



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 05:55 PM UTC

PDB ID : 6PGK / pdb_00006pgk
Title : Membrane Protein Megahertz Crystallography at the European XFEL, Photosystem I XFEL at 2.9 Å
Authors : Fromme, R.; Gisriel, C.; Fromme, P.
Deposited on : 2019-06-24
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

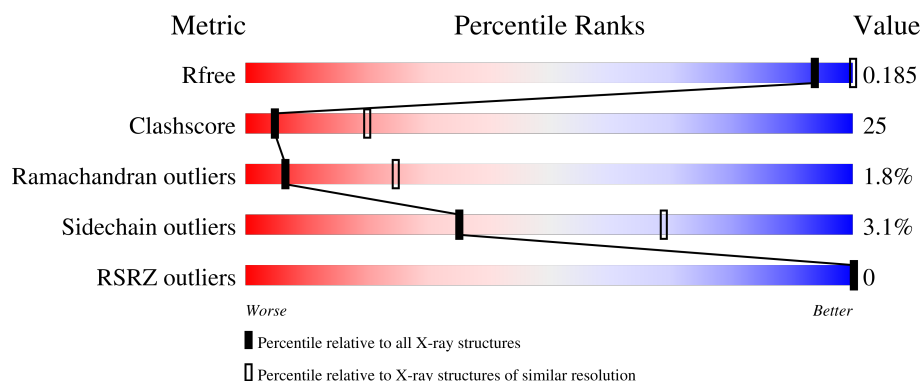
1 Overall quality at a glance

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	55% 42% ..
1	G	755	52% 45% ..
1	Y	755	48% 47% ..
2	B	741	53% 44% .
2	H	741	53% 45% .

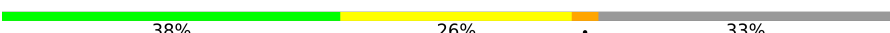
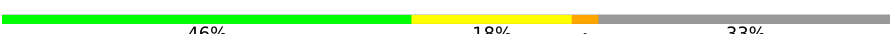
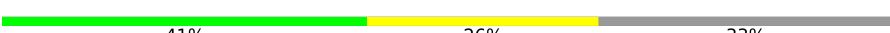
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Mol	Chain	Length	Quality of chain
2	Z	741	
3	C	81	
3	N	81	
3	a	81	
4	D	139	
4	O	139	
4	b	139	
5	E	76	
5	P	76	
5	c	76	
6	F	164	
6	Q	164	
6	d	164	
7	I	38	
7	R	38	
7	e	38	
8	J	41	
8	S	41	
8	f	41	
9	K	83	
9	T	83	
9	g	83	
10	L	155	
10	U	155	
10	h	155	

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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	-	-	-
14	CLA	A	830	X	-	-	-
14	CLA	A	831	X	-	-	-
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	839	X	-	-	-
14	CLA	A	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	842	X	-	-	-
14	CLA	A	852	X	-	-	-
14	CLA	B	801	X	-	-	-
14	CLA	B	802	X	-	-	-
14	CLA	B	803	X	-	-	-
14	CLA	B	804	X	-	-	-
14	CLA	B	805	X	-	-	-
14	CLA	B	806	X	-	-	-
14	CLA	B	807	X	-	-	-
14	CLA	B	808	X	-	-	-
14	CLA	B	809	X	-	-	-
14	CLA	B	810	X	-	-	-
14	CLA	B	811	X	-	-	-
14	CLA	B	812	X	-	-	-
14	CLA	B	813	X	-	-	-
14	CLA	B	814	X	-	-	-
14	CLA	B	815	X	-	-	-
14	CLA	B	816	X	-	-	-
14	CLA	B	817	X	-	-	-
14	CLA	B	818	X	-	-	-
14	CLA	B	819	X	-	-	-
14	CLA	B	820	X	-	-	-
14	CLA	B	821	X	-	-	-
14	CLA	B	822	X	-	-	-
14	CLA	B	823	X	-	-	-
14	CLA	B	824	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	825	X	-	-	-
14	CLA	B	826	X	-	-	-
14	CLA	B	827	X	-	-	-
14	CLA	B	828	X	-	-	-
14	CLA	B	829	X	-	-	-
14	CLA	B	830	X	-	-	-
14	CLA	B	831	X	-	-	-
14	CLA	B	832	X	-	-	-
14	CLA	B	833	X	-	-	-
14	CLA	B	834	X	-	-	-
14	CLA	B	835	X	-	-	-
14	CLA	B	836	X	-	-	-
14	CLA	B	837	X	-	-	-
14	CLA	B	838	X	-	-	-
14	CLA	B	839	X	-	-	-
14	CLA	B	840	X	-	-	-
14	CLA	B	841	X	-	-	-
14	CLA	F	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	843	X	-	-	-
14	CLA	G	853	X	-	-	-
14	CLA	H	801	X	-	X	-
14	CLA	H	802	X	-	-	-
14	CLA	H	803	X	-	-	-
14	CLA	H	804	X	-	-	-
14	CLA	H	805	X	-	-	-
14	CLA	H	806	X	-	-	-
14	CLA	H	807	X	-	-	-
14	CLA	H	808	X	-	-	-
14	CLA	H	809	X	-	-	-
14	CLA	H	810	X	-	-	-
14	CLA	H	811	X	-	-	-
14	CLA	H	812	X	-	-	-
14	CLA	H	813	X	-	-	-
14	CLA	H	814	X	-	-	-
14	CLA	H	815	X	-	-	-
14	CLA	H	816	X	-	-	-
14	CLA	H	817	X	-	-	-
14	CLA	H	818	X	-	-	-
14	CLA	H	819	X	-	-	-
14	CLA	H	820	X	-	-	-
14	CLA	H	821	X	-	-	-
14	CLA	H	822	X	-	-	-
14	CLA	H	823	X	-	-	-

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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	J	101	X	-	-	-
14	CLA	J	102	X	-	-	-
14	CLA	K	101	X	-	-	-
14	CLA	K	103	X	-	-	-
14	CLA	L	201	X	-	-	-
14	CLA	L	202	X	-	-	-
14	CLA	L	205	X	-	-	-
14	CLA	L	206	X	-	-	-
14	CLA	L	207	X	-	-	-
14	CLA	Q	201	X	-	-	-
14	CLA	Q	203	X	-	-	-
14	CLA	S	1101	X	-	-	-
14	CLA	S	1102	X	-	-	-
14	CLA	S	1103	X	-	-	-
14	CLA	T	101	X	-	-	-
14	CLA	T	103	X	-	-	-
14	CLA	U	1002	X	-	-	-
14	CLA	U	1003	X	-	-	-
14	CLA	U	1004	X	-	-	-
14	CLA	U	1006	X	-	-	-
14	CLA	V	1201	X	-	-	-
14	CLA	W	1701	X	-	-	-
14	CLA	X	1701	X	-	-	-
14	CLA	Y	802	X	-	-	-
14	CLA	Y	803	X	-	-	-
14	CLA	Y	804	X	-	-	-
14	CLA	Y	805	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	Y	842	X	-	-	-
14	CLA	Y	843	X	-	-	-
14	CLA	Y	854	X	-	-	-
14	CLA	Y	855	X	-	-	-
14	CLA	Z	801	X	-	-	-
14	CLA	Z	802	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	Z	803	X	-	-	-
14	CLA	Z	804	X	-	-	-
14	CLA	Z	805	X	-	-	-
14	CLA	Z	806	X	-	-	-
14	CLA	Z	807	X	-	-	-
14	CLA	Z	808	X	-	-	-
14	CLA	Z	809	X	-	-	-
14	CLA	Z	810	X	-	-	-
14	CLA	Z	811	X	-	-	-
14	CLA	Z	812	X	-	-	-
14	CLA	Z	813	X	-	-	-
14	CLA	Z	814	X	-	-	-
14	CLA	Z	815	X	-	-	-
14	CLA	Z	816	X	-	-	-
14	CLA	Z	817	X	-	-	-
14	CLA	Z	818	X	-	-	-
14	CLA	Z	819	X	-	-	-
14	CLA	Z	820	X	-	-	-
14	CLA	Z	821	X	-	-	-
14	CLA	Z	822	X	-	-	-
14	CLA	Z	823	X	-	-	-
14	CLA	Z	824	X	-	-	-
14	CLA	Z	825	X	-	-	-
14	CLA	Z	826	X	-	-	-
14	CLA	Z	827	X	-	-	-
14	CLA	Z	828	X	-	-	-
14	CLA	Z	829	X	-	-	-
14	CLA	Z	830	X	-	-	-
14	CLA	Z	831	X	-	-	-
14	CLA	Z	832	X	-	-	-
14	CLA	Z	833	X	-	-	-
14	CLA	Z	834	X	-	-	-
14	CLA	Z	835	X	-	-	-
14	CLA	Z	836	X	-	-	-
14	CLA	Z	837	X	-	-	-
14	CLA	Z	838	X	-	-	-
14	CLA	Z	839	X	-	-	-
14	CLA	d	201	X	-	-	-
14	CLA	d	202	X	-	-	-
14	CLA	f	101	X	-	-	-
14	CLA	f	102	X	-	-	-
14	CLA	g	101	X	-	-	-

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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	205	X	-	-	-
14	CLA	h	206	X	-	-	-
14	CLA	h	207	X	-	-	-
14	CLA	j	102	X	-	-	-
16	SF4	C	101	-	-	X	-
16	SF4	C	102	-	-	X	-
16	SF4	N	102	-	-	X	-

2 Entry composition

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	741	Total	C	N	O	S	0	0	0
			5791	3799	989	977	26			
1	G	741	Total	C	N	O	S	0	0	0
			5791	3799	989	977	26			
1	Y	741	Total	C	N	O	S	0	0	0
			5791	3799	989	977	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	739	Total	C	N	O	S	0	0	0
			5889	3876	987	1005	21			
2	H	739	Total	C	N	O	S	0	0	0
			5889	3876	987	1005	21			
2	Z	739	Total	C	N	O	S	0	0	0
			5889	3876	987	1005	21			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

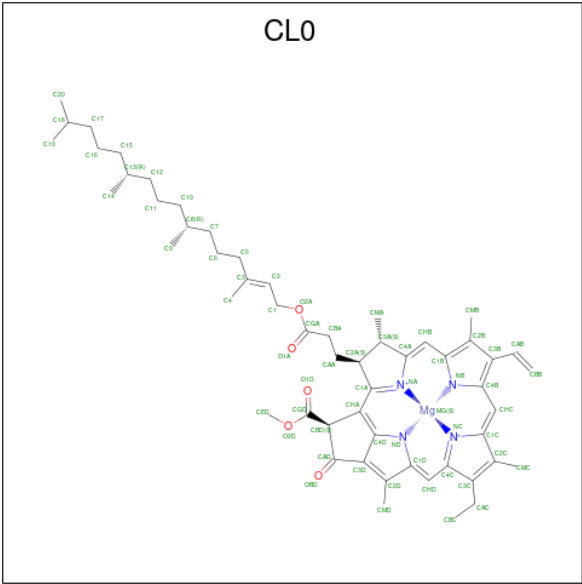
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

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

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

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

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	Y	1	Total 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	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 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 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
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0	0

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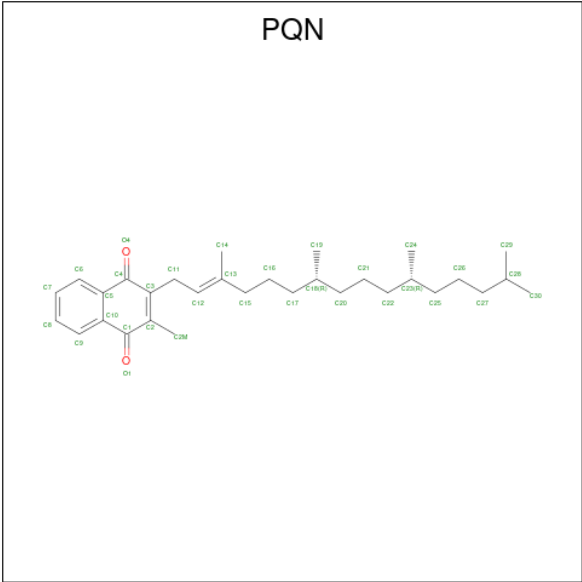
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
14	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
14	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
14	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
14	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
14	Z	1	Total 55	C 45	Mg 1	N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

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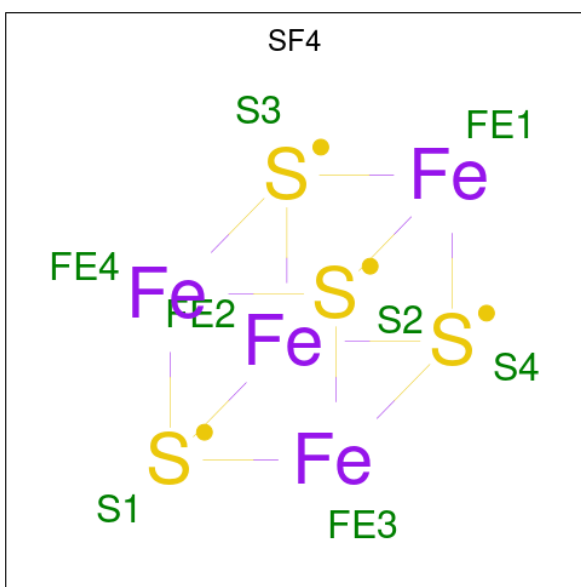
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	Z	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	Z	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	d	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5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

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



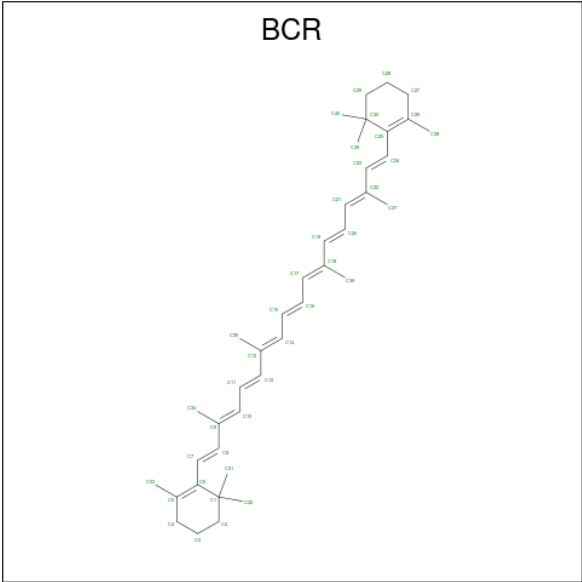
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	A	1	Total	C	O	0	0
			33	31	2		
15	B	1	Total	C	O	0	0
			33	31	2		
15	G	1	Total	C	O	0	0
			33	31	2		
15	H	1	Total	C	O	0	0
			33	31	2		
15	Y	1	Total	C	O	0	0
			33	31	2		
15	Z	1	Total	C	O	0	0
			33	31	2		

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (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	B	1	Total C 30 30	0	0
17	B	1	Total C 40 40	0	0
17	B	1	Total C 40 40	0	0
17	B	1	Total C 25 25	0	0
17	B	1	Total C 40 40	0	0
17	B	1	Total C 40 40	0	0
17	B	1	Total C 40 40	0	0
17	B	1	Total C 40 40	0	0
17	F	1	Total C 40 40	0	0
17	F	1	Total C 40 40	0	0

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

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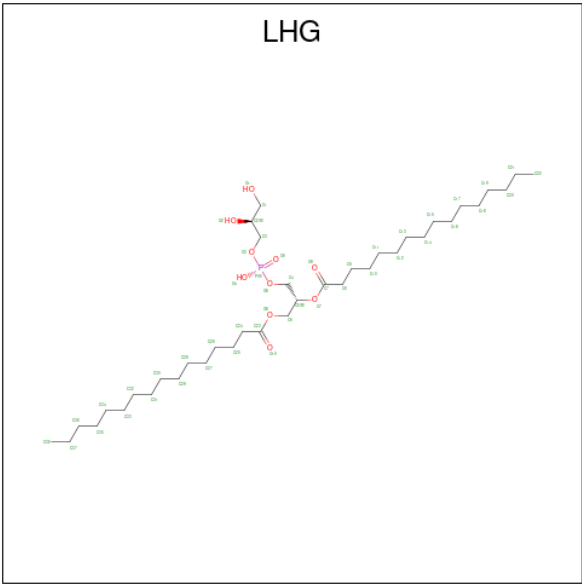
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	Q	1	Total C 40 40	0	0
17	Q	1	Total C 40 40	0	0
17	R	1	Total C 40 40	0	0
17	R	1	Total C 40 40	0	0
17	S	1	Total C 40 40	0	0
17	T	1	Total C 40 40	0	0
17	U	1	Total C 40 40	0	0
17	U	1	Total C 40 40	0	0
17	U	1	Total C 40 40	0	0
17	V	1	Total C 40 40	0	0
17	Y	1	Total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

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



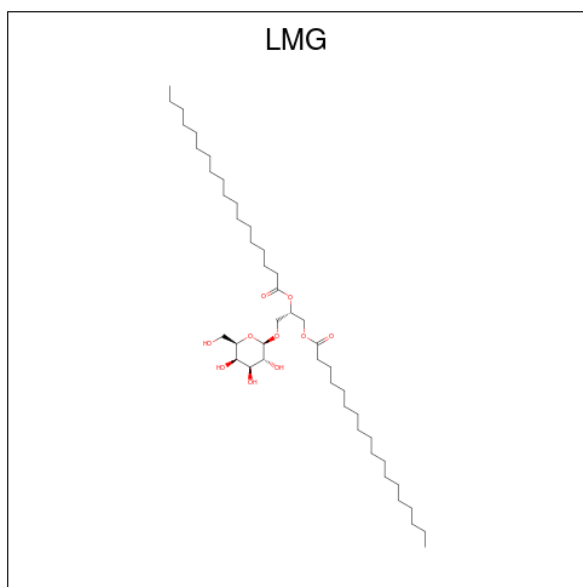
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O P 49 38 10 1	0	0

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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: $C_{45}H_{86}O_{10}$).



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

- Molecule 20 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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	9	Total O 9 9	0	0
21	B	9	Total O 9 9	0	0
21	C	1	Total O 1 1	0	0
21	D	2	Total O 2 2	0	0
21	E	1	Total O 1 1	0	0
21	G	8	Total O 8 8	0	0
21	H	3	Total O 3 3	0	0
21	J	1	Total O 1 1	0	0
21	K	1	Total O 1 1	0	0
21	L	5	Total O 5 5	0	0
21	N	1	Total O 1 1	0	0
21	O	2	Total O 2 2	0	0
21	Q	2	Total O 2 2	0	0
21	T	1	Total O 1 1	0	0
21	U	4	Total O 4 4	0	0
21	W	1	Total O 1 1	0	0

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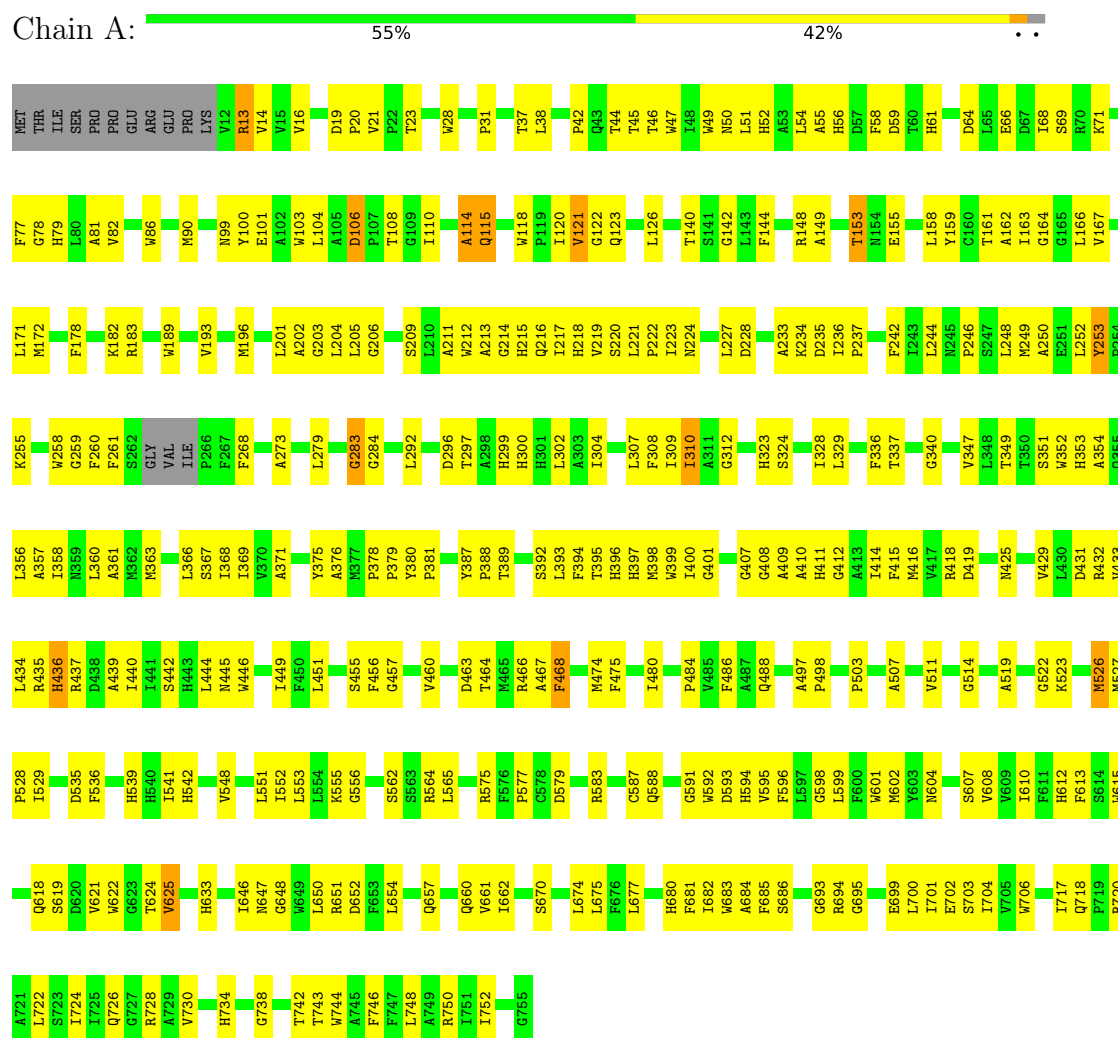
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	Y	8	Total 8	O 8	0	0
21	Z	2	Total 2	O 2	0	0
21	b	4	Total 4	O 4	0	0
21	c	1	Total 1	O 1	0	0
21	d	2	Total 2	O 2	0	0
21	f	1	Total 1	O 1	0	0
21	h	1	Total 1	O 1	0	0
21	j	1	Total 1	O 1	0	0

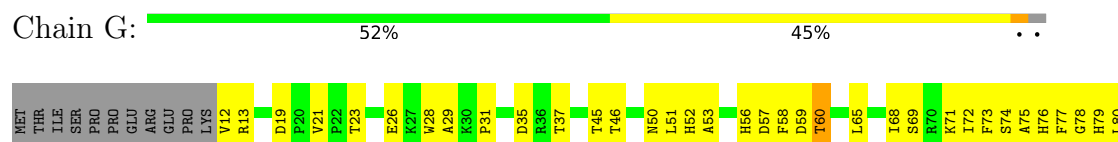
3 Residue-property plots

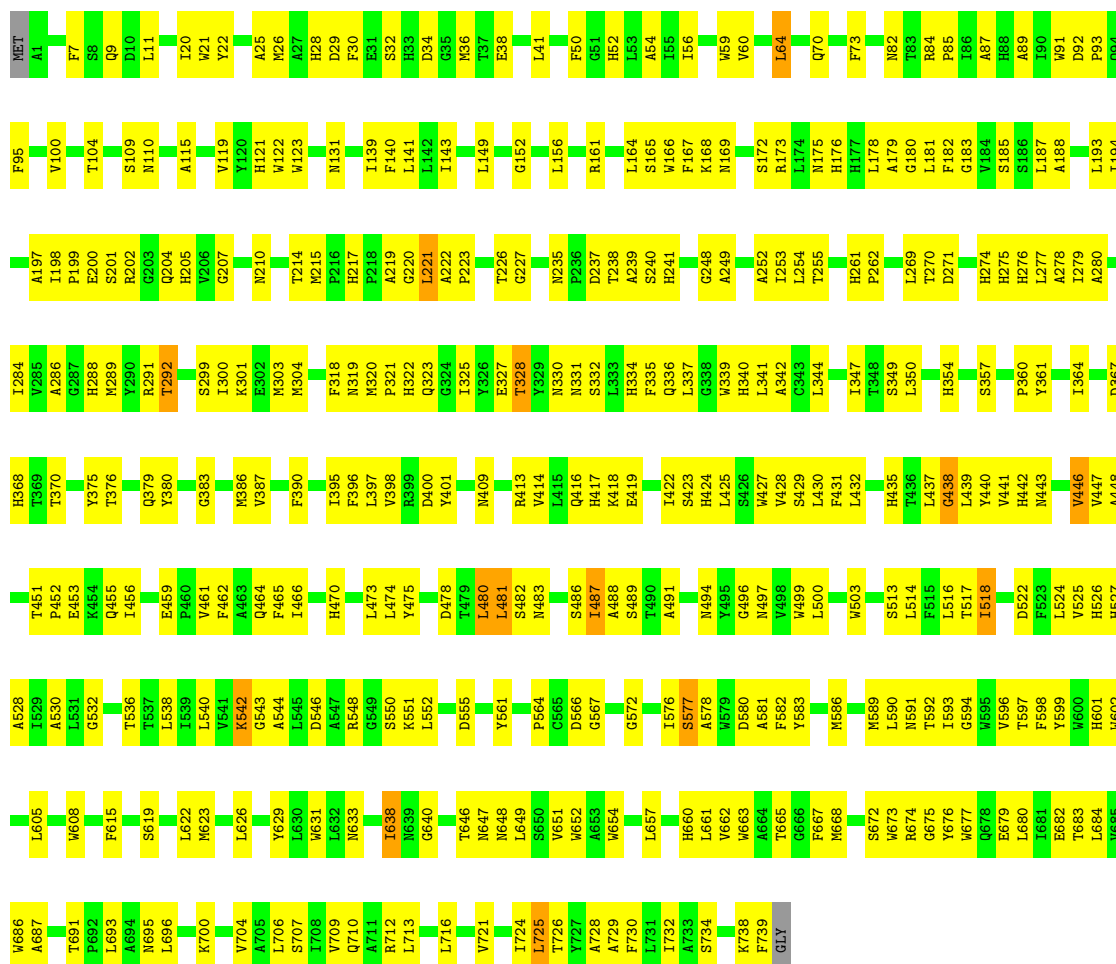
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



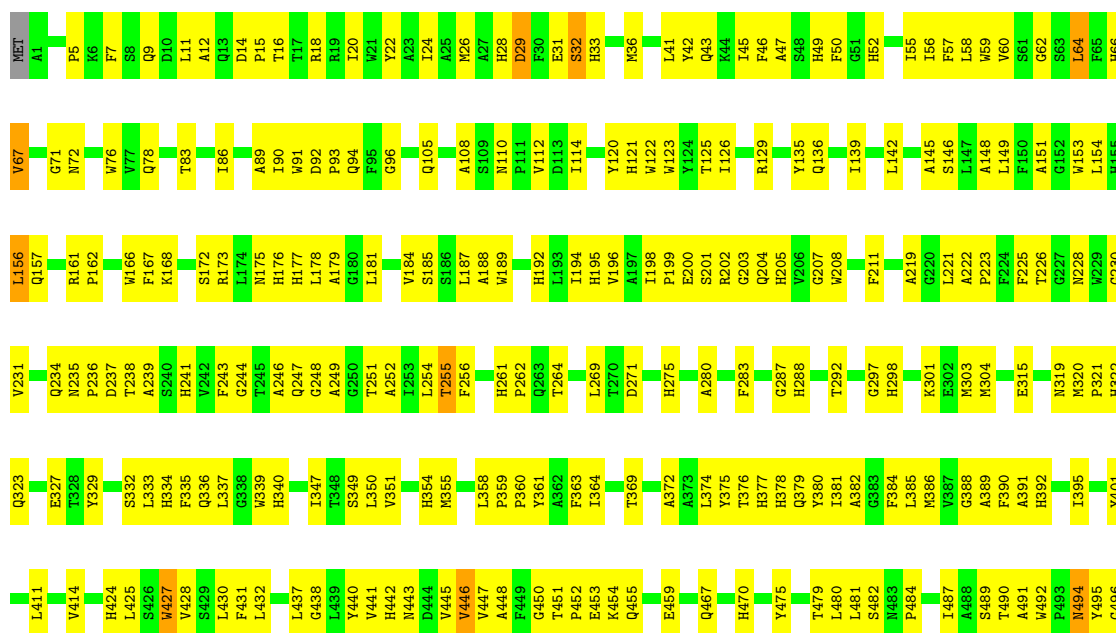
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

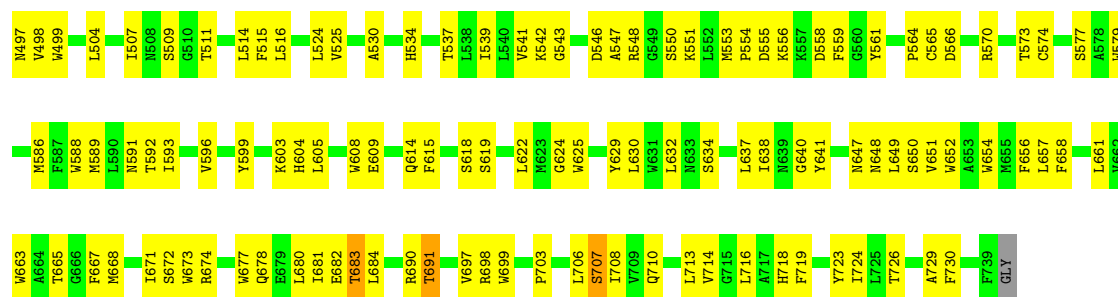




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain Z: 52% 46%

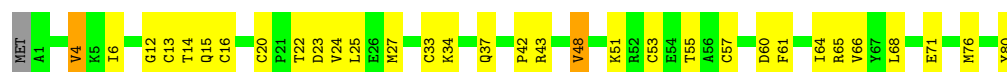




• Molecule 3: Photosystem I iron-sulfur center



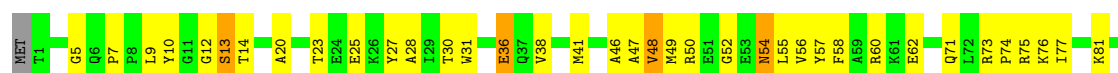
• Molecule 3: Photosystem I iron-sulfur center



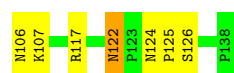
• Molecule 3: Photosystem I iron-sulfur center



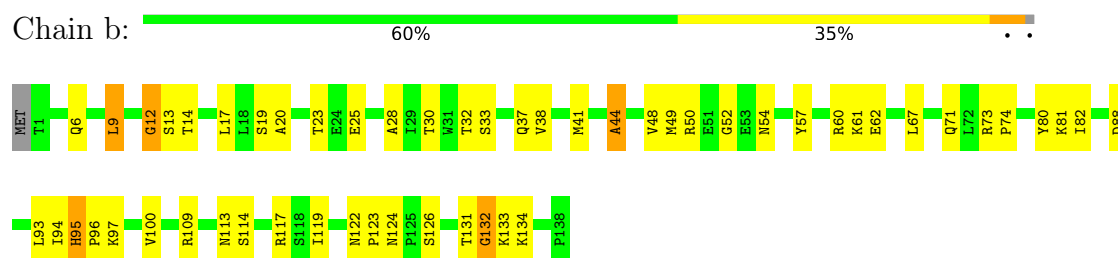
• Molecule 4: Photosystem I reaction center subunit II



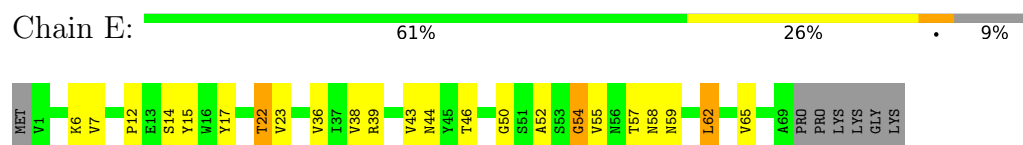
• Molecule 4: Photosystem I reaction center subunit II



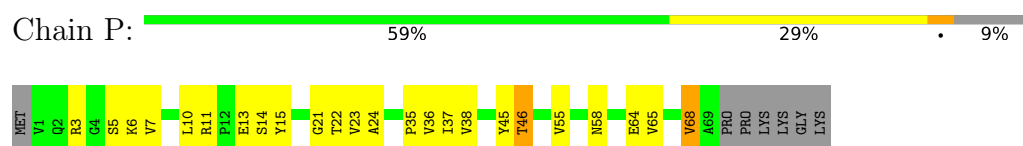
- Molecule 4: Photosystem I reaction center subunit II



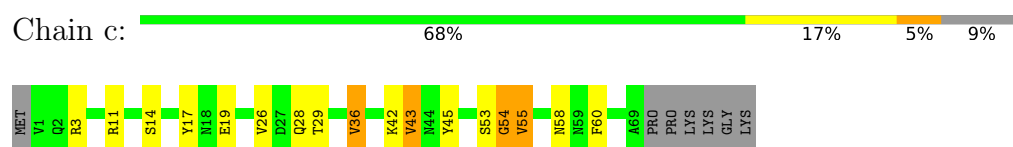
- Molecule 5: Photosystem I reaction center subunit IV



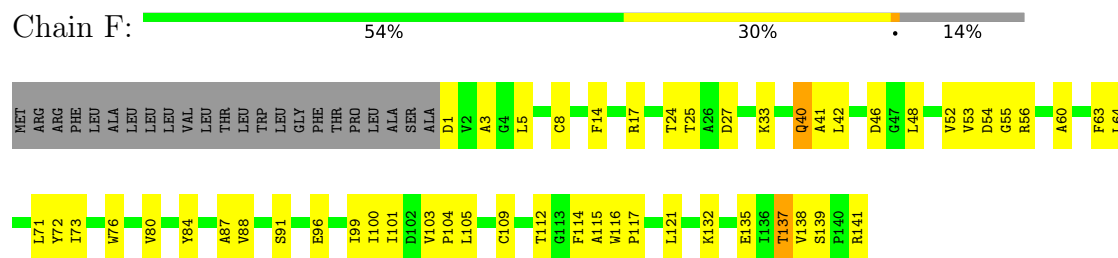
- Molecule 5: Photosystem I reaction center subunit IV



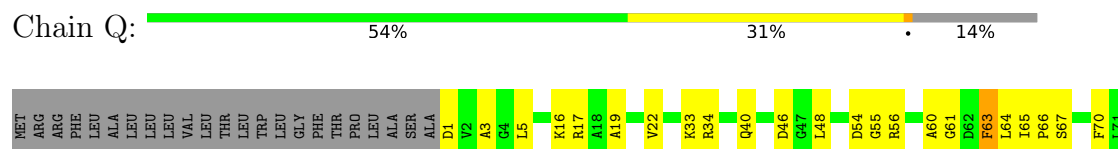
- Molecule 5: Photosystem I reaction center subunit IV



- Molecule 6: Photosystem I reaction center subunit III

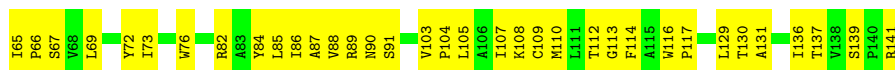


- Molecule 6: Photosystem I reaction center subunit III

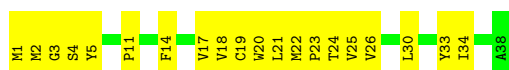




- Molecule 6: Photosystem I reaction center subunit III



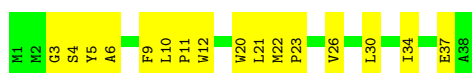
- Molecule 7: Photosystem I reaction center subunit VIII



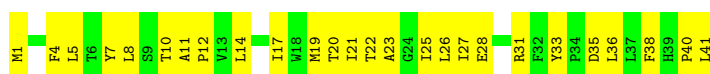
- Molecule 7: Photosystem I reaction center subunit VIII



- Molecule 7: Photosystem I reaction center subunit VIII



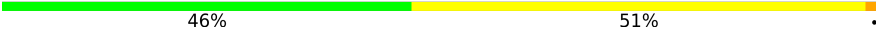
- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 8: Photosystem I reaction center subunit IX

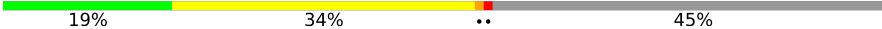


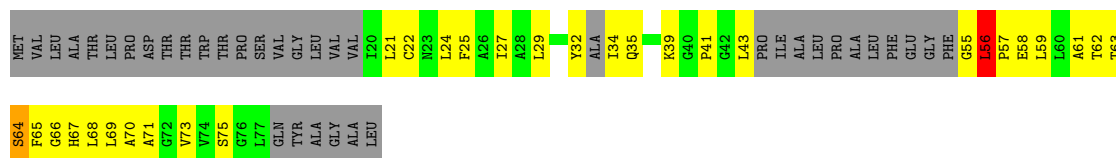
- Molecule 8: Photosystem I reaction center subunit IX

Chain f:  46% 51% .



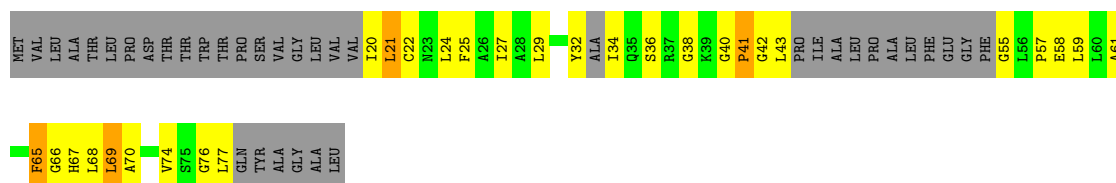
• Molecule 9: Photosystem I reaction center subunit Psak

Chain K:  19% 34% .. 45%



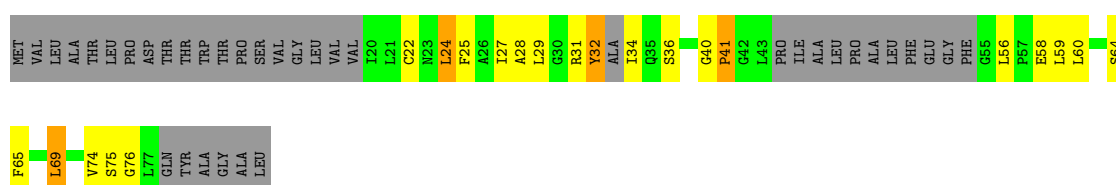
• Molecule 9: Photosystem I reaction center subunit Psak

Chain T:  20% 30% 5% 45%



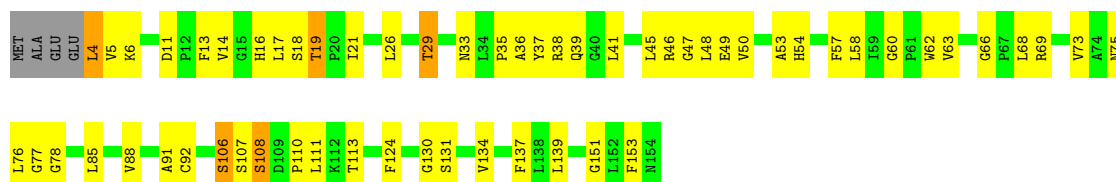
• Molecule 9: Photosystem I reaction center subunit Psak

Chain g:  29% 22% 5% 45%



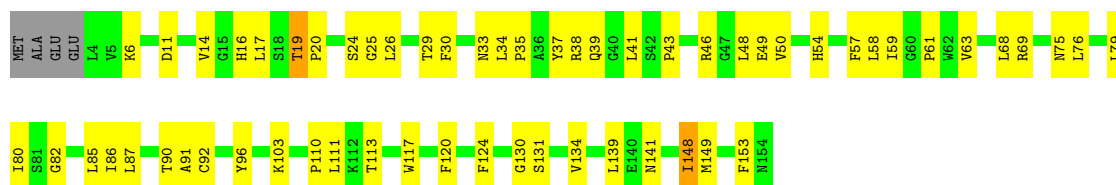
• Molecule 10: Photosystem I reaction center subunit XI

Chain L:  59% 35% ..



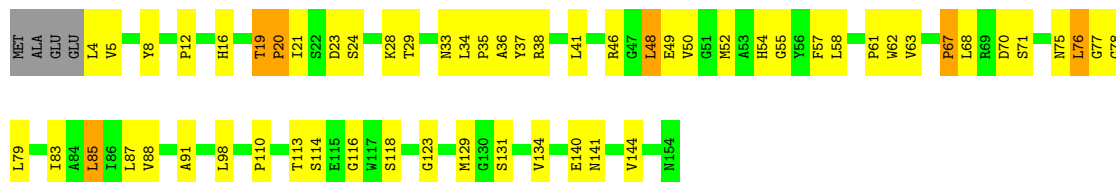
• Molecule 10: Photosystem I reaction center subunit XI

Chain U:  59% 37% ..



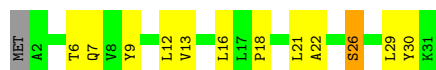
- Molecule 10: Photosystem I reaction center subunit XI

Chain h: 60% 34%



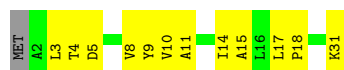
- Molecule 11: Photosystem I reaction center subunit XII

Chain M: 58% 35%



- Molecule 11: Photosystem I reaction center subunit XII

Chain V: 58% 39%



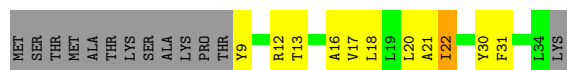
- Molecule 11: Photosystem I reaction center subunit XII

Chain i: 55% 39%



- Molecule 12: Photosystem I 4.8K protein

Chain W: 38% 26% 33%

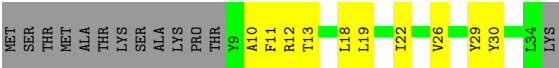


- Molecule 12: Photosystem I 4.8K protein

Chain X: 46% 18% 33%



● Molecule 12: Photosystem I 4.8K protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	279.10Å 164.60Å 284.10Å 90.00° 119.25° 90.00°	Depositor
Resolution (Å)	39.88 – 2.90 39.88 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.88-2.90) 92.7 (39.88-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.298 , 0.336 (Not available) , 0.185	Depositor DCC
R_{free} test set	24635 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	72.2	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 77.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.27$, $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	0.268 for -h-l,k,h 0.268 for l,k,-h-l 0.347 for h,-k,-h-l 0.260 for -h-l,-k,l 0.259 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	72532	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, LMG, LHG, CL0, BCR, PQN, CLA, CA

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	1.00	1/5990 (0.0%)	1.44	0/8168
1	G	1.00	0/5990	1.45	4/8168 (0.0%)
1	Y	1.00	0/5990	1.46	7/8168 (0.1%)
2	B	0.97	0/6107	1.42	2/8345 (0.0%)
2	H	0.99	0/6107	1.42	1/8345 (0.0%)
2	Z	0.98	0/6107	1.42	4/8345 (0.0%)
3	C	1.07	0/608	1.41	0/824
3	N	1.02	0/608	1.37	0/824
3	a	1.05	0/608	1.35	0/824
4	D	0.97	0/1101	1.30	0/1492
4	O	0.96	0/1101	1.26	0/1492
4	b	0.98	0/1101	1.28	1/1492 (0.1%)
5	E	1.04	0/551	1.29	0/750
5	P	1.03	0/551	1.26	0/750
5	c	1.03	0/551	1.30	1/750 (0.1%)
6	F	1.04	0/1087	1.45	2/1476 (0.1%)
6	Q	1.02	0/1087	1.44	2/1476 (0.1%)
6	d	1.02	0/1087	1.44	0/1476
7	I	1.00	0/312	1.41	0/425
7	R	1.01	0/312	1.33	0/425
7	e	0.95	0/312	1.38	0/425
8	J	0.98	0/350	1.38	0/477
8	S	0.98	0/350	1.47	0/477
8	f	0.97	0/350	1.45	2/477 (0.4%)
9	K	1.03	0/331	1.45	0/444
9	T	1.05	0/331	1.59	2/444 (0.5%)
9	g	1.10	0/331	1.64	0/444
10	L	1.01	0/1148	1.50	0/1558
10	U	1.02	0/1148	1.52	0/1558
10	h	1.01	0/1148	1.47	0/1558
11	M	1.01	0/236	1.43	0/322
11	V	1.04	0/236	1.54	0/322

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	i	1.05	0/236	1.51	0/322
12	W	0.94	0/227	1.44	0/310
12	X	0.96	0/227	1.46	0/310
12	j	0.95	0/227	1.37	0/310
All	All	1.00	1/54144 (0.0%)	1.43	28/73773 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	VAL	N-CA	5.01	1.49	1.45

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	297	GLY	CA-C-O	-6.24	117.92	122.23
4	b	12	GLY	CA-C-O	-5.78	117.61	122.29
2	B	568	PRO	CA-C-N	5.78	126.21	120.31
2	B	568	PRO	C-N-CA	5.78	126.21	120.31
6	Q	102	ASP	CA-C-N	5.76	124.94	120.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	K	56	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5791	0	5648	338	0
1	G	5791	0	5648	355	0
1	Y	5791	0	5649	357	0
2	B	5889	0	5651	360	0
2	H	5889	0	5650	362	0
2	Z	5889	0	5651	335	0
3	C	598	0	582	36	0
3	N	598	0	582	36	0
3	a	598	0	582	35	0
4	D	1075	0	1077	51	0
4	O	1075	0	1077	37	0
4	b	1075	0	1077	51	0
5	E	539	0	528	16	0
5	P	539	0	528	12	0
5	c	539	0	528	10	1
6	F	1065	0	1077	45	0
6	Q	1065	0	1077	52	0
6	d	1065	0	1077	50	1
7	I	301	0	306	22	0
7	R	301	0	306	17	0
7	e	301	0	306	13	0
8	J	338	0	347	29	0
8	S	338	0	347	29	0
8	f	338	0	347	23	0
9	K	328	0	348	32	0
9	T	328	0	348	23	0
9	g	328	0	348	16	0
10	L	1119	0	1125	54	0
10	U	1119	0	1125	58	0
10	h	1119	0	1125	61	0
11	M	233	0	252	10	0
11	V	233	0	252	7	0
11	i	233	0	252	14	0
12	W	219	0	221	9	0
12	X	219	0	221	7	0
12	j	219	0	221	12	0
13	A	65	0	72	10	0
13	G	65	0	72	11	0
13	Y	65	0	72	8	0
14	A	2489	0	2488	234	0
14	B	2389	0	2373	218	0
14	F	45	0	32	2	0
14	G	2534	0	2522	251	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	H	2220	0	2211	239	0
14	J	100	0	81	1	0
14	K	86	0	61	4	0
14	L	325	0	360	27	0
14	Q	110	0	104	11	0
14	S	165	0	154	11	0
14	T	86	0	62	3	0
14	U	260	0	287	30	0
14	V	54	0	48	3	0
14	W	45	0	33	4	0
14	X	45	0	33	0	0
14	Y	2640	0	2675	252	0
14	Z	2254	0	2219	203	0
14	d	95	0	70	10	0
14	f	100	0	82	3	0
14	g	86	0	62	2	0
14	h	260	0	287	24	0
14	j	45	0	33	2	0
15	A	33	0	46	6	0
15	B	33	0	46	9	0
15	G	33	0	46	3	0
15	H	33	0	46	4	0
15	Y	33	0	46	5	0
15	Z	33	0	46	2	0
16	A	8	0	0	1	0
16	C	16	0	0	5	0
16	G	8	0	0	0	0
16	N	16	0	0	3	0
16	Y	8	0	0	0	0
16	a	16	0	0	1	0
17	A	200	0	243	33	0
17	B	255	0	302	52	0
17	F	80	0	98	9	0
17	G	240	0	288	61	0
17	H	265	0	320	46	0
17	I	40	0	48	6	0
17	J	80	0	96	22	0
17	K	40	0	48	3	0
17	L	120	0	145	21	0
17	M	40	0	48	7	0
17	Q	80	0	98	9	0
17	R	80	0	96	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	S	40	0	47	9	0
17	T	40	0	49	8	0
17	U	120	0	145	23	0
17	V	40	0	49	5	0
17	Y	280	0	337	60	0
17	Z	225	0	271	32	0
17	d	40	0	48	5	0
17	e	40	0	48	5	0
17	f	120	0	145	34	0
17	h	80	0	97	10	0
17	i	40	0	47	6	0
18	A	81	0	108	5	0
18	B	39	0	48	0	0
18	G	81	0	108	11	0
18	H	37	0	44	2	0
18	Y	74	0	94	8	0
18	j	28	0	26	2	0
19	B	52	0	77	6	0
19	H	49	0	68	4	0
19	Z	49	0	68	3	0
20	L	1	0	0	0	0
20	U	1	0	0	0	0
20	h	1	0	0	0	0
21	A	9	0	0	0	0
21	B	9	0	0	0	0
21	C	1	0	0	1	0
21	D	2	0	0	0	0
21	E	1	0	0	0	0
21	G	8	0	0	17	0
21	H	3	0	0	0	0
21	J	1	0	0	0	0
21	K	1	0	0	0	0
21	L	5	0	0	0	0
21	N	1	0	0	1	0
21	O	2	0	0	0	0
21	Q	2	0	0	0	0
21	T	1	0	0	0	0
21	U	4	0	0	0	0
21	W	1	0	0	1	0
21	Y	8	0	0	18	0
21	Z	2	0	0	0	0
21	b	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	c	1	0	0	0	0
21	d	2	0	0	0	0
21	f	1	0	0	0	0
21	h	1	0	0	0	0
21	j	1	0	0	0	0
All	All	72532	0	72009	3673	1

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

The worst 5 of 3673 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:819:CLA:HBB1	21:G:907:HOH:O	1.23	1.26
1:G:373:HIS:ND1	14:G:818:CLA:OBD	1.80	1.15
14:Y:821:CLA:C3B	21:Y:904:HOH:O	1.92	1.14
9:K:32:TYR:C	9:K:34:ILE:N	2.07	1.13
1:A:399:TRP:CD1	14:A:828:CLA:HAB	1.84	1.12

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:c:28:GLN:OE1	6:d:1:ASP:N[2_545]	2.13	0.07

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	737/755 (98%)	634 (86%)	89 (12%)	14 (2%)	6	23
1	G	737/755 (98%)	634 (86%)	86 (12%)	17 (2%)	5	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	737/755 (98%)	627 (85%)	98 (13%)	12 (2%)	7	27
2	B	737/741 (100%)	639 (87%)	84 (11%)	14 (2%)	6	23
2	H	737/741 (100%)	658 (89%)	69 (9%)	10 (1%)	9	30
2	Z	737/741 (100%)	642 (87%)	86 (12%)	9 (1%)	10	34
3	C	78/81 (96%)	72 (92%)	4 (5%)	2 (3%)	4	17
3	N	78/81 (96%)	69 (88%)	8 (10%)	1 (1%)	9	32
3	a	78/81 (96%)	64 (82%)	12 (15%)	2 (3%)	4	17
4	D	136/139 (98%)	119 (88%)	14 (10%)	3 (2%)	5	20
4	O	136/139 (98%)	122 (90%)	11 (8%)	3 (2%)	5	20
4	b	136/139 (98%)	117 (86%)	15 (11%)	4 (3%)	3	15
5	E	67/76 (88%)	58 (87%)	6 (9%)	3 (4%)	2	8
5	P	67/76 (88%)	56 (84%)	6 (9%)	5 (8%)	1	2
5	c	67/76 (88%)	56 (84%)	8 (12%)	3 (4%)	2	8
6	F	139/164 (85%)	126 (91%)	12 (9%)	1 (1%)	18	48
6	Q	139/164 (85%)	124 (89%)	14 (10%)	1 (1%)	18	48
6	d	139/164 (85%)	118 (85%)	18 (13%)	3 (2%)	5	20
7	I	36/38 (95%)	30 (83%)	6 (17%)	0	100	100
7	R	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
7	e	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	4	15
8	J	39/41 (95%)	34 (87%)	5 (13%)	0	100	100
8	S	39/41 (95%)	34 (87%)	5 (13%)	0	100	100
8	f	39/41 (95%)	38 (97%)	0	1 (3%)	4	17
9	K	40/83 (48%)	31 (78%)	7 (18%)	2 (5%)	1	6
9	T	40/83 (48%)	33 (82%)	4 (10%)	3 (8%)	1	2
9	g	40/83 (48%)	30 (75%)	8 (20%)	2 (5%)	1	6
10	L	149/155 (96%)	124 (83%)	22 (15%)	3 (2%)	6	22
10	U	149/155 (96%)	138 (93%)	11 (7%)	0	100	100
10	h	149/155 (96%)	129 (87%)	17 (11%)	3 (2%)	6	22
11	M	28/31 (90%)	26 (93%)	2 (7%)	0	100	100
11	V	28/31 (90%)	26 (93%)	2 (7%)	0	100	100
11	i	28/31 (90%)	28 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	W	24/39 (62%)	23 (96%)	1 (4%)	0	100	100
12	X	24/39 (62%)	24 (100%)	0	0	100	100
12	j	24/39 (62%)	23 (96%)	1 (4%)	0	100	100
All	All	6630/7029 (94%)	5768 (87%)	740 (11%)	122 (2%)	6	25

5 of 122 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	VAL
4	D	95	HIS
5	E	55	VAL
1	G	320	GLY
1	G	508	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	590/603 (98%)	582 (99%)	8 (1%)	59	85
1	G	590/603 (98%)	574 (97%)	16 (3%)	39	73
1	Y	590/603 (98%)	569 (96%)	21 (4%)	31	65
2	B	597/598 (100%)	580 (97%)	17 (3%)	38	72
2	H	597/598 (100%)	583 (98%)	14 (2%)	44	76
2	Z	597/598 (100%)	579 (97%)	18 (3%)	36	70
3	C	67/68 (98%)	64 (96%)	3 (4%)	24	58
3	N	67/68 (98%)	64 (96%)	3 (4%)	24	58
3	a	67/68 (98%)	67 (100%)	0	100	100
4	D	115/116 (99%)	110 (96%)	5 (4%)	26	60
4	O	115/116 (99%)	110 (96%)	5 (4%)	26	60
4	b	115/116 (99%)	112 (97%)	3 (3%)	40	73
5	E	59/65 (91%)	55 (93%)	4 (7%)	14	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	P	59/65 (91%)	56 (95%)	3 (5%)	21	53
5	c	59/65 (91%)	56 (95%)	3 (5%)	21	53
6	F	109/128 (85%)	106 (97%)	3 (3%)	38	72
6	Q	109/128 (85%)	107 (98%)	2 (2%)	51	80
6	d	109/128 (85%)	107 (98%)	2 (2%)	51	80
7	I	32/32 (100%)	32 (100%)	0	100	100
7	R	32/32 (100%)	32 (100%)	0	100	100
7	e	32/32 (100%)	31 (97%)	1 (3%)	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%)	36 (100%)	0	100	100
9	K	33/61 (54%)	31 (94%)	2 (6%)	17	46
9	T	33/61 (54%)	31 (94%)	2 (6%)	17	46
9	g	33/61 (54%)	28 (85%)	5 (15%)	3	9
10	L	117/120 (98%)	112 (96%)	5 (4%)	26	60
10	U	117/120 (98%)	112 (96%)	5 (4%)	26	60
10	h	117/120 (98%)	108 (92%)	9 (8%)	12	35
11	M	25/26 (96%)	23 (92%)	2 (8%)	11	34
11	V	25/26 (96%)	23 (92%)	2 (8%)	11	34
11	i	25/26 (96%)	23 (92%)	2 (8%)	11	34
12	W	20/31 (64%)	19 (95%)	1 (5%)	22	53
12	X	20/31 (64%)	19 (95%)	1 (5%)	22	53
12	j	20/31 (64%)	20 (100%)	0	100	100
All	All	5400/5652 (96%)	5230 (97%)	170 (3%)	35	69

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	347	VAL
2	Z	691	THR
1	Y	478	THR
2	Z	67	VAL
5	c	53	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 132 such sidechains are listed below:

Mol	Chain	Res	Type
2	Z	353	GLN
2	Z	494	ASN
10	h	141	ASN
1	G	547	HIS
1	G	426	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	A	826	-	64,68,73	2.31	22 (34%)	76,107,113	2.54	24 (31%)
14	CLA	G	805	-	69,73,73	2.16	21 (30%)	82,113,113	2.56	27 (32%)
14	CLA	G	834	-	59,63,73	2.44	22 (37%)	70,101,113	2.53	27 (38%)
14	CLA	G	815	-	54,58,73	2.51	22 (40%)	64,95,113	3.03	29 (45%)
14	CLA	B	803	-	69,73,73	2.17	21 (30%)	82,113,113	2.42	29 (35%)
14	CLA	B	814	-	69,73,73	2.34	24 (34%)	82,113,113	2.36	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	Z	811	-	69,73,73	2.21	21 (30%)	82,113,113	2.41	27 (32%)
14	CLA	B	828	-	69,73,73	2.25	22 (31%)	82,113,113	2.43	28 (34%)
14	CLA	Y	826	-	64,68,73	2.33	23 (35%)	76,107,113	2.59	28 (36%)
14	CLA	B	817	-	69,73,73	2.19	22 (31%)	82,113,113	2.45	28 (34%)
14	CLA	A	819	-	69,73,73	2.20	23 (33%)	82,113,113	2.35	24 (29%)
14	CLA	B	806	-	69,73,73	2.17	21 (30%)	82,113,113	2.65	24 (29%)
14	CLA	Z	838	-	69,73,73	2.25	22 (31%)	82,113,113	2.40	26 (31%)
14	CLA	B	830	-	49,53,73	2.46	21 (42%)	58,89,113	2.99	27 (46%)
14	CLA	Z	816	-	64,68,73	2.34	22 (34%)	76,107,113	2.49	28 (36%)
14	CLA	H	822	-	64,68,73	2.27	17 (26%)	76,107,113	2.66	26 (34%)
14	CLA	U	1002	10	69,73,73	2.24	22 (31%)	82,113,113	2.61	30 (36%)
17	BCR	Y	847	-	41,41,41	2.53	6 (14%)	56,56,56	7.26	30 (53%)
14	CLA	Z	809	-	59,63,73	2.46	22 (37%)	70,101,113	2.60	27 (38%)
14	CLA	G	824	-	64,68,73	2.33	21 (32%)	76,107,113	2.43	25 (32%)
14	CLA	G	813	-	64,68,73	2.28	23 (35%)	76,107,113	2.66	29 (38%)
14	CLA	U	1006	2	69,73,73	2.28	21 (30%)	82,113,113	2.59	33 (40%)
17	BCR	B	844	-	41,41,41	2.61	6 (14%)	56,56,56	7.46	25 (44%)
14	CLA	Z	826	-	69,73,73	2.20	20 (28%)	82,113,113	2.38	23 (28%)
14	CLA	G	843	18	54,58,73	2.58	22 (40%)	64,95,113	2.74	29 (45%)
14	CLA	Y	831	-	54,58,73	2.53	22 (40%)	64,95,113	2.81	29 (45%)
14	CLA	Y	835	-	59,63,73	2.54	23 (38%)	70,101,113	2.57	24 (34%)
17	BCR	G	854	-	41,41,41	2.71	6 (14%)	56,56,56	7.28	27 (48%)
19	LMG	H	846	-	49,49,55	1.46	7 (14%)	57,57,63	1.18	5 (8%)
14	CLA	Z	810	-	49,53,73	2.51	18 (36%)	58,89,113	2.70	25 (43%)
14	CLA	Z	823	-	69,73,73	2.31	22 (31%)	82,113,113	2.63	30 (36%)
14	CLA	B	820	-	49,53,73	2.57	22 (44%)	58,89,113	2.77	24 (41%)
17	BCR	G	848	-	41,41,41	2.54	7 (17%)	56,56,56	7.37	30 (53%)
14	CLA	A	813	-	64,68,73	2.32	22 (34%)	76,107,113	2.50	26 (34%)
14	CLA	G	837	-	69,73,73	2.22	21 (30%)	82,113,113	2.51	26 (31%)
14	CLA	G	804	-	63,67,73	2.35	22 (34%)	74,105,113	2.58	24 (32%)
14	CLA	T	101	-	45,49,73	2.53	19 (42%)	54,83,113	2.79	22 (40%)
15	PQN	H	839	-	34,34,34	1.64	2 (5%)	43,45,45	1.31	7 (16%)
17	BCR	d	203	-	41,41,41	2.48	6 (14%)	56,56,56	7.14	27 (48%)
14	CLA	G	822	-	69,73,73	2.23	21 (30%)	82,113,113	2.67	27 (32%)
14	CLA	Z	832	-	49,53,73	2.68	23 (46%)	58,89,113	2.85	26 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	H	819	-	49,53,73	2.50	20 (40%)	58,89,113	2.93	23 (39%)
14	CLA	H	838	-	69,73,73	2.23	20 (28%)	82,113,113	2.58	29 (35%)
19	LMG	B	849	-	52,52,55	1.39	7 (13%)	60,60,63	1.00	3 (5%)
14	CLA	Z	835	-	64,68,73	2.32	22 (34%)	76,107,113	2.41	24 (31%)
14	CLA	A	816	-	54,58,73	2.61	22 (40%)	64,95,113	2.72	24 (37%)
14	CLA	A	832	-	69,73,73	2.27	23 (33%)	82,113,113	2.39	25 (30%)
14	CLA	A	827	-	69,73,73	2.25	23 (33%)	82,113,113	2.33	27 (32%)
14	CLA	H	836	-	49,53,73	2.54	23 (46%)	58,89,113	3.04	27 (46%)
14	CLA	F	202	-	49,53,73	2.54	19 (38%)	58,89,113	2.70	25 (43%)
14	CLA	A	833	-	69,73,73	2.27	20 (28%)	82,113,113	2.44	32 (39%)
17	BCR	B	847	-	41,41,41	2.65	6 (14%)	56,56,56	7.15	25 (44%)
14	CLA	A	814	-	54,58,73	2.54	22 (40%)	64,95,113	2.82	27 (42%)
14	CLA	A	836	-	54,58,73	2.62	22 (40%)	64,95,113	2.67	24 (37%)
17	BCR	Z	846	-	41,41,41	2.52	7 (17%)	56,56,56	7.20	22 (39%)
14	CLA	Z	813	-	49,53,73	2.58	22 (44%)	58,89,113	2.94	26 (44%)
14	CLA	H	834	-	64,68,73	2.23	21 (32%)	76,107,113	2.54	27 (35%)
14	CLA	Y	819	-	69,73,73	2.25	22 (31%)	82,113,113	2.51	25 (30%)
14	CLA	H	823	2	59,63,73	2.51	23 (38%)	70,101,113	2.62	27 (38%)
17	BCR	G	849	-	41,41,41	2.60	6 (14%)	56,56,56	7.10	26 (46%)
14	CLA	Z	820	-	59,63,73	2.49	21 (35%)	70,101,113	2.40	28 (40%)
14	CLA	Y	822	-	69,73,73	2.30	22 (31%)	82,113,113	2.52	24 (29%)
17	BCR	H	845	-	41,41,41	2.61	7 (17%)	56,56,56	7.25	26 (46%)
14	CLA	Y	817	-	64,68,73	2.41	23 (35%)	76,107,113	2.36	25 (32%)
14	CLA	T	103	-	49,53,73	2.61	21 (42%)	58,89,113	2.76	20 (34%)
17	BCR	H	841	-	41,41,41	2.78	6 (14%)	56,56,56	7.10	26 (46%)
14	CLA	A	820	-	64,68,73	2.35	24 (37%)	76,107,113	2.54	26 (34%)
14	CLA	d	201	-	54,58,73	2.59	20 (37%)	64,95,113	2.76	27 (42%)
14	CLA	G	853	-	49,53,73	2.60	22 (44%)	58,89,113	2.61	22 (37%)
17	BCR	Z	843	-	41,41,41	2.44	6 (14%)	56,56,56	7.46	29 (51%)
14	CLA	Z	806	-	69,73,73	2.24	21 (30%)	82,113,113	2.53	26 (31%)
16	SF4	a	101	3	0,12,12	-	-	-	-	-
14	CLA	Z	833	-	49,53,73	2.61	19 (38%)	58,89,113	2.65	22 (37%)
14	CLA	L	205	10	69,73,73	2.32	22 (31%)	82,113,113	2.31	25 (30%)
14	CLA	B	829	-	69,73,73	2.21	21 (30%)	82,113,113	2.46	25 (30%)
14	CLA	G	841	-	69,73,73	2.31	22 (31%)	82,113,113	2.39	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	B	845	-	41,41,41	2.55	6 (14%)	56,56,56	7.20	27 (48%)
14	CLA	h	205	10	69,73,73	2.30	21 (30%)	82,113,113	2.49	27 (32%)
14	CLA	H	817	-	64,68,73	2.32	23 (35%)	76,107,113	2.55	26 (34%)
14	CLA	H	802	-	69,73,73	2.25	19 (27%)	82,113,113	2.32	28 (34%)
14	CLA	H	813	-	69,73,73	2.28	20 (28%)	82,113,113	2.40	26 (31%)
14	CLA	A	830	-	69,73,73	2.26	23 (33%)	82,113,113	2.46	26 (31%)
14	CLA	H	812	-	69,73,73	2.28	21 (30%)	82,113,113	2.38	23 (28%)
14	CLA	H	804	-	69,73,73	2.31	21 (30%)	82,113,113	2.40	27 (32%)
14	CLA	A	805	-	69,73,73	2.20	22 (31%)	82,113,113	2.40	25 (30%)
14	CLA	G	820	-	64,68,73	2.37	22 (34%)	76,107,113	2.53	26 (34%)
14	CLA	B	833	-	59,63,73	2.39	23 (38%)	70,101,113	2.73	29 (41%)
14	CLA	Y	809	-	69,73,73	2.26	22 (31%)	82,113,113	2.37	26 (31%)
17	BCR	Q	202	-	41,41,41	2.58	6 (14%)	56,56,56	6.90	27 (48%)
17	BCR	A	846	-	41,41,41	2.47	6 (14%)	56,56,56	7.18	26 (46%)
14	CLA	B	826	-	69,73,73	2.25	21 (30%)	82,113,113	2.46	32 (39%)
14	CLA	G	803	-	69,73,73	2.23	20 (28%)	82,113,113	2.43	31 (37%)
14	CLA	G	814	-	54,58,73	2.56	21 (38%)	64,95,113	3.12	33 (51%)
14	CLA	G	816	-	54,58,73	2.58	22 (40%)	64,95,113	2.75	25 (39%)
14	CLA	A	809	1	69,73,73	2.24	21 (30%)	82,113,113	2.54	25 (30%)
14	CLA	G	817	-	64,68,73	2.41	22 (34%)	76,107,113	2.43	29 (38%)
14	CLA	B	812	-	54,58,73	2.56	22 (40%)	64,95,113	2.75	27 (42%)
14	CLA	Y	823	-	54,58,73	2.61	22 (40%)	64,95,113	2.62	27 (42%)
14	CLA	B	811	-	59,63,73	2.41	21 (35%)	70,101,113	2.60	29 (41%)
14	CLA	B	839	-	49,53,73	2.60	20 (40%)	58,89,113	2.68	22 (37%)
14	CLA	S	1102	8	49,53,73	2.53	20 (40%)	58,89,113	2.66	21 (36%)
14	CLA	G	842	-	69,73,73	2.21	21 (30%)	82,113,113	2.22	25 (30%)
14	CLA	A	841	-	69,73,73	2.27	21 (30%)	82,113,113	2.37	29 (35%)
14	CLA	B	838	-	69,73,73	2.20	21 (30%)	82,113,113	2.55	28 (34%)
14	CLA	H	821	-	59,63,73	2.49	24 (40%)	70,101,113	2.65	25 (35%)
14	CLA	Y	832	-	69,73,73	2.24	23 (33%)	82,113,113	2.54	29 (35%)
17	BCR	R	101	-	41,41,41	2.54	6 (14%)	56,56,56	7.63	24 (42%)
18	LHG	G	852	14	31,31,48	1.26	2 (6%)	34,37,54	1.33	4 (11%)
14	CLA	H	830	-	59,63,73	2.42	21 (35%)	70,101,113	2.48	25 (35%)
14	CLA	G	807	-	55,59,73	2.56	22 (40%)	64,96,113	2.83	27 (42%)
14	CLA	G	818	-	69,73,73	2.28	22 (31%)	82,113,113	2.49	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	Y	825	-	69,73,73	2.30	22 (31%)	82,113,113	2.41	24 (29%)
17	BCR	L	209	-	41,41,41	2.56	6 (14%)	56,56,56	7.24	26 (46%)
14	CLA	L	206	-	69,73,73	2.31	20 (28%)	82,113,113	2.41	25 (30%)
14	CLA	G	806	-	69,73,73	2.20	22 (31%)	82,113,113	2.50	24 (29%)
14	CLA	G	830	-	69,73,73	2.25	21 (30%)	82,113,113	2.37	22 (26%)
18	LHG	G	851	-	48,48,48	0.93	2 (4%)	51,54,54	1.12	3 (5%)
14	CLA	A	852	-	69,73,73	2.25	21 (30%)	82,113,113	2.52	28 (34%)
14	CLA	Y	812	-	59,63,73	2.40	20 (33%)	70,101,113	2.63	29 (41%)
14	CLA	Y	808	1	69,73,73	2.25	21 (30%)	82,113,113	2.51	28 (34%)
14	CLA	G	840	-	54,58,73	2.60	19 (35%)	64,95,113	2.52	24 (37%)
14	CLA	K	103	-	49,53,73	2.52	20 (40%)	58,89,113	2.79	23 (39%)
14	CLA	Y	855	-	69,73,73	2.19	20 (28%)	82,113,113	2.33	27 (32%)
17	BCR	Z	844	-	25,25,41	2.25	2 (8%)	33,33,56	8.00	20 (60%)
14	CLA	L	207	-	69,73,73	2.26	23 (33%)	82,113,113	2.39	26 (31%)
14	CLA	Y	816	-	54,58,73	2.50	21 (38%)	64,95,113	2.84	27 (42%)
14	CLA	h	207	-	69,73,73	2.30	22 (31%)	82,113,113	2.44	27 (32%)
17	BCR	H	844	-	41,41,41	2.56	6 (14%)	56,56,56	7.19	29 (51%)
14	CLA	G	831	-	54,58,73	2.49	21 (38%)	64,95,113	2.77	26 (40%)
14	CLA	B	840	-	69,73,73	2.28	23 (33%)	82,113,113	2.38	28 (34%)
14	CLA	Y	833	-	69,73,73	2.27	22 (31%)	82,113,113	2.44	26 (31%)
14	CLA	Y	843	18	54,58,73	2.62	22 (40%)	64,95,113	2.89	28 (43%)
14	CLA	h	206	-	69,73,73	2.29	22 (31%)	82,113,113	2.71	28 (34%)
14	CLA	A	811	14	69,73,73	2.25	22 (31%)	82,113,113	2.32	23 (28%)
17	BCR	M	101	-	41,41,41	2.63	6 (14%)	56,56,56	7.28	26 (46%)
14	CLA	A	808	1	69,73,73	2.25	21 (30%)	82,113,113	2.54	25 (30%)
14	CLA	B	805	-	58,62,73	2.47	24 (41%)	68,99,113	2.80	26 (38%)
14	CLA	L	201	-	69,73,73	2.23	20 (28%)	82,113,113	2.56	31 (37%)
17	BCR	S	1104	-	41,41,41	2.66	6 (14%)	56,56,56	7.35	28 (50%)
14	CLA	B	821	-	49,53,73	2.55	21 (42%)	58,89,113	2.87	25 (43%)
14	CLA	G	812	-	58,62,73	2.50	21 (36%)	68,99,113	2.53	23 (33%)
14	CLA	B	802	-	69,73,73	2.21	21 (30%)	82,113,113	2.42	28 (34%)
14	CLA	Y	839	-	54,58,73	2.57	23 (42%)	64,95,113	2.87	27 (42%)
14	CLA	h	201	-	69,73,73	2.24	22 (31%)	82,113,113	2.32	26 (31%)
14	CLA	B	819	-	64,68,73	2.34	24 (37%)	76,107,113	2.49	30 (39%)
14	CLA	Y	827	-	69,73,73	2.33	23 (33%)	82,113,113	2.48	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	Z	815	-	69,73,73	2.22	23 (33%)	82,113,113	2.48	25 (30%)
14	CLA	H	815	-	59,63,73	2.43	21 (35%)	70,101,113	2.74	26 (37%)
14	CLA	Y	813	-	64,68,73	2.32	23 (35%)	76,107,113	2.40	26 (34%)
17	BCR	U	1005	-	41,41,41	2.55	7 (17%)	56,56,56	7.04	21 (37%)
18	LHG	B	850	-	38,38,48	1.10	2 (5%)	41,44,54	1.30	4 (9%)
15	PQN	Y	844	-	34,34,34	1.85	2 (5%)	43,45,45	0.84	1 (2%)
14	CLA	Z	802	-	69,73,73	2.25	21 (30%)	82,113,113	2.41	27 (32%)
14	CLA	A	802	-	69,73,73	2.22	22 (31%)	82,113,113	2.57	34 (41%)
14	CLA	Z	837	-	49,53,73	2.55	21 (42%)	58,89,113	2.96	24 (41%)
17	BCR	J	103	-	41,41,41	2.45	6 (14%)	56,56,56	7.02	29 (51%)
17	BCR	Z	845	-	41,41,41	2.47	8 (19%)	56,56,56	7.41	29 (51%)
14	CLA	Y	836	1	49,53,73	2.57	20 (40%)	58,89,113	2.83	24 (41%)
14	CLA	B	809	-	69,73,73	2.22	20 (28%)	82,113,113	2.56	26 (31%)
14	CLA	f	102	-	59,63,73	2.49	21 (35%)	70,101,113	2.62	29 (41%)
14	CLA	B	815	-	49,53,73	2.50	19 (38%)	58,89,113	2.80	27 (46%)
14	CLA	G	826	-	64,68,73	2.31	22 (34%)	76,107,113	2.63	26 (34%)
17	BCR	B	848	-	41,41,41	2.58	7 (17%)	56,56,56	7.02	29 (51%)
14	CLA	B	841	-	69,73,73	2.18	21 (30%)	82,113,113	2.73	32 (39%)
14	CLA	A	822	-	69,73,73	2.29	22 (31%)	82,113,113	2.63	26 (31%)
17	BCR	Y	856	-	41,41,41	2.57	7 (17%)	56,56,56	7.14	32 (57%)
17	BCR	Y	846	-	41,41,41	2.38	6 (14%)	56,56,56	7.33	23 (41%)
16	SF4	C	101	21,3	0,12,12	-	-	-	-	-
14	CLA	G	811	-	69,73,73	2.31	21 (30%)	82,113,113	2.34	23 (28%)
14	CLA	Z	804	-	69,73,73	2.21	22 (31%)	82,113,113	2.52	30 (36%)
14	CLA	G	839	-	69,73,73	2.26	23 (33%)	82,113,113	2.56	30 (36%)
14	CLA	B	822	-	59,63,73	2.47	21 (35%)	70,101,113	2.61	28 (40%)
14	CLA	B	832	-	69,73,73	2.19	21 (30%)	82,113,113	2.56	23 (28%)
13	CL0	Y	801	-	58,73,73	3.18	16 (27%)	60,113,113	2.70	15 (25%)
14	CLA	H	832	-	49,53,73	2.60	21 (42%)	58,89,113	2.77	23 (39%)
14	CLA	B	835	-	49,53,73	2.59	21 (42%)	58,89,113	2.73	25 (43%)
17	BCR	U	1008	-	41,41,41	2.42	6 (14%)	56,56,56	7.32	27 (48%)
14	CLA	G	835	1	49,53,73	2.55	21 (42%)	58,89,113	2.81	25 (43%)
14	CLA	H	827	-	69,73,73	2.19	23 (33%)	82,113,113	2.54	28 (34%)
14	CLA	H	831	-	49,53,73	2.60	22 (44%)	58,89,113	2.84	23 (39%)
14	CLA	J	102	-	59,63,73	2.52	22 (37%)	70,101,113	2.70	27 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	i	101	-	41,41,41	2.63	7 (17%)	56,56,56	7.75	32 (57%)
17	BCR	H	840	-	41,41,41	2.64	6 (14%)	56,56,56	7.27	21 (37%)
14	CLA	B	810	2	69,73,73	2.28	22 (31%)	82,113,113	2.72	30 (36%)
14	CLA	H	825	-	69,73,73	2.27	23 (33%)	82,113,113	2.38	27 (32%)
18	LHG	H	847	-	36,36,48	1.11	2 (5%)	39,42,54	0.93	3 (7%)
14	CLA	Y	815	-	54,58,73	2.58	21 (38%)	64,95,113	2.88	27 (42%)
14	CLA	Y	805	-	69,73,73	2.17	21 (30%)	82,113,113	2.58	31 (37%)
13	CL0	A	801	-	58,73,73	3.16	18 (31%)	60,113,113	2.66	16 (26%)
14	CLA	Y	820	-	64,68,73	2.30	21 (32%)	76,107,113	2.45	24 (31%)
14	CLA	Y	854	-	69,73,73	2.20	20 (28%)	82,113,113	2.50	29 (35%)
14	CLA	A	807	-	55,59,73	2.51	23 (41%)	64,96,113	2.84	25 (39%)
14	CLA	Z	836	-	69,73,73	2.21	21 (30%)	82,113,113	2.44	26 (31%)
17	BCR	G	850	-	41,41,41	2.52	6 (14%)	56,56,56	7.47	28 (50%)
17	BCR	F	203	-	41,41,41	2.53	7 (17%)	56,56,56	7.26	29 (51%)
14	CLA	H	810	-	59,63,73	2.37	22 (37%)	70,101,113	2.65	22 (31%)
14	CLA	H	829	-	49,53,73	2.52	20 (40%)	58,89,113	2.82	24 (41%)
14	CLA	U	1003	-	69,73,73	2.28	22 (31%)	82,113,113	2.40	23 (28%)
14	CLA	G	802	-	69,73,73	2.25	21 (30%)	82,113,113	2.47	25 (30%)
18	LHG	Y	853	14	24,24,48	1.53	2 (8%)	27,30,54	1.65	4 (14%)
14	CLA	B	825	-	69,73,73	2.30	21 (30%)	82,113,113	2.55	28 (34%)
14	CLA	g	102	-	49,53,73	2.58	20 (40%)	58,89,113	2.74	24 (41%)
17	BCR	Q	204	-	41,41,41	2.55	7 (17%)	56,56,56	7.27	28 (50%)
14	CLA	A	810	-	49,53,73	2.57	21 (42%)	58,89,113	2.71	22 (37%)
14	CLA	A	829	-	69,73,73	2.23	22 (31%)	82,113,113	2.19	25 (30%)
14	CLA	H	818	-	64,68,73	2.40	22 (34%)	76,107,113	2.49	26 (34%)
14	CLA	H	805	-	69,73,73	2.26	20 (28%)	82,113,113	2.38	26 (31%)
17	BCR	A	849	-	41,41,41	2.51	6 (14%)	56,56,56	7.51	26 (46%)
14	CLA	Y	841	-	69,73,73	2.24	22 (31%)	82,113,113	2.31	21 (25%)
14	CLA	S	1101	-	69,73,73	2.24	21 (30%)	82,113,113	2.54	25 (30%)
14	CLA	H	833	-	49,53,73	2.54	20 (40%)	58,89,113	2.73	25 (43%)
14	CLA	H	803	-	69,73,73	2.20	22 (31%)	82,113,113	2.48	26 (31%)
14	CLA	Y	834	-	69,73,73	2.22	22 (31%)	82,113,113	2.45	32 (39%)
14	CLA	G	828	-	69,73,73	2.20	20 (28%)	82,113,113	2.42	29 (35%)
14	CLA	A	824	-	64,68,73	2.38	23 (35%)	76,107,113	2.48	29 (38%)
16	SF4	N	102	21,3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	Y	848	-	41,41,41	2.43	6 (14%)	56,56,56	7.36	29 (51%)
18	LHG	j	101	-	27,27,48	1.28	2 (7%)	30,33,54	1.38	4 (13%)
14	CLA	Y	837	-	54,58,73	2.54	22 (40%)	64,95,113	2.74	25 (39%)
14	CLA	H	811	-	49,53,73	2.56	21 (42%)	58,89,113	2.71	25 (43%)
14	CLA	B	827	-	69,73,73	2.23	22 (31%)	82,113,113	2.47	28 (34%)
17	BCR	B	843	-	30,30,41	3.16	6 (20%)	39,39,56	8.30	18 (46%)
14	CLA	B	831	-	49,53,73	2.57	21 (42%)	58,89,113	2.81	25 (43%)
14	CLA	G	819	-	69,73,73	2.28	22 (31%)	82,113,113	2.53	27 (32%)
14	CLA	Z	834	-	49,53,73	2.58	23 (46%)	58,89,113	2.94	26 (44%)
14	CLA	G	808	1	69,73,73	2.25	22 (31%)	82,113,113	2.54	27 (32%)
14	CLA	Y	824	-	64,68,73	2.39	23 (35%)	76,107,113	2.51	25 (32%)
14	CLA	A	823	-	54,58,73	2.57	22 (40%)	64,95,113	2.78	27 (42%)
17	BCR	H	848	-	41,41,41	2.58	6 (14%)	56,56,56	7.19	28 (50%)
14	CLA	X	1701	-	49,53,73	2.59	22 (44%)	58,89,113	2.79	23 (39%)
14	CLA	A	838	-	54,58,73	2.44	21 (38%)	64,95,113	2.76	23 (35%)
17	BCR	U	1007	-	41,41,41	2.63	6 (14%)	56,56,56	7.26	21 (37%)
14	CLA	A	818	-	69,73,73	2.28	23 (33%)	82,113,113	2.51	29 (35%)
14	CLA	B	823	-	64,68,73	2.39	22 (34%)	76,107,113	2.36	23 (30%)
17	BCR	h	202	-	41,41,41	2.38	8 (19%)	56,56,56	7.44	28 (50%)
16	SF4	A	844	1,2	0,12,12	-	-	-	-	-
14	CLA	G	809	-	69,73,73	2.20	22 (31%)	82,113,113	2.46	28 (34%)
14	CLA	A	839	-	54,58,73	2.57	22 (40%)	64,95,113	2.57	25 (39%)
17	BCR	L	208	-	41,41,41	2.80	6 (14%)	56,56,56	7.06	24 (42%)
17	BCR	I	101	-	41,41,41	2.45	7 (17%)	56,56,56	7.45	26 (46%)
17	BCR	B	851	-	41,41,41	2.58	6 (14%)	56,56,56	7.22	28 (50%)
14	CLA	A	828	-	69,73,73	2.24	22 (31%)	82,113,113	2.38	25 (30%)
14	CLA	B	807	-	69,73,73	2.21	22 (31%)	82,113,113	2.42	28 (34%)
18	LHG	A	851	14	31,31,48	1.19	2 (6%)	34,37,54	1.22	4 (11%)
14	CLA	G	823	-	54,58,73	2.53	21 (38%)	64,95,113	2.81	27 (42%)
14	CLA	B	818	-	64,68,73	2.30	23 (35%)	76,107,113	2.51	27 (35%)
14	CLA	V	1201	-	58,62,73	2.49	20 (34%)	68,99,113	2.60	24 (35%)
14	CLA	Y	828	-	69,73,73	2.18	22 (31%)	82,113,113	2.31	27 (32%)
17	BCR	Z	841	-	41,41,41	2.70	6 (14%)	56,56,56	7.28	26 (46%)
17	BCR	f	103	-	41,41,41	2.41	6 (14%)	56,56,56	7.33	28 (50%)
14	CLA	J	101	8	49,53,73	2.57	19 (38%)	58,89,113	2.78	23 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	A	847	-	41,41,41	2.53	6 (14%)	56,56,56	7.24	26 (46%)
14	CLA	G	825	-	69,73,73	2.22	21 (30%)	82,113,113	2.45	28 (34%)
14	CLA	H	808	2	69,73,73	2.19	21 (30%)	82,113,113	2.51	27 (32%)
14	CLA	G	832	-	69,73,73	2.21	20 (28%)	82,113,113	2.41	27 (32%)
14	CLA	Z	839	-	69,73,73	2.31	23 (33%)	82,113,113	2.56	26 (31%)
14	CLA	A	831	-	54,58,73	2.50	21 (38%)	64,95,113	2.69	26 (40%)
14	CLA	Z	818	-	49,53,73	2.57	20 (40%)	58,89,113	2.83	29 (50%)
14	CLA	H	824	-	69,73,73	2.25	24 (34%)	82,113,113	2.78	34 (41%)
14	CLA	U	1004	-	69,73,73	2.21	21 (30%)	82,113,113	2.50	21 (25%)
17	BCR	R	102	-	41,41,41	2.75	6 (14%)	56,56,56	7.07	23 (41%)
14	CLA	G	810	-	49,53,73	2.56	22 (44%)	58,89,113	2.83	25 (43%)
14	CLA	G	829	-	69,73,73	2.26	21 (30%)	82,113,113	2.31	29 (35%)
18	LHG	Y	852	-	48,48,48	1.01	2 (4%)	51,54,54	1.01	2 (3%)
17	BCR	B	846	-	25,25,41	2.15	2 (8%)	33,33,56	8.09	15 (45%)
14	CLA	A	835	1	49,53,73	2.58	22 (44%)	58,89,113	2.79	26 (44%)
14	CLA	B	808	-	69,73,73	2.21	21 (30%)	82,113,113	2.45	29 (35%)
17	BCR	G	847	-	41,41,41	2.59	6 (14%)	56,56,56	7.12	26 (46%)
14	CLA	Z	829	-	49,53,73	2.58	23 (46%)	58,89,113	2.94	28 (48%)
14	CLA	H	801	-	69,73,73	2.30	21 (30%)	82,113,113	2.57	27 (32%)
16	SF4	Y	845	1,2	0,12,12	-	-	-	-	-
14	CLA	Z	827	-	69,73,73	2.19	21 (30%)	82,113,113	2.57	25 (30%)
14	CLA	Z	831	-	59,63,73	2.38	20 (33%)	70,101,113	2.57	29 (41%)
14	CLA	Q	203	-	49,53,73	2.50	21 (42%)	58,89,113	2.77	22 (37%)
14	CLA	K	101	-	45,49,73	2.58	19 (42%)	54,83,113	2.81	25 (46%)
14	CLA	B	836	-	49,53,73	2.55	21 (42%)	58,89,113	2.94	27 (46%)
14	CLA	H	816	-	69,73,73	2.21	23 (33%)	82,113,113	2.62	31 (37%)
15	PQN	Z	840	-	34,34,34	1.69	2 (5%)	43,45,45	1.12	5 (11%)
14	CLA	f	101	8	49,53,73	2.61	23 (46%)	58,89,113	2.75	23 (39%)
14	CLA	Z	828	-	49,53,73	2.50	21 (42%)	58,89,113	2.72	25 (43%)
17	BCR	F	201	-	41,41,41	2.58	6 (14%)	56,56,56	7.03	22 (39%)
14	CLA	Z	814	-	59,63,73	2.45	21 (35%)	70,101,113	2.72	27 (38%)
17	BCR	J	104	-	41,41,41	2.68	6 (14%)	56,56,56	7.22	27 (48%)
18	LHG	A	850	-	48,48,48	1.00	2 (4%)	51,54,54	1.06	3 (5%)
14	CLA	H	809	2	69,73,73	2.22	21 (30%)	82,113,113	2.55	29 (35%)
14	CLA	A	803	-	69,73,73	2.26	23 (33%)	82,113,113	2.58	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	SF4	N	101	3	0,12,12	-	-	-		
14	CLA	B	834	-	49,53,73	2.62	23 (46%)	58,89,113	3.11	27 (46%)
13	CL0	G	801	-	58,73,73	3.23	18 (31%)	60,113,113	2.96	21 (35%)
19	LMG	Z	847	-	49,49,55	1.36	7 (14%)	57,57,63	1.26	5 (8%)
17	BCR	V	1202	-	41,41,41	2.56	7 (17%)	56,56,56	7.42	30 (53%)
17	BCR	Y	851	-	41,41,41	2.72	6 (14%)	56,56,56	7.47	29 (51%)
14	CLA	G	838	-	54,58,73	2.57	22 (40%)	64,95,113	2.76	26 (40%)
15	PQN	B	842	-	34,34,34	1.56	3 (8%)	43,45,45	1.28	7 (16%)
14	CLA	Y	803	-	69,73,73	2.34	21 (30%)	82,113,113	2.47	28 (34%)
14	CLA	Y	814	-	59,63,73	2.49	23 (38%)	70,101,113	2.62	25 (35%)
14	CLA	Y	807	-	55,59,73	2.59	24 (43%)	64,96,113	2.80	25 (39%)
14	CLA	Y	821	-	69,73,73	2.34	22 (31%)	82,113,113	2.26	24 (29%)
14	CLA	A	842	18	54,58,73	2.60	21 (38%)	64,95,113	2.99	24 (37%)
14	CLA	L	202	-	69,73,73	2.21	21 (30%)	82,113,113	2.71	31 (37%)
14	CLA	Y	806	-	69,73,73	2.24	19 (27%)	82,113,113	2.50	26 (31%)
14	CLA	g	101	-	45,49,73	2.57	17 (37%)	54,83,113	2.69	23 (42%)
14	CLA	Y	804	14	63,67,73	2.36	21 (33%)	74,105,113	2.81	27 (36%)
14	CLA	Y	830	-	69,73,73	2.26	20 (28%)	82,113,113	2.55	28 (34%)
14	CLA	A	821	-	69,73,73	2.29	21 (30%)	82,113,113	2.42	24 (29%)
14	CLA	Q	201	-	69,73,73	2.18	21 (30%)	82,113,113	2.57	25 (30%)
14	CLA	Z	805	-	69,73,73	2.27	23 (33%)	82,113,113	2.49	28 (34%)
14	CLA	S	1103	-	59,63,73	2.45	22 (37%)	70,101,113	2.74	27 (38%)
14	CLA	A	812	-	58,62,73	2.49	22 (37%)	68,99,113	2.54	25 (36%)
14	CLA	G	827	-	69,73,73	2.25	20 (28%)	82,113,113	2.27	29 (35%)
17	BCR	A	845	-	41,41,41	2.41	6 (14%)	56,56,56	7.30	28 (50%)
14	CLA	A	837	-	69,73,73	2.24	21 (30%)	82,113,113	2.52	28 (34%)
14	CLA	A	804	14	63,67,73	2.29	21 (33%)	74,105,113	2.72	26 (35%)
14	CLA	A	806	-	69,73,73	2.26	24 (34%)	82,113,113	2.49	26 (31%)
17	BCR	L	203	-	41,41,41	2.71	6 (14%)	56,56,56	7.11	28 (50%)
14	CLA	Y	842	-	69,73,73	2.24	20 (28%)	82,113,113	2.44	26 (31%)
14	CLA	B	824	2	59,63,73	2.44	21 (35%)	70,101,113	2.58	27 (38%)
14	CLA	B	813	-	69,73,73	2.25	22 (31%)	82,113,113	2.57	28 (34%)
16	SF4	G	845	1,2	0,12,12	-	-	-		
17	BCR	f	104	-	41,41,41	2.72	7 (17%)	56,56,56	7.09	28 (50%)
14	CLA	G	833	-	69,73,73	2.26	21 (30%)	82,113,113	2.47	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	Z	803	-	58,62,73	2.45	22 (37%)	68,99,113	2.83	28 (41%)
14	CLA	Z	807	-	69,73,73	2.26	20 (28%)	82,113,113	2.57	28 (34%)
14	CLA	H	807	-	69,73,73	2.31	22 (31%)	82,113,113	2.59	30 (36%)
14	CLA	Z	821	-	64,68,73	2.40	21 (32%)	76,107,113	2.40	28 (36%)
14	CLA	Z	817	-	64,68,73	2.38	22 (34%)	76,107,113	2.36	27 (35%)
15	PQN	A	843	-	34,34,34	1.63	2 (5%)	43,45,45	1.12	4 (9%)
14	CLA	Y	829	-	69,73,73	2.31	22 (31%)	82,113,113	2.32	22 (26%)
14	CLA	H	835	-	69,73,73	2.22	22 (31%)	82,113,113	2.51	25 (30%)
14	CLA	A	817	-	64,68,73	2.32	22 (34%)	76,107,113	2.53	29 (38%)
14	CLA	B	837	-	64,68,73	2.30	22 (34%)	76,107,113	2.56	26 (34%)
14	CLA	B	804	-	69,73,73	2.19	21 (30%)	82,113,113	2.43	26 (31%)
14	CLA	Z	812	-	69,73,73	2.40	21 (30%)	82,113,113	2.27	24 (29%)
14	CLA	Z	830	-	69,73,73	2.19	20 (28%)	82,113,113	2.41	26 (31%)
14	CLA	H	820	-	49,53,73	2.59	22 (44%)	58,89,113	2.92	27 (46%)
16	SF4	C	102	3	0,12,12	-	-	-	-	-
14	CLA	W	1701	-	49,53,73	2.53	22 (44%)	58,89,113	2.75	22 (37%)
16	SF4	a	102	3	0,12,12	-	-	-	-	-
14	CLA	H	837	-	69,73,73	2.29	23 (33%)	82,113,113	2.19	28 (34%)
14	CLA	H	814	-	49,53,73	2.57	22 (44%)	58,89,113	2.93	30 (51%)
14	CLA	A	815	-	54,58,73	2.53	22 (40%)	64,95,113	3.01	26 (40%)
14	CLA	H	828	-	69,73,73	2.26	21 (30%)	82,113,113	2.61	28 (34%)
17	BCR	e	101	-	41,41,41	2.56	6 (14%)	56,56,56	7.60	27 (48%)
14	CLA	A	834	-	59,63,73	2.47	23 (38%)	70,101,113	2.53	28 (40%)
14	CLA	H	806	-	69,73,73	2.26	21 (30%)	82,113,113	2.35	23 (28%)
17	BCR	h	203	-	41,41,41	2.77	6 (14%)	56,56,56	7.21	27 (48%)
17	BCR	f	105	-	41,41,41	2.56	6 (14%)	56,56,56	7.20	26 (46%)
17	BCR	Y	849	-	41,41,41	2.56	6 (14%)	56,56,56	7.35	25 (44%)
14	CLA	Y	802	-	69,73,73	2.16	20 (28%)	82,113,113	2.38	27 (32%)
14	CLA	G	821	-	69,73,73	2.28	23 (33%)	82,113,113	2.37	27 (32%)
14	CLA	Y	840	-	69,73,73	2.27	22 (31%)	82,113,113	2.51	25 (30%)
14	CLA	d	202	-	49,53,73	2.58	20 (40%)	58,89,113	2.61	23 (39%)
14	CLA	j	102	-	49,53,73	2.55	20 (40%)	58,89,113	2.74	22 (37%)
14	CLA	A	825	-	69,73,73	2.28	22 (31%)	82,113,113	2.57	27 (32%)
17	BCR	G	846	-	41,41,41	2.61	6 (14%)	56,56,56	7.40	29 (51%)
14	CLA	B	801	-	69,73,73	2.17	20 (28%)	82,113,113	2.48	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	840	-	69,73,73	2.29	23 (33%)	82,113,113	2.38	24 (29%)
17	BCR	Z	842	-	41,41,41	2.54	7 (17%)	56,56,56	7.19	27 (48%)
14	CLA	B	816	-	59,63,73	2.46	21 (35%)	70,101,113	2.50	25 (35%)
17	BCR	H	842	-	41,41,41	2.56	6 (14%)	56,56,56	7.28	24 (42%)
14	CLA	Z	819	-	49,53,73	2.58	20 (40%)	58,89,113	2.90	25 (43%)
17	BCR	H	843	-	25,25,41	2.01	2 (8%)	33,33,56	8.21	17 (51%)
14	CLA	Z	801	-	69,73,73	2.22	21 (30%)	82,113,113	2.39	25 (30%)
15	PQN	G	844	-	34,34,34	1.56	2 (5%)	43,45,45	1.27	6 (13%)
14	CLA	Z	808	2	69,73,73	2.20	20 (28%)	82,113,113	2.35	23 (28%)
17	BCR	T	102	-	41,41,41	2.35	6 (14%)	56,56,56	7.54	23 (41%)
14	CLA	Z	822	2	59,63,73	2.43	22 (37%)	70,101,113	2.69	30 (42%)
14	CLA	Y	811	14	69,73,73	2.30	20 (28%)	82,113,113	2.41	25 (30%)
17	BCR	A	848	-	41,41,41	2.41	6 (14%)	56,56,56	7.21	22 (39%)
17	BCR	Y	850	-	41,41,41	2.53	6 (14%)	56,56,56	7.26	25 (44%)
14	CLA	Y	810	-	49,53,73	2.53	22 (44%)	58,89,113	2.81	21 (36%)
14	CLA	Z	824	-	69,73,73	2.22	21 (30%)	82,113,113	2.35	28 (34%)
14	CLA	H	826	-	69,73,73	2.21	20 (28%)	82,113,113	2.47	28 (34%)
14	CLA	G	836	-	54,58,73	2.58	22 (40%)	64,95,113	2.70	24 (37%)
14	CLA	Y	818	-	69,73,73	2.31	22 (31%)	82,113,113	2.60	29 (35%)
14	CLA	Y	838	-	69,73,73	2.26	20 (28%)	82,113,113	2.45	26 (31%)
17	BCR	K	102	-	41,41,41	2.58	6 (14%)	56,56,56	7.35	24 (42%)
14	CLA	Z	825	-	69,73,73	2.25	22 (31%)	82,113,113	2.34	25 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	826	-	1/1/14/20	10/33/109/115	-
14	CLA	G	805	-	1/1/15/20	20/39/115/115	-
14	CLA	G	834	-	1/1/13/20	8/27/103/115	-
14	CLA	G	815	-	1/1/12/20	4/21/97/115	-
14	CLA	B	803	-	1/1/15/20	14/39/115/115	-
14	CLA	B	814	-	1/1/15/20	21/39/115/115	-
14	CLA	Z	811	-	1/1/15/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	828	-	1/1/15/20	14/39/115/115	-
14	CLA	Y	826	-	1/1/14/20	9/33/109/115	-
14	CLA	B	817	-	1/1/15/20	11/39/115/115	-
14	CLA	A	819	-	1/1/15/20	14/39/115/115	-
14	CLA	B	806	-	1/1/15/20	15/39/115/115	-
14	CLA	Z	838	-	1/1/15/20	14/39/115/115	-
14	CLA	B	830	-	1/1/11/20	6/15/91/115	-
14	CLA	Z	816	-	1/1/14/20	15/33/109/115	-
14	CLA	H	822	-	1/1/14/20	12/33/109/115	-
14	CLA	U	1002	10	1/1/15/20	23/39/115/115	-
17	BCR	Y	847	-	-	6/29/63/63	0/2/2/2
14	CLA	Z	809	-	1/1/13/20	12/27/103/115	-
14	CLA	G	824	-	1/1/14/20	14/33/109/115	-
14	CLA	G	813	-	1/1/14/20	11/33/109/115	-
14	CLA	U	1006	2	1/1/15/20	14/39/115/115	-
17	BCR	B	844	-	-	8/29/63/63	0/2/2/2
14	CLA	Z	826	-	1/1/15/20	12/39/115/115	-
14	CLA	G	843	18	1/1/12/20	9/21/97/115	-
14	CLA	Y	831	-	1/1/12/20	7/21/97/115	-
14	CLA	Y	835	-	1/1/13/20	9/27/103/115	-
17	BCR	G	854	-	-	8/29/63/63	0/2/2/2
19	LMG	H	846	-	-	10/44/64/70	0/1/1/1
14	CLA	Z	810	-	1/1/11/20	6/15/91/115	-
14	CLA	Z	823	-	1/1/15/20	15/39/115/115	-
14	CLA	B	820	-	1/1/11/20	4/15/91/115	-
17	BCR	G	848	-	-	8/29/63/63	0/2/2/2
14	CLA	A	813	-	1/1/14/20	10/33/109/115	-
14	CLA	G	837	-	1/1/15/20	19/39/115/115	-
14	CLA	G	804	-	1/1/13/20	12/32/108/115	-
14	CLA	T	101	-	1/1/9/20	9/9/81/115	-
15	PQN	H	839	-	-	8/23/43/43	0/2/2/2
17	BCR	d	203	-	-	10/29/63/63	0/2/2/2
14	CLA	G	822	-	1/1/15/20	11/39/115/115	-
14	CLA	Z	832	-	1/1/11/20	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	819	-	1/1/11/20	11/15/91/115	-
14	CLA	H	838	-	1/1/15/20	15/39/115/115	-
19	LMG	B	849	-	-	14/47/67/70	0/1/1/1
14	CLA	Z	835	-	1/1/14/20	10/33/109/115	-
14	CLA	A	816	-	1/1/12/20	9/21/97/115	-
14	CLA	A	832	-	1/1/15/20	15/39/115/115	-
14	CLA	A	827	-	1/1/15/20	14/39/115/115	-
14	CLA	H	836	-	1/1/11/20	1/15/91/115	-
14	CLA	F	202	-	1/1/11/20	4/15/91/115	-
14	CLA	A	833	-	1/1/15/20	14/39/115/115	-
17	BCR	B	847	-	-	11/29/63/63	0/2/2/2
14	CLA	A	814	-	1/1/12/20	7/21/97/115	-
14	CLA	A	836	-	1/1/12/20	5/21/97/115	-
17	BCR	Z	846	-	-	10/29/63/63	0/2/2/2
14	CLA	Z	813	-	1/1/11/20	2/15/91/115	-
14	CLA	H	834	-	1/1/14/20	11/33/109/115	-
14	CLA	Y	819	-	1/1/15/20	19/39/115/115	-
14	CLA	H	823	2	1/1/13/20	10/27/103/115	-
17	BCR	G	849	-	-	8/29/63/63	0/2/2/2
14	CLA	Z	820	-	1/1/13/20	10/27/103/115	-
14	CLA	Y	822	-	1/1/15/20	18/39/115/115	-
17	BCR	H	845	-	-	8/29/63/63	0/2/2/2
14	CLA	Y	817	-	1/1/14/20	11/33/109/115	-
14	CLA	T	103	-	1/1/11/20	6/15/91/115	-
17	BCR	H	841	-	-	13/29/63/63	0/2/2/2
14	CLA	A	820	-	1/1/14/20	16/33/109/115	-
14	CLA	d	201	-	1/1/12/20	2/21/97/115	-
14	CLA	G	853	-	1/1/11/20	5/15/91/115	-
17	BCR	Z	843	-	-	7/29/63/63	0/2/2/2
14	CLA	Z	806	-	1/1/15/20	18/39/115/115	-
16	SF4	a	101	3	-	-	0/6/5/5
14	CLA	Z	833	-	1/1/11/20	8/15/91/115	-
14	CLA	L	205	10	1/1/15/20	22/39/115/115	-
14	CLA	B	829	-	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	841	-	1/1/15/20	16/39/115/115	-
17	BCR	B	845	-	-	9/29/63/63	0/2/2/2
14	CLA	h	205	10	1/1/15/20	23/39/115/115	-
14	CLA	H	817	-	1/1/14/20	13/33/109/115	-
14	CLA	H	802	-	1/1/15/20	17/39/115/115	-
14	CLA	H	813	-	1/1/15/20	19/39/115/115	-
14	CLA	A	830	-	1/1/15/20	10/39/115/115	-
14	CLA	H	812	-	1/1/15/20	17/39/115/115	-
14	CLA	H	804	-	1/1/15/20	11/39/115/115	-
14	CLA	A	805	-	1/1/15/20	23/39/115/115	-
14	CLA	G	820	-	1/1/14/20	16/33/109/115	-
14	CLA	B	833	-	1/1/13/20	12/27/103/115	-
14	CLA	Y	809	-	1/1/15/20	18/39/115/115	-
17	BCR	Q	202	-	-	10/29/63/63	0/2/2/2
17	BCR	A	846	-	-	12/29/63/63	0/2/2/2
14	CLA	B	826	-	1/1/15/20	15/39/115/115	-
14	CLA	G	803	-	1/1/15/20	12/39/115/115	-
14	CLA	G	814	-	1/1/12/20	3/21/97/115	-
14	CLA	G	816	-	1/1/12/20	11/21/97/115	-
14	CLA	A	809	1	1/1/15/20	17/39/115/115	-
14	CLA	G	817	-	1/1/14/20	11/33/109/115	-
14	CLA	B	812	-	1/1/12/20	9/21/97/115	-
14	CLA	Y	823	-	1/1/12/20	8/21/97/115	-
14	CLA	B	811	-	1/1/13/20	17/27/103/115	-
14	CLA	B	839	-	1/1/11/20	3/15/91/115	-
14	CLA	S	1102	8	1/1/11/20	7/15/91/115	-
14	CLA	G	842	-	1/1/15/20	19/39/115/115	-
14	CLA	A	841	-	1/1/15/20	11/39/115/115	-
14	CLA	B	838	-	1/1/15/20	15/39/115/115	-
14	CLA	H	821	-	1/1/13/20	9/27/103/115	-
14	CLA	Y	832	-	1/1/15/20	22/39/115/115	-
17	BCR	R	101	-	-	11/29/63/63	0/2/2/2
18	LHG	G	852	14	-	15/36/36/53	-
14	CLA	H	830	-	1/1/13/20	15/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	807	-	1/1/12/20	10/23/99/115	-
14	CLA	G	818	-	1/1/15/20	17/39/115/115	-
14	CLA	Y	825	-	1/1/15/20	14/39/115/115	-
17	BCR	L	209	-	-	9/29/63/63	0/2/2/2
14	CLA	L	206	-	1/1/15/20	14/39/115/115	-
14	CLA	G	806	-	1/1/15/20	18/39/115/115	-
14	CLA	G	830	-	1/1/15/20	14/39/115/115	-
18	LHG	G	851	-	-	27/53/53/53	-
14	CLA	A	852	-	1/1/15/20	13/39/115/115	-
14	CLA	Y	812	-	1/1/13/20	11/27/103/115	-
14	CLA	Y	808	1	1/1/15/20	20/39/115/115	-
14	CLA	G	840	-	1/1/12/20	5/21/97/115	-
14	CLA	K	103	-	1/1/11/20	6/15/91/115	-
14	CLA	Y	855	-	1/1/15/20	11/39/115/115	-
17	BCR	Z	844	-	-	8/18/35/63	0/1/1/2
14	CLA	L	207	-	1/1/15/20	18/39/115/115	-
14	CLA	Y	816	-	1/1/12/20	6/21/97/115	-
14	CLA	h	207	-	1/1/15/20	15/39/115/115	-
17	BCR	H	844	-	-	8/29/63/63	0/2/2/2
14	CLA	G	831	-	1/1/12/20	8/21/97/115	-
14	CLA	B	840	-	1/1/15/20	13/39/115/115	-
14	CLA	Y	833	-	1/1/15/20	15/39/115/115	-
14	CLA	Y	843	18	1/1/12/20	11/21/97/115	-
14	CLA	h	206	-	1/1/15/20	13/39/115/115	-
14	CLA	A	811	14	1/1/15/20	16/39/115/115	-
17	BCR	M	101	-	-	9/29/63/63	0/2/2/2
14	CLA	A	808	1	1/1/15/20	22/39/115/115	-
14	CLA	B	805	-	1/1/12/20	12/26/102/115	-
14	CLA	L	201	-	1/1/15/20	15/39/115/115	-
17	BCR	S	1104	-	-	11/29/63/63	0/2/2/2
14	CLA	B	821	-	1/1/11/20	10/15/91/115	-
14	CLA	G	812	-	1/1/12/20	12/26/102/115	-
14	CLA	B	802	-	1/1/15/20	16/39/115/115	-
14	CLA	Y	839	-	1/1/12/20	9/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	h	201	-	1/1/15/20	12/39/115/115	-
14	CLA	B	819	-	1/1/14/20	19/33/109/115	-
14	CLA	Y	827	-	1/1/15/20	17/39/115/115	-
14	CLA	Z	815	-	1/1/15/20	19/39/115/115	-
14	CLA	H	815	-	1/1/13/20	9/27/103/115	-
14	CLA	Y	813	-	1/1/14/20	9/33/109/115	-
17	BCR	U	1005	-	-	12/29/63/63	0/2/2/2
18	LHG	B	850	-	-	24/43/43/53	-
15	PQN	Y	844	-	-	6/23/43/43	0/2/2/2
14	CLA	Z	802	-	1/1/15/20	18/39/115/115	-
14	CLA	A	802	-	1/1/15/20	11/39/115/115	-
14	CLA	Z	837	-	1/1/11/20	5/15/91/115	-
17	BCR	J	103	-	-	6/29/63/63	0/2/2/2
17	BCR	Z	845	-	-	8/29/63/63	0/2/2/2
14	CLA	Y	836	1	1/1/11/20	4/15/91/115	-
14	CLA	B	809	-	1/1/15/20	22/39/115/115	-
14	CLA	f	102	-	1/1/13/20	15/27/103/115	-
14	CLA	B	815	-	1/1/11/20	2/15/91/115	-
14	CLA	G	826	-	1/1/14/20	16/33/109/115	-
17	BCR	B	848	-	-	3/29/63/63	0/2/2/2
14	CLA	B	841	-	1/1/15/20	20/39/115/115	-
14	CLA	A	822	-	1/1/15/20	15/39/115/115	-
17	BCR	Y	856	-	-	10/29/63/63	0/2/2/2
17	BCR	Y	846	-	-	9/29/63/63	0/2/2/2
16	SF4	C	101	21,3	-	-	0/6/5/5
14	CLA	G	811	-	1/1/15/20	17/39/115/115	-
14	CLA	Z	804	-	1/1/15/20	14/39/115/115	-
14	CLA	G	839	-	1/1/15/20	15/39/115/115	-
14	CLA	B	822	-	1/1/13/20	9/27/103/115	-
14	CLA	B	832	-	1/1/15/20	20/39/115/115	-
13	CL0	Y	801	-	3/3/20/25	13/37/135/135	-
14	CLA	H	832	-	1/1/11/20	6/15/91/115	-
14	CLA	B	835	-	1/1/11/20	2/15/91/115	-
17	BCR	U	1008	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	835	1	1/1/11/20	6/15/91/115	-
14	CLA	H	827	-	1/1/15/20	14/39/115/115	-
14	CLA	H	831	-	1/1/11/20	8/15/91/115	-
14	CLA	J	102	-	1/1/13/20	14/27/103/115	-
17	BCR	i	101	-	-	9/29/63/63	0/2/2/2
17	BCR	H	840	-	-	8/29/63/63	0/2/2/2
14	CLA	B	810	2	1/1/15/20	13/39/115/115	-
14	CLA	H	825	-	1/1/15/20	10/39/115/115	-
18	LHG	H	847	-	-	17/41/41/53	-
14	CLA	Y	815	-	1/1/12/20	8/21/97/115	-
14	CLA	Y	805	-	1/1/15/20	14/39/115/115	-
13	CL0	A	801	-	3/3/20/25	16/37/135/135	-
14	CLA	Y	820	-	1/1/14/20	11/33/109/115	-
14	CLA	Y	854	-	1/1/15/20	16/39/115/115	-
14	CLA	A	807	-	1/1/12/20	7/23/99/115	-
14	CLA	Z	836	-	1/1/15/20	10/39/115/115	-
17	BCR	G	850	-	-	9/29/63/63	0/2/2/2
17	BCR	F	203	-	-	6/29/63/63	0/2/2/2
14	CLA	H	810	-	1/1/13/20	13/27/103/115	-
14	CLA	H	829	-	1/1/11/20	8/15/91/115	-
14	CLA	U	1003	-	1/1/15/20	13/39/115/115	-
14	CLA	G	802	-	1/1/15/20	18/39/115/115	-
18	LHG	Y	853	14	-	20/28/28/53	-
14	CLA	B	825	-	1/1/15/20	14/39/115/115	-
14	CLA	g	102	-	1/1/11/20	5/15/91/115	-
17	BCR	Q	204	-	-	7/29/63/63	0/2/2/2
14	CLA	A	810	-	1/1/11/20	4/15/91/115	-
14	CLA	A	829	-	1/1/15/20	11/39/115/115	-
14	CLA	H	818	-	1/1/14/20	15/33/109/115	-
14	CLA	H	805	-	1/1/15/20	19/39/115/115	-
17	BCR	A	849	-	-	10/29/63/63	0/2/2/2
14	CLA	Y	841	-	1/1/15/20	14/39/115/115	-
14	CLA	S	1101	-	1/1/15/20	20/39/115/115	-
14	CLA	H	833	-	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	803	-	1/1/15/20	12/39/115/115	-
14	CLA	Y	834	-	1/1/15/20	15/39/115/115	-
14	CLA	G	828	-	1/1/15/20	13/39/115/115	-
14	CLA	A	824	-	1/1/14/20	15/33/109/115	-
16	SF4	N	102	21,3	-	-	0/6/5/5
17	BCR	Y	848	-	-	10/29/63/63	0/2/2/2
18	LHG	j	101	-	-	15/32/32/53	-
14	CLA	Y	837	-	1/1/12/20	5/21/97/115	-
14	CLA	H	811	-	1/1/11/20	7/15/91/115	-
14	CLA	B	827	-	1/1/15/20	16/39/115/115	-
17	BCR	B	843	-	-	3/24/41/63	0/1/1/2
14	CLA	B	831	-	1/1/11/20	7/15/91/115	-
14	CLA	G	819	-	1/1/15/20	15/39/115/115	-
14	CLA	Z	834	-	1/1/11/20	8/15/91/115	-
14	CLA	G	808	1	1/1/15/20	19/39/115/115	-
14	CLA	Y	824	-	1/1/14/20	20/33/109/115	-
14	CLA	A	823	-	1/1/12/20	10/21/97/115	-
17	BCR	H	848	-	-	8/29/63/63	0/2/2/2
14	CLA	X	1701	-	1/1/11/20	5/15/91/115	-
14	CLA	A	838	-	1/1/12/20	7/21/97/115	-
17	BCR	U	1007	-	-	16/29/63/63	0/2/2/2
14	CLA	A	818	-	1/1/15/20	23/39/115/115	-
14	CLA	B	823	-	1/1/14/20	13/33/109/115	-
17	BCR	h	202	-	-	7/29/63/63	0/2/2/2
16	SF4	A	844	1,2	-	-	0/6/5/5
14	CLA	G	809	-	1/1/15/20	14/39/115/115	-
14	CLA	A	839	-	1/1/12/20	2/21/97/115	-
17	BCR	L	208	-	-	11/29/63/63	0/2/2/2
17	BCR	I	101	-	-	7/29/63/63	0/2/2/2
17	BCR	B	851	-	-	7/29/63/63	0/2/2/2
14	CLA	A	828	-	1/1/15/20	14/39/115/115	-
14	CLA	B	807	-	1/1/15/20	18/39/115/115	-
18	LHG	A	851	14	-	16/36/36/53	-
14	CLA	G	823	-	1/1/12/20	6/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	818	-	1/1/14/20	10/33/109/115	-
14	CLA	V	1201	-	1/1/12/20	9/26/102/115	-
14	CLA	Y	828	-	1/1/15/20	14/39/115/115	-
17	BCR	Z	841	-	-	14/29/63/63	0/2/2/2
17	BCR	f	103	-	-	8/29/63/63	0/2/2/2
14	CLA	J	101	8	1/1/11/20	5/15/91/115	-
17	BCR	A	847	-	-	4/29/63/63	0/2/2/2
14	CLA	G	825	-	1/1/15/20	17/39/115/115	-
14	CLA	H	808	2	1/1/15/20	9/39/115/115	-
14	CLA	G	832	-	1/1/15/20	16/39/115/115	-
14	CLA	Z	839	-	1/1/15/20	17/39/115/115	-
14	CLA	A	831	-	1/1/12/20	7/21/97/115	-
14	CLA	Z	818	-	1/1/11/20	7/15/91/115	-
14	CLA	H	824	-	1/1/15/20	21/39/115/115	-
14	CLA	U	1004	-	1/1/15/20	19/39/115/115	-
17	BCR	R	102	-	-	10/29/63/63	0/2/2/2
14	CLA	G	810	-	1/1/11/20	6/15/91/115	-
14	CLA	G	829	-	1/1/15/20	17/39/115/115	-
18	LHG	Y	852	-	-	26/53/53/53	-
17	BCR	B	846	-	-	3/18/35/63	0/1/1/2
14	CLA	A	835	1	1/1/11/20	3/15/91/115	-
14	CLA	B	808	-	1/1/15/20	12/39/115/115	-
17	BCR	G	847	-	-	9/29/63/63	0/2/2/2
14	CLA	Z	829	-	1/1/11/20	11/15/91/115	-
14	CLA	H	801	-	1/1/15/20	16/39/115/115	-
16	SF4	Y	845	1,2	-	-	0/6/5/5
14	CLA	Z	827	-	1/1/15/20	13/39/115/115	-
14	CLA	Z	831	-	1/1/13/20	14/27/103/115	-
14	CLA	Q	203	-	1/1/11/20	2/15/91/115	-
14	CLA	K	101	-	1/1/9/20	7/9/81/115	-
14	CLA	B	836	-	1/1/11/20	6/15/91/115	-
14	CLA	H	816	-	1/1/15/20	12/39/115/115	-
15	PQN	Z	840	-	-	10/23/43/43	0/2/2/2
14	CLA	f	101	8	1/1/11/20	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	Z	828	-	1/1/11/20	7/15/91/115	-
17	BCR	F	201	-	-	13/29/63/63	0/2/2/2
14	CLA	Z	814	-	1/1/13/20	10/27/103/115	-
17	BCR	J	104	-	-	13/29/63/63	0/2/2/2
18	LHG	A	850	-	-	27/53/53/53	-
14	CLA	H	809	2	1/1/15/20	17/39/115/115	-
14	CLA	A	803	-	1/1/15/20	19/39/115/115	-
16	SF4	N	101	3	-	-	0/6/5/5
14	CLA	B	834	-	1/1/11/20	2/15/91/115	-
13	CL0	G	801	-	3/3/20/25	13/37/135/135	-
19	LMG	Z	847	-	-	15/44/64/70	0/1/1/1
17	BCR	V	1202	-	-	8/29/63/63	0/2/2/2
17	BCR	Y	851	-	-	10/29/63/63	0/2/2/2
14	CLA	G	838	-	1/1/12/20	2/21/97/115	-
15	PQN	B	842	-	-	12/23/43/43	0/2/2/2
14	CLA	Y	803	-	1/1/15/20	17/39/115/115	-
14	CLA	Y	814	-	1/1/13/20	11/27/103/115	-
14	CLA	Y	807	-	1/1/12/20	10/23/99/115	-
14	CLA	Y	821	-	1/1/15/20	16/39/115/115	-
14	CLA	A	842	18	1/1/12/20	10/21/97/115	-
14	CLA	L	202	-	1/1/15/20	17/39/115/115	-
14	CLA	Y	806	-	1/1/15/20	14/39/115/115	-
14	CLA	g	101	-	1/1/9/20	5/9/81/115	-
14	CLA	Y	804	14	1/1/13/20	15/32/108/115	-
14	CLA	Y	830	-	1/1/15/20	10/39/115/115	-
14	CLA	A	821	-	1/1/15/20	14/39/115/115	-
14	CLA	Q	201	-	1/1/15/20	20/39/115/115	-
14	CLA	Z	805	-	1/1/15/20	18/39/115/115	-
14	CLA	S	1103	-	1/1/13/20	17/27/103/115	-
14	CLA	A	812	-	1/1/12/20	9/26/102/115	-
14	CLA	G	827	-	1/1/15/20	18/39/115/115	-
17	BCR	A	845	-	-	11/29/63/63	0/2/2/2
14	CLA	A	837	-	1/1/15/20	16/39/115/115	-
14	CLA	A	804	14	1/1/13/20	14/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	806	-	1/1/15/20	17/39/115/115	-
17	BCR	L	203	-	-	13/29/63/63	0/2/2/2
14	CLA	Y	842	-	1/1/15/20	15/39/115/115	-
14	CLA	B	824	2	1/1/13/20	10/27/103/115	-
14	CLA	B	813	-	1/1/15/20	19/39/115/115	-
16	SF4	G	845	1,2	-	-	0/6/5/5
17	BCR	f	104	-	-	6/29/63/63	0/2/2/2
14	CLA	G	833	-	1/1/15/20	17/39/115/115	-
14	CLA	Z	803	-	1/1/12/20	9/26/102/115	-
14	CLA	Z	807	-	1/1/15/20	13/39/115/115	-
14	CLA	H	807	-	1/1/15/20	11/39/115/115	-
14	CLA	Z	821	-	1/1/14/20	11/33/109/115	-
14	CLA	Z	817	-	1/1/14/20	16/33/109/115	-
15	PQN	A	843	-	-	5/23/43/43	0/2/2/2
14	CLA	Y	829	-	1/1/15/20	15/39/115/115	-
14	CLA	H	835	-	1/1/15/20	18/39/115/115	-
14	CLA	A	817	-	1/1/14/20	13/33/109/115	-
14	CLA	B	837	-	1/1/14/20	8/33/109/115	-
14	CLA	B	804	-	1/1/15/20	6/39/115/115	-
14	CLA	Z	812	-	1/1/15/20	10/39/115/115	-
14	CLA	Z	830	-	1/1/15/20	12/39/115/115	-
14	CLA	H	820	-	1/1/11/20	4/15/91/115	-
16	SF4	C	102	3	-	-	0/6/5/5
14	CLA	W	1701	-	1/1/11/20	6/15/91/115	-
16	SF4	a	102	3	-	-	0/6/5/5
14	CLA	H	837	-	1/1/15/20	13/39/115/115	-
14	CLA	H	814	-	1/1/11/20	8/15/91/115	-
14	CLA	A	815	-	1/1/12/20	6/21/97/115	-
14	CLA	H	828	-	1/1/15/20	13/39/115/115	-
17	BCR	e	101	-	-	9/29/63/63	0/2/2/2
14	CLA	A	834	-	1/1/13/20	9/27/103/115	-
14	CLA	H	806	-	1/1/15/20	9/39/115/115	-
17	BCR	h	203	-	-	10/29/63/63	0/2/2/2
17	BCR	f	105	-	-	6/29/63/63	0/2/2/2
17	BCR	Y	849	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	Y	802	-	1/1/15/20	11/39/115/115	-
14	CLA	G	821	-	1/1/15/20	15/39/115/115	-
14	CLA	Y	840	-	1/1/15/20	12/39/115/115	-
14	CLA	d	202	-	1/1/11/20	2/15/91/115	-
14	CLA	j	102	-	1/1/11/20	6/15/91/115	-
14	CLA	A	825	-	1/1/15/20	15/39/115/115	-
17	BCR	G	846	-	-	7/29/63/63	0/2/2/2
14	CLA	B	801	-	1/1/15/20	20/39/115/115	-
14	CLA	A	840	-	1/1/15/20	15/39/115/115	-
17	BCR	Z	842	-	-	6/29/63/63	0/2/2/2
14	CLA	B	816	-	1/1/13/20	8/27/103/115	-
17	BCR	H	842	-	-	8/29/63/63	0/2/2/2
14	CLA	Z	819	-	1/1/11/20	7/15/91/115	-
17	BCR	H	843	-	-	6/18/35/63	0/1/1/2
14	CLA	Z	801	-	1/1/15/20	20/39/115/115	-
15	PQN	G	844	-	-	9/23/43/43	0/2/2/2
14	CLA	Z	808	2	1/1/15/20	14/39/115/115	-
17	BCR	T	102	-	-	9/29/63/63	0/2/2/2
14	CLA	Z	822	2	1/1/13/20	9/27/103/115	-
14	CLA	Y	811	14	1/1/15/20	20/39/115/115	-
17	BCR	A	848	-	-	7/29/63/63	0/2/2/2
17	BCR	Y	850	-	-	7/29/63/63	0/2/2/2
14	CLA	Y	810	-	1/1/11/20	4/15/91/115	-
14	CLA	Z	824	-	1/1/15/20	18/39/115/115	-
14	CLA	H	826	-	1/1/15/20	14/39/115/115	-
14	CLA	G	836	-	1/1/12/20	8/21/97/115	-
14	CLA	Y	818	-	1/1/15/20	16/39/115/115	-
14	CLA	Y	838	-	1/1/15/20	20/39/115/115	-
17	BCR	K	102	-	-	8/29/63/63	0/2/2/2
14	CLA	Z	825	-	1/1/15/20	17/39/115/115	-

The worst 5 of 6557 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Y	801	CL0	C1B-C2B	10.24	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	801	CL0	C1D-C2D	9.78	1.50	1.39
13	A	801	CL0	C1A-CHA	9.77	1.51	1.40
13	G	801	CL0	C1A-CHA	9.33	1.50	1.40
13	Y	801	CL0	C1A-CHA	9.10	1.50	1.40

The worst 5 of 9259 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	i	101	BCR	C16-C17-C18	30.64	170.25	127.28
17	A	845	BCR	C16-C17-C18	29.81	169.09	127.28
17	G	846	BCR	C16-C17-C18	29.27	168.33	127.28
17	R	101	BCR	C16-C17-C18	28.90	167.81	127.28
17	A	849	BCR	C16-C17-C18	28.57	167.35	127.28

5 of 291 chirality outliers are listed below:

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

5 of 4327 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	G	801	CL0	CBD-CGD-O2D-CED
13	Y	801	CL0	C3A-C2A-CAA-CBA
13	Y	801	CL0	CBD-CGD-O2D-CED
14	A	802	CLA	C4B-C3B-CAB-CBB
14	A	803	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

364 monomers are involved in 1864 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	826	CLA	12	0
14	G	805	CLA	10	0
14	G	834	CLA	5	0
14	G	815	CLA	4	0
14	B	803	CLA	19	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	814	CLA	3	0
14	Z	811	CLA	5	0
14	B	828	CLA	8	0
14	Y	826	CLA	6	0
14	B	817	CLA	6	0
14	A	819	CLA	11	0
14	B	806	CLA	6	0
14	Z	838	CLA	5	0
14	B	830	CLA	4	0
14	Z	816	CLA	9	0
14	H	822	CLA	5	0
14	U	1002	CLA	9	0
17	Y	847	BCR	9	0
14	Z	809	CLA	3	0
14	G	824	CLA	9	0
14	G	813	CLA	12	0
14	U	1006	CLA	12	0
17	B	844	BCR	3	0
14	Z	826	CLA	7	0
14	G	843	CLA	2	0
14	Y	831	CLA	5	0
14	Y	835	CLA	2	0
17	G	854	BCR	11	0
19	H	846	LMG	4	0
14	Z	810	CLA	2	0
14	Z	823	CLA	8	0
14	B	820	CLA	3	0
17	G	848	BCR	5	0
14	A	813	CLA	8	0
14	G	837	CLA	6	0
14	G	804	CLA	9	0
14	T	101	CLA	1	0
15	H	839	PQN	4	0
17	d	203	BCR	5	0
14	G	822	CLA	4	0
14	Z	832	CLA	8	0
14	H	819	CLA	4	0
14	H	838	CLA	1	0
19	B	849	LMG	6	0
14	Z	835	CLA	10	0
14	A	832	CLA	3	0
14	A	827	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	836	CLA	10	0
14	F	202	CLA	2	0
14	A	833	CLA	5	0
17	B	847	BCR	15	0
14	A	814	CLA	2	0
14	A	836	CLA	7	0
17	Z	846	BCR	6	0
14	Z	813	CLA	3	0
14	H	834	CLA	6	0
14	Y	819	CLA	13	0
14	H	823	CLA	8	0
17	G	849	BCR	15	0
14	Z	820	CLA	6	0
14	Y	822	CLA	1	0
17	H	845	BCR	10	0
14	Y	817	CLA	3	0
14	T	103	CLA	2	0
17	H	841	BCR	5	0
14	A	820	CLA	4	0
14	d	201	CLA	9	0
14	G	853	CLA	3	0
17	Z	843	BCR	5	0
14	Z	806	CLA	8	0
14	Z	833	CLA	5	0
14	L	205	CLA	5	0
14	B	829	CLA	6	0
14	G	841	CLA	5	0
17	B	845	BCR	7	0
14	h	205	CLA	10	0
14	H	817	CLA	7	0
14	H	802	CLA	17	0
14	H	813	CLA	2	0
14	A	830	CLA	6	0
14	H	812	CLA	6	0
14	H	804	CLA	4	0
14	A	805	CLA	10	0
14	G	820	CLA	5	0
14	B	833	CLA	5	0
14	Y	809	CLA	3	0
17	Q	202	BCR	5	0
17	A	846	BCR	9	0
14	B	826	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	G	803	CLA	13	0
14	G	814	CLA	6	0
14	A	809	CLA	2	0
14	G	817	CLA	6	0
14	Y	823	CLA	2	0
14	B	811	CLA	2	0
14	B	839	CLA	7	0
14	S	1102	CLA	1	0
14	G	842	CLA	7	0
14	A	841	CLA	11	0
14	B	838	CLA	6	0
14	H	821	CLA	8	0
14	Y	832	CLA	6	0
17	R	101	BCR	4	0
18	G	852	LHG	4	0
14	H	830	CLA	7	0
14	G	807	CLA	4	0
14	G	818	CLA	14	0
14	Y	825	CLA	8	0
17	L	209	BCR	8	0
14	L	206	CLA	7	0
14	G	806	CLA	6	0
14	G	830	CLA	8	0
18	G	851	LHG	7	0
14	A	852	CLA	12	0
14	Y	812	CLA	2	0
14	Y	808	CLA	10	0
14	G	840	CLA	2	0
14	K	103	CLA	3	0
14	Y	855	CLA	19	0
17	Z	844	BCR	8	0
14	L	207	CLA	3	0
14	Y	816	CLA	2	0
14	h	207	CLA	4	0
17	H	844	BCR	9	0
14	G	831	CLA	5	0
14	B	840	CLA	7	0
14	Y	833	CLA	8	0
14	Y	843	CLA	4	0
14	h	206	CLA	4	0
14	A	811	CLA	6	0
17	M	101	BCR	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	808	CLA	7	0
14	B	805	CLA	7	0
14	L	201	CLA	5	0
17	S	1104	BCR	9	0
14	B	821	CLA	2	0
14	G	812	CLA	1	0
14	B	802	CLA	7	0
14	Y	839	CLA	4	0
14	h	201	CLA	7	0
14	B	819	CLA	4	0
14	Y	827	CLA	10	0
14	Z	815	CLA	5	0
14	H	815	CLA	1	0
14	Y	813	CLA	4	0
17	U	1005	BCR	3	0
15	Y	844	PQN	5	0
14	Z	802	CLA	9	0
14	A	802	CLA	10	0
14	Z	837	CLA	9	0
17	J	103	BCR	12	0
17	Z	845	BCR	6	0
14	Y	836	CLA	3	0
14	B	809	CLA	8	0
14	f	102	CLA	3	0
14	B	815	CLA	7	0
14	G	826	CLA	5	0
17	B	848	BCR	11	0
14	B	841	CLA	3	0
14	A	822	CLA	8	0
17	Y	856	BCR	6	0
17	Y	846	BCR	9	0
16	C	101	SF4	2	0
14	G	811	CLA	10	0
14	Z	804	CLA	6	0
14	G	839	CLA	9	0
14	B	822	CLA	5	0
14	B	832	CLA	8	0
13	Y	801	CL0	8	0
14	H	832	CLA	5	0
14	B	835	CLA	4	0
17	U	1008	BCR	8	0
14	G	835	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	827	CLA	8	0
14	H	831	CLA	6	0
14	J	102	CLA	1	0
17	i	101	BCR	6	0
17	H	840	BCR	8	0
14	B	810	CLA	11	0
14	H	825	CLA	5	0
18	H	847	LHG	2	0
14	Y	815	CLA	1	0
14	Y	805	CLA	12	0
13	A	801	CL0	10	0
14	Y	820	CLA	4	0
14	Y	854	CLA	10	0
14	A	807	CLA	4	0
14	Z	836	CLA	4	0
17	G	850	BCR	14	0
14	H	810	CLA	4	0
14	H	829	CLA	5	0
14	U	1003	CLA	5	0
14	G	802	CLA	19	0
18	Y	853	LHG	5	0
14	B	825	CLA	9	0
14	g	102	CLA	1	0
17	Q	204	BCR	4	0
14	A	810	CLA	5	0
14	A	829	CLA	12	0
14	H	818	CLA	6	0
14	H	805	CLA	8	0
17	A	849	BCR	11	0
14	Y	841	CLA	10	0
14	S	1101	CLA	7	0
14	H	833	CLA	3	0
14	H	803	CLA	14	0
14	Y	834	CLA	15	0
14	G	828	CLA	13	0
14	A	824	CLA	3	0
16	N	102	SF4	2	0
17	Y	848	BCR	5	0
18	j	101	LHG	2	0
14	Y	837	CLA	4	0
14	H	811	CLA	3	0
14	B	827	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	843	BCR	2	0
14	B	831	CLA	3	0
14	G	819	CLA	14	0
14	Z	834	CLA	3	0
14	G	808	CLA	10	0
14	Y	824	CLA	5	0
17	H	848	BCR	5	0
14	A	838	CLA	6	0
17	U	1007	BCR	12	0
14	A	818	CLA	5	0
14	B	823	CLA	1	0
17	h	202	BCR	7	0
16	A	844	SF4	1	0
14	G	809	CLA	4	0
14	A	839	CLA	6	0
17	L	208	BCR	6	0
17	I	101	BCR	6	0
17	B	851	BCR	12	0
14	A	828	CLA	16	0
14	B	807	CLA	10	0
18	A	851	LHG	1	0
14	G	823	CLA	2	0
14	B	818	CLA	6	0
14	V	1201	CLA	3	0
14	Y	828	CLA	15	0
17	Z	841	BCR	3	0
17	f	103	BCR	11	0
17	A	847	BCR	3	0
14	G	825	CLA	11	0
14	H	808	CLA	13	0
14	G	832	CLA	2	0
14	Z	839	CLA	3	0
14	A	831	CLA	5	0
14	Z	818	CLA	4	0
14	H	824	CLA	12	0
14	U	1004	CLA	6	0
17	R	102	BCR	9	0
14	G	810	CLA	2	0
14	G	829	CLA	12	0
18	Y	852	LHG	3	0
17	B	846	BCR	2	0
14	A	835	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	808	CLA	5	0
17	G	847	BCR	11	0
14	Z	829	CLA	3	0
14	H	801	CLA	24	0
14	Z	827	CLA	8	0
14	Z	831	CLA	8	0
14	Q	203	CLA	2	0
14	K	101	CLA	1	0
14	B	836	CLA	4	0
14	H	816	CLA	11	0
15	Z	840	PQN	2	0
14	Z	828	CLA	8	0
17	F	201	BCR	9	0
14	Z	814	CLA	1	0
17	J	104	BCR	10	0
18	A	850	LHG	4	0
14	H	809	CLA	11	0
14	A	803	CLA	6	0
16	N	101	SF4	1	0
14	B	834	CLA	3	0
13	G	801	CL0	11	0
19	Z	847	LMG	3	0
17	V	1202	BCR	5	0
17	Y	851	BCR	14	0
14	G	838	CLA	2	0
15	B	842	PQN	9	0
14	Y	803	CLA	8	0
14	Y	814	CLA	1	0
14	Y	807	CLA	1	0
14	Y	821	CLA	13	0
14	L	202	CLA	8	0
14	Y	806	CLA	8	0
14	g	101	CLA	1	0
14	Y	804	CLA	4	0
14	Y	830	CLA	11	0
14	A	821	CLA	7	0
14	Q	201	CLA	9	0
14	Z	805	CLA	6	0
14	S	1103	CLA	3	0
14	A	812	CLA	6	0
14	G	827	CLA	7	0
17	A	845	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	837	CLA	10	0
14	A	804	CLA	6	0
14	A	806	CLA	12	0
17	L	203	BCR	7	0
14	Y	842	CLA	11	0
14	B	824	CLA	4	0
14	B	813	CLA	13	0
17	f	104	BCR	16	0
14	G	833	CLA	4	0
14	Z	803	CLA	1	0
14	Z	807	CLA	5	0
14	H	807	CLA	11	0
14	Z	821	CLA	4	0
14	Z	817	CLA	4	0
15	A	843	PQN	6	0
14	Y	829	CLA	9	0
14	H	835	CLA	10	0
14	A	817	CLA	3	0
14	B	837	CLA	6	0
14	B	804	CLA	12	0
14	Z	812	CLA	2	0
14	Z	830	CLA	5	0
14	H	820	CLA	3	0
16	C	102	SF4	3	0
14	W	1701	CLA	4	0
16	a	102	SF4	1	0
14	H	837	CLA	5	0
14	H	814	CLA	5	0
14	A	815	CLA	2	0
14	H	828	CLA	11	0
17	e	101	BCR	5	0
14	A	834	CLA	7	0
14	H	806	CLA	6	0
17	h	203	BCR	3	0
17	f	105	BCR	7	0
17	Y	849	BCR	7	0
14	Y	802	CLA	8	0
14	G	821	CLA	11	0
14	Y	840	CLA	6	0
14	d	202	CLA	2	0
14	j	102	CLA	2	0
14	A	825	CLA	5	0

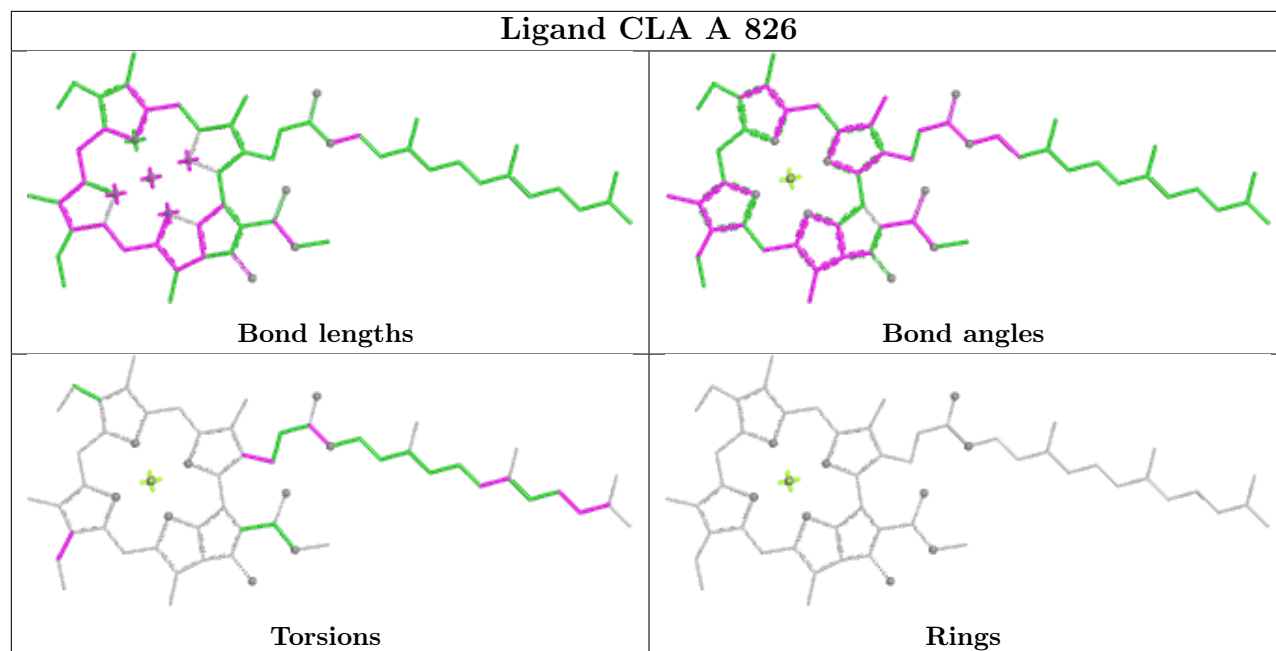
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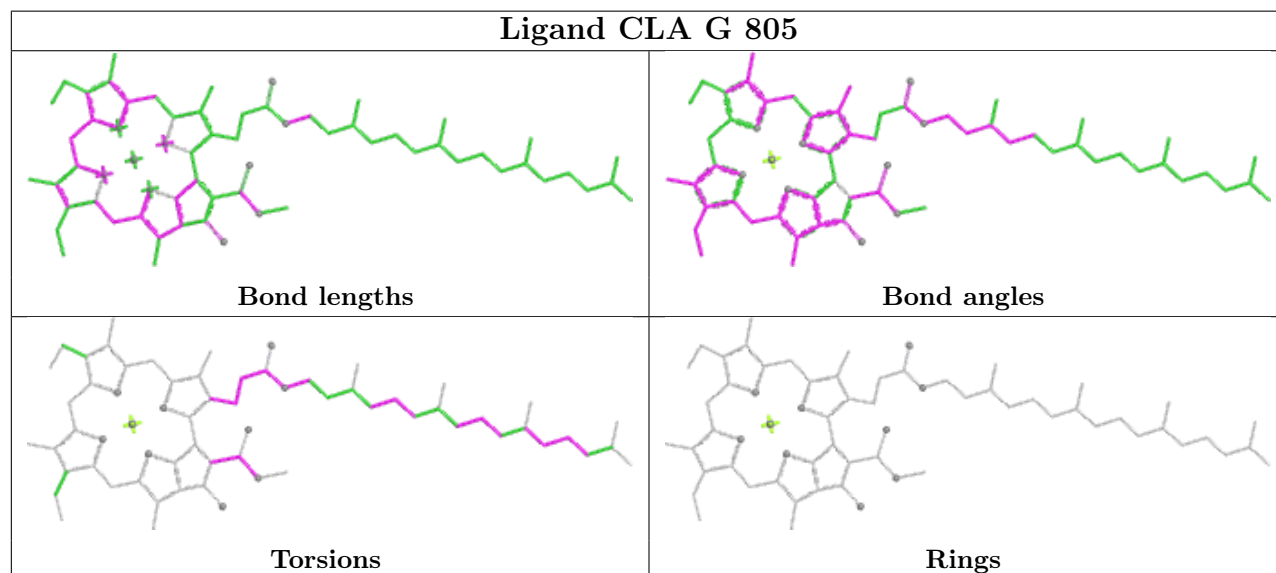
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	G	846	BCR	5	0
14	B	801	CLA	11	0
14	A	840	CLA	16	0
17	Z	842	BCR	4	0
17	H	842	BCR	5	0
14	Z	819	CLA	3	0
17	H	843	BCR	5	0
14	Z	801	CLA	18	0
15	G	844	PQN	3	0
14	Z	808	CLA	12	0
17	T	102	BCR	8	0
14	Z	822	CLA	6	0
14	Y	811	CLA	8	0
17	A	848	BCR	8	0
17	Y	850	BCR	10	0
14	Y	810	CLA	4	0
14	Z	824	CLA	6	0
14	H	826	CLA	9	0
14	G	836	CLA	3	0
14	Y	818	CLA	4	0
14	Y	838	CLA	6	0
17	K	102	BCR	3	0
14	Z	825	CLA	12	0

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

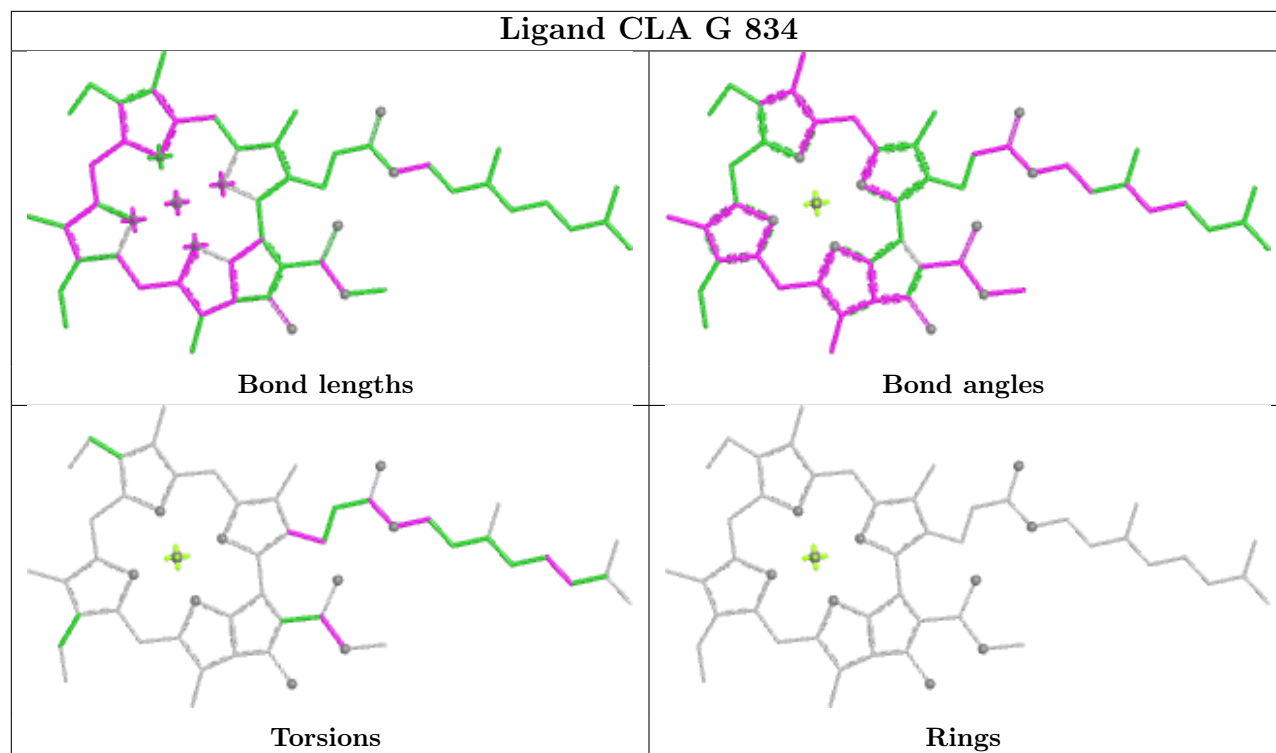
Ligand CLA A 826



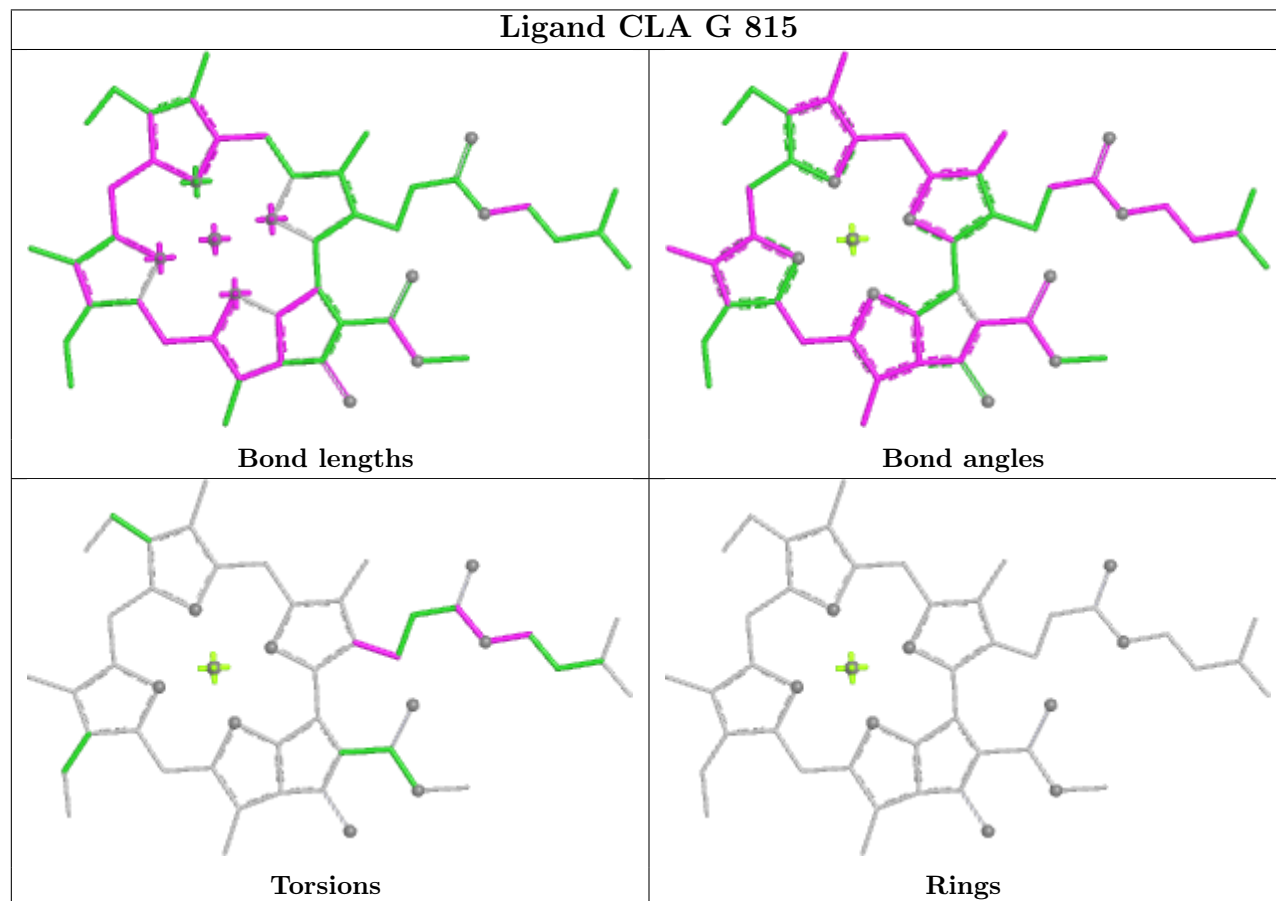
Ligand CLA G 805



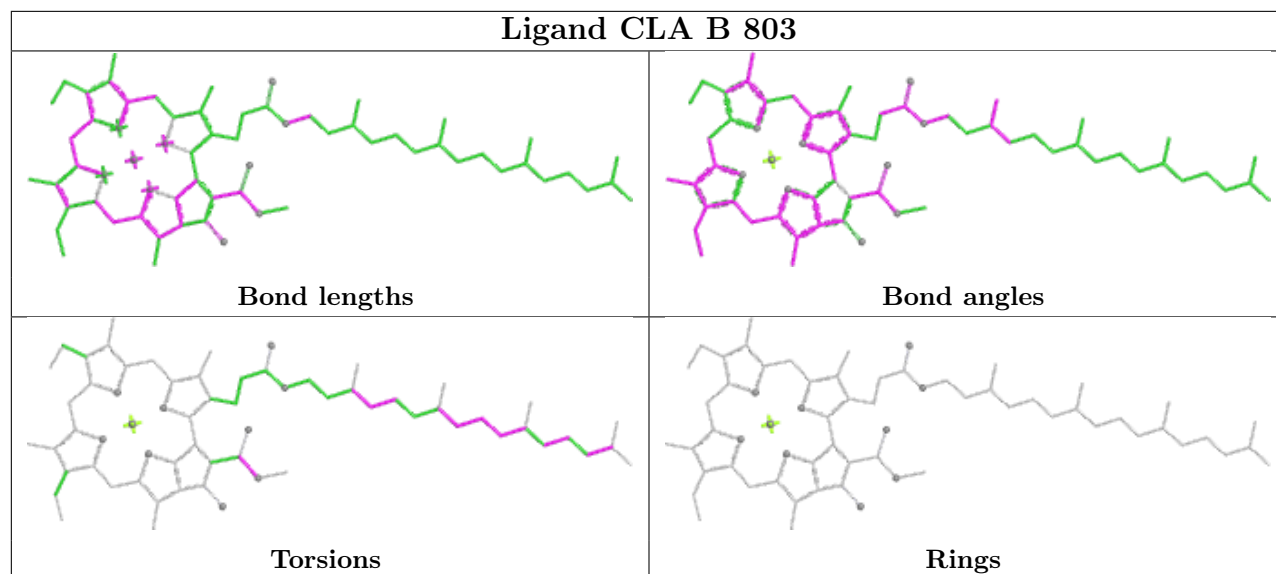
Ligand CLA G 834



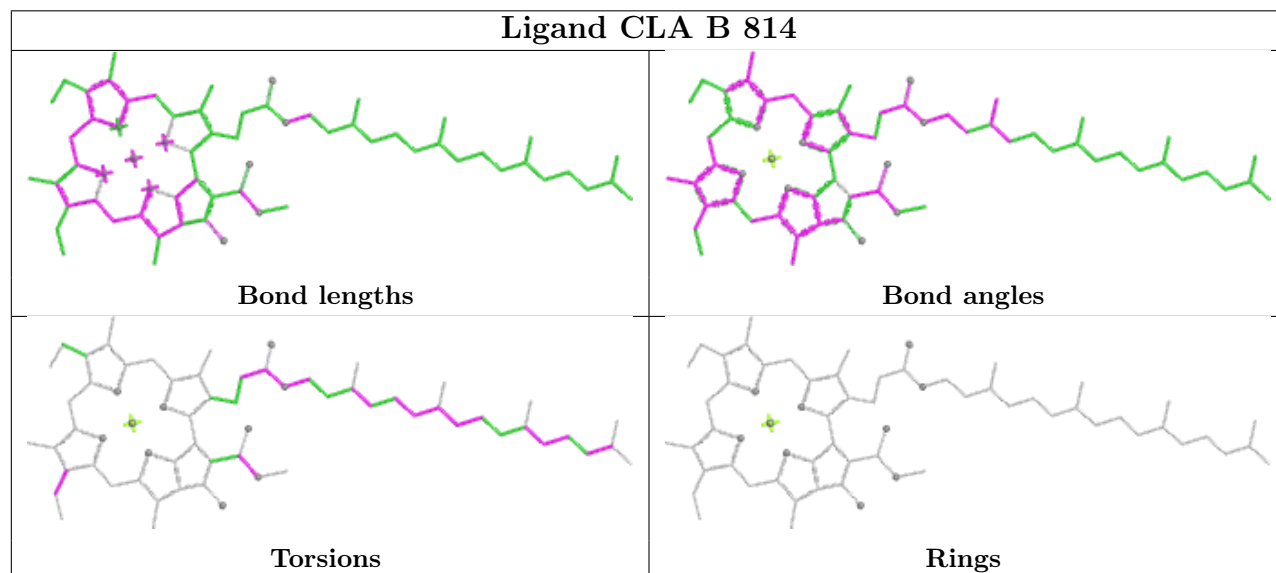
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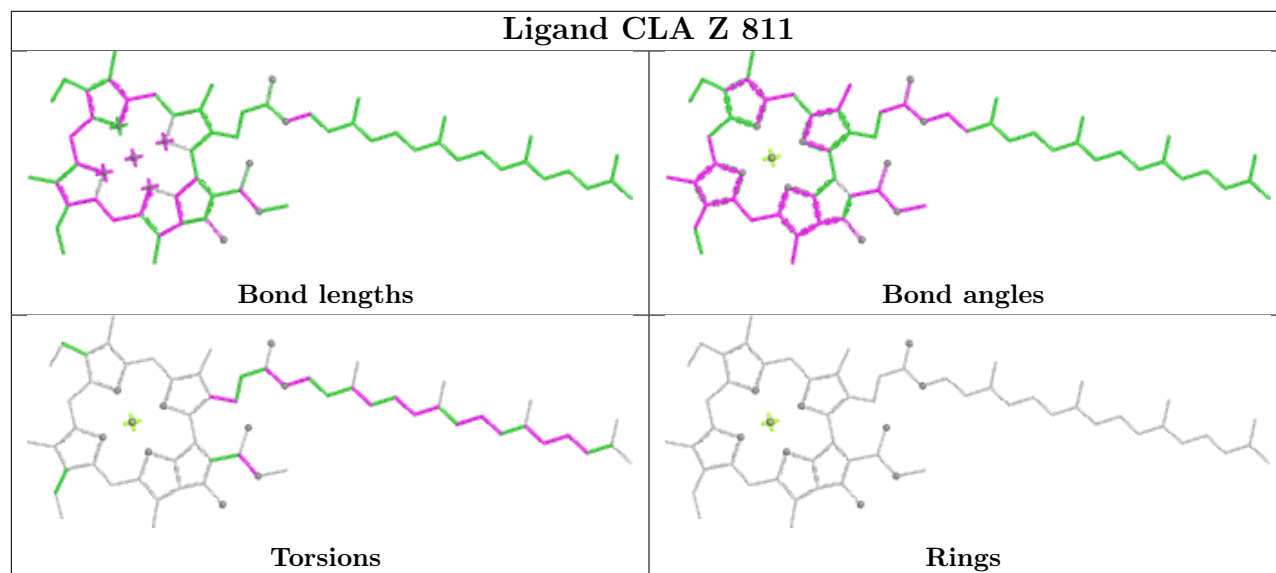
Ligand CLA B 803



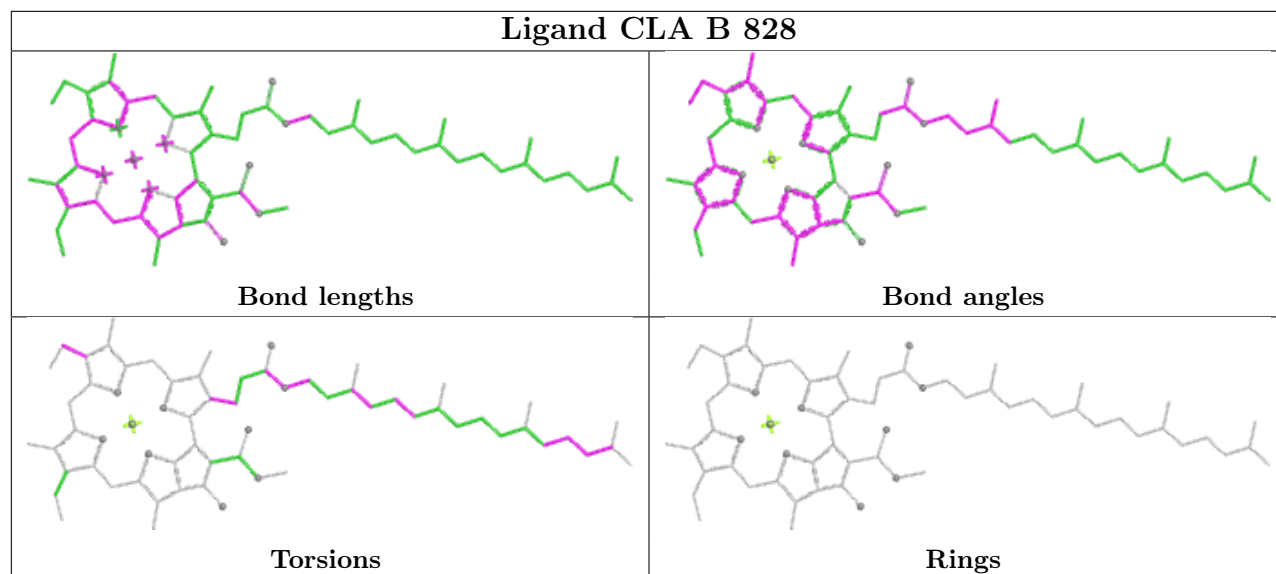
Ligand CLA B 814



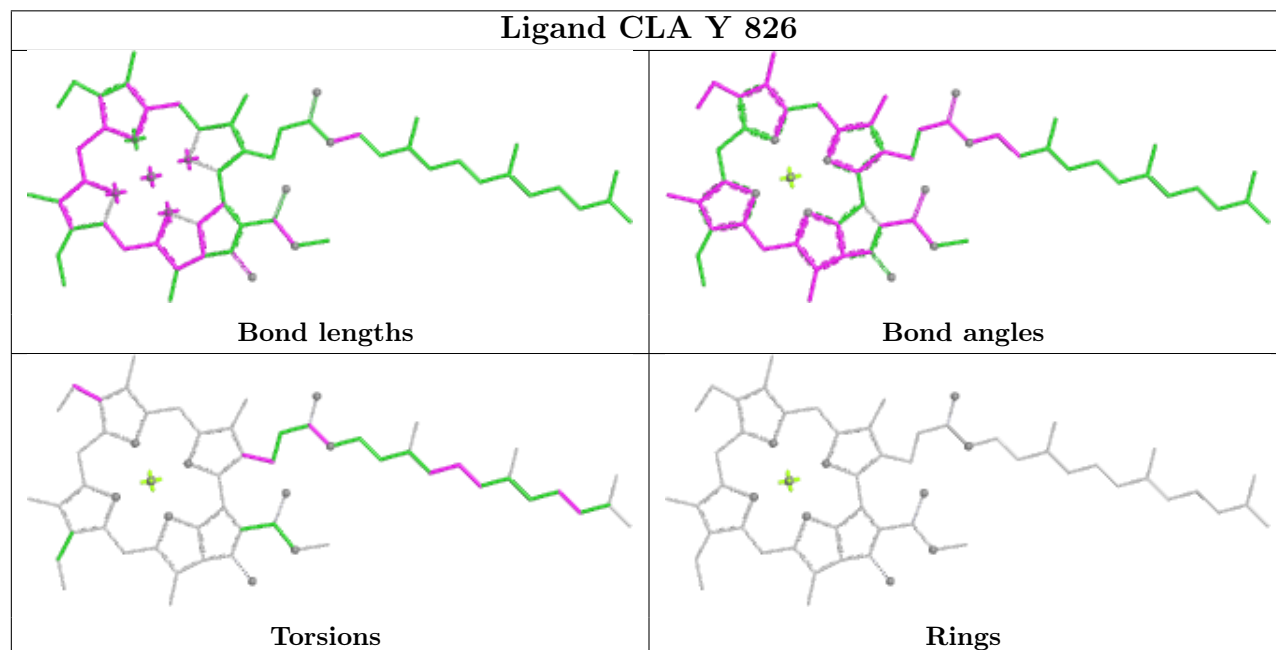
Ligand CLA Z 811

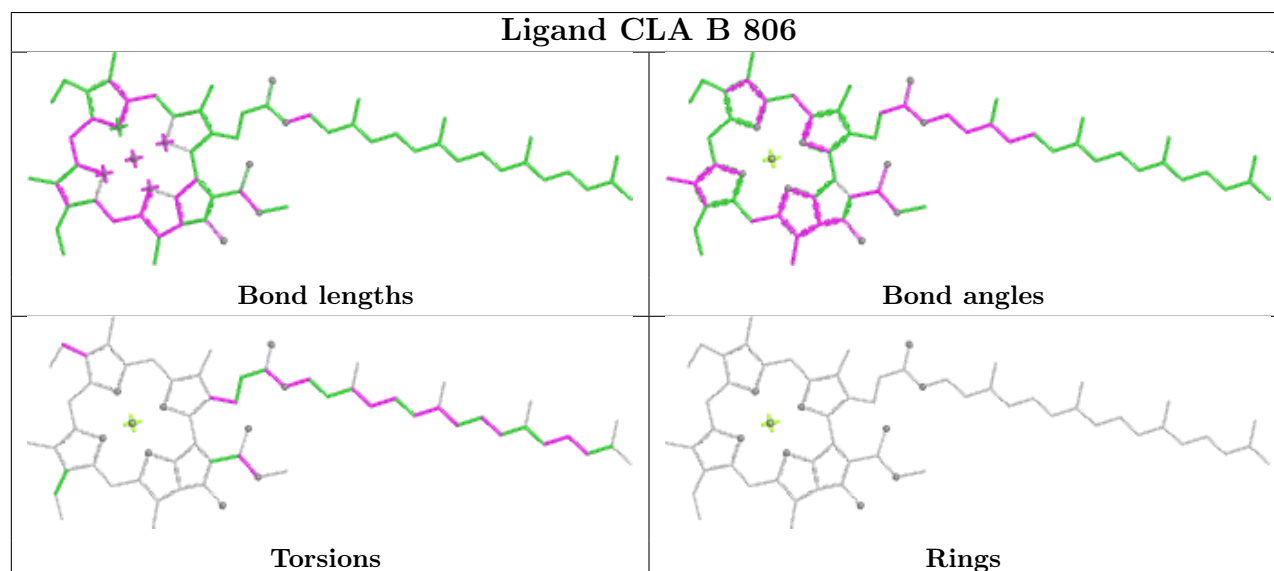
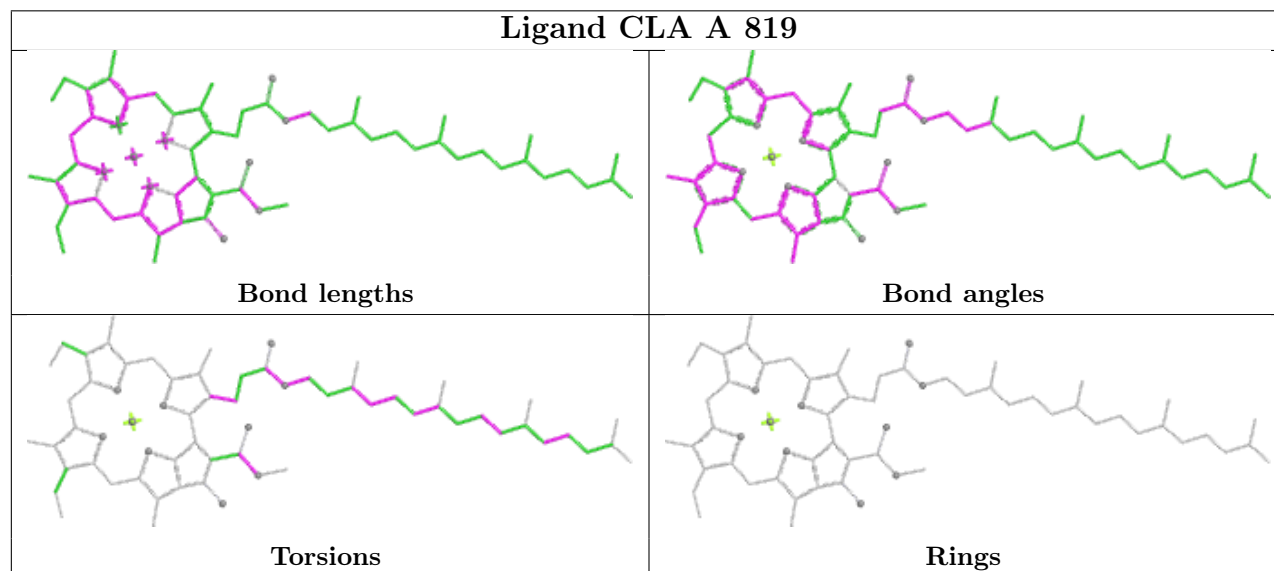
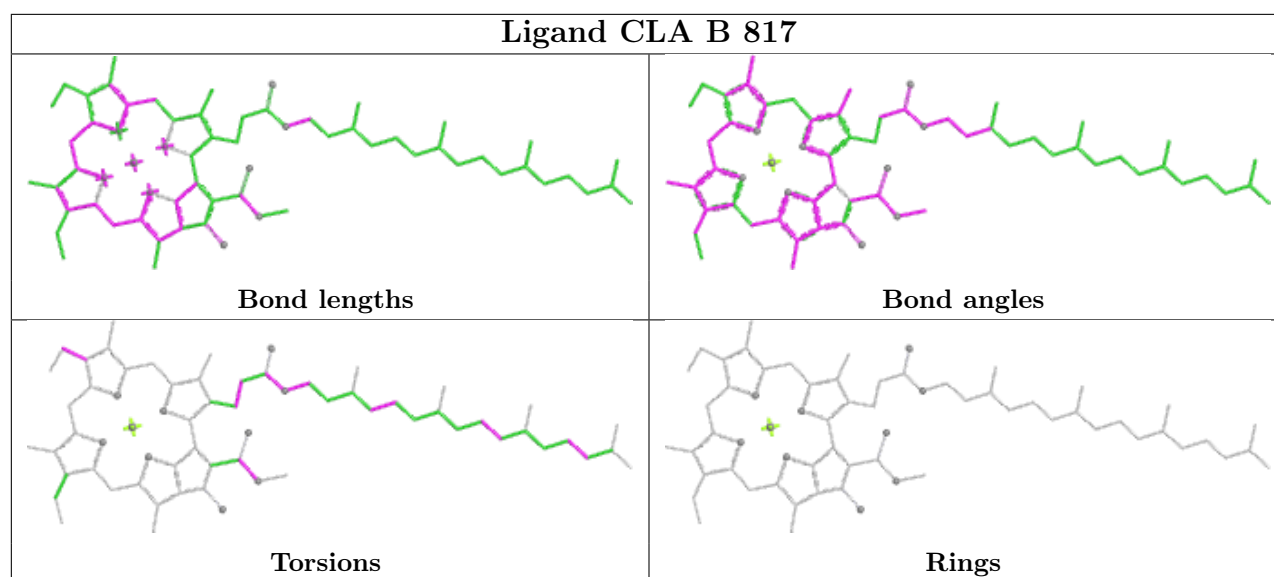


Ligand CLA B 828

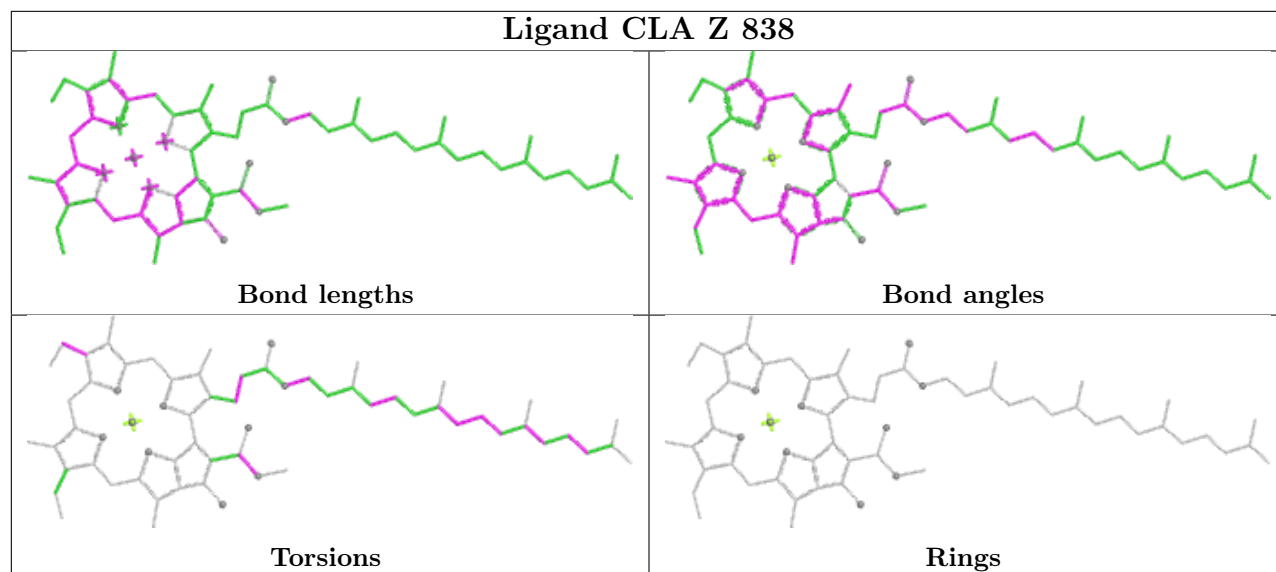


Ligand CLA Y 826

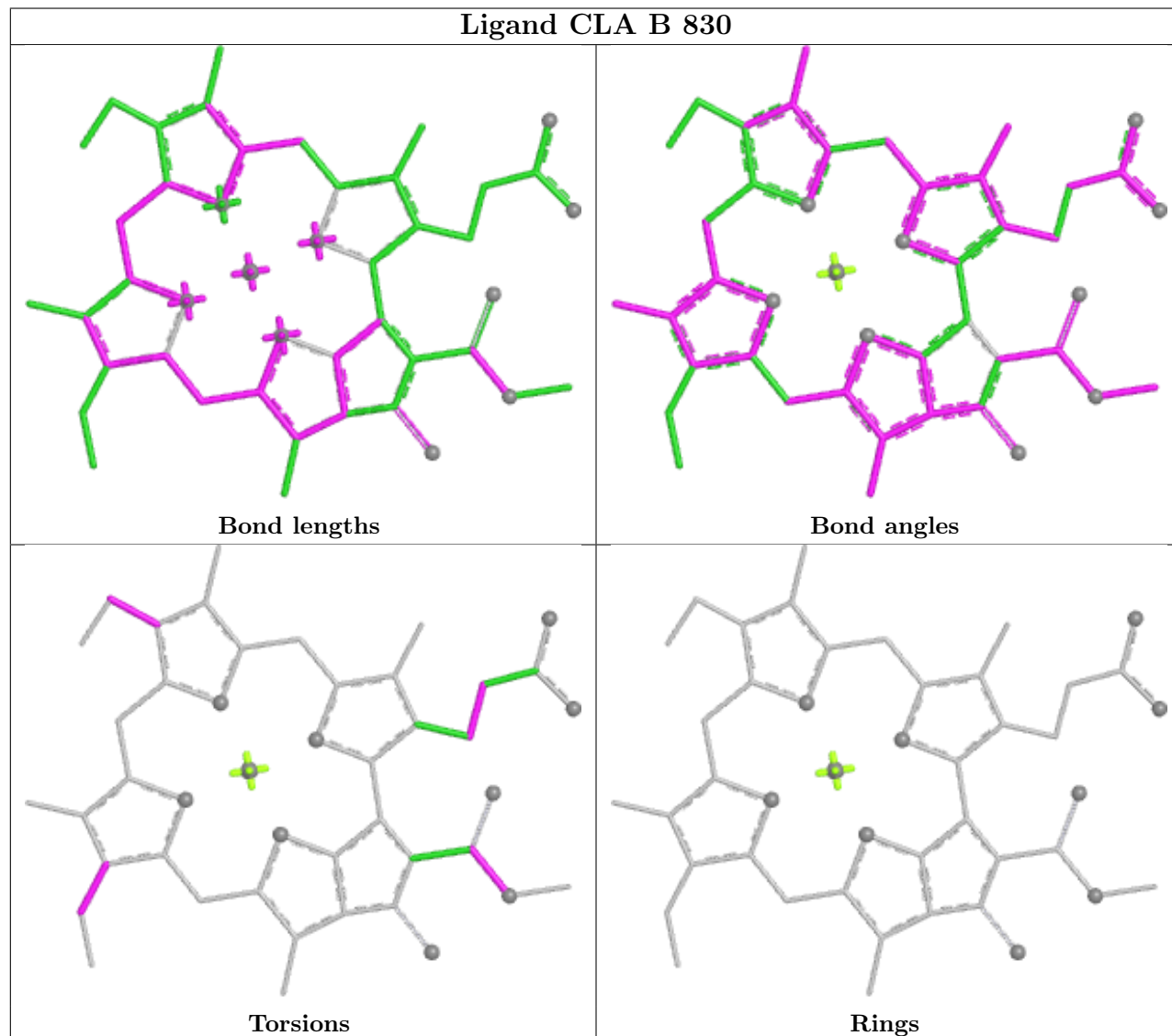




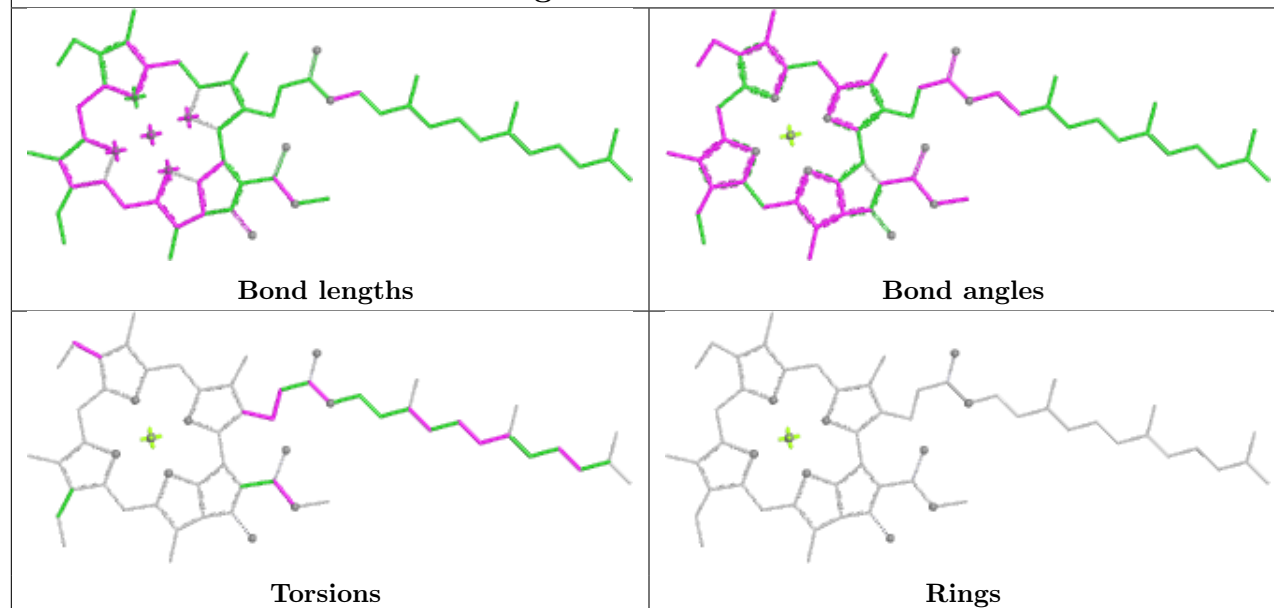
Ligand CLA Z 838



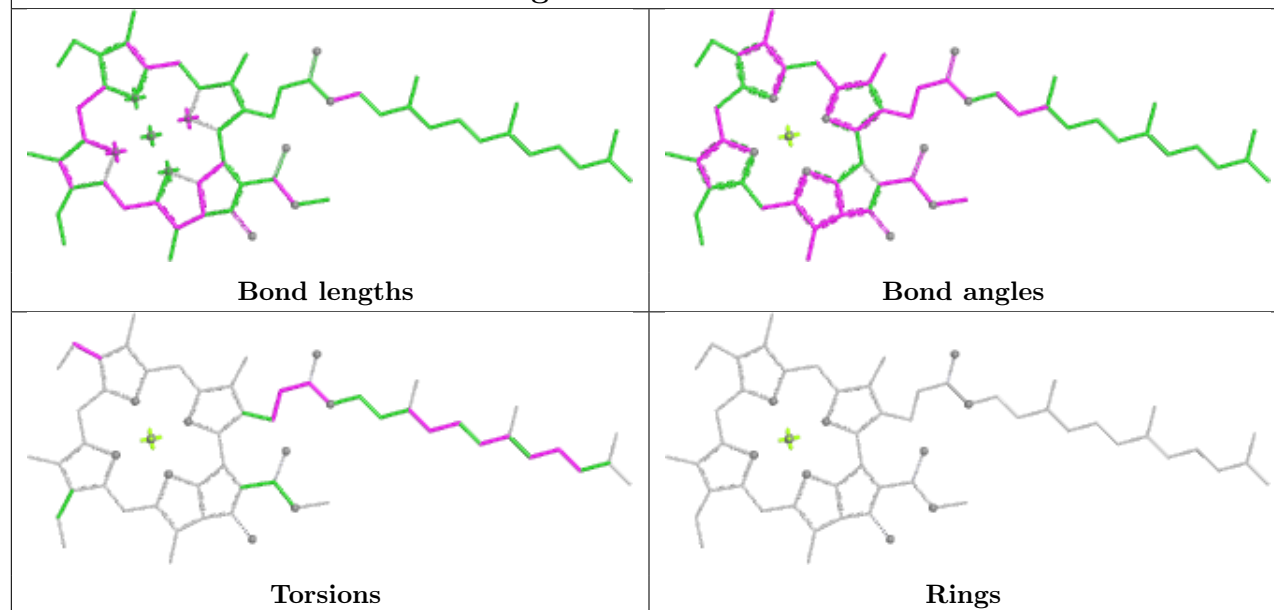
Ligand CLA B 830



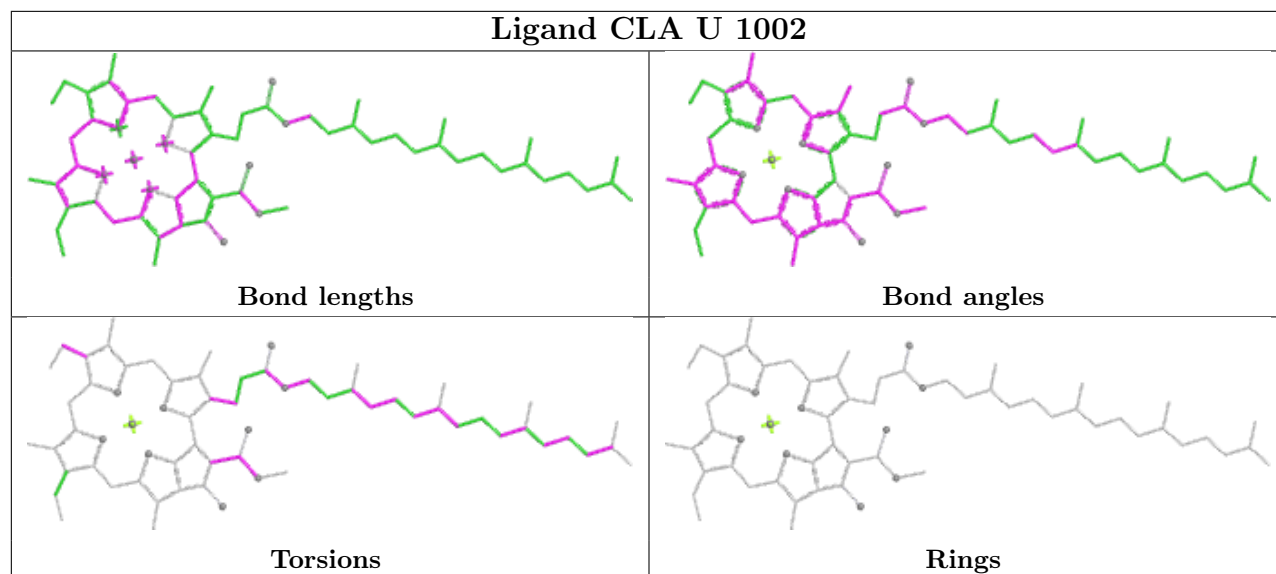
Ligand CLA Z 816



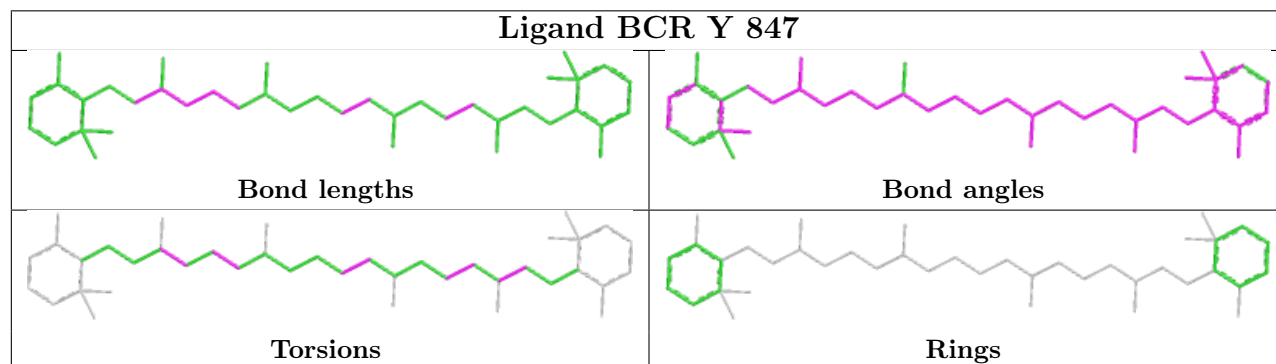
Ligand CLA H 822



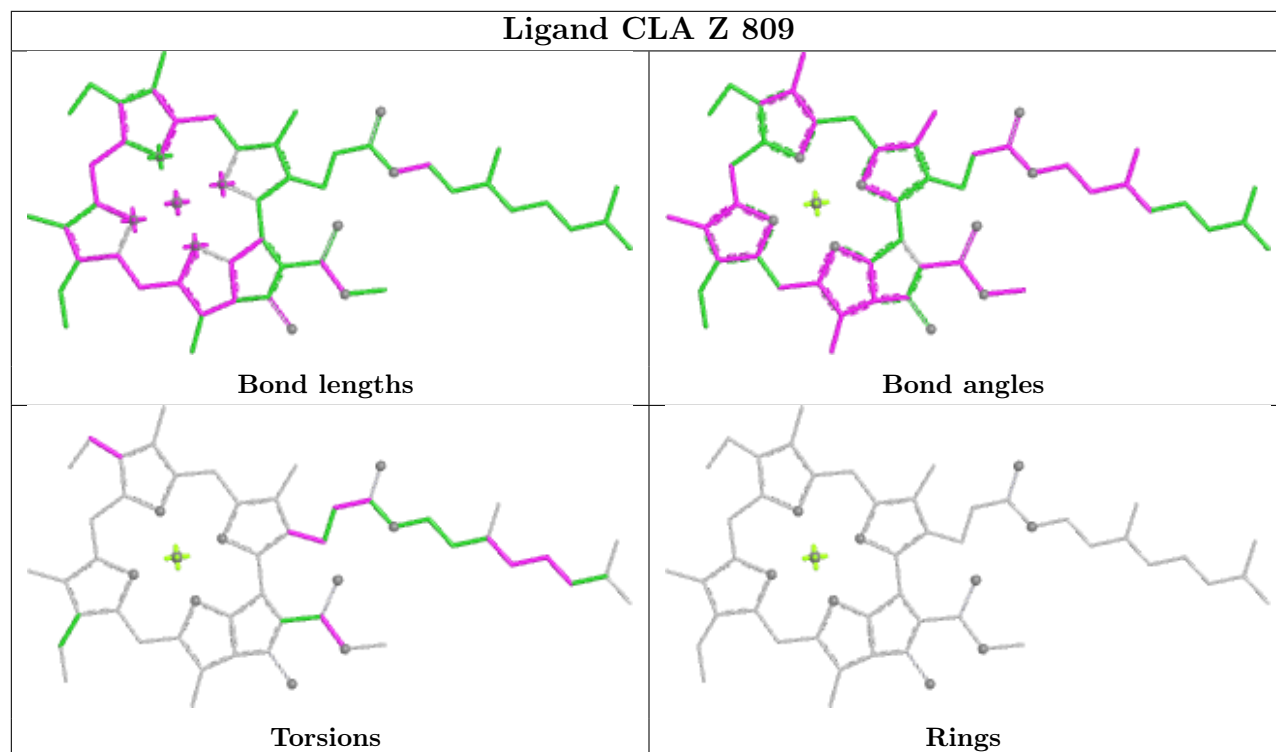
Ligand CLA U 1002



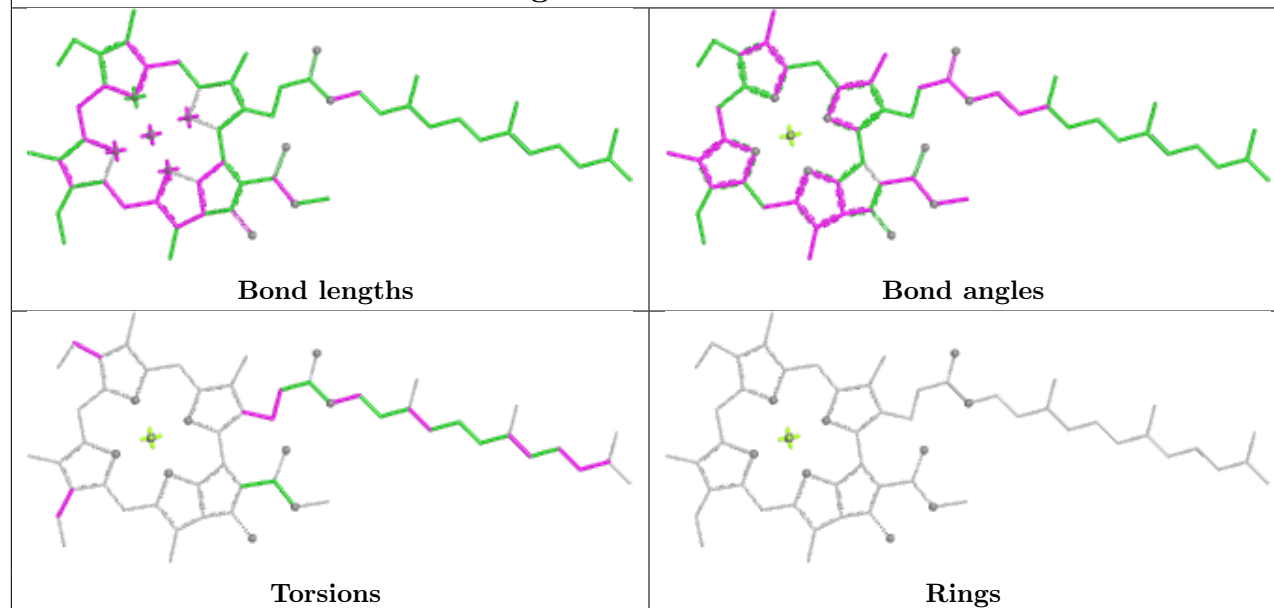
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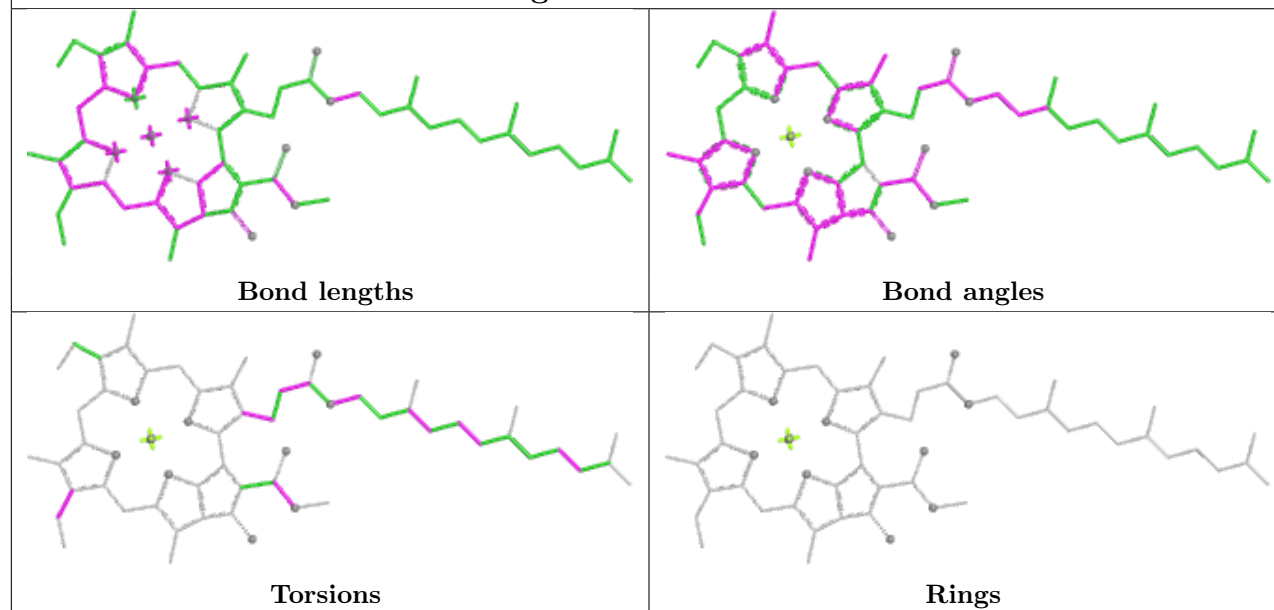
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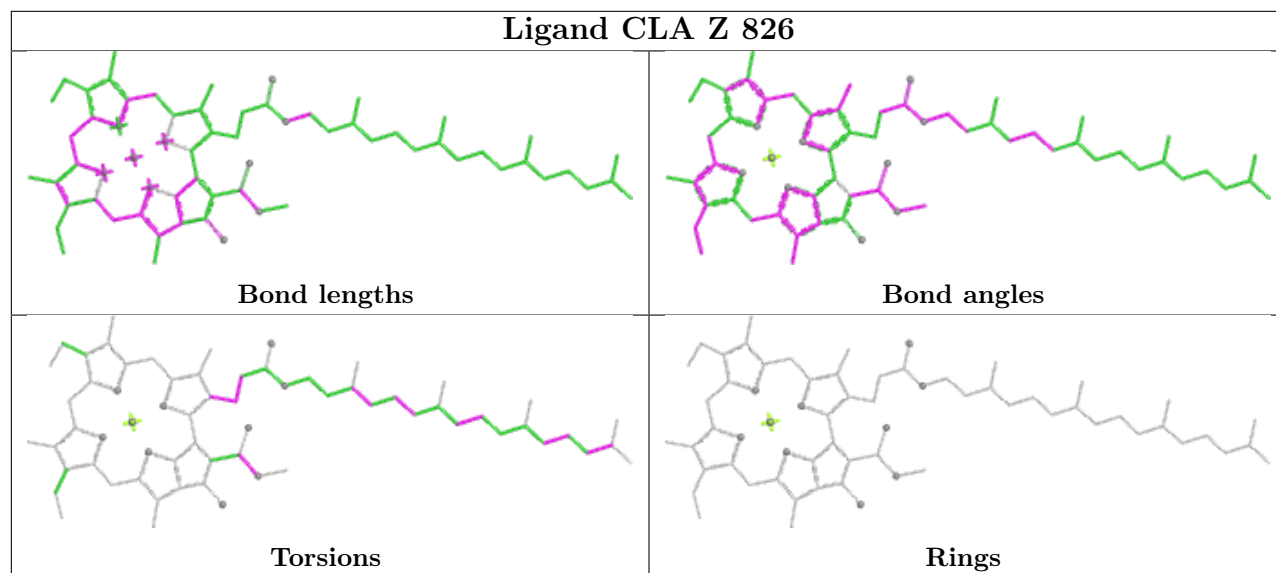
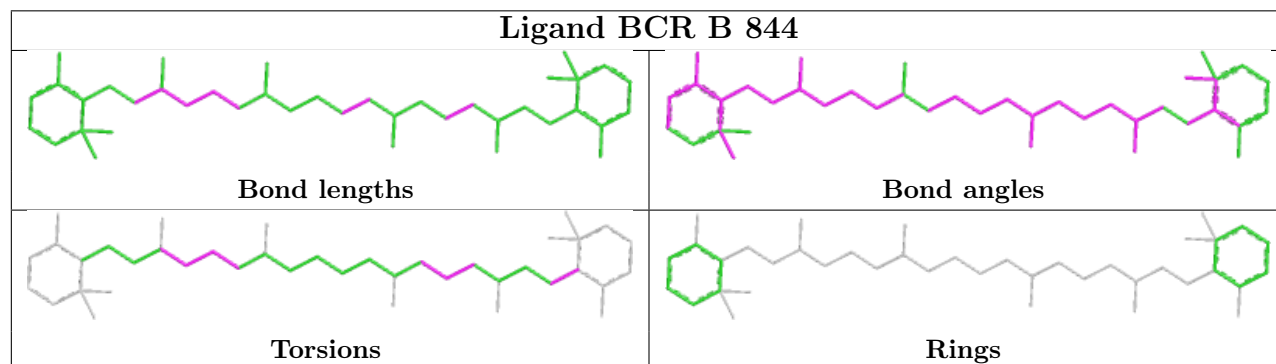
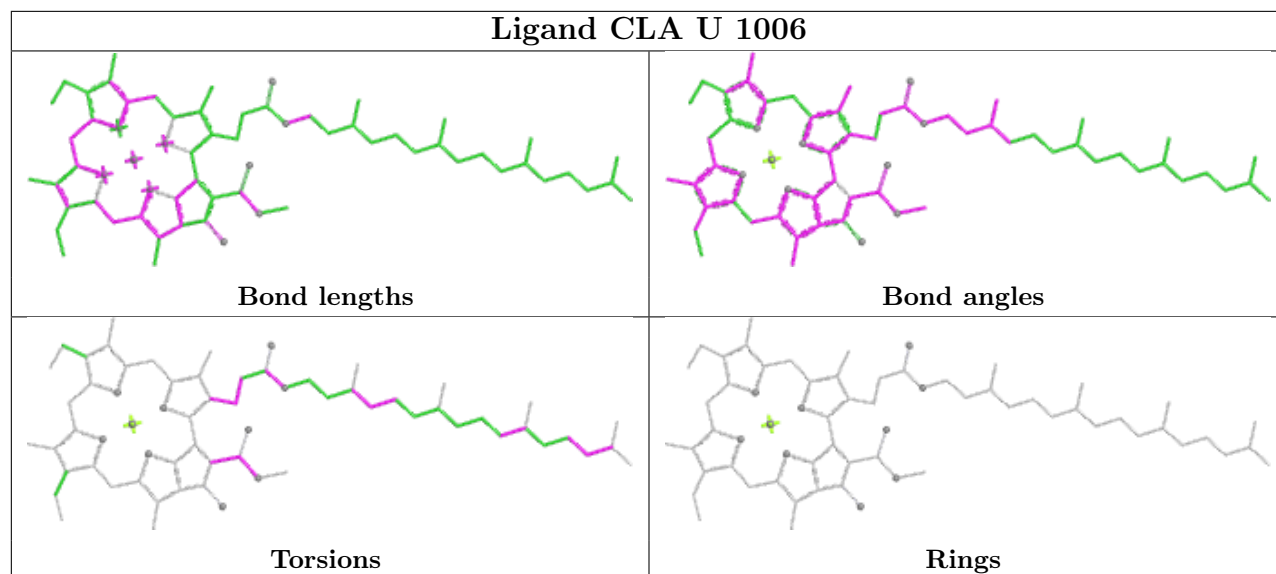


Ligand CLA G 824

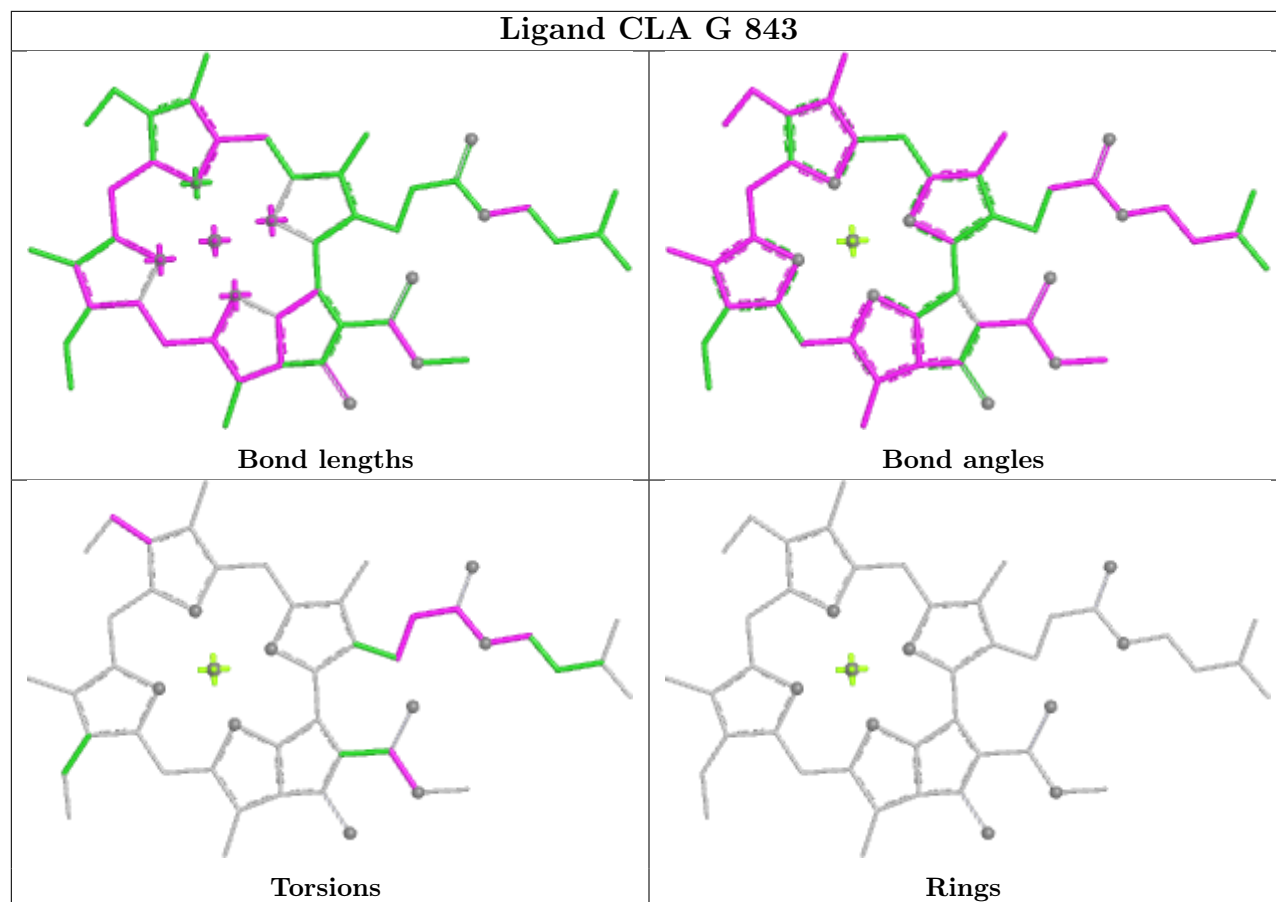


Ligand CLA G 813

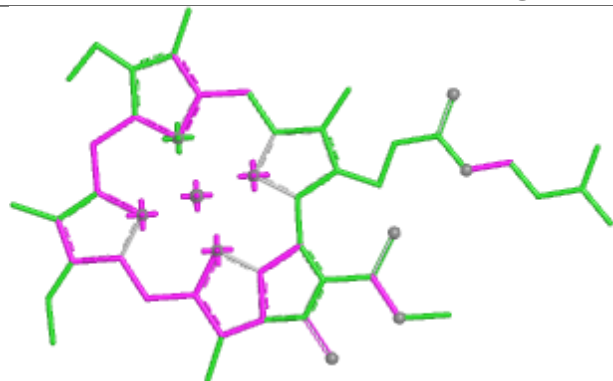




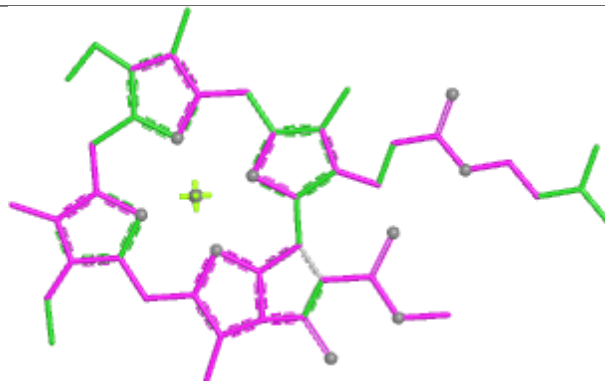
Ligand CLA G 843



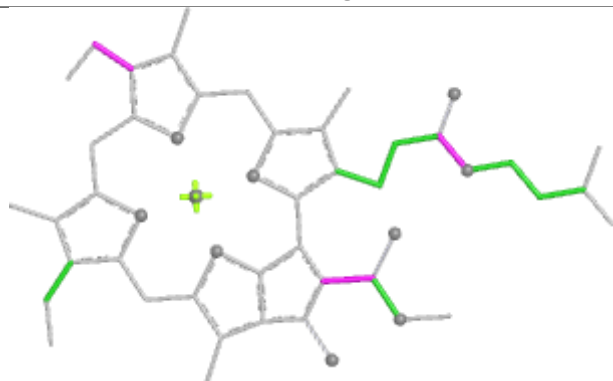
Ligand CLA Y 831



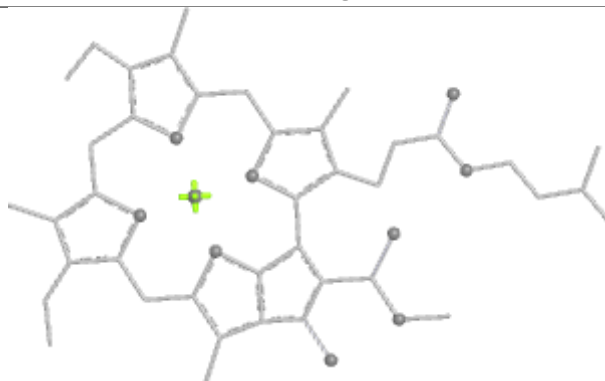
Bond lengths



Bond angles

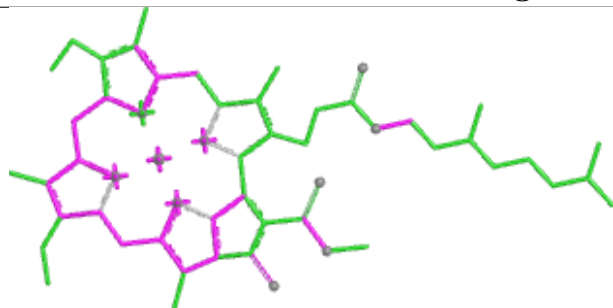


Torsions

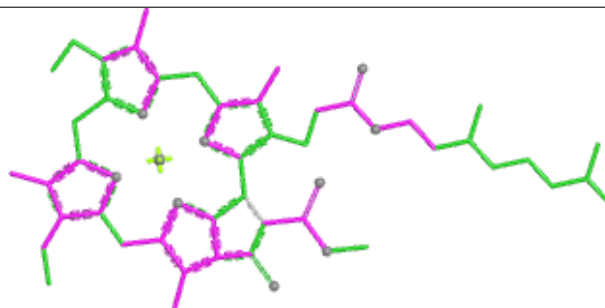


Rings

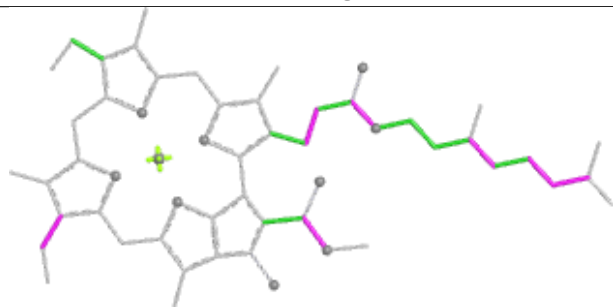
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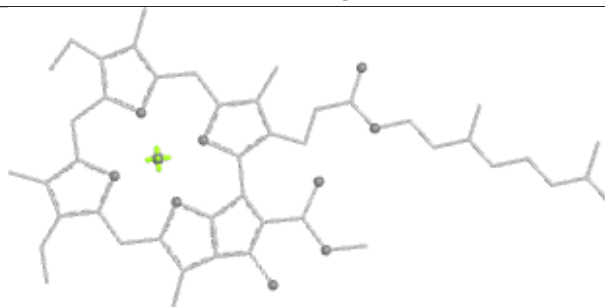
Bond lengths



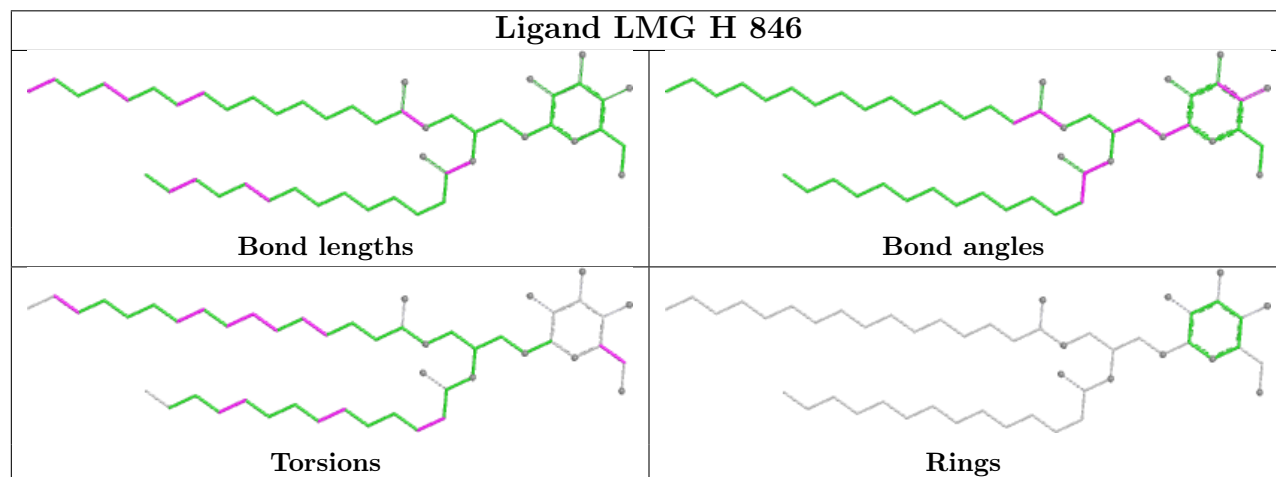
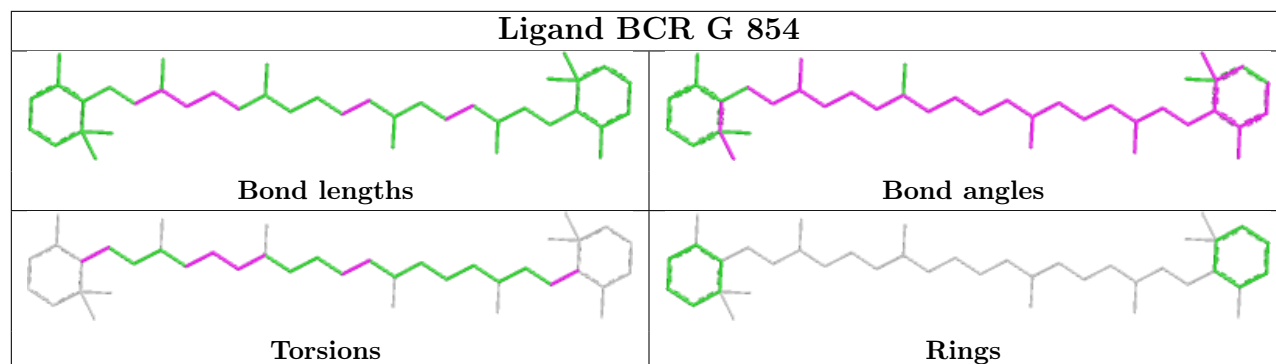
Bond angles



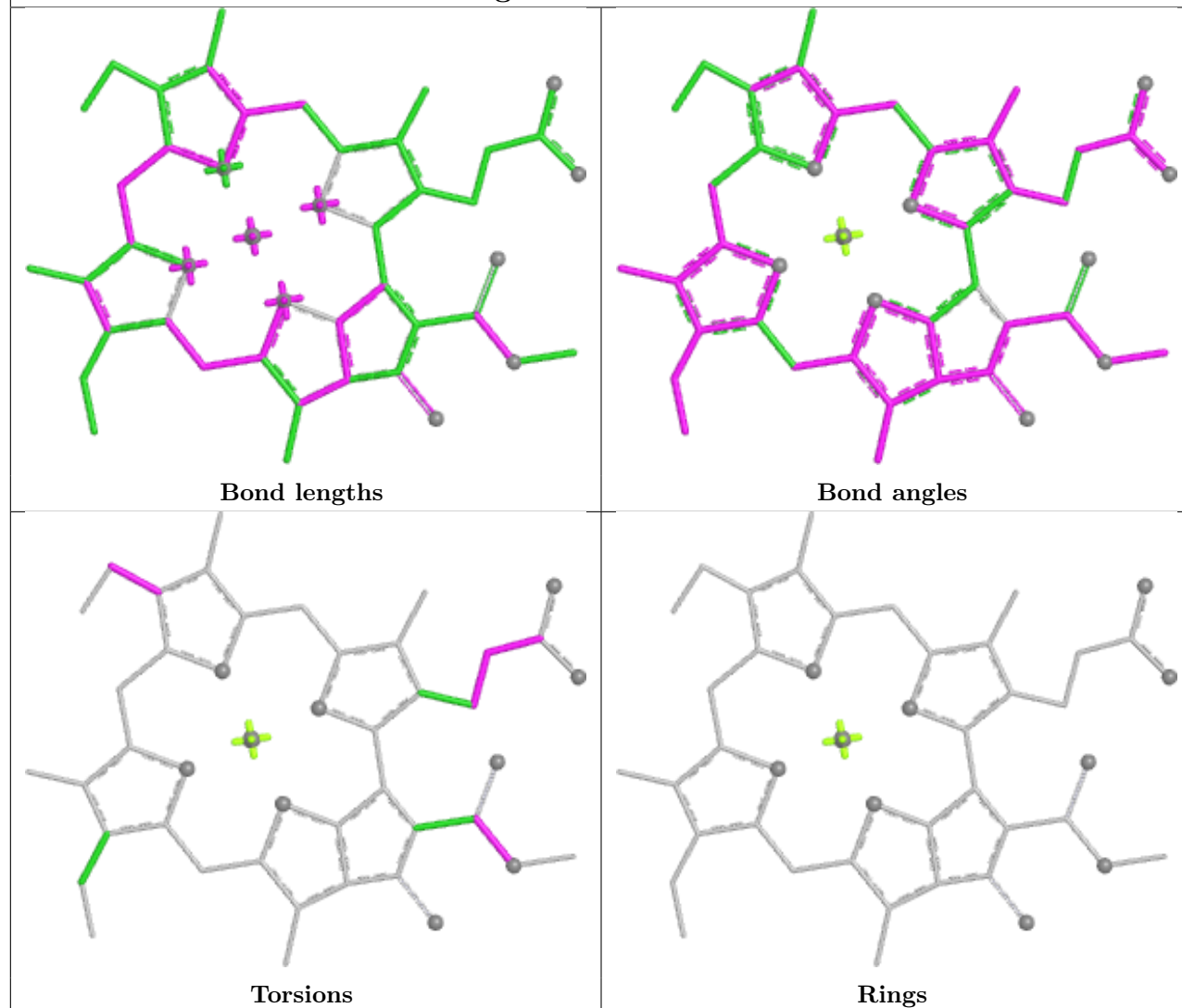
Torsions



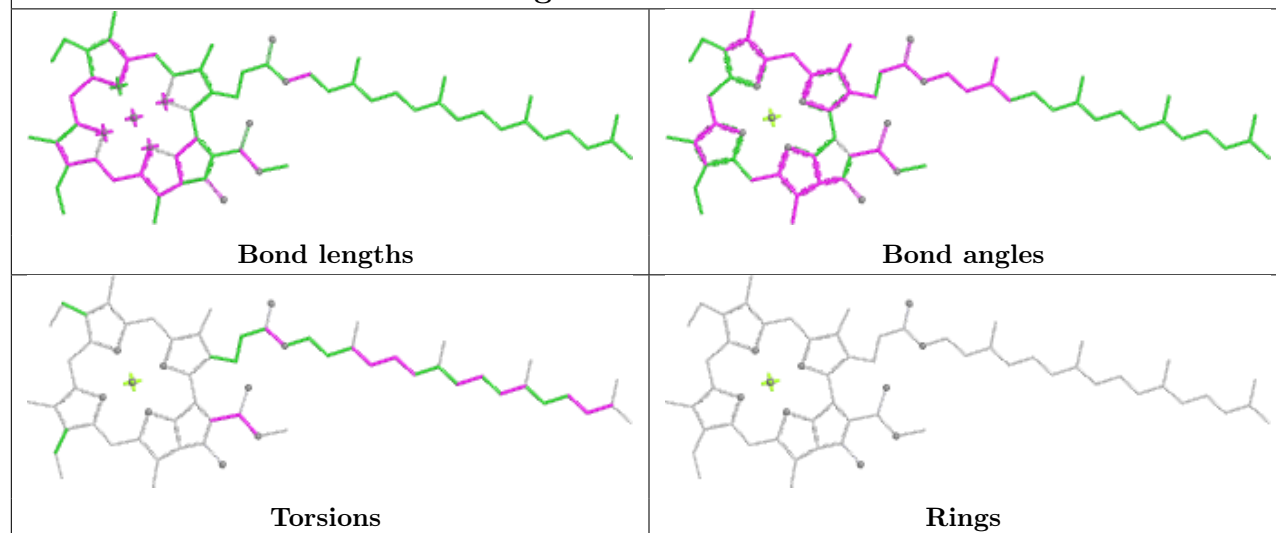
Rings



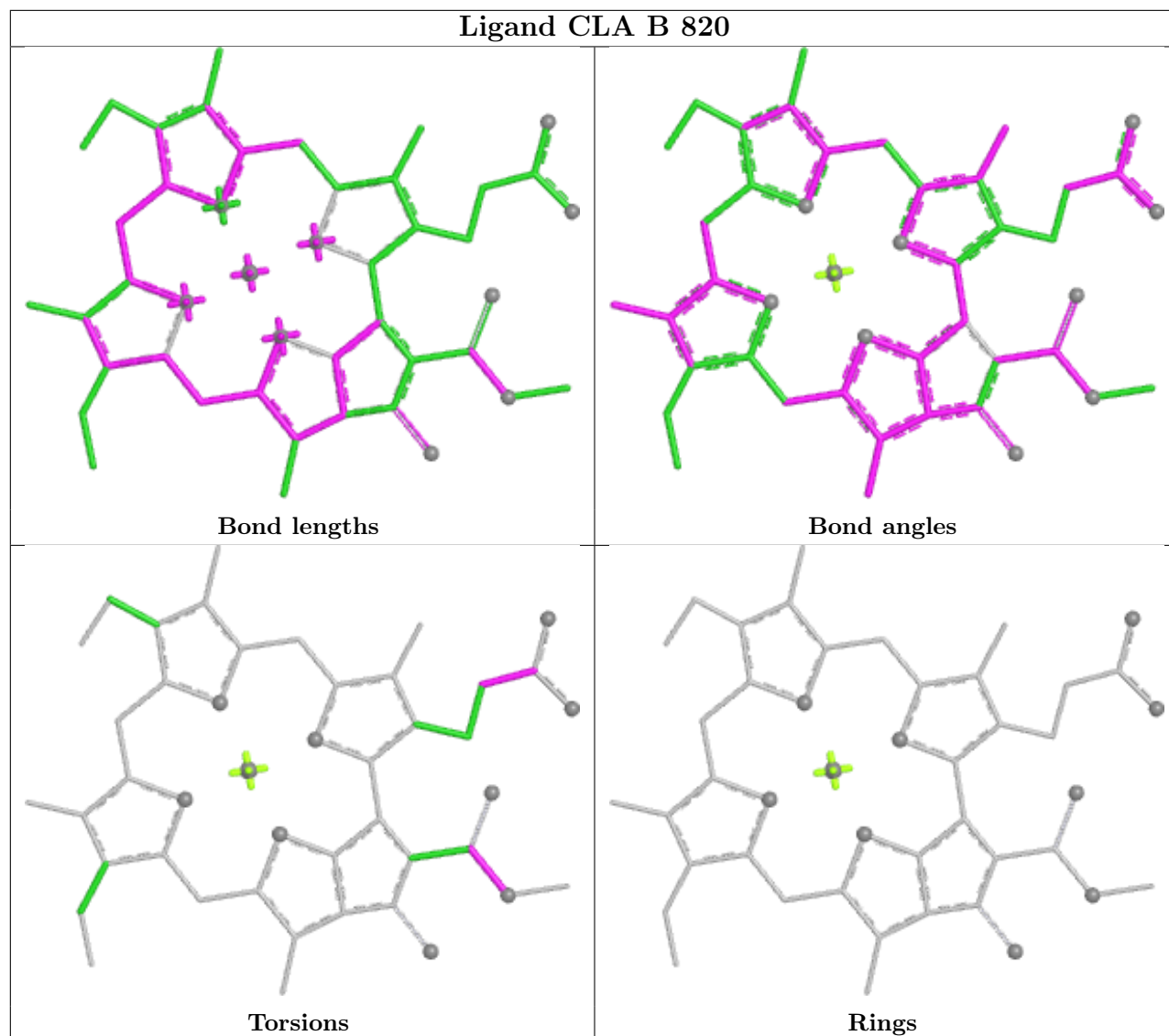
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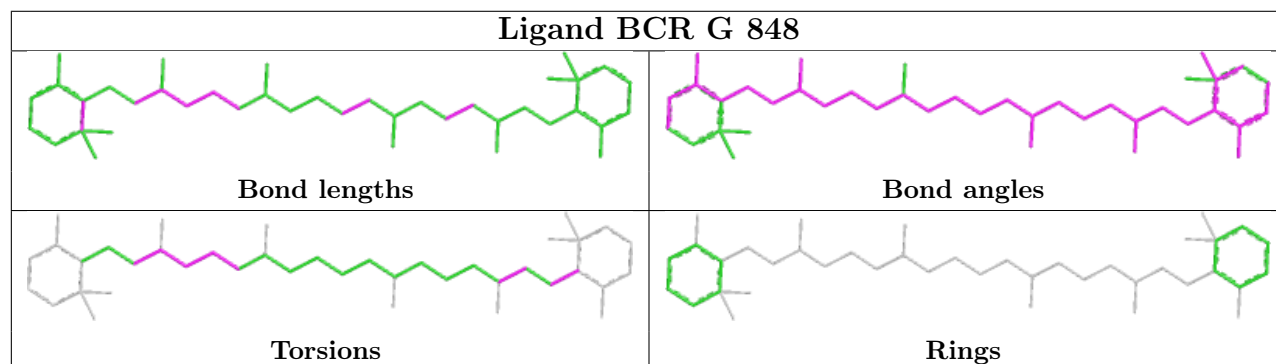
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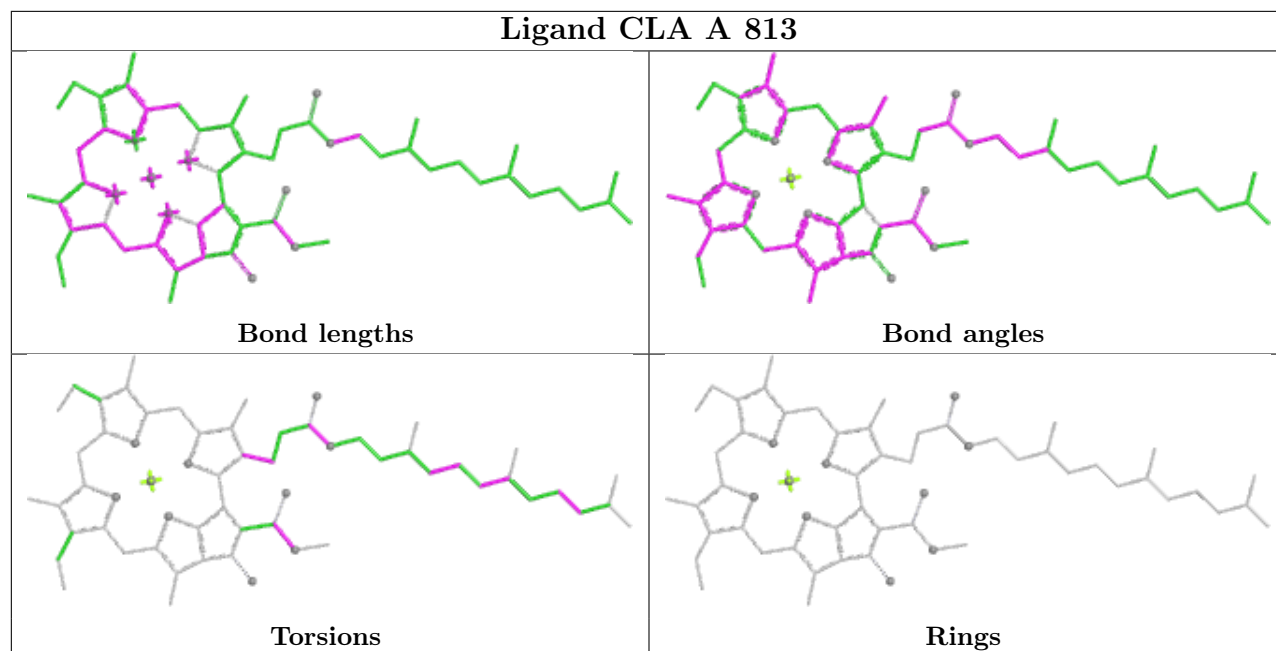
Ligand CLA B 820



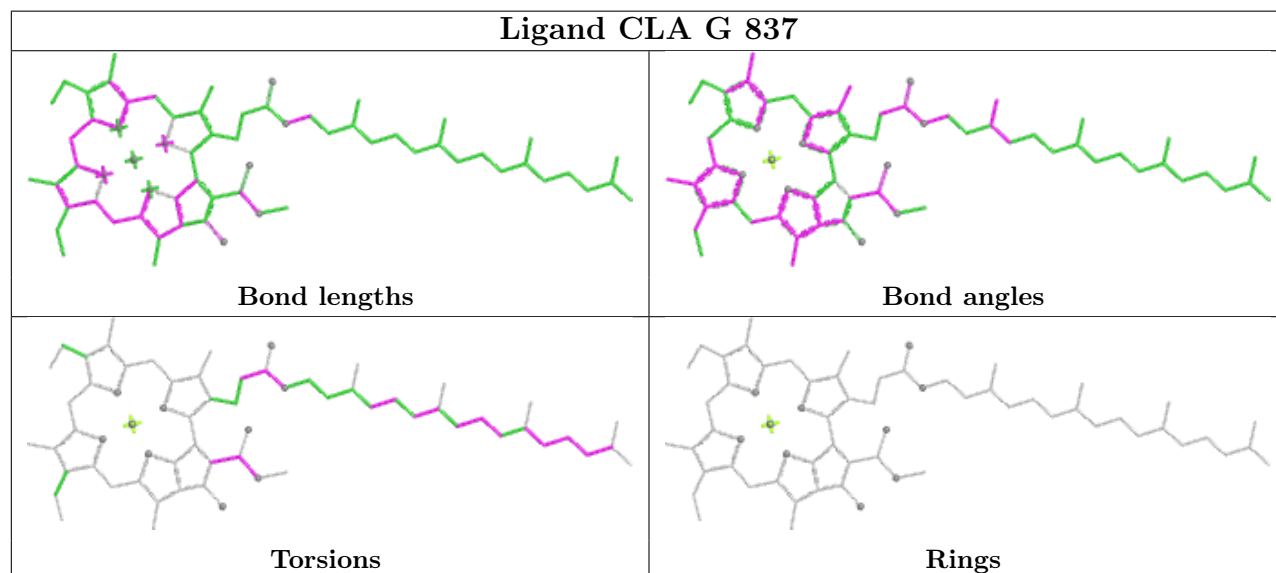
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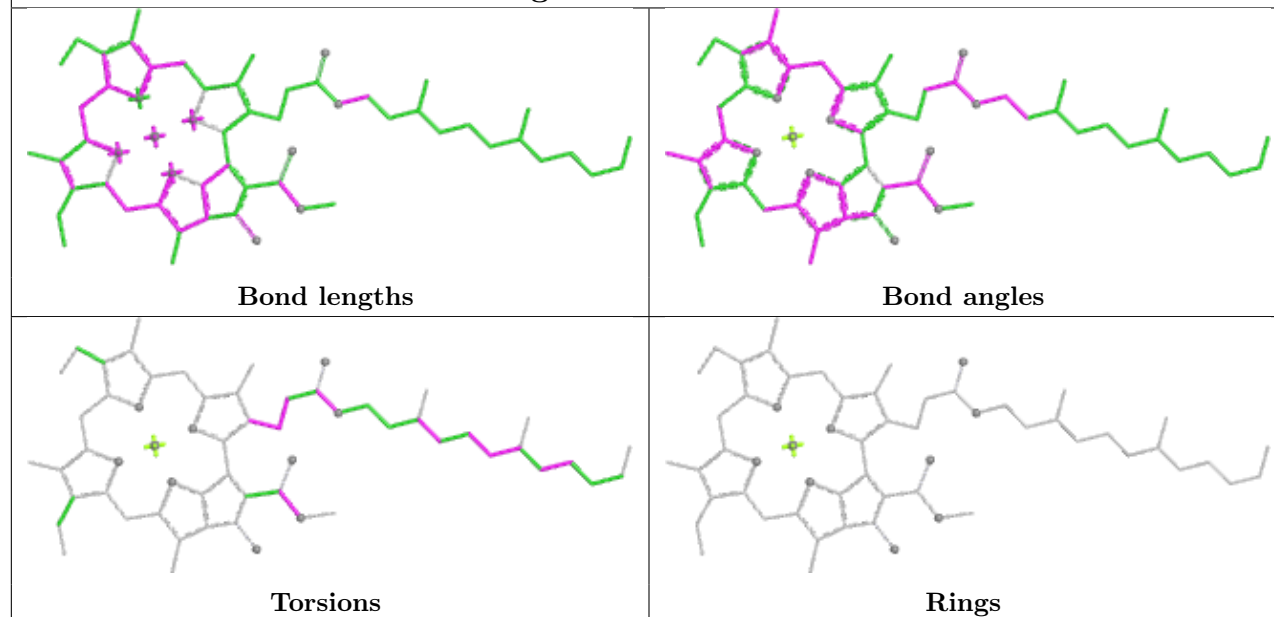
Ligand CLA A 813



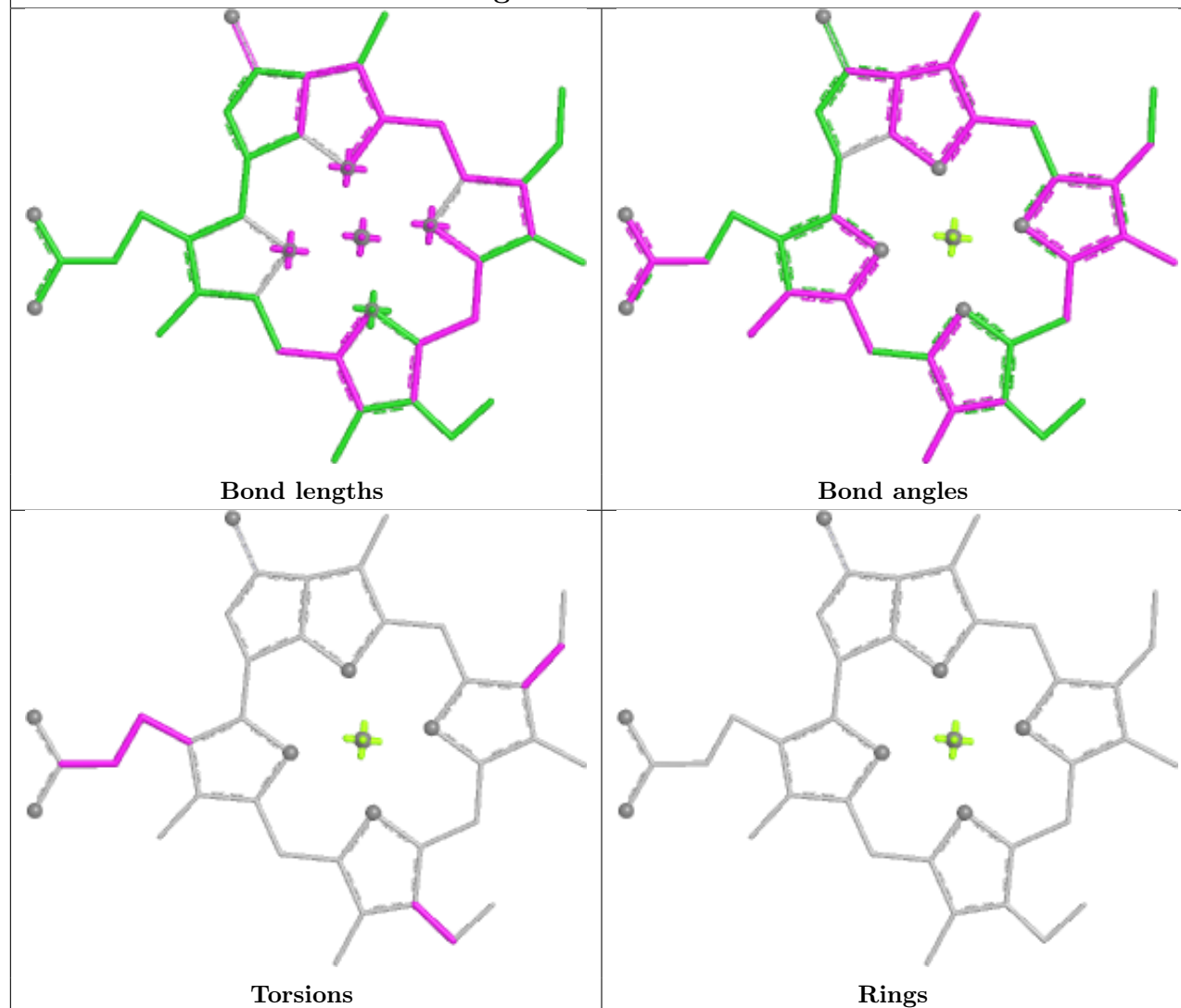
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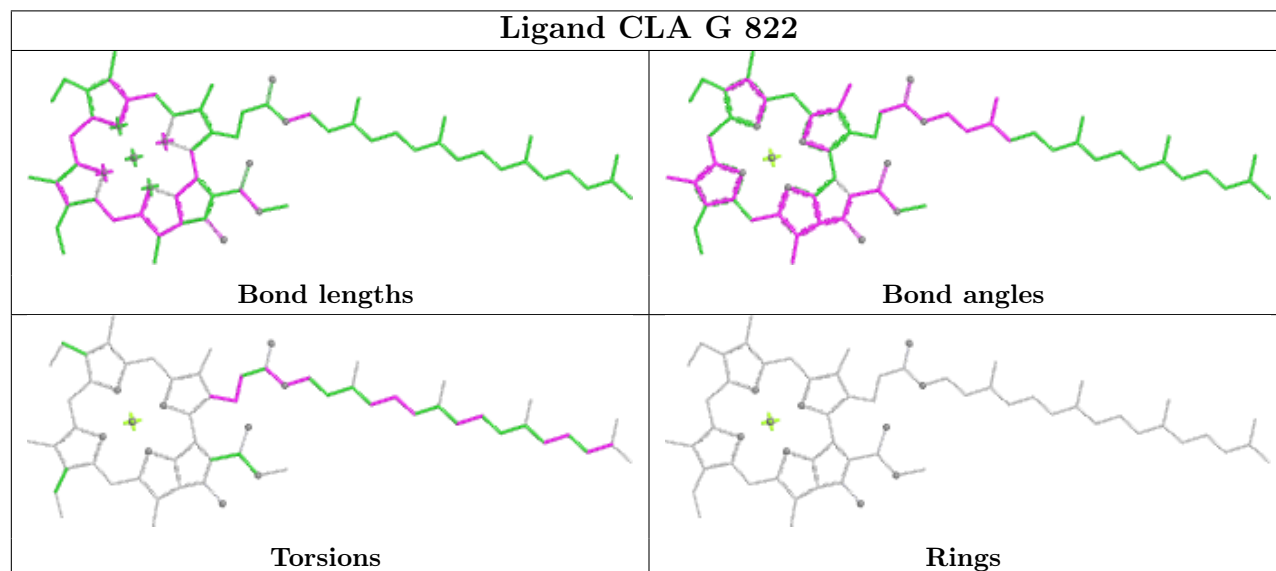
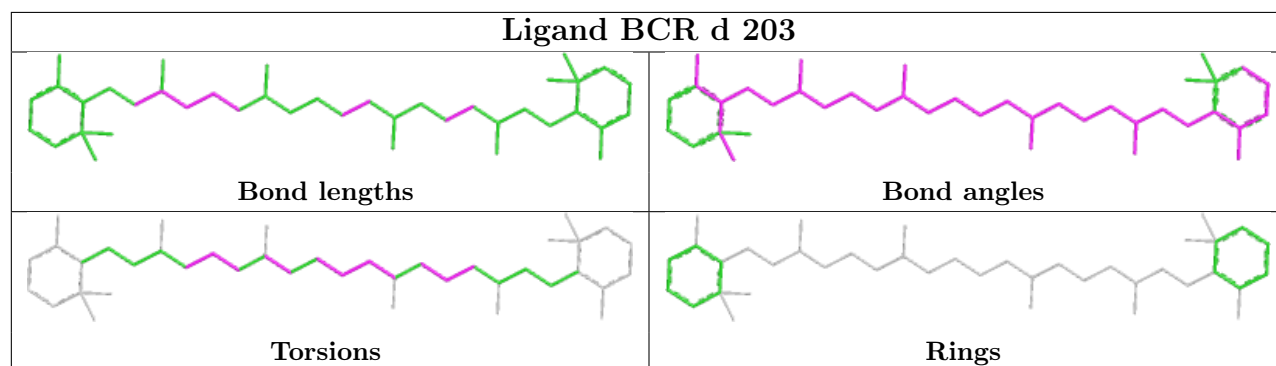
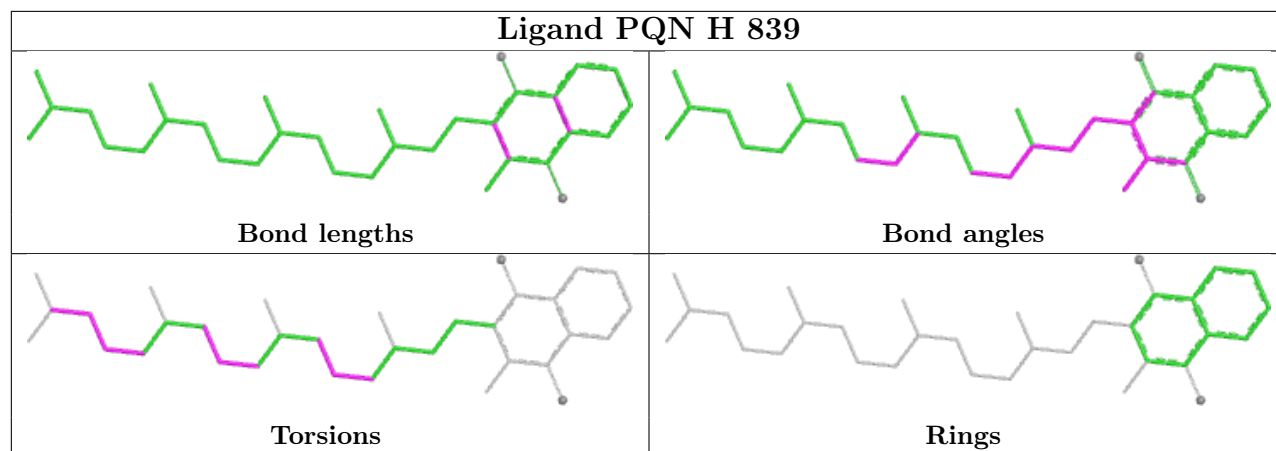


Ligand CLA G 804

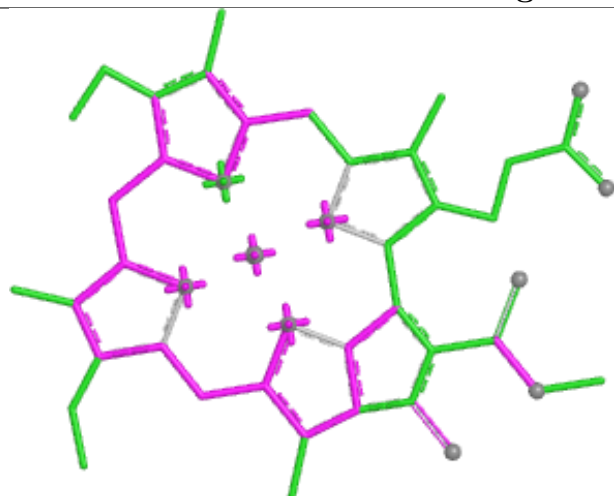


Ligand CLA T 101

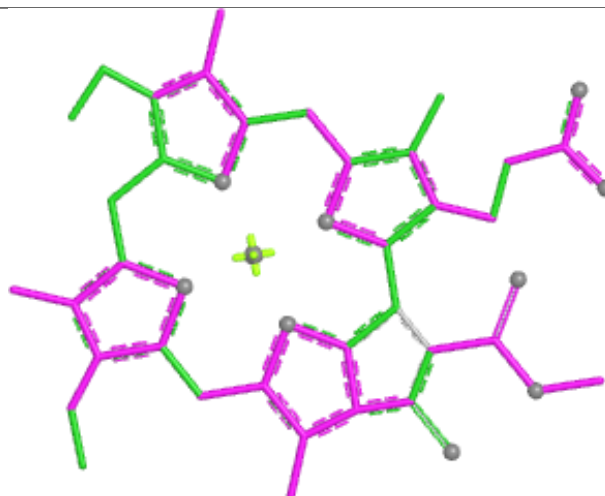




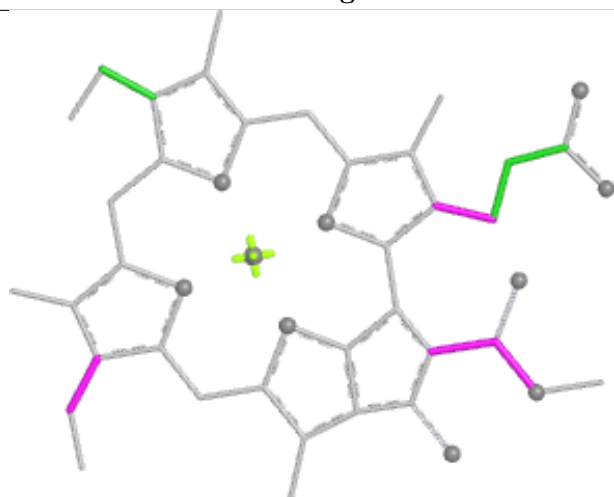
Ligand CLA Z 832



Bond lengths



Bond angles

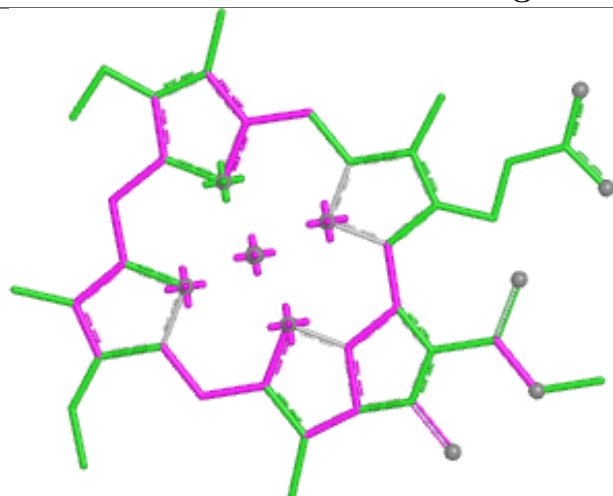


Torsions

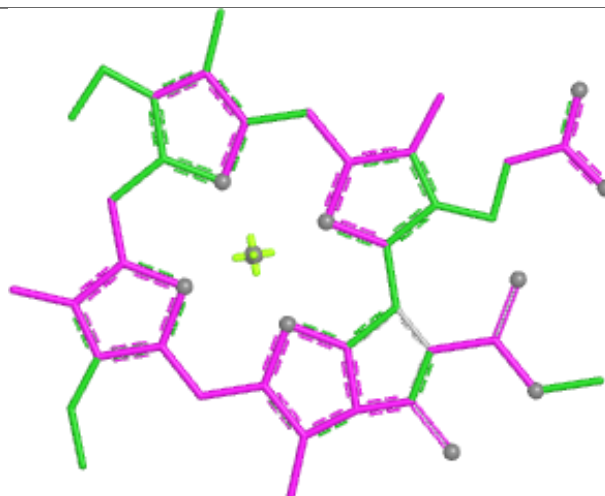


Rings

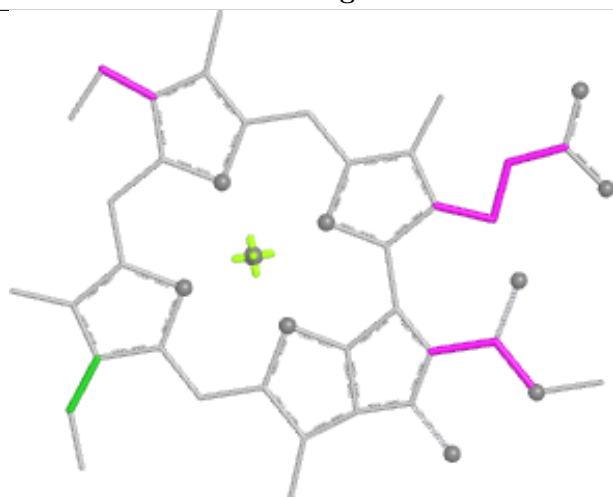
Ligand CLA H 819



Bond lengths



Bond angles

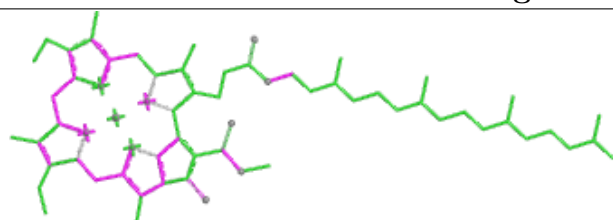


Torsions

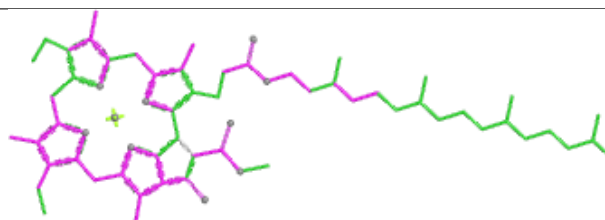


Rings

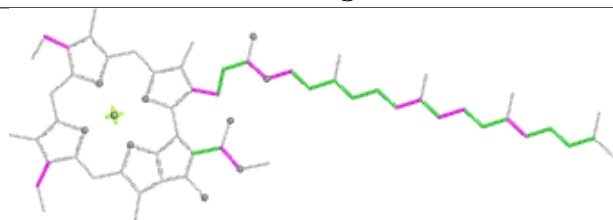
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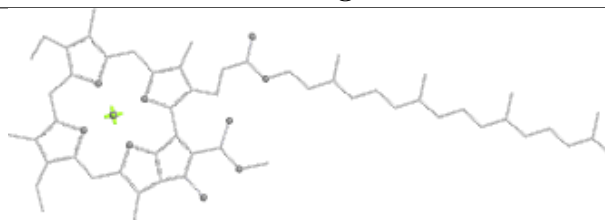
Bond lengths



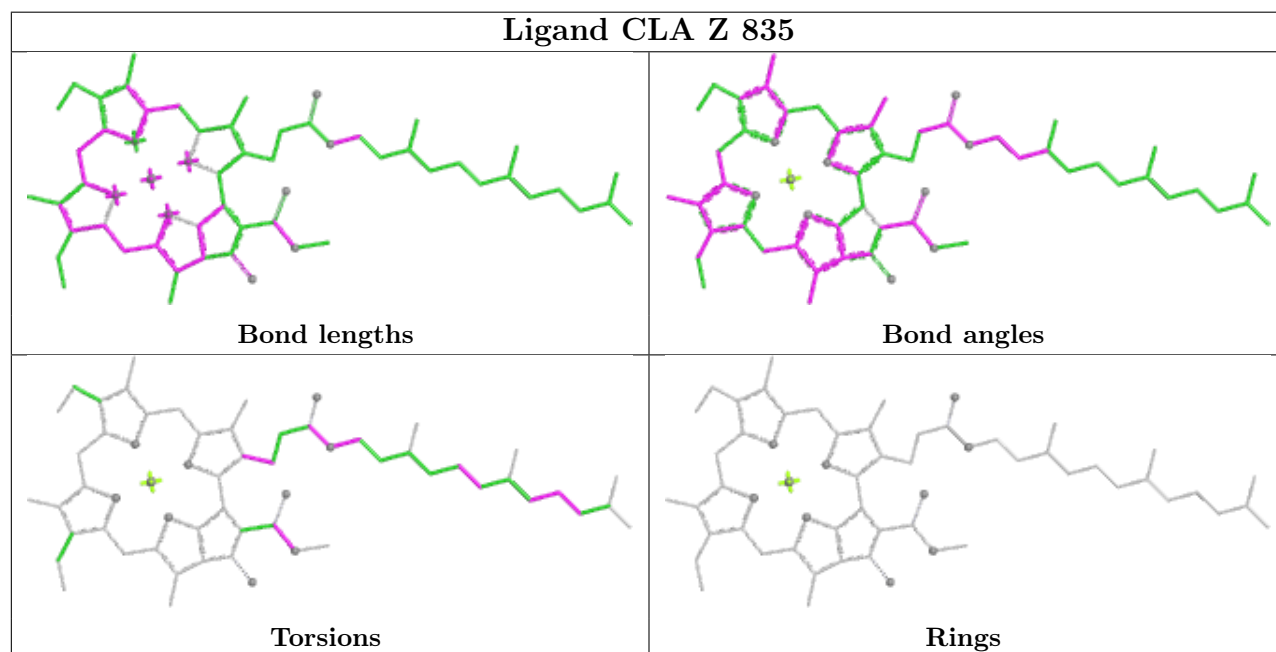
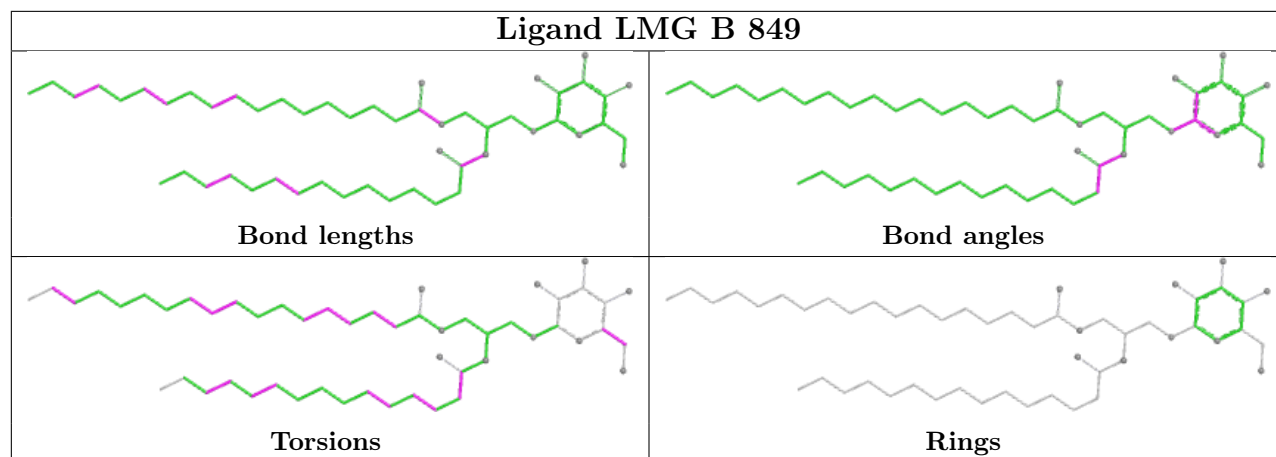
Bond angles



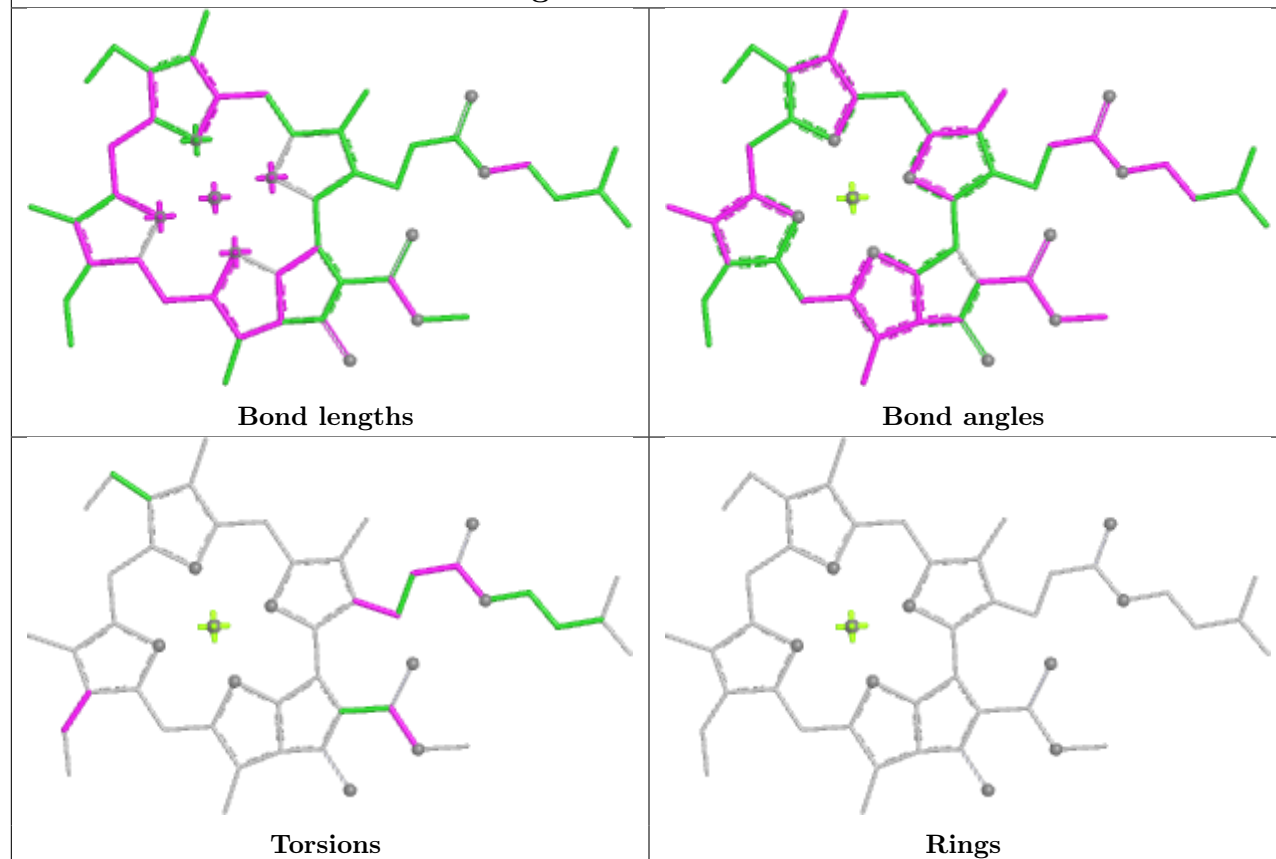
Torsions



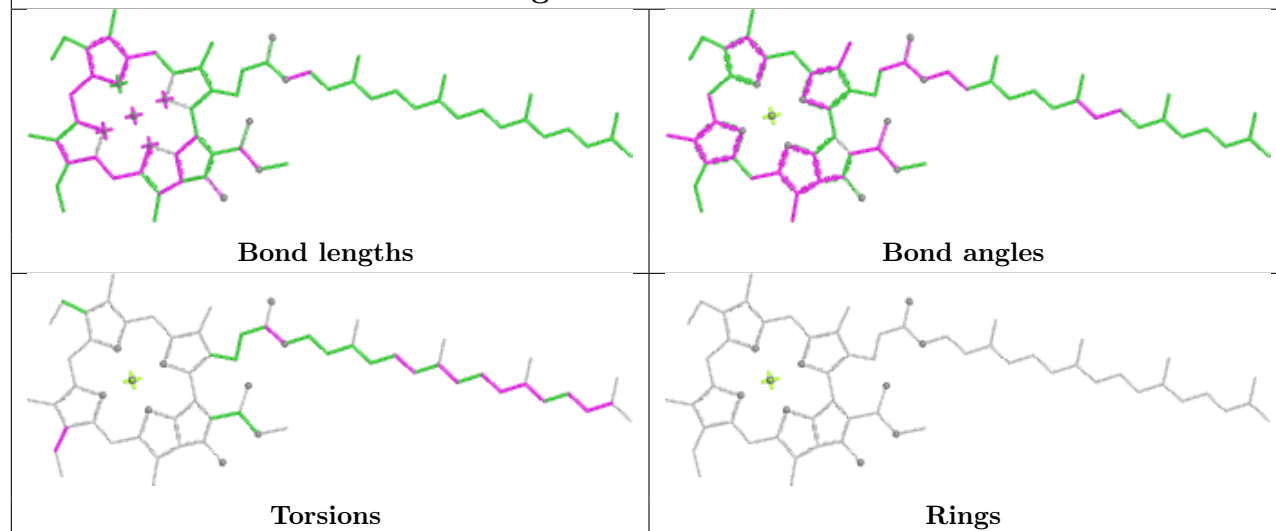
Rings



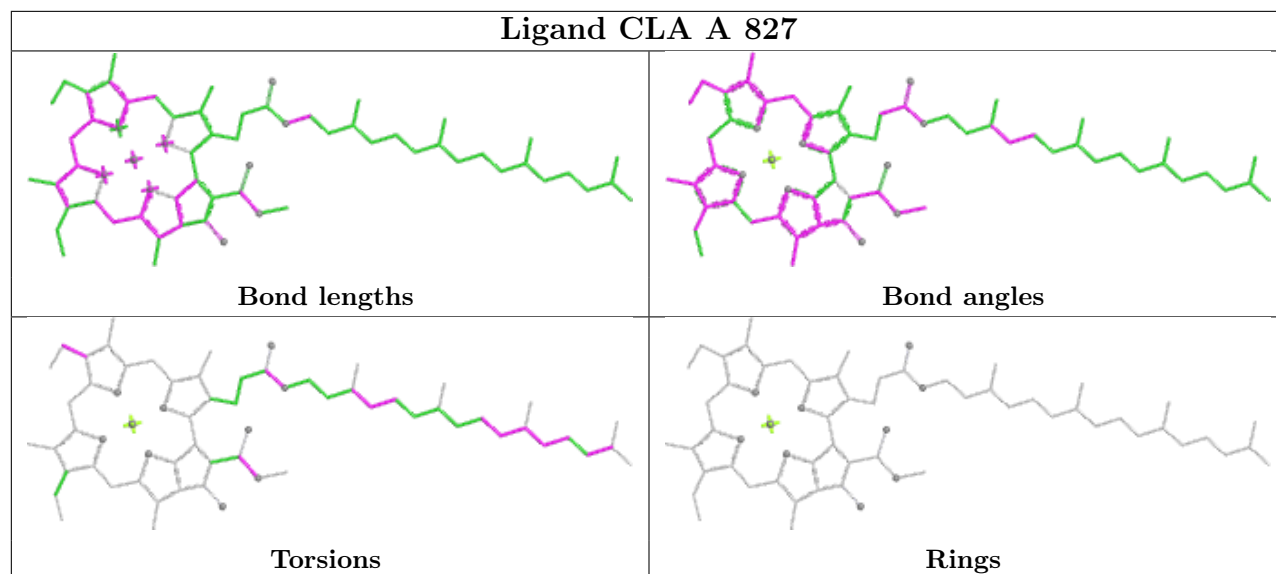
Ligand CLA A 816



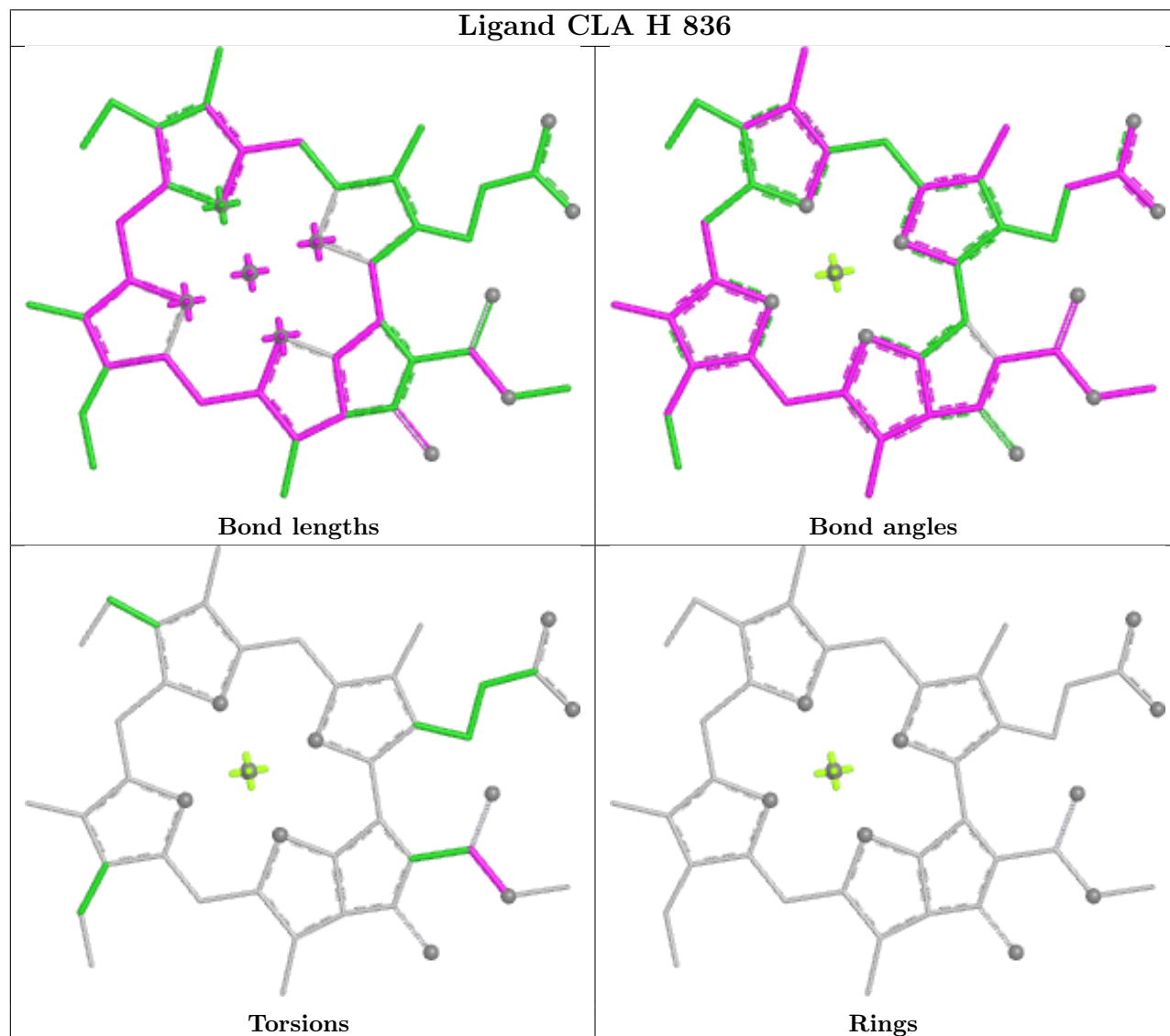
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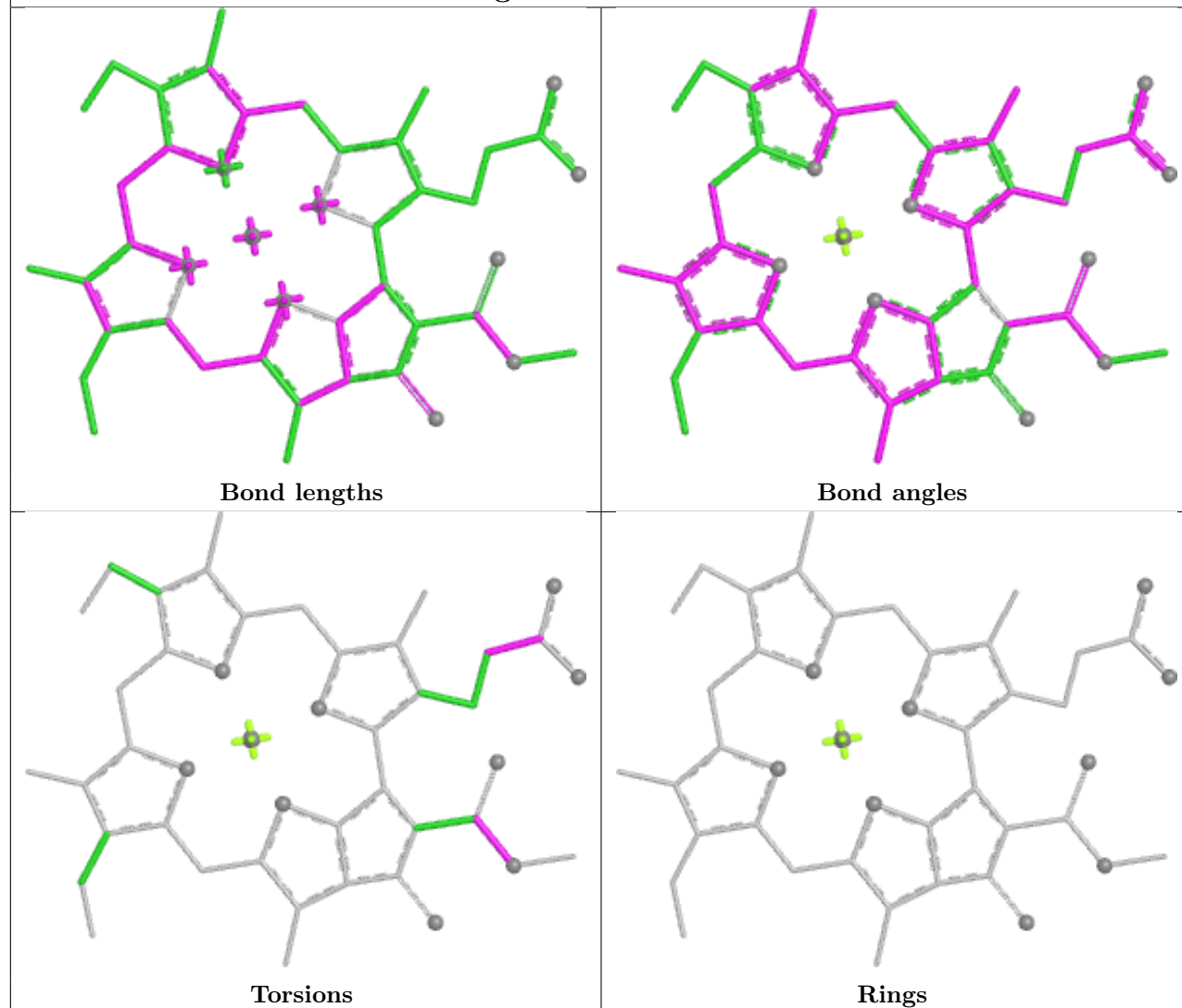
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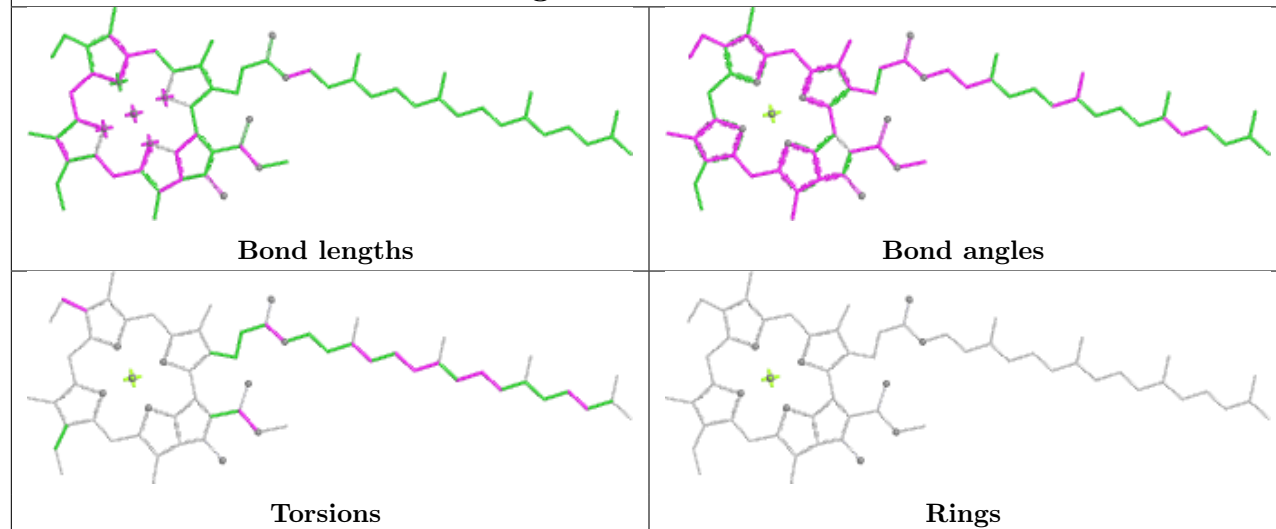
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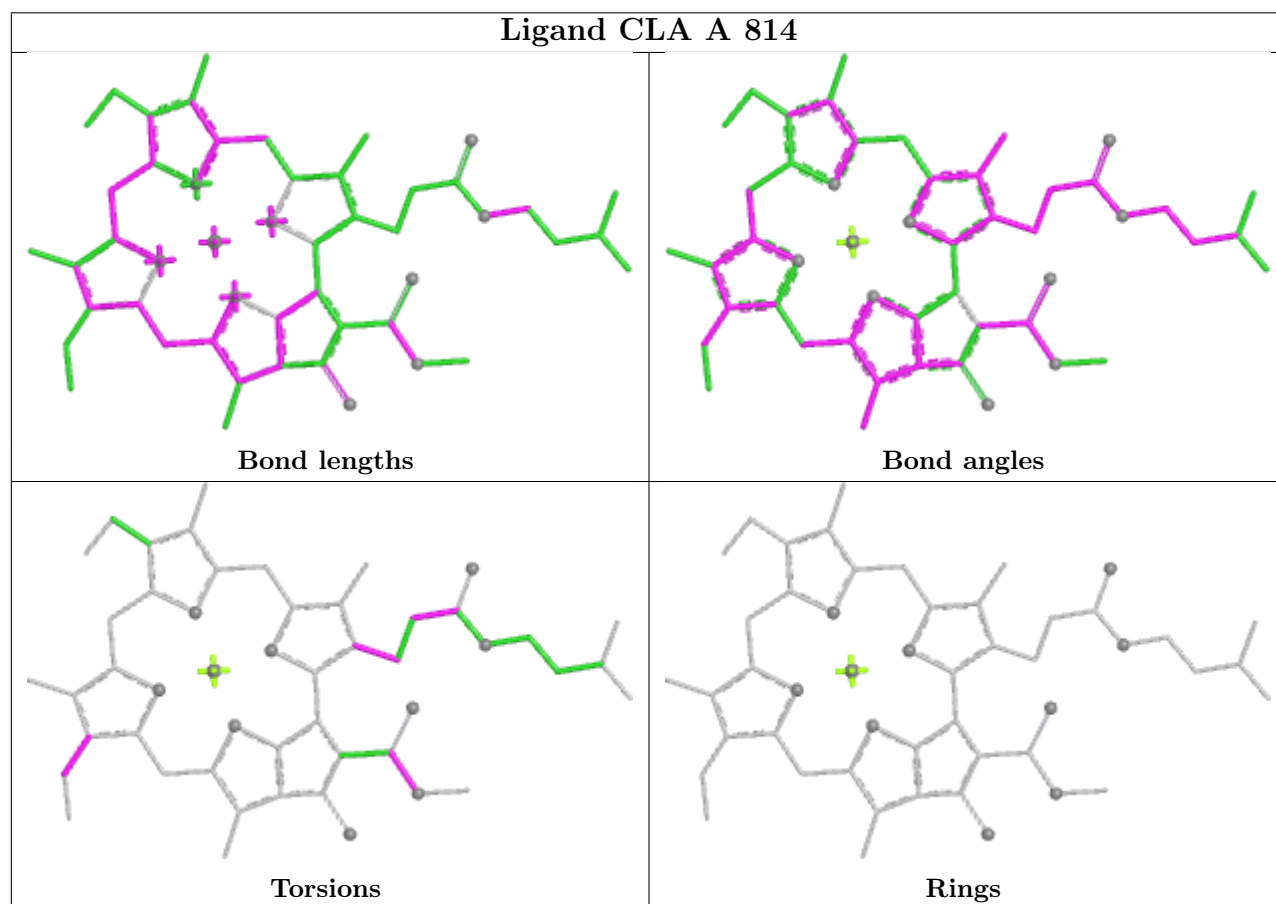
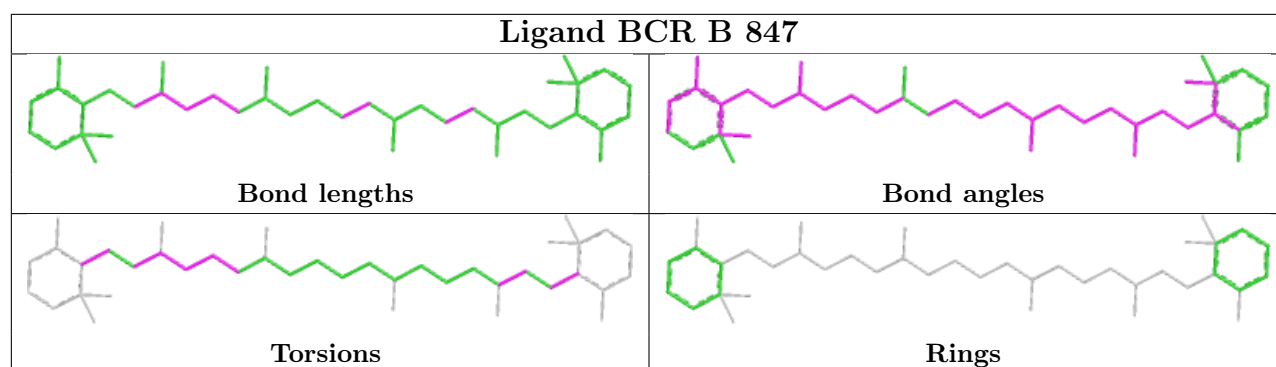


Ligand CLA F 202

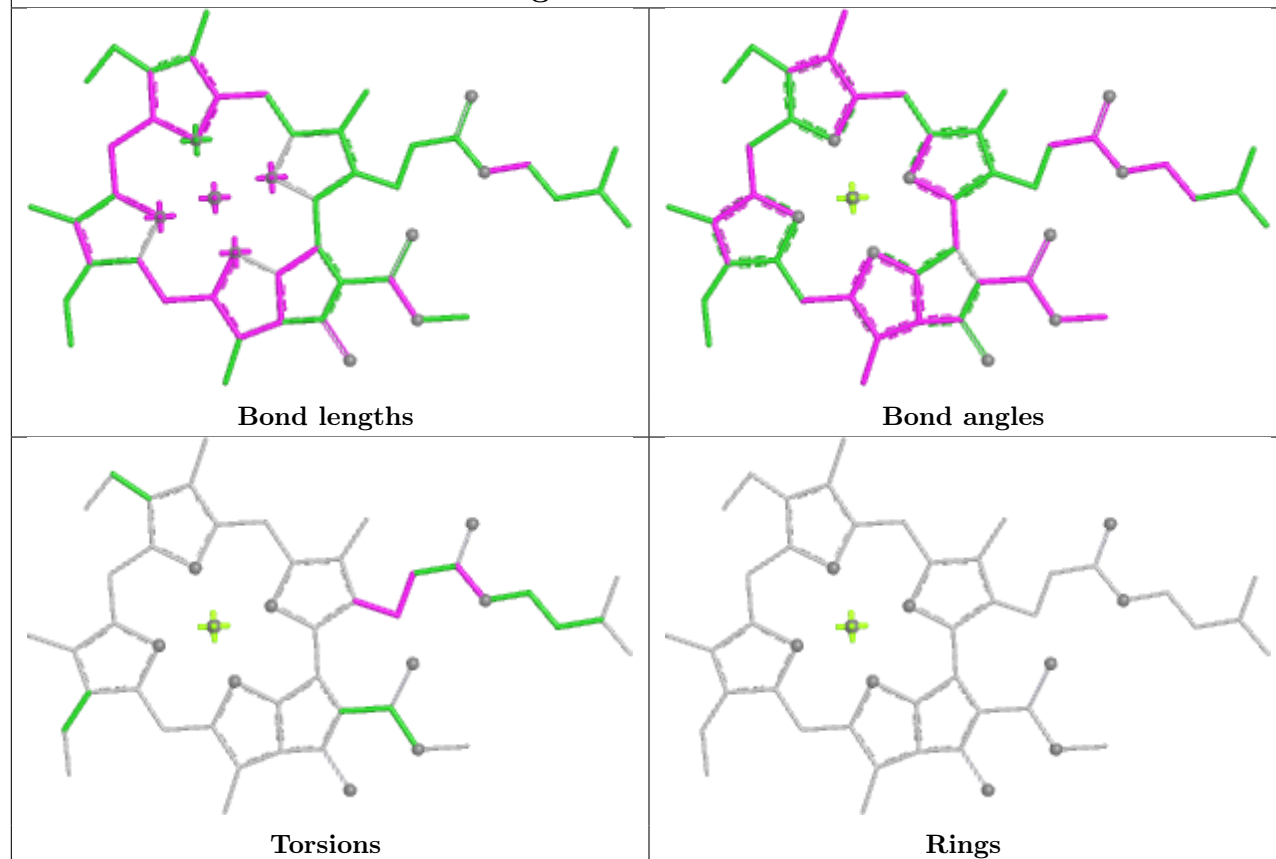


Ligand CLA A 833

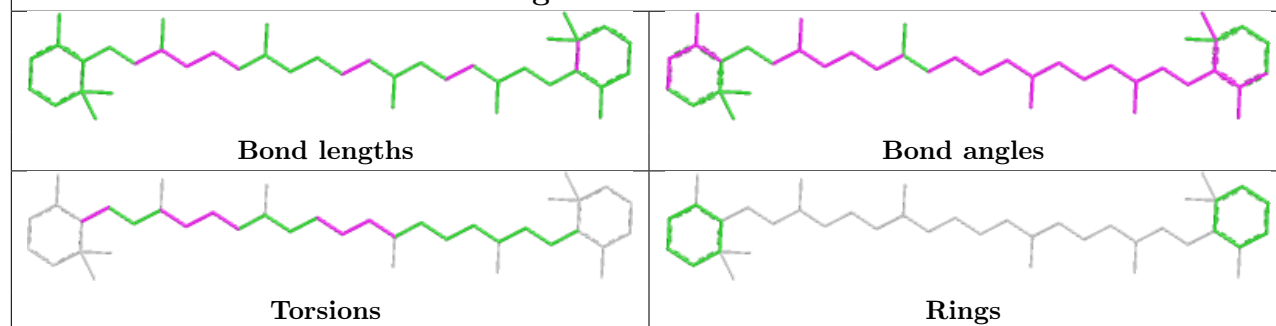




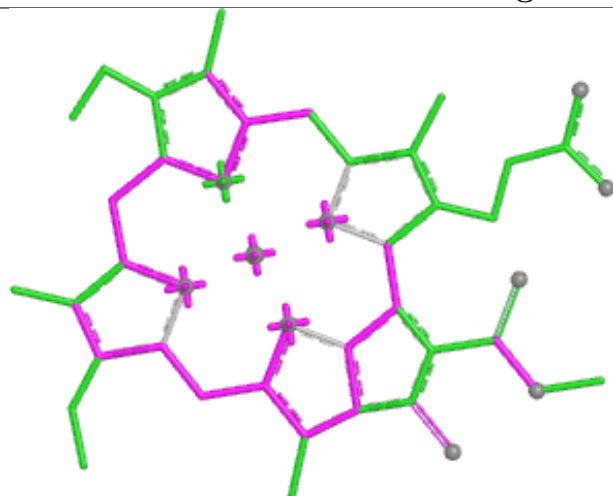
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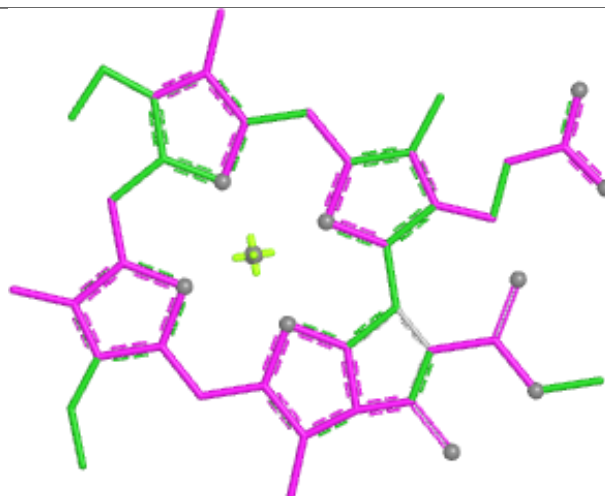
Ligand BCR Z 846



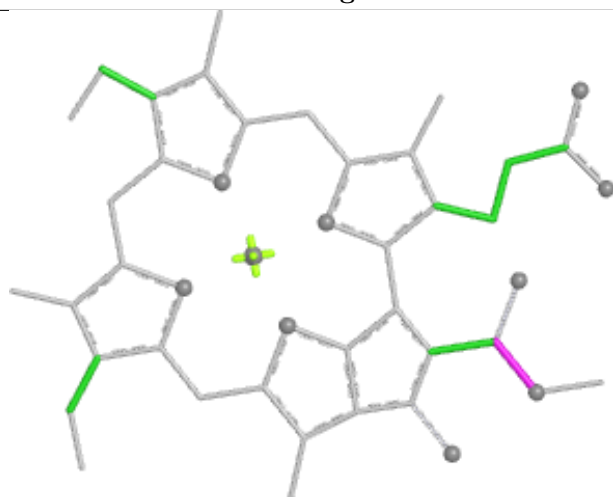
Ligand CLA Z 813



Bond lengths



Bond angles

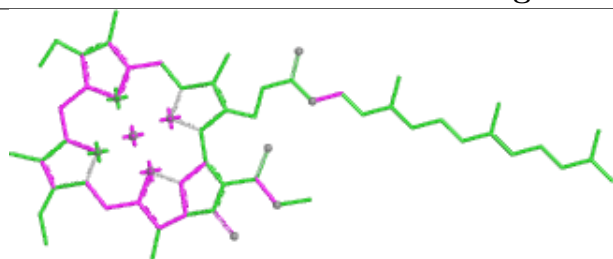


Torsions

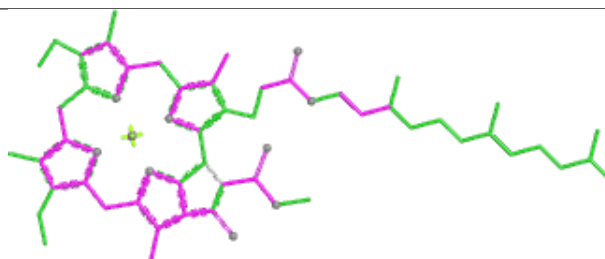


Rings

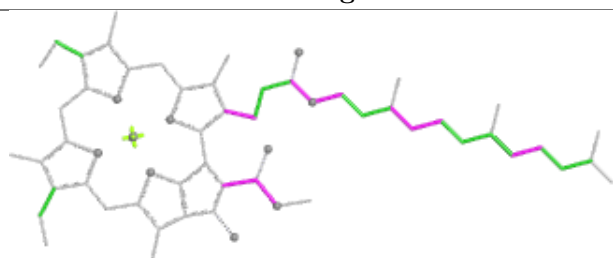
Ligand CLA H 834



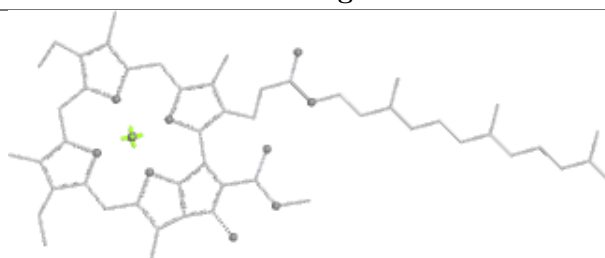
Bond lengths



Bond angles

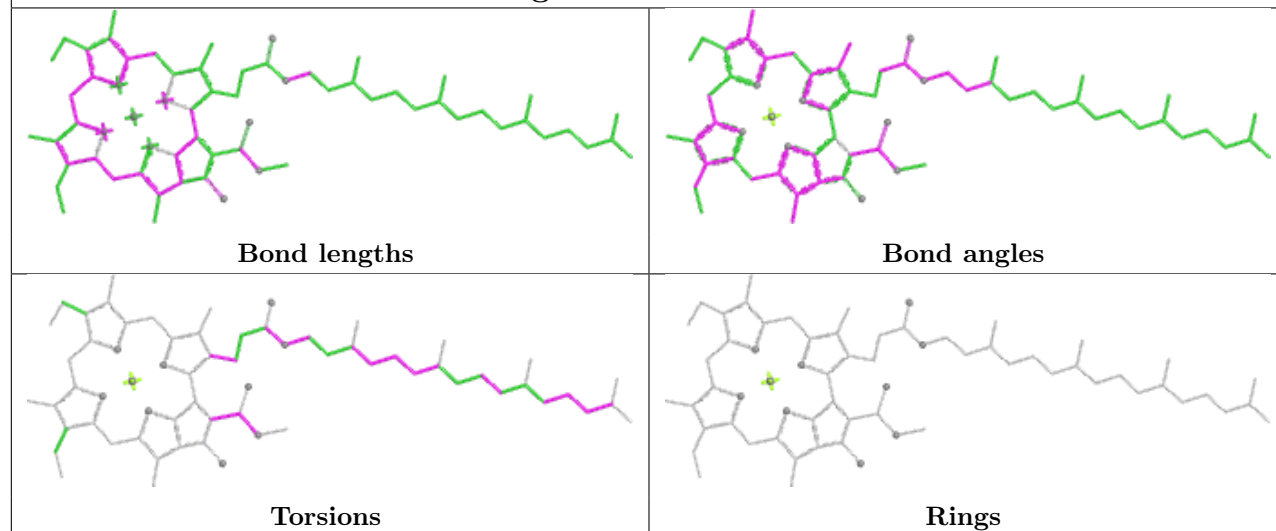


Torsions

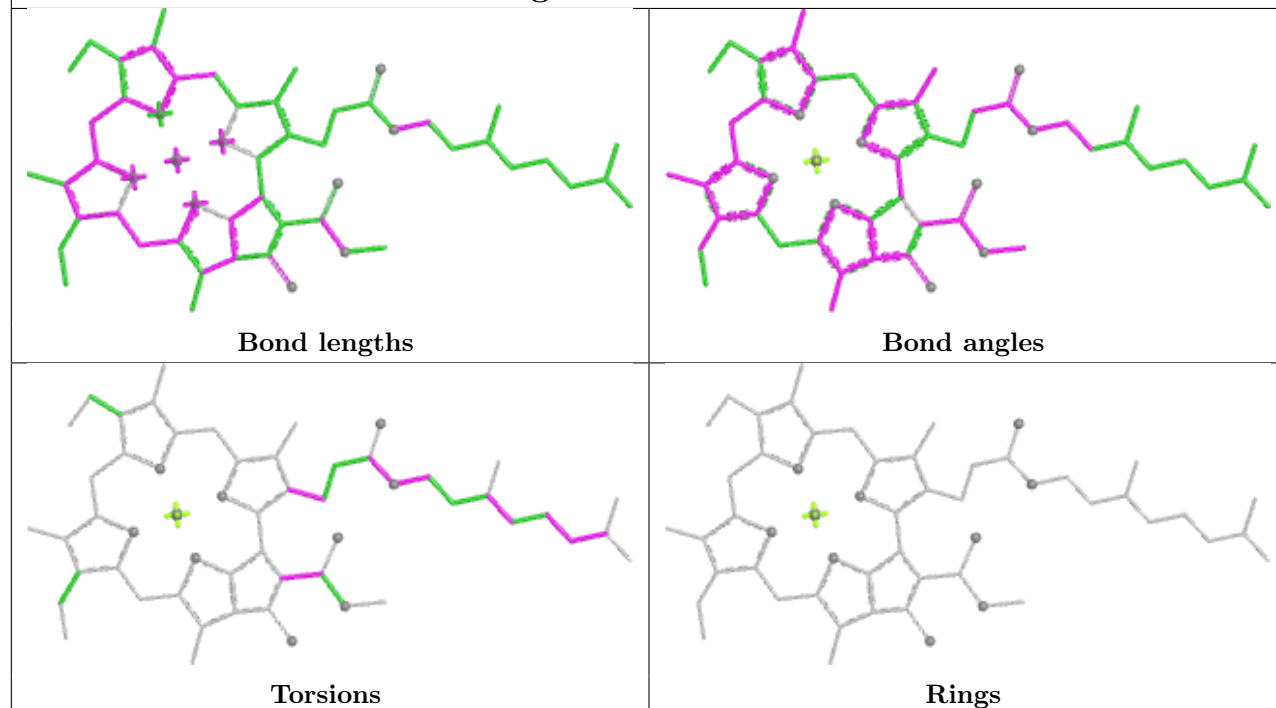


Rings

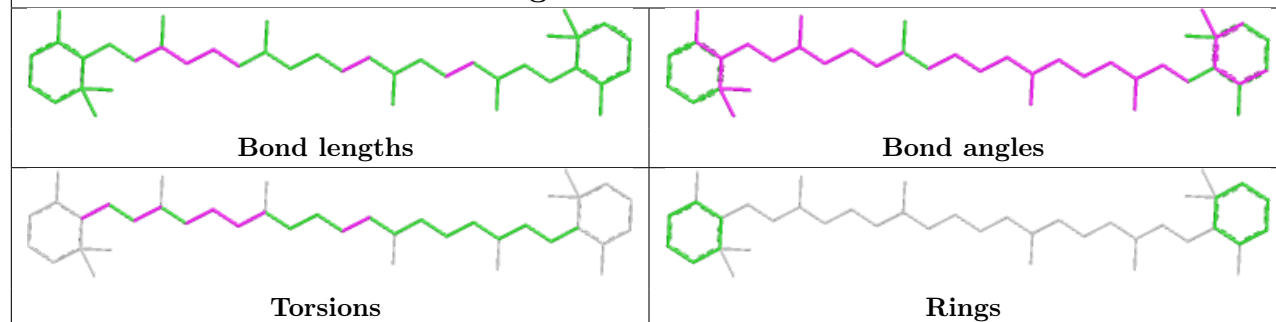
Ligand CLA Y 819



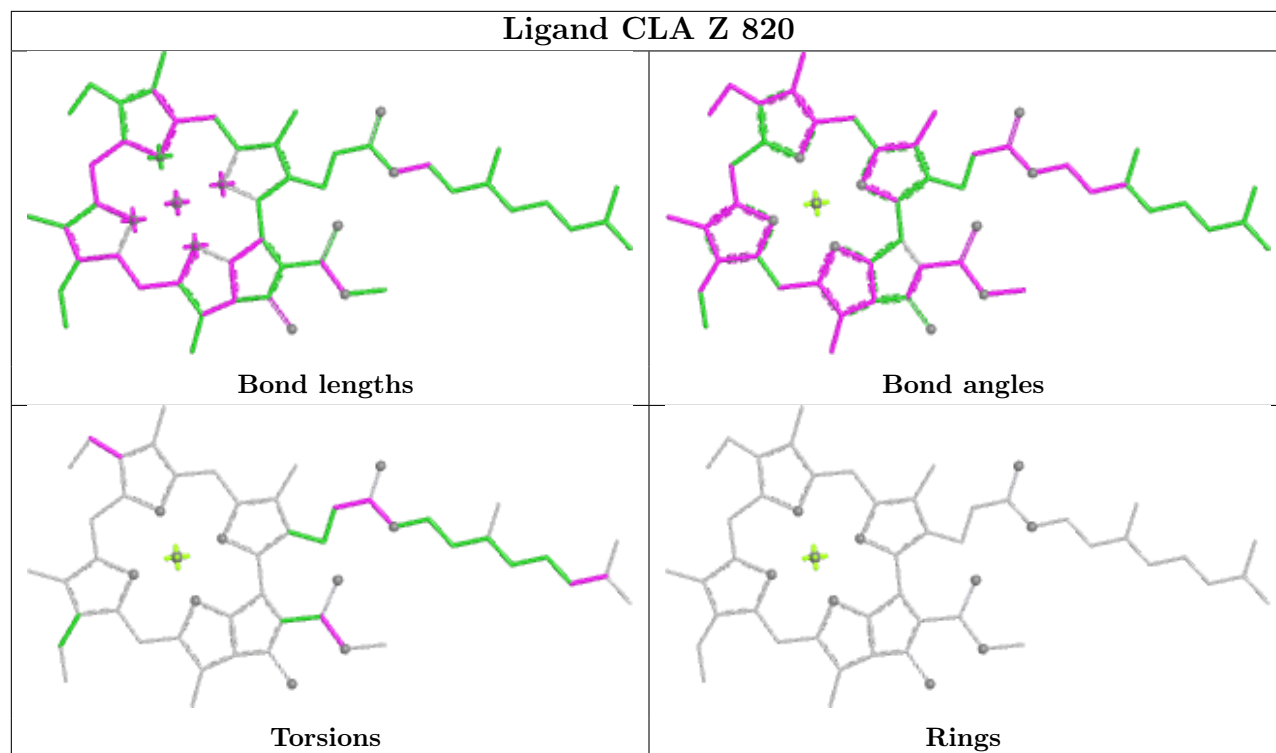
Ligand CLA H 823



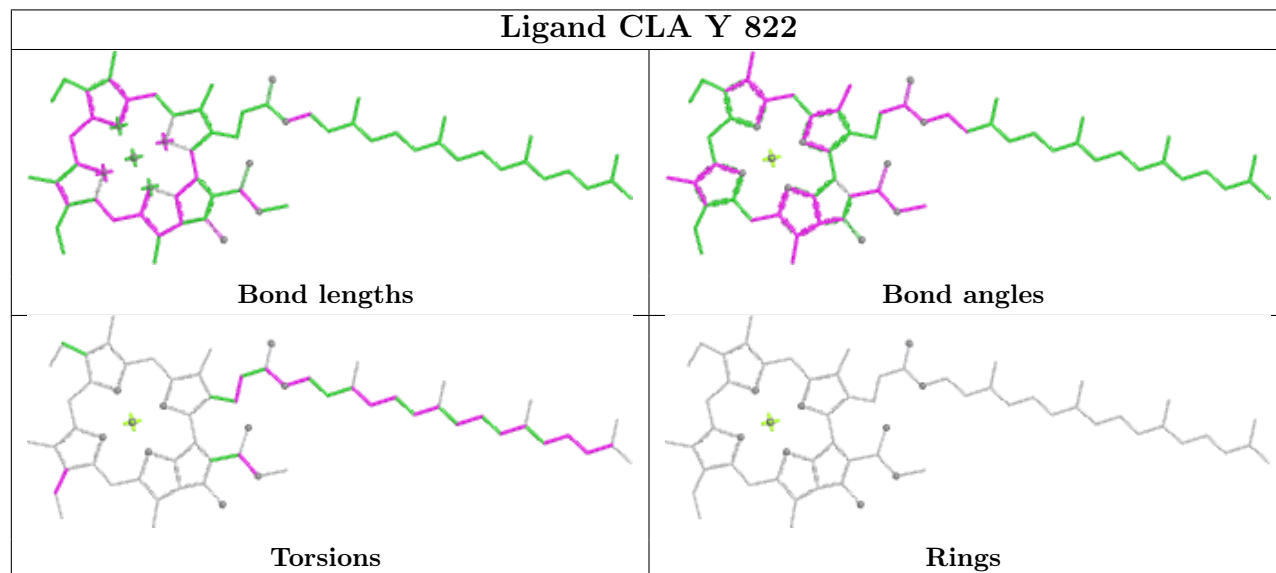
Ligand BCR G 849



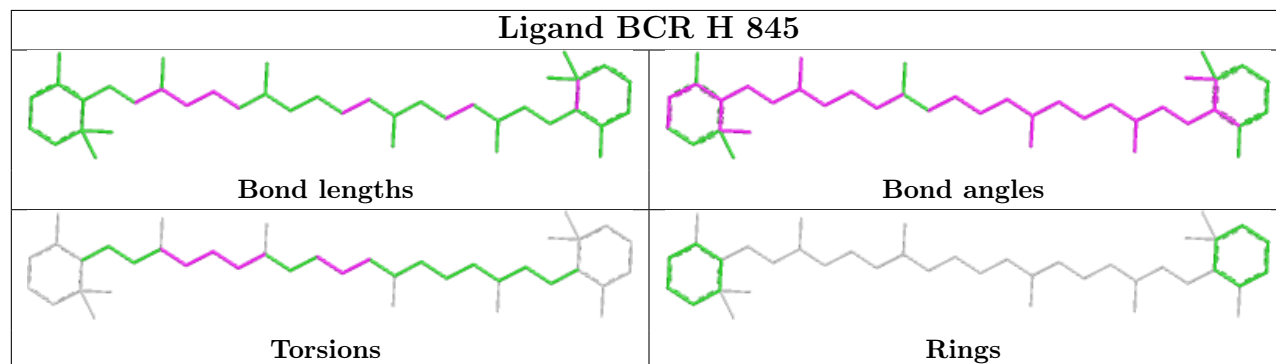
Ligand CLA Z 820



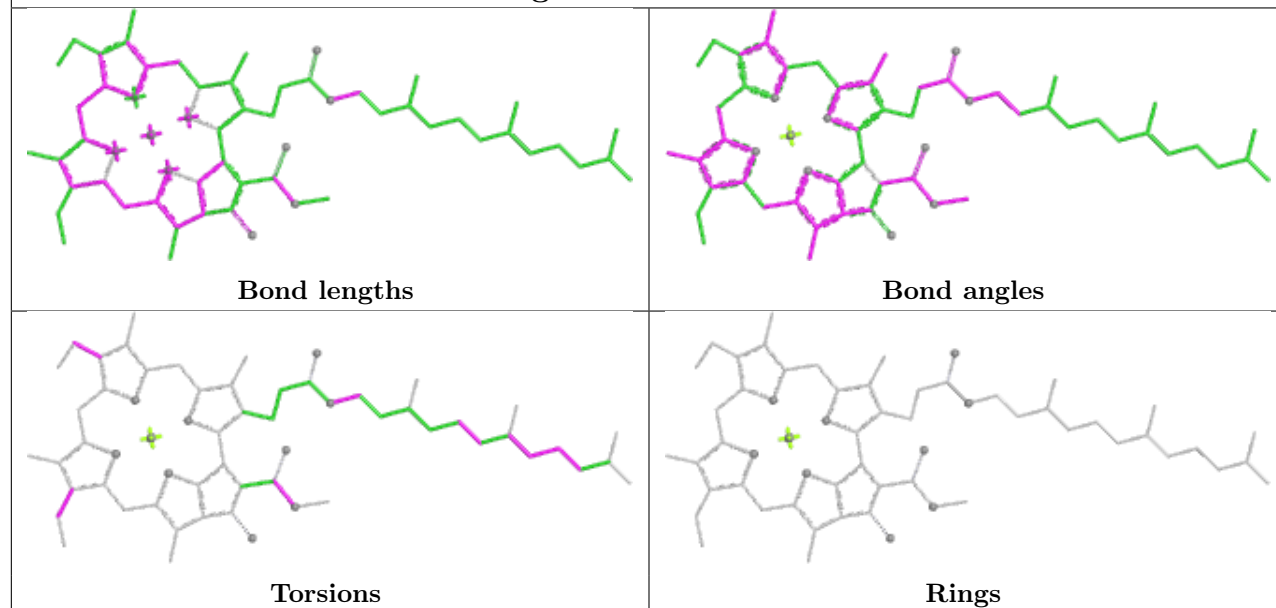
Ligand CLA Y 822



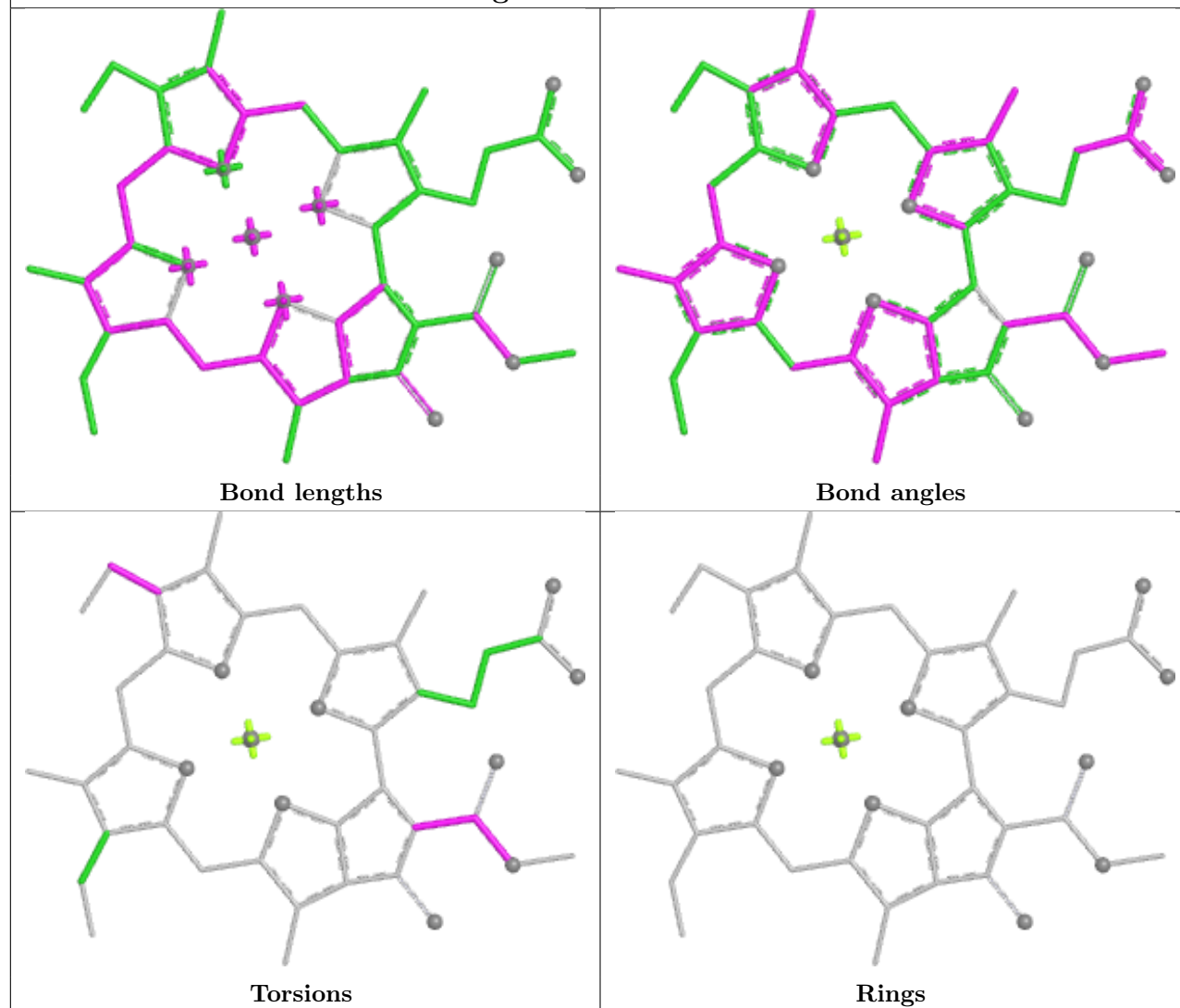
Ligand BCR H 845

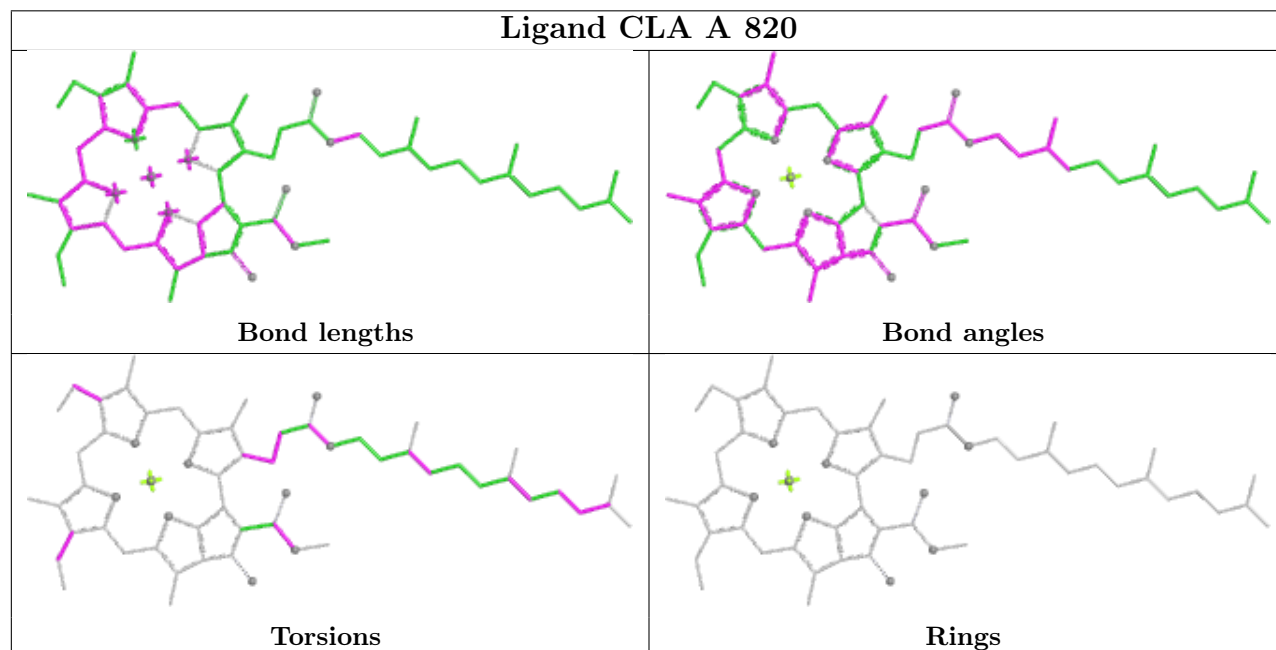
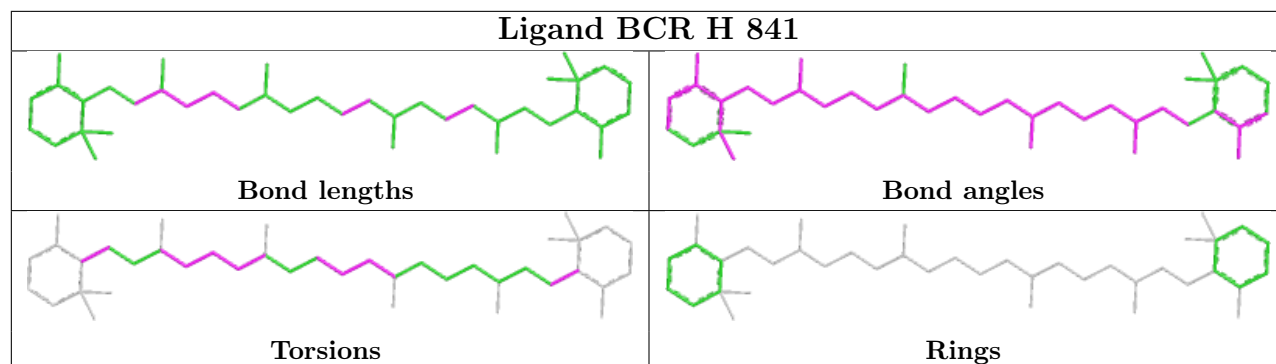


Ligand CLA Y 817

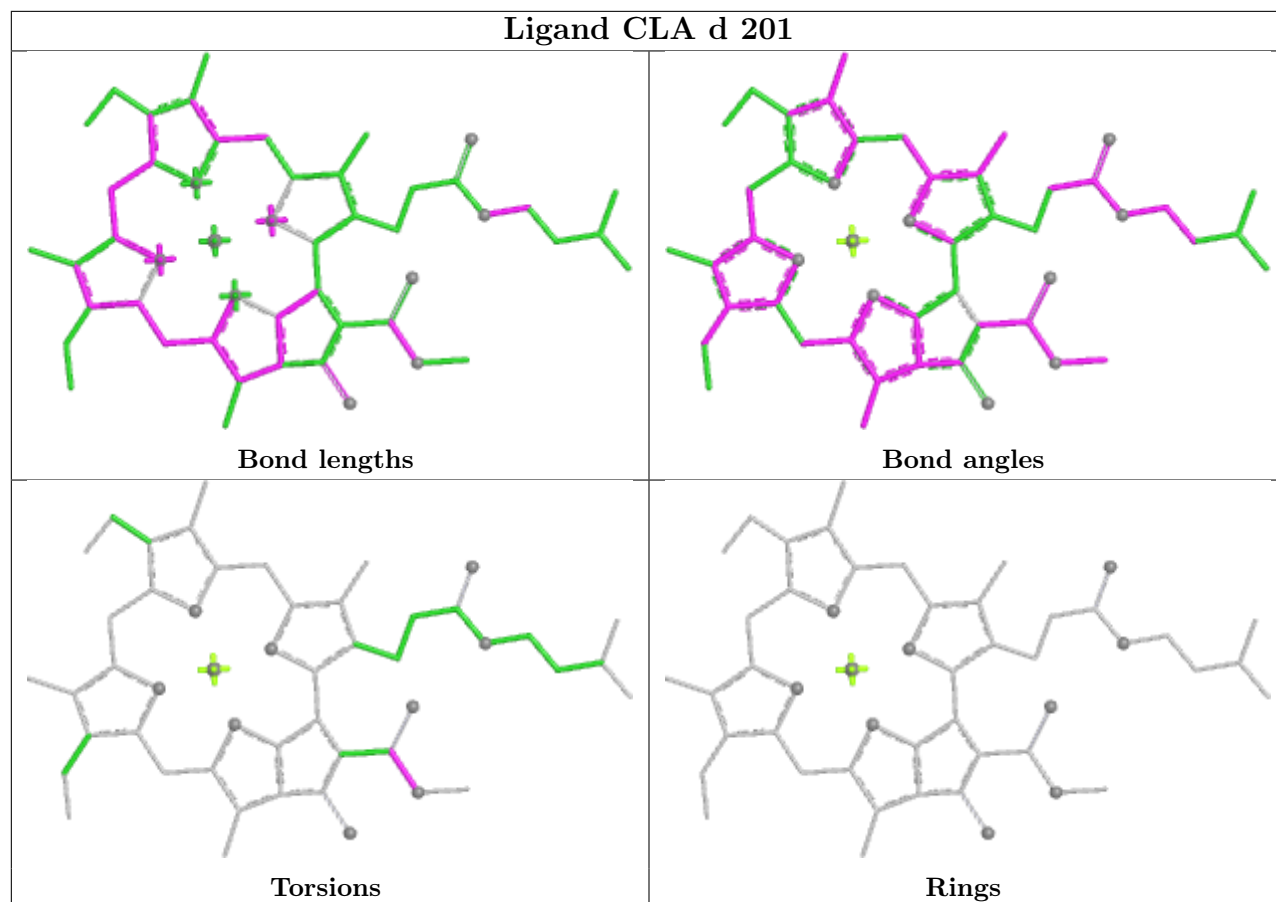


Ligand CLA T 103

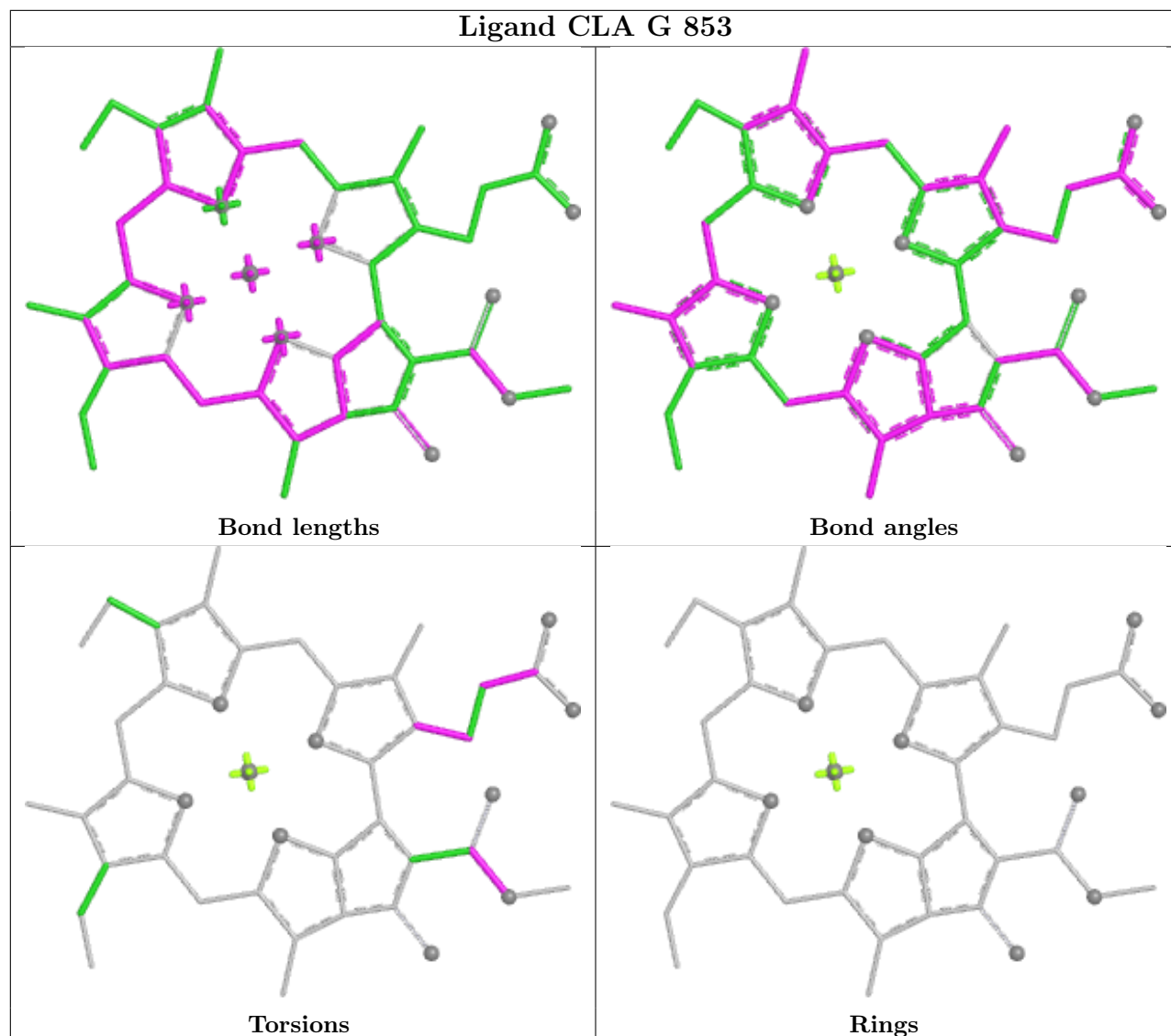




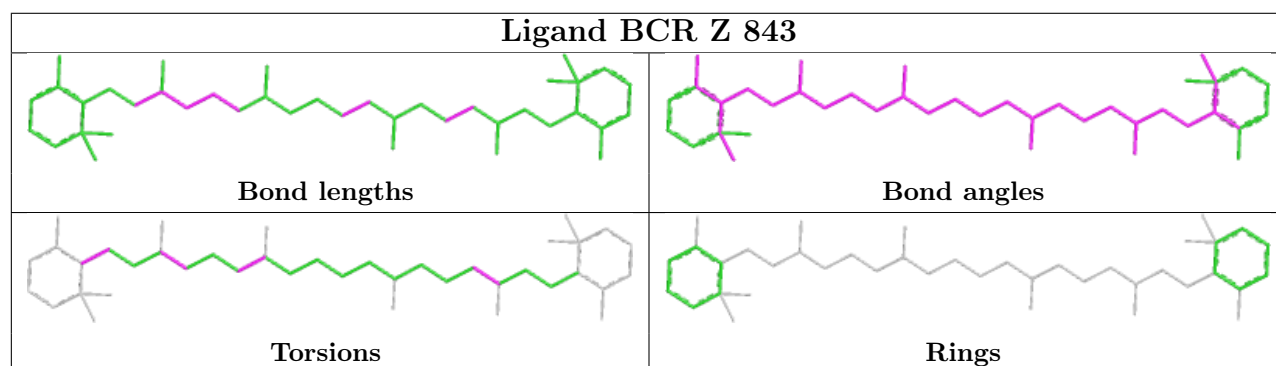
Ligand CLA d 201



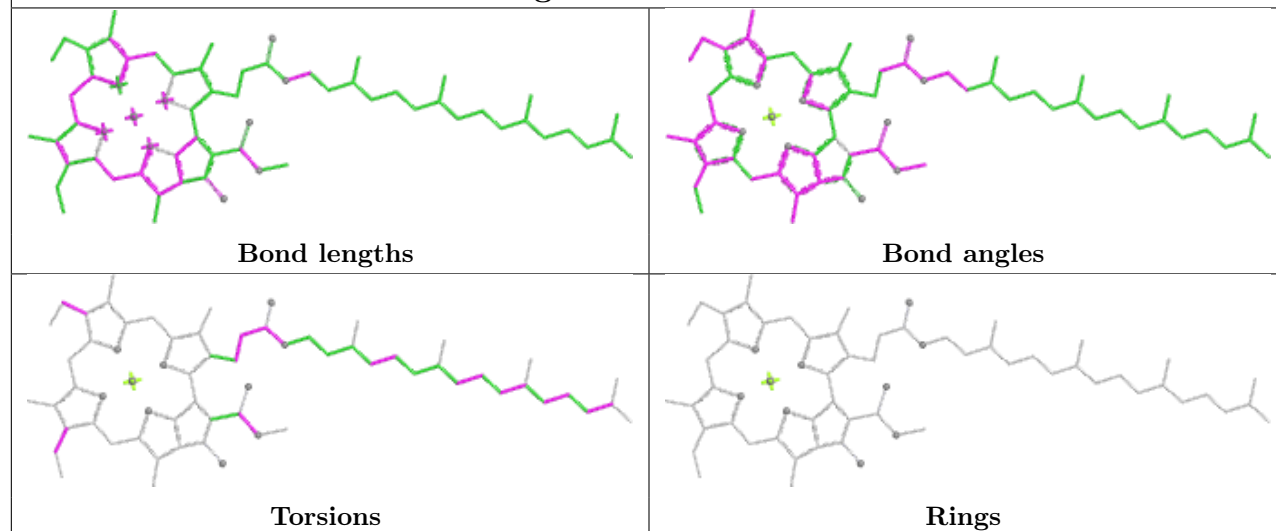
Ligand CLA G 853



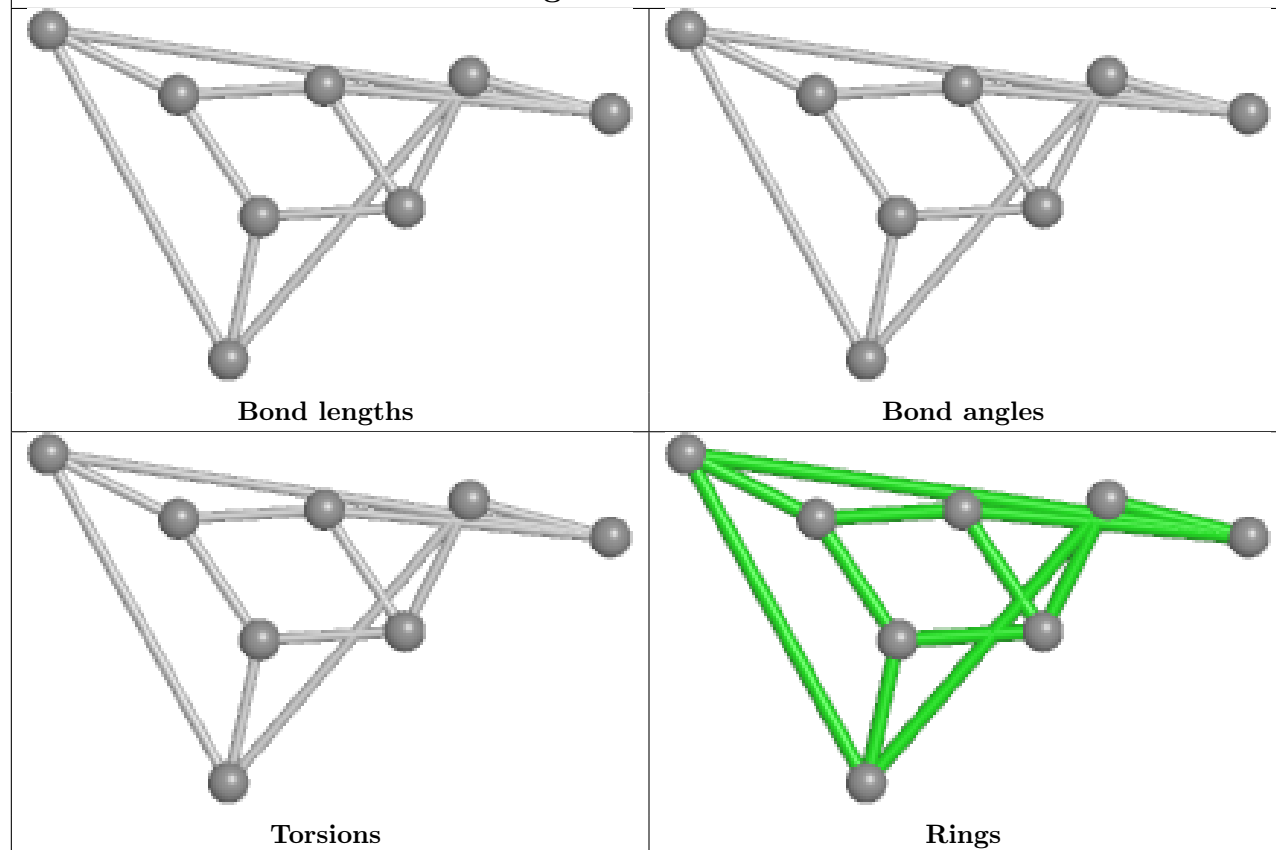
Ligand BCR Z 843



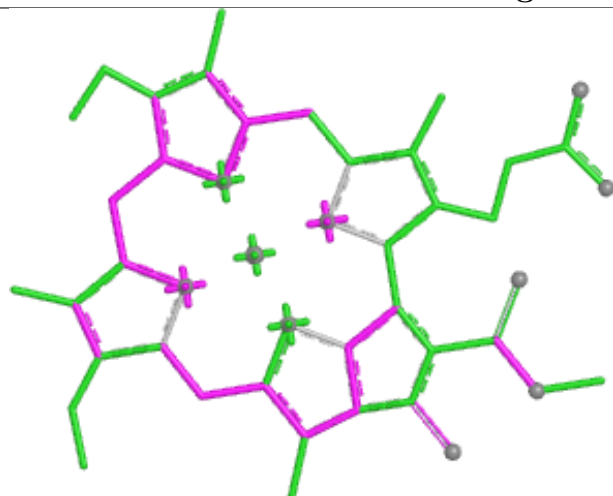
Ligand CLA Z 806



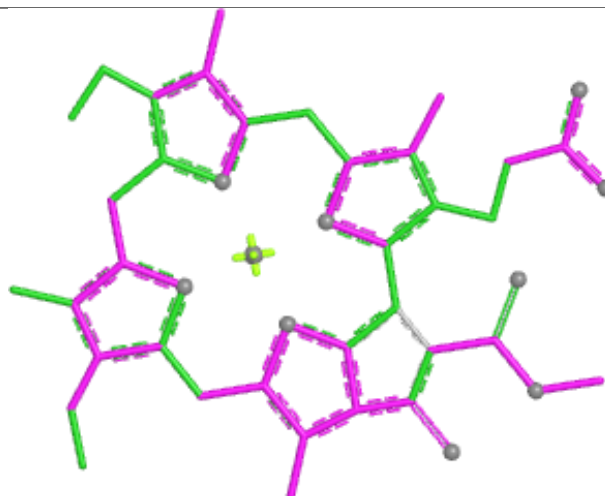
Ligand SF4 a 101



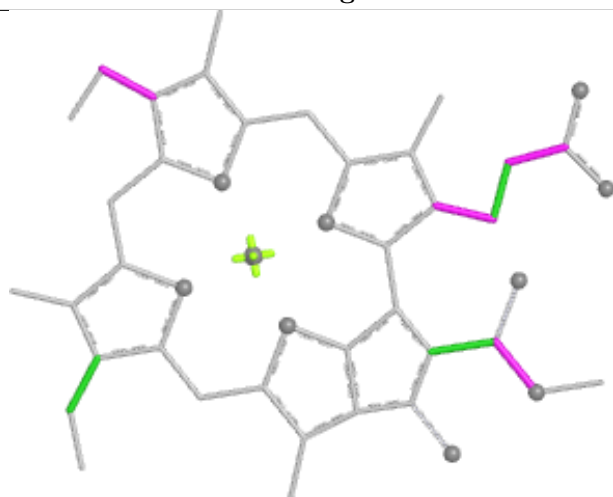
Ligand CLA Z 833



Bond lengths



Bond angles

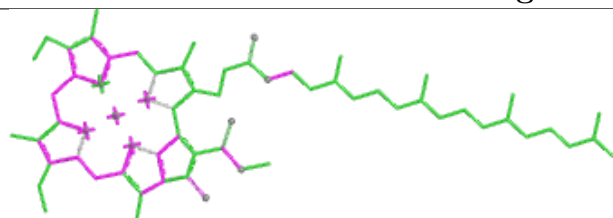


Torsions

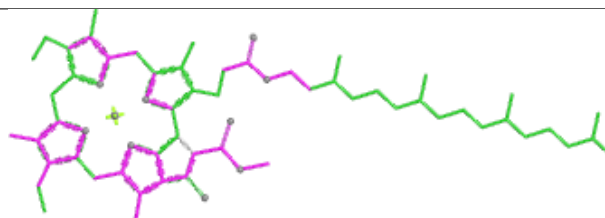


Rings

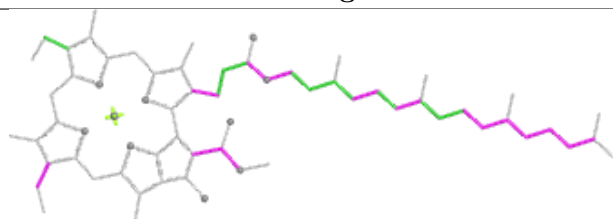
Ligand CLA L 205



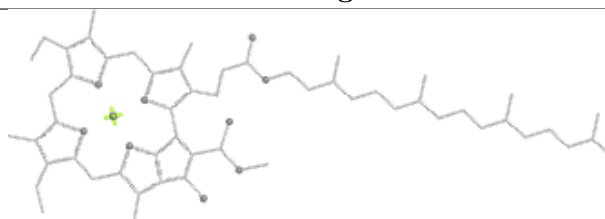
Bond lengths



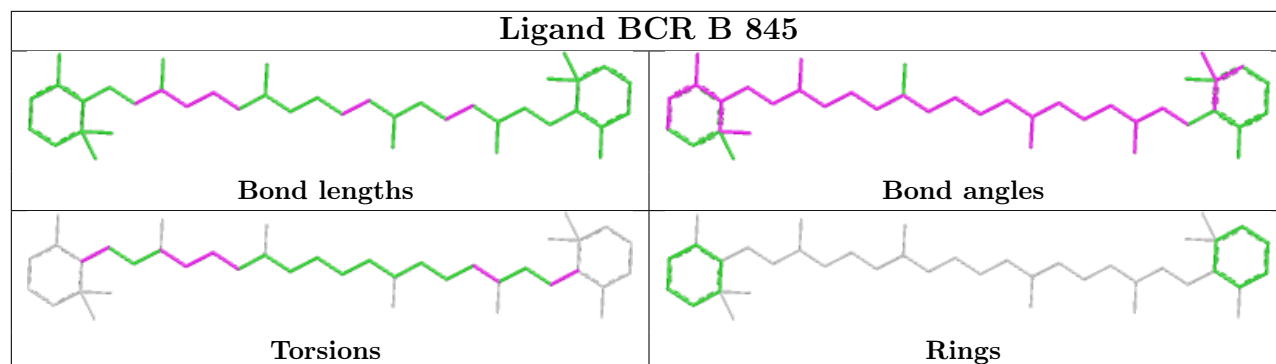
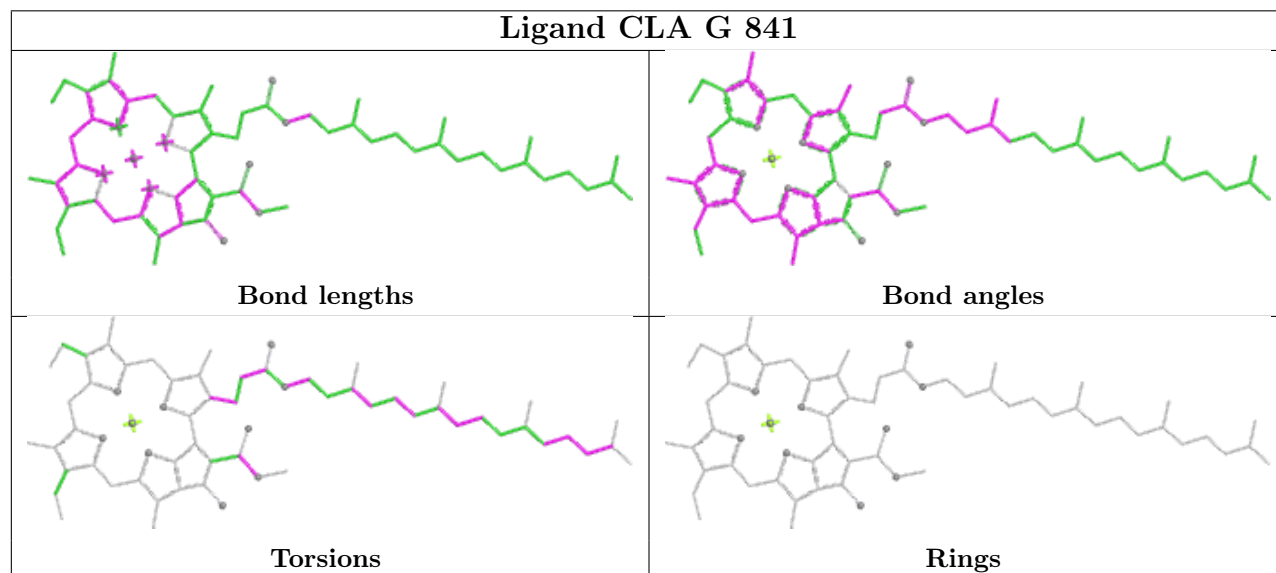
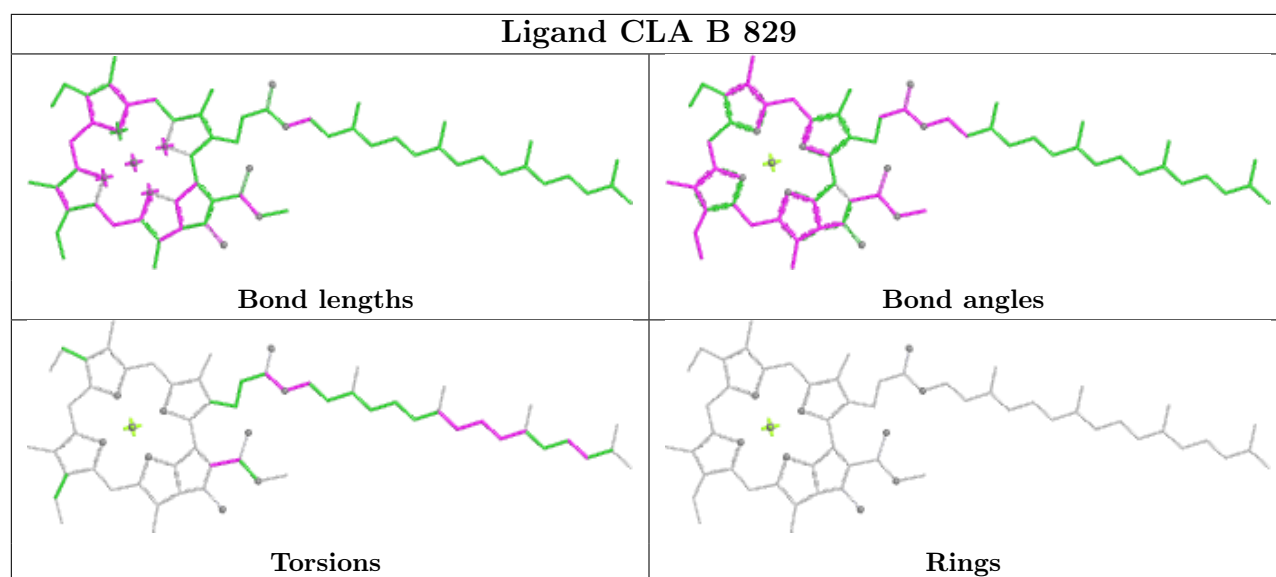
Bond angles



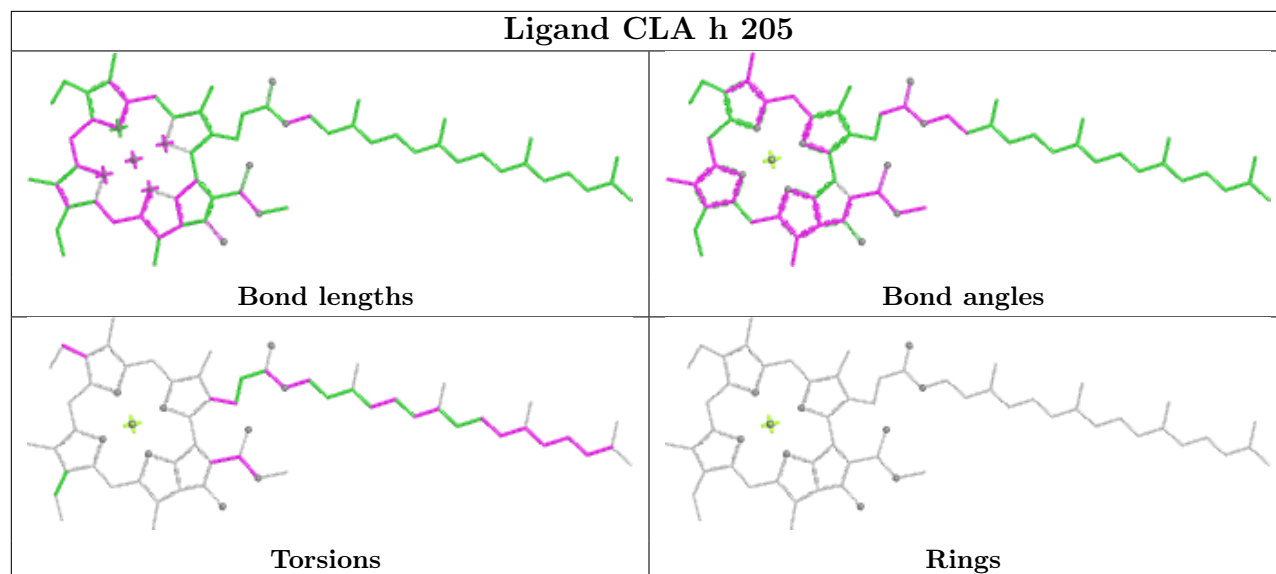
Torsions



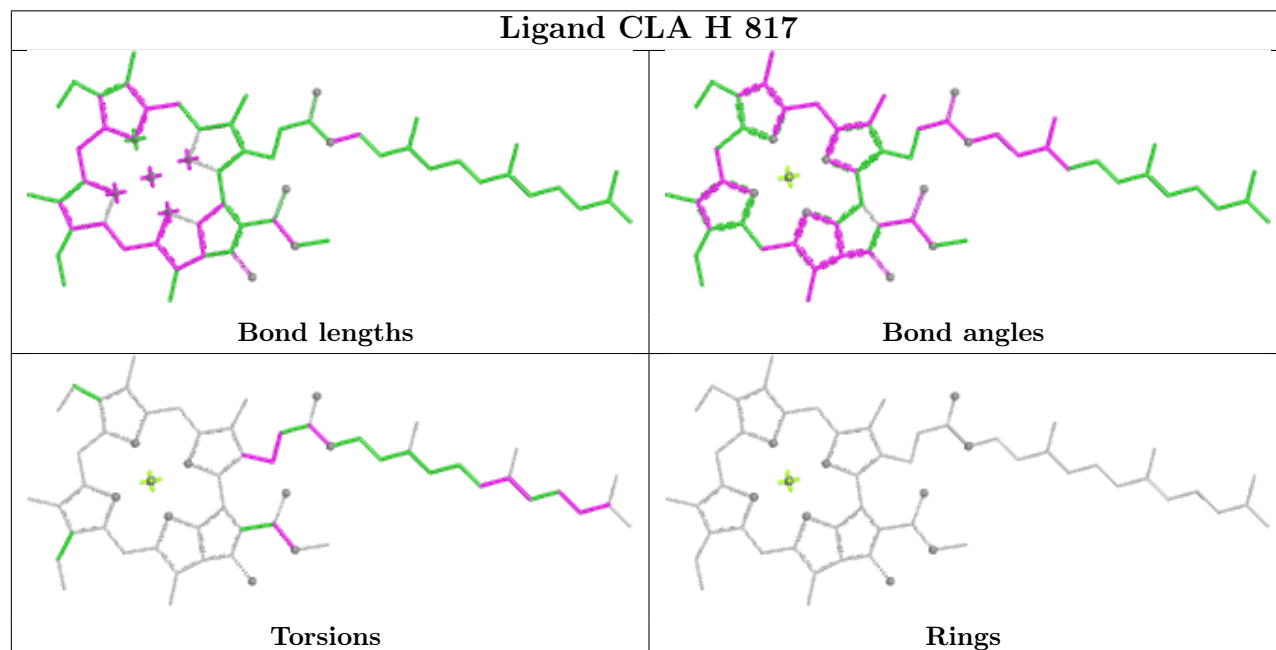
Rings

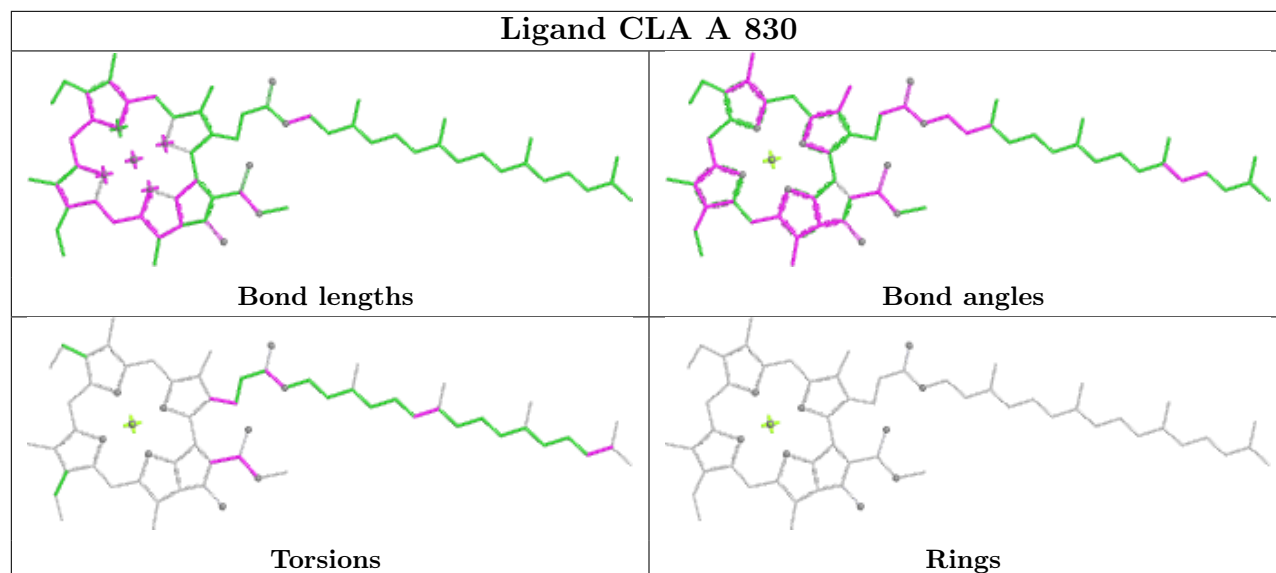
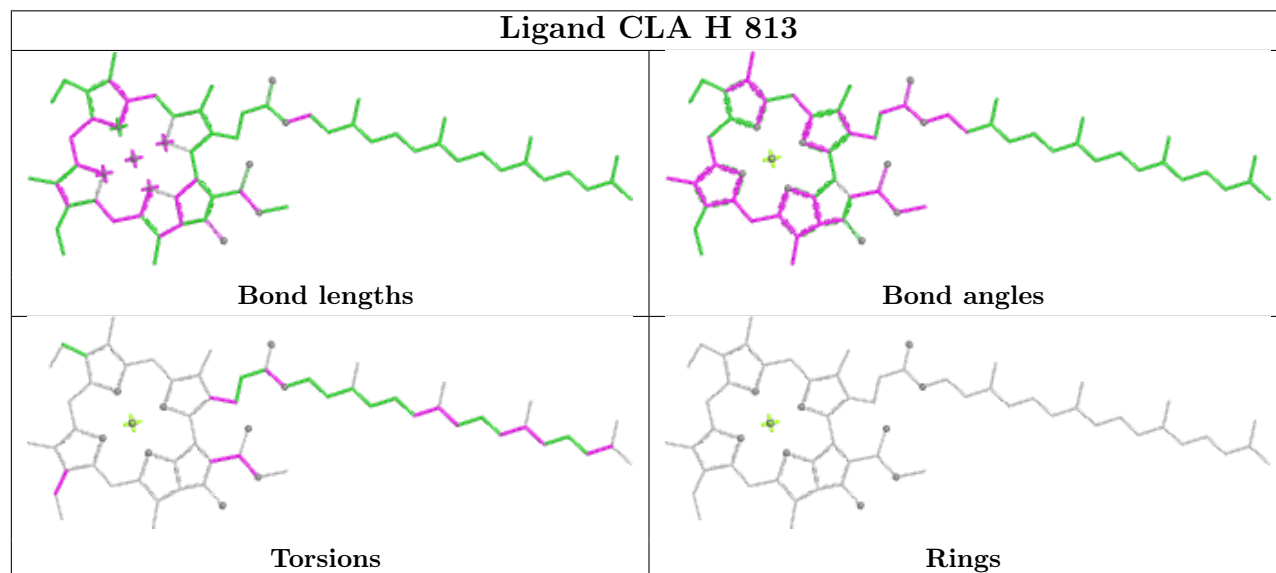
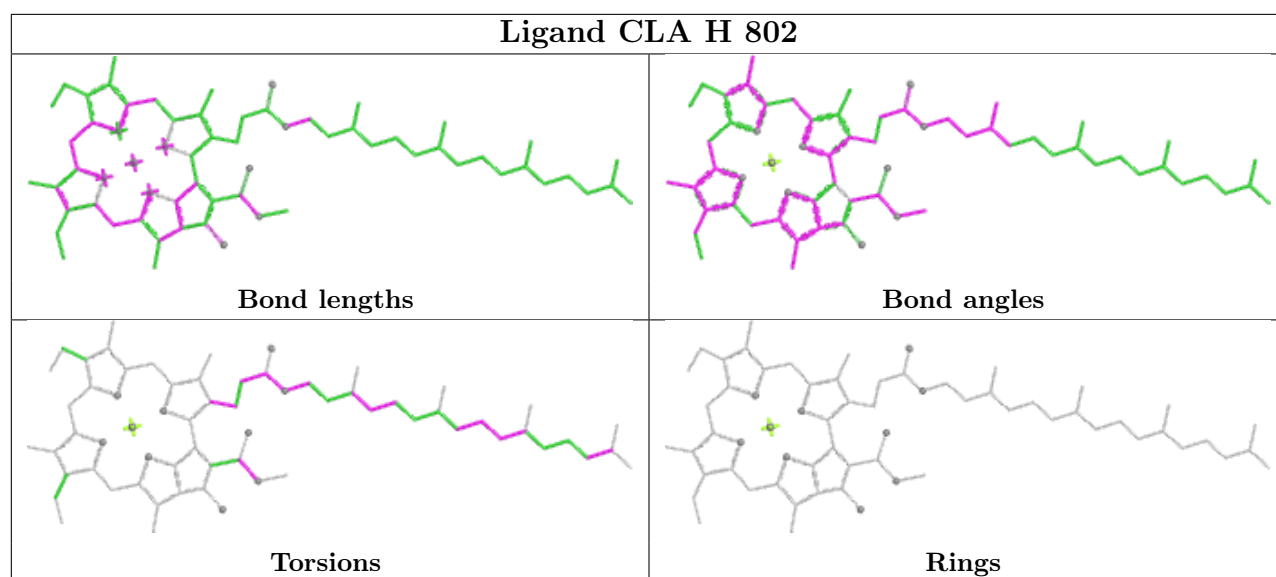


Ligand CLA h 205

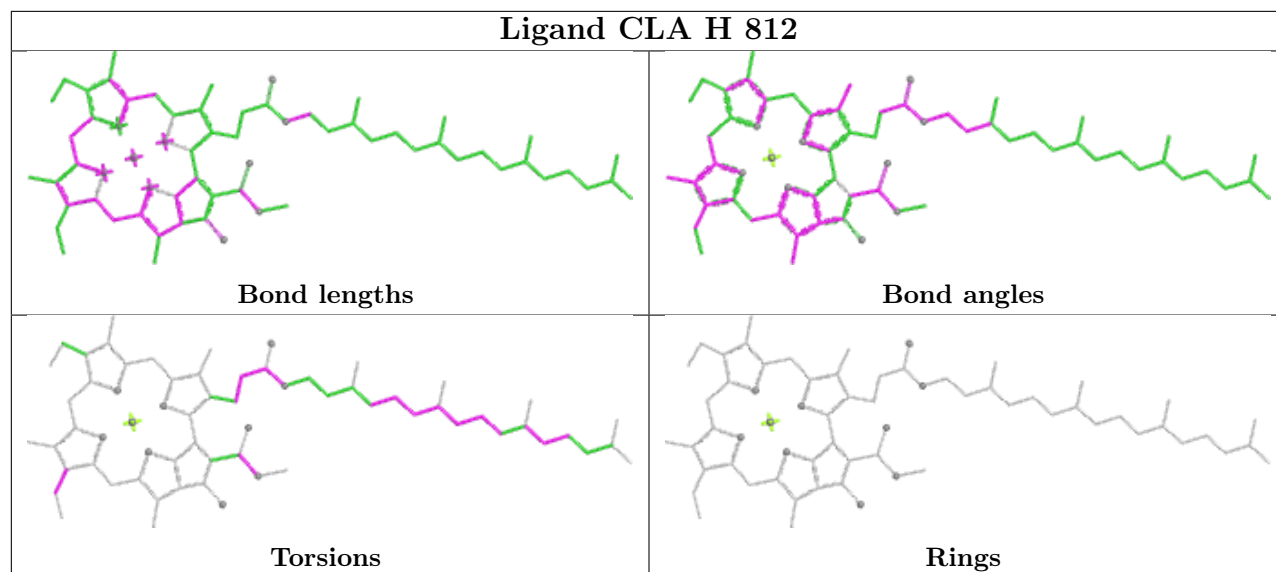


Ligand CLA H 817

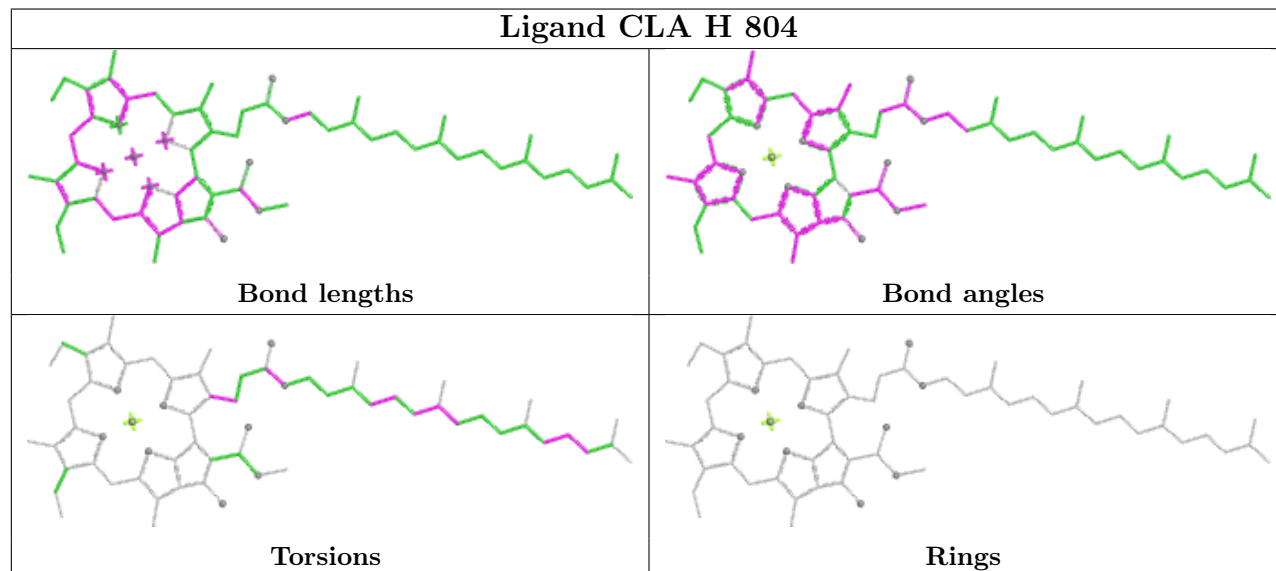




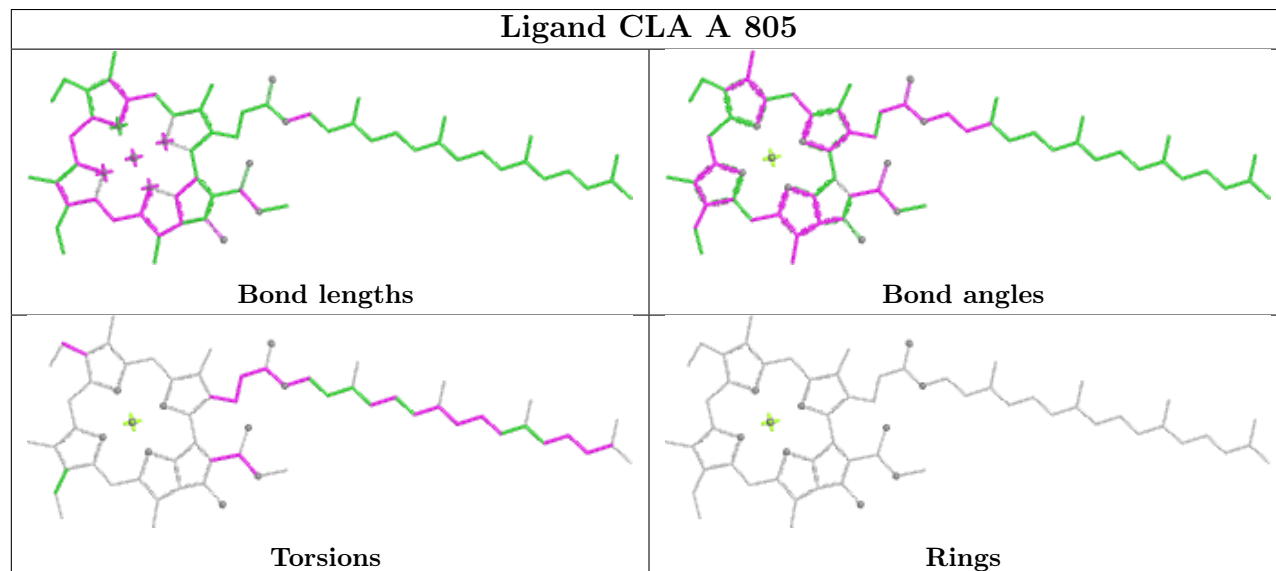
Ligand CLA H 812



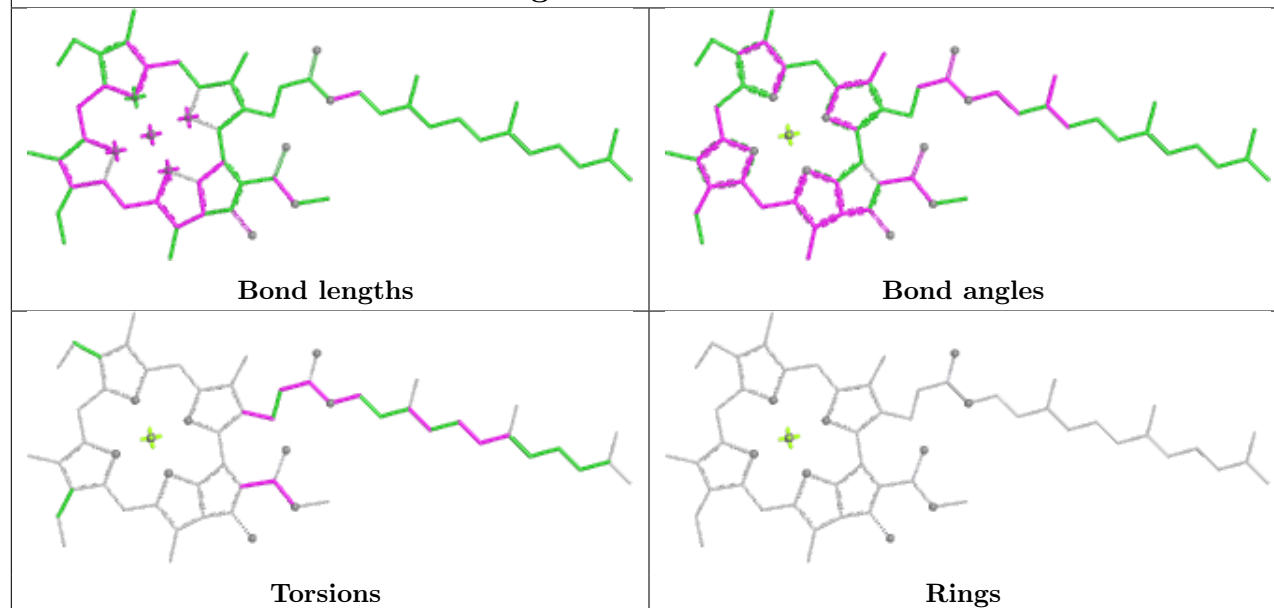
Ligand CLA H 804



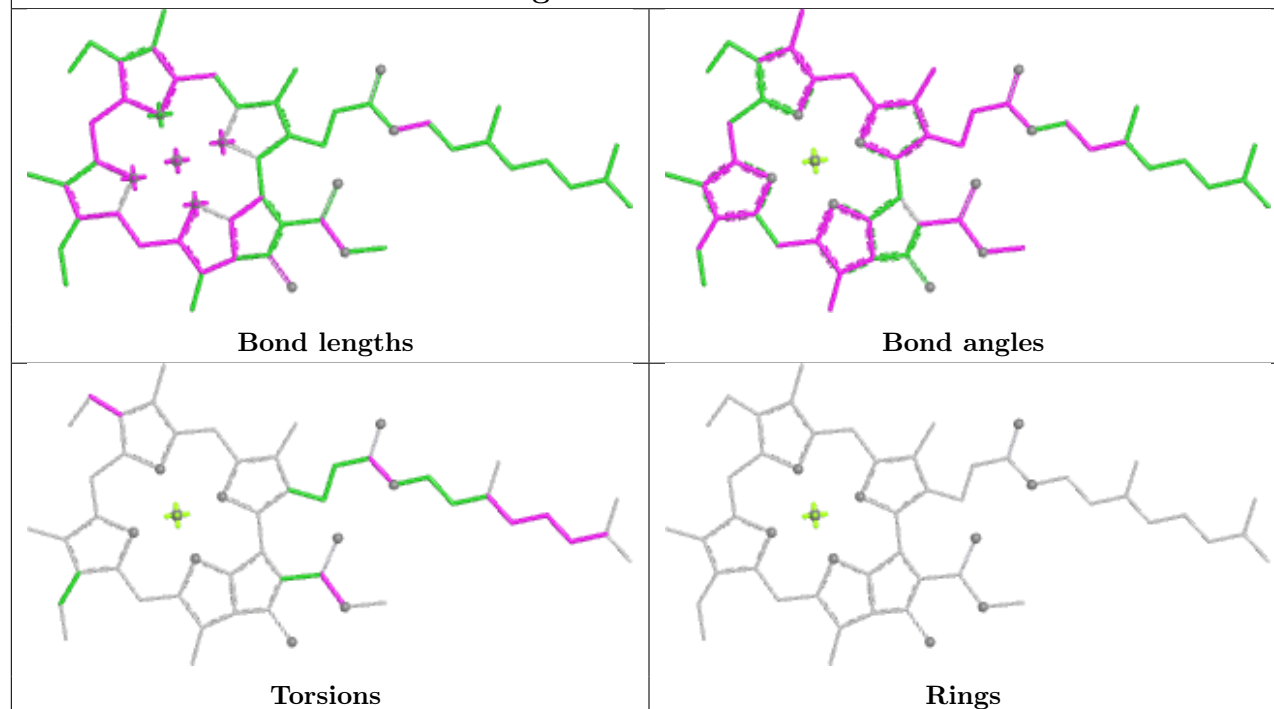
Ligand CLA A 805

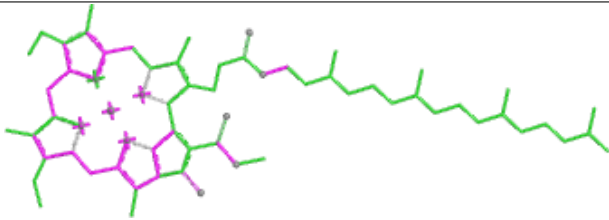
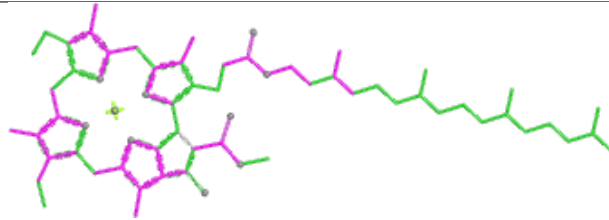
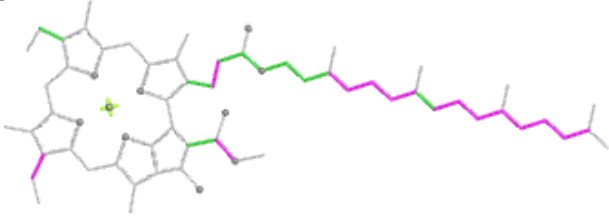
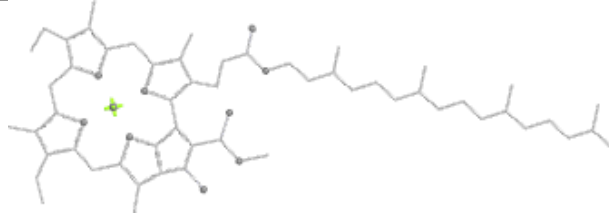


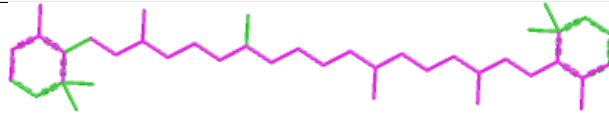
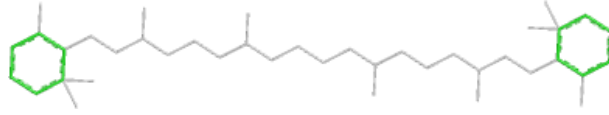
Ligand CLA G 820

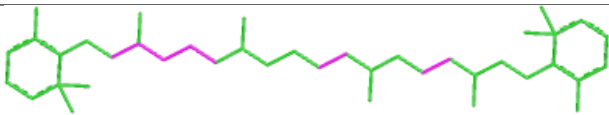
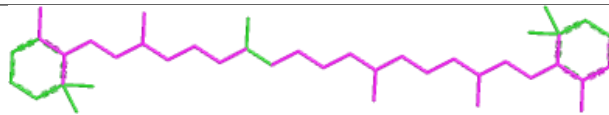
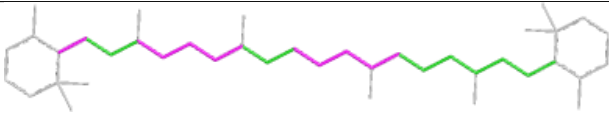
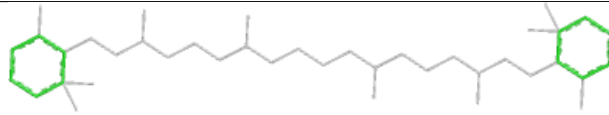


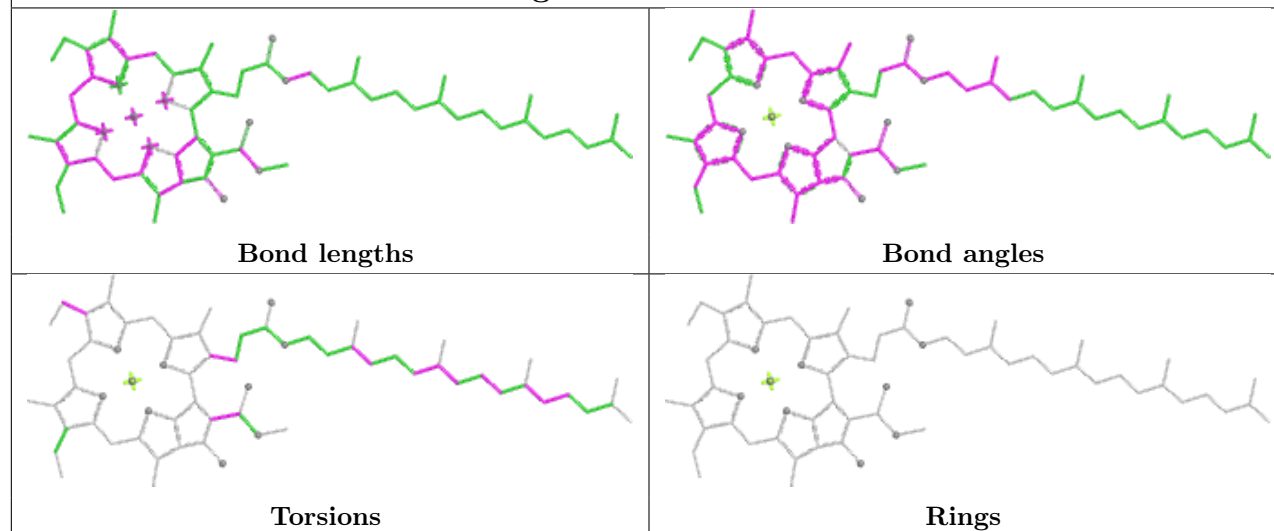
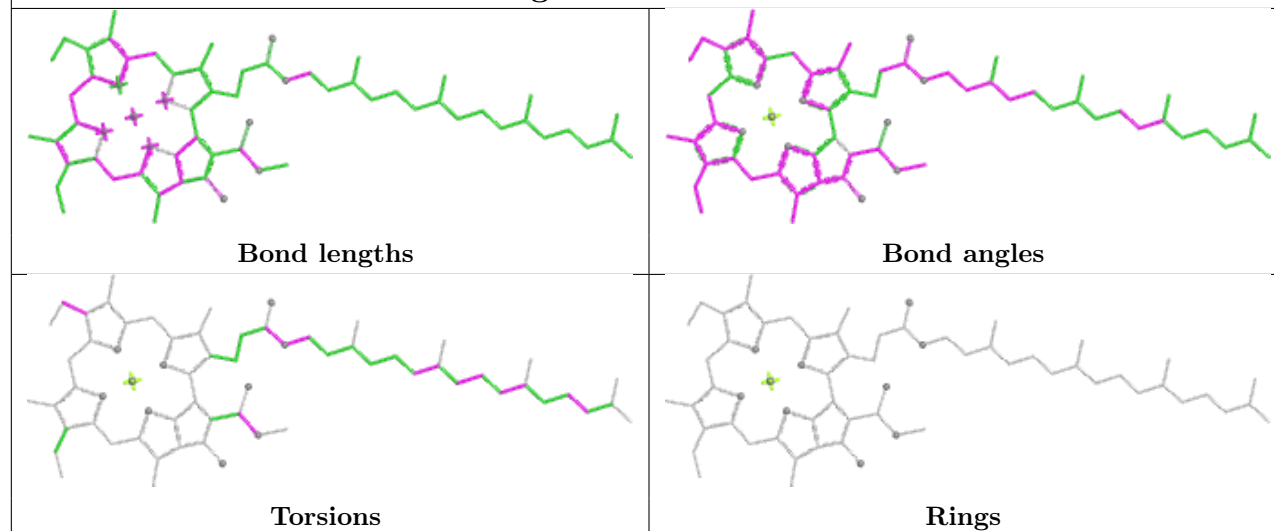
Ligand CLA B 833

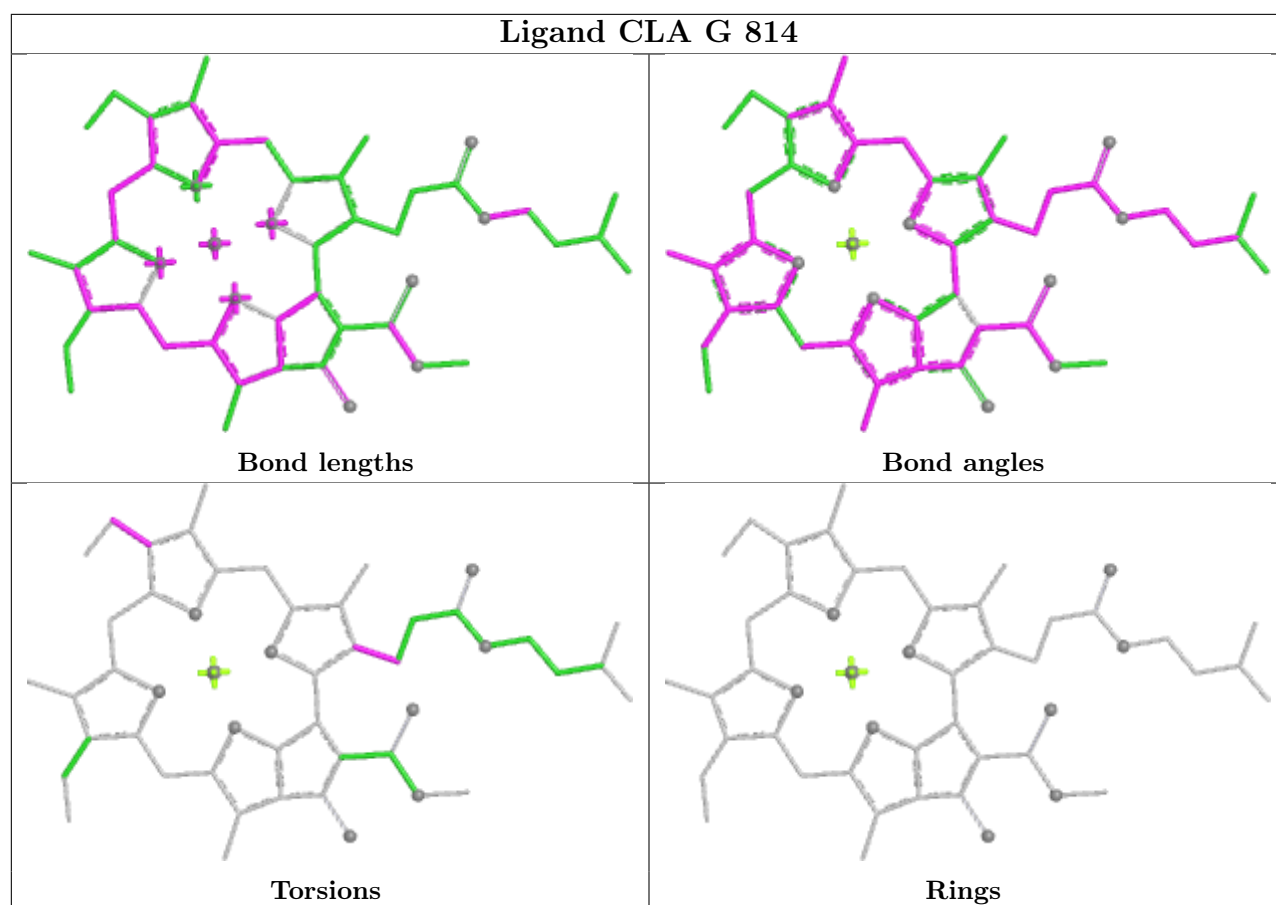


Ligand CLA Y 809	
	
Bond lengths	Bond angles
	
Torsions	Rings

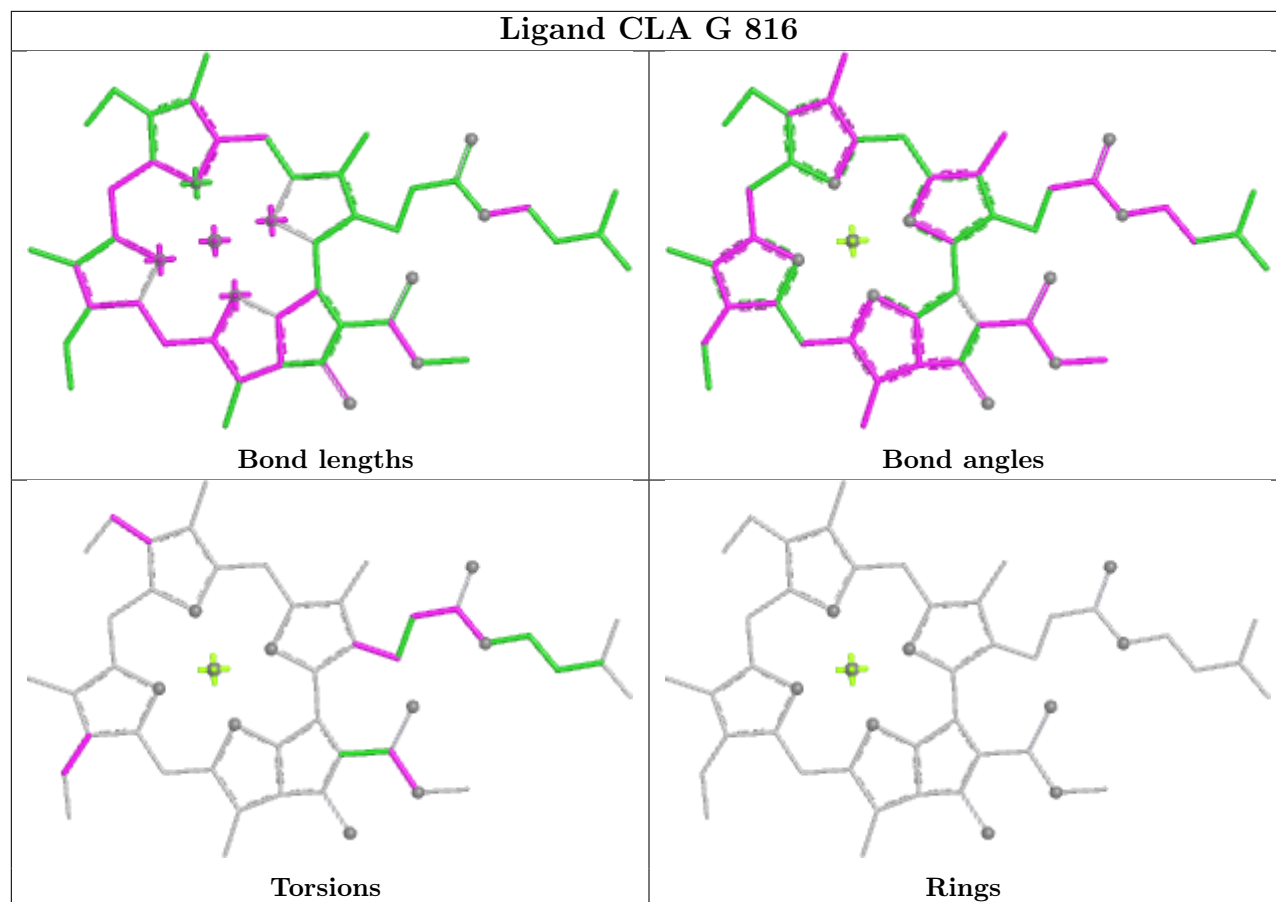
Ligand BCR Q 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

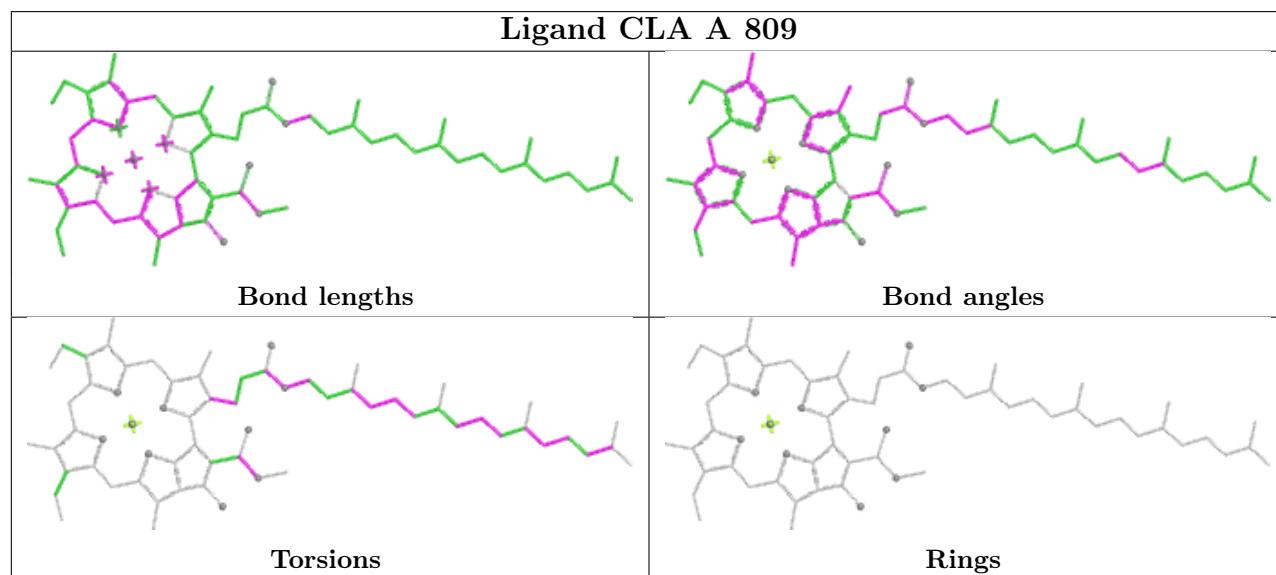
Ligand CLA B 826**Ligand CLA G 803**



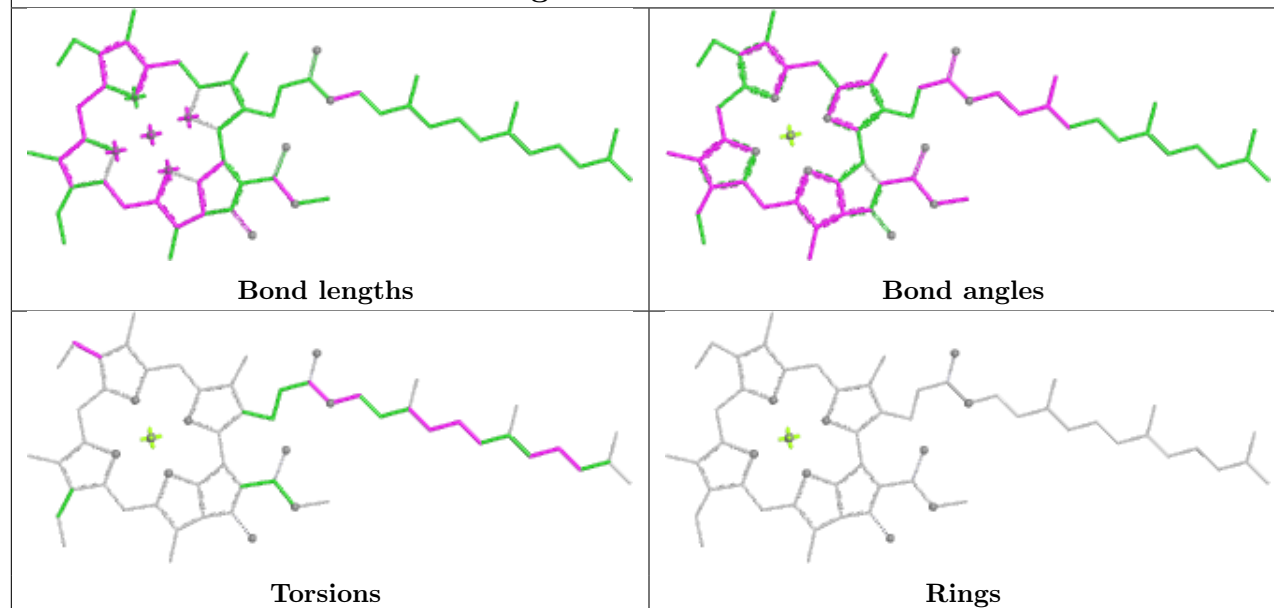
Ligand CLA G 816



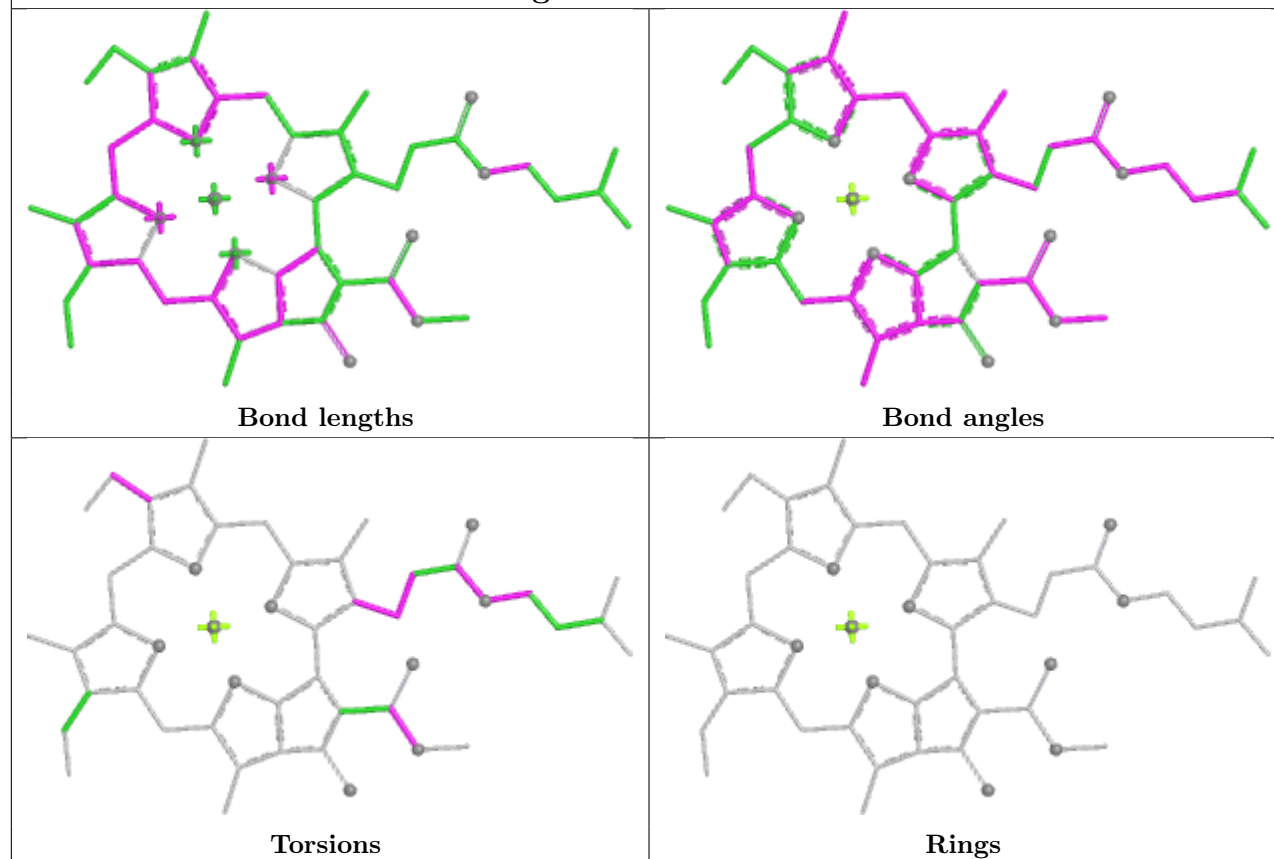
Ligand CLA A 809



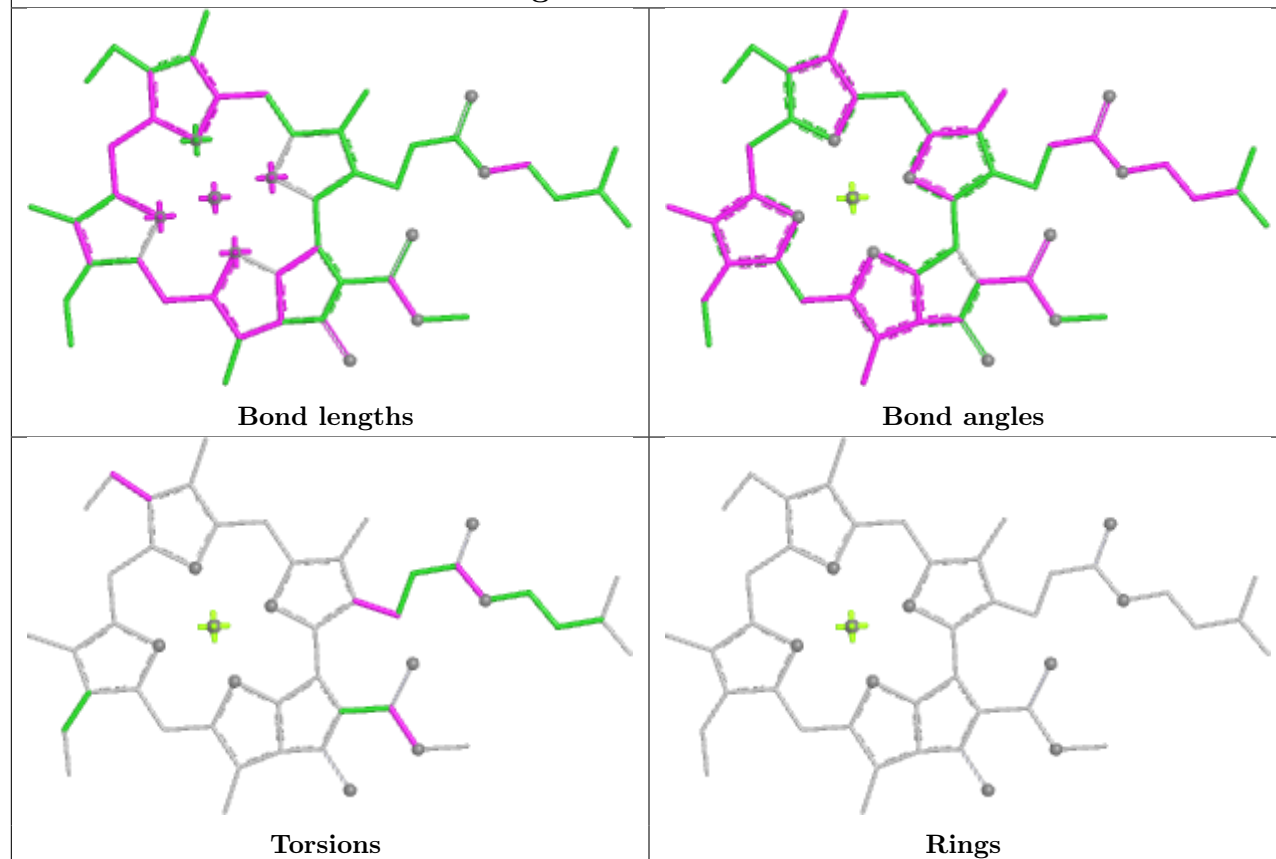
Ligand CLA G 817



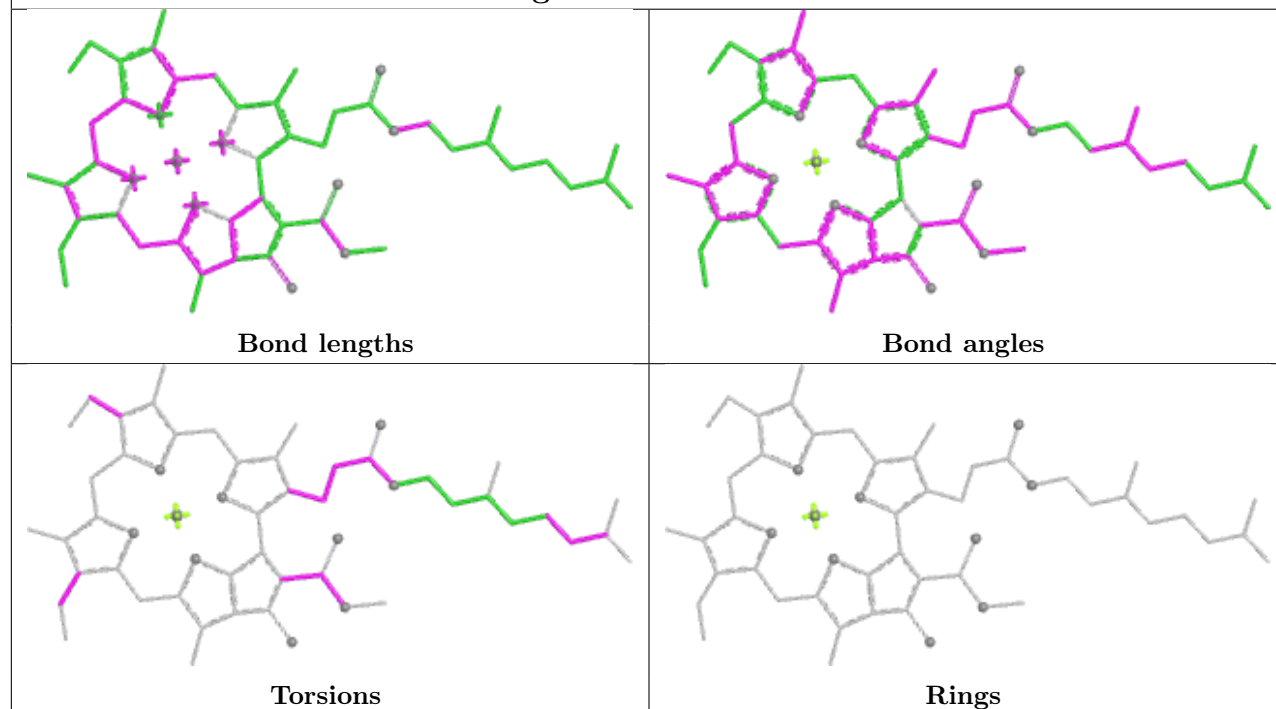
Ligand CLA B 812



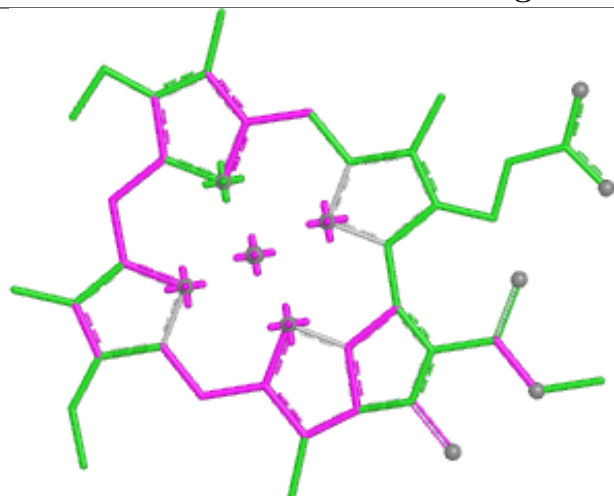
Ligand CLA Y 823



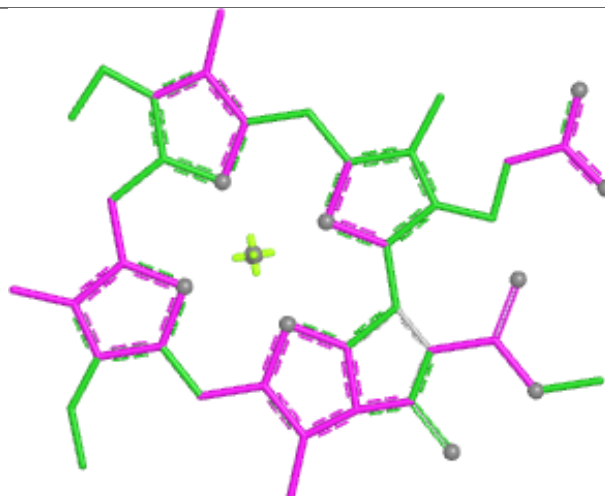
Ligand CLA B 811



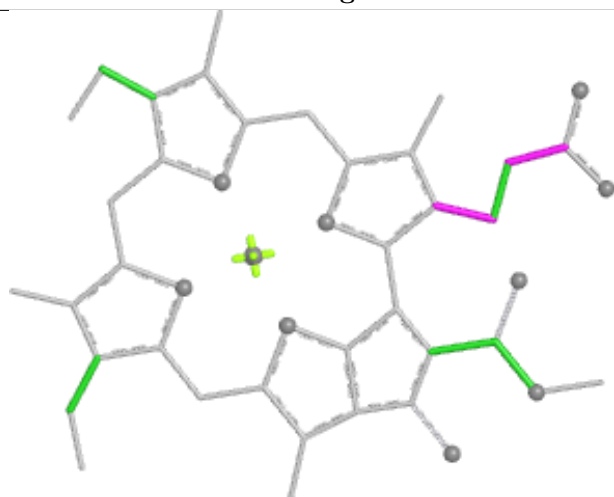
Ligand CLA B 839



Bond lengths



Bond angles

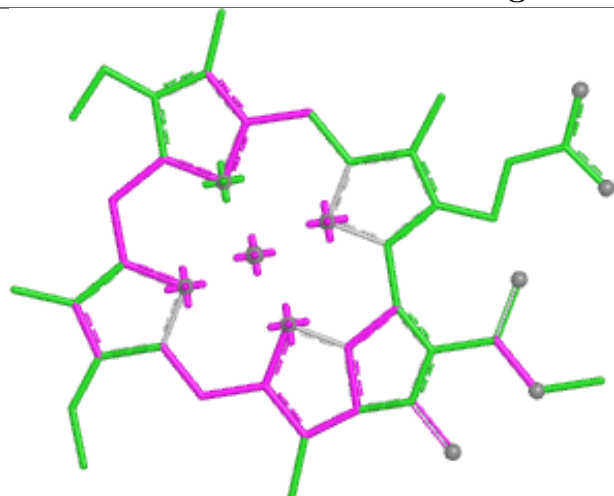


Torsions

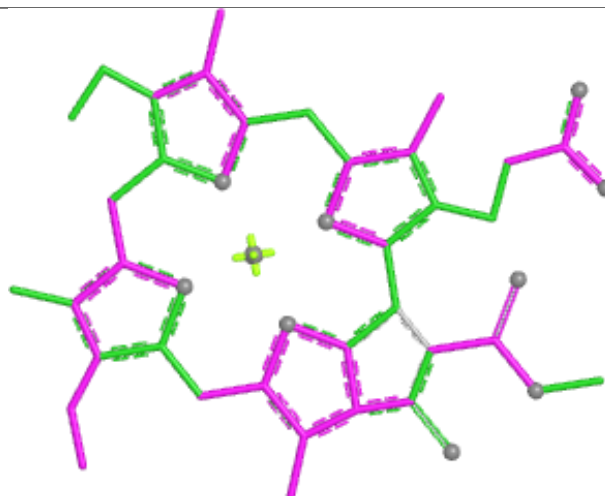


Rings

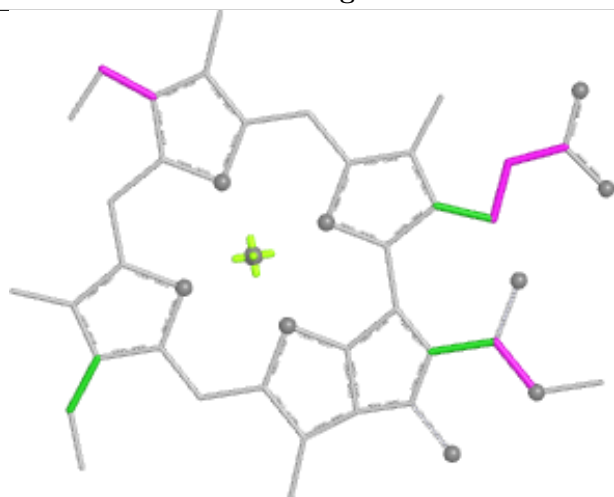
Ligand CLA S 1102



Bond lengths



Bond angles

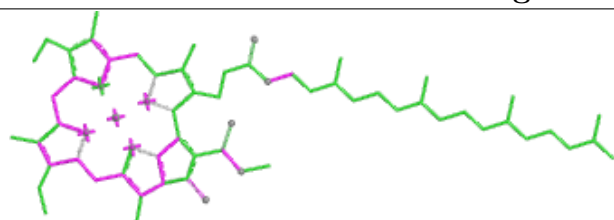


Torsions

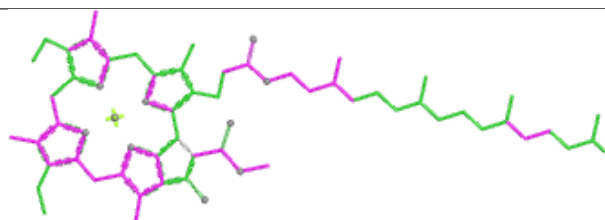


Rings

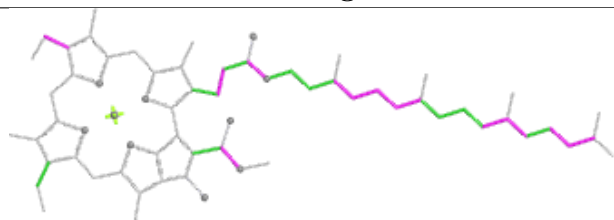
Ligand CLA G 842



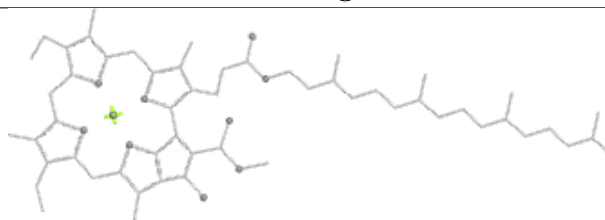
Bond lengths



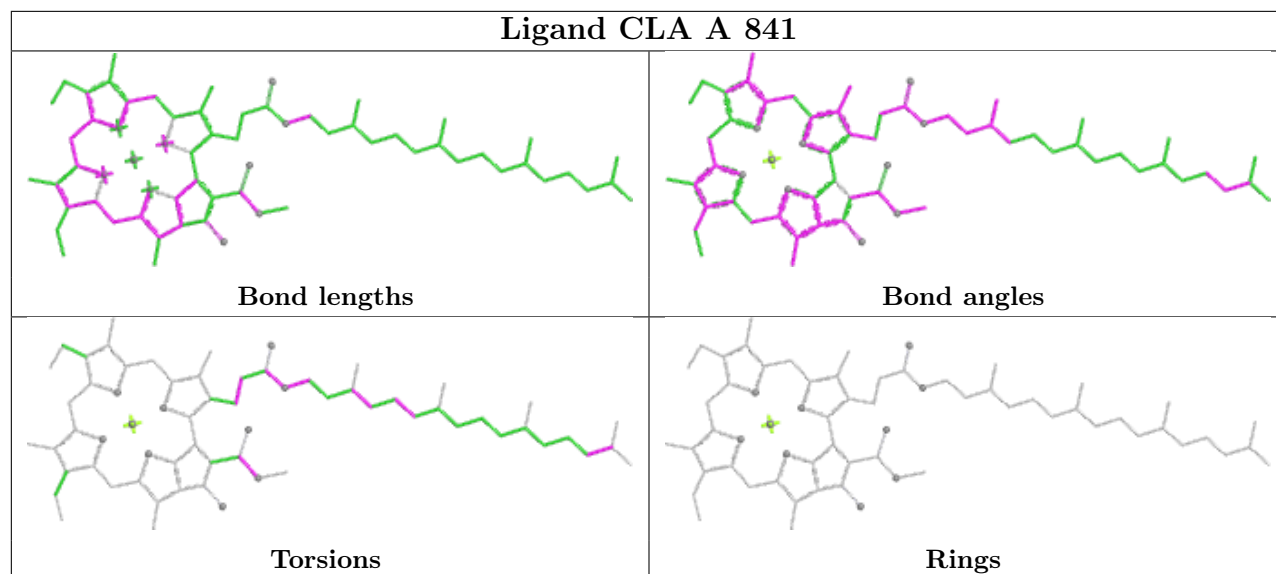
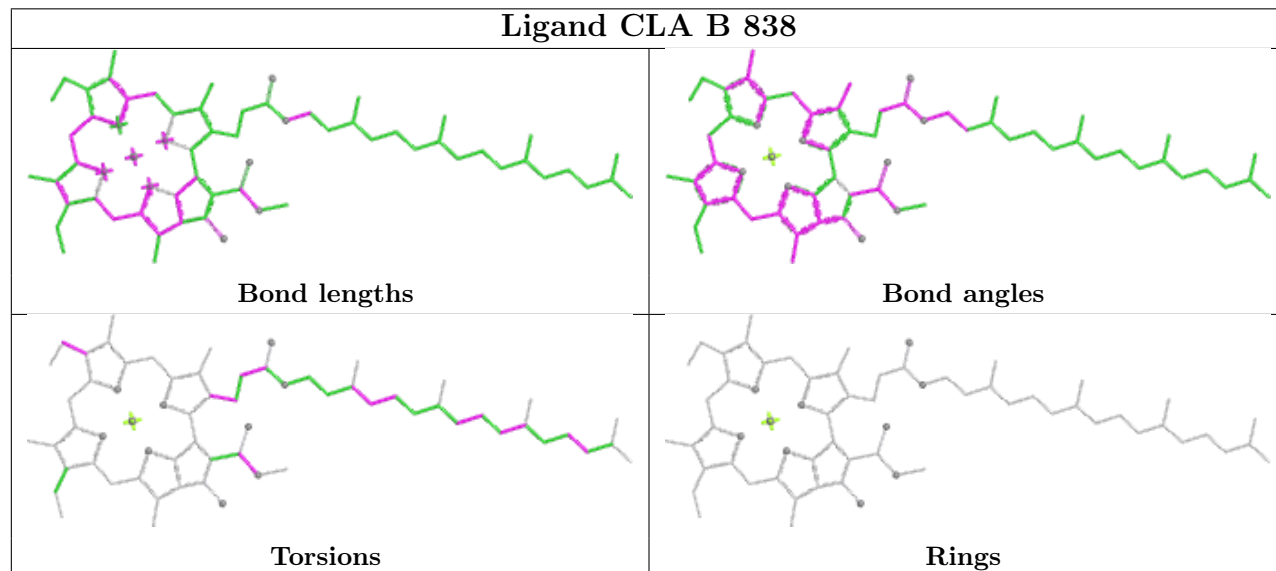
Bond angles



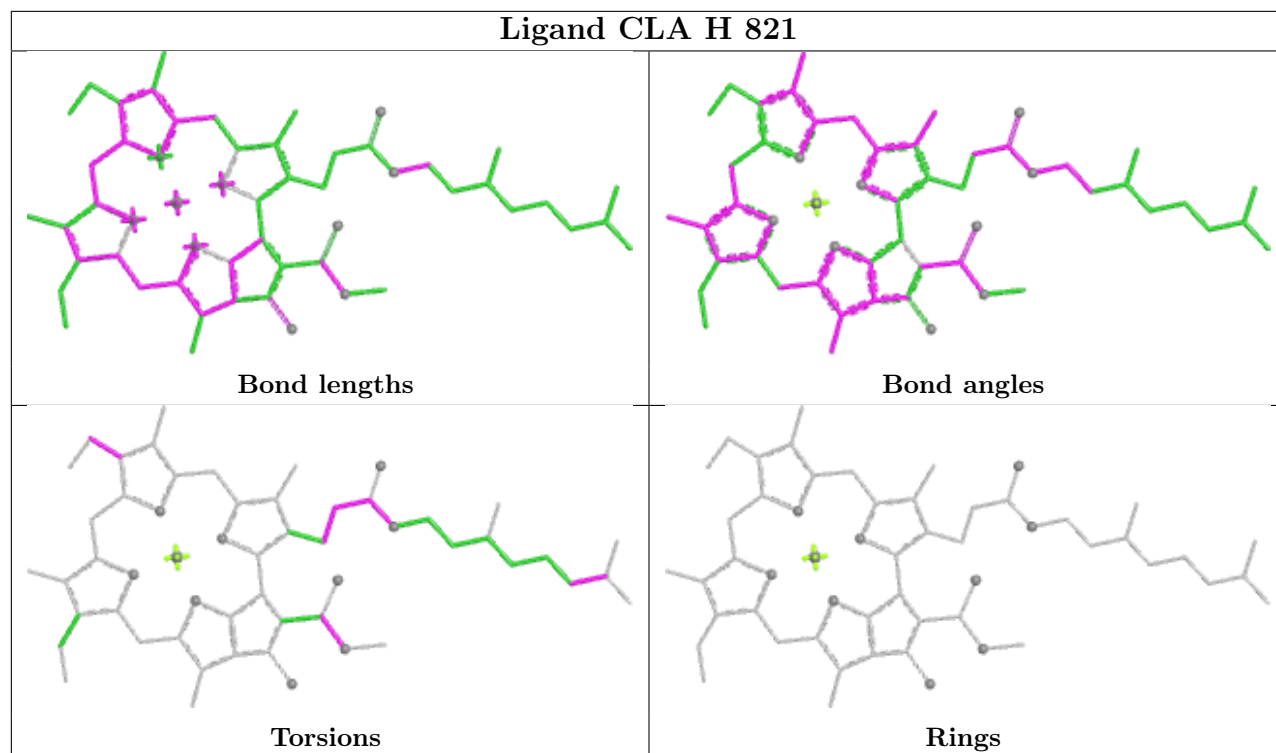
Torsions



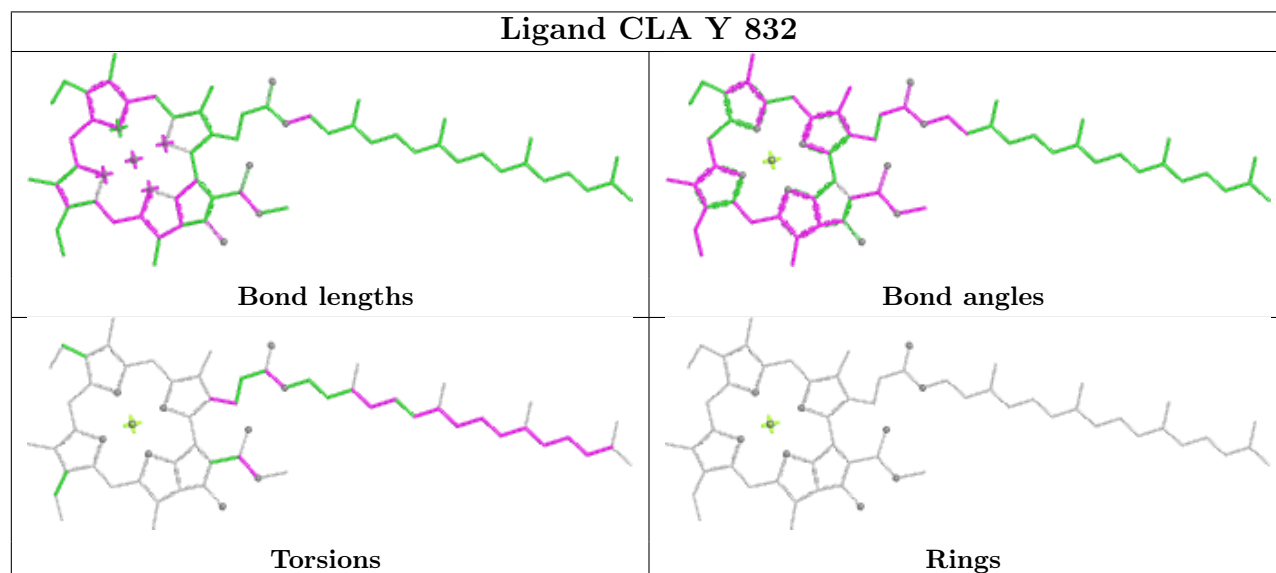
Rings

Ligand CLA A 841**Ligand CLA B 838**

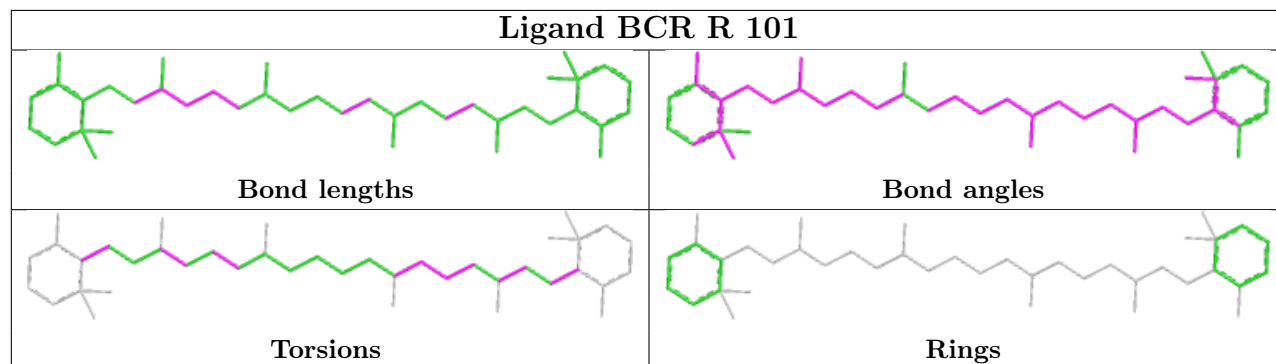
Ligand CLA H 821

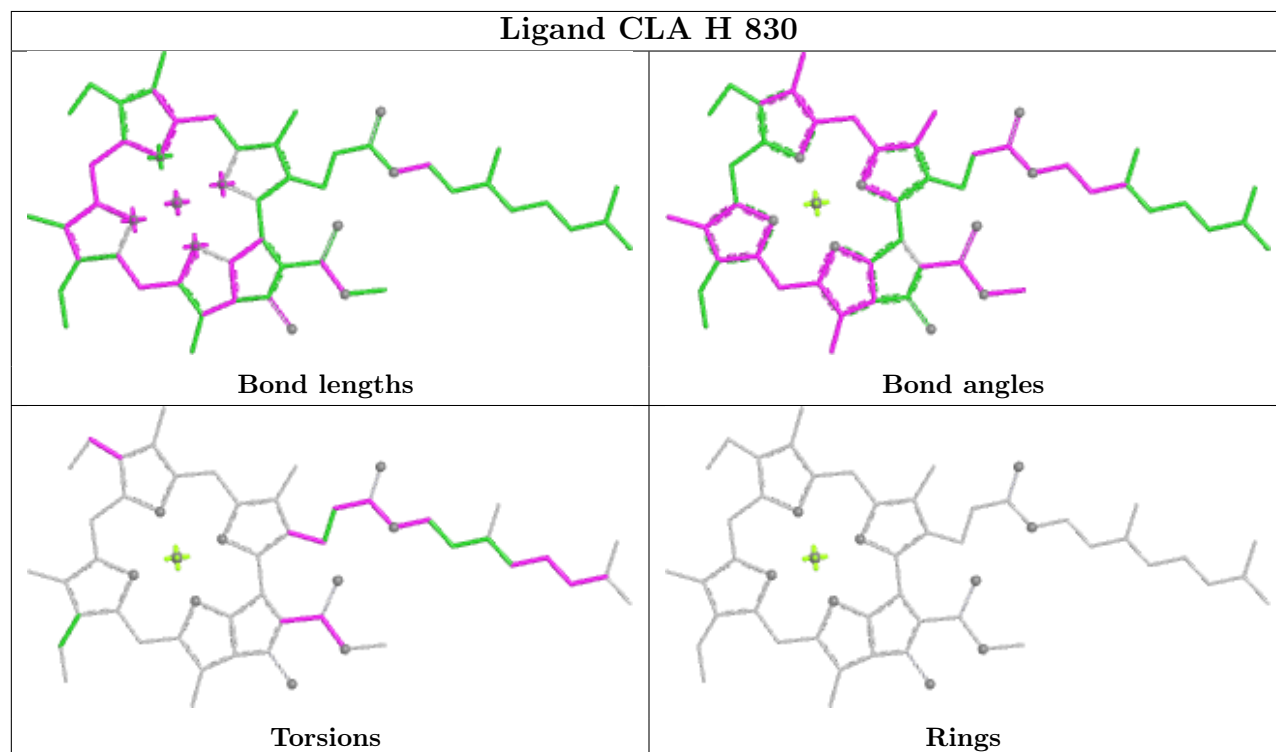
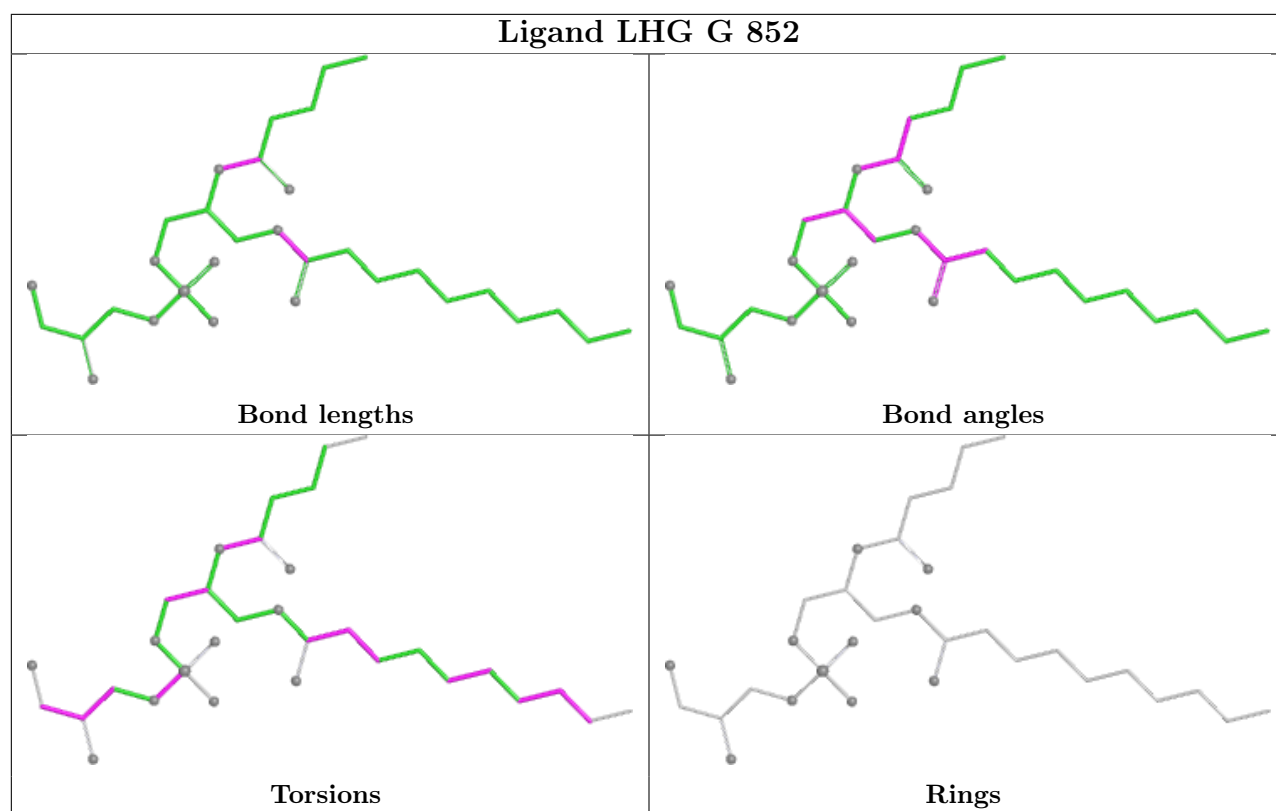


Ligand CLA Y 832

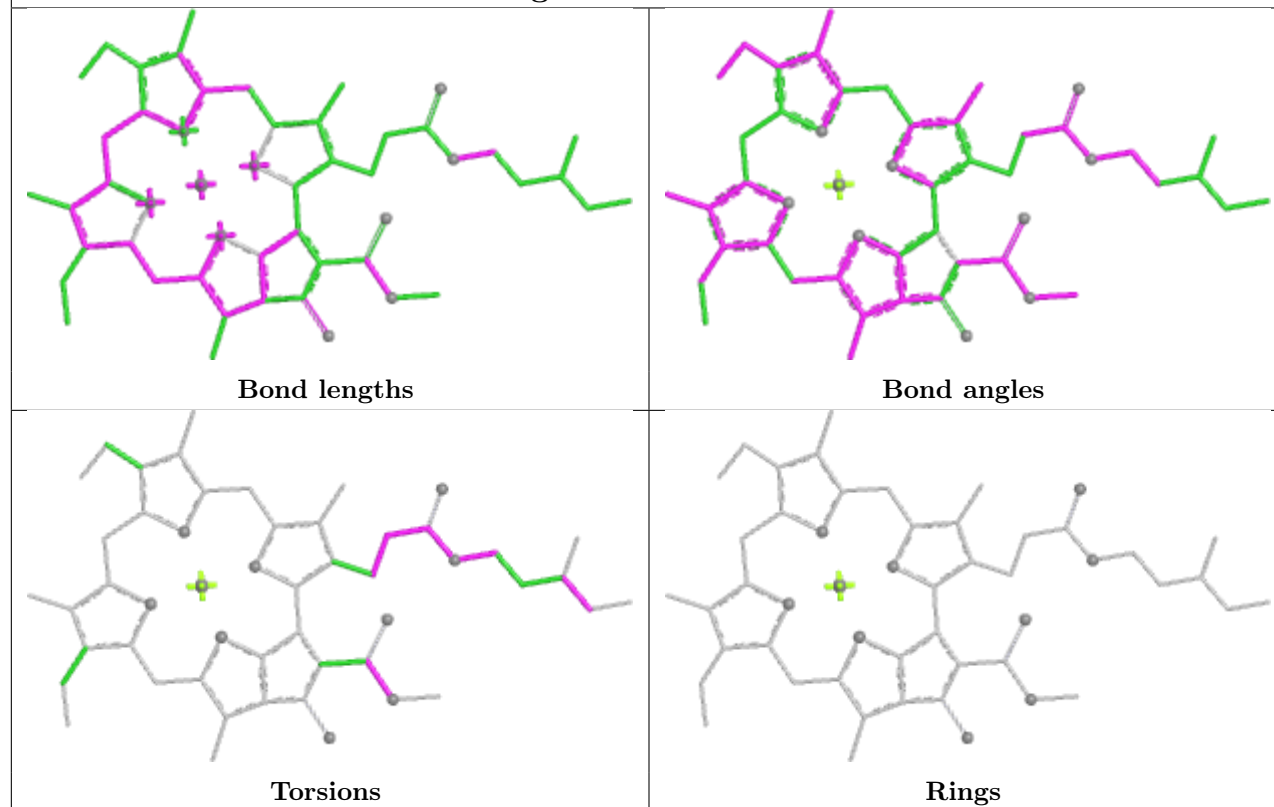


Ligand BCR R 101

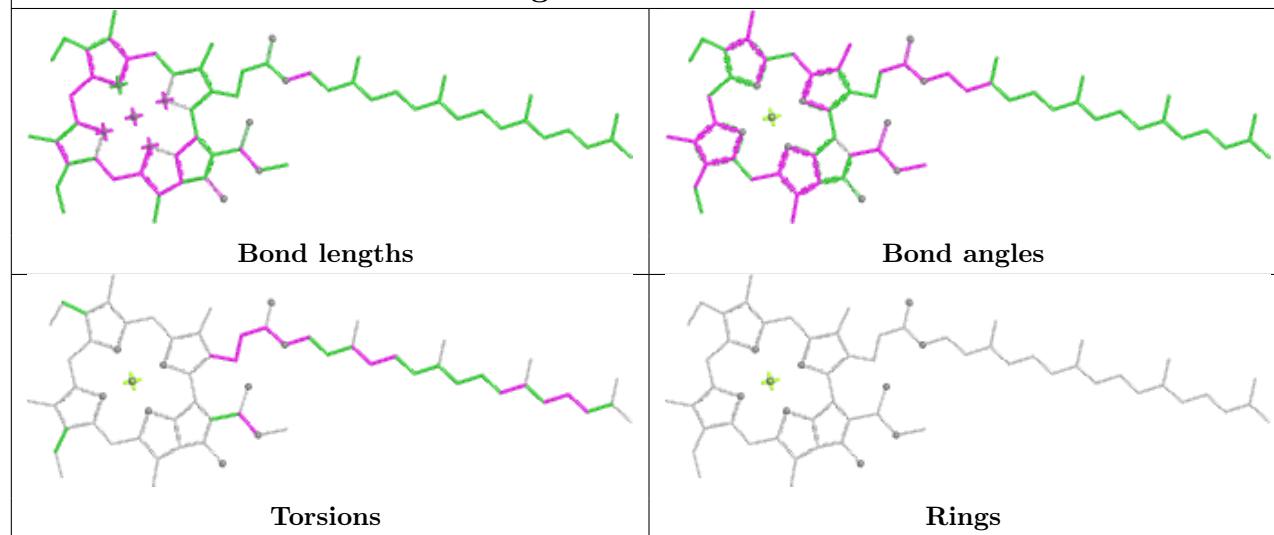


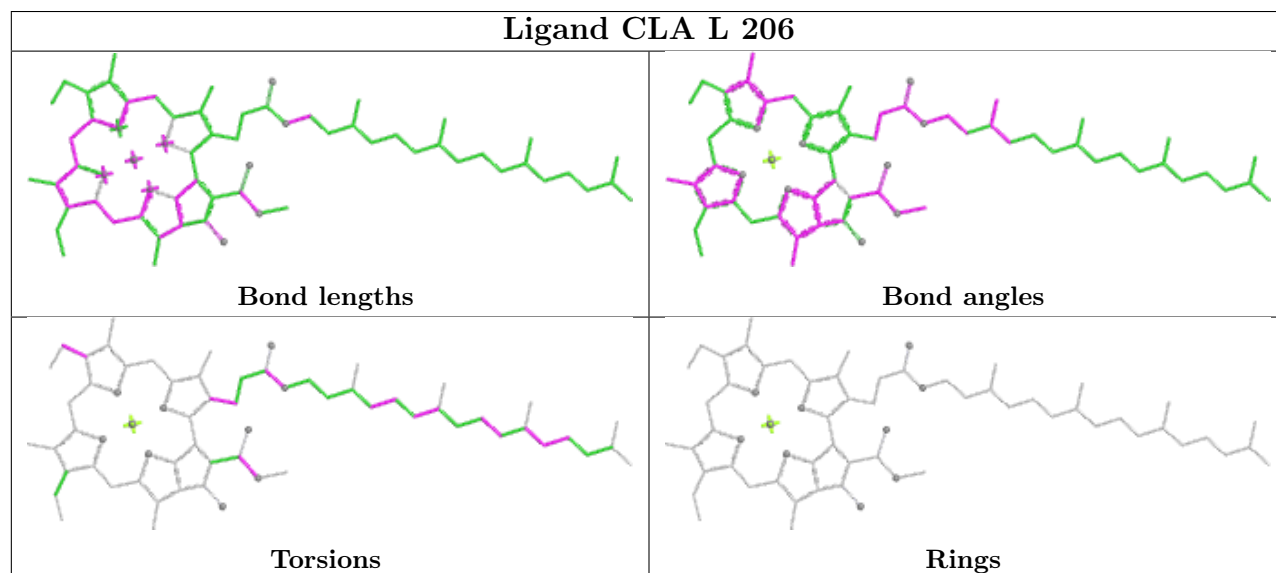
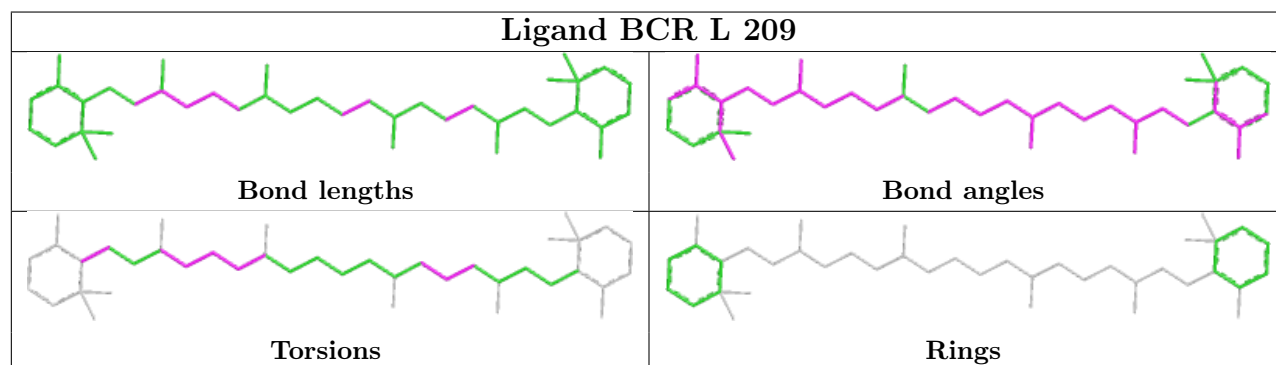
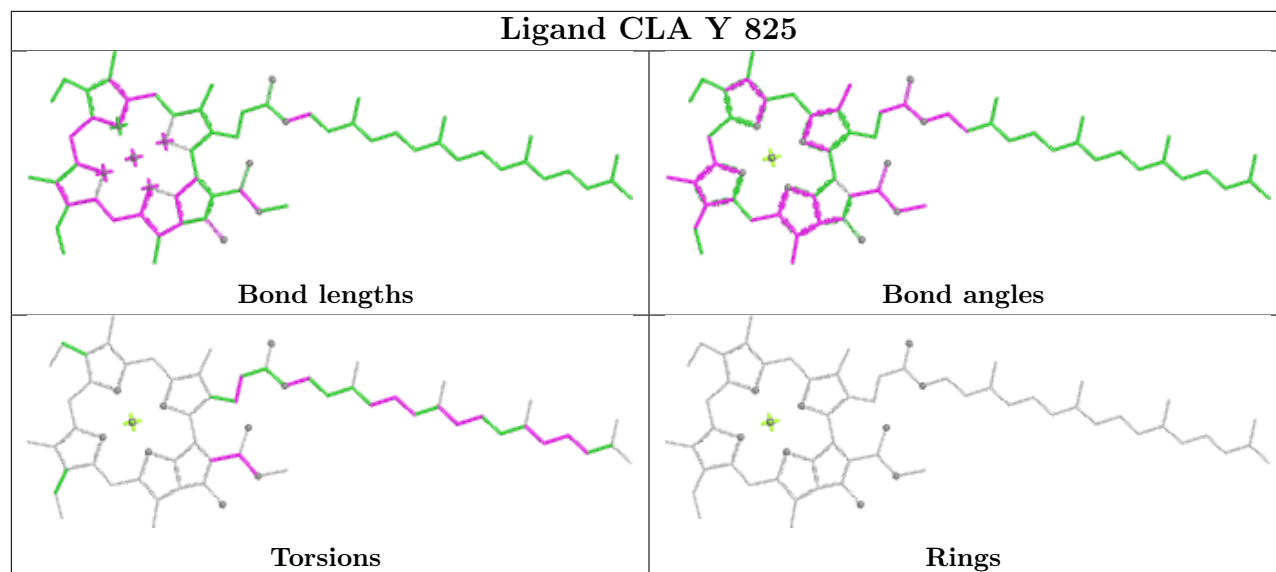


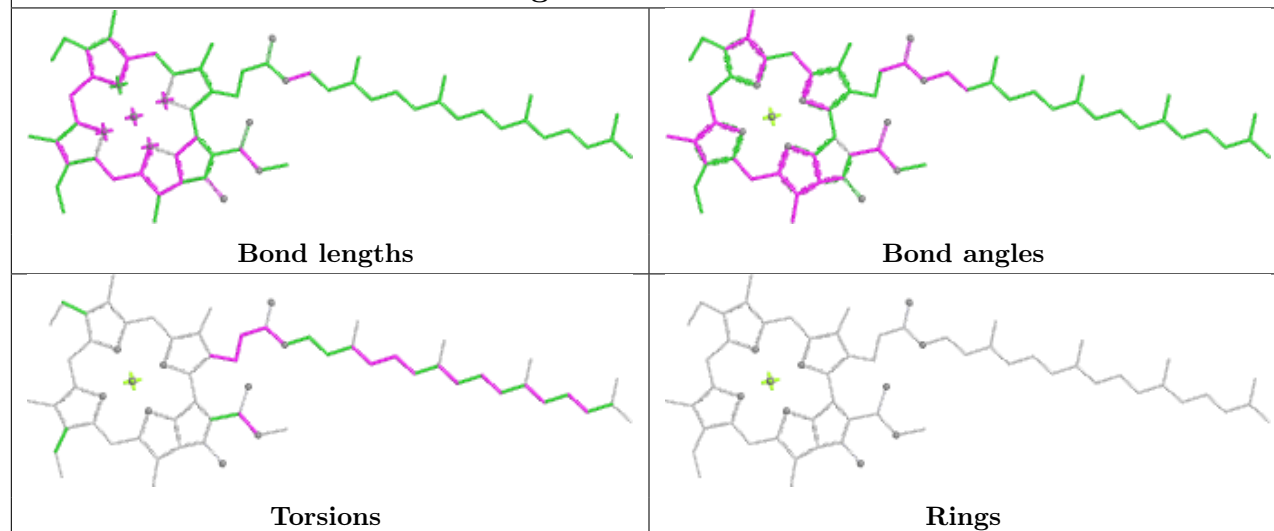
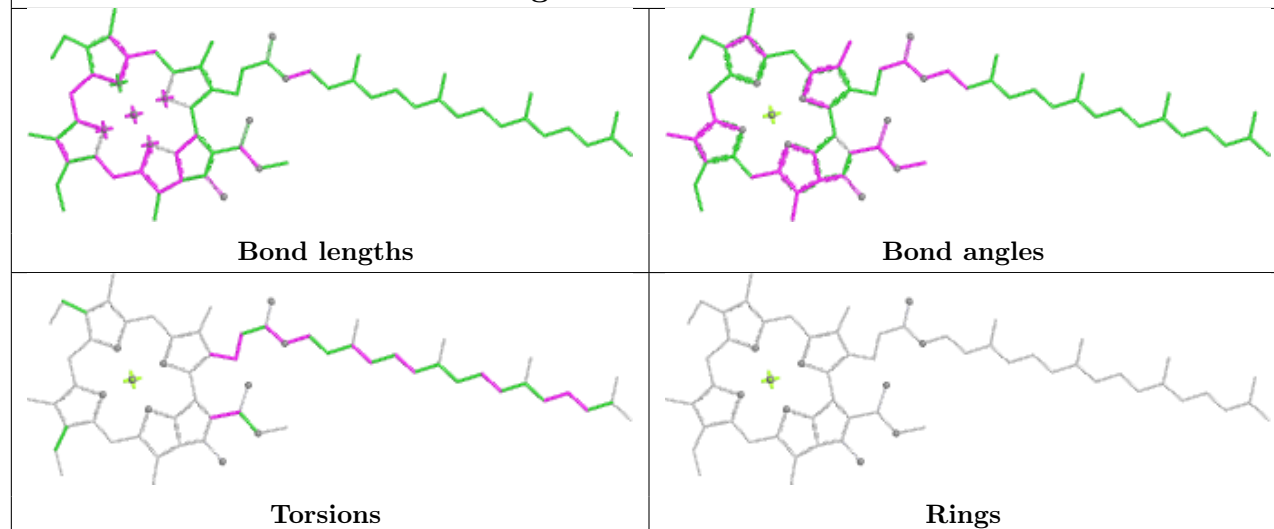
Ligand CLA G 807

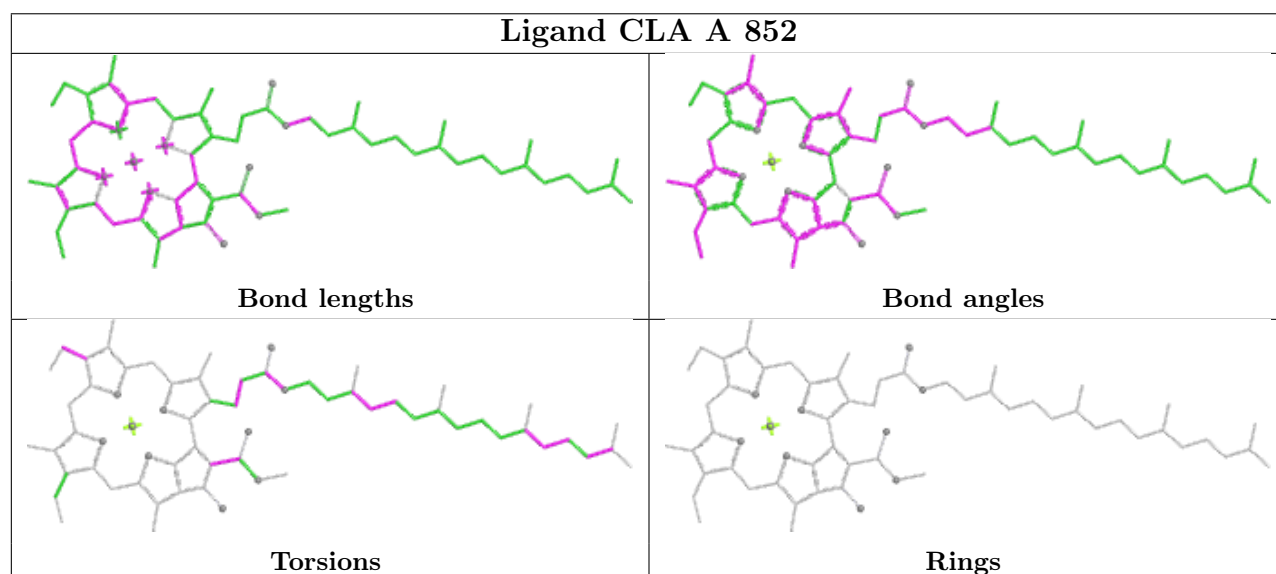
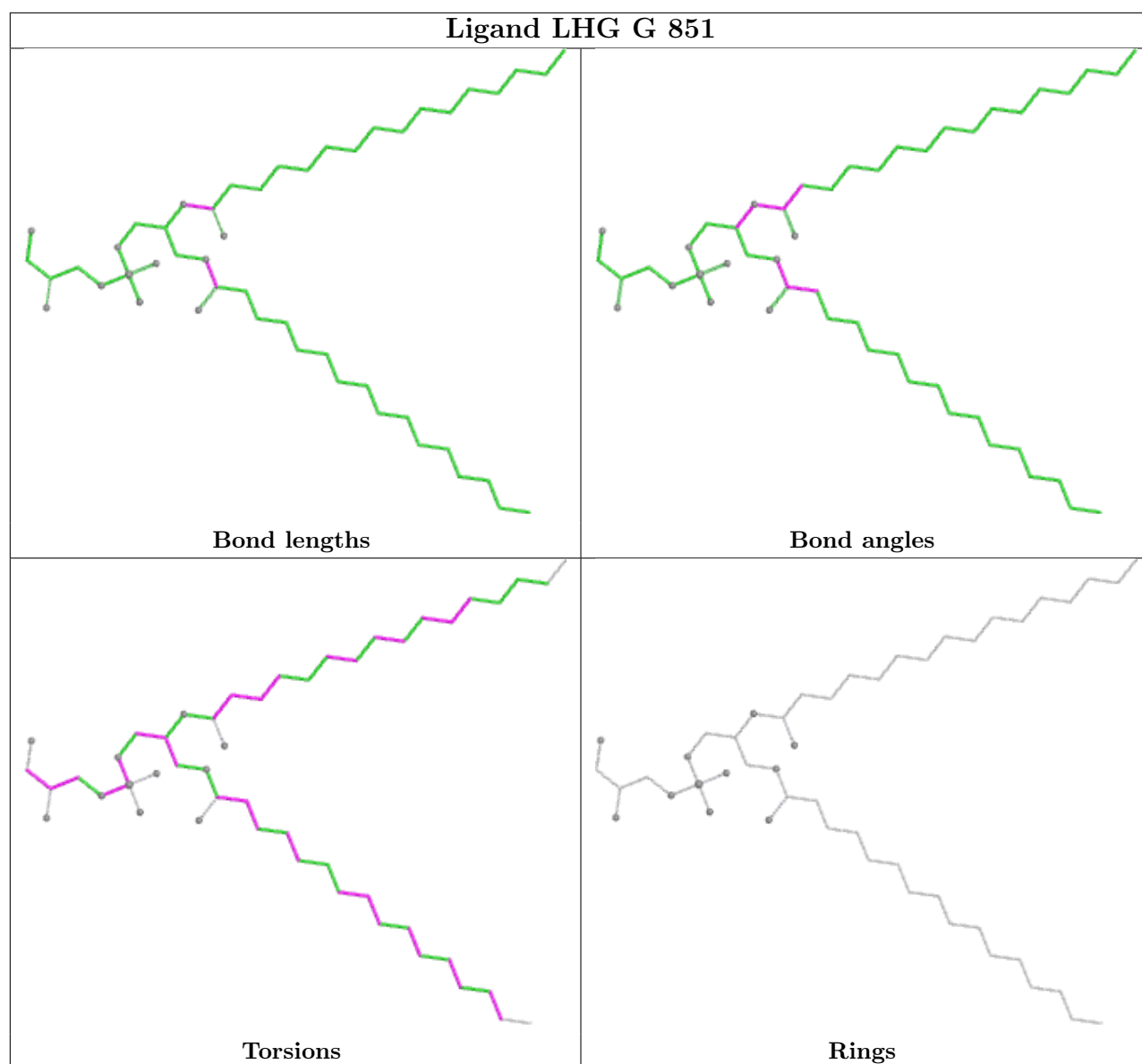


Ligand CLA G 818

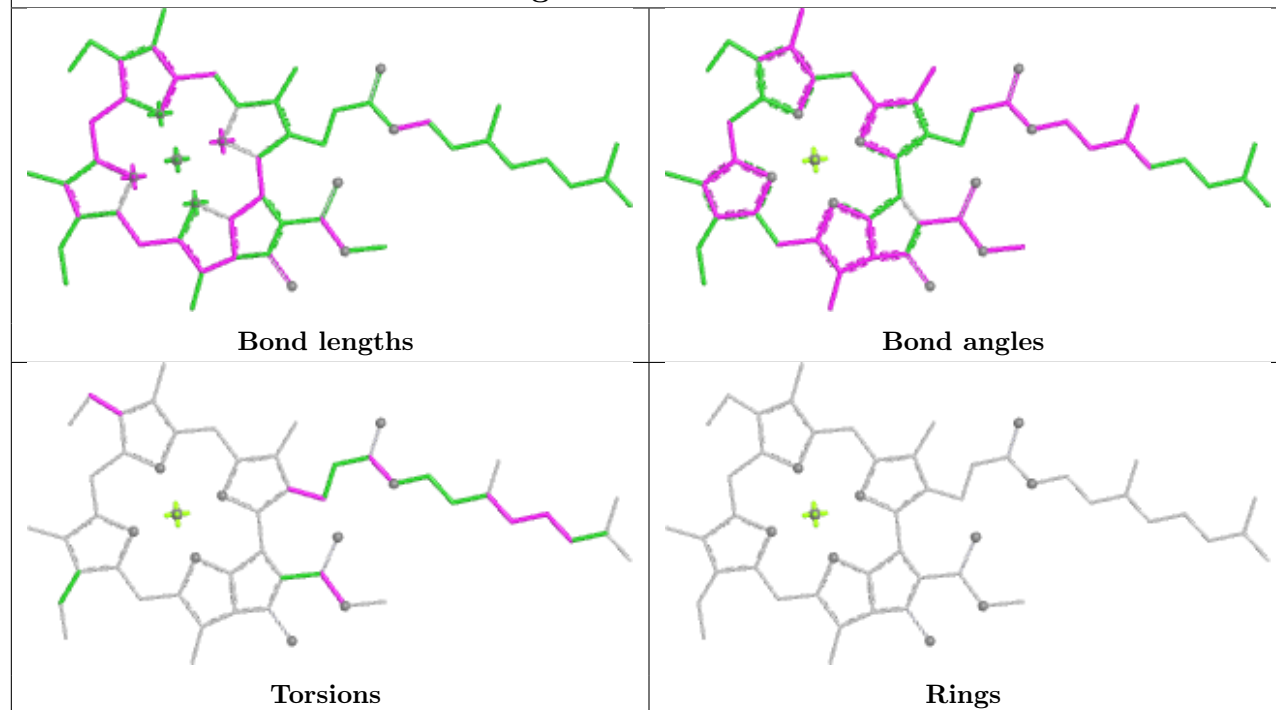




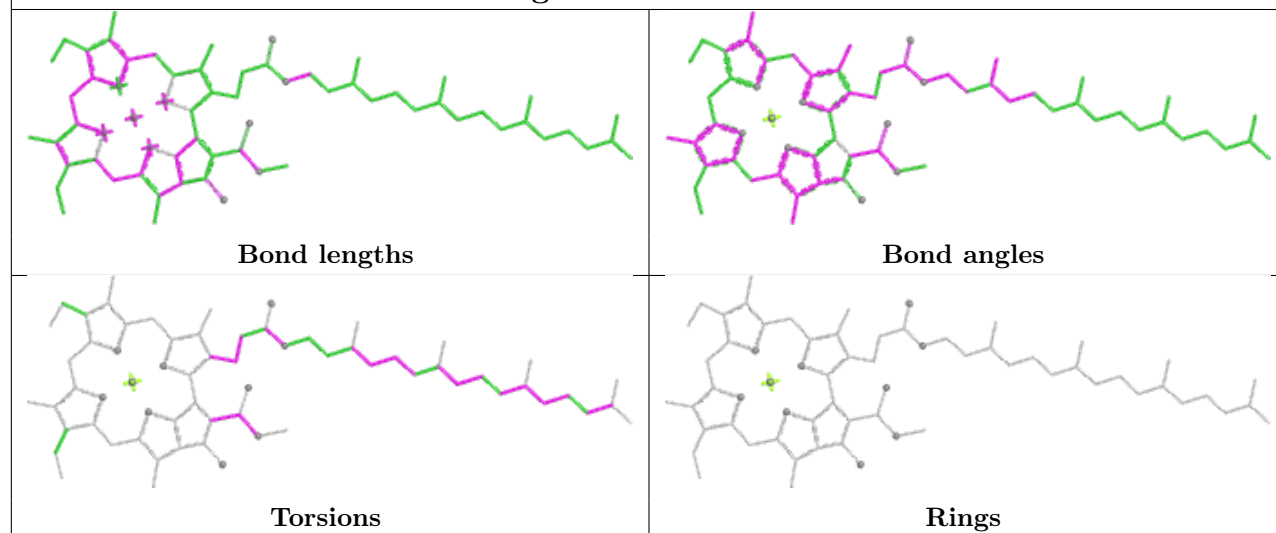
Ligand CLA G 806**Ligand CLA G 830**

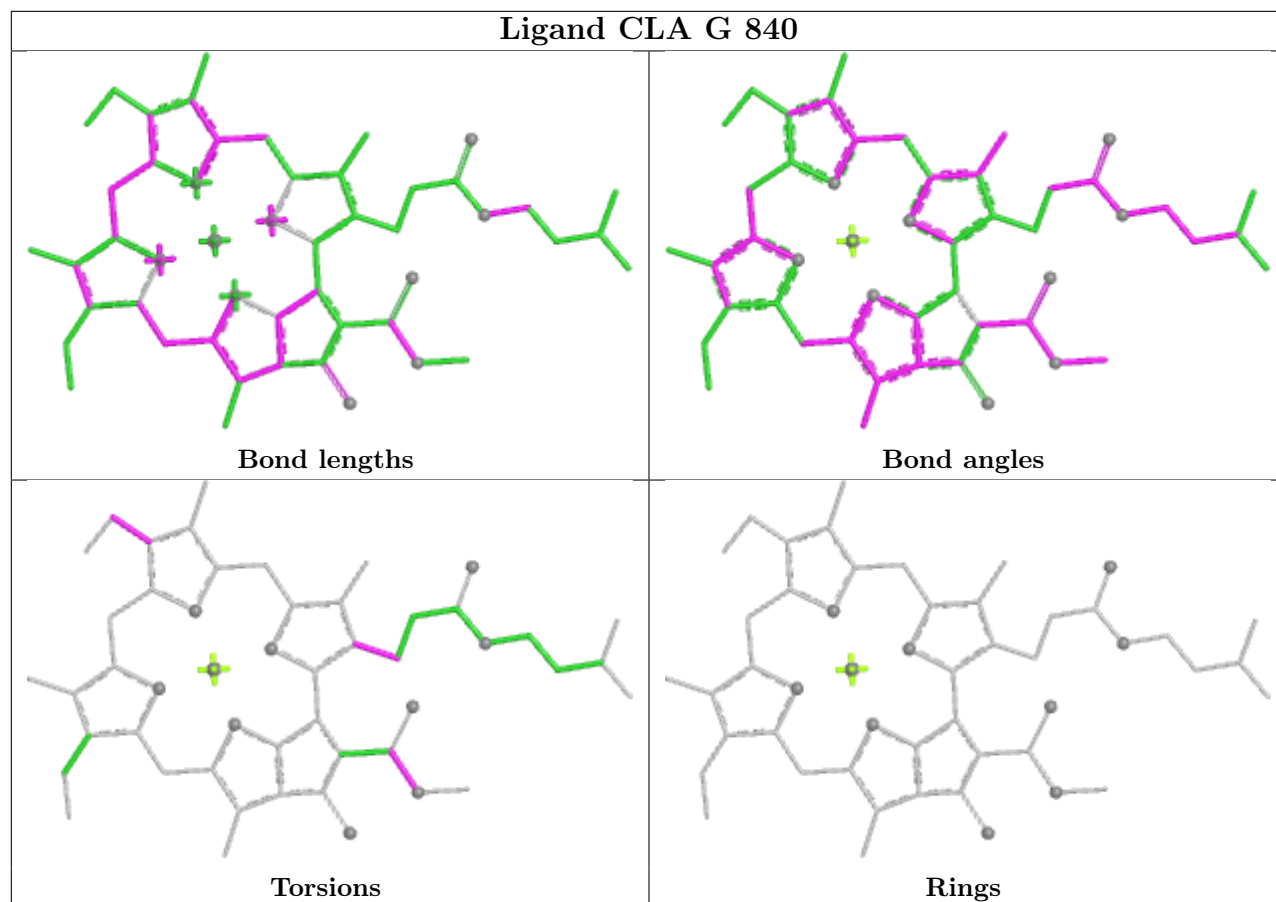


Ligand CLA Y 812

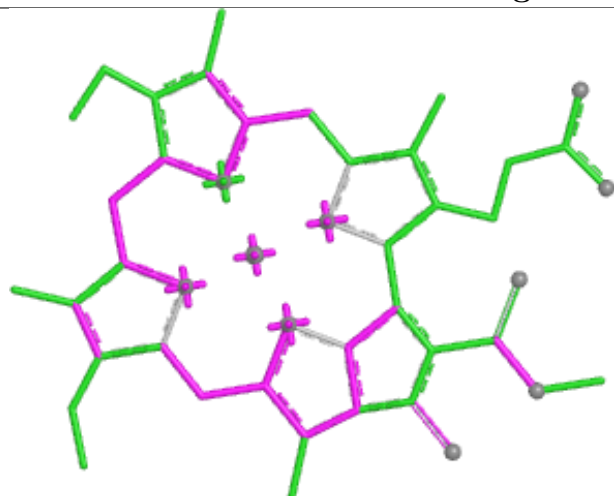


Ligand CLA Y 808

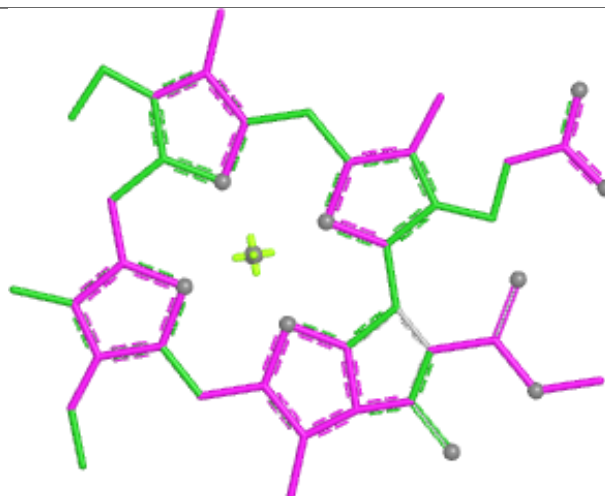




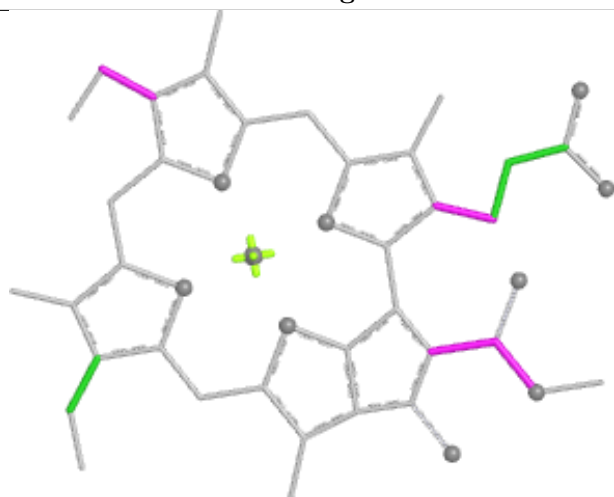
Ligand CLA K 103



Bond lengths



Bond angles

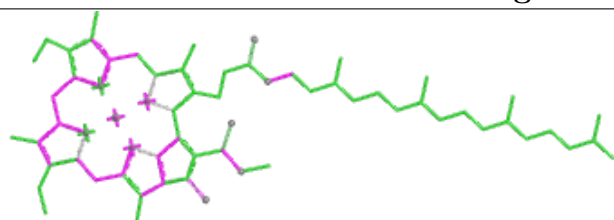


Torsions

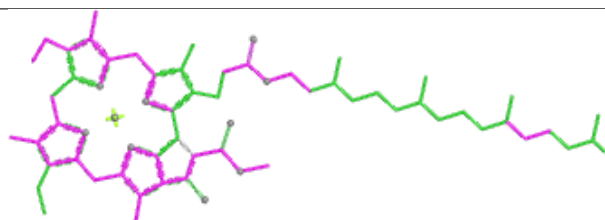


Rings

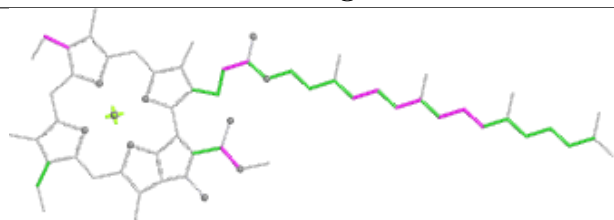
Ligand CLA Y 855



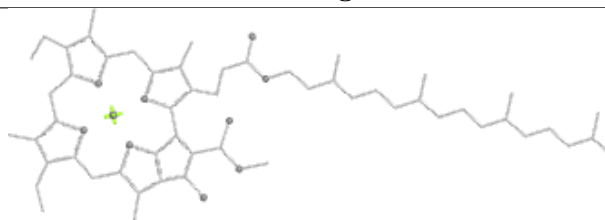
Bond lengths



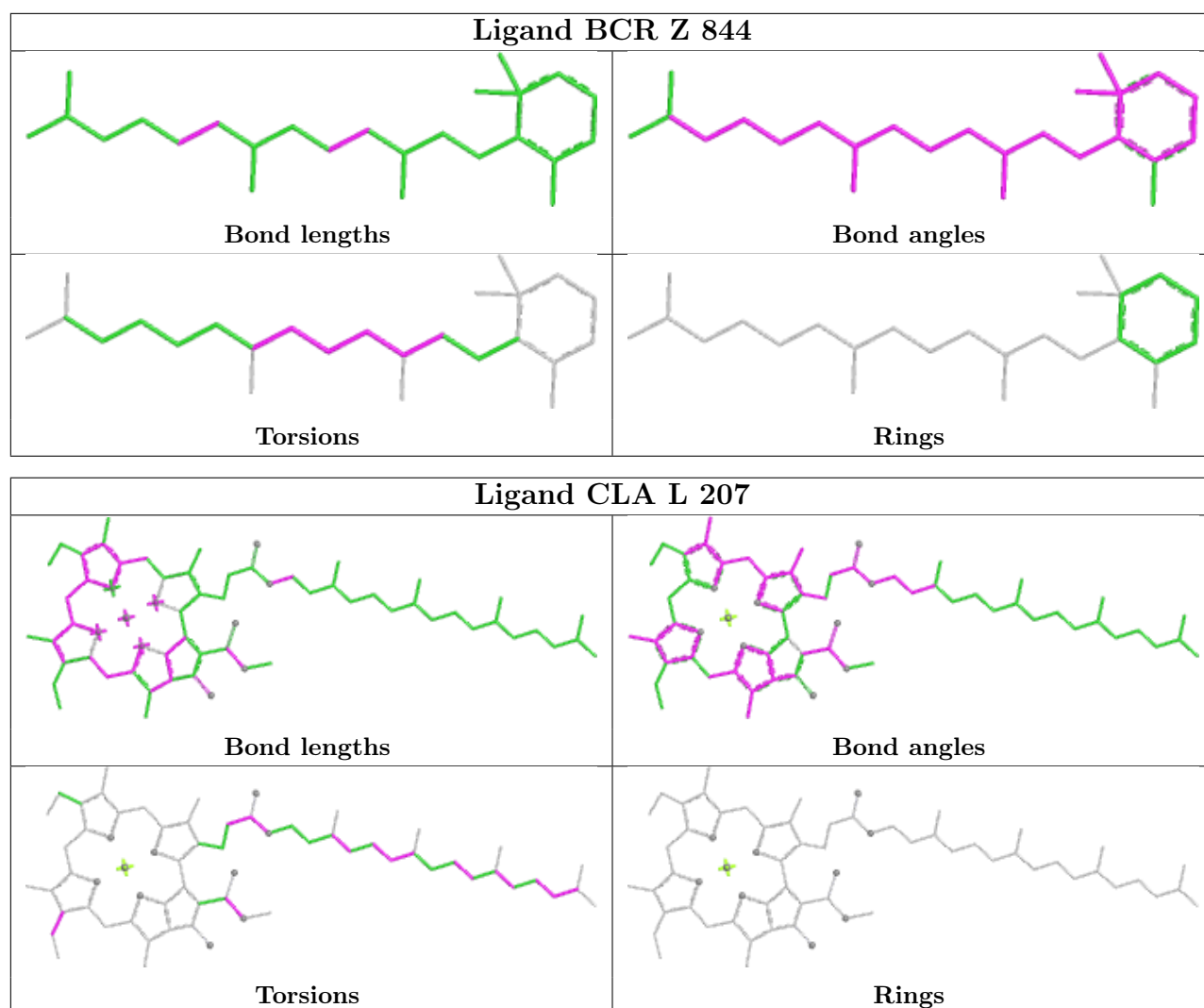
Bond angles



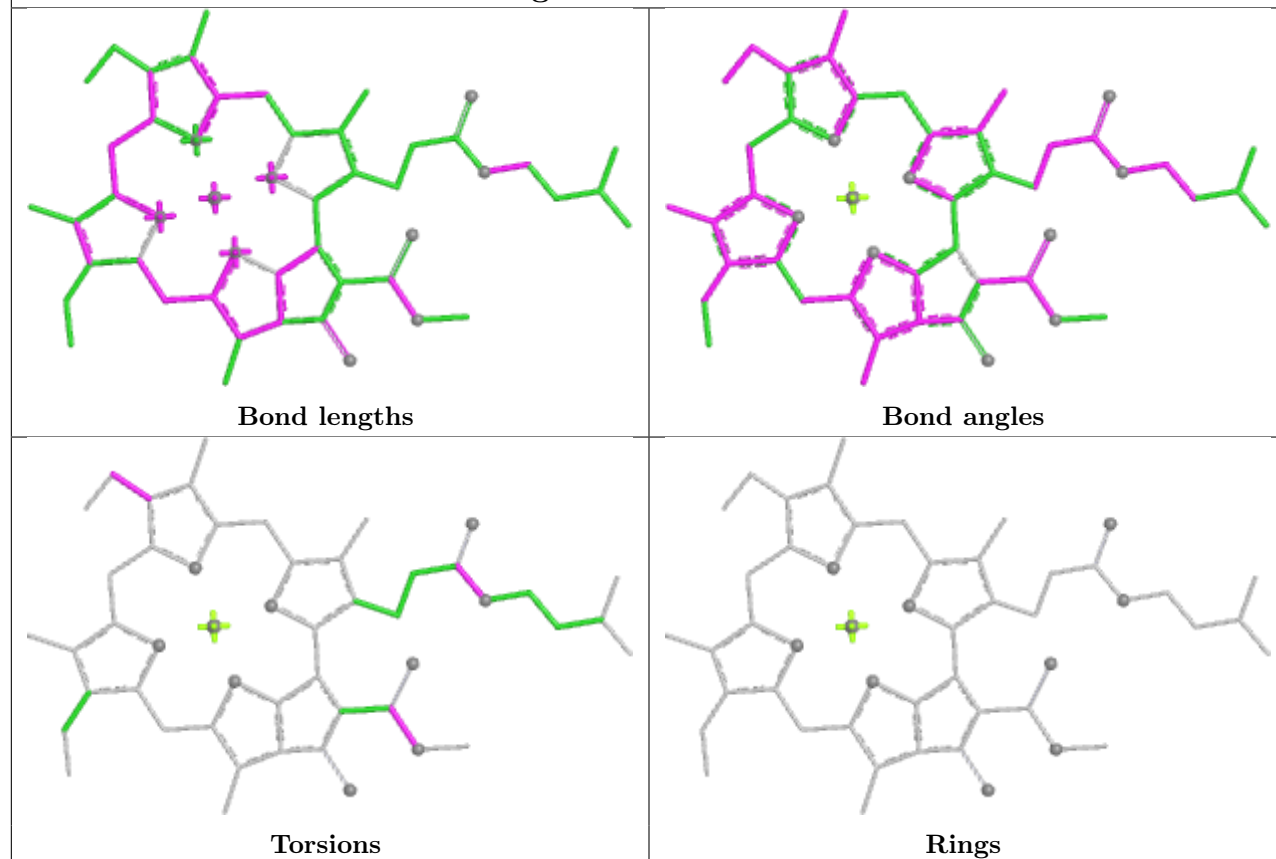
Torsions



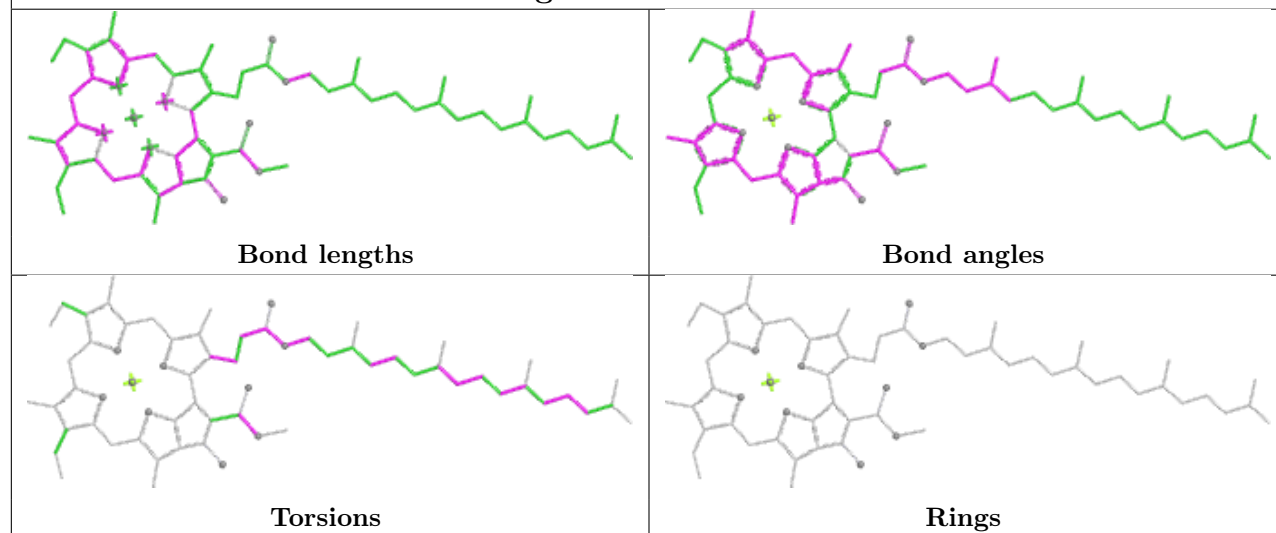
Rings

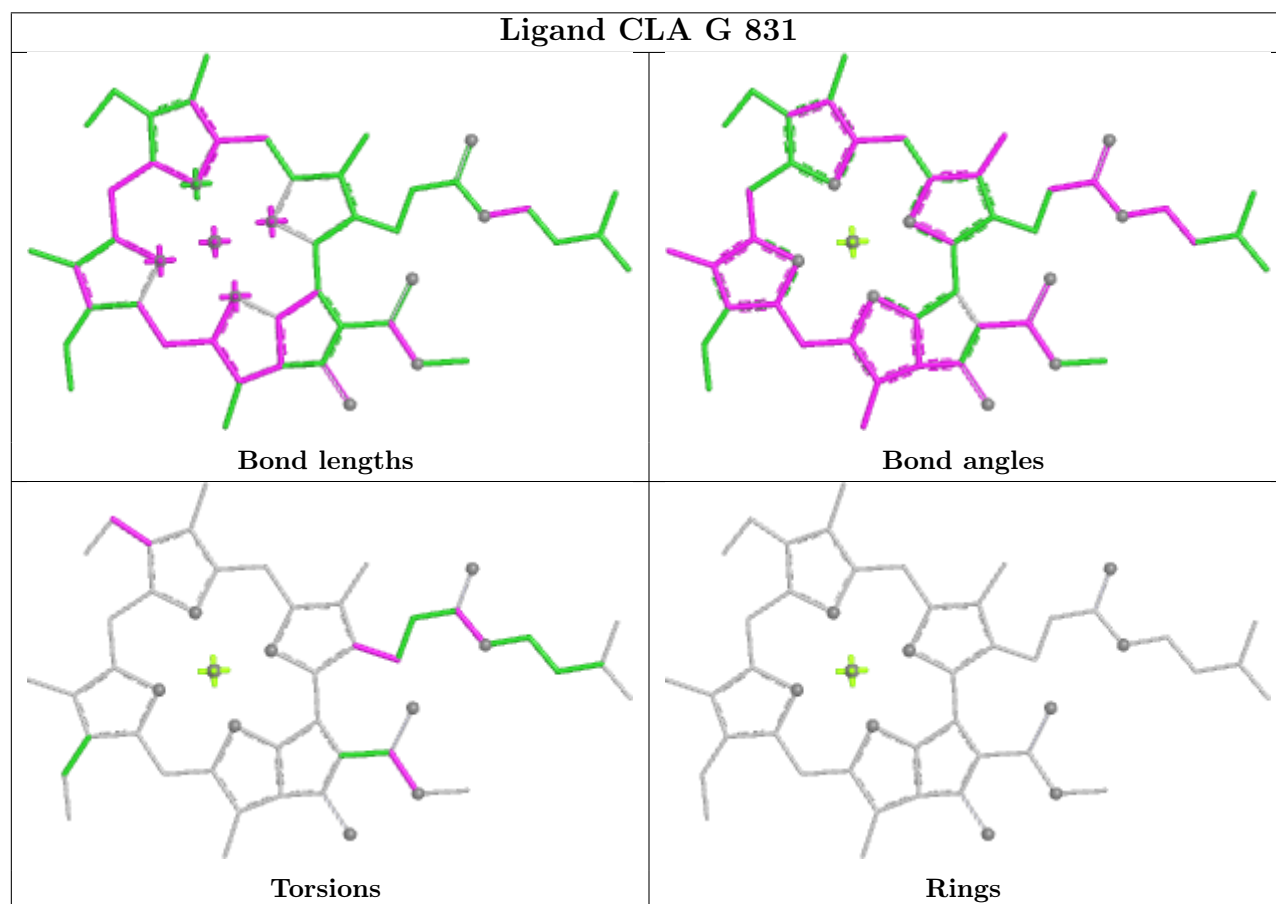
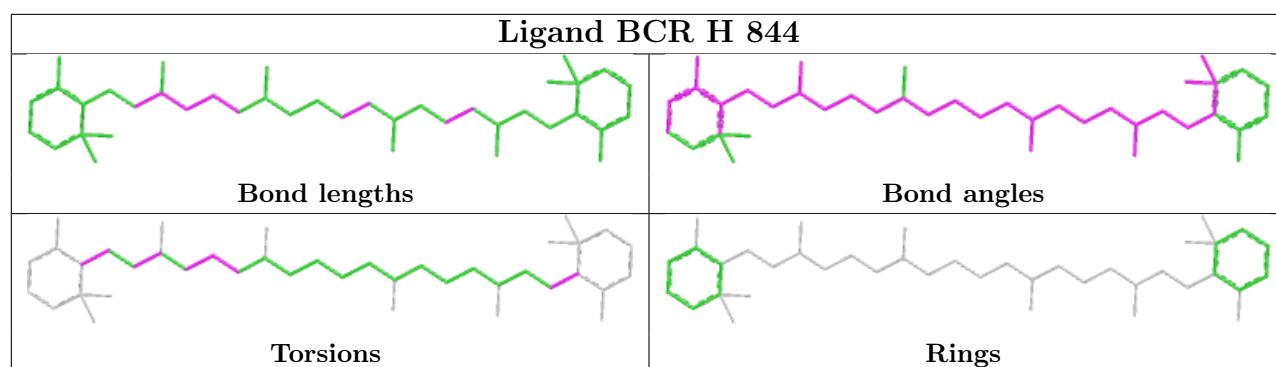


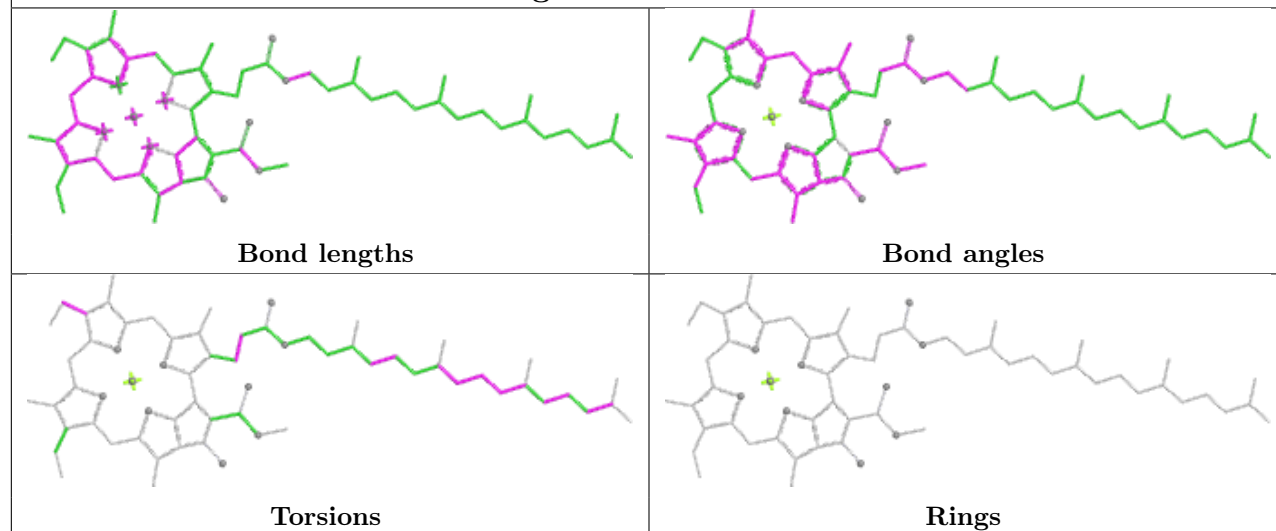
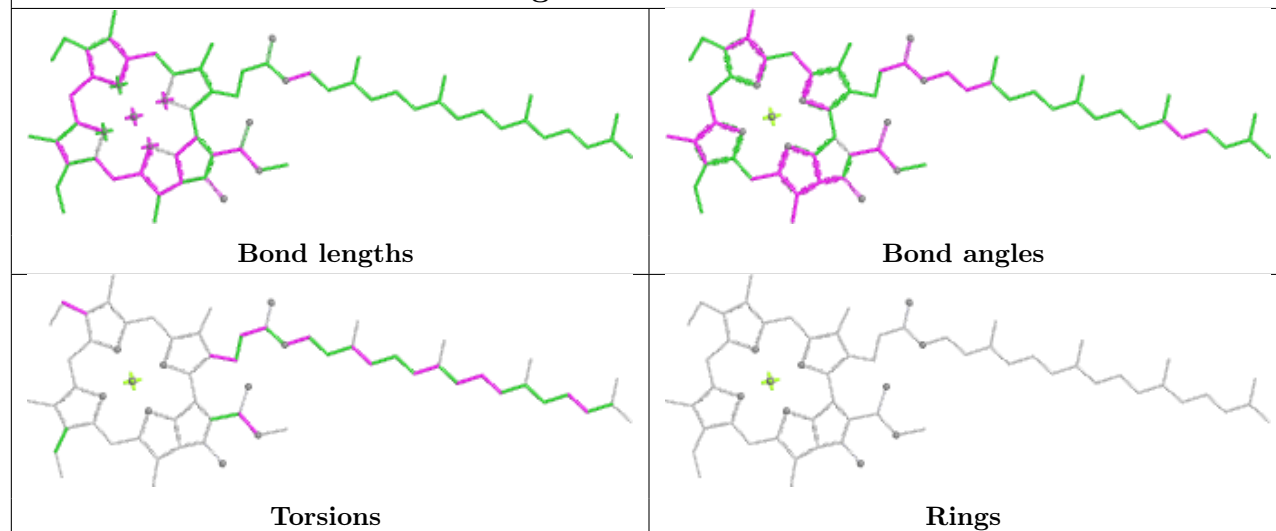
Ligand CLA Y 816



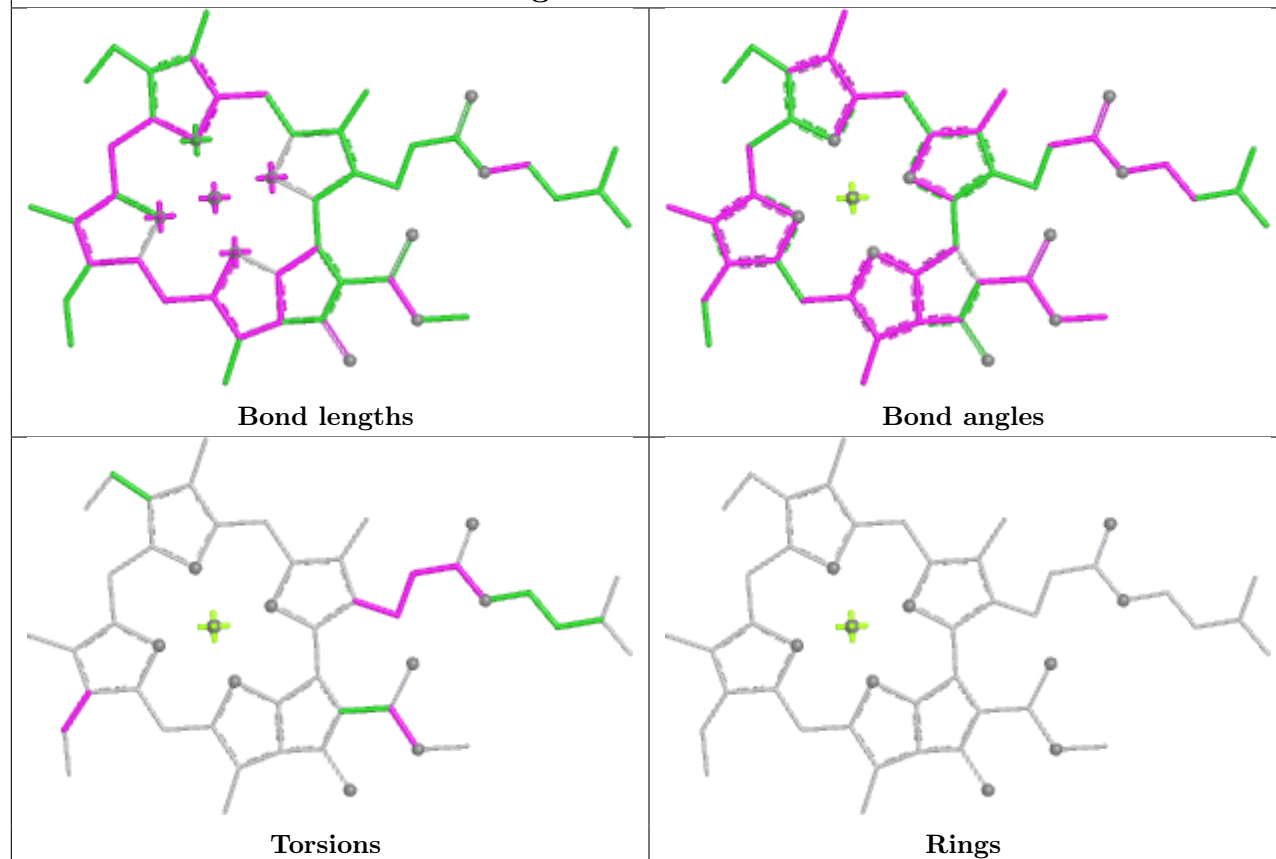
Ligand CLA h 207



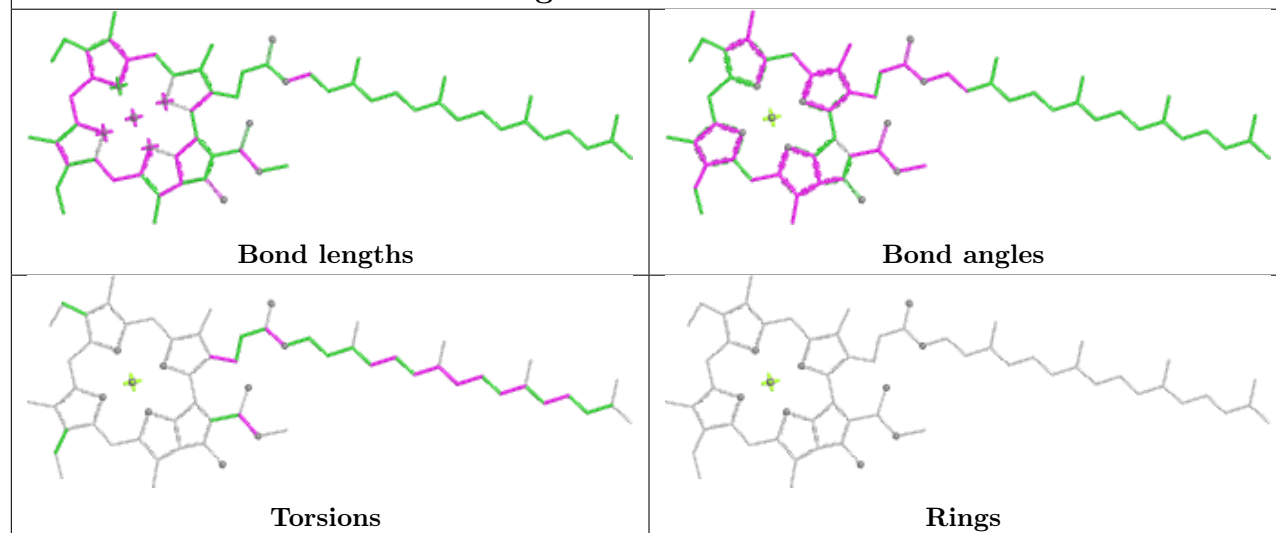


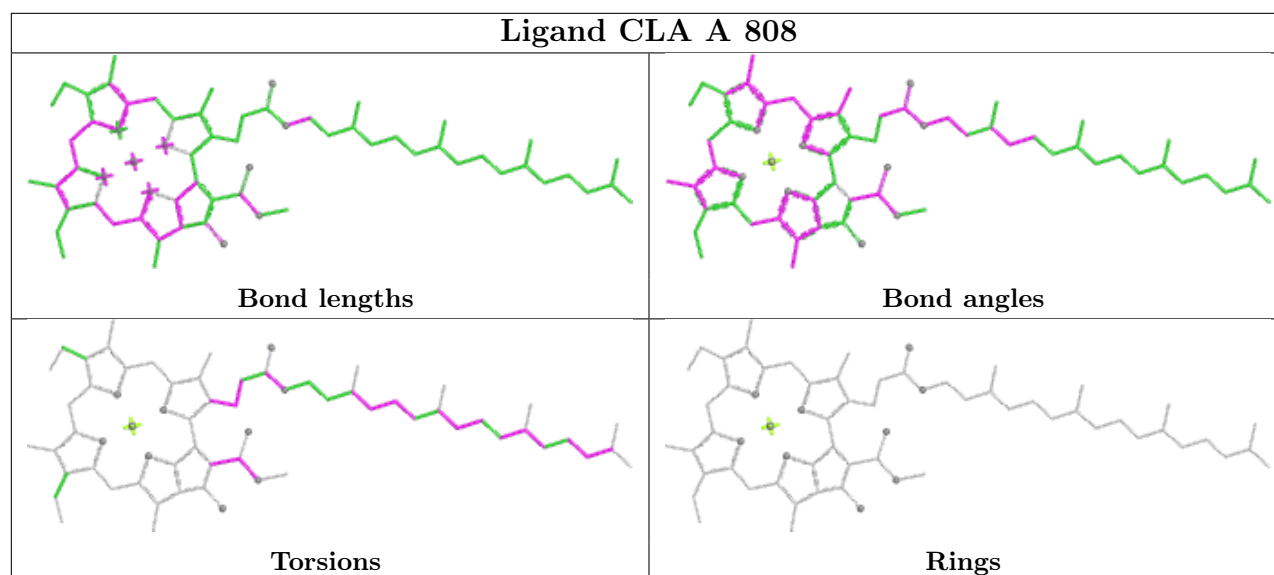
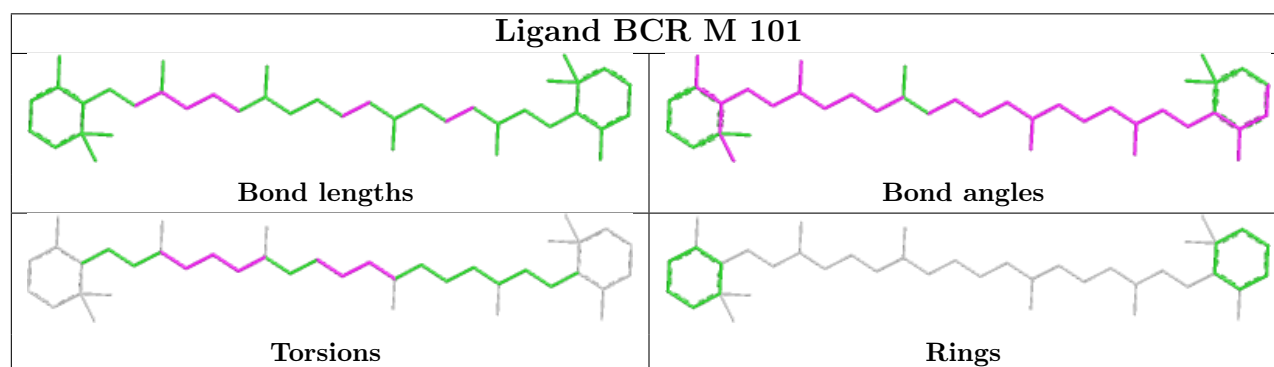
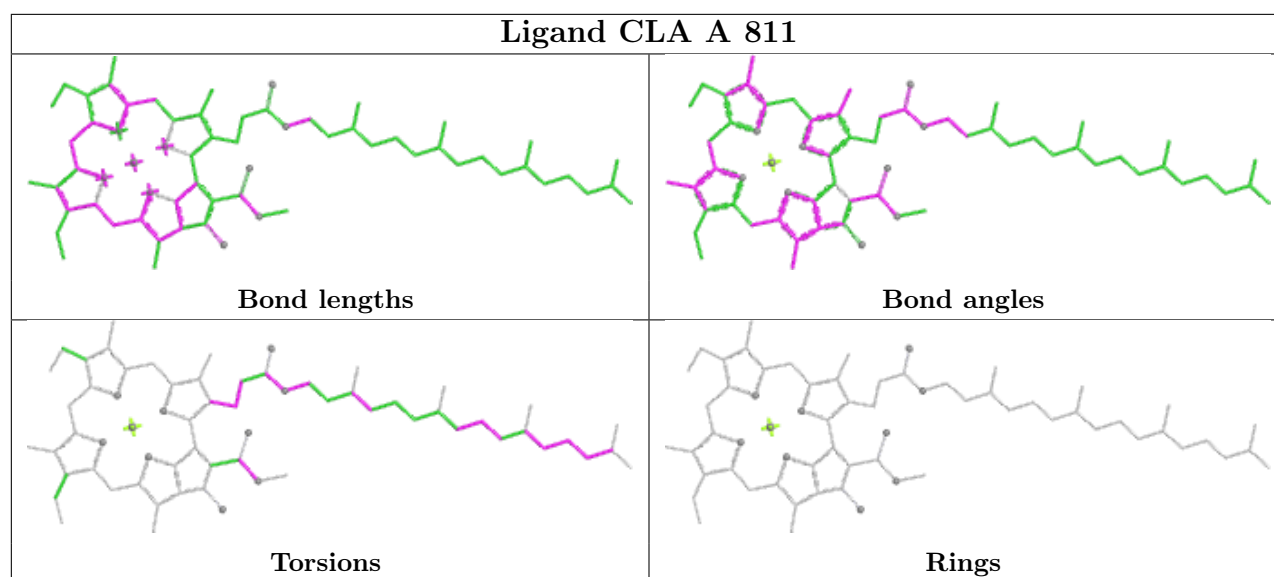
Ligand CLA B 840**Ligand CLA Y 833**

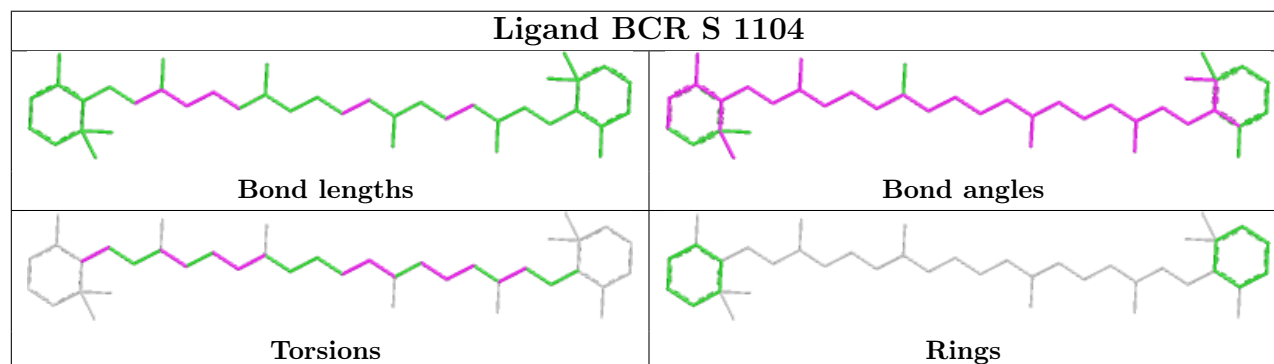
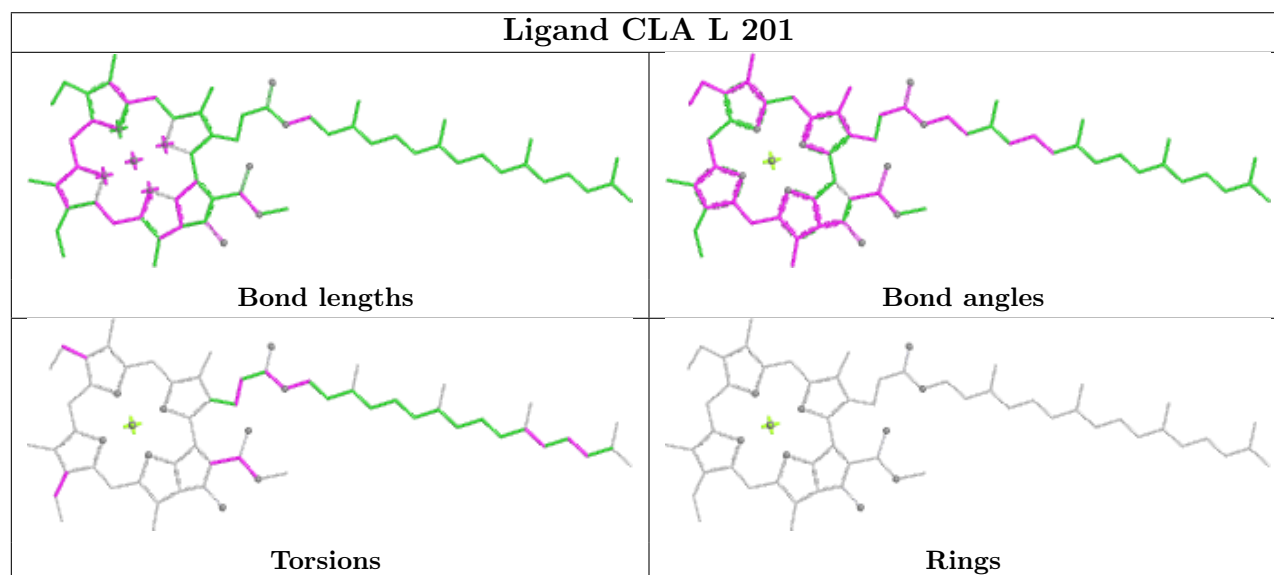
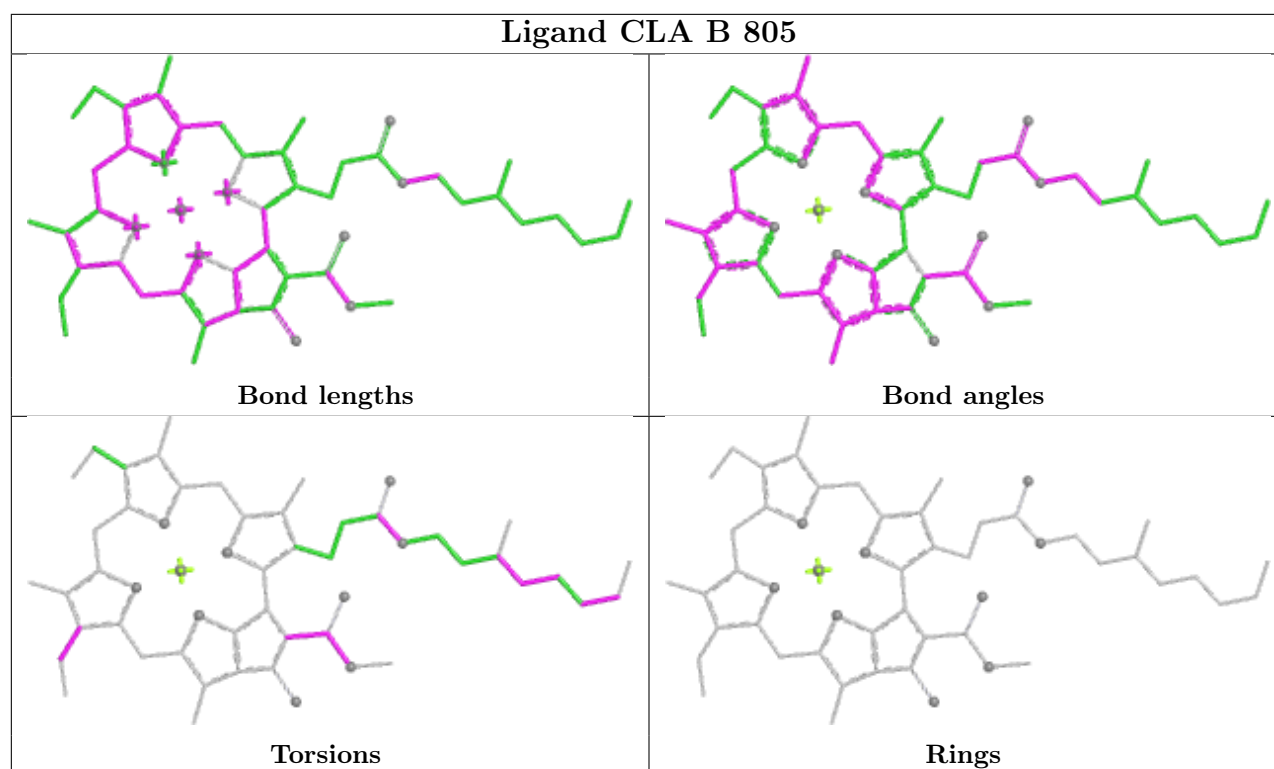
Ligand CLA Y 843



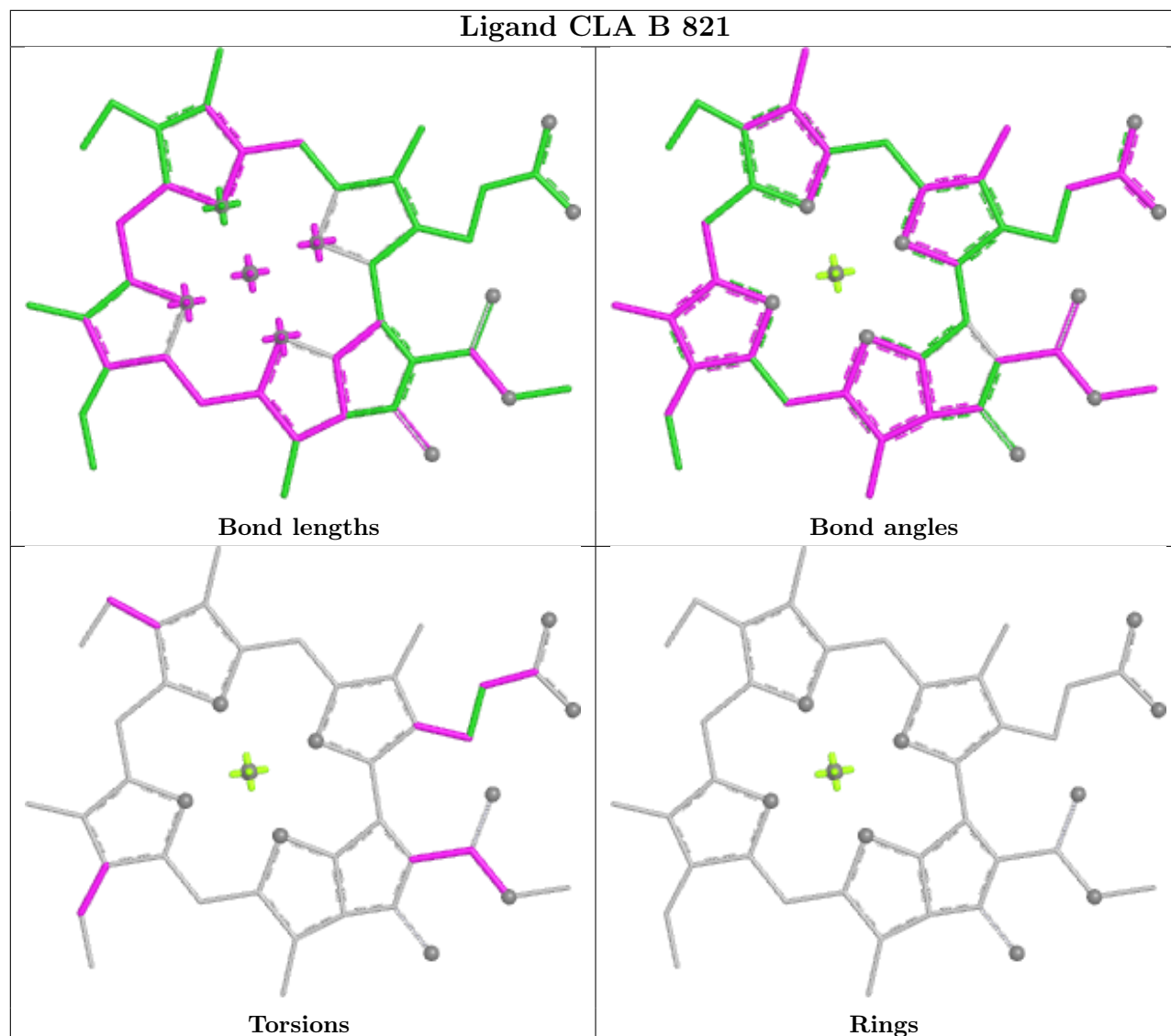
Ligand CLA h 206



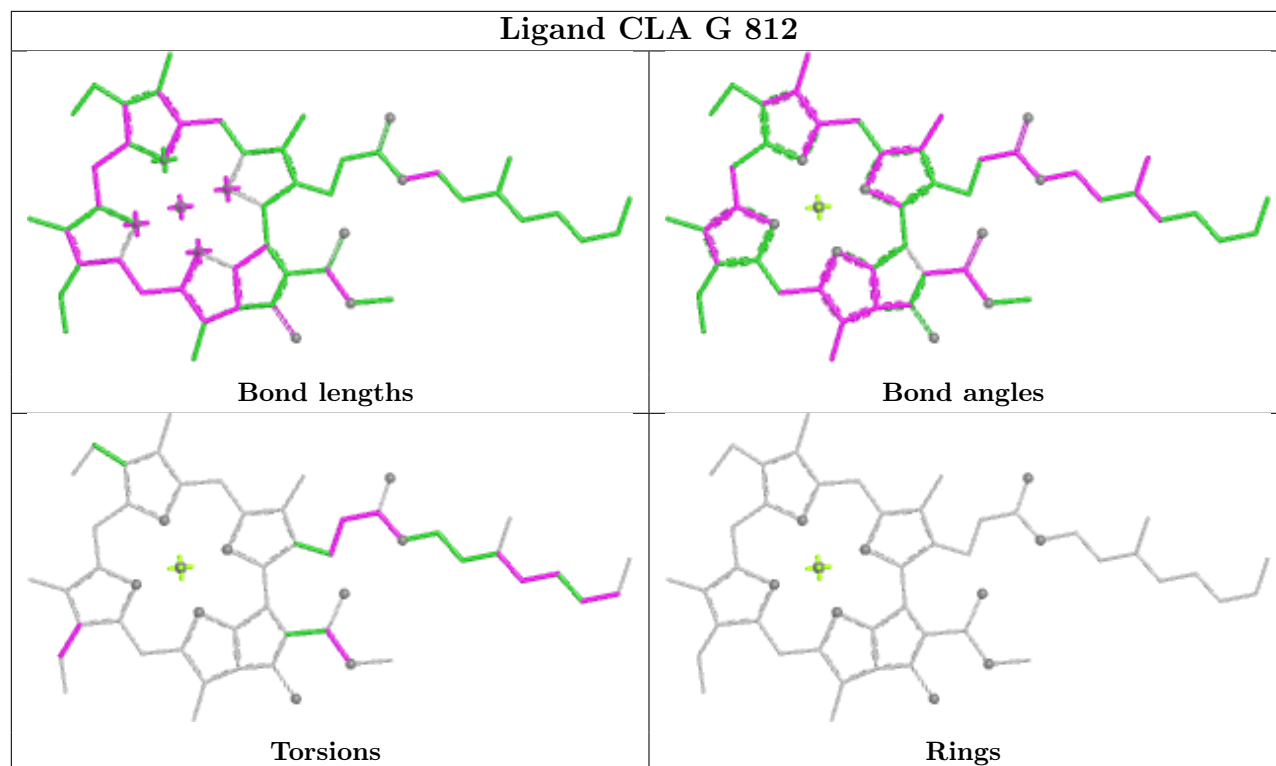




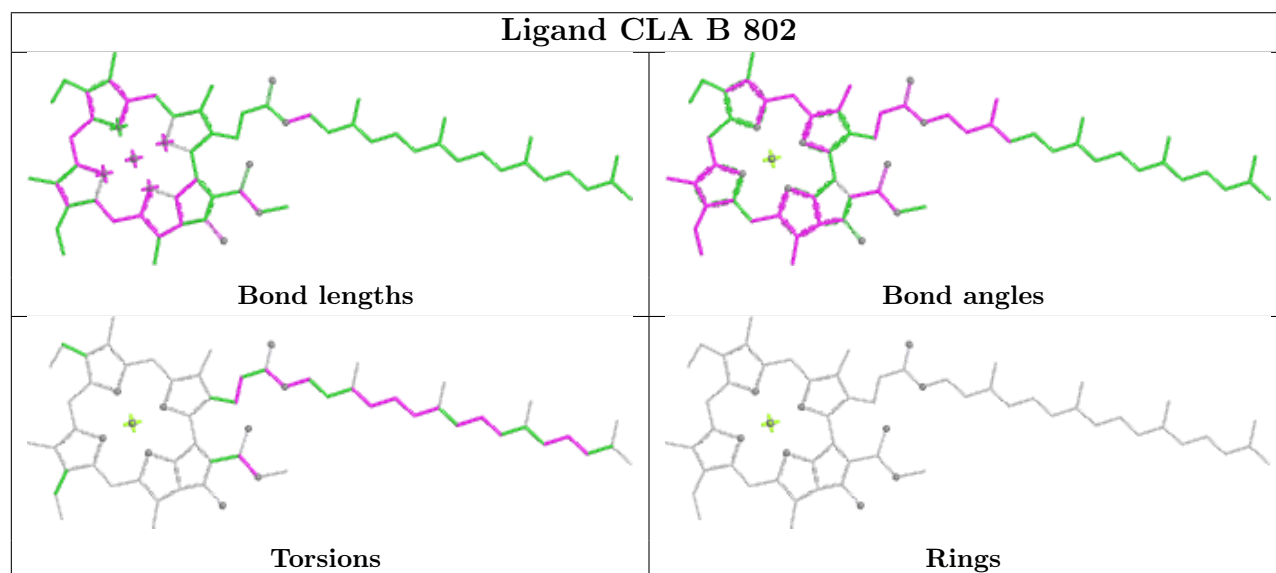
Ligand CLA B 821



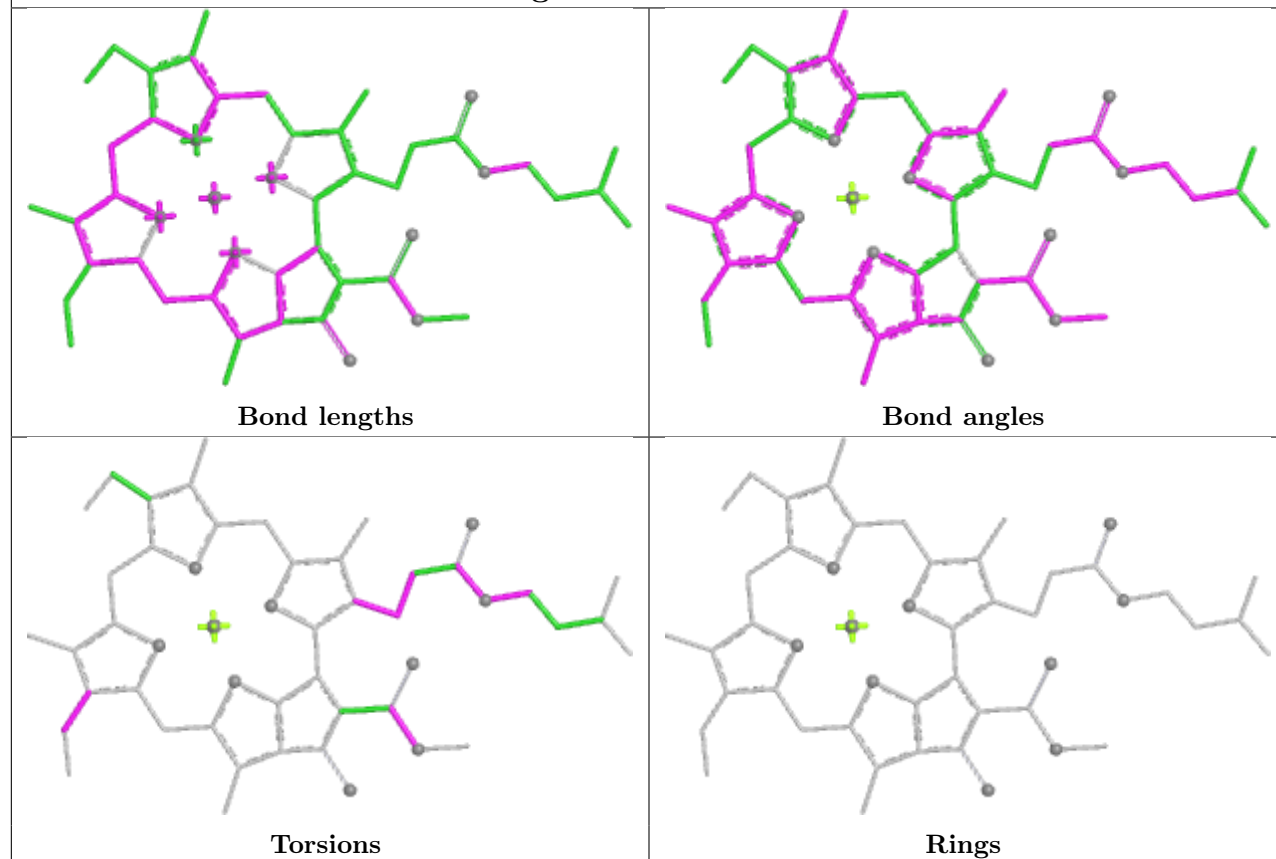
Ligand CLA G 812



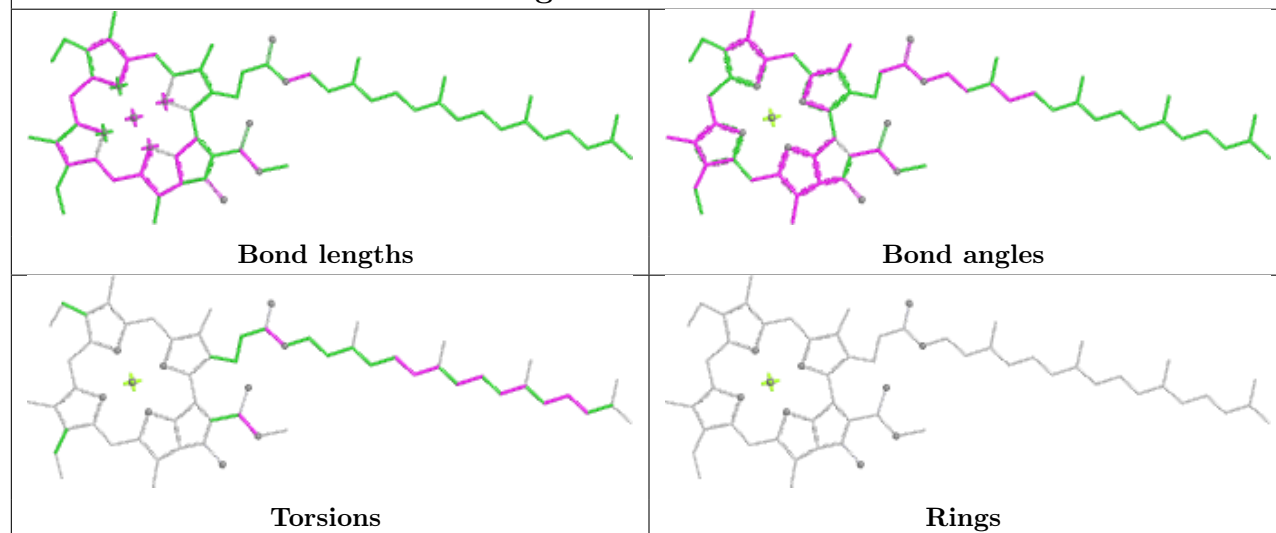
Ligand CLA B 802

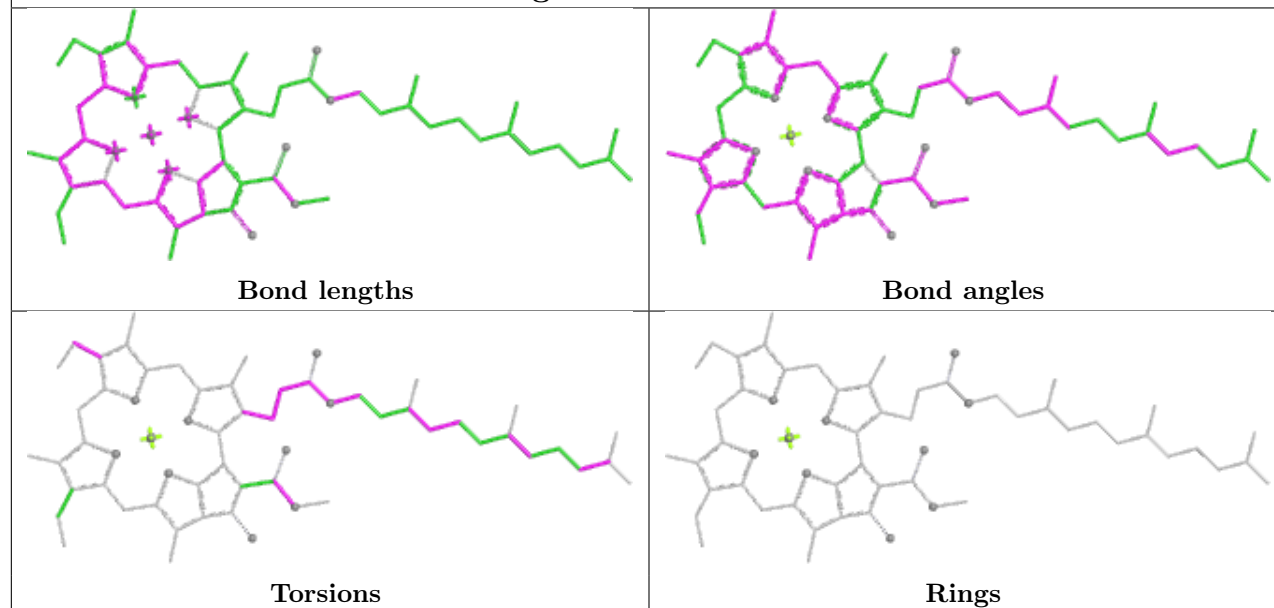
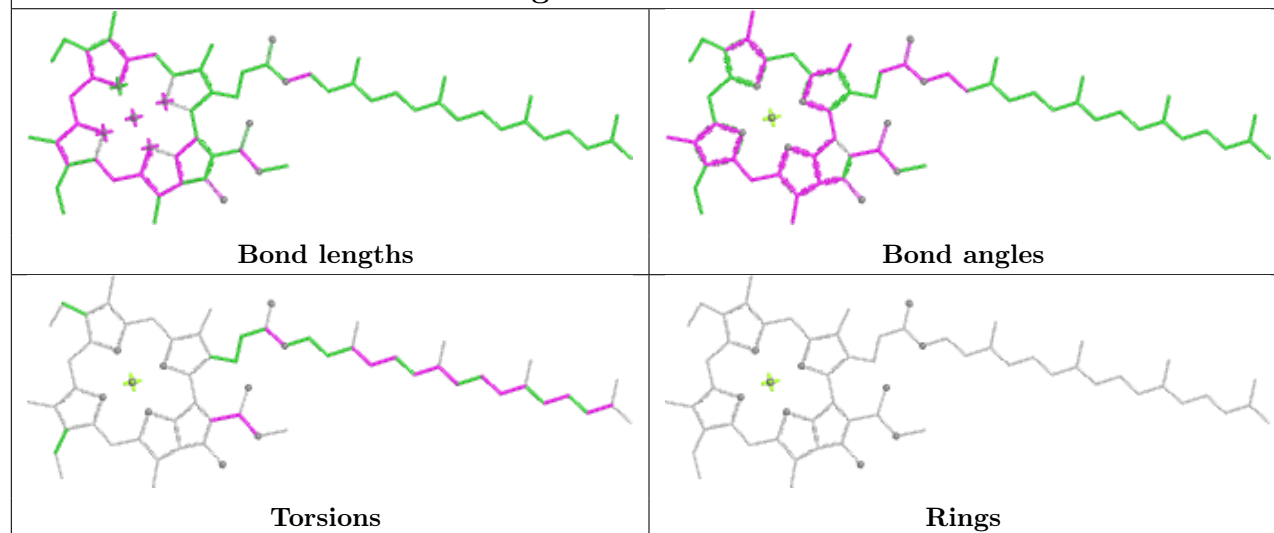


Ligand CLA Y 839

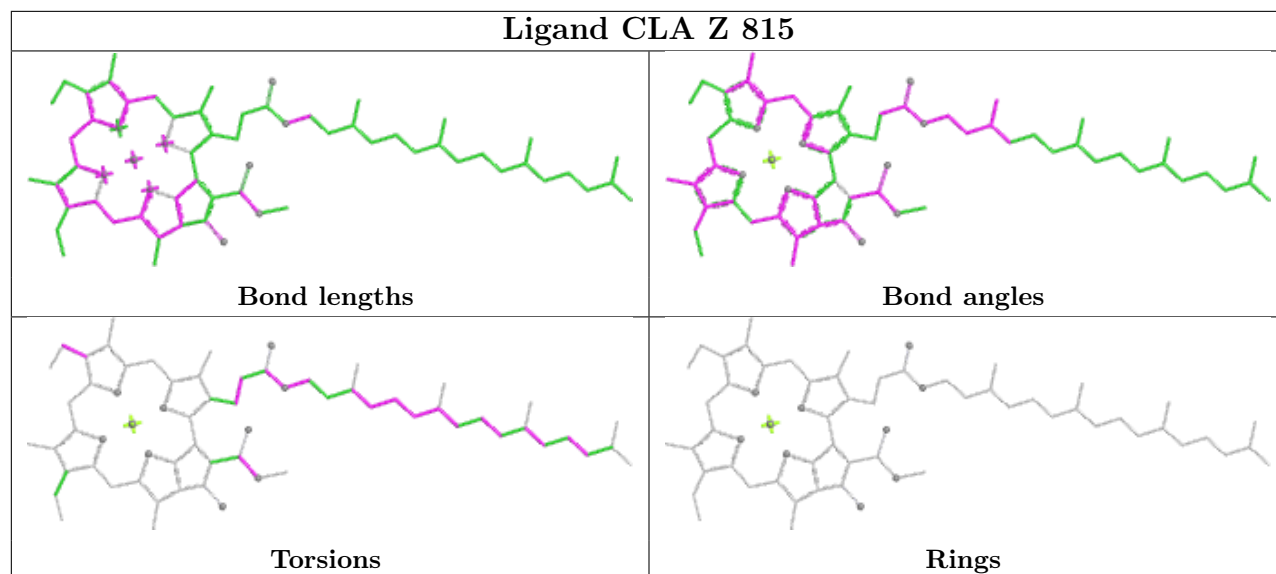


Ligand CLA h 201

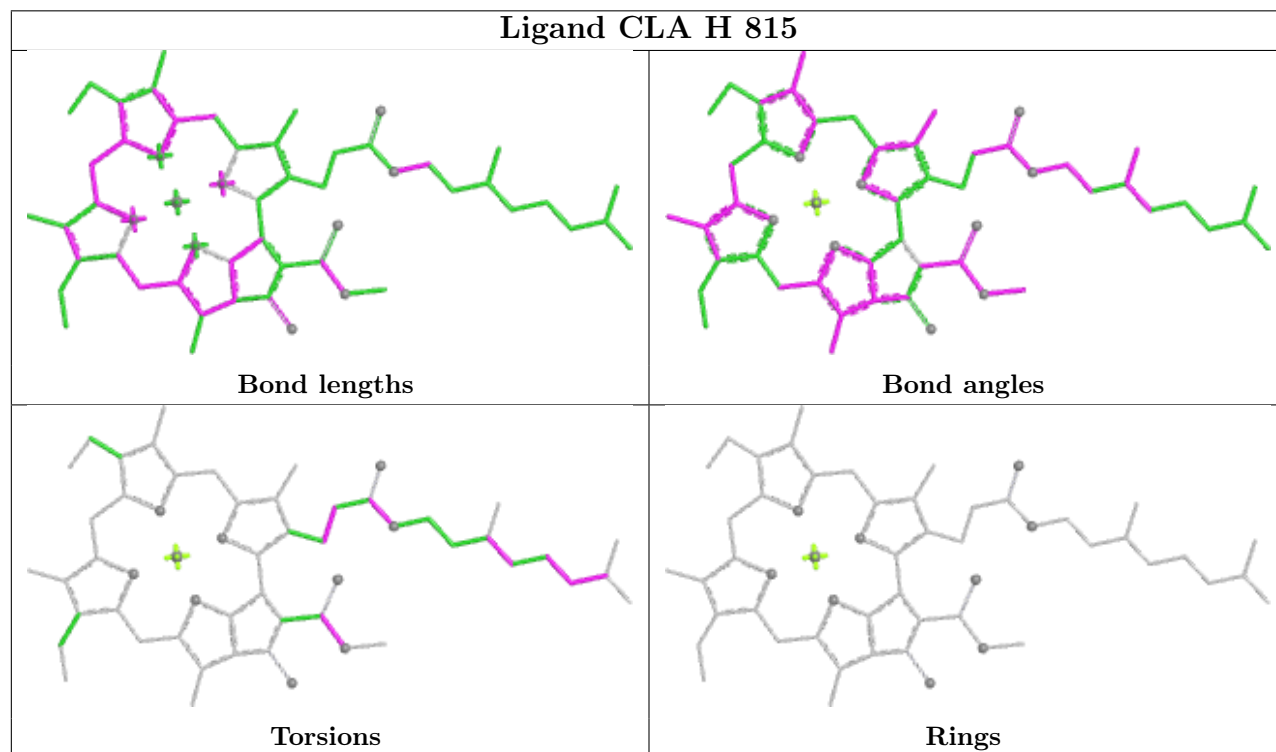


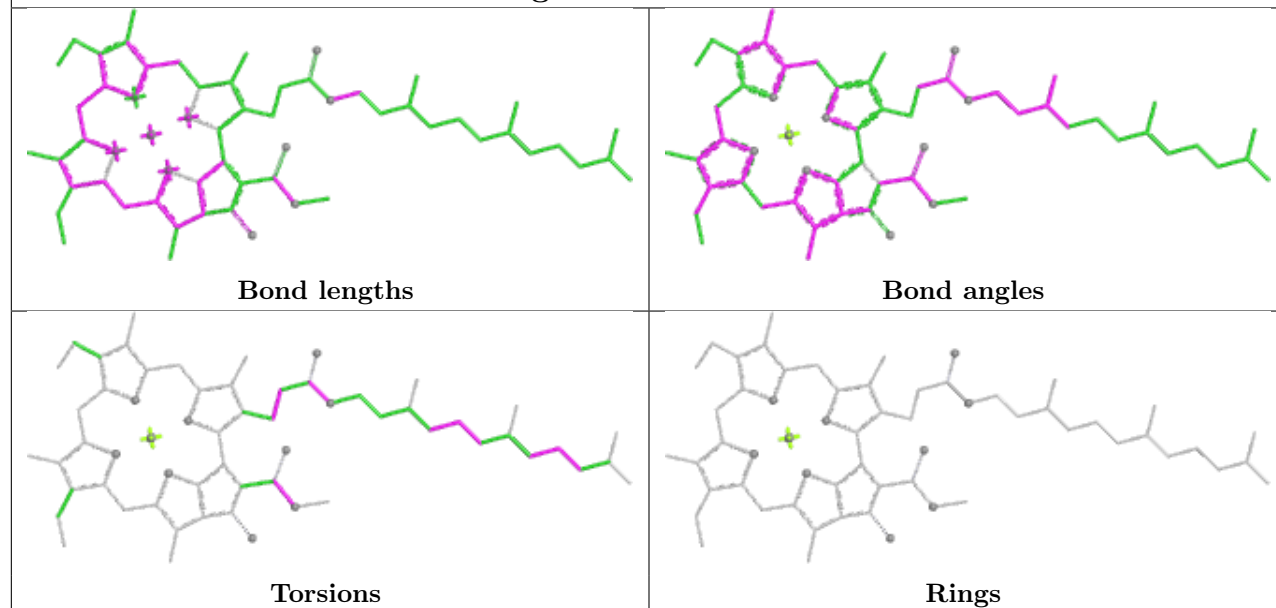
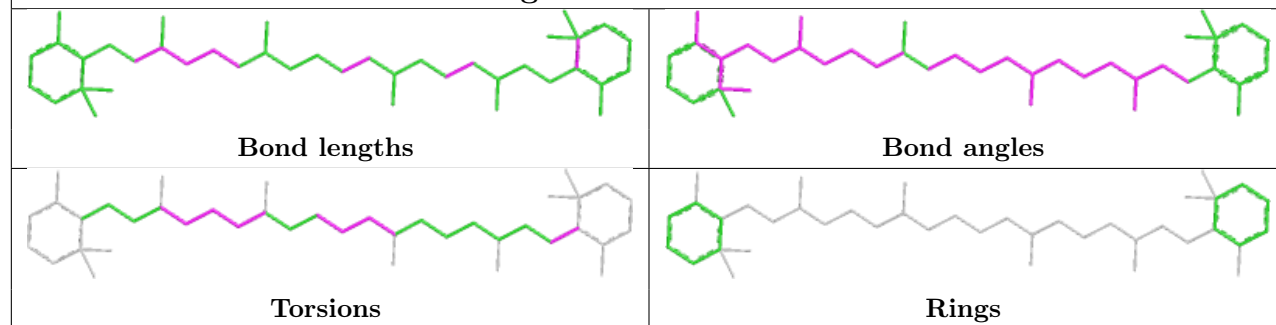
Ligand CLA B 819**Ligand CLA Y 827**

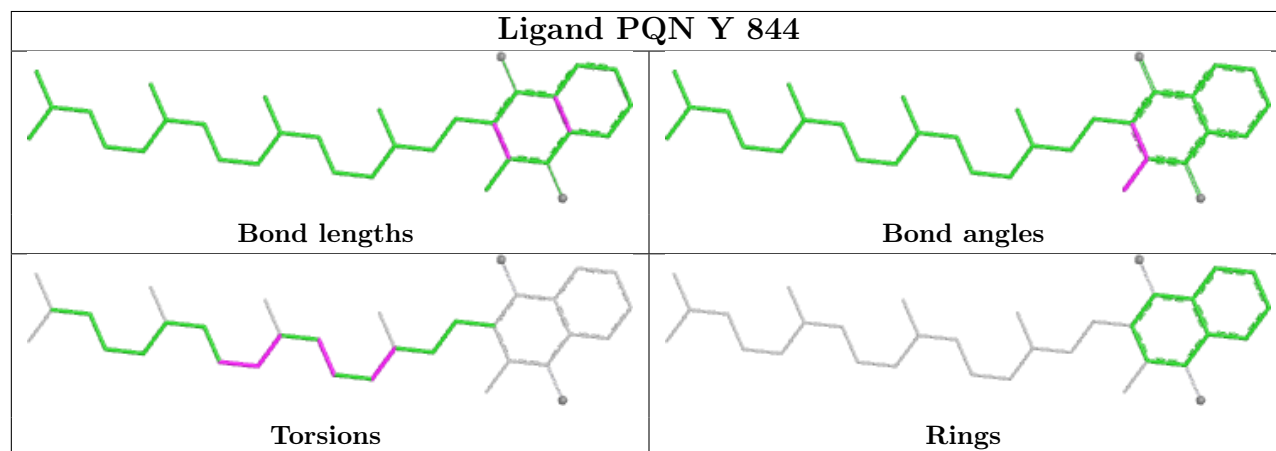
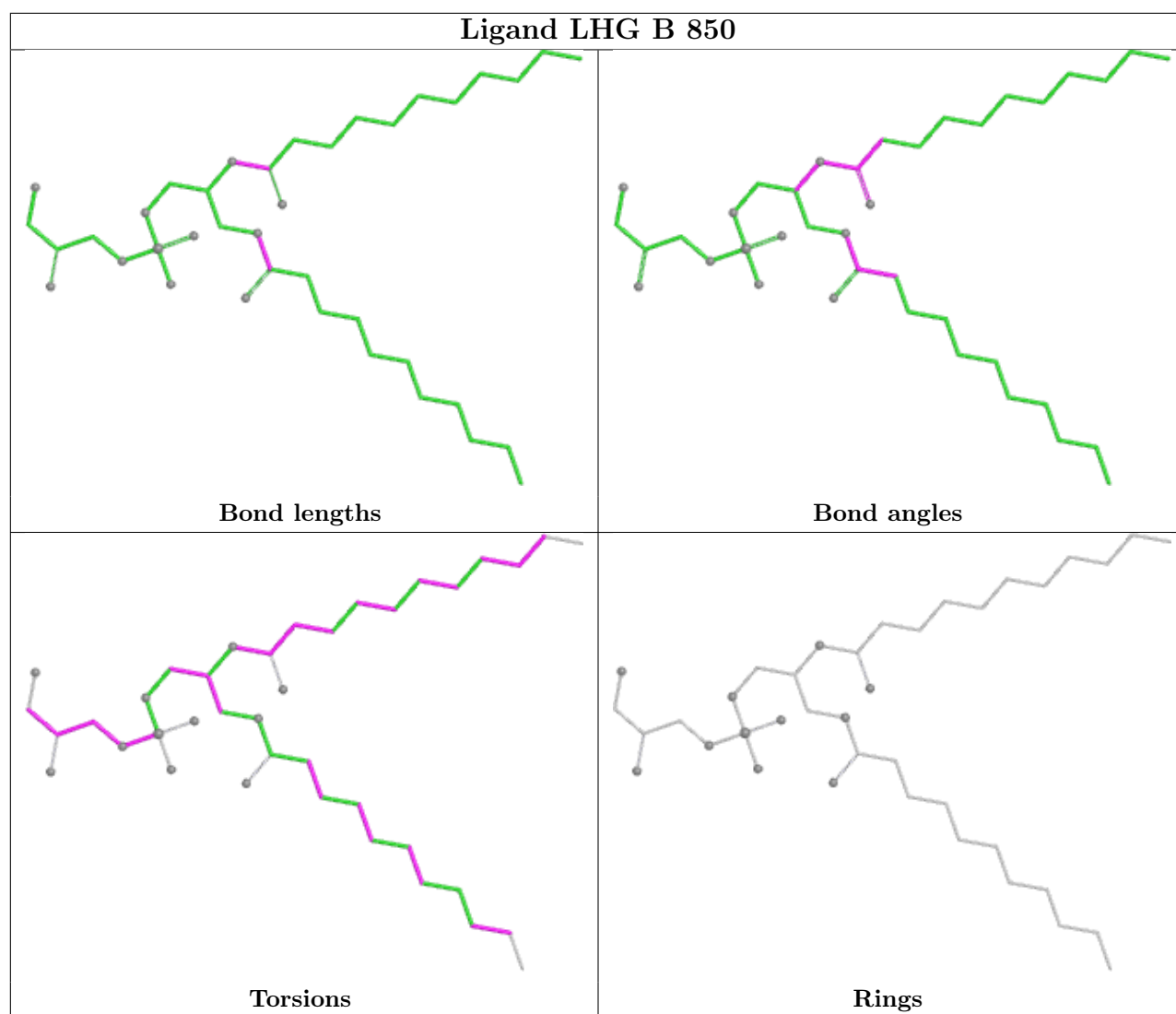
Ligand CLA Z 815



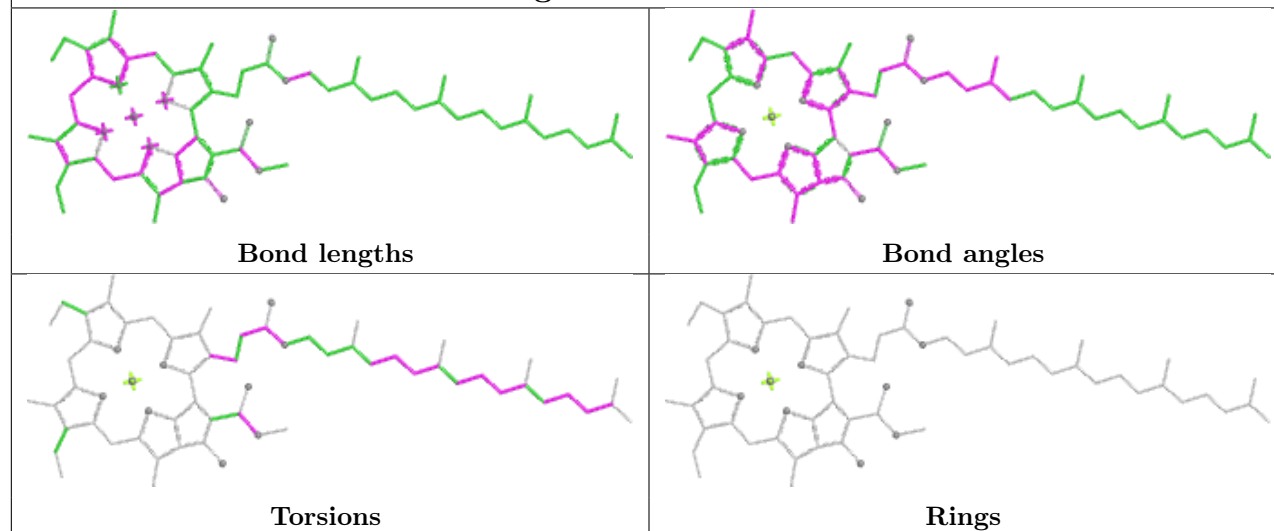
Ligand CLA H 815



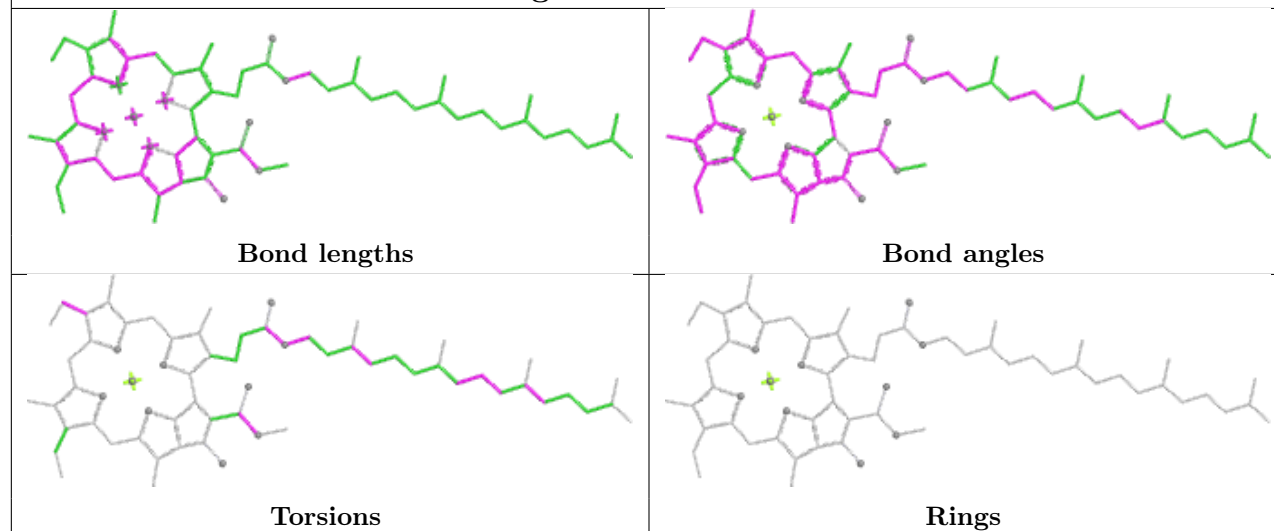
Ligand CLA Y 813**Ligand BCR U 1005**



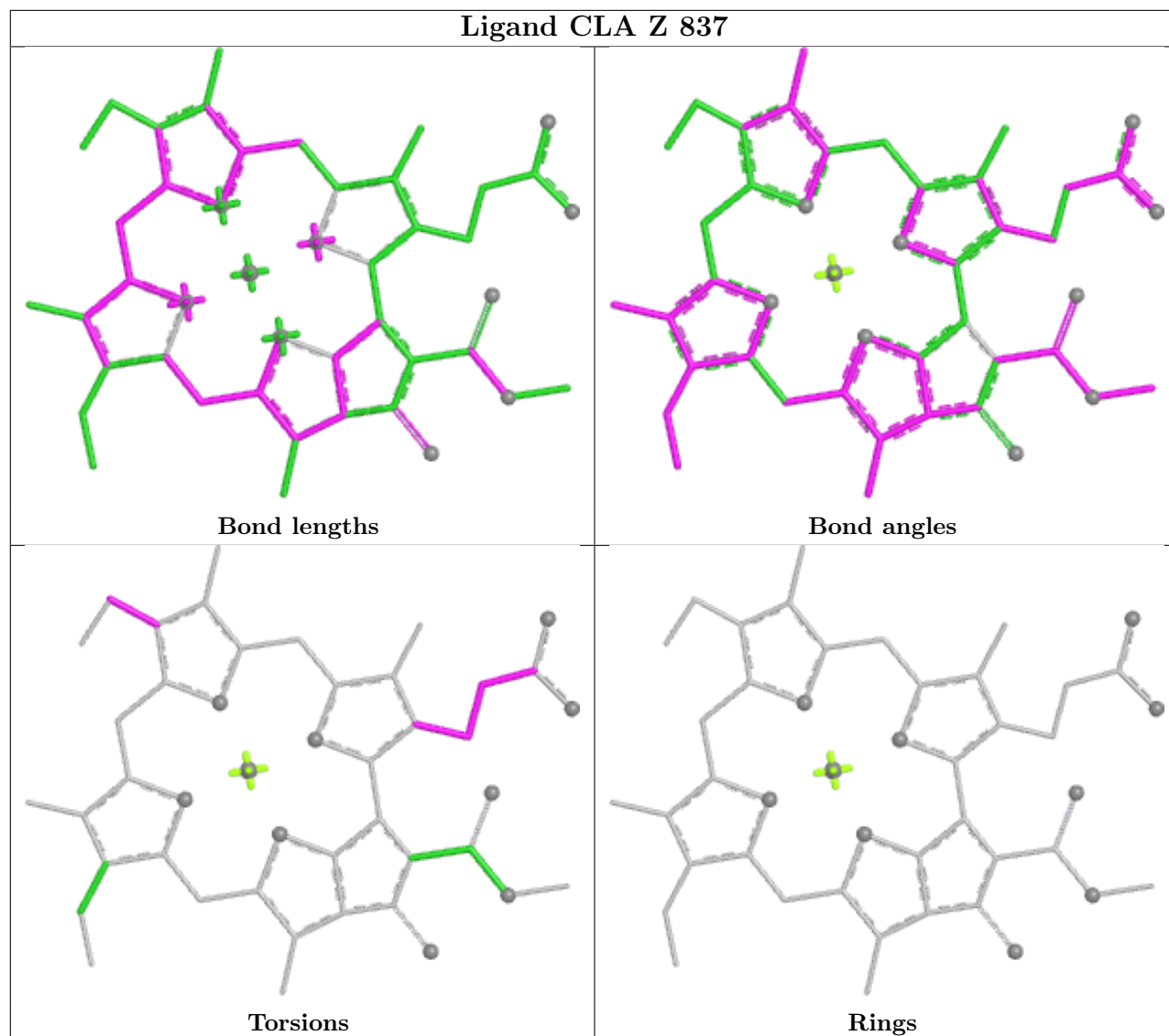
Ligand CLA Z 802



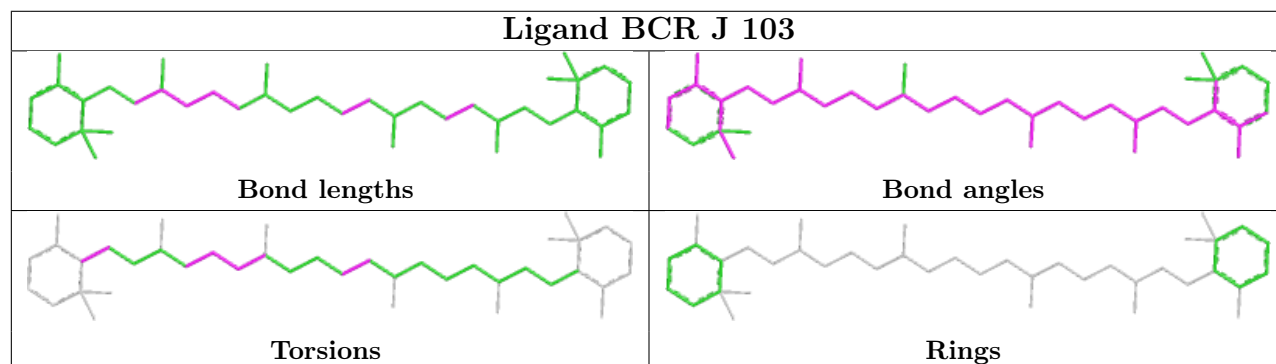
Ligand CLA A 802



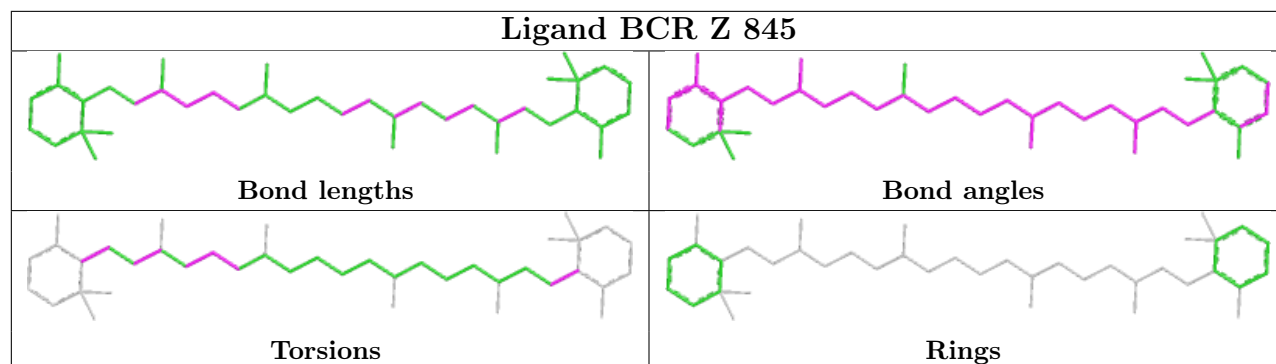
Ligand CLA Z 837



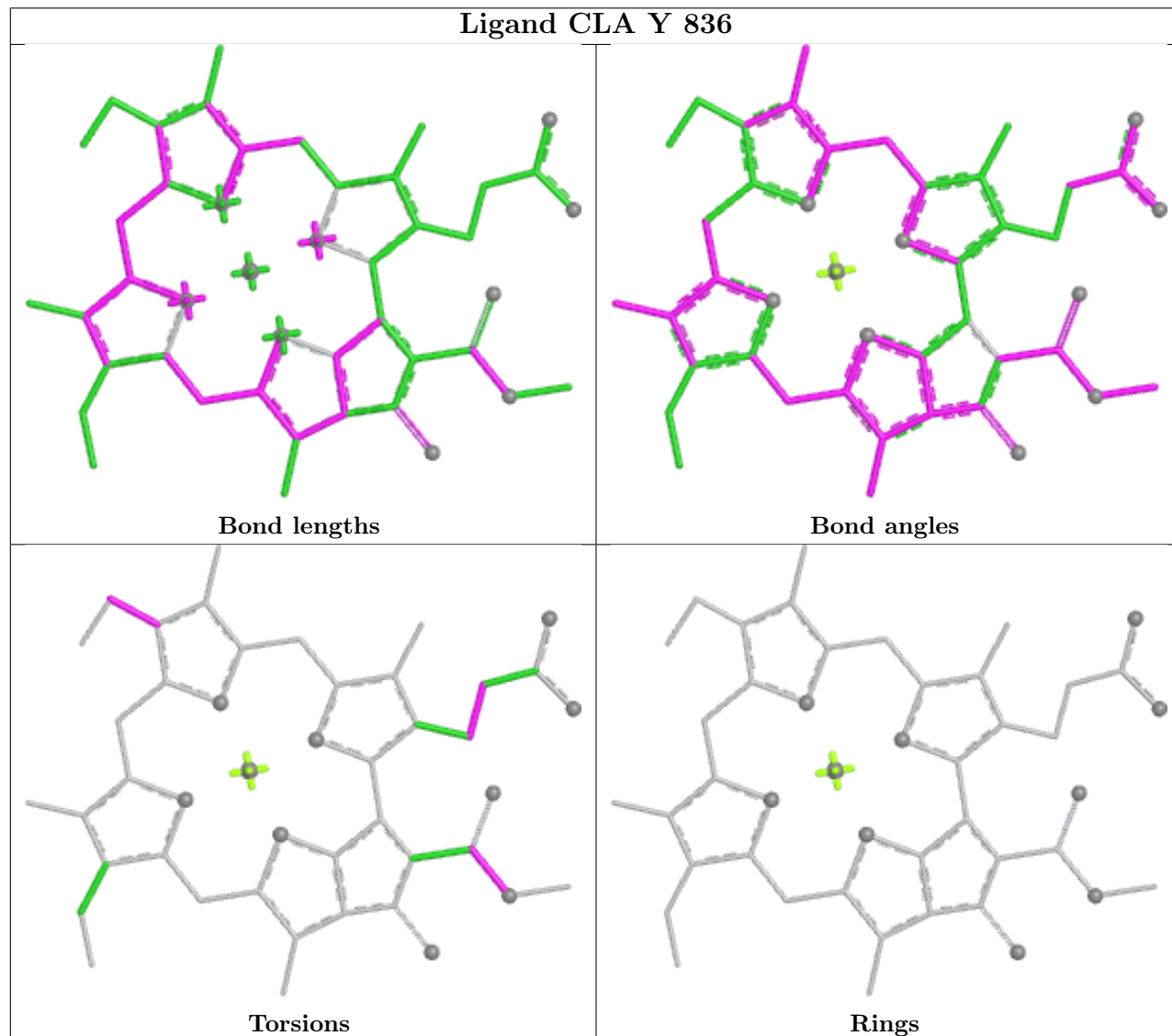
Ligand BCR J 103



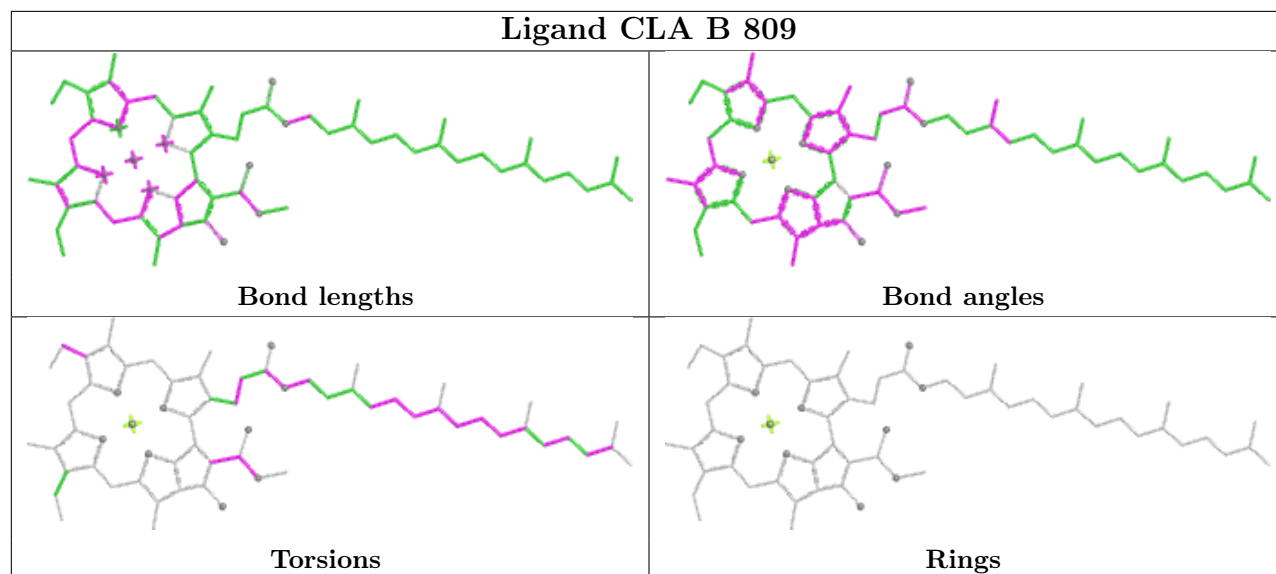
Ligand BCR Z 845



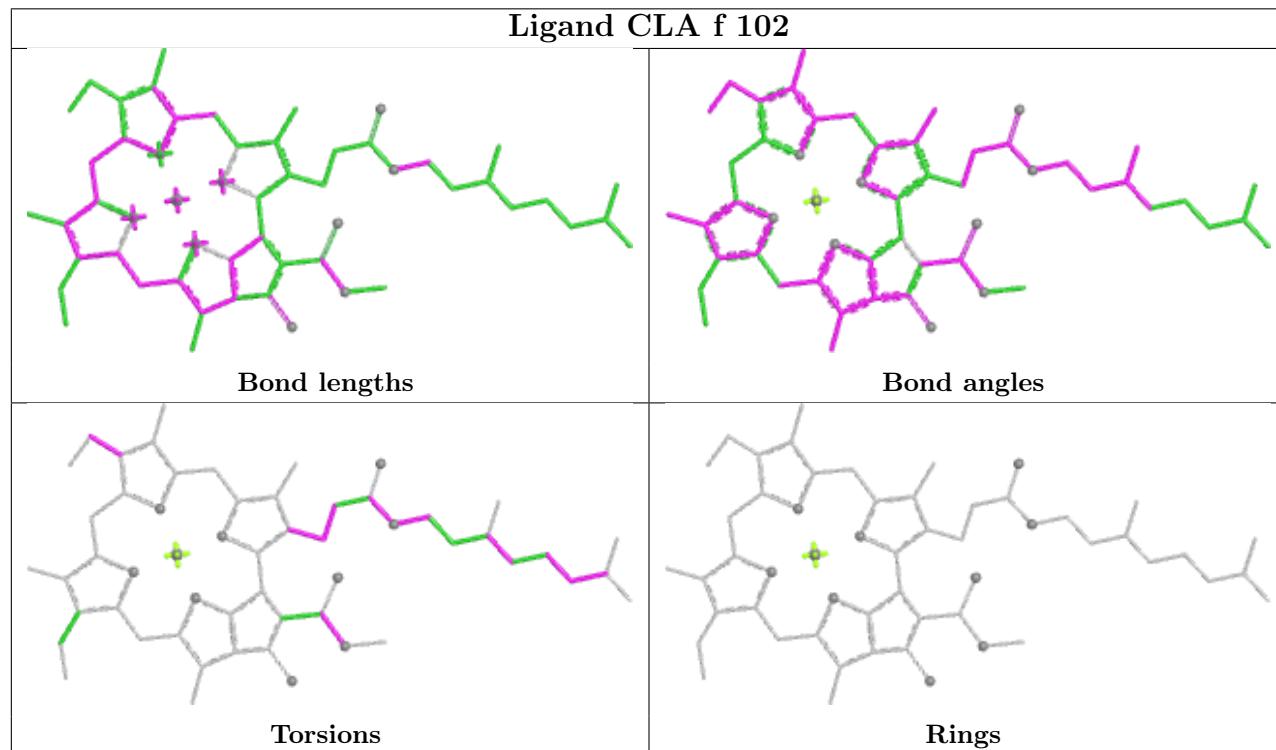
Ligand CLA Y 836



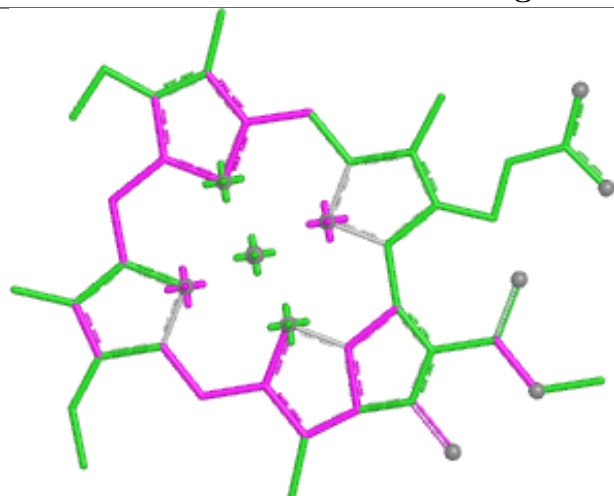
Ligand CLA B 809



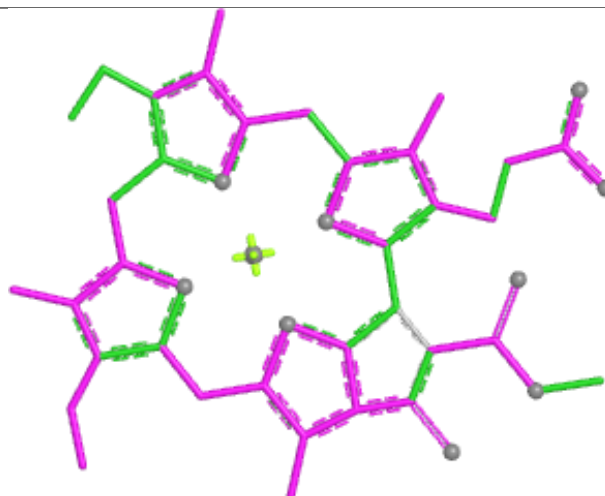
Ligand CLA f 102



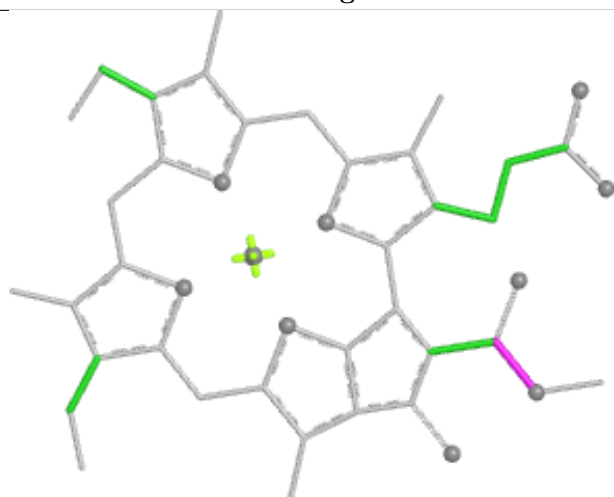
Ligand CLA B 815



Bond lengths



Bond angles

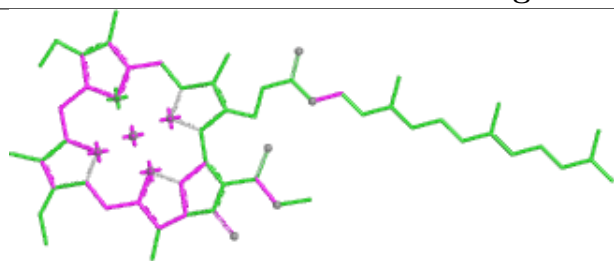


Torsions

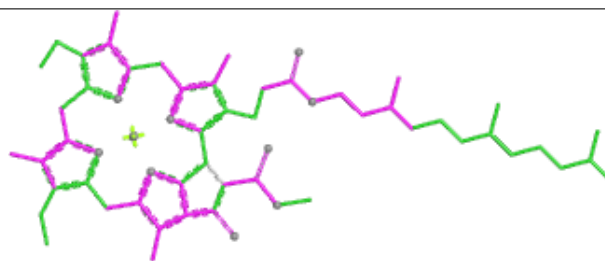


Rings

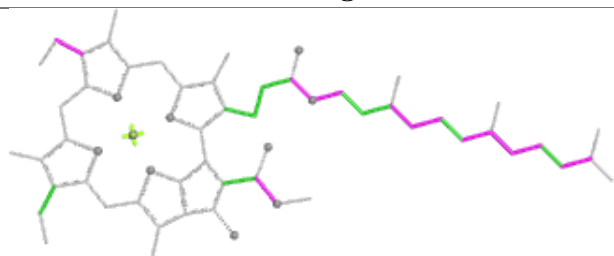
Ligand CLA G 826



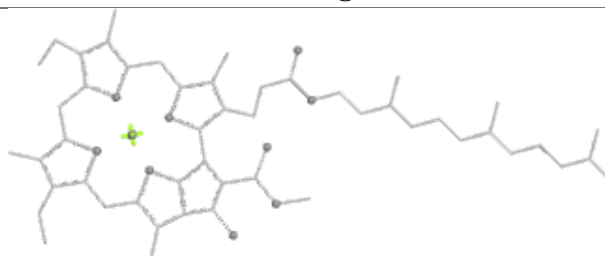
Bond lengths



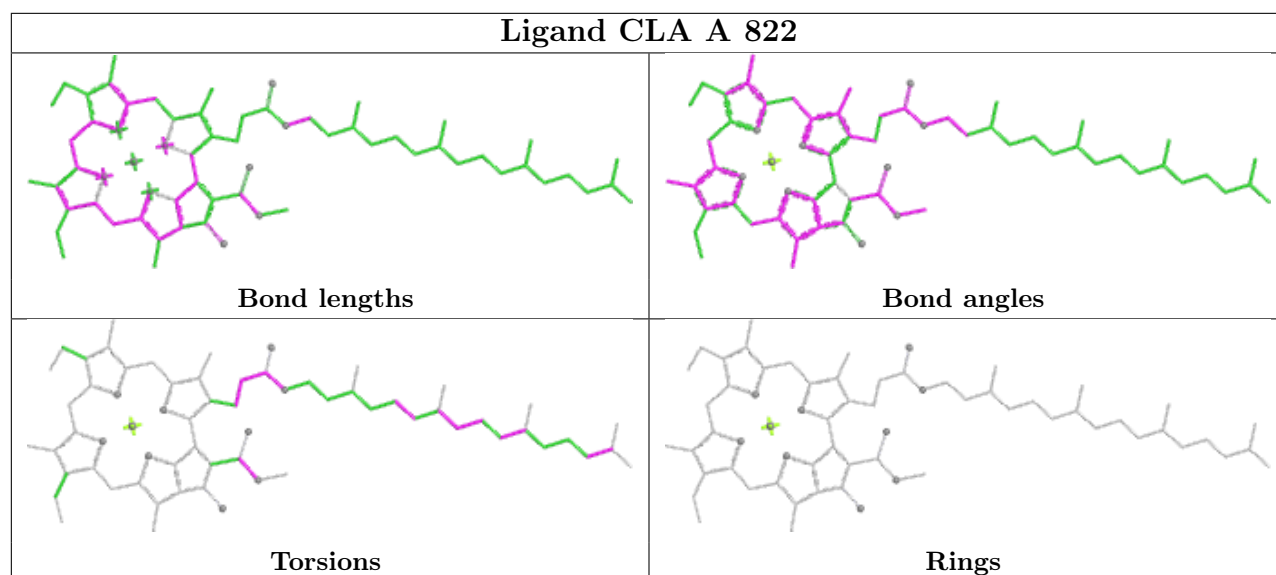
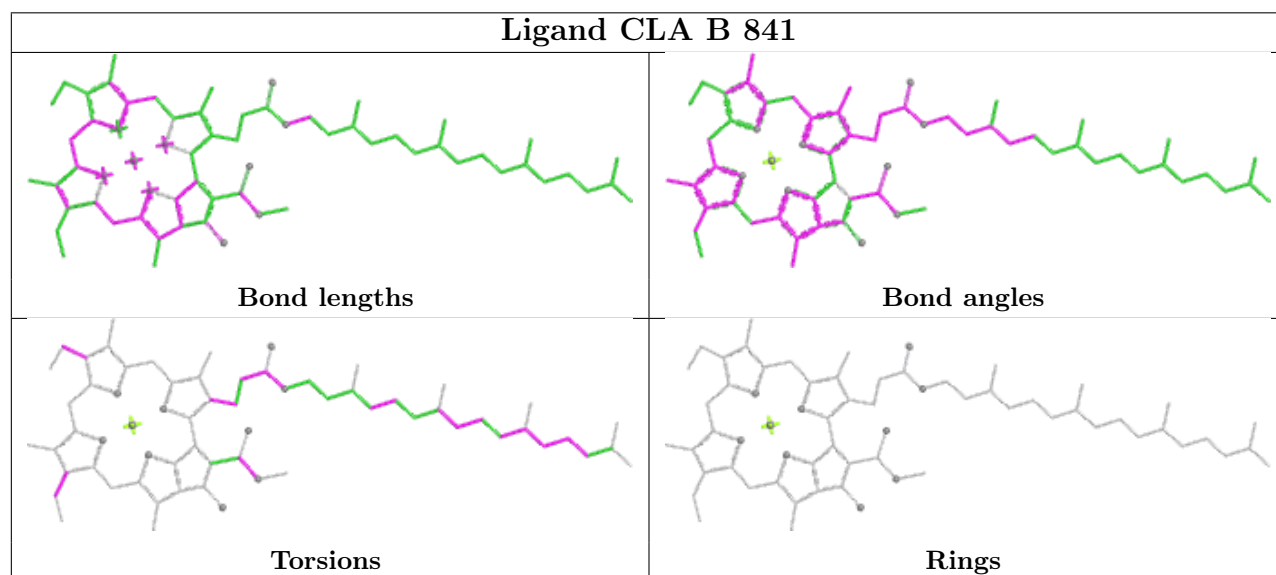
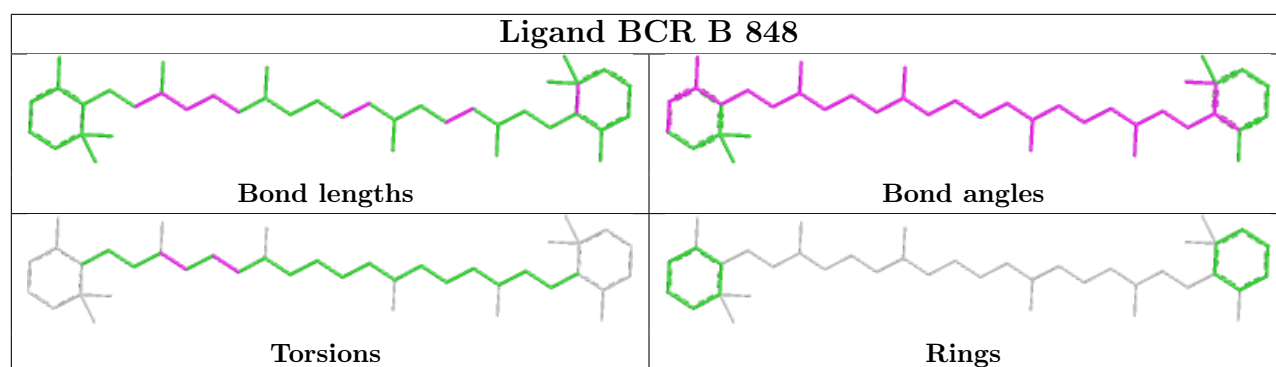
Bond angles

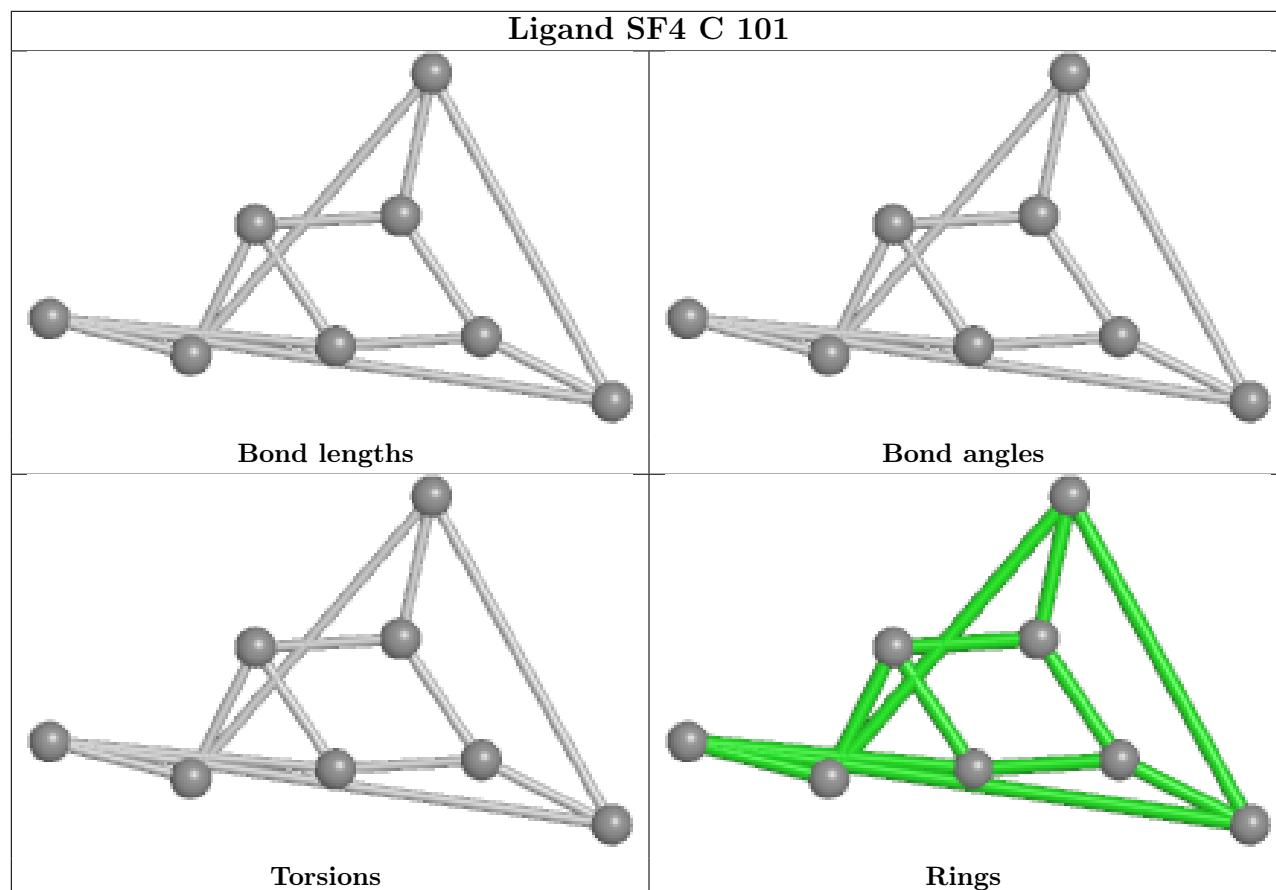
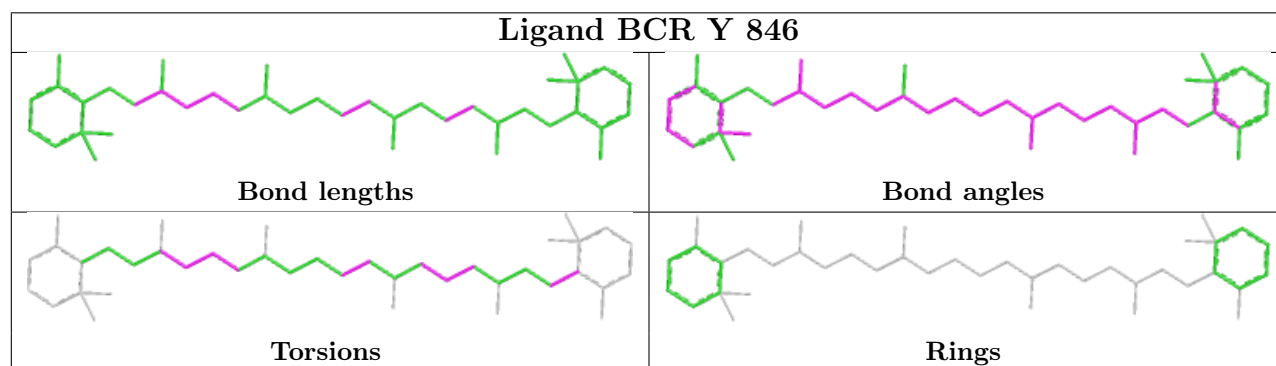
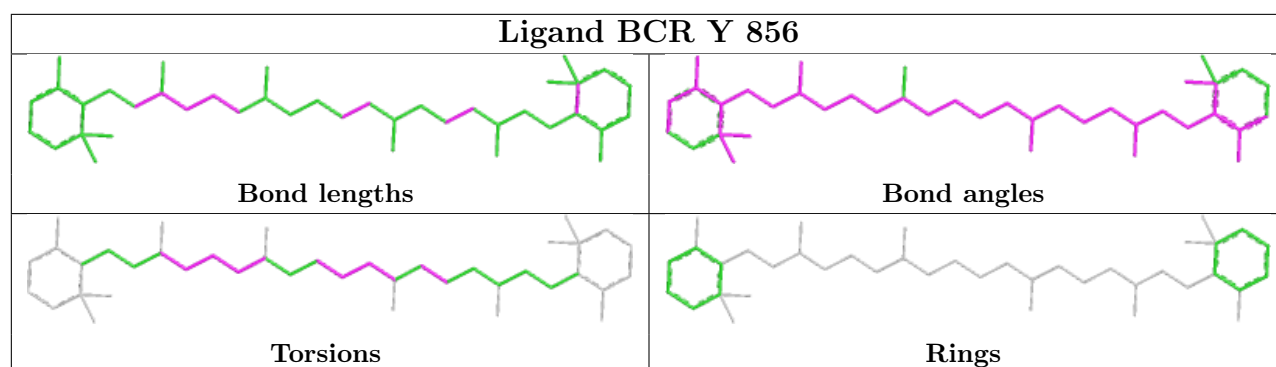


Torsions

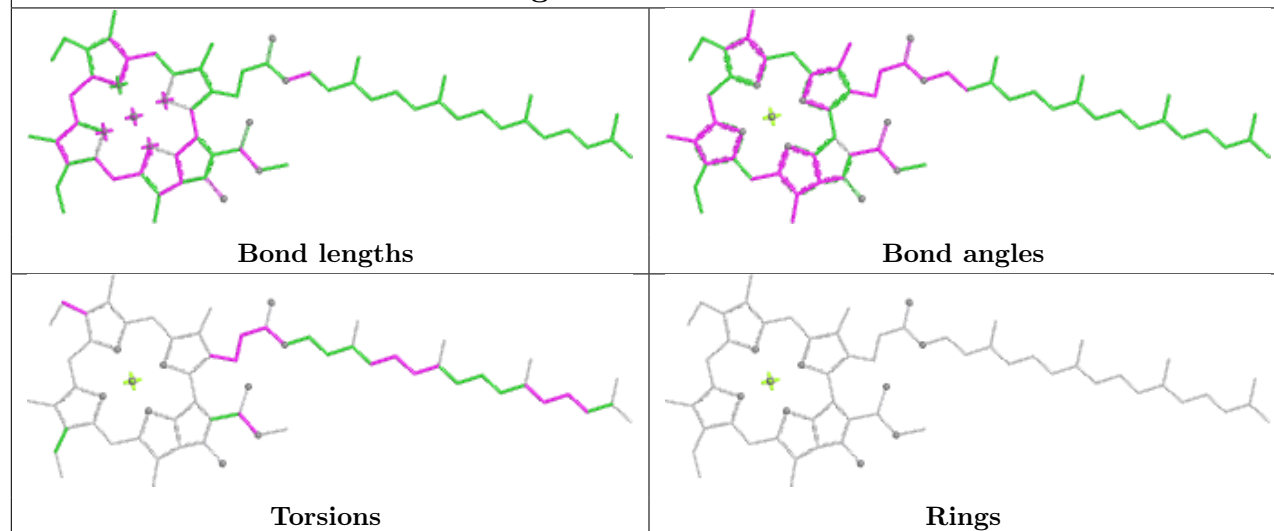


Rings

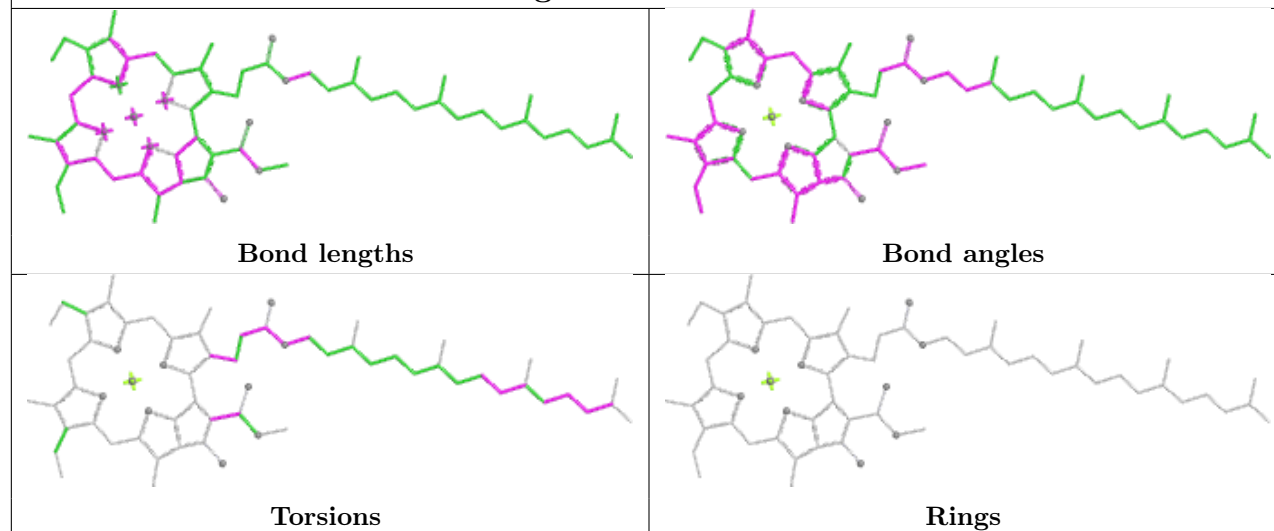




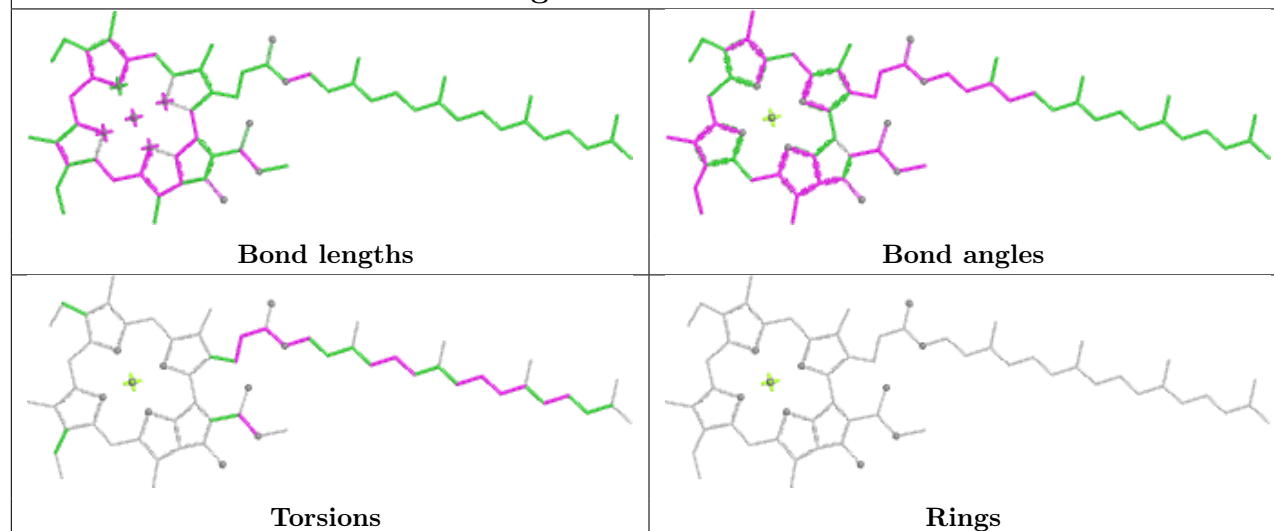
Ligand CLA G 811



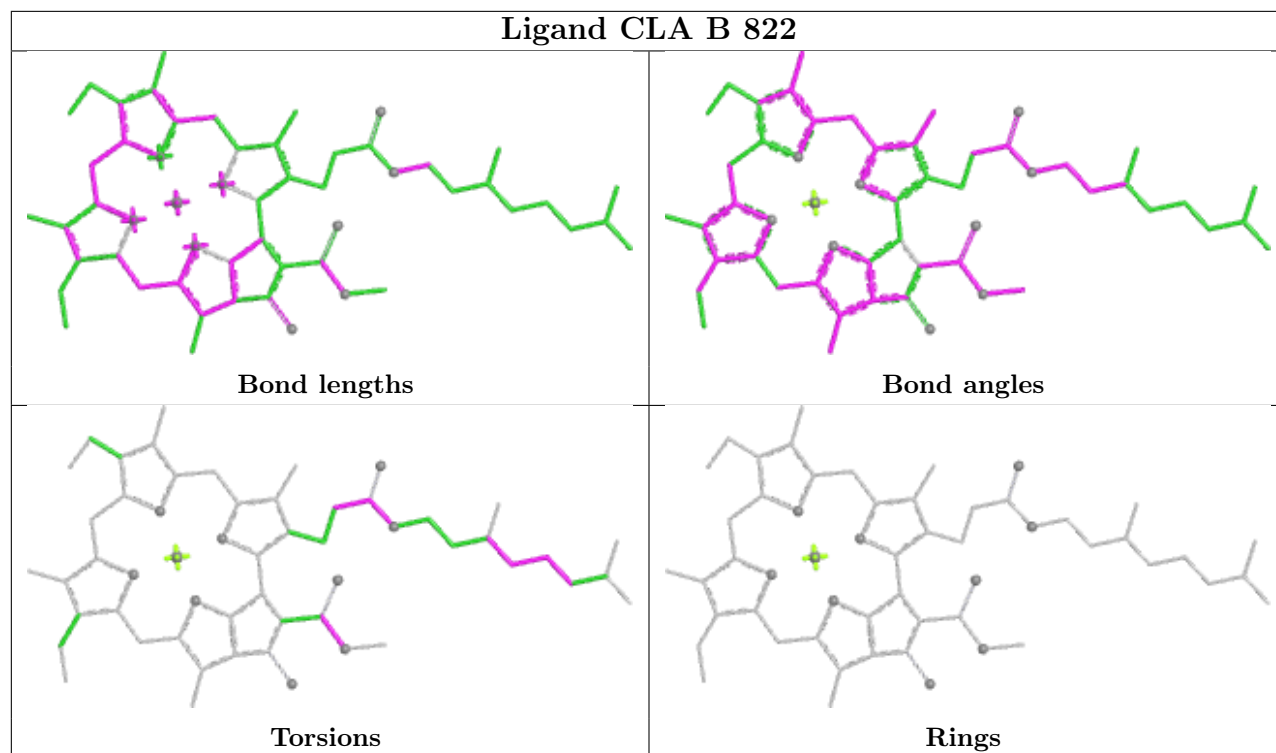
Ligand CLA Z 804



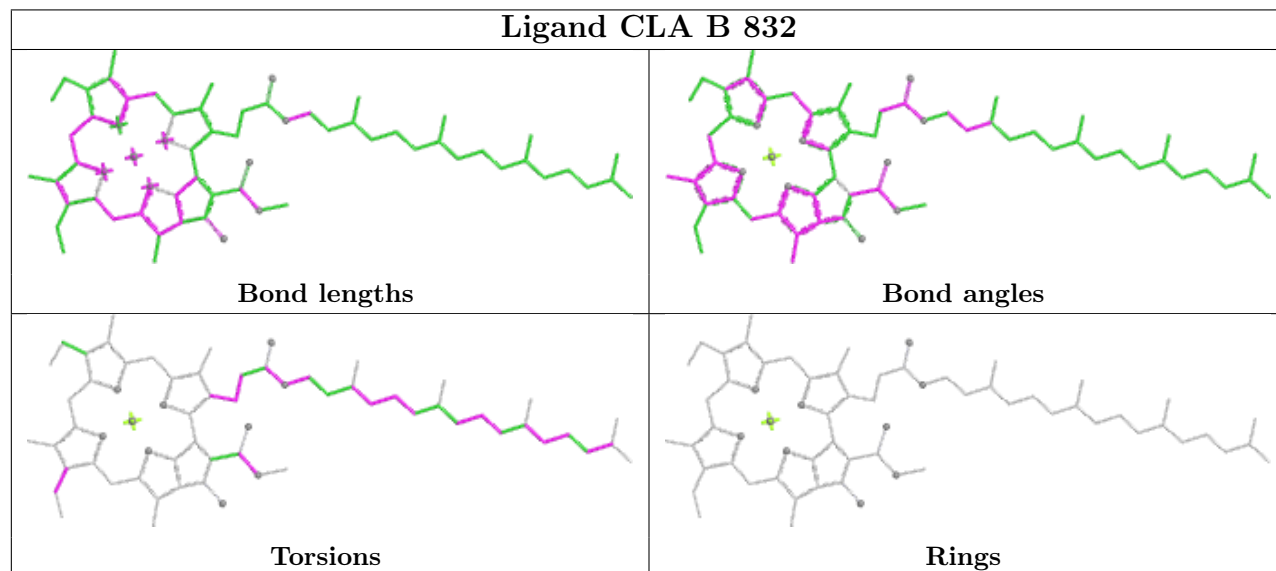
Ligand CLA G 839



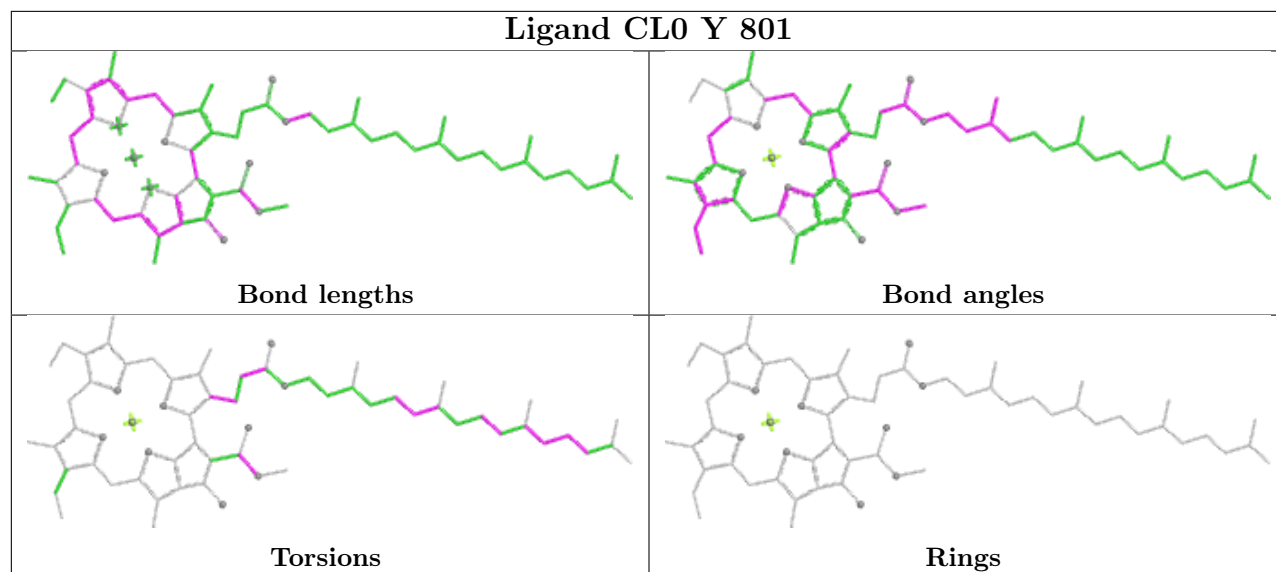
Ligand CLA B 822



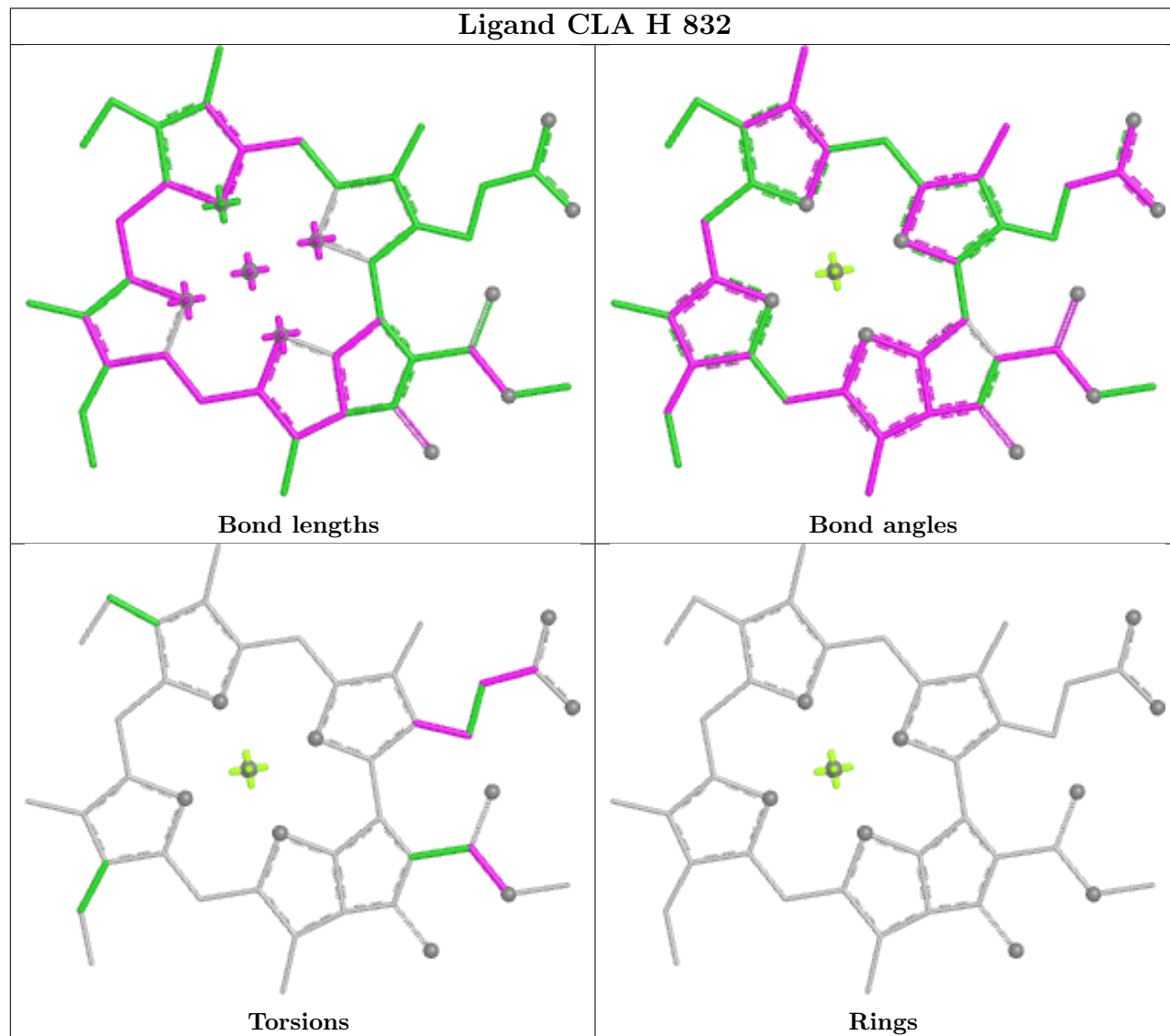
Ligand CLA B 832



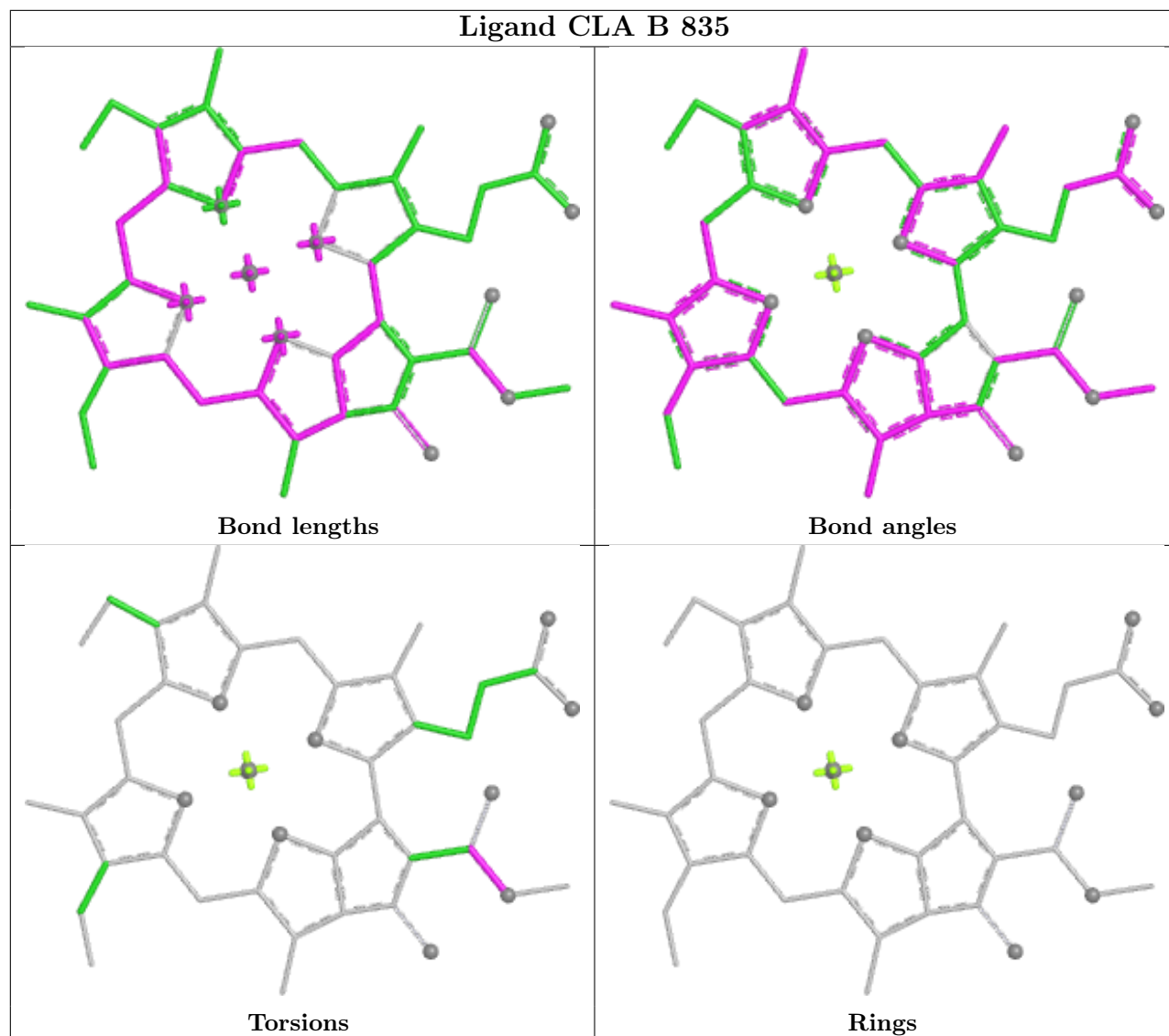
Ligand CL0 Y 801



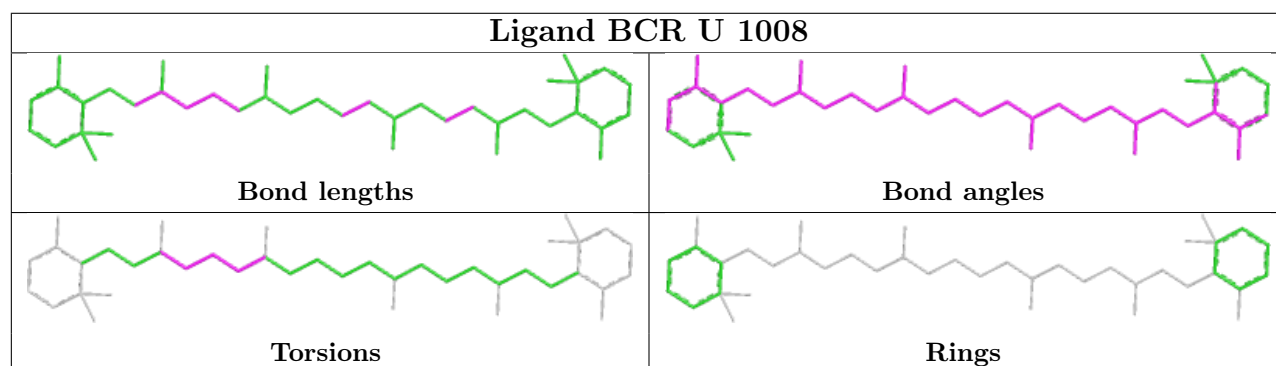
Ligand CLA H 832



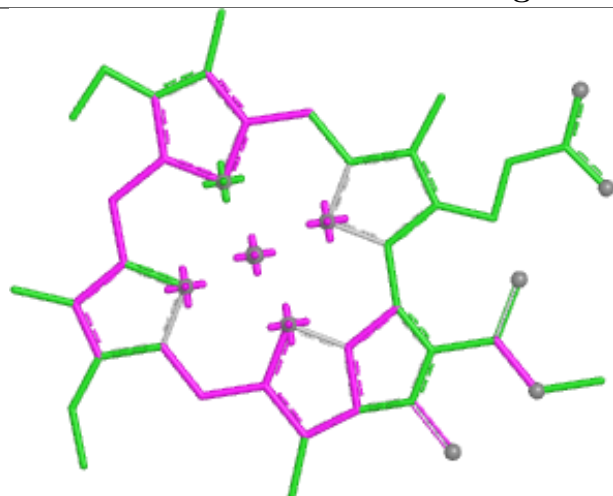
Ligand CLA B 835



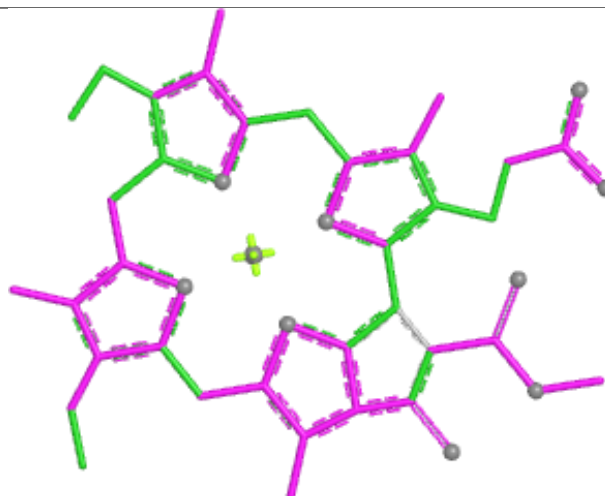
Ligand BCR U 1008



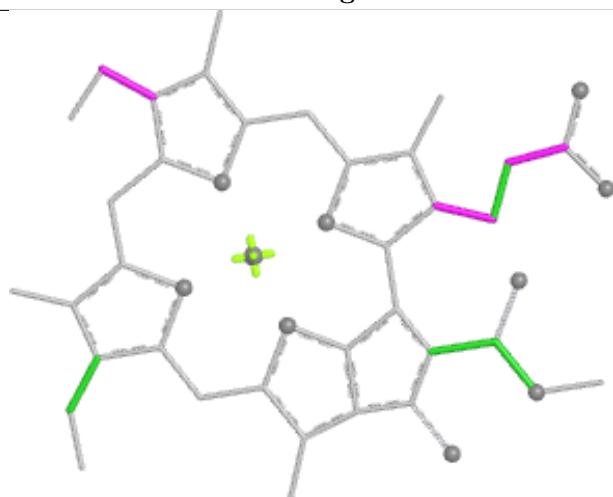
Ligand CLA G 835



Bond lengths



Bond angles

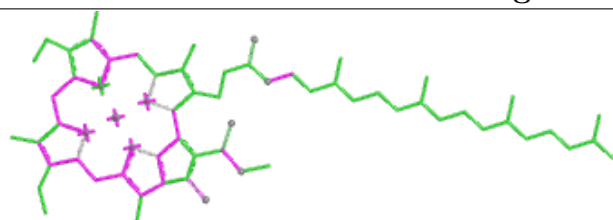


Torsions

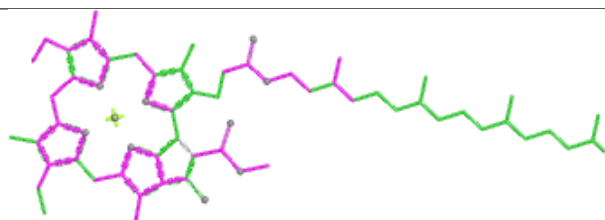


Rings

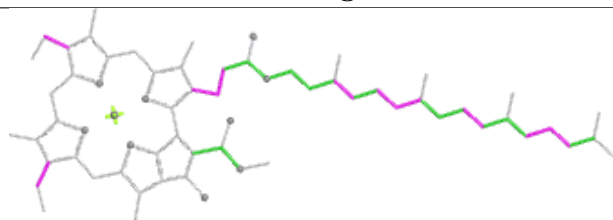
Ligand CLA H 827



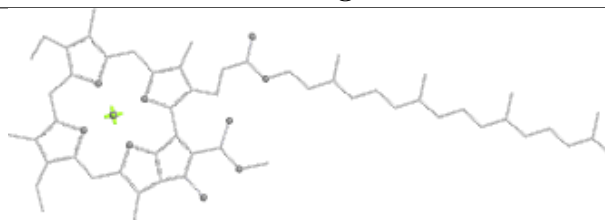
Bond lengths



Bond angles

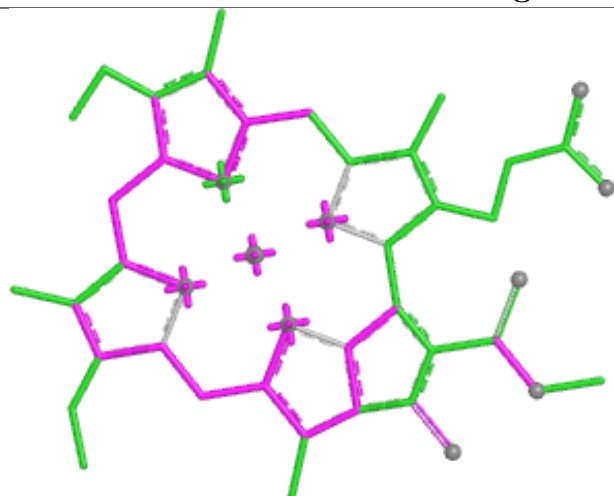


Torsions

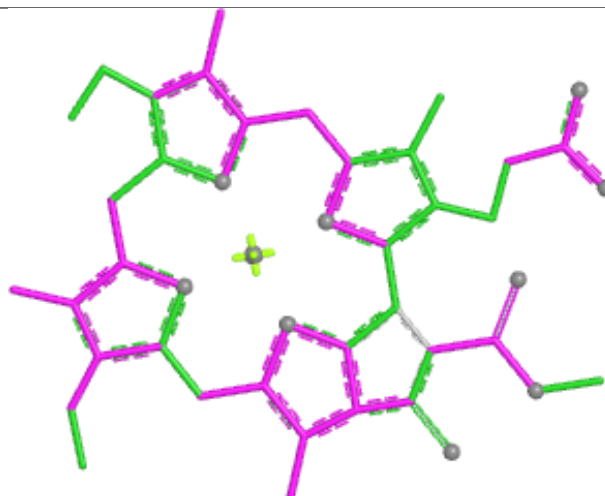


Rings

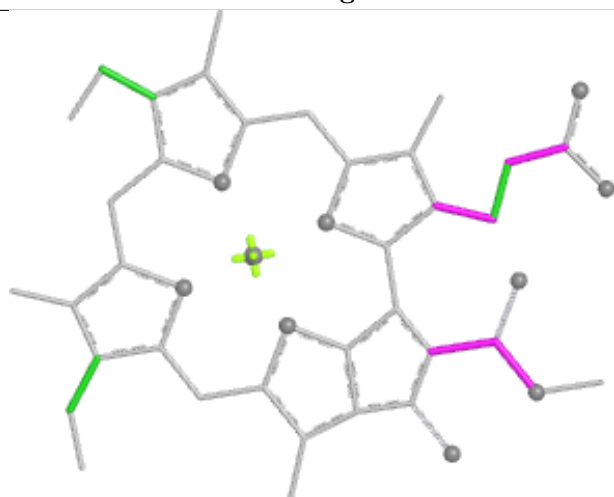
Ligand CLA H 831



Bond lengths



Bond angles

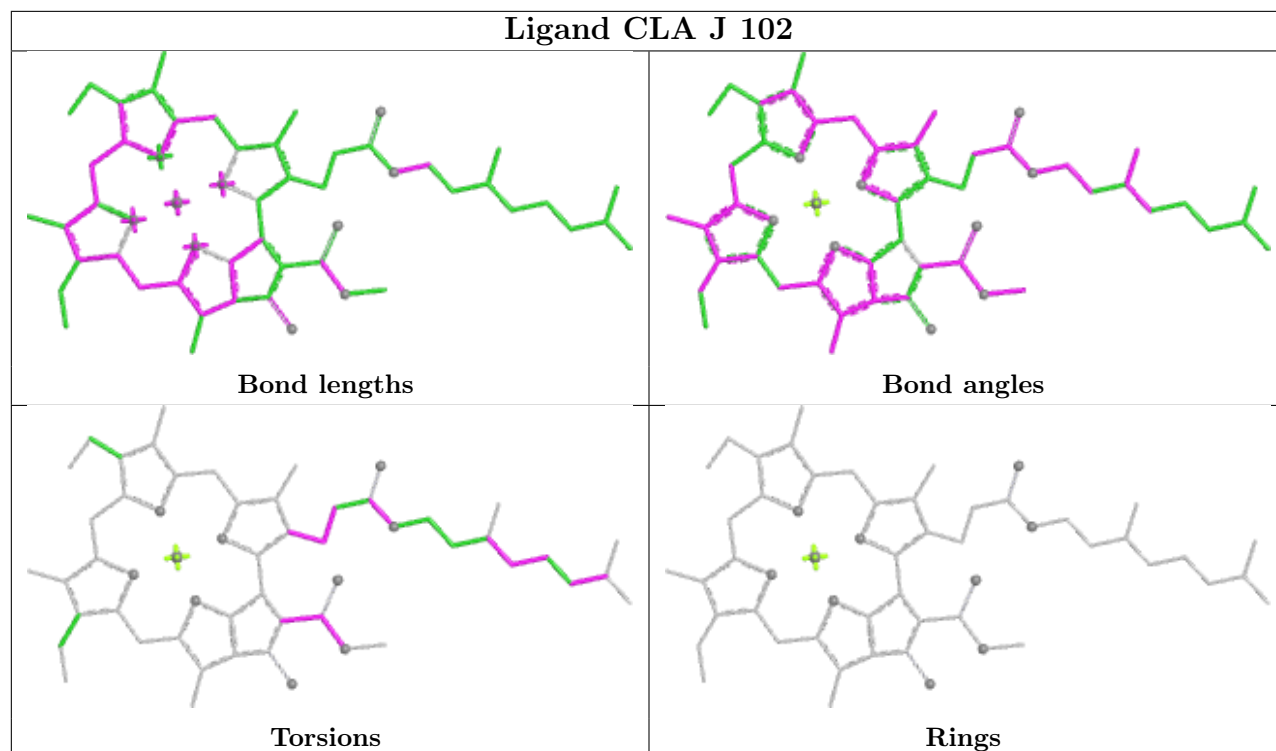


Torsions

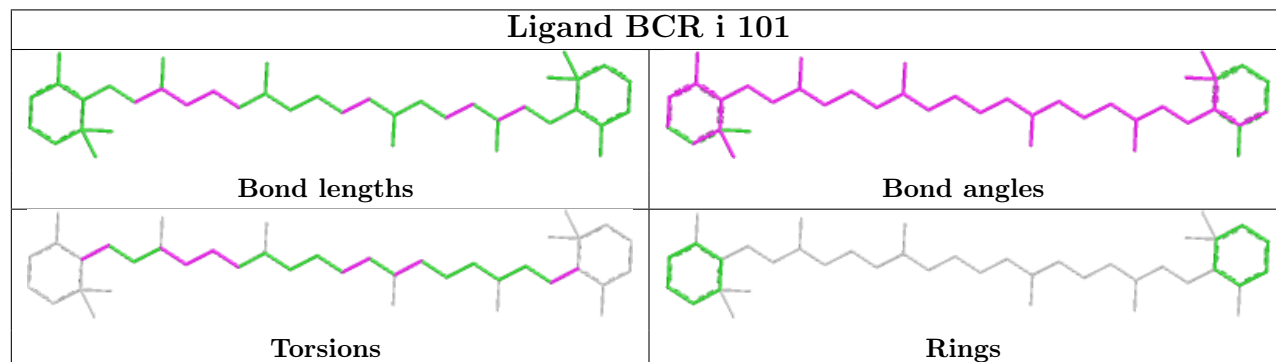


Rings

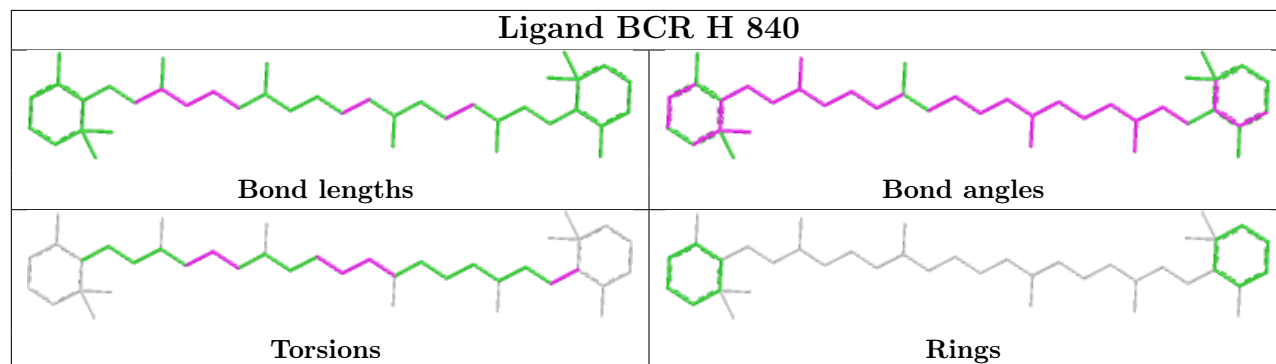
Ligand CLA J 102



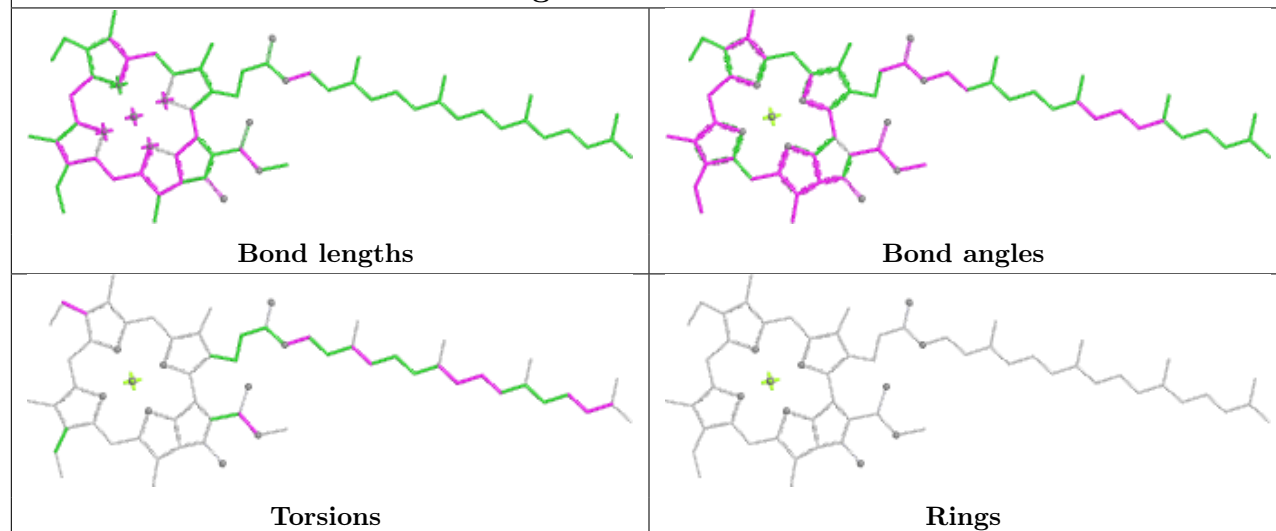
Ligand BCR i 101



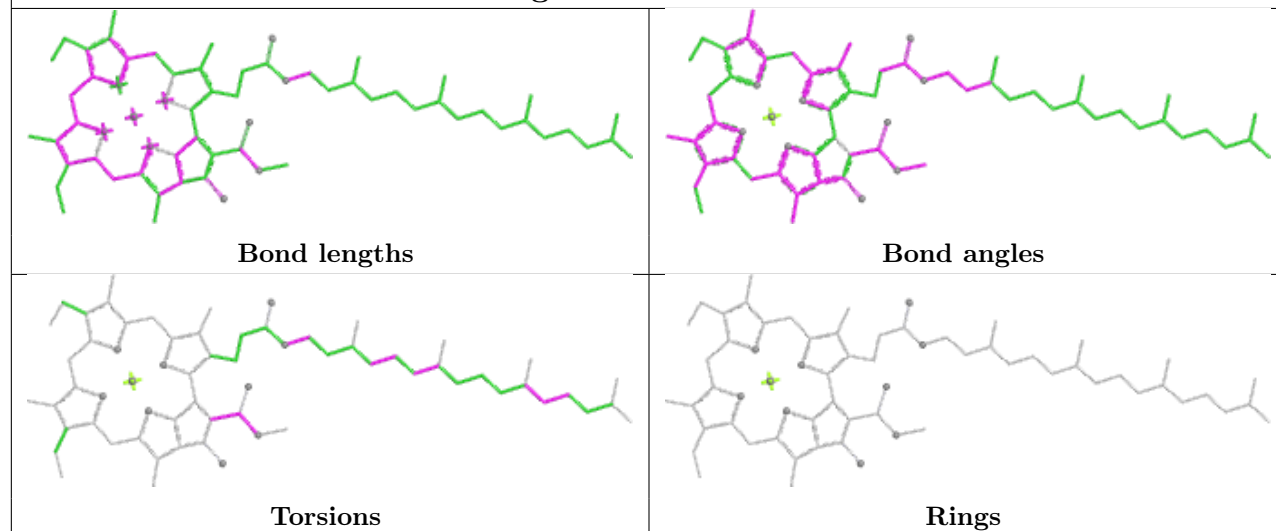
Ligand BCR H 840

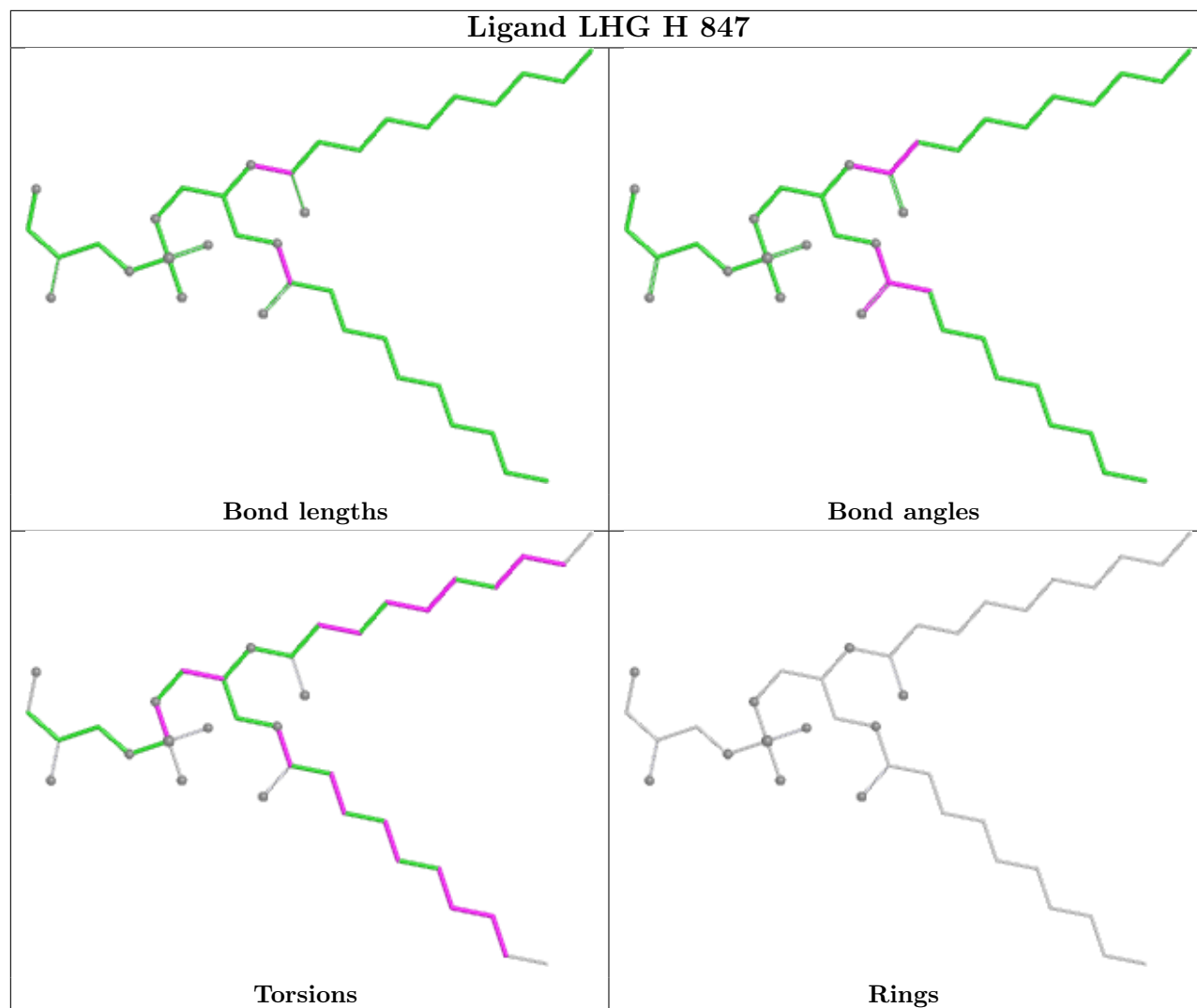


Ligand CLA B 810

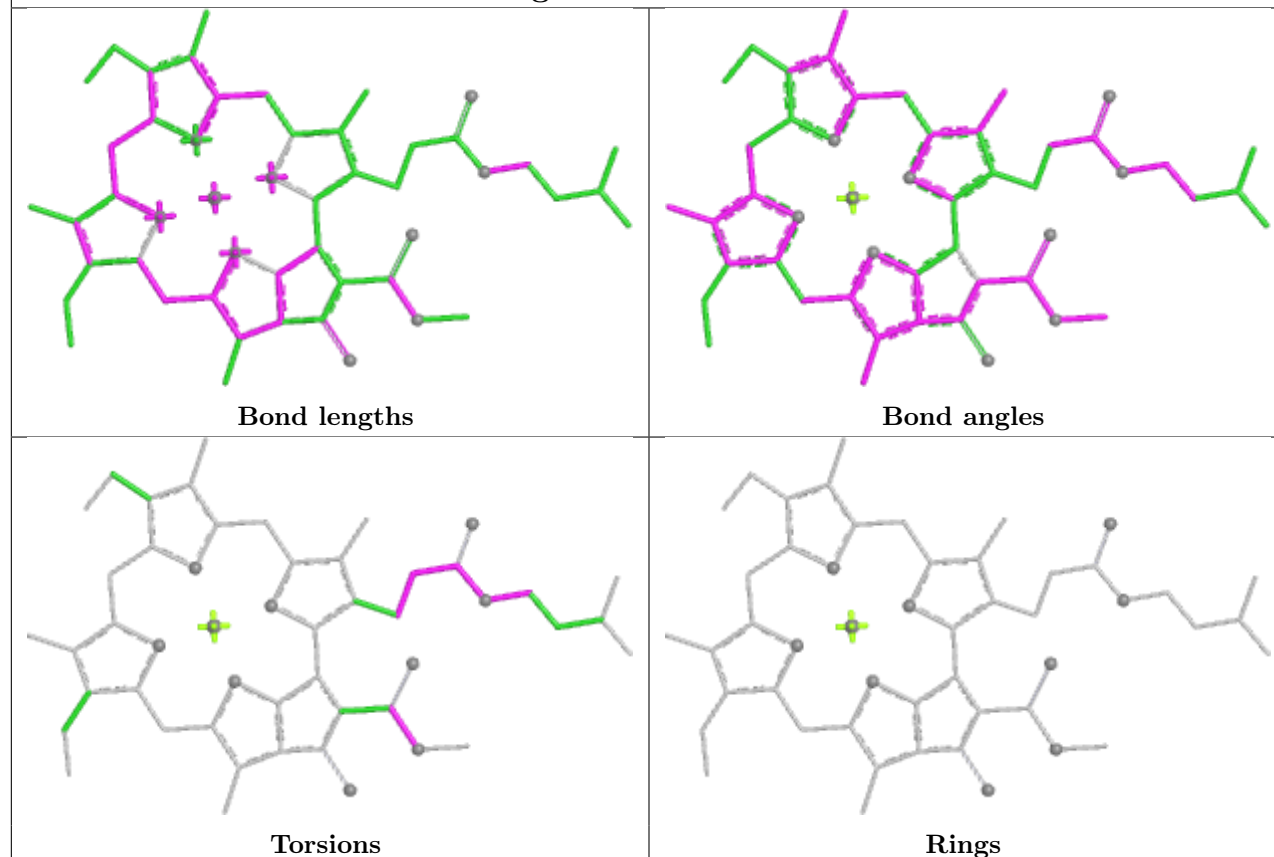


Ligand CLA H 825

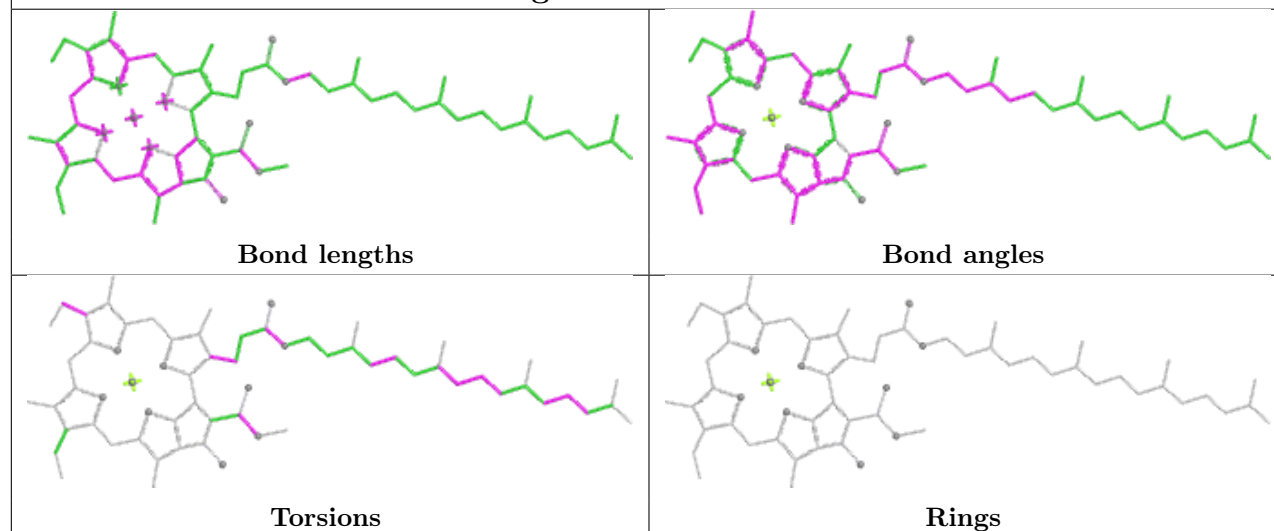




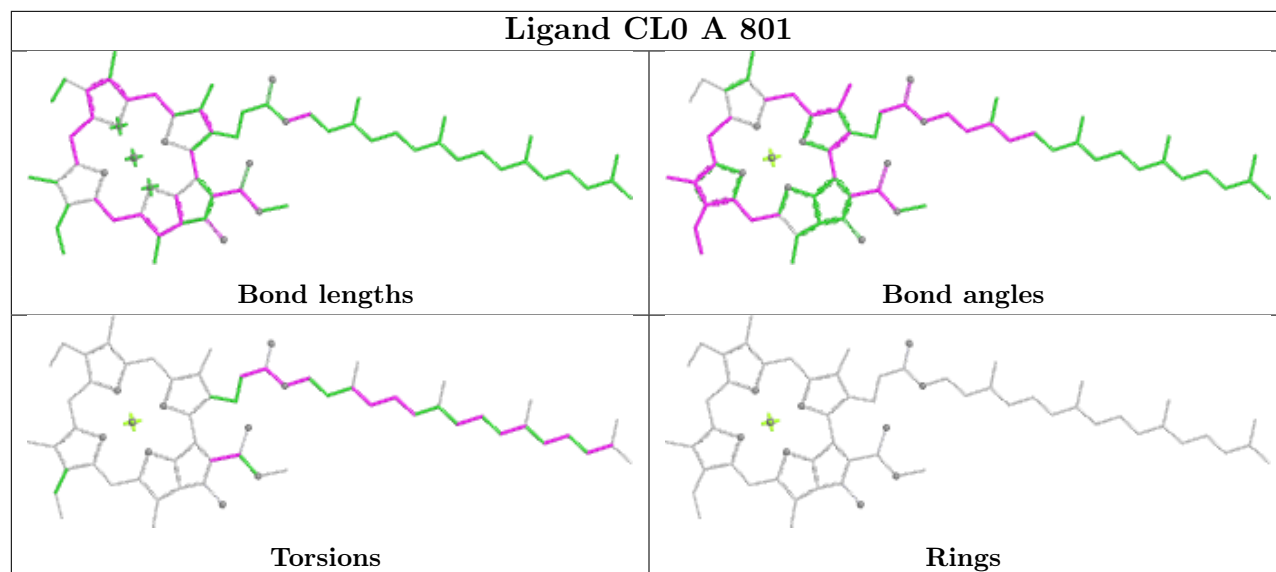
Ligand CLA Y 815



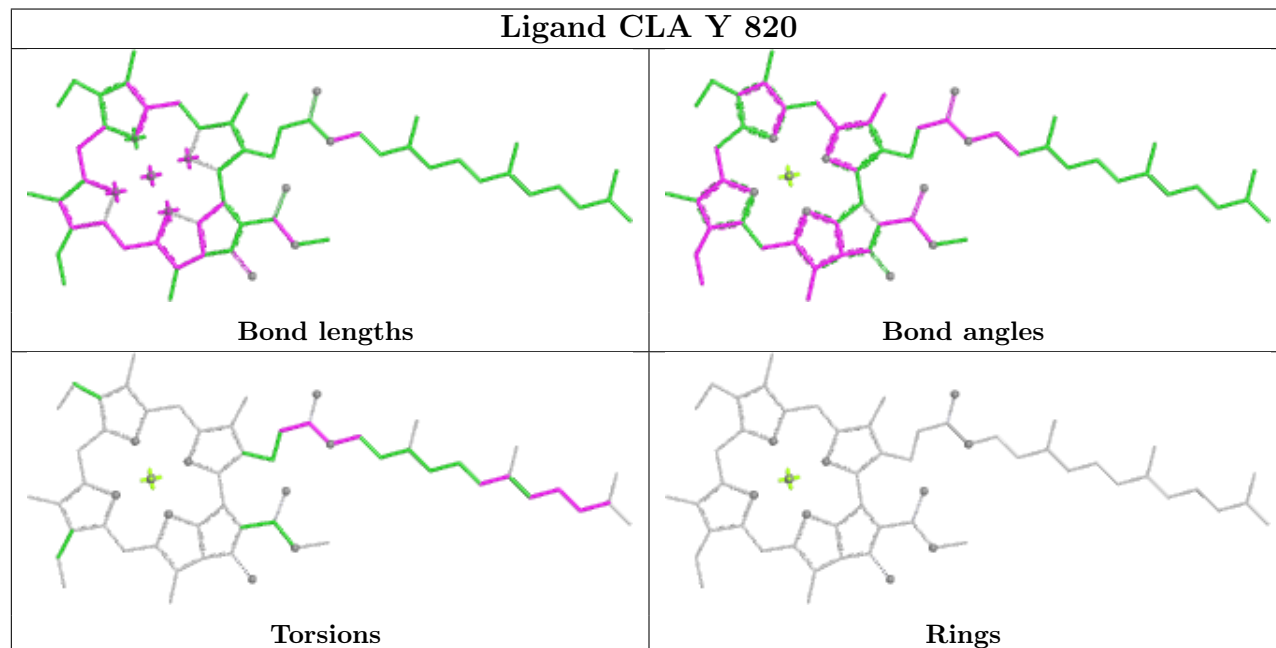
Ligand CLA Y 805



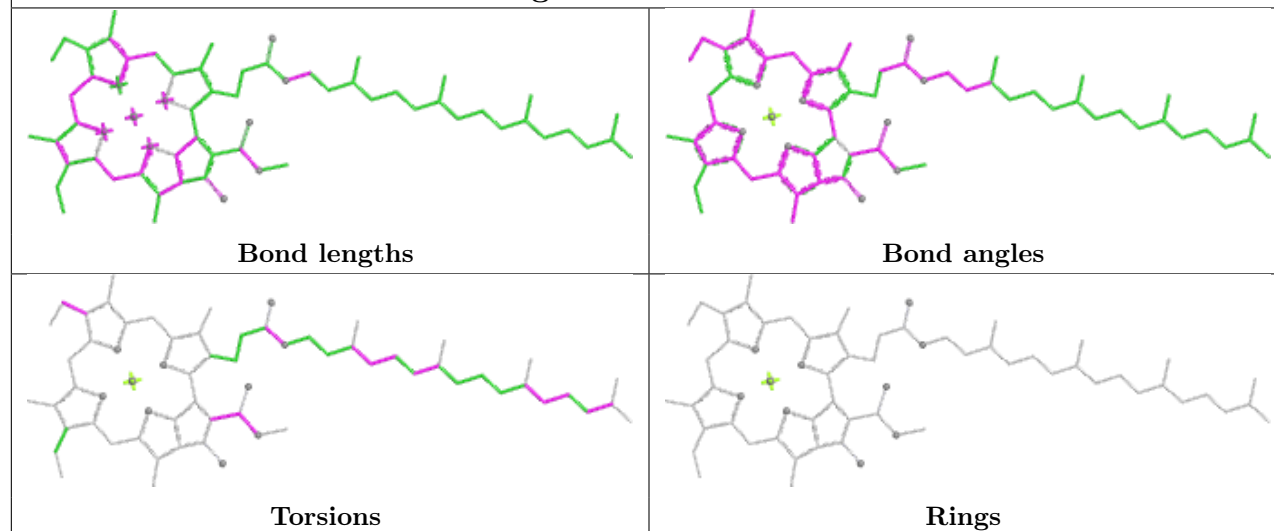
Ligand CL0 A 801



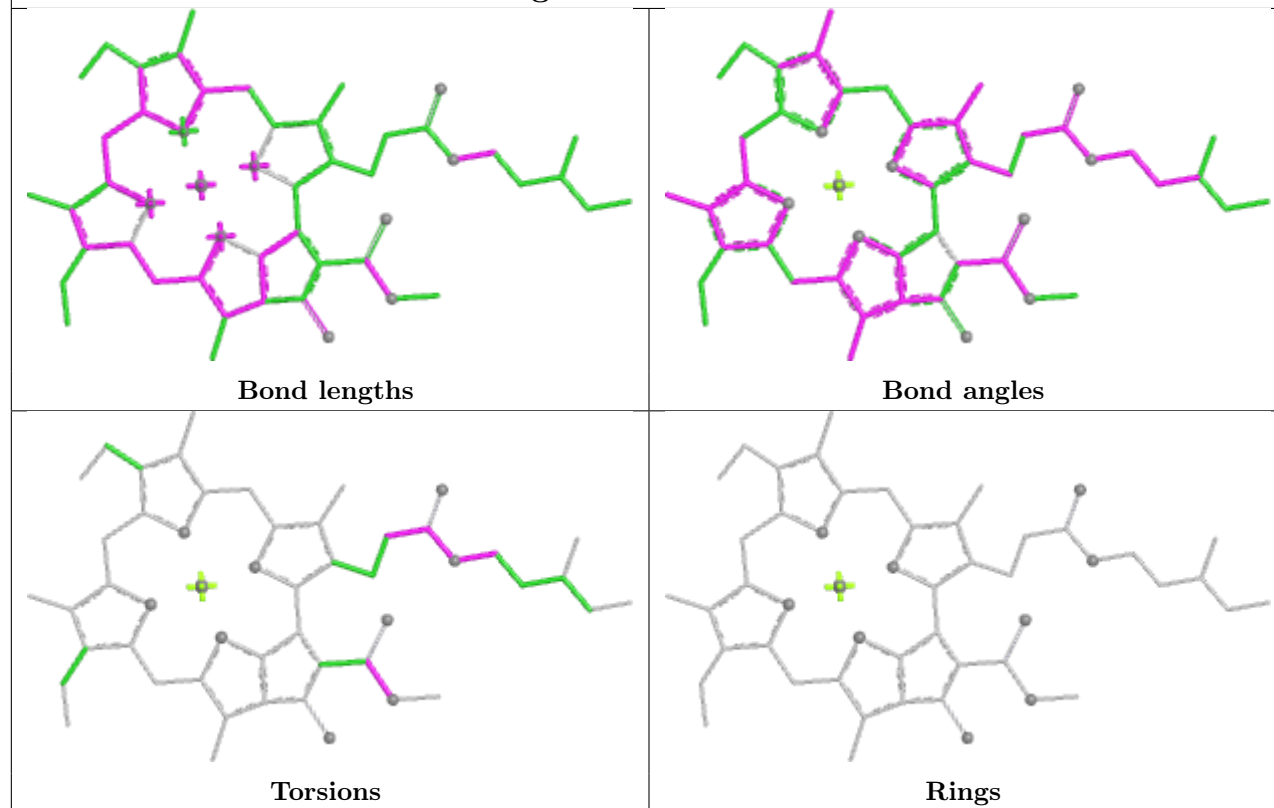
Ligand CLA Y 820

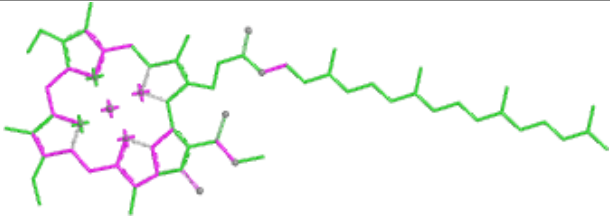
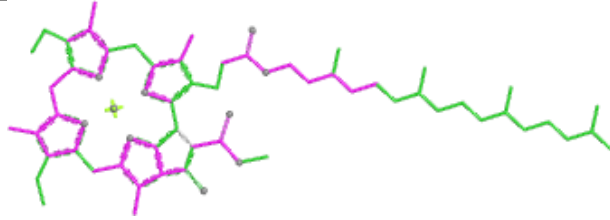
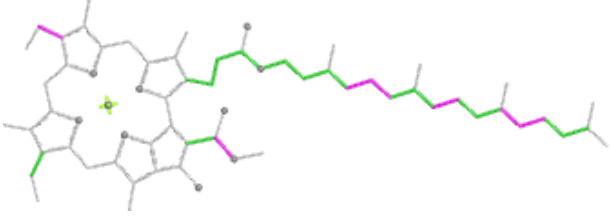
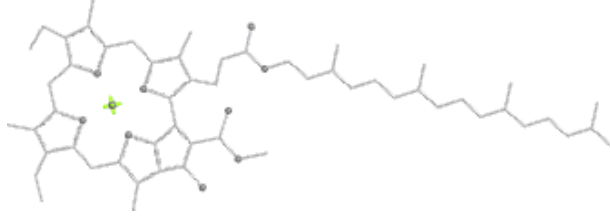
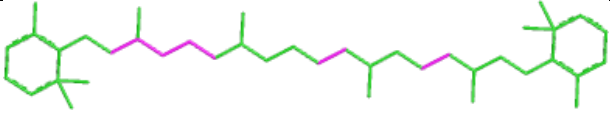
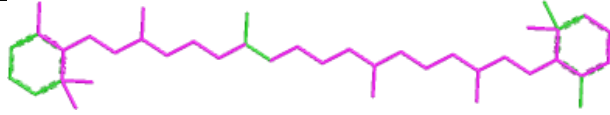
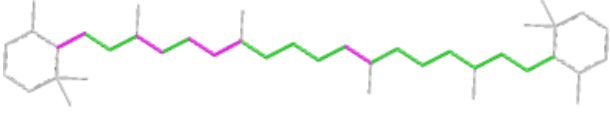
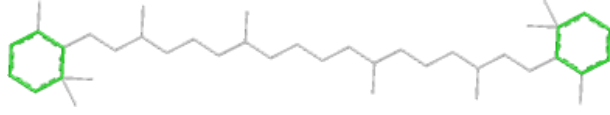
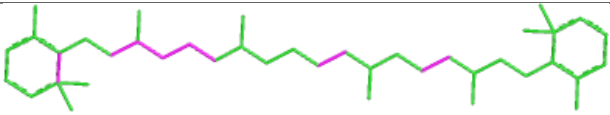
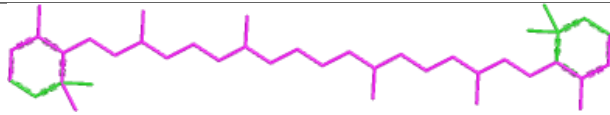
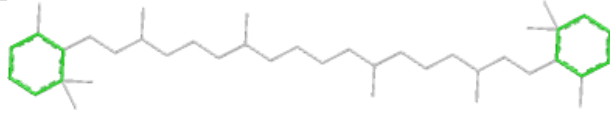


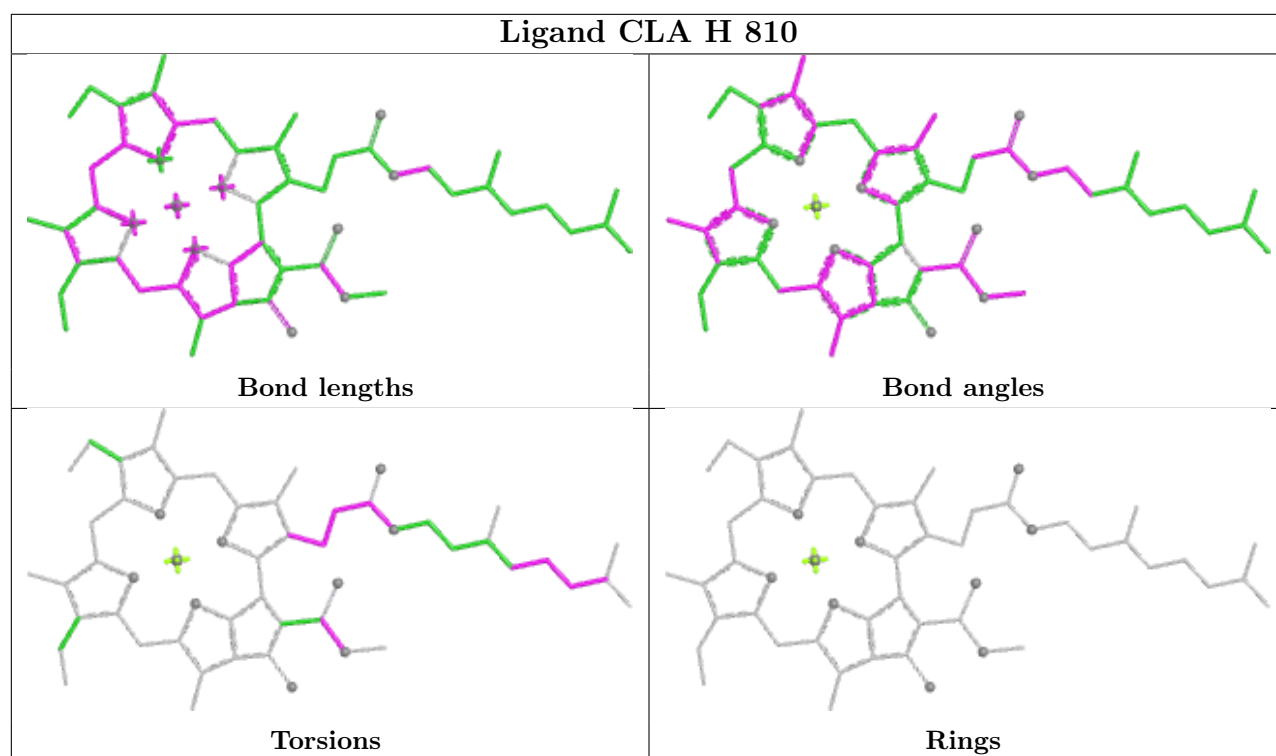
Ligand CLA Y 854



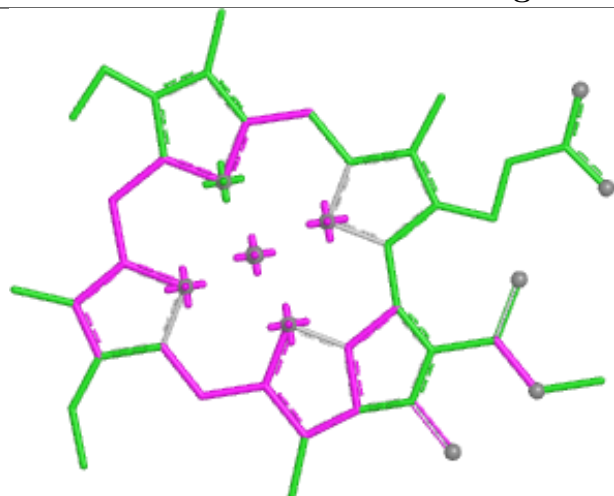
Ligand CLA A 807



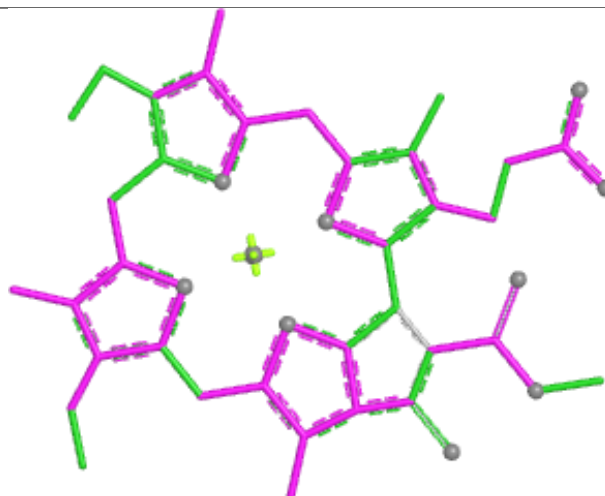
Ligand CLA Z 836	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR G 850	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR F 203	
 Bond lengths	 Bond angles
 Torsions	 Rings



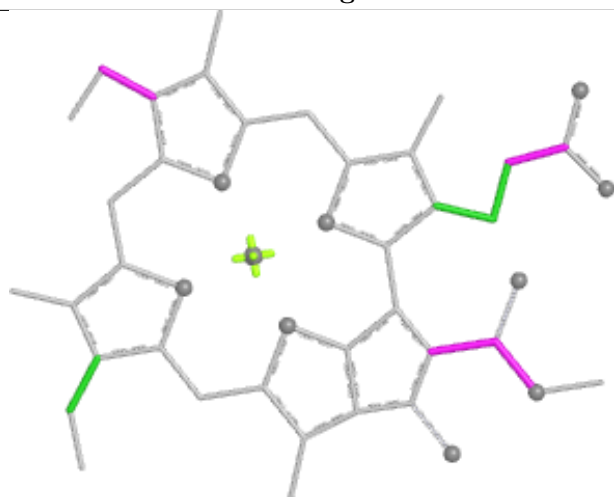
Ligand CLA H 829



Bond lengths



Bond angles

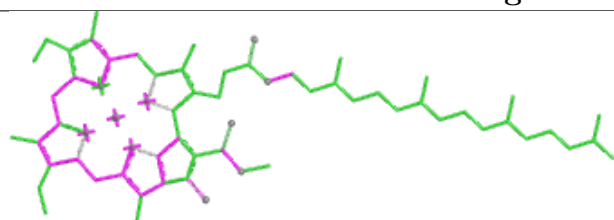


Torsions

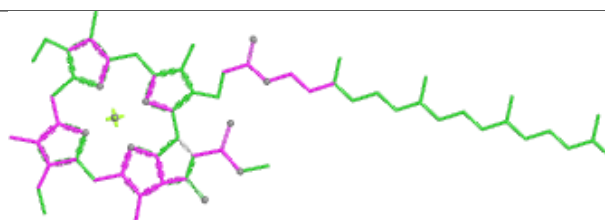


Rings

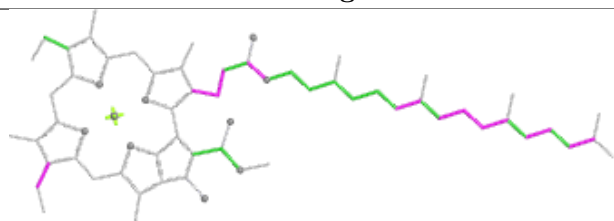
Ligand CLA U 1003



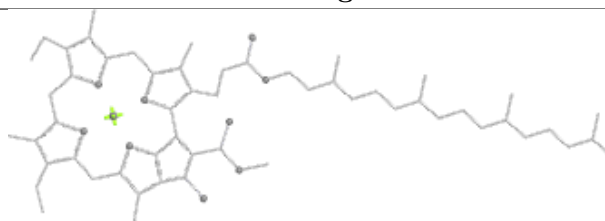
Bond lengths



Bond angles

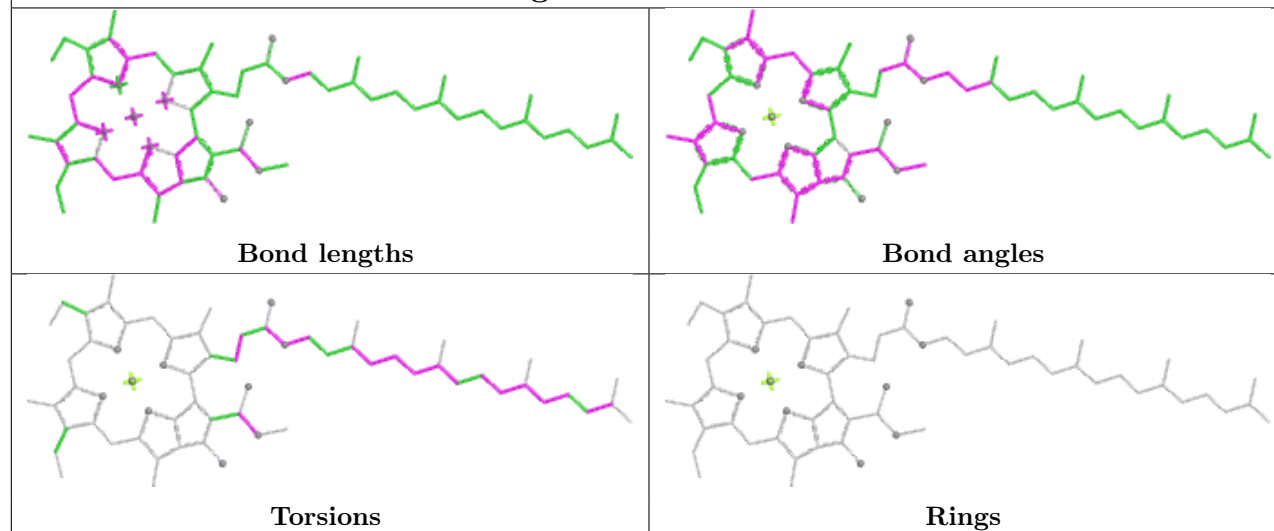


Torsions

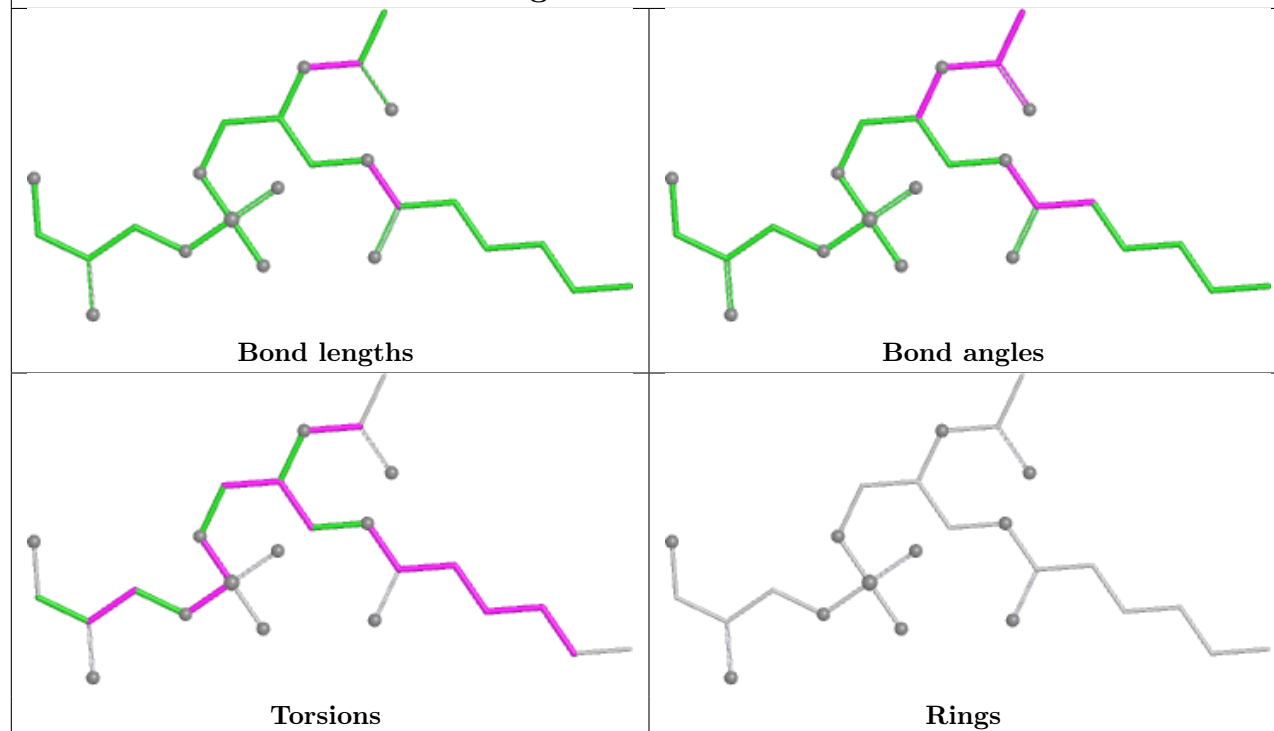


Rings

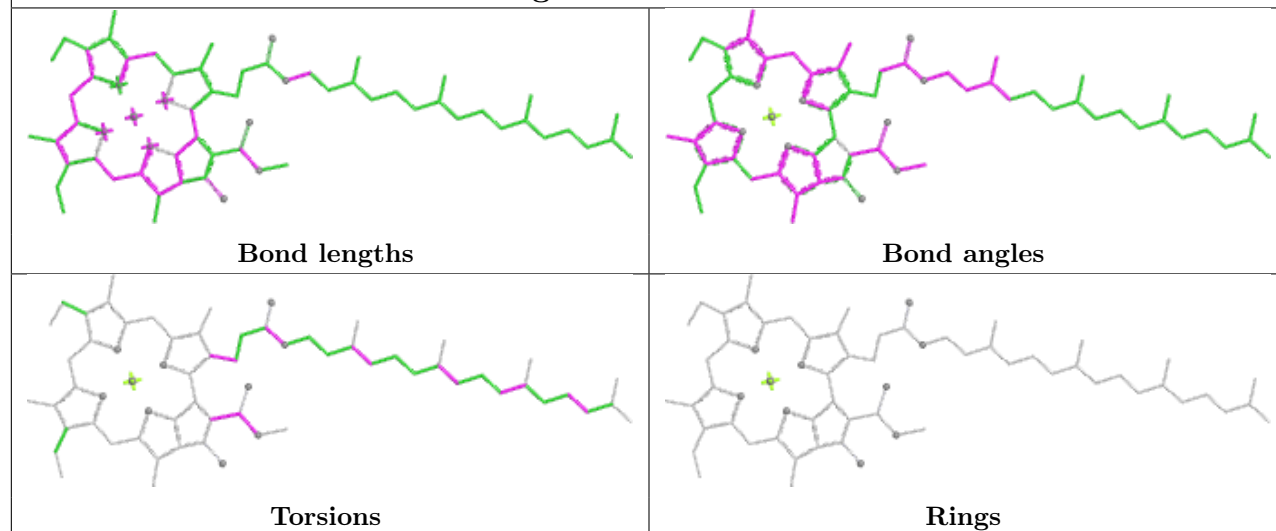
Ligand CLA G 802



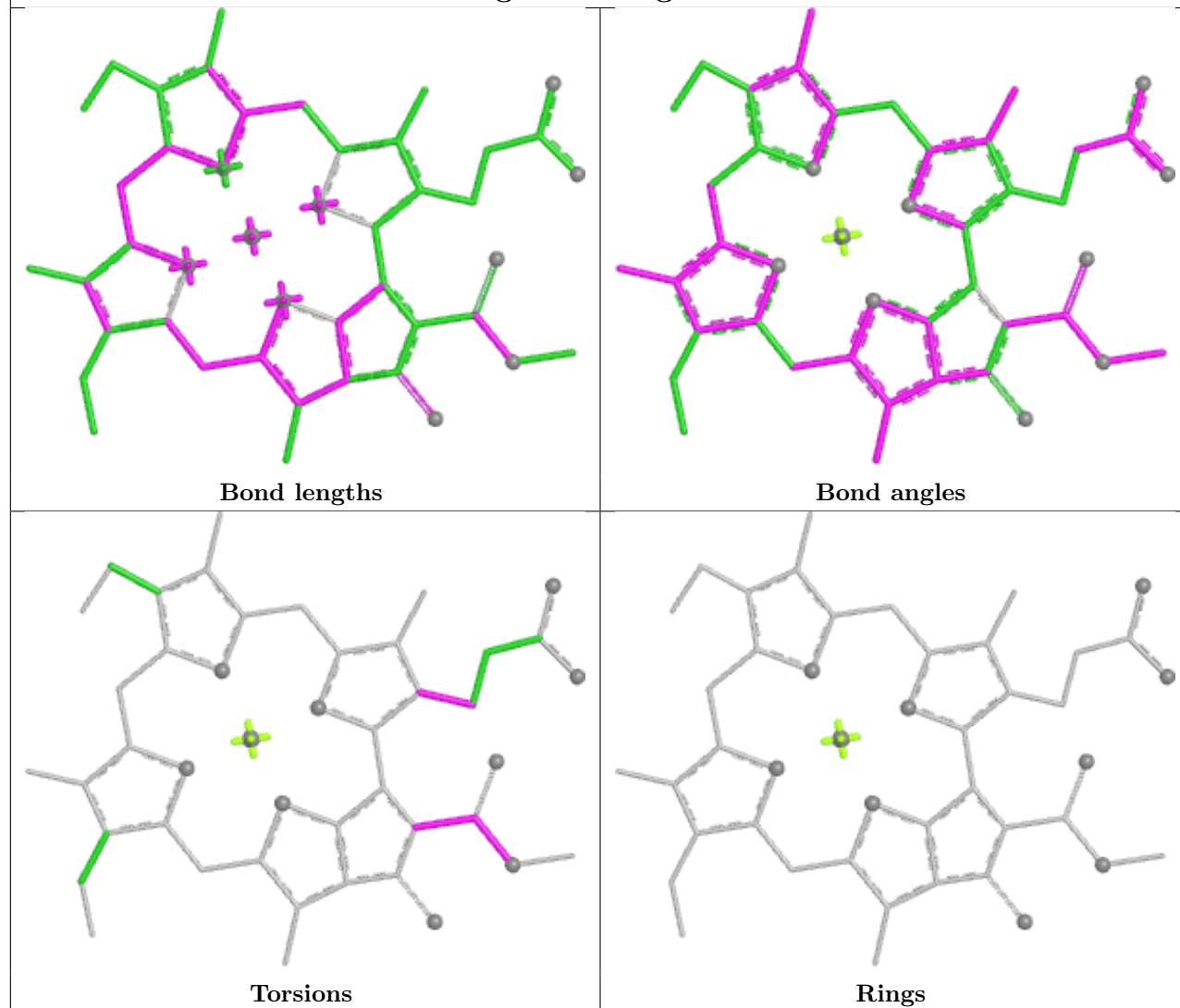
Ligand LHG Y 853

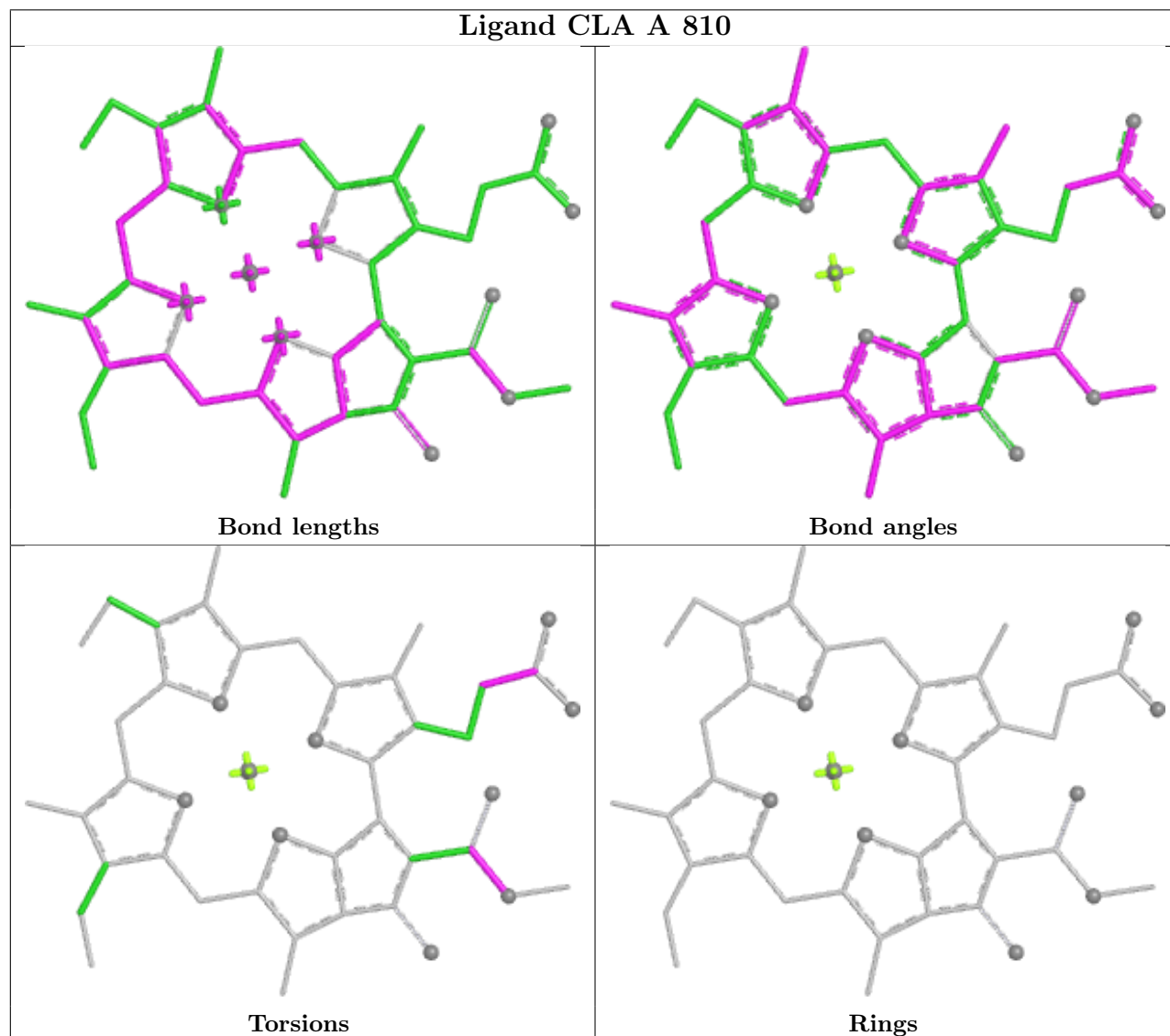
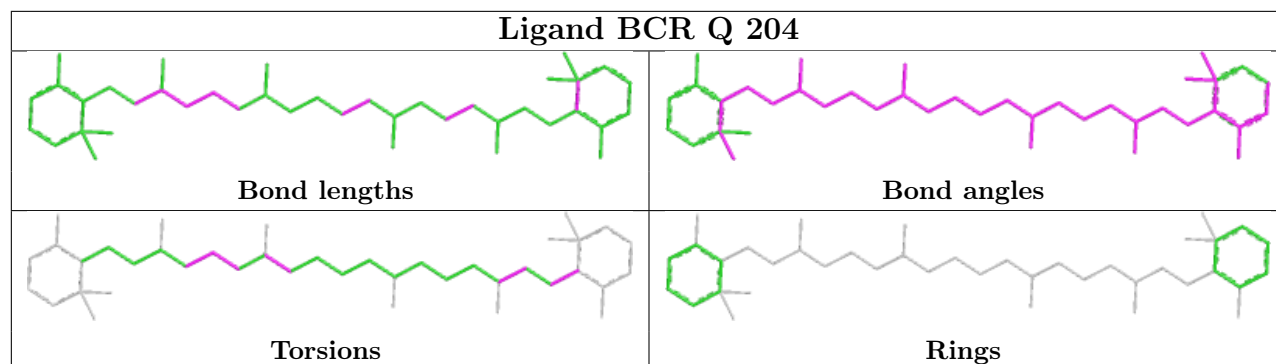


Ligand CLA B 825

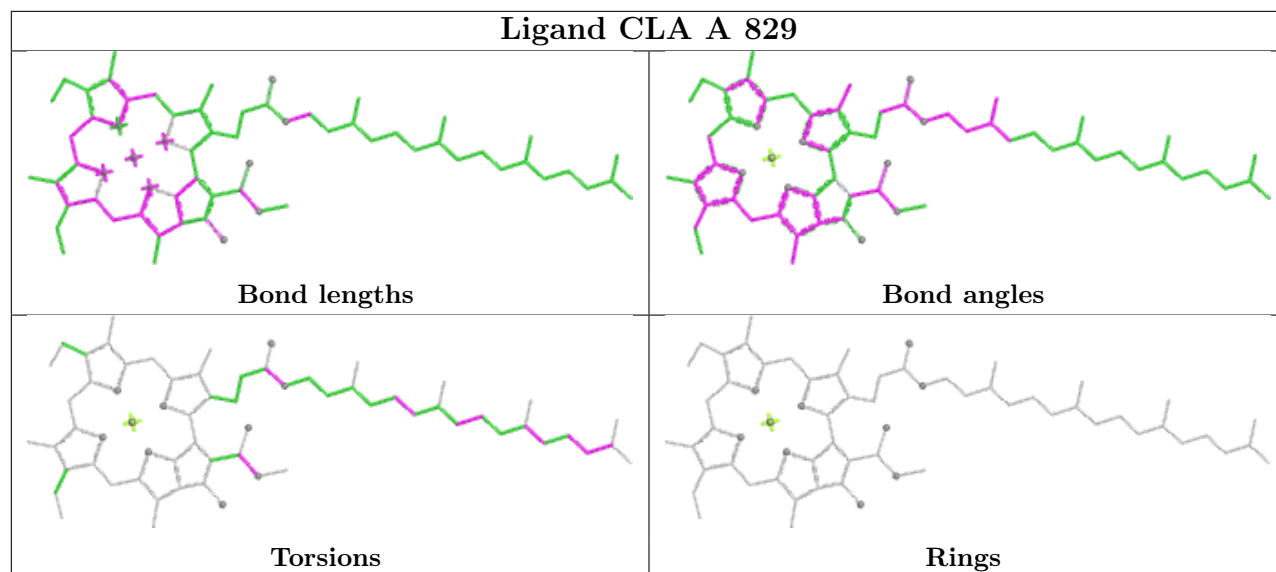


Ligand CLA g 102

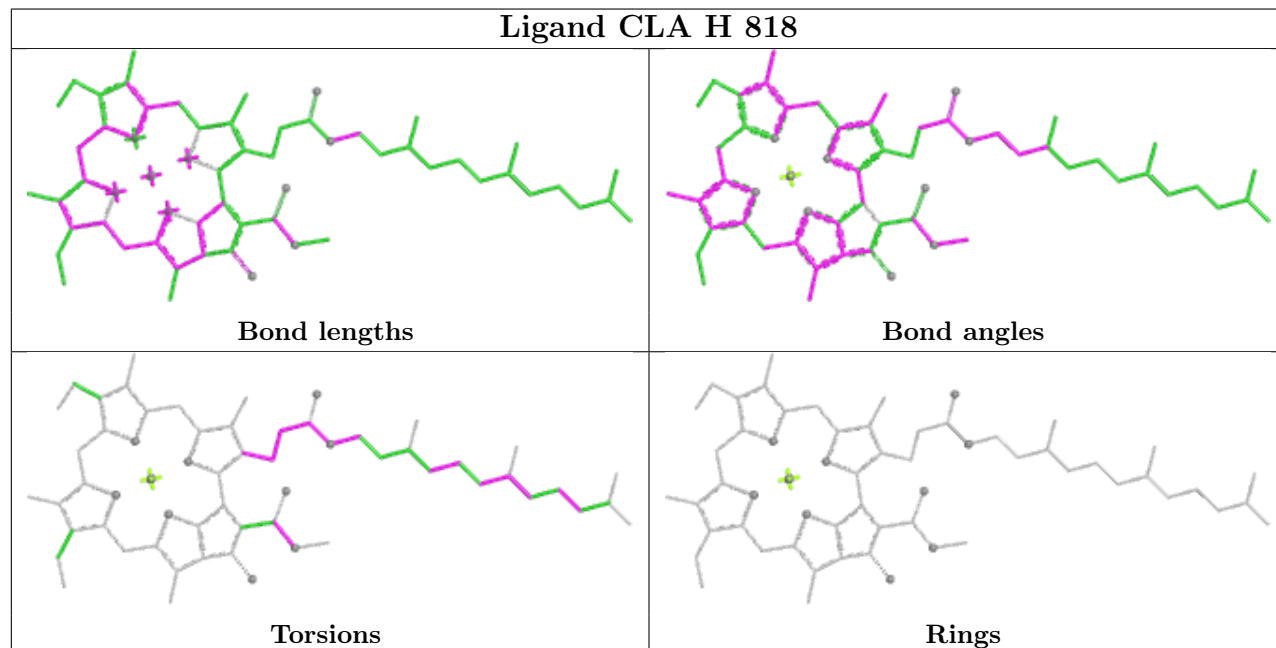


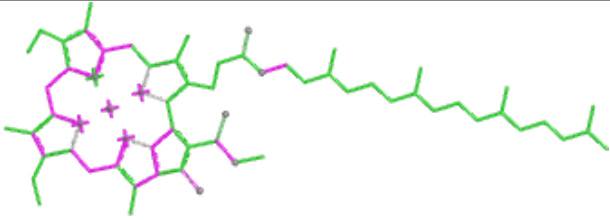
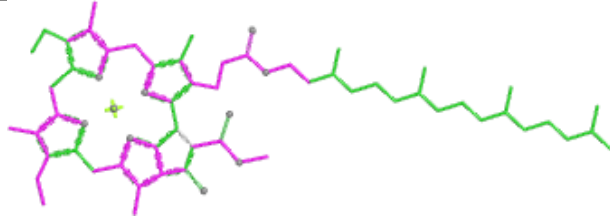
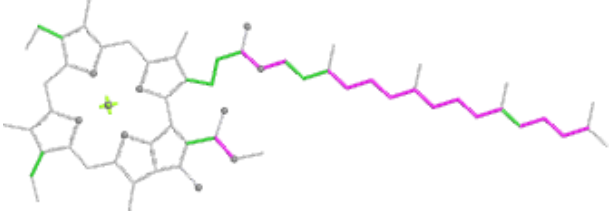
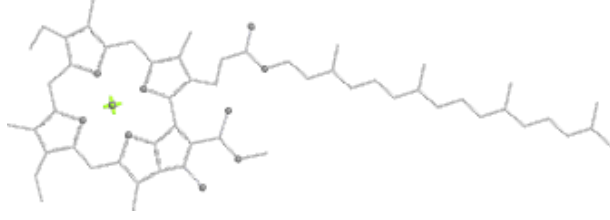
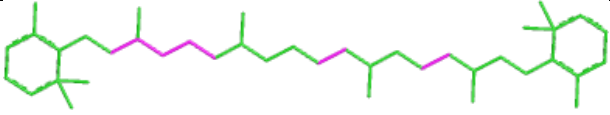
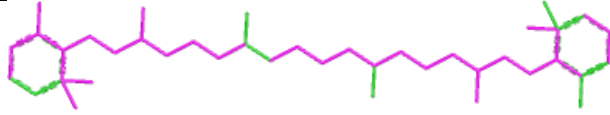
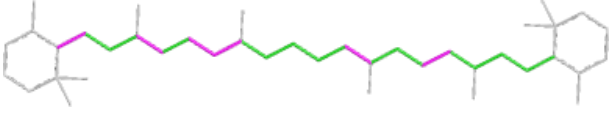
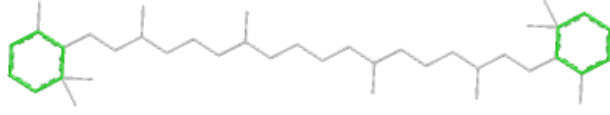
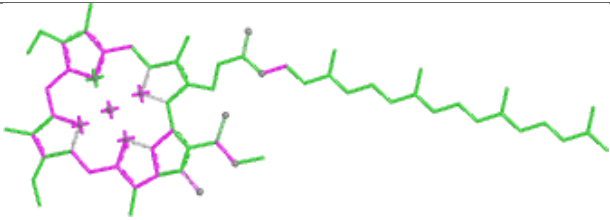
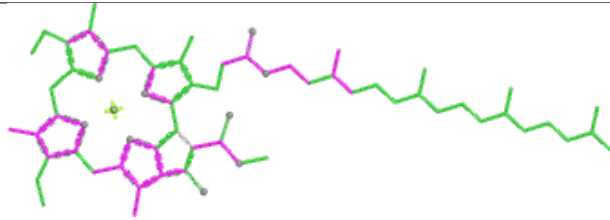
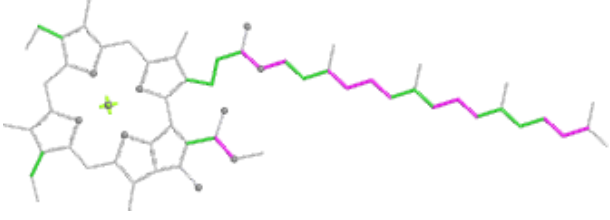
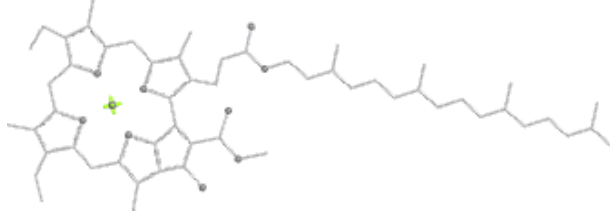


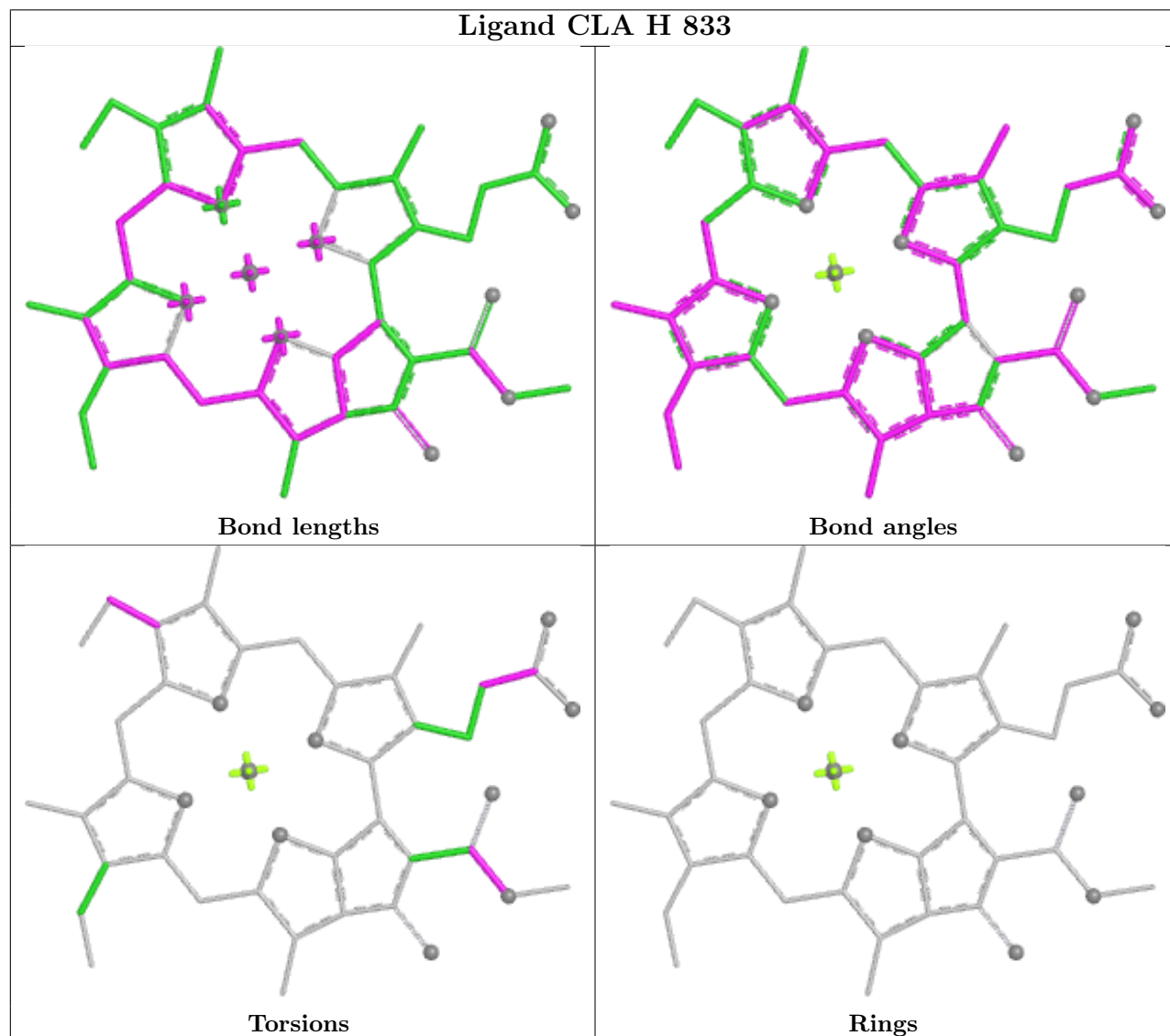
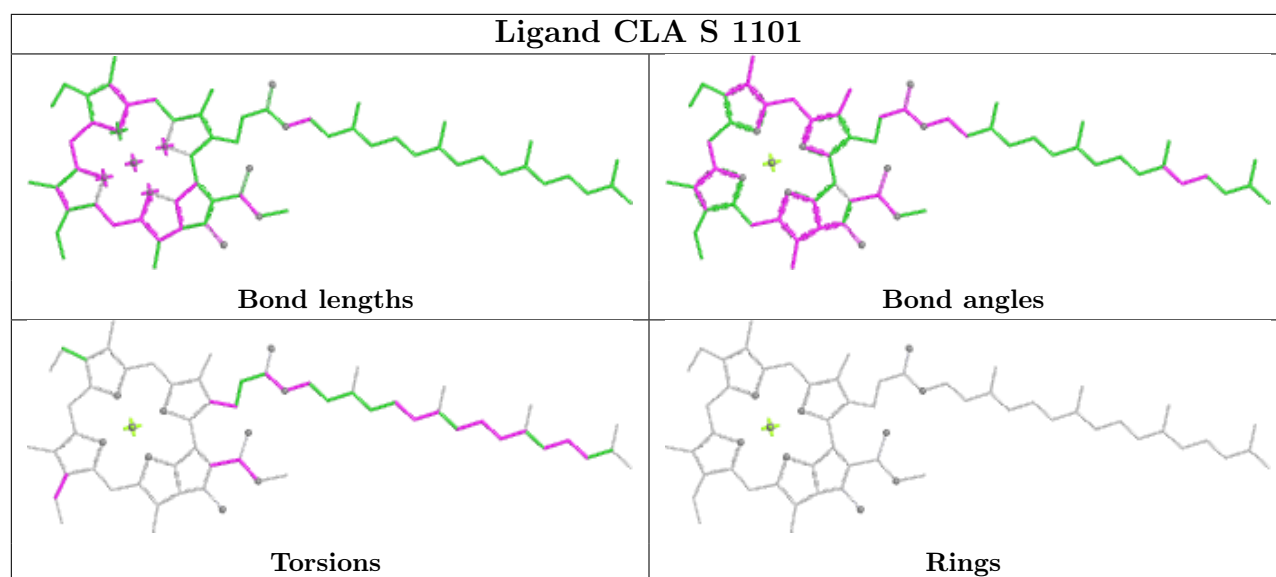
Ligand CLA A 829



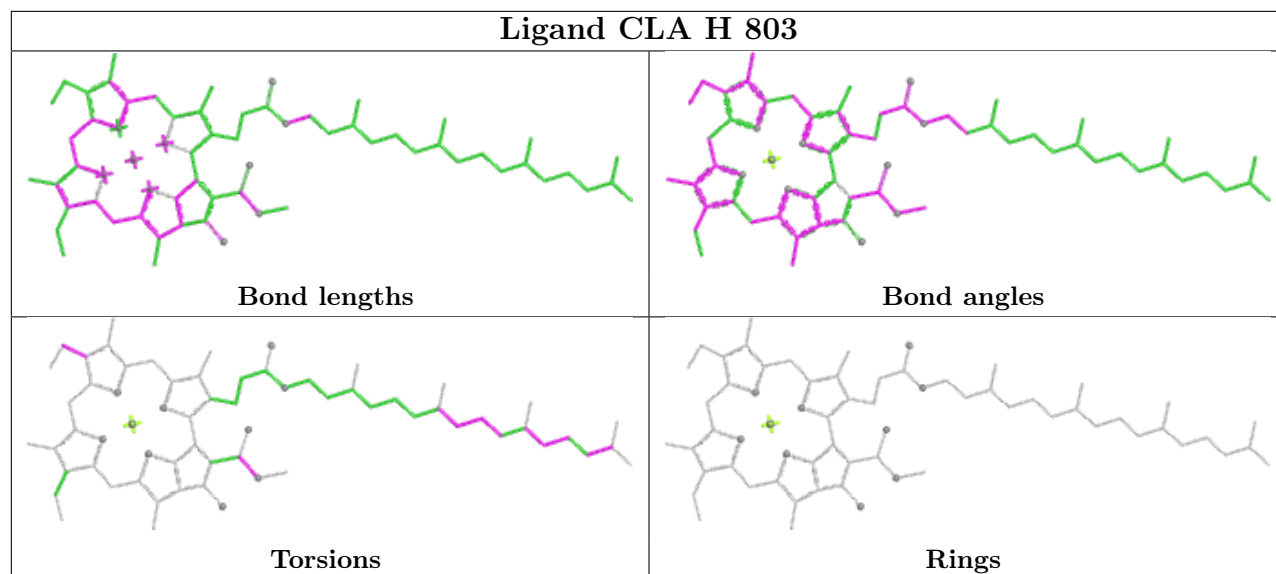
Ligand CLA H 818



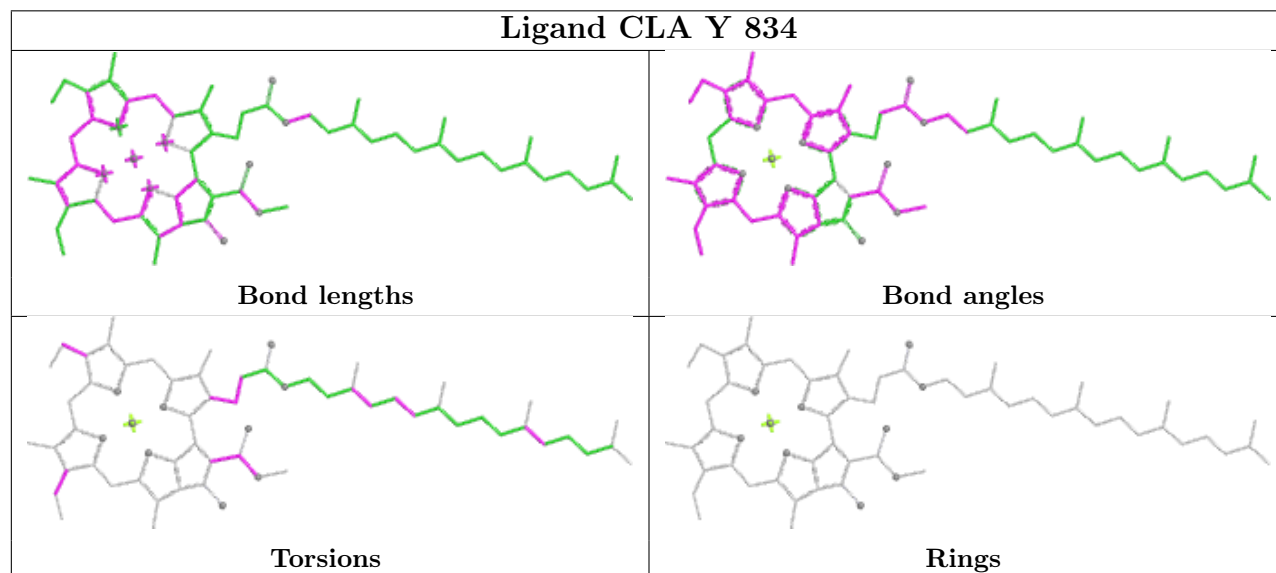
Ligand CLA H 805	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 849	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA Y 841	
 Bond lengths	 Bond angles
 Torsions	 Rings



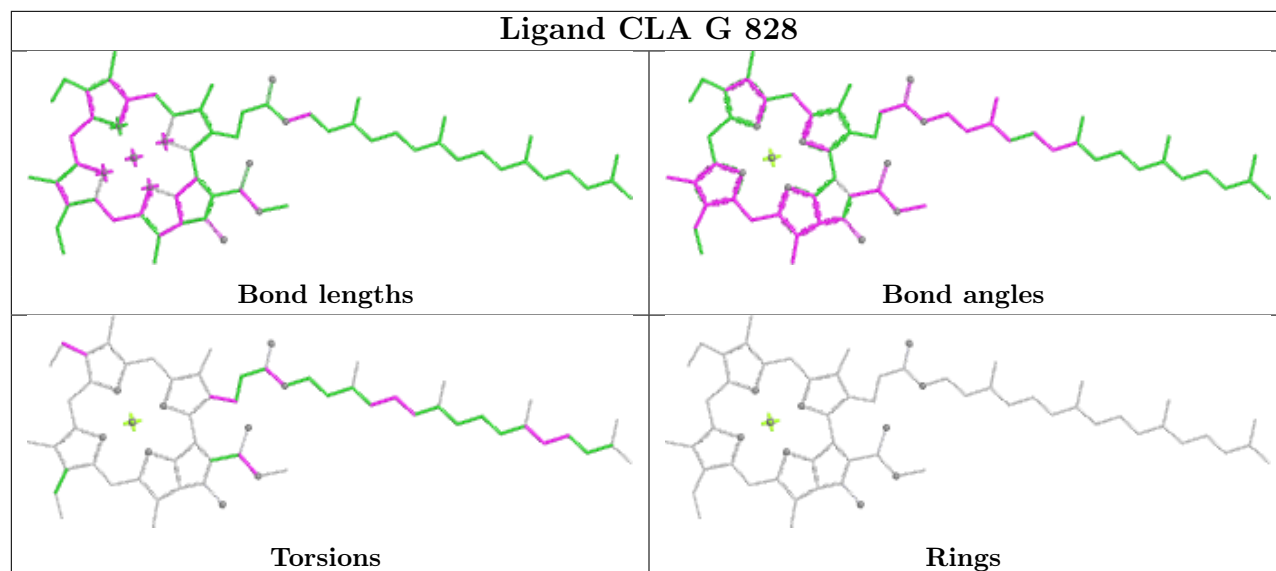
Ligand CLA H 803



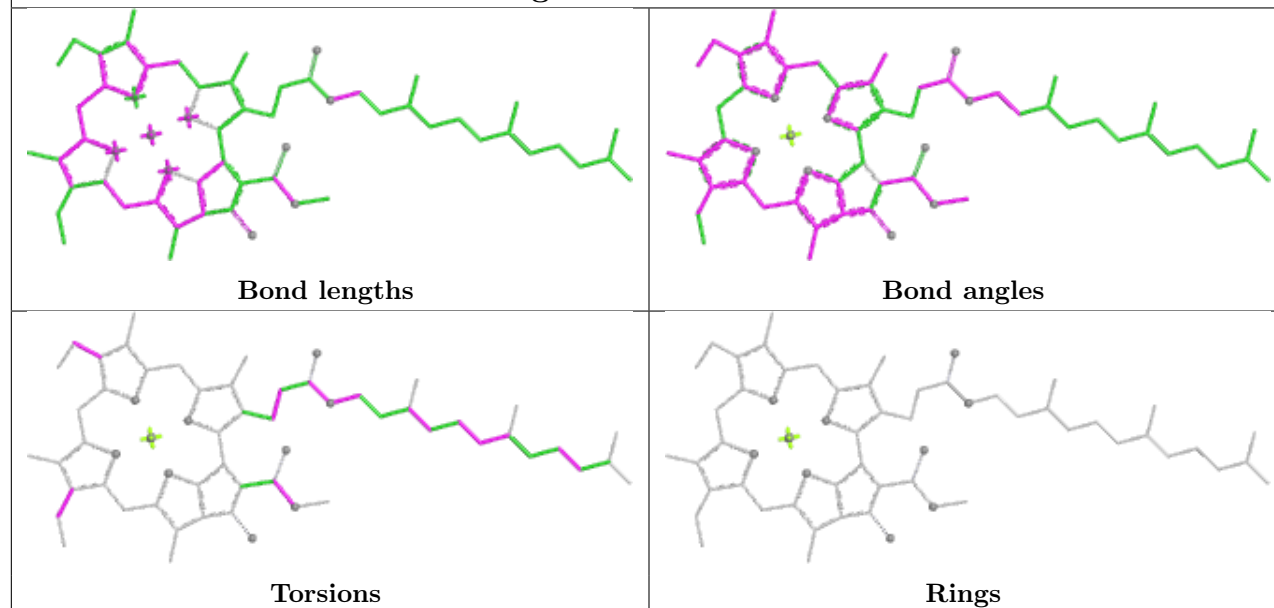
Ligand CLA Y 834



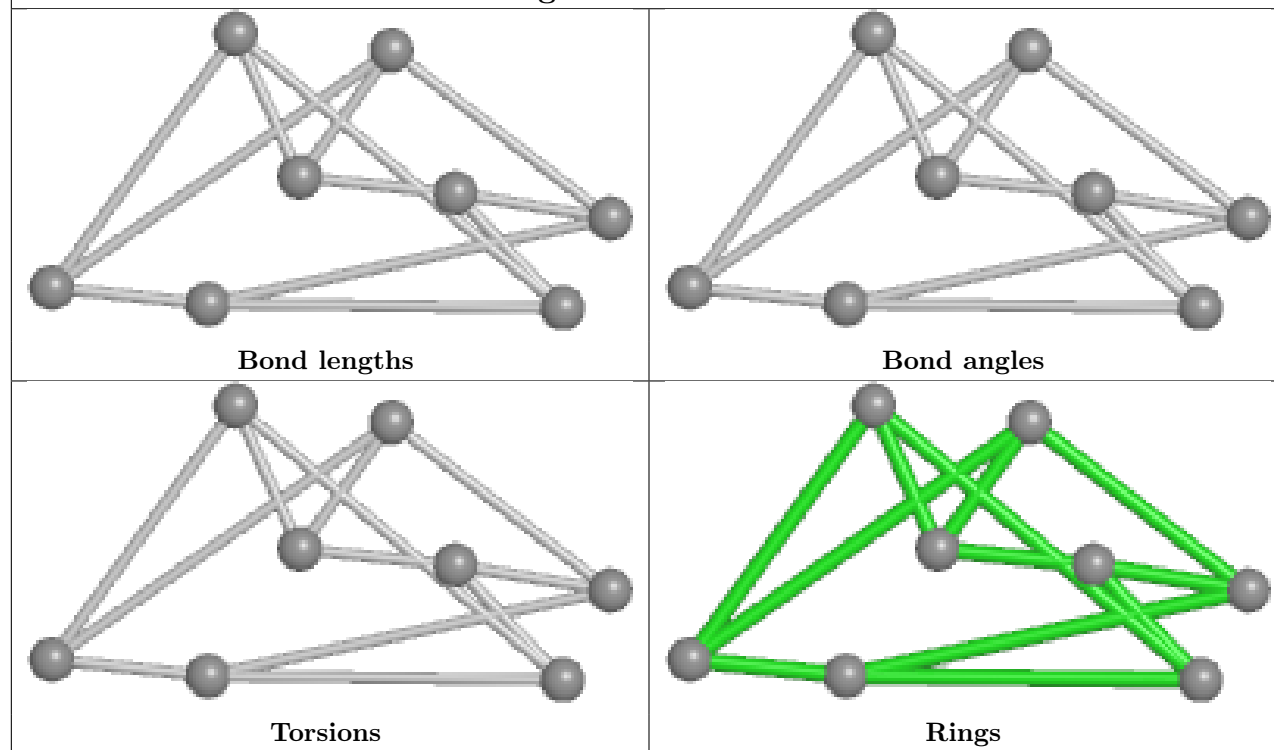
Ligand CLA G 828

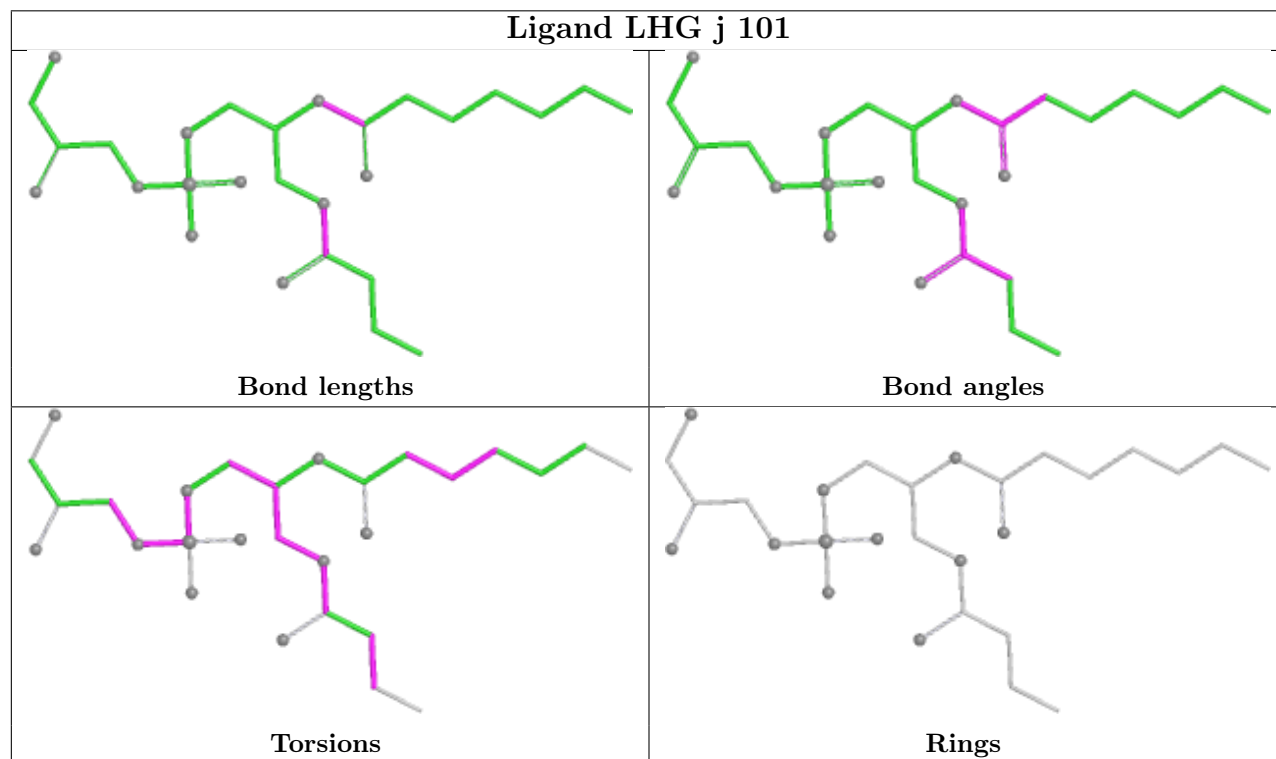
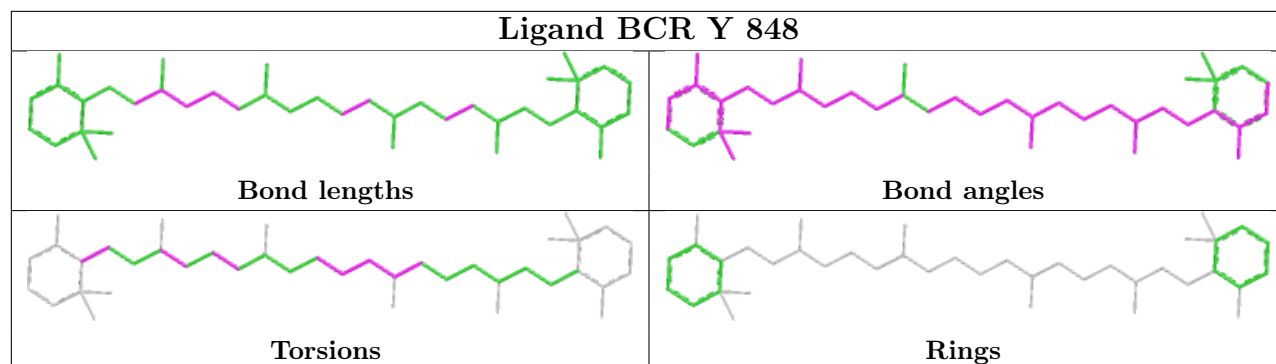


Ligand CLA A 824

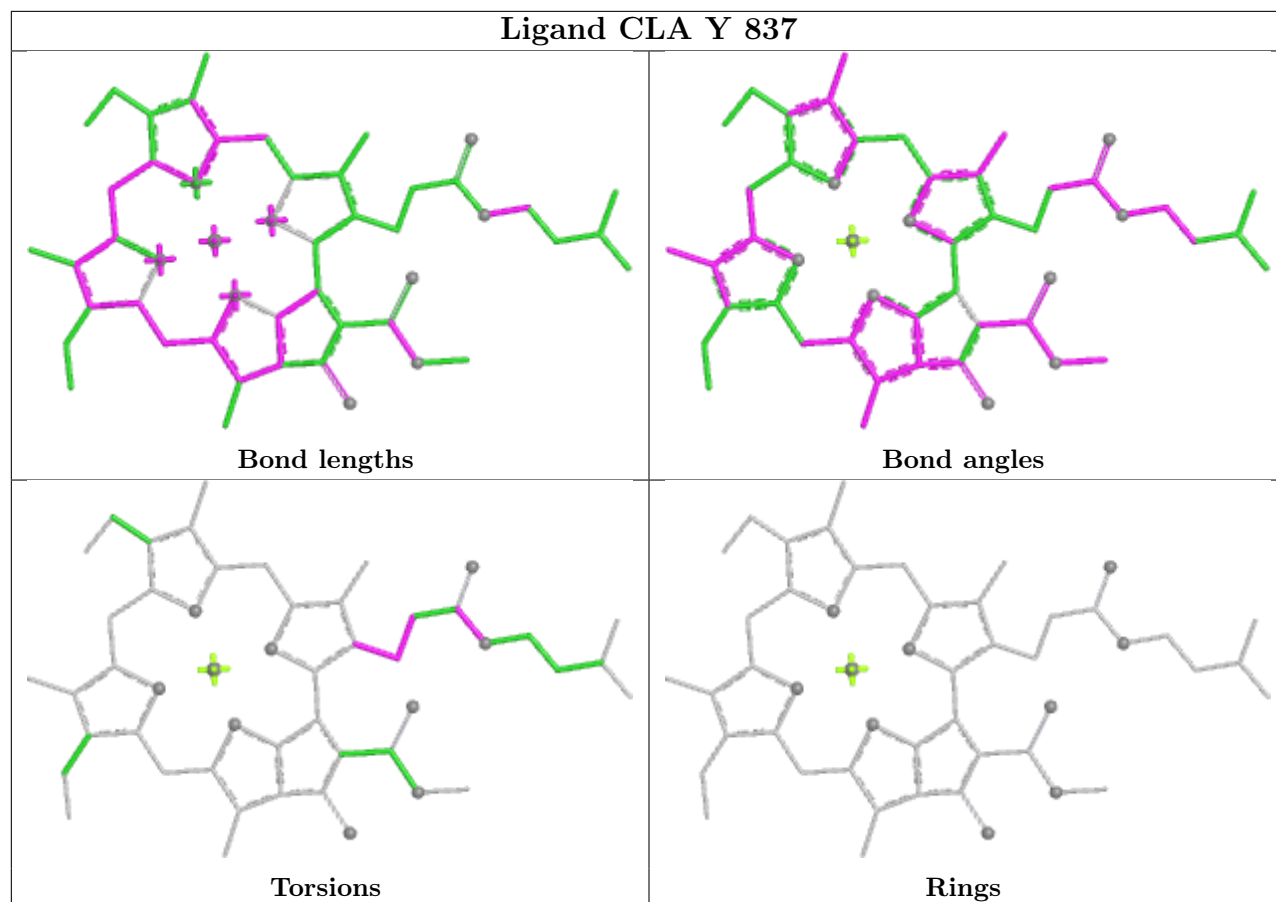


Ligand SF4 N 102

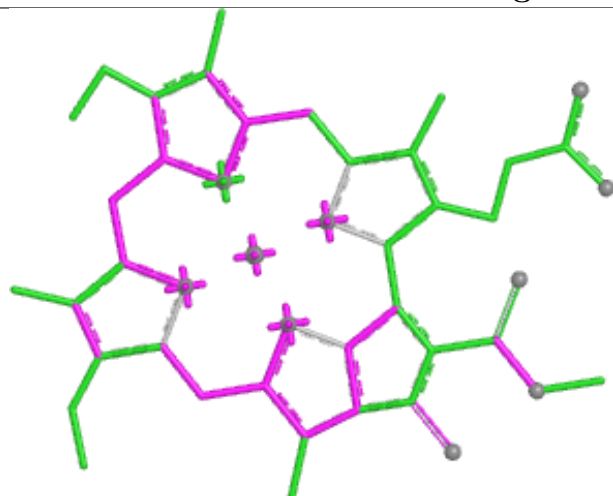




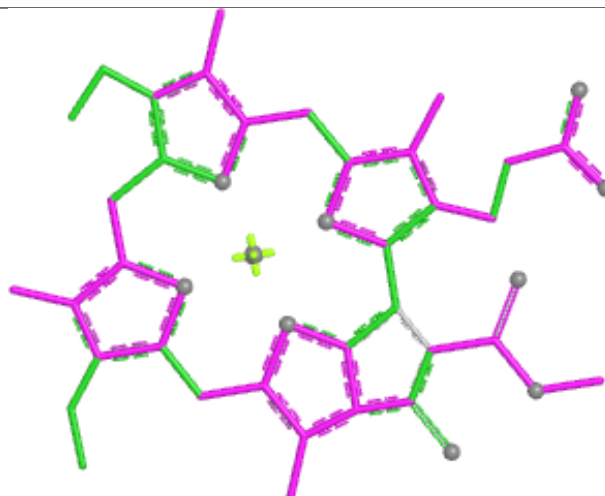
Ligand CLA Y 837



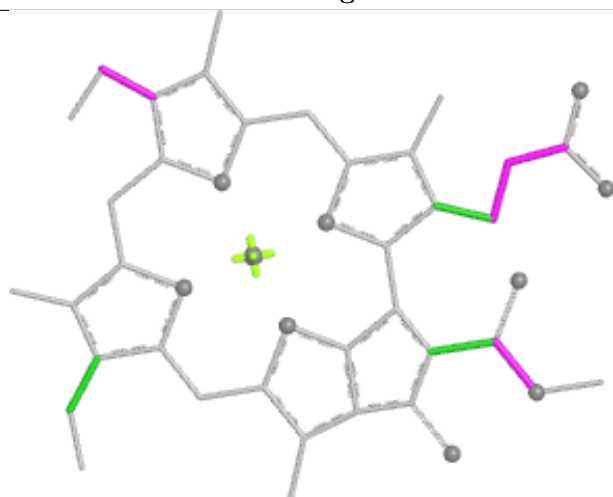
Ligand CLA H 811



Bond lengths



Bond angles

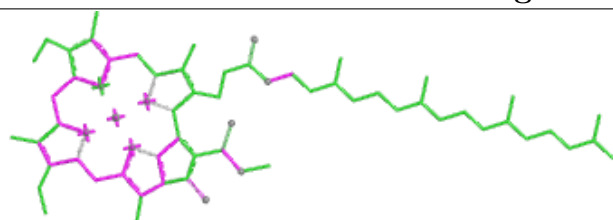


Torsions

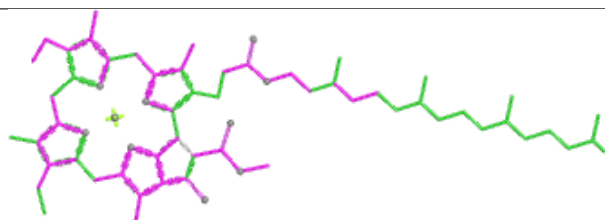


Rings

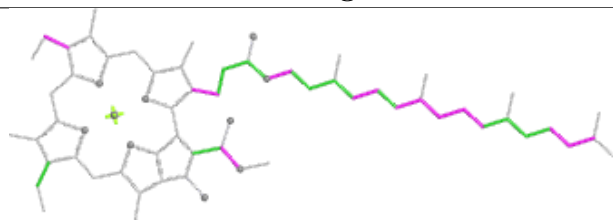
Ligand CLA B 827



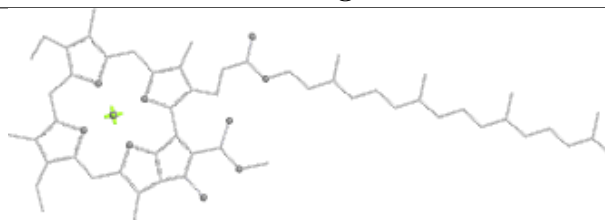
Bond lengths



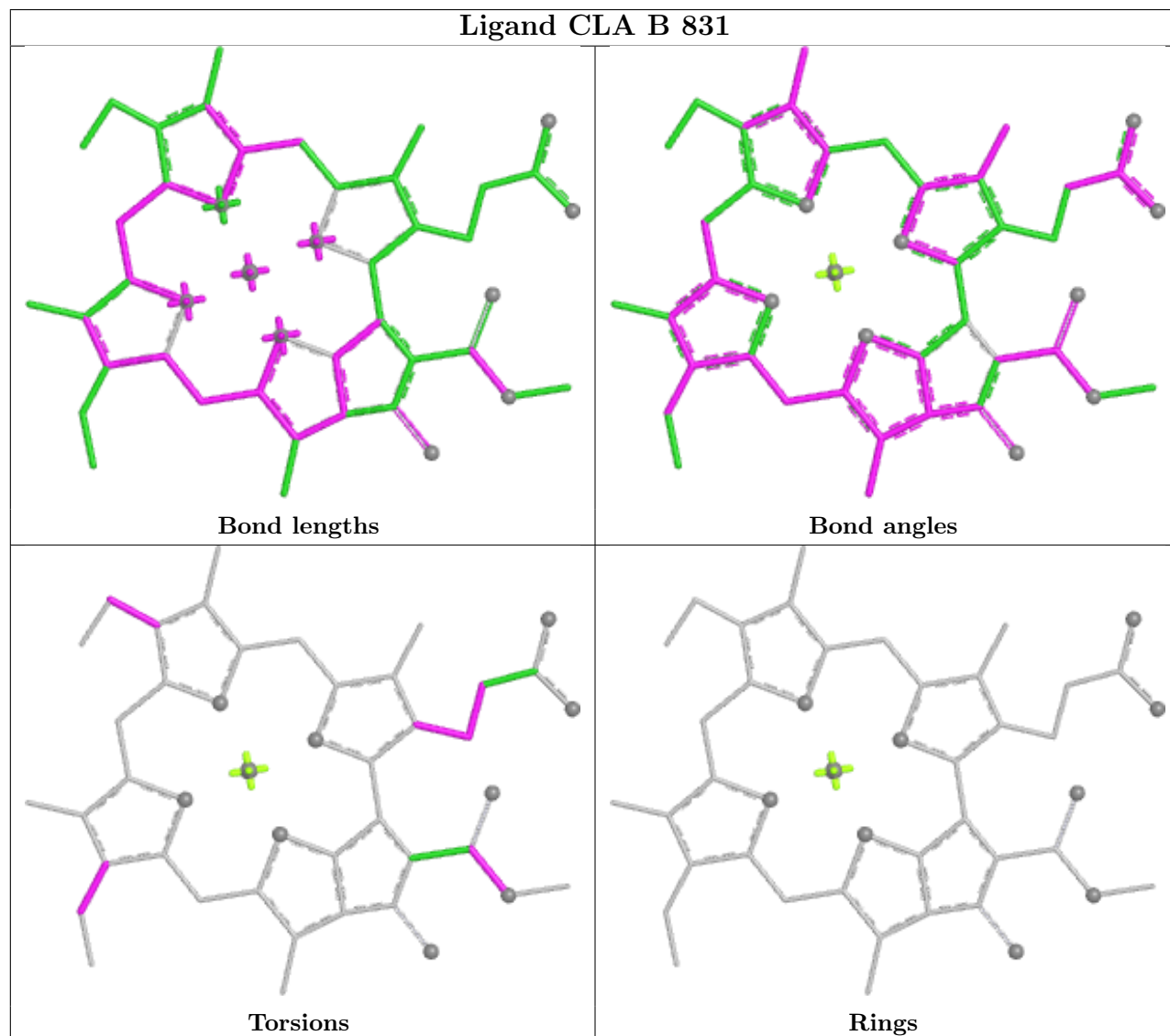
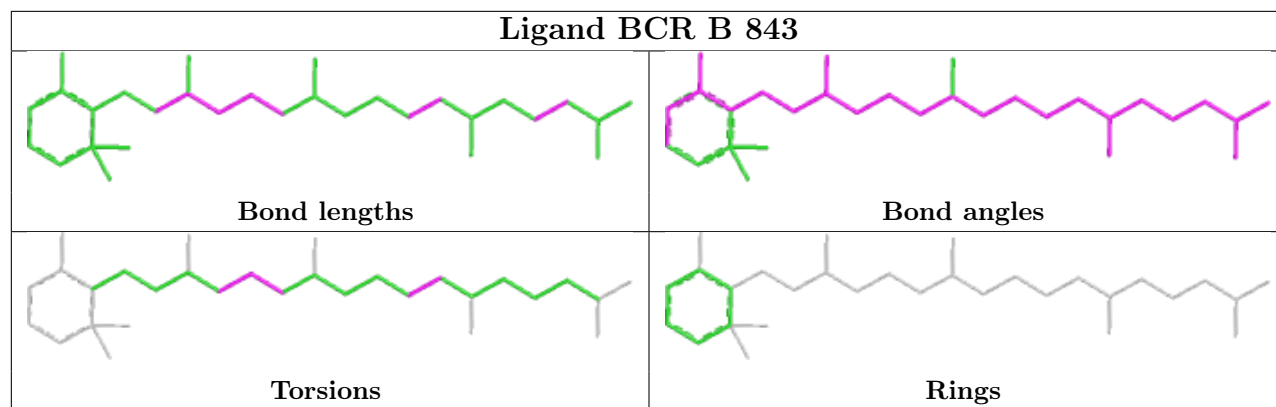
Bond angles



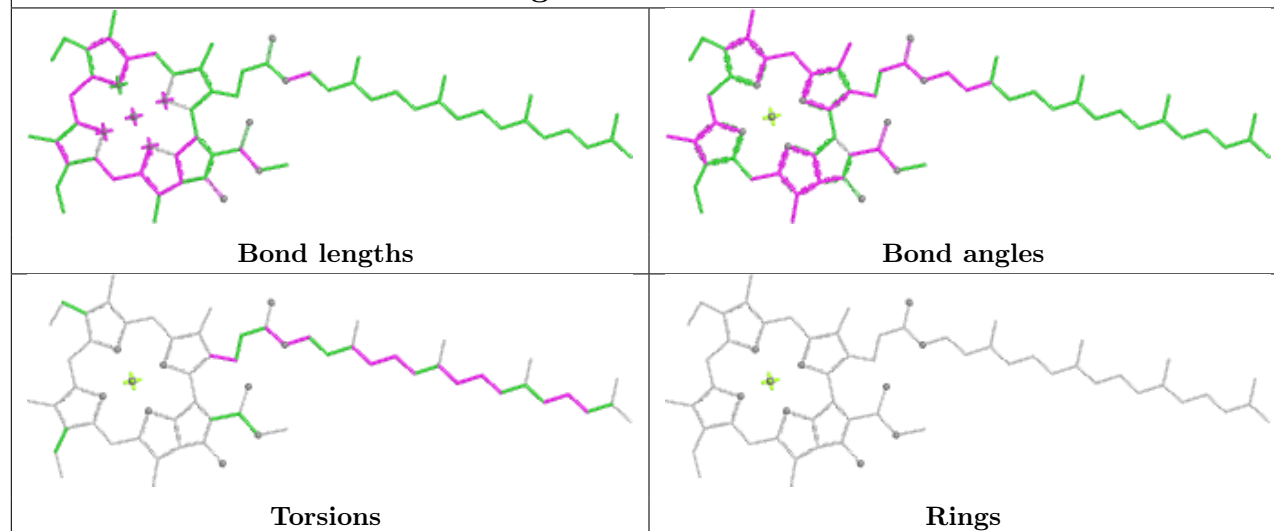
Torsions



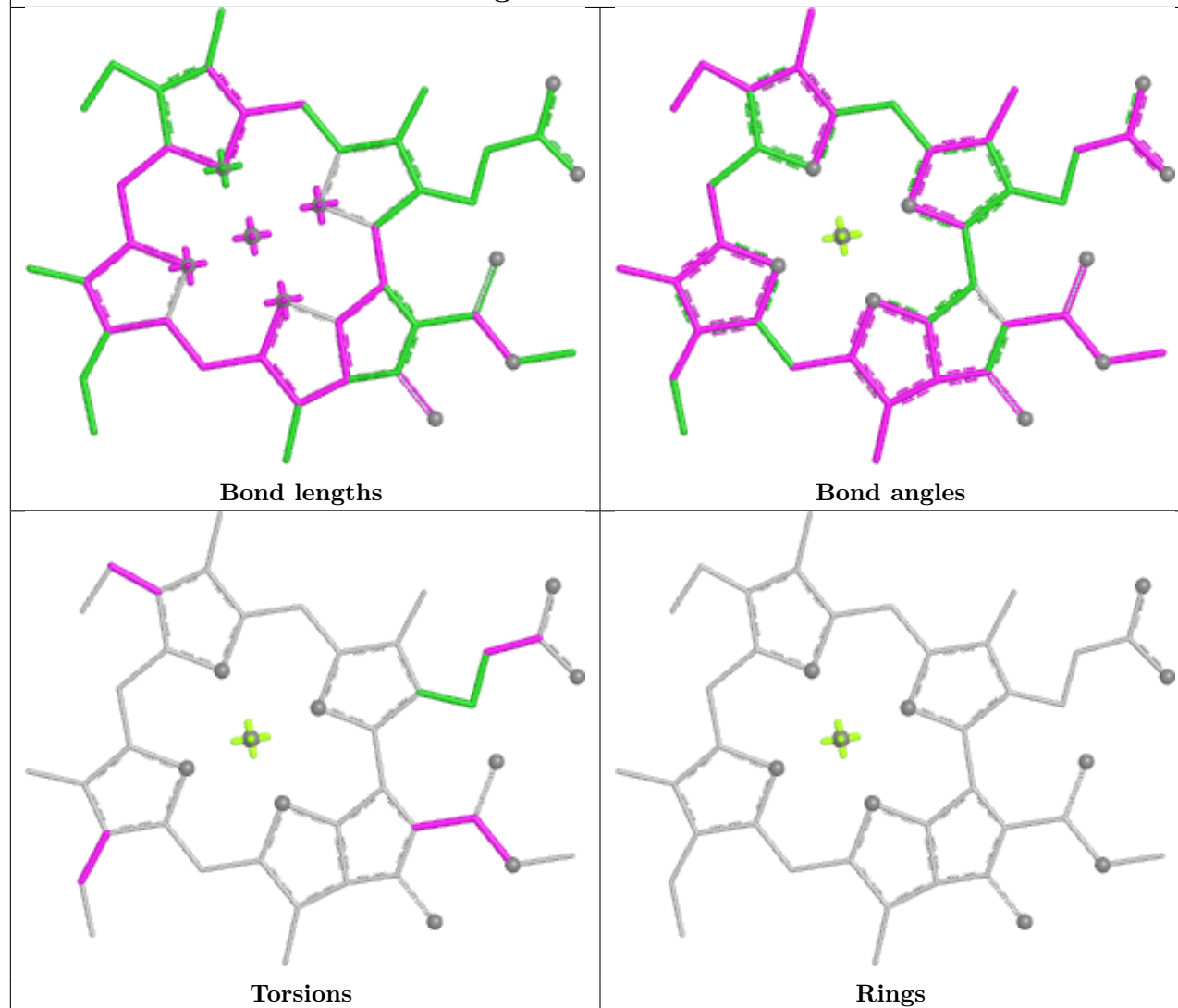
Rings



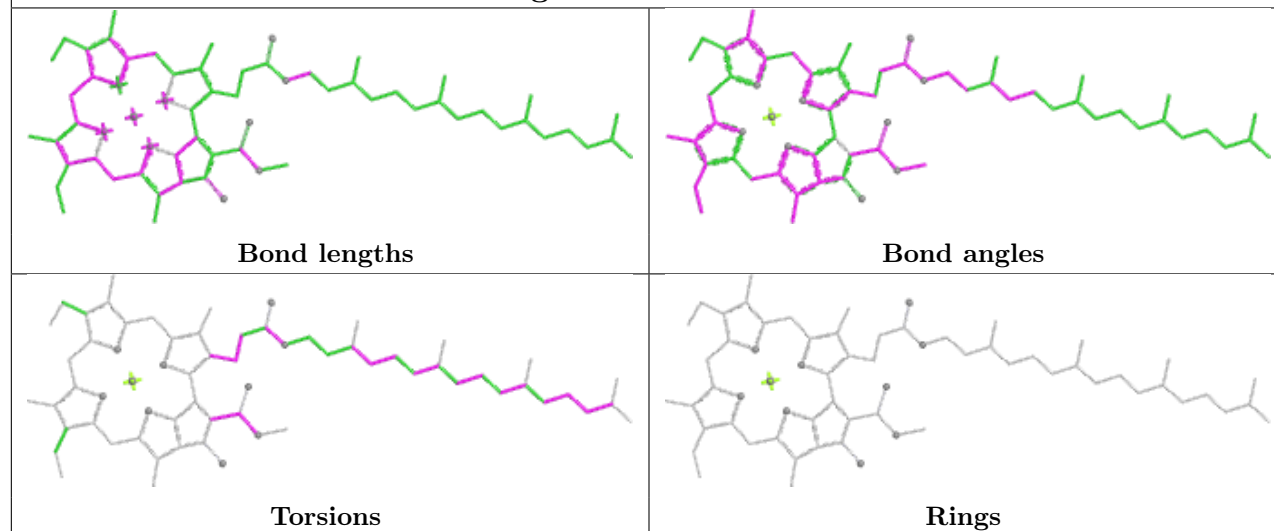
Ligand CLA G 819



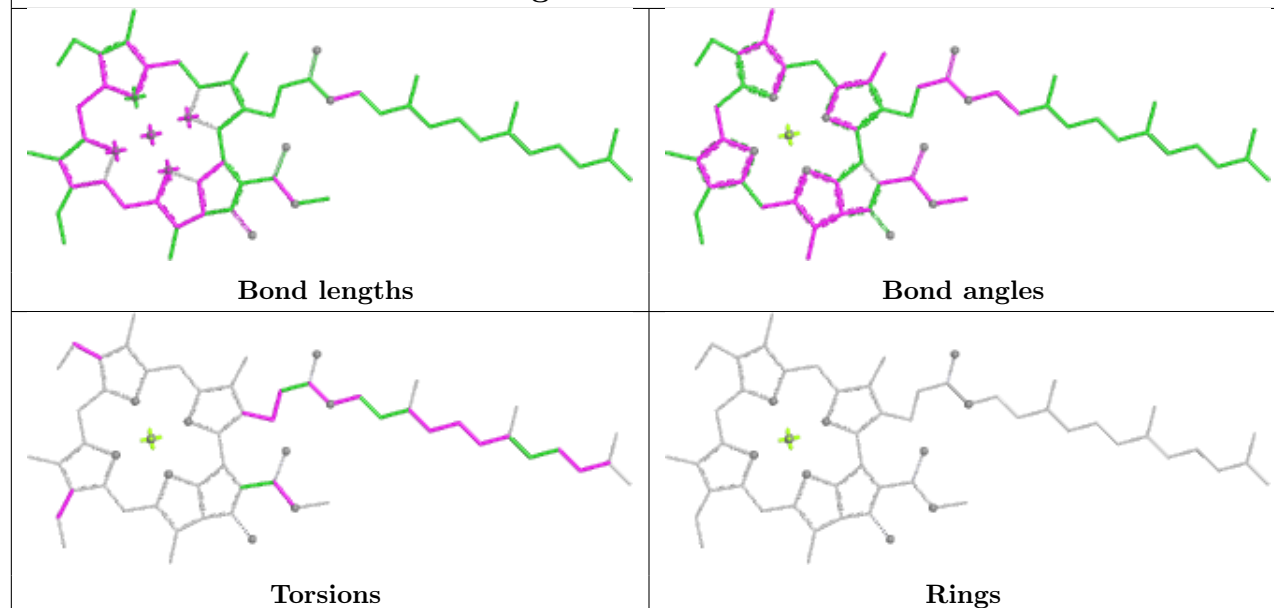
Ligand CLA Z 834

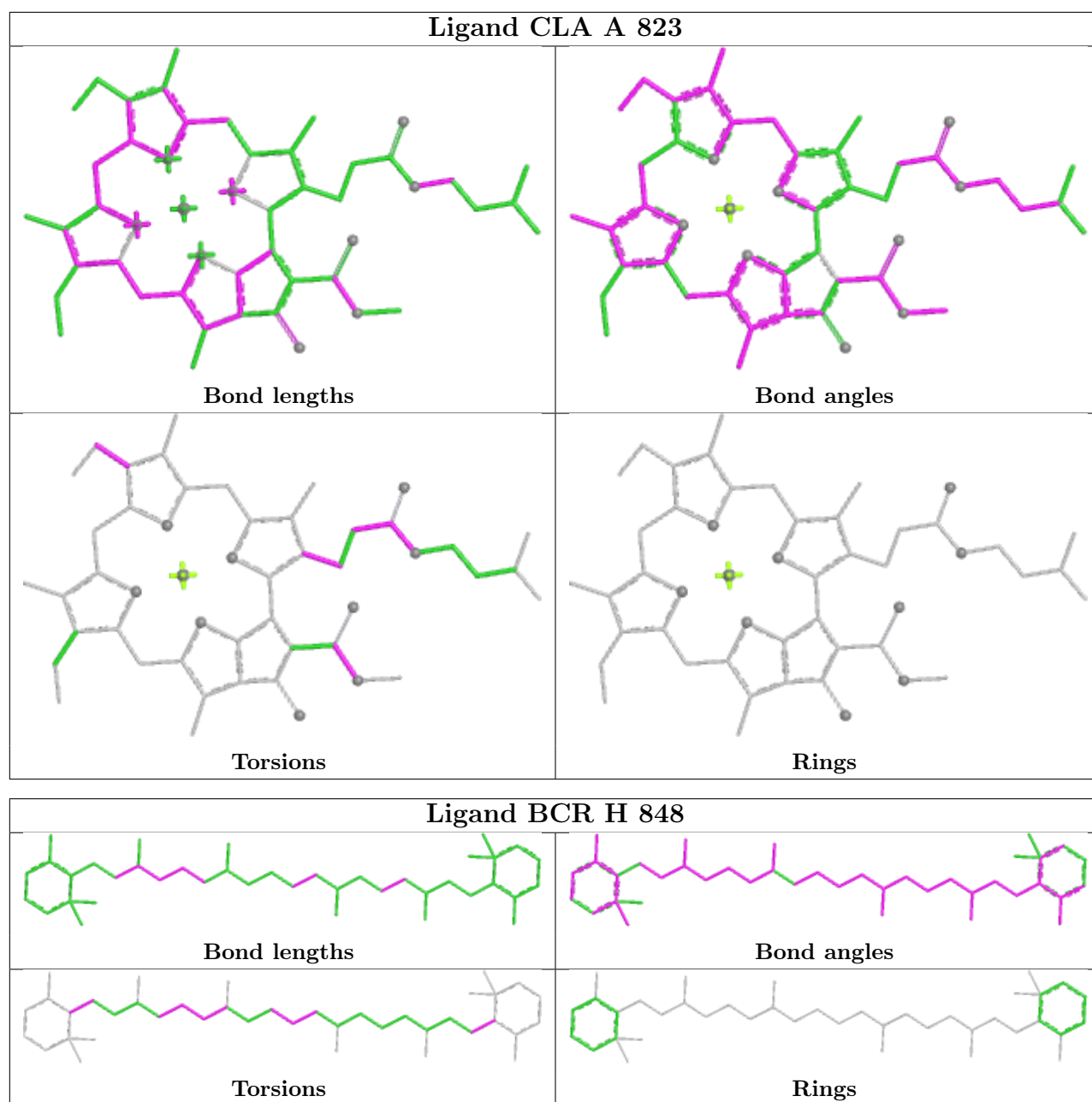


Ligand CLA G 808

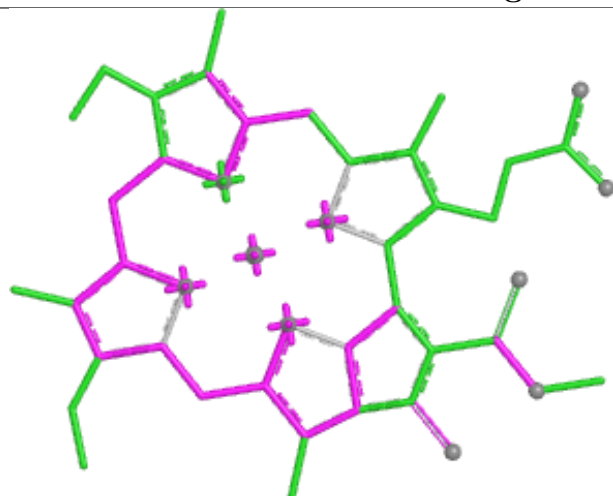


Ligand CLA Y 824

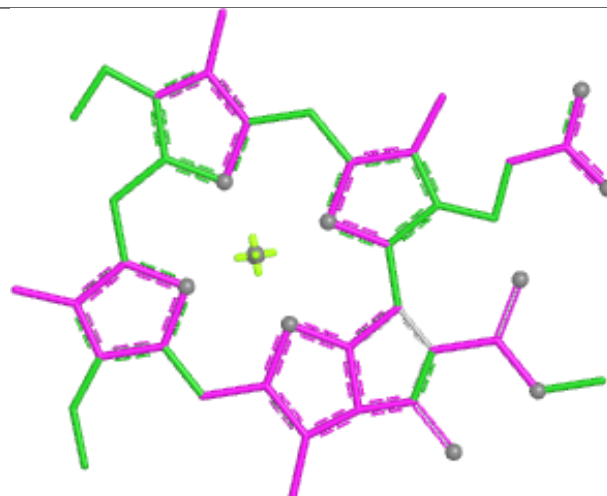




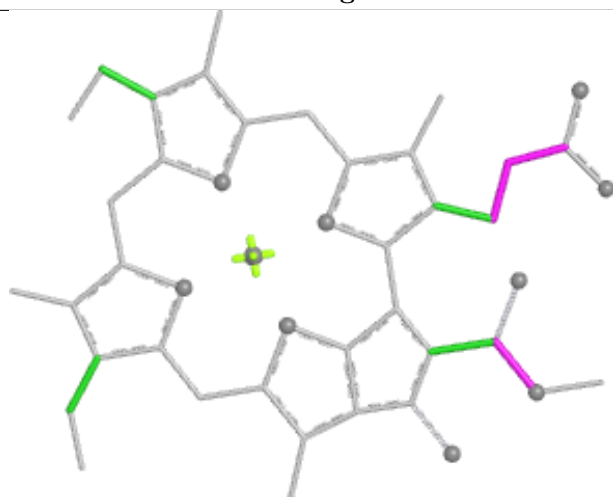
Ligand CLA X 1701



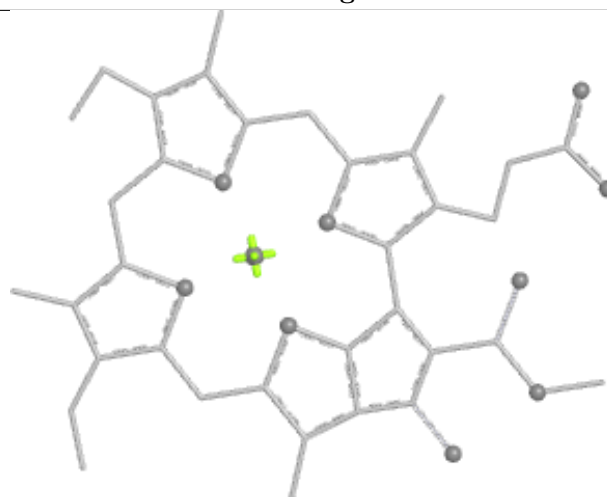
Bond lengths



Bond angles

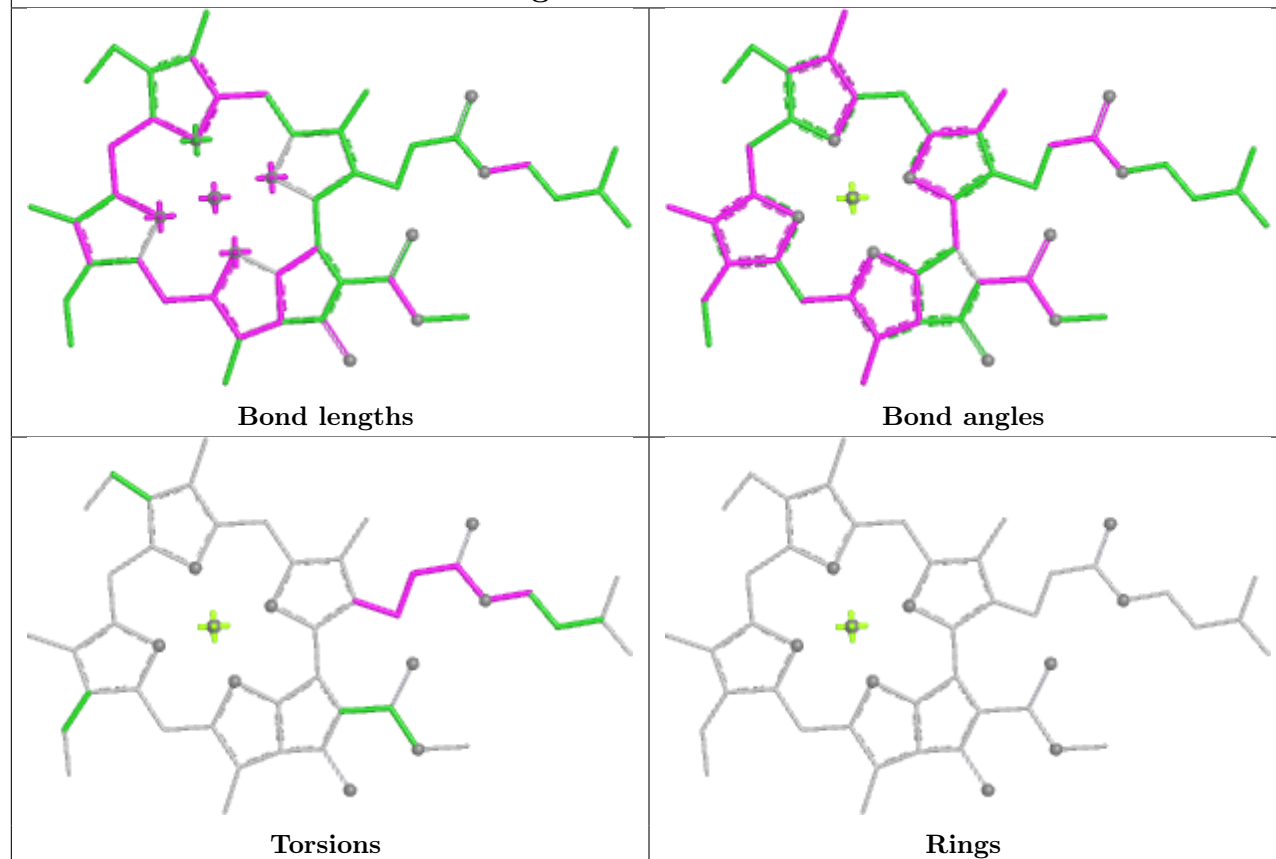


Torsions

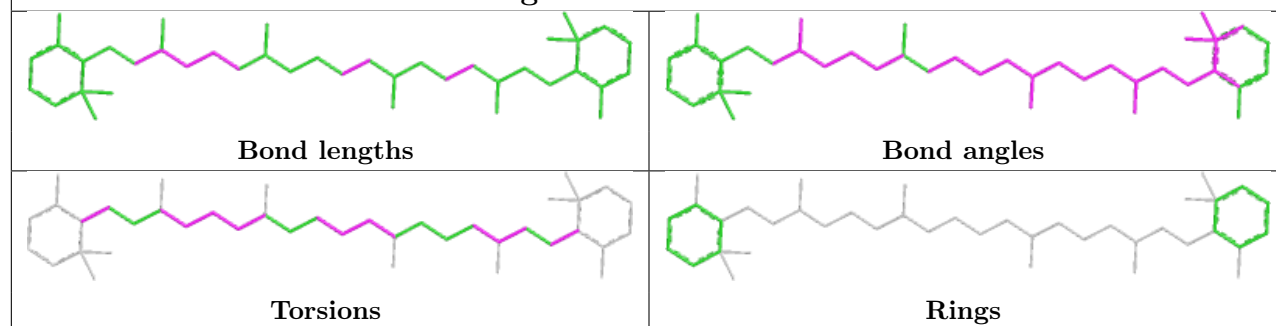


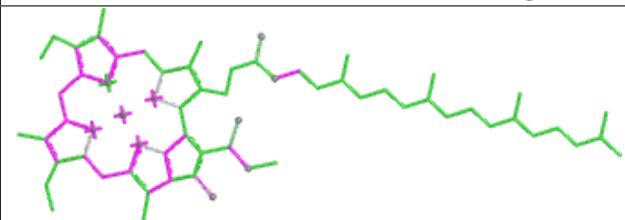
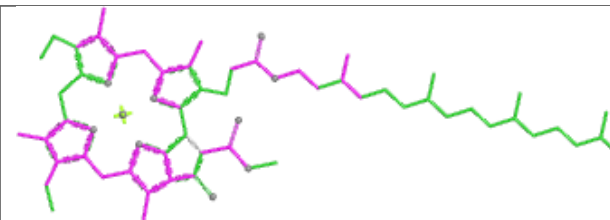
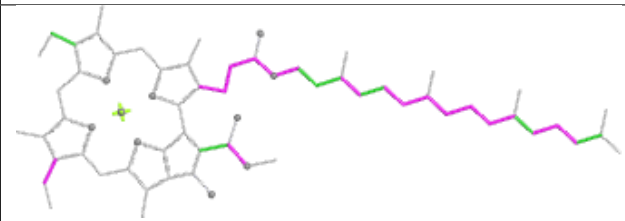
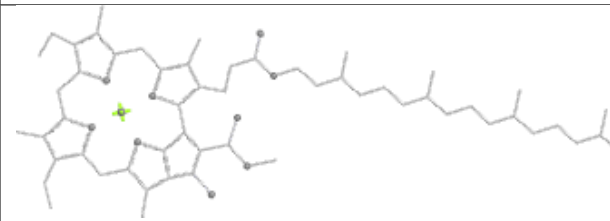
Rings

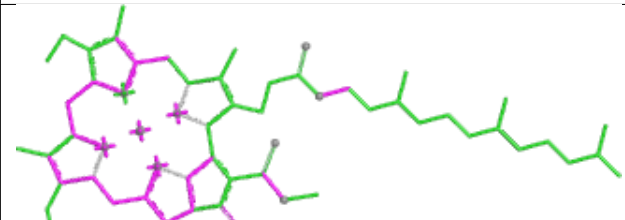
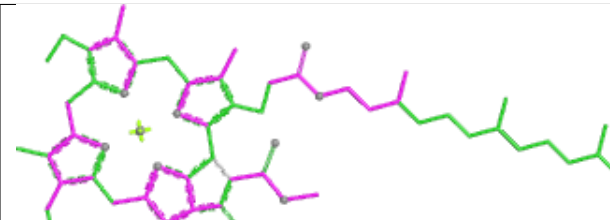
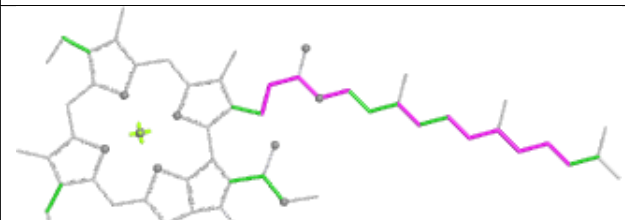
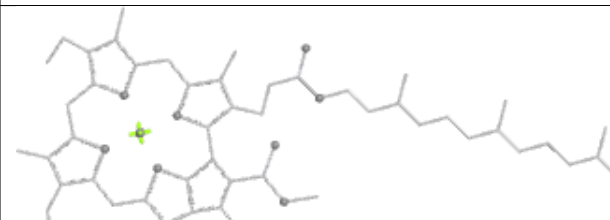
Ligand CLA A 838

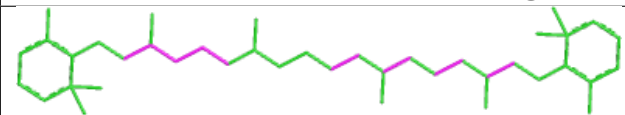
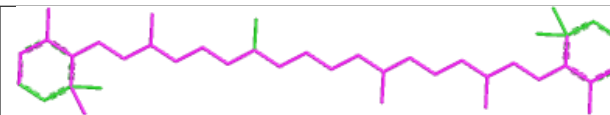
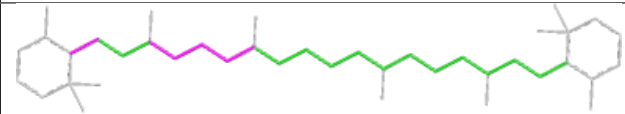
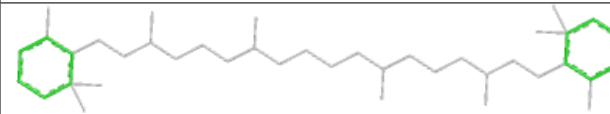


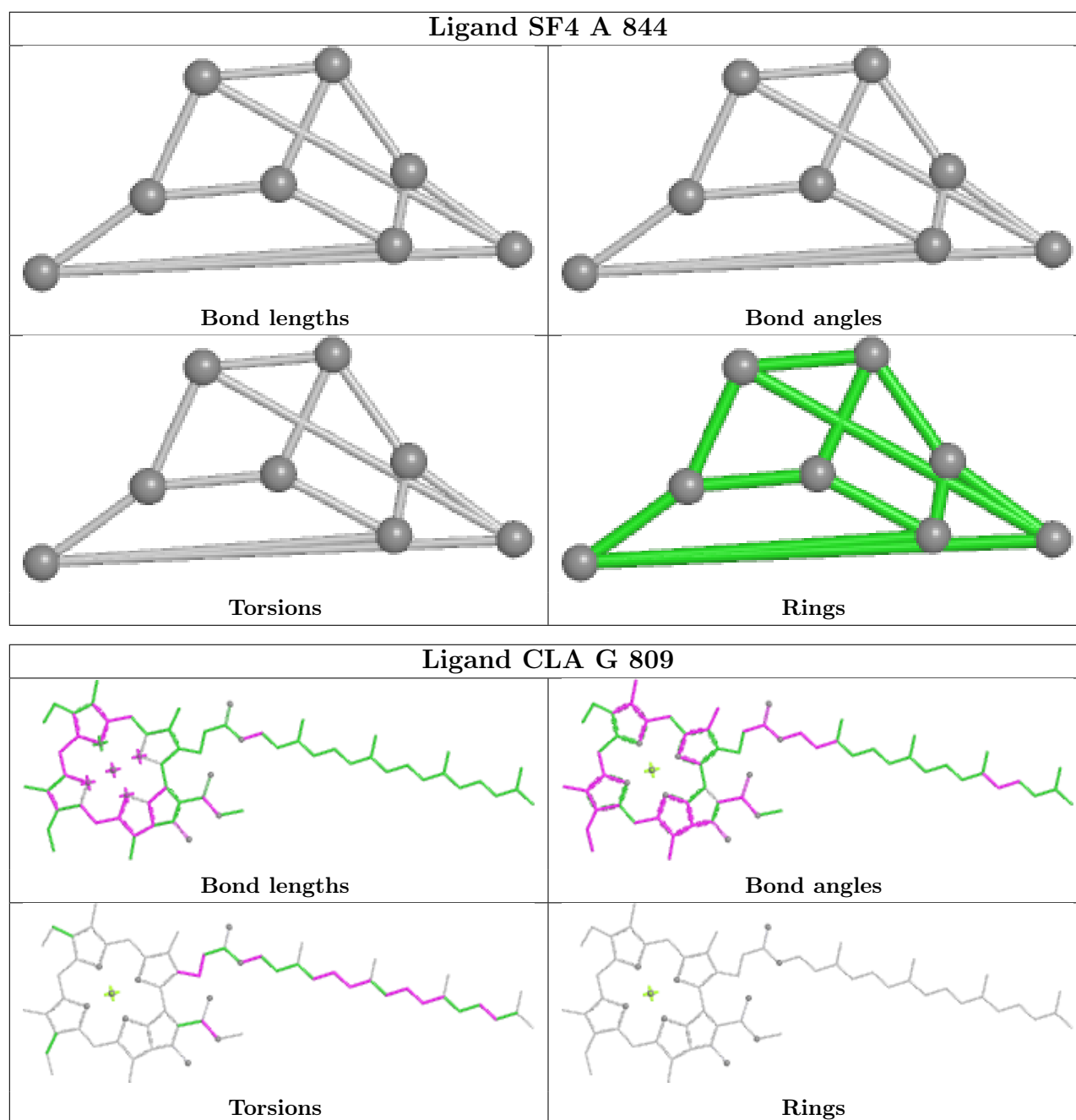
Ligand BCR U 1007

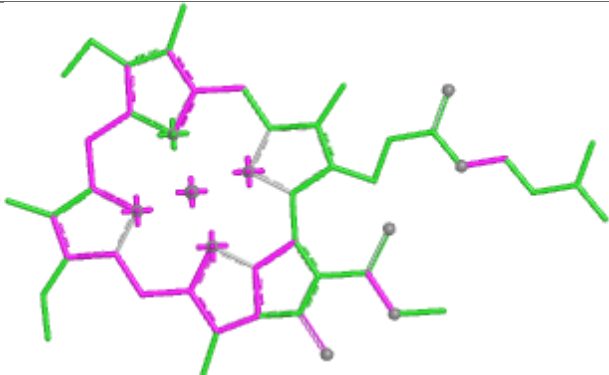
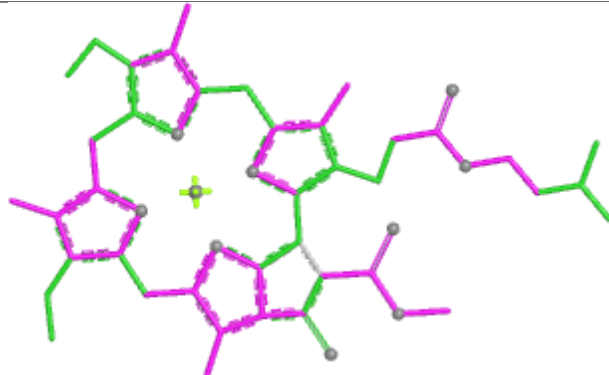
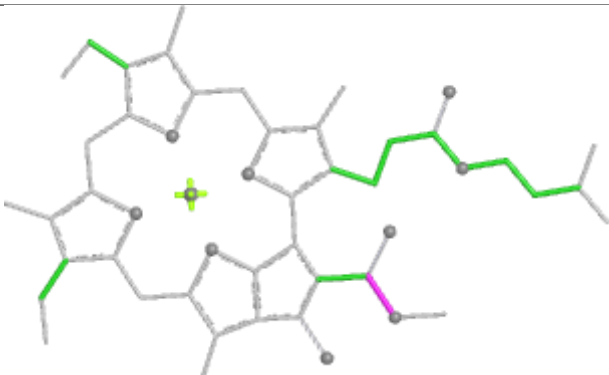
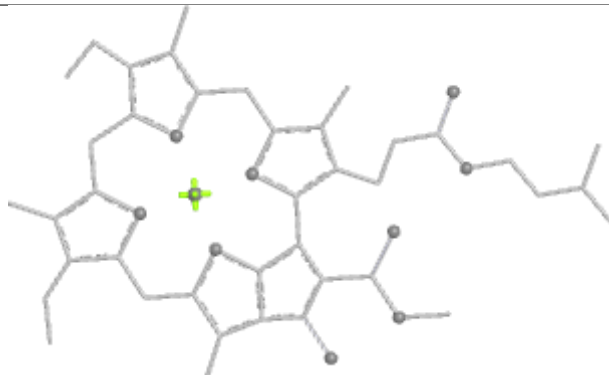


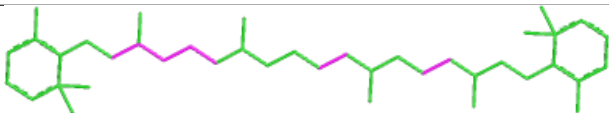
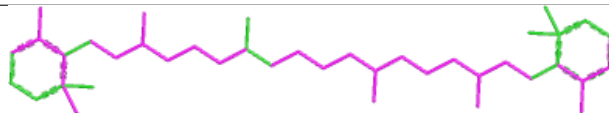
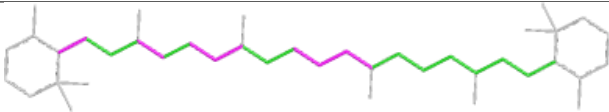
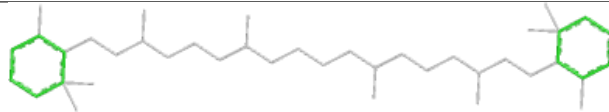
Ligand CLA A 818	
	
Bond lengths	Bond angles
	
Torsions	Rings

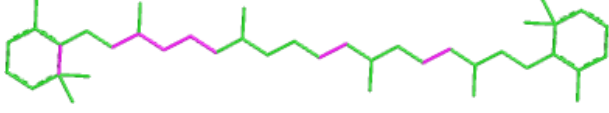
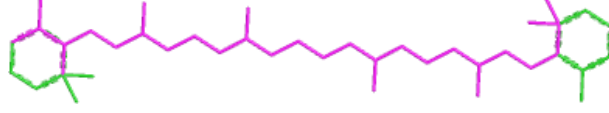
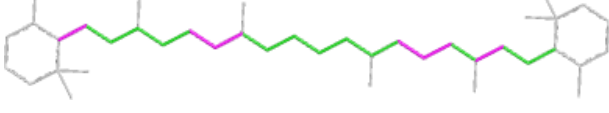
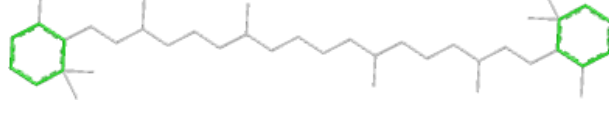
Ligand CLA B 823	
	
Bond lengths	Bond angles
	
Torsions	Rings

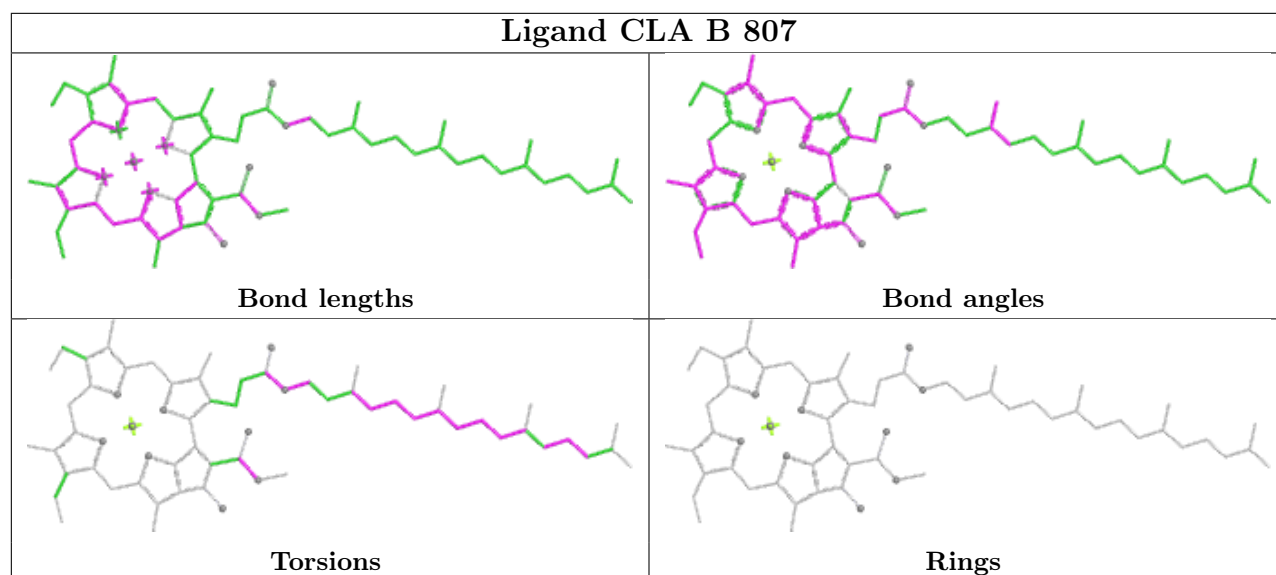
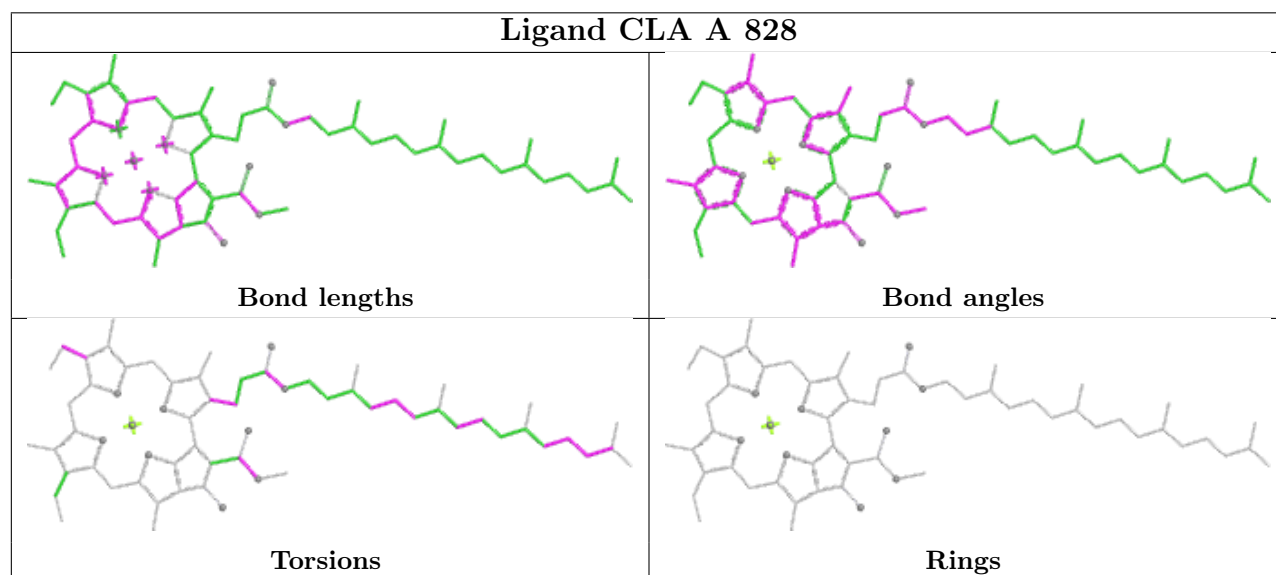
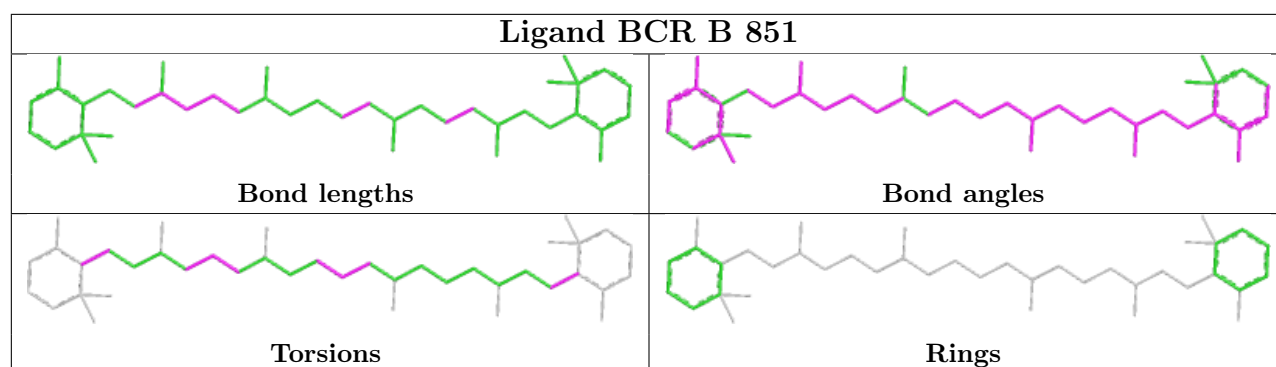
Ligand BCR h 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

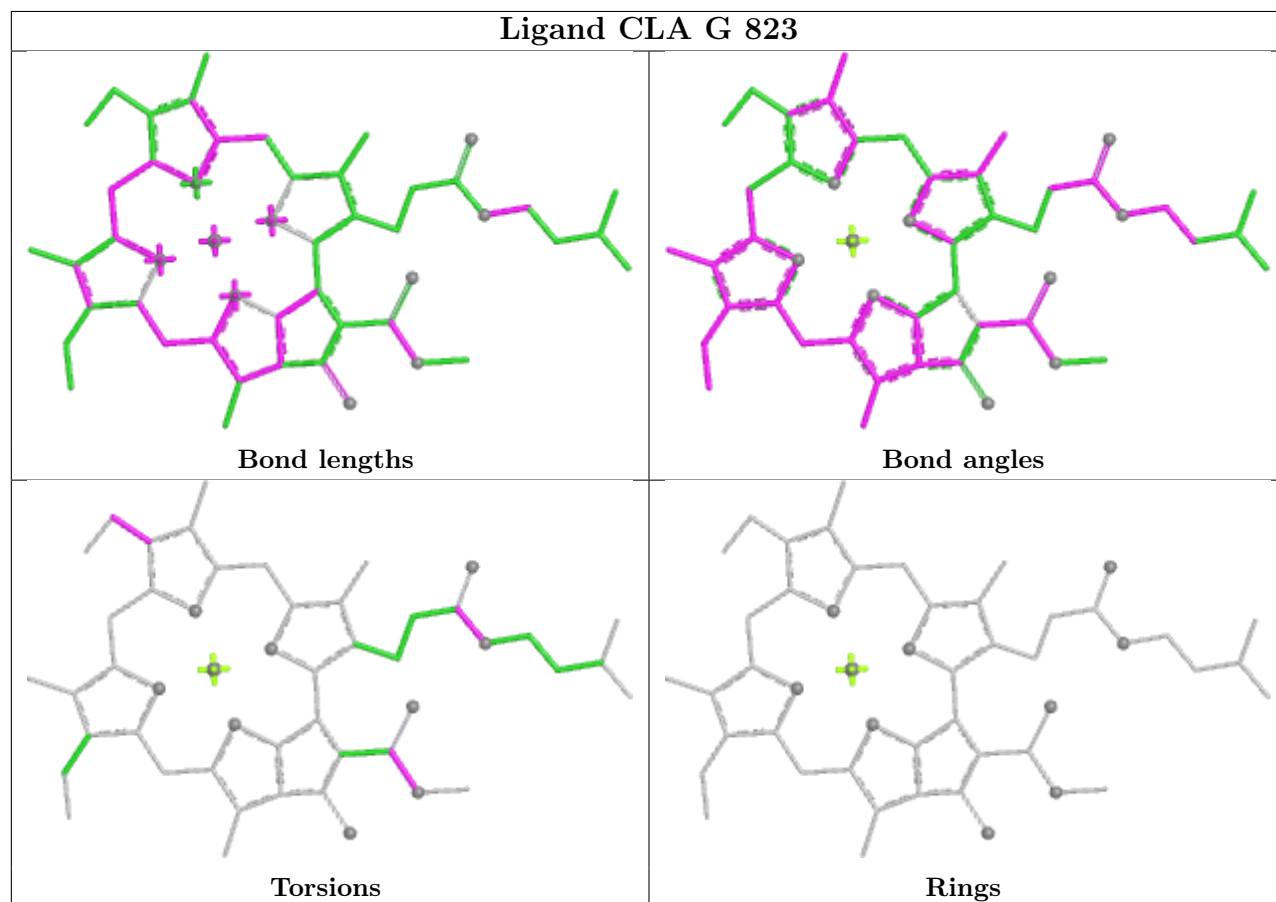
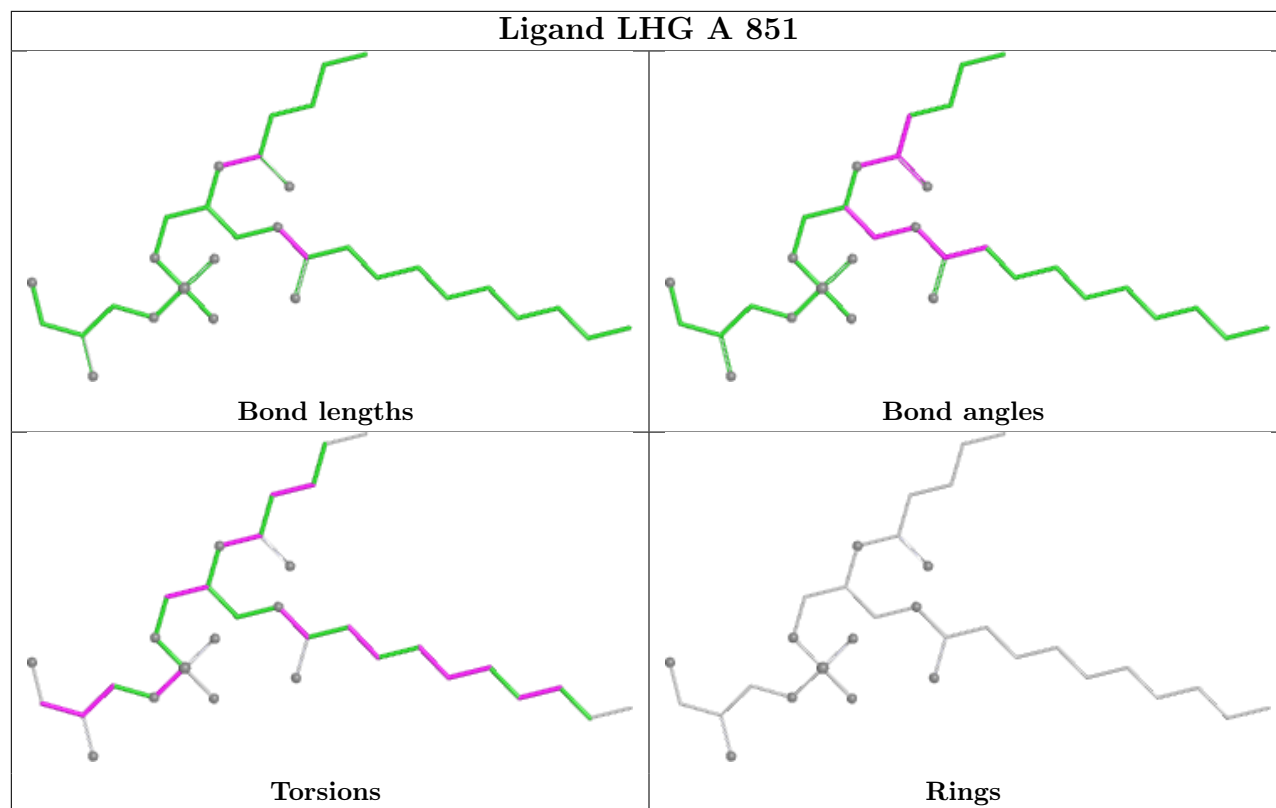


Ligand CLA A 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

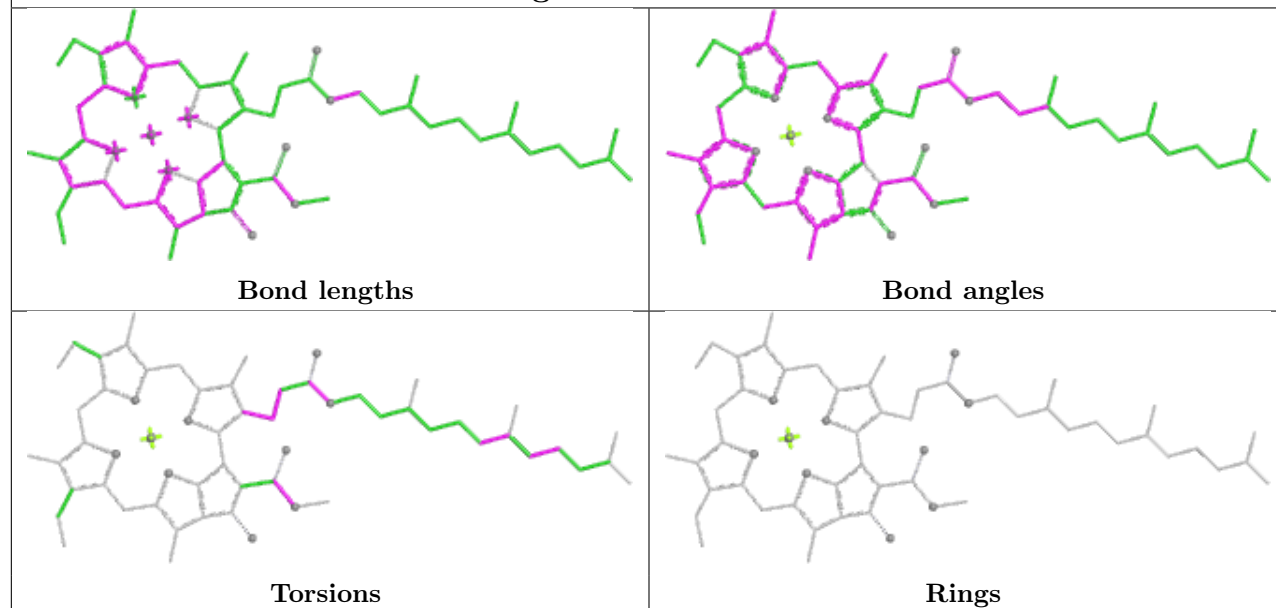
Ligand BCR L 208	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

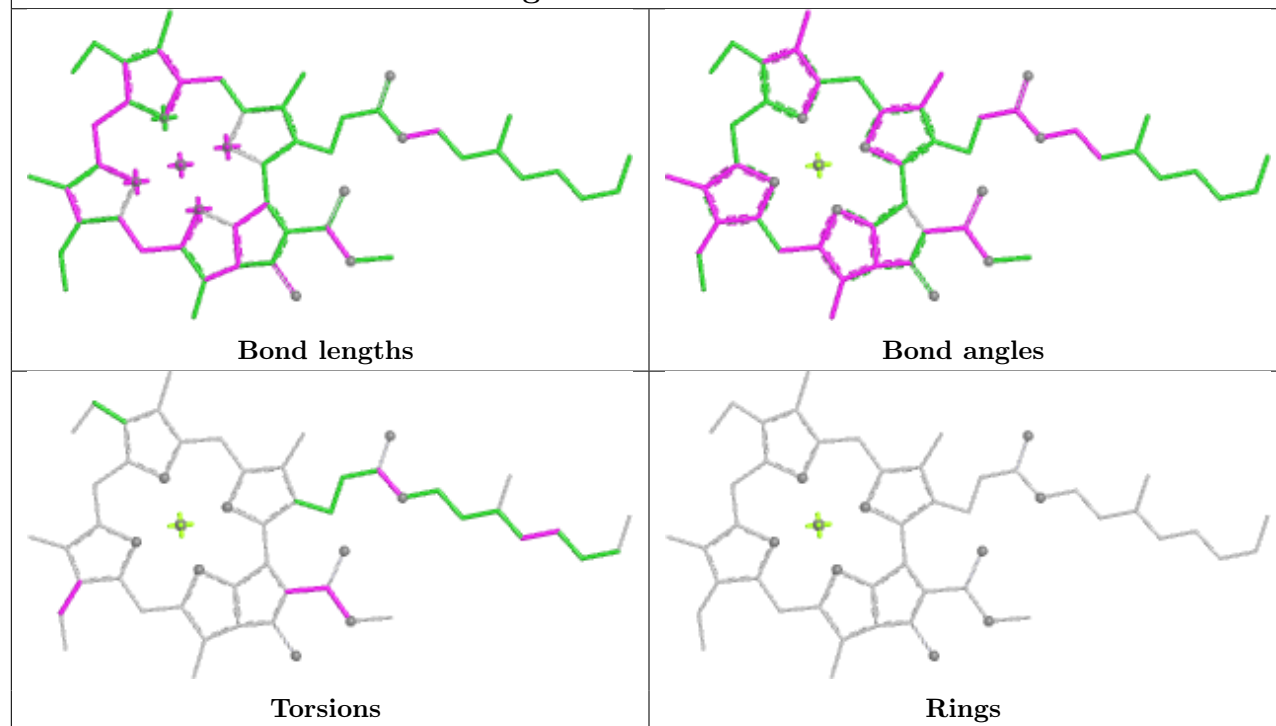


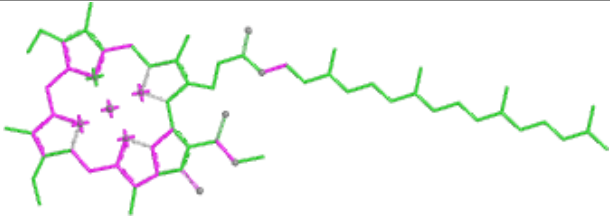
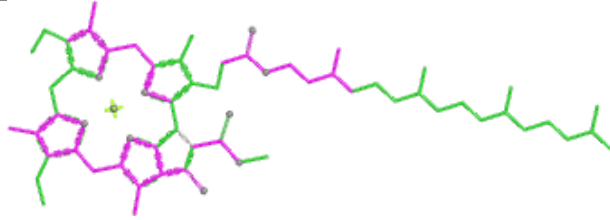
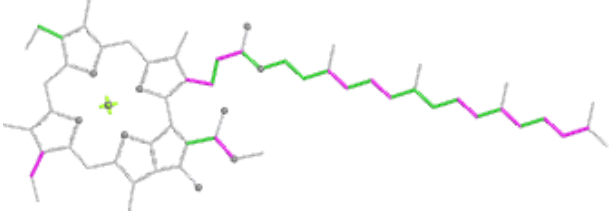
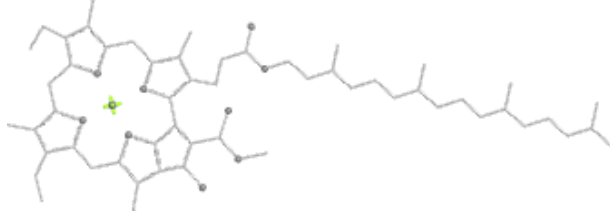
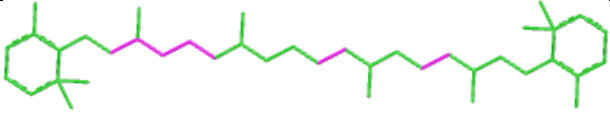
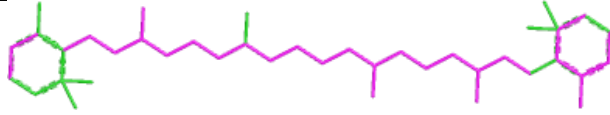
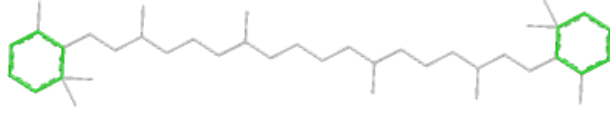
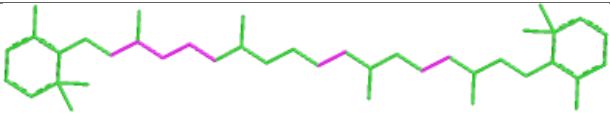
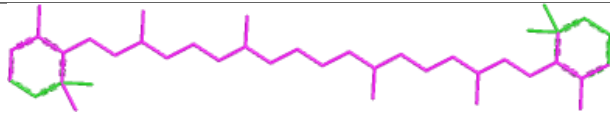
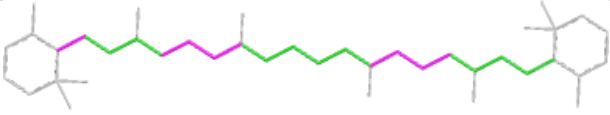
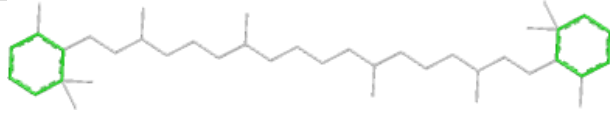


Ligand CLA B 818

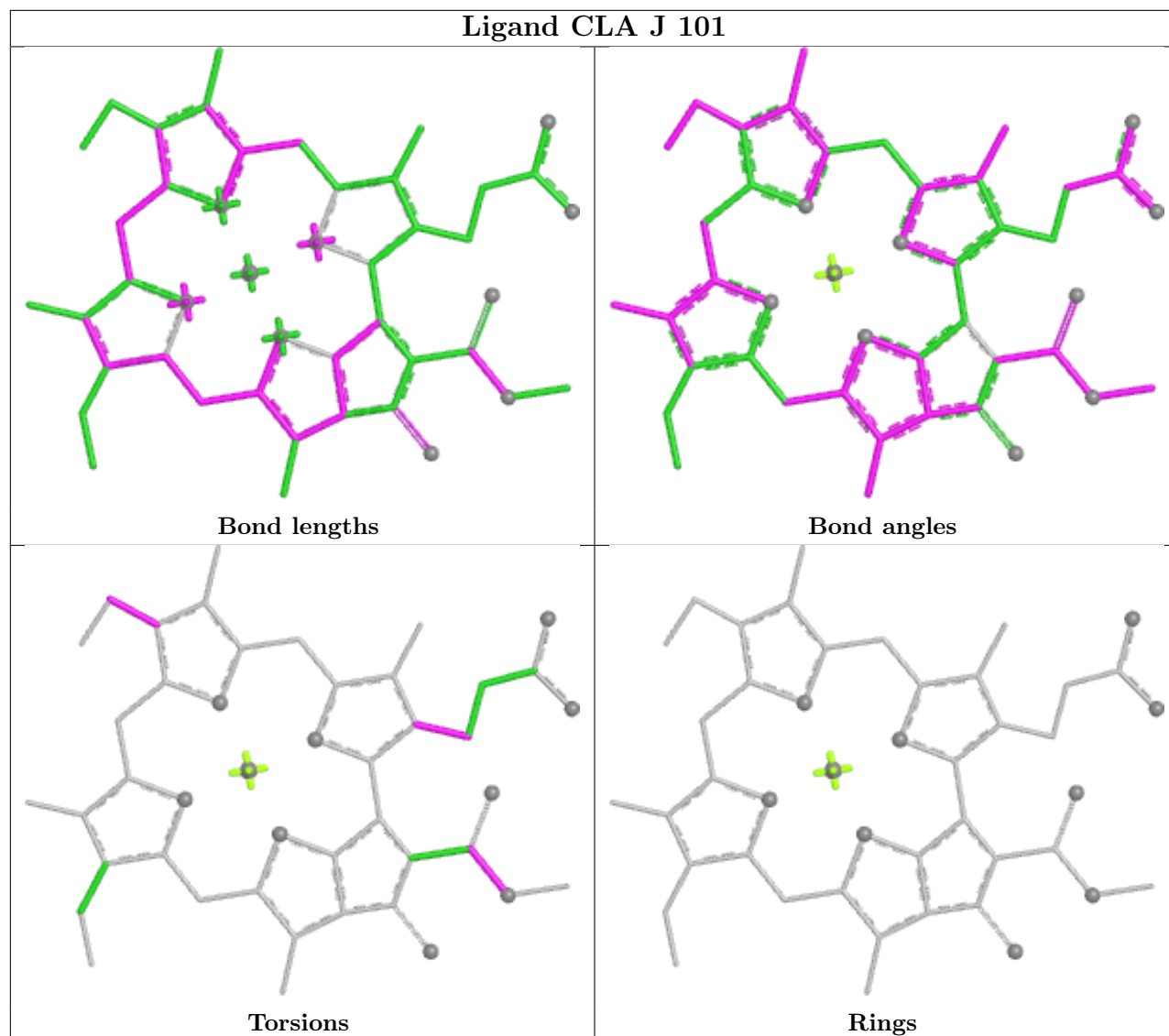


Ligand CLA V 1201

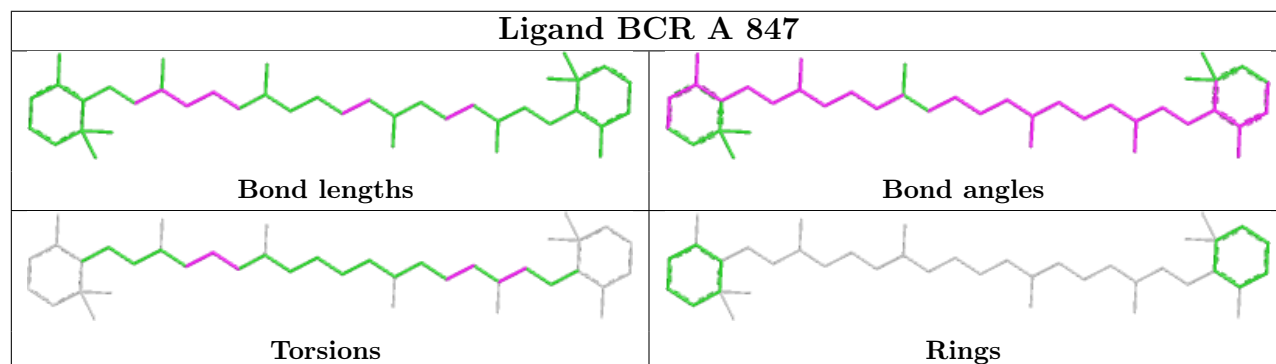


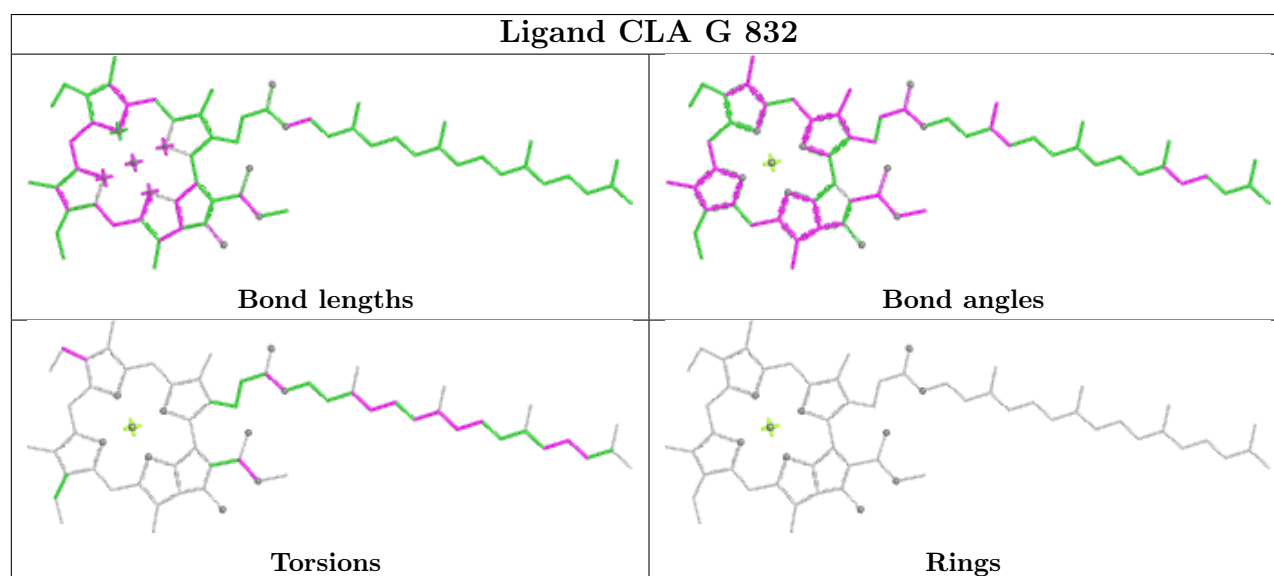
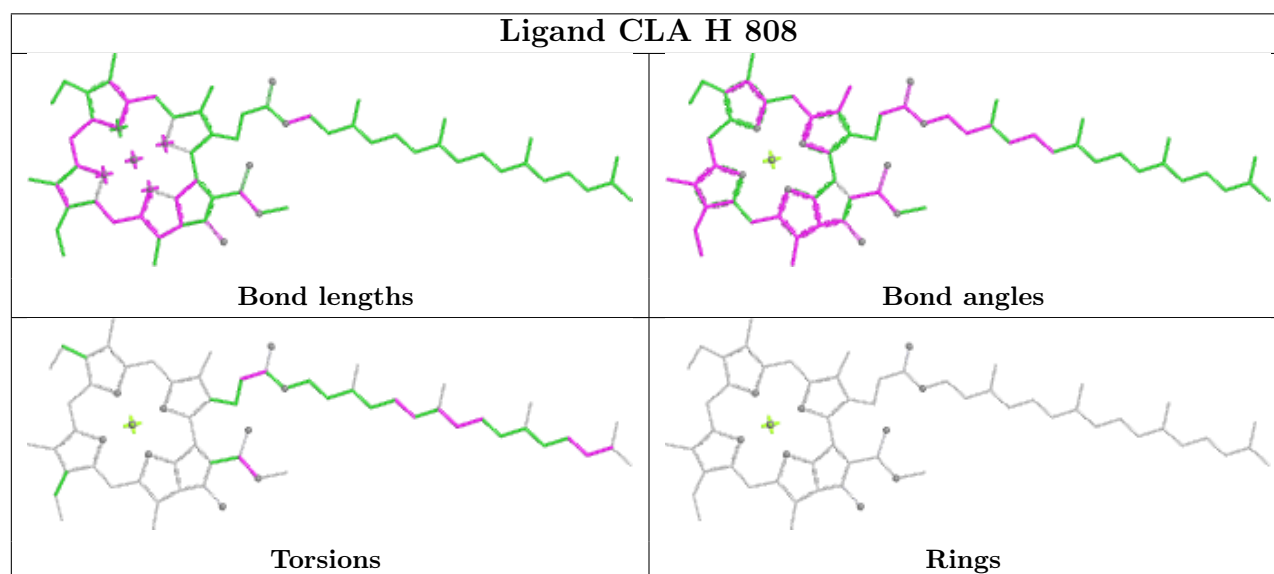
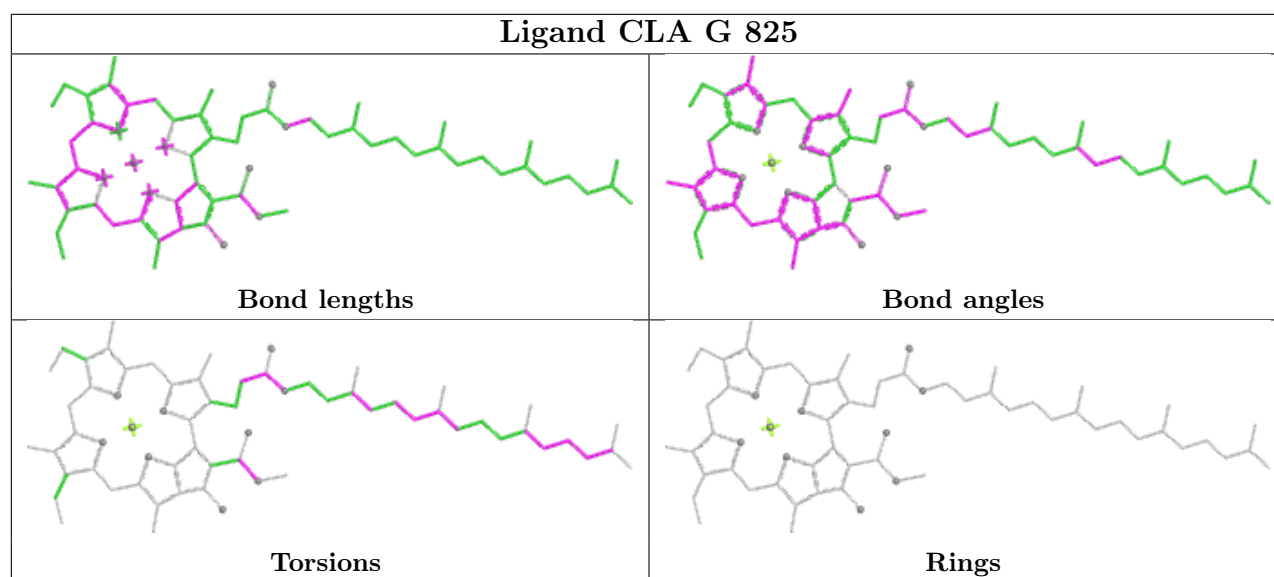
Ligand CLA Y 828	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR Z 841	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR f 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA J 101

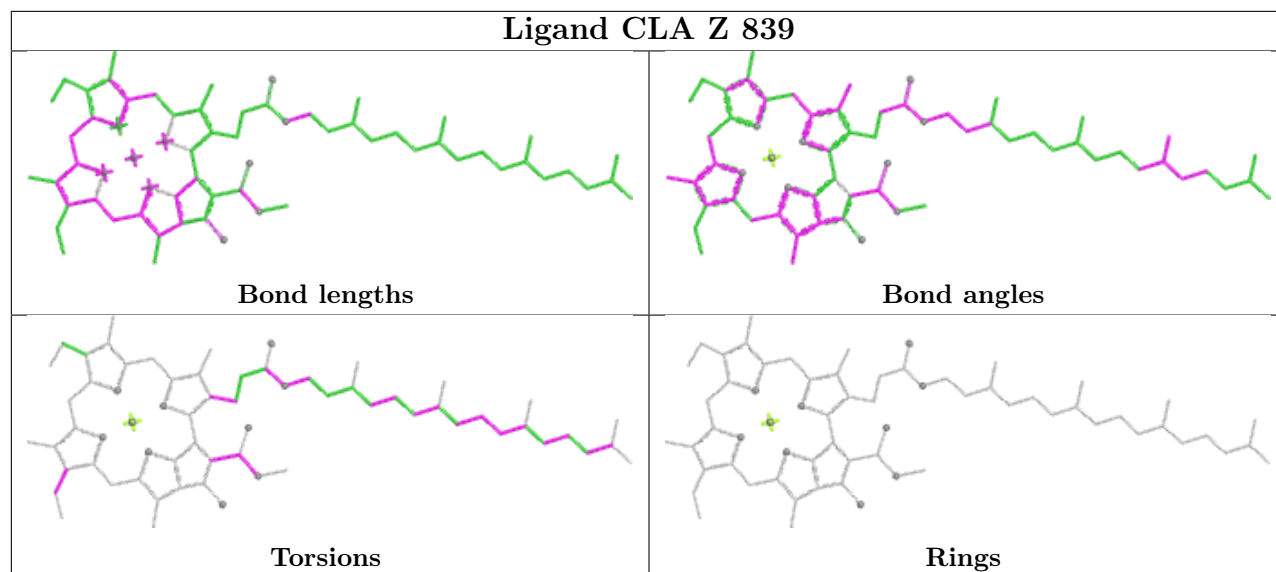


Ligand BCR A 847

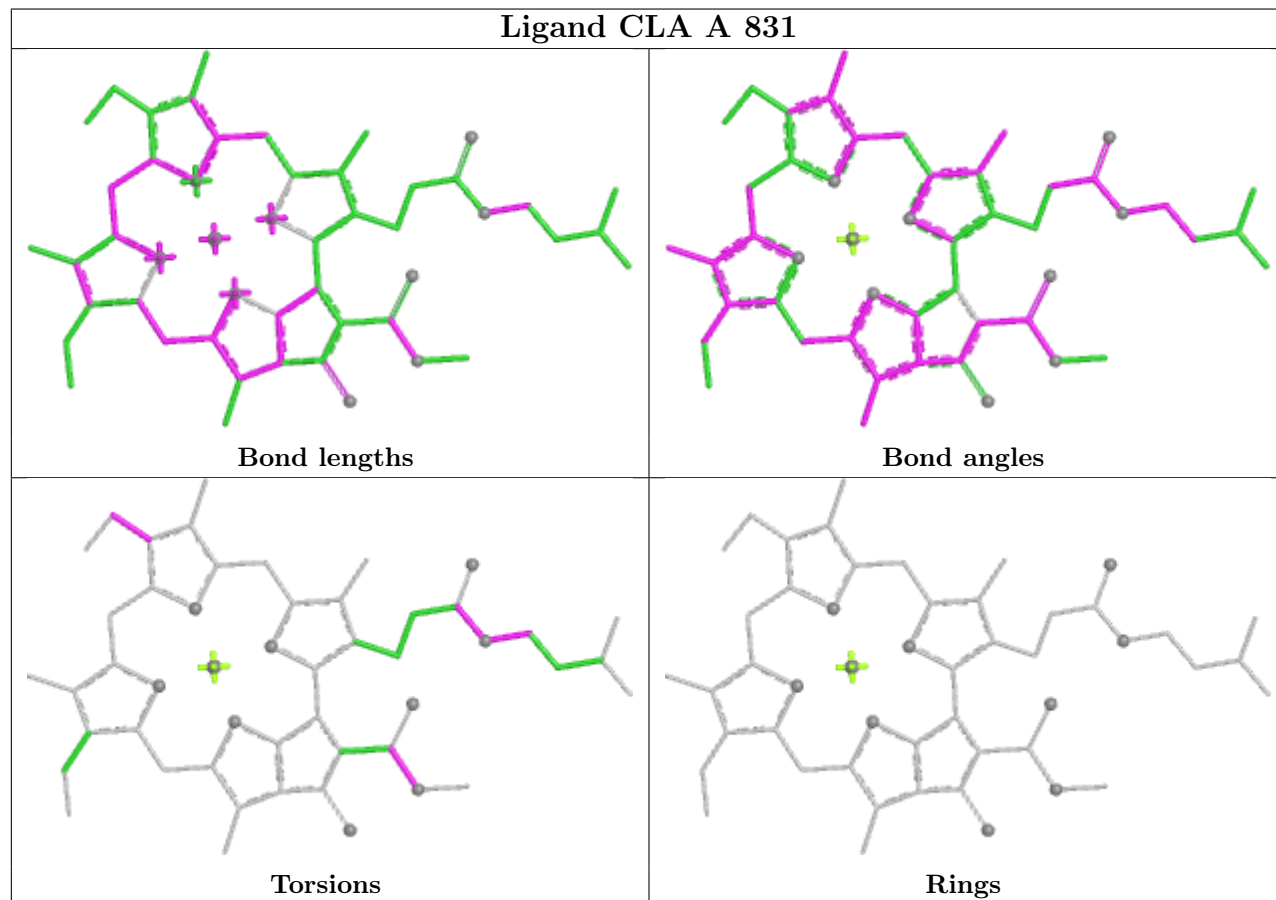




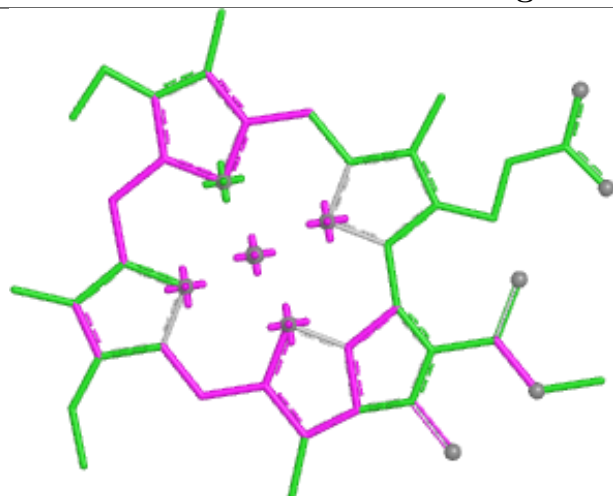
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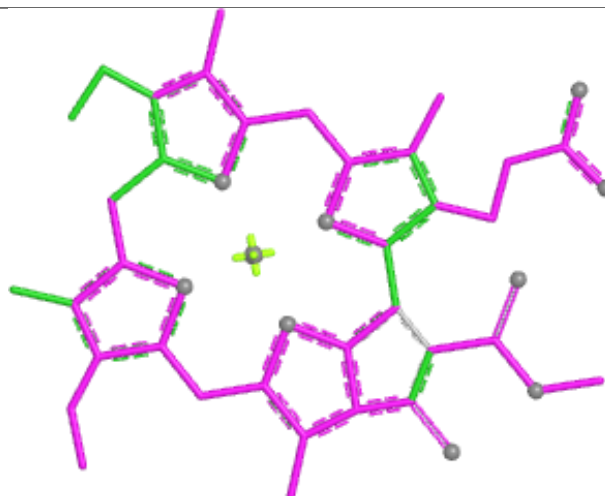
Ligand CLA A 831



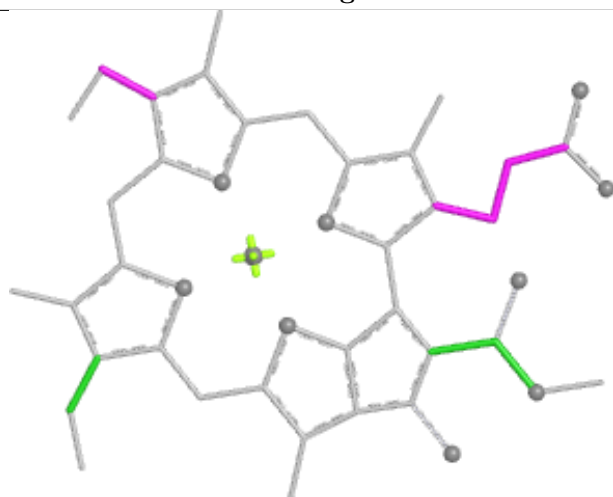
Ligand CLA Z 818



Bond lengths



Bond angles

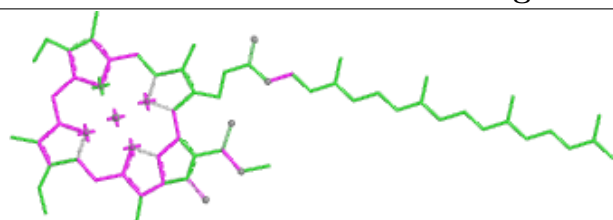


Torsions

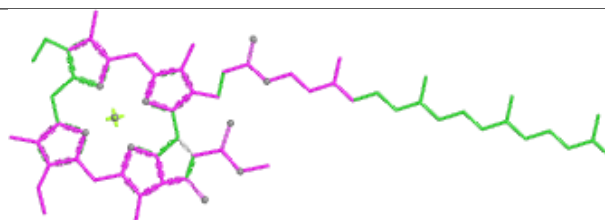


Rings

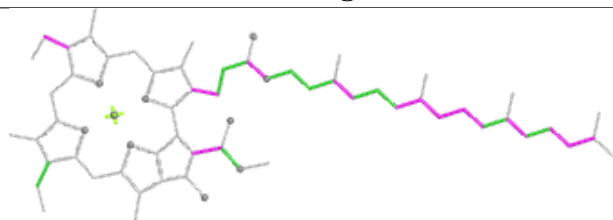
Ligand CLA H 824



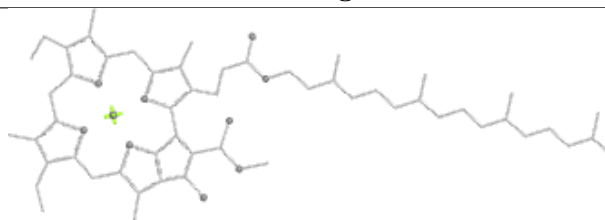
Bond lengths



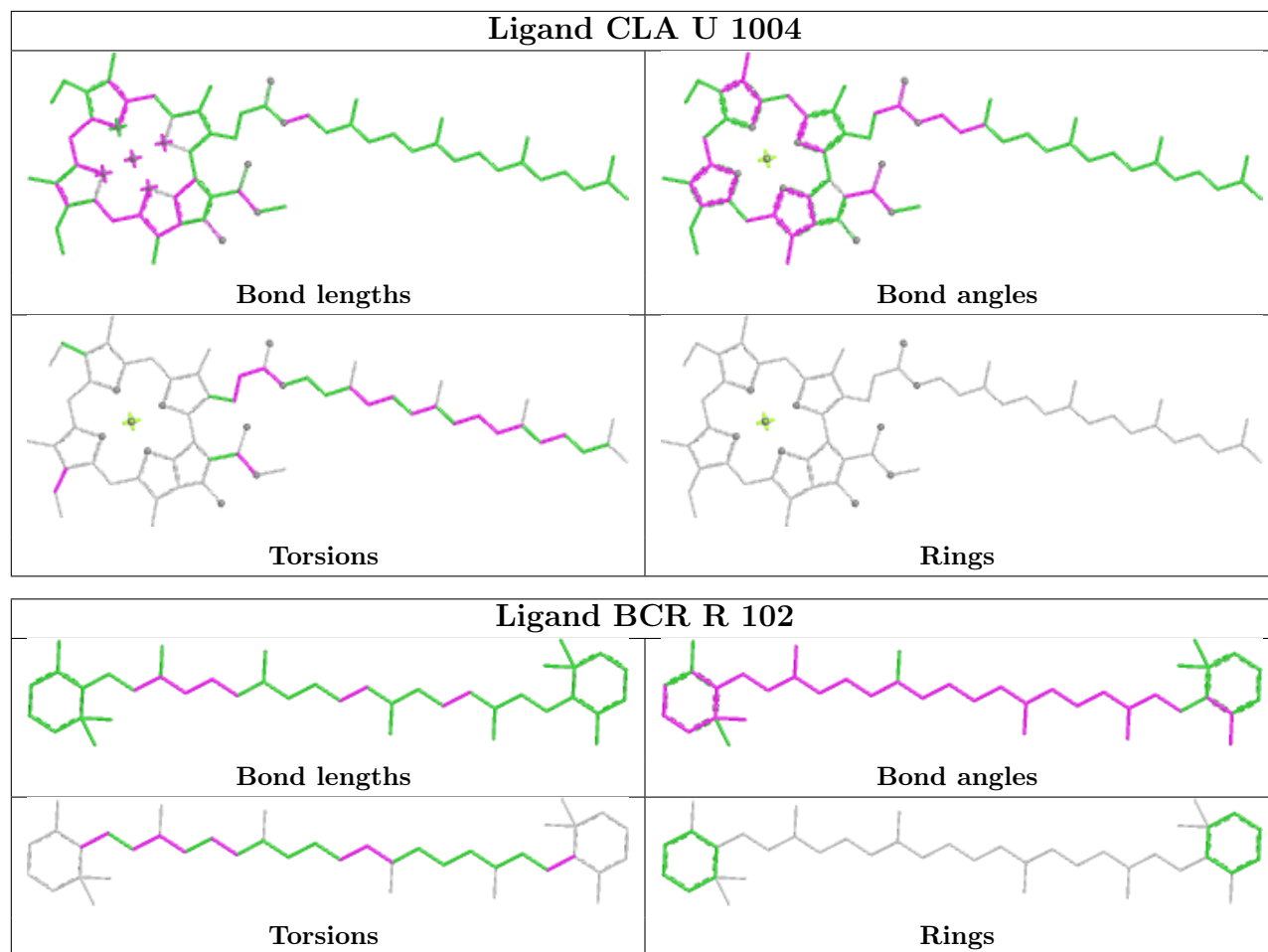
Bond angles



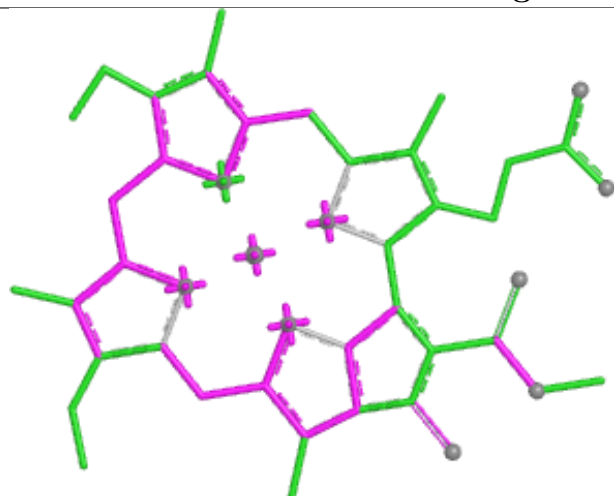
Torsions



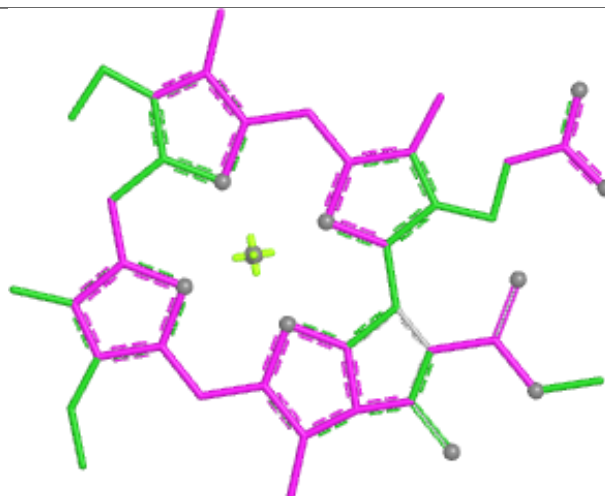
Rings



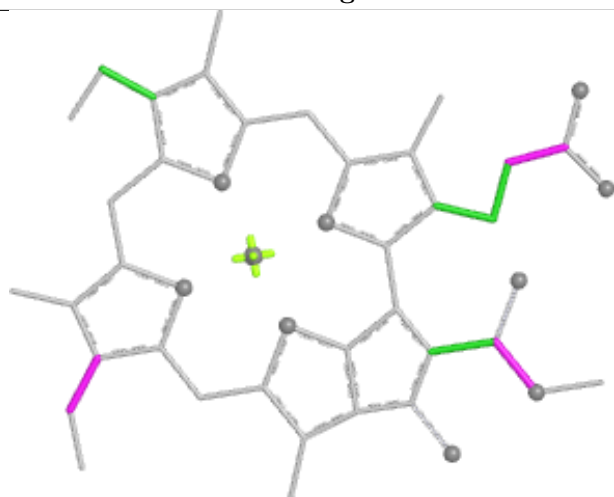
Ligand CLA G 810



Bond lengths



Bond angles

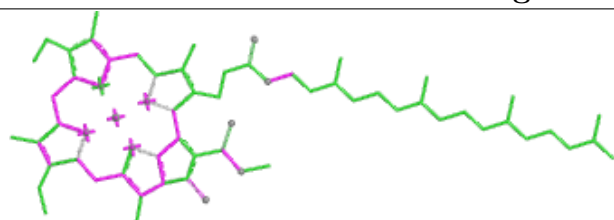


Torsions

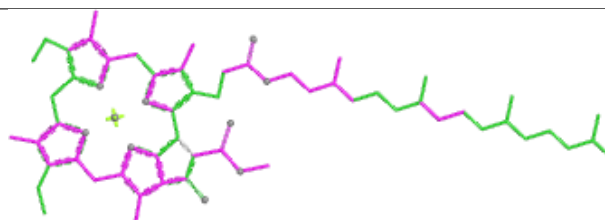


Rings

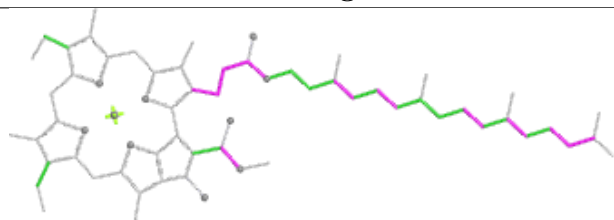
Ligand CLA G 829



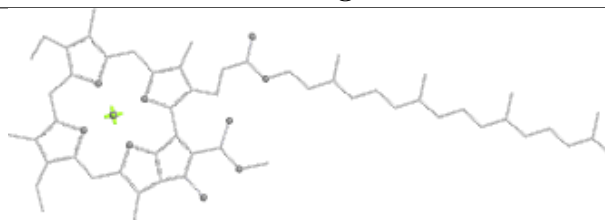
Bond lengths



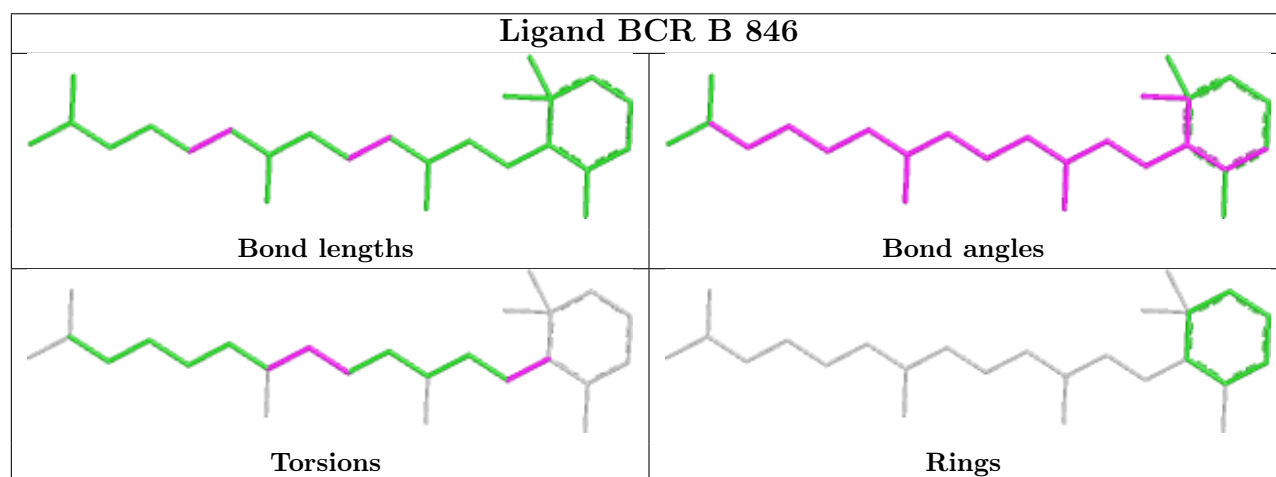
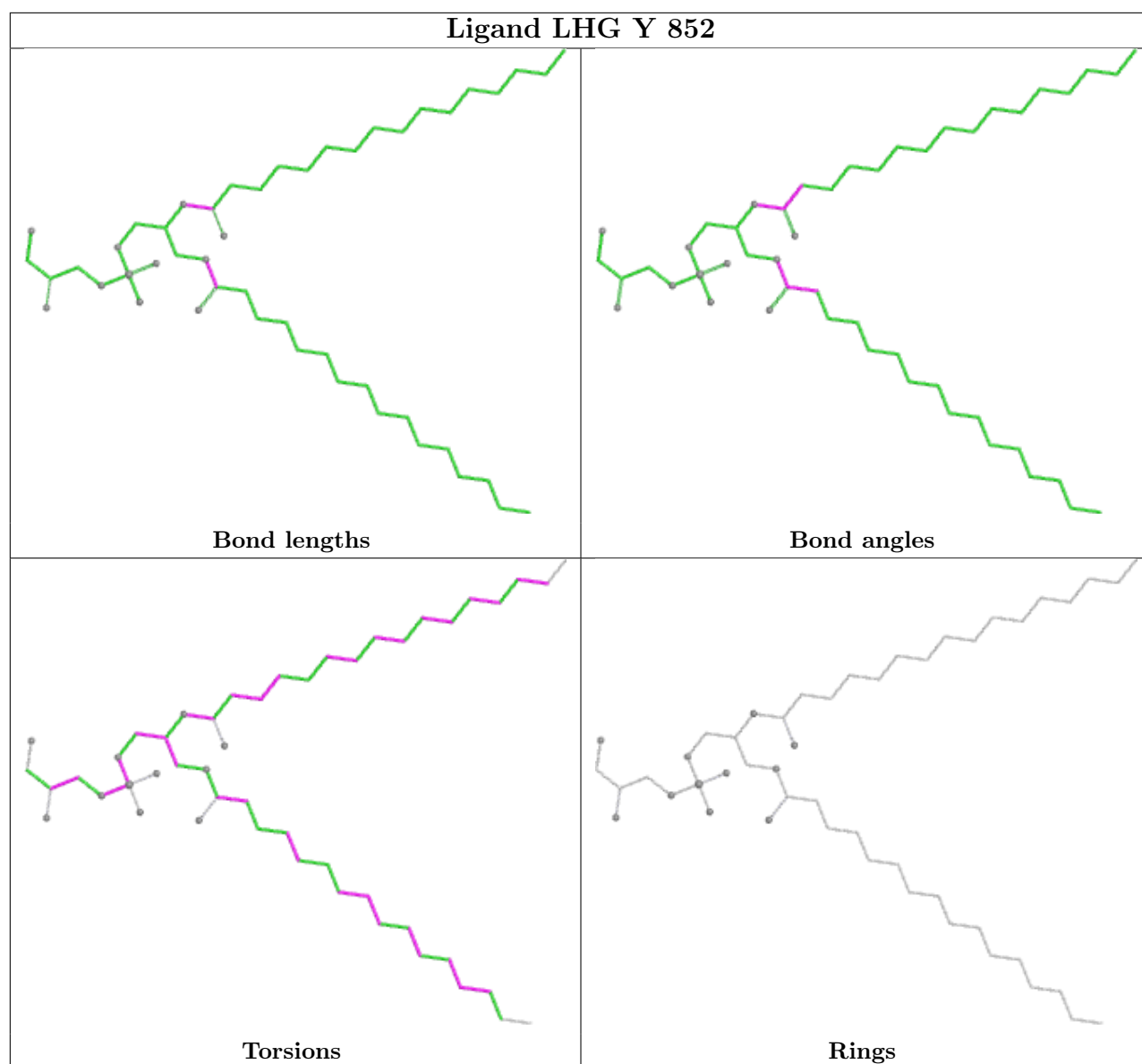
Bond angles



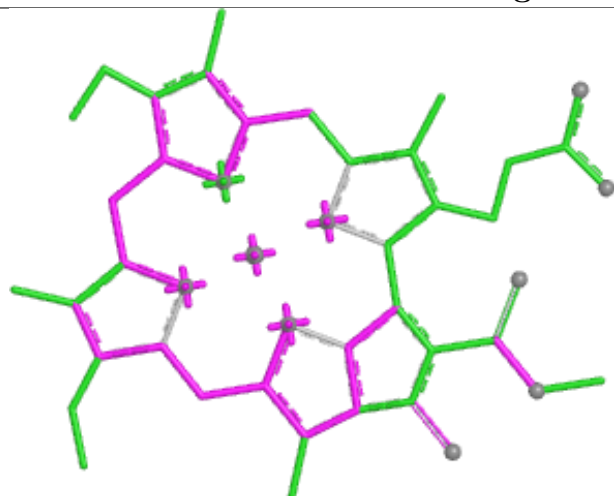
Torsions



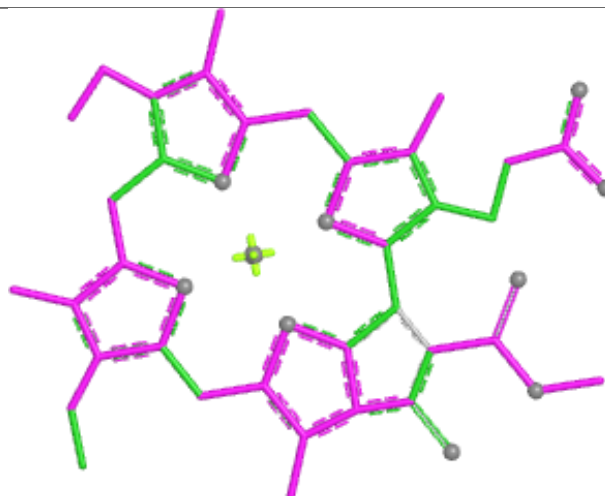
Rings



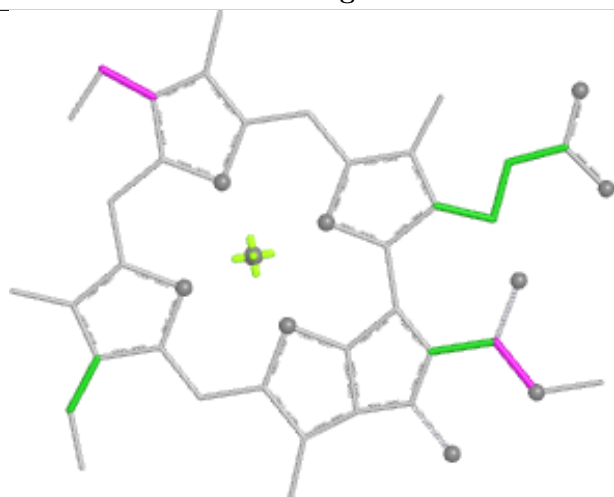
Ligand CLA A 835



Bond lengths



Bond angles

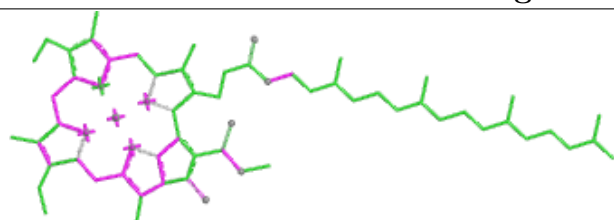


Torsions

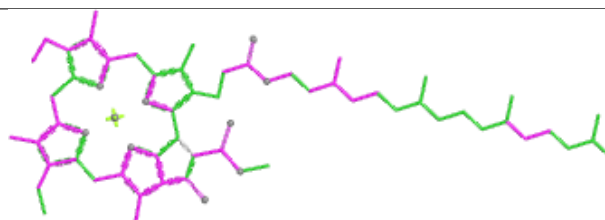


Rings

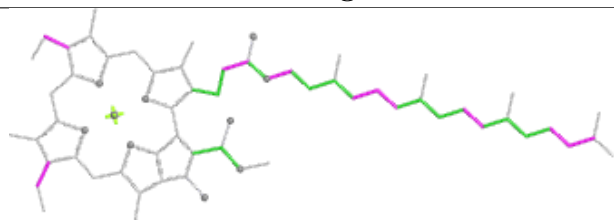
Ligand CLA B 808



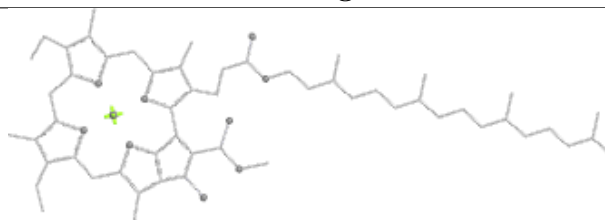
Bond lengths



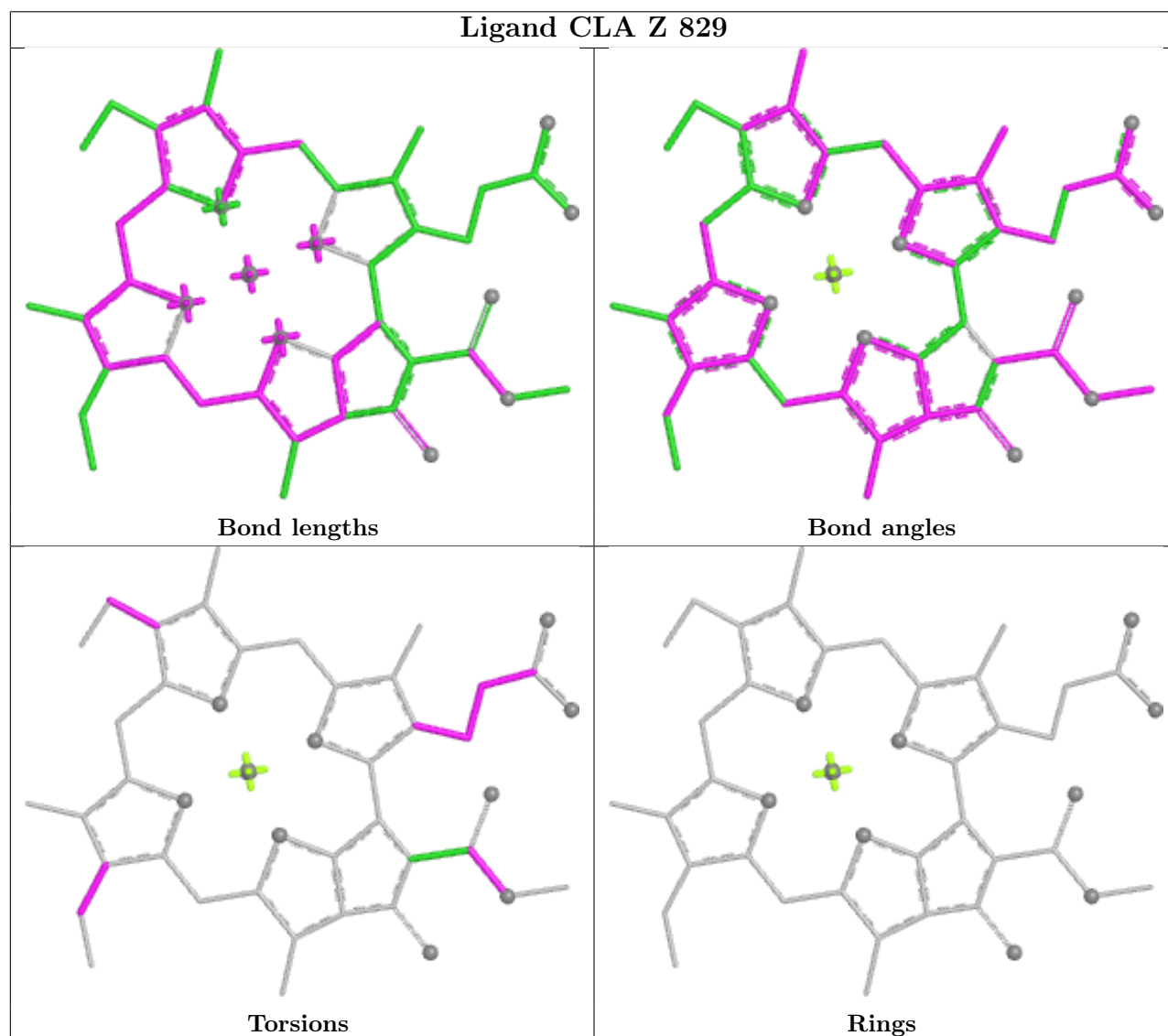
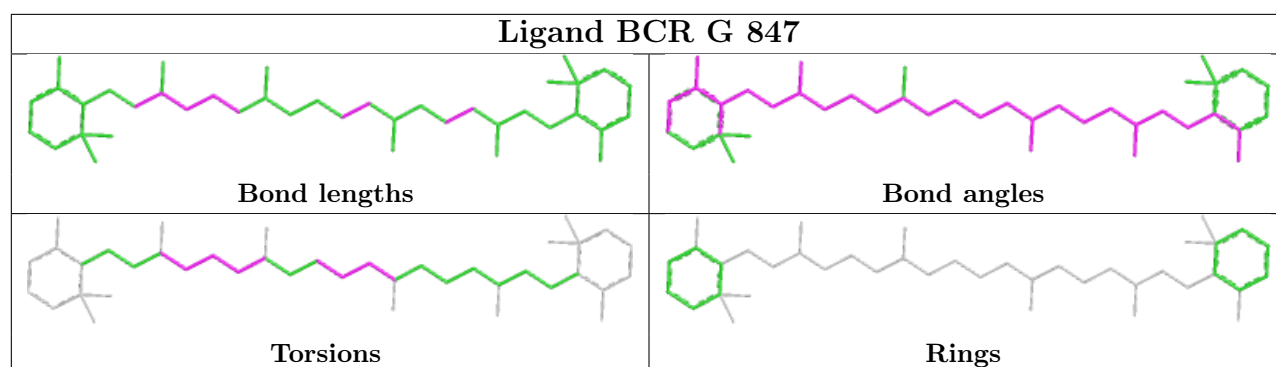
Bond angles



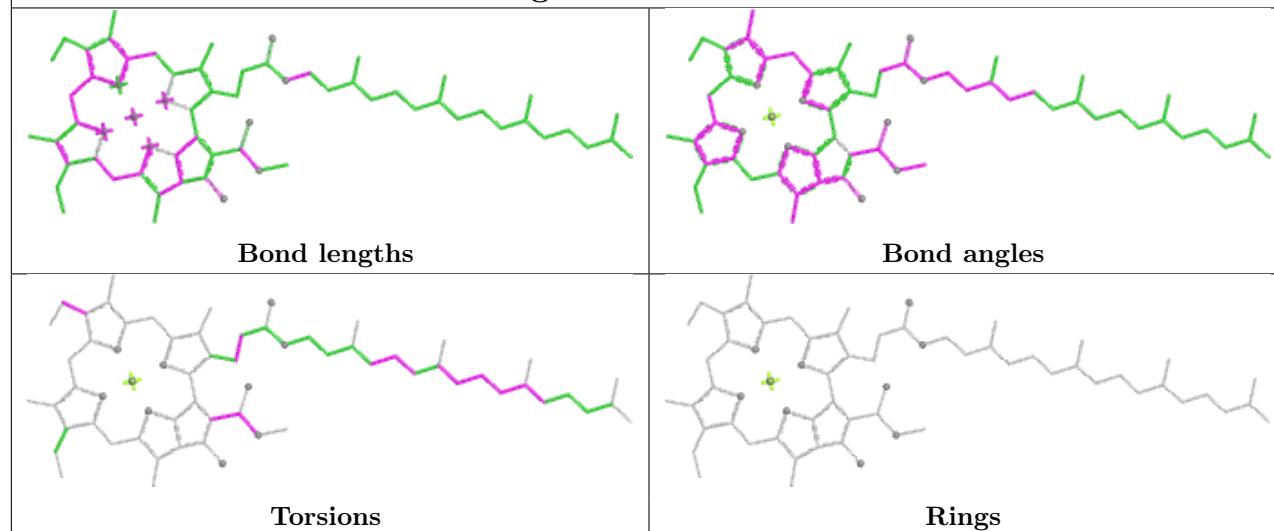
Torsions



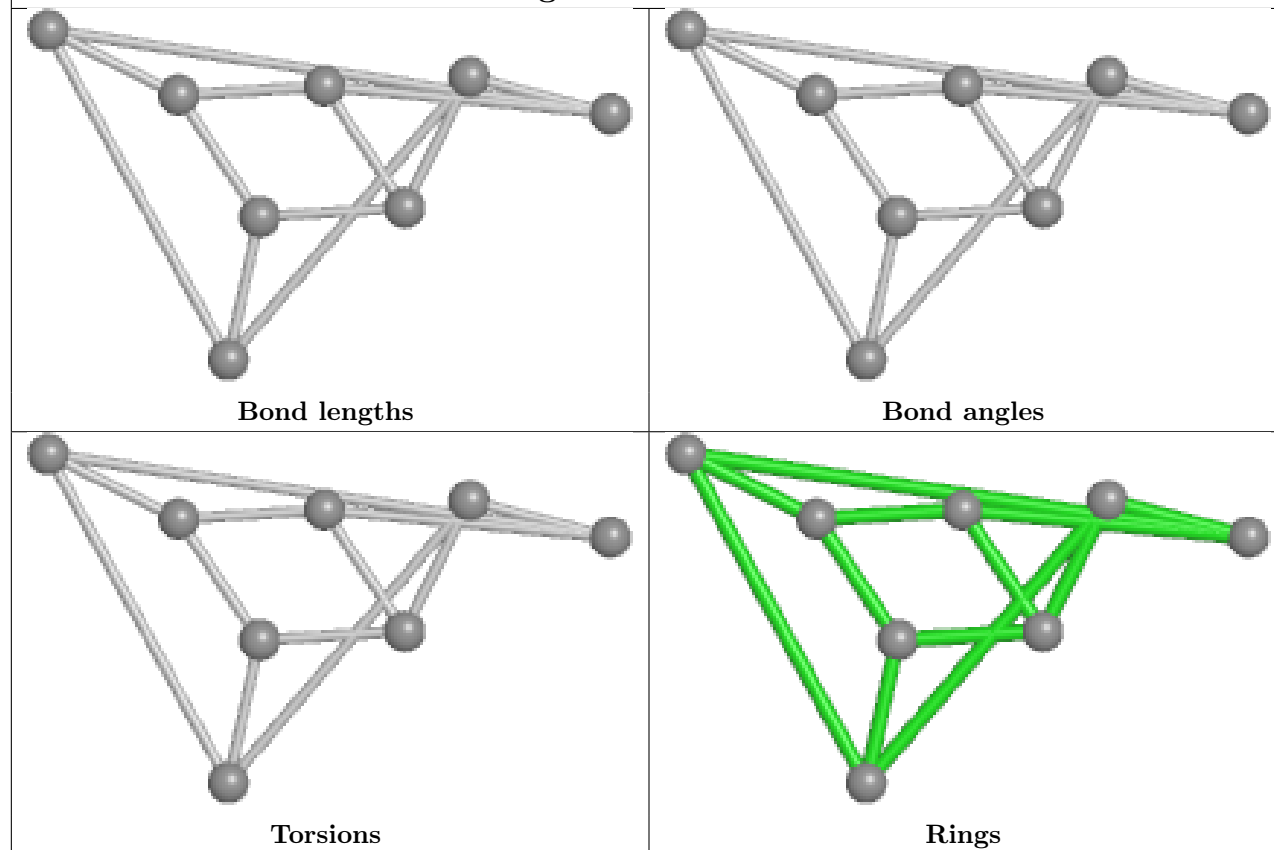
Rings



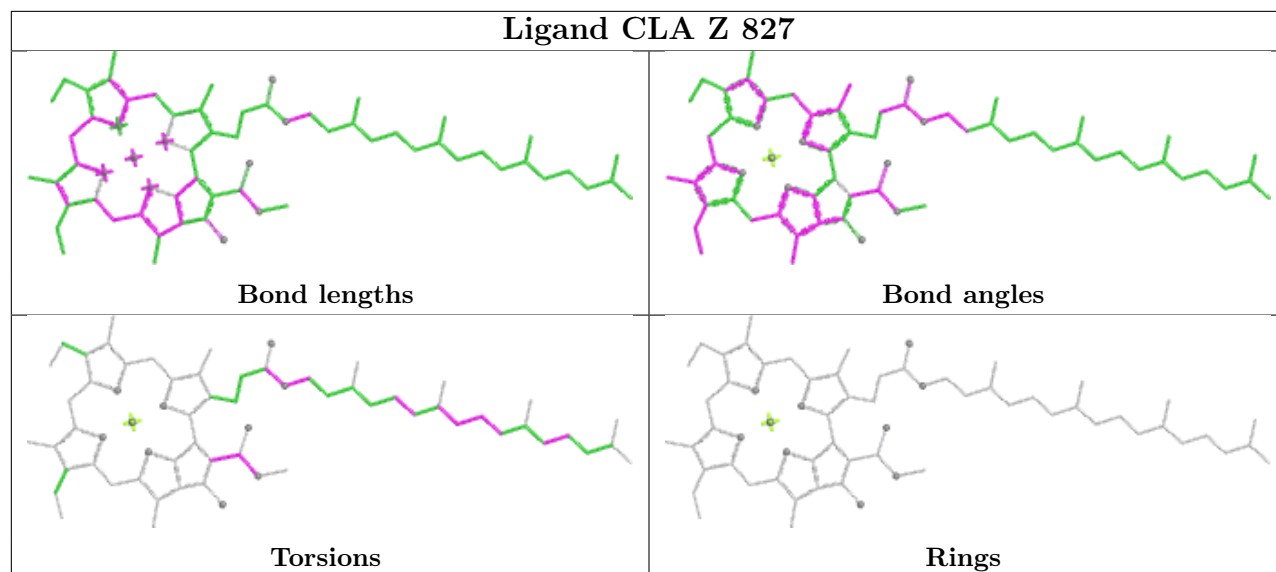
Ligand CLA H 801



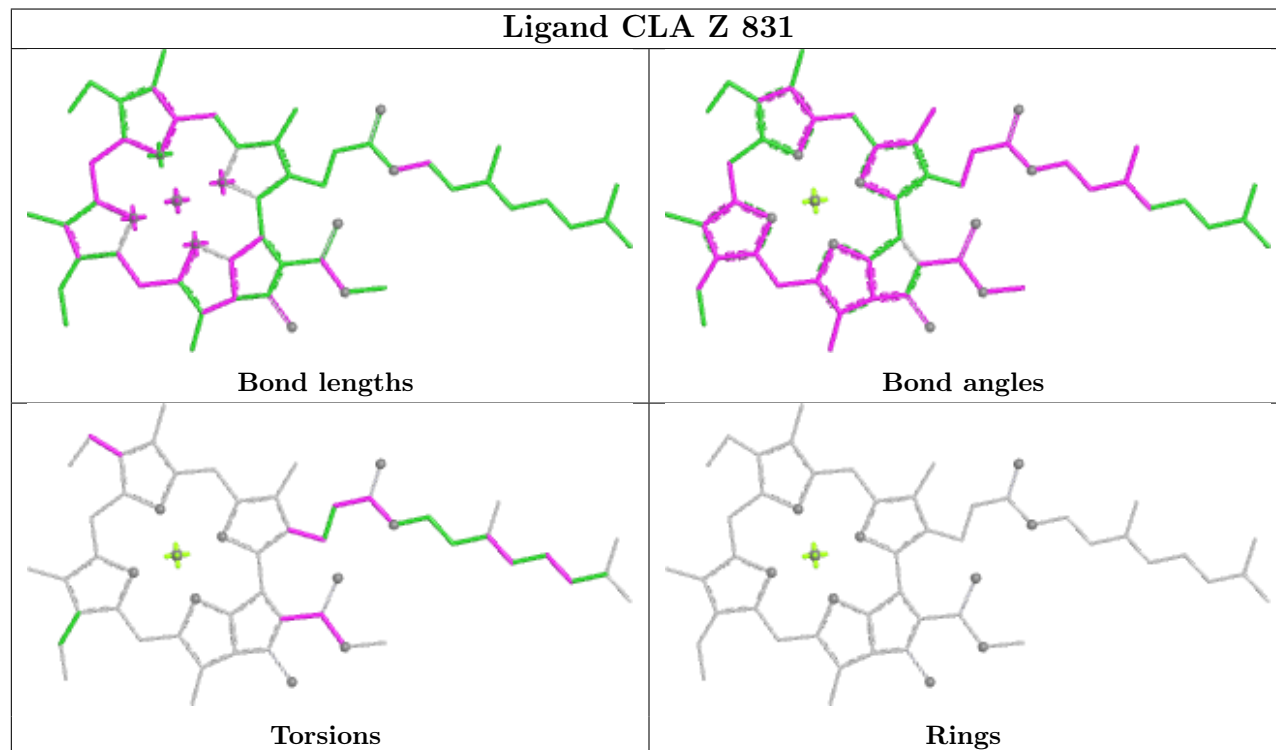
Ligand SF4 Y 845



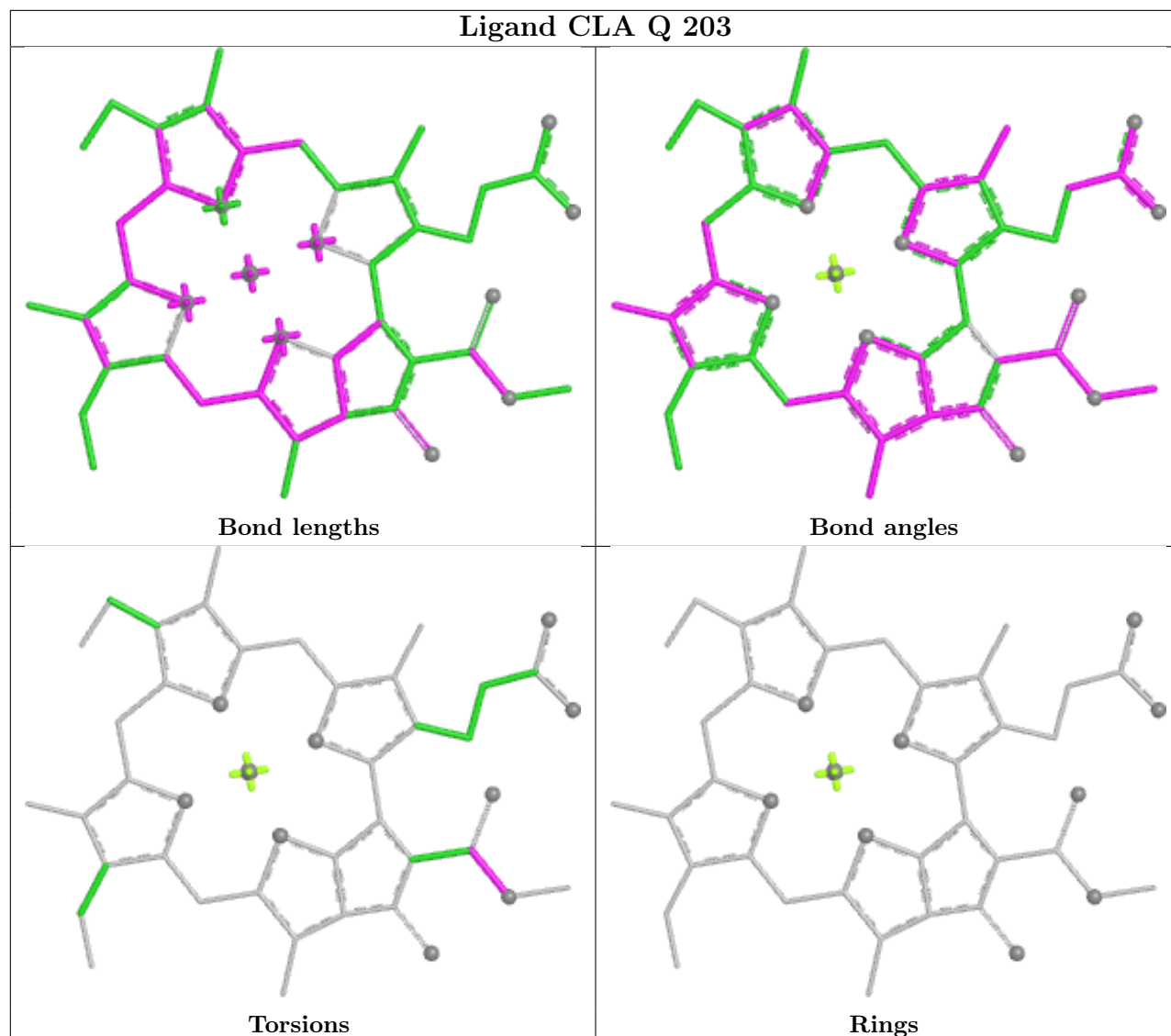
Ligand CLA Z 827

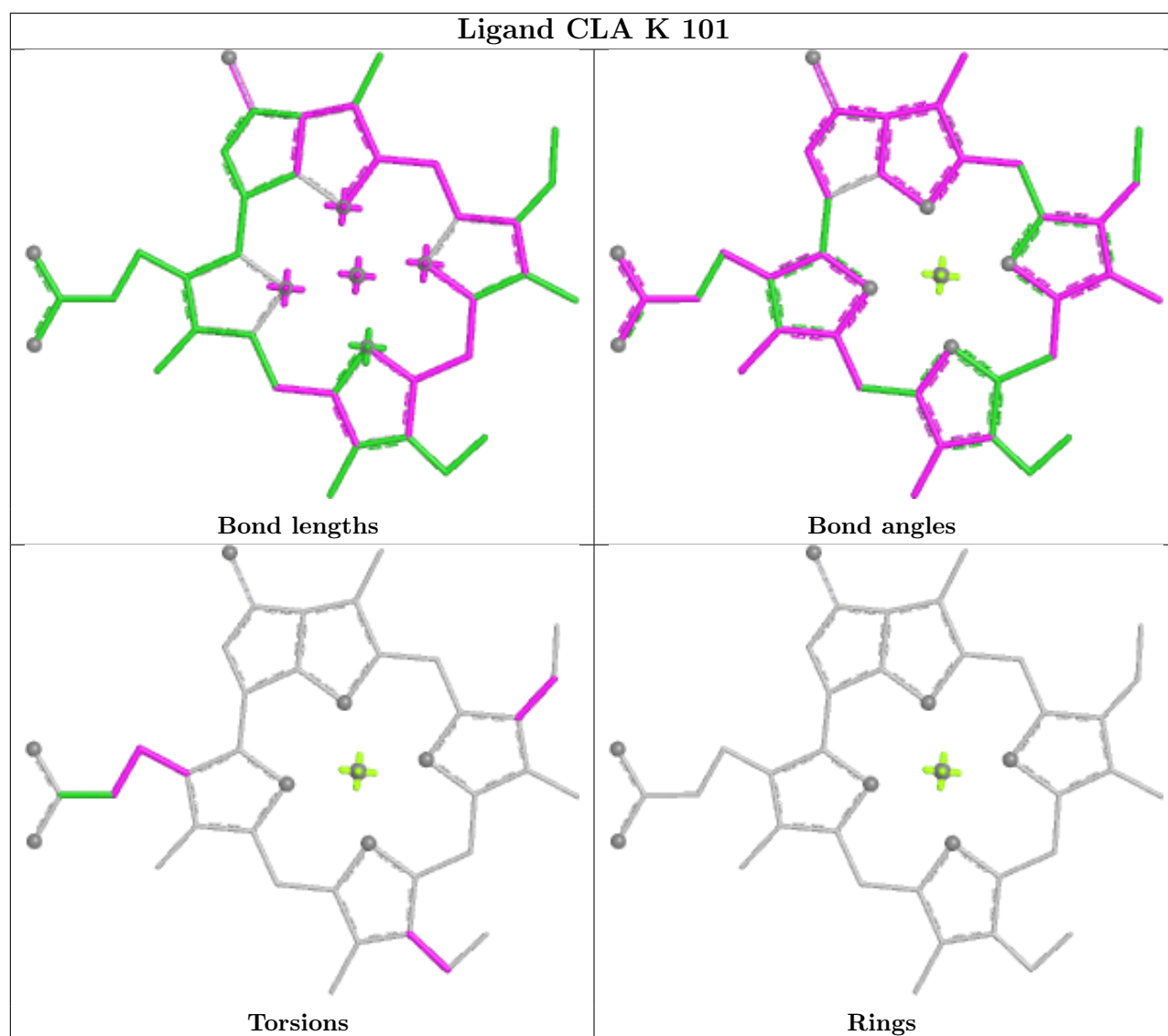


Ligand CLA Z 831

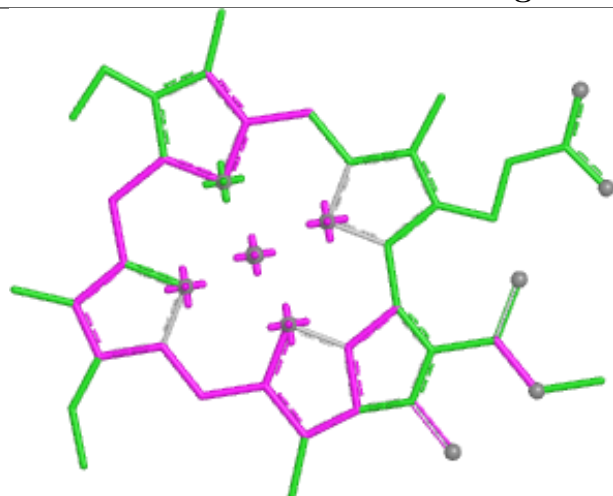


Ligand CLA Q 203

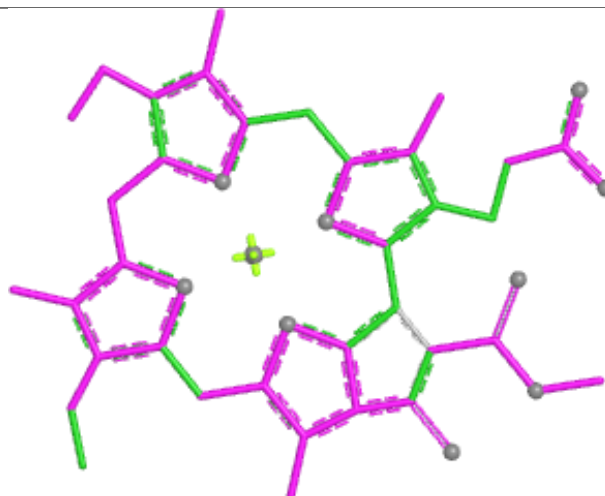




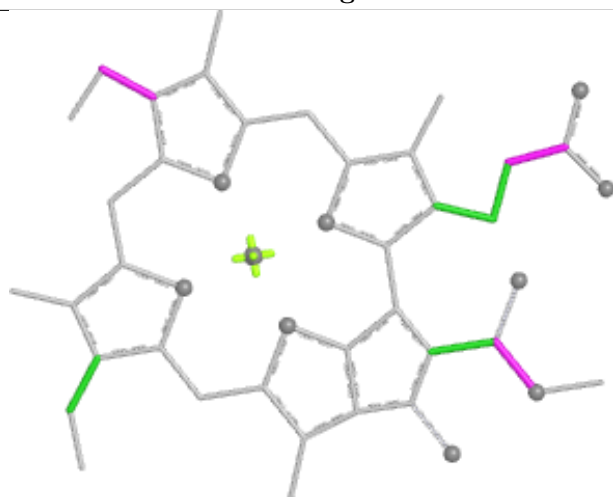
Ligand CLA B 836



Bond lengths



Bond angles

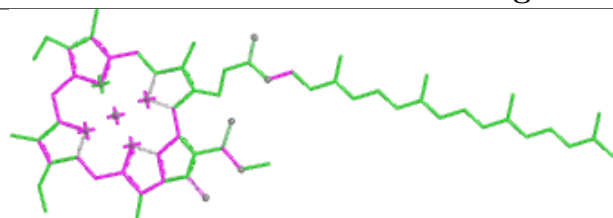


Torsions

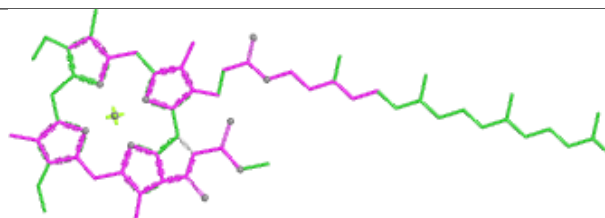


Rings

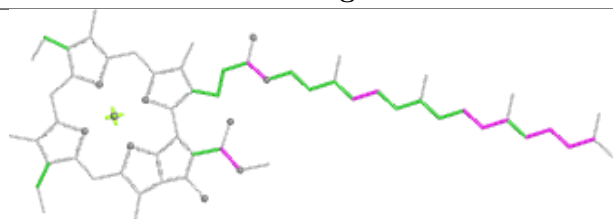
Ligand CLA H 816



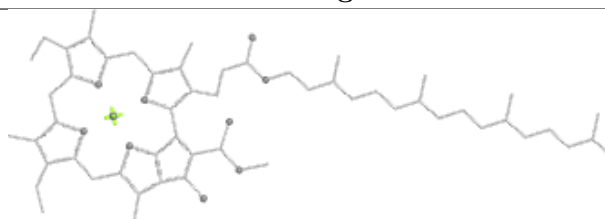
Bond lengths



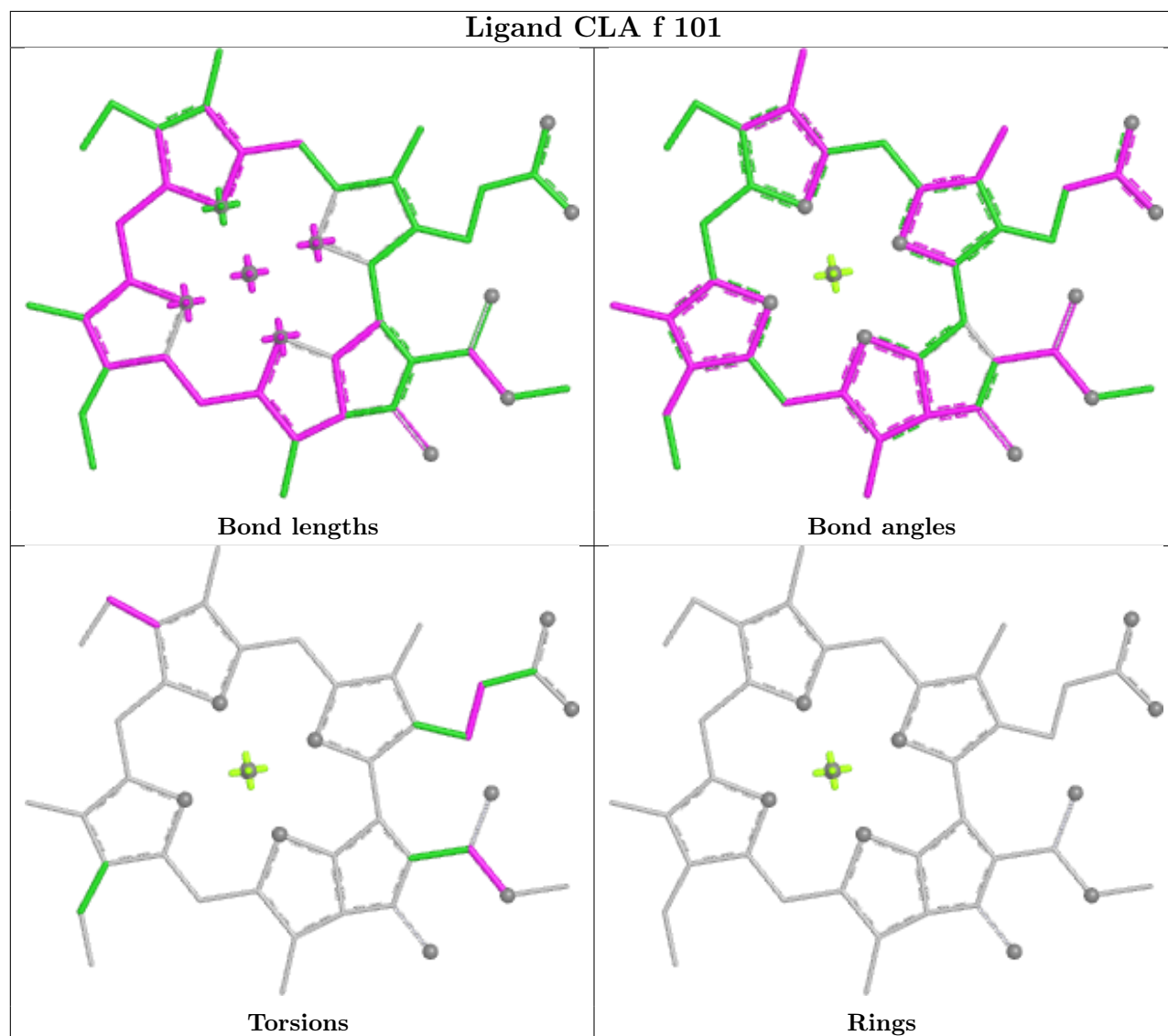
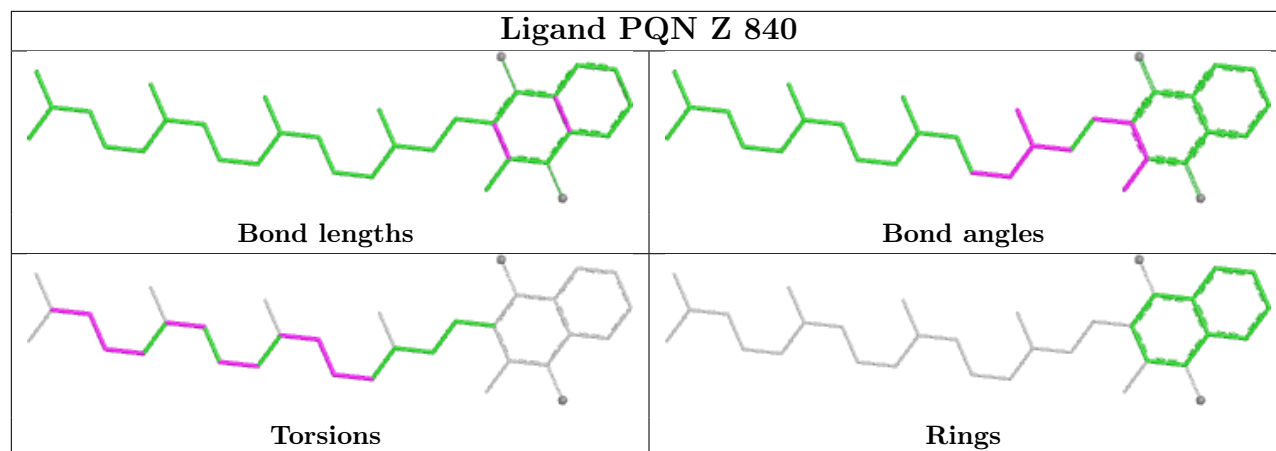
Bond angles



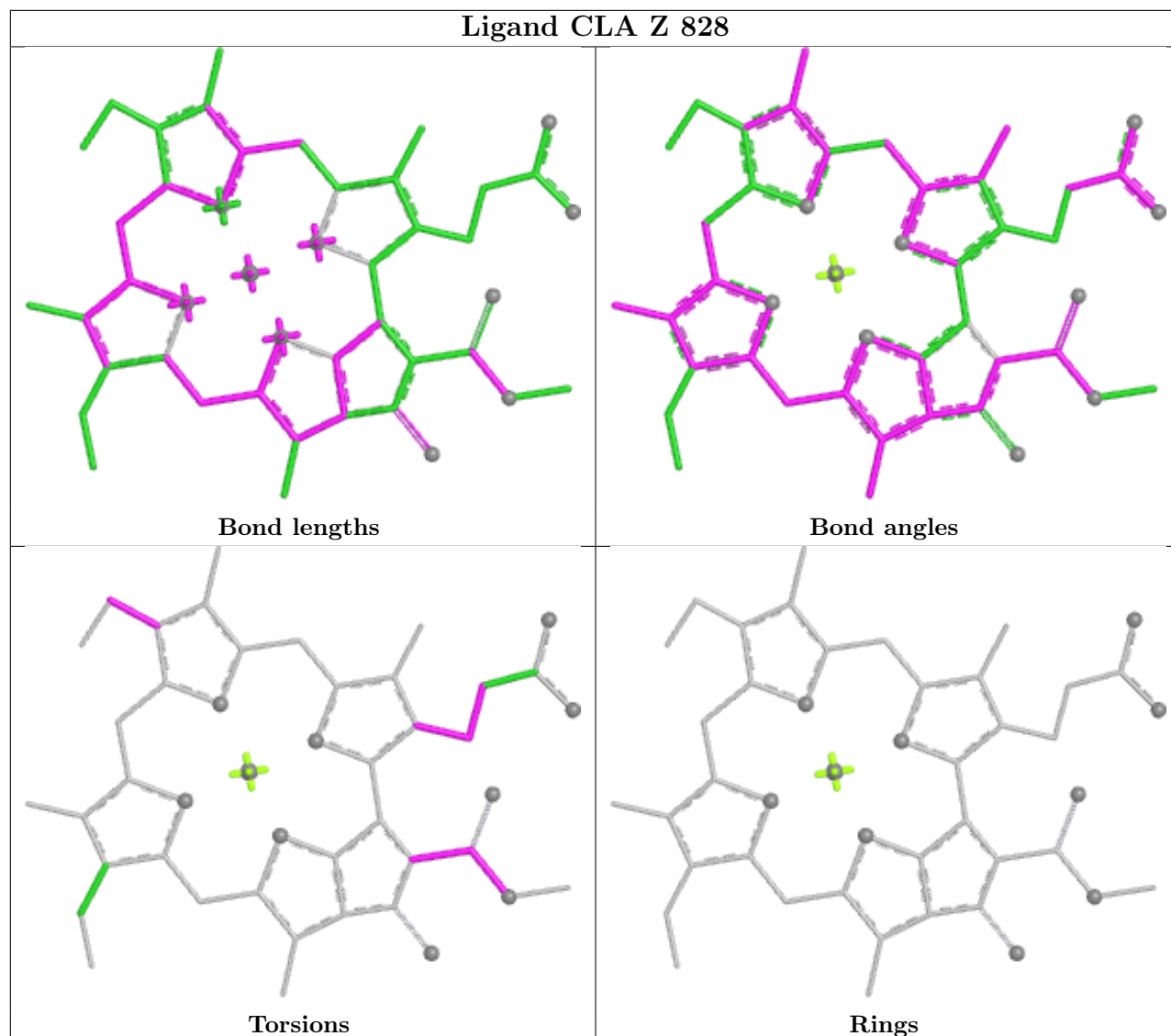
Torsions



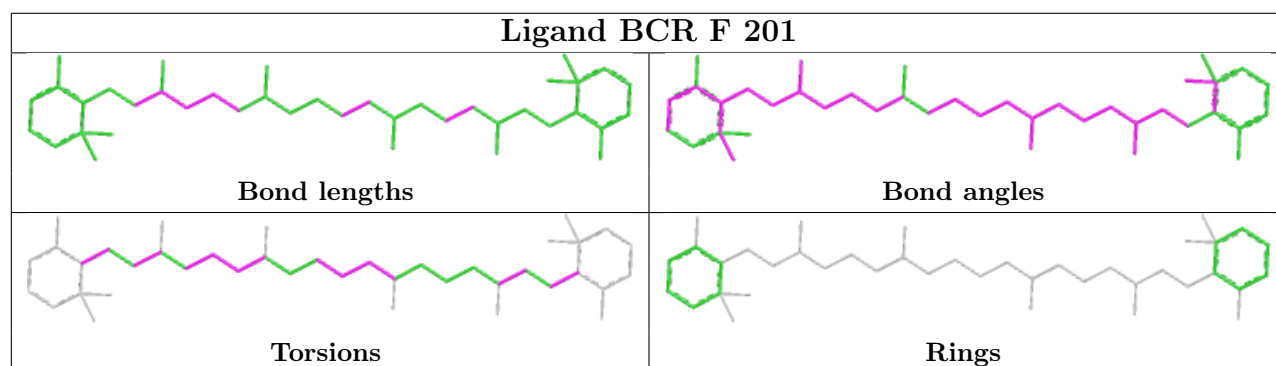
Rings



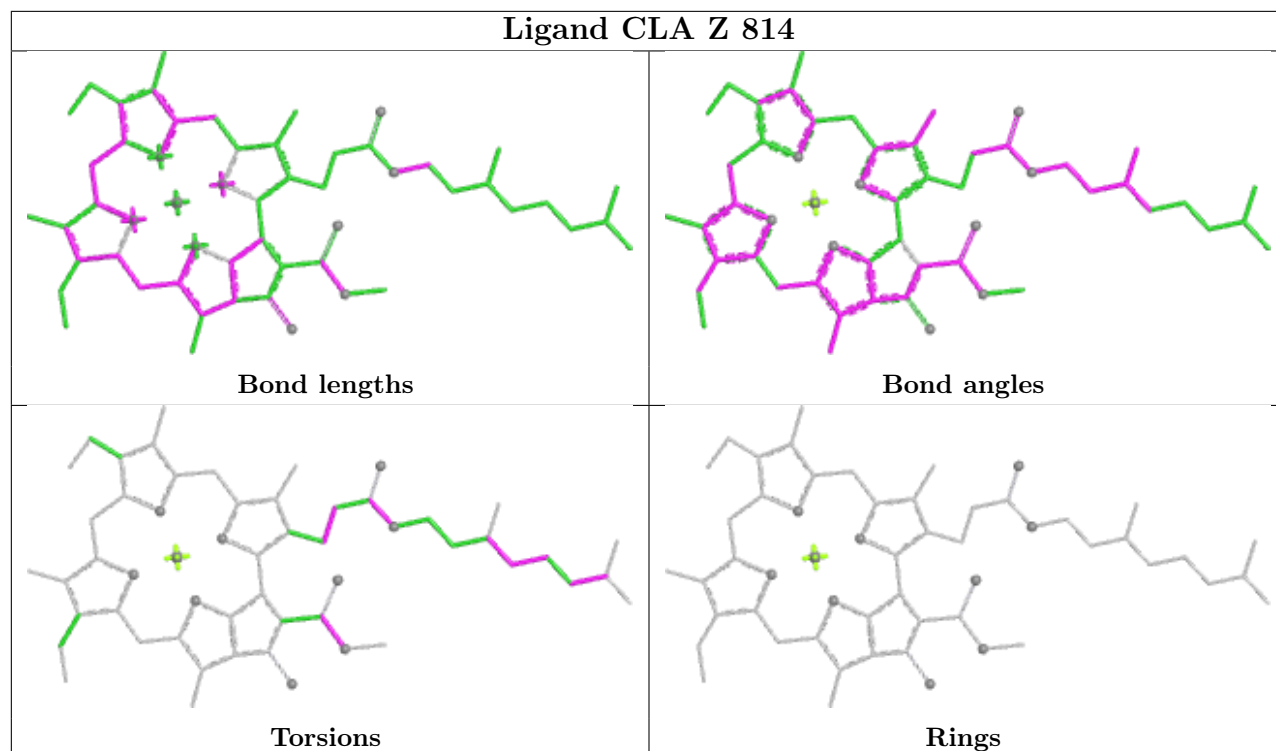
Ligand CLA Z 828



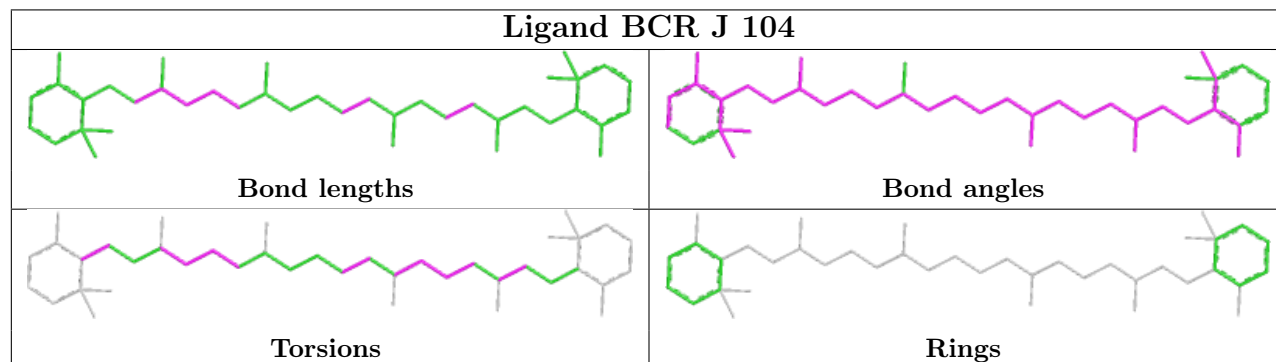
Ligand BCR F 201

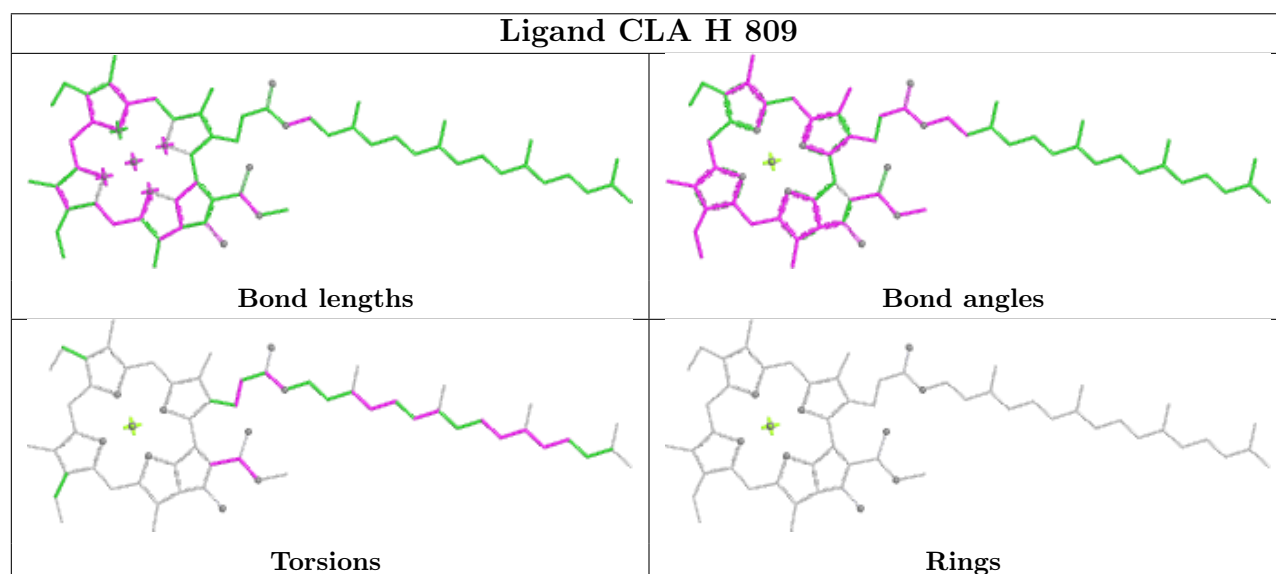
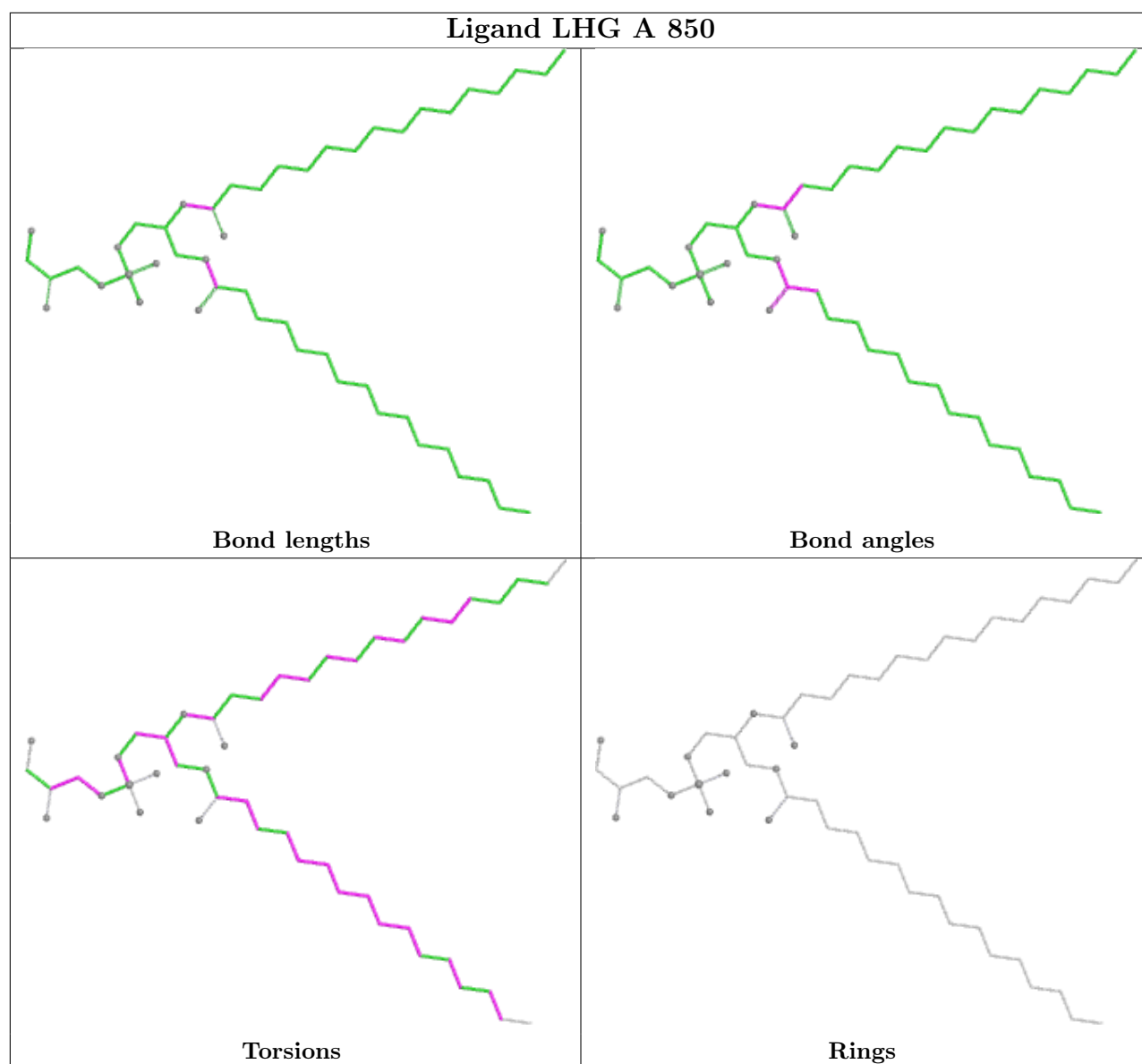


Ligand CLA Z 814

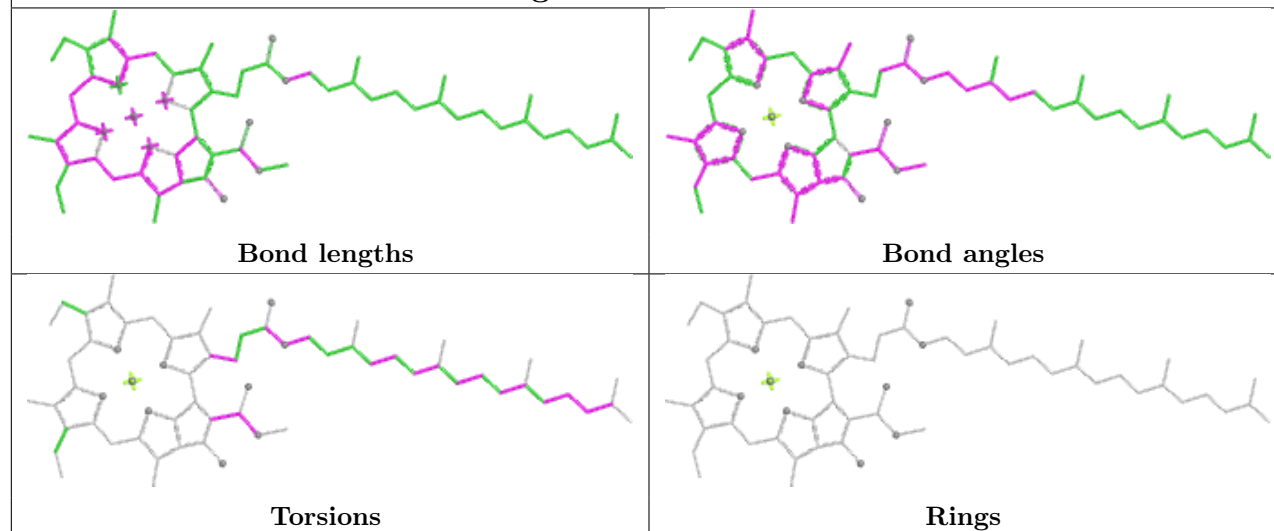


Ligand BCR J 104

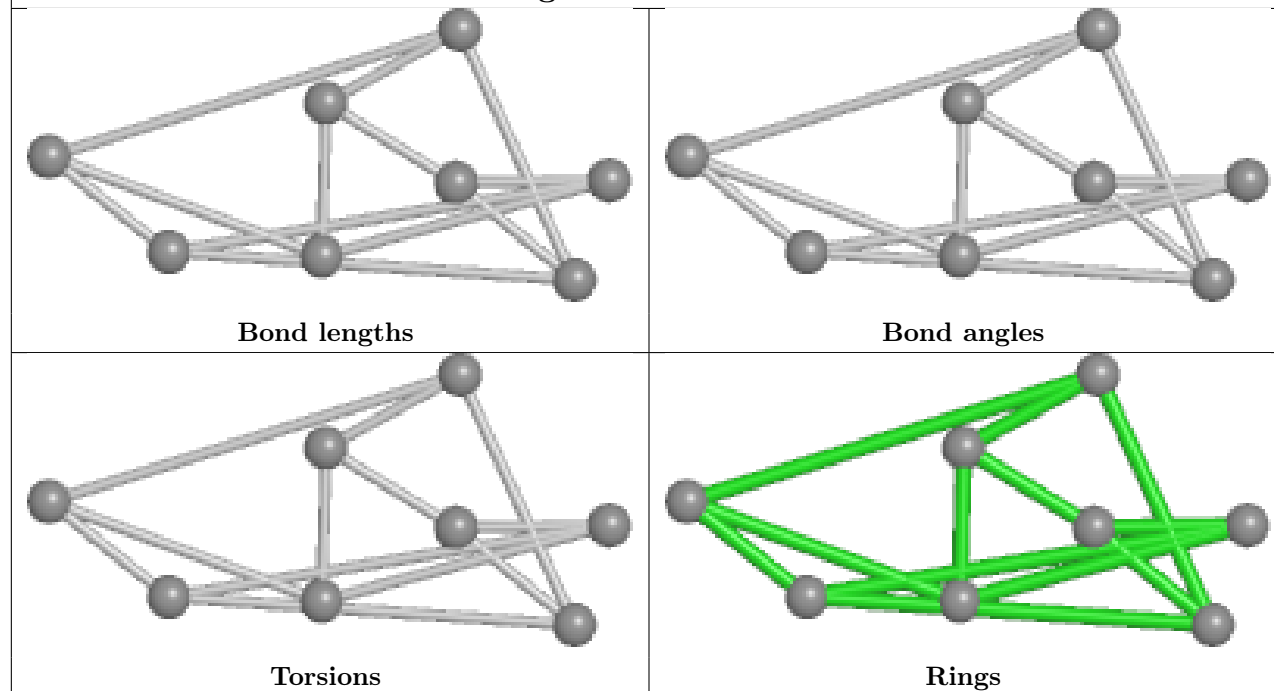




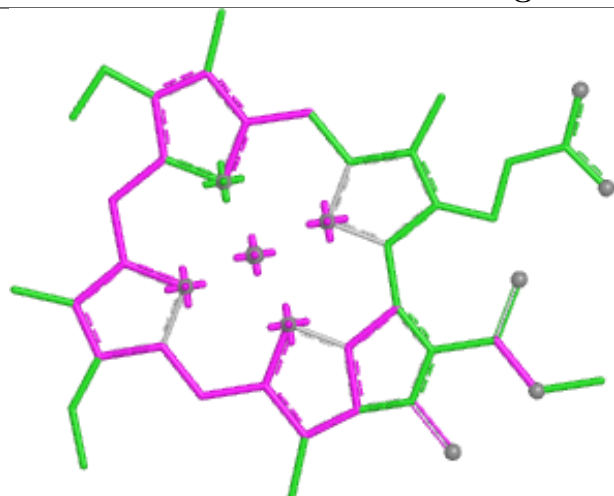
Ligand CLA A 803



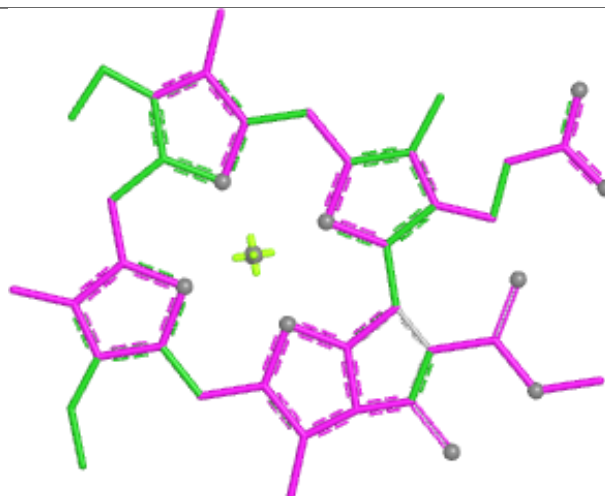
Ligand SF4 N 101



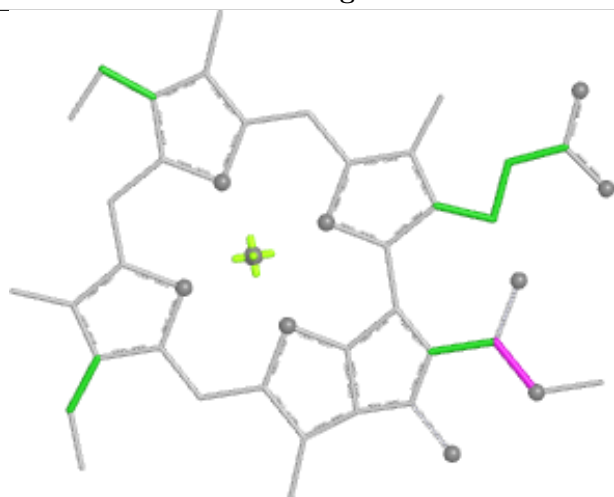
Ligand CLA B 834



Bond lengths



Bond angles

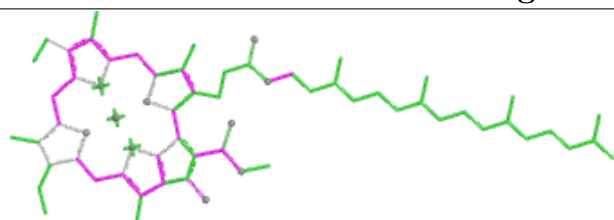


Torsions

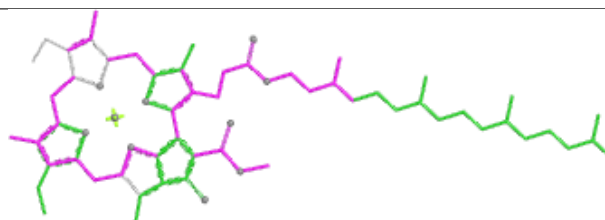


Rings

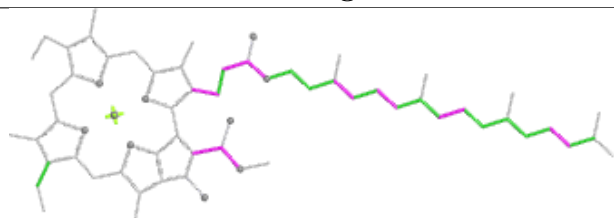
Ligand CL0 G 801



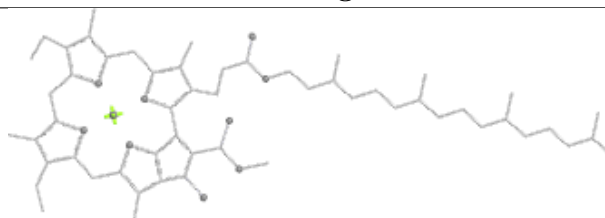
Bond lengths



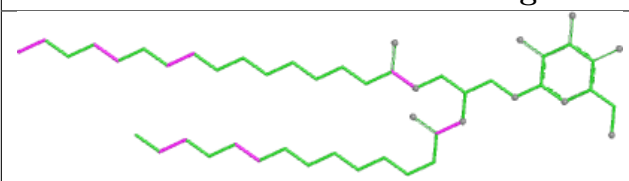
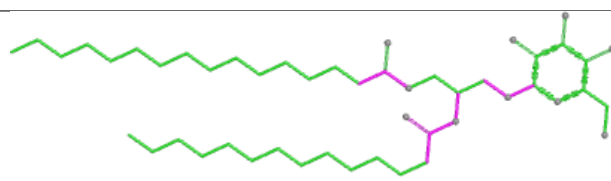
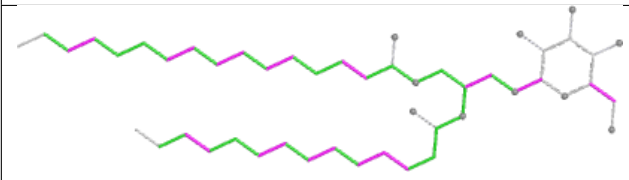
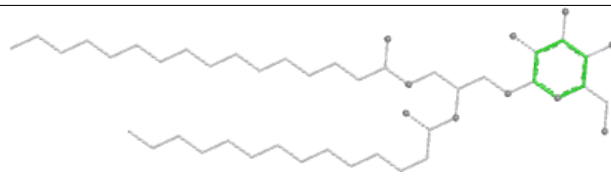
Bond angles

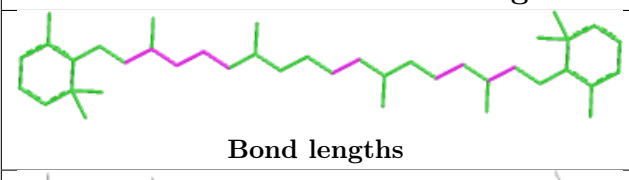
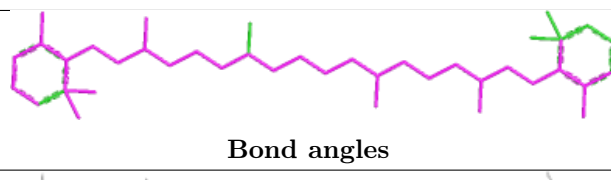
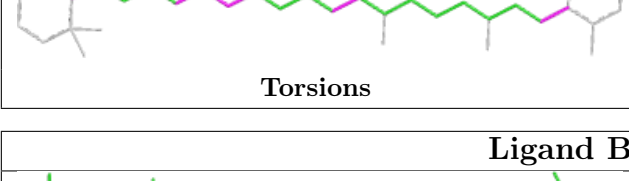
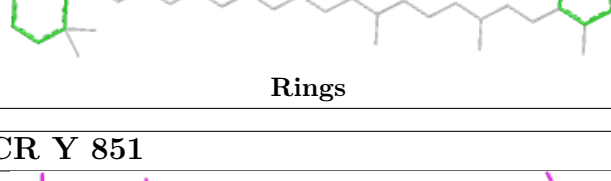


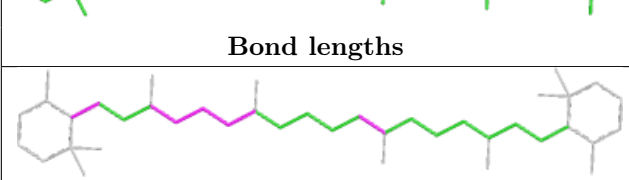
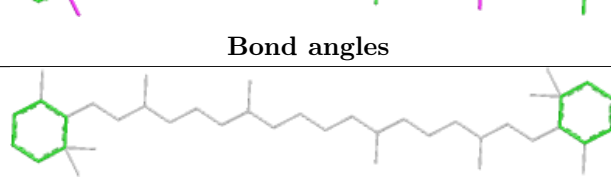
Torsions



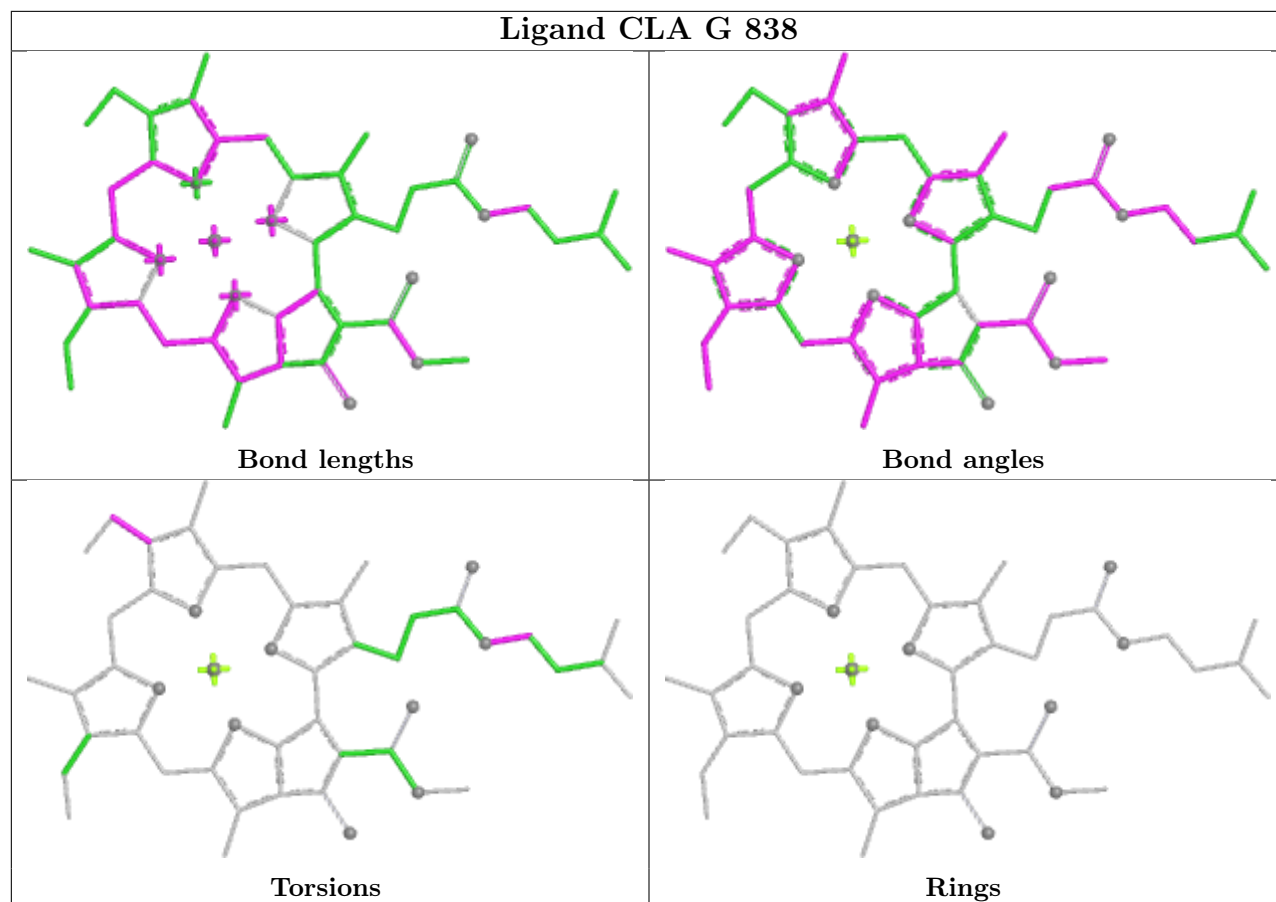
Rings

Ligand LMG Z 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

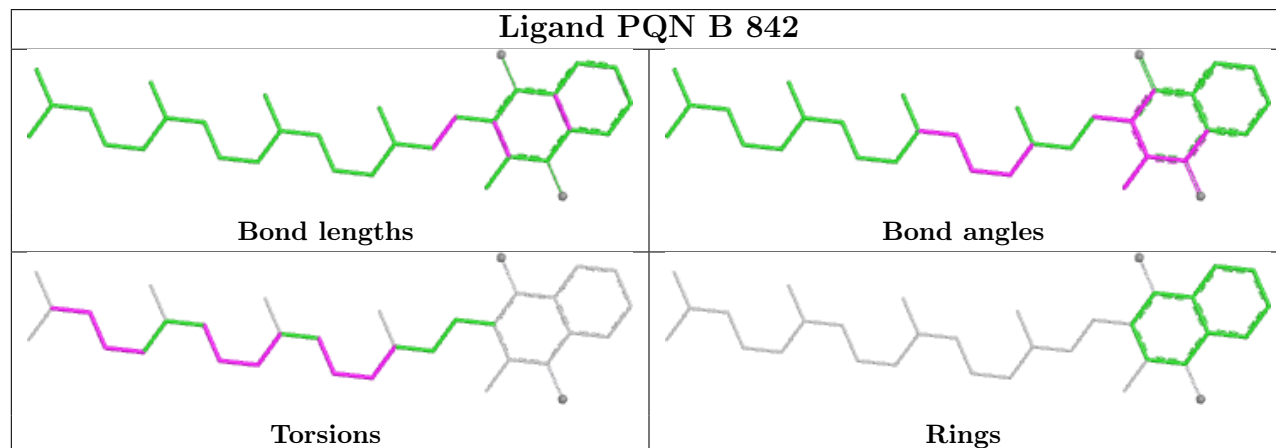
Ligand BCR V 1202	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR Y 851	
	
Bond lengths	Bond angles
Torsions	Rings

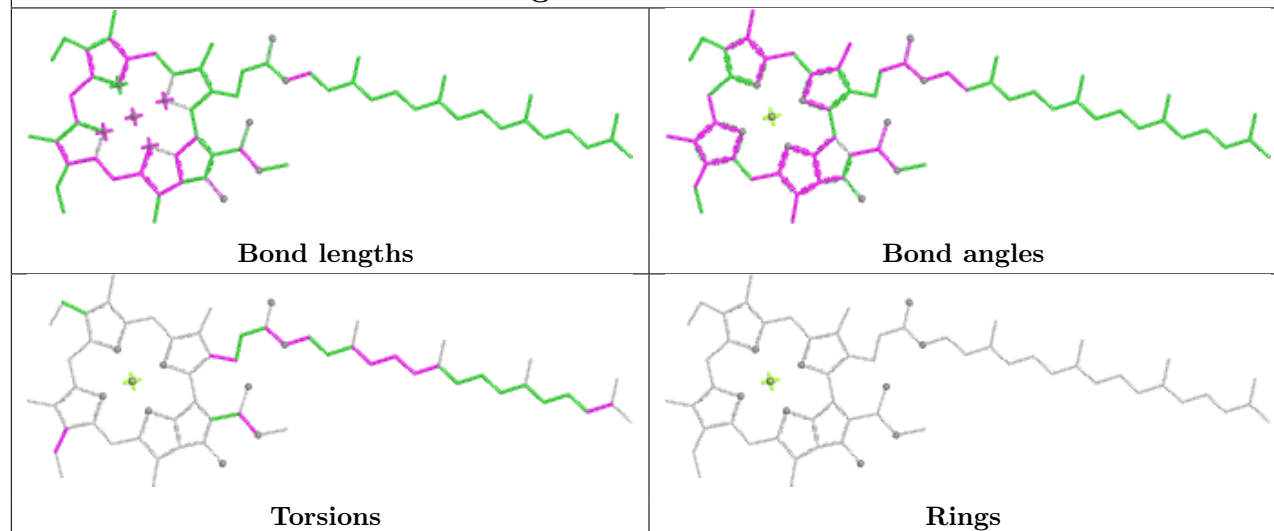
Ligand CLA G 838



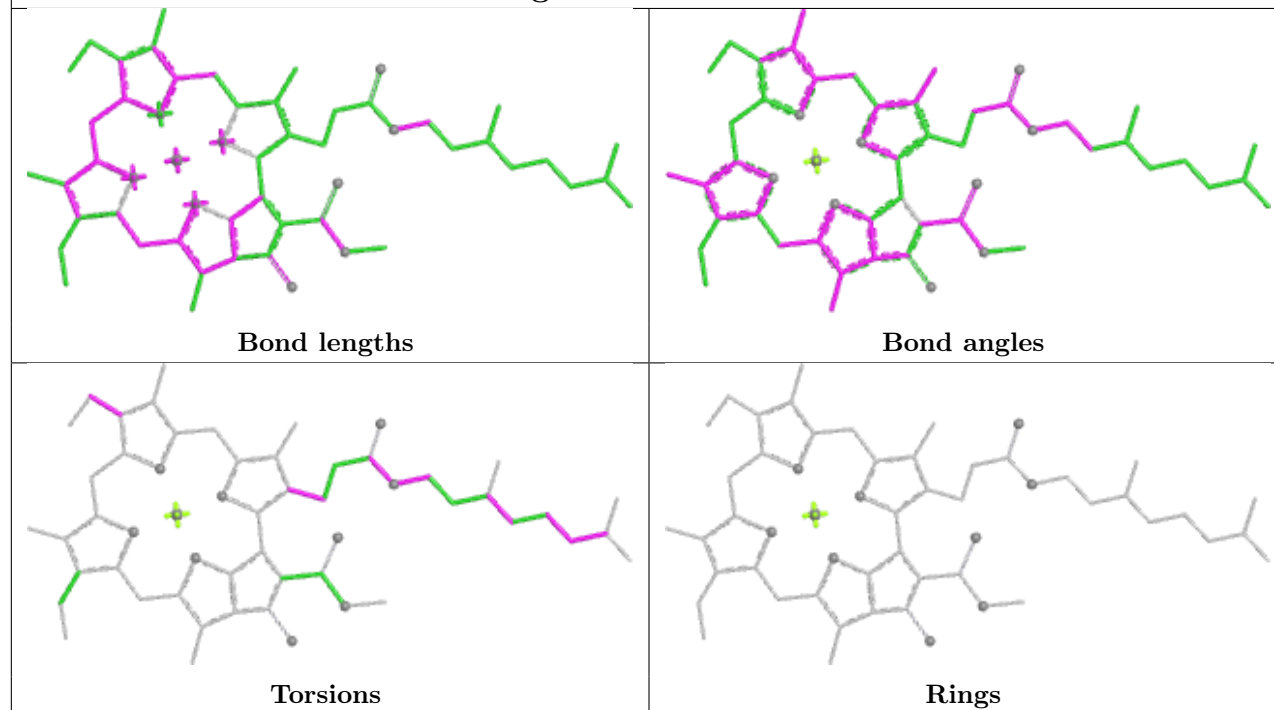
Ligand PQN B 842



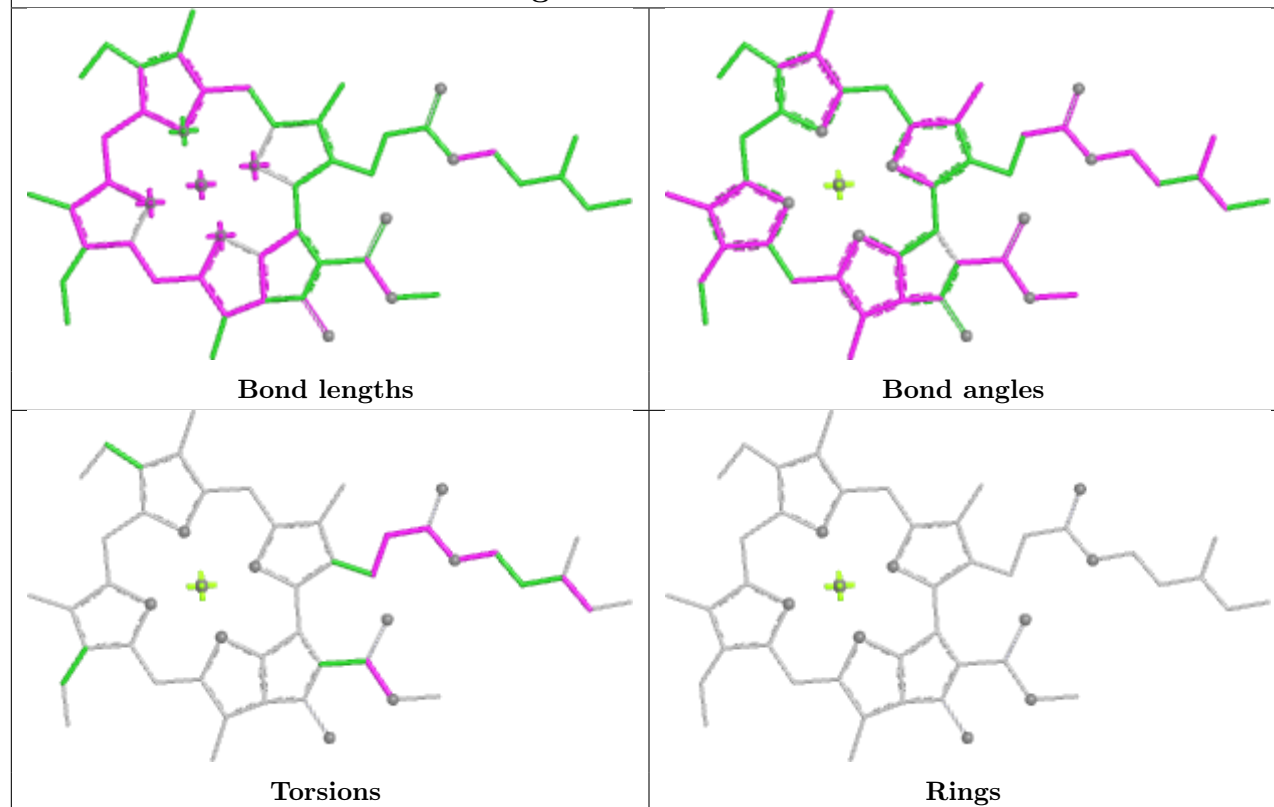
Ligand CLA Y 803



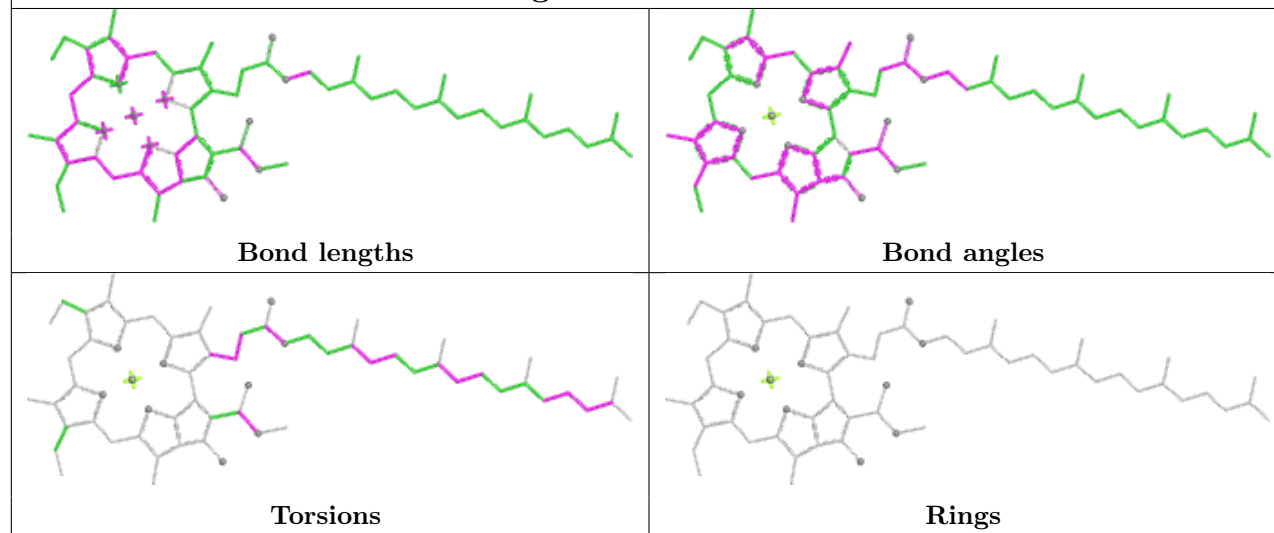
Ligand CLA Y 814



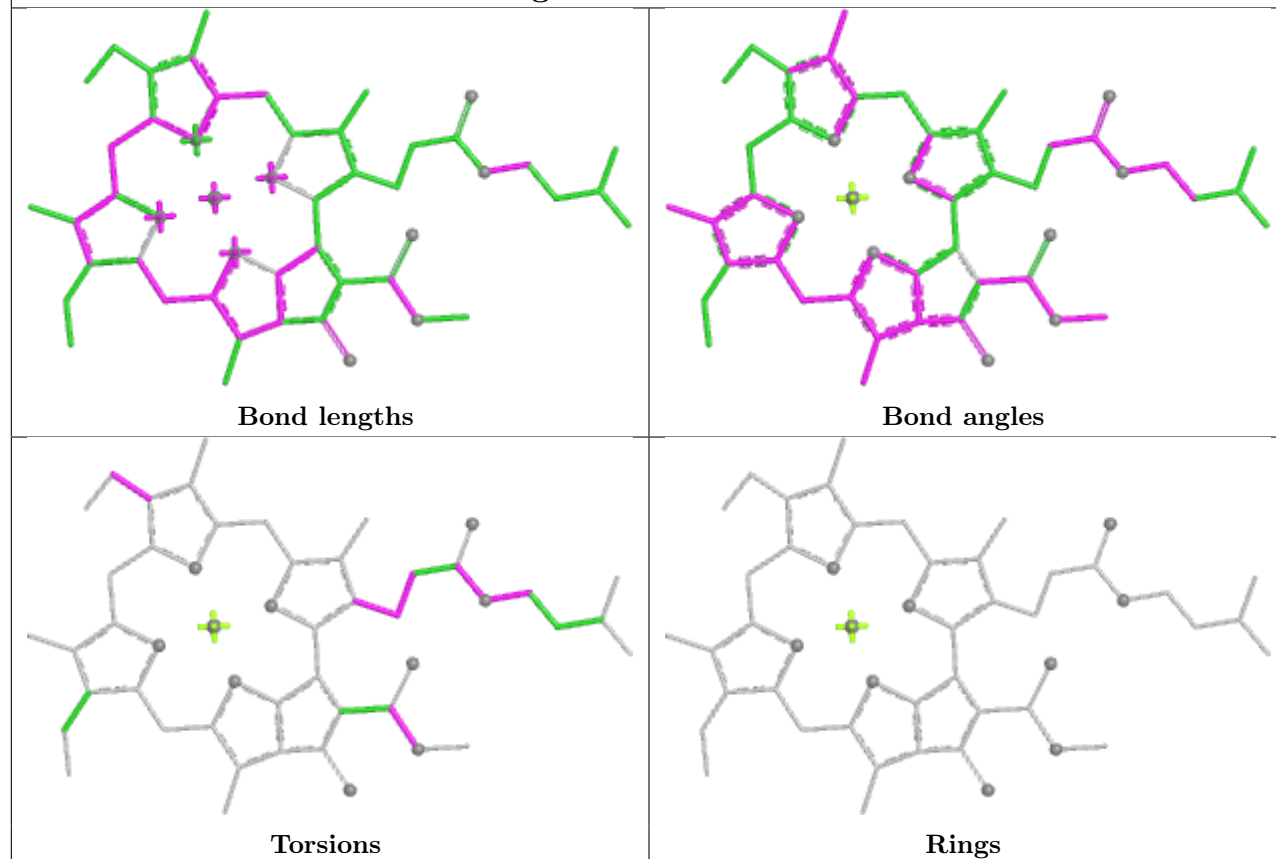
Ligand CLA Y 807



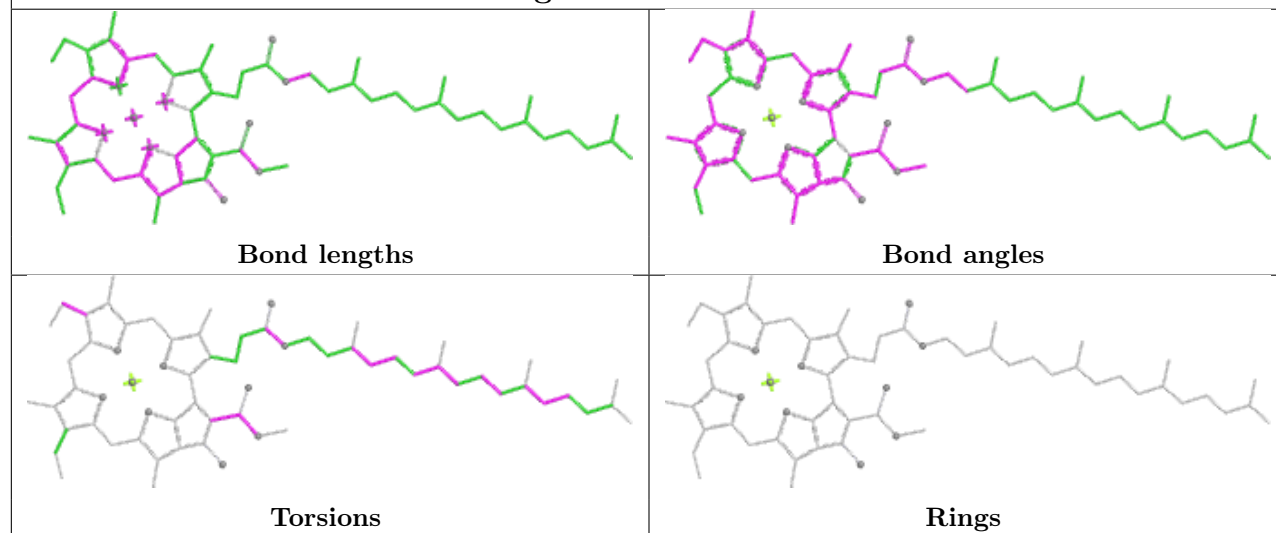
Ligand CLA Y 821



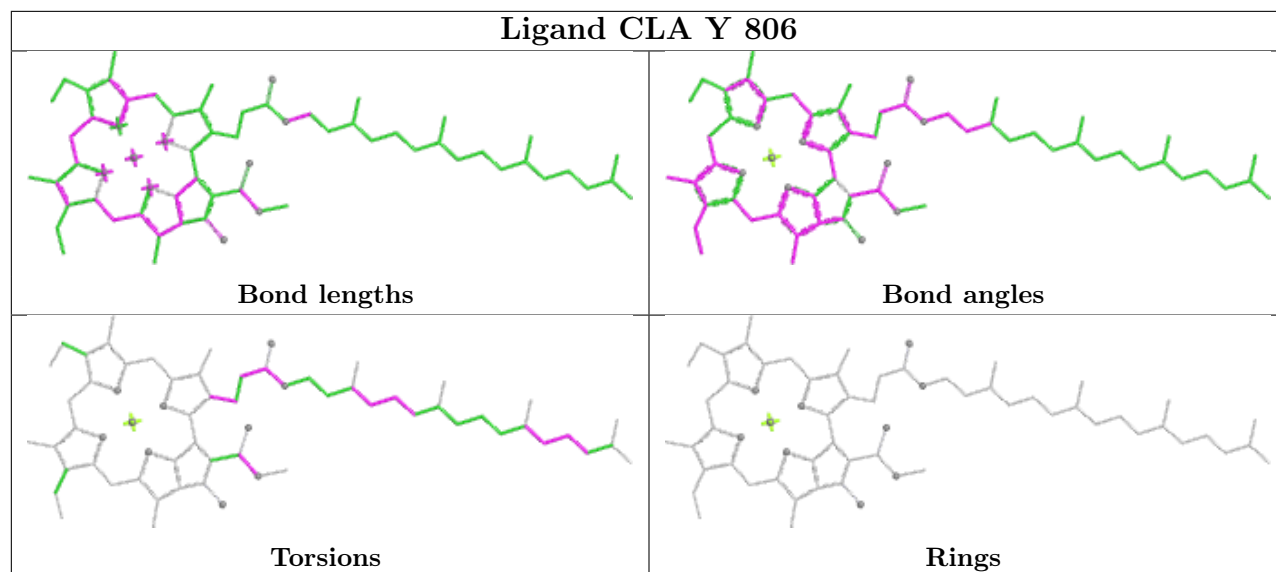
Ligand CLA A 842



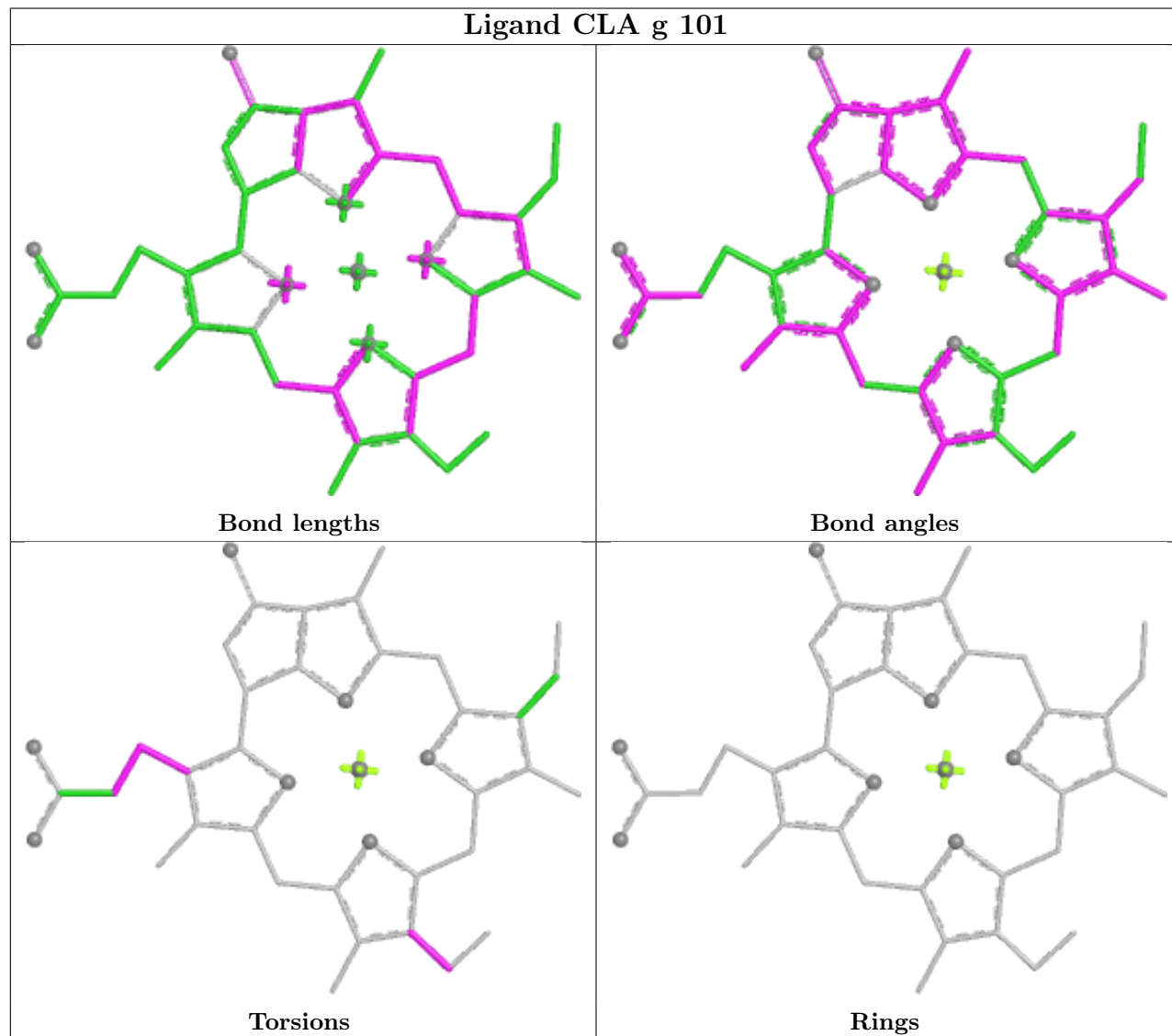
Ligand CLA L 202

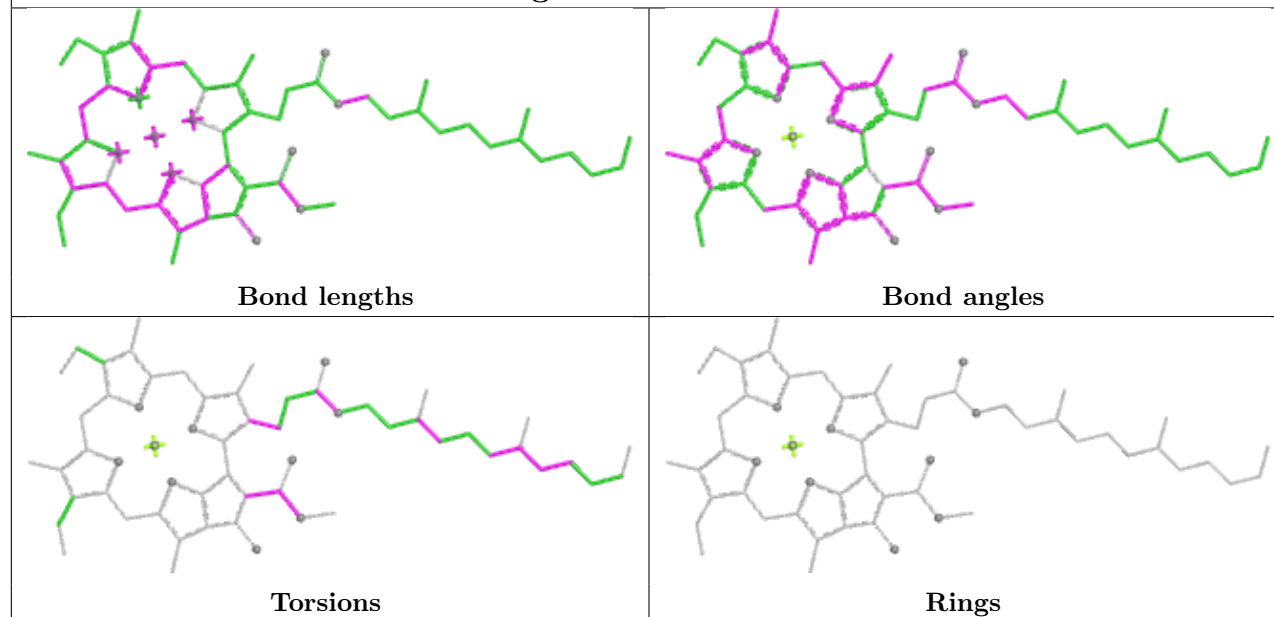
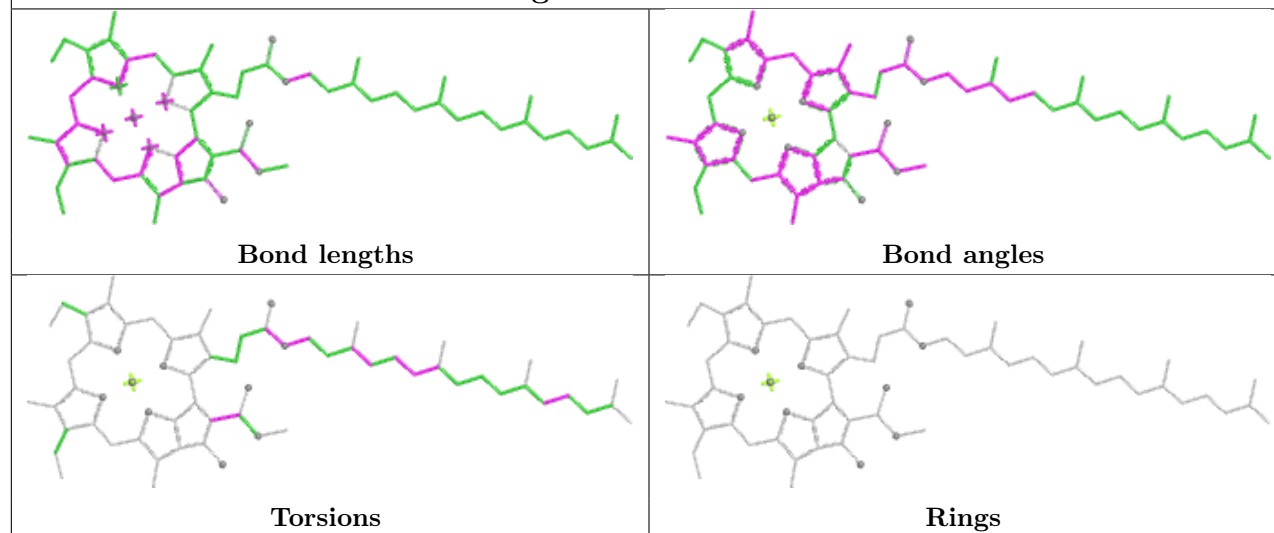


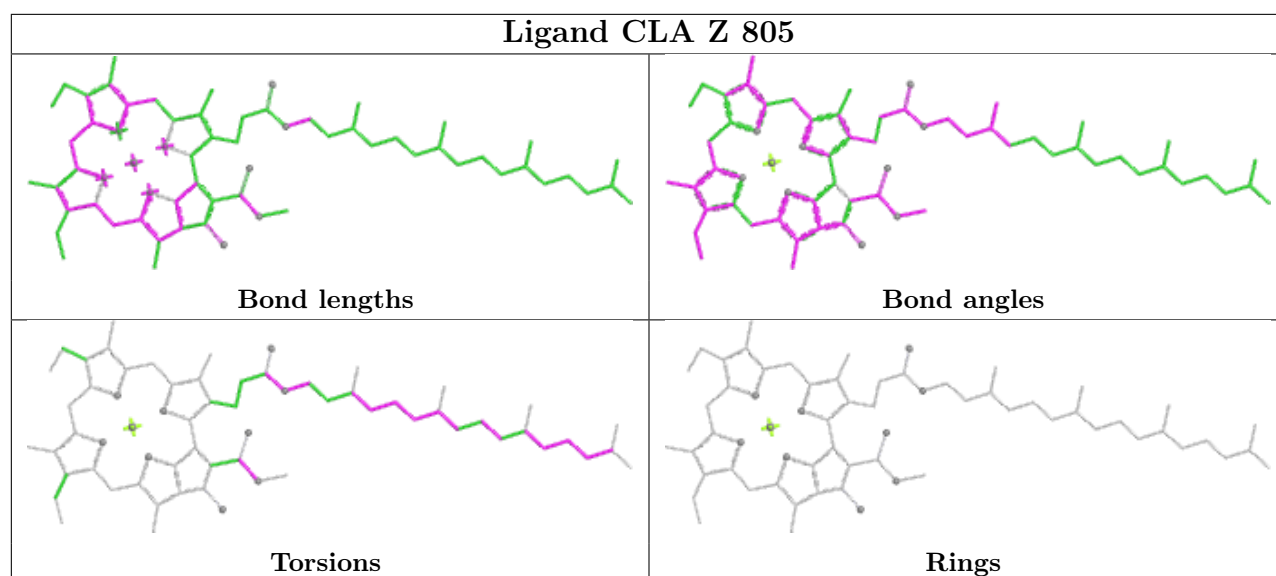
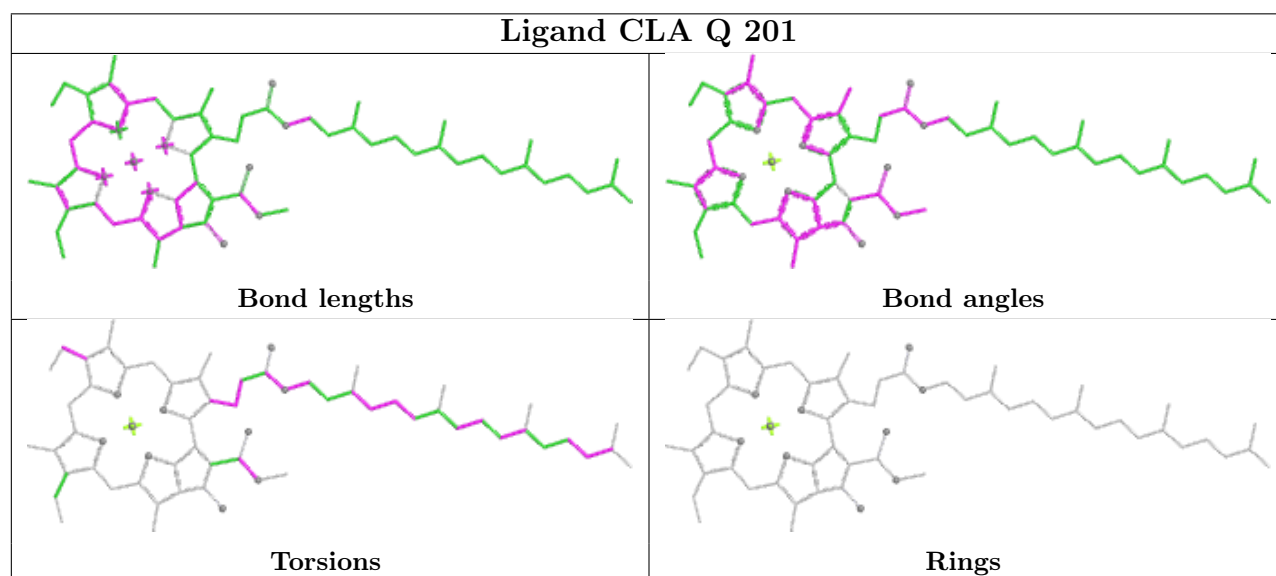
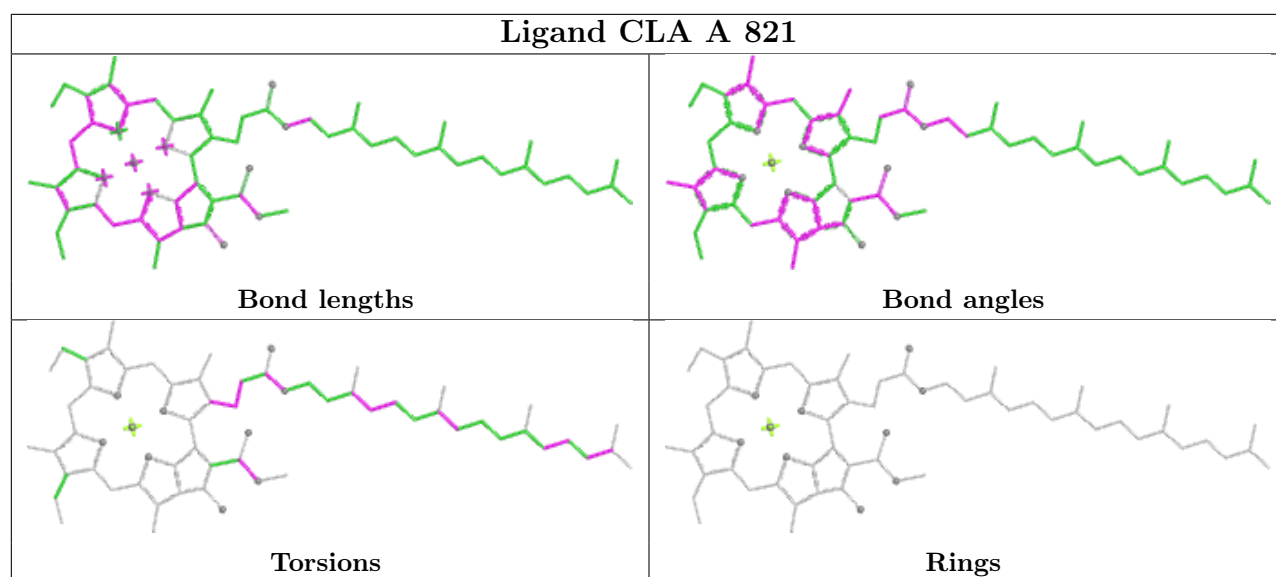
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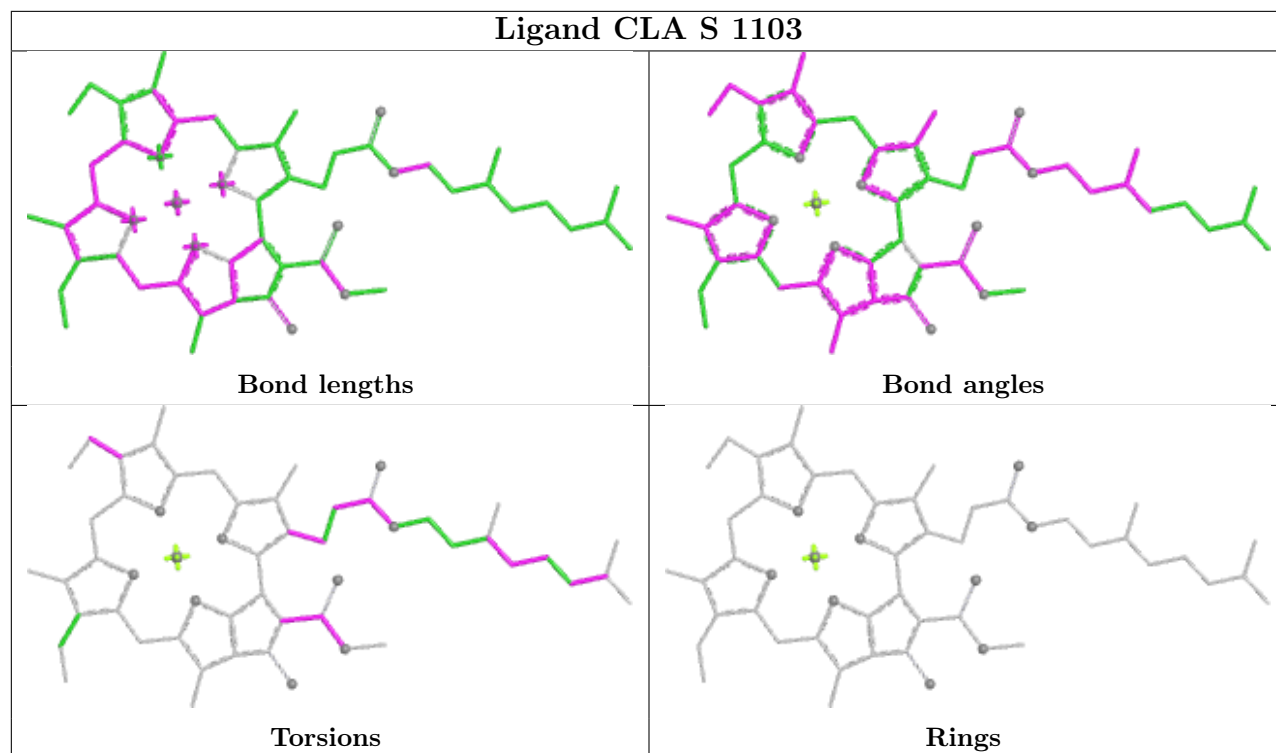
Ligand CLA g 101



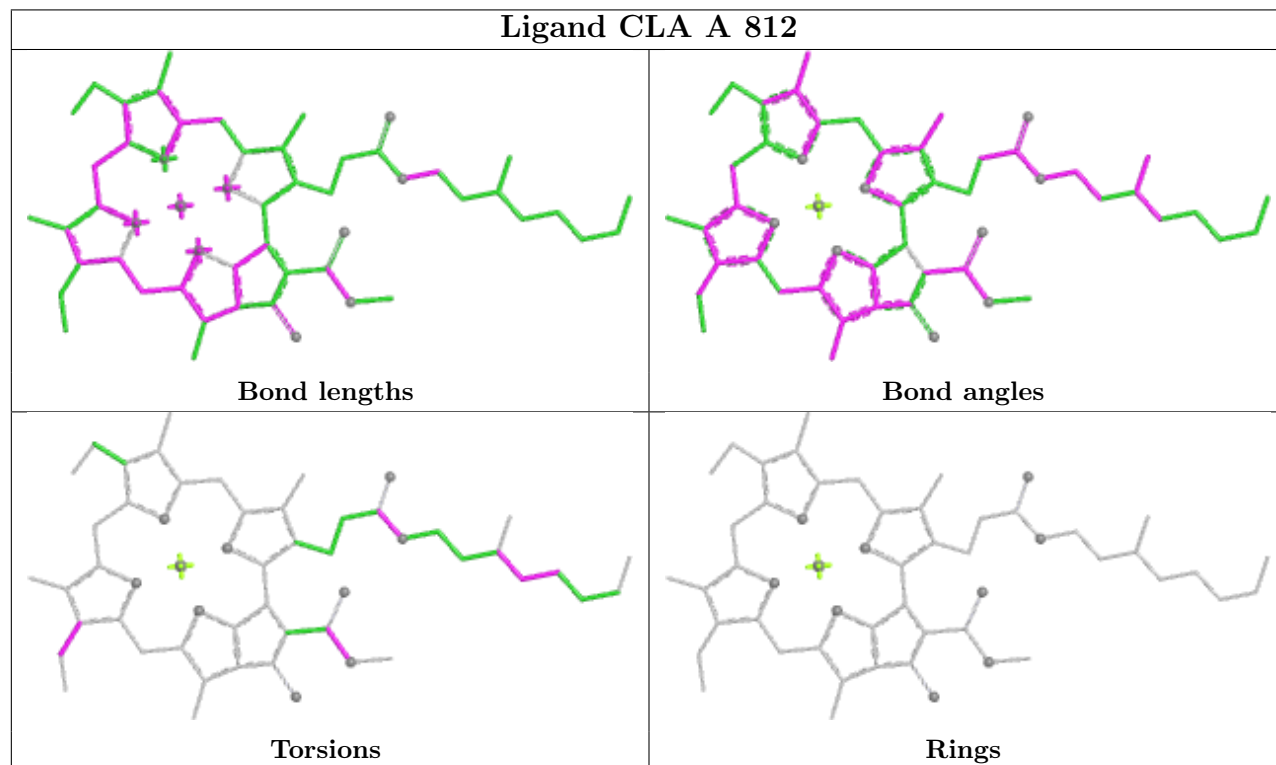
Ligand CLA Y 804**Ligand CLA Y 830**

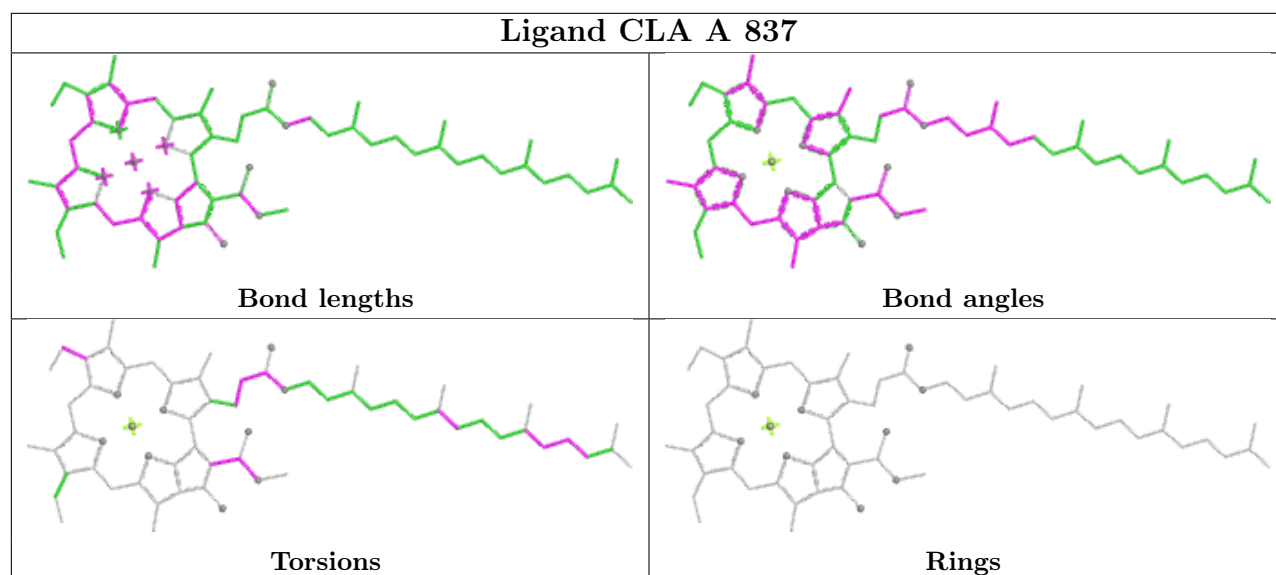
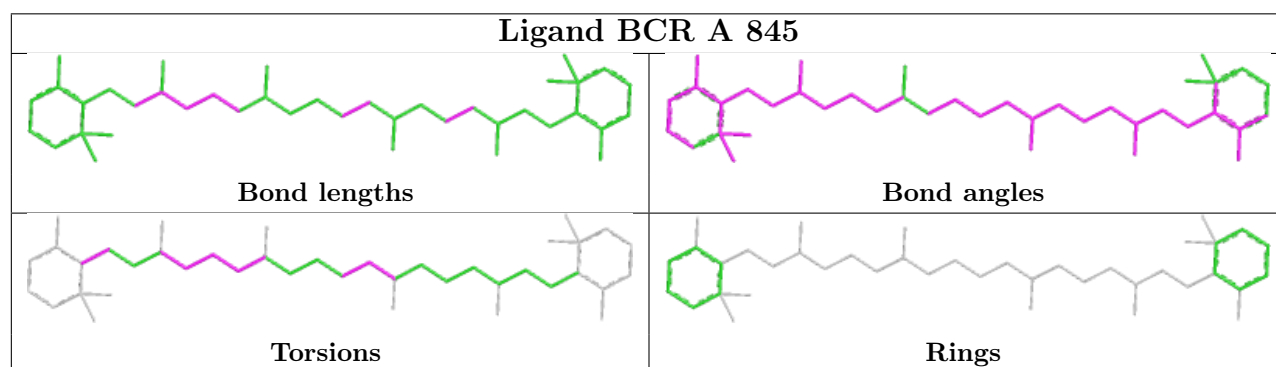
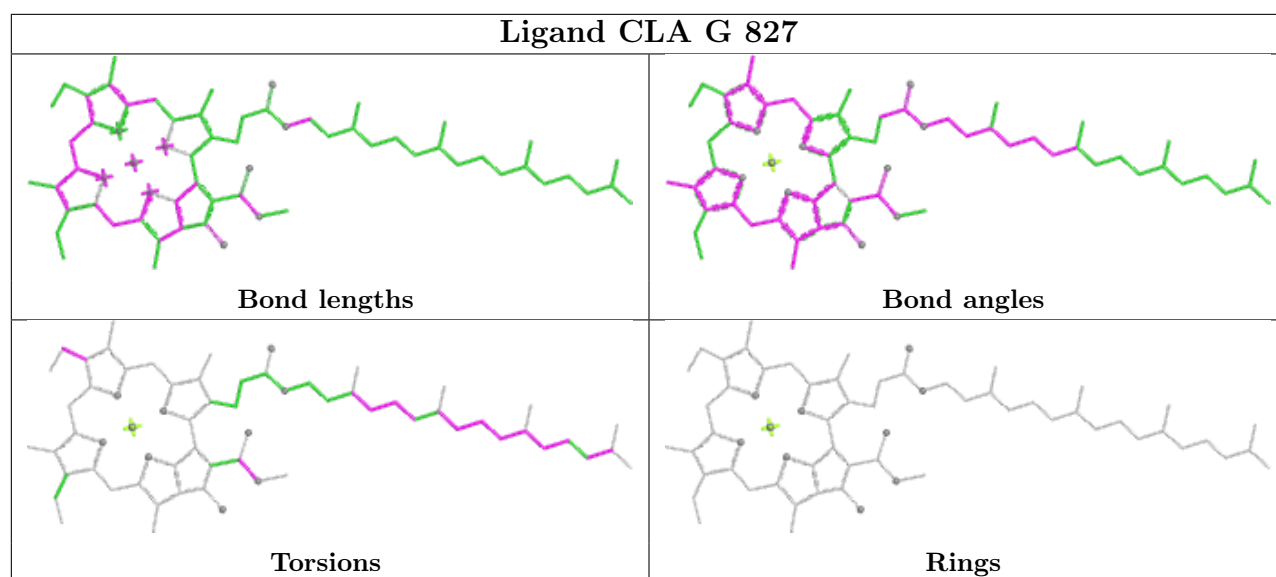


Ligand CLA S 1103

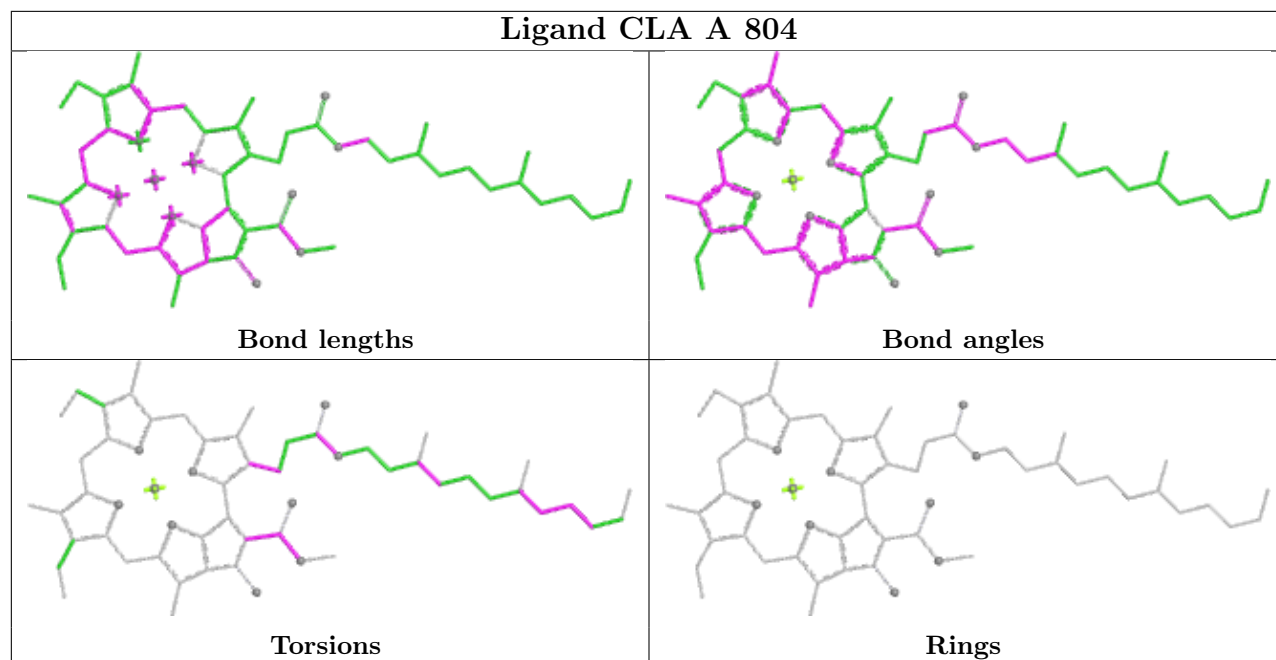


Ligand CLA A 812

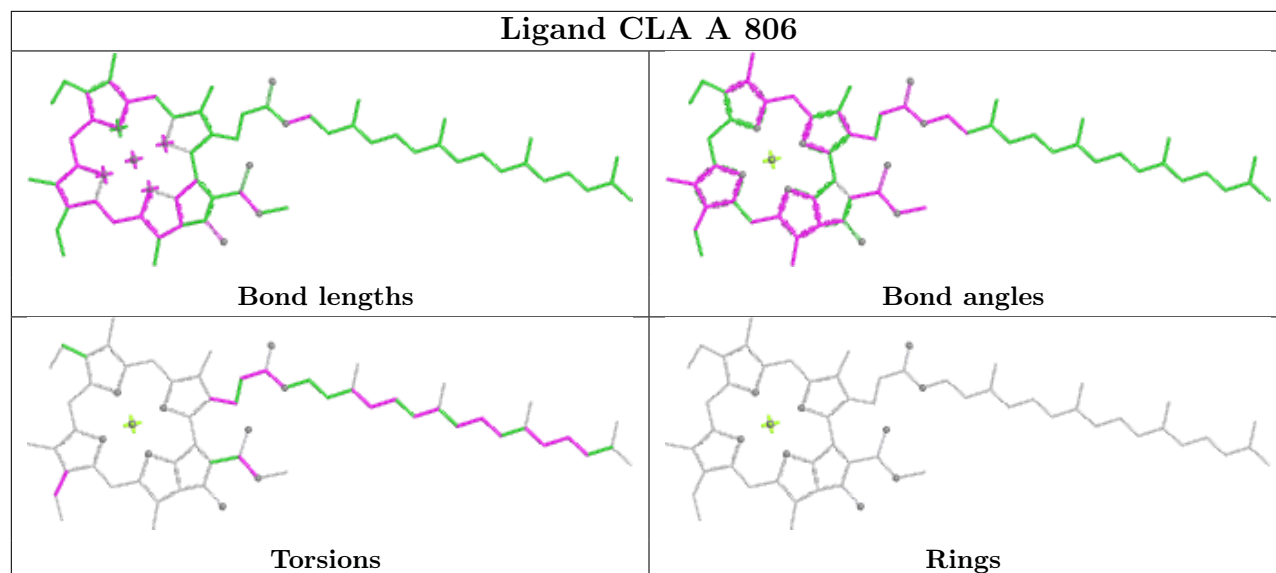




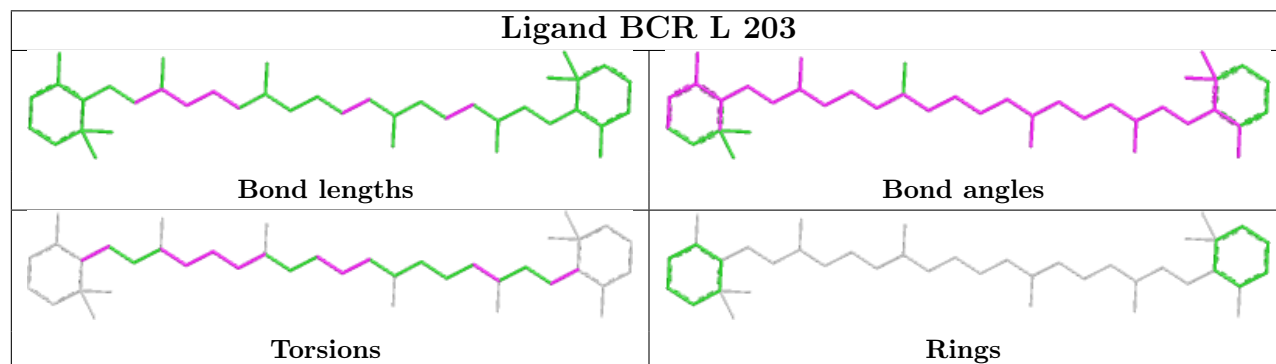
Ligand CLA A 804

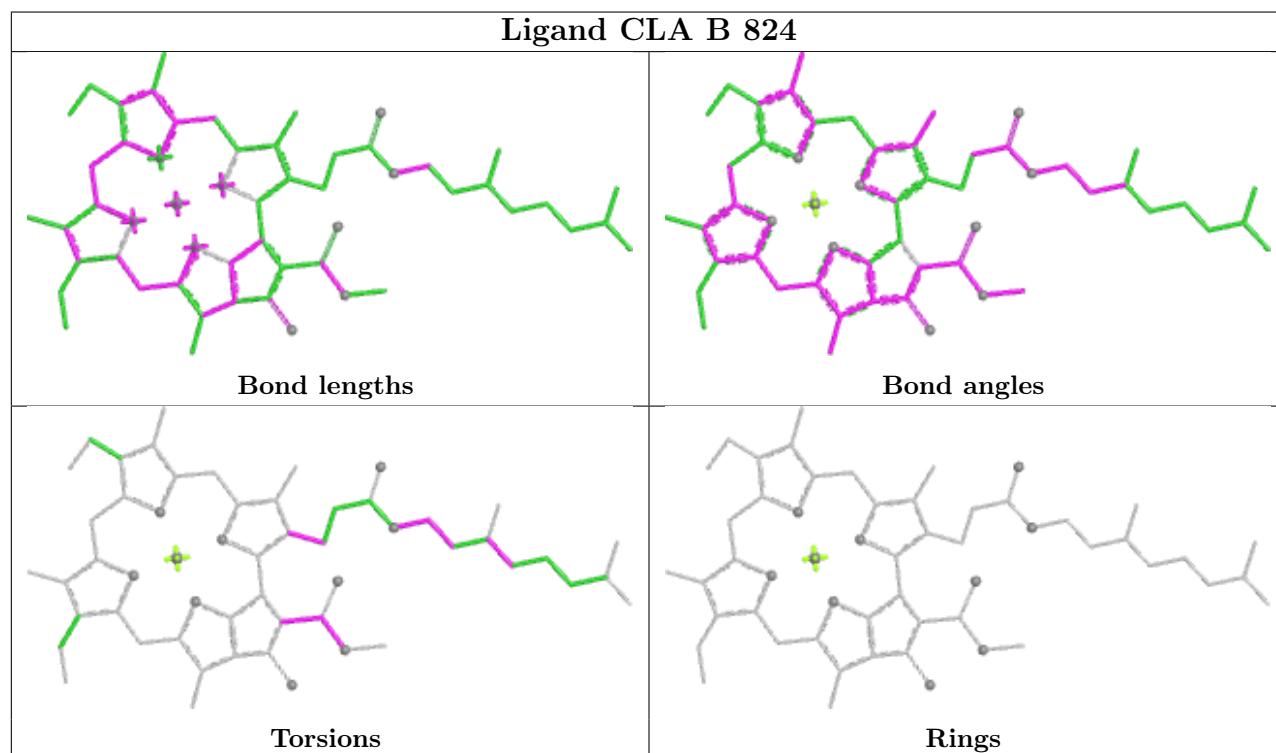
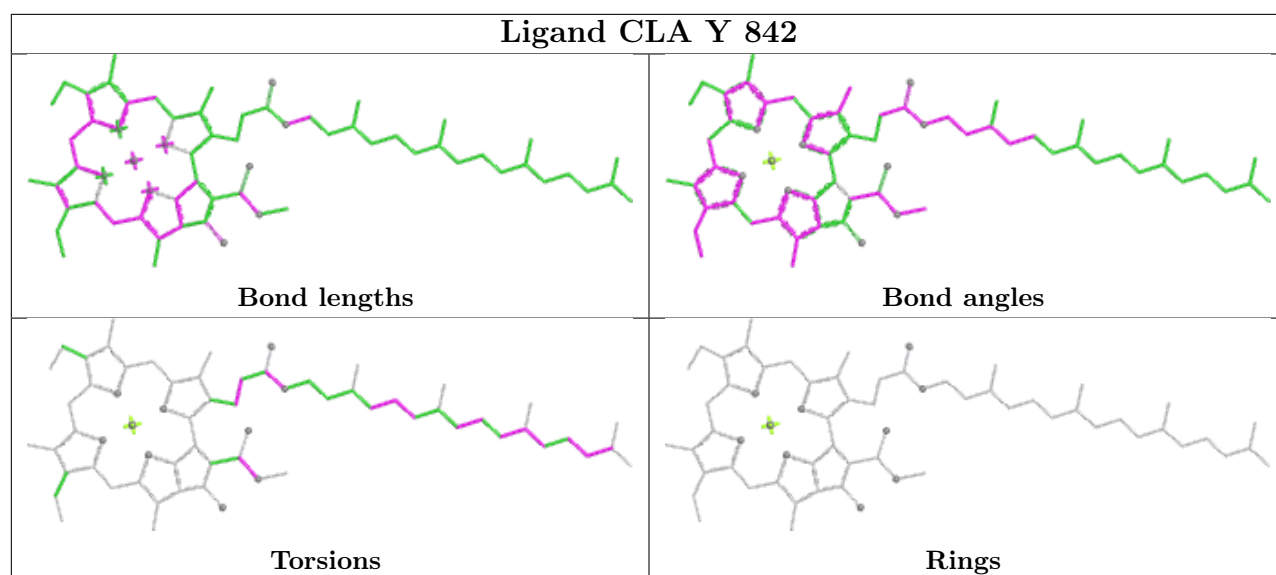


Ligand CLA A 806

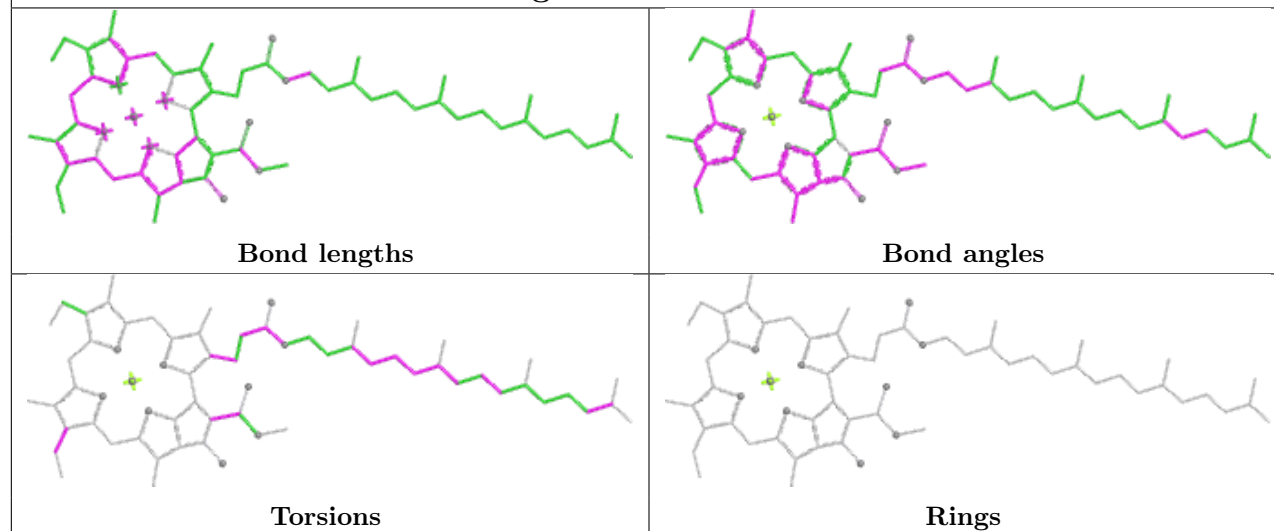


Ligand BCR L 203

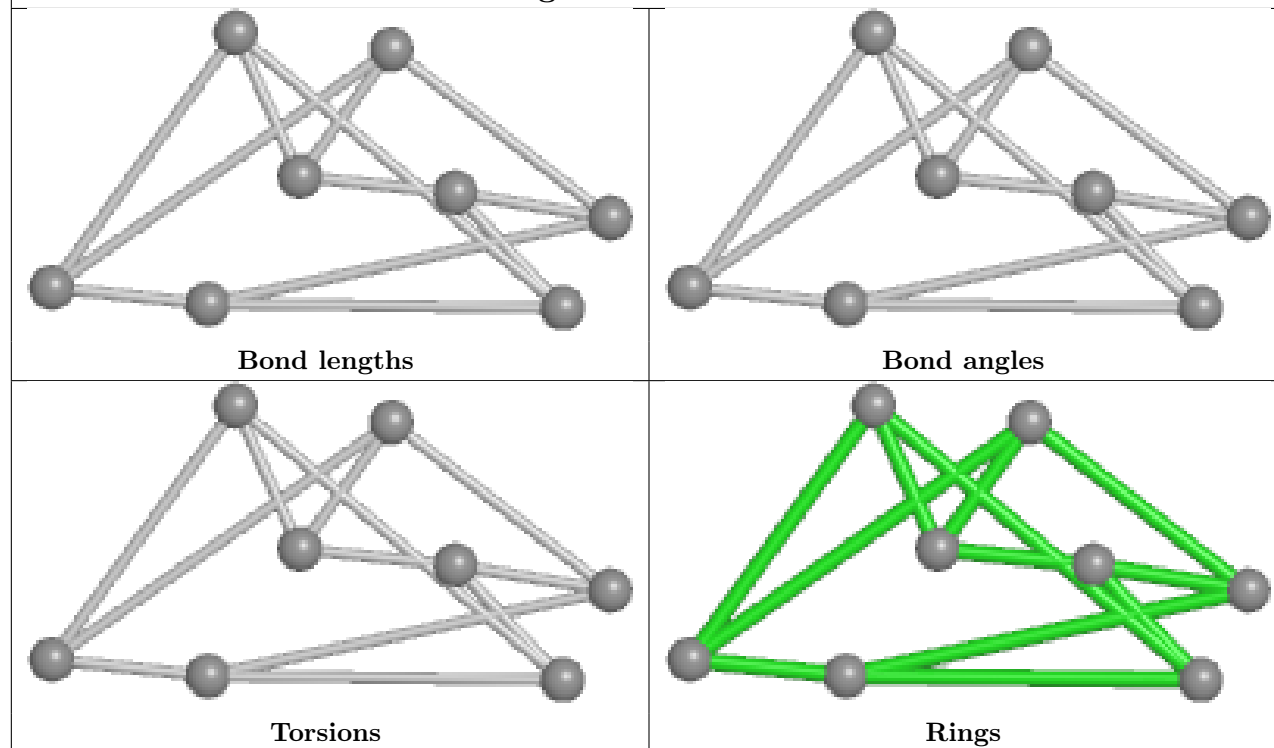




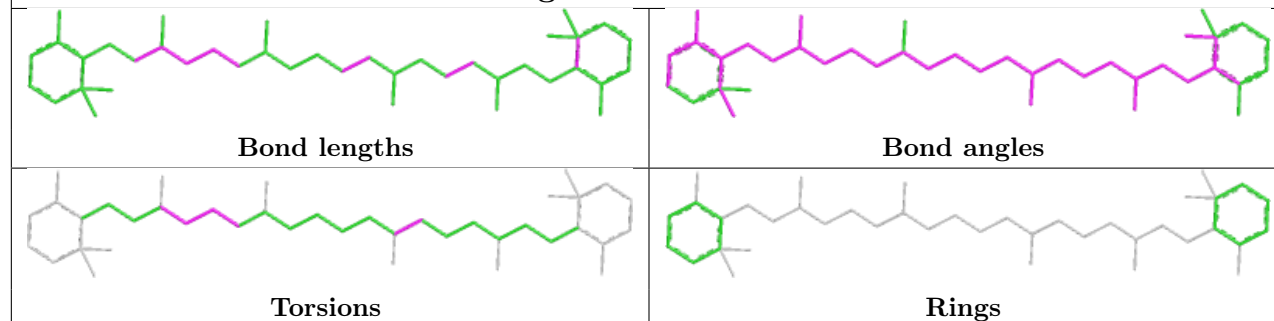
Ligand CLA B 813



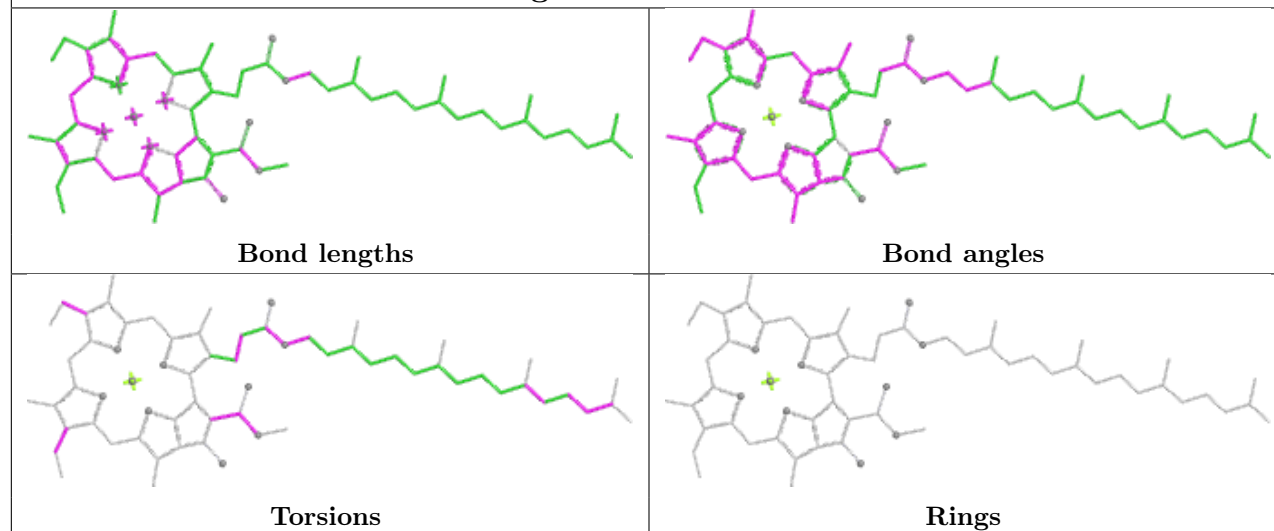
Ligand SF4 G 845



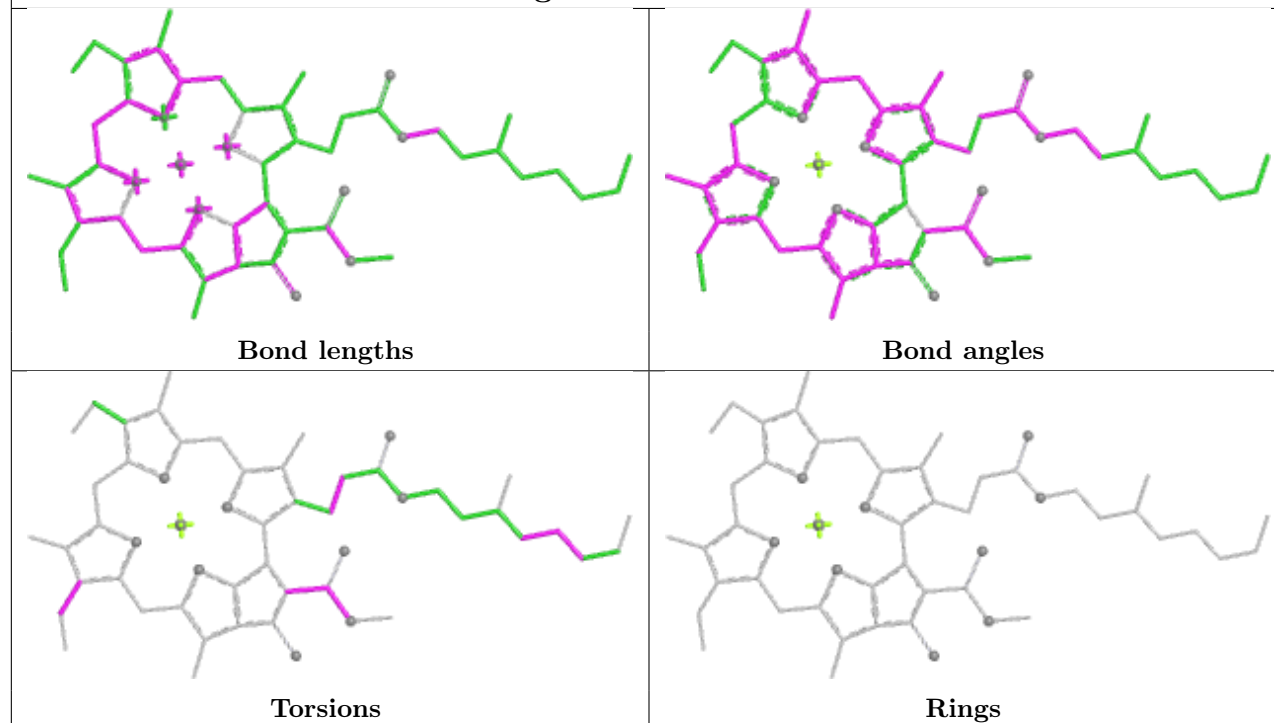
Ligand BCR f 104



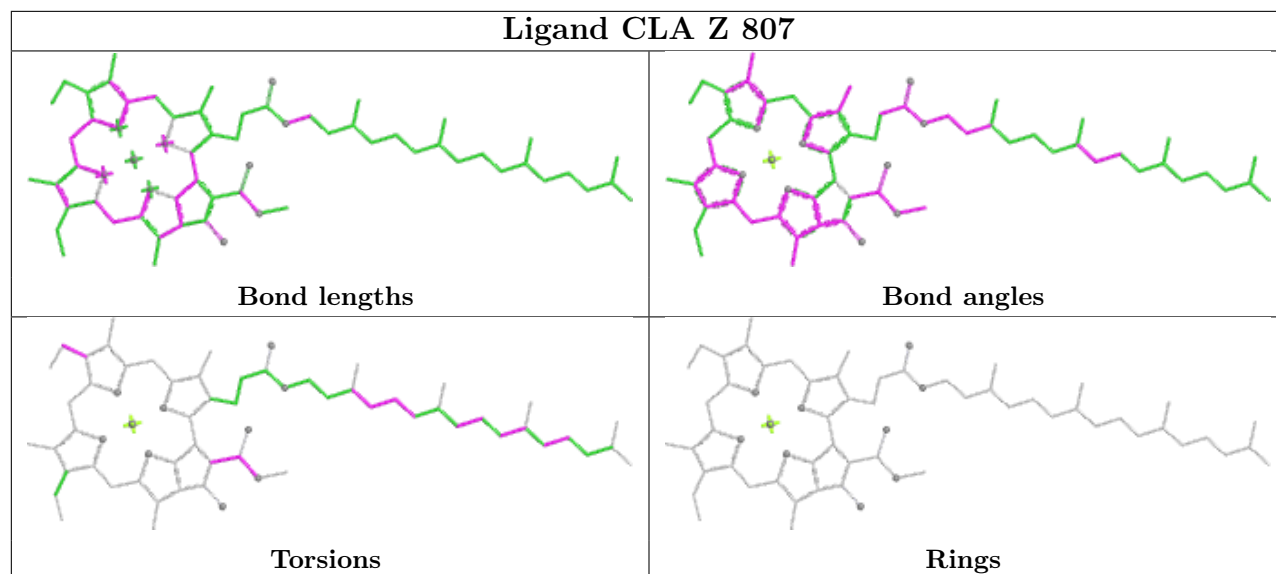
Ligand CLA G 833



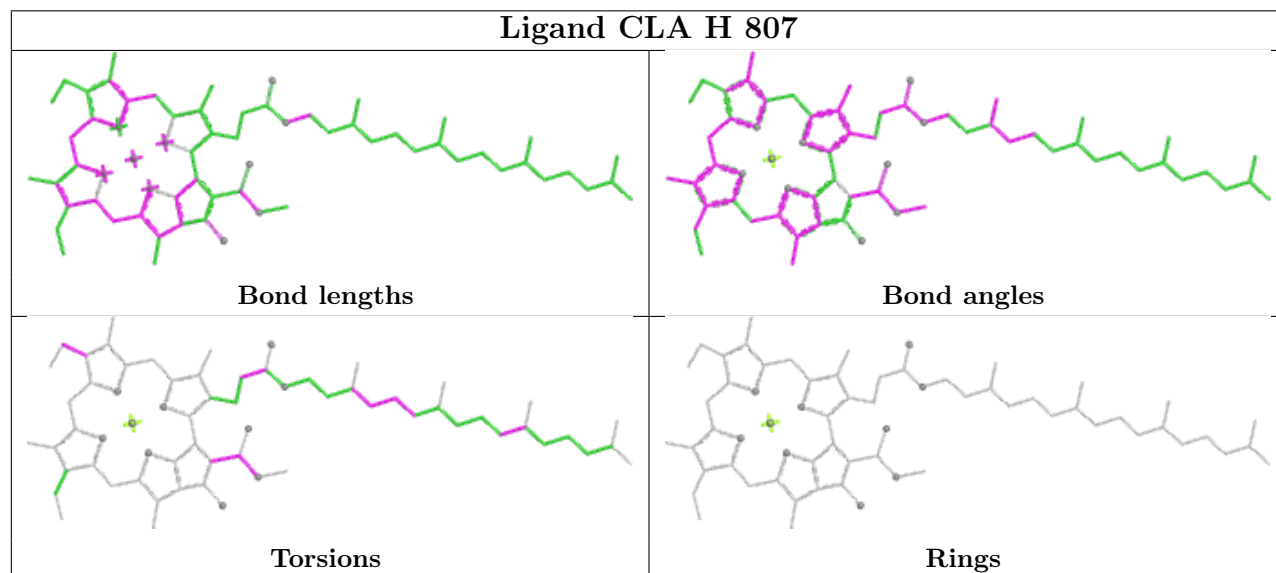
Ligand CLA Z 803



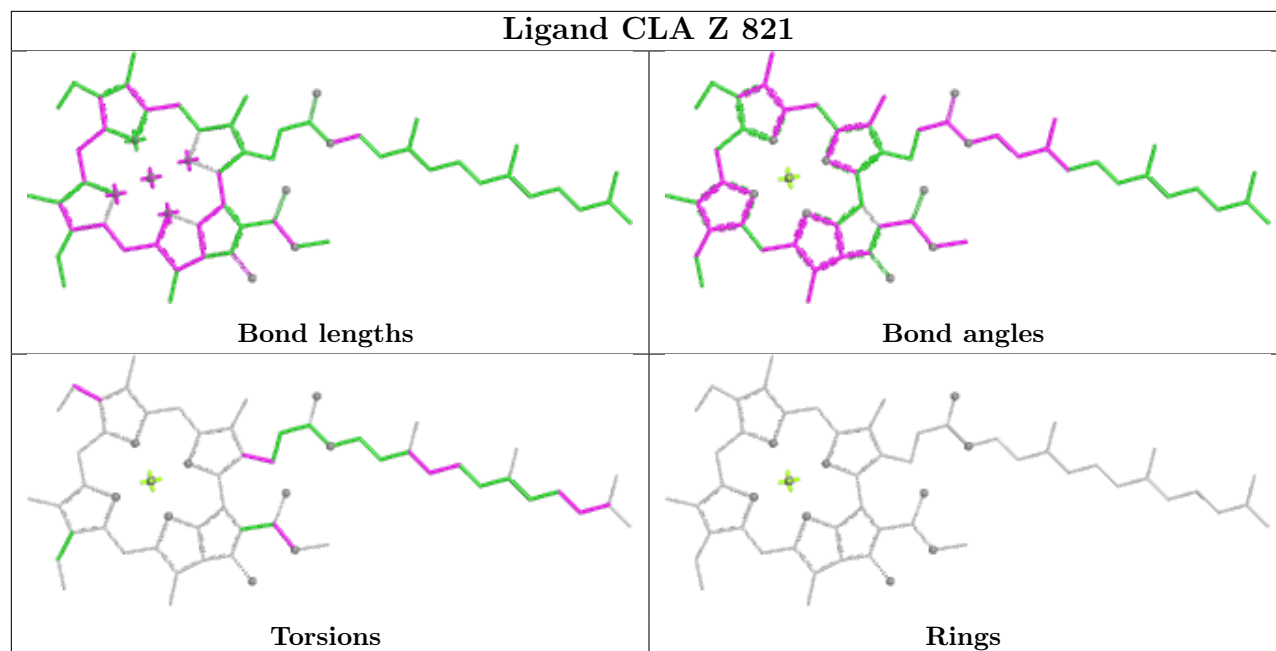
Ligand CLA Z 807



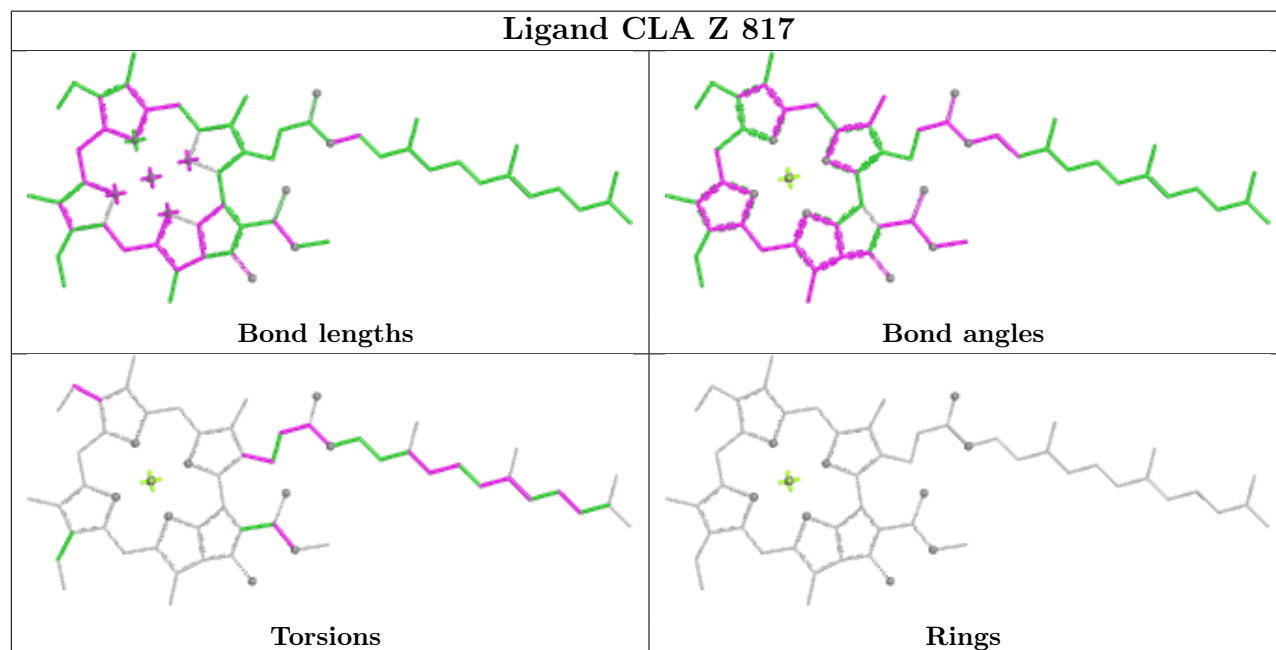
Ligand CLA H 807



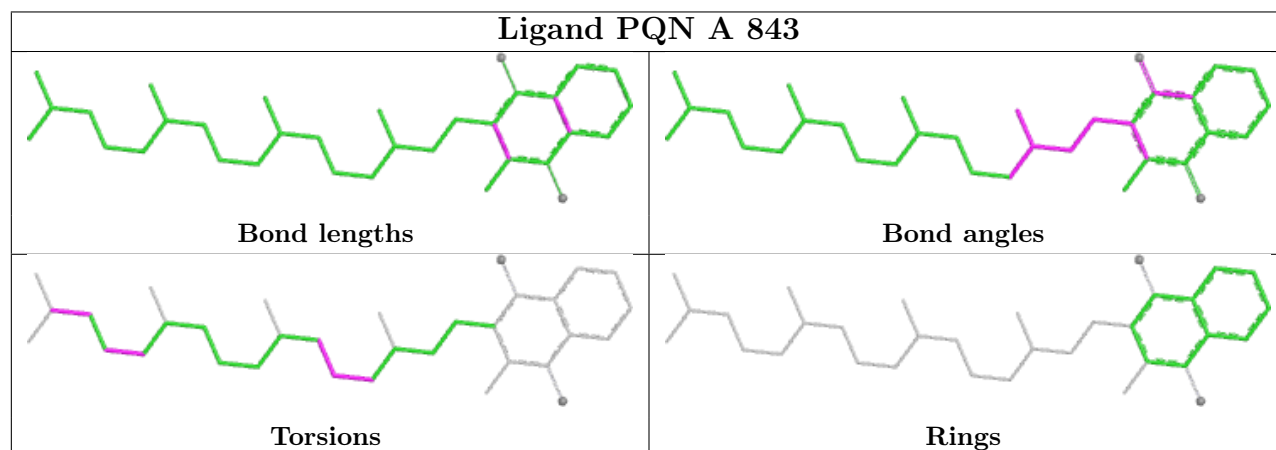
Ligand CLA Z 821



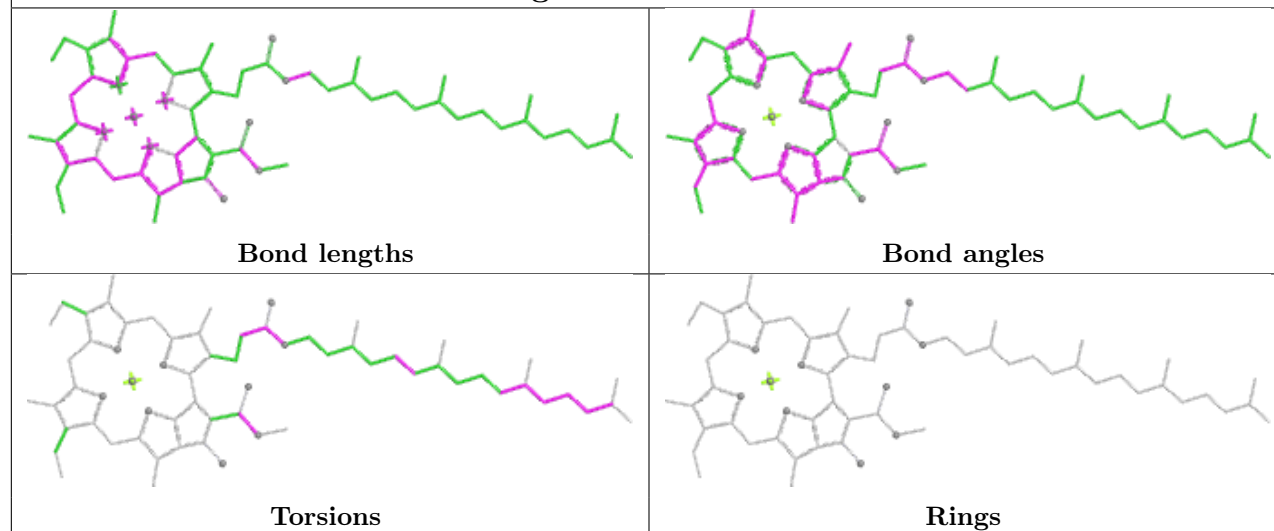
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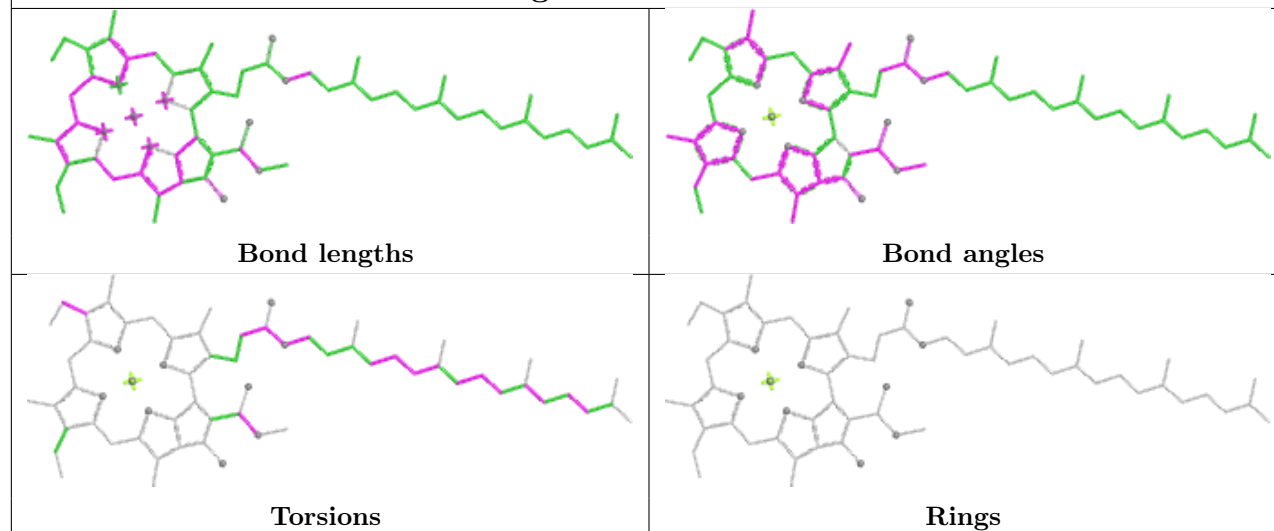
Ligand PQN A 843



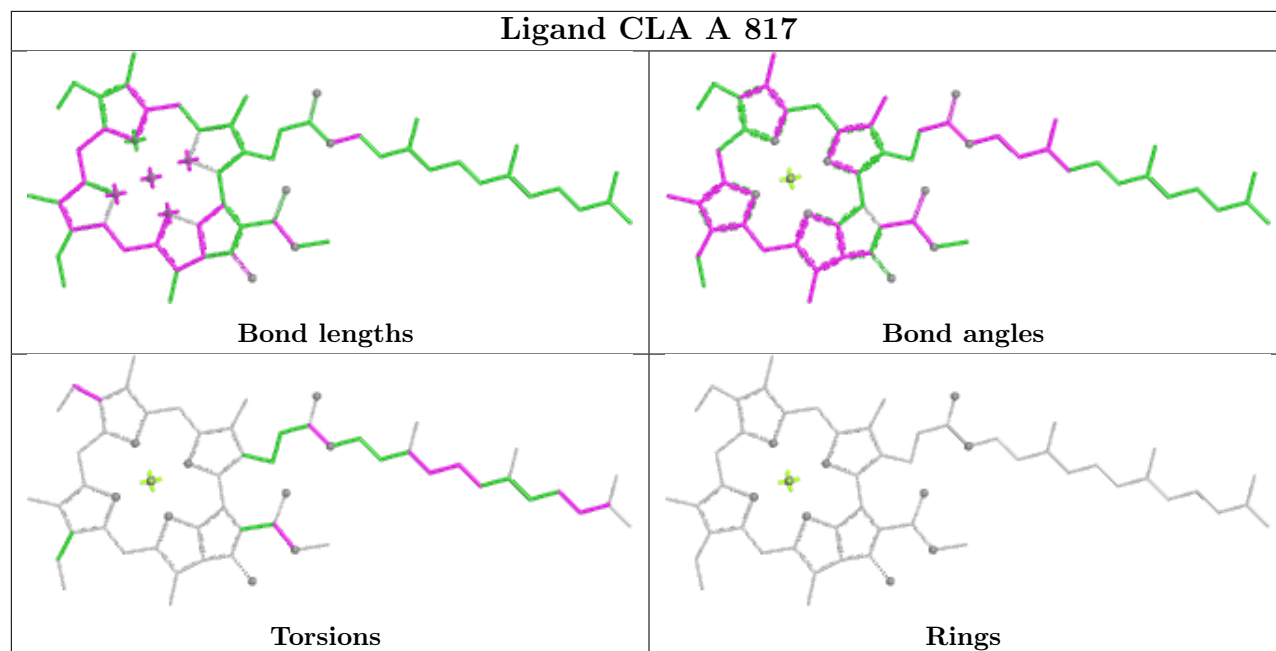
Ligand CLA Y 829



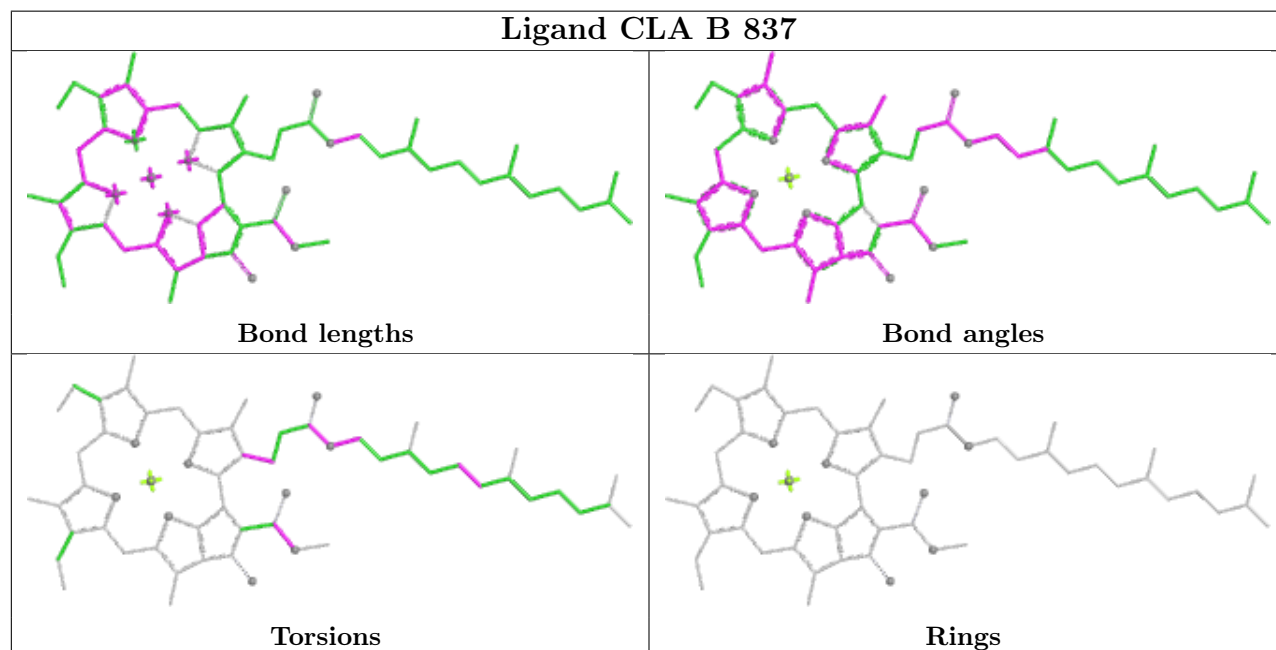
Ligand CLA H 835

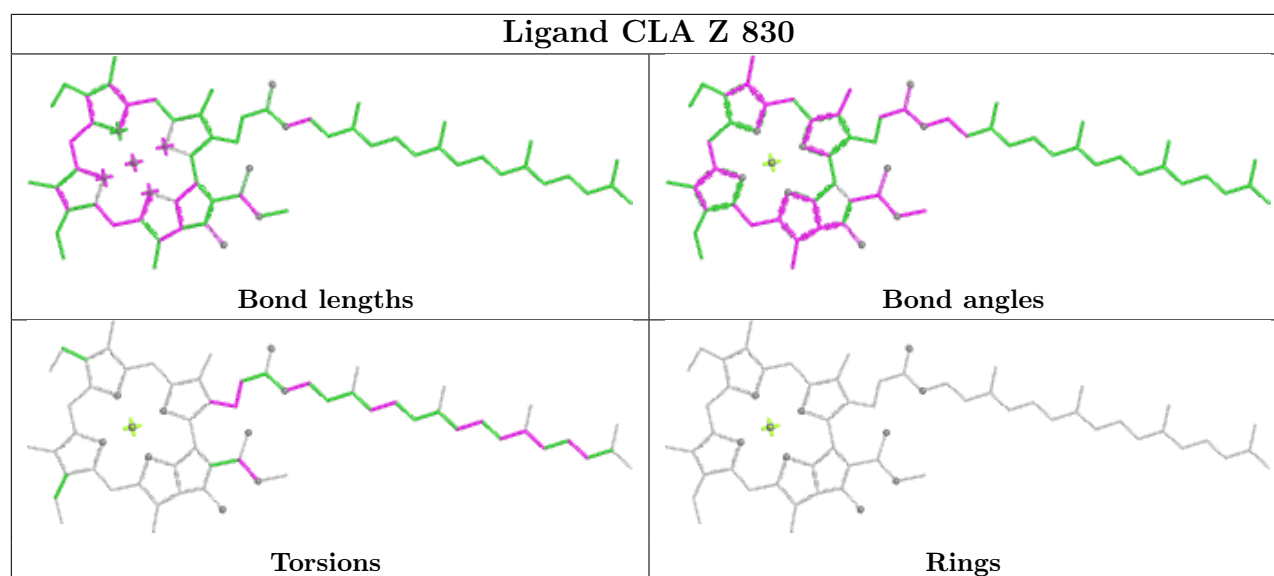
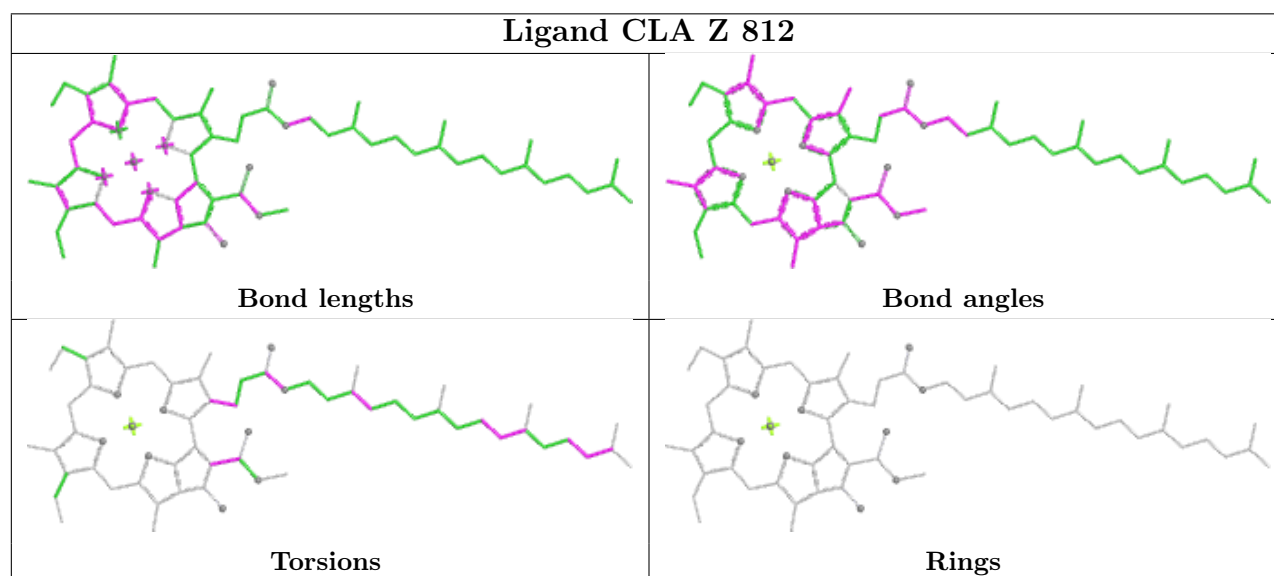
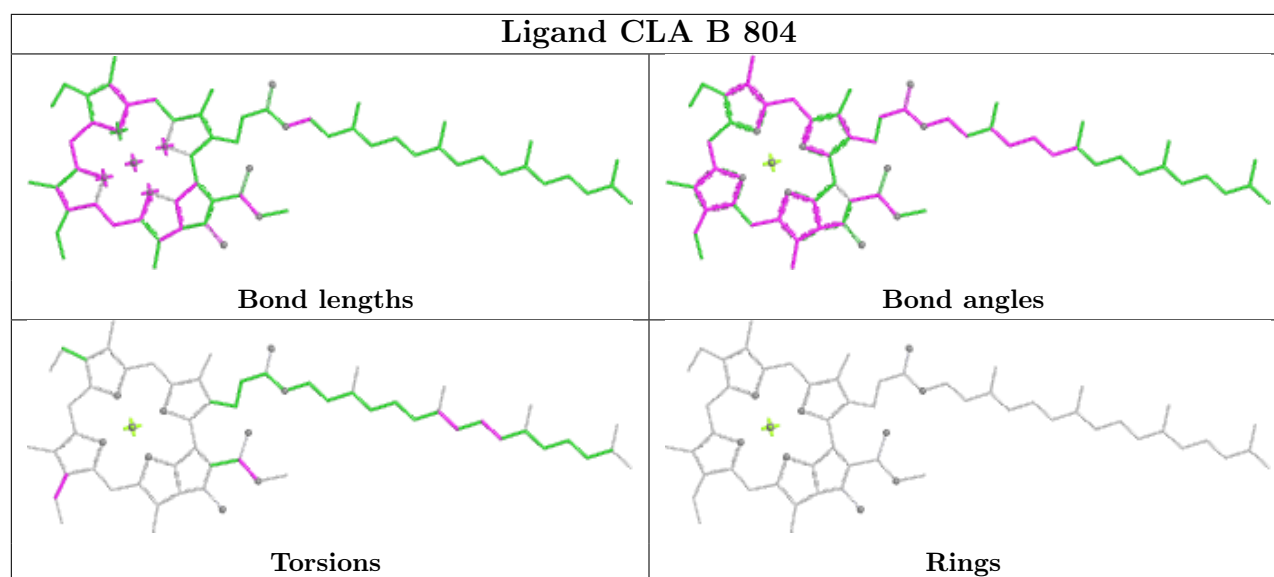


Ligand CLA A 817

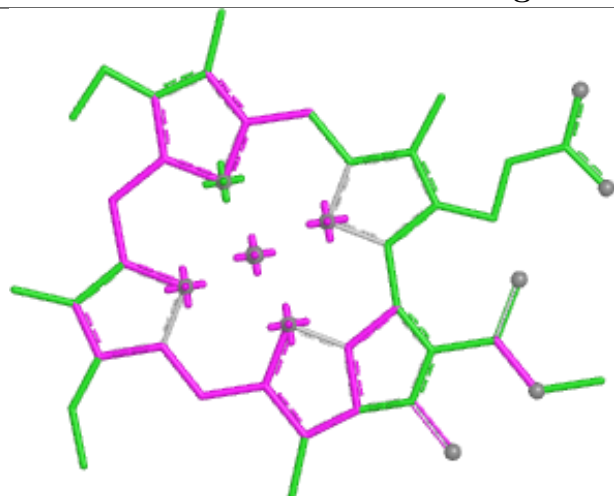


Ligand CLA B 837

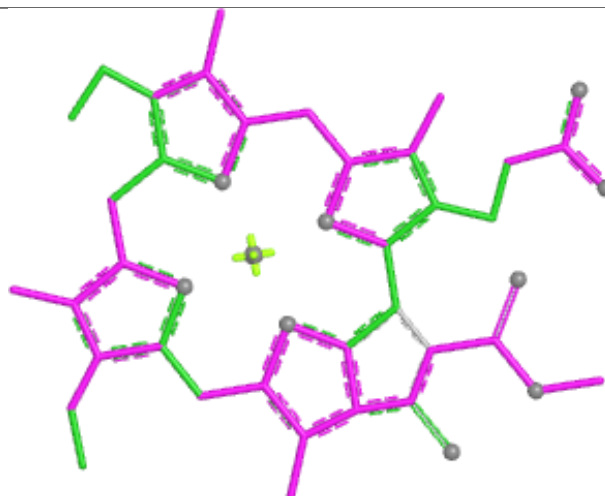




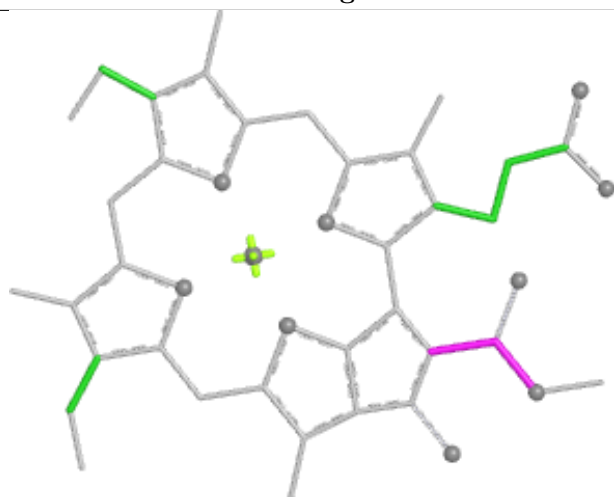
Ligand CLA H 820



Bond lengths



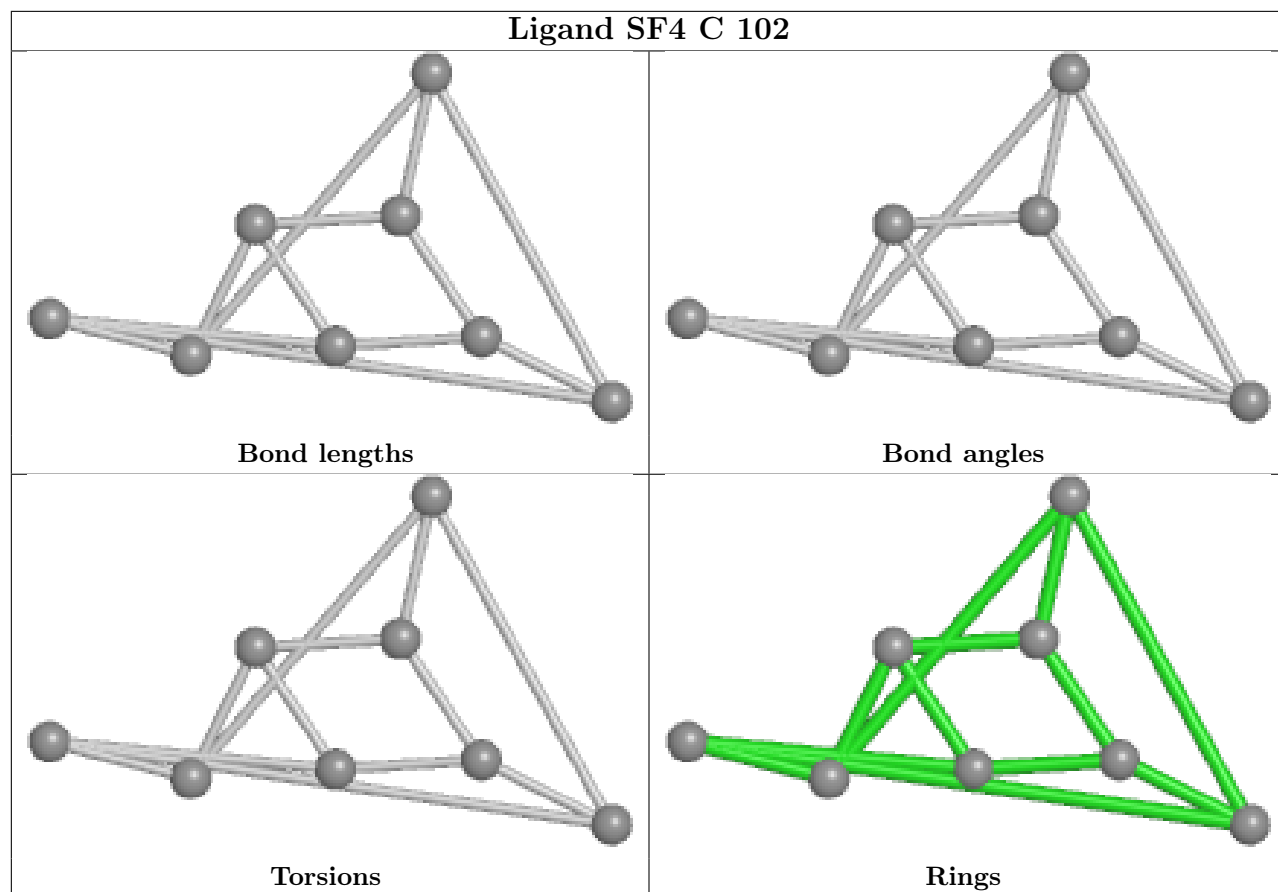
Bond angles



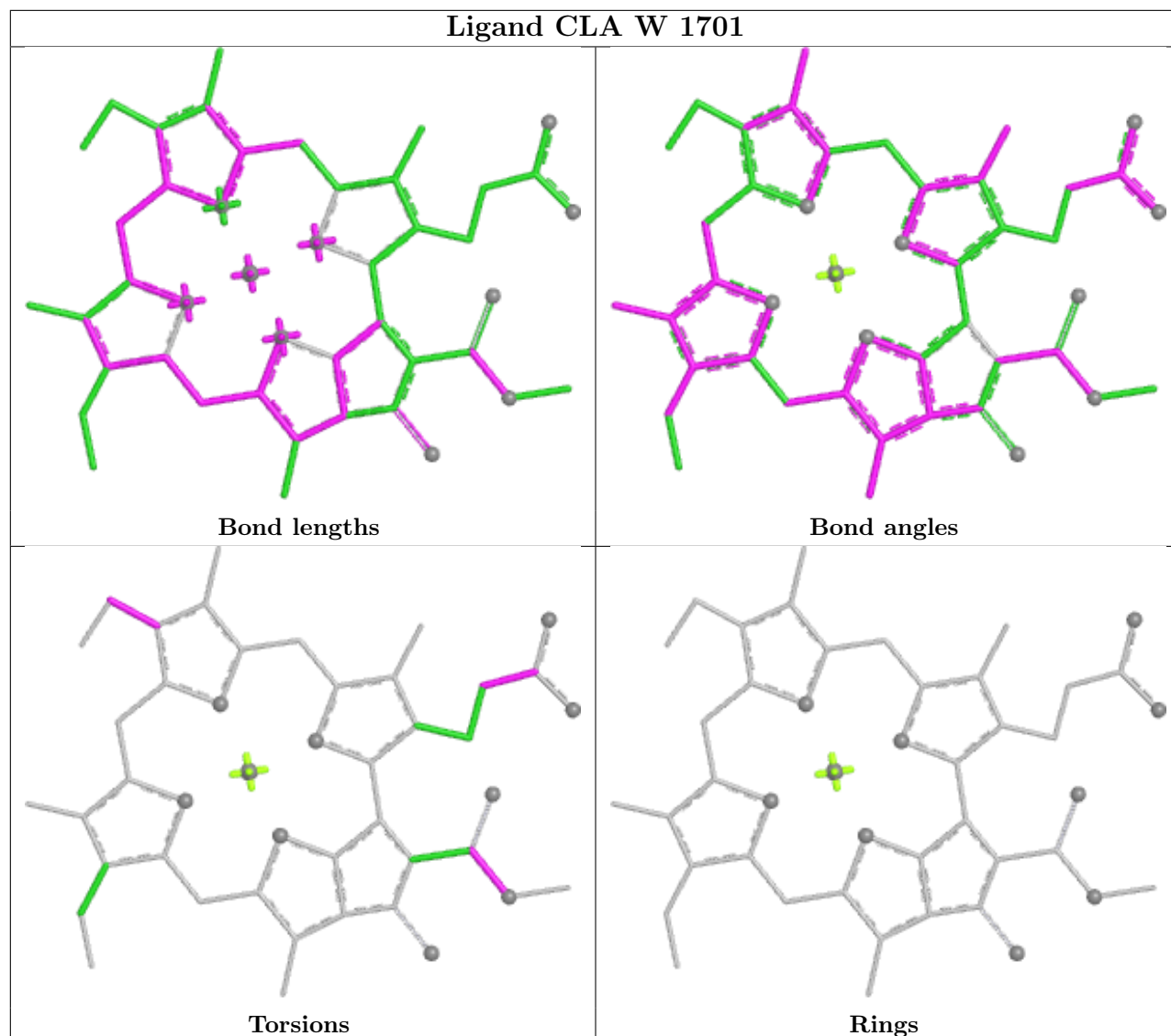
Torsions



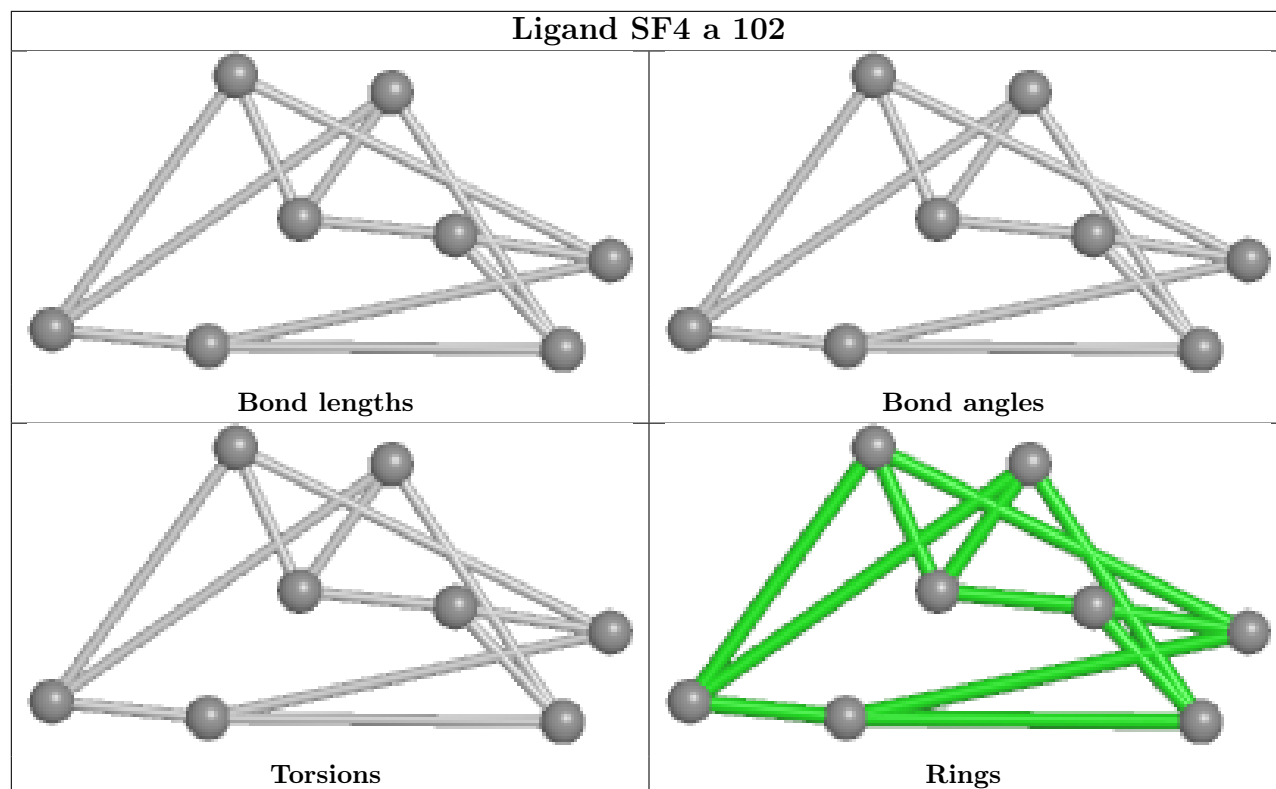
Rings



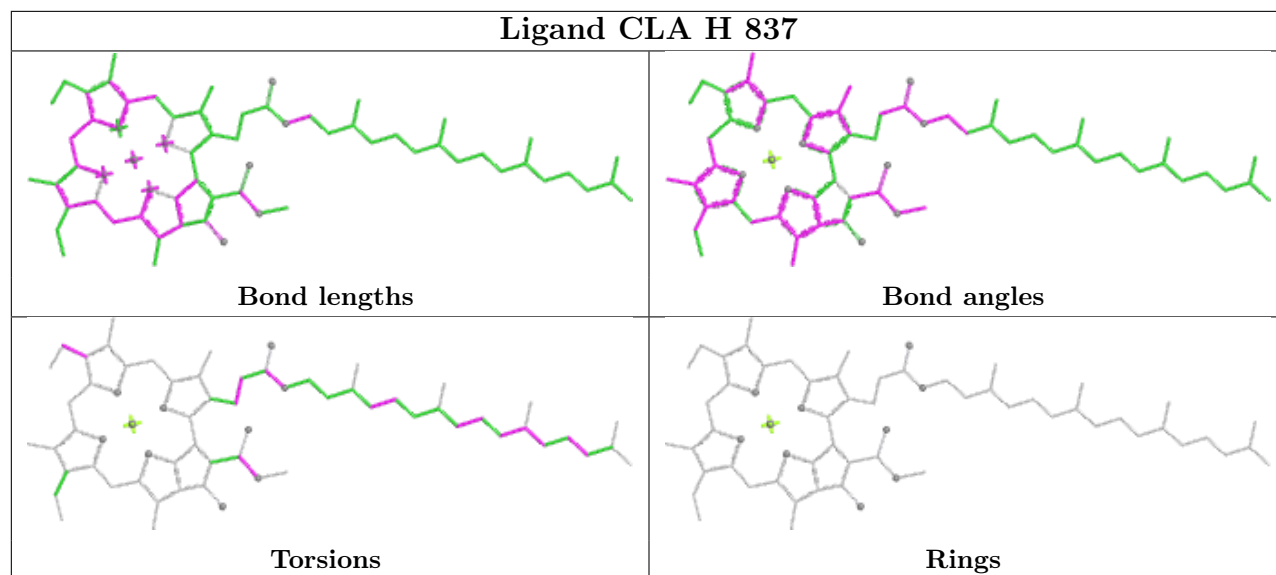
Ligand CLA W 1701



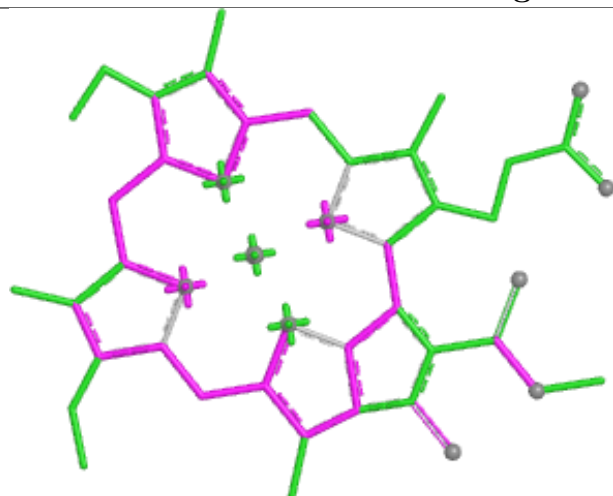
Ligand SF4 a 102



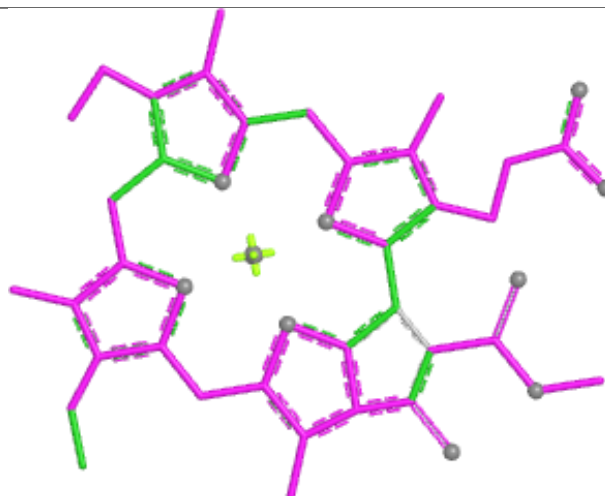
Ligand CLA H 837



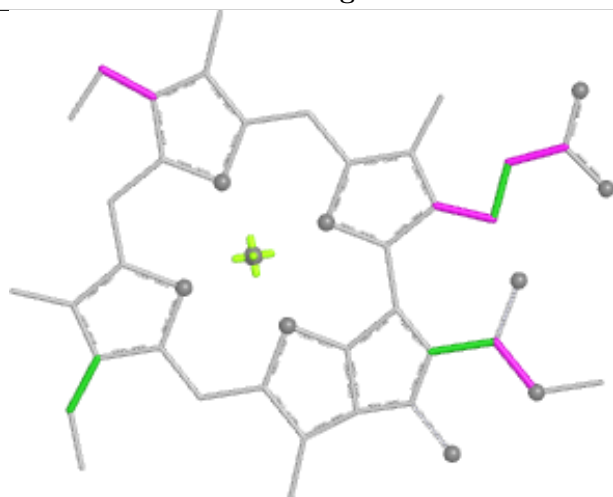
Ligand CLA H 814



Bond lengths



Bond angles

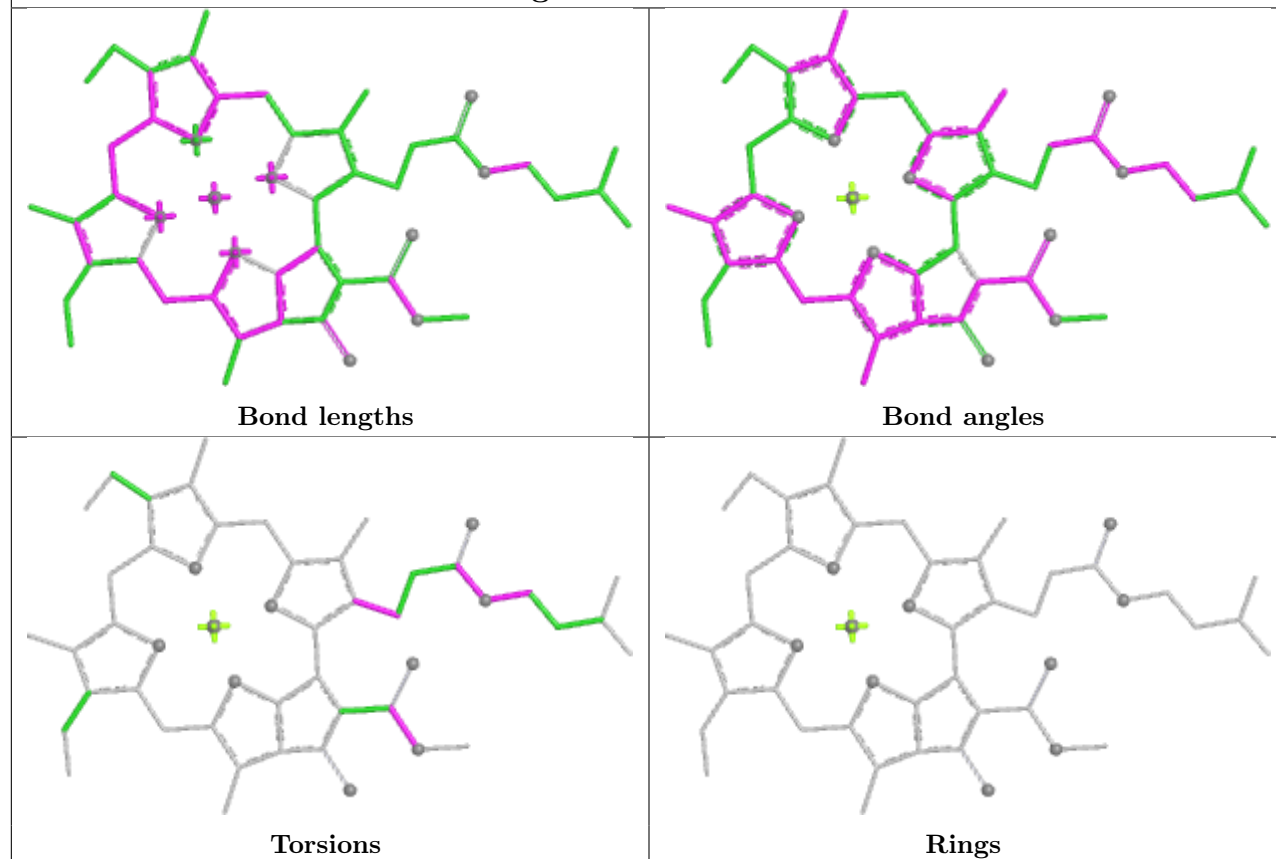


Torsions

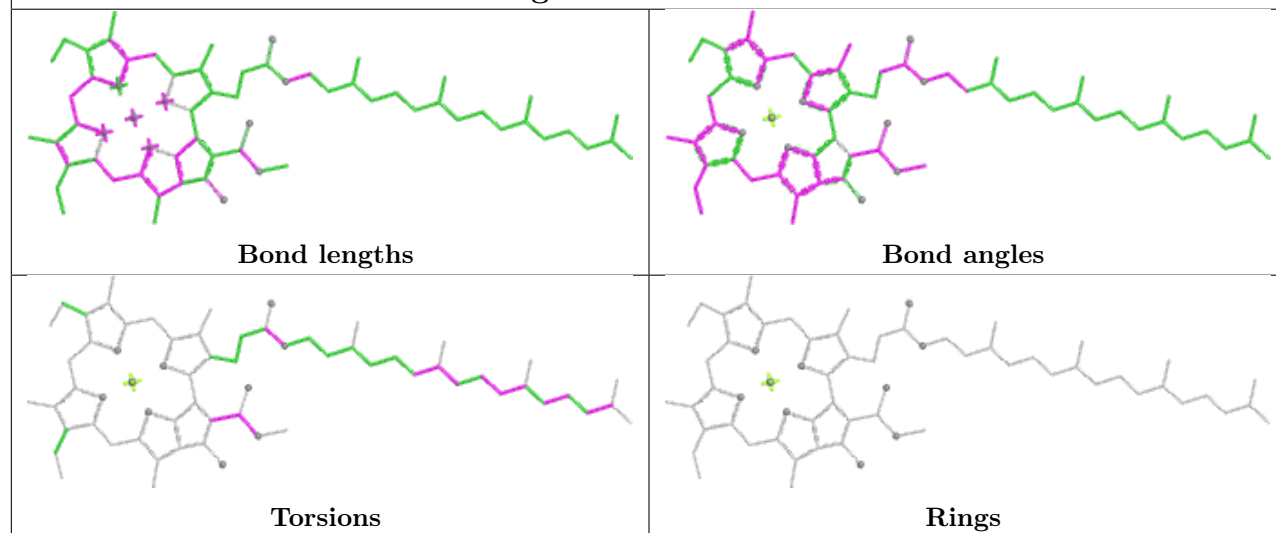


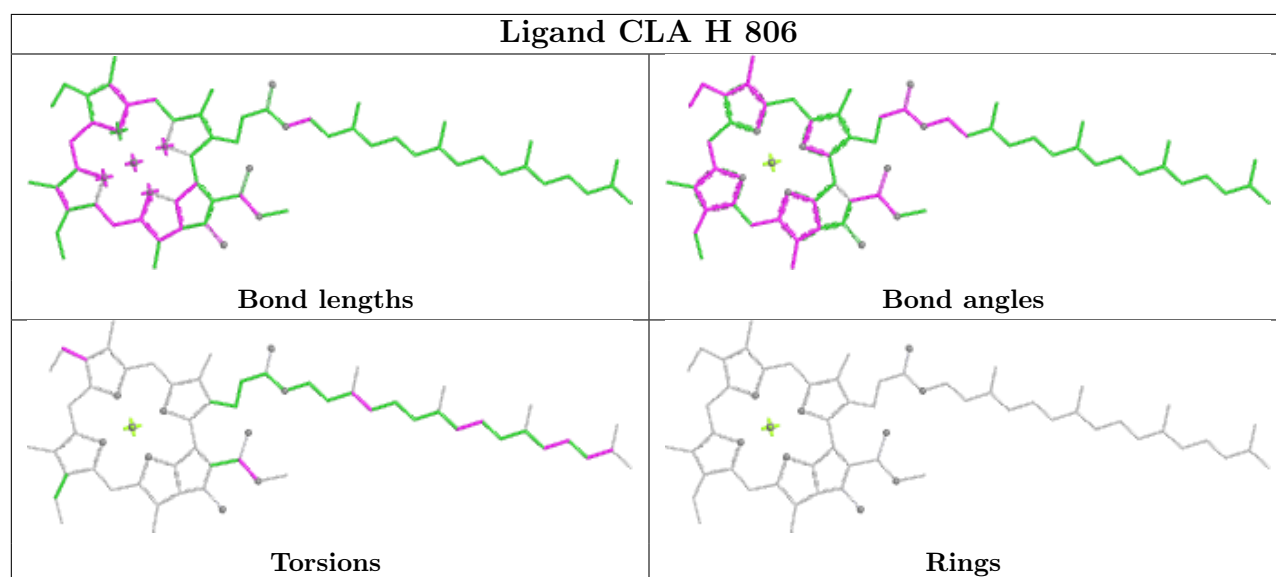
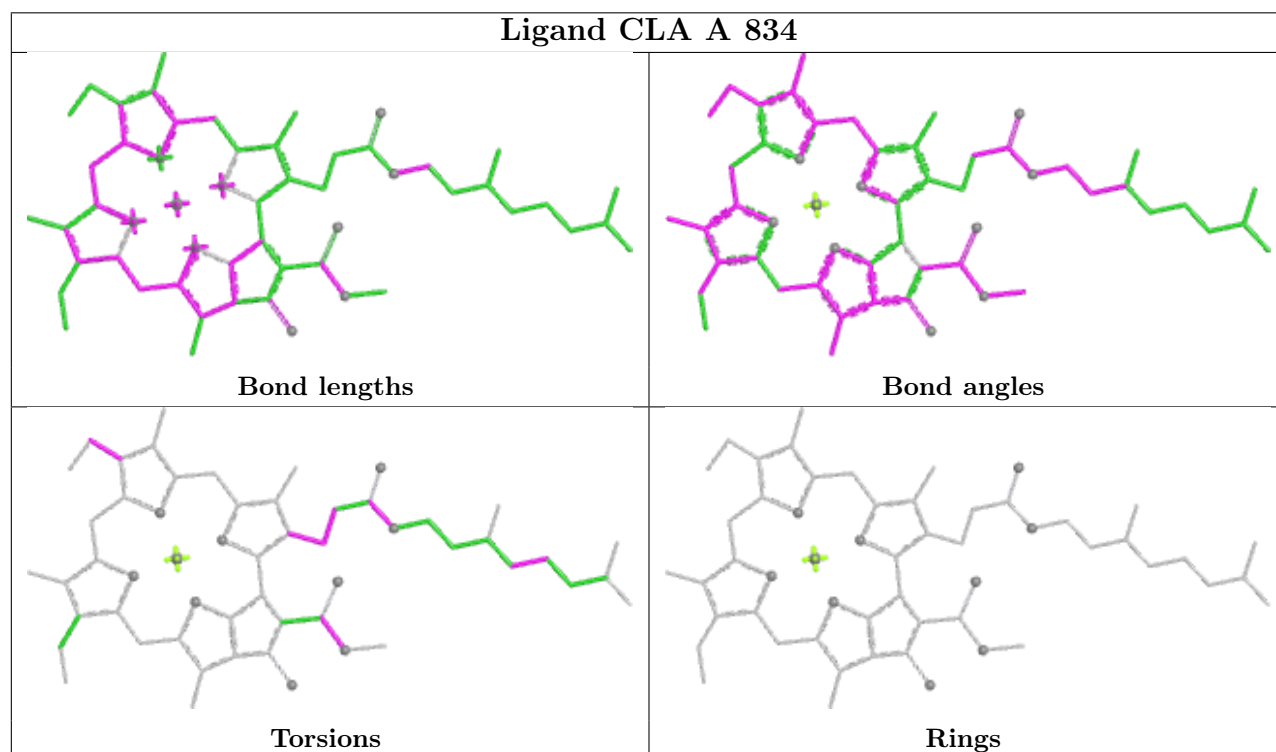
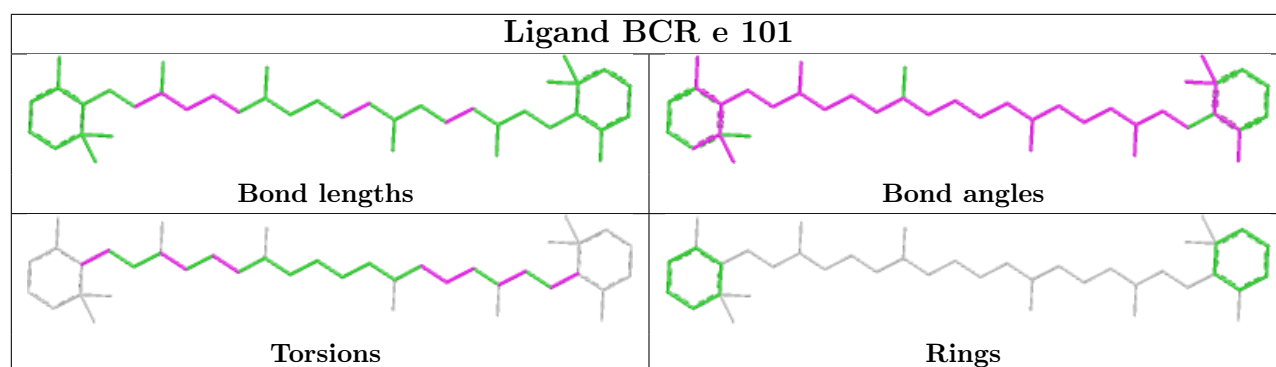
Rings

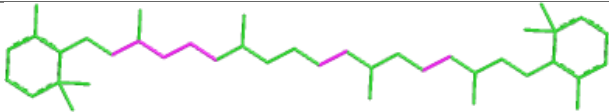
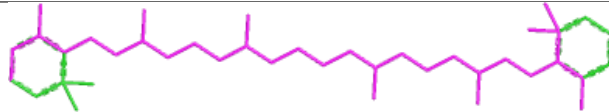
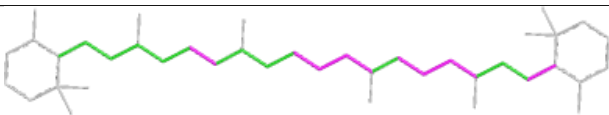
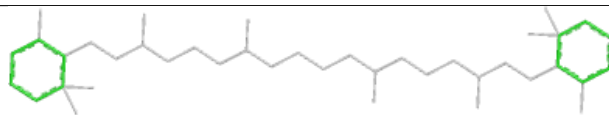
Ligand CLA A 815

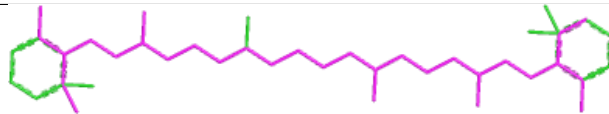
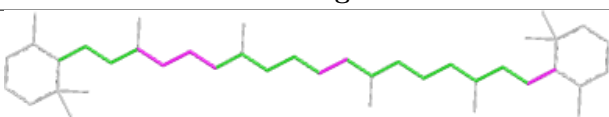
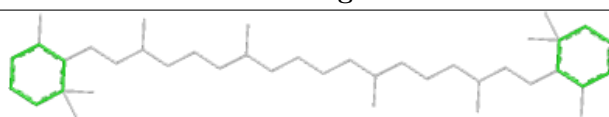


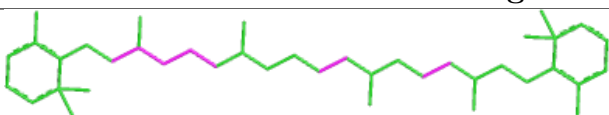
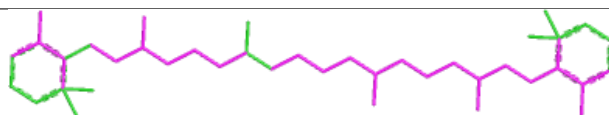
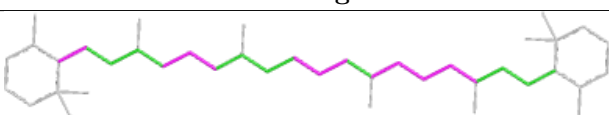
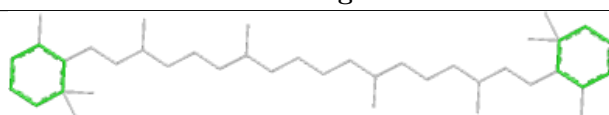
Ligand CLA H 828

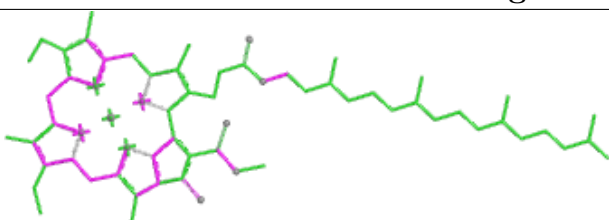
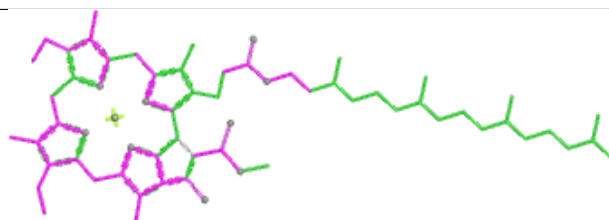
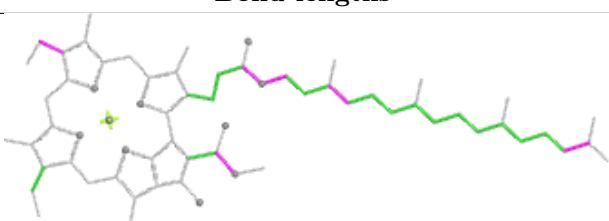
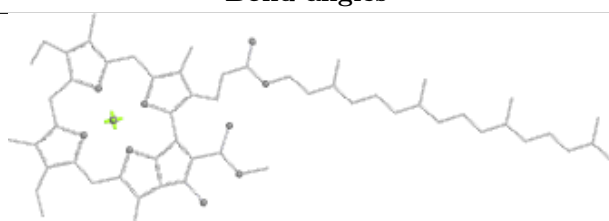




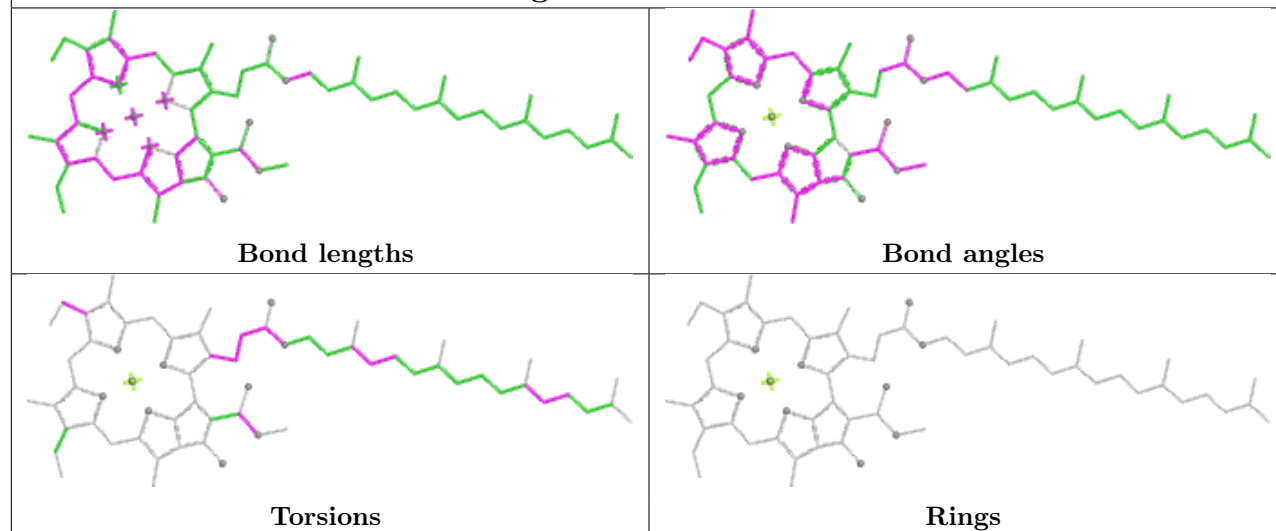
Ligand BCR h 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR f 105	
	
Bond lengths	Bond angles
	
Torsions	Rings

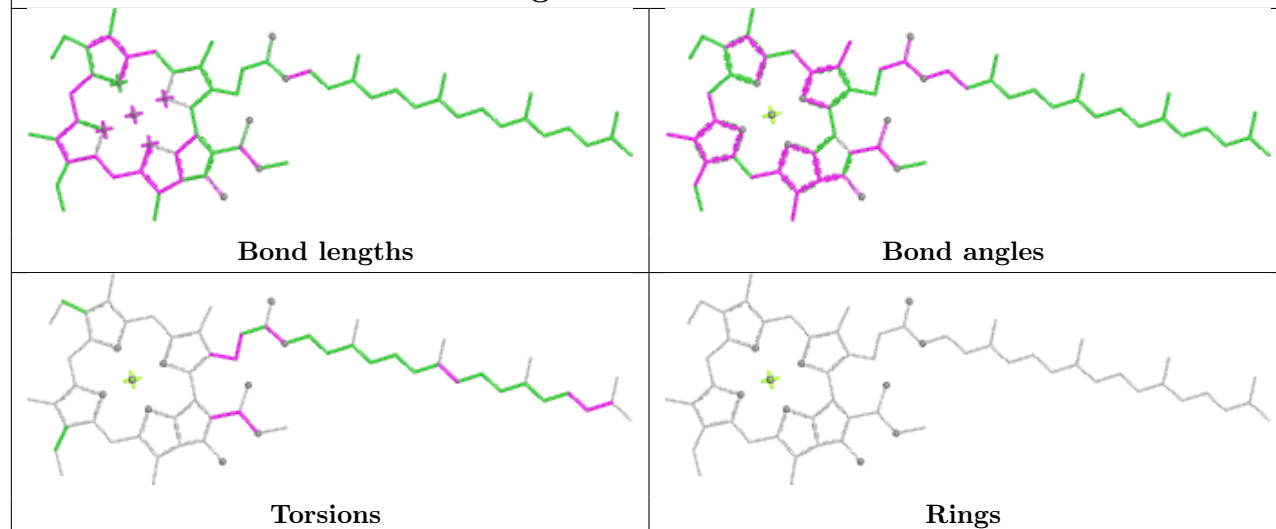
Ligand BCR Y 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Y 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

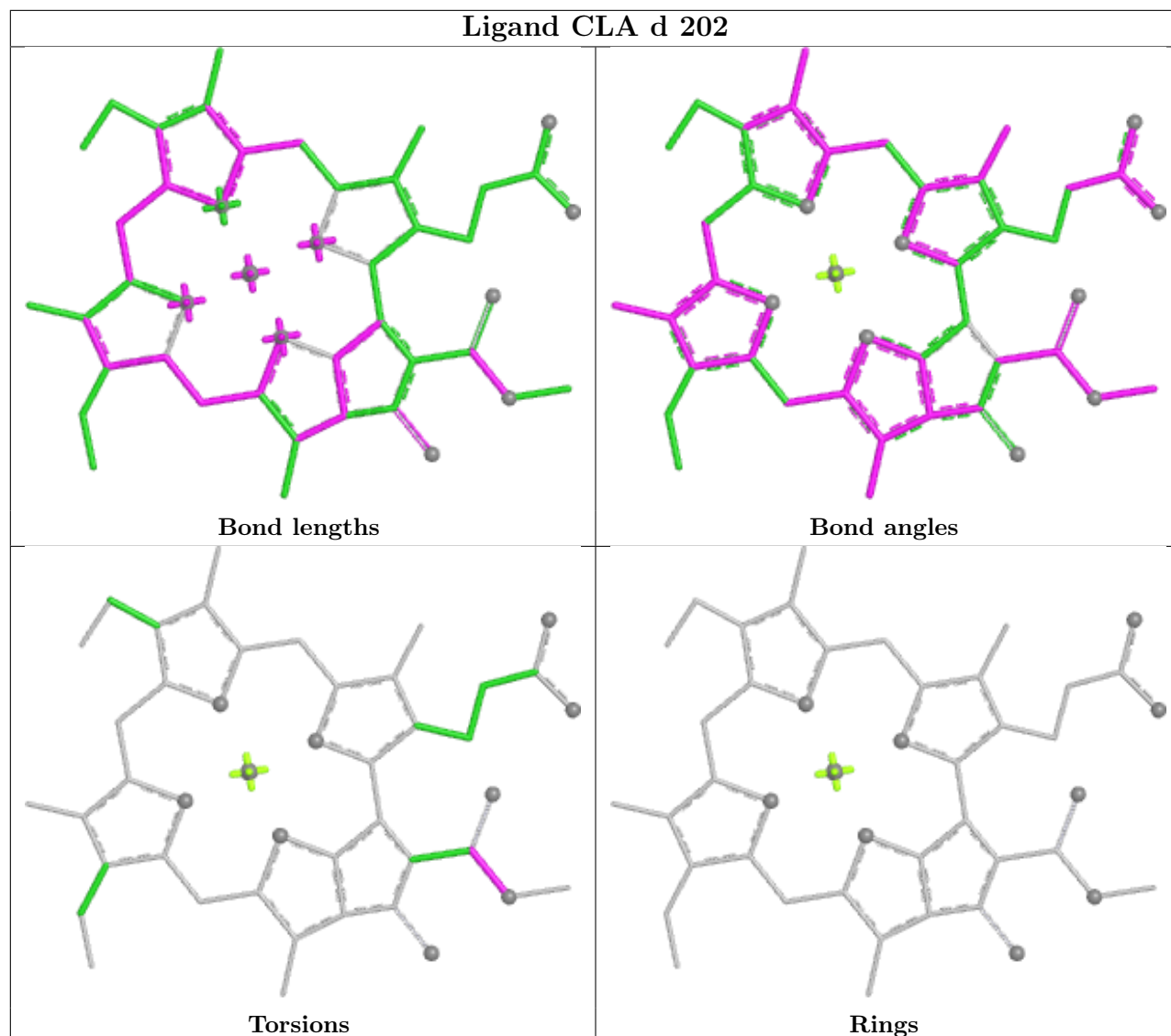
Ligand CLA G 821



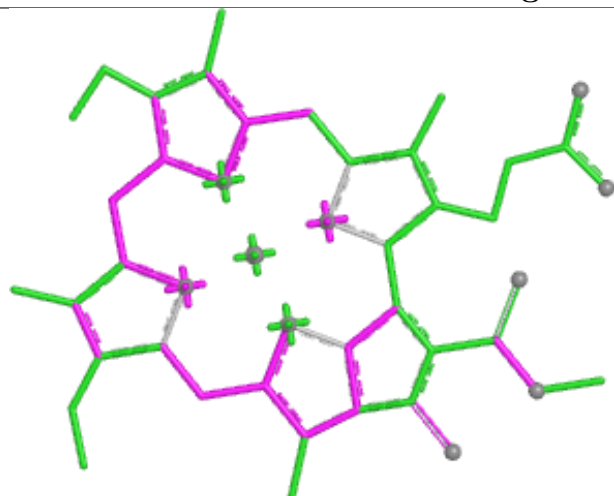
Ligand CLA Y 840



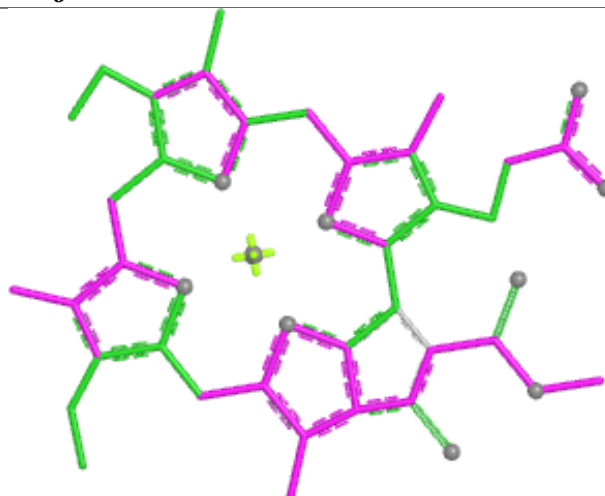
Ligand CLA d 202



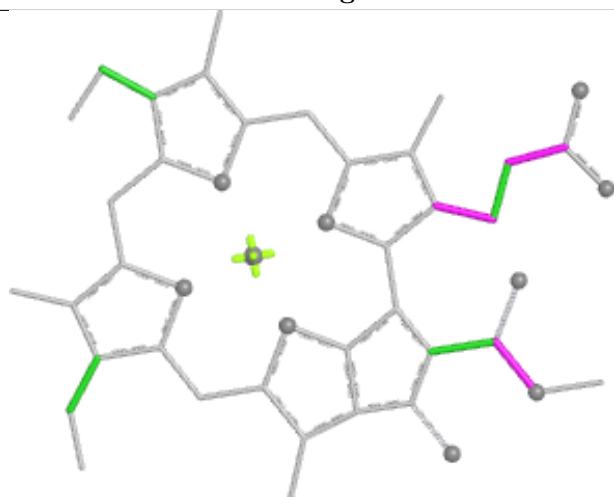
Ligand CLA j 102



Bond lengths



Bond angles

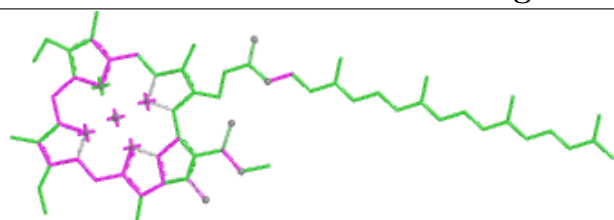


Torsions

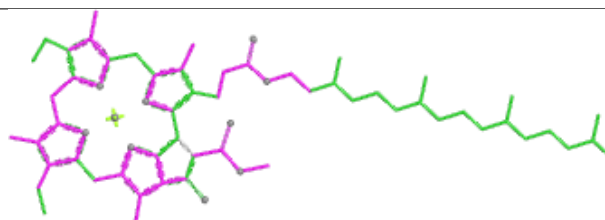


Rings

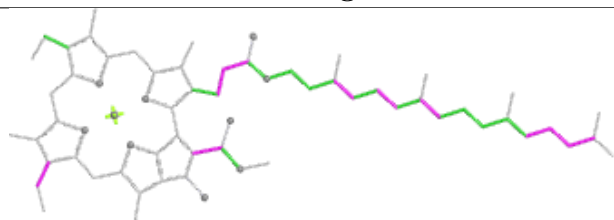
Ligand CLA A 825



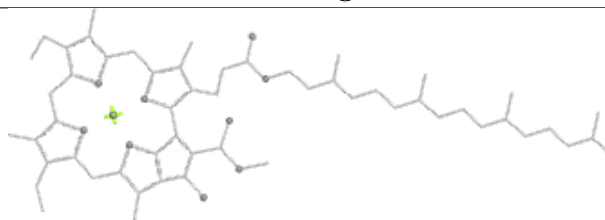
Bond lengths



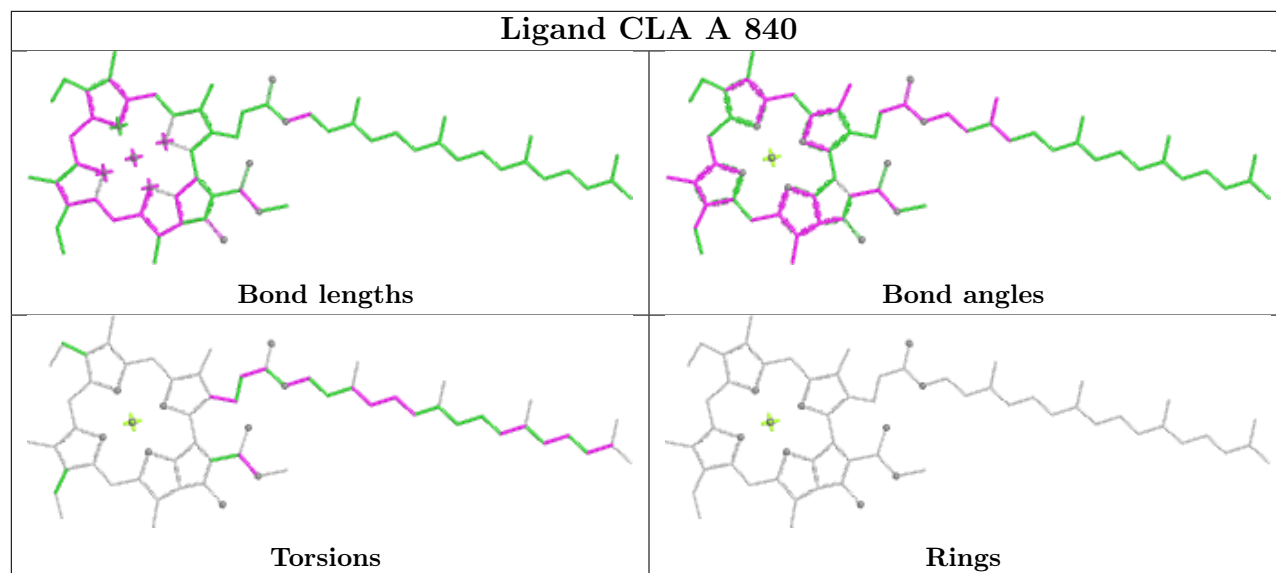
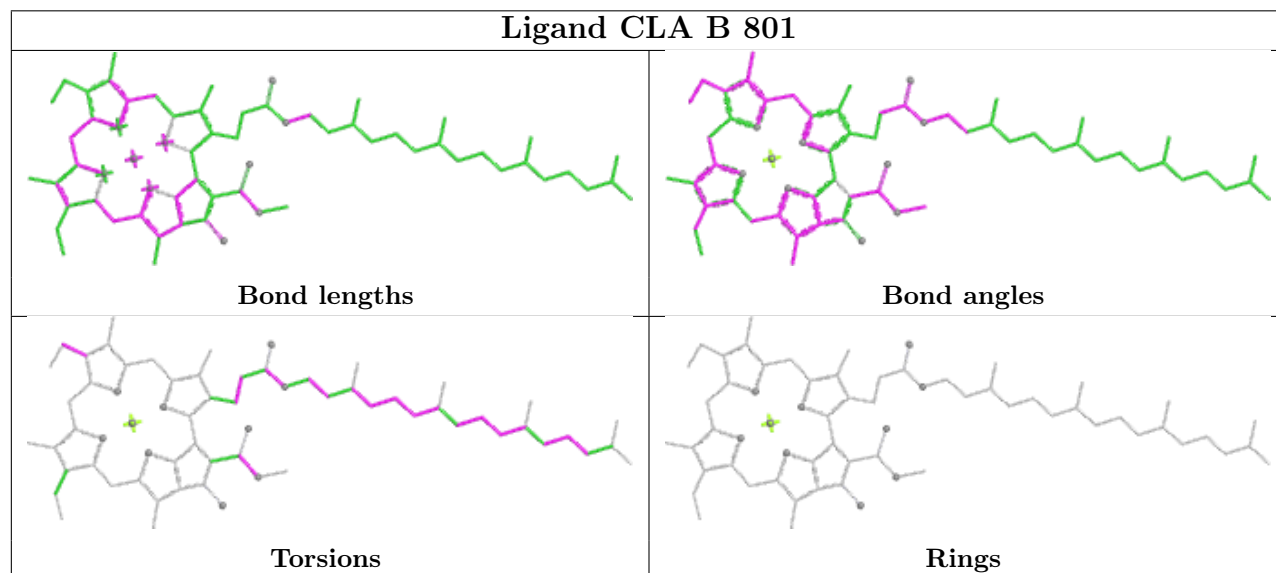
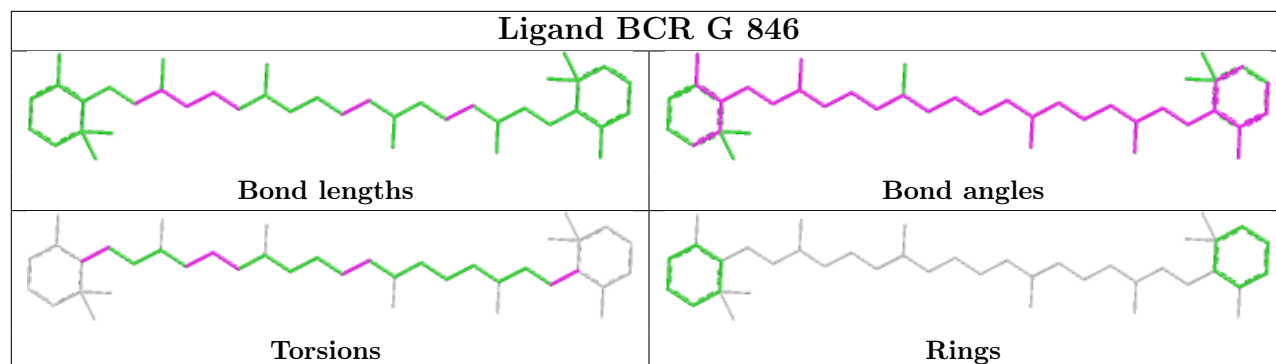
Bond angles

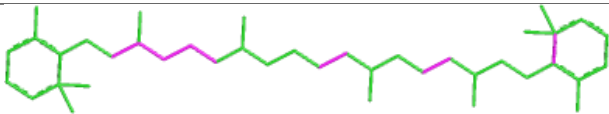
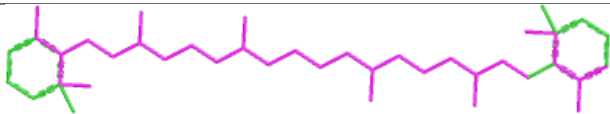
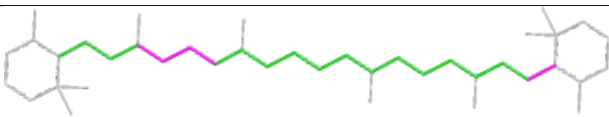
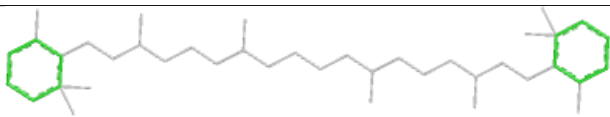


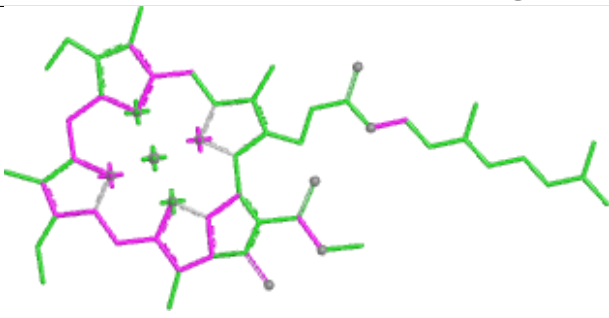
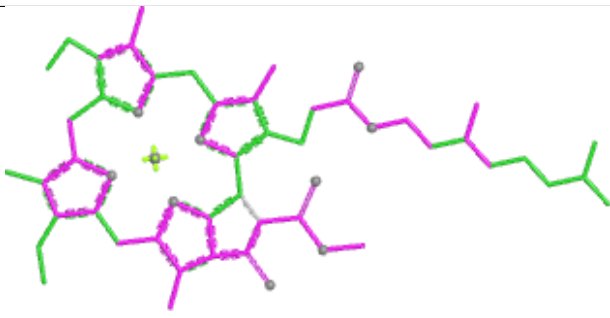
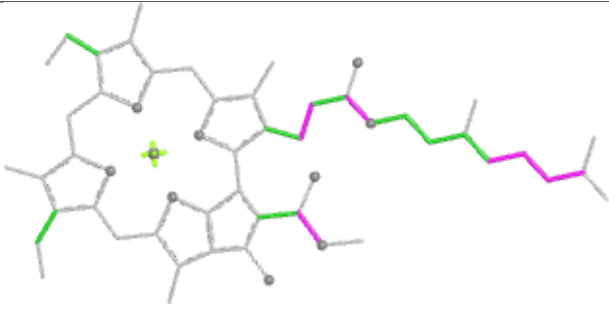
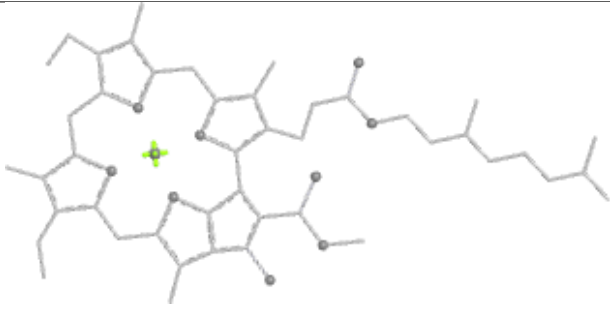
Torsions

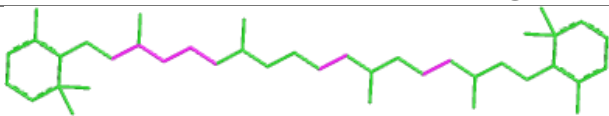
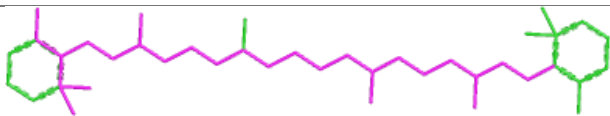
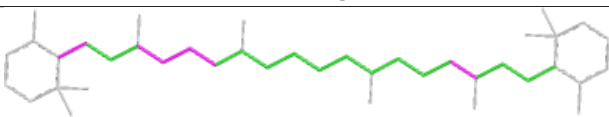
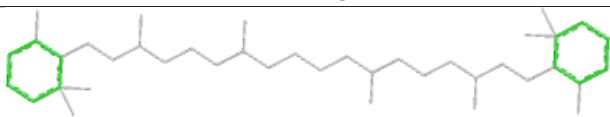


Rings

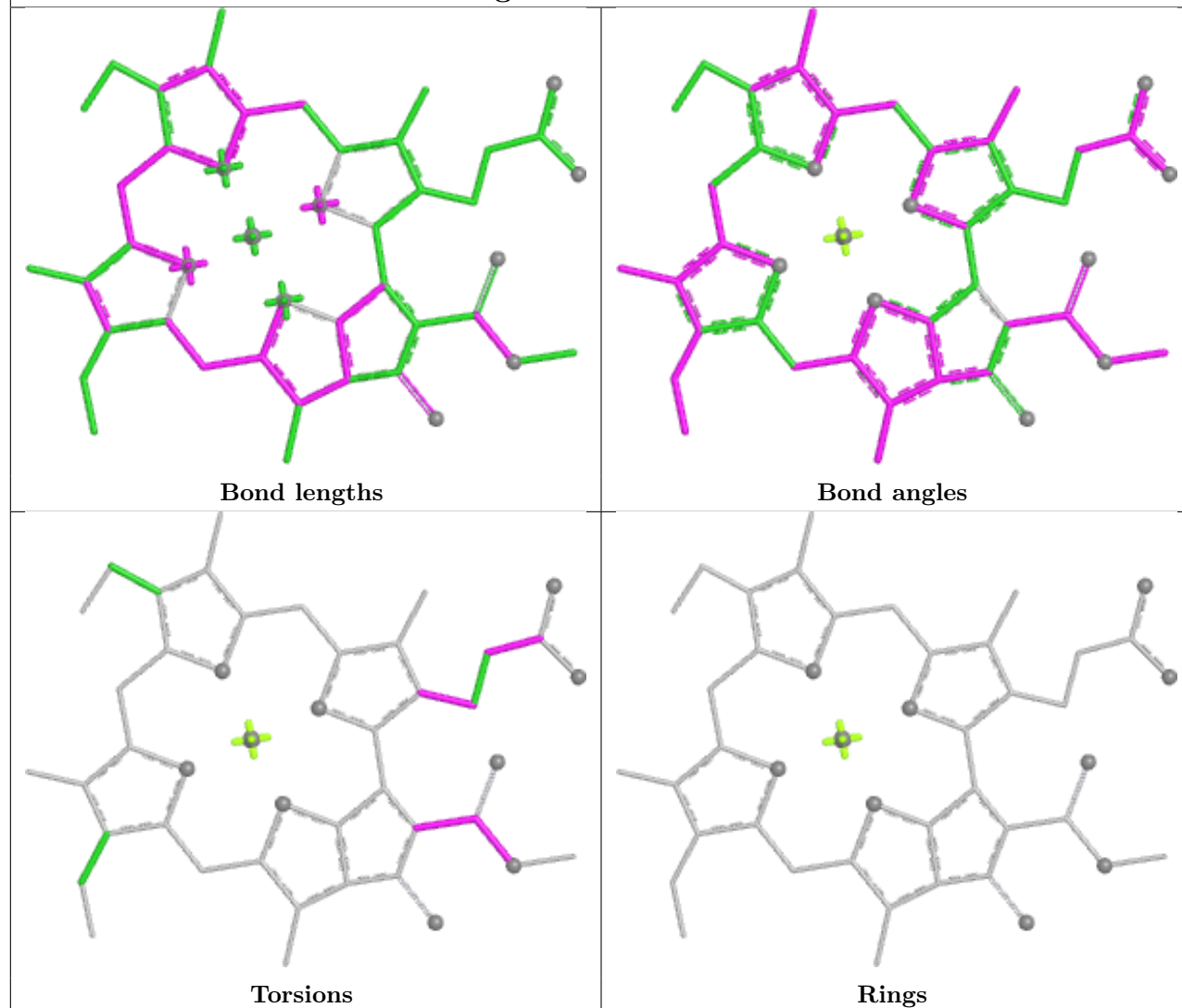


Ligand BCR Z 842	
	
Bond lengths	Bond angles
	
Torsions	Rings

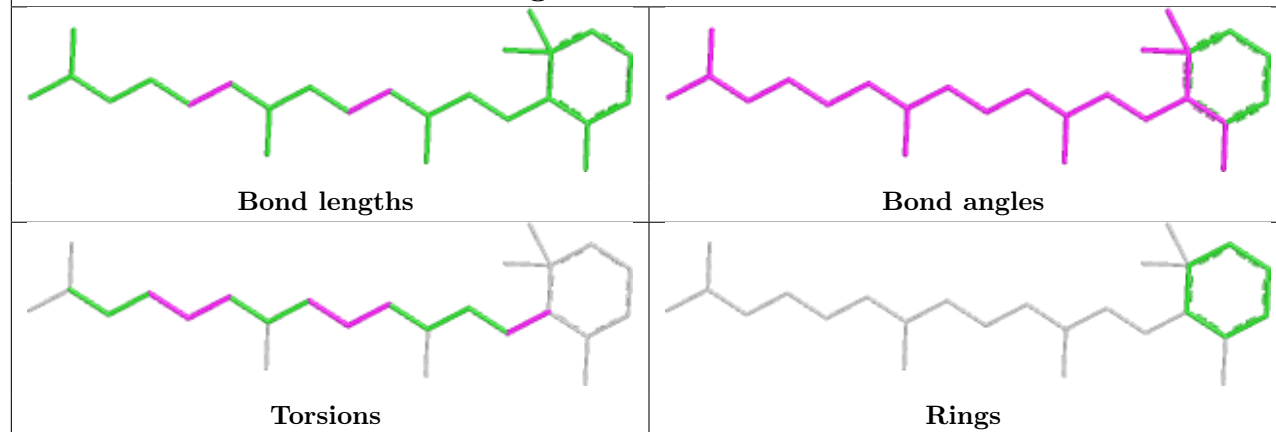
Ligand CLA B 816	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR H 842	
	
Bond lengths	Bond angles
	
Torsions	Rings

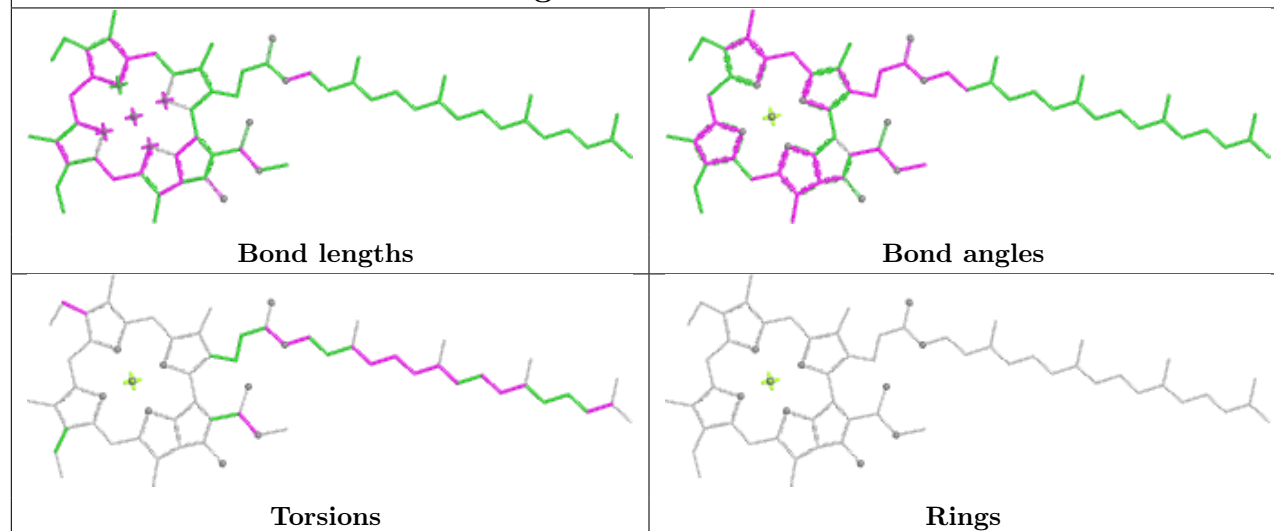
Ligand CLA Z 819



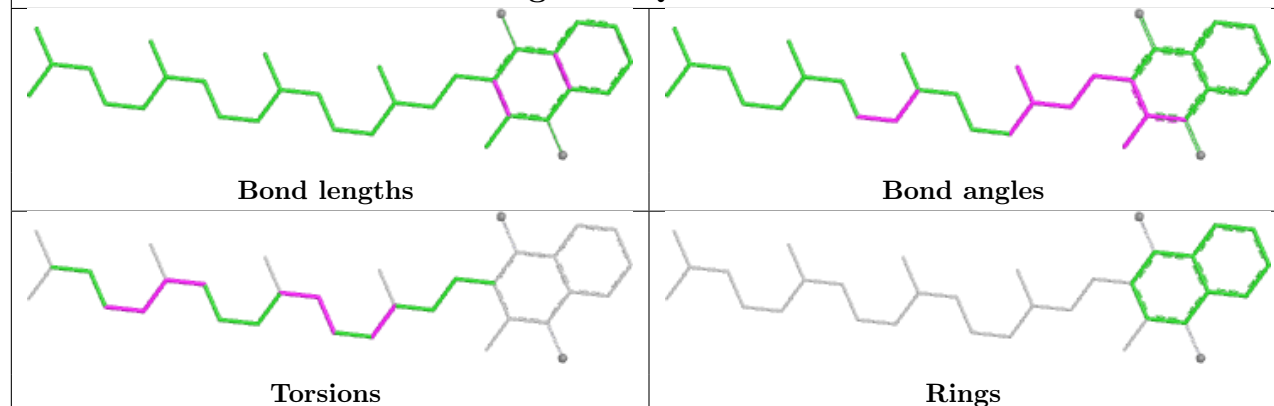
Ligand BCR H 843



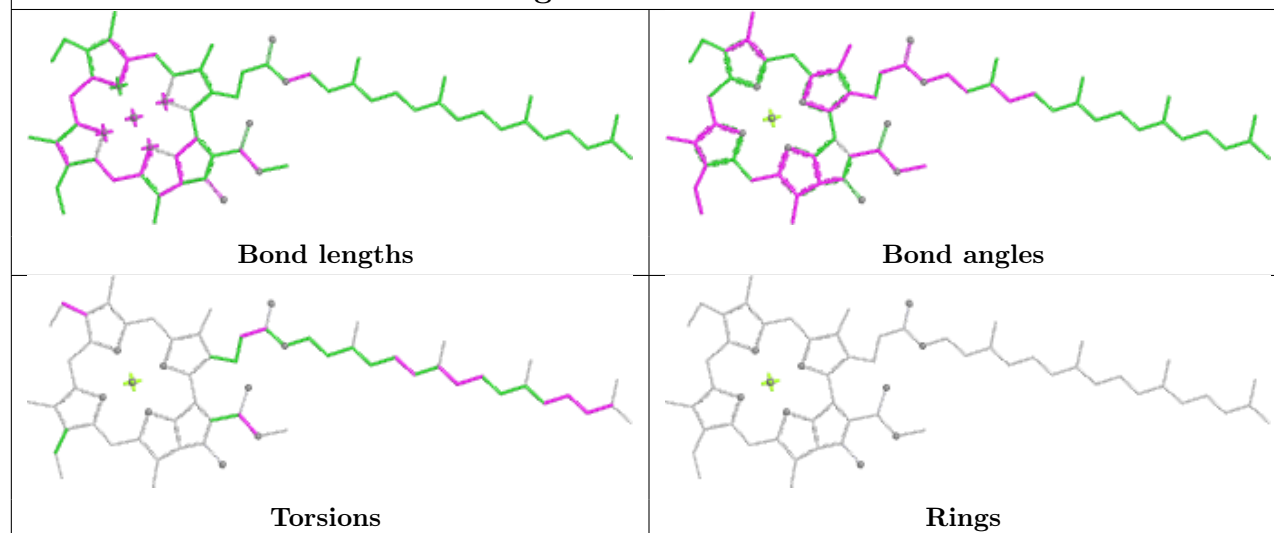
Ligand CLA Z 801

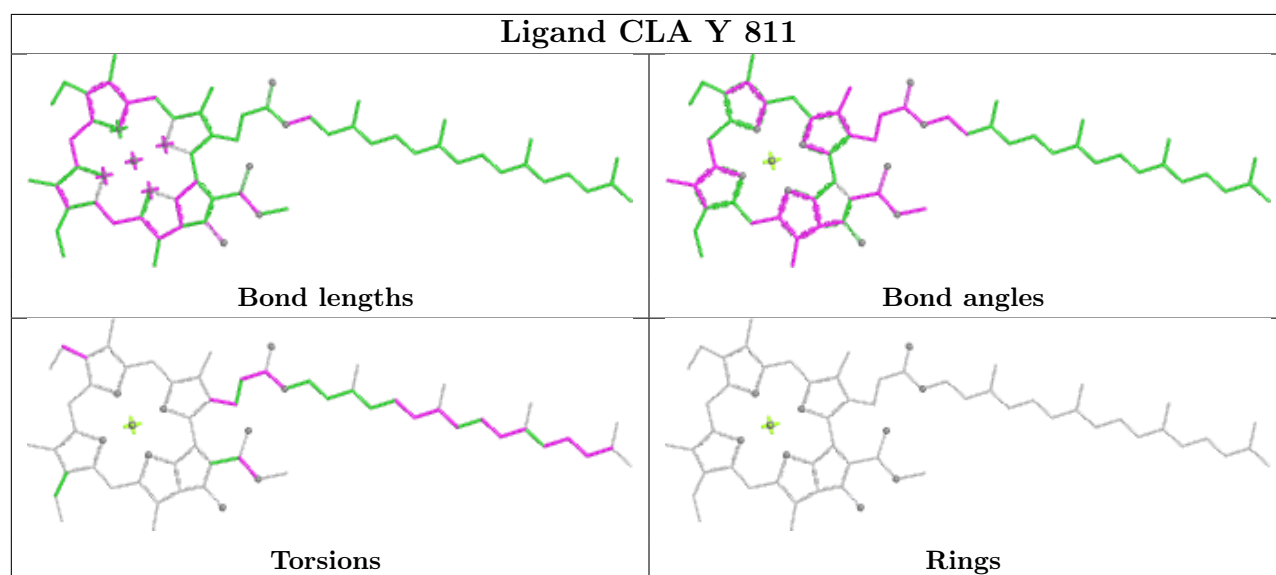
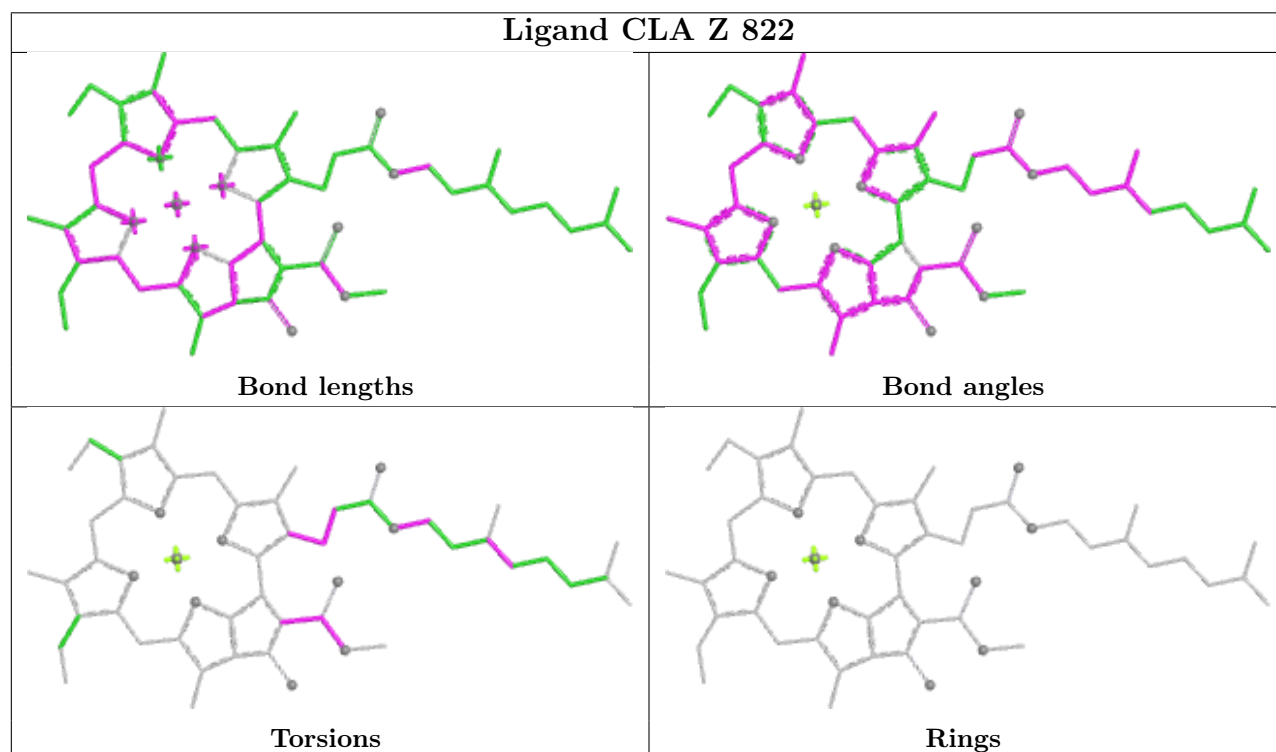
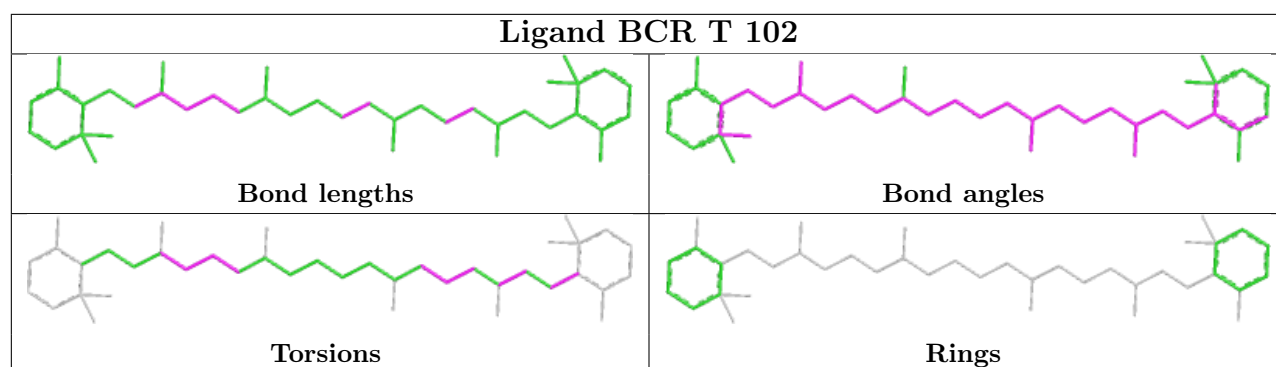


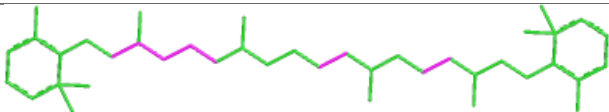
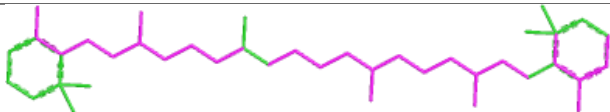
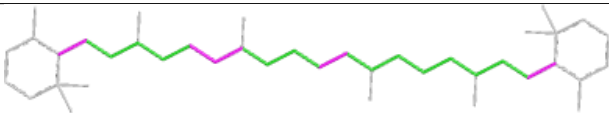
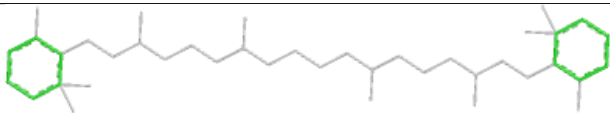
Ligand PQN G 844

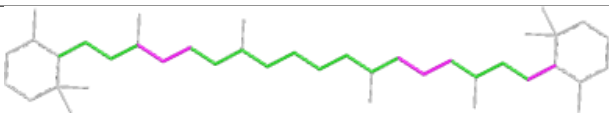
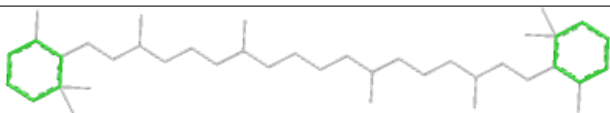


Ligand CLA Z 808

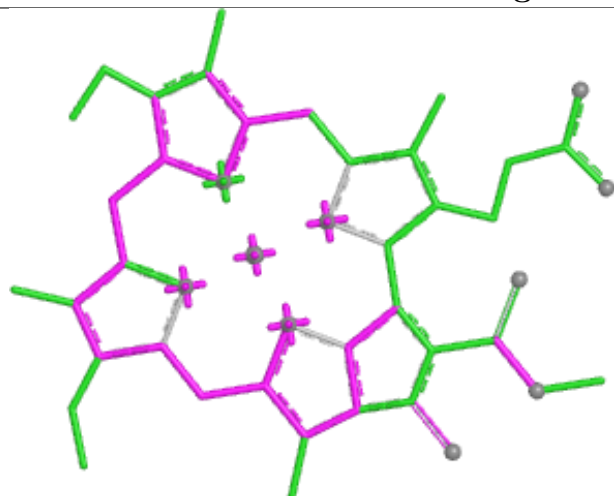




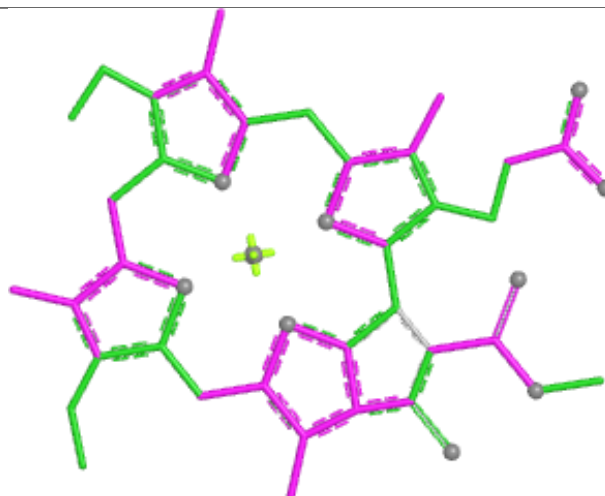
Ligand BCR A 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR Y 850	
	
Bond lengths	Bond angles
	
Torsions	Rings

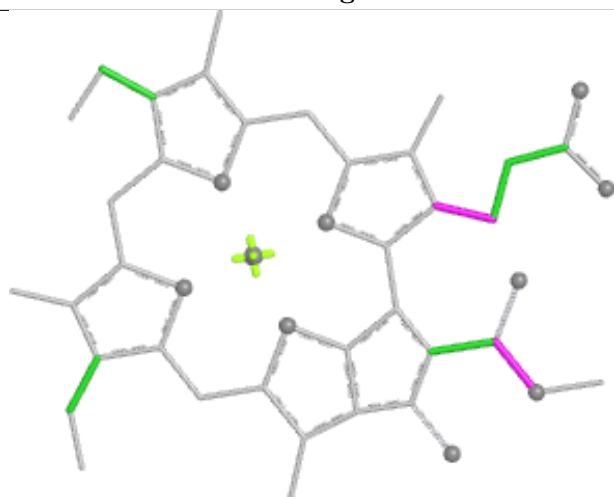
Ligand CLA Y 810



Bond lengths



Bond angles

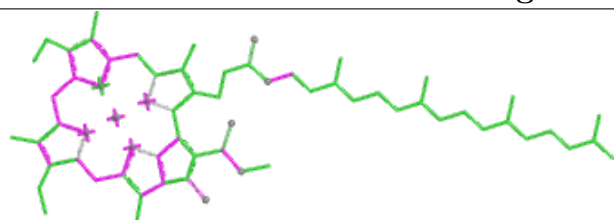


Torsions

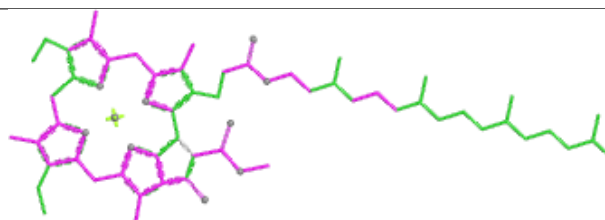


Rings

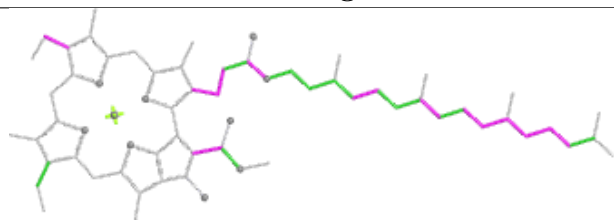
Ligand CLA Z 824



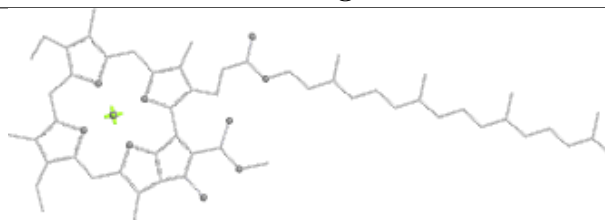
Bond lengths



Bond angles

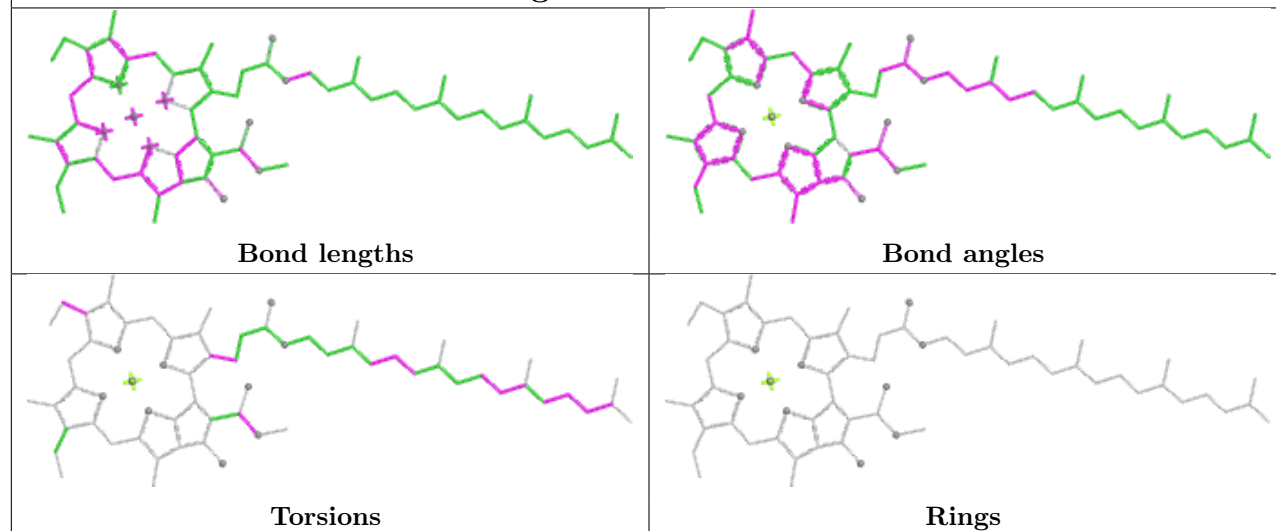


Torsions

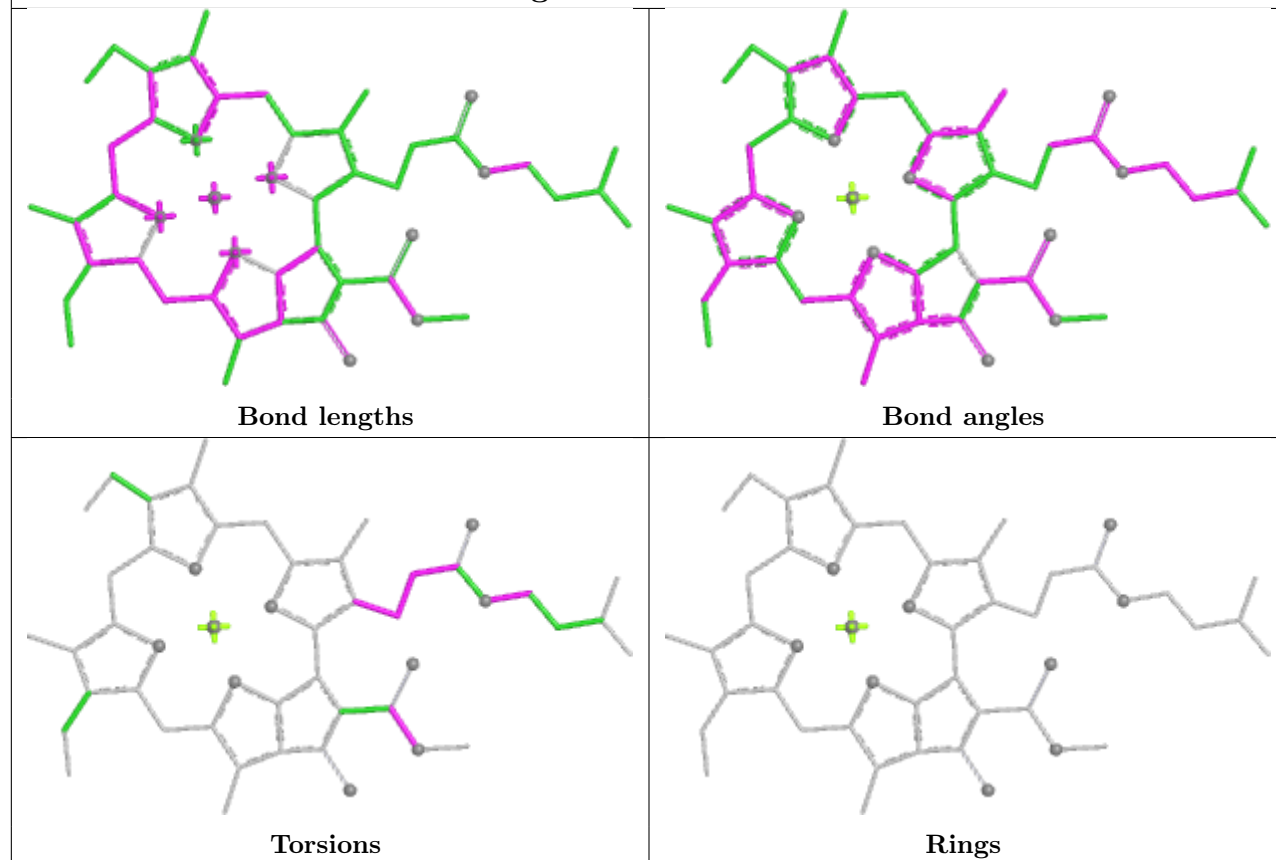


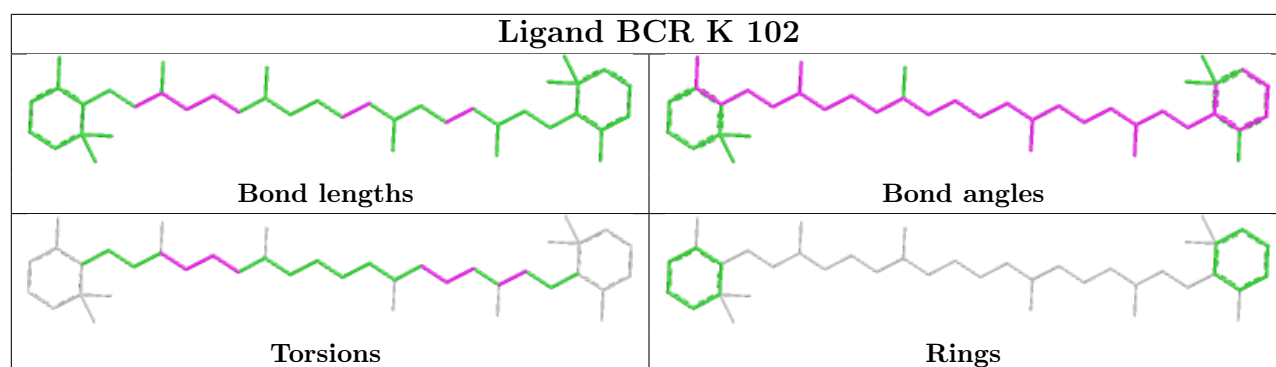
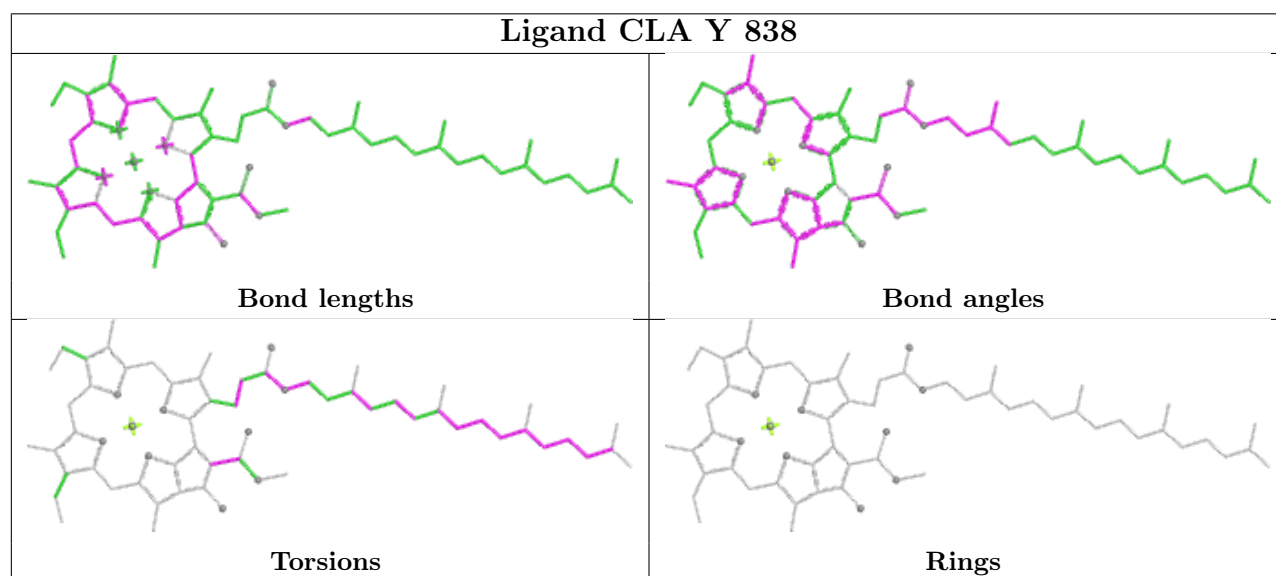
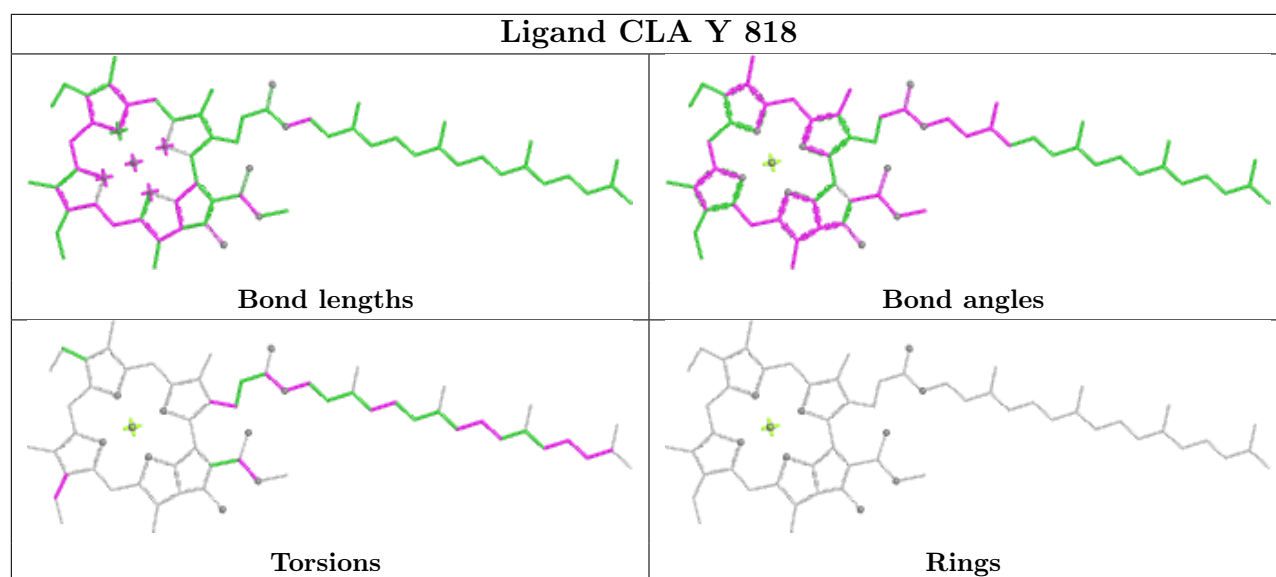
Rings

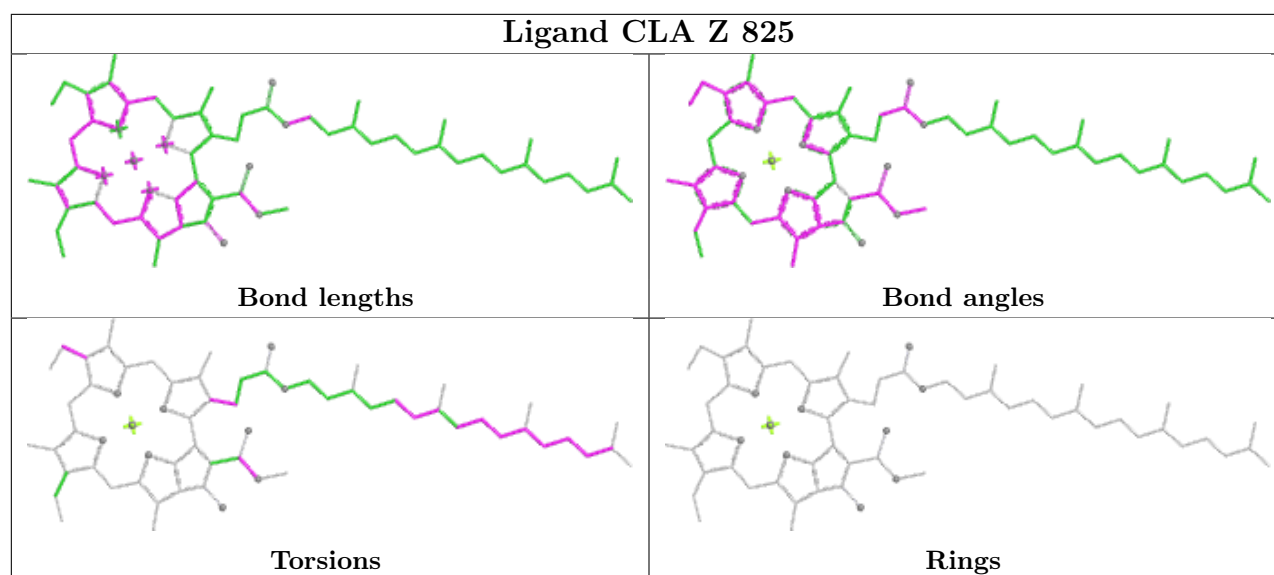
Ligand CLA H 826



Ligand CLA G 836







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-1.52	0 100 100	34, 61, 86, 106	0
1	G	741/755 (98%)	-1.52	0 100 100	34, 62, 89, 120	0
1	Y	741/755 (98%)	-1.49	0 100 100	33, 63, 86, 99	0
2	B	739/741 (99%)	-1.58	0 100 100	33, 54, 74, 94	0
2	H	739/741 (99%)	-1.55	0 100 100	31, 56, 77, 117	0
2	Z	739/741 (99%)	-1.56	0 100 100	30, 58, 77, 95	0
3	C	80/81 (98%)	-1.62	0 100 100	37, 52, 68, 75	0
3	N	80/81 (98%)	-1.56	0 100 100	40, 56, 75, 78	0
3	a	80/81 (98%)	-1.58	0 100 100	42, 55, 66, 82	0
4	D	138/139 (99%)	-1.63	0 100 100	35, 55, 72, 83	0
4	O	138/139 (99%)	-1.55	0 100 100	43, 60, 77, 115	0
4	b	138/139 (99%)	-1.58	0 100 100	41, 60, 76, 108	0
5	E	69/76 (90%)	-1.47	0 100 100	45, 61, 75, 91	0
5	P	69/76 (90%)	-1.55	0 100 100	45, 61, 80, 85	0
5	c	69/76 (90%)	-1.43	0 100 100	51, 65, 81, 86	0
6	F	141/164 (85%)	-1.57	0 100 100	48, 67, 79, 84	0
6	Q	141/164 (85%)	-1.46	0 100 100	48, 70, 89, 108	0
6	d	141/164 (85%)	-1.50	0 100 100	50, 72, 88, 106	0
7	I	38/38 (100%)	-1.41	0 100 100	37, 48, 70, 73	0
7	R	38/38 (100%)	-1.43	0 100 100	36, 51, 70, 75	0
7	e	38/38 (100%)	-1.54	0 100 100	38, 49, 66, 87	0
8	J	41/41 (100%)	-1.40	0 100 100	55, 69, 84, 89	0
8	S	41/41 (100%)	-1.39	0 100 100	62, 71, 86, 93	0
8	f	41/41 (100%)	-1.25	0 100 100	65, 74, 89, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)	Q<0.9		
9	K	46/83 (55%)	-1.18	0	100	100	70, 89, 118, 125	0
9	T	46/83 (55%)	-1.27	0	100	100	71, 90, 103, 116	0
9	g	46/83 (55%)	-1.21	0	100	100	66, 85, 99, 108	0
10	L	151/155 (97%)	-1.58	0	100	100	32, 48, 62, 82	0
10	U	151/155 (97%)	-1.61	0	100	100	33, 47, 67, 83	0
10	h	151/155 (97%)	-1.61	0	100	100	36, 47, 68, 97	0
11	M	30/31 (96%)	-1.70	0	100	100	40, 50, 64, 69	0
11	V	30/31 (96%)	-1.63	0	100	100	41, 49, 65, 73	0
11	i	30/31 (96%)	-1.57	0	100	100	44, 54, 63, 66	0
12	W	26/39 (66%)	-1.35	0	100	100	52, 66, 81, 83	0
12	X	26/39 (66%)	-1.36	0	100	100	54, 62, 69, 70	0
12	j	26/39 (66%)	-1.41	0	100	100	60, 70, 88, 95	0
All	All	6720/7029 (95%)	-1.53	0	100	100	30, 59, 84, 125	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
15	PQN	H	839	33/33	0.98	0.07	38,49,63,66	0
14	CLA	A	803	65/65	0.99	0.05	52,61,70,77	0
14	CLA	A	804	59/65	0.99	0.04	52,60,79,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	A	807	51/65	0.99	0.04	63,72,78,83	0
14	CLA	A	808	65/65	0.99	0.05	46,56,81,83	0
14	CLA	A	810	45/65	0.99	0.04	71,86,89,92	0
14	CLA	A	811	65/65	0.99	0.04	56,80,89,93	0
14	CLA	A	812	54/65	0.99	0.04	58,66,80,89	0
14	CLA	A	813	60/65	0.99	0.05	53,64,82,85	0
14	CLA	A	815	50/65	0.99	0.05	64,78,84,92	0
14	CLA	A	816	50/65	0.99	0.05	68,78,108,115	0
14	CLA	A	820	60/65	0.99	0.04	61,68,78,79	0
14	CLA	A	822	65/65	0.99	0.06	72,84,105,109	0
14	CLA	A	823	50/65	0.99	0.04	53,69,81,92	0
14	CLA	A	824	60/65	0.99	0.04	42,68,71,72	0
14	CLA	A	825	65/65	0.99	0.05	55,68,74,76	0
14	CLA	A	827	65/65	0.99	0.04	38,50,67,73	0
14	CLA	A	828	65/65	0.99	0.04	43,52,68,69	0
14	CLA	A	829	65/65	0.99	0.04	53,62,81,84	0
14	CLA	A	830	65/65	0.99	0.04	42,48,67,72	0
14	CLA	A	831	50/65	0.99	0.04	43,46,60,61	0
14	CLA	A	834	55/65	0.99	0.04	49,66,70,75	0
14	CLA	A	835	45/65	0.99	0.05	58,71,75,79	0
14	CLA	A	840	65/65	0.99	0.04	42,45,81,84	0
14	CLA	A	842	50/65	0.99	0.04	49,61,64,68	0
14	CLA	A	852	65/65	0.99	0.04	44,53,63,69	0
14	CLA	B	801	65/65	0.99	0.04	49,58,65,72	0
14	CLA	B	804	65/65	0.99	0.04	40,48,52,53	0
14	CLA	B	810	65/65	0.99	0.04	37,45,51,54	0
14	CLA	B	812	50/65	0.99	0.04	50,61,66,72	0
14	CLA	B	814	65/65	0.99	0.04	50,54,85,87	0
14	CLA	B	820	45/65	0.99	0.04	50,53,58,63	0
14	CLA	B	821	45/65	0.99	0.03	54,58,68,75	0
14	CLA	B	822	55/65	0.99	0.04	52,59,70,73	0
14	CLA	B	823	60/65	0.99	0.05	57,63,67,74	0
14	CLA	B	829	65/65	0.99	0.04	35,45,57,59	0
14	CLA	B	830	45/65	0.99	0.03	37,44,46,53	0
14	CLA	B	833	55/65	0.99	0.05	59,72,77,78	0
14	CLA	B	835	45/65	0.99	0.04	63,69,74,77	0
14	CLA	B	836	45/65	0.99	0.04	52,62,66,67	0
14	CLA	B	837	60/65	0.99	0.04	47,59,63,64	0
14	CLA	B	841	65/65	0.99	0.04	37,43,48,55	0
14	CLA	G	803	65/65	0.99	0.04	34,52,56,59	0
14	CLA	G	807	51/65	0.99	0.04	70,77,82,86	0
14	CLA	G	808	65/65	0.99	0.05	49,55,82,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	G	809	65/65	0.99	0.04	56,68,81,86	0
14	CLA	G	810	45/65	0.99	0.04	66,73,90,94	0
14	CLA	G	811	65/65	0.99	0.04	59,75,82,85	0
14	CLA	G	815	50/65	0.99	0.04	74,85,95,100	0
14	CLA	G	816	50/65	0.99	0.04	68,79,83,85	0
14	CLA	G	817	60/65	0.99	0.05	56,70,85,87	0
14	CLA	G	818	65/65	0.99	0.04	59,72,87,93	0
14	CLA	G	820	60/65	0.99	0.04	66,80,86,91	0
14	CLA	G	821	65/65	0.99	0.04	47,63,67,70	0
14	CLA	G	822	65/65	0.99	0.05	59,66,89,92	0
14	CLA	G	823	50/65	0.99	0.04	57,72,97,101	0
14	CLA	G	824	60/65	0.99	0.04	51,59,67,70	0
14	CLA	G	825	65/65	0.99	0.04	58,62,66,68	0
14	CLA	G	827	65/65	0.99	0.04	52,62,87,91	0
14	CLA	G	828	65/65	0.99	0.04	51,64,73,74	0
14	CLA	G	830	65/65	0.99	0.04	43,53,76,78	0
14	CLA	G	832	65/65	0.99	0.04	41,48,54,60	0
14	CLA	G	834	55/65	0.99	0.04	50,61,69,72	0
14	CLA	G	836	50/65	0.99	0.04	47,59,62,64	0
14	CLA	G	837	65/65	0.99	0.03	42,53,58,64	0
14	CLA	G	838	50/65	0.99	0.04	46,51,57,59	0
14	CLA	G	841	65/65	0.99	0.04	49,56,63,65	0
14	CLA	G	843	50/65	0.99	0.04	49,58,86,94	0
14	CLA	H	801	65/65	0.99	0.04	42,51,55,66	0
14	CLA	H	803	65/65	0.99	0.04	38,42,47,52	0
14	CLA	H	808	65/65	0.99	0.05	40,48,54,55	0
14	CLA	H	810	55/65	0.99	0.04	49,55,64,66	0
14	CLA	H	815	55/65	0.99	0.04	56,65,90,93	0
14	CLA	H	816	65/65	0.99	0.04	46,60,73,76	0
14	CLA	H	818	60/65	0.99	0.05	50,61,67,70	0
14	CLA	H	821	55/65	0.99	0.04	54,64,68,72	0
14	CLA	H	822	60/65	0.99	0.04	49,60,72,75	0
14	CLA	H	823	55/65	0.99	0.04	47,56,59,61	0
14	CLA	H	824	65/65	0.99	0.04	53,69,73,73	0
14	CLA	H	827	65/65	0.99	0.05	46,54,61,64	0
14	CLA	H	829	45/65	0.99	0.04	37,48,58,60	0
14	CLA	H	830	55/65	0.99	0.04	70,76,84,92	0
14	CLA	H	831	45/65	0.99	0.04	55,71,78,81	0
14	CLA	H	832	45/65	0.99	0.04	60,74,84,89	0
14	CLA	H	833	45/65	0.99	0.03	59,66,72,74	0
14	CLA	H	834	60/65	0.99	0.05	46,60,80,82	0
14	CLA	J	101	45/65	0.99	0.04	68,81,99,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	J	102	55/65	0.99	0.05	73,84,130,134	0
14	CLA	K	101	41/65	0.99	0.04	50,61,66,67	0
14	CLA	L	202	65/65	0.99	0.04	32,39,48,52	0
14	CLA	L	205	65/65	0.99	0.04	42,51,56,57	0
14	CLA	Q	203	45/65	0.99	0.04	52,69,74,76	0
14	CLA	S	1101	65/65	0.99	0.06	57,64,71,74	0
14	CLA	S	1102	45/65	0.99	0.04	81,88,94,103	0
14	CLA	S	1103	55/65	0.99	0.04	60,74,114,118	0
14	CLA	T	101	41/65	0.99	0.04	60,75,81,84	0
14	CLA	T	103	45/65	0.99	0.04	68,83,88,89	0
14	CLA	U	1006	65/65	0.99	0.03	32,38,45,56	0
14	CLA	W	1701	45/65	0.99	0.04	58,65,68,69	0
14	CLA	Y	802	65/65	0.99	0.04	32,43,47,51	0
14	CLA	Y	803	65/65	0.99	0.04	53,67,75,77	0
14	CLA	Y	804	59/65	0.99	0.04	63,70,82,85	0
14	CLA	Y	807	51/65	0.99	0.05	63,86,92,93	0
14	CLA	Y	808	65/65	0.99	0.04	41,50,68,70	0
14	CLA	Y	809	65/65	0.99	0.04	60,72,78,84	0
14	CLA	Y	810	45/65	0.99	0.04	71,80,84,86	0
14	CLA	Y	811	65/65	0.99	0.04	59,72,77,82	0
14	CLA	Y	814	55/65	0.99	0.04	50,71,74,78	0
14	CLA	Y	815	50/65	0.99	0.05	71,80,84,86	0
14	CLA	Y	816	50/65	0.99	0.04	63,74,124,130	0
14	CLA	Y	817	60/65	0.99	0.04	45,75,86,89	0
14	CLA	Y	818	65/65	0.99	0.05	56,65,76,85	0
14	CLA	Y	820	60/65	0.99	0.04	56,71,87,92	0
14	CLA	Y	822	65/65	0.99	0.05	64,80,95,98	0
14	CLA	Y	823	50/65	0.99	0.04	64,73,90,93	0
14	CLA	Y	824	60/65	0.99	0.04	58,70,87,89	0
14	CLA	Y	825	65/65	0.99	0.05	43,65,70,71	0
14	CLA	Y	826	60/65	0.99	0.04	38,44,55,56	0
14	CLA	Y	827	65/65	0.99	0.04	49,63,68,70	0
14	CLA	Y	828	65/65	0.99	0.04	56,66,73,78	0
14	CLA	Y	834	65/65	0.99	0.04	35,40,49,56	0
14	CLA	Y	836	45/65	0.99	0.04	58,77,81,81	0
14	CLA	Y	837	50/65	0.99	0.04	40,50,58,61	0
14	CLA	Y	838	65/65	0.99	0.03	44,53,56,63	0
14	CLA	Y	841	65/65	0.99	0.04	50,57,75,77	0
14	CLA	Y	843	50/65	0.99	0.04	62,71,87,95	0
14	CLA	Y	854	65/65	0.99	0.05	46,58,65,68	0
14	CLA	Y	855	65/65	0.99	0.04	36,50,54,62	0
14	CLA	Z	801	65/65	0.99	0.04	45,52,62,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	Z	803	54/65	0.99	0.04	40,43,47,57	0
14	CLA	Z	804	65/65	0.99	0.04	41,48,52,54	0
14	CLA	Z	805	65/65	0.99	0.04	40,47,54,65	0
14	CLA	Z	806	65/65	0.99	0.04	36,45,62,67	0
14	CLA	Z	807	65/65	0.99	0.04	50,58,61,65	0
14	CLA	Z	808	65/65	0.99	0.04	41,51,57,61	0
14	CLA	Z	810	45/65	0.99	0.03	57,63,75,92	0
14	CLA	Z	813	45/65	0.99	0.04	58,64,72,80	0
14	CLA	Z	814	55/65	0.99	0.04	56,74,86,91	0
14	CLA	Z	815	65/65	0.99	0.05	48,56,81,85	0
14	CLA	Z	816	60/65	0.99	0.04	49,59,65,68	0
14	CLA	Z	817	60/65	0.99	0.04	54,63,84,87	0
14	CLA	Z	818	45/65	0.99	0.04	57,64,80,84	0
14	CLA	Z	820	55/65	0.99	0.04	52,78,84,86	0
14	CLA	Z	821	60/65	0.99	0.05	58,73,90,91	0
14	CLA	Z	823	65/65	0.99	0.04	44,57,70,71	0
14	CLA	Z	827	65/65	0.99	0.04	39,47,57,62	0
14	CLA	Z	828	45/65	0.99	0.04	51,64,77,91	0
14	CLA	Z	834	45/65	0.99	0.04	67,75,78,81	0
14	CLA	Z	835	60/65	0.99	0.04	40,53,62,65	0
14	CLA	Z	837	45/65	0.99	0.04	51,56,59,72	0
14	CLA	d	202	45/65	0.99	0.04	67,73,80,87	0
14	CLA	f	101	45/65	0.99	0.05	84,99,109,114	0
14	CLA	f	102	55/65	0.99	0.05	74,88,104,106	0
14	CLA	g	101	41/65	0.99	0.03	54,70,74,75	0
14	CLA	j	102	45/65	0.99	0.04	58,69,73,78	0
15	PQN	A	843	33/33	0.99	0.06	54,59,63,64	0
15	PQN	B	842	33/33	0.99	0.05	43,51,63,68	0
15	PQN	G	844	33/33	0.99	0.06	51,58,63,65	0
14	CLA	A	802	65/65	0.99	0.04	28,48,52,54	0
15	PQN	Y	844	33/33	0.99	0.05	45,55,67,67	0
15	PQN	Z	840	33/33	0.99	0.06	49,54,64,65	0
17	BCR	A	846	40/40	0.99	0.06	75,83,93,97	0
17	BCR	A	847	40/40	0.99	0.06	45,60,79,83	0
17	BCR	A	848	40/40	0.99	0.05	35,53,60,61	0
17	BCR	A	849	40/40	0.99	0.05	45,51,56,58	0
17	BCR	B	843	30/40	0.99	0.06	70,79,87,90	0
17	BCR	B	845	40/40	0.99	0.05	55,64,82,84	0
17	BCR	B	846	25/40	0.99	0.04	26,41,46,49	0
17	BCR	B	847	40/40	0.99	0.05	39,46,51,52	0
17	BCR	B	848	40/40	0.99	0.04	38,44,70,71	0
17	BCR	B	851	40/40	0.99	0.05	56,65,81,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	BCR	F	201	40/40	0.99	0.05	44,77,86,88	0
17	BCR	F	203	40/40	0.99	0.04	44,49,74,74	0
17	BCR	G	846	40/40	0.99	0.05	67,72,76,77	0
17	BCR	G	847	40/40	0.99	0.05	70,80,109,111	0
17	BCR	G	848	40/40	0.99	0.05	51,61,90,92	0
17	BCR	H	840	40/40	0.99	0.05	73,87,96,97	0
17	BCR	H	841	40/40	0.99	0.04	46,58,68,69	0
17	BCR	H	842	40/40	0.99	0.05	38,71,81,83	0
17	BCR	H	843	25/40	0.99	0.04	28,57,59,60	0
17	BCR	H	844	40/40	0.99	0.05	43,57,63,63	0
17	BCR	H	848	40/40	0.99	0.05	54,72,79,87	0
17	BCR	I	101	40/40	0.99	0.03	33,35,40,41	0
17	BCR	J	103	40/40	0.99	0.05	52,62,77,79	0
17	BCR	J	104	40/40	0.99	0.06	57,73,83,85	0
17	BCR	K	102	40/40	0.99	0.05	62,82,92,94	0
17	BCR	L	208	40/40	0.99	0.04	36,39,43,43	0
17	BCR	L	209	40/40	0.99	0.05	41,44,80,82	0
17	BCR	Q	202	40/40	0.99	0.06	55,66,72,73	0
17	BCR	Q	204	40/40	0.99	0.04	50,58,64,66	0
17	BCR	R	102	40/40	0.99	0.05	36,42,57,60	0
17	BCR	S	1104	40/40	0.99	0.05	57,68,73,77	0
17	BCR	U	1005	40/40	0.99	0.03	30,36,52,53	0
17	BCR	U	1008	40/40	0.99	0.04	33,41,69,70	0
17	BCR	V	1202	40/40	0.99	0.04	49,56,64,69	0
17	BCR	Y	846	40/40	0.99	0.05	60,70,77,78	0
17	BCR	Y	848	40/40	0.99	0.04	58,75,79,81	0
17	BCR	Y	849	40/40	0.99	0.05	53,68,135,141	0
17	BCR	Y	850	40/40	0.99	0.04	46,52,65,66	0
17	BCR	Y	856	40/40	0.99	0.04	40,43,45,46	0
17	BCR	Z	841	40/40	0.99	0.05	58,66,94,97	0
17	BCR	Z	842	40/40	0.99	0.04	46,54,68,69	0
17	BCR	Z	845	40/40	0.99	0.05	48,53,59,65	0
17	BCR	d	203	40/40	0.99	0.06	52,59,63,64	0
17	BCR	e	101	40/40	0.99	0.04	32,40,49,51	0
17	BCR	f	104	40/40	0.99	0.05	57,68,82,88	0
18	LHG	A	850	49/49	0.99	0.04	41,52,62,63	0
18	LHG	B	850	39/49	0.99	0.04	53,60,97,99	0
18	LHG	G	851	49/49	0.99	0.04	49,58,63,68	0
18	LHG	H	847	37/49	0.99	0.04	59,76,103,115	0
18	LHG	Y	852	49/49	0.99	0.05	49,60,69,70	0
18	LHG	j	101	28/49	0.99	0.04	53,60,67,71	0
19	LMG	B	849	52/55	0.99	0.04	28,44,68,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	LMG	H	846	49/55	0.99	0.04	35,43,58,61	0
19	LMG	Z	847	49/55	0.99	0.05	46,57,68,73	0
14	CLA	B	817	65/65	1.00	0.04	48,55,62,63	0
14	CLA	G	833	65/65	1.00	0.03	37,41,52,59	0
14	CLA	B	818	60/65	1.00	0.03	45,52,56,57	0
14	CLA	Y	829	65/65	1.00	0.03	47,57,79,85	0
14	CLA	Y	830	65/65	1.00	0.04	45,55,64,67	0
14	CLA	Y	831	50/65	1.00	0.04	48,52,71,75	0
14	CLA	Y	832	65/65	1.00	0.03	46,52,77,79	0
14	CLA	Y	833	65/65	1.00	0.03	34,37,55,61	0
14	CLA	G	835	45/65	1.00	0.03	51,65,70,74	0
14	CLA	Y	835	55/65	1.00	0.04	60,67,75,76	0
14	CLA	B	819	60/65	1.00	0.03	50,57,60,65	0
14	CLA	A	818	65/65	1.00	0.03	42,52,64,66	0
14	CLA	A	819	65/65	1.00	0.03	59,67,78,82	0
14	CLA	Y	839	50/65	1.00	0.03	44,50,62,66	0
14	CLA	Y	840	65/65	1.00	0.03	51,56,73,75	0
14	CLA	G	839	65/65	1.00	0.04	56,62,70,73	0
14	CLA	Y	842	65/65	1.00	0.03	30,36,49,50	0
14	CLA	G	840	50/65	1.00	0.03	46,52,58,63	0
14	CLA	A	832	65/65	1.00	0.03	37,42,89,96	0
14	CLA	G	842	65/65	1.00	0.02	31,33,40,46	0
14	CLA	A	833	65/65	1.00	0.03	31,36,47,57	0
14	CLA	Z	802	65/65	1.00	0.04	53,60,66,73	0
14	CLA	G	853	45/65	1.00	0.03	49,59,71,74	0
14	CLA	B	824	55/65	1.00	0.03	40,53,57,59	0
14	CLA	H	802	65/65	1.00	0.03	45,49,63,66	0
14	CLA	B	825	65/65	1.00	0.03	44,51,60,61	0
14	CLA	H	804	65/65	1.00	0.04	45,54,59,61	0
14	CLA	H	805	65/65	1.00	0.03	50,57,61,62	0
14	CLA	Z	809	55/65	1.00	0.03	45,62,69,73	0
14	CLA	H	806	65/65	1.00	0.03	36,40,56,61	0
14	CLA	Z	811	65/65	1.00	0.03	44,53,86,96	0
14	CLA	Z	812	65/65	1.00	0.04	45,54,63,67	0
14	CLA	H	807	65/65	1.00	0.03	43,48,55,57	0
14	CLA	B	826	65/65	1.00	0.03	40,44,48,51	0
14	CLA	H	809	65/65	1.00	0.03	33,41,49,51	0
14	CLA	B	827	65/65	1.00	0.03	39,47,65,66	0
14	CLA	H	811	45/65	1.00	0.03	58,64,70,72	0
14	CLA	H	812	65/65	1.00	0.03	50,59,65,67	0
14	CLA	Z	819	45/65	1.00	0.03	57,65,75,81	0
14	CLA	H	813	65/65	1.00	0.03	49,55,66,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	H	814	45/65	1.00	0.04	66,75,85,86	0
14	CLA	Z	822	55/65	1.00	0.03	44,50,53,55	0
14	CLA	B	828	65/65	1.00	0.04	46,51,54,59	0
14	CLA	Z	824	65/65	1.00	0.03	43,49,56,59	0
14	CLA	Z	825	65/65	1.00	0.03	47,52,70,74	0
14	CLA	Z	826	65/65	1.00	0.04	43,54,64,66	0
13	CL0	Y	801	65/65	1.00	0.04	44,54,60,63	0
14	CLA	H	817	60/65	1.00	0.04	43,53,78,80	0
14	CLA	Z	829	45/65	1.00	0.03	46,61,65,66	0
14	CLA	Z	830	65/65	1.00	0.04	53,62,81,83	0
14	CLA	Z	831	55/65	1.00	0.04	58,67,71,77	0
14	CLA	Z	832	45/65	1.00	0.03	51,63,75,86	0
14	CLA	Z	833	45/65	1.00	0.04	52,67,71,73	0
14	CLA	A	821	65/65	1.00	0.04	51,62,69,73	0
14	CLA	H	819	45/65	1.00	0.04	59,69,73,75	0
14	CLA	Z	836	65/65	1.00	0.04	48,60,68,69	0
14	CLA	H	820	45/65	1.00	0.03	66,72,77,81	0
14	CLA	Z	838	65/65	1.00	0.03	31,34,48,50	0
14	CLA	Z	839	65/65	1.00	0.03	33,45,48,49	0
14	CLA	d	201	50/65	1.00	0.03	51,57,62,66	0
14	CLA	B	831	45/65	1.00	0.02	40,44,51,55	0
14	CLA	B	832	65/65	1.00	0.03	38,47,69,75	0
14	CLA	A	836	50/65	1.00	0.03	43,52,68,74	0
14	CLA	B	834	45/65	1.00	0.04	57,66,71,77	0
14	CLA	g	102	45/65	1.00	0.03	50,62,65,75	0
14	CLA	h	201	65/65	1.00	0.04	45,49,83,86	0
14	CLA	h	205	65/65	1.00	0.03	40,45,57,71	0
14	CLA	h	206	65/65	1.00	0.03	42,51,56,58	0
14	CLA	h	207	65/65	1.00	0.03	32,36,58,60	0
14	CLA	H	825	65/65	1.00	0.03	46,59,65,68	0
14	CLA	H	826	65/65	1.00	0.03	42,48,63,65	0
14	CLA	A	837	65/65	1.00	0.03	45,57,63,66	0
14	CLA	H	828	65/65	1.00	0.03	42,49,63,69	0
14	CLA	A	838	50/65	1.00	0.03	47,57,62,75	0
14	CLA	A	839	50/65	1.00	0.03	47,57,78,83	0
14	CLA	B	838	65/65	1.00	0.03	46,64,69,84	0
16	SF4	A	844	8/8	1.00	0.01	49,50,55,55	0
16	SF4	C	101	8/8	1.00	0.01	41,44,50,51	0
16	SF4	C	102	8/8	1.00	0.01	61,63,68,73	0
16	SF4	G	845	8/8	1.00	0.01	63,69,74,82	0
16	SF4	N	101	8/8	1.00	0.01	54,61,66,68	0
16	SF4	N	102	8/8	1.00	0.01	62,65,71,78	0

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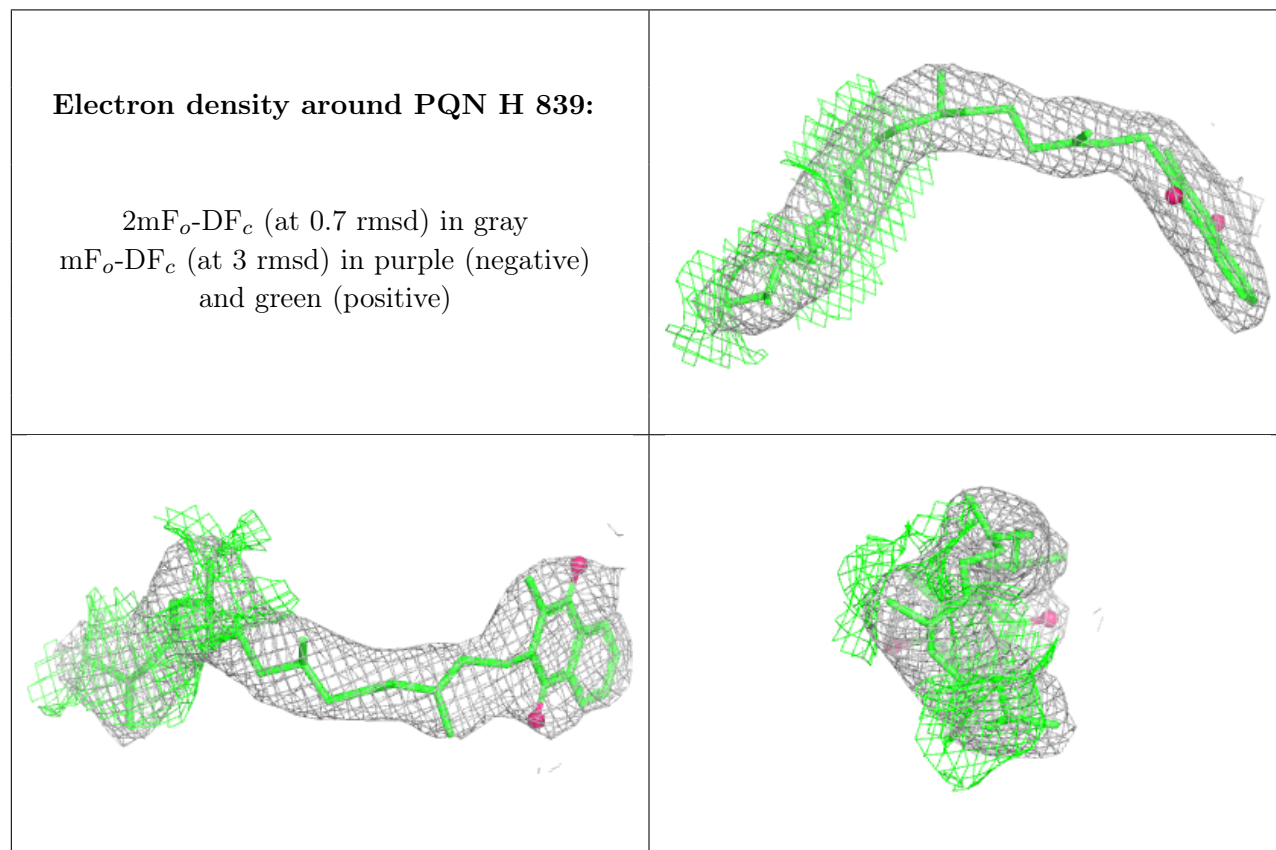
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	SF4	Y	845	8/8	1.00	0.01	54,60,61,65	0
16	SF4	a	101	8/8	1.00	0.01	43,50,59,59	0
16	SF4	a	102	8/8	1.00	0.01	46,52,56,56	0
17	BCR	A	845	40/40	1.00	0.04	63,69,73,74	0
14	CLA	B	839	45/65	1.00	0.03	45,57,65,72	0
14	CLA	B	840	65/65	1.00	0.03	31,34,39,42	0
14	CLA	A	805	65/65	1.00	0.05	53,62,93,95	0
14	CLA	H	835	65/65	1.00	0.03	50,58,74,76	0
14	CLA	H	836	45/65	1.00	0.03	45,58,60,63	0
17	BCR	B	844	40/40	1.00	0.04	47,58,78,79	0
14	CLA	H	837	65/65	1.00	0.03	32,35,42,44	0
14	CLA	H	838	65/65	1.00	0.04	35,44,50,53	0
14	CLA	F	202	45/65	1.00	0.03	51,62,66,70	0
14	CLA	G	802	65/65	1.00	0.04	47,58,63,70	0
14	CLA	A	841	65/65	1.00	0.03	28,31,43,47	0
14	CLA	K	103	45/65	1.00	0.04	65,69,75,79	0
14	CLA	L	201	65/65	1.00	0.03	33,37,52,54	0
14	CLA	G	804	59/65	1.00	0.04	59,69,75,78	0
14	CLA	G	805	65/65	1.00	0.03	58,67,74,82	0
14	CLA	L	206	65/65	1.00	0.03	41,47,77,82	0
17	BCR	G	849	40/40	1.00	0.04	36,60,73,73	0
17	BCR	G	850	40/40	1.00	0.03	47,56,66,68	0
17	BCR	G	854	40/40	1.00	0.04	63,72,81,82	0
14	CLA	L	207	65/65	1.00	0.03	38,42,56,65	0
14	CLA	Q	201	65/65	1.00	0.03	52,59,71,75	0
14	CLA	G	806	65/65	1.00	0.03	60,66,70,73	0
14	CLA	A	806	65/65	1.00	0.03	57,65,74,79	0
13	CL0	A	801	65/65	1.00	0.04	40,47,51,54	0
17	BCR	H	845	40/40	1.00	0.03	37,43,48,49	0
14	CLA	A	814	50/65	1.00	0.04	74,80,87,94	0
14	CLA	B	802	65/65	1.00	0.03	51,56,66,73	0
14	CLA	B	803	65/65	1.00	0.04	38,45,59,60	0
14	CLA	U	1002	65/65	1.00	0.03	38,45,54,55	0
14	CLA	U	1003	65/65	1.00	0.03	33,38,57,58	0
17	BCR	L	203	40/40	1.00	0.03	44,49,58,58	0
14	CLA	U	1004	65/65	1.00	0.03	30,35,47,51	0
14	CLA	G	812	54/65	1.00	0.04	61,70,84,89	0
17	BCR	M	101	40/40	1.00	0.03	42,49,56,57	0
14	CLA	V	1201	54/65	1.00	0.03	41,49,55,60	0
14	CLA	G	813	60/65	1.00	0.04	55,68,75,80	0
17	BCR	R	101	40/40	1.00	0.03	38,42,50,50	0
14	CLA	X	1701	45/65	1.00	0.03	53,75,79,84	0

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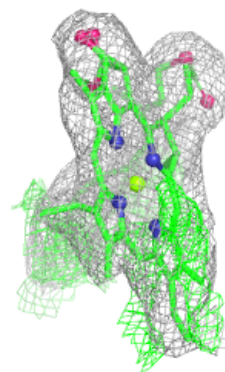
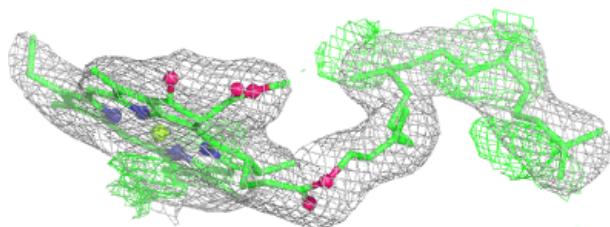
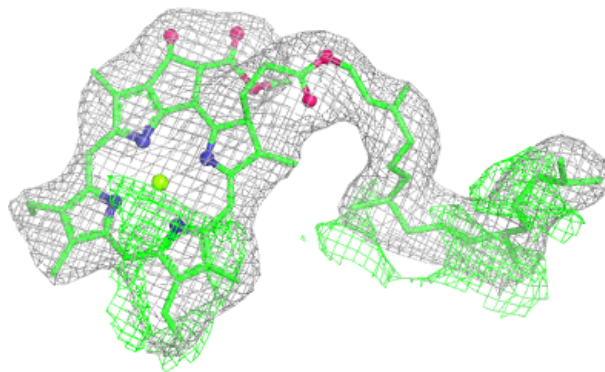
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	G	814	50/65	1.00	0.03	67,75,80,85	0
17	BCR	T	102	40/40	1.00	0.04	58,69,78,81	0
14	CLA	A	826	60/65	1.00	0.03	40,46,83,85	0
17	BCR	U	1007	40/40	1.00	0.03	33,39,48,49	0
14	CLA	B	805	54/65	1.00	0.03	37,41,44,50	0
14	CLA	Y	805	65/65	1.00	0.03	46,53,76,80	0
14	CLA	Y	806	65/65	1.00	0.04	53,57,67,71	0
17	BCR	Y	847	40/40	1.00	0.04	60,70,82,83	0
14	CLA	B	806	65/65	1.00	0.04	30,43,55,56	0
14	CLA	B	807	65/65	1.00	0.04	36,49,54,56	0
14	CLA	G	819	65/65	1.00	0.03	48,66,72,76	0
17	BCR	Y	851	40/40	1.00	0.03	42,49,59,62	0
14	CLA	B	808	65/65	1.00	0.03	37,41,46,49	0
14	CLA	B	809	65/65	1.00	0.03	38,44,50,54	0
14	CLA	Y	812	55/65	1.00	0.03	56,61,66,67	0
17	BCR	Z	843	40/40	1.00	0.04	50,57,81,82	0
17	BCR	Z	844	25/40	1.00	0.03	26,48,54,55	0
14	CLA	Y	813	60/65	1.00	0.04	51,59,91,96	0
17	BCR	Z	846	40/40	1.00	0.04	52,60,86,89	0
13	CL0	G	801	65/65	1.00	0.04	32,46,53,55	0
14	CLA	B	811	55/65	1.00	0.04	57,60,73,76	0
17	BCR	f	103	40/40	1.00	0.04	62,70,75,77	0
14	CLA	A	809	65/65	1.00	0.03	54,64,81,84	0
17	BCR	f	105	40/40	1.00	0.04	54,59,67,72	0
17	BCR	h	202	40/40	1.00	0.04	39,47,83,86	0
17	BCR	h	203	40/40	1.00	0.03	37,43,48,50	0
17	BCR	i	101	40/40	1.00	0.03	39,48,54,55	0
14	CLA	B	813	65/65	1.00	0.04	35,40,54,56	0
18	LHG	A	851	32/49	1.00	0.03	44,48,56,57	0
14	CLA	G	826	60/65	1.00	0.04	45,58,88,90	0
14	CLA	Y	819	65/65	1.00	0.03	53,62,71,75	0
18	LHG	G	852	32/49	1.00	0.04	53,63,77,81	0
14	CLA	A	817	60/65	1.00	0.03	55,67,73,76	0
14	CLA	Y	821	65/65	1.00	0.04	56,67,77,81	0
18	LHG	Y	853	25/49	1.00	0.03	41,48,58,59	0
14	CLA	B	815	45/65	1.00	0.03	59,66,72,76	0
14	CLA	G	829	65/65	1.00	0.04	62,68,95,102	0
14	CLA	B	816	55/65	1.00	0.03	52,62,80,82	0
14	CLA	G	831	50/65	1.00	0.03	42,46,49,54	0
20	CA	L	204	1/1	1.00	0.01	49,49,49,49	0
20	CA	U	1001	1/1	1.00	0.01	64,64,64,64	0
20	CA	h	204	1/1	1.00	0.01	52,52,52,52	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.



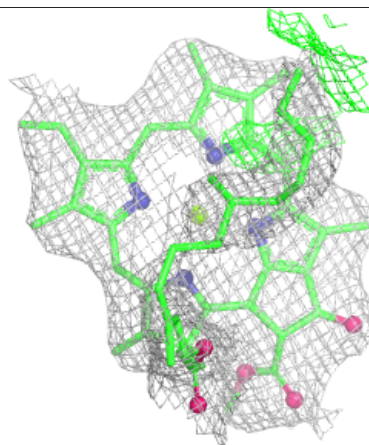
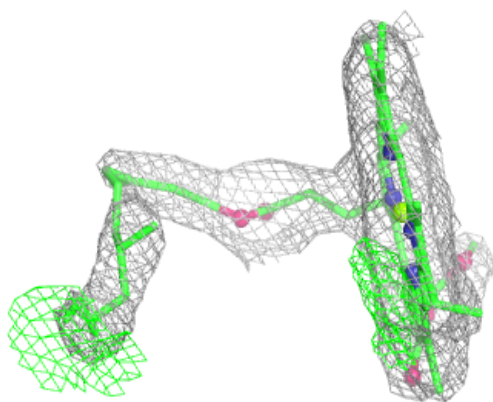
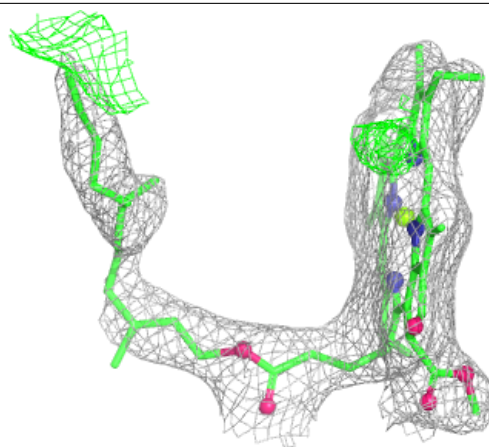
Electron density around CLA A 803:

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



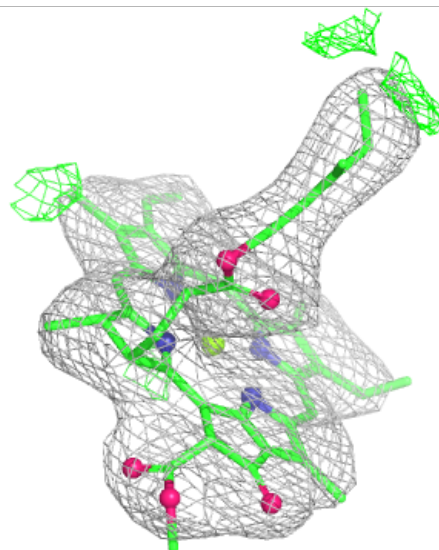
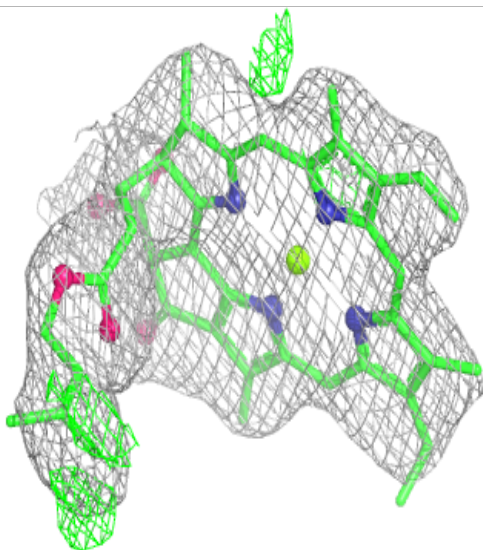
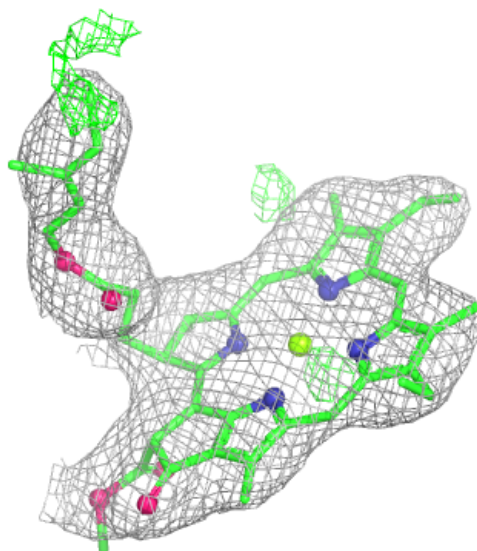
Electron density around CLA A 804:

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



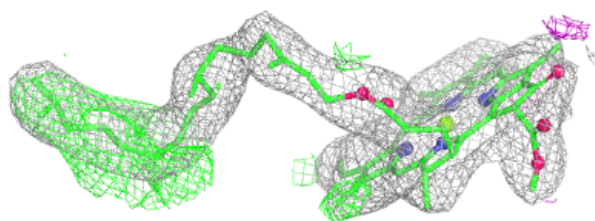
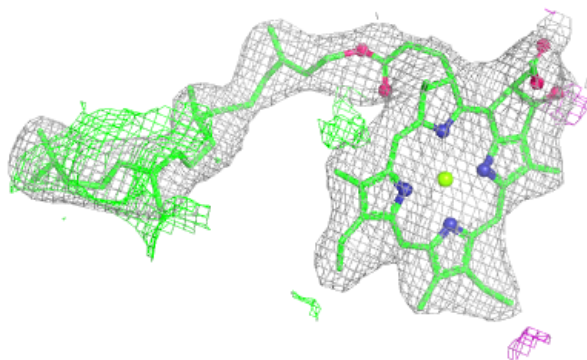
Electron density around CLA A 807:

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



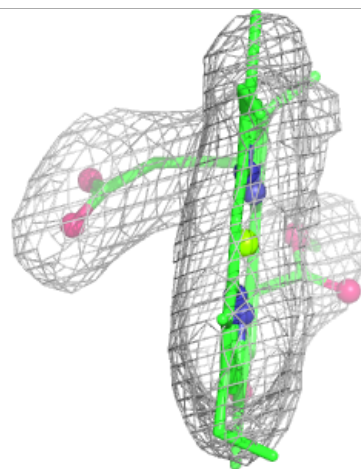
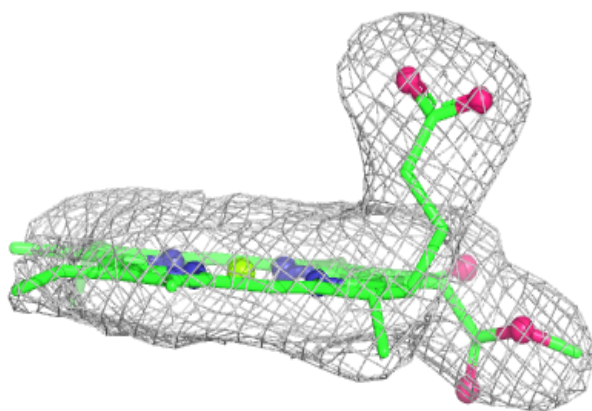
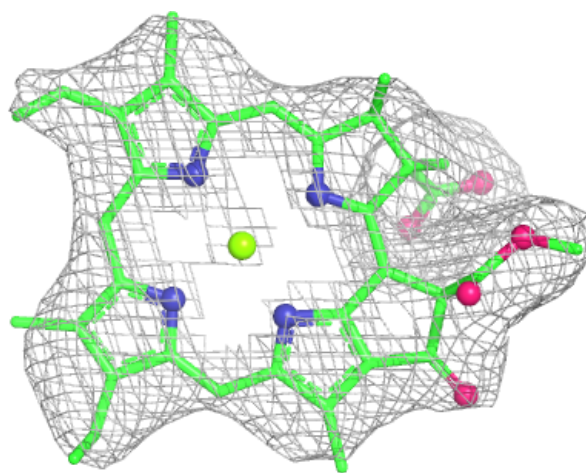
Electron density around CLA A 808:

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



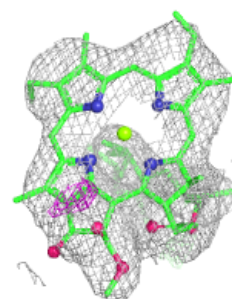
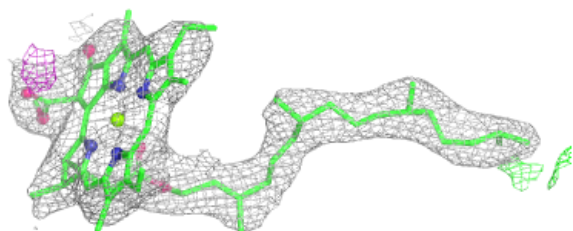
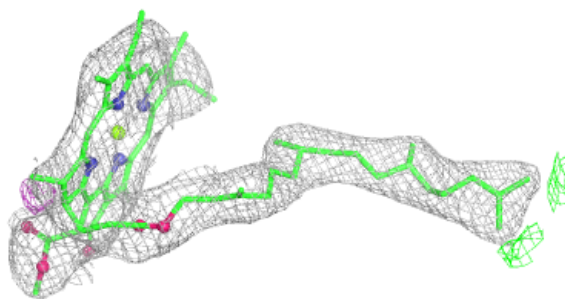
Electron density around CLA A 810:

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

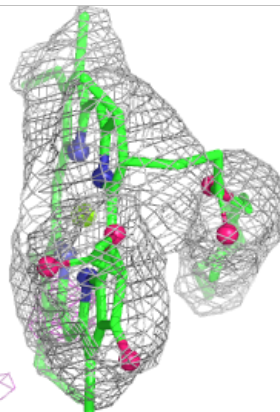
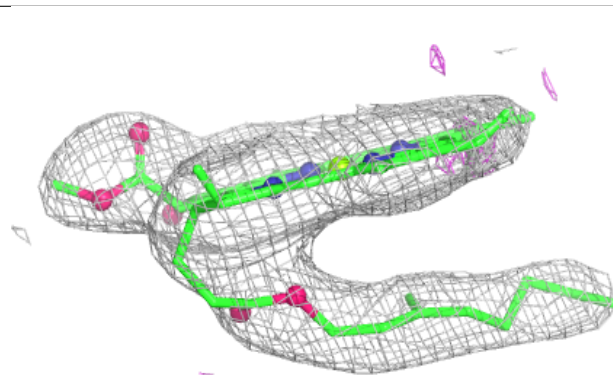
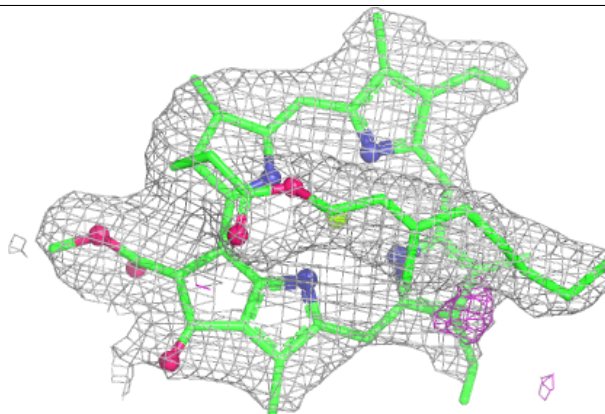


Electron density around CLA A 811:

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

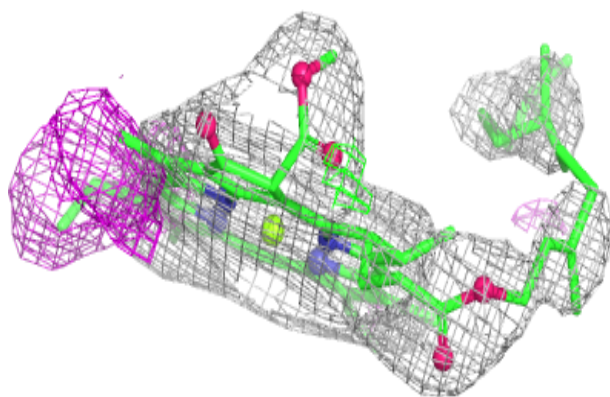
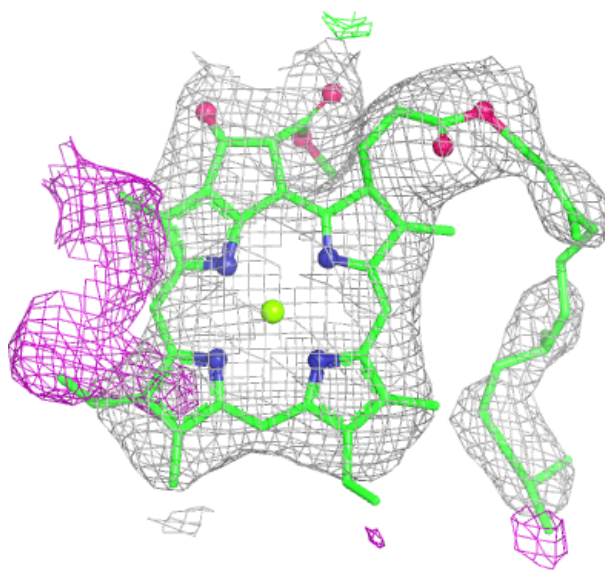
**Electron density around CLA A 812:**

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



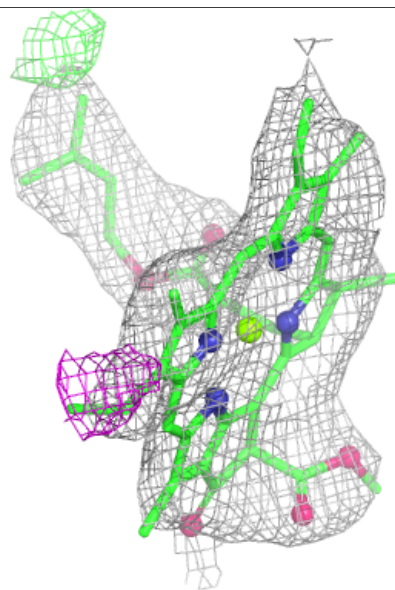
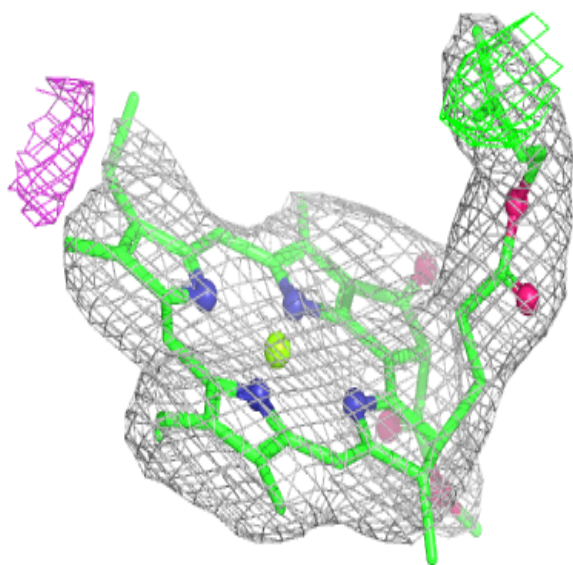
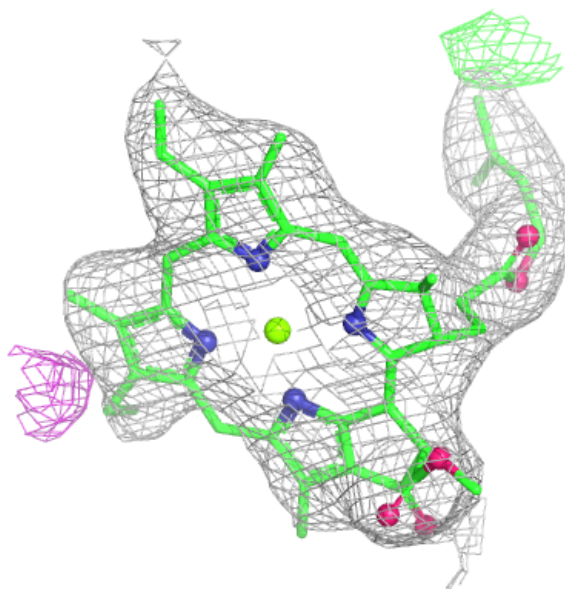
Electron density around CLA A 813:

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



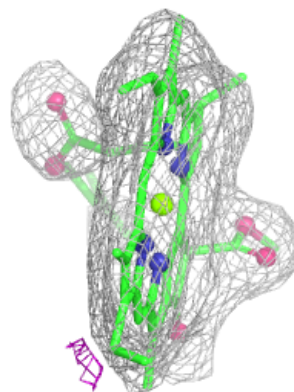
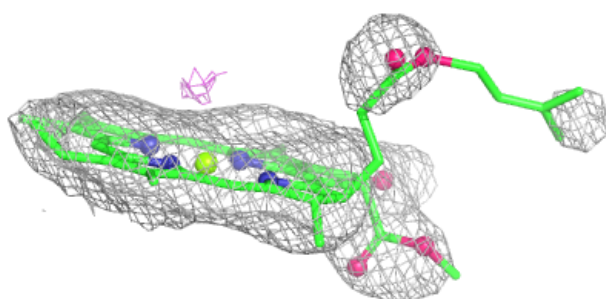
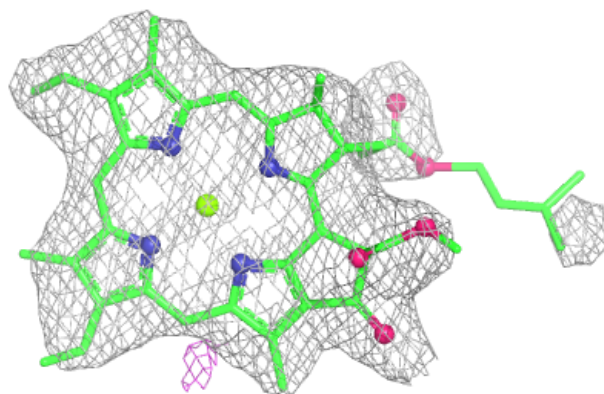
Electron density around CLA A 815:

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



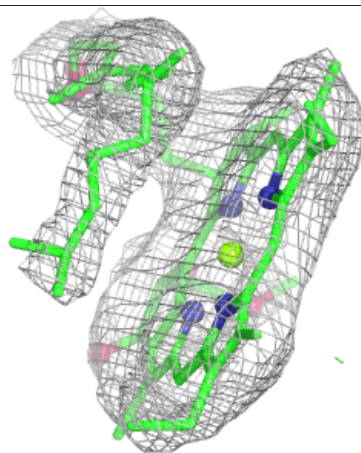
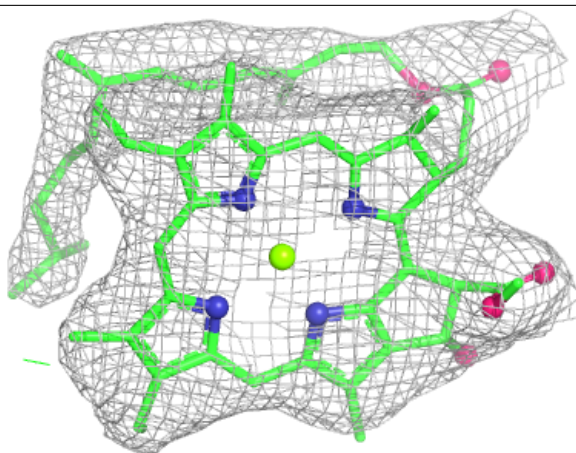
Electron density around CLA A 816:

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



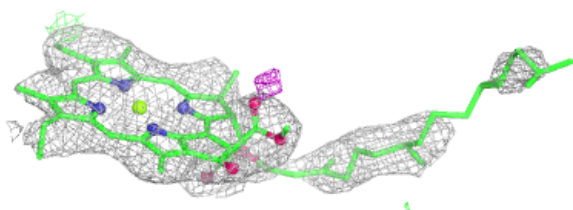
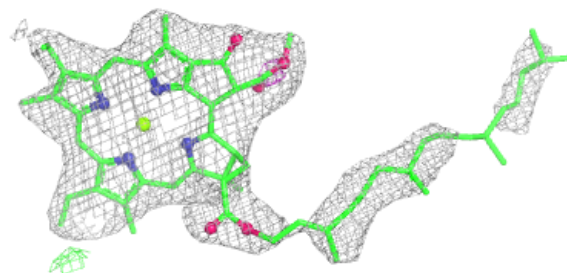
Electron density around CLA A 820:

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



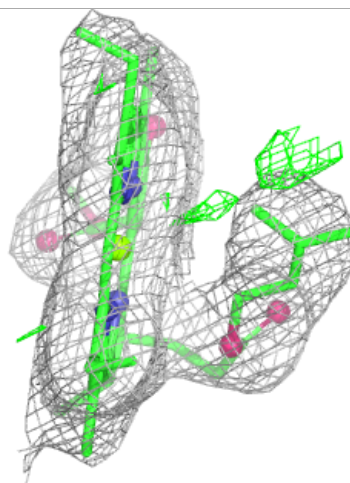
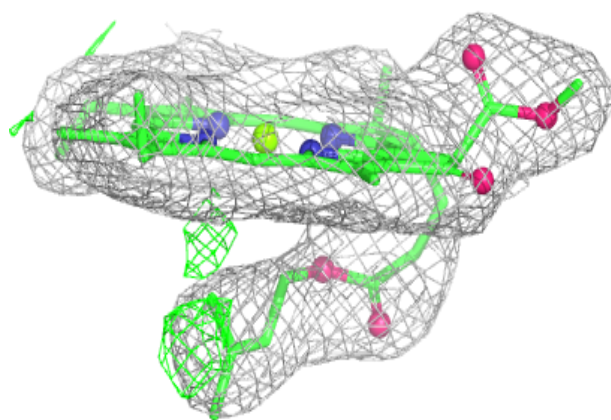
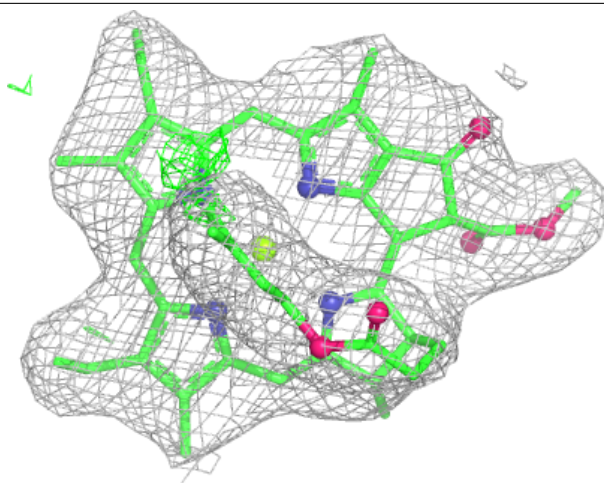
Electron density around CLA A 822:

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



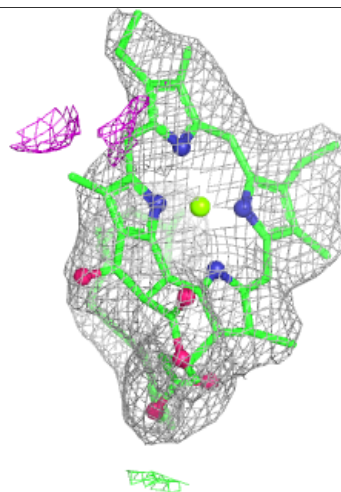
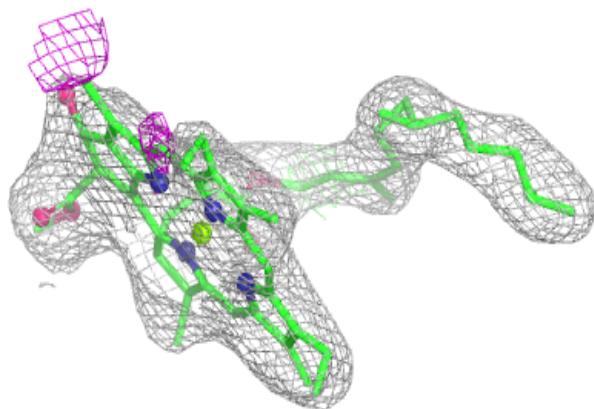
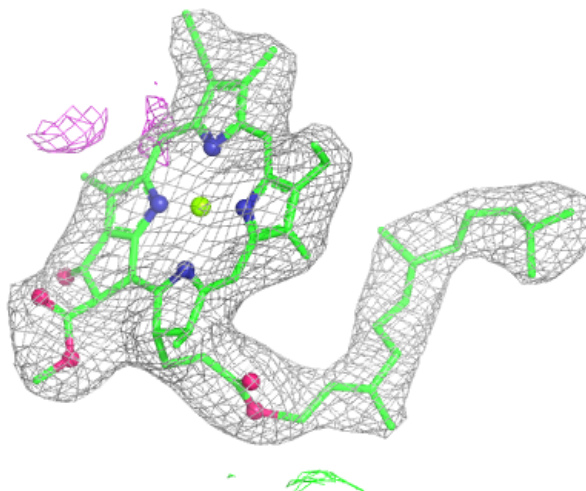
Electron density around CLA A 823:

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



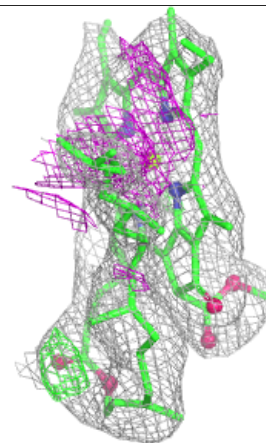
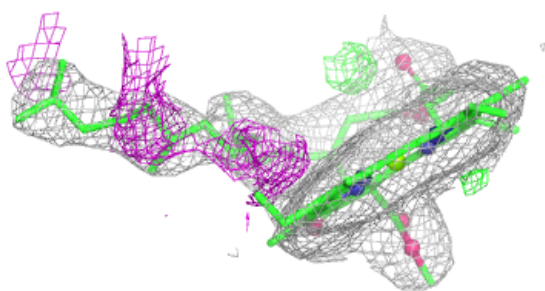
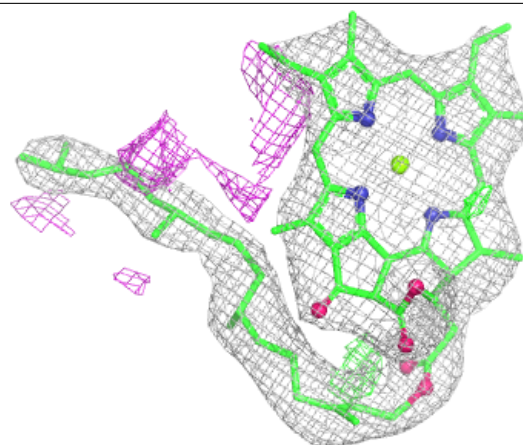
Electron density around CLA A 824:

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

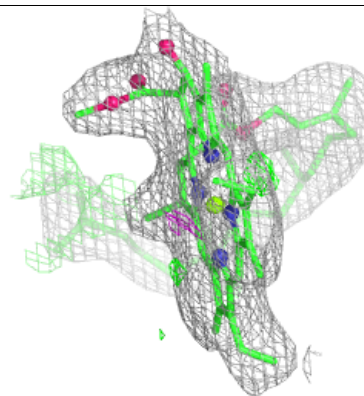
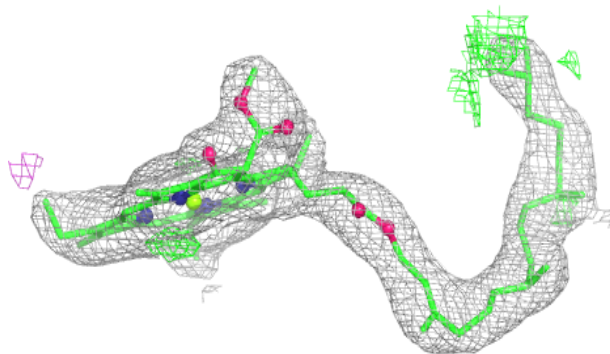
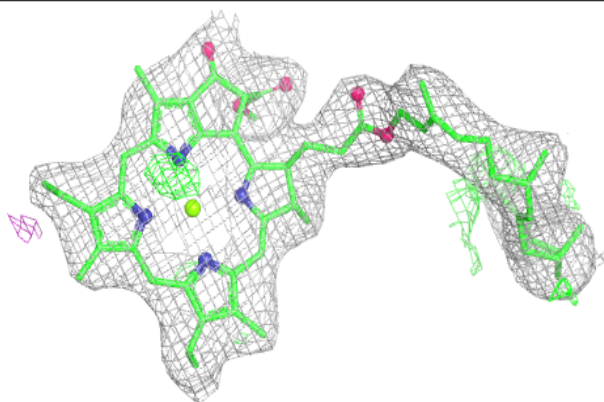


Electron density around CLA A 825:

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

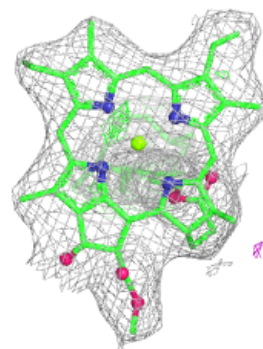
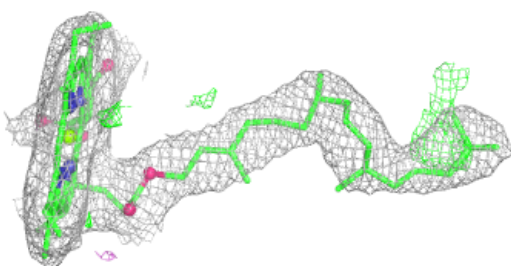
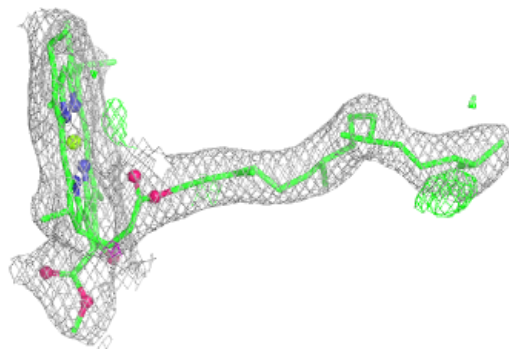
**Electron density around CLA A 827:**

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

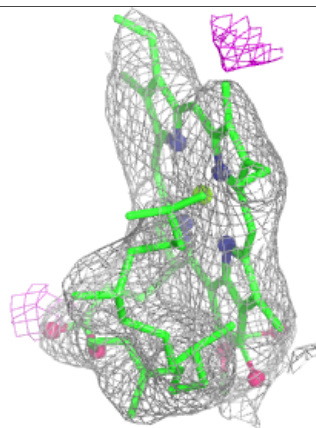
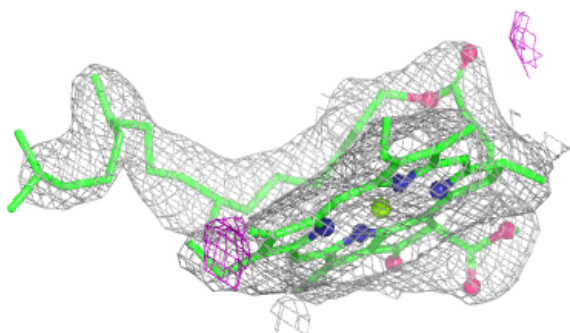
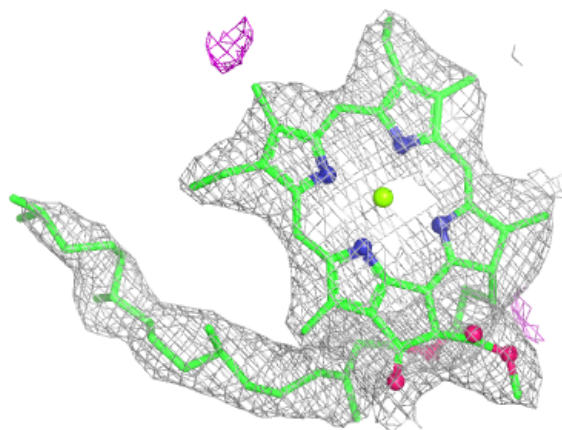


Electron density around CLA A 828:

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

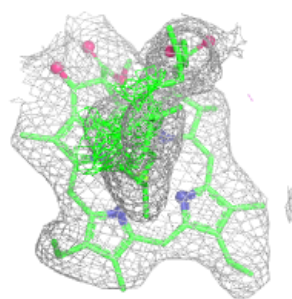
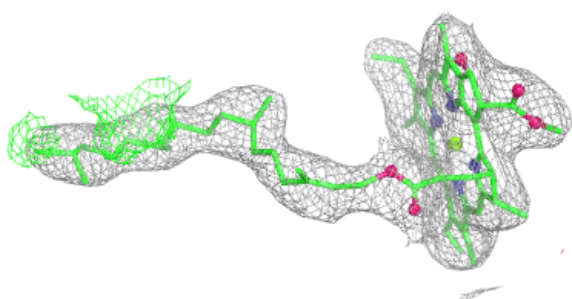
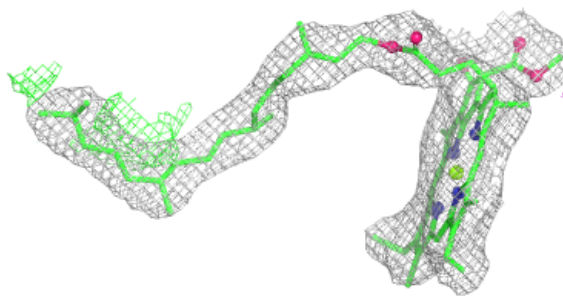
**Electron density around CLA A 829:**

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



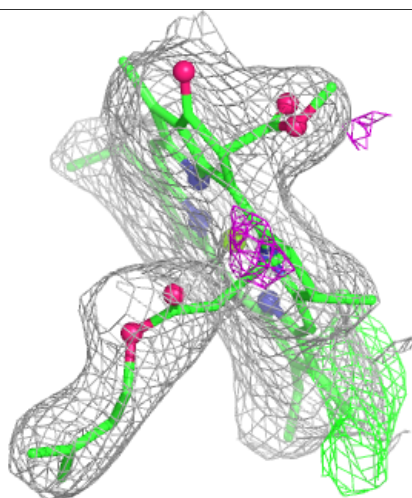
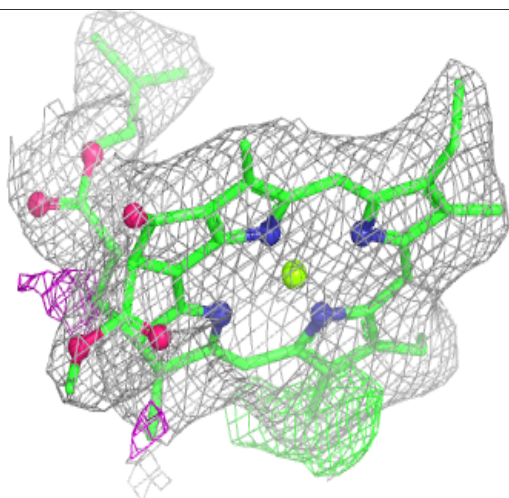
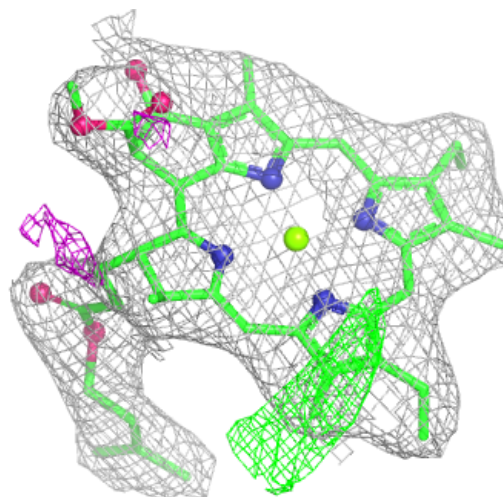
Electron density around CLA A 830:

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



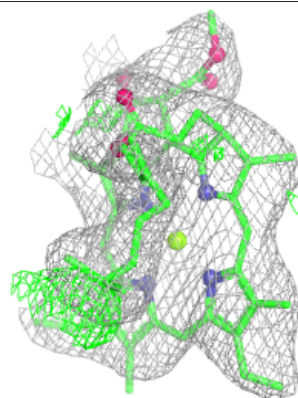
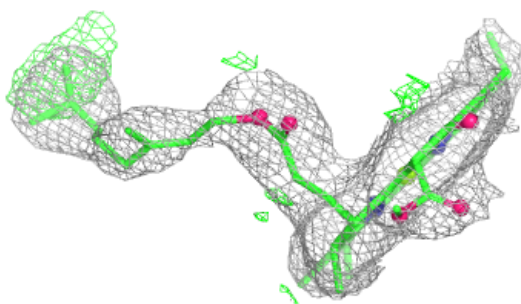
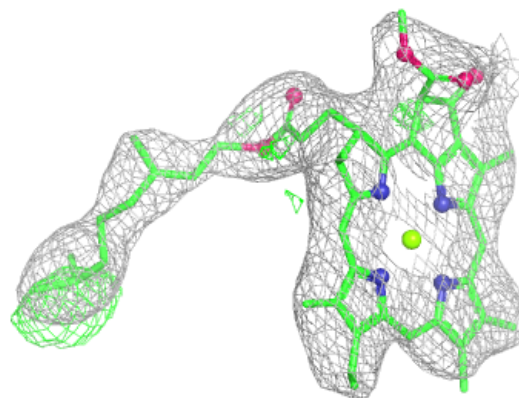
Electron density around CLA A 831:

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



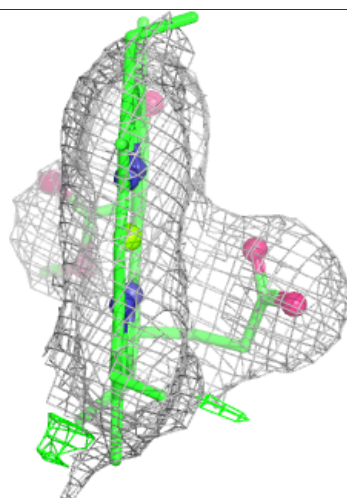
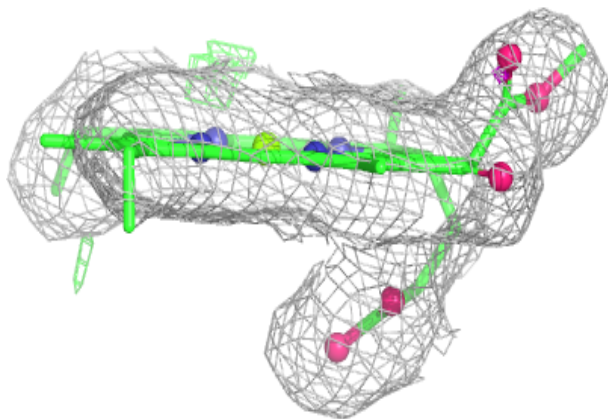
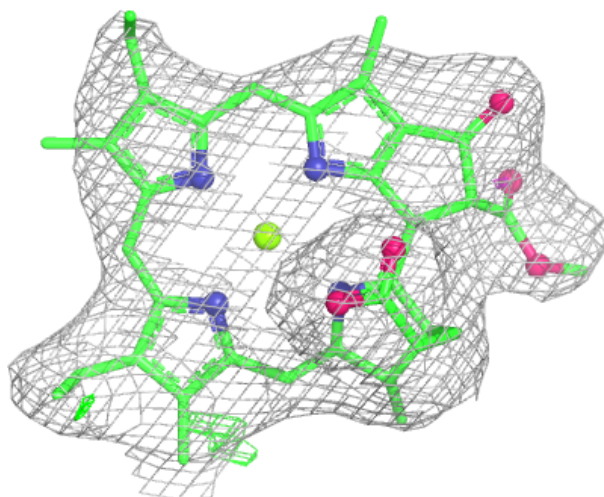
Electron density around CLA A 834:

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



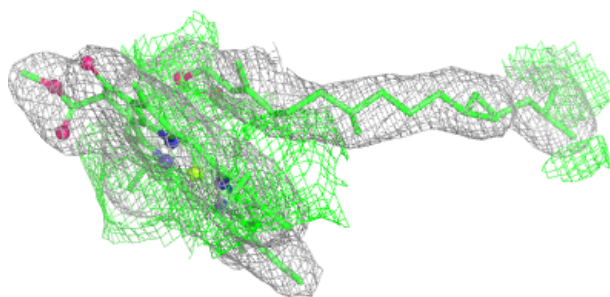
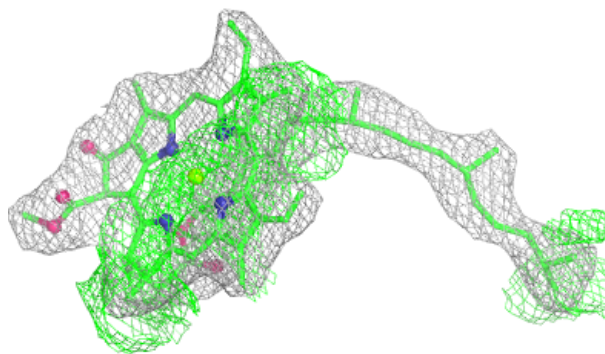
Electron density around CLA A 835:

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



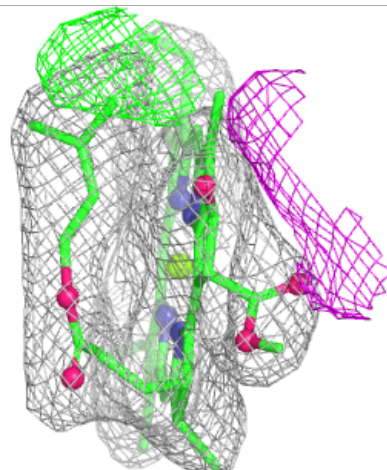
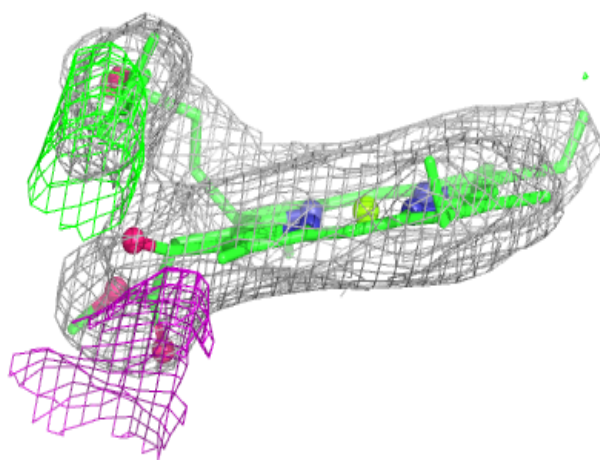
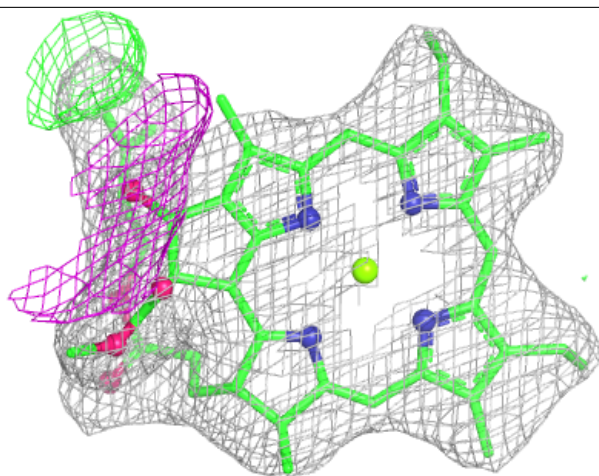
Electron density around CLA A 840:

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



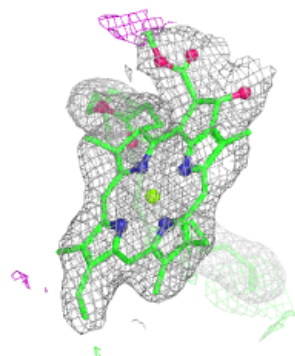
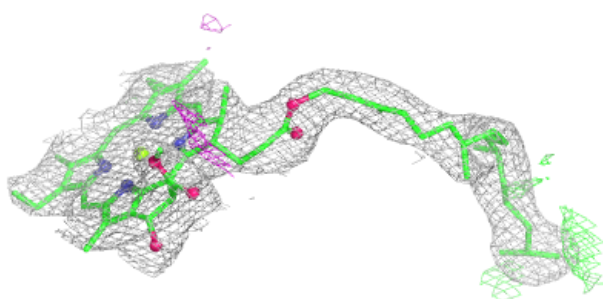
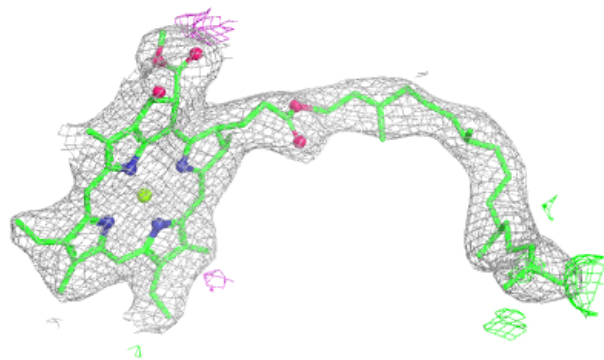
Electron density around CLA A 842:

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

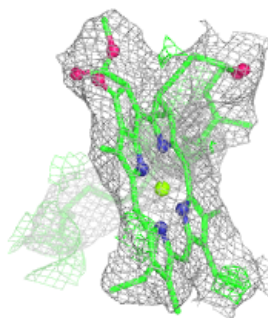
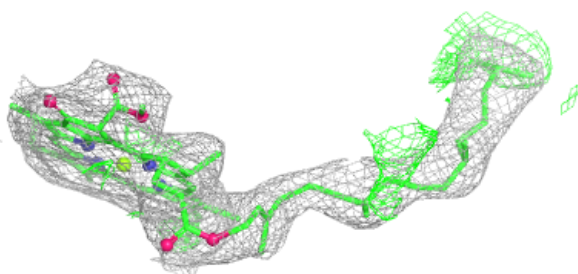
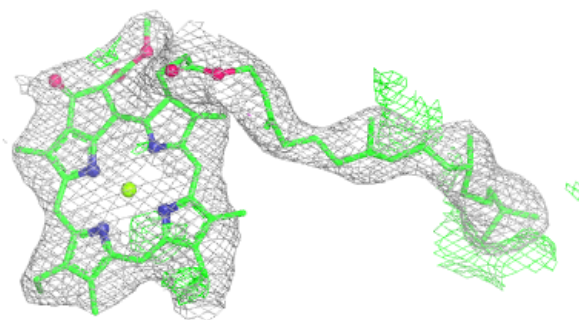


Electron density around CLA A 852:

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

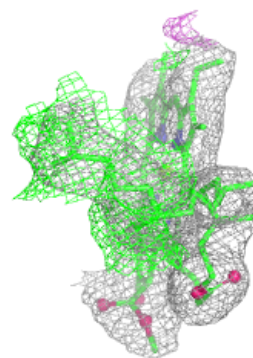
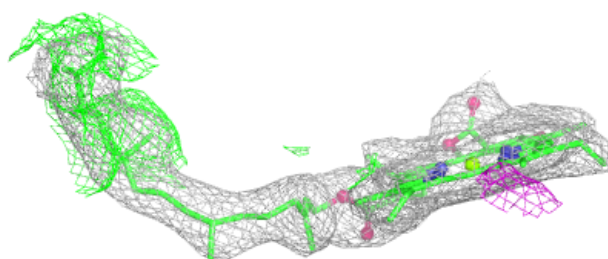
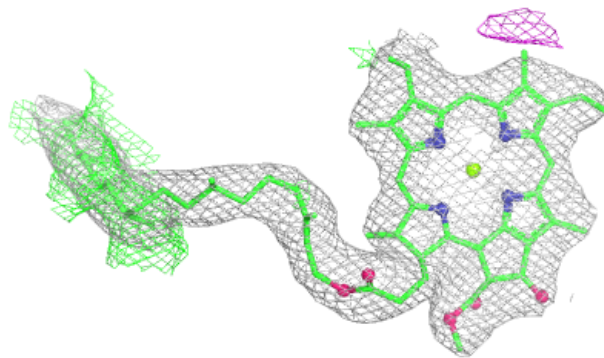
**Electron density around CLA B 801:**

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

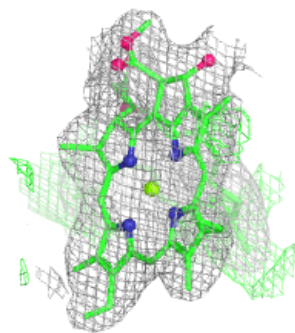
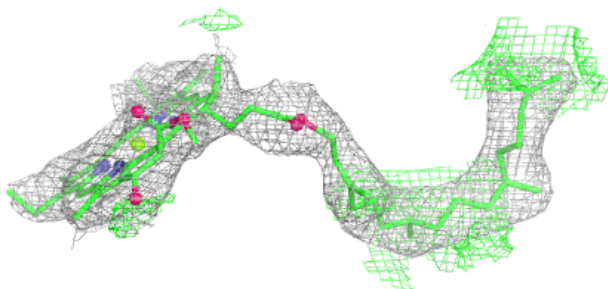
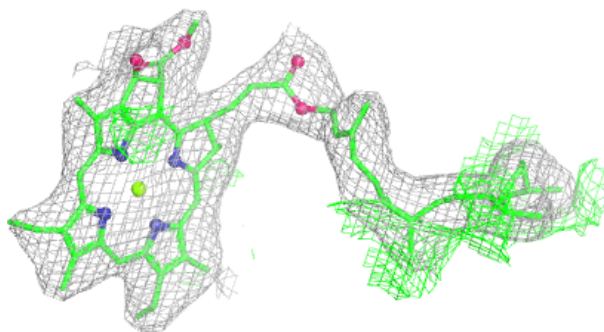


Electron density around CLA B 804:

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

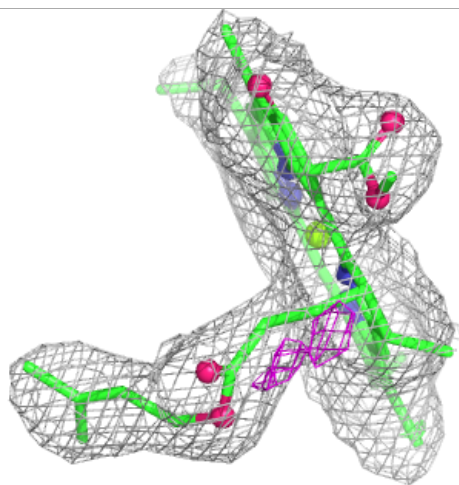
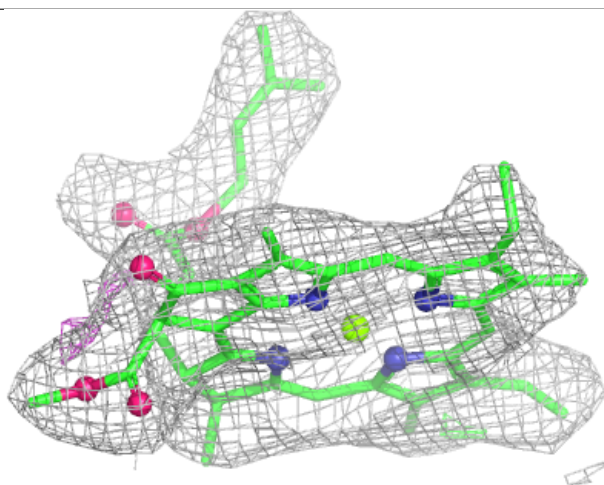
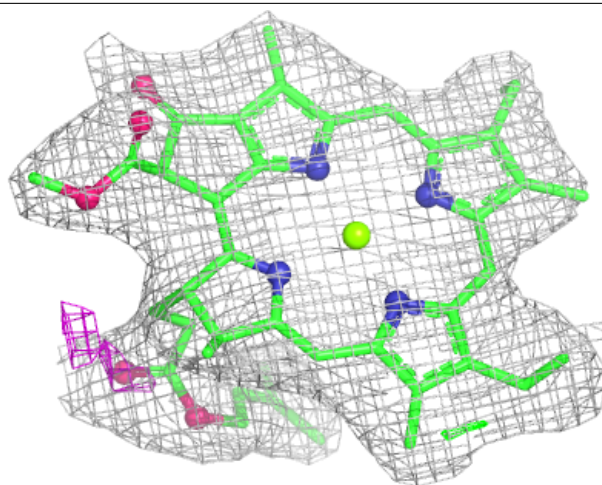
**Electron density around CLA B 810:**

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



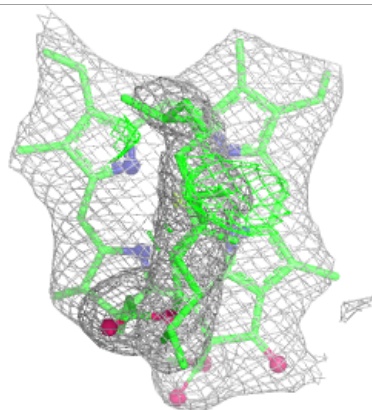
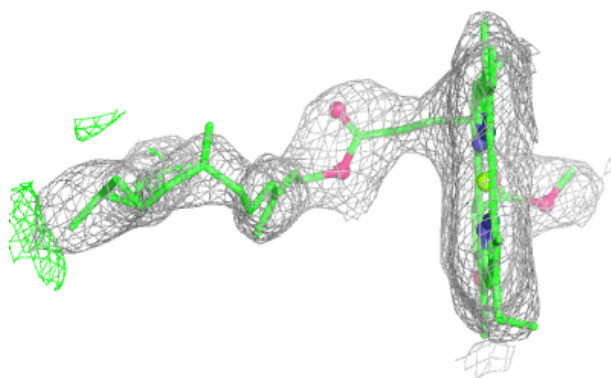
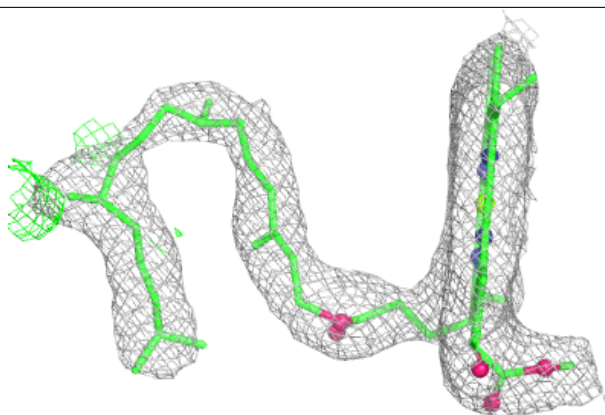
Electron density around CLA B 812:

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



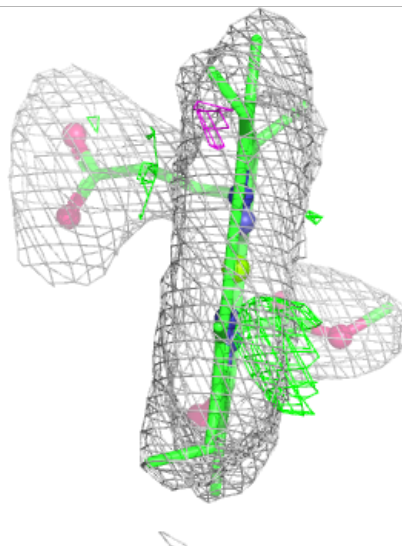
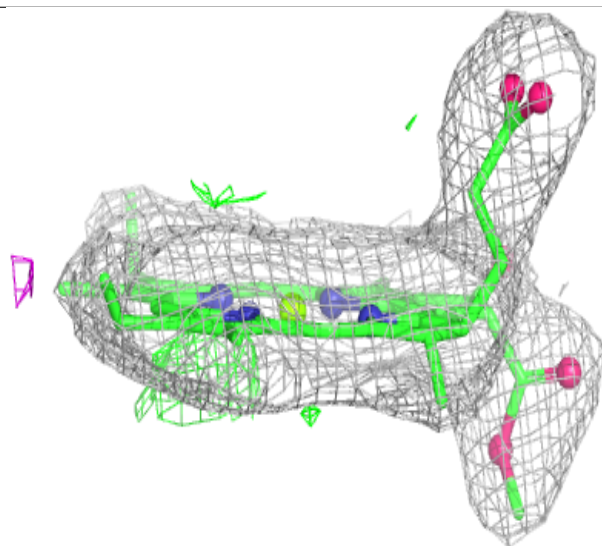
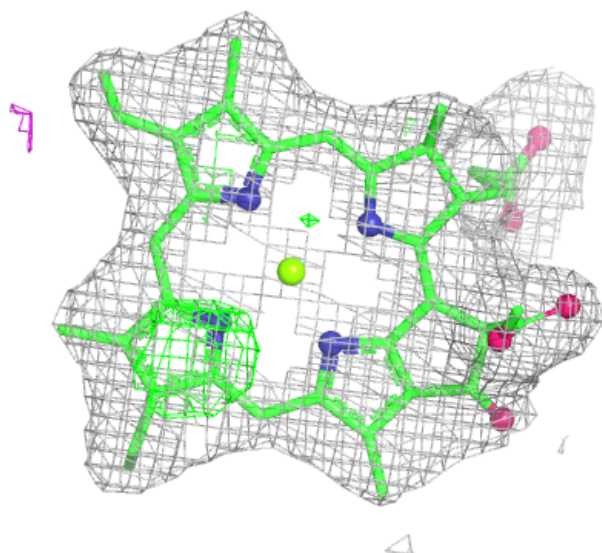
Electron density around CLA B 814:

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



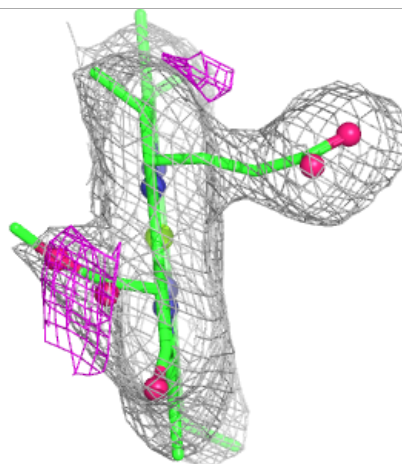
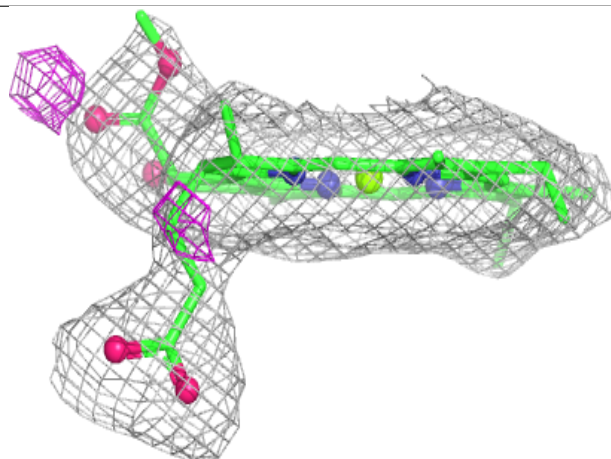
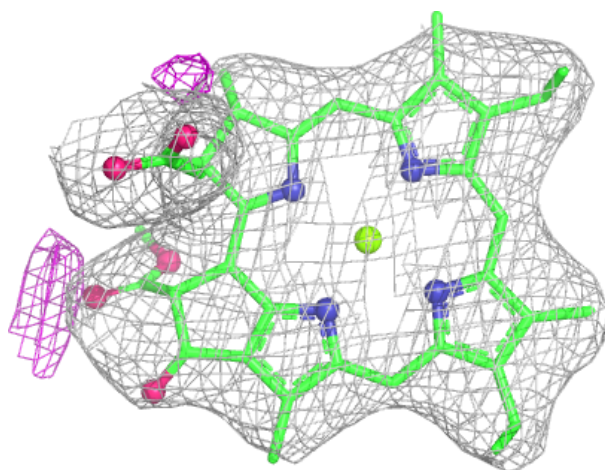
Electron density around CLA B 820:

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



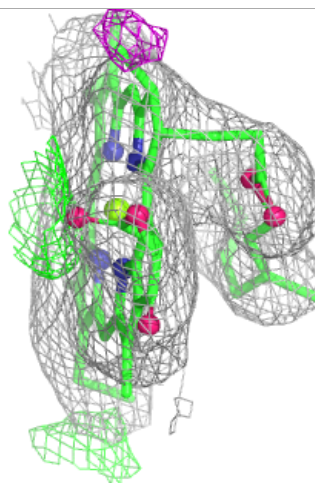
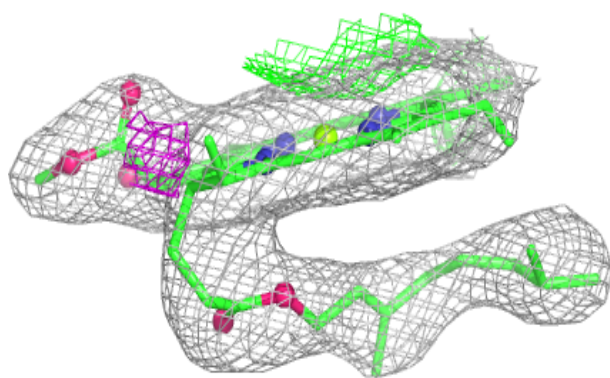
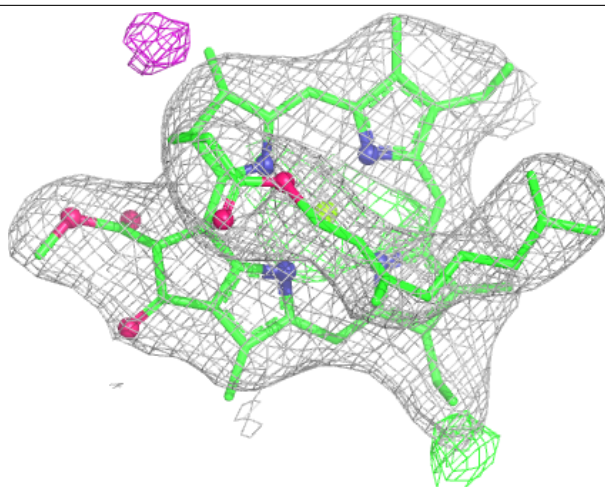
Electron density around CLA B 821:

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



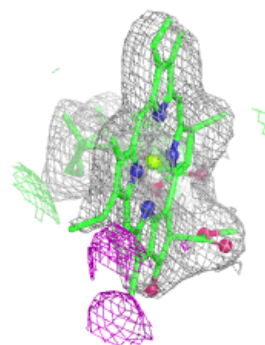
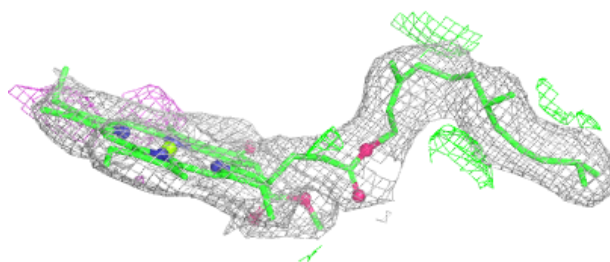
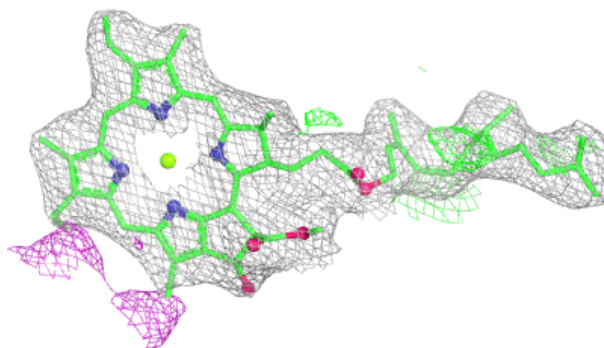
Electron density around CLA B 822:

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

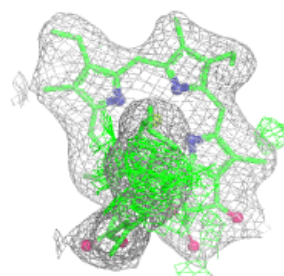
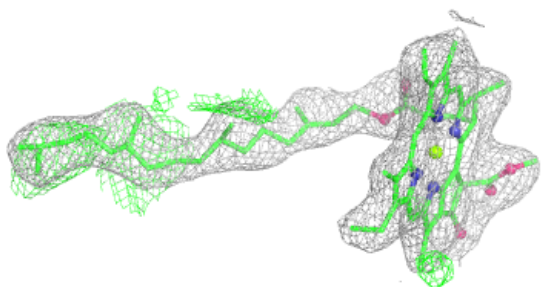
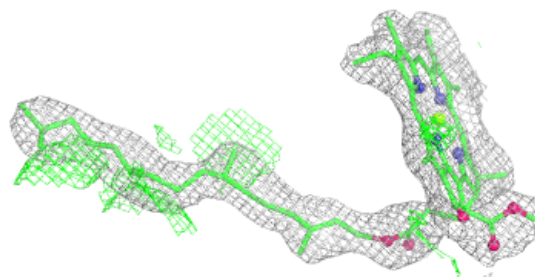


Electron density around CLA B 823:

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

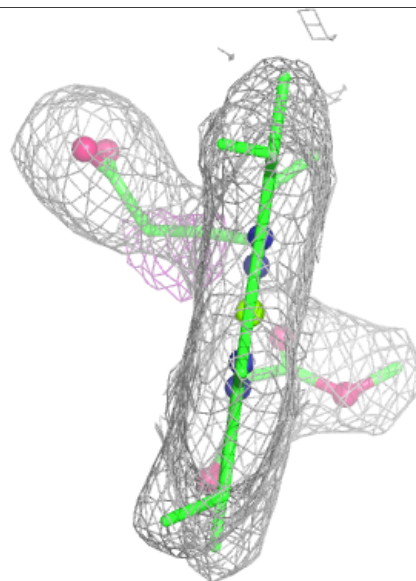
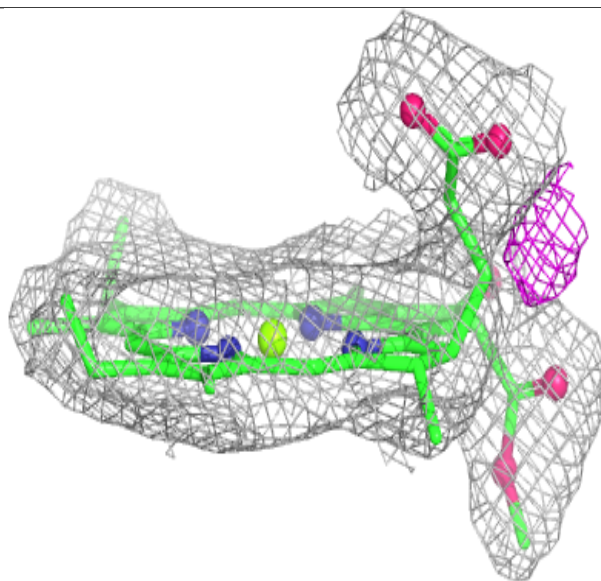
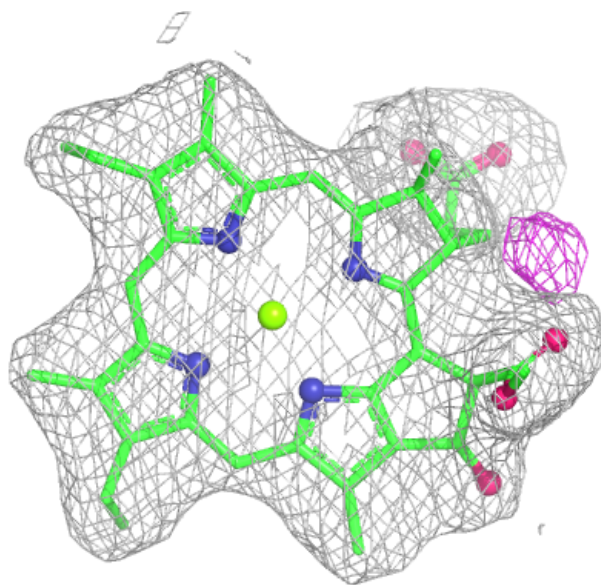
**Electron density around CLA B 829:**

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



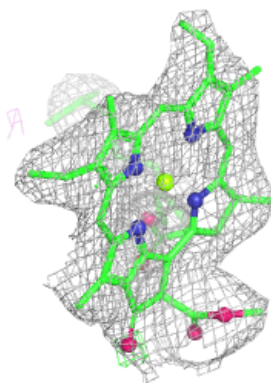
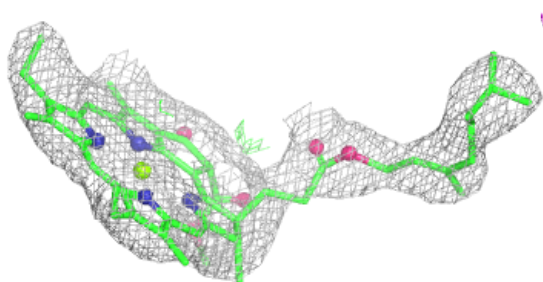
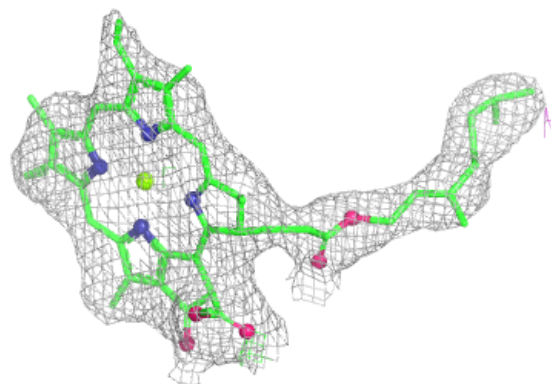
Electron density around CLA B 830:

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



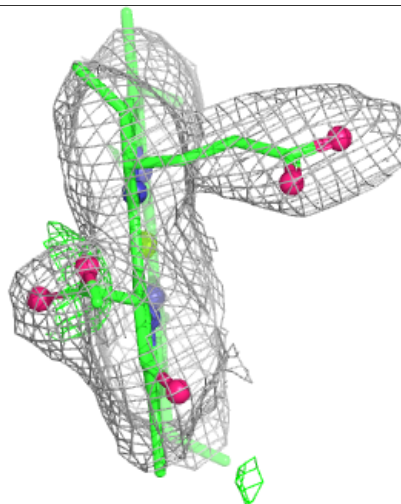
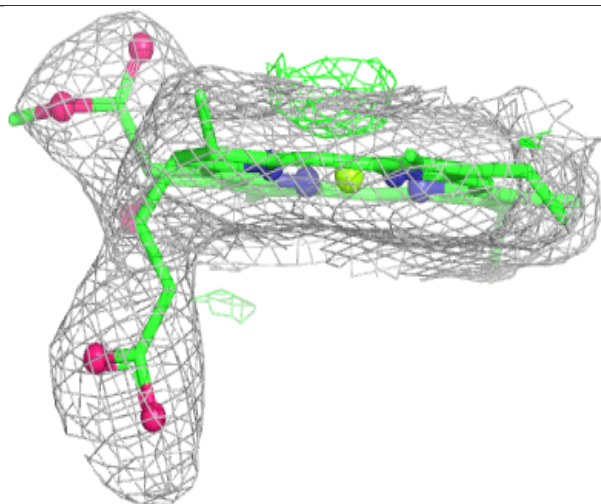
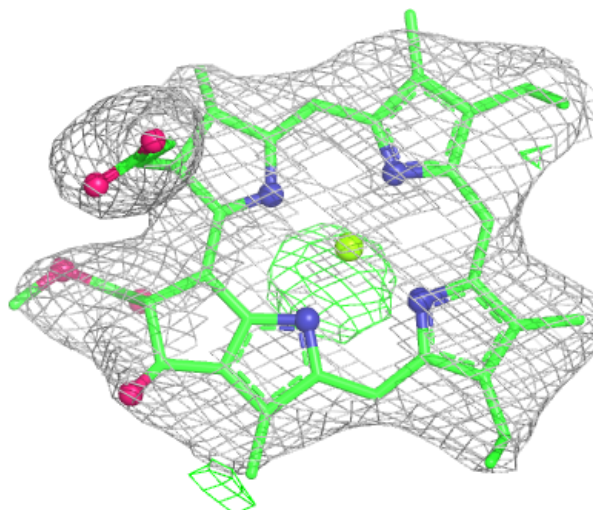
Electron density around CLA B 833:

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



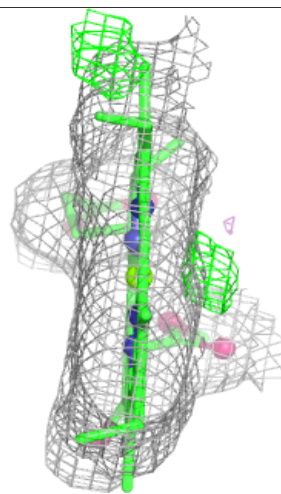
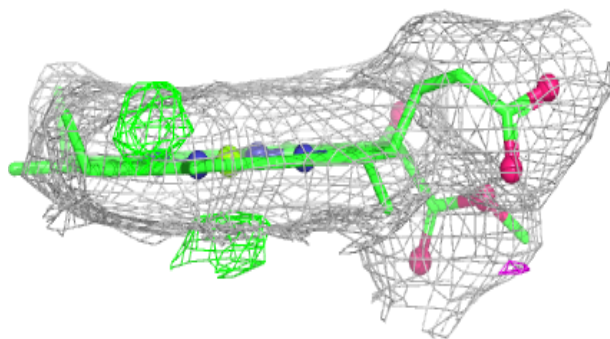
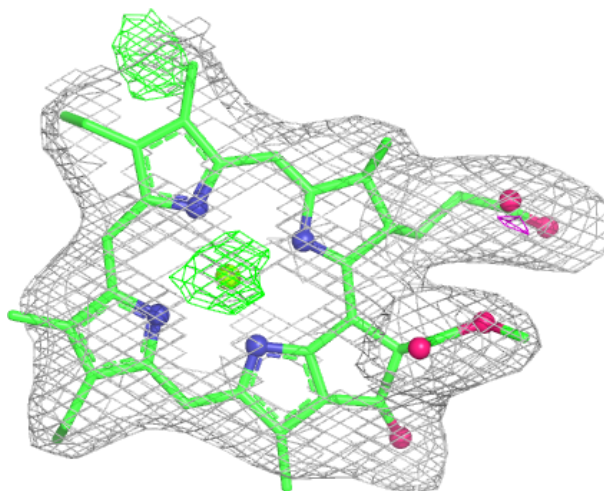
Electron density around CLA B 835:

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



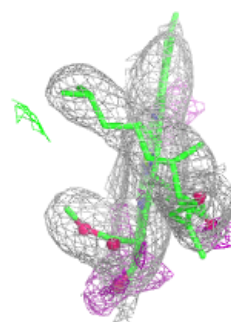
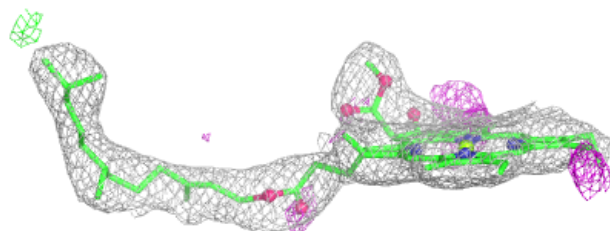
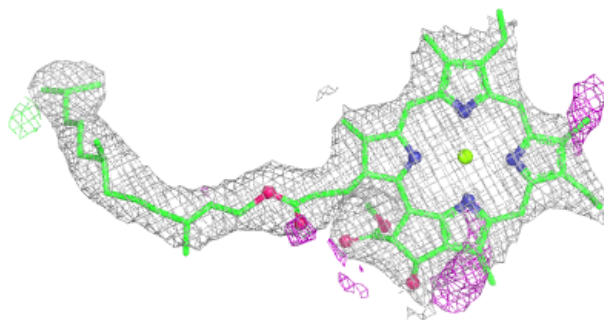
Electron density around CLA B 836:

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

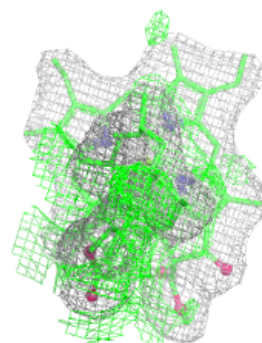
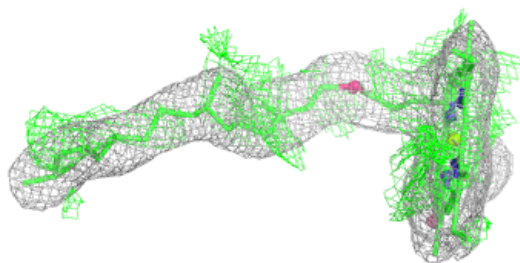
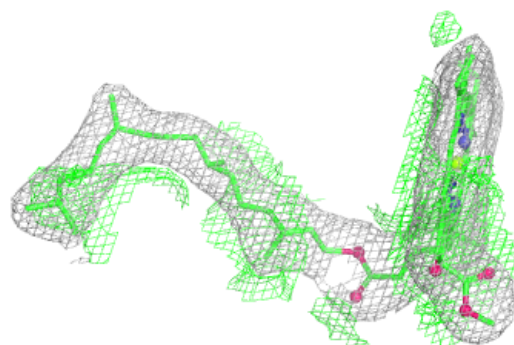


Electron density around CLA B 837:

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

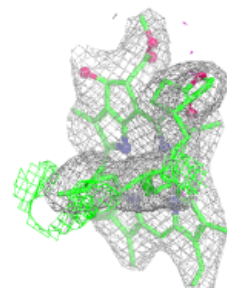
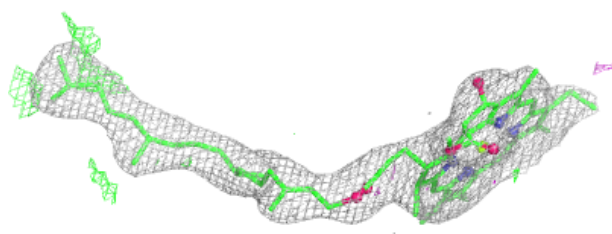
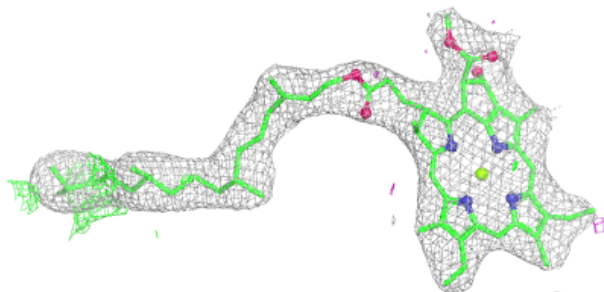
**Electron density around CLA B 841:**

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

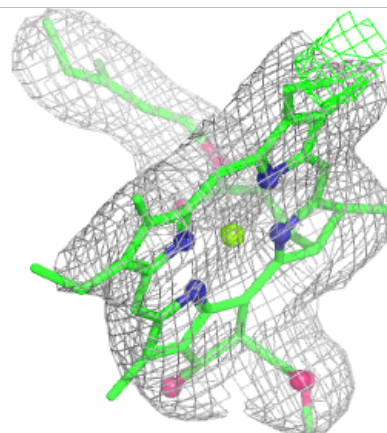
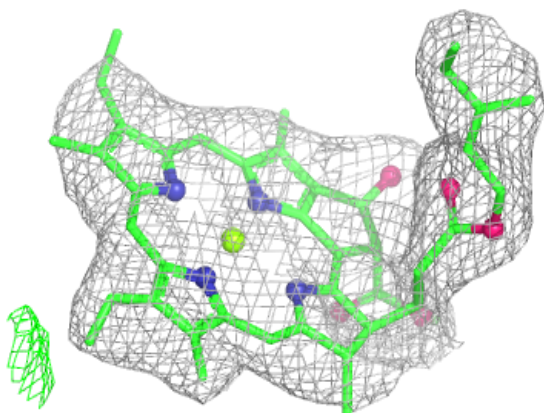
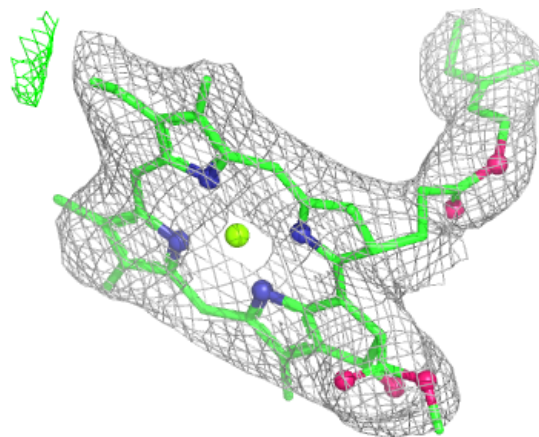


Electron density around CLA G 803:

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

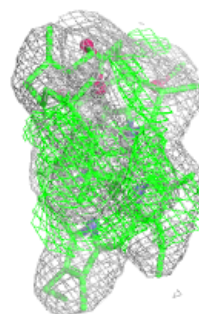
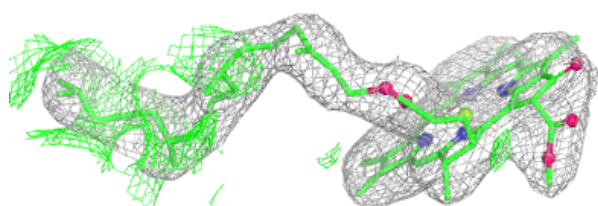
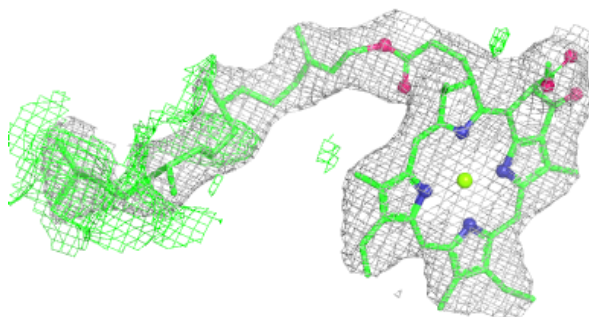
**Electron density around CLA G 807:**

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

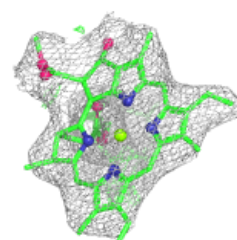
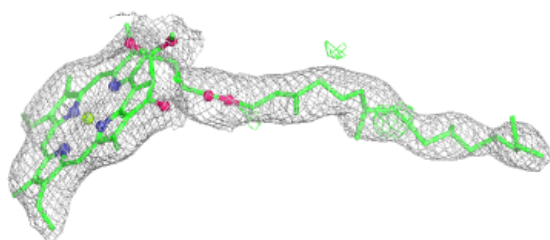
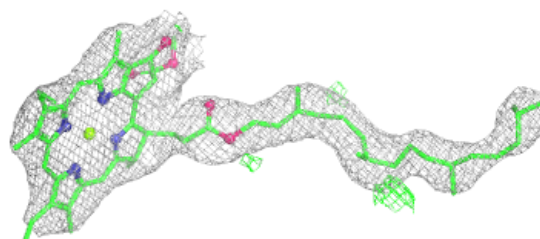


Electron density around CLA G 808:

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

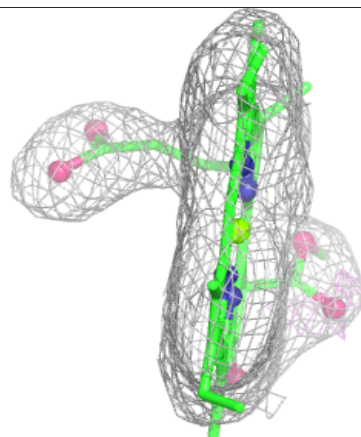
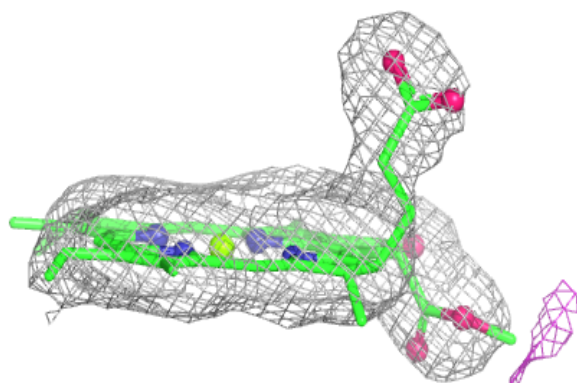
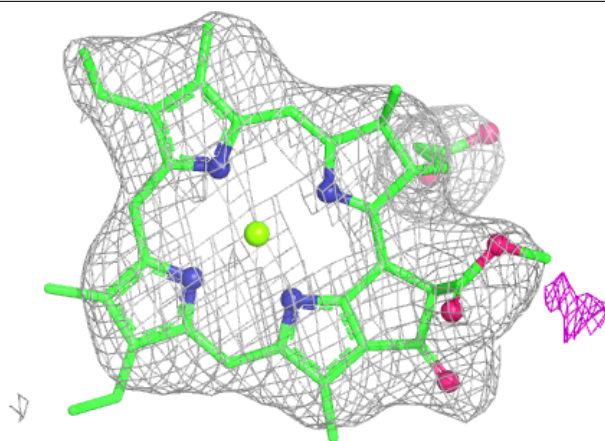
**Electron density around CLA G 809:**

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



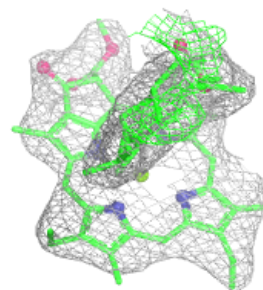
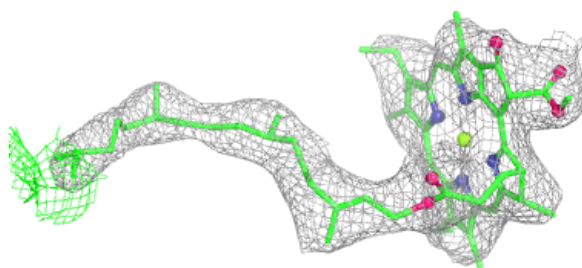
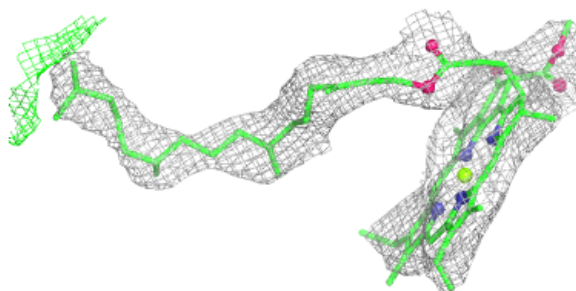
Electron density around CLA G 810:

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



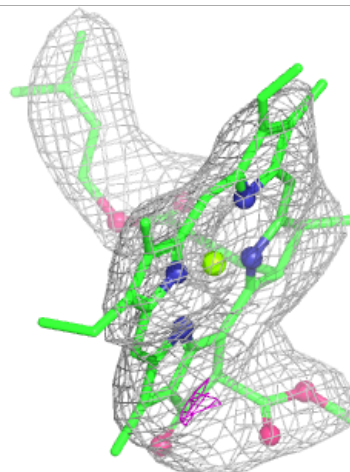
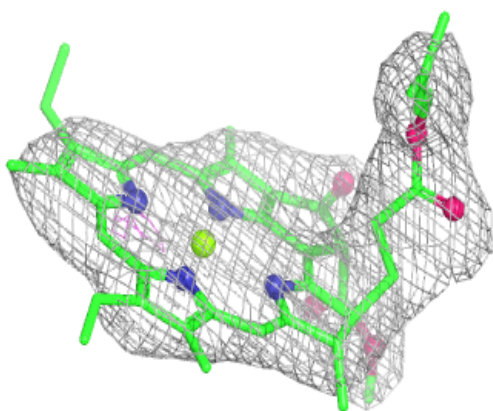
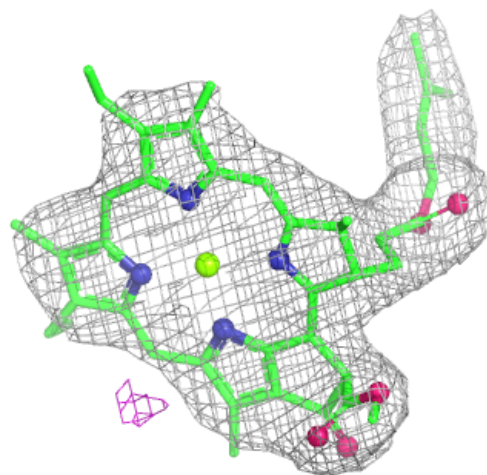
Electron density around CLA G 811:

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



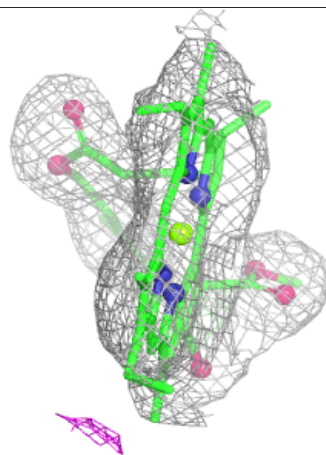
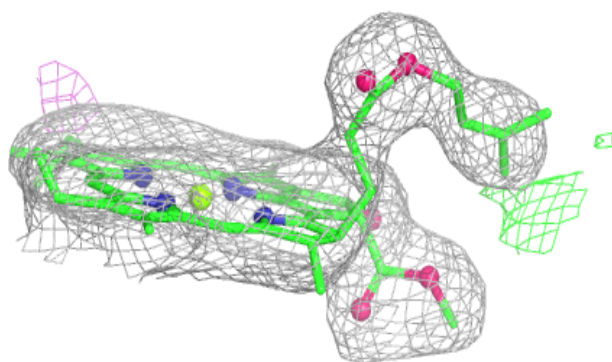
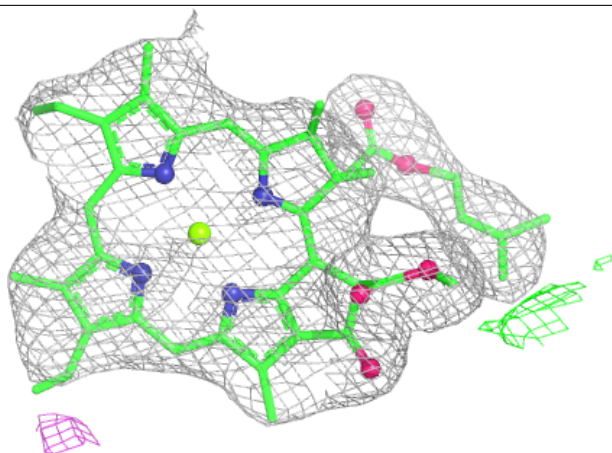
Electron density around CLA G 815:

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



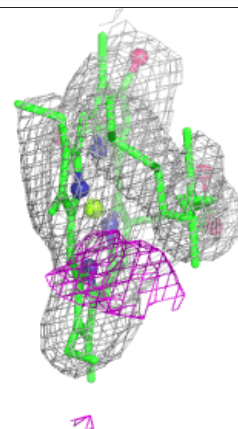
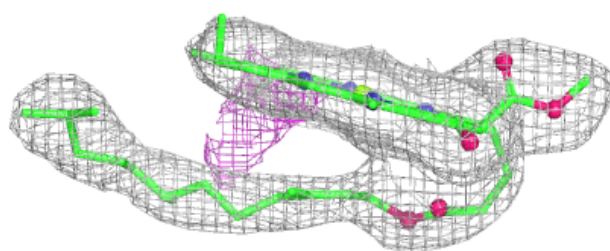
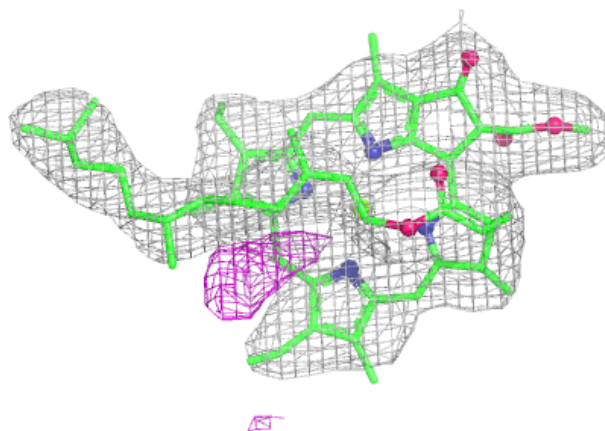
Electron density around CLA G 816:

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

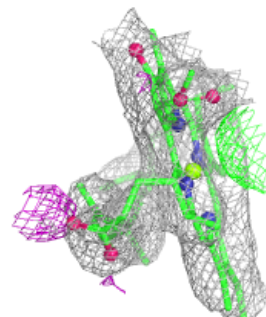
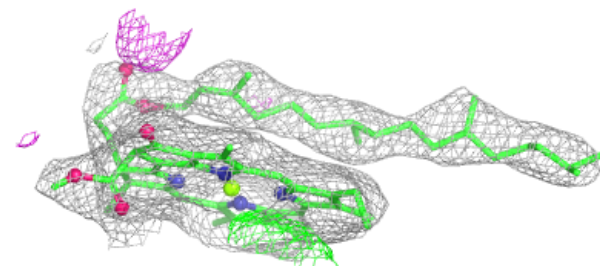
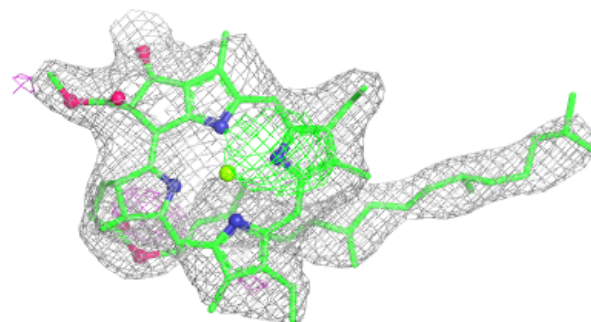


Electron density around CLA G 817:

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

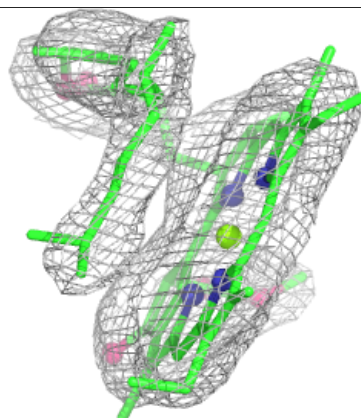
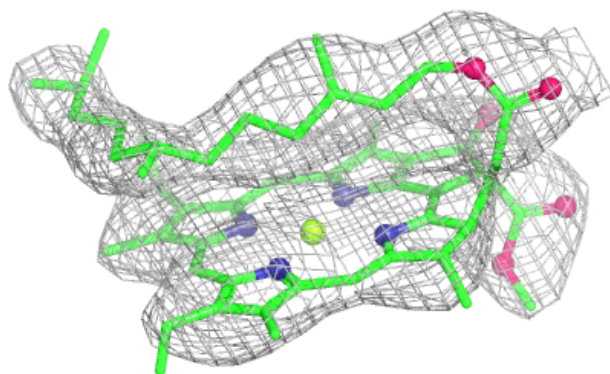
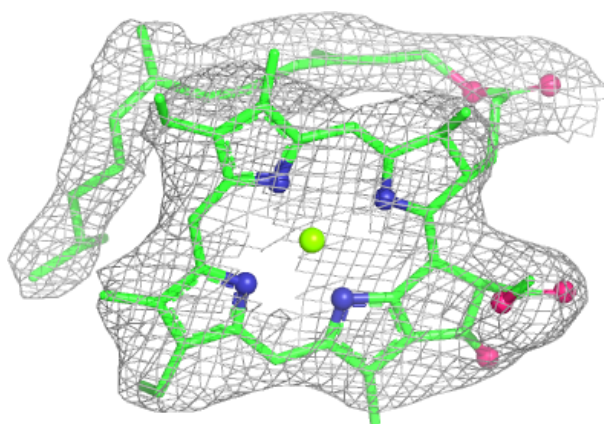
**Electron density around CLA G 818:**

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

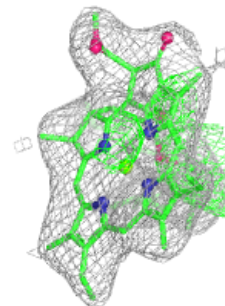
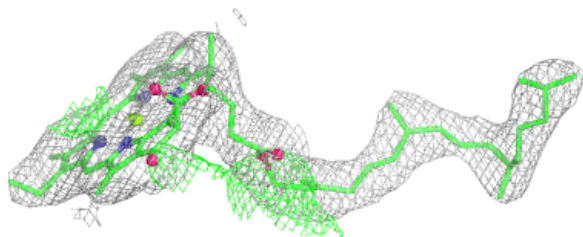
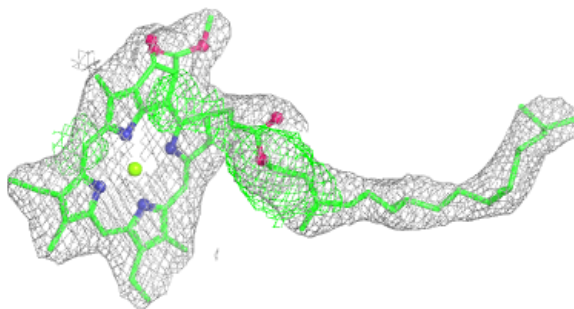


Electron density around CLA G 820:

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

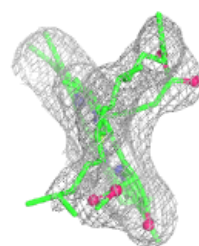
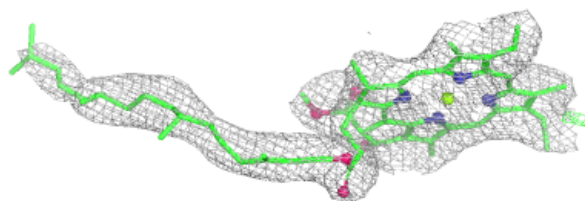
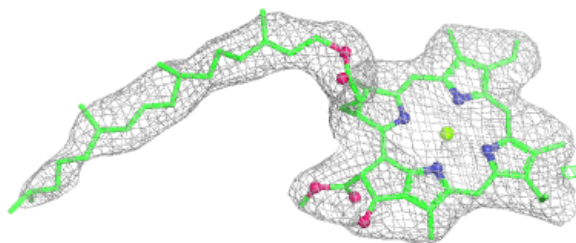
**Electron density around CLA G 821:**

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



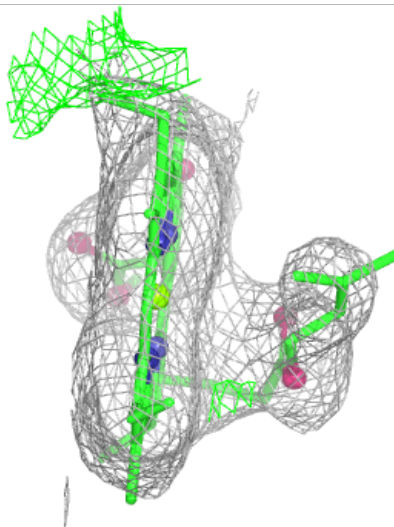
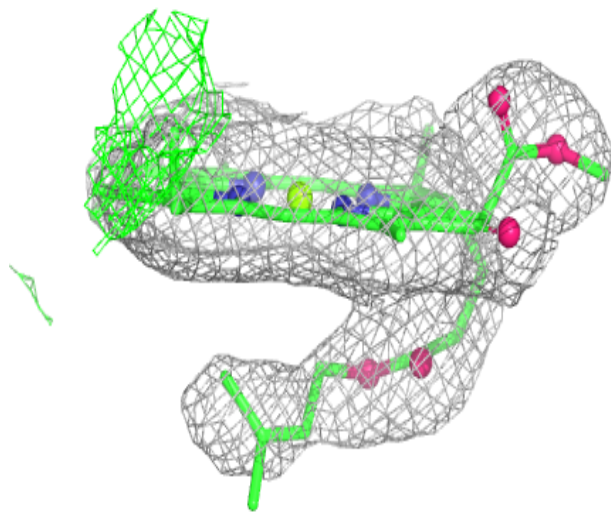
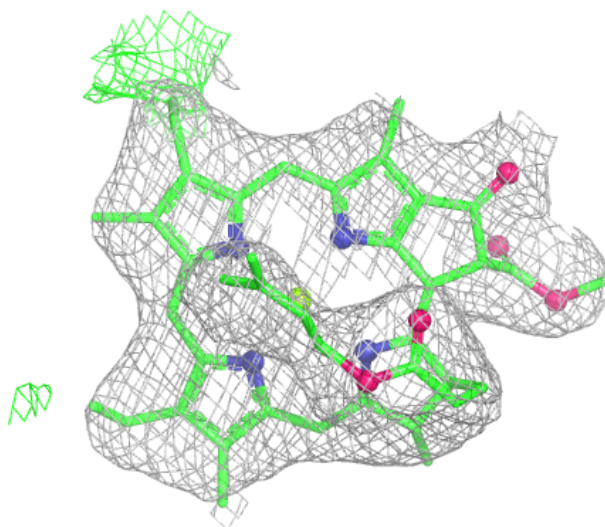
Electron density around CLA G 822:

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



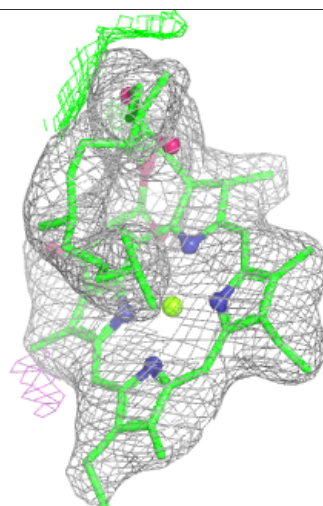
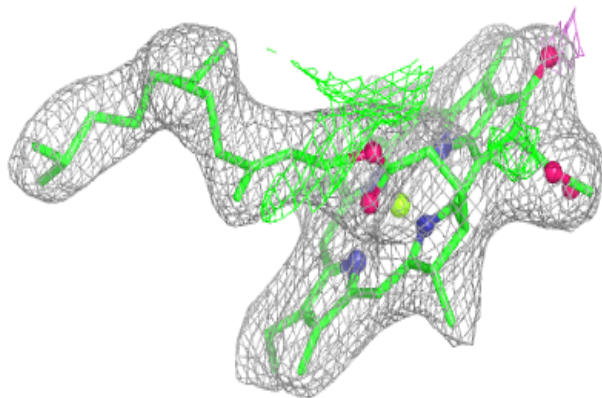
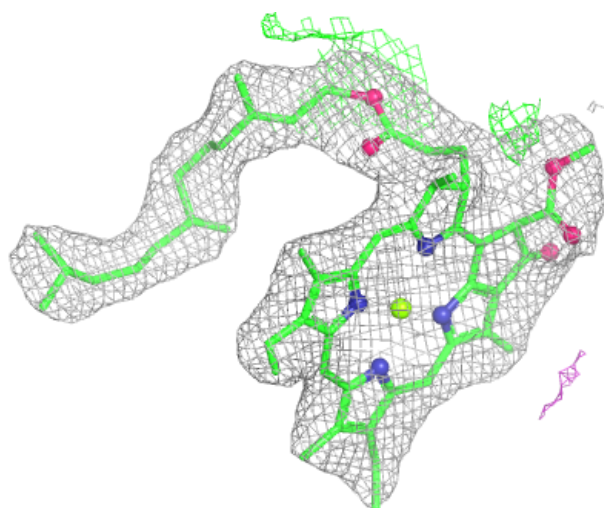
Electron density around CLA G 823:

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



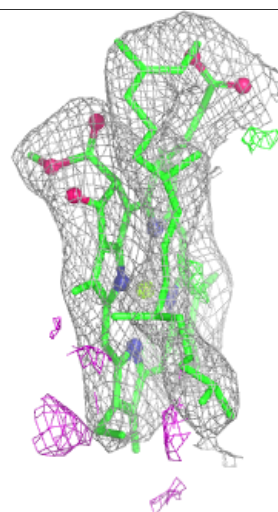
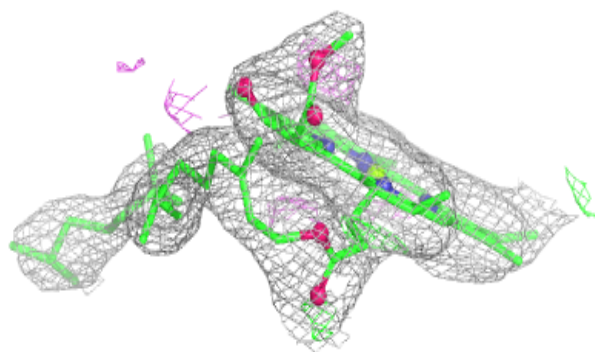
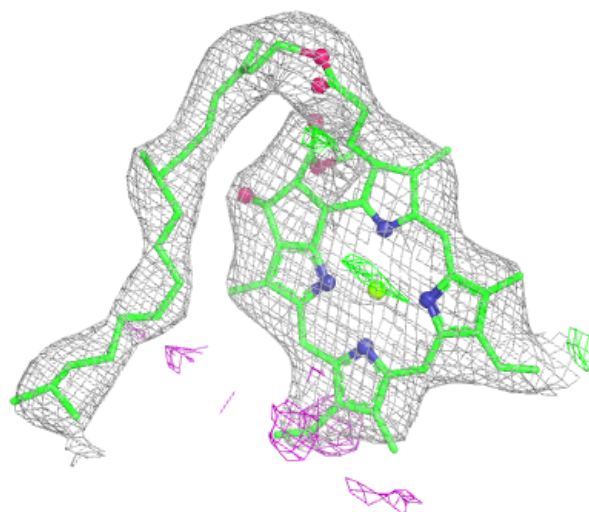
Electron density around CLA G 824:

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



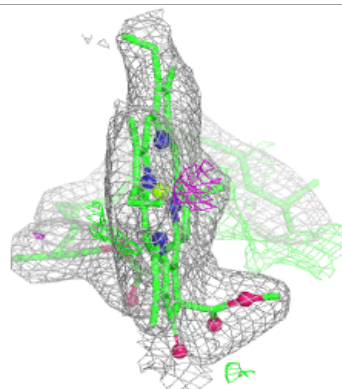
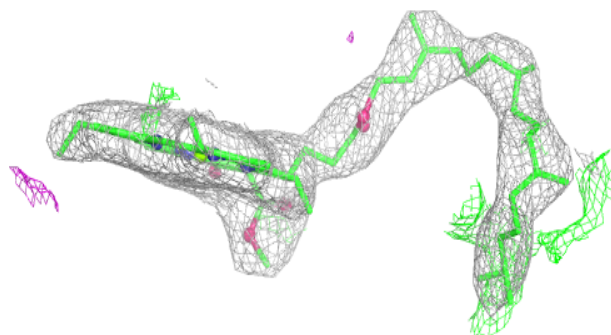
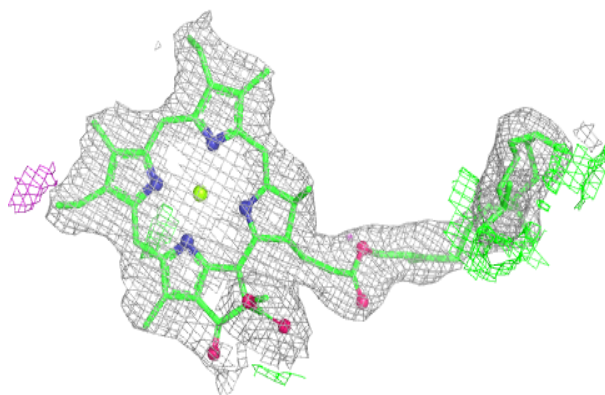
Electron density around CLA G 825:

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

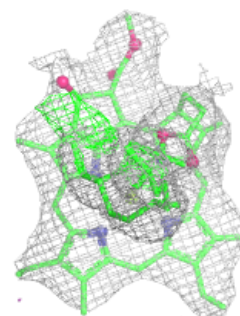
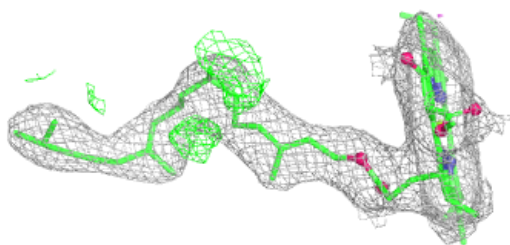
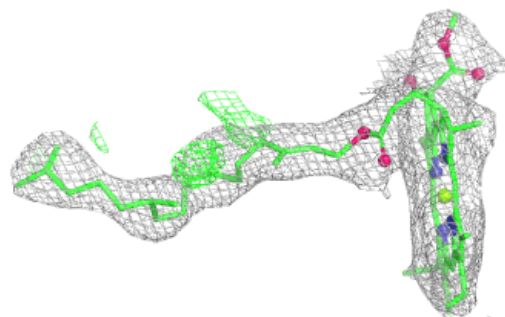


Electron density around CLA G 827:

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

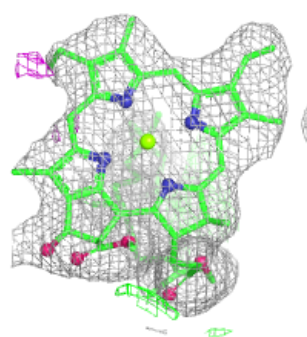
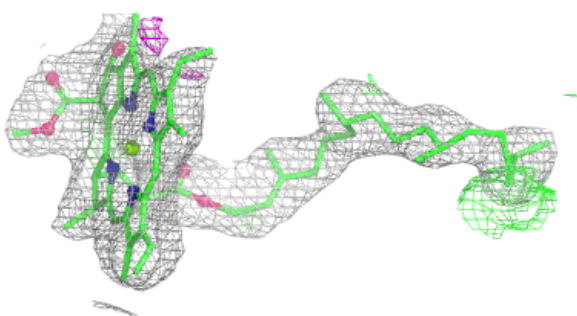
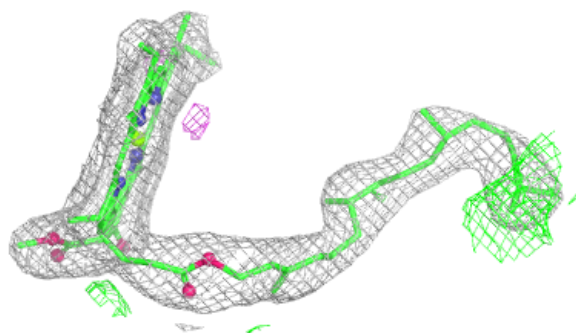
**Electron density around CLA G 828:**

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

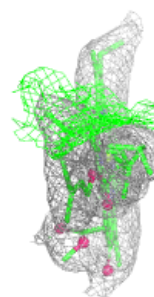
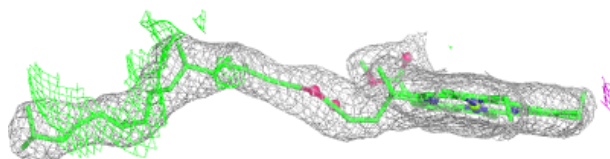
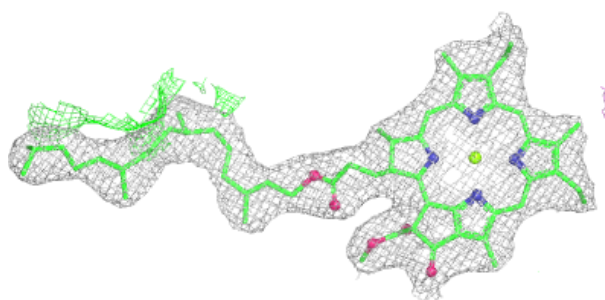


Electron density around CLA G 830:

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

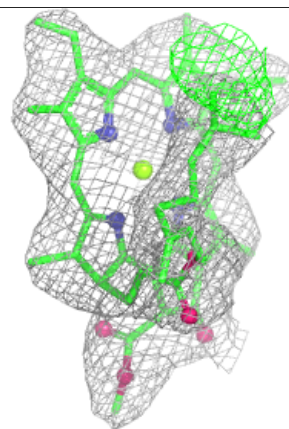
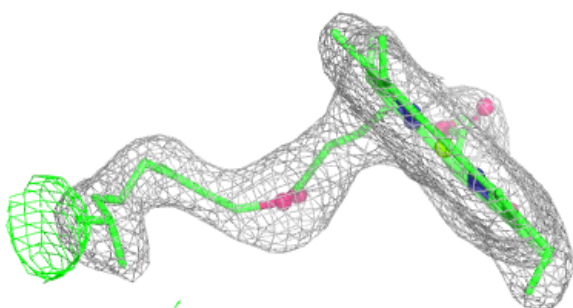
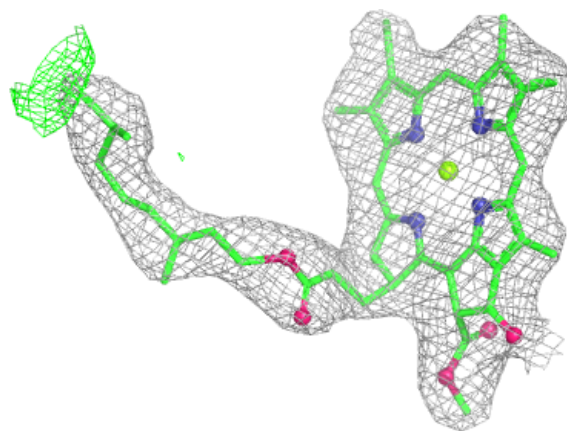
**Electron density around CLA G 832:**

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

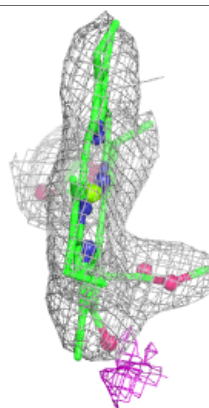
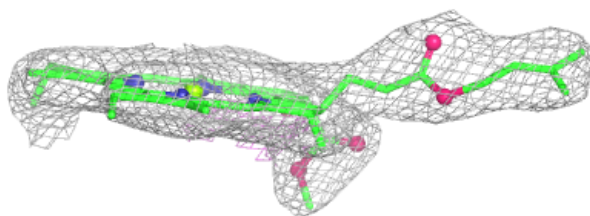
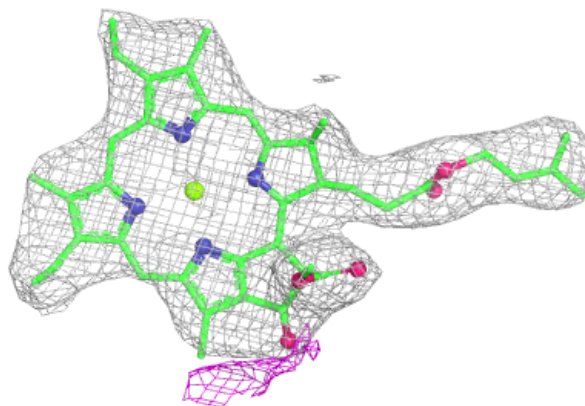


Electron density around CLA G 834:

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

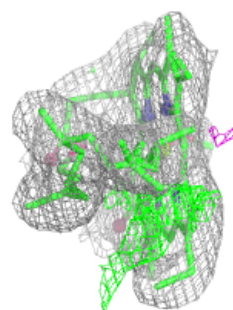
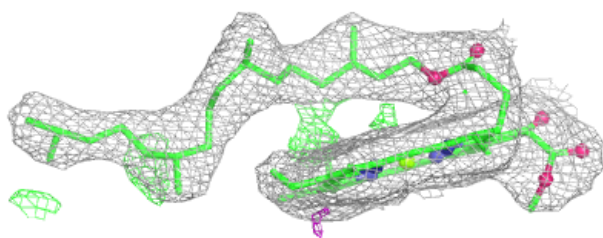
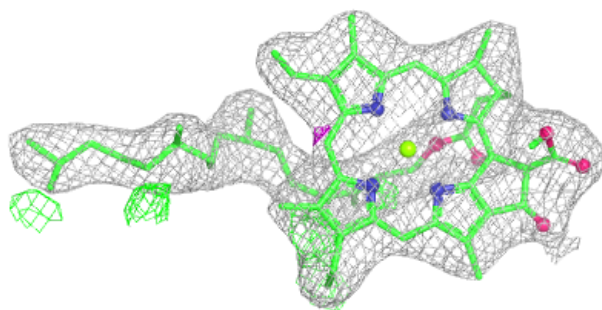
**Electron density around CLA G 836:**

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

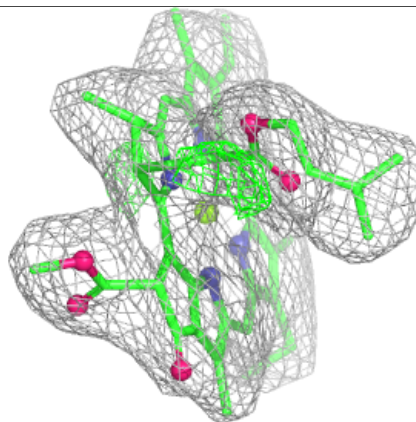
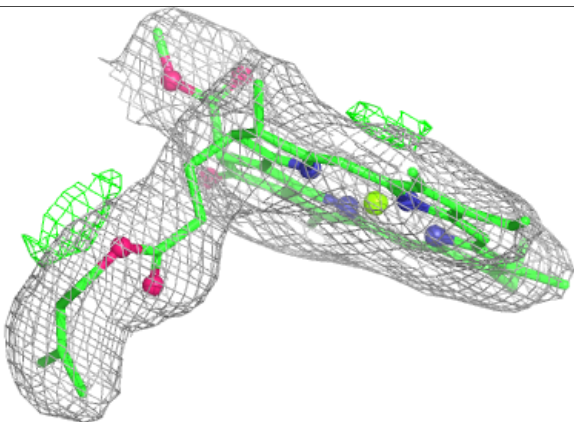
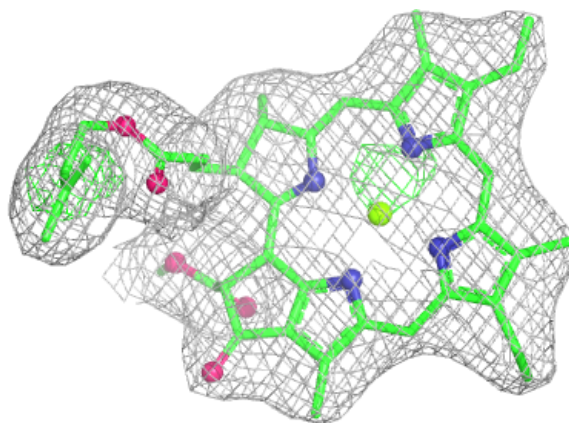


Electron density around CLA G 837:

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

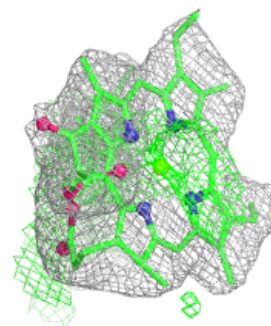
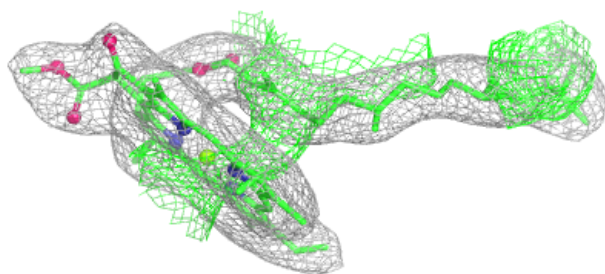
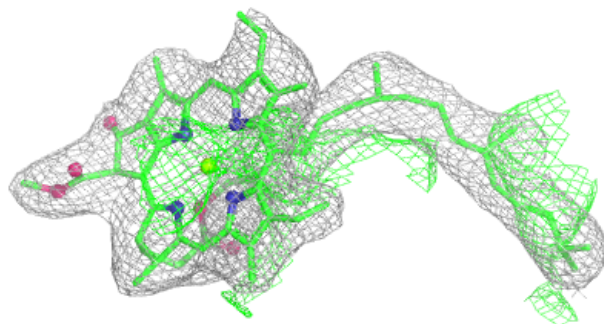
**Electron density around CLA G 838:**

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



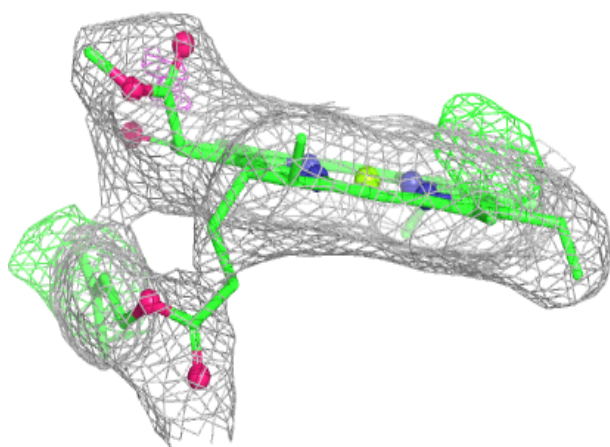
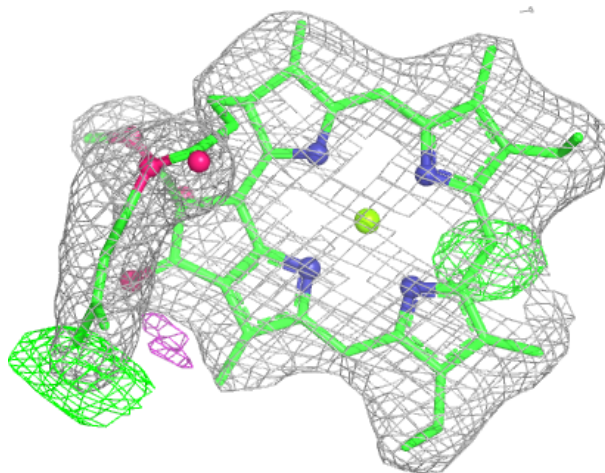
Electron density around CLA G 841:

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



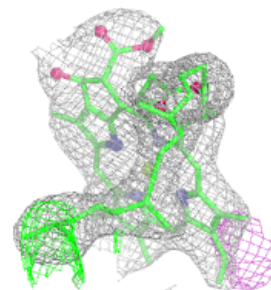
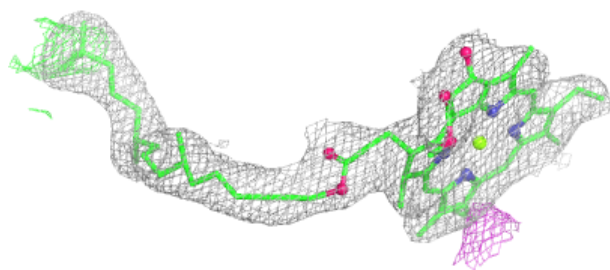
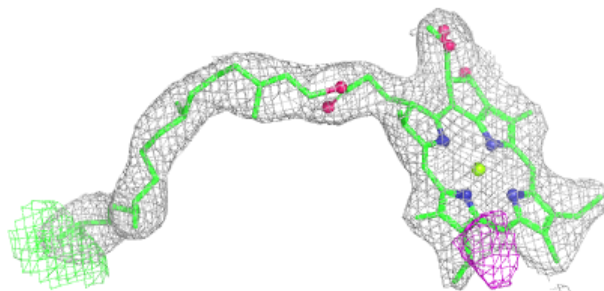
Electron density around CLA G 843:

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

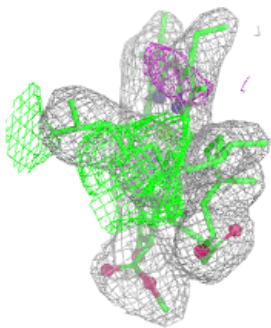
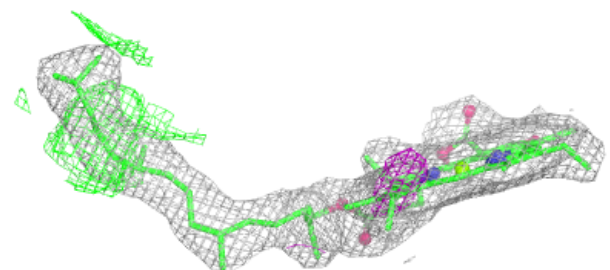
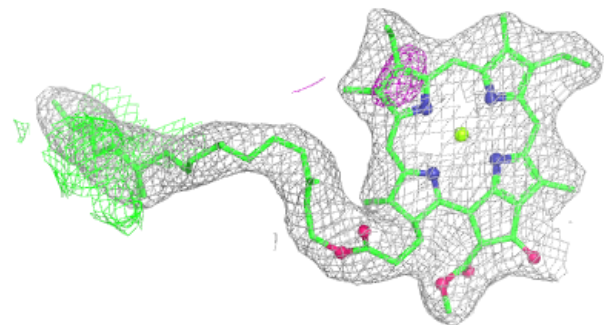


Electron density around CLA H 801:

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

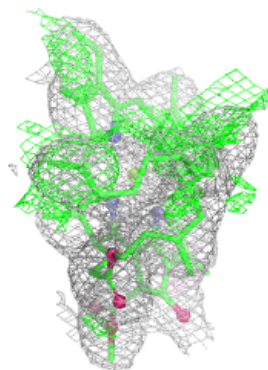
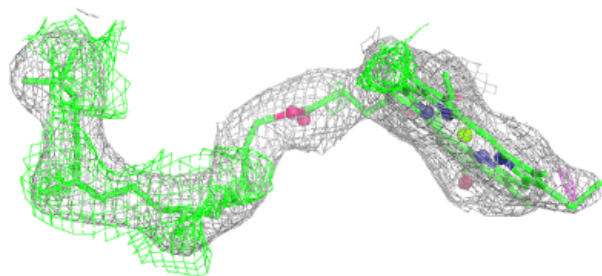
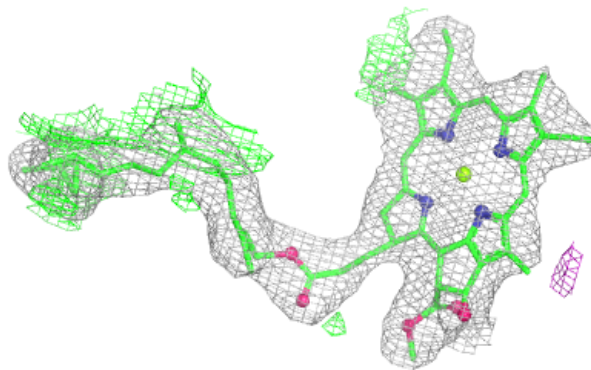
**Electron density around CLA H 803:**

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



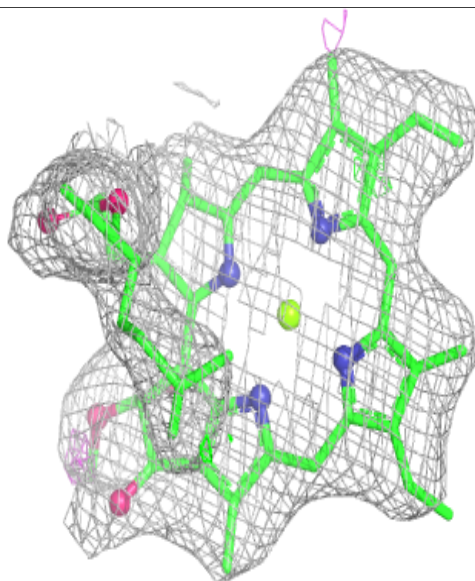
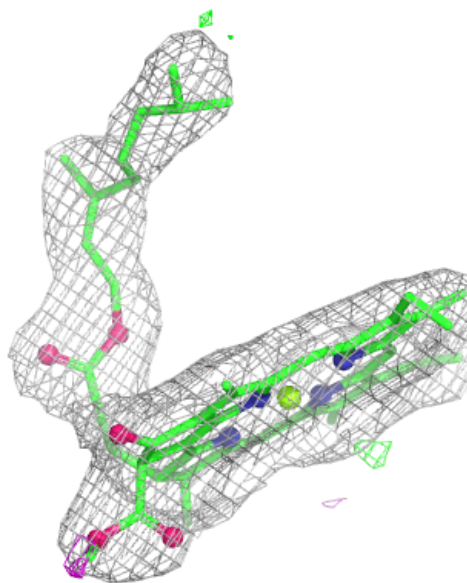
Electron density around CLA H 808:

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



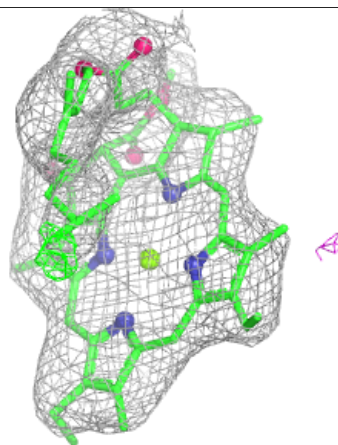
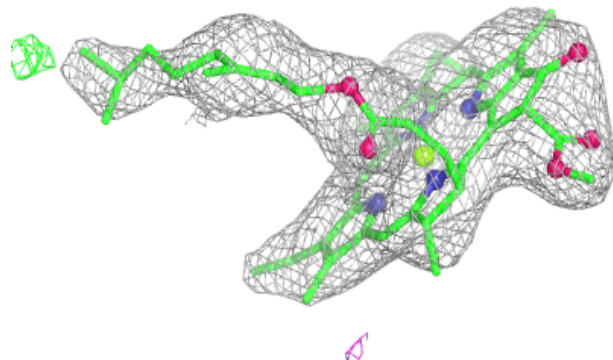
Electron density around CLA H 810:

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

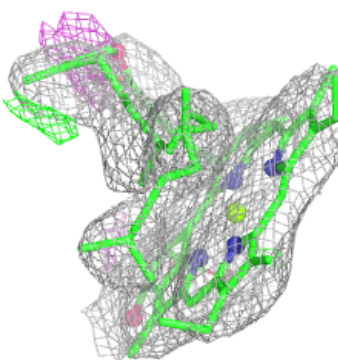
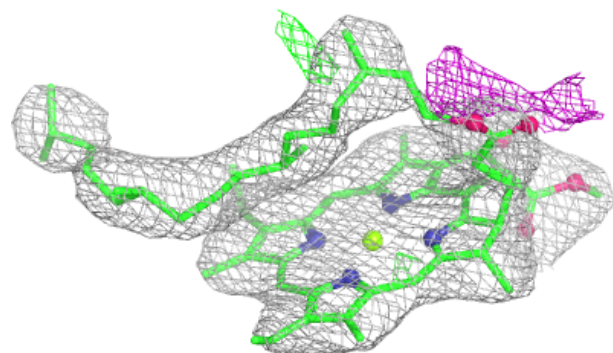
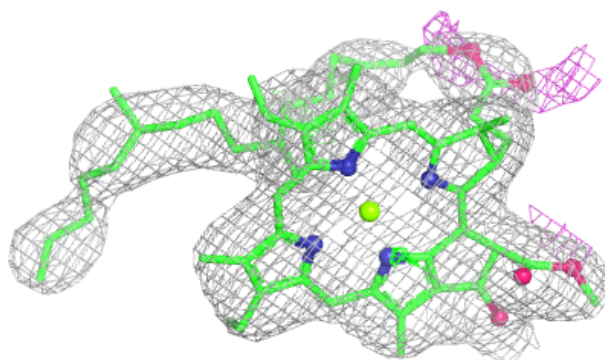


Electron density around CLA H 815:

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

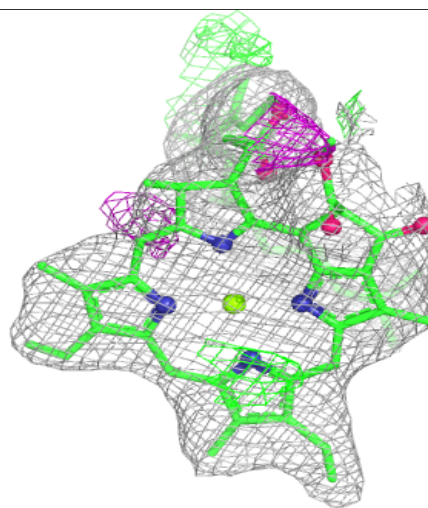
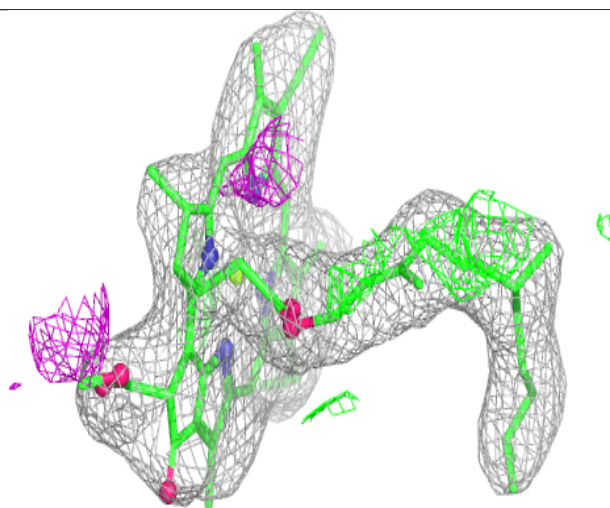
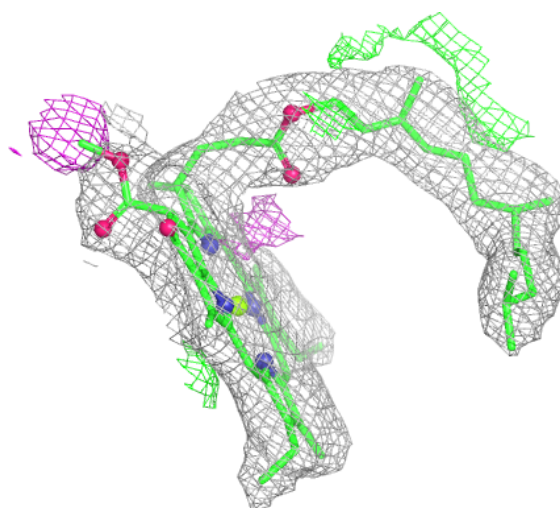
**Electron density around CLA H 816:**

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



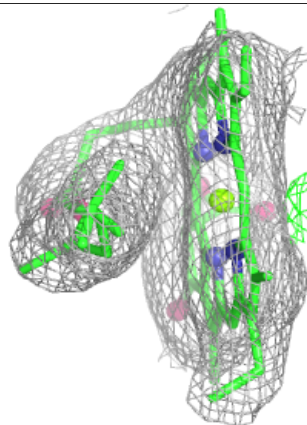
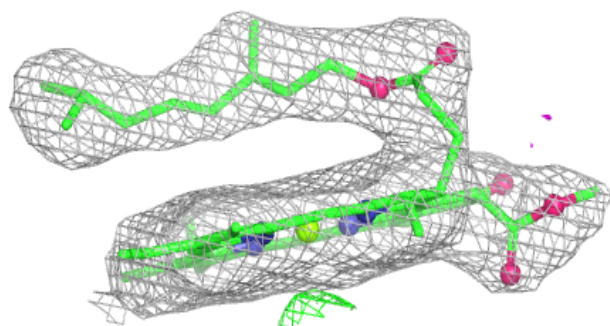
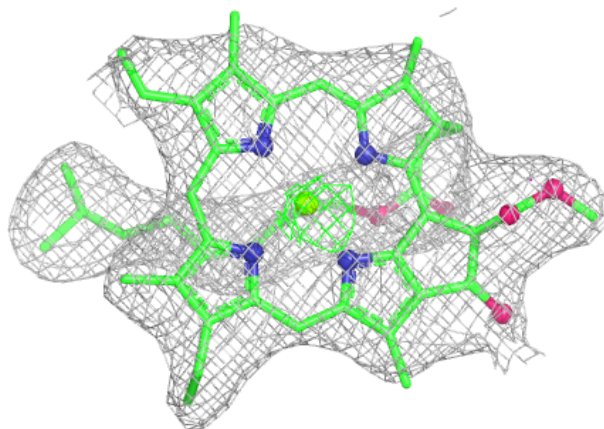
Electron density around CLA H 818:

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

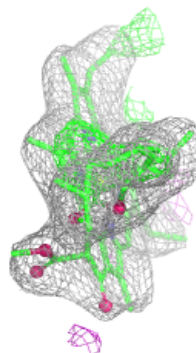
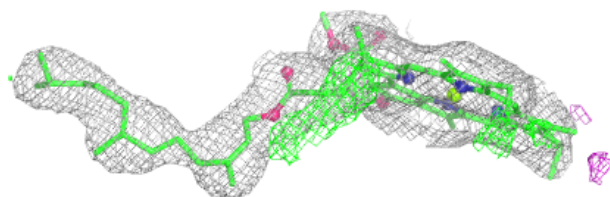
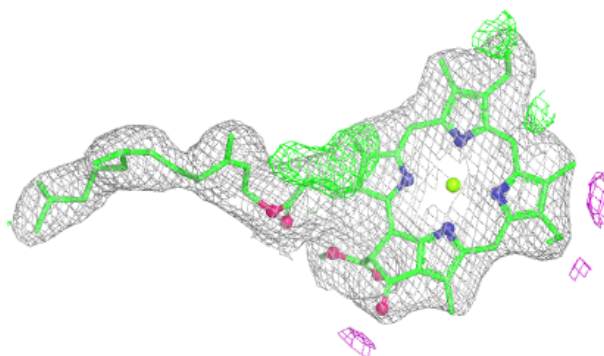


Electron density around CLA H 821:

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

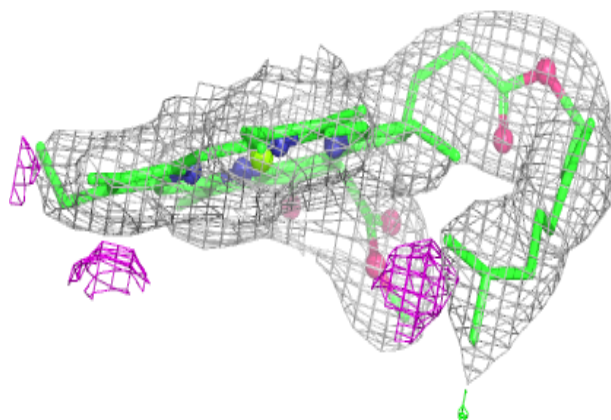
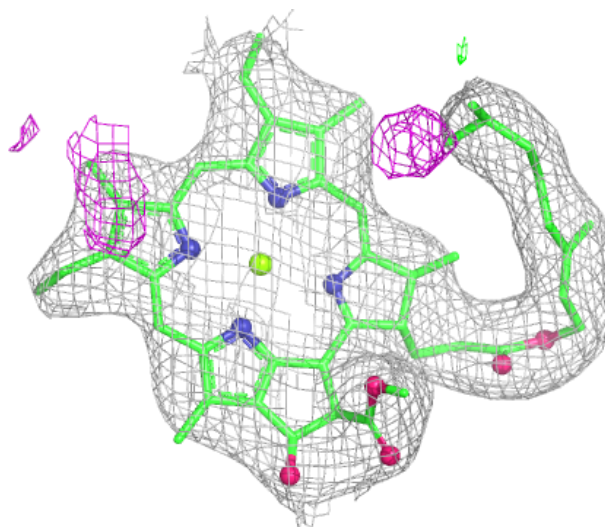
**Electron density around CLA H 822:**

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



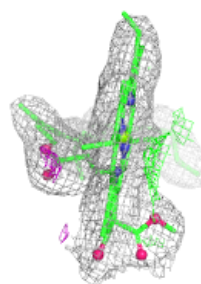
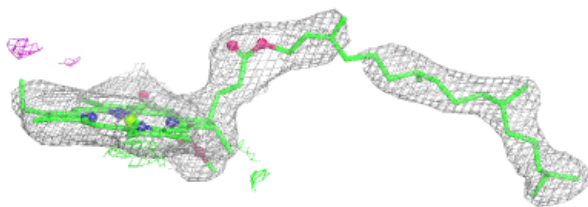
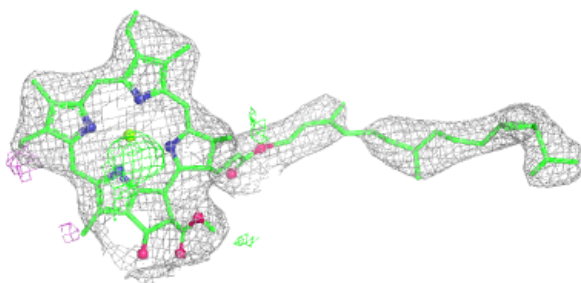
Electron density around CLA H 823:

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

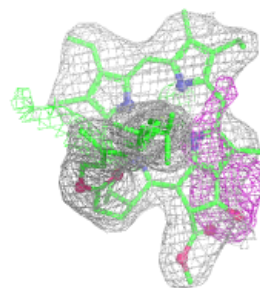
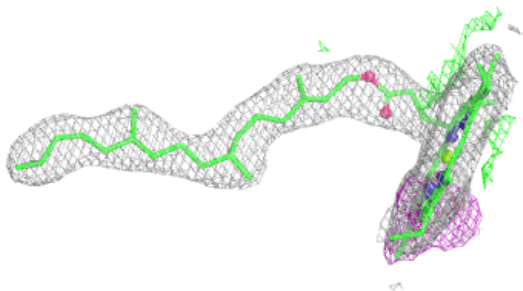
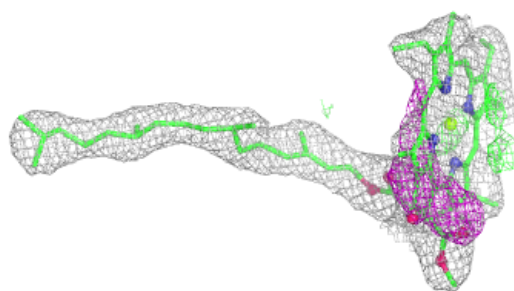


Electron density around CLA H 824:

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

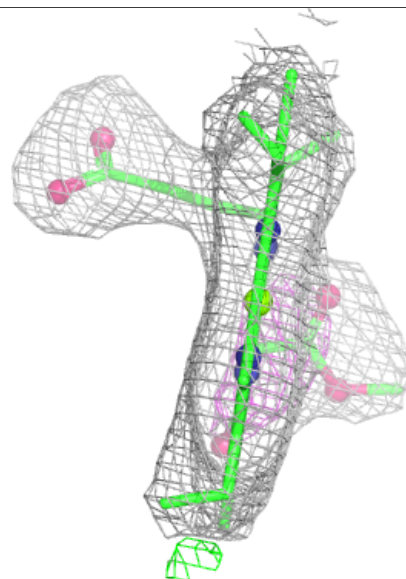
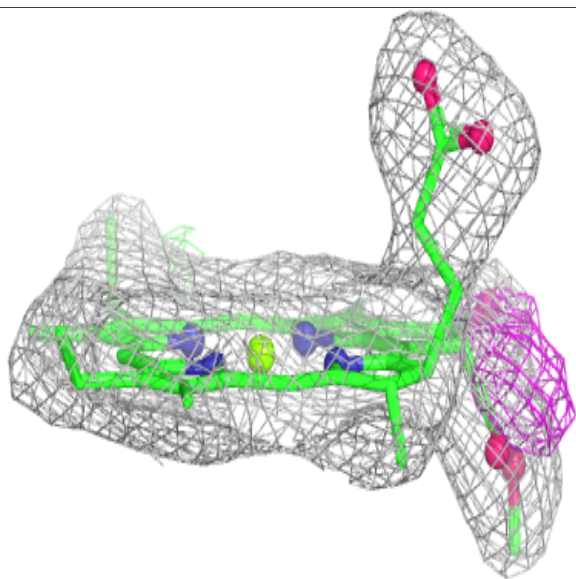
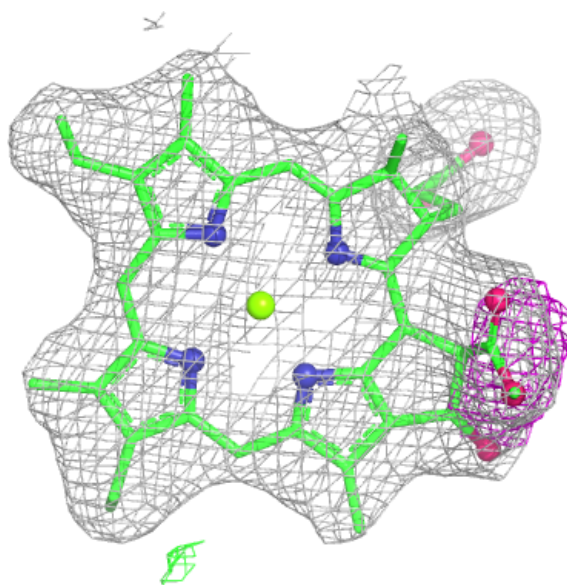
**Electron density around CLA H 827:**

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



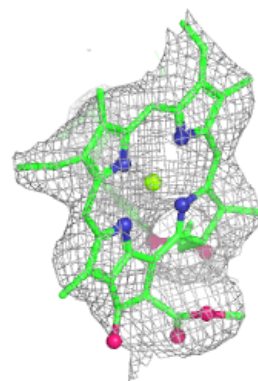
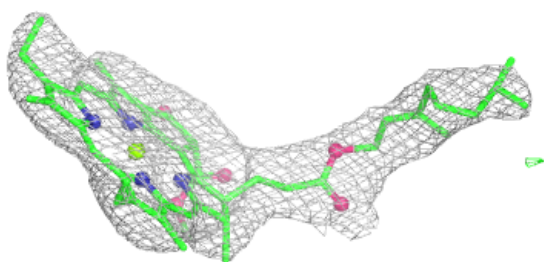
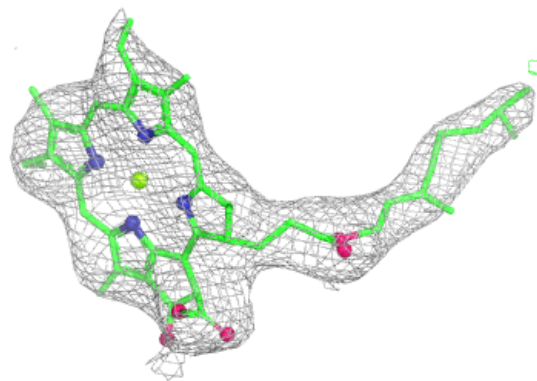
Electron density around CLA H 829:

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



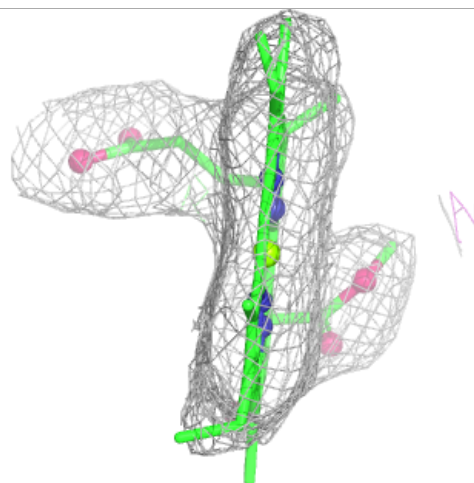
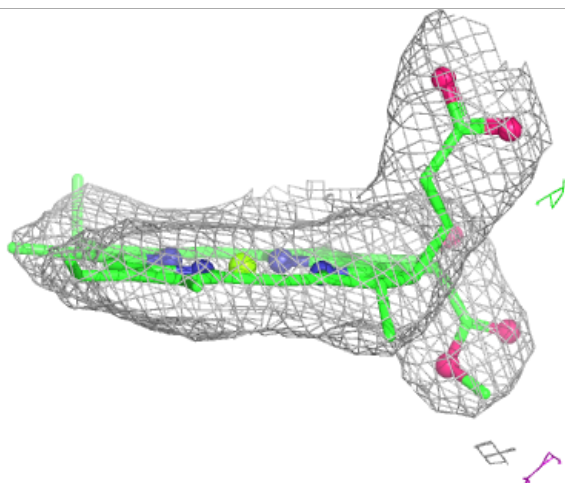
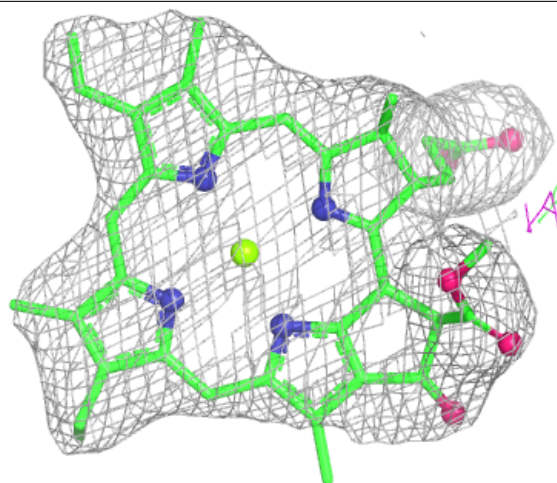
Electron density around CLA H 830:

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



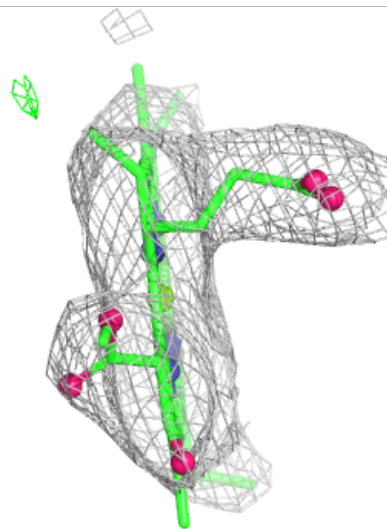
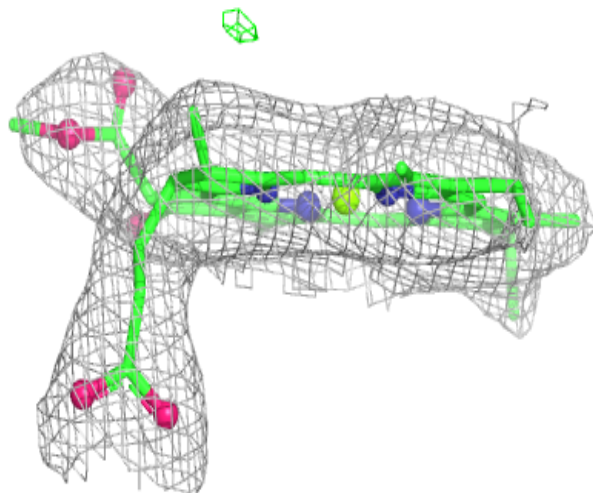
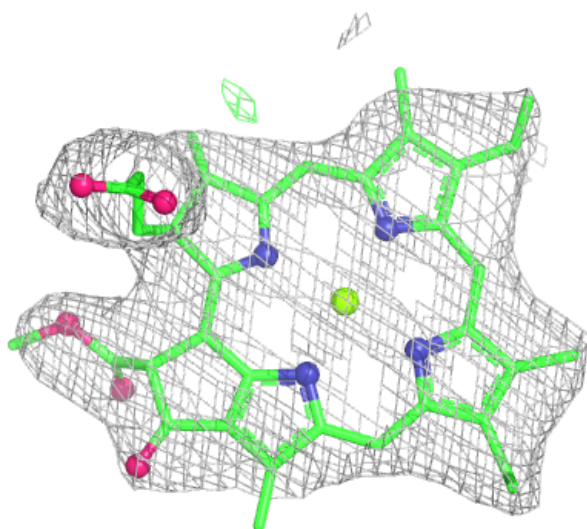
Electron density around CLA H 831:

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



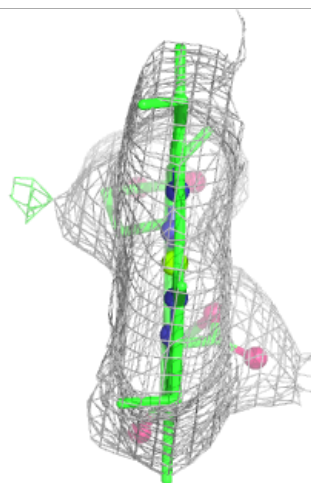
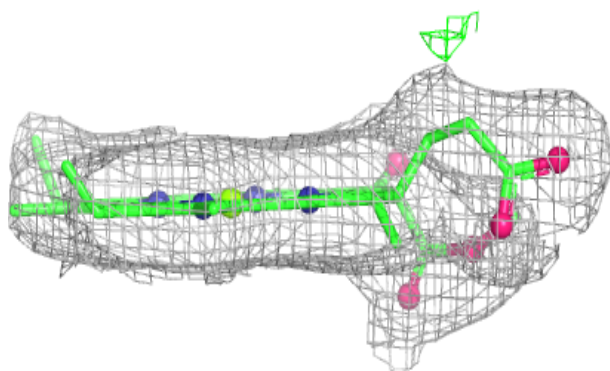
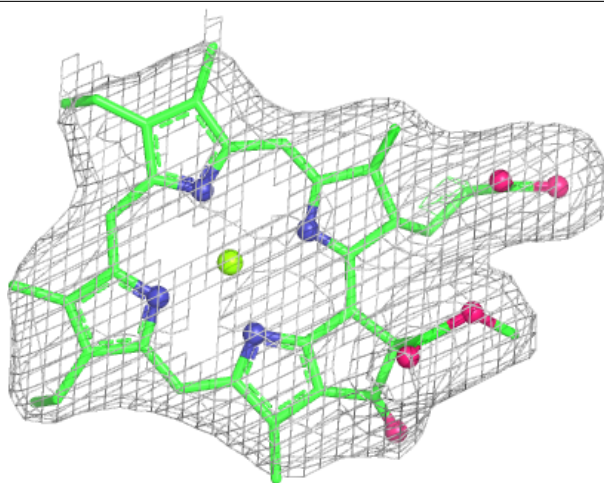
Electron density around CLA H 832:

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



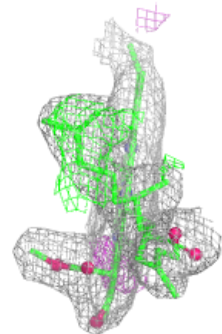
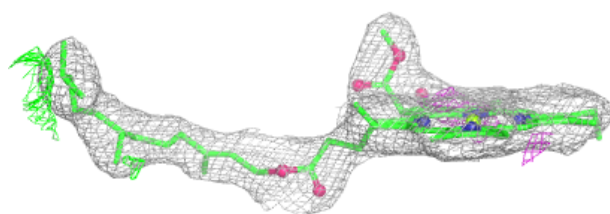
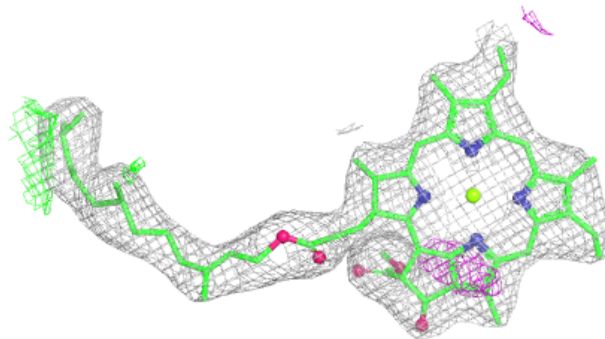
Electron density around CLA H 833:

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



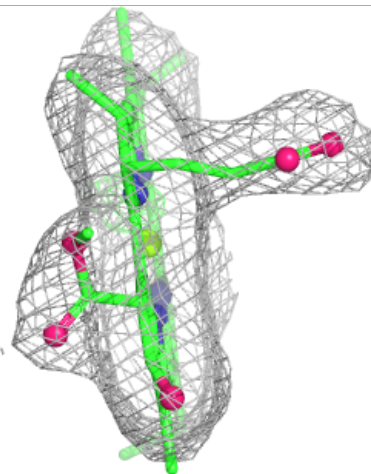
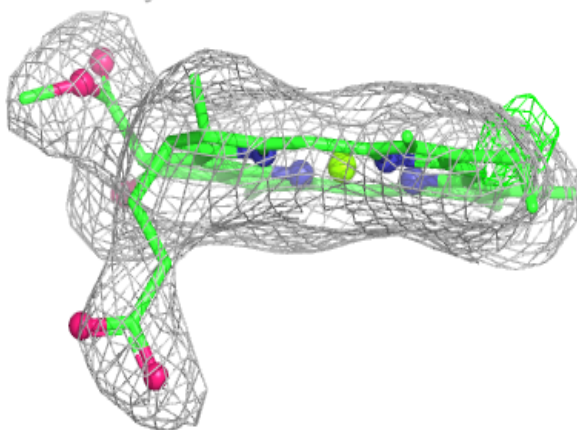
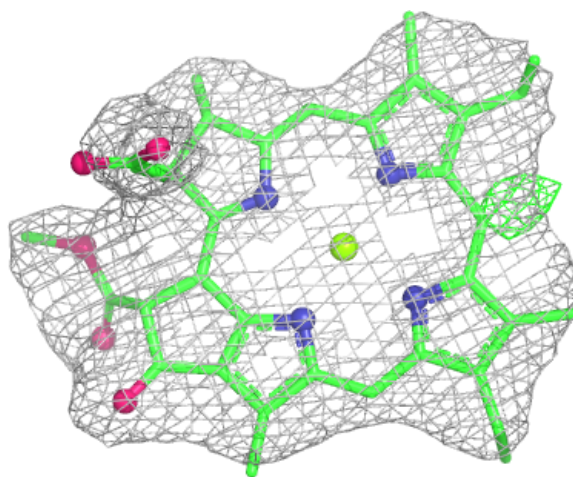
Electron density around CLA H 834:

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



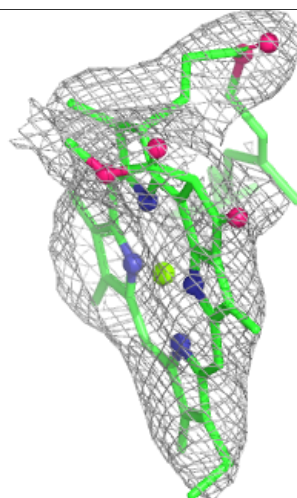
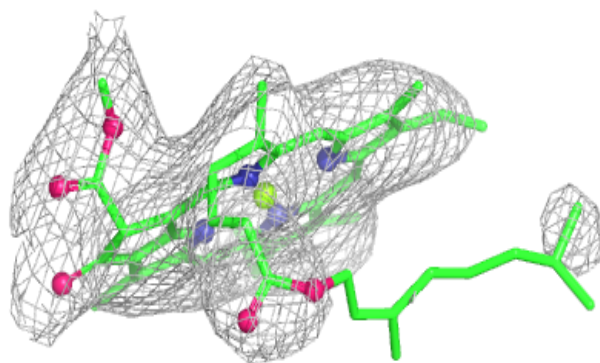
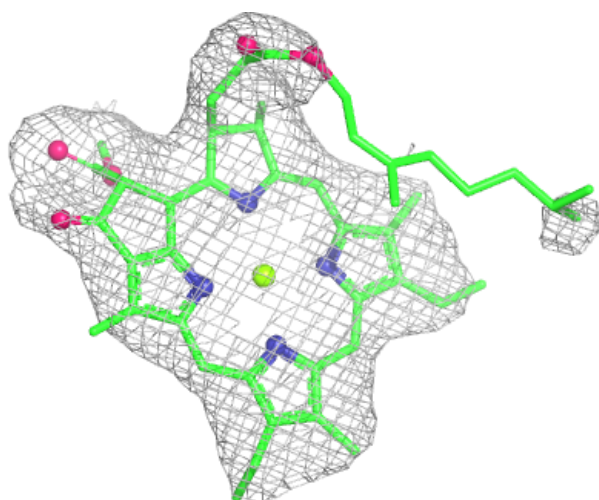
Electron density around CLA J 101:

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



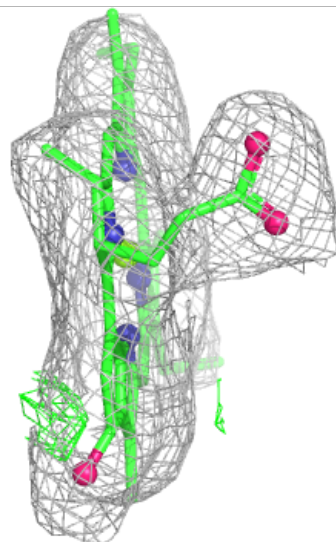
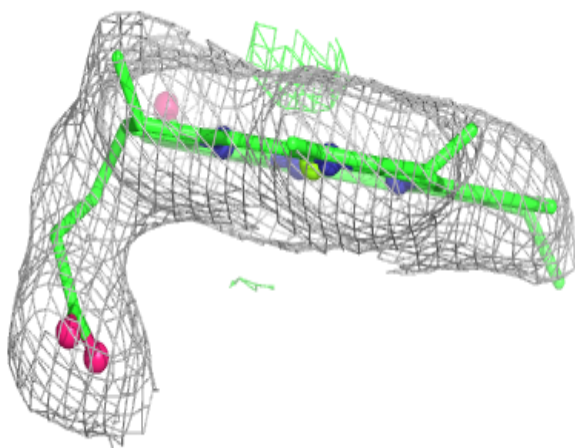
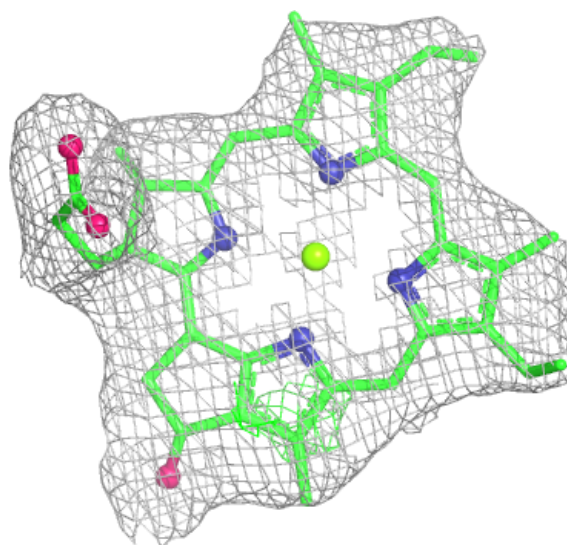
Electron density around CLA J 102:

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



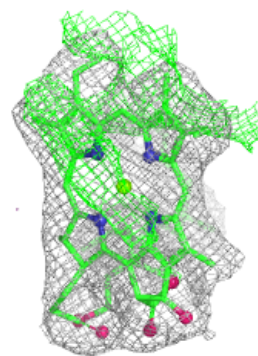
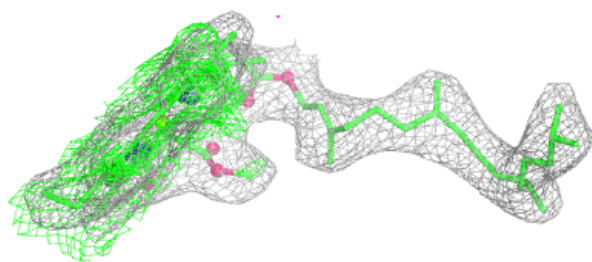
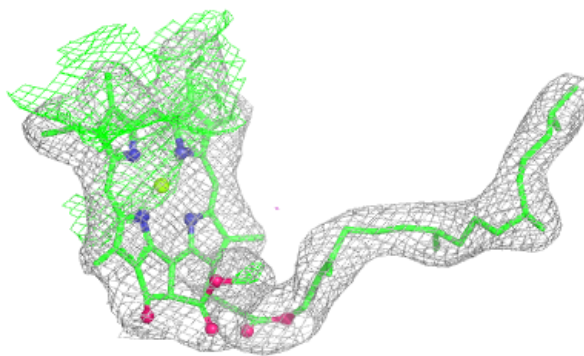
Electron density around CLA K 101:

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



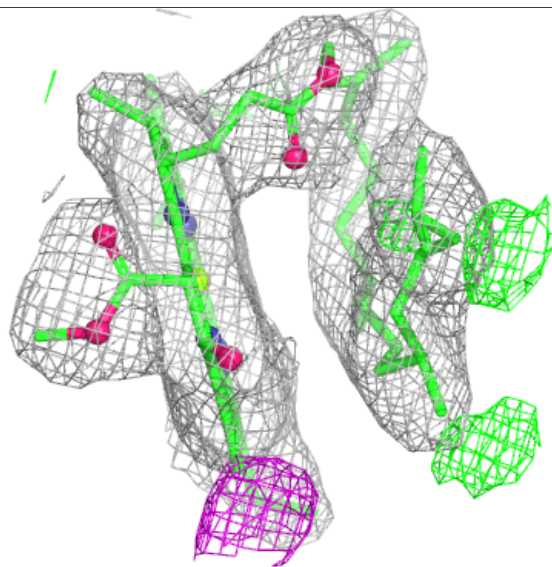
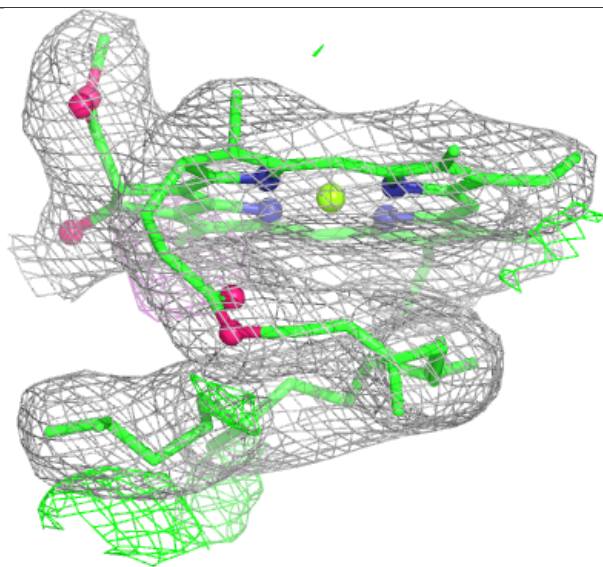
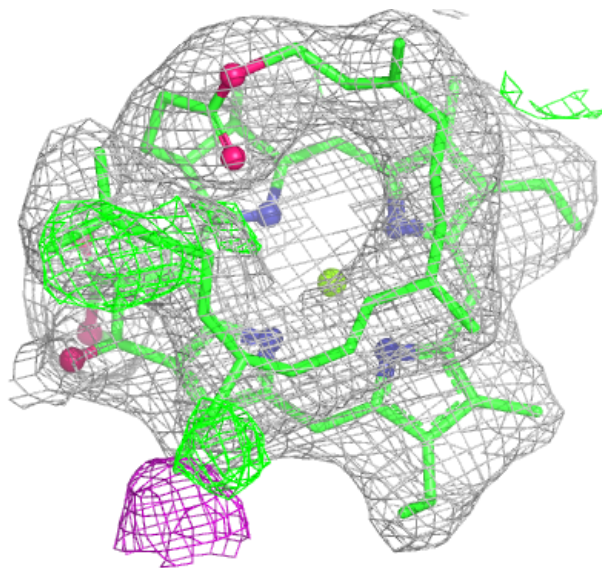
Electron density around CLA L 202:

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



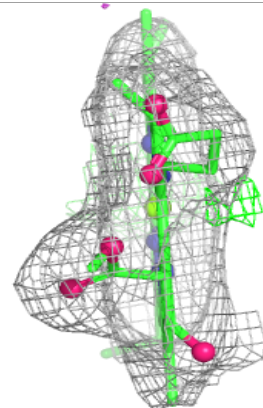
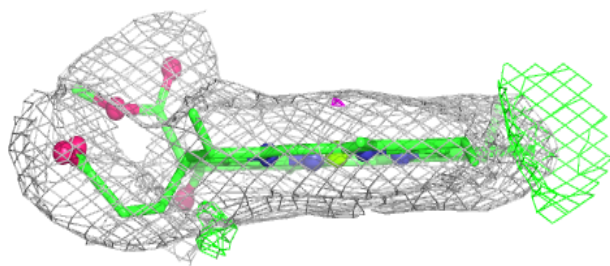
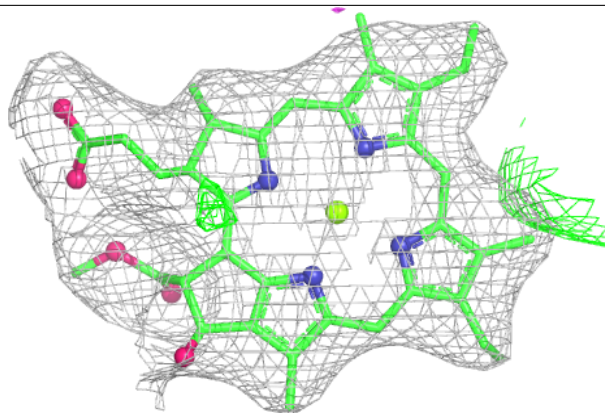
Electron density around CLA L 205:

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

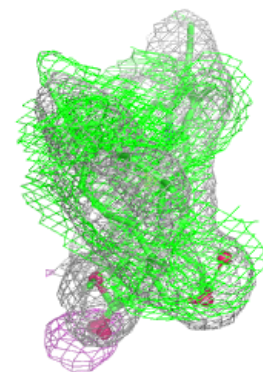
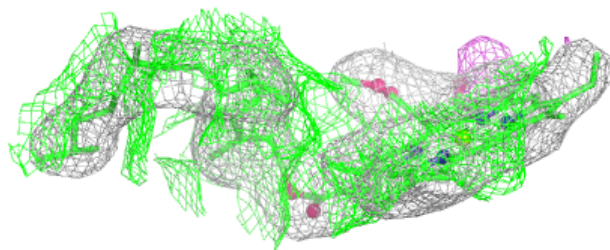
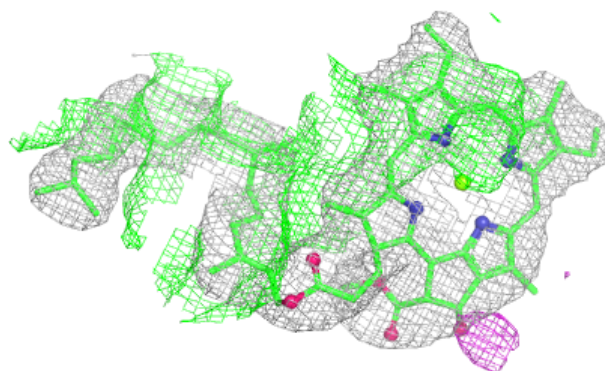


Electron density around CLA Q 203:

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

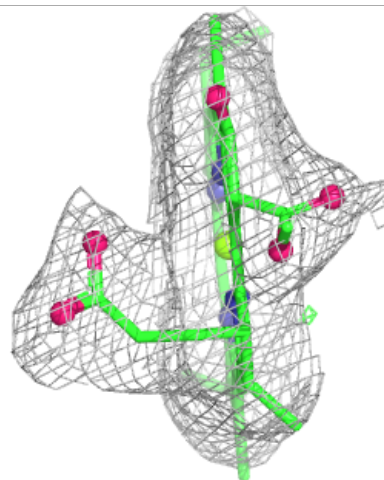
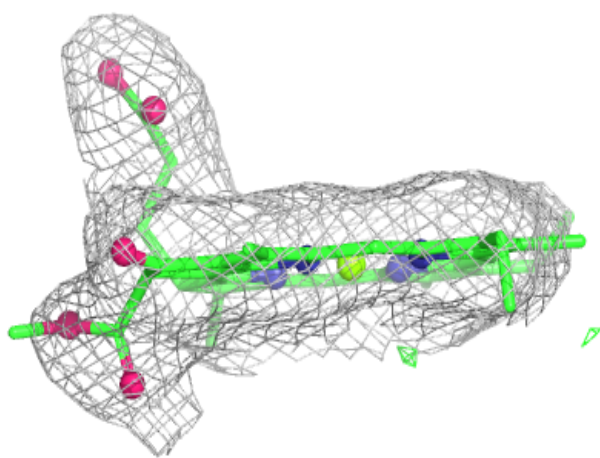
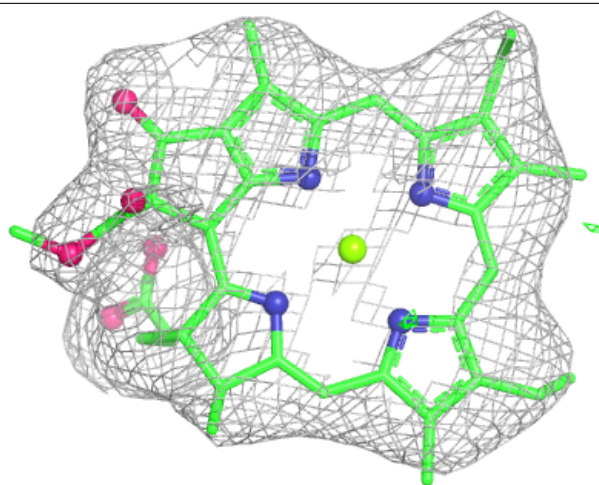
**Electron density around CLA S 1101:**

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



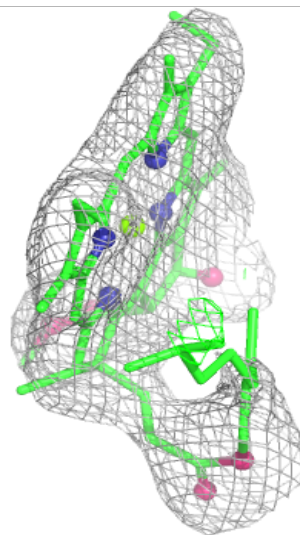
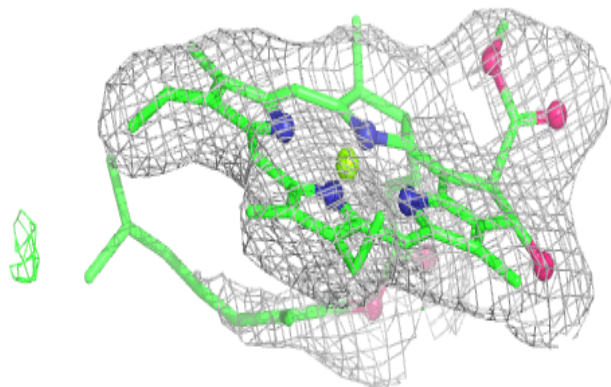
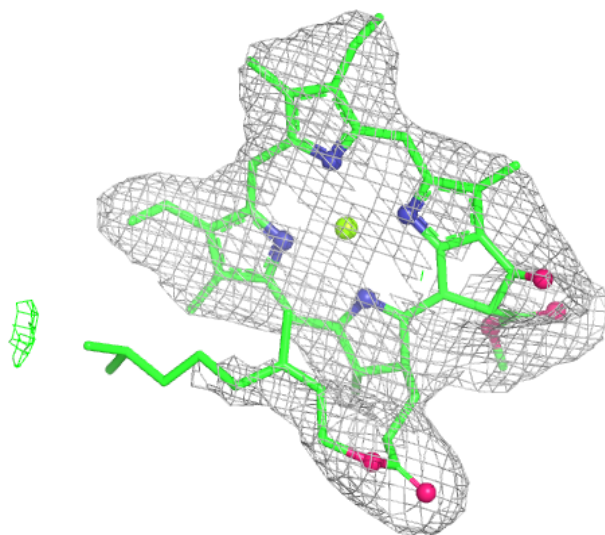
Electron density around CLA S 1102:

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



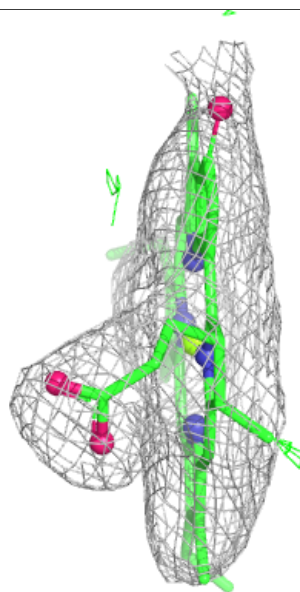
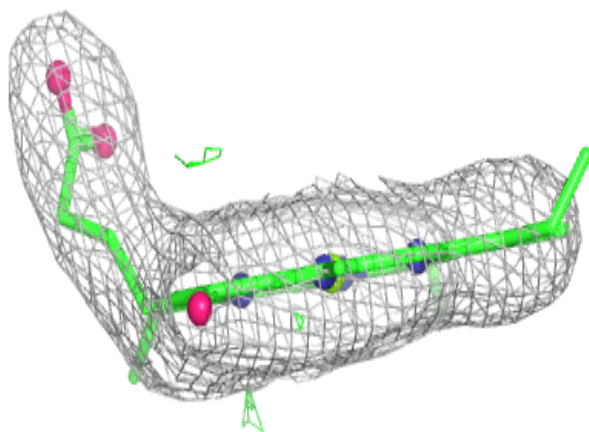
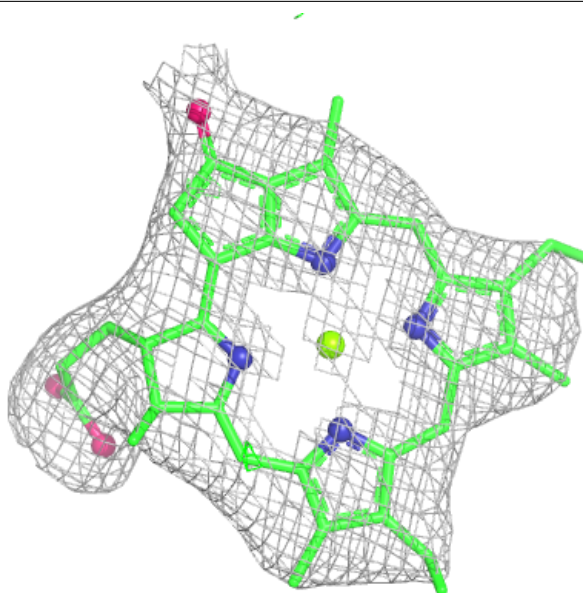
Electron density around CLA S 1103:

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



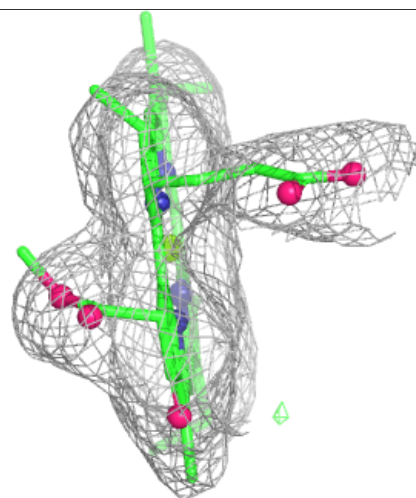
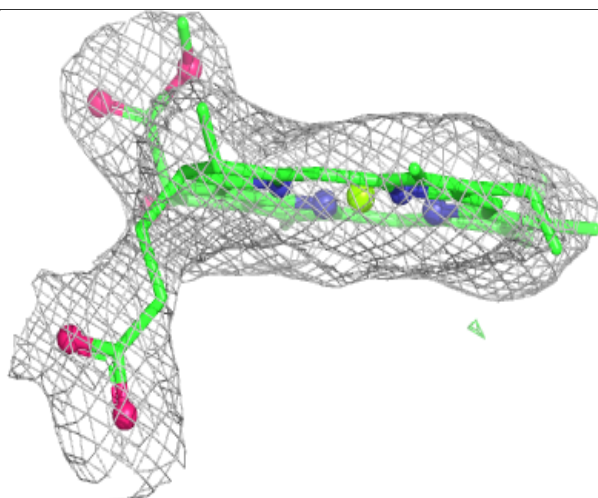
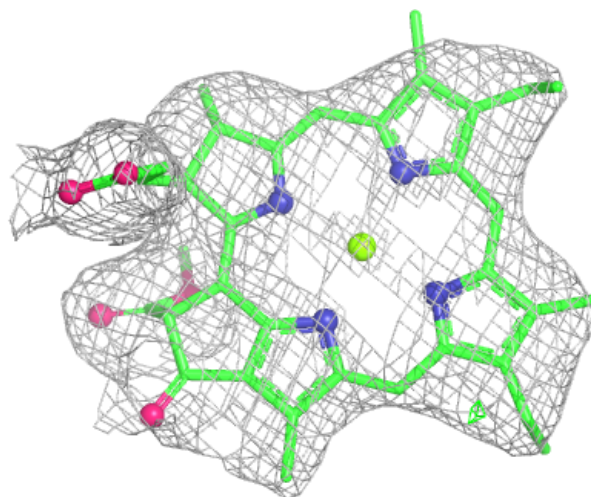
Electron density around CLA T 101:

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



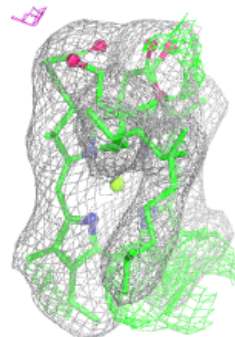
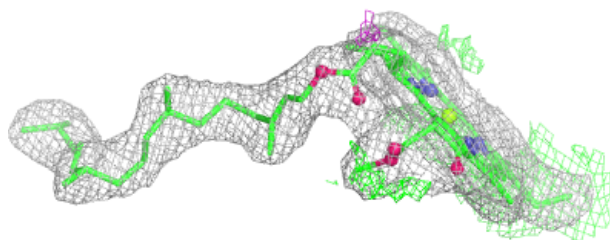
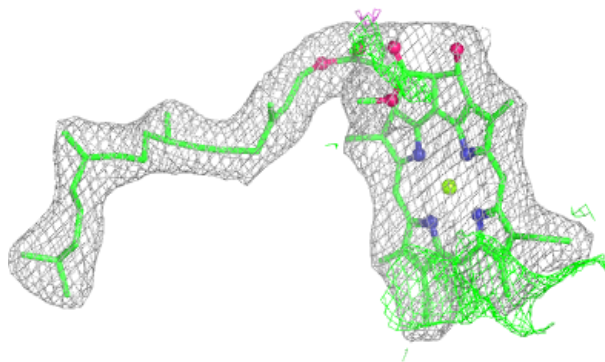
Electron density around CLA T 103:

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



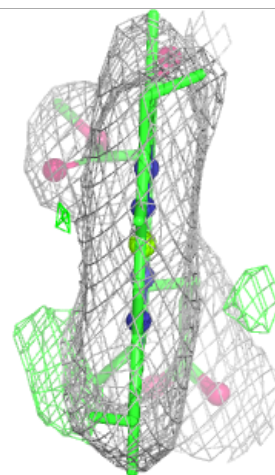
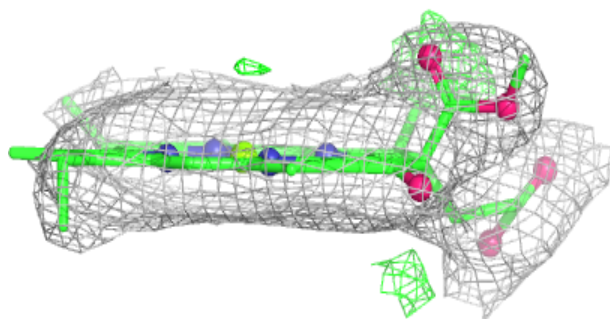
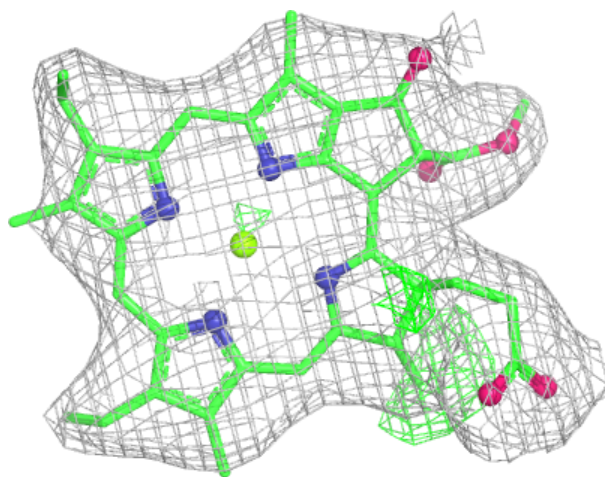
Electron density around CLA U 1006:

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



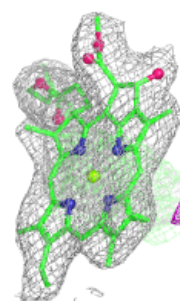
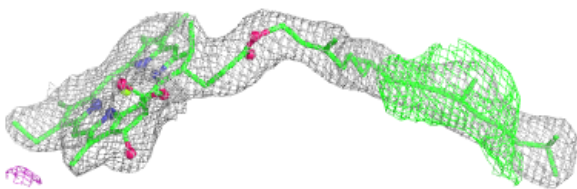
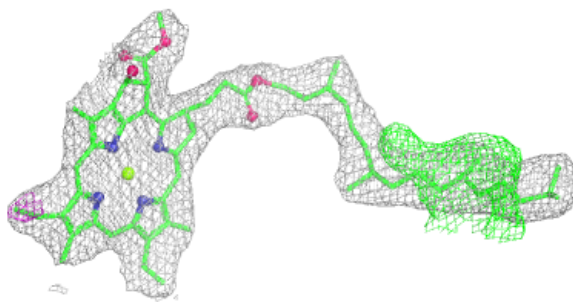
Electron density around CLA W 1701:

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

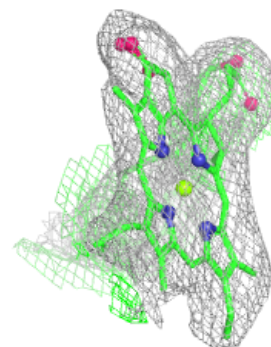
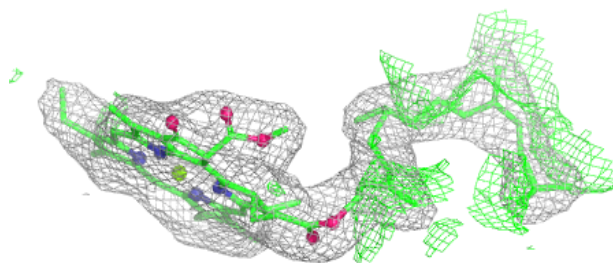
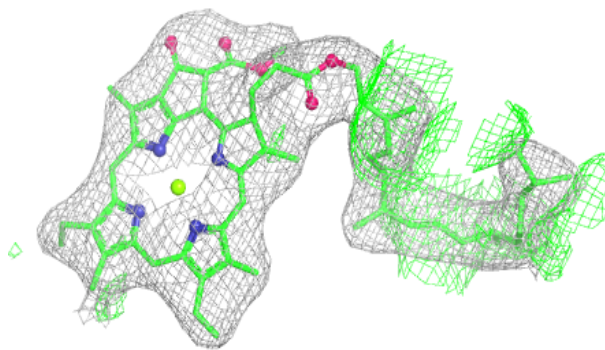


Electron density around CLA Y 802:

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

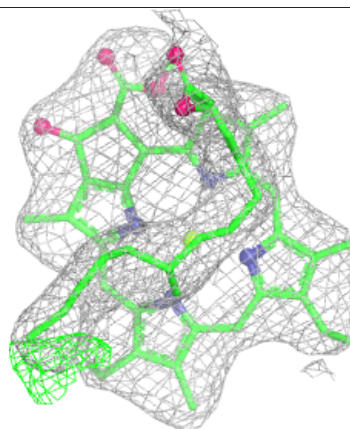
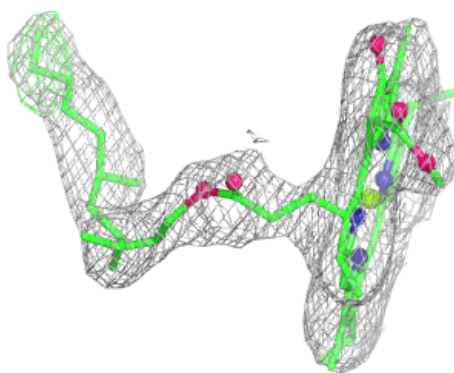
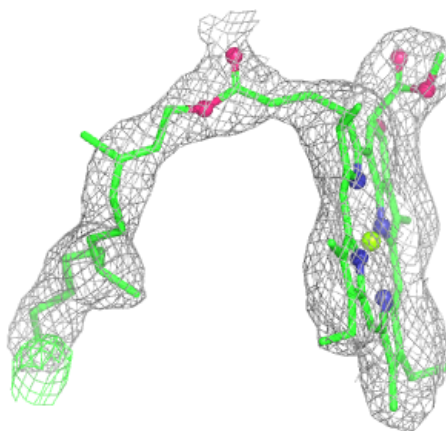
**Electron density around CLA Y 803:**

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



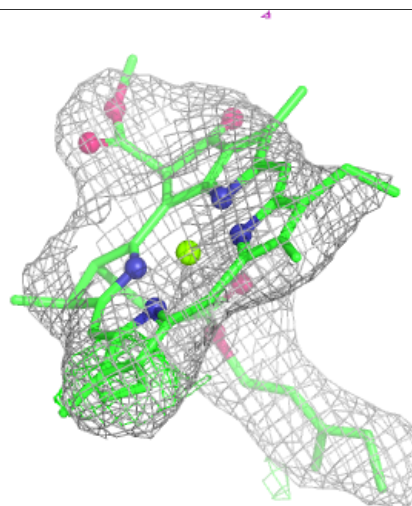
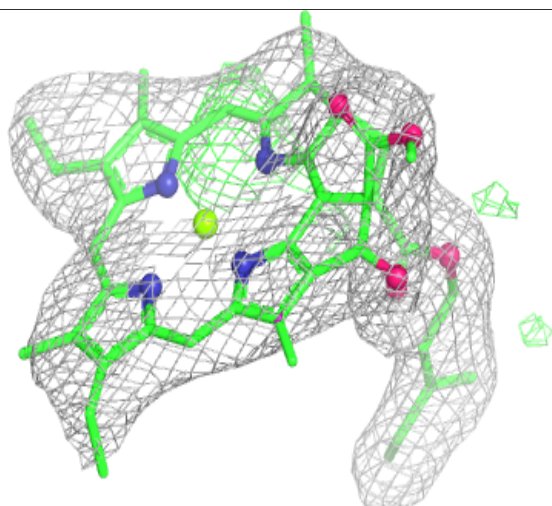
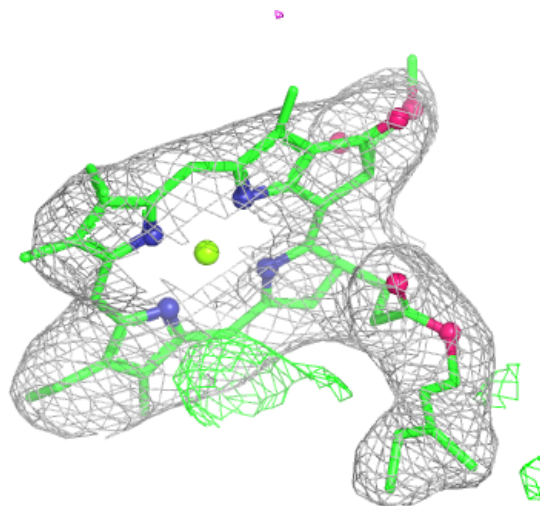
Electron density around CLA Y 804:

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



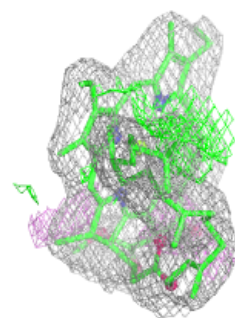
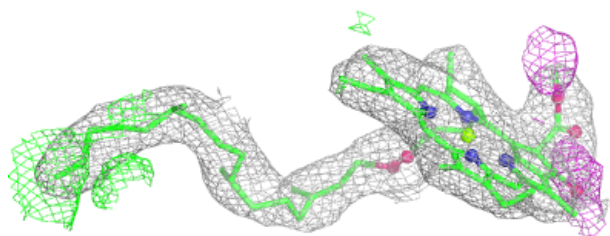
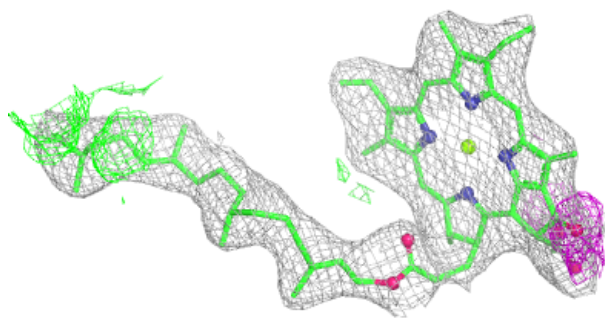
Electron density around CLA Y 807:

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

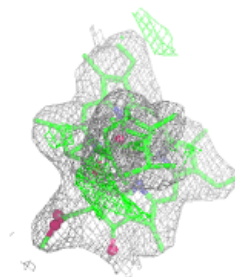
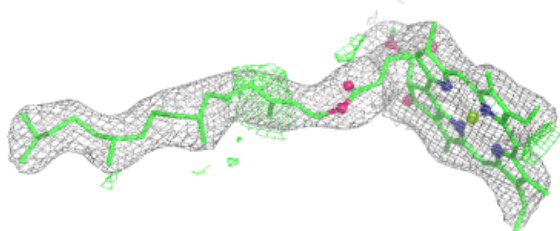
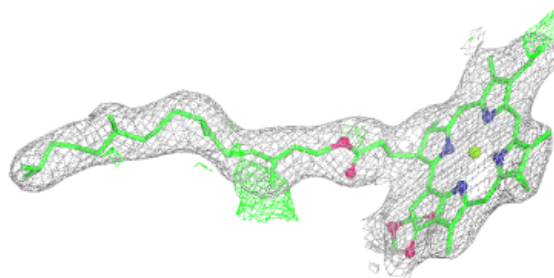


Electron density around CLA Y 808:

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

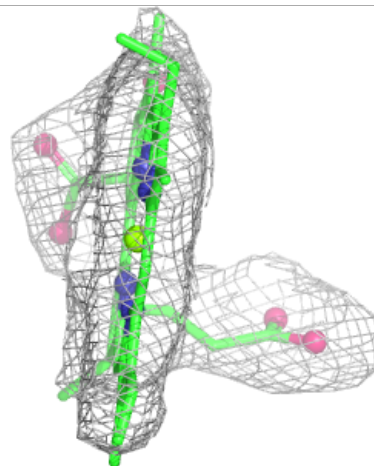
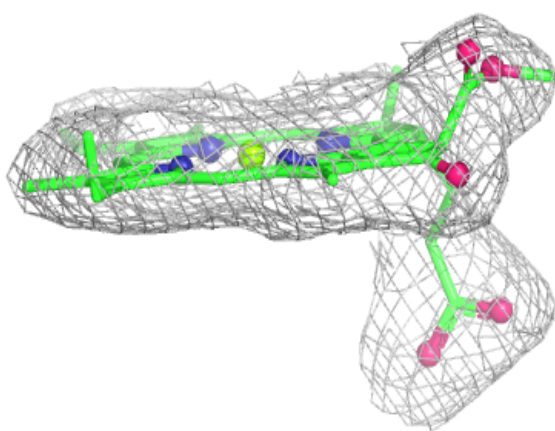
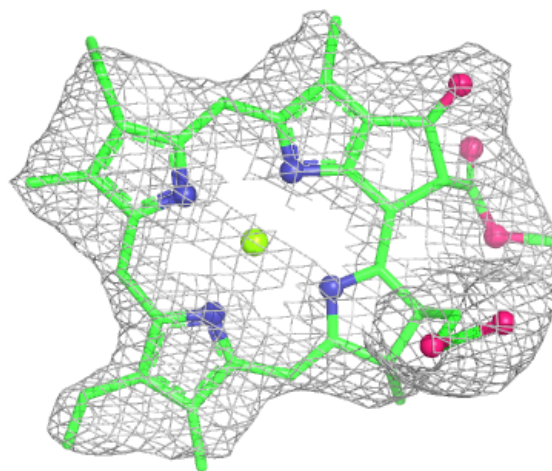
**Electron density around CLA Y 809:**

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



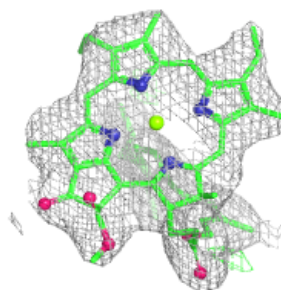
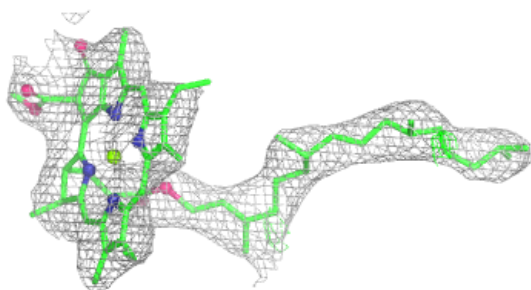
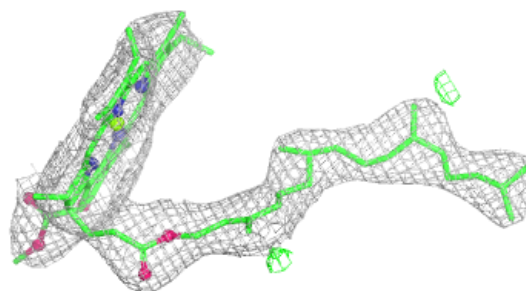
Electron density around CLA Y 810:

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

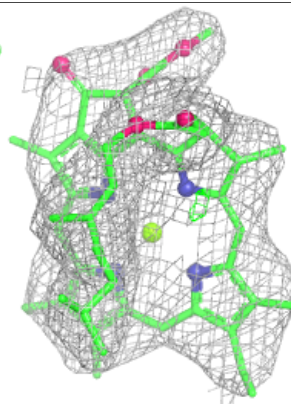
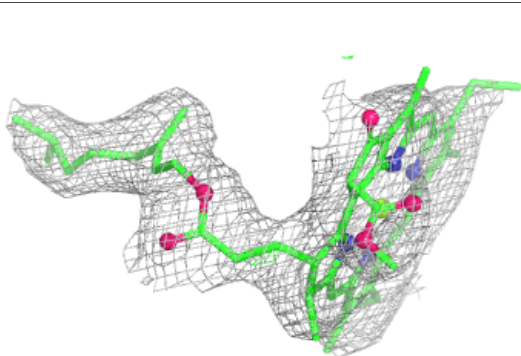
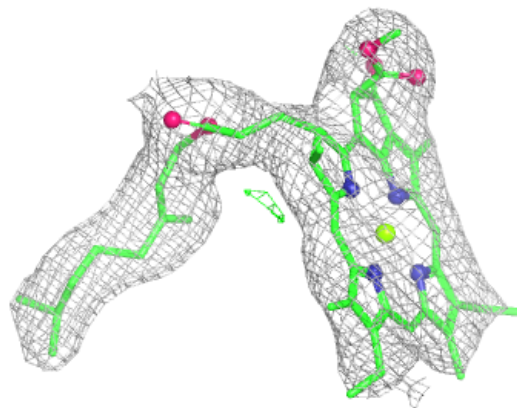


Electron density around CLA Y 811:

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

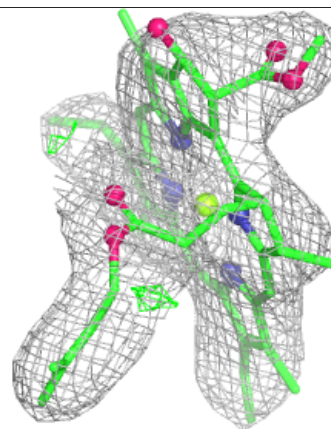
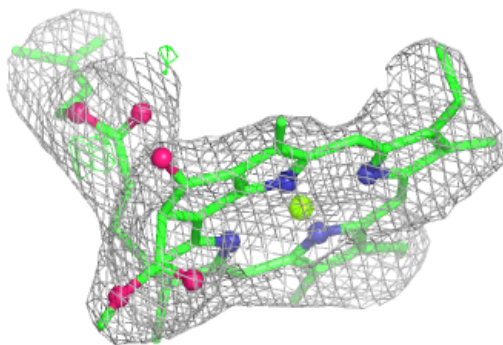
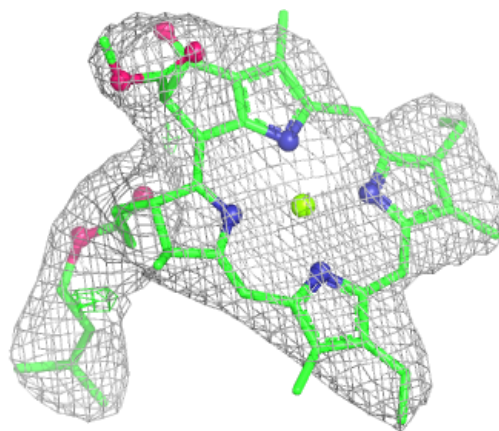
**Electron density around CLA Y 814:**

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

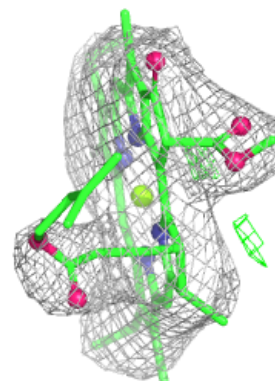
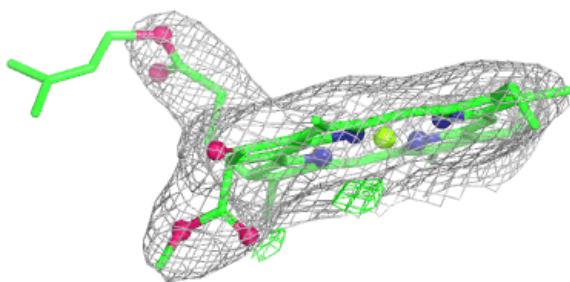
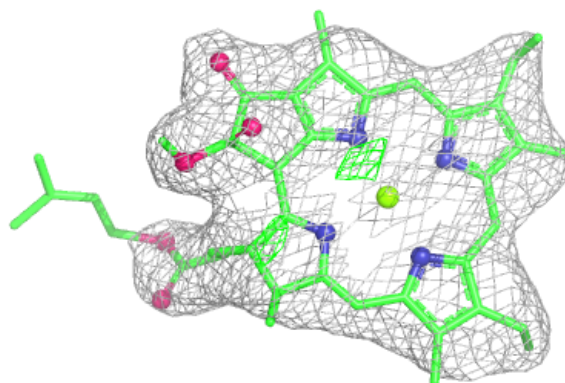


Electron density around CLA Y 815:

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

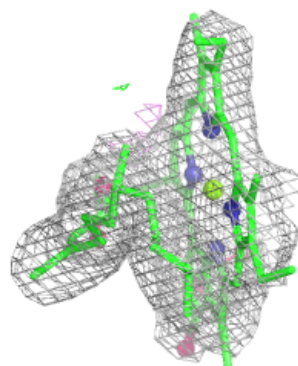
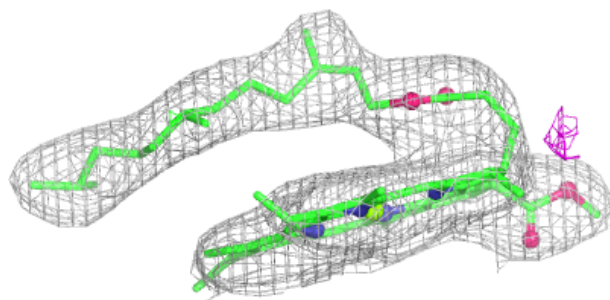
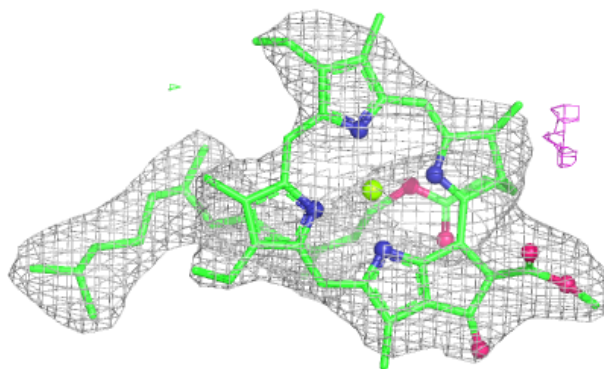
**Electron density around CLA Y 816:**

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

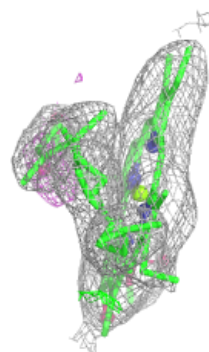
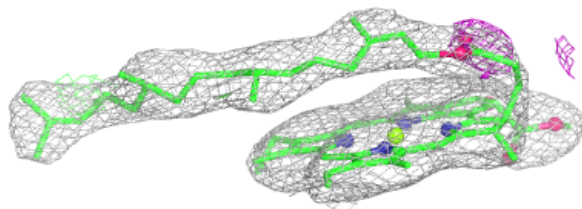
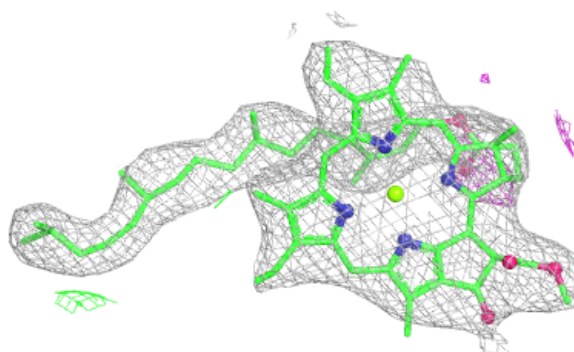


Electron density around CLA Y 817:

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

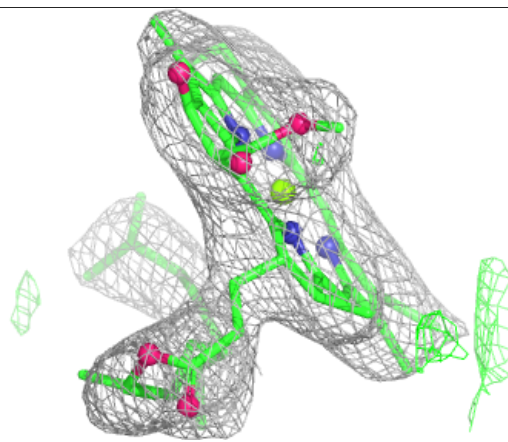
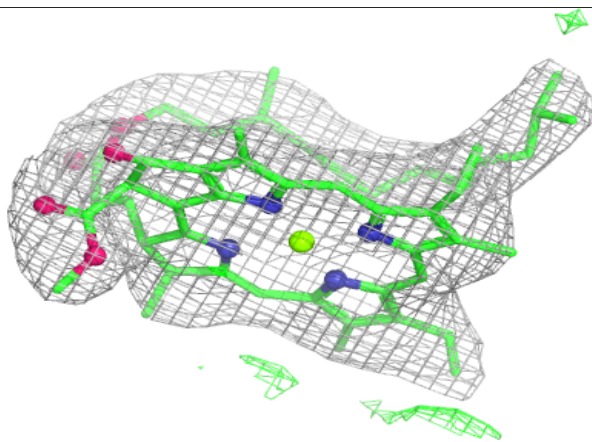
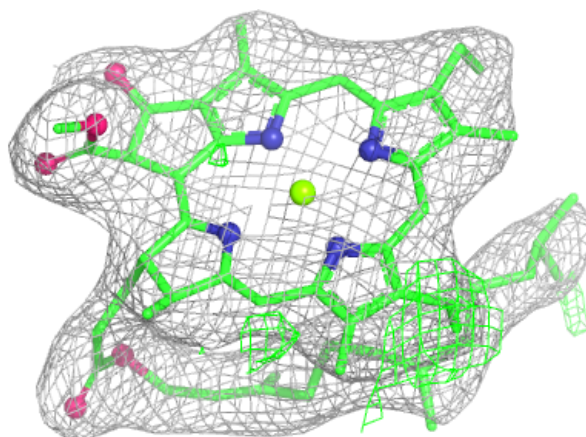
**Electron density around CLA Y 818:**

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



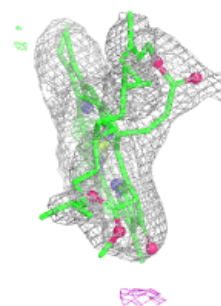
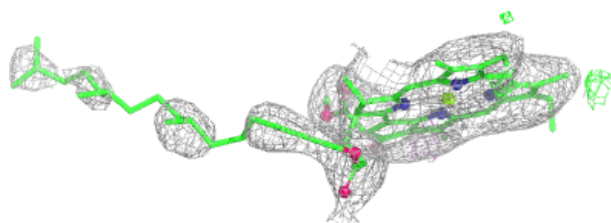
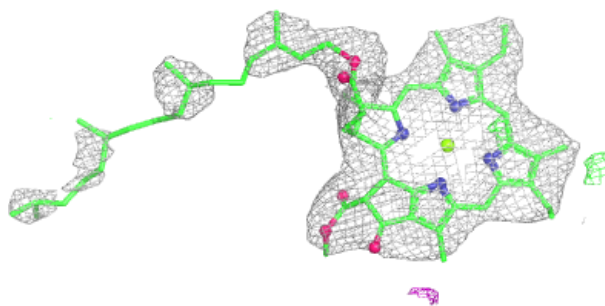
Electron density around CLA Y 820:

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



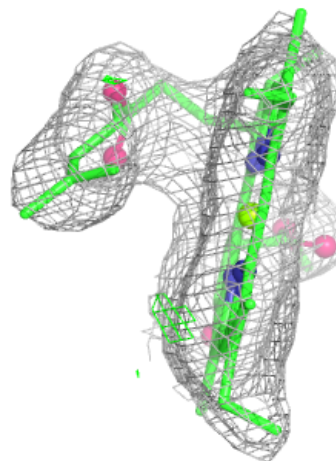
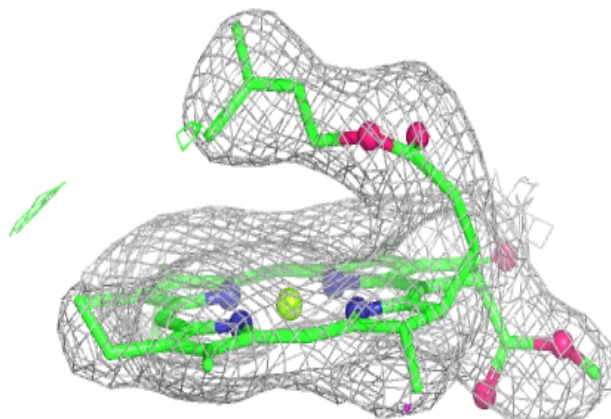
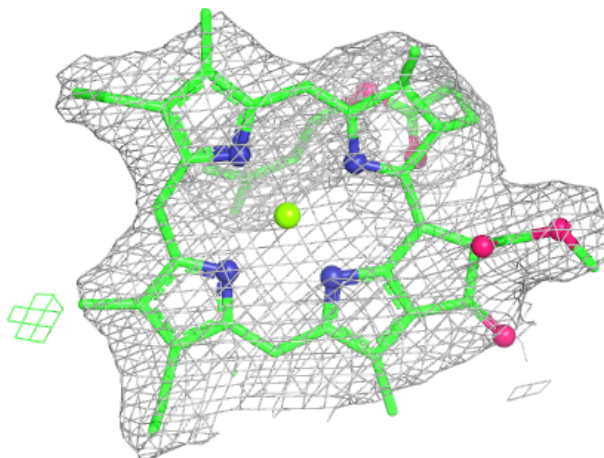
Electron density around CLA Y 822:

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



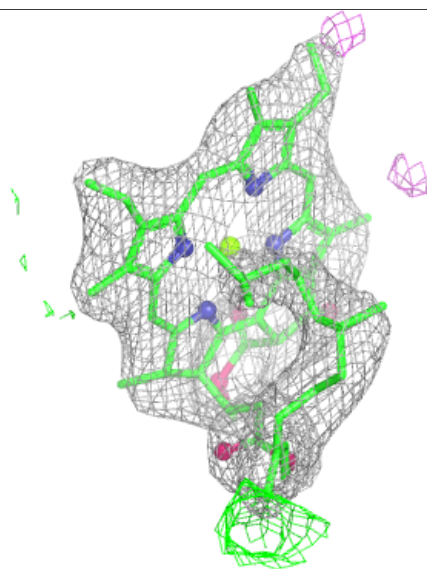
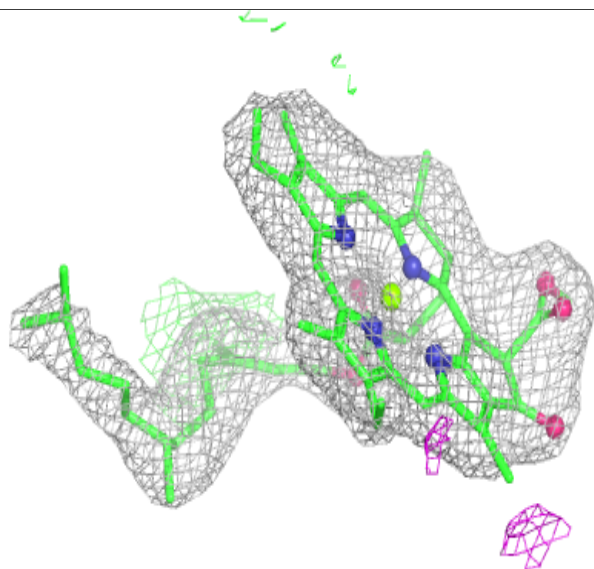
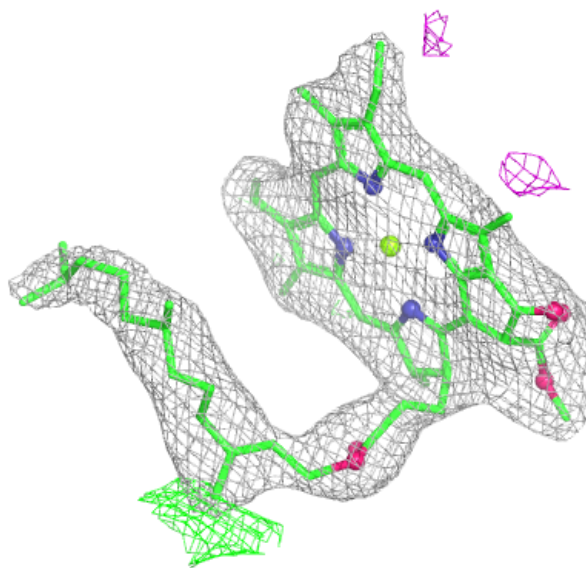
Electron density around CLA Y 823:

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



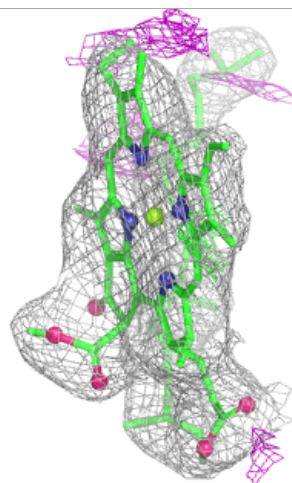
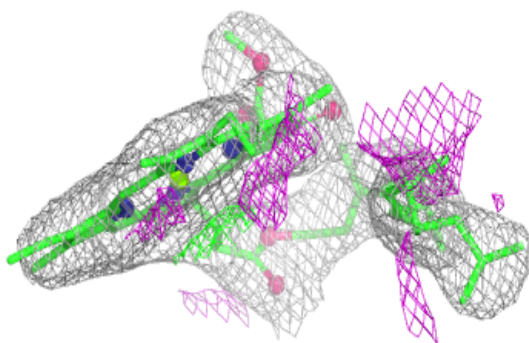
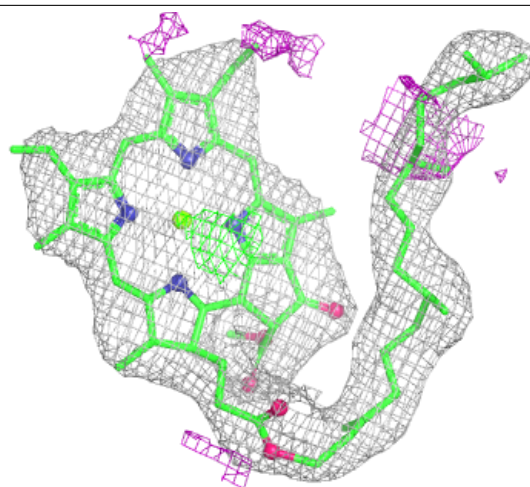
Electron density around CLA Y 824:

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



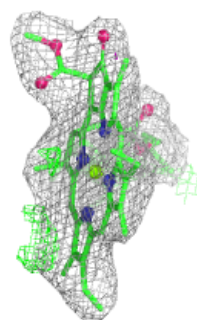
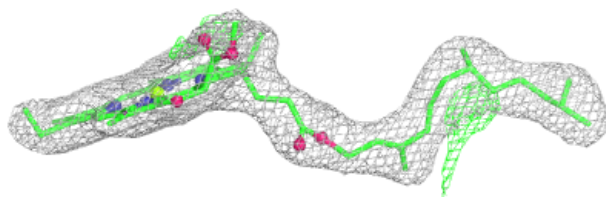
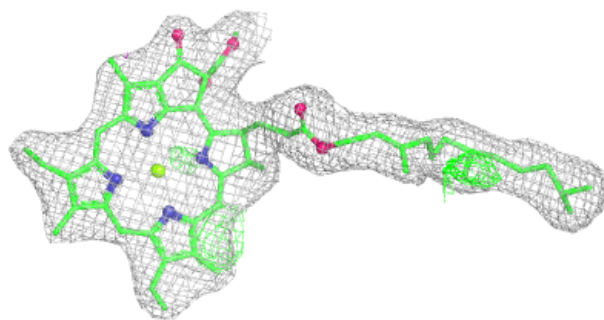
Electron density around CLA Y 825:

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

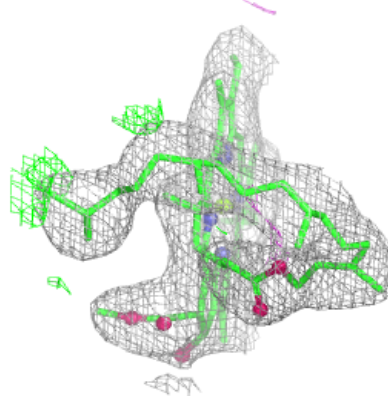
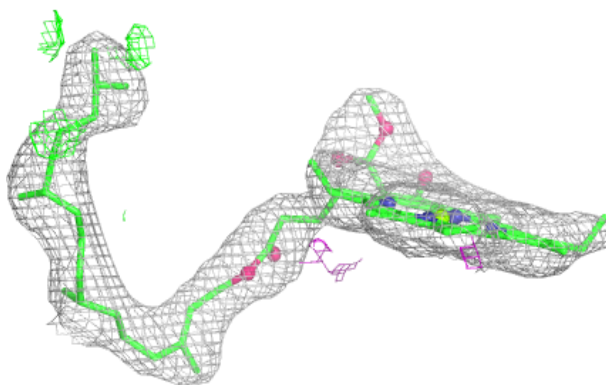
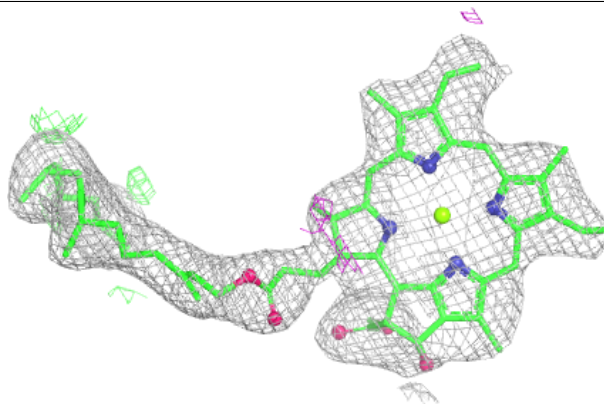


Electron density around CLA Y 826:

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

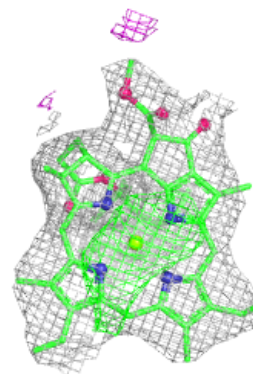
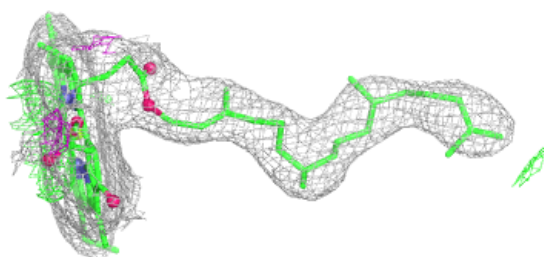
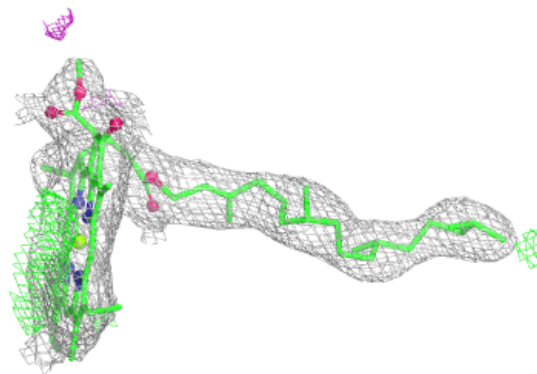
**Electron density around CLA Y 827:**

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

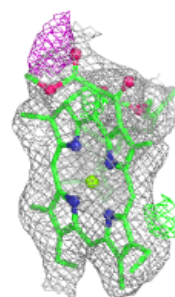
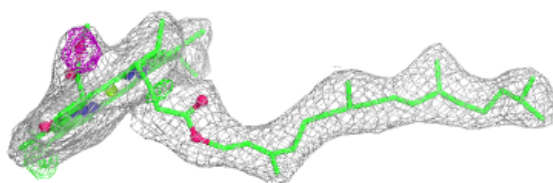
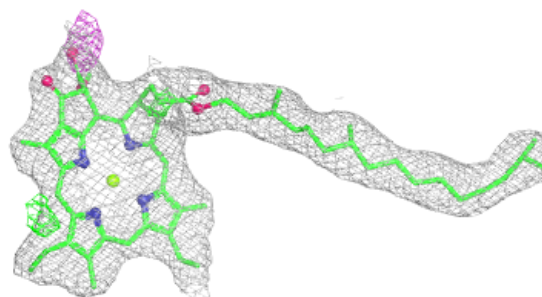


Electron density around CLA Y 828:

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

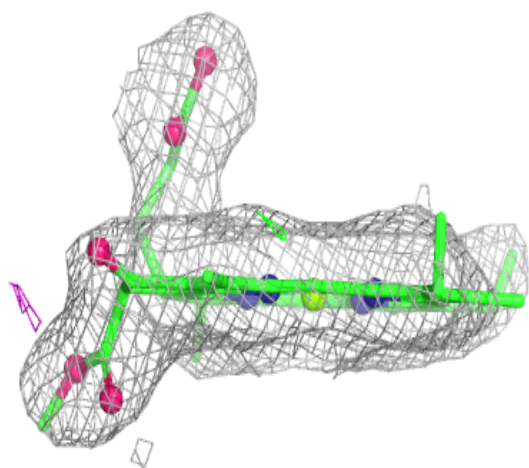
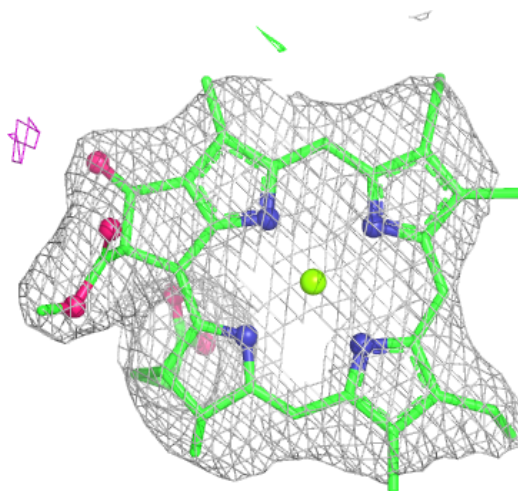
**Electron density around CLA Y 834:**

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



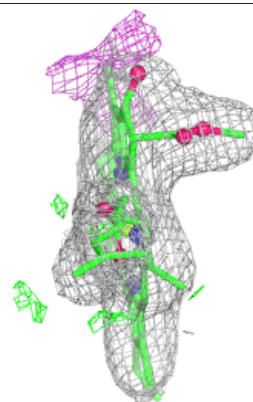
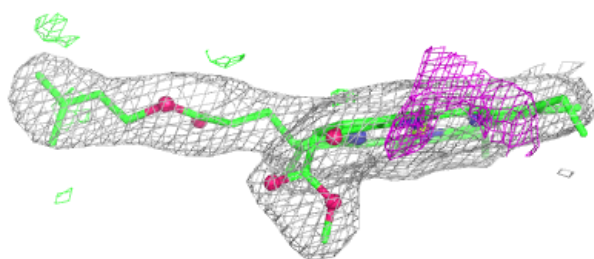
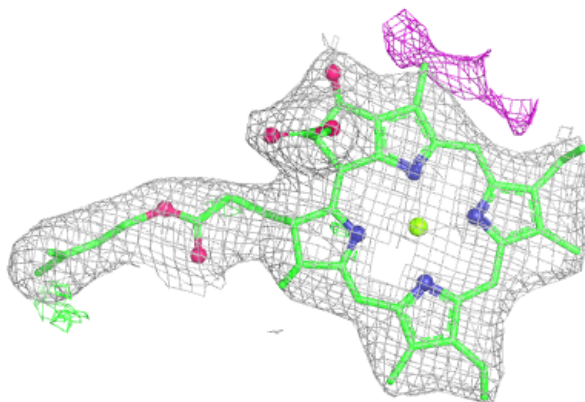
Electron density around CLA Y 836:

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

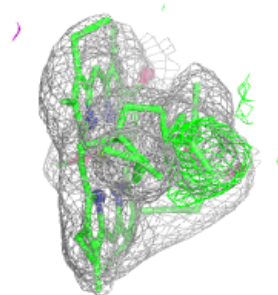
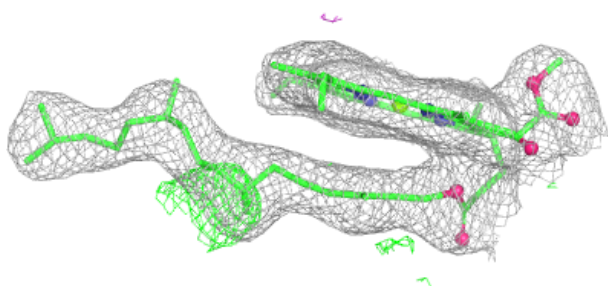
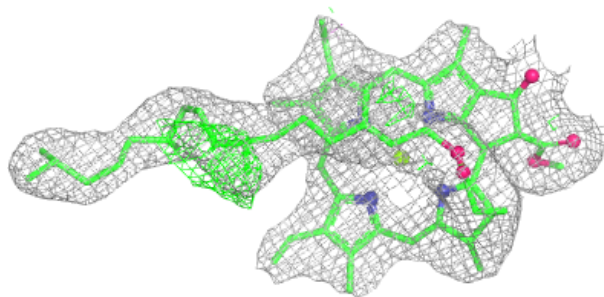


Electron density around CLA Y 837:

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

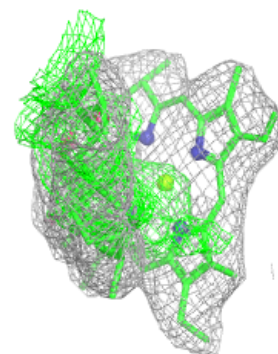
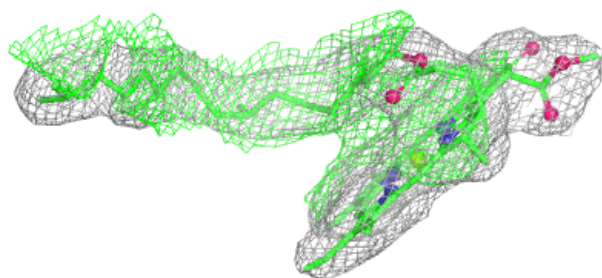
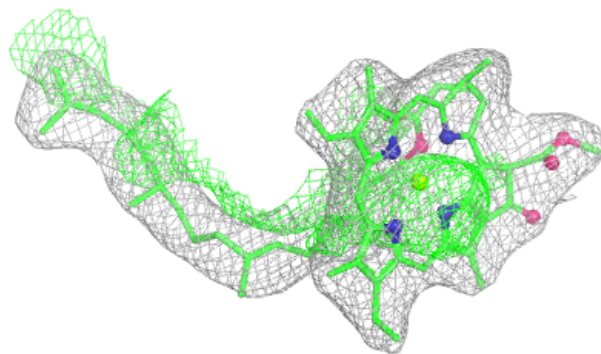
**Electron density around CLA Y 838:**

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



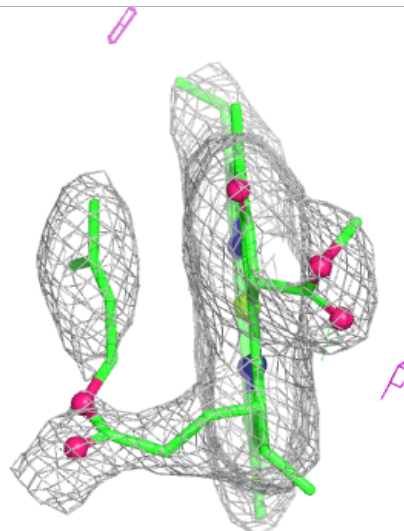
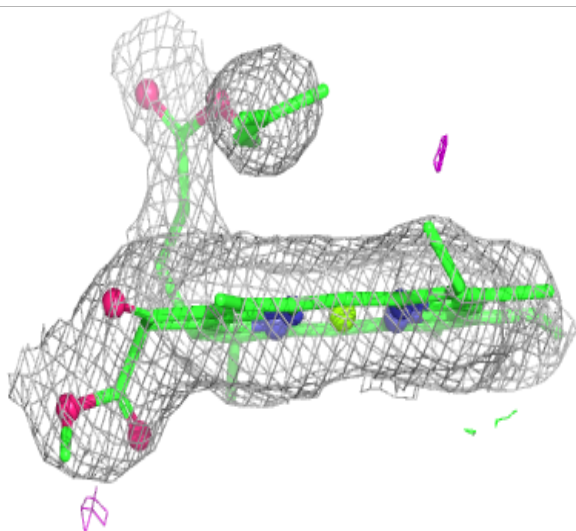
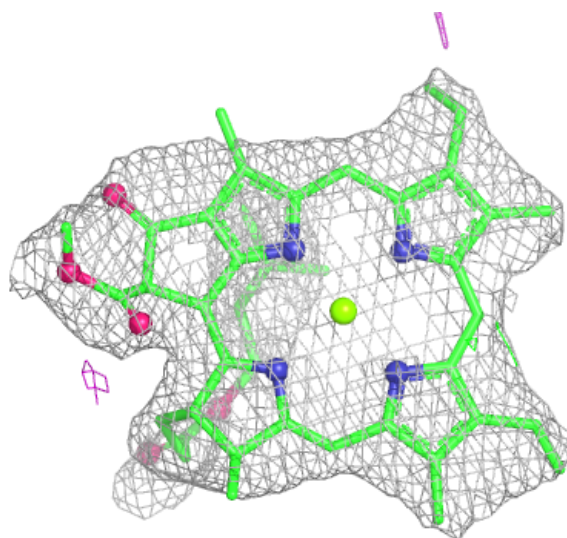
Electron density around CLA Y 841:

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



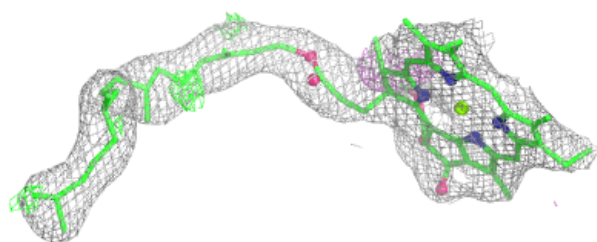
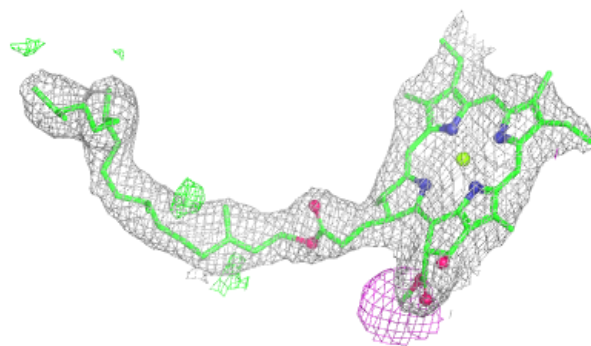
Electron density around CLA Y 843:

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

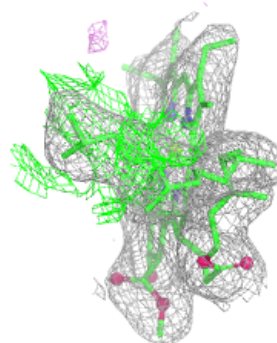
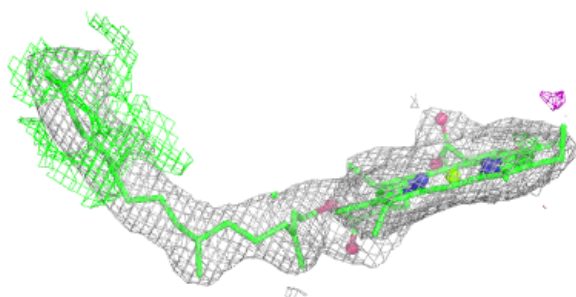
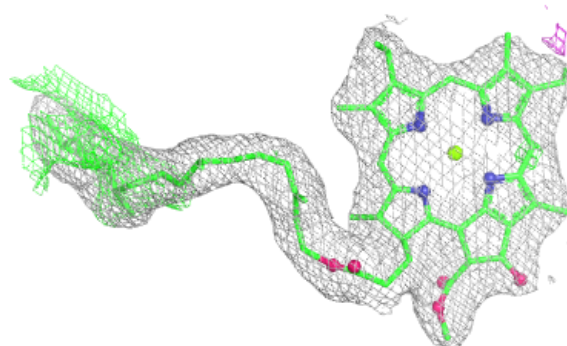


Electron density around CLA Y 854:

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

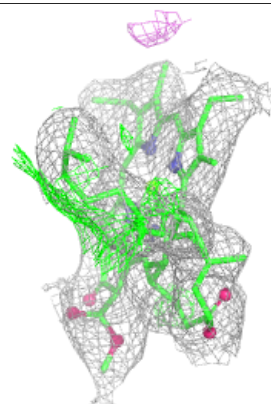
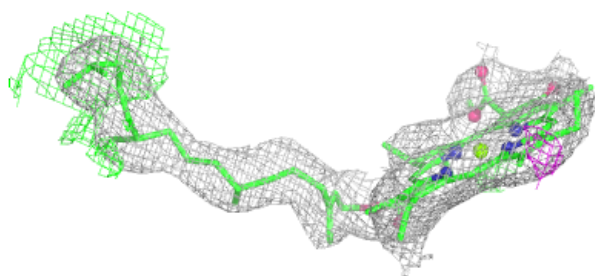
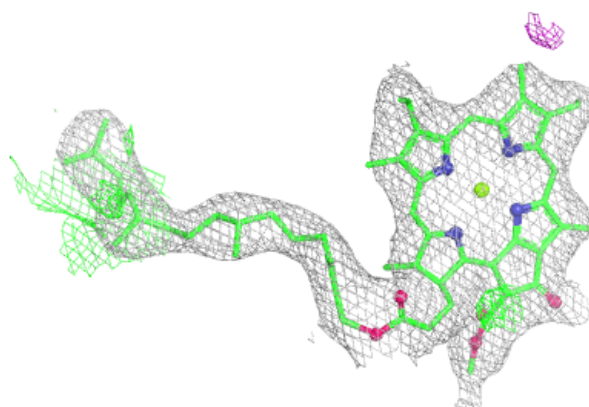
**Electron density around CLA Y 855:**

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



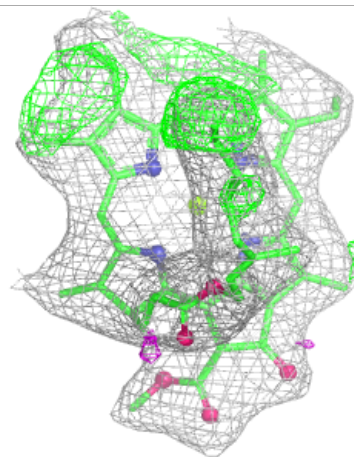
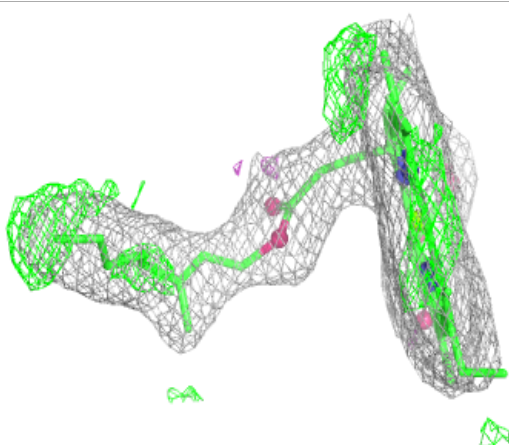
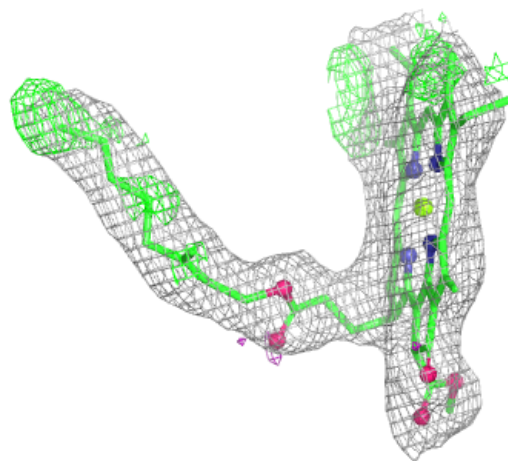
Electron density around CLA Z 801:

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



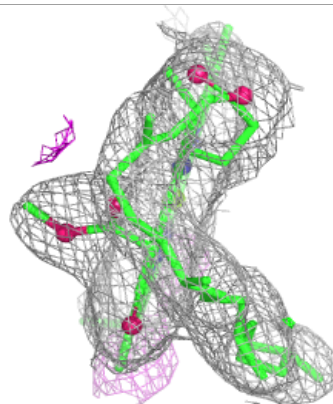
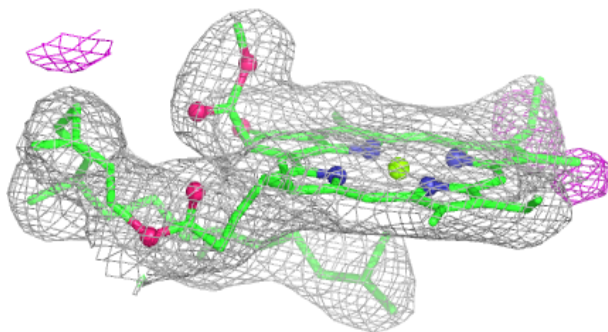
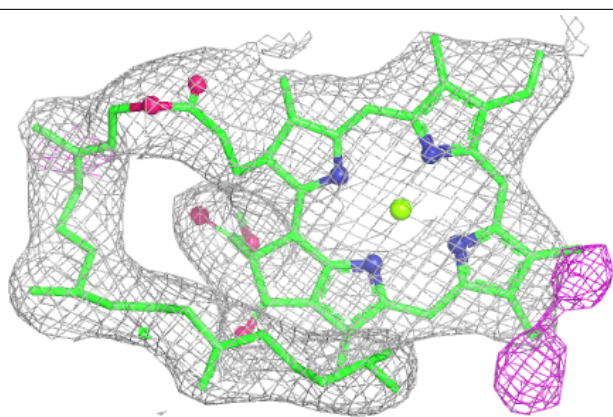
Electron density around CLA Z 803:

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



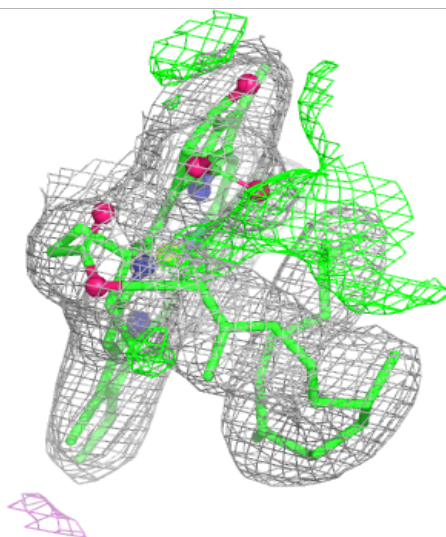
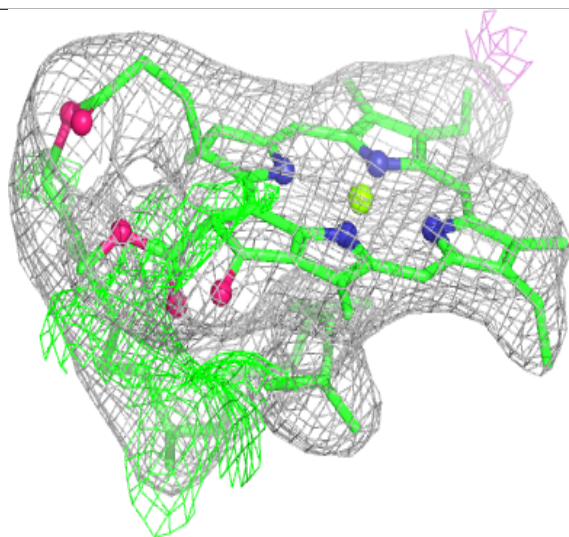
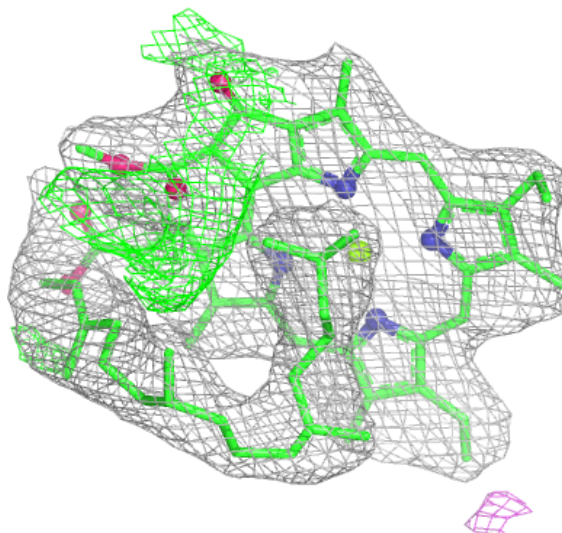
Electron density around CLA Z 804:

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



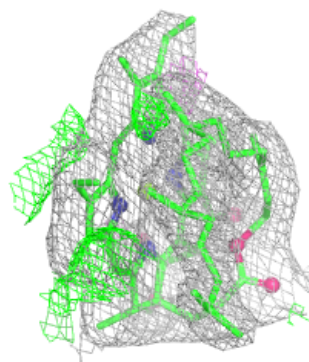
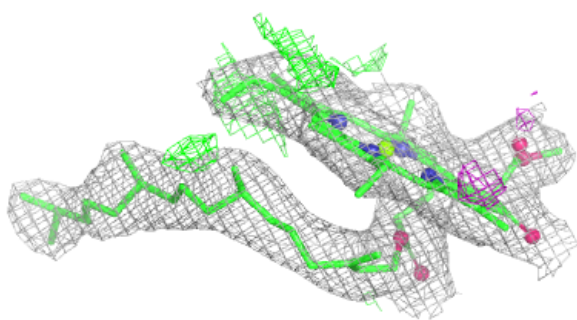
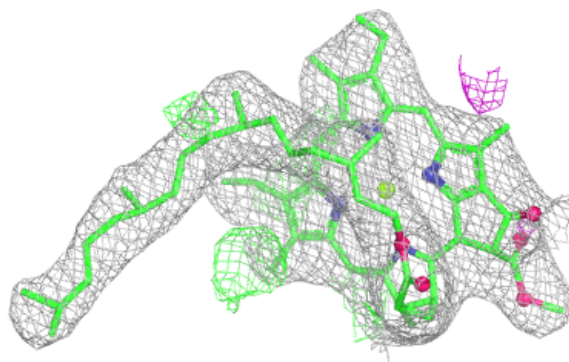
Electron density around CLA Z 805:

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



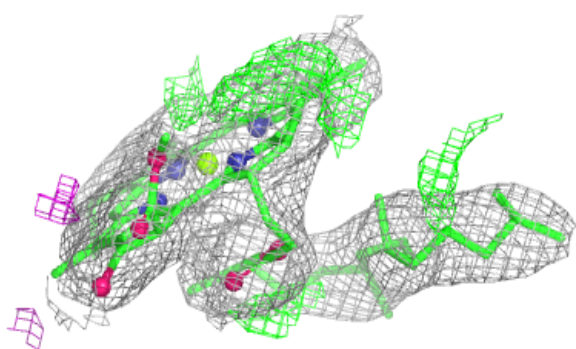
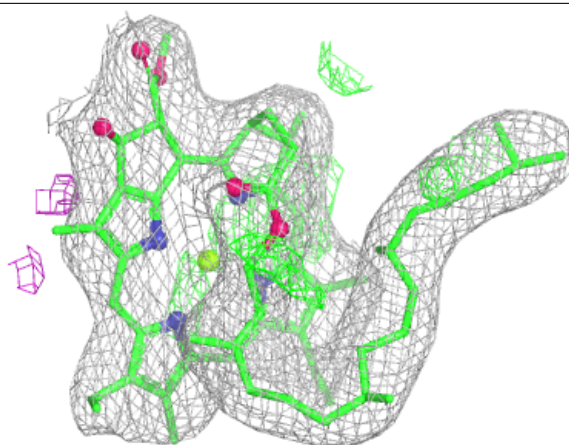
Electron density around CLA Z 806:

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

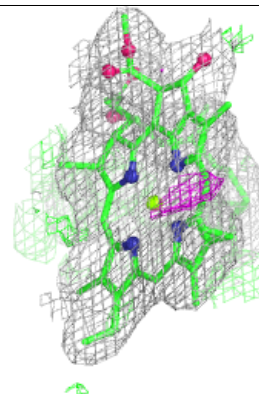
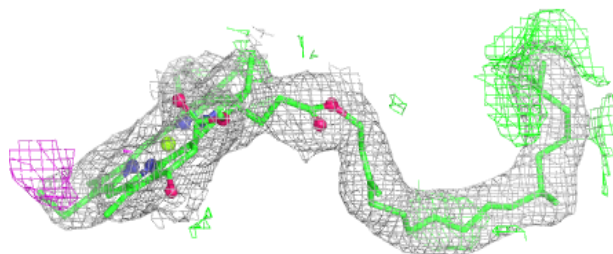
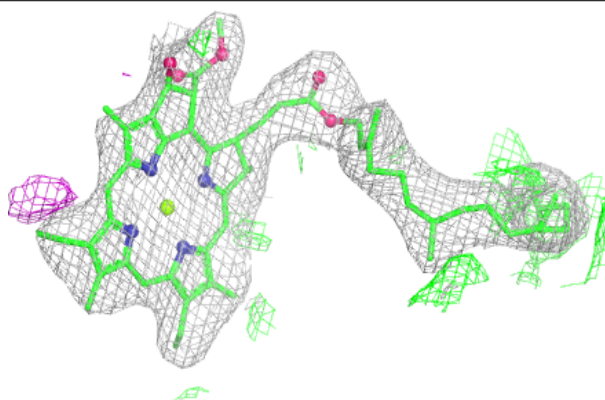


Electron density around CLA Z 807:

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

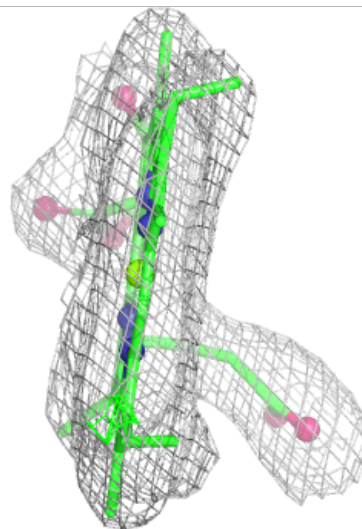
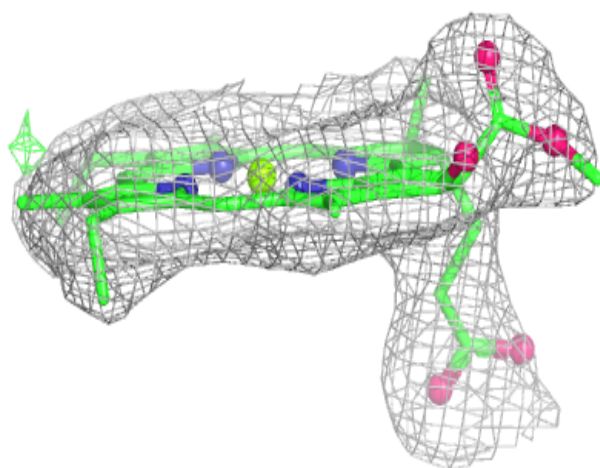
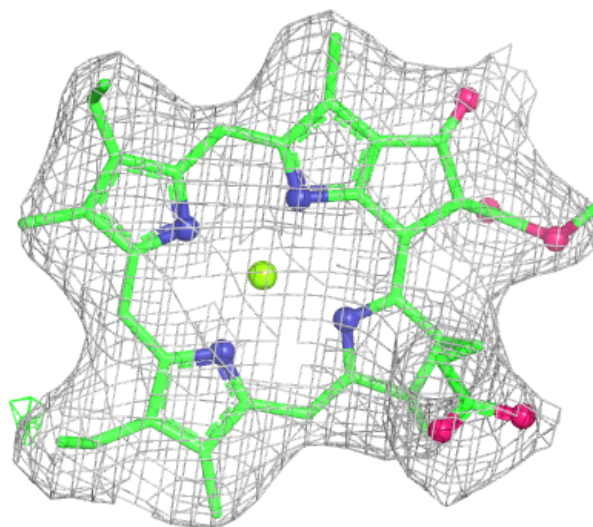
**Electron density around CLA Z 808:**

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



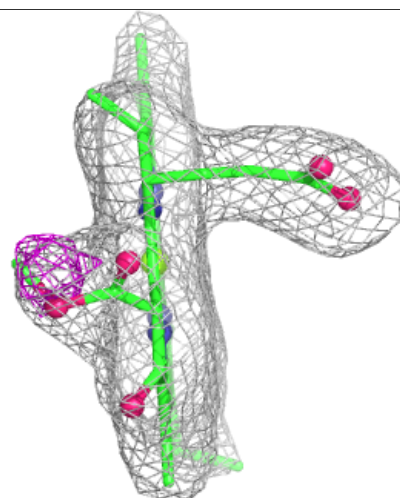
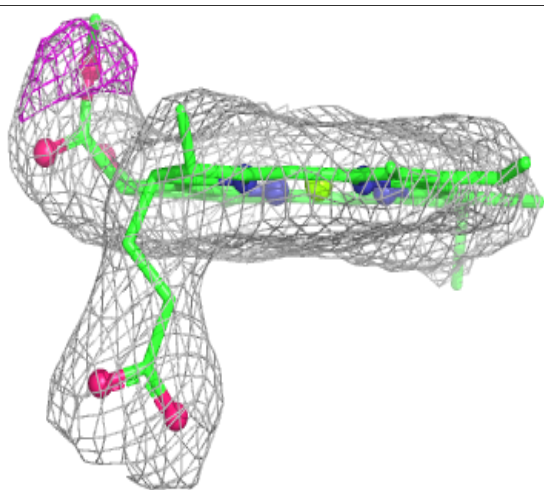
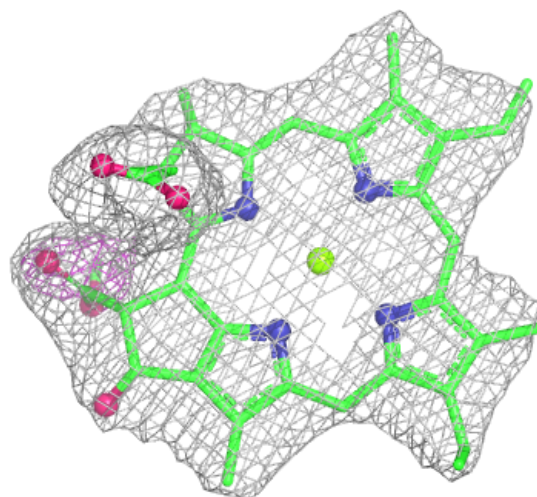
Electron density around CLA Z 810:

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



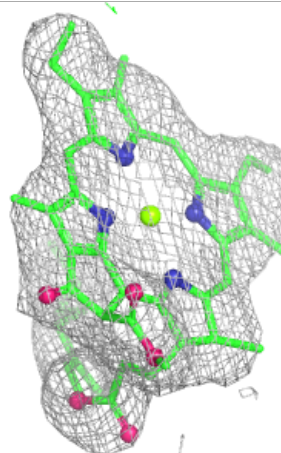
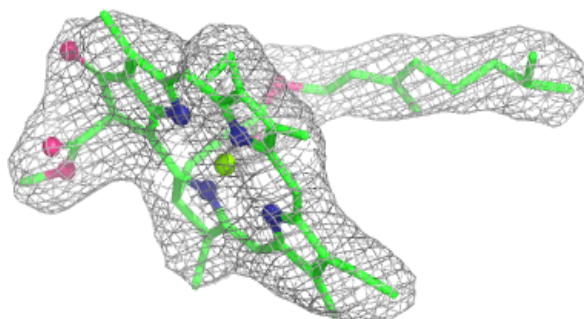
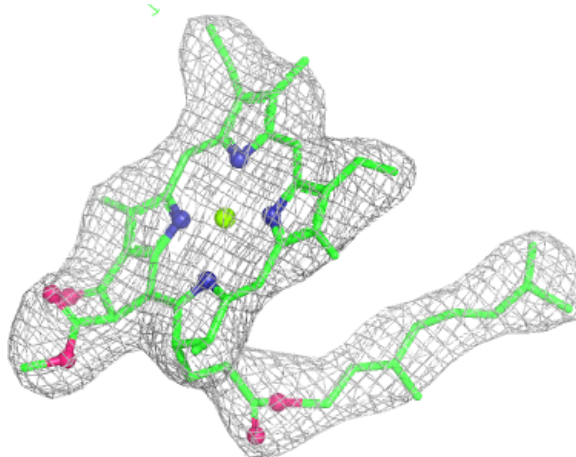
Electron density around CLA Z 813:

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



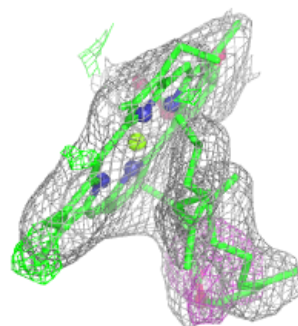
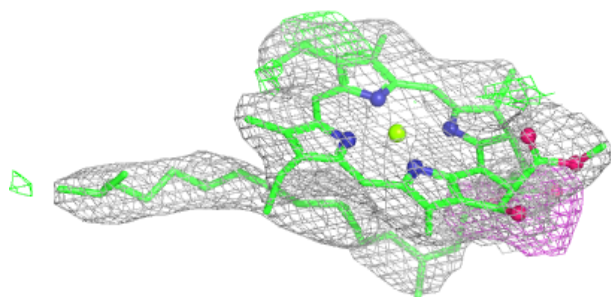
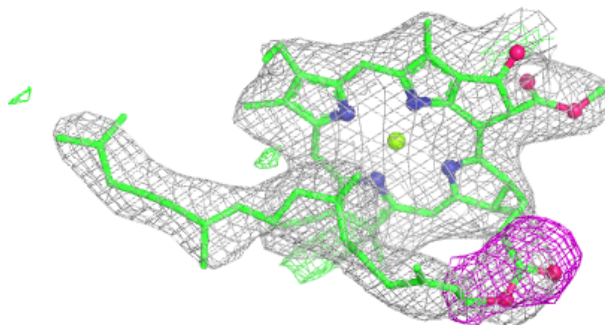
Electron density around CLA Z 814:

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

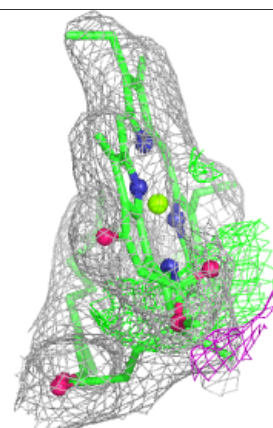
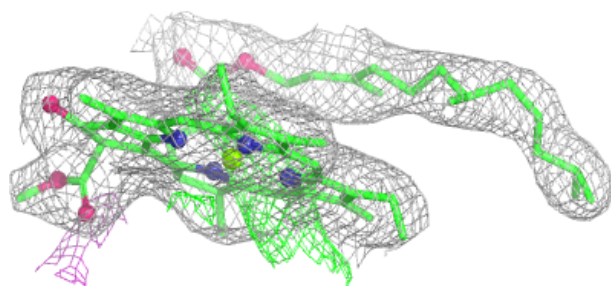
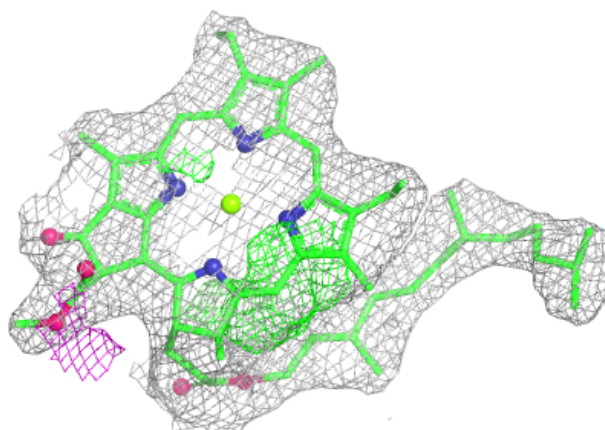


Electron density around CLA Z 815:

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

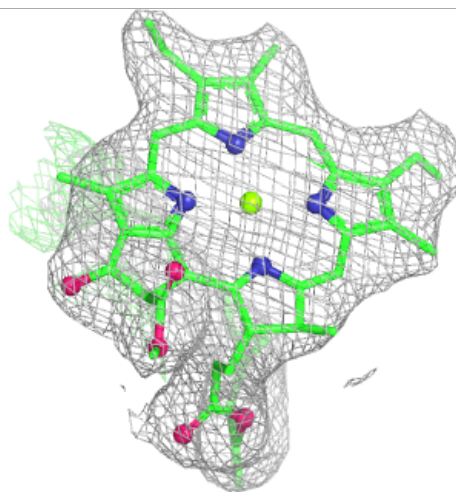
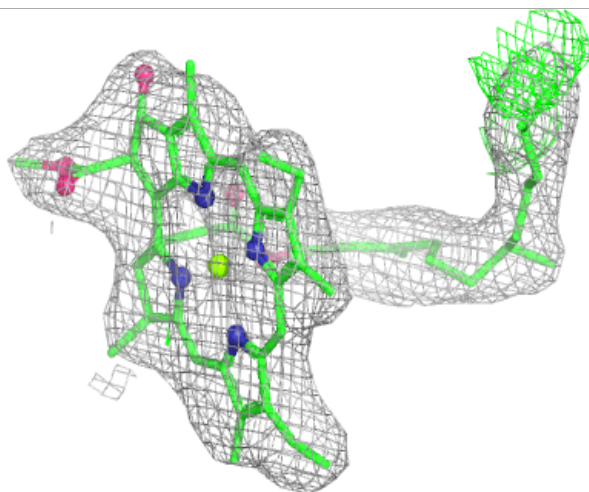
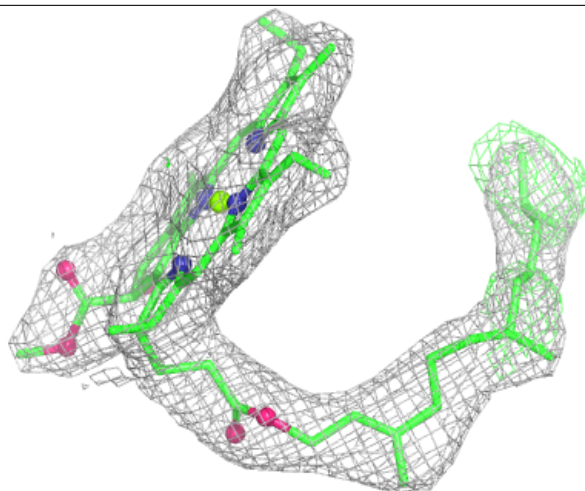
**Electron density around CLA Z 816:**

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



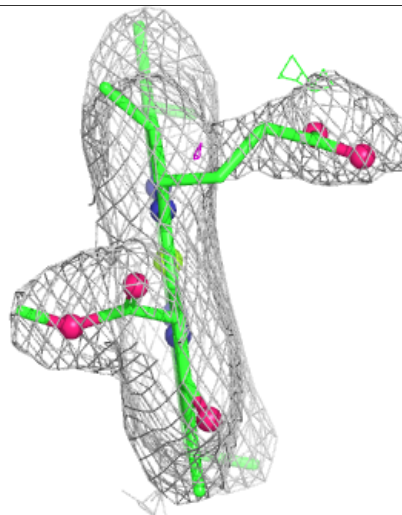
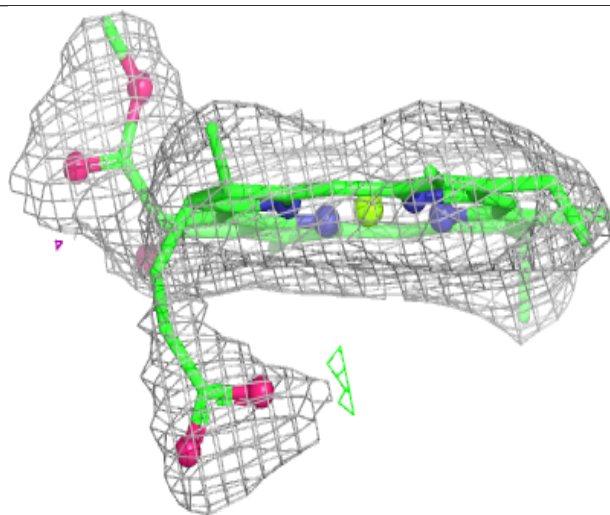
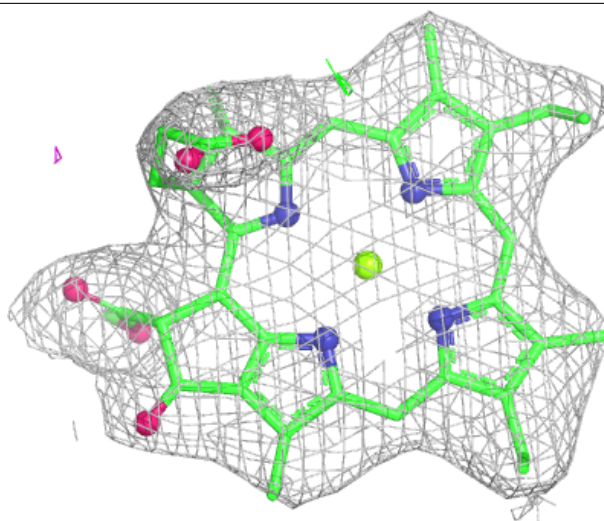
Electron density around CLA Z 817:

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



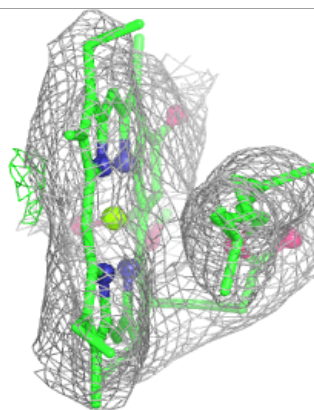
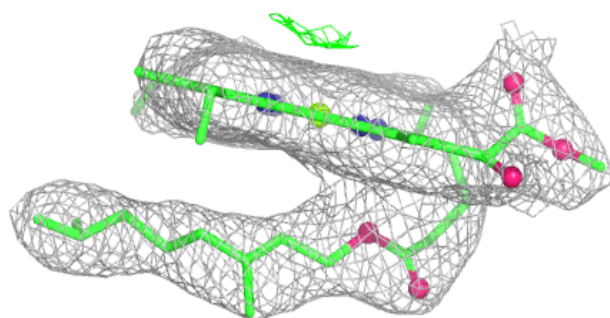
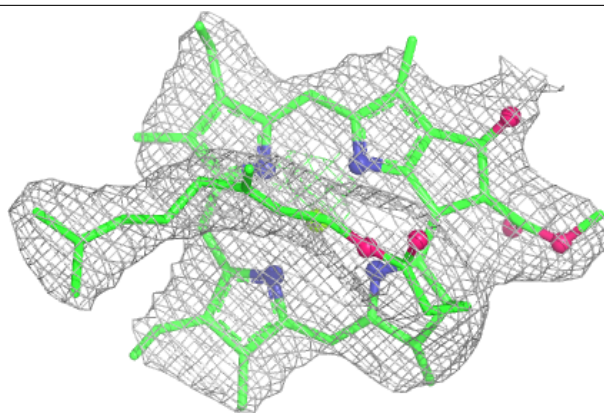
Electron density around CLA Z 818:

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

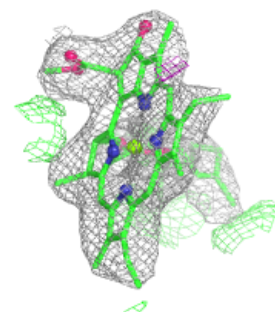
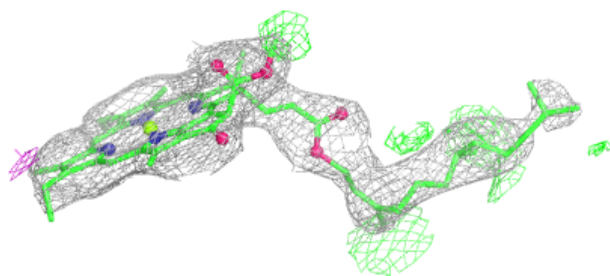
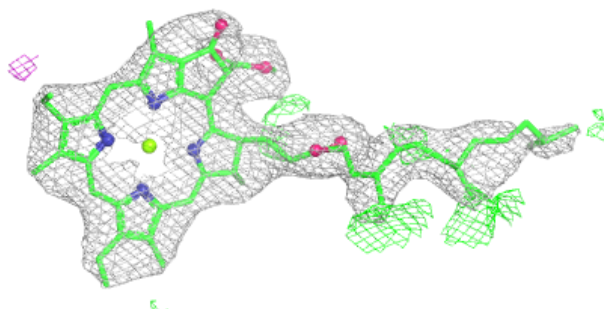


Electron density around CLA Z 820:

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

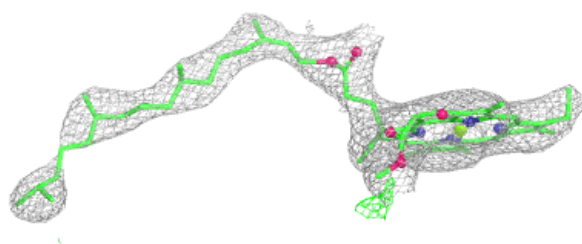
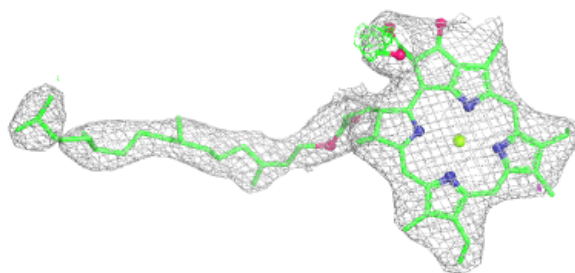
**Electron density around CLA Z 821:**

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

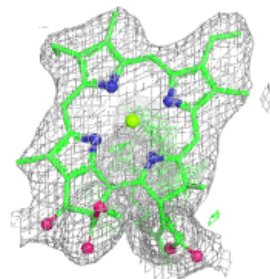
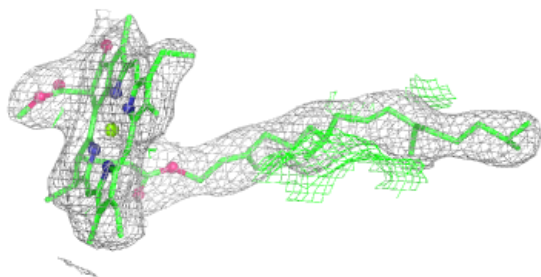
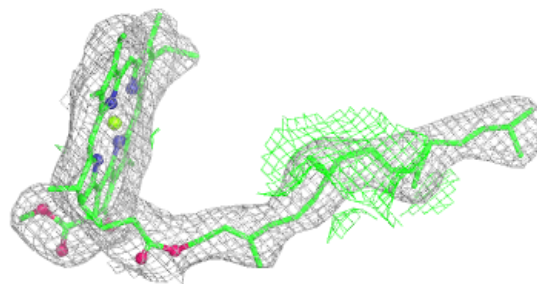


Electron density around CLA Z 823:

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

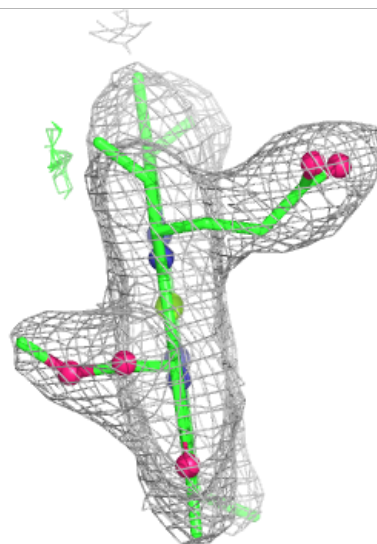
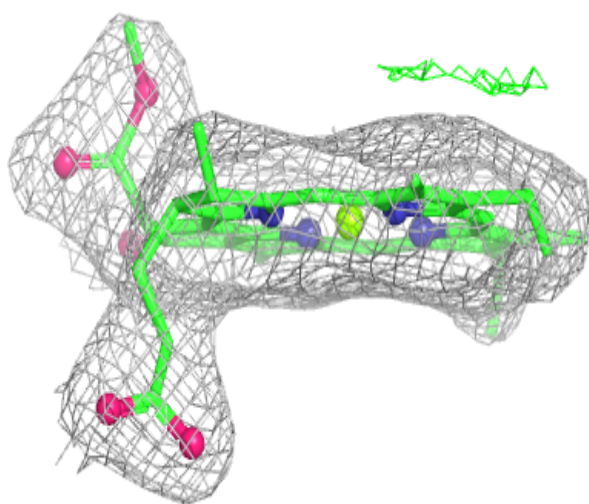
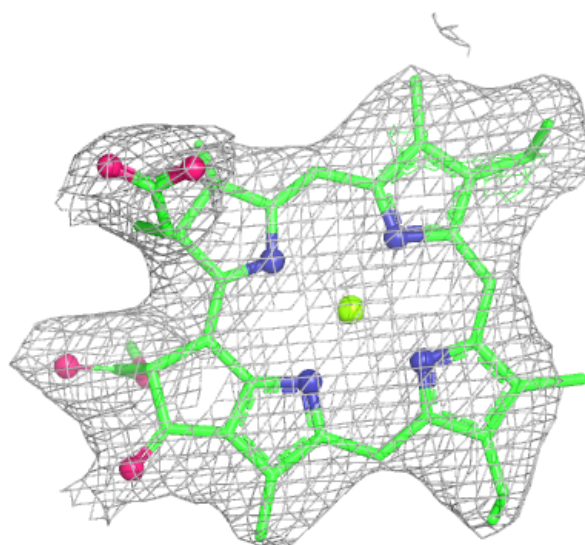
**Electron density around CLA Z 827:**

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



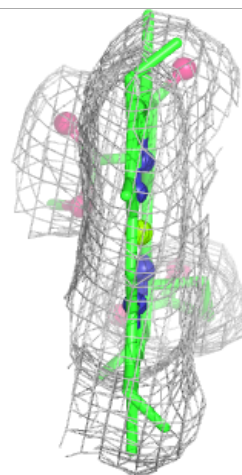
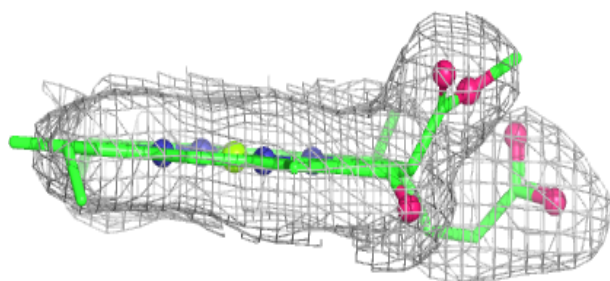
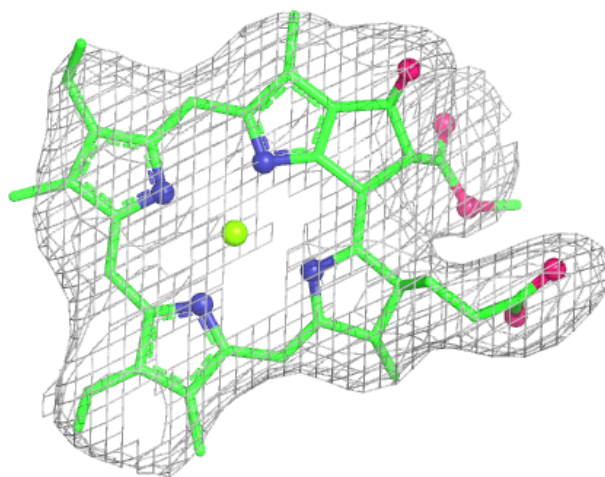
Electron density around CLA Z 828:

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



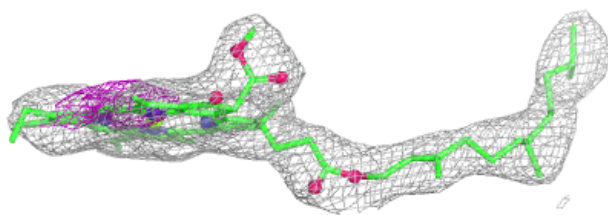
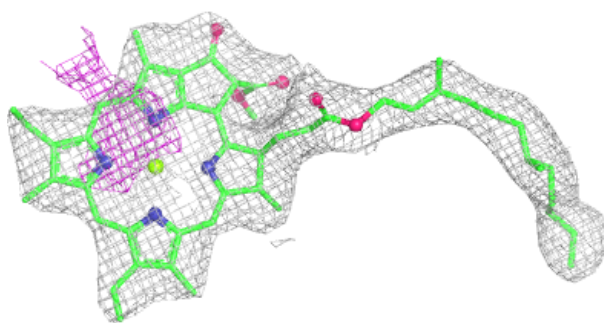
Electron density around CLA Z 834:

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



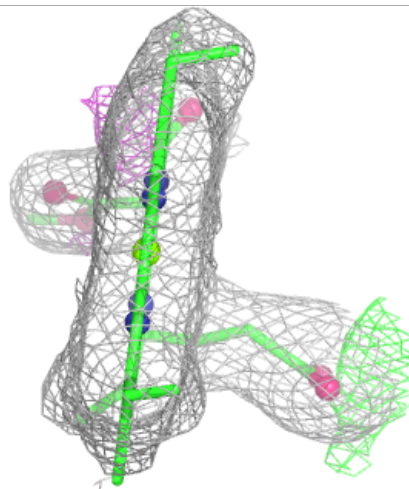
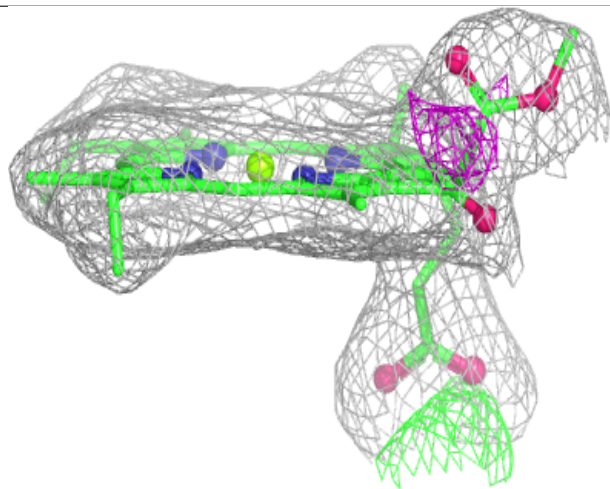
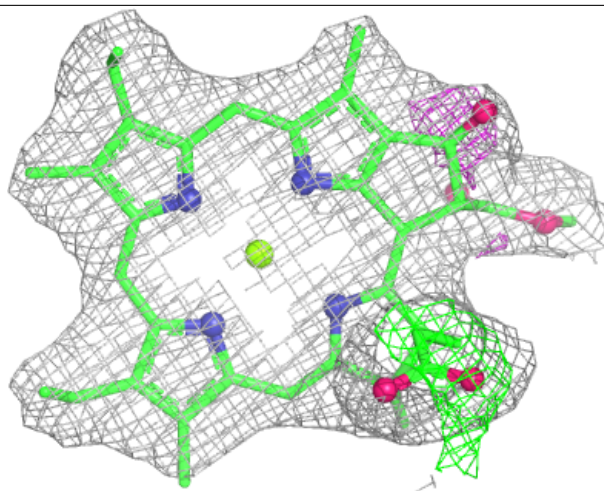
Electron density around CLA Z 835:

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



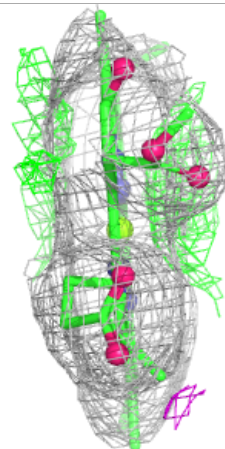
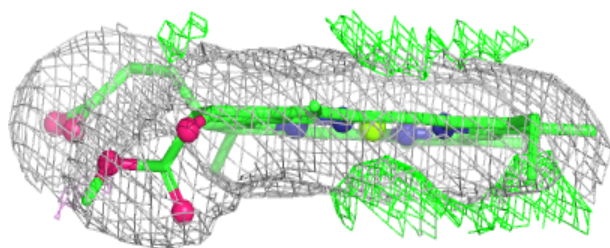
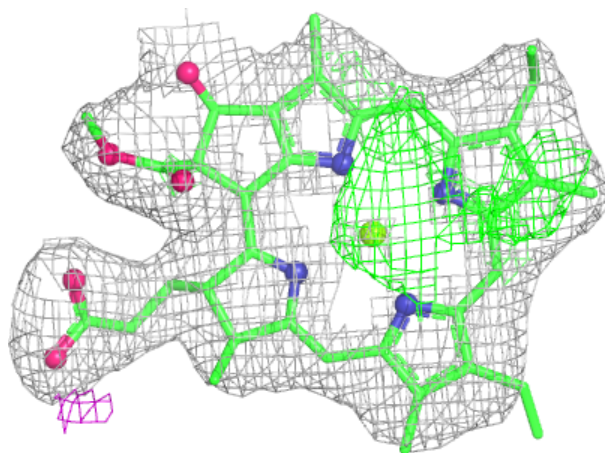
Electron density around CLA Z 837:

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



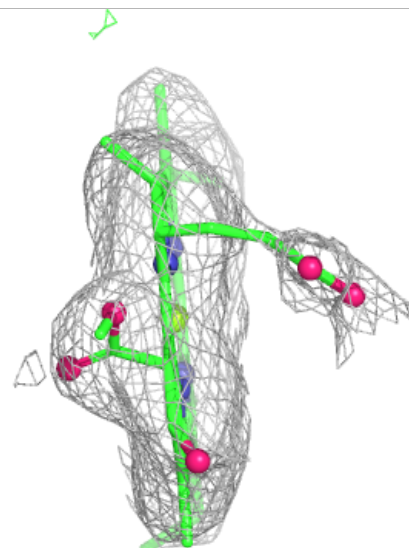
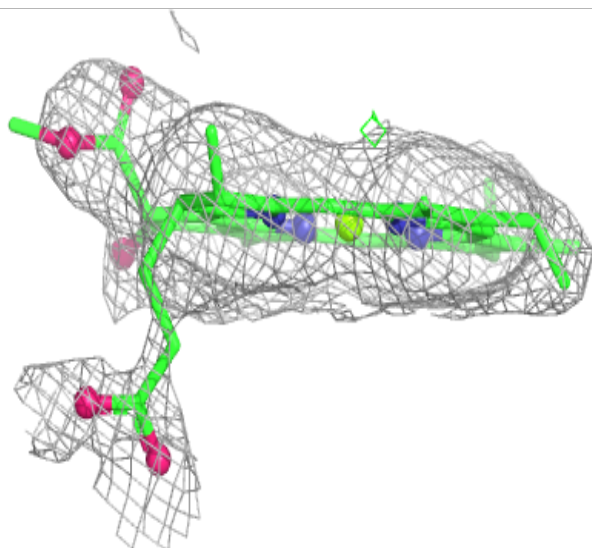
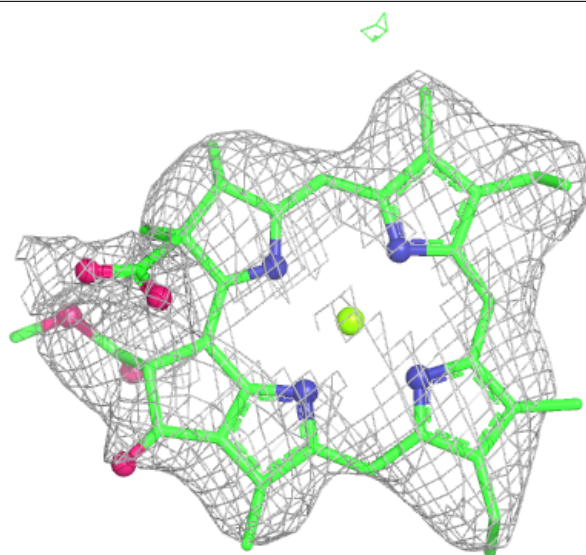
Electron density around CLA d 202:

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



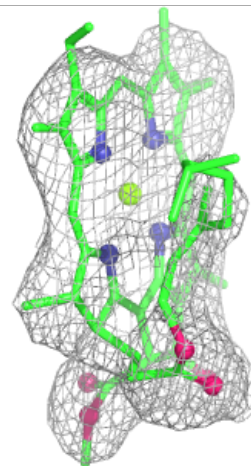
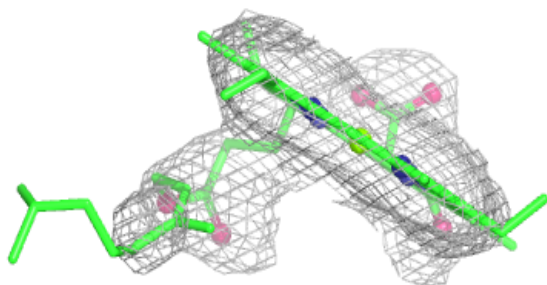
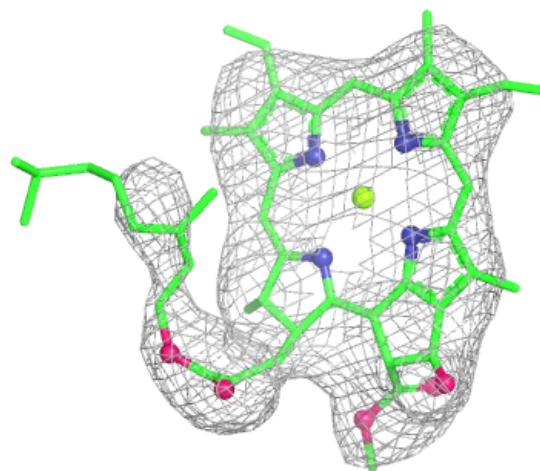
Electron density around CLA f 101:

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



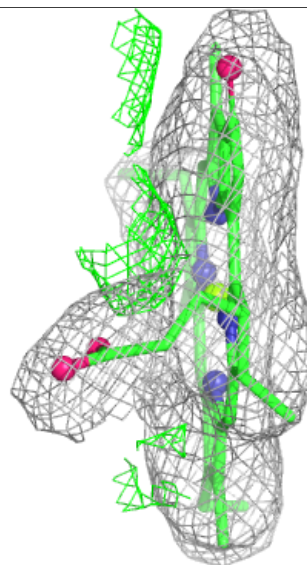
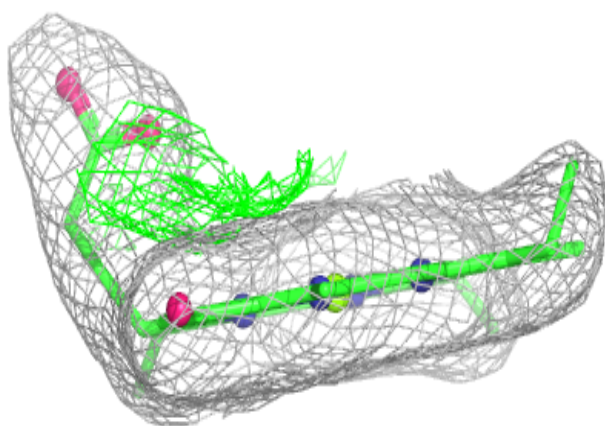
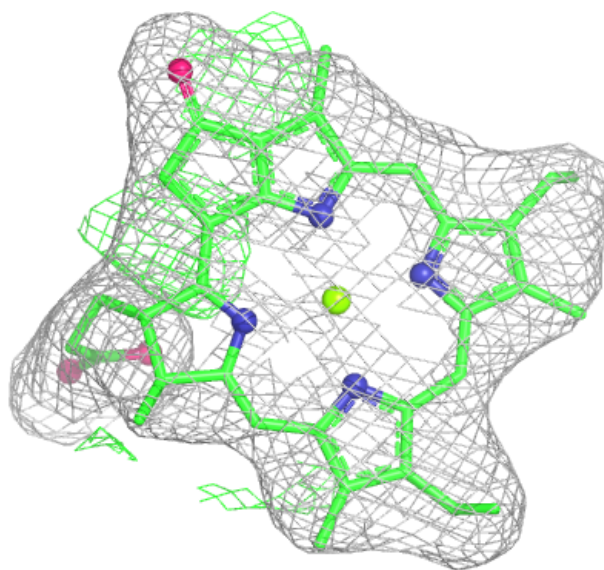
Electron density around CLA f 102:

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



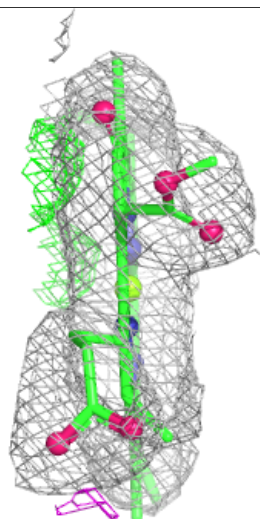
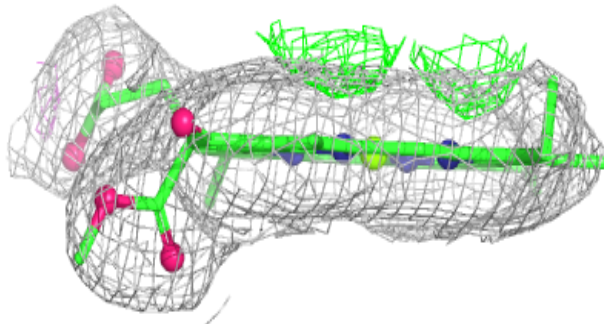
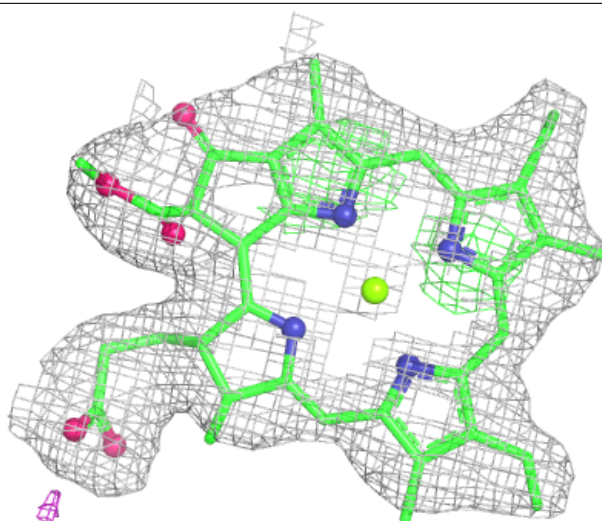
Electron density around CLA g 101:

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



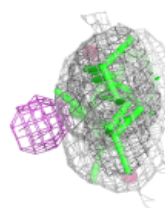
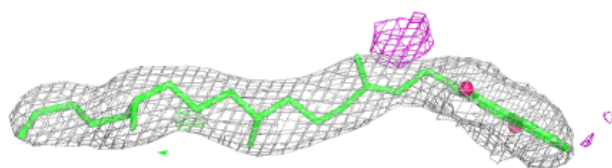
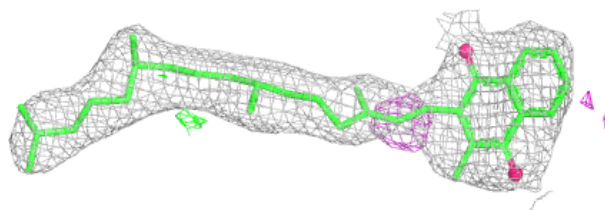
Electron density around CLA j 102:

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

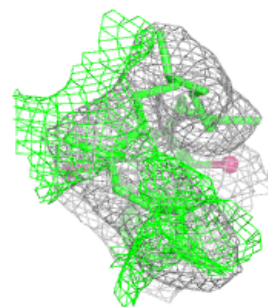
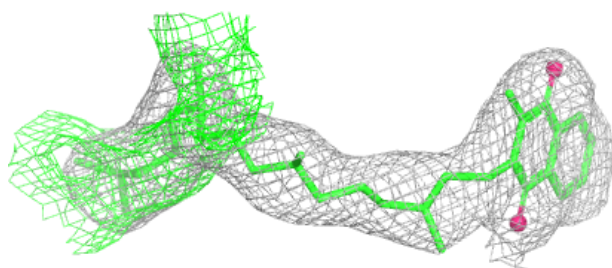
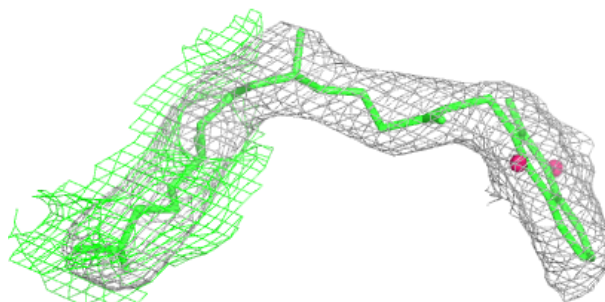


Electron density around PQN A 843:

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

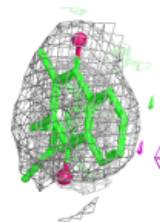
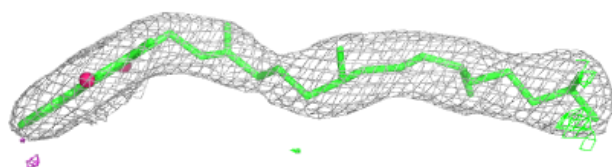
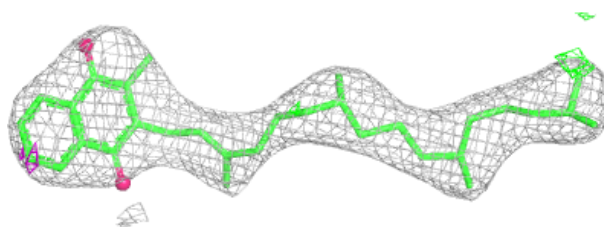
**Electron density around PQN B 842:**

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

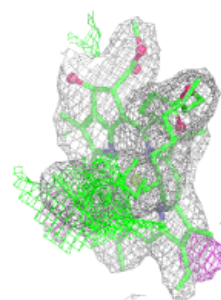
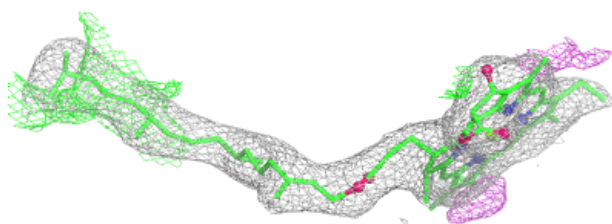
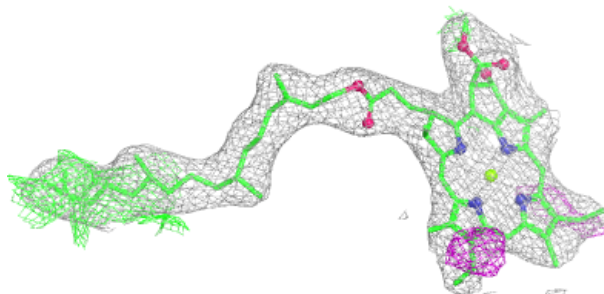


Electron density around PQN G 844:

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

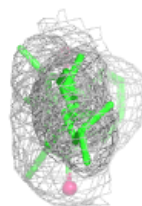
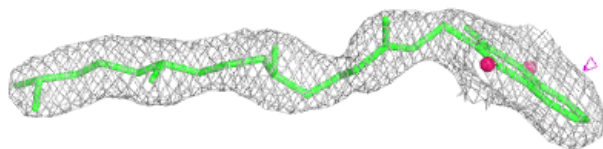
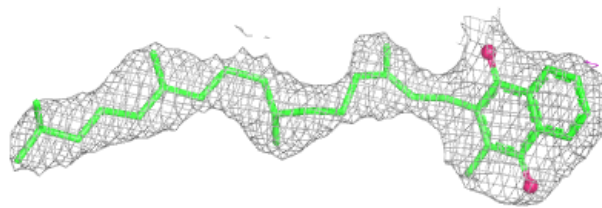
**Electron density around CLA A 802:**

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

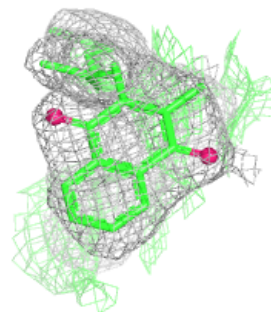
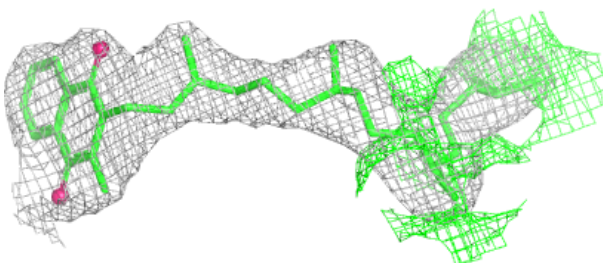
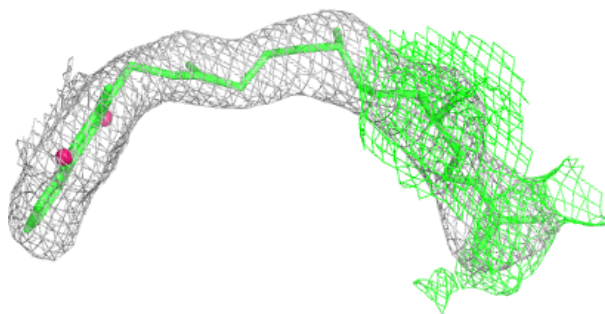


Electron density around PQN Y 844:

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

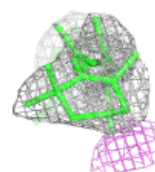
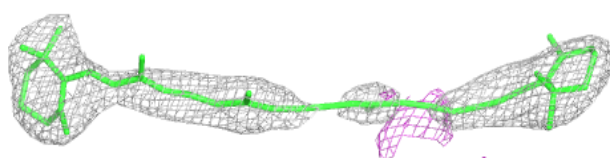
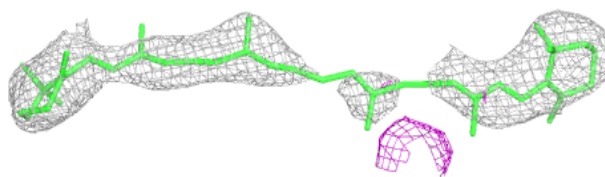
**Electron density around PQN Z 840:**

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

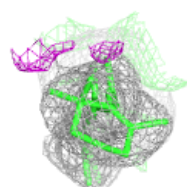
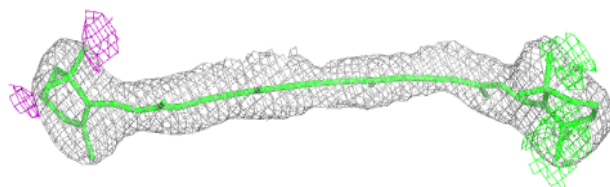
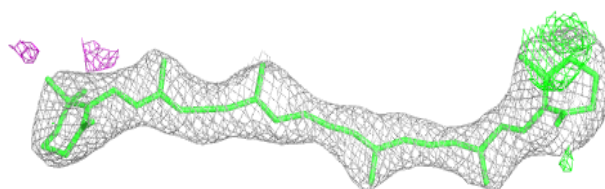


Electron density around BCR A 846:

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

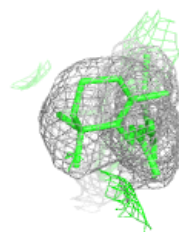
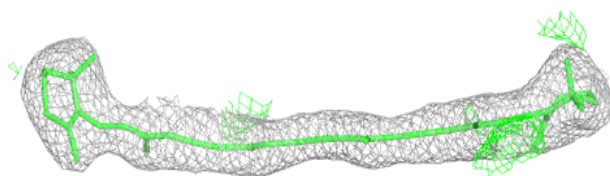
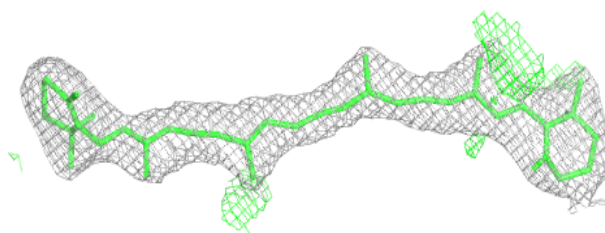
**Electron density around BCR A 847:**

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

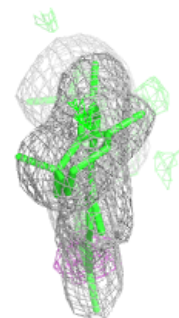
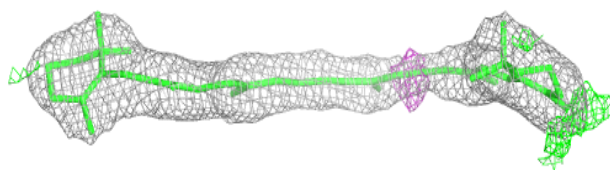
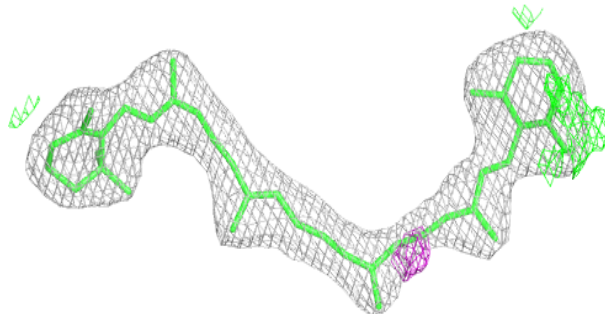


Electron density around BCR A 848:

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

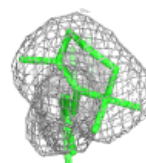
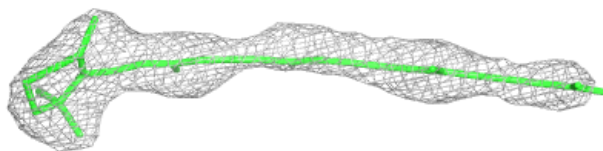
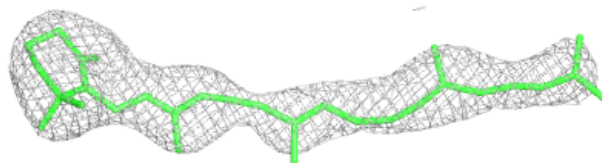
**Electron density around BCR A 849:**

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

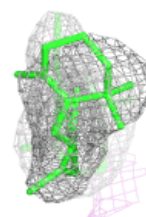
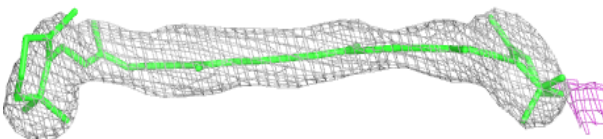
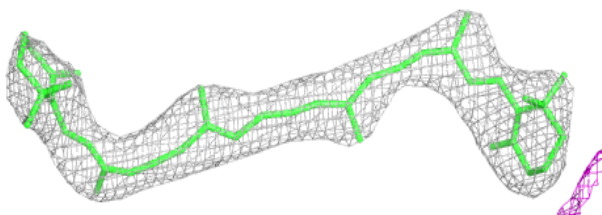


Electron density around BCR B 843:

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

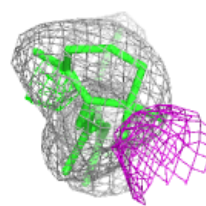
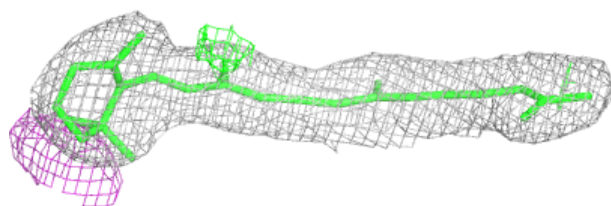
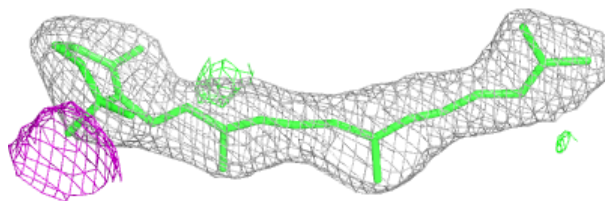
**Electron density around BCR B 845:**

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

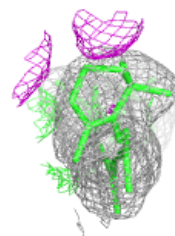
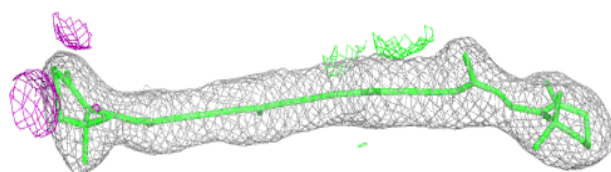
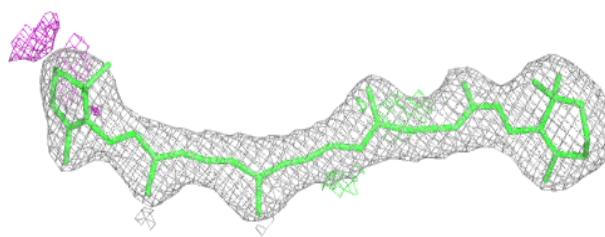


Electron density around BCR B 846:

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

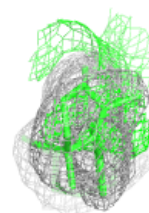
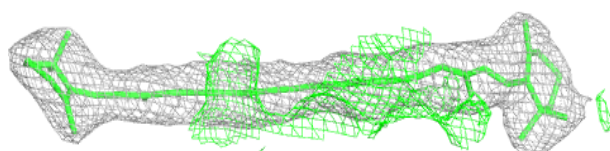
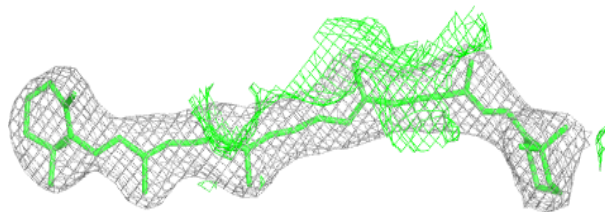
**Electron density around BCR B 847:**

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

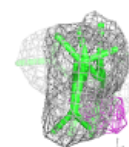
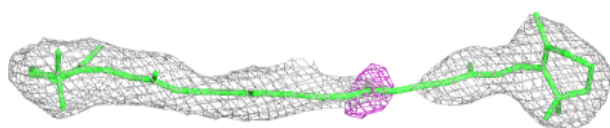
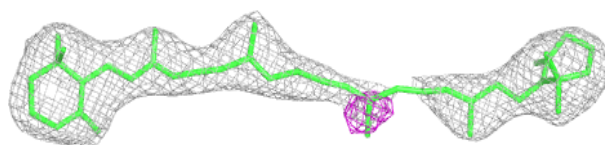


Electron density around BCR B 848:

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

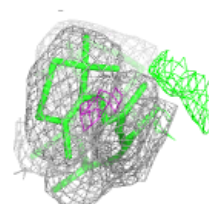
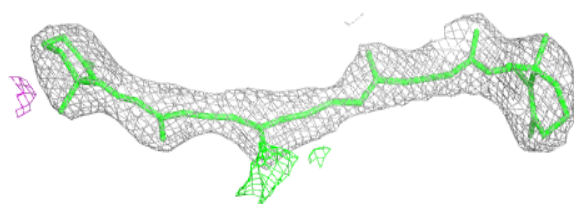
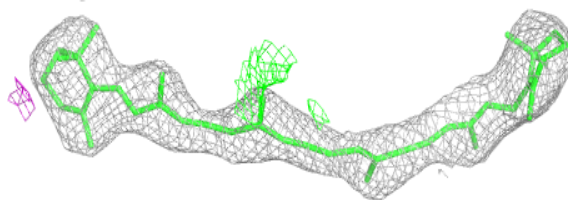
**Electron density around BCR B 851:**

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

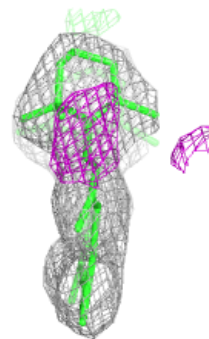
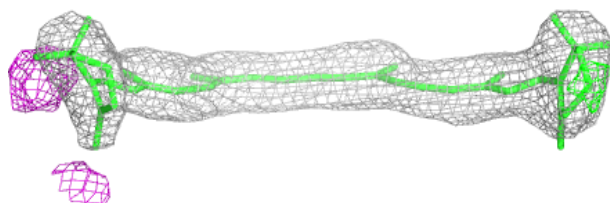
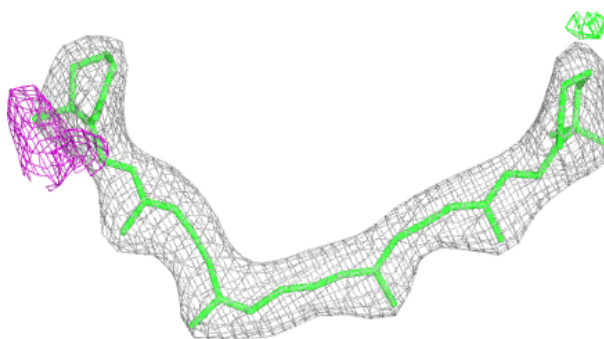


Electron density around BCR F 201:

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

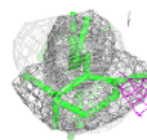
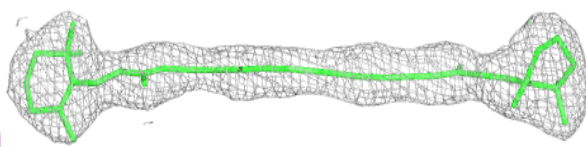
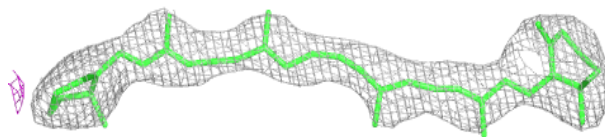
**Electron density around BCR F 203:**

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

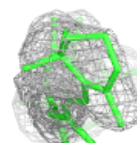
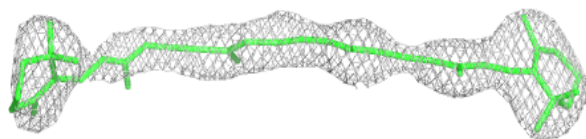
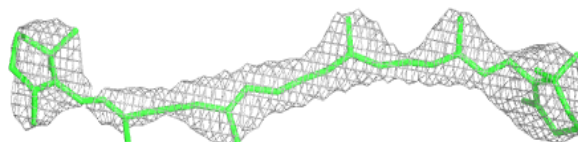


Electron density around BCR G 846:

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

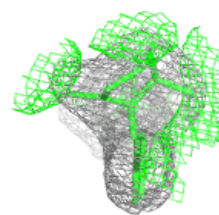
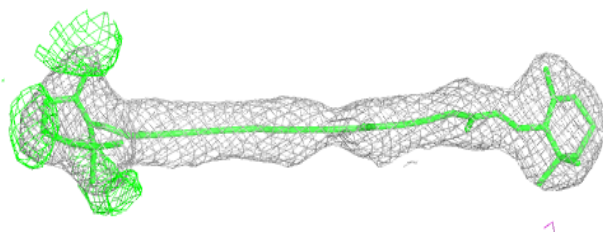
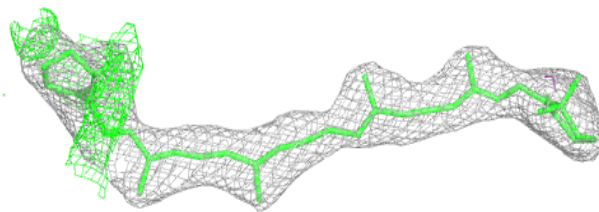
**Electron density around BCR G 847:**

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

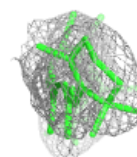
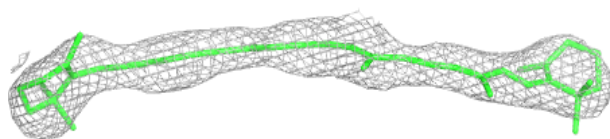
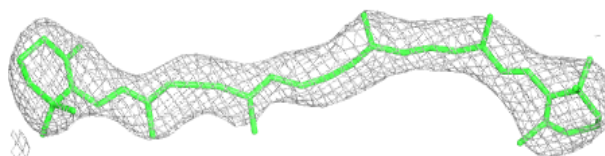


Electron density around BCR G 848:

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

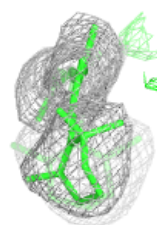
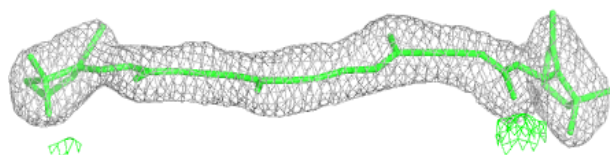
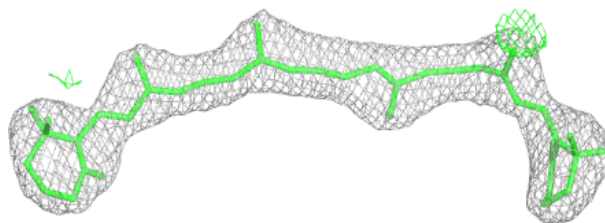
**Electron density around BCR H 840:**

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

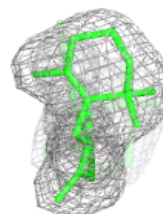
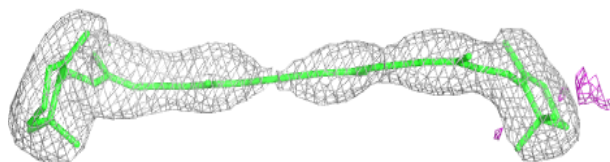
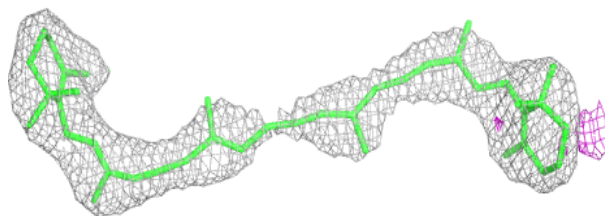


Electron density around BCR H 841:

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

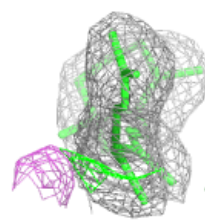
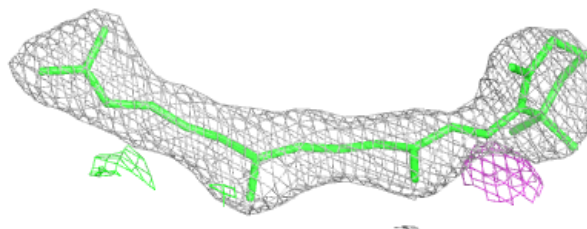
**Electron density around BCR H 842:**

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

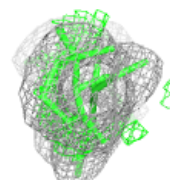
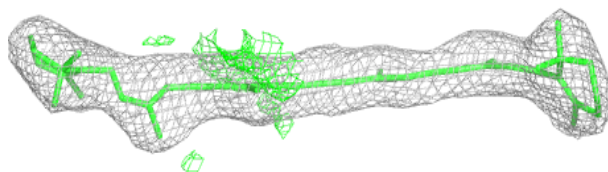
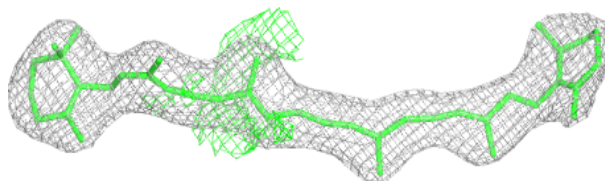


Electron density around BCR H 843:

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

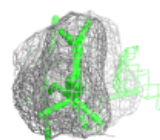
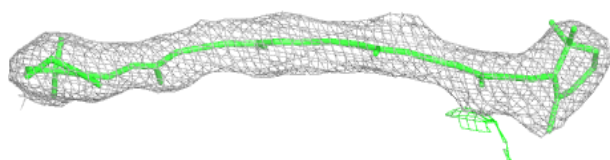
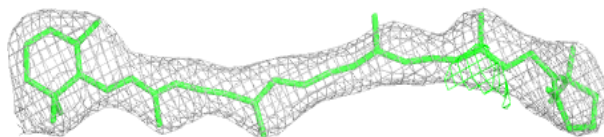
**Electron density around BCR H 844:**

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

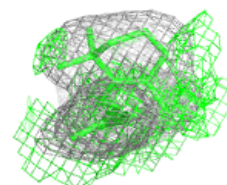
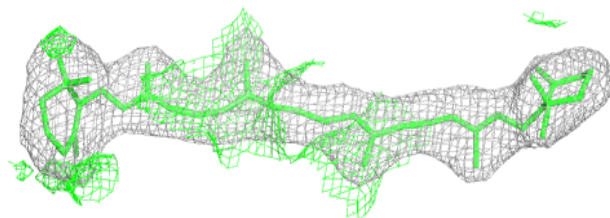
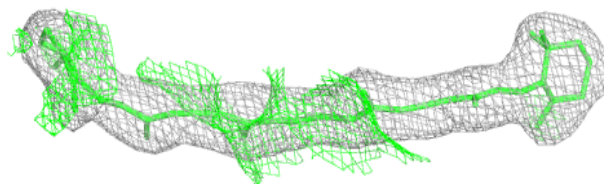


Electron density around BCR H 848:

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

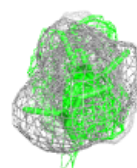
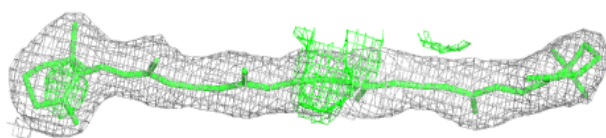
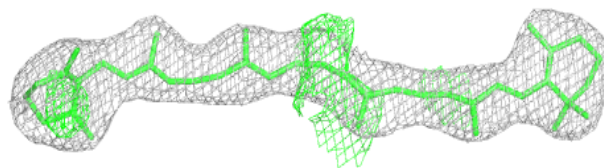
**Electron density around BCR I 101:**

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

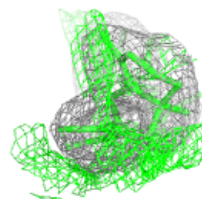
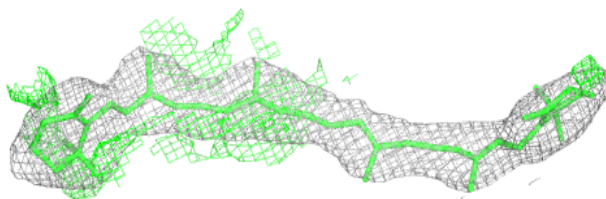
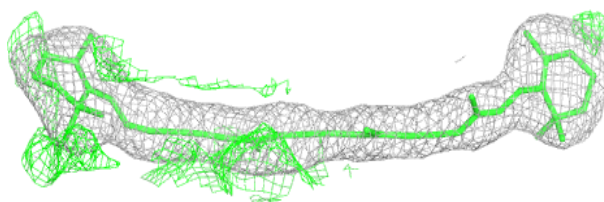


Electron density around BCR J 103:

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

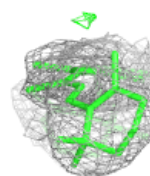
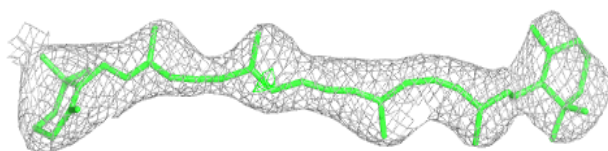
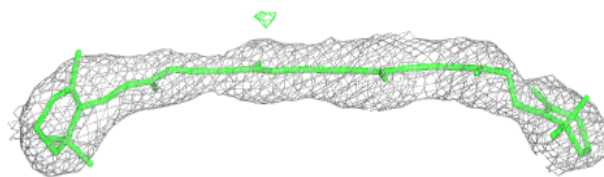
**Electron density around BCR J 104:**

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

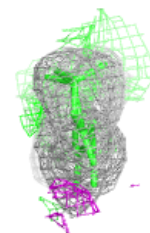
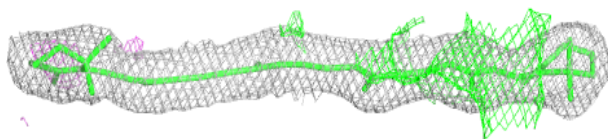
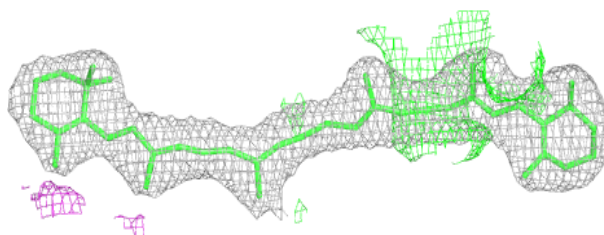


Electron density around BCR K 102:

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

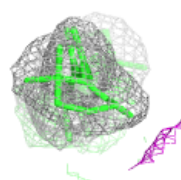
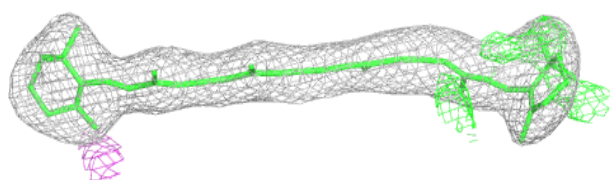
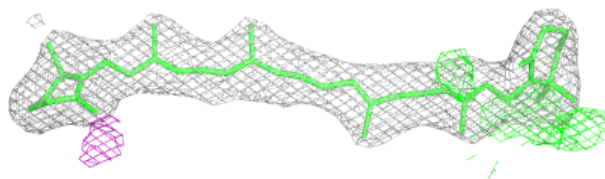
**Electron density around BCR L 208:**

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

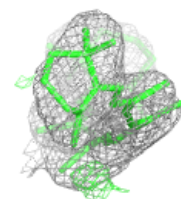
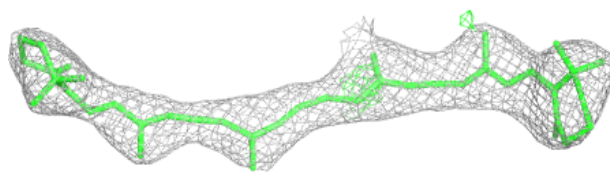
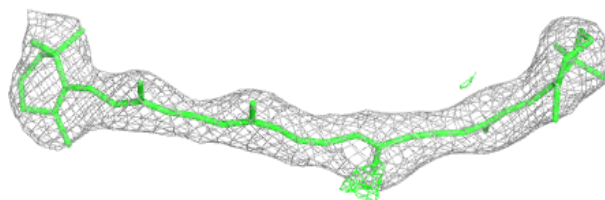


Electron density around BCR L 209:

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

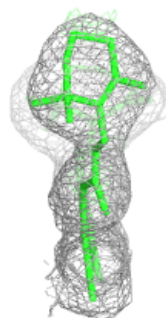
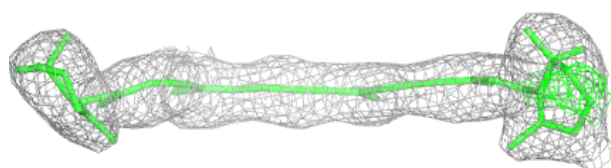
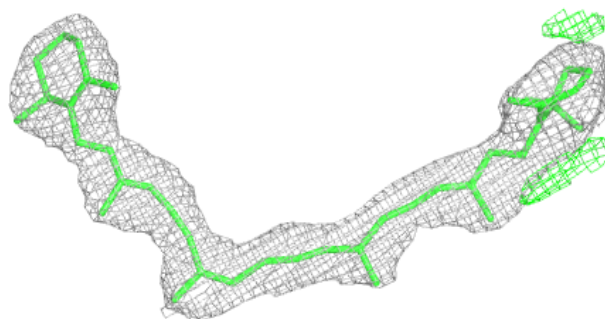
**Electron density around BCR Q 202:**

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

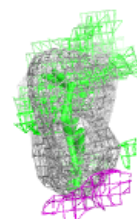
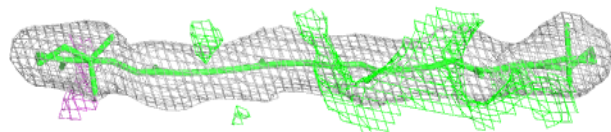
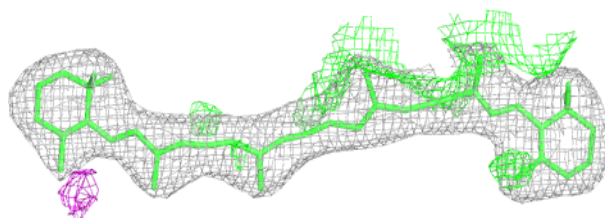


Electron density around BCR Q 204:

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

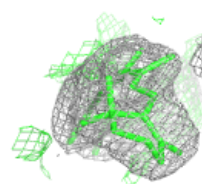
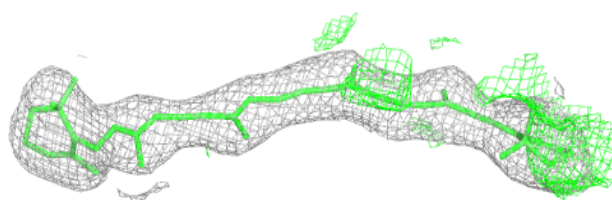
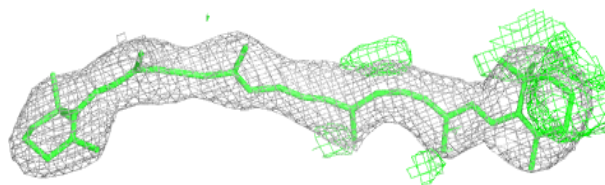
**Electron density around BCR R 102:**

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

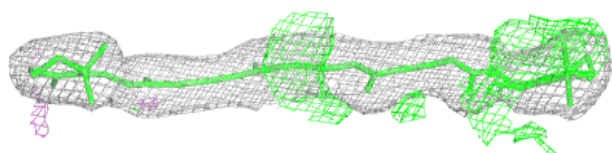
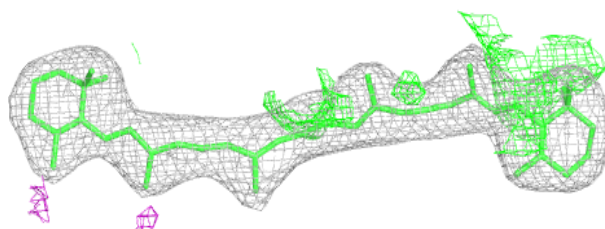


Electron density around BCR S 1104:

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

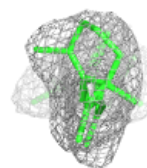
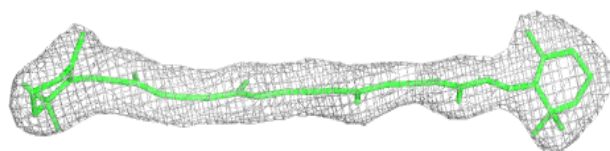
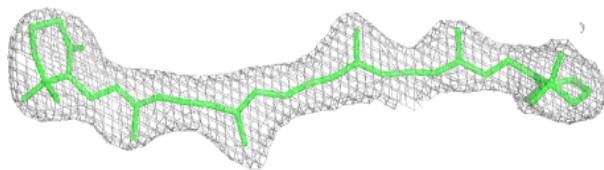
**Electron density around BCR U 1005:**

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

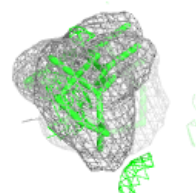
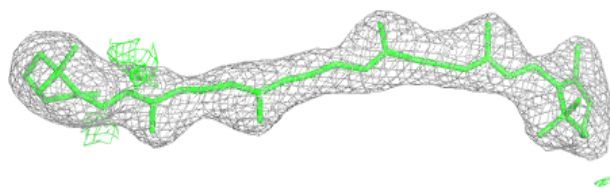
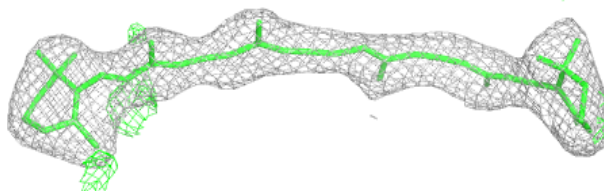


Electron density around BCR U 1008:

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

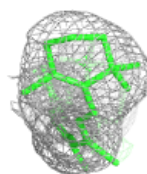
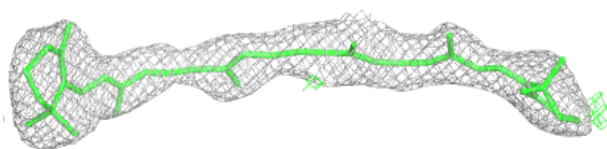
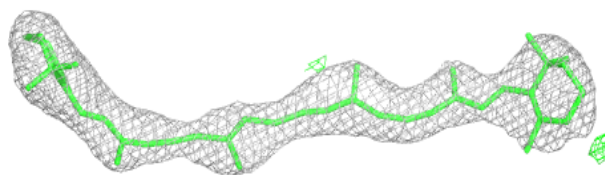
**Electron density around BCR V 1202:**

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

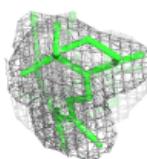
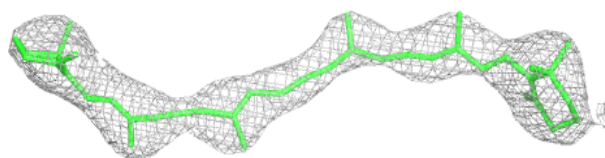


Electron density around BCR Y 846:

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

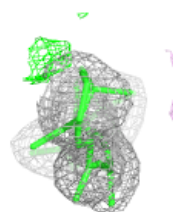
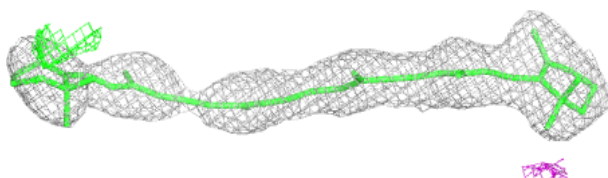
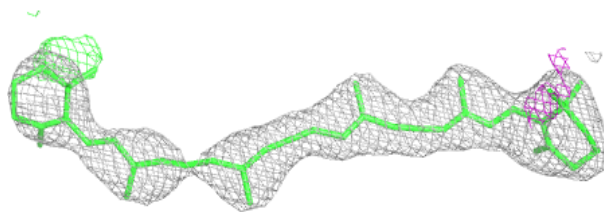
**Electron density around BCR Y 848:**

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

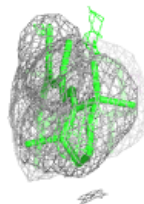
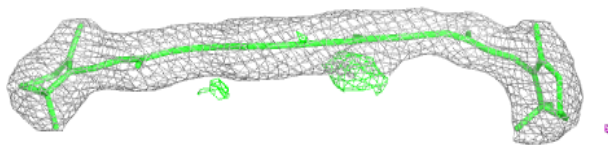
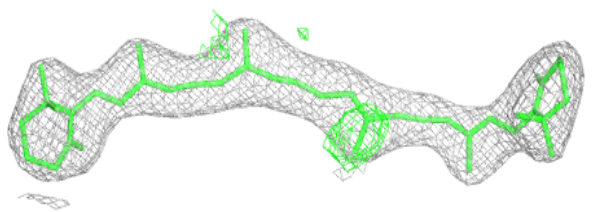


Electron density around BCR Y 849:

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

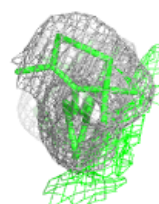
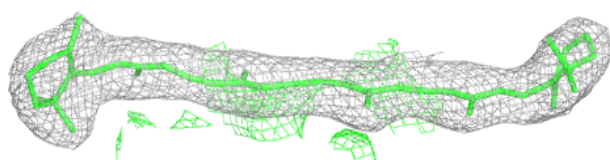
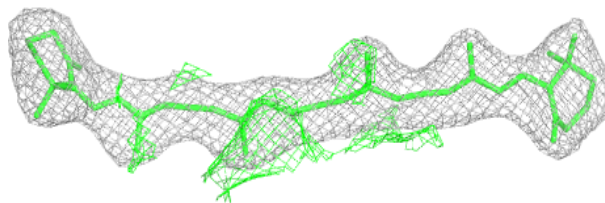
**Electron density around BCR Y 850:**

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

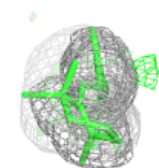
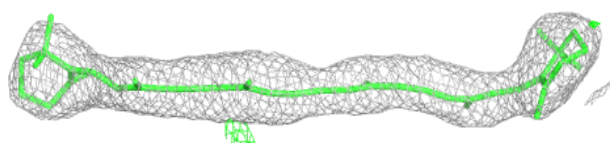
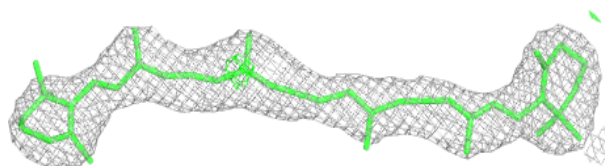


Electron density around BCR Y 856:

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

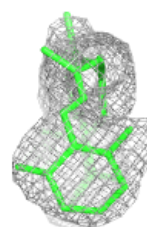
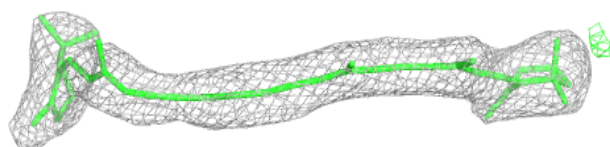
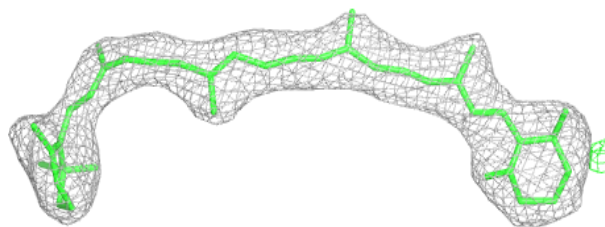
**Electron density around BCR Z 841:**

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

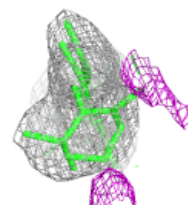
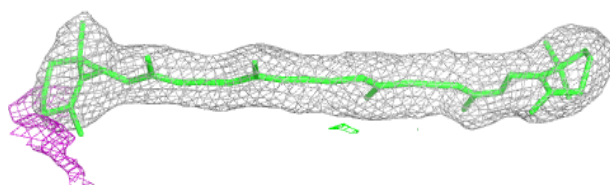
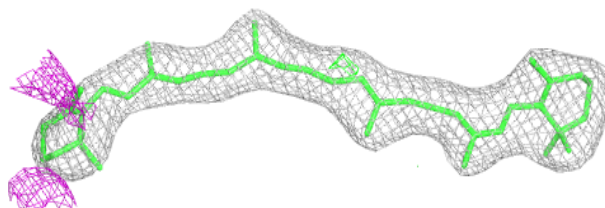


Electron density around BCR Z 842:

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

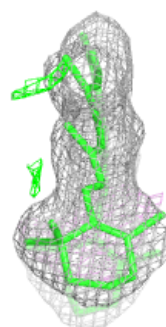
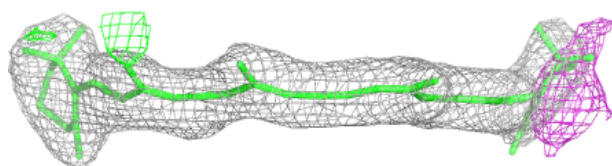
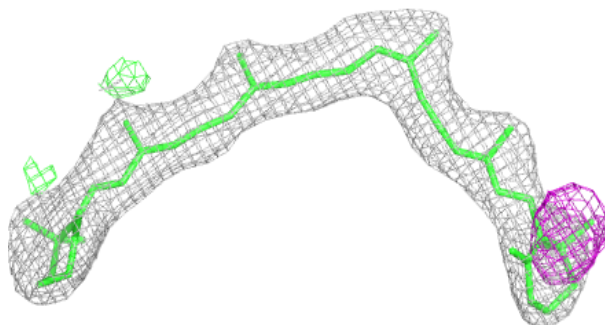
**Electron density around BCR Z 845:**

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

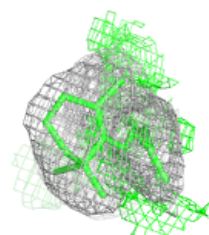
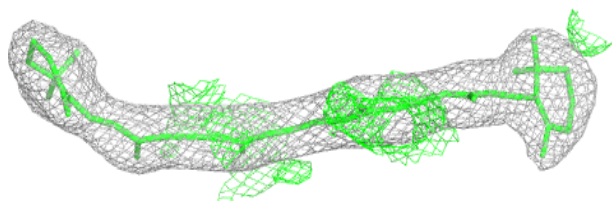
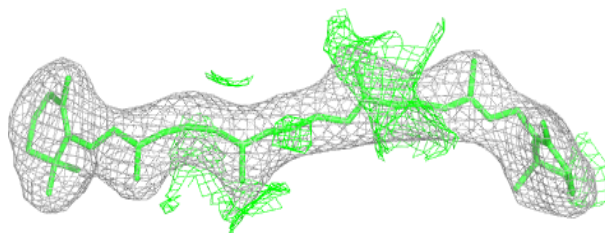


Electron density around BCR d 203:

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

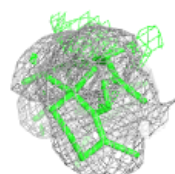
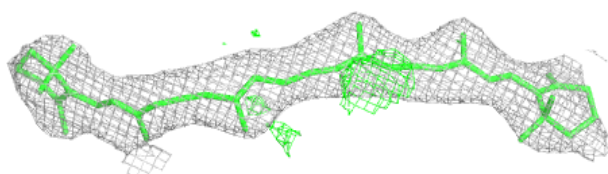
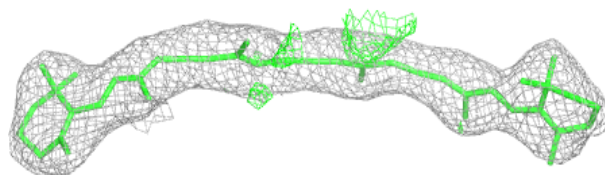
**Electron density around BCR e 101:**

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

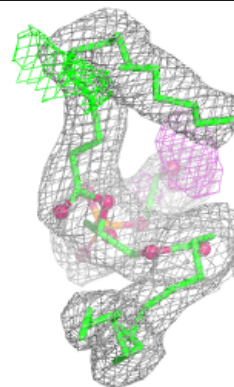
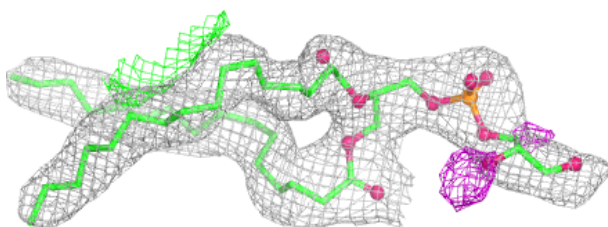
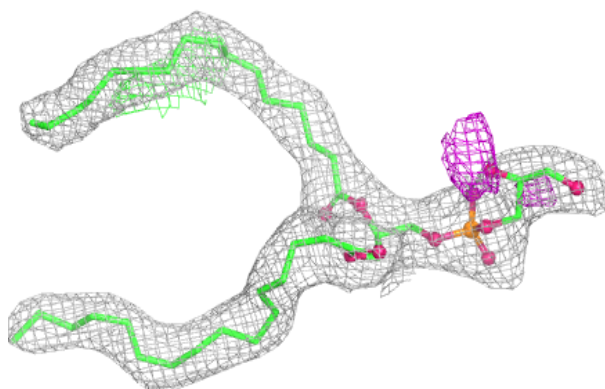


Electron density around BCR f 104:

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

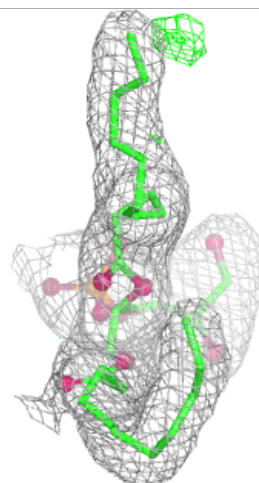
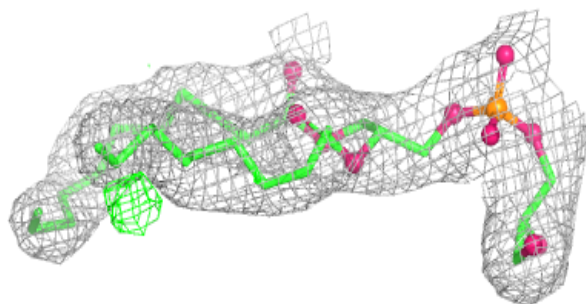
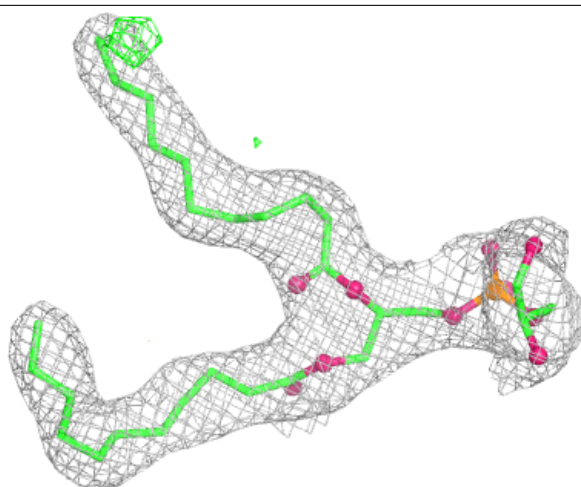
**Electron density around LHG A 850:**

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



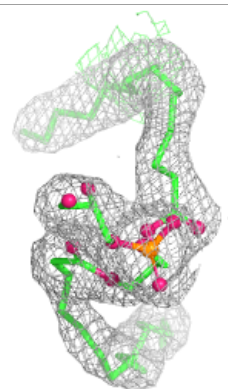
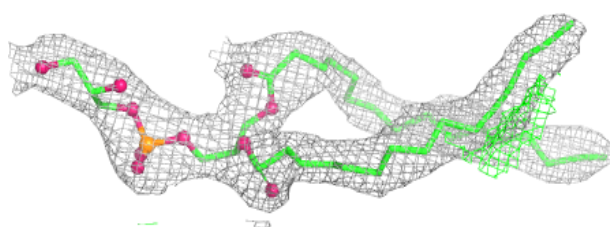
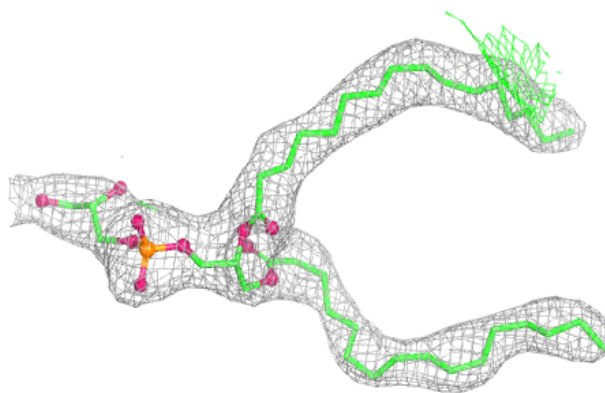
Electron density around LHG B 850:

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

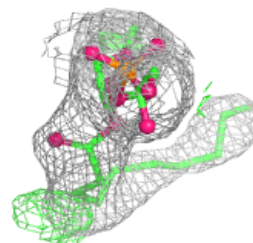
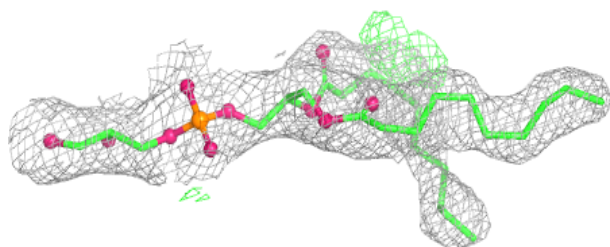
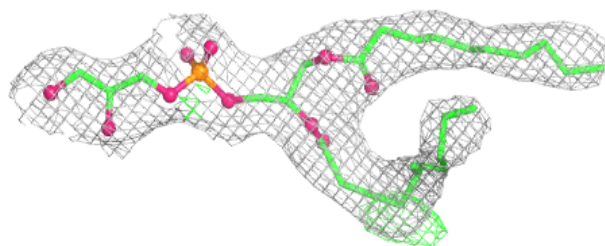


Electron density around LHG G 851:

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

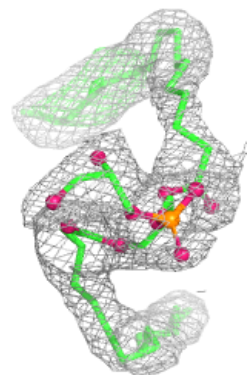
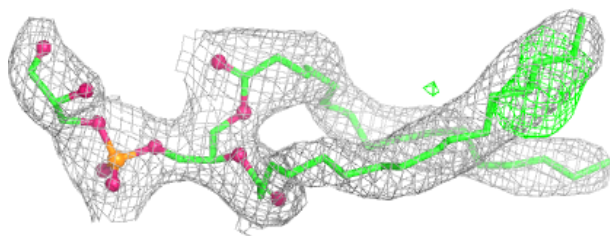
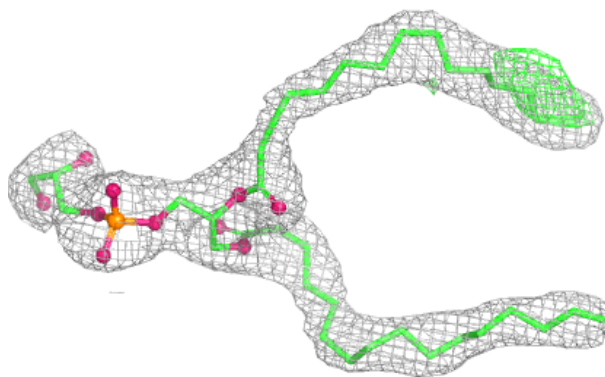
**Electron density around LHG H 847:**

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

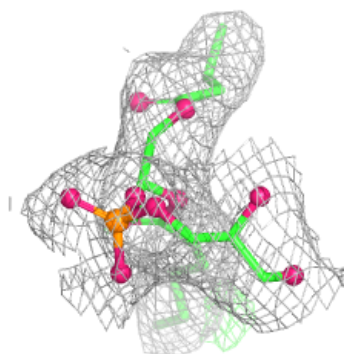
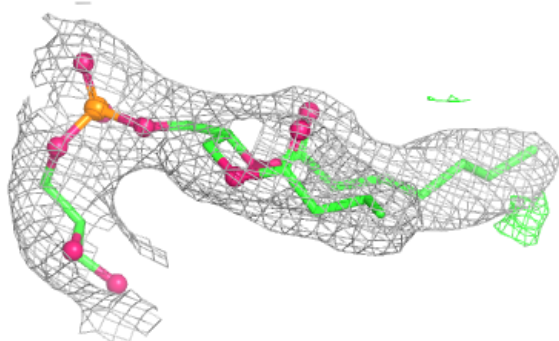
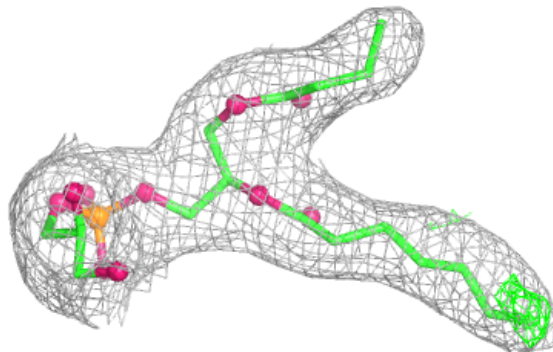


Electron density around LHG Y 852:

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

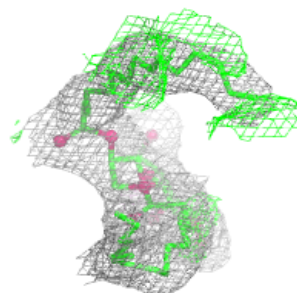
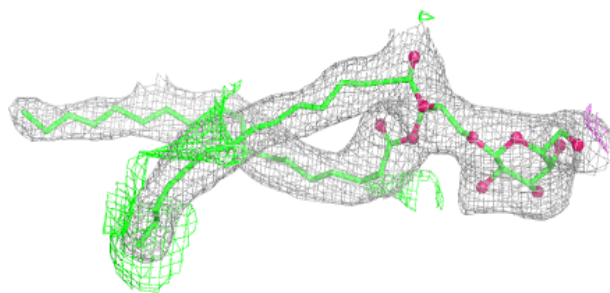
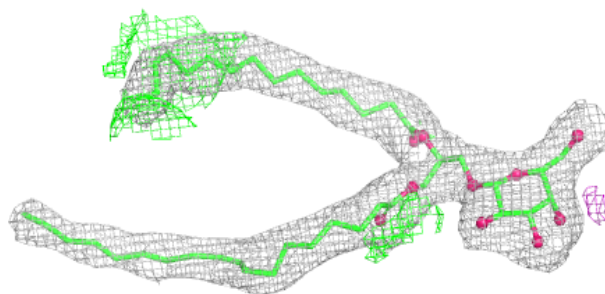
**Electron density around LHG j 101:**

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

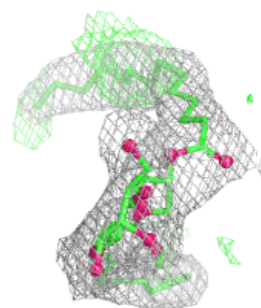
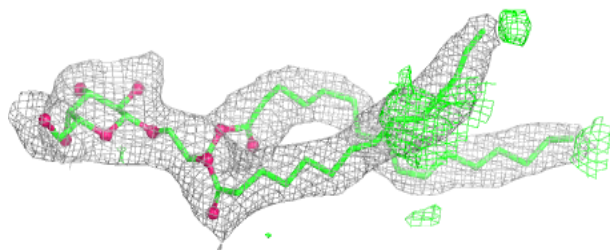
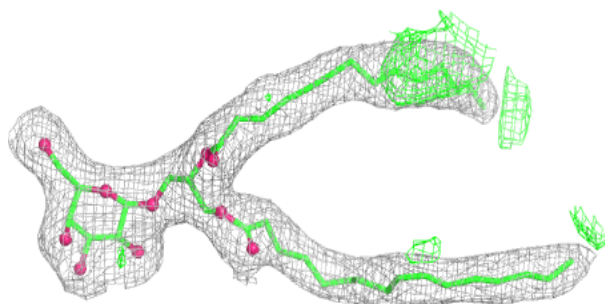


Electron density around LMG B 849:

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

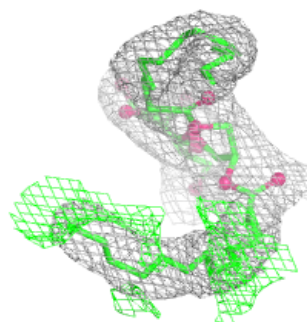
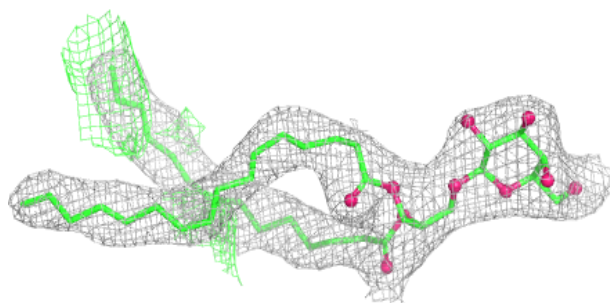
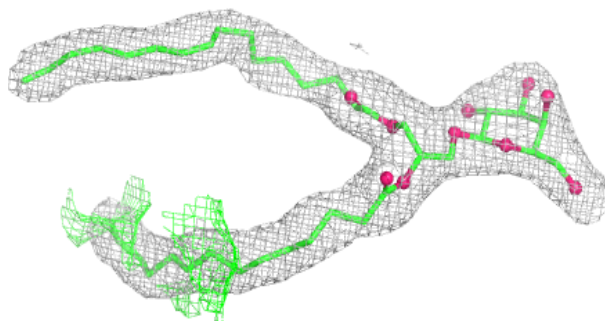
**Electron density around LMG H 846:**

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

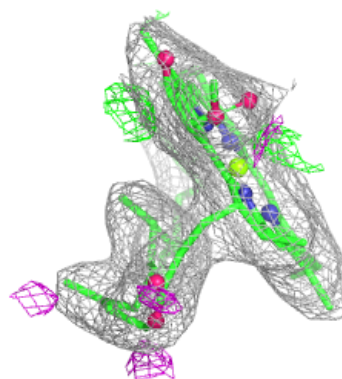
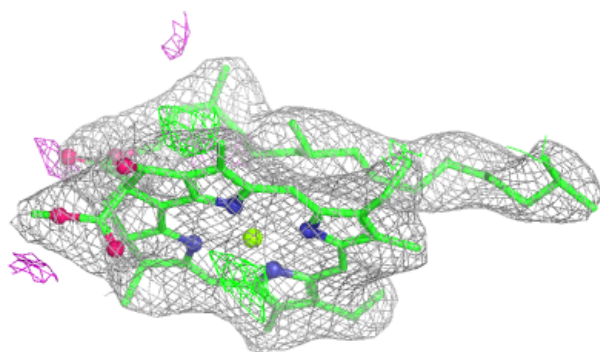
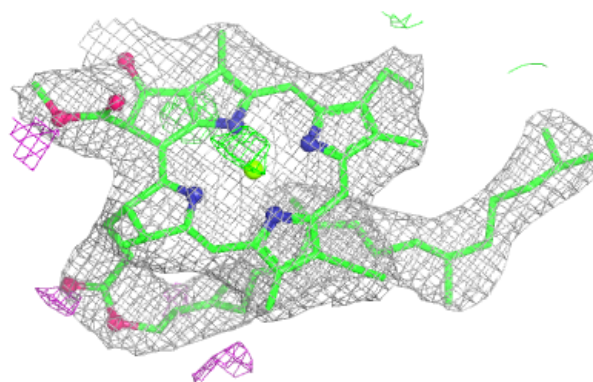


Electron density around LMG Z 847:

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

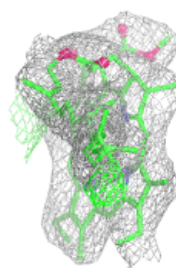
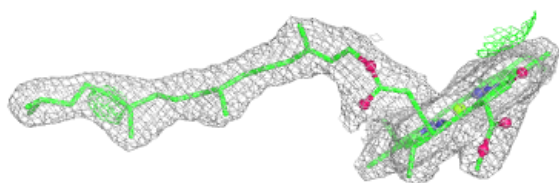
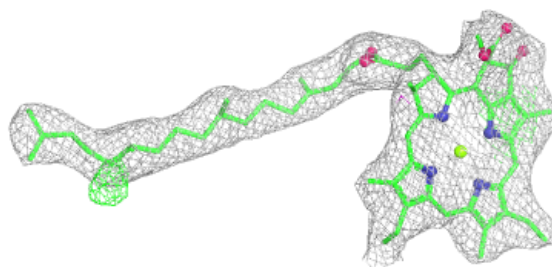
**Electron density around CLA B 817:**

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

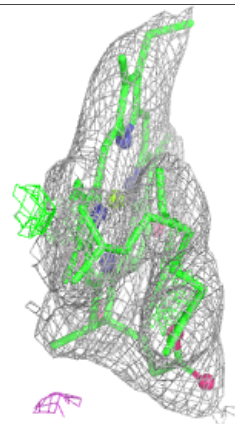
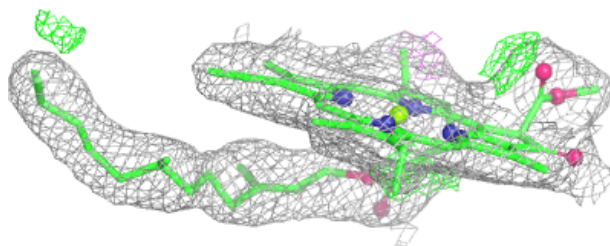
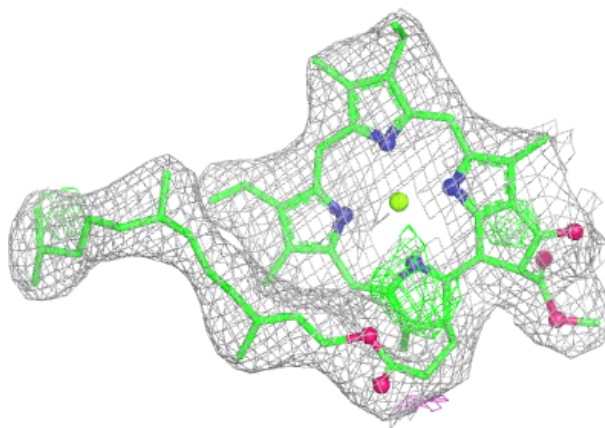


Electron density around CLA G 833:

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

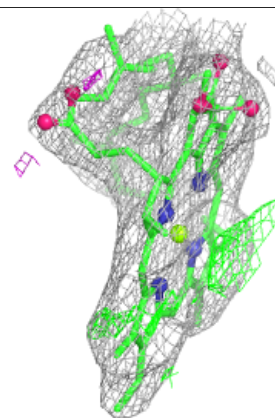
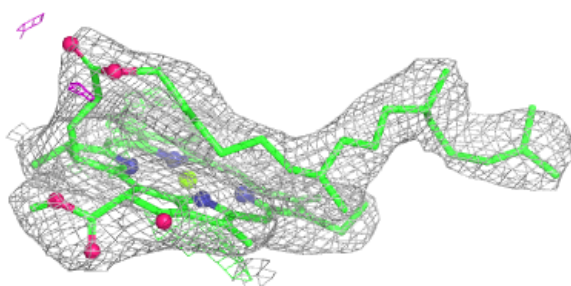
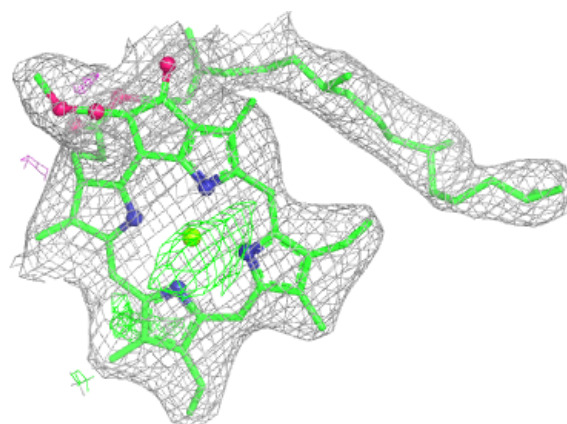
**Electron density around CLA B 818:**

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

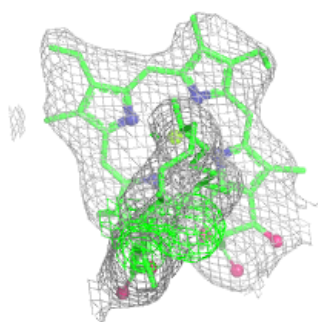
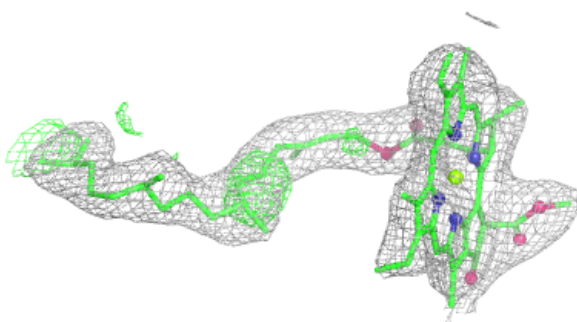
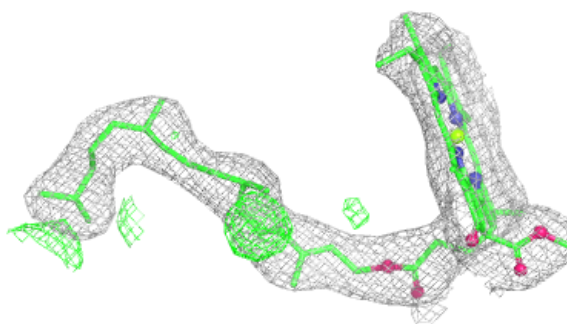


Electron density around CLA Y 829:

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

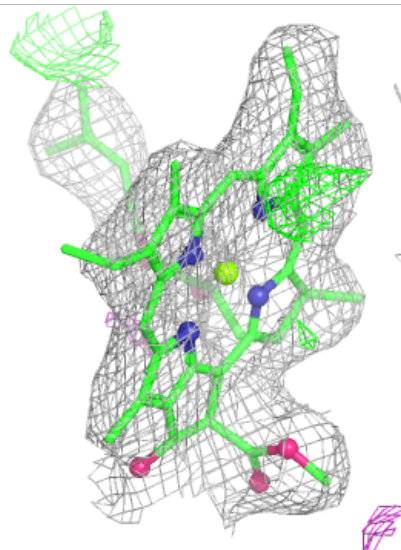
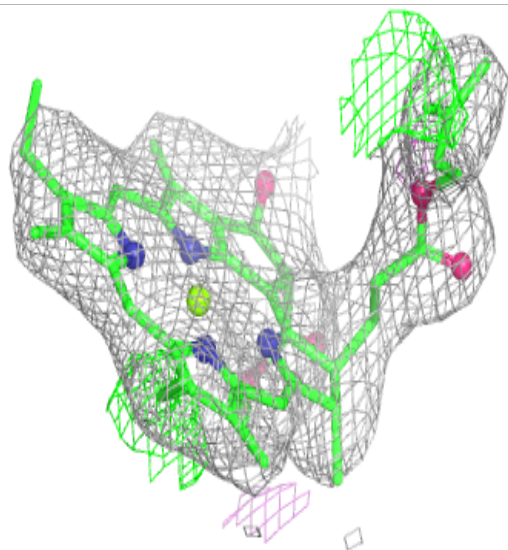
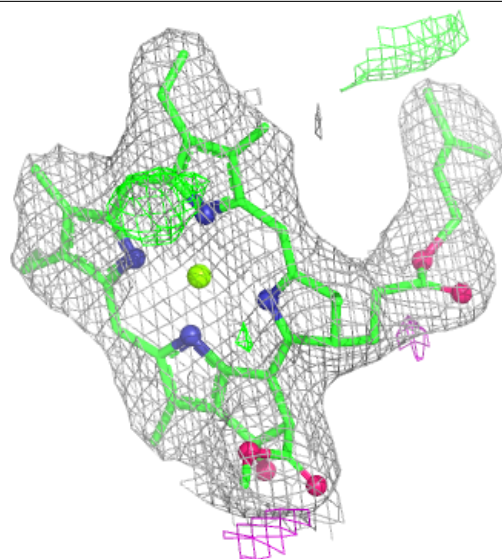
**Electron density around CLA Y 830:**

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



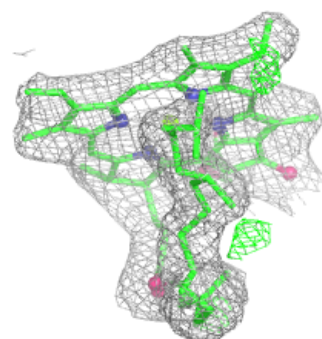
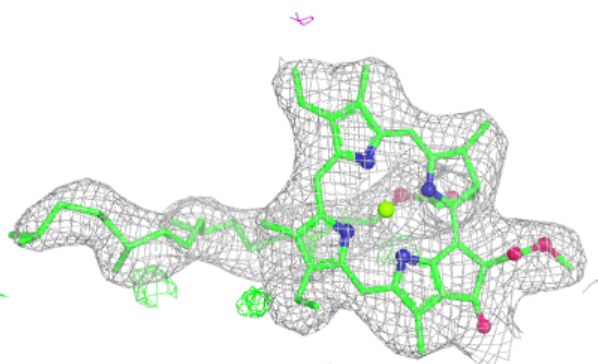
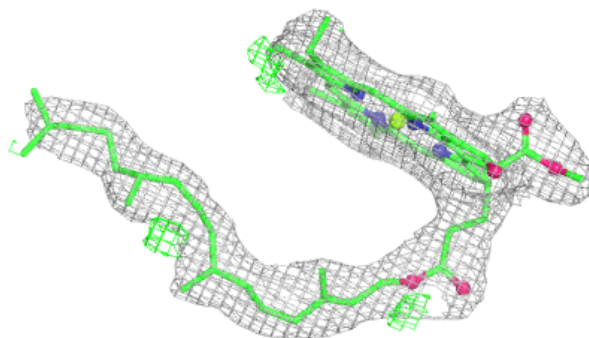
Electron density around CLA Y 831:

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

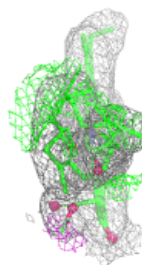
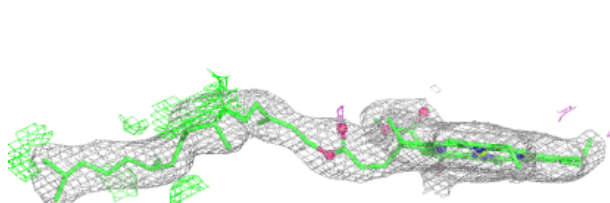
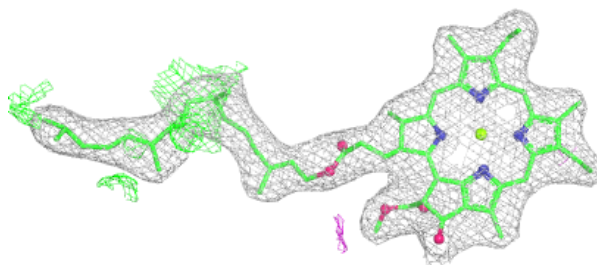


Electron density around CLA Y 832:

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

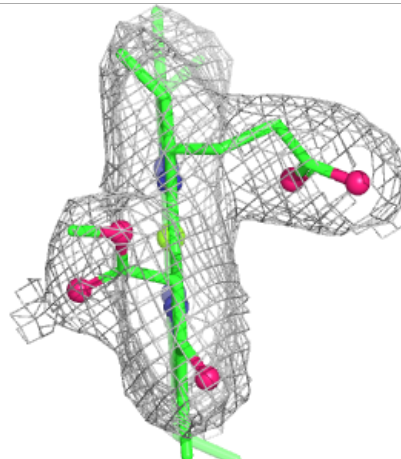
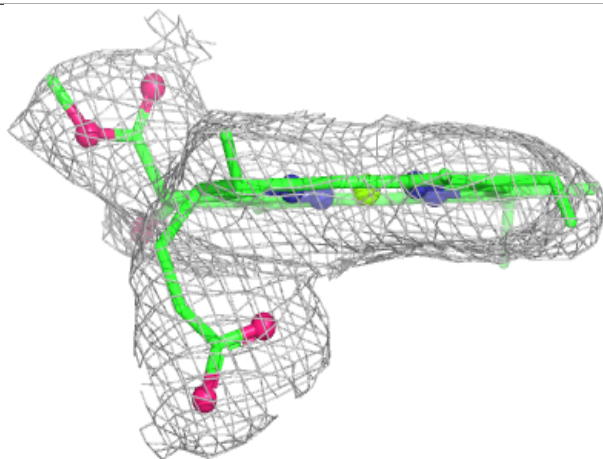
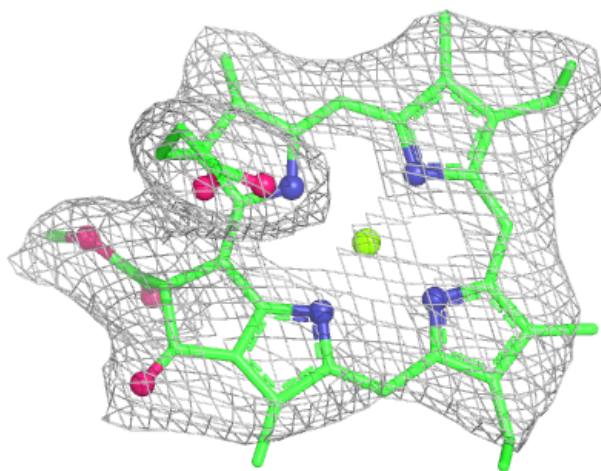
**Electron density around CLA Y 833:**

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



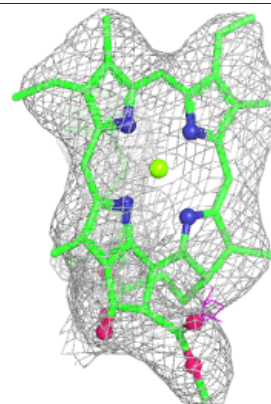
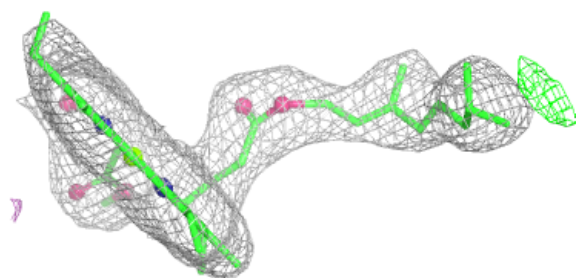
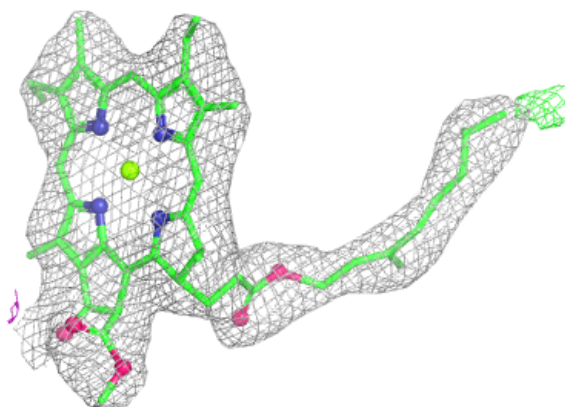
Electron density around CLA G 835:

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



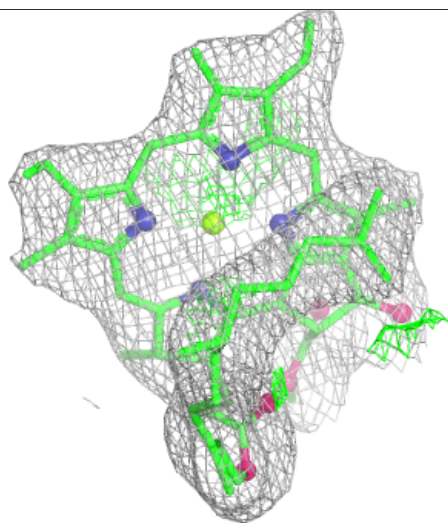
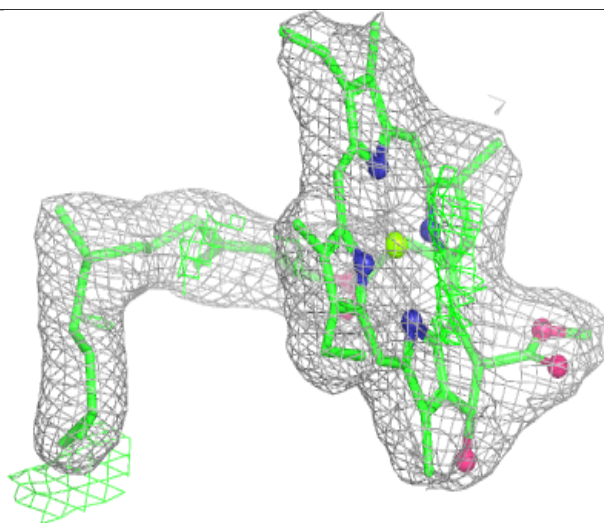
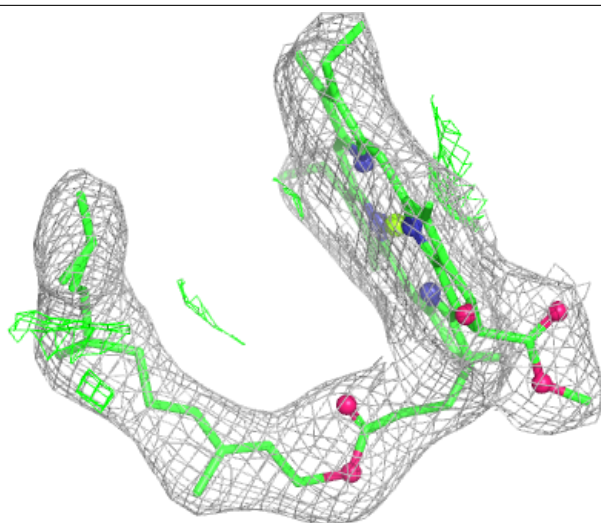
Electron density around CLA Y 835:

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



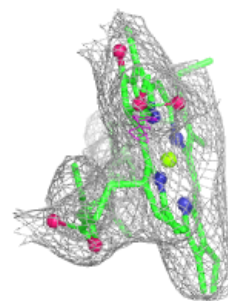
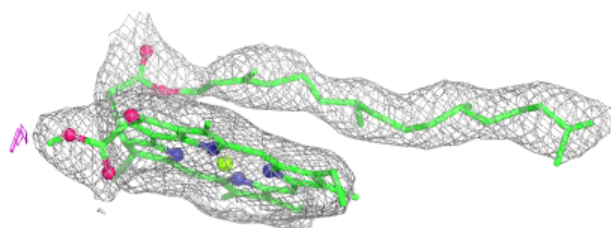
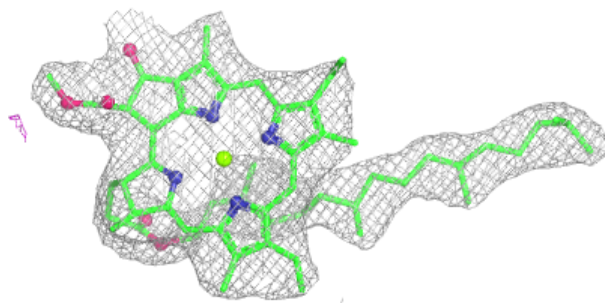
Electron density around CLA B 819:

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

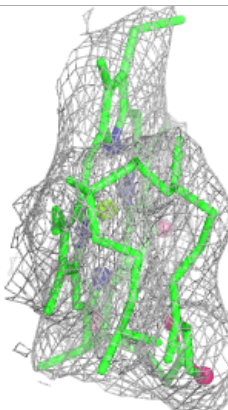
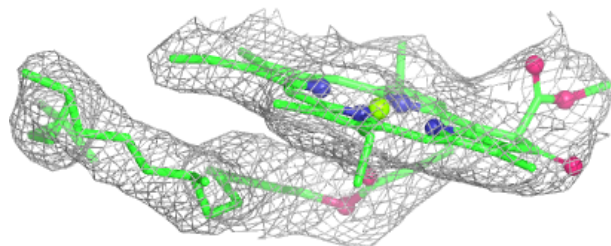
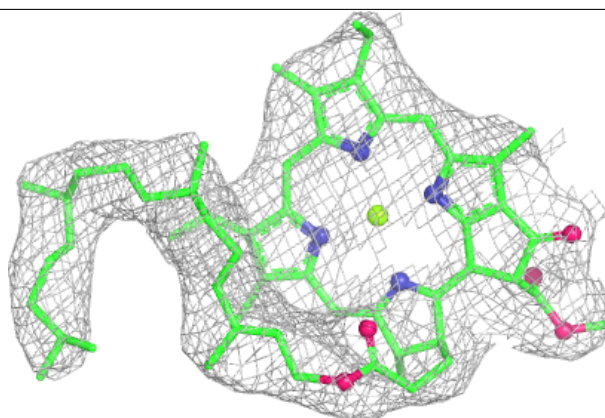


Electron density around CLA A 818:

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

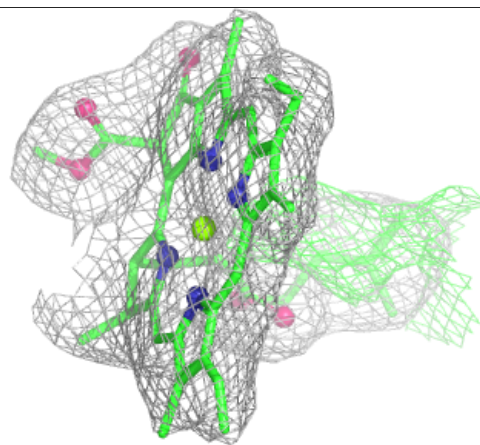
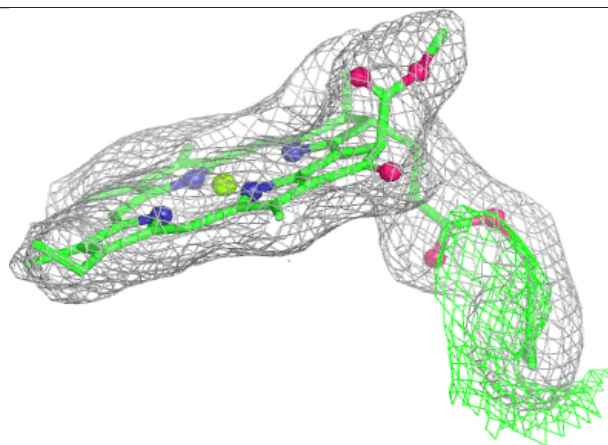
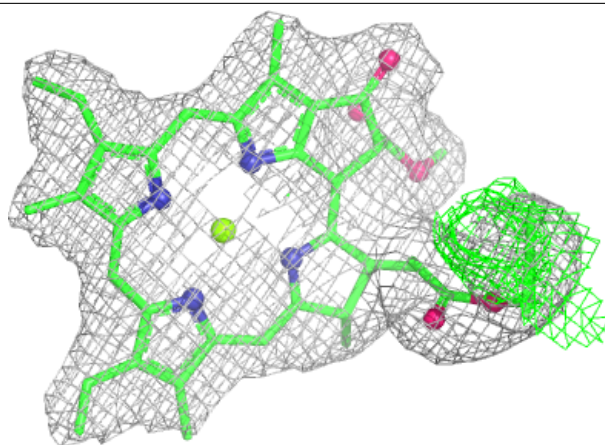
**Electron density around CLA A 819:**

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



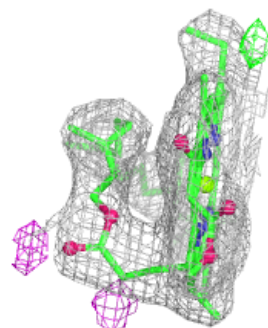
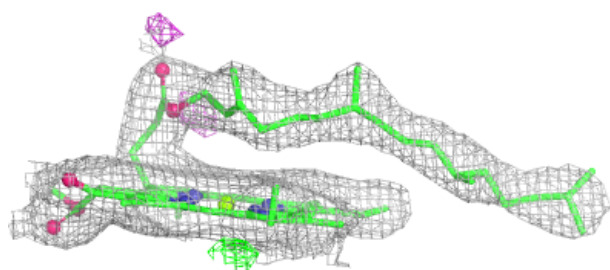
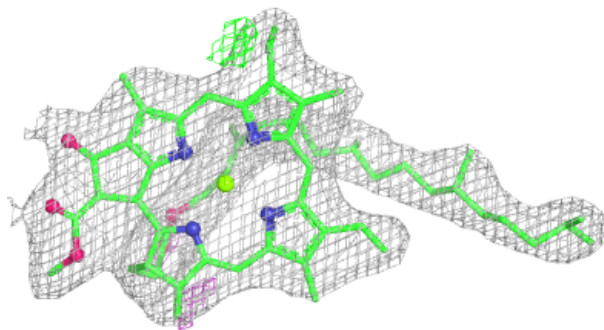
Electron density around CLA Y 839:

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

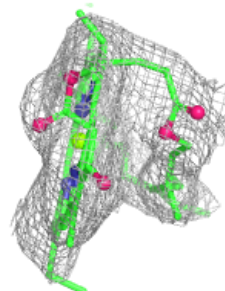
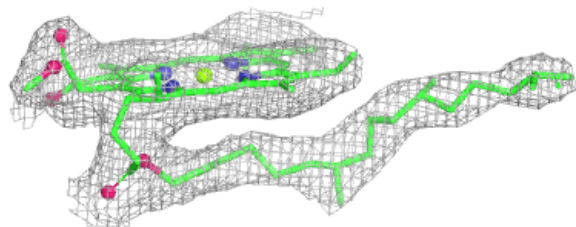
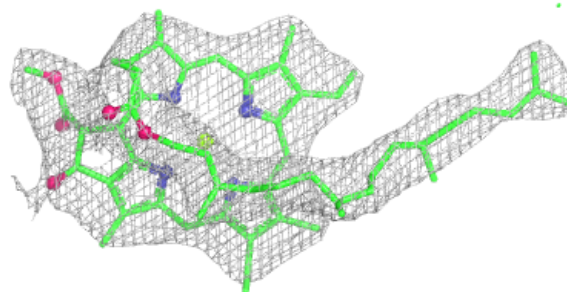


Electron density around CLA Y 840:

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

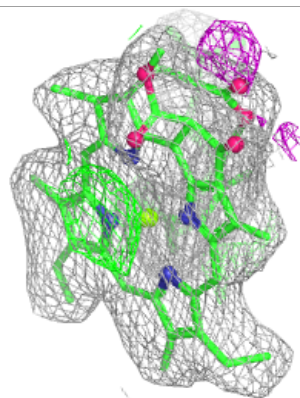
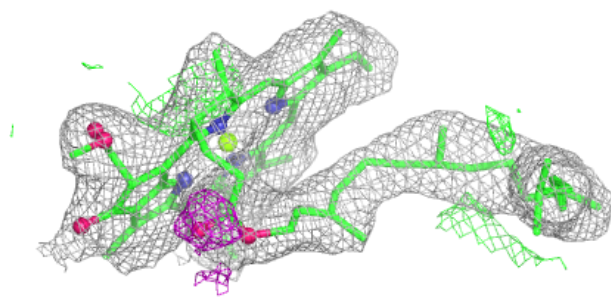
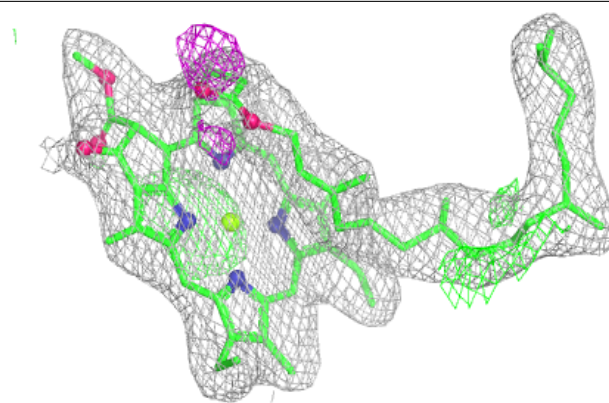
**Electron density around CLA G 839:**

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

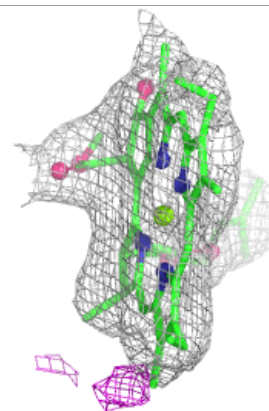
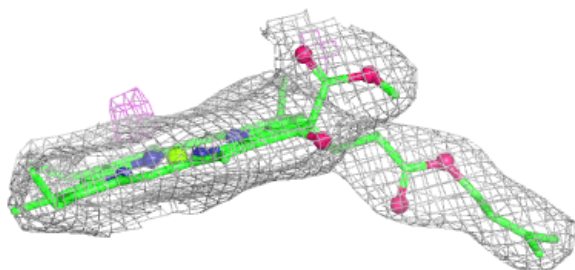
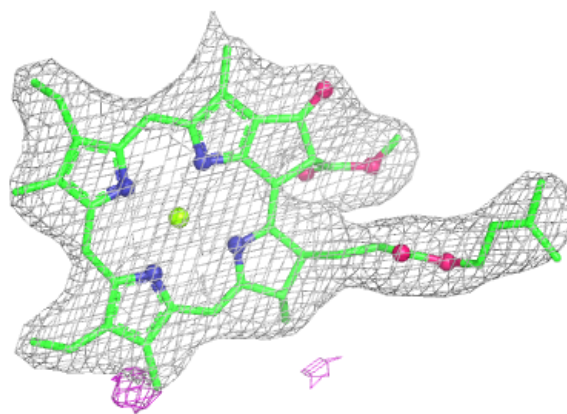


Electron density around CLA Y 842:

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

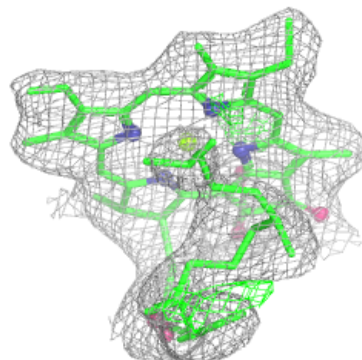
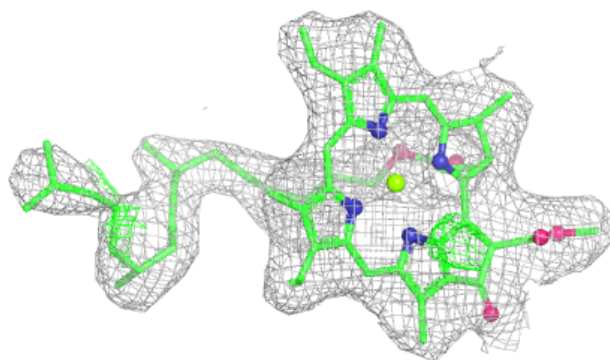
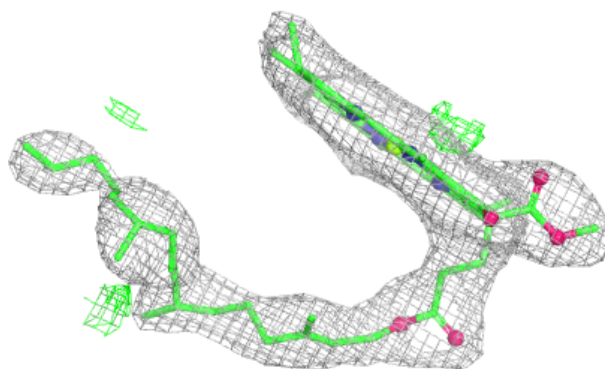
**Electron density around CLA G 840:**

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

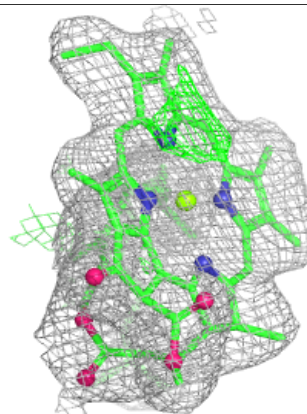
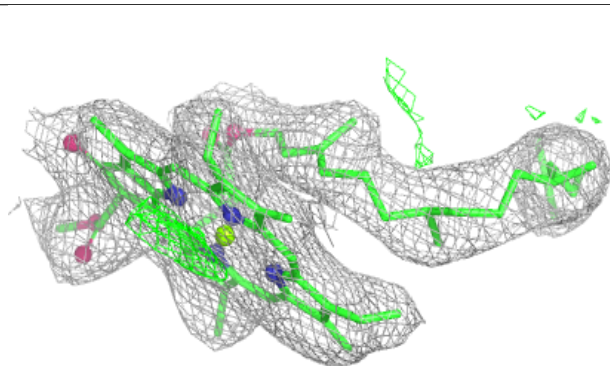
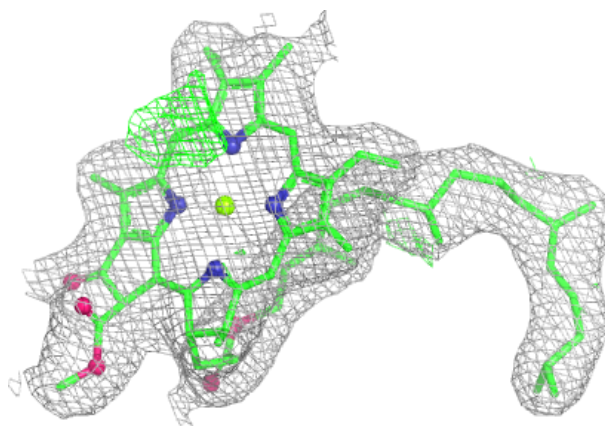


Electron density around CLA A 832:

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

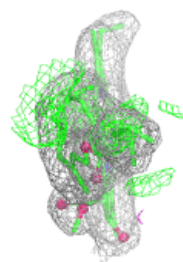
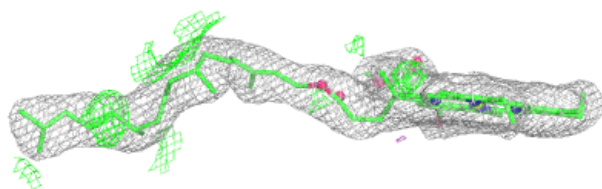
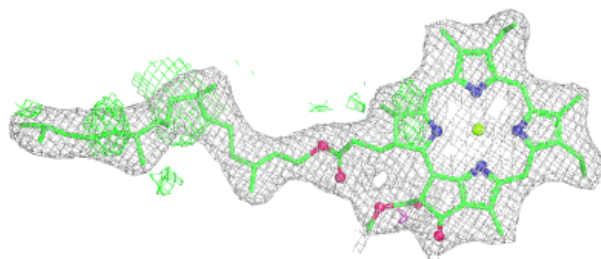
**Electron density around CLA G 842:**

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

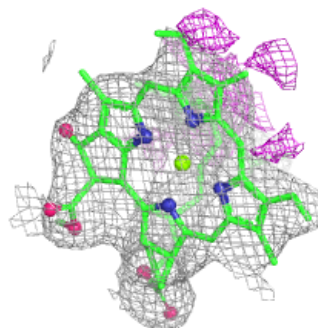
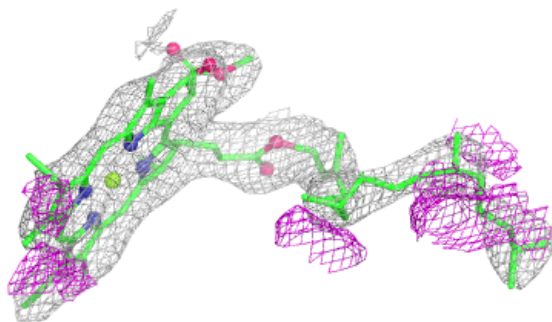
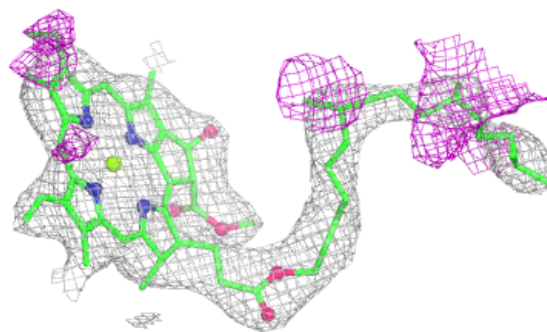


Electron density around CLA A 833:

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

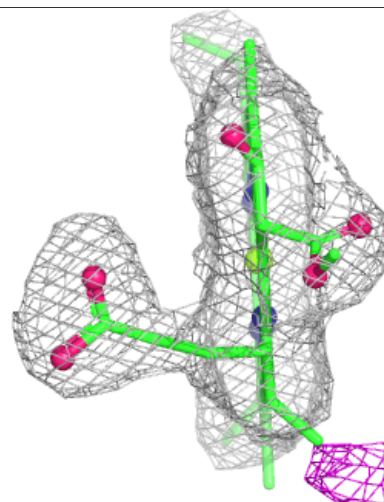
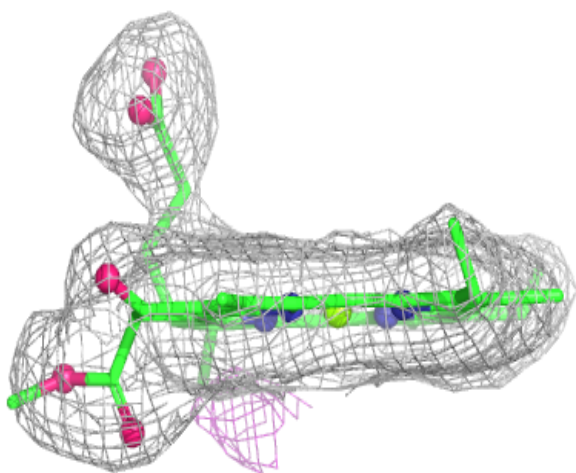
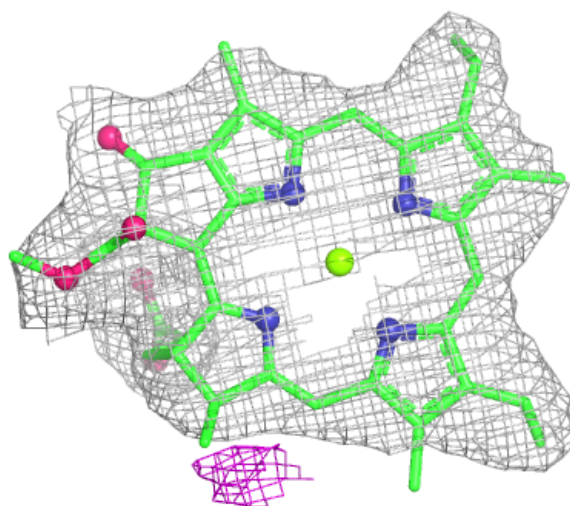
**Electron density around CLA Z 802:**

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



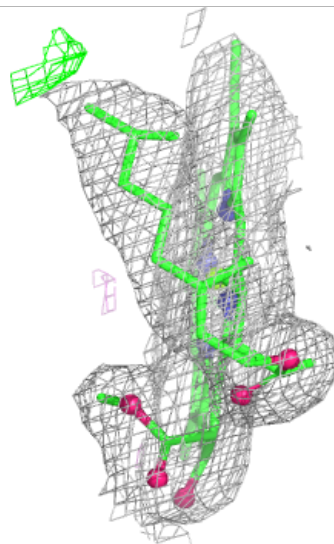
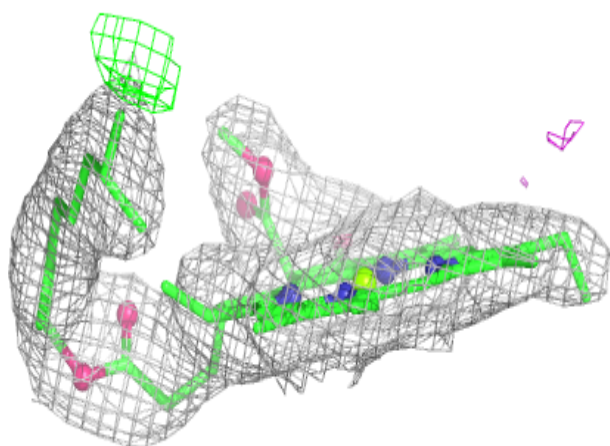
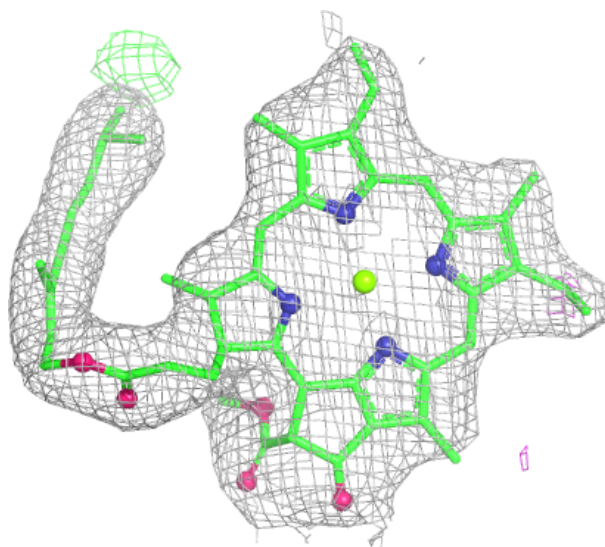
Electron density around CLA G 853:

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



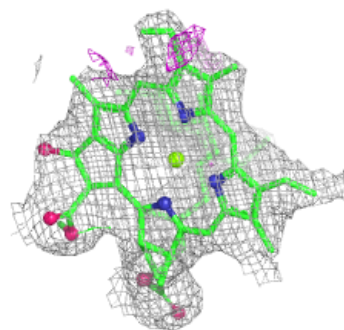
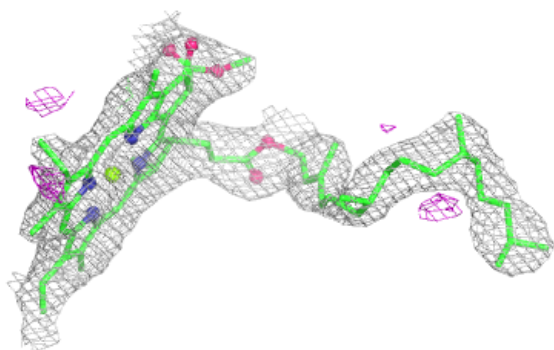
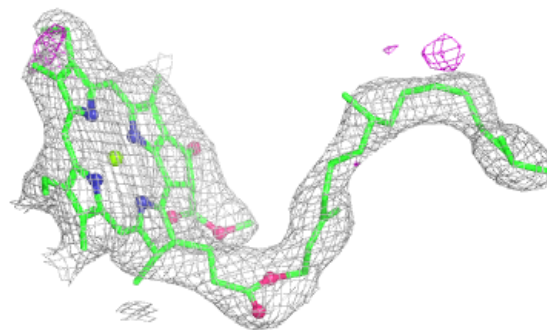
Electron density around CLA B 824:

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

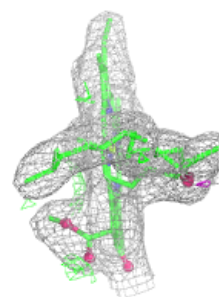
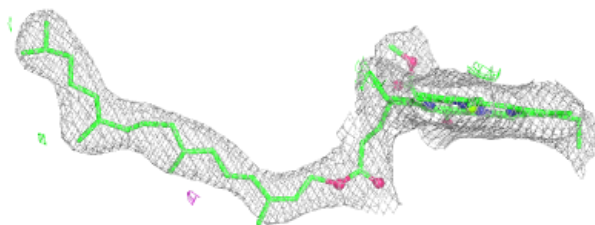
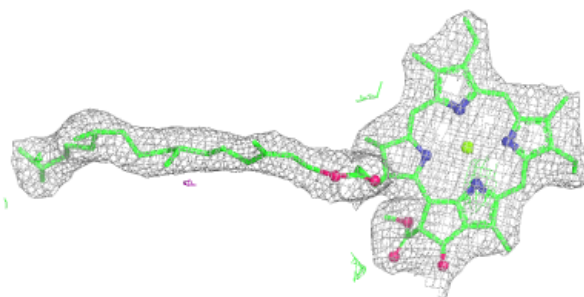


Electron density around CLA H 802:

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

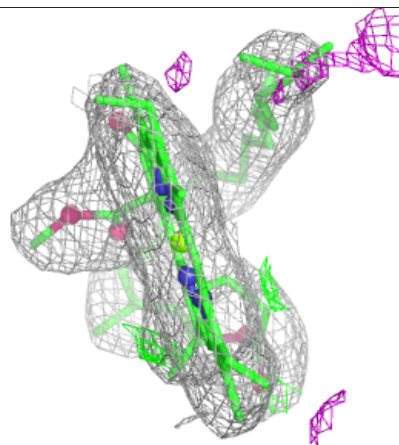
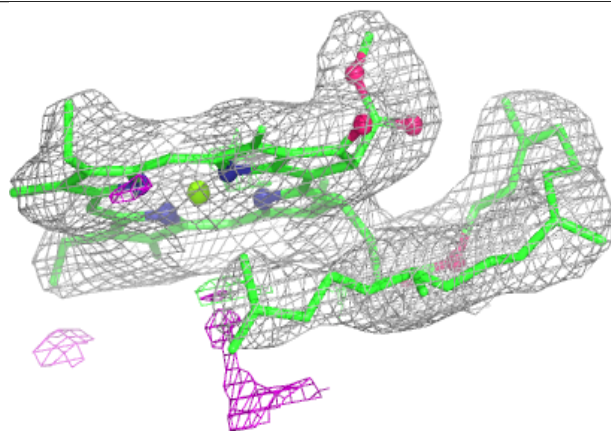
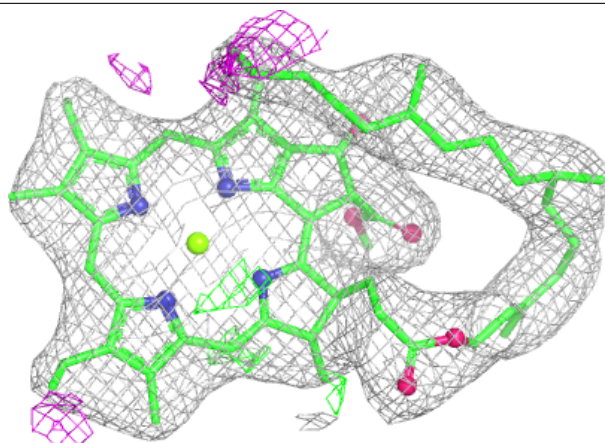
**Electron density around CLA B 825:**

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



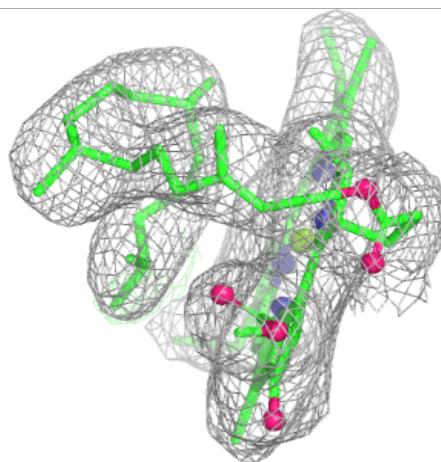
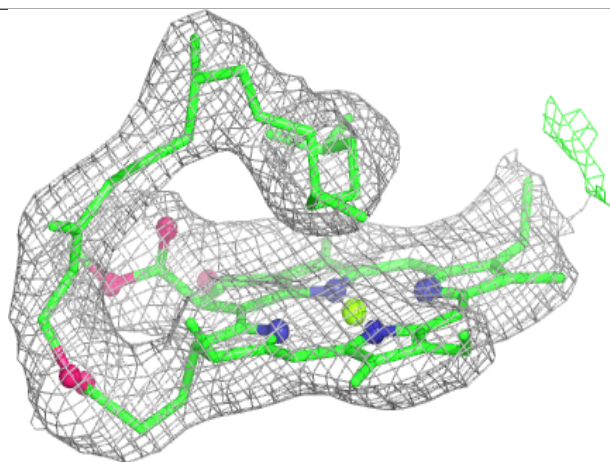
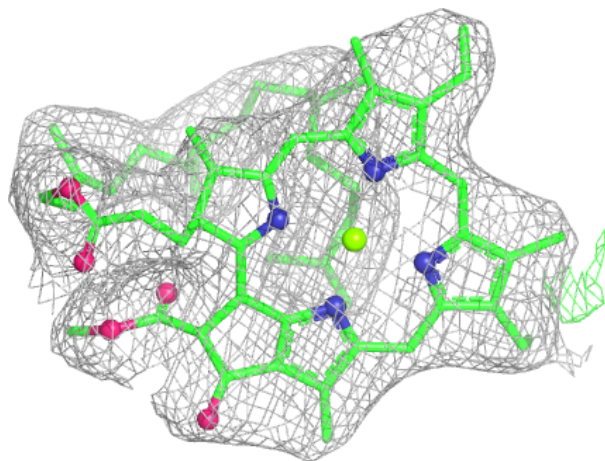
Electron density around CLA H 804:

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



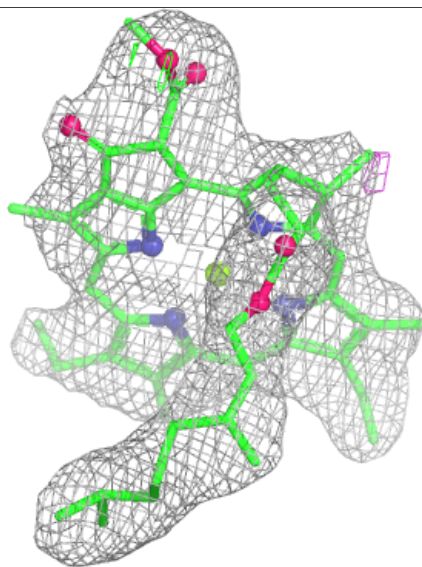
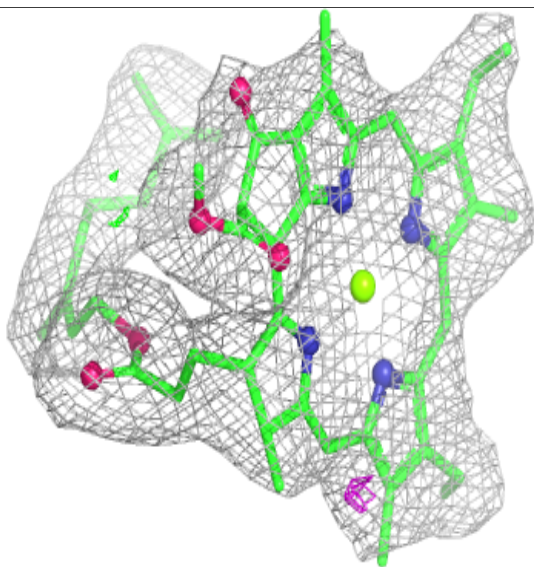
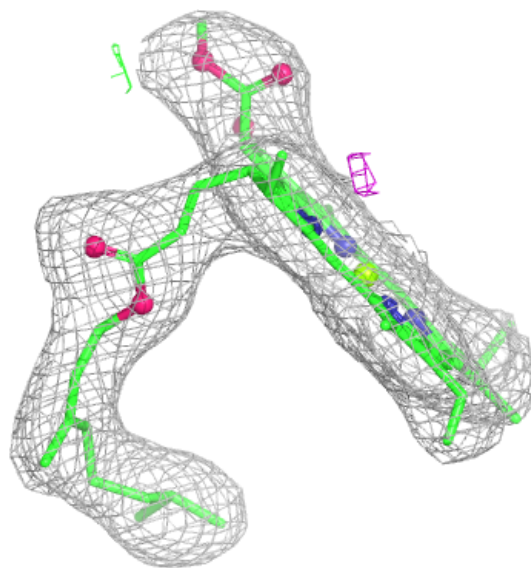
Electron density around CLA H 805:

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



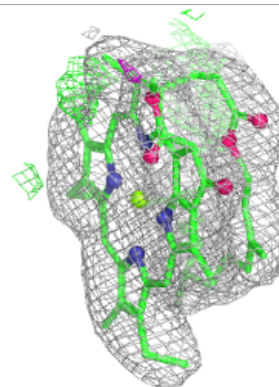
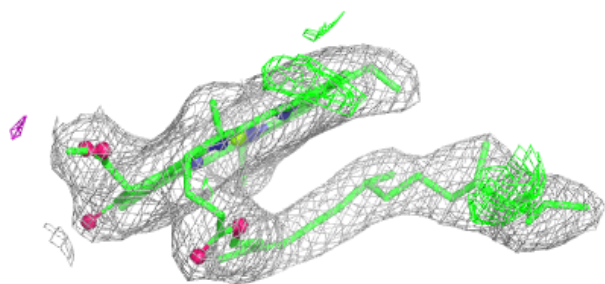
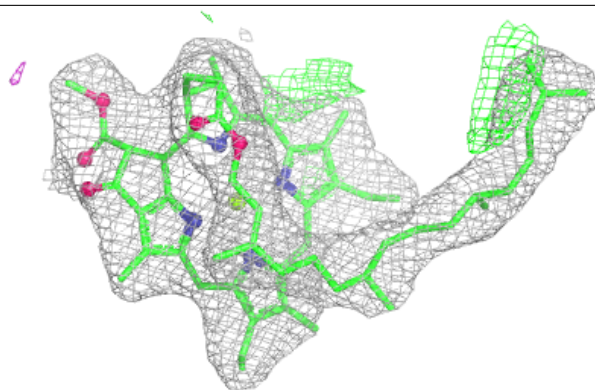
Electron density around CLA Z 809:

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

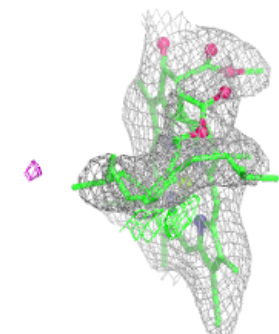
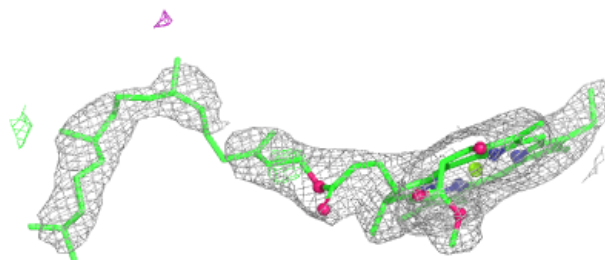
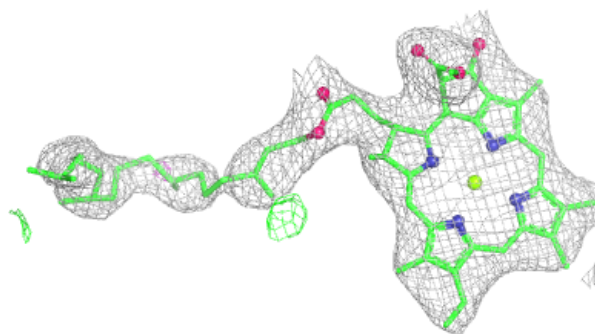


Electron density around CLA H 806:

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

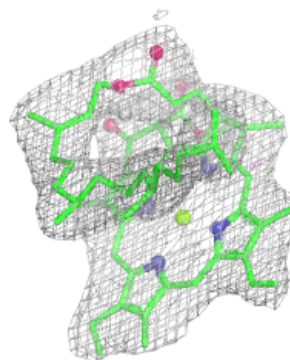
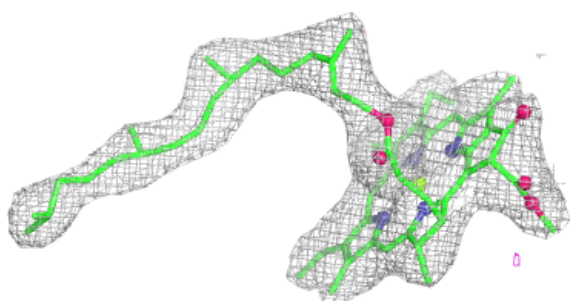
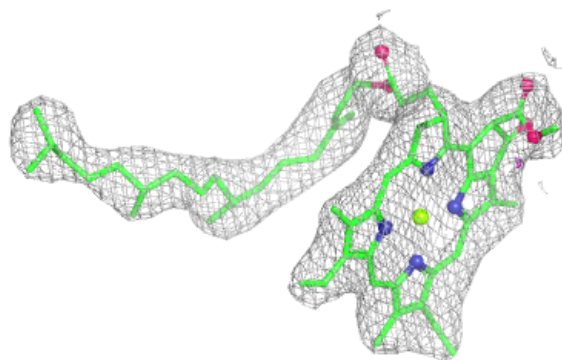
**Electron density around CLA Z 811:**

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



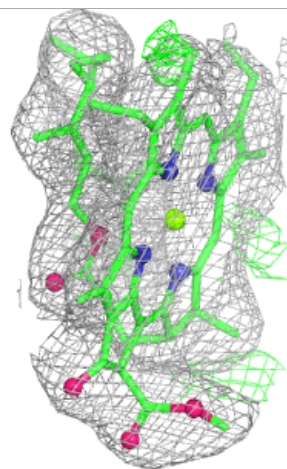
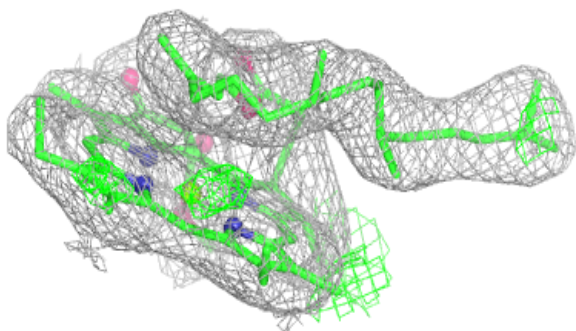
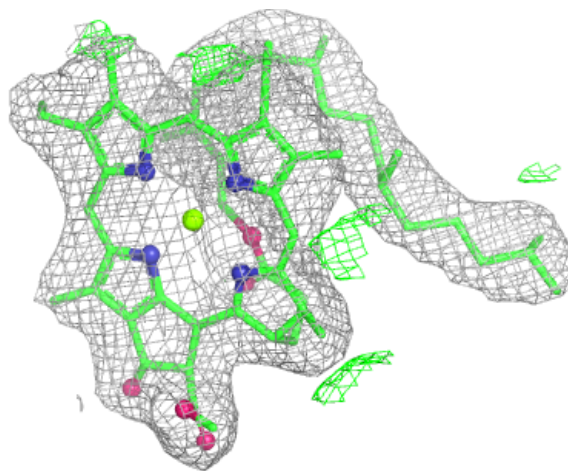
Electron density around CLA Z 812:

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



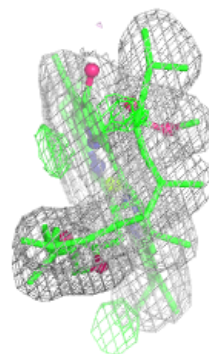
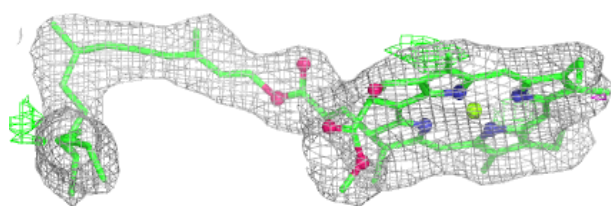
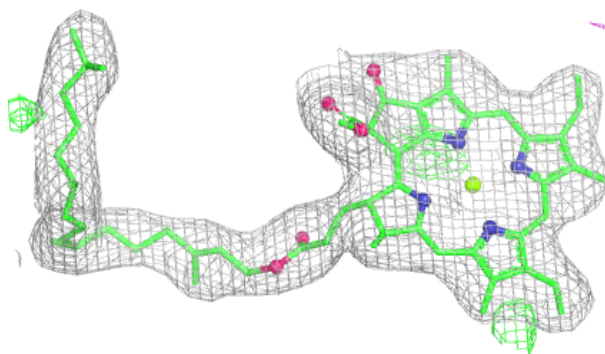
Electron density around CLA H 807:

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

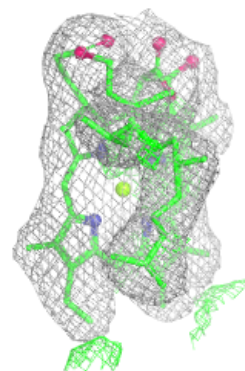
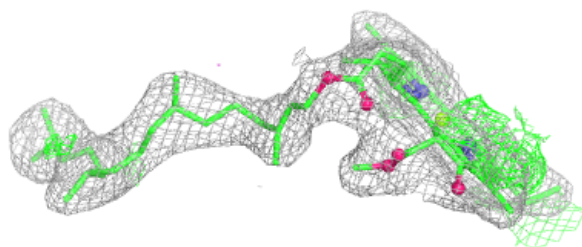
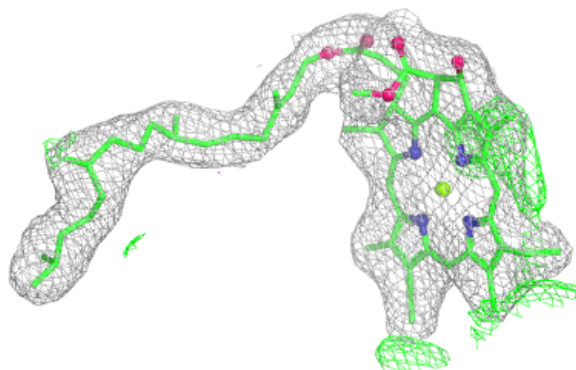


Electron density around CLA B 826:

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

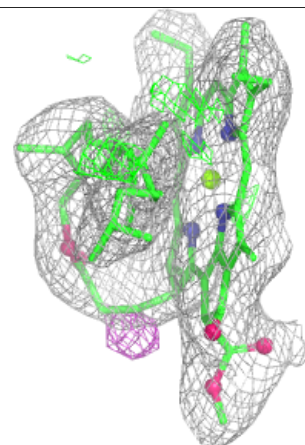
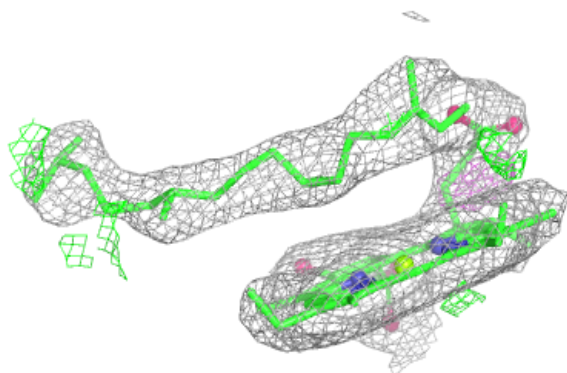
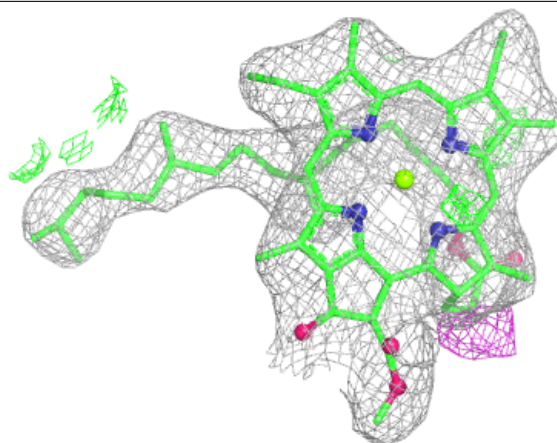
**Electron density around CLA H 809:**

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



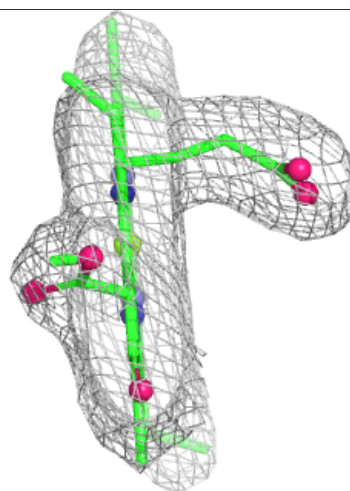
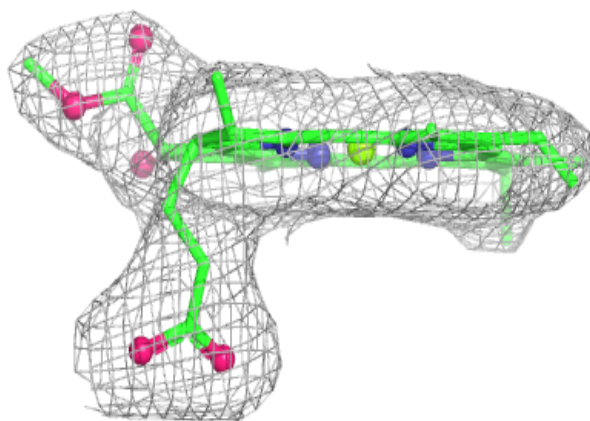
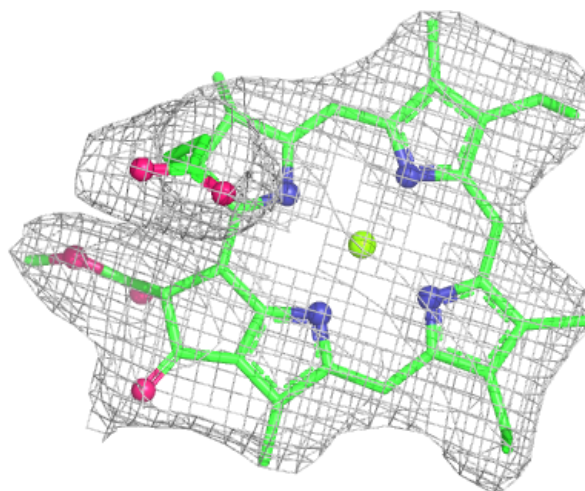
Electron density around CLA B 827:

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



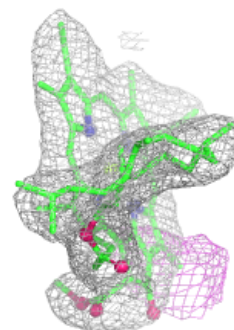
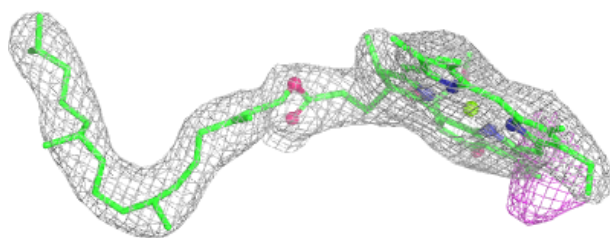
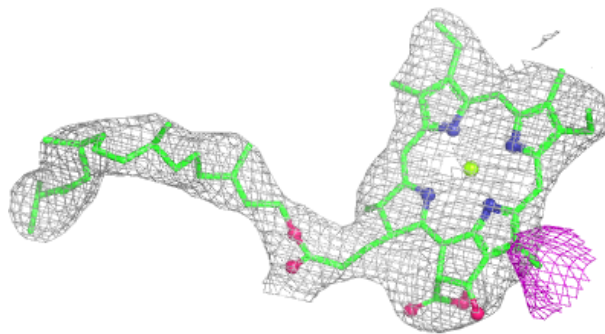
Electron density around CLA H 811:

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



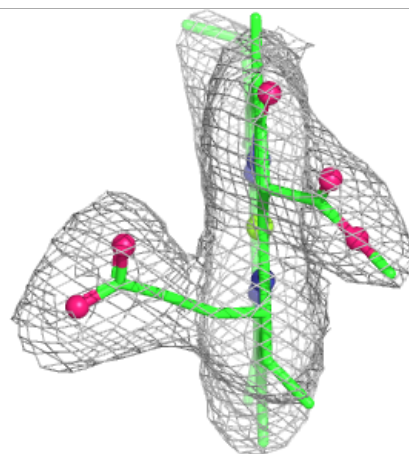
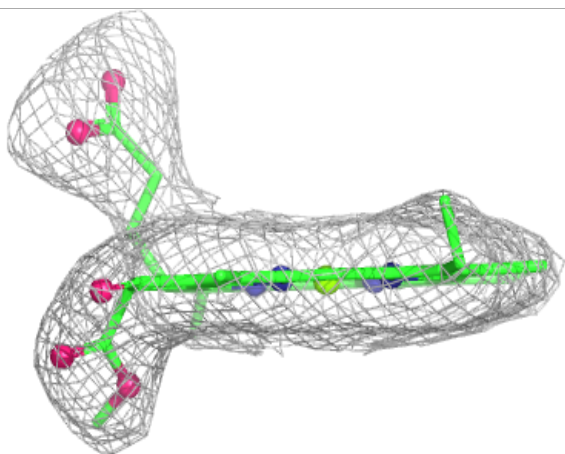
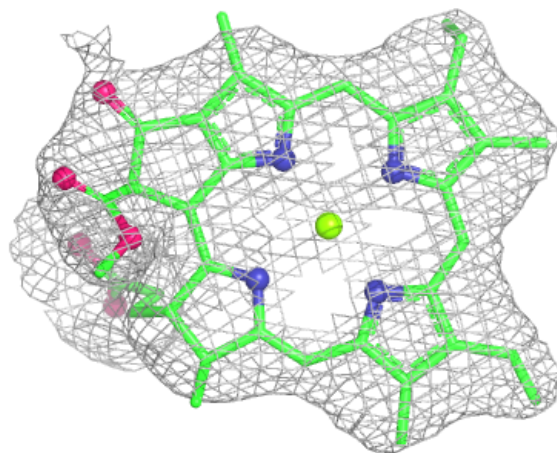
Electron density around CLA H 812:

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



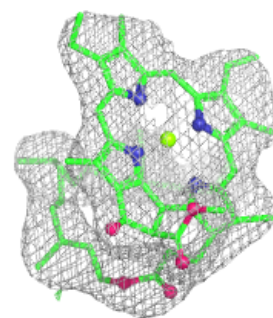
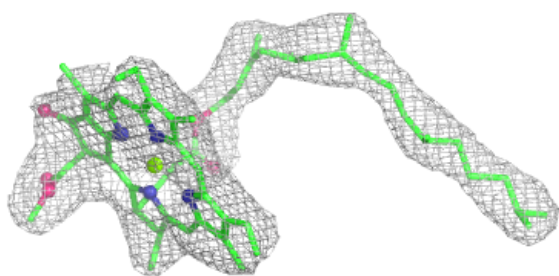
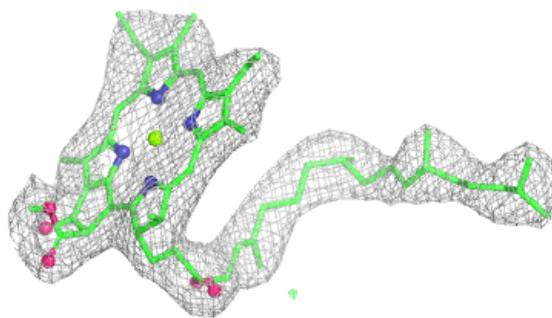
Electron density around CLA Z 819:

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



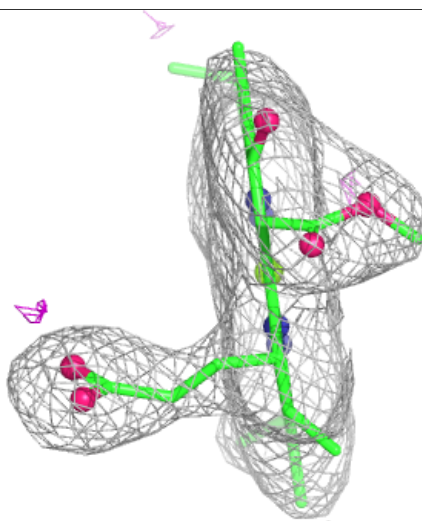
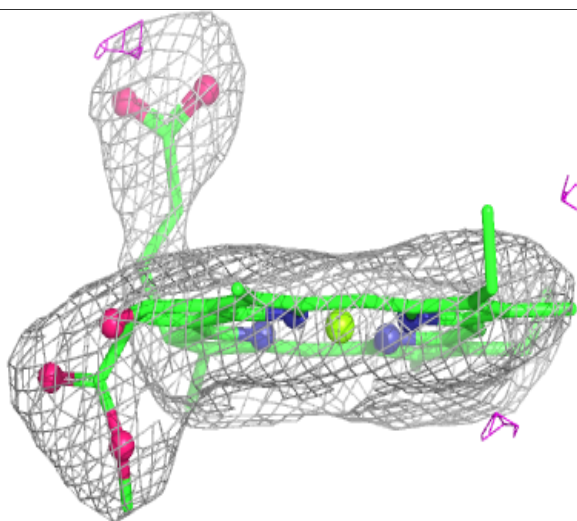
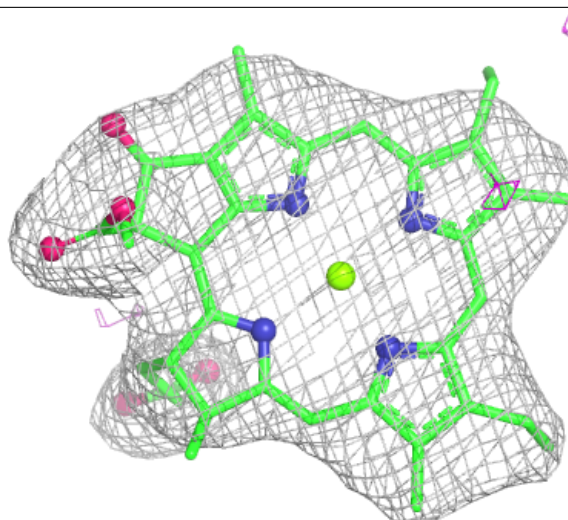
Electron density around CLA H 813:

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



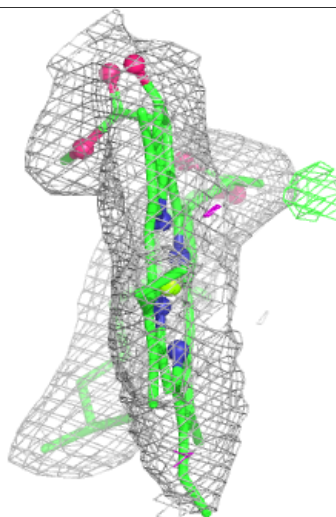
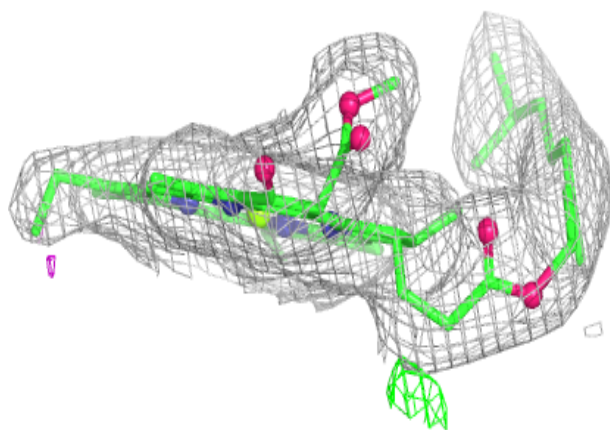
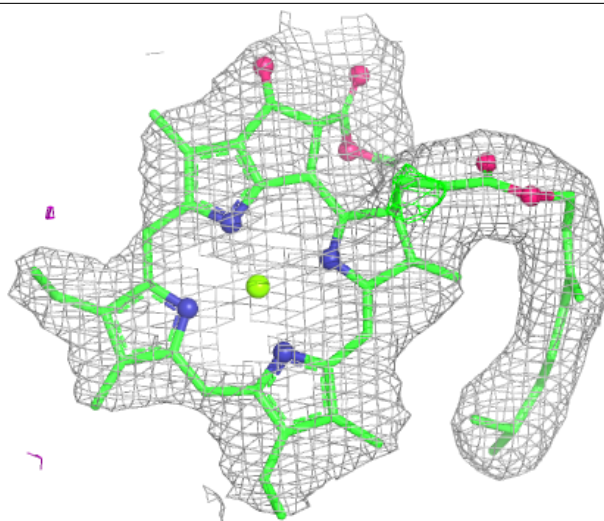
Electron density around CLA H 814:

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



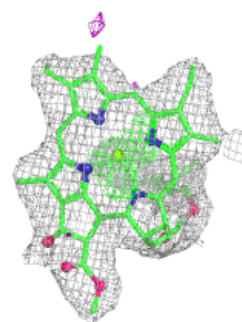
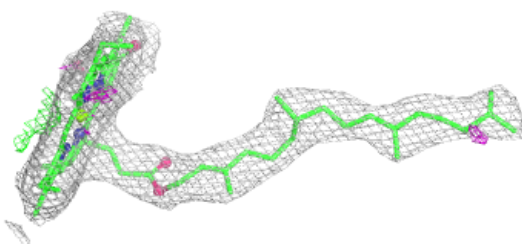
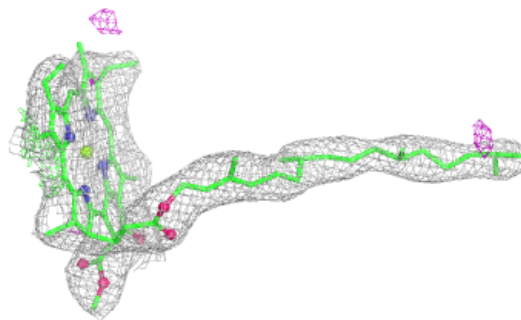
Electron density around CLA Z 822:

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

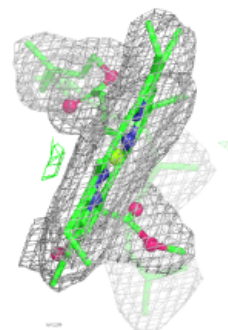
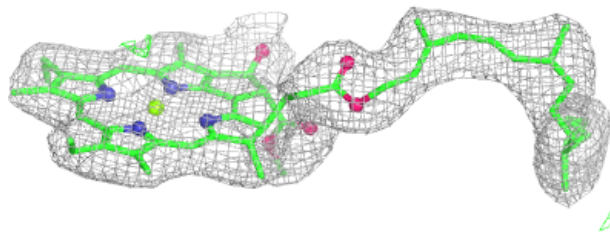
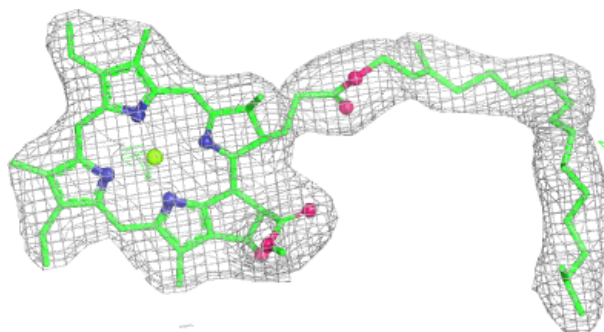


Electron density around CLA B 828:

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

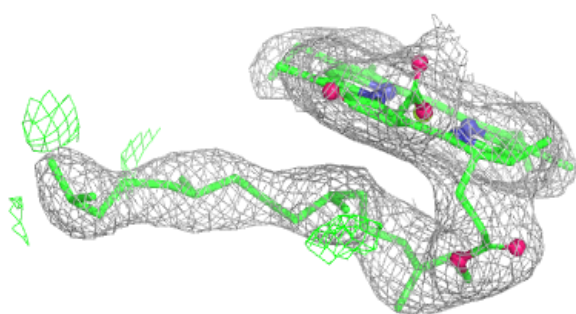
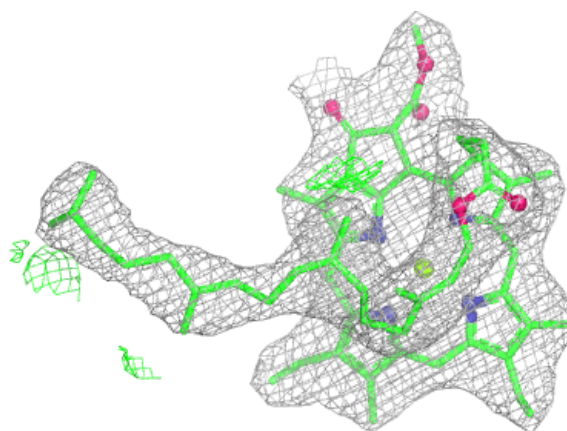
**Electron density around CLA Z 824:**

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

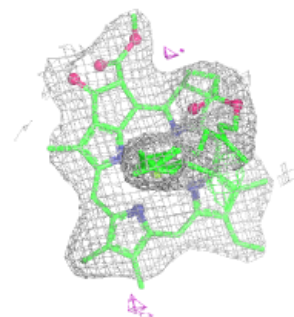
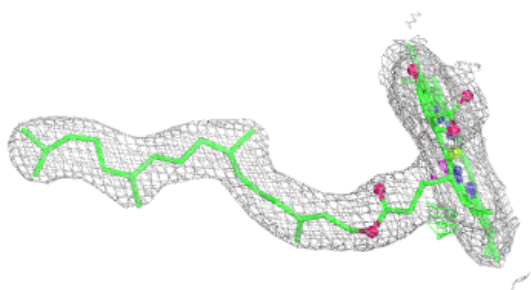
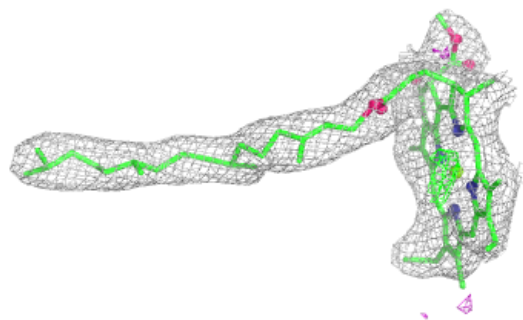


Electron density around CLA Z 825:

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

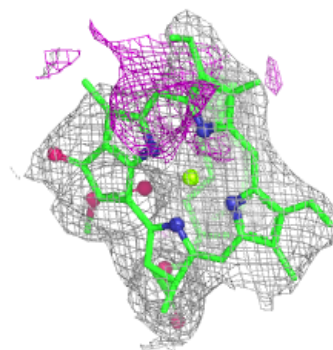
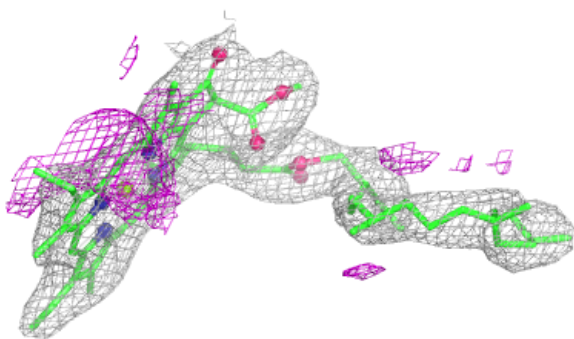
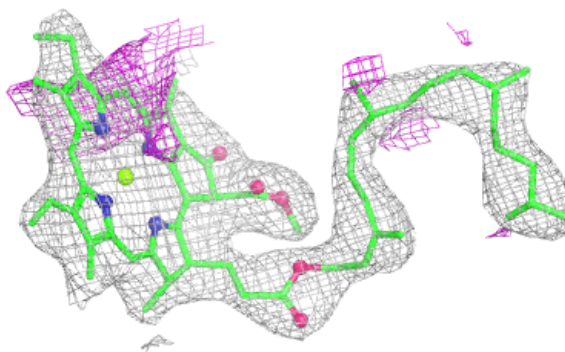
**Electron density around CLA Z 826:**

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

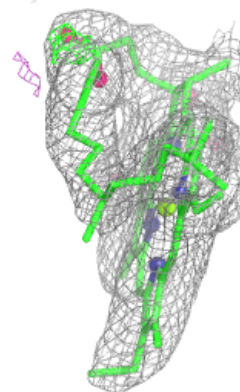
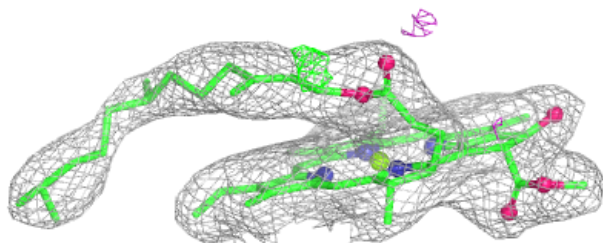
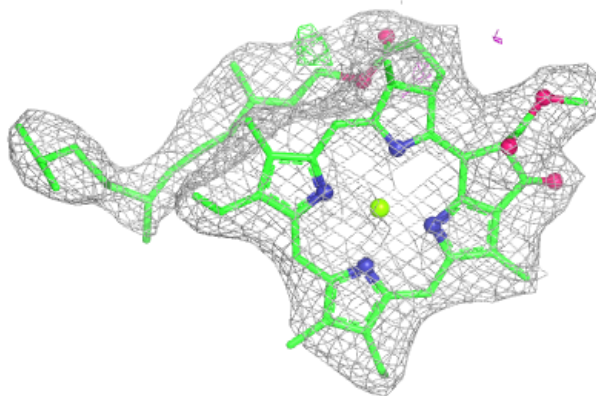


Electron density around CL0 Y 801:

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

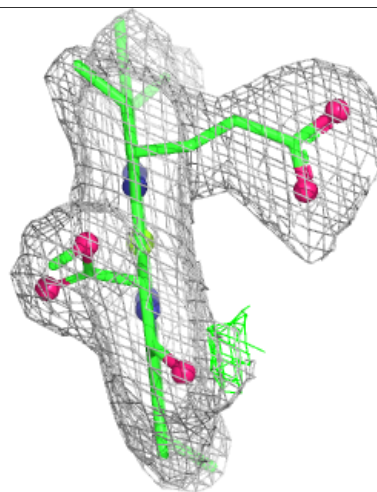
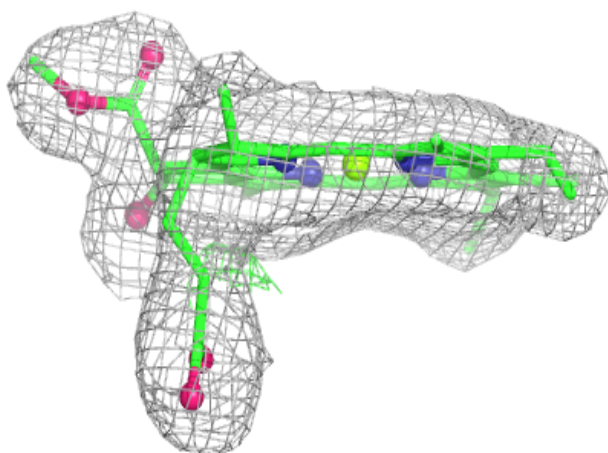
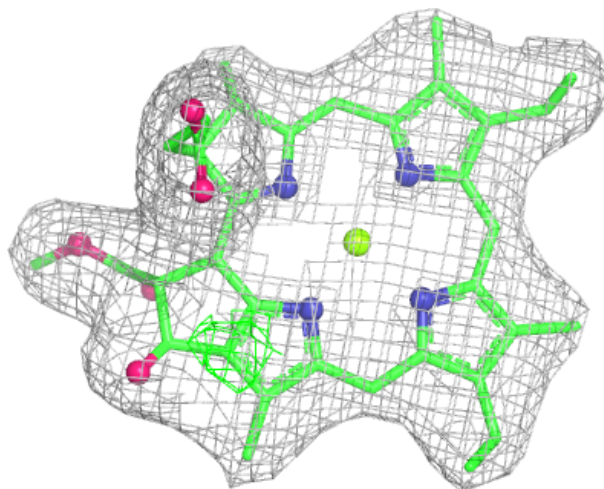
**Electron density around CLA H 817:**

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



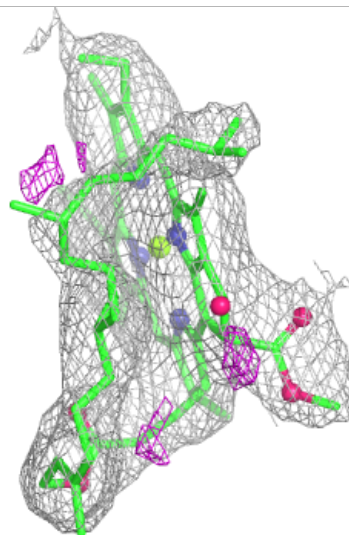
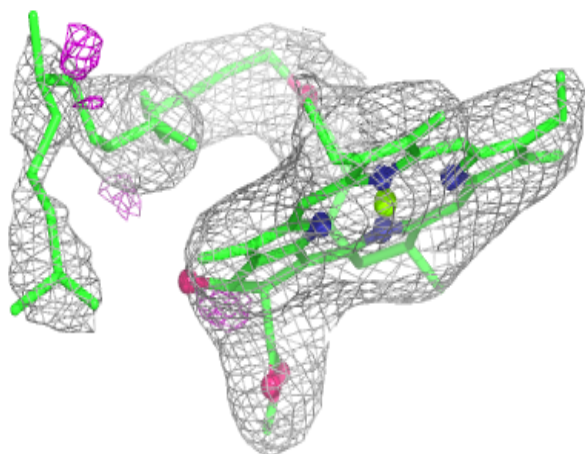
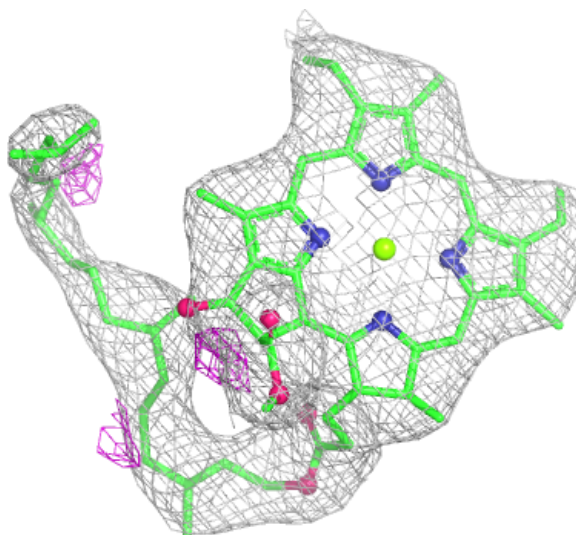
Electron density around CLA Z 829:

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



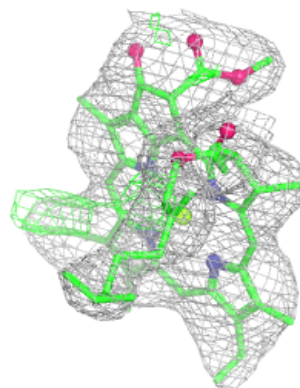
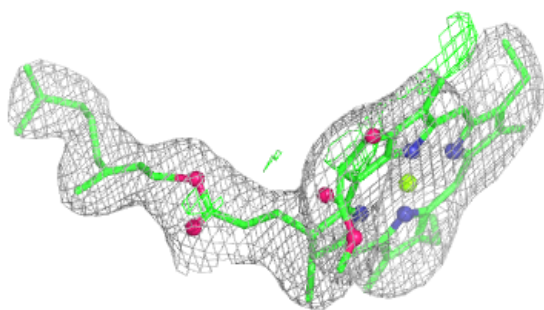
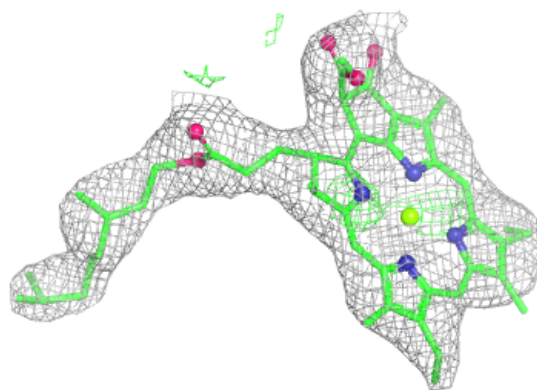
Electron density around CLA Z 830:

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



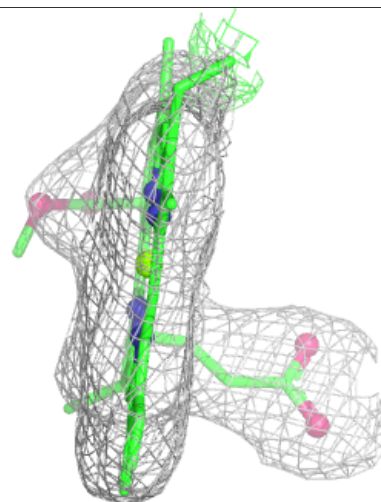
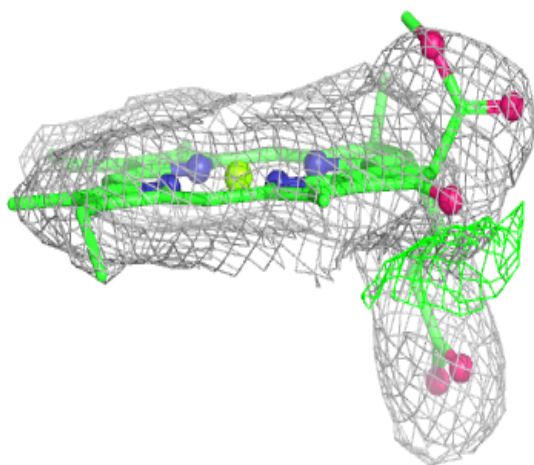
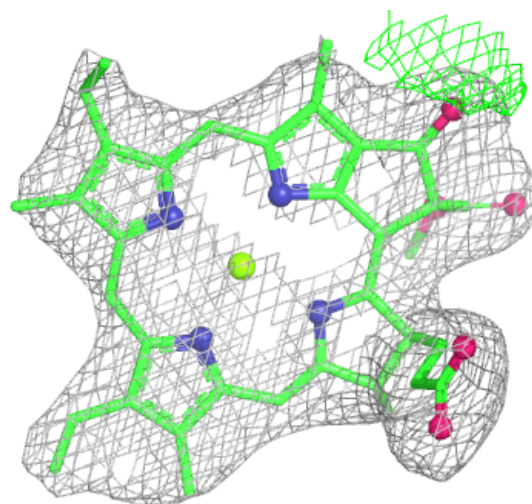
Electron density around CLA Z 831:

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



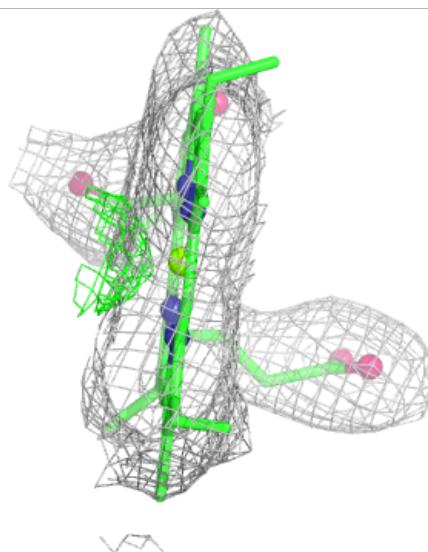
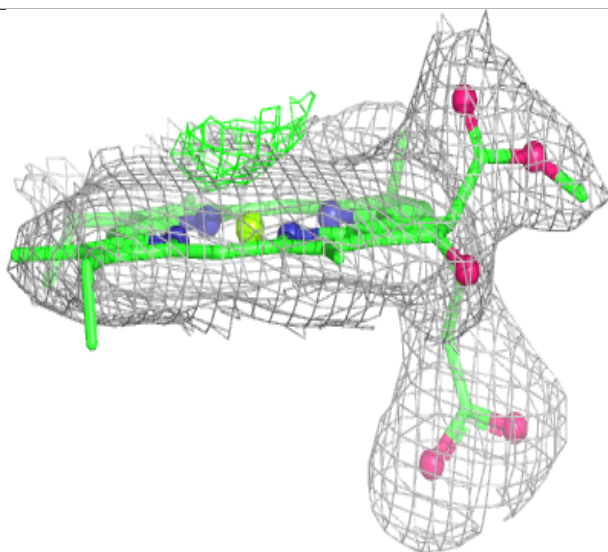
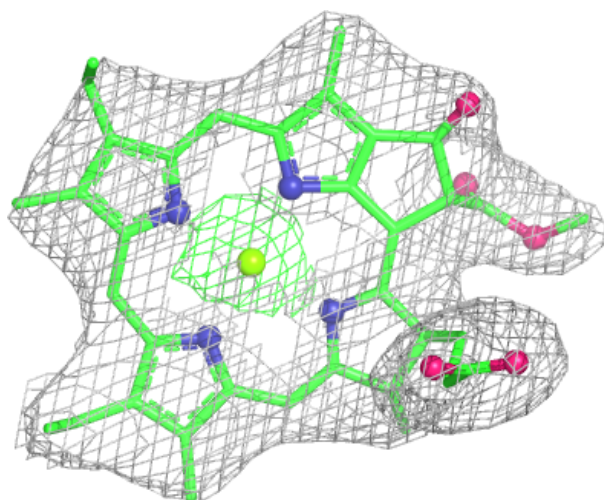
Electron density around CLA Z 832:

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



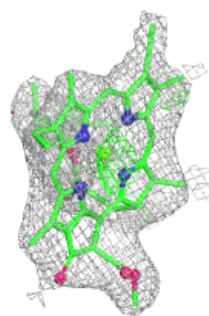
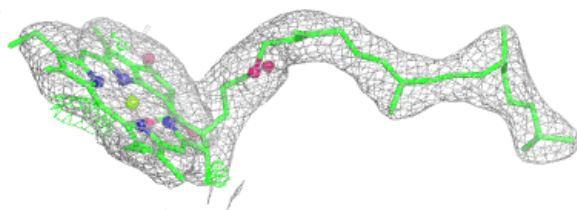
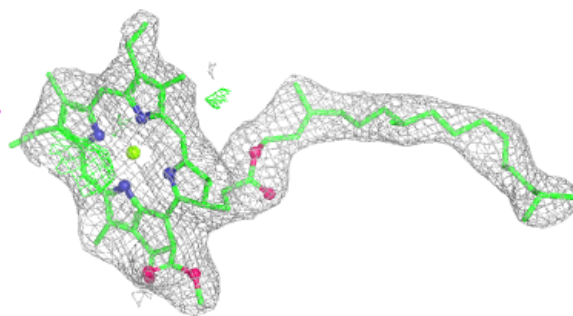
Electron density around CLA Z 833:

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



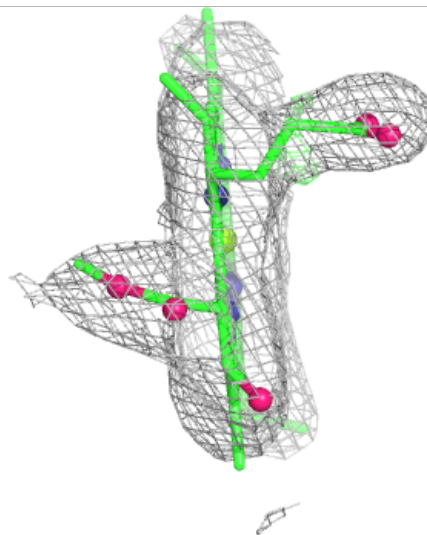
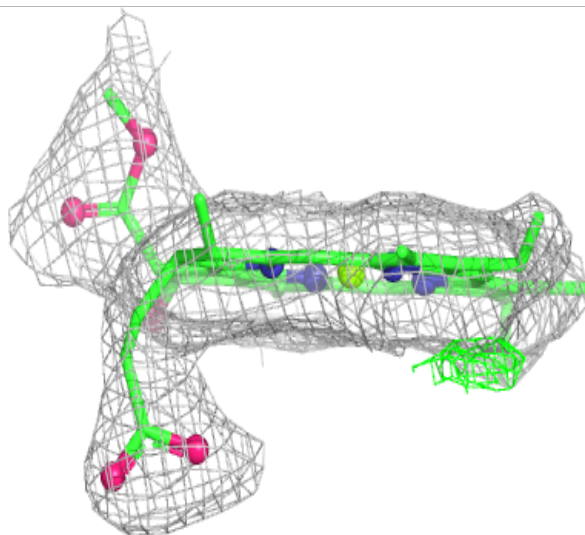
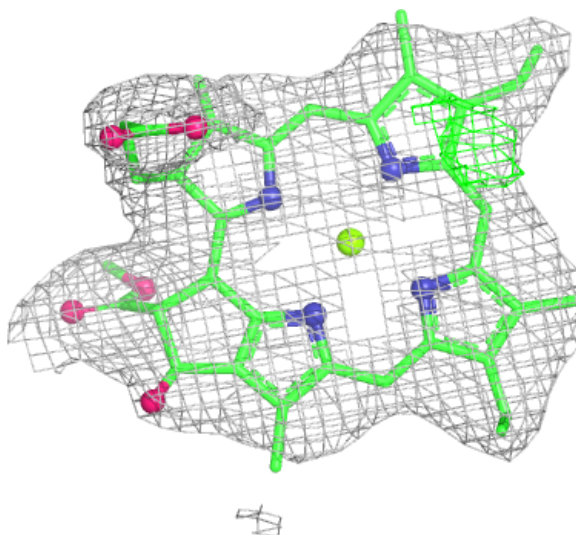
Electron density around CLA A 821:

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



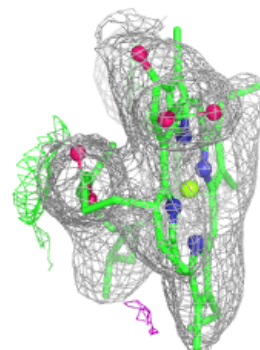
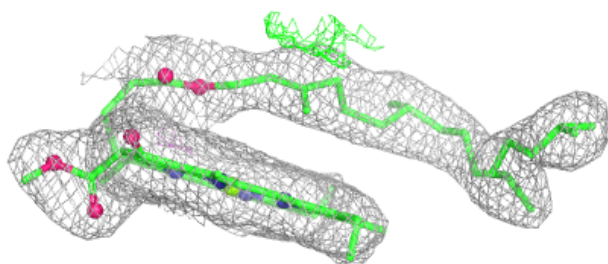
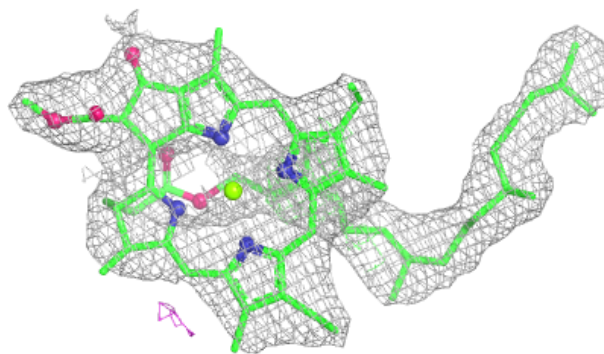
Electron density around CLA H 819:

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



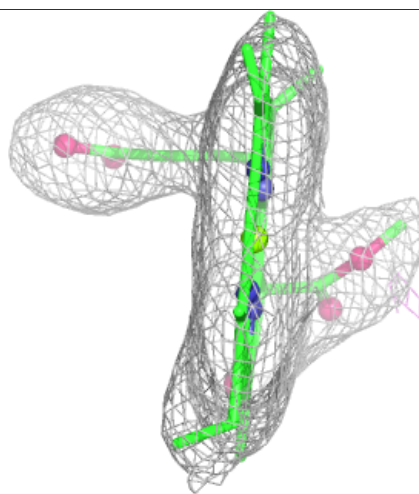
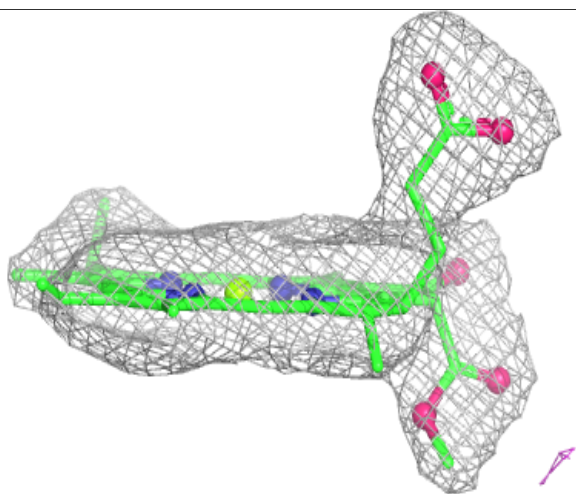
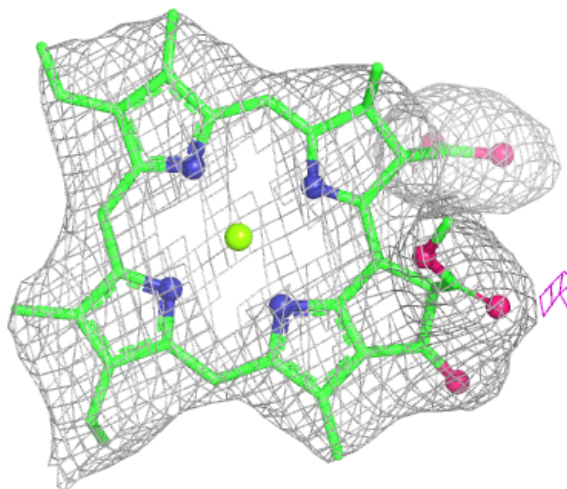
Electron density around CLA Z 836:

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



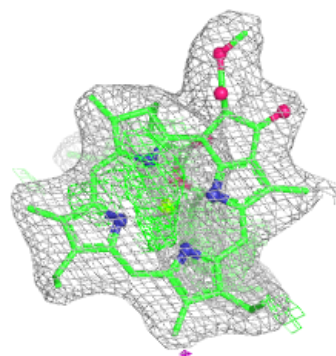
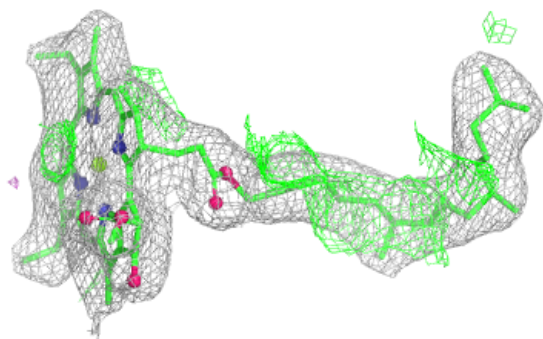
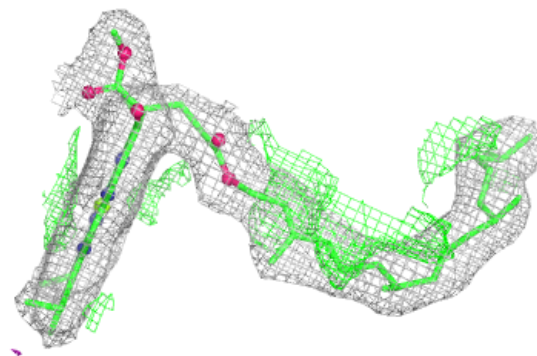
Electron density around CLA H 820:

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

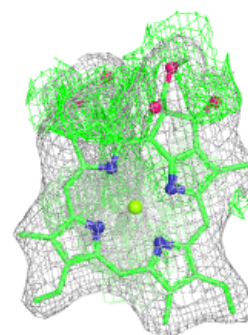
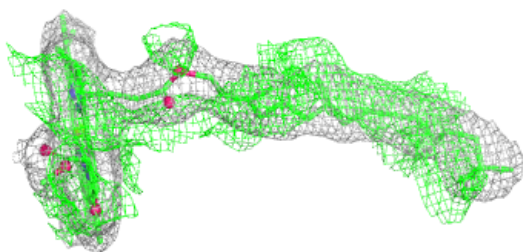
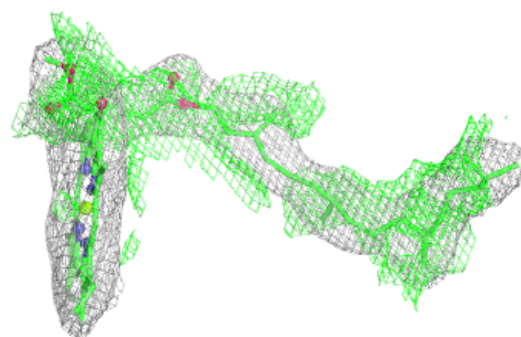


Electron density around CLA Z 838:

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

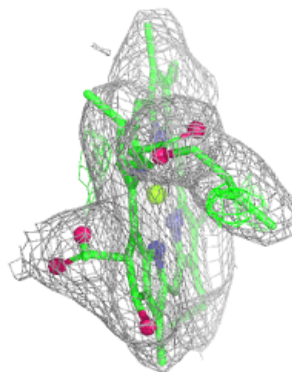
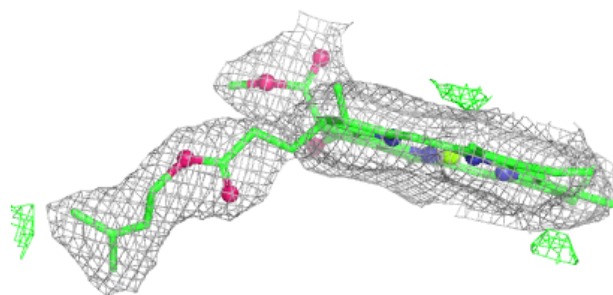
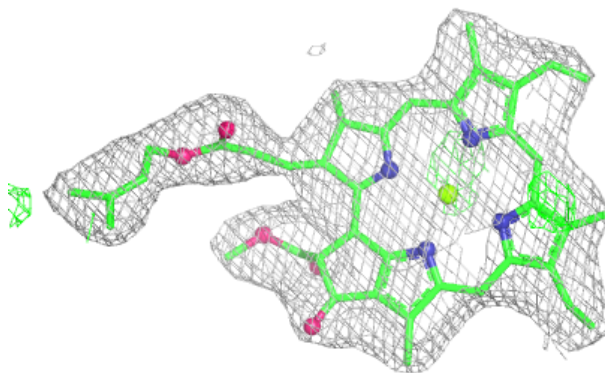
**Electron density around CLA Z 839:**

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



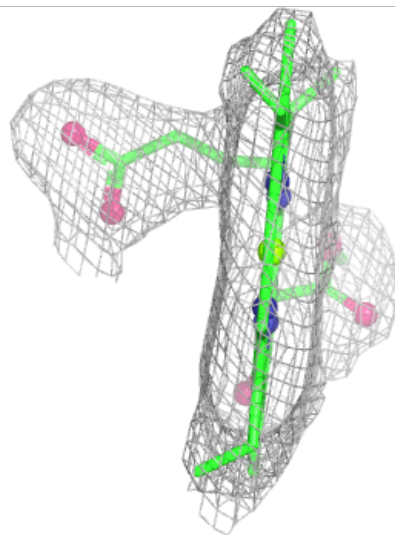
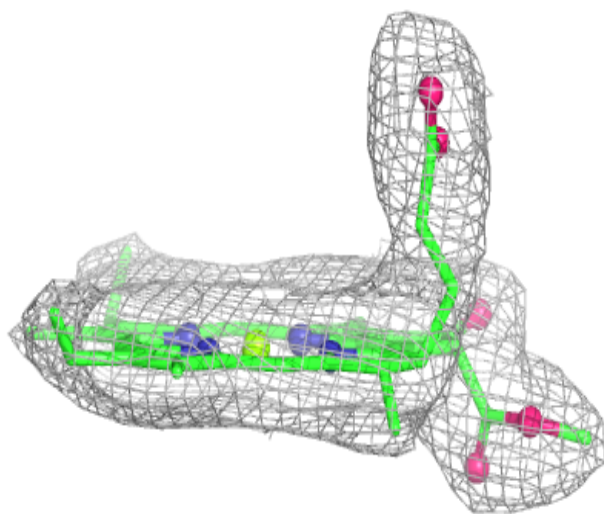
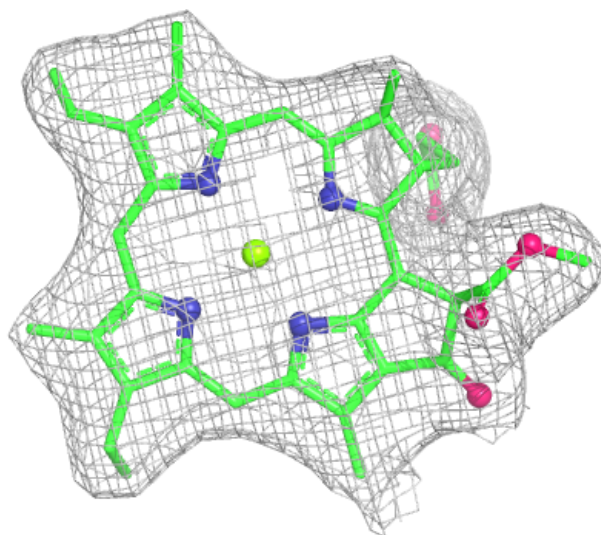
Electron density around CLA d 201:

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



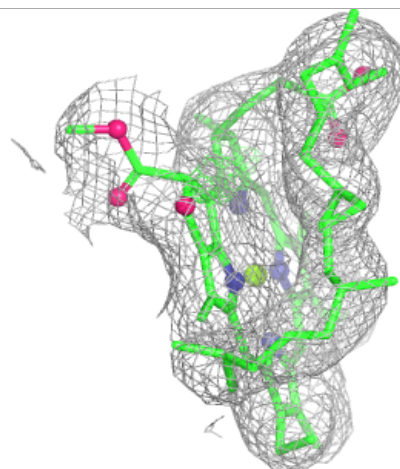
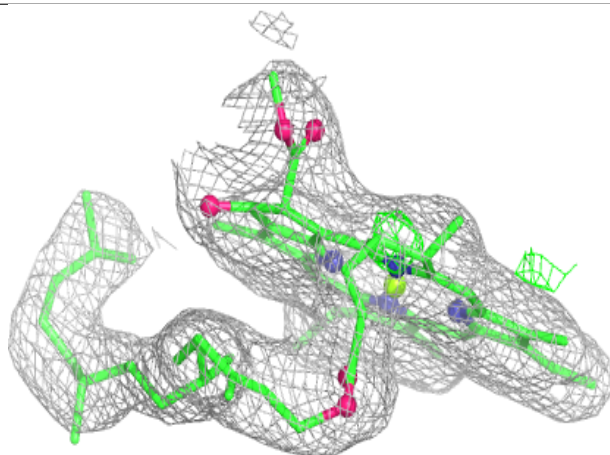
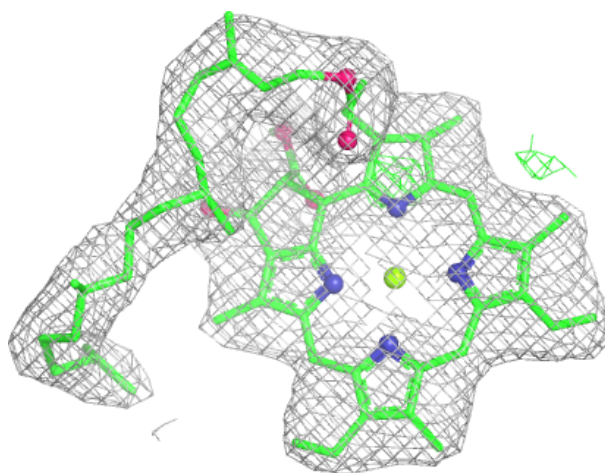
Electron density around CLA B 831:

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



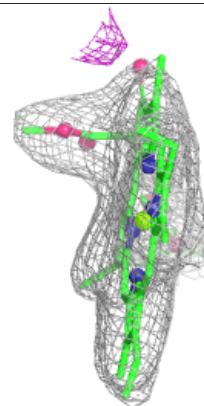
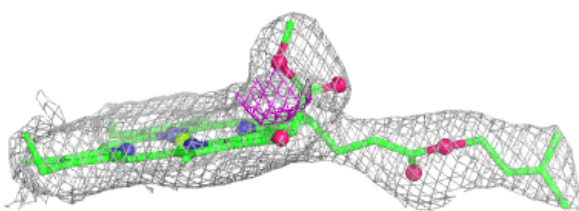
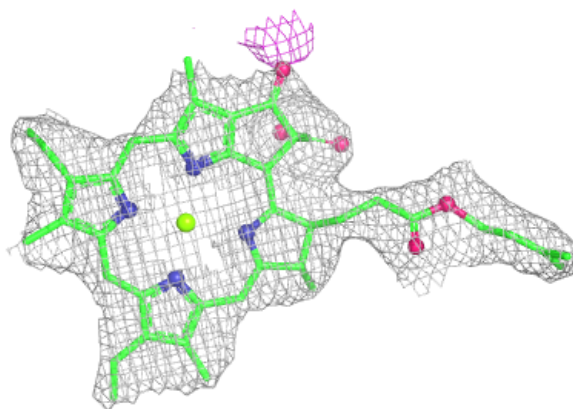
Electron density around CLA B 832:

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



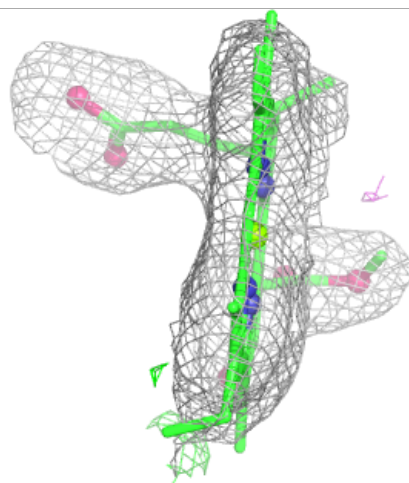
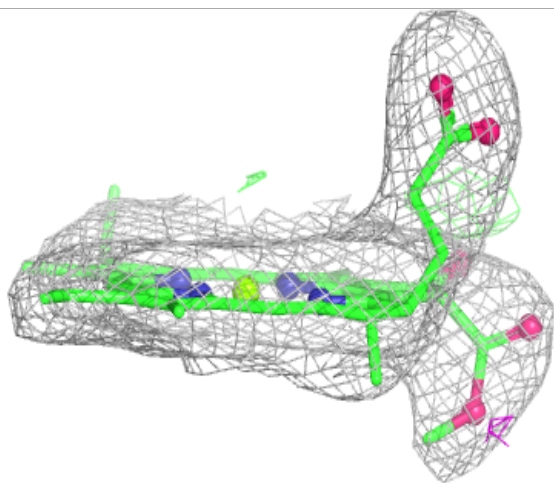
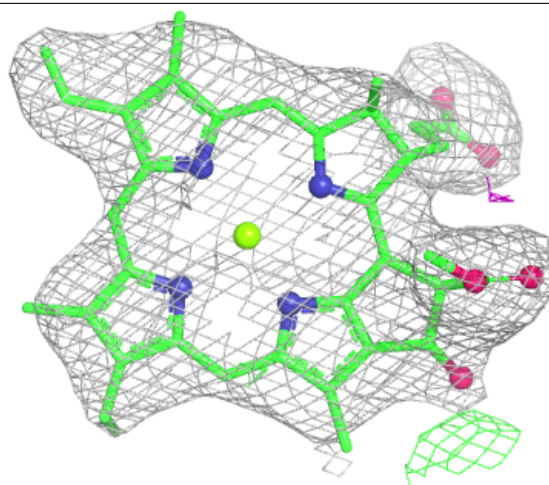
Electron density around CLA A 836:

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



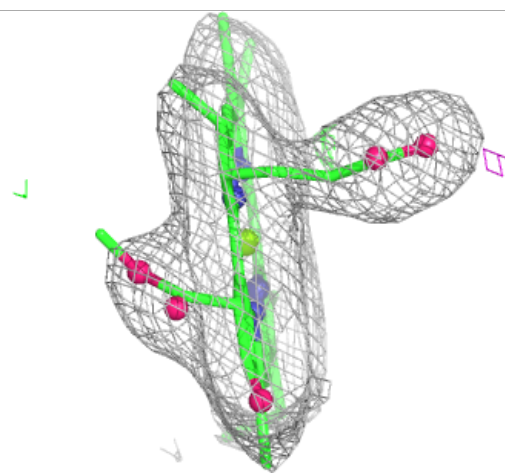
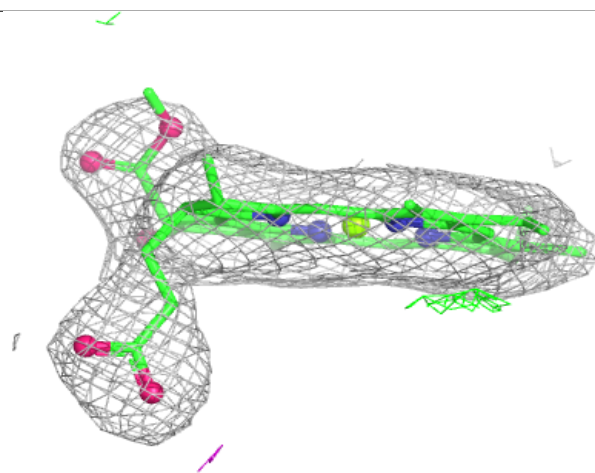
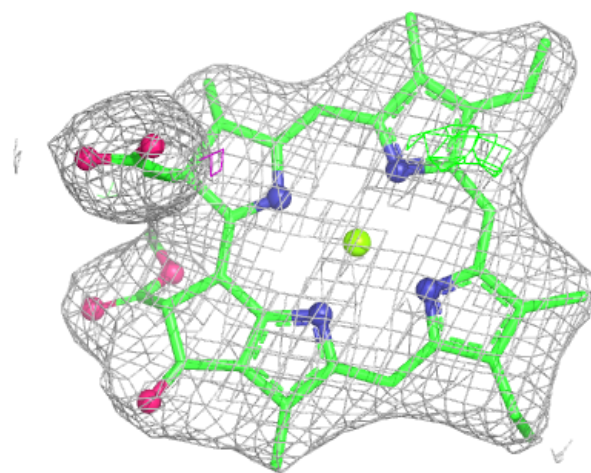
Electron density around CLA B 834:

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



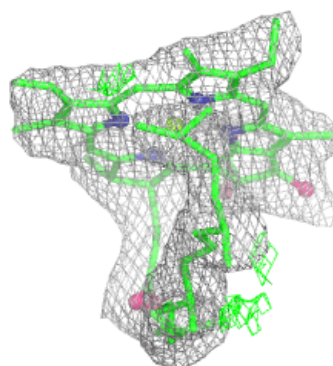
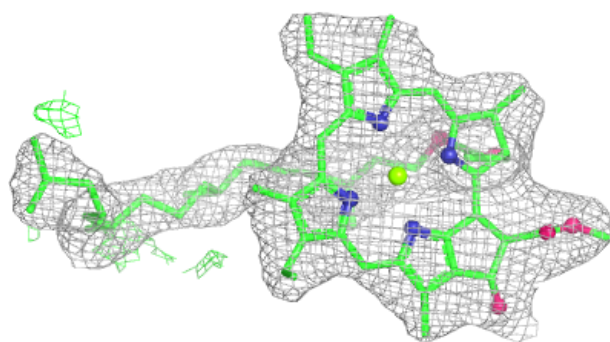
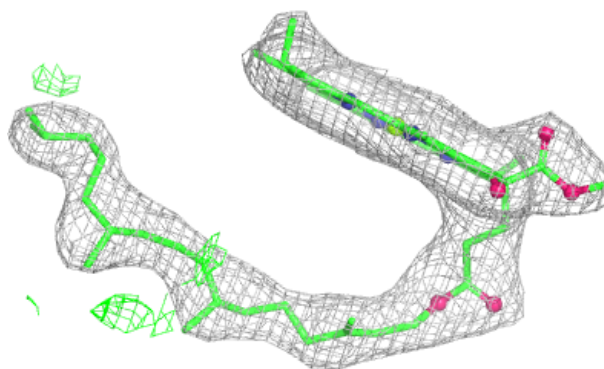
Electron density around CLA g 102:

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



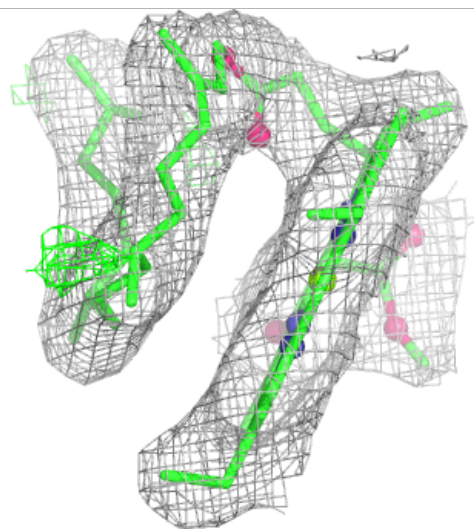
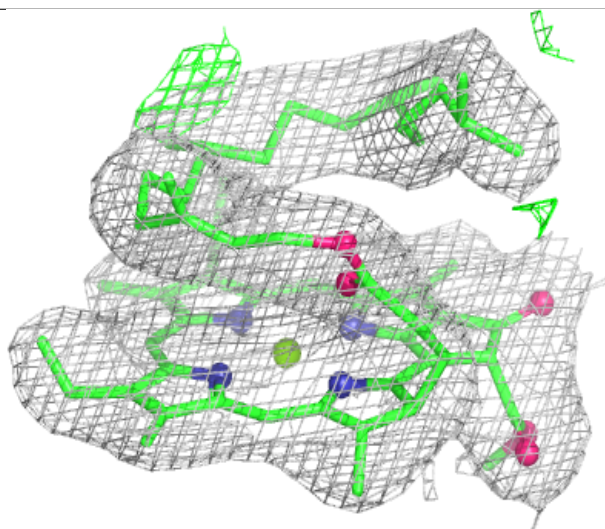
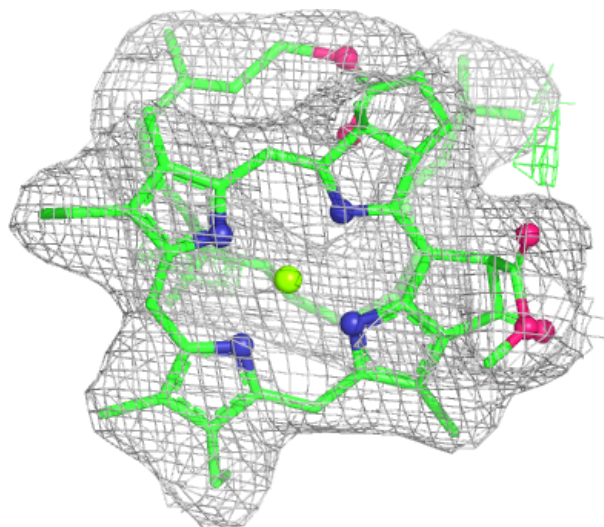
Electron density around CLA h 201:

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



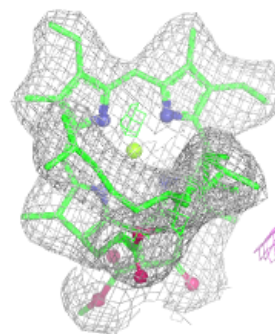
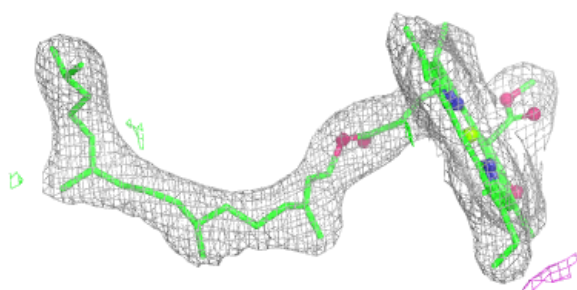
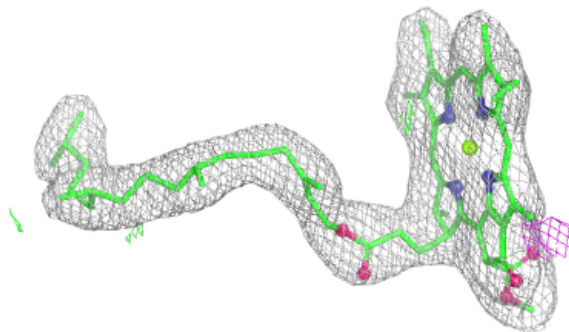
Electron density around CLA h 205:

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

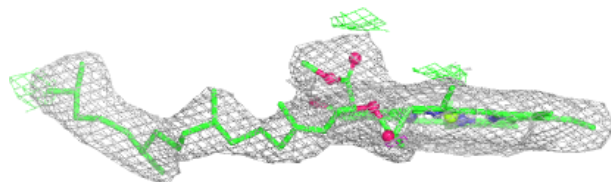
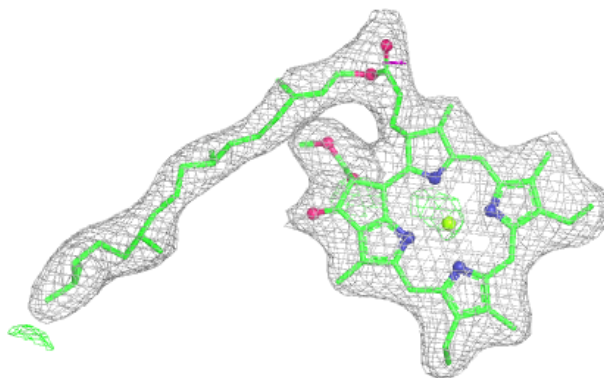


Electron density around CLA h 206:

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

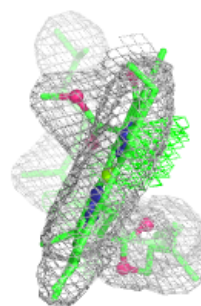
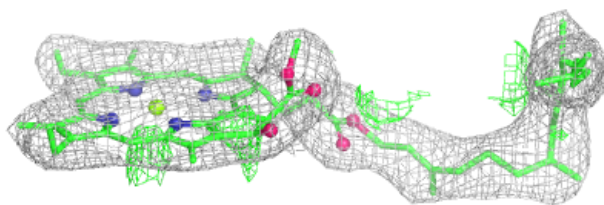
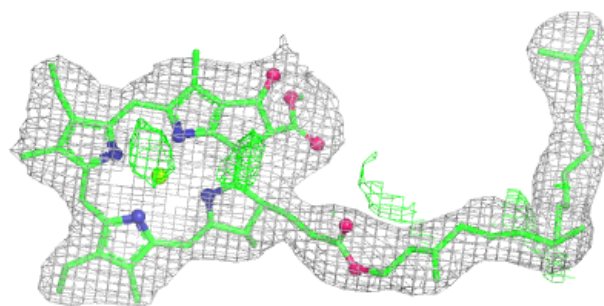
**Electron density around CLA h 207:**

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



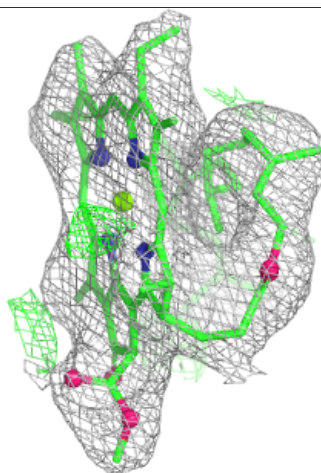
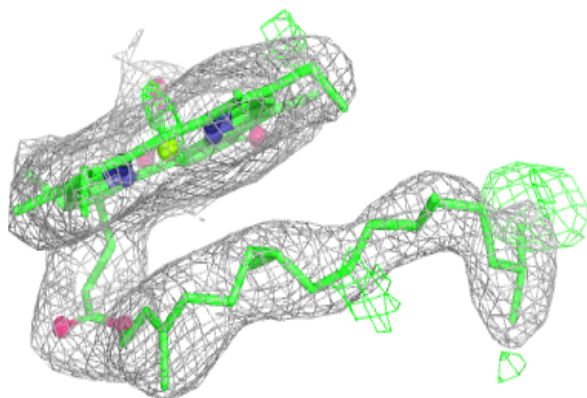
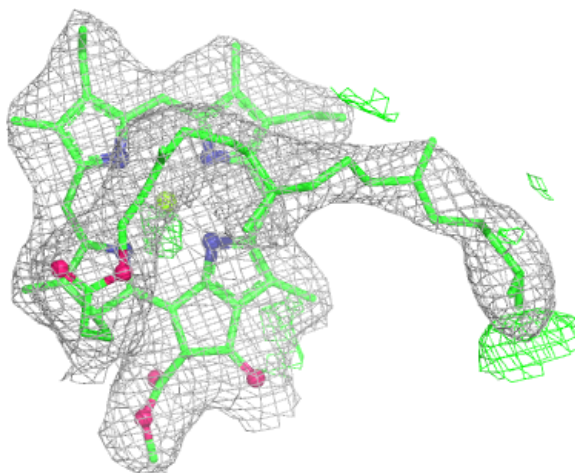
Electron density around CLA H 825:

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



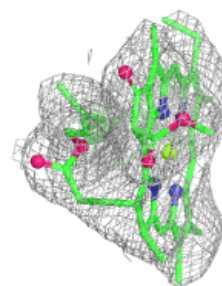
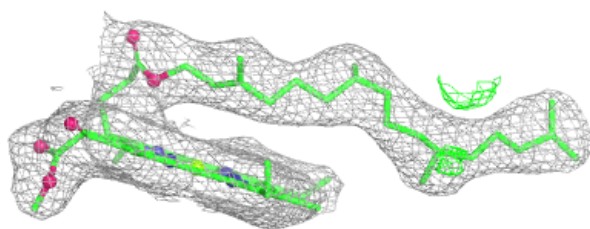
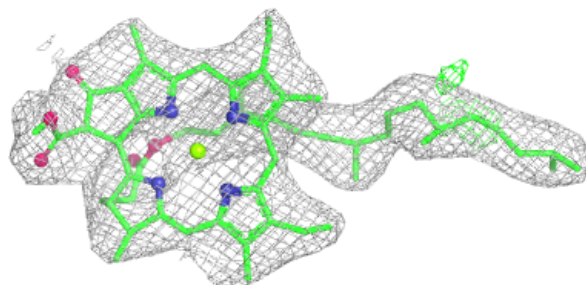
Electron density around CLA H 826:

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

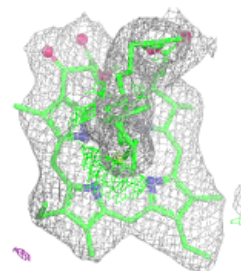
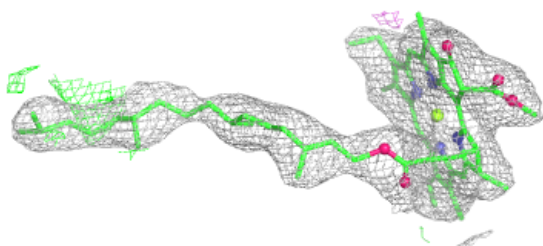
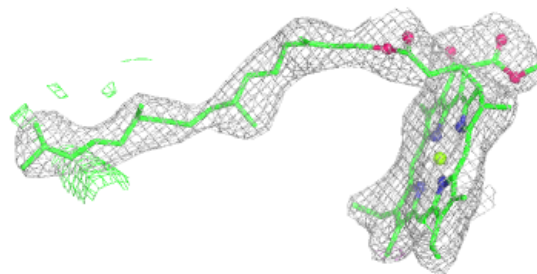


Electron density around CLA A 837:

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

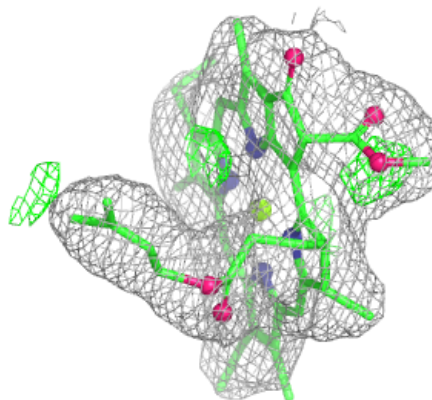
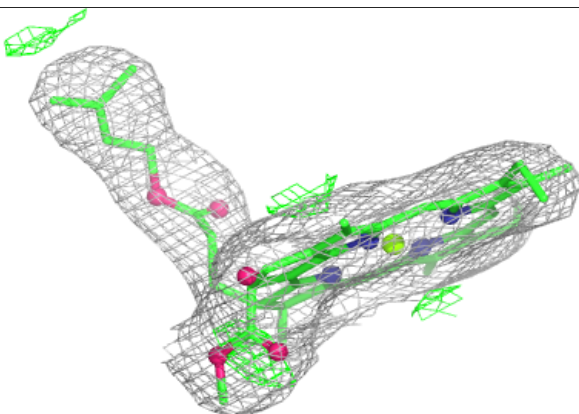
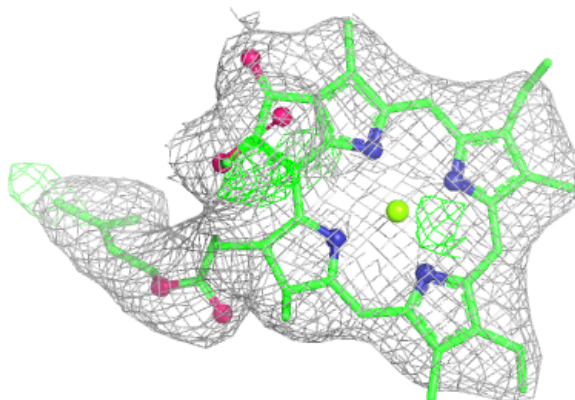
**Electron density around CLA H 828:**

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

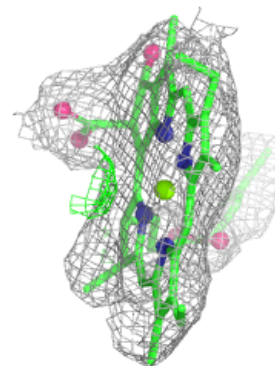
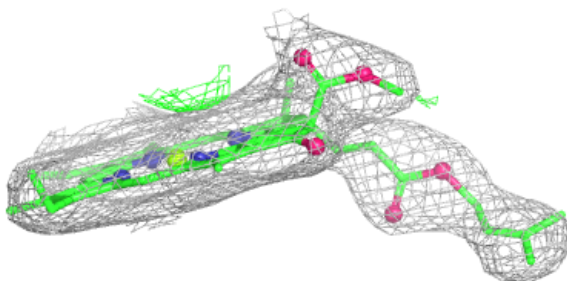
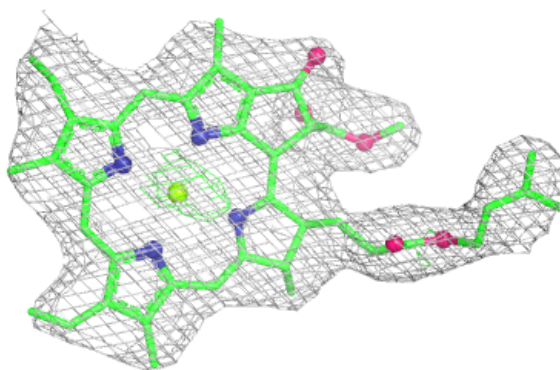


Electron density around CLA A 838:

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

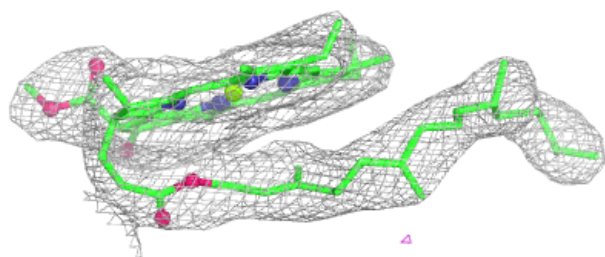
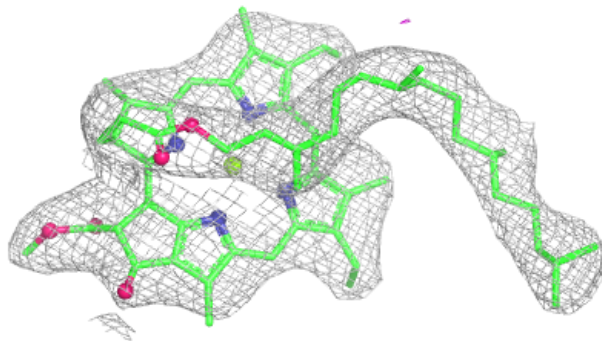
**Electron density around CLA A 839:**

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



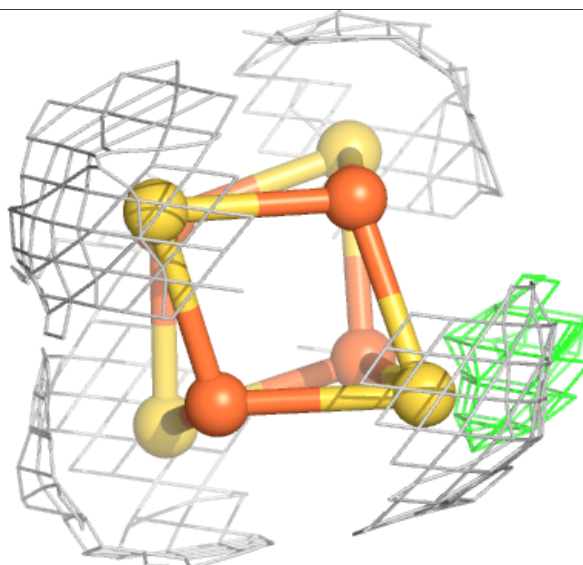
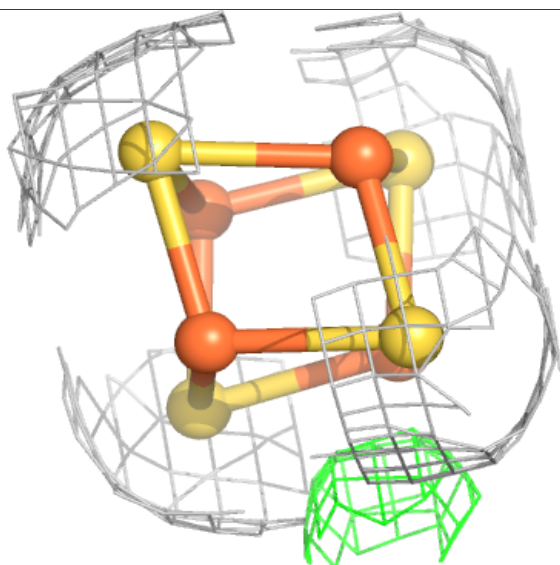
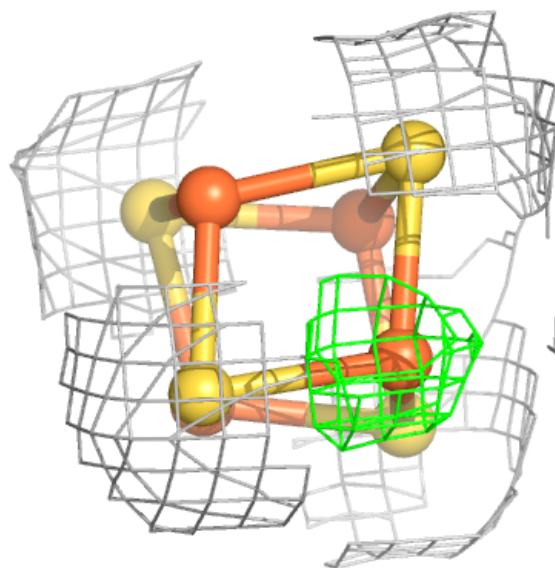
Electron density around CLA B 838:

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



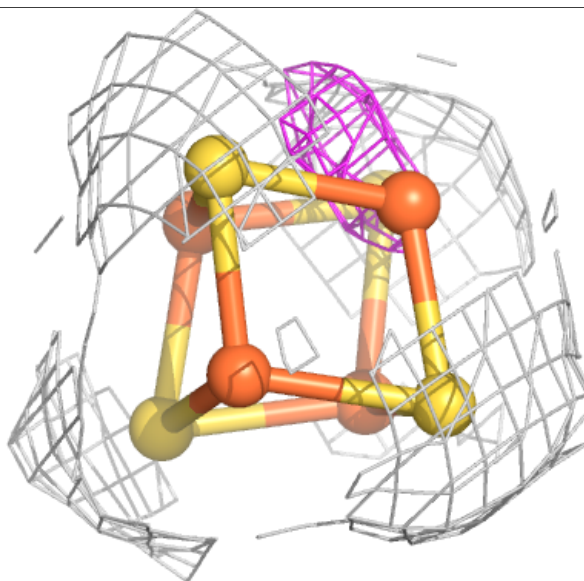
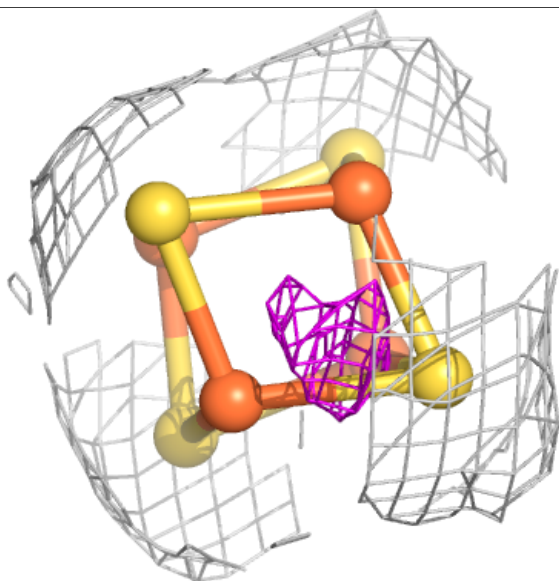
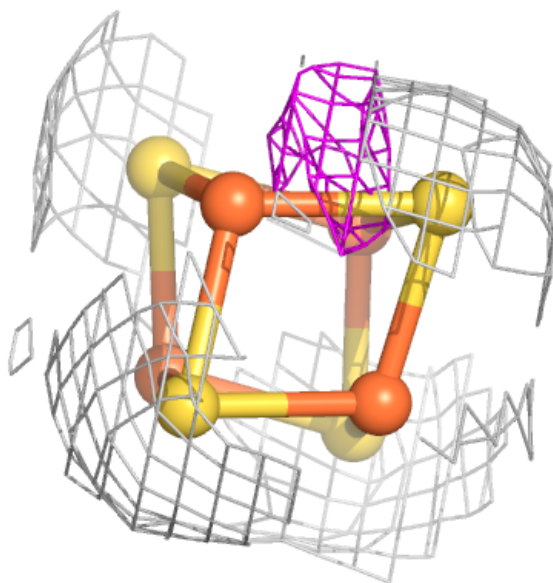
Electron density around SF4 A 844:

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



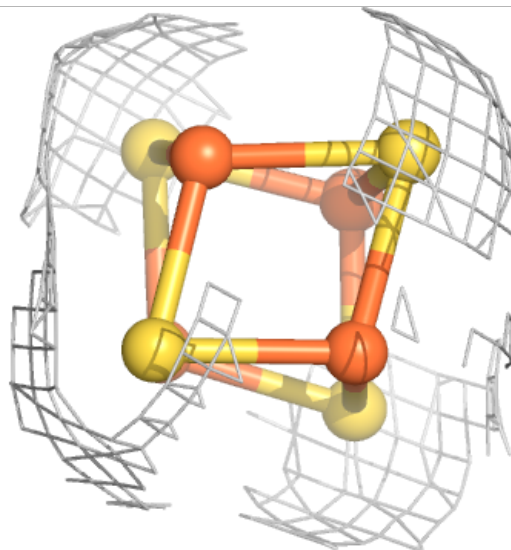
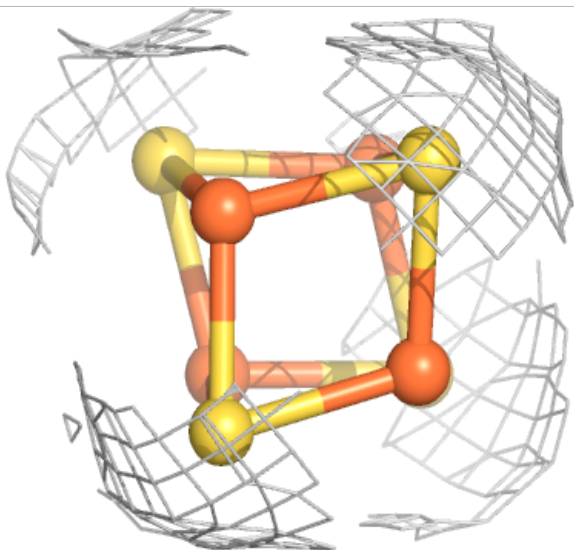
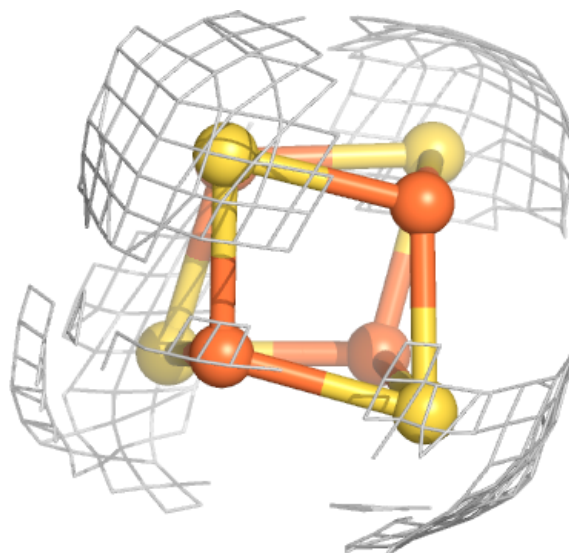
Electron density around SF4 C 101:

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



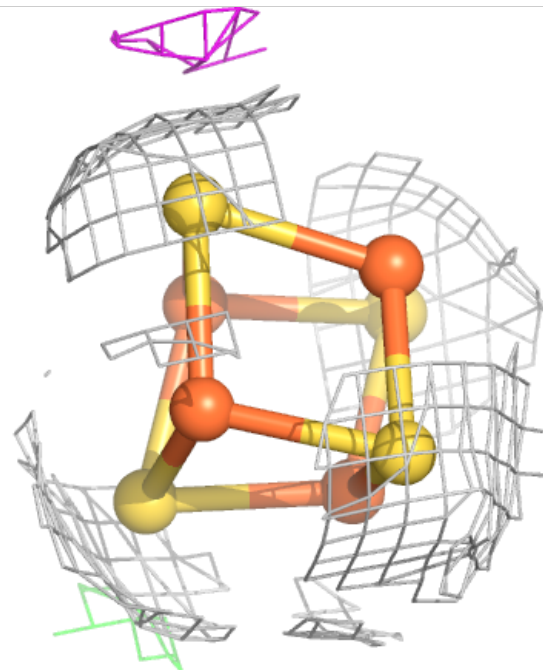
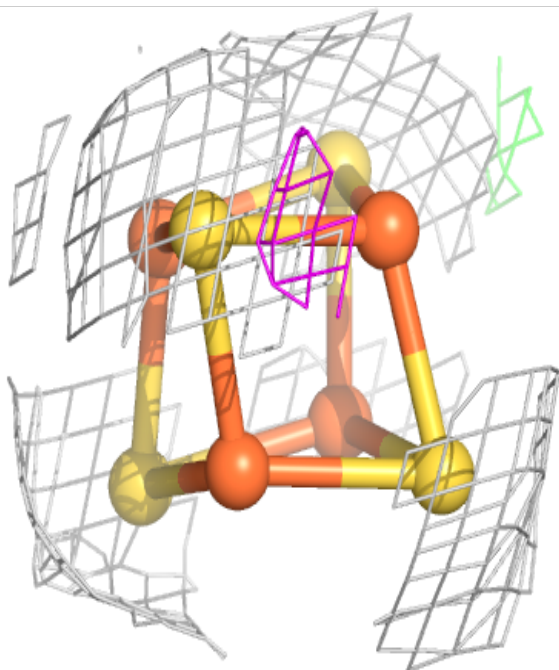
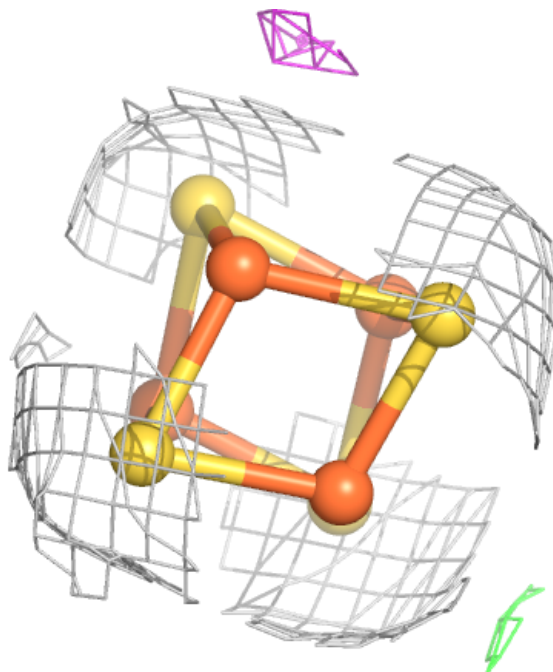
Electron density around SF4 C 102:

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



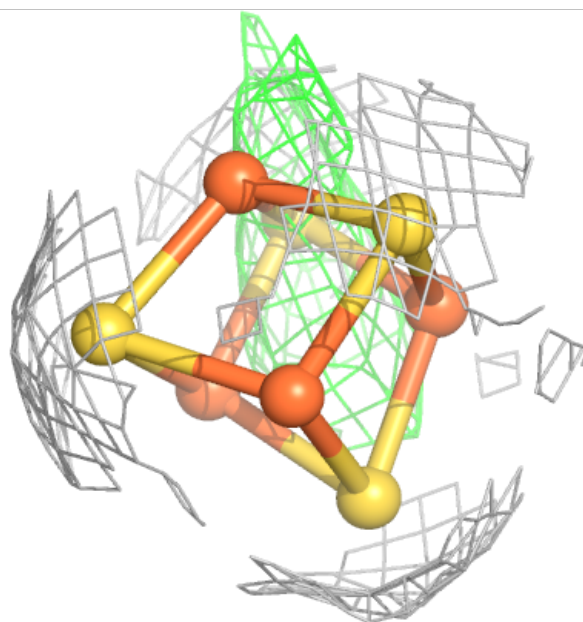
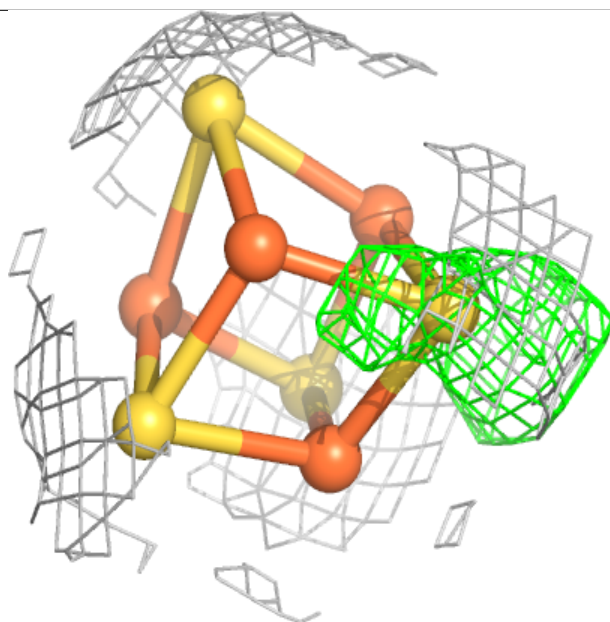
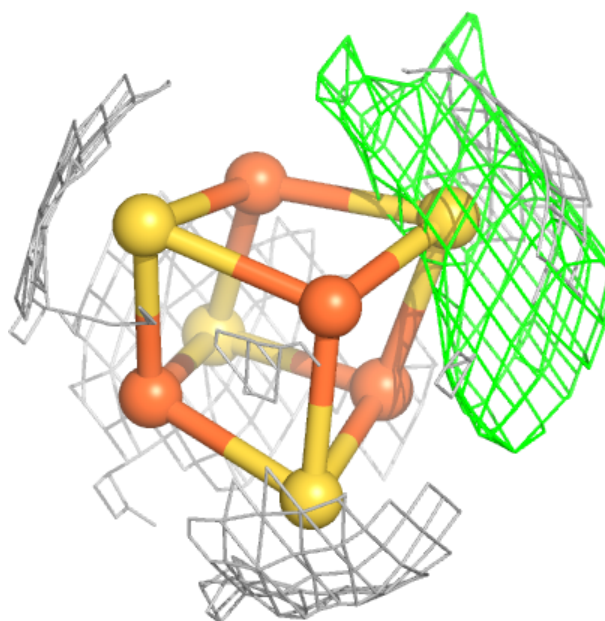
Electron density around SF4 G 845:

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



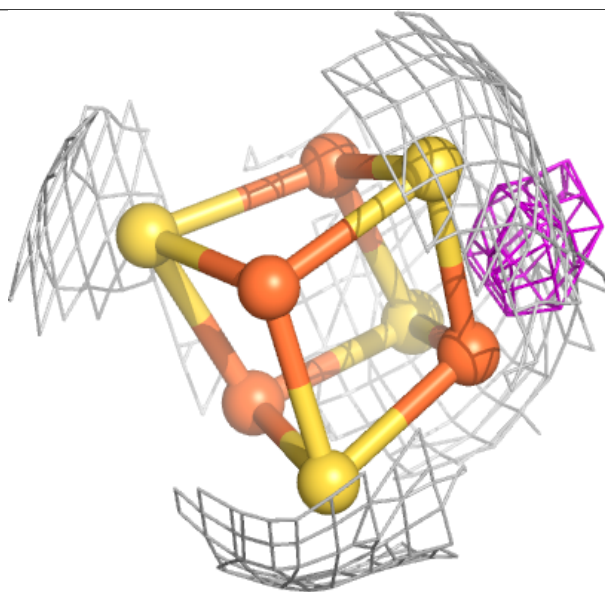
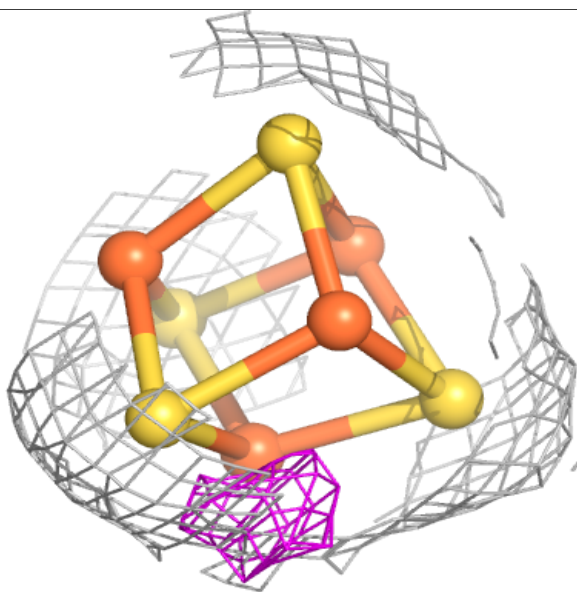
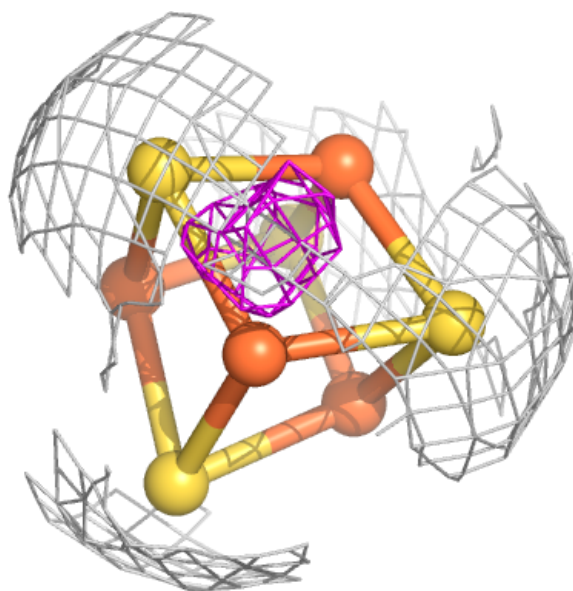
Electron density around SF4 N 101:

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



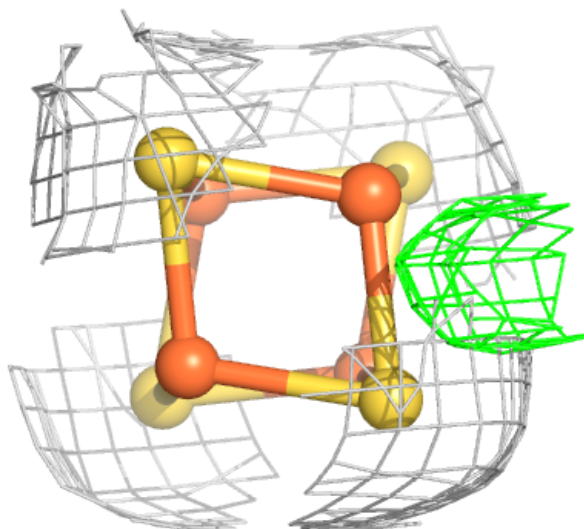
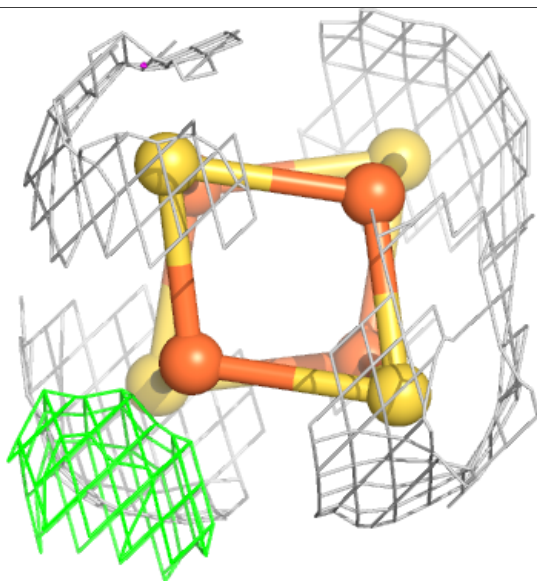
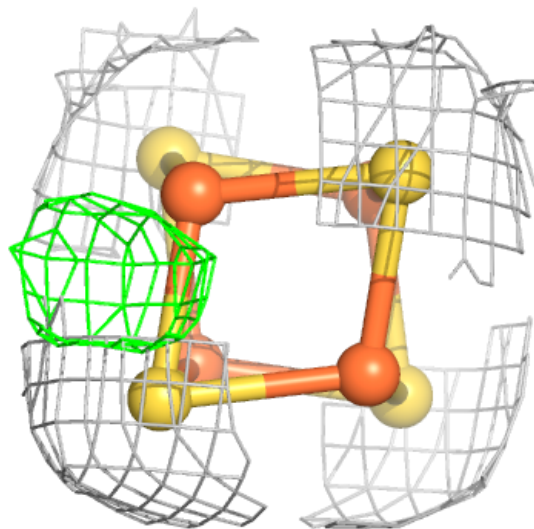
Electron density around SF4 N 102:

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



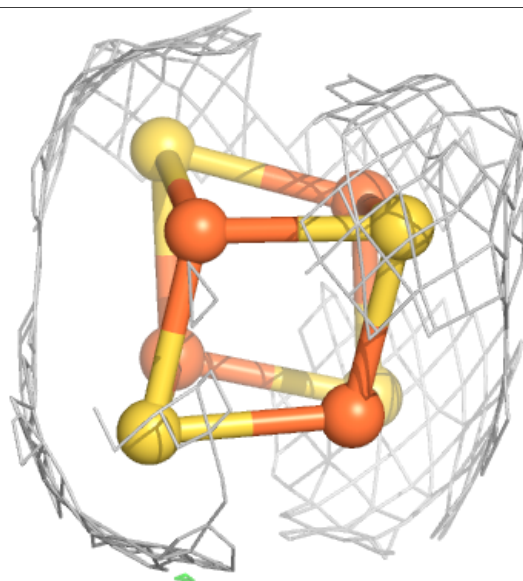
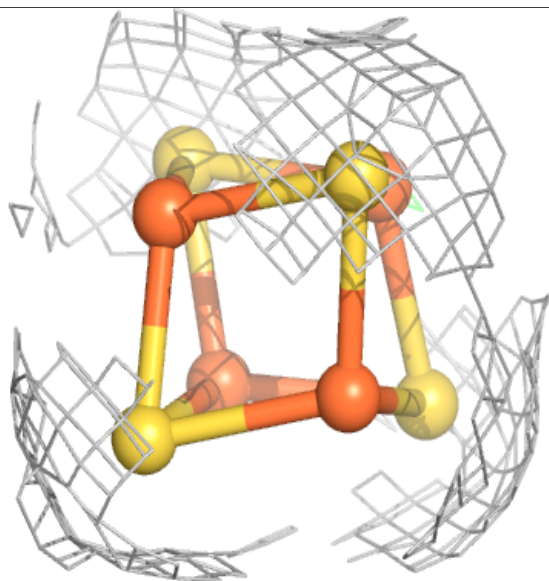
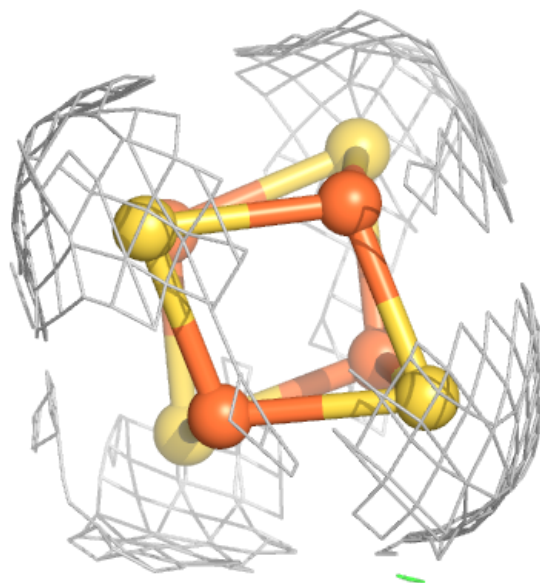
Electron density around SF4 Y 845:

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



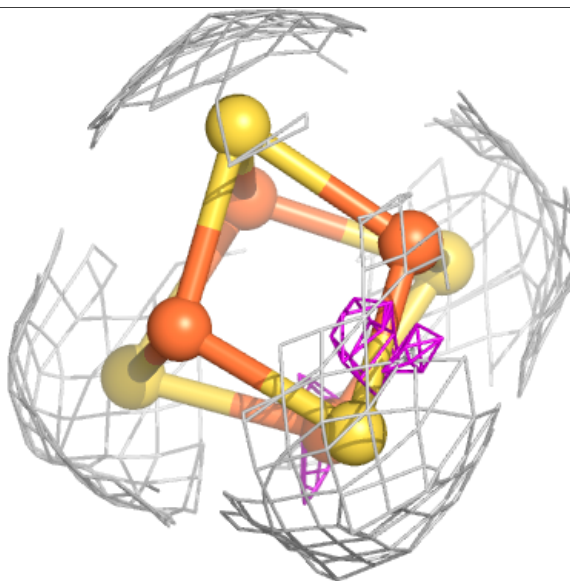
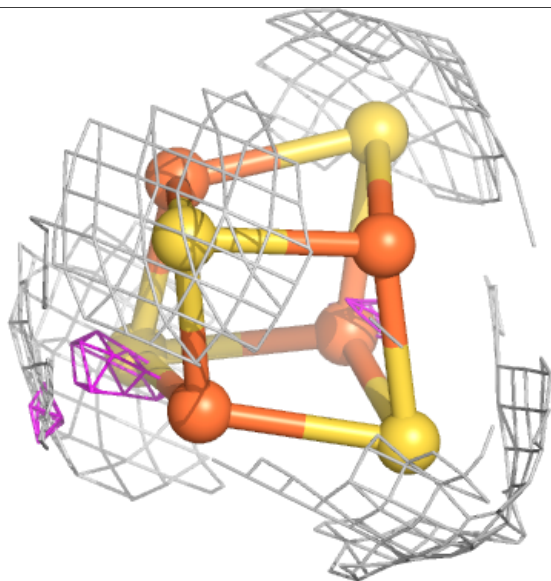
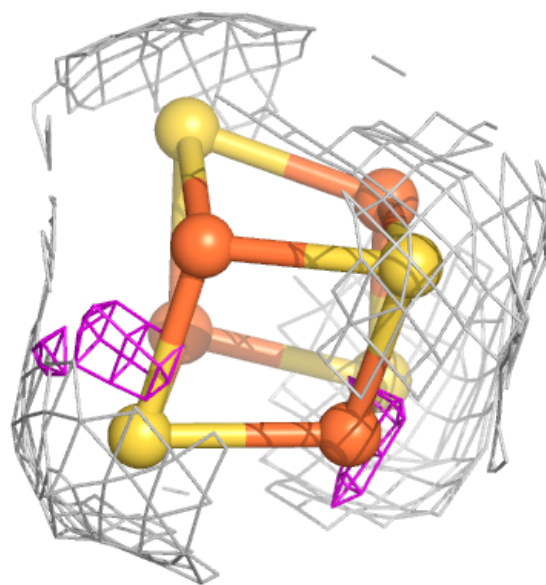
Electron density around SF4 a 101:

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



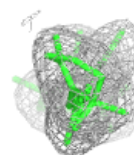
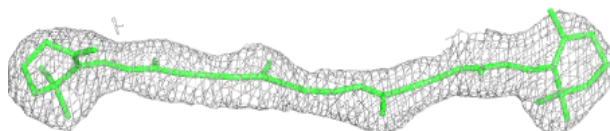
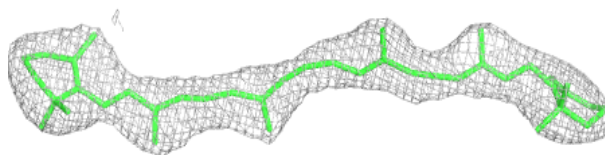
Electron density around SF4 a 102:

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



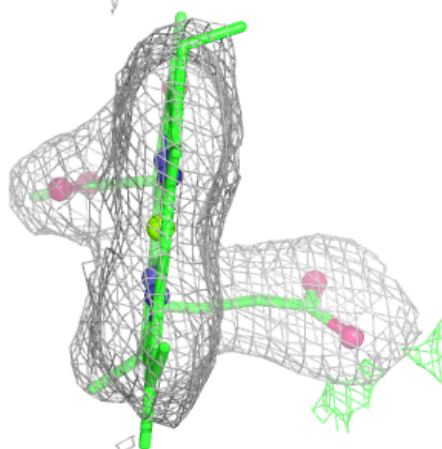
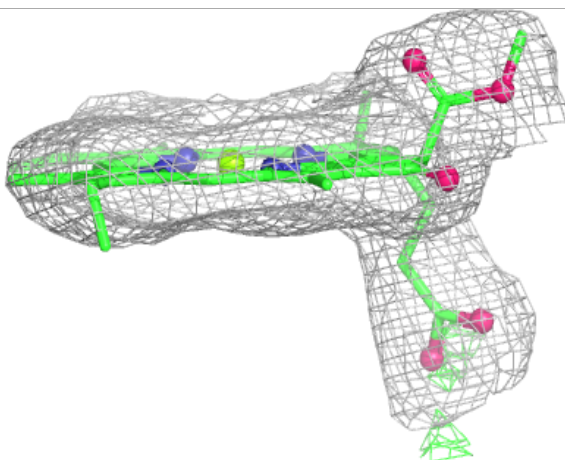
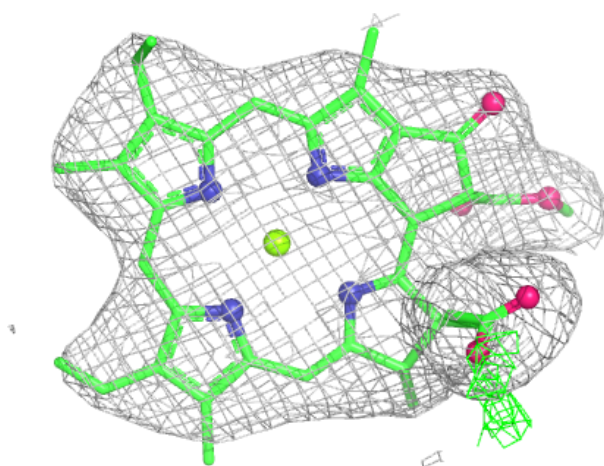
Electron density around BCR A 845:

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



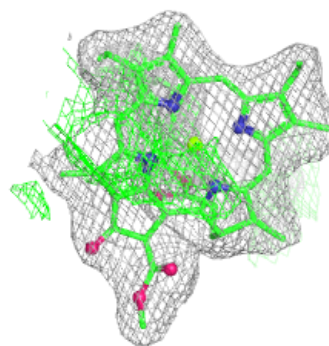
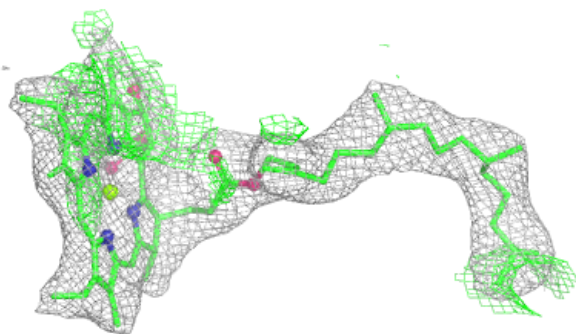
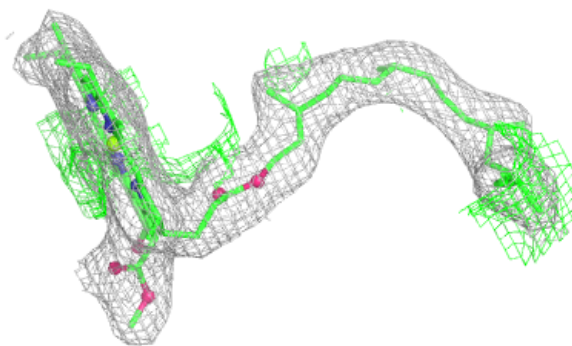
Electron density around CLA B 839:

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

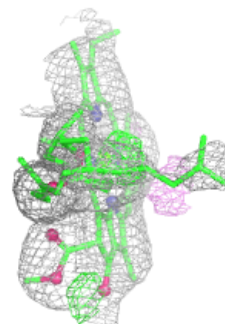
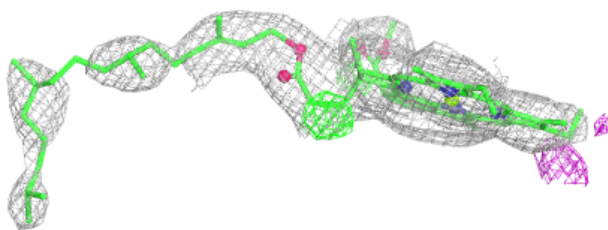
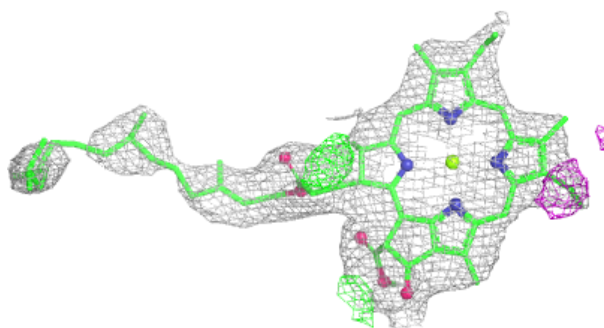


Electron density around CLA B 840:

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

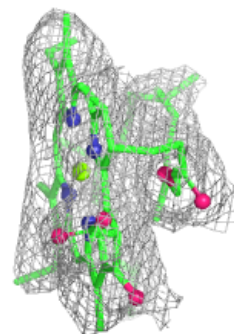
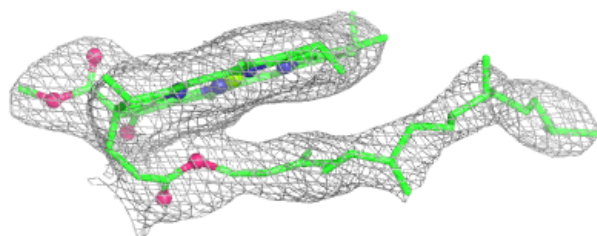
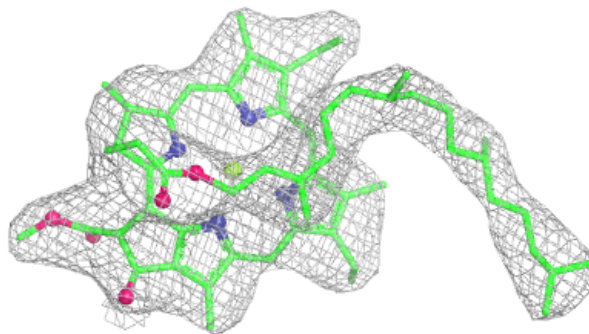
**Electron density around CLA A 805:**

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



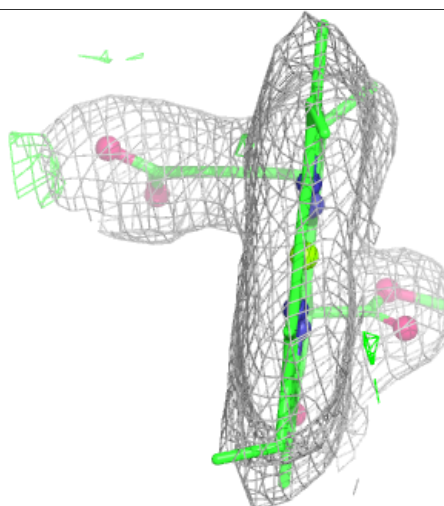
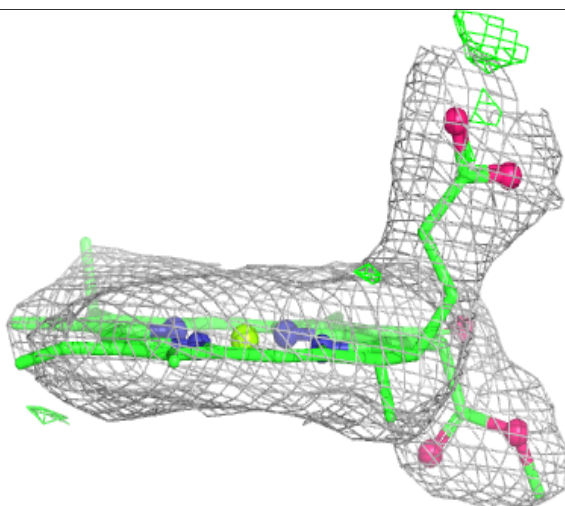
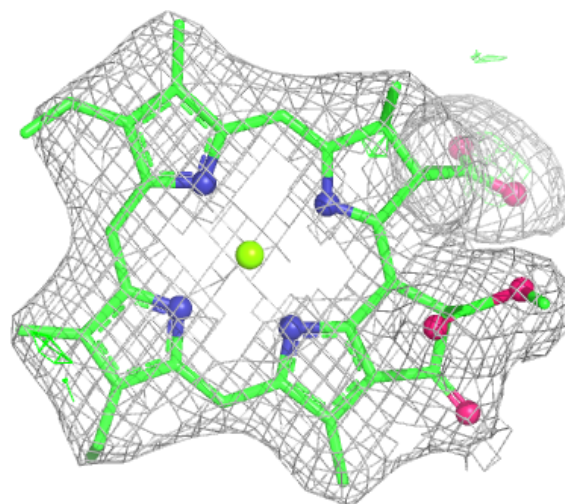
Electron density around CLA H 835:

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



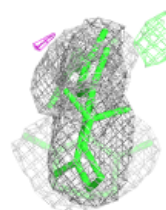
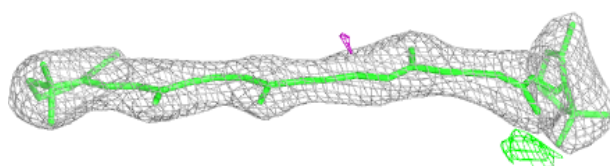
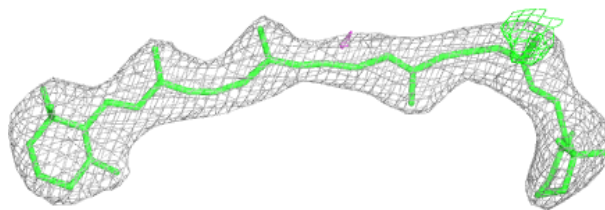
Electron density around CLA H 836:

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

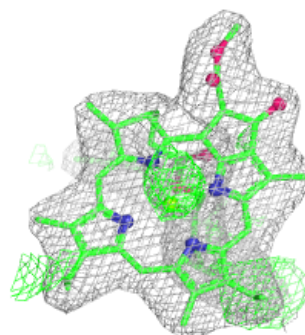
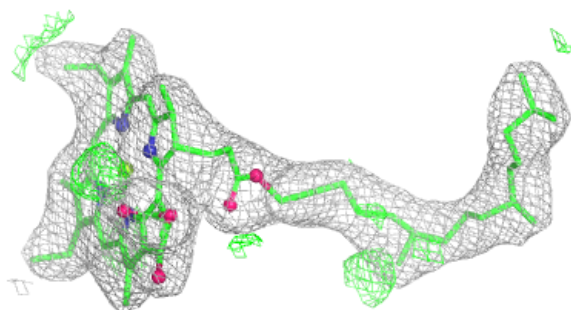
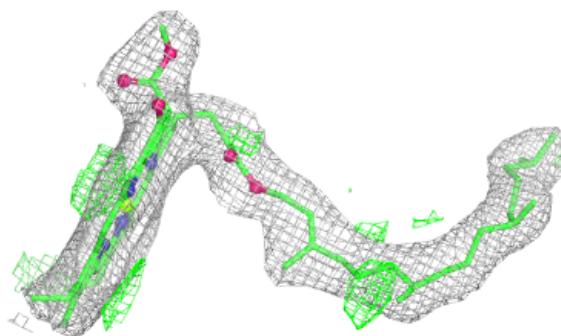


Electron density around BCR B 844:

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

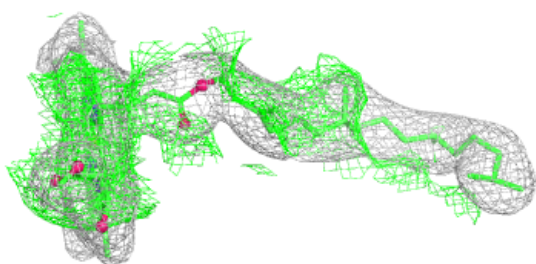
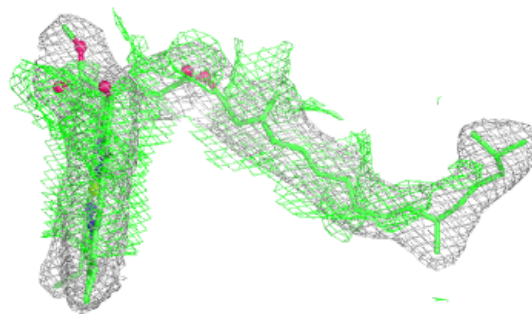
**Electron density around CLA H 837:**

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



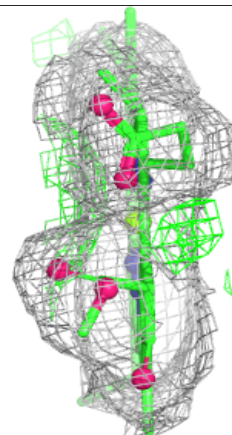
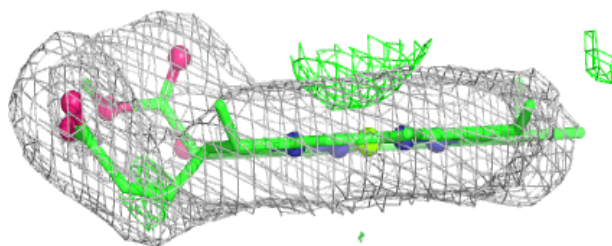
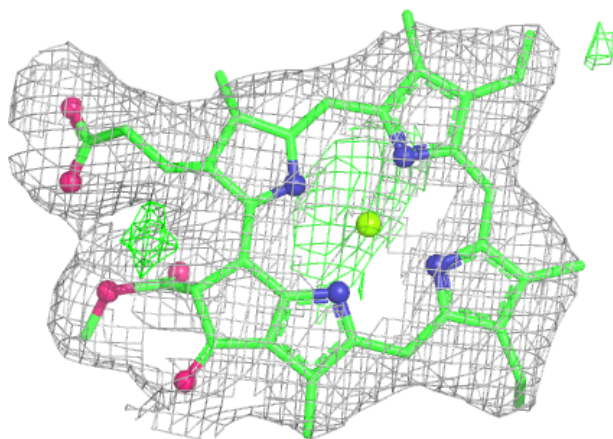
Electron density around CLA H 838:

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



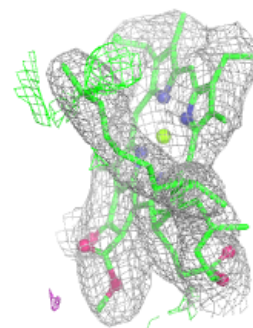
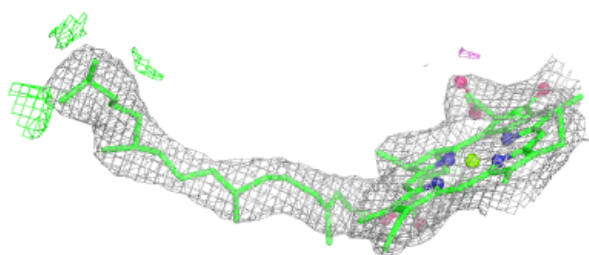
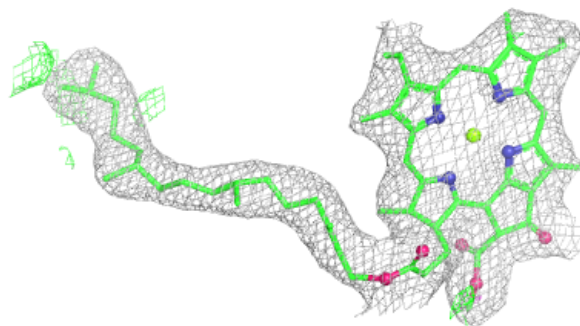
Electron density around CLA F 202:

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

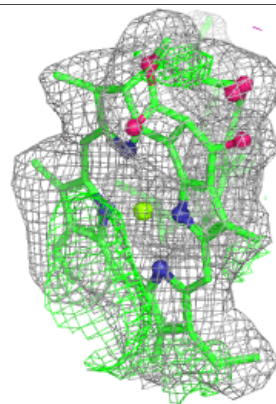
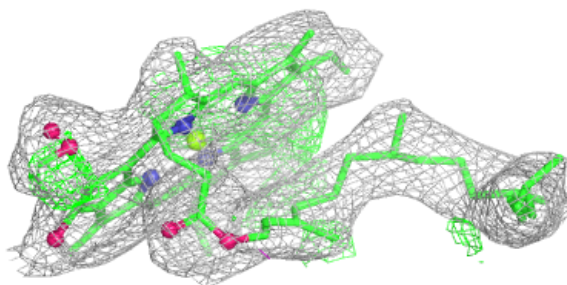
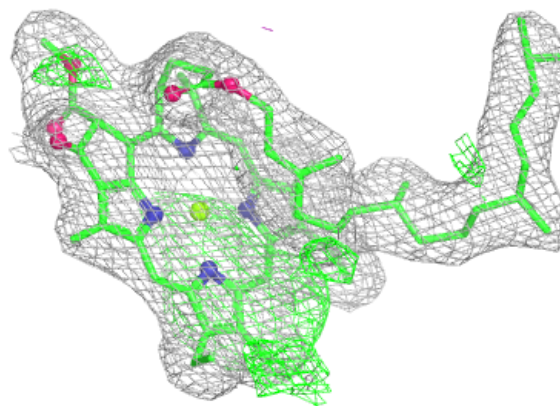


Electron density around CLA G 802:

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

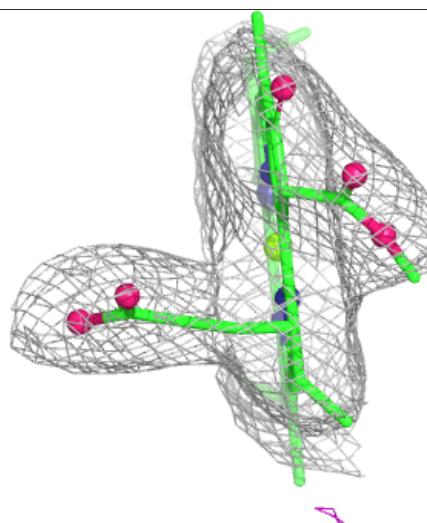
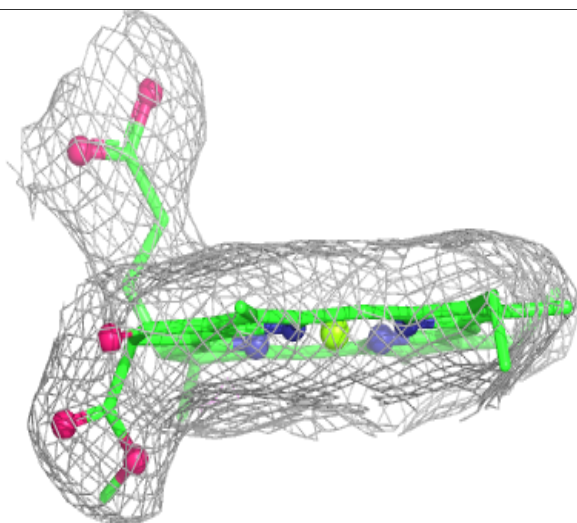
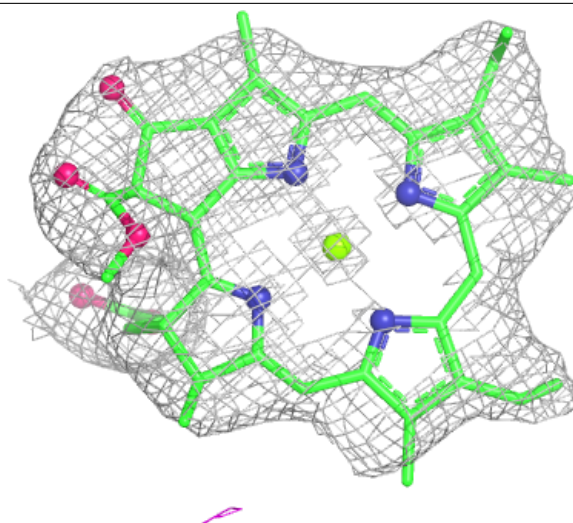
**Electron density around CLA A 841:**

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



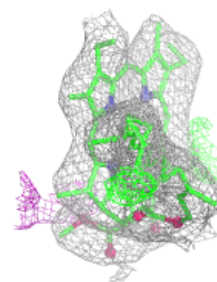
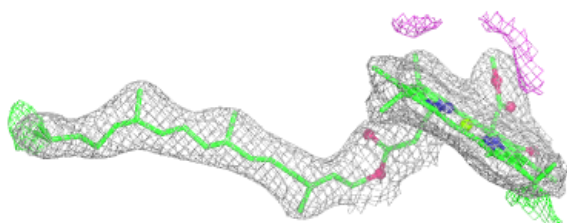
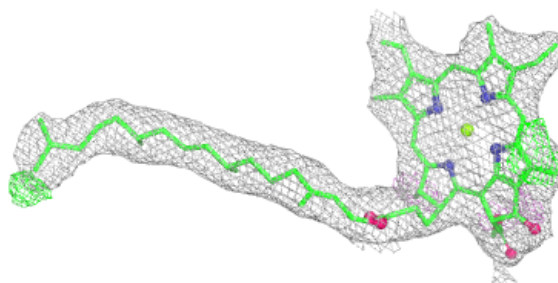
Electron density around CLA K 103:

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

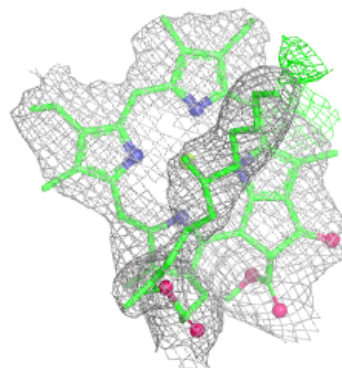
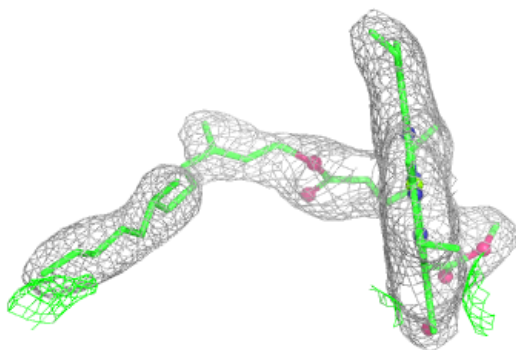
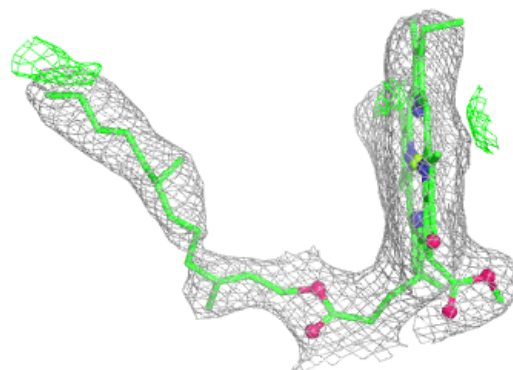


Electron density around CLA L 201:

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

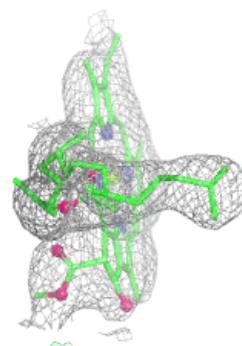
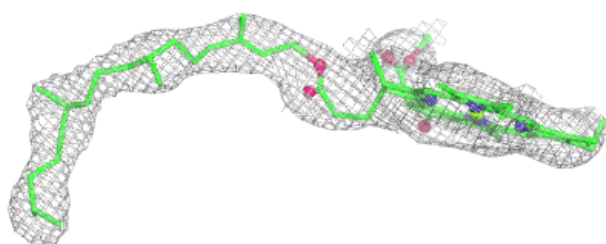
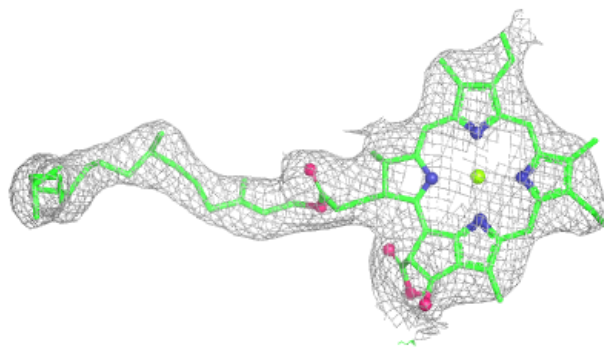
**Electron density around CLA G 804:**

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

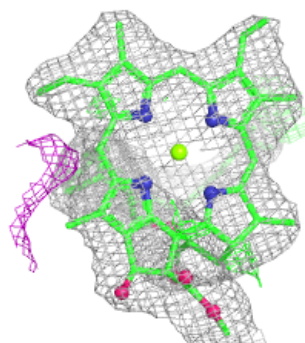
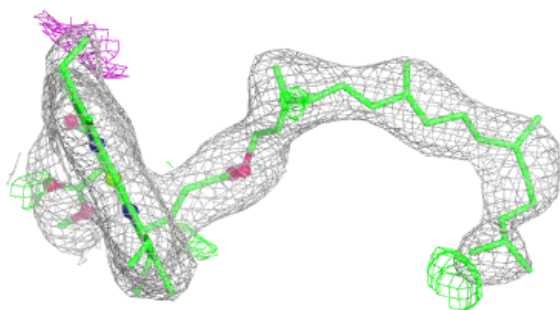
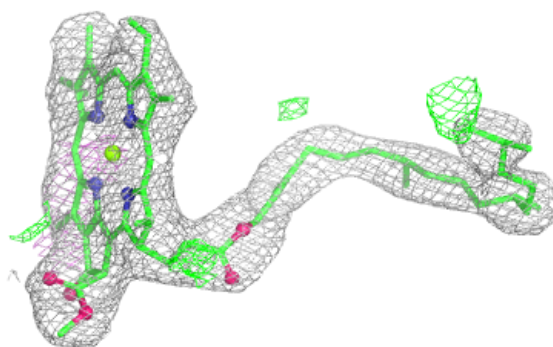


Electron density around CLA G 805:

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

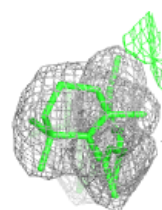
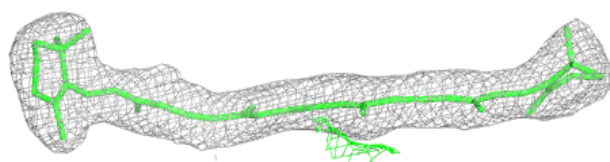
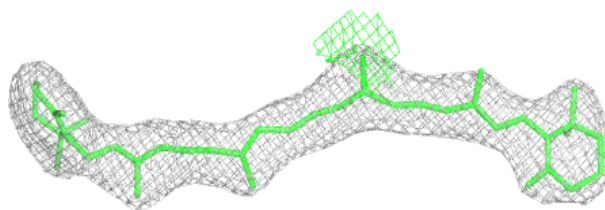
**Electron density around CLA L 206:**

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

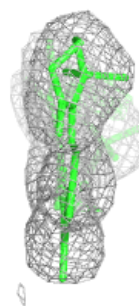
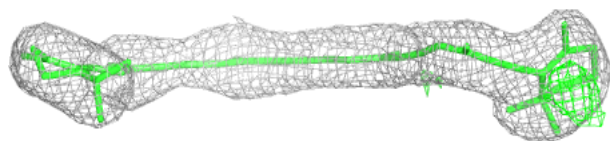
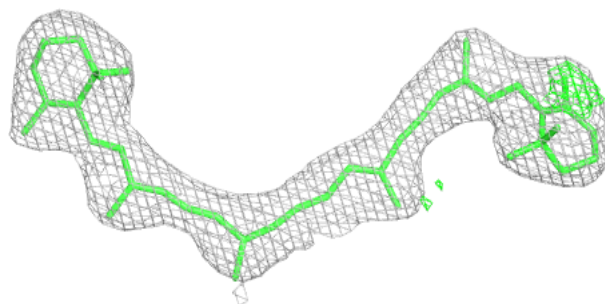


Electron density around BCR G 849:

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

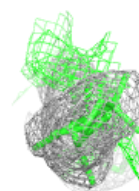
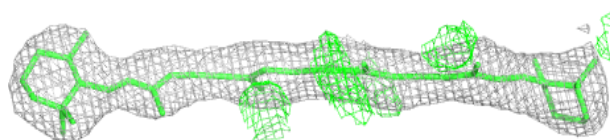
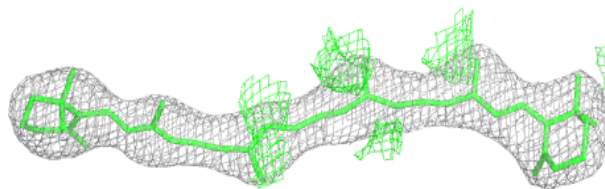
**Electron density around BCR G 850:**

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

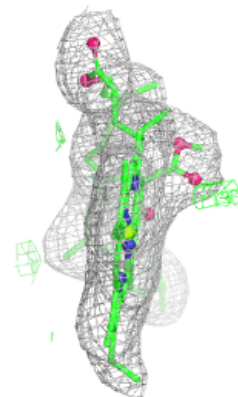
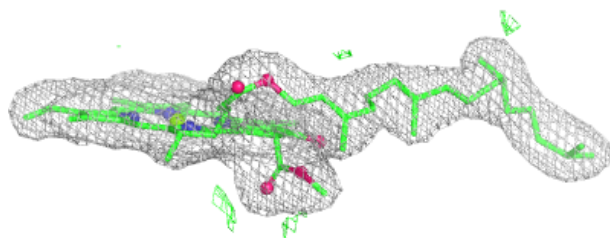
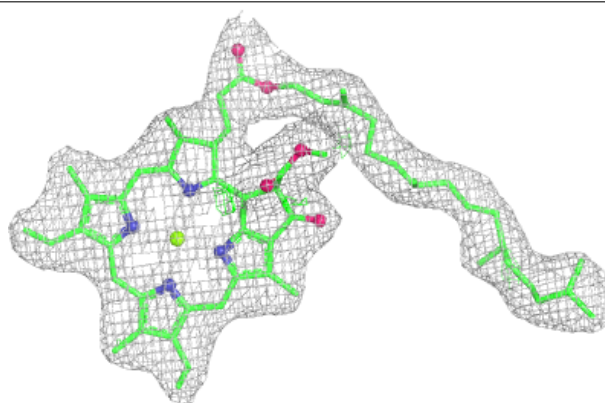


Electron density around BCR G 854:

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

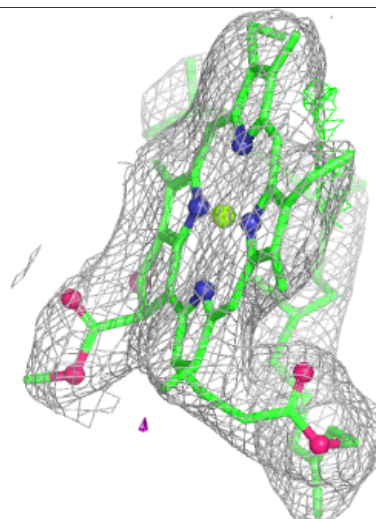
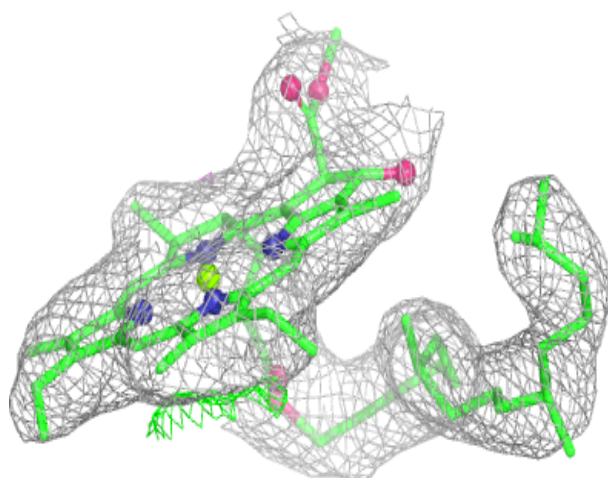
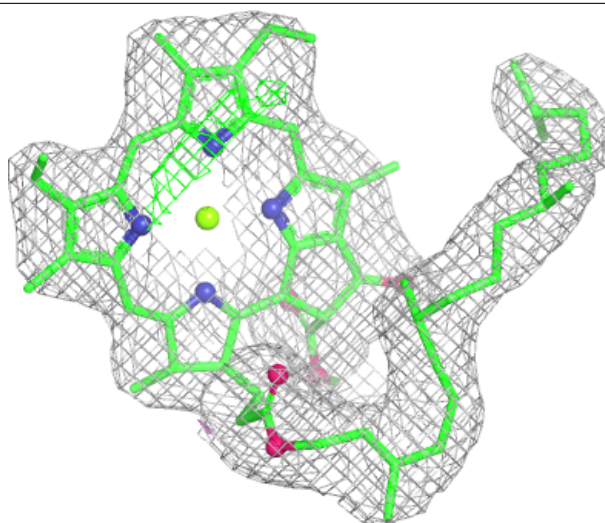
**Electron density around CLA L 207:**

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



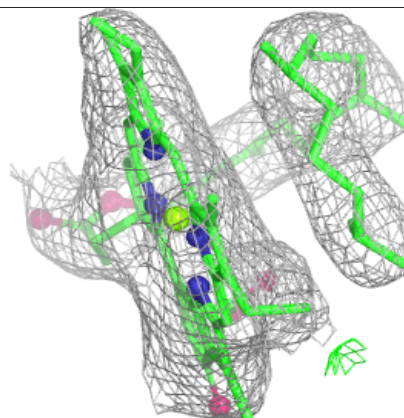
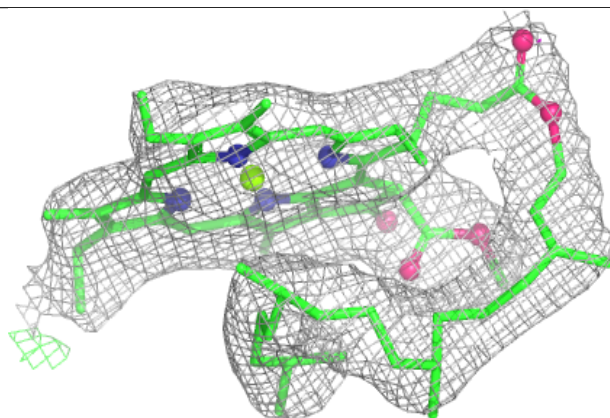
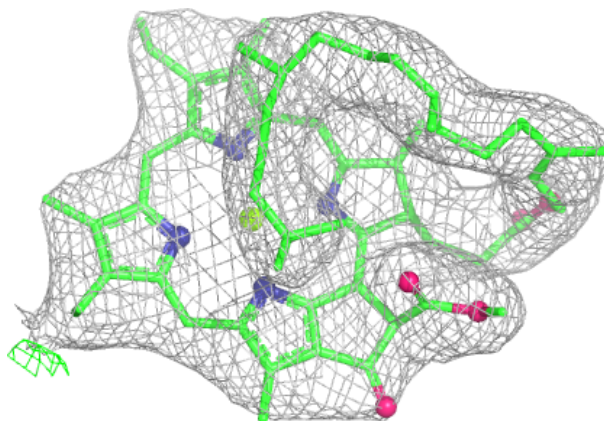
Electron density around CLA Q 201:

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



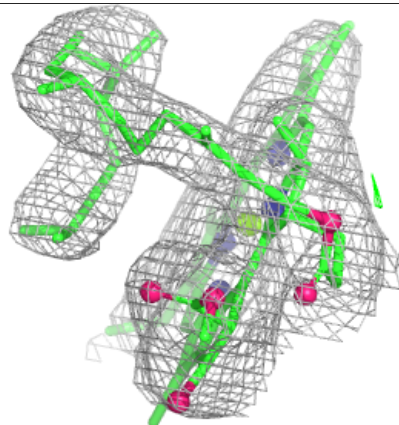
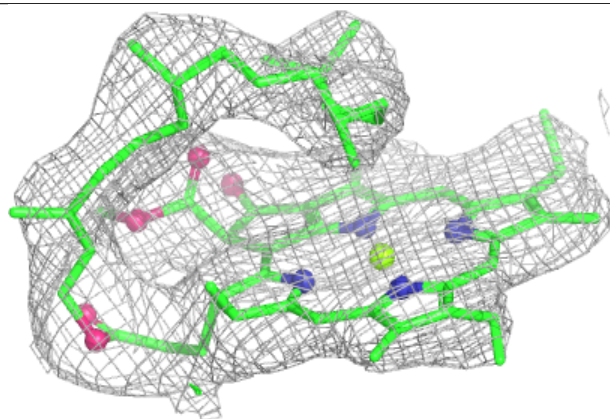
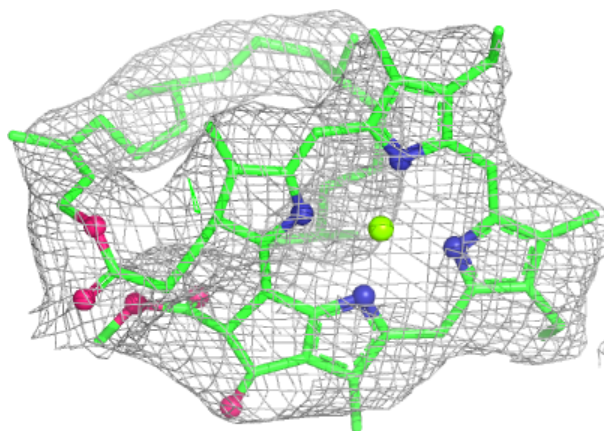
Electron density around CLA G 806:

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

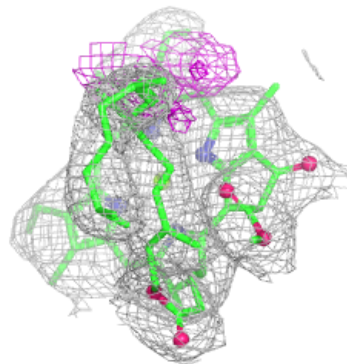
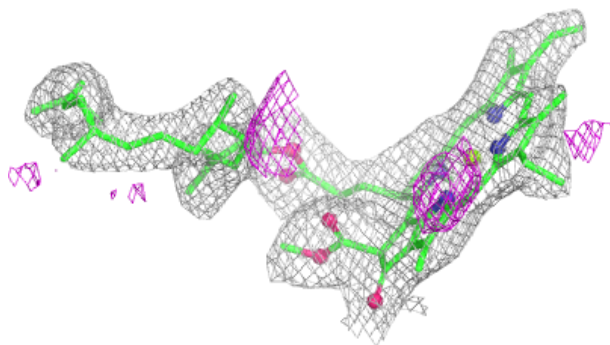
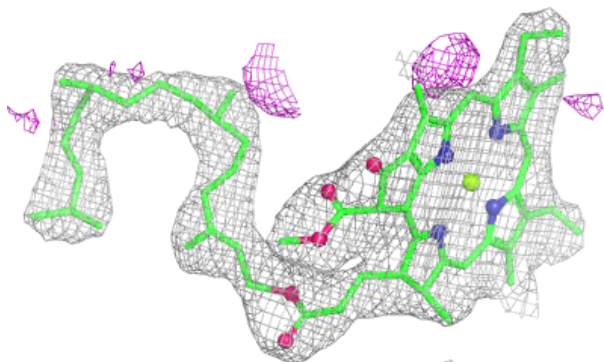


Electron density around CLA A 806:

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

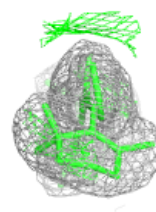
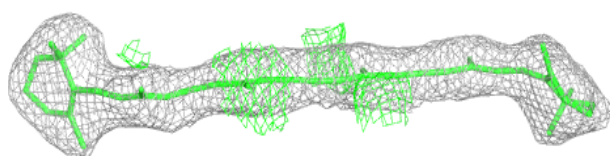
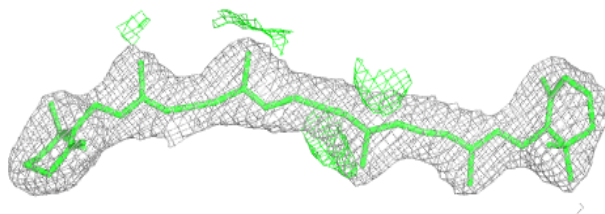
**Electron density around CL0 A 801:**

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



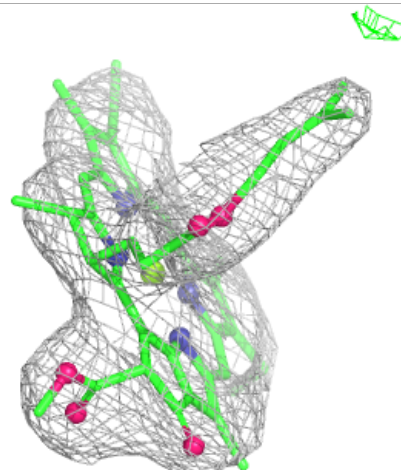
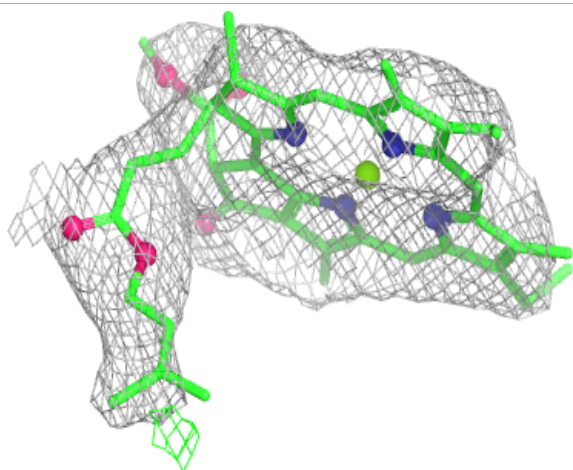
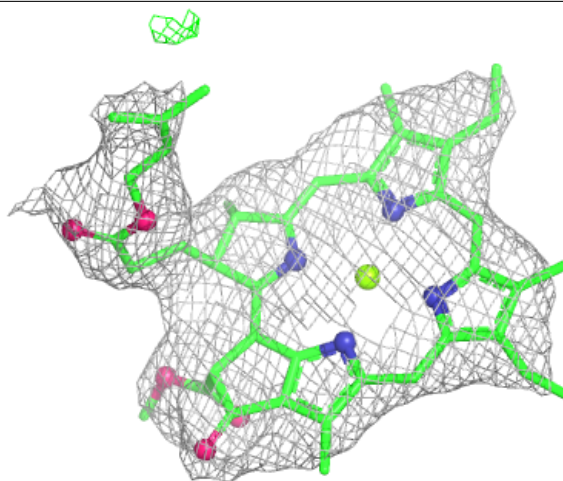
Electron density around BCR H 845:

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



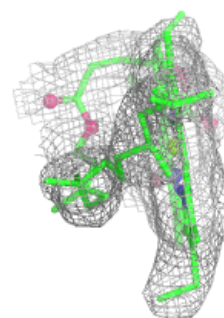
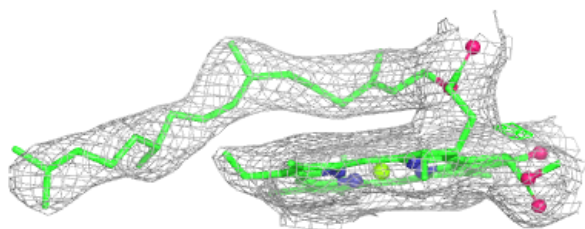
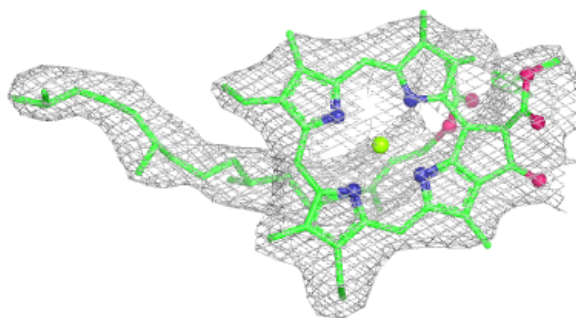
Electron density around CLA A 814:

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

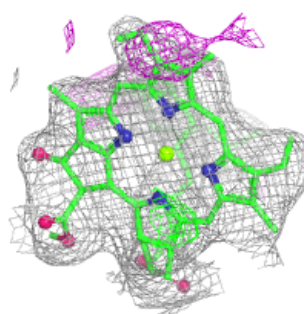
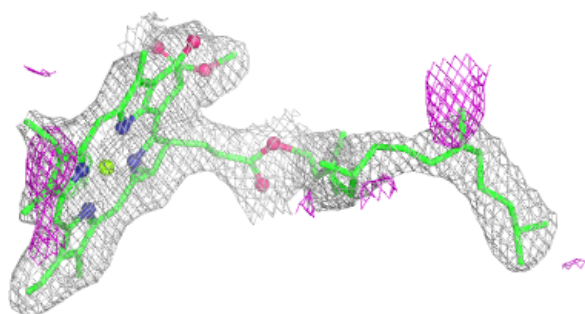
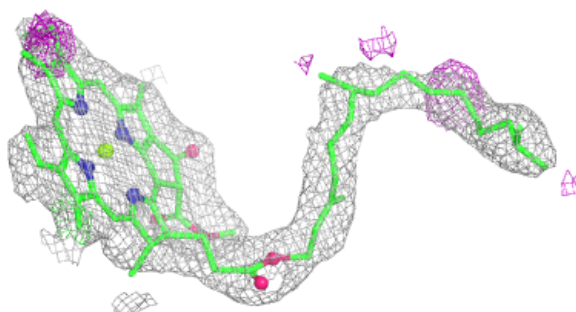


Electron density around CLA B 802:

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

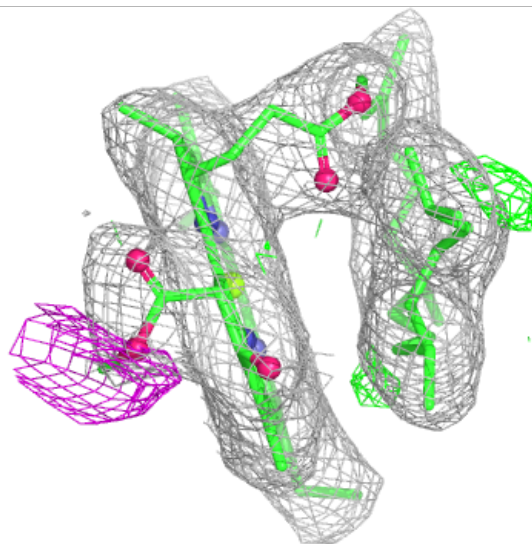
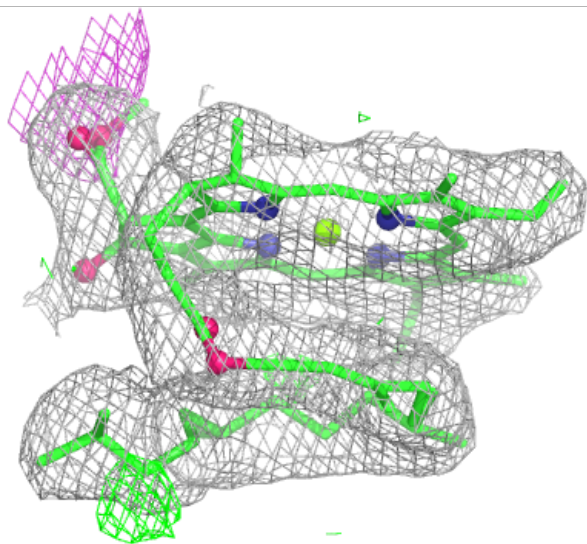
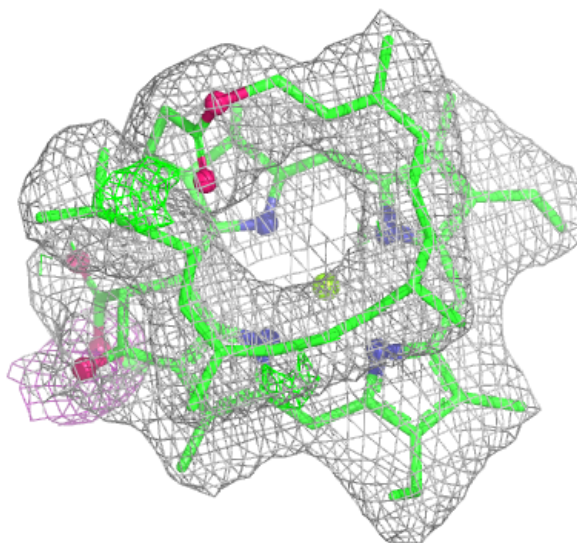
**Electron density around CLA B 803:**

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



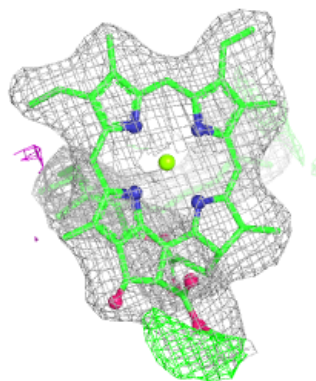
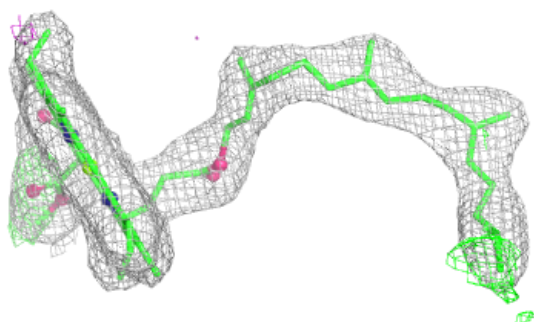
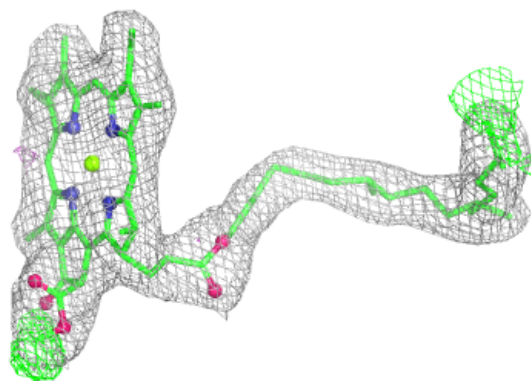
Electron density around CLA U 1002:

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

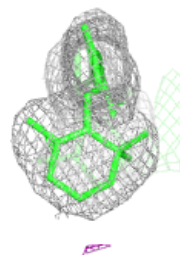
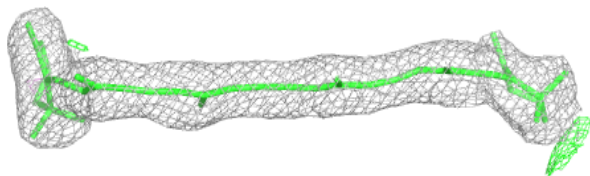
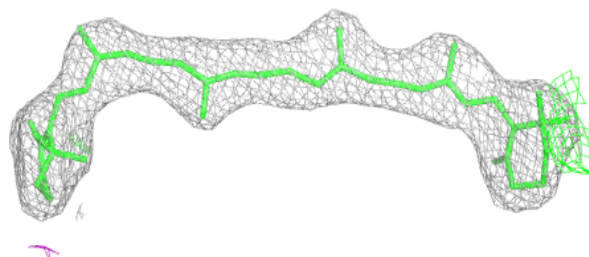


Electron density around CLA U 1003:

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

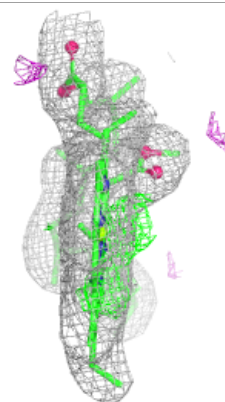
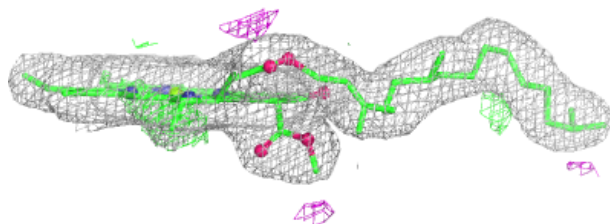
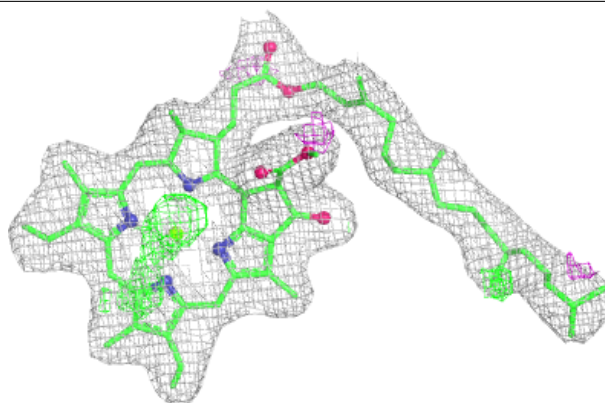
**Electron density around BCR L 203:**

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

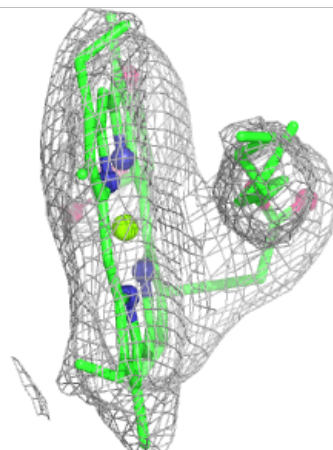
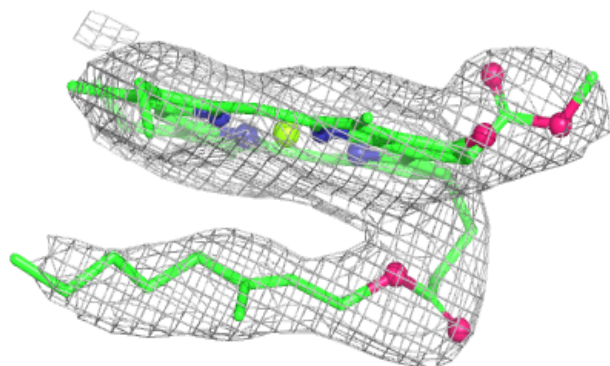
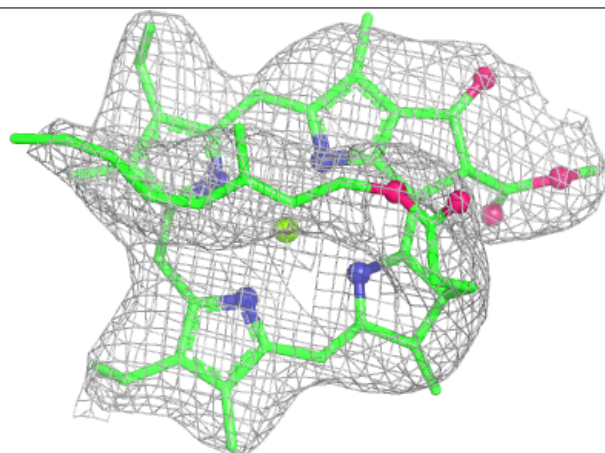


Electron density around CLA U 1004:

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

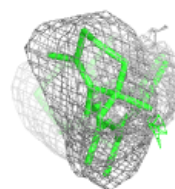
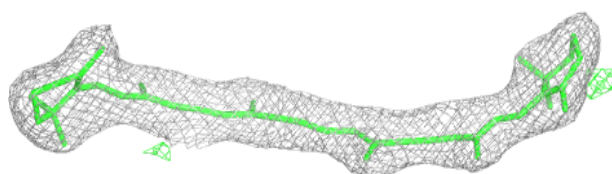
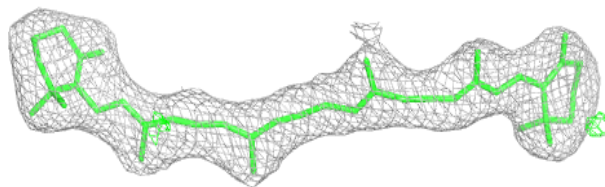
**Electron density around CLA G 812:**

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

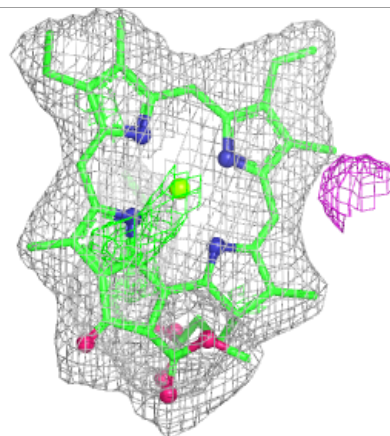
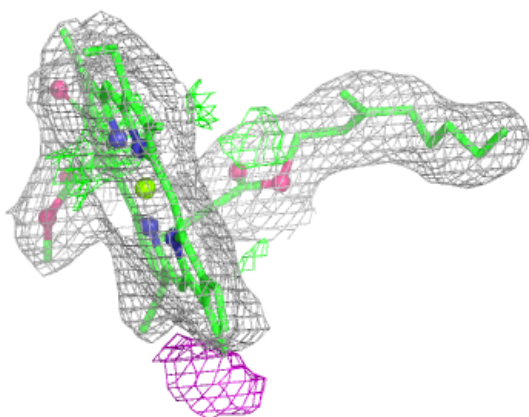
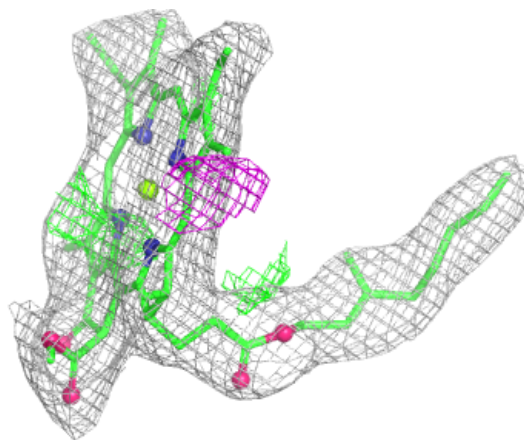


Electron density around BCR M 101:

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

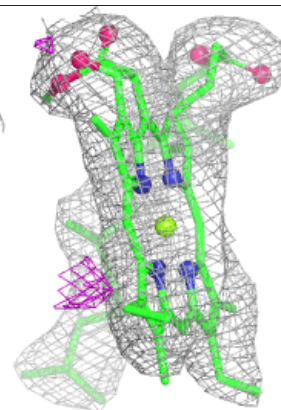
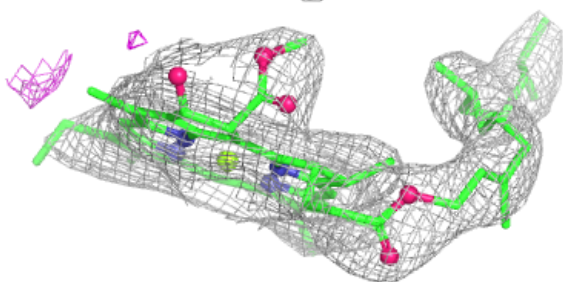
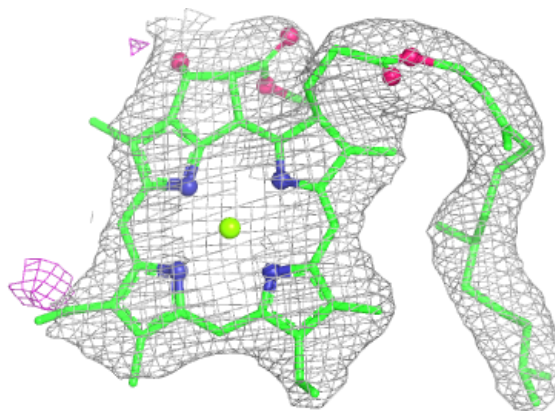
**Electron density around CLA V 1201:**

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

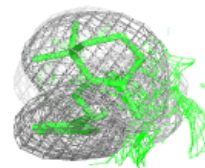
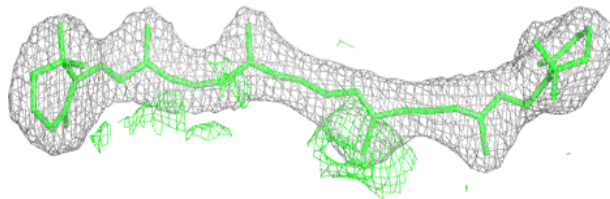
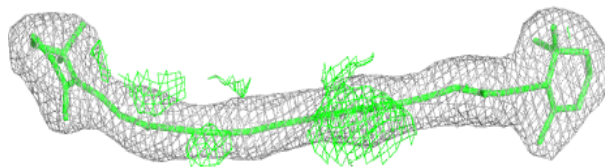


Electron density around CLA G 813:

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

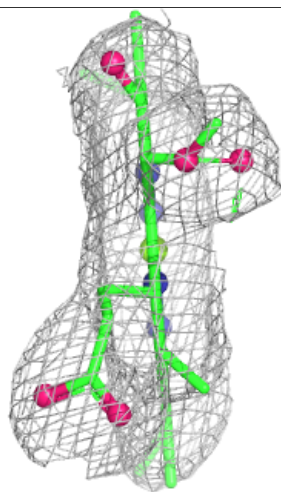
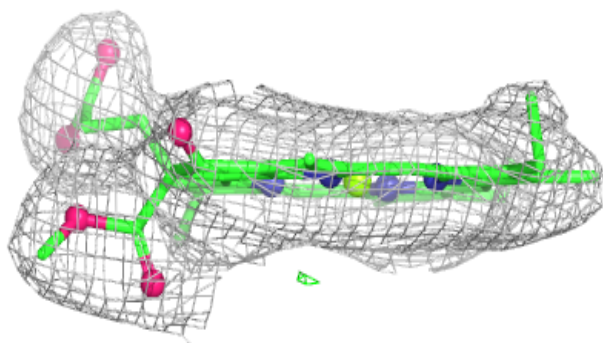
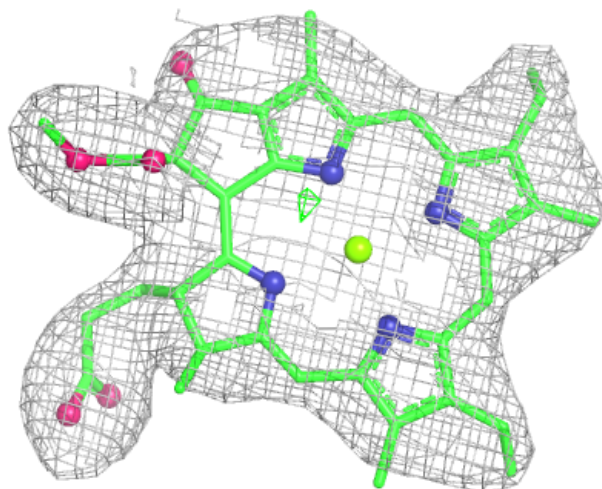
**Electron density around BCR R 101:**

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



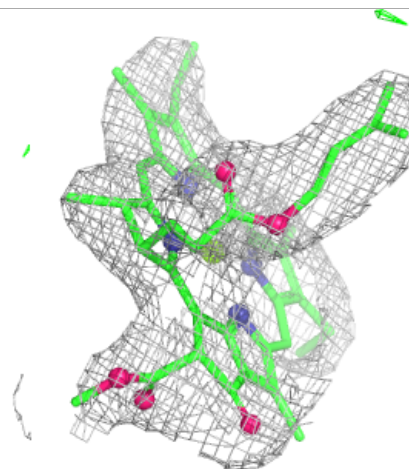
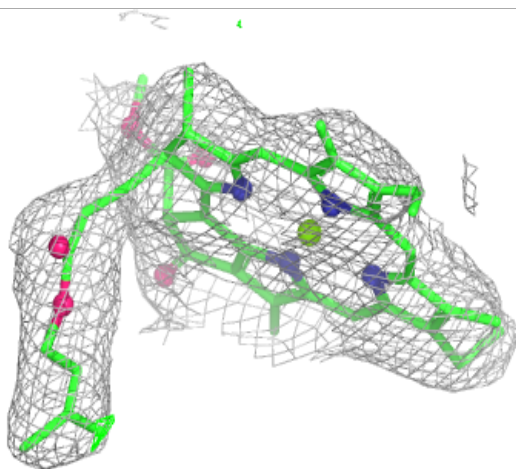
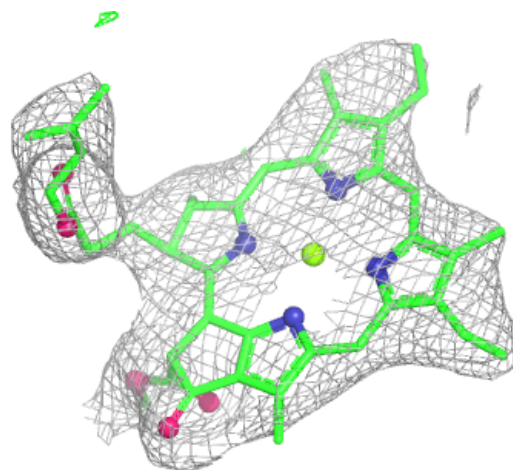
Electron density around CLA X 1701:

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



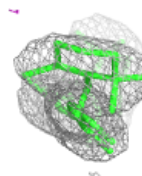
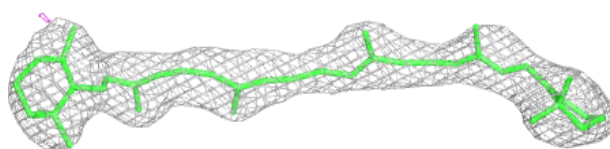
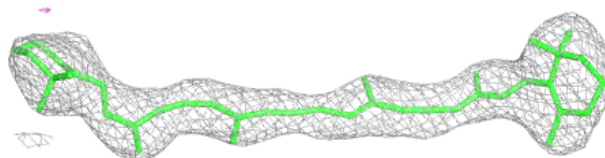
Electron density around CLA G 814:

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

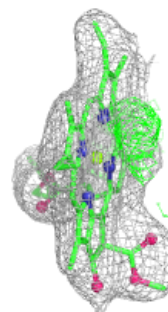
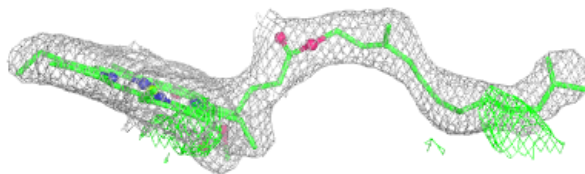
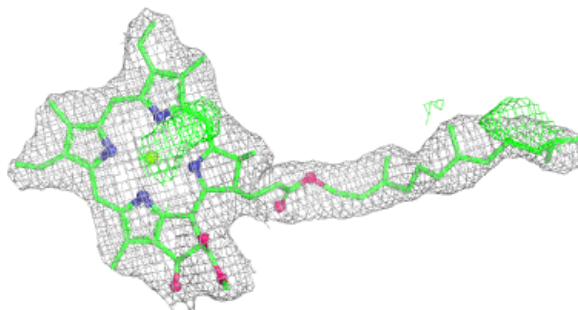


Electron density around BCR T 102:

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

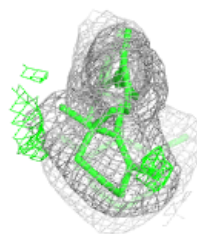
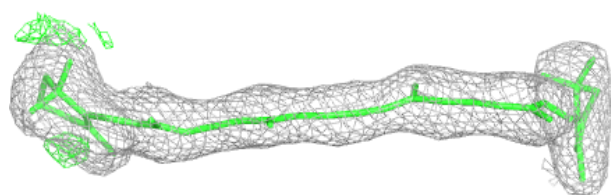
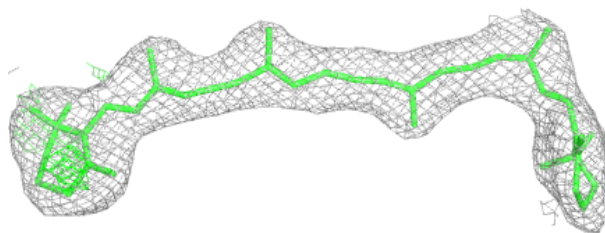
**Electron density around CLA A 826:**

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

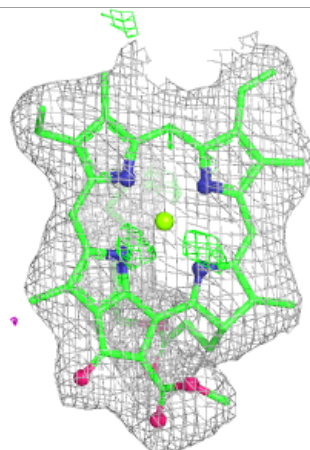
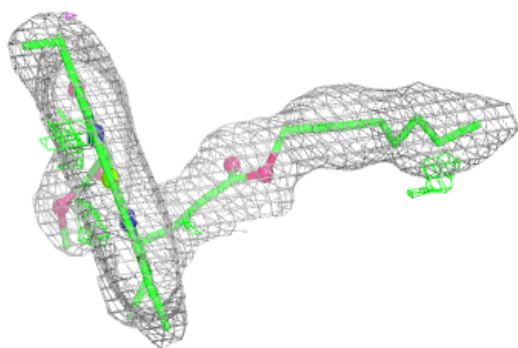
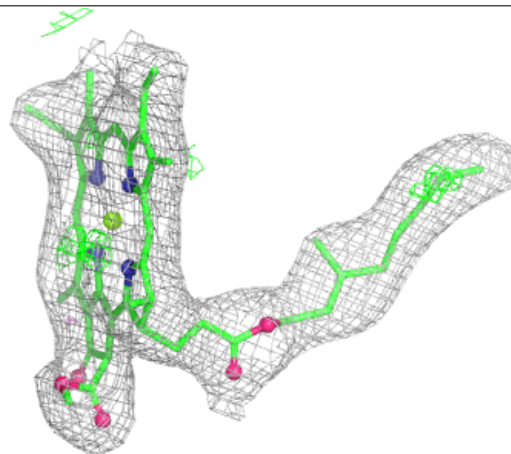


Electron density around BCR U 1007:

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

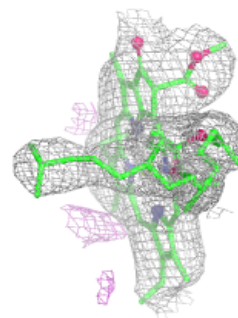
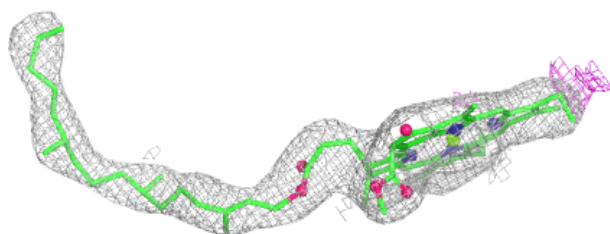
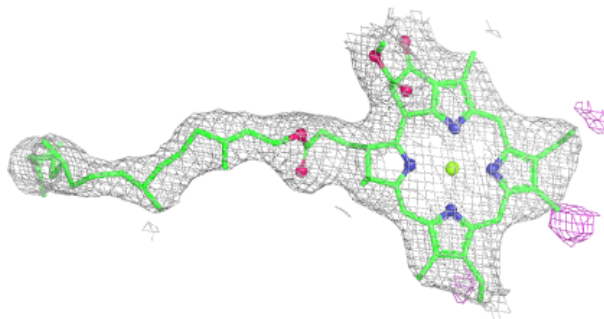
**Electron density around CLA B 805:**

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

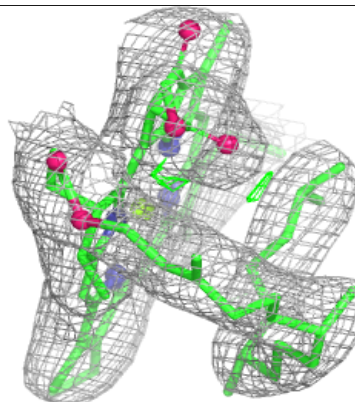
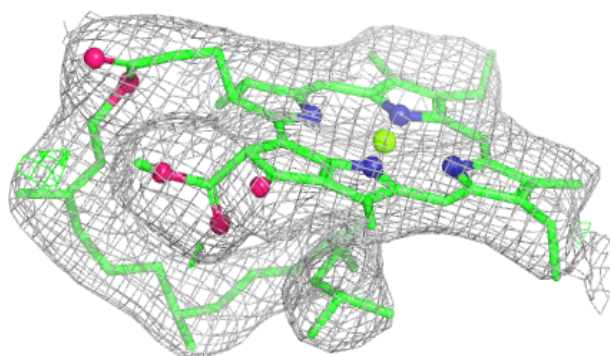
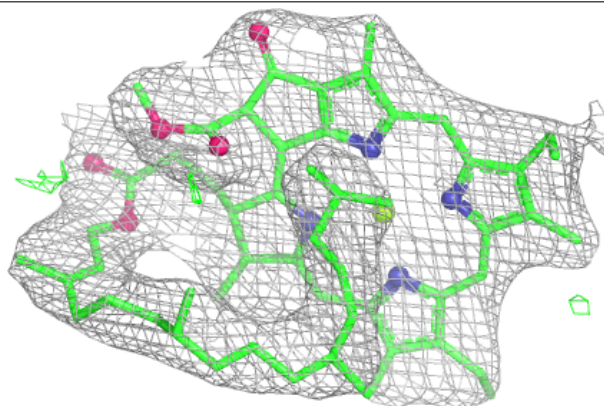


Electron density around CLA Y 805:

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

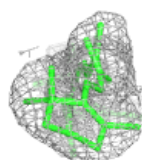
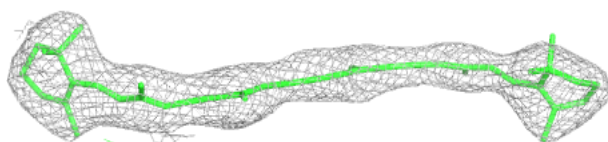
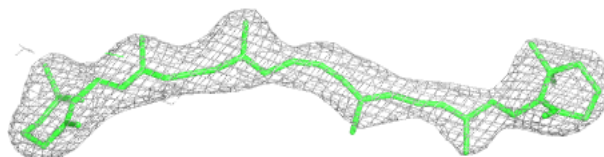
**Electron density around CLA Y 806:**

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



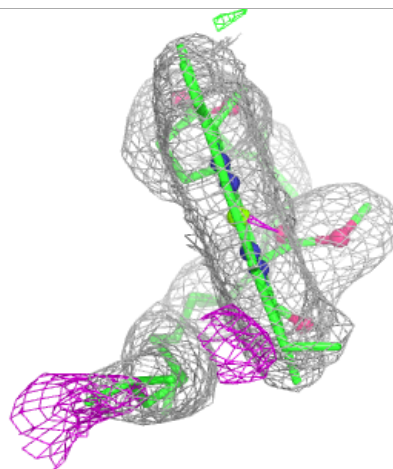
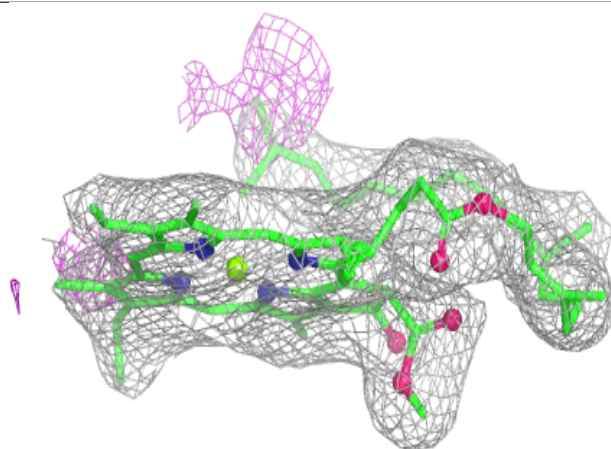
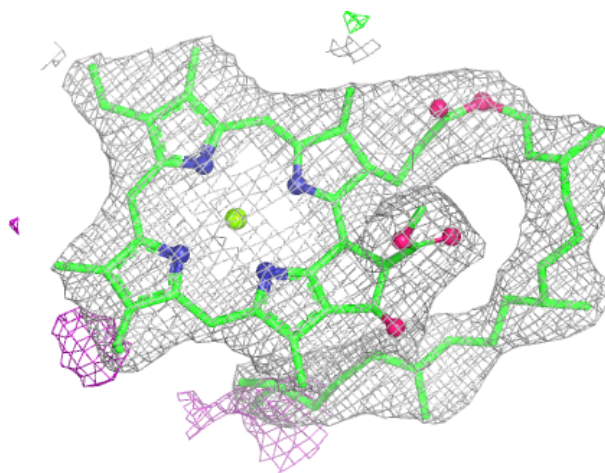
Electron density around BCR Y 847:

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



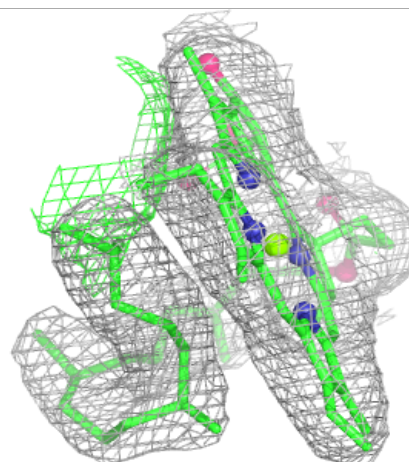
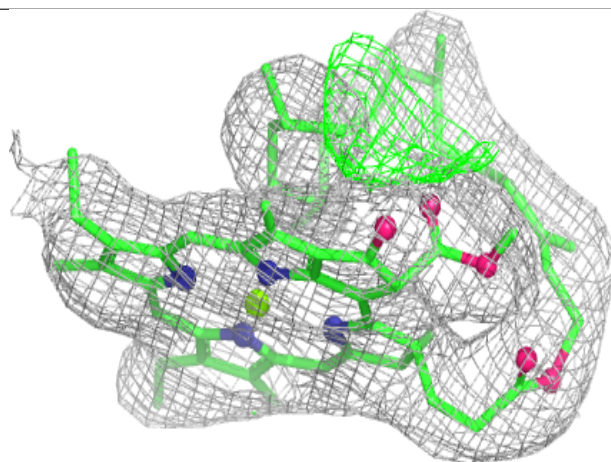
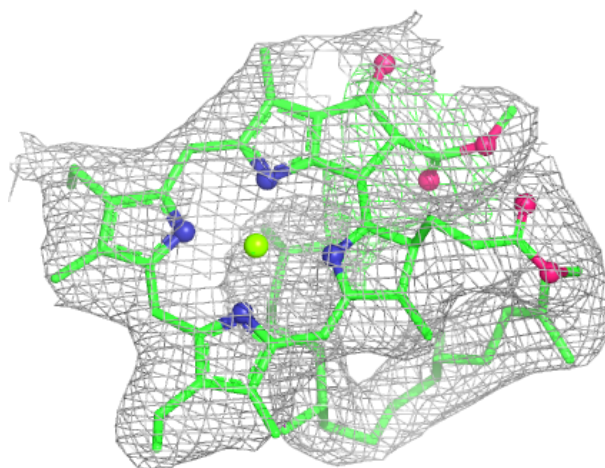
Electron density around CLA B 806:

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



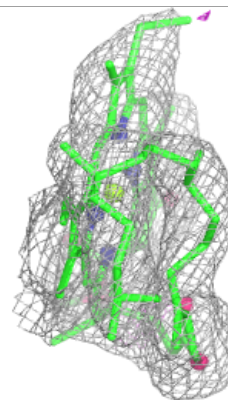
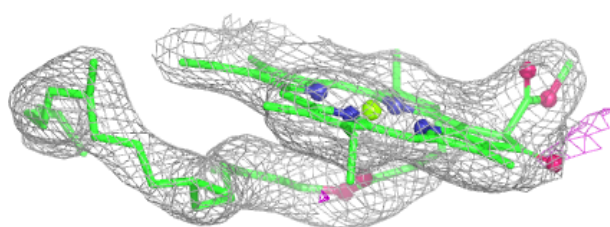
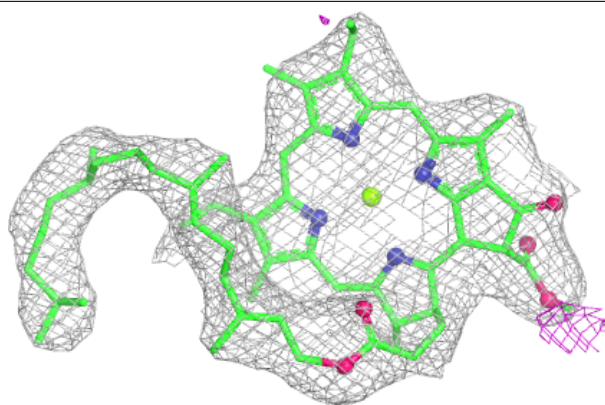
Electron density around CLA B 807:

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

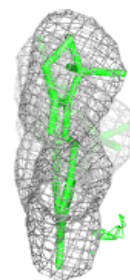
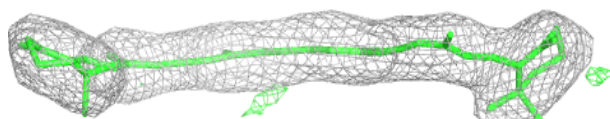
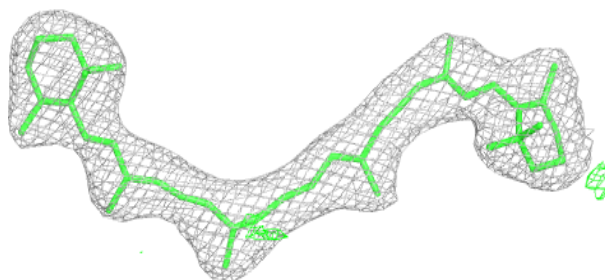


Electron density around CLA G 819:

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

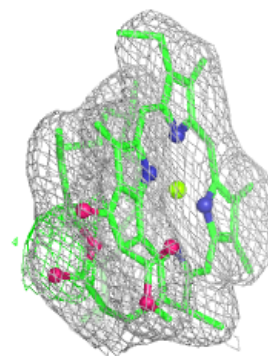
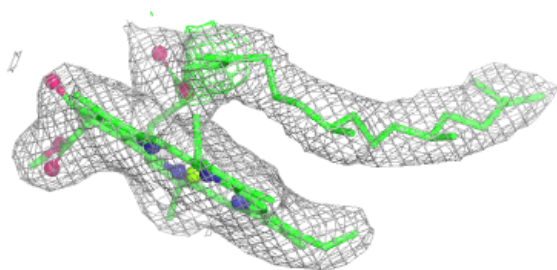
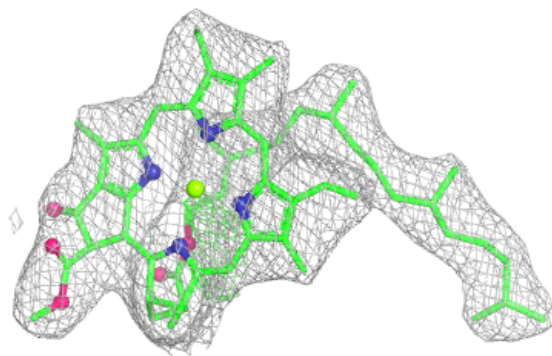
**Electron density around BCR Y 851:**

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



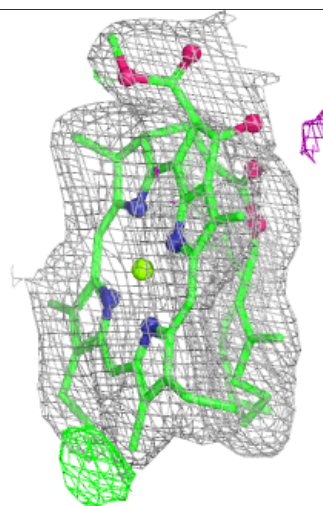
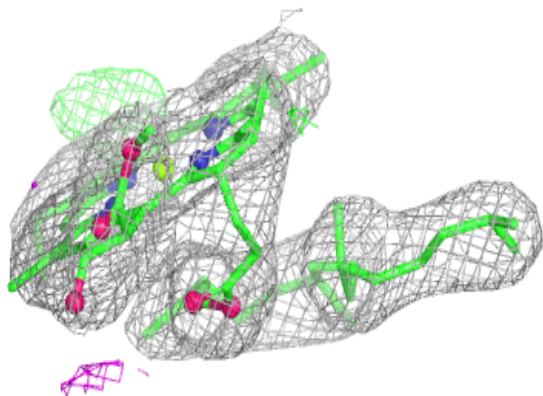
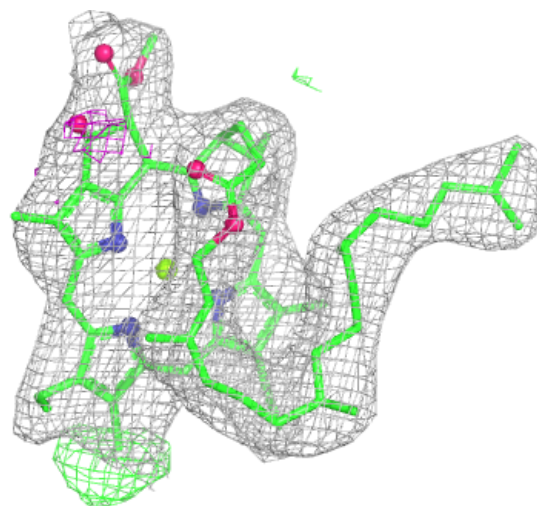
Electron density around CLA B 808:

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



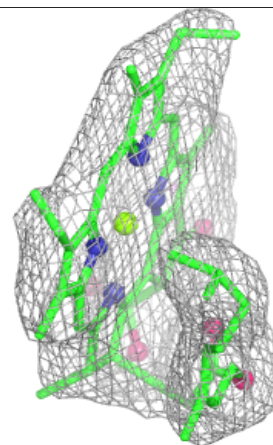
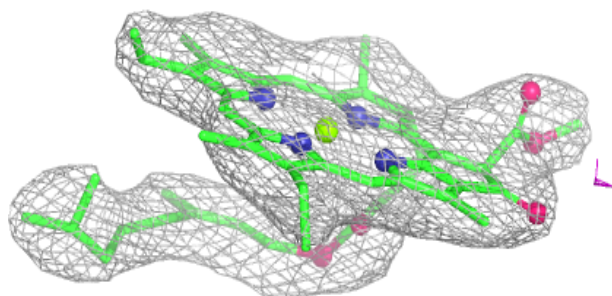
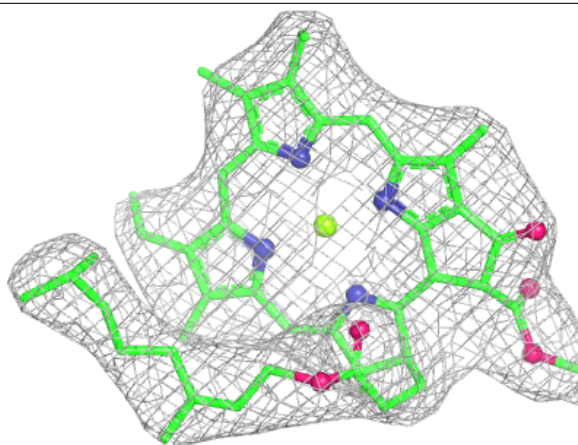
Electron density around CLA B 809:

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

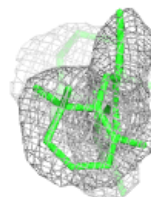
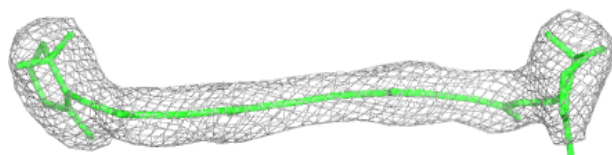
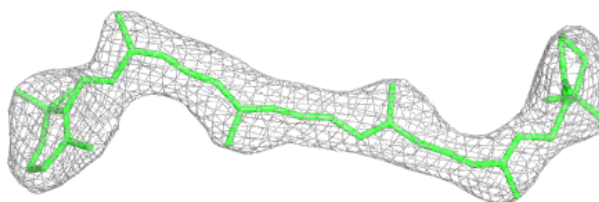


Electron density around CLA Y 812:

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

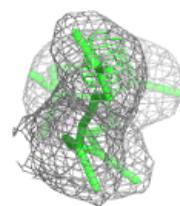
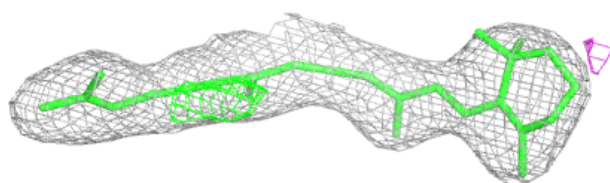
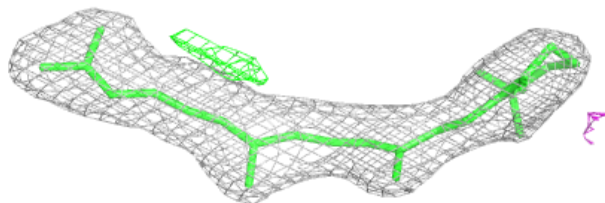
**Electron density around BCR Z 843:**

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

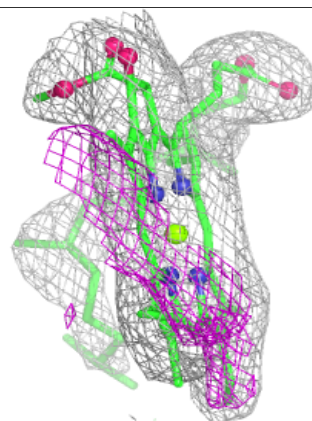
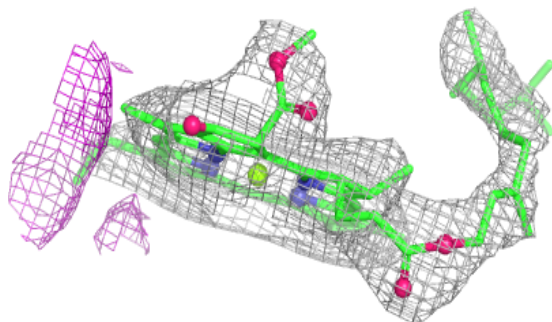
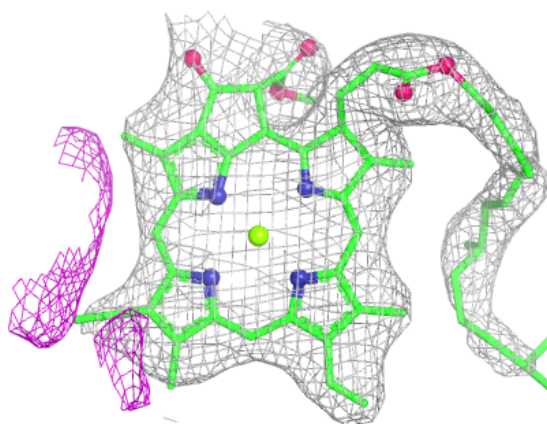


Electron density around BCR Z 844:

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

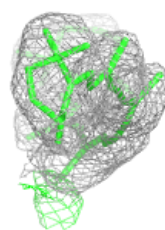
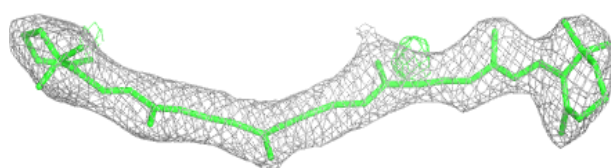
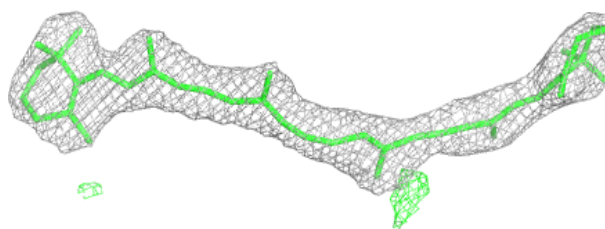
**Electron density around CLA Y 813:**

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

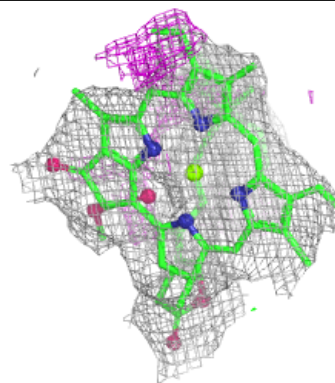
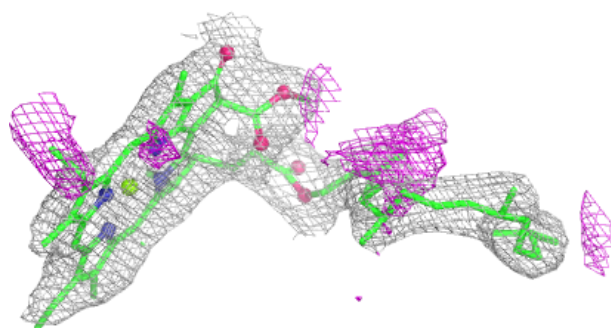
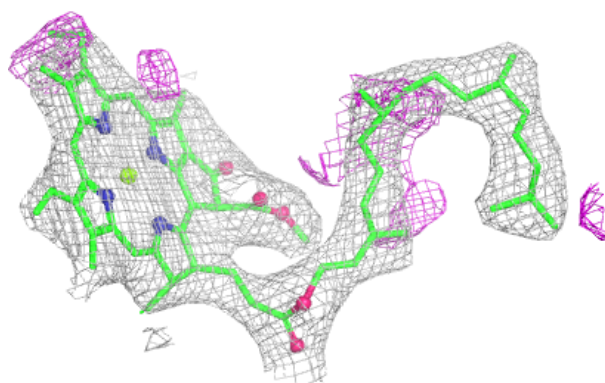


Electron density around BCR Z 846:

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

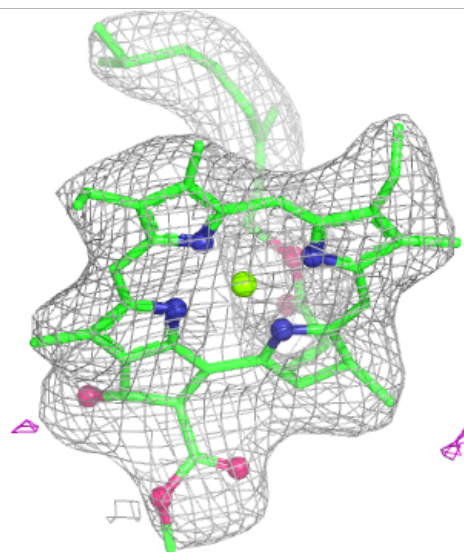
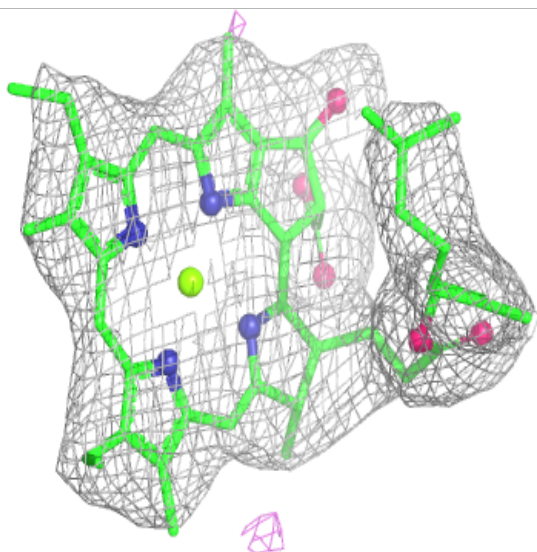
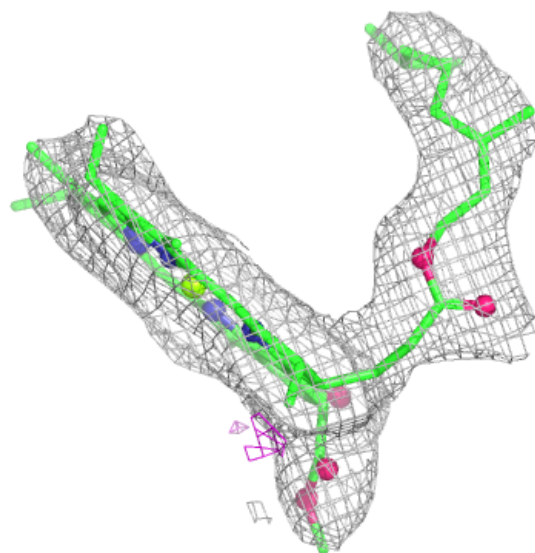
**Electron density around CL0 G 801:**

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



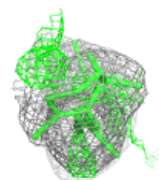
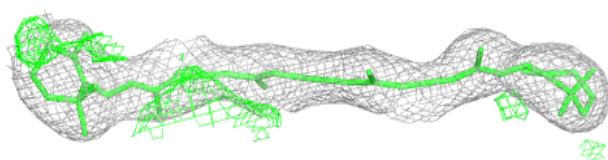
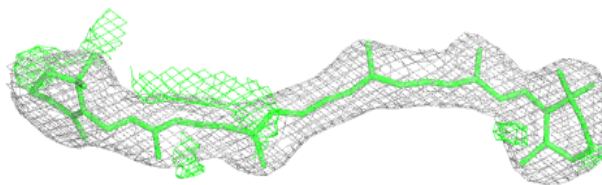
Electron density around CLA B 811:

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

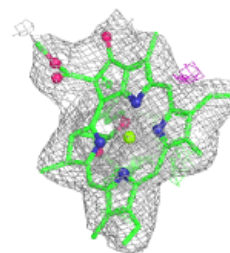
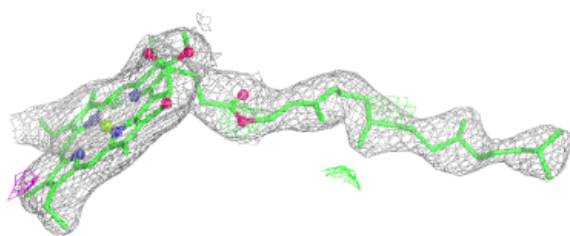
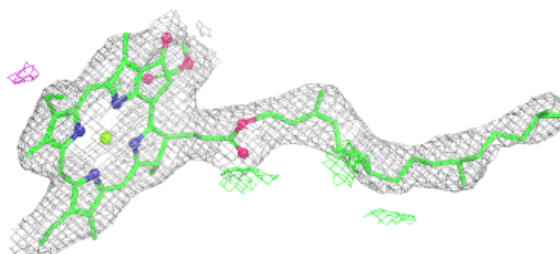


Electron density around BCR f 103:

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

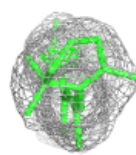
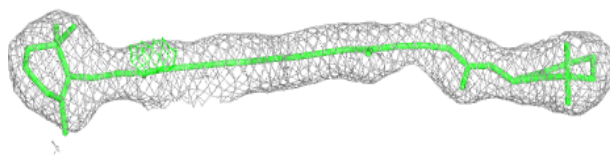
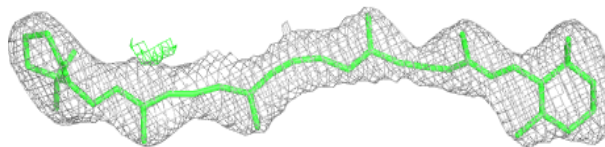
**Electron density around CLA A 809:**

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

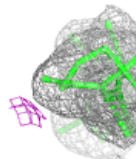
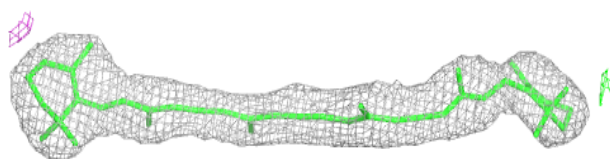
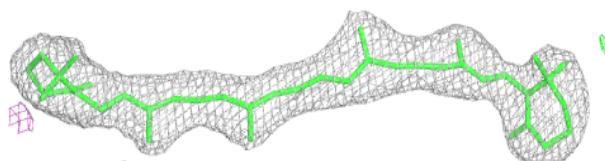


Electron density around BCR f 105:

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

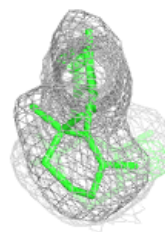
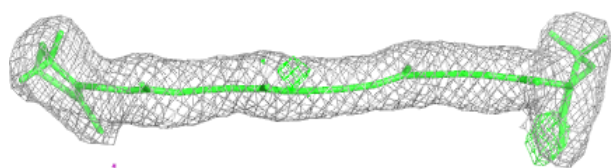
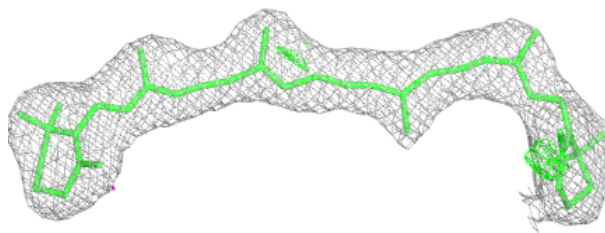
**Electron density around BCR h 202:**

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

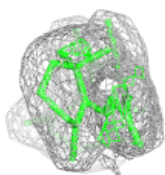
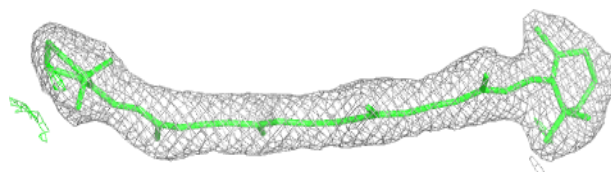
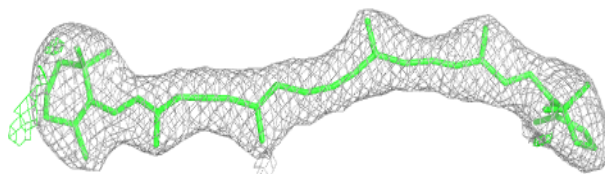


Electron density around BCR h 203:

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

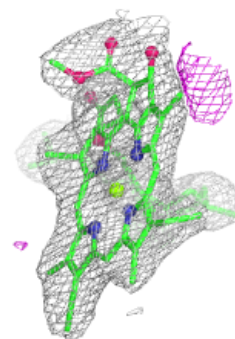
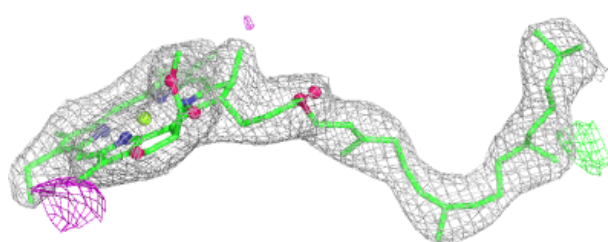
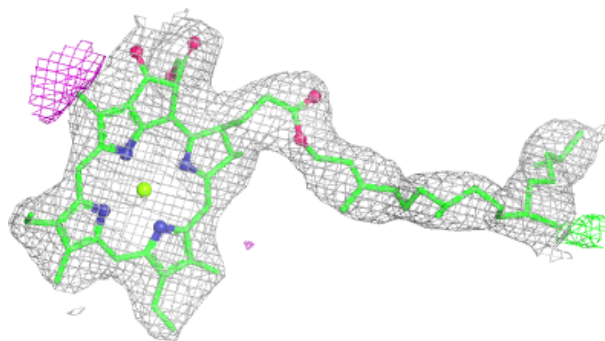
**Electron density around BCR i 101:**

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

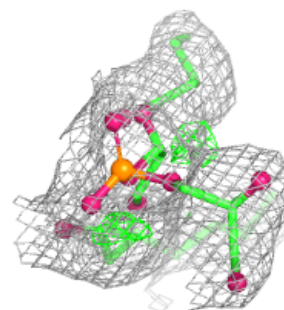
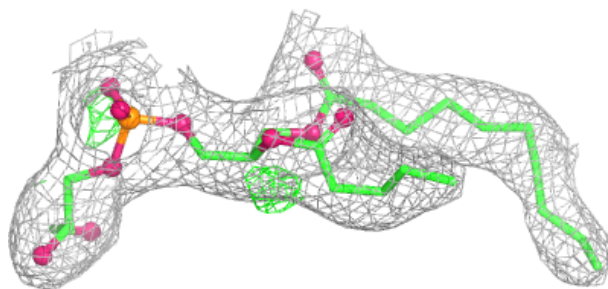
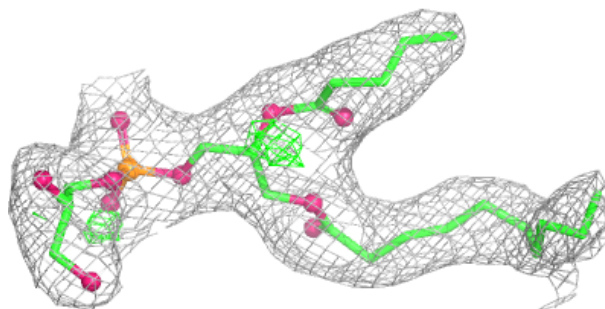


Electron density around CLA B 813:

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

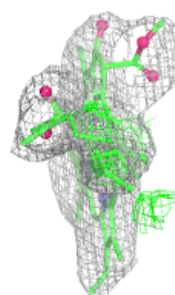
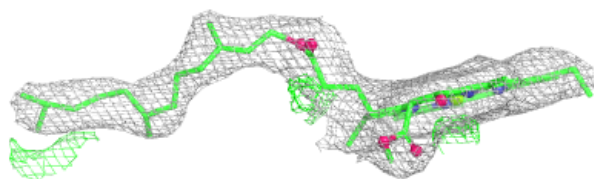
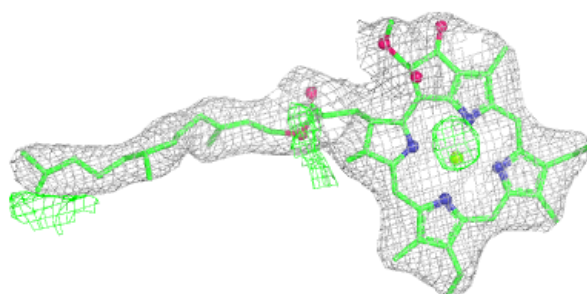
**Electron density around LHG A 851:**

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

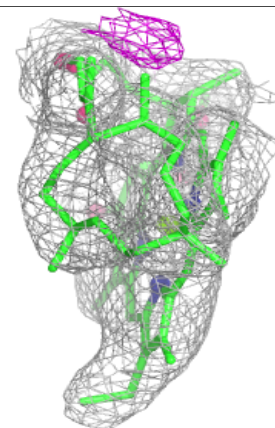
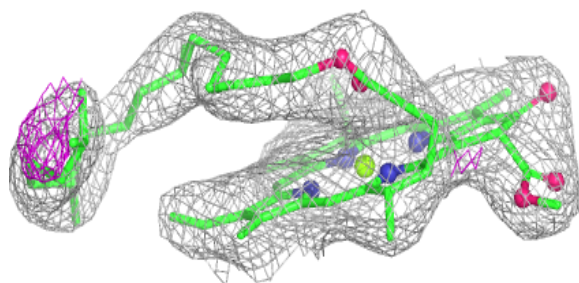
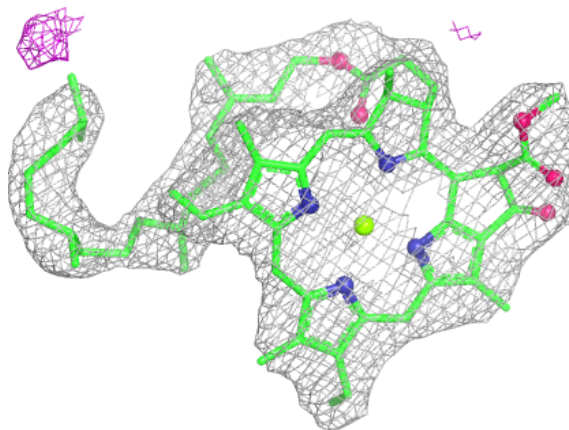


Electron density around CLA G 826:

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

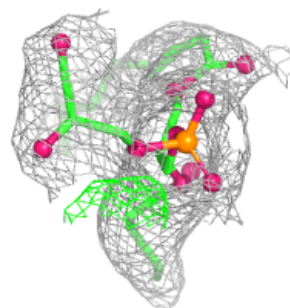
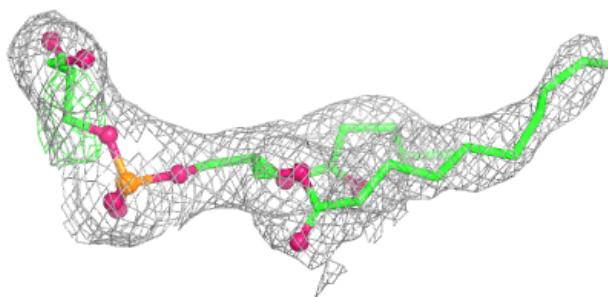
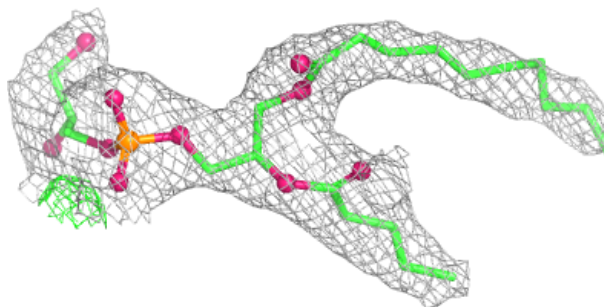
**Electron density around CLA Y 819:**

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

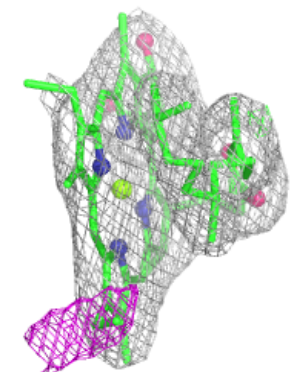
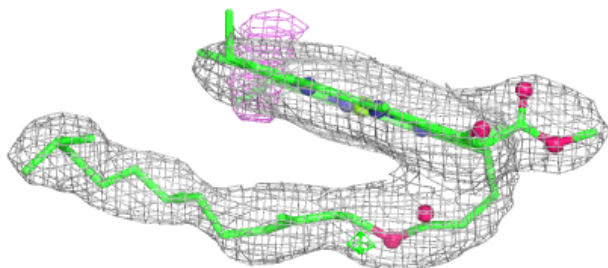
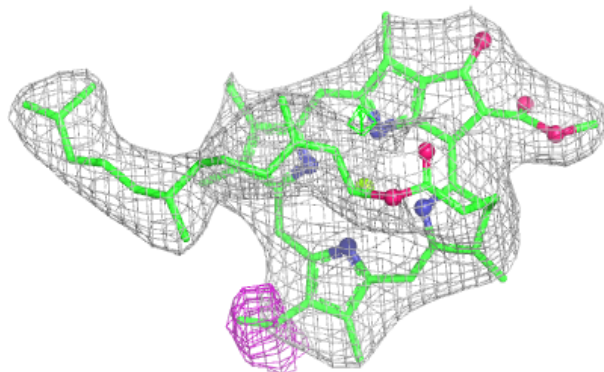


Electron density around LHG G 852:

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

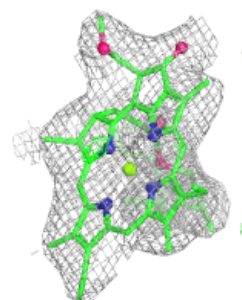
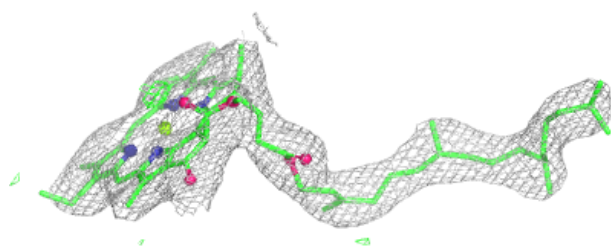
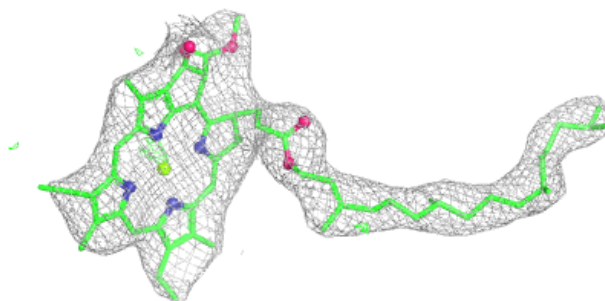
**Electron density around CLA A 817:**

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

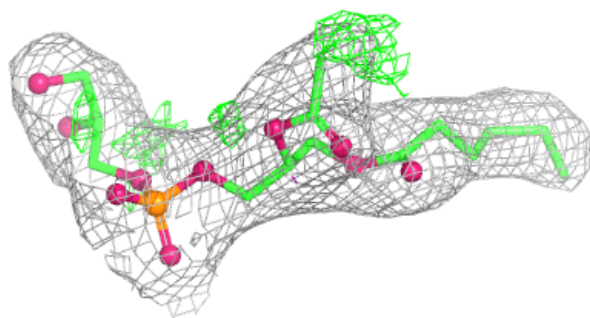
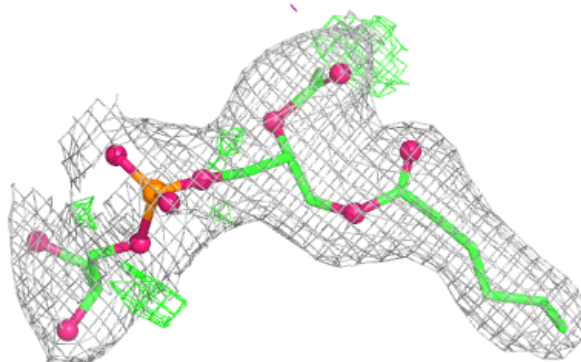


Electron density around CLA Y 821:

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

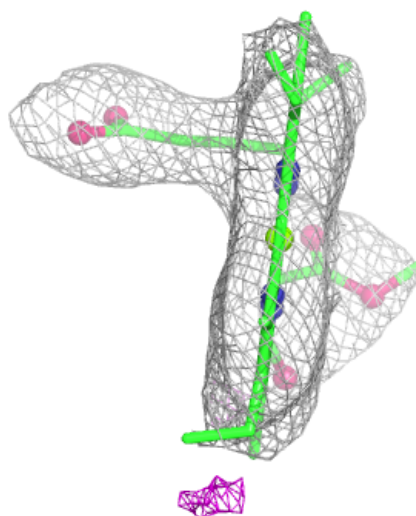
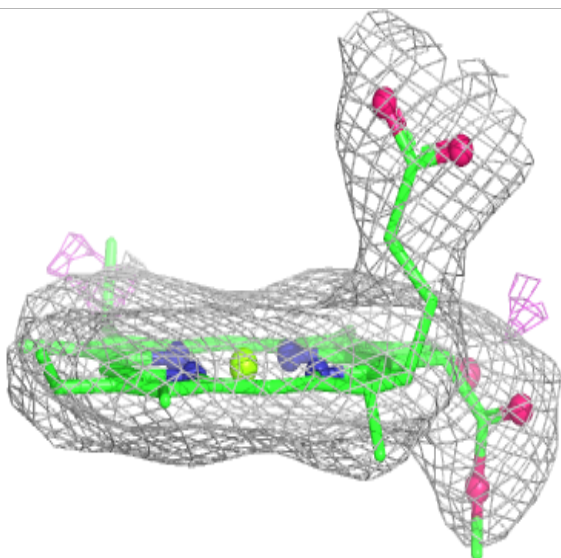
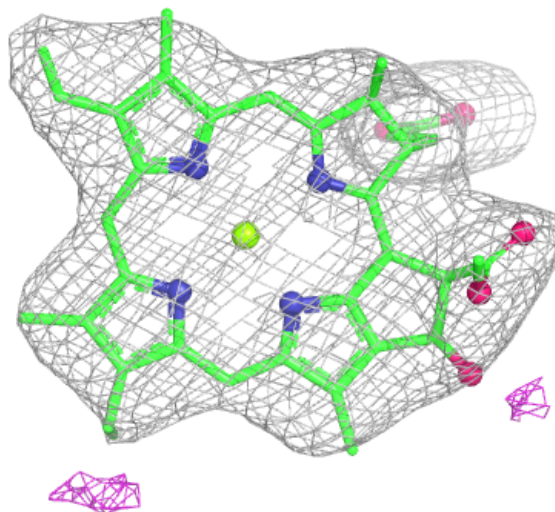
**Electron density around LHG Y 853:**

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



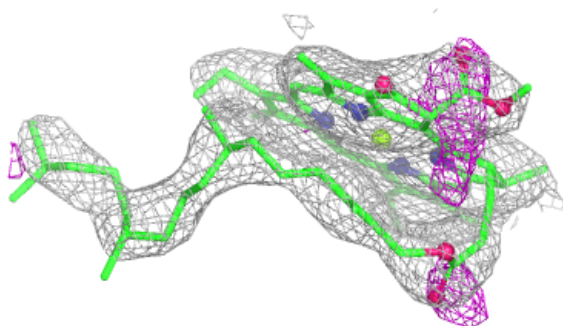
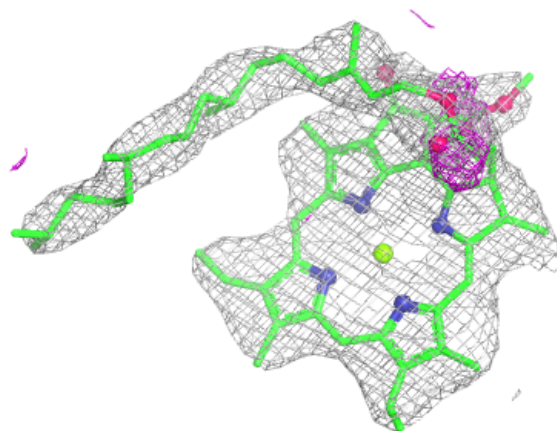
Electron density around CLA B 815:

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



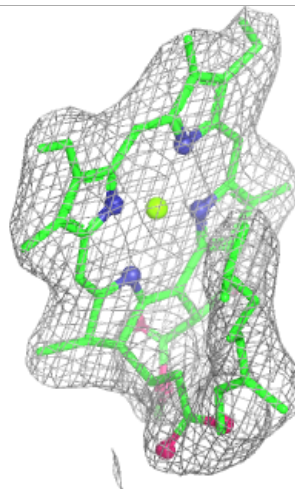
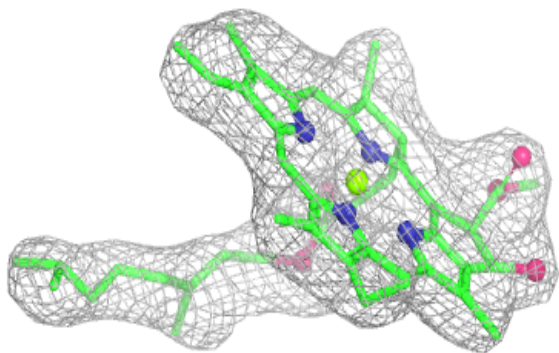
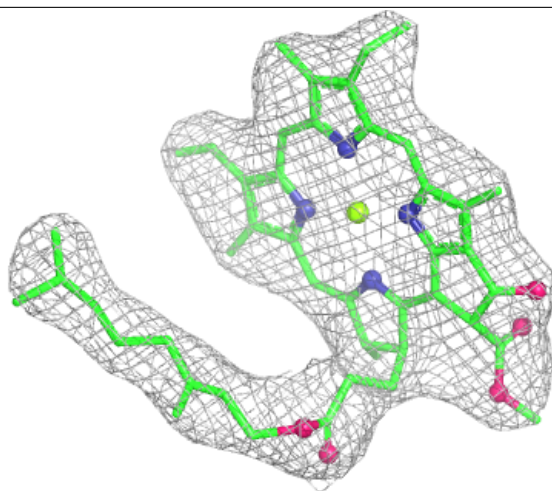
Electron density around CLA G 829:

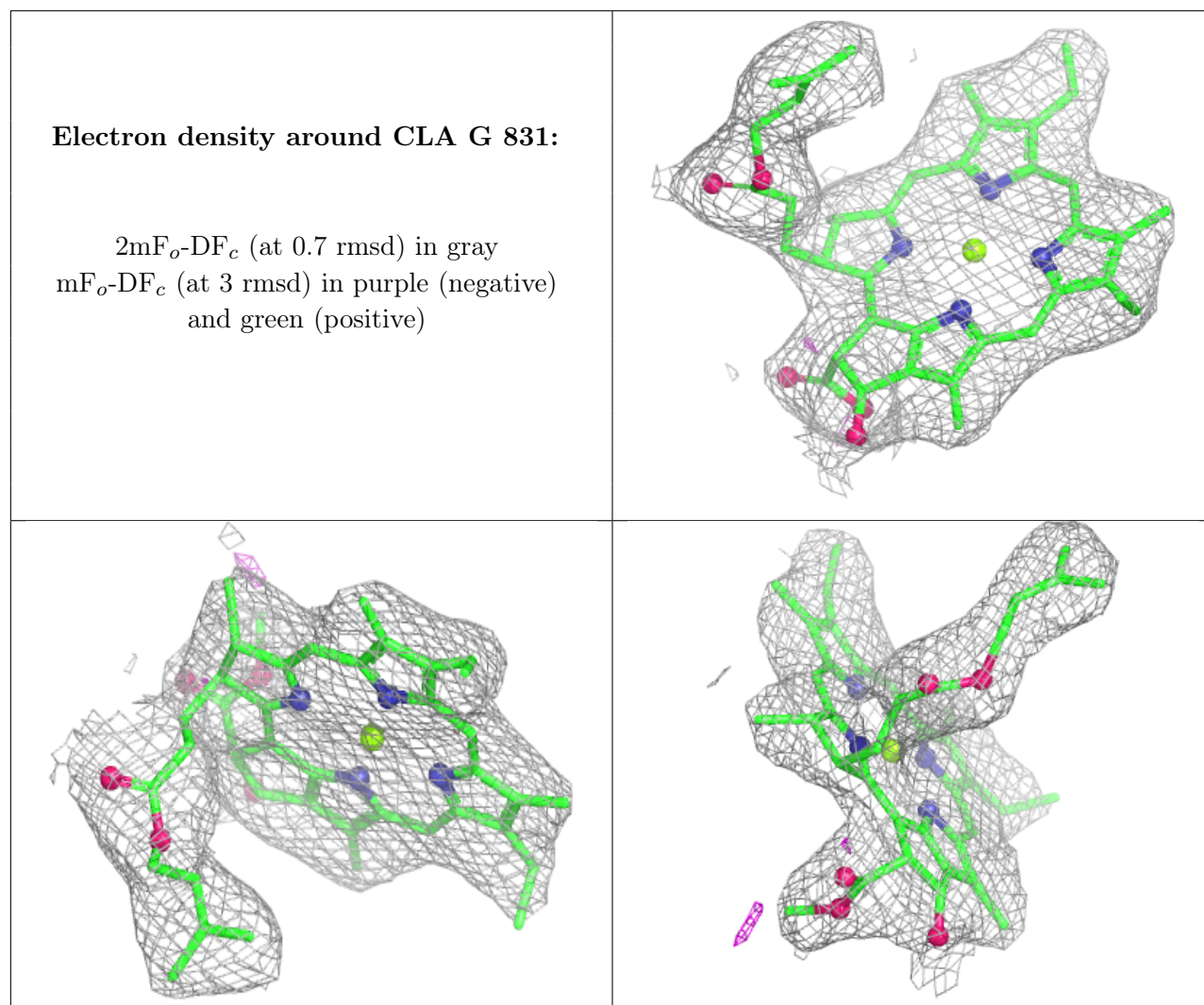
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.