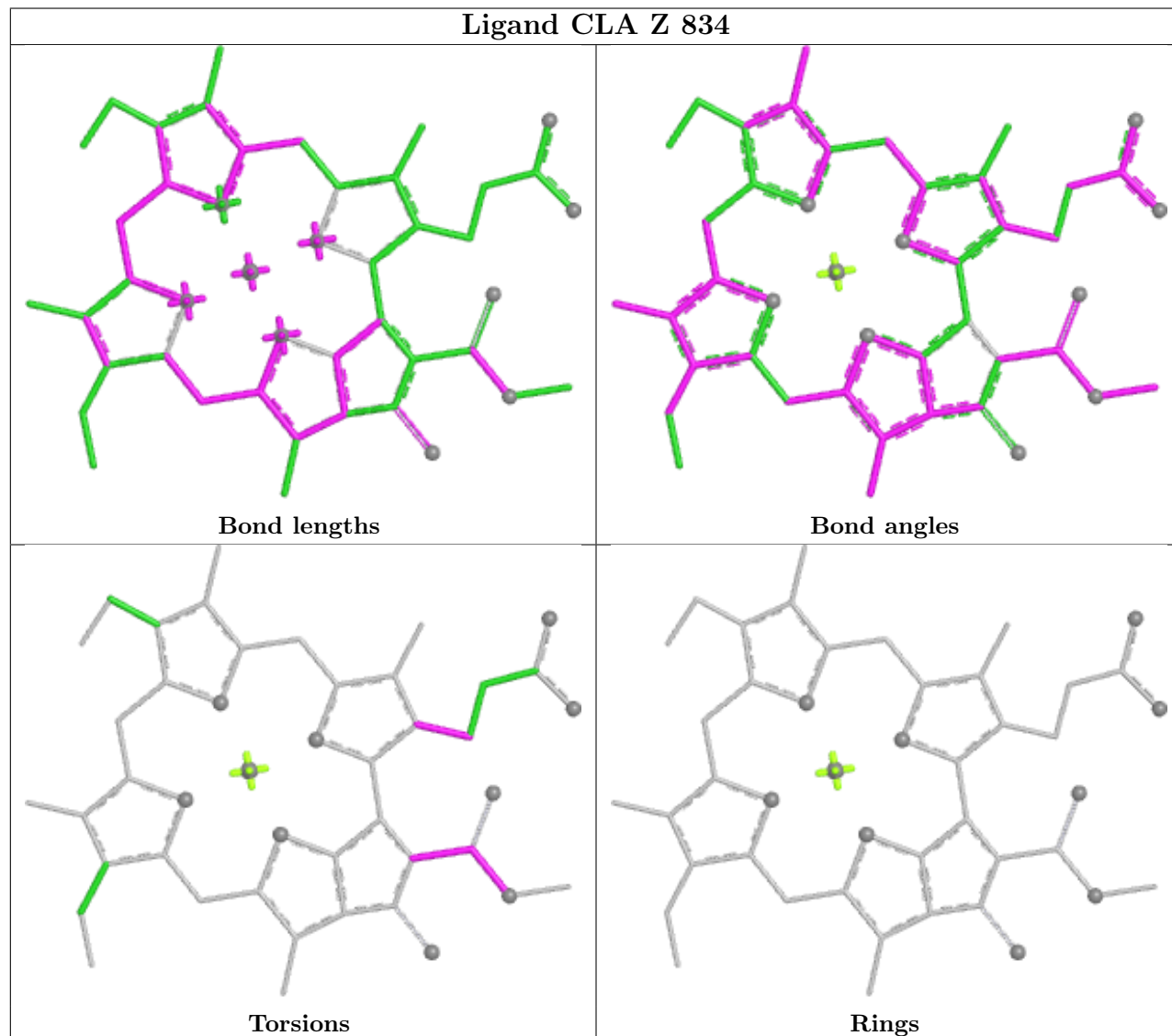
Ligand BCR i 101



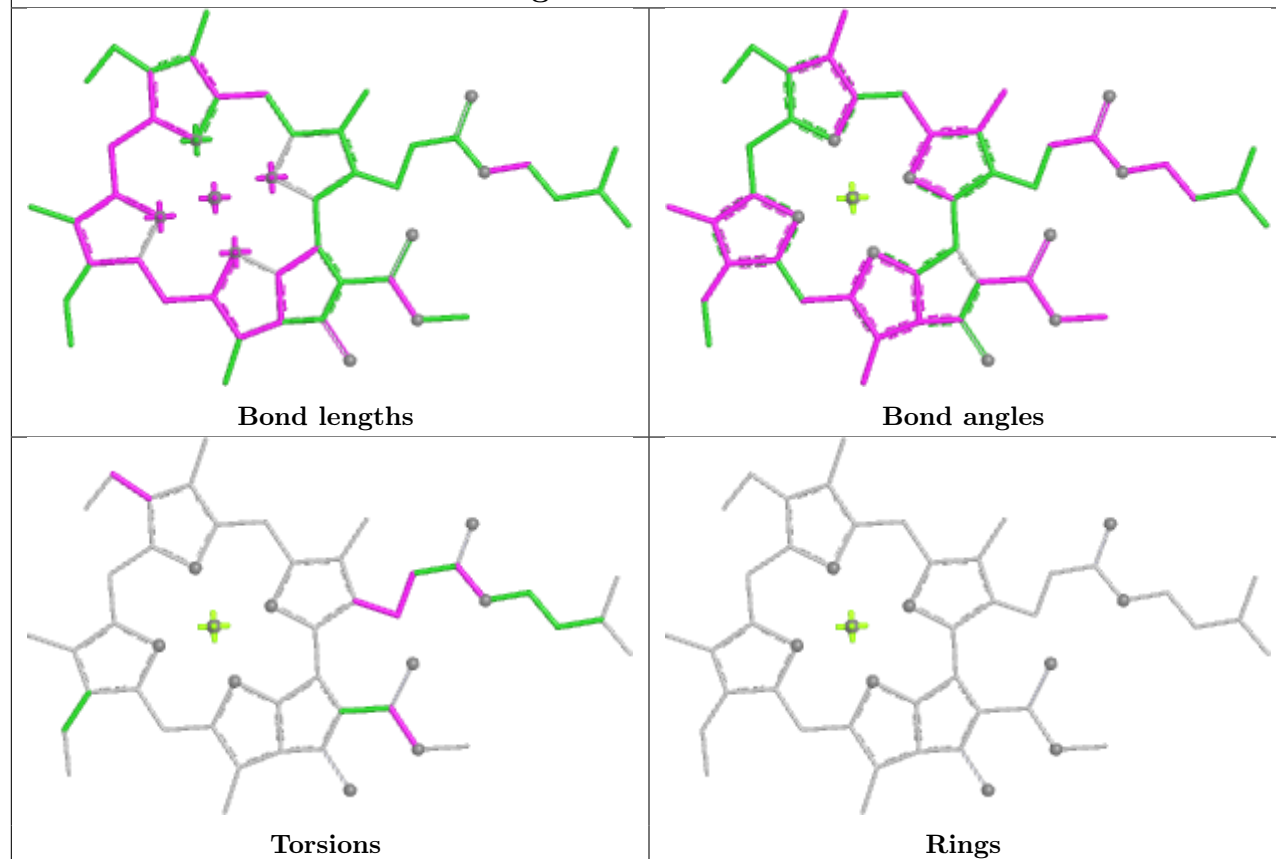
Ligand CLA G 830



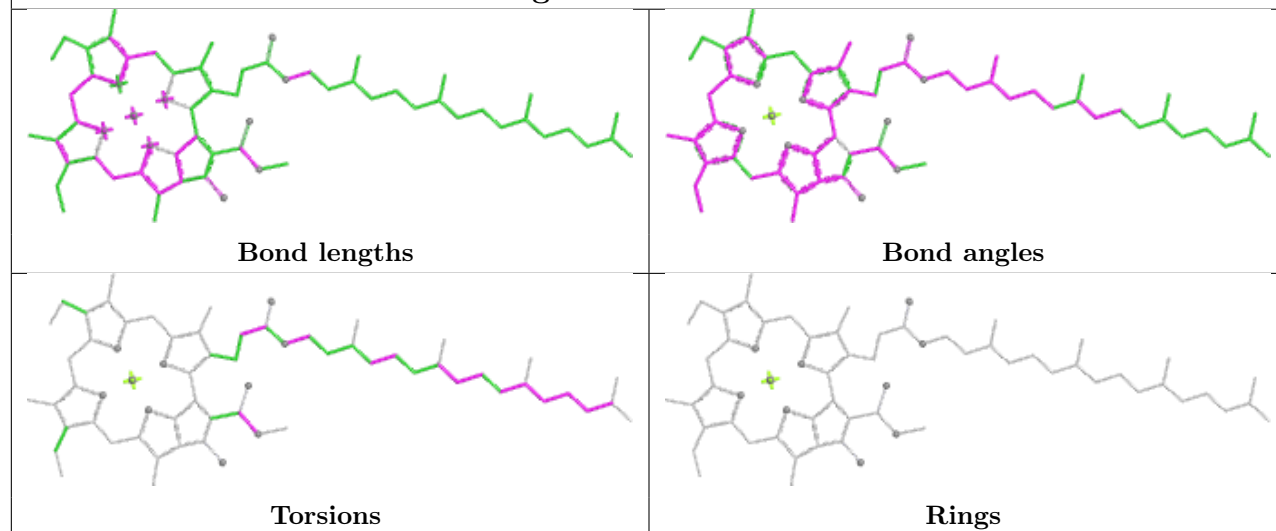
Ligand CLA Z 834



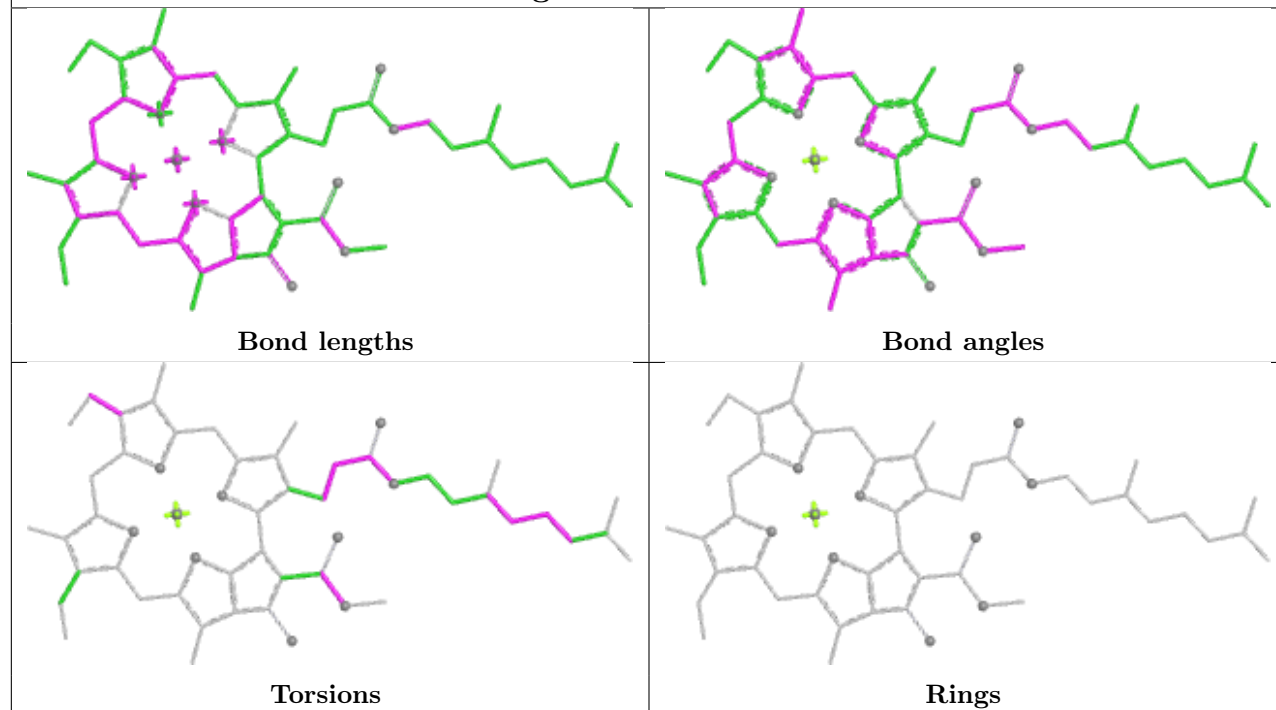
Ligand CLA A 843



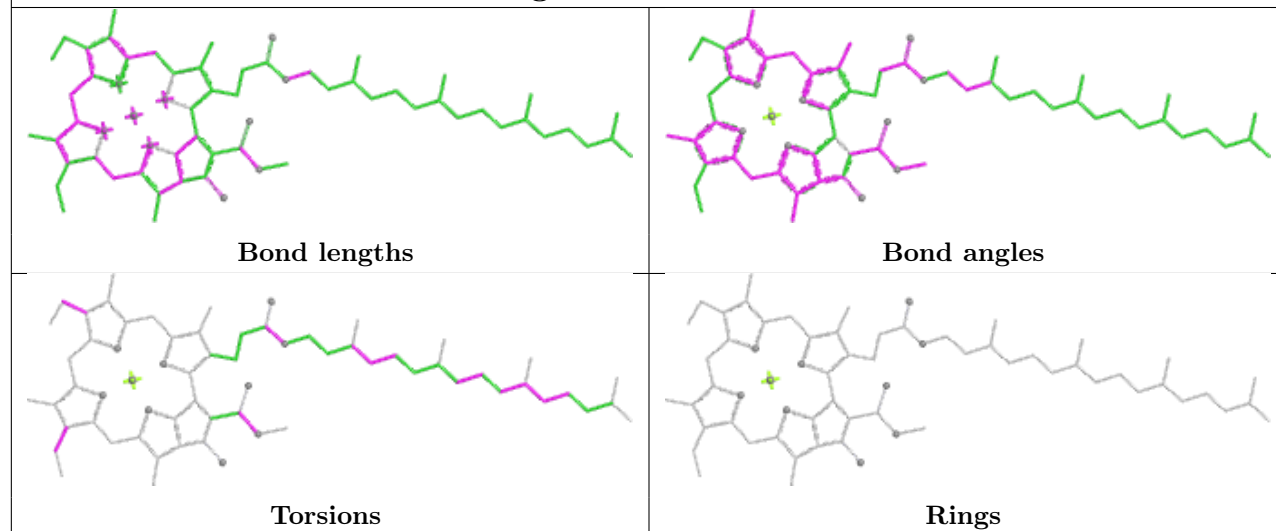
Ligand CLA B 808

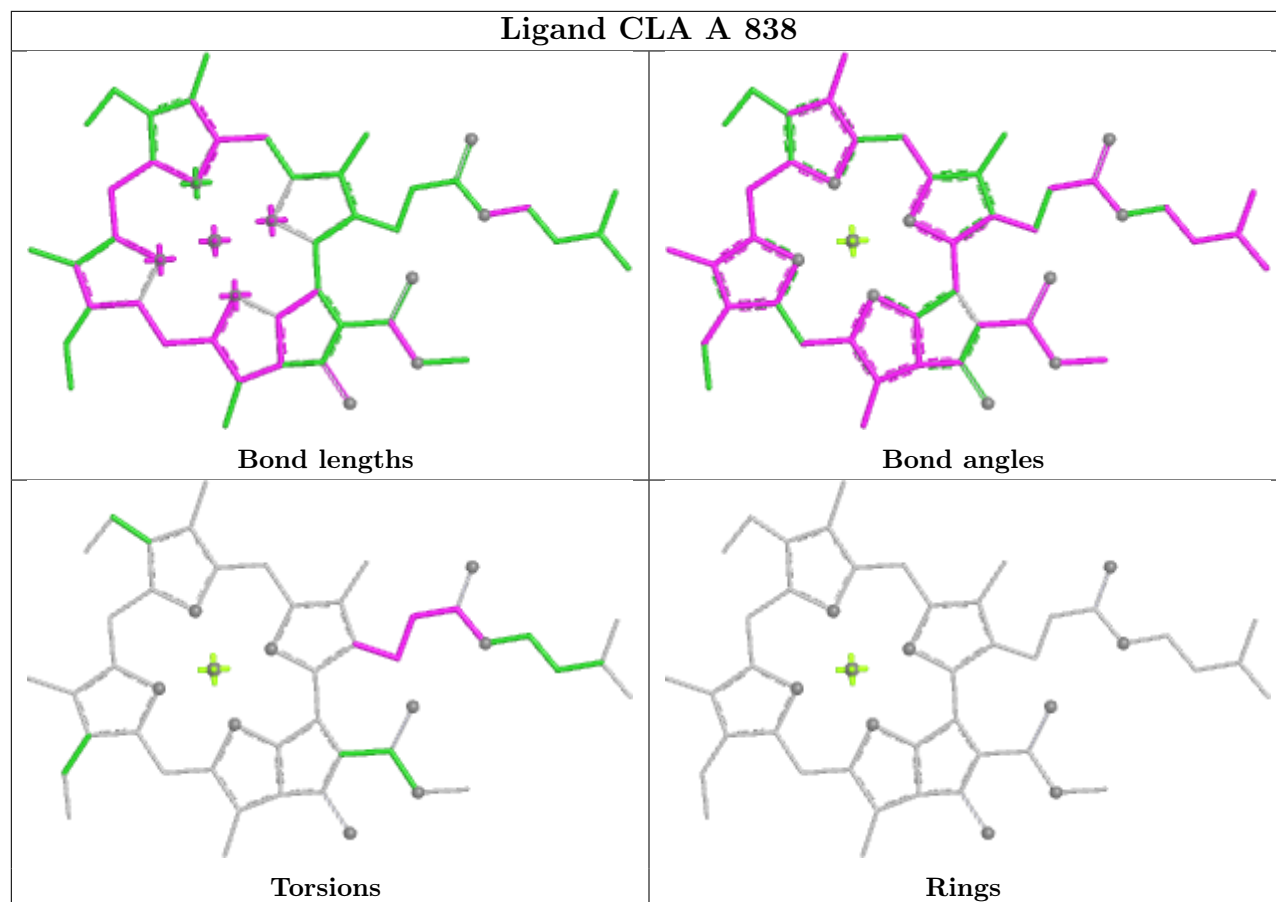


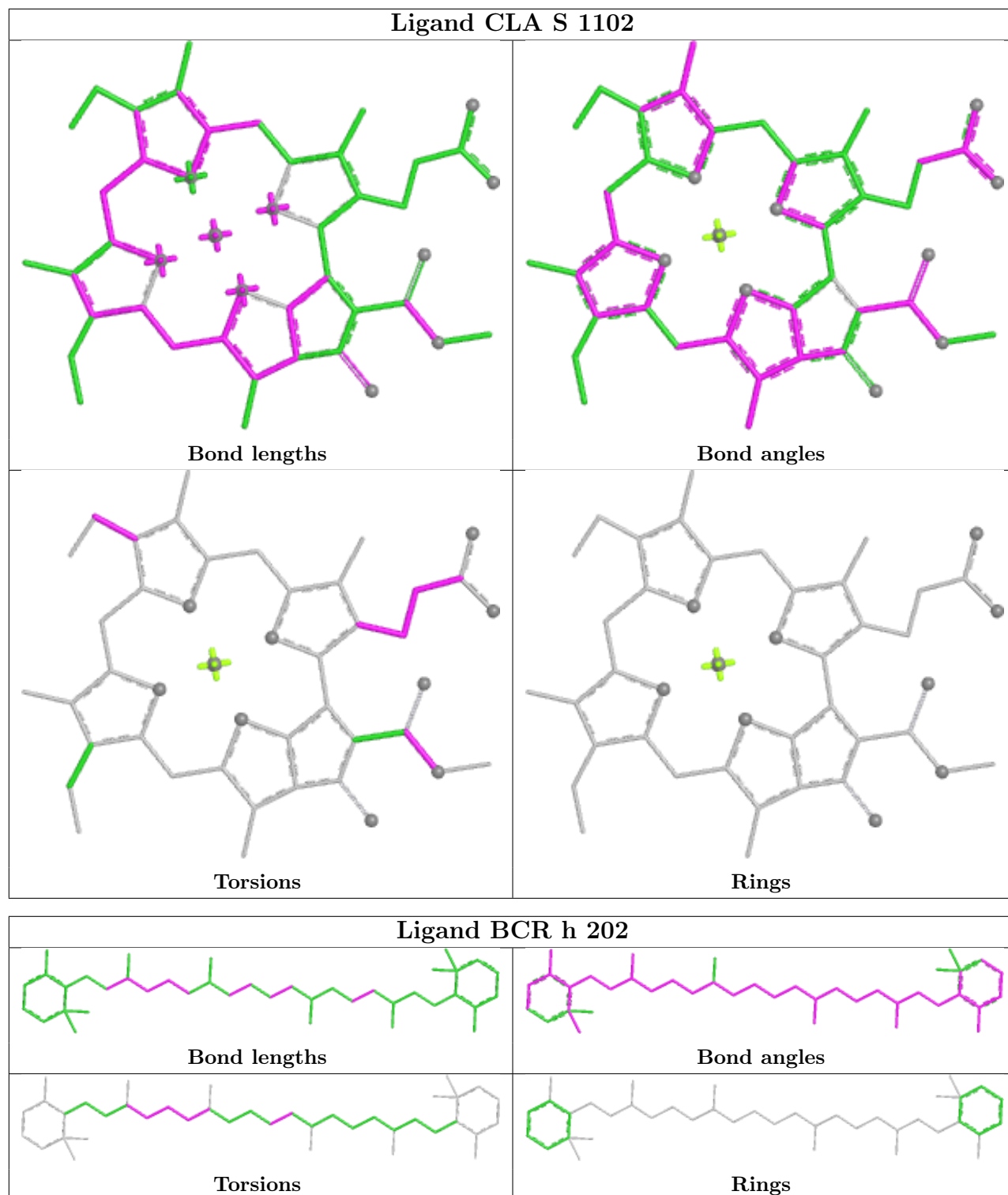
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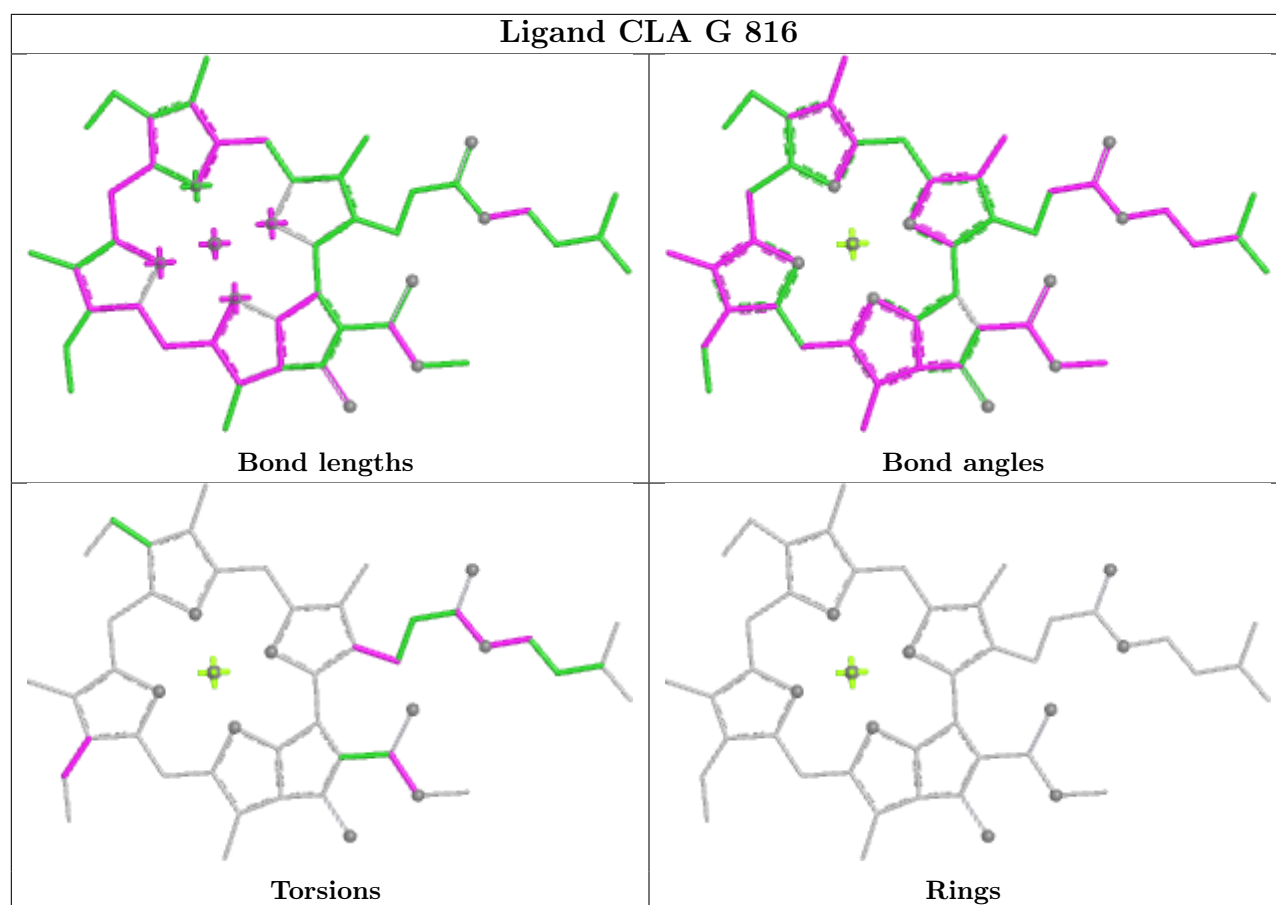


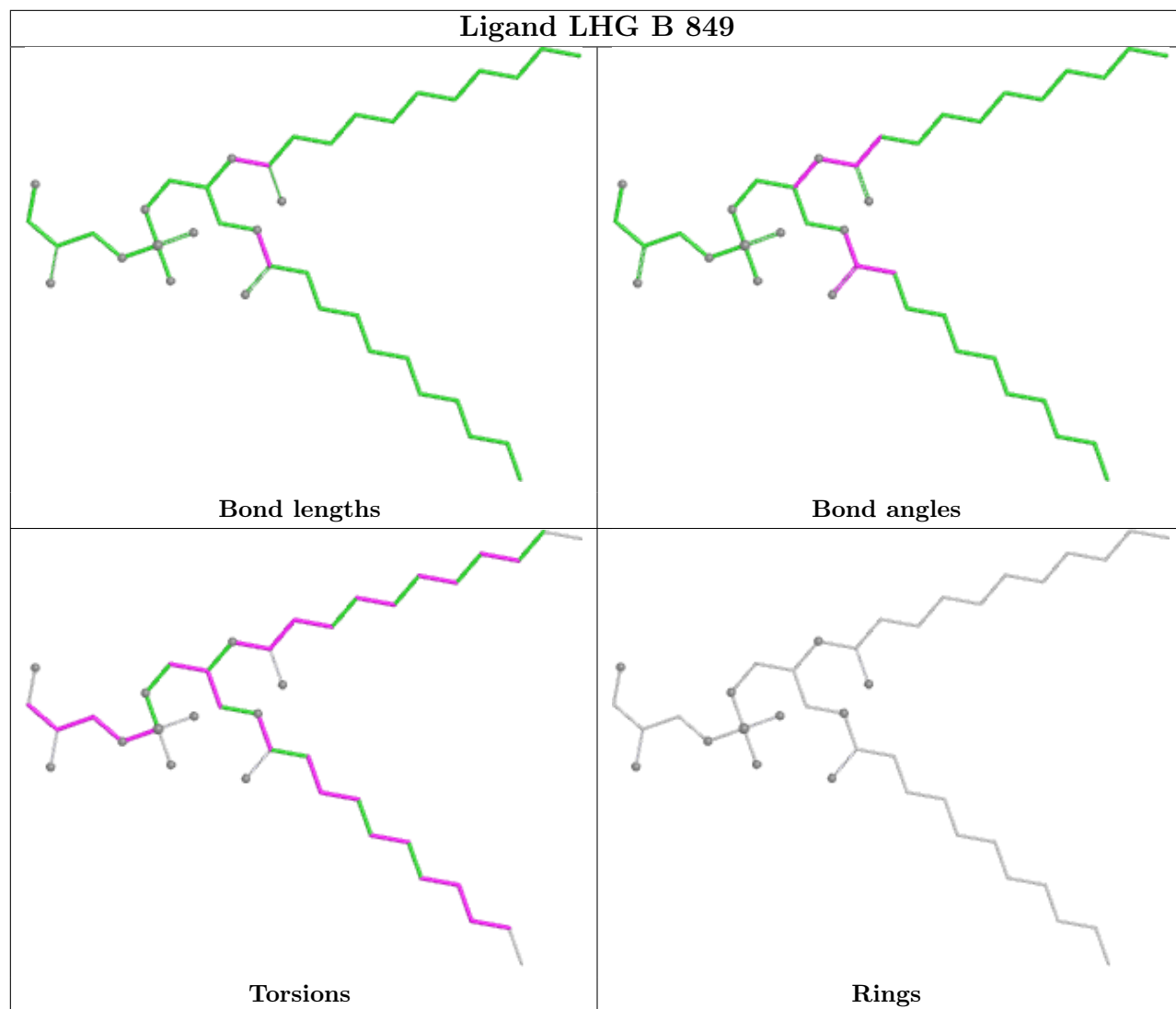
Ligand CLA G 827

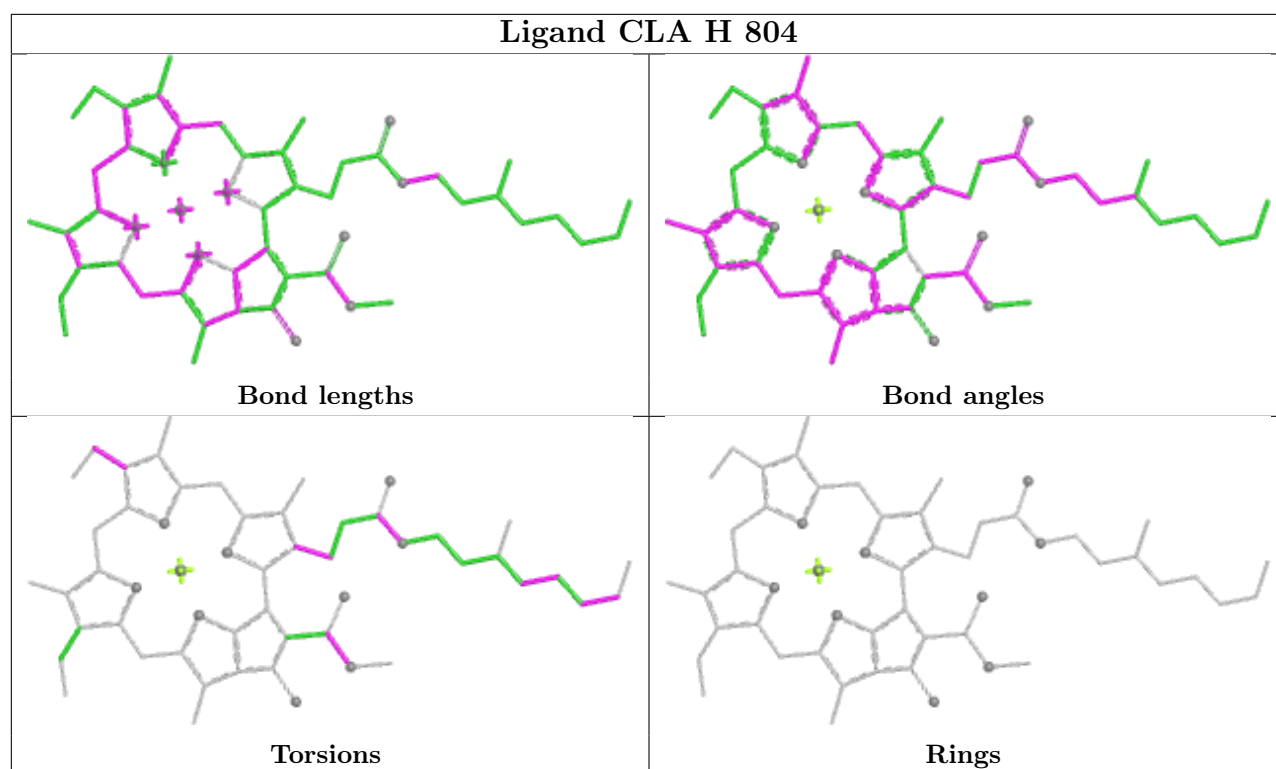




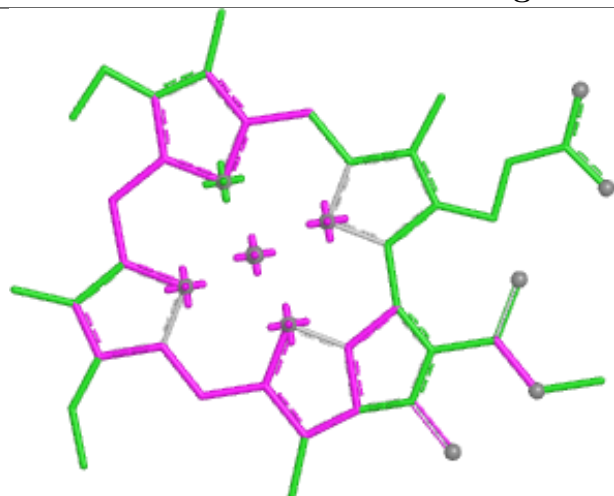




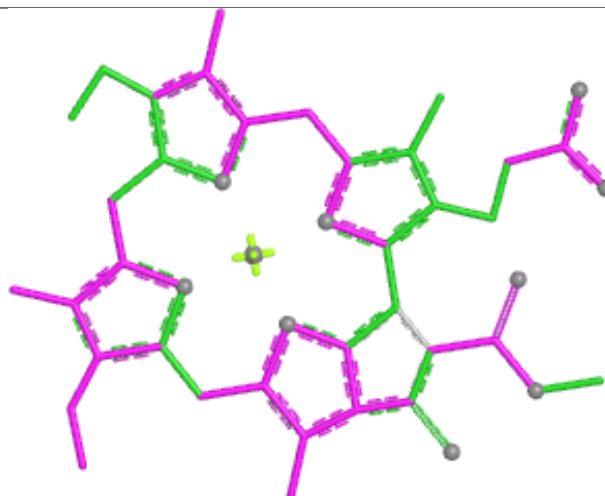




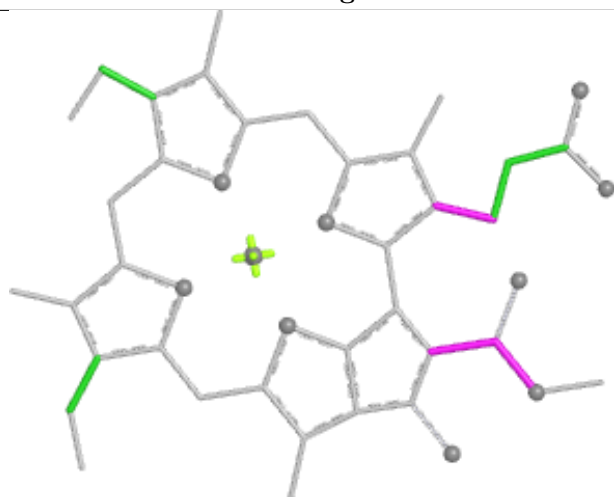
Ligand CLA H 833



Bond lengths



Bond angles

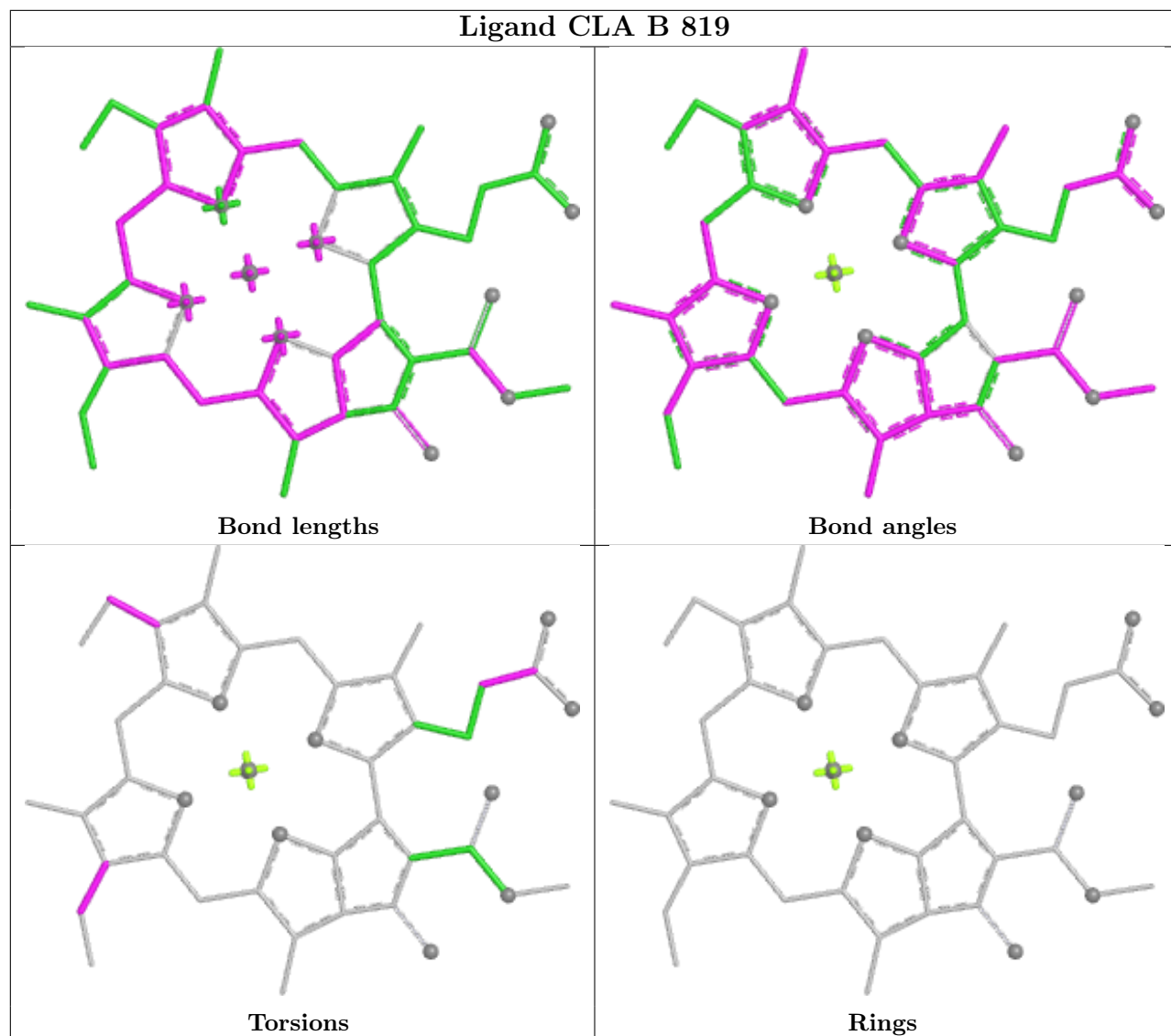


Torsions

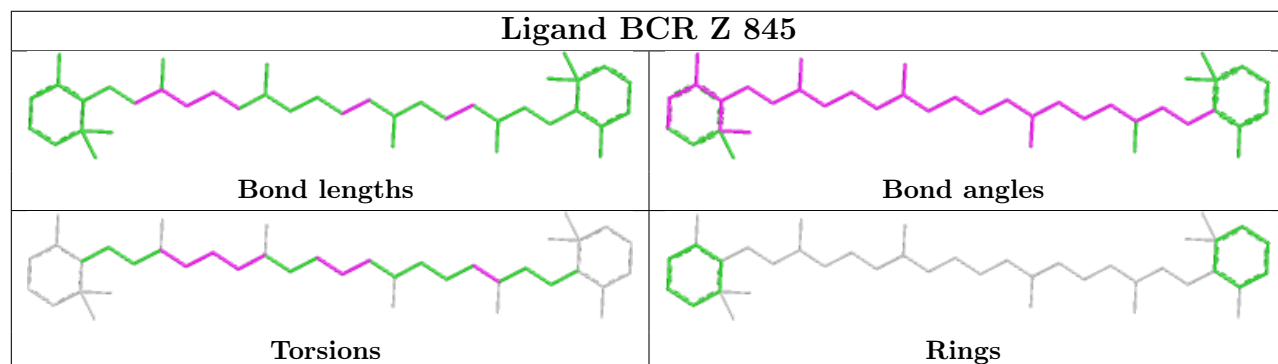


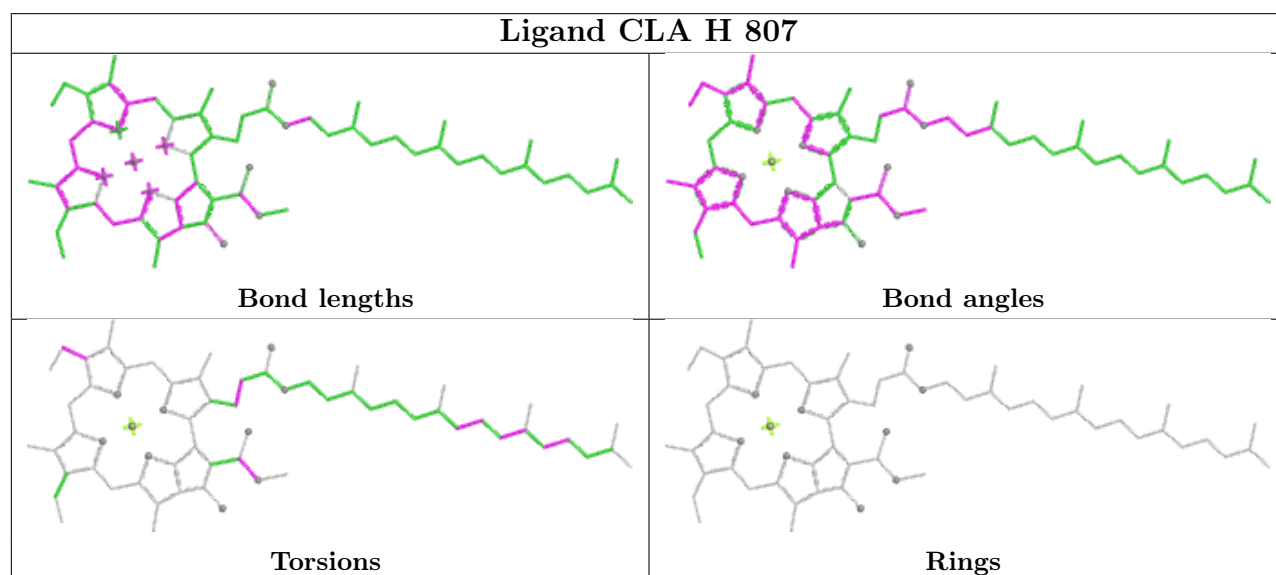
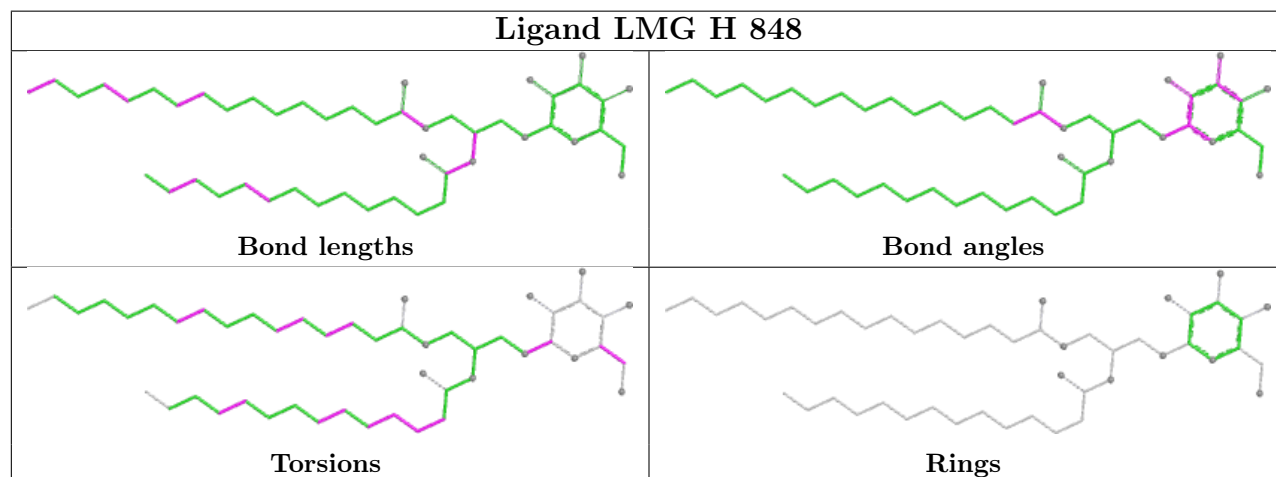
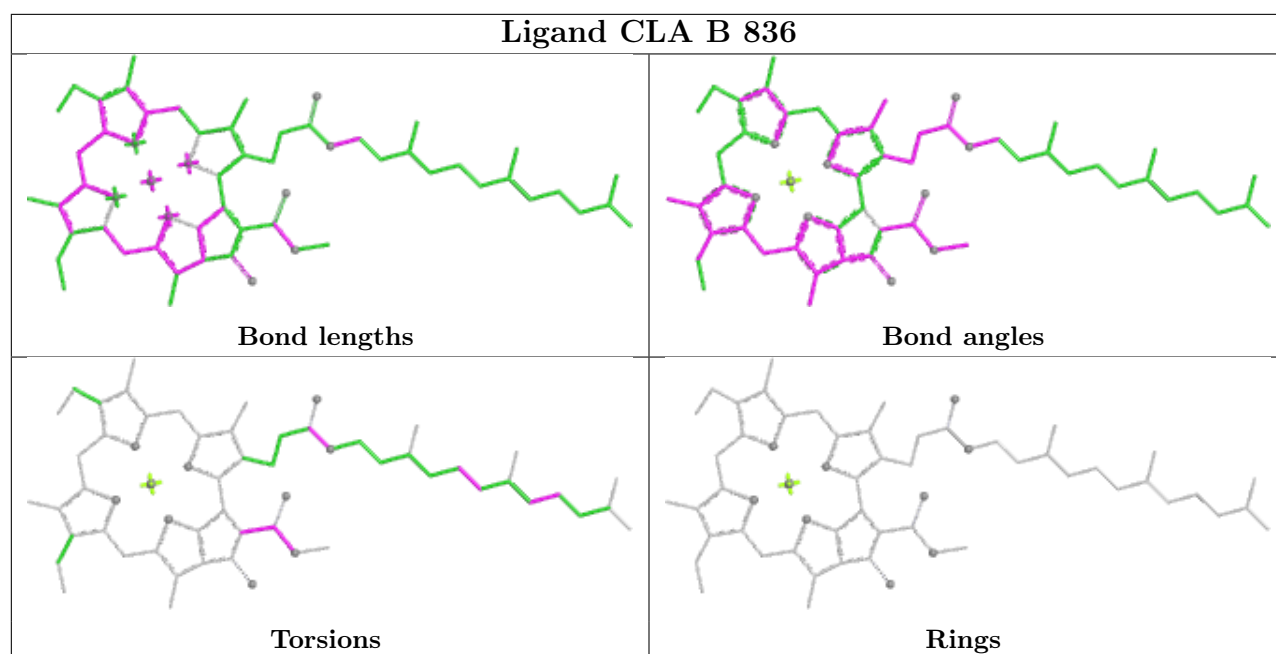
Rings

Ligand CLA B 819

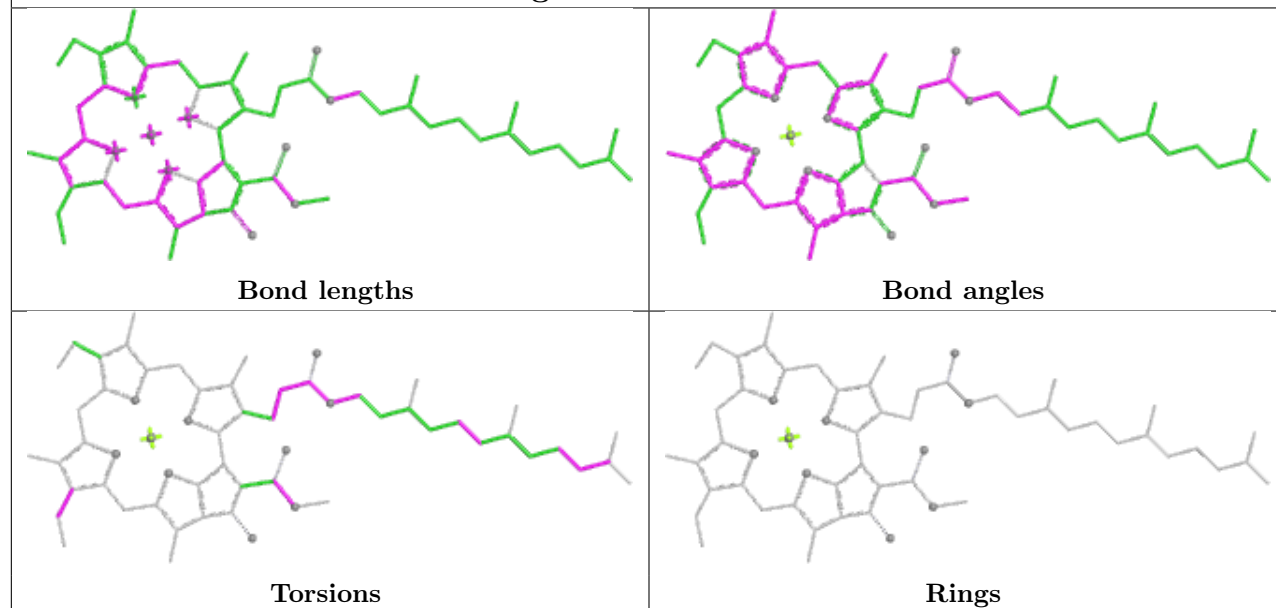


Ligand BCR Z 845

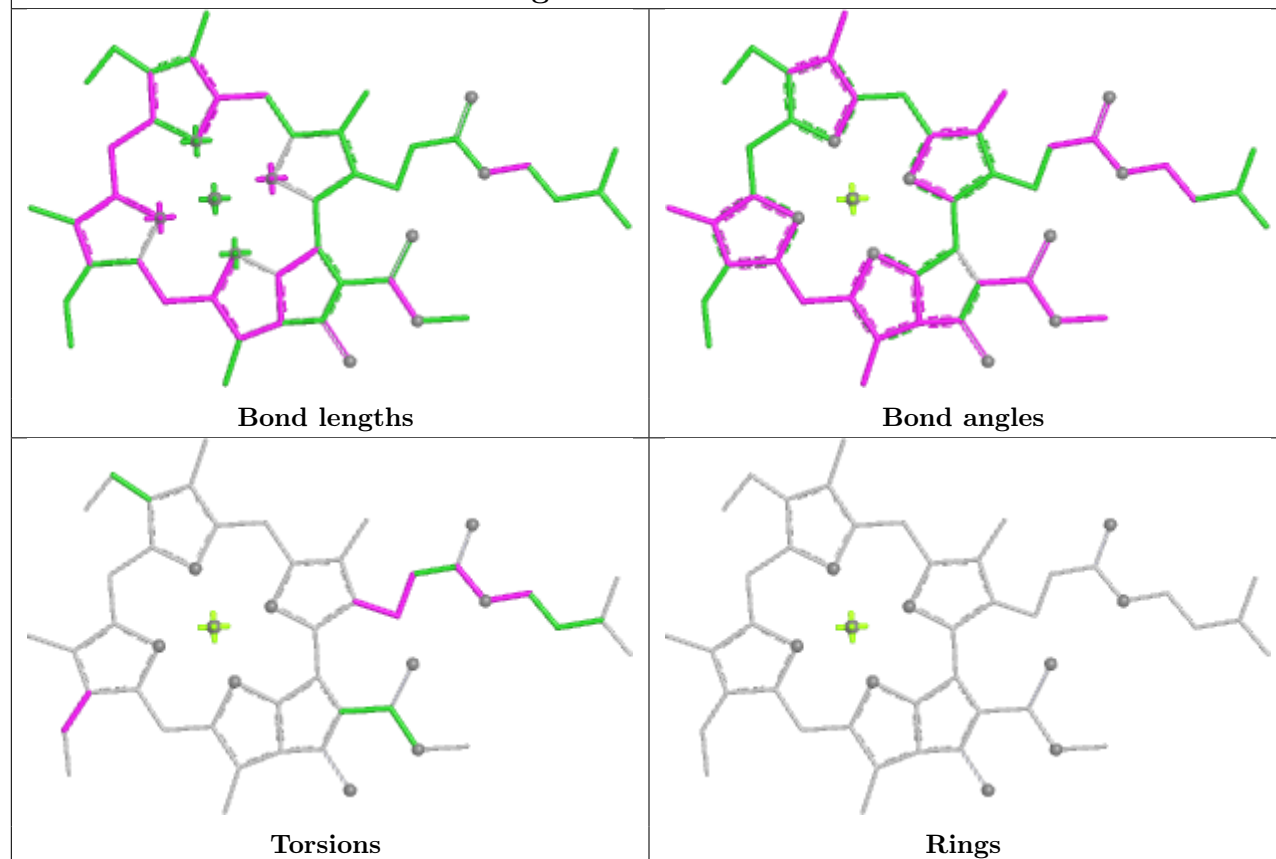




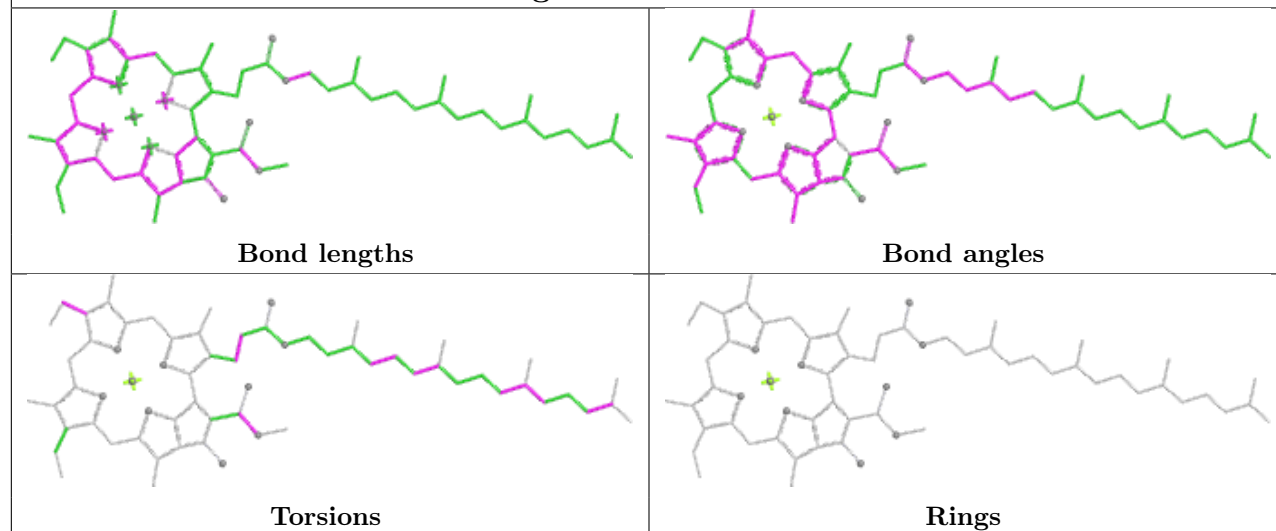
Ligand CLA A 825



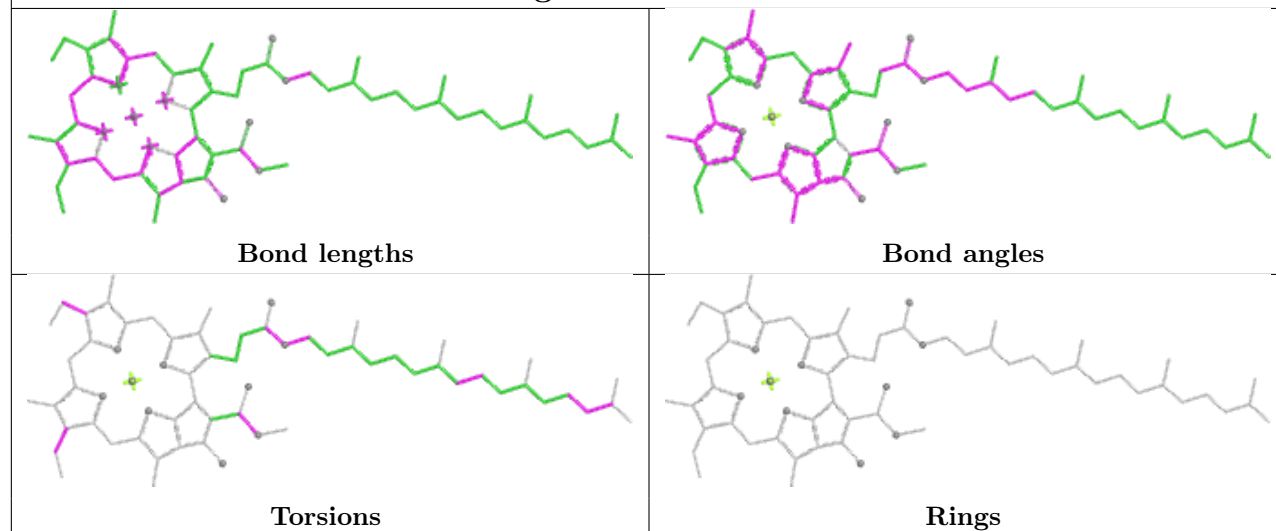
Ligand CLA Y 835



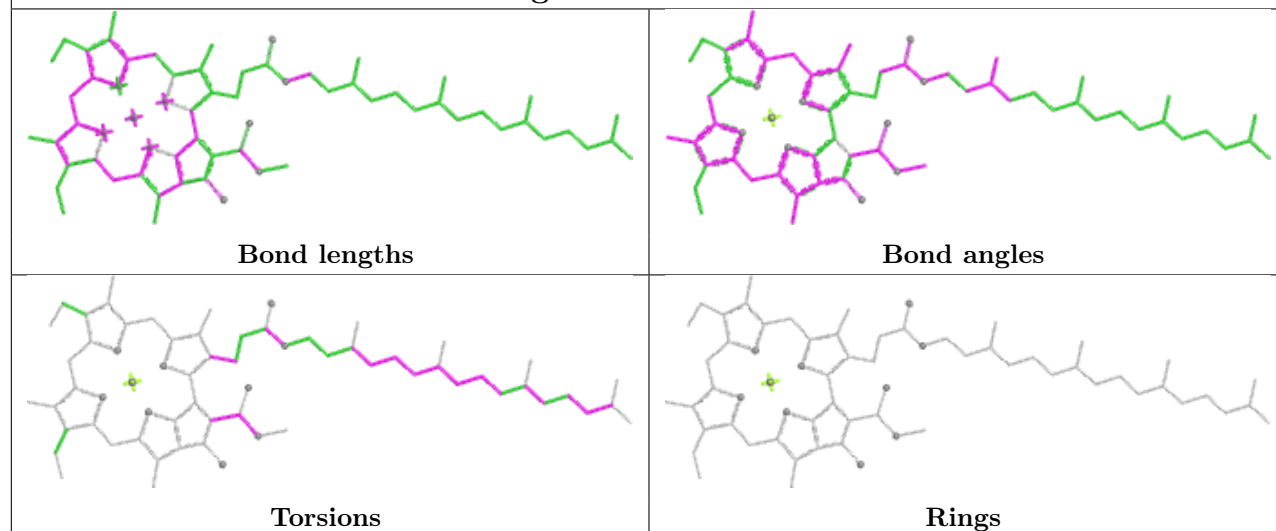
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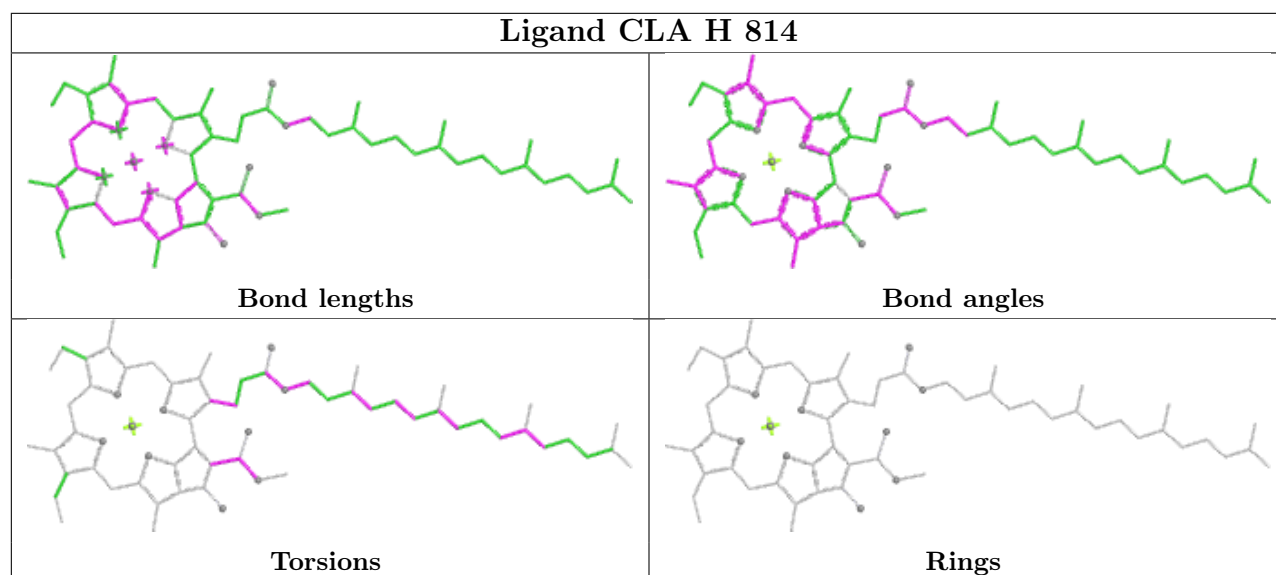
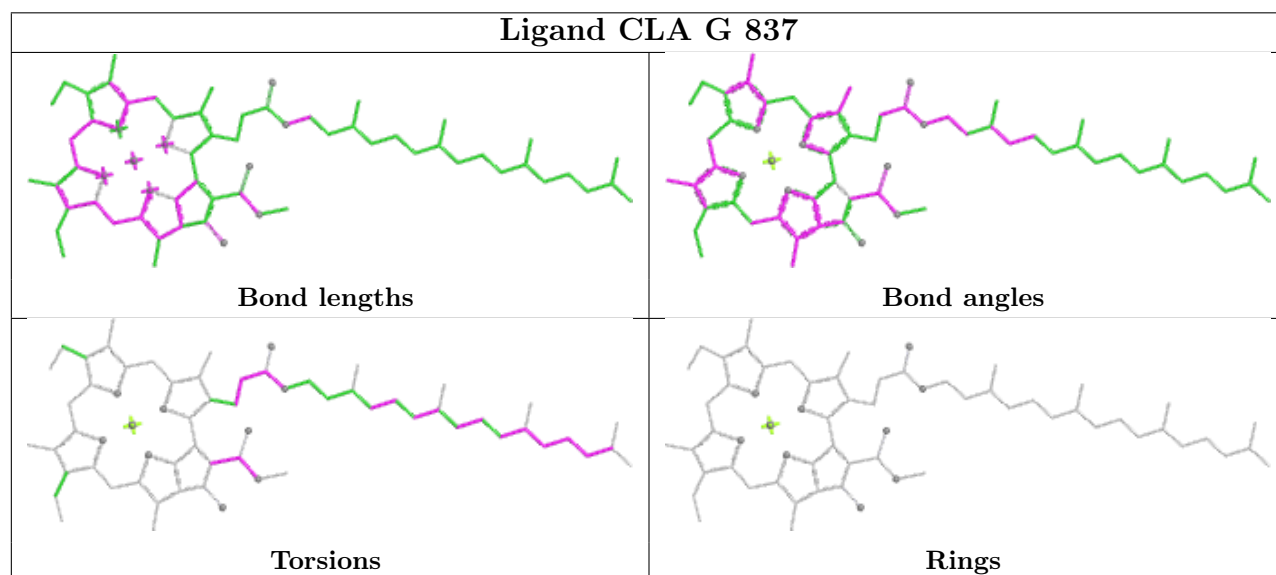
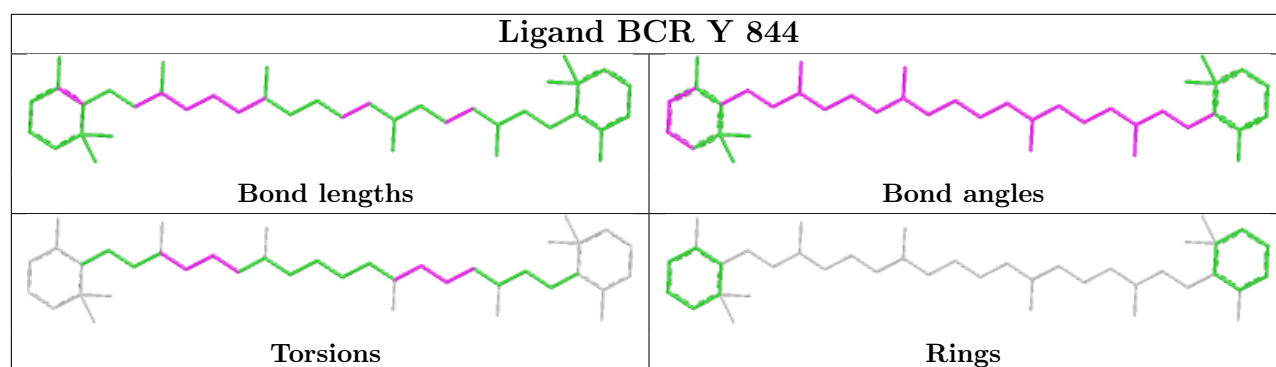


Ligand CLA Z 841

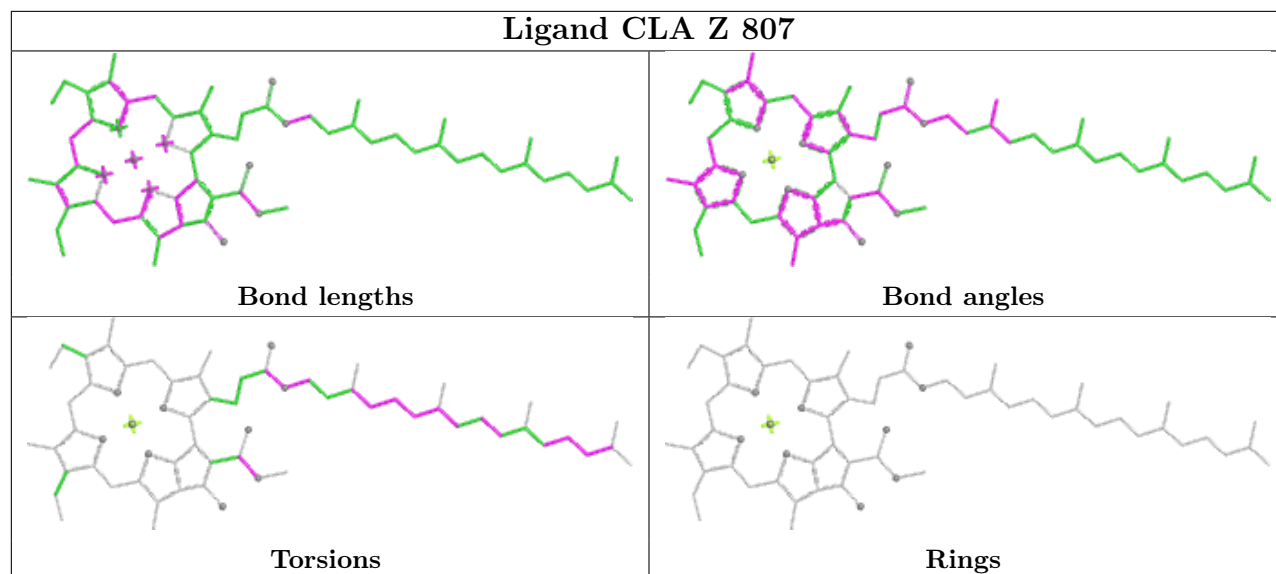


Ligand CLA H 825

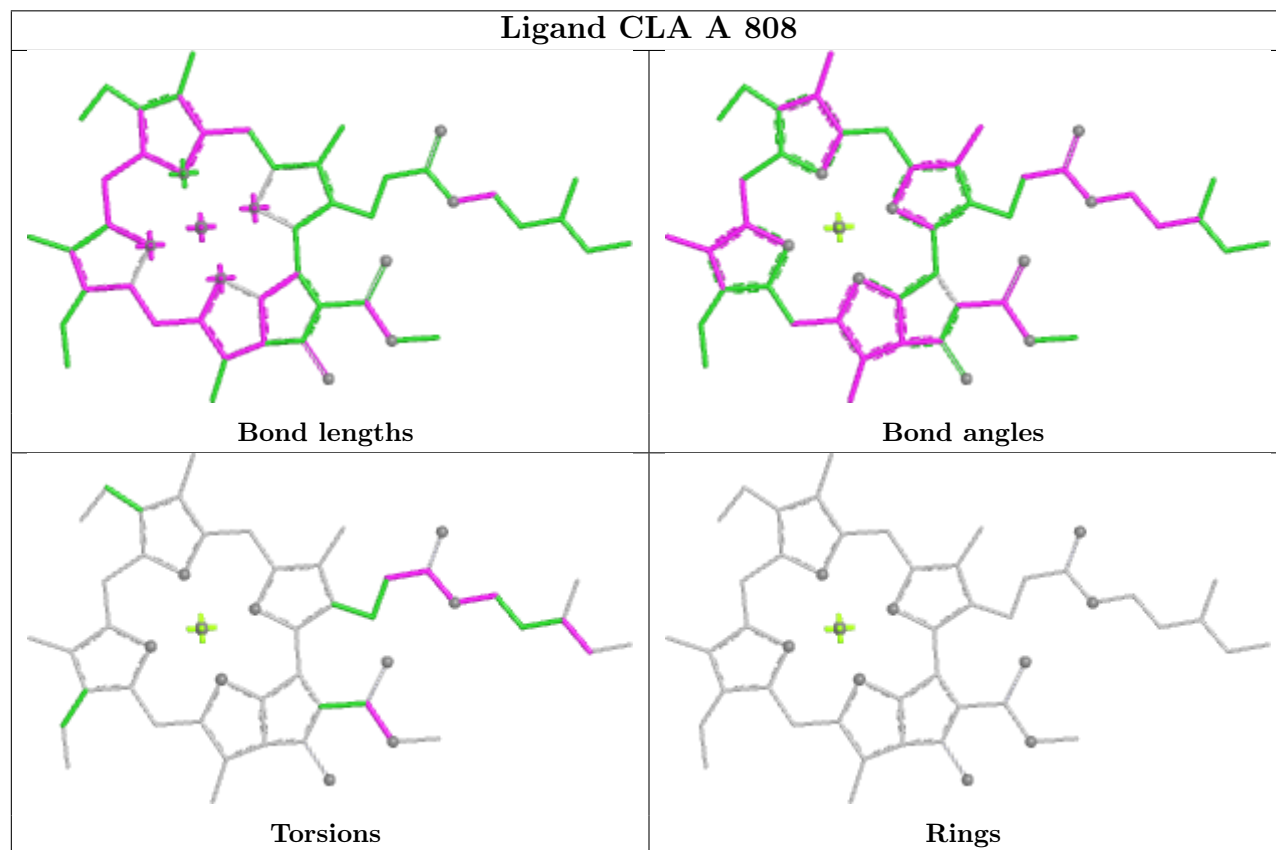


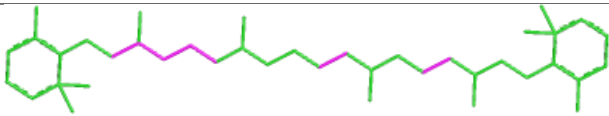
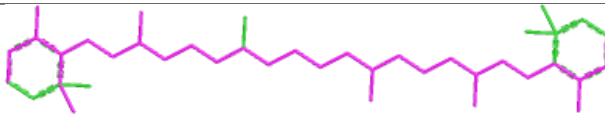
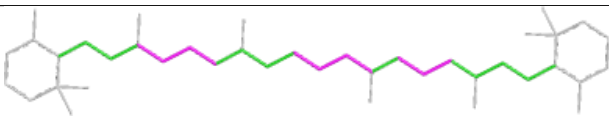
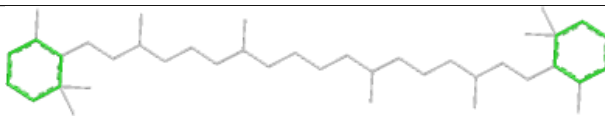


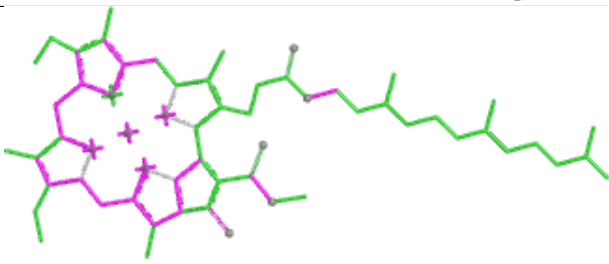
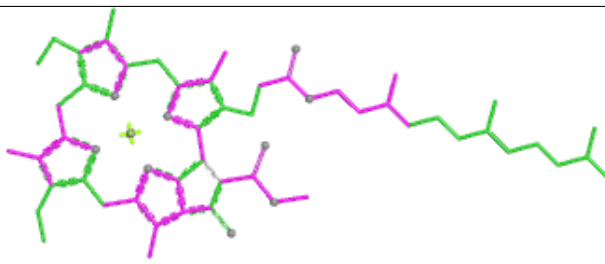
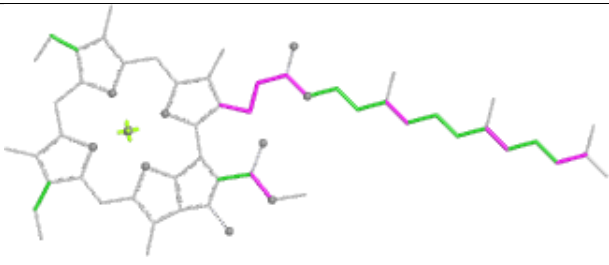
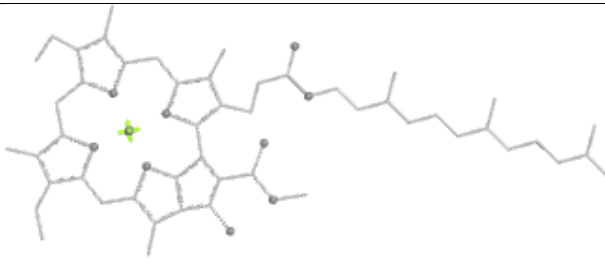
Ligand CLA Z 807

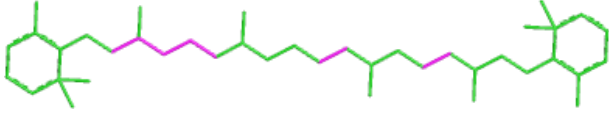
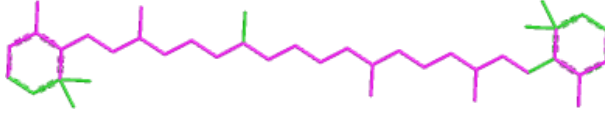
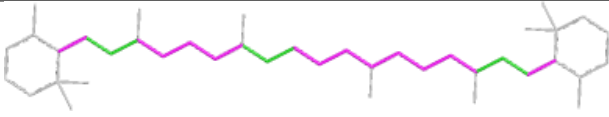
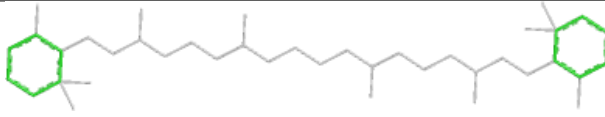


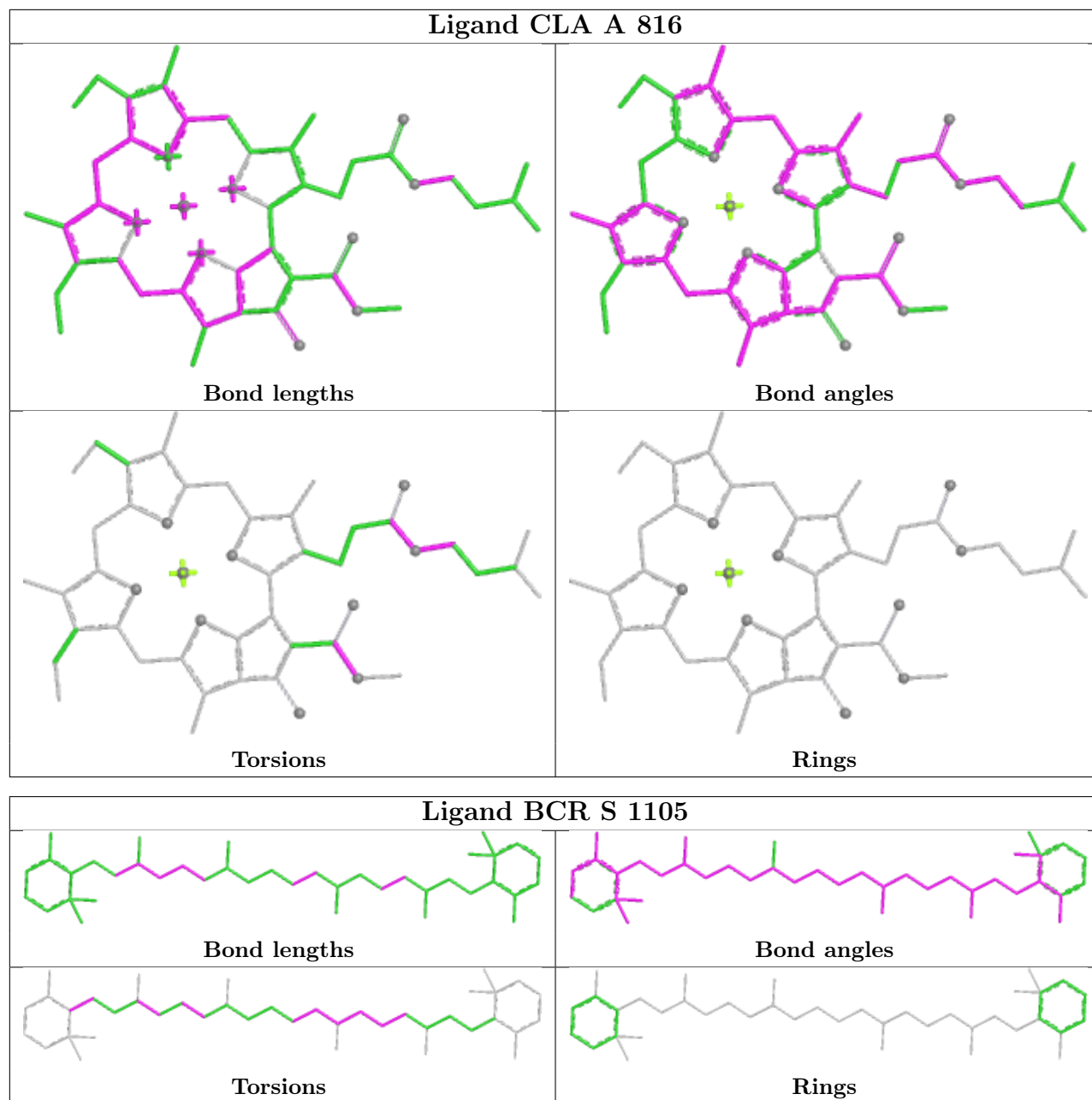
Ligand CLA A 808

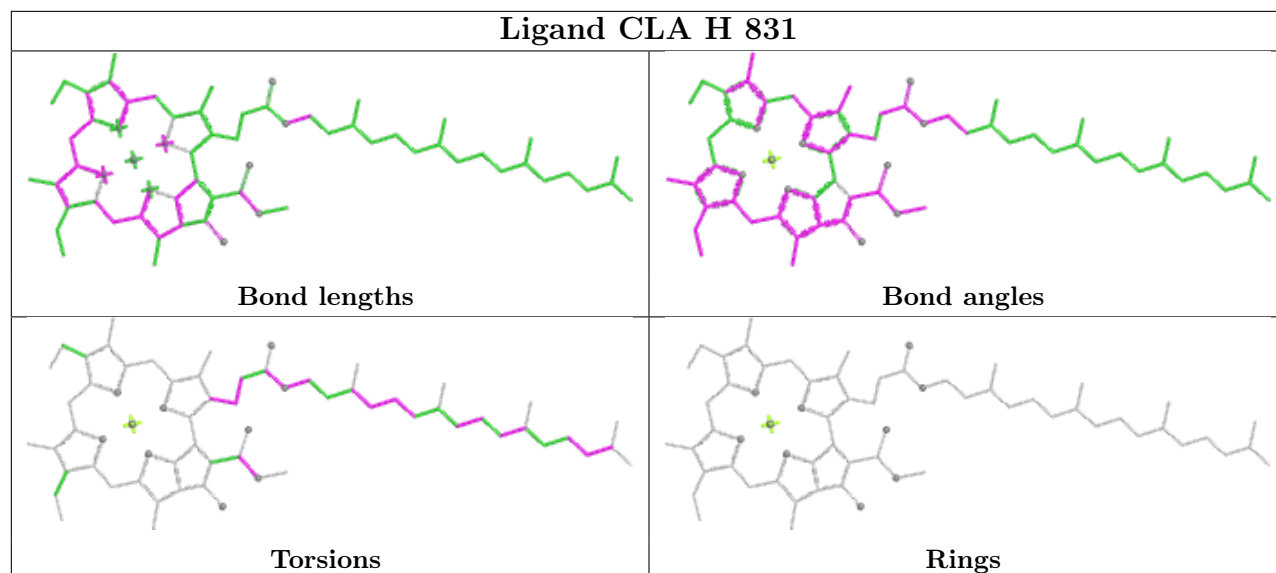
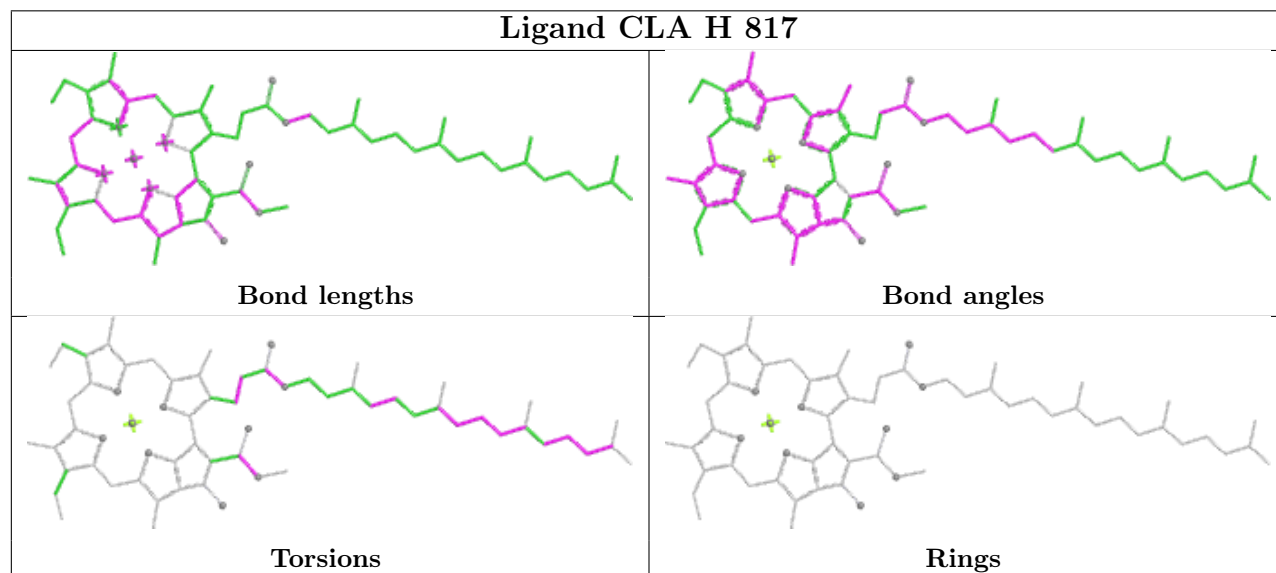
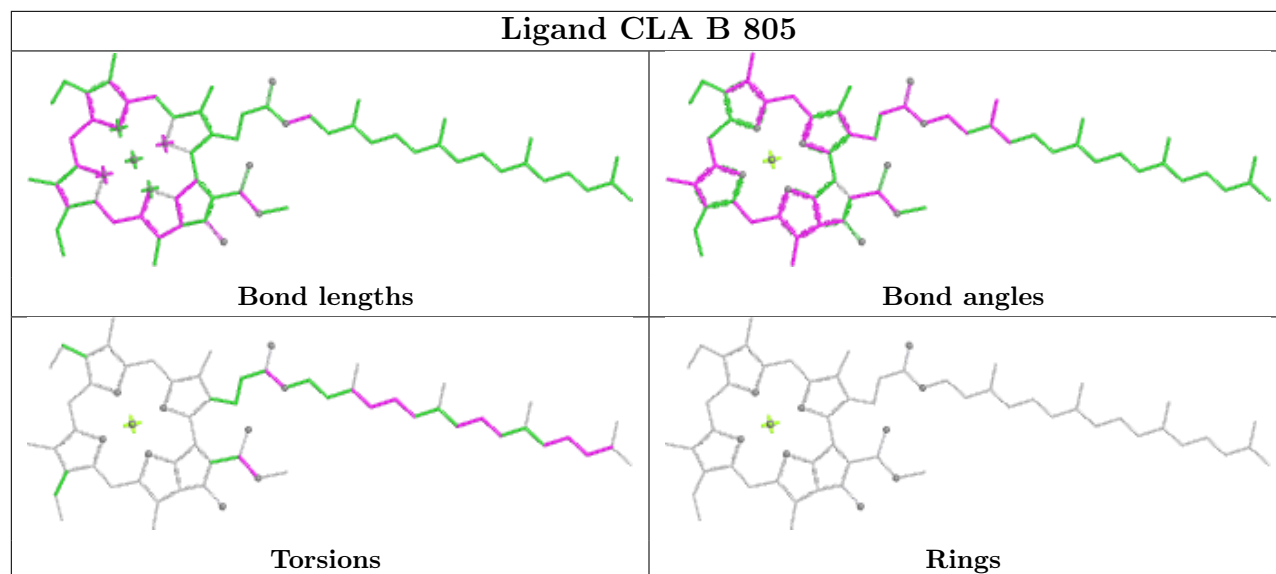


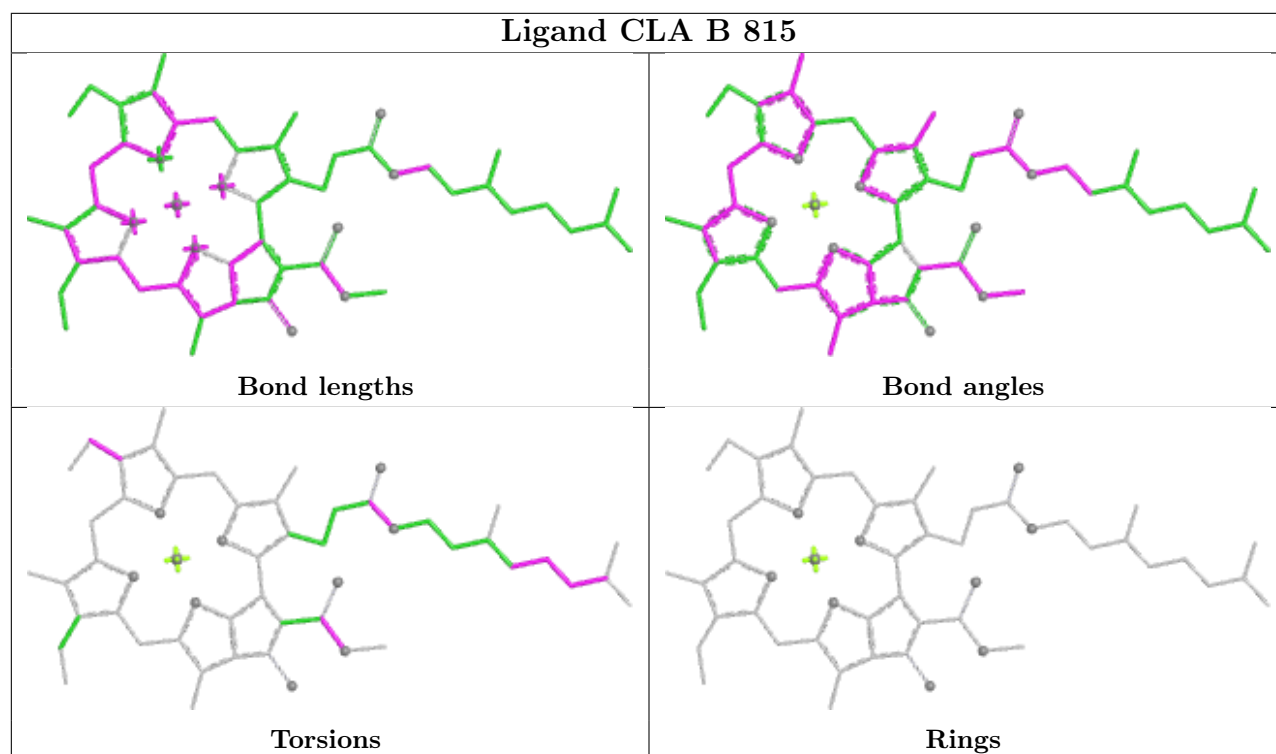
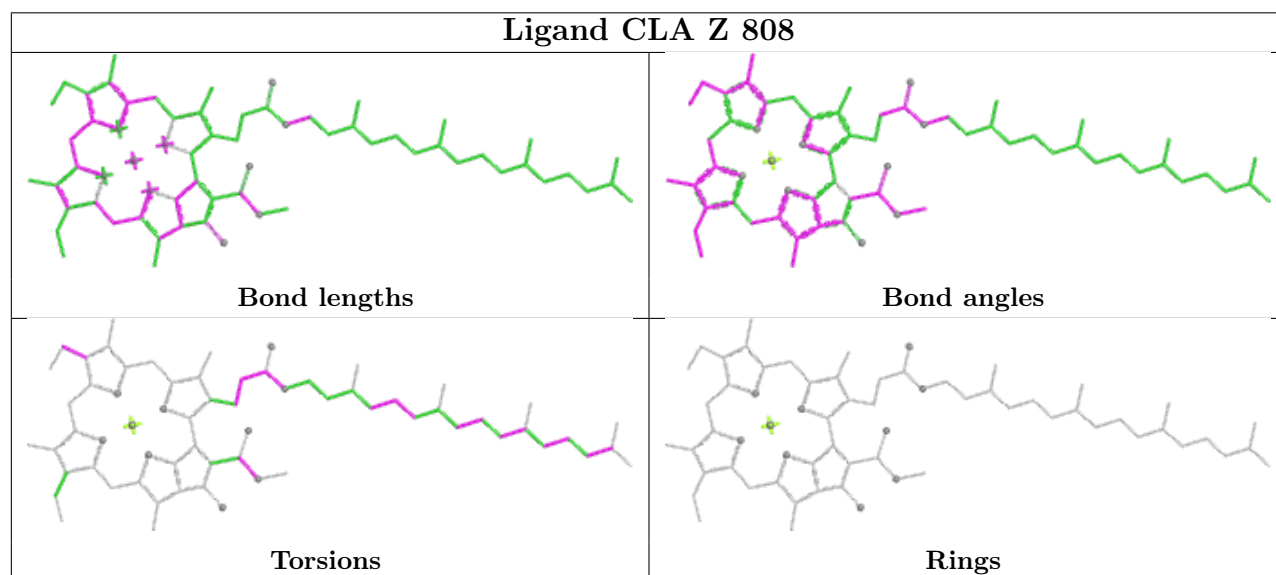
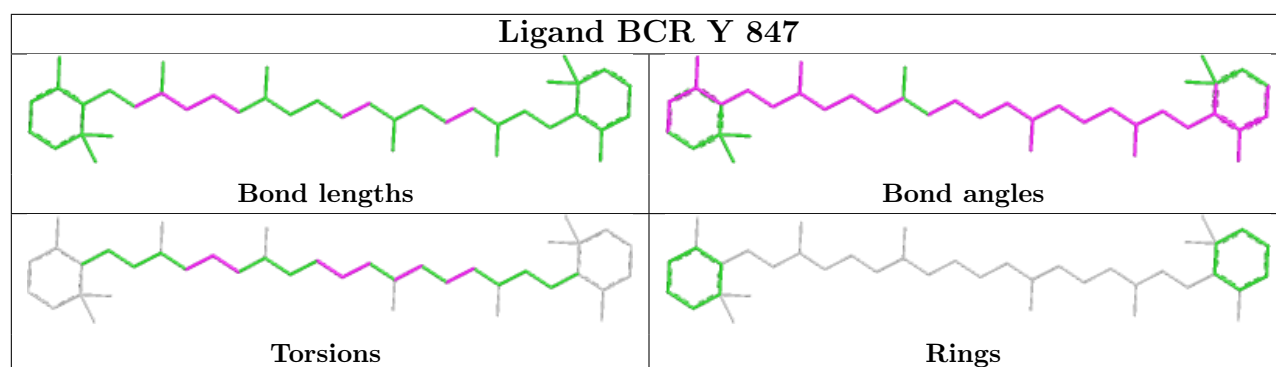
Ligand BCR G 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

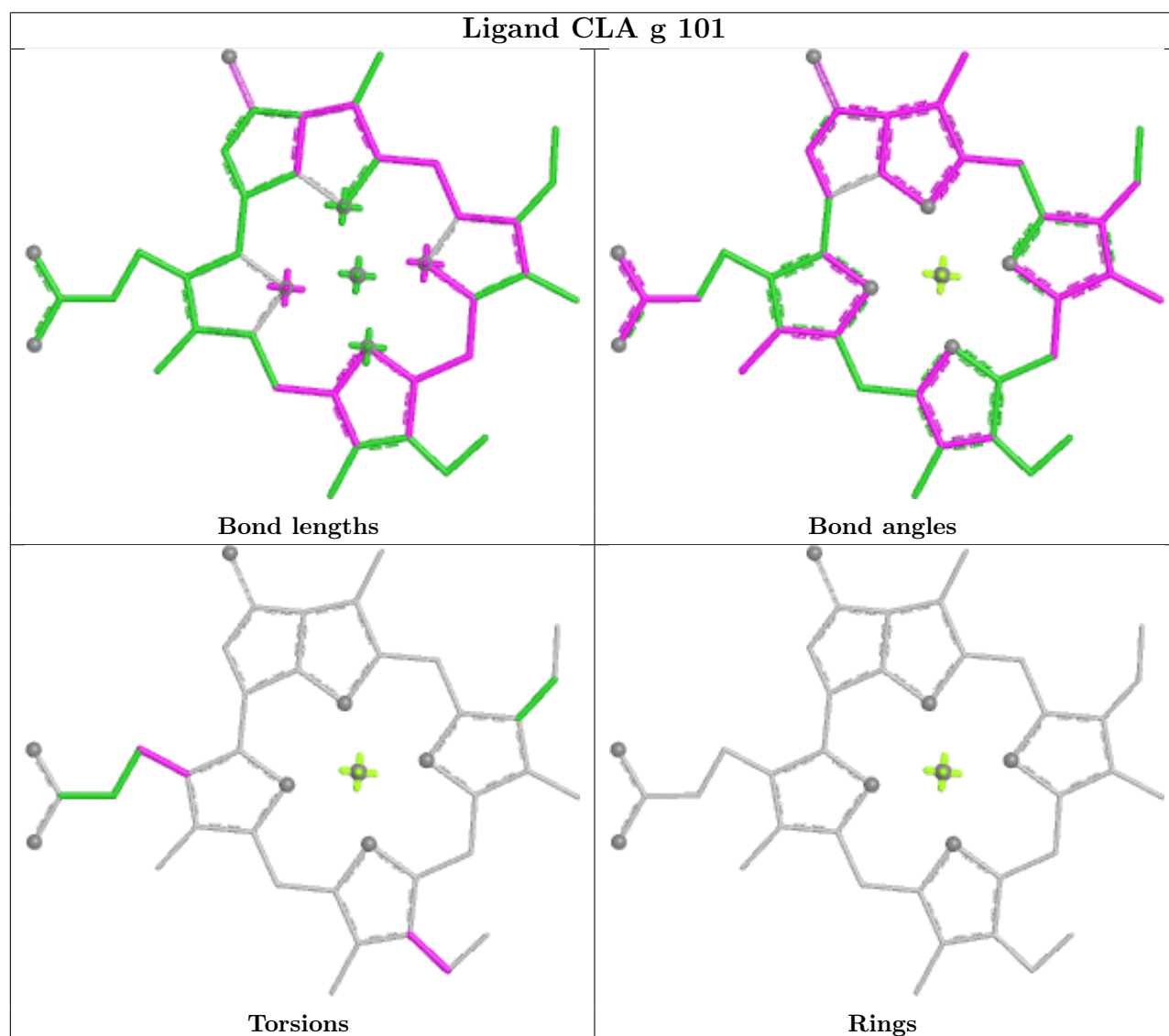
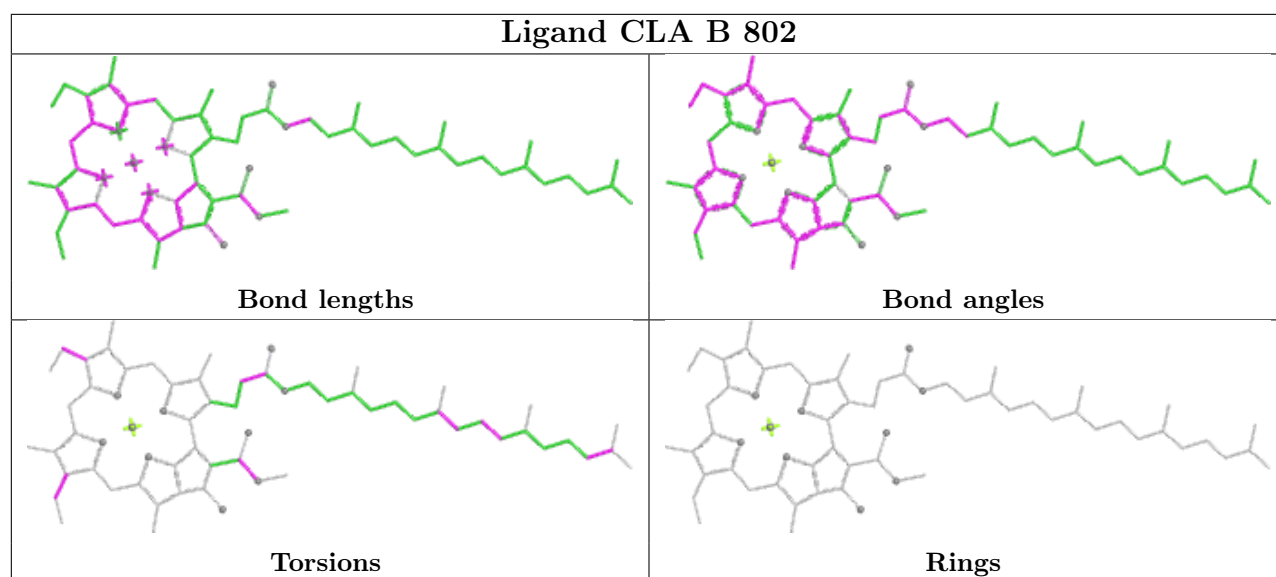
Ligand CLA A 821	
	
Bond lengths	Bond angles
	
Torsions	Rings

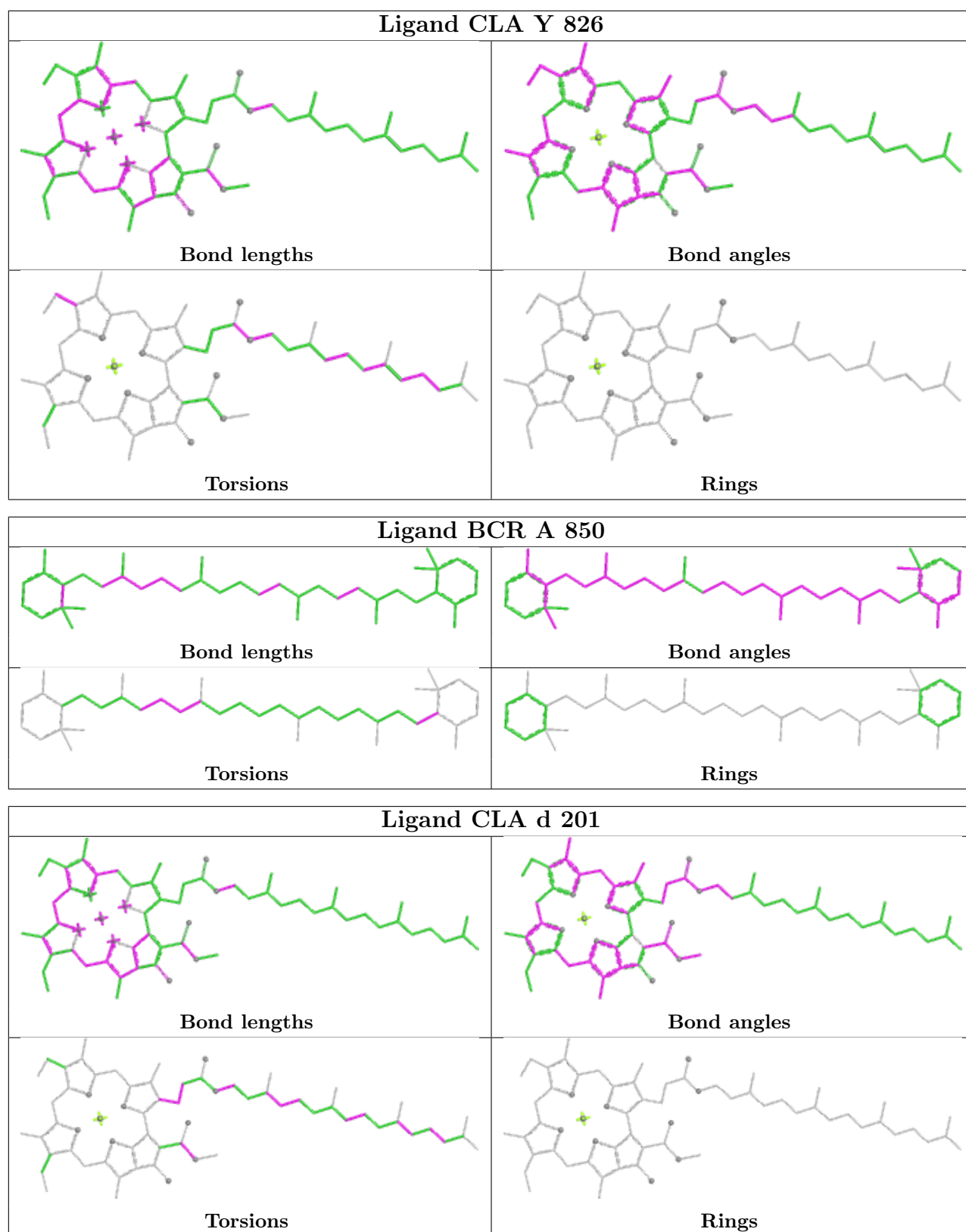
Ligand BCR Y 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

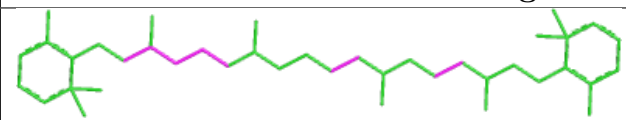
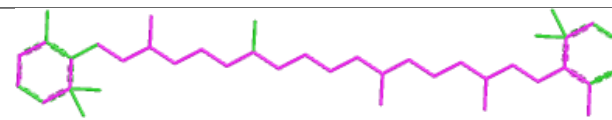
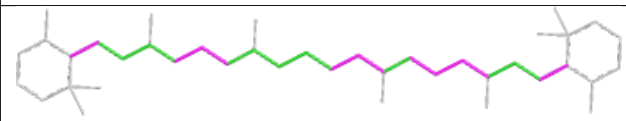
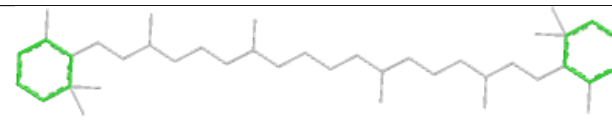


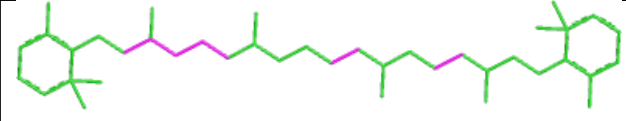
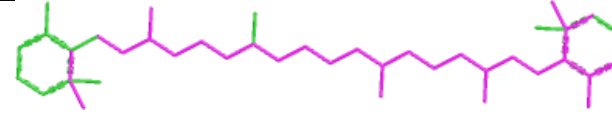
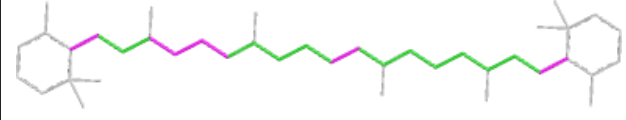
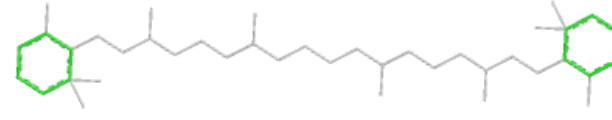


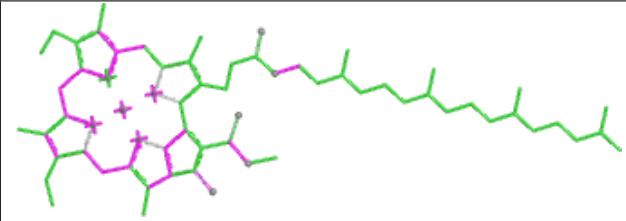
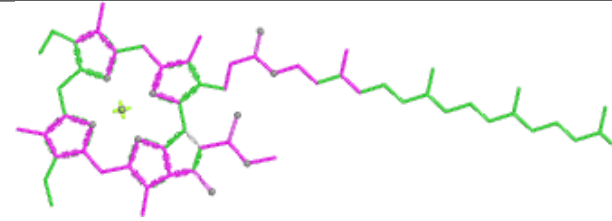
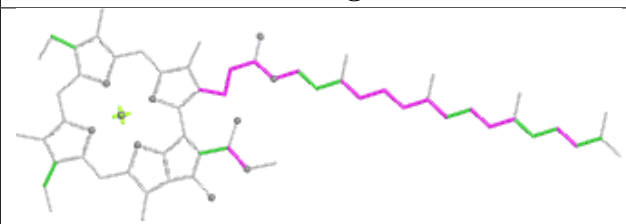
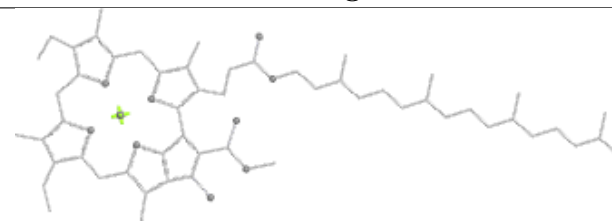




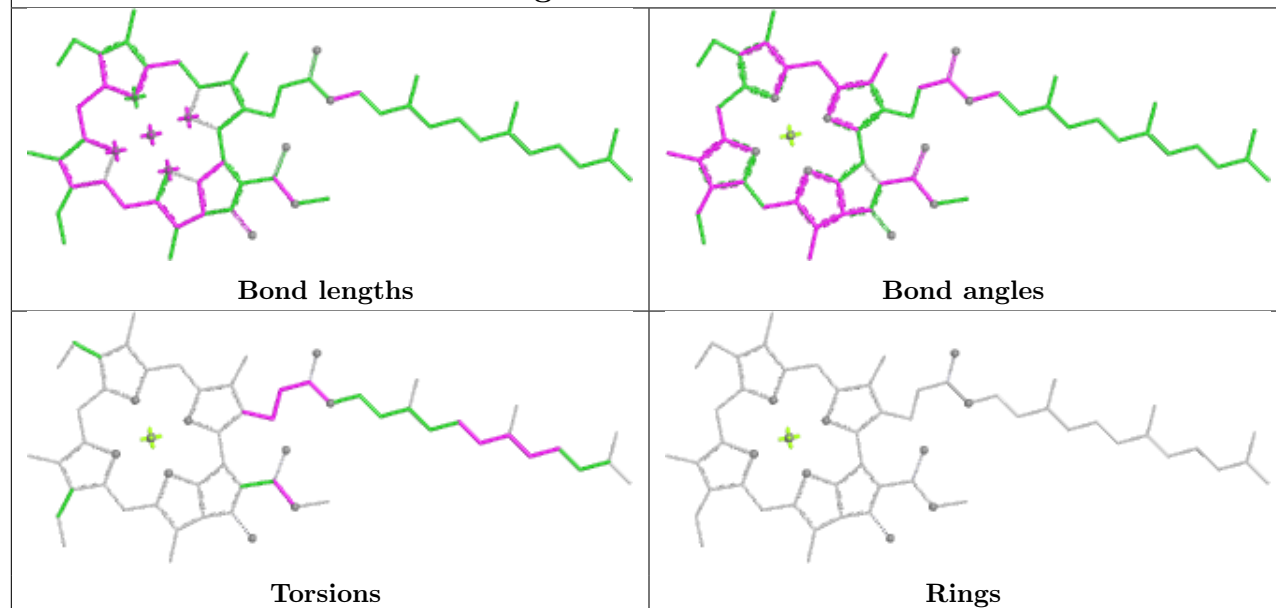


Ligand BCR R 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

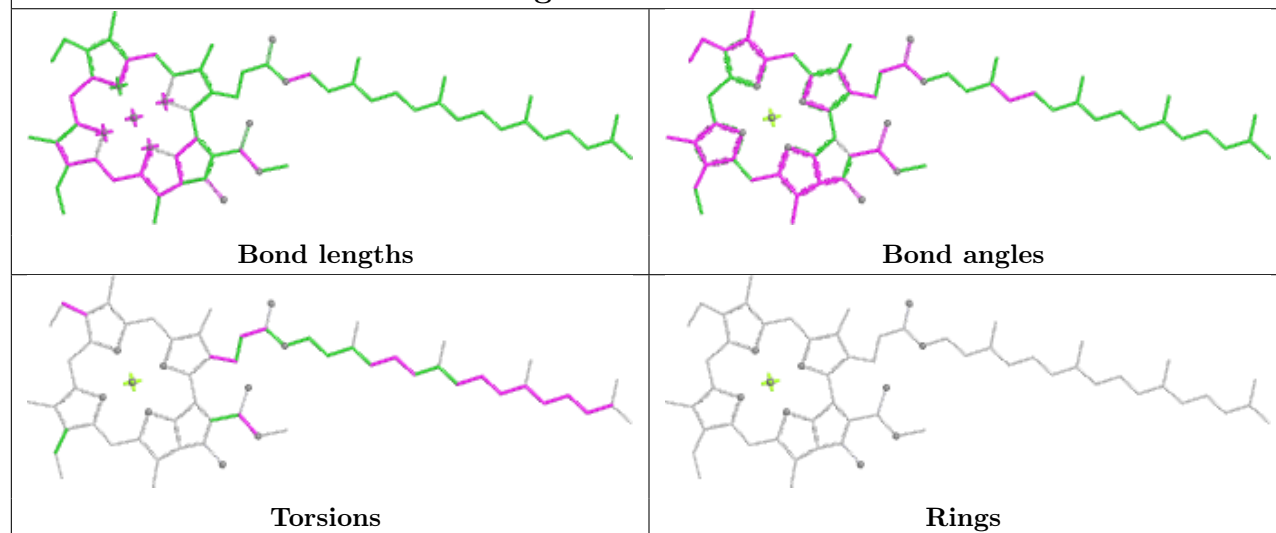
Ligand BCR S 1104	
	
Bond lengths	Bond angles
	
Torsions	Rings

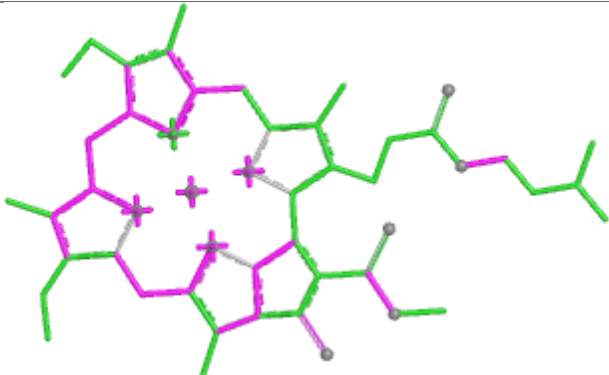
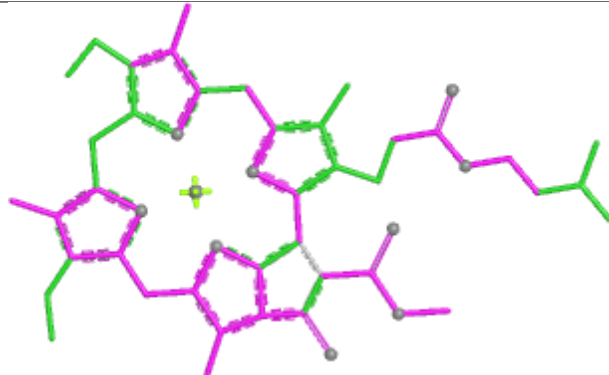
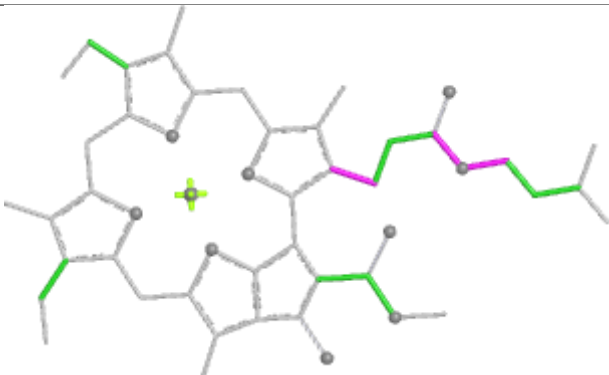
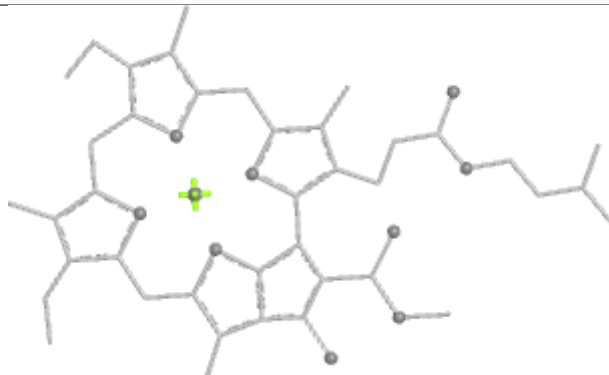
Ligand CLA A 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

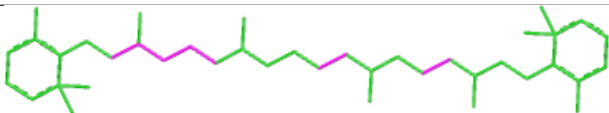
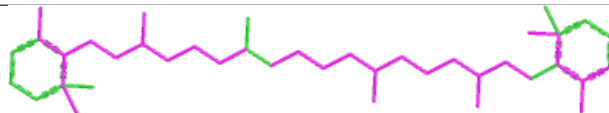
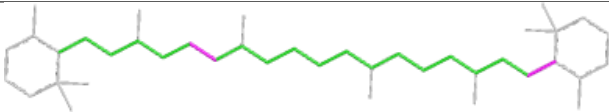
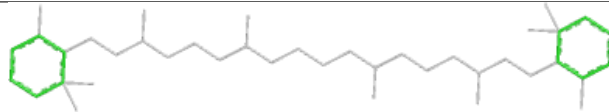
Ligand CLA Z 819

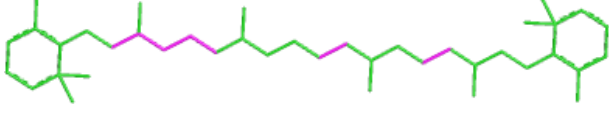
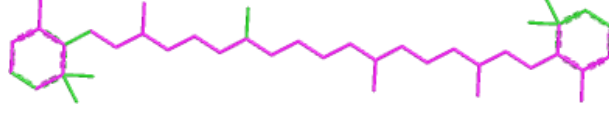
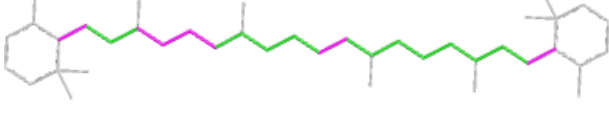
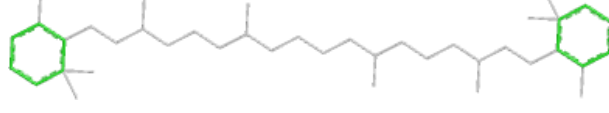


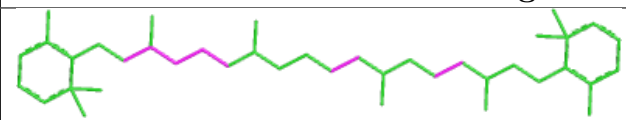
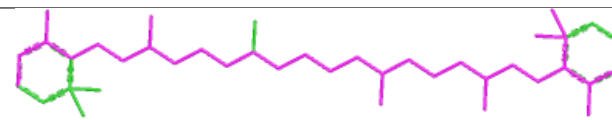
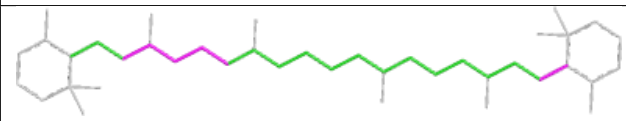
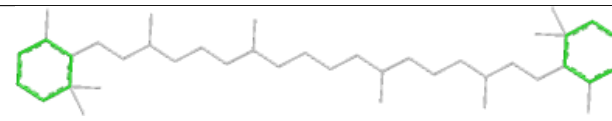
Ligand CLA Z 828

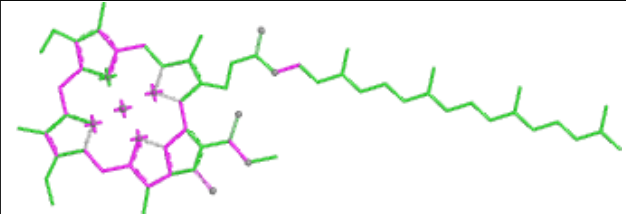
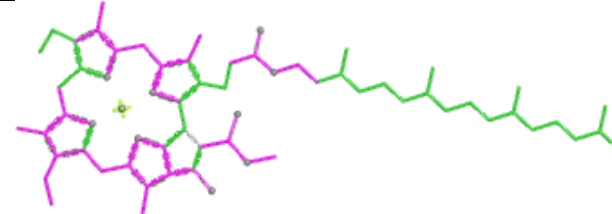
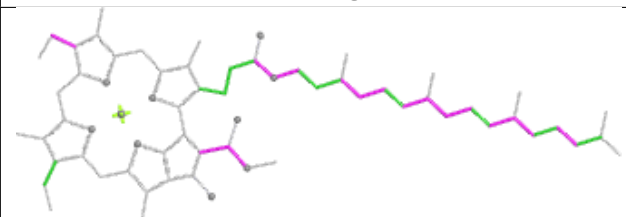
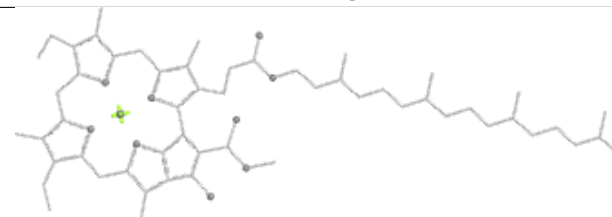


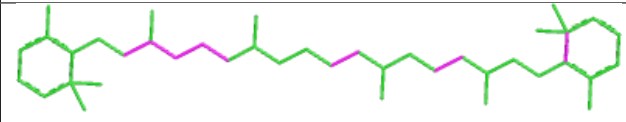
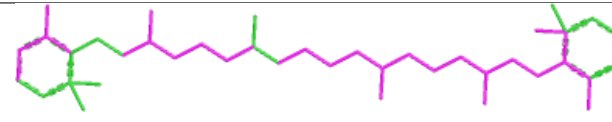
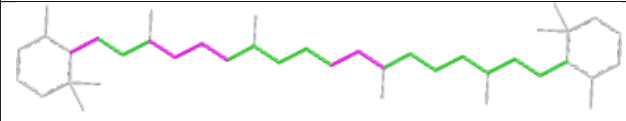
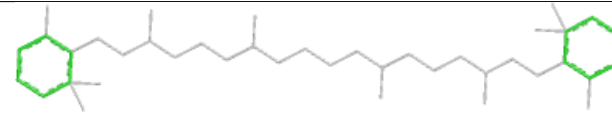
Ligand CLA A 836	
	
Bond lengths	Bond angles
	
Torsions	Rings

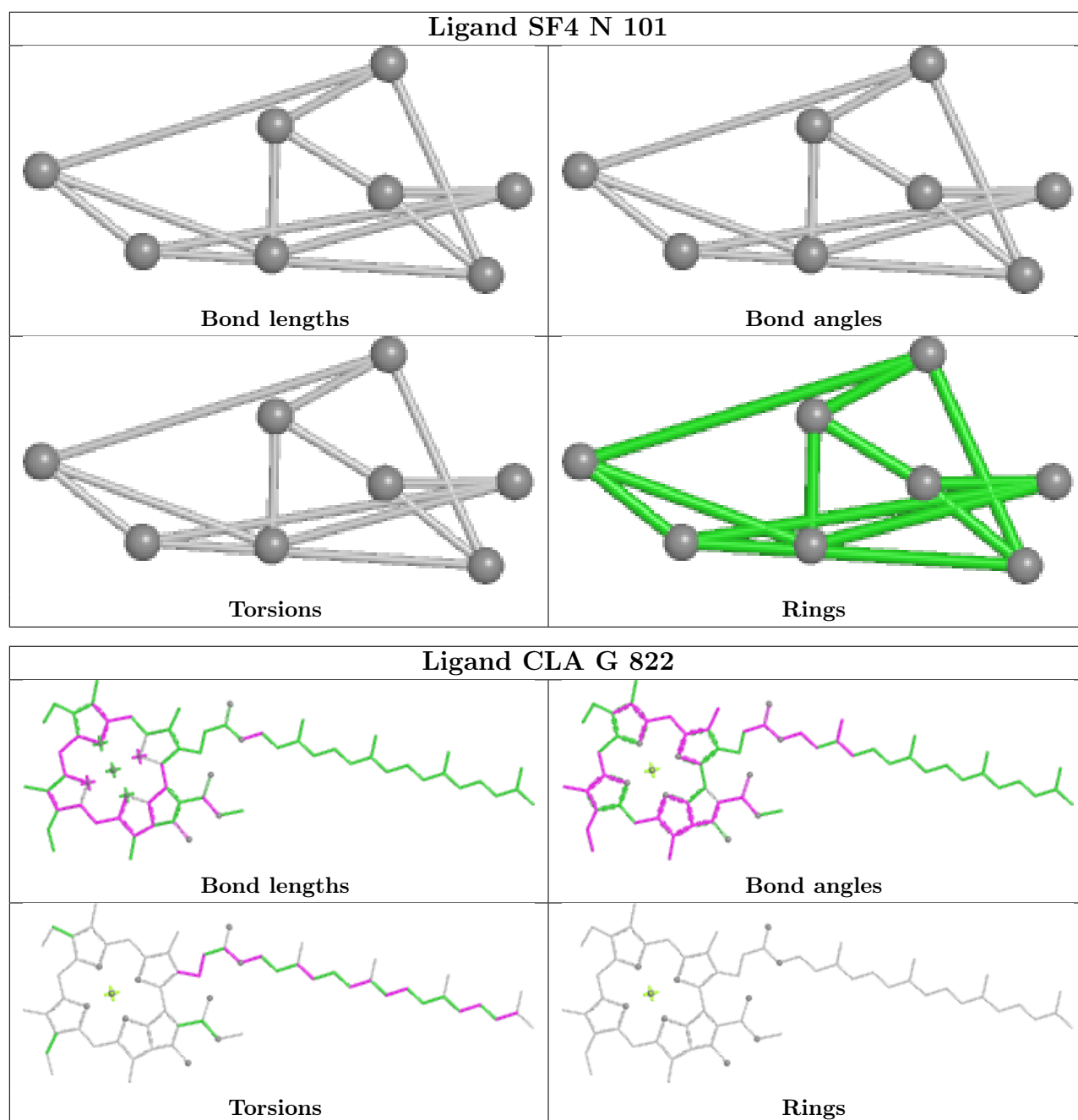
Ligand BCR Y 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

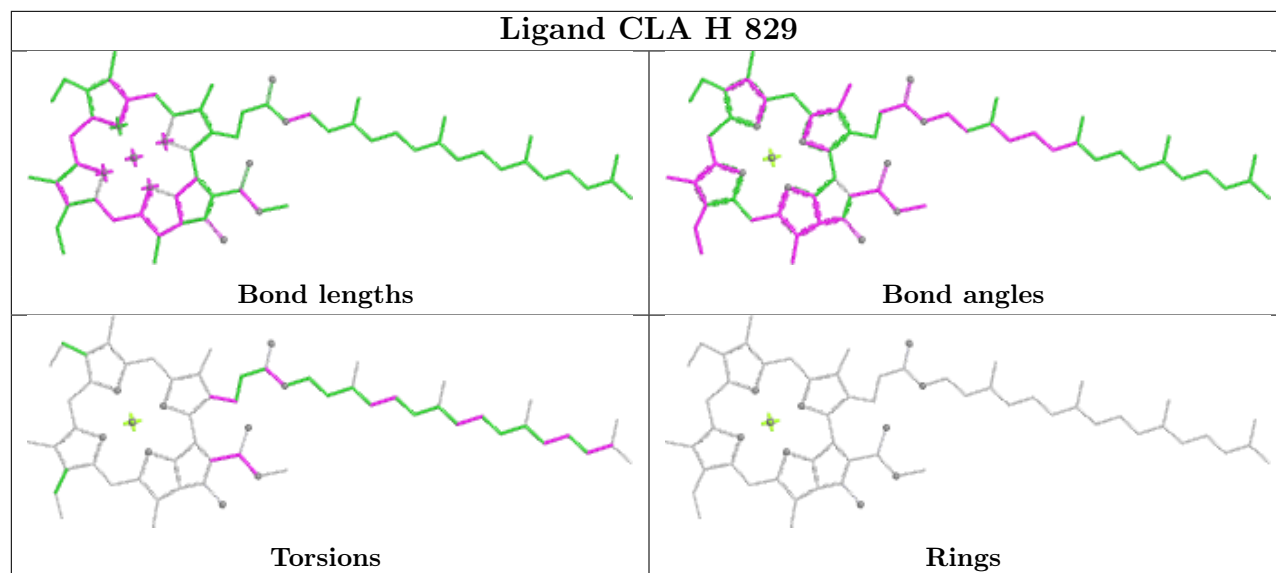
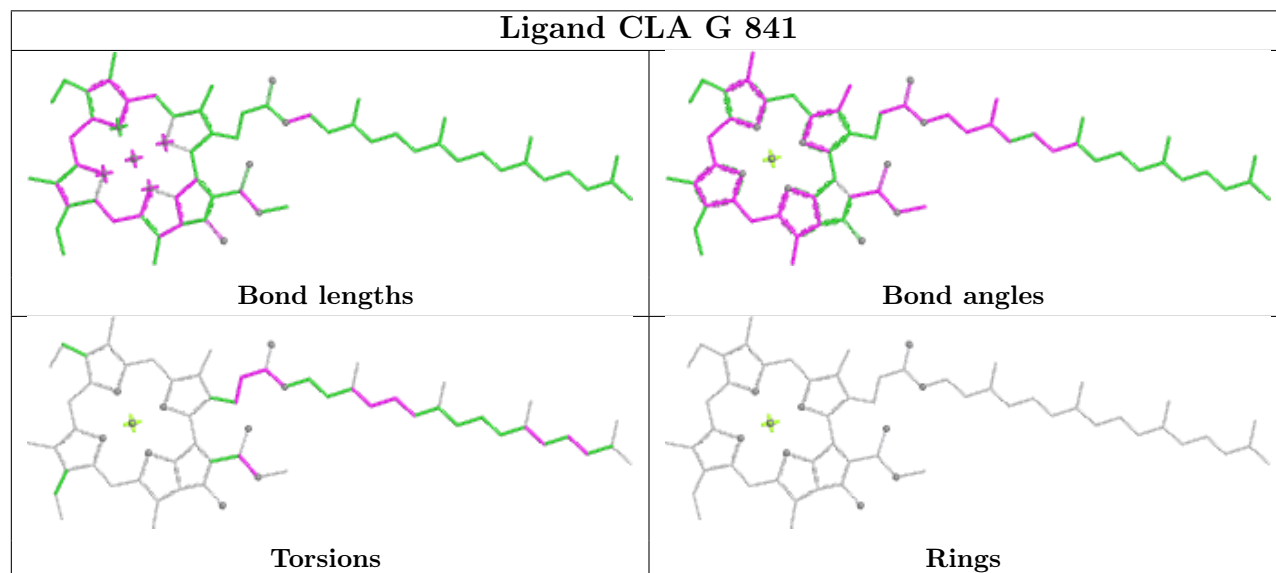
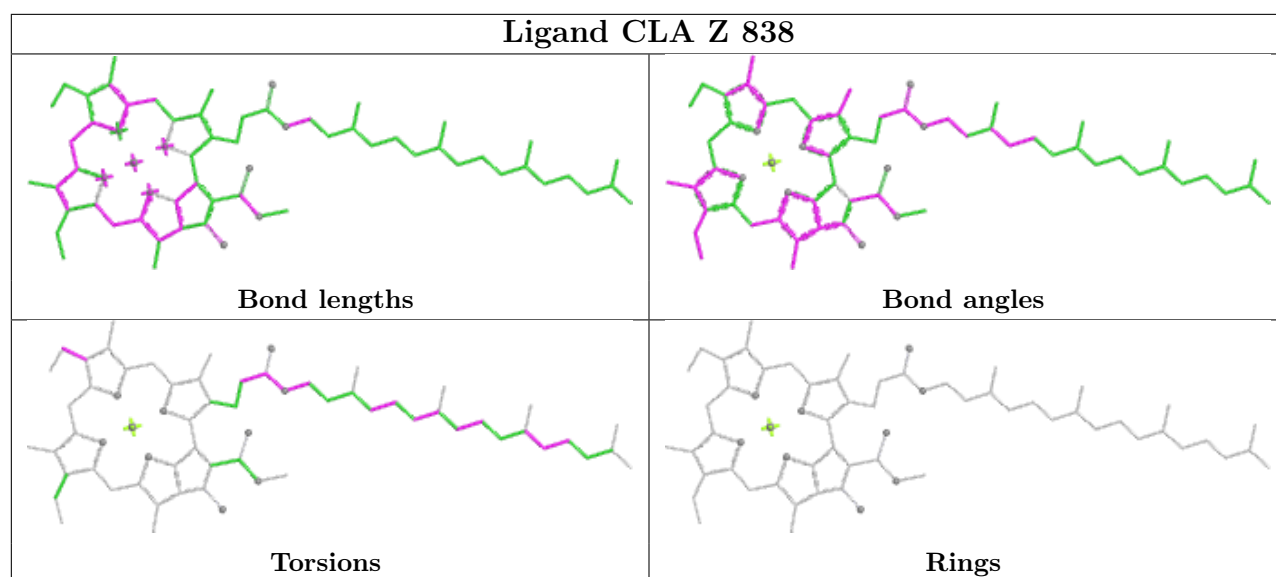
Ligand BCR H 843	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR G 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

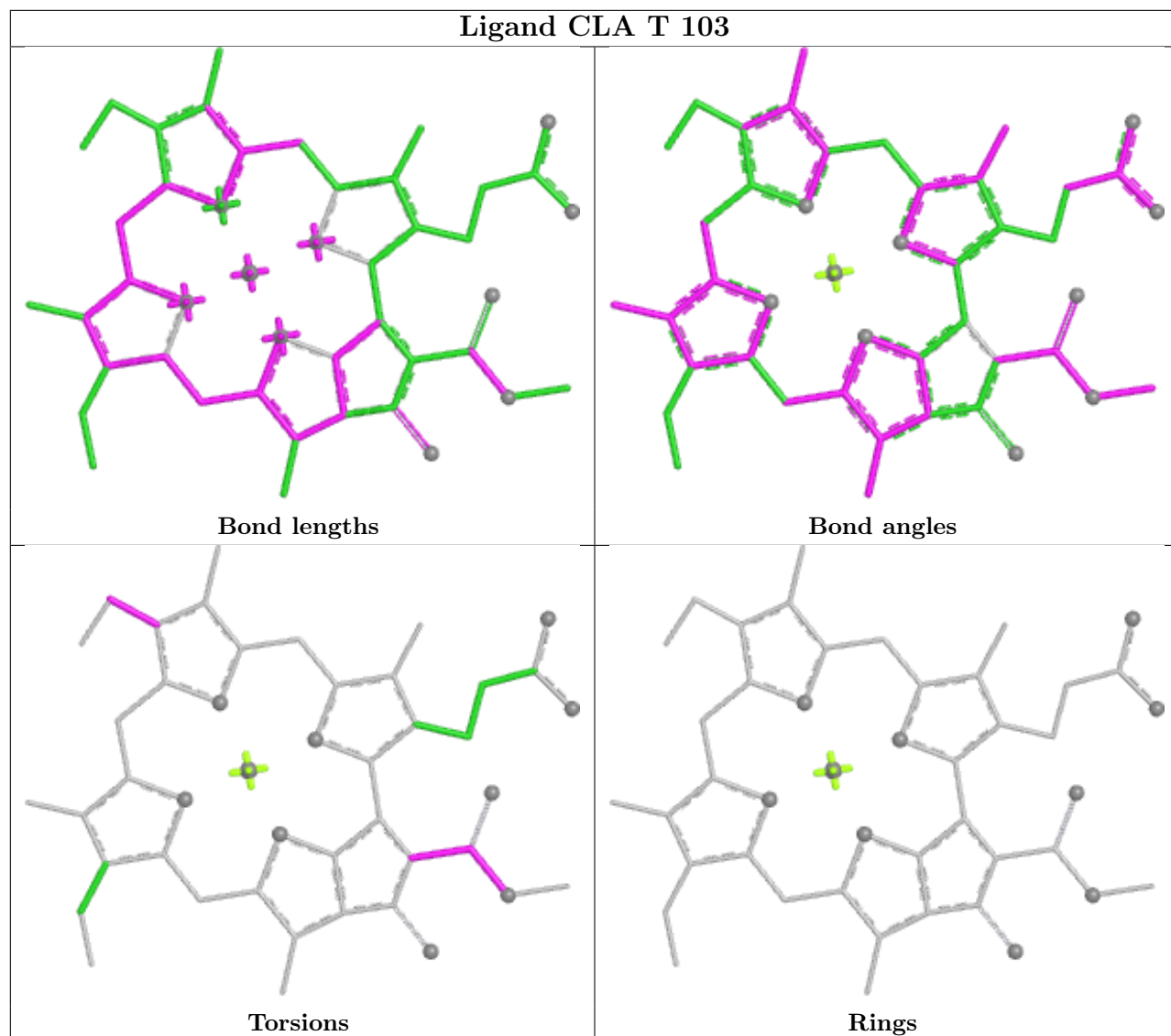
Ligand CLA H 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR Z 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

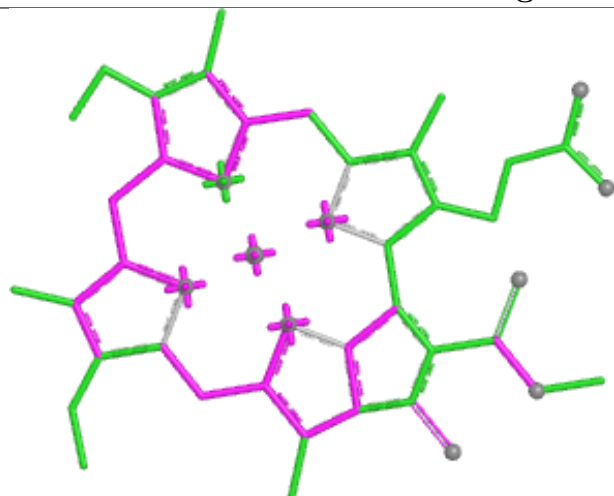




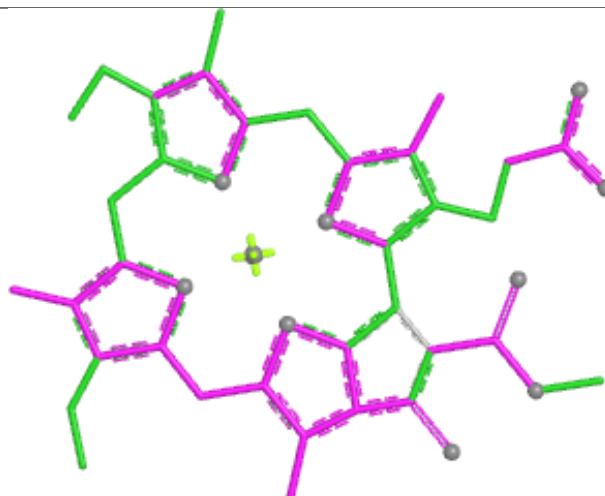
Ligand CLA T 103



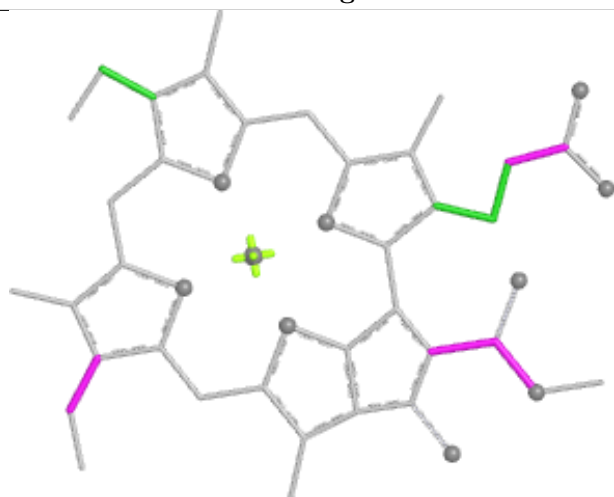
Ligand CLA Z 836



Bond lengths



Bond angles

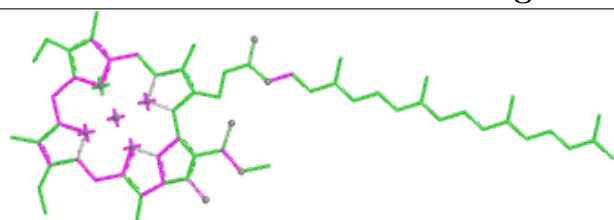


Torsions

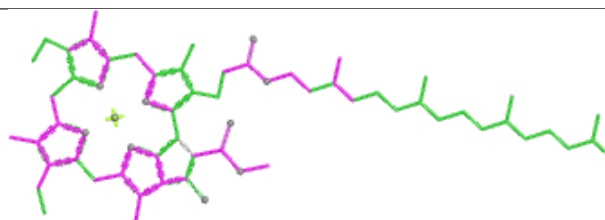


Rings

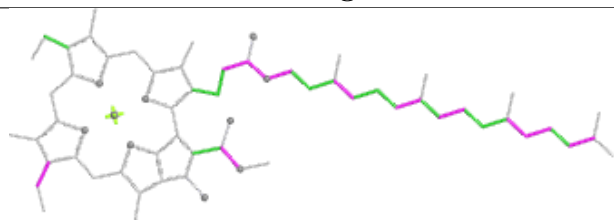
Ligand CLA B 813



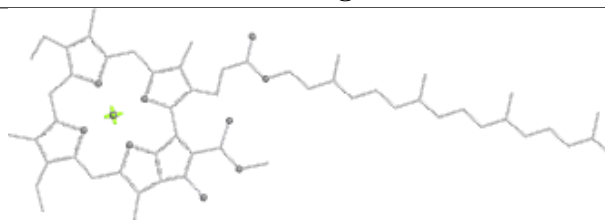
Bond lengths



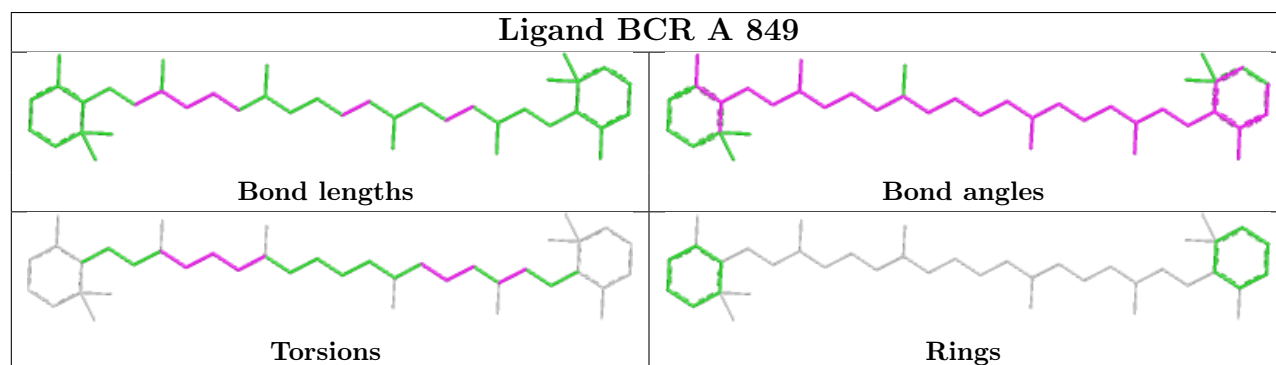
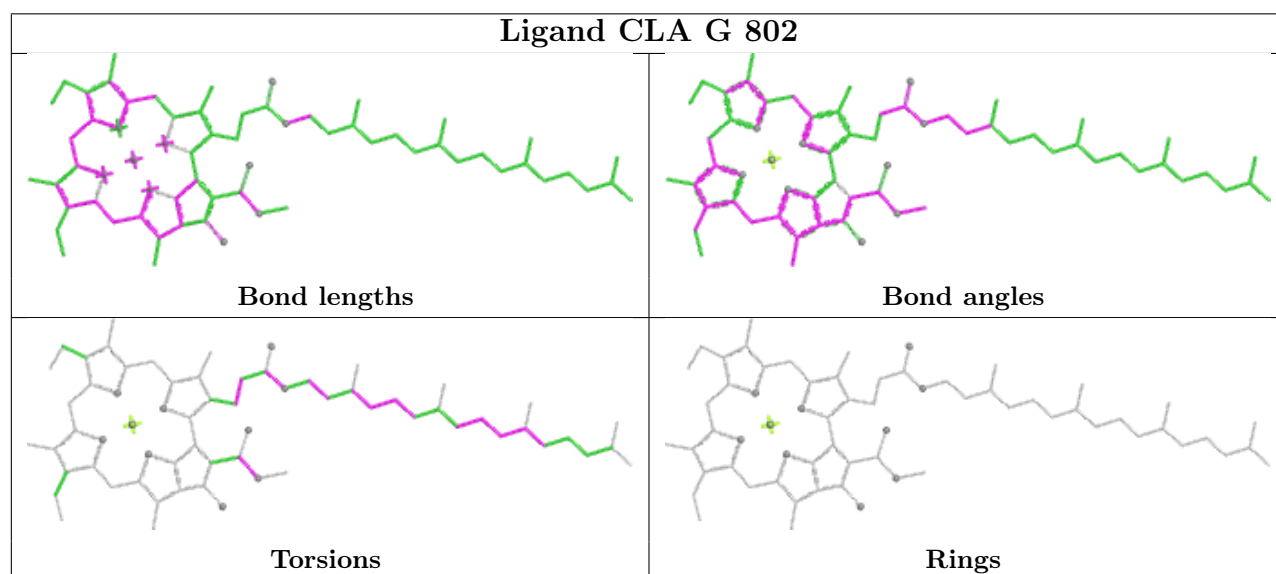
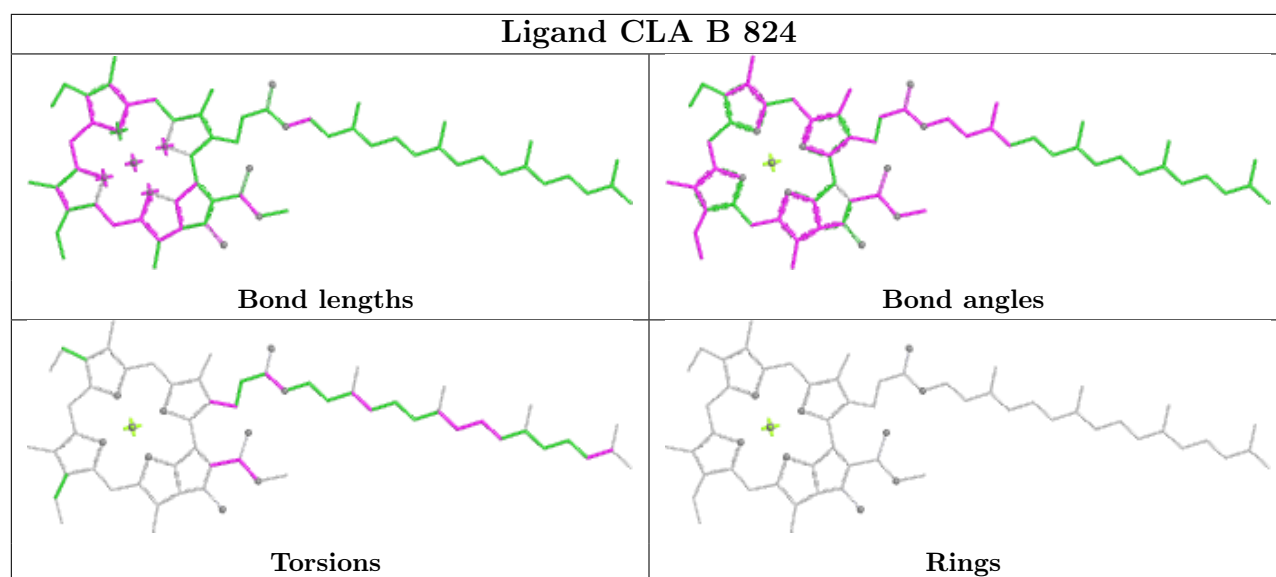
Bond angles

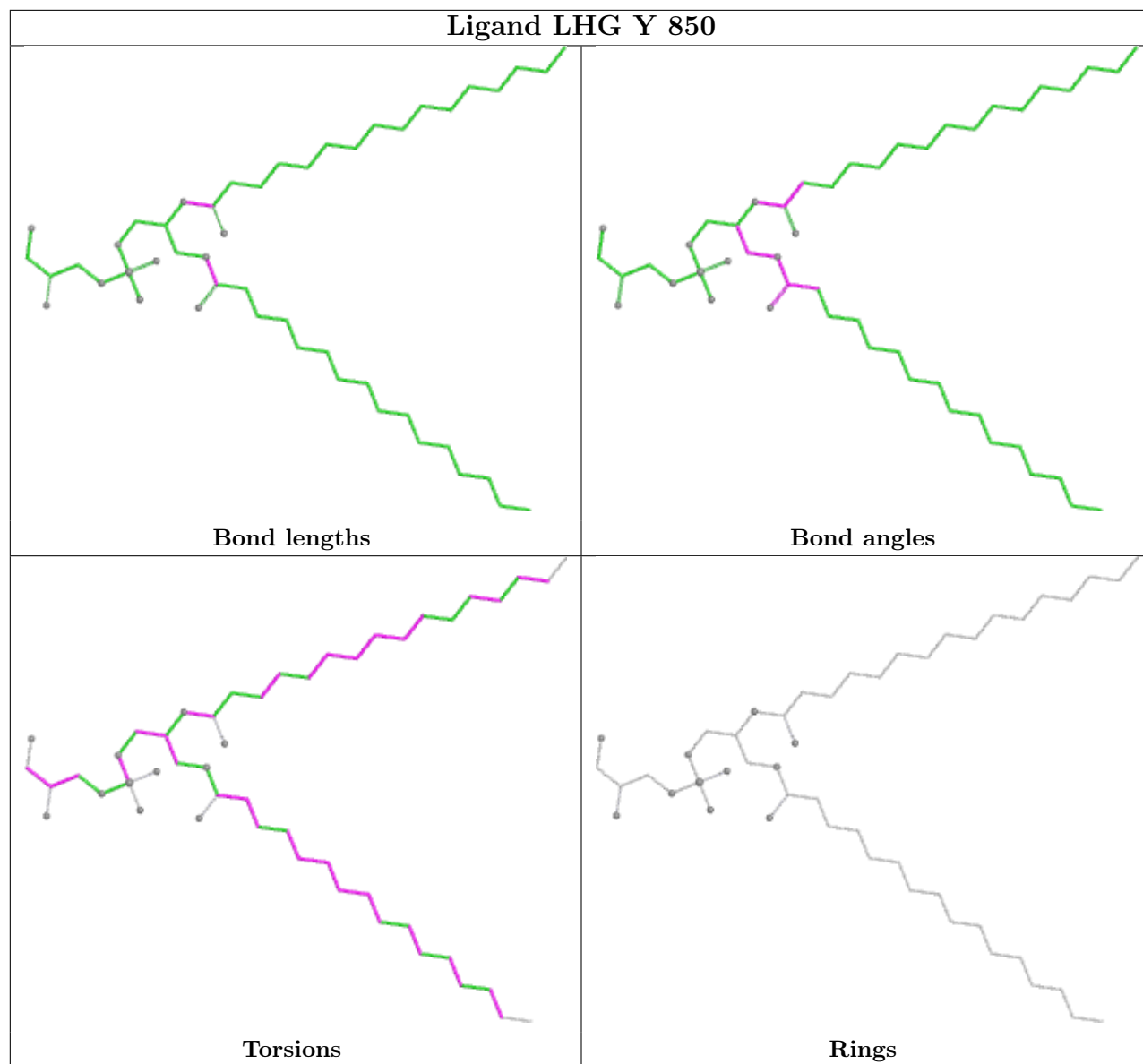


Torsions

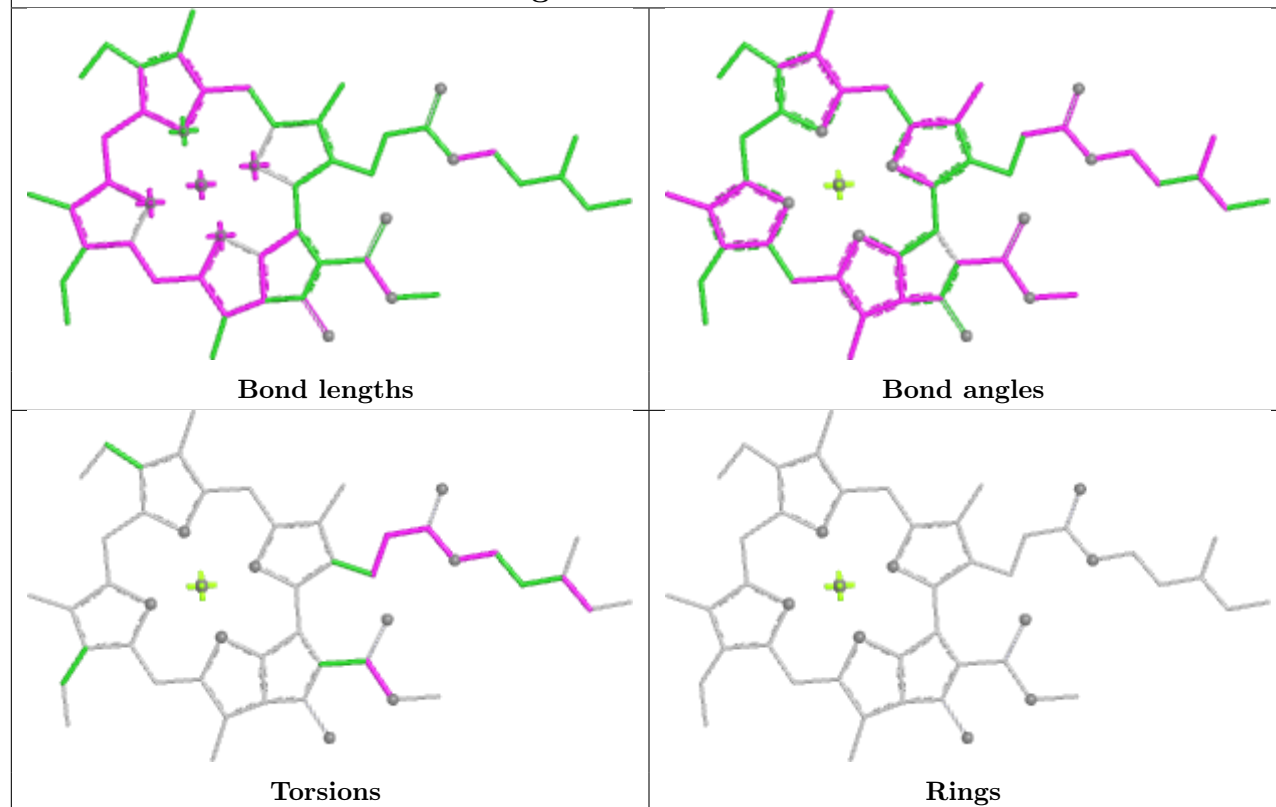


Rings

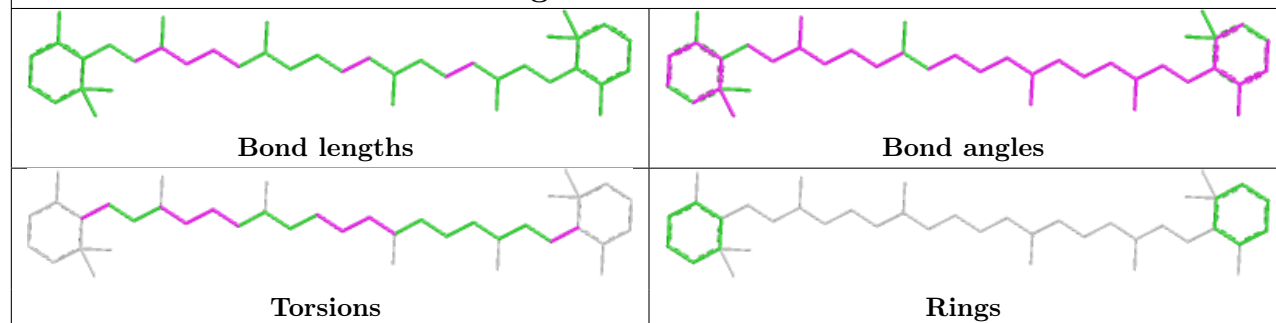




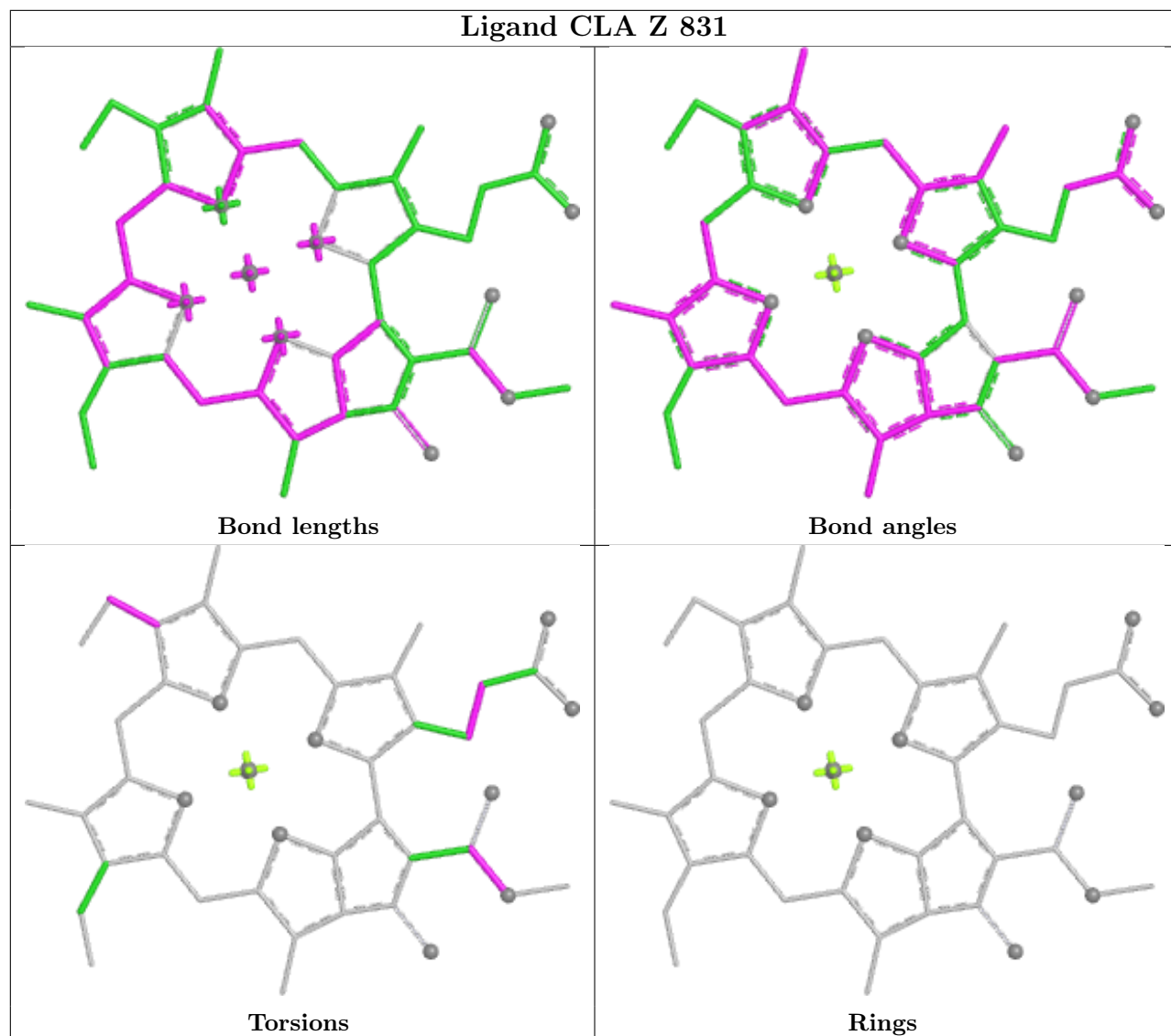
Ligand CLA Y 807

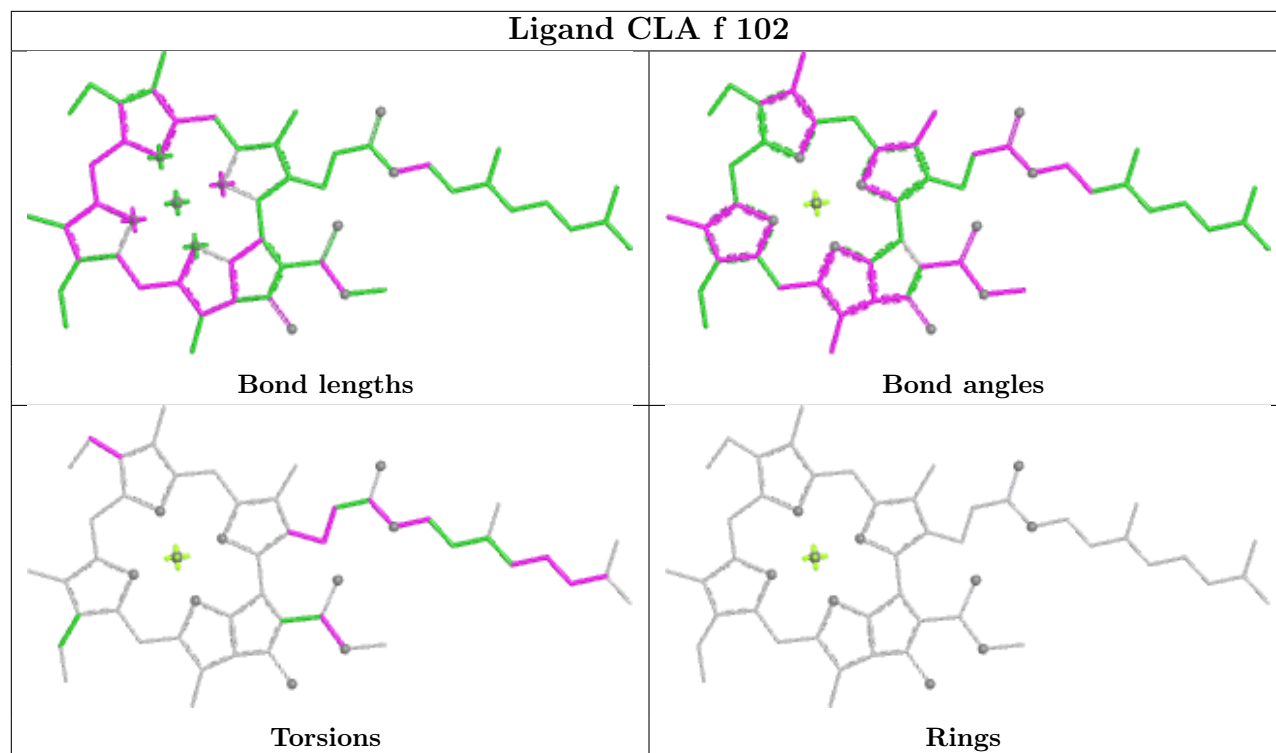


Ligand BCR B 850

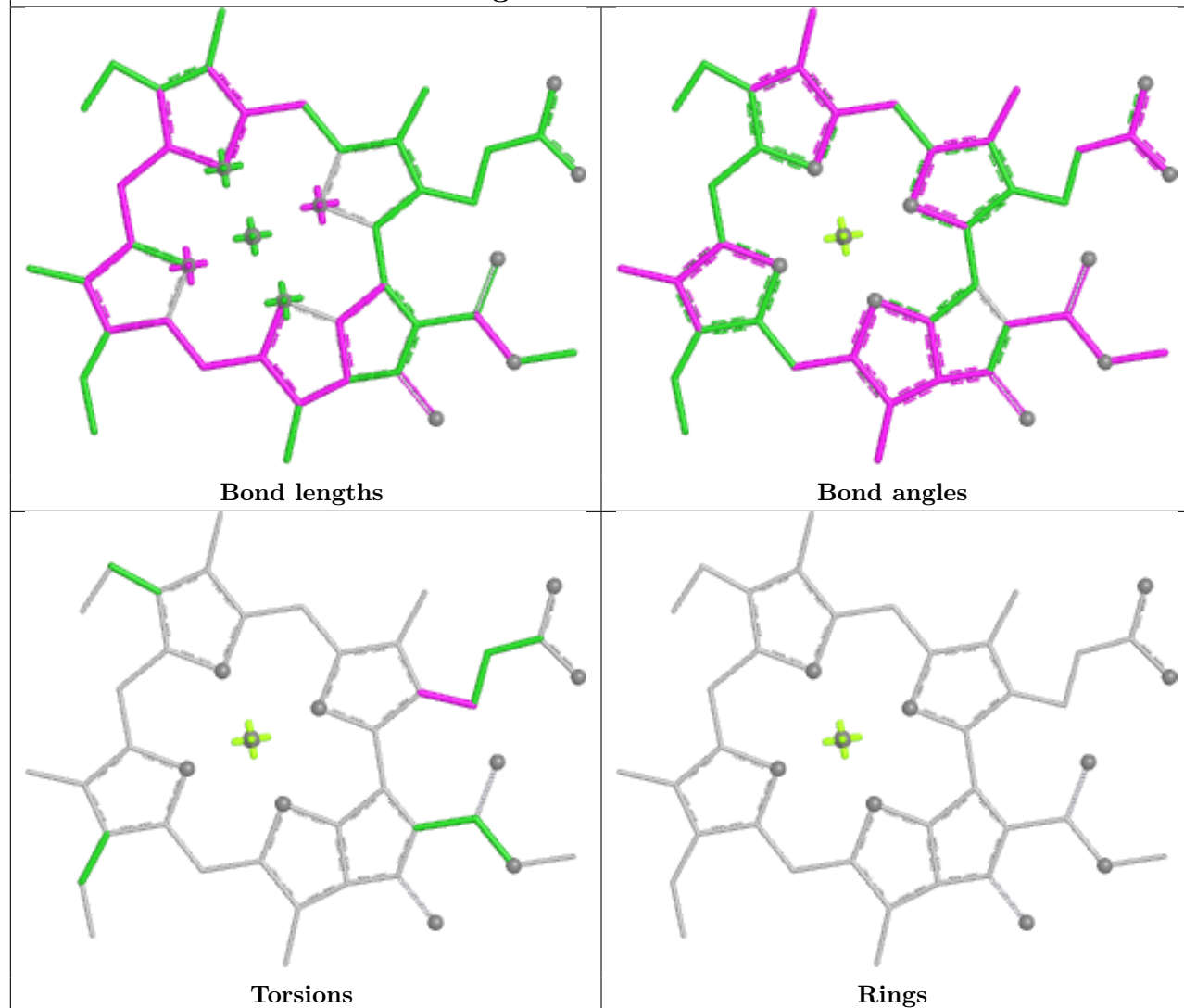


Ligand CLA Z 831

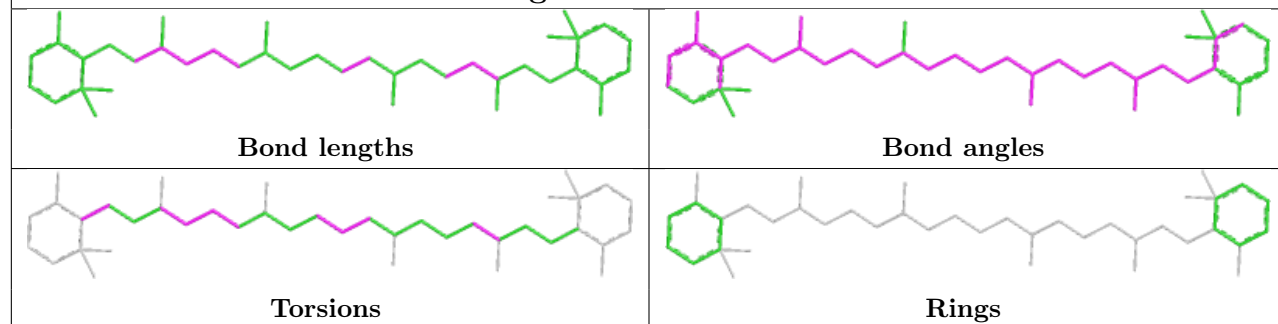


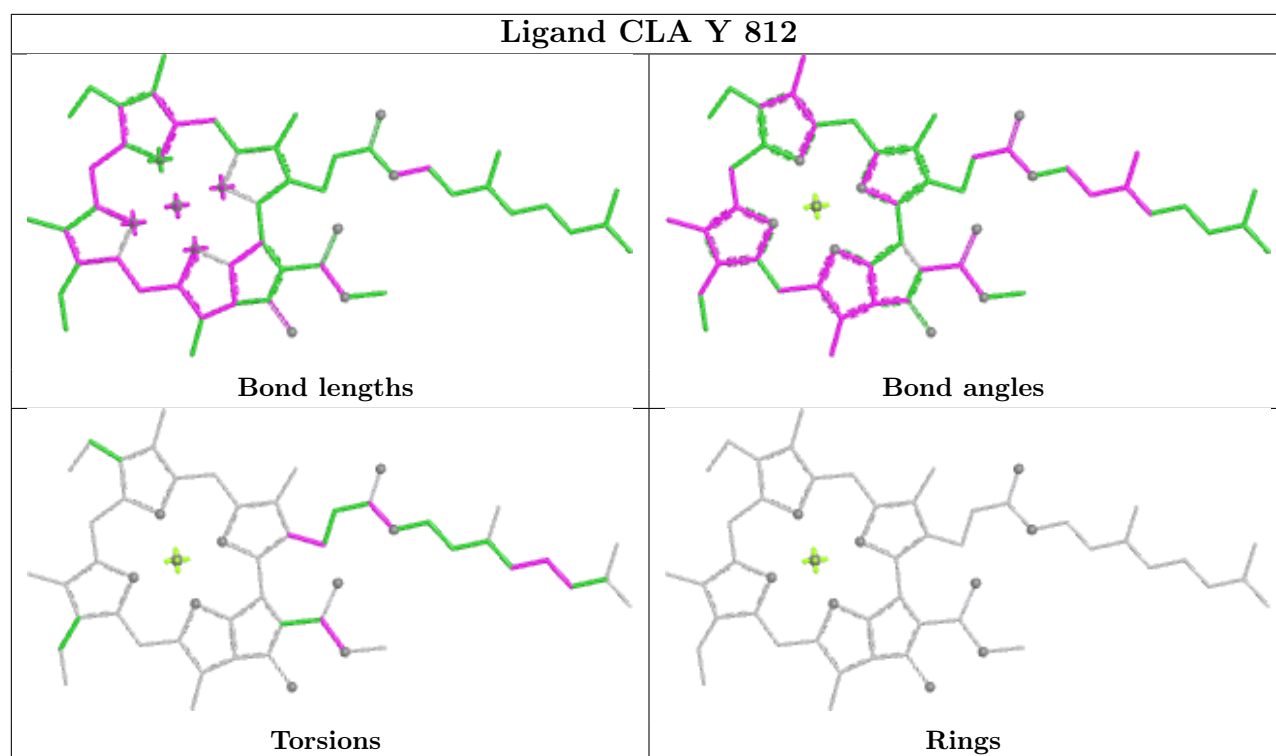


Ligand CLA A 835

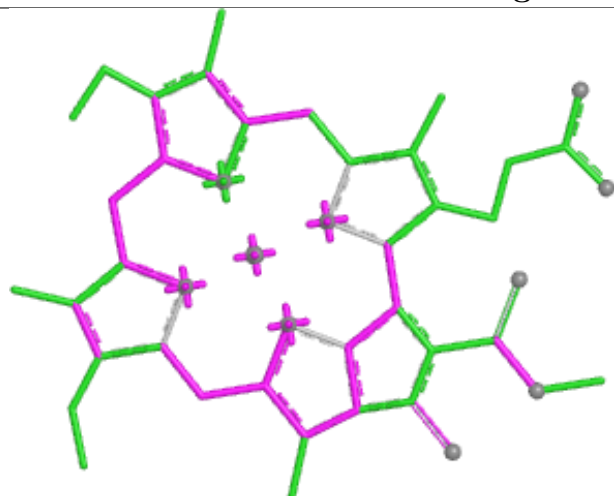


Ligand BCR H 844

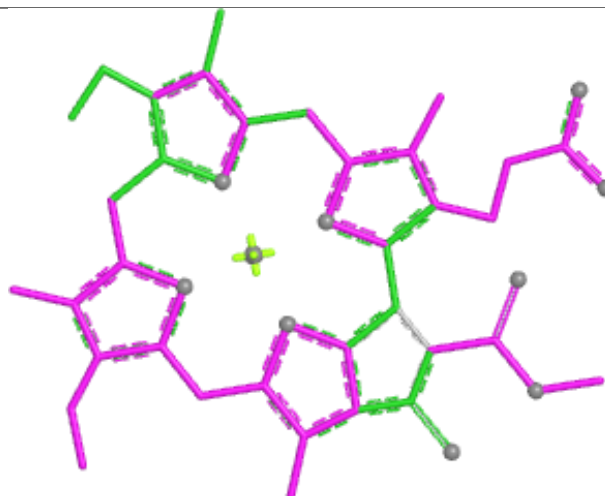




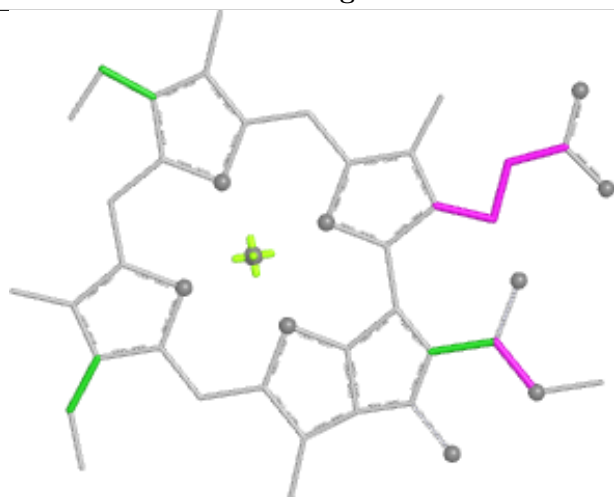
Ligand CLA H 815



Bond lengths



Bond angles

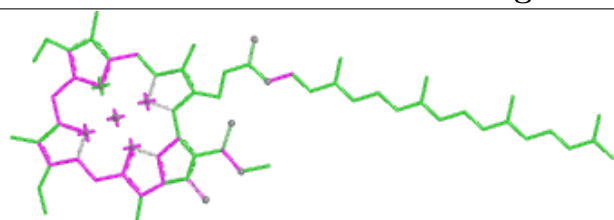


Torsions

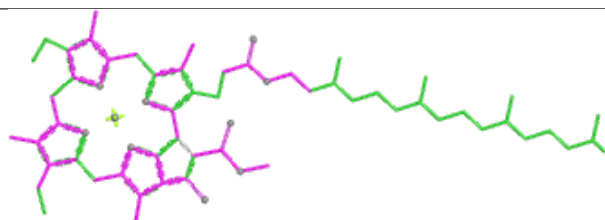


Rings

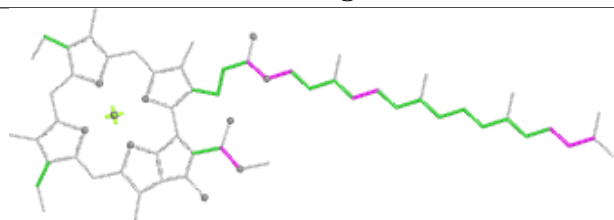
Ligand CLA B 816



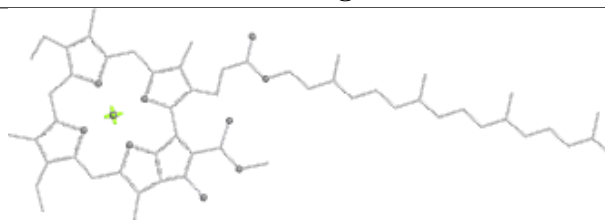
Bond lengths



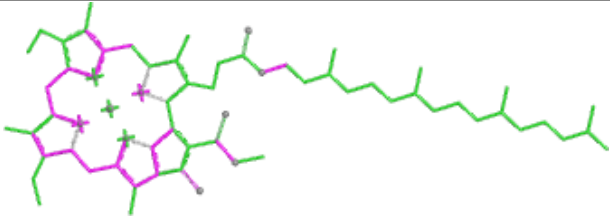
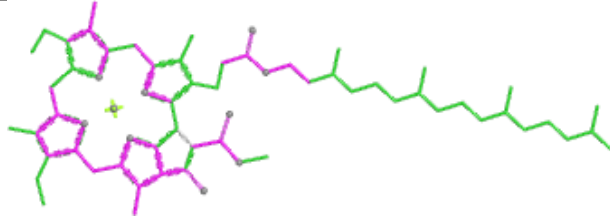
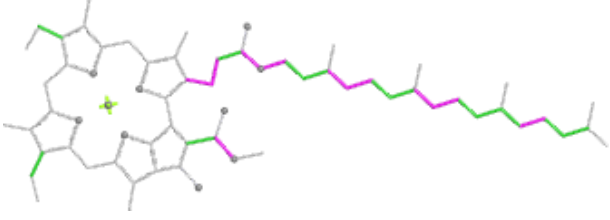
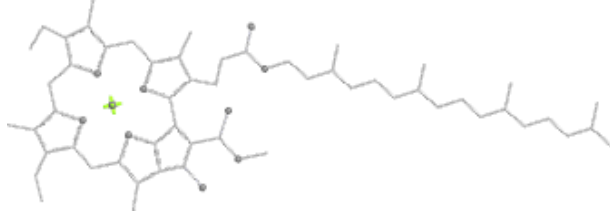
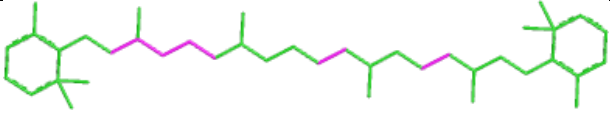
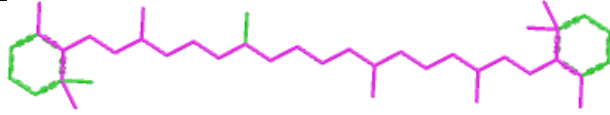
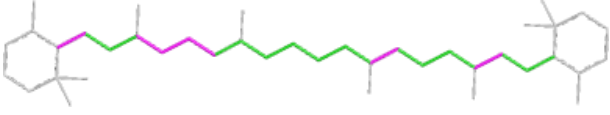
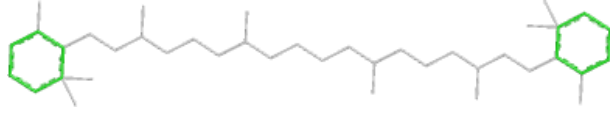
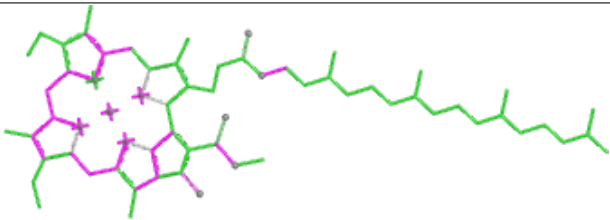
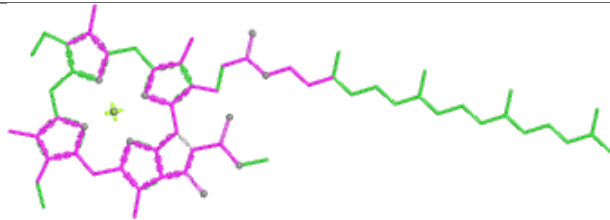
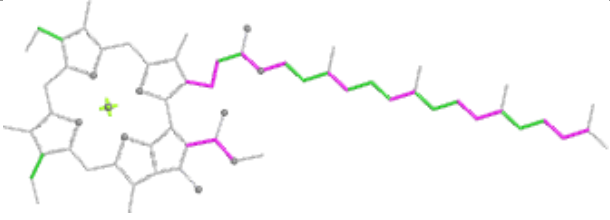
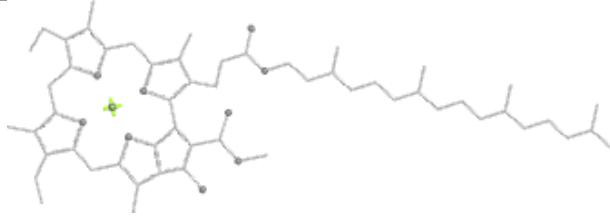
Bond angles



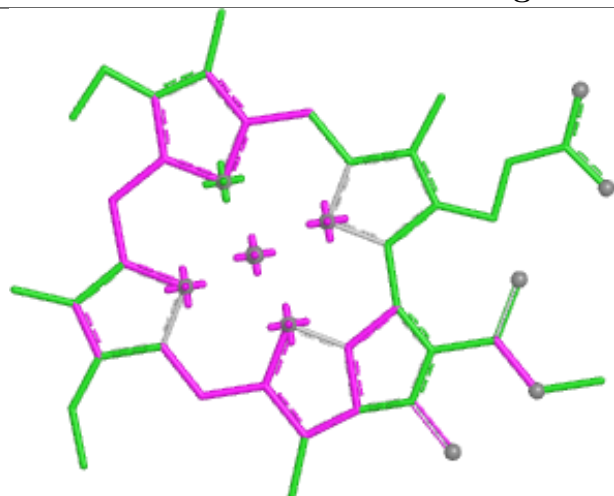
Torsions



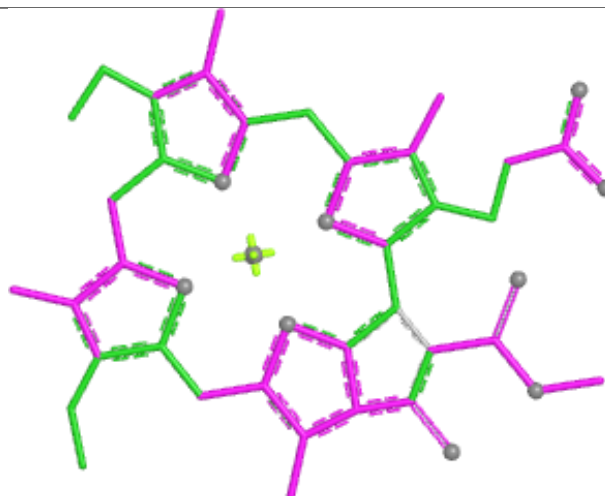
Rings

Ligand CLA h 206	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR J 104	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA Z 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

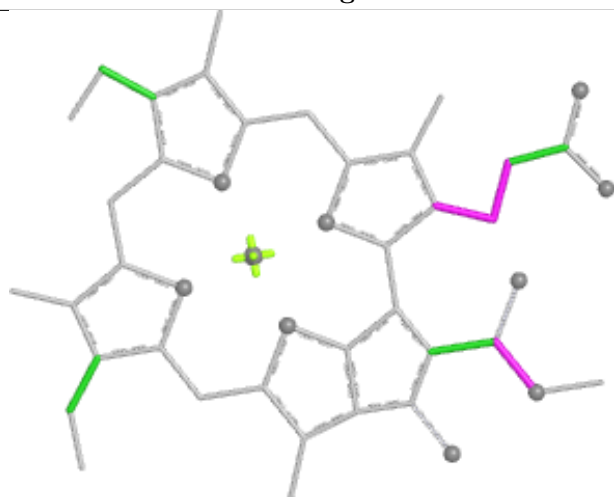
Ligand CLA H 834



Bond lengths



Bond angles

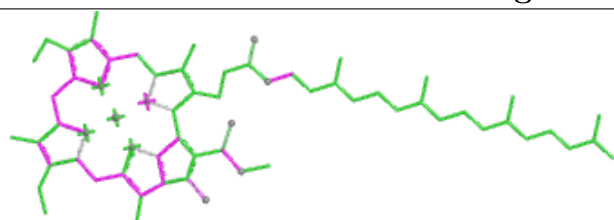


Torsions

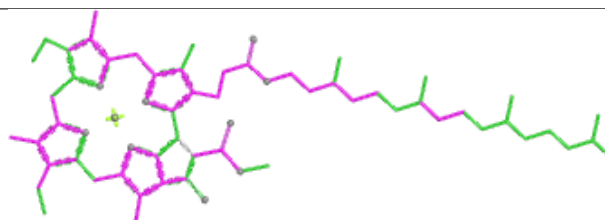


Rings

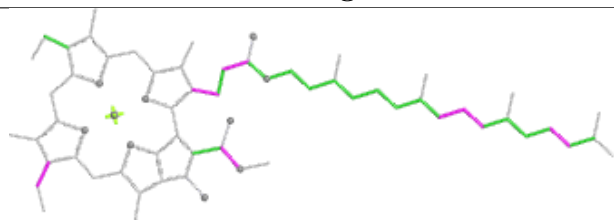
Ligand CLA B 840



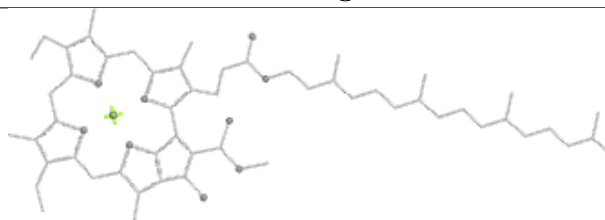
Bond lengths



Bond angles

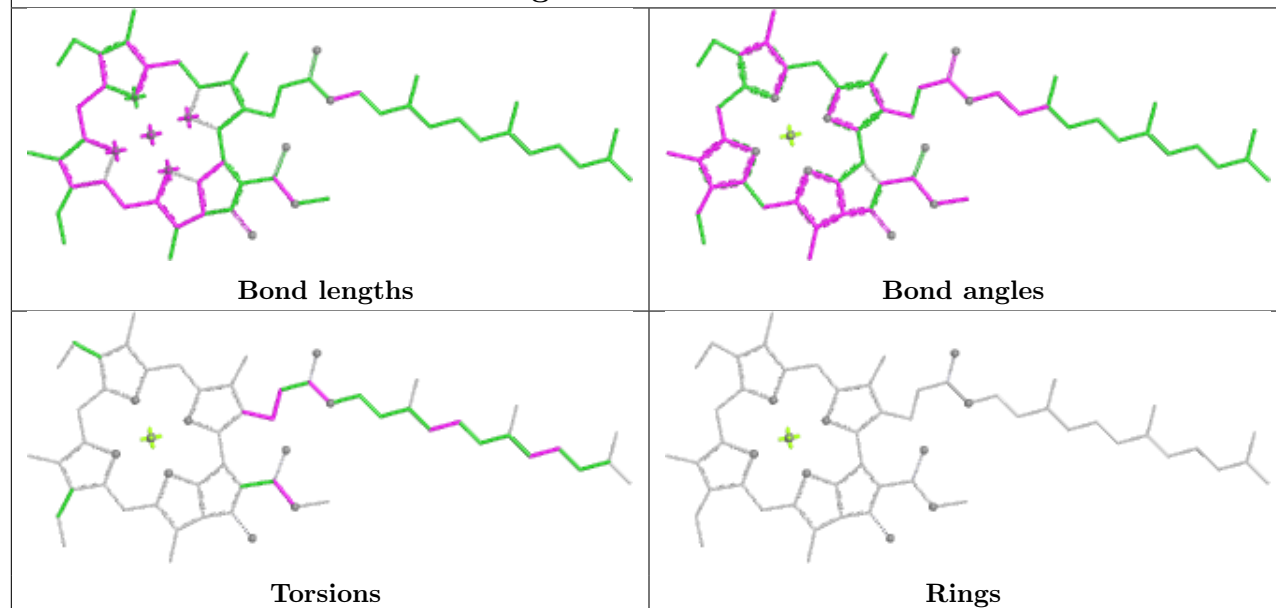


Torsions

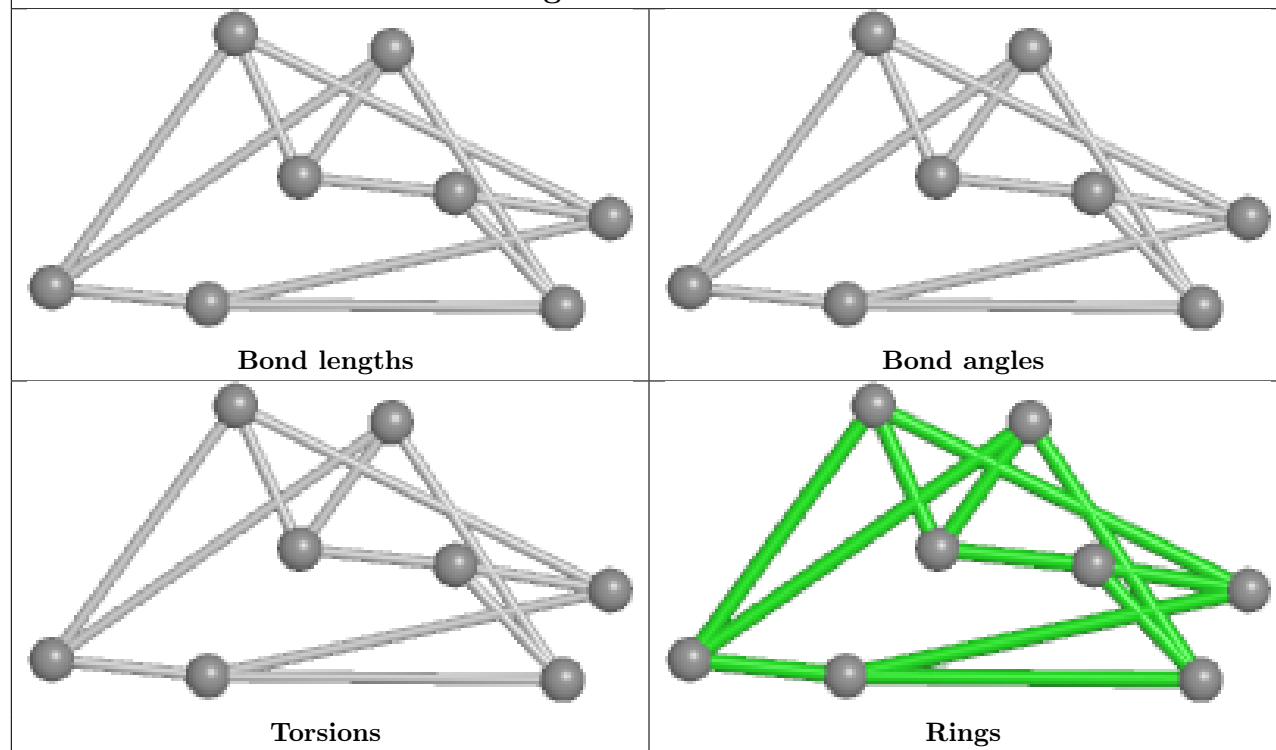


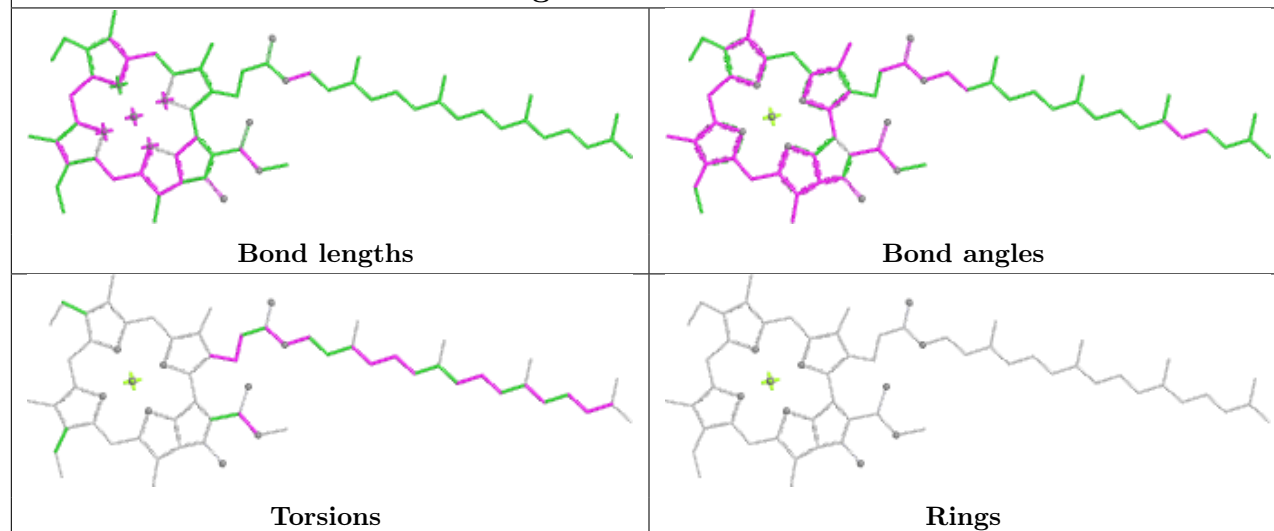
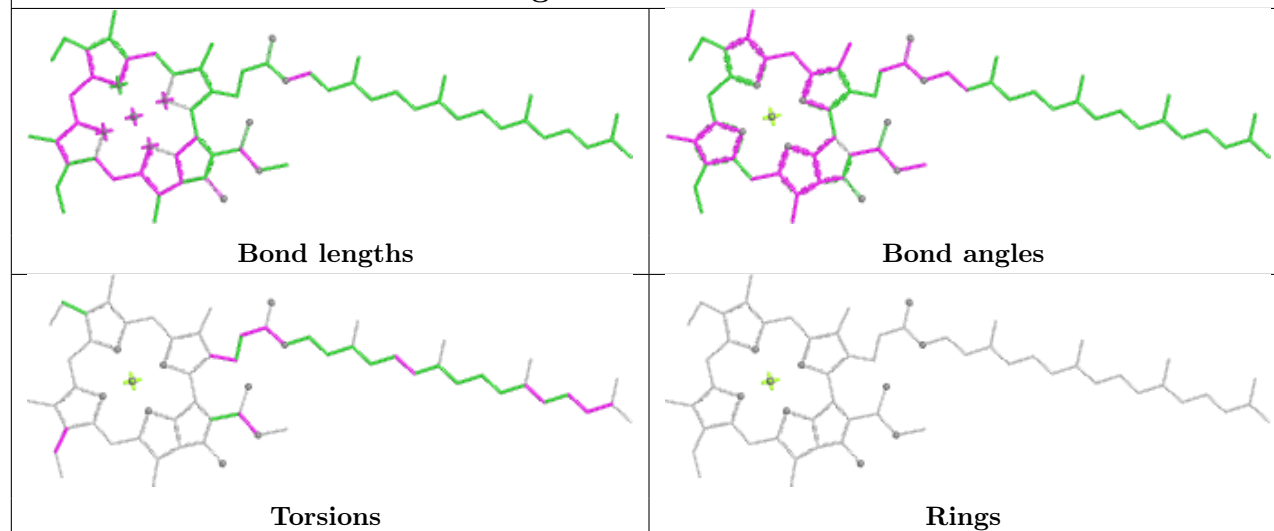
Rings

Ligand CLA Y 813

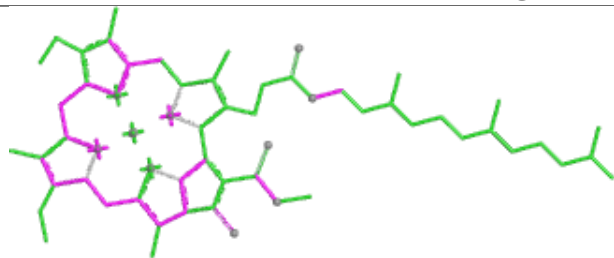


Ligand SF4 a 102

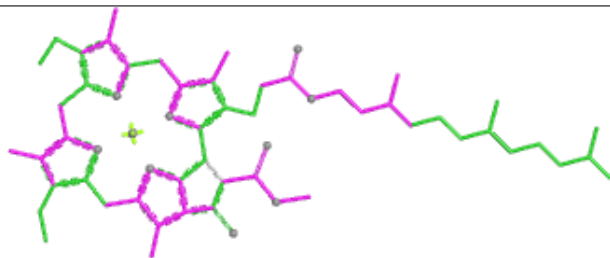


Ligand CLA B 831**Ligand CLA Y 828**

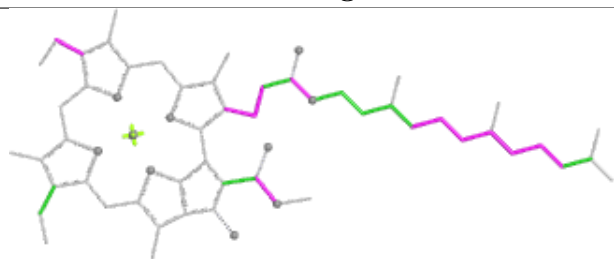
Ligand CLA H 818



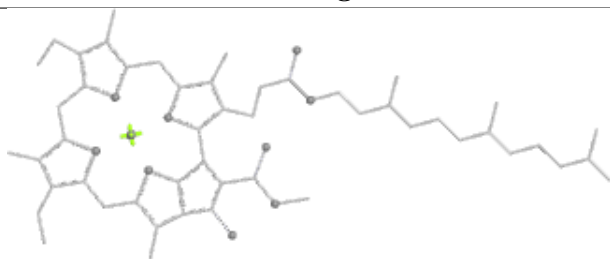
Bond lengths



Bond angles

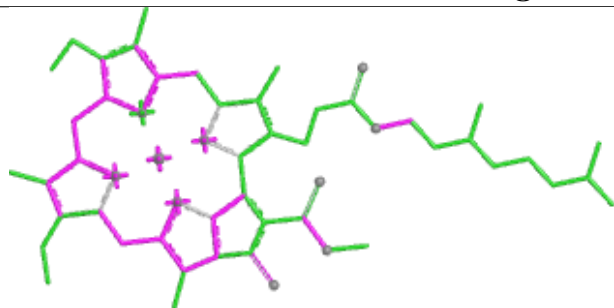


Torsions

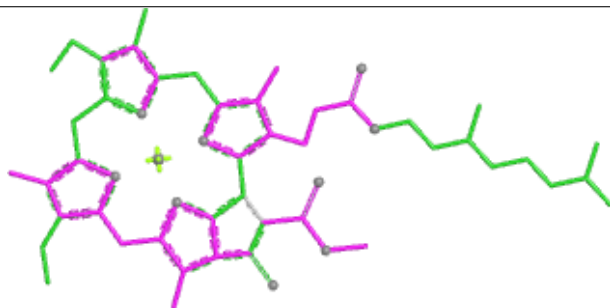


Rings

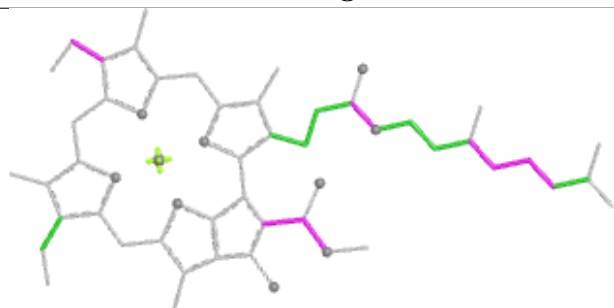
Ligand CLA B 832



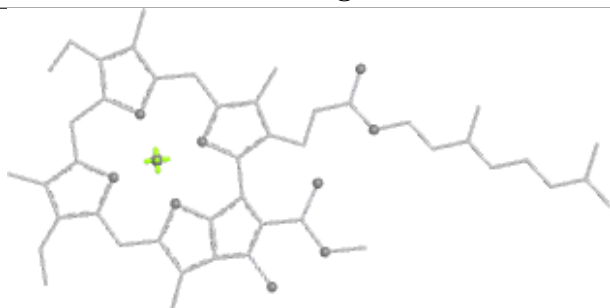
Bond lengths



Bond angles

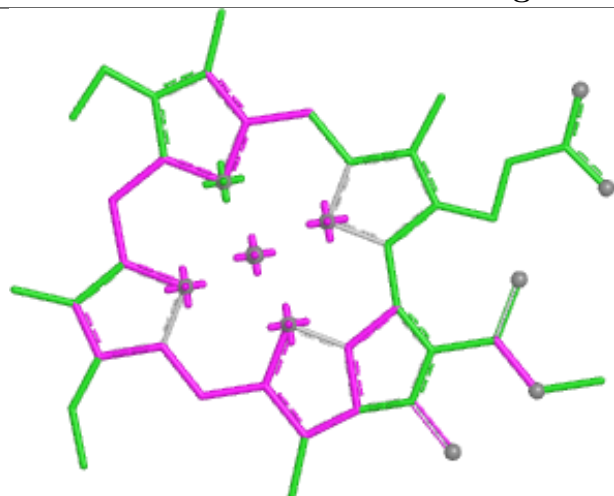


Torsions

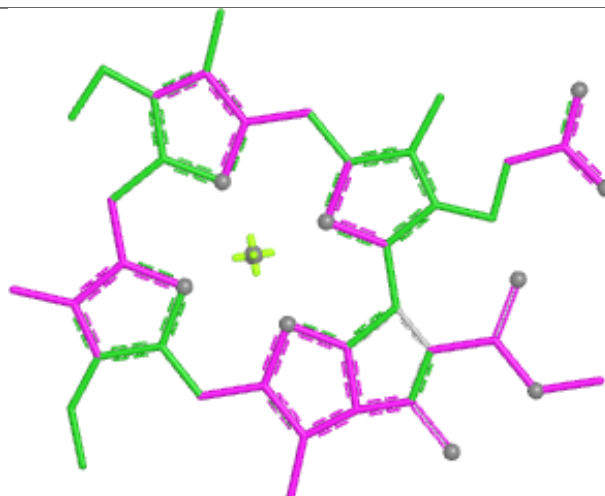


Rings

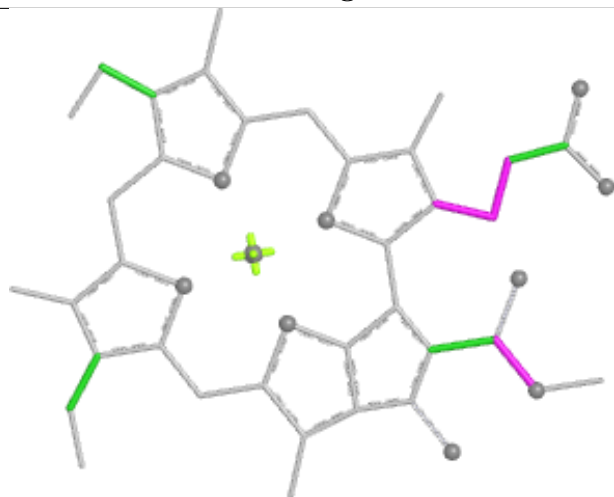
Ligand CLA G 835



Bond lengths



Bond angles

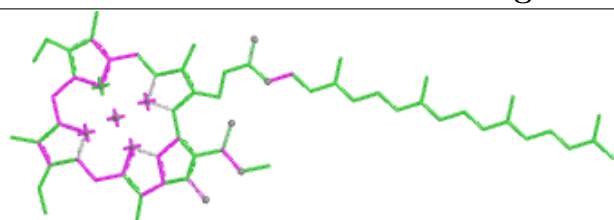


Torsions

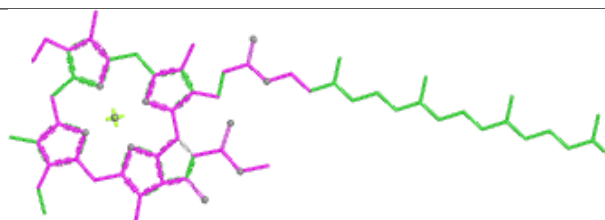


Rings

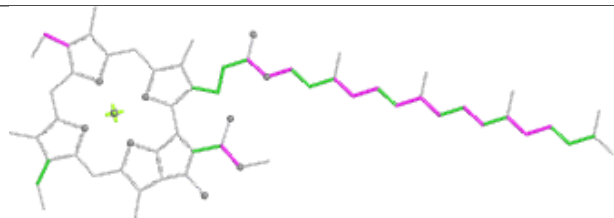
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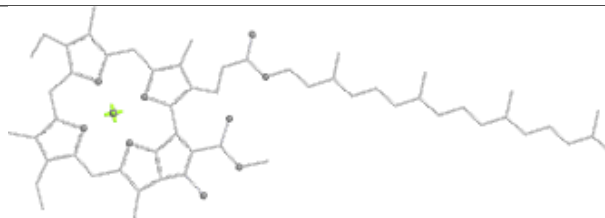
Bond lengths



Bond angles

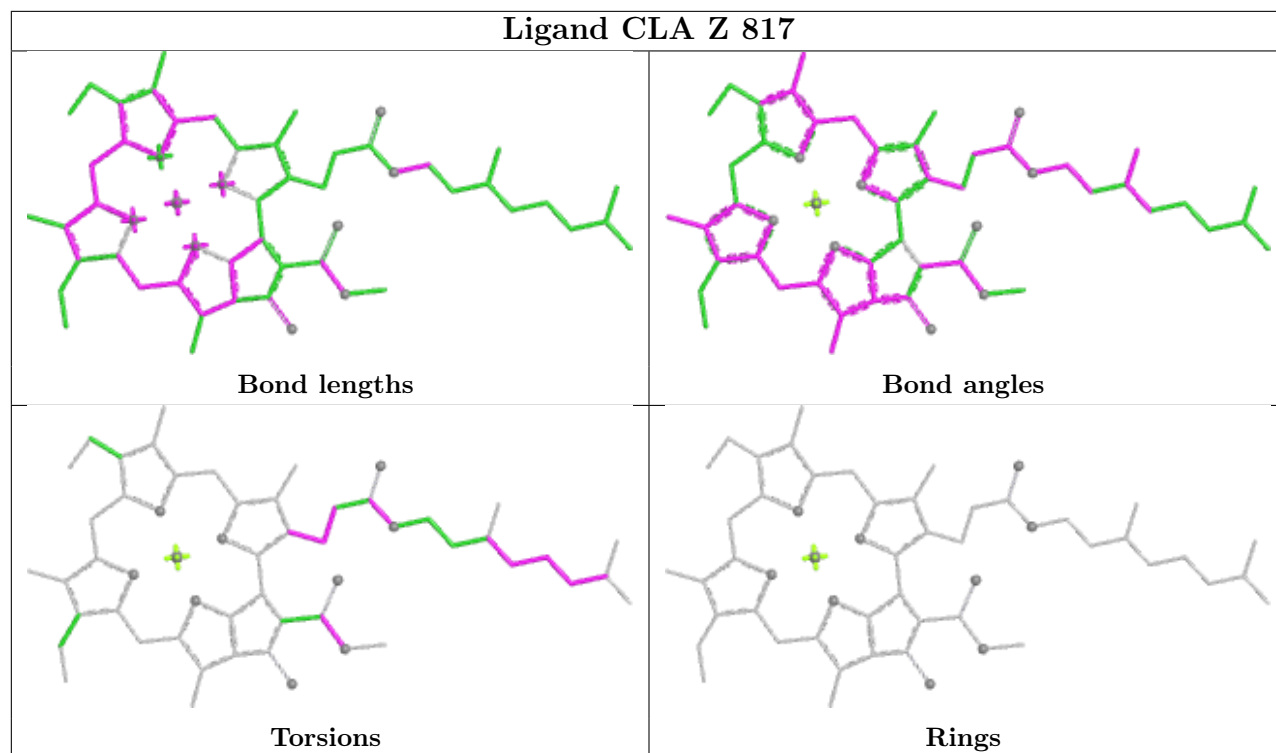


Torsions

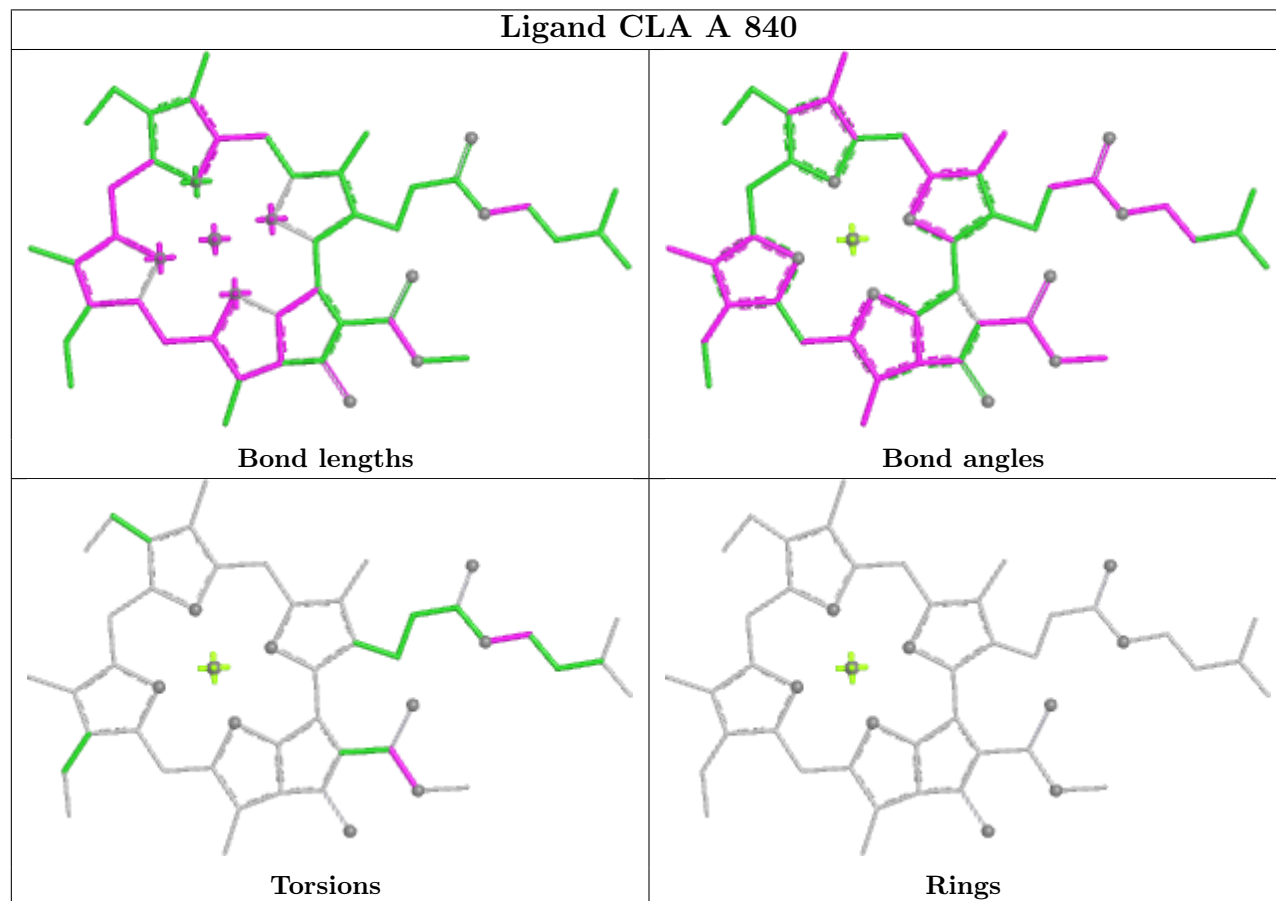


Rings

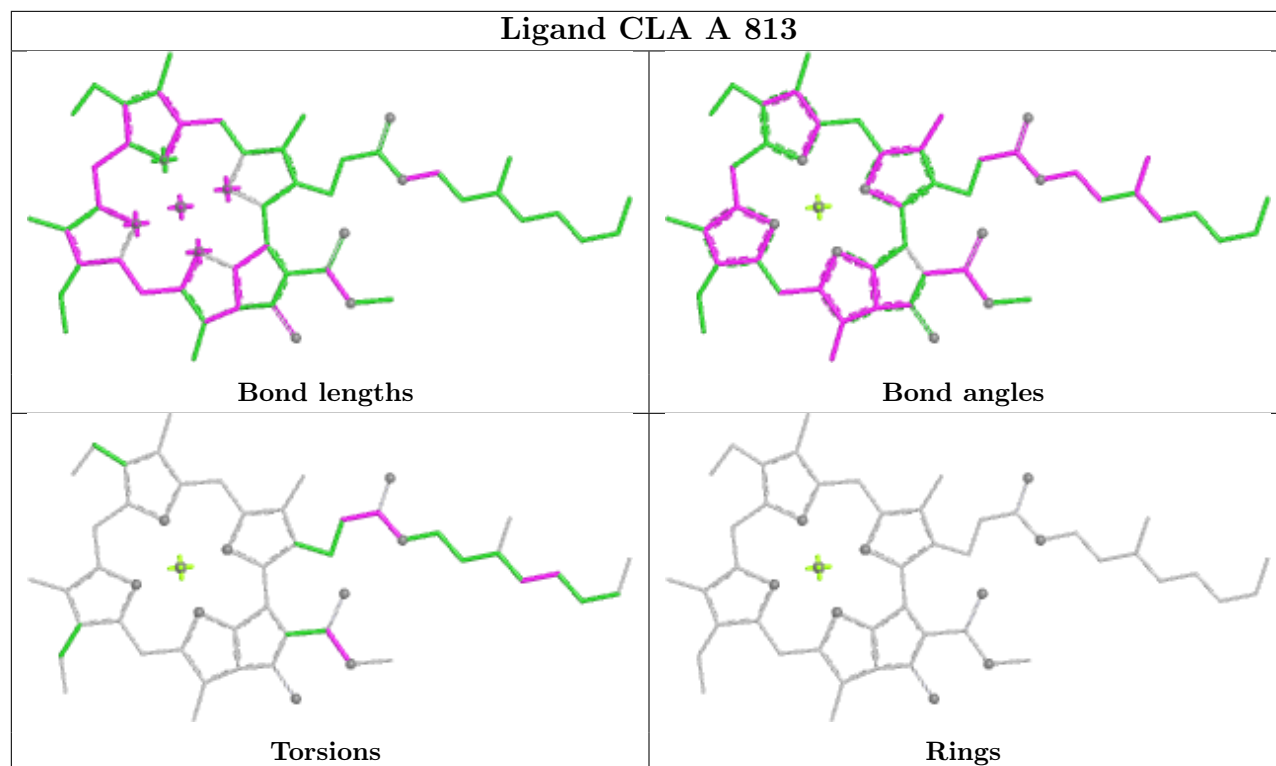
Ligand CLA Z 817



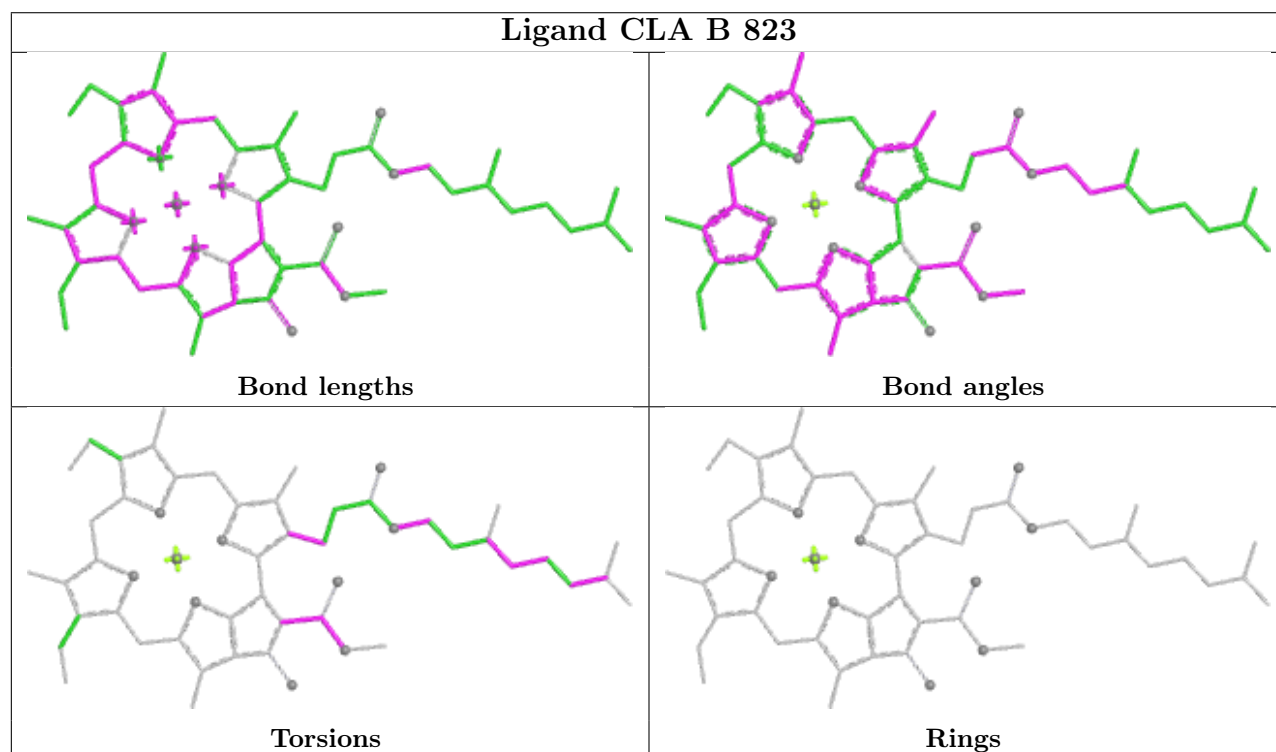
Ligand CLA A 840

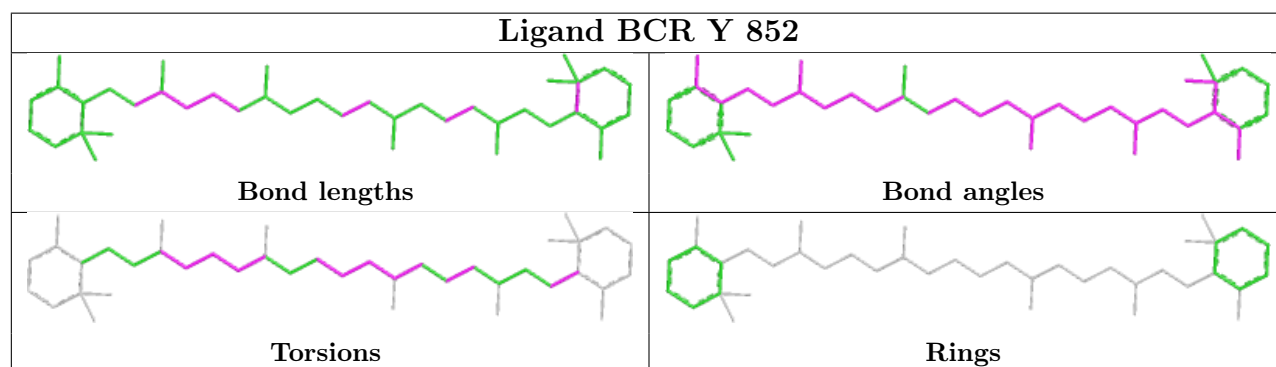
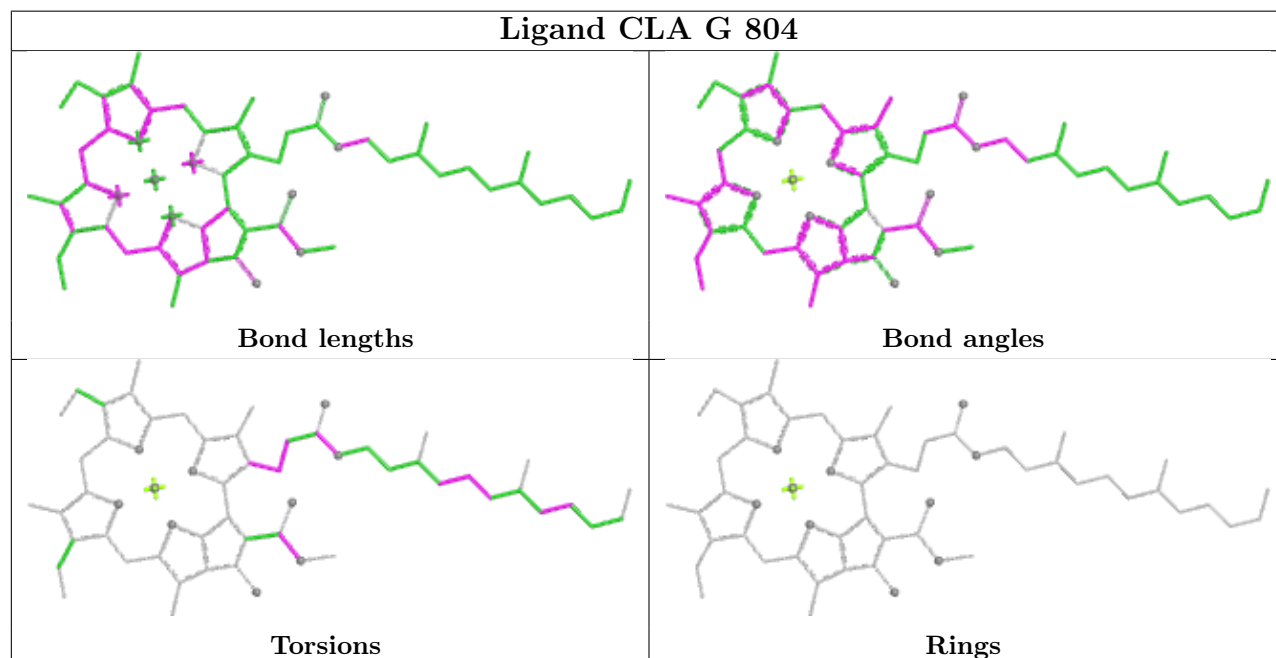
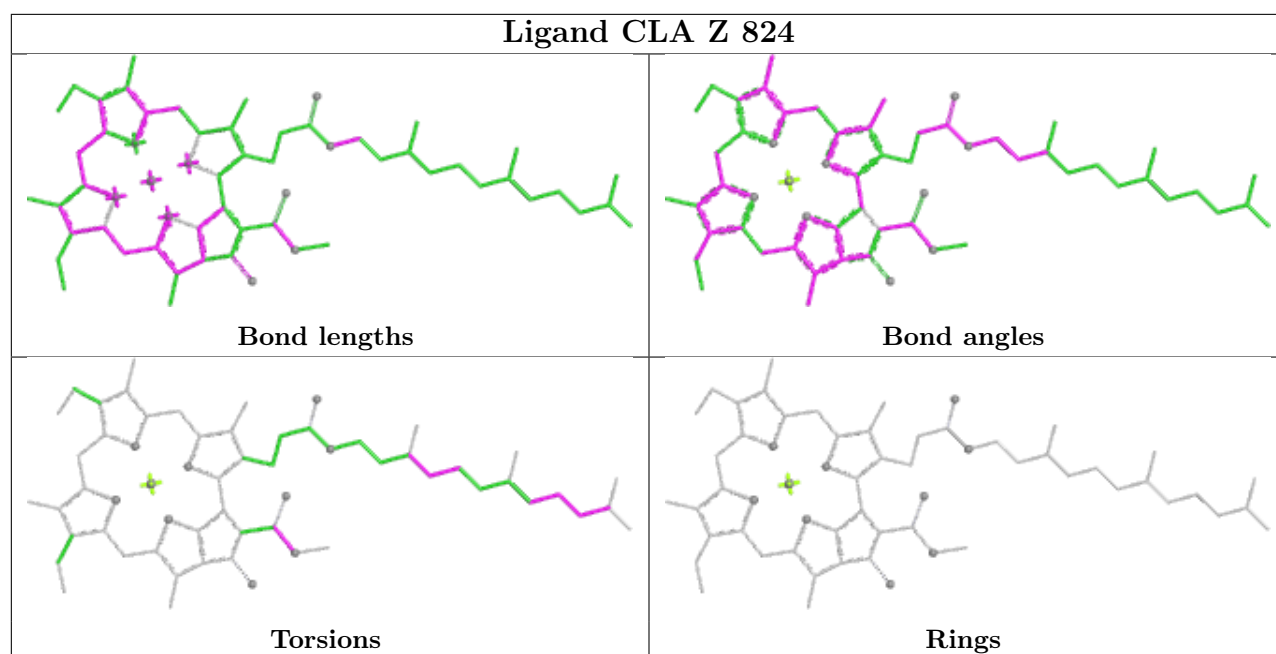


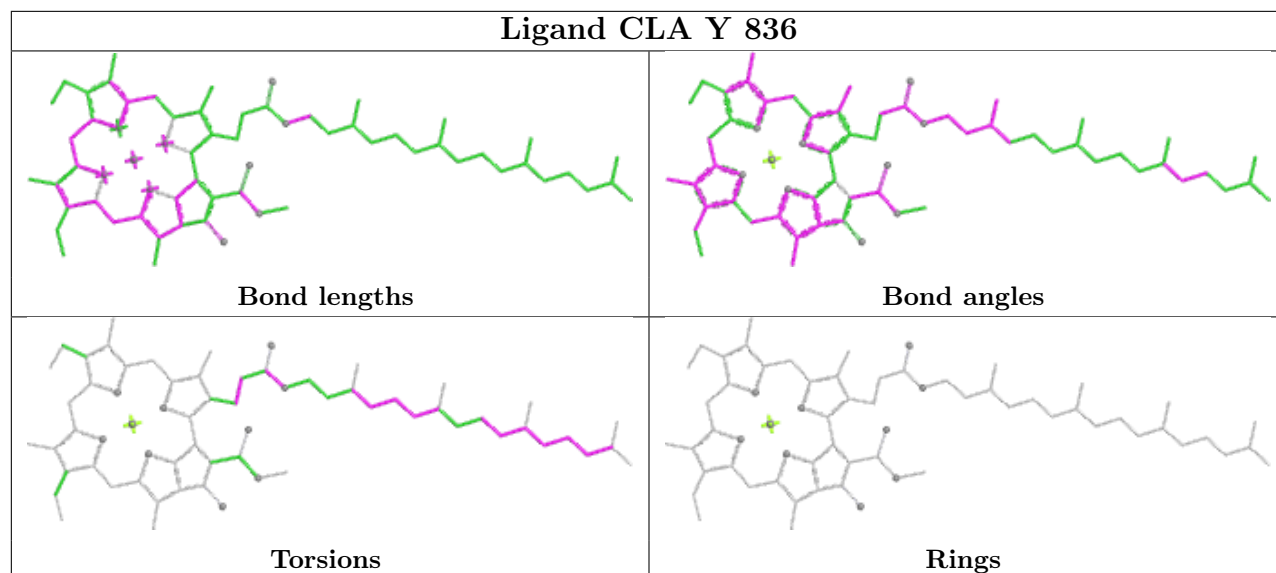
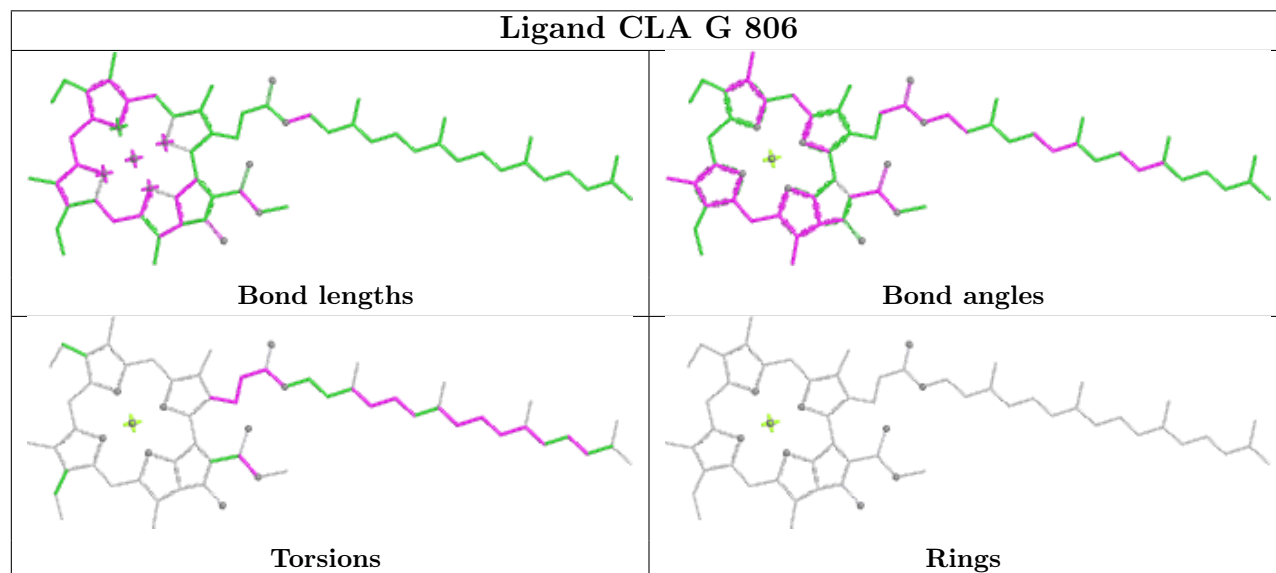
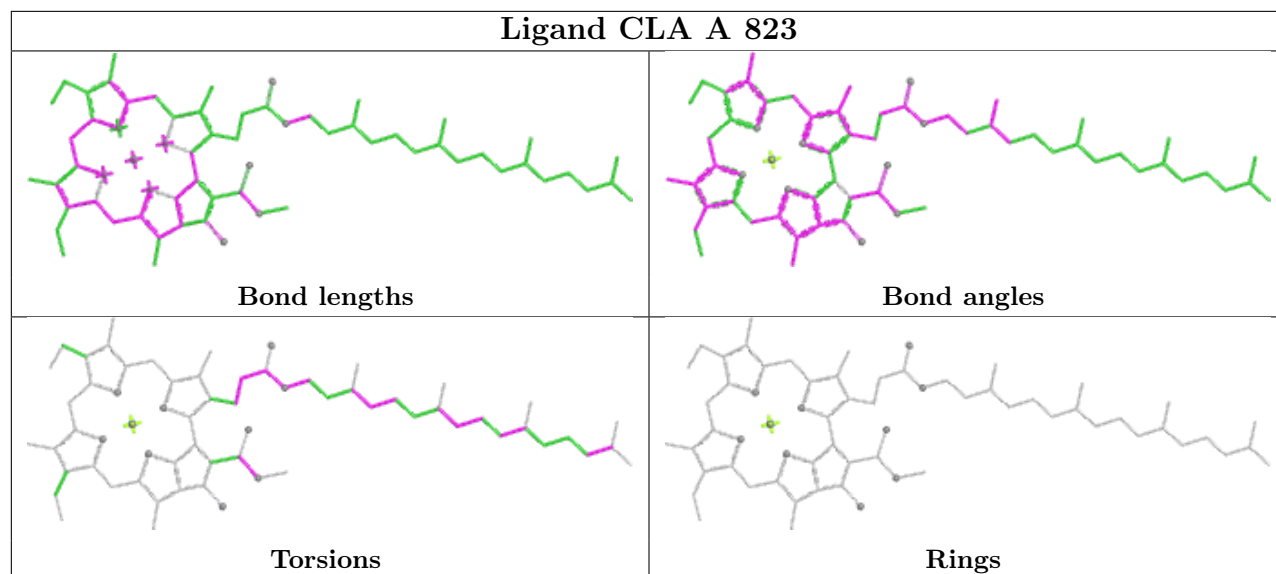
Ligand CLA A 813

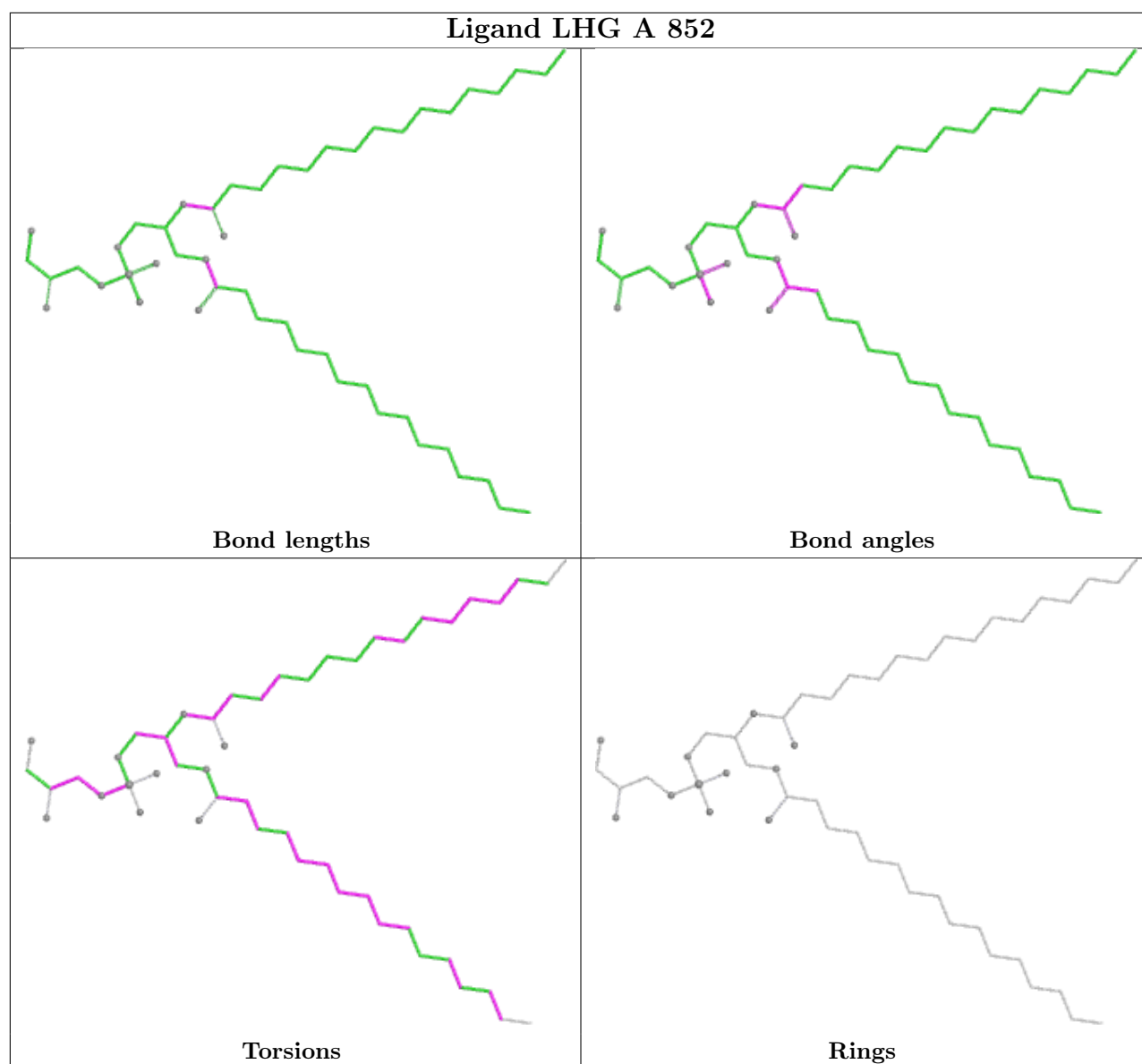


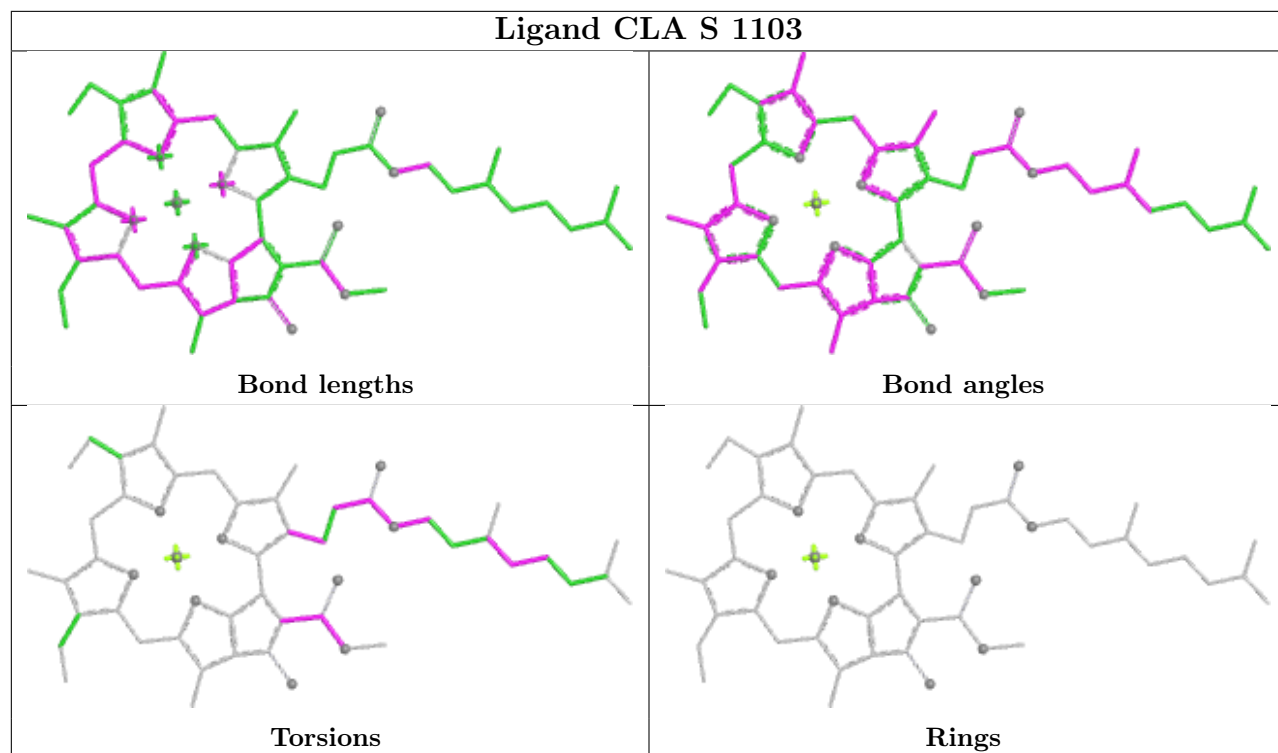
Ligand CLA B 823



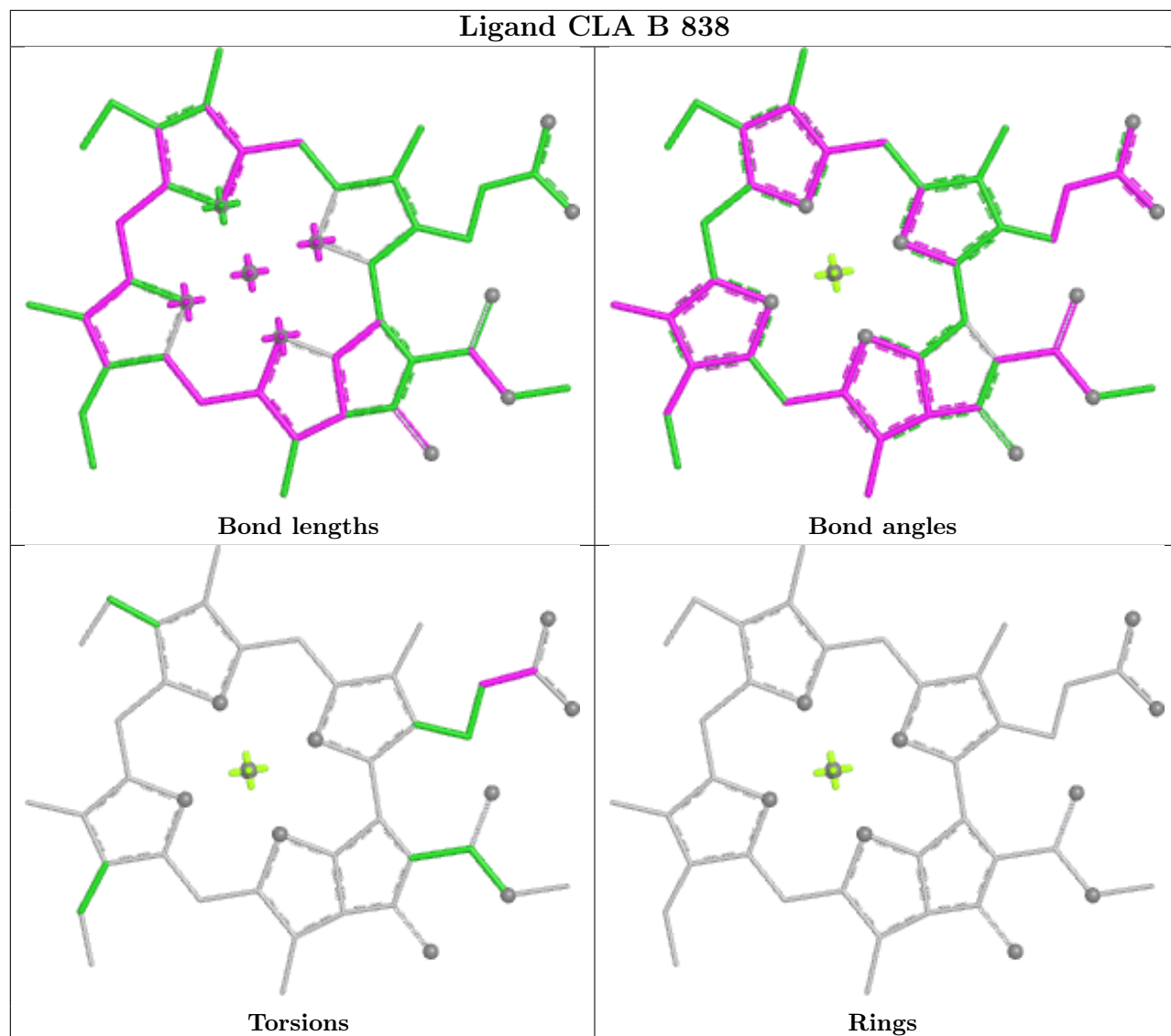




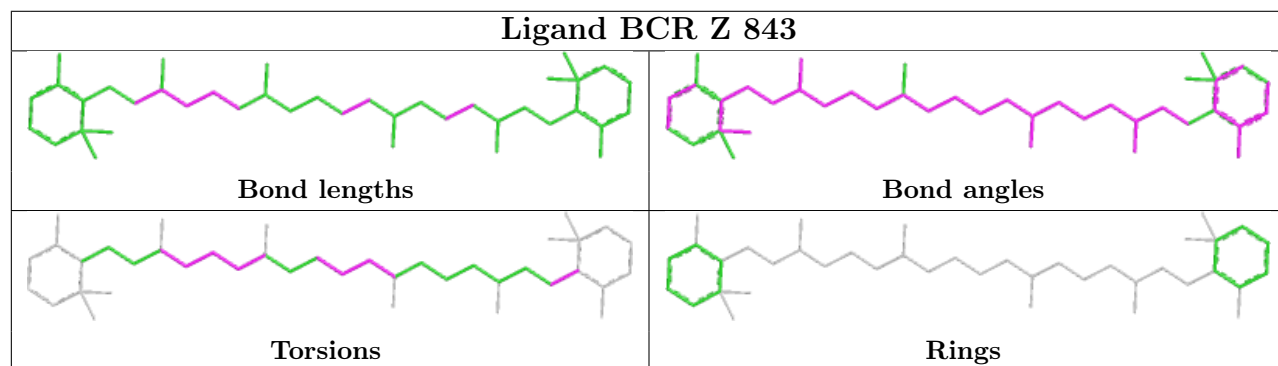


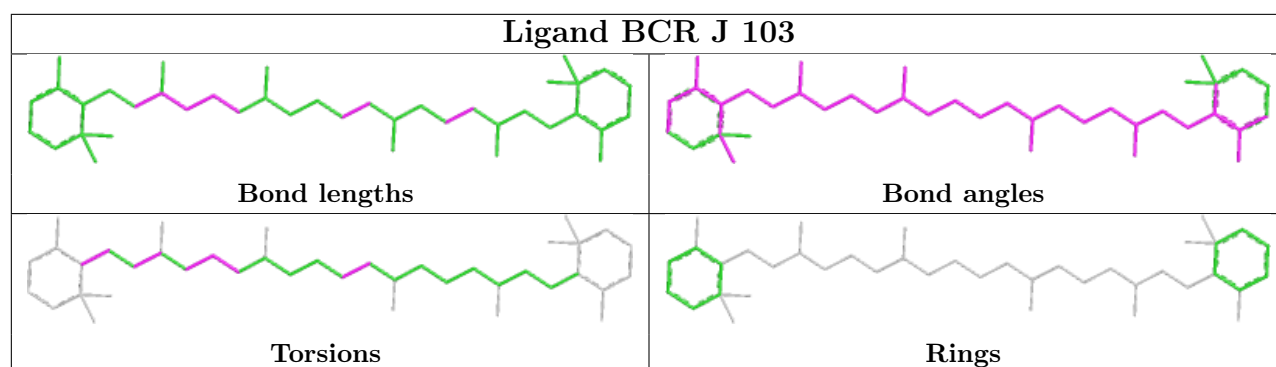
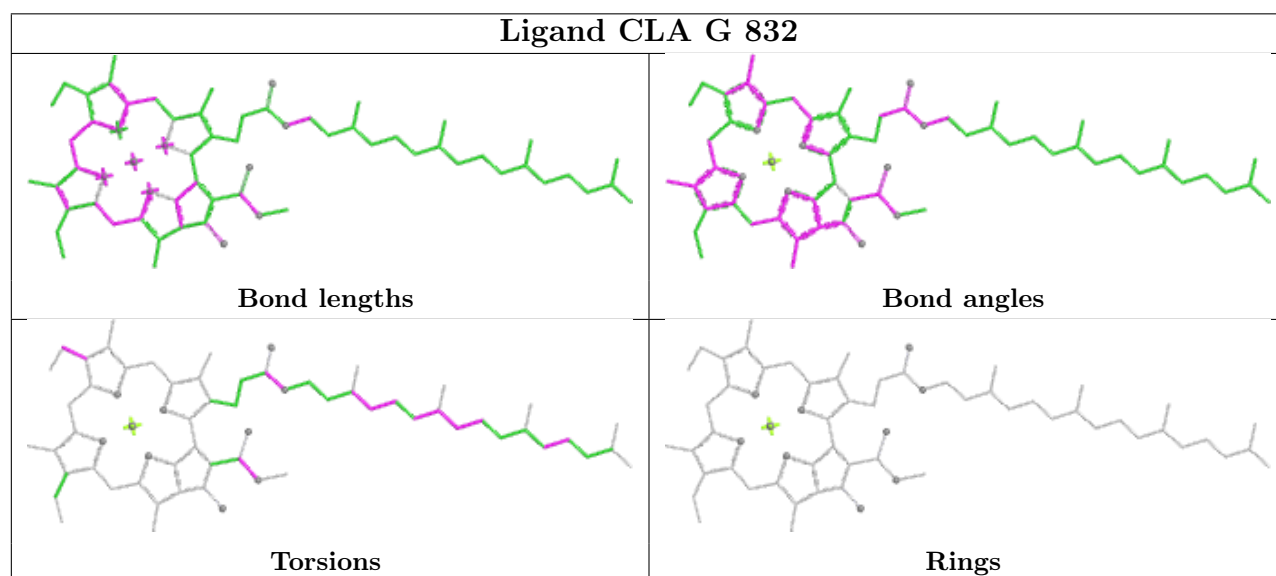
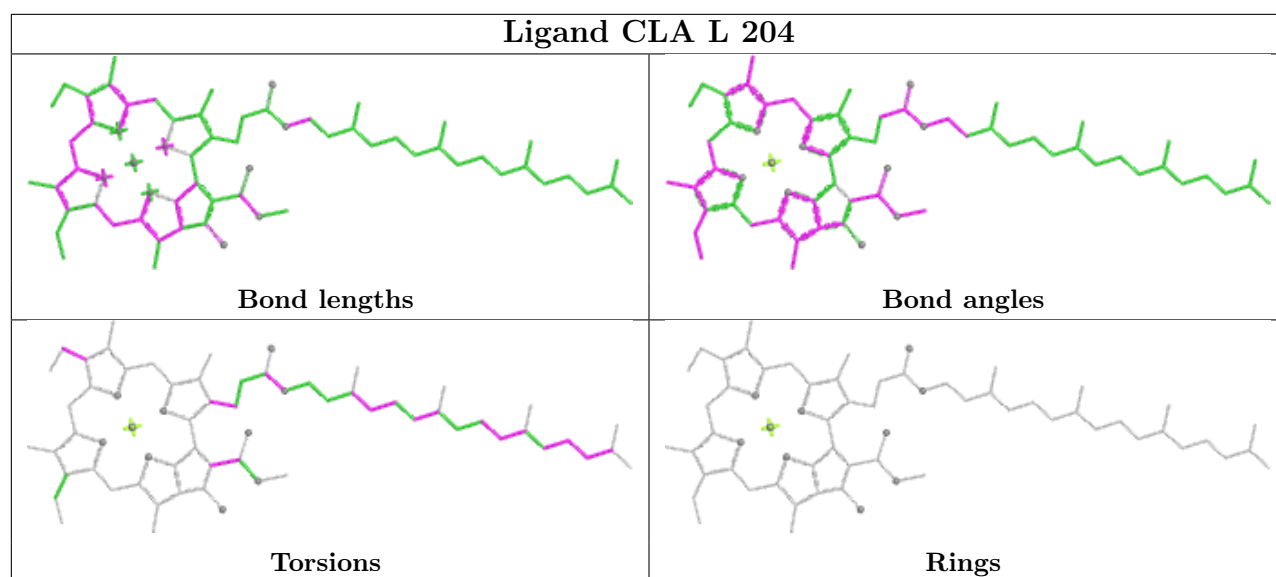


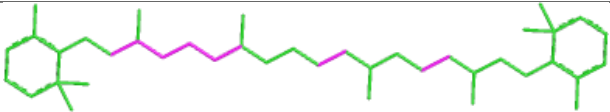
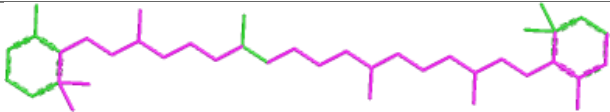
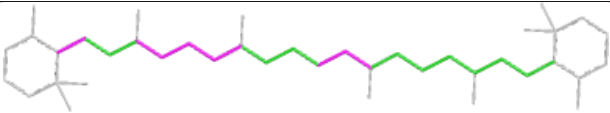
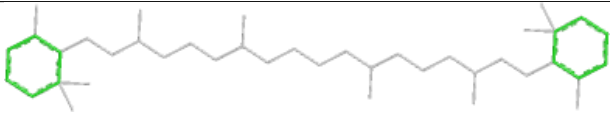
Ligand CLA B 838

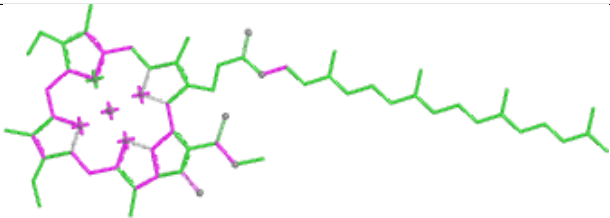
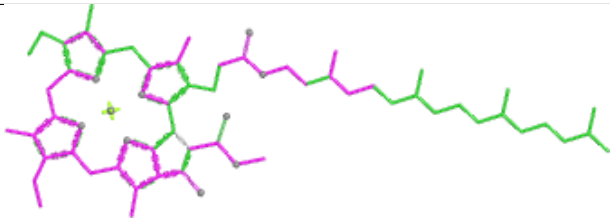
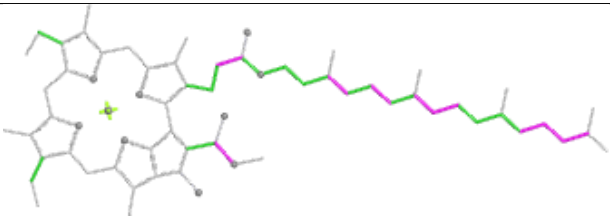
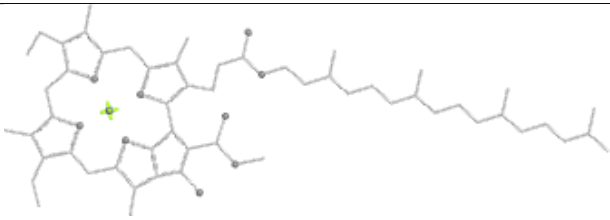


Ligand BCR Z 843

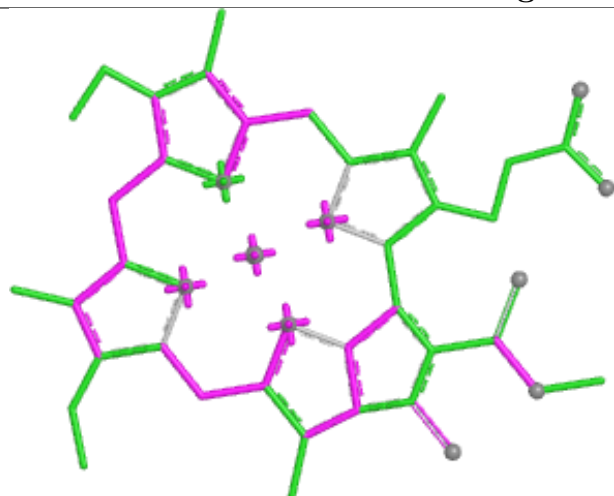




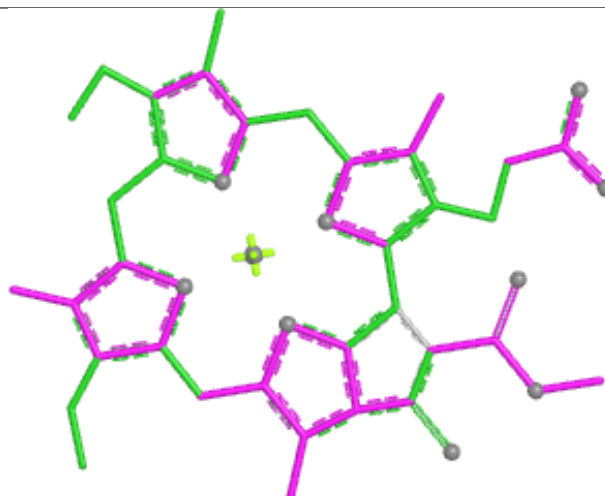
Ligand BCR A 847			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand CLA Z 810			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

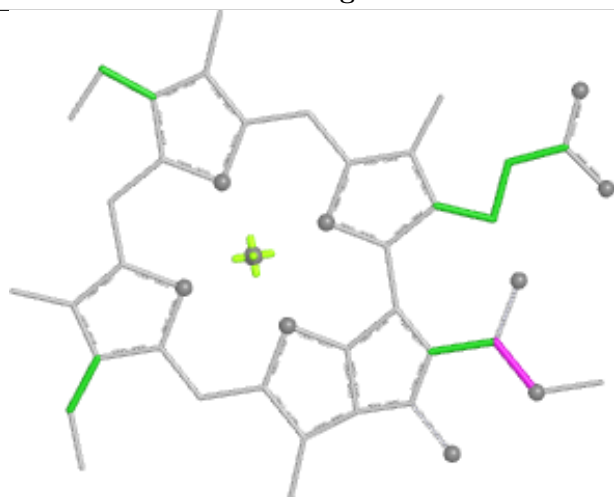
Ligand CLA d 202



Bond lengths



Bond angles

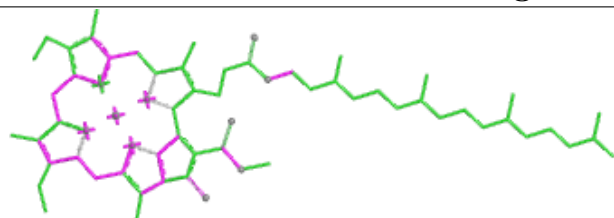


Torsions

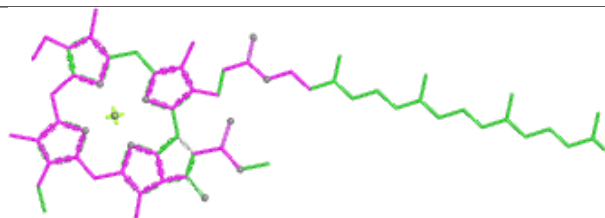


Rings

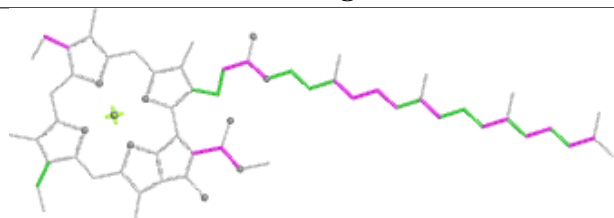
Ligand CLA H 808



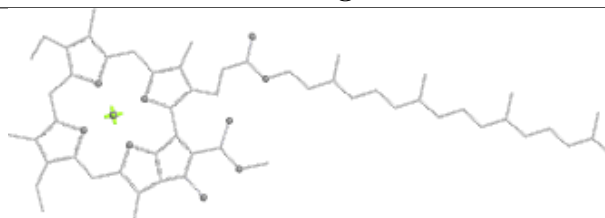
Bond lengths



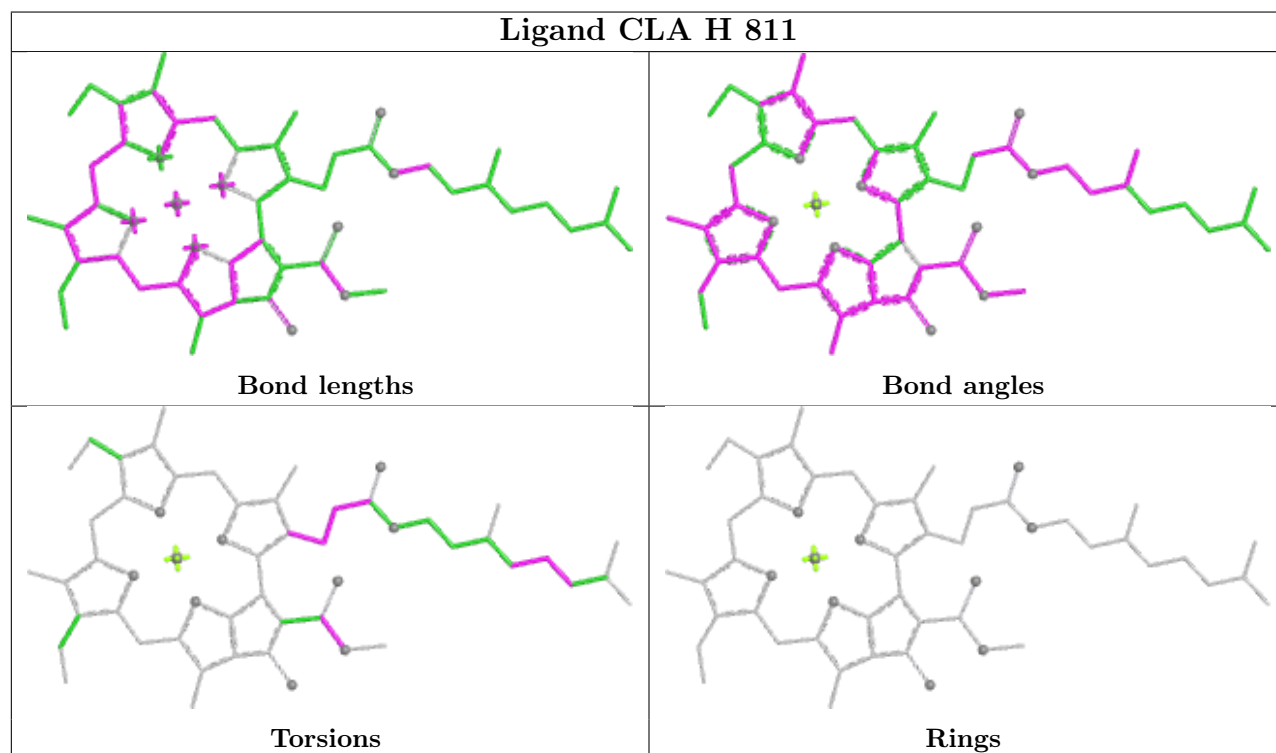
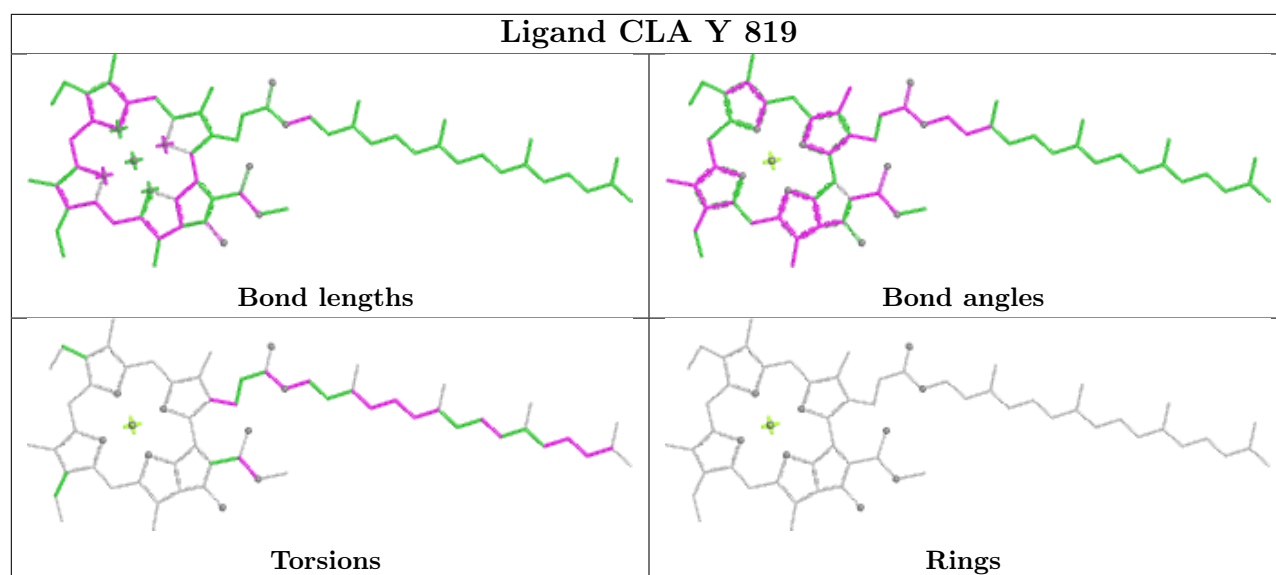
Bond angles



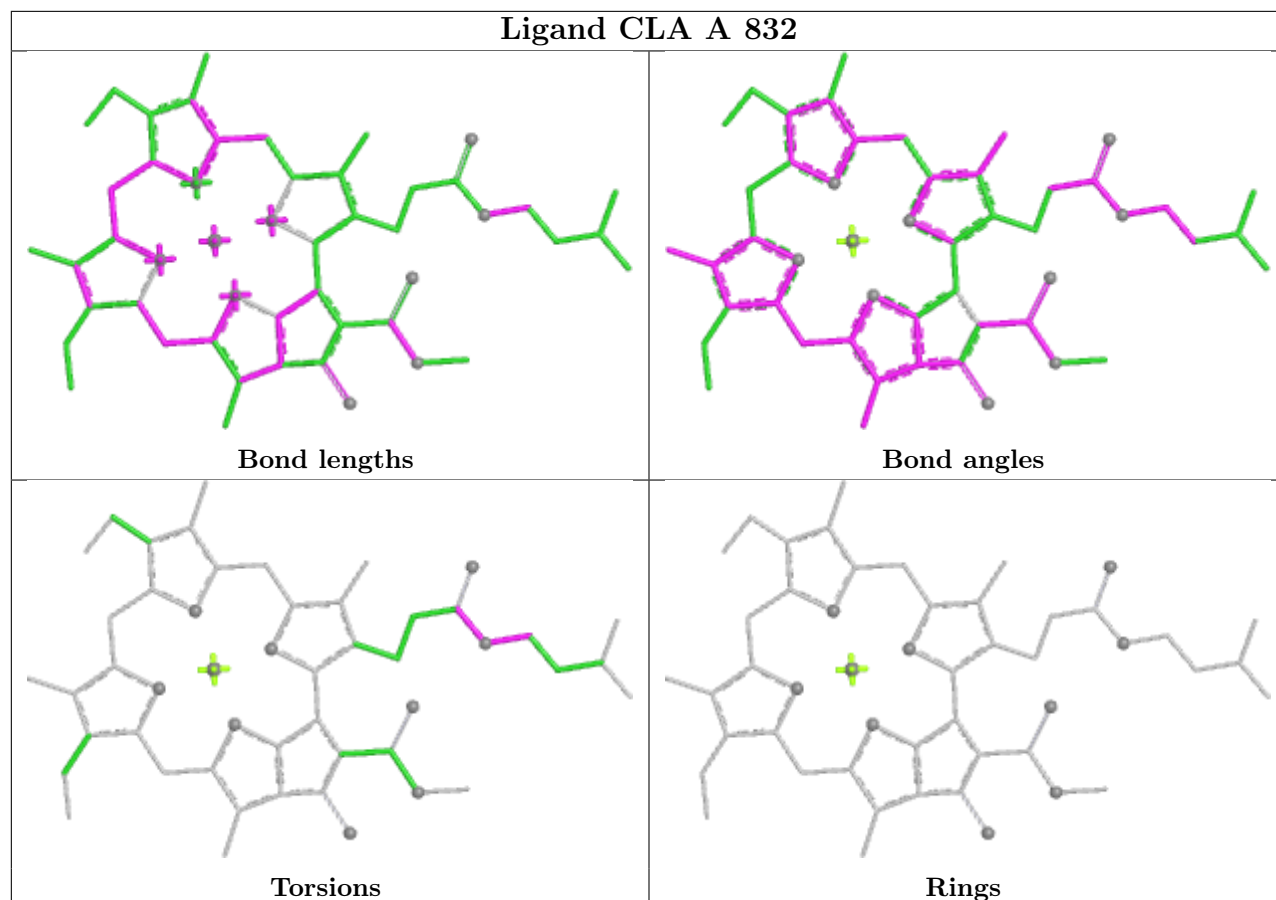
Torsions



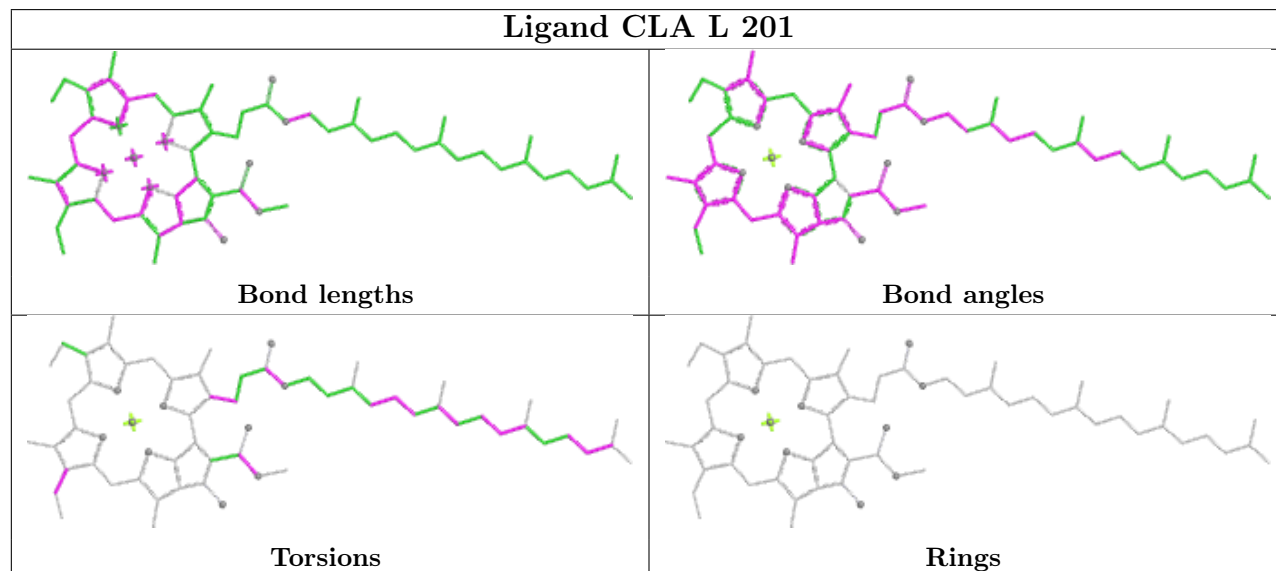
Rings



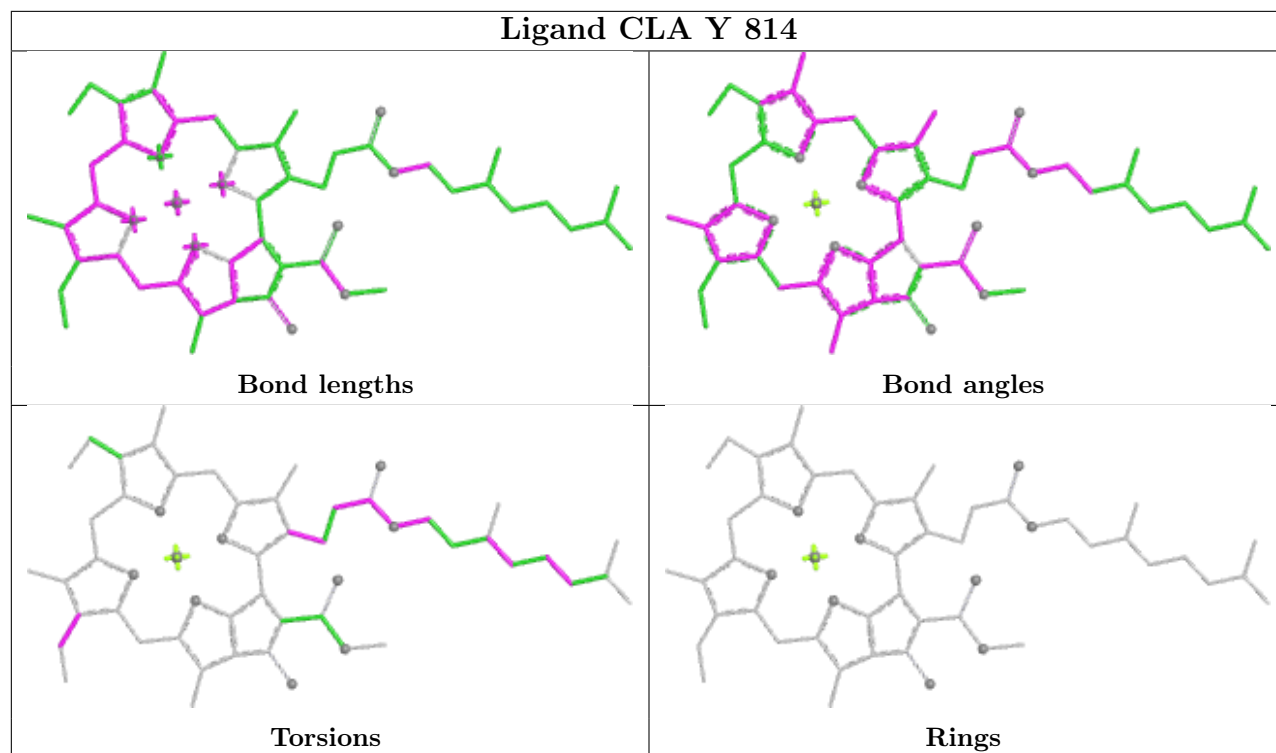
Ligand CLA A 832



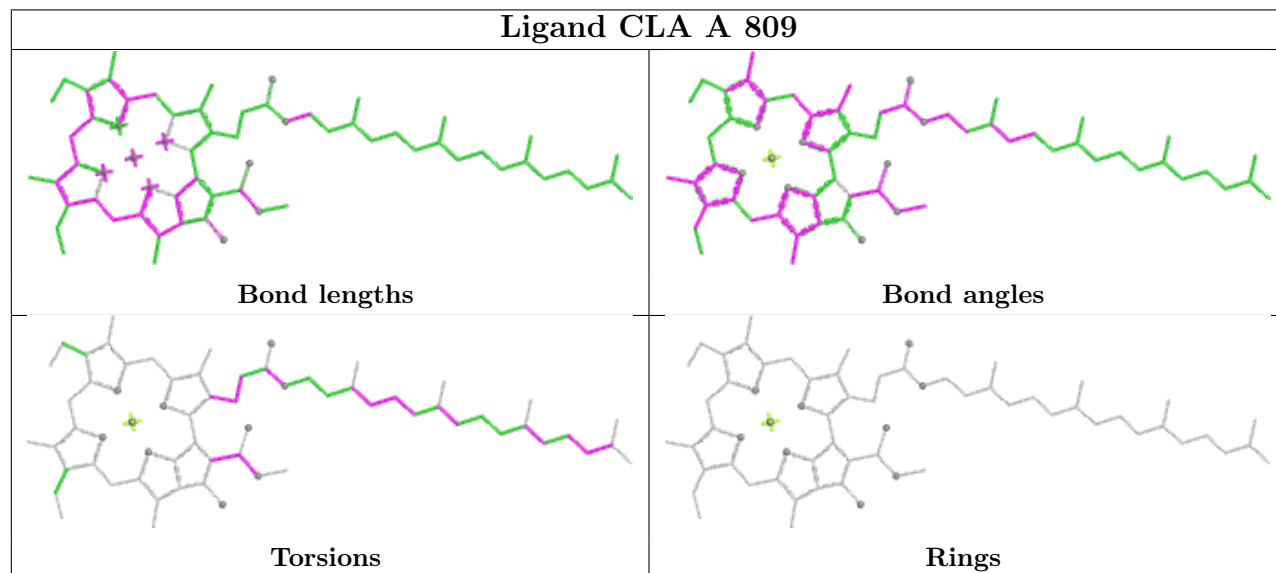
Ligand CLA L 201



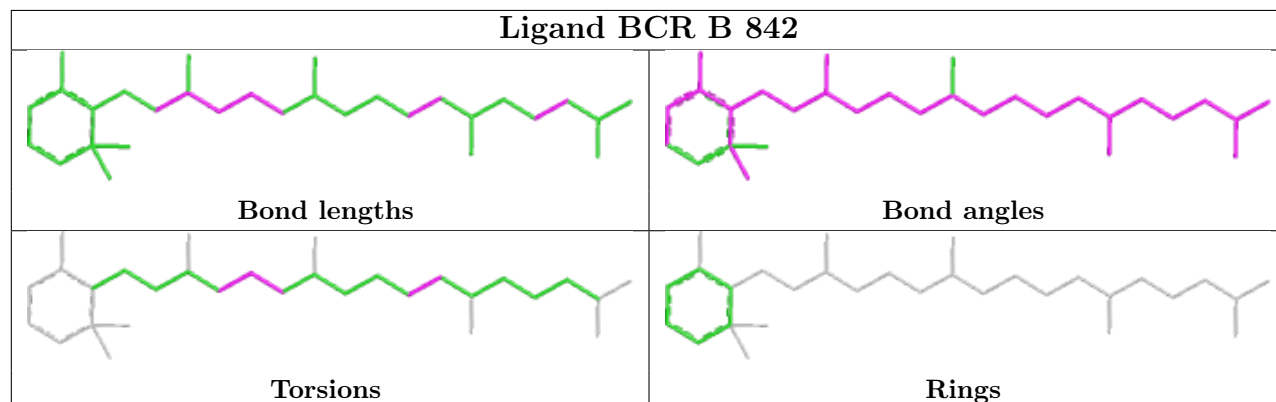
Ligand CLA Y 814

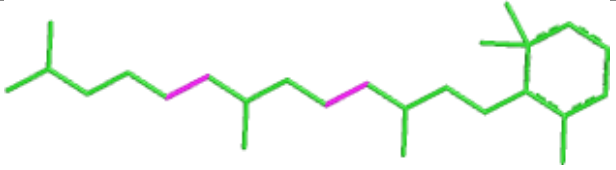
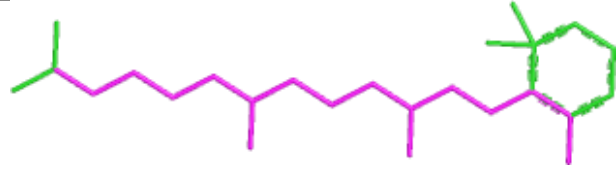
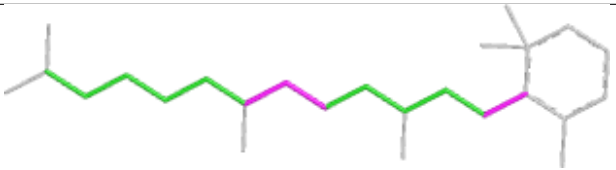
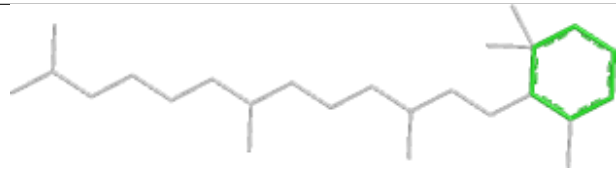


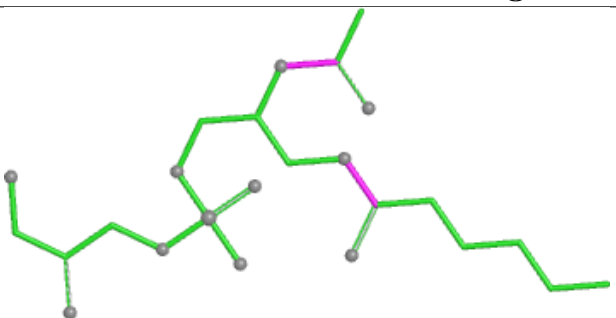
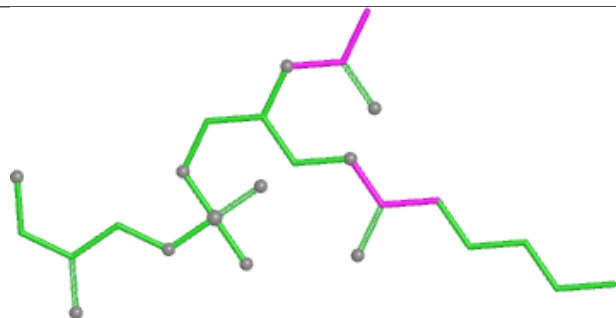
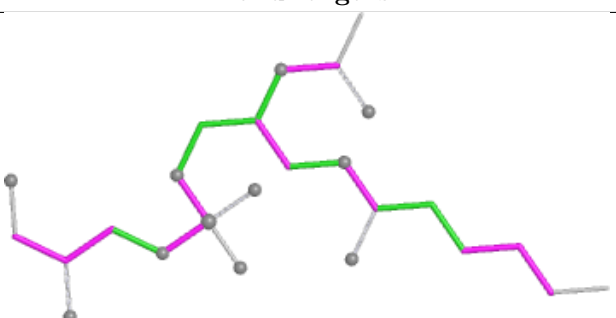
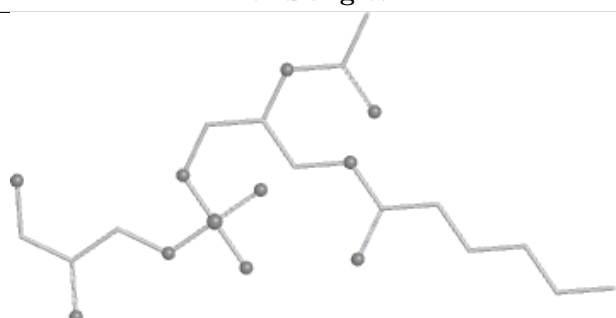
Ligand CLA A 809

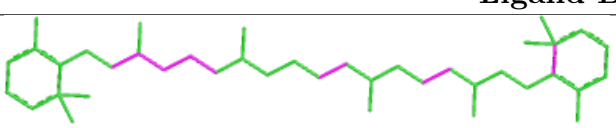
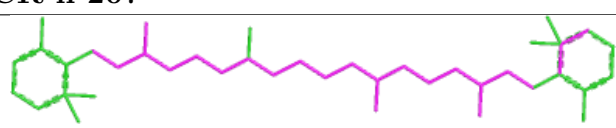
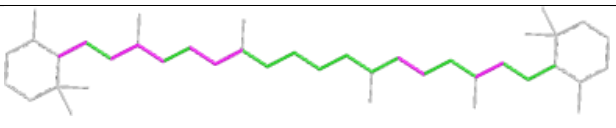
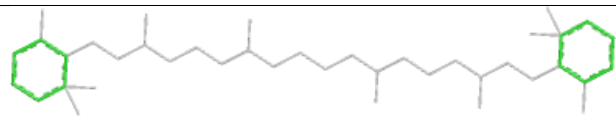


Ligand BCR B 842

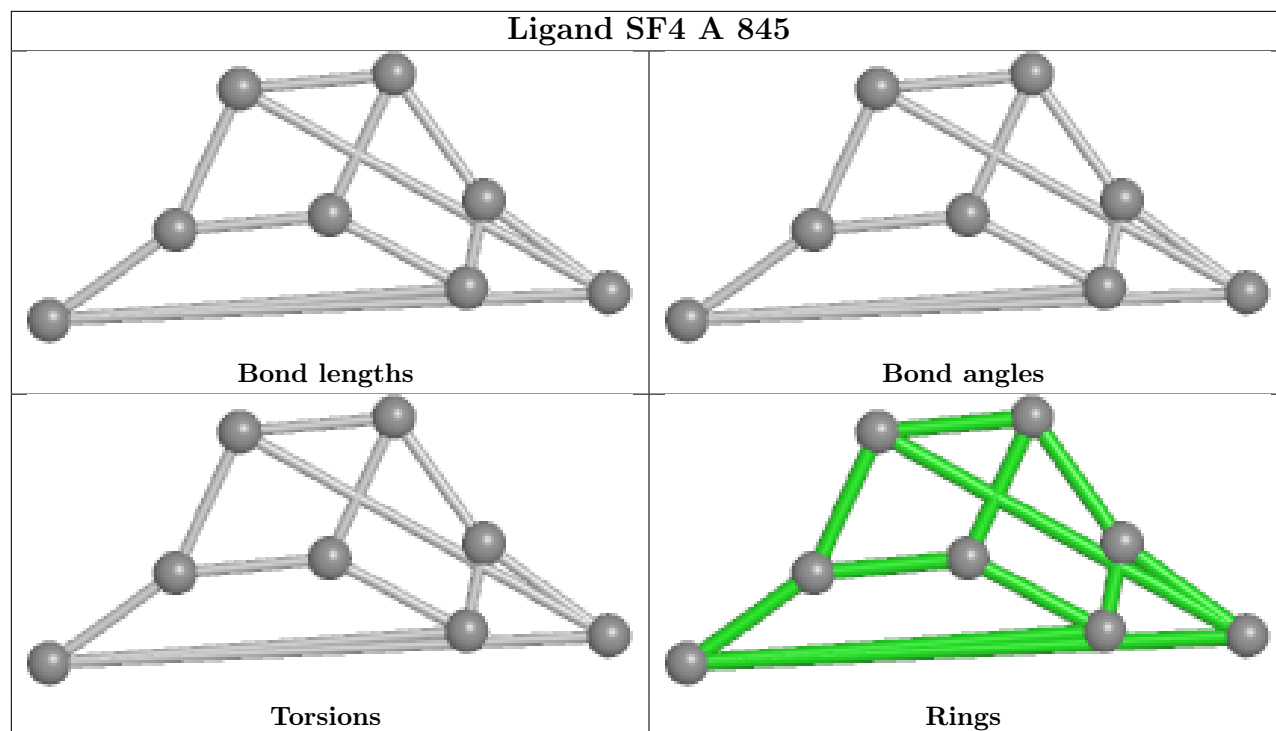


Ligand BCR B 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

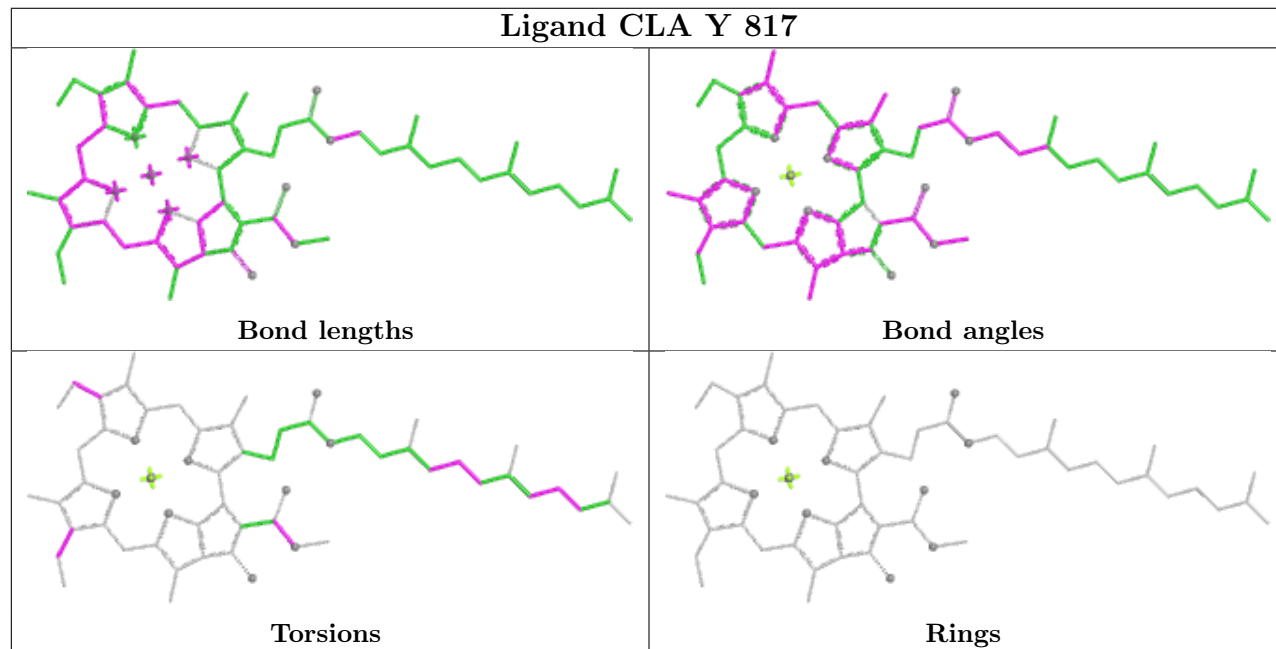
Ligand LHG Y 851	
	
Bond lengths	Bond angles
	
Torsions	Rings

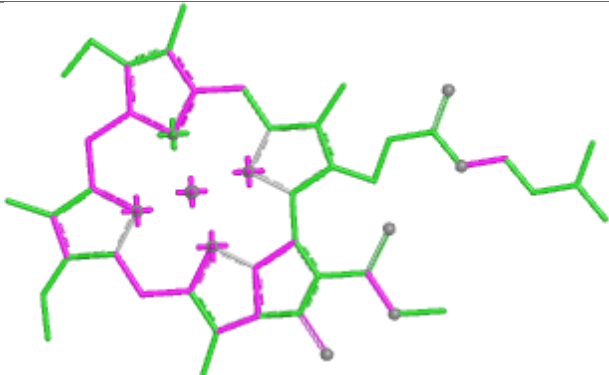
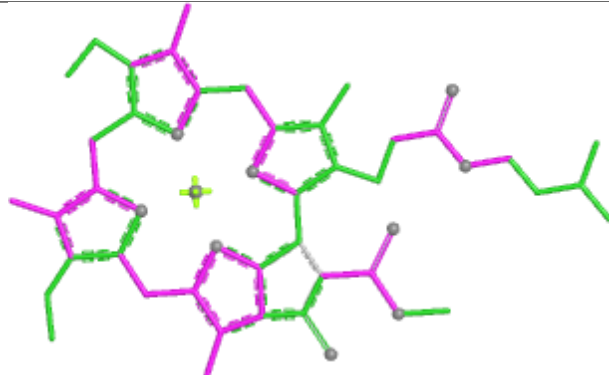
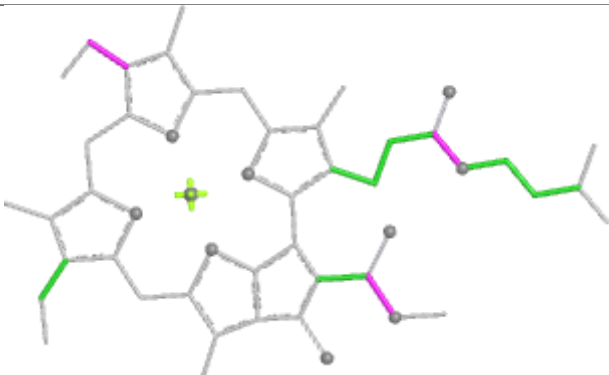
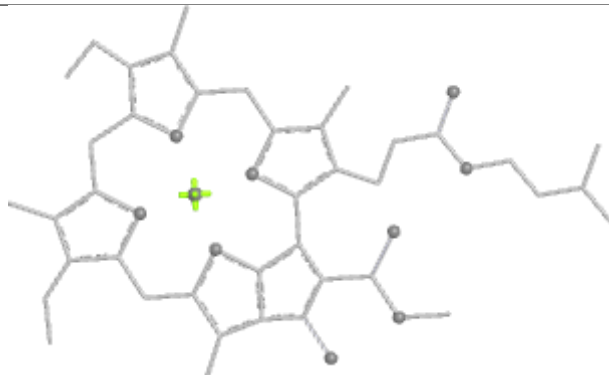
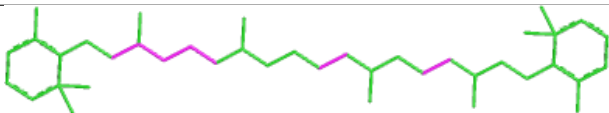
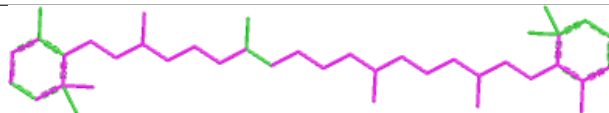
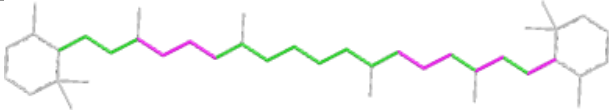
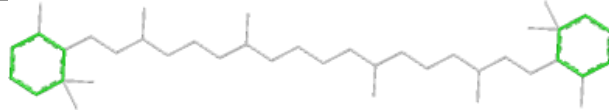
Ligand BCR h 207	
	
Bond lengths	Bond angles
	
Torsions	Rings

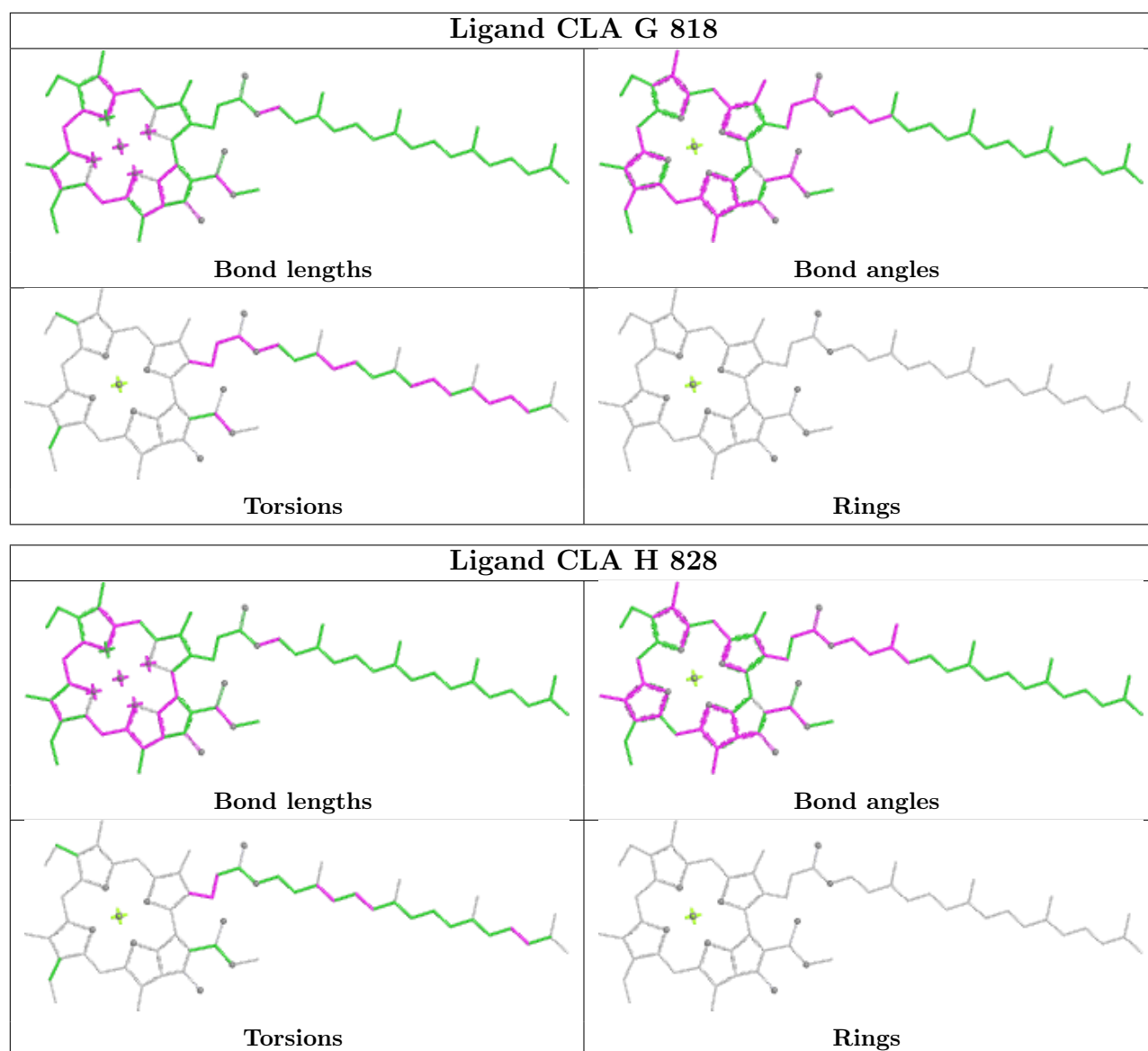
Ligand SF4 A 845



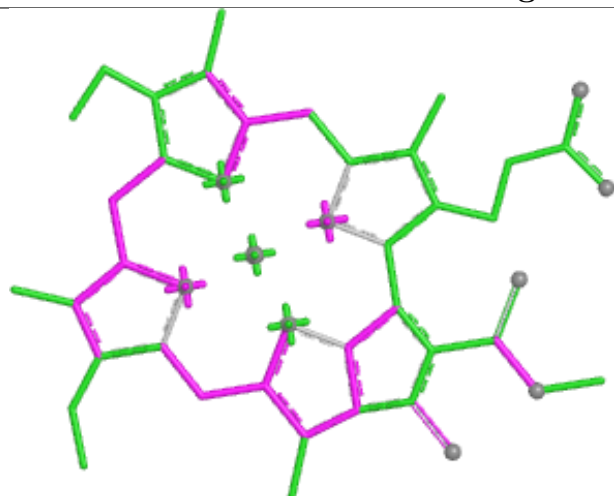
Ligand CLA Y 817



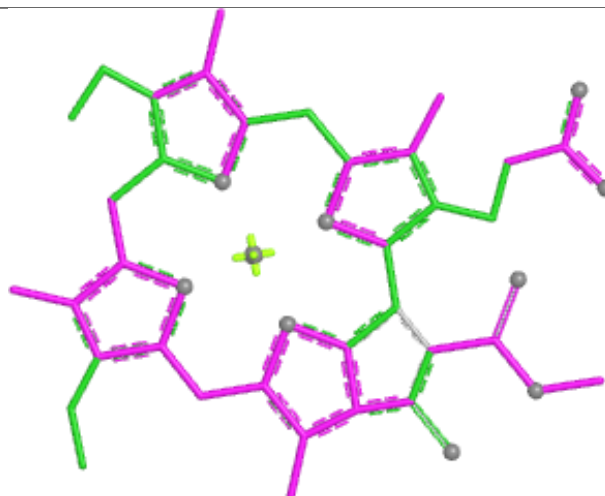
Ligand CLA Y 831	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR T 102	
	
Bond lengths	Bond angles
	
Torsions	Rings



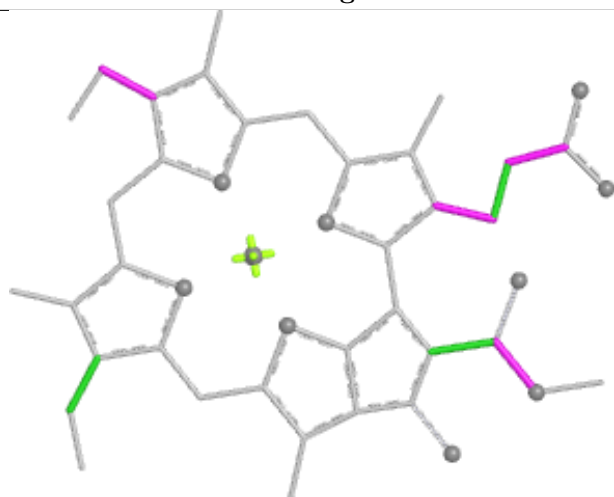
Ligand CLA J 101



Bond lengths



Bond angles

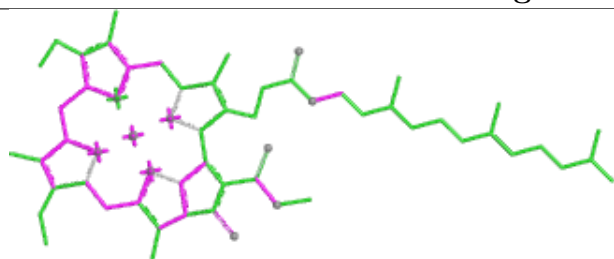


Torsions

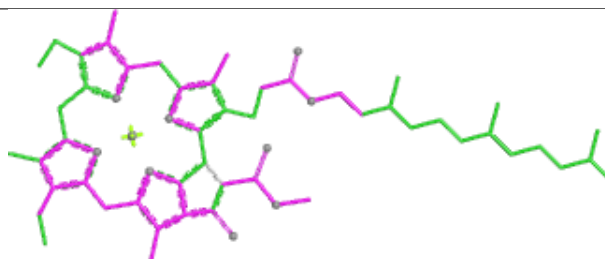


Rings

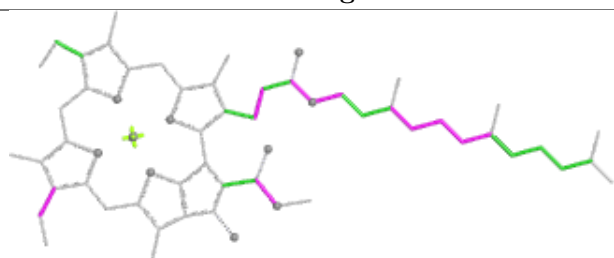
Ligand CLA Y 824



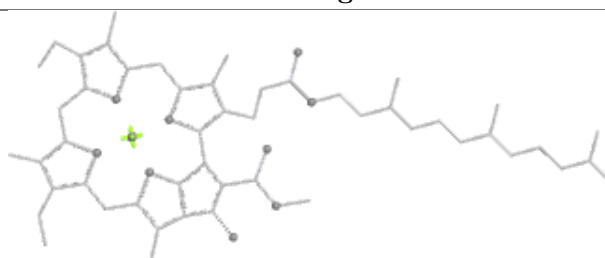
Bond lengths



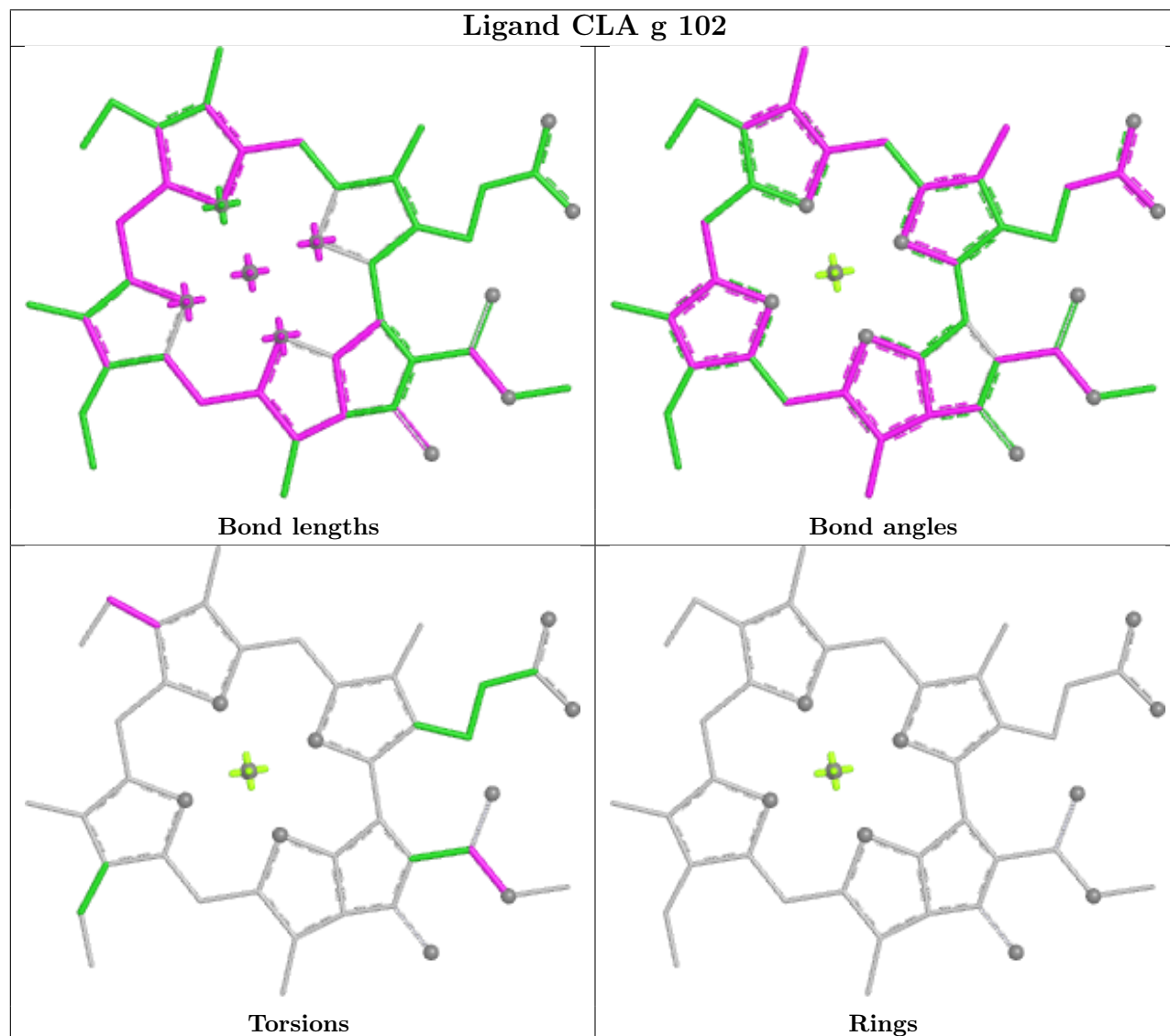
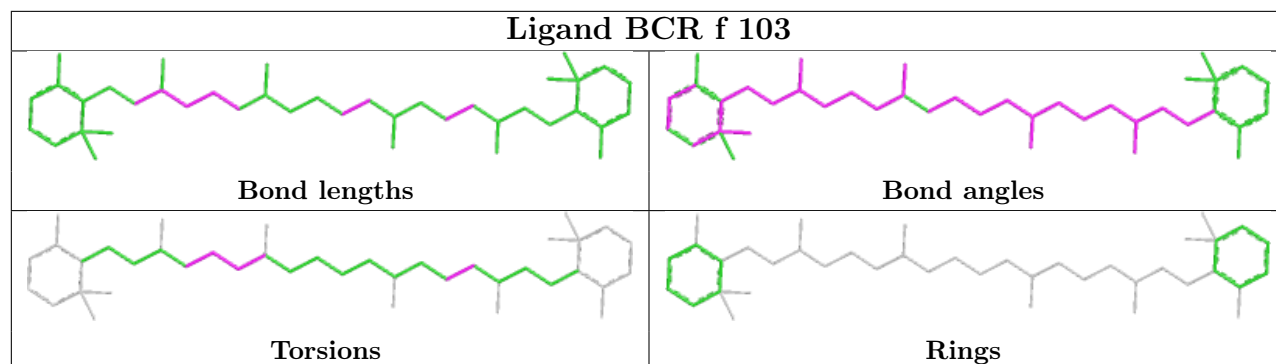
Bond angles



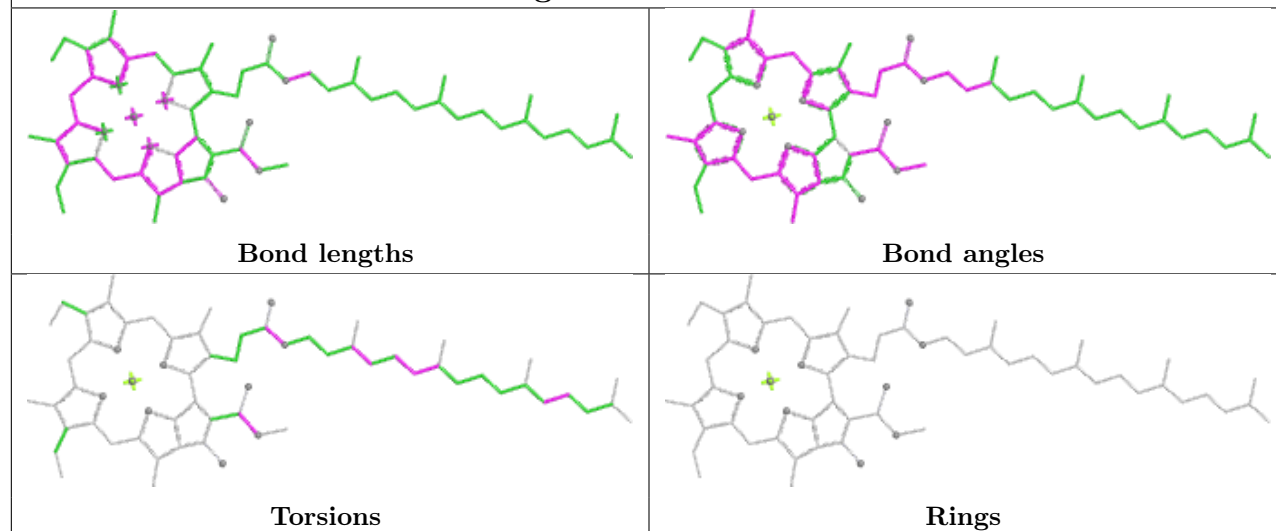
Torsions



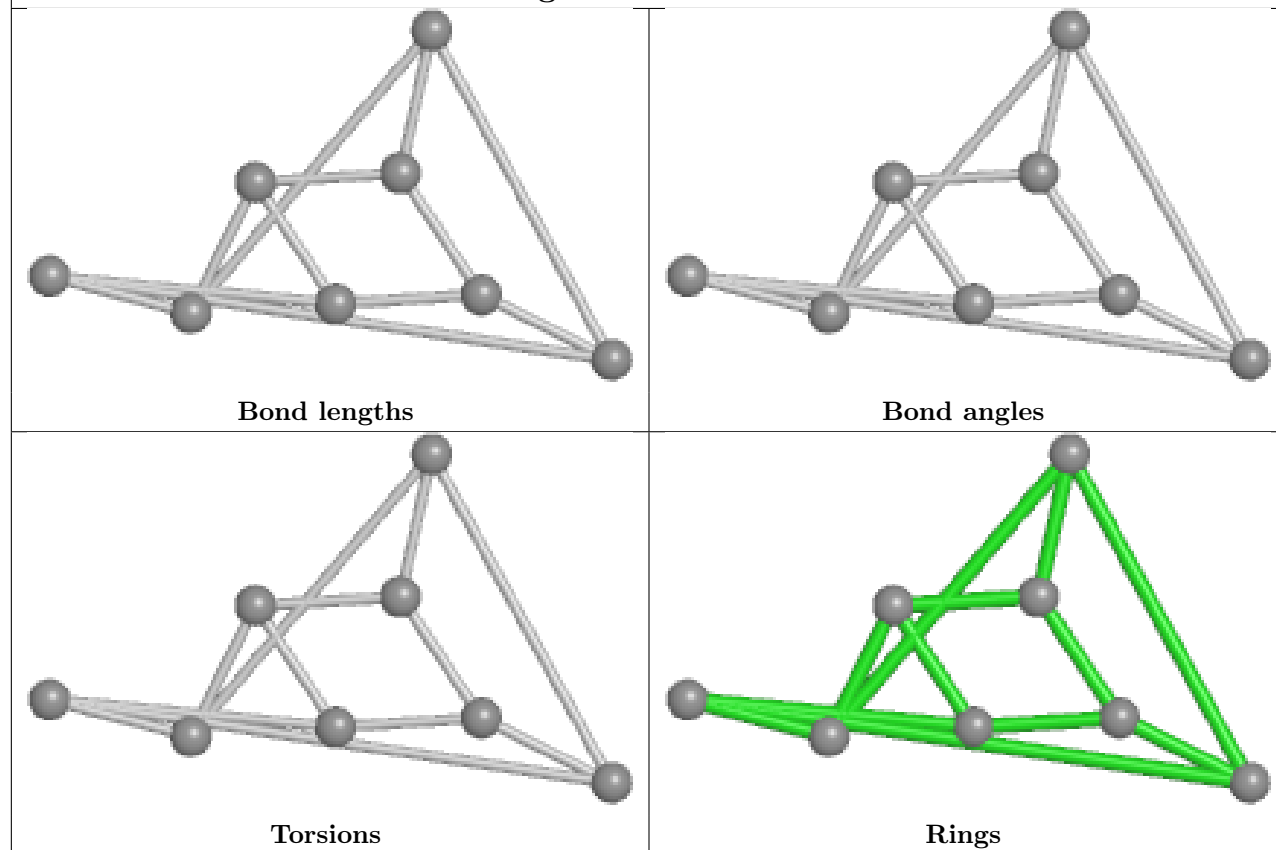
Rings

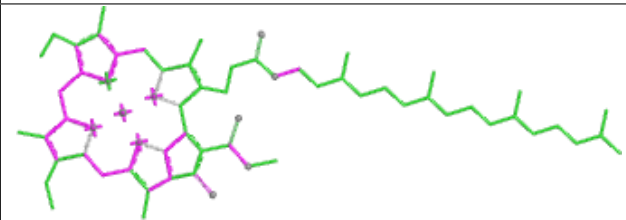
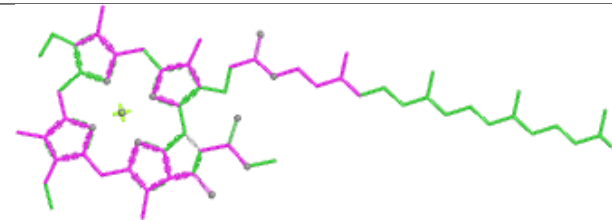
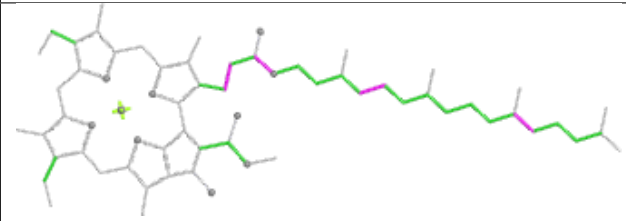
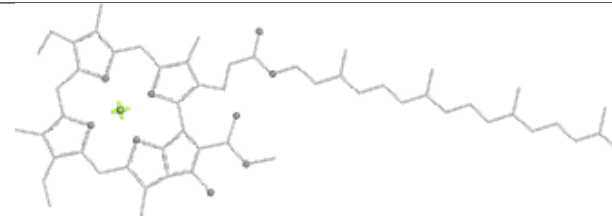


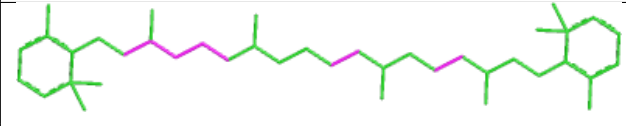
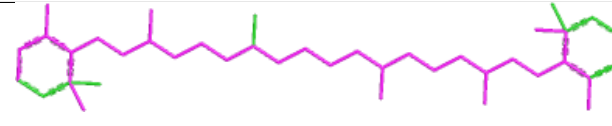
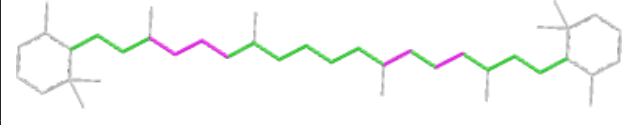
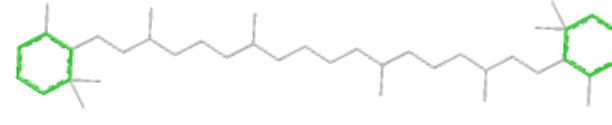
Ligand CLA L 206



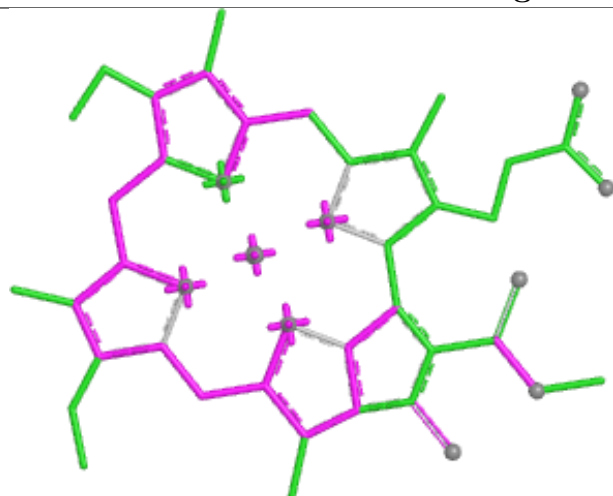
Ligand SF4 G 844



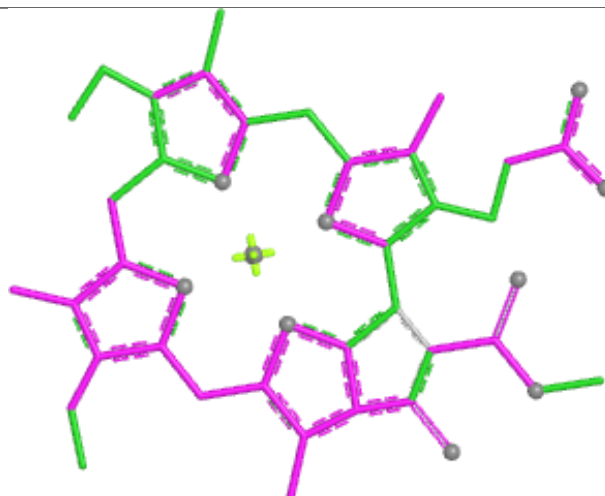
Ligand CLA H 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR Y 853	
	
Bond lengths	Bond angles
	
Torsions	Rings

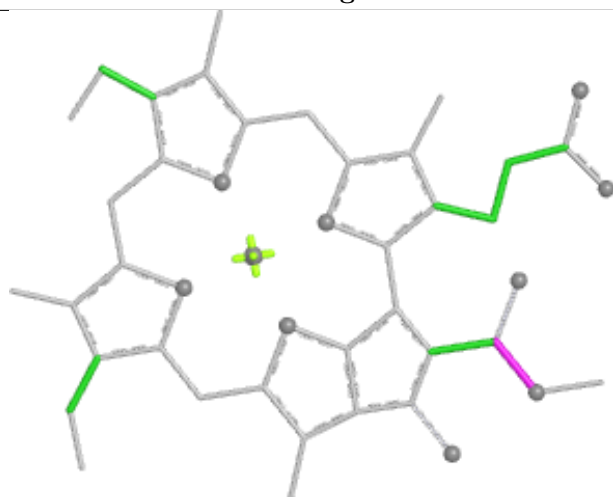
Ligand CLA Y 810



Bond lengths



Bond angles

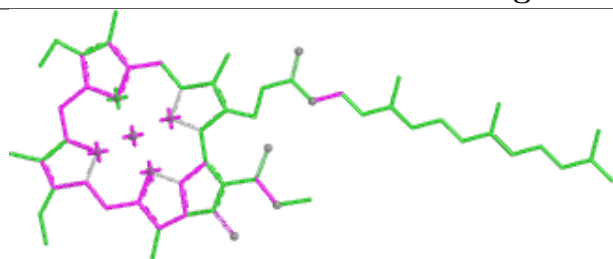


Torsions

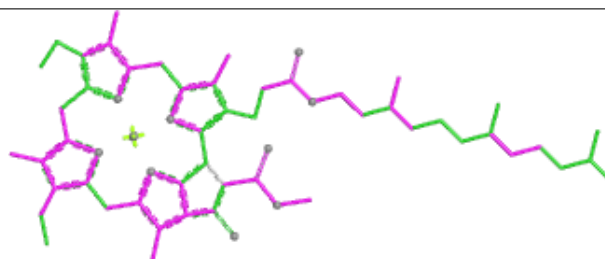


Rings

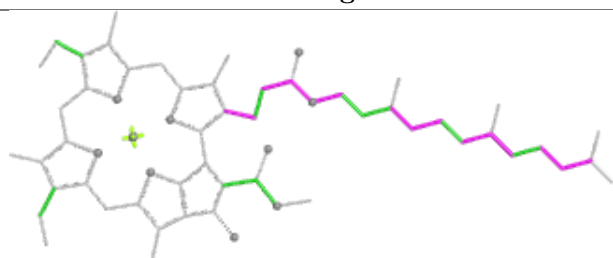
Ligand CLA H 819



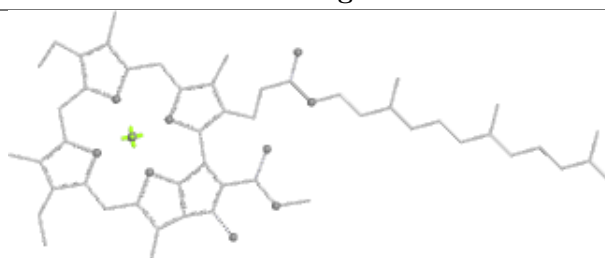
Bond lengths



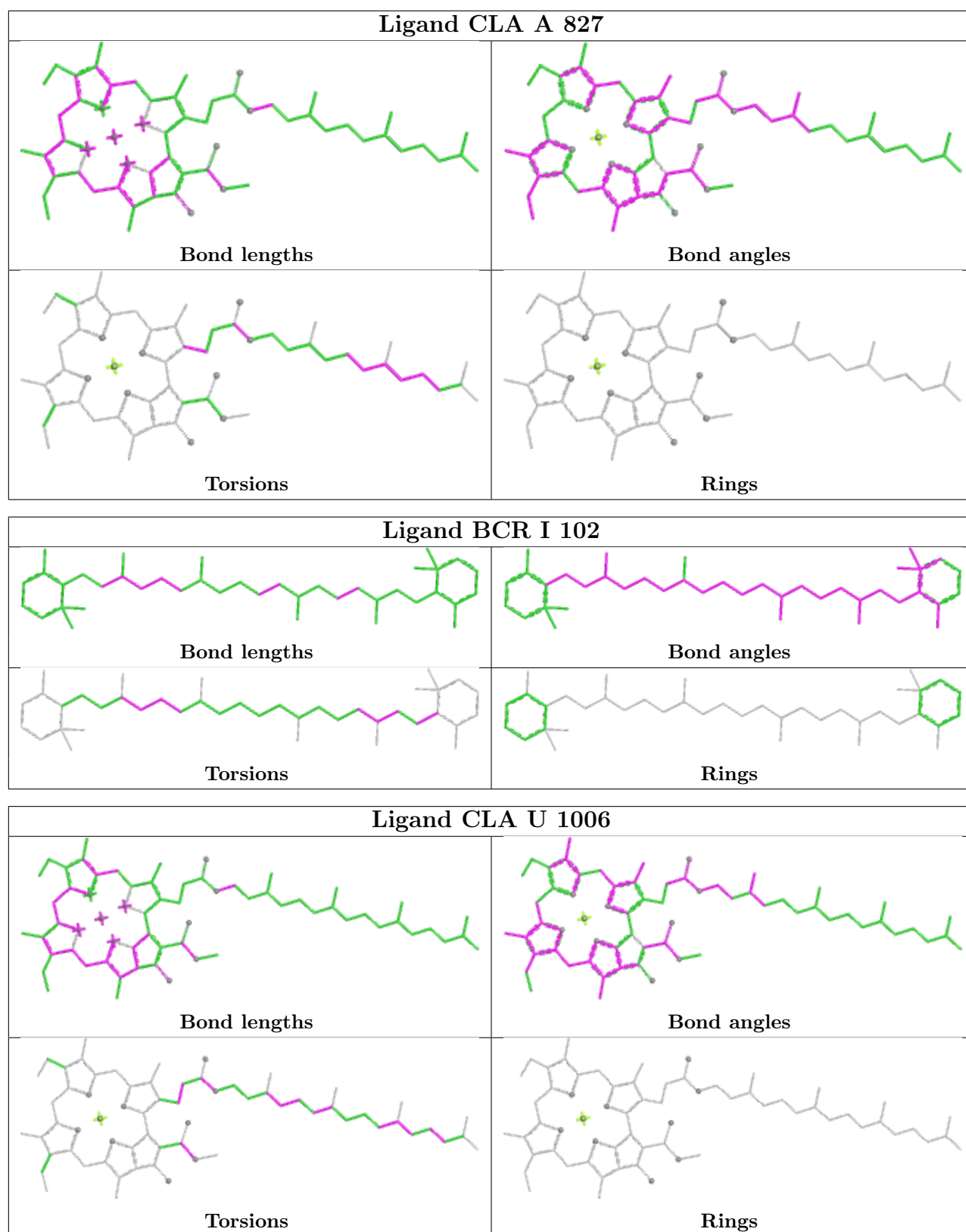
Bond angles

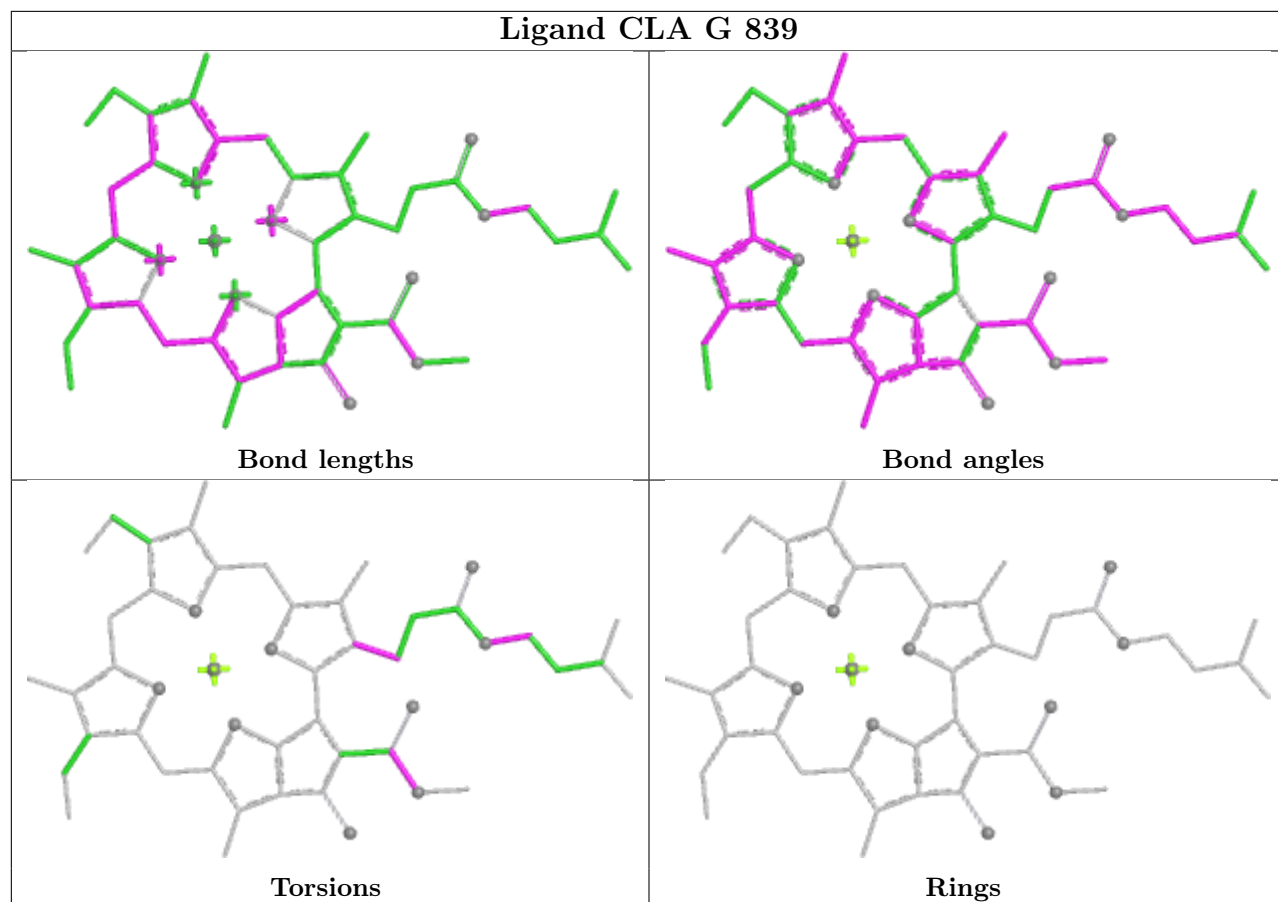


Torsions

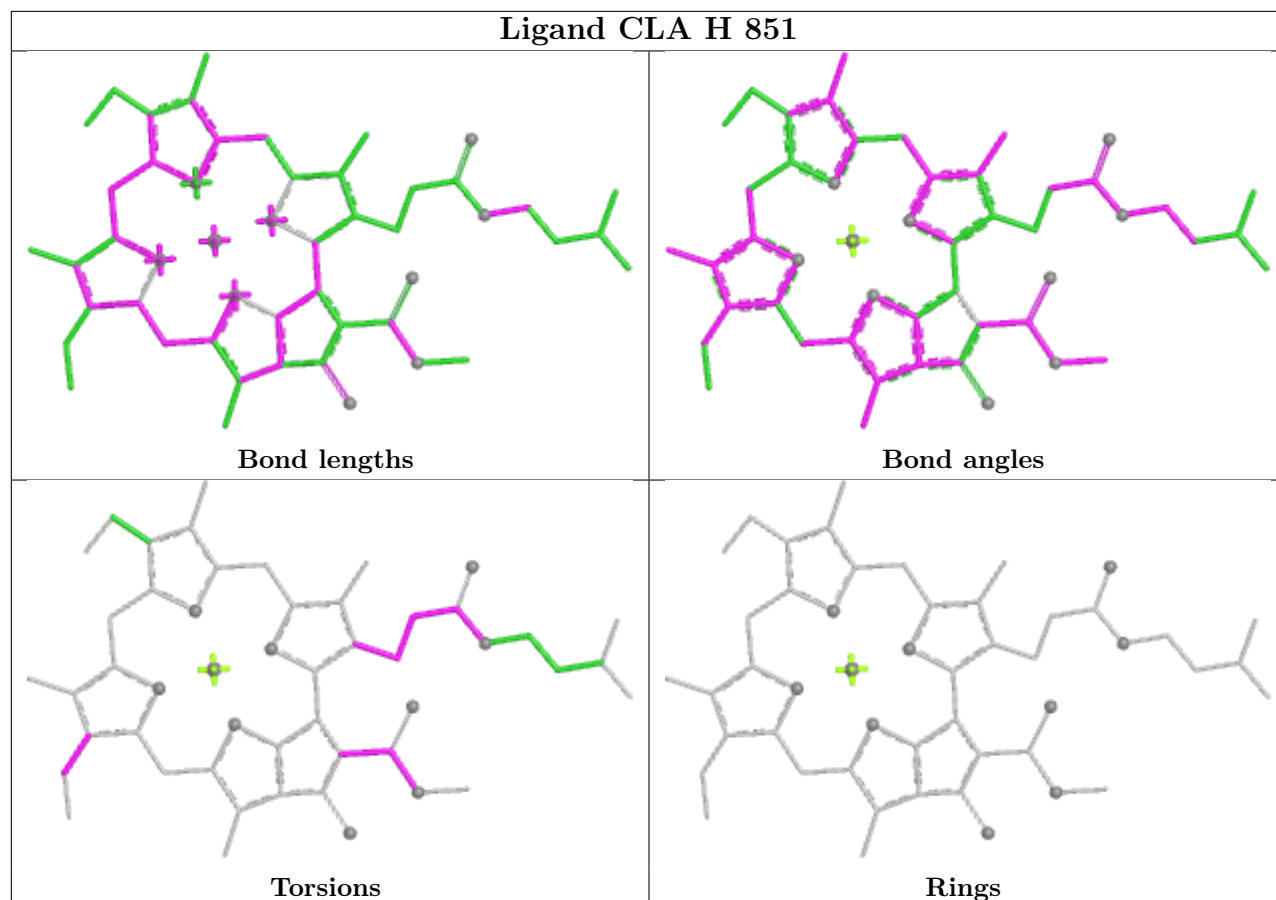


Rings

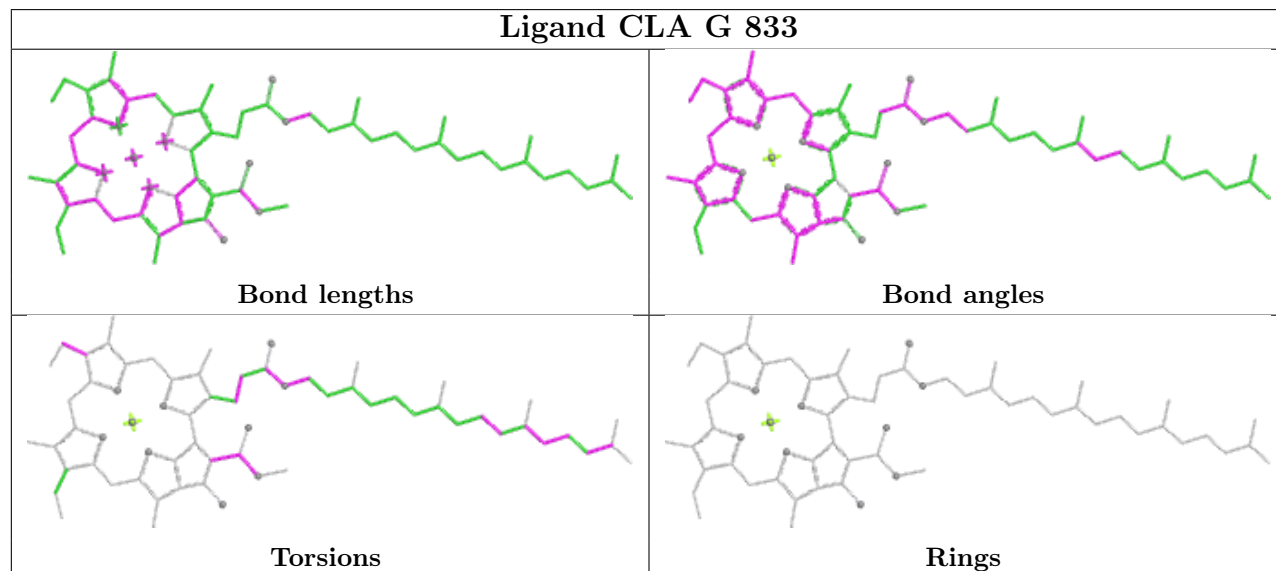


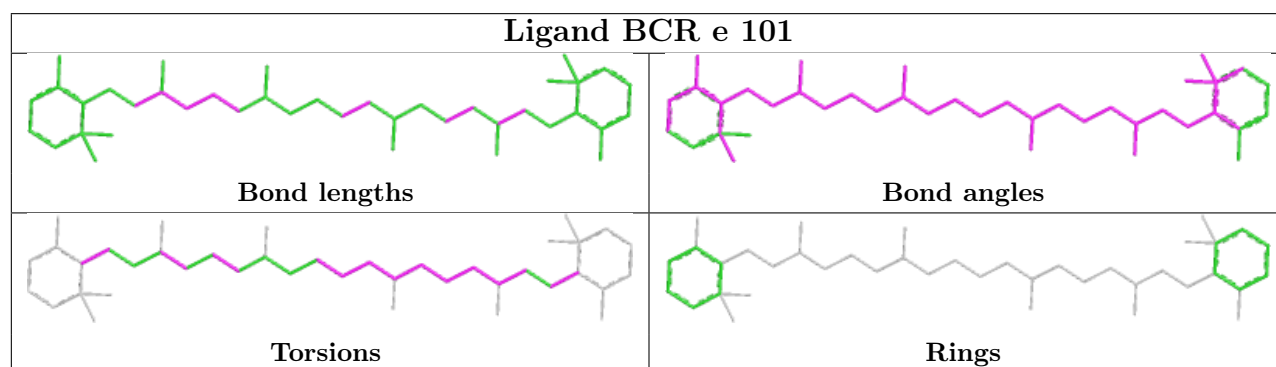
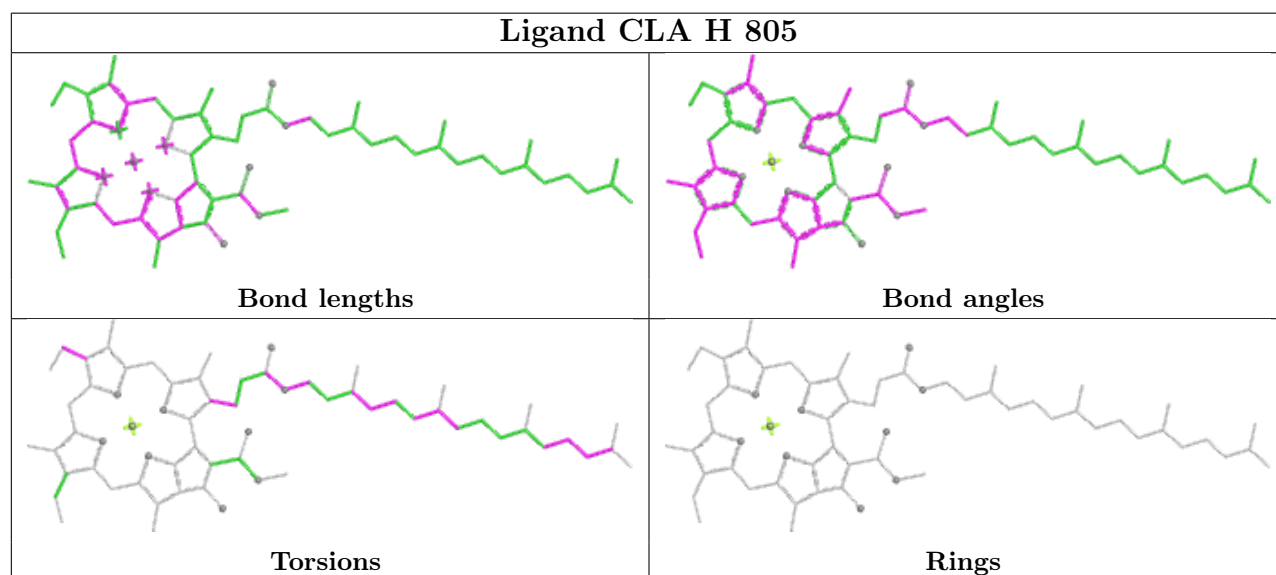
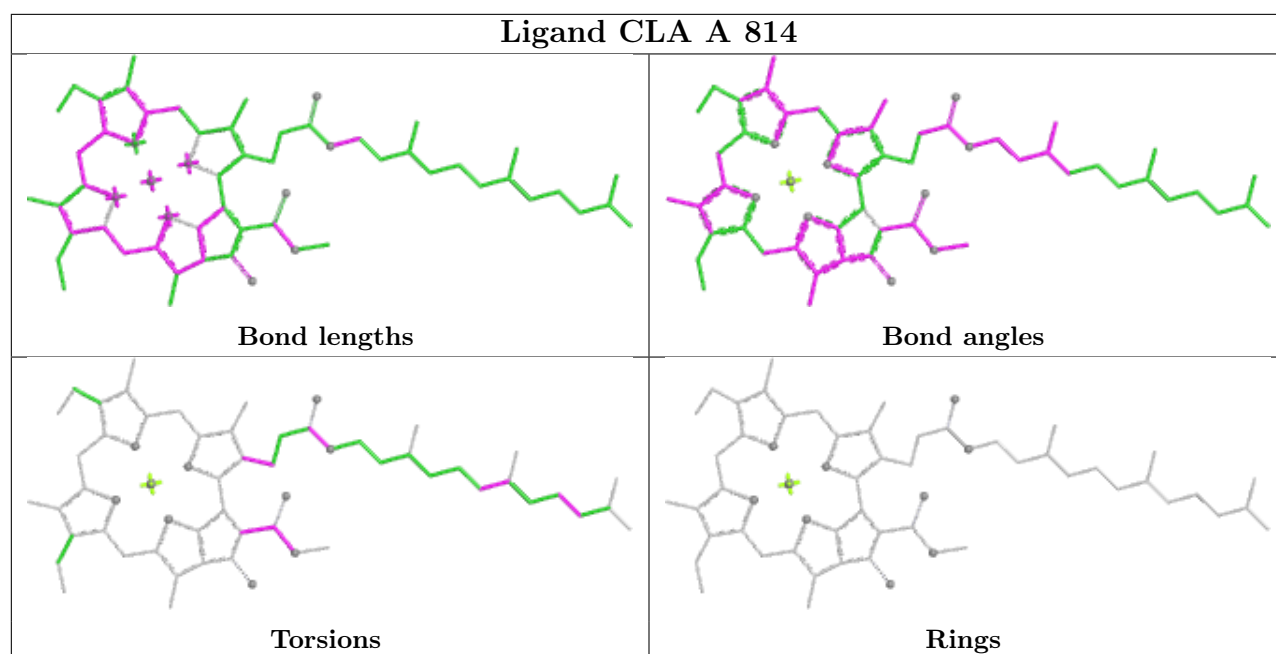


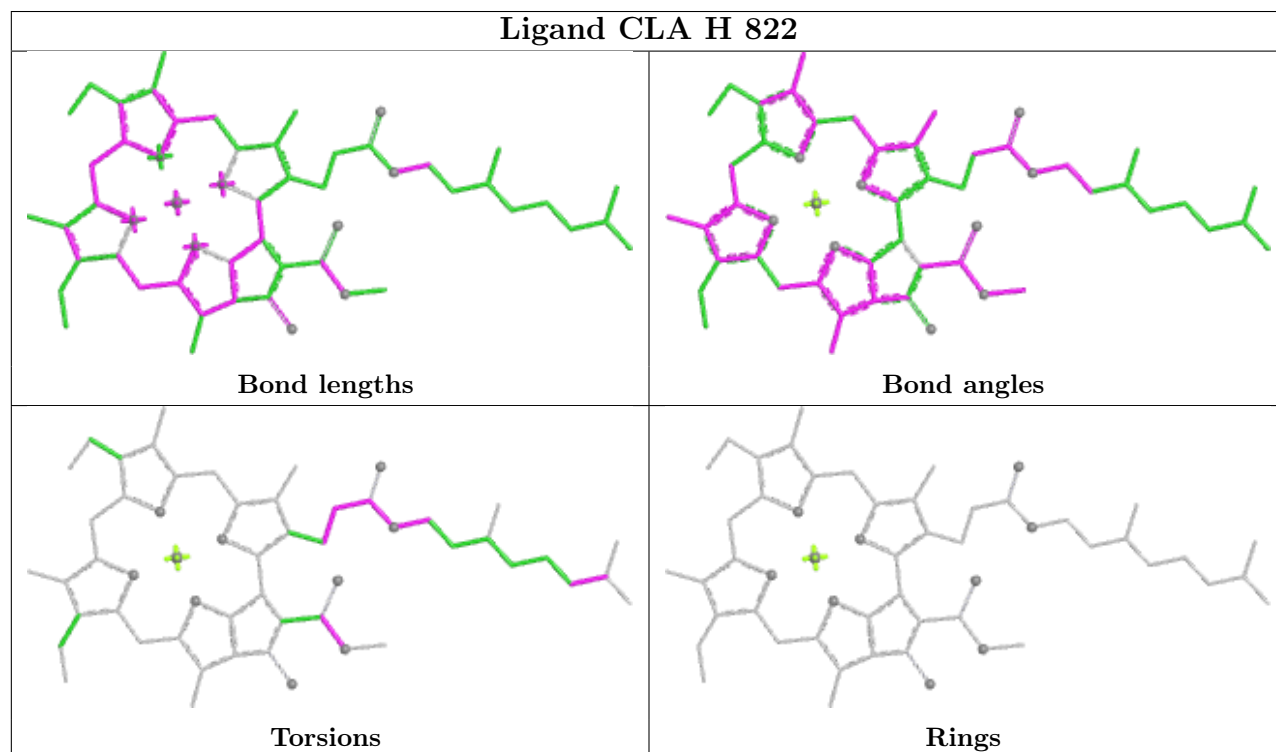
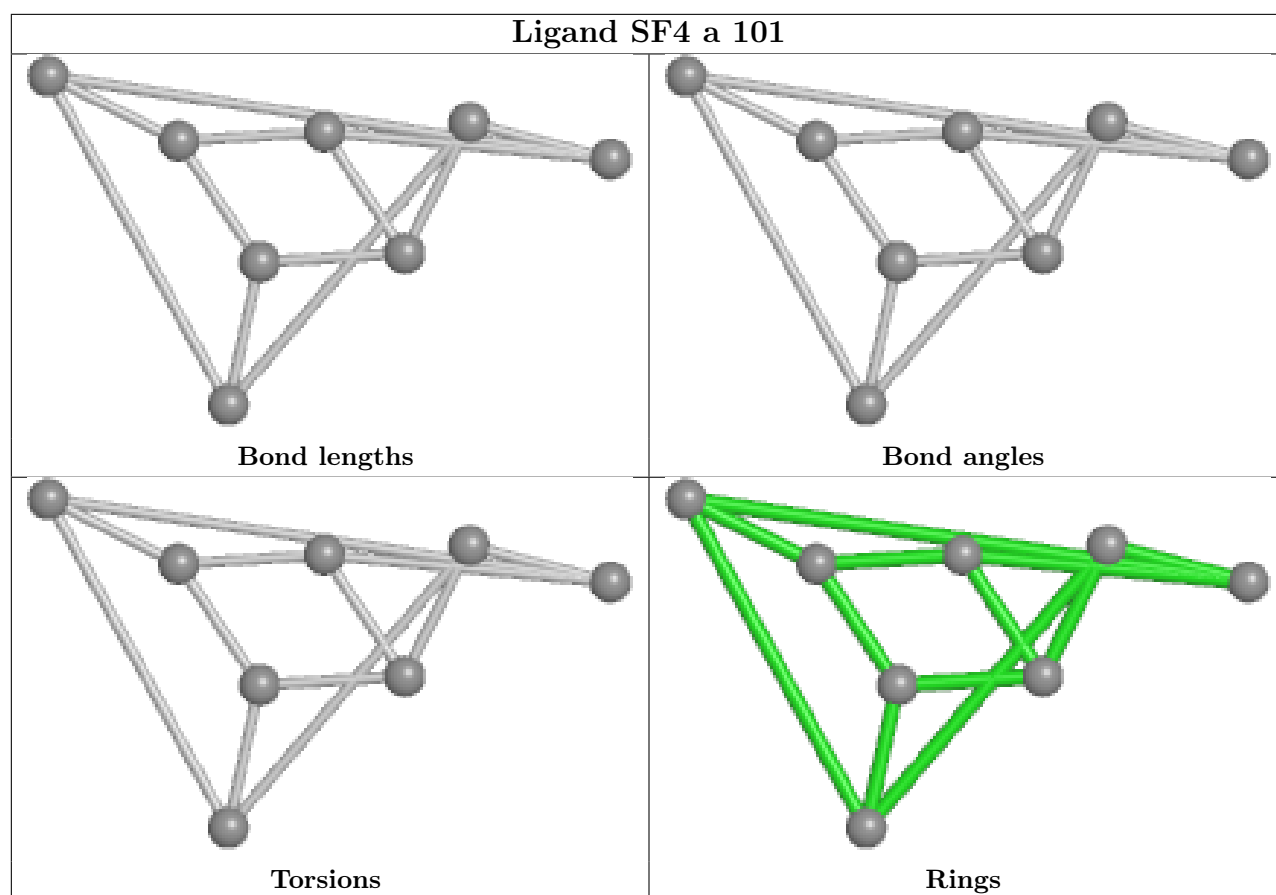
Ligand CLA H 851

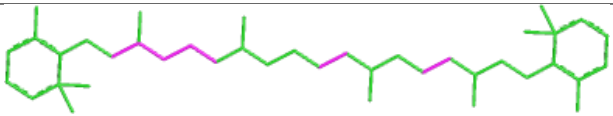
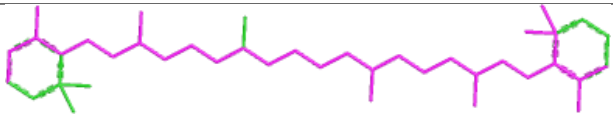
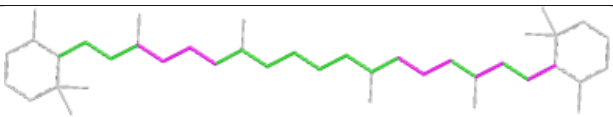
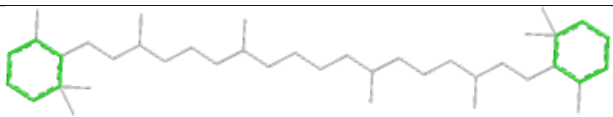


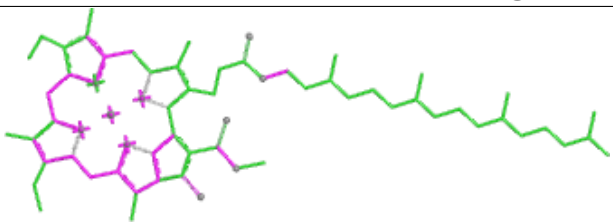
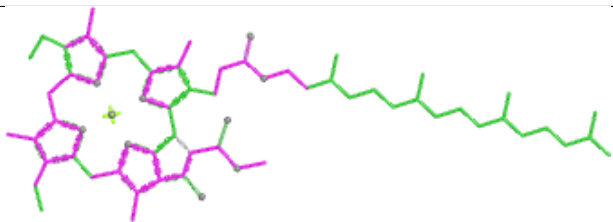
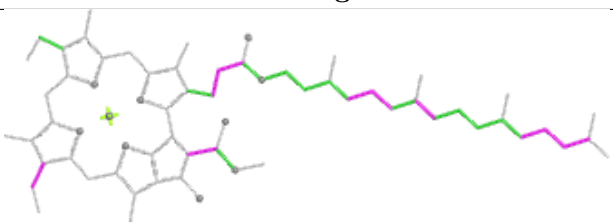
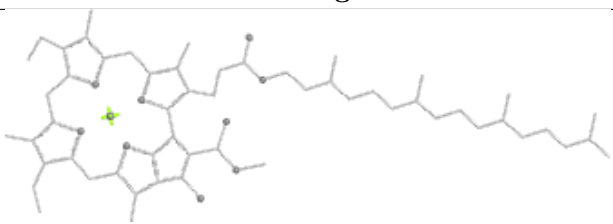
Ligand CLA G 833

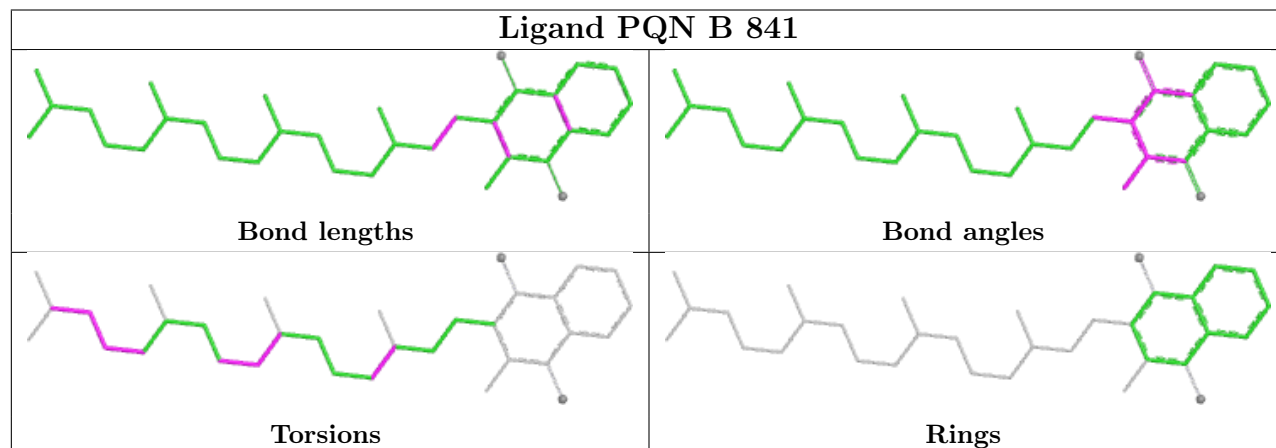
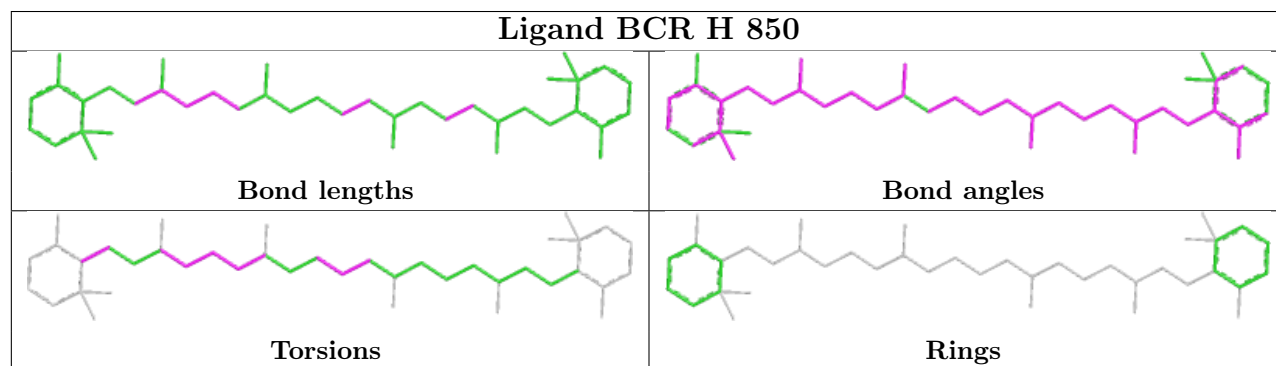
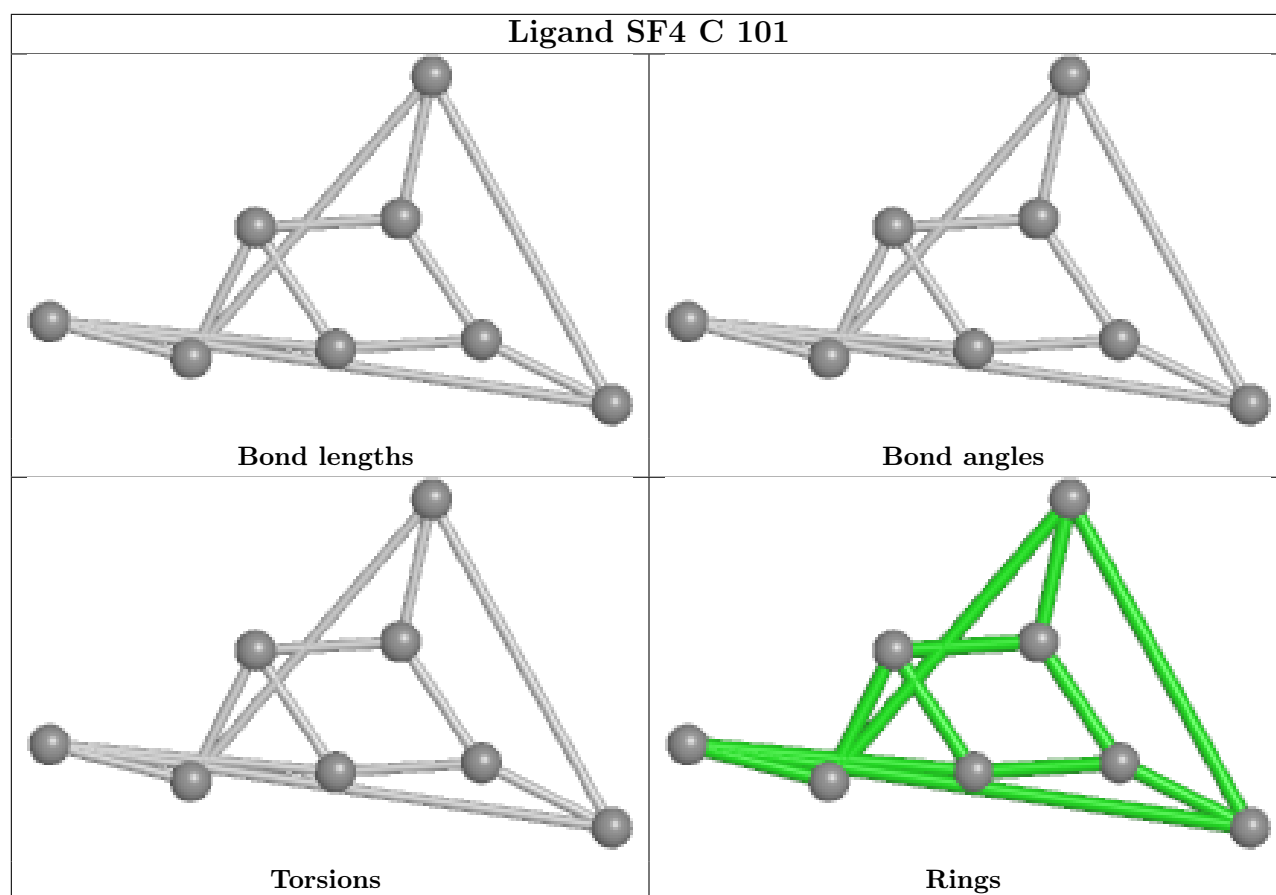


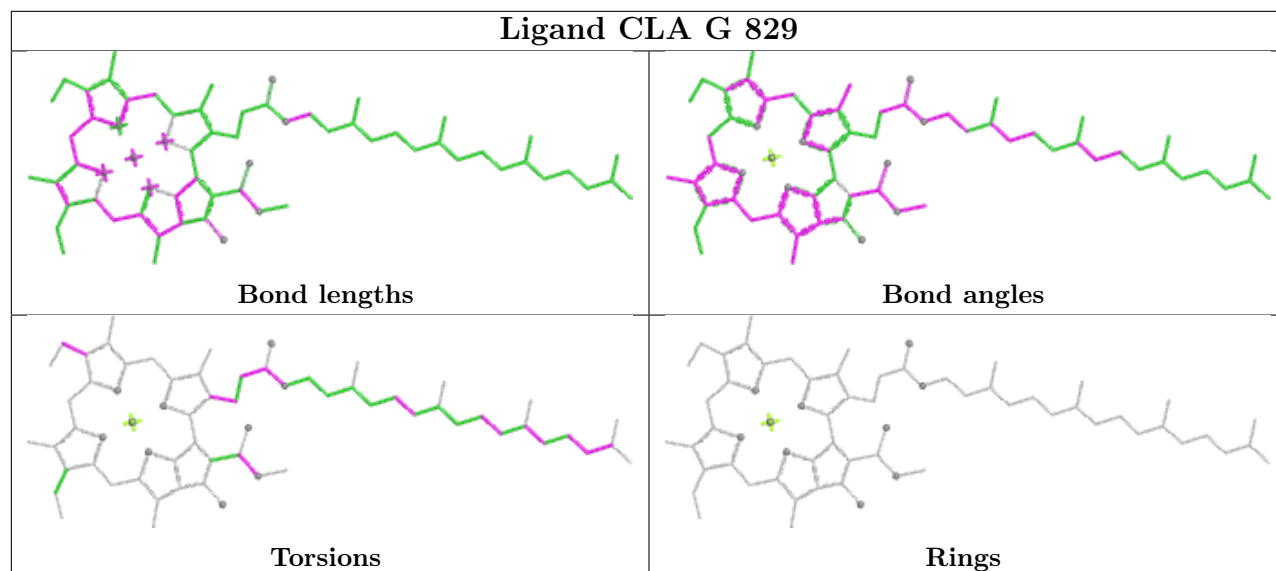
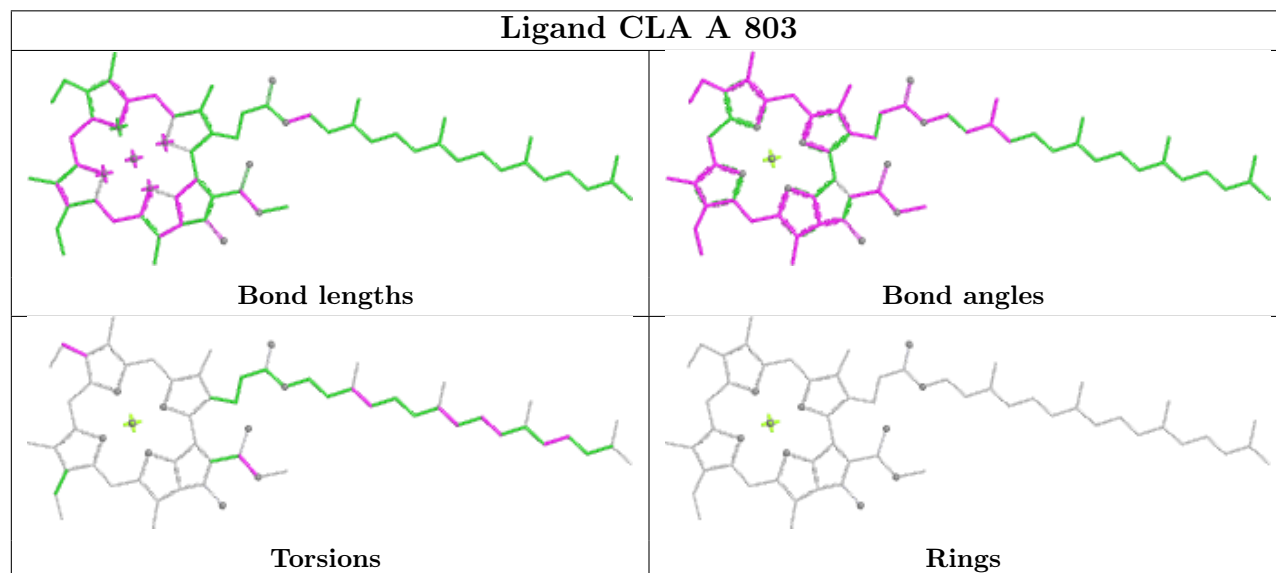
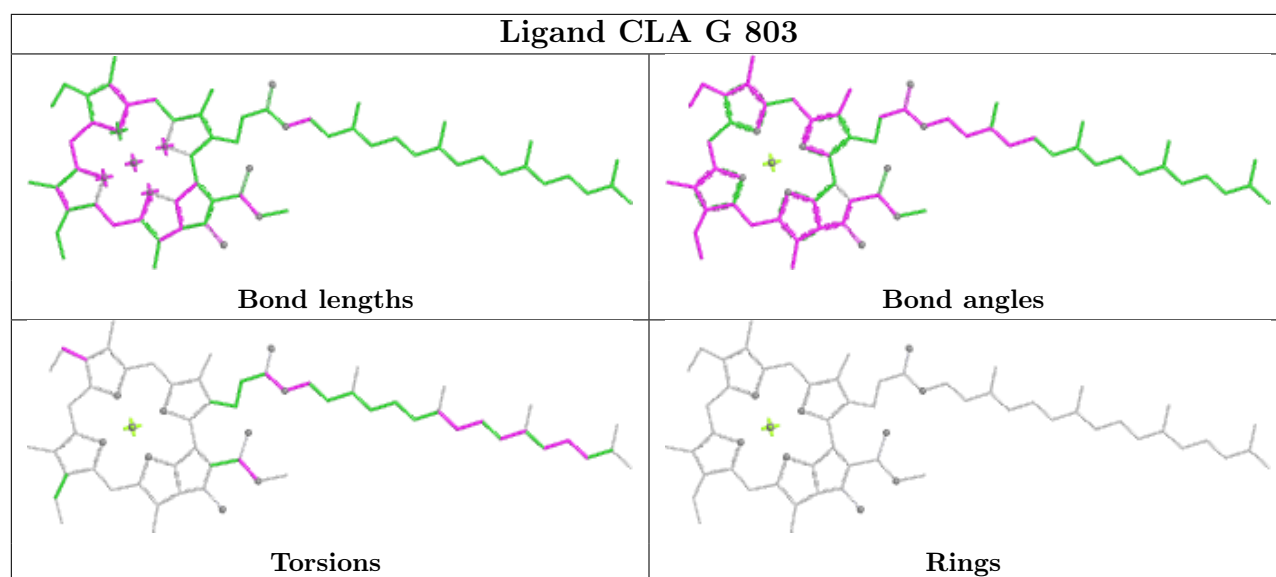




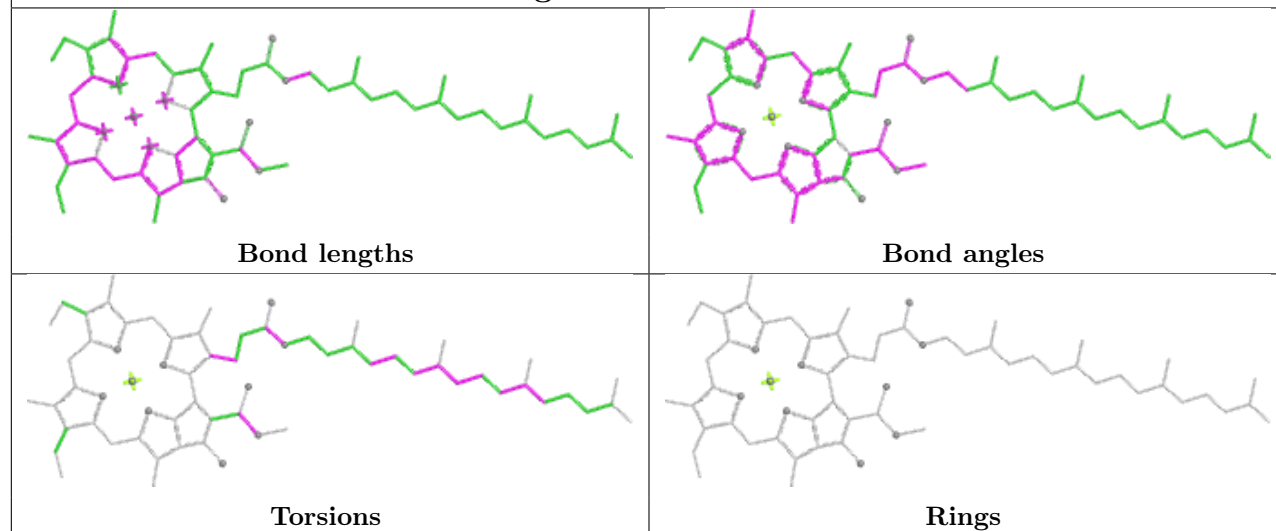
Ligand BCR A 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 826	
	
Bond lengths	Bond angles
	
Torsions	Rings

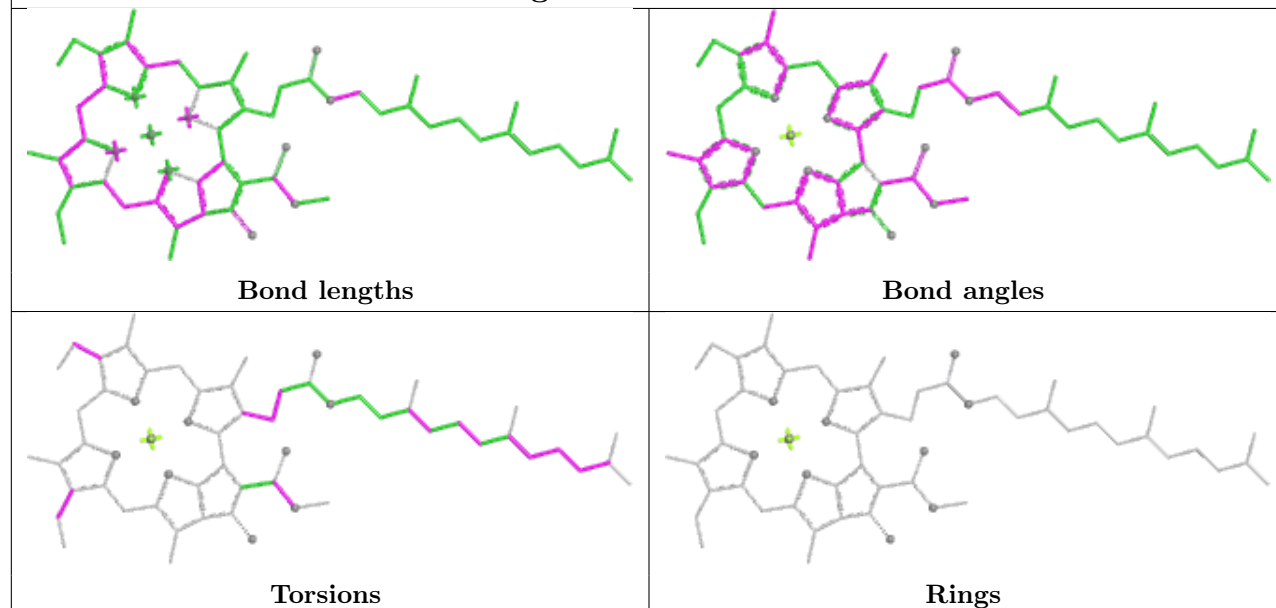


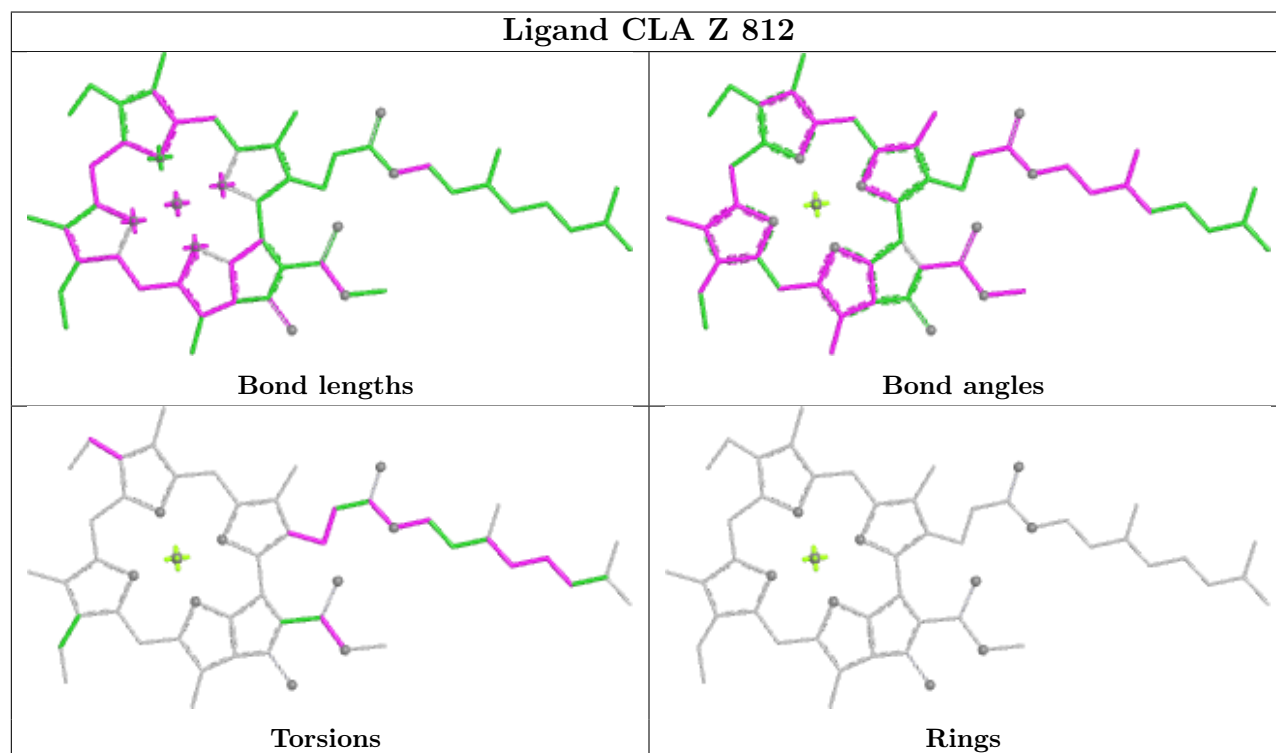
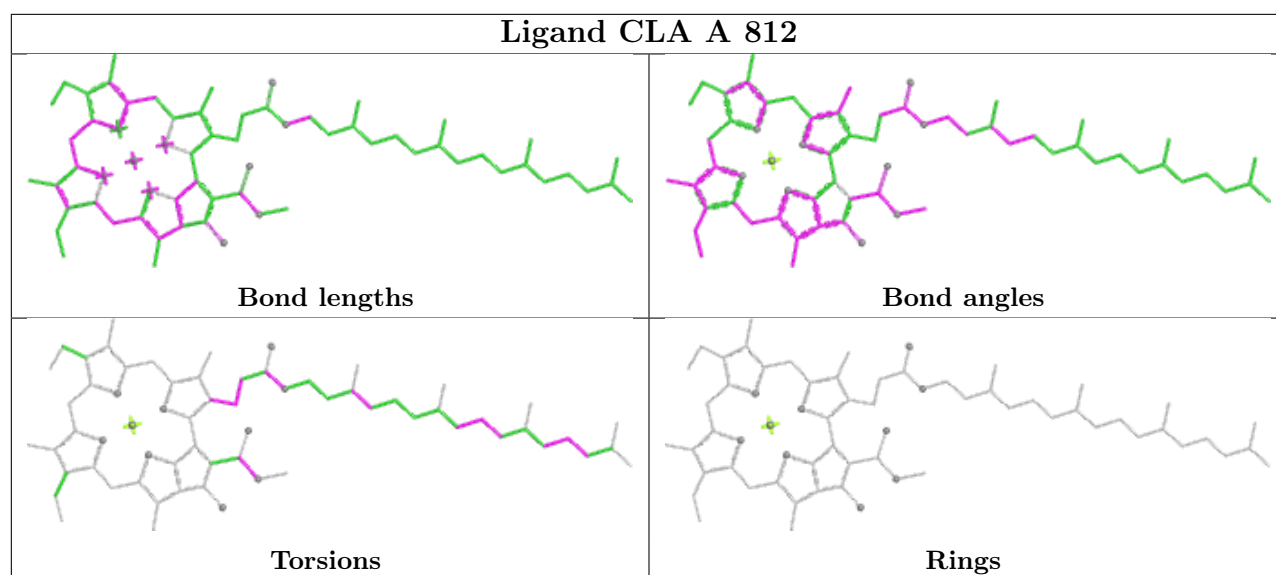


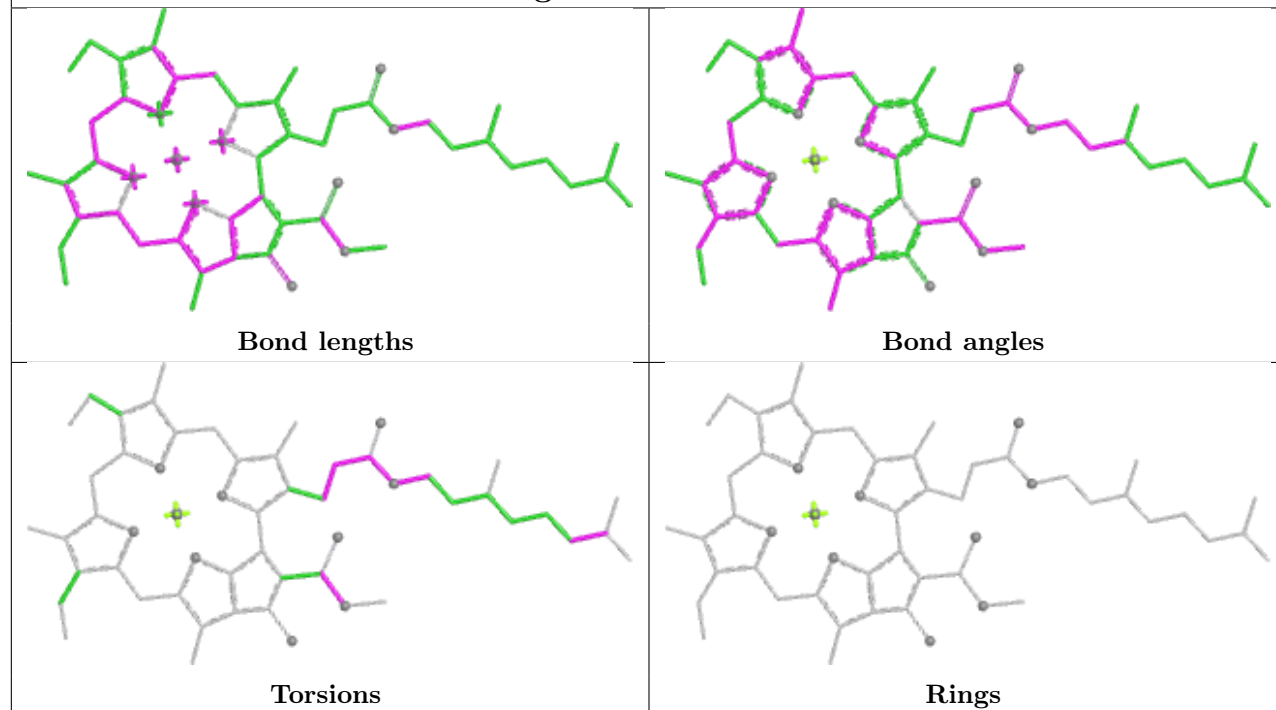
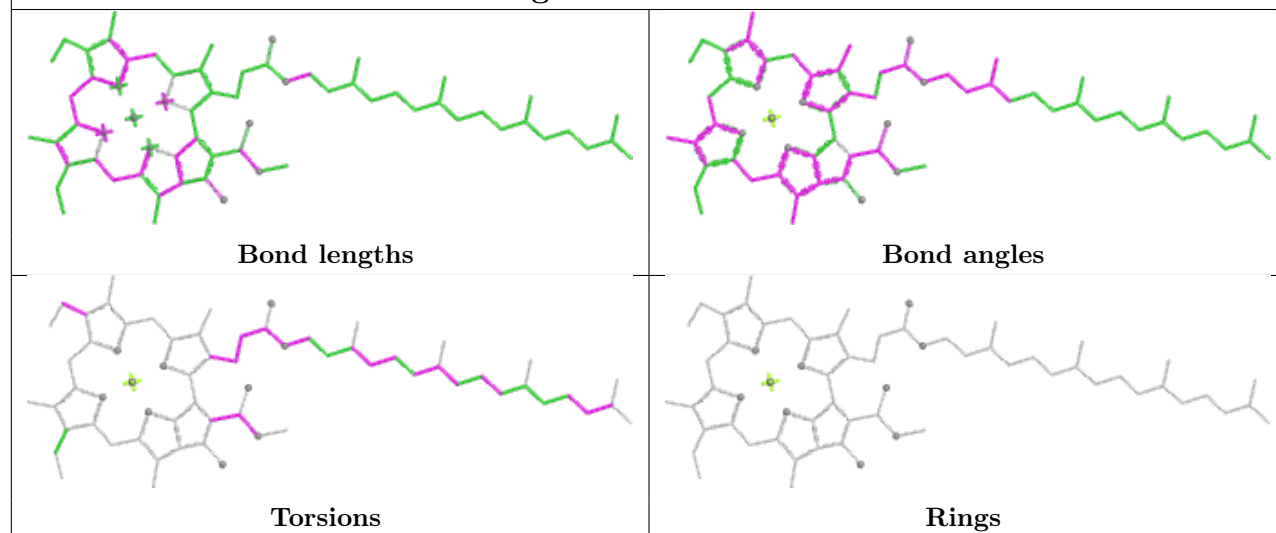
Ligand CLA L 205

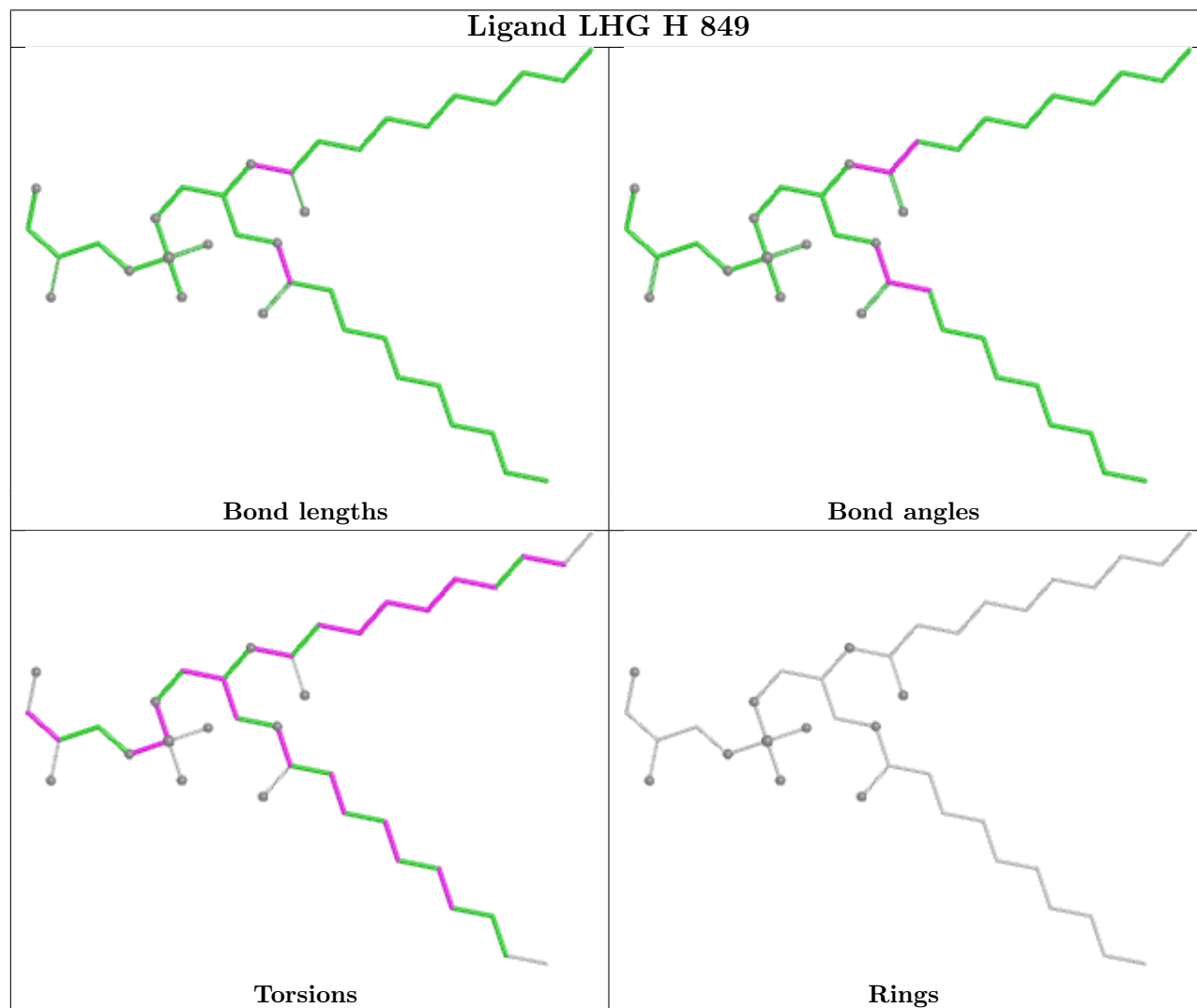
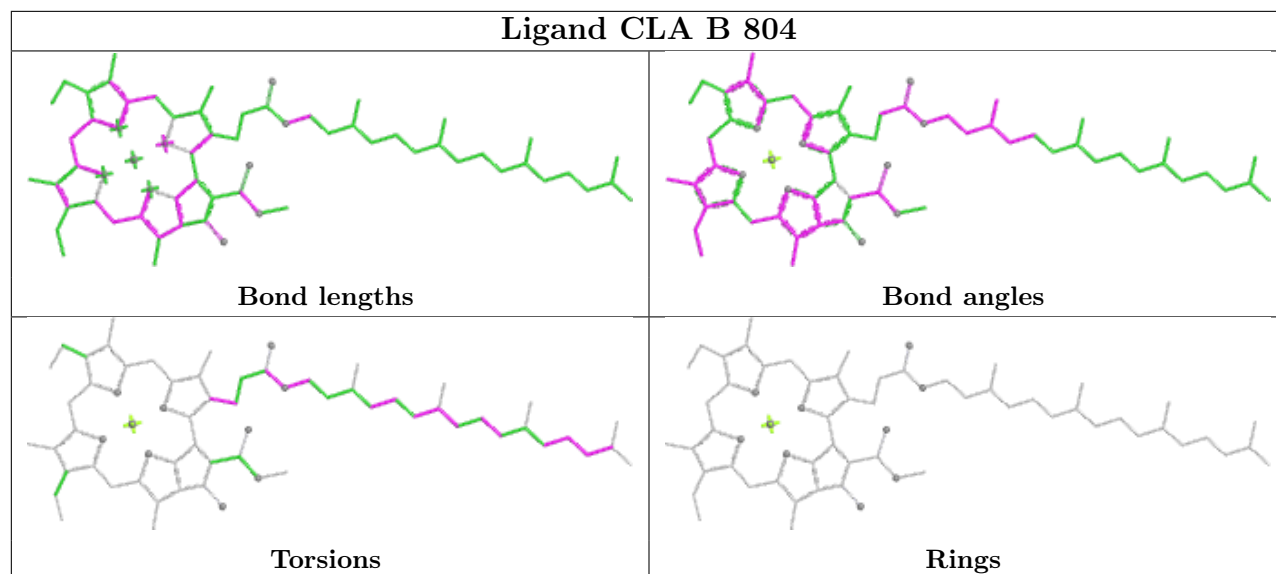


Ligand CLA G 824

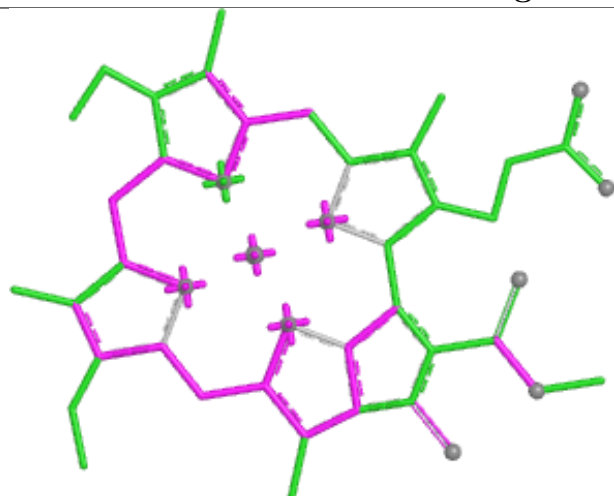




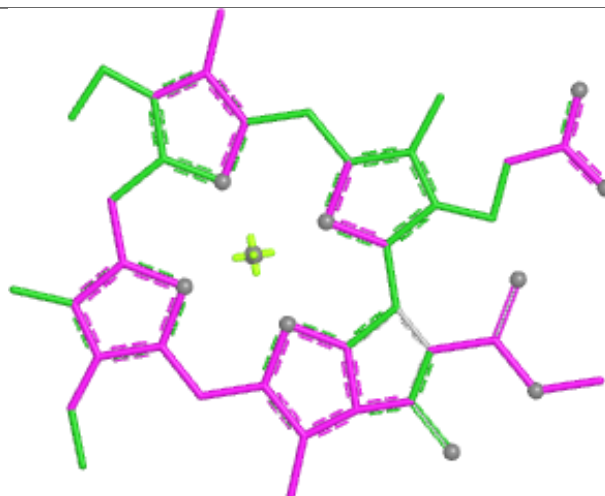
Ligand CLA Z 823**Ligand CLA A 806**



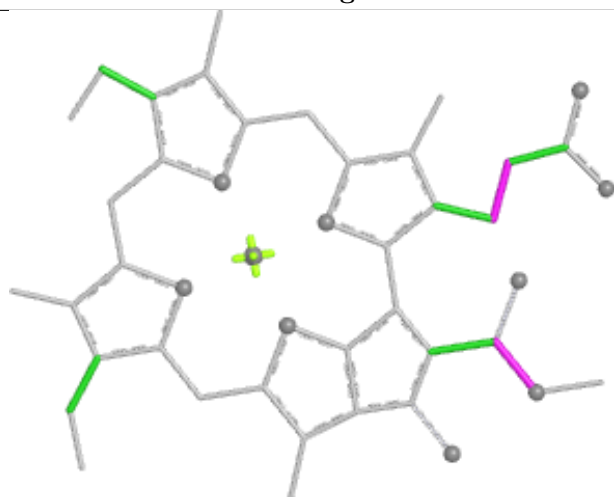
Ligand CLA B 830



Bond lengths



Bond angles

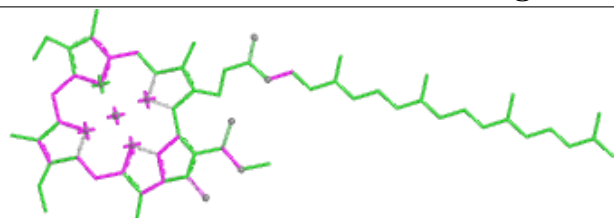


Torsions

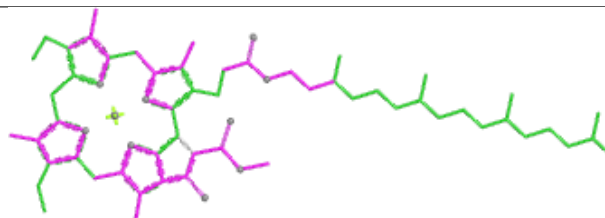


Rings

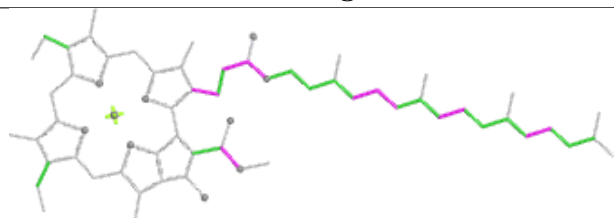
Ligand CLA A 829



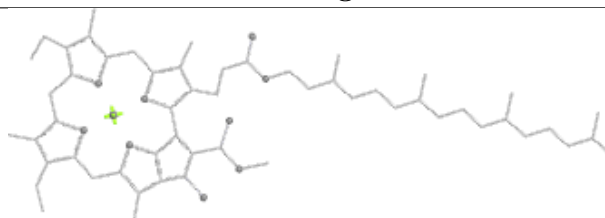
Bond lengths



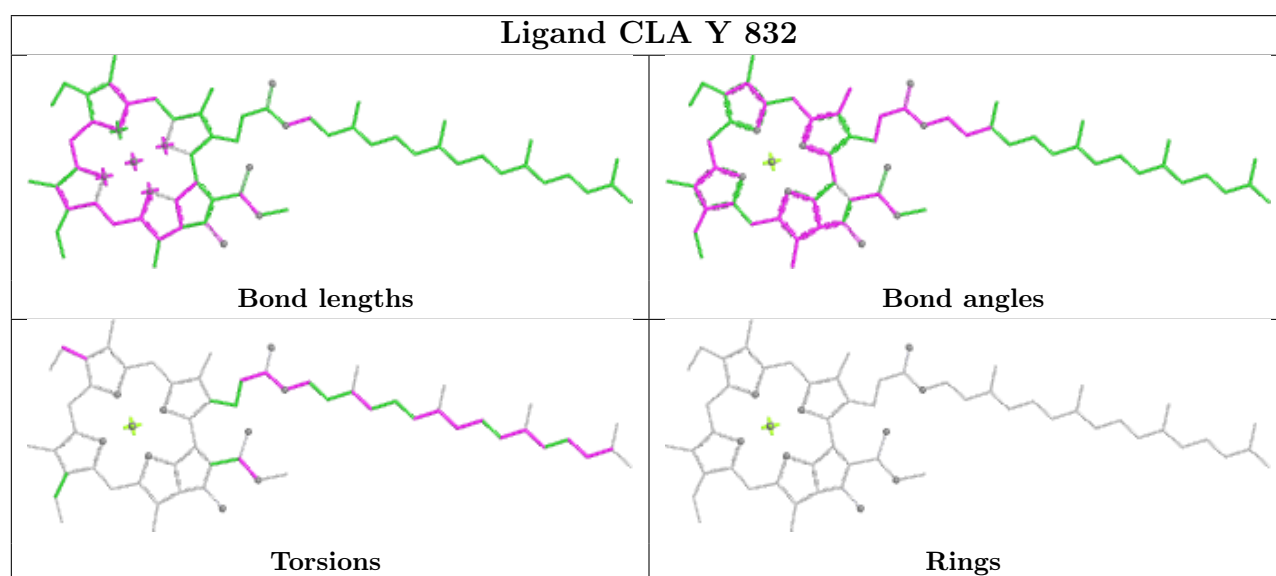
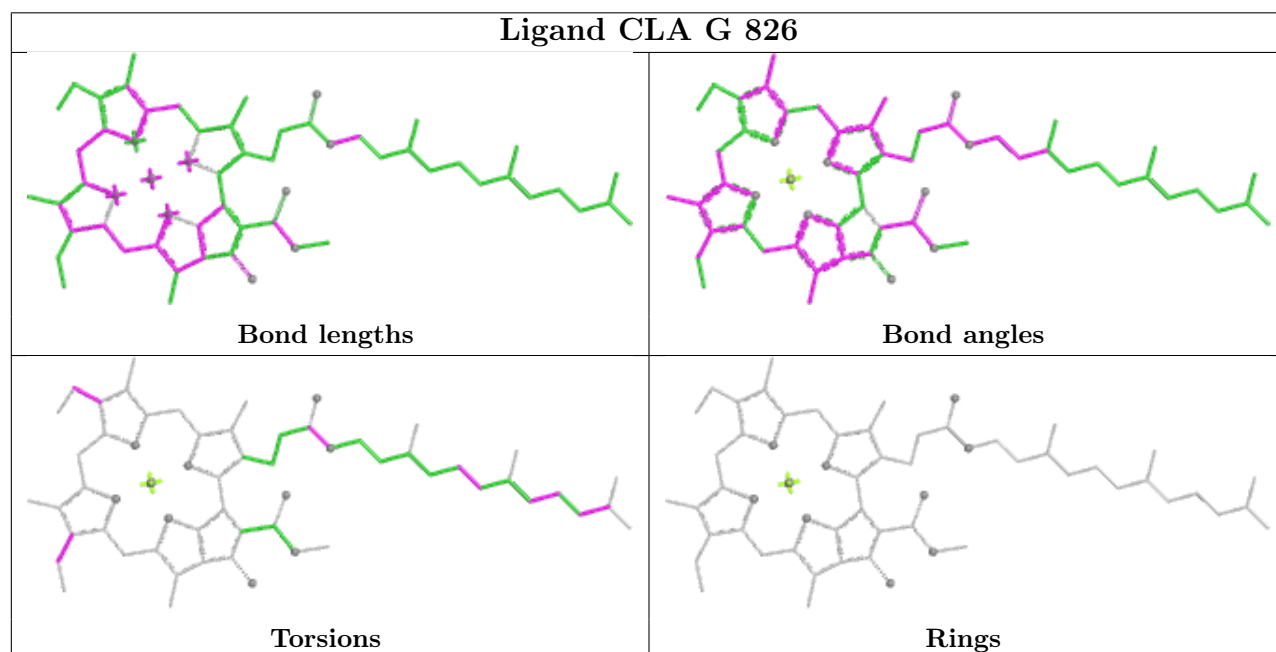
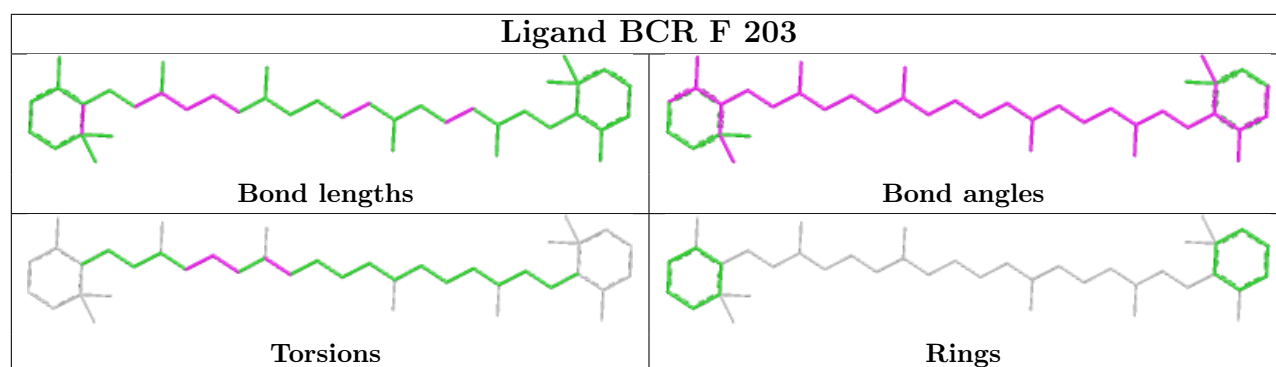
Bond angles

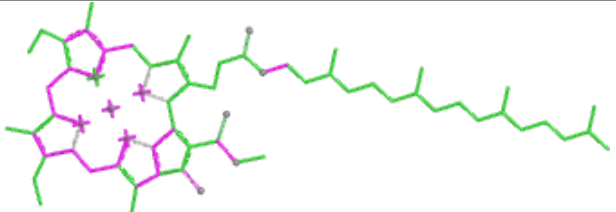
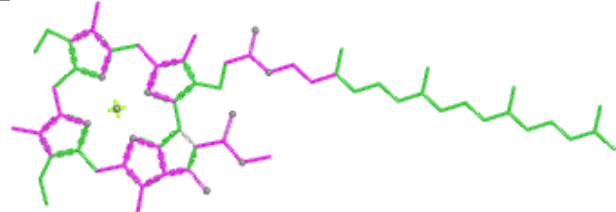
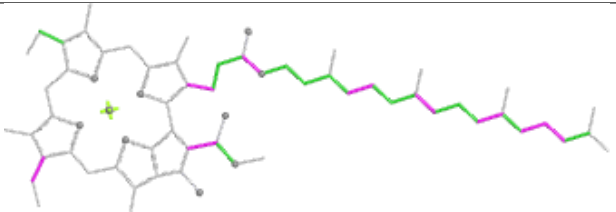
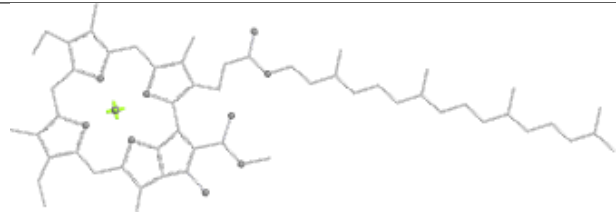


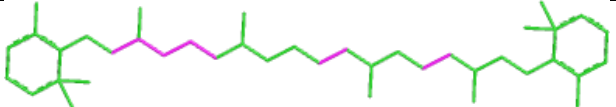
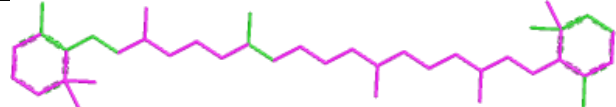
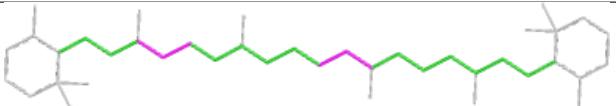
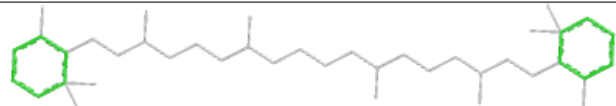
Torsions



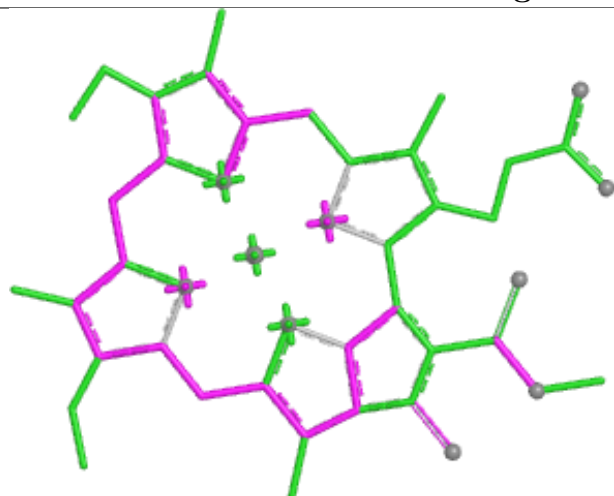
Rings



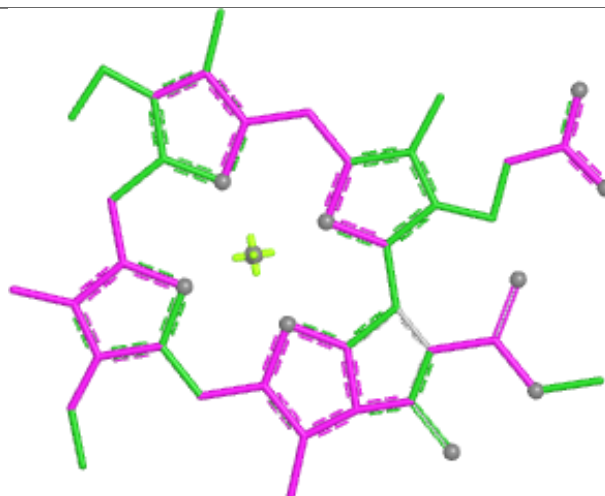
Ligand CLA Z 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR U 1005	
	
Bond lengths	Bond angles
	
Torsions	Rings

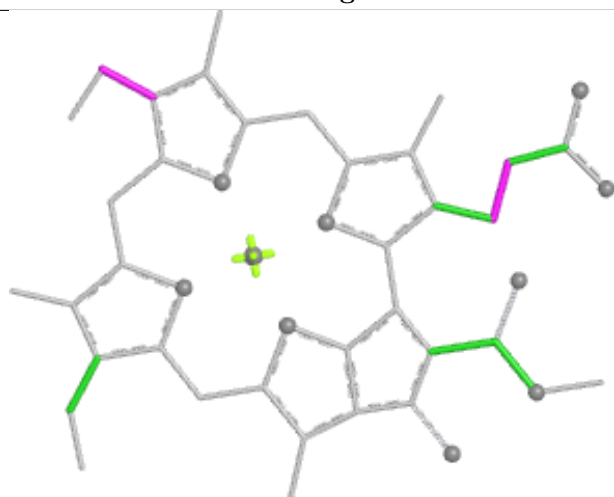
Ligand CLA Y 834



Bond lengths



Bond angles

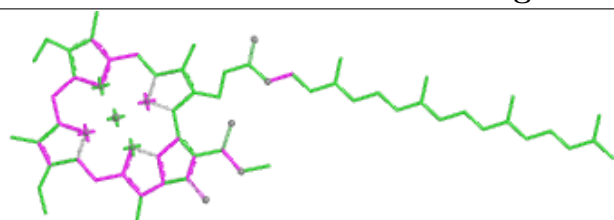


Torsions

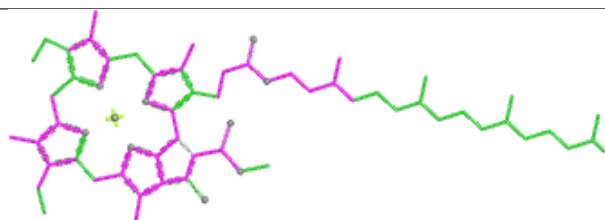


Rings

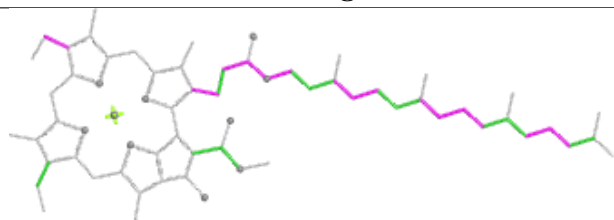
Ligand CLA Y 805



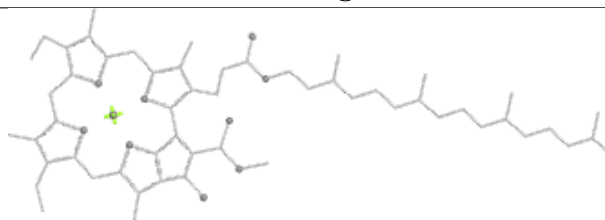
Bond lengths



Bond angles

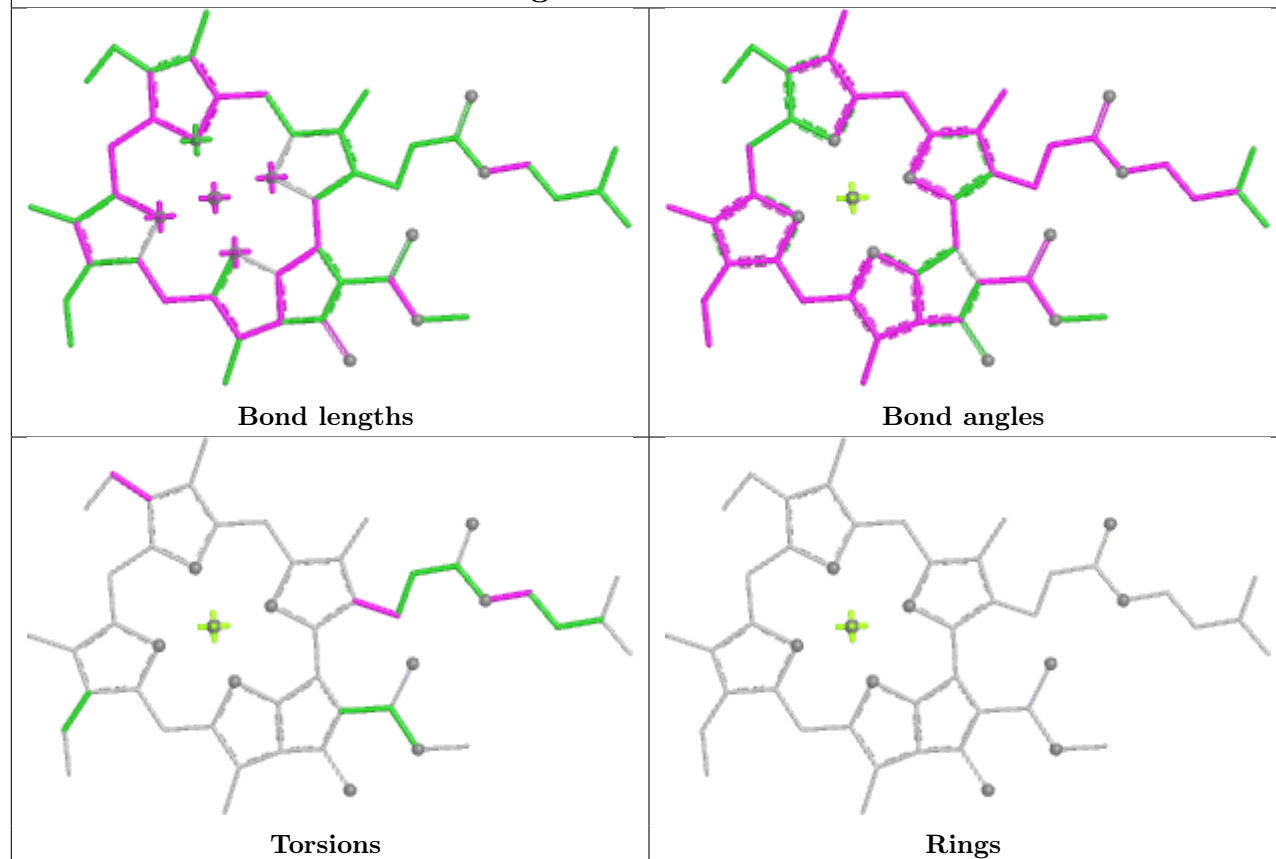


Torsions

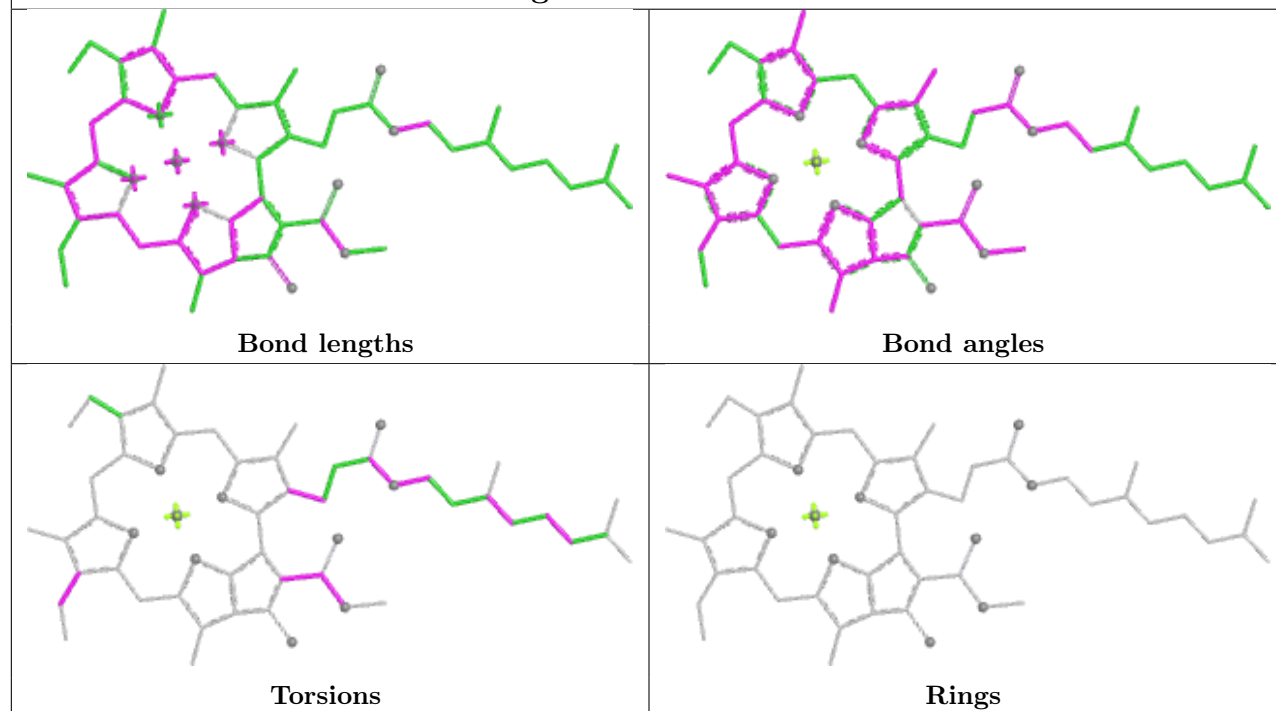


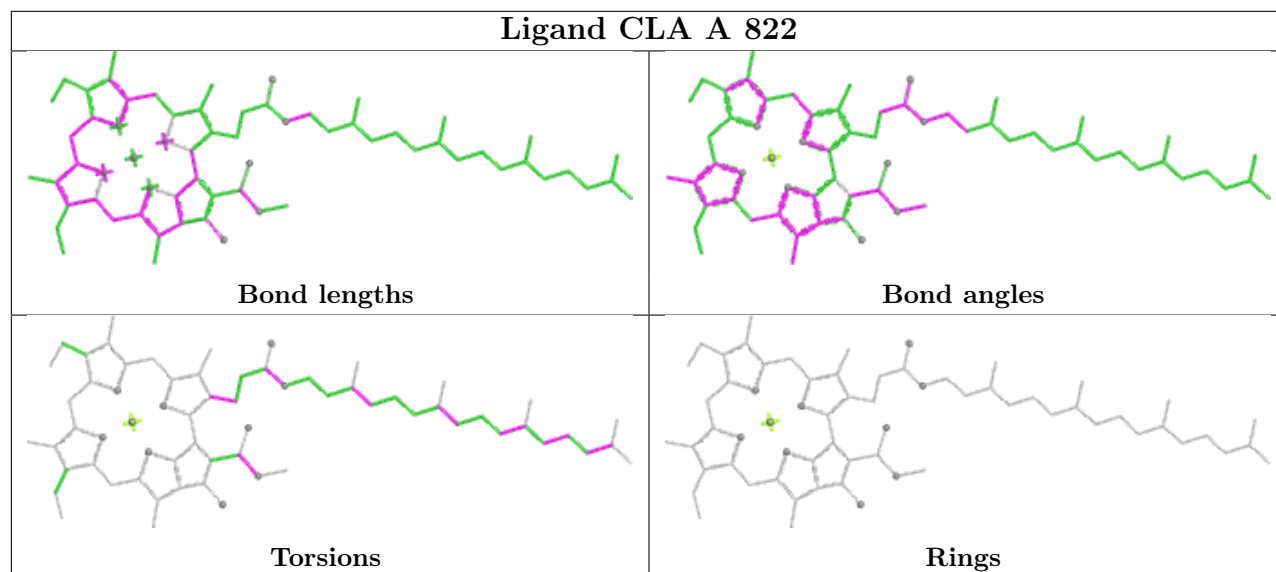
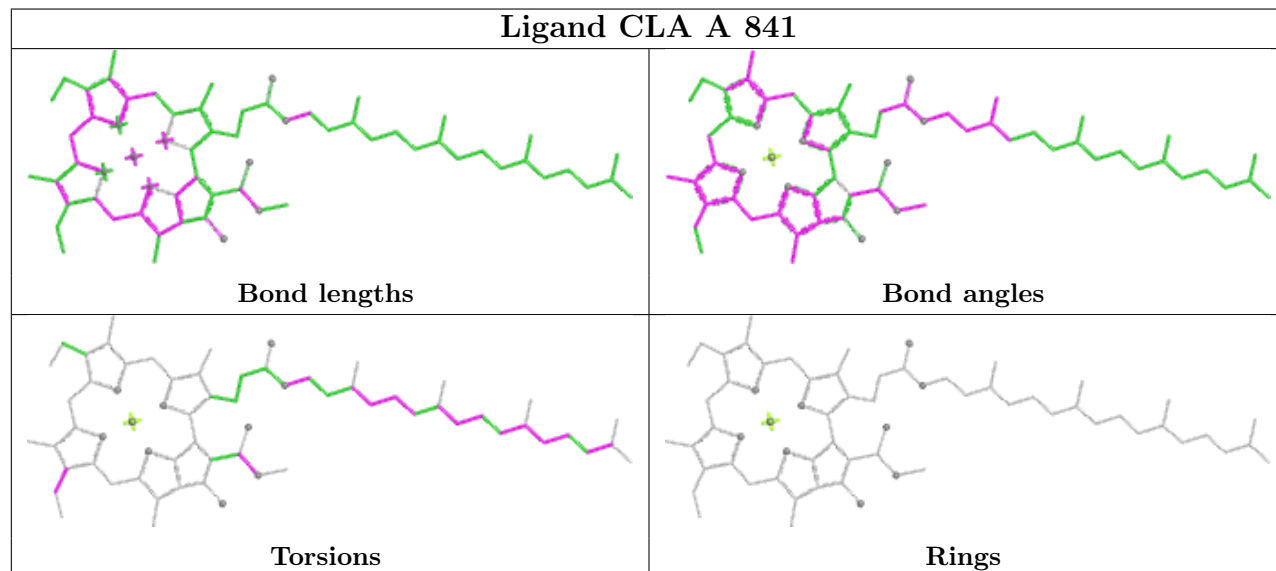
Rings

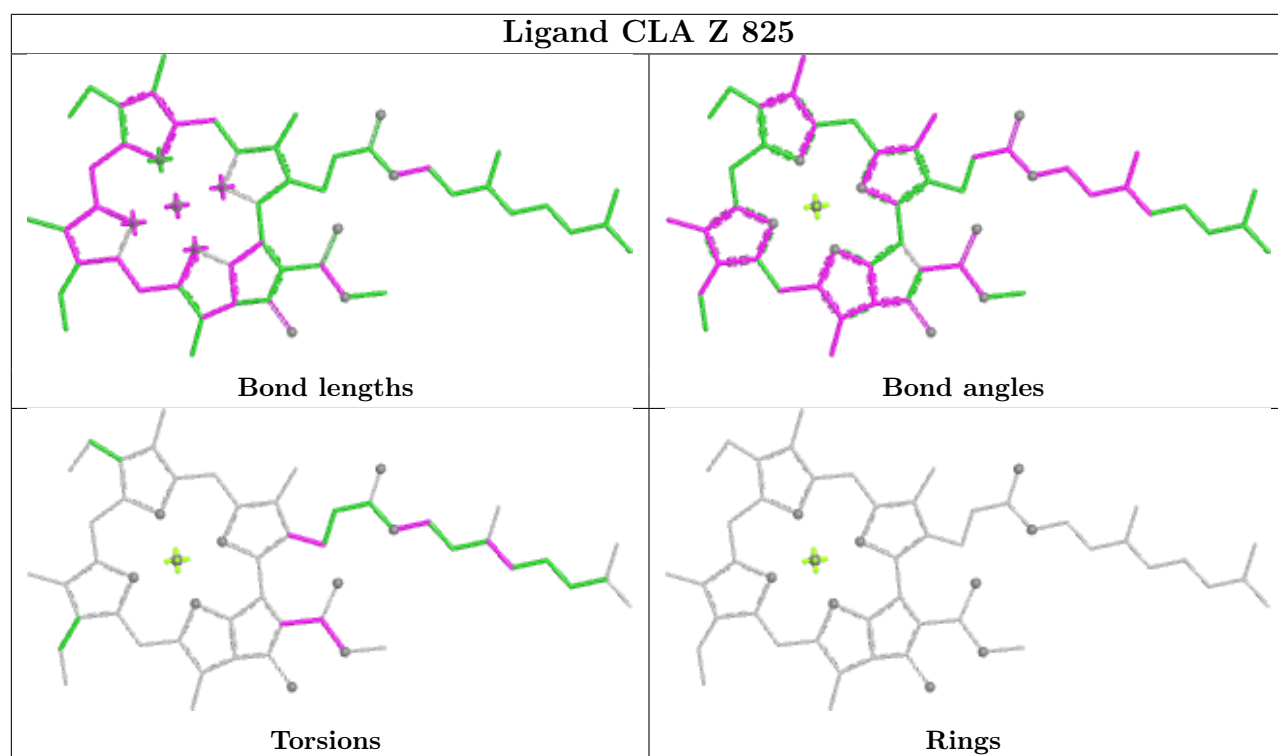
Ligand CLA G 814



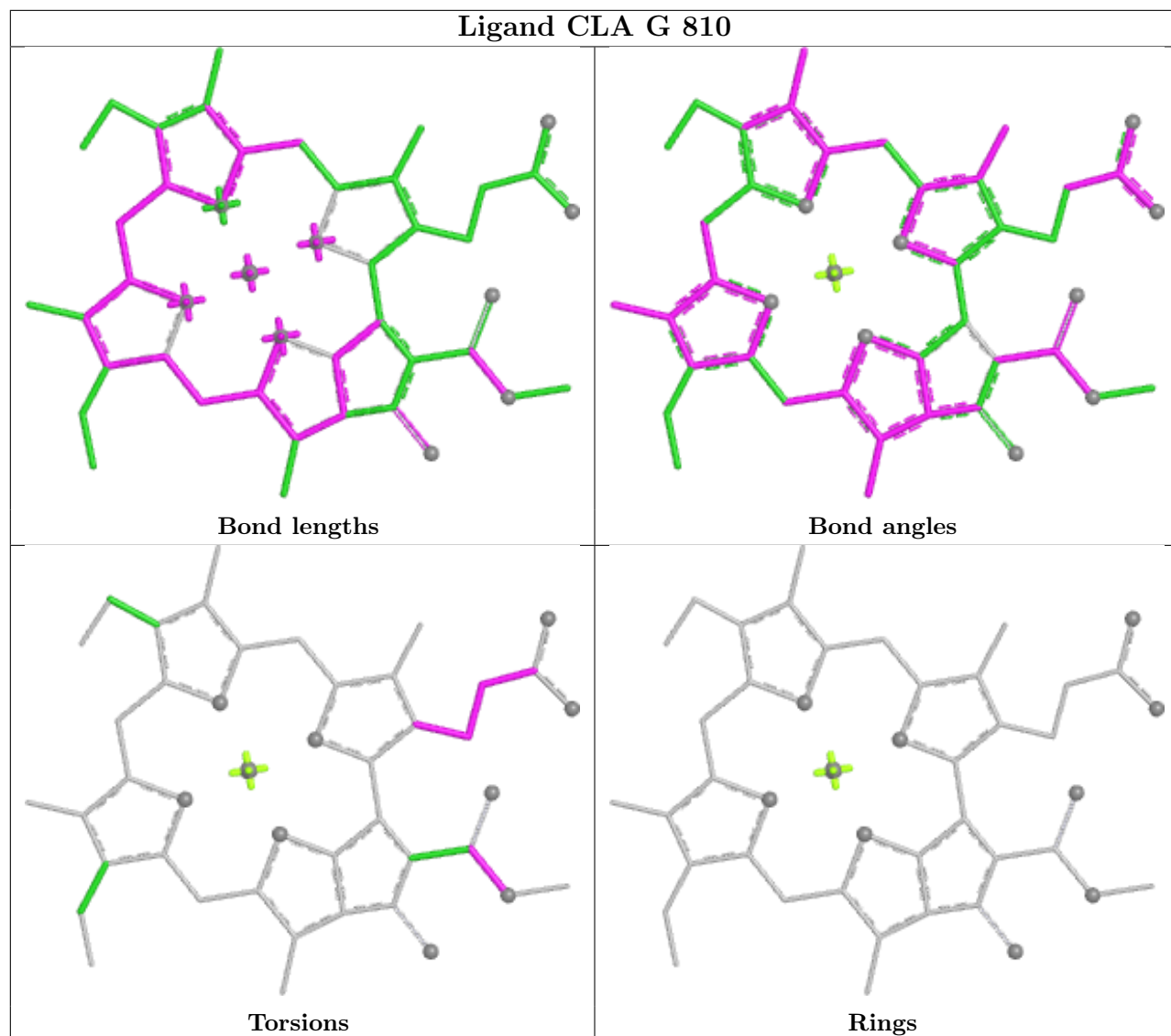
Ligand CLA H 824



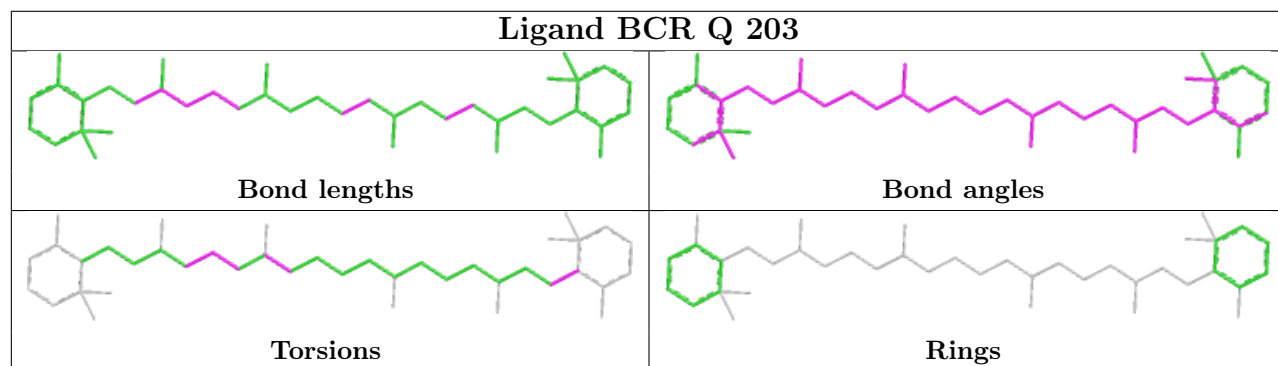
Ligand CLA A 822**Ligand CLA A 841**



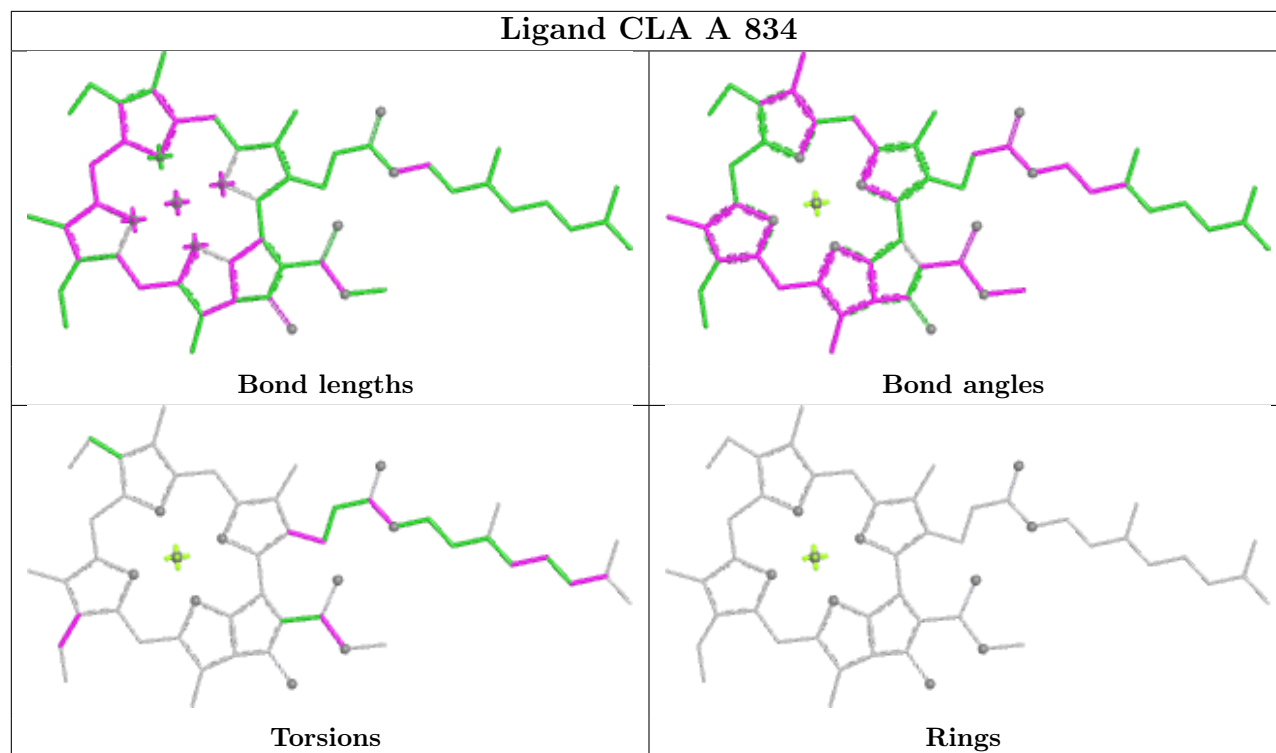
Ligand CLA G 810



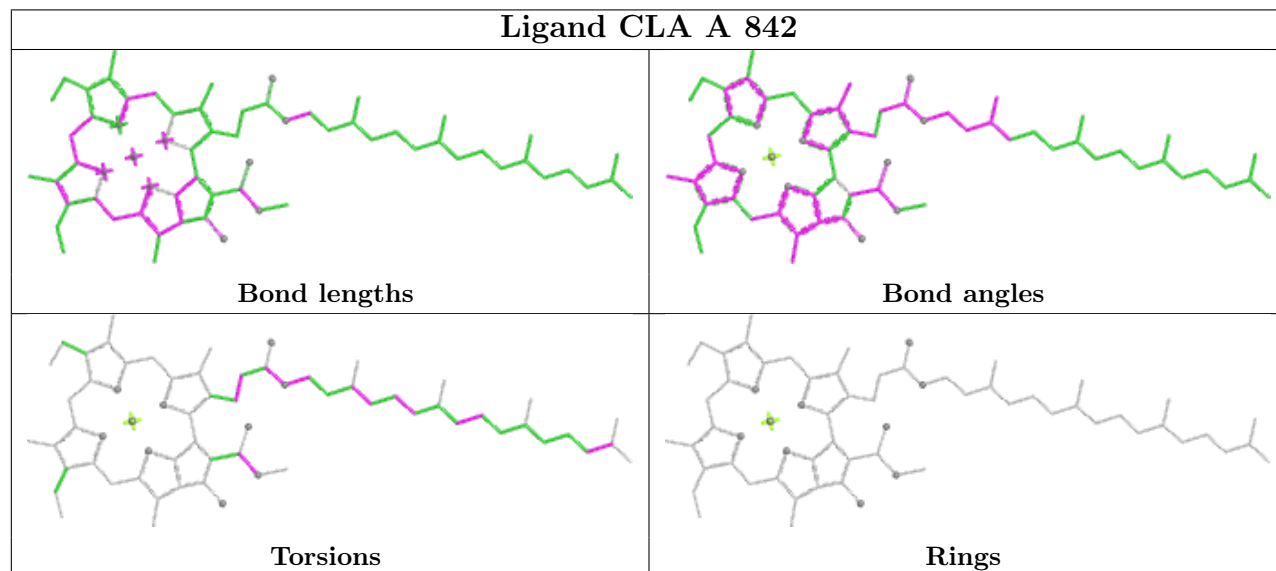
Ligand BCR Q 203



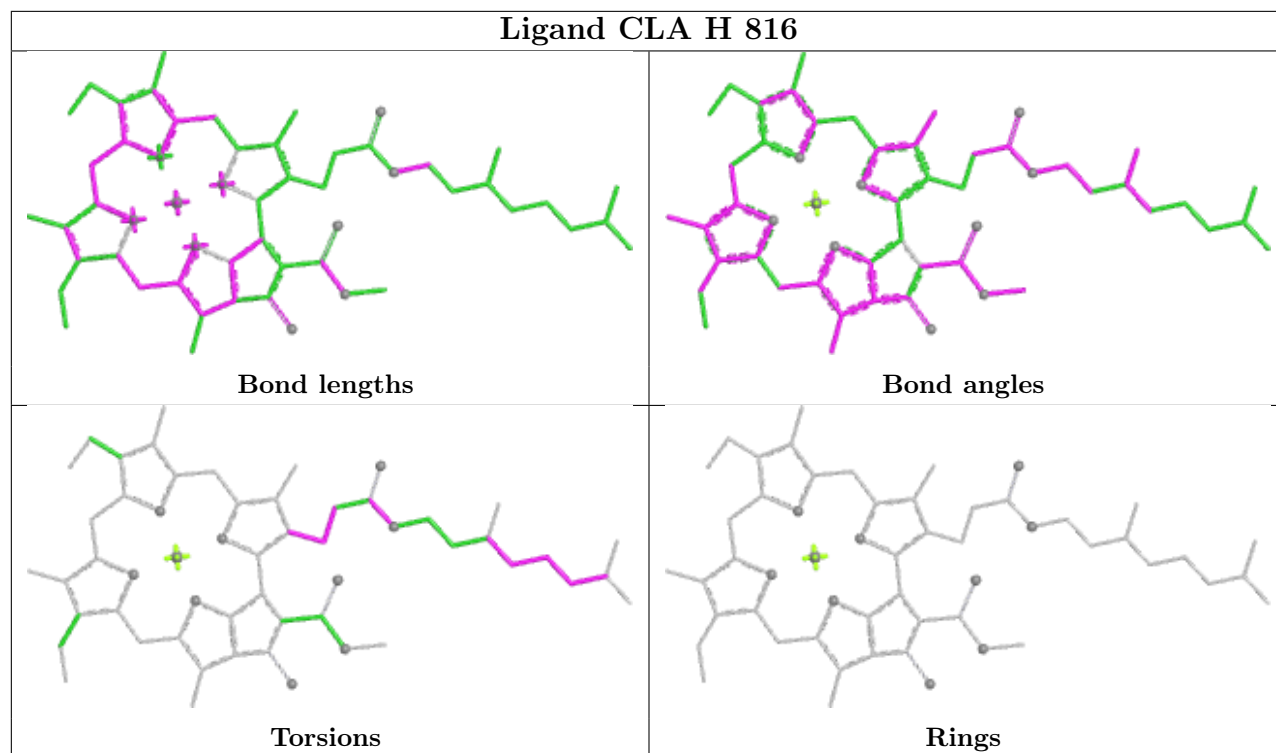
Ligand CLA A 834



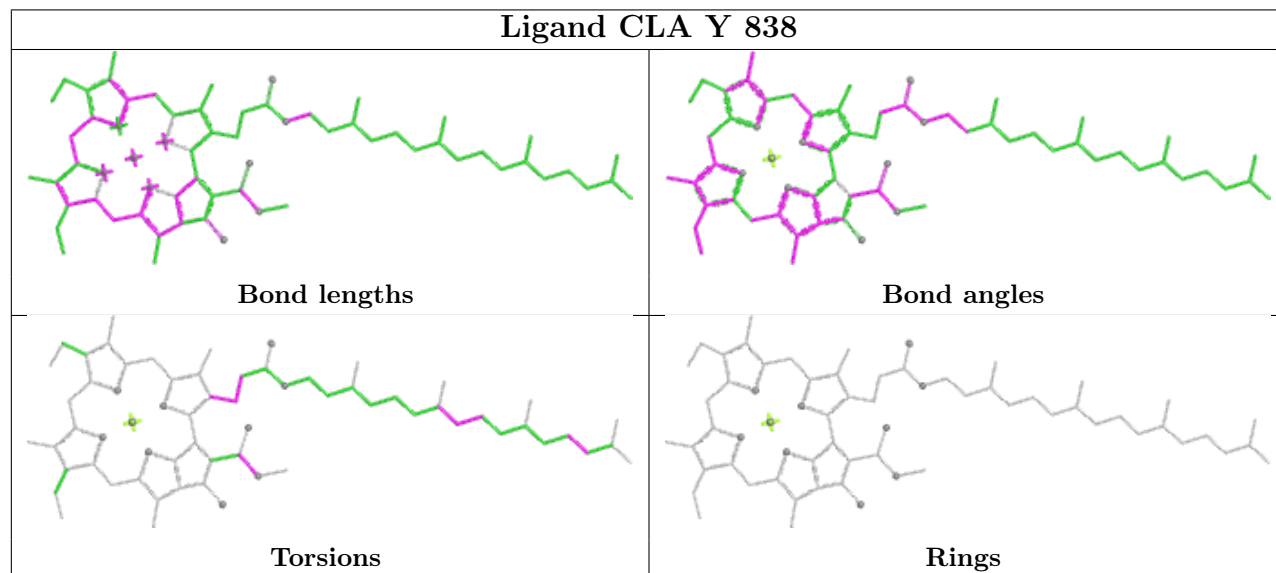
Ligand CLA A 842

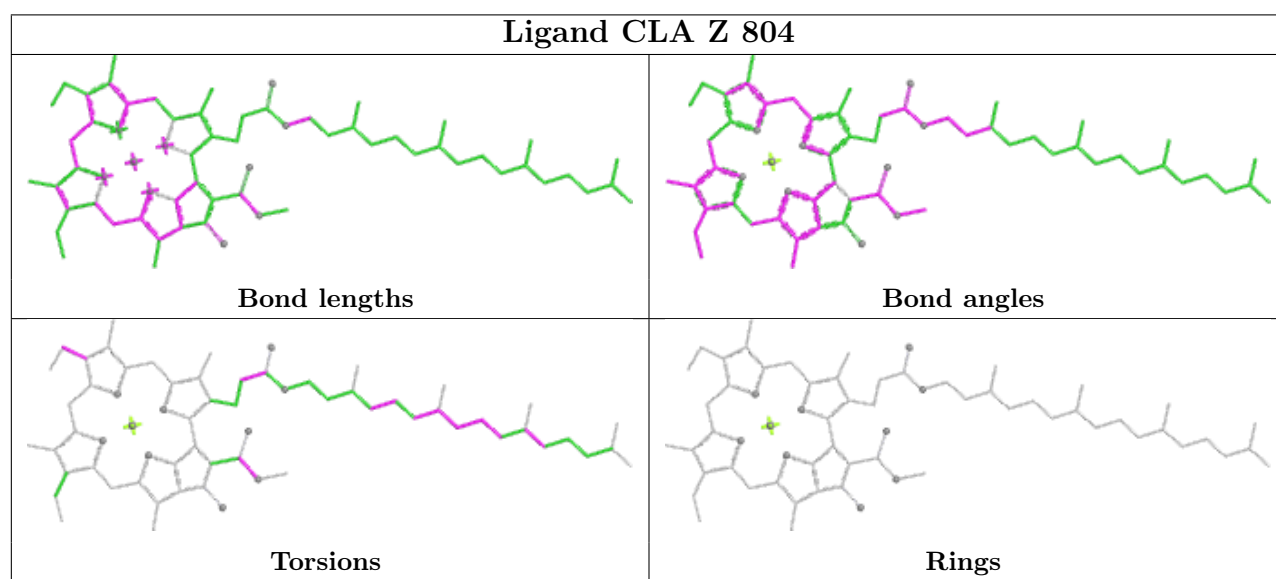
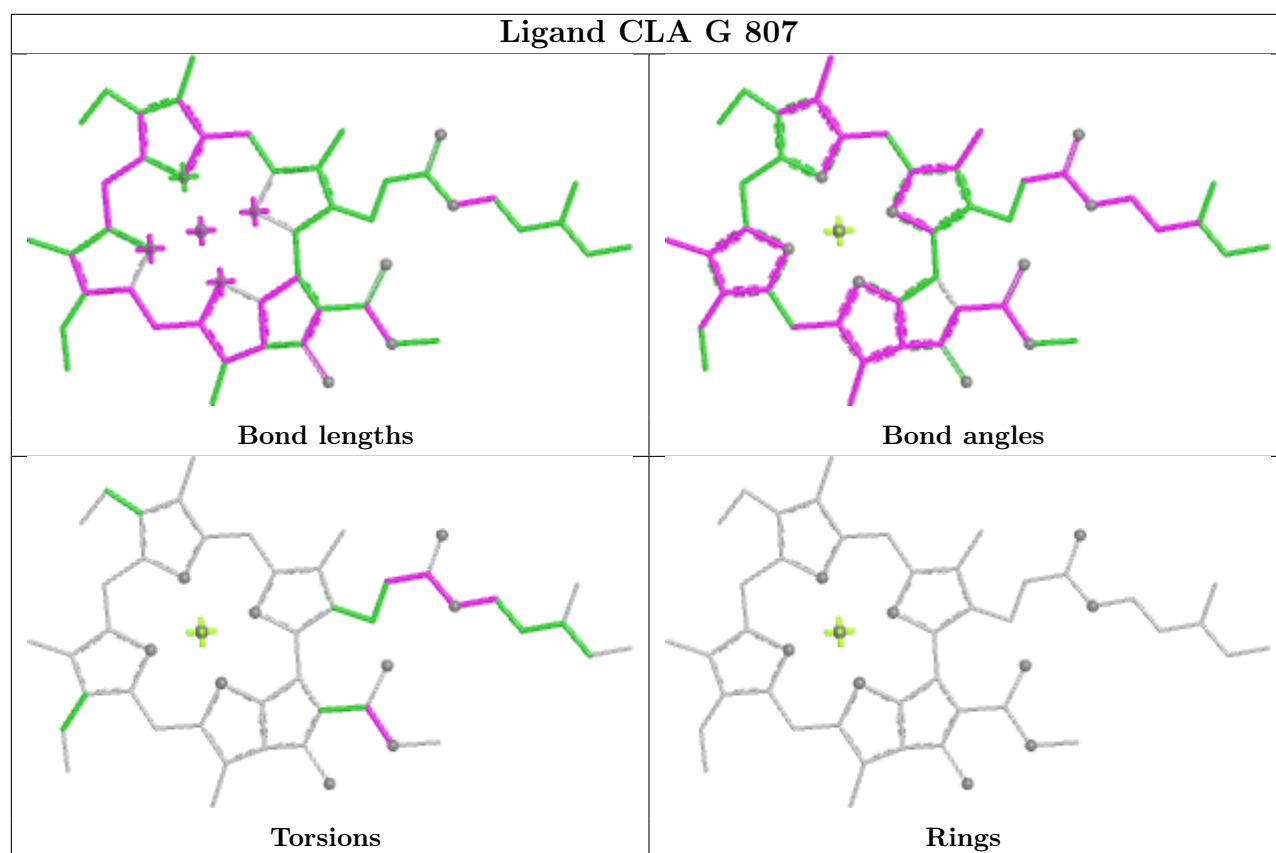


Ligand CLA H 816

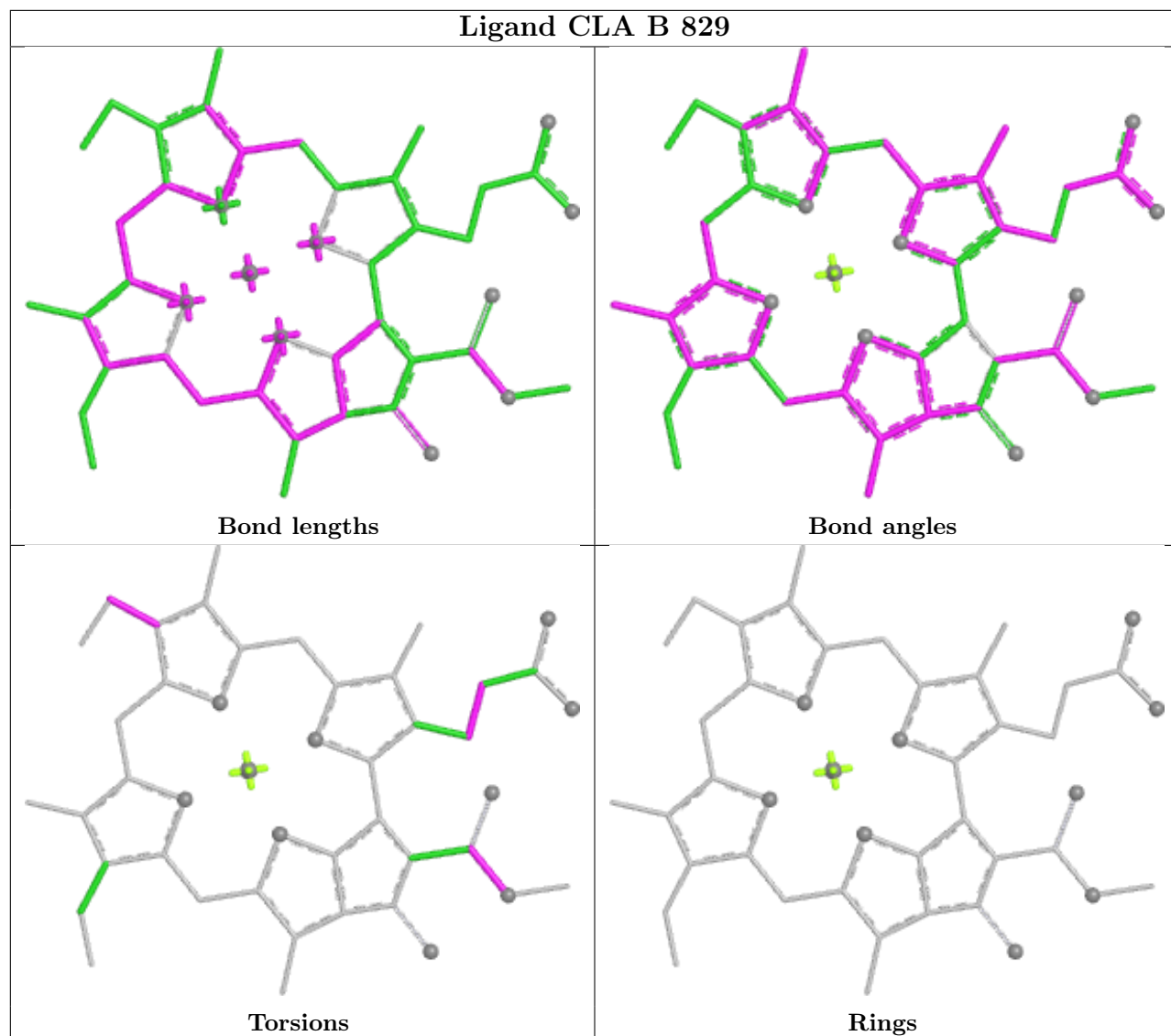


Ligand CLA Y 838

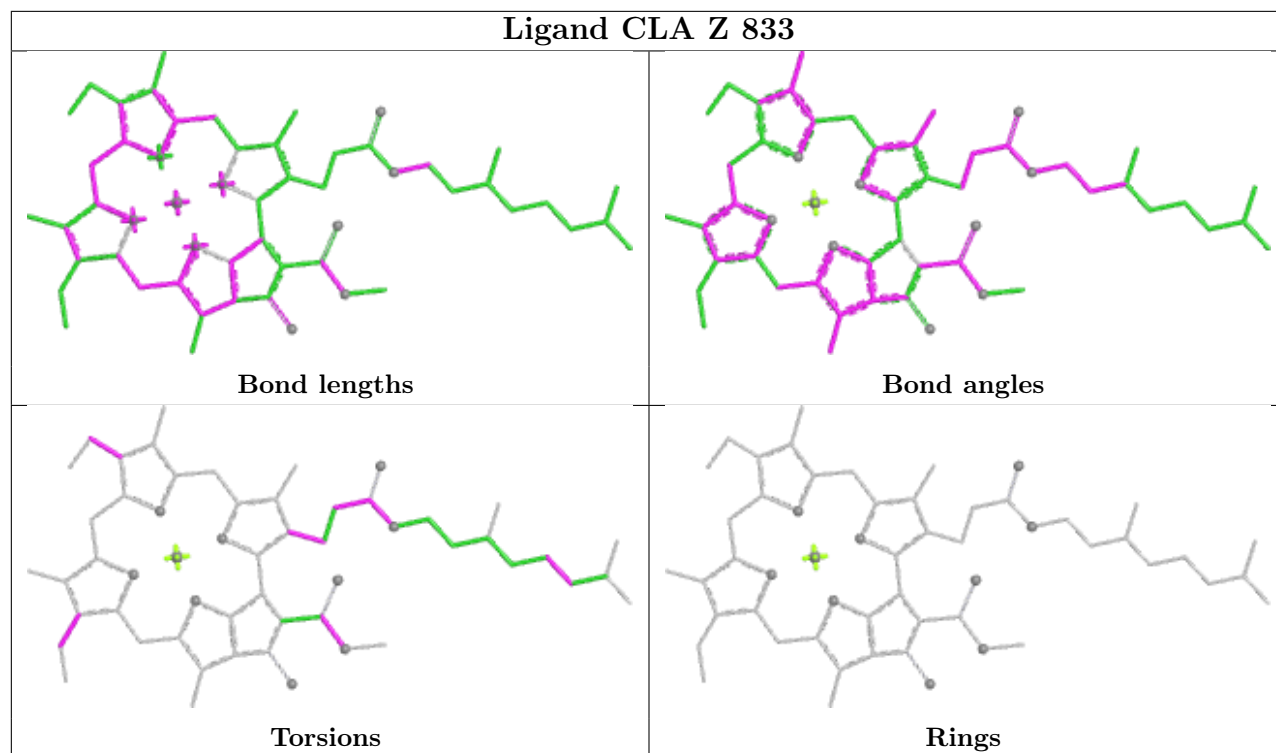




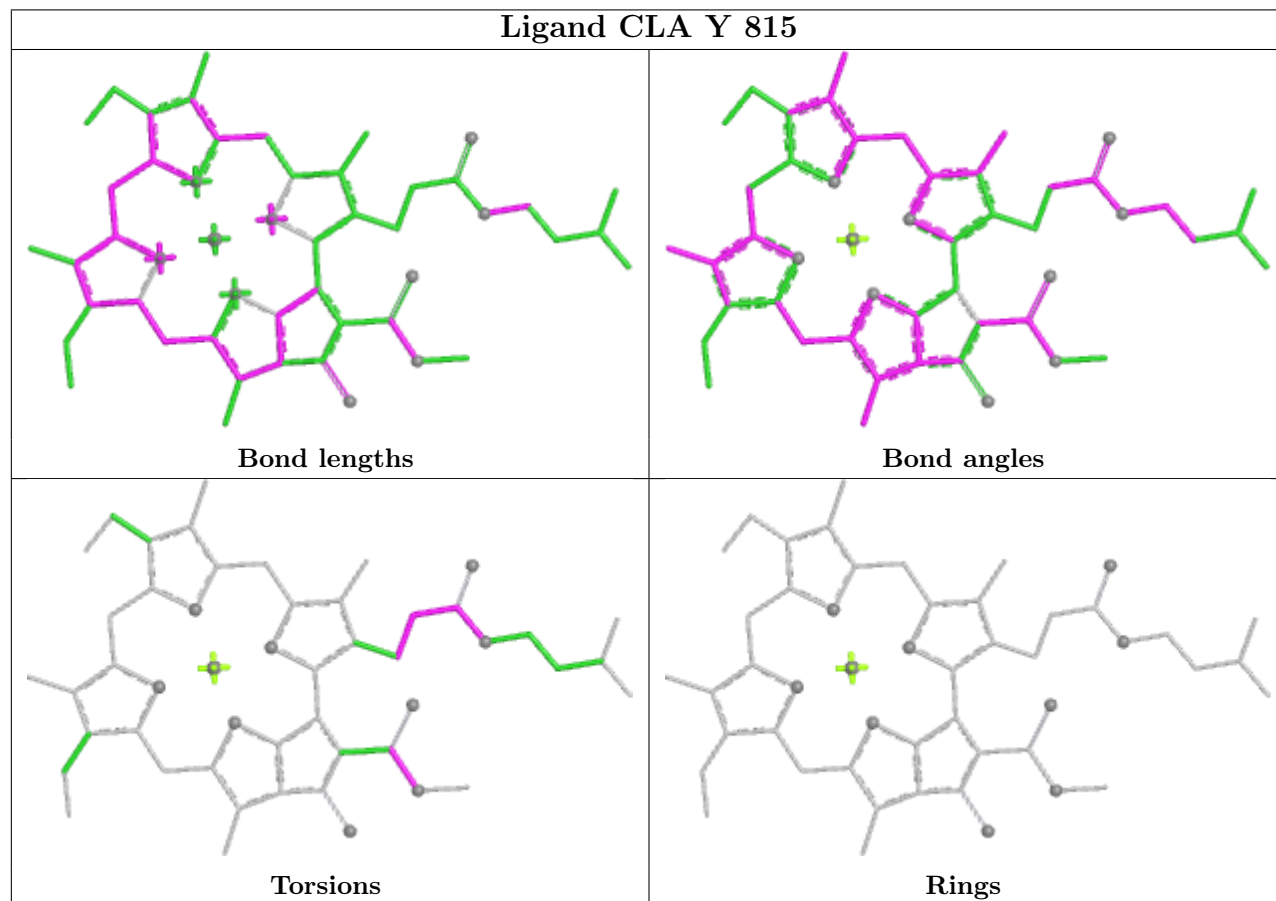
Ligand CLA B 829



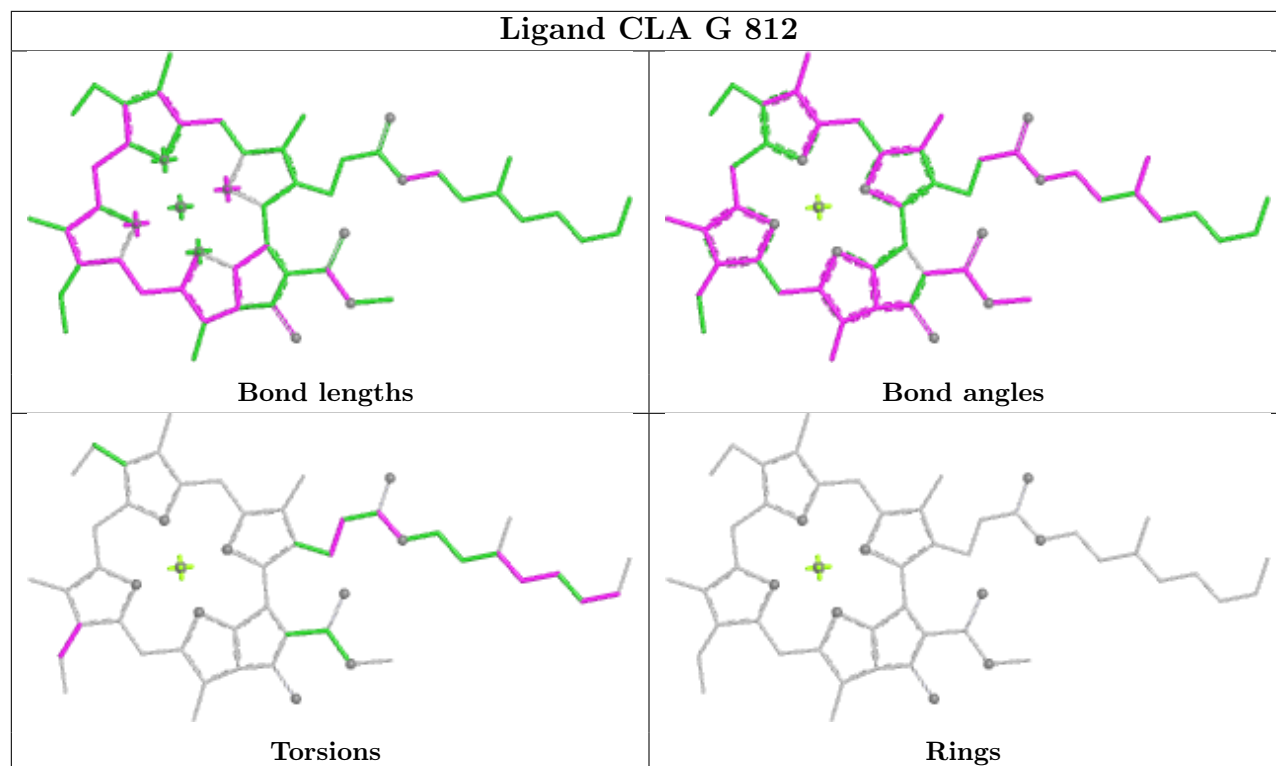
Ligand CLA Z 833



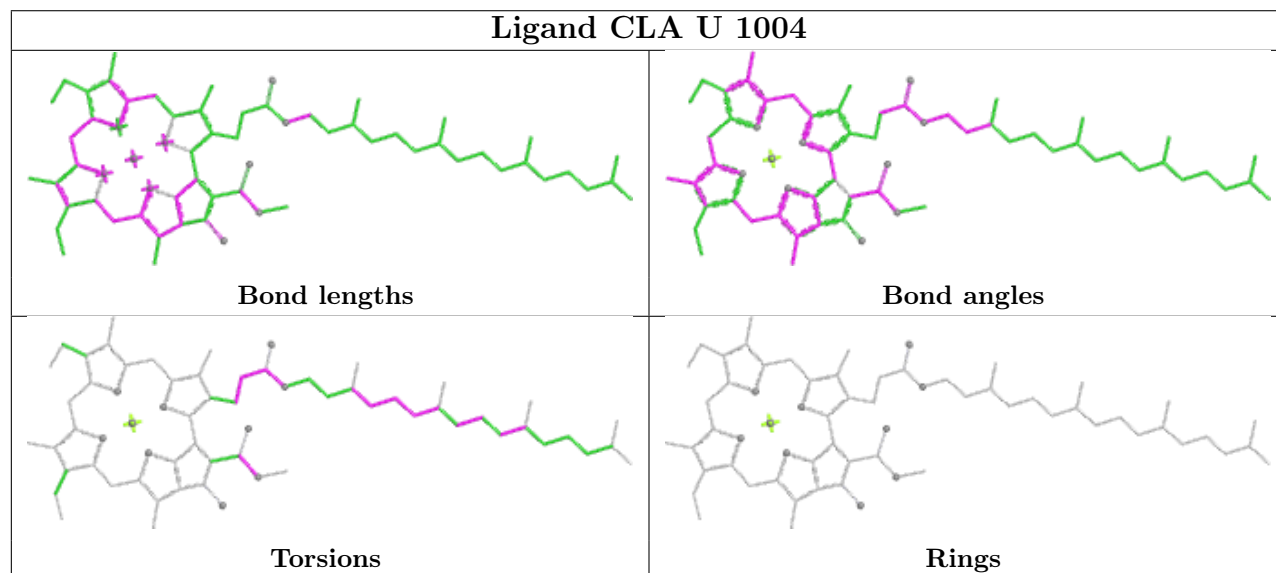
Ligand CLA Y 815

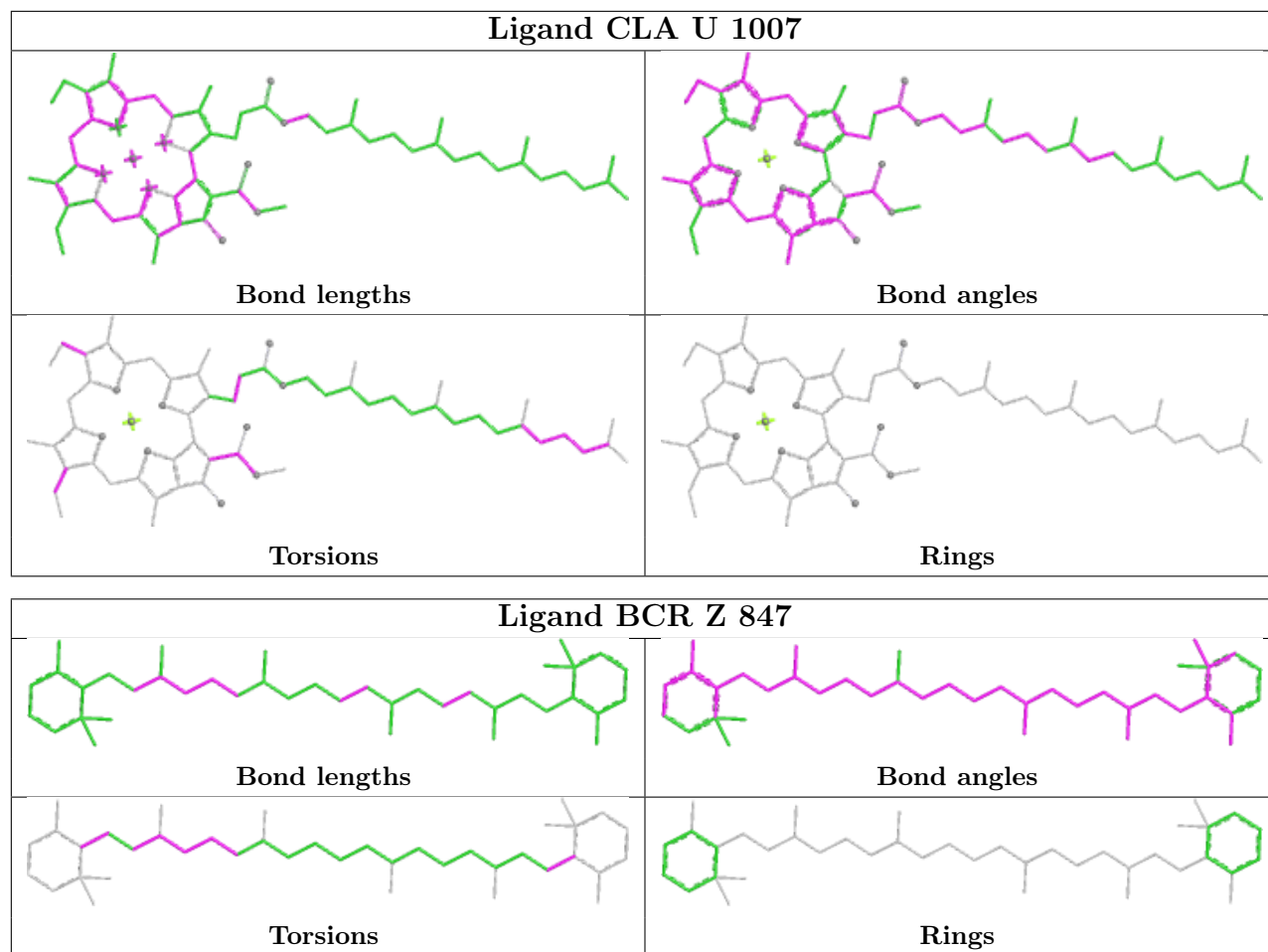


Ligand CLA G 812

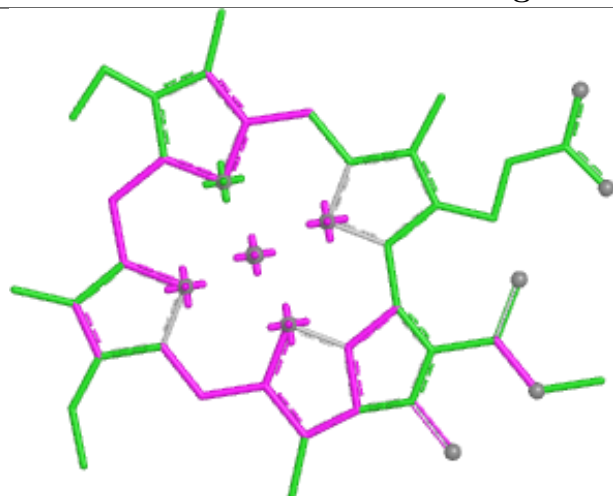


Ligand CLA U 1004

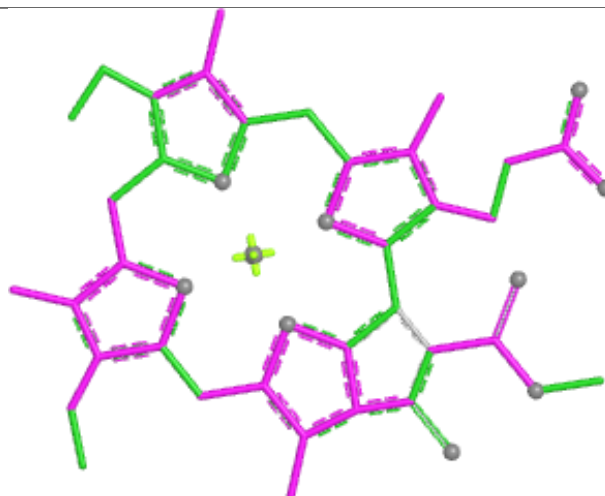




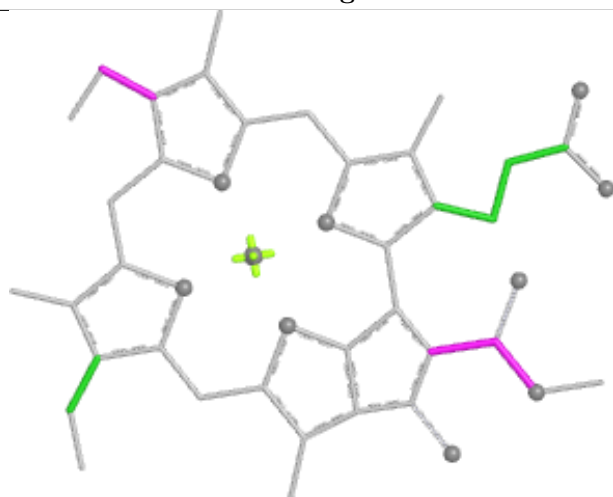
Ligand CLA K 102



Bond lengths



Bond angles

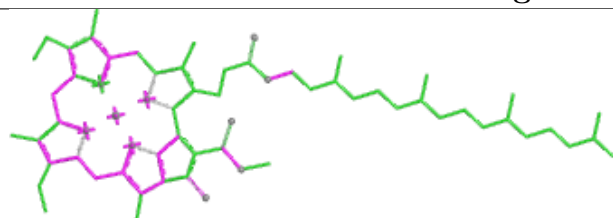


Torsions

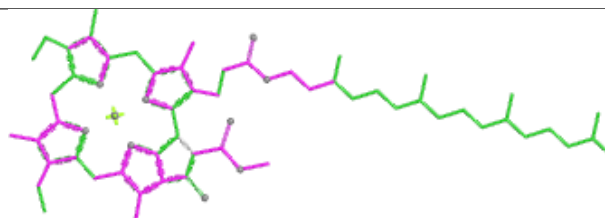


Rings

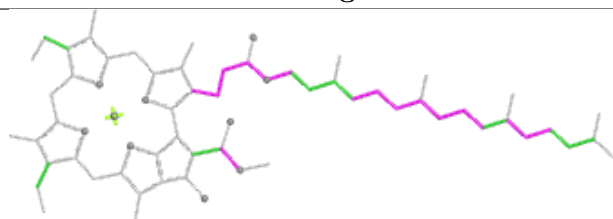
Ligand CLA H 813



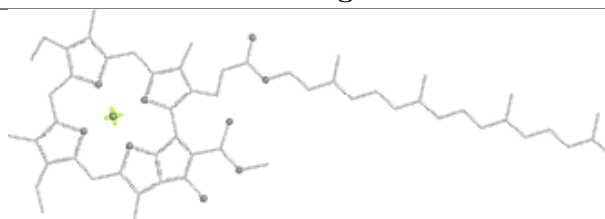
Bond lengths



Bond angles

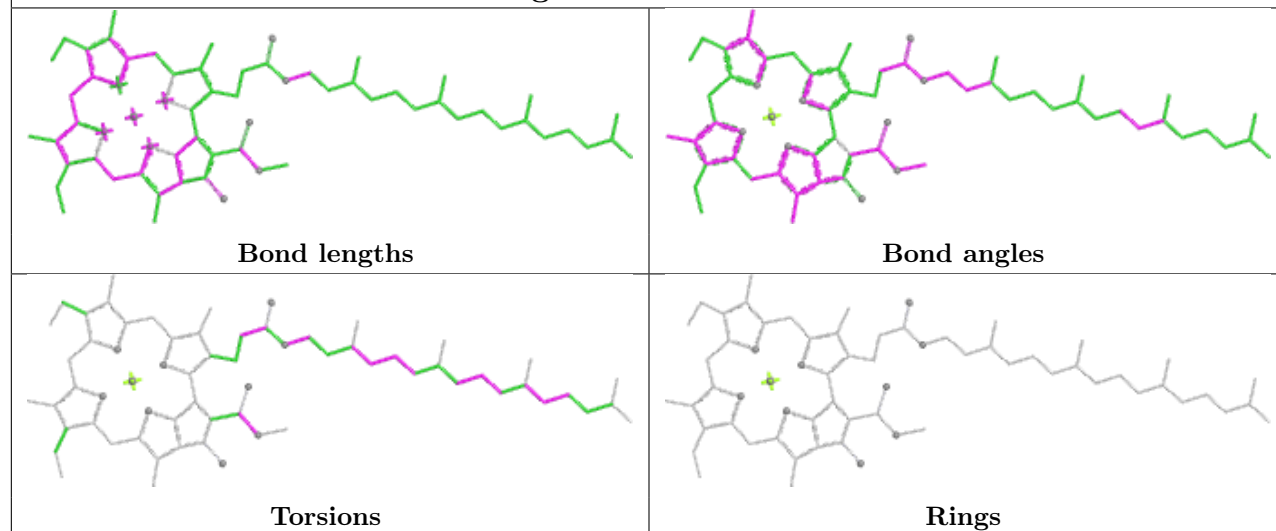


Torsions

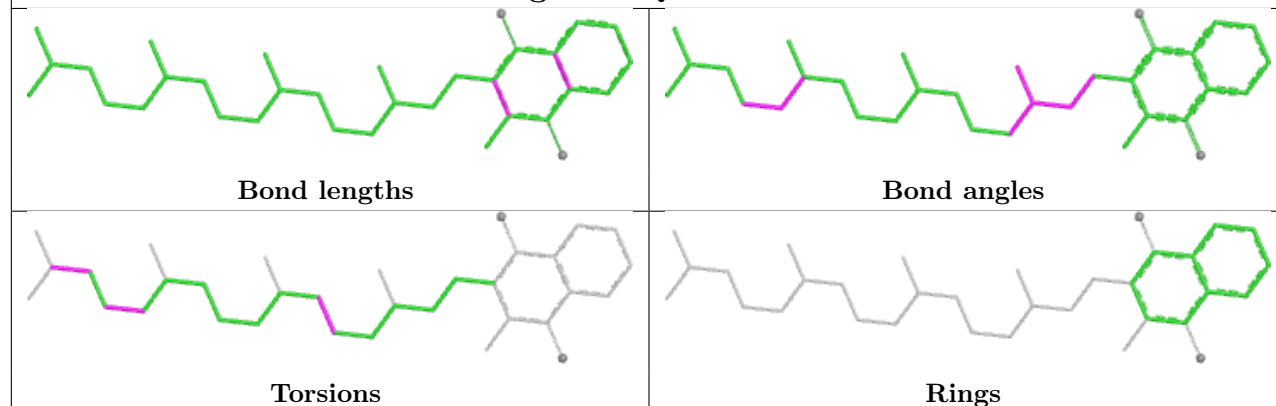


Rings

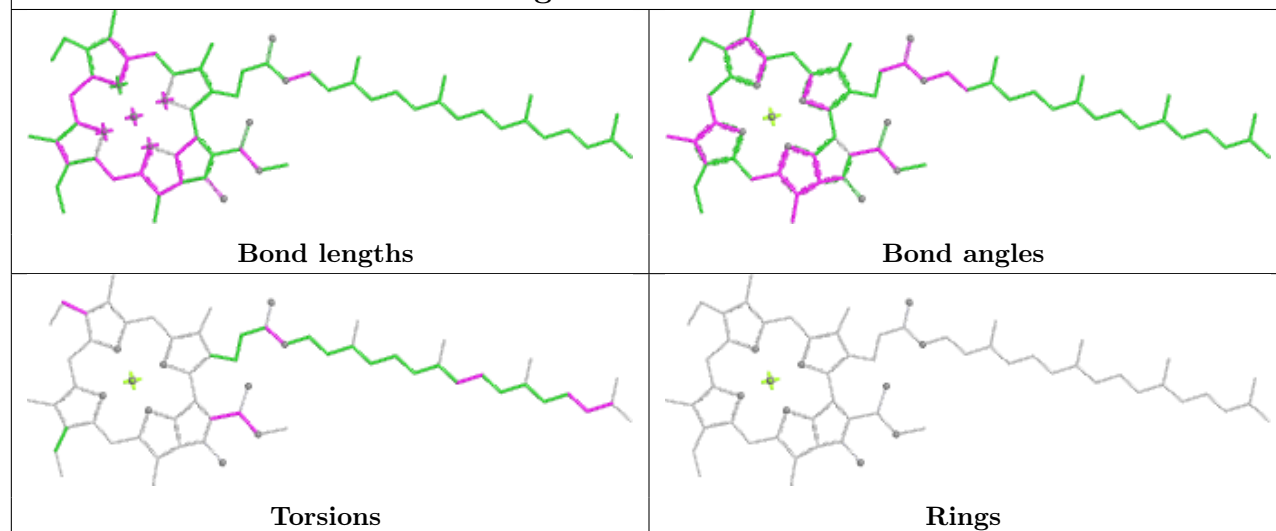
Ligand CLA A 810

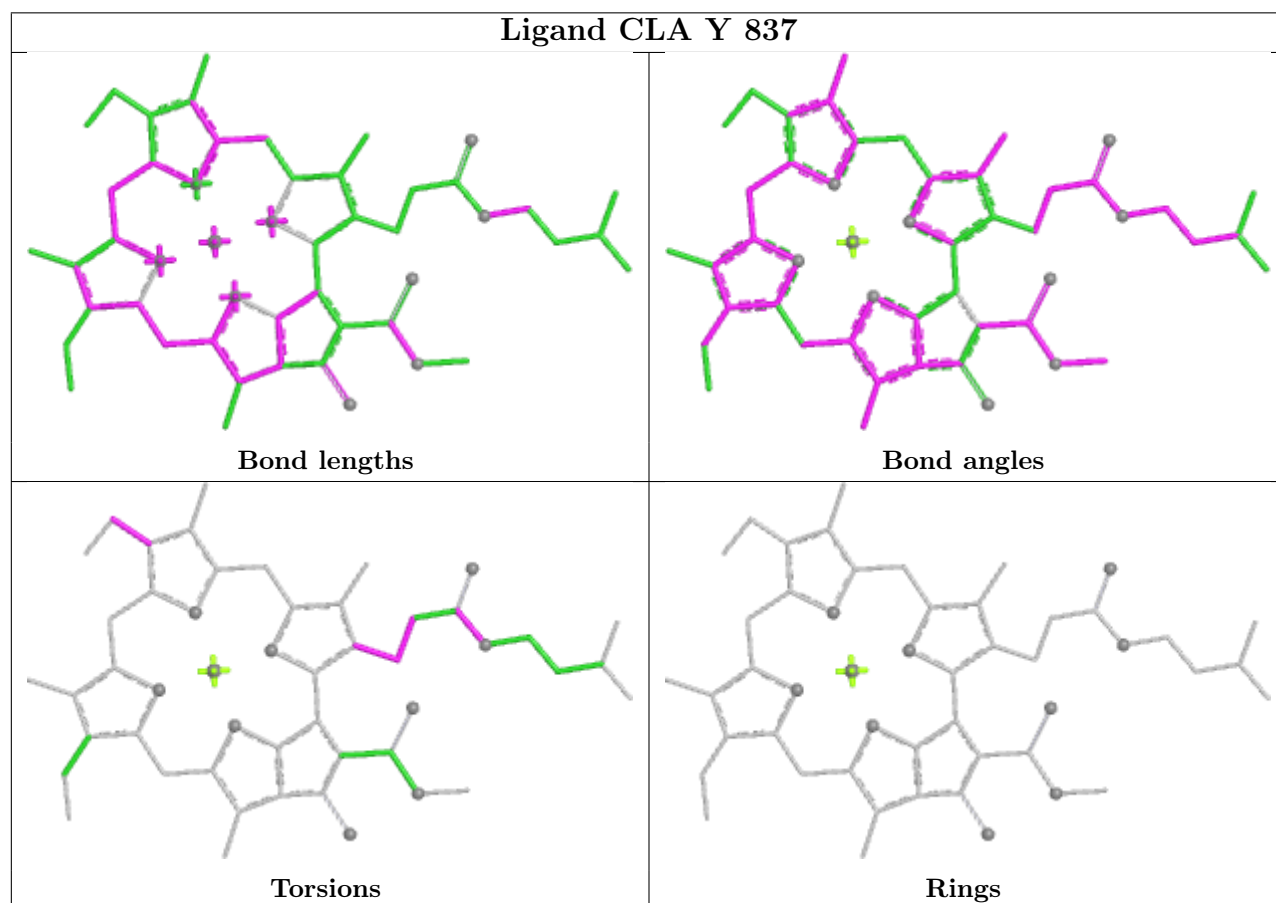
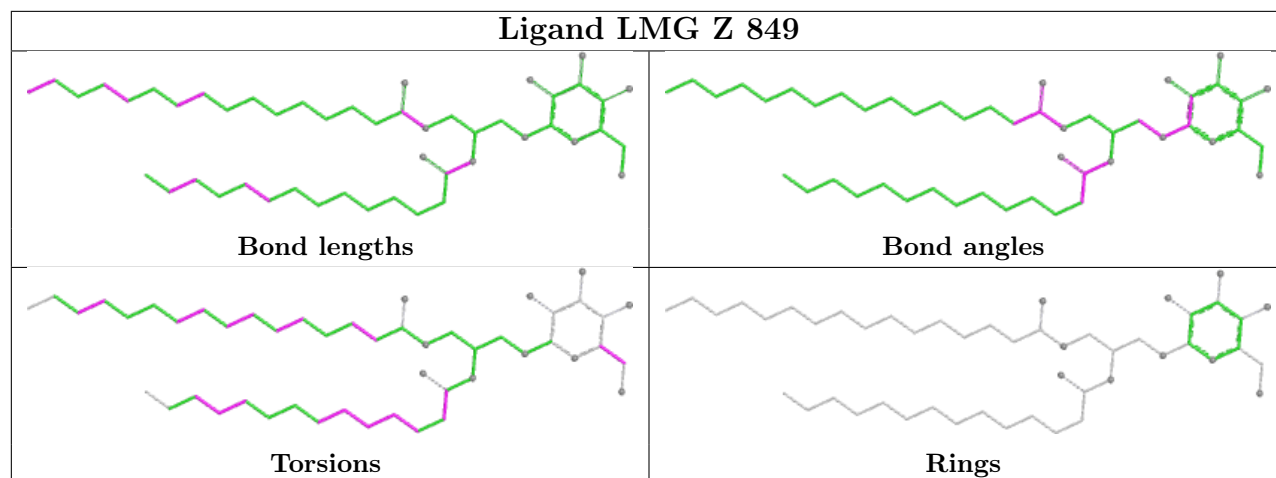


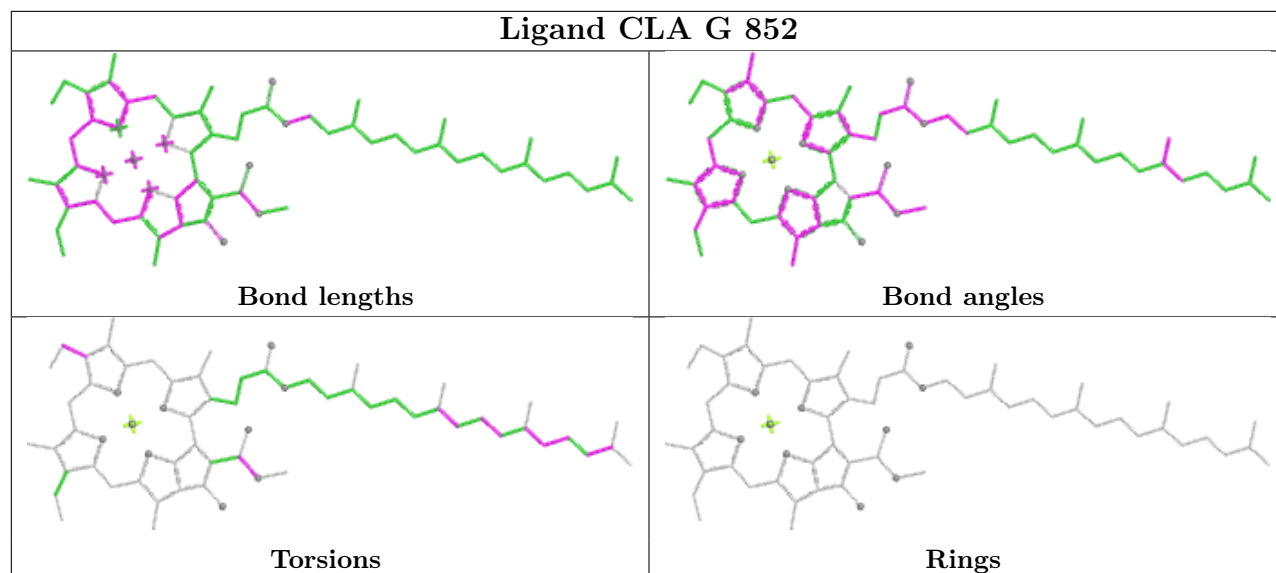
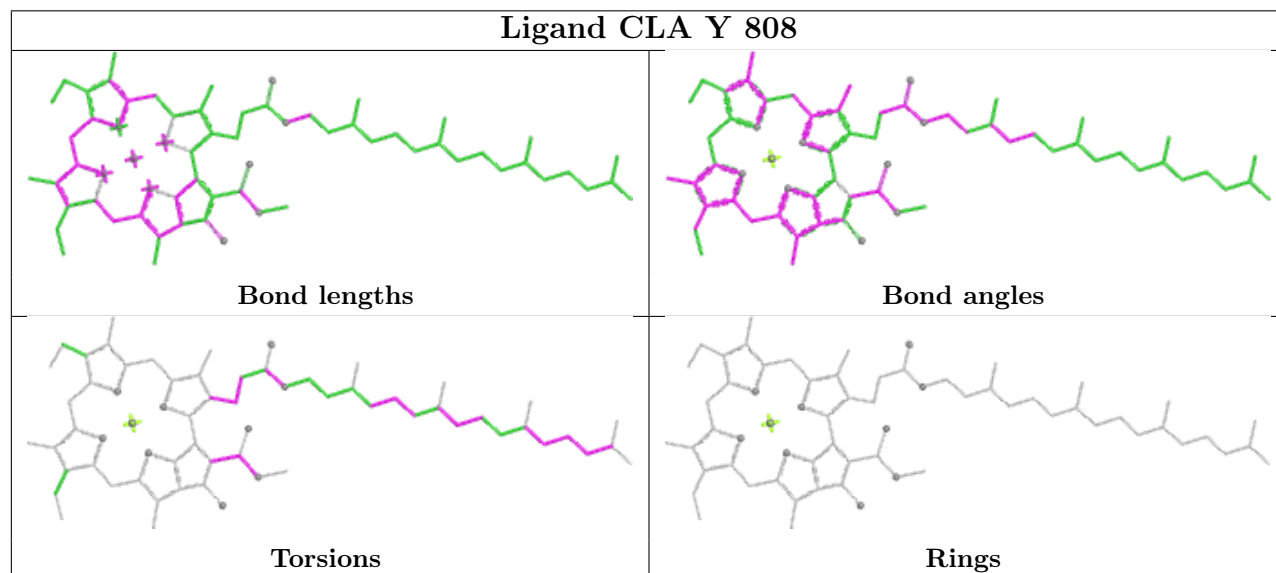
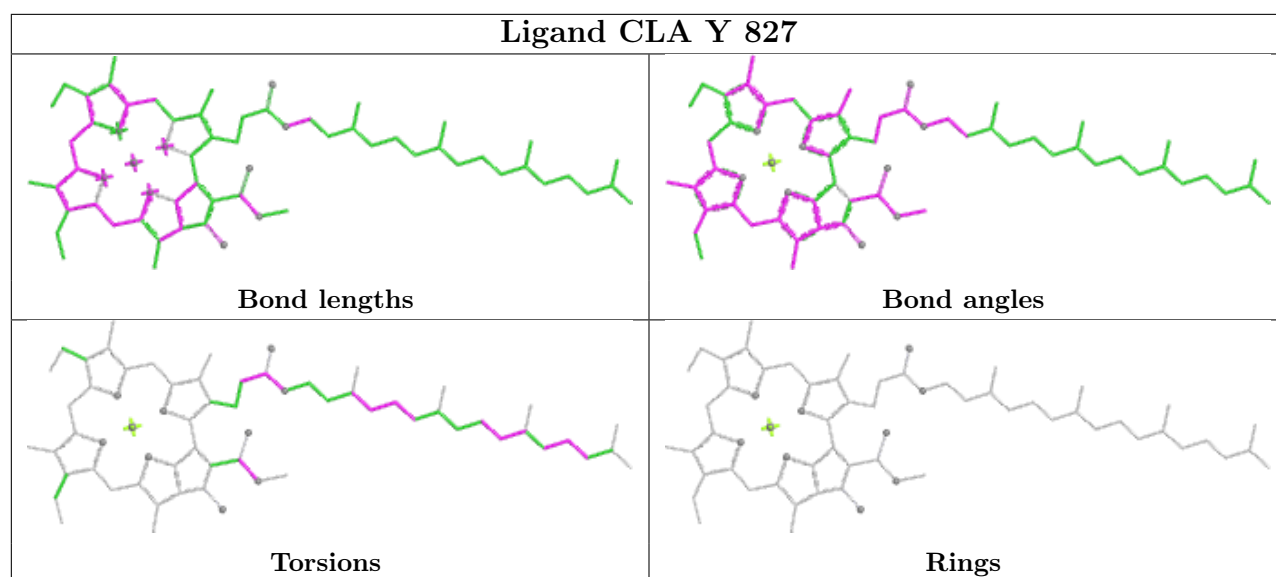
Ligand PQN A 844



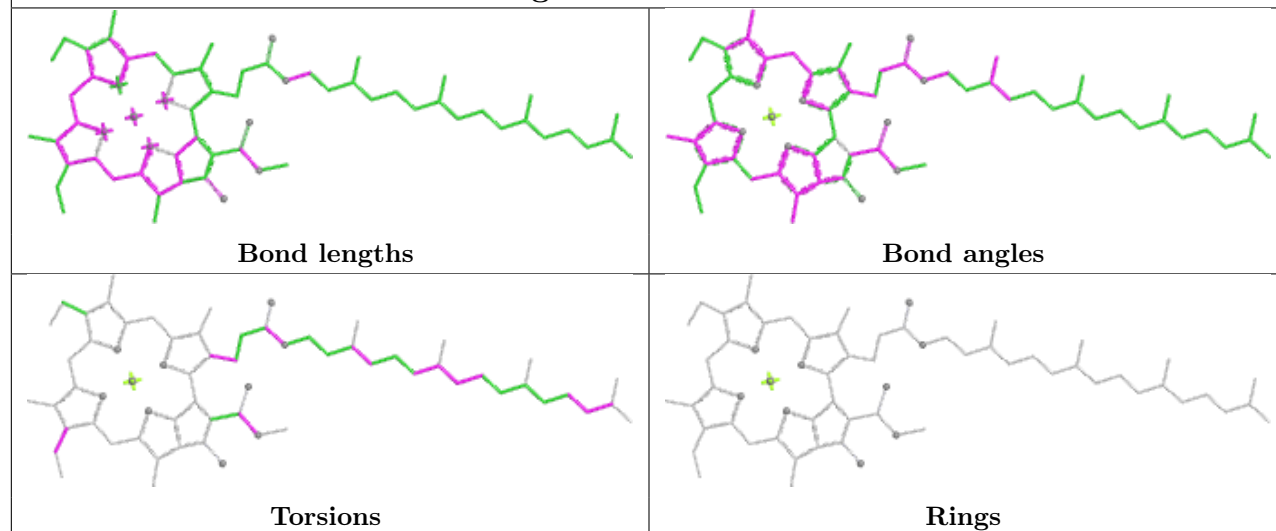
Ligand CLA Z 815



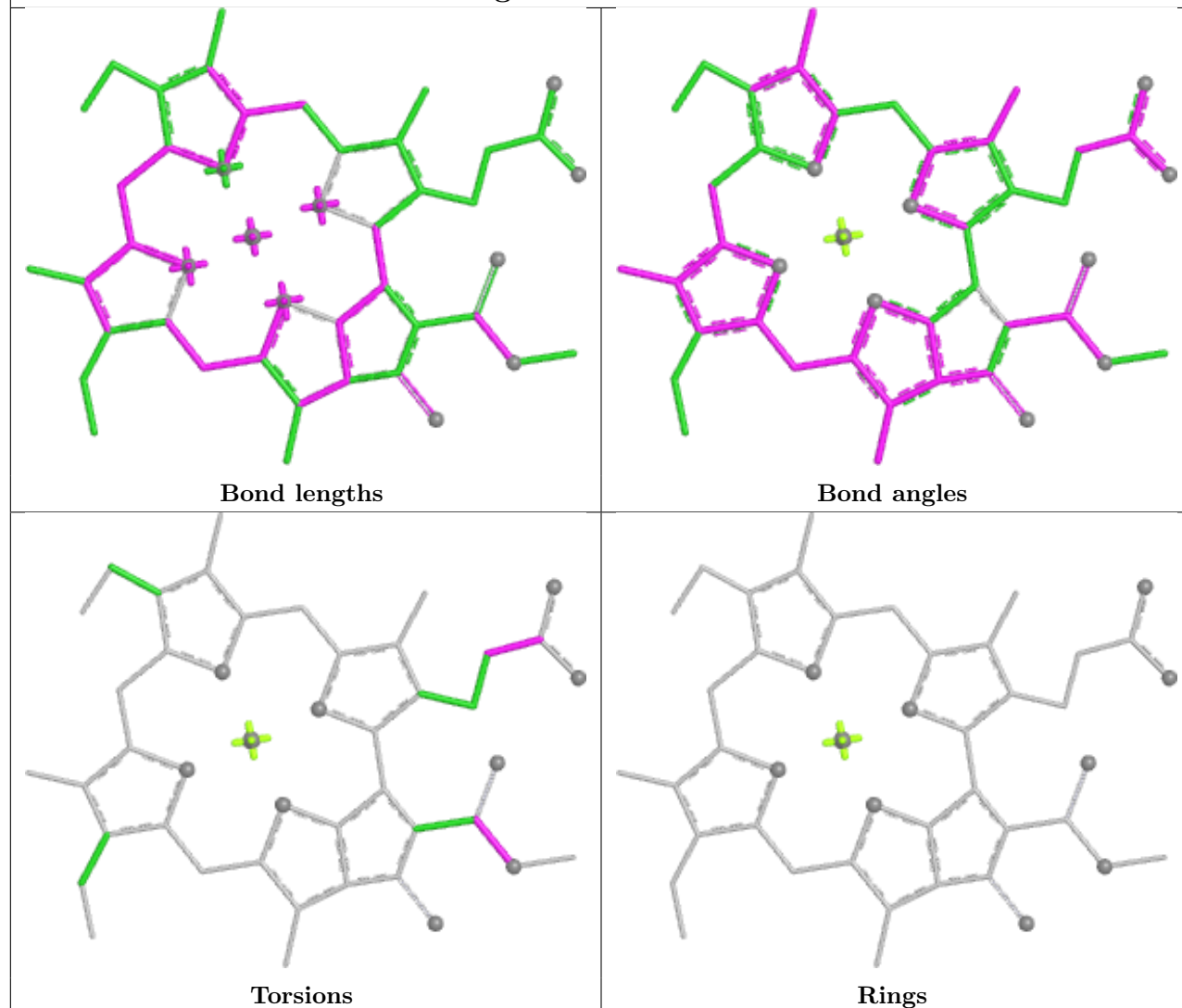




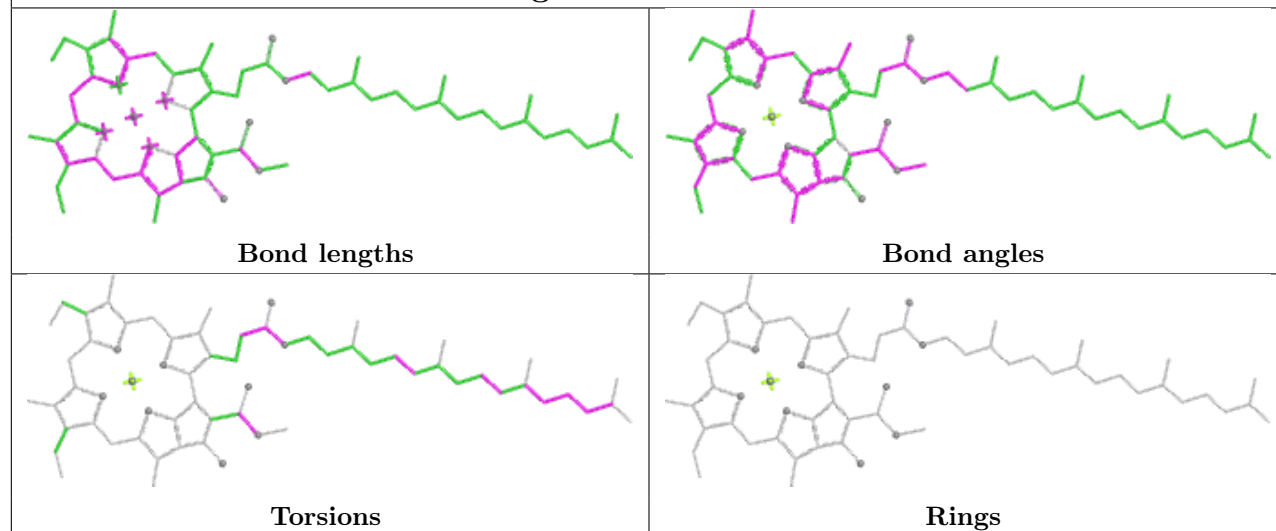
Ligand CLA Y 821



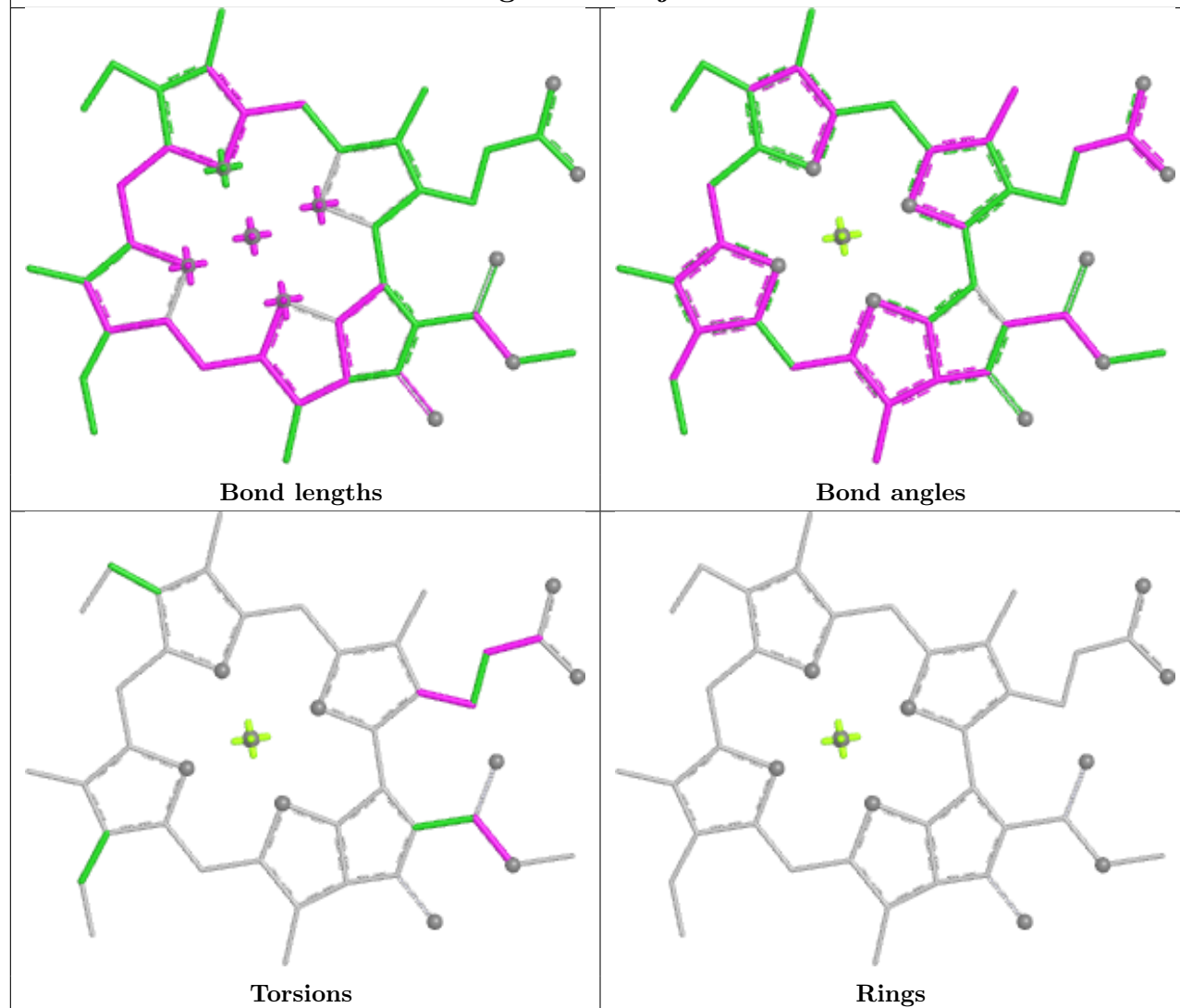
Ligand CLA F 202



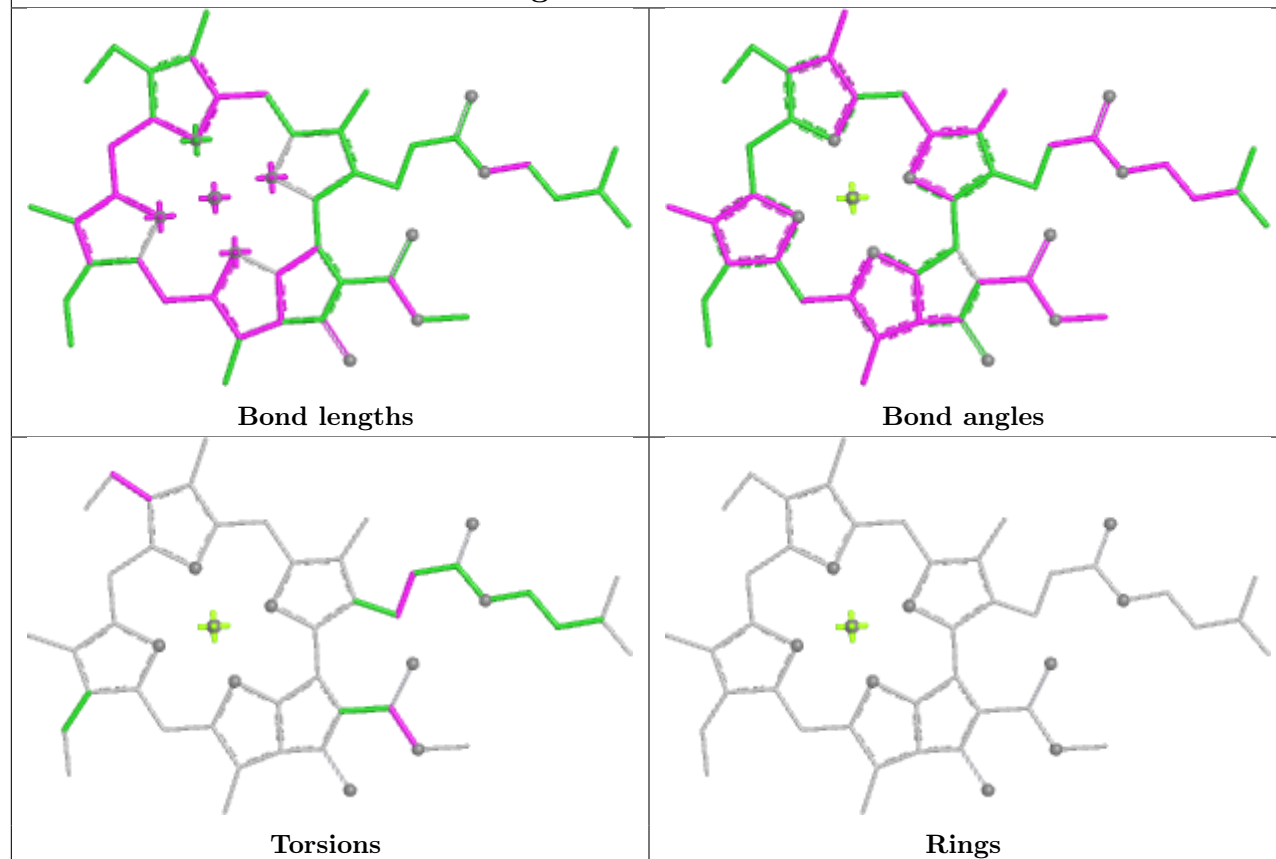
Ligand CLA Y 829



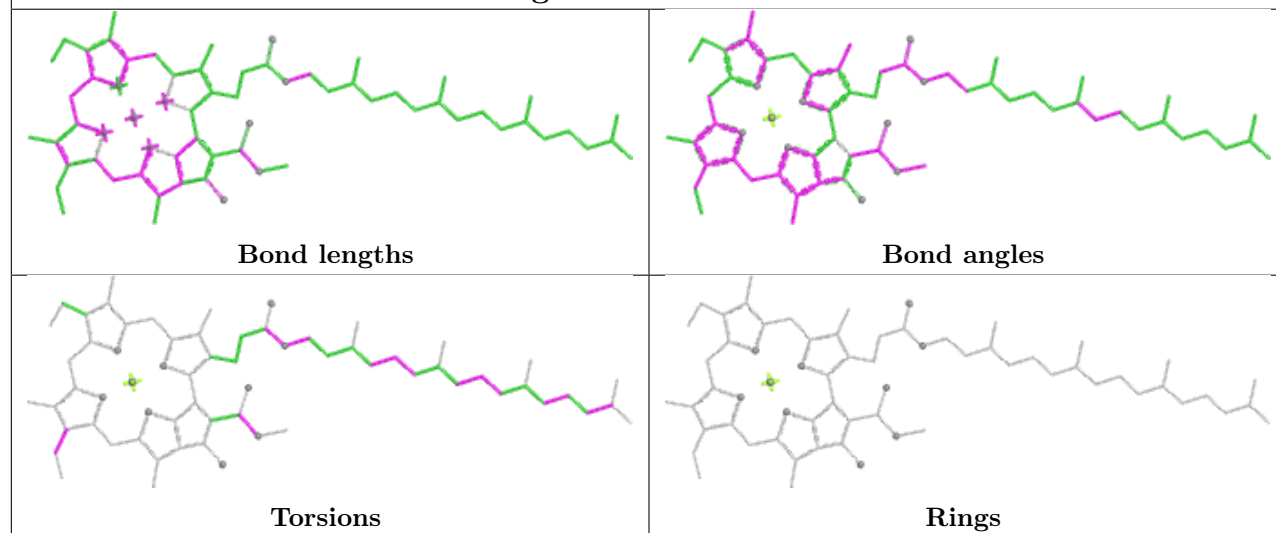
Ligand CLA j 102

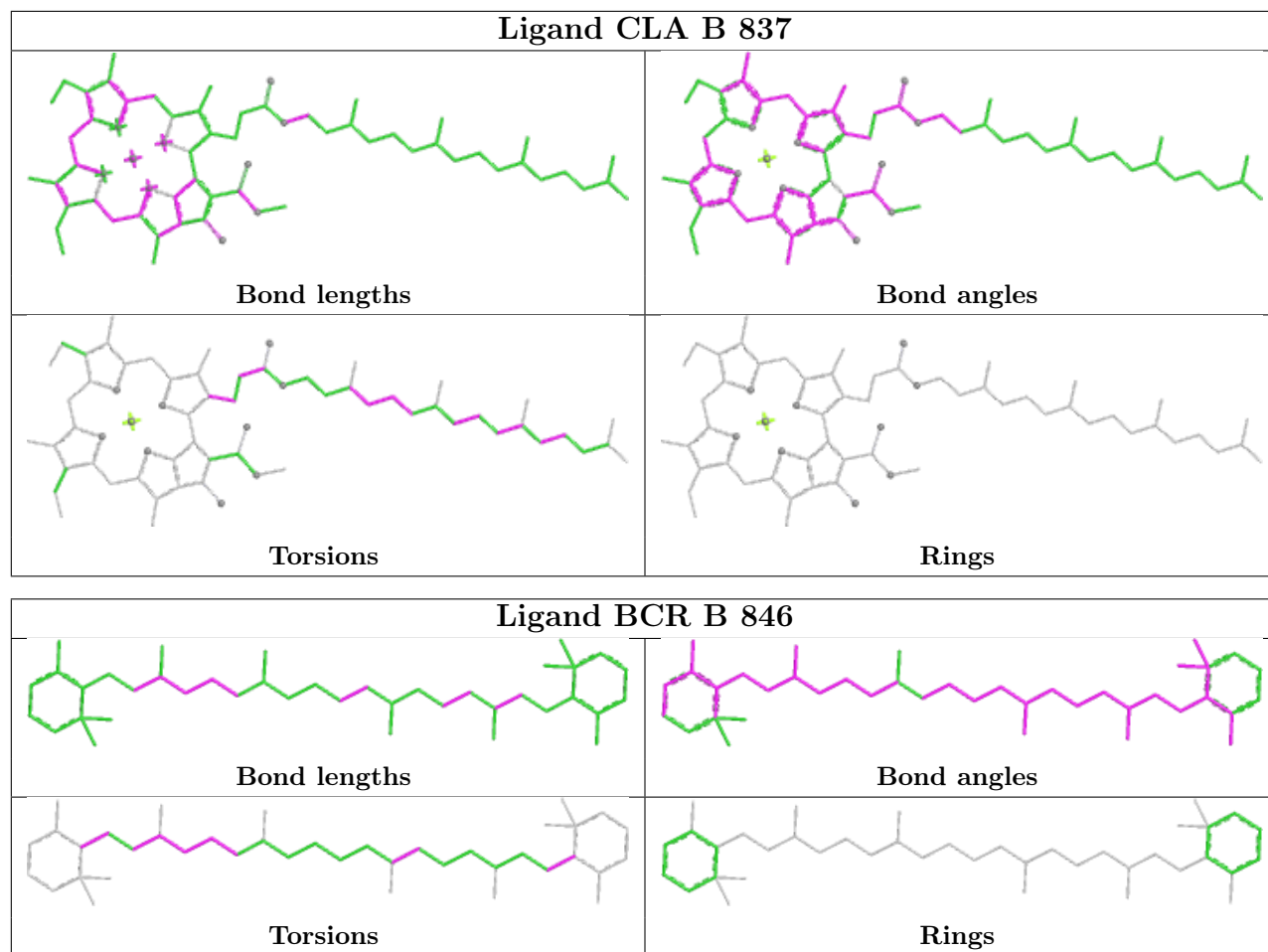


Ligand CLA G 842

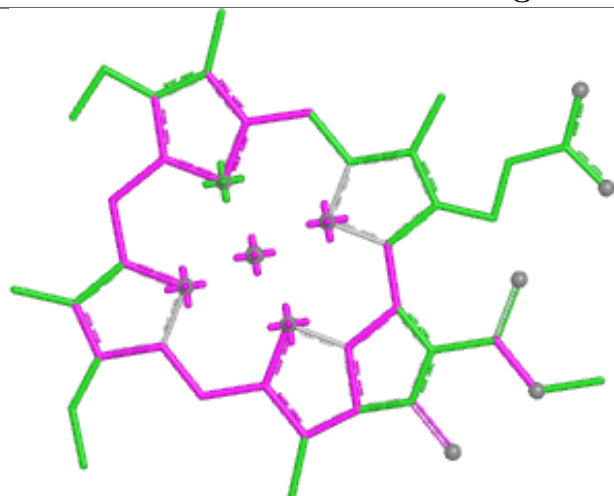


Ligand CLA Y 825

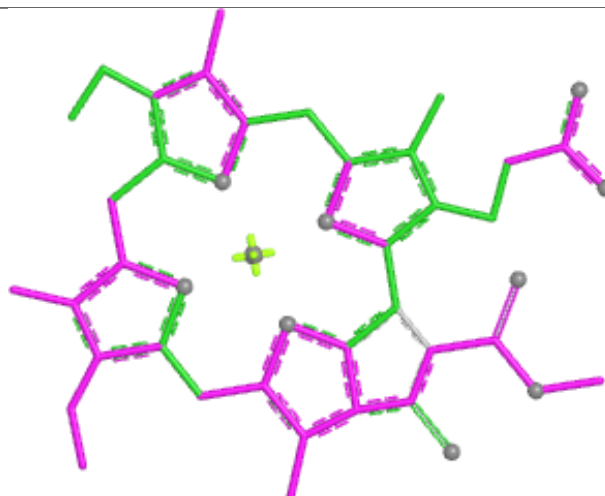




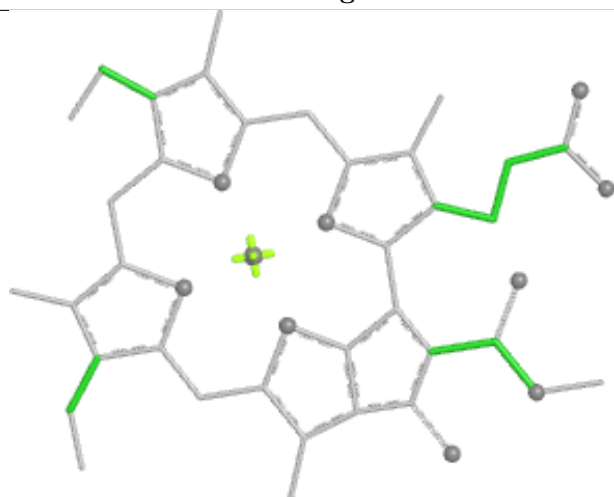
Ligand CLA H 838



Bond lengths



Bond angles

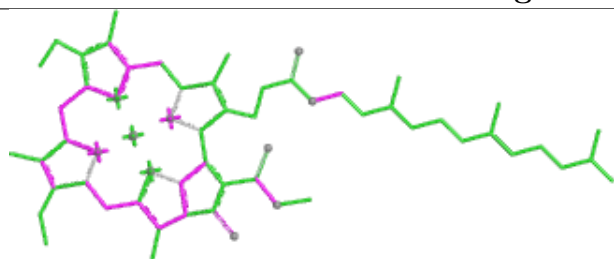


Torsions

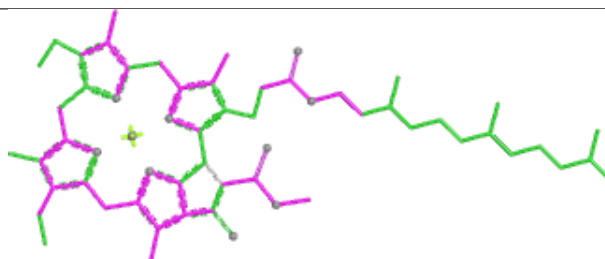


Rings

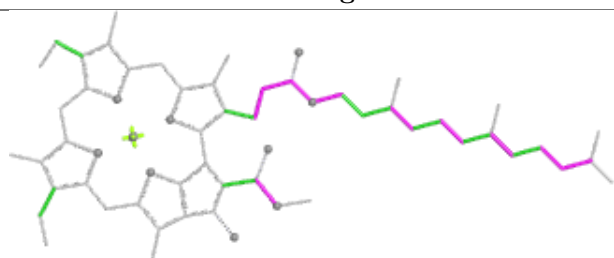
Ligand CLA B 822



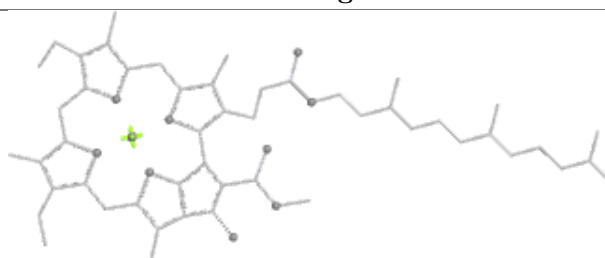
Bond lengths



Bond angles

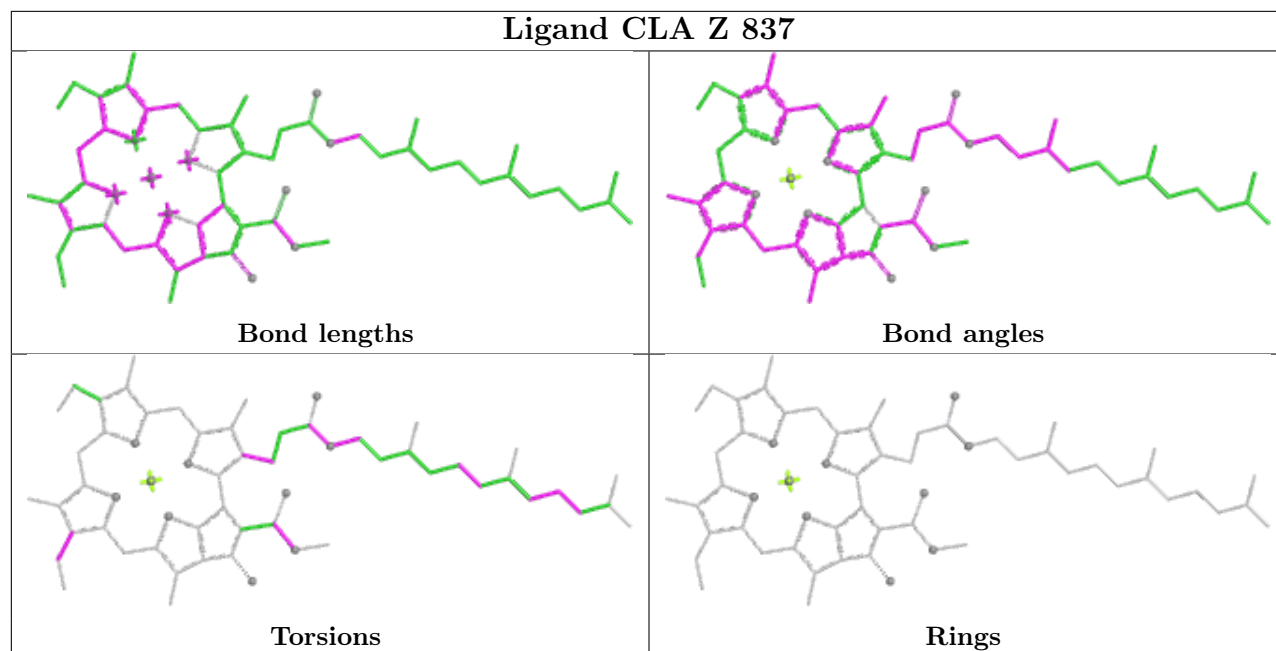


Torsions

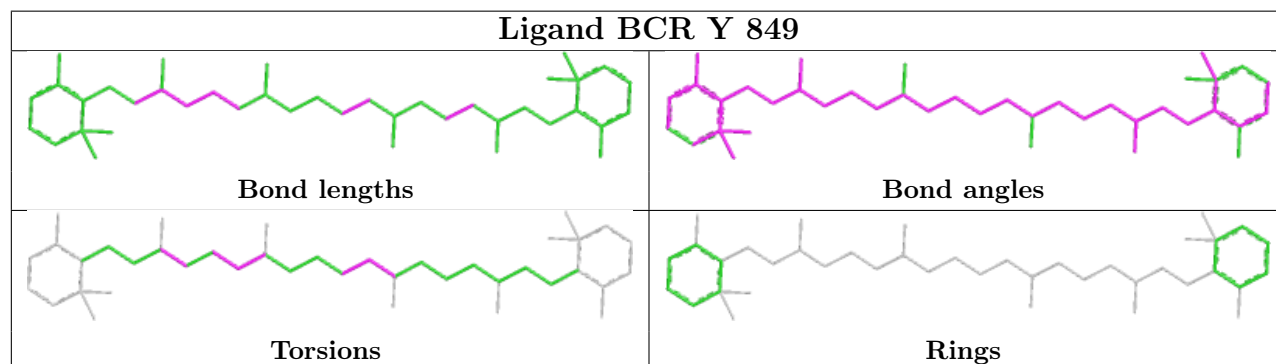


Rings

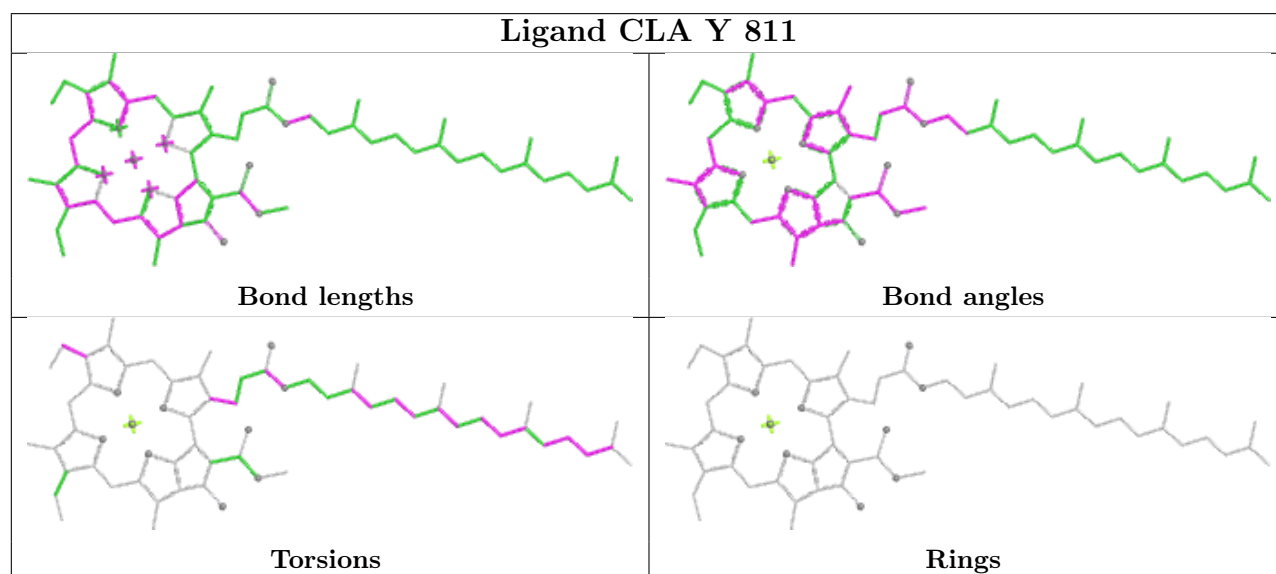
Ligand CLA Z 837

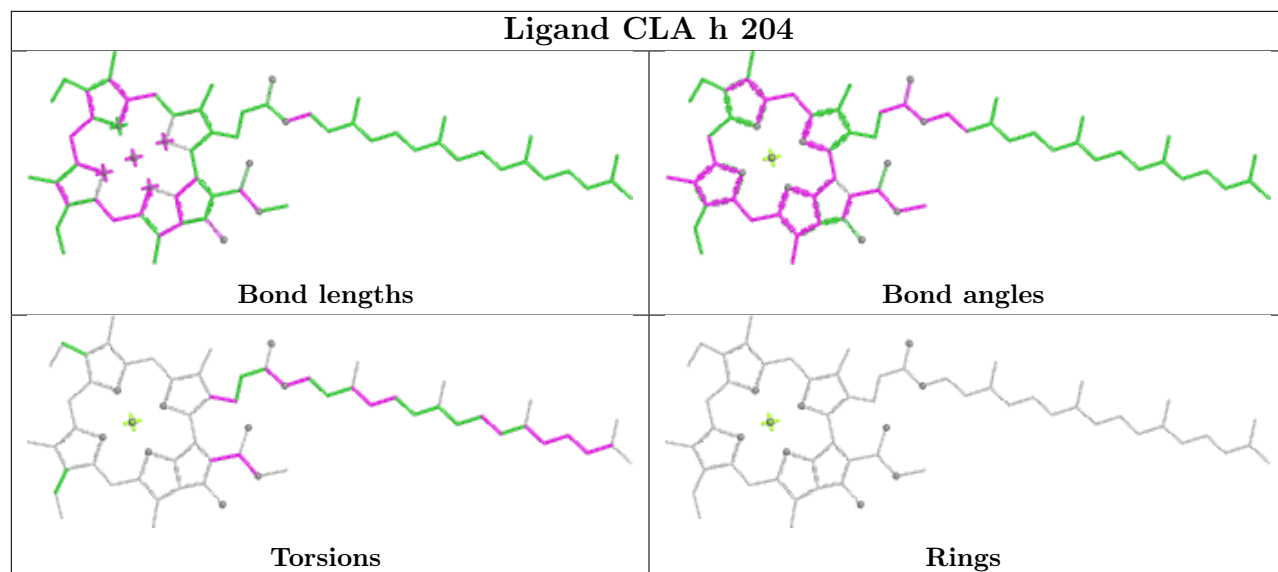
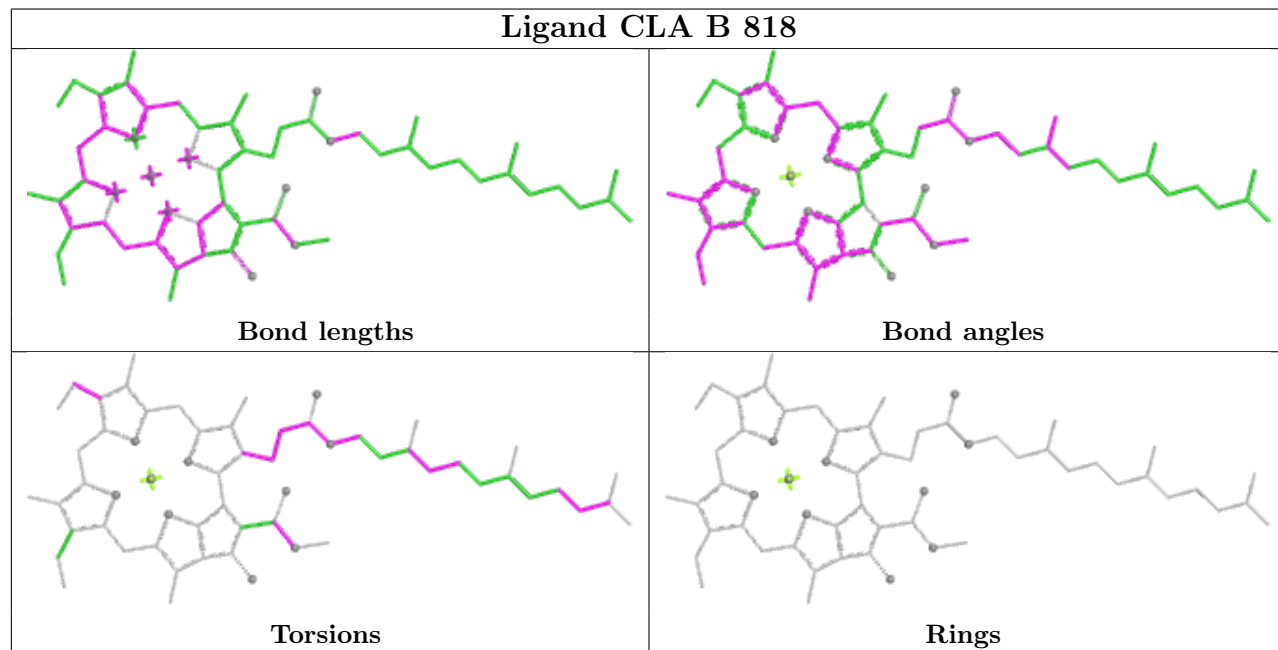


Ligand BCR Y 849

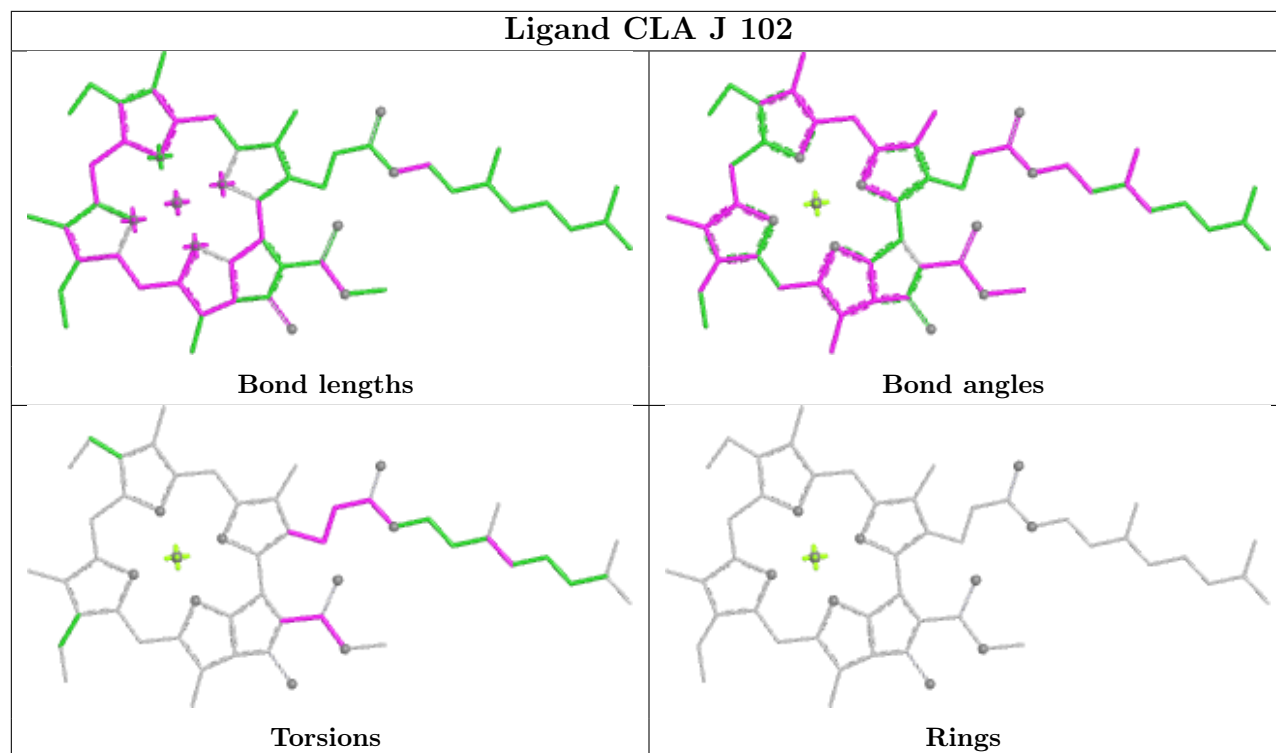


Ligand CLA Y 811

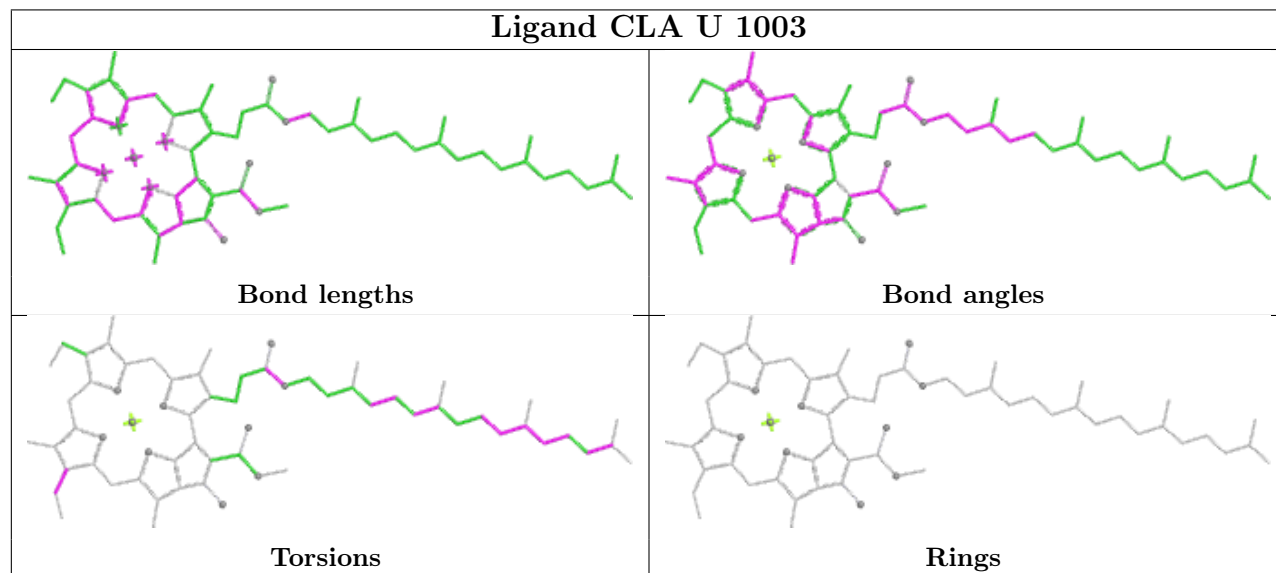


Ligand CLA h 204**Ligand CLA B 818**

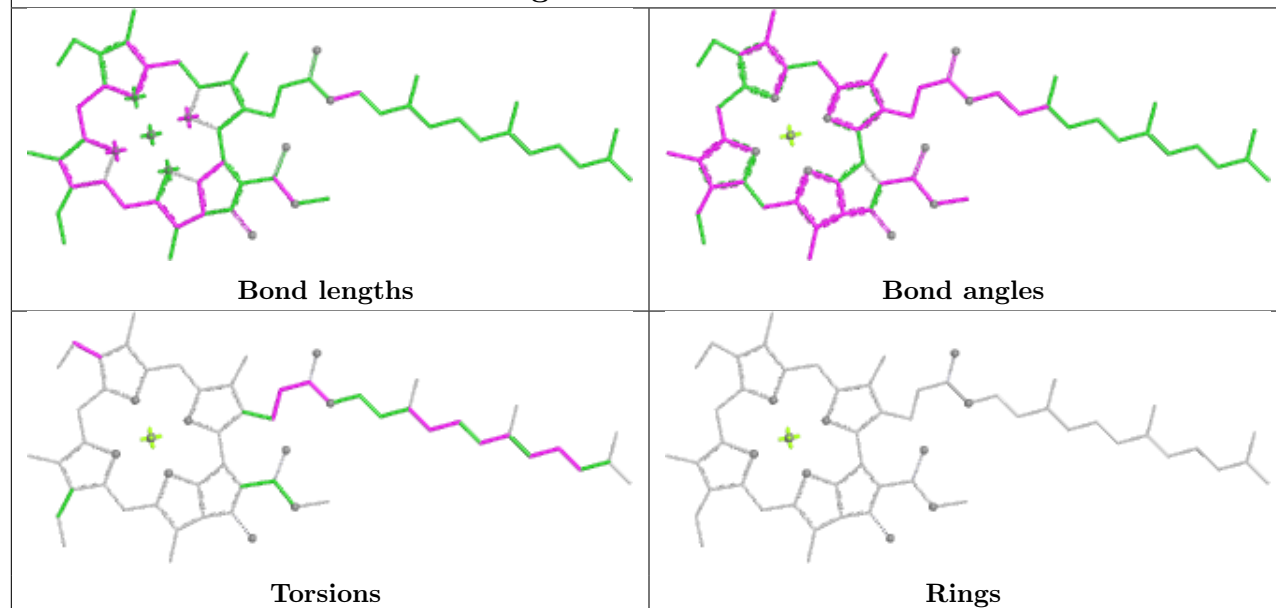
Ligand CLA J 102



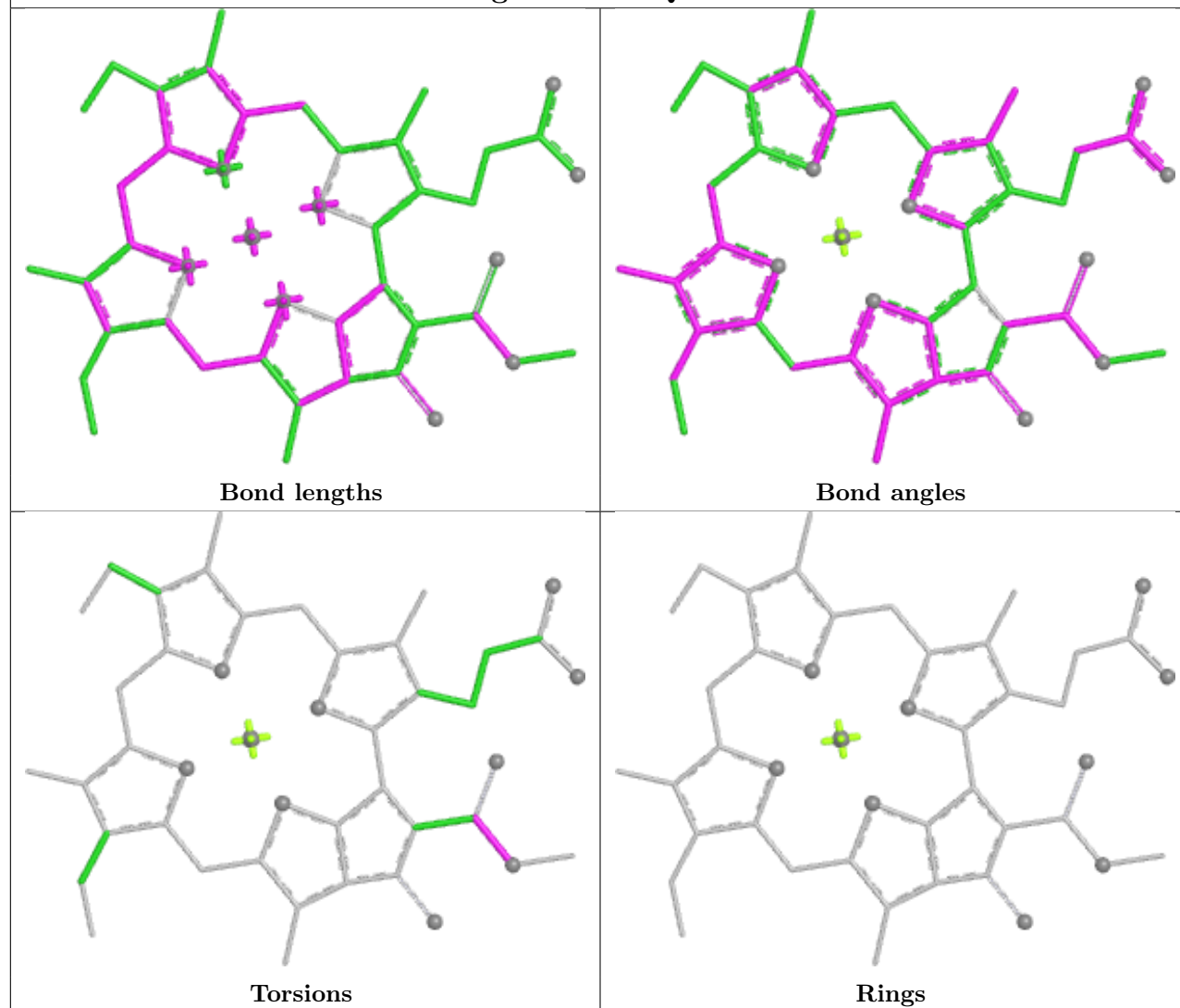
Ligand CLA U 1003

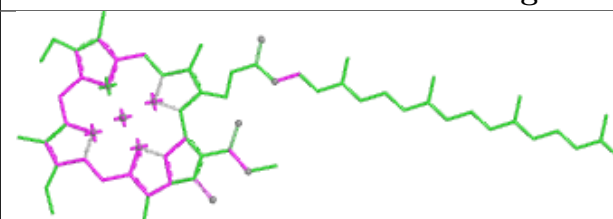
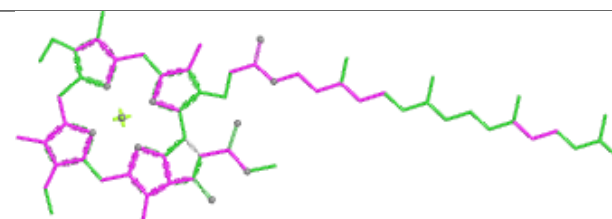
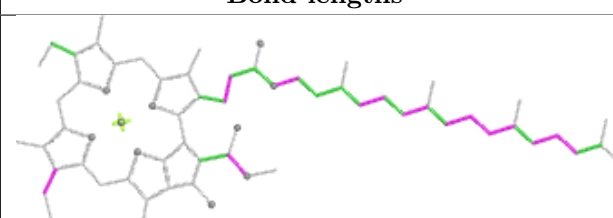
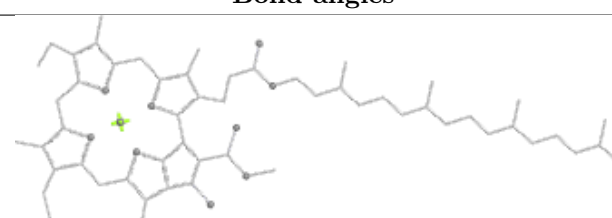


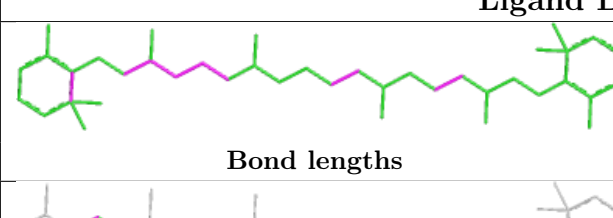
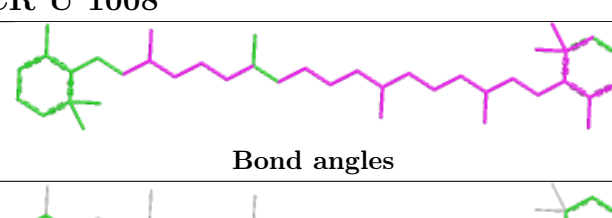
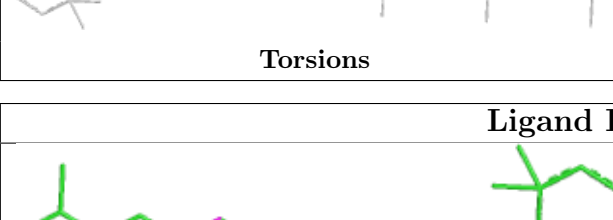
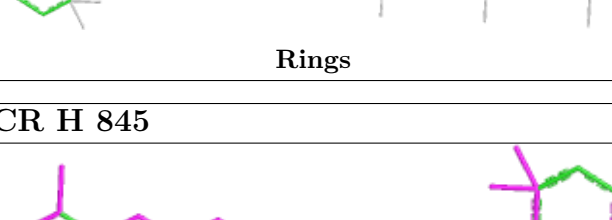
Ligand CLA H 823

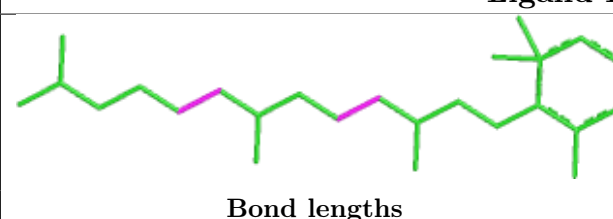
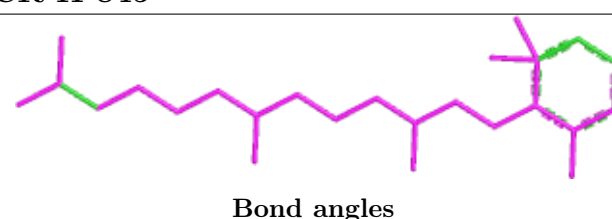
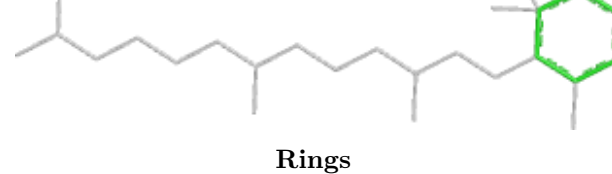


Ligand CLA Q 202

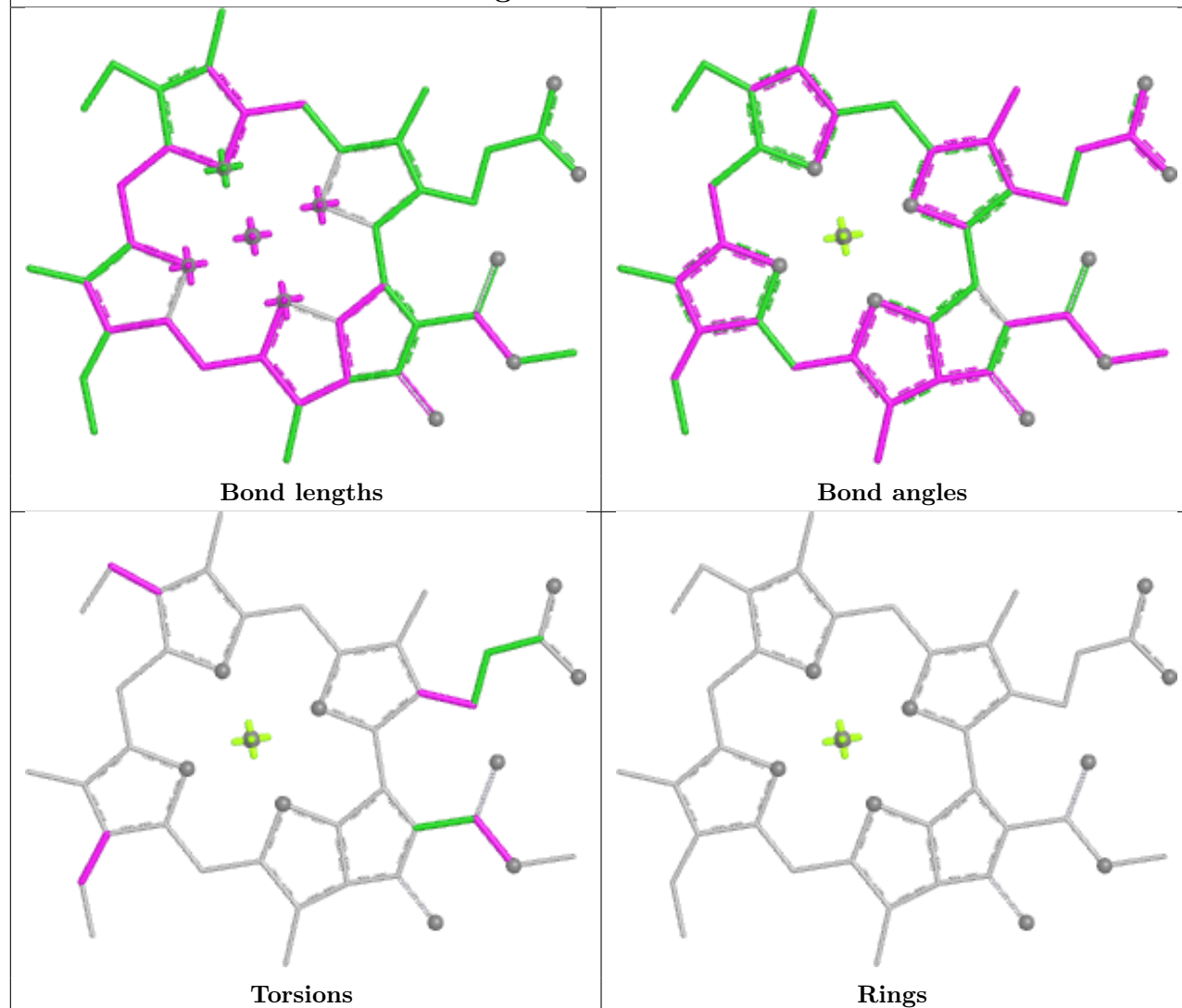


Ligand CLA Y 809	
	
Bond lengths	Bond angles
	
Torsions	Rings

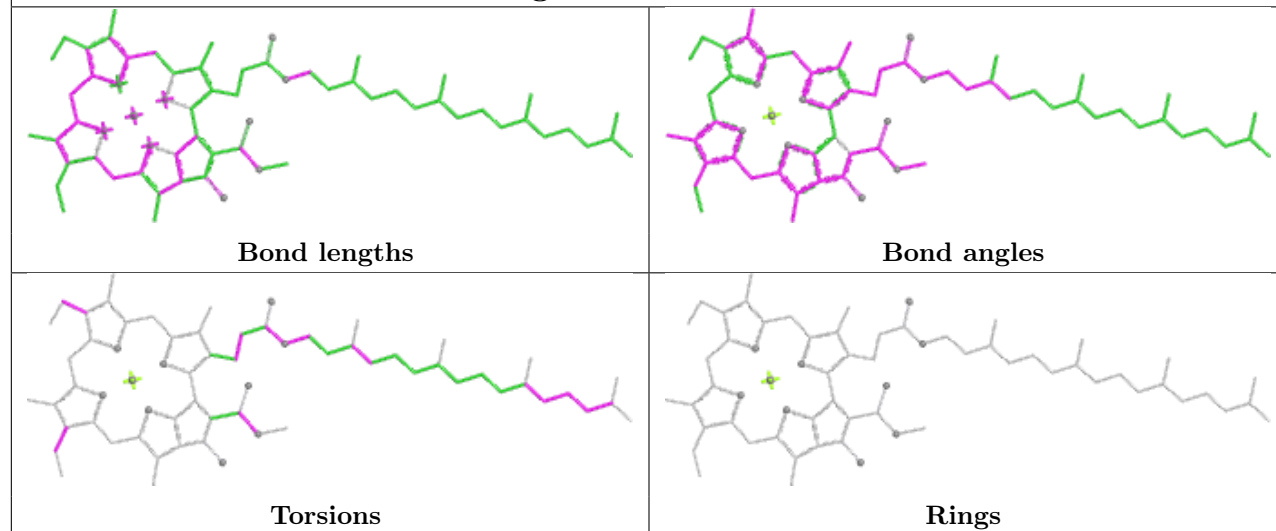
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Bond lengths	Bond angles
	
Torsions	Rings

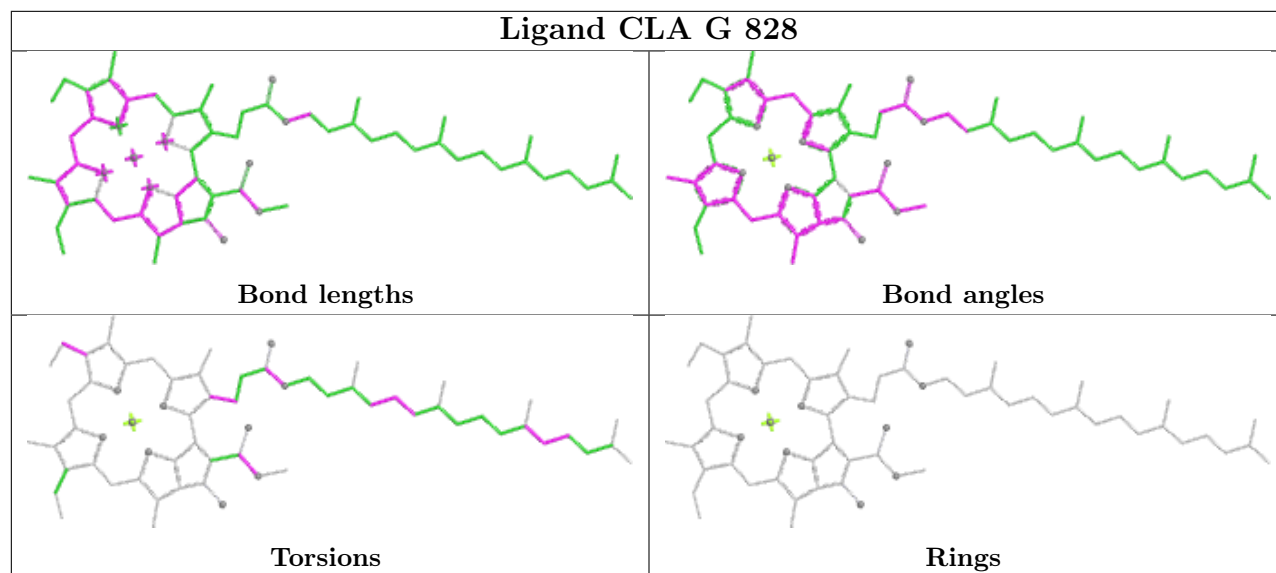
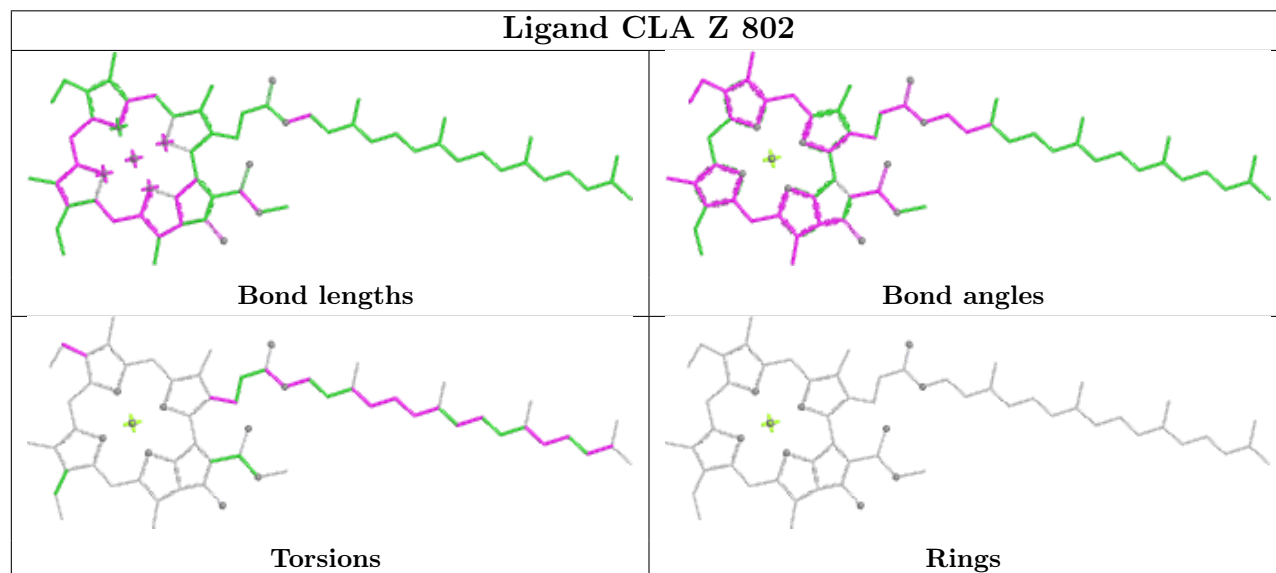
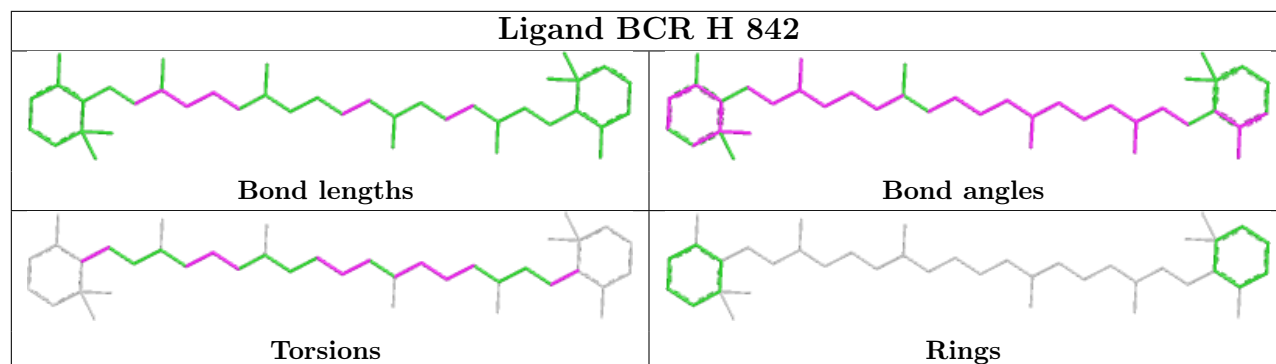
Ligand BCR H 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Z 813

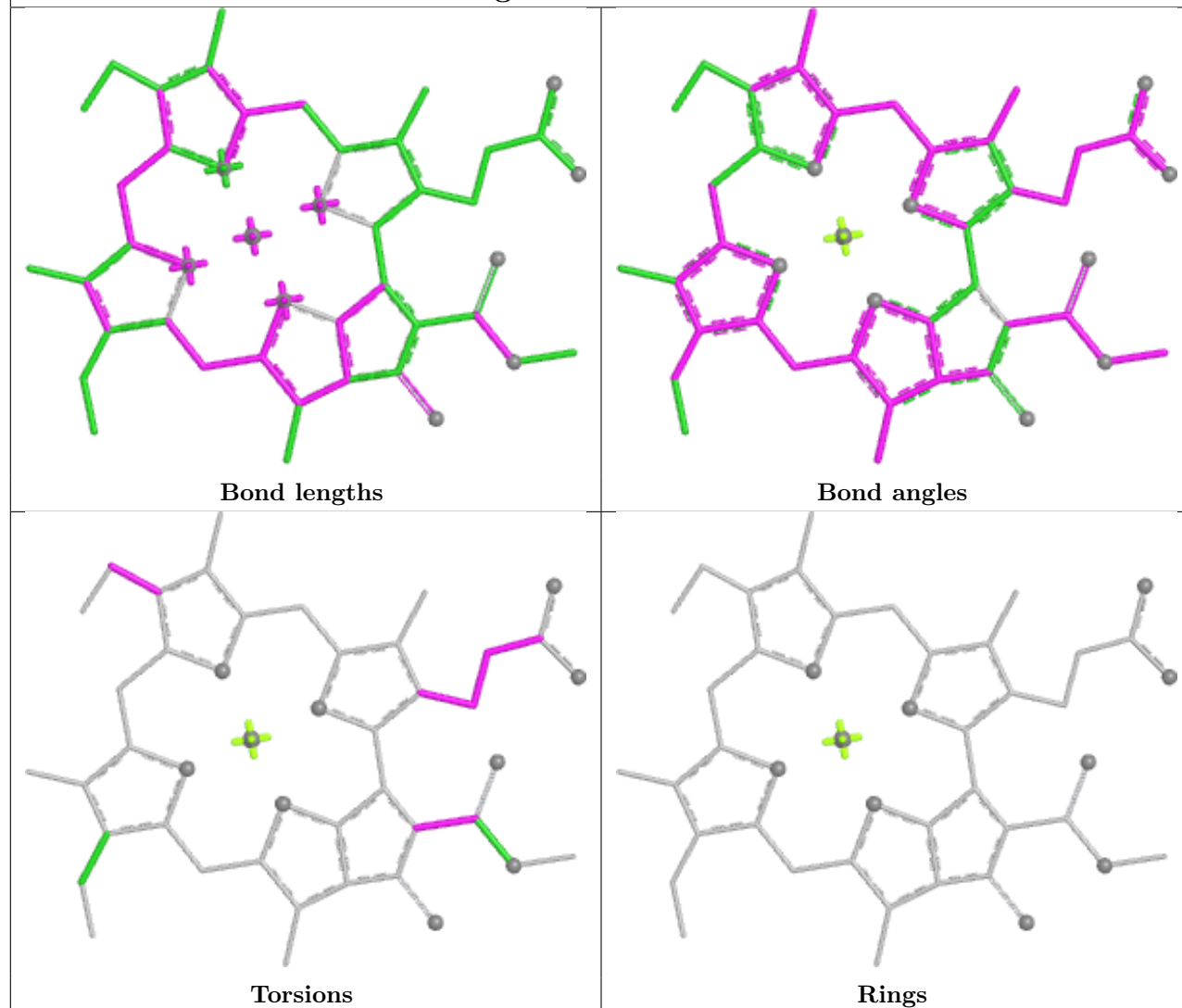


Ligand CLA H 810

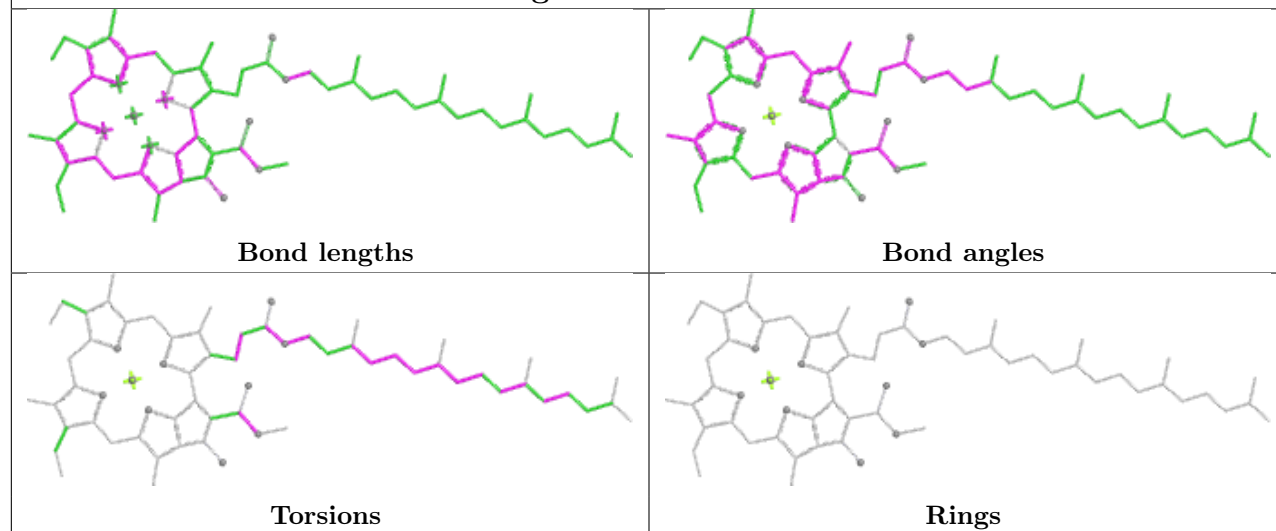




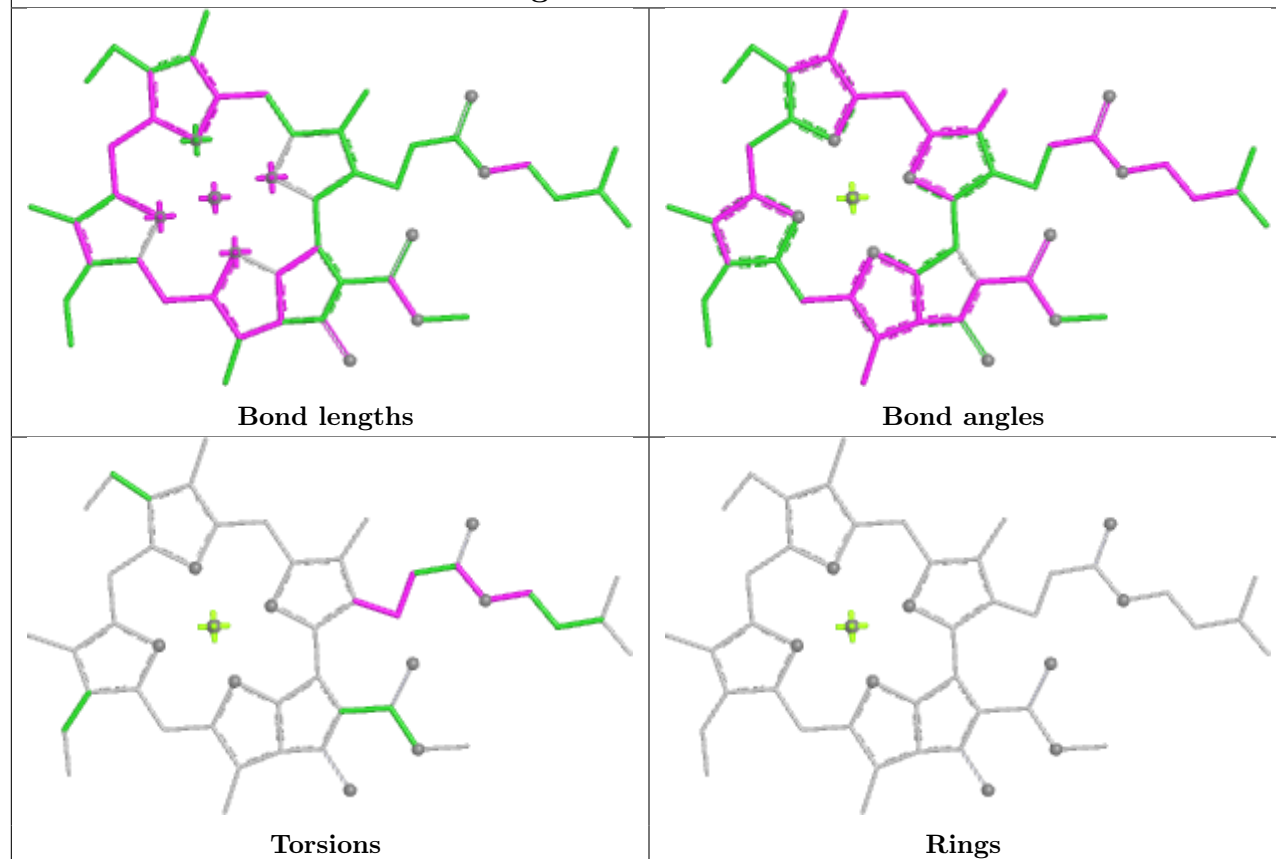
Ligand CLA Z 821



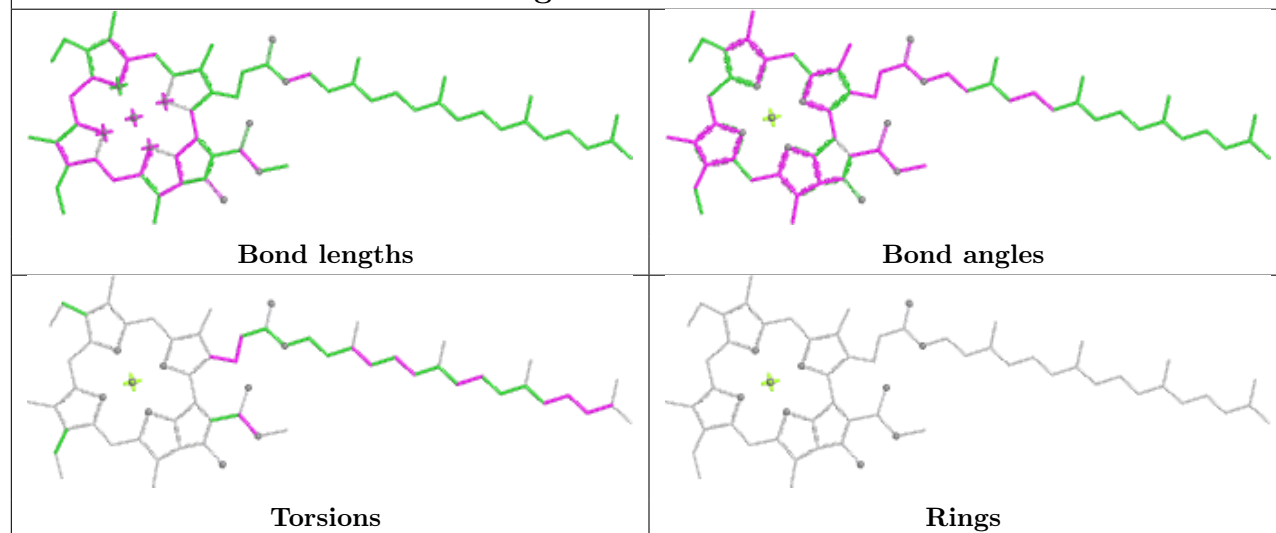
Ligand CLA Y 822



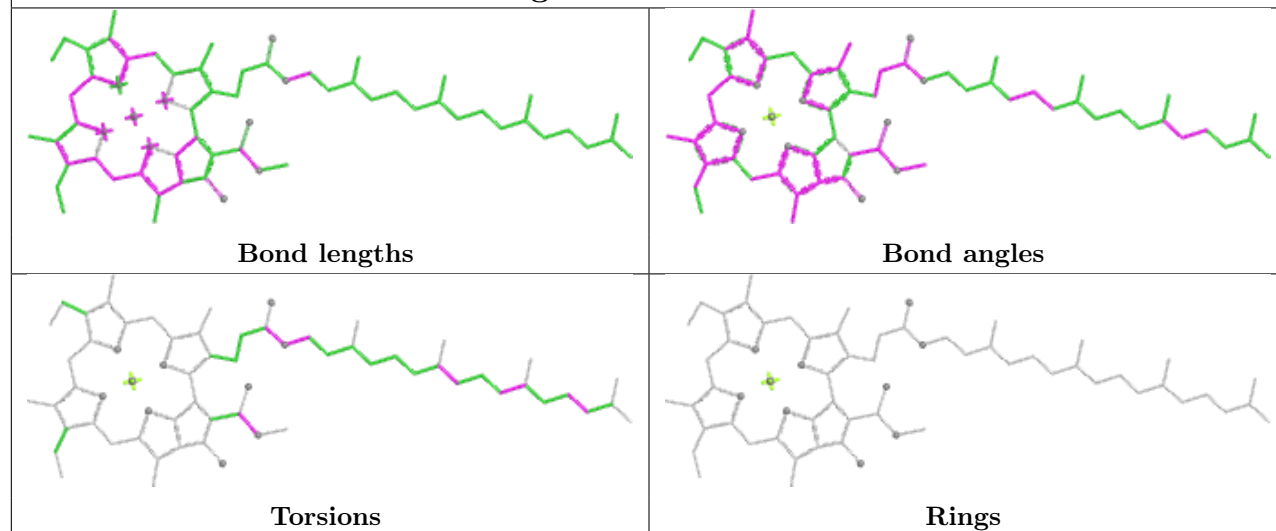
Ligand CLA G 815



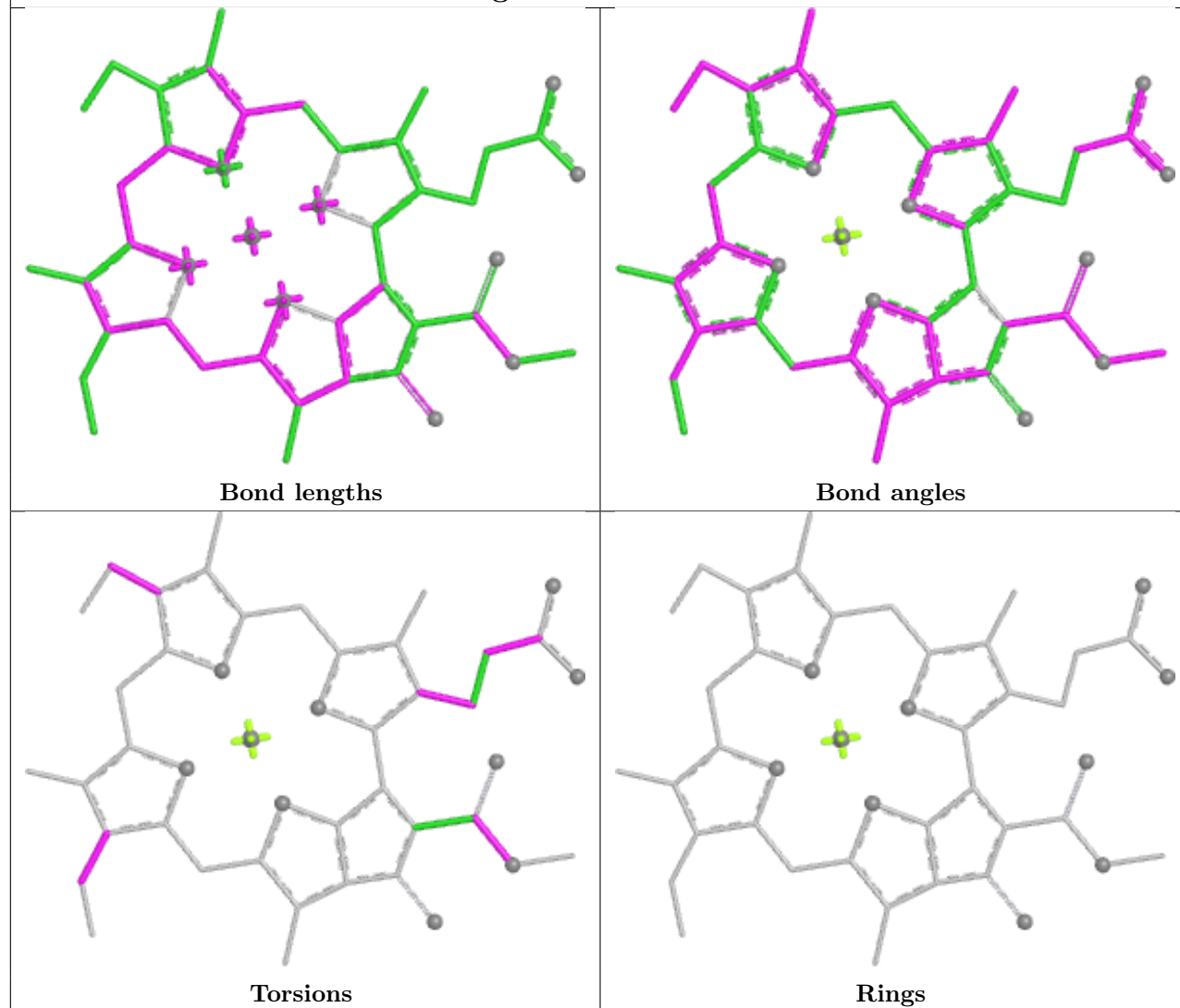
Ligand CLA Z 829



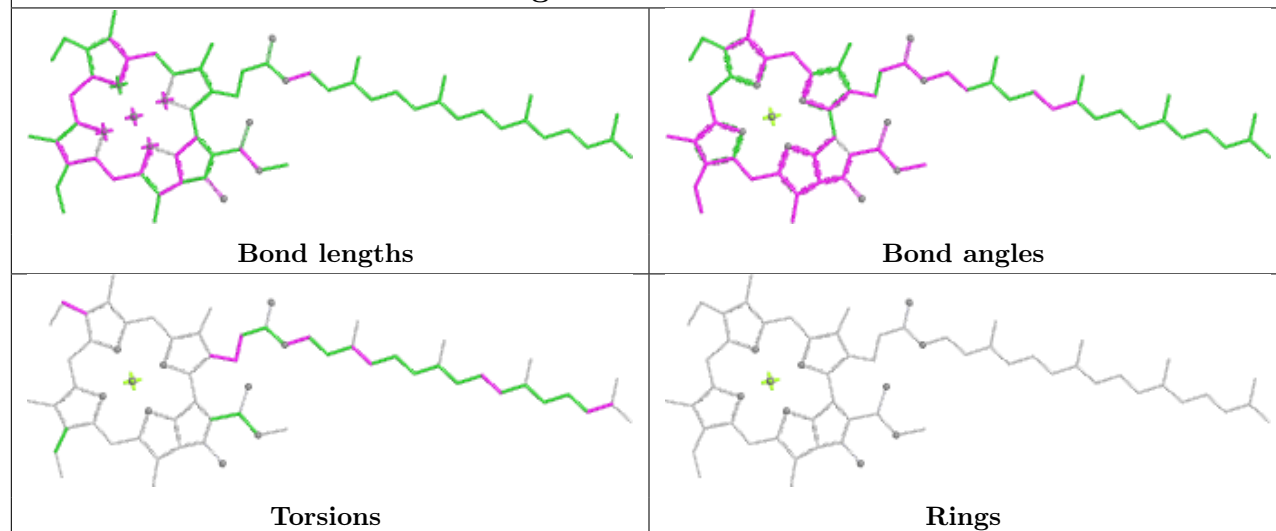
Ligand CLA G 825



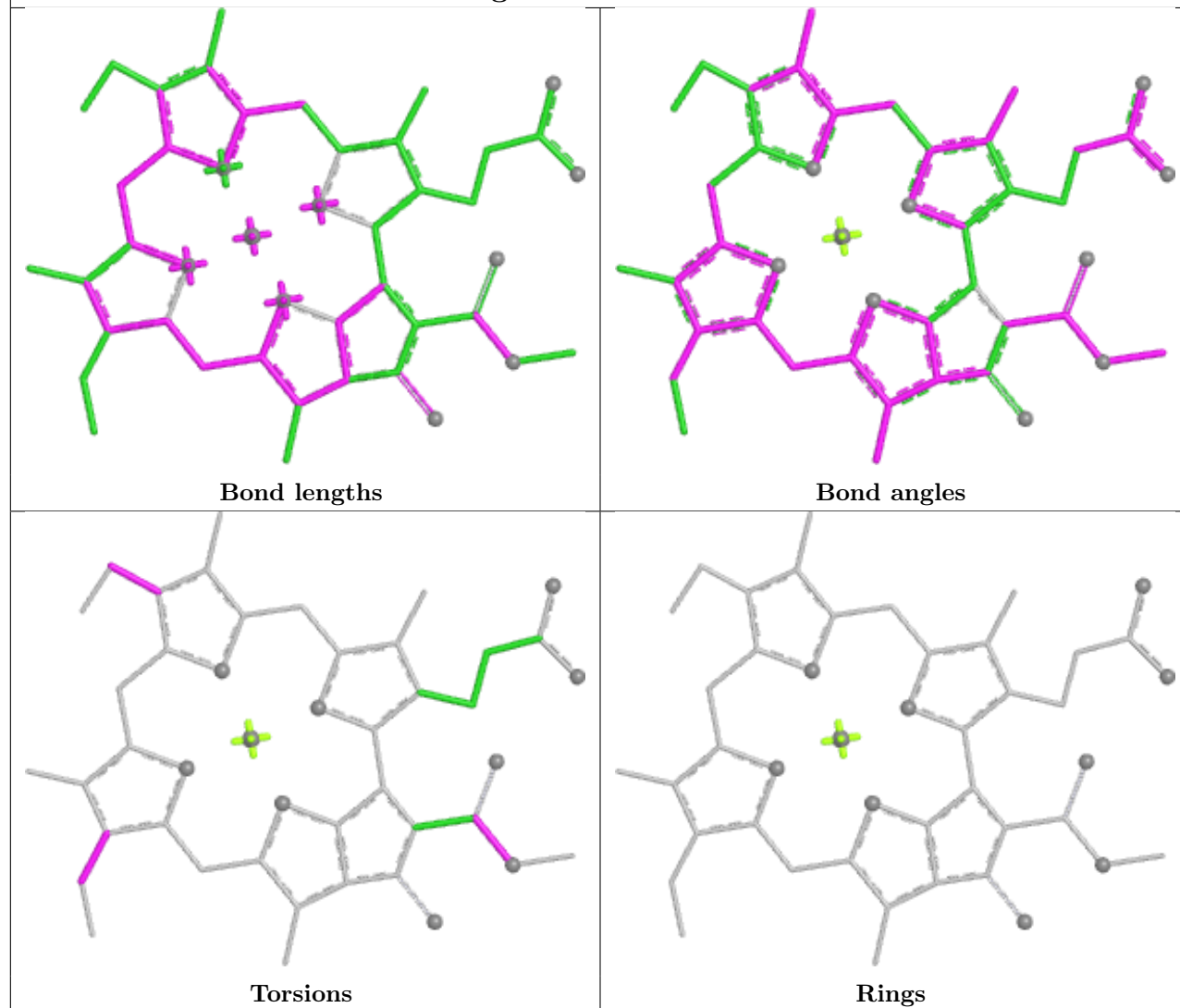
Ligand CLA B 820



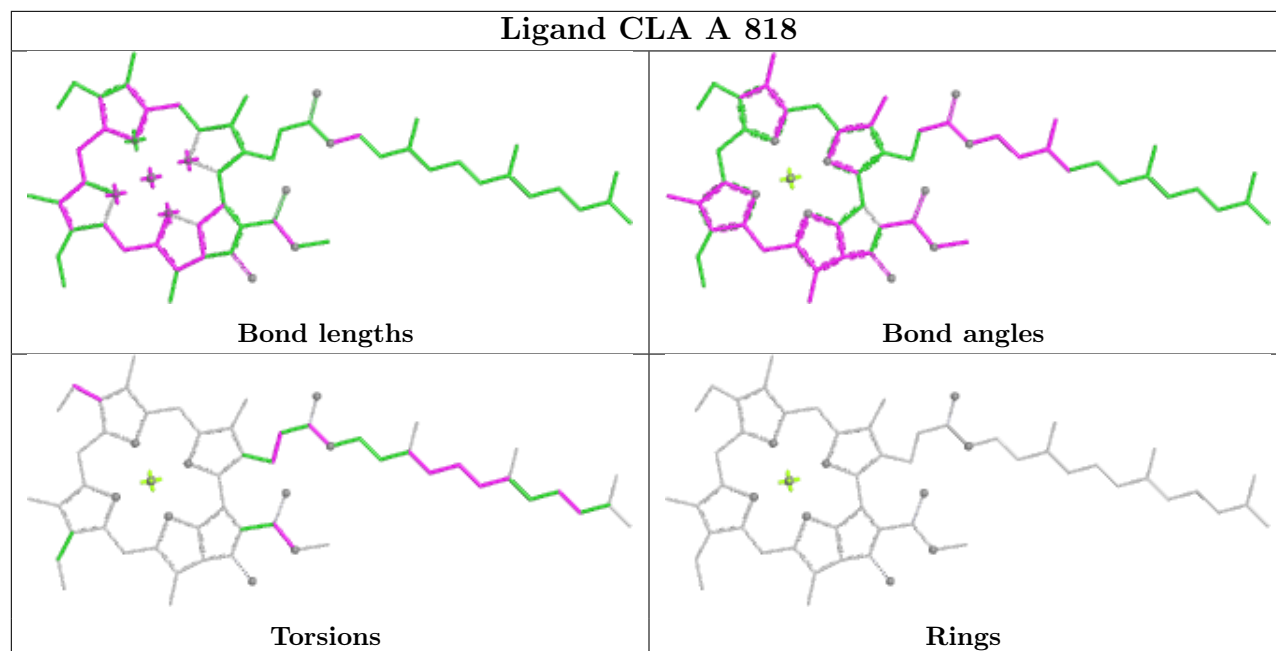
Ligand CLA Y 802



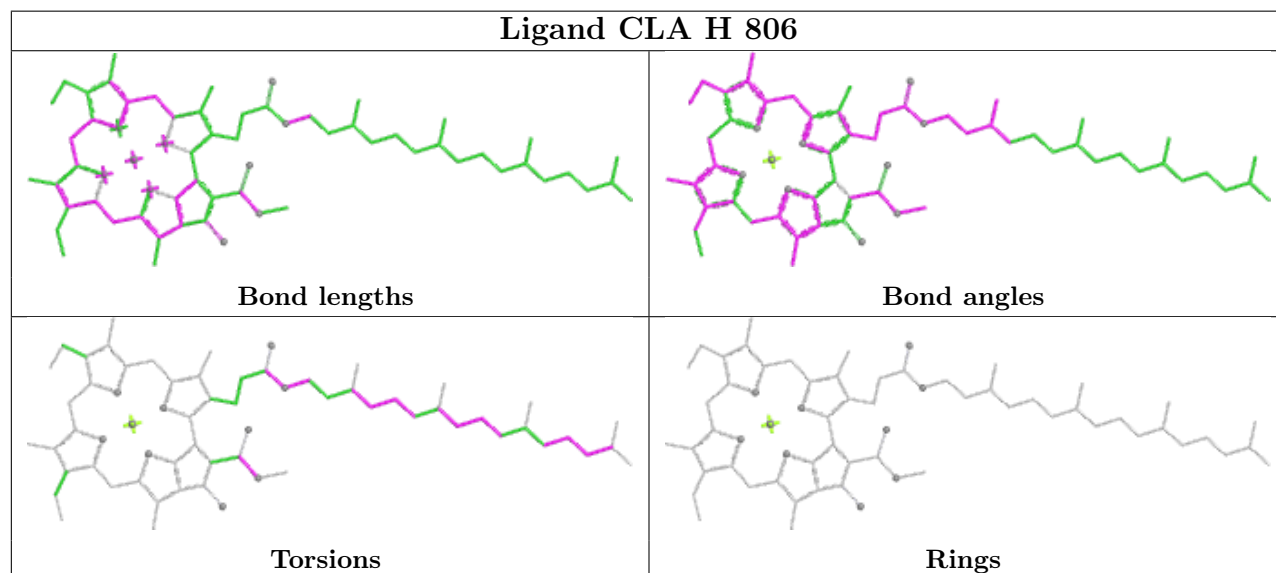
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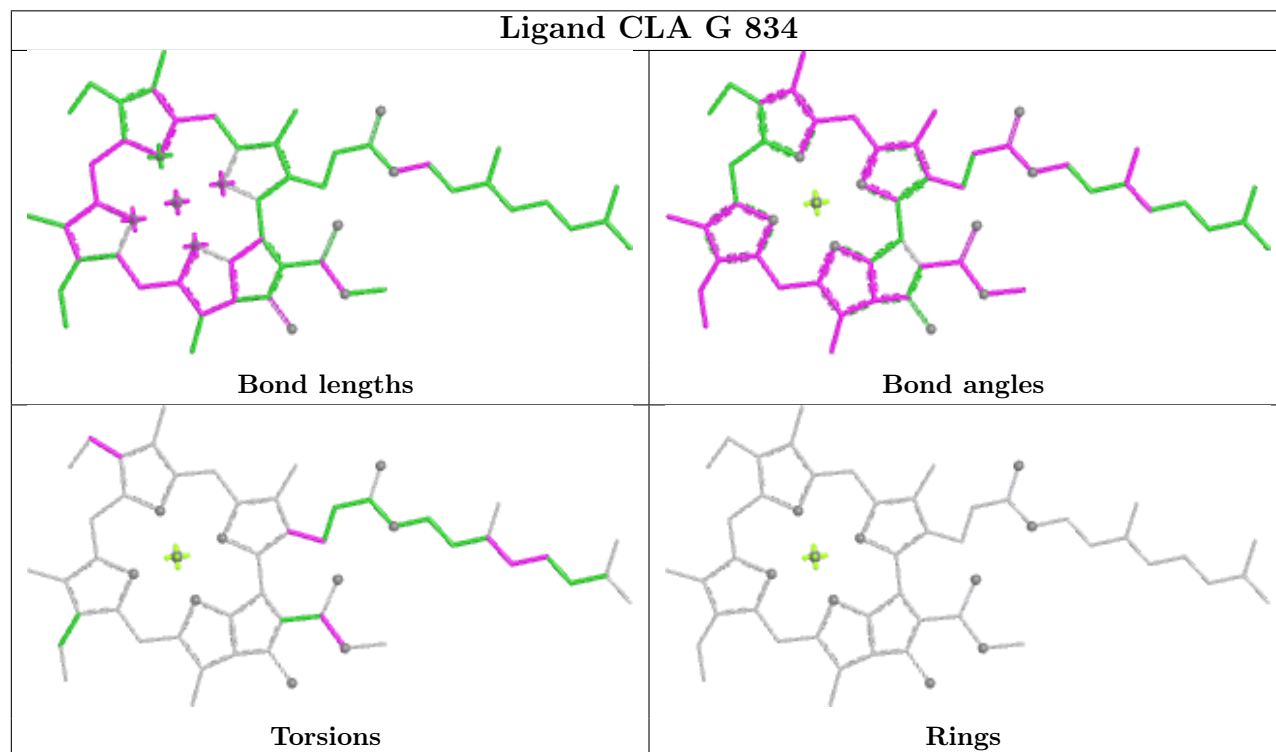
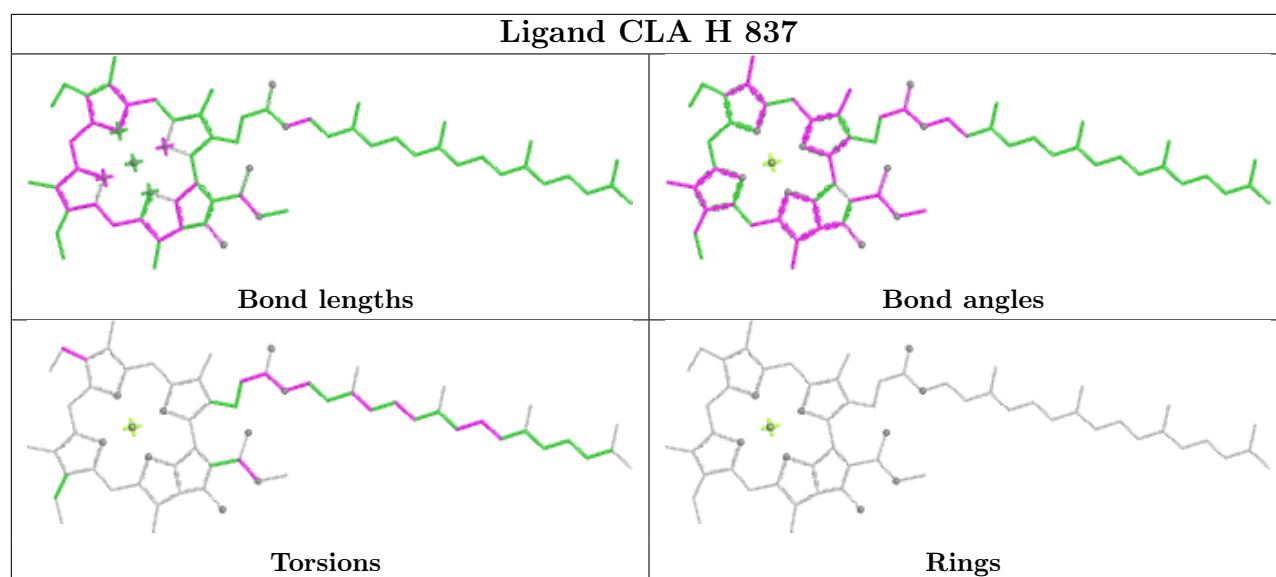


Ligand CLA A 818

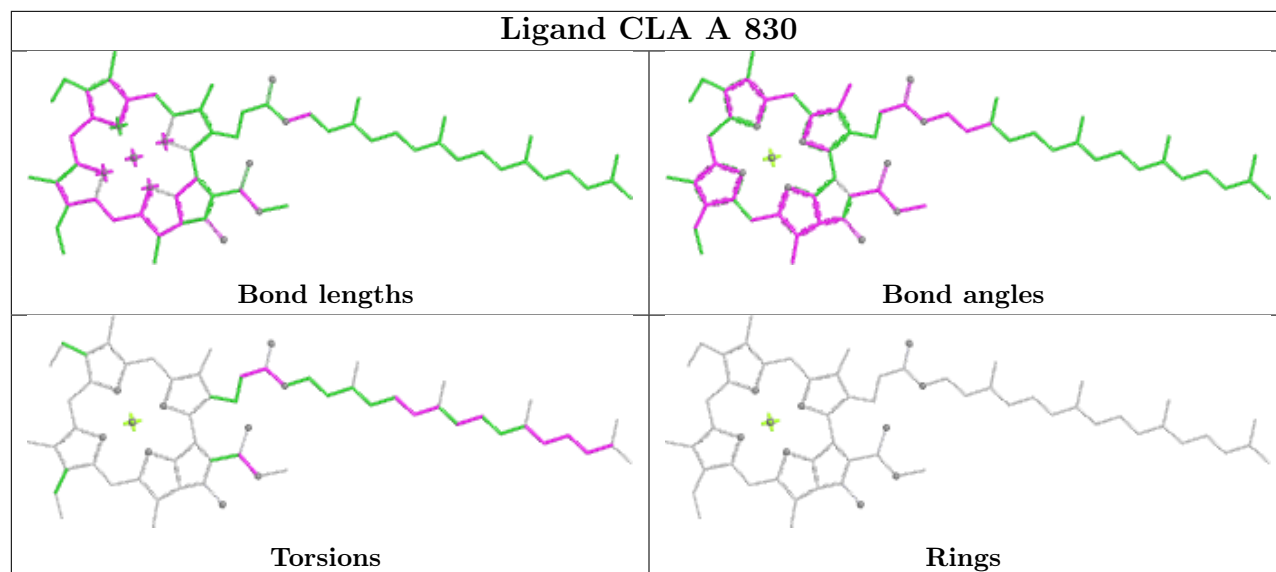


Ligand CLA H 806

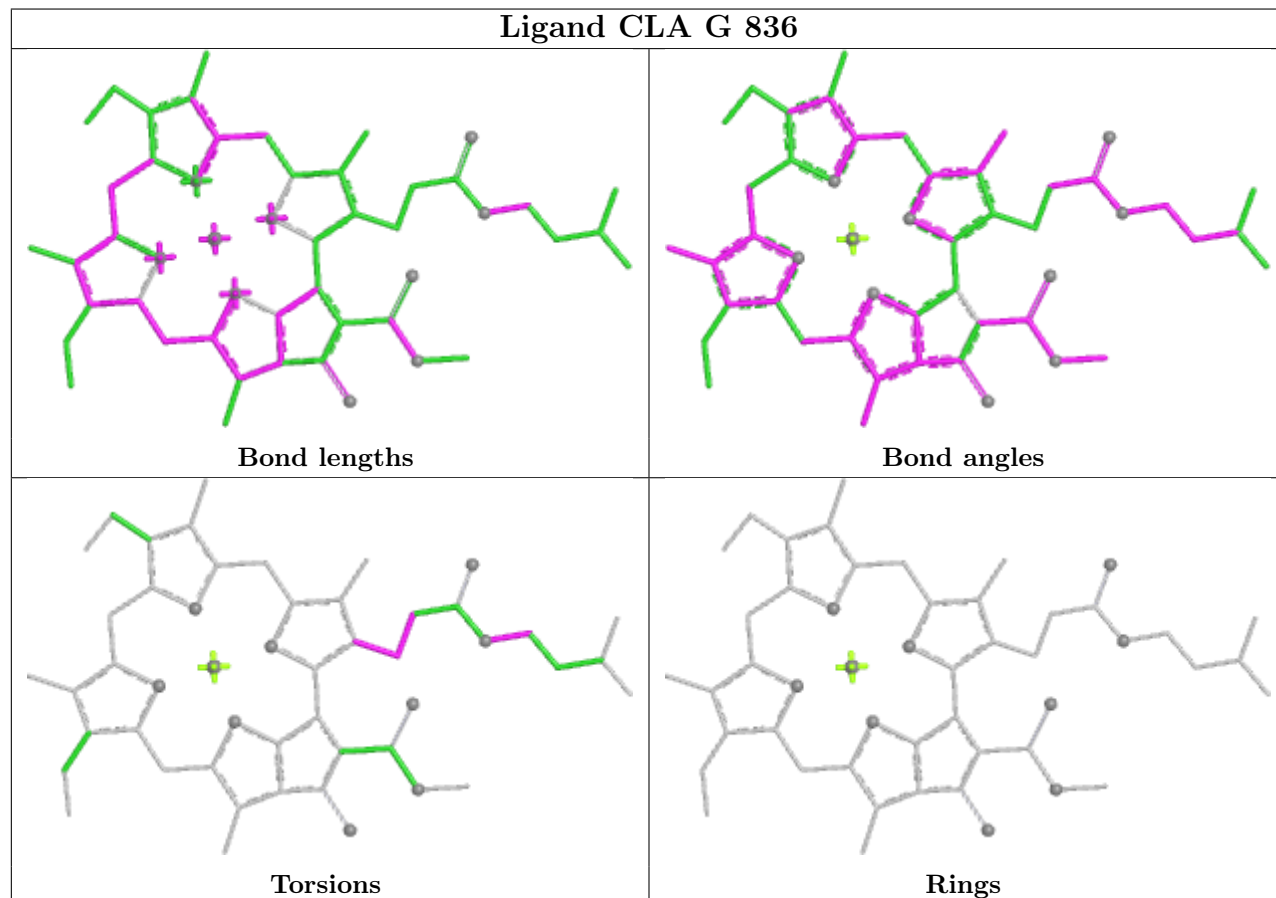




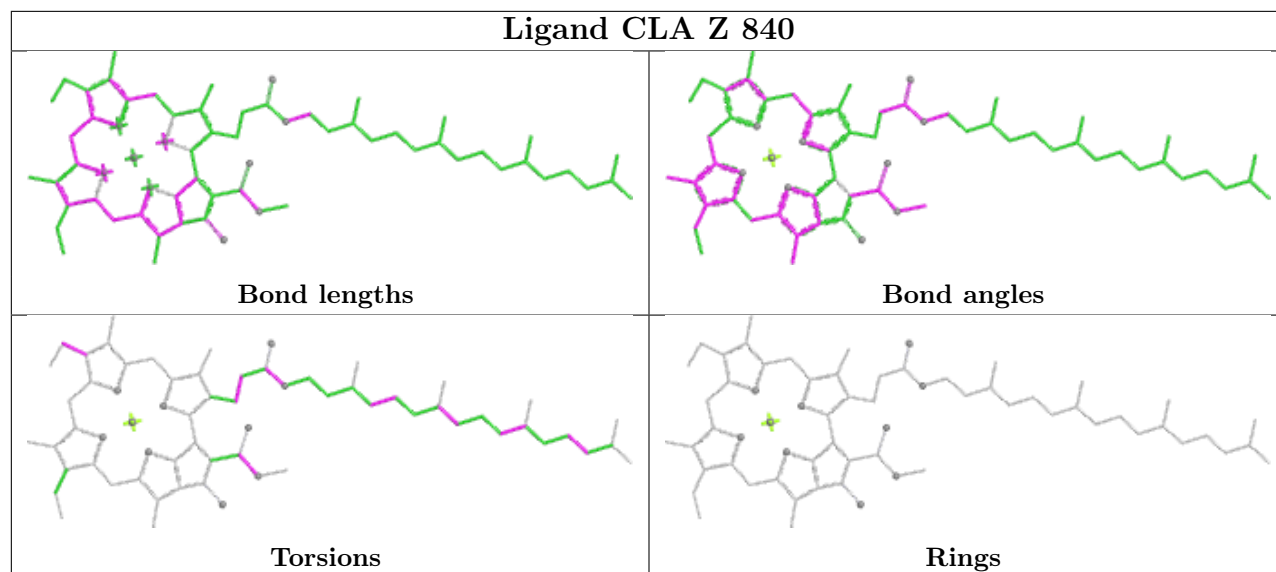
Ligand CLA A 830



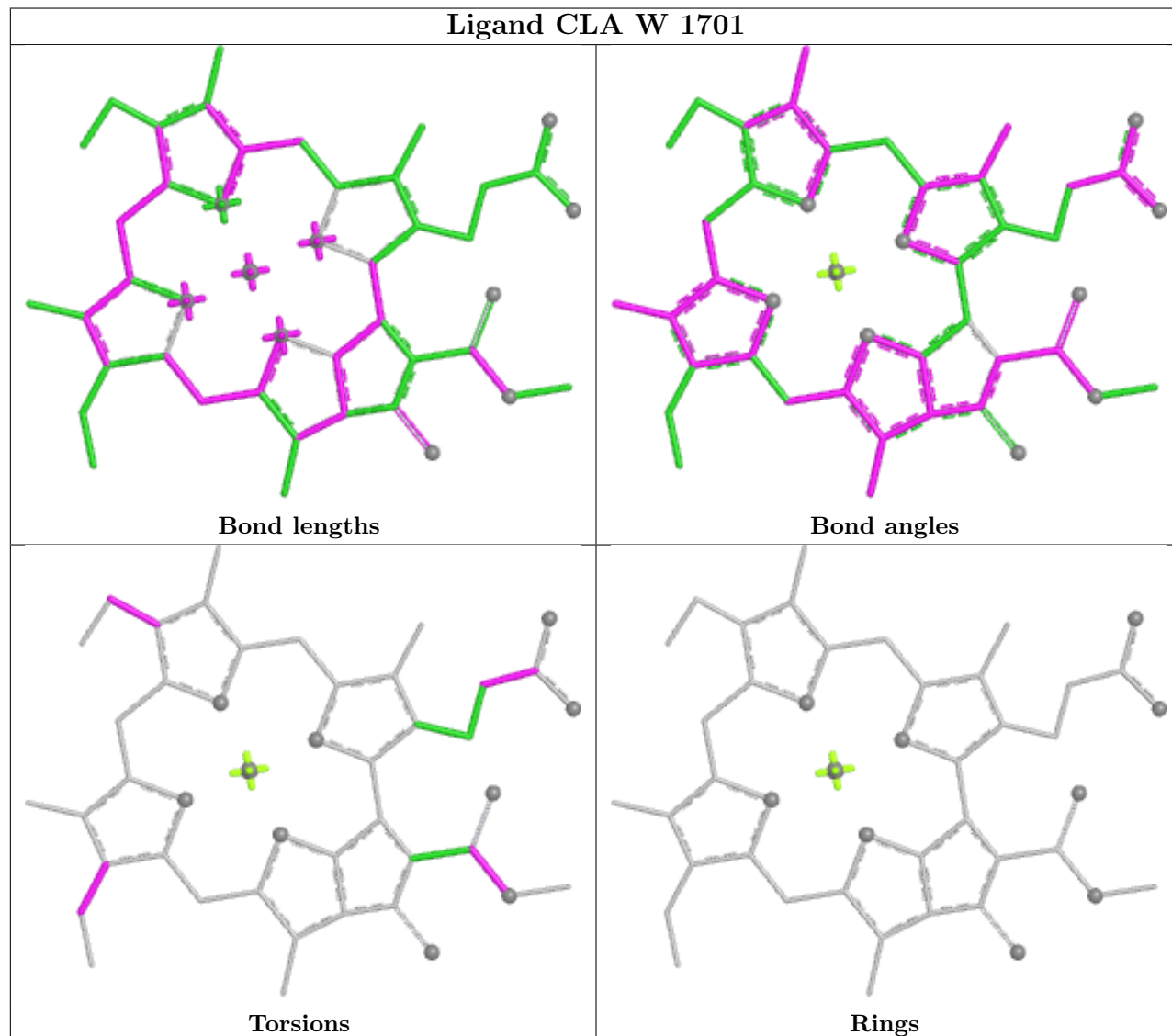
Ligand CLA G 836



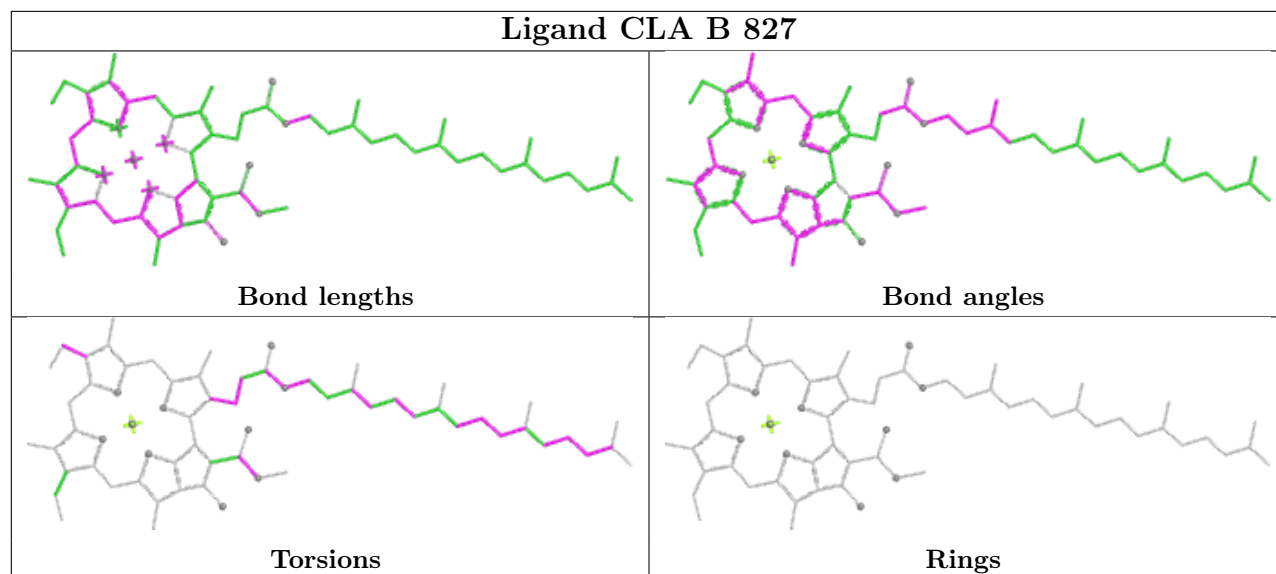
Ligand CLA Z 840



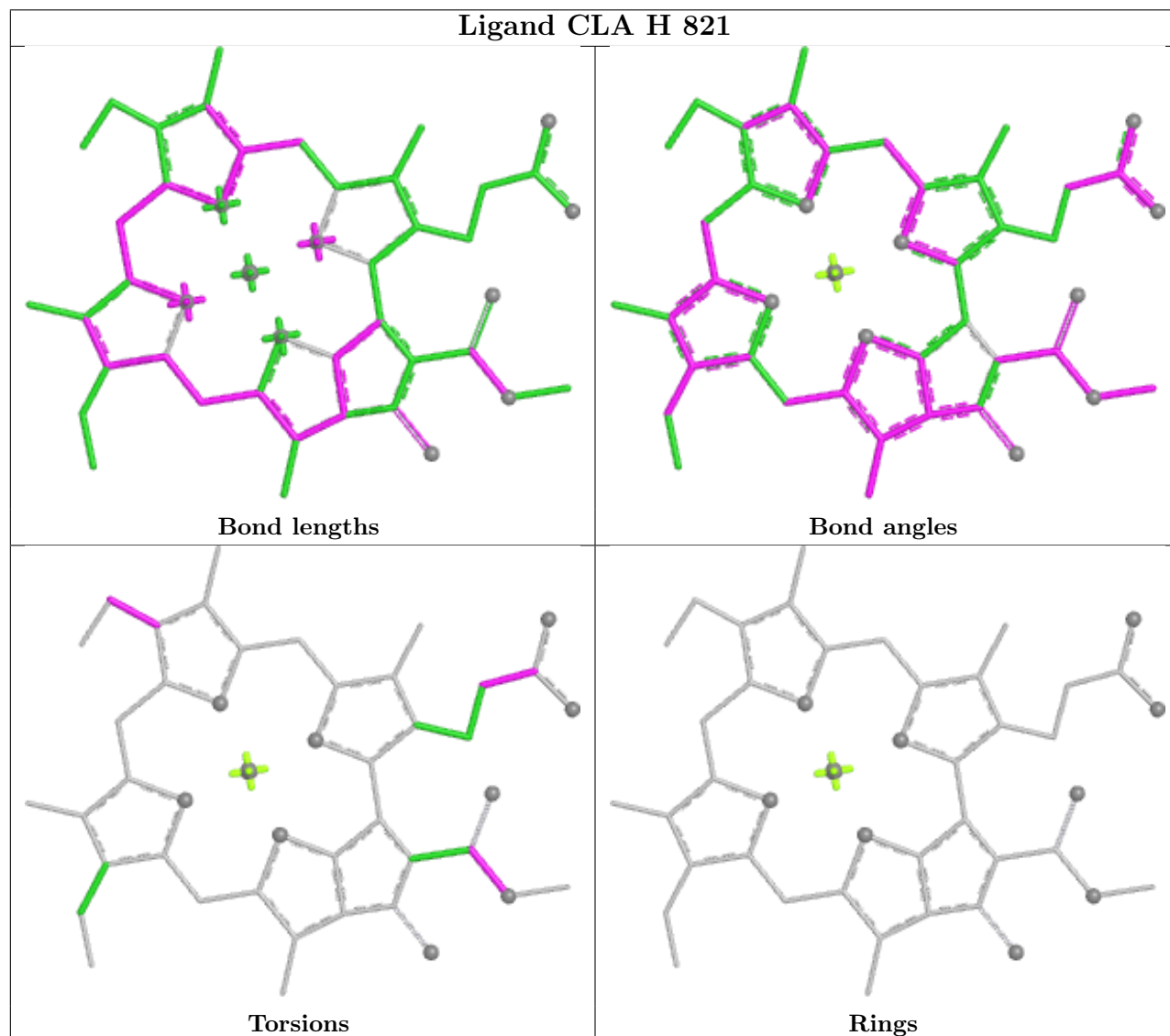
Ligand CLA W 1701

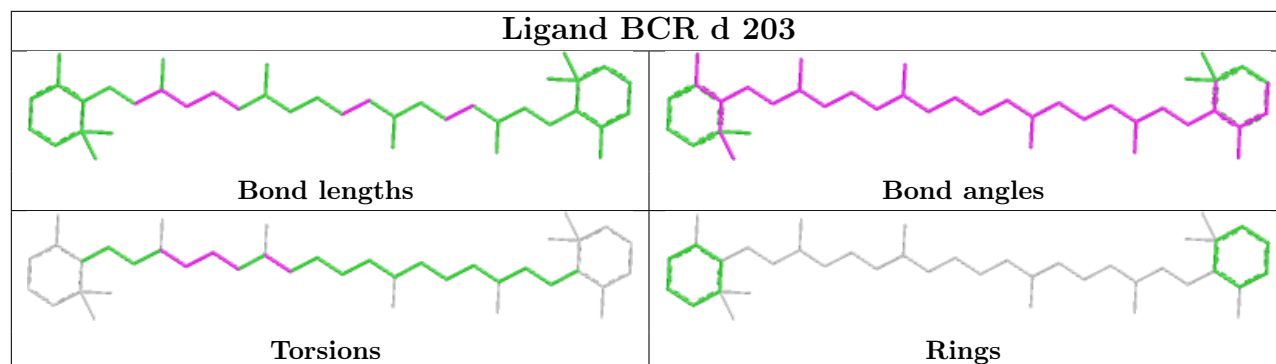
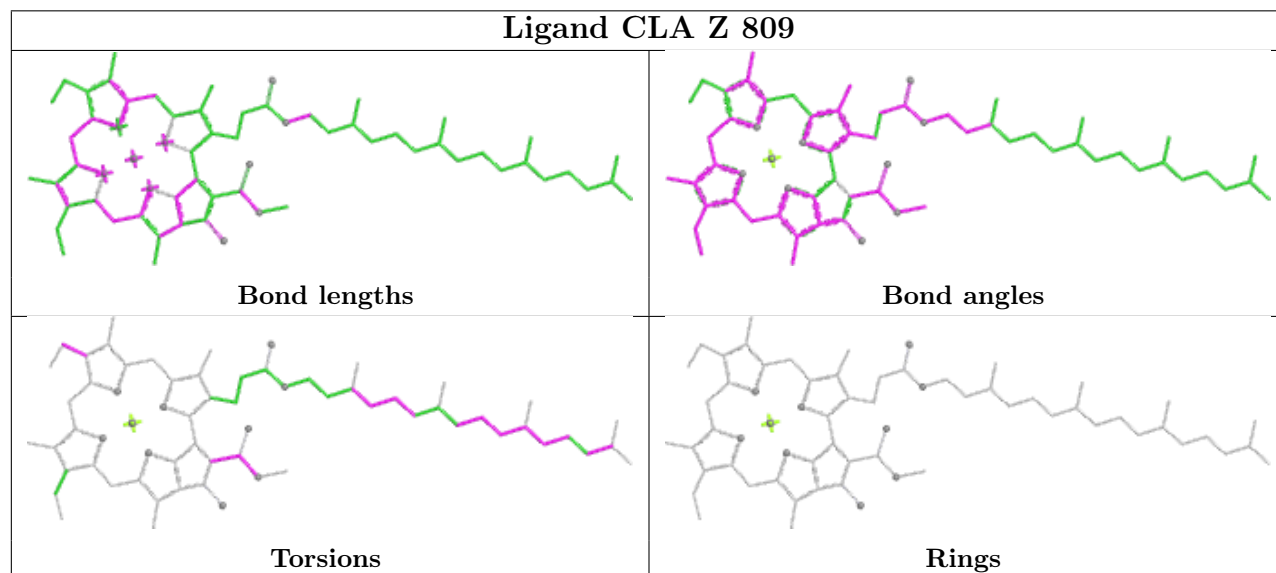
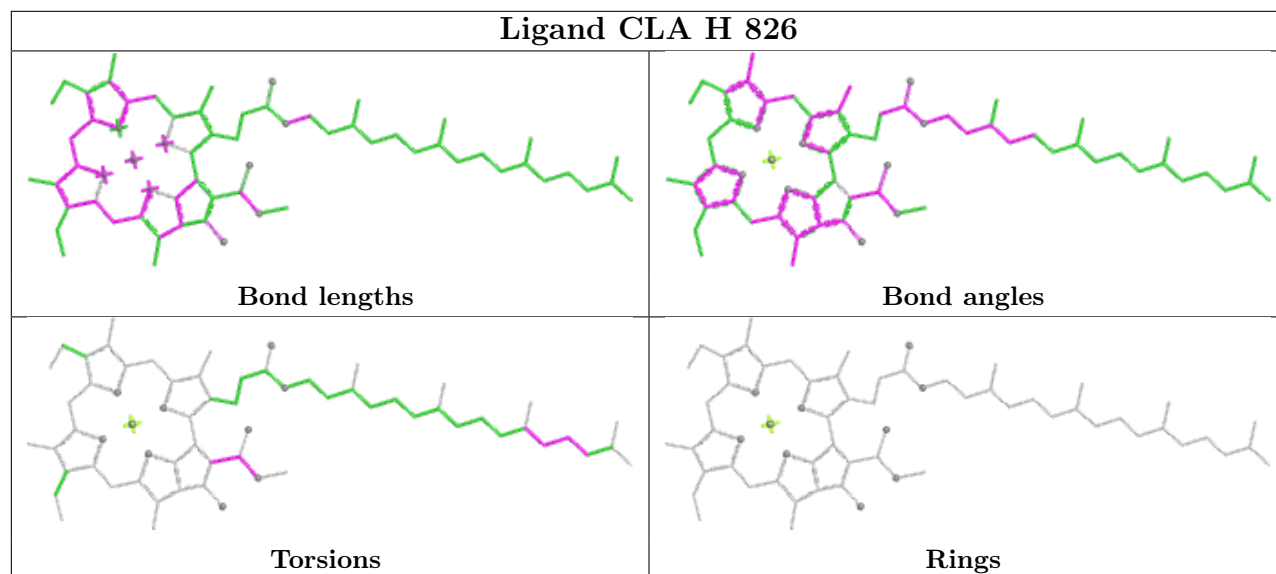


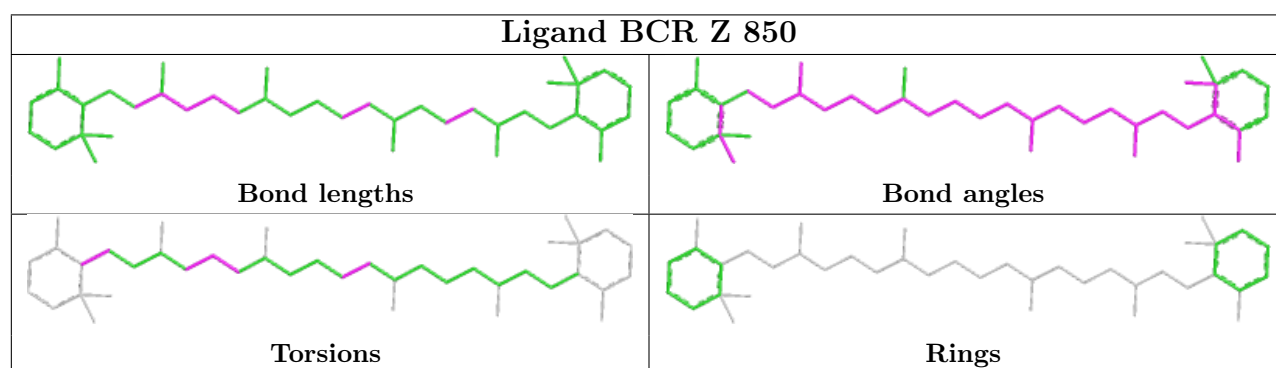
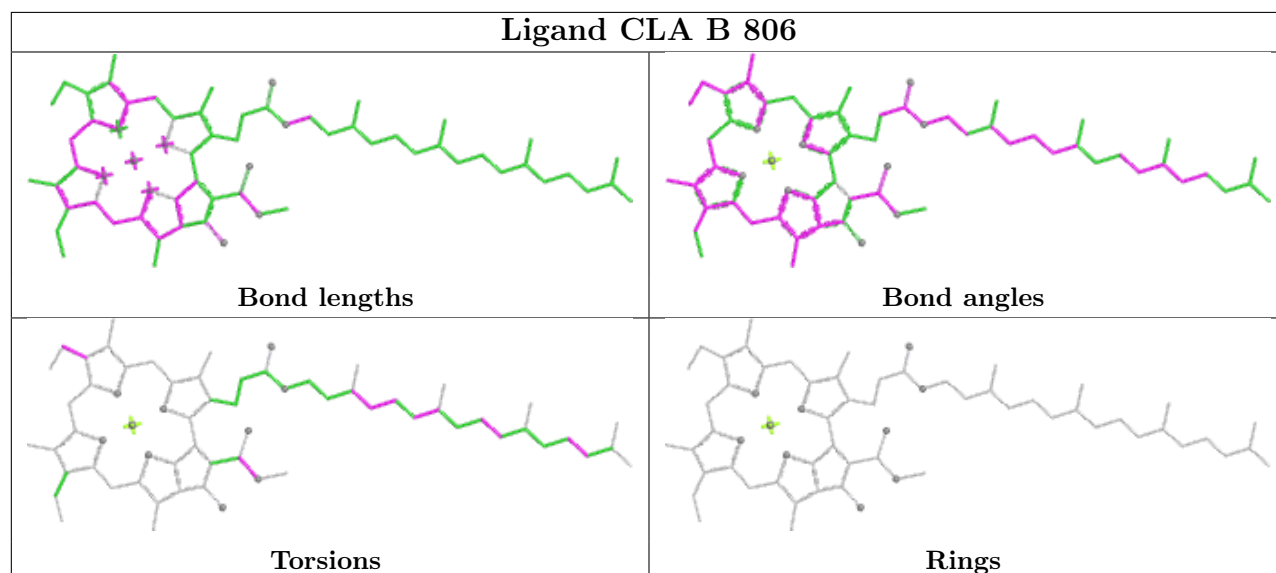
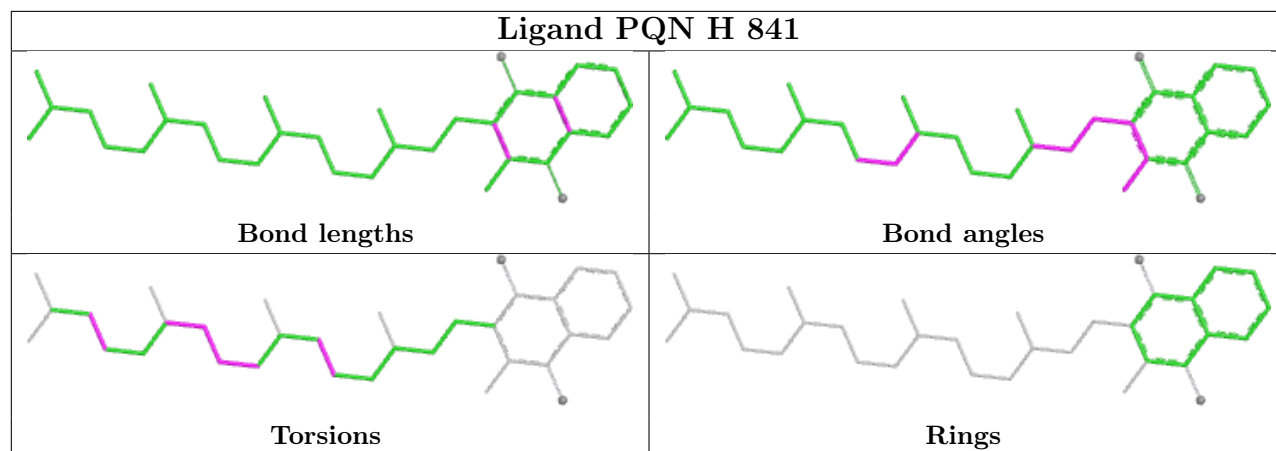
Ligand CLA B 827



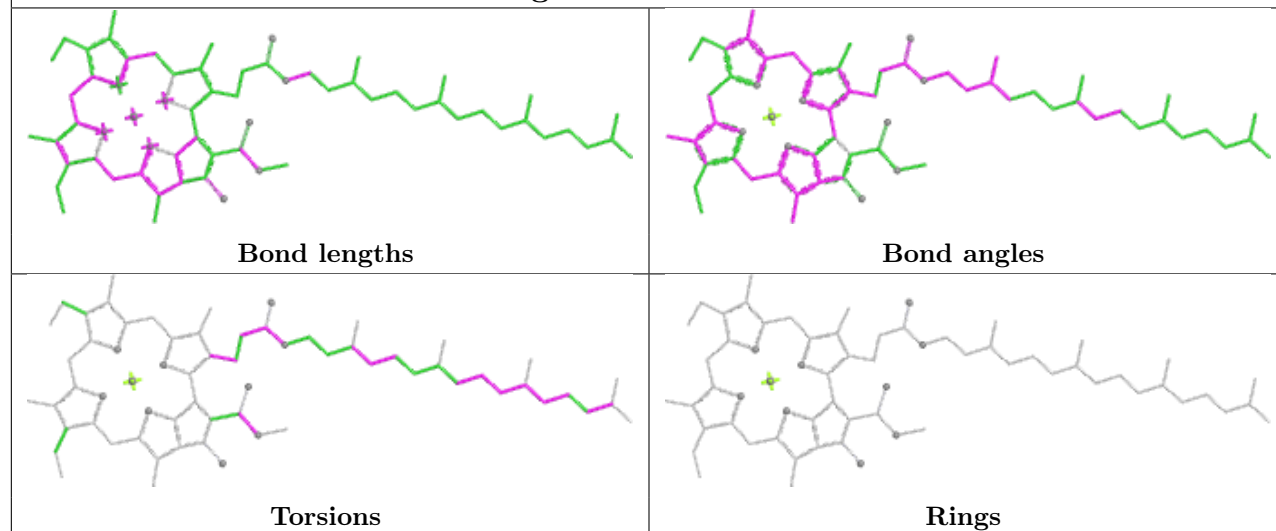
Ligand CLA H 821



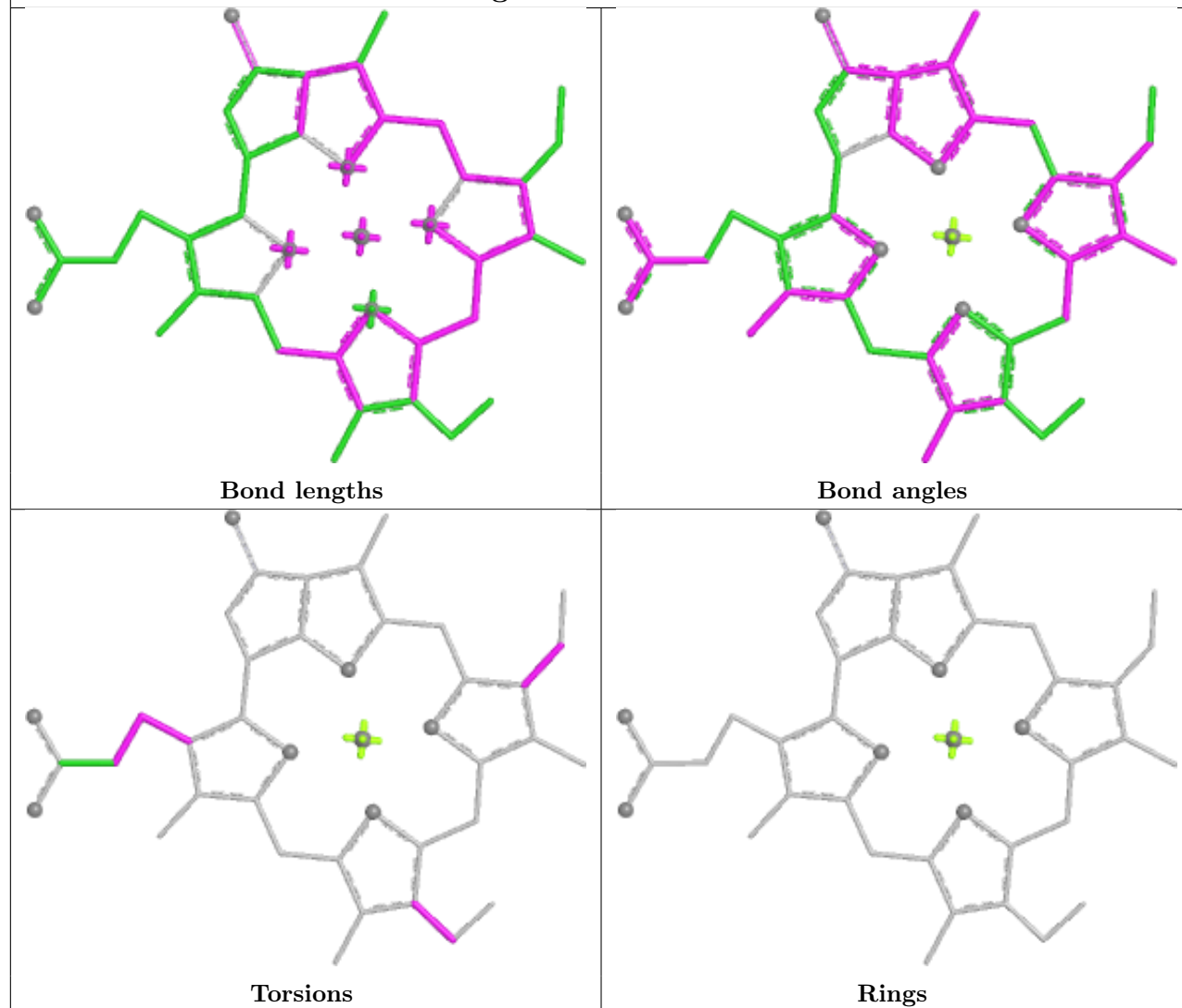


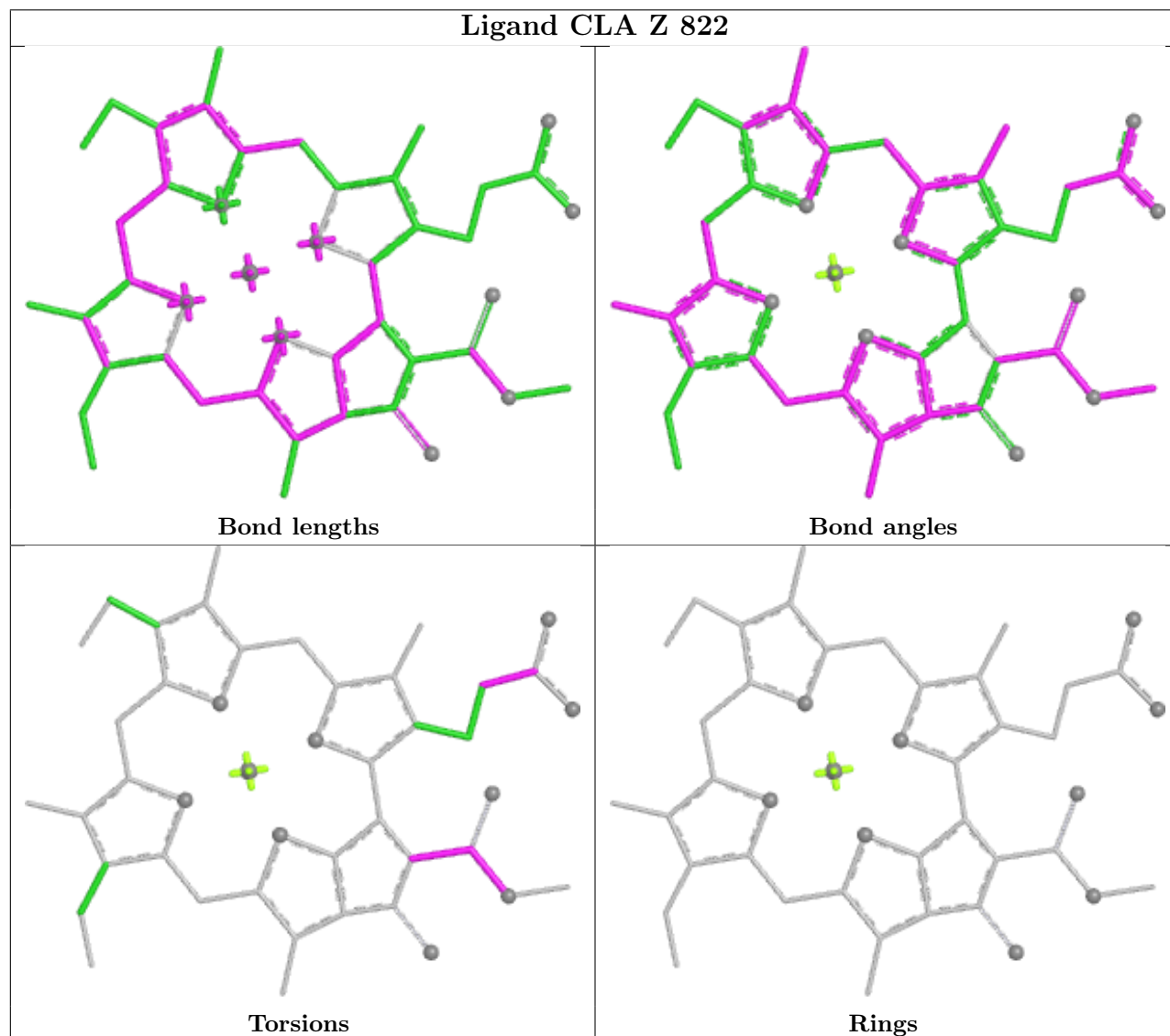
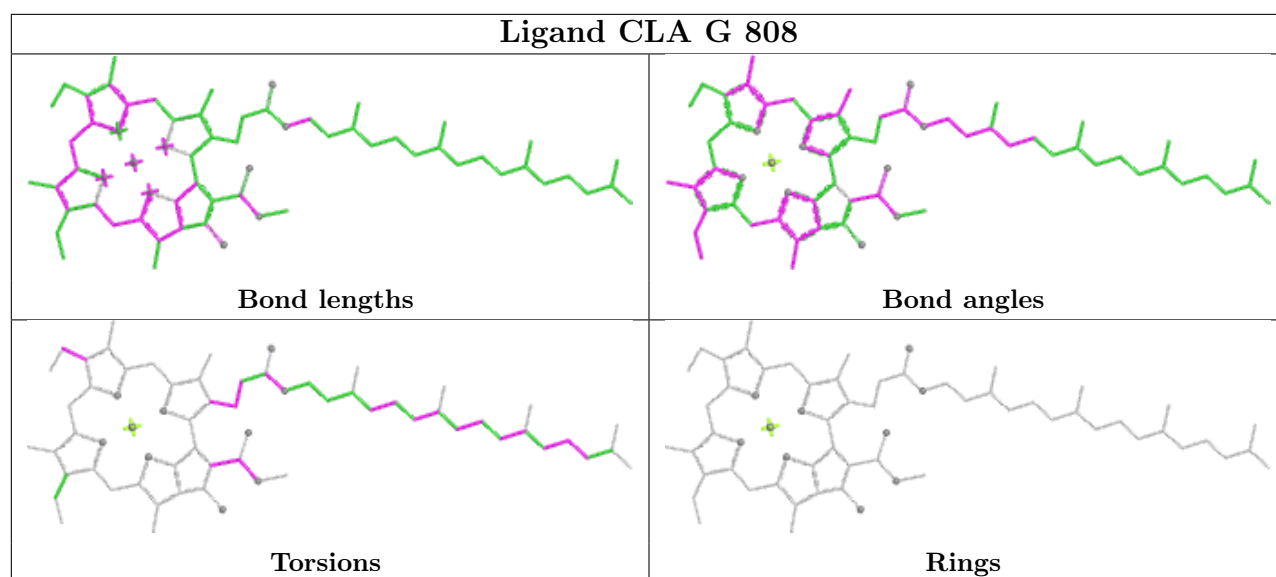


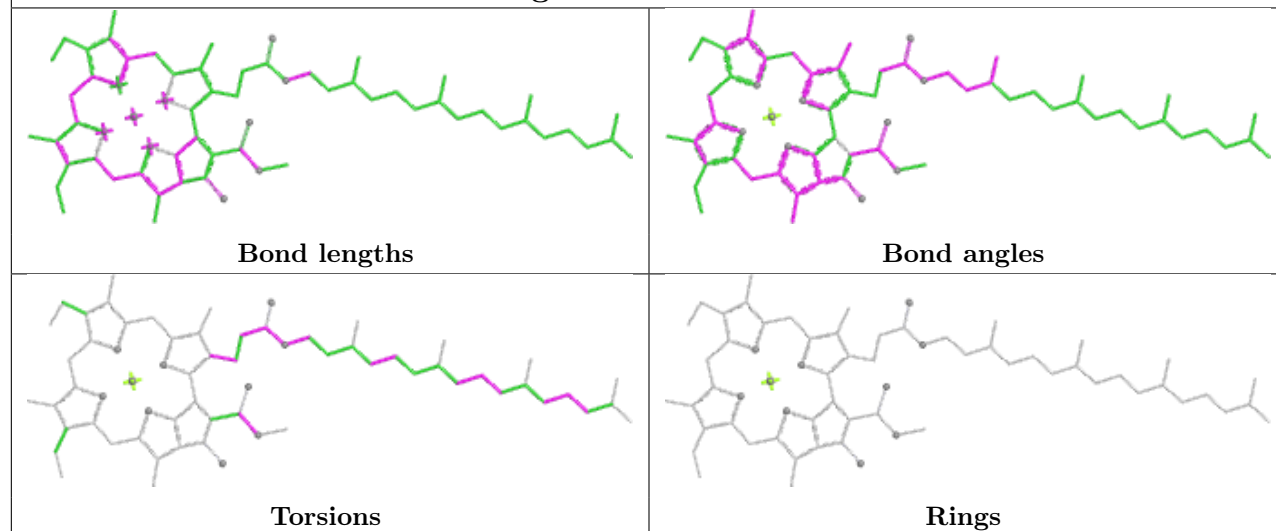
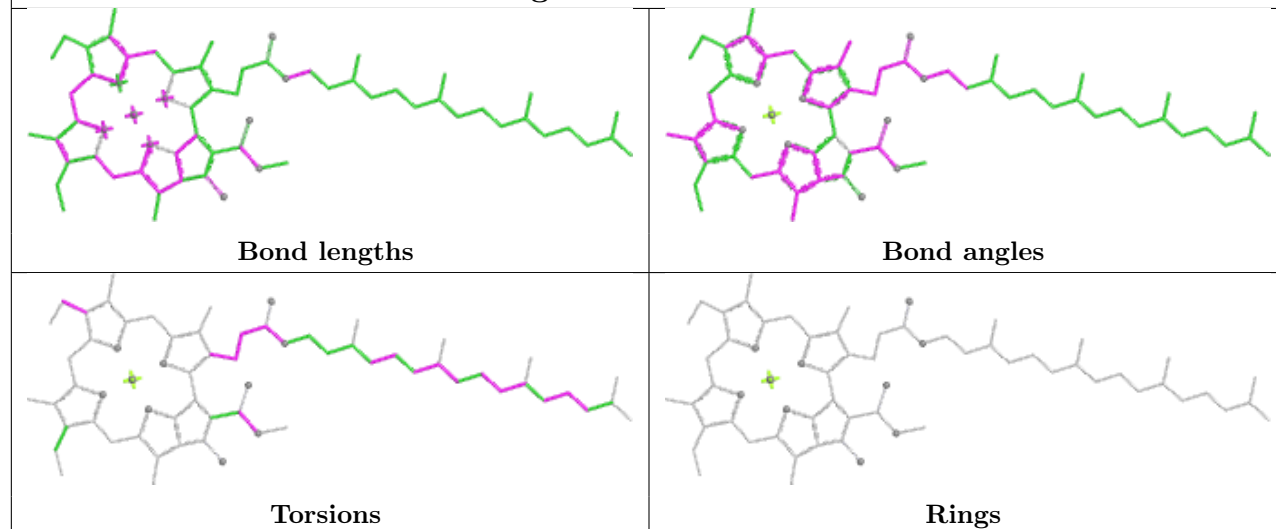
Ligand CLA H 803

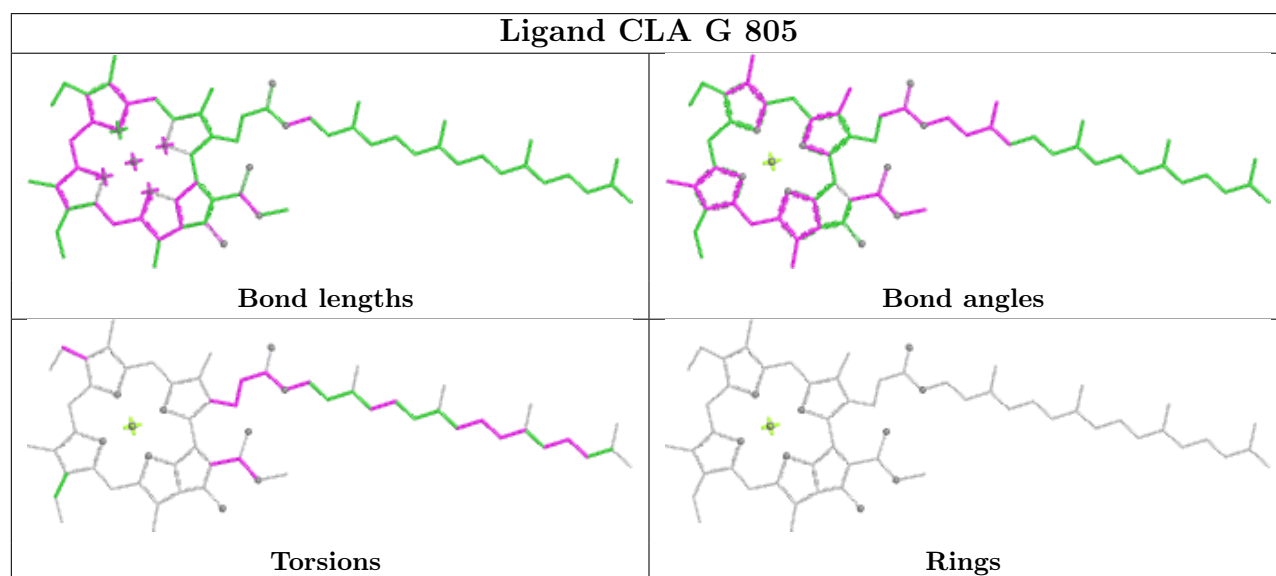
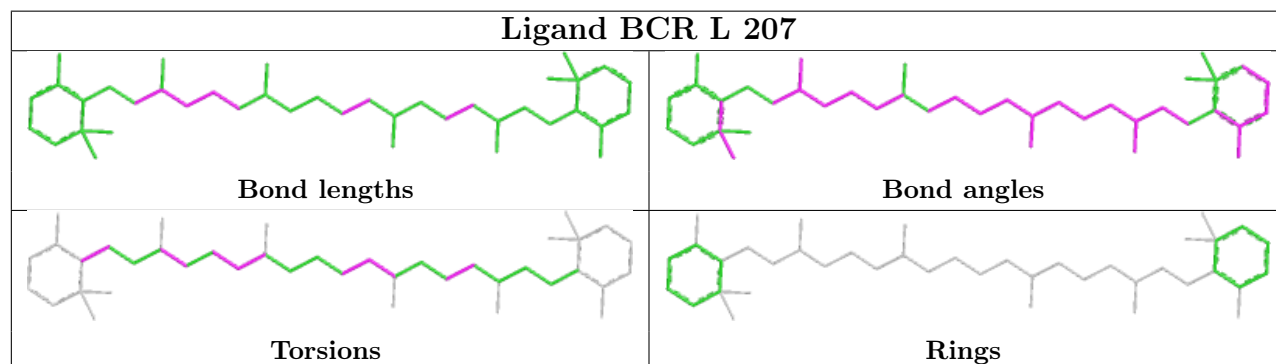
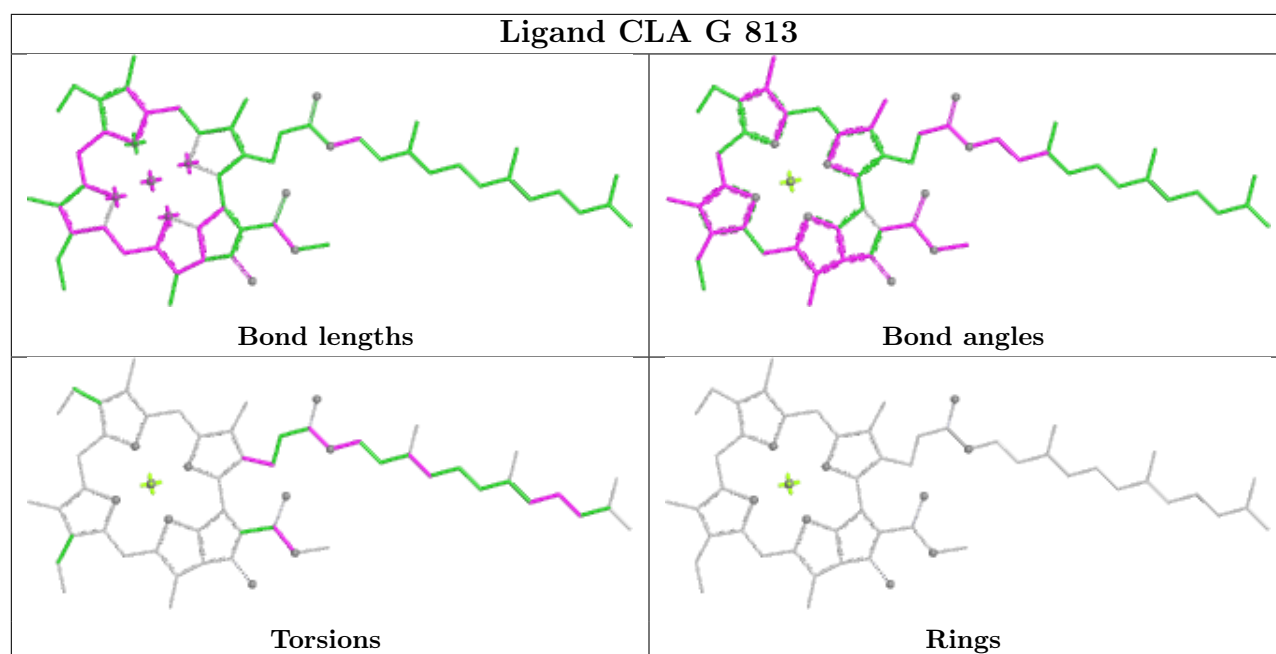


Ligand CLA K 101

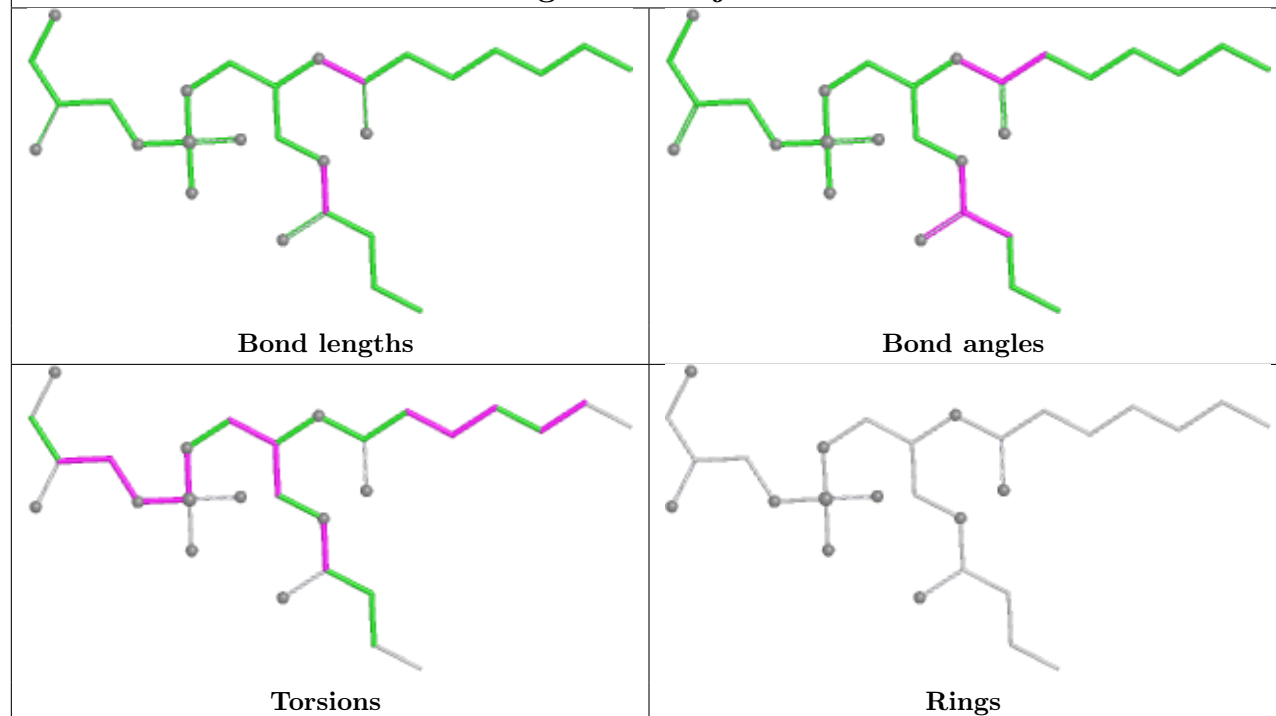




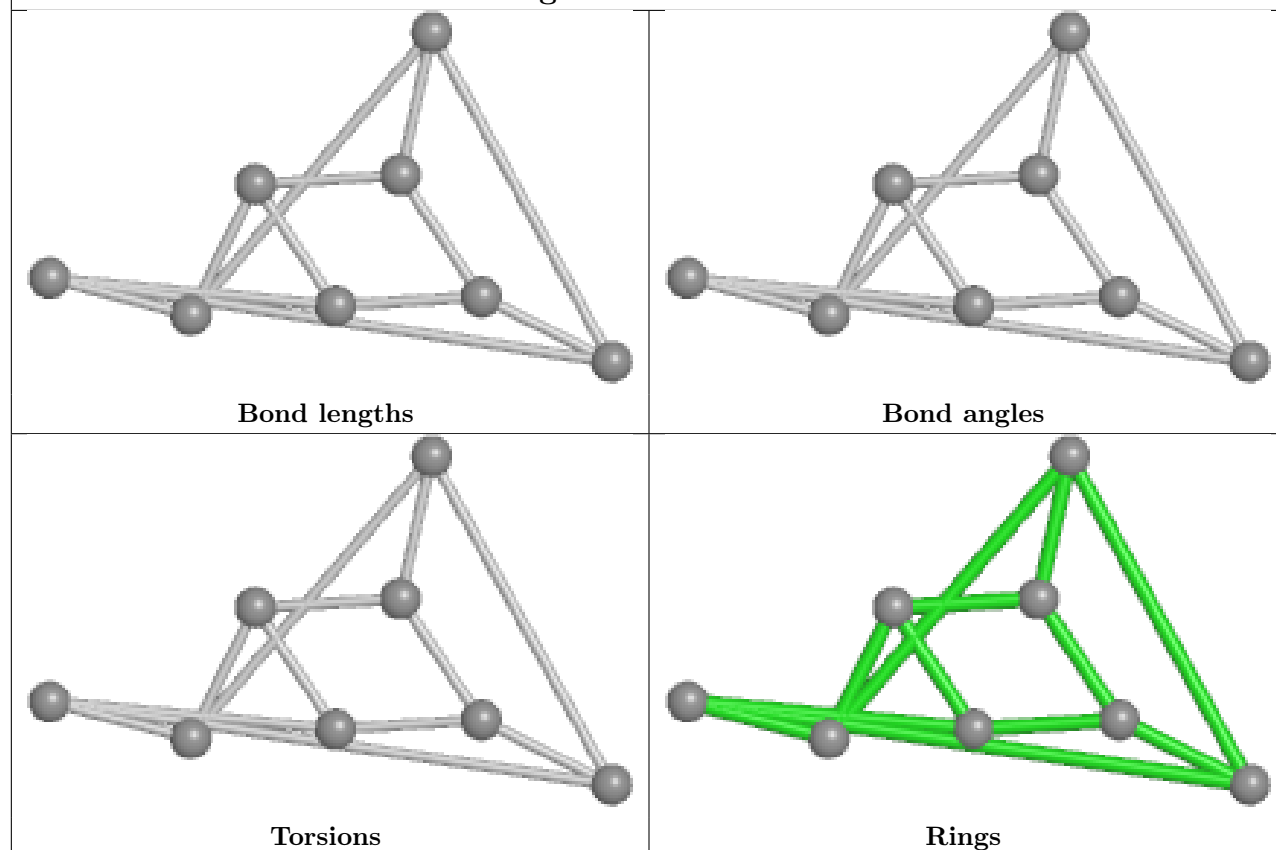
Ligand CLA Y 818**Ligand CLA G 811**

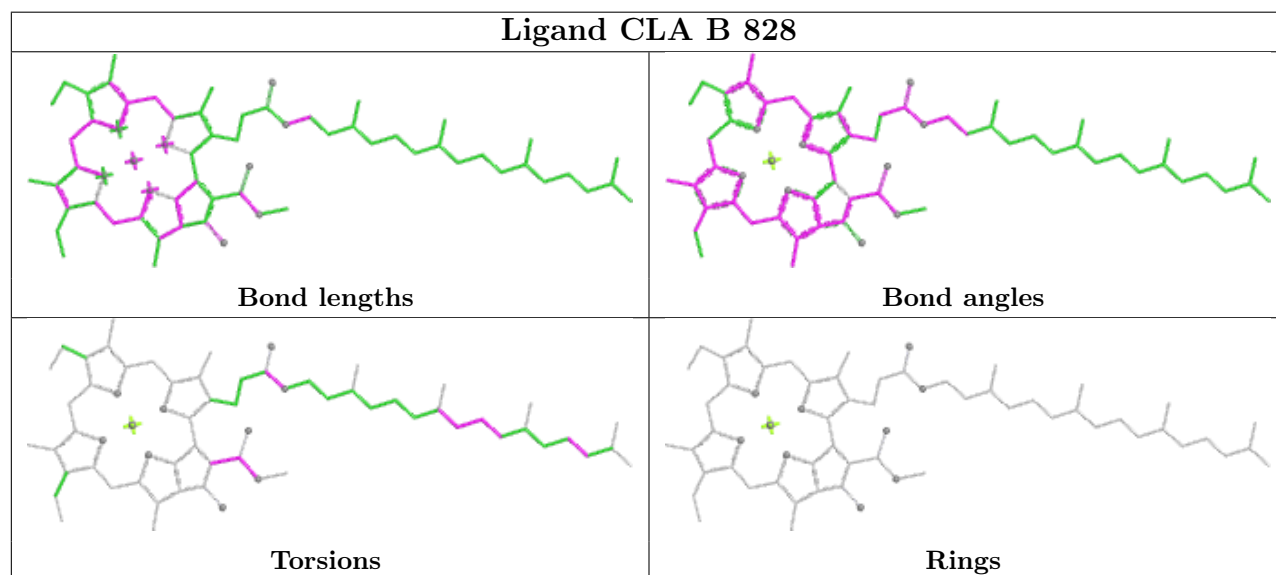
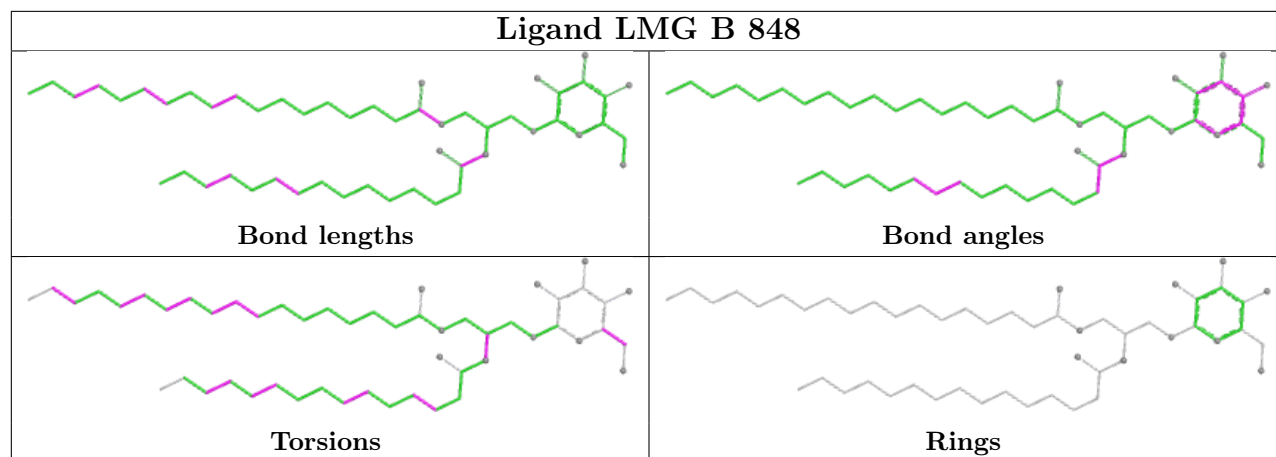


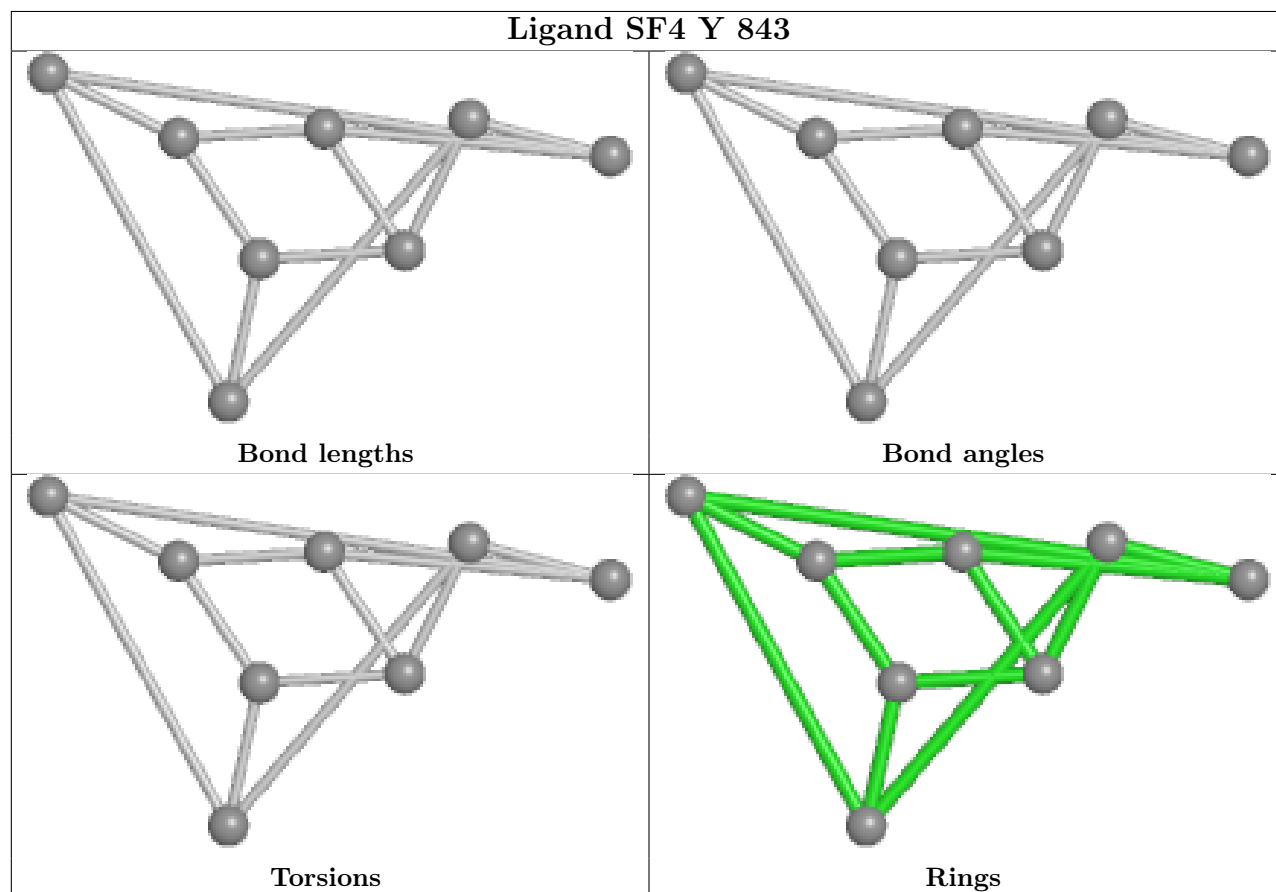
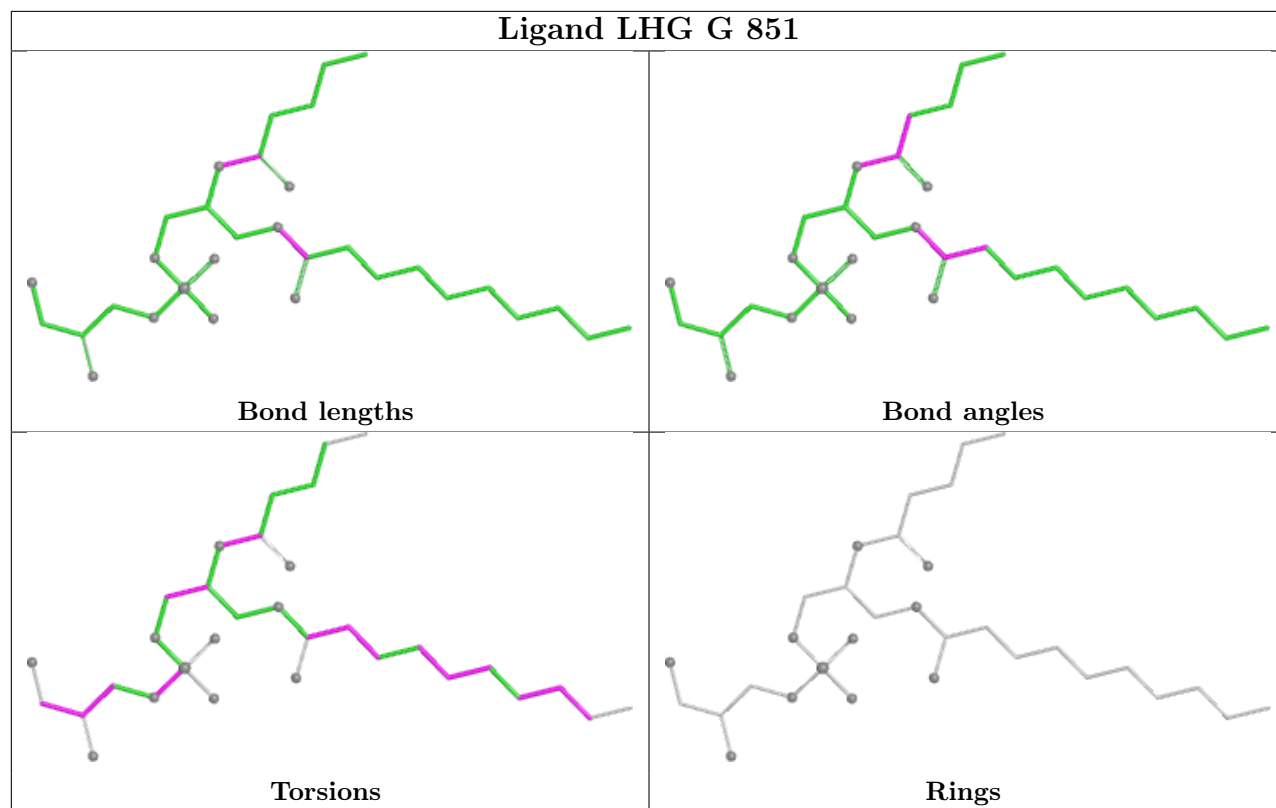
Ligand LHG j 101

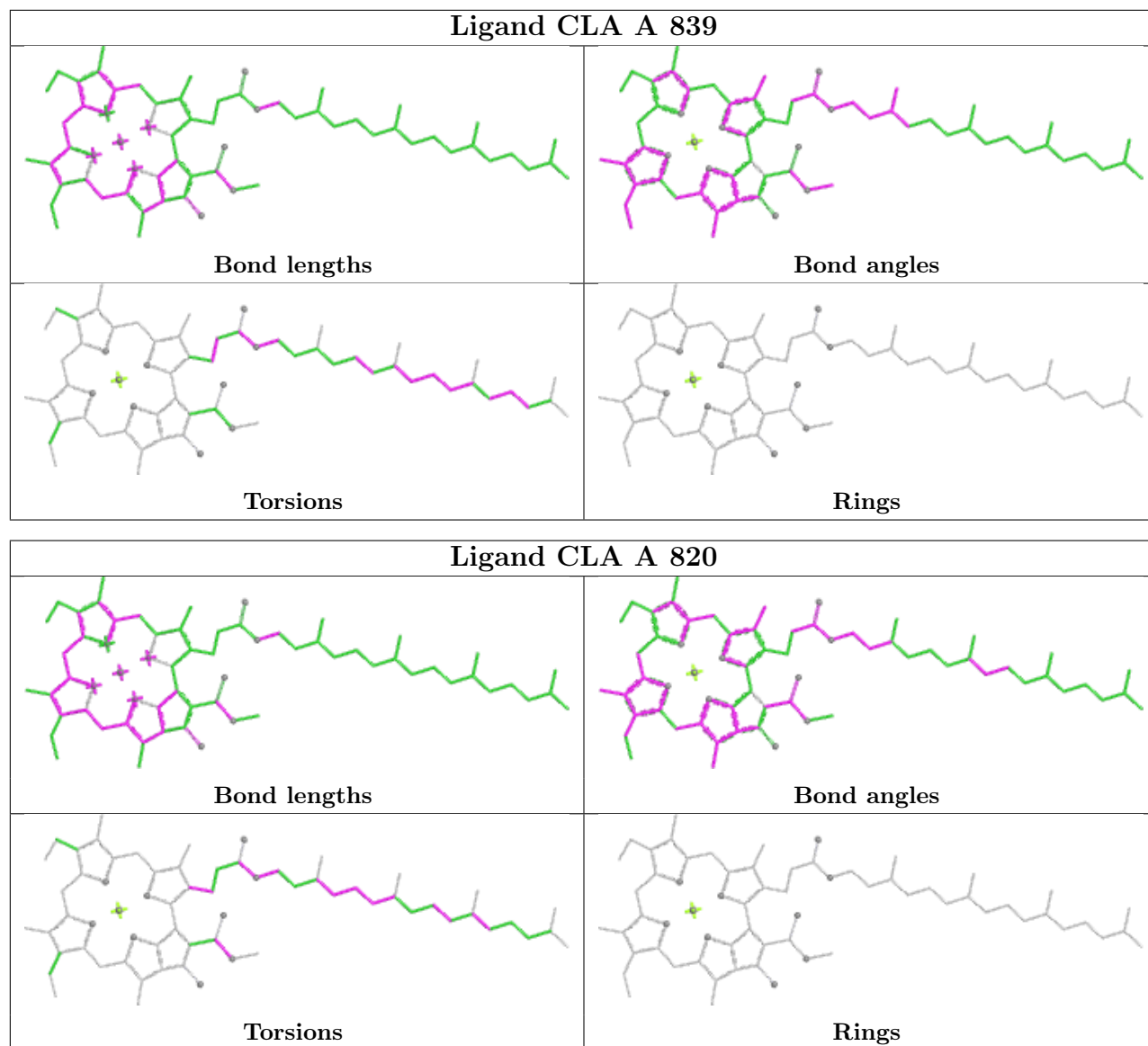


Ligand SF4 C 102

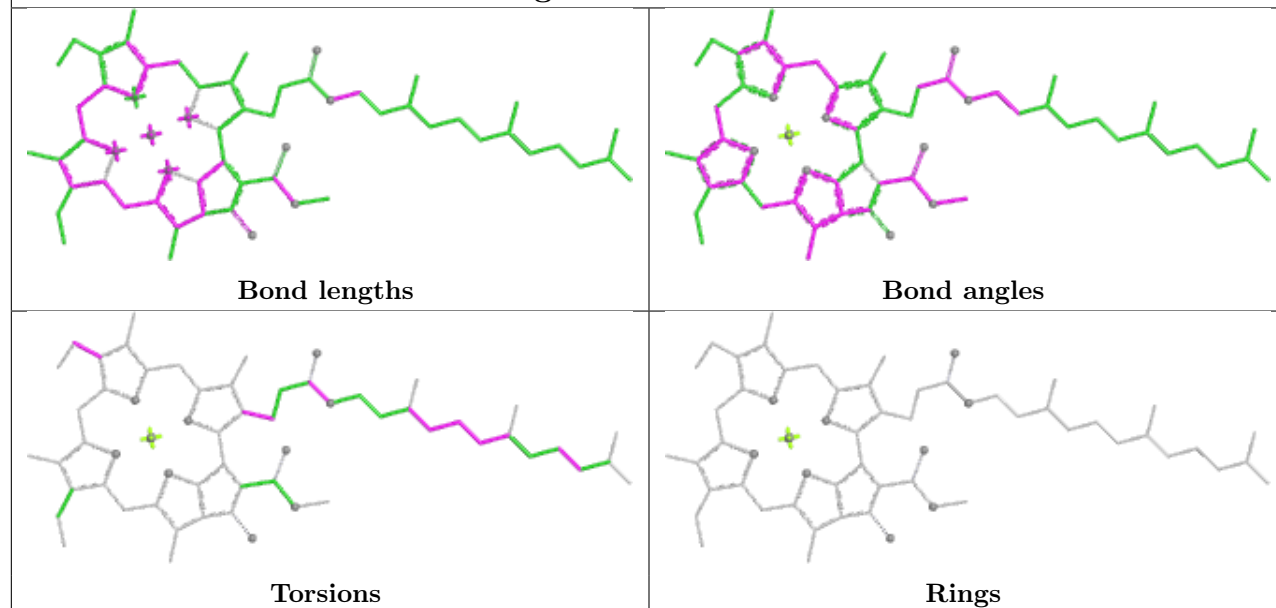




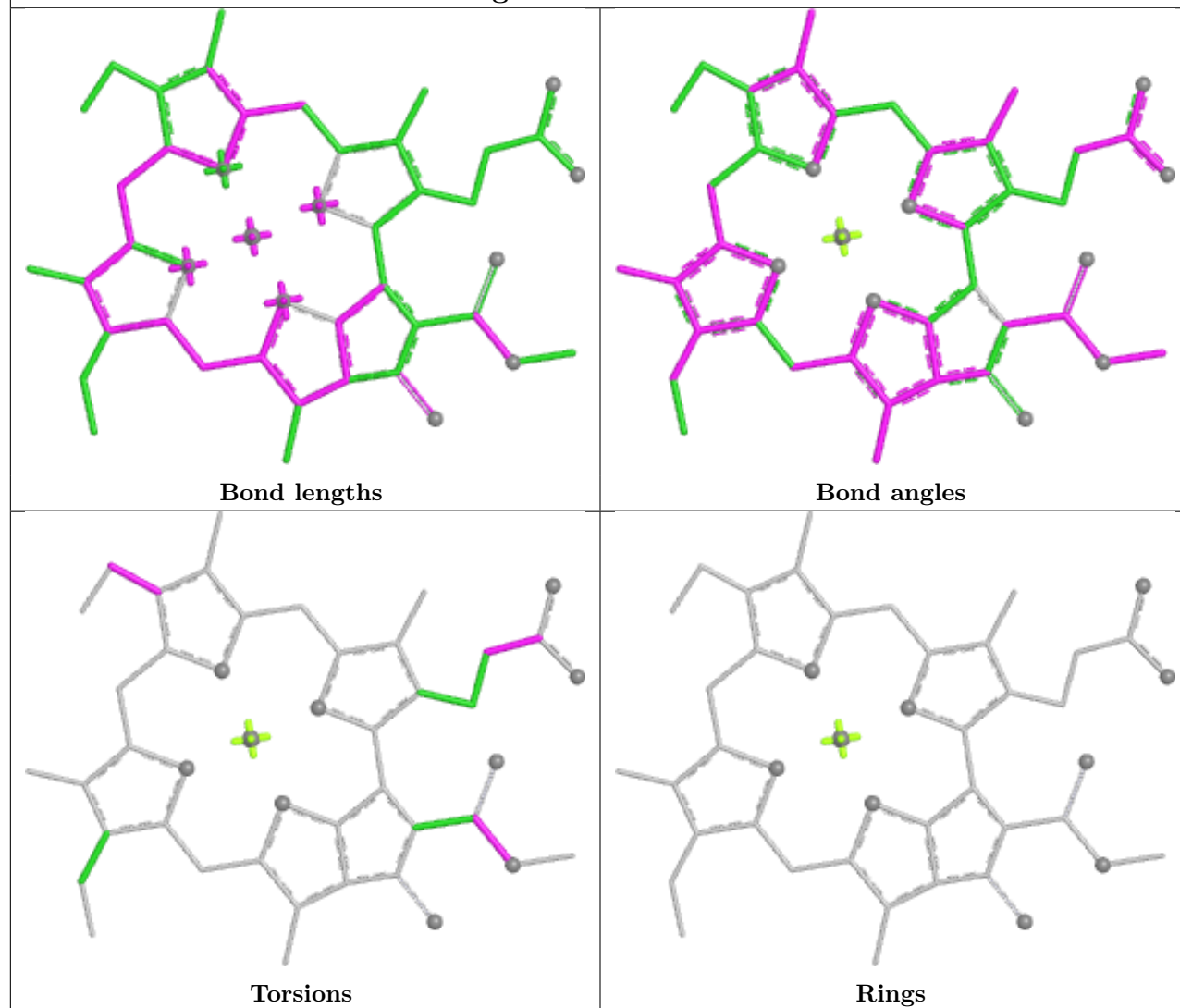


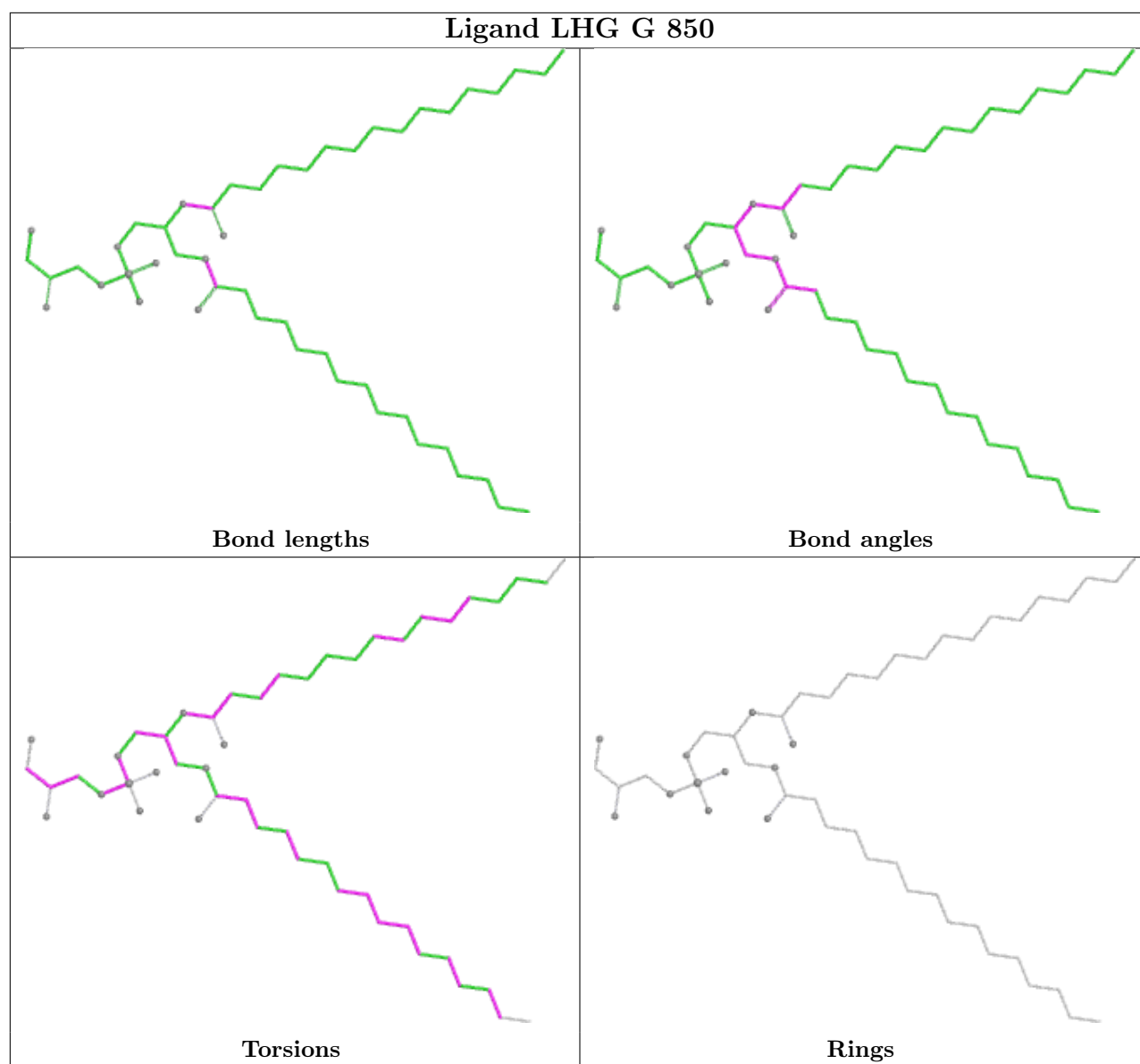


Ligand CLA Z 820

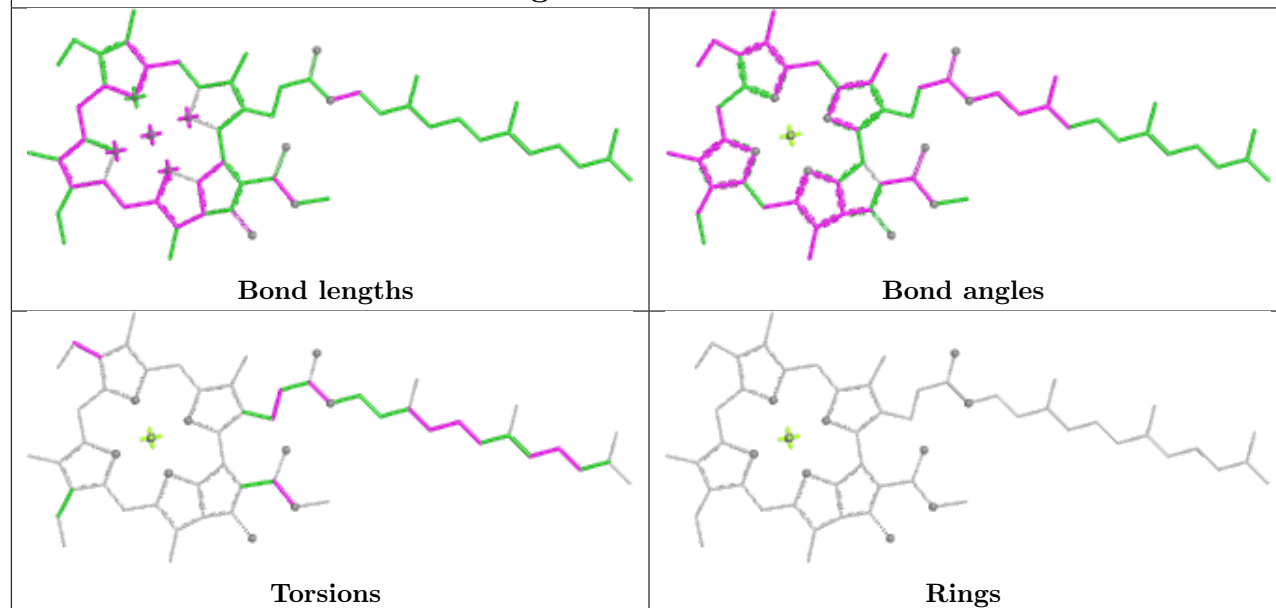


Ligand CLA B 835

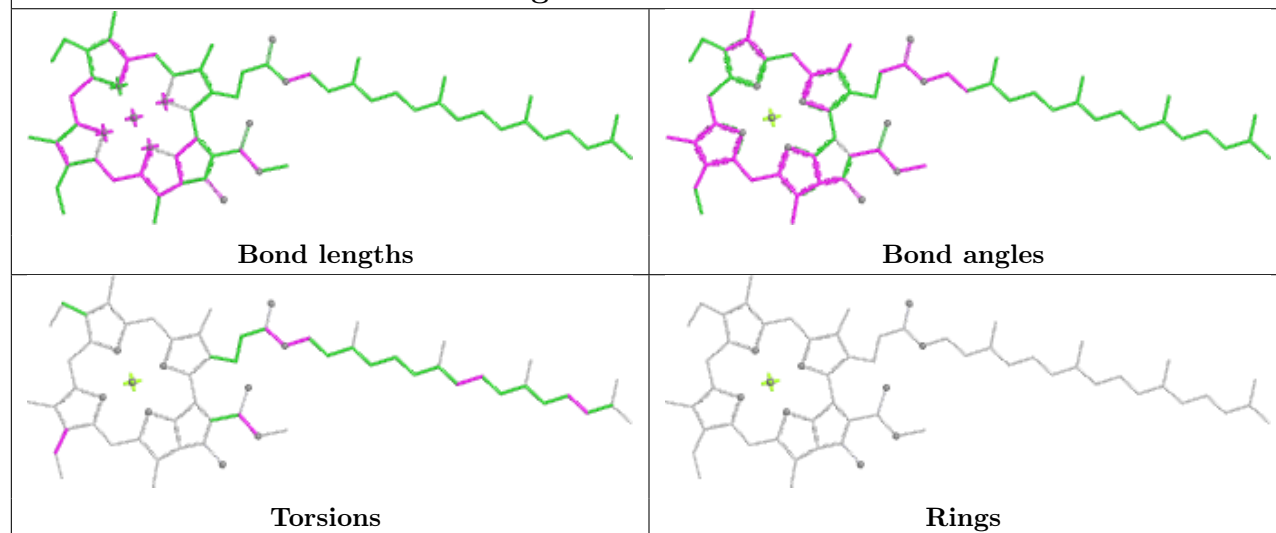


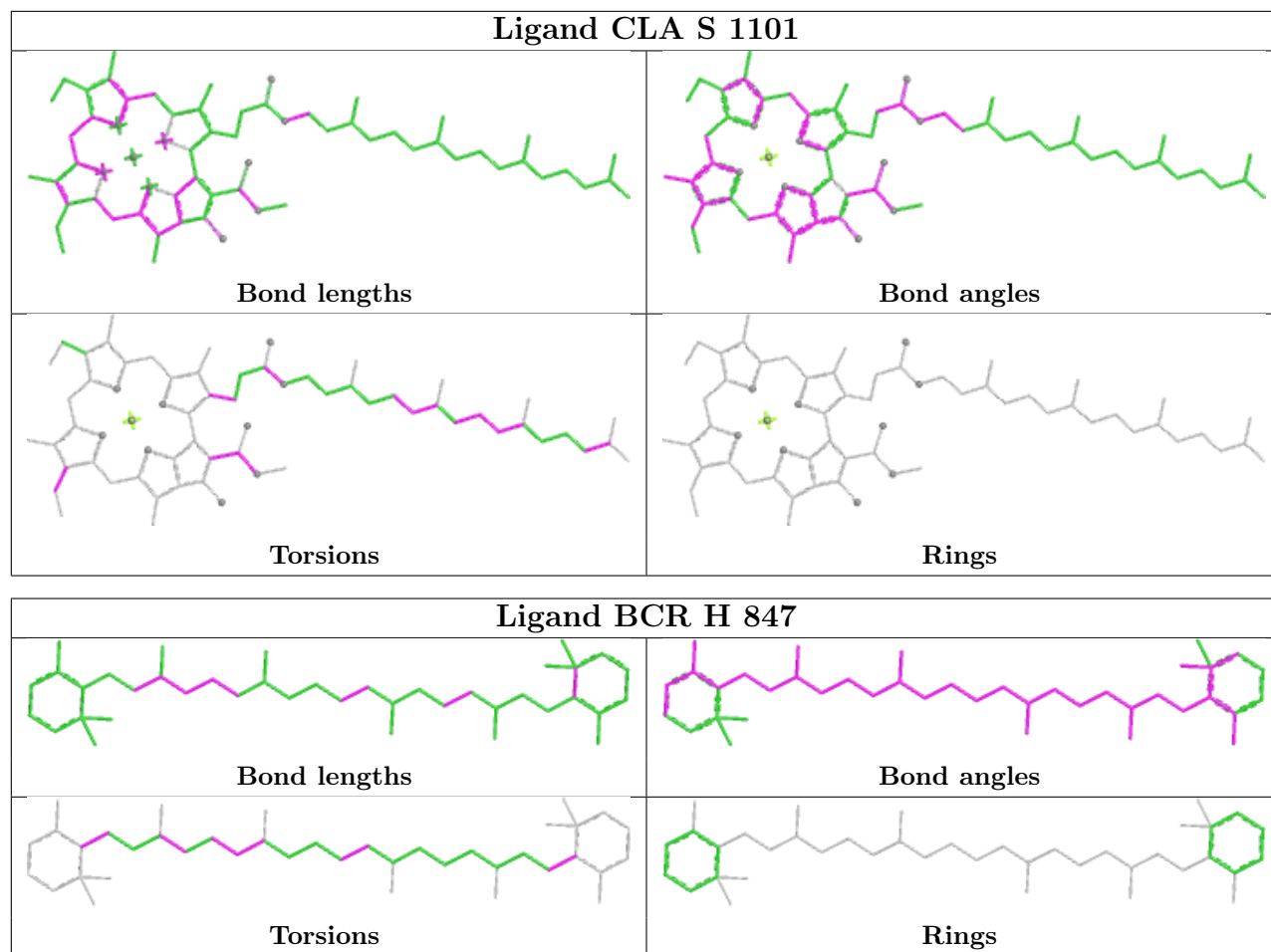


Ligand CLA G 817

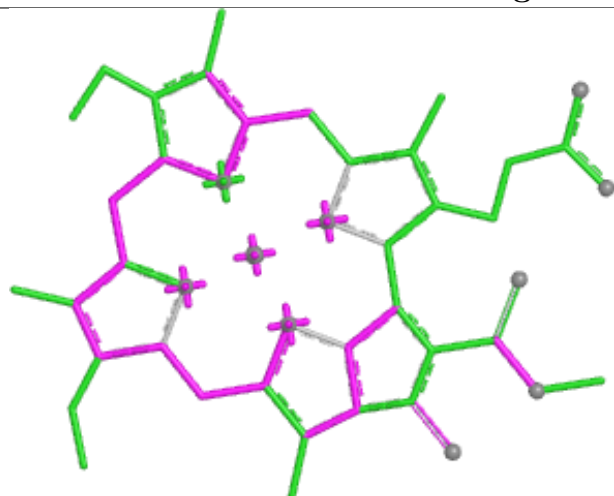


Ligand CLA H 840

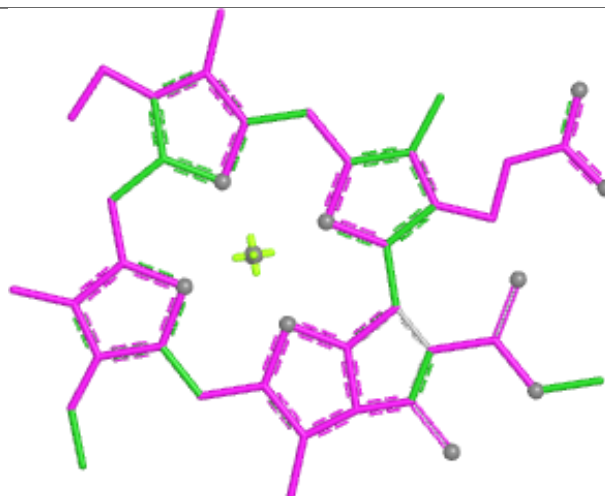




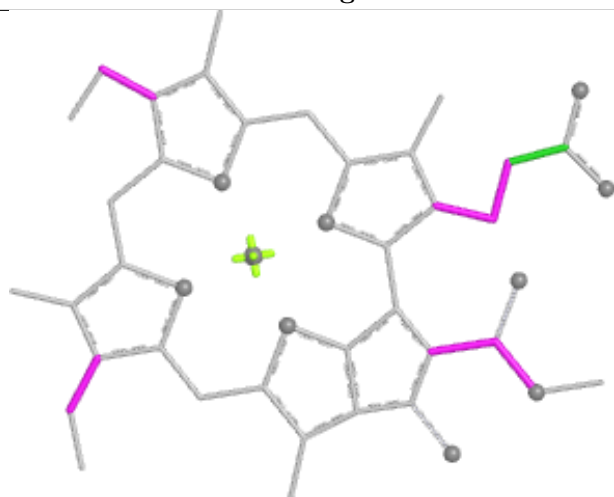
Ligand CLA H 830



Bond lengths



Bond angles

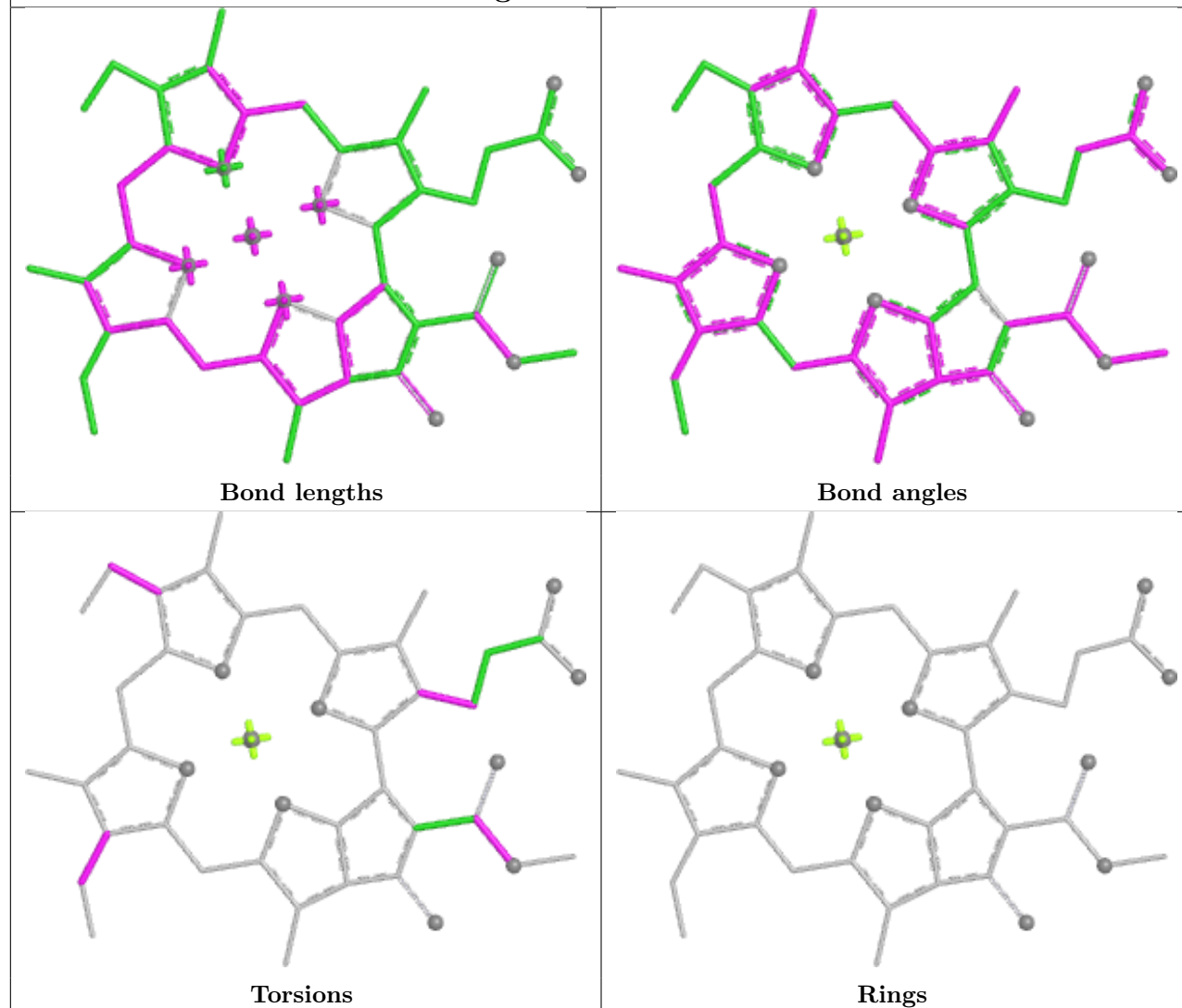


Torsions

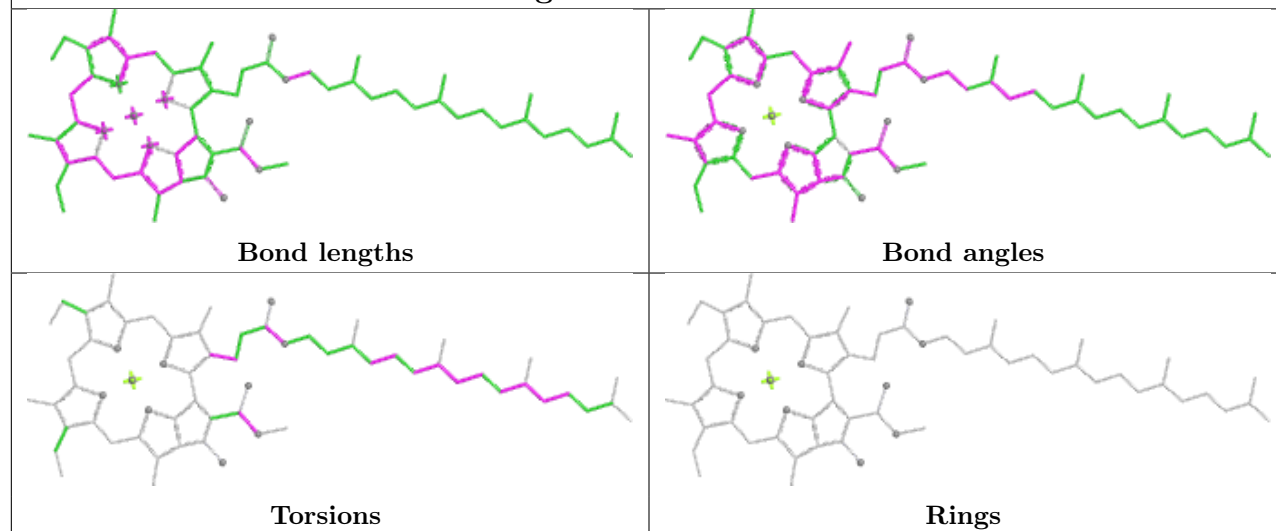


Rings

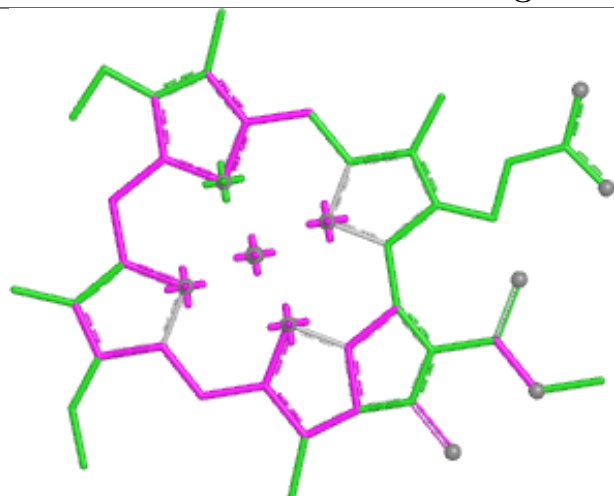
Ligand CLA Z 832



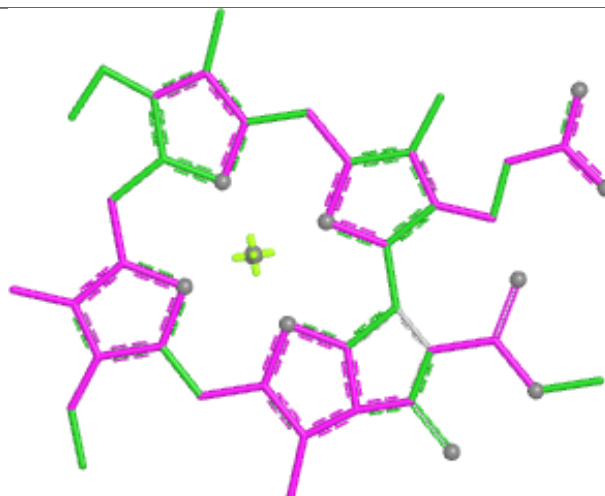
Ligand CLA h 205



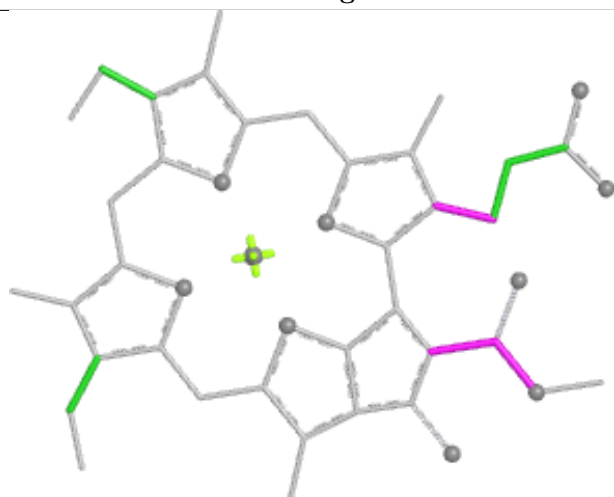
Ligand CLA B 833



Bond lengths



Bond angles

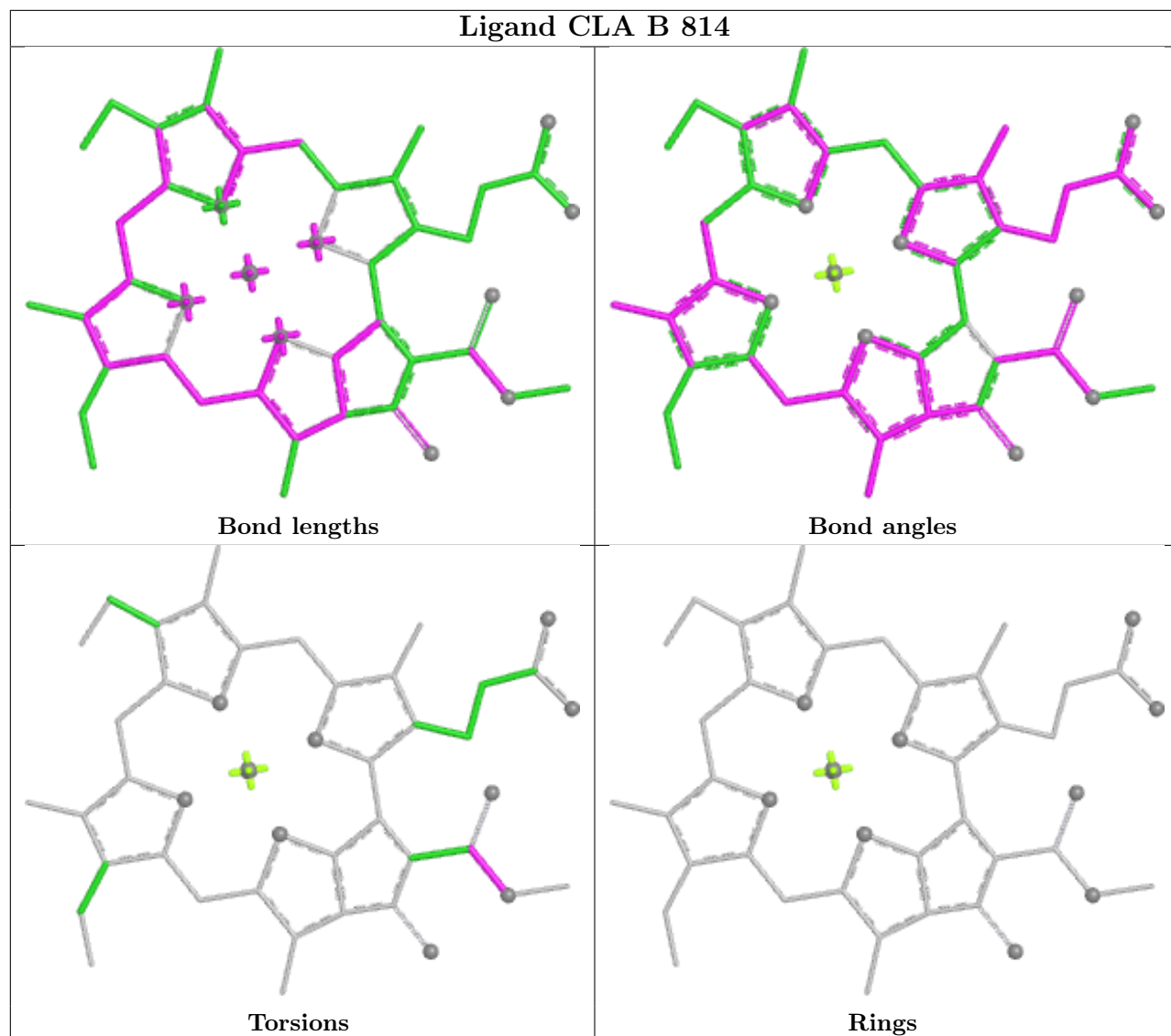


Torsions

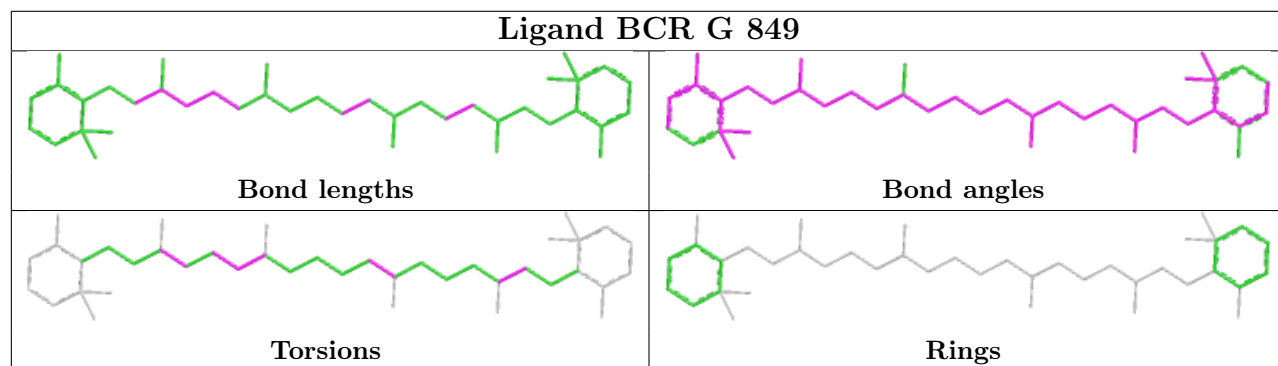


Rings

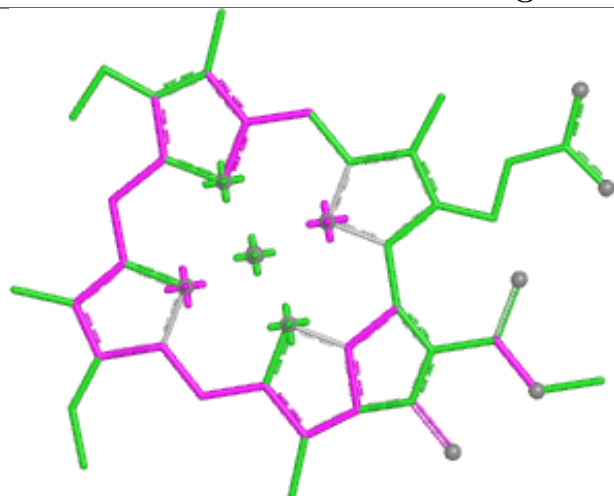
Ligand CLA B 814



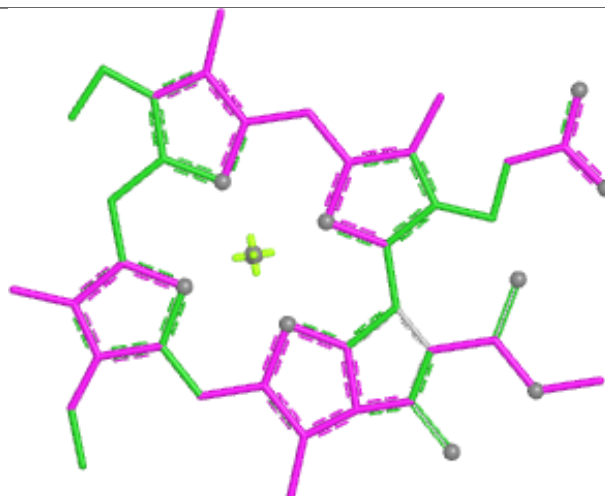
Ligand BCR G 849



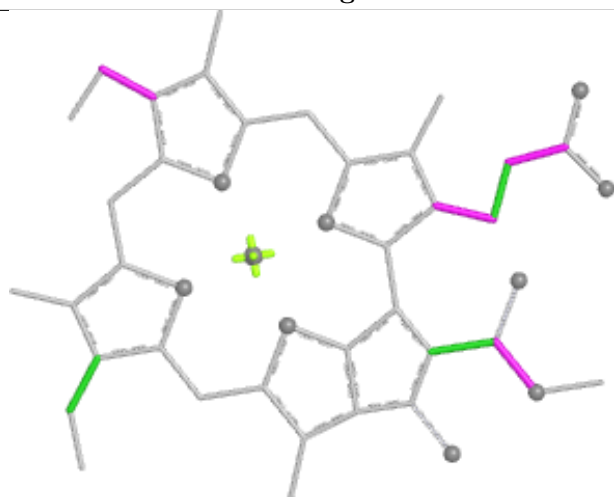
Ligand CLA Z 835



Bond lengths



Bond angles

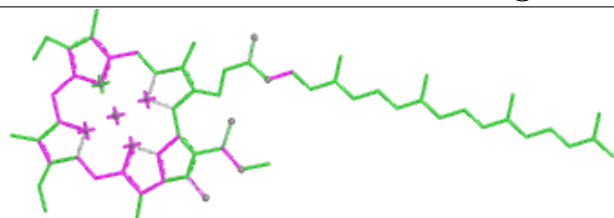


Torsions

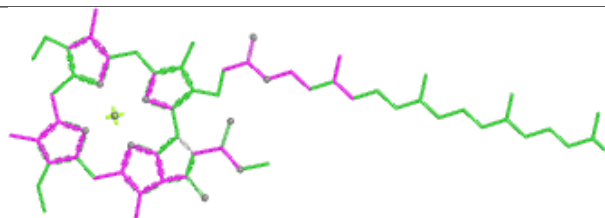


Rings

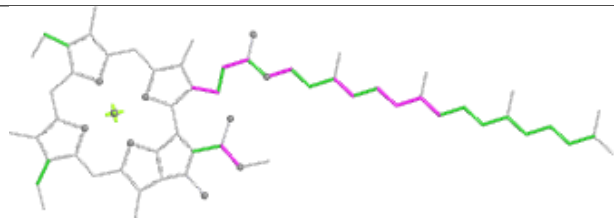
Ligand CLA Y 840



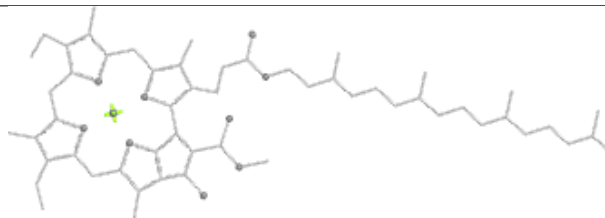
Bond lengths



Bond angles

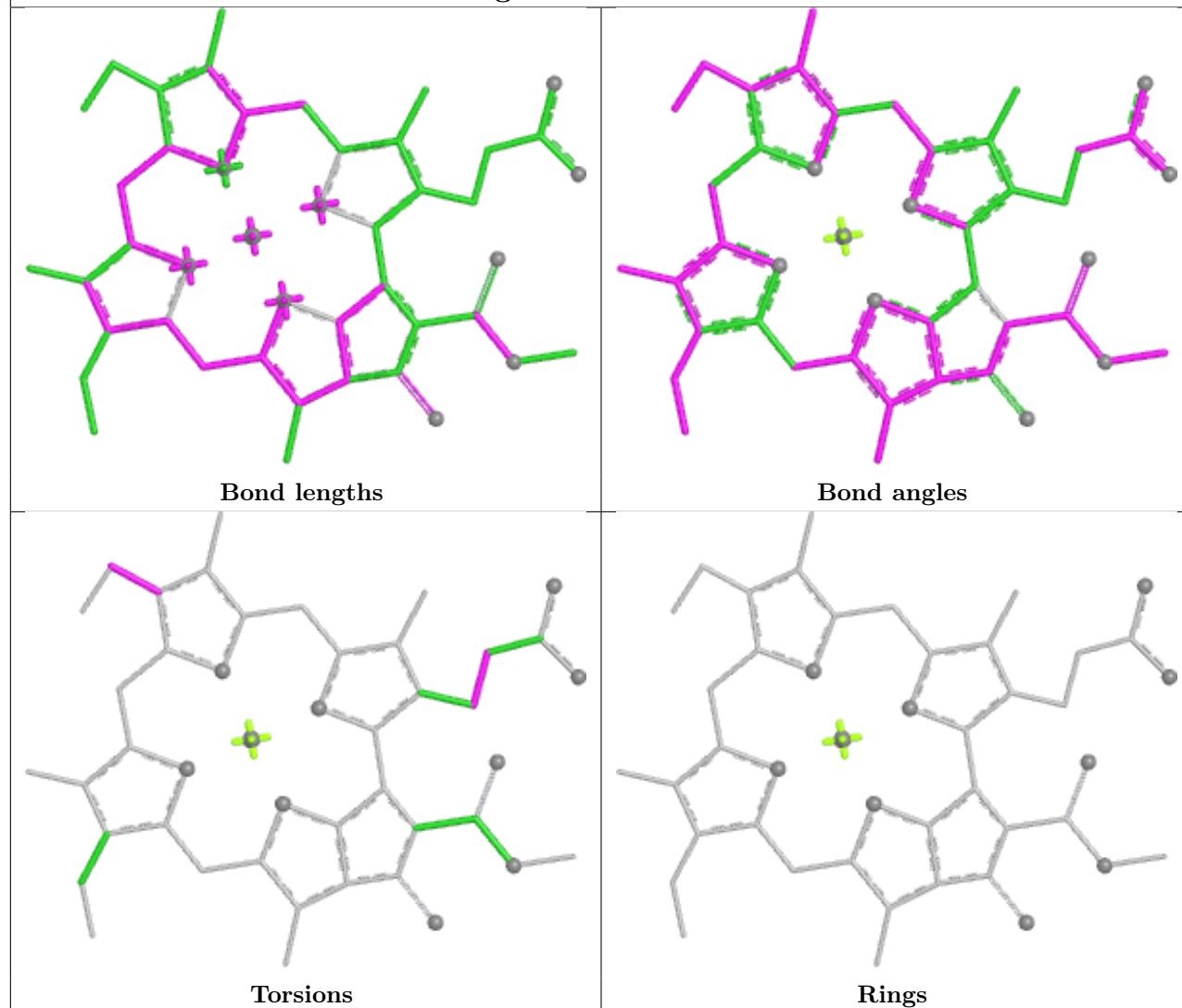


Torsions

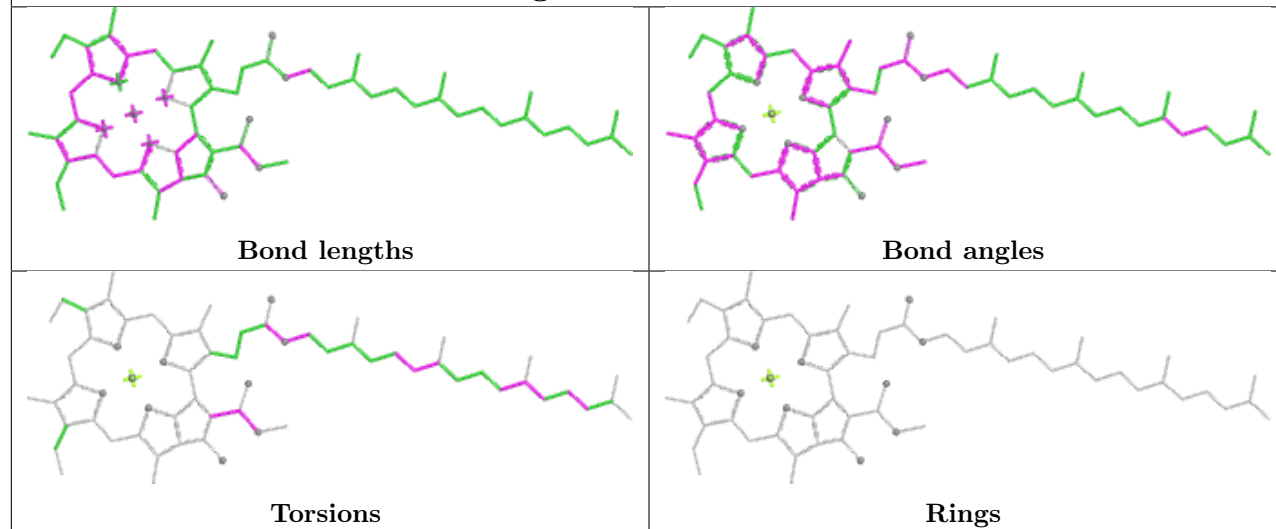


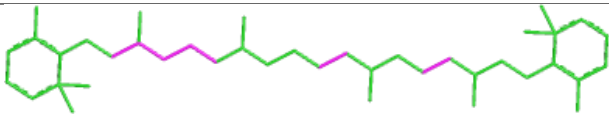
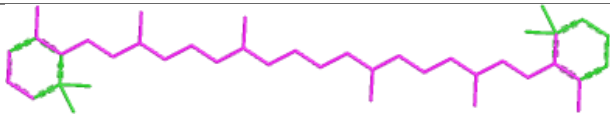
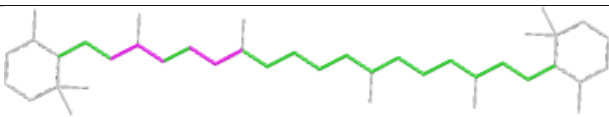
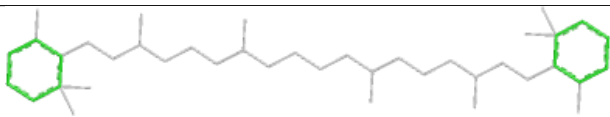
Rings

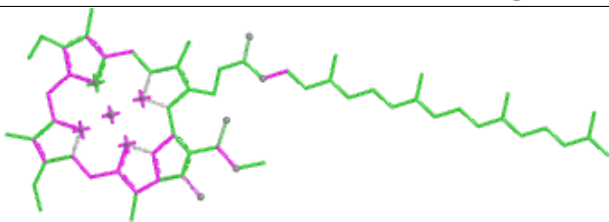
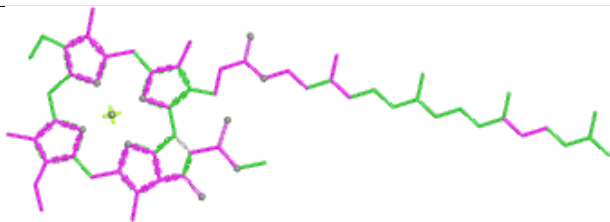
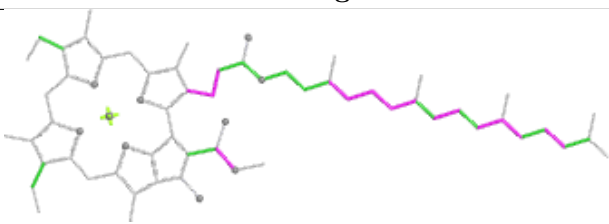
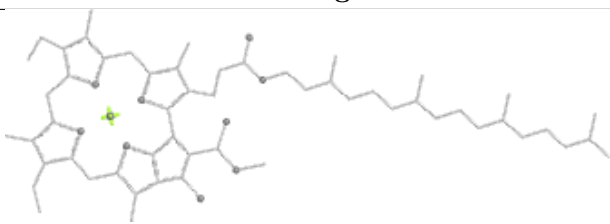
Ligand CLA Z 839

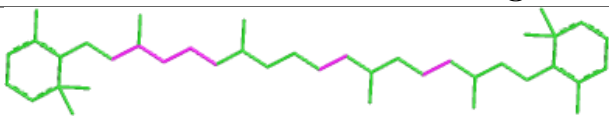
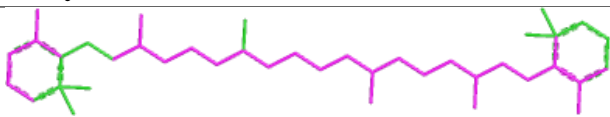
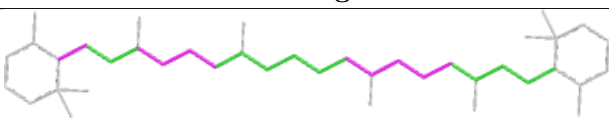
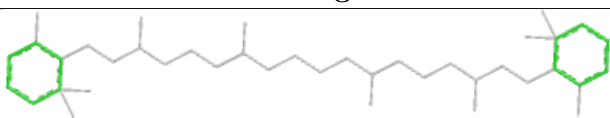


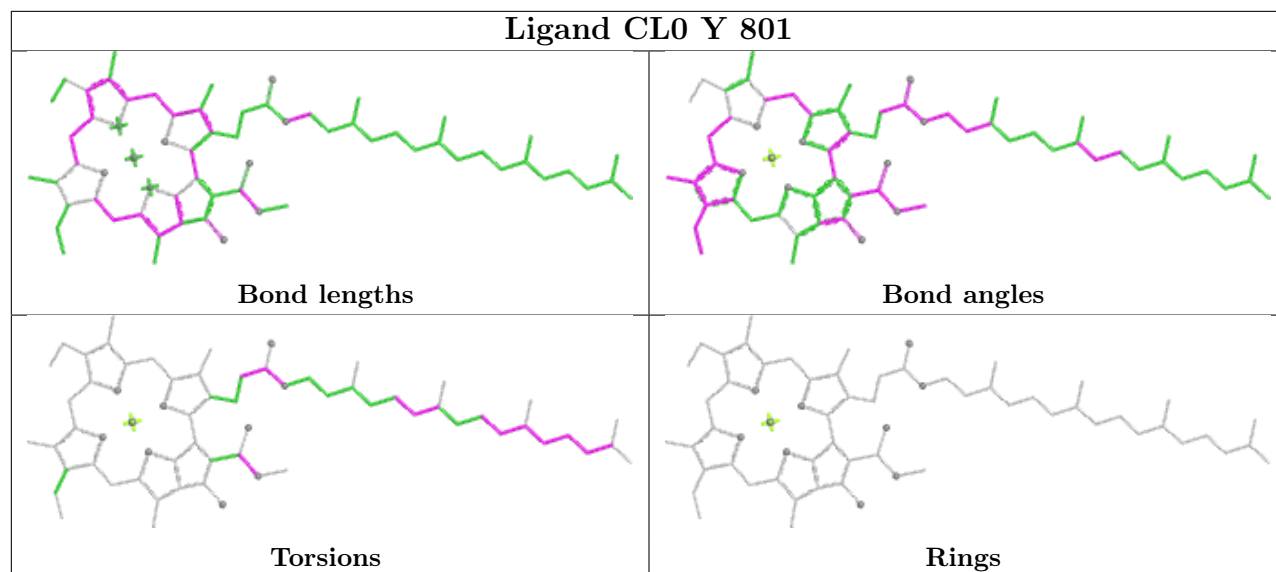
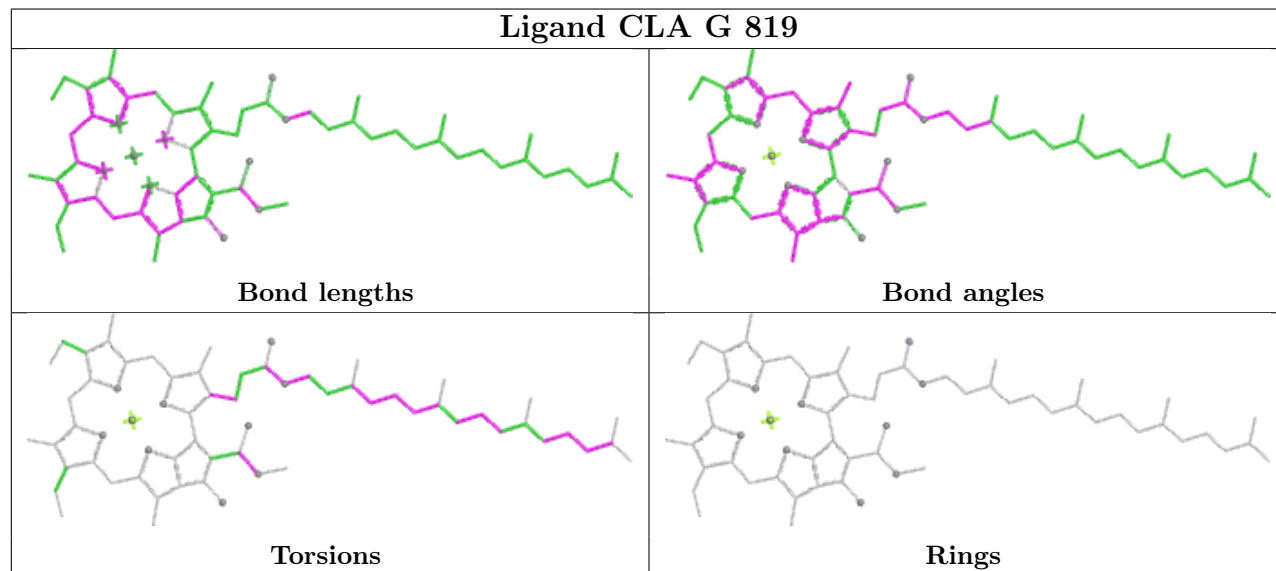
Ligand CLA A 831



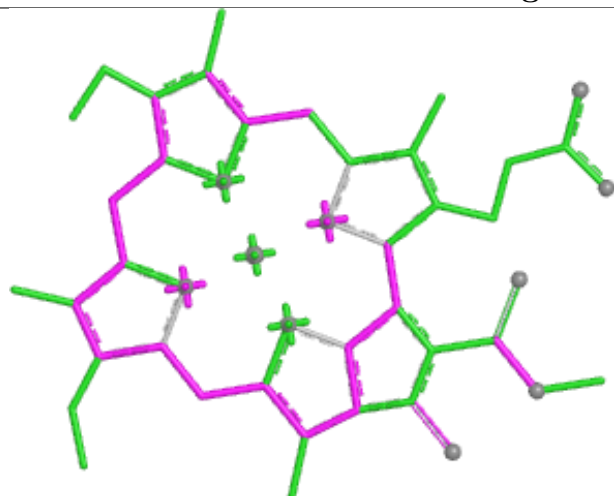
Ligand BCR B 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 809	
	
Bond lengths	Bond angles
	
Torsions	Rings

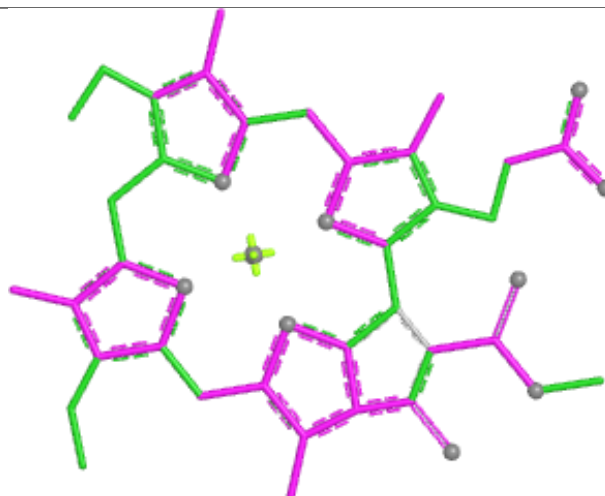
Ligand BCR Q 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CL0 Y 801**Ligand CLA G 819**

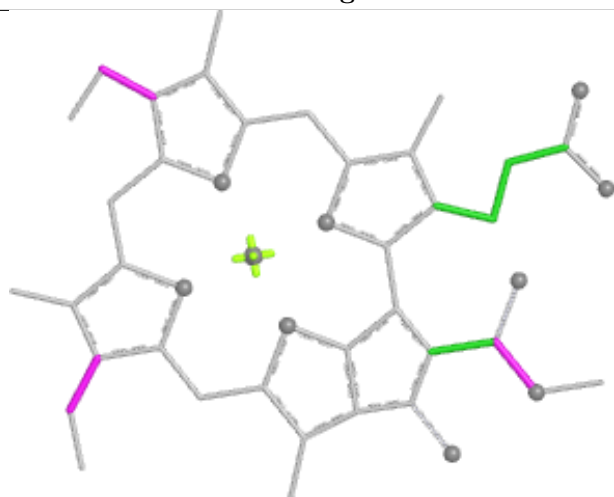
Ligand CLA f 101



Bond lengths



Bond angles

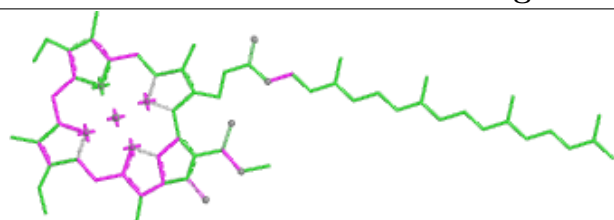


Torsions

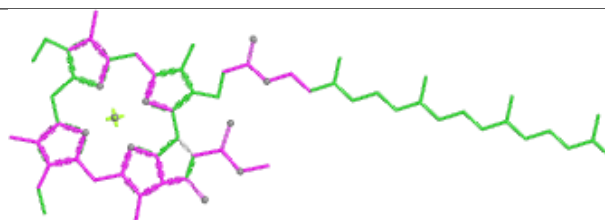


Rings

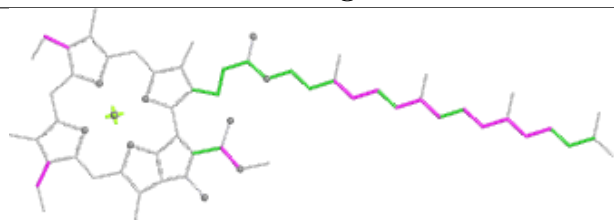
Ligand CLA A 828



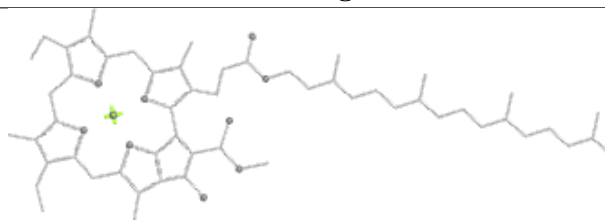
Bond lengths



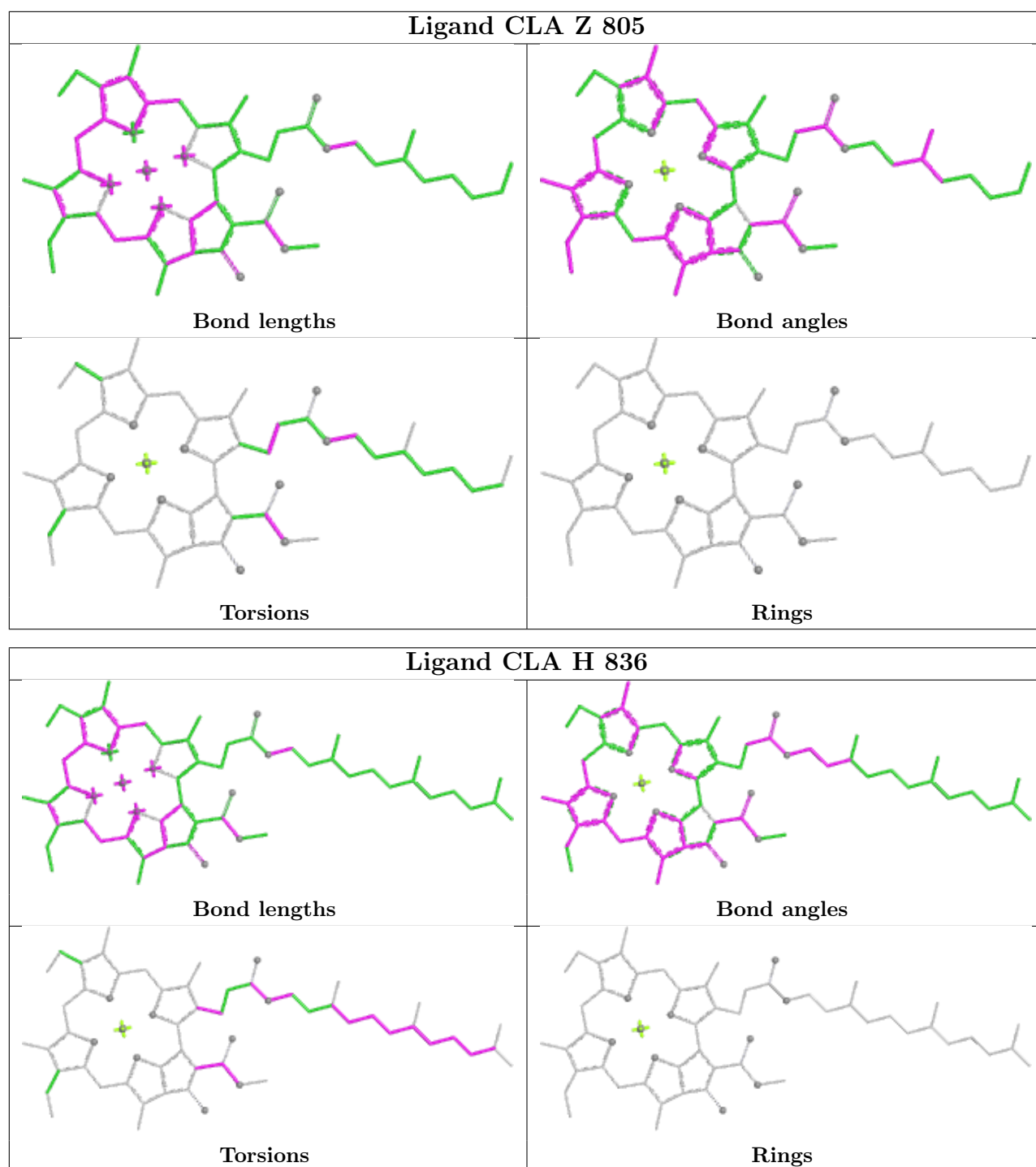
Bond angles



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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	741/755 (98%)	-0.99	0 100 100	23, 46, 71, 91	0
1	G	741/755 (98%)	-0.96	0 100 100	20, 49, 76, 99	0
1	Y	741/755 (98%)	-0.94	0 100 100	27, 52, 73, 93	0
2	B	739/741 (99%)	-1.06	0 100 100	21, 38, 61, 81	0
2	H	739/741 (99%)	-0.97	0 100 100	22, 42, 64, 89	0
2	Z	739/741 (99%)	-1.04	0 100 100	24, 44, 63, 77	0
3	C	80/81 (98%)	-1.15	0 100 100	25, 36, 51, 59	0
3	N	80/81 (98%)	-0.99	0 100 100	24, 39, 55, 64	0
3	a	80/81 (98%)	-1.07	0 100 100	29, 39, 50, 55	0
4	D	138/139 (99%)	-1.09	0 100 100	27, 42, 56, 75	0
4	O	138/139 (99%)	-1.05	0 100 100	25, 43, 59, 76	0
4	b	138/139 (99%)	-1.06	0 100 100	31, 45, 57, 74	0
5	E	69/76 (90%)	-1.00	0 100 100	27, 42, 58, 66	0
5	P	69/76 (90%)	-0.93	0 100 100	32, 44, 57, 63	0
5	c	69/76 (90%)	-0.90	1 (1%) 73 65	36, 51, 68, 81	0
6	F	141/164 (85%)	-0.93	0 100 100	32, 51, 64, 75	0
6	Q	141/164 (85%)	-0.87	0 100 100	36, 52, 65, 79	0
6	d	141/164 (85%)	-0.90	1 (0%) 84 79	34, 60, 71, 76	0
7	I	38/38 (100%)	-1.04	0 100 100	27, 37, 48, 57	0
7	R	38/38 (100%)	-0.96	0 100 100	28, 35, 49, 56	0
7	e	38/38 (100%)	-1.06	0 100 100	22, 35, 46, 53	0
8	J	41/41 (100%)	-0.92	0 100 100	44, 58, 74, 80	0
8	S	41/41 (100%)	-0.85	0 100 100	42, 58, 72, 78	0
8	f	41/41 (100%)	-0.79	0 100 100	58, 67, 80, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
9	K	46/83 (55%)	-0.62	0 100 100	46, 76, 97, 108	0
9	T	46/83 (55%)	-0.55	0 100 100	64, 86, 100, 106	0
9	g	46/83 (55%)	-0.53	1 (2%) 62 53	51, 76, 91, 94	0
10	L	151/155 (97%)	-1.10	0 100 100	20, 32, 54, 75	0
10	U	151/155 (97%)	-1.10	0 100 100	20, 32, 47, 76	0
10	h	151/155 (97%)	-1.12	0 100 100	19, 31, 46, 70	0
11	M	30/31 (96%)	-1.06	0 100 100	30, 39, 42, 47	0
11	V	30/31 (96%)	-0.98	0 100 100	28, 38, 46, 53	0
11	i	30/31 (96%)	-1.14	0 100 100	28, 37, 54, 56	0
12	W	26/39 (66%)	-0.95	0 100 100	39, 48, 58, 61	0
12	X	26/39 (66%)	-0.94	0 100 100	44, 50, 56, 60	0
12	j	26/39 (66%)	-1.07	0 100 100	40, 52, 68, 74	0
All	All	6720/7029 (95%)	-0.99	3 (0%) 100 100	19, 45, 71, 108	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	g	35	GLN	2.6
6	d	13	ALA	2.1
5	c	69	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	A	817	50/65	0.97	0.08	66,75,78,81	0
14	CLA	A	823	65/65	0.97	0.09	52,65,82,85	0
14	CLA	H	812	45/65	0.97	0.06	36,41,42,47	0
14	CLA	J	101	45/65	0.97	0.08	57,72,93,102	0
14	CLA	S	1102	45/65	0.97	0.09	67,86,90,94	0
14	CLA	S	1103	55/65	0.97	0.09	54,67,109,112	0
14	CLA	W	1701	45/65	0.97	0.07	45,64,68,70	0
14	CLA	Y	818	65/65	0.97	0.09	53,61,78,81	0
14	CLA	f	101	45/65	0.97	0.08	82,90,103,106	0
14	CLA	f	102	55/65	0.97	0.10	78,90,105,112	0
17	BCR	B	842	30/40	0.97	0.11	49,70,86,90	0
18	LHG	H	849	37/49	0.97	0.09	42,67,86,92	0
14	CLA	A	835	45/65	0.98	0.07	48,58,61,62	0
14	CLA	A	838	50/65	0.98	0.06	31,38,57,63	0
14	CLA	A	843	50/65	0.98	0.07	50,56,59,61	0
14	CLA	B	810	55/65	0.98	0.06	45,49,57,63	0
14	CLA	B	811	50/65	0.98	0.06	36,40,58,62	0
14	CLA	B	814	45/65	0.98	0.06	58,65,69,74	0
14	CLA	B	815	55/65	0.98	0.08	50,58,78,80	0
14	CLA	B	816	65/65	0.98	0.07	32,39,61,63	0
14	CLA	B	818	60/65	0.98	0.07	40,47,50,53	0
14	CLA	B	819	45/65	0.98	0.06	51,57,65,70	0
14	CLA	B	820	45/65	0.98	0.06	47,60,63,64	0
14	CLA	B	823	55/65	0.98	0.06	30,45,50,51	0
14	CLA	B	824	65/65	0.98	0.06	26,34,53,55	0
14	CLA	B	825	65/65	0.98	0.06	24,32,37,41	0
14	CLA	B	826	65/65	0.98	0.06	28,35,53,58	0
14	CLA	B	832	55/65	0.98	0.06	39,51,56,60	0
14	CLA	B	834	45/65	0.98	0.07	48,51,60,72	0
14	CLA	B	835	45/65	0.98	0.05	47,52,59,64	0
14	CLA	G	803	65/65	0.98	0.06	22,36,41,42	0
14	CLA	G	804	59/65	0.98	0.07	48,56,63,65	0
14	CLA	G	805	65/65	0.98	0.07	39,46,65,68	0
14	CLA	G	806	65/65	0.98	0.07	43,57,64,67	0
14	CLA	G	807	51/65	0.98	0.07	48,52,73,75	0
14	CLA	G	810	45/65	0.98	0.06	61,66,74,92	0
14	CLA	G	812	54/65	0.98	0.07	49,54,75,81	0
14	CLA	G	813	60/65	0.98	0.06	46,57,62,66	0
14	CLA	G	815	50/65	0.98	0.07	62,81,86,89	0
14	CLA	G	816	50/65	0.98	0.08	57,73,76,80	0
14	CLA	G	817	60/65	0.98	0.07	51,58,64,69	0
14	CLA	G	819	65/65	0.98	0.06	44,55,65,70	0
14	CLA	G	820	60/65	0.98	0.06	50,59,66,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	G	822	65/65	0.98	0.07	45,53,65,66	0
14	CLA	G	826	60/65	0.98	0.07	34,38,64,68	0
14	CLA	G	827	65/65	0.98	0.07	31,42,64,65	0
14	CLA	G	829	65/65	0.98	0.07	49,55,61,66	0
14	CLA	G	834	55/65	0.98	0.06	39,52,54,55	0
14	CLA	G	835	45/65	0.98	0.07	58,66,69,73	0
14	CLA	G	837	65/65	0.98	0.06	35,40,48,51	0
14	CLA	G	839	50/65	0.98	0.07	34,39,58,60	0
14	CLA	G	840	65/65	0.98	0.06	29,37,48,49	0
14	CLA	G	842	50/65	0.98	0.08	46,51,71,82	0
14	CLA	H	802	65/65	0.98	0.07	35,53,60,64	0
14	CLA	H	804	54/65	0.98	0.06	27,29,38,39	0
14	CLA	H	805	65/65	0.98	0.07	34,42,47,48	0
14	CLA	A	810	65/65	0.98	0.06	32,37,58,60	0
14	CLA	H	815	45/65	0.98	0.07	55,66,70,74	0
14	CLA	H	816	55/65	0.98	0.08	48,57,67,69	0
14	CLA	H	818	60/65	0.98	0.08	41,56,61,63	0
14	CLA	H	819	60/65	0.98	0.07	40,52,59,62	0
14	CLA	H	821	45/65	0.98	0.07	49,56,61,64	0
14	CLA	H	822	55/65	0.98	0.06	45,50,63,65	0
14	CLA	H	823	60/65	0.98	0.07	38,44,86,91	0
14	CLA	H	824	55/65	0.98	0.06	36,43,48,48	0
14	CLA	H	825	65/65	0.98	0.07	37,47,53,54	0
14	CLA	H	828	65/65	0.98	0.08	34,45,50,59	0
14	CLA	H	829	65/65	0.98	0.07	32,37,51,55	0
14	CLA	H	830	45/65	0.98	0.06	34,42,46,56	0
14	CLA	H	831	65/65	0.98	0.07	42,50,56,60	0
14	CLA	H	832	55/65	0.98	0.07	50,61,92,94	0
14	CLA	H	833	45/65	0.98	0.06	36,44,47,49	0
14	CLA	H	834	45/65	0.98	0.06	48,58,62,65	0
14	CLA	H	835	45/65	0.98	0.06	53,59,64,69	0
14	CLA	H	836	60/65	0.98	0.08	41,48,69,73	0
14	CLA	H	837	65/65	0.98	0.06	33,39,44,45	0
14	CLA	H	838	45/65	0.98	0.06	31,49,52,55	0
14	CLA	H	851	50/65	0.98	0.07	41,48,68,72	0
14	CLA	A	811	45/65	0.98	0.06	57,65,72,73	0
14	CLA	J	102	55/65	0.98	0.07	66,73,98,111	0
14	CLA	K	101	41/65	0.98	0.06	46,61,64,66	0
14	CLA	K	102	45/65	0.98	0.07	68,75,79,80	0
14	CLA	L	204	65/65	0.98	0.05	28,37,42,44	0
14	CLA	Q	202	45/65	0.98	0.06	53,63,66,69	0
14	CLA	S	1101	65/65	0.98	0.07	38,45,58,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	A	813	54/65	0.98	0.07	43,51,59,64	0
14	CLA	A	804	65/65	0.98	0.07	41,45,49,52	0
14	CLA	T	101	41/65	0.98	0.08	50,76,83,88	0
14	CLA	T	103	45/65	0.98	0.07	63,75,78,82	0
14	CLA	U	1004	65/65	0.98	0.06	26,29,35,36	0
14	CLA	A	818	60/65	0.98	0.07	57,63,67,71	0
14	CLA	X	1701	45/65	0.98	0.06	45,56,59,60	0
14	CLA	Y	804	59/65	0.98	0.07	47,65,69,71	0
14	CLA	Y	805	65/65	0.98	0.07	39,43,82,84	0
14	CLA	Y	807	51/65	0.98	0.06	60,72,74,78	0
14	CLA	Y	810	45/65	0.98	0.06	59,69,72,73	0
14	CLA	Y	811	65/65	0.98	0.07	54,71,77,79	0
14	CLA	Y	812	55/65	0.98	0.06	37,52,58,63	0
14	CLA	Y	813	60/65	0.98	0.07	56,65,69,71	0
14	CLA	Y	814	55/65	0.98	0.07	59,71,76,78	0
14	CLA	Y	816	50/65	0.98	0.08	79,87,98,101	0
14	CLA	Y	817	60/65	0.98	0.07	50,54,61,63	0
14	CLA	A	819	65/65	0.98	0.07	36,48,58,59	0
14	CLA	Y	819	65/65	0.98	0.07	45,58,62,65	0
14	CLA	Y	820	60/65	0.98	0.07	51,66,70,73	0
14	CLA	Y	821	65/65	0.98	0.07	39,55,65,70	0
14	CLA	Y	822	65/65	0.98	0.07	51,60,89,92	0
14	CLA	Y	823	50/65	0.98	0.06	46,49,56,61	0
14	CLA	Y	832	65/65	0.98	0.06	27,35,39,45	0
14	CLA	Y	833	55/65	0.98	0.07	50,55,63,65	0
14	CLA	Y	834	45/65	0.98	0.07	49,56,59,59	0
14	CLA	Y	838	65/65	0.98	0.06	40,49,54,60	0
14	CLA	Y	839	50/65	0.98	0.06	44,53,57,58	0
14	CLA	Z	806	65/65	0.98	0.07	34,40,44,46	0
14	CLA	Z	811	65/65	0.98	0.05	25,35,39,44	0
14	CLA	Z	813	45/65	0.98	0.06	50,55,64,72	0
14	CLA	Z	818	65/65	0.98	0.07	40,44,57,60	0
14	CLA	Z	822	45/65	0.98	0.07	42,44,51,55	0
14	CLA	Z	824	60/65	0.98	0.07	47,53,75,77	0
14	CLA	Z	826	65/65	0.98	0.07	37,48,69,73	0
14	CLA	Z	832	45/65	0.98	0.05	27,31,41,44	0
14	CLA	Z	834	45/65	0.98	0.06	36,48,50,52	0
14	CLA	Z	836	45/65	0.98	0.06	50,75,79,82	0
14	CLA	Z	837	60/65	0.98	0.06	41,59,66,71	0
14	CLA	d	201	65/65	0.98	0.07	40,59,66,71	0
14	CLA	A	820	65/65	0.98	0.07	43,54,60,61	0
14	CLA	A	821	60/65	0.98	0.07	55,62,72,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	g	101	41/65	0.98	0.07	47,64,71,73	0
14	CLA	g	102	45/65	0.98	0.06	49,59,67,74	0
14	CLA	h	205	65/65	0.98	0.06	28,32,36,38	0
15	PQN	B	841	33/33	0.98	0.06	34,37,39,40	0
15	PQN	Z	842	33/33	0.98	0.06	32,36,38,40	0
17	BCR	A	846	40/40	0.98	0.08	54,62,72,74	0
17	BCR	A	847	40/40	0.98	0.09	50,70,85,86	0
17	BCR	A	848	40/40	0.98	0.09	52,67,81,84	0
17	BCR	A	850	40/40	0.98	0.08	31,42,56,58	0
14	CLA	A	808	51/65	0.98	0.07	47,56,61,66	0
17	BCR	B	846	40/40	0.98	0.06	31,34,36,38	0
17	BCR	B	847	40/40	0.98	0.06	22,26,30,31	0
17	BCR	B	850	40/40	0.98	0.08	46,57,79,80	0
17	BCR	F	201	40/40	0.98	0.06	30,45,56,59	0
17	BCR	G	845	40/40	0.98	0.08	55,68,75,77	0
17	BCR	G	846	40/40	0.98	0.09	47,59,95,97	0
17	BCR	G	847	40/40	0.98	0.09	47,57,81,83	0
17	BCR	G	848	40/40	0.98	0.07	28,48,59,61	0
17	BCR	H	842	40/40	0.98	0.08	64,69,89,93	0
17	BCR	H	843	40/40	0.98	0.08	38,46,69,69	0
17	BCR	H	846	40/40	0.98	0.08	36,40,47,48	0
17	BCR	H	847	40/40	0.98	0.06	24,26,30,32	0
17	BCR	H	850	40/40	0.98	0.07	36,52,68,68	0
17	BCR	I	102	40/40	0.98	0.06	29,32,41,43	0
17	BCR	J	104	40/40	0.98	0.07	56,60,75,75	0
17	BCR	L	208	40/40	0.98	0.06	27,30,62,63	0
17	BCR	M	101	40/40	0.98	0.06	30,35,44,45	0
17	BCR	Q	201	40/40	0.98	0.09	46,58,70,72	0
17	BCR	Q	203	40/40	0.98	0.07	28,35,44,45	0
17	BCR	S	1105	40/40	0.98	0.06	45,51,58,61	0
17	BCR	T	102	40/40	0.98	0.09	51,64,73,76	0
17	BCR	U	1008	40/40	0.98	0.06	23,26,30,31	0
17	BCR	U	1009	40/40	0.98	0.06	25,33,44,46	0
17	BCR	V	101	40/40	0.98	0.07	28,36,52,53	0
17	BCR	Y	844	40/40	0.98	0.07	50,56,61,64	0
17	BCR	Y	845	40/40	0.98	0.09	50,64,97,99	0
17	BCR	Y	846	40/40	0.98	0.09	56,70,91,92	0
17	BCR	Y	847	40/40	0.98	0.09	39,47,93,94	0
17	BCR	Y	849	40/40	0.98	0.06	33,39,45,45	0
17	BCR	Y	852	40/40	0.98	0.07	28,35,41,42	0
17	BCR	Y	853	40/40	0.98	0.08	59,67,84,87	0
17	BCR	Z	843	40/40	0.98	0.07	45,48,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	BCR	Z	844	40/40	0.98	0.08	38,47,65,67	0
17	BCR	Z	845	40/40	0.98	0.08	40,61,78,81	0
17	BCR	Z	846	25/40	0.98	0.07	22,44,50,51	0
17	BCR	Z	847	40/40	0.98	0.07	37,43,47,48	0
17	BCR	Z	850	40/40	0.98	0.08	50,67,72,74	0
17	BCR	d	203	40/40	0.98	0.07	40,45,55,56	0
17	BCR	e	101	40/40	0.98	0.05	22,28,38,39	0
17	BCR	h	202	40/40	0.98	0.07	31,34,68,70	0
17	BCR	i	101	40/40	0.98	0.06	30,36,41,42	0
18	LHG	A	852	49/49	0.98	0.08	26,41,52,55	0
18	LHG	B	849	39/49	0.98	0.08	49,61,79,80	0
14	CLA	A	824	50/65	0.98	0.07	48,63,73,76	0
18	LHG	j	101	28/49	0.98	0.07	50,58,69,73	0
19	LMG	B	848	52/55	0.98	0.07	21,27,50,52	0
19	LMG	H	848	49/55	0.98	0.07	22,32,39,40	0
19	LMG	Z	849	49/55	0.98	0.06	26,36,41,42	0
14	CLA	A	829	65/65	0.99	0.05	30,37,57,61	0
14	CLA	U	1002	65/65	0.99	0.05	22,28,35,46	0
14	CLA	U	1003	65/65	0.99	0.05	25,29,46,47	0
14	CLA	A	830	65/65	0.99	0.06	33,41,57,60	0
14	CLA	U	1006	65/65	0.99	0.05	27,30,48,52	0
14	CLA	U	1007	65/65	0.99	0.05	29,33,37,39	0
14	CLA	A	831	65/65	0.99	0.06	33,41,45,46	0
14	CLA	A	832	50/65	0.99	0.06	37,40,61,62	0
14	CLA	Y	802	65/65	0.99	0.06	28,36,44,47	0
14	CLA	Y	803	65/65	0.99	0.06	49,60,65,66	0
14	CLA	A	833	65/65	0.99	0.05	25,28,36,41	0
14	CLA	G	808	65/65	0.99	0.06	31,36,63,66	0
14	CLA	Y	806	65/65	0.99	0.06	38,52,60,62	0
14	CLA	G	809	65/65	0.99	0.06	38,44,58,62	0
14	CLA	Y	808	65/65	0.99	0.05	38,49,60,63	0
14	CLA	Y	809	65/65	0.99	0.06	45,52,66,68	0
14	CLA	A	834	55/65	0.99	0.06	39,49,58,66	0
14	CLA	G	811	65/65	0.99	0.07	43,66,72,75	0
14	CLA	A	802	65/65	0.99	0.06	40,44,51,59	0
14	CLA	A	836	50/65	0.99	0.05	27,31,42,43	0
14	CLA	G	814	50/65	0.99	0.05	55,70,76,86	0
14	CLA	Y	815	50/65	0.99	0.06	43,60,65,71	0
14	CLA	A	837	65/65	0.99	0.05	32,41,45,49	0
14	CLA	A	812	65/65	0.99	0.06	39,58,63,65	0
14	CLA	A	839	65/65	0.99	0.06	35,39,58,66	0
14	CLA	G	818	65/65	0.99	0.06	47,53,68,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	A	840	50/65	0.99	0.06	40,46,55,69	0
14	CLA	A	841	65/65	0.99	0.05	24,27,47,52	0
14	CLA	G	821	65/65	0.99	0.06	39,53,59,61	0
14	CLA	A	842	65/65	0.99	0.05	20,24,27,28	0
14	CLA	Y	824	60/65	0.99	0.07	37,44,78,80	0
14	CLA	Y	825	65/65	0.99	0.06	34,39,50,52	0
14	CLA	Y	826	60/65	0.99	0.06	41,44,53,56	0
14	CLA	Y	827	65/65	0.99	0.07	51,66,71,73	0
14	CLA	Y	828	65/65	0.99	0.06	43,46,55,59	0
14	CLA	Y	829	65/65	0.99	0.06	40,49,59,65	0
14	CLA	Y	830	65/65	0.99	0.06	36,48,51,58	0
14	CLA	Y	831	50/65	0.99	0.06	35,38,56,61	0
14	CLA	G	823	50/65	0.99	0.06	40,51,71,75	0
14	CLA	G	824	60/65	0.99	0.06	42,46,55,56	0
14	CLA	G	825	65/65	0.99	0.06	38,47,51,53	0
14	CLA	Y	835	50/65	0.99	0.06	43,49,51,53	0
14	CLA	Y	836	65/65	0.99	0.06	30,38,44,52	0
14	CLA	Y	837	50/65	0.99	0.05	34,39,67,68	0
14	CLA	A	803	65/65	0.99	0.05	18,30,33,35	0
14	CLA	A	854	65/65	0.99	0.06	34,40,58,61	0
14	CLA	Y	840	65/65	0.99	0.06	44,52,78,87	0
14	CLA	Y	841	65/65	0.99	0.05	22,25,31,34	0
14	CLA	Z	801	65/65	0.99	0.06	35,47,51,53	0
14	CLA	Z	802	65/65	0.99	0.06	46,56,59,65	0
14	CLA	Z	803	65/65	0.99	0.06	37,52,57,65	0
14	CLA	Z	804	65/65	0.99	0.05	24,36,38,43	0
14	CLA	Z	805	54/65	0.99	0.05	25,30,32,33	0
14	CLA	G	828	65/65	0.99	0.07	39,51,58,64	0
14	CLA	Z	807	65/65	0.99	0.06	30,37,56,57	0
14	CLA	Z	808	65/65	0.99	0.05	31,35,46,53	0
14	CLA	Z	809	65/65	0.99	0.06	39,47,51,54	0
14	CLA	Z	810	65/65	0.99	0.05	29,33,43,49	0
14	CLA	B	801	65/65	0.99	0.05	22,28,33,34	0
14	CLA	Z	812	55/65	0.99	0.06	37,43,54,55	0
14	CLA	G	830	65/65	0.99	0.06	32,40,57,58	0
14	CLA	Z	814	65/65	0.99	0.06	34,37,50,52	0
14	CLA	Z	815	65/65	0.99	0.05	37,44,57,61	0
14	CLA	Z	816	45/65	0.99	0.06	51,59,70,76	0
14	CLA	Z	817	55/65	0.99	0.06	39,49,62,70	0
14	CLA	G	831	50/65	0.99	0.05	31,34,46,50	0
14	CLA	Z	819	60/65	0.99	0.06	37,47,51,55	0
14	CLA	Z	820	60/65	0.99	0.06	42,52,71,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	Z	821	45/65	0.99	0.06	38,47,61,72	0
14	CLA	G	832	65/65	0.99	0.05	22,27,34,35	0
14	CLA	Z	823	55/65	0.99	0.05	40,44,48,48	0
14	CLA	G	833	65/65	0.99	0.05	18,22,32,34	0
14	CLA	Z	825	55/65	0.99	0.05	36,44,48,51	0
14	CLA	B	802	65/65	0.99	0.04	25,35,38,39	0
14	CLA	Z	827	65/65	0.99	0.05	34,37,47,48	0
14	CLA	Z	828	65/65	0.99	0.06	36,41,48,51	0
14	CLA	Z	829	65/65	0.99	0.06	33,40,44,45	0
14	CLA	Z	830	65/65	0.99	0.06	29,34,44,45	0
14	CLA	Z	831	45/65	0.99	0.06	42,46,64,66	0
14	CLA	B	803	54/65	0.99	0.05	26,29,39,40	0
14	CLA	Z	833	55/65	0.99	0.06	51,66,71,75	0
14	CLA	G	836	50/65	0.99	0.06	34,41,50,54	0
14	CLA	Z	835	45/65	0.99	0.05	51,59,61,62	0
14	CLA	B	804	65/65	0.99	0.05	26,31,39,41	0
14	CLA	G	838	50/65	0.99	0.06	32,41,56,58	0
14	CLA	Z	838	65/65	0.99	0.05	35,39,55,58	0
14	CLA	Z	839	45/65	0.99	0.05	36,40,42,44	0
14	CLA	Z	840	65/65	0.99	0.05	17,20,27,28	0
14	CLA	Z	841	65/65	0.99	0.05	21,31,34,35	0
14	CLA	B	805	65/65	0.99	0.05	34,38,56,60	0
14	CLA	d	202	45/65	0.99	0.06	63,75,80,81	0
14	CLA	B	806	65/65	0.99	0.04	25,30,37,41	0
14	CLA	G	841	65/65	0.99	0.05	20,23,30,32	0
14	CLA	B	807	65/65	0.99	0.05	27,30,40,43	0
14	CLA	G	852	65/65	0.99	0.06	27,36,38,41	0
14	CLA	h	201	65/65	0.99	0.06	25,29,72,74	0
14	CLA	h	204	65/65	0.99	0.05	22,28,42,47	0
14	CLA	G	853	45/65	0.99	0.05	26,29,39,44	0
14	CLA	h	206	65/65	0.99	0.05	26,31,45,47	0
14	CLA	j	102	45/65	0.99	0.06	47,64,68,69	0
15	PQN	A	844	33/33	0.99	0.06	35,38,42,42	0
14	CLA	H	801	65/65	0.99	0.05	30,34,49,53	0
15	PQN	G	843	33/33	0.99	0.07	44,51,55,56	0
15	PQN	H	841	33/33	0.99	0.07	29,39,60,61	0
15	PQN	Y	842	33/33	0.99	0.06	38,45,52,52	0
14	CLA	B	808	65/65	0.99	0.05	27,29,41,45	0
16	SF4	G	844	8/8	0.99	0.03	45,45,48,58	0
14	CLA	H	803	65/65	0.99	0.06	24,30,51,54	0
14	CLA	B	809	65/65	0.99	0.05	21,25,33,41	0
14	CLA	A	814	60/65	0.99	0.06	42,48,78,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	BCR	A	849	40/40	0.99	0.07	38,48,70,72	0
14	CLA	H	806	65/65	0.99	0.06	40,45,59,62	0
17	BCR	A	851	40/40	0.99	0.05	28,36,42,46	0
14	CLA	H	807	65/65	0.99	0.05	22,27,40,45	0
17	BCR	B	843	40/40	0.99	0.07	34,46,66,69	0
17	BCR	B	844	40/40	0.99	0.07	30,50,68,70	0
17	BCR	B	845	25/40	0.99	0.06	21,28,34,36	0
14	CLA	H	808	65/65	0.99	0.06	29,34,44,47	0
14	CLA	H	809	65/65	0.99	0.05	27,29,44,49	0
14	CLA	H	810	65/65	0.99	0.05	20,22,31,35	0
14	CLA	H	811	55/65	0.99	0.05	37,43,52,54	0
17	BCR	F	203	40/40	0.99	0.06	35,48,51,52	0
14	CLA	A	815	50/65	0.99	0.07	67,76,99,102	0
14	CLA	H	813	65/65	0.99	0.06	32,38,43,51	0
14	CLA	H	814	65/65	0.99	0.06	31,35,51,53	0
14	CLA	B	812	65/65	0.99	0.05	29,34,45,50	0
17	BCR	G	849	40/40	0.99	0.06	27,34,40,41	0
14	CLA	B	813	65/65	0.99	0.06	39,45,63,67	0
14	CLA	H	817	65/65	0.99	0.07	34,44,65,66	0
17	BCR	H	844	40/40	0.99	0.06	33,44,76,78	0
17	BCR	H	845	25/40	0.99	0.07	23,49,56,59	0
14	CLA	A	816	50/65	0.99	0.07	53,66,69,73	0
13	CL0	A	801	65/65	0.99	0.05	26,30,34,40	0
14	CLA	H	820	45/65	0.99	0.06	46,53,64,71	0
17	BCR	I	101	40/40	0.99	0.04	18,24,29,29	0
14	CLA	A	805	59/65	0.99	0.06	41,47,72,76	0
17	BCR	J	103	40/40	0.99	0.07	45,51,57,59	0
14	CLA	B	817	60/65	0.99	0.05	33,47,49,50	0
17	BCR	L	207	40/40	0.99	0.05	23,26,30,31	0
14	CLA	A	806	65/65	0.99	0.06	39,43,66,69	0
14	CLA	A	807	65/65	0.99	0.06	40,51,61,62	0
13	CL0	G	801	65/65	0.99	0.05	22,24,31,34	0
14	CLA	H	826	65/65	0.99	0.05	28,34,40,43	0
17	BCR	R	101	40/40	0.99	0.04	18,24,30,30	0
17	BCR	R	102	40/40	0.99	0.05	18,25,31,33	0
17	BCR	S	1104	40/40	0.99	0.07	45,48,57,59	0
14	CLA	H	827	65/65	0.99	0.06	29,34,40,43	0
14	CLA	B	821	55/65	0.99	0.06	49,53,71,72	0
17	BCR	U	1005	40/40	0.99	0.06	26,29,37,39	0
14	CLA	B	822	60/65	0.99	0.07	43,51,76,80	0
14	CLA	A	822	65/65	0.99	0.06	32,46,54,57	0
14	CLA	A	809	65/65	0.99	0.06	36,40,57,61	0

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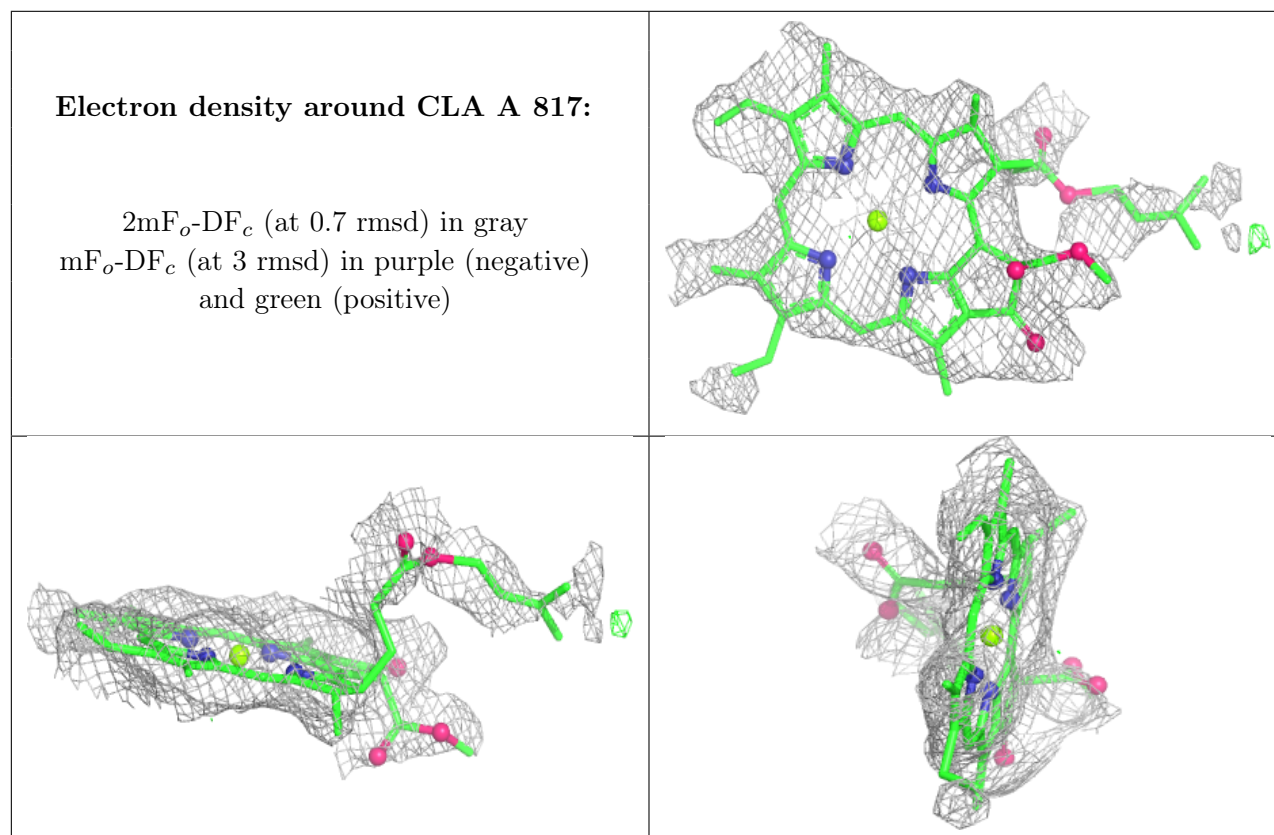
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	CL0	Y	801	65/65	0.99	0.06	37,45,50,55	0
14	CLA	A	825	60/65	0.99	0.06	38,42,54,57	0
14	CLA	B	827	65/65	0.99	0.06	33,37,60,62	0
14	CLA	B	828	65/65	0.99	0.06	29,33,41,44	0
17	BCR	Y	848	40/40	0.99	0.07	41,49,53,53	0
14	CLA	B	829	45/65	0.99	0.05	34,37,41,46	0
14	CLA	B	830	45/65	0.99	0.05	32,36,49,56	0
14	CLA	B	831	65/65	0.99	0.06	30,36,53,58	0
14	CLA	H	839	65/65	0.99	0.05	16,18,25,26	0
14	CLA	H	840	65/65	0.99	0.05	24,28,40,43	0
14	CLA	A	826	65/65	0.99	0.06	40,49,51,53	0
14	CLA	B	833	45/65	0.99	0.06	47,51,54,57	0
14	CLA	A	827	60/65	0.99	0.06	28,33,76,78	0
17	BCR	Z	848	40/40	0.99	0.06	36,56,70,72	0
14	CLA	A	828	65/65	0.99	0.06	38,45,61,69	0
14	CLA	B	836	60/65	0.99	0.06	40,50,57,58	0
14	CLA	L	201	65/65	0.99	0.06	25,30,63,64	0
17	BCR	f	103	40/40	0.99	0.07	56,64,70,72	0
14	CLA	L	202	65/65	0.99	0.04	18,20,35,36	0
17	BCR	h	207	40/40	0.99	0.06	23,29,37,39	0
14	CLA	B	837	65/65	0.99	0.05	38,45,61,66	0
14	CLA	L	205	65/65	0.99	0.05	25,29,46,51	0
18	LHG	A	853	32/49	0.99	0.06	37,43,56,57	0
14	CLA	L	206	65/65	0.99	0.05	23,26,52,54	0
18	LHG	G	850	49/49	0.99	0.07	30,44,50,51	0
18	LHG	G	851	32/49	0.99	0.07	46,51,70,73	0
14	CLA	B	838	45/65	0.99	0.05	40,47,54,57	0
18	LHG	Y	850	49/49	0.99	0.06	38,42,50,55	0
18	LHG	Y	851	25/49	0.99	0.04	40,45,49,50	0
14	CLA	B	839	65/65	0.99	0.04	18,20,24,26	0
14	CLA	B	840	65/65	0.99	0.05	21,25,32,37	0
14	CLA	F	202	45/65	0.99	0.05	41,56,59,64	0
14	CLA	G	802	65/65	0.99	0.06	27,41,46,48	0
20	CA	L	203	1/1	0.99	0.03	55,55,55,55	0
20	CA	U	1001	1/1	0.99	0.03	37,37,37,37	0
20	CA	h	203	1/1	0.99	0.05	65,65,65,65	0
16	SF4	C	102	8/8	1.00	0.03	37,42,47,52	0
16	SF4	A	845	8/8	1.00	0.02	36,38,41,43	0
16	SF4	N	101	8/8	1.00	0.03	40,44,49,51	0
16	SF4	N	102	8/8	1.00	0.02	46,50,57,57	0
16	SF4	Y	843	8/8	1.00	0.03	48,51,57,61	0
16	SF4	a	101	8/8	1.00	0.02	42,44,45,46	0

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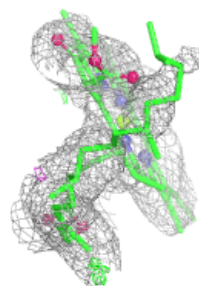
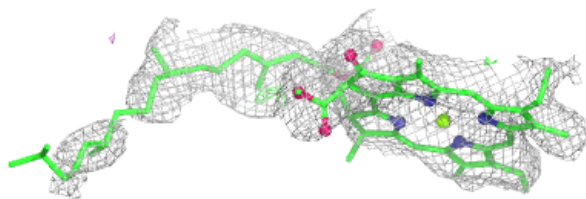
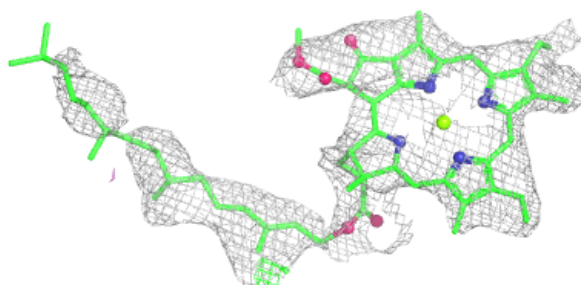
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	SF4	a	102	8/8	1.00	0.02	41,44,46,48	0
16	SF4	C	101	8/8	1.00	0.01	31,33,34,36	0

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



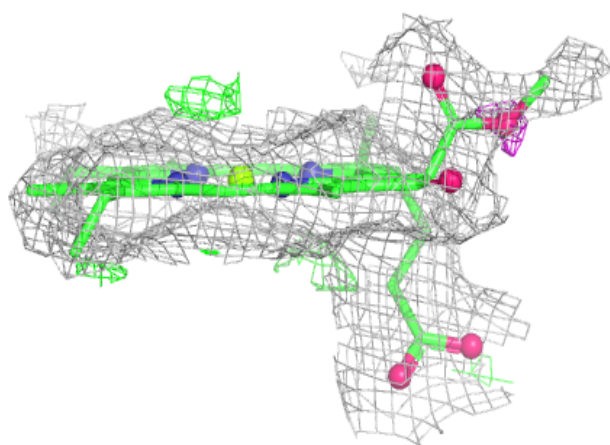
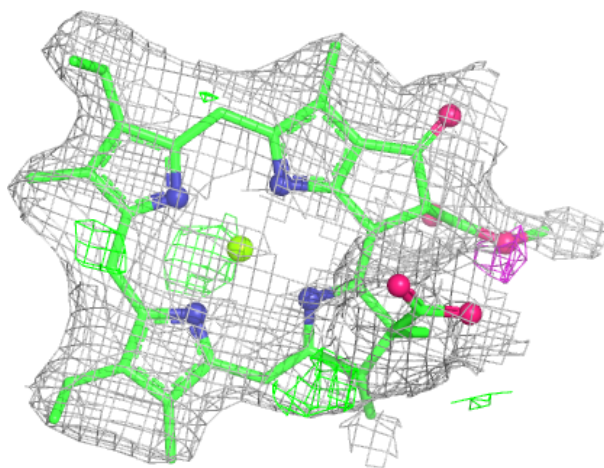
Electron density around CLA A 823:

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



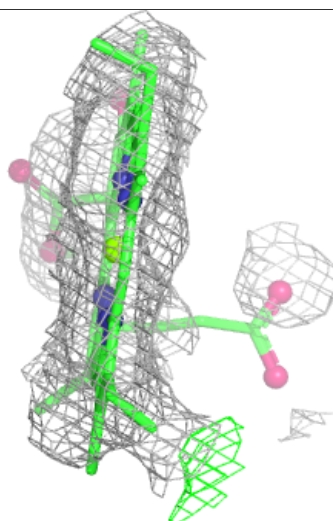
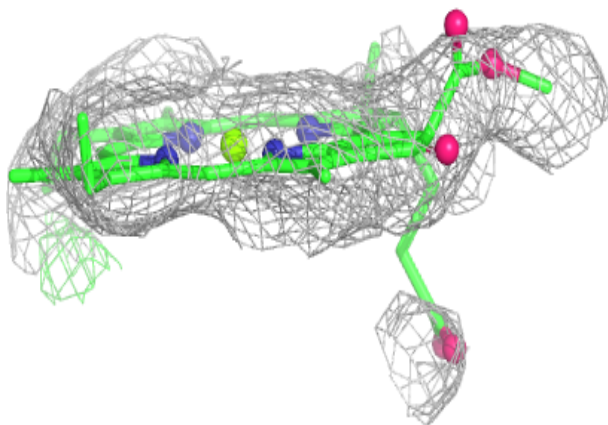
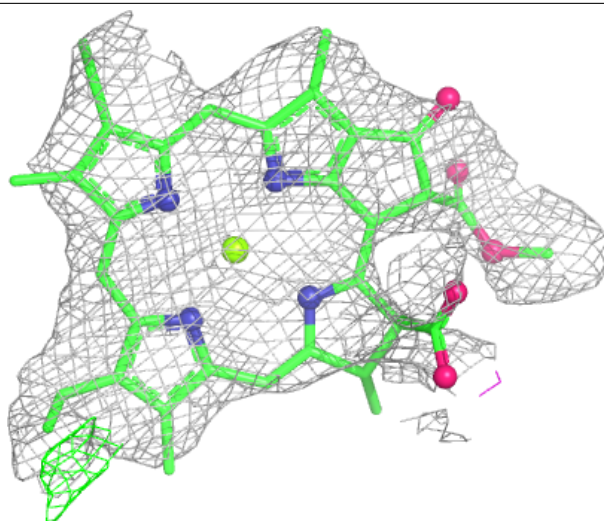
Electron density around CLA H 812:

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



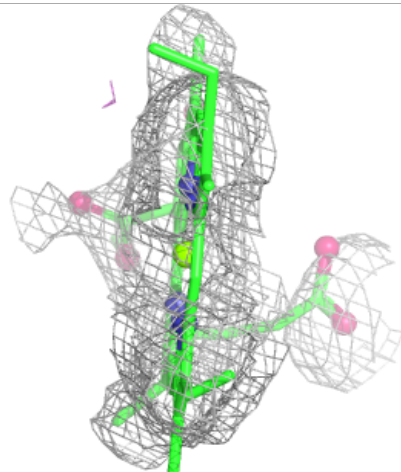
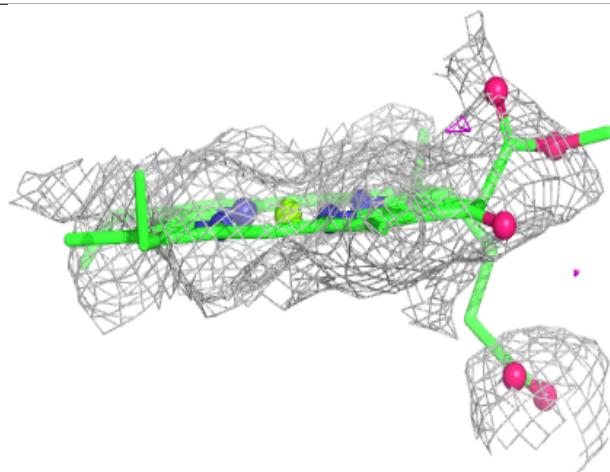
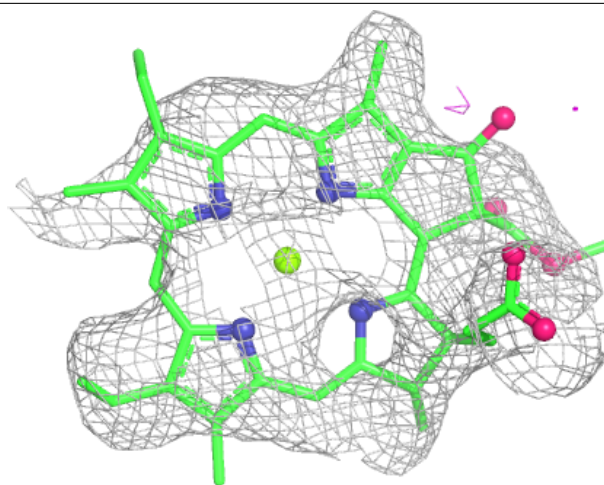
Electron density around CLA J 101:

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



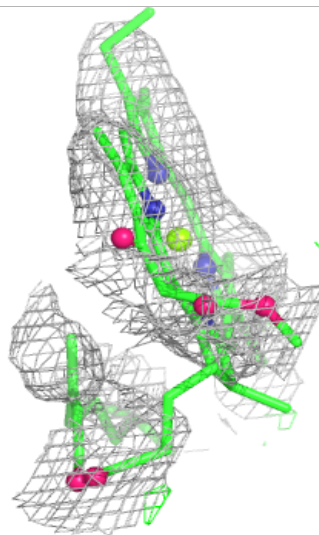
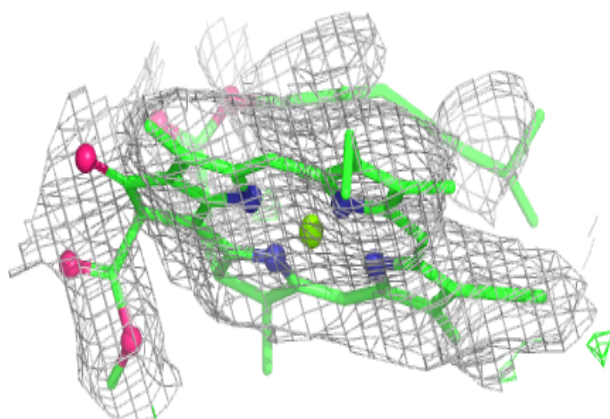
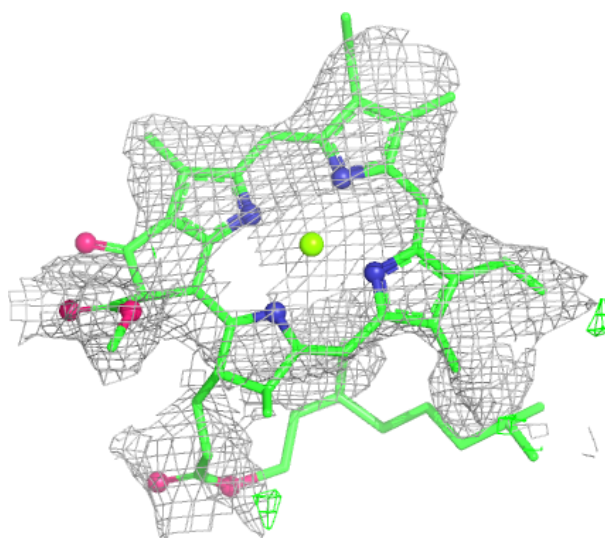
Electron density around CLA S 1102:

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



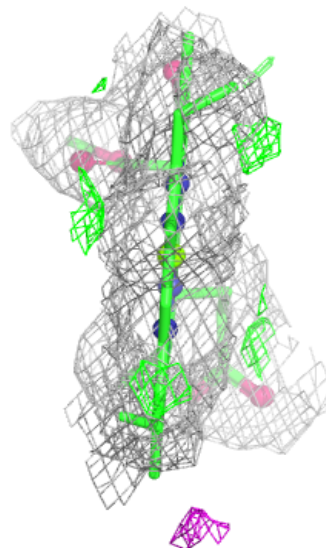
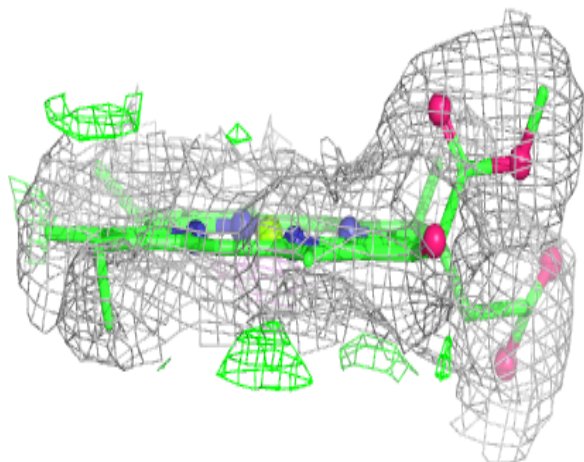
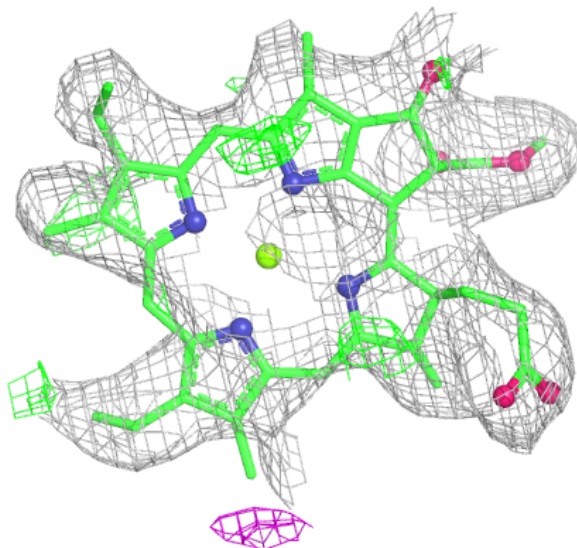
Electron density around CLA S 1103:

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



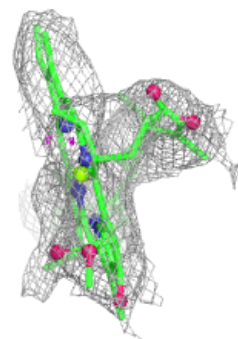
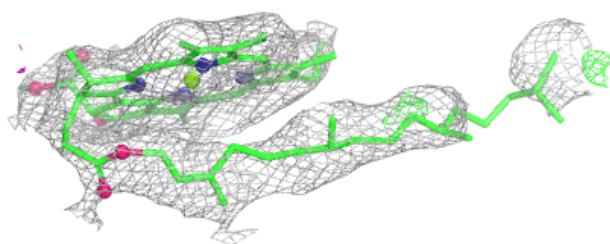
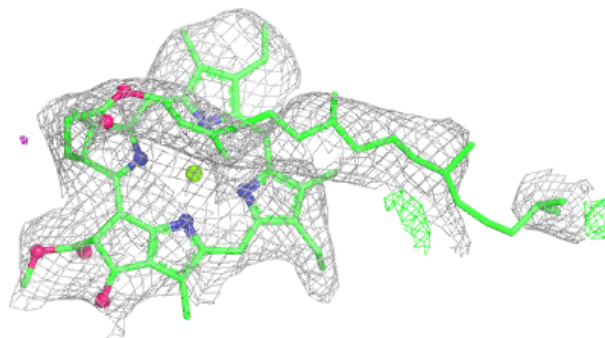
Electron density around CLA W 1701:

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



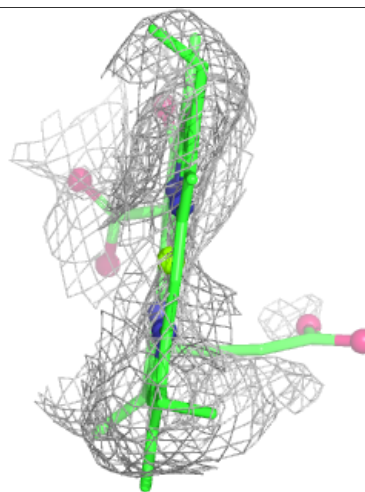
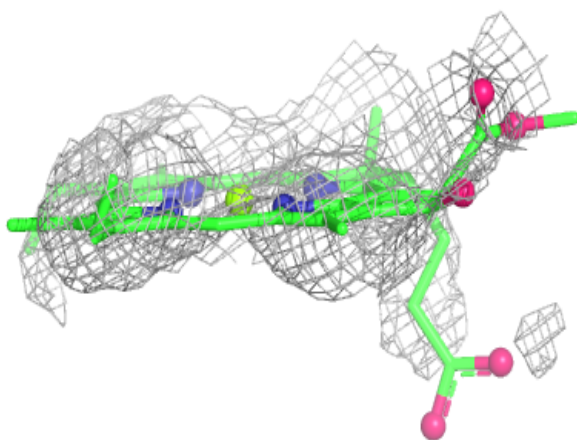
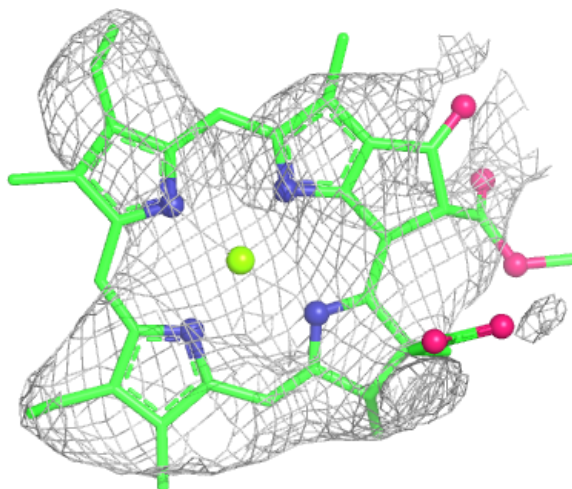
Electron density around CLA Y 818:

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



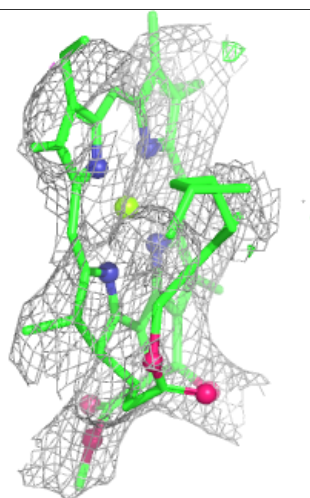
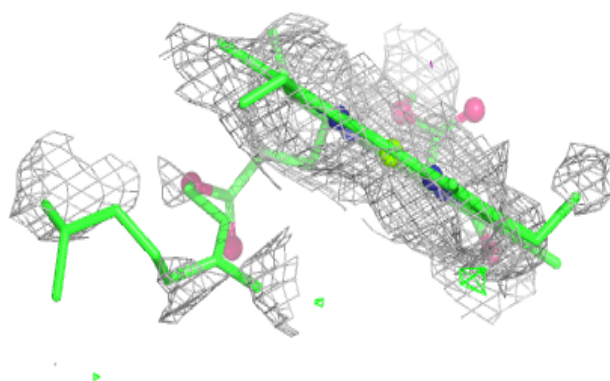
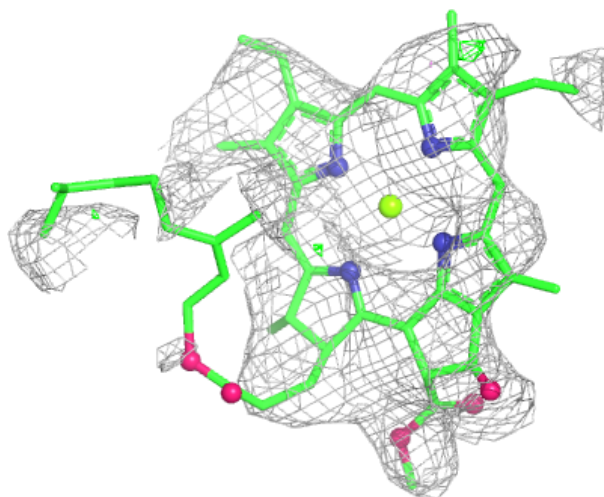
Electron density around CLA f 101:

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



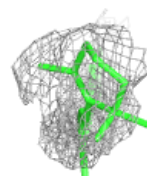
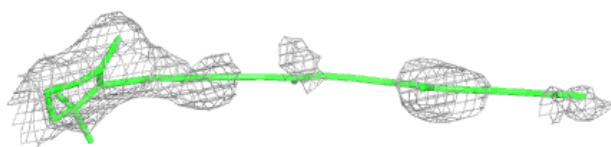
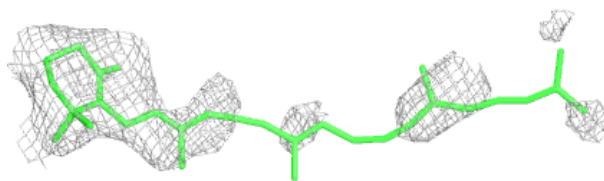
Electron density around CLA f 102:

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and green (positive)

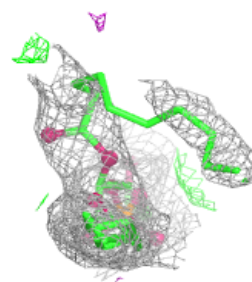
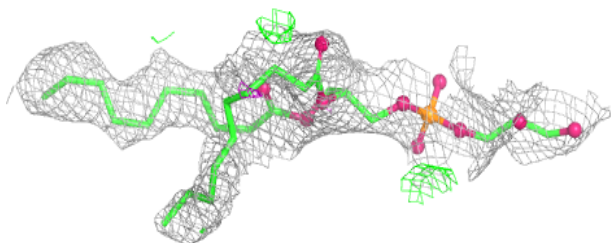
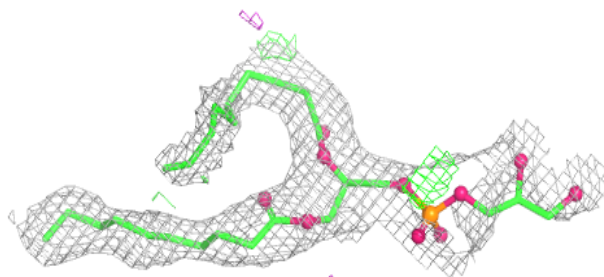


Electron density around BCR B 842:

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

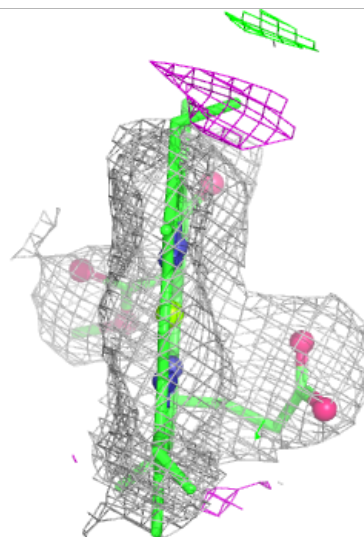
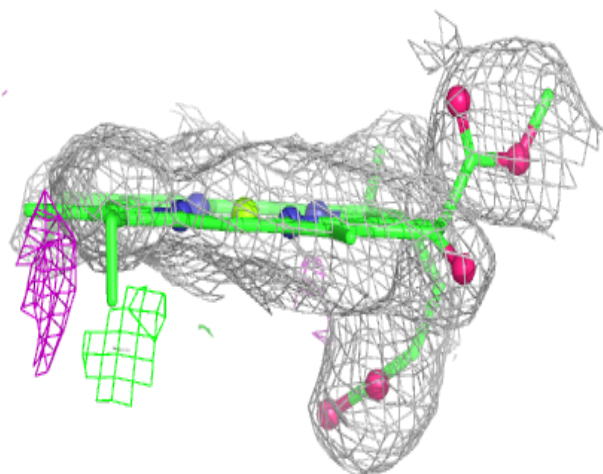
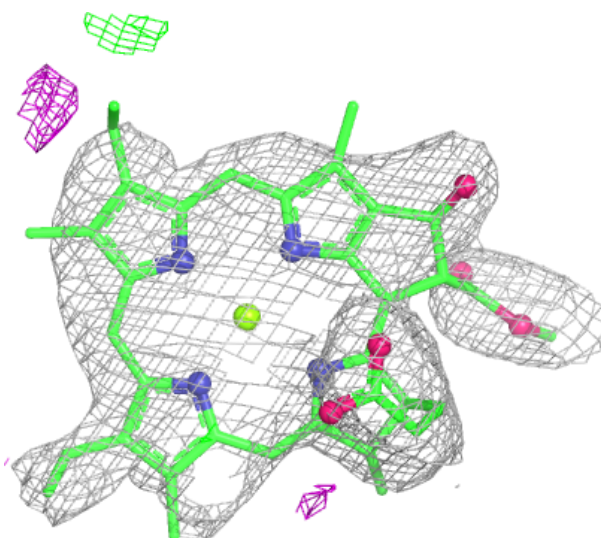
**Electron density around LHG H 849:**

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



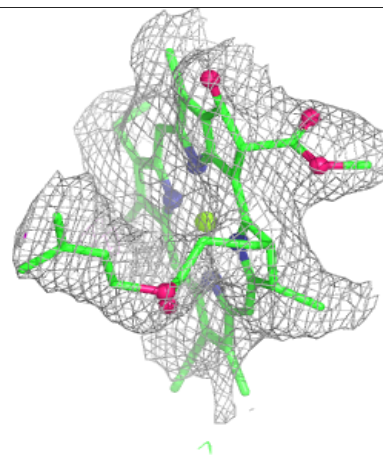
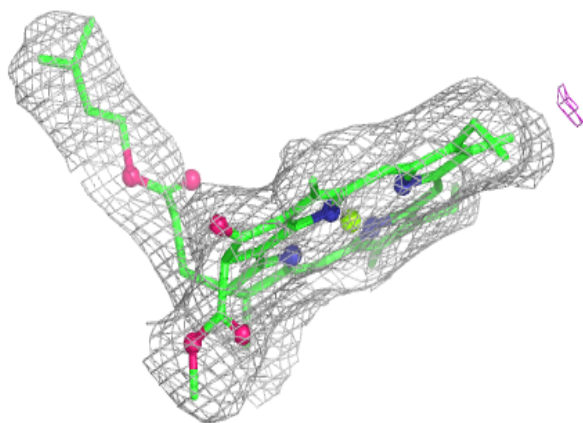
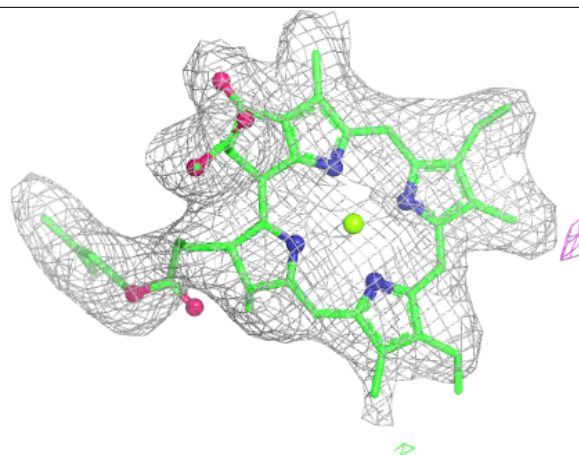
Electron density around CLA A 835:

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and green (positive)



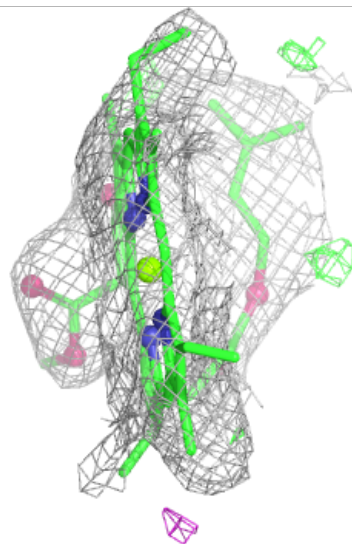
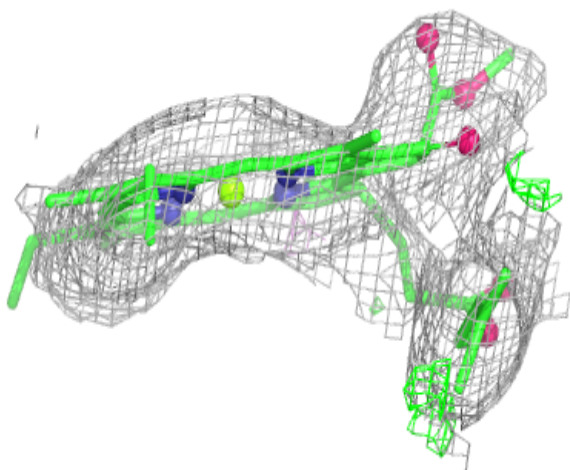
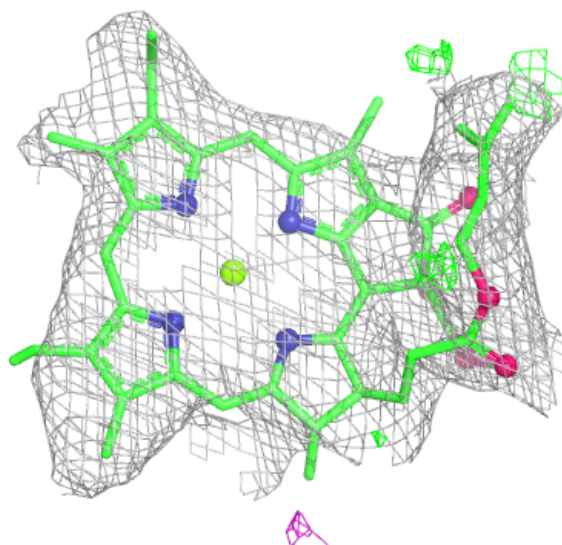
Electron density around CLA A 838:

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



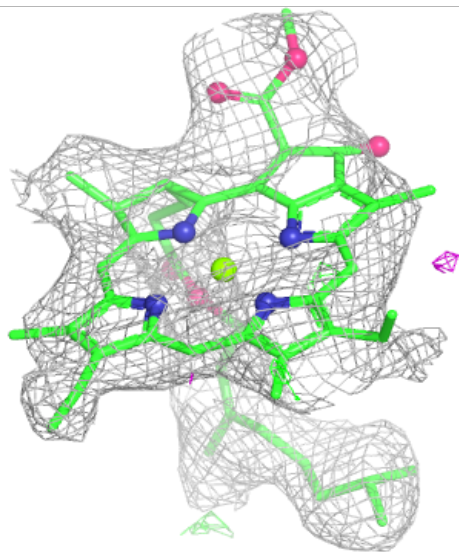
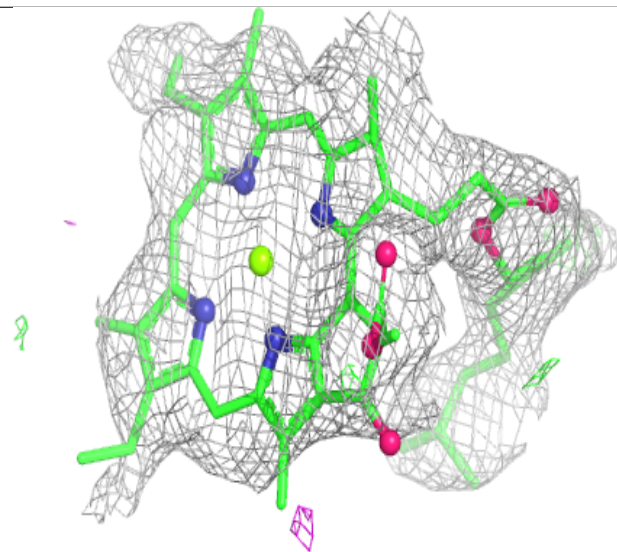
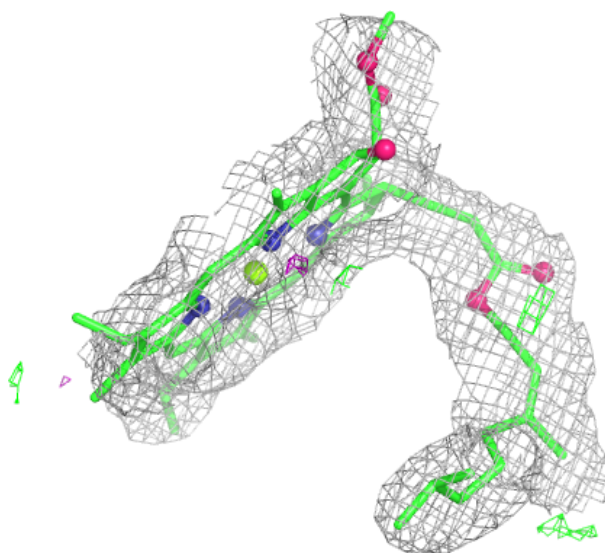
Electron density around CLA A 843:

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



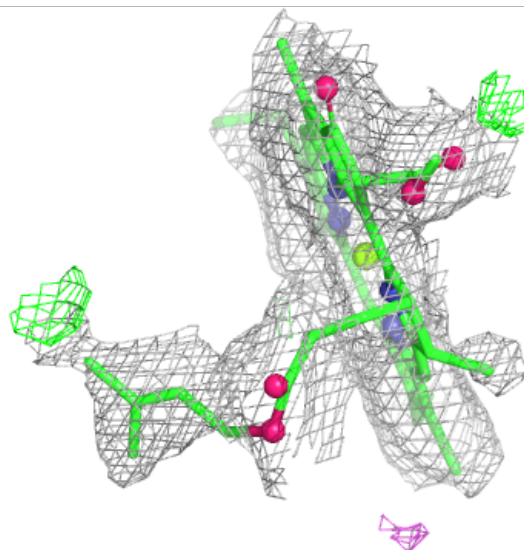
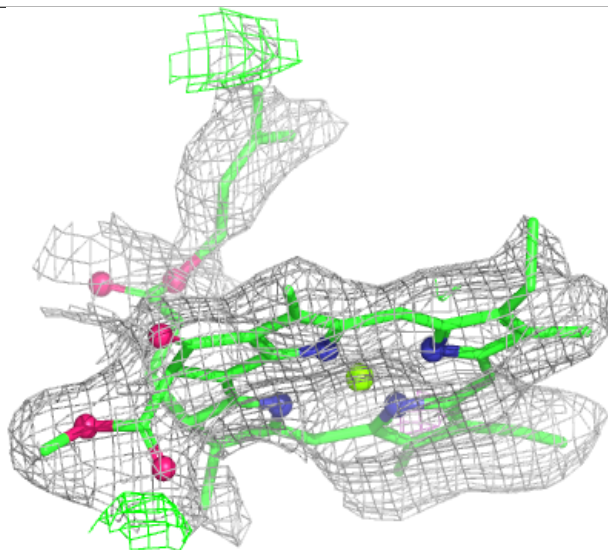
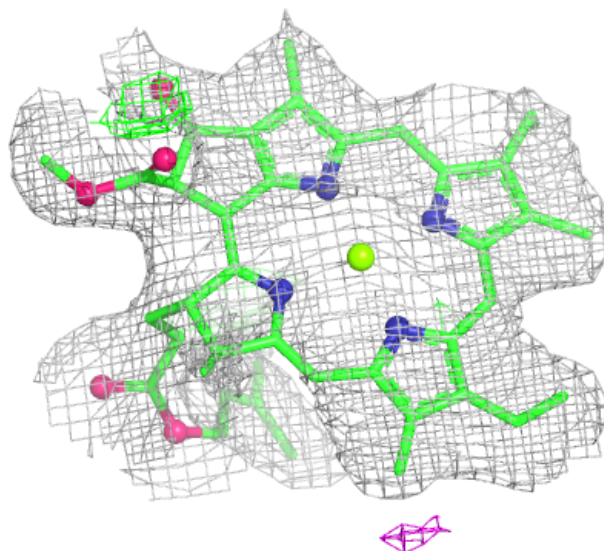
Electron density around CLA B 810:

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



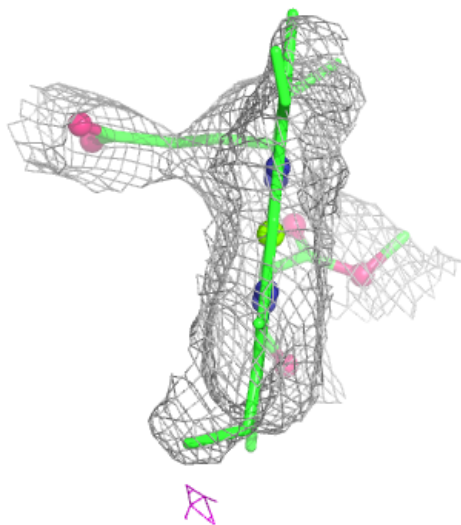
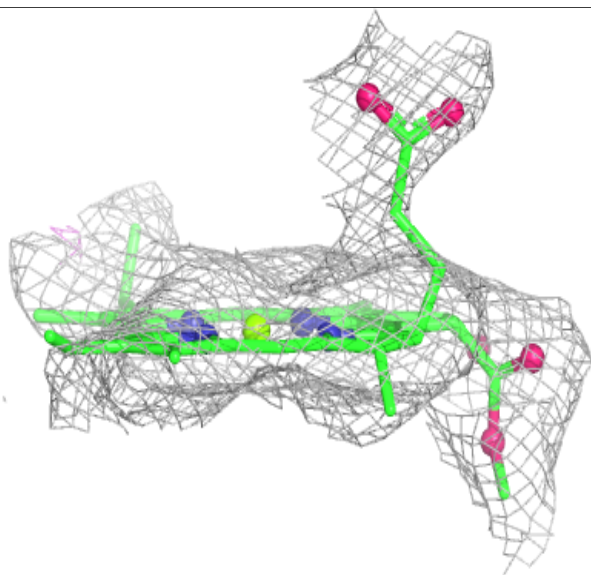
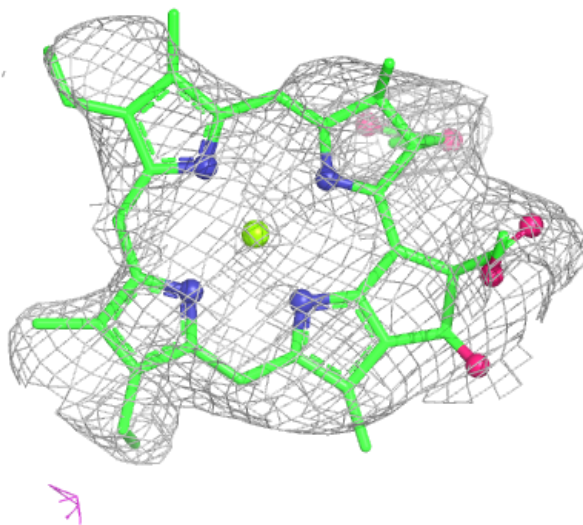
Electron density around CLA B 811:

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and green (positive)



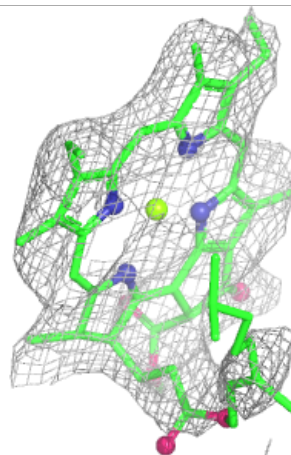
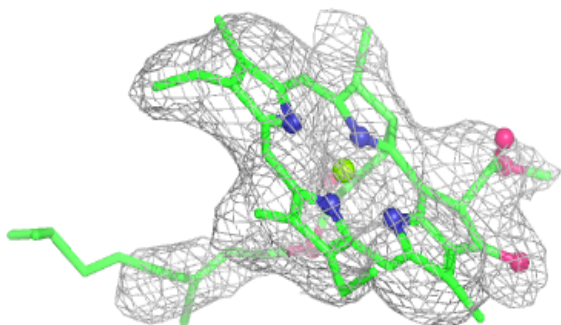
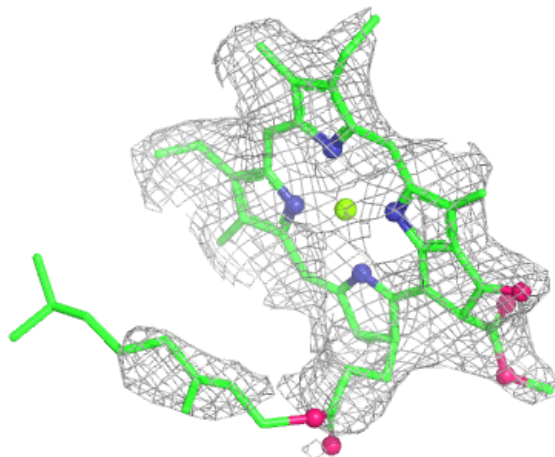
Electron density around CLA B 814:

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



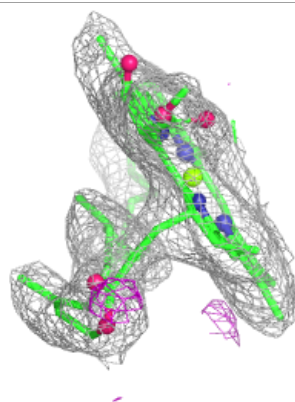
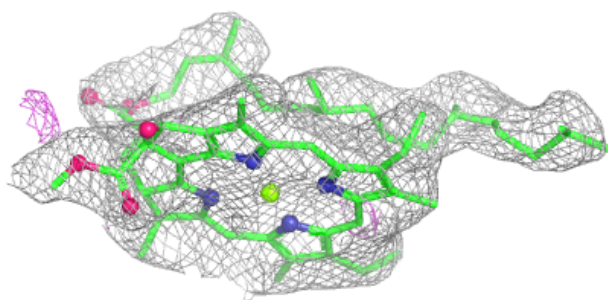
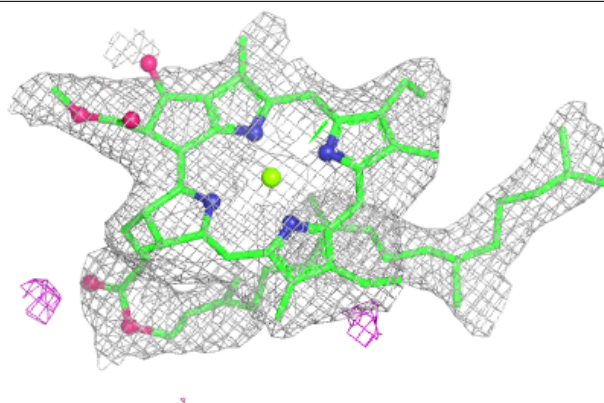
Electron density around CLA B 815:

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



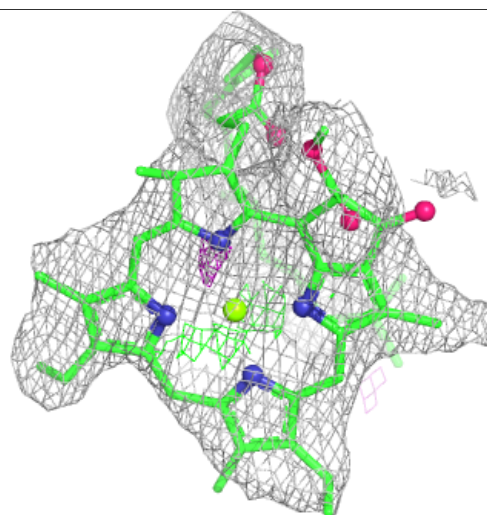
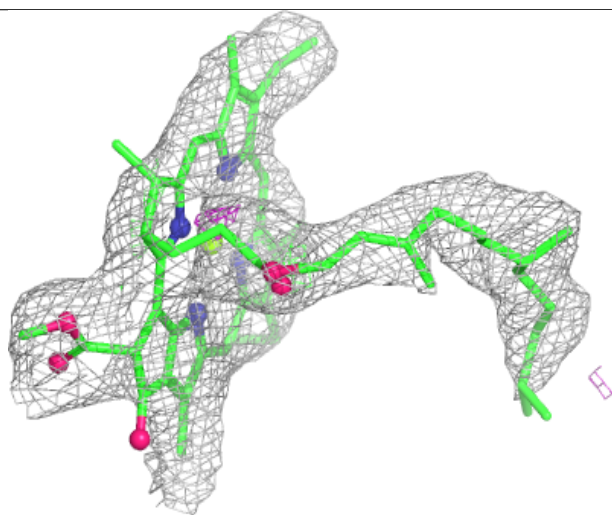
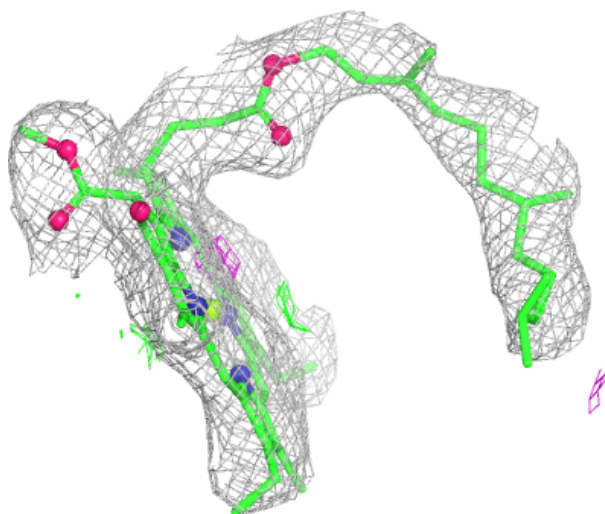
Electron density around CLA B 816:

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



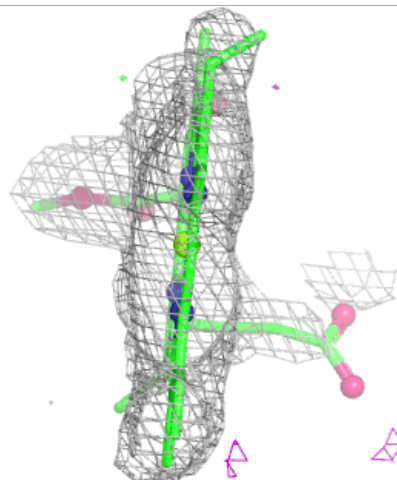
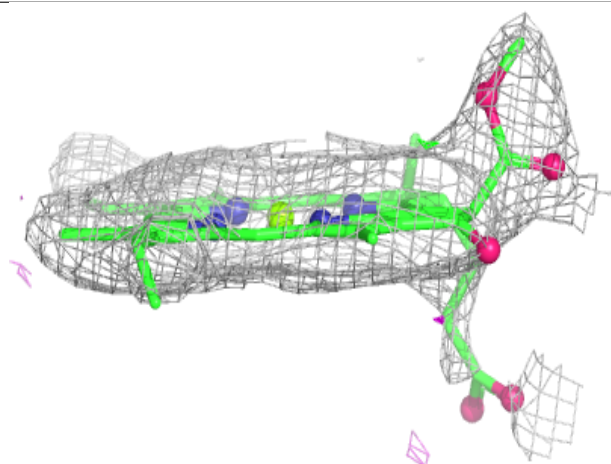
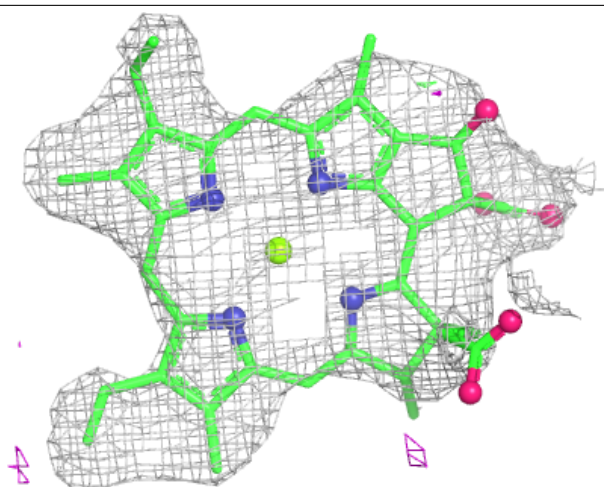
Electron density around CLA B 818:

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



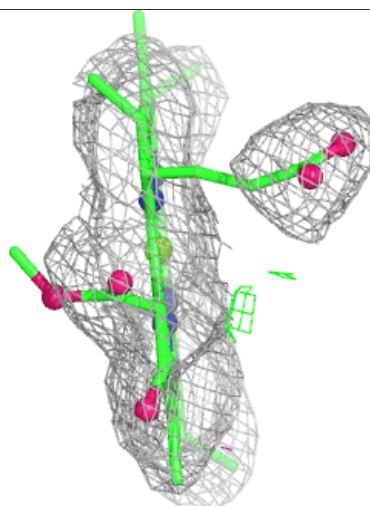
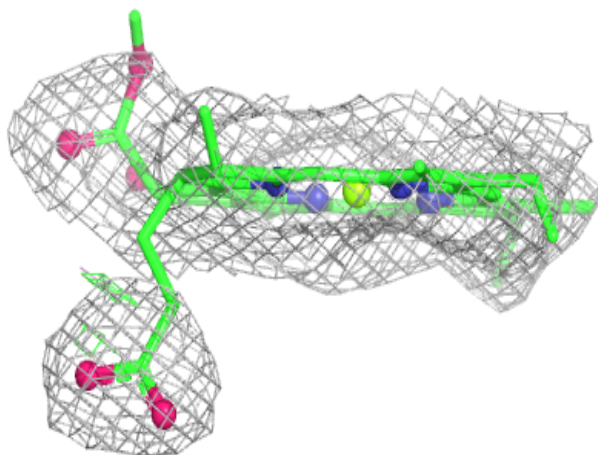
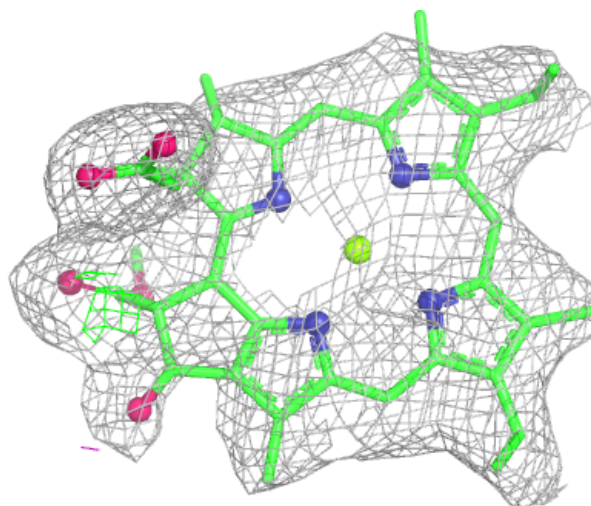
Electron density around CLA B 819:

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



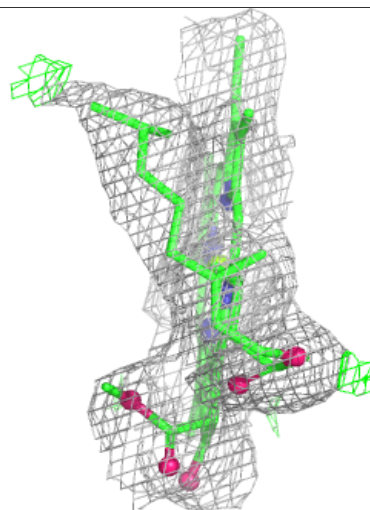
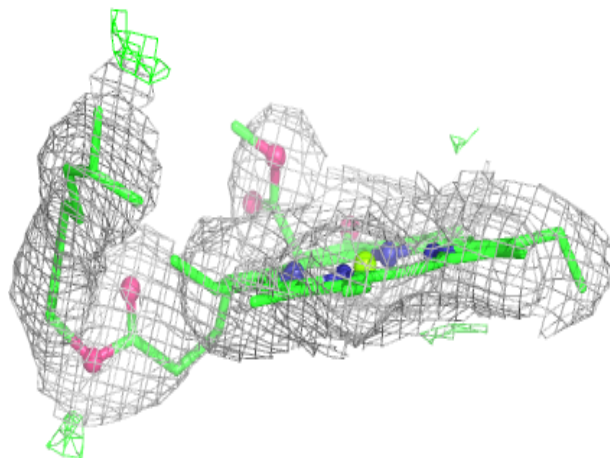
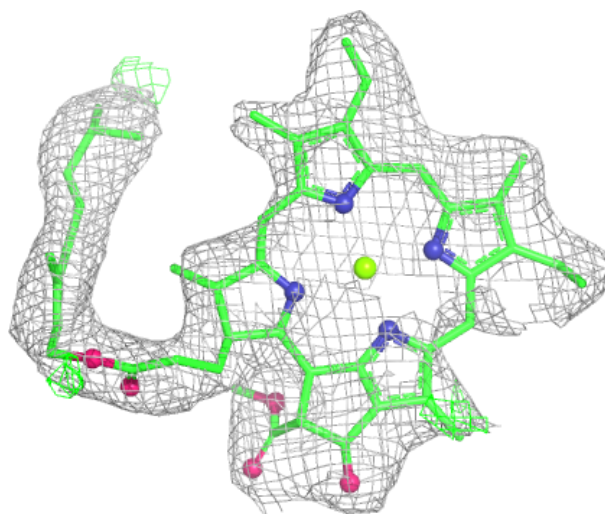
Electron density around CLA B 820:

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



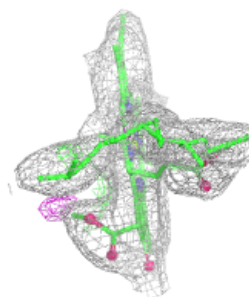
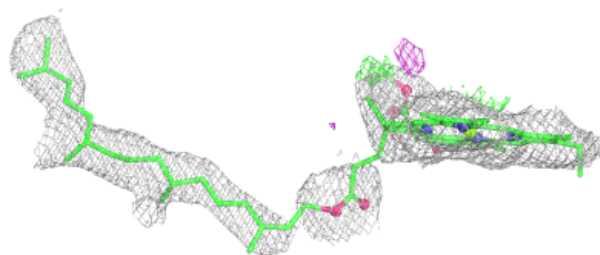
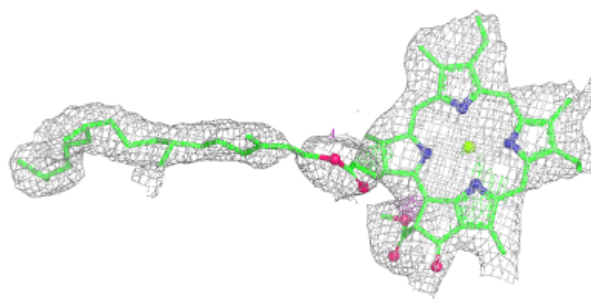
Electron density around CLA B 823:

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

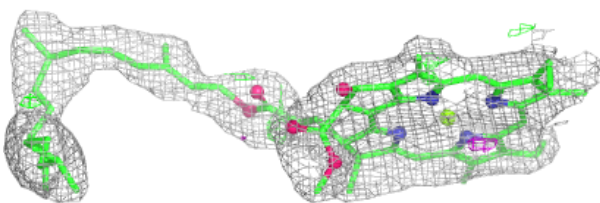
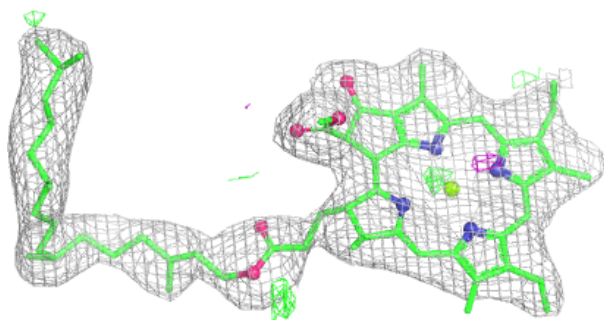


Electron density around CLA B 824:

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

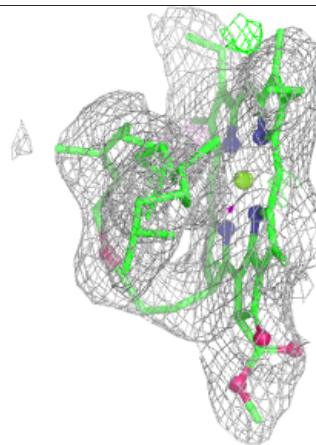
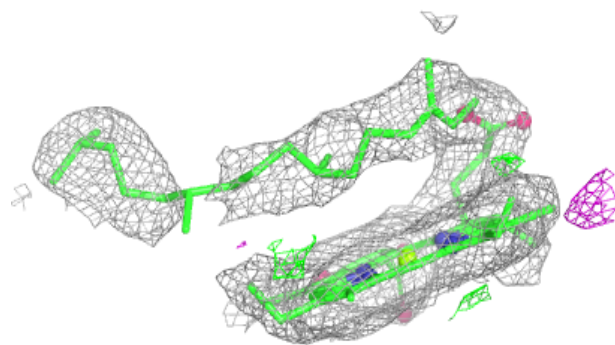
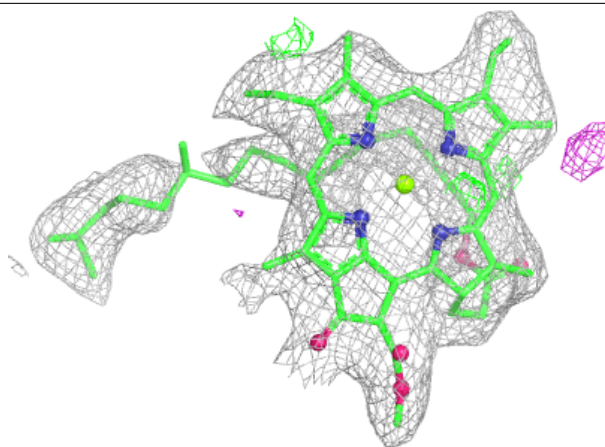
**Electron density around CLA B 825:**

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



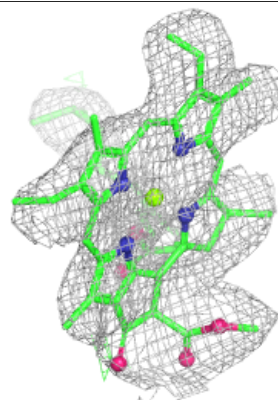
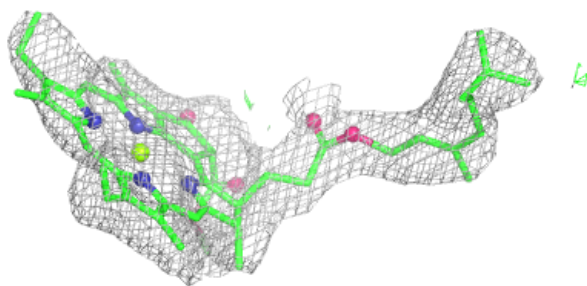
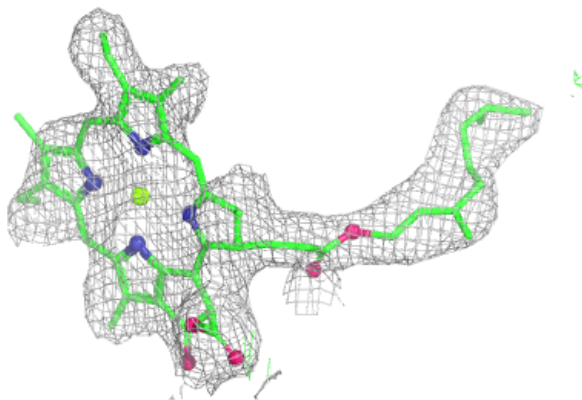
Electron density around CLA B 826:

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



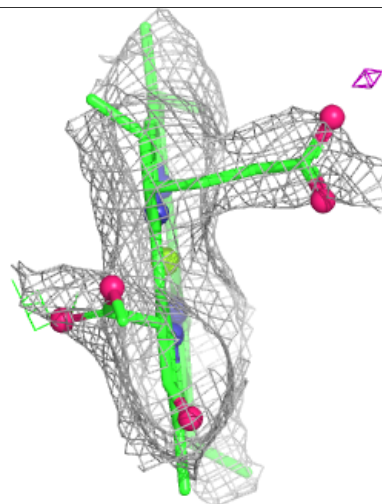
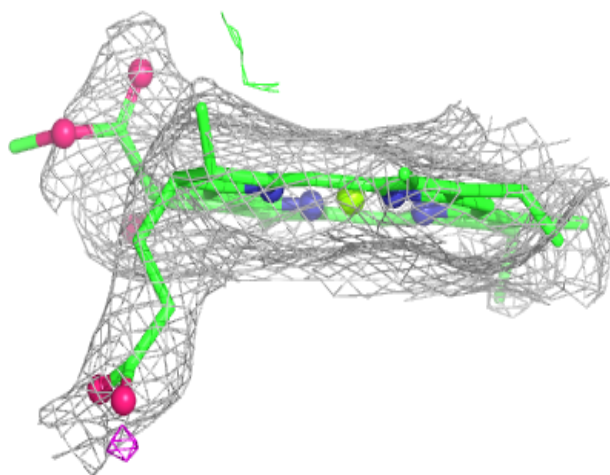
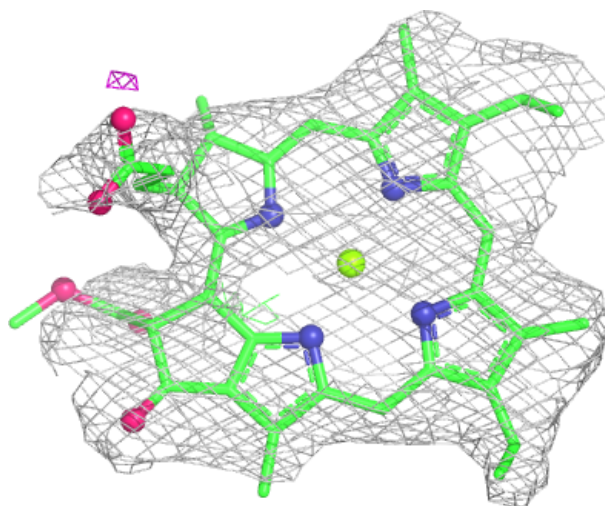
Electron density around CLA B 832:

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



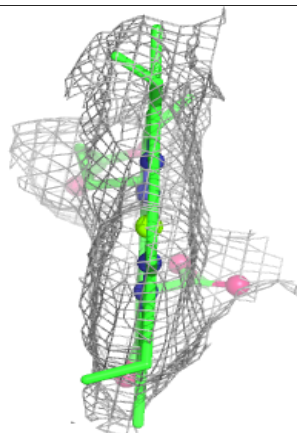
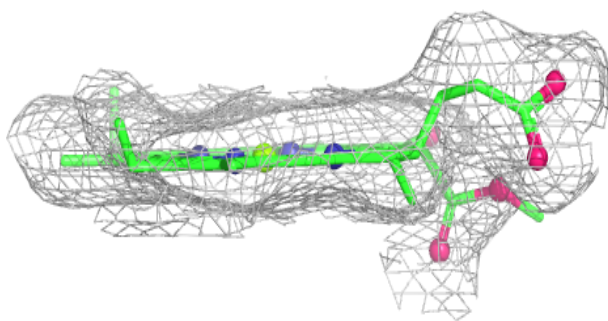
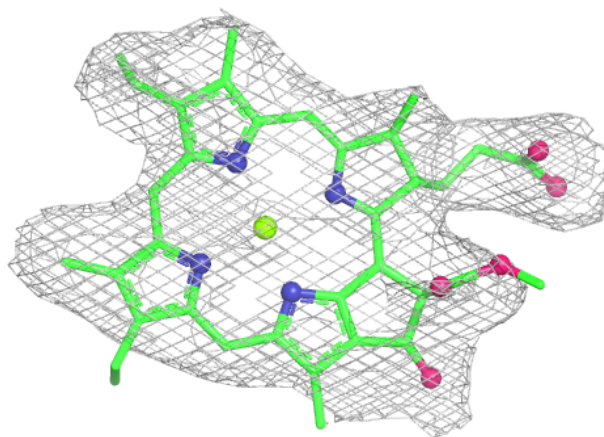
Electron density around CLA B 834:

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

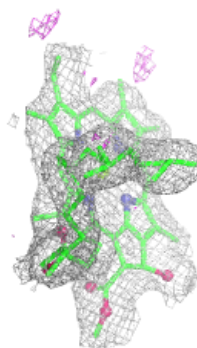
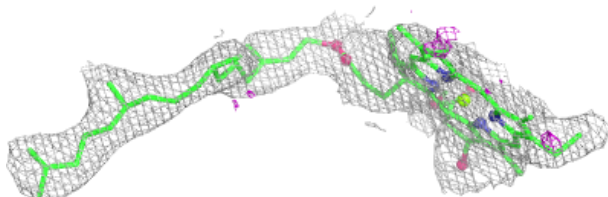
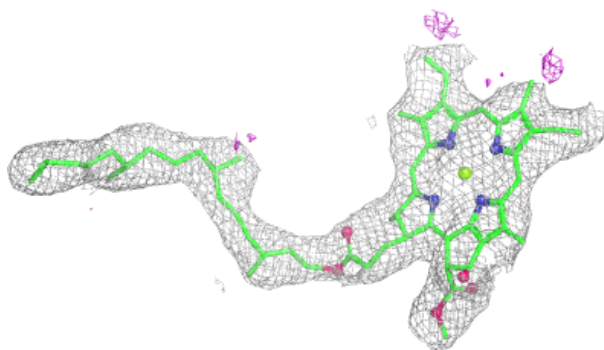


Electron density around CLA B 835:

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

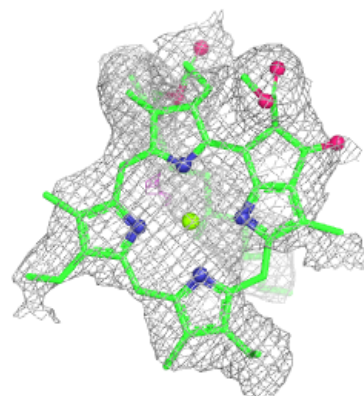
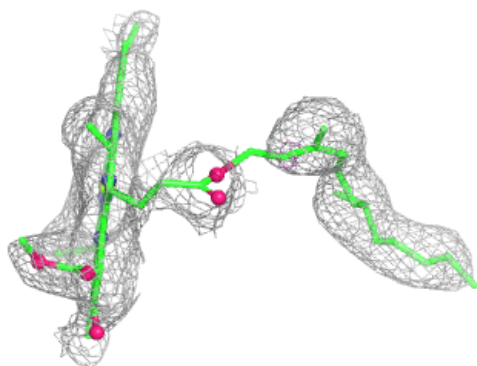
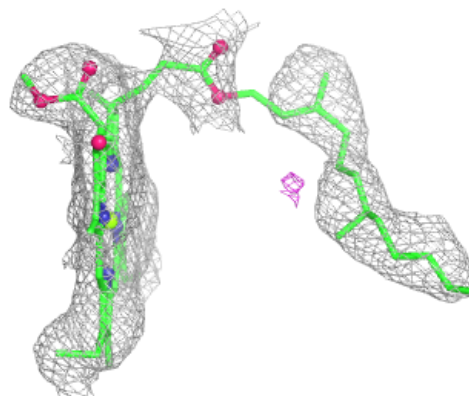
**Electron density around CLA G 803:**

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

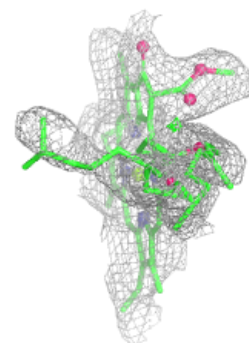
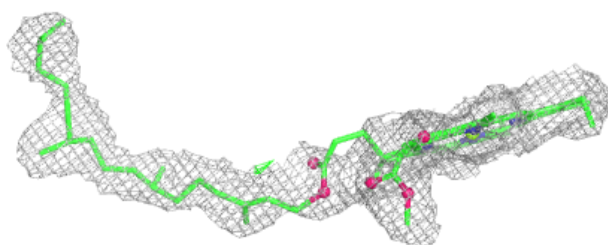
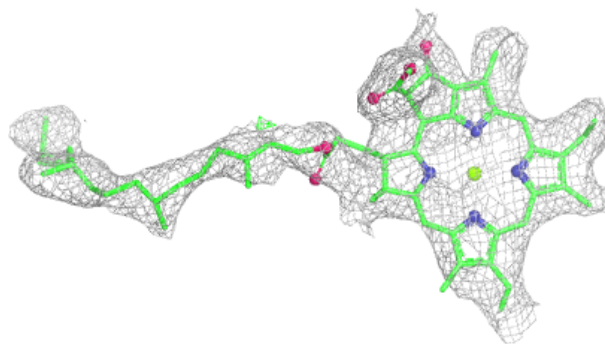


Electron density around CLA G 804:

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

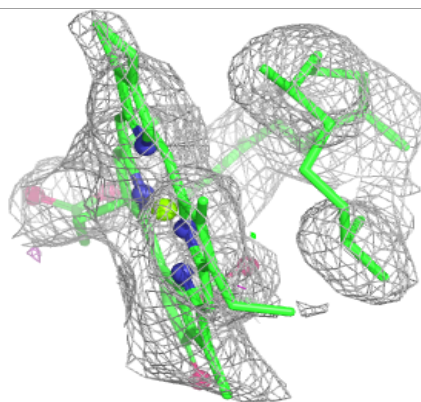
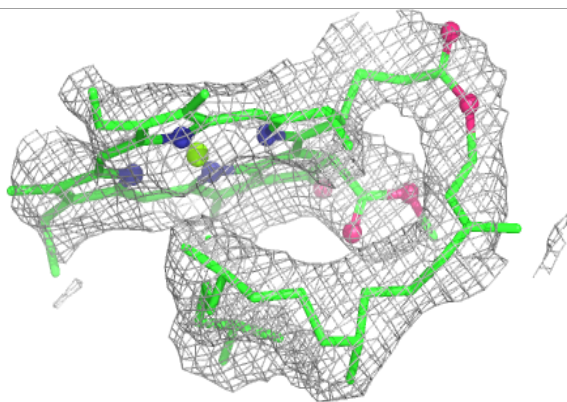
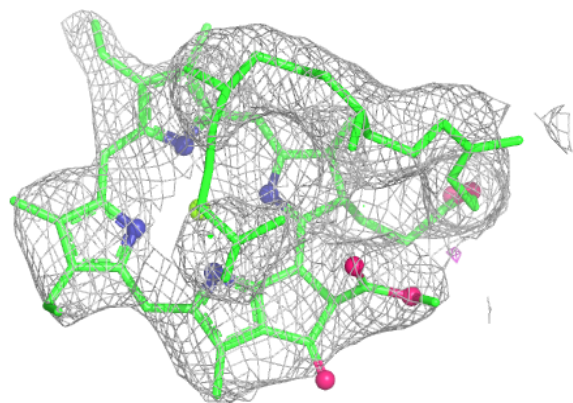
**Electron density around CLA G 805:**

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



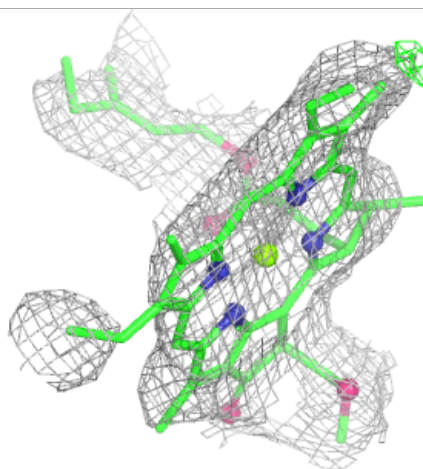
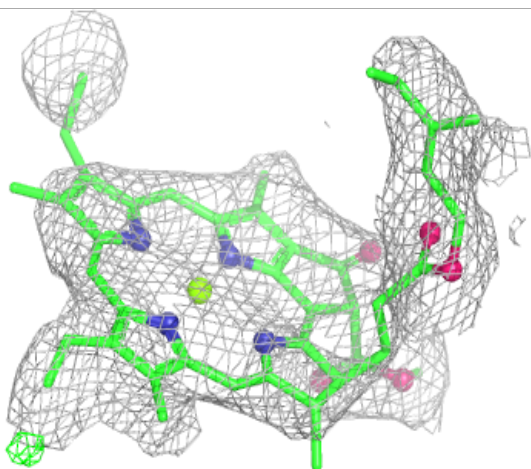
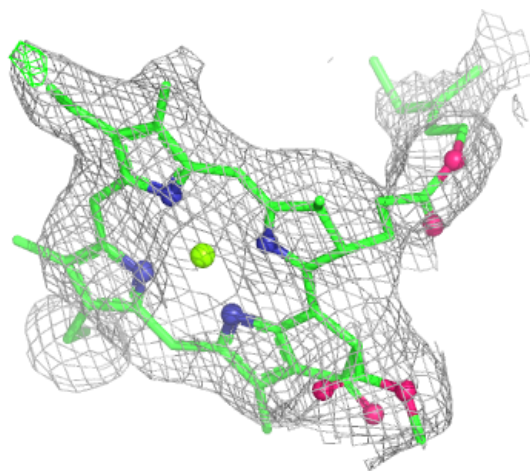
Electron density around CLA G 806:

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



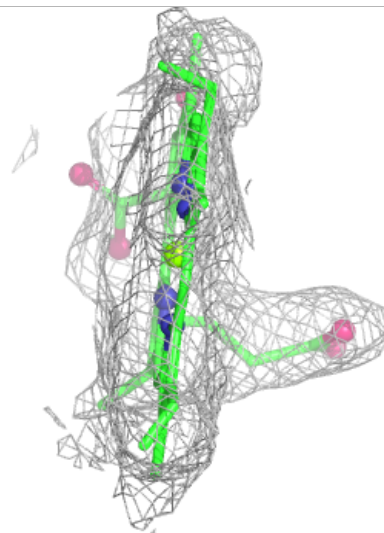
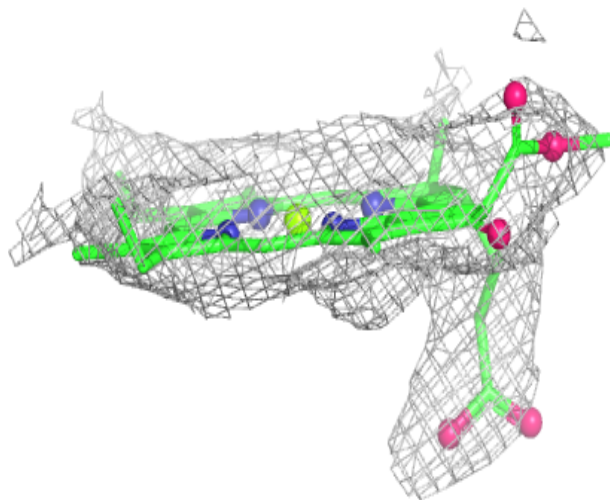
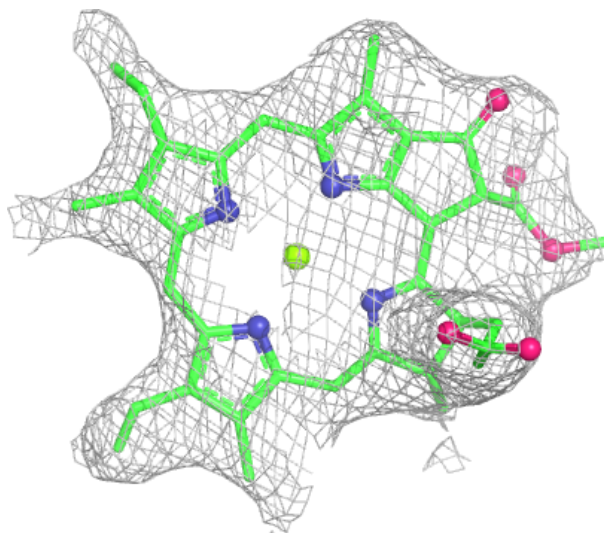
Electron density around CLA G 807:

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



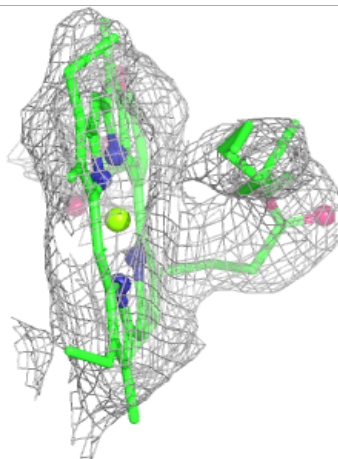
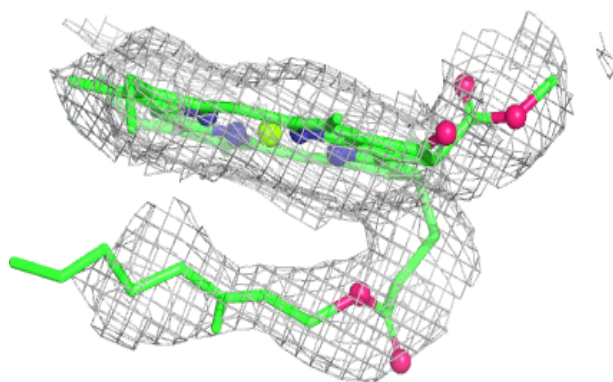
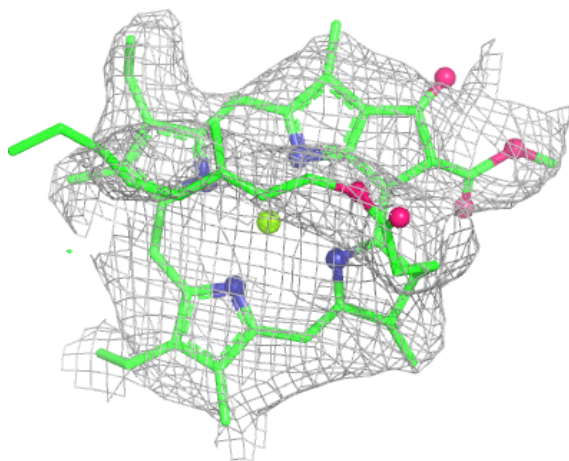
Electron density around CLA G 810:

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



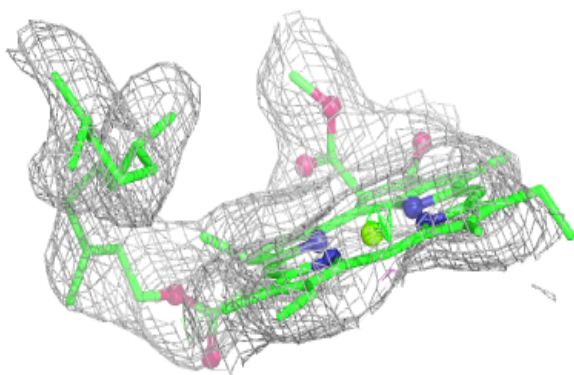
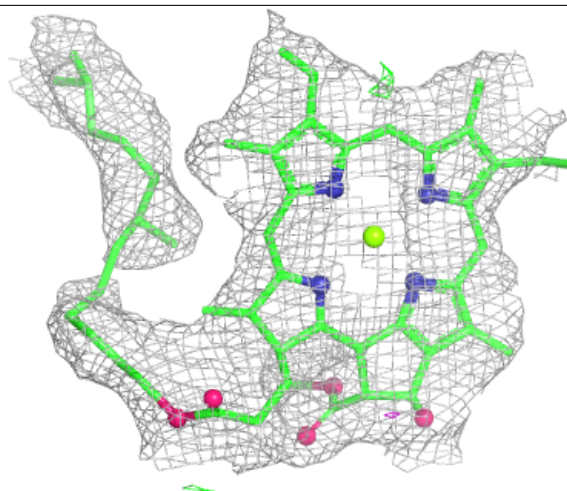
Electron density around CLA G 812:

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



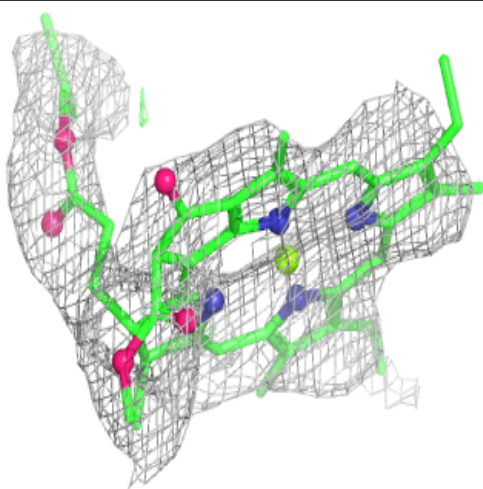
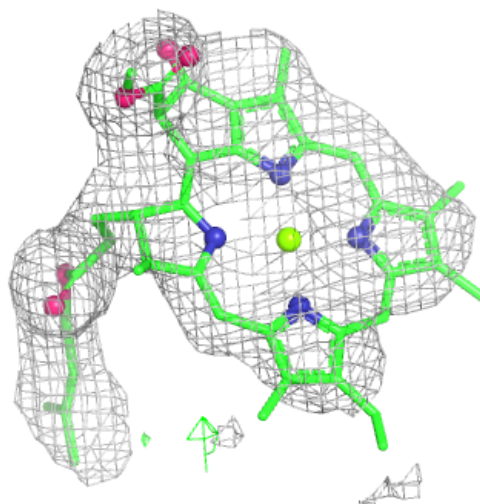
Electron density around CLA G 813:

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



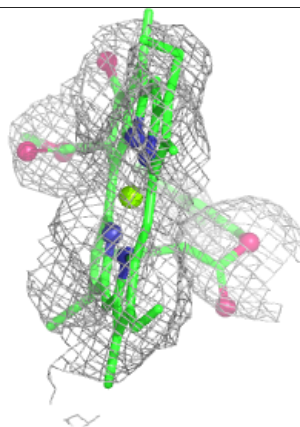
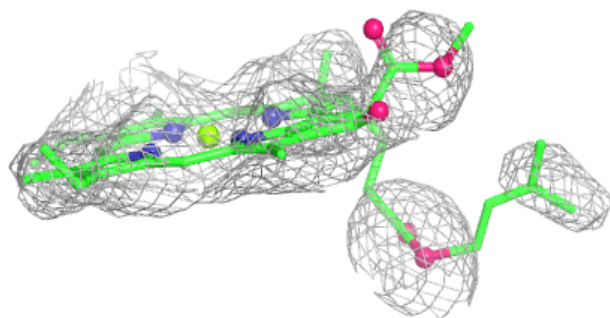
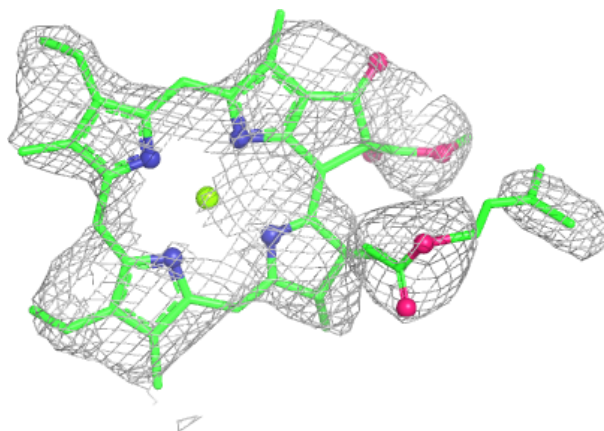
Electron density around CLA G 815:

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

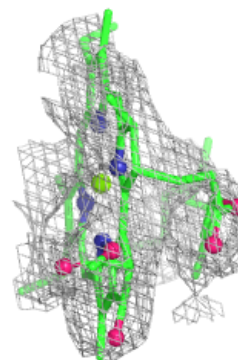
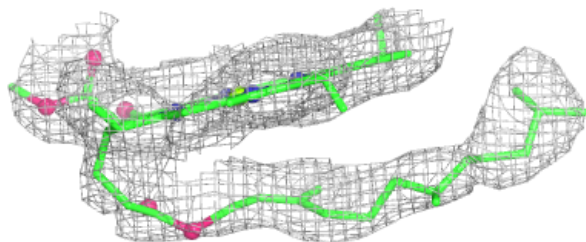
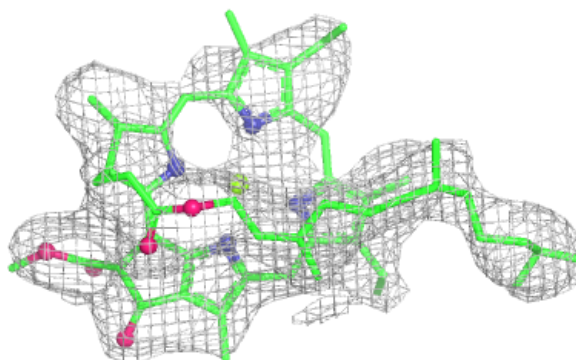


Electron density around CLA G 816:

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

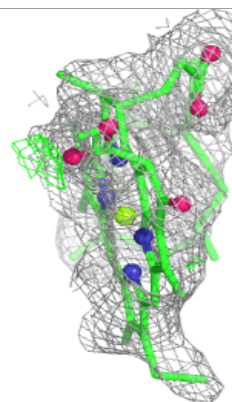
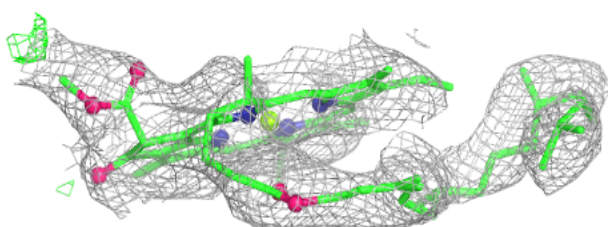
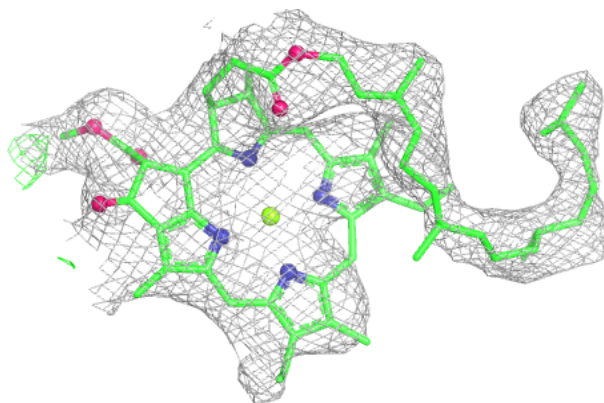
**Electron density around CLA G 817:**

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

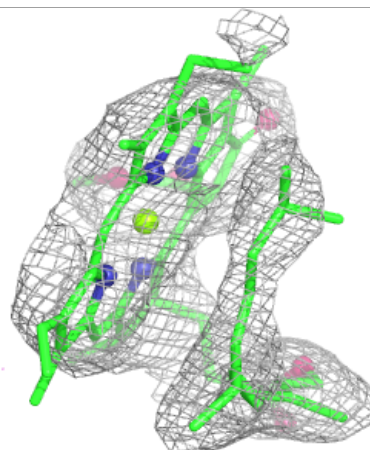
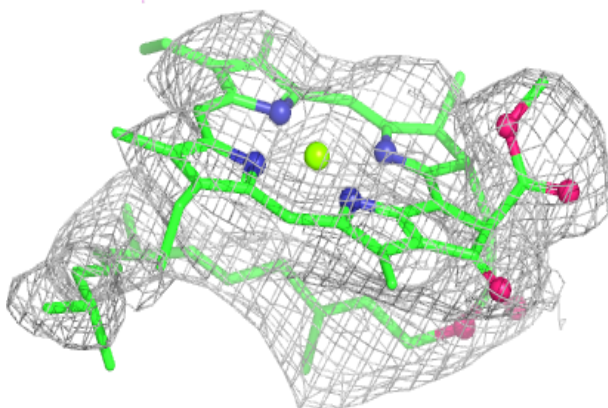
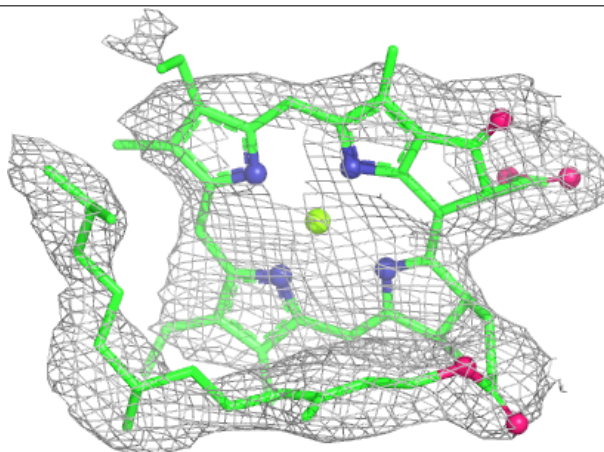


Electron density around CLA G 819:

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

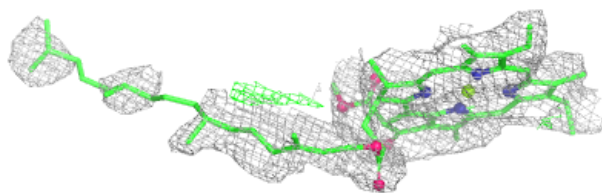
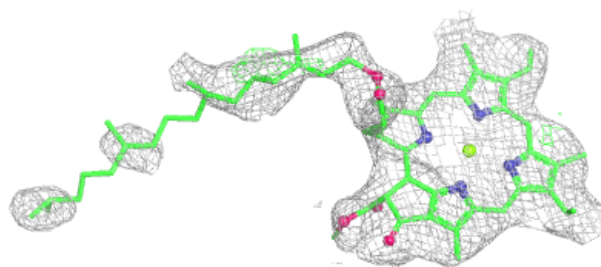
**Electron density around CLA G 820:**

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

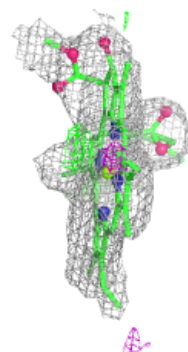
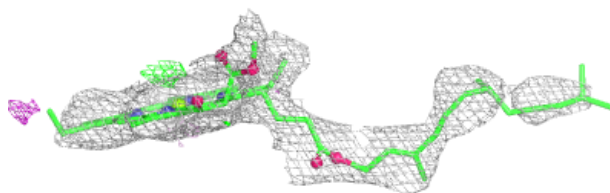
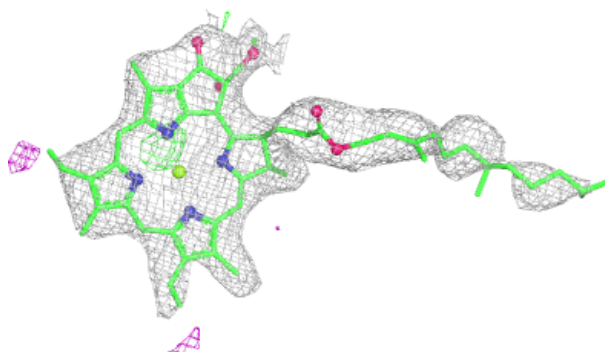


Electron density around CLA G 822:

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

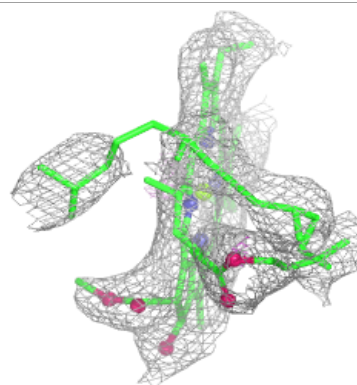
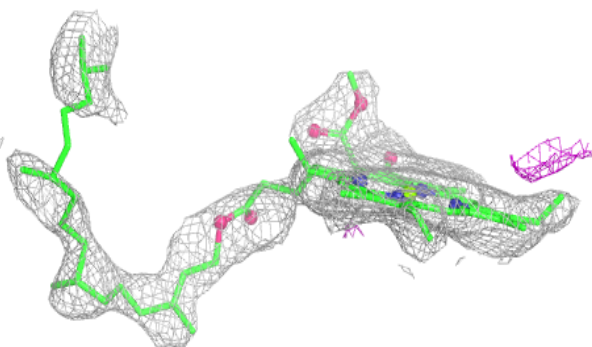
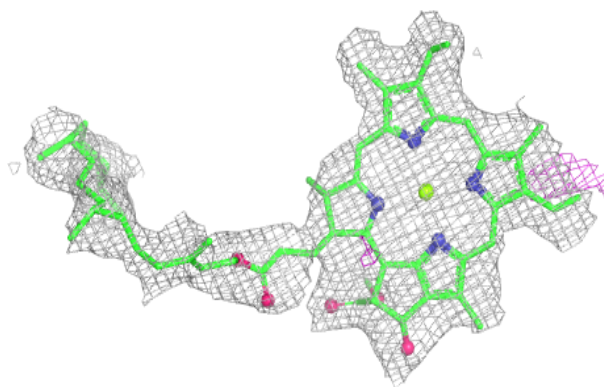
**Electron density around CLA G 826:**

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

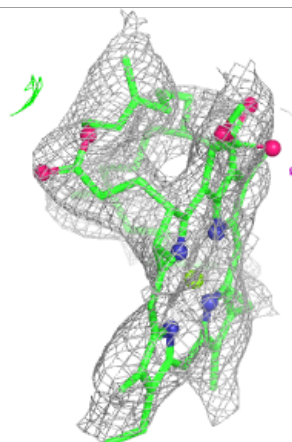
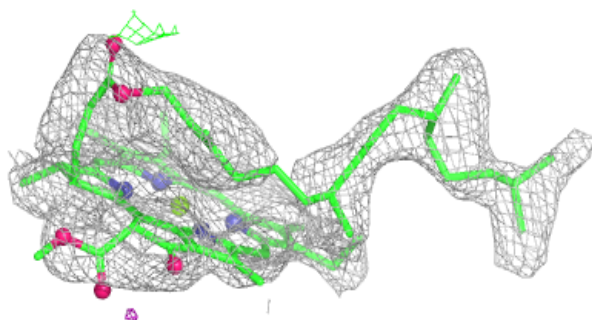
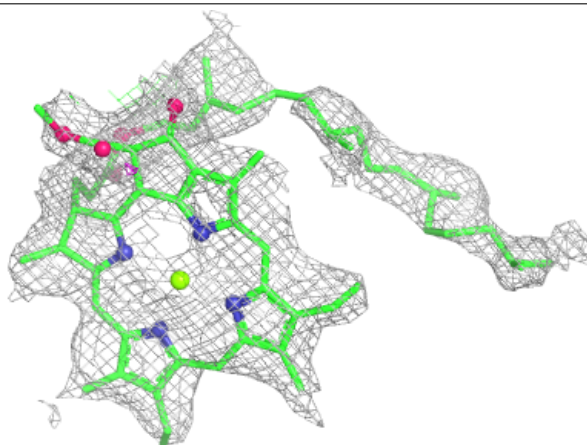


Electron density around CLA G 827:

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

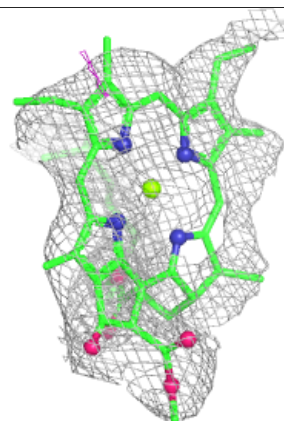
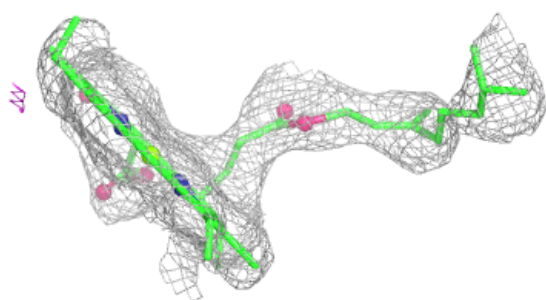
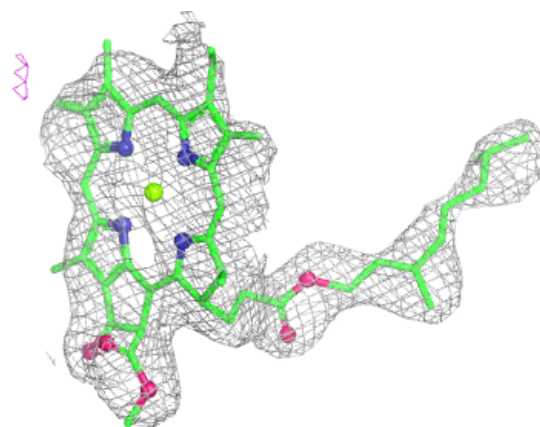
**Electron density around CLA G 829:**

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



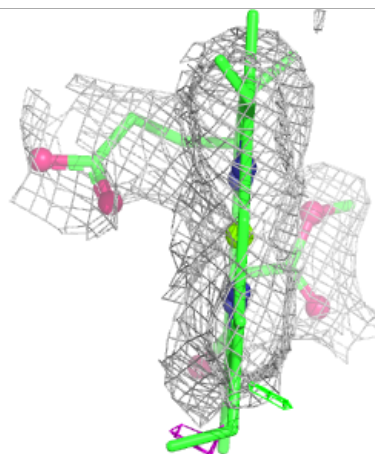
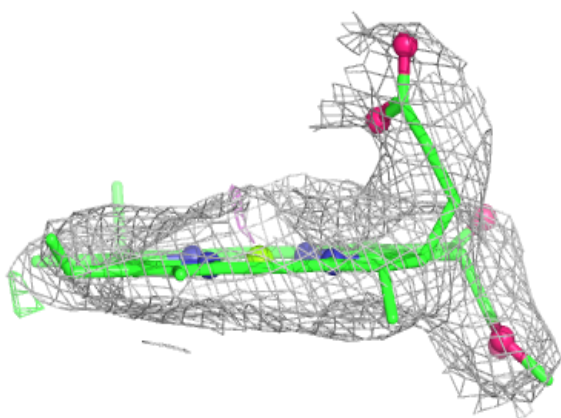
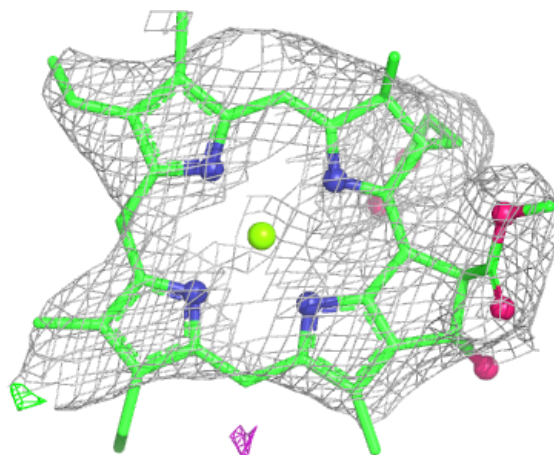
Electron density around CLA G 834:

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



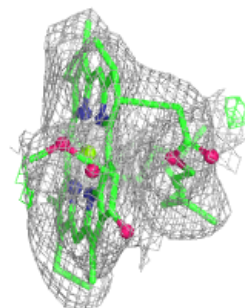
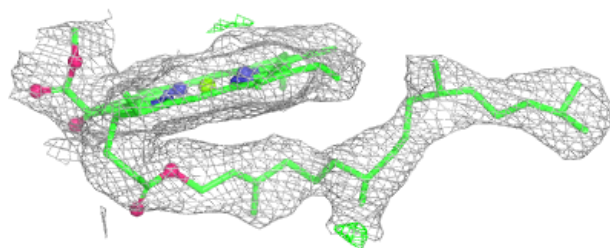
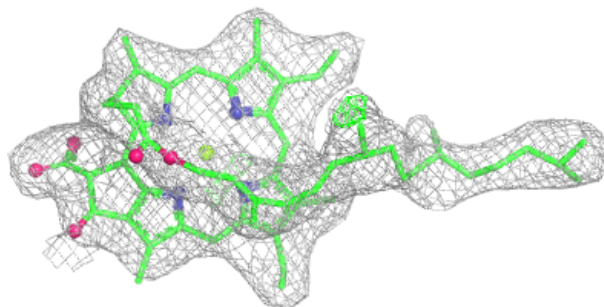
Electron density around CLA G 835:

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

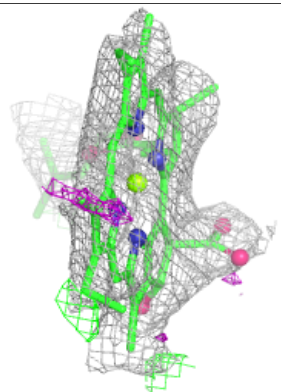
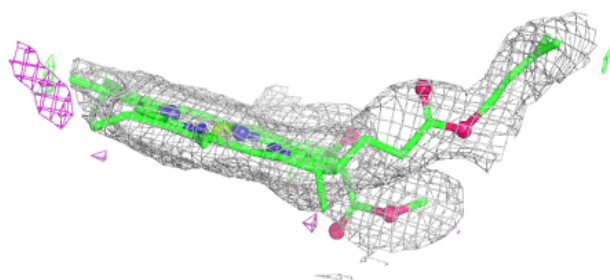
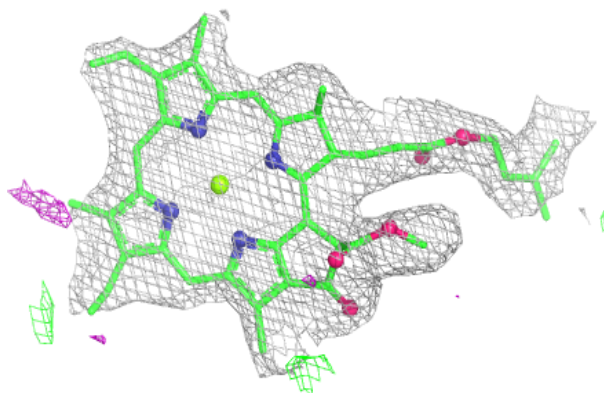


Electron density around CLA G 837:

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

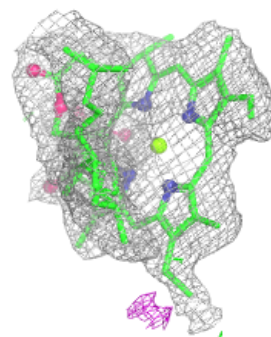
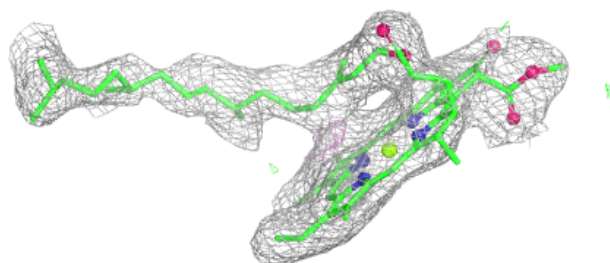
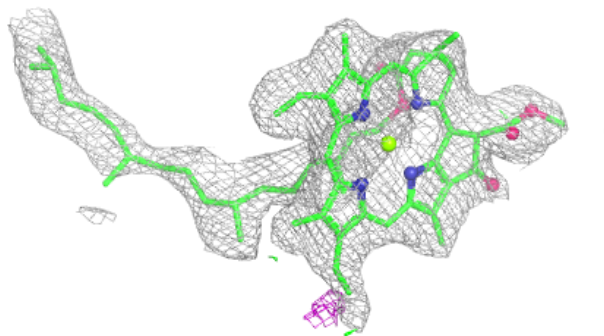
**Electron density around CLA G 839:**

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



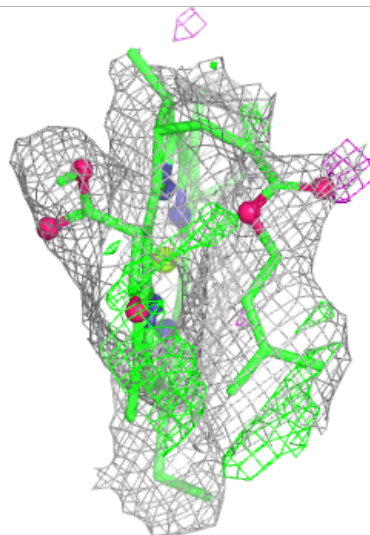
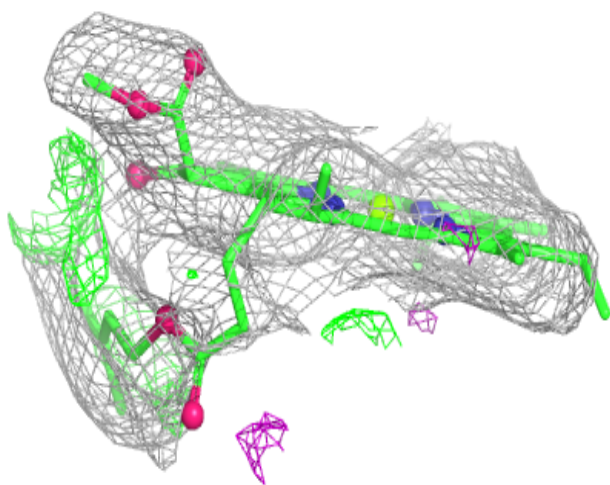
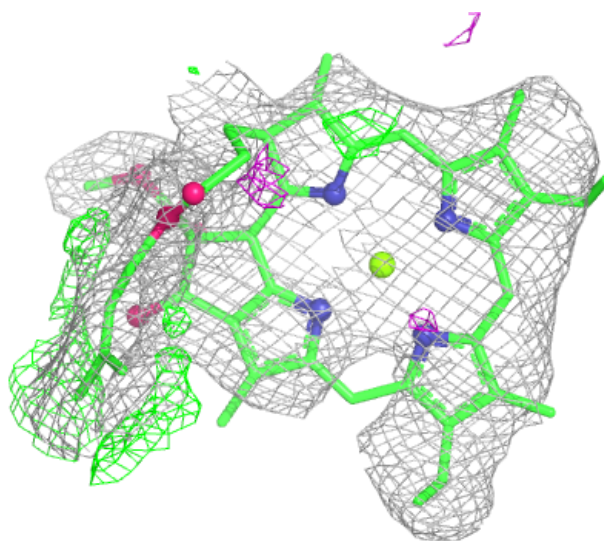
Electron density around CLA G 840:

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



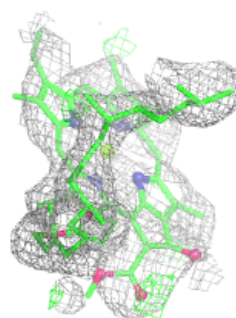
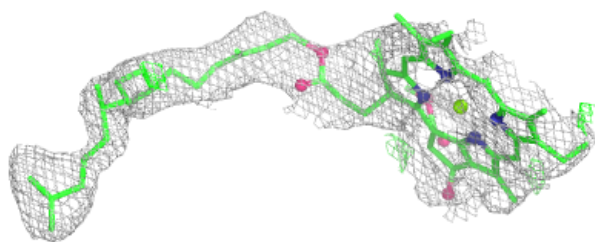
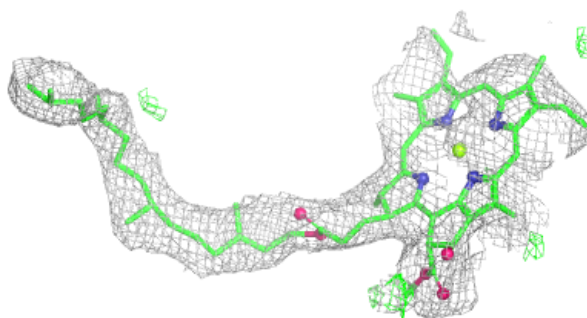
Electron density around CLA G 842:

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



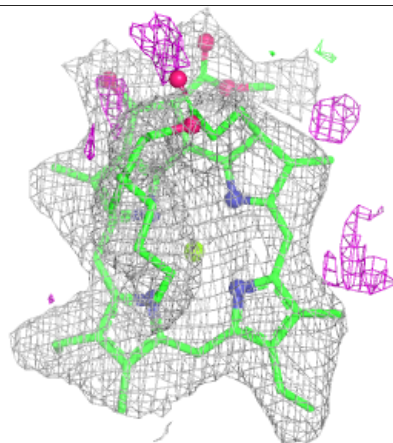
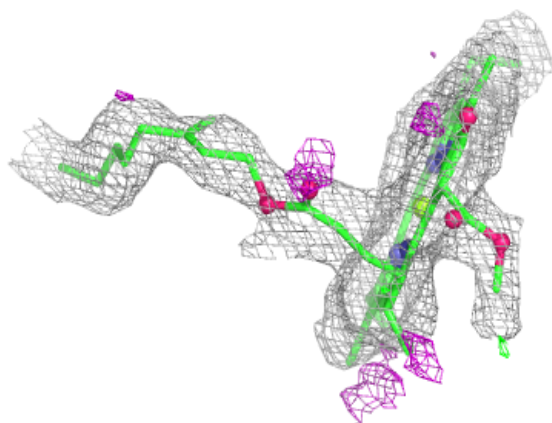
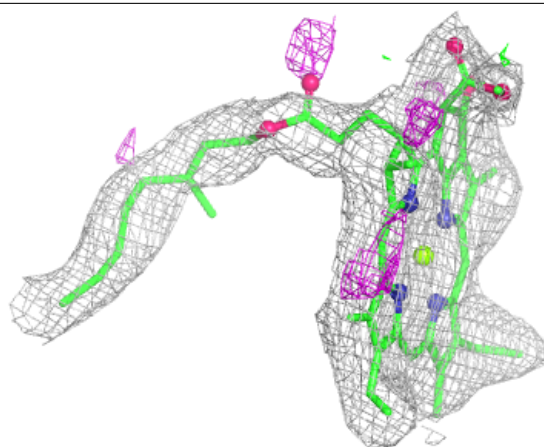
Electron density around CLA H 802:

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



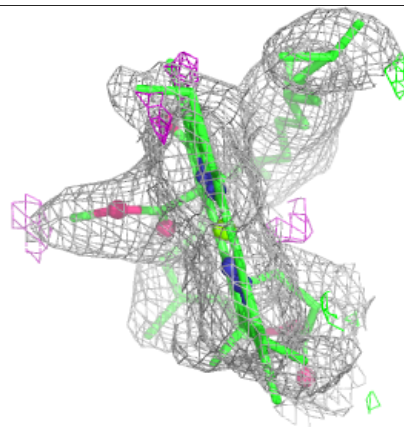
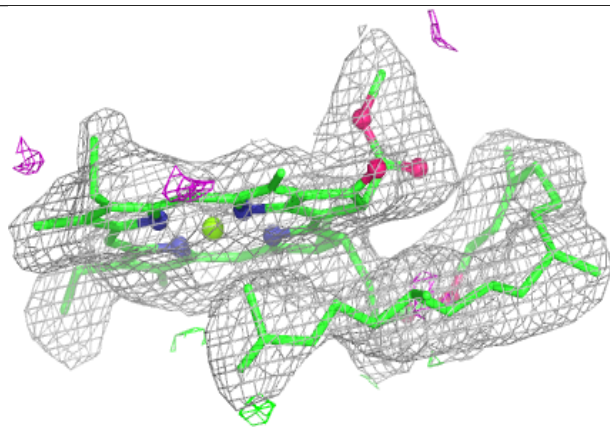
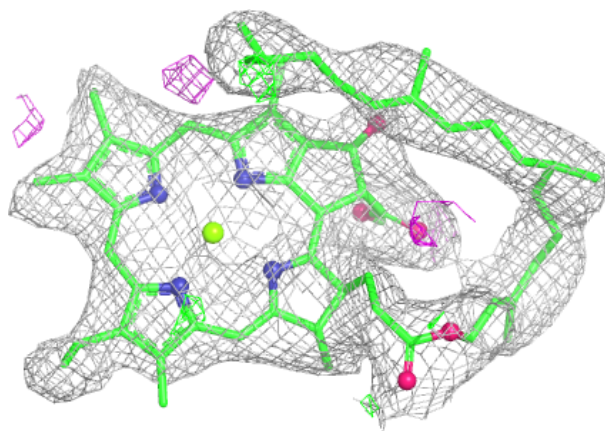
Electron density around CLA H 804:

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

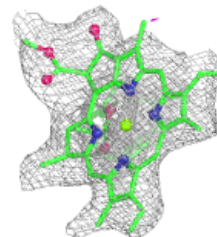
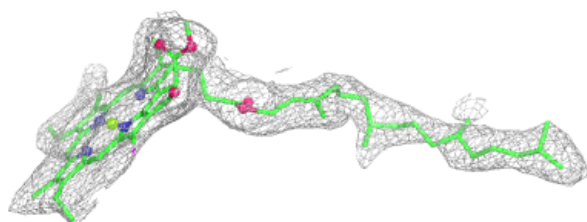
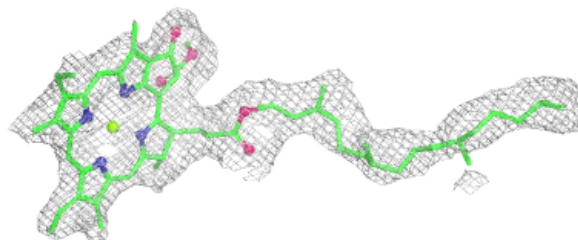


Electron density around CLA H 805:

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

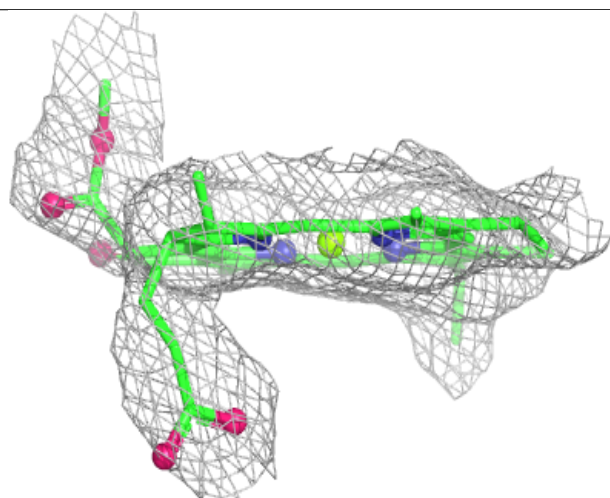
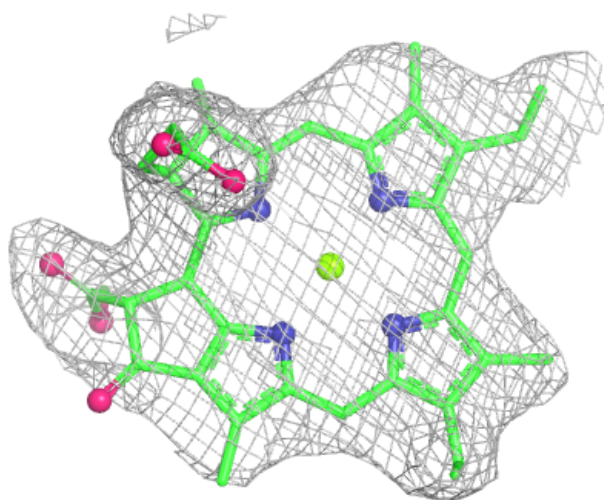
**Electron density around CLA A 810:**

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



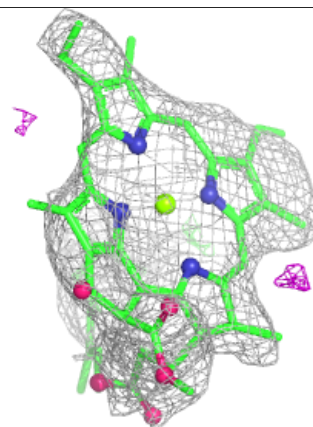
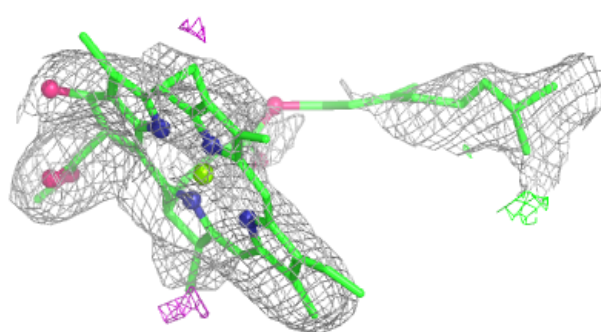
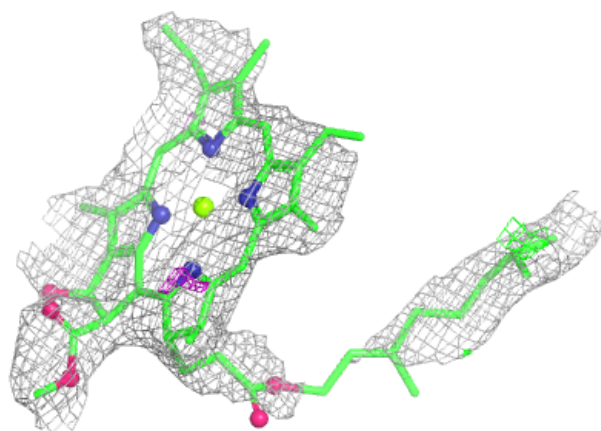
Electron density around CLA H 815:

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

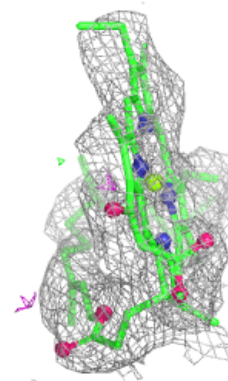
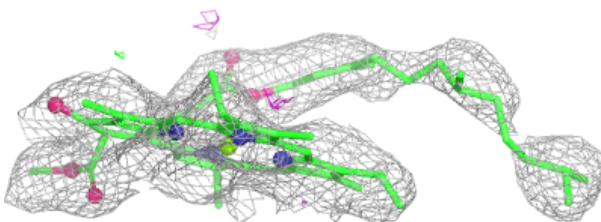
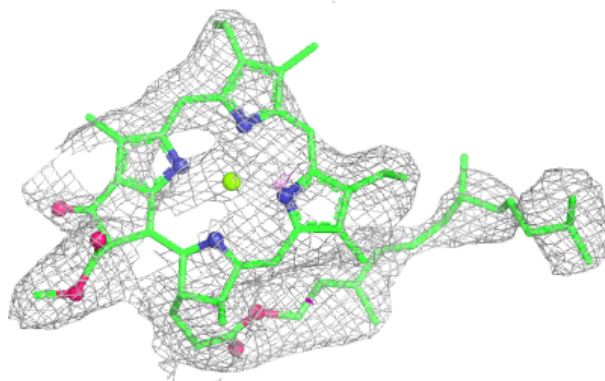


Electron density around CLA H 816:

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

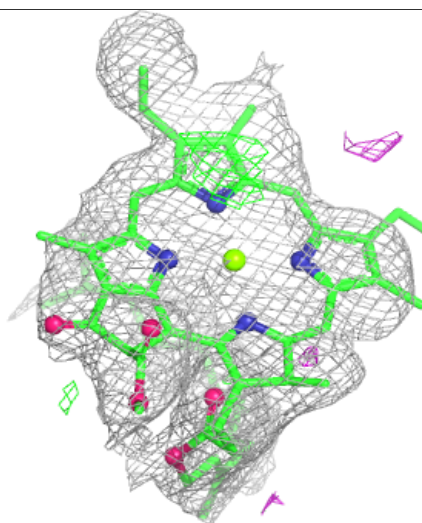
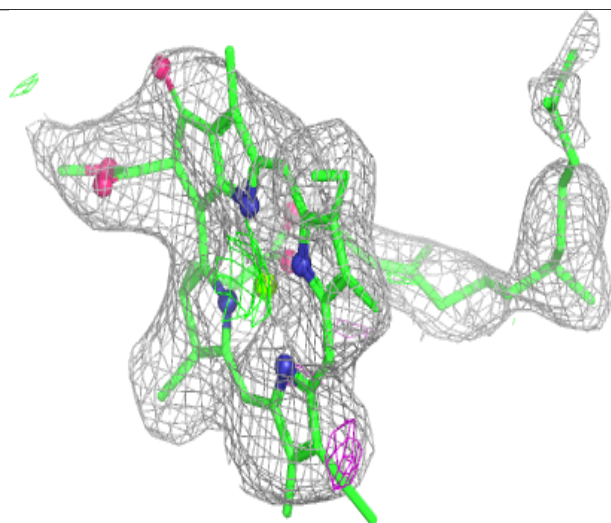
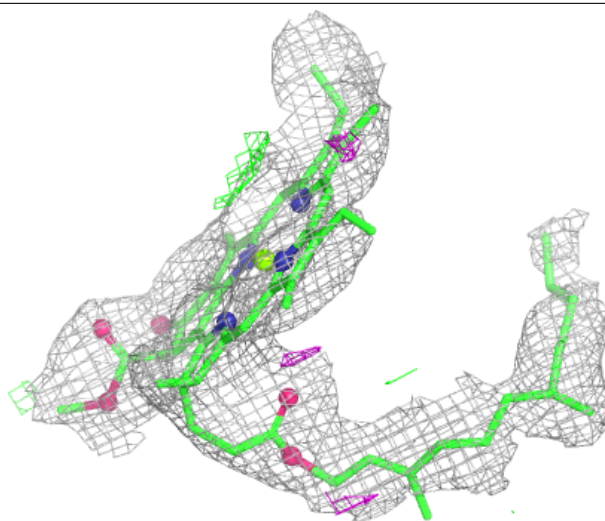
**Electron density around CLA H 818:**

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



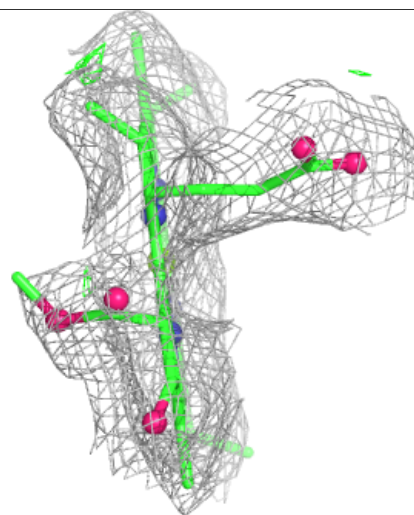
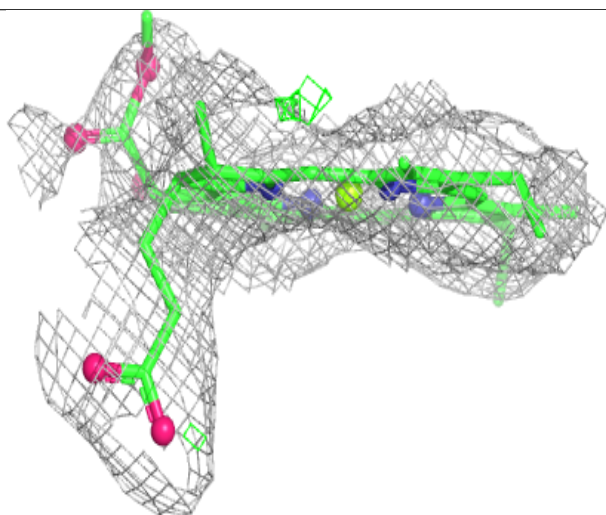
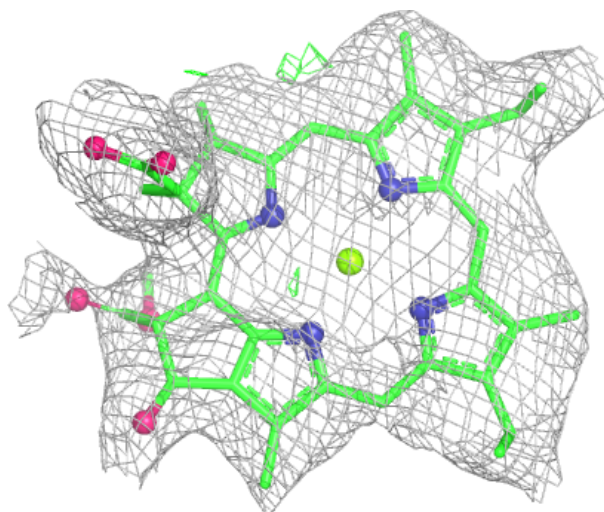
Electron density around CLA H 819:

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



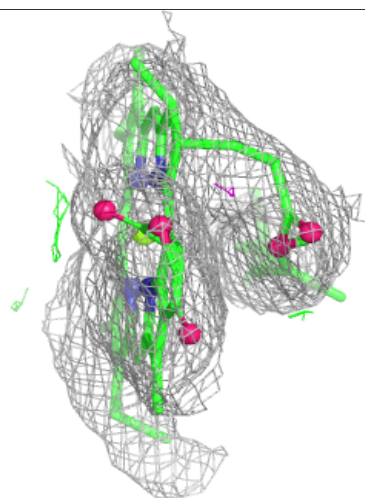
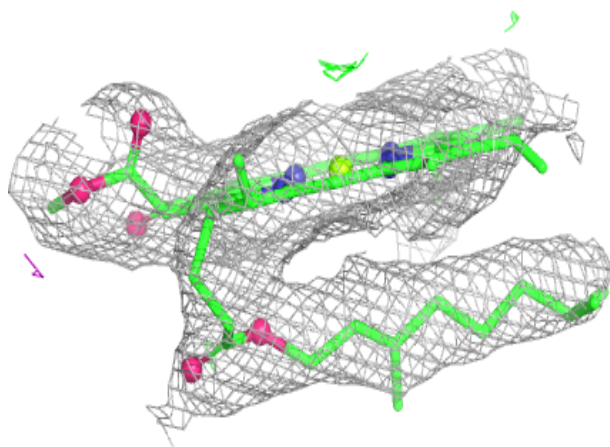
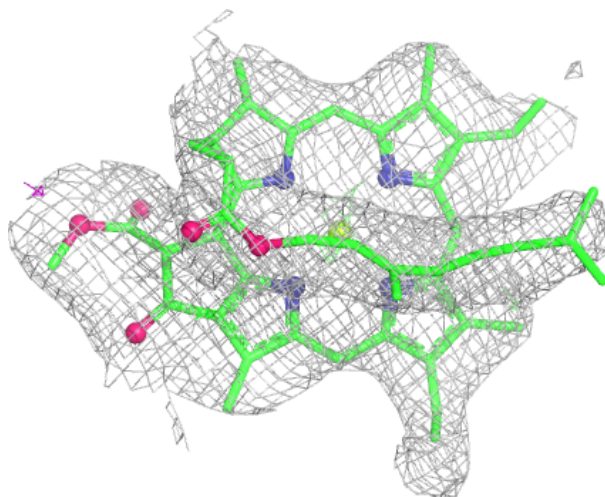
Electron density around CLA H 821:

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



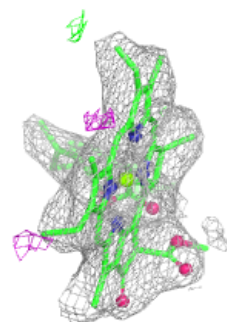
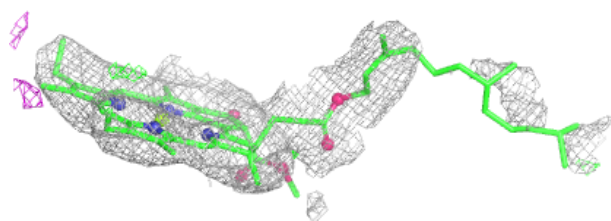
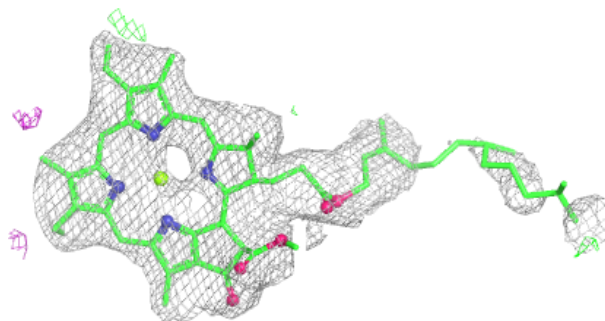
Electron density around CLA H 822:

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



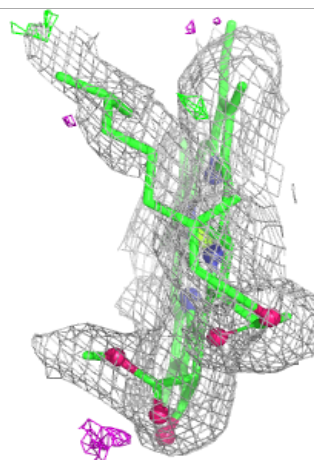
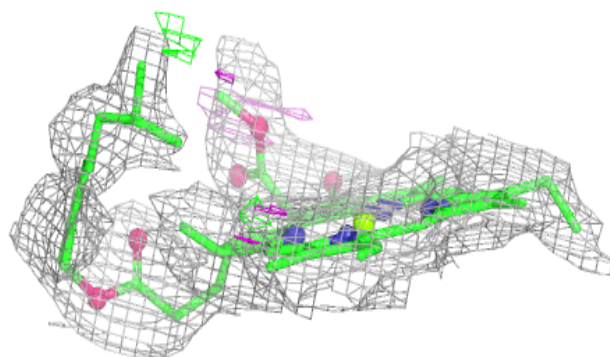
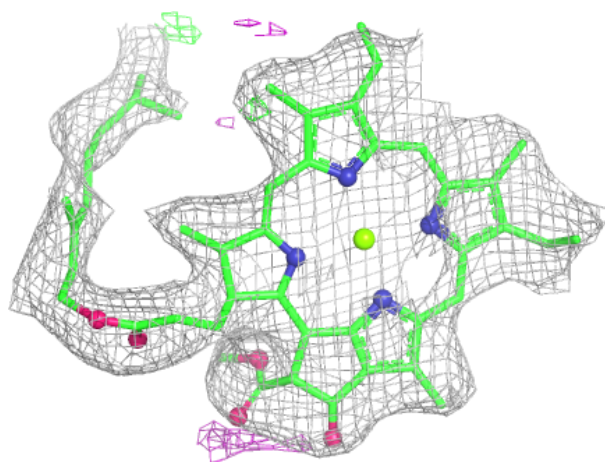
Electron density around CLA H 823:

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



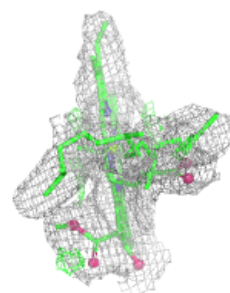
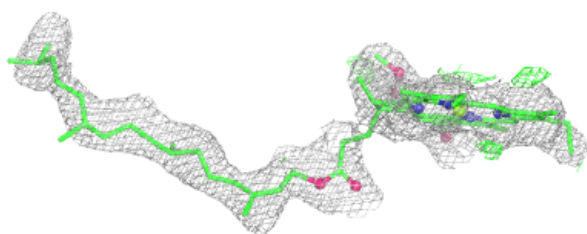
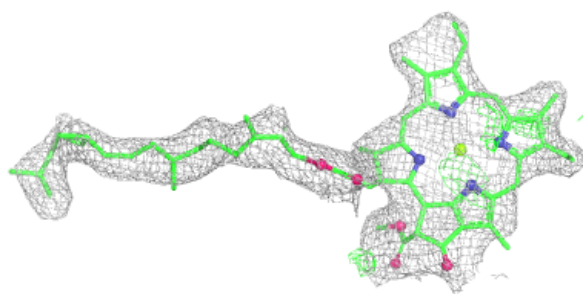
Electron density around CLA H 824:

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

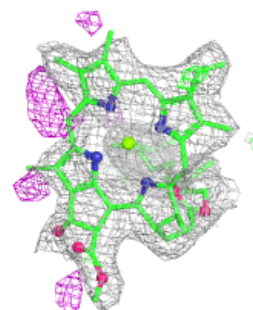
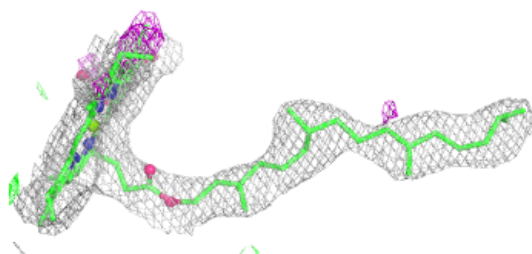
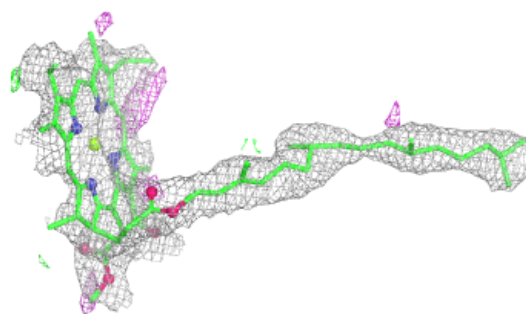


Electron density around CLA H 825:

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

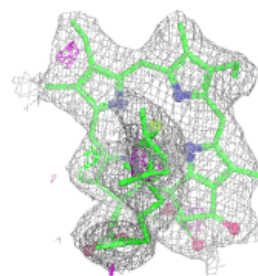
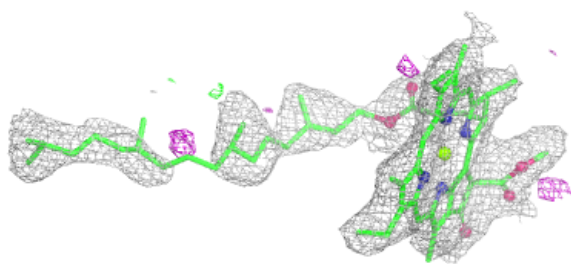
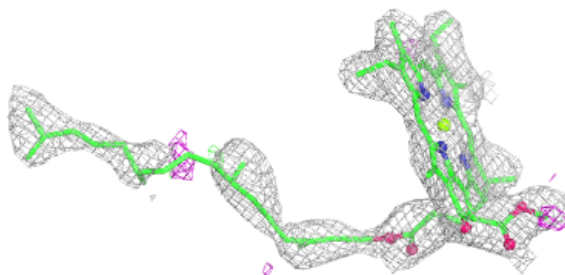
**Electron density around CLA H 828:**

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



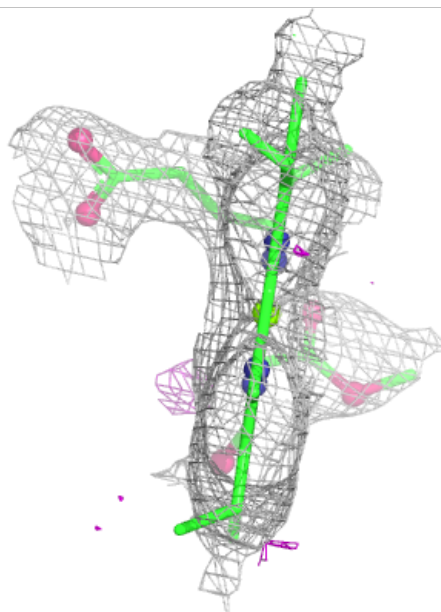
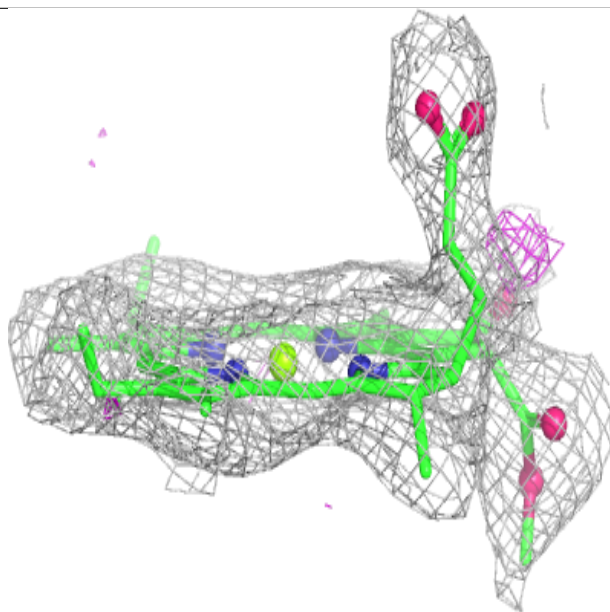
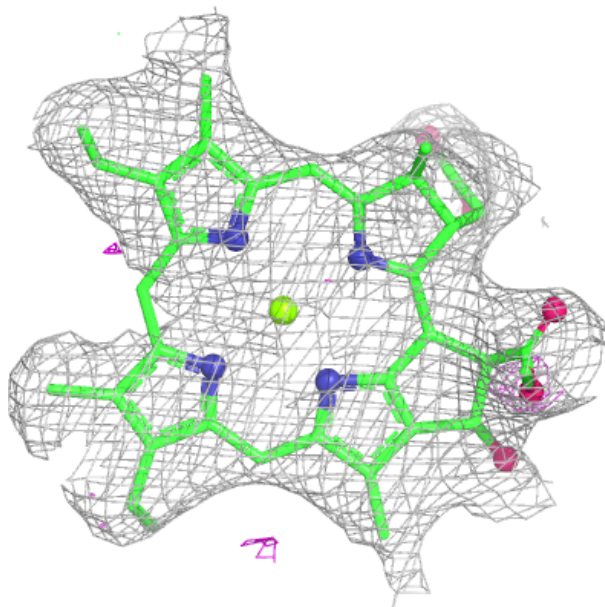
Electron density around CLA H 829:

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



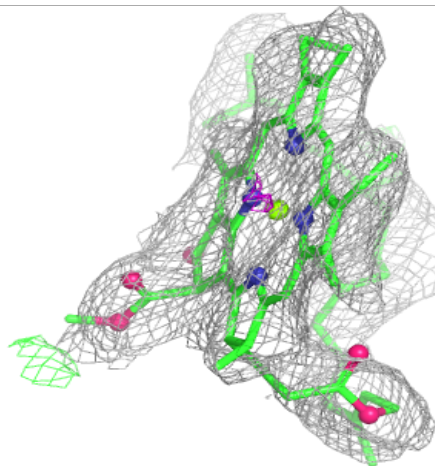
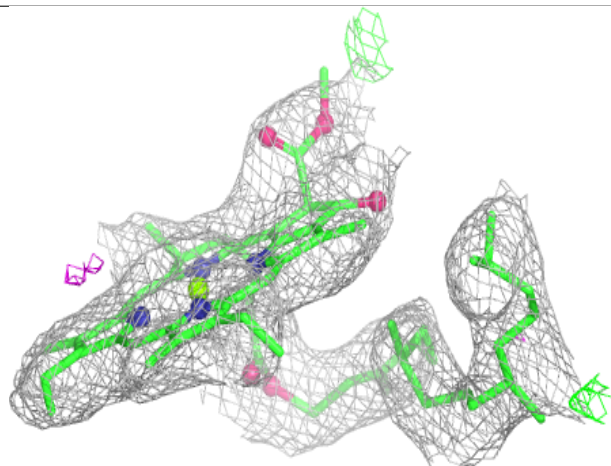
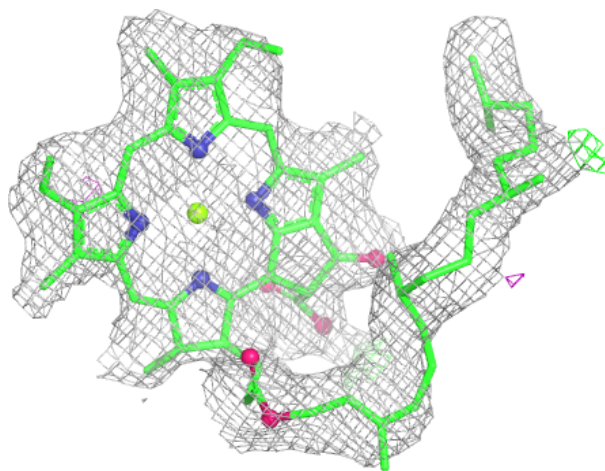
Electron density around CLA H 830:

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



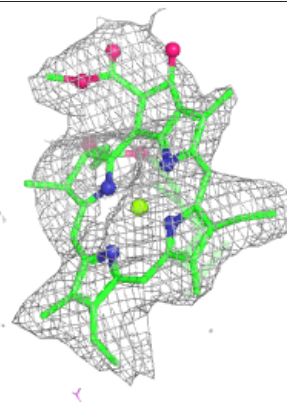
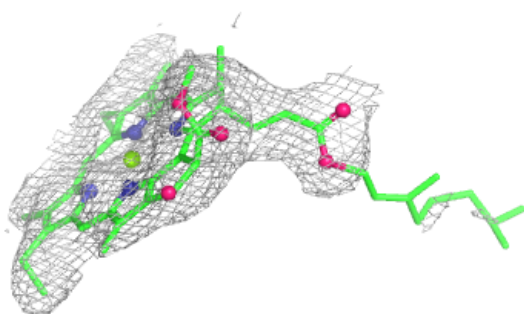
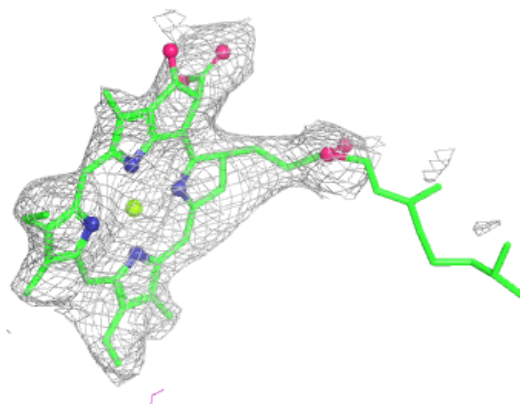
Electron density around CLA H 831:

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



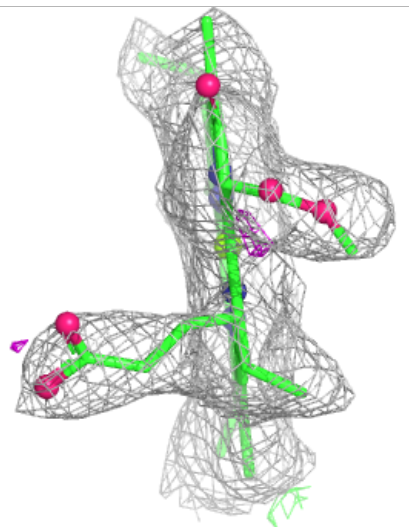
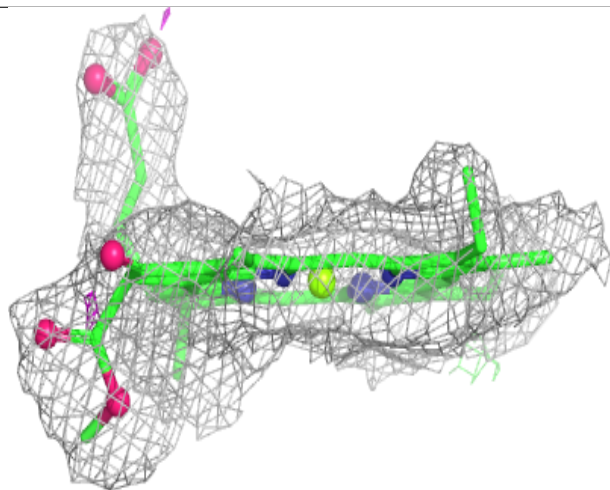
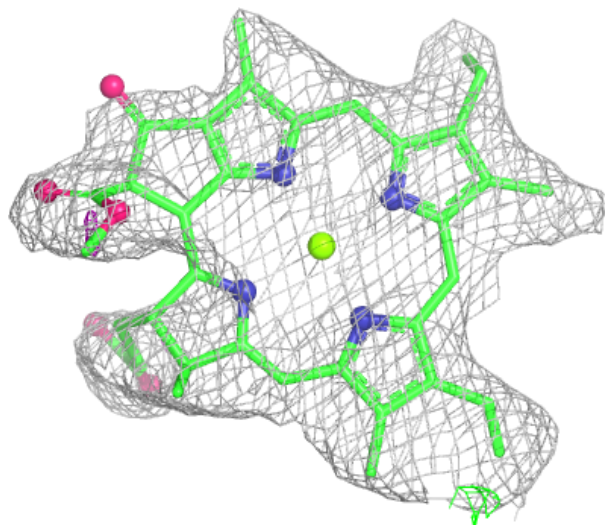
Electron density around CLA H 832:

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



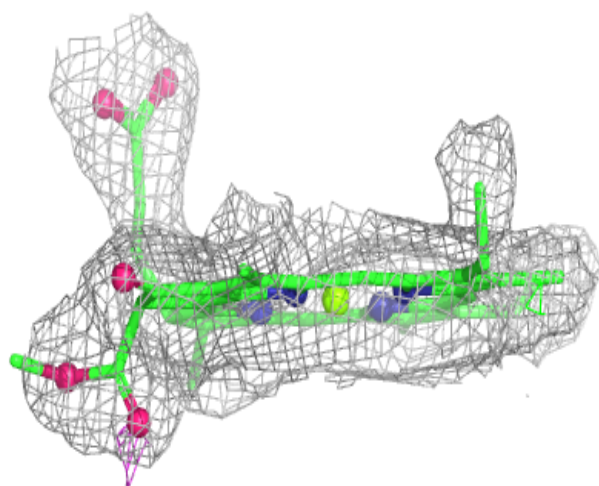
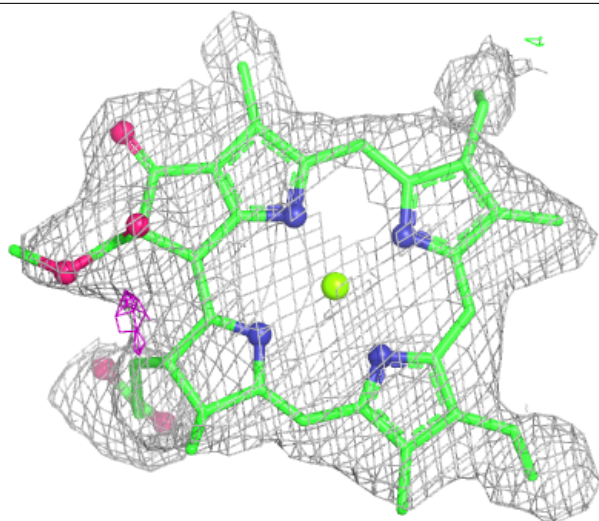
Electron density around CLA H 833:

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



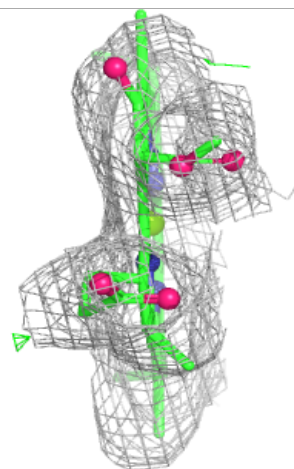
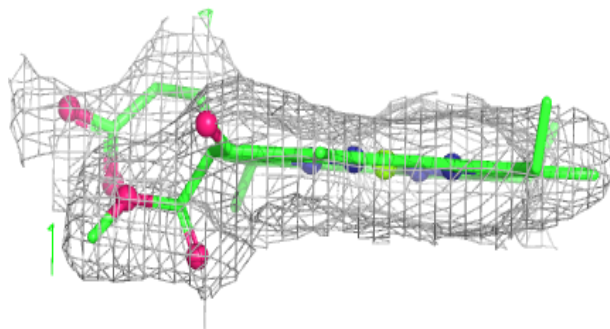
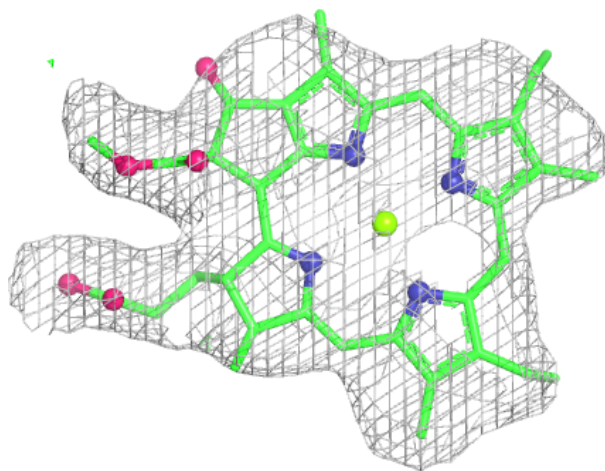
Electron density around CLA H 834:

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



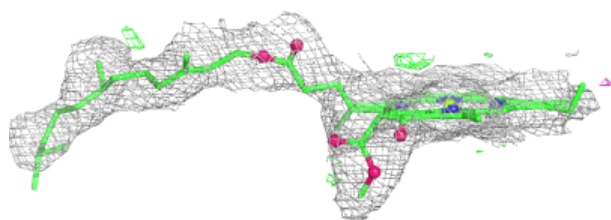
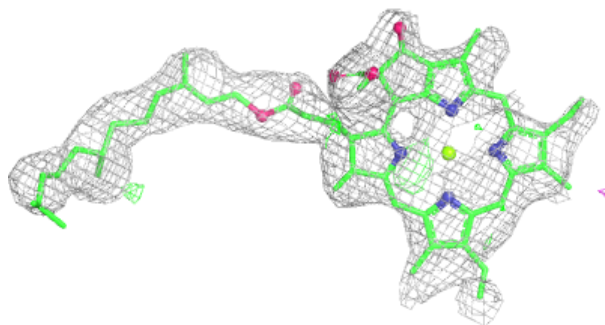
Electron density around CLA H 835:

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

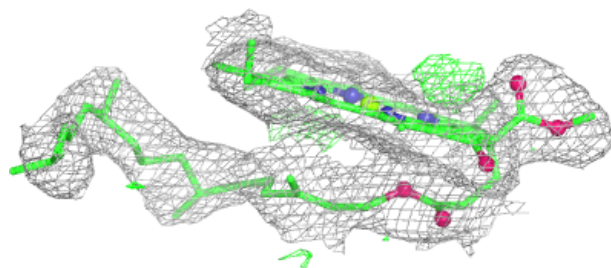
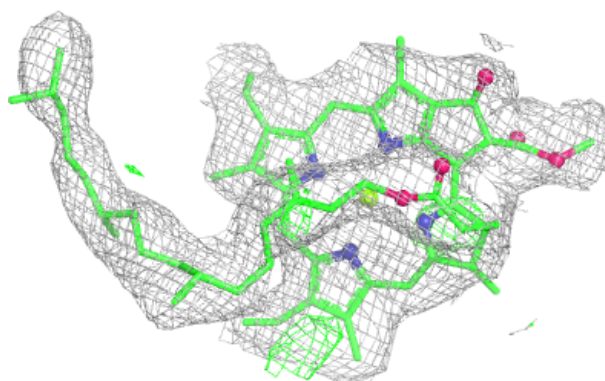


Electron density around CLA H 836:

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

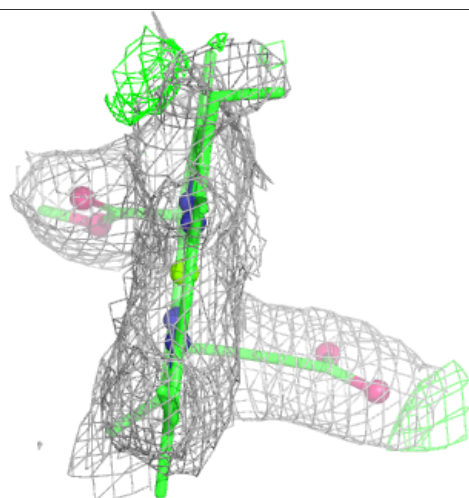
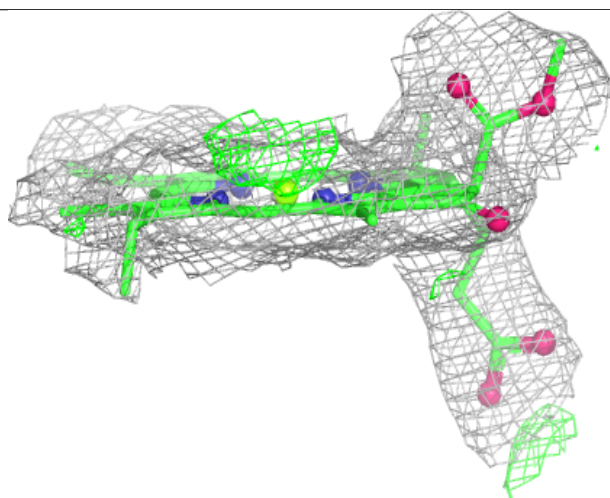
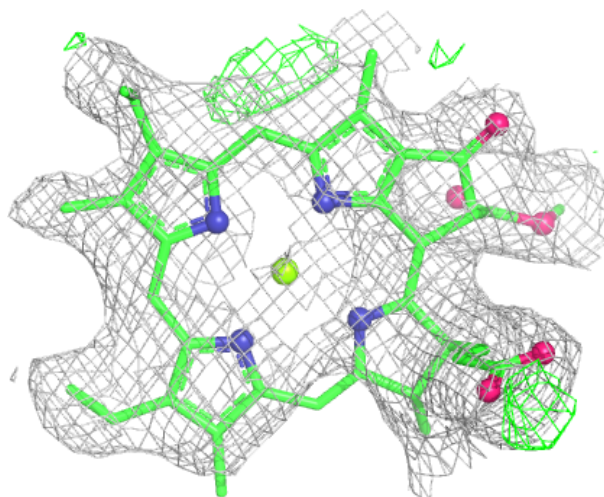
**Electron density around CLA H 837:**

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



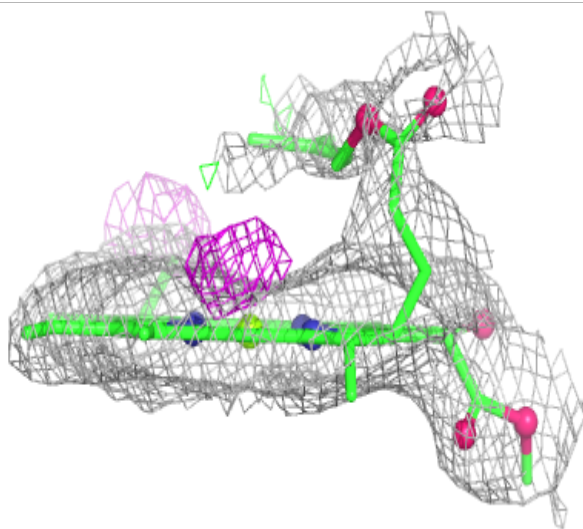
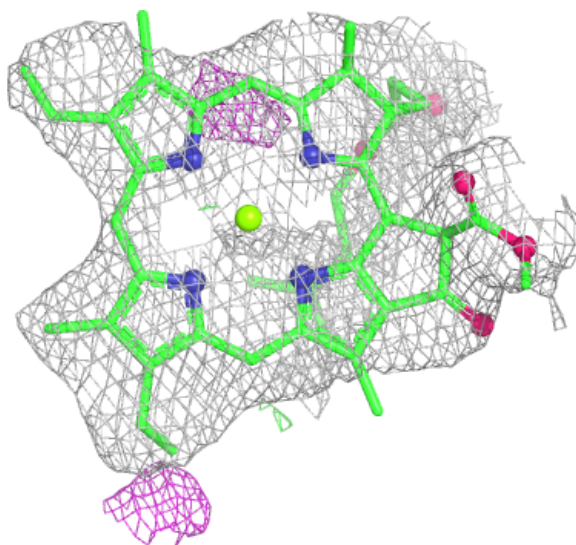
Electron density around CLA H 838:

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



Electron density around CLA H 851:

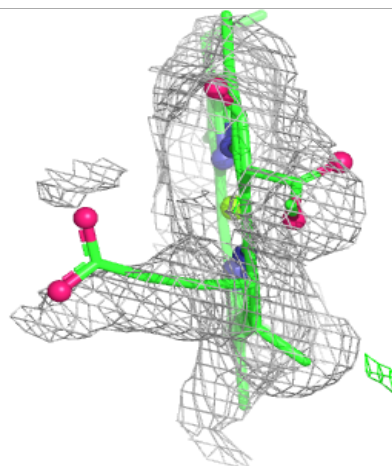
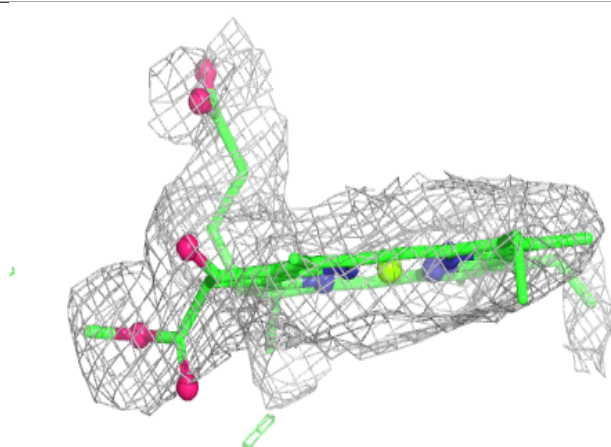
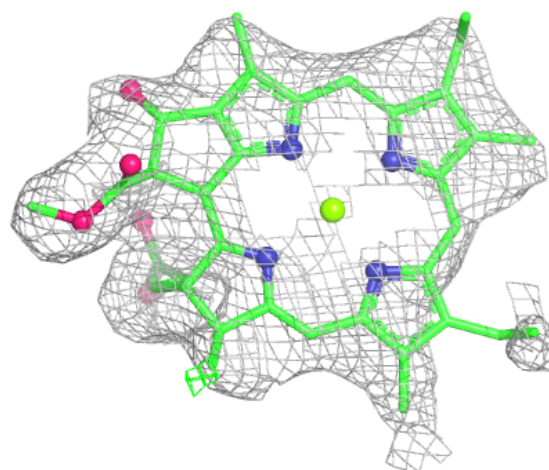
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA A 811:

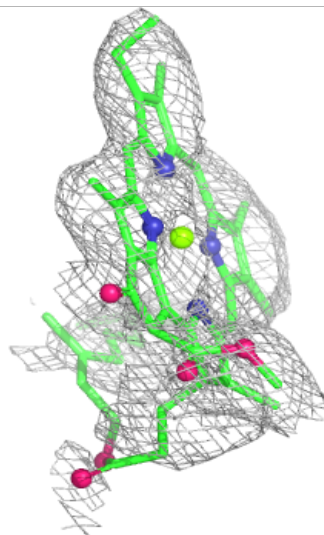
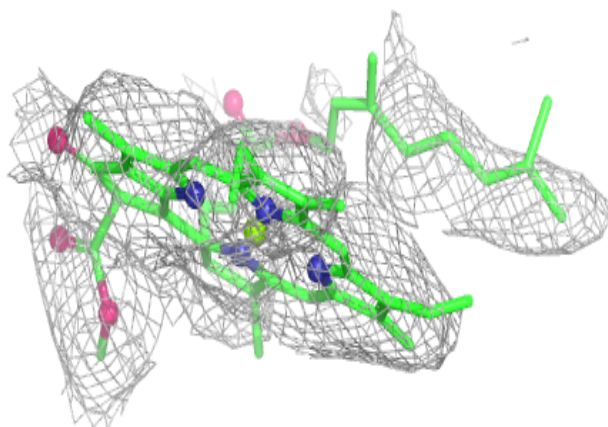
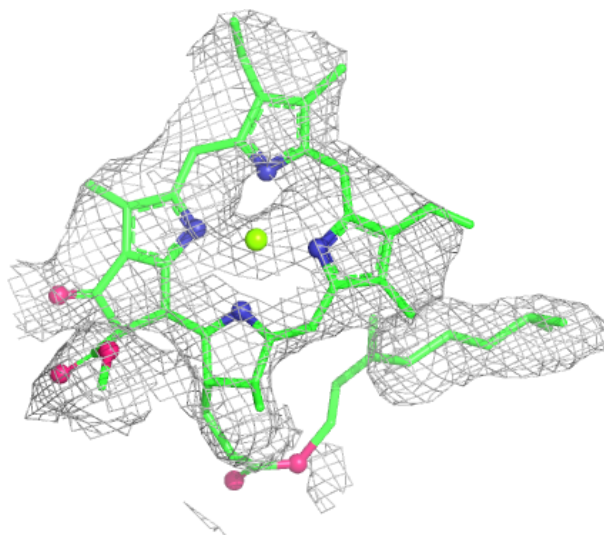
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

1



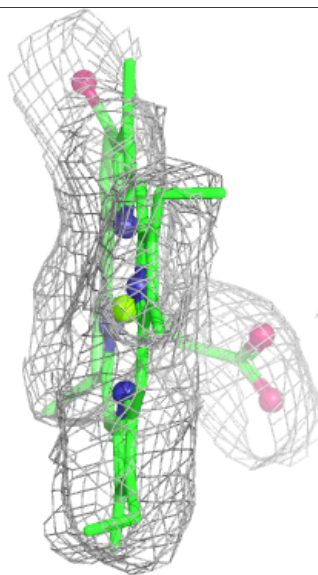
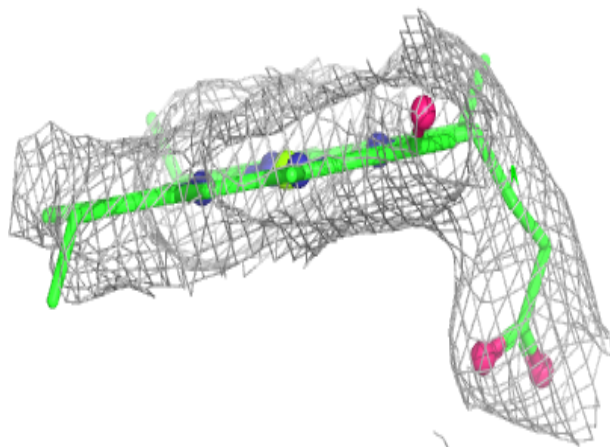
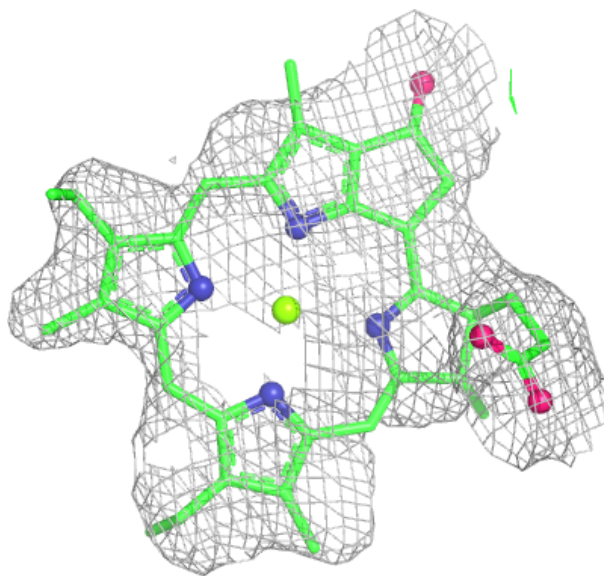
Electron density around CLA J 102:

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



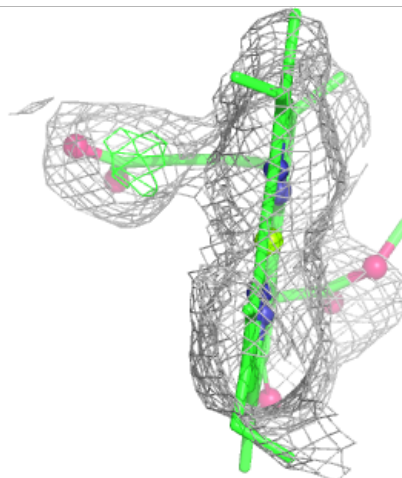
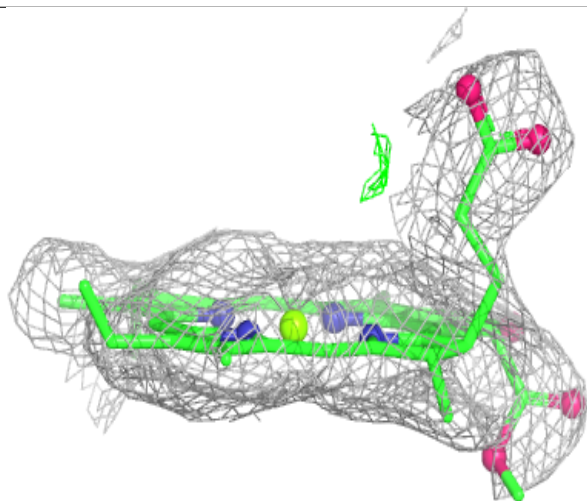
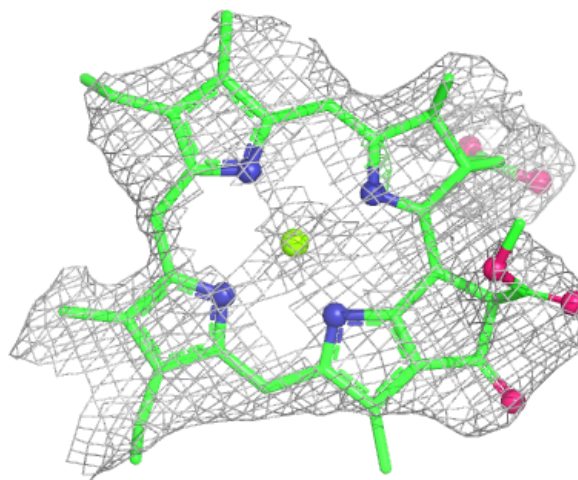
Electron density around CLA K 101:

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



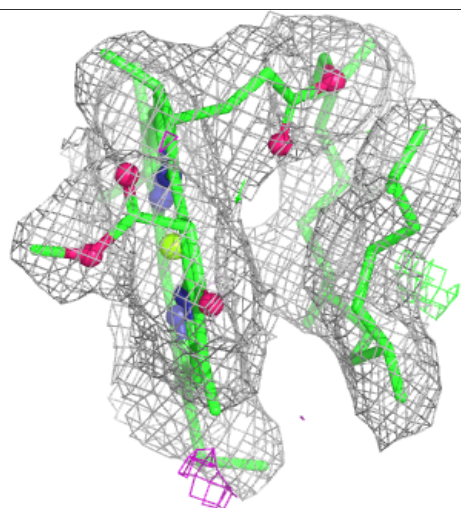
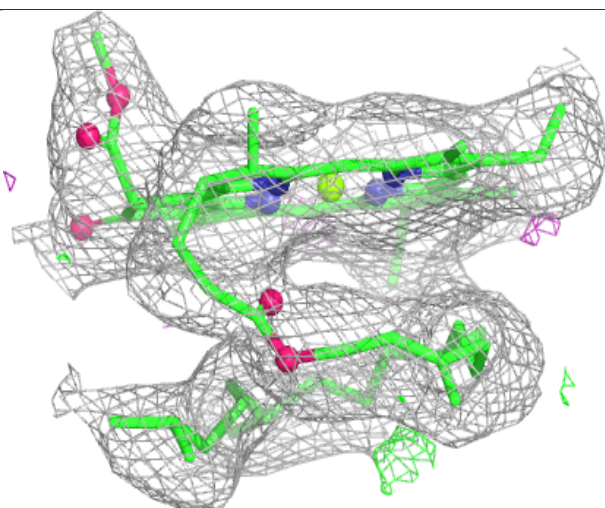
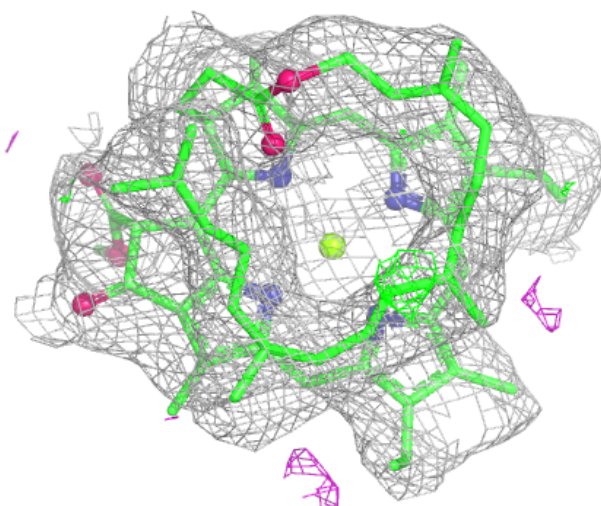
Electron density around CLA K 102:

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



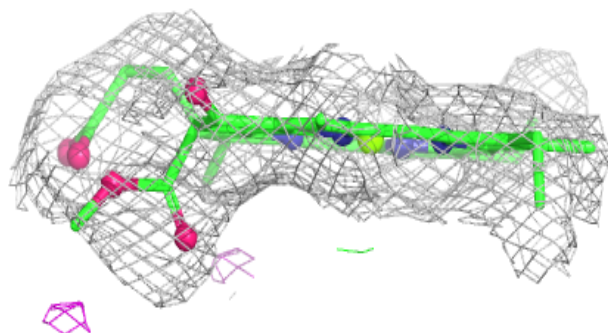
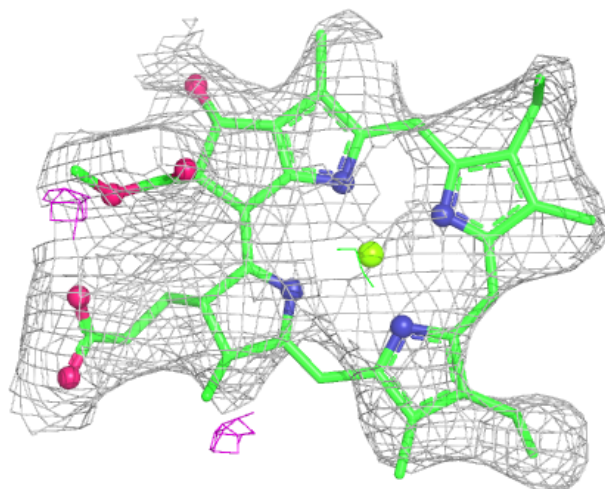
Electron density around CLA L 204:

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



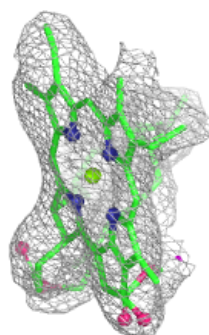
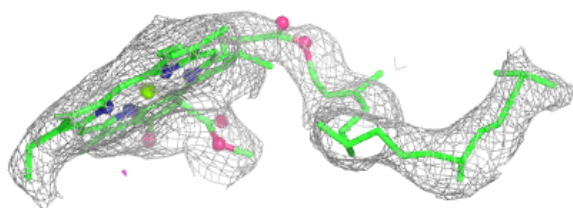
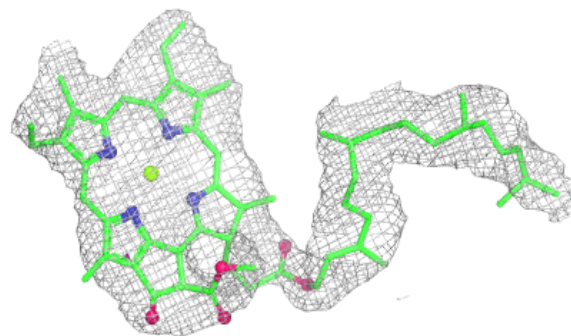
Electron density around CLA Q 202:

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

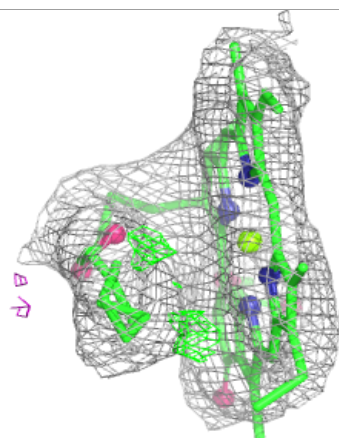
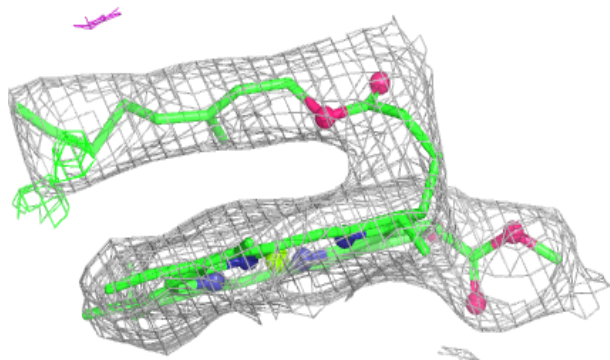
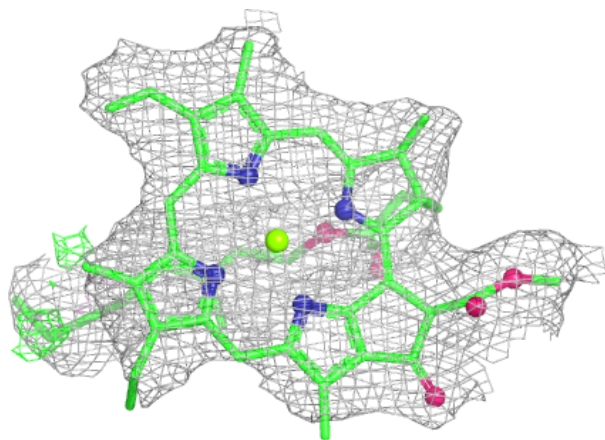


Electron density around CLA S 1101:

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

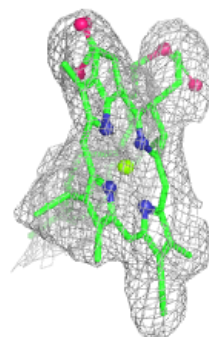
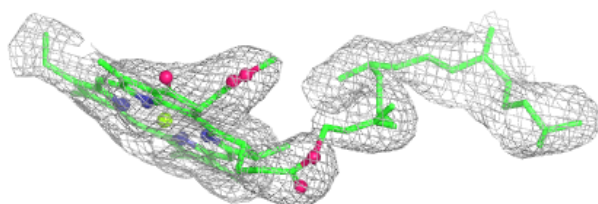
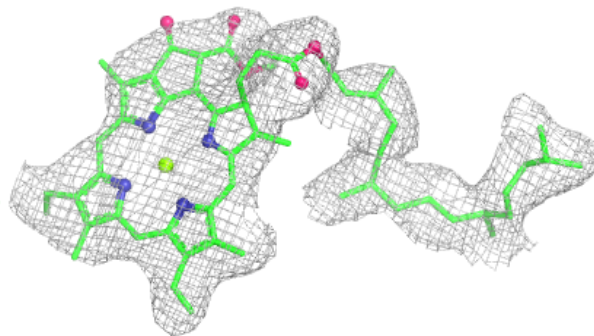
**Electron density around CLA A 813:**

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



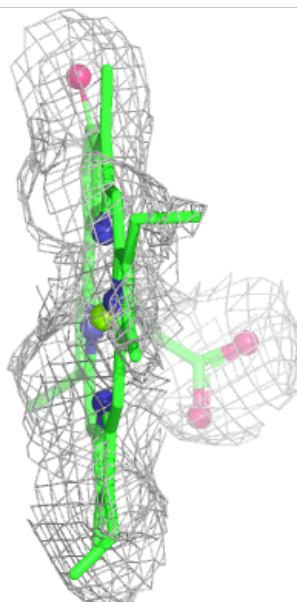
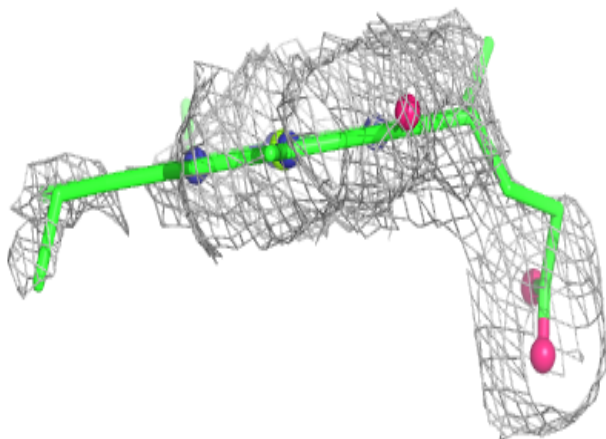
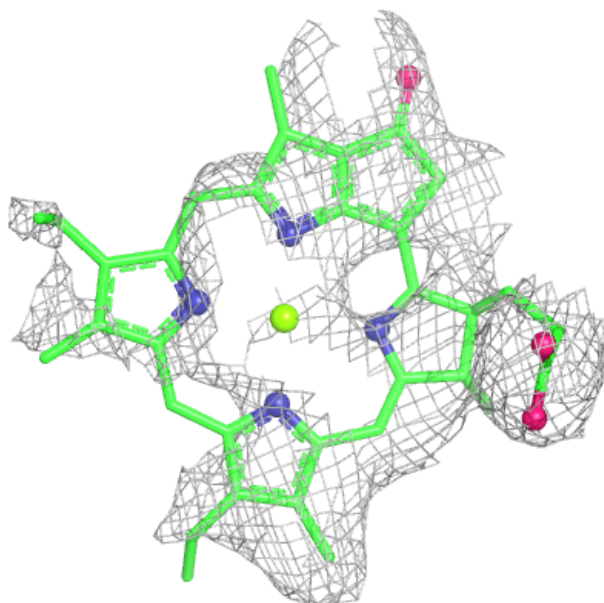
Electron density around CLA A 804:

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



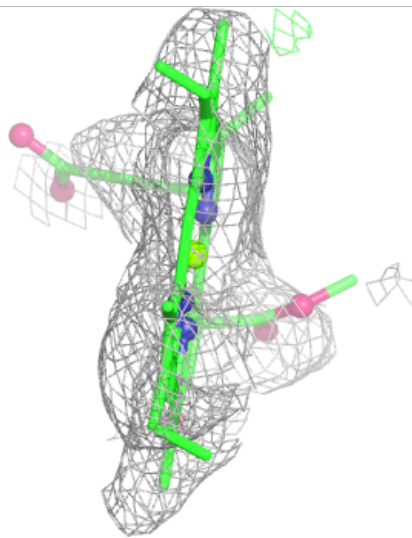
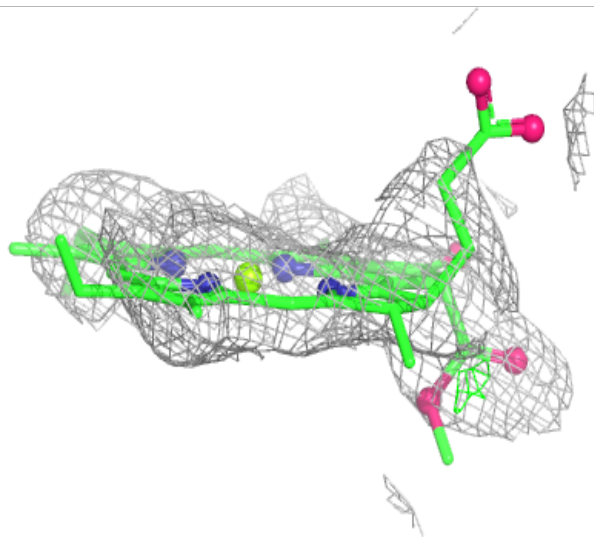
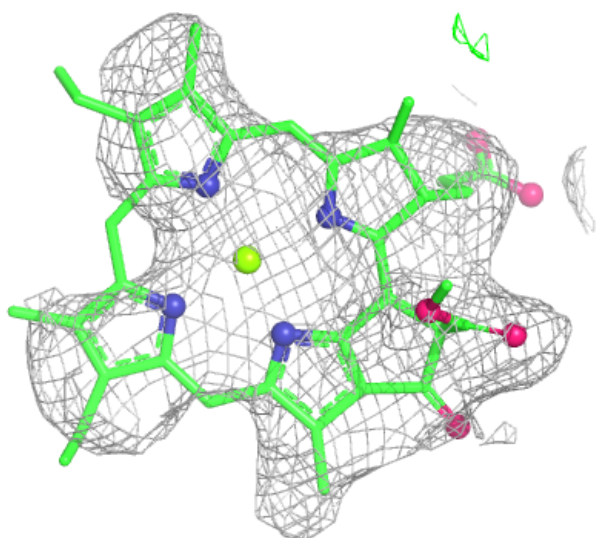
Electron density around CLA T 101:

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



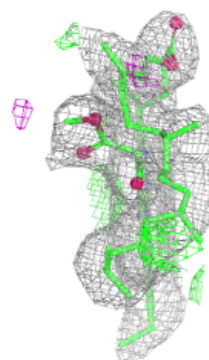
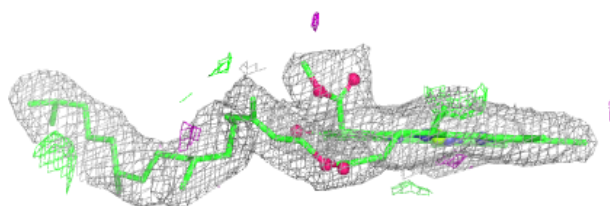
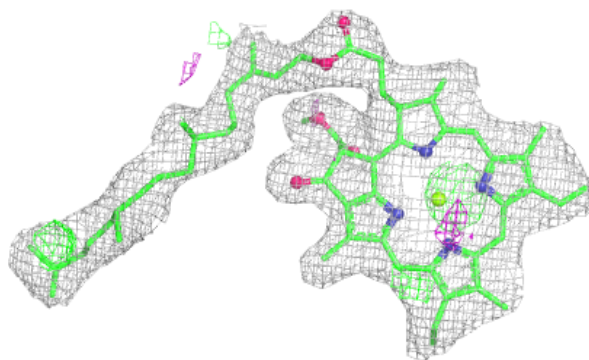
Electron density around CLA T 103:

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

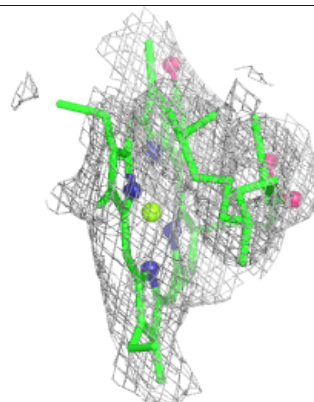
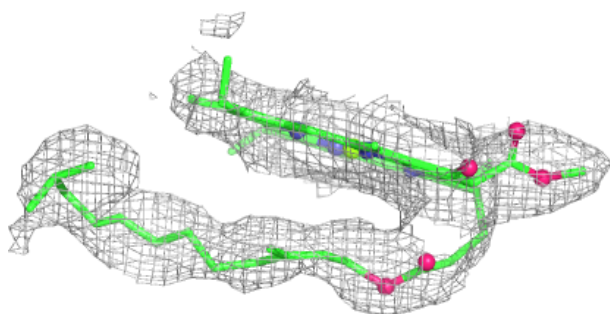
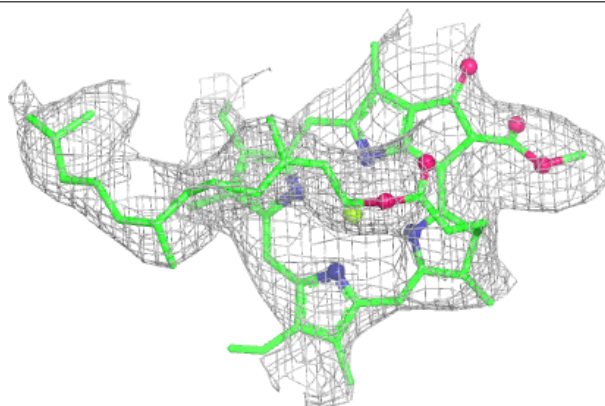


Electron density around CLA U 1004:

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

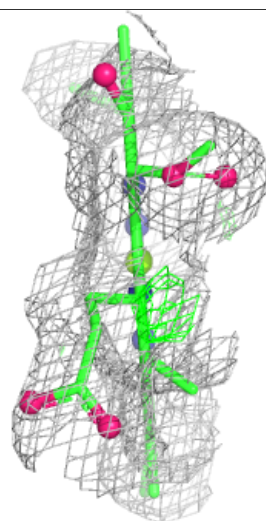
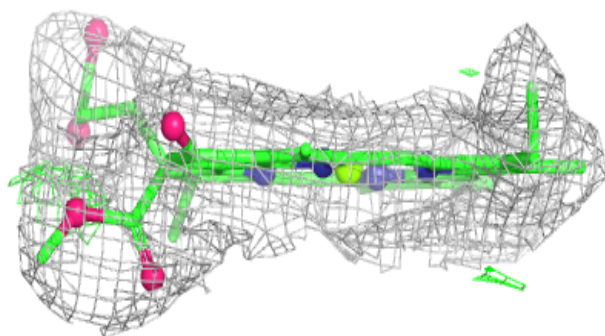
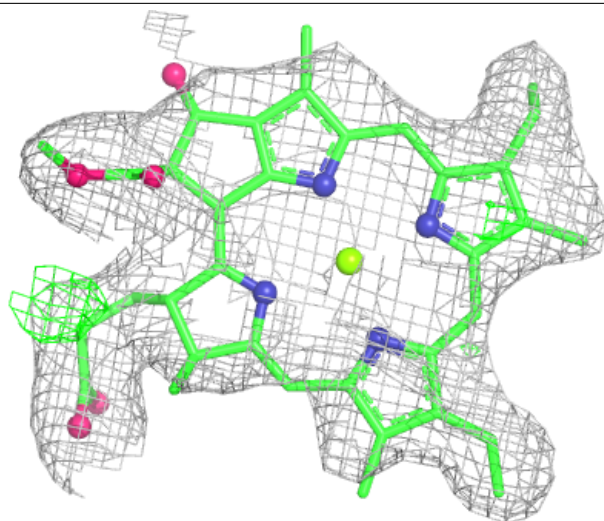
**Electron density around CLA A 818:**

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



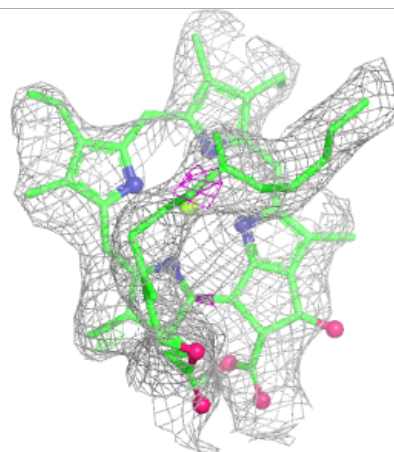
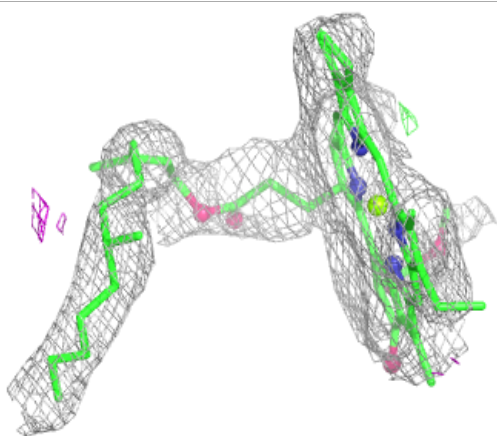
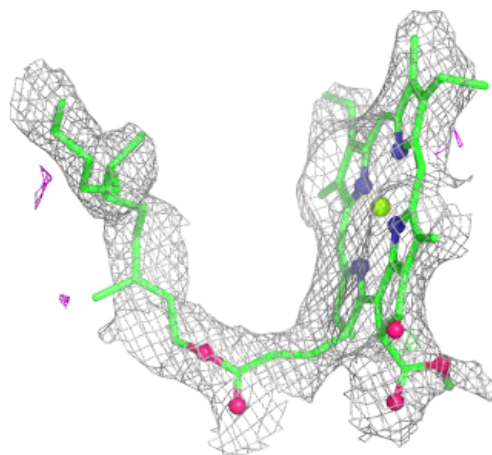
Electron density around CLA X 1701:

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



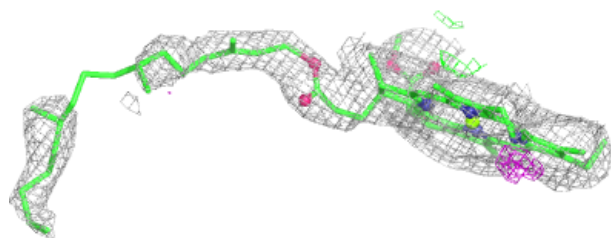
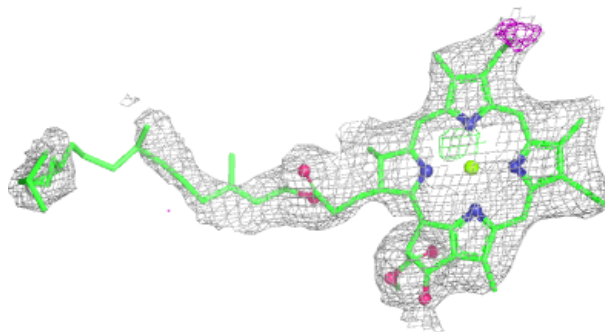
Electron density around CLA Y 804:

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



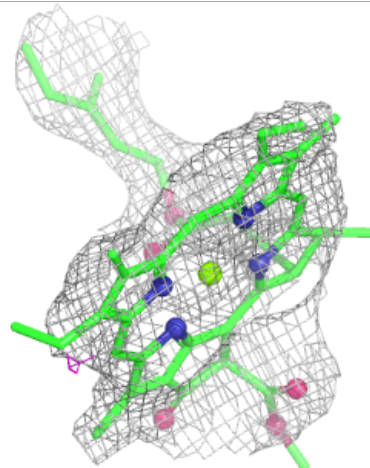
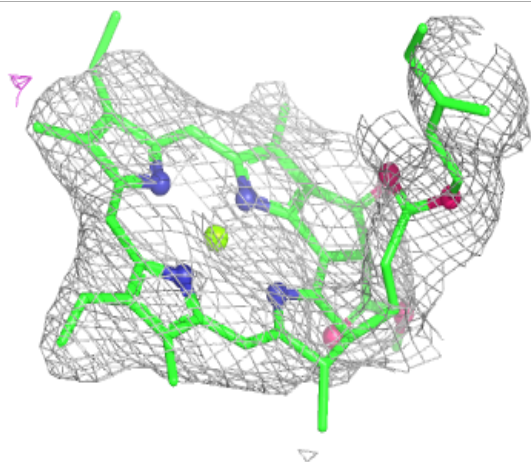
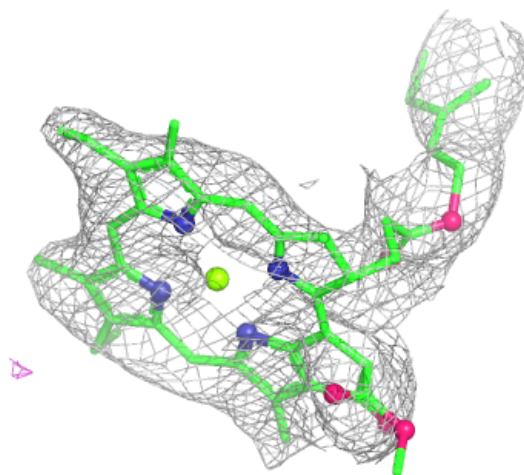
Electron density around CLA Y 805:

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



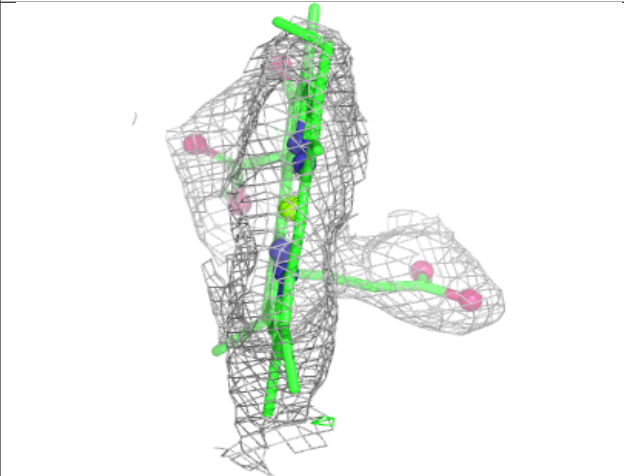
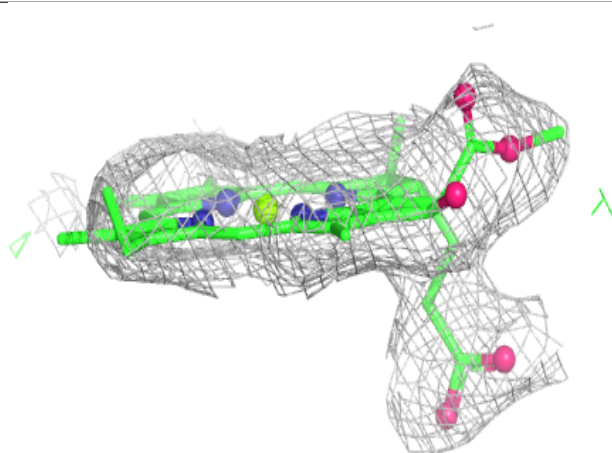
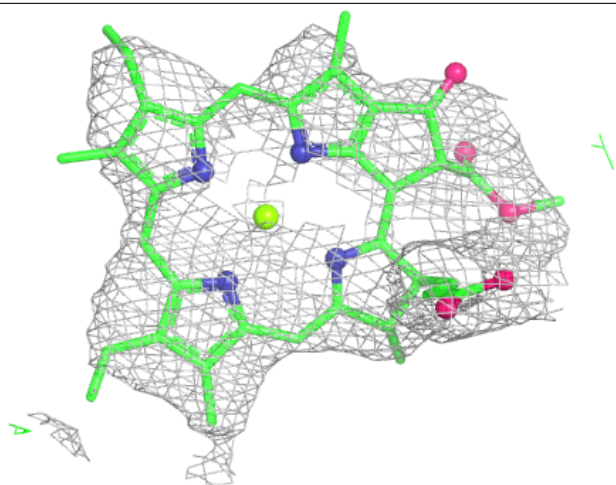
Electron density around CLA Y 807:

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



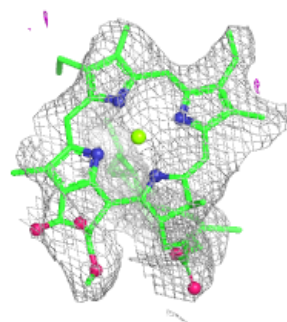
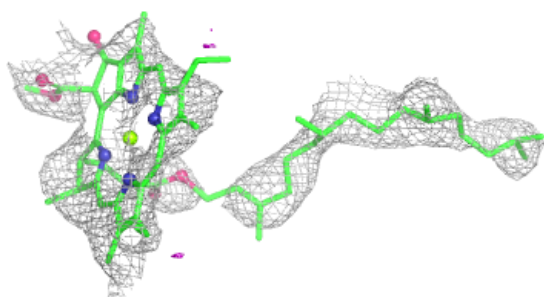
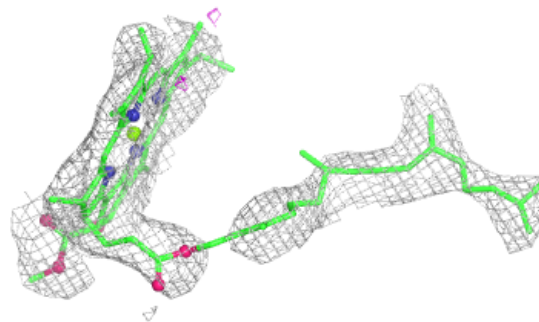
Electron density around CLA Y 810:

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

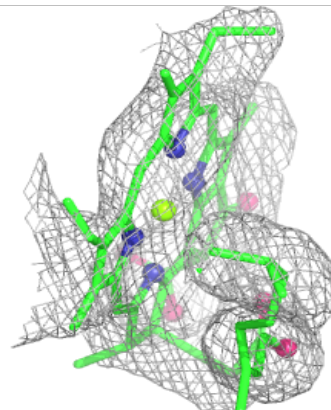
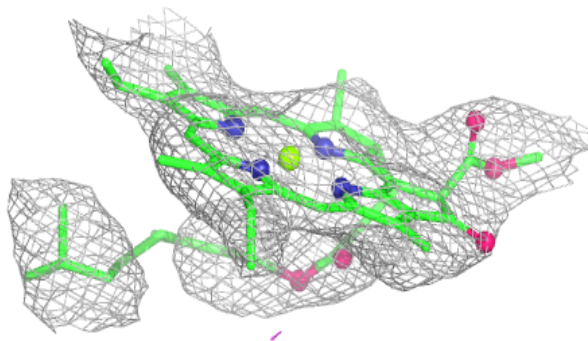
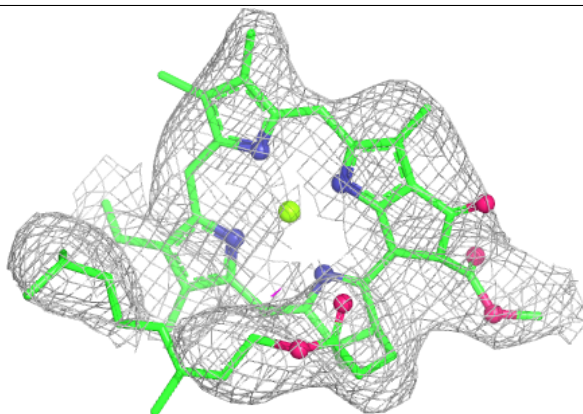


Electron density around CLA Y 811:

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

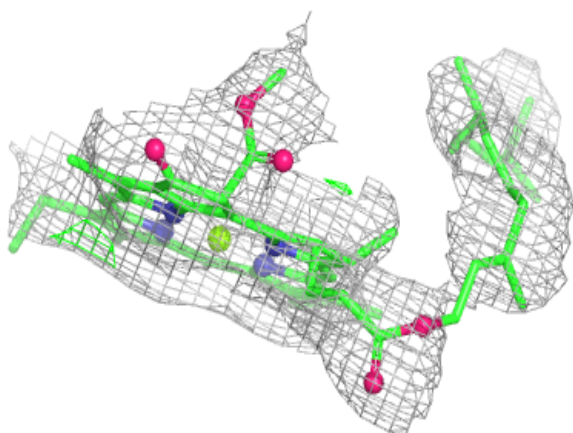
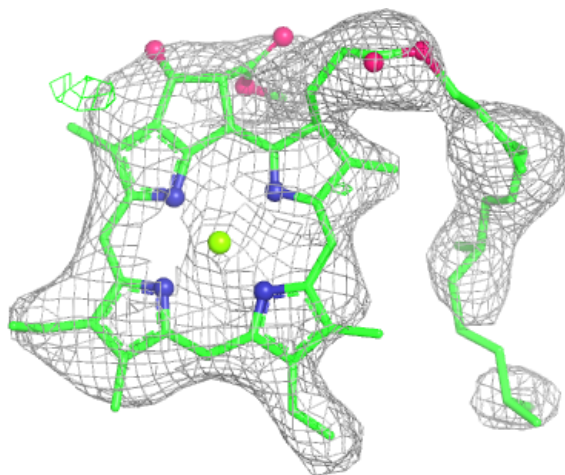
**Electron density around CLA Y 812:**

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



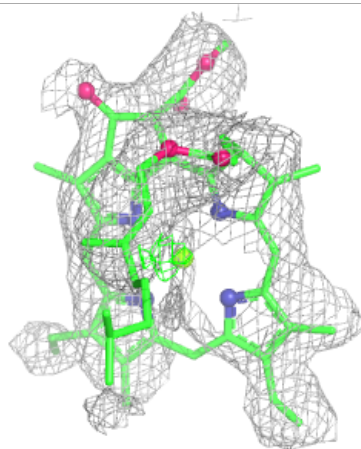
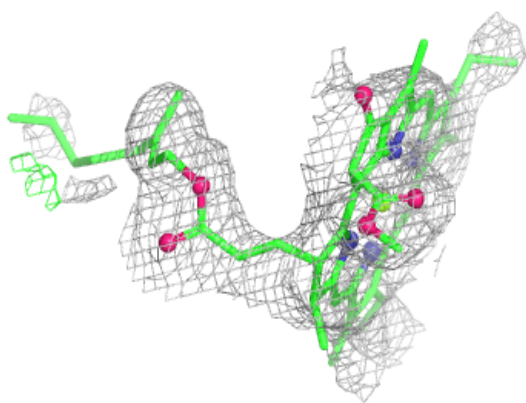
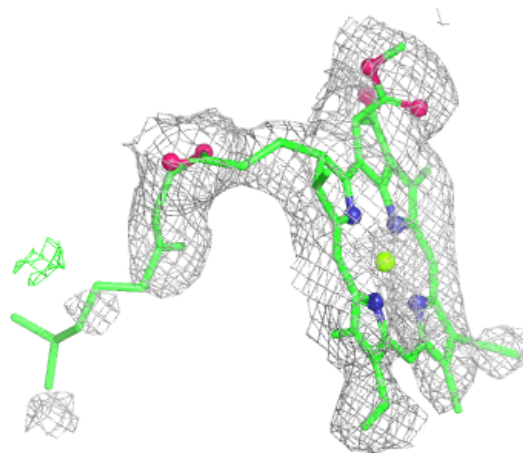
Electron density around CLA Y 813:

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



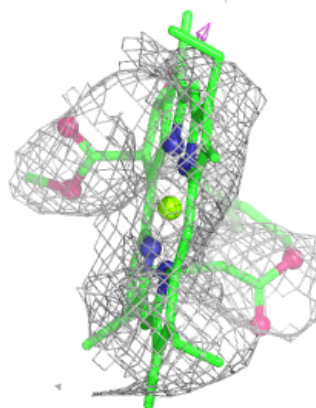
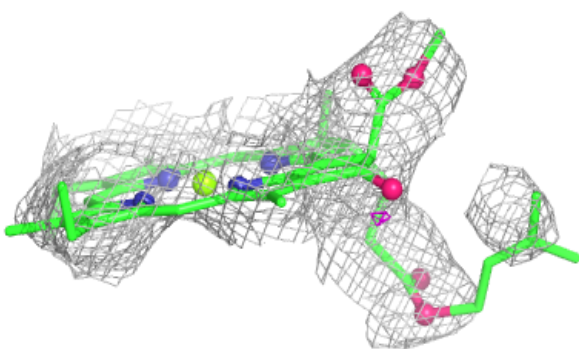
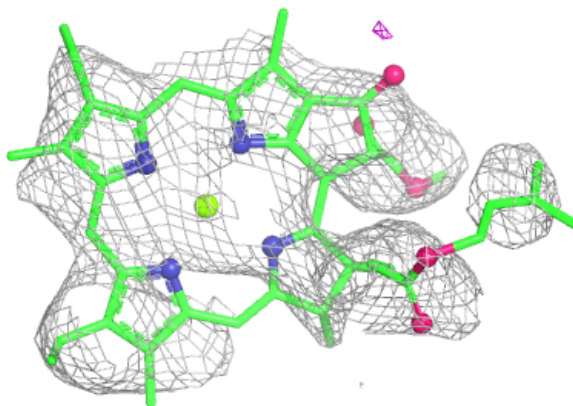
Electron density around CLA Y 814:

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



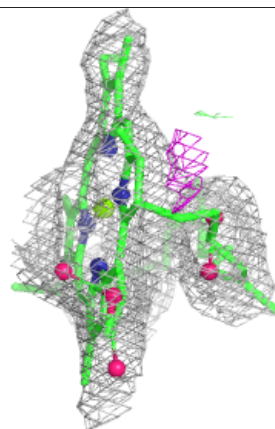
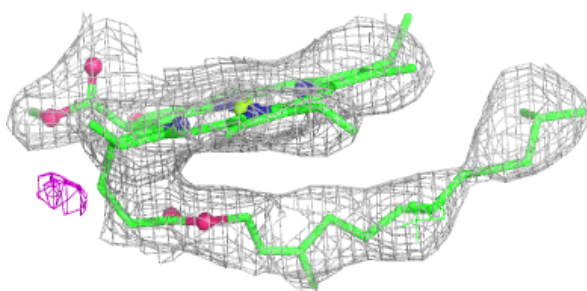
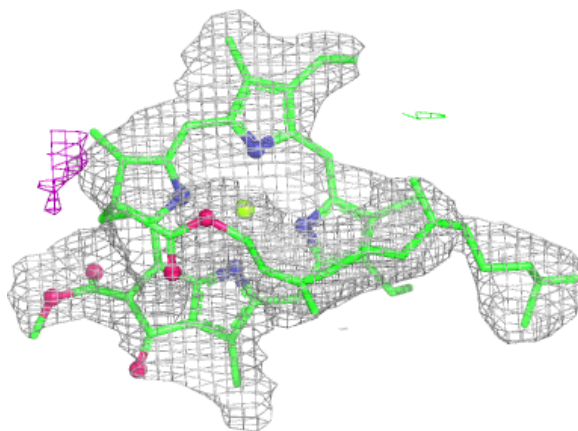
Electron density around CLA Y 816:

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

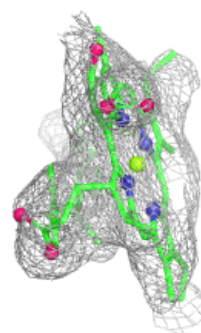
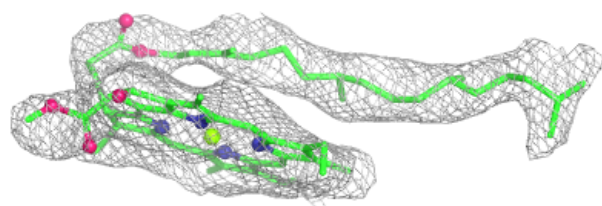
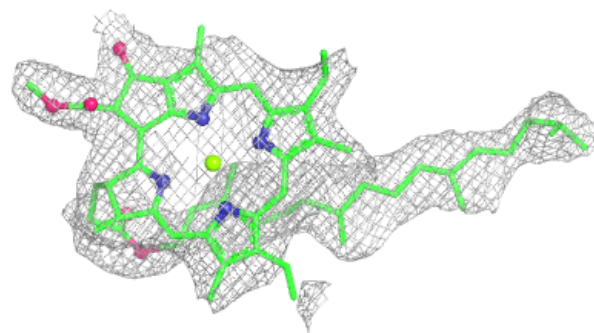


Electron density around CLA Y 817:

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

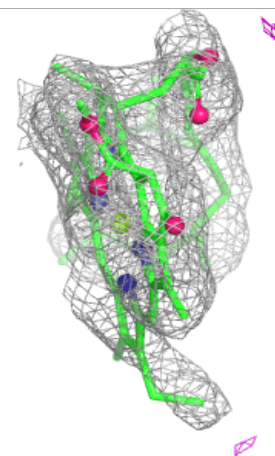
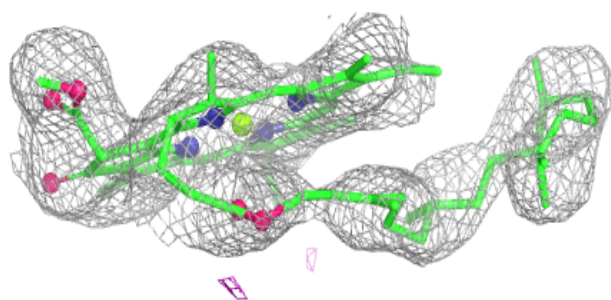
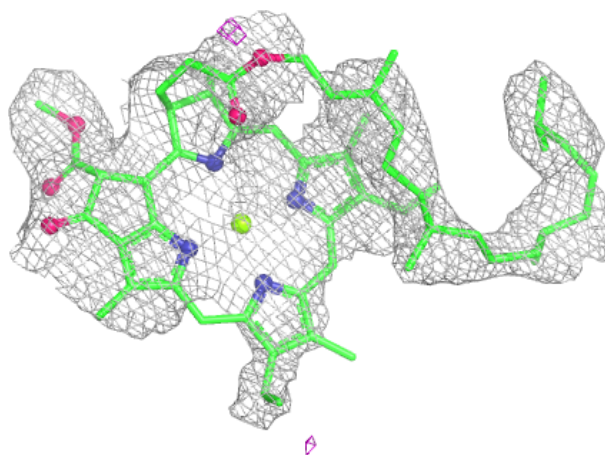
**Electron density around CLA A 819:**

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



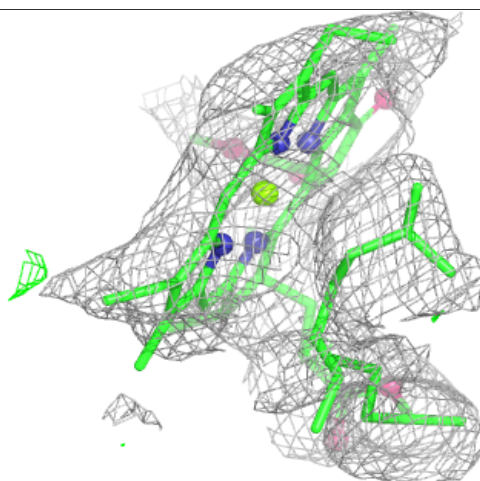
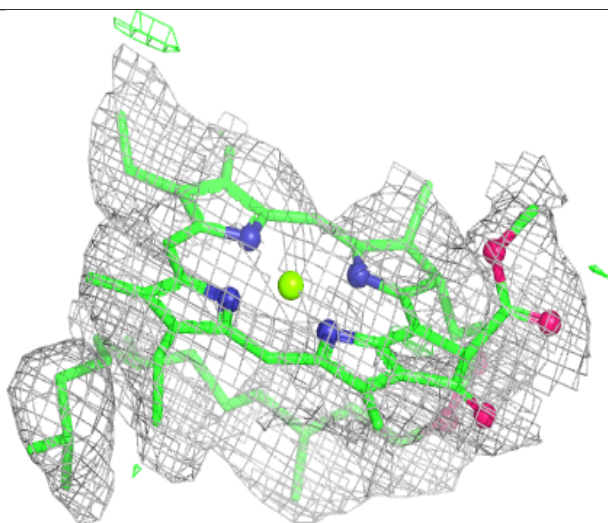
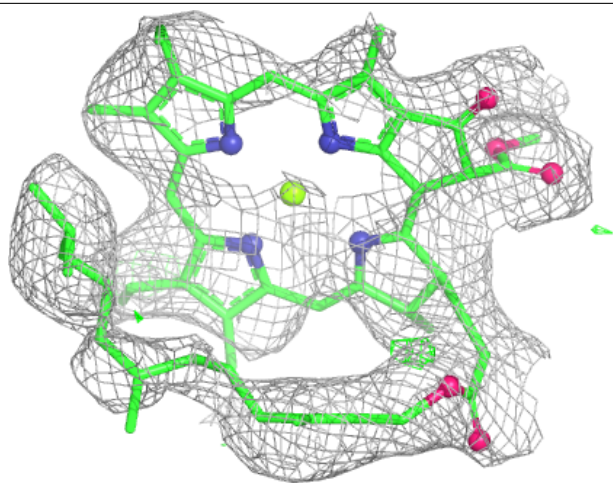
Electron density around CLA Y 819:

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



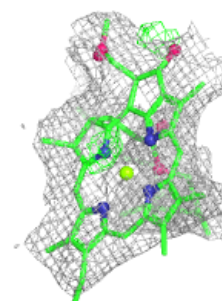
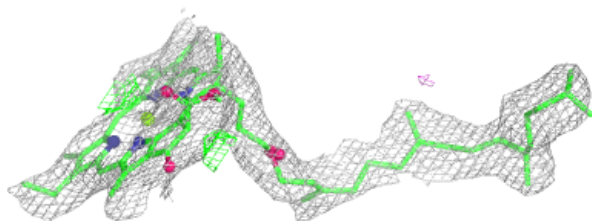
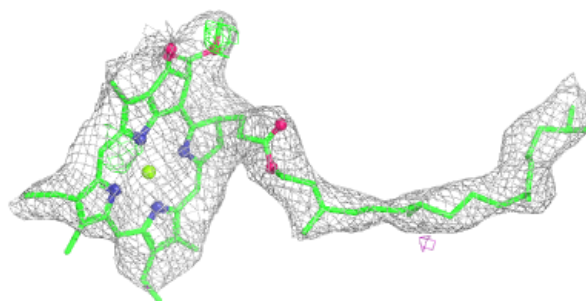
Electron density around CLA Y 820:

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

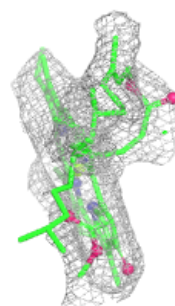
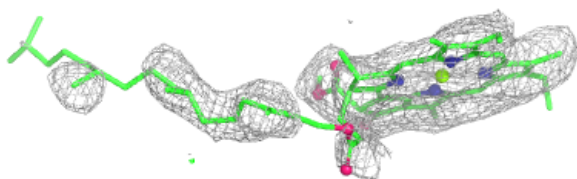
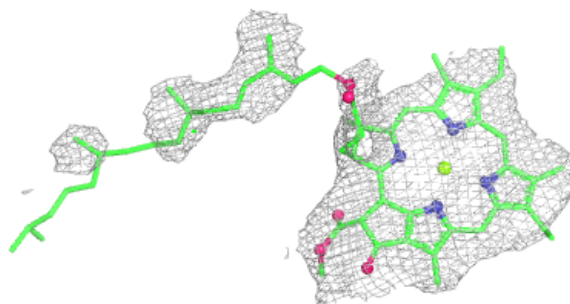


Electron density around CLA Y 821:

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

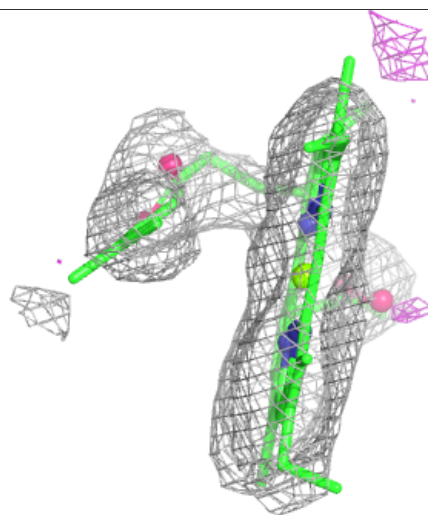
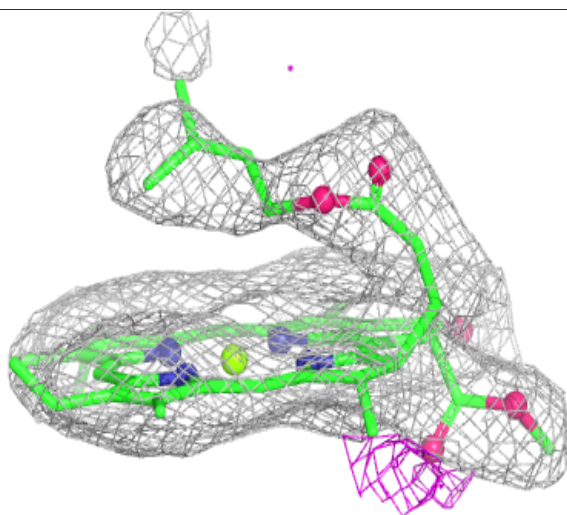
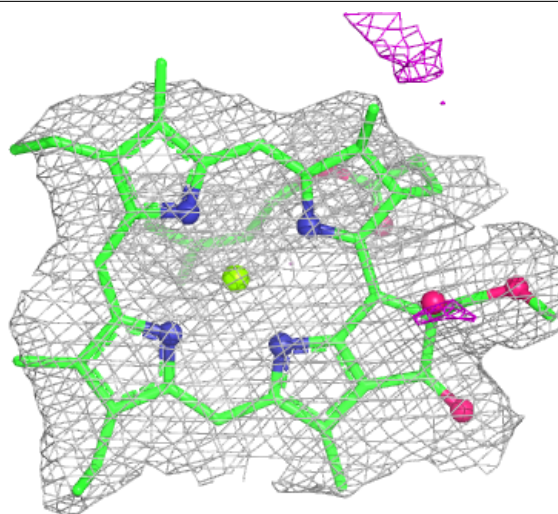
**Electron density around CLA Y 822:**

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



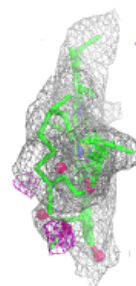
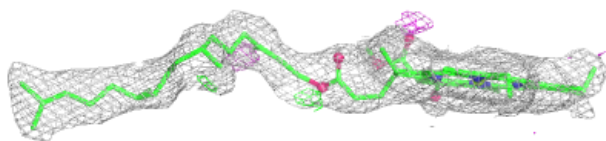
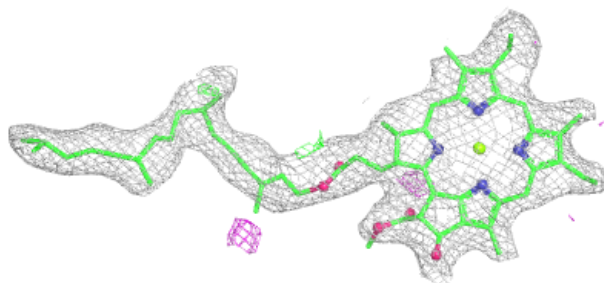
Electron density around CLA Y 823:

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



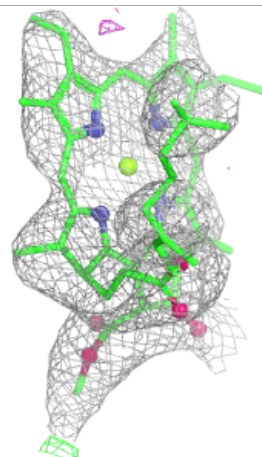
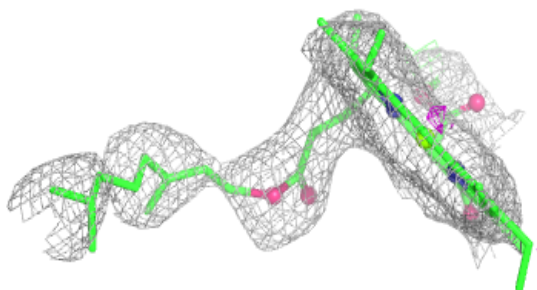
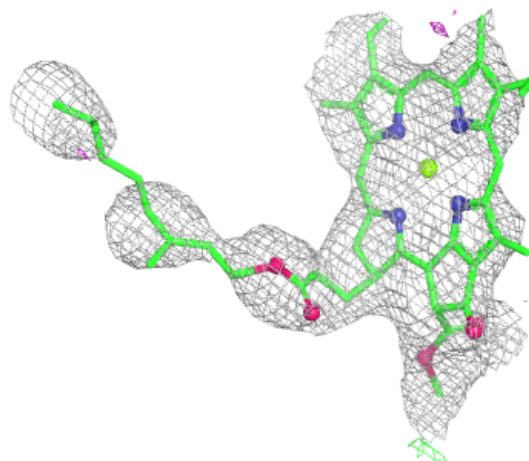
Electron density around CLA Y 832:

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



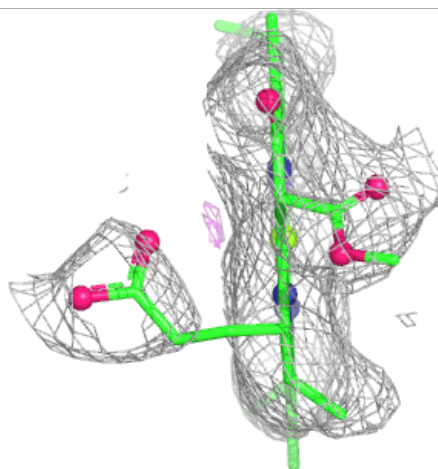
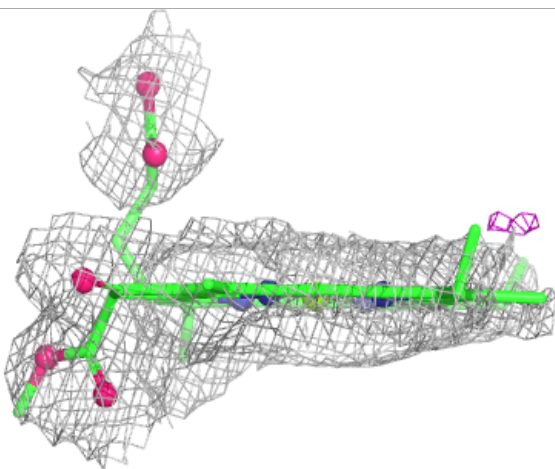
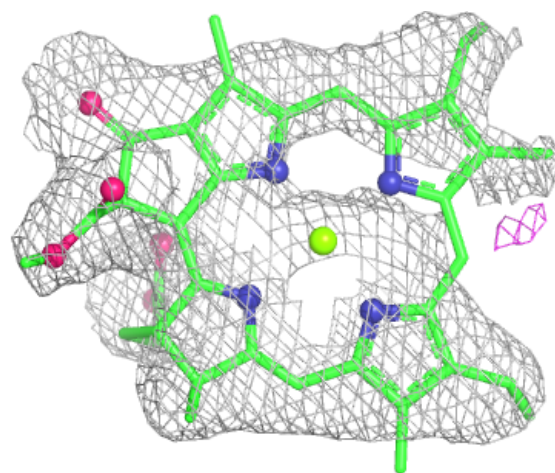
Electron density around CLA Y 833:

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



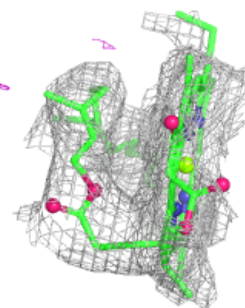
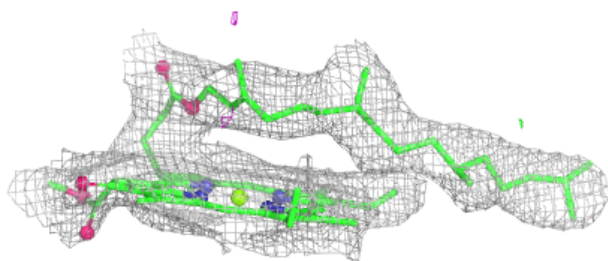
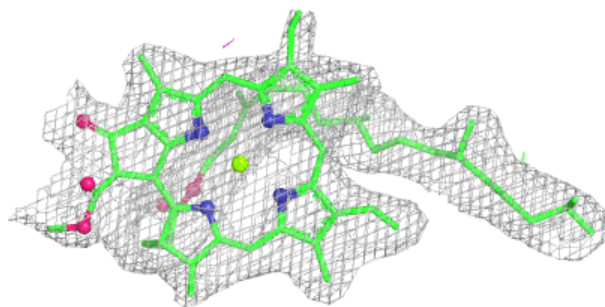
Electron density around CLA Y 834:

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

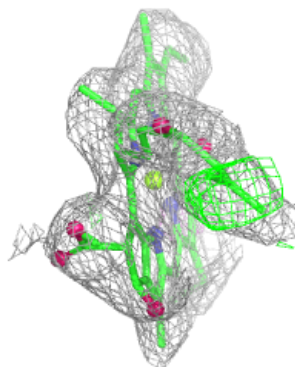
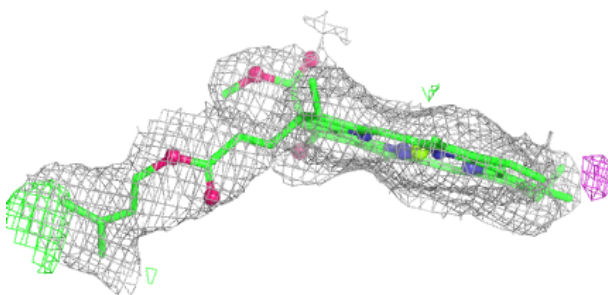
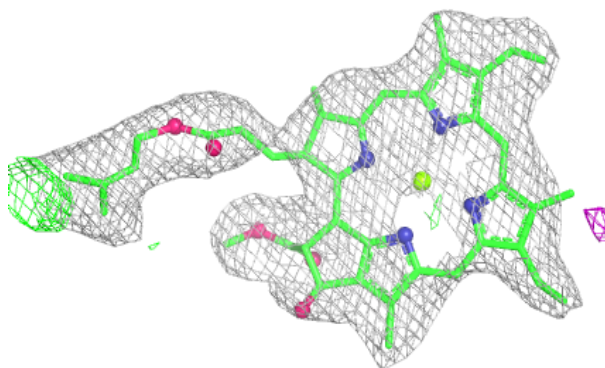


Electron density around CLA Y 838:

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

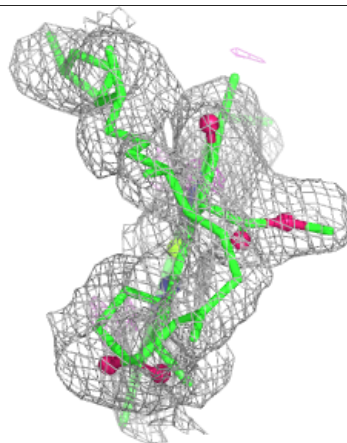
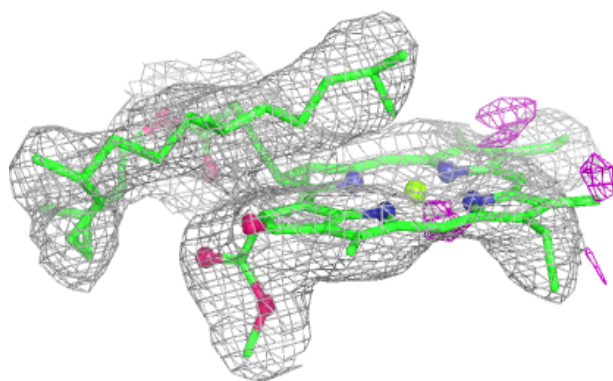
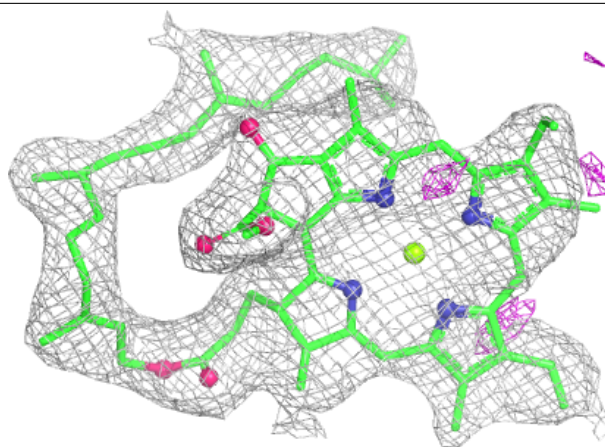
**Electron density around CLA Y 839:**

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



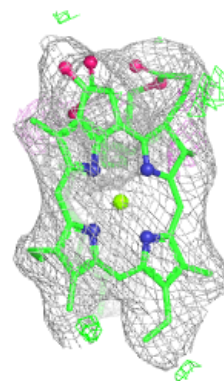
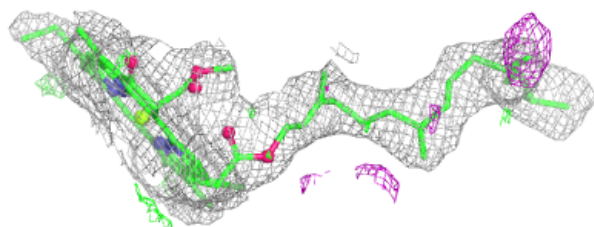
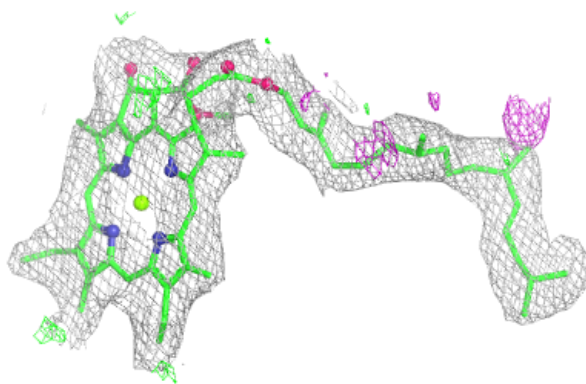
Electron density around CLA Z 806:

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



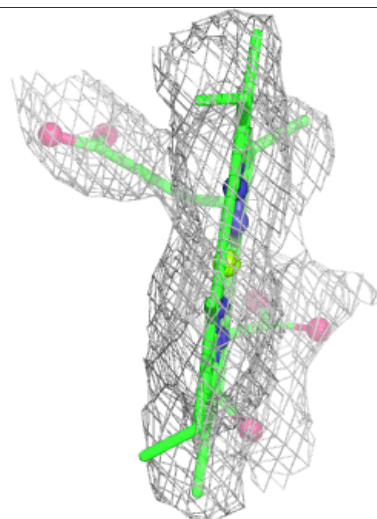
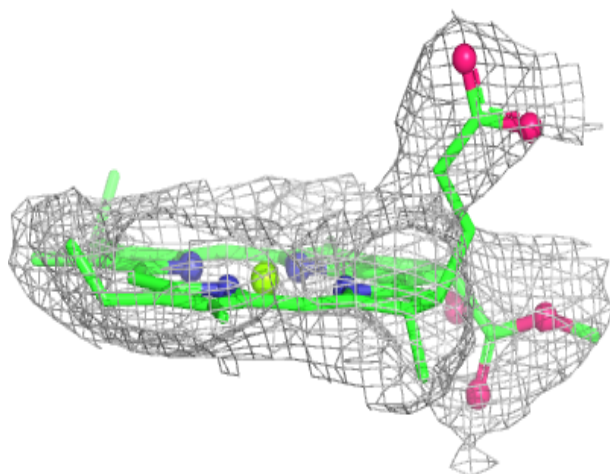
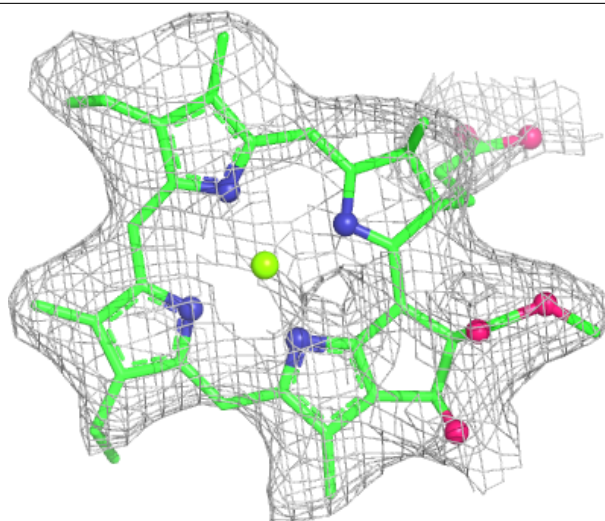
Electron density around CLA Z 811:

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



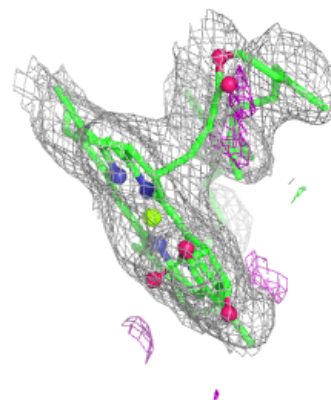
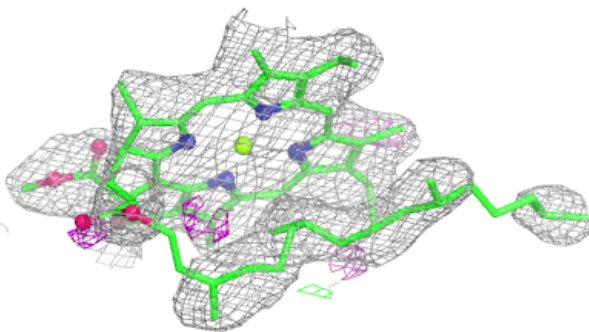
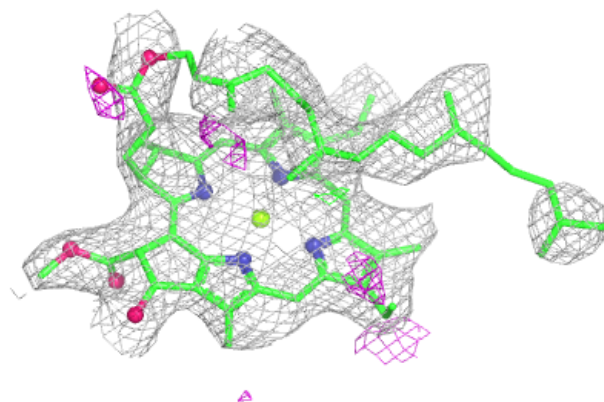
Electron density around CLA Z 813:

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



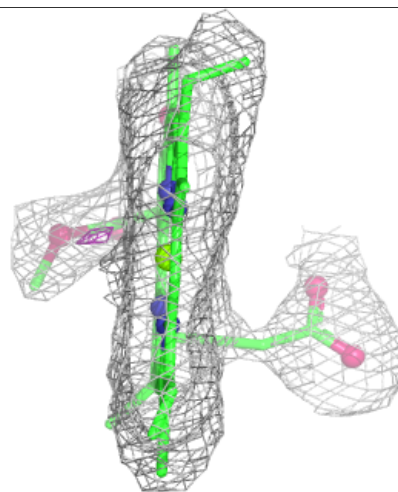
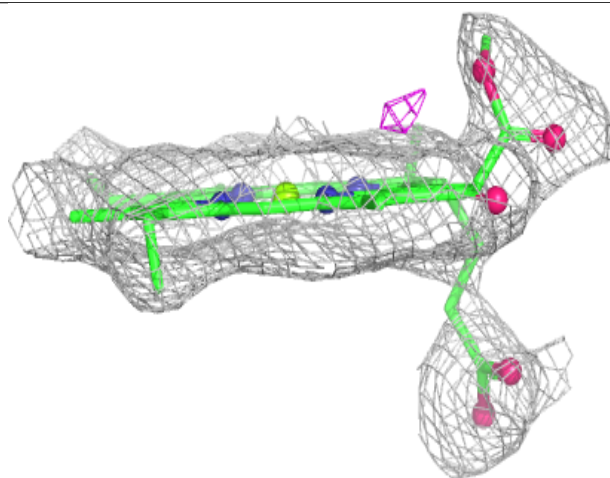
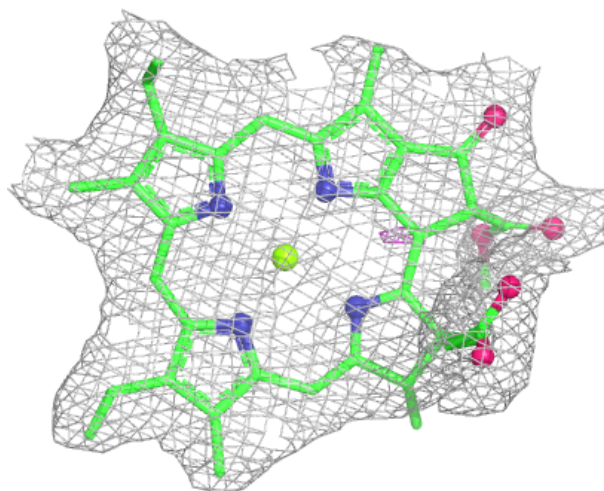
Electron density around CLA Z 818:

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



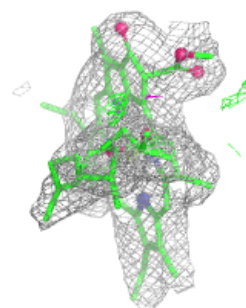
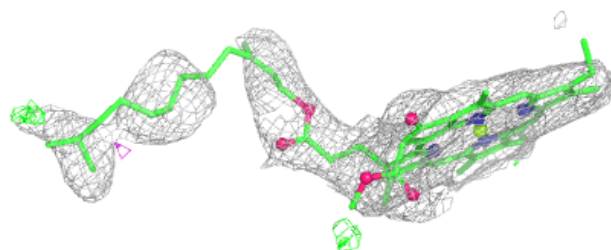
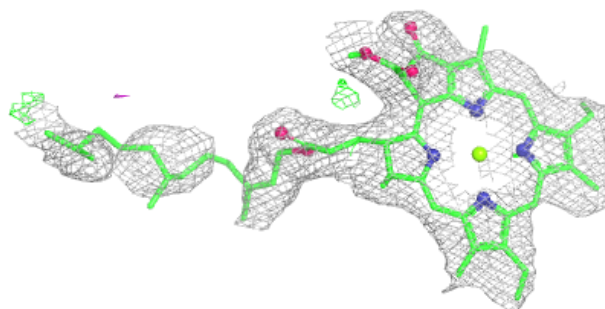
Electron density around CLA Z 822:

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

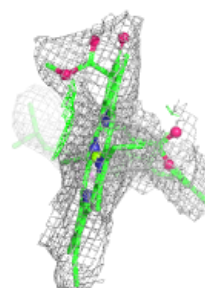
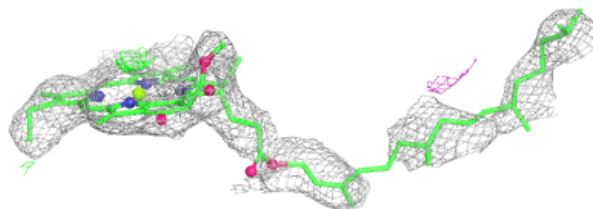
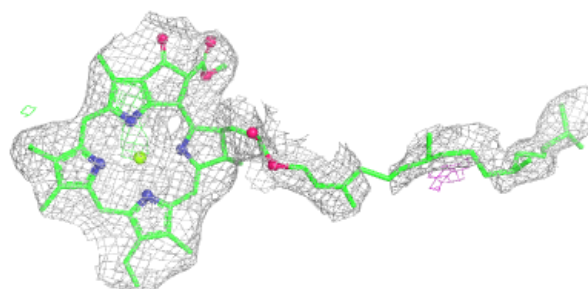


Electron density around CLA Z 824:

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

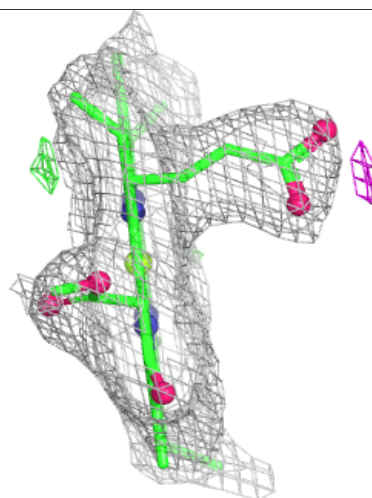
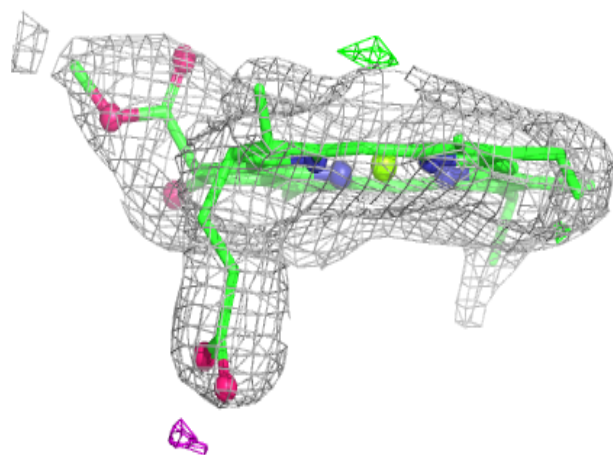
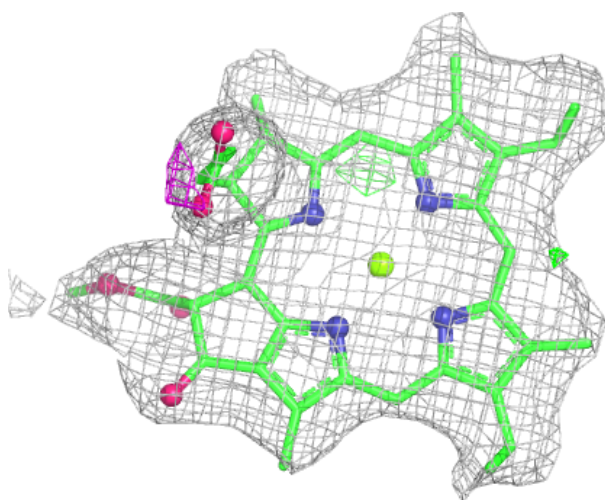
**Electron density around CLA Z 826:**

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



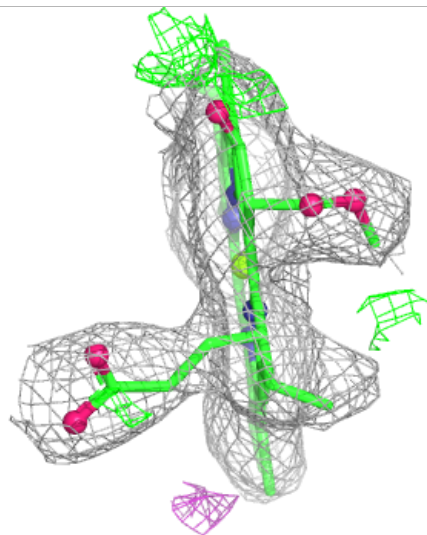
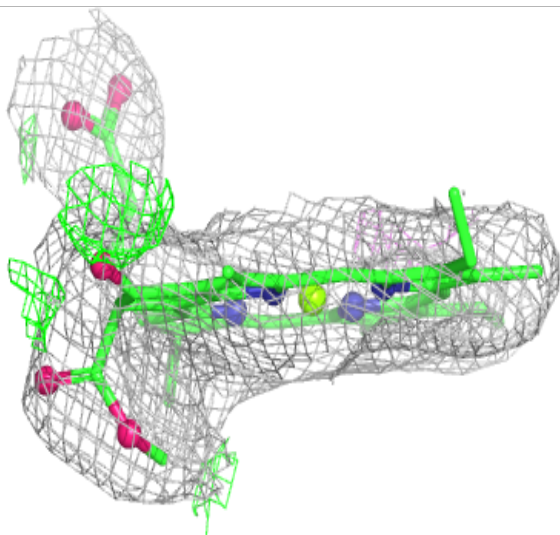
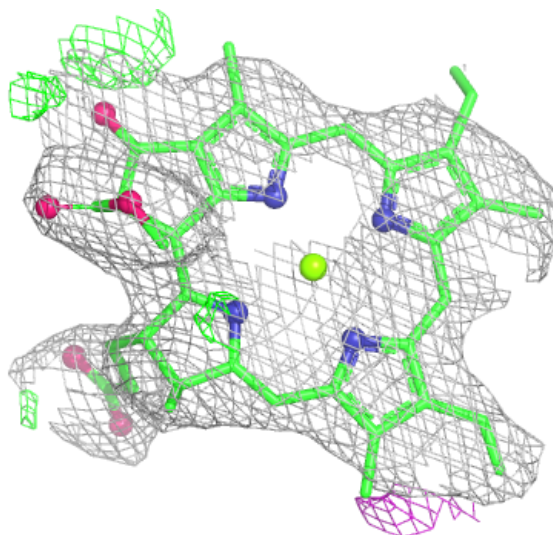
Electron density around CLA Z 832:

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



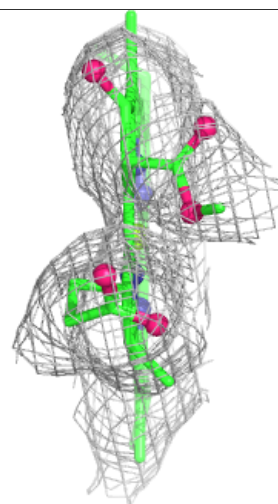
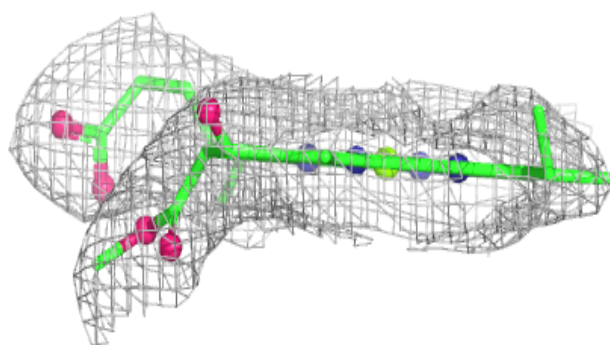
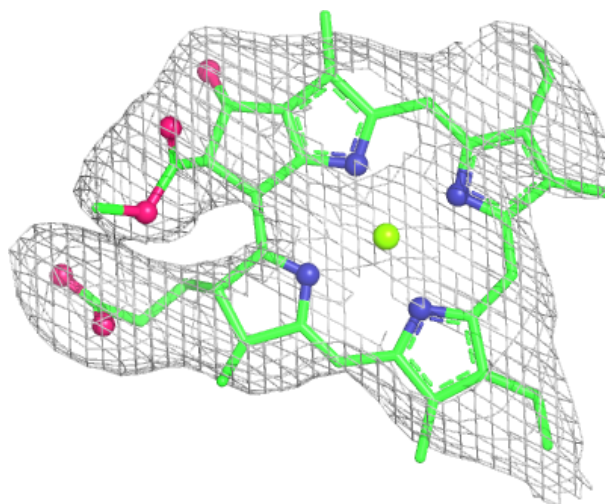
Electron density around CLA Z 834:

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



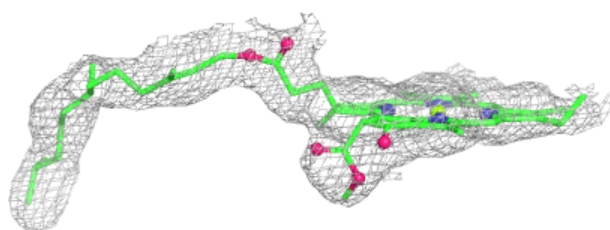
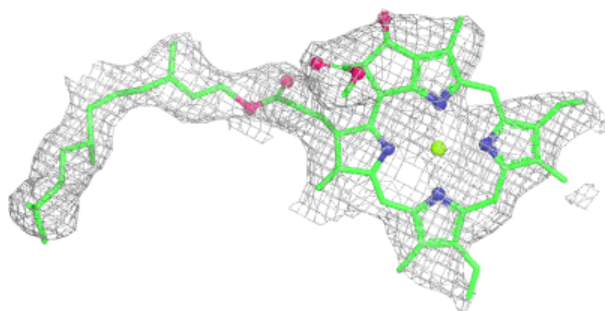
Electron density around CLA Z 836:

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



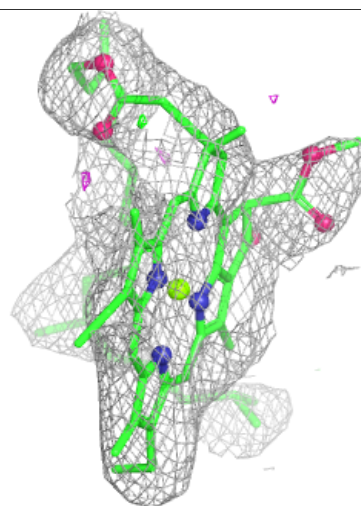
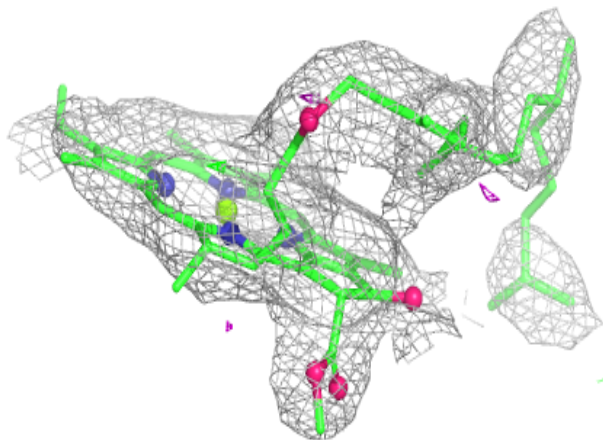
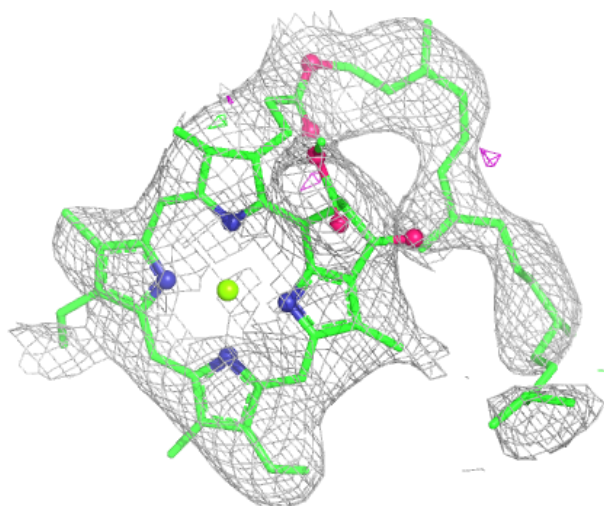
Electron density around CLA Z 837:

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



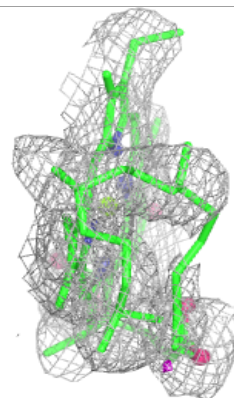
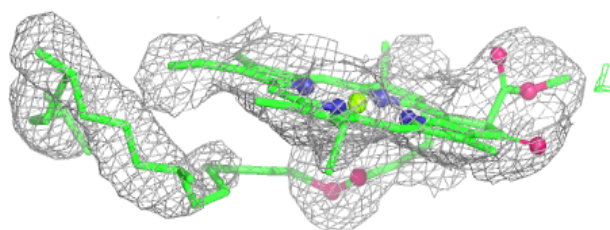
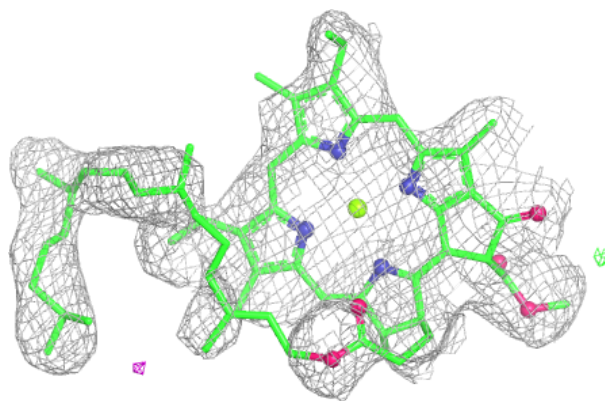
Electron density around CLA d 201:

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



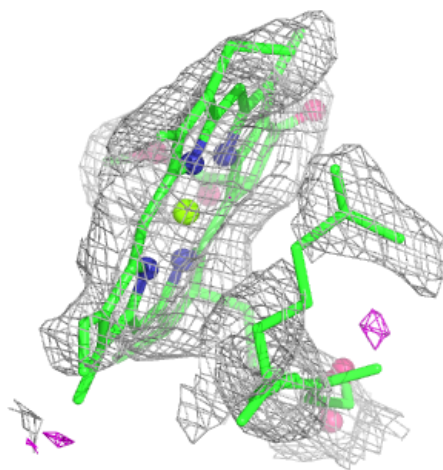
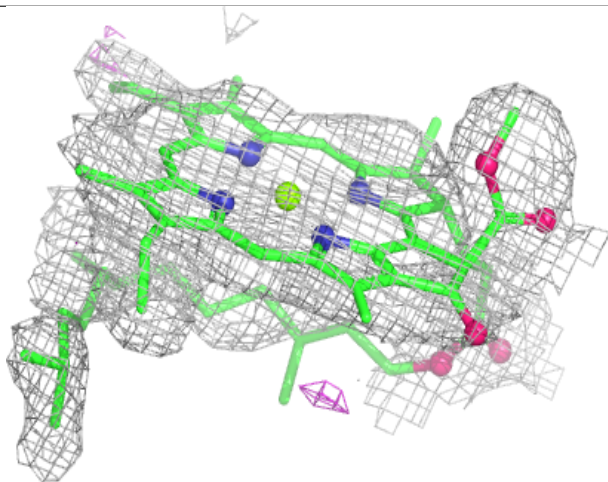
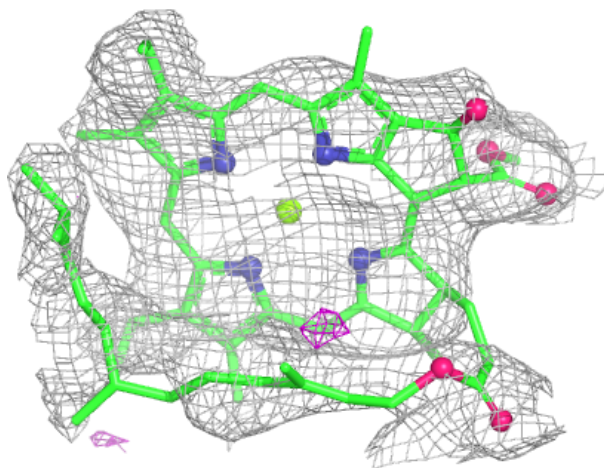
Electron density around CLA A 820:

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



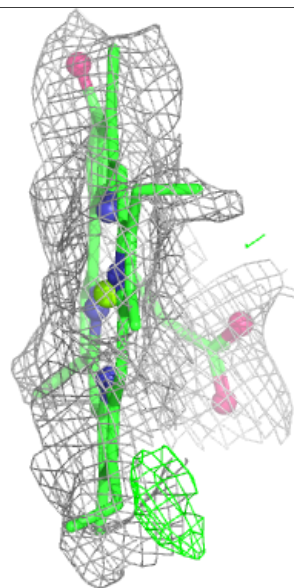
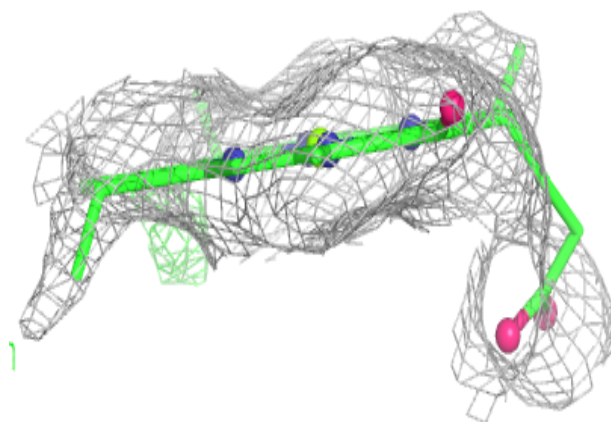
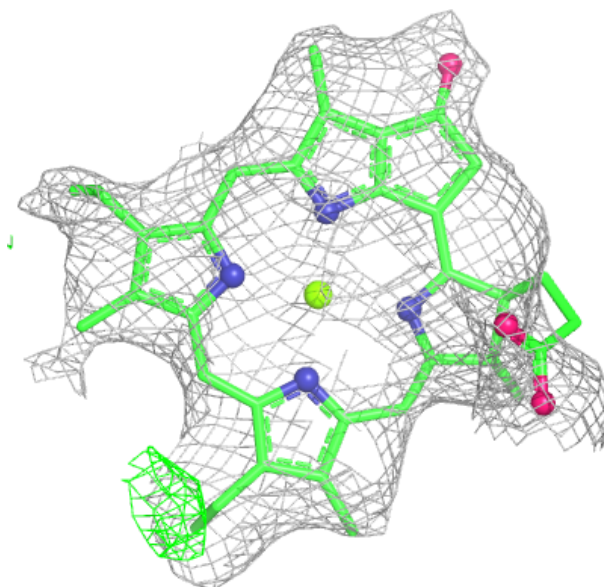
Electron density around CLA A 821:

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



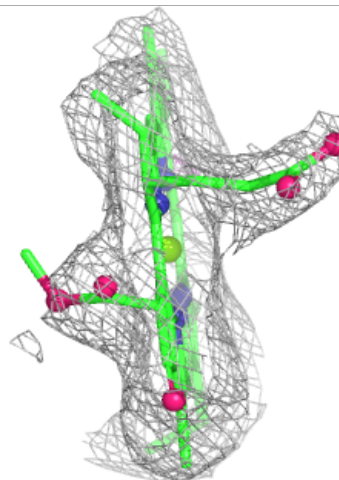
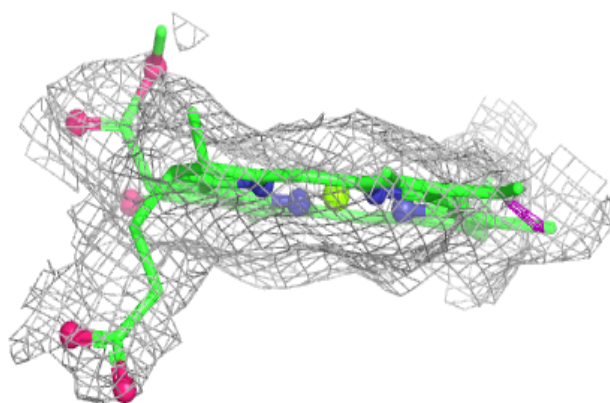
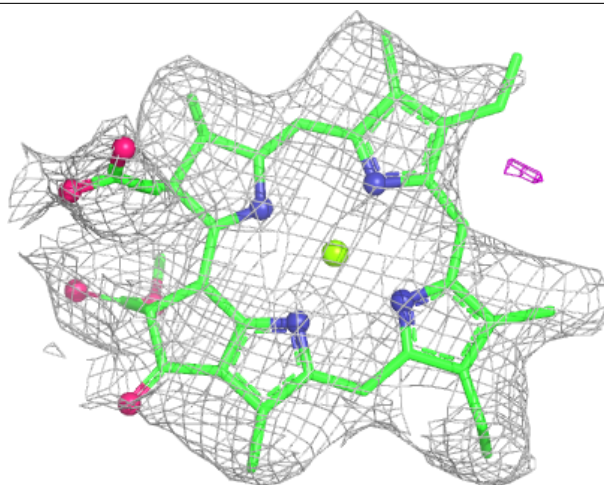
Electron density around CLA g 101:

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



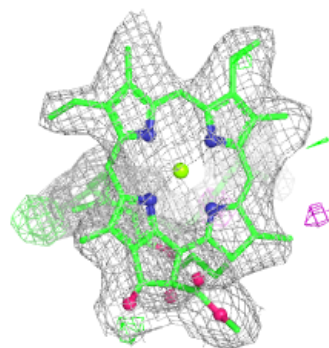
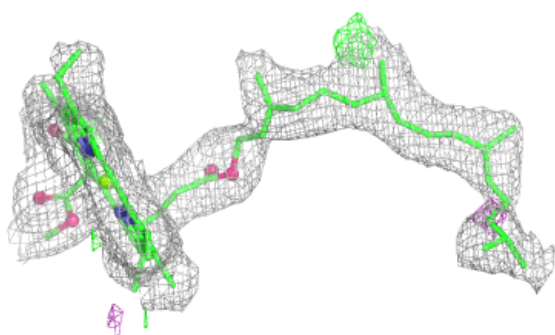
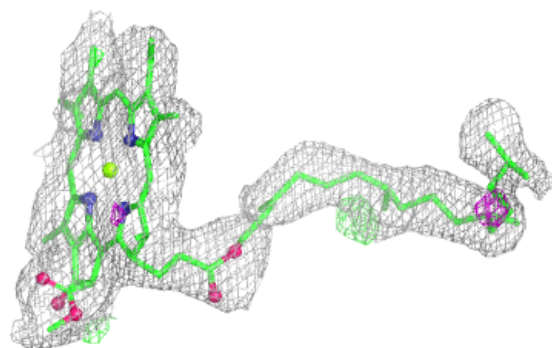
Electron density around CLA g 102:

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

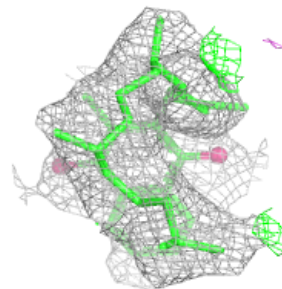
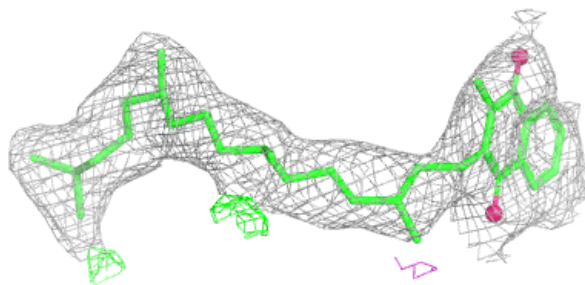
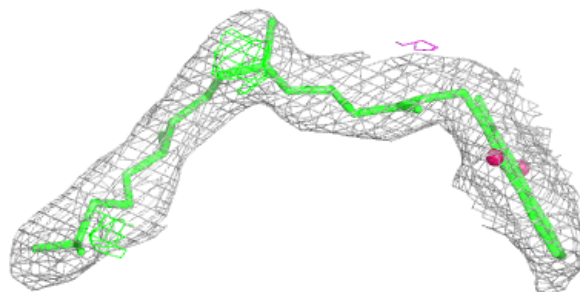


Electron density around CLA h 205:

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

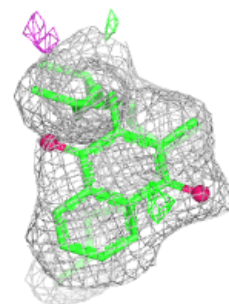
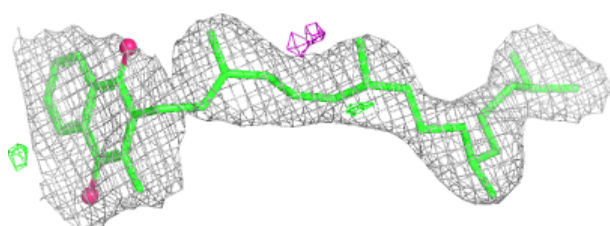
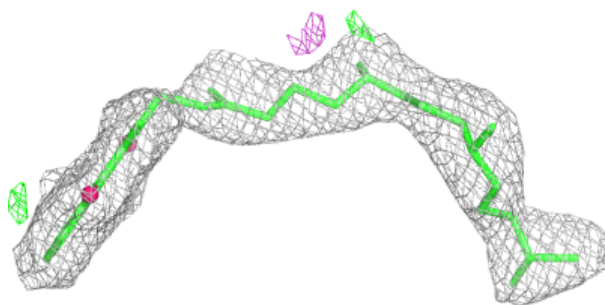
**Electron density around PQN B 841:**

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

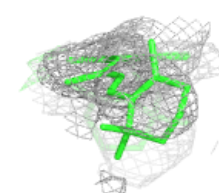
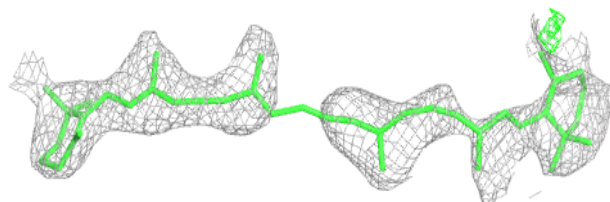
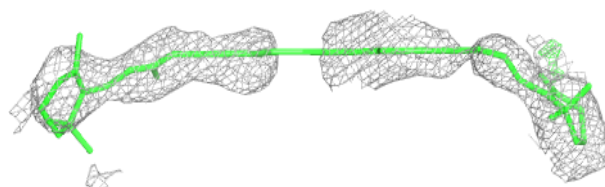


Electron density around PQN Z 842:

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

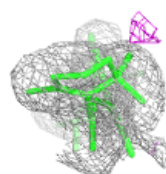
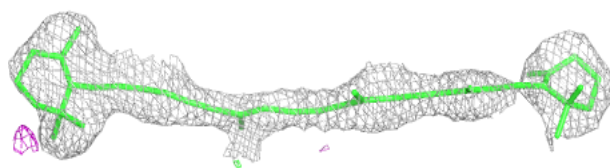
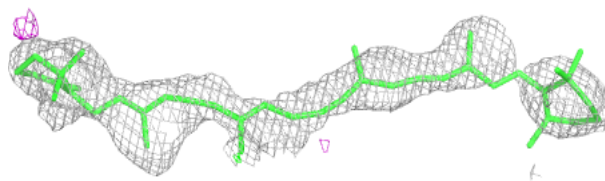
**Electron density around BCR A 846:**

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

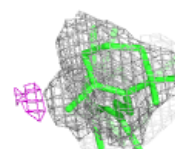
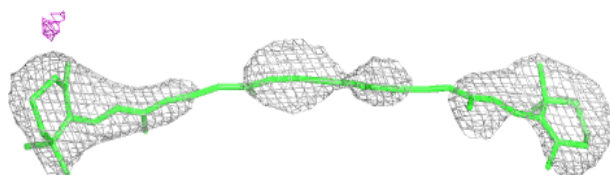
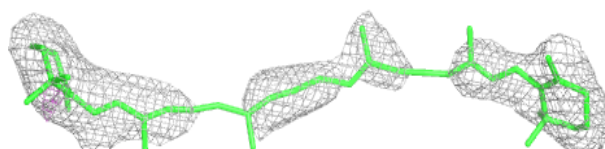


Electron density around BCR A 847:

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

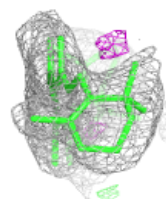
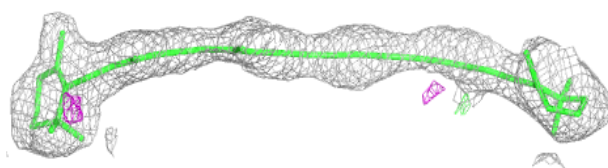
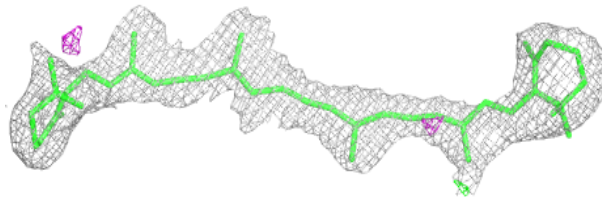
**Electron density around BCR A 848:**

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



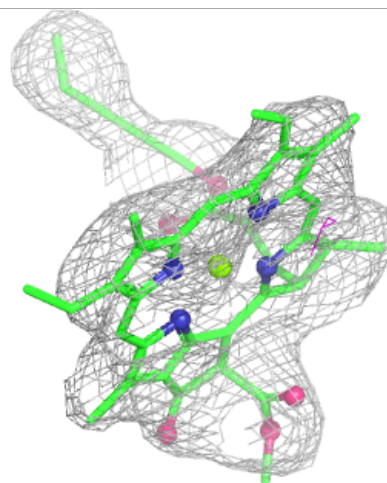
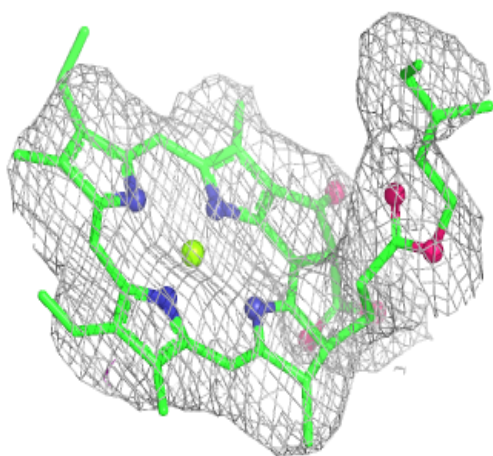
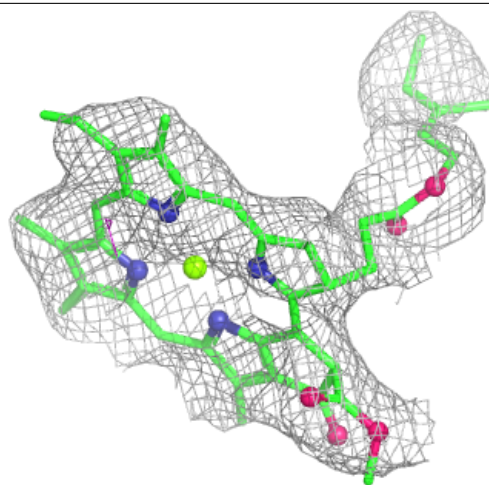
Electron density around BCR A 850:

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



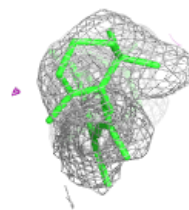
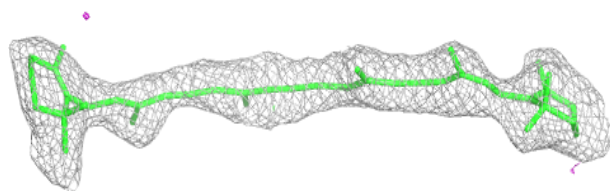
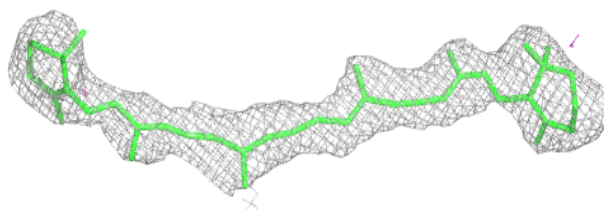
Electron density around CLA A 808:

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

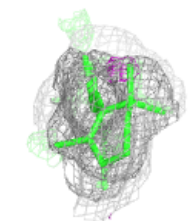
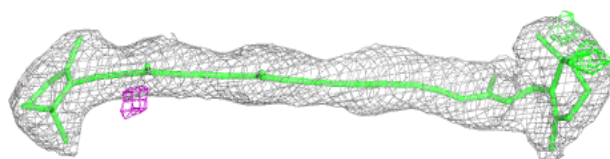
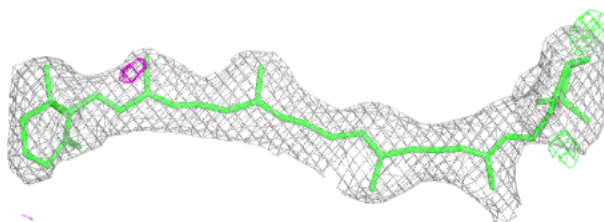


Electron density around BCR B 846:

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

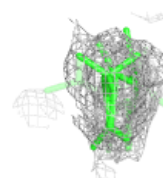
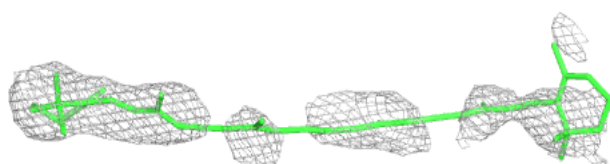
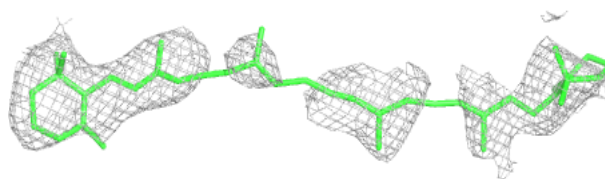
**Electron density around BCR B 847:**

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

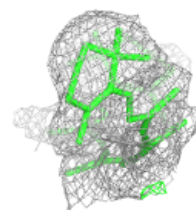
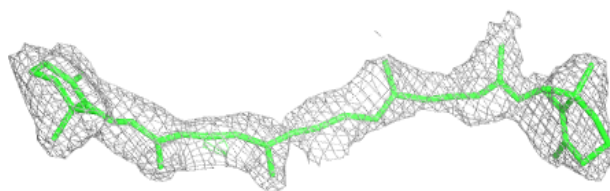
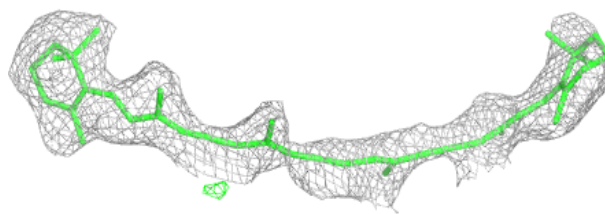


Electron density around BCR B 850:

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

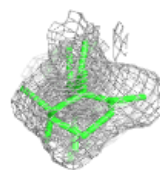
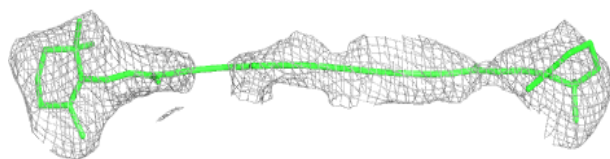
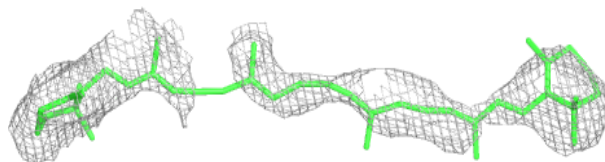
**Electron density around BCR F 201:**

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

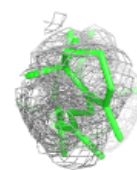
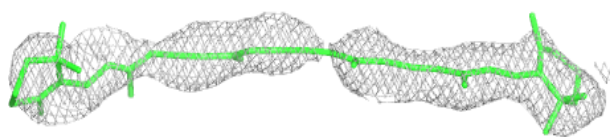
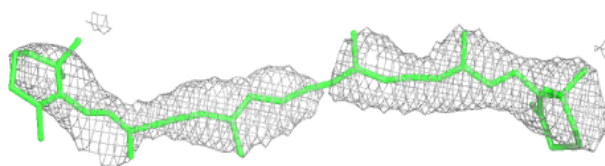


Electron density around BCR G 845:

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

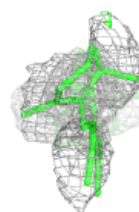
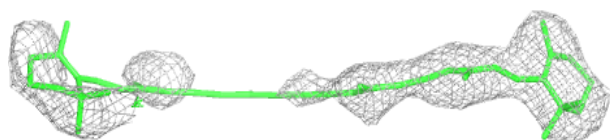
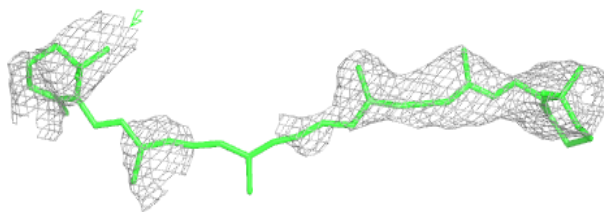
**Electron density around BCR G 846:**

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

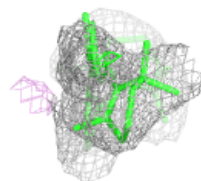
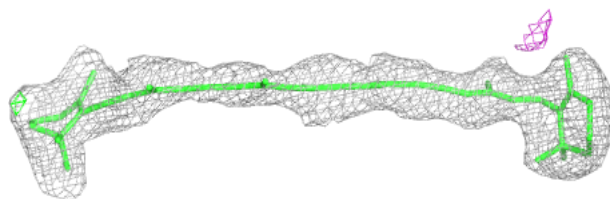
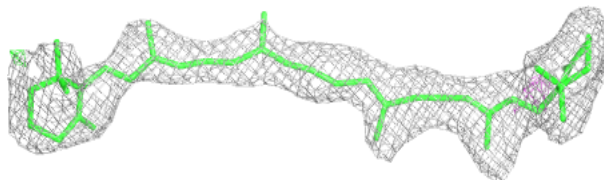


Electron density around BCR G 847:

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

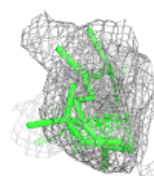
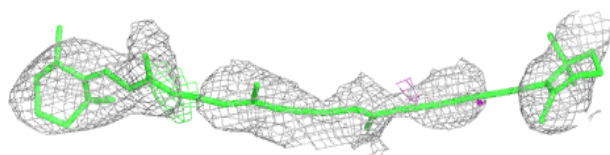
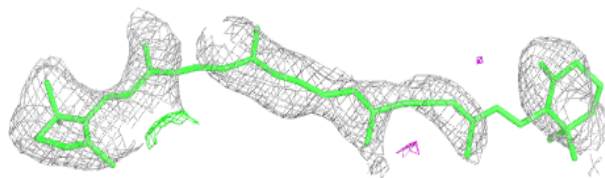
**Electron density around BCR G 848:**

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

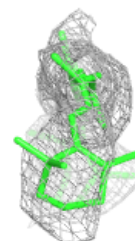
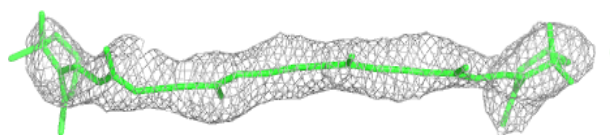
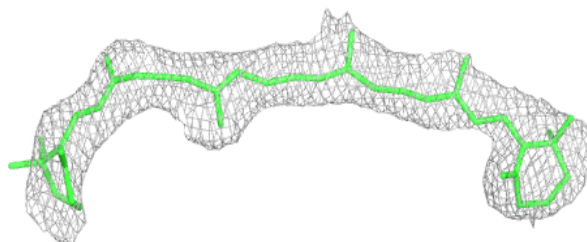


Electron density around BCR H 842:

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

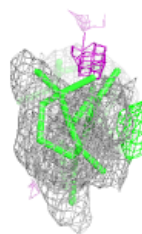
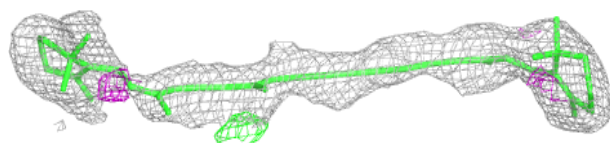
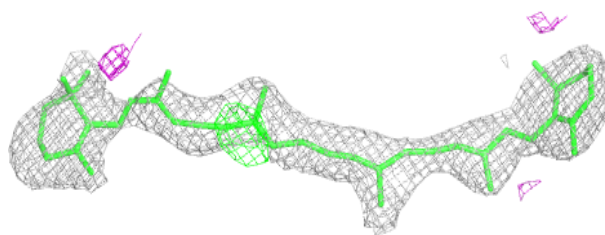
**Electron density around BCR H 843:**

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

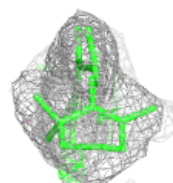
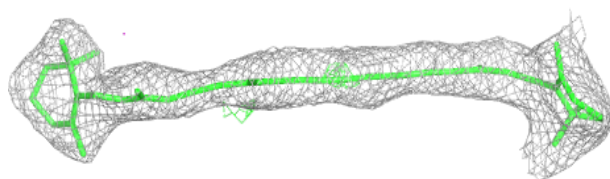


Electron density around BCR H 846:

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

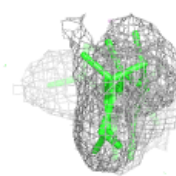
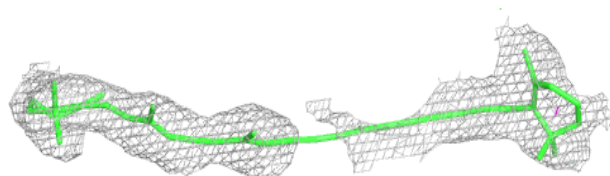
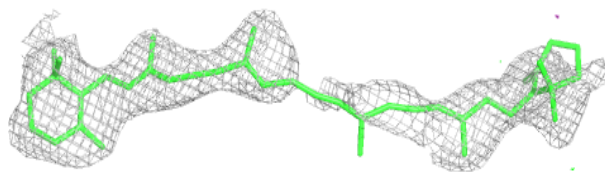
**Electron density around BCR H 847:**

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

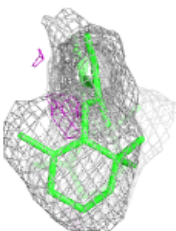
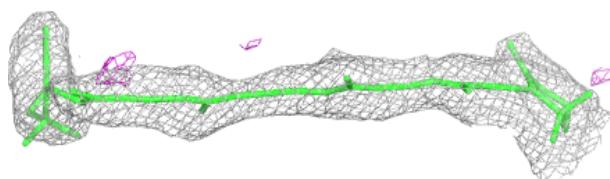
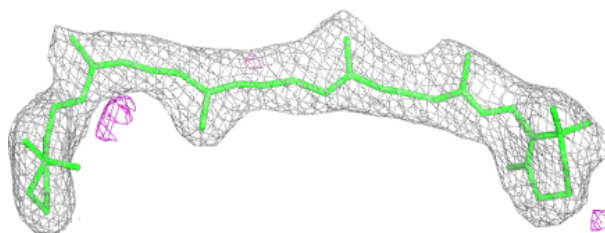


Electron density around BCR H 850:

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

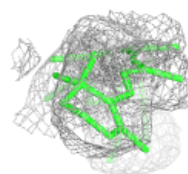
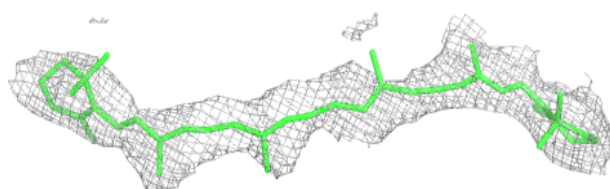
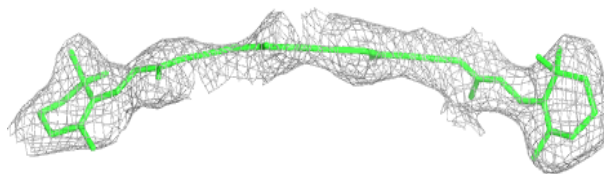
**Electron density around BCR I 102:**

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

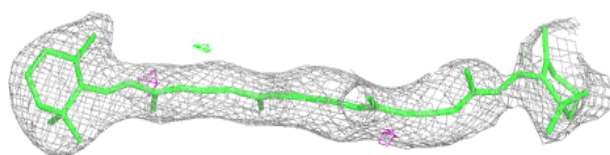


Electron density around BCR J 104:

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

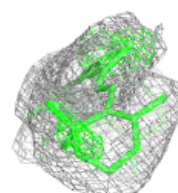
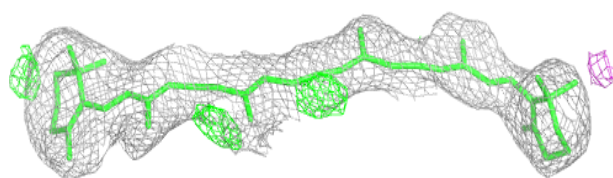
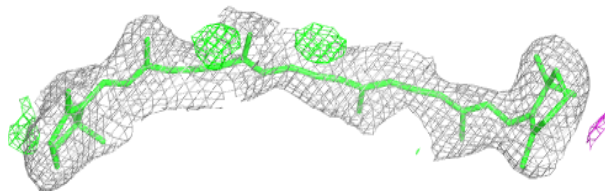
**Electron density around BCR L 208:**

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

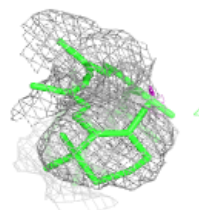
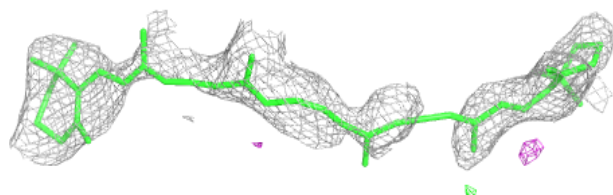
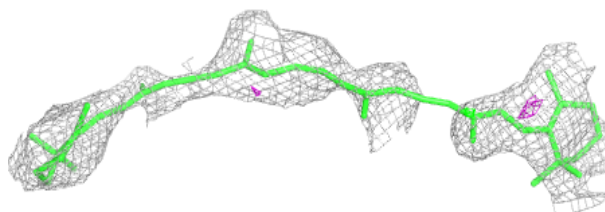


Electron density around BCR M 101:

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

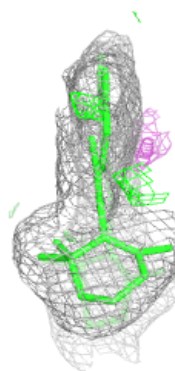
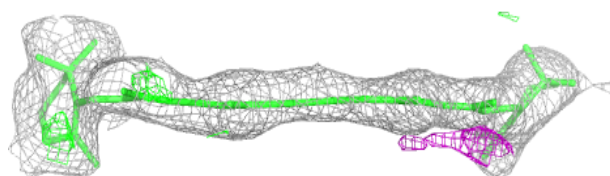
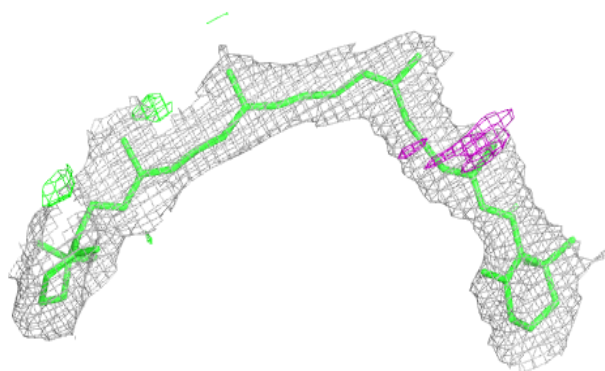
**Electron density around BCR Q 201:**

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

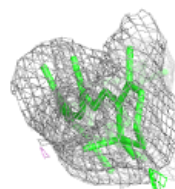
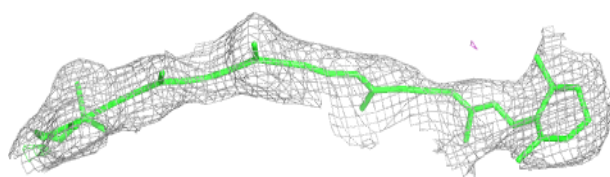
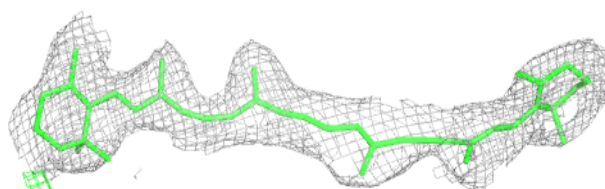


Electron density around BCR Q 203:

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

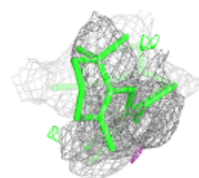
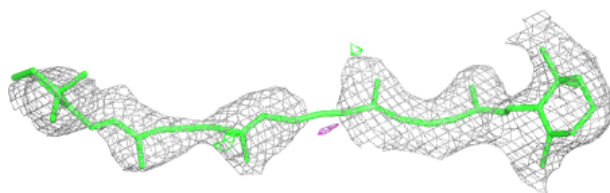
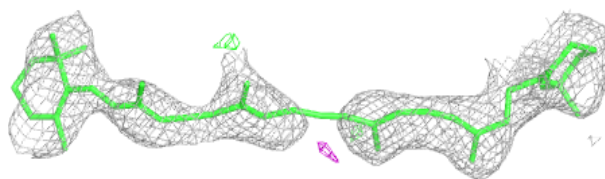
**Electron density around BCR S 1105:**

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

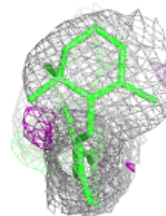
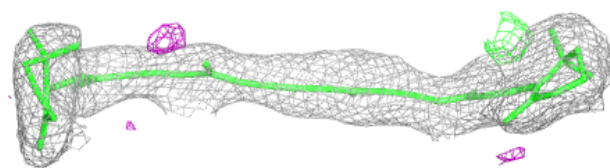
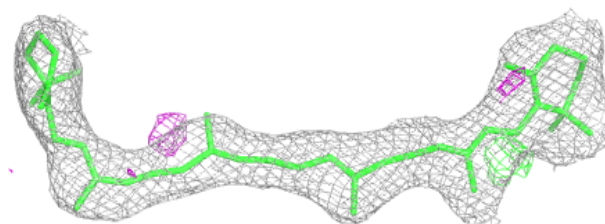


Electron density around BCR T 102:

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

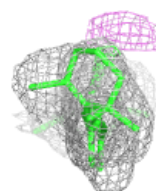
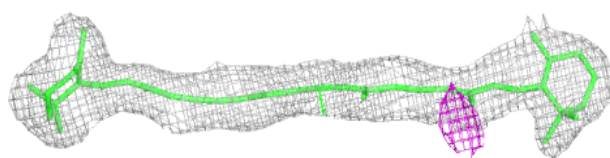
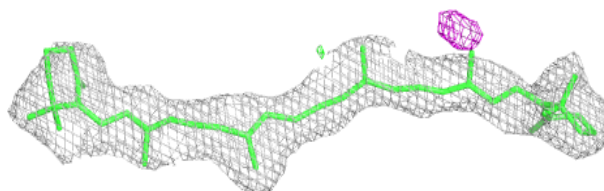
**Electron density around BCR U 1008:**

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

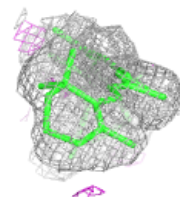
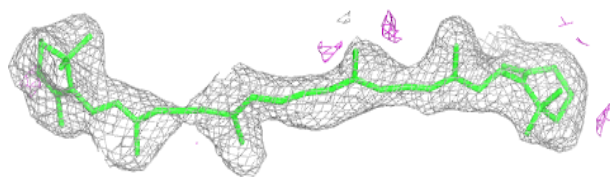
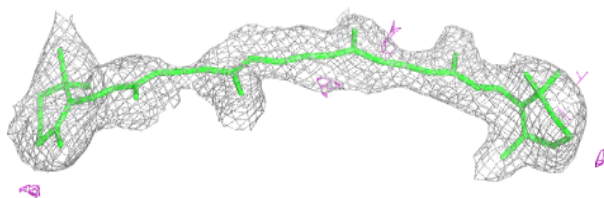


Electron density around BCR U 1009:

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

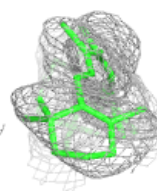
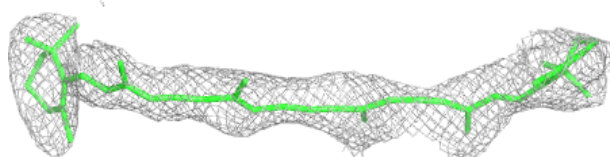
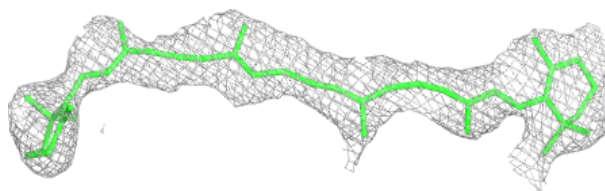
**Electron density around BCR V 101:**

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

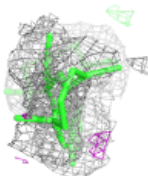
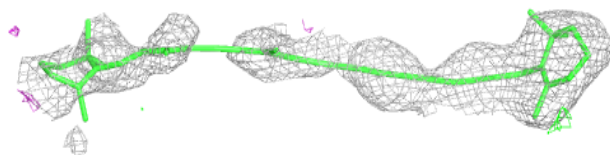
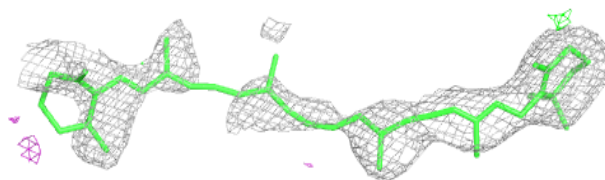


Electron density around BCR Y 844:

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

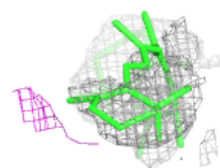
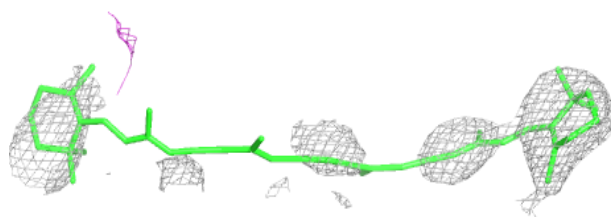
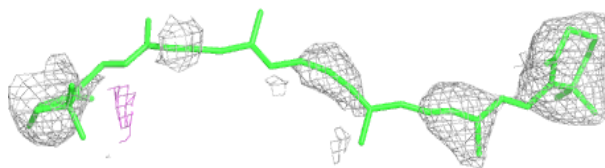
**Electron density around BCR Y 845:**

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

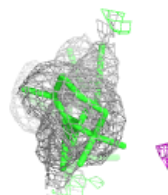
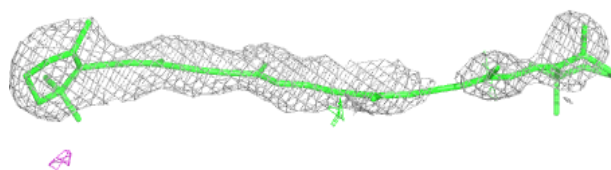
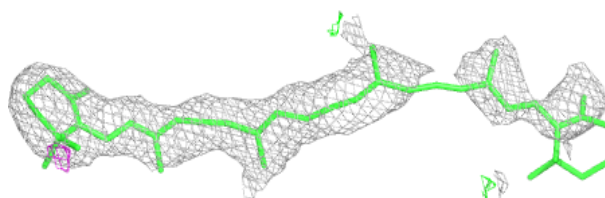


Electron density around BCR Y 846:

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

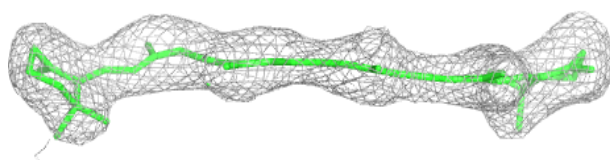
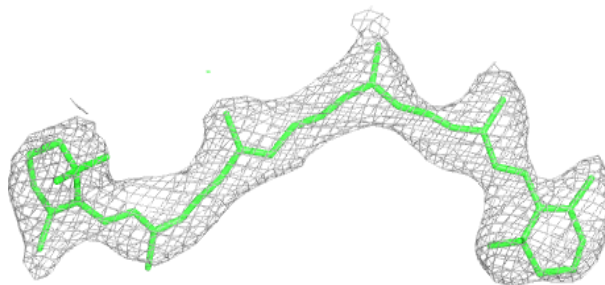
**Electron density around BCR Y 847:**

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

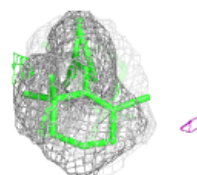
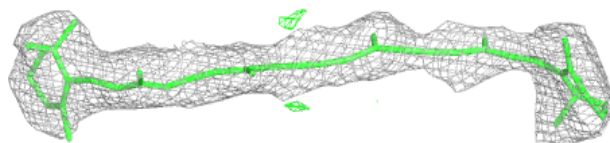
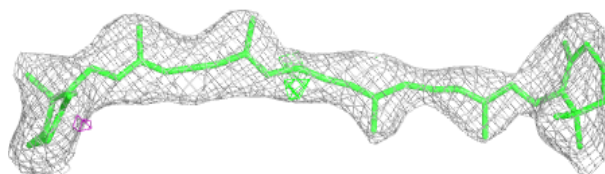


Electron density around BCR Y 849:

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

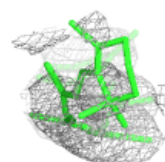
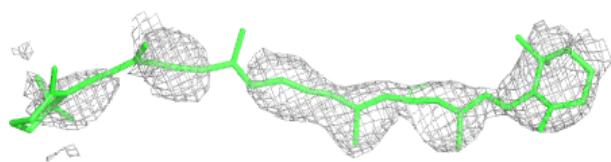
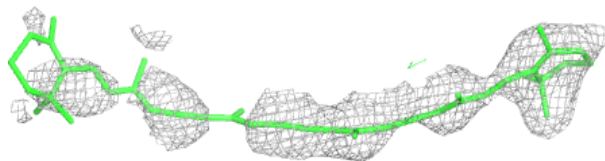
**Electron density around BCR Y 852:**

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

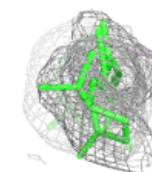
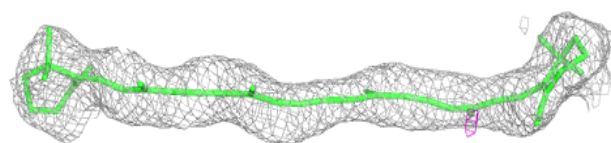
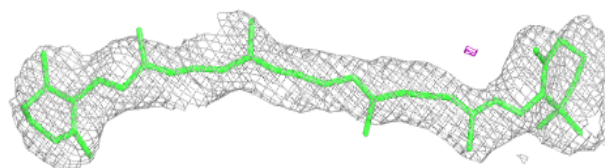


Electron density around BCR Y 853:

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

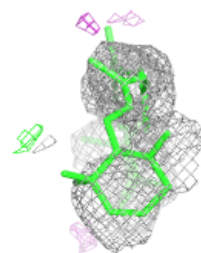
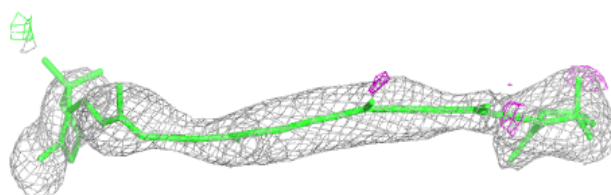
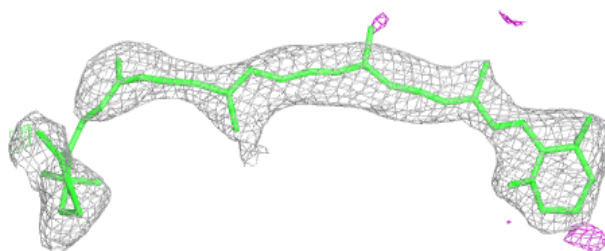
**Electron density around BCR Z 843:**

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

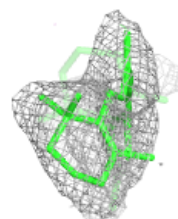
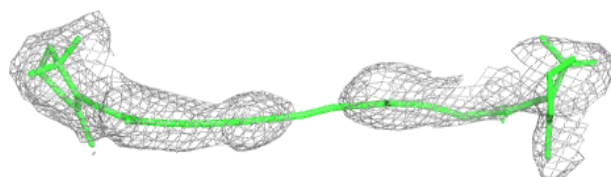
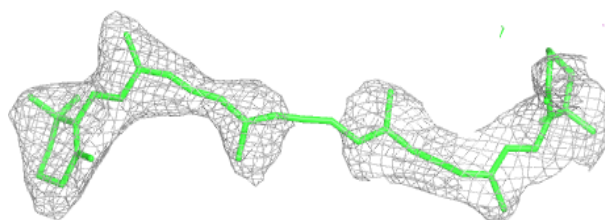


Electron density around BCR Z 844:

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

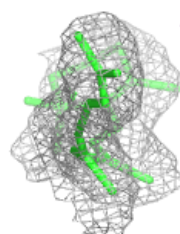
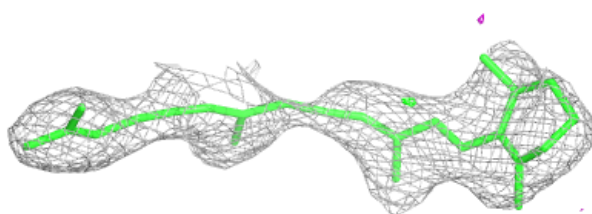
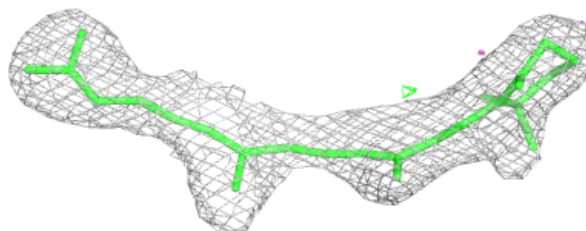
**Electron density around BCR Z 845:**

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

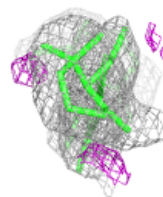
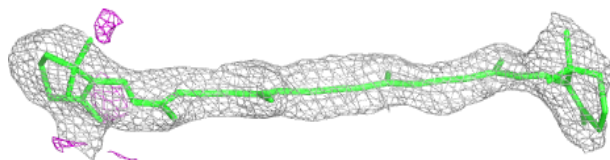
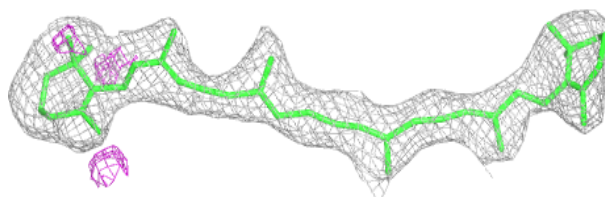


Electron density around BCR Z 846:

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

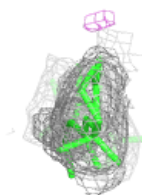
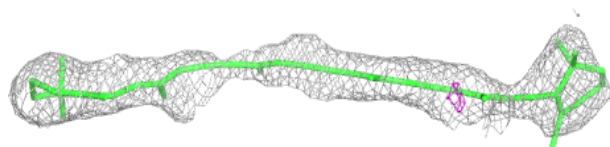
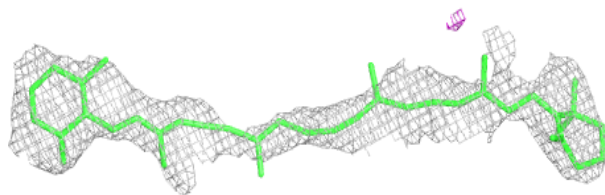
**Electron density around BCR Z 847:**

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

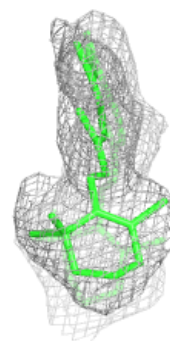
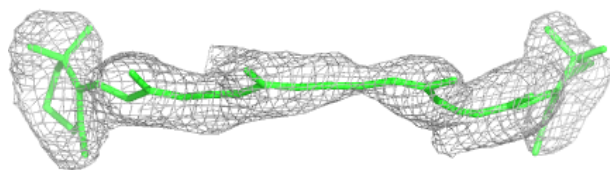
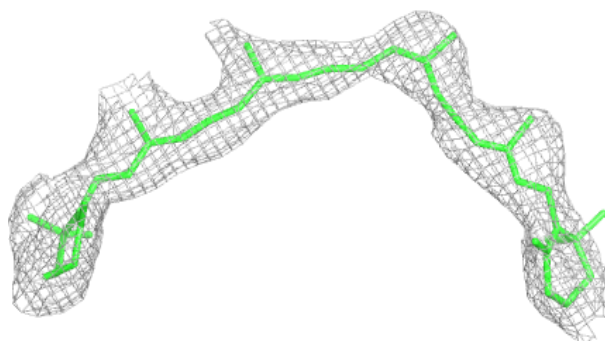


Electron density around BCR Z 850:

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

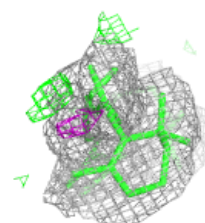
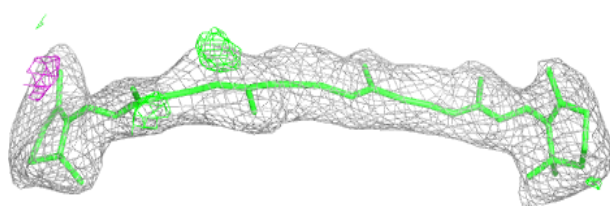
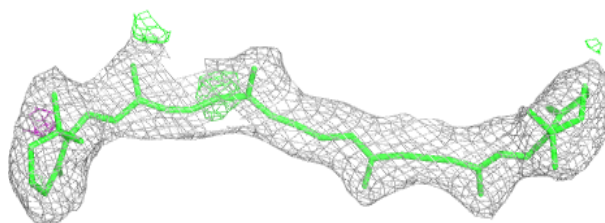
**Electron density around BCR d 203:**

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

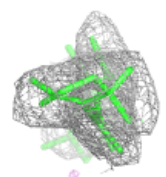
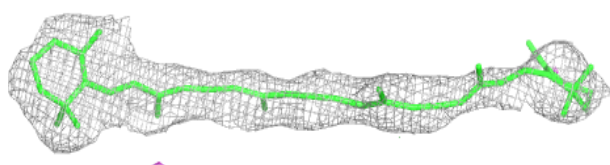
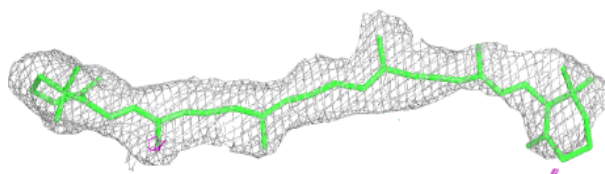


Electron density around BCR e 101:

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

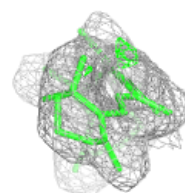
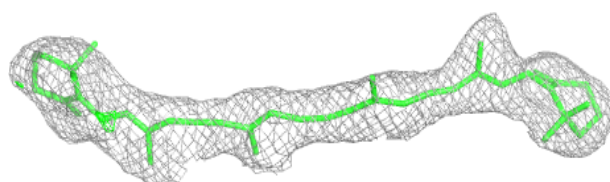
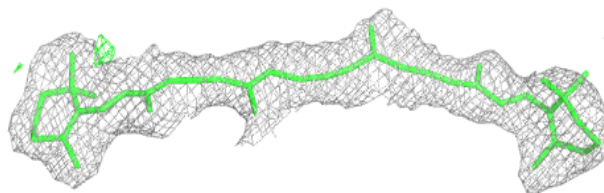
**Electron density around BCR h 202:**

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

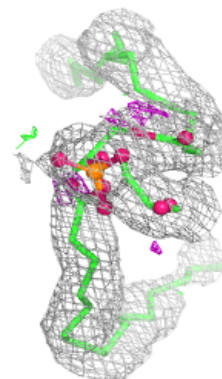
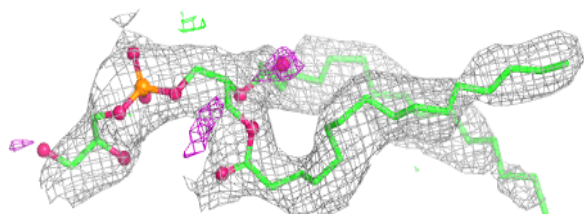
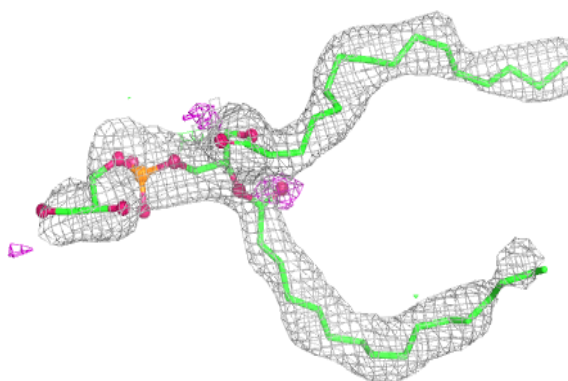


Electron density around BCR i 101:

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

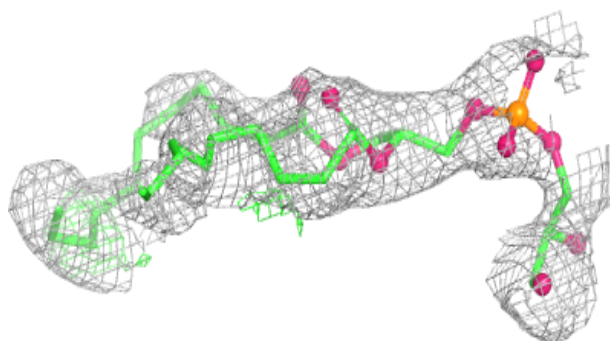
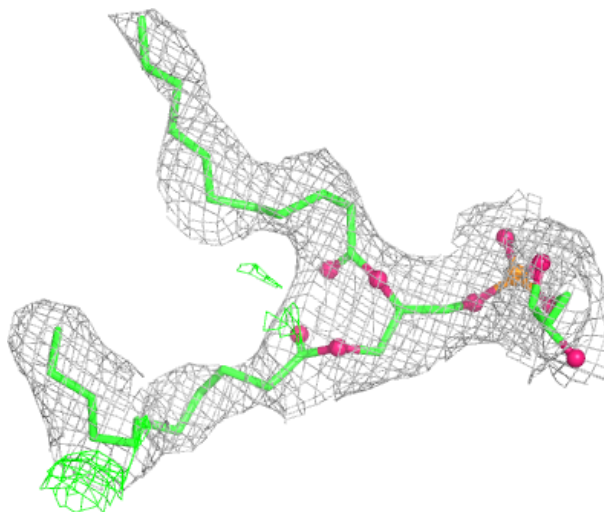
**Electron density around LHG A 852:**

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



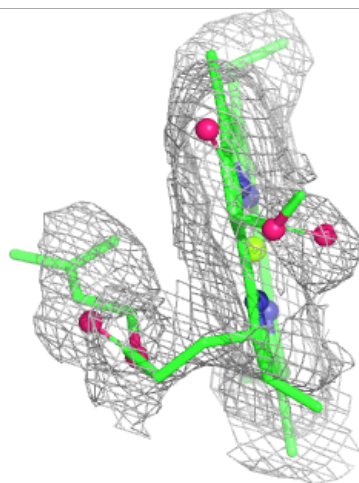
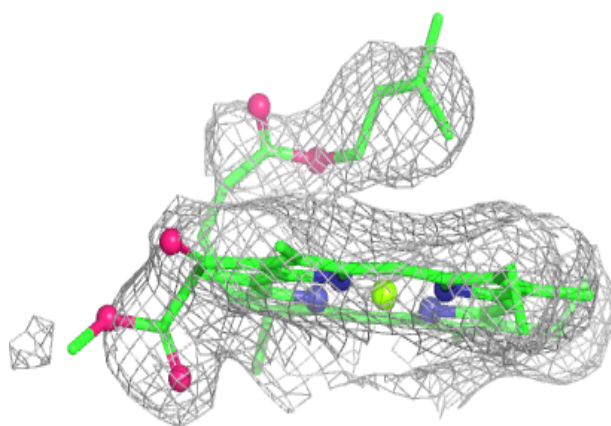
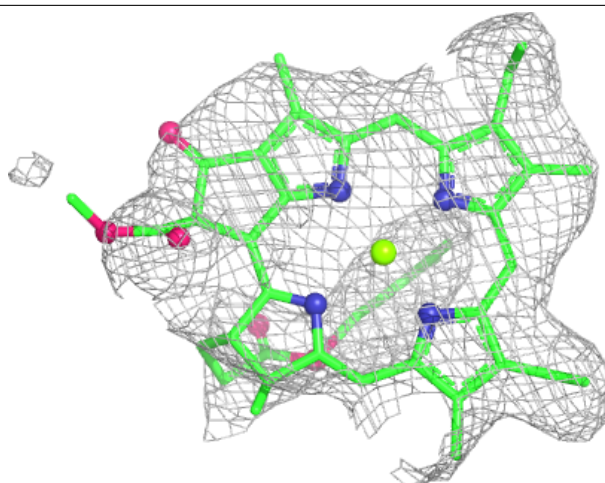
Electron density around LHG B 849:

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



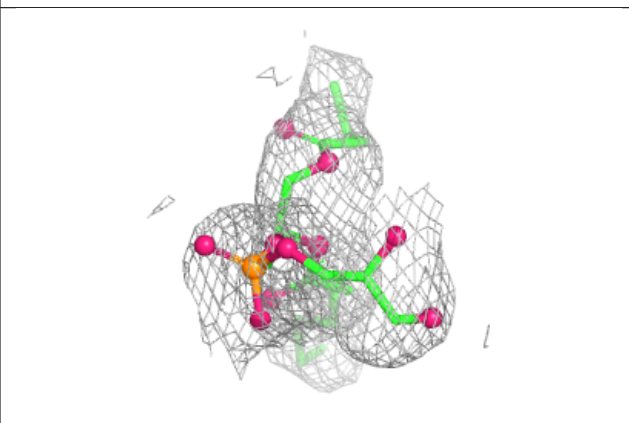
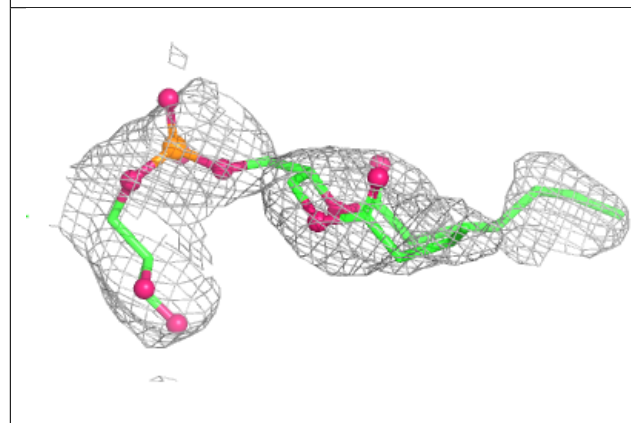
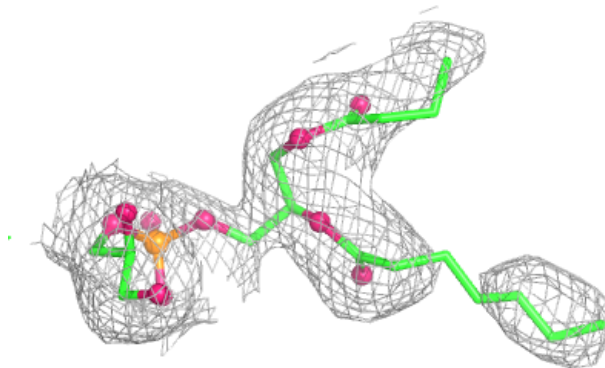
Electron density around CLA A 824:

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

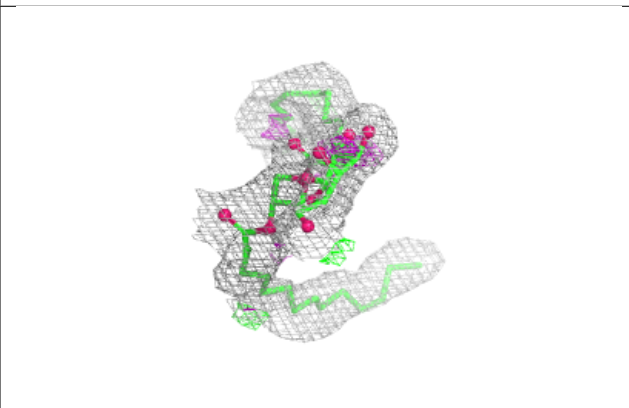
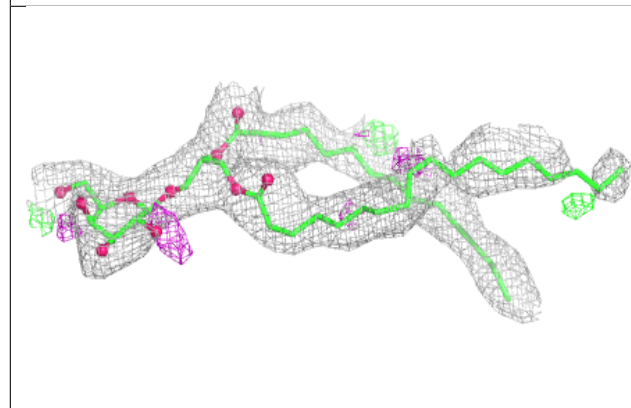
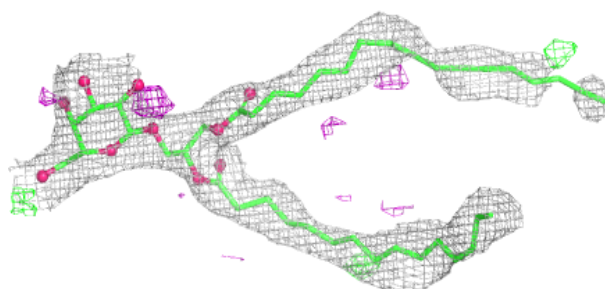


Electron density around LHG j 101:

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

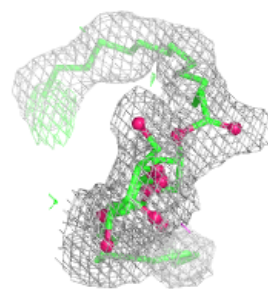
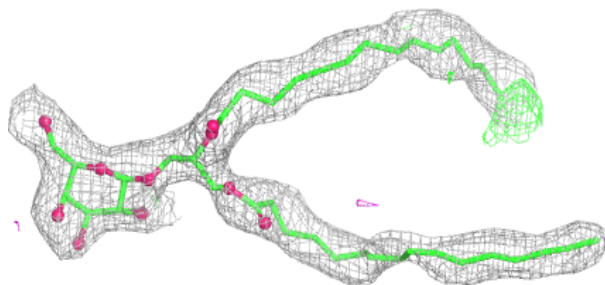
**Electron density around LMG B 848:**

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

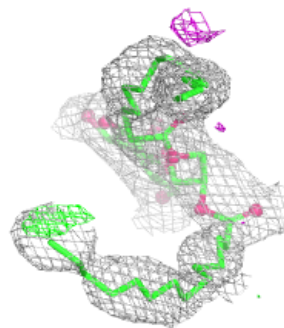
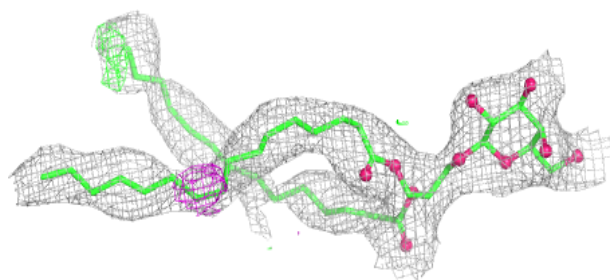
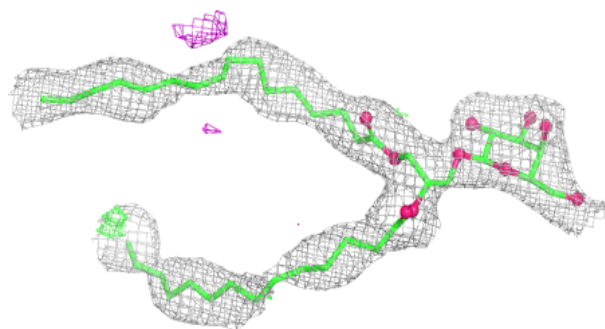


Electron density around LMG H 848:

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

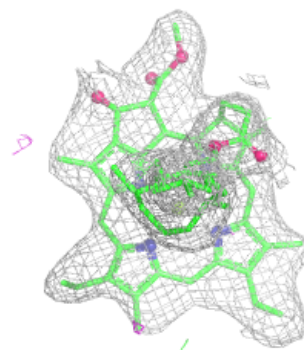
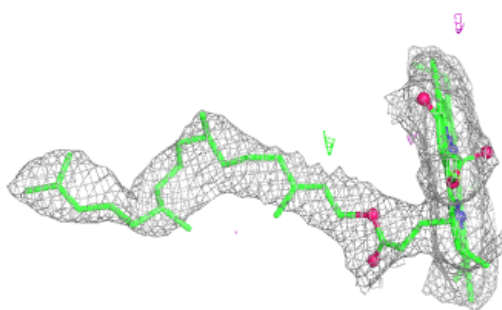
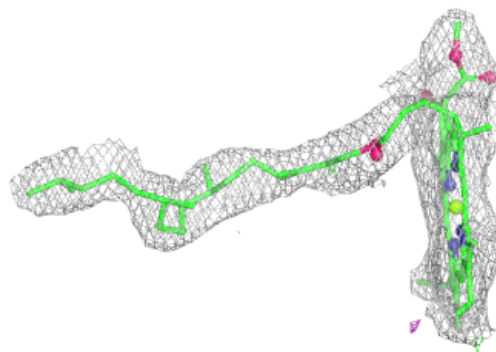
**Electron density around LMG Z 849:**

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



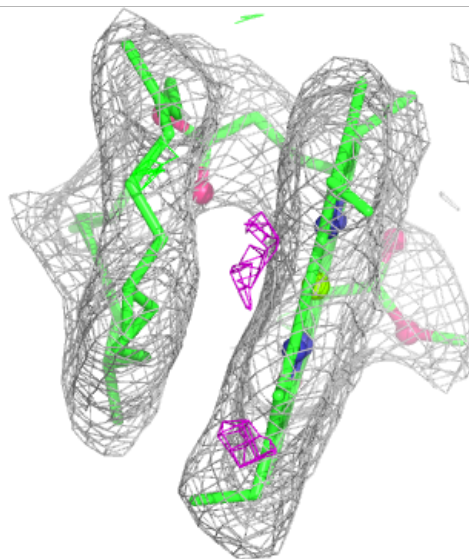
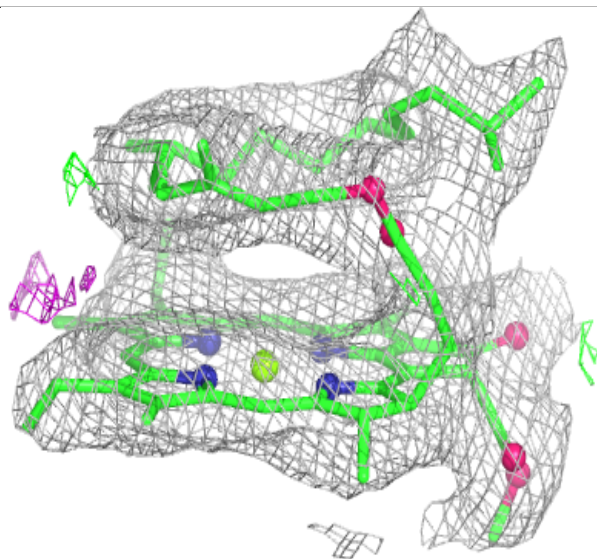
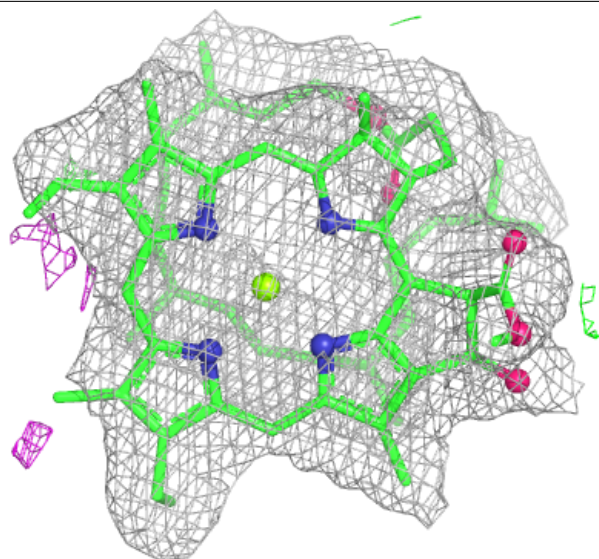
Electron density around CLA A 829:

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



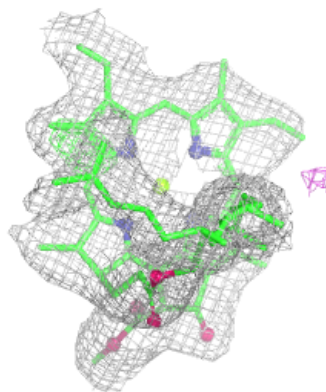
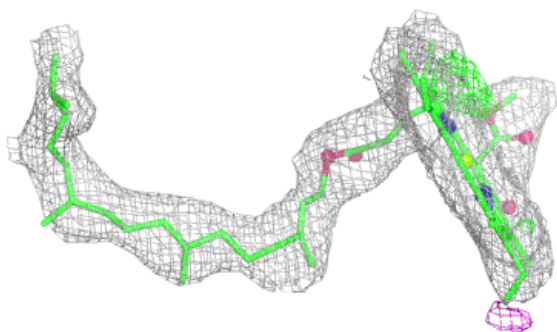
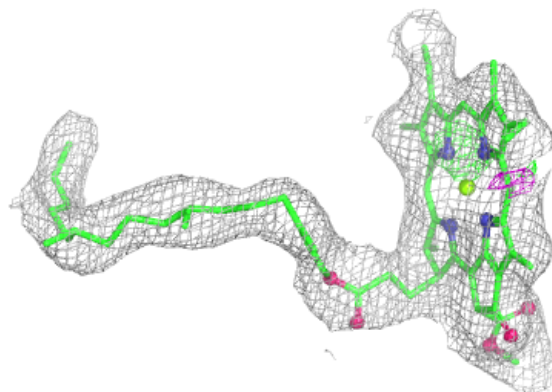
Electron density around CLA U 1002:

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



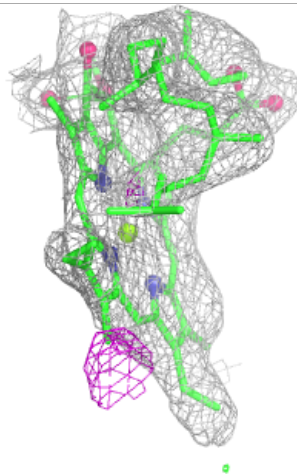
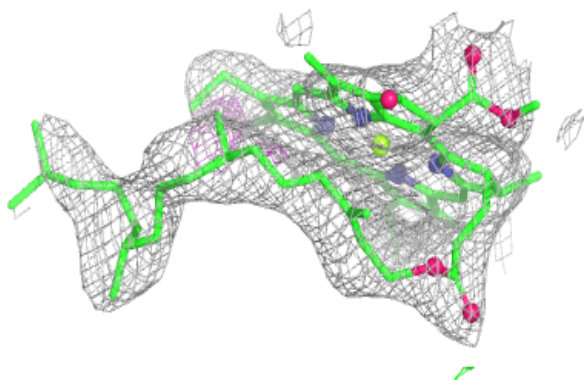
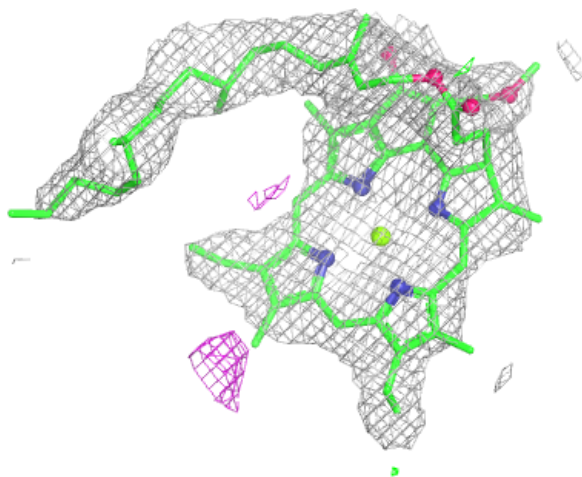
Electron density around CLA U 1003:

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



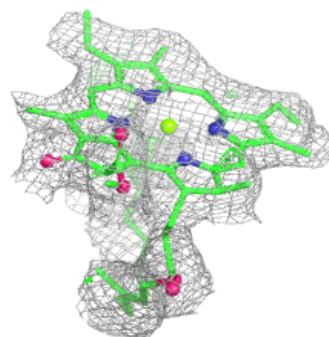
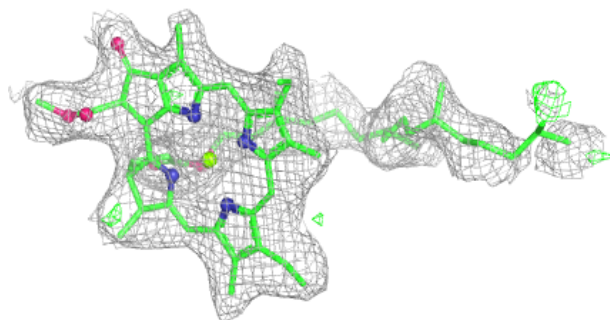
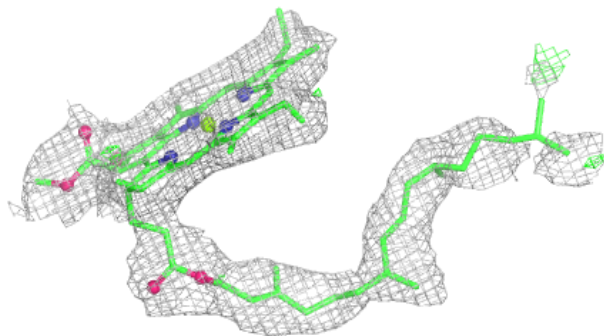
Electron density around CLA A 830:

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

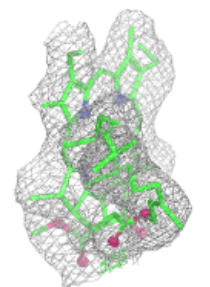
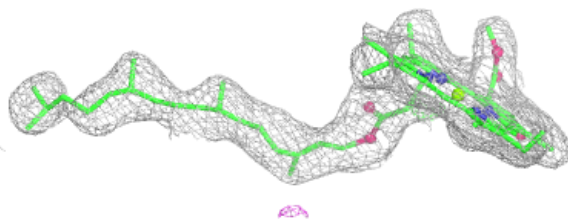
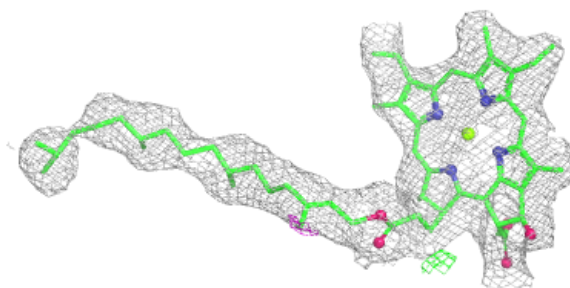


Electron density around CLA U 1006:

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

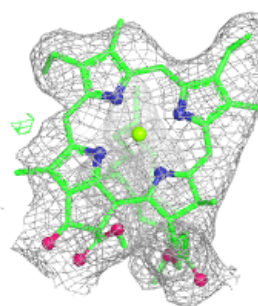
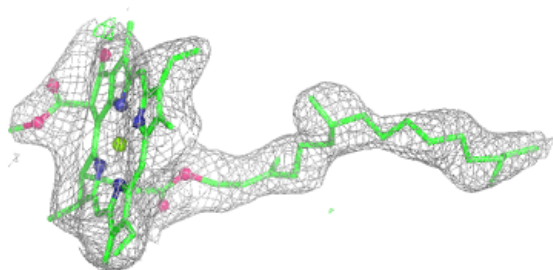
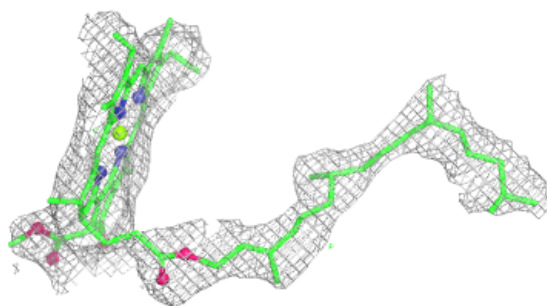
**Electron density around CLA U 1007:**

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



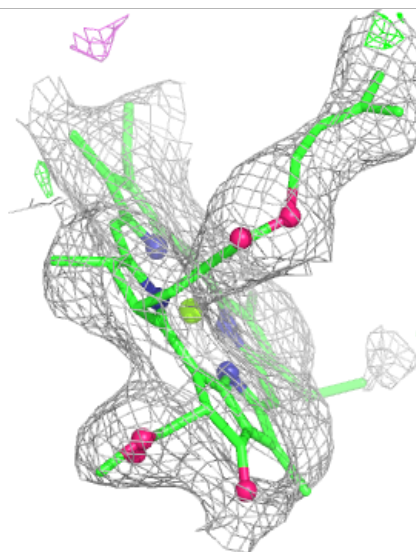
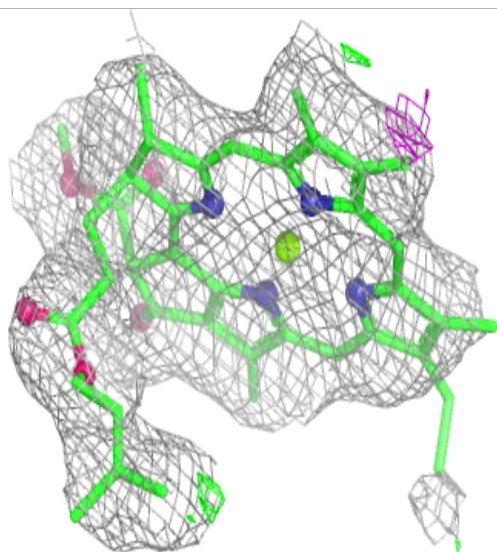
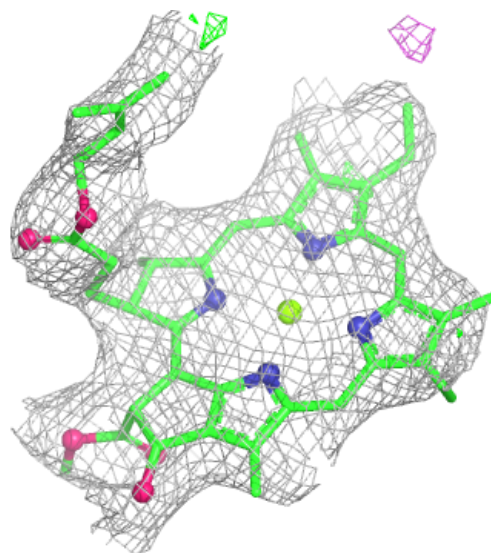
Electron density around CLA A 831:

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



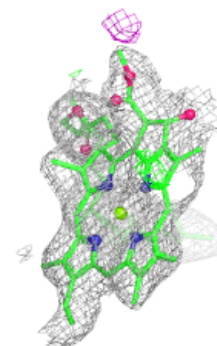
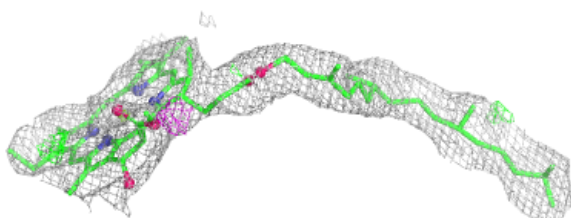
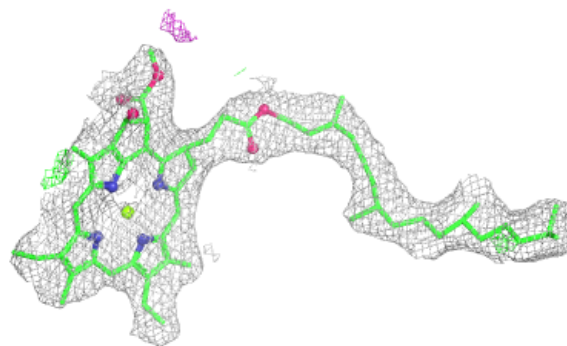
Electron density around CLA A 832:

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

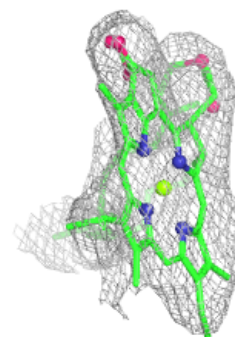
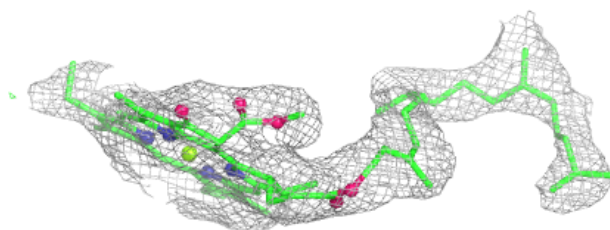
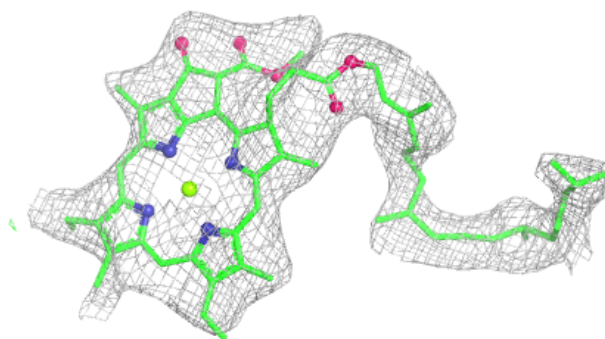


Electron density around CLA Y 802:

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

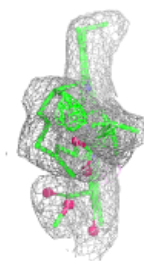
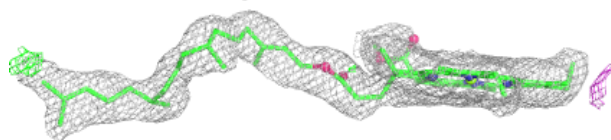
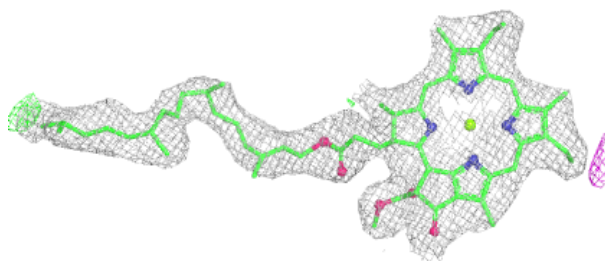
**Electron density around CLA Y 803:**

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

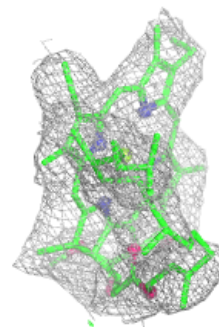
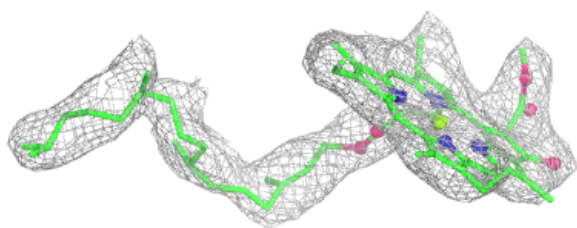
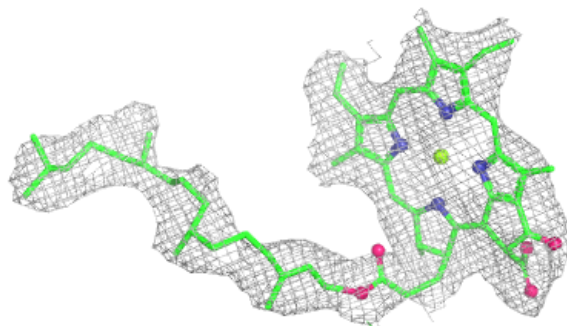


Electron density around CLA A 833:

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

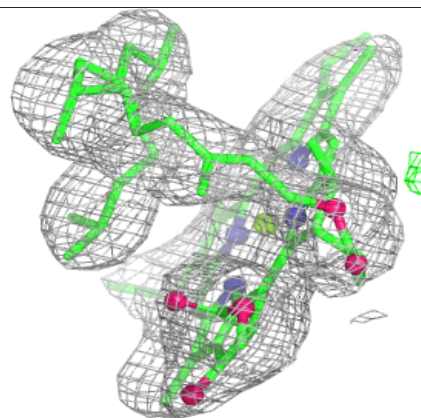
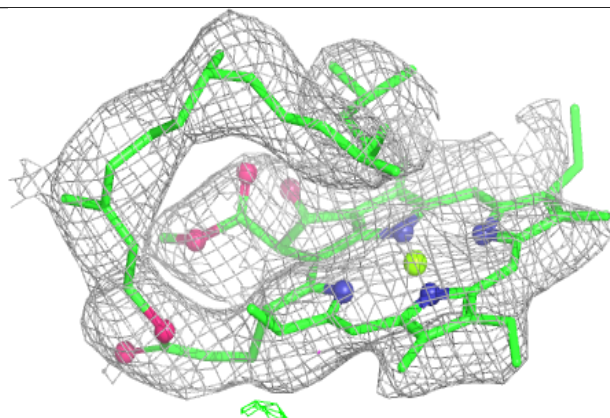
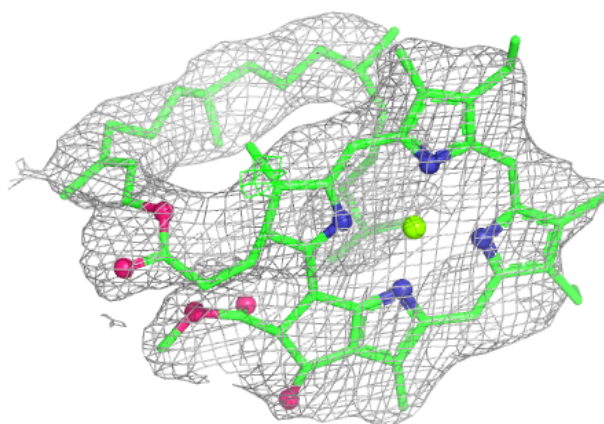
**Electron density around CLA G 808:**

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

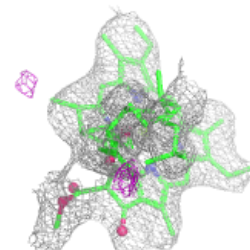
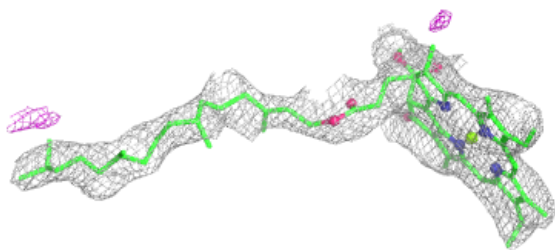
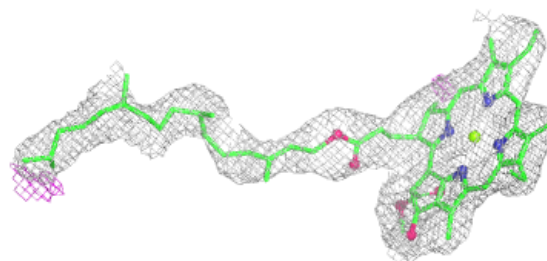


Electron density around CLA Y 806:

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

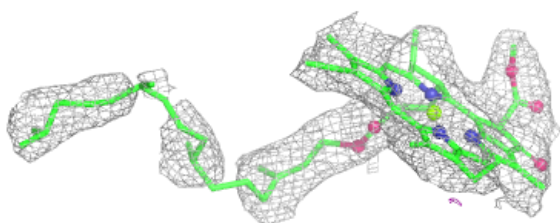
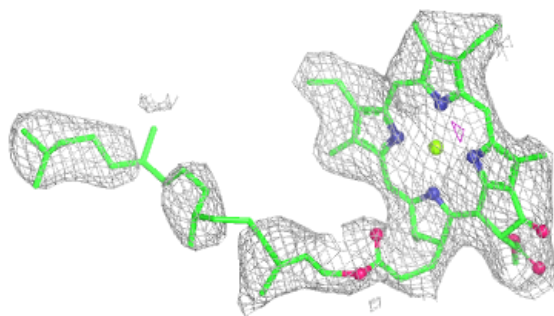
**Electron density around CLA G 809:**

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

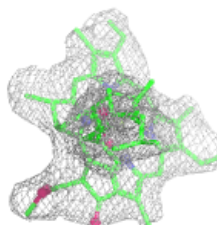
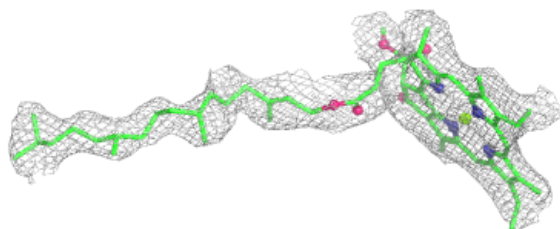
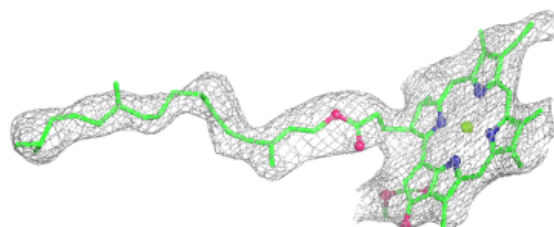


Electron density around CLA Y 808:

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

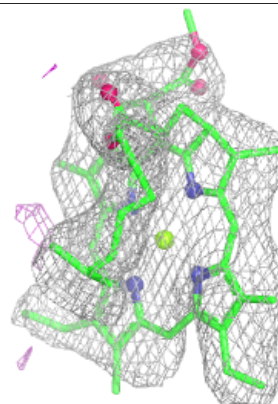
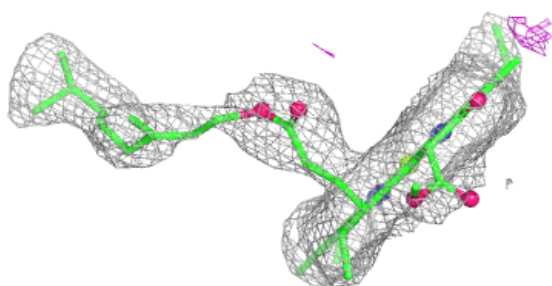
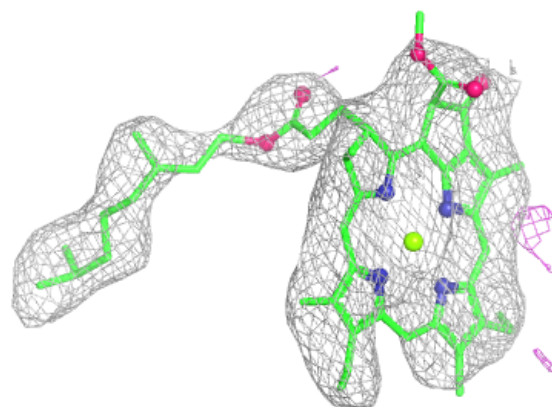
**Electron density around CLA Y 809:**

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

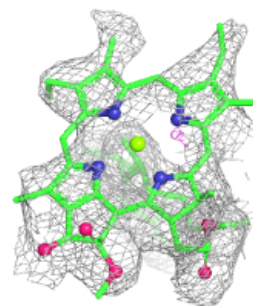
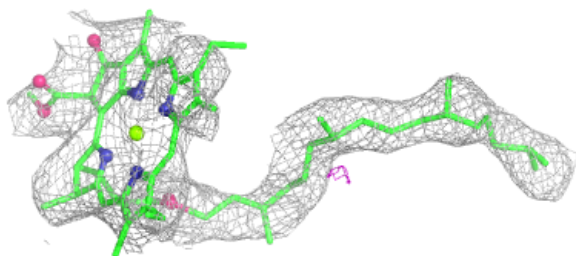
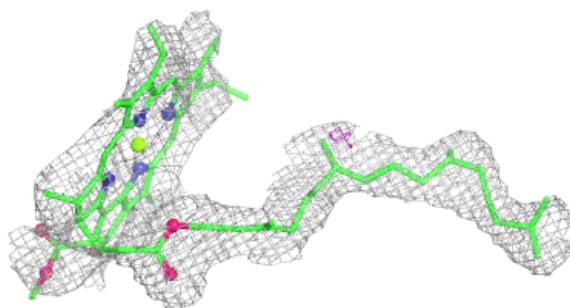


Electron density around CLA A 834:

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

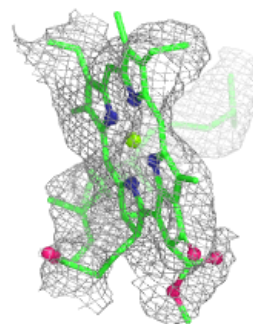
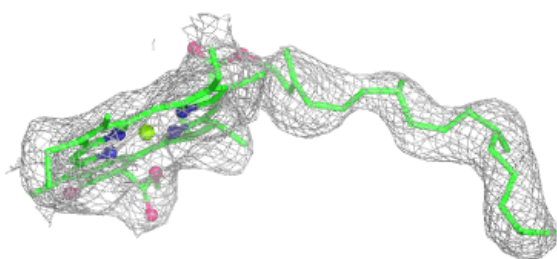
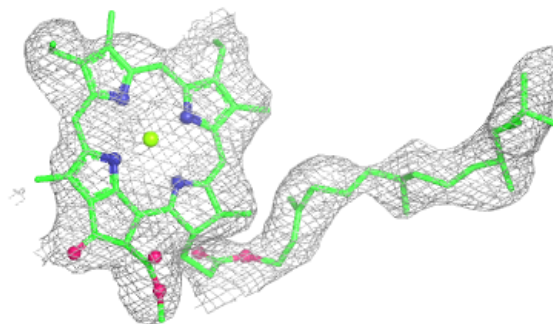
**Electron density around CLA G 811:**

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

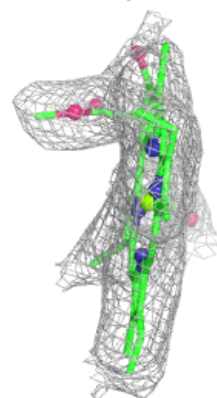
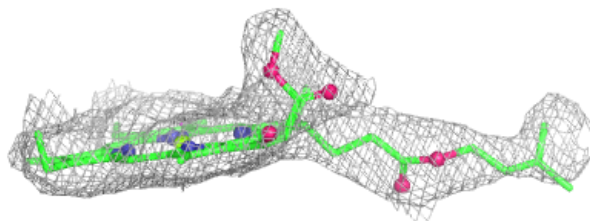
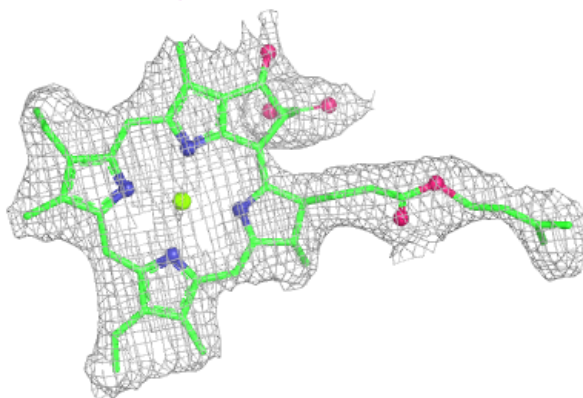


Electron density around CLA A 802:

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

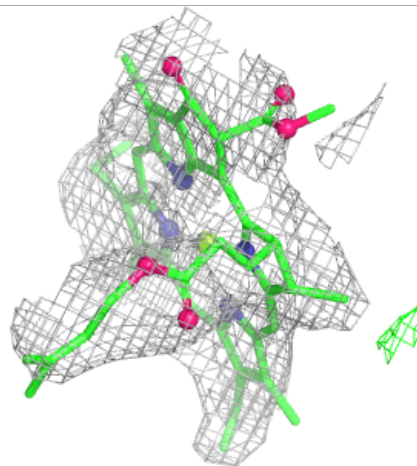
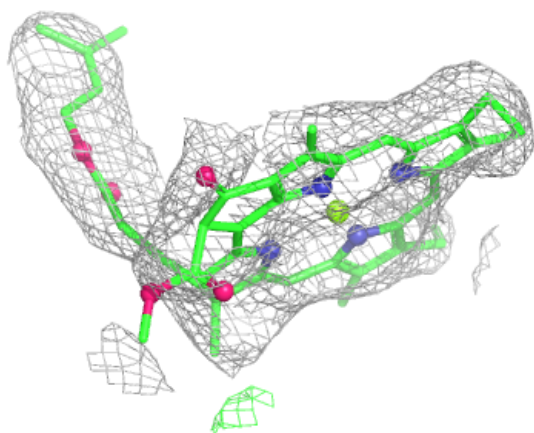
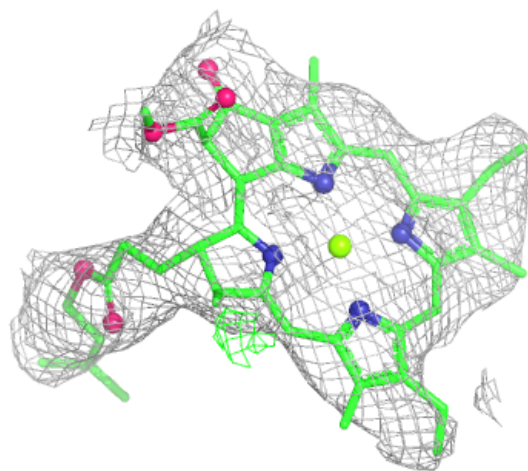
**Electron density around CLA A 836:**

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



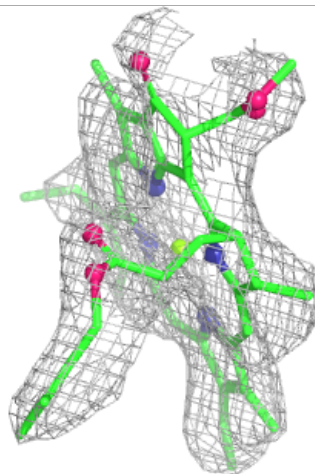
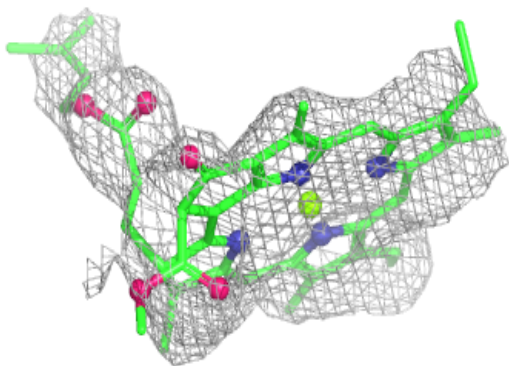
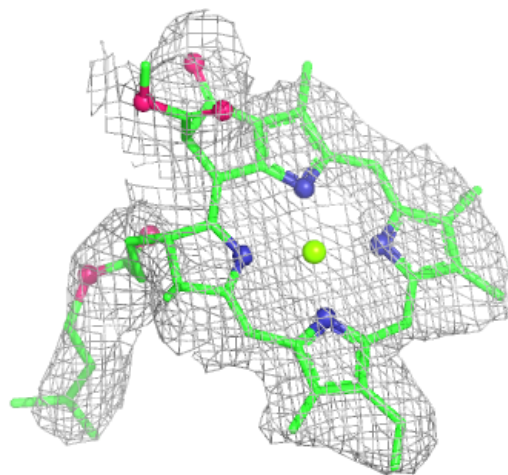
Electron density around CLA G 814:

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



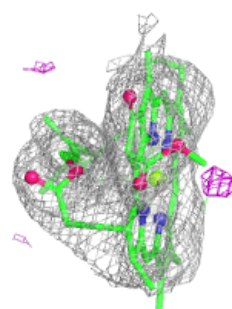
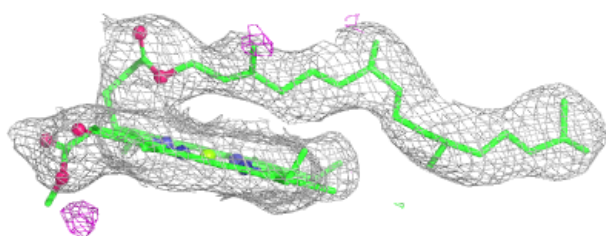
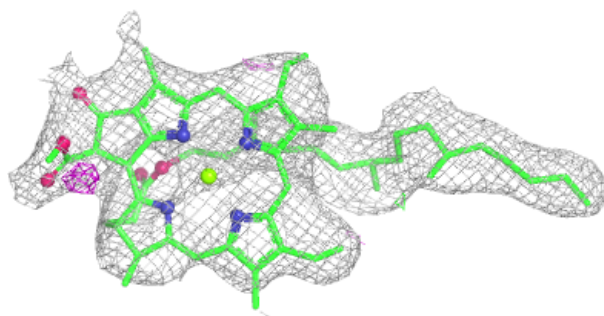
Electron density around CLA Y 815:

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

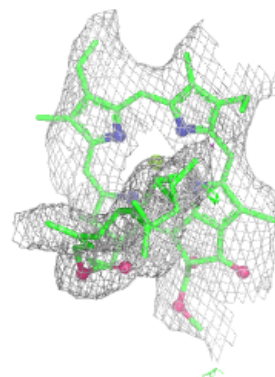
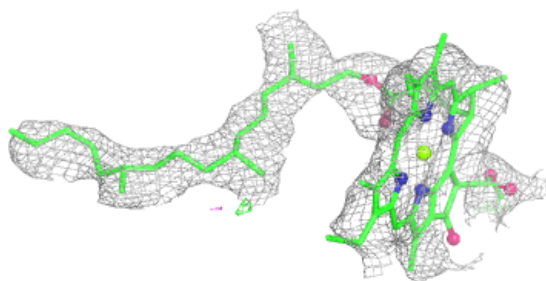
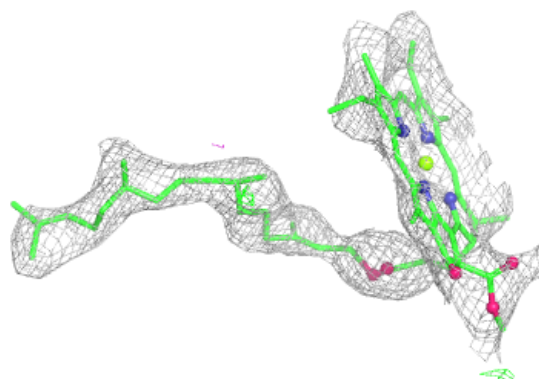


Electron density around CLA A 837:

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

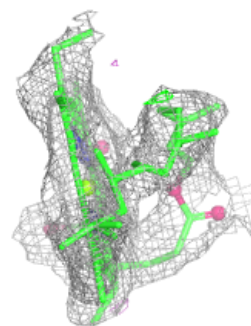
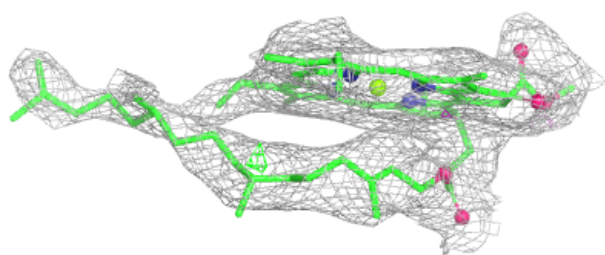
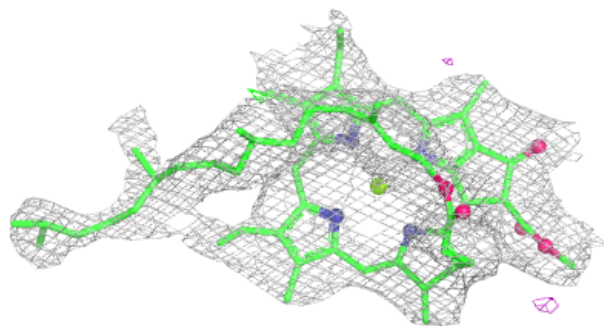
**Electron density around CLA A 812:**

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

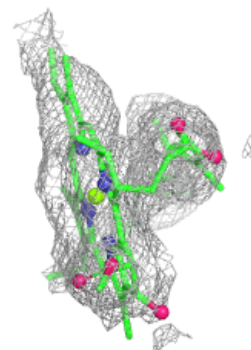
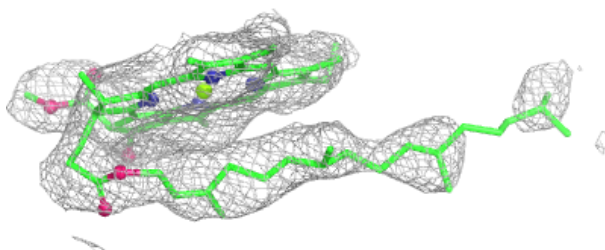
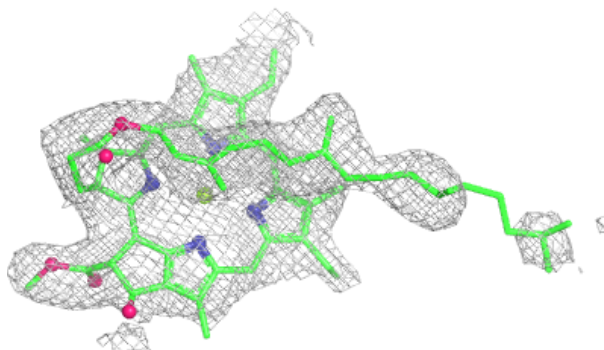


Electron density around CLA A 839:

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

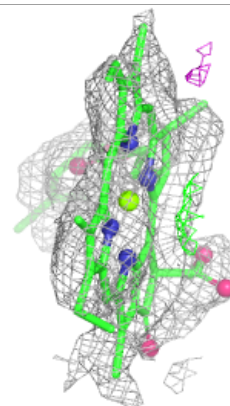
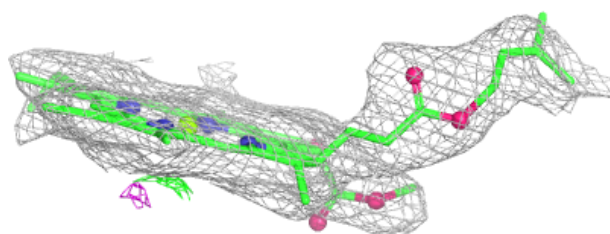
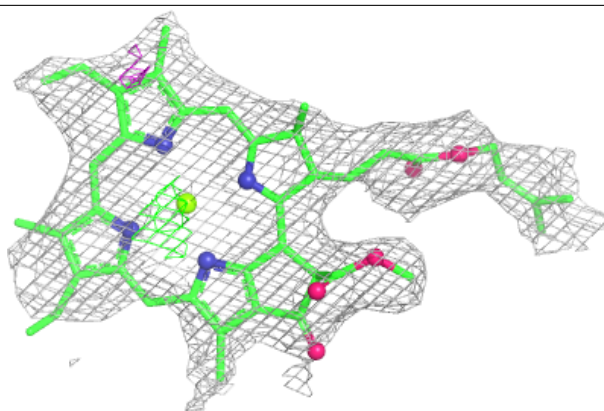
**Electron density around CLA G 818:**

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

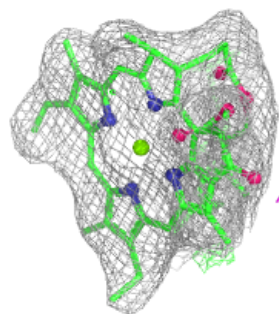
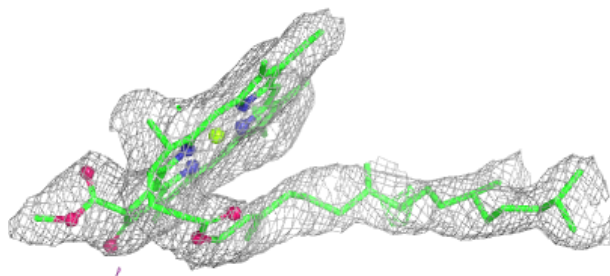
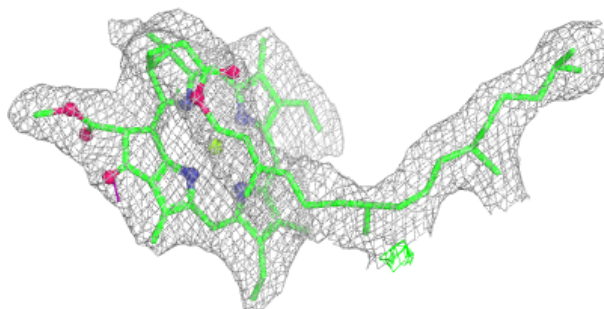


Electron density around CLA A 840:

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

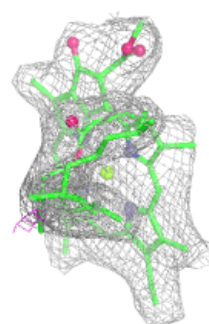
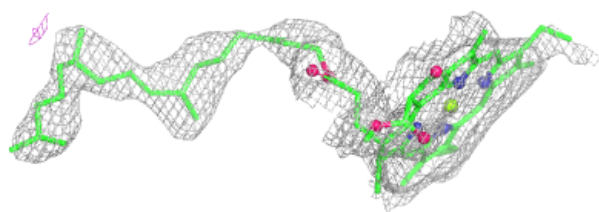
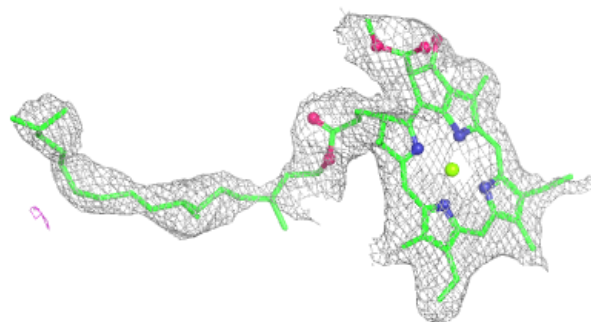
**Electron density around CLA A 841:**

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

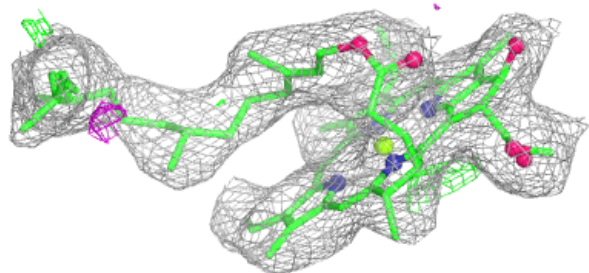
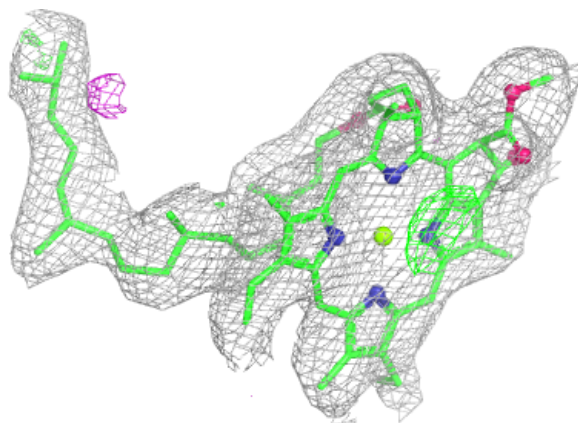


Electron density around CLA G 821:

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

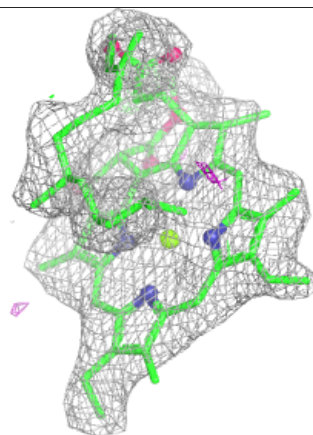
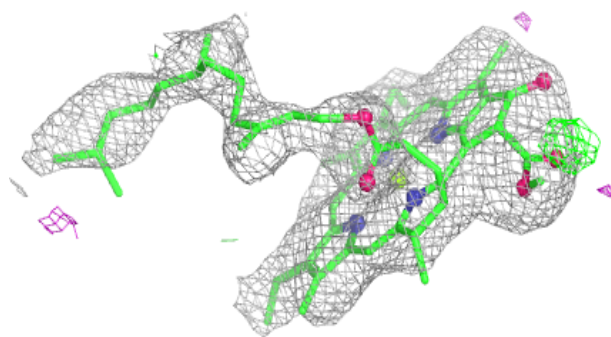
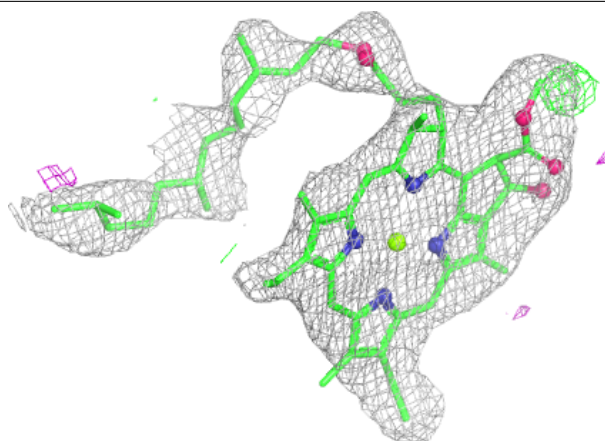
**Electron density around CLA A 842:**

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



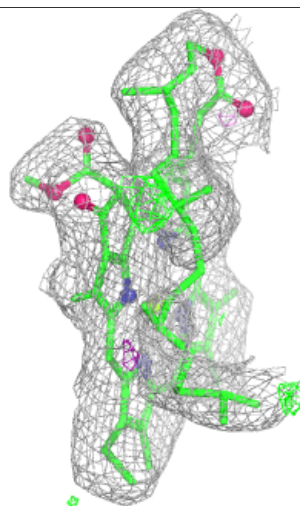
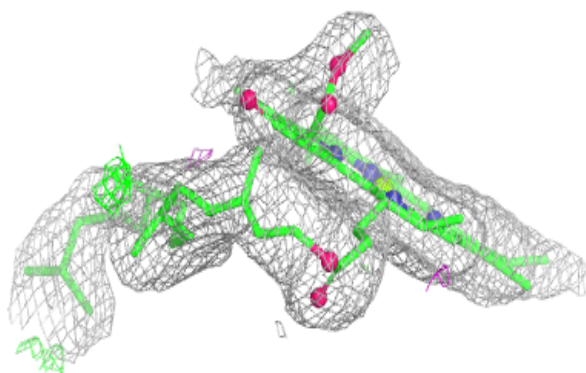
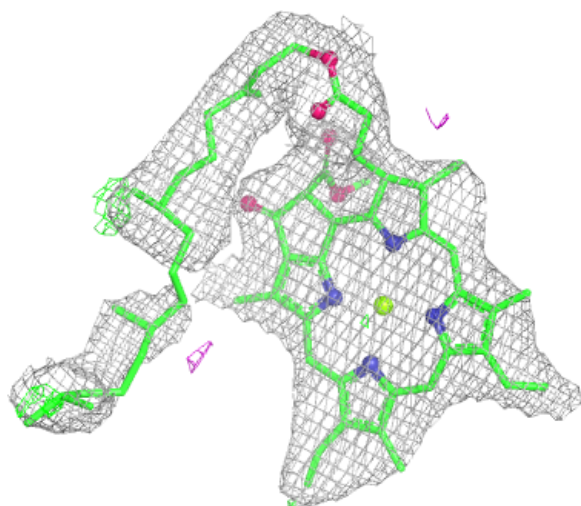
Electron density around CLA Y 824:

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



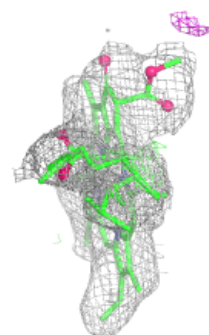
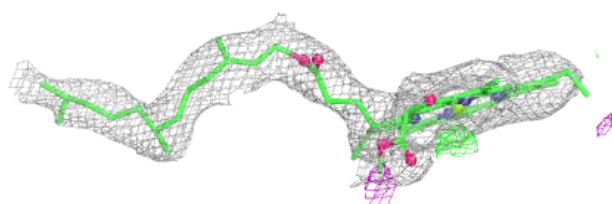
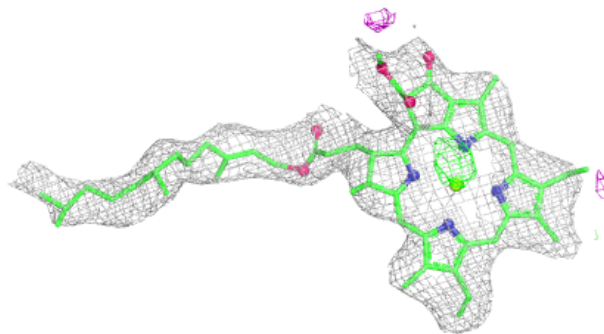
Electron density around CLA Y 825:

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

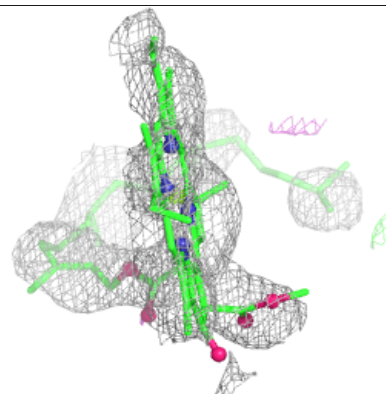
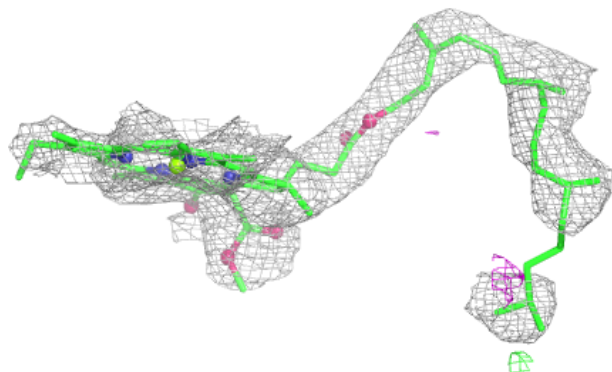
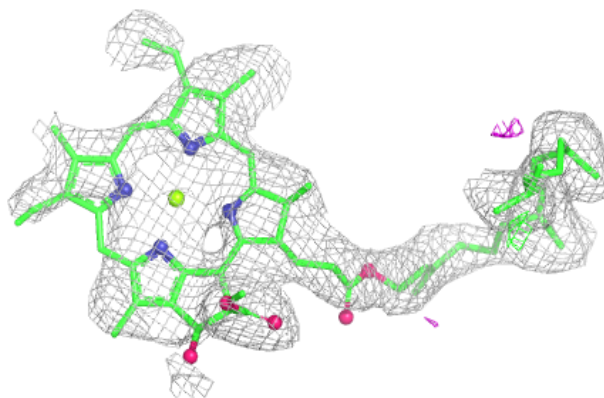


Electron density around CLA Y 826:

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

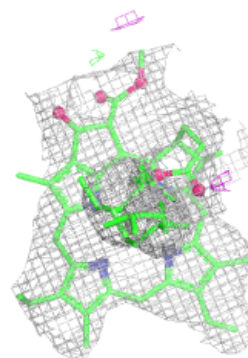
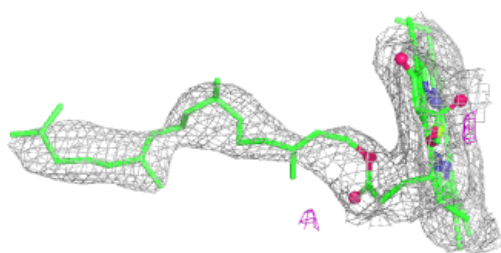
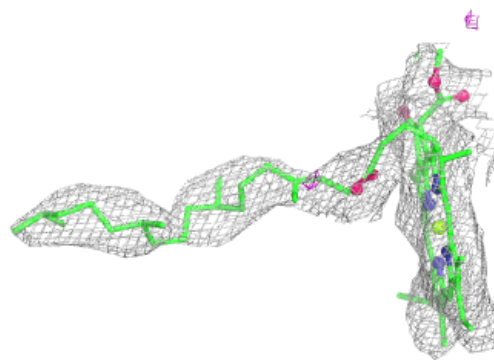
**Electron density around CLA Y 827:**

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

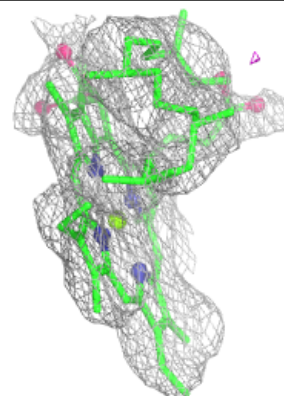
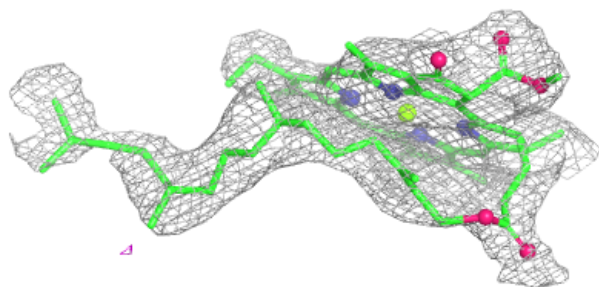
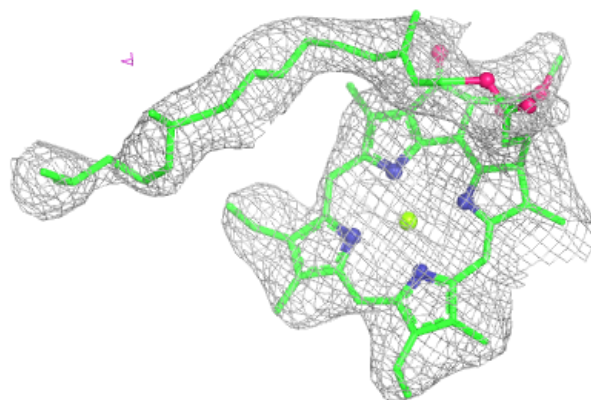


Electron density around CLA Y 828:

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

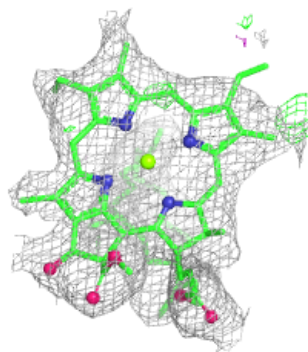
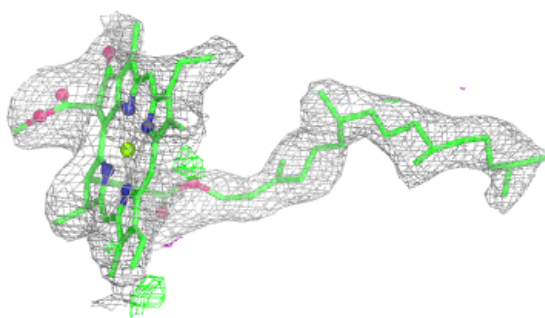
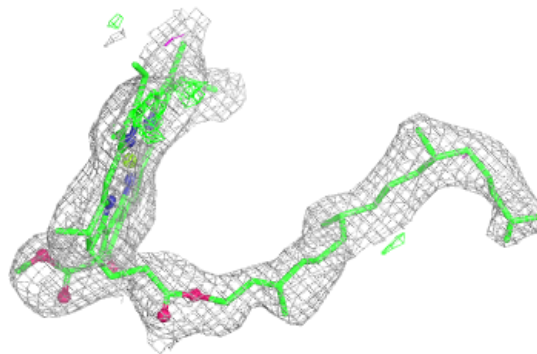
**Electron density around CLA Y 829:**

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



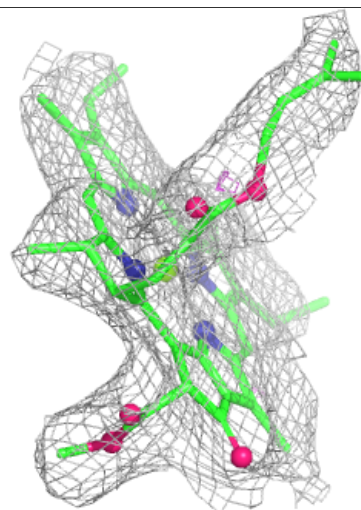
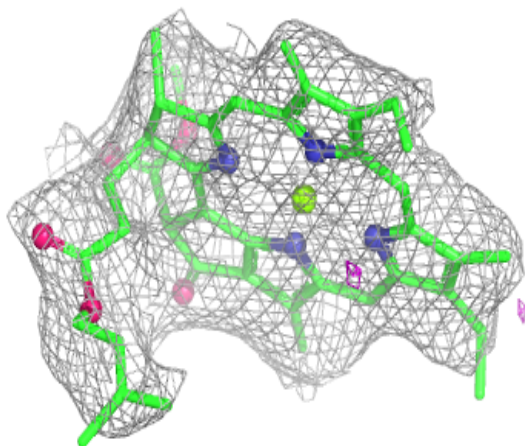
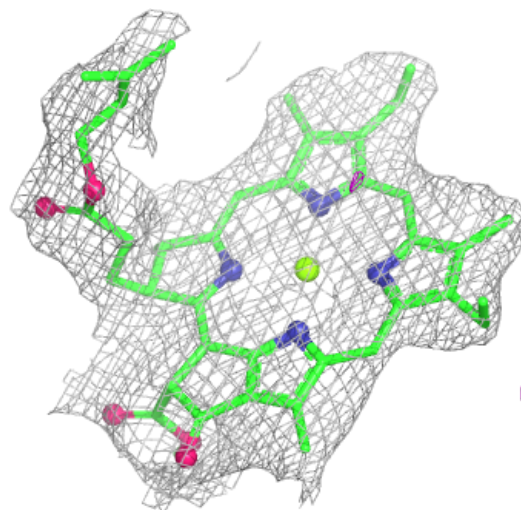
Electron density around CLA Y 830:

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



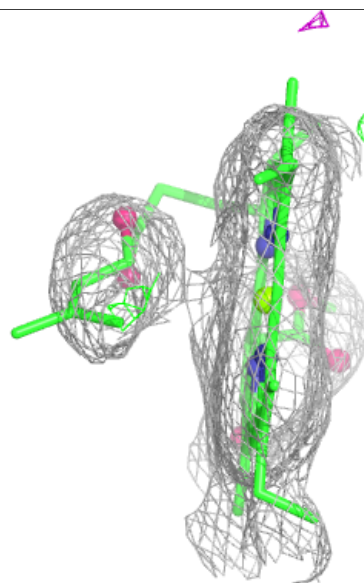
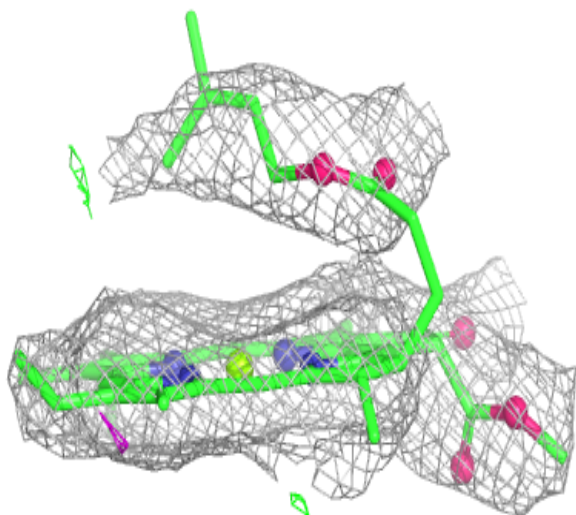
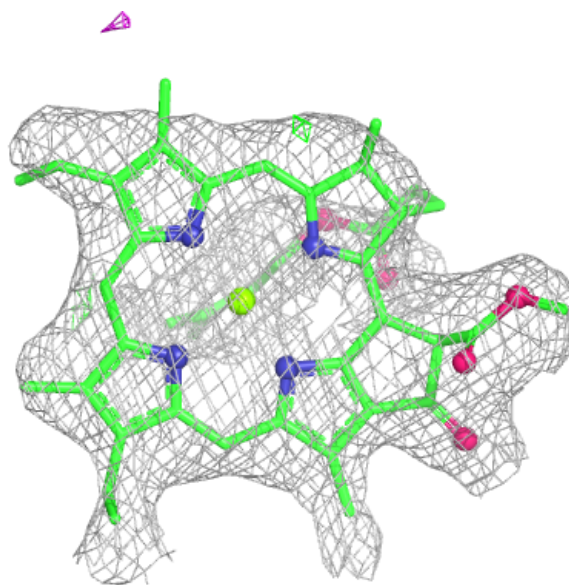
Electron density around CLA Y 831:

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



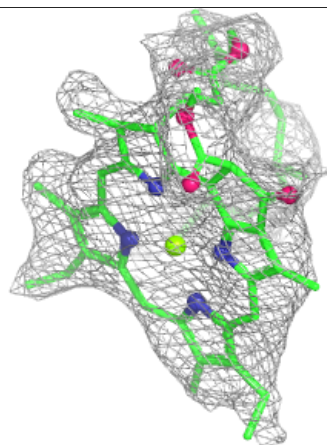
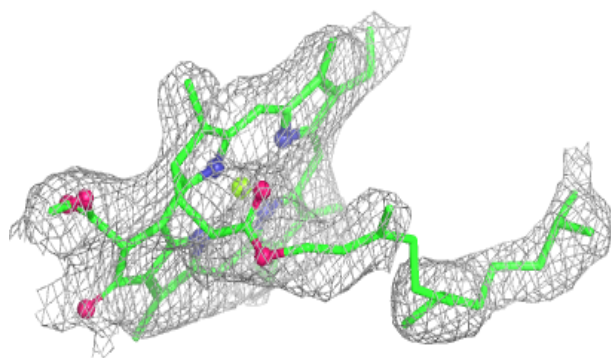
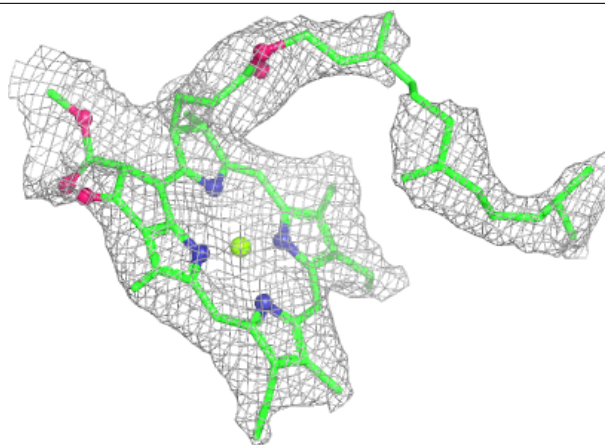
Electron density around CLA G 823:

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



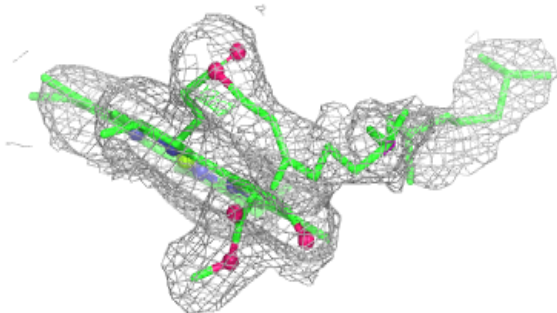
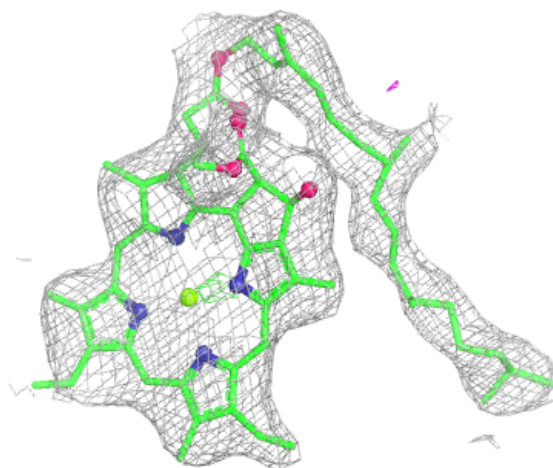
Electron density around CLA G 824:

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



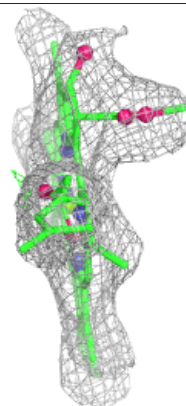
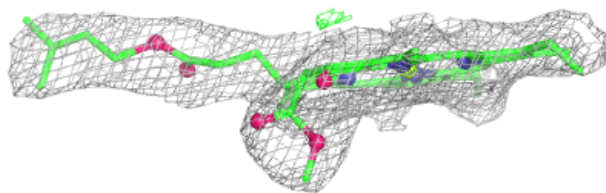
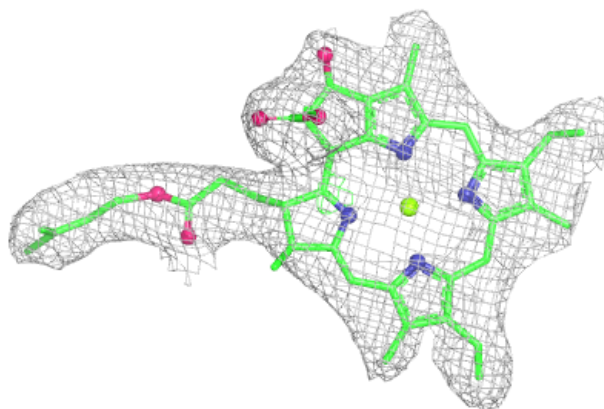
Electron density around CLA G 825:

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

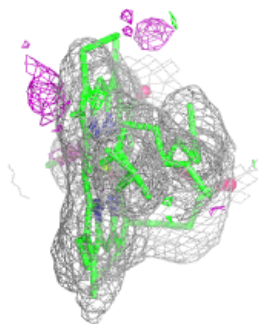
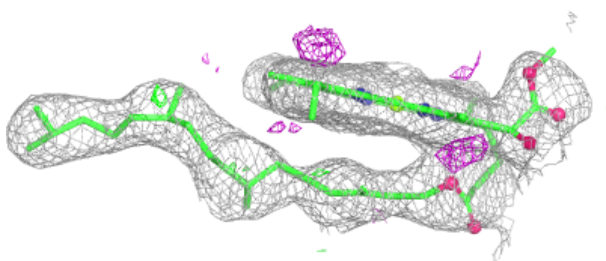
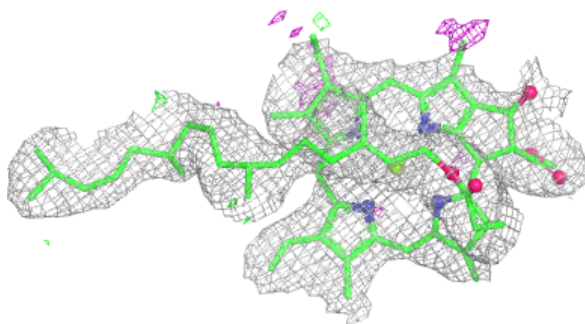


Electron density around CLA Y 835:

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

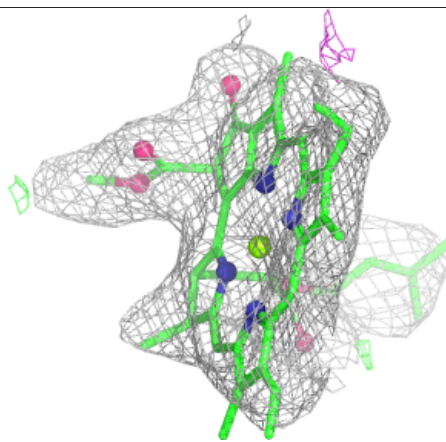
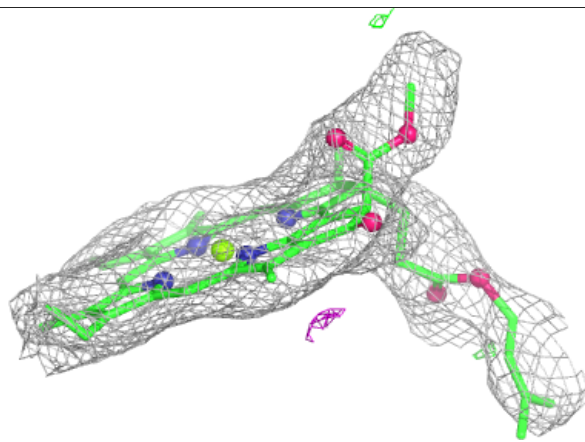
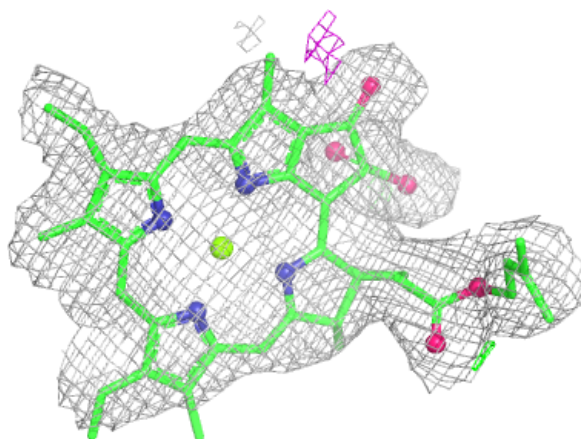
**Electron density around CLA Y 836:**

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



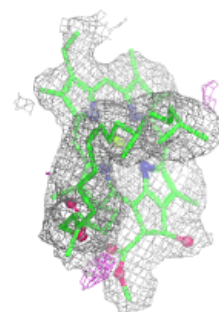
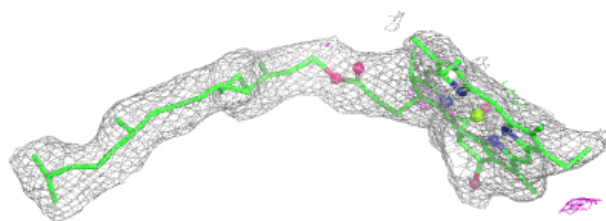
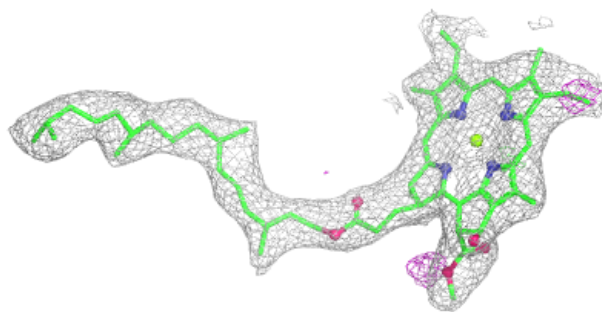
Electron density around CLA Y 837:

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

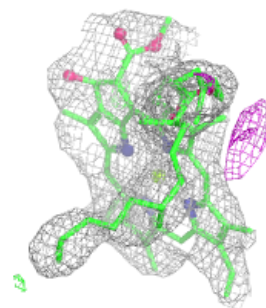
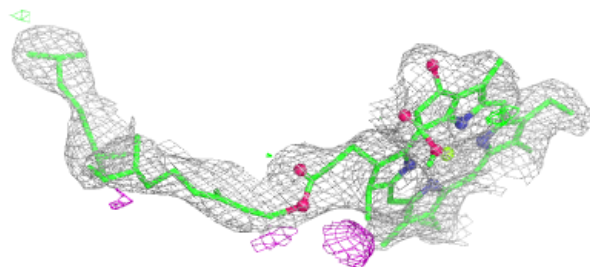
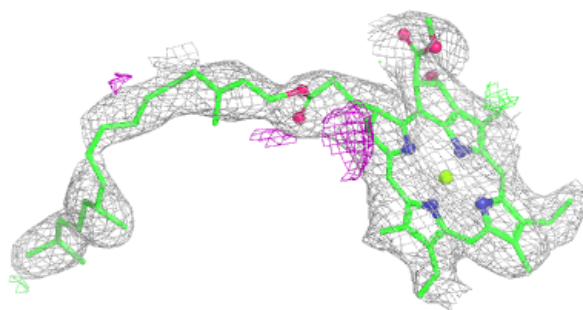


Electron density around CLA A 803:

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

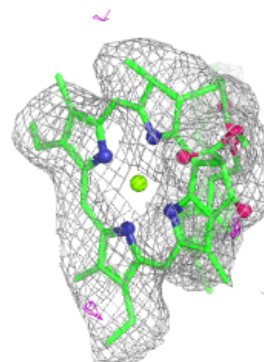
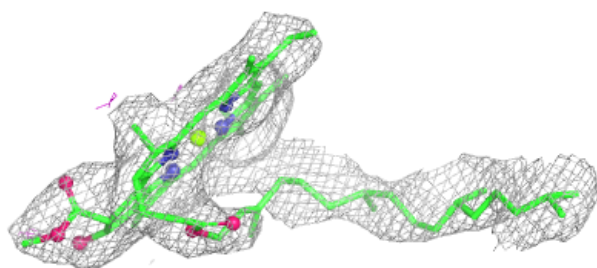
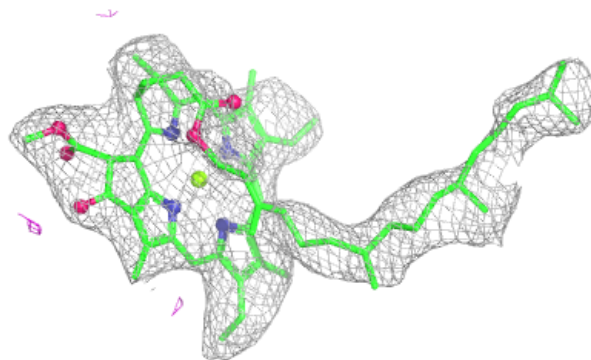
**Electron density around CLA A 854:**

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

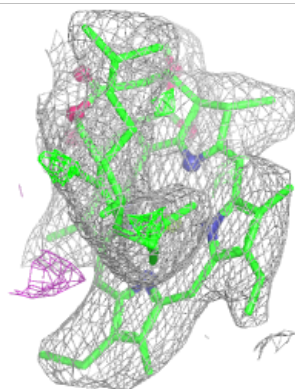
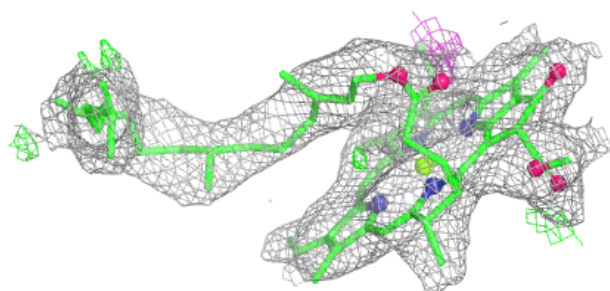
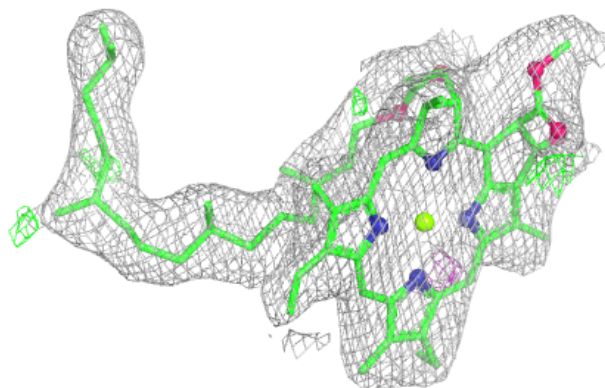


Electron density around CLA Y 840:

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

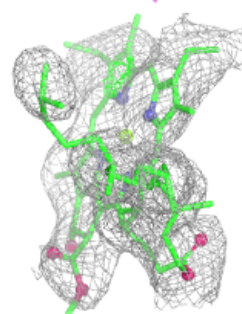
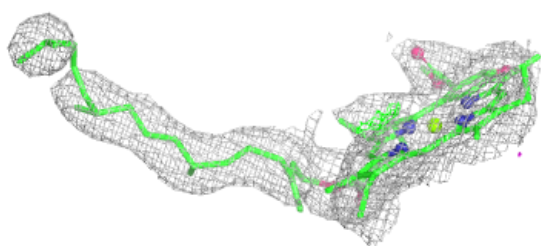
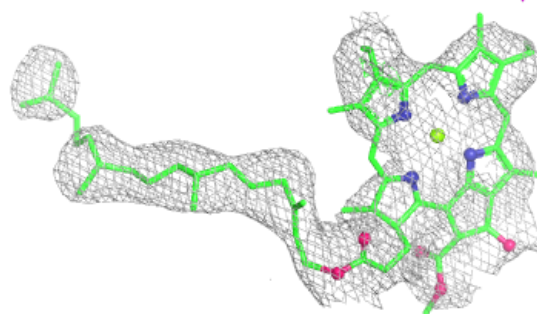
**Electron density around CLA Y 841:**

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

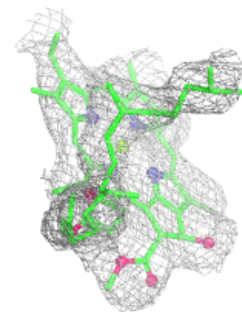
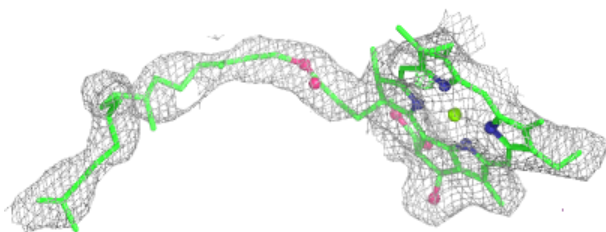
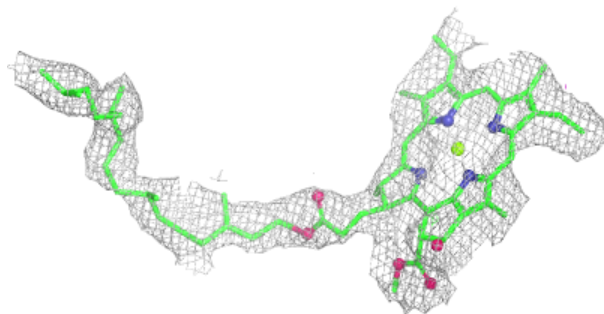


Electron density around CLA Z 801:

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

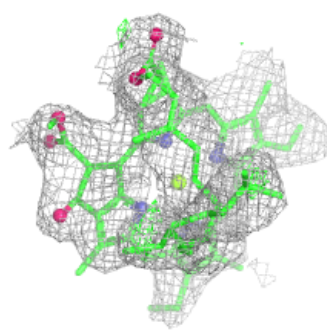
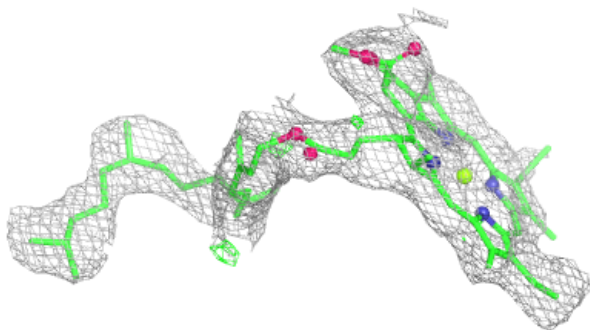
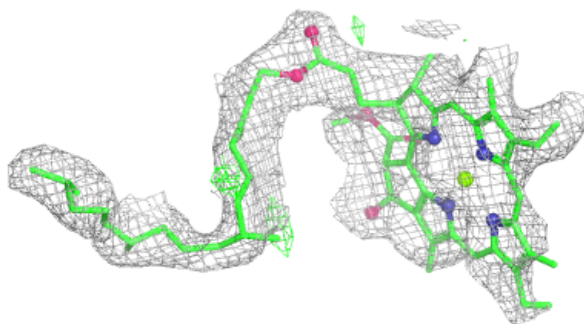
**Electron density around CLA Z 802:**

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

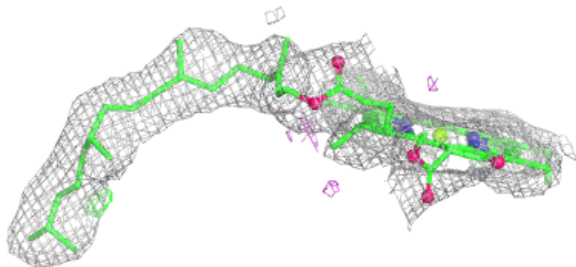
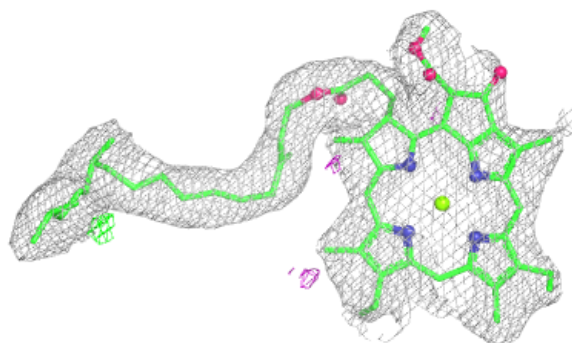


Electron density around CLA Z 803:

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

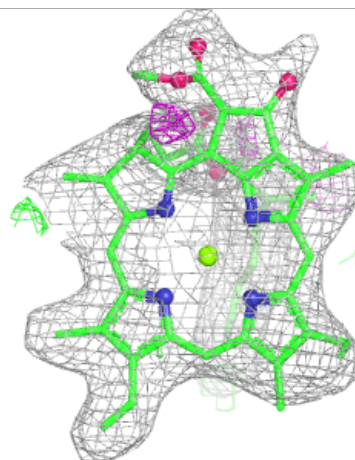
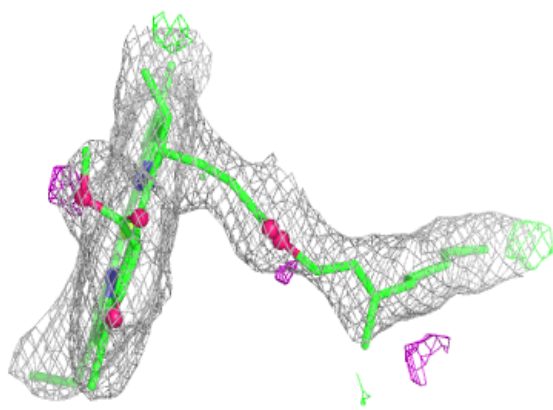
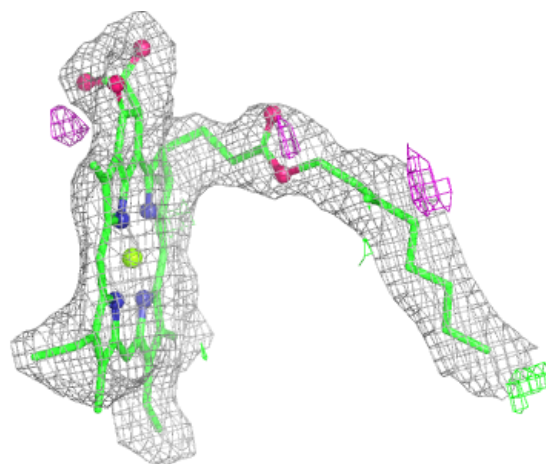
**Electron density around CLA Z 804:**

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



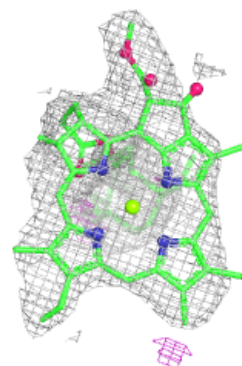
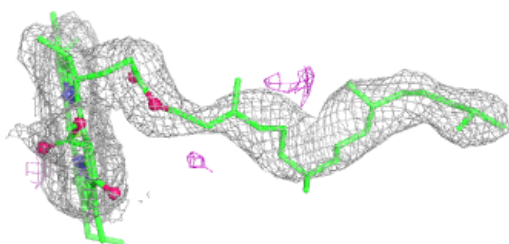
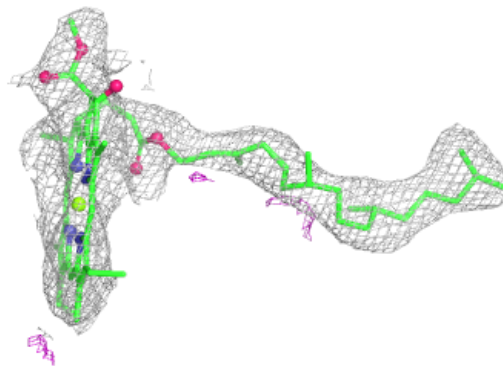
Electron density around CLA Z 805:

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



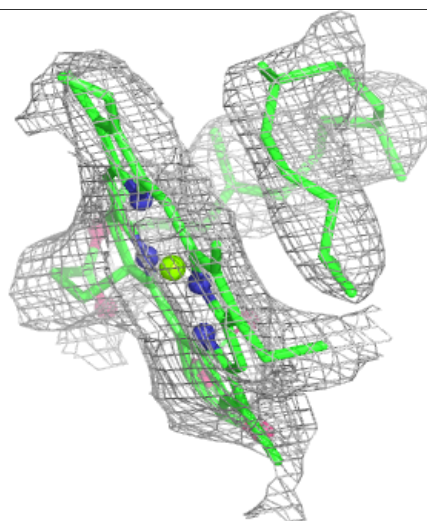
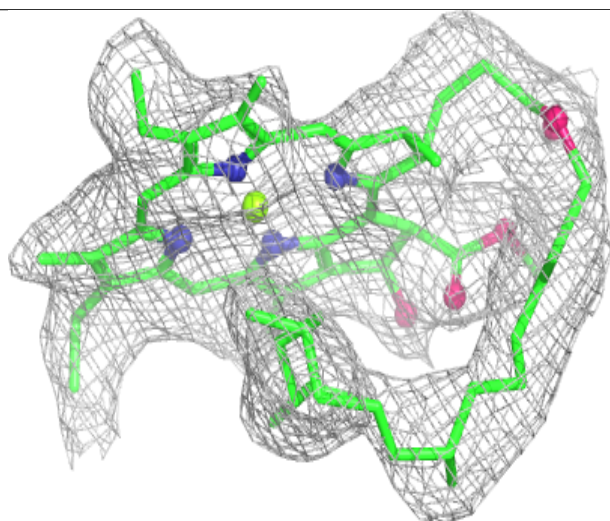
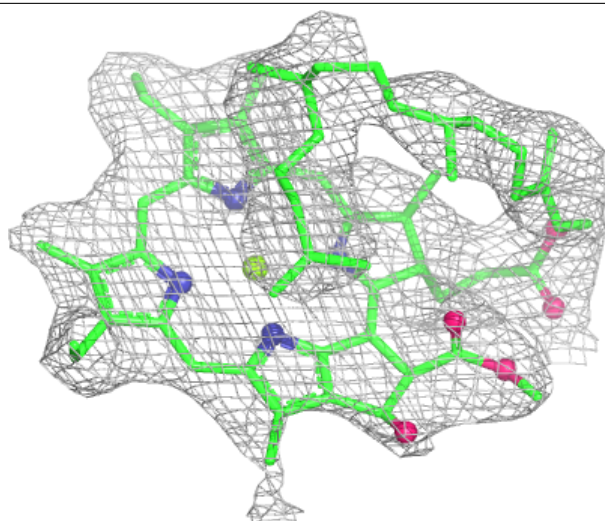
Electron density around CLA G 828:

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



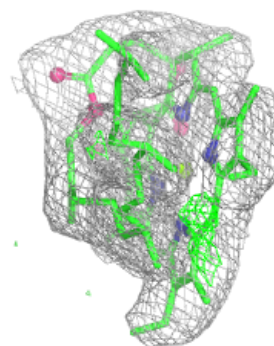
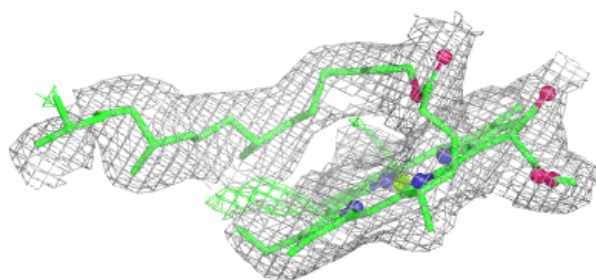
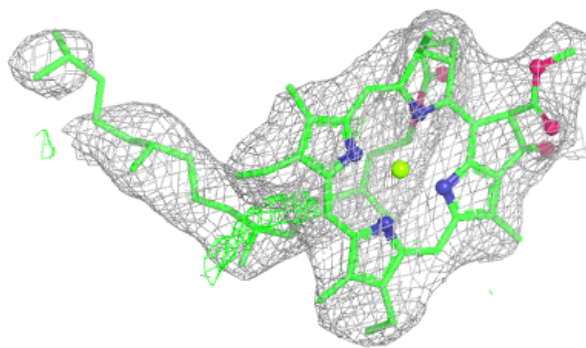
Electron density around CLA Z 807:

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



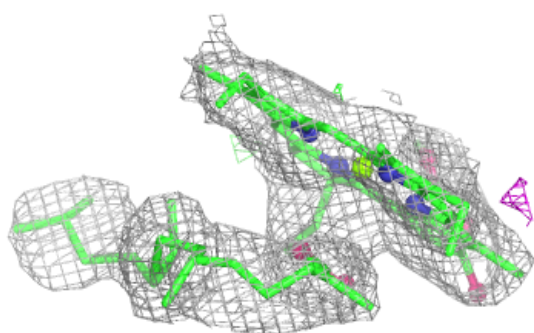
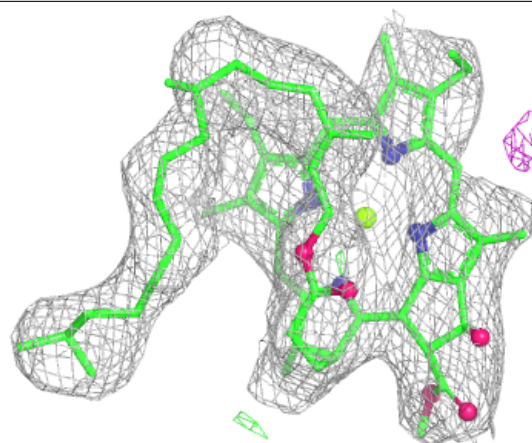
Electron density around CLA Z 808:

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

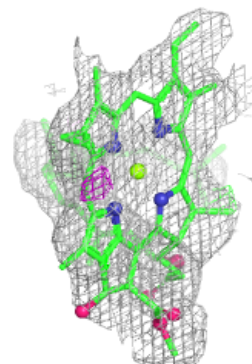
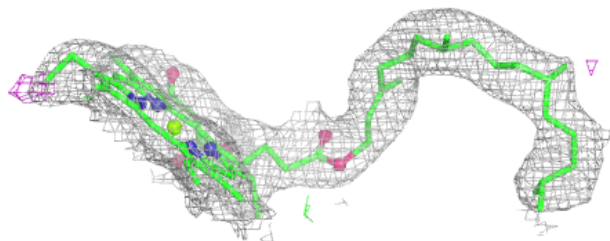
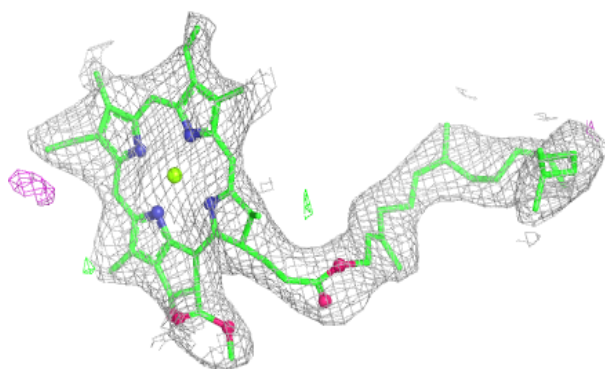


Electron density around CLA Z 809:

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

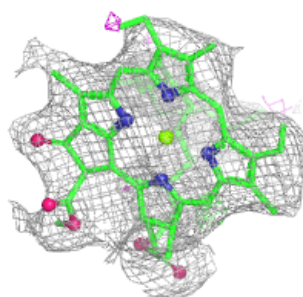
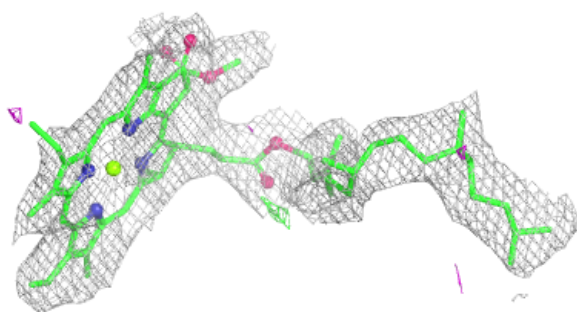
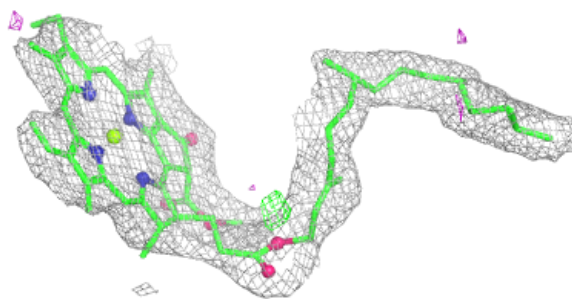
**Electron density around CLA Z 810:**

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



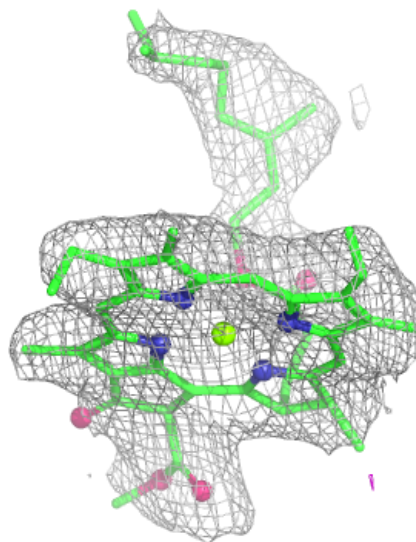
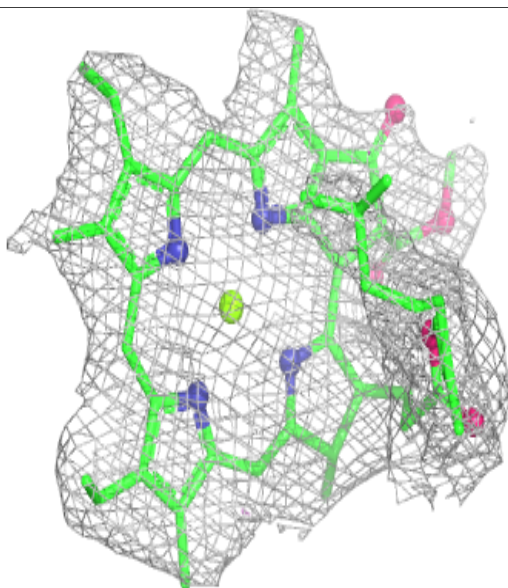
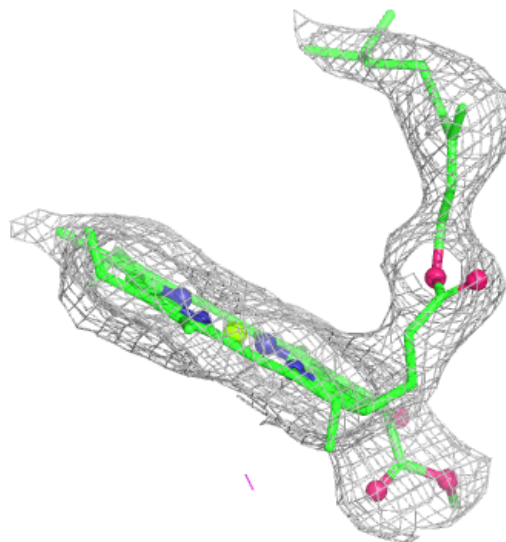
Electron density around CLA B 801:

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



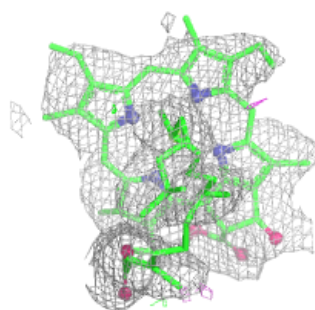
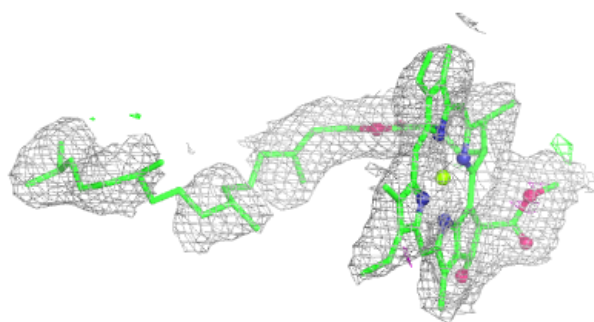
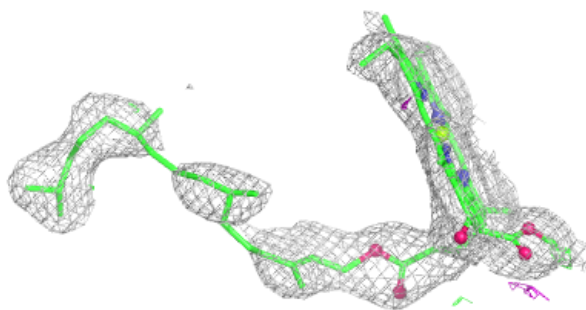
Electron density around CLA Z 812:

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

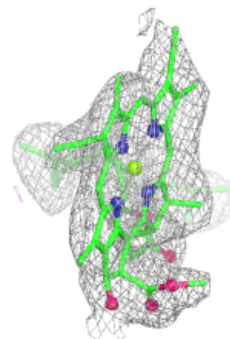
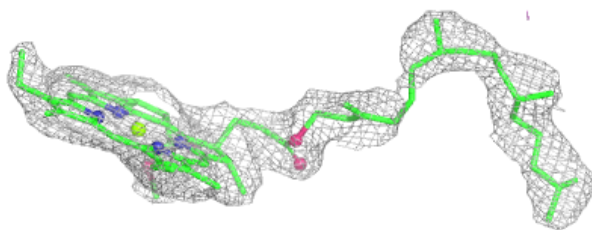
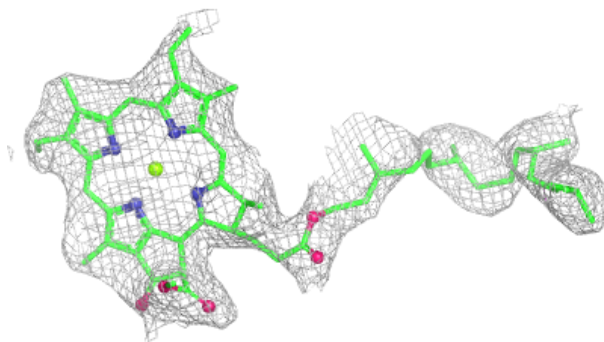


Electron density around CLA G 830:

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

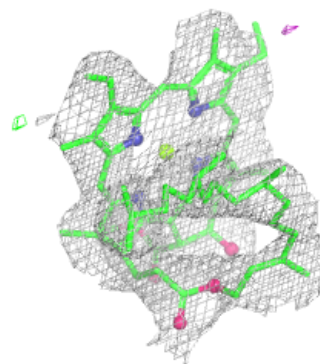
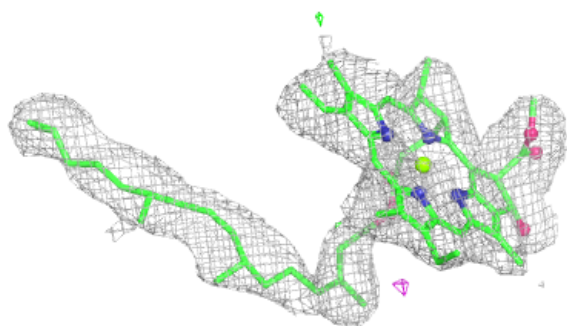
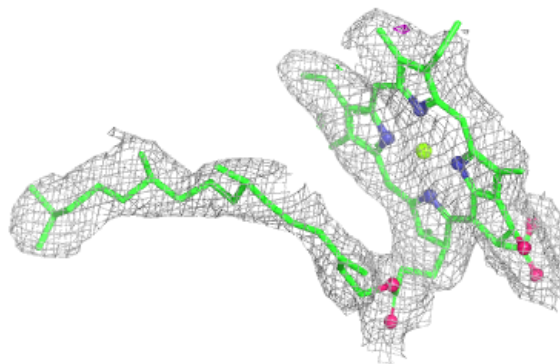
**Electron density around CLA Z 814:**

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



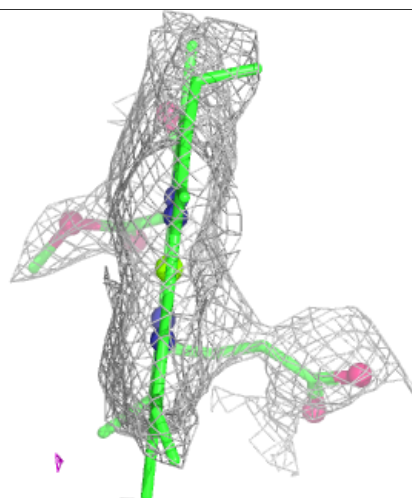
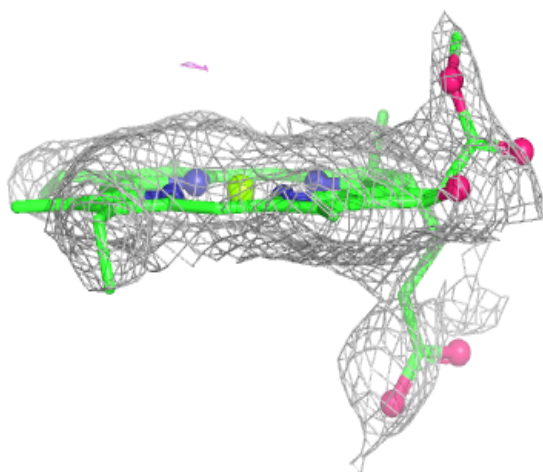
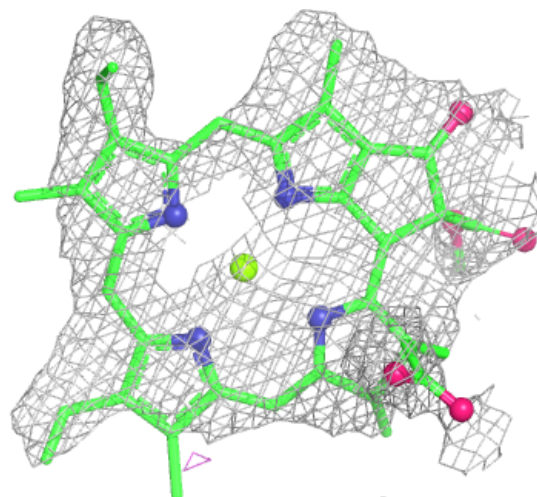
Electron density around CLA Z 815:

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



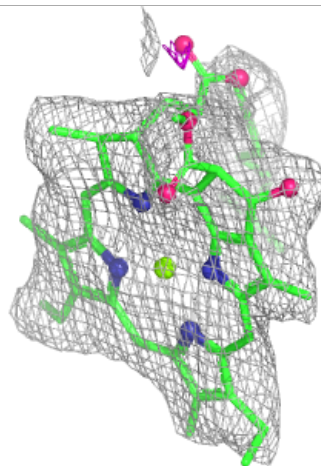
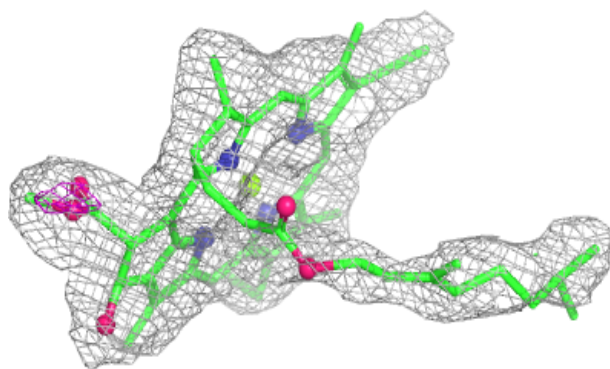
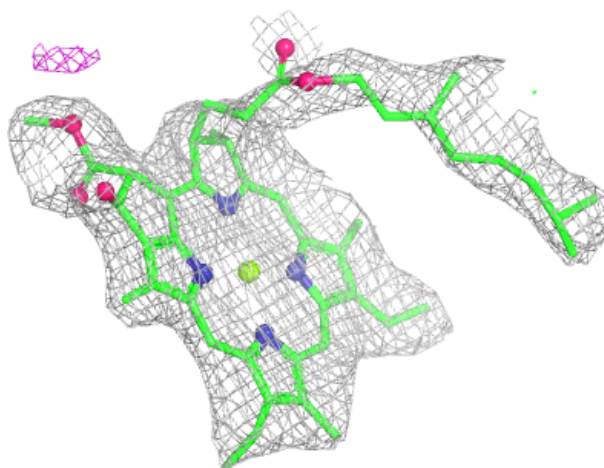
Electron density around CLA Z 816:

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



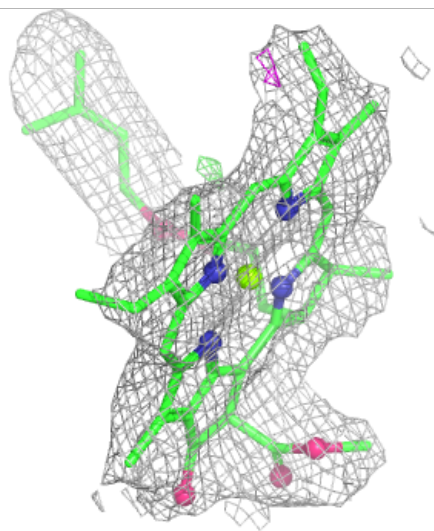
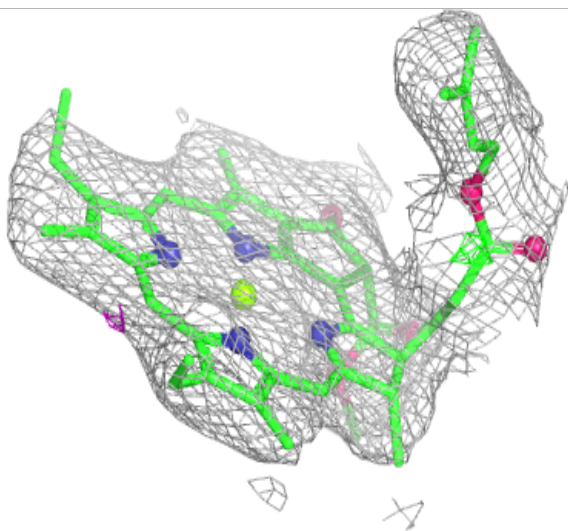
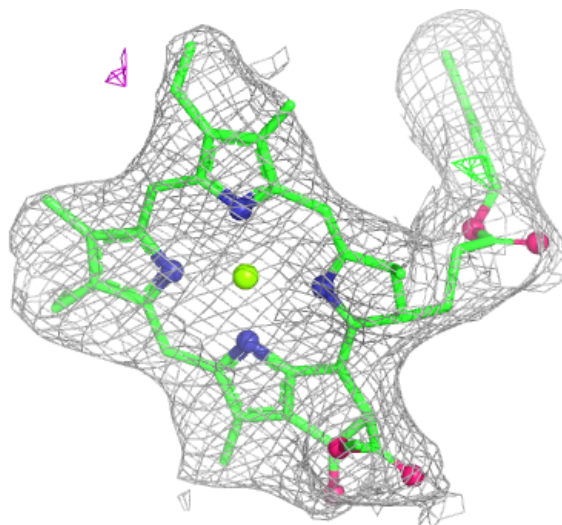
Electron density around CLA Z 817:

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



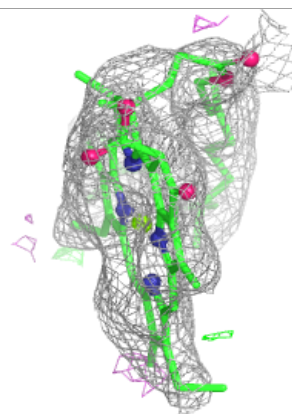
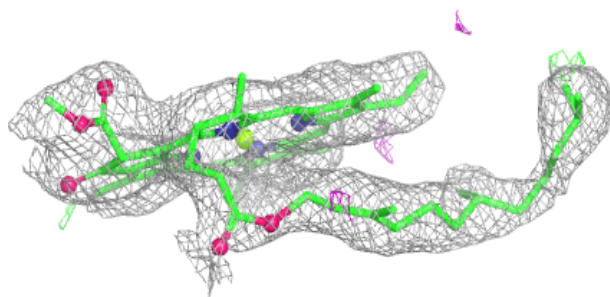
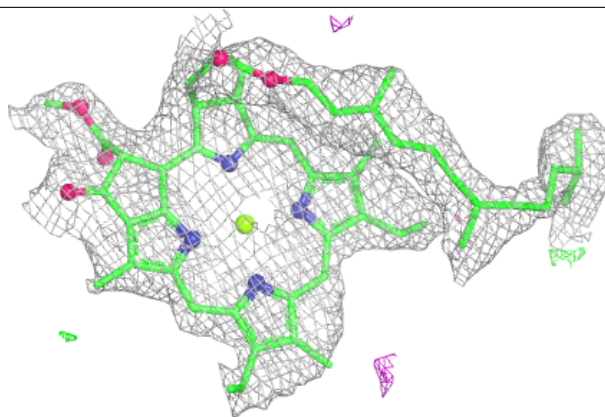
Electron density around CLA G 831:

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



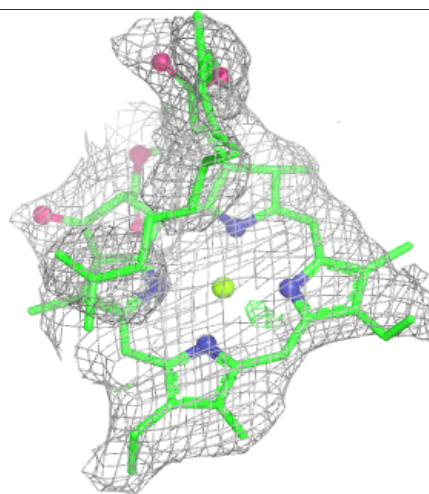
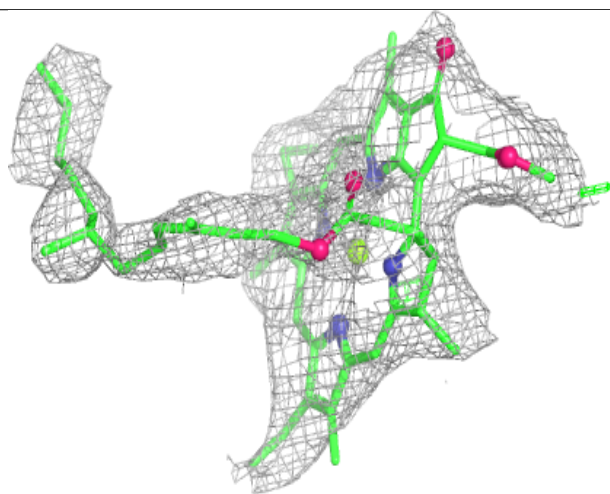
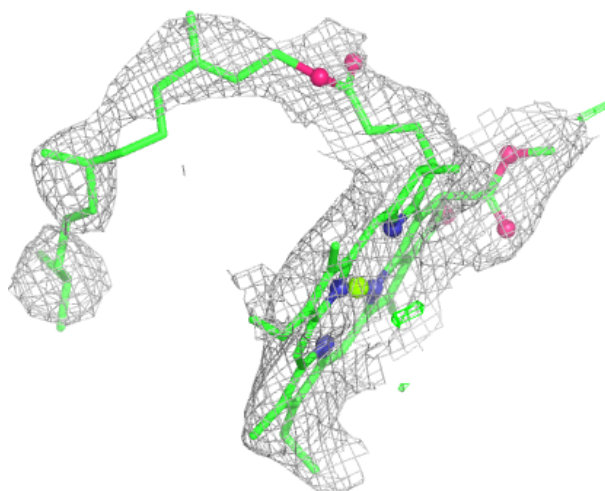
Electron density around CLA Z 819:

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



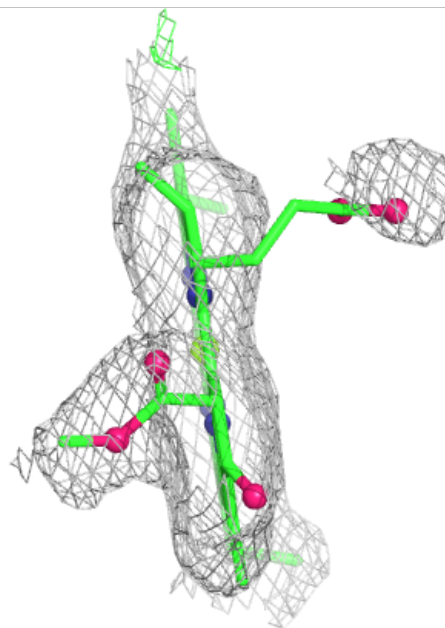
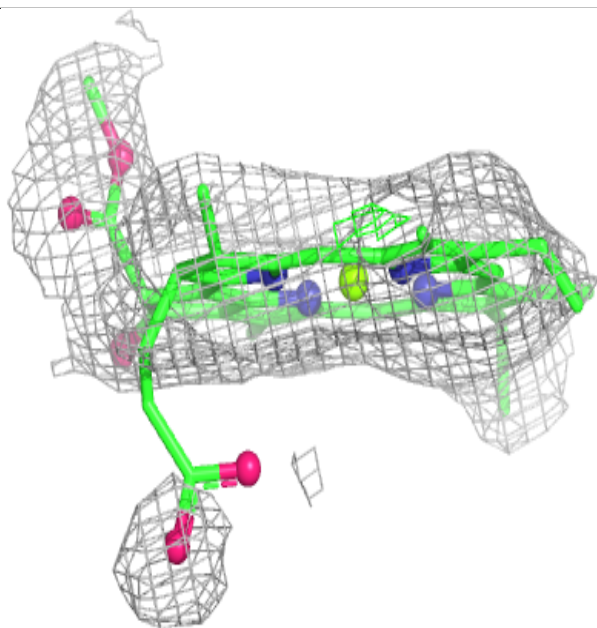
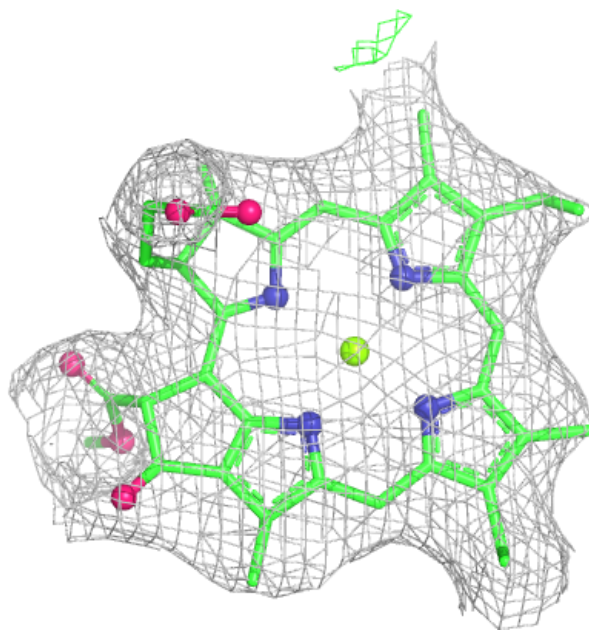
Electron density around CLA Z 820:

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



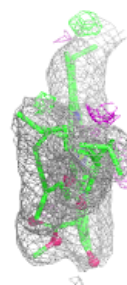
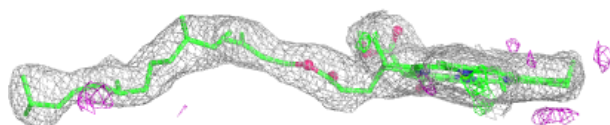
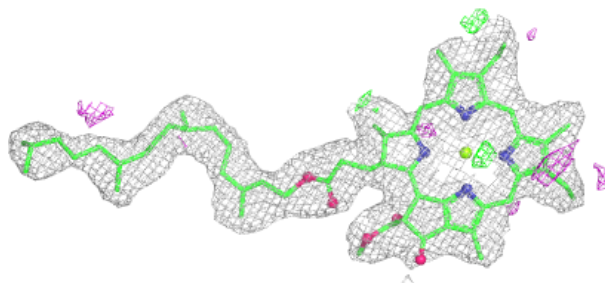
Electron density around CLA Z 821:

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

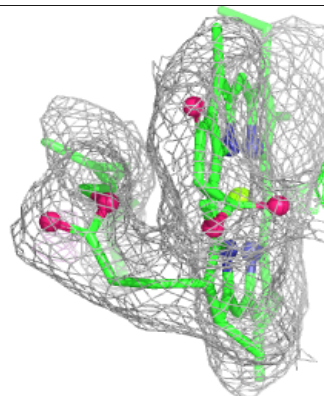
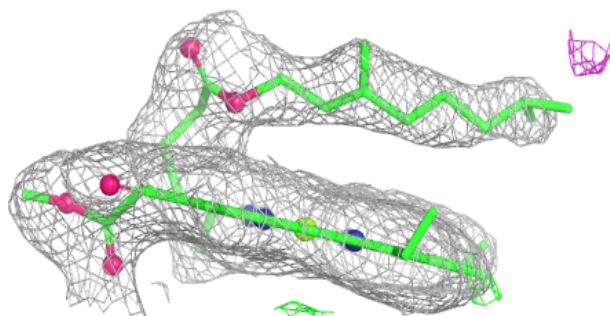
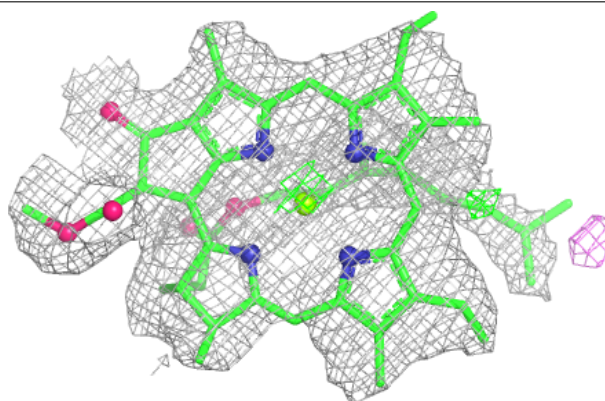


Electron density around CLA G 832:

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

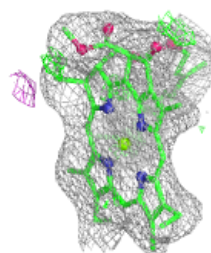
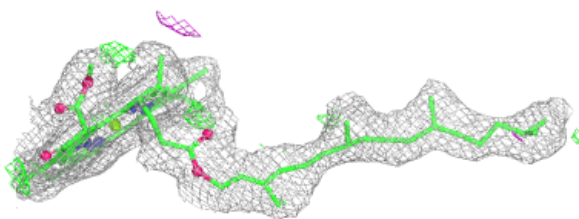
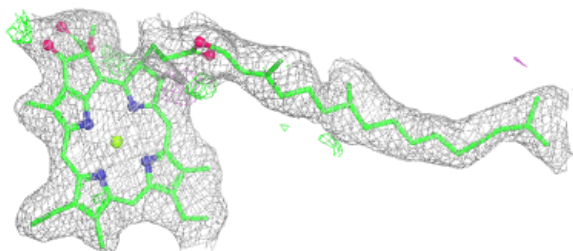
**Electron density around CLA Z 823:**

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



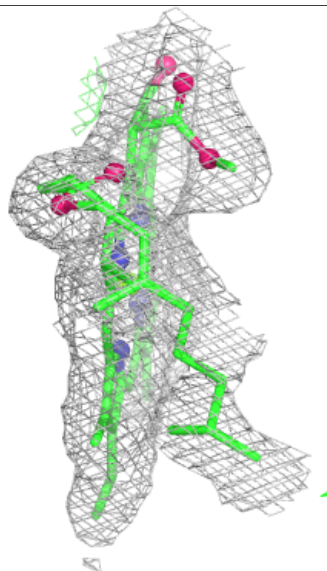
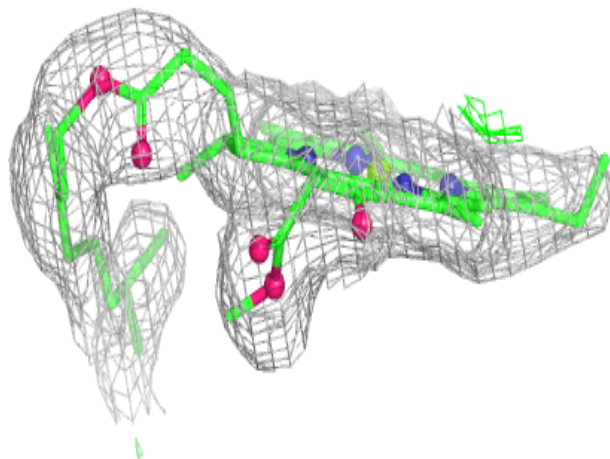
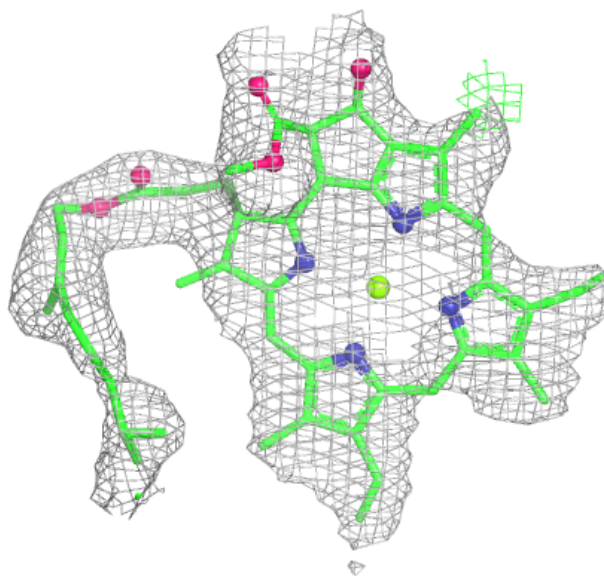
Electron density around CLA G 833:

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



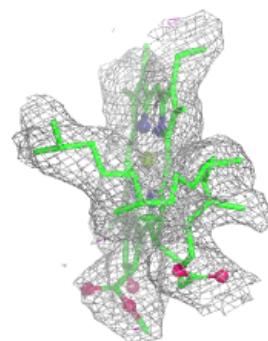
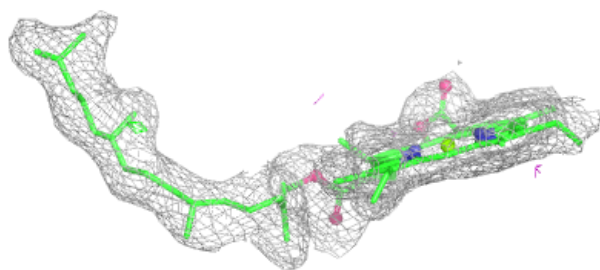
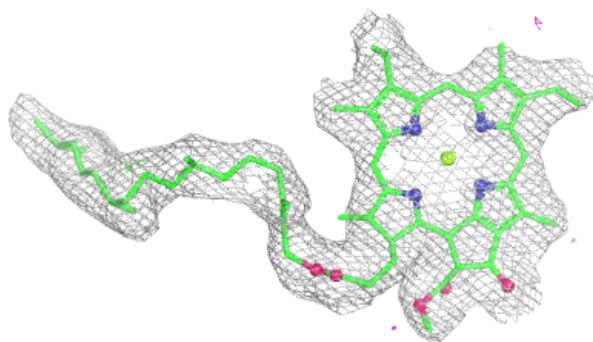
Electron density around CLA Z 825:

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

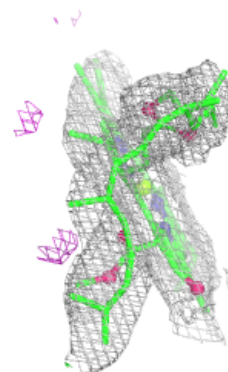
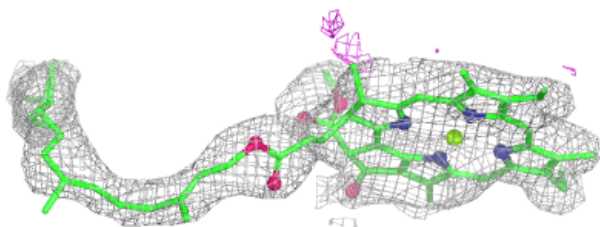
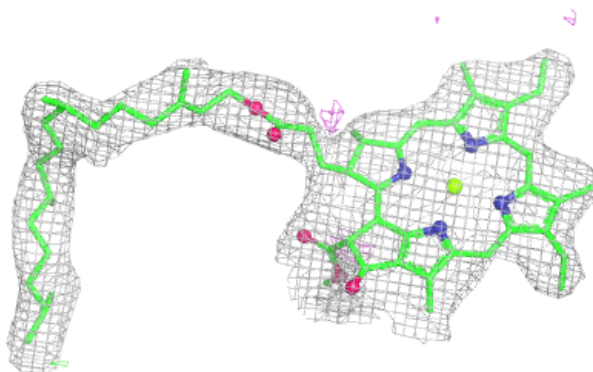


Electron density around CLA B 802:

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

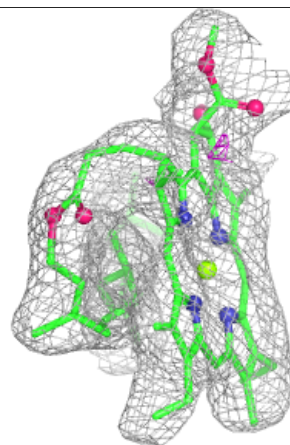
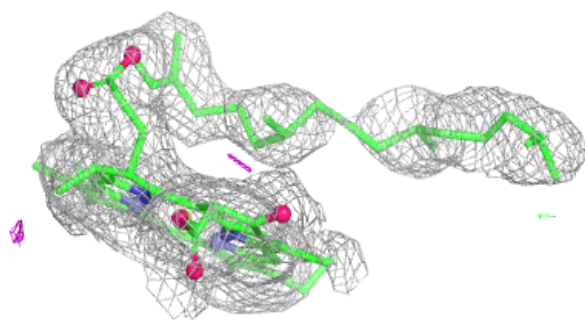
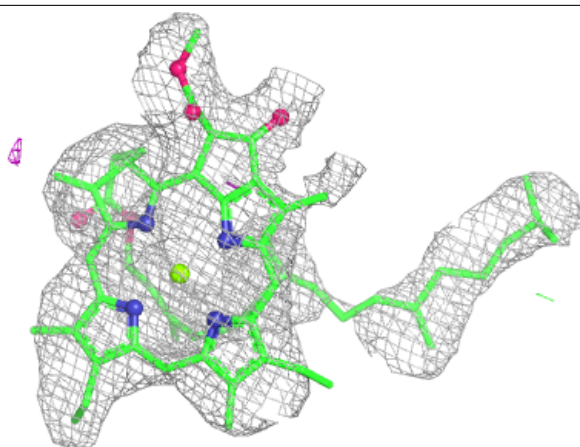
**Electron density around CLA Z 827:**

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



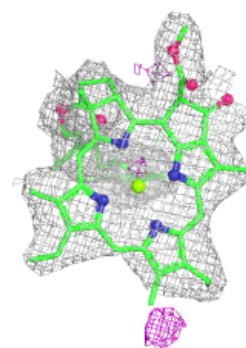
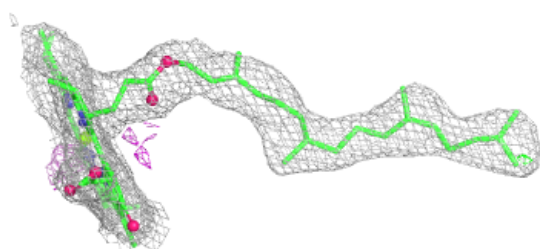
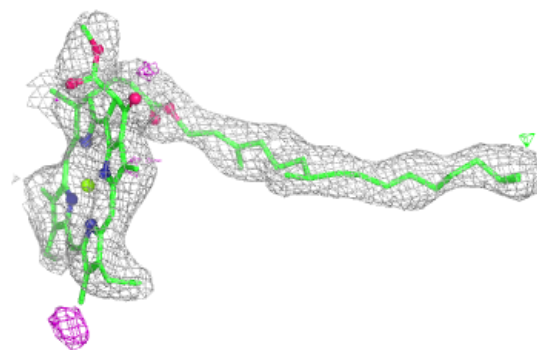
Electron density around CLA Z 828:

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

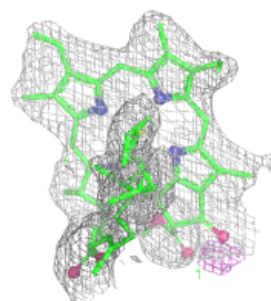
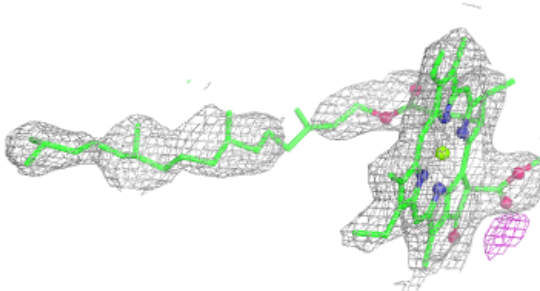
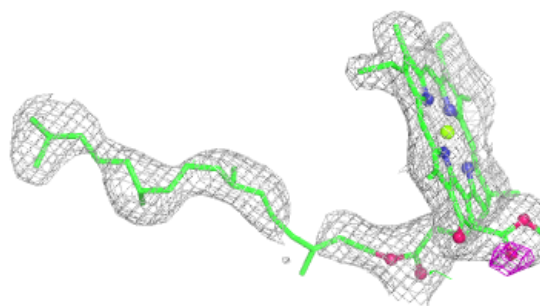


Electron density around CLA Z 829:

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

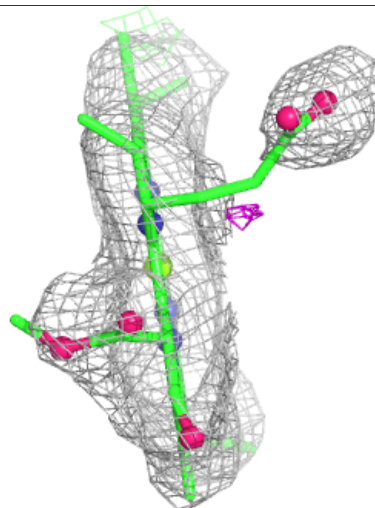
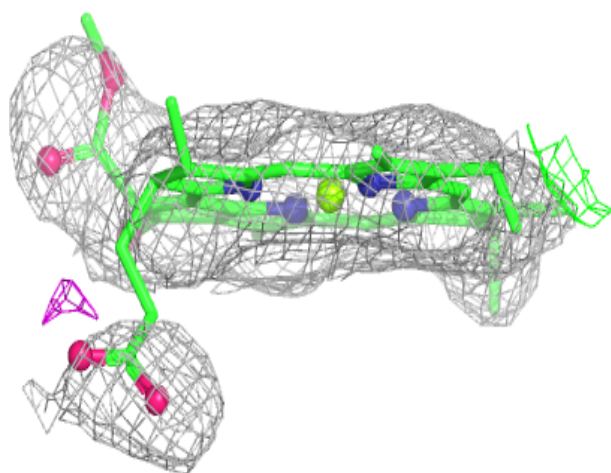
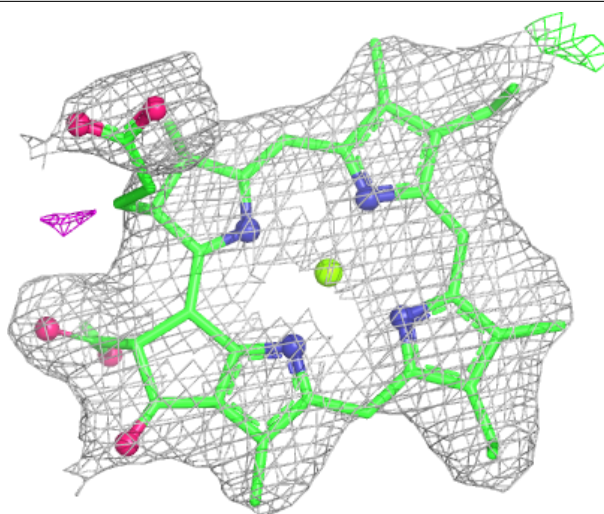
**Electron density around CLA Z 830:**

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



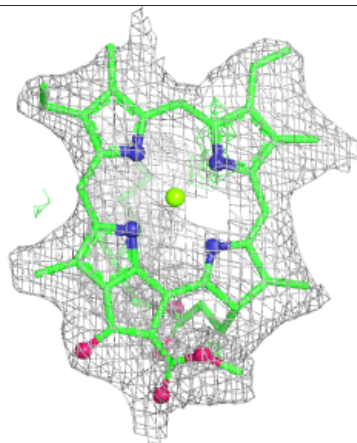
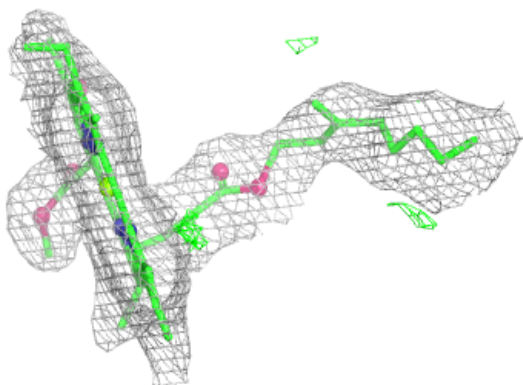
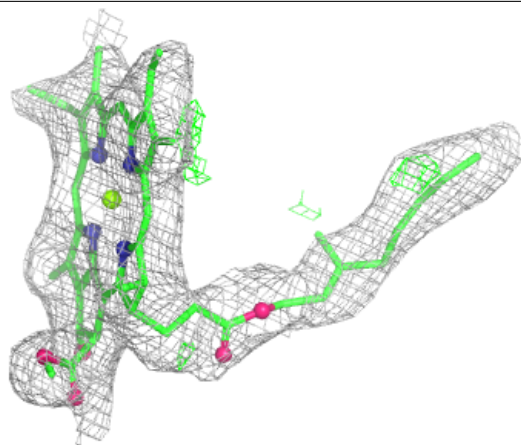
Electron density around CLA Z 831:

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



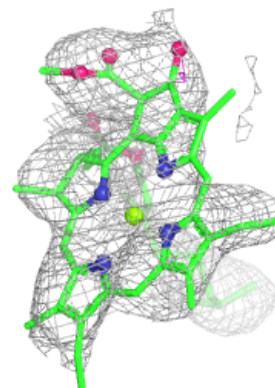
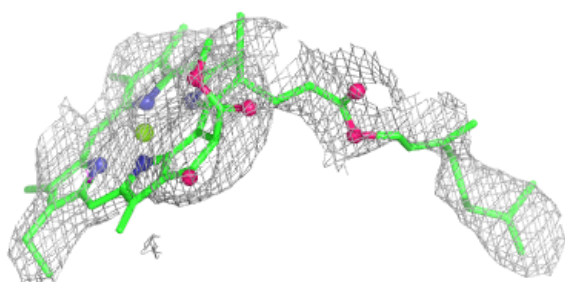
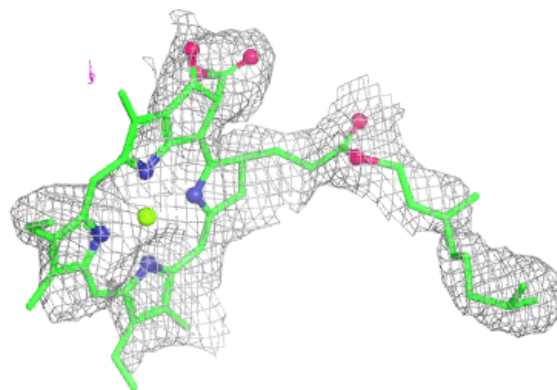
Electron density around CLA B 803:

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

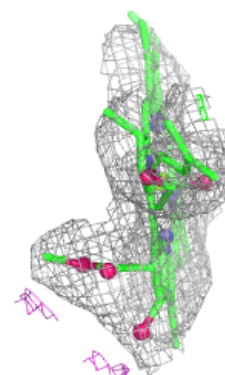
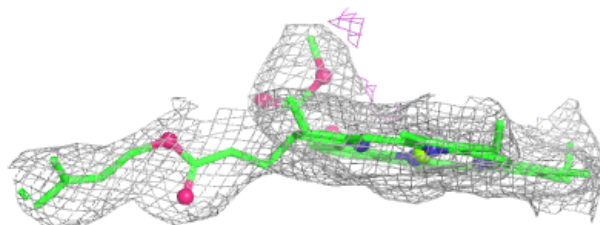
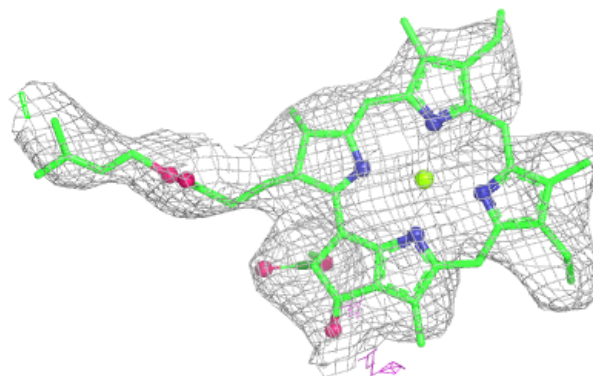


Electron density around CLA Z 833:

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

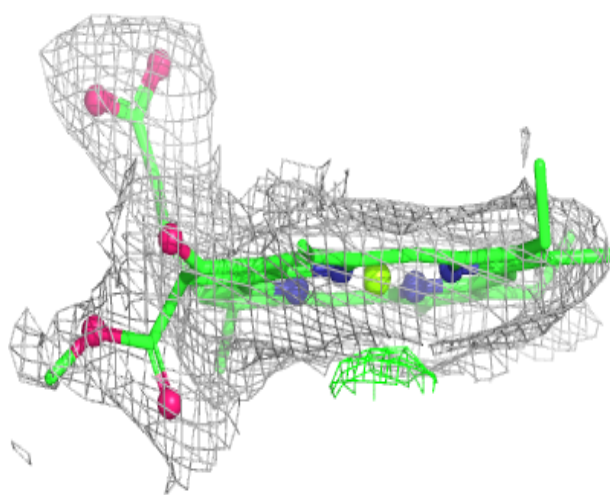
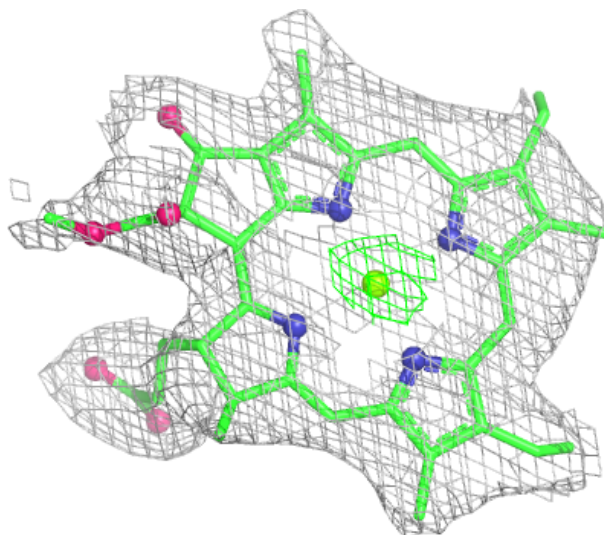
**Electron density around CLA G 836:**

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



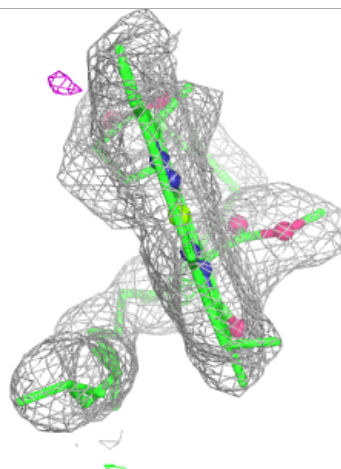
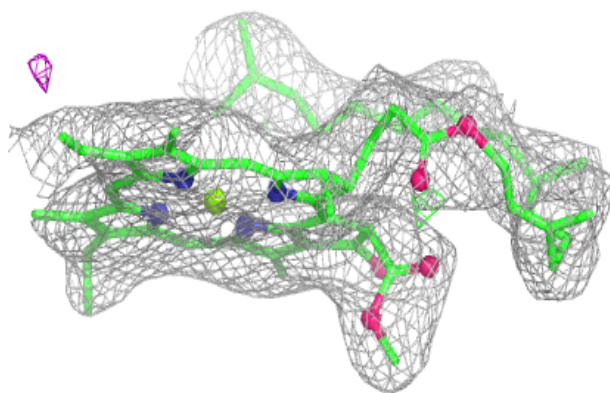
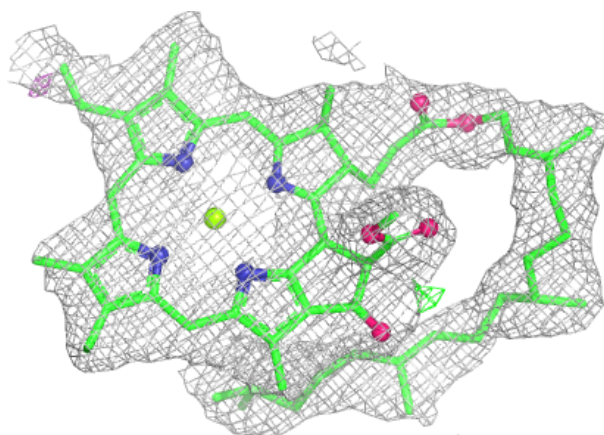
Electron density around CLA Z 835:

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



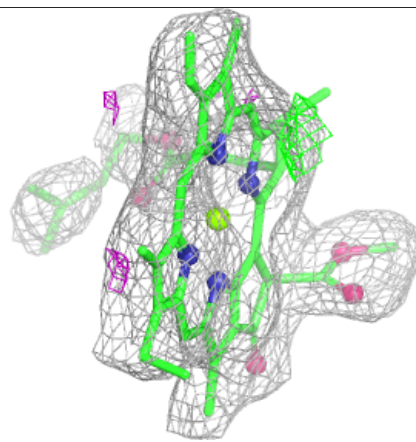
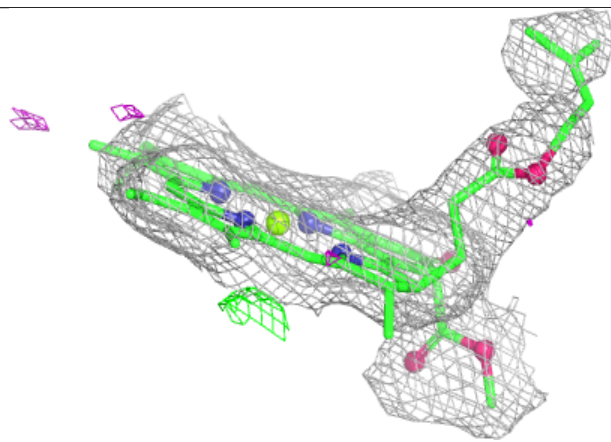
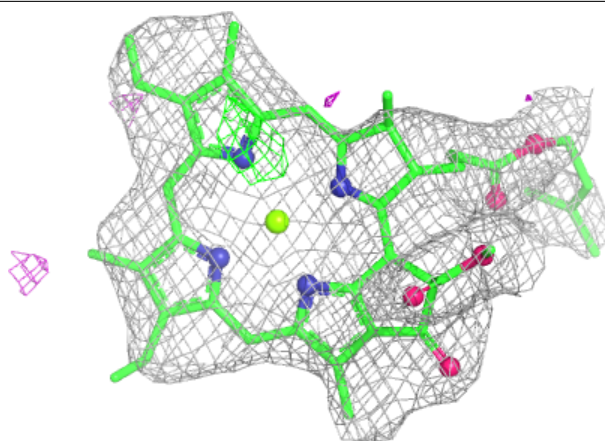
Electron density around CLA B 804:

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

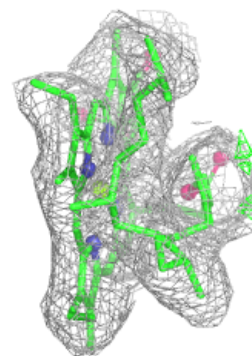
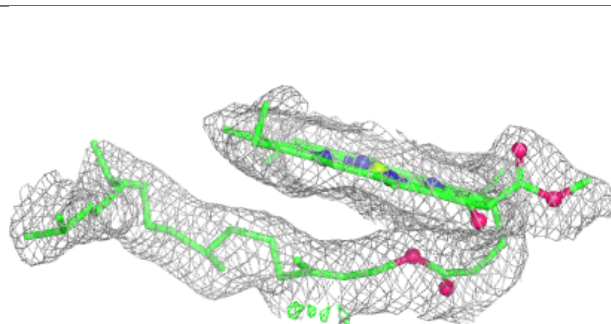
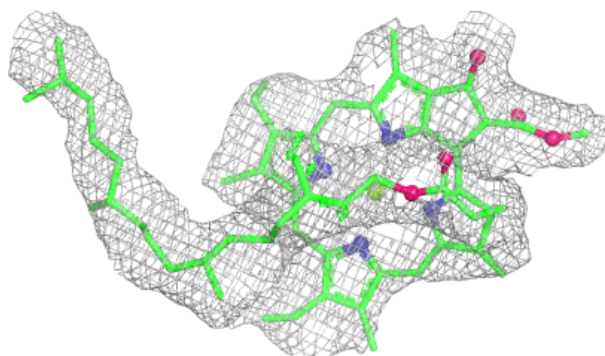


Electron density around CLA G 838:

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

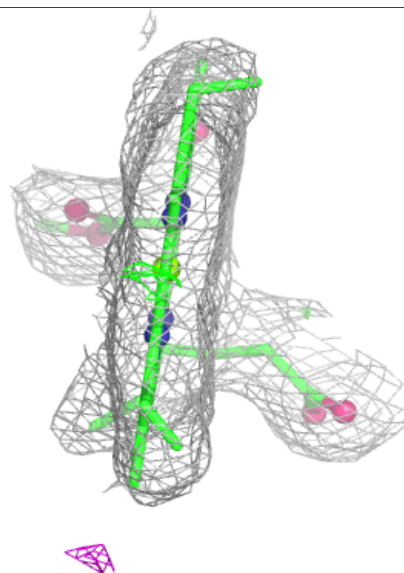
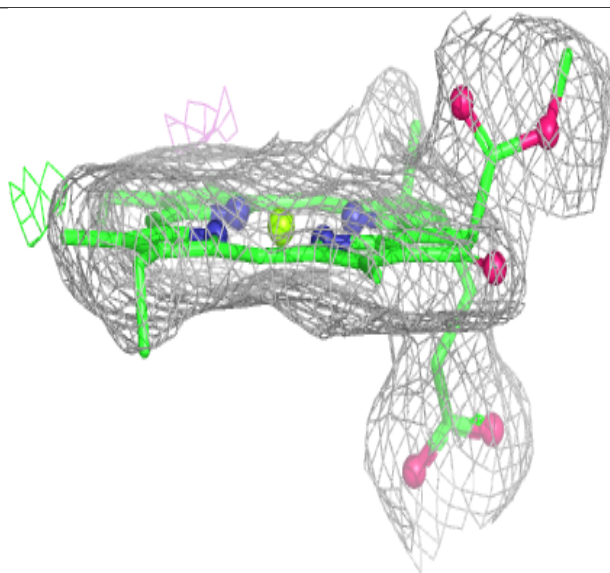
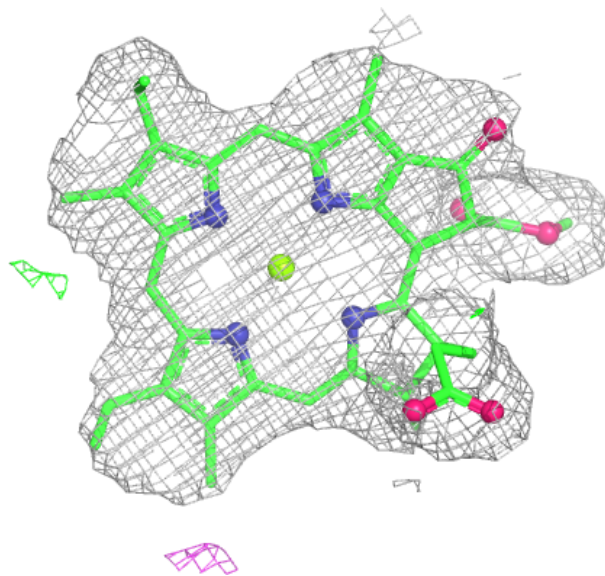
**Electron density around CLA Z 838:**

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



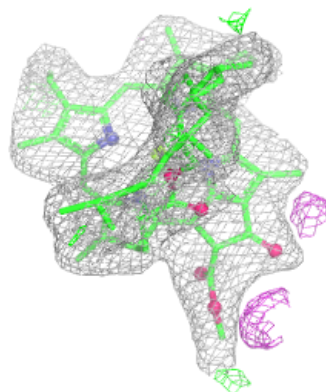
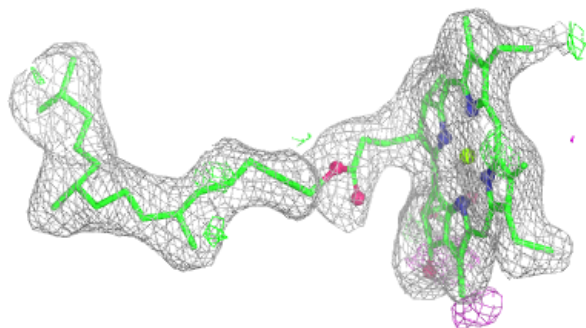
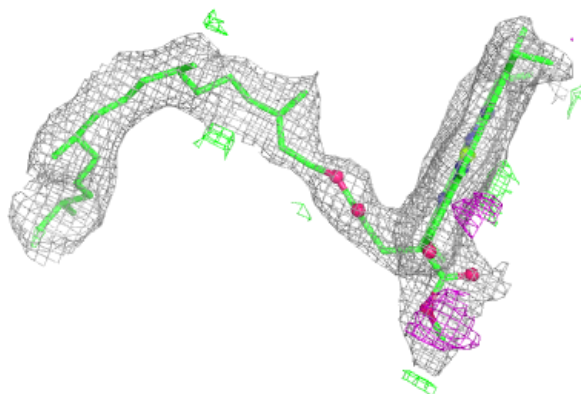
Electron density around CLA Z 839:

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

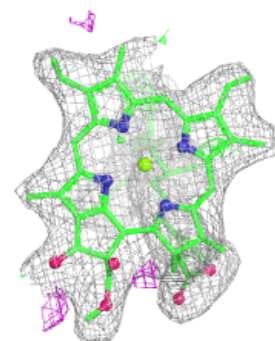
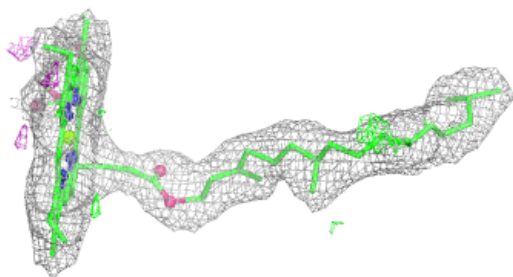
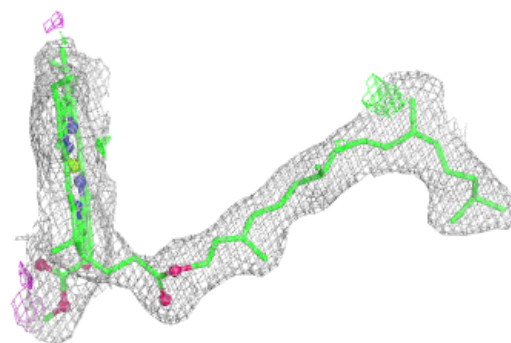


Electron density around CLA Z 840:

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

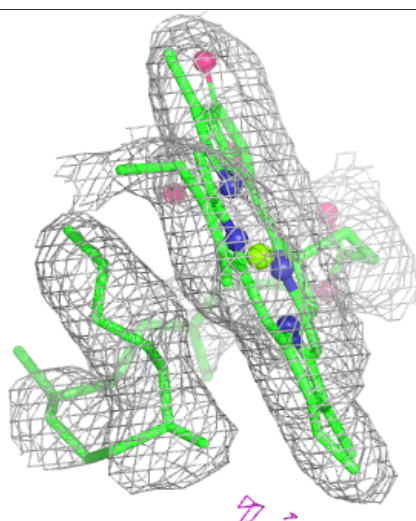
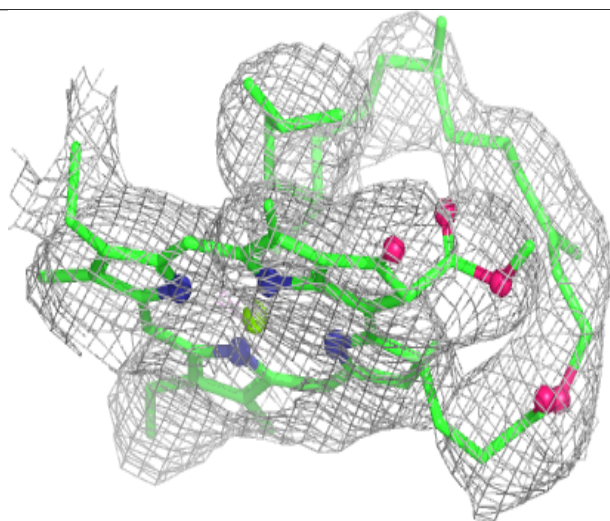
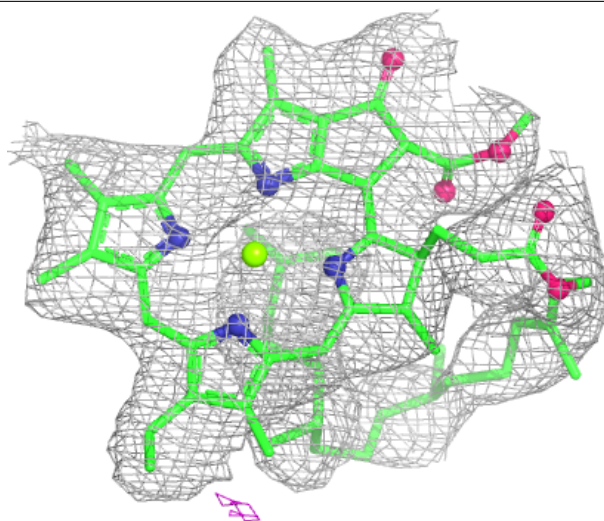
**Electron density around CLA Z 841:**

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



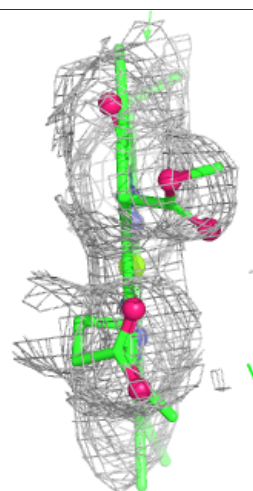
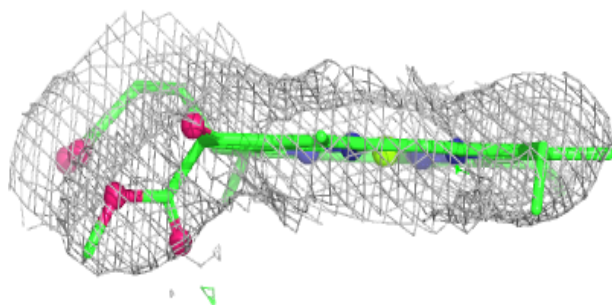
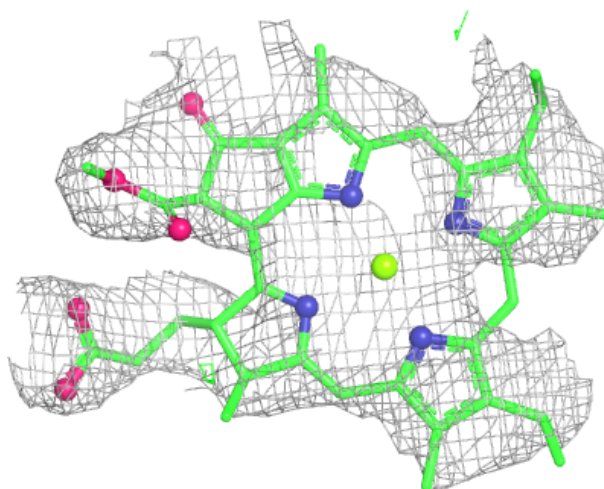
Electron density around CLA B 805:

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



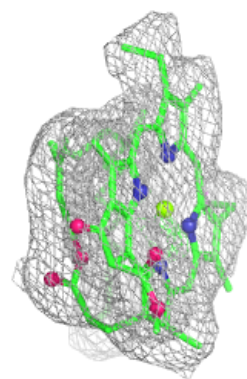
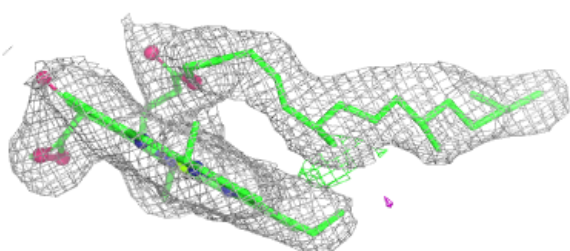
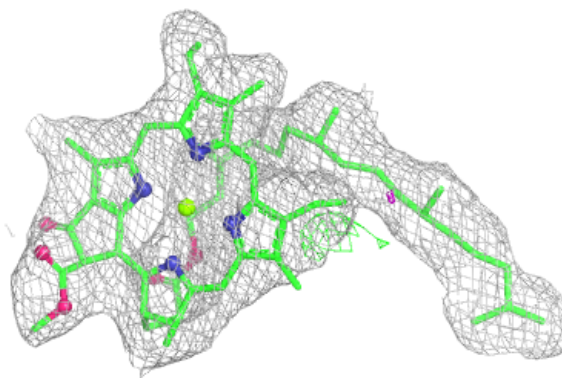
Electron density around CLA d 202:

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

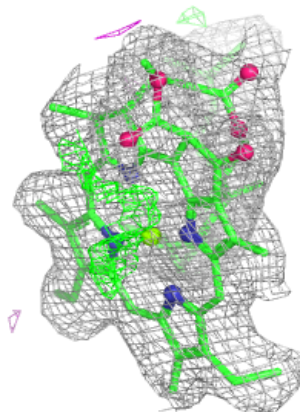
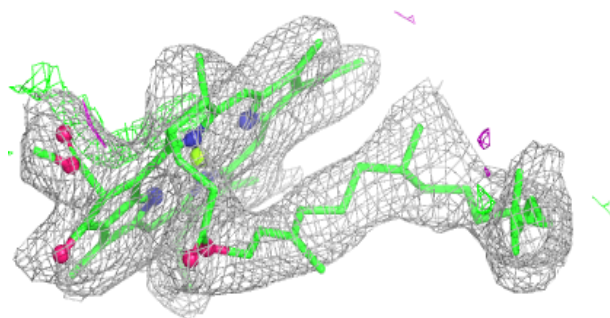
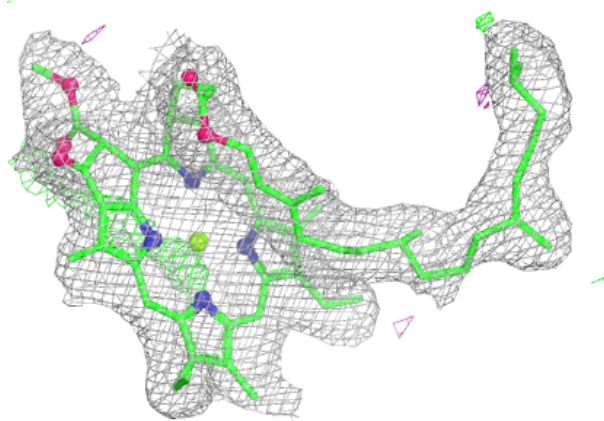


Electron density around CLA B 806:

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

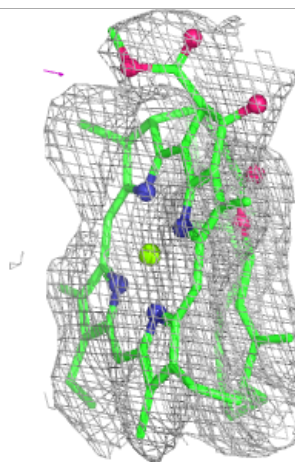
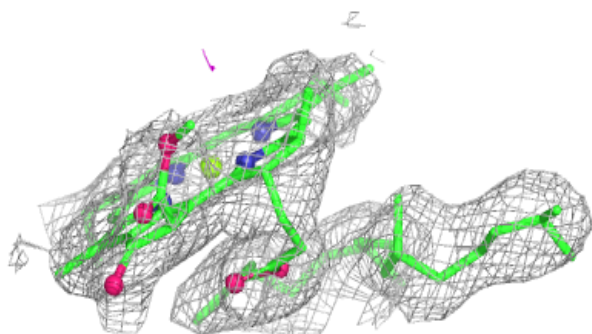
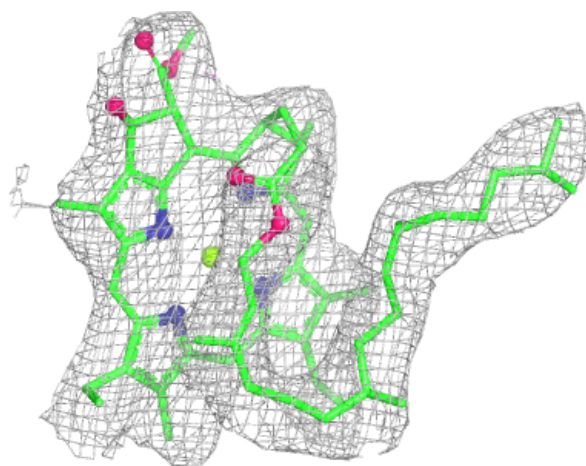
**Electron density around CLA G 841:**

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



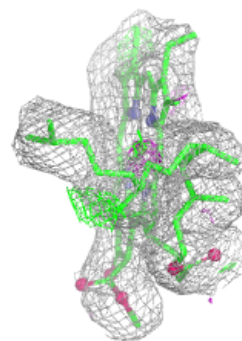
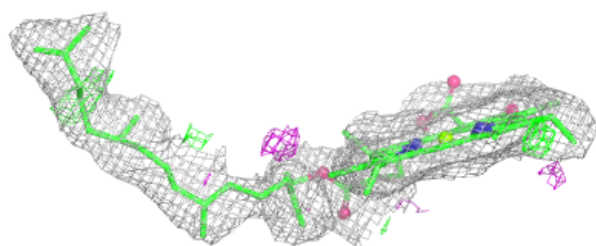
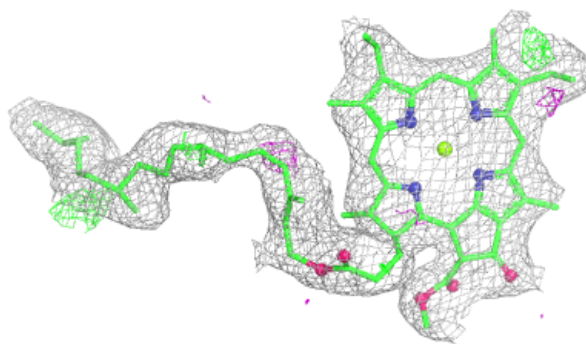
Electron density around CLA B 807:

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

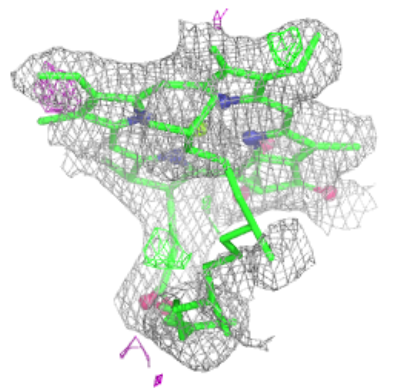
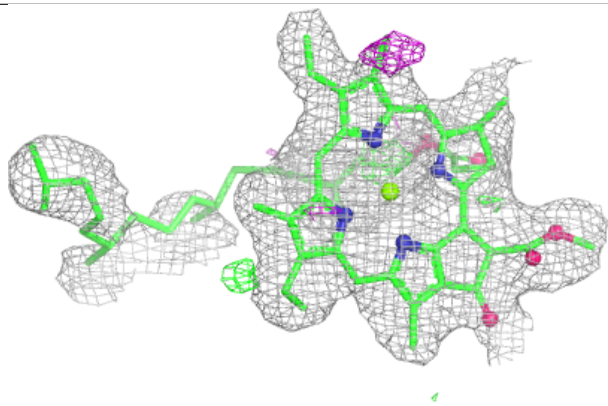
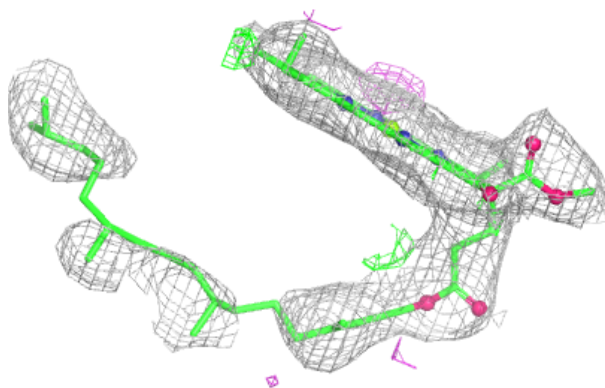


Electron density around CLA G 852:

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

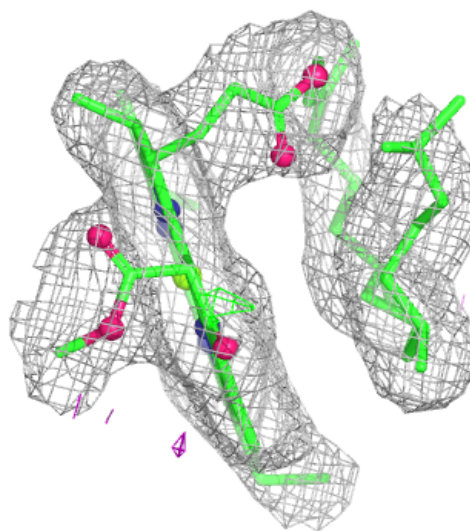
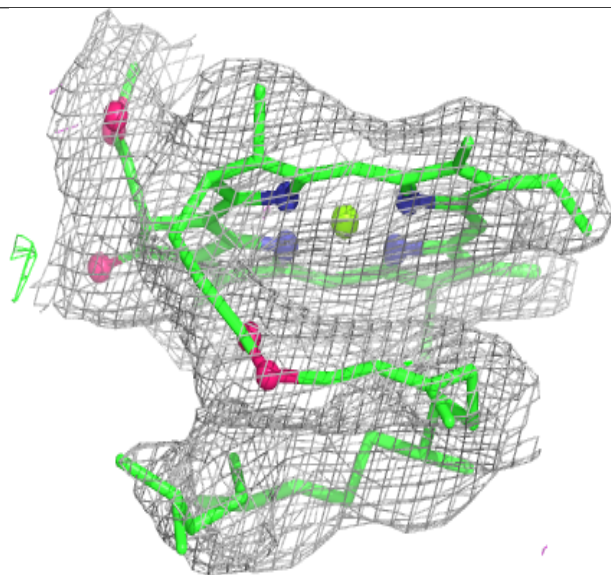
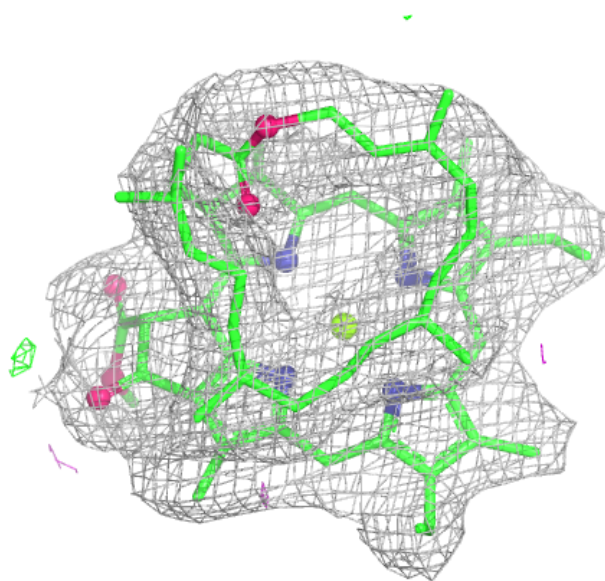
**Electron density around CLA h 201:**

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



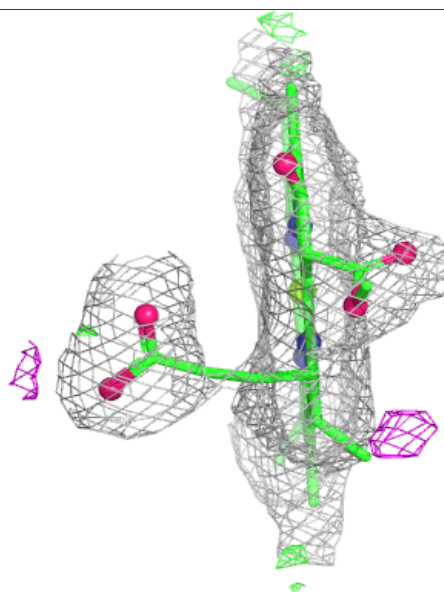
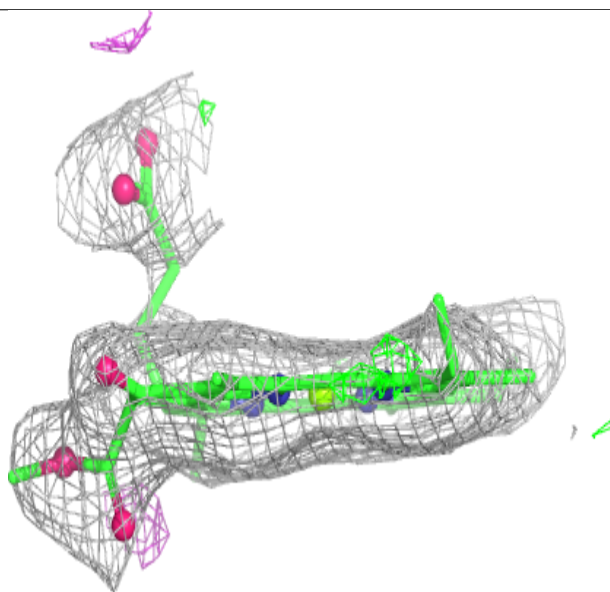
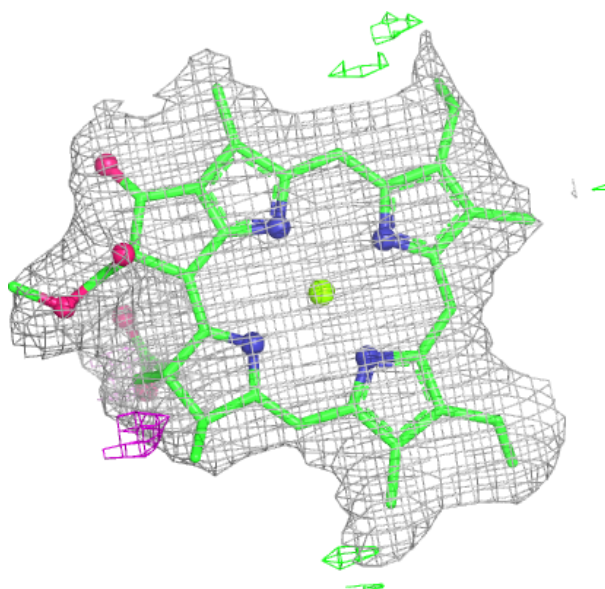
Electron density around CLA h 204:

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



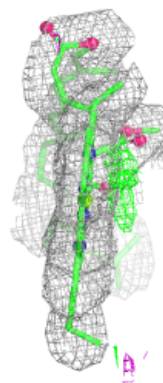
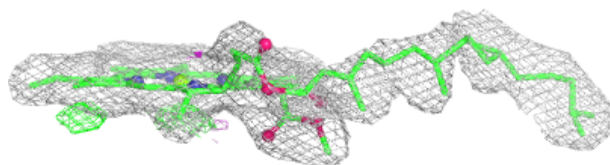
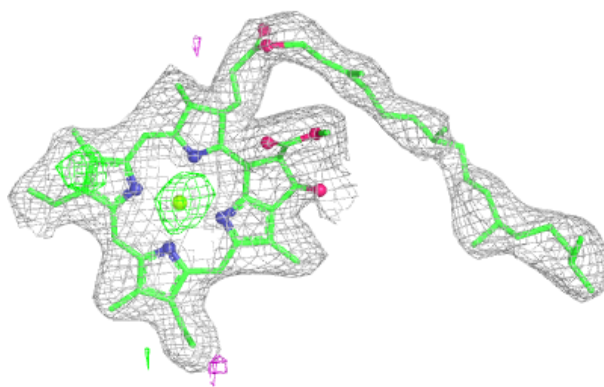
Electron density around CLA G 853:

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



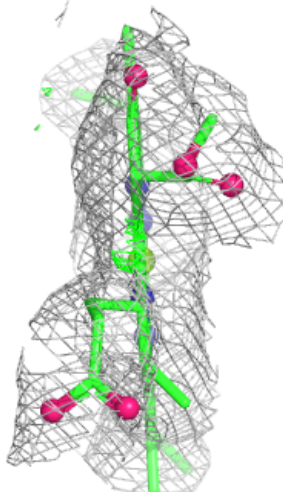
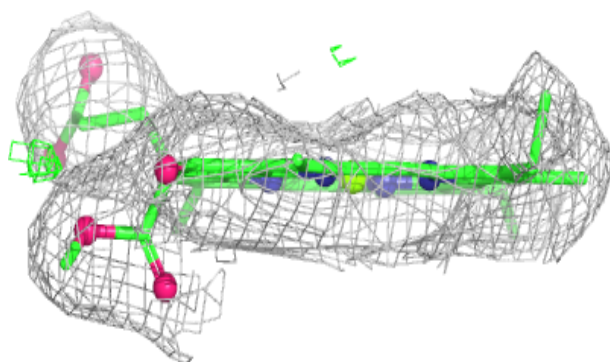
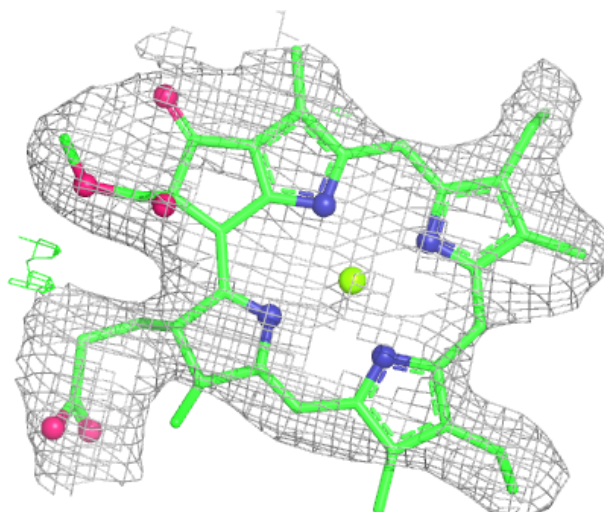
Electron density around CLA h 206:

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



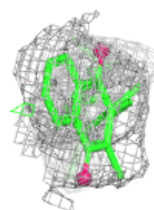
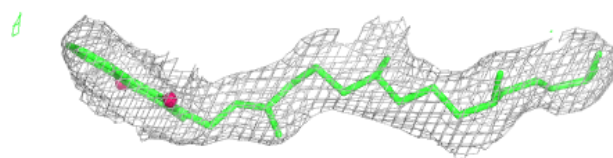
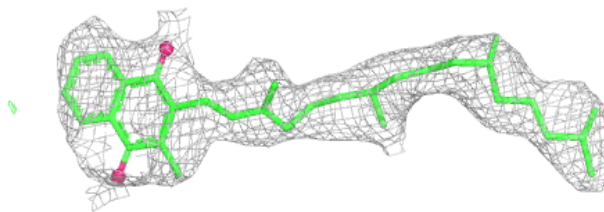
Electron density around CLA j 102:

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

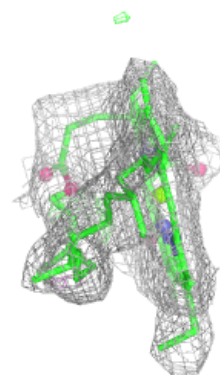
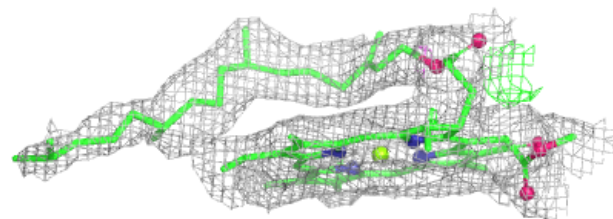
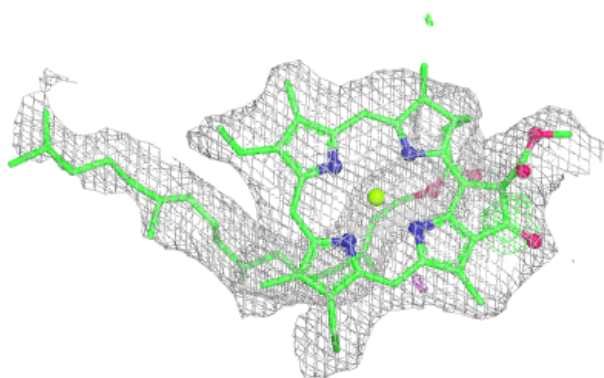


Electron density around PQN A 844:

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

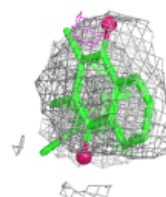
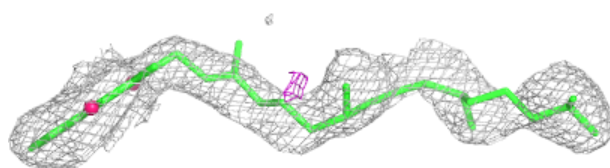
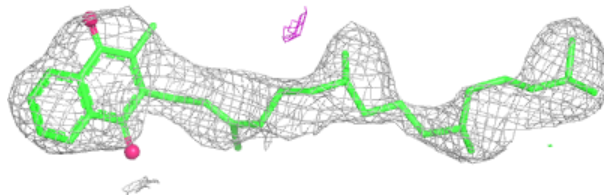
**Electron density around CLA H 801:**

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

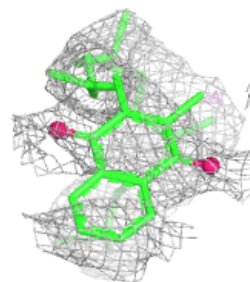
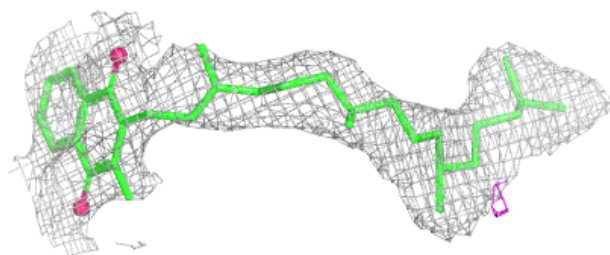
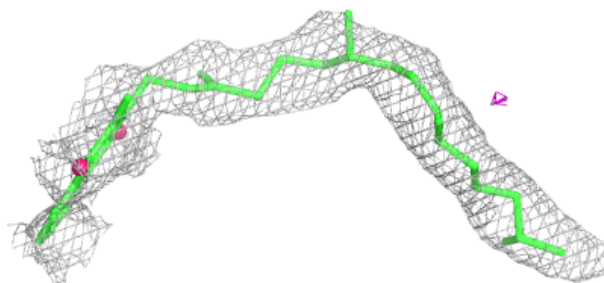


Electron density around PQN G 843:

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

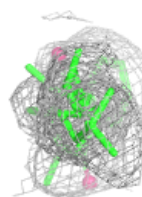
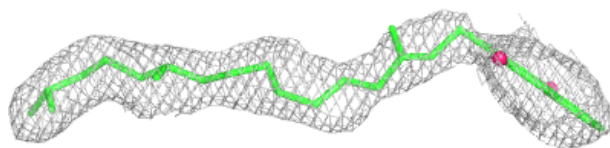
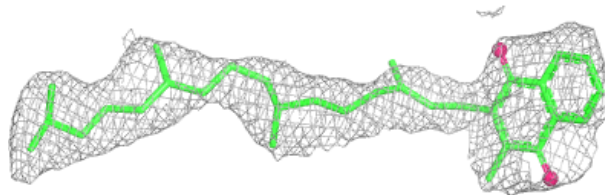
**Electron density around PQN H 841:**

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

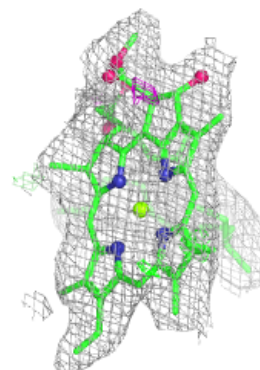
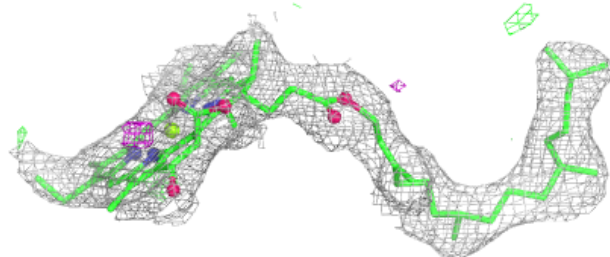
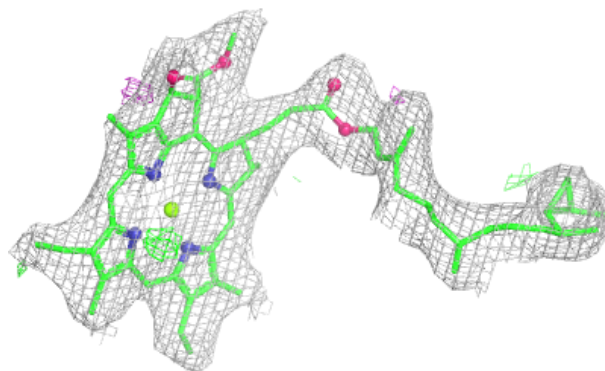


Electron density around PQN Y 842:

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

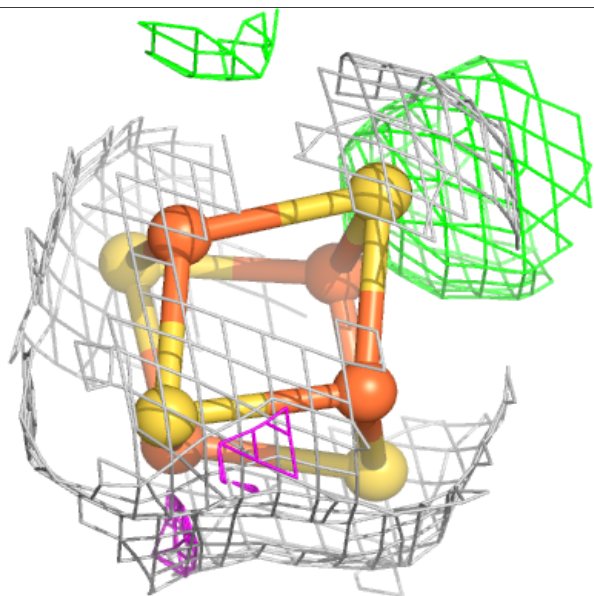
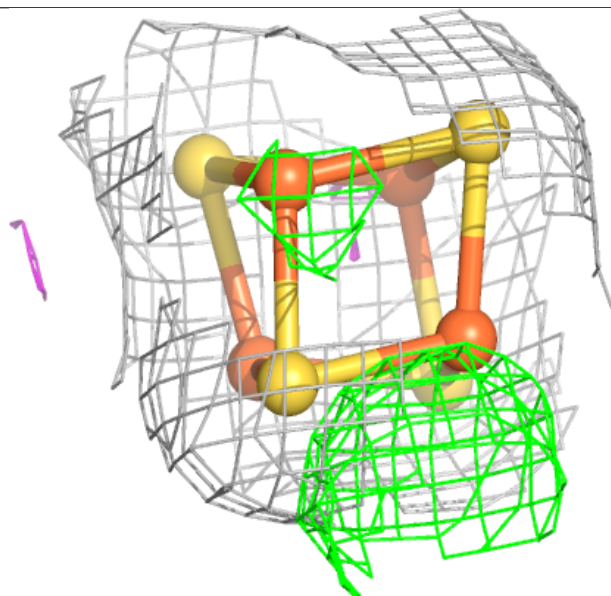
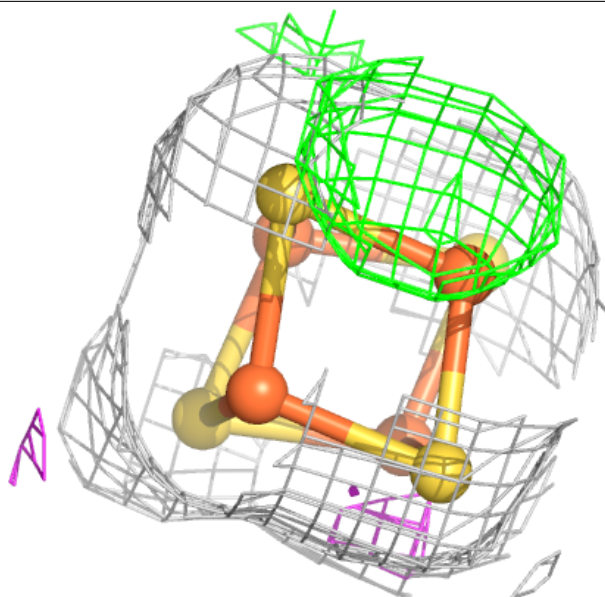
**Electron density around CLA B 808:**

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



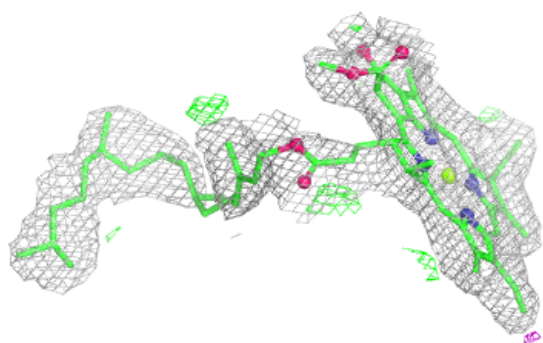
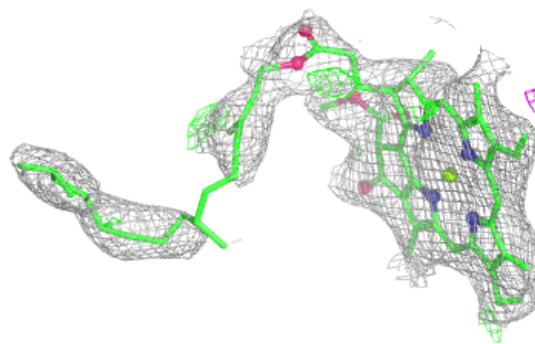
Electron density around SF4 G 844:

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

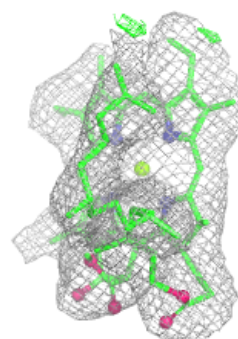
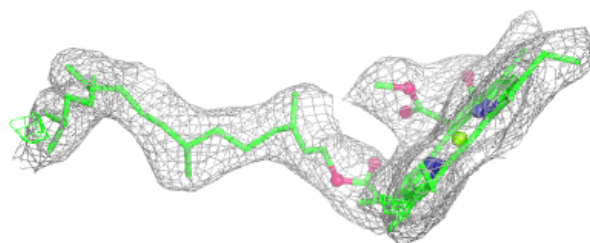
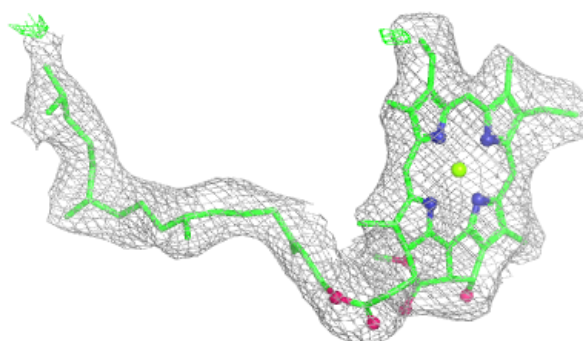


Electron density around CLA H 803:

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

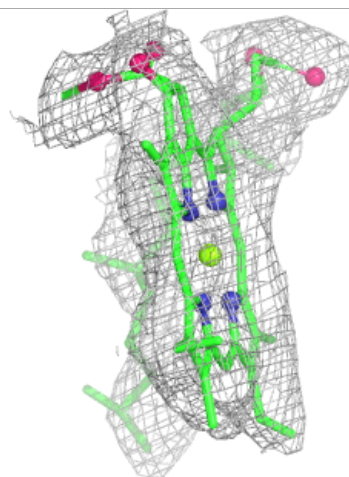
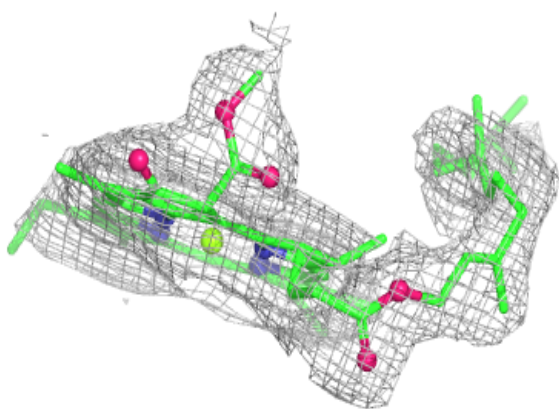
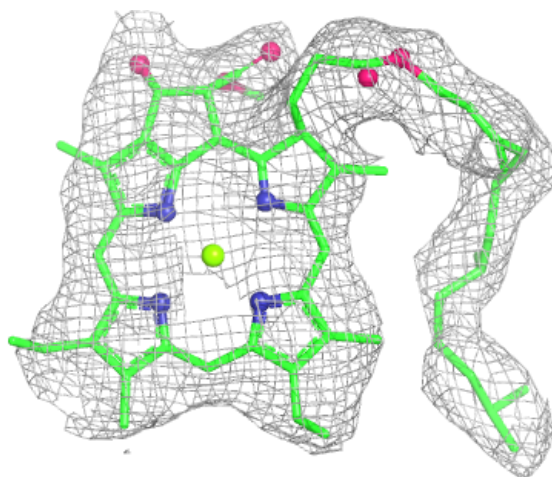
**Electron density around CLA B 809:**

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



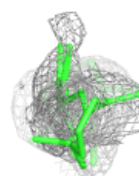
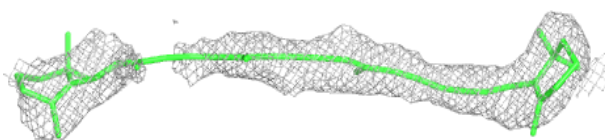
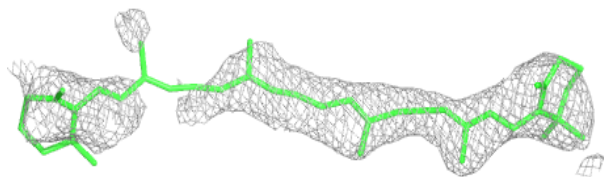
Electron density around CLA A 814:

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



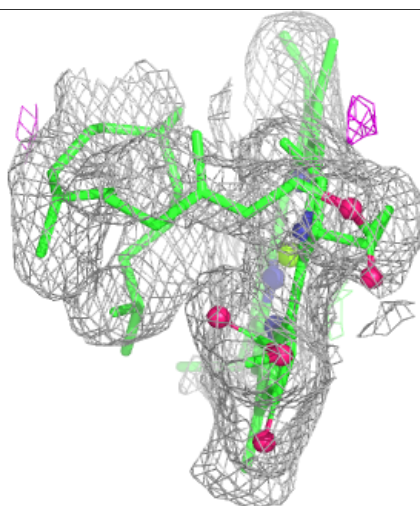
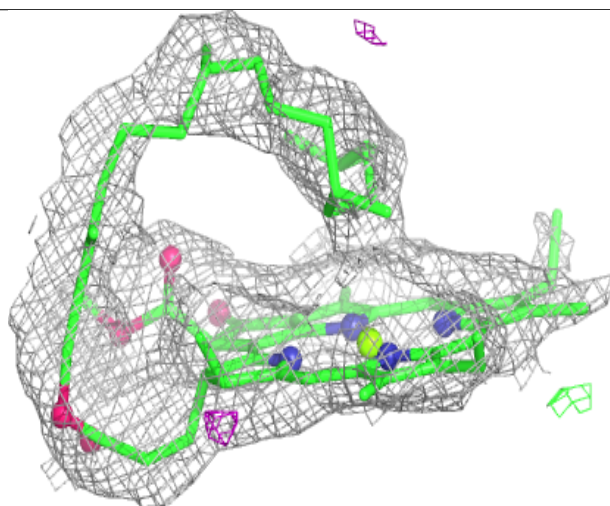
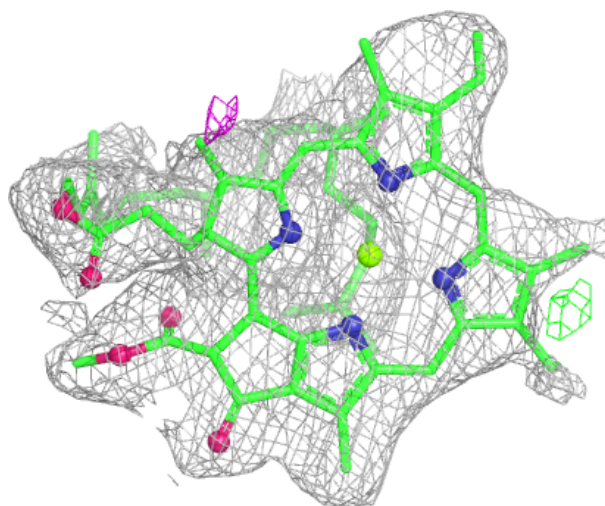
Electron density around BCR A 849:

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



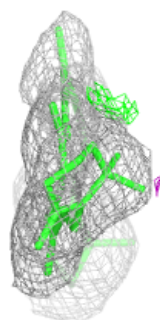
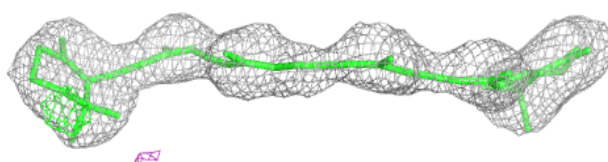
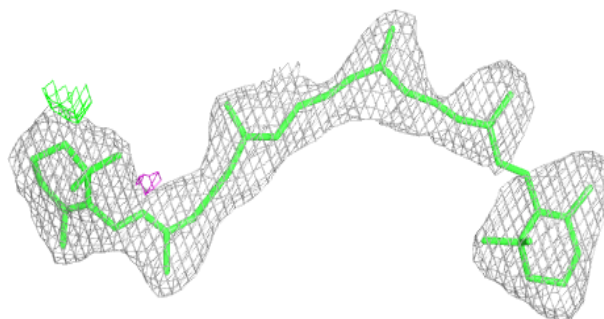
Electron density around CLA H 806:

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

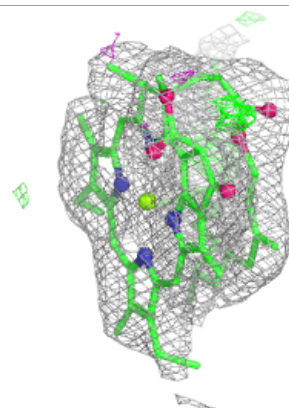
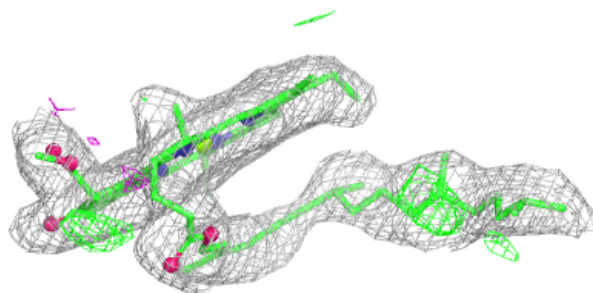
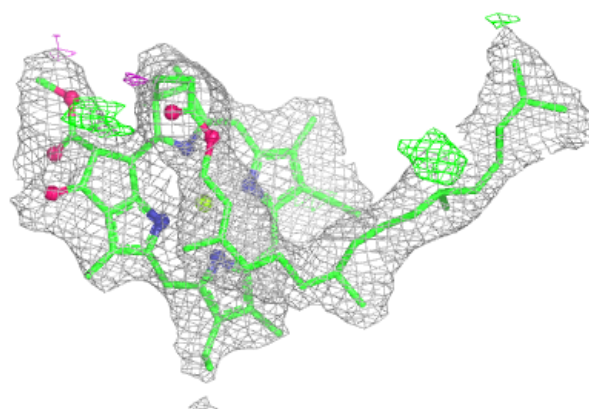


Electron density around BCR A 851:

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

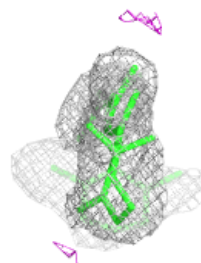
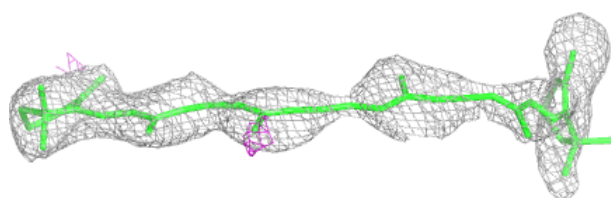
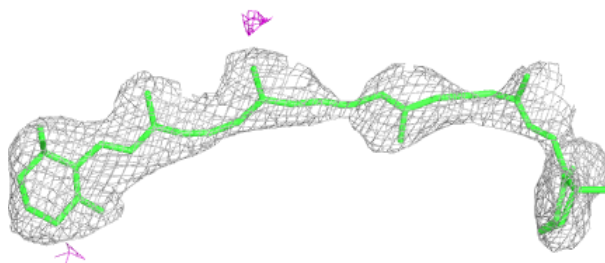
**Electron density around CLA H 807:**

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

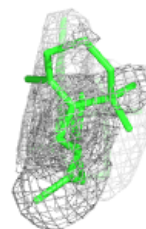
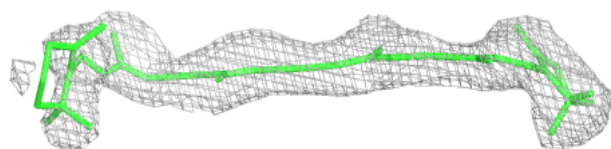
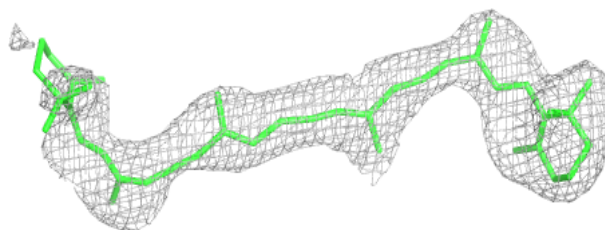


Electron density around BCR B 843:

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

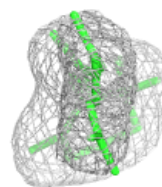
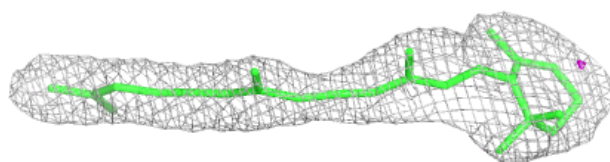
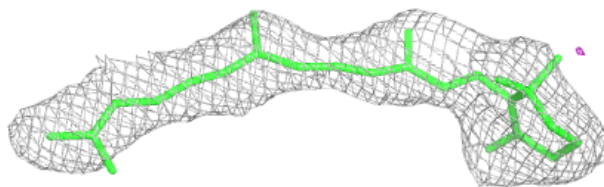
**Electron density around BCR B 844:**

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



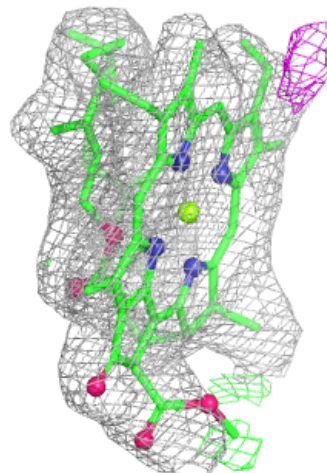
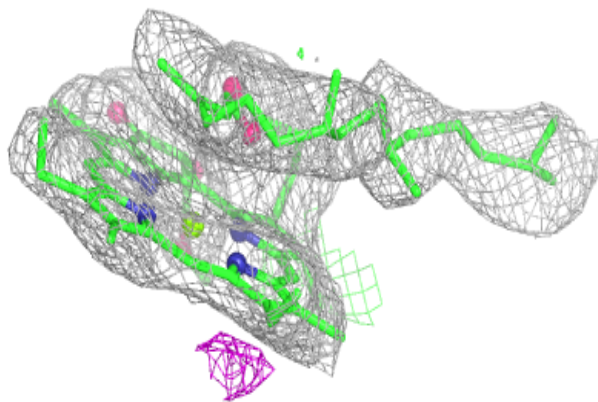
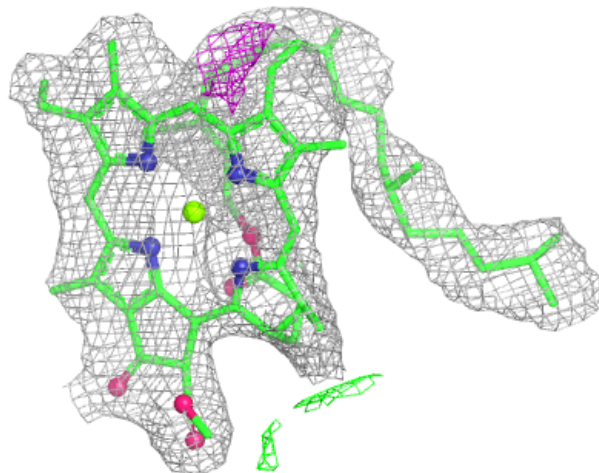
Electron density around BCR B 845:

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



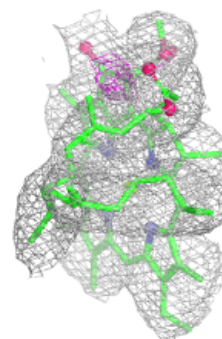
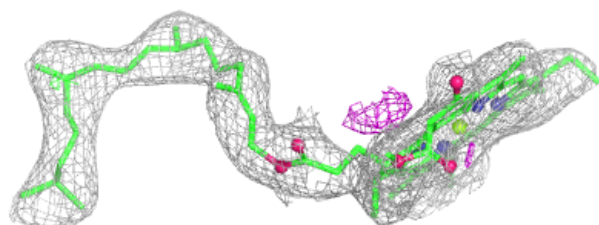
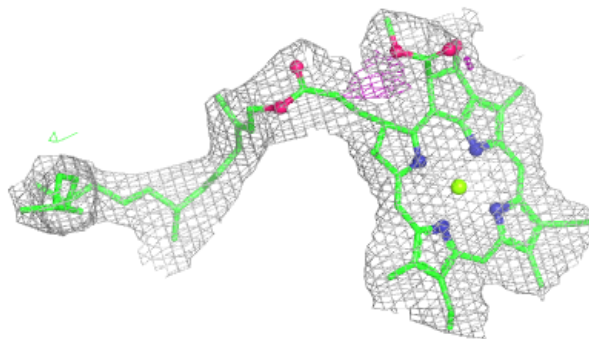
Electron density around CLA H 808:

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

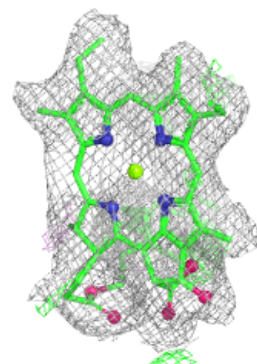
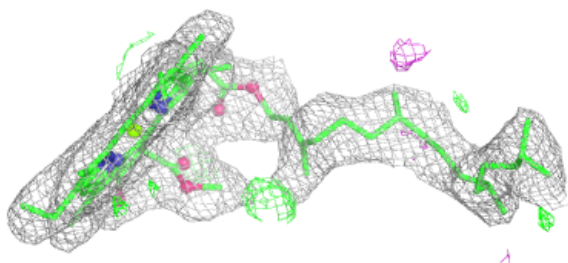
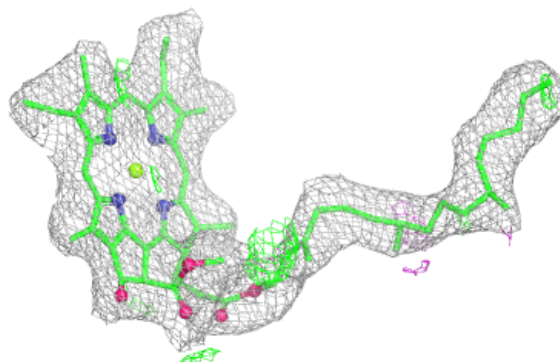


Electron density around CLA H 809:

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

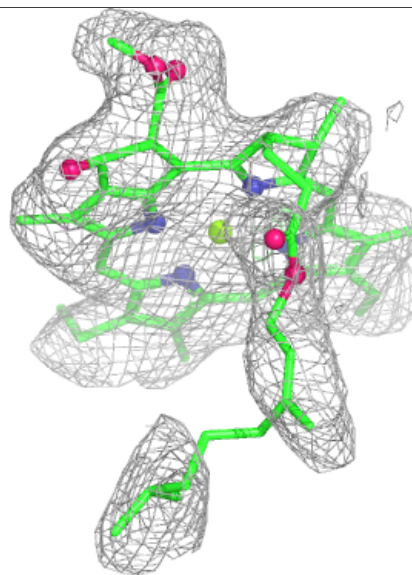
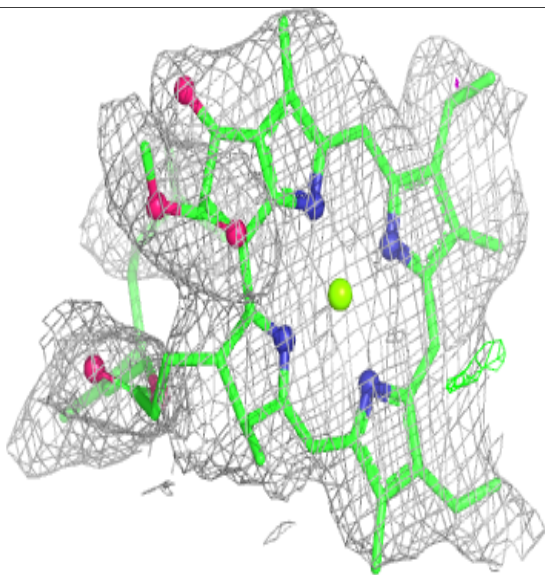
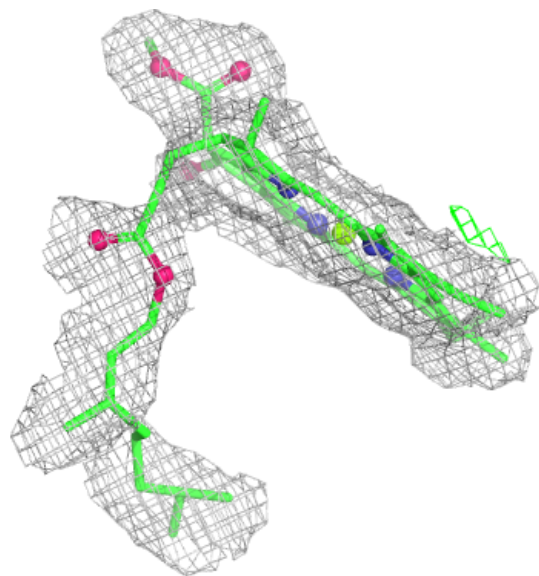
**Electron density around CLA H 810:**

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



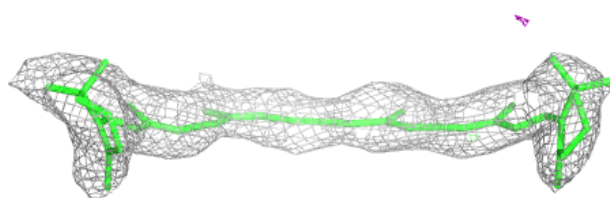
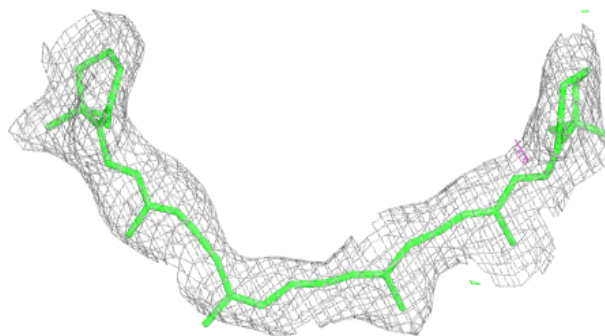
Electron density around CLA H 811:

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

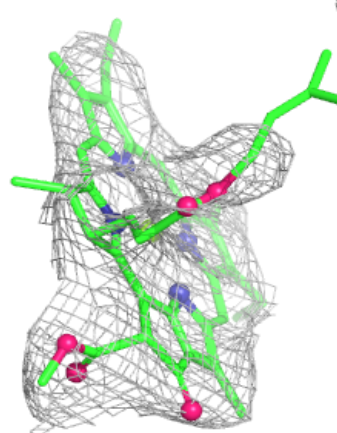
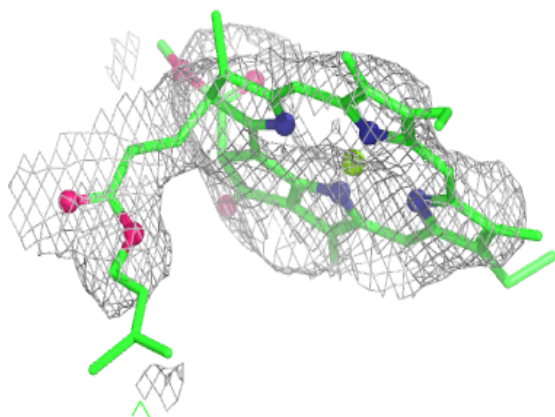
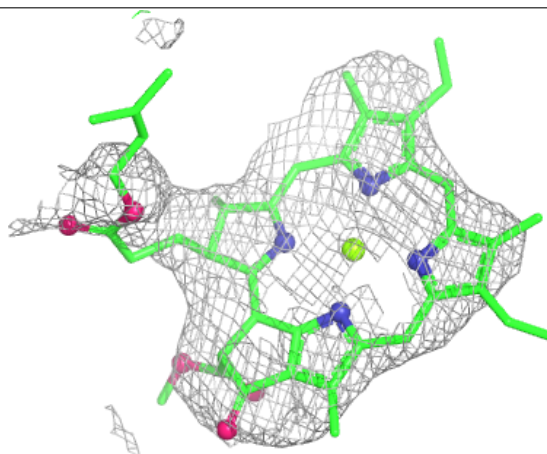


Electron density around BCR F 203:

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

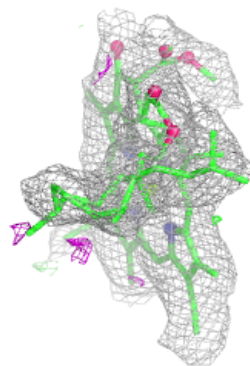
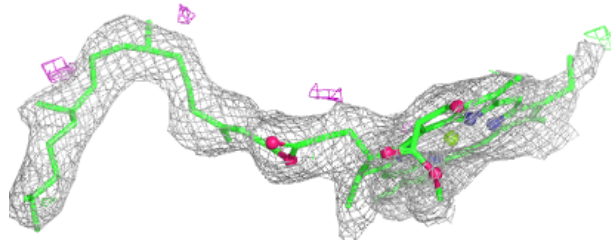
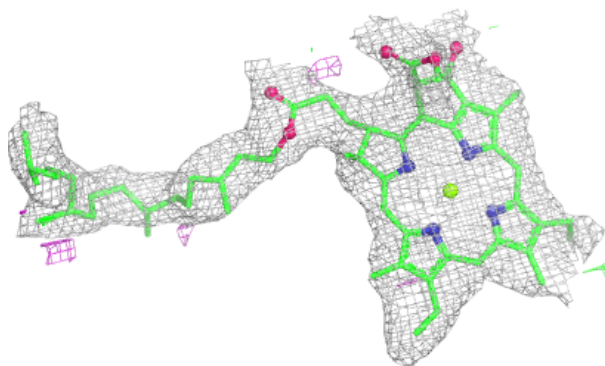
**Electron density around CLA A 815:**

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

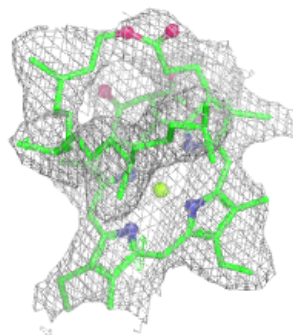
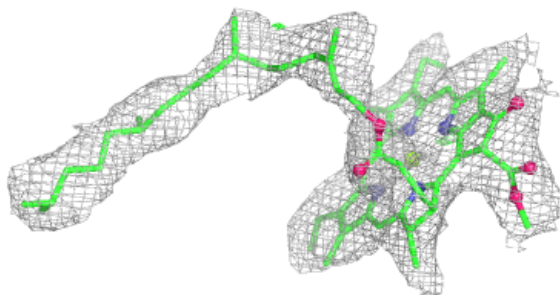
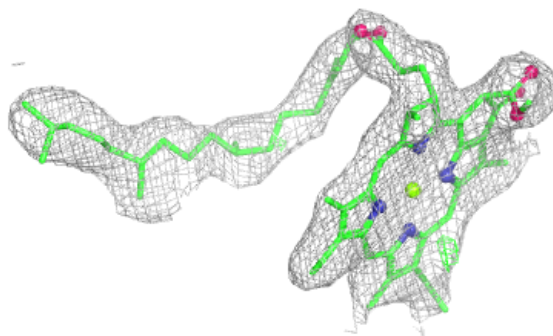


Electron density around CLA H 813:

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

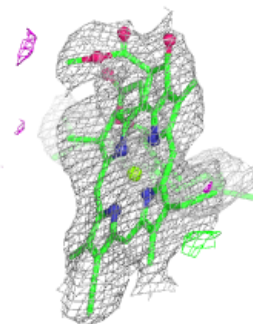
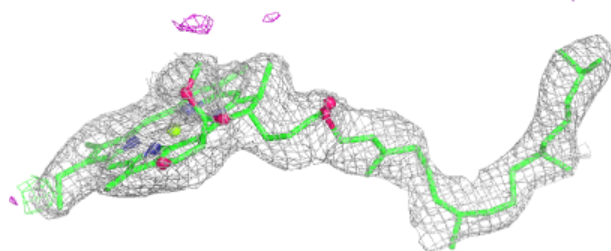
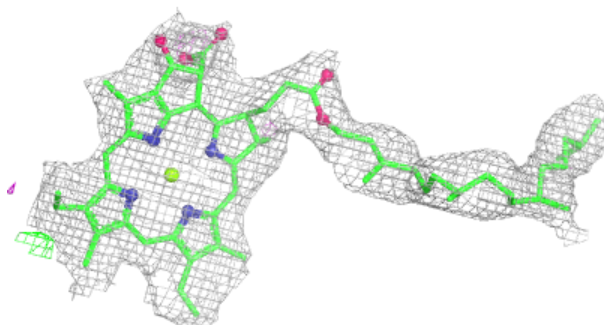
**Electron density around CLA H 814:**

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

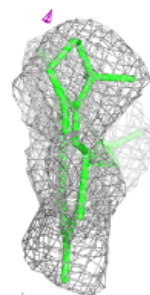
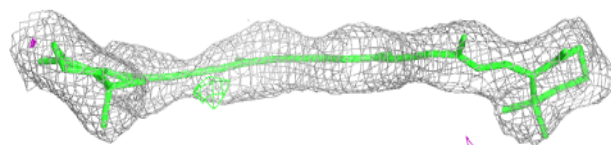
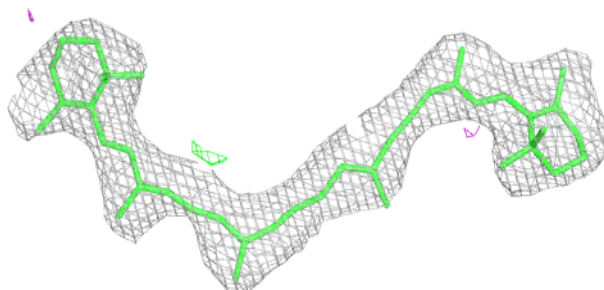


Electron density around CLA B 812:

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

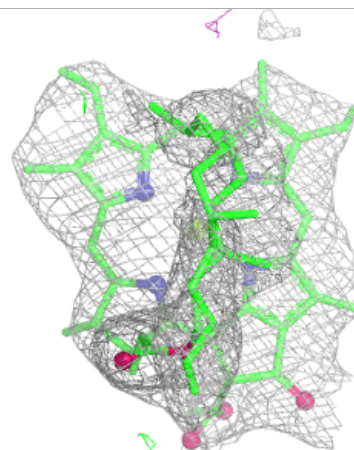
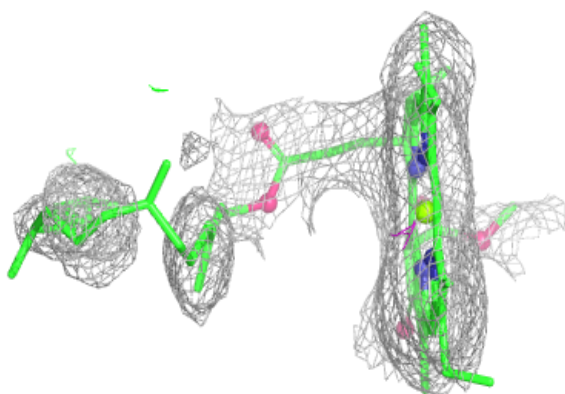
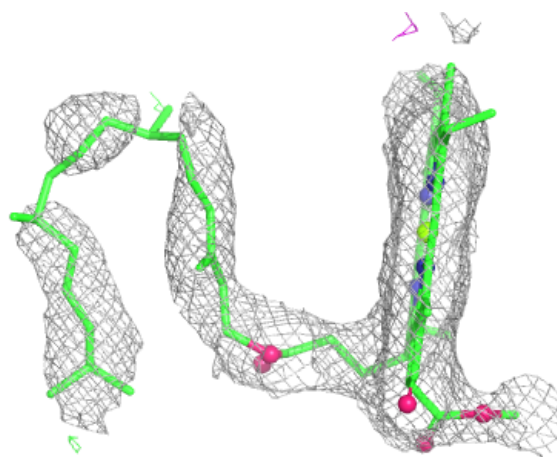
**Electron density around BCR G 849:**

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



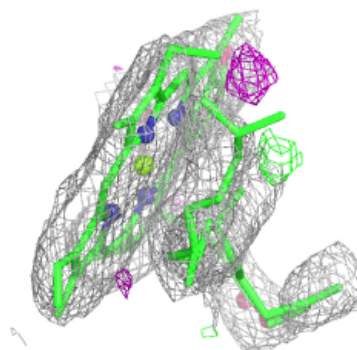
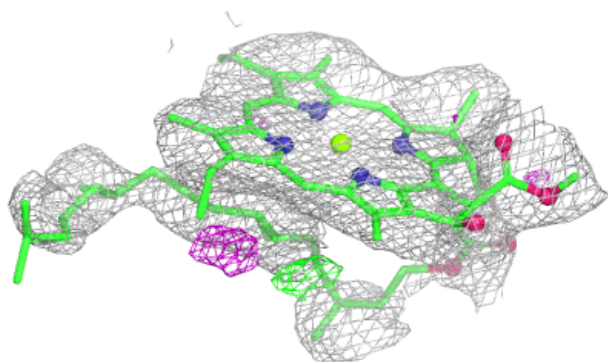
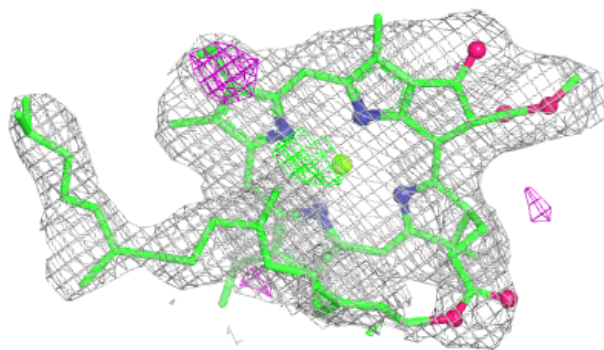
Electron density around CLA B 813:

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

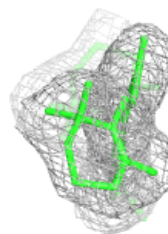
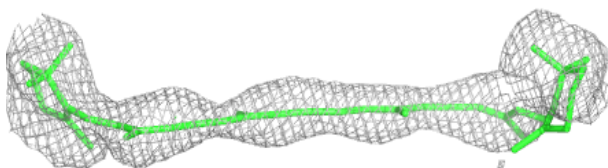
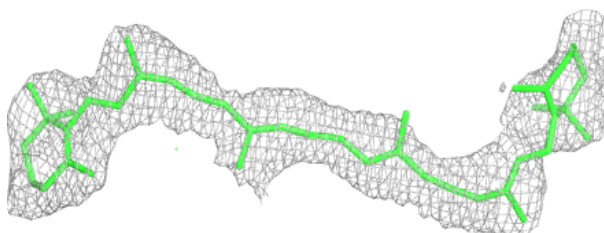


Electron density around CLA H 817:

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

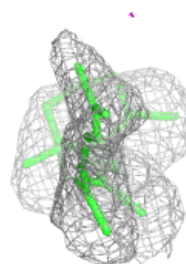
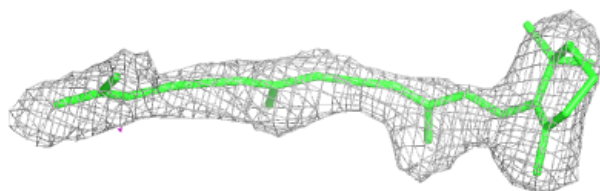
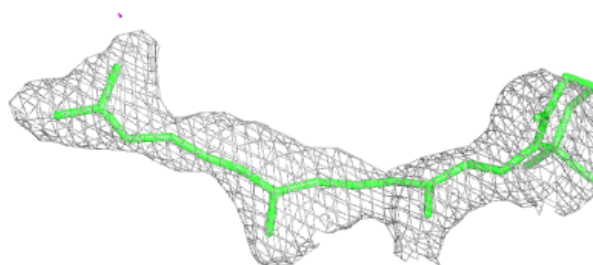
**Electron density around BCR H 844:**

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



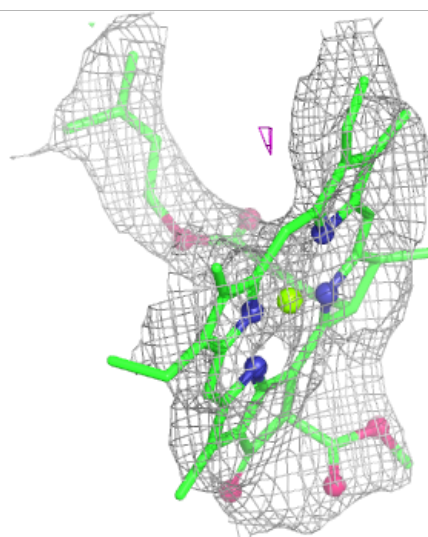
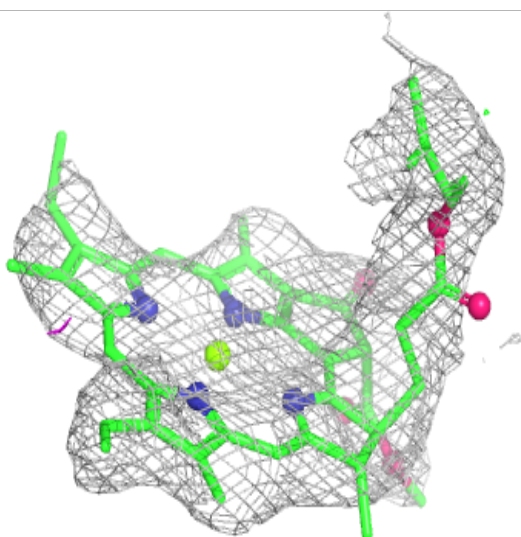
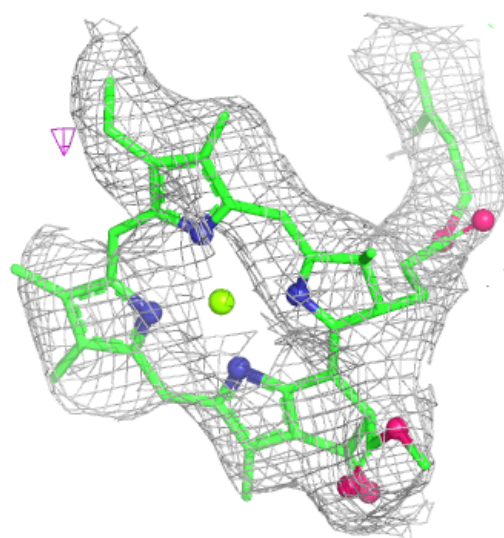
Electron density around BCR H 845:

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



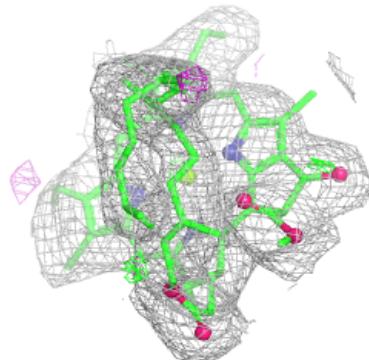
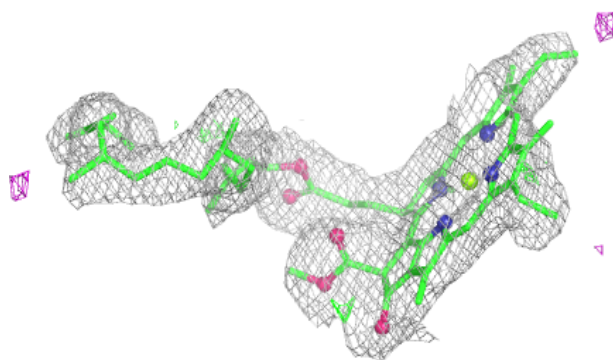
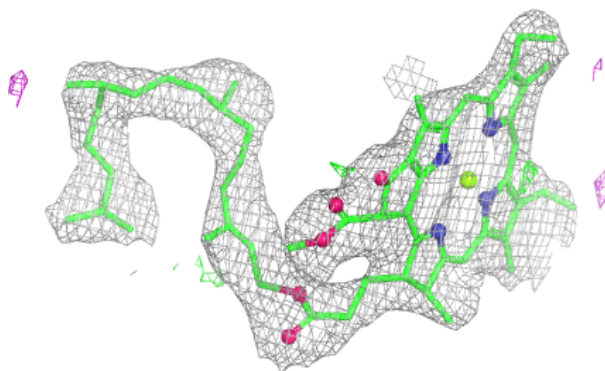
Electron density around CLA A 816:

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



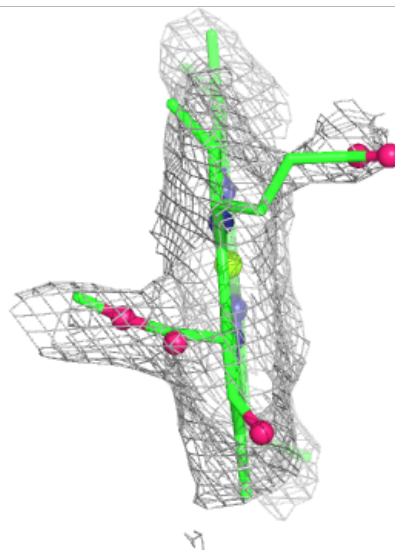
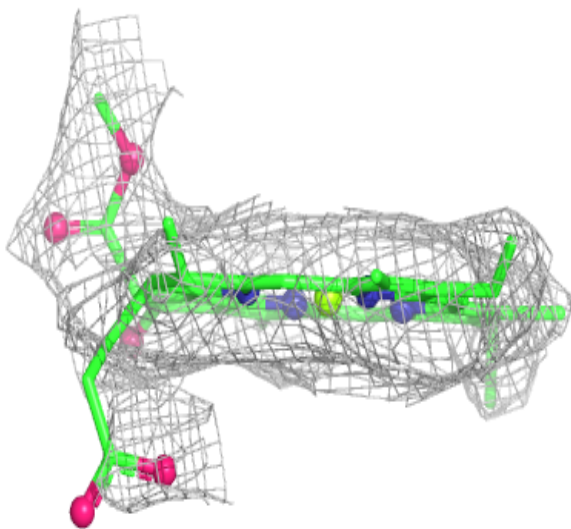
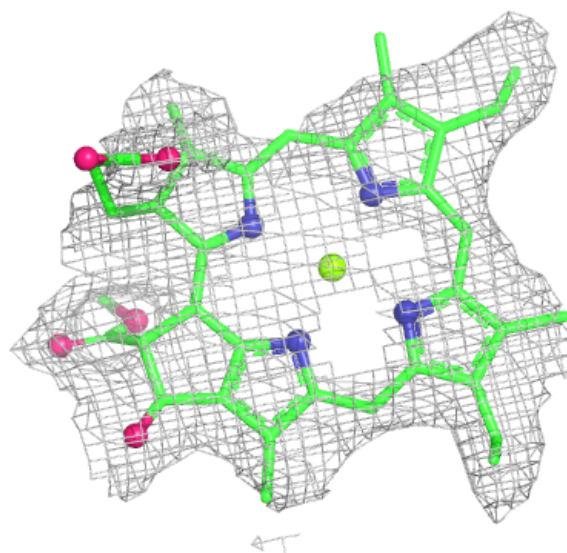
Electron density around CL0 A 801:

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



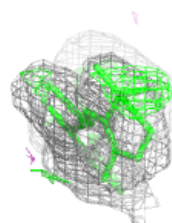
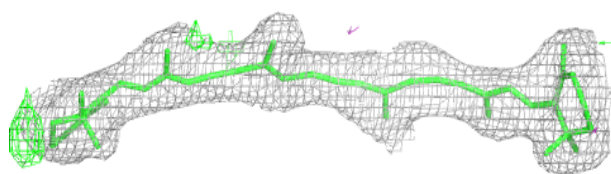
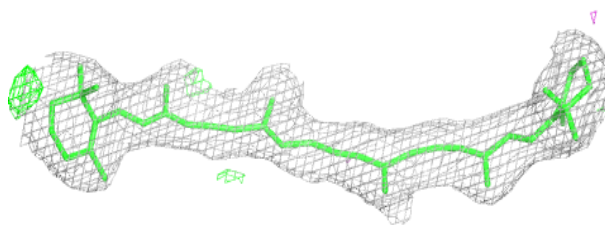
Electron density around CLA H 820:

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

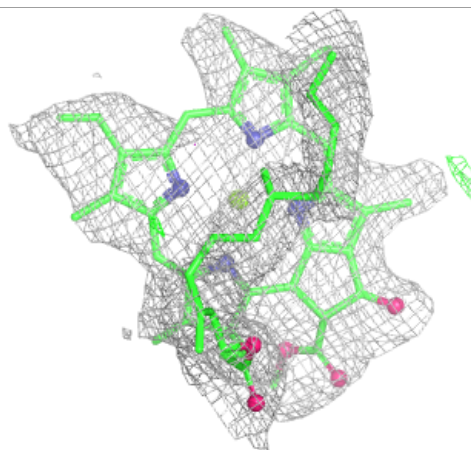
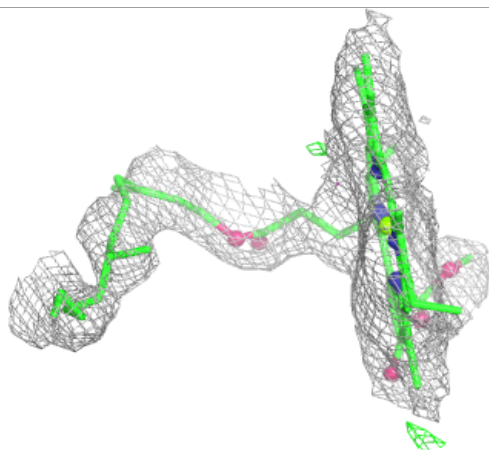
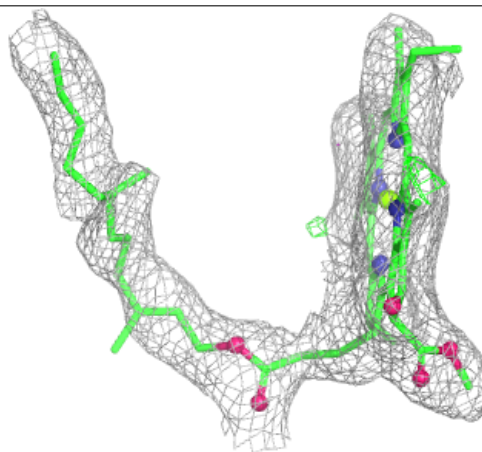


Electron density around BCR I 101:

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

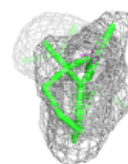
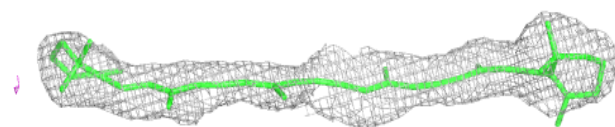
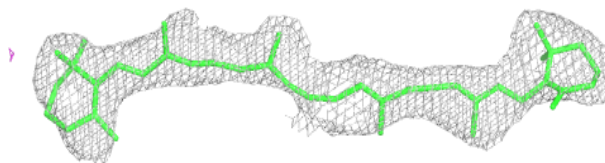
**Electron density around CLA A 805:**

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

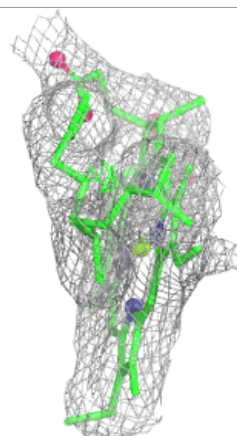
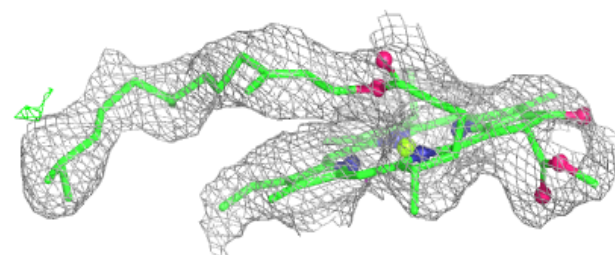
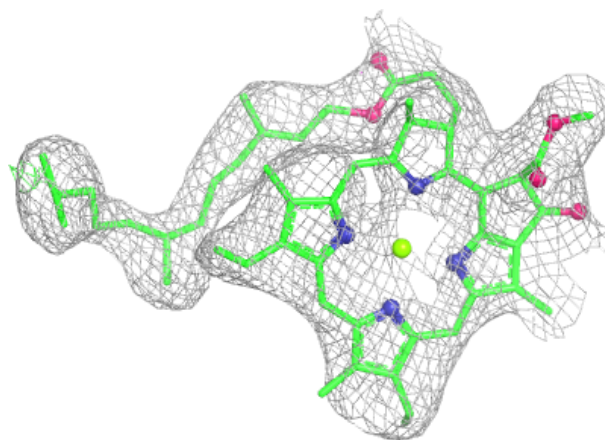


Electron density around BCR J 103:

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

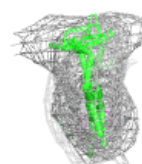
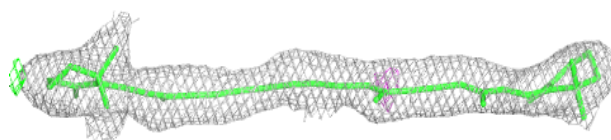
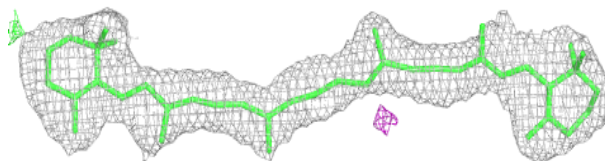
**Electron density around CLA B 817:**

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

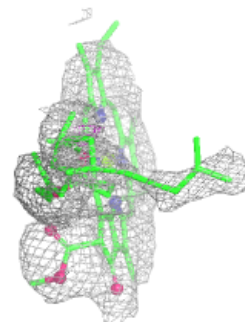
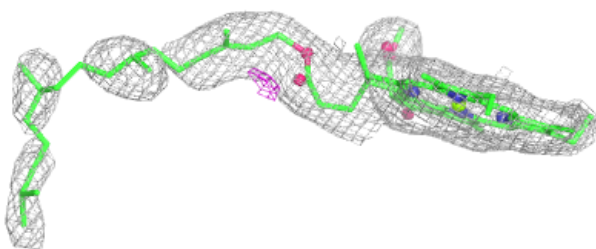
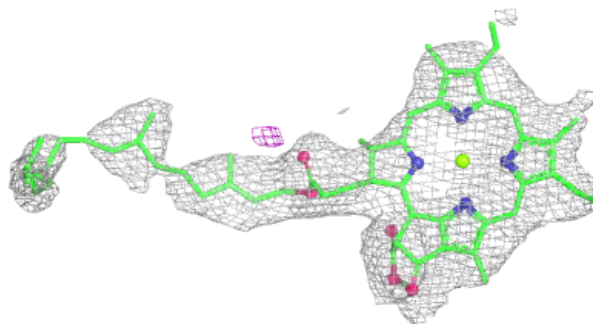


Electron density around BCR L 207:

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

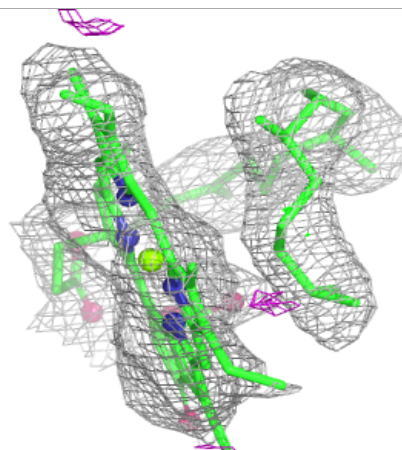
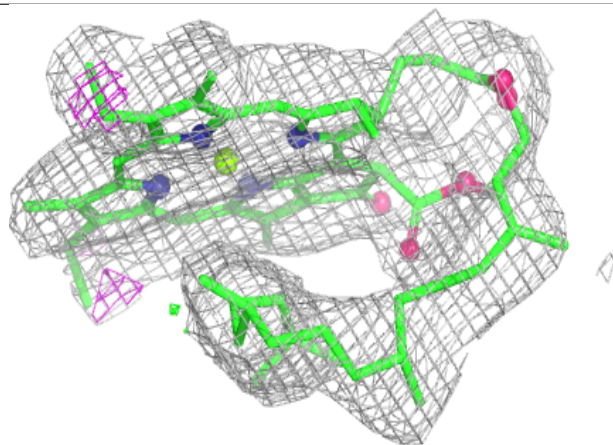
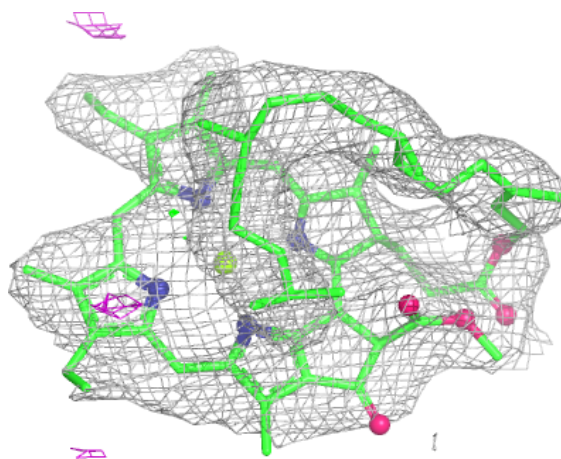
**Electron density around CLA A 806:**

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



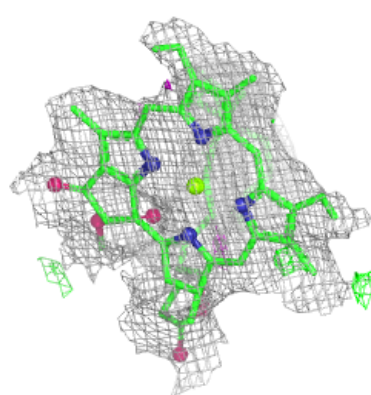
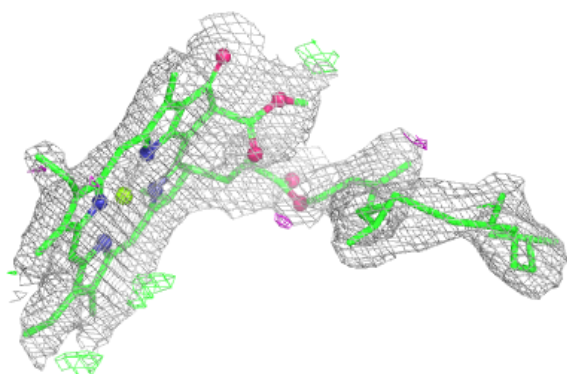
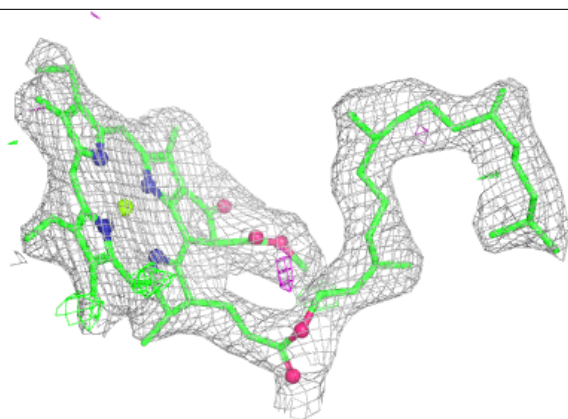
Electron density around CLA A 807:

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

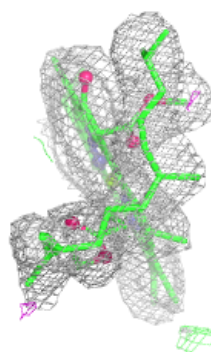
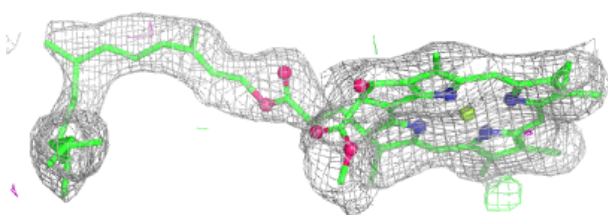
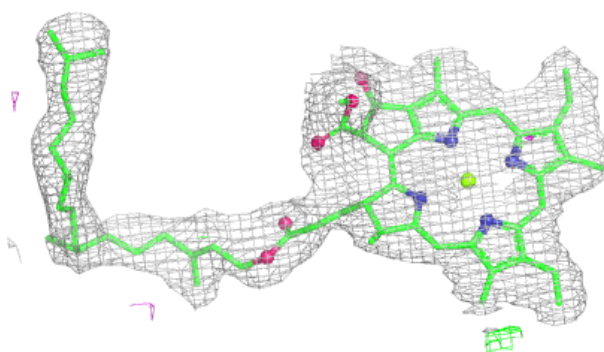


Electron density around CL0 G 801:

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

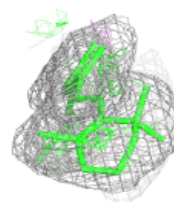
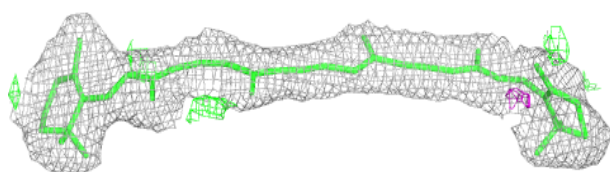
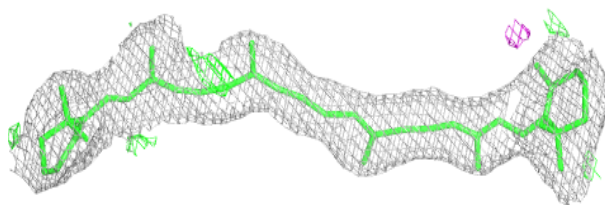
**Electron density around CLA H 826:**

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

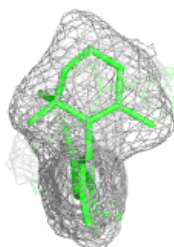
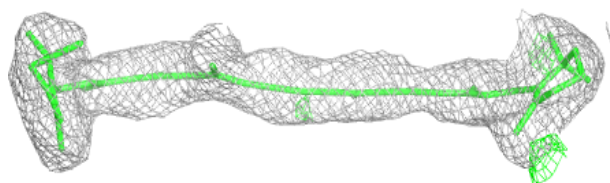
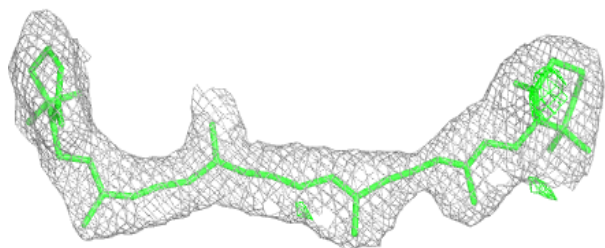


Electron density around BCR R 101:

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

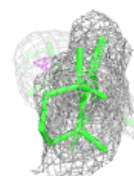
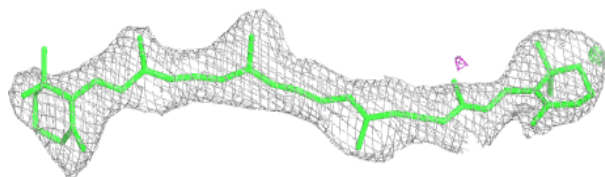
**Electron density around BCR R 102:**

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



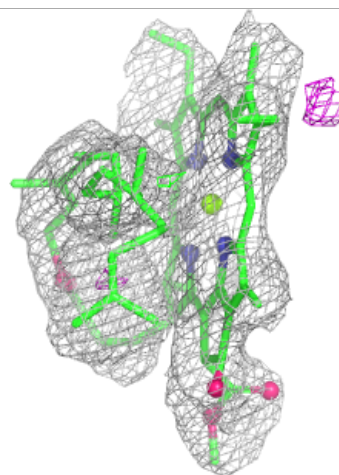
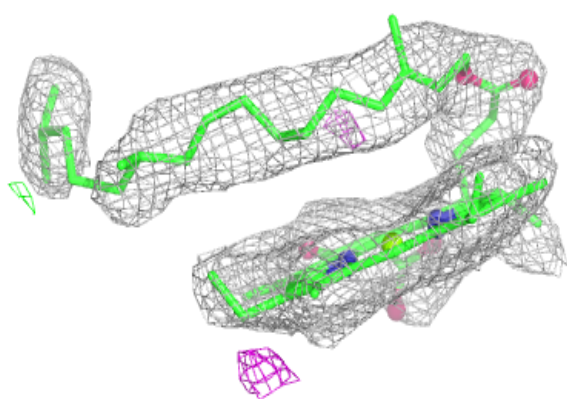
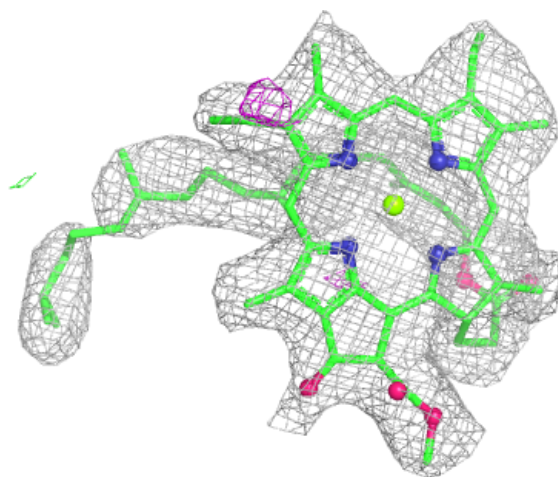
Electron density around BCR S 1104:

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



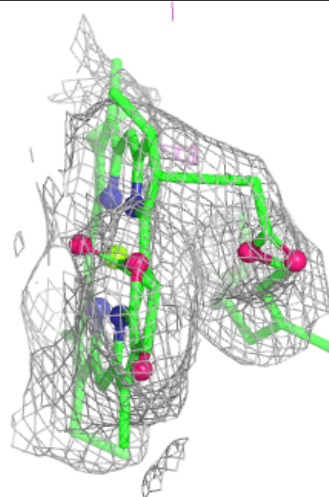
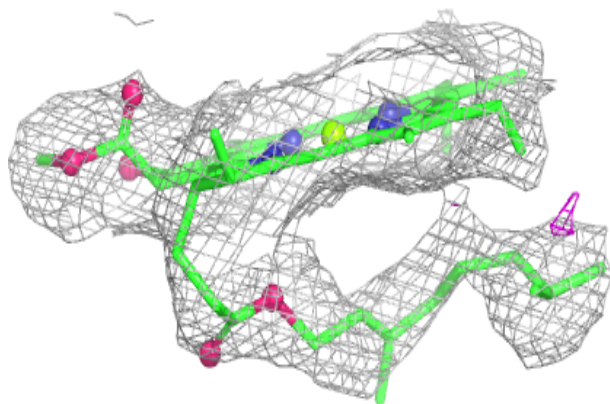
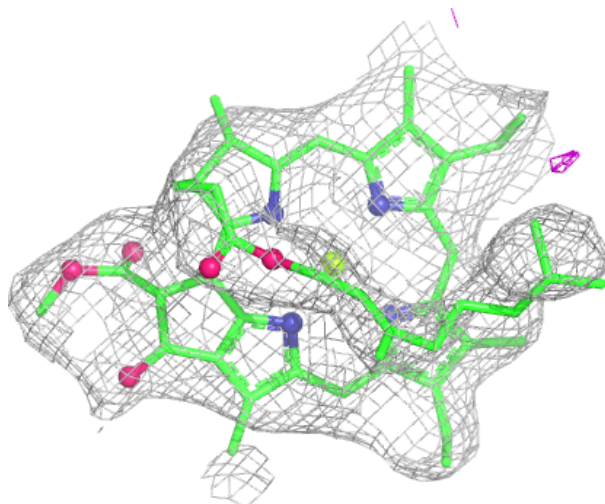
Electron density around CLA H 827:

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



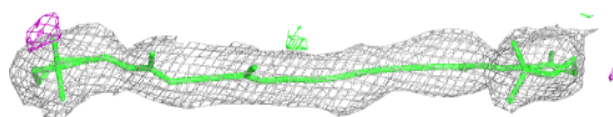
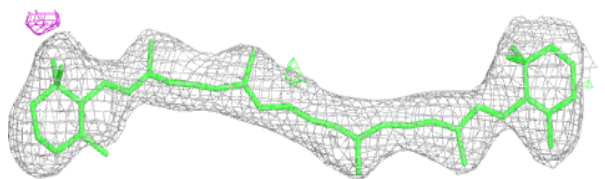
Electron density around CLA B 821:

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

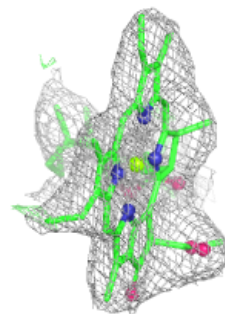
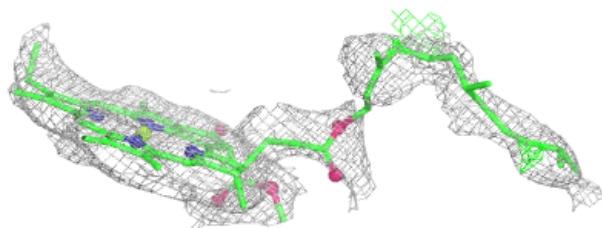
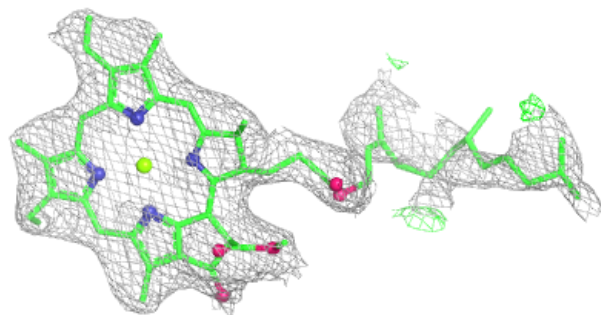


Electron density around BCR U 1005:

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

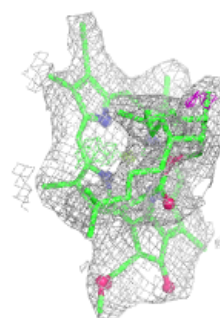
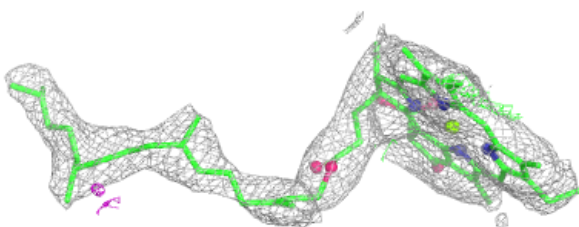
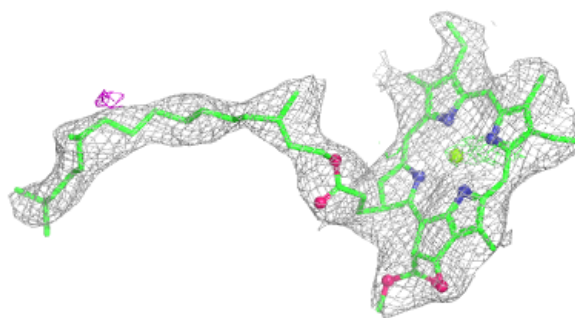
**Electron density around CLA B 822:**

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

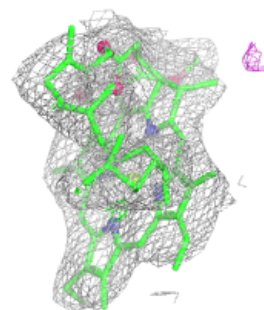
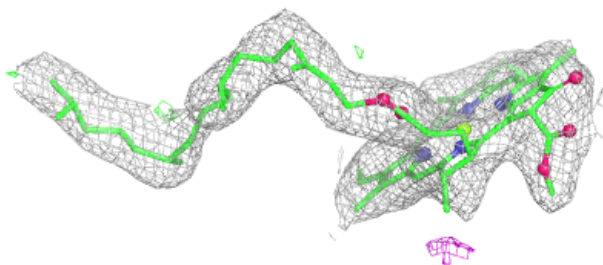
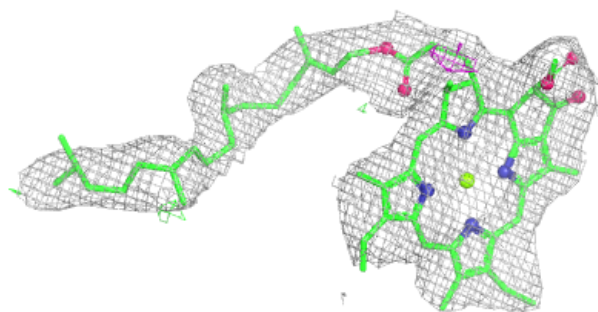


Electron density around CLA A 822:

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

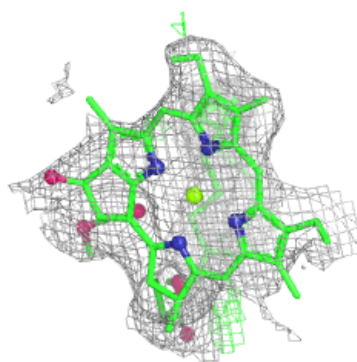
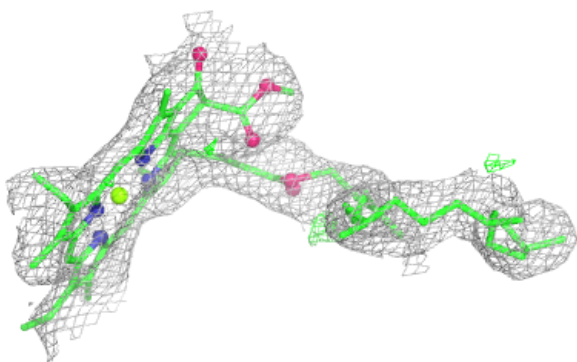
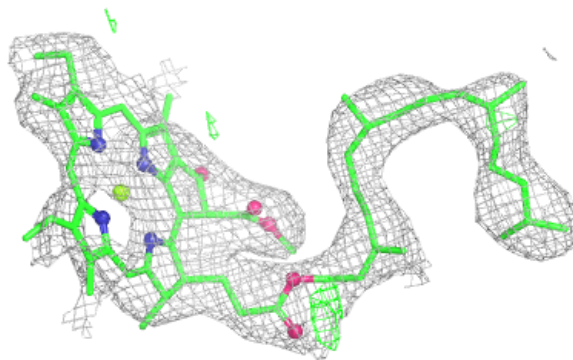
**Electron density around CLA A 809:**

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



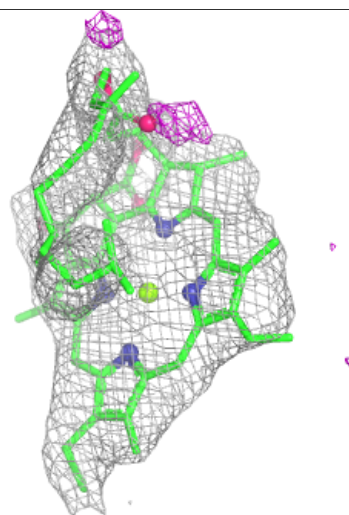
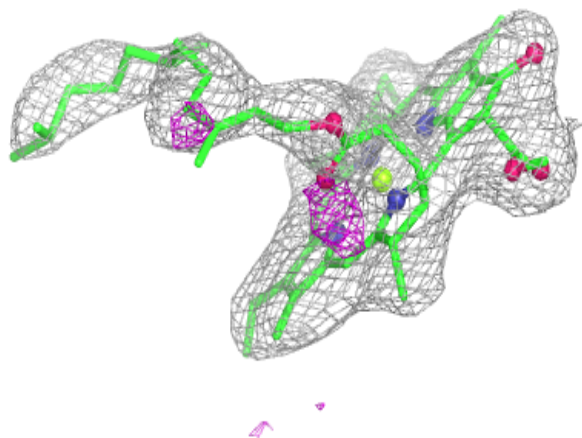
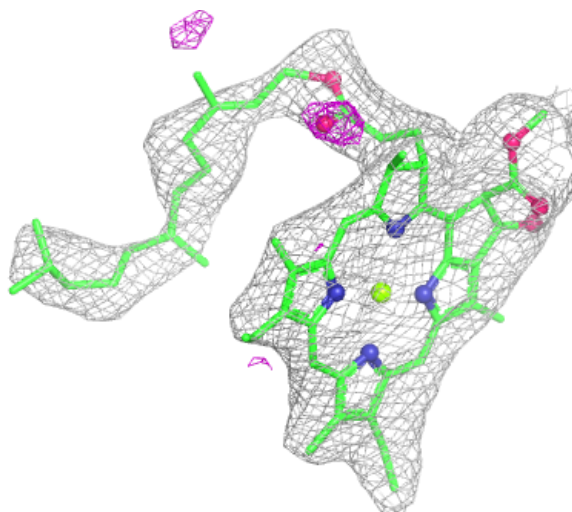
Electron density around CL0 Y 801:

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



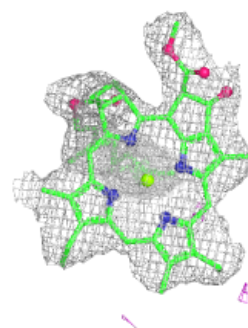
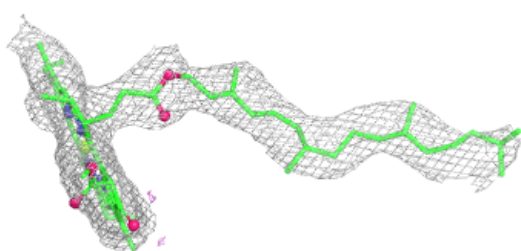
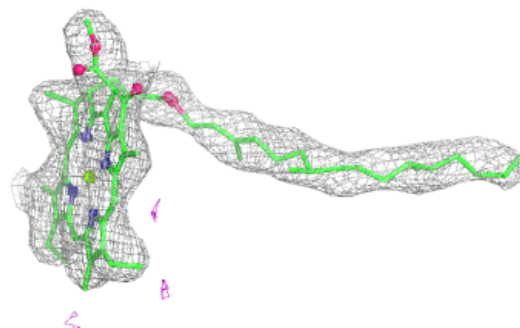
Electron density around CLA A 825:

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

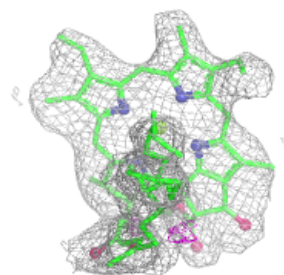
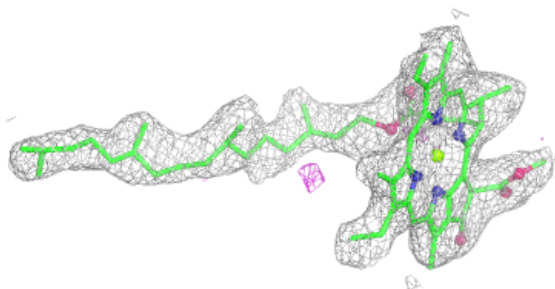
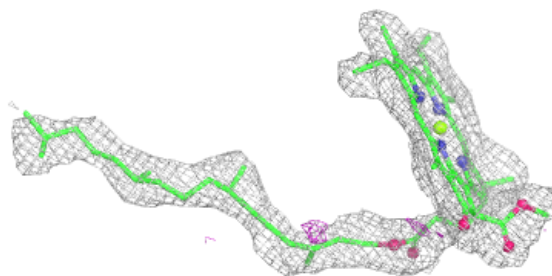


Electron density around CLA B 827:

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

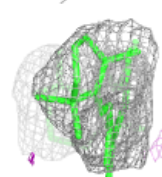
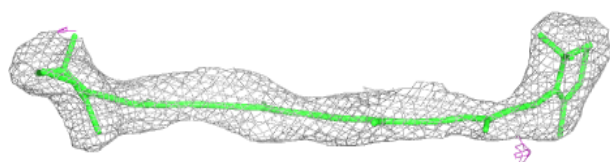
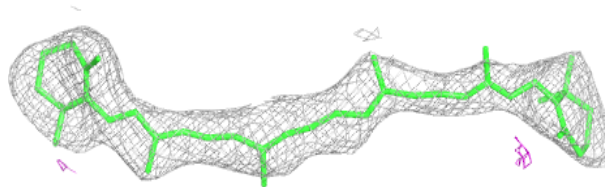
**Electron density around CLA B 828:**

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



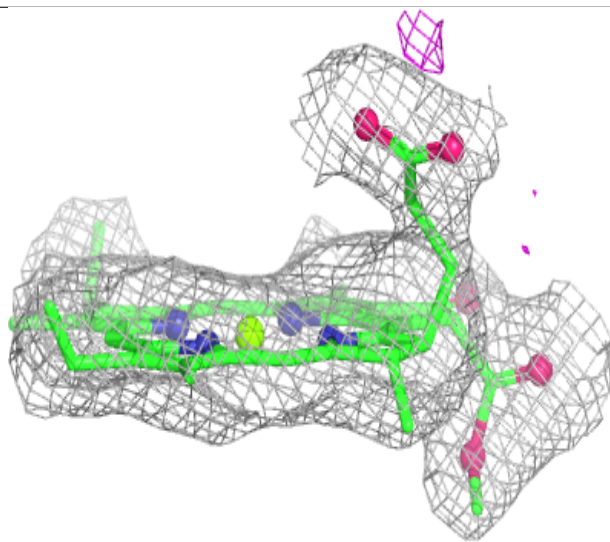
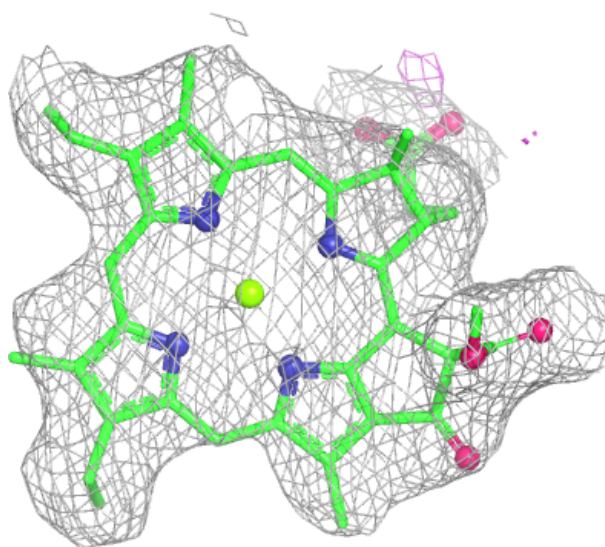
Electron density around BCR Y 848:

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



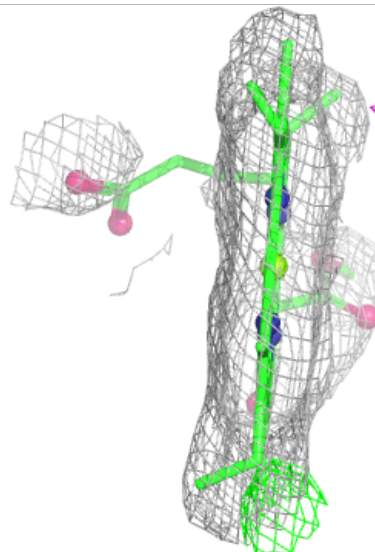
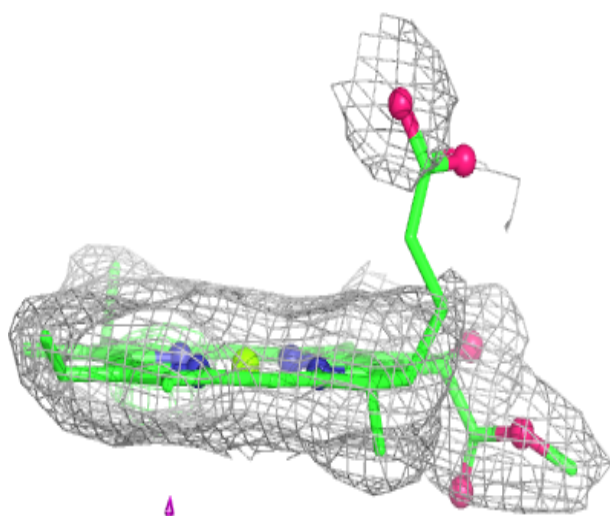
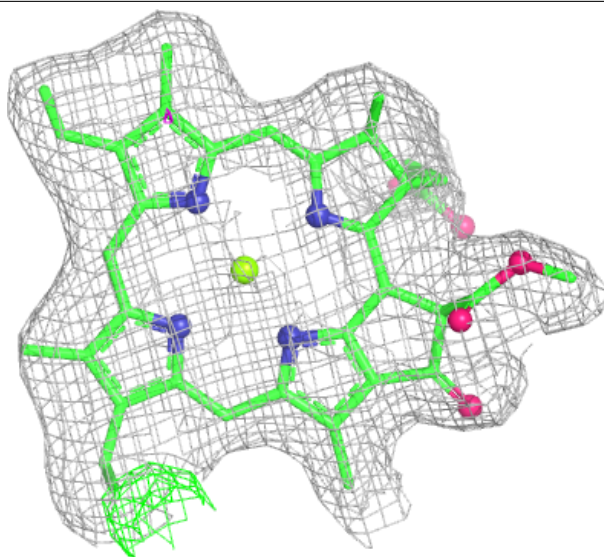
Electron density around CLA B 829:

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



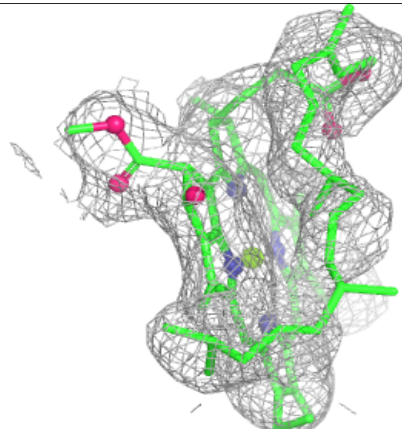
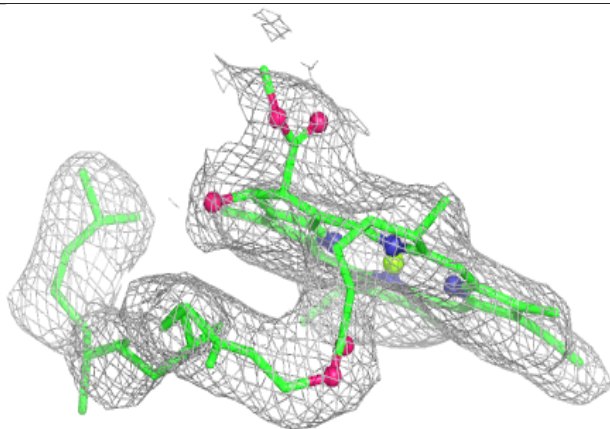
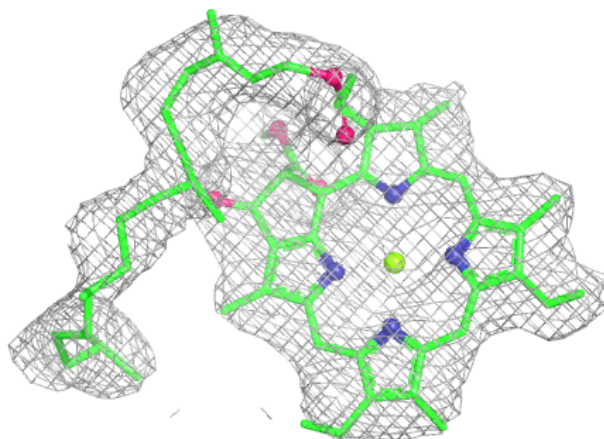
Electron density around CLA B 830:

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



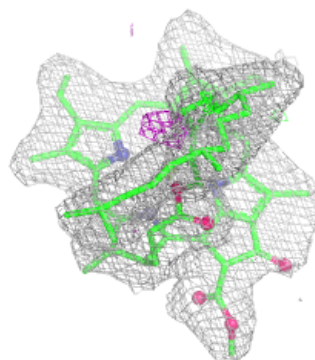
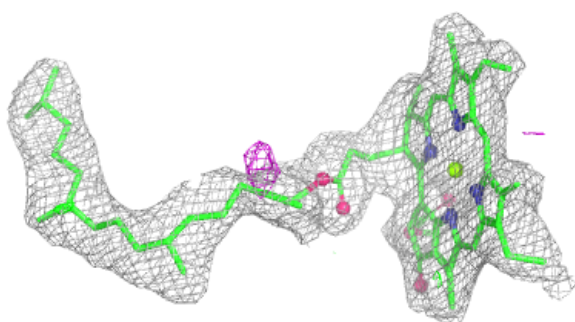
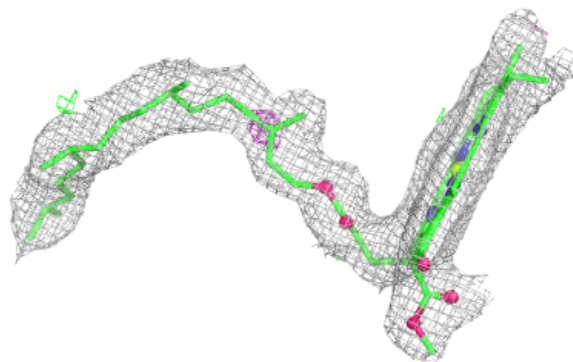
Electron density around CLA B 831:

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

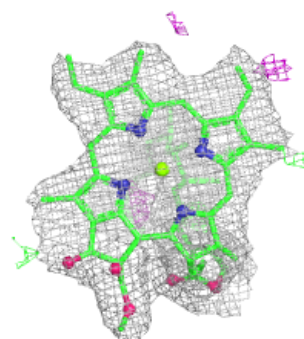
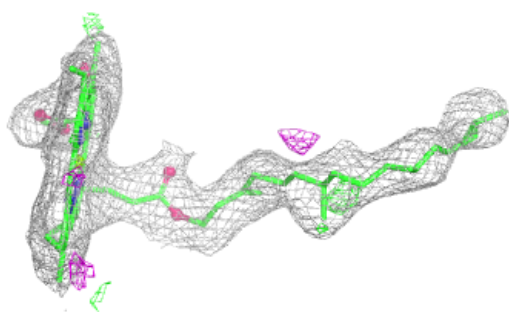
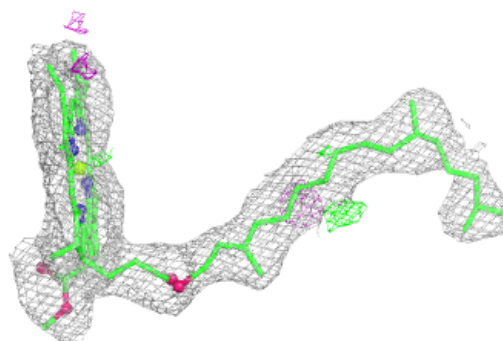


Electron density around CLA H 839:

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

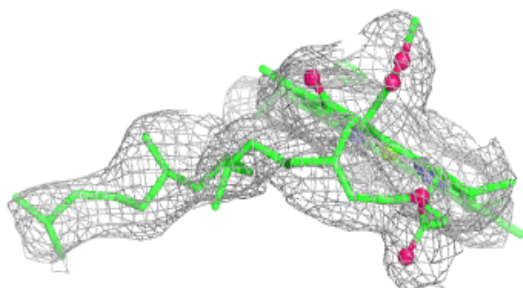
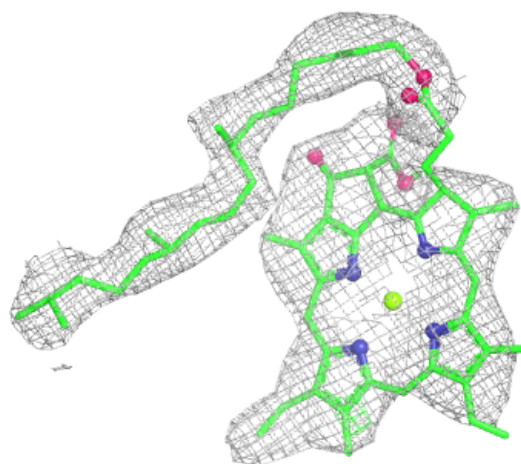
**Electron density around CLA H 840:**

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



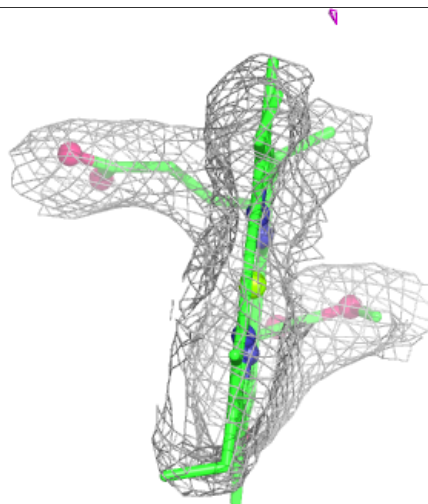
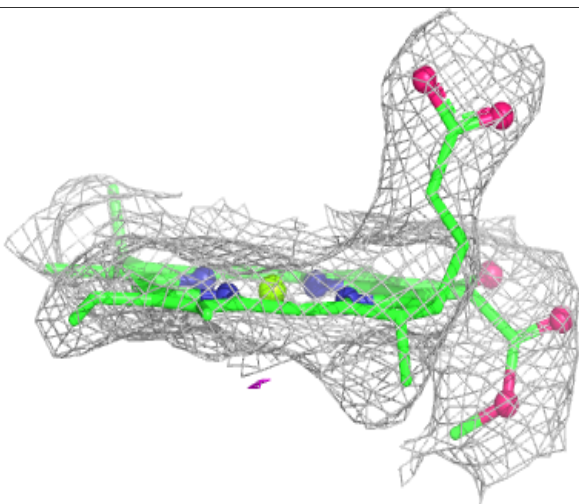
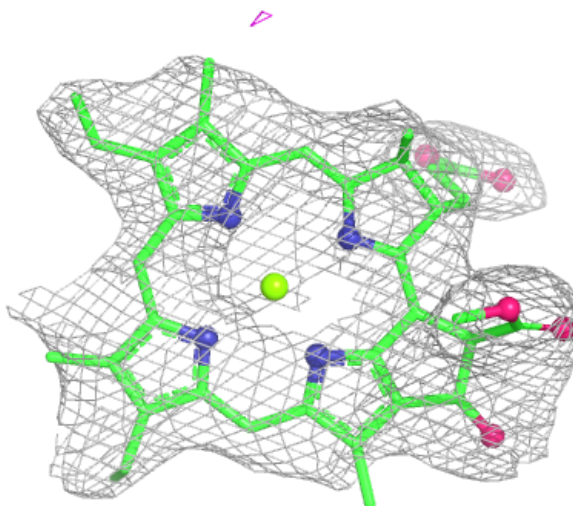
Electron density around CLA A 826:

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



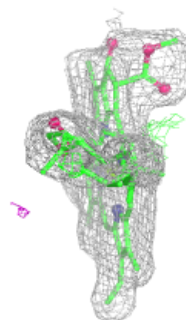
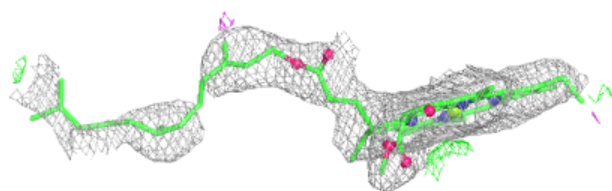
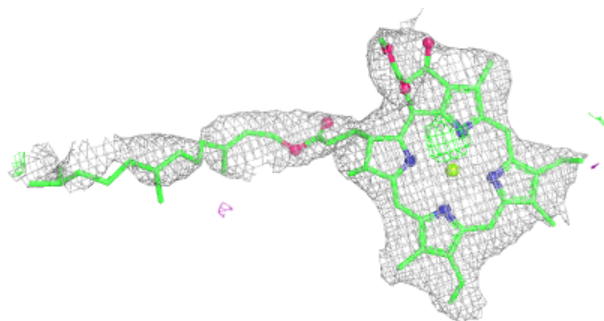
Electron density around CLA B 833:

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

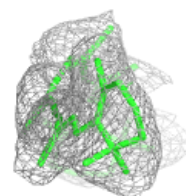
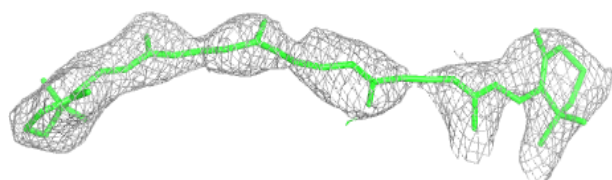
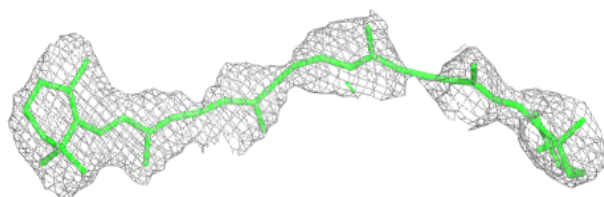


Electron density around CLA A 827:

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

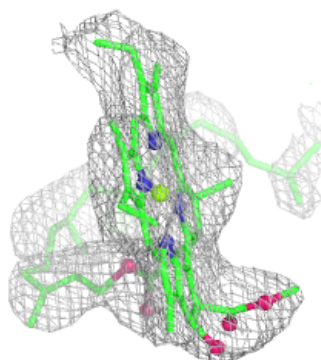
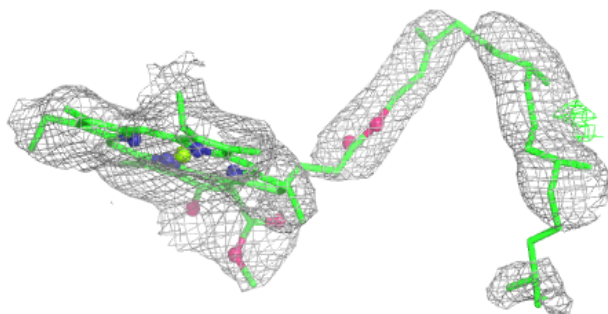
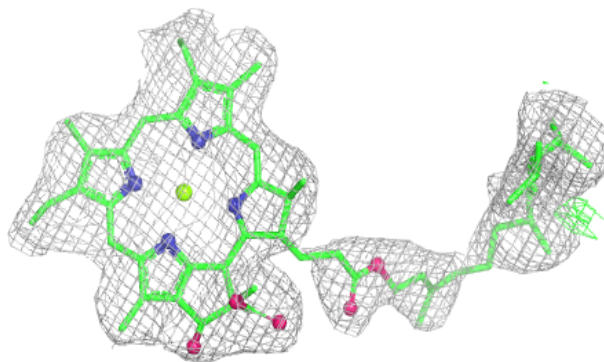
**Electron density around BCR Z 848:**

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

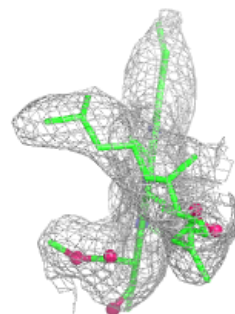
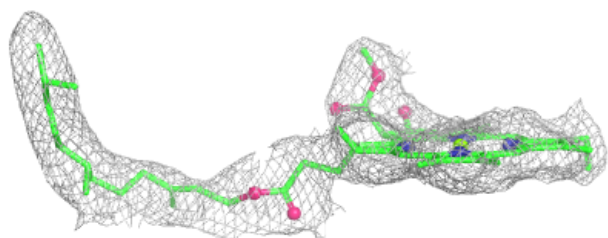
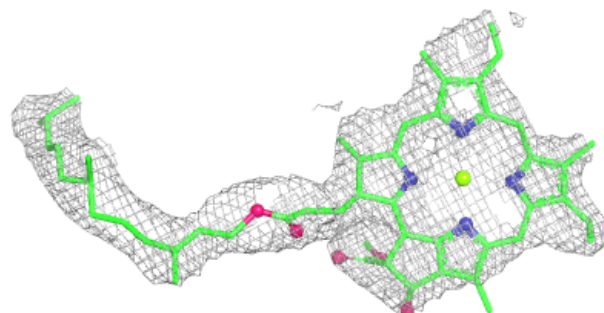


Electron density around CLA A 828:

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

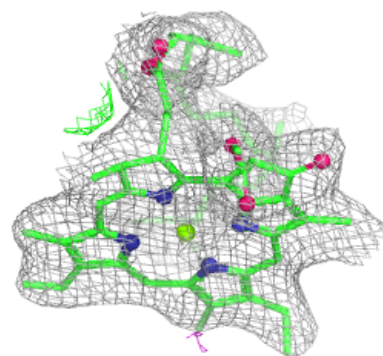
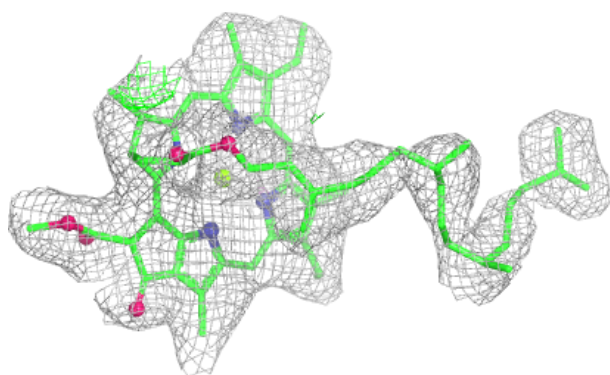
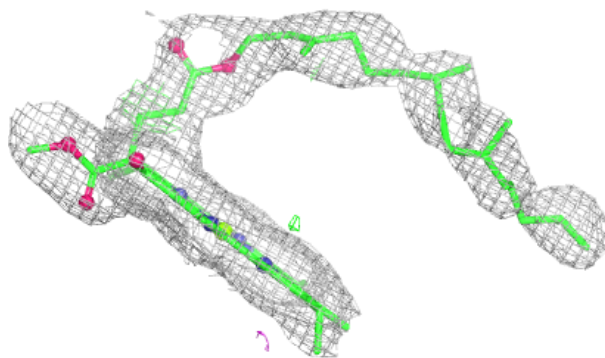
**Electron density around CLA B 836:**

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

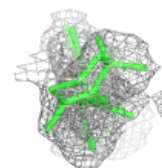
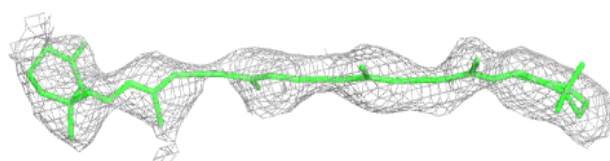
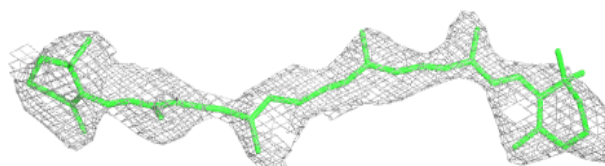


Electron density around CLA L 201:

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

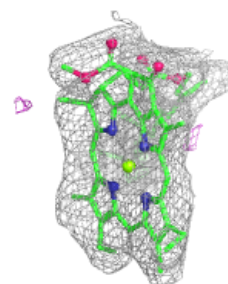
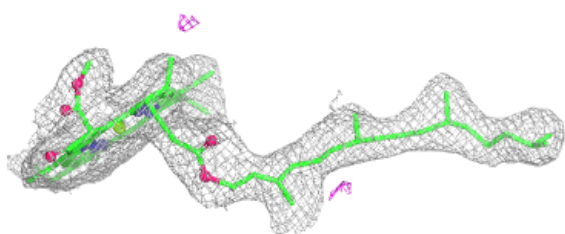
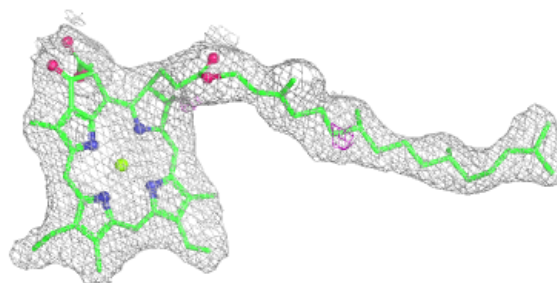
**Electron density around BCR f 103:**

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

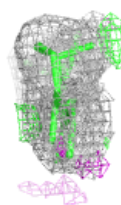
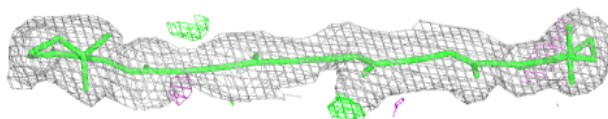
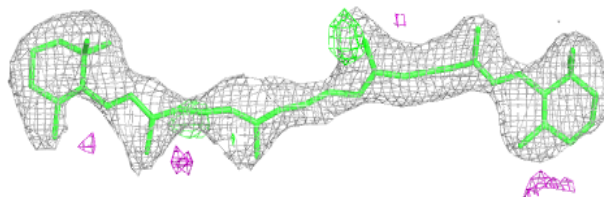


Electron density around CLA L 202:

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

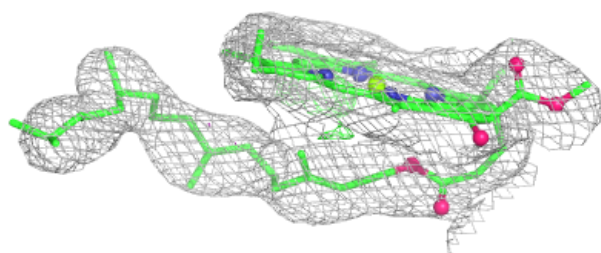
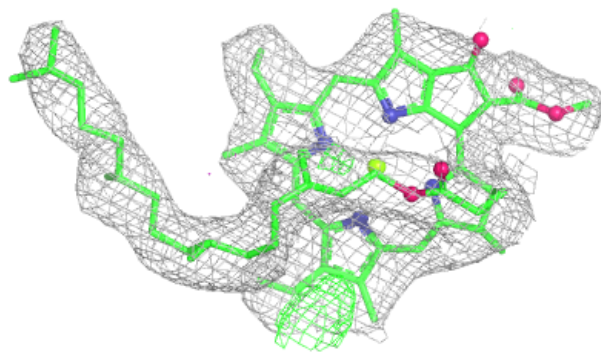
**Electron density around BCR h 207:**

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

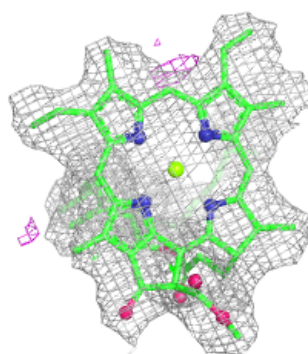
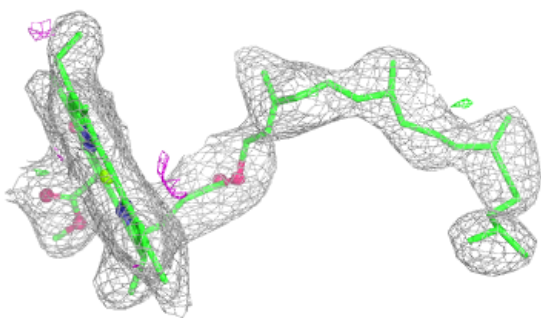
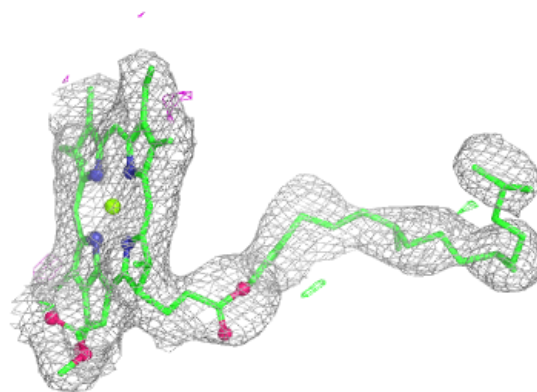


Electron density around CLA B 837:

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

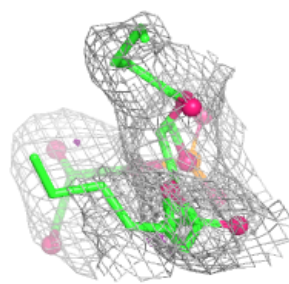
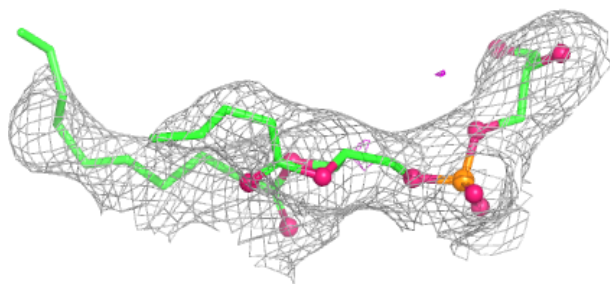
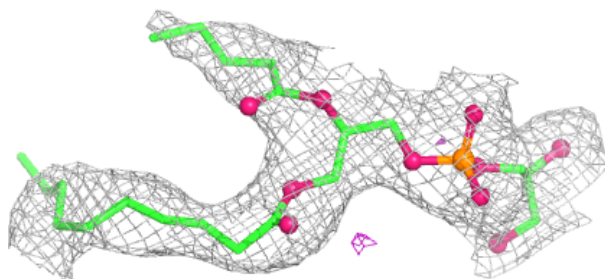
**Electron density around CLA L 205:**

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

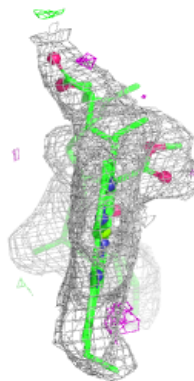
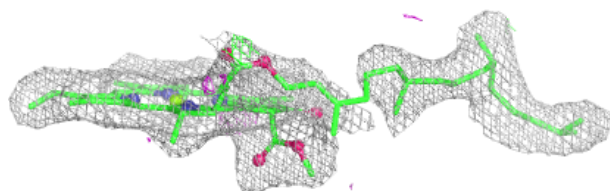
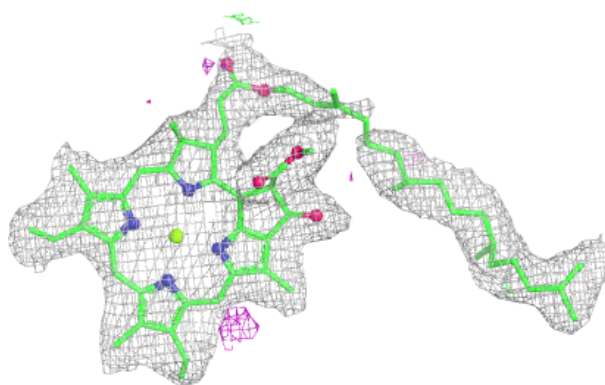


Electron density around LHG A 853:

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

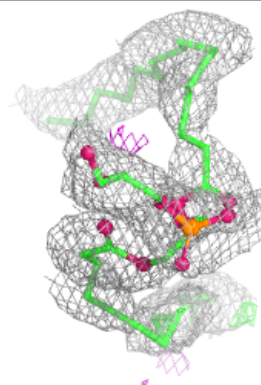
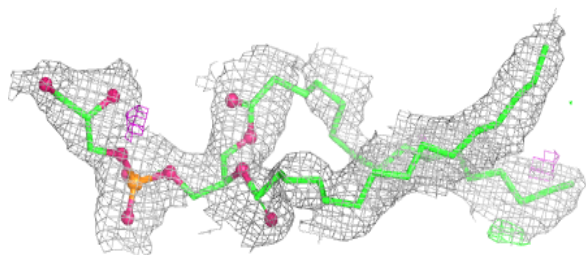
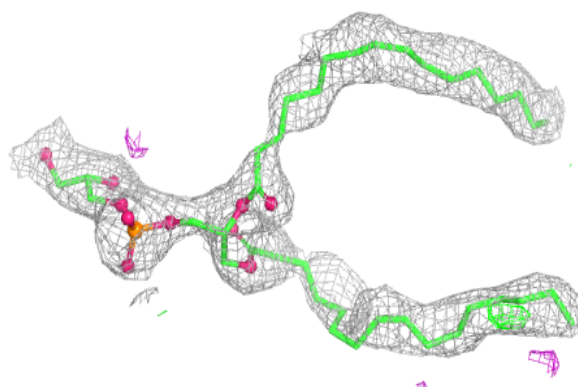
**Electron density around CLA L 206:**

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

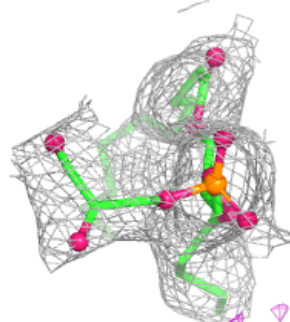
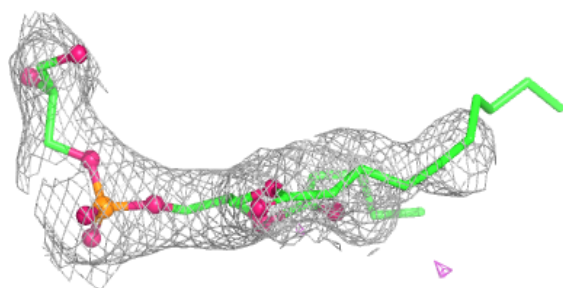


Electron density around LHG G 850:

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

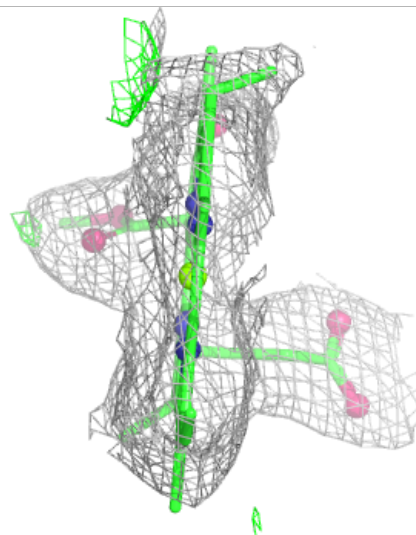
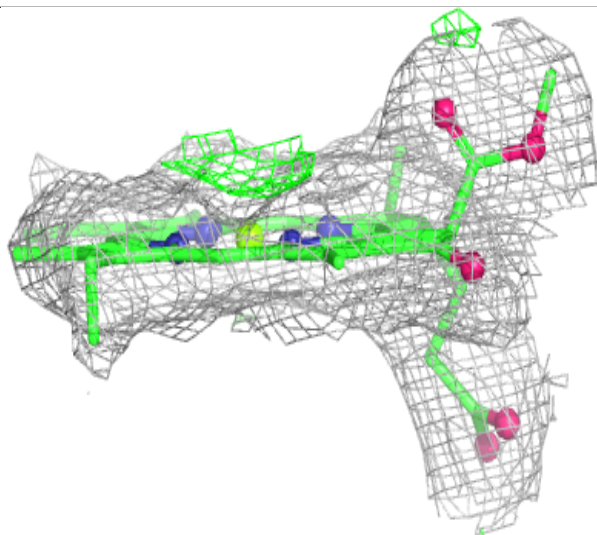
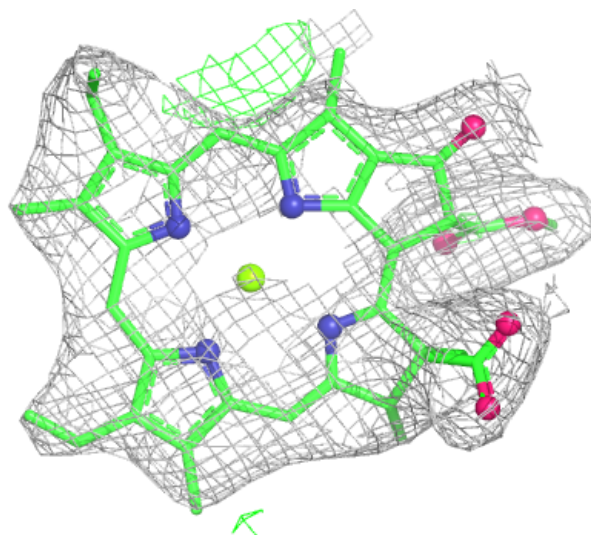
**Electron density around LHG G 851:**

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



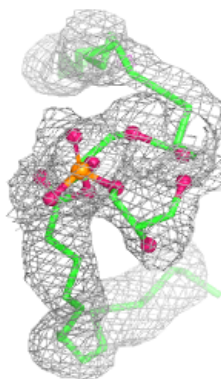
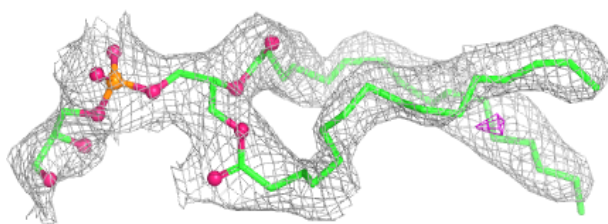
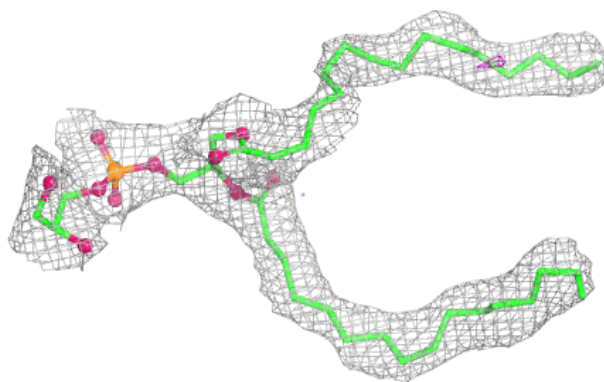
Electron density around CLA B 838:

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

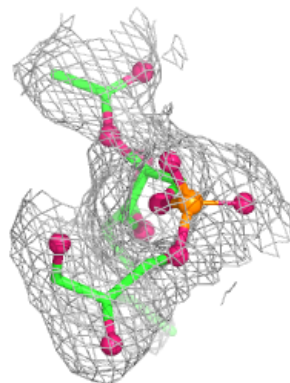
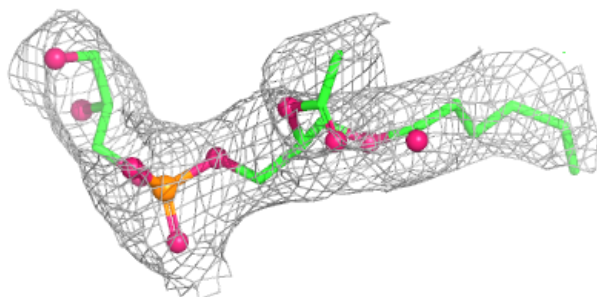
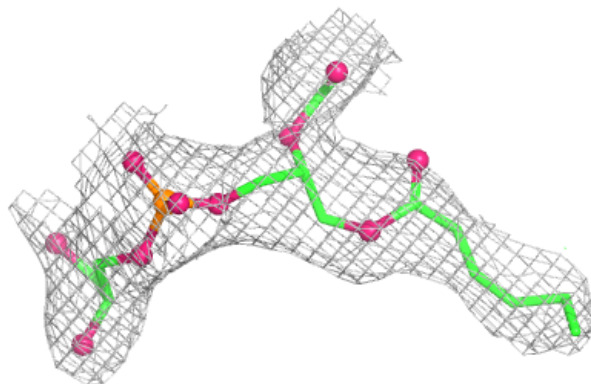


Electron density around LHG Y 850:

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

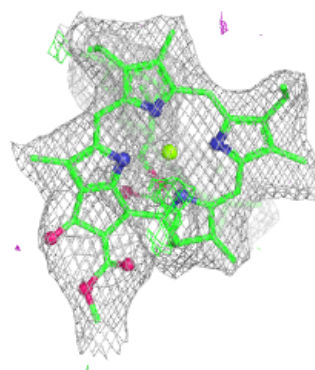
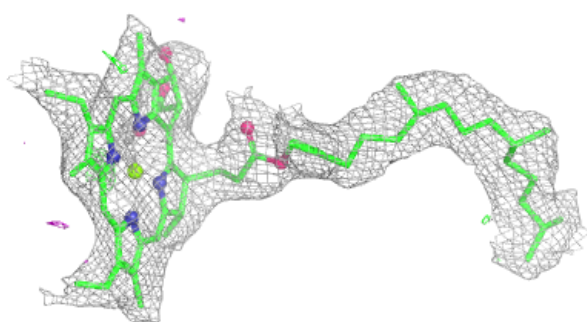
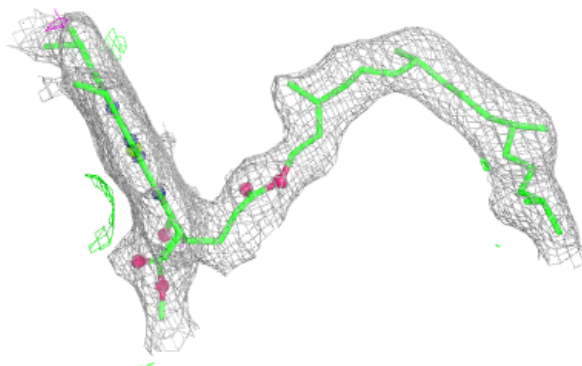
**Electron density around LHG Y 851:**

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

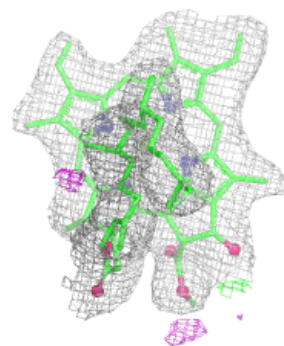
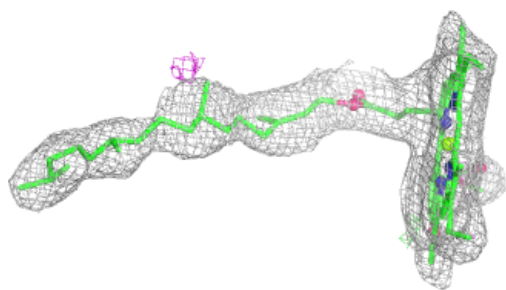
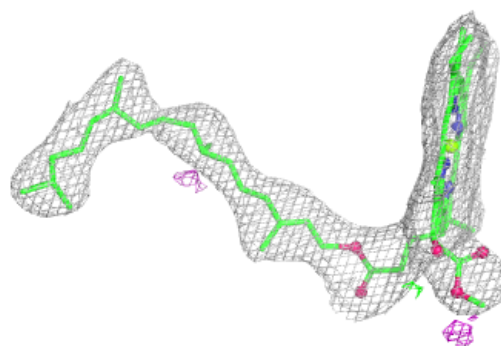


Electron density around CLA B 839:

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

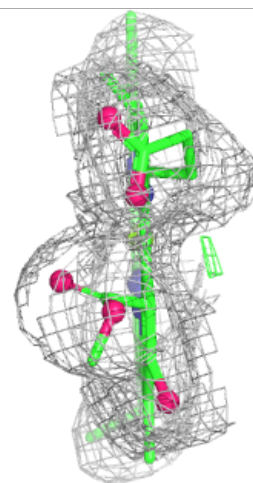
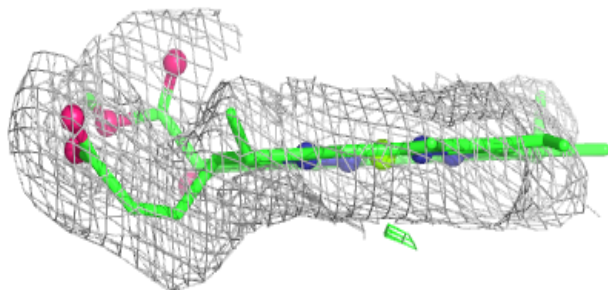
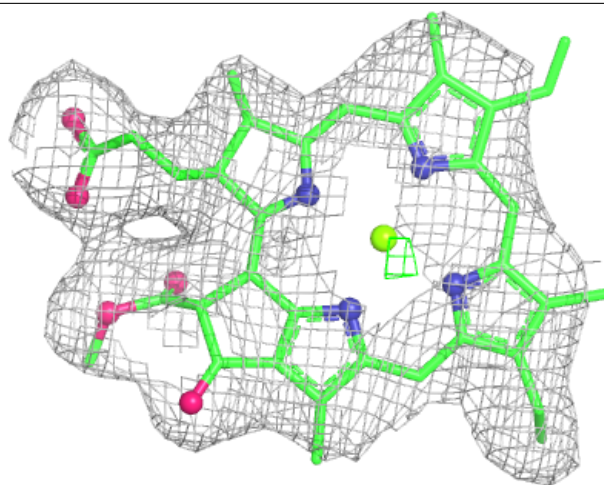
**Electron density around CLA B 840:**

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



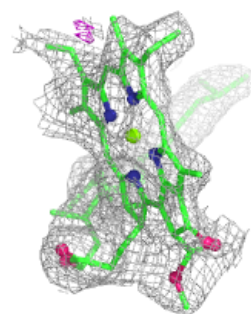
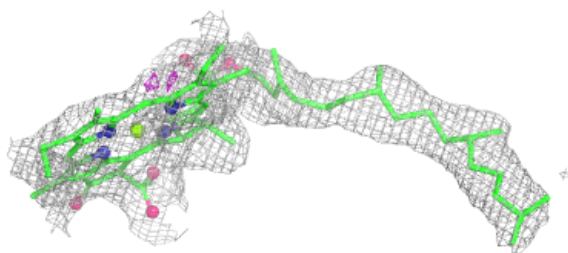
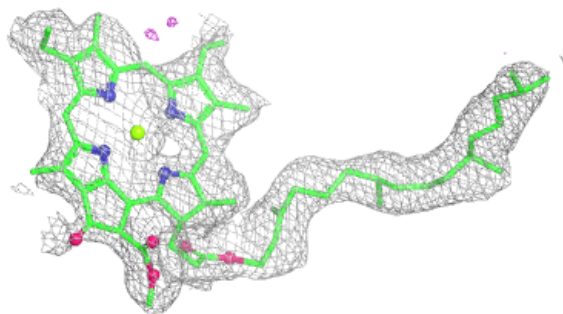
Electron density around CLA F 202:

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



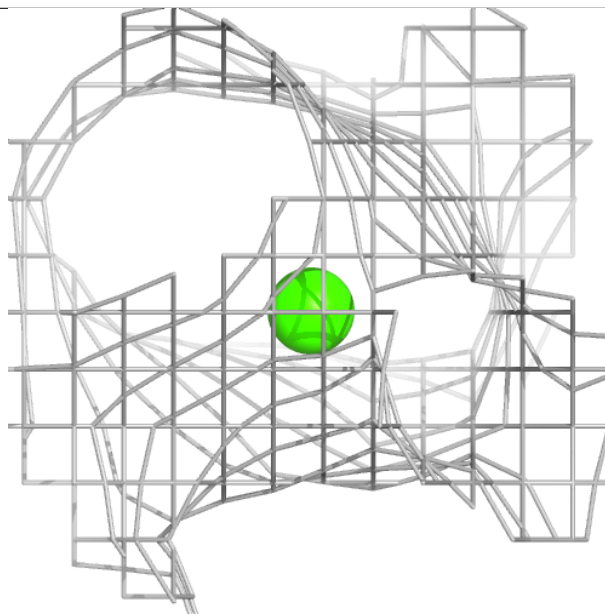
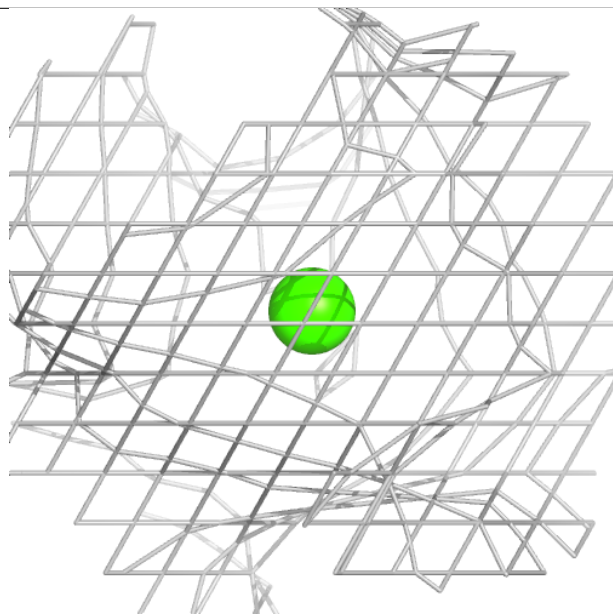
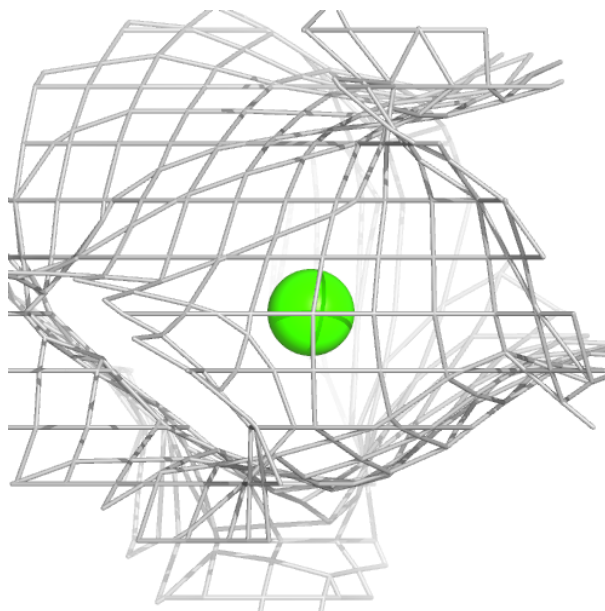
Electron density around CLA G 802:

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



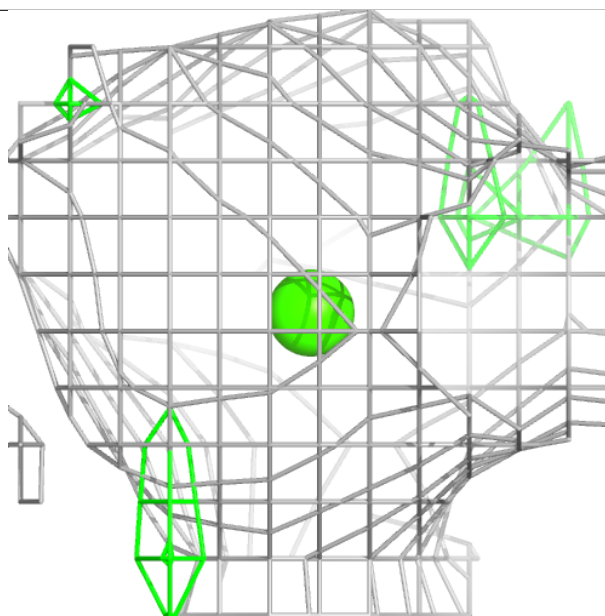
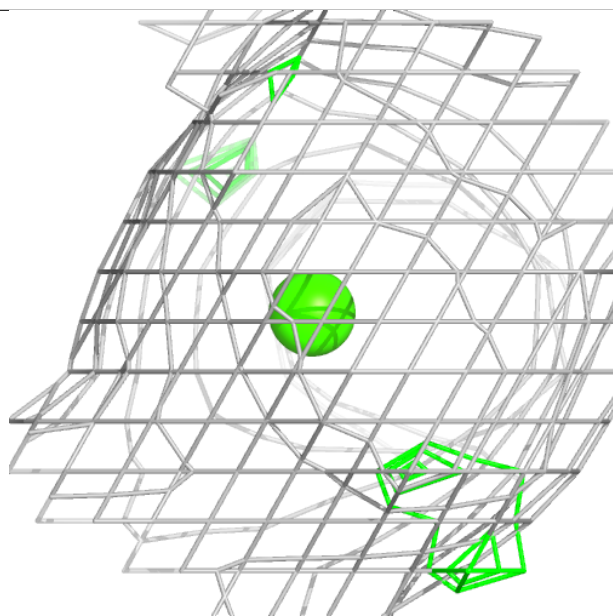
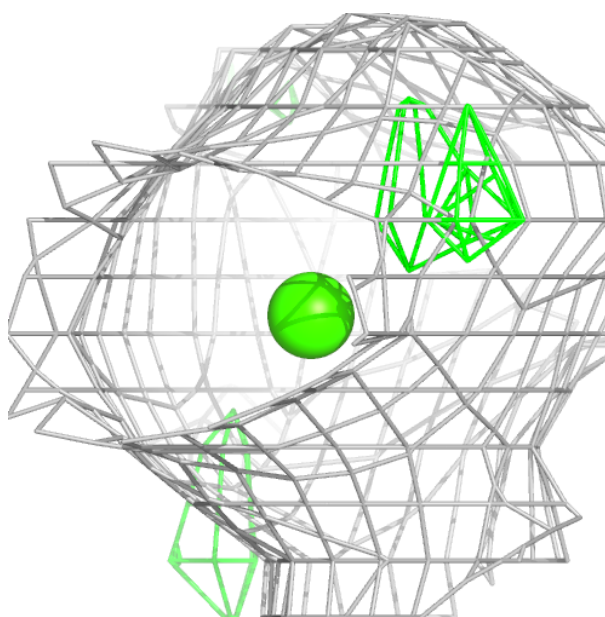
Electron density around CA L 203:

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



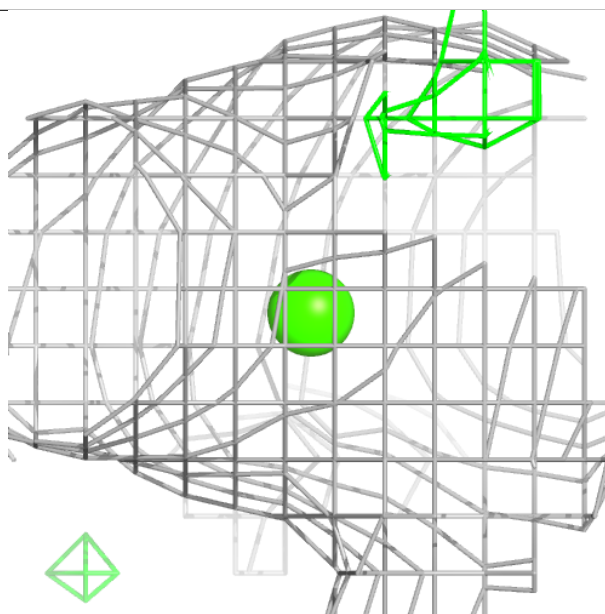
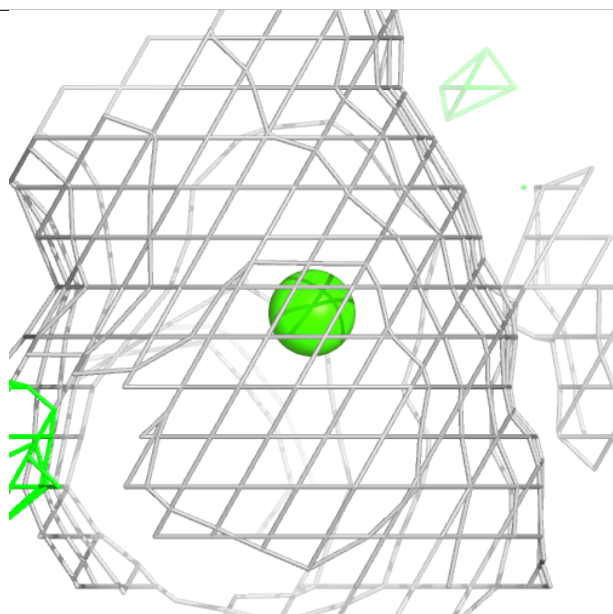
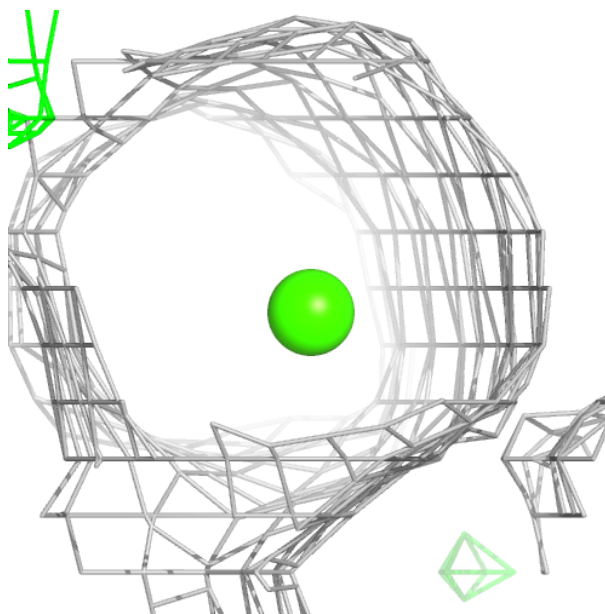
Electron density around CA U 1001:

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



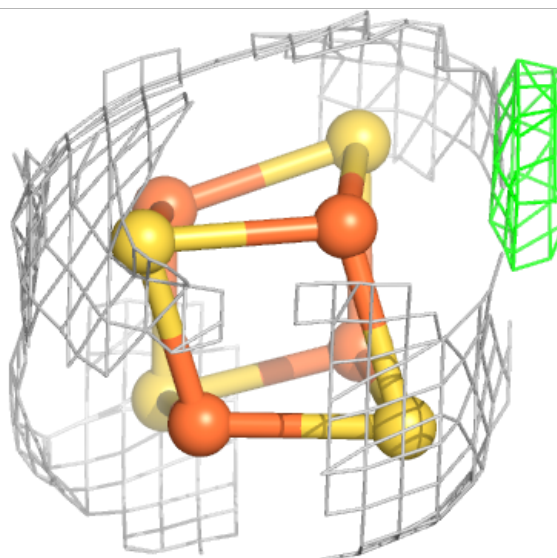
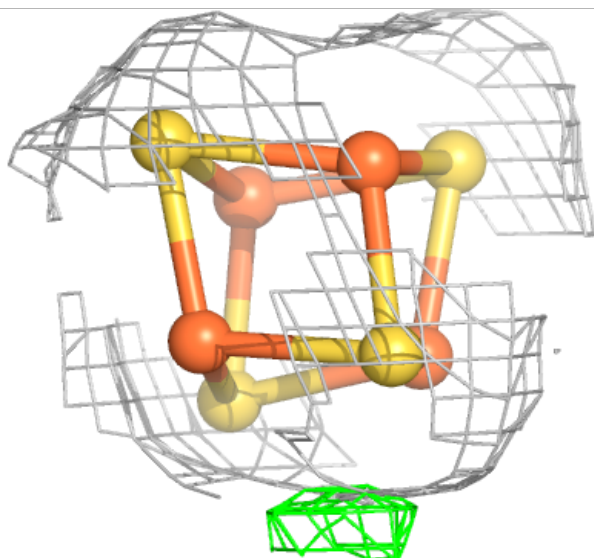
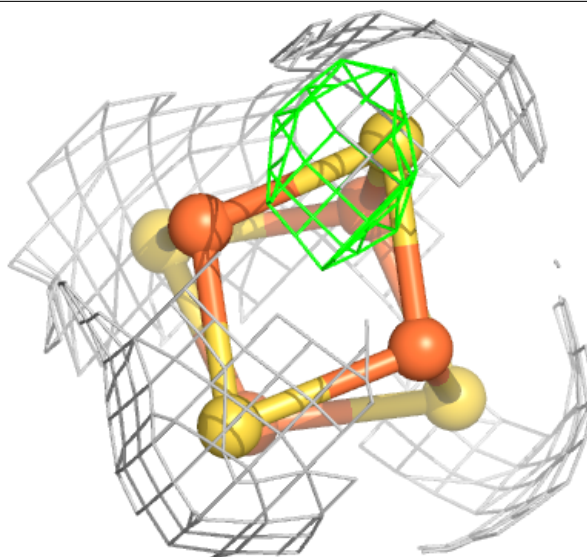
Electron density around CA h 203:

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



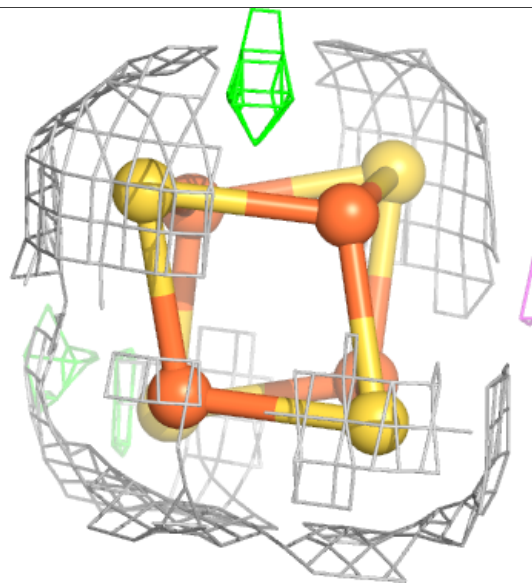
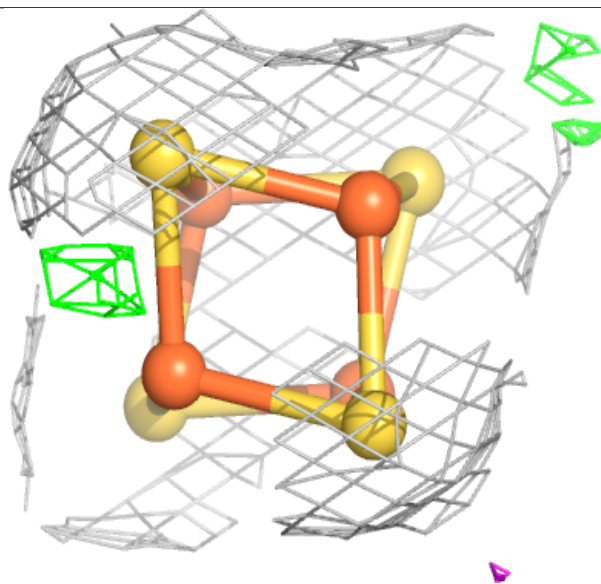
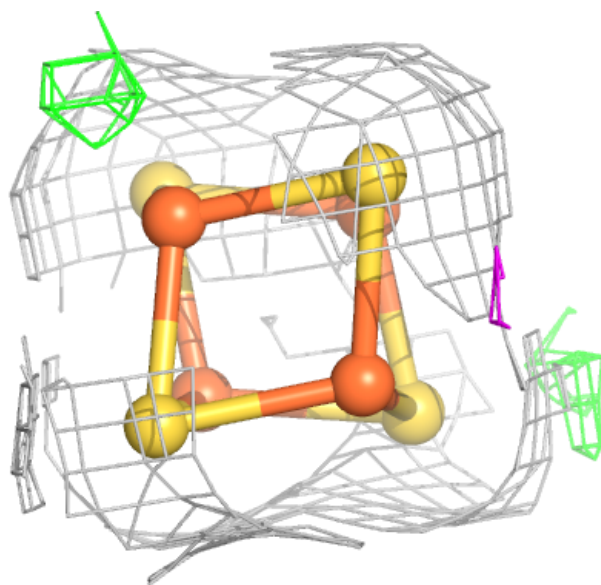
Electron density around SF4 C 102:

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



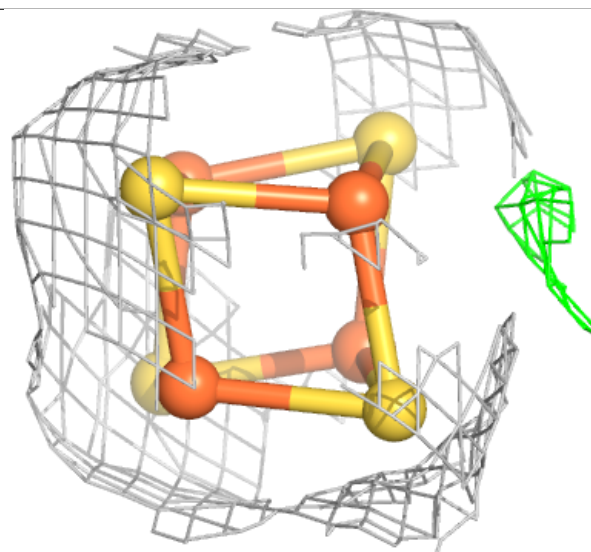
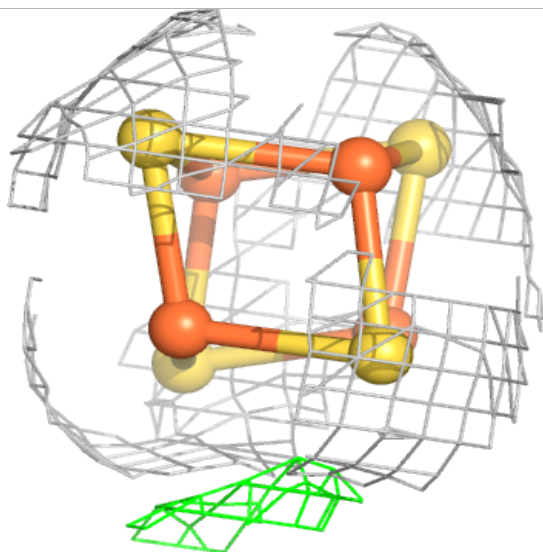
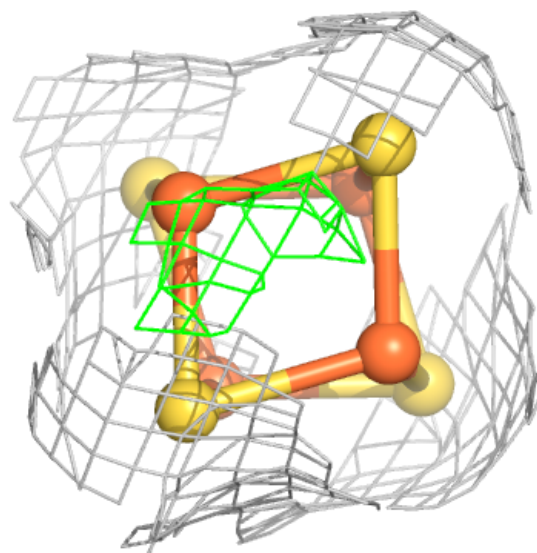
Electron density around SF4 A 845:

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



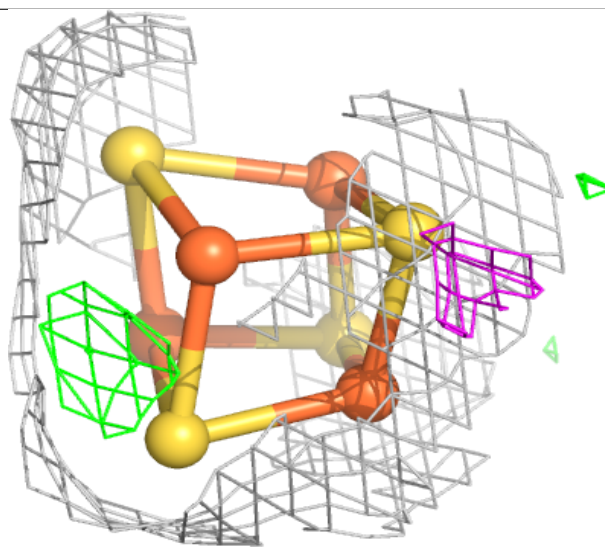
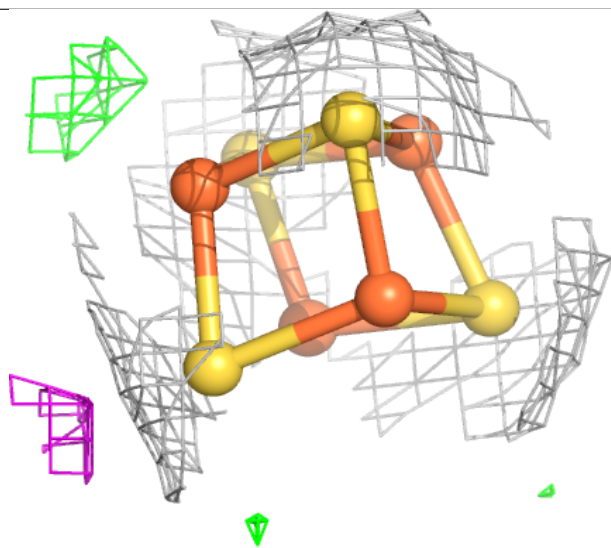
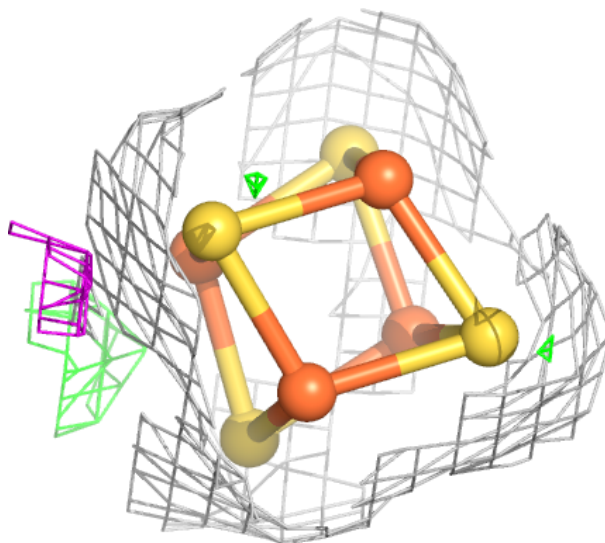
Electron density around SF4 N 101:

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



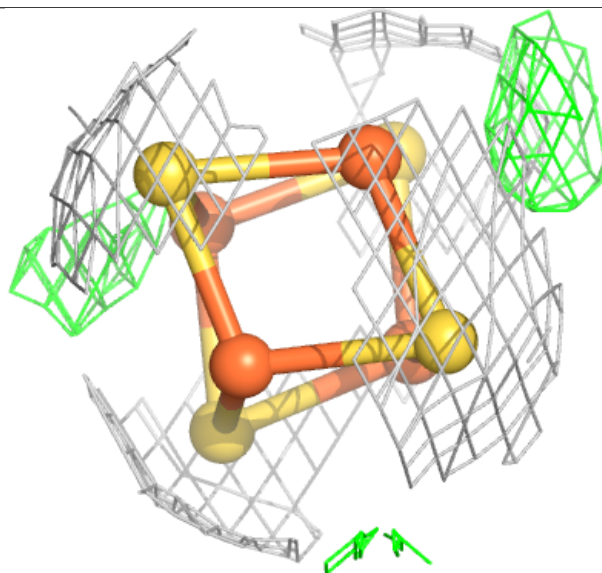
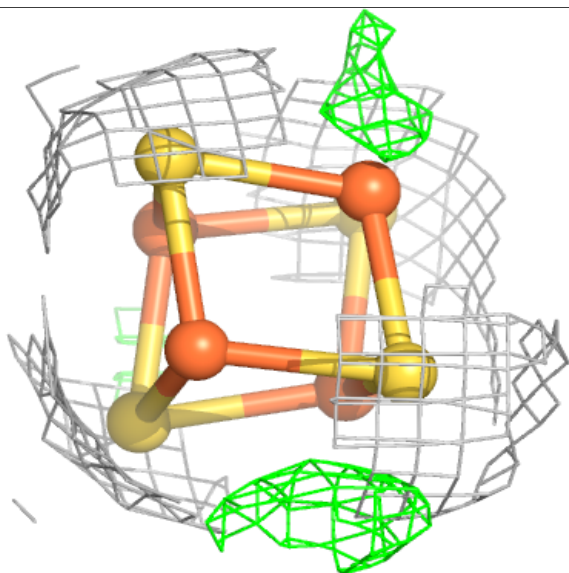
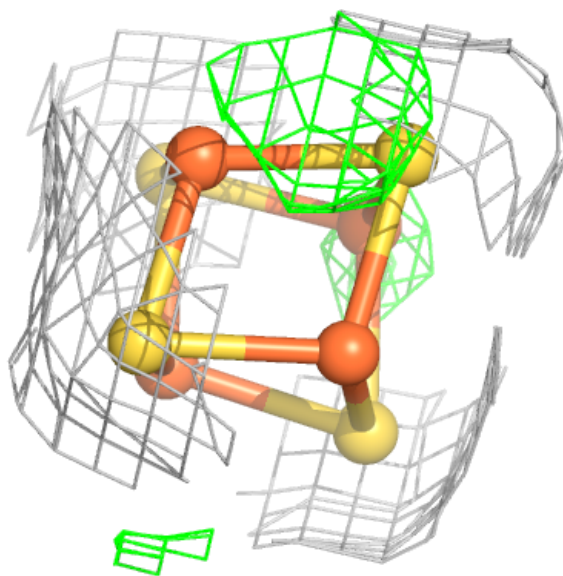
Electron density around SF4 N 102:

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



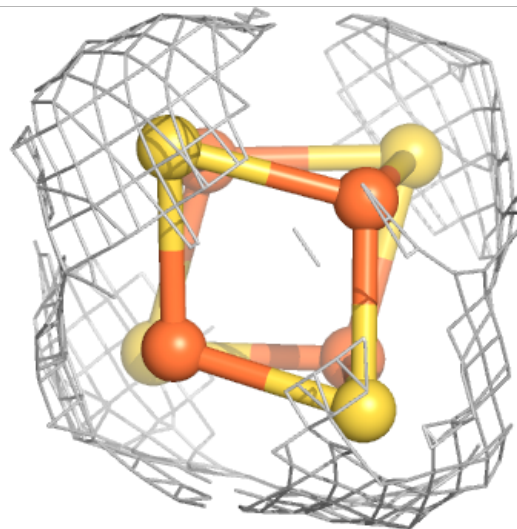
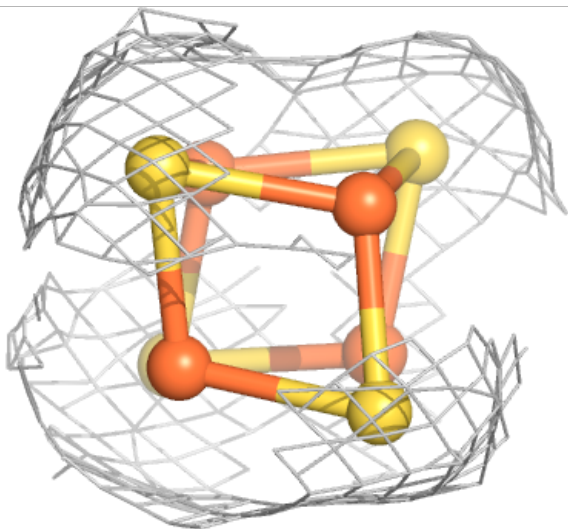
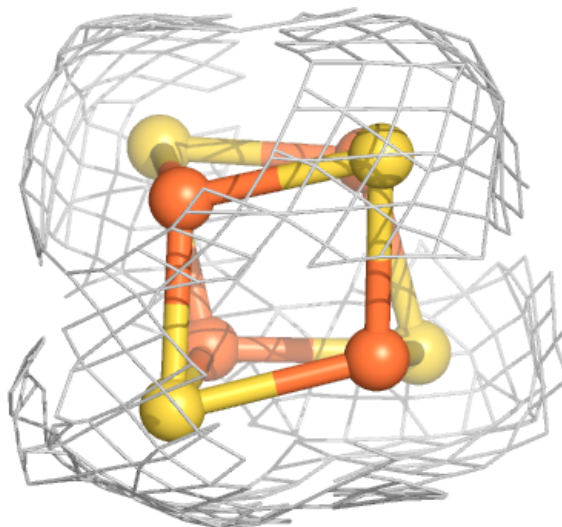
Electron density around SF4 Y 843:

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



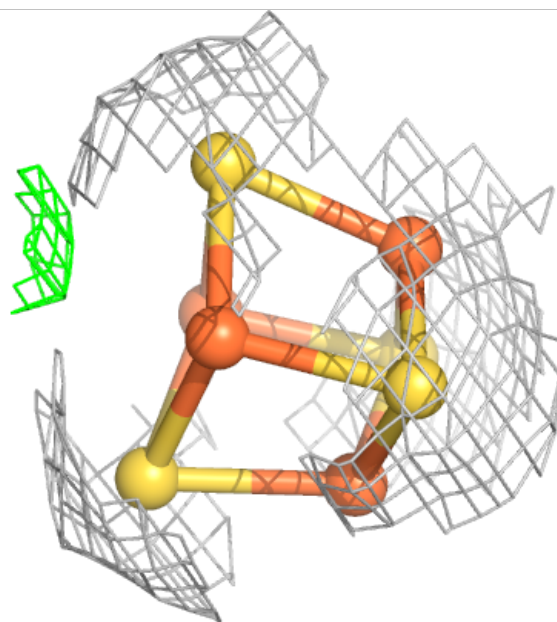
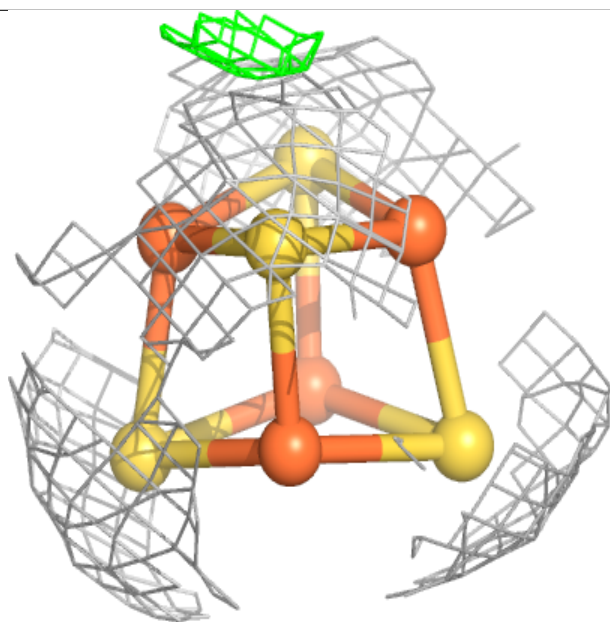
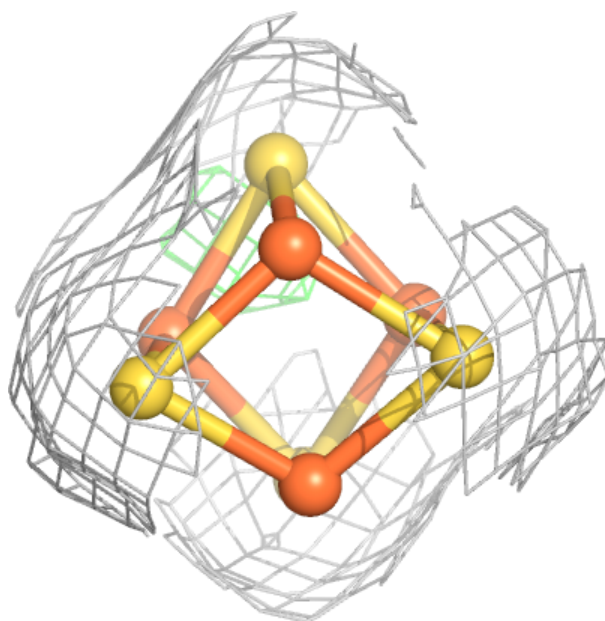
Electron density around SF4 a 101:

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



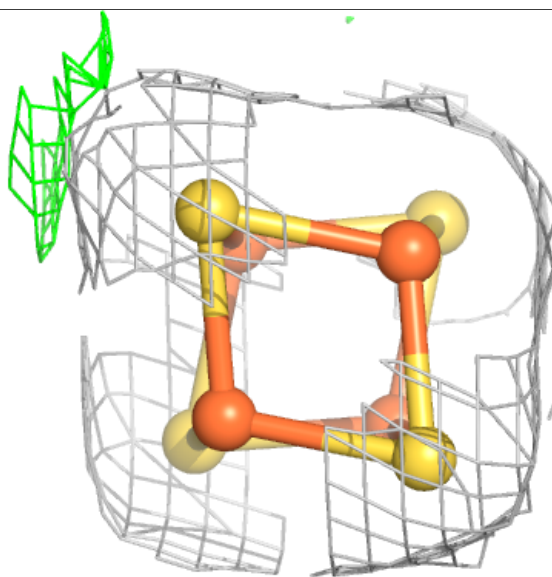
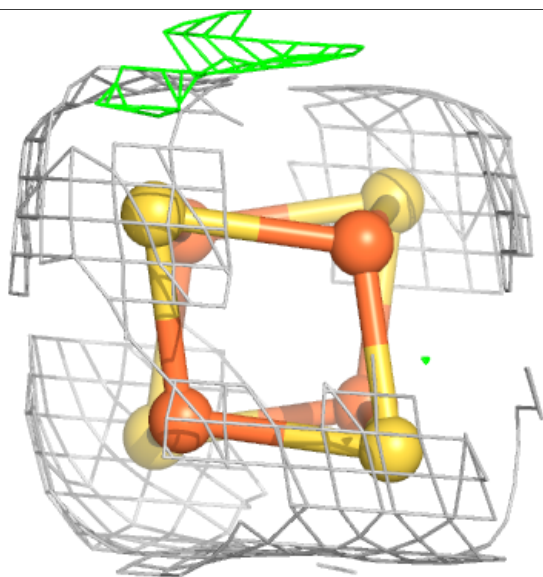
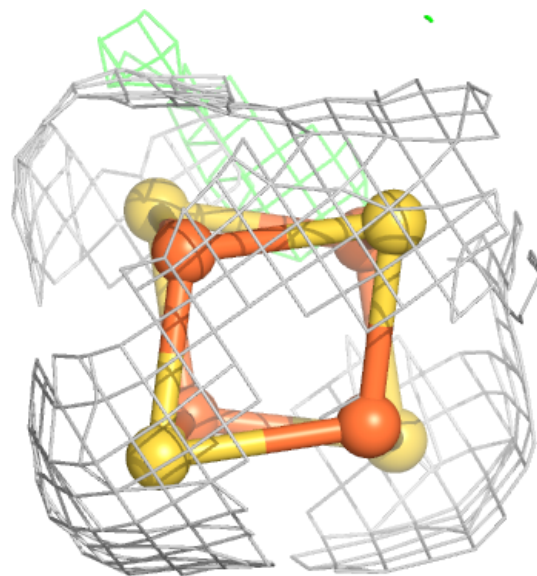
Electron density around SF4 a 102:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.