



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 11, 2024 – 09:08 AM JST

PDB ID : 4XK8  
Title : Crystal structure of plant photosystem I-LHCI super-complex at 2.8 angstrom resolution  
Authors : Suga, M.; Qin, X.; Kuang, T.; Shen, J.R.  
Deposited on : 2015-01-10  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

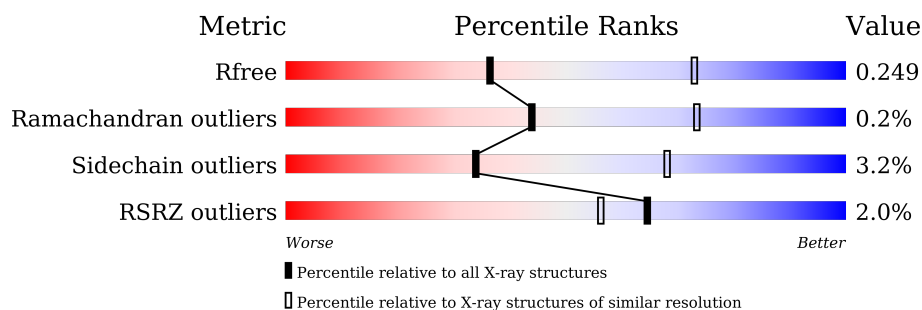
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	164625	3657 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	742	<div> <div></div> <div>98%</div> <div>.</div> </div>
1	a	742	<div> <div></div> <div>98%</div> <div>.</div> </div>
2	B	733	<div> <div>2%</div> <div>98%</div> <div>.</div> </div>
2	b	733	<div> <div></div> <div>98%</div> <div>.</div> </div>
3	C	80	<div> <div></div> <div>98%</div> <div>.</div> </div>
3	c	80	<div> <div></div> <div>98%</div> <div>.</div> </div>
4	D	141	<div> <div>2%</div> <div>96%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
4	d	141	 3% 94% 5%
5	E	64	 98%
5	e	64	 98%
6	F	151	 2% 98%
6	f	151	 2% 97%
7	G	95	 2% 99%
7	g	95	 6% 100%
8	H	90	 2% 97%
8	h	90	 4% 97%
9	I	30	 3% 93%
9	i	30	 7% 97%
10	J	39	 3% 95% 5%
10	j	39	 3% 95% 5%
11	K	84	 % 51% 46%
11	k	84	 2% 52% 45%
12	L	153	 4% 93% 7%
12	l	153	 % 92% 7%
13	1	195	 4% 97%
13	6	195	 7% 97%
14	2	206	 4% 96%
14	7	206	 4% 96%
15	3	218	 2% 97%
15	8	218	 % 97%
16	4	196	 3% 96%
16	9	196	 6% 96%

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
17	CLA	1	303	X	-	-	-
17	CLA	1	304	X	-	-	-
17	CLA	1	305	X	-	-	-
17	CLA	1	306	X	-	-	-
17	CLA	1	308	X	-	-	-
17	CLA	1	309	X	-	-	-
17	CLA	1	310	X	-	-	-
17	CLA	1	311	X	-	-	-
17	CLA	1	312	X	-	-	-
17	CLA	1	313	X	-	-	-
17	CLA	1	315	X	-	-	-
17	CLA	2	602	X	-	-	-
17	CLA	2	603	X	-	-	-
17	CLA	2	604	X	-	-	-
17	CLA	2	608	X	-	-	-
17	CLA	2	609	X	-	-	-
17	CLA	2	610	X	-	-	-
17	CLA	2	611	X	-	-	-
17	CLA	2	612	X	-	-	-
17	CLA	2	613	X	-	-	-
17	CLA	3	301	X	-	-	-
17	CLA	3	302	X	-	-	-
17	CLA	3	303	X	-	-	-
17	CLA	3	304	X	-	-	-
17	CLA	3	305	X	-	-	-
17	CLA	3	306	X	-	-	-
17	CLA	3	308	X	-	-	-
17	CLA	3	309	X	-	-	-
17	CLA	3	310	X	-	-	-
17	CLA	3	311	X	-	-	-
17	CLA	3	312	X	-	-	-
17	CLA	3	313	X	-	-	-
17	CLA	3	314	X	-	-	-
17	CLA	3	315	X	-	-	-
17	CLA	4	601	X	-	-	-
17	CLA	4	602	X	-	-	-
17	CLA	4	603	X	-	-	-
17	CLA	4	604	X	-	-	-
17	CLA	4	608	X	-	-	-
17	CLA	4	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	4	610	X	-	-	-
17	CLA	4	611	X	-	-	-
17	CLA	4	612	X	-	-	-
17	CLA	4	613	X	-	-	-
17	CLA	4	614	X	-	-	-
17	CLA	6	304	X	-	-	-
17	CLA	6	305	X	-	-	-
17	CLA	6	306	X	-	-	-
17	CLA	6	307	X	-	-	-
17	CLA	6	309	X	-	-	-
17	CLA	6	310	X	-	-	-
17	CLA	6	311	X	-	-	-
17	CLA	6	312	X	-	-	-
17	CLA	6	313	X	-	-	-
17	CLA	6	314	X	-	-	-
17	CLA	6	315	X	-	-	-
17	CLA	6	316	X	-	-	-
17	CLA	7	602	X	-	-	-
17	CLA	7	603	X	-	-	-
17	CLA	7	604	X	-	-	-
17	CLA	7	608	X	-	-	-
17	CLA	7	609	X	-	-	-
17	CLA	7	610	X	-	-	-
17	CLA	7	611	X	-	-	-
17	CLA	7	612	X	-	-	-
17	CLA	8	301	X	-	-	-
17	CLA	8	302	X	-	-	-
17	CLA	8	303	X	-	-	-
17	CLA	8	304	X	-	-	-
17	CLA	8	305	X	-	-	-
17	CLA	8	307	X	-	-	-
17	CLA	8	308	X	-	-	-
17	CLA	8	309	X	-	-	-
17	CLA	8	310	X	-	-	-
17	CLA	8	311	X	-	-	-
17	CLA	8	312	X	-	-	-
17	CLA	8	313	X	-	-	-
17	CLA	9	601	X	-	-	-
17	CLA	9	602	X	-	-	-
17	CLA	9	603	X	-	-	-
17	CLA	9	604	X	-	-	-
17	CLA	9	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	9	609	X	-	-	-
17	CLA	9	610	X	-	-	-
17	CLA	9	611	X	-	-	-
17	CLA	9	612	X	-	-	-
17	CLA	9	613	X	-	-	-
17	CLA	9	614	X	-	-	-
17	CLA	A	801	X	-	-	-
17	CLA	A	802	X	-	-	-
17	CLA	A	803	X	-	-	-
17	CLA	A	804	X	-	-	-
17	CLA	A	805	X	-	-	-
17	CLA	A	806	X	-	-	-
17	CLA	A	807	X	-	-	-
17	CLA	A	808	X	-	-	-
17	CLA	A	809	X	-	-	-
17	CLA	A	810	X	-	-	-
17	CLA	A	811	X	-	-	-
17	CLA	A	812	X	-	-	-
17	CLA	A	813	X	-	-	-
17	CLA	A	814	X	-	-	-
17	CLA	A	815	X	-	-	-
17	CLA	A	816	X	-	-	-
17	CLA	A	818	X	-	-	-
17	CLA	A	819	X	-	-	-
17	CLA	A	820	X	-	-	-
17	CLA	A	821	X	-	-	-
17	CLA	A	822	X	-	-	-
17	CLA	A	823	X	-	-	-
17	CLA	A	824	X	-	-	-
17	CLA	A	825	X	-	-	-
17	CLA	A	826	X	-	-	-
17	CLA	A	827	X	-	-	-
17	CLA	A	828	X	-	-	-
17	CLA	A	829	X	-	-	-
17	CLA	A	830	X	-	-	-
17	CLA	A	831	X	-	-	-
17	CLA	A	832	X	-	-	-
17	CLA	A	833	X	-	-	-
17	CLA	A	834	X	-	-	-
17	CLA	A	835	X	-	-	-
17	CLA	A	836	X	-	-	-
17	CLA	A	837	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A	838	X	-	-	-
17	CLA	A	839	X	-	-	-
17	CLA	A	840	X	-	-	-
17	CLA	A	841	X	-	-	-
17	CLA	A	842	X	-	-	-
17	CLA	A	843	X	-	-	-
17	CLA	A	845	X	-	-	-
17	CLA	A	854	X	-	-	-
17	CLA	B	802	X	-	-	-
17	CLA	B	803	X	-	-	-
17	CLA	B	804	X	-	-	-
17	CLA	B	805	X	-	-	-
17	CLA	B	806	X	-	-	-
17	CLA	B	807	X	-	-	-
17	CLA	B	808	X	-	-	-
17	CLA	B	809	X	-	-	-
17	CLA	B	810	X	-	-	-
17	CLA	B	811	X	-	-	-
17	CLA	B	812	X	-	-	-
17	CLA	B	813	X	-	-	-
17	CLA	B	814	X	-	-	-
17	CLA	B	815	X	-	-	-
17	CLA	B	816	X	-	-	-
17	CLA	B	817	X	-	-	-
17	CLA	B	818	X	-	-	-
17	CLA	B	819	X	-	-	-
17	CLA	B	820	X	-	-	-
17	CLA	B	821	X	-	-	-
17	CLA	B	822	X	-	-	-
17	CLA	B	823	X	-	-	-
17	CLA	B	825	X	-	-	-
17	CLA	B	826	X	-	-	-
17	CLA	B	827	X	-	-	-
17	CLA	B	828	X	-	-	-
17	CLA	B	829	X	-	-	-
17	CLA	B	830	X	-	-	-
17	CLA	B	831	X	-	-	-
17	CLA	B	832	X	-	-	-
17	CLA	B	833	X	-	-	-
17	CLA	B	834	X	-	-	-
17	CLA	B	835	X	-	-	-
17	CLA	B	836	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B	837	X	-	-	-
17	CLA	B	838	X	-	-	-
17	CLA	B	839	X	-	-	-
17	CLA	B	841	X	-	-	-
17	CLA	F	301	X	-	-	-
17	CLA	F	303	X	-	-	-
17	CLA	F	304	X	-	-	-
17	CLA	G	101	X	-	-	-
17	CLA	G	103	X	-	-	-
17	CLA	G	104	X	-	-	-
17	CLA	J	3002	X	-	-	-
17	CLA	K	4002	X	-	-	-
17	CLA	K	4003	X	-	-	-
17	CLA	L	202	X	-	-	-
17	CLA	L	203	X	-	-	-
17	CLA	L	204	X	-	-	-
17	CLA	a	801	X	-	-	-
17	CLA	a	802	X	-	-	-
17	CLA	a	803	X	-	-	-
17	CLA	a	804	X	-	-	-
17	CLA	a	805	X	-	-	-
17	CLA	a	806	X	-	-	-
17	CLA	a	807	X	-	-	-
17	CLA	a	808	X	-	-	-
17	CLA	a	809	X	-	-	-
17	CLA	a	810	X	-	-	-
17	CLA	a	811	X	-	-	-
17	CLA	a	812	X	-	-	-
17	CLA	a	813	X	-	-	-
17	CLA	a	814	X	-	-	-
17	CLA	a	815	X	-	-	-
17	CLA	a	816	X	-	-	-
17	CLA	a	817	X	-	-	-
17	CLA	a	818	X	-	-	-
17	CLA	a	819	X	-	-	-
17	CLA	a	820	X	-	-	-
17	CLA	a	821	X	-	-	-
17	CLA	a	822	X	-	-	-
17	CLA	a	823	X	-	-	-
17	CLA	a	824	X	-	-	-
17	CLA	a	825	X	-	-	-
17	CLA	a	826	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	a	827	X	-	-	-
17	CLA	a	828	X	-	-	-
17	CLA	a	829	X	-	-	-
17	CLA	a	830	X	-	-	-
17	CLA	a	831	X	-	-	-
17	CLA	a	832	X	-	-	-
17	CLA	a	833	X	-	-	-
17	CLA	a	834	X	-	-	-
17	CLA	a	835	X	-	-	-
17	CLA	a	836	X	-	-	-
17	CLA	a	837	X	-	-	-
17	CLA	a	838	X	-	-	-
17	CLA	a	839	X	-	-	-
17	CLA	a	840	X	-	-	-
17	CLA	a	841	X	-	-	-
17	CLA	a	842	X	-	-	-
17	CLA	a	843	X	-	-	-
17	CLA	a	844	X	-	-	-
17	CLA	a	846	X	-	-	-
17	CLA	a	856	X	-	-	-
17	CLA	b	802	X	-	-	-
17	CLA	b	803	X	-	-	-
17	CLA	b	804	X	-	-	-
17	CLA	b	805	X	-	-	-
17	CLA	b	806	X	-	-	-
17	CLA	b	807	X	-	-	-
17	CLA	b	808	X	-	-	-
17	CLA	b	809	X	-	-	-
17	CLA	b	810	X	-	-	-
17	CLA	b	811	X	-	-	-
17	CLA	b	812	X	-	-	-
17	CLA	b	813	X	-	-	-
17	CLA	b	814	X	-	-	-
17	CLA	b	815	X	-	-	-
17	CLA	b	816	X	-	-	-
17	CLA	b	817	X	-	-	-
17	CLA	b	818	X	-	-	-
17	CLA	b	819	X	-	-	-
17	CLA	b	820	X	-	-	-
17	CLA	b	821	X	-	-	-
17	CLA	b	822	X	-	-	-
17	CLA	b	823	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	b	824	X	-	-	-
17	CLA	b	825	X	-	-	-
17	CLA	b	826	X	-	-	-
17	CLA	b	827	X	-	-	-
17	CLA	b	828	X	-	-	-
17	CLA	b	829	X	-	-	-
17	CLA	b	830	X	-	-	-
17	CLA	b	831	X	-	-	-
17	CLA	b	832	X	-	-	-
17	CLA	b	833	X	-	-	-
17	CLA	b	834	X	-	-	-
17	CLA	b	835	X	-	-	-
17	CLA	b	836	X	-	-	-
17	CLA	b	837	X	-	-	-
17	CLA	b	838	X	-	-	-
17	CLA	b	839	X	-	-	-
17	CLA	b	840	X	-	-	-
17	CLA	b	841	X	-	-	-
17	CLA	f	7002	X	-	-	-
17	CLA	g	102	X	-	-	-
17	CLA	g	103	X	-	-	-
17	CLA	j	3002	X	-	-	-
17	CLA	k	1401	X	-	-	-
17	CLA	k	1402	X	-	-	-
17	CLA	k	1403	X	-	-	-
17	CLA	l	202	X	-	-	-
17	CLA	l	203	X	-	-	-
17	CLA	l	204	X	-	-	-
26	CHL	1	302	X	-	-	-
26	CHL	1	307	X	-	-	-
26	CHL	2	601	X	-	-	-
26	CHL	2	605	X	-	-	-
26	CHL	2	606	X	-	-	-
26	CHL	2	607	X	-	-	-
26	CHL	2	614	X	-	-	-
26	CHL	3	307	X	-	-	-
26	CHL	4	605	X	-	-	-
26	CHL	4	606	X	-	-	-
26	CHL	4	607	X	-	-	-
26	CHL	4	615	X	-	-	-
26	CHL	6	303	X	-	-	-
26	CHL	6	308	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CHL	7	601	X	-	-	-
26	CHL	7	605	X	-	-	-
26	CHL	7	606	X	-	-	-
26	CHL	7	607	X	-	-	-
26	CHL	7	614	X	-	-	-
26	CHL	8	306	X	-	-	-
26	CHL	9	605	X	-	-	-
26	CHL	9	606	X	-	-	-
26	CHL	9	607	X	-	-	-
26	CHL	9	615	X	-	-	-

## 2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 71157 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	742	Total	C	N	O	S	0	0	0
			5846	3831	994	1003	18			
1	a	742	Total	C	N	O	S	0	0	0
			5846	3831	994	1003	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	733	Total	C	N	O	S	0	0	0
			5863	3853	1002	994	14			
2	b	733	Total	C	N	O	S	0	0	0
			5863	3853	1002	994	14			

- 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
			611	379	107	114	11			
3	c	80	Total	C	N	O	S	0	0	0
			611	379	107	114	11			

- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	141	Total	C	N	O	S	0	0	0
			1114	716	193	202	3			
4	d	140	Total	C	N	O	S	0	0	0
			1107	712	192	200	3			

- Molecule 5 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	63	Total	C	N	O	0	0	0
			507	321	90	96			
5	e	63	Total	C	N	O	0	0	0
			506	322	90	94			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	151	Total	C	N	O	S	0	0	0
			1193	776	204	210	3			
6	f	151	Total	C	N	O	S	0	0	0
			1193	776	204	210	3			

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	95	Total	C	N	O	0	0	0
			741	480	121	140			
7	g	95	Total	C	N	O	0	0	0
			737	478	121	138			

- Molecule 8 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	90	Total	C	N	O	0	0	0
			678	439	110	129			
8	h	90	Total	C	N	O	0	0	0
			682	442	111	129			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	29	Total	C	N	O	S	0	0	0
			221	153	33	34	1			
9	i	30	Total	C	N	O	S	0	0	0
			226	156	34	35	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	39	Total	C	N	O	S	0	0	0
			311	211	48	51	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	j	39	Total	C	N	O	S	0	0	0
			311	211	48	51	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	45	Total	C	N	O	S	0	0	0
			311	204	48	56	3			
11	k	46	Total	C	N	O	S	0	0	0
			316	207	49	57	3			

- Molecule 12 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	153	Total	C	N	O	S	0	0	0
			1136	746	183	206	1			
12	l	151	Total	C	N	O	S	0	0	0
			1122	738	180	203	1			

- Molecule 13 is a protein called Chlorophyll a-b binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1	195	Total	C	N	O	S	0	0	0
			1491	969	249	268	5			
13	6	195	Total	C	N	O	S	0	0	0
			1483	963	247	268	5			

- Molecule 14 is a protein called Type II chlorophyll a/b binding protein from photosystem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	2	206	Total	C	N	O	S	0	0	0
			1610	1055	263	288	4			
14	7	206	Total	C	N	O	S	0	0	0
			1610	1055	263	288	4			

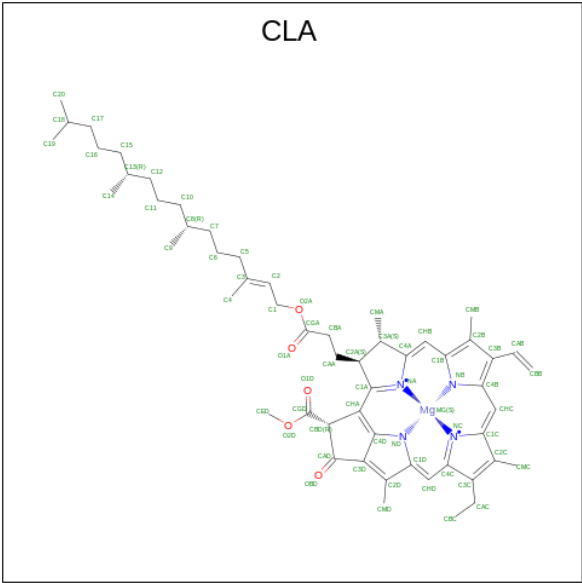
- Molecule 15 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	3	218	Total	C	N	O	S	0	0	0
			1680	1100	273	302	5			
15	8	217	Total	C	N	O	S	0	0	0
			1672	1094	272	301	5			

- Molecule 16 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	4	196	Total	C	N	O	S	0	0	0
			1540	1009	251	277	3			
16	9	196	Total	C	N	O	S	0	0	0
			1540	1009	251	277	3			

- Molecule 17 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	A	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	A	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	F	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	G	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	G	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	G	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	J	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	K	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
17	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	L	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	1	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
17	1	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
17	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	1	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
17	1	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
17	1	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
17	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	1	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
17	1	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
17	2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	2	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
17	2	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	2	1	Total 60	C 50	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	2	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	2	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			43	35	1	4	3		
17	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	3	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			37	31	1	4	1		
17	3	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
17	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	a	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	a	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
17	a	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
17	a	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	b	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 58	C 48	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	b	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	f	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	f	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
17	g	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
17	g	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	g	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
17	j	1	Total 42	C 34	Mg 1	N 4	O 3	0	0
17	k	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	k	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
17	k	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
17	l	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	l	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	6	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	6	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	7	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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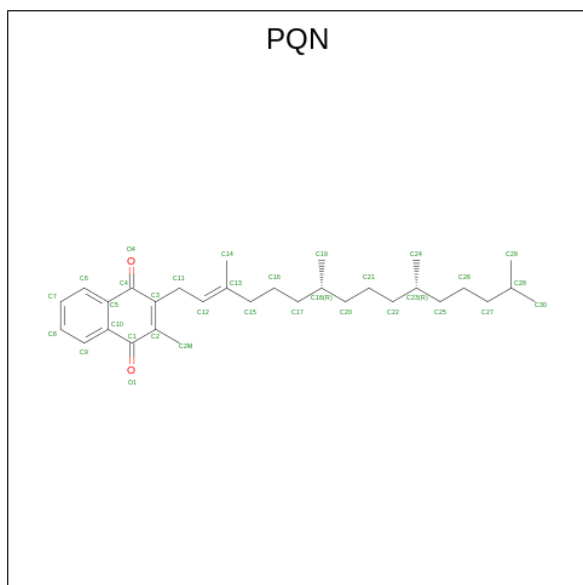
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	7	1	Total	C	Mg	N	O	0	0
			43	35	1	4	3		
17	8	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	8	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	8	1	Total	C	Mg	N		0	0
			25	20	1	4			
17	9	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	9	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		

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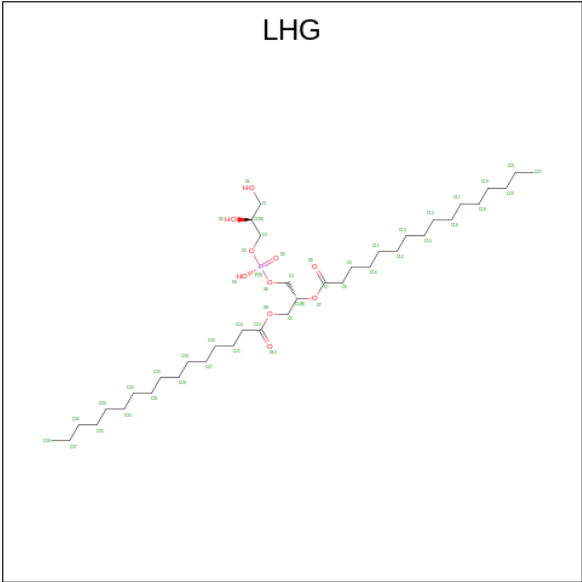
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	9	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		

- Molecule 18 is PHYLLOQUINONE (three-letter code: PQN) (formula:  $C_{31}H_{46}O_2$ ).



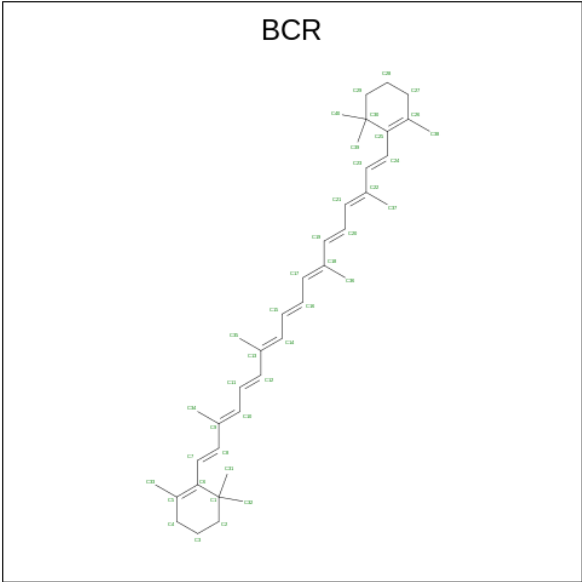
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			33	31	2		
18	B	1	Total	C	O	0	0
			33	31	2		
18	a	1	Total	C	O	0	0
			33	31	2		
18	b	1	Total	C	O	0	0
			33	31	2		

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			49	38	10	1		
19	A	1	Total	C	O	P	0	0
			27	16	10	1		
19	1	1	Total	C	O	P	0	0
			23	12	10	1		
19	1	1	Total	C	O	P	0	0
			49	38	10	1		
19	2	1	Total	C	O	P	0	0
			37	26	10	1		
19	3	1	Total	C	O	P	0	0
			20	10	9	1		
19	a	1	Total	C	O	P	0	0
			49	38	10	1		
19	a	1	Total	C	O	P	0	0
			27	16	10	1		
19	6	1	Total	C	O	P	0	0
			23	12	10	1		
19	6	1	Total	C	O	P	0	0
			49	38	10	1		
19	7	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 20 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C 40 40	0	0
20	A	1	Total C 40 40	0	0
20	A	1	Total C 40 40	0	0
20	A	1	Total C 40 40	0	0
20	A	1	Total C 40 40	0	0
20	A	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	F	1	Total C 40 40	0	0

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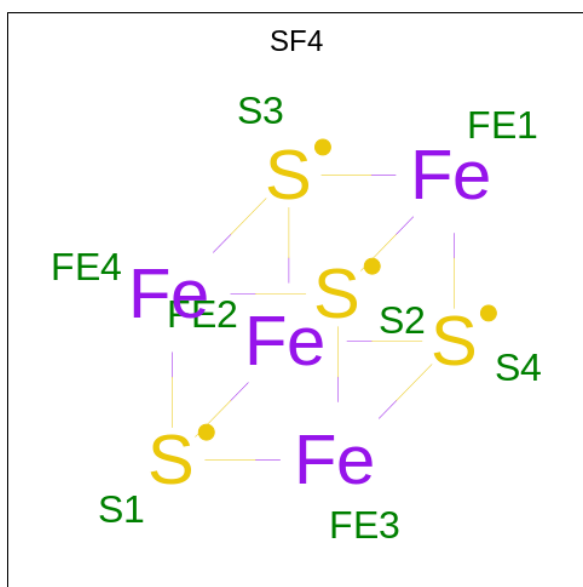
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	G	1	Total C 40 40	0	0
20	I	1	Total C 40 40	0	0
20	J	1	Total C 40 40	0	0
20	K	1	Total C 40 40	0	0
20	K	1	Total C 40 40	0	0
20	L	1	Total C 40 40	0	0
20	L	1	Total C 40 40	0	0
20	L	1	Total C 40 40	0	0
20	1	1	Total C 40 40	0	0
20	2	1	Total C 40 40	0	0
20	3	1	Total C 40 40	0	0
20	4	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	f	1	Total C 40 40	0	0
20	g	1	Total C 40 40	0	0
20	i	1	Total C 40 40	0	0
20	j	1	Total C 40 40	0	0
20	j	1	Total C 40 40	0	0
20	k	1	Total C 40 40	0	0
20	l	1	Total C 40 40	0	0
20	l	1	Total C 40 40	0	0
20	l	1	Total C 40 40	0	0
20	6	1	Total C 40 40	0	0
20	7	1	Total C 40 40	0	0
20	8	1	Total C 40 40	0	0
20	9	1	Total C 40 40	0	0

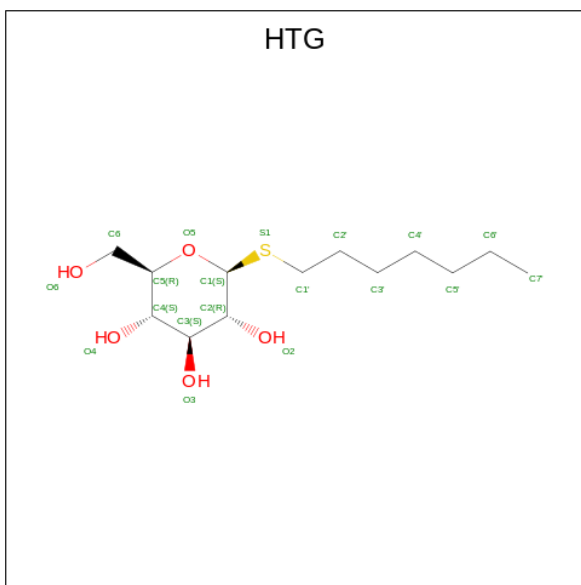
- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	Fe	S	0	0
			8	4	4		
21	C	1	Total	Fe	S	0	0
			8	4	4		
21	C	1	Total	Fe	S	0	0
			8	4	4		
21	a	1	Total	Fe	S	0	0
			8	4	4		
21	c	1	Total	Fe	S	0	0
			8	4	4		
21	c	1	Total	Fe	S	0	0
			8	4	4		

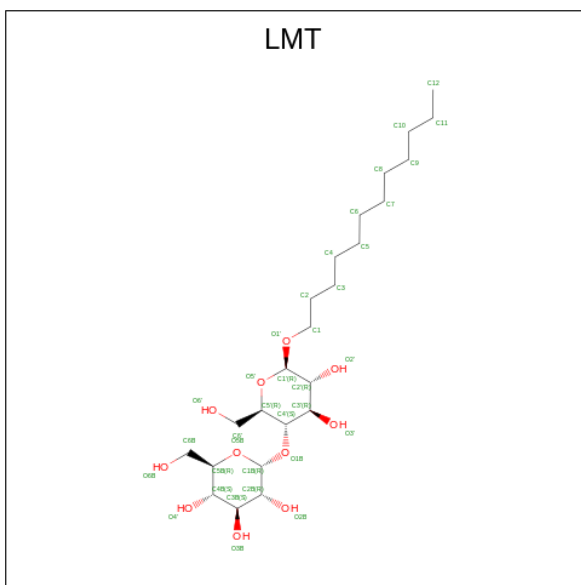
- Molecule 22 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C<sub>13</sub>H<sub>26</sub>O<sub>5</sub>S).





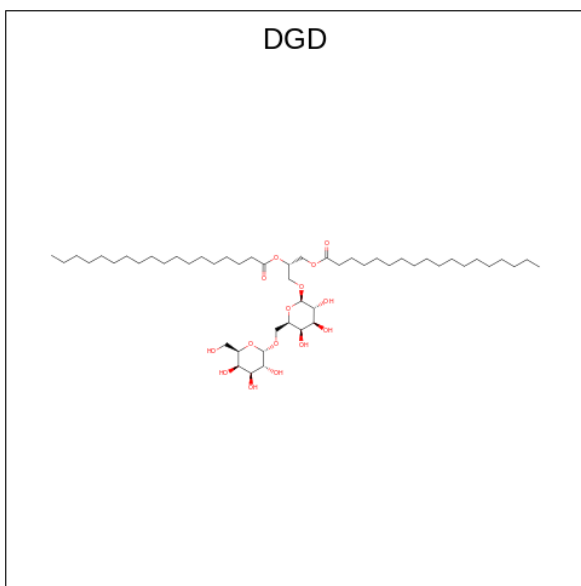
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	O	S	0	0
			19	13	5	1		
22	F	1	Total	C	O	S	0	0
			19	13	5	1		
22	J	1	Total	C	O	S	0	0
			19	13	5	1		
22	a	1	Total	C	O	S	0	0
			19	13	5	1		
22	f	1	Total	C	O	S	0	0
			19	13	5	1		
22	j	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 23 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



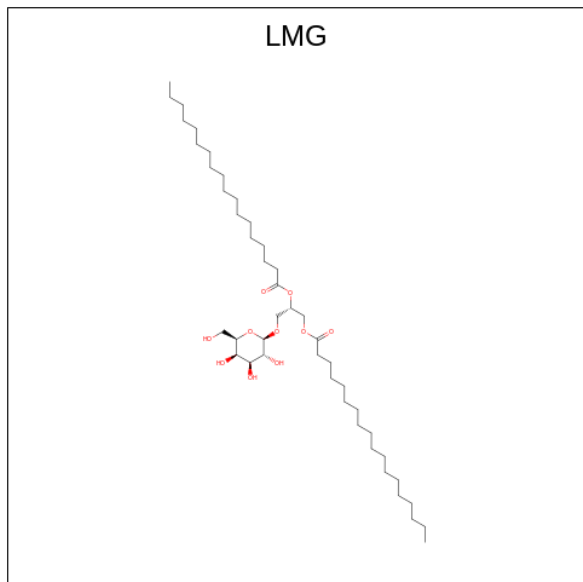
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			35	24	11		

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



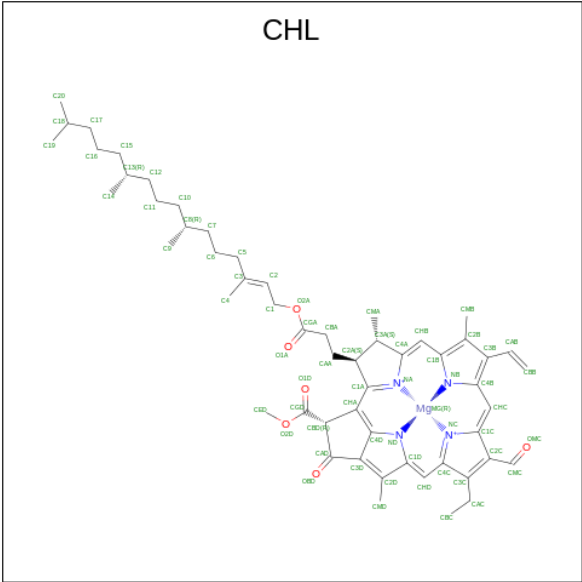
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total 66	C 51	O 15	0	0
24	b	1	Total 66	C 51	O 15	0	0

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	G	1	Total	C	O	0	0
			44	34	10		
25	4	1	Total	C	O	0	0
			44	34	10		
25	4	1	Total	C	O	0	0
			44	34	10		
25	6	1	Total	C	O	0	0
			40	30	10		
25	9	1	Total	C	O	0	0
			50	40	10		

- Molecule 26 is CHLOROPHYLL B (three-letter code: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ).



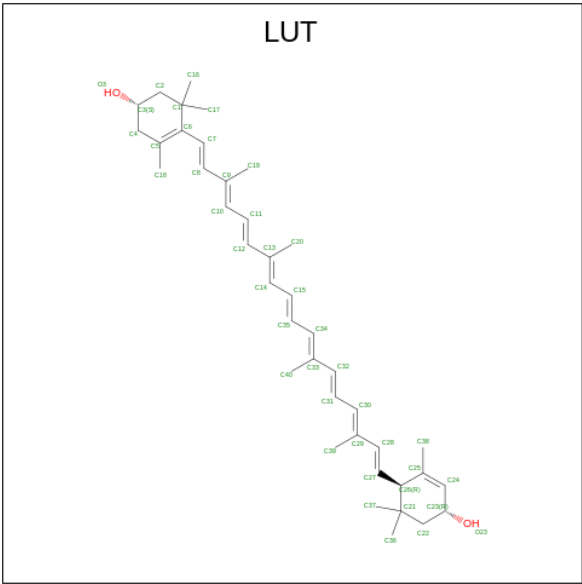
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	1	1	Total 61	C 50	Mg 1	N 4	O 6	0	0
26	1	1	Total 48	C 37	Mg 1	N 4	O 6	0	0
26	2	1	Total 61	C 50	Mg 1	N 4	O 6	0	0
26	2	1	Total 43	C 34	Mg 1	N 4	O 4	0	0
26	2	1	Total 48	C 37	Mg 1	N 4	O 6	0	0
26	2	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
26	2	1	Total 43	C 34	Mg 1	N 4	O 4	0	0
26	3	1	Total 47	C 36	Mg 1	N 4	O 6	0	0
26	4	1	Total 56	C 45	Mg 1	N 4	O 6	0	0
26	4	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
26	4	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
26	4	1	Total 43	C 34	Mg 1	N 4	O 4	0	0
26	6	1	Total 61	C 50	Mg 1	N 4	O 6	0	0
26	6	1	Total 47	C 36	Mg 1	N 4	O 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	7	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
26	7	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
26	7	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
26	7	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
26	7	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
26	8	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
26	9	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
26	9	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
26	9	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
26	9	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		

- Molecule 27 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



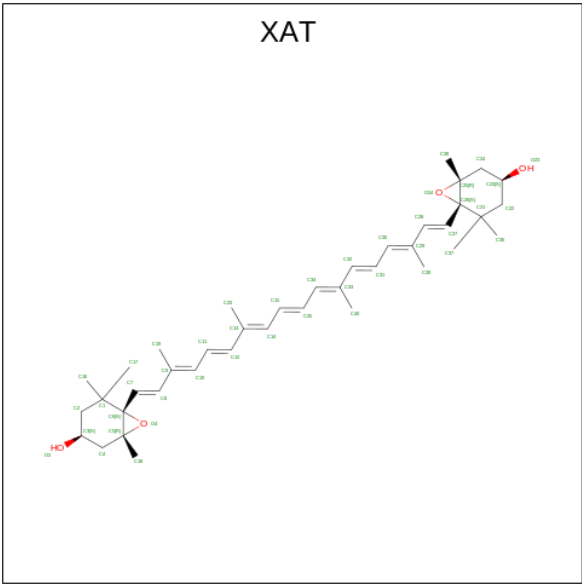
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	1	1	Total	C	O	0	0
			42	40	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	1	1	Total	C	O	0	0
			42	40	2		
27	2	1	Total	C	O	0	0
			42	40	2		
27	3	1	Total	C	O	0	0
			42	40	2		
27	4	1	Total	C	O	0	0
			42	40	2		
27	6	1	Total	C	O	0	0
			42	40	2		
27	6	1	Total	C	O	0	0
			42	40	2		
27	7	1	Total	C	O	0	0
			42	40	2		
27	8	1	Total	C	O	0	0
			42	40	2		
27	9	1	Total	C	O	0	0
			42	40	2		

- Molecule 28 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	1	1	Total	C	O	0	0
			44	40	4		
28	2	1	Total	C	O	0	0
			44	40	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	3	1	Total	C	O	0	0
			44	40	4		
28	4	1	Total	C	O	0	0
			44	40	4		
28	6	1	Total	C	O	0	0
			44	40	4		
28	7	1	Total	C	O	0	0
			44	40	4		
28	8	1	Total	C	O	0	0
			44	40	4		
28	9	1	Total	C	O	0	0
			44	40	4		

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	29	Total	O	0	0
			29	29		
29	B	42	Total	O	0	0
			42	42		
29	C	1	Total	O	0	0
			1	1		
29	D	2	Total	O	0	0
			2	2		
29	F	5	Total	O	0	0
			5	5		
29	I	1	Total	O	0	0
			1	1		
29	L	1	Total	O	0	0
			1	1		
29	1	3	Total	O	0	0
			3	3		
29	2	4	Total	O	0	0
			4	4		
29	3	3	Total	O	0	0
			3	3		
29	4	6	Total	O	0	0
			6	6		
29	a	30	Total	O	0	0
			30	30		
29	b	32	Total	O	0	0
			32	32		

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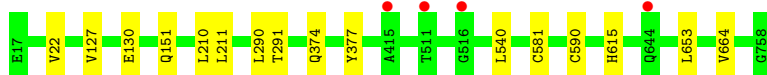
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	d	1	Total 1	O 1	0	0
29	f	4	Total 4	O 4	0	0
29	h	1	Total 1	O 1	0	0
29	l	3	Total 3	O 3	0	0
29	6	3	Total 3	O 3	0	0
29	7	6	Total 6	O 6	0	0
29	8	3	Total 3	O 3	0	0
29	9	5	Total 5	O 5	0	0



### 3 Residue-property plots [i](#)

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.

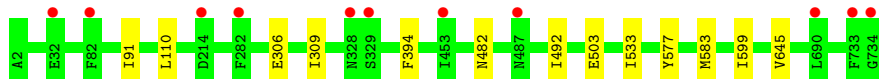
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center



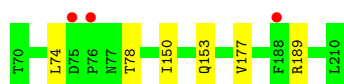
- Molecule 3: Photosystem I iron-sulfur center

Chain c:  98% .



- Molecule 4: Uncharacterized protein

Chain D:  96% .



- Molecule 4: Uncharacterized protein

Chain d:  94% 5% .



- Molecule 5: Putative uncharacterized protein

Chain E:  98% .



- Molecule 5: Putative uncharacterized protein

Chain e:  98% .



- Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain F:  98% .

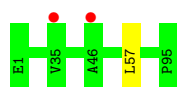


- Molecule 6: Photosystem I reaction center subunit III, chloroplastic

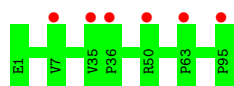
Chain f:  97% .



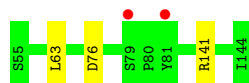
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



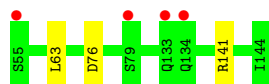
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



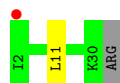
- Molecule 8: Putative uncharacterized protein



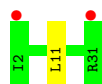
- Molecule 8: Putative uncharacterized protein



- Molecule 9: Photosystem I reaction center subunit VIII



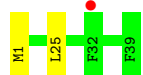
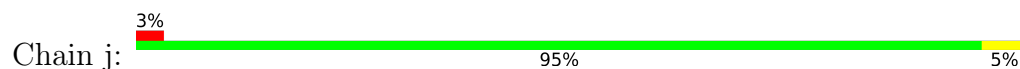
- Molecule 9: Photosystem I reaction center subunit VIII



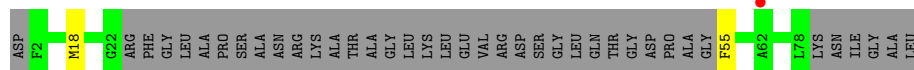
- Molecule 10: Photosystem I reaction center subunit IX



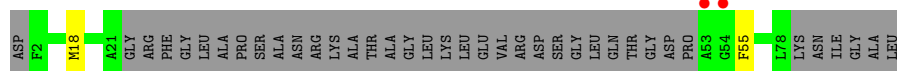
- Molecule 10: Photosystem I reaction center subunit IX



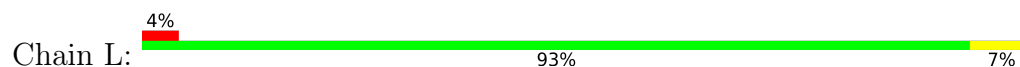
- Molecule 11: Photosystem I reaction center subunit X psaK



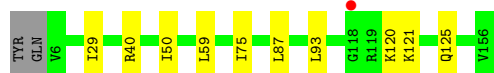
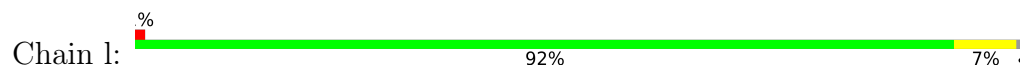
- Molecule 11: Photosystem I reaction center subunit X psaK



- Molecule 12: Putative uncharacterized protein



- Molecule 12: Putative uncharacterized protein

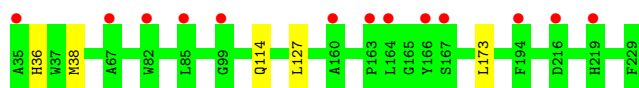


- Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic

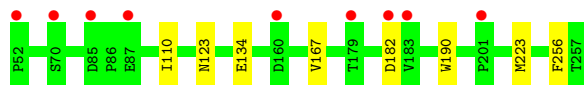


- Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic

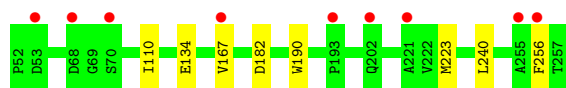




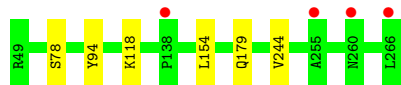
- Molecule 14: Type II chlorophyll a/b binding protein from photosystem I



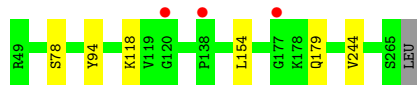
- Molecule 14: Type II chlorophyll a/b binding protein from photosystem I



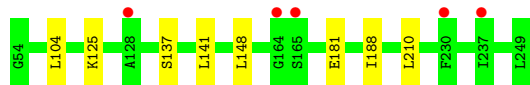
- Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic



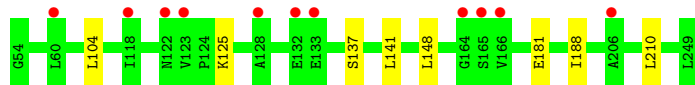
- Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic



- Molecule 16: Chlorophyll a-b binding protein P4, chloroplastic



- Molecule 16: Chlorophyll a-b binding protein P4, chloroplastic



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	165.62Å 192.22Å 175.09Å 90.00° 91.41° 90.00°	Depositor
Resolution (Å)	49.15 – 2.80 49.15 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.15-2.80) 99.8 (49.15-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, $R_{free}$	0.210 , 0.248 0.212 , 0.249	Depositor DCC
$R_{free}$ test set	13503 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.2	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 57.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	71157	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, HTG, DGD, SF4, LMG, PQN, LHG, LUT, CLA, CHL, XAT, LMT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/6043	0.41	0/8245
1	a	0.26	0/6043	0.42	0/8245
2	B	0.25	0/6077	0.42	0/8299
2	b	0.25	0/6077	0.42	0/8299
3	C	0.22	0/624	0.41	0/846
3	c	0.23	0/624	0.43	0/846
4	D	0.23	0/1143	0.42	0/1545
4	d	0.24	0/1136	0.43	0/1534
5	E	0.21	0/517	0.39	0/701
5	e	0.21	0/516	0.39	0/700
6	F	0.23	0/1221	0.40	0/1648
6	f	0.24	0/1221	0.40	0/1648
7	G	0.24	0/759	0.39	0/1033
7	g	0.24	0/755	0.40	0/1028
8	H	0.22	0/697	0.39	0/950
8	h	0.22	0/701	0.40	0/954
9	I	0.26	0/227	0.44	0/310
9	i	0.26	0/232	0.44	0/317
10	J	0.24	0/319	0.40	0/434
10	j	0.24	0/319	0.41	0/434
11	K	0.22	0/314	0.37	0/426
11	k	0.24	0/319	0.38	0/433
12	L	0.23	0/1167	0.43	0/1596
12	l	0.25	0/1153	0.44	0/1577
13	1	0.24	0/1539	0.40	0/2099
13	6	0.23	0/1531	0.38	0/2091
14	2	0.23	0/1670	0.40	0/2288
14	7	0.23	0/1670	0.39	0/2288
15	3	0.25	0/1732	0.39	0/2352
15	8	0.25	0/1724	0.39	0/2341
16	4	0.24	0/1589	0.40	0/2168
16	9	0.23	0/1589	0.39	0/2168

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.24	0/51248	0.41	0/69843

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

## 5.3 Torsion angles [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	740/742 (100%)	710 (96%)	28 (4%)	2 (0%)	37	67
1	a	740/742 (100%)	709 (96%)	29 (4%)	2 (0%)	37	67
2	B	731/733 (100%)	700 (96%)	30 (4%)	1 (0%)	48	77
2	b	731/733 (100%)	700 (96%)	30 (4%)	1 (0%)	48	77
3	C	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
3	c	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
4	D	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
4	d	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
5	E	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
5	e	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
6	F	149/151 (99%)	147 (99%)	1 (1%)	1 (1%)	19	48
6	f	149/151 (99%)	147 (99%)	1 (1%)	1 (1%)	19	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
7	g	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
8	H	88/90 (98%)	87 (99%)	1 (1%)	0	100	100
8	h	88/90 (98%)	87 (99%)	1 (1%)	0	100	100
9	I	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
9	i	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
10	J	37/39 (95%)	37 (100%)	0	0	100	100
10	j	37/39 (95%)	37 (100%)	0	0	100	100
11	K	41/84 (49%)	41 (100%)	0	0	100	100
11	k	42/84 (50%)	42 (100%)	0	0	100	100
12	L	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
12	l	149/153 (97%)	143 (96%)	6 (4%)	0	100	100
13	1	193/195 (99%)	187 (97%)	6 (3%)	0	100	100
13	6	193/195 (99%)	189 (98%)	4 (2%)	0	100	100
14	2	204/206 (99%)	196 (96%)	8 (4%)	0	100	100
14	7	204/206 (99%)	195 (96%)	9 (4%)	0	100	100
15	3	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
15	8	215/218 (99%)	204 (95%)	11 (5%)	0	100	100
16	4	194/196 (99%)	184 (95%)	9 (5%)	1 (0%)	25	56
16	9	194/196 (99%)	183 (94%)	10 (5%)	1 (0%)	25	56
All	All	6282/6434 (98%)	6041 (96%)	231 (4%)	10 (0%)	44	73

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	159	PHE
6	f	159	PHE
1	A	581	CYS
16	9	137	SER
16	4	137	SER

### 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	602/602 (100%)	588 (98%)	14 (2%)	45	78
1	a	602/602 (100%)	587 (98%)	15 (2%)	42	75
2	B	597/597 (100%)	585 (98%)	12 (2%)	50	81
2	b	597/597 (100%)	582 (98%)	15 (2%)	42	75
3	C	69/69 (100%)	67 (97%)	2 (3%)	37	71
3	c	69/69 (100%)	67 (97%)	2 (3%)	37	71
4	D	119/120 (99%)	113 (95%)	6 (5%)	20	51
4	d	118/120 (98%)	111 (94%)	7 (6%)	16	44
5	E	55/56 (98%)	55 (100%)	0	100	100
5	e	55/56 (98%)	55 (100%)	0	100	100
6	F	123/125 (98%)	121 (98%)	2 (2%)	58	85
6	f	123/125 (98%)	120 (98%)	3 (2%)	44	77
7	G	81/81 (100%)	80 (99%)	1 (1%)	67	89
7	g	80/81 (99%)	80 (100%)	0	100	100
8	H	72/73 (99%)	69 (96%)	3 (4%)	25	58
8	h	73/73 (100%)	70 (96%)	3 (4%)	26	59
9	I	25/26 (96%)	24 (96%)	1 (4%)	27	60
9	i	25/26 (96%)	24 (96%)	1 (4%)	27	60
10	J	33/33 (100%)	31 (94%)	2 (6%)	15	43
10	j	33/33 (100%)	31 (94%)	2 (6%)	15	43
11	K	34/62 (55%)	32 (94%)	2 (6%)	16	44
11	k	34/62 (55%)	32 (94%)	2 (6%)	16	44
12	L	118/119 (99%)	108 (92%)	10 (8%)	8	27
12	l	117/119 (98%)	107 (92%)	10 (8%)	8	27
13	1	149/153 (97%)	144 (97%)	5 (3%)	32	66
13	6	147/153 (96%)	142 (97%)	5 (3%)	32	66
14	2	166/166 (100%)	158 (95%)	8 (5%)	21	53
14	7	166/166 (100%)	158 (95%)	8 (5%)	21	53
15	3	169/169 (100%)	163 (96%)	6 (4%)	30	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	8	168/169 (99%)	162 (96%)	6 (4%)	30	64
16	4	161/161 (100%)	154 (96%)	7 (4%)	25	57
16	9	161/161 (100%)	154 (96%)	7 (4%)	25	57
All	All	5141/5224 (98%)	4974 (97%)	167 (3%)	34	68

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	145	ARG
13	6	114	GLN
4	d	189	ARG
11	k	55	PHE
14	7	190	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
15	3	99	ASN
16	9	150	HIS
16	4	168	GLN
16	9	232	ASN
13	6	114	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

414 ligands are modelled in this entry.

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$
17	CLA	B	820	2	50,58,73	2.40	17 (34%)	58,95,113	3.04	27 (46%)
17	CLA	A	834	1	65,73,73	2.08	17 (26%)	76,113,113	2.74	27 (35%)
17	CLA	a	809	1	65,73,73	2.07	15 (23%)	76,113,113	2.80	26 (34%)
20	BCR	9	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.81	16 (28%)
17	CLA	a	814	1	65,73,73	2.10	16 (24%)	76,113,113	2.68	25 (32%)
17	CLA	1	314	13	55,63,73	2.29	17 (30%)	64,101,113	2.97	28 (43%)
20	BCR	A	852	-	41,41,41	1.05	1 (2%)	56,56,56	1.78	14 (25%)
17	CLA	k	1402	11	46,54,73	2.48	17 (36%)	53,90,113	3.10	23 (43%)
17	CLA	8	305	15	47,55,73	2.48	17 (36%)	54,91,113	3.10	24 (44%)
17	CLA	3	305	29	42,50,73	2.52	16 (38%)	48,85,113	3.26	24 (50%)
17	CLA	L	204	29	50,58,73	2.40	17 (34%)	58,95,113	3.09	27 (46%)
17	CLA	b	803	2	65,73,73	2.07	16 (24%)	76,113,113	2.52	26 (34%)
26	CHL	6	308	13	47,55,74	2.38	17 (36%)	50,91,114	3.28	21 (42%)
20	BCR	8	316	-	41,41,41	1.07	1 (2%)	56,56,56	1.92	17 (30%)
17	CLA	A	822	29	65,73,73	2.09	16 (24%)	76,113,113	2.60	27 (35%)
17	CLA	2	609	14	60,68,73	2.20	17 (28%)	70,107,113	2.79	30 (42%)
17	CLA	7	613	14	43,51,73	2.50	16 (37%)	49,86,113	3.27	24 (48%)
17	CLA	b	834	2	65,73,73	2.10	17 (26%)	76,113,113	2.73	27 (35%)
20	BCR	A	856	-	41,41,41	1.03	1 (2%)	56,56,56	2.03	16 (28%)
17	CLA	3	313	15	45,53,73	2.55	17 (37%)	52,89,113	3.15	24 (46%)
17	CLA	a	840	1	65,73,73	2.09	16 (24%)	76,113,113	2.74	26 (34%)
17	CLA	g	101	-	41,49,73	2.55	17 (41%)	47,84,113	3.44	24 (51%)
17	CLA	A	854	29	65,73,73	2.05	16 (24%)	76,113,113	2.81	30 (39%)
20	BCR	L	205	-	41,41,41	1.03	1 (2%)	56,56,56	1.66	11 (19%)
17	CLA	2	608	14	50,58,73	2.40	17 (34%)	58,95,113	3.06	29 (50%)
20	BCR	L	201	-	41,41,41	1.06	1 (2%)	56,56,56	1.88	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	B	834	2	65,73,73	2.13	17 (26%)	76,113,113	2.66	27 (35%)
27	LUT	6	321	-	42,43,43	0.74	0	51,60,60	1.69	9 (17%)
26	CHL	2	614	14	43,51,74	2.39	16 (37%)	45,86,114	3.51	20 (44%)
17	CLA	7	602	14	65,73,73	2.08	17 (26%)	76,113,113	2.74	28 (36%)
17	CLA	A	842	1	65,73,73	2.11	17 (26%)	76,113,113	2.73	27 (35%)
17	CLA	9	609	16	60,68,73	2.19	17 (28%)	70,107,113	2.79	30 (42%)
17	CLA	b	808	2	65,73,73	2.07	16 (24%)	76,113,113	2.78	30 (39%)
26	CHL	1	302	13	61,69,74	2.05	17 (27%)	67,108,114	2.97	25 (37%)
17	CLA	2	602	14	65,73,73	2.11	17 (26%)	76,113,113	2.71	28 (36%)
17	CLA	A	833	1	65,73,73	2.09	17 (26%)	76,113,113	2.70	26 (34%)
17	CLA	a	824	1	51,59,73	2.35	16 (31%)	59,96,113	3.08	25 (42%)
17	CLA	b	802	2	65,73,73	2.06	16 (24%)	76,113,113	2.72	29 (38%)
17	CLA	b	824	29	65,73,73	2.09	16 (24%)	76,113,113	2.67	27 (35%)
17	CLA	b	827	2	65,73,73	2.06	16 (24%)	76,113,113	2.73	26 (34%)
17	CLA	B	814	2	65,73,73	2.06	16 (24%)	76,113,113	2.73	29 (38%)
17	CLA	b	832	2	65,73,73	2.06	17 (26%)	76,113,113	2.78	27 (35%)
20	BCR	4	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.79	15 (26%)
17	CLA	b	838	2	47,55,73	2.47	16 (34%)	54,91,113	3.17	24 (44%)
20	BCR	b	801	-	41,41,41	1.03	1 (2%)	56,56,56	1.43	6 (10%)
17	CLA	A	805	1	55,63,73	2.26	16 (29%)	64,101,113	3.01	29 (45%)
17	CLA	A	837	1	45,53,73	2.54	17 (37%)	52,89,113	3.14	24 (46%)
17	CLA	8	310	15	55,63,73	2.29	17 (30%)	64,101,113	2.90	27 (42%)
17	CLA	A	821	1	45,53,73	2.50	16 (35%)	52,89,113	3.21	26 (50%)
17	CLA	a	839	1	65,73,73	2.06	16 (24%)	76,113,113	2.75	25 (32%)
17	CLA	b	836	2	60,68,73	2.18	16 (26%)	70,107,113	2.88	25 (35%)
17	CLA	A	835	1	65,73,73	2.10	17 (26%)	76,113,113	2.74	28 (36%)
17	CLA	B	809	2	65,73,73	2.05	17 (26%)	76,113,113	2.69	24 (31%)
20	BCR	b	847	-	41,41,41	1.05	1 (2%)	56,56,56	1.82	15 (26%)
19	LHG	1	319	17	48,48,48	0.94	2 (4%)	51,54,54	1.03	3 (5%)
17	CLA	a	828	1	65,73,73	2.04	16 (24%)	76,113,113	2.74	25 (32%)
17	CLA	3	310	19	38,45,73	2.50	15 (39%)	43,78,113	3.36	23 (53%)
28	XAT	2	616	-	39,47,47	0.87	0	54,74,74	2.62	19 (35%)
17	CLA	7	609	14	60,68,73	2.18	16 (26%)	70,107,113	2.79	29 (41%)
17	CLA	B	827	2	65,73,73	2.07	17 (26%)	76,113,113	2.76	27 (35%)
17	CLA	9	603	16	46,54,73	2.45	17 (36%)	53,90,113	3.23	25 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	9	612	16	56,64,73	2.27	17 (30%)	65,102,113	2.89	26 (40%)
17	CLA	g	102	7	50,58,73	2.41	17 (34%)	58,95,113	3.10	27 (46%)
17	CLA	A	802	1	65,73,73	2.08	15 (23%)	76,113,113	2.67	26 (34%)
25	LMG	G	102	-	44,44,55	1.01	2 (4%)	52,52,63	0.98	3 (5%)
22	HTG	F	302	-	19,19,19	1.01	2 (10%)	23,24,24	0.61	0
20	BCR	a	853	-	41,41,41	1.05	1 (2%)	56,56,56	1.93	14 (25%)
17	CLA	A	831	1	65,73,73	2.07	16 (24%)	76,113,113	2.69	26 (34%)
20	BCR	f	7004	-	41,41,41	1.03	1 (2%)	56,56,56	1.75	18 (32%)
17	CLA	a	819	1	65,73,73	2.12	16 (24%)	76,113,113	2.63	26 (34%)
17	CLA	b	807	2	65,73,73	2.11	17 (26%)	76,113,113	2.69	26 (34%)
17	CLA	4	611	16	52,60,73	2.33	16 (30%)	60,97,113	3.01	26 (43%)
17	CLA	4	609	16	60,68,73	2.18	17 (28%)	70,107,113	2.84	29 (41%)
20	BCR	A	848	-	41,41,41	1.02	1 (2%)	56,56,56	1.82	13 (23%)
17	CLA	B	822	2	55,63,73	2.30	17 (30%)	64,101,113	2.89	27 (42%)
17	CLA	B	833	2	58,66,73	2.20	16 (27%)	67,104,113	2.90	26 (38%)
17	CLA	3	301	-	46,54,73	2.50	17 (36%)	53,90,113	3.16	25 (47%)
17	CLA	a	818	1	65,73,73	2.10	17 (26%)	76,113,113	2.76	28 (36%)
20	BCR	A	850	-	41,41,41	1.04	1 (2%)	56,56,56	1.94	15 (26%)
17	CLA	g	103	7	46,54,73	2.49	17 (36%)	53,90,113	3.18	25 (47%)
27	LUT	1	320	-	42,43,43	0.74	0	51,60,60	1.65	11 (21%)
17	CLA	a	832	1	50,58,73	2.39	16 (32%)	58,95,113	3.05	27 (46%)
17	CLA	2	613	14	43,51,73	2.50	16 (37%)	49,86,113	3.26	23 (46%)
17	CLA	A	815	1	45,53,73	2.51	17 (37%)	52,89,113	3.17	24 (46%)
17	CLA	8	301	15	60,68,73	2.19	17 (28%)	70,107,113	2.83	28 (40%)
28	XAT	3	317	-	39,47,47	0.88	0	54,74,74	2.67	20 (37%)
17	CLA	B	803	2	65,73,73	2.10	17 (26%)	76,113,113	2.67	29 (38%)
17	CLA	a	806	1	65,73,73	2.08	16 (24%)	76,113,113	2.75	28 (36%)
23	LMT	B	849	-	36,36,36	0.48	0	47,47,47	0.94	3 (6%)
17	CLA	a	805	1	55,63,73	2.27	17 (30%)	64,101,113	2.91	27 (42%)
17	CLA	b	804	2	45,53,73	2.48	16 (35%)	52,89,113	3.26	24 (46%)
17	CLA	B	831	2	49,57,73	2.40	16 (32%)	55,93,113	3.06	26 (47%)
17	CLA	a	844	29	65,73,73	2.04	16 (24%)	76,113,113	2.71	25 (32%)
17	CLA	A	803	29	65,73,73	2.06	16 (24%)	76,113,113	2.75	28 (36%)
17	CLA	b	825	29	65,73,73	2.08	16 (24%)	76,113,113	2.71	28 (36%)
17	CLA	7	610	19	41,49,73	2.57	17 (41%)	47,84,113	3.36	24 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	4	602	16	60,68,73	2.18	17 (28%)	70,107,113	2.82	30 (42%)
17	CLA	A	818	1	65,73,73	2.09	16 (24%)	76,113,113	2.76	28 (36%)
22	HTG	J	3001	-	19,19,19	1.05	2 (10%)	23,24,24	0.53	0
20	BCR	G	105	-	41,41,41	1.05	1 (2%)	56,56,56	1.85	15 (26%)
17	CLA	b	815	2	55,63,73	2.25	16 (29%)	64,101,113	2.90	28 (43%)
17	CLA	3	306	15	47,55,73	2.48	16 (34%)	54,91,113	3.07	24 (44%)
17	CLA	a	821	1	45,53,73	2.48	16 (35%)	52,89,113	3.25	25 (48%)
19	LHG	A	847	17	26,26,48	1.28	2 (7%)	29,32,54	1.26	3 (10%)
25	LMG	6	302	-	40,40,55	1.05	2 (5%)	48,48,63	1.10	3 (6%)
17	CLA	A	832	1	50,58,73	2.38	17 (34%)	58,95,113	3.08	27 (46%)
17	CLA	1	304	13	65,73,73	2.11	17 (26%)	76,113,113	2.70	26 (34%)
17	CLA	3	315	-	27,32,73	3.00	13 (48%)	30,54,113	4.59	24 (80%)
26	CHL	9	605	29	56,64,74	2.16	18 (32%)	61,102,114	3.09	27 (44%)
26	CHL	6	303	13	61,69,74	2.05	18 (29%)	67,108,114	2.93	26 (38%)
18	PQN	B	842	-	34,34,34	1.60	2 (5%)	42,45,45	1.12	3 (7%)
17	CLA	3	303	15	50,58,73	2.39	17 (34%)	58,95,113	3.06	25 (43%)
21	SF4	c	102	3	0,12,12	-	-	-	-	-
17	CLA	8	307	15	50,58,73	2.38	16 (32%)	58,95,113	2.97	27 (46%)
26	CHL	4	605	29	56,64,74	2.16	18 (32%)	61,102,114	3.09	27 (44%)
17	CLA	8	308	15	50,58,73	2.41	17 (34%)	58,95,113	3.05	28 (48%)
17	CLA	a	817	29	45,53,73	2.51	17 (37%)	52,89,113	3.16	23 (44%)
17	CLA	9	613	16	45,53,73	2.53	17 (37%)	52,89,113	3.19	25 (48%)
20	BCR	B	845	-	41,41,41	1.01	1 (2%)	56,56,56	2.01	18 (32%)
18	PQN	A	844	-	34,34,34	1.61	2 (5%)	42,45,45	1.21	4 (9%)
17	CLA	A	819	1	65,73,73	2.08	16 (24%)	76,113,113	2.70	27 (35%)
25	LMG	4	619	-	44,44,55	1.01	2 (4%)	52,52,63	1.00	3 (5%)
17	CLA	a	834	1	65,73,73	2.09	17 (26%)	76,113,113	2.74	28 (36%)
17	CLA	4	610	29	55,63,73	2.28	16 (29%)	64,101,113	2.87	28 (43%)
21	SF4	C	101	3	0,12,12	-	-	-	-	-
17	CLA	a	816	1	50,58,73	2.38	16 (32%)	58,95,113	3.05	27 (46%)
17	CLA	f	7003	6	55,63,73	2.30	17 (30%)	64,101,113	2.96	28 (43%)
17	CLA	a	820	1	65,73,73	2.12	17 (26%)	76,113,113	2.70	26 (34%)
17	CLA	4	603	16	46,54,73	2.42	16 (34%)	53,90,113	3.24	25 (47%)
17	CLA	6	304	13	65,73,73	2.11	17 (26%)	76,113,113	2.72	28 (36%)
20	BCR	a	851	-	41,41,41	1.03	1 (2%)	56,56,56	1.72	14 (25%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	A	813	1	54,62,73	2.30	17 (31%)	62,99,113	2.95	28 (45%)
17	CLA	b	816	2	55,63,73	2.27	17 (30%)	64,101,113	2.92	28 (43%)
17	CLA	a	837	1	45,53,73	2.53	17 (37%)	52,89,113	3.17	25 (48%)
17	CLA	B	815	2	60,68,73	2.17	16 (26%)	70,107,113	2.76	27 (38%)
17	CLA	G	101	29	45,53,73	2.50	17 (37%)	52,89,113	3.25	23 (44%)
24	DGD	b	849	-	67,67,67	0.86	2 (2%)	81,81,81	1.00	4 (4%)
17	CLA	6	307	-	42,50,73	2.52	16 (38%)	48,85,113	3.25	24 (50%)
17	CLA	A	830	1	65,73,73	2.10	16 (24%)	76,113,113	2.69	27 (35%)
17	CLA	3	311	-	52,60,73	2.37	17 (32%)	60,97,113	3.02	26 (43%)
17	CLA	A	816	1	50,58,73	2.38	17 (34%)	58,95,113	3.11	26 (44%)
17	CLA	A	807	1	65,73,73	2.09	16 (24%)	76,113,113	2.71	28 (36%)
17	CLA	B	824	29	65,73,73	2.06	16 (24%)	76,113,113	2.70	26 (34%)
17	CLA	a	841	1	65,73,73	2.09	16 (24%)	76,113,113	2.66	28 (36%)
17	CLA	A	811	1	65,73,73	2.10	17 (26%)	76,113,113	2.70	27 (35%)
17	CLA	3	308	15	50,58,73	2.39	16 (32%)	58,95,113	3.03	27 (46%)
20	BCR	b	848	-	41,41,41	1.05	1 (2%)	56,56,56	1.55	10 (17%)
17	CLA	A	839	1	65,73,73	2.05	16 (24%)	76,113,113	2.74	25 (32%)
17	CLA	B	813	2	65,73,73	2.08	16 (24%)	76,113,113	2.69	27 (35%)
19	LHG	6	301	17	22,22,48	1.17	2 (9%)	25,28,54	1.22	2 (8%)
17	CLA	6	314	13	60,68,73	2.18	16 (26%)	70,107,113	2.77	26 (37%)
27	LUT	9	616	-	42,43,43	0.74	0	51,60,60	1.62	12 (23%)
17	CLA	l	204	29	50,58,73	2.38	16 (32%)	58,95,113	3.07	28 (48%)
20	BCR	i	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.60	12 (21%)
17	CLA	A	827	29	65,73,73	2.10	17 (26%)	76,113,113	2.71	26 (34%)
17	CLA	b	829	2	65,73,73	2.04	17 (26%)	76,113,113	2.78	29 (38%)
19	LHG	6	320	17	48,48,48	0.94	2 (4%)	51,54,54	1.08	3 (5%)
27	LUT	1	316	-	42,43,43	0.74	0	51,60,60	1.55	12 (23%)
17	CLA	b	819	29	65,73,73	2.09	17 (26%)	76,113,113	2.65	26 (34%)
17	CLA	A	801	1	65,73,73	2.07	16 (24%)	76,113,113	2.71	32 (42%)
17	CLA	B	830	2	50,58,73	2.37	17 (34%)	58,95,113	3.08	26 (44%)
17	CLA	b	811	2	54,62,73	2.16	16 (29%)	67,100,113	2.98	28 (41%)
26	CHL	4	606	29	51,59,74	2.32	18 (35%)	55,96,114	3.22	22 (40%)
17	CLA	B	811	2	54,62,73	2.18	17 (31%)	67,100,113	2.94	28 (41%)
26	CHL	2	601	14	61,69,74	2.06	17 (27%)	67,108,114	3.00	25 (37%)
17	CLA	F	301	29	65,73,73	2.10	16 (24%)	76,113,113	2.68	25 (32%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	BCR	b	843	-	41,41,41	1.06	1 (2%)	56,56,56	1.93	14 (25%)
27	LUT	4	616	-	42,43,43	0.76	0	51,60,60	1.64	13 (25%)
26	CHL	7	605	29	43,51,74	2.38	16 (37%)	45,86,114	3.51	23 (51%)
17	CLA	B	804	2	45,53,73	2.50	17 (37%)	52,89,113	3.18	25 (48%)
17	CLA	a	842	29	65,73,73	2.08	16 (24%)	76,113,113	2.67	26 (34%)
17	CLA	a	856	29	65,73,73	2.04	17 (26%)	76,113,113	2.85	30 (39%)
17	CLA	3	312	15	55,63,73	2.29	16 (29%)	64,101,113	2.91	27 (42%)
17	CLA	A	814	1	65,73,73	2.09	16 (24%)	76,113,113	2.70	26 (34%)
17	CLA	B	836	2	60,68,73	2.19	16 (26%)	70,107,113	2.87	25 (35%)
22	HTG	A	855	-	19,19,19	1.03	2 (10%)	23,24,24	0.69	0
17	CLA	8	311	15	45,53,73	2.54	17 (37%)	52,89,113	3.17	25 (48%)
20	BCR	b	846	-	41,41,41	1.08	1 (2%)	56,56,56	1.66	13 (23%)
17	CLA	B	832	2	65,73,73	2.06	16 (24%)	76,113,113	2.78	25 (32%)
17	CLA	A	809	1	65,73,73	2.10	16 (24%)	76,113,113	2.73	27 (35%)
17	CLA	b	828	2	65,73,73	2.08	16 (24%)	76,113,113	2.70	26 (34%)
17	CLA	a	835	1	65,73,73	2.10	17 (26%)	76,113,113	2.77	29 (38%)
20	BCR	k	1404	-	41,41,41	1.04	1 (2%)	56,56,56	1.78	12 (21%)
17	CLA	a	822	29	65,73,73	2.08	16 (24%)	76,113,113	2.66	28 (36%)
17	CLA	a	825	1	55,63,73	2.29	16 (29%)	64,101,113	2.88	27 (42%)
20	BCR	B	847	-	41,41,41	1.06	1 (2%)	56,56,56	1.73	15 (26%)
17	CLA	8	303	29	45,53,73	2.52	17 (37%)	52,89,113	3.16	24 (46%)
20	BCR	K	4001	-	41,41,41	1.05	1 (2%)	56,56,56	1.80	11 (19%)
26	CHL	7	606	-	48,56,74	2.34	17 (35%)	51,92,114	3.34	23 (45%)
20	BCR	l	205	-	41,41,41	1.02	1 (2%)	56,56,56	1.59	10 (17%)
17	CLA	A	825	1	55,63,73	2.30	17 (30%)	64,101,113	2.88	27 (42%)
17	CLA	B	807	2	65,73,73	2.11	17 (26%)	76,113,113	2.74	29 (38%)
17	CLA	6	313	13	52,60,73	2.35	16 (30%)	60,97,113	3.01	26 (43%)
17	CLA	1	309	13	65,73,73	2.10	16 (24%)	76,113,113	2.67	26 (34%)
17	CLA	J	3002	10	42,50,73	2.56	16 (38%)	48,85,113	3.23	25 (52%)
17	CLA	8	302	15	50,58,73	2.39	16 (32%)	58,95,113	3.12	27 (46%)
17	CLA	A	840	1	65,73,73	2.09	16 (24%)	76,113,113	2.75	27 (35%)
17	CLA	7	611	14	52,60,73	2.34	16 (30%)	60,97,113	3.02	26 (43%)
17	CLA	3	302	15	60,68,73	2.18	17 (28%)	70,107,113	2.83	28 (40%)
17	CLA	L	202	12	65,73,73	2.10	17 (26%)	76,113,113	2.68	26 (34%)
17	CLA	6	311	13	60,68,73	2.19	17 (28%)	70,107,113	2.82	29 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	B	802	2	65,73,73	2.06	16 (24%)	76,113,113	2.75	29 (38%)
17	CLA	9	614	16	47,55,73	2.43	17 (36%)	54,91,113	3.20	24 (44%)
17	CLA	b	818	2	60,68,73	2.16	17 (28%)	70,107,113	2.80	26 (37%)
17	CLA	b	820	2	50,58,73	2.38	16 (32%)	58,95,113	3.10	27 (46%)
17	CLA	6	316	13	46,54,73	2.50	17 (36%)	53,90,113	3.14	24 (45%)
21	SF4	C	102	3	0,12,12	-	-	-		
27	LUT	8	314	-	42,43,43	0.74	0	51,60,60	1.47	11 (21%)
25	LMG	4	620	-	44,44,55	1.02	3 (6%)	52,52,63	1.18	4 (7%)
17	CLA	6	306	29	51,59,73	2.38	17 (33%)	59,96,113	3.04	27 (45%)
26	CHL	9	606	29	51,59,74	2.26	17 (33%)	55,96,114	3.24	24 (43%)
17	CLA	A	824	1	51,59,73	2.37	17 (33%)	59,96,113	3.03	27 (45%)
26	CHL	1	307	13	48,56,74	2.35	17 (35%)	51,92,114	3.27	21 (41%)
17	CLA	2	611	14	52,60,73	2.35	16 (30%)	60,97,113	3.04	26 (43%)
17	CLA	9	611	16	52,60,73	2.36	17 (32%)	60,97,113	3.04	26 (43%)
22	HTG	j	3001	-	19,19,19	1.11	2 (10%)	23,24,24	0.59	0
17	CLA	a	838	1	51,59,73	2.34	15 (29%)	59,96,113	3.12	29 (49%)
20	BCR	b	844	-	41,41,41	1.03	1 (2%)	56,56,56	2.08	14 (25%)
17	CLA	B	816	2	55,63,73	2.28	17 (30%)	64,101,113	2.94	27 (42%)
17	CLA	b	813	2	65,73,73	2.09	16 (24%)	76,113,113	2.69	25 (32%)
17	CLA	A	828	1	65,73,73	2.05	16 (24%)	76,113,113	2.74	26 (34%)
25	LMG	9	619	-	50,50,55	0.93	2 (4%)	58,58,63	0.98	3 (5%)
17	CLA	7	612	14	65,73,73	2.10	17 (26%)	76,113,113	2.69	26 (34%)
17	CLA	a	826	29	65,73,73	2.07	16 (24%)	76,113,113	2.76	25 (32%)
20	BCR	l	201	-	41,41,41	1.04	1 (2%)	56,56,56	1.85	15 (26%)
17	CLA	B	805	2	65,73,73	2.07	17 (26%)	76,113,113	2.74	26 (34%)
17	CLA	A	838	1	51,59,73	2.34	16 (31%)	59,96,113	3.12	27 (45%)
21	SF4	a	855	2,1	0,12,12	-	-	-		
17	CLA	b	830	2	50,58,73	2.39	17 (34%)	58,95,113	3.10	29 (50%)
20	BCR	L	206	-	41,41,41	1.06	1 (2%)	56,56,56	1.84	12 (21%)
17	CLA	F	304	6	55,63,73	2.30	17 (30%)	64,101,113	2.89	29 (45%)
17	CLA	B	821	2	46,54,73	2.48	17 (36%)	53,90,113	3.18	23 (43%)
17	CLA	2	610	19	41,49,73	2.57	17 (41%)	47,84,113	3.37	25 (53%)
17	CLA	1	305	29	52,60,73	2.36	17 (32%)	60,97,113	3.07	28 (46%)
20	BCR	7	617	-	41,41,41	1.09	1 (2%)	56,56,56	2.09	13 (23%)
17	CLA	9	610	29	41,49,73	2.57	16 (39%)	47,84,113	3.32	24 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	CHL	8	306	29	47,55,74	2.33	16 (34%)	50,91,114	3.36	22 (44%)
17	CLA	b	840	2	65,73,73	2.07	16 (24%)	76,113,113	2.77	27 (35%)
17	CLA	a	823	1	49,57,73	2.41	16 (32%)	55,93,113	3.09	25 (45%)
17	CLA	a	807	1	65,73,73	2.07	16 (24%)	76,113,113	2.77	29 (38%)
17	CLA	b	833	2	58,66,73	2.21	16 (27%)	67,104,113	2.93	26 (38%)
17	CLA	A	826	29	65,73,73	2.05	16 (24%)	76,113,113	2.70	24 (31%)
17	CLA	4	612	16	56,64,73	2.27	17 (30%)	65,102,113	2.92	26 (40%)
17	CLA	F	303	29	45,53,73	2.50	16 (35%)	52,89,113	3.14	24 (46%)
20	BCR	b	845	-	41,41,41	1.05	1 (2%)	56,56,56	1.94	13 (23%)
17	CLA	b	809	2	65,73,73	2.03	17 (26%)	76,113,113	2.70	27 (35%)
20	BCR	B	848	-	41,41,41	1.05	1 (2%)	56,56,56	1.64	12 (21%)
19	LHG	A	846	-	48,48,48	0.93	2 (4%)	51,54,54	1.07	3 (5%)
17	CLA	A	812	1	65,73,73	2.08	16 (24%)	76,113,113	2.76	28 (36%)
20	BCR	6	319	-	41,41,41	1.07	1 (2%)	56,56,56	1.88	14 (25%)
19	LHG	1	301	17	22,22,48	1.18	2 (9%)	25,28,54	1.29	2 (8%)
17	CLA	A	806	1	65,73,73	2.09	16 (24%)	76,113,113	2.69	29 (38%)
27	LUT	2	615	-	42,43,43	0.75	0	51,60,60	1.62	11 (21%)
17	CLA	l	203	12	65,73,73	2.08	16 (24%)	76,113,113	2.76	29 (38%)
17	CLA	6	305	13	65,73,73	2.09	17 (26%)	76,113,113	2.70	26 (34%)
17	CLA	a	810	1	65,73,73	2.10	16 (24%)	76,113,113	2.69	27 (35%)
17	CLA	1	308	29	65,73,73	2.10	17 (26%)	76,113,113	2.69	26 (34%)
17	CLA	8	309	-	52,60,73	2.38	17 (32%)	60,97,113	3.01	25 (41%)
20	BCR	F	305	-	41,41,41	1.04	1 (2%)	56,56,56	1.74	16 (28%)
17	CLA	9	601	16	46,54,73	2.48	17 (36%)	53,90,113	3.14	26 (49%)
17	CLA	b	814	2	65,73,73	2.09	17 (26%)	76,113,113	2.75	26 (34%)
17	CLA	a	843	1	65,73,73	2.06	16 (24%)	76,113,113	2.75	29 (38%)
17	CLA	L	203	12	65,73,73	2.08	17 (26%)	76,113,113	2.80	28 (36%)
17	CLA	4	608	16	50,58,73	2.38	16 (32%)	58,95,113	3.00	27 (46%)
17	CLA	a	804	1	65,73,73	2.10	17 (26%)	76,113,113	2.76	28 (36%)
17	CLA	a	829	1	65,73,73	2.06	16 (24%)	76,113,113	2.71	26 (34%)
17	CLA	B	828	2	65,73,73	2.09	16 (24%)	76,113,113	2.72	26 (34%)
17	CLA	A	843	29	65,73,73	2.07	17 (26%)	76,113,113	2.68	25 (32%)
21	SF4	A	853	2,1	0,12,12	-	-	-	-	-
17	CLA	8	312	15	46,54,73	2.47	17 (36%)	53,90,113	3.17	25 (47%)
17	CLA	b	826	2	65,73,73	2.06	16 (24%)	76,113,113	2.71	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	BCR	l	206	-	41,41,41	1.06	1 (2%)	56,56,56	1.80	12 (21%)
17	CLA	A	829	1	65,73,73	2.04	16 (24%)	76,113,113	2.70	27 (35%)
17	CLA	B	819	29	65,73,73	2.09	17 (26%)	76,113,113	2.66	29 (38%)
17	CLA	B	812	2	55,63,73	2.28	17 (30%)	64,101,113	2.87	25 (39%)
17	CLA	j	3002	10	42,50,73	2.55	16 (38%)	48,85,113	3.27	25 (52%)
20	BCR	A	851	-	41,41,41	1.06	1 (2%)	56,56,56	2.02	14 (25%)
17	CLA	k	1401	-	45,53,73	2.52	16 (35%)	52,89,113	3.19	23 (44%)
20	BCR	K	4004	-	41,41,41	1.04	1 (2%)	56,56,56	1.81	14 (25%)
20	BCR	I	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.93	15 (26%)
17	CLA	B	806	2	65,73,73	2.09	17 (26%)	76,113,113	2.70	26 (34%)
26	CHL	3	307	29	47,55,74	2.34	18 (38%)	50,91,114	3.27	23 (46%)
17	CLA	B	837	2	65,73,73	2.08	17 (26%)	76,113,113	2.75	29 (38%)
27	LUT	3	316	-	42,43,43	0.74	0	51,60,60	1.63	14 (27%)
26	CHL	4	607	29	51,59,74	2.23	17 (33%)	55,96,114	3.21	23 (41%)
20	BCR	a	852	-	41,41,41	1.04	1 (2%)	56,56,56	1.94	17 (30%)
20	BCR	g	104	-	41,41,41	1.05	1 (2%)	56,56,56	1.89	16 (28%)
17	CLA	A	820	1	65,73,73	2.09	17 (26%)	76,113,113	2.73	26 (34%)
17	CLA	a	801	1	65,73,73	2.05	16 (24%)	76,113,113	2.74	29 (38%)
18	PQN	a	845	-	34,34,34	1.63	2 (5%)	42,45,45	1.09	4 (9%)
17	CLA	k	1403	-	46,54,73	2.52	17 (36%)	53,90,113	3.17	26 (49%)
17	CLA	6	309	29	46,54,73	2.49	17 (36%)	53,90,113	3.13	24 (45%)
17	CLA	9	602	16	60,68,73	2.17	17 (28%)	70,107,113	2.85	30 (42%)
20	BCR	B	843	-	41,41,41	1.06	1 (2%)	56,56,56	1.88	14 (25%)
17	CLA	B	810	2	65,73,73	2.09	17 (26%)	76,113,113	2.72	29 (38%)
17	CLA	A	810	1	65,73,73	2.05	16 (24%)	76,113,113	2.70	26 (34%)
17	CLA	4	614	16	50,58,73	2.39	17 (34%)	58,95,113	3.14	27 (46%)
17	CLA	b	812	2	55,63,73	2.28	16 (29%)	64,101,113	2.88	26 (40%)
17	CLA	6	310	13	65,73,73	2.10	16 (24%)	76,113,113	2.65	25 (32%)
17	CLA	b	806	2	65,73,73	2.08	16 (24%)	76,113,113	2.73	26 (34%)
17	CLA	b	823	2	60,68,73	2.18	16 (26%)	70,107,113	2.74	26 (37%)
17	CLA	b	837	2	65,73,73	2.10	17 (26%)	76,113,113	2.75	29 (38%)
17	CLA	G	104	7	46,54,73	2.49	17 (36%)	53,90,113	3.15	24 (45%)
17	CLA	b	835	29	45,53,73	2.52	17 (37%)	52,89,113	3.13	25 (48%)
17	CLA	B	817	2	59,67,73	2.19	17 (28%)	68,105,113	2.85	29 (42%)
20	BCR	J	3003	-	41,41,41	1.03	1 (2%)	56,56,56	1.76	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	B	829	2	65,73,73	2.08	16 (24%)	76,113,113	2.75	29 (38%)
28	XAT	6	318	-	39,47,47	0.89	0	54,74,74	2.62	19 (35%)
26	CHL	2	606	-	48,56,74	2.34	17 (35%)	51,92,114	3.32	22 (43%)
17	CLA	b	821	2	46,54,73	2.49	17 (36%)	53,90,113	3.14	24 (45%)
17	CLA	a	808	1	65,73,73	2.08	16 (24%)	76,113,113	2.72	26 (34%)
26	CHL	9	615	16	43,51,74	2.39	17 (39%)	45,86,114	3.55	21 (46%)
20	BCR	B	801	-	41,41,41	1.06	1 (2%)	56,56,56	1.49	8 (14%)
27	LUT	7	615	-	42,43,43	0.74	0	51,60,60	1.56	13 (25%)
26	CHL	9	607	29	51,59,74	2.25	17 (33%)	55,96,114	3.19	25 (45%)
17	CLA	a	831	1	65,73,73	2.04	17 (26%)	76,113,113	2.75	28 (36%)
17	CLA	b	805	2	65,73,73	2.07	17 (26%)	76,113,113	2.72	28 (36%)
17	CLA	9	608	16	50,58,73	2.36	16 (32%)	58,95,113	3.01	27 (46%)
22	HTG	f	7001	-	19,19,19	1.05	2 (10%)	23,24,24	0.58	0
17	CLA	1	310	13	60,68,73	2.19	17 (28%)	70,107,113	2.80	29 (41%)
17	CLA	1	312	13	52,60,73	2.33	16 (30%)	60,97,113	3.05	25 (41%)
17	CLA	3	314	15	46,54,73	2.49	16 (34%)	53,90,113	3.17	23 (43%)
17	CLA	K	4002	-	45,53,73	2.53	17 (37%)	52,89,113	3.20	23 (44%)
17	CLA	B	818	2	60,68,73	2.16	16 (26%)	70,107,113	2.81	25 (35%)
17	CLA	1	313	13	65,73,73	2.10	17 (26%)	76,113,113	2.70	27 (35%)
17	CLA	a	803	29	65,73,73	2.07	17 (26%)	76,113,113	2.71	27 (35%)
22	HTG	a	857	-	19,19,19	1.05	2 (10%)	23,24,24	0.55	0
17	CLA	3	309	15	50,58,73	2.38	16 (32%)	58,95,113	3.10	30 (51%)
17	CLA	a	802	1	65,73,73	2.07	14 (21%)	76,113,113	2.65	32 (42%)
17	CLA	1	311	19	41,49,73	2.57	16 (39%)	47,84,113	3.34	24 (51%)
17	CLA	b	810	2	65,73,73	2.09	16 (24%)	76,113,113	2.68	26 (34%)
17	CLA	4	604	29	50,58,73	2.39	17 (34%)	58,95,113	3.06	28 (48%)
28	XAT	8	315	-	39,47,47	0.88	0	54,74,74	2.71	21 (38%)
17	CLA	B	823	2	60,68,73	2.16	16 (26%)	70,107,113	2.78	30 (42%)
20	BCR	a	850	-	41,41,41	1.01	1 (2%)	56,56,56	1.86	15 (26%)
17	CLA	6	315	13	55,63,73	2.29	17 (30%)	64,101,113	2.95	28 (43%)
17	CLA	A	808	1	65,73,73	2.12	16 (24%)	76,113,113	2.72	26 (34%)
17	CLA	a	815	1	45,53,73	2.52	17 (37%)	52,89,113	3.15	25 (48%)
17	CLA	A	845	19	52,60,73	2.37	17 (32%)	60,97,113	3.05	24 (40%)
28	XAT	1	317	-	39,47,47	0.86	0	54,74,74	2.69	21 (38%)
20	BCR	a	854	-	41,41,41	1.04	1 (2%)	56,56,56	1.74	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	f	7002	29	45,53,73	2.48	16 (35%)	52,89,113	3.16	26 (50%)
17	CLA	7	603	14	51,59,73	2.36	16 (31%)	59,96,113	3.02	27 (45%)
17	CLA	B	840	2	65,73,73	2.09	17 (26%)	76,113,113	2.76	26 (34%)
19	LHG	3	319	17	19,19,48	1.10	1 (5%)	21,24,54	0.99	1 (4%)
19	LHG	a	847	-	48,48,48	0.93	2 (4%)	51,54,54	1.06	3 (5%)
20	BCR	1	318	-	41,41,41	1.07	1 (2%)	56,56,56	1.88	16 (28%)
17	CLA	B	808	2	65,73,73	2.09	16 (24%)	76,113,113	2.71	30 (39%)
21	SF4	c	101	3	0,12,12	-	-	-		
19	LHG	2	618	17	36,36,48	1.08	2 (5%)	39,42,54	1.16	3 (7%)
26	CHL	2	605	29	43,51,74	2.38	17 (39%)	45,86,114	3.46	22 (48%)
17	CLA	b	817	2	59,67,73	2.21	17 (28%)	68,105,113	2.84	29 (42%)
19	LHG	7	618	17	36,36,48	1.08	2 (5%)	39,42,54	1.16	4 (10%)
17	CLA	A	836	1	50,58,73	2.36	16 (32%)	58,95,113	3.03	28 (48%)
17	CLA	8	304	29	42,50,73	2.52	16 (38%)	48,85,113	3.25	24 (50%)
20	BCR	2	617	-	41,41,41	1.07	1 (2%)	56,56,56	1.86	18 (32%)
17	CLA	B	825	29	65,73,73	2.08	16 (24%)	76,113,113	2.74	30 (39%)
26	CHL	4	615	16	43,51,74	2.39	16 (37%)	45,86,114	3.48	19 (42%)
20	BCR	B	844	-	41,41,41	1.04	1 (2%)	56,56,56	1.97	13 (23%)
17	CLA	3	304	29	45,53,73	2.52	17 (37%)	52,89,113	3.16	24 (46%)
17	CLA	a	812	1	65,73,73	2.09	17 (26%)	76,113,113	2.76	28 (36%)
19	LHG	a	848	17	26,26,48	1.26	2 (7%)	29,32,54	1.32	3 (10%)
17	CLA	B	839	29	65,73,73	2.10	17 (26%)	76,113,113	2.69	25 (32%)
17	CLA	2	603	14	65,73,73	2.09	17 (26%)	76,113,113	2.68	25 (32%)
17	CLA	2	612	14	65,73,73	2.12	17 (26%)	76,113,113	2.69	27 (35%)
17	CLA	a	846	19	52,60,73	2.38	17 (32%)	60,97,113	3.03	24 (40%)
17	CLA	9	604	29	50,58,73	2.39	17 (34%)	58,95,113	3.13	28 (48%)
17	CLA	1	315	13	46,54,73	2.49	16 (34%)	53,90,113	3.13	23 (43%)
17	CLA	B	826	2	65,73,73	2.07	16 (24%)	76,113,113	2.75	26 (34%)
17	CLA	a	813	1	54,62,73	2.32	17 (31%)	62,99,113	2.96	25 (40%)
17	CLA	b	839	29	65,73,73	2.10	16 (24%)	76,113,113	2.71	23 (30%)
20	BCR	j	3003	-	41,41,41	1.02	1 (2%)	56,56,56	1.71	13 (23%)
17	CLA	7	608	14	50,58,73	2.39	17 (34%)	58,95,113	3.05	29 (50%)
17	CLA	A	823	1	49,57,73	2.43	17 (34%)	55,93,113	3.12	26 (47%)
17	CLA	a	836	1	50,58,73	2.35	16 (32%)	58,95,113	3.01	27 (46%)
17	CLA	a	827	29	65,73,73	2.09	16 (24%)	76,113,113	2.69	26 (34%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	CLA	8	313	-	27,32,73	3.00	13 (48%)	30,54,113	4.60	24 (80%)
17	CLA	4	613	16	45,53,73	2.53	17 (37%)	52,89,113	3.20	24 (46%)
17	CLA	2	604	29	60,68,73	2.19	17 (28%)	70,107,113	2.79	28 (40%)
17	CLA	b	831	2	49,57,73	2.38	17 (34%)	55,93,113	3.10	26 (47%)
17	CLA	7	604	29	60,68,73	2.20	17 (28%)	70,107,113	2.79	28 (40%)
17	CLA	a	830	1	65,73,73	2.09	16 (24%)	76,113,113	2.70	26 (34%)
26	CHL	2	607	29	51,59,74	2.24	17 (33%)	55,96,114	3.19	24 (43%)
26	CHL	7	601	14	61,69,74	2.07	17 (27%)	67,108,114	3.05	26 (38%)
17	CLA	B	841	19	65,73,73	2.09	17 (26%)	76,113,113	2.77	27 (35%)
28	XAT	9	617	-	39,47,47	0.86	1 (2%)	54,74,74	2.61	17 (31%)
17	CLA	b	822	2	55,63,73	2.28	17 (30%)	64,101,113	2.93	26 (40%)
20	BCR	B	846	-	41,41,41	1.04	1 (2%)	56,56,56	1.76	18 (32%)
17	CLA	A	817	29	45,53,73	2.53	17 (37%)	52,89,113	3.17	23 (44%)
17	CLA	K	4003	11	46,54,73	2.50	17 (36%)	53,90,113	3.14	24 (45%)
26	CHL	7	607	29	51,59,74	2.25	17 (33%)	55,96,114	3.21	21 (38%)
17	CLA	G	103	7	50,58,73	2.39	17 (34%)	58,95,113	3.07	26 (44%)
26	CHL	7	614	14	43,51,74	2.40	16 (37%)	45,86,114	3.47	20 (44%)
24	DGD	B	850	-	67,67,67	0.86	2 (2%)	81,81,81	0.93	4 (4%)
17	CLA	a	811	1	65,73,73	2.10	17 (26%)	76,113,113	2.72	27 (35%)
17	CLA	4	601	16	46,54,73	2.47	16 (34%)	53,90,113	3.16	24 (45%)
20	BCR	3	318	-	41,41,41	1.06	1 (2%)	56,56,56	1.88	14 (25%)
17	CLA	6	312	19	41,49,73	2.56	16 (39%)	47,84,113	3.38	25 (53%)
20	BCR	a	849	-	41,41,41	1.06	1 (2%)	56,56,56	1.96	14 (25%)
27	LUT	6	317	-	42,43,43	0.75	0	51,60,60	1.66	14 (27%)
17	CLA	B	835	29	45,53,73	2.51	17 (37%)	52,89,113	3.11	25 (48%)
17	CLA	l	202	12	65,73,73	2.10	16 (24%)	76,113,113	2.70	26 (34%)
17	CLA	1	306	-	52,60,73	2.34	17 (32%)	60,97,113	3.00	27 (45%)
17	CLA	b	841	19	65,73,73	2.10	17 (26%)	76,113,113	2.78	27 (35%)
17	CLA	B	838	2	47,55,73	2.42	16 (34%)	54,91,113	3.17	26 (48%)
20	BCR	j	3004	-	41,41,41	1.05	1 (2%)	56,56,56	2.15	18 (32%)
17	CLA	1	303	13	65,73,73	2.10	17 (26%)	76,113,113	2.71	27 (35%)
28	XAT	4	617	-	39,47,47	0.88	0	54,74,74	2.59	18 (33%)
28	XAT	7	616	-	39,47,47	0.85	0	54,74,74	2.60	19 (35%)
20	BCR	A	849	-	41,41,41	1.07	1 (2%)	56,56,56	1.65	13 (23%)
17	CLA	A	804	1	65,73,73	2.06	16 (24%)	76,113,113	2.77	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	PQN	b	842	-	34,34,34	1.62	2 (5%)	42,45,45	1.07	3 (7%)
17	CLA	a	833	1	65,73,73	2.09	17 (26%)	76,113,113	2.71	26 (34%)
17	CLA	A	841	1	65,73,73	2.10	17 (26%)	76,113,113	2.71	23 (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
17	CLA	B	820	2	1/1/12/20	3/19/97/115	-
17	CLA	A	834	1	1/1/15/20	10/37/115/115	-
17	CLA	a	809	1	1/1/15/20	13/37/115/115	-
20	BCR	9	618	-	-	6/29/63/63	0/2/2/2
17	CLA	a	814	1	1/1/15/20	11/37/115/115	-
17	CLA	1	314	13	-	4/25/103/115	-
20	BCR	A	852	-	-	6/29/63/63	0/2/2/2
17	CLA	k	1402	11	1/1/11/20	0/15/93/115	-
17	CLA	8	305	15	1/1/11/20	3/16/94/115	-
17	CLA	3	305	29	1/1/10/20	2/10/88/115	-
17	CLA	L	204	29	1/1/12/20	3/19/97/115	-
17	CLA	b	803	2	1/1/15/20	6/37/115/115	-
26	CHL	6	308	13	3/3/16/26	1/17/115/137	-
20	BCR	8	316	-	-	4/29/63/63	0/2/2/2
17	CLA	A	822	29	1/1/15/20	5/37/115/115	-
17	CLA	2	609	14	1/1/14/20	8/31/109/115	-
17	CLA	7	613	14	-	0/11/89/115	-
17	CLA	b	834	2	1/1/15/20	13/37/115/115	-
20	BCR	A	856	-	-	4/29/63/63	0/2/2/2
17	CLA	3	313	15	1/1/11/20	4/13/91/115	-
17	CLA	a	840	1	1/1/15/20	9/37/115/115	-
17	CLA	g	101	-	-	3/8/86/115	-
17	CLA	A	854	29	1/1/15/20	10/37/115/115	-
20	BCR	L	205	-	-	6/29/63/63	0/2/2/2
17	CLA	2	608	14	1/1/12/20	3/19/97/115	-
20	BCR	L	201	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	834	2	1/1/15/20	16/37/115/115	-
27	LUT	6	321	-	-	2/29/67/67	0/2/2/2
26	CHL	2	614	14	3/3/15/26	0/12/110/137	-
17	CLA	7	602	14	1/1/15/20	8/37/115/115	-
17	CLA	A	842	1	1/1/15/20	13/37/115/115	-
17	CLA	9	609	16	1/1/14/20	4/31/109/115	-
17	CLA	b	808	2	1/1/15/20	8/37/115/115	-
26	CHL	1	302	13	3/3/19/26	7/33/131/137	-
17	CLA	2	602	14	1/1/15/20	13/37/115/115	-
17	CLA	A	833	1	1/1/15/20	7/37/115/115	-
17	CLA	a	824	1	1/1/12/20	8/21/99/115	-
17	CLA	b	802	2	1/1/15/20	5/37/115/115	-
17	CLA	b	824	29	1/1/15/20	10/37/115/115	-
17	CLA	b	827	2	1/1/15/20	14/37/115/115	-
17	CLA	B	814	2	1/1/15/20	12/37/115/115	-
17	CLA	b	832	2	1/1/15/20	12/37/115/115	-
20	BCR	4	618	-	-	6/29/63/63	0/2/2/2
17	CLA	b	838	2	1/1/11/20	2/16/94/115	-
20	BCR	b	801	-	-	0/29/63/63	0/2/2/2
17	CLA	A	805	1	1/1/13/20	8/25/103/115	-
17	CLA	A	837	1	1/1/11/20	5/13/91/115	-
17	CLA	8	310	15	1/1/13/20	8/25/103/115	-
17	CLA	A	821	1	1/1/11/20	2/13/91/115	-
17	CLA	a	839	1	1/1/15/20	10/37/115/115	-
17	CLA	b	836	2	1/1/14/20	5/31/109/115	-
17	CLA	A	835	1	1/1/15/20	10/37/115/115	-
17	CLA	B	809	2	1/1/15/20	7/37/115/115	-
20	BCR	b	847	-	-	3/29/63/63	0/2/2/2
19	LHG	1	319	17	-	10/53/53/53	-
17	CLA	a	828	1	1/1/15/20	10/37/115/115	-
17	CLA	3	310	19	1/1/8/20	0/2/76/115	-
28	XAT	2	616	-	-	0/31/93/93	0/4/4/4
17	CLA	7	609	14	1/1/14/20	7/31/109/115	-
17	CLA	B	827	2	1/1/15/20	8/37/115/115	-
17	CLA	9	603	16	1/1/11/20	4/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	9	612	16	1/1/13/20	10/27/105/115	-
17	CLA	g	102	7	1/1/12/20	1/19/97/115	-
17	CLA	A	802	1	1/1/15/20	5/37/115/115	-
25	LMG	G	102	-	-	10/39/59/70	0/1/1/1
22	HTG	F	302	-	-	2/10/30/30	0/1/1/1
20	BCR	a	853	-	-	7/29/63/63	0/2/2/2
17	CLA	A	831	1	1/1/15/20	13/37/115/115	-
20	BCR	f	7004	-	-	4/29/63/63	0/2/2/2
17	CLA	a	819	1	1/1/15/20	14/37/115/115	-
17	CLA	b	807	2	1/1/15/20	6/37/115/115	-
17	CLA	4	611	16	1/1/12/20	7/22/100/115	-
17	CLA	4	609	16	1/1/14/20	5/31/109/115	-
20	BCR	A	848	-	-	6/29/63/63	0/2/2/2
17	CLA	B	822	2	1/1/13/20	11/25/103/115	-
17	CLA	B	833	2	1/1/13/20	9/29/107/115	-
17	CLA	3	301	-	1/1/11/20	2/15/93/115	-
17	CLA	a	818	1	1/1/15/20	12/37/115/115	-
20	BCR	A	850	-	-	3/29/63/63	0/2/2/2
17	CLA	g	103	7	1/1/11/20	2/15/93/115	-
27	LUT	1	320	-	-	2/29/67/67	0/2/2/2
17	CLA	a	832	1	1/1/12/20	4/19/97/115	-
17	CLA	2	613	14	1/1/10/20	6/11/89/115	-
17	CLA	A	815	1	1/1/11/20	1/13/91/115	-
17	CLA	8	301	15	1/1/14/20	11/31/109/115	-
28	XAT	3	317	-	-	2/31/93/93	0/4/4/4
17	CLA	B	803	2	1/1/15/20	5/37/115/115	-
17	CLA	a	806	1	1/1/15/20	16/37/115/115	-
23	LMT	B	849	-	-	3/21/61/61	0/2/2/2
17	CLA	a	805	1	1/1/13/20	9/25/103/115	-
17	CLA	b	804	2	1/1/11/20	4/13/91/115	-
17	CLA	B	831	2	1/1/11/20	8/18/96/115	-
17	CLA	a	844	29	1/1/15/20	12/37/115/115	-
17	CLA	A	803	29	1/1/15/20	2/37/115/115	-
17	CLA	b	825	29	1/1/15/20	8/37/115/115	-
17	CLA	7	610	19	1/1/10/20	0/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	4	602	16	1/1/14/20	6/31/109/115	-
17	CLA	A	818	1	1/1/15/20	12/37/115/115	-
22	HTG	J	3001	-	-	4/10/30/30	0/1/1/1
20	BCR	G	105	-	-	3/29/63/63	0/2/2/2
17	CLA	b	815	2	1/1/13/20	7/25/103/115	-
17	CLA	3	306	15	1/1/11/20	3/16/94/115	-
17	CLA	a	821	1	1/1/11/20	4/13/91/115	-
19	LHG	A	847	17	-	9/31/31/53	-
25	LMG	6	302	-	-	6/35/55/70	0/1/1/1
17	CLA	A	832	1	1/1/12/20	2/19/97/115	-
17	CLA	1	304	13	1/1/15/20	12/37/115/115	-
17	CLA	3	315	-	1/1/4/20	-	-
26	CHL	9	605	29	2/2/18/26	8/27/125/137	-
26	CHL	6	303	13	3/3/19/26	15/33/131/137	-
18	PQN	B	842	-	-	3/23/43/43	0/2/2/2
17	CLA	3	303	15	1/1/12/20	2/19/97/115	-
26	CHL	4	605	29	2/2/18/26	8/27/125/137	-
17	CLA	8	307	15	1/1/12/20	5/19/97/115	-
21	SF4	c	102	3	-	-	0/6/5/5
17	CLA	8	308	15	1/1/12/20	1/19/97/115	-
17	CLA	a	817	29	1/1/11/20	2/13/91/115	-
17	CLA	9	613	16	1/1/11/20	0/13/91/115	-
20	BCR	B	845	-	-	6/29/63/63	0/2/2/2
18	PQN	A	844	-	-	8/23/43/43	0/2/2/2
17	CLA	A	819	1	1/1/15/20	13/37/115/115	-
25	LMG	4	619	-	-	9/39/59/70	0/1/1/1
17	CLA	a	834	1	1/1/15/20	10/37/115/115	-
17	CLA	4	610	29	1/1/13/20	5/25/103/115	-
21	SF4	C	101	3	-	-	0/6/5/5
17	CLA	a	816	1	1/1/12/20	9/19/97/115	-
17	CLA	f	7003	6	-	9/25/103/115	-
17	CLA	a	820	1	1/1/15/20	11/37/115/115	-
17	CLA	4	603	16	1/1/11/20	2/15/93/115	-
17	CLA	6	304	13	1/1/15/20	9/37/115/115	-
20	BCR	a	851	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	813	1	1/1/12/20	7/24/102/115	-
17	CLA	b	816	2	1/1/13/20	11/25/103/115	-
17	CLA	a	837	1	1/1/11/20	5/13/91/115	-
17	CLA	B	815	2	1/1/14/20	10/31/109/115	-
17	CLA	G	101	29	1/1/11/20	2/13/91/115	-
24	DGD	b	849	-	-	10/55/95/95	0/2/2/2
17	CLA	6	307	-	1/1/10/20	4/10/88/115	-
17	CLA	A	830	1	1/1/15/20	13/37/115/115	-
17	CLA	3	311	-	1/1/12/20	6/22/100/115	-
17	CLA	A	816	1	1/1/12/20	3/19/97/115	-
17	CLA	A	807	1	1/1/15/20	12/37/115/115	-
17	CLA	B	824	29	-	7/37/115/115	-
17	CLA	a	841	1	1/1/15/20	12/37/115/115	-
17	CLA	A	811	1	1/1/15/20	9/37/115/115	-
17	CLA	3	308	15	1/1/12/20	5/19/97/115	-
20	BCR	b	848	-	-	2/29/63/63	0/2/2/2
17	CLA	A	839	1	1/1/15/20	5/37/115/115	-
17	CLA	B	813	2	1/1/15/20	16/37/115/115	-
19	LHG	6	301	17	-	7/26/26/53	-
17	CLA	6	314	13	1/1/14/20	6/31/109/115	-
27	LUT	9	616	-	-	2/29/67/67	0/2/2/2
17	CLA	l	204	29	1/1/12/20	4/19/97/115	-
20	BCR	i	101	-	-	1/29/63/63	0/2/2/2
17	CLA	A	827	29	1/1/15/20	7/37/115/115	-
17	CLA	b	829	2	1/1/15/20	6/37/115/115	-
19	LHG	6	320	17	-	14/53/53/53	-
27	LUT	1	316	-	-	2/29/67/67	0/2/2/2
17	CLA	b	819	29	1/1/15/20	5/37/115/115	-
17	CLA	A	801	1	2/2/15/20	7/37/115/115	-
17	CLA	B	830	2	1/1/12/20	5/19/97/115	-
17	CLA	b	811	2	1/1/13/20	10/25/101/115	-
26	CHL	4	606	29	3/3/17/26	6/21/119/137	-
17	CLA	B	811	2	1/1/13/20	4/25/101/115	-
26	CHL	2	601	14	2/2/19/26	11/33/131/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	F	301	29	1/1/15/20	8/37/115/115	-
20	BCR	b	843	-	-	0/29/63/63	0/2/2/2
27	LUT	4	616	-	-	2/29/67/67	0/2/2/2
26	CHL	7	605	29	3/3/15/26	4/12/110/137	-
17	CLA	B	804	2	1/1/11/20	8/13/91/115	-
17	CLA	a	842	29	1/1/15/20	5/37/115/115	-
17	CLA	a	856	29	1/1/15/20	11/37/115/115	-
17	CLA	3	312	15	1/1/13/20	9/25/103/115	-
17	CLA	A	814	1	1/1/15/20	16/37/115/115	-
17	CLA	B	836	2	1/1/14/20	5/31/109/115	-
22	HTG	A	855	-	-	1/10/30/30	0/1/1/1
17	CLA	8	311	15	1/1/11/20	3/13/91/115	-
20	BCR	b	846	-	-	5/29/63/63	0/2/2/2
17	CLA	B	832	2	1/1/15/20	14/37/115/115	-
17	CLA	A	809	1	1/1/15/20	18/37/115/115	-
17	CLA	b	828	2	1/1/15/20	9/37/115/115	-
17	CLA	a	835	1	1/1/15/20	10/37/115/115	-
20	BCR	k	1404	-	-	6/29/63/63	0/2/2/2
17	CLA	a	822	29	1/1/15/20	3/37/115/115	-
17	CLA	a	825	1	1/1/13/20	6/25/103/115	-
20	BCR	B	847	-	-	5/29/63/63	0/2/2/2
17	CLA	8	303	29	1/1/11/20	1/13/91/115	-
20	BCR	K	4001	-	-	1/29/63/63	0/2/2/2
26	CHL	7	606	-	3/3/16/26	0/18/116/137	-
20	BCR	l	205	-	-	6/29/63/63	0/2/2/2
17	CLA	A	825	1	1/1/13/20	7/25/103/115	-
17	CLA	B	807	2	1/1/15/20	14/37/115/115	-
17	CLA	6	313	13	1/1/12/20	10/22/100/115	-
17	CLA	1	309	13	1/1/15/20	10/37/115/115	-
17	CLA	J	3002	10	1/1/10/20	4/10/88/115	-
17	CLA	8	302	15	1/1/12/20	1/19/97/115	-
17	CLA	A	840	1	1/1/15/20	7/37/115/115	-
17	CLA	7	611	14	1/1/12/20	5/22/100/115	-
17	CLA	3	302	15	1/1/14/20	8/31/109/115	-
17	CLA	L	202	12	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	6	311	13	1/1/14/20	9/31/109/115	-
17	CLA	B	802	2	1/1/15/20	13/37/115/115	-
17	CLA	9	614	16	1/1/11/20	4/16/94/115	-
17	CLA	b	818	2	1/1/14/20	13/31/109/115	-
17	CLA	b	820	2	1/1/12/20	2/19/97/115	-
17	CLA	6	316	13	1/1/11/20	3/15/93/115	-
21	SF4	C	102	3	-	-	0/6/5/5
27	LUT	8	314	-	-	2/29/67/67	0/2/2/2
25	LMG	4	620	-	-	11/39/59/70	0/1/1/1
17	CLA	6	306	29	1/1/12/20	3/21/99/115	-
26	CHL	9	606	29	3/3/17/26	4/21/119/137	-
17	CLA	A	824	1	1/1/12/20	9/21/99/115	-
26	CHL	1	307	13	3/3/16/26	3/18/116/137	-
17	CLA	2	611	14	1/1/12/20	5/22/100/115	-
17	CLA	9	611	16	1/1/12/20	6/22/100/115	-
22	HTG	j	3001	-	-	1/10/30/30	0/1/1/1
17	CLA	a	838	1	1/1/12/20	9/21/99/115	-
20	BCR	b	844	-	-	6/29/63/63	0/2/2/2
17	CLA	B	816	2	1/1/13/20	9/25/103/115	-
17	CLA	b	813	2	1/1/15/20	13/37/115/115	-
17	CLA	A	828	1	1/1/15/20	13/37/115/115	-
25	LMG	9	619	-	-	10/45/65/70	0/1/1/1
17	CLA	7	612	14	1/1/15/20	8/37/115/115	-
17	CLA	a	826	29	1/1/15/20	6/37/115/115	-
20	BCR	l	201	-	-	8/29/63/63	0/2/2/2
17	CLA	B	805	2	1/1/15/20	16/37/115/115	-
17	CLA	A	838	1	1/1/12/20	3/21/99/115	-
21	SF4	a	855	2,1	-	-	0/6/5/5
17	CLA	b	830	2	1/1/12/20	3/19/97/115	-
20	BCR	L	206	-	-	3/29/63/63	0/2/2/2
17	CLA	F	304	6	1/1/13/20	8/25/103/115	-
17	CLA	B	821	2	1/1/11/20	1/15/93/115	-
17	CLA	2	610	19	1/1/10/20	0/8/86/115	-
17	CLA	1	305	29	1/1/12/20	6/22/100/115	-
20	BCR	7	617	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	9	610	29	1/1/10/20	0/8/86/115	-
26	CHL	8	306	29	3/3/16/26	3/17/115/137	-
17	CLA	b	840	2	1/1/15/20	5/37/115/115	-
17	CLA	a	823	1	1/1/11/20	5/18/96/115	-
17	CLA	a	807	1	1/1/15/20	14/37/115/115	-
17	CLA	b	833	2	1/1/13/20	8/29/107/115	-
17	CLA	A	826	29	1/1/15/20	14/37/115/115	-
17	CLA	4	612	16	1/1/13/20	9/27/105/115	-
17	CLA	F	303	29	1/1/11/20	2/13/91/115	-
20	BCR	b	845	-	-	6/29/63/63	0/2/2/2
17	CLA	b	809	2	1/1/15/20	8/37/115/115	-
20	BCR	B	848	-	-	2/29/63/63	0/2/2/2
19	LHG	A	846	-	-	10/53/53/53	-
17	CLA	A	812	1	1/1/15/20	13/37/115/115	-
20	BCR	6	319	-	-	4/29/63/63	0/2/2/2
19	LHG	1	301	17	-	9/26/26/53	-
17	CLA	A	806	1	1/1/15/20	19/37/115/115	-
27	LUT	2	615	-	-	2/29/67/67	0/2/2/2
17	CLA	l	203	12	1/1/15/20	6/37/115/115	-
17	CLA	6	305	13	1/1/15/20	10/37/115/115	-
17	CLA	a	810	1	1/1/15/20	2/37/115/115	-
17	CLA	1	308	29	1/1/15/20	5/37/115/115	-
17	CLA	8	309	-	1/1/12/20	5/22/100/115	-
20	BCR	F	305	-	-	4/29/63/63	0/2/2/2
17	CLA	9	601	16	1/1/11/20	5/15/93/115	-
17	CLA	b	814	2	1/1/15/20	10/37/115/115	-
17	CLA	a	843	1	1/1/15/20	14/37/115/115	-
17	CLA	L	203	12	1/1/15/20	5/37/115/115	-
17	CLA	4	608	16	1/1/12/20	3/19/97/115	-
17	CLA	a	804	1	1/1/15/20	16/37/115/115	-
17	CLA	a	829	1	1/1/15/20	12/37/115/115	-
17	CLA	B	828	2	1/1/15/20	5/37/115/115	-
17	CLA	A	843	29	1/1/15/20	16/37/115/115	-
21	SF4	A	853	2,1	-	-	0/6/5/5
17	CLA	8	312	15	1/1/11/20	1/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	b	826	2	1/1/15/20	8/37/115/115	-
20	BCR	l	206	-	-	0/29/63/63	0/2/2/2
17	CLA	A	829	1	1/1/15/20	11/37/115/115	-
17	CLA	B	819	29	1/1/15/20	9/37/115/115	-
17	CLA	B	812	2	1/1/13/20	8/25/103/115	-
17	CLA	j	3002	10	1/1/10/20	1/10/88/115	-
20	BCR	A	851	-	-	5/29/63/63	0/2/2/2
17	CLA	k	1401	-	1/1/11/20	5/13/91/115	-
20	BCR	K	4004	-	-	4/29/63/63	0/2/2/2
20	BCR	I	101	-	-	3/29/63/63	0/2/2/2
17	CLA	B	806	2	1/1/15/20	16/37/115/115	-
26	CHL	3	307	29	3/3/16/26	2/17/115/137	-
17	CLA	B	837	2	1/1/15/20	9/37/115/115	-
27	LUT	3	316	-	-	2/29/67/67	0/2/2/2
26	CHL	4	607	29	3/3/17/26	3/21/119/137	-
20	BCR	a	852	-	-	6/29/63/63	0/2/2/2
20	BCR	g	104	-	-	2/29/63/63	0/2/2/2
17	CLA	A	820	1	1/1/15/20	12/37/115/115	-
17	CLA	a	801	1	2/2/15/20	8/37/115/115	-
18	PQN	a	845	-	-	5/23/43/43	0/2/2/2
17	CLA	k	1403	-	1/1/11/20	4/15/93/115	-
17	CLA	6	309	29	1/1/11/20	3/15/93/115	-
17	CLA	9	602	16	1/1/14/20	10/31/109/115	-
20	BCR	B	843	-	-	0/29/63/63	0/2/2/2
17	CLA	B	810	2	1/1/15/20	9/37/115/115	-
17	CLA	A	810	1	1/1/15/20	4/37/115/115	-
17	CLA	4	614	16	1/1/12/20	2/19/97/115	-
17	CLA	b	812	2	1/1/13/20	11/25/103/115	-
17	CLA	6	310	13	1/1/15/20	7/37/115/115	-
17	CLA	b	806	2	1/1/15/20	9/37/115/115	-
17	CLA	b	823	2	1/1/14/20	6/31/109/115	-
17	CLA	b	837	2	1/1/15/20	9/37/115/115	-
17	CLA	G	104	7	1/1/11/20	2/15/93/115	-
17	CLA	b	835	29	1/1/11/20	2/13/91/115	-
17	CLA	B	817	2	1/1/13/20	10/30/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	J	3003	-	-	2/29/63/63	0/2/2/2
17	CLA	B	829	2	1/1/15/20	9/37/115/115	-
28	XAT	6	318	-	-	1/31/93/93	0/4/4/4
26	CHL	2	606	-	3/3/16/26	2/18/116/137	-
17	CLA	b	821	2	1/1/11/20	3/15/93/115	-
17	CLA	a	808	1	1/1/15/20	8/37/115/115	-
26	CHL	9	615	16	3/3/15/26	0/12/110/137	-
20	BCR	B	801	-	-	1/29/63/63	0/2/2/2
27	LUT	7	615	-	-	1/29/67/67	0/2/2/2
26	CHL	9	607	29	3/3/17/26	3/21/119/137	-
17	CLA	a	831	1	1/1/15/20	16/37/115/115	-
17	CLA	b	805	2	1/1/15/20	19/37/115/115	-
17	CLA	9	608	16	1/1/12/20	4/19/97/115	-
22	HTG	f	7001	-	-	1/10/30/30	0/1/1/1
17	CLA	1	310	13	1/1/14/20	3/31/109/115	-
17	CLA	1	312	13	1/1/12/20	8/22/100/115	-
17	CLA	3	314	15	1/1/11/20	1/15/93/115	-
17	CLA	K	4002	-	1/1/11/20	4/13/91/115	-
17	CLA	B	818	2	1/1/14/20	10/31/109/115	-
17	CLA	1	313	13	1/1/15/20	5/37/115/115	-
17	CLA	a	803	29	1/1/15/20	1/37/115/115	-
22	HTG	a	857	-	-	0/10/30/30	0/1/1/1
17	CLA	3	309	15	1/1/12/20	1/19/97/115	-
17	CLA	a	802	1	1/1/15/20	16/37/115/115	-
17	CLA	1	311	19	1/1/10/20	0/8/86/115	-
17	CLA	b	810	2	1/1/15/20	14/37/115/115	-
17	CLA	4	604	29	1/1/12/20	5/19/97/115	-
28	XAT	8	315	-	-	0/31/93/93	0/4/4/4
17	CLA	B	823	2	1/1/14/20	12/31/109/115	-
20	BCR	a	850	-	-	6/29/63/63	0/2/2/2
17	CLA	6	315	13	1/1/13/20	6/25/103/115	-
17	CLA	A	808	1	1/1/15/20	8/37/115/115	-
17	CLA	a	815	1	1/1/11/20	3/13/91/115	-
17	CLA	A	845	19	1/1/12/20	10/22/100/115	-
28	XAT	1	317	-	-	0/31/93/93	0/4/4/4
20	BCR	a	854	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	f	7002	29	1/1/11/20	1/13/91/115	-
17	CLA	7	603	14	1/1/12/20	3/21/99/115	-
17	CLA	B	840	2	-	9/37/115/115	-
19	LHG	3	319	17	-	11/23/23/53	-
19	LHG	a	847	-	-	10/53/53/53	-
20	BCR	1	318	-	-	6/29/63/63	0/2/2/2
17	CLA	B	808	2	1/1/15/20	7/37/115/115	-
21	SF4	c	101	3	-	-	0/6/5/5
19	LHG	2	618	17	-	9/41/41/53	-
26	CHL	2	605	29	2/2/15/26	0/12/110/137	-
17	CLA	b	817	2	1/1/13/20	11/30/108/115	-
19	LHG	7	618	17	-	10/41/41/53	-
17	CLA	A	836	1	1/1/12/20	0/19/97/115	-
17	CLA	8	304	29	1/1/10/20	0/10/88/115	-
20	BCR	2	617	-	-	3/29/63/63	0/2/2/2
17	CLA	B	825	29	1/1/15/20	7/37/115/115	-
26	CHL	4	615	16	3/3/15/26	0/12/110/137	-
20	BCR	B	844	-	-	6/29/63/63	0/2/2/2
17	CLA	3	304	29	1/1/11/20	1/13/91/115	-
17	CLA	a	812	1	1/1/15/20	13/37/115/115	-
19	LHG	a	848	17	-	12/31/31/53	-
17	CLA	B	839	29	1/1/15/20	7/37/115/115	-
17	CLA	2	603	14	1/1/15/20	11/37/115/115	-
17	CLA	2	612	14	1/1/15/20	9/37/115/115	-
17	CLA	a	846	19	1/1/12/20	13/22/100/115	-
17	CLA	9	604	29	1/1/12/20	5/19/97/115	-
17	CLA	1	315	13	1/1/11/20	1/15/93/115	-
17	CLA	B	826	2	1/1/15/20	10/37/115/115	-
17	CLA	a	813	1	1/1/12/20	6/24/102/115	-
17	CLA	b	839	29	1/1/15/20	9/37/115/115	-
20	BCR	j	3003	-	-	6/29/63/63	0/2/2/2
17	CLA	7	608	14	1/1/12/20	6/19/97/115	-
17	CLA	A	823	1	1/1/11/20	5/18/96/115	-
17	CLA	a	836	1	1/1/12/20	2/19/97/115	-
17	CLA	a	827	29	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	8	313	-	1/1/4/20	-	-
17	CLA	4	613	16	1/1/11/20	2/13/91/115	-
17	CLA	2	604	29	1/1/14/20	9/31/109/115	-
17	CLA	b	831	2	1/1/11/20	7/18/96/115	-
17	CLA	7	604	29	1/1/14/20	11/31/109/115	-
17	CLA	a	830	1	1/1/15/20	11/37/115/115	-
26	CHL	2	607	29	3/3/17/26	5/21/119/137	-
26	CHL	7	601	14	3/3/19/26	8/33/131/137	-
17	CLA	B	841	19	1/1/15/20	8/37/115/115	-
28	XAT	9	617	-	-	0/31/93/93	0/4/4/4
17	CLA	b	822	2	1/1/13/20	10/25/103/115	-
20	BCR	B	846	-	-	4/29/63/63	0/2/2/2
17	CLA	A	817	29	-	3/13/91/115	-
17	CLA	K	4003	11	1/1/11/20	2/15/93/115	-
26	CHL	7	607	29	3/3/17/26	4/21/119/137	-
17	CLA	G	103	7	1/1/12/20	1/19/97/115	-
26	CHL	7	614	14	3/3/15/26	3/12/110/137	-
24	DGD	B	850	-	-	12/55/95/95	0/2/2/2
17	CLA	a	811	1	1/1/15/20	9/37/115/115	-
17	CLA	4	601	16	1/1/11/20	3/15/93/115	-
20	BCR	3	318	-	-	6/29/63/63	0/2/2/2
17	CLA	6	312	19	1/1/10/20	0/8/86/115	-
20	BCR	a	849	-	-	2/29/63/63	0/2/2/2
27	LUT	6	317	-	-	2/29/67/67	0/2/2/2
17	CLA	B	835	29	1/1/11/20	1/13/91/115	-
17	CLA	l	202	12	1/1/15/20	10/37/115/115	-
17	CLA	1	306	-	1/1/12/20	2/22/100/115	-
17	CLA	b	841	19	1/1/15/20	4/37/115/115	-
17	CLA	B	838	2	1/1/11/20	0/16/94/115	-
20	BCR	j	3004	-	-	9/29/63/63	0/2/2/2
17	CLA	1	303	13	1/1/15/20	9/37/115/115	-
28	XAT	4	617	-	-	0/31/93/93	0/4/4/4
28	XAT	7	616	-	-	1/31/93/93	0/4/4/4
20	BCR	A	849	-	-	2/29/63/63	0/2/2/2
17	CLA	A	804	1	1/1/15/20	7/37/115/115	-
18	PQN	b	842	-	-	3/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	a	833	1	1/1/15/20	5/37/115/115	-
17	CLA	A	841	1	1/1/15/20	10/37/115/115	-

The worst 5 of 5213 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	845	PQN	C3-C2	7.78	1.49	1.35
18	b	842	PQN	C3-C2	7.70	1.49	1.35
18	A	844	PQN	C3-C2	7.61	1.49	1.35
18	B	842	PQN	C3-C2	7.59	1.49	1.35
17	3	315	CLA	C3D-C2D	6.56	1.49	1.35

The worst 5 of 9160 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	832	CLA	C1D-ND-C4D	-10.07	99.18	106.33
26	4	607	CHL	C2D-C1D-ND	10.04	117.50	110.10
17	L	203	CLA	C1D-ND-C4D	-10.01	99.23	106.33
26	7	606	CHL	C2D-C1D-ND	9.96	117.44	110.10
26	1	302	CHL	C2D-C1D-ND	9.90	117.40	110.10

5 of 348 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	801	CLA	CBD
17	A	801	CLA	ND
17	A	802	CLA	ND
17	A	803	CLA	ND
17	A	804	CLA	ND

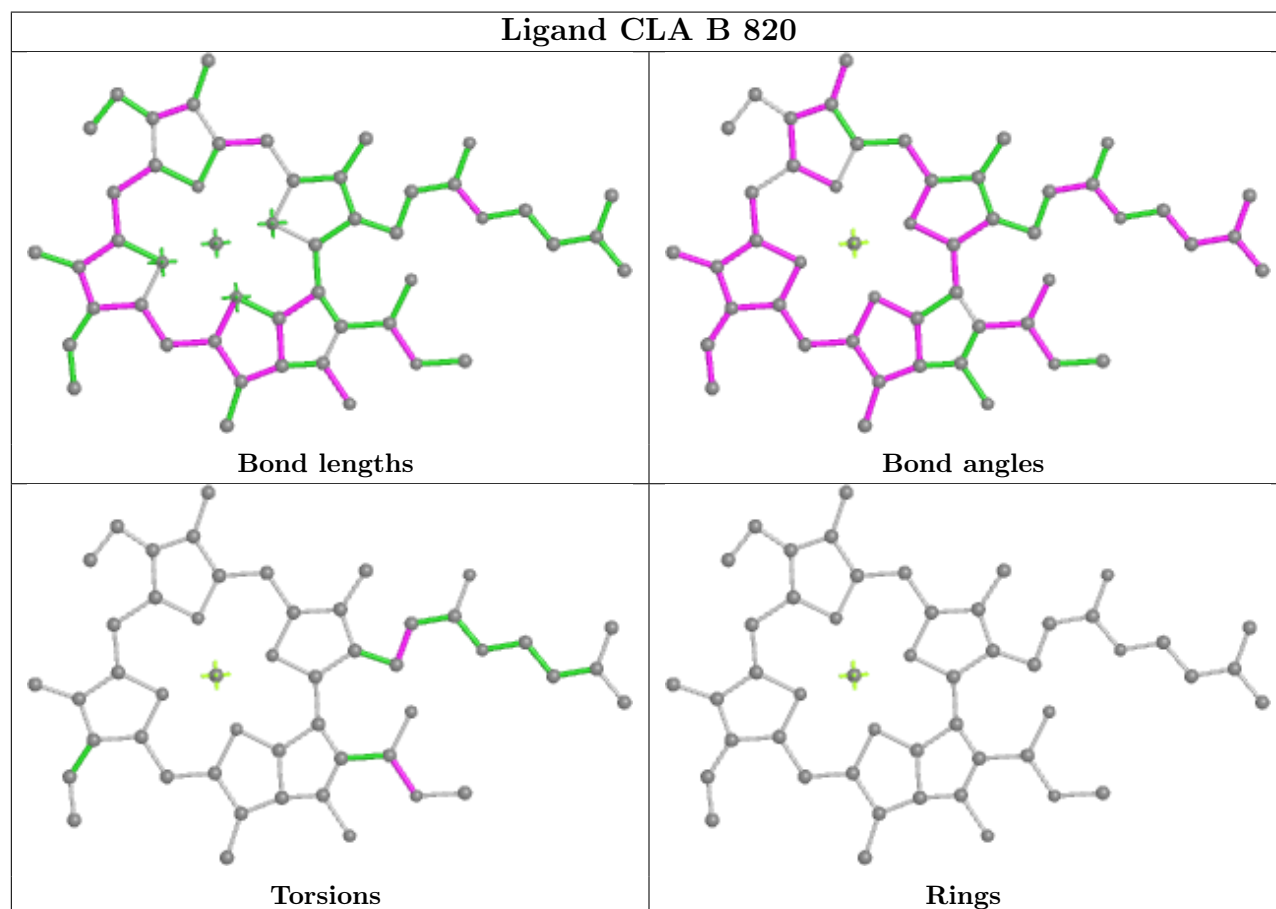
5 of 2543 torsion outliers are listed below:

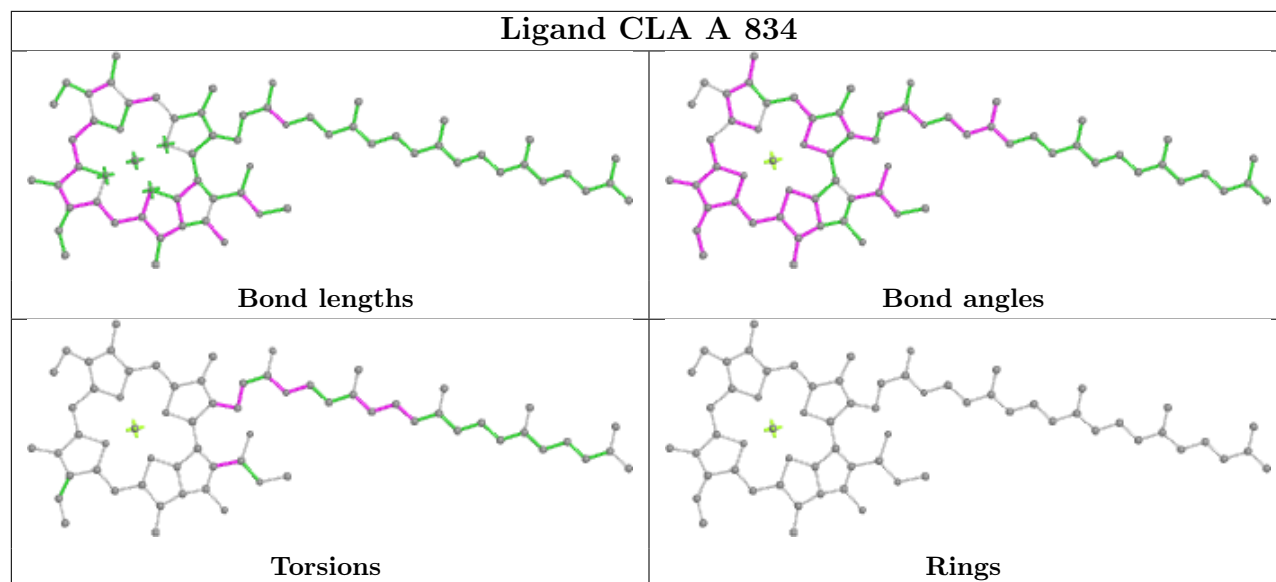
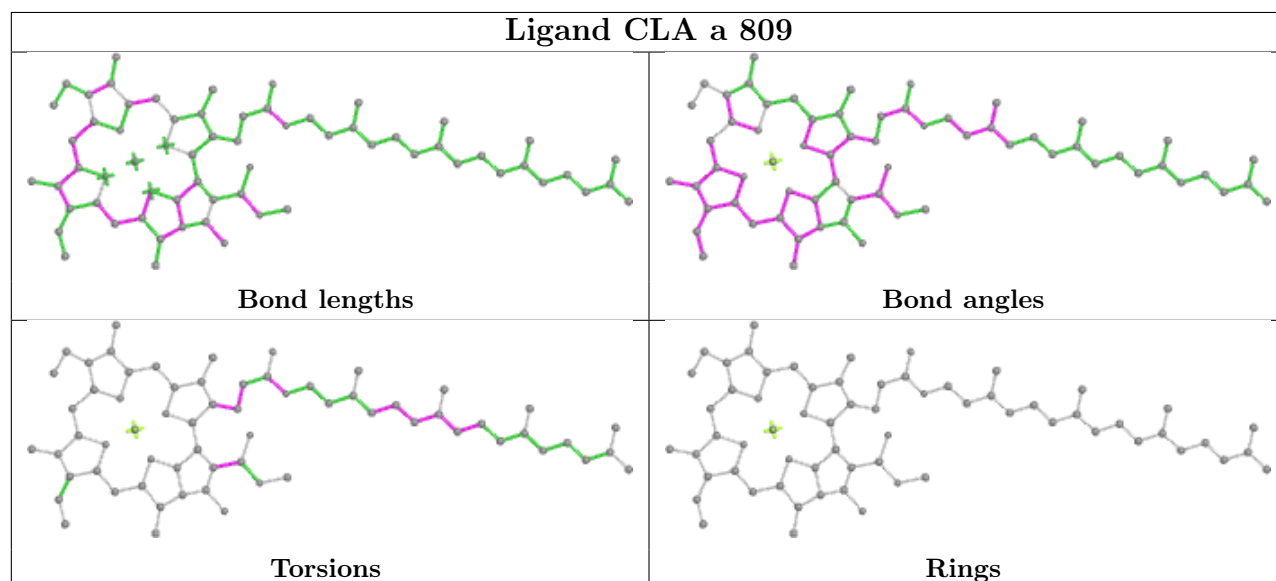
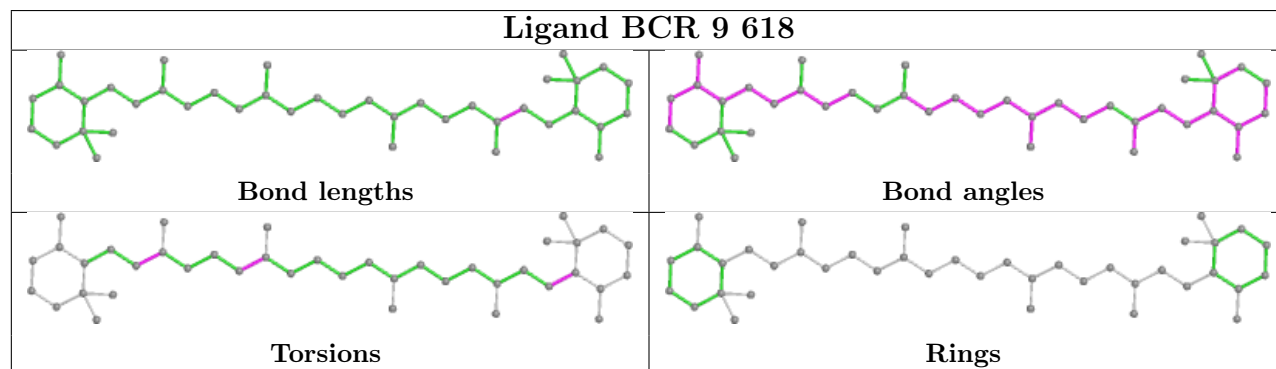
Mol	Chain	Res	Type	Atoms
17	A	805	CLA	CHA-CBD-CGD-O1D
17	A	809	CLA	C3A-C2A-CAA-CBA
17	A	809	CLA	CHA-CBD-CGD-O1D
17	A	809	CLA	CHA-CBD-CGD-O2D
17	A	811	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

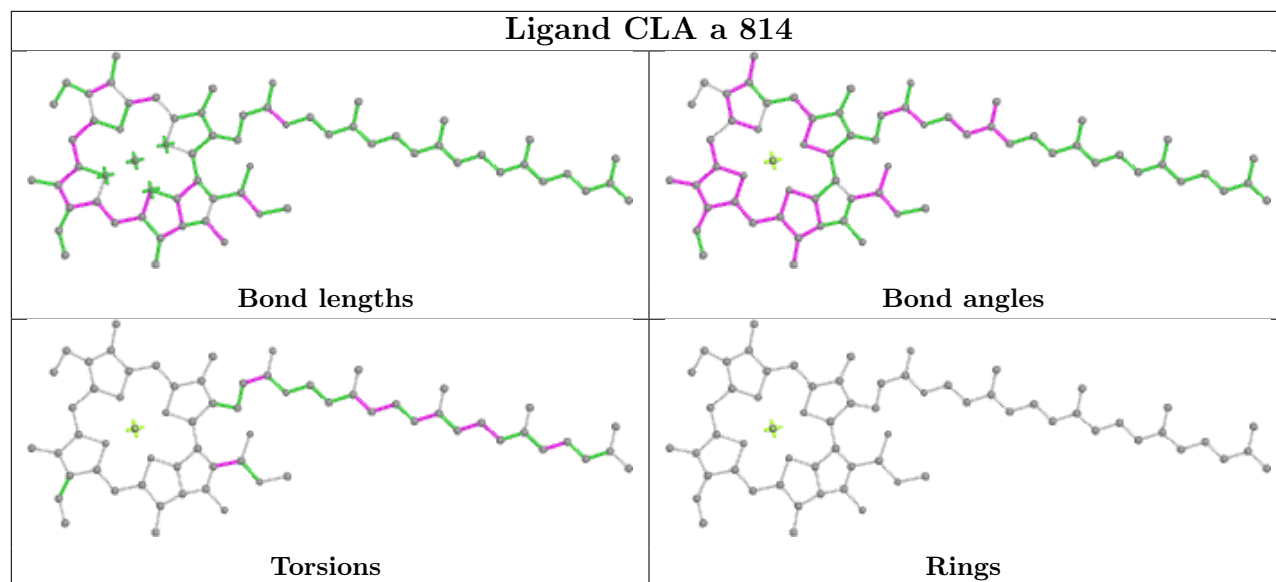
No monomer is involved in short contacts.

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

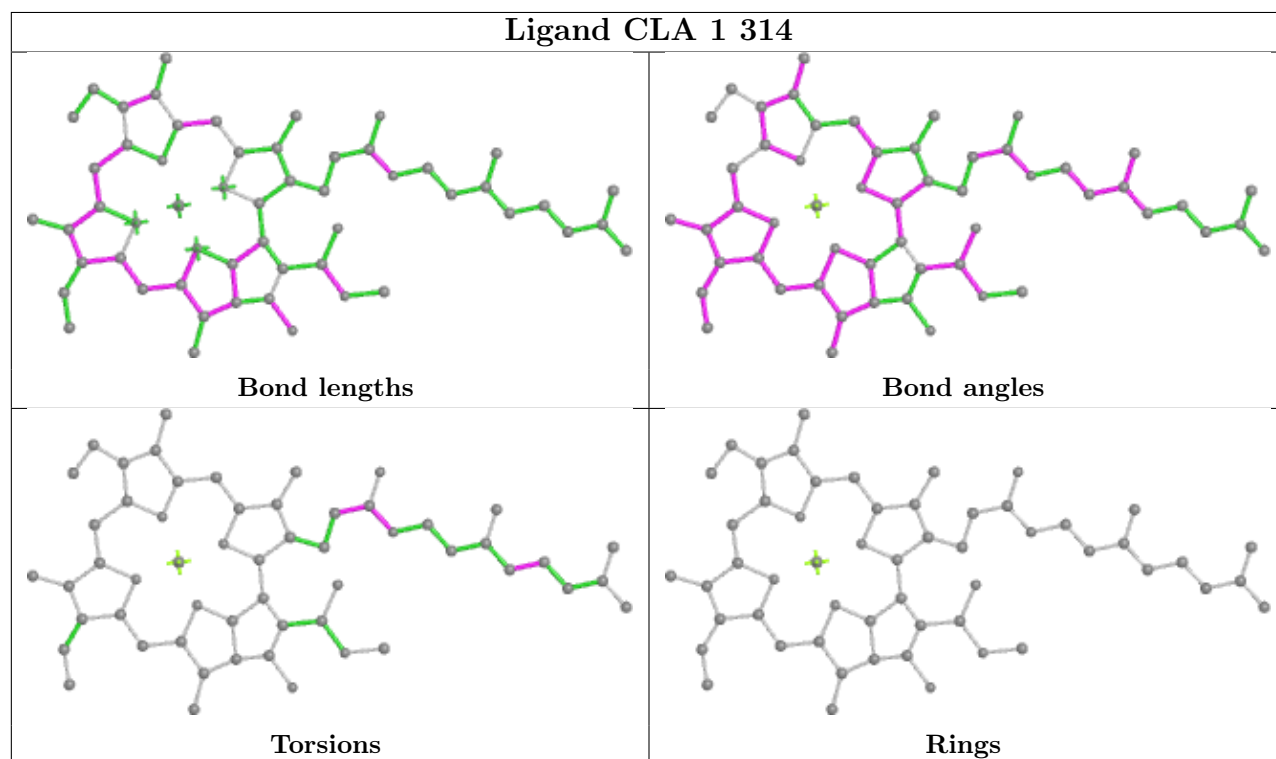


**Ligand CLA A 834****Ligand CLA a 809****Ligand BCR 9 618**

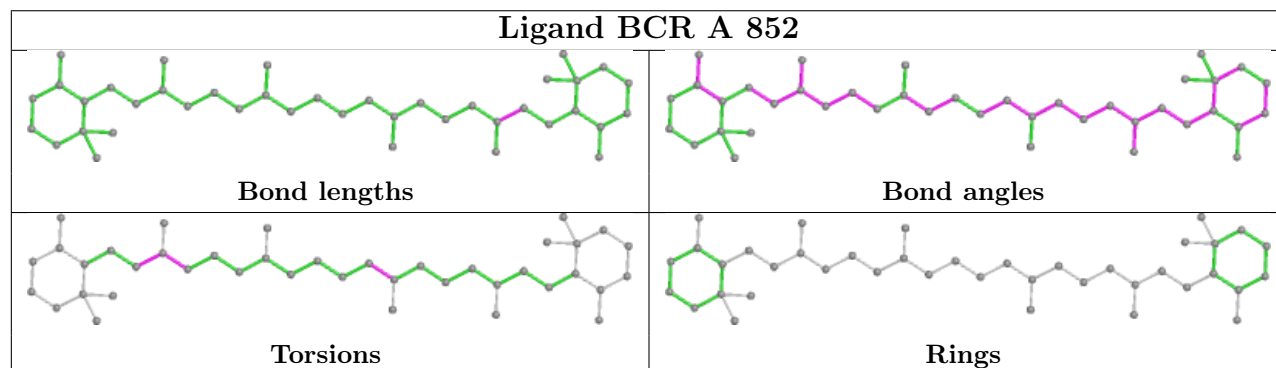
## Ligand CLA a 814

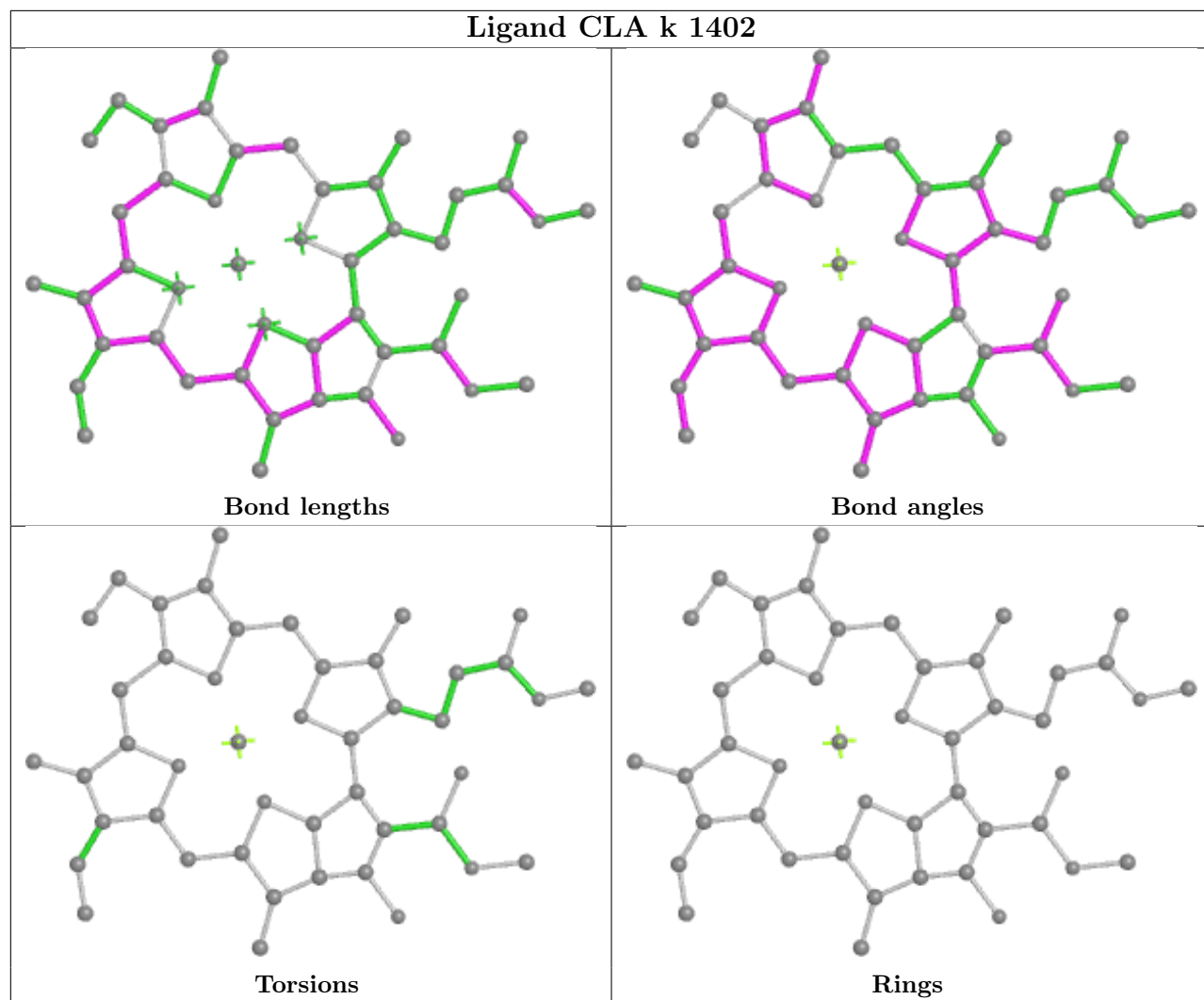


## Ligand CLA 1 314



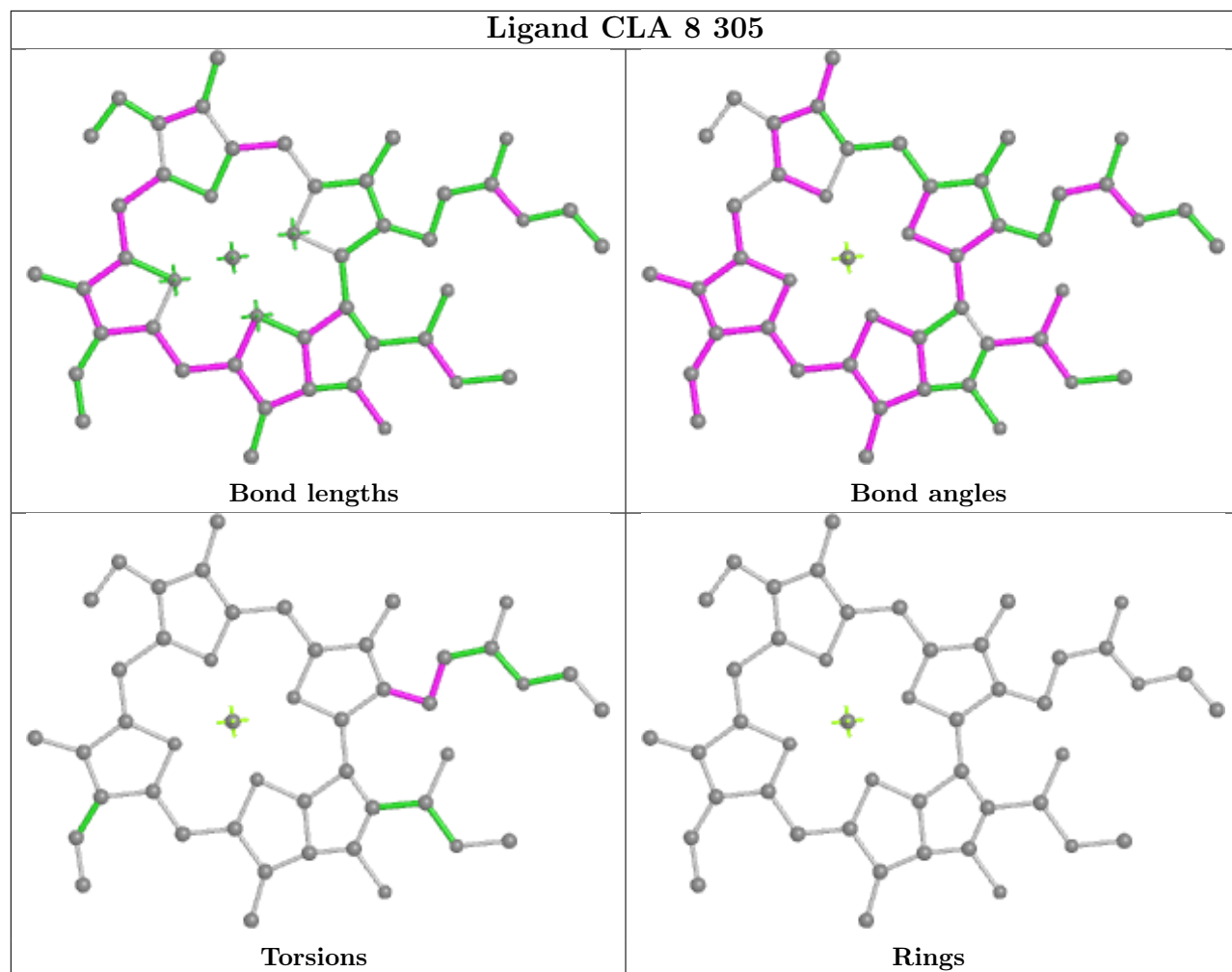
## Ligand BCR A 852



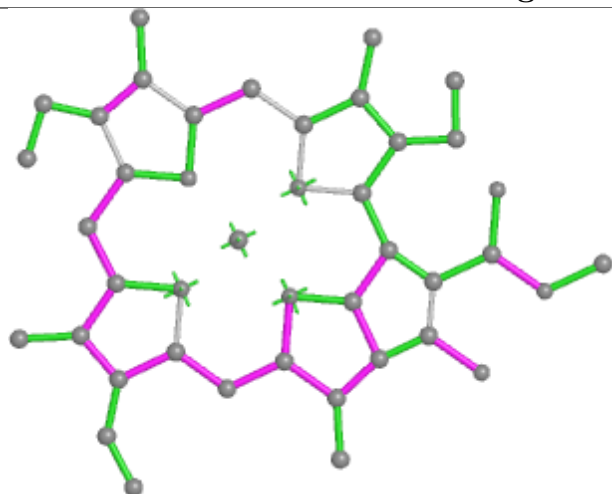




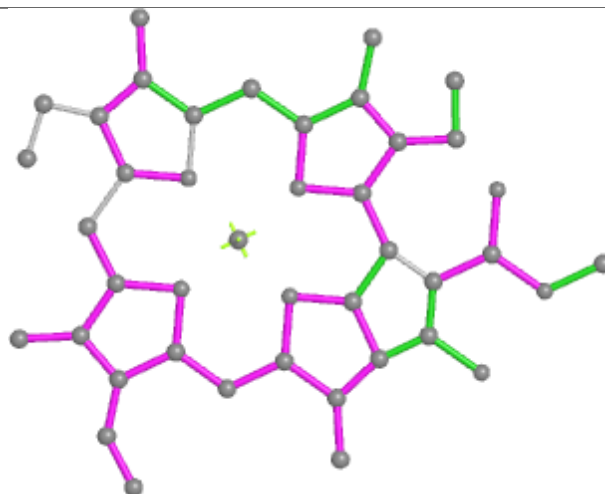
## Ligand CLA 8 305



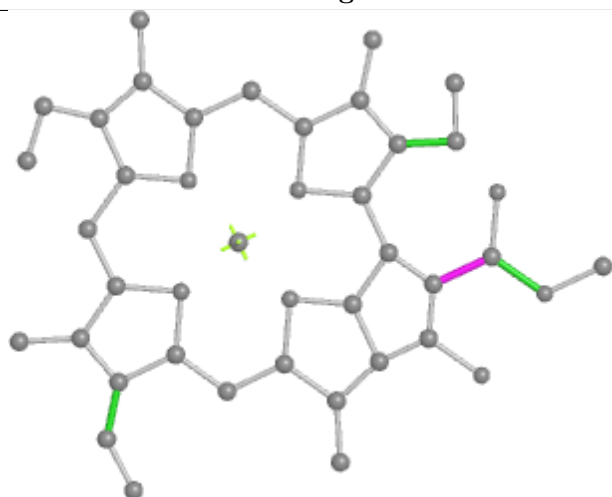
## Ligand CLA 3 305



Bond lengths



Bond angles

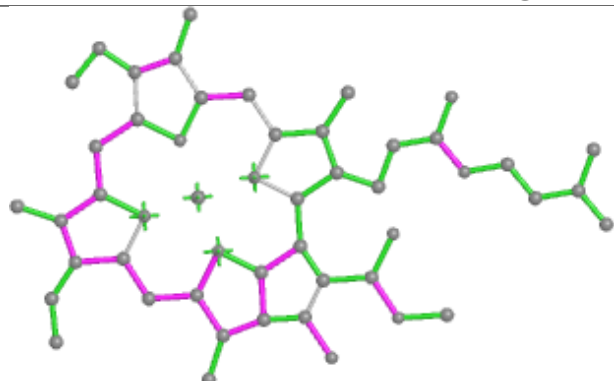


Torsions

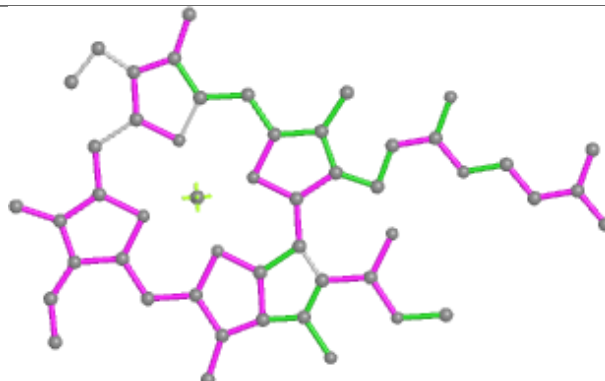


Rings

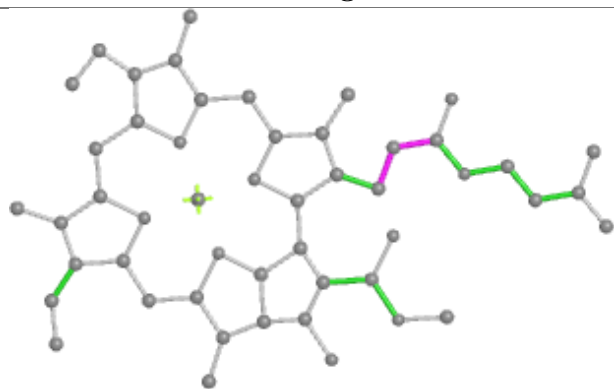
## Ligand CLA L 204



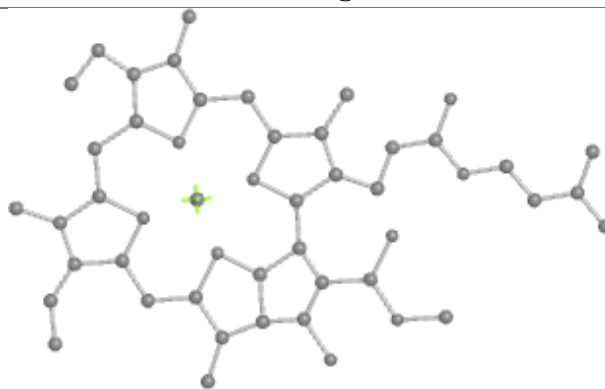
Bond lengths



Bond angles

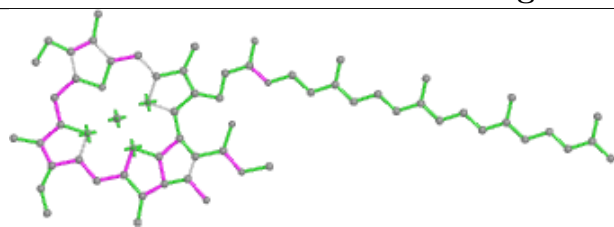


Torsions

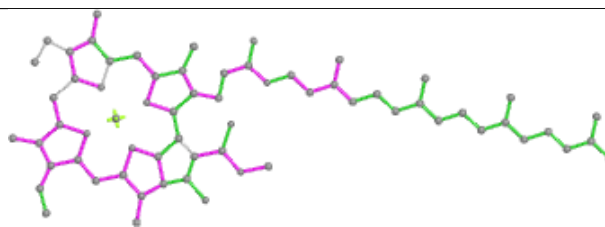


Rings

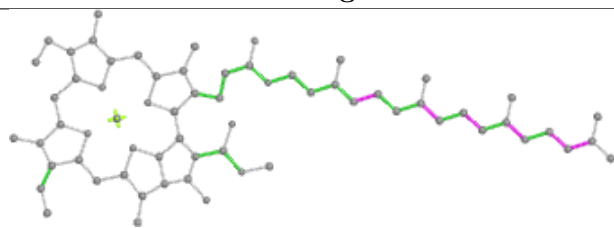
## Ligand CLA b 803



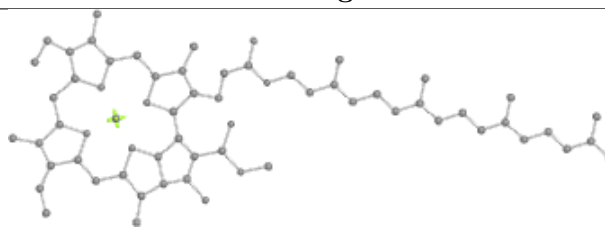
Bond lengths



Bond angles

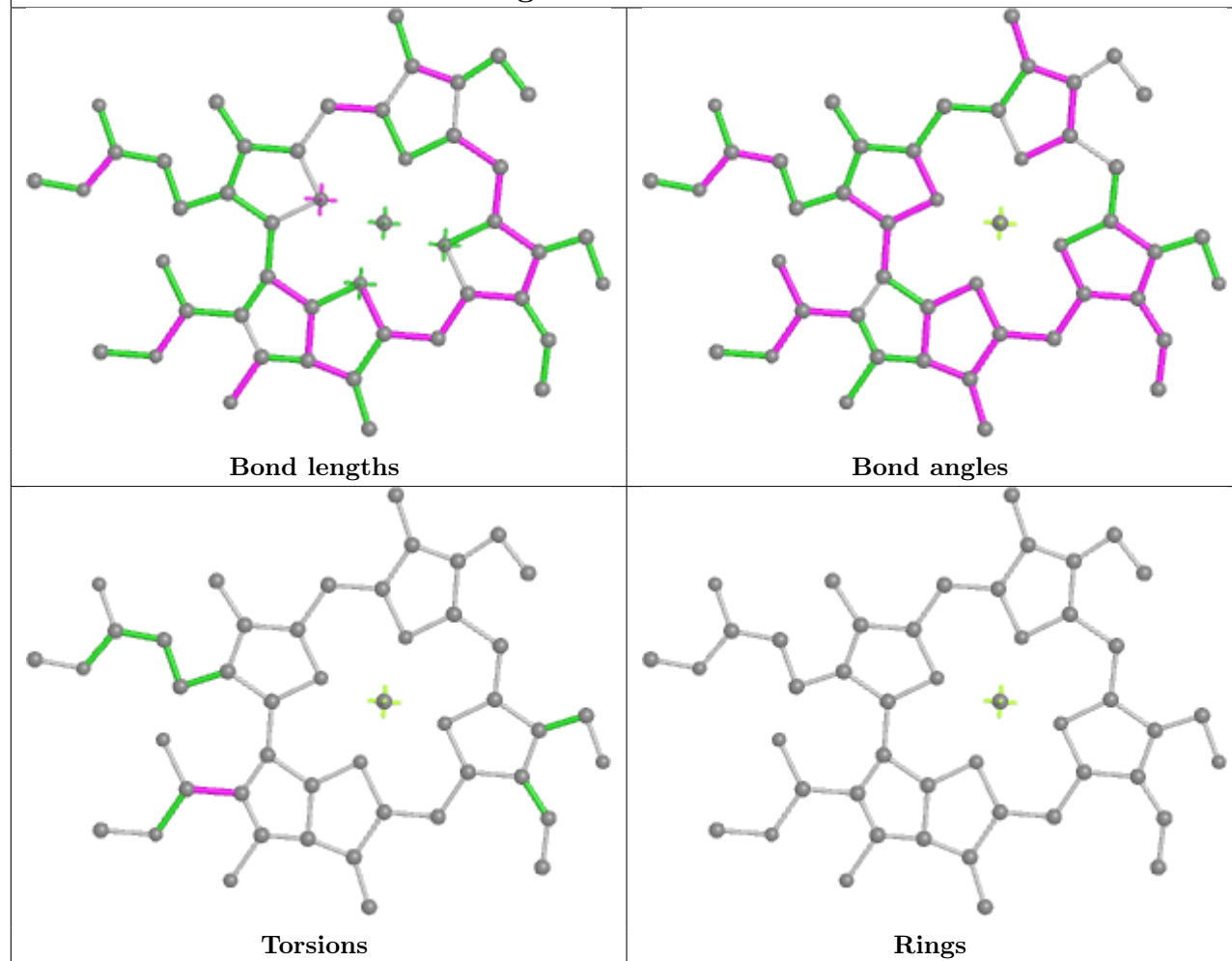


Torsions

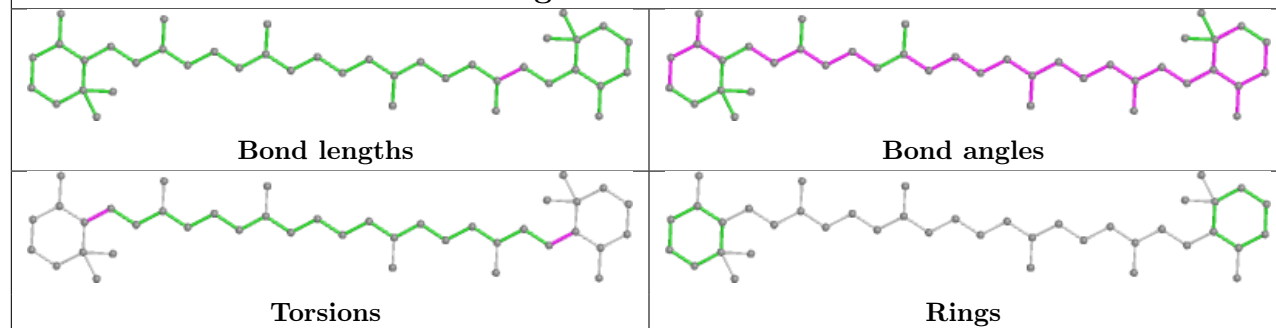


Rings

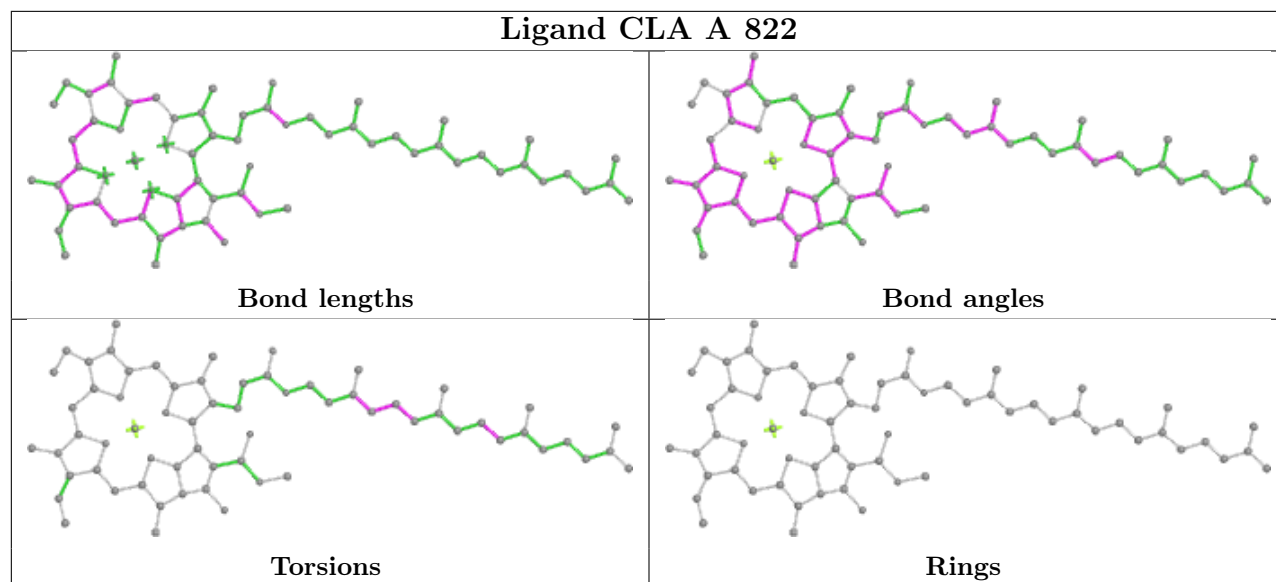
## Ligand CHL 6 308



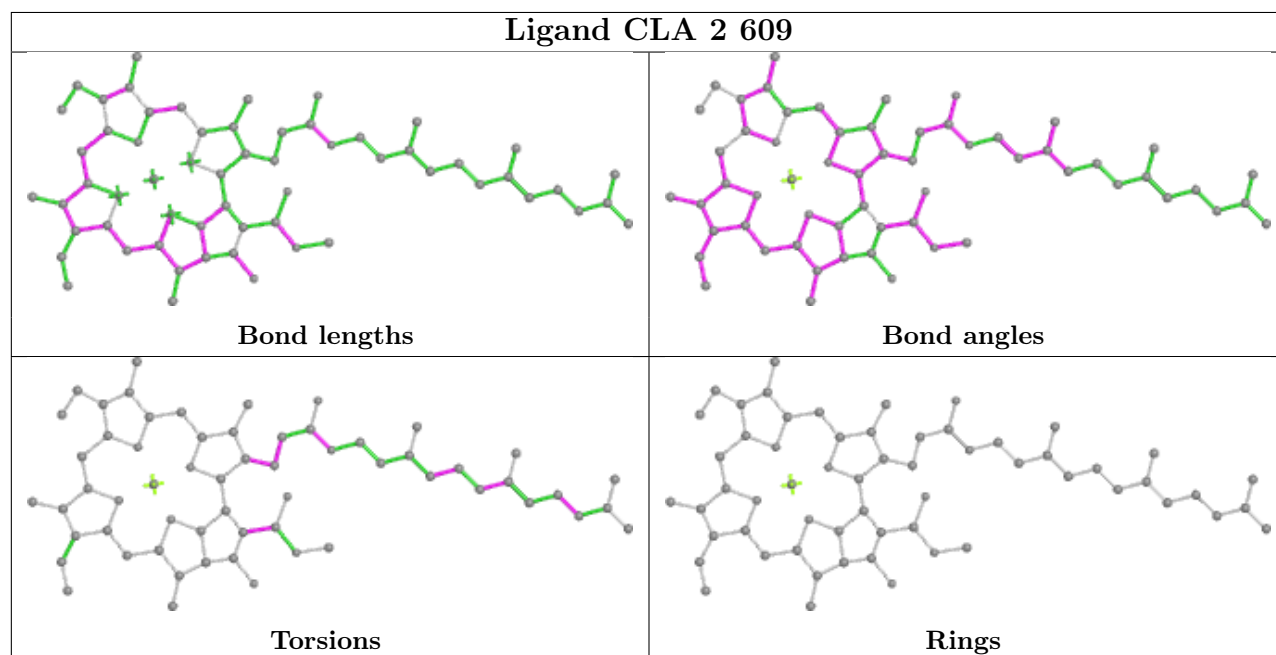
## Ligand BCR 8 316



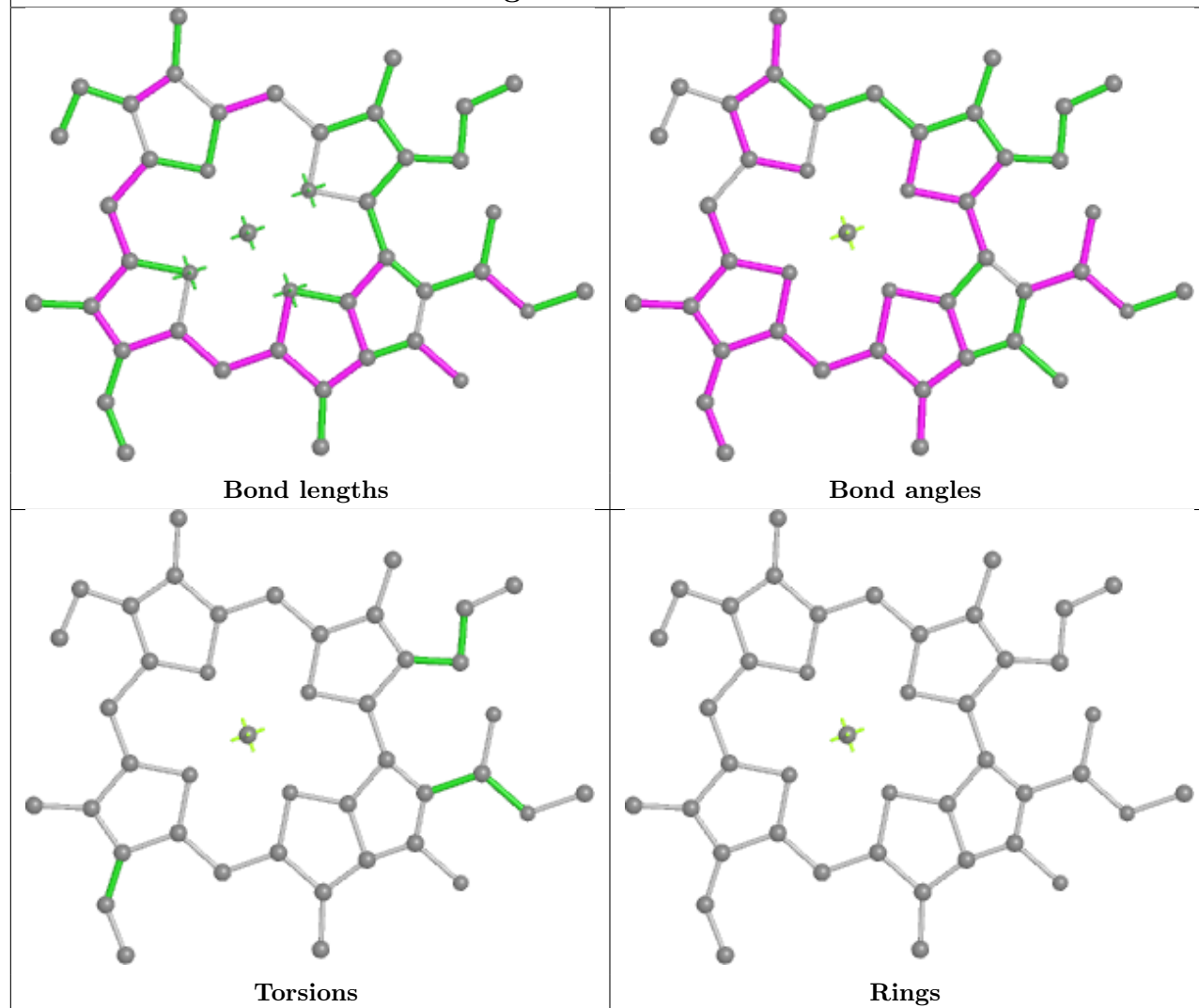
## Ligand CLA A 822



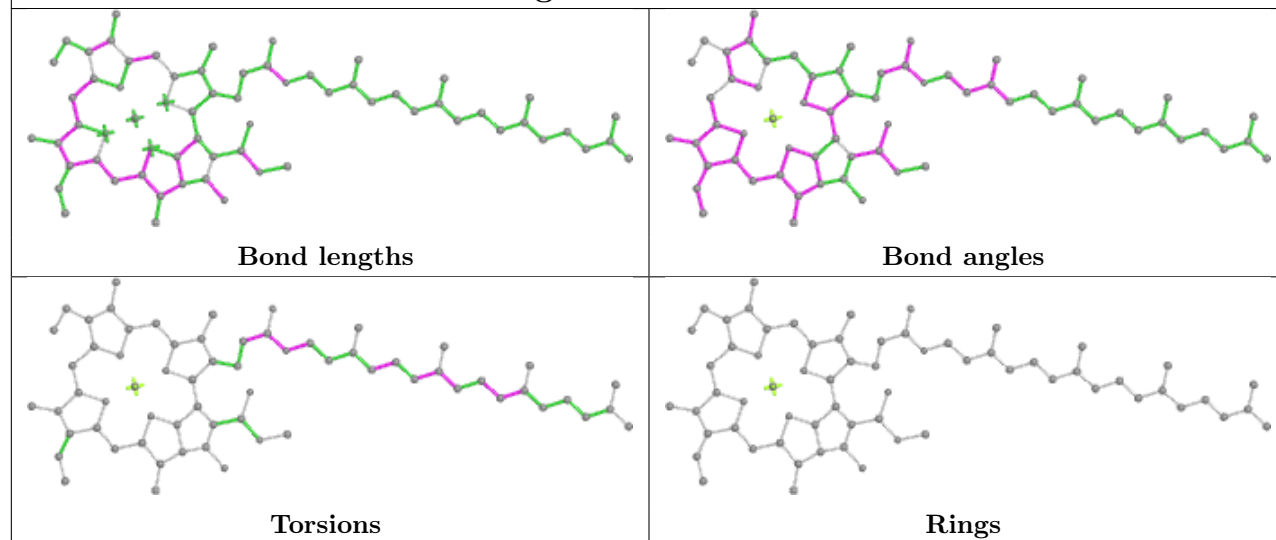
## Ligand CLA 2 609

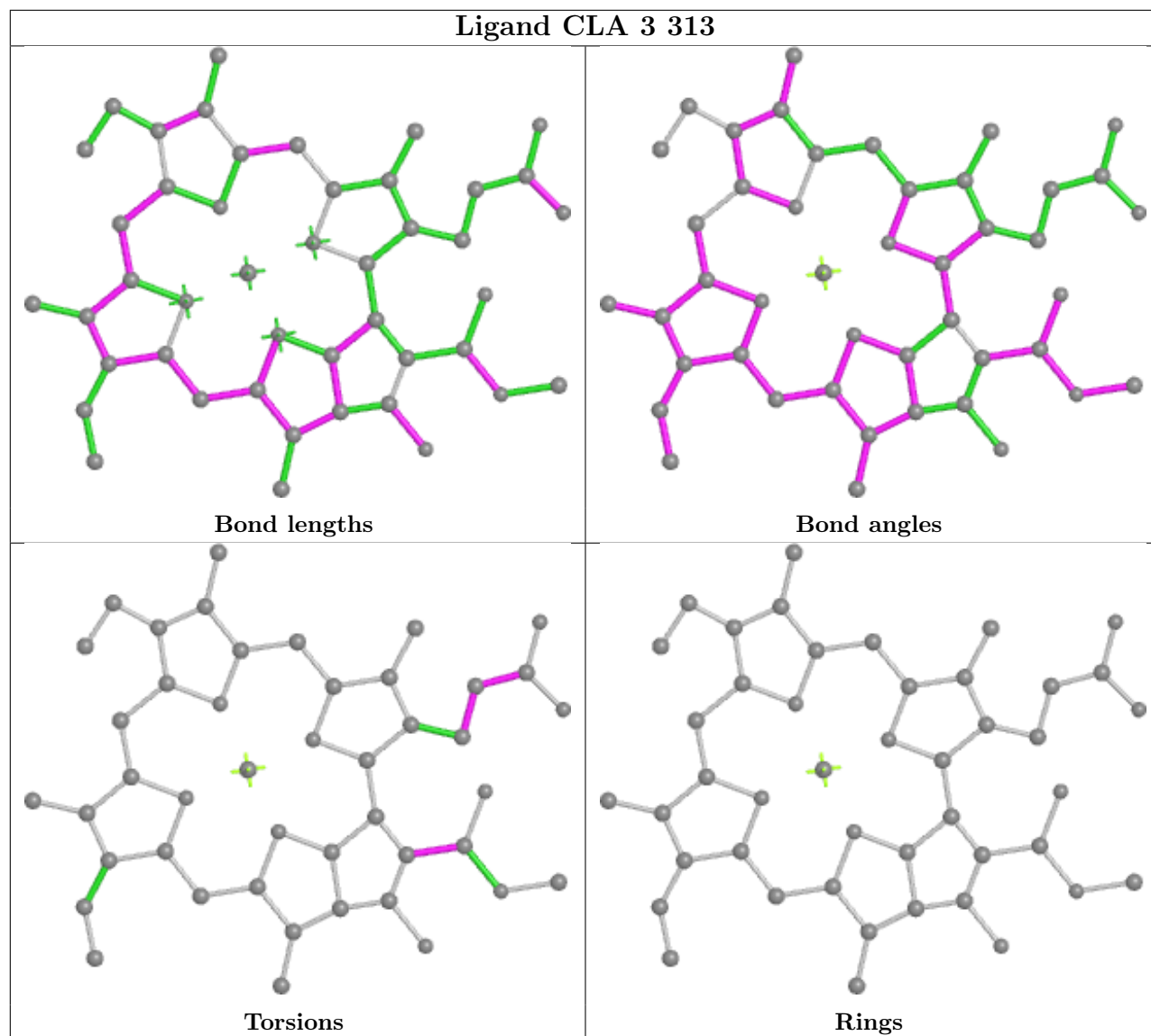
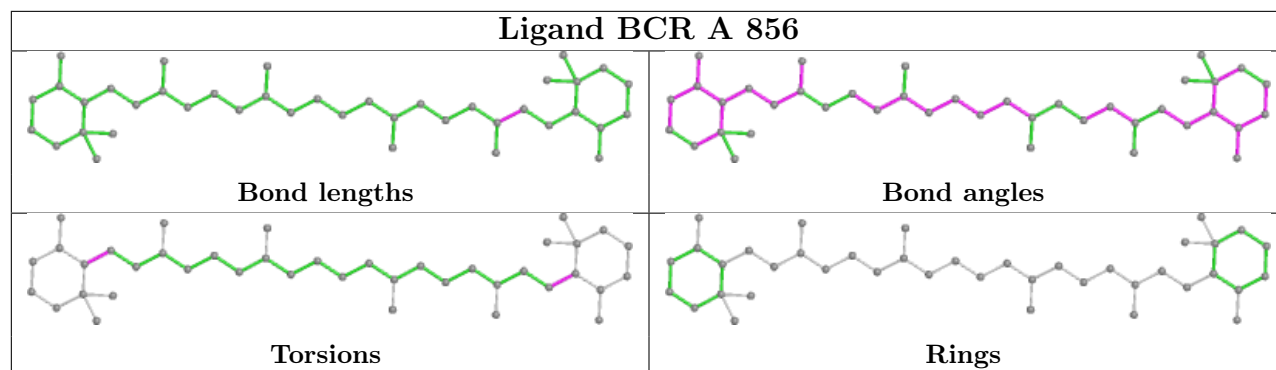


## Ligand CLA 7 613

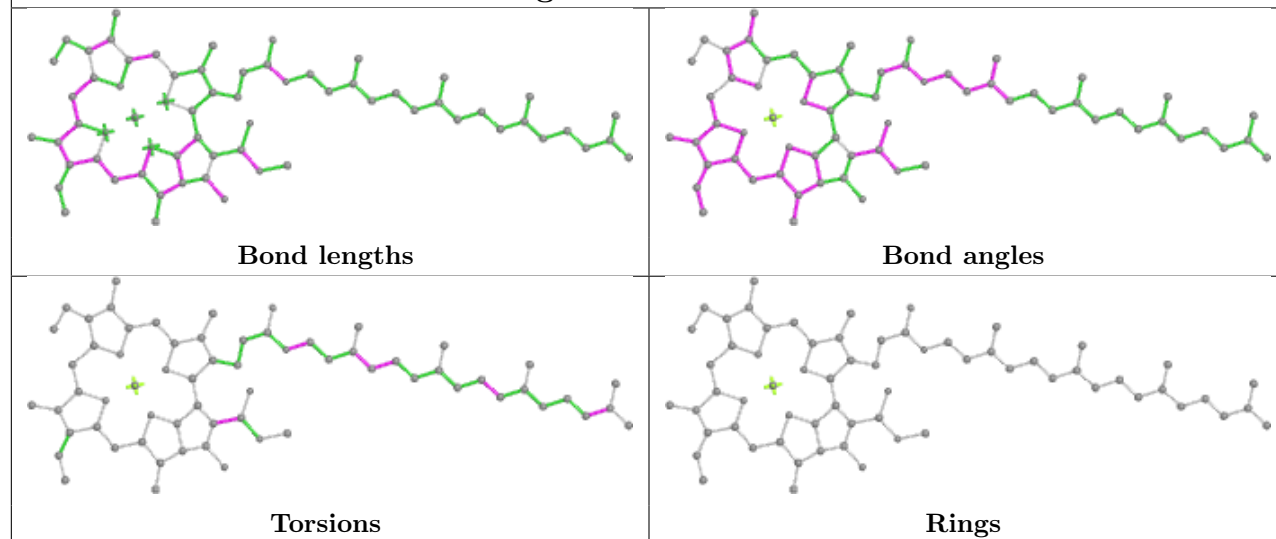


## Ligand CLA b 834

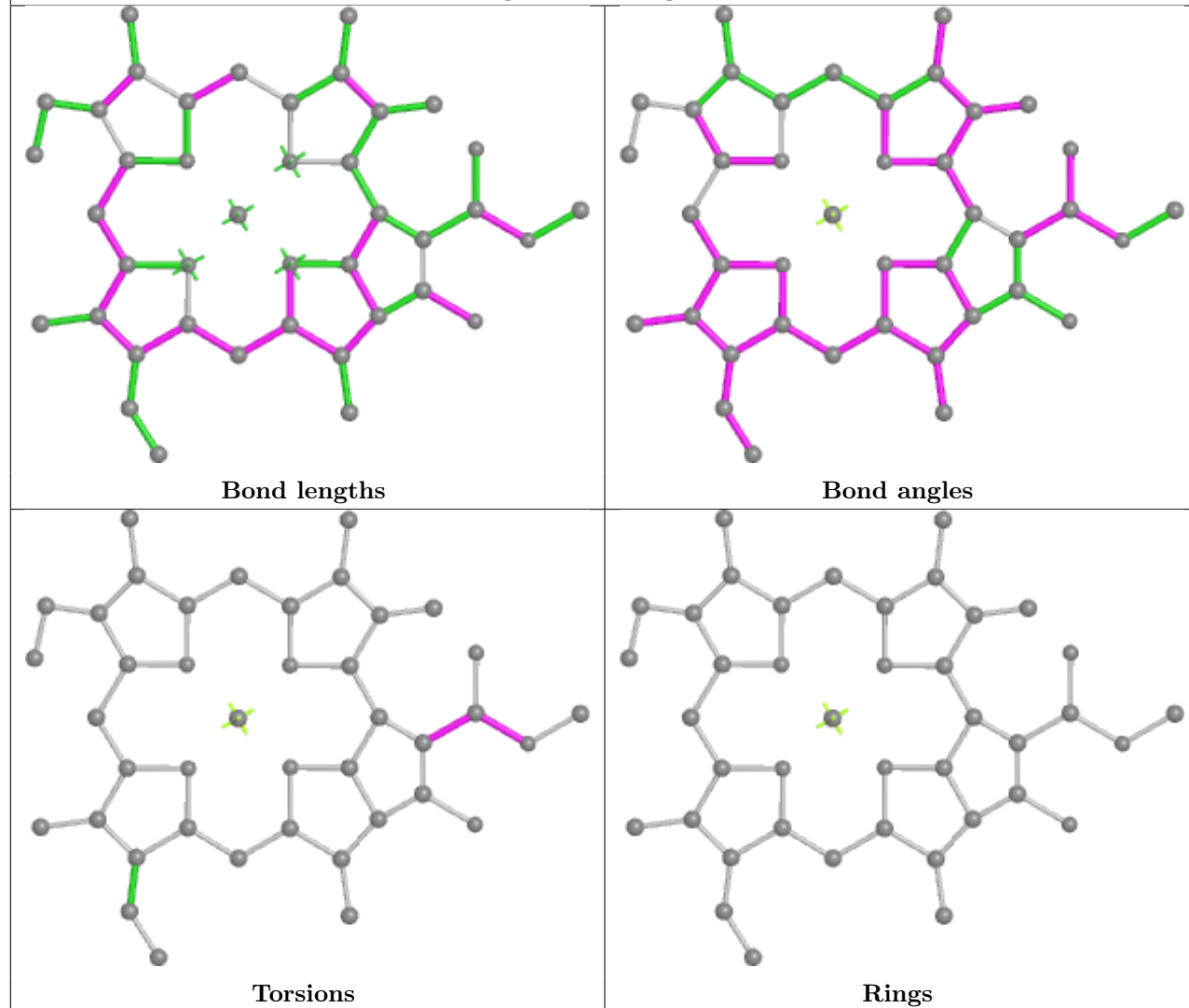




## Ligand CLA a 840

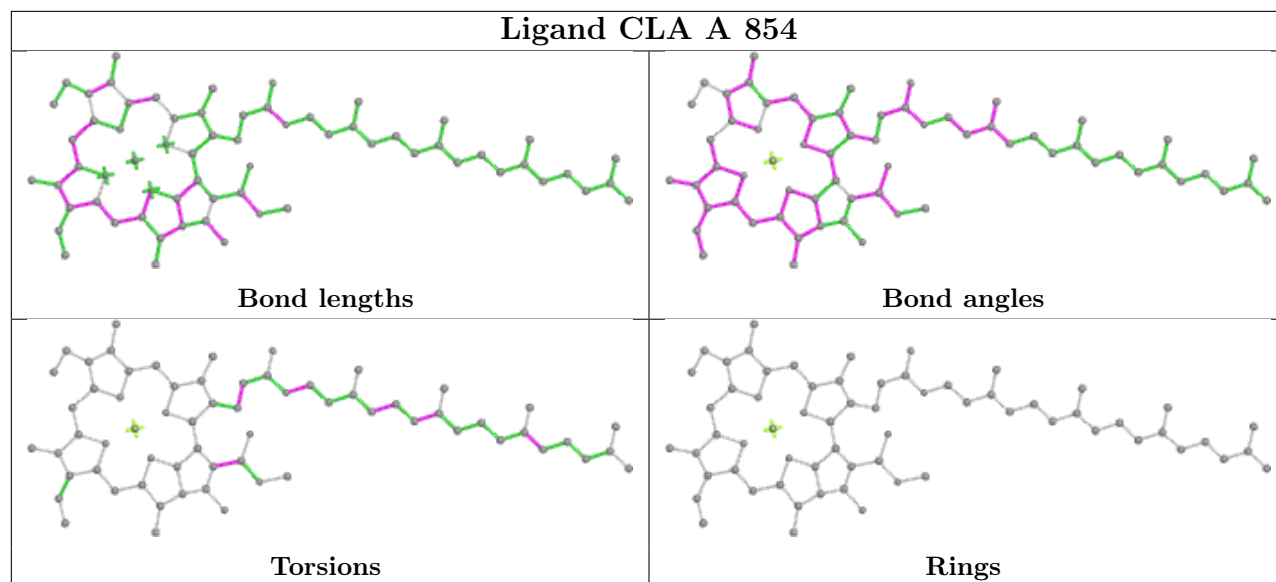


## Ligand CLA g 101

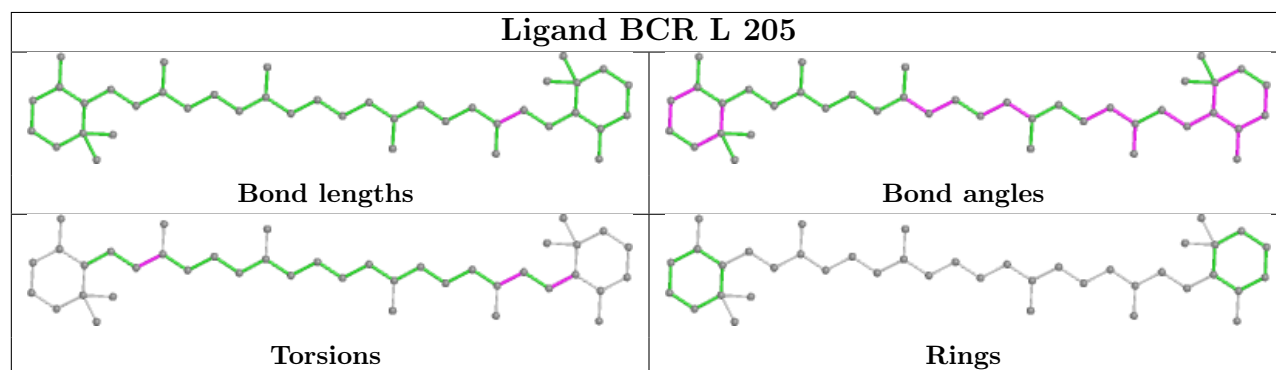




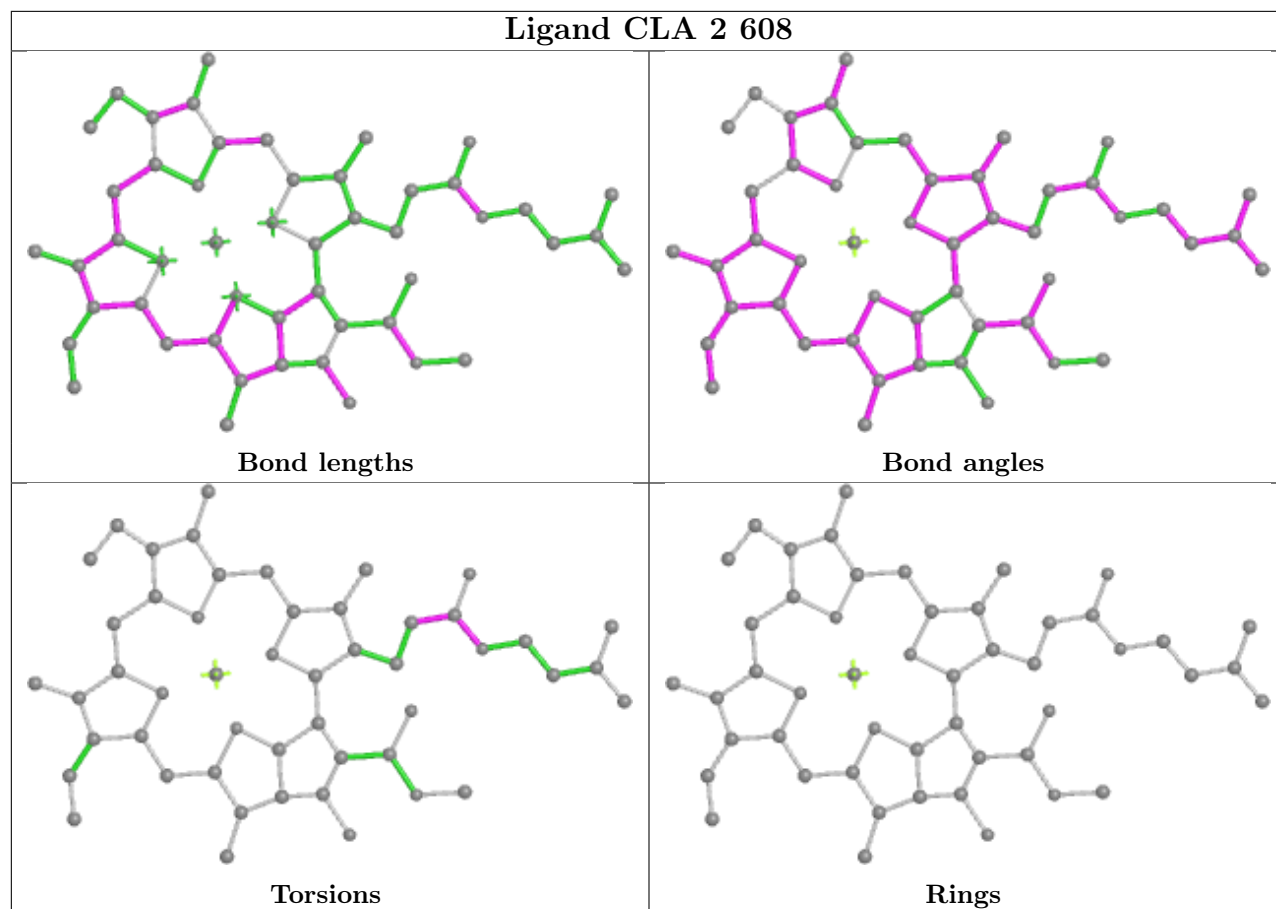
## Ligand CLA A 854



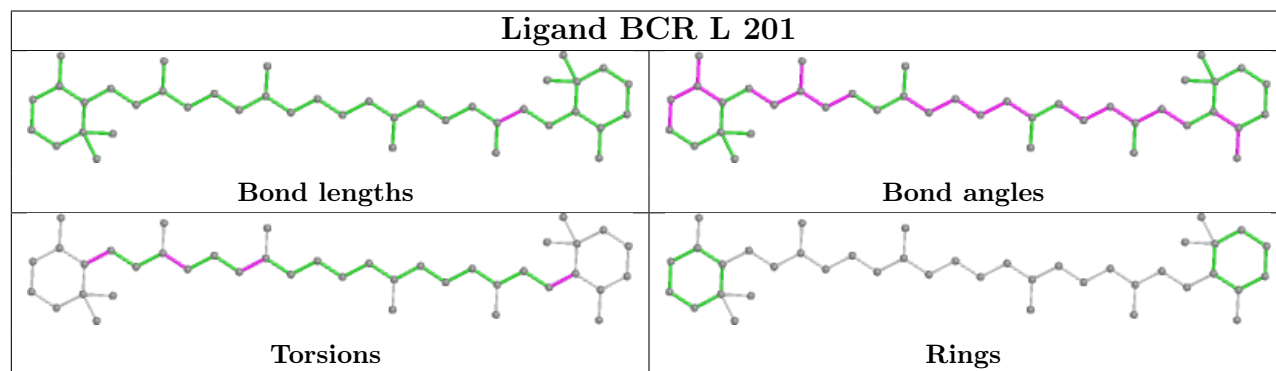
## Ligand BCR L 205

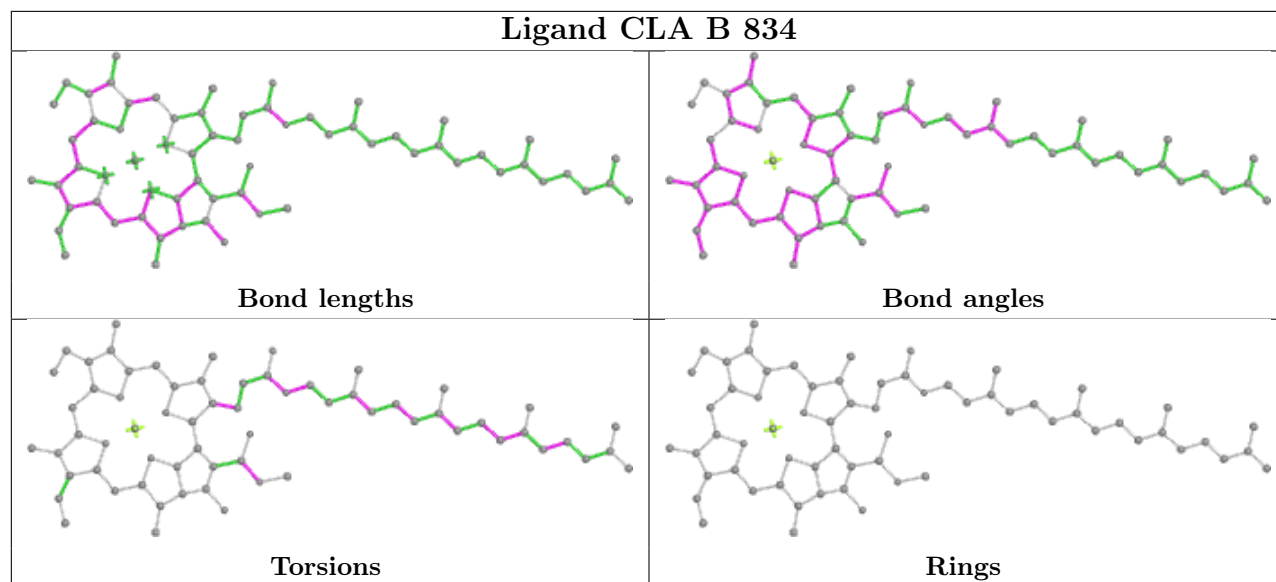
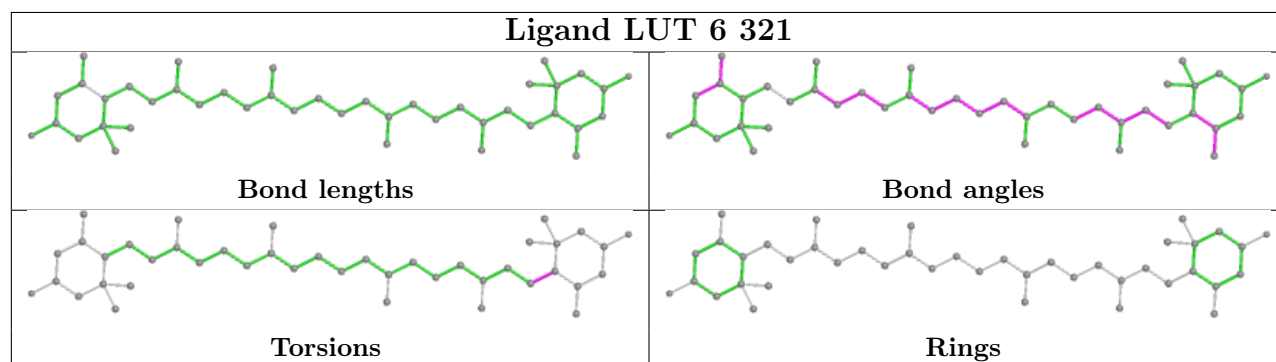


## Ligand CLA 2 608

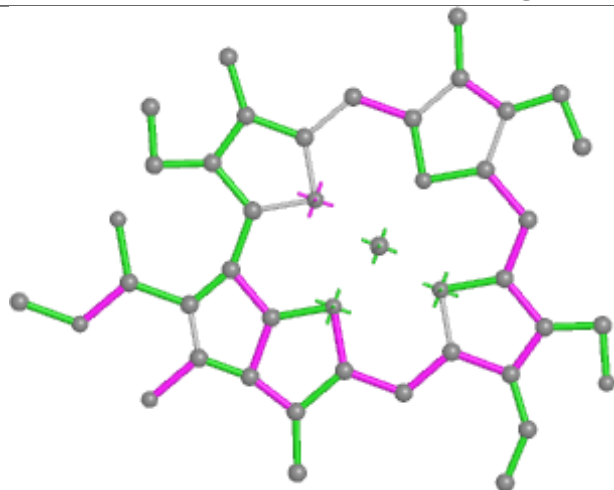


## Ligand BCR L 201

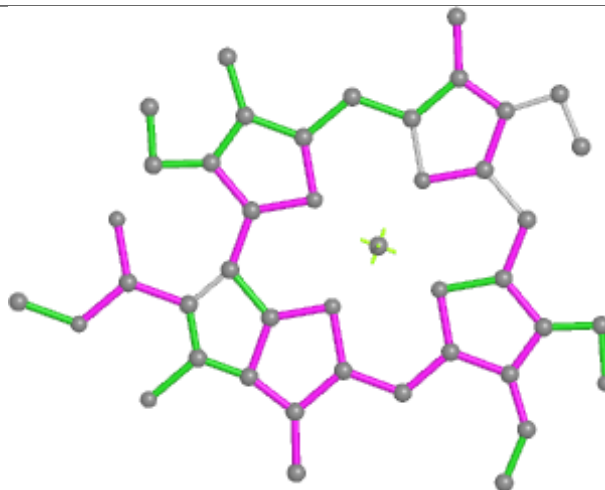


**Ligand CLA B 834****Ligand LUT 6 321**

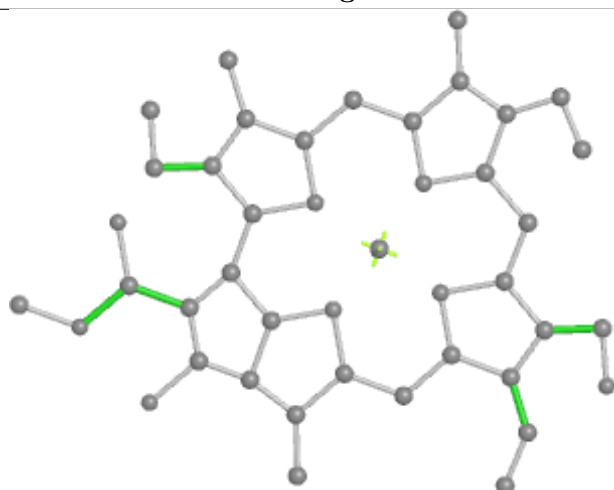
## Ligand CHL 2 614



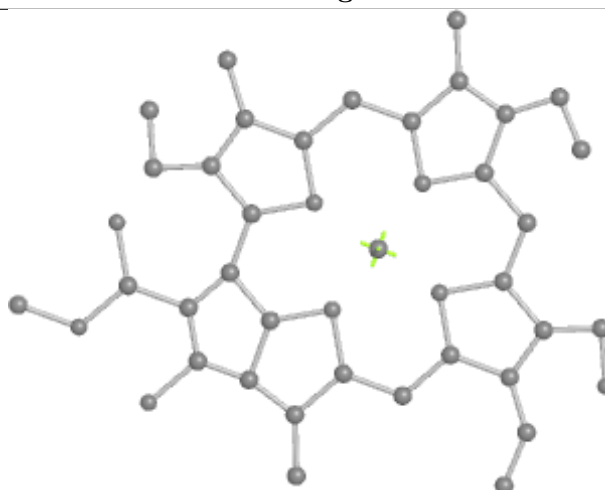
Bond lengths



Bond angles

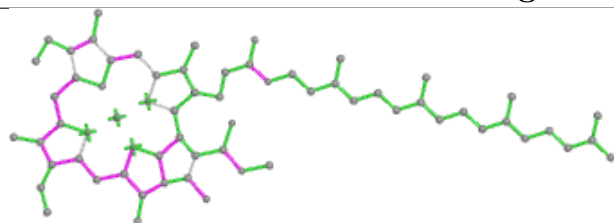


Torsions

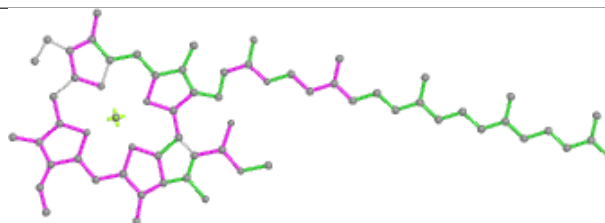


Rings

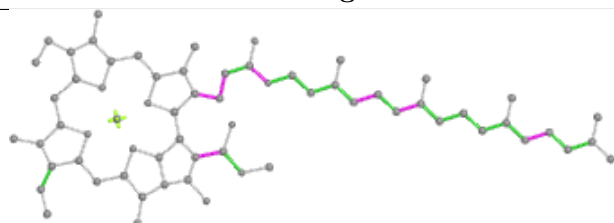
## Ligand CLA 7 602



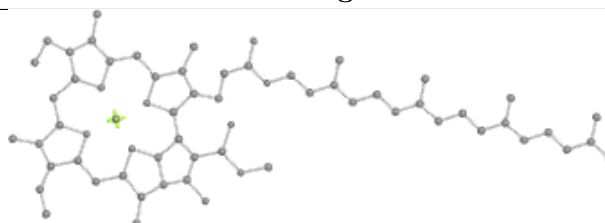
Bond lengths



Bond angles

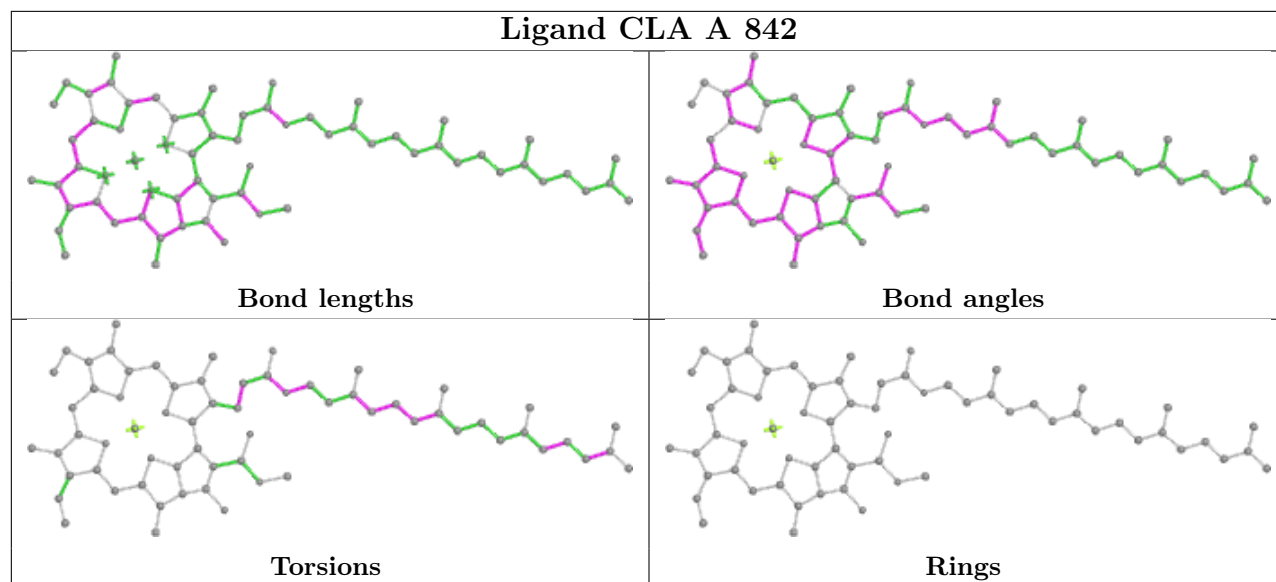


Torsions

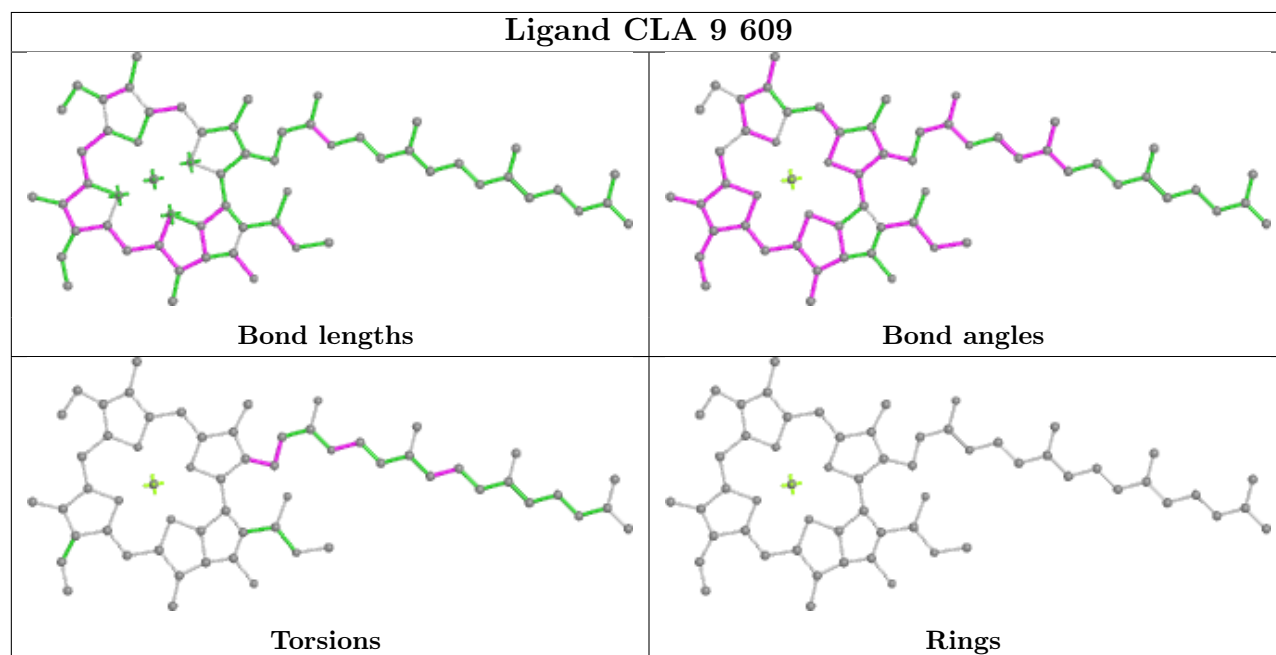


Rings

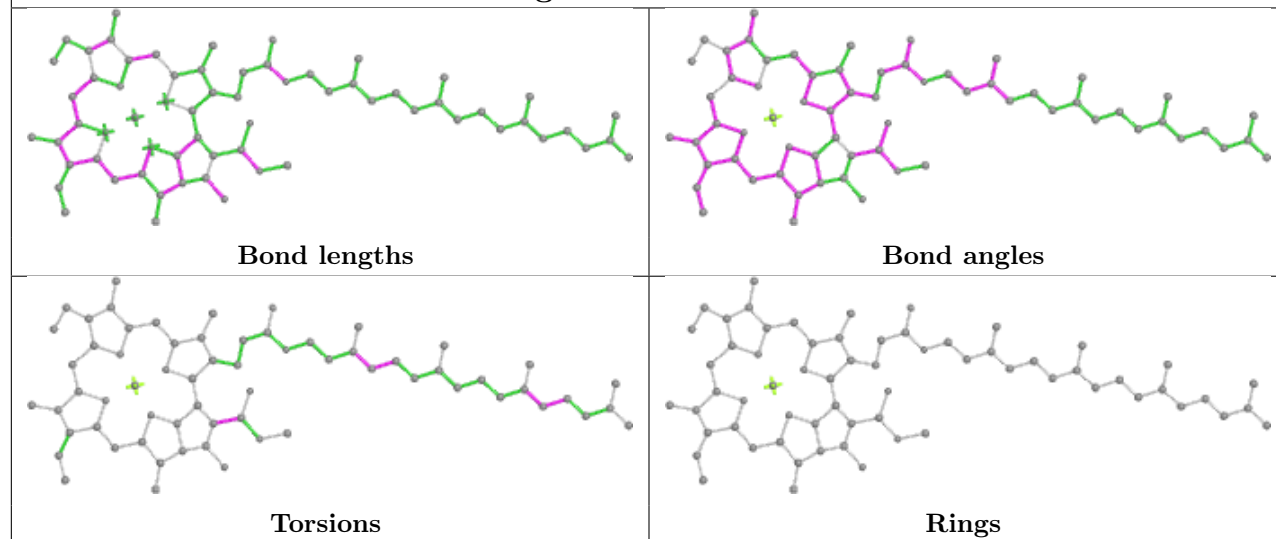
## Ligand CLA A 842



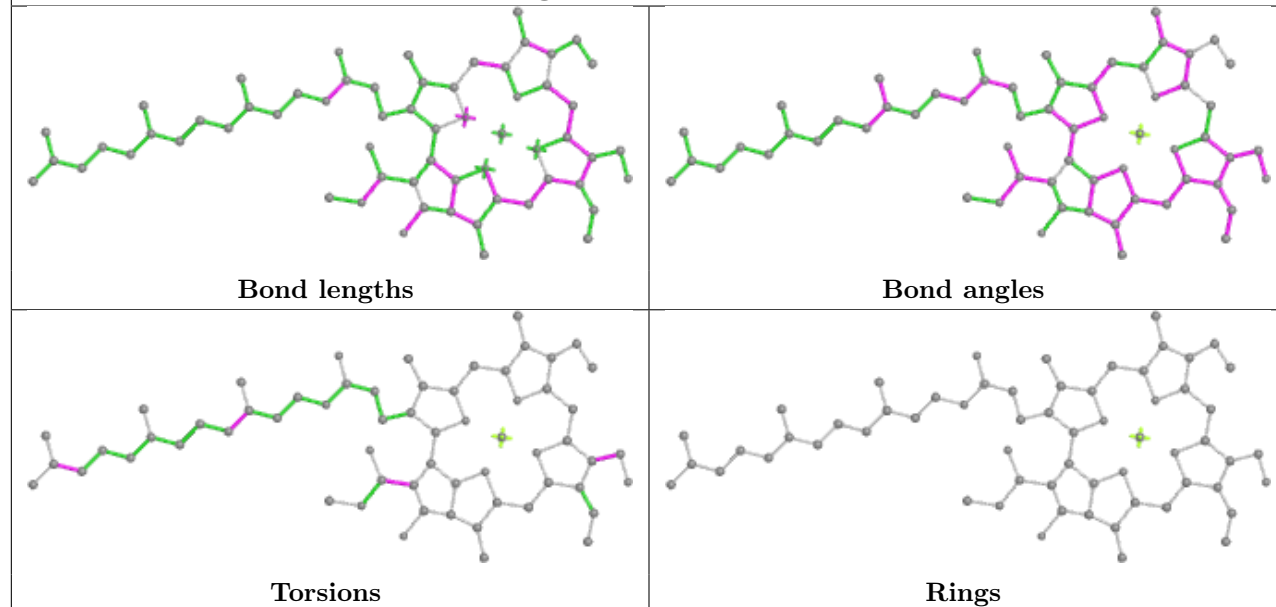
## Ligand CLA 9 609

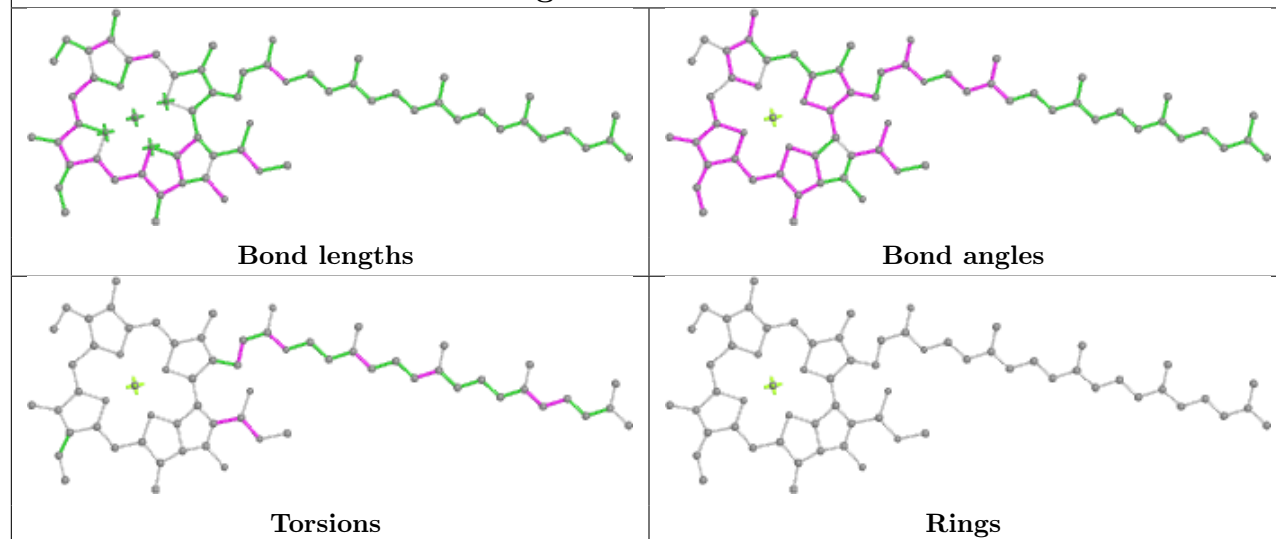
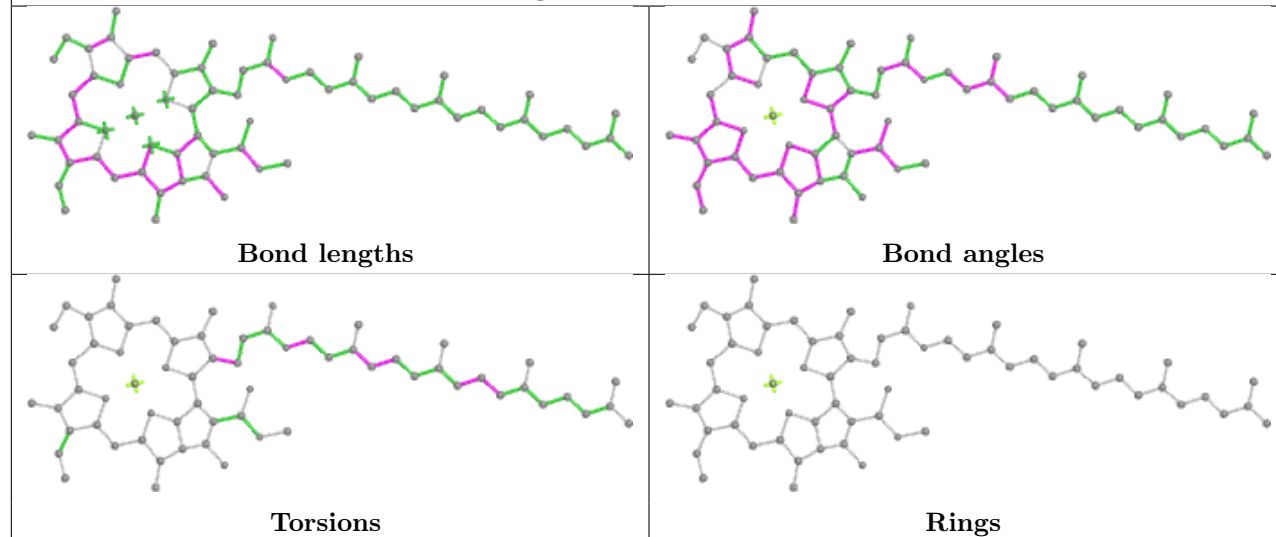


## Ligand CLA b 808

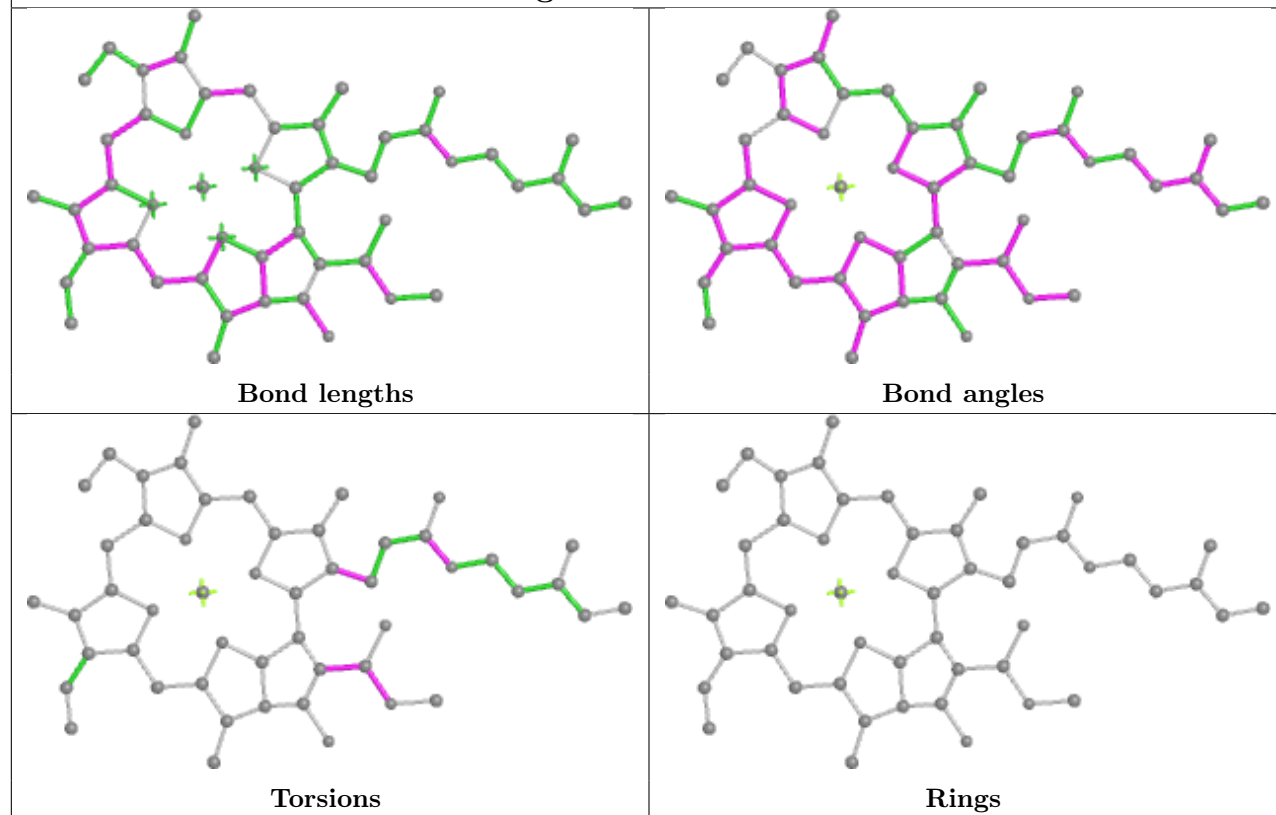


## Ligand CHL 1 302

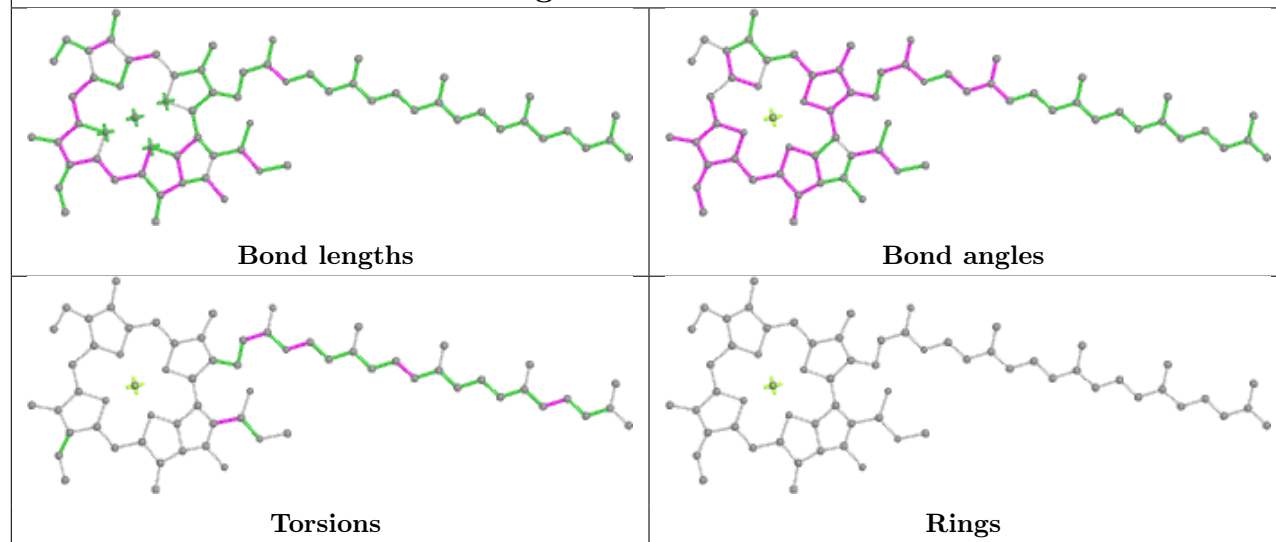


**Ligand CLA 2 602****Ligand CLA A 833**

## Ligand CLA a 824

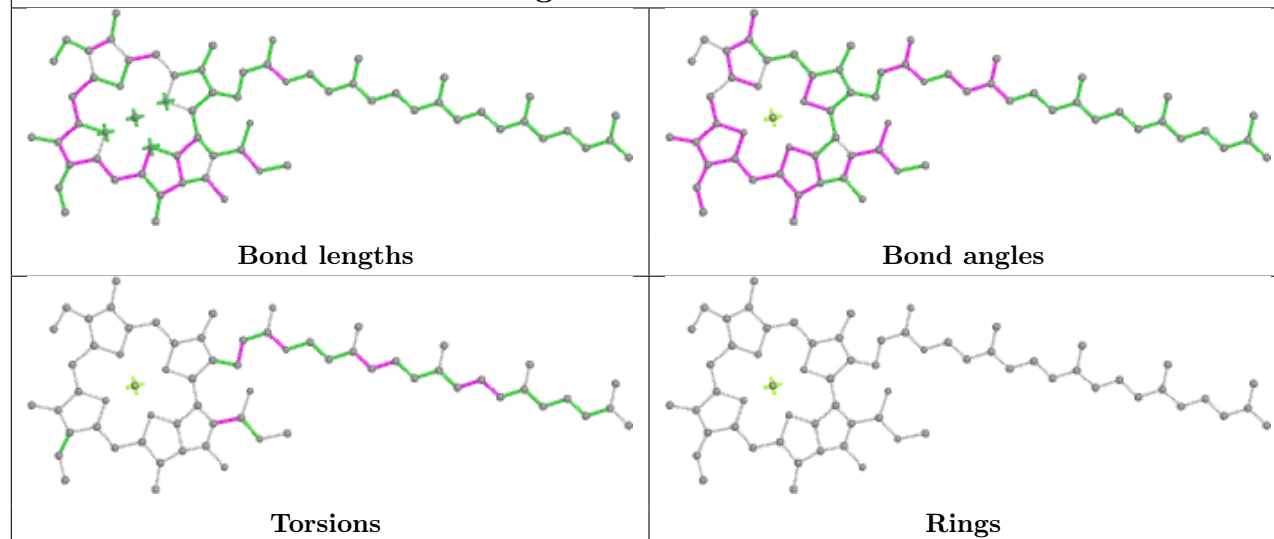


## Ligand CLA b 802

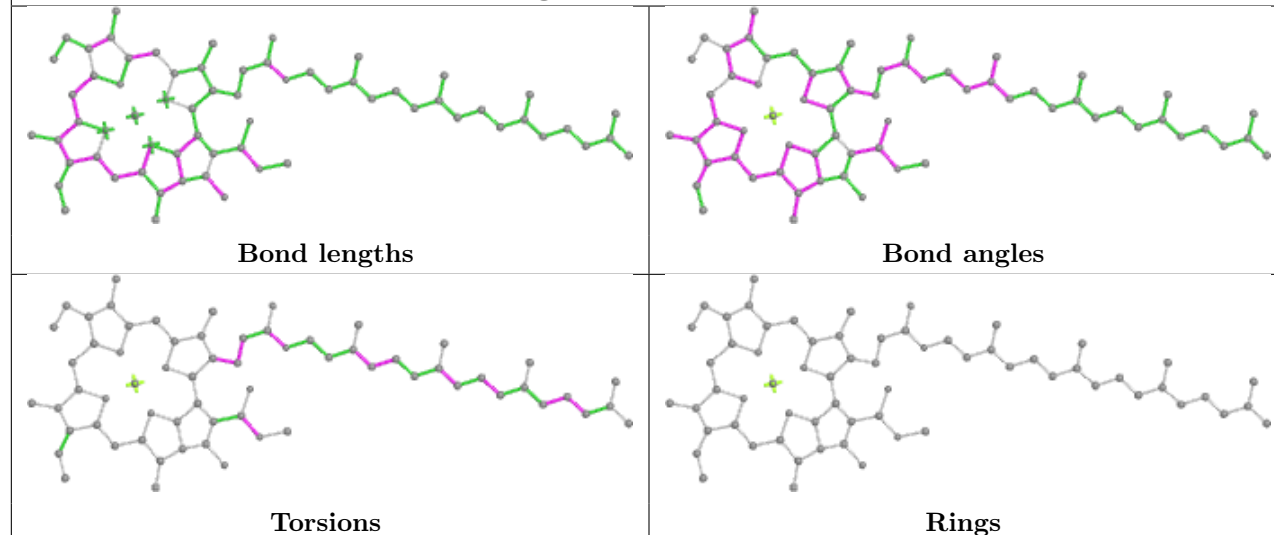




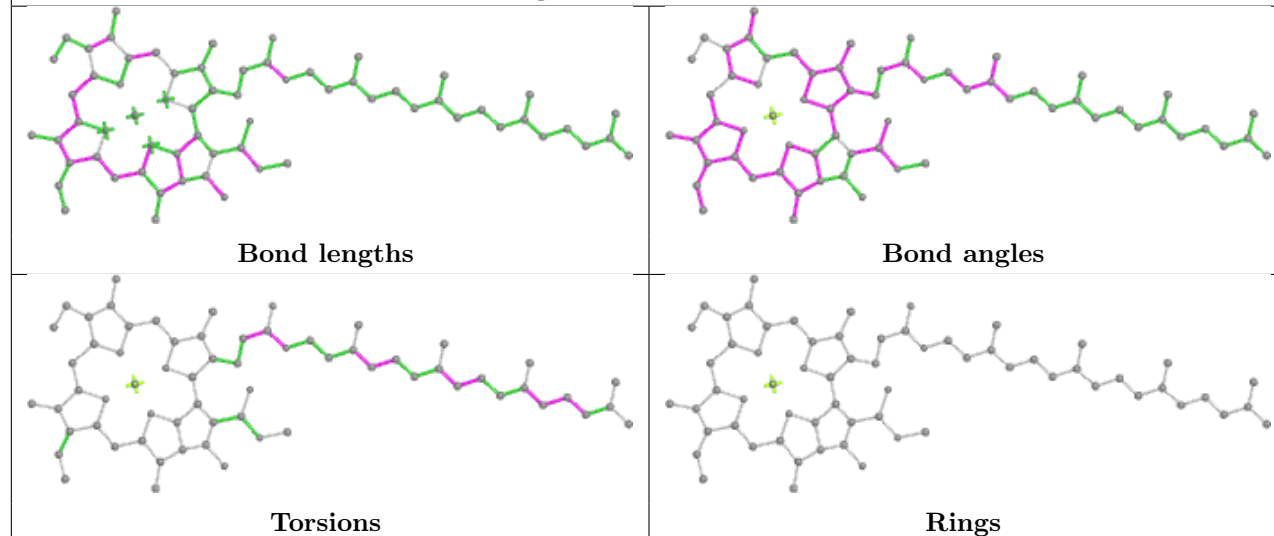
## Ligand CLA b 824

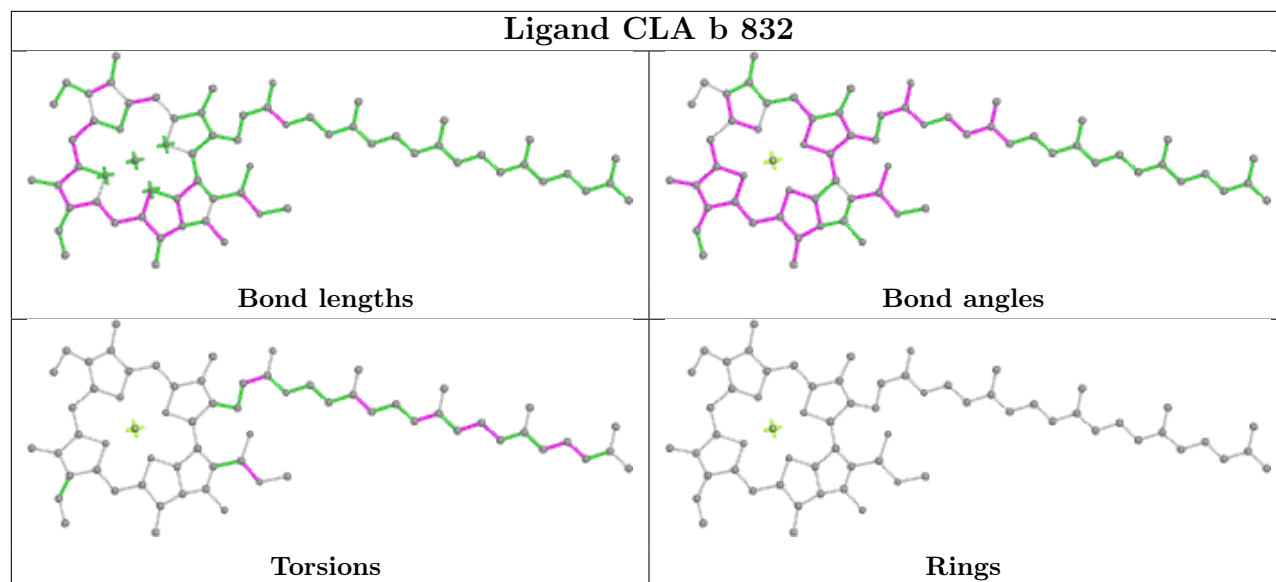
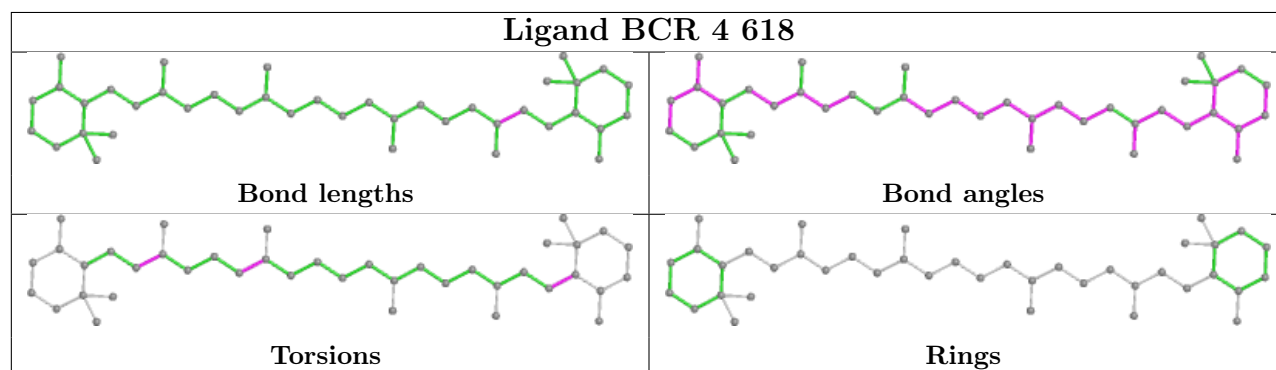


## Ligand CLA b 827

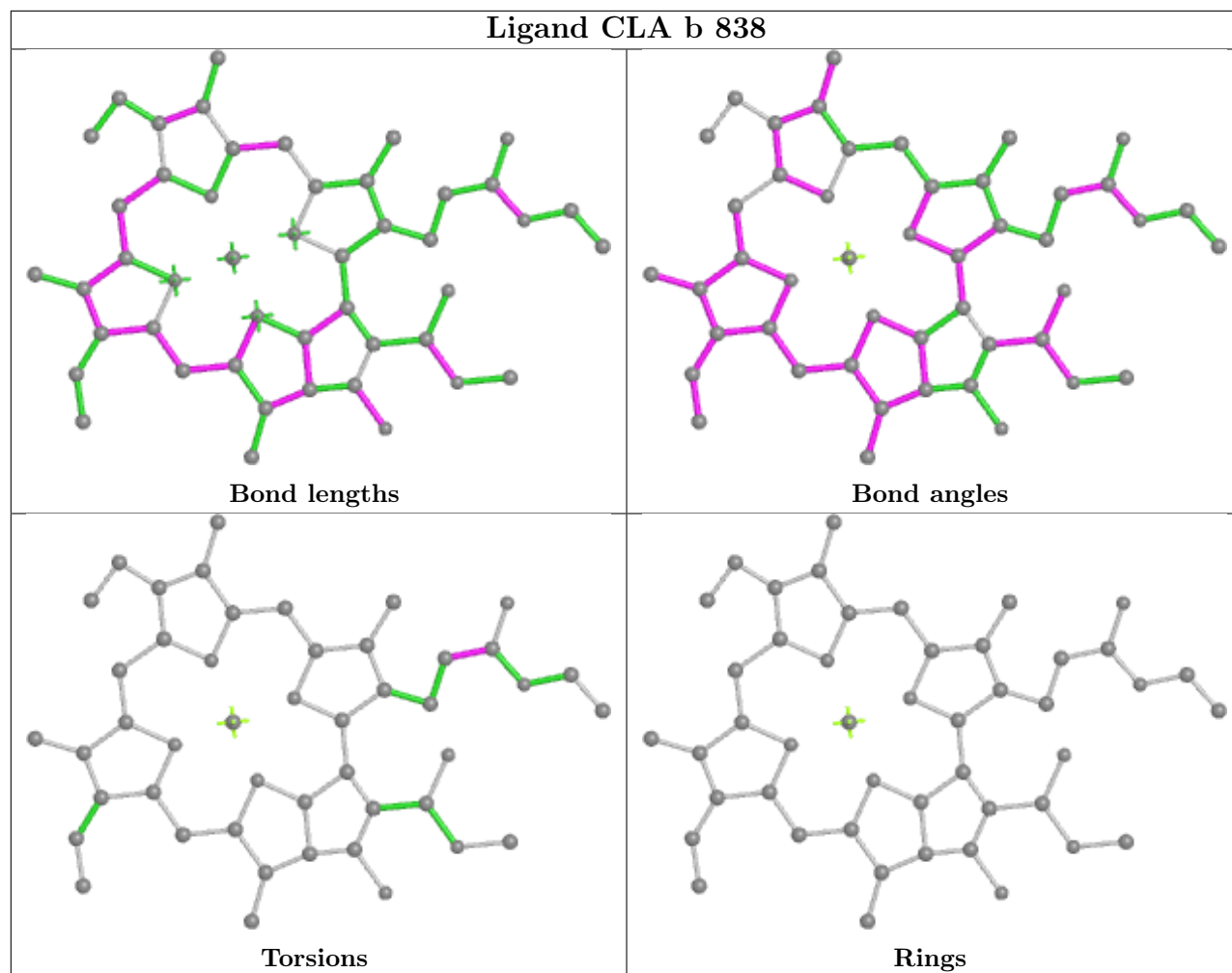


## Ligand CLA B 814

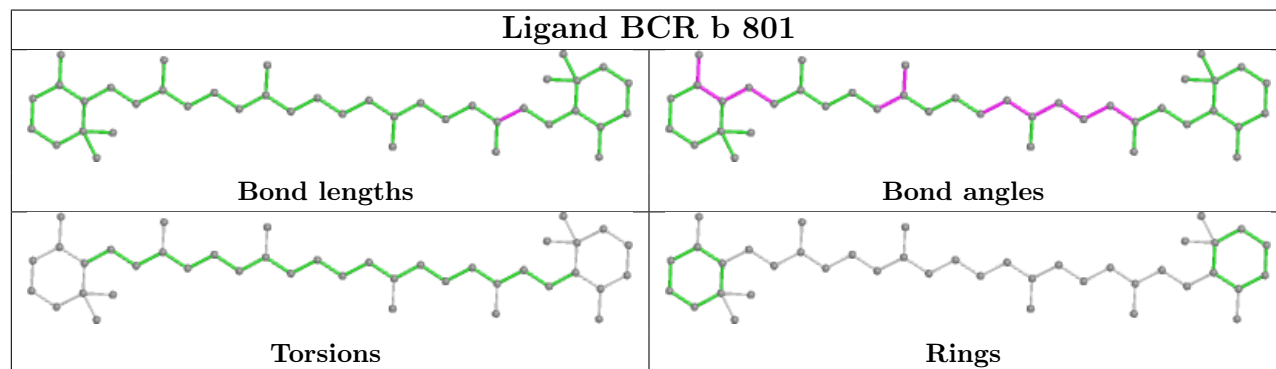


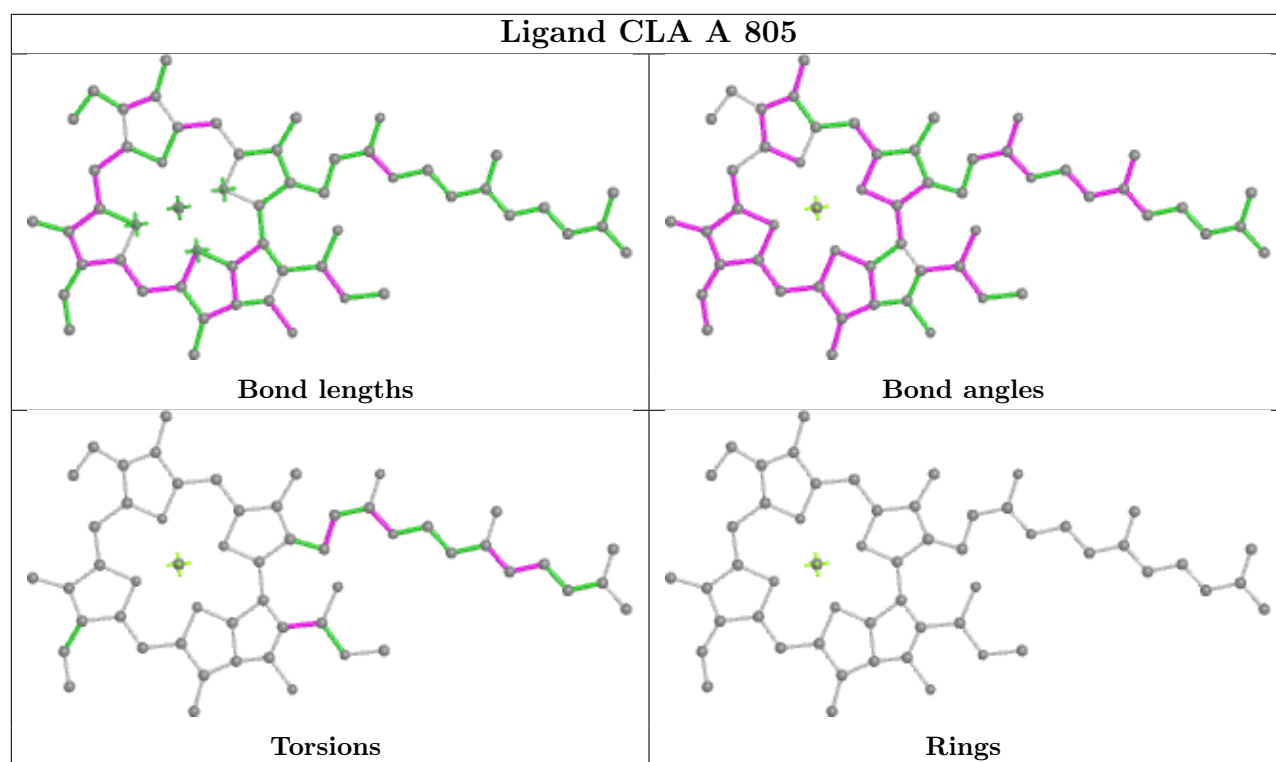
**Ligand CLA b 832****Ligand BCR 4 618**

## Ligand CLA b 838

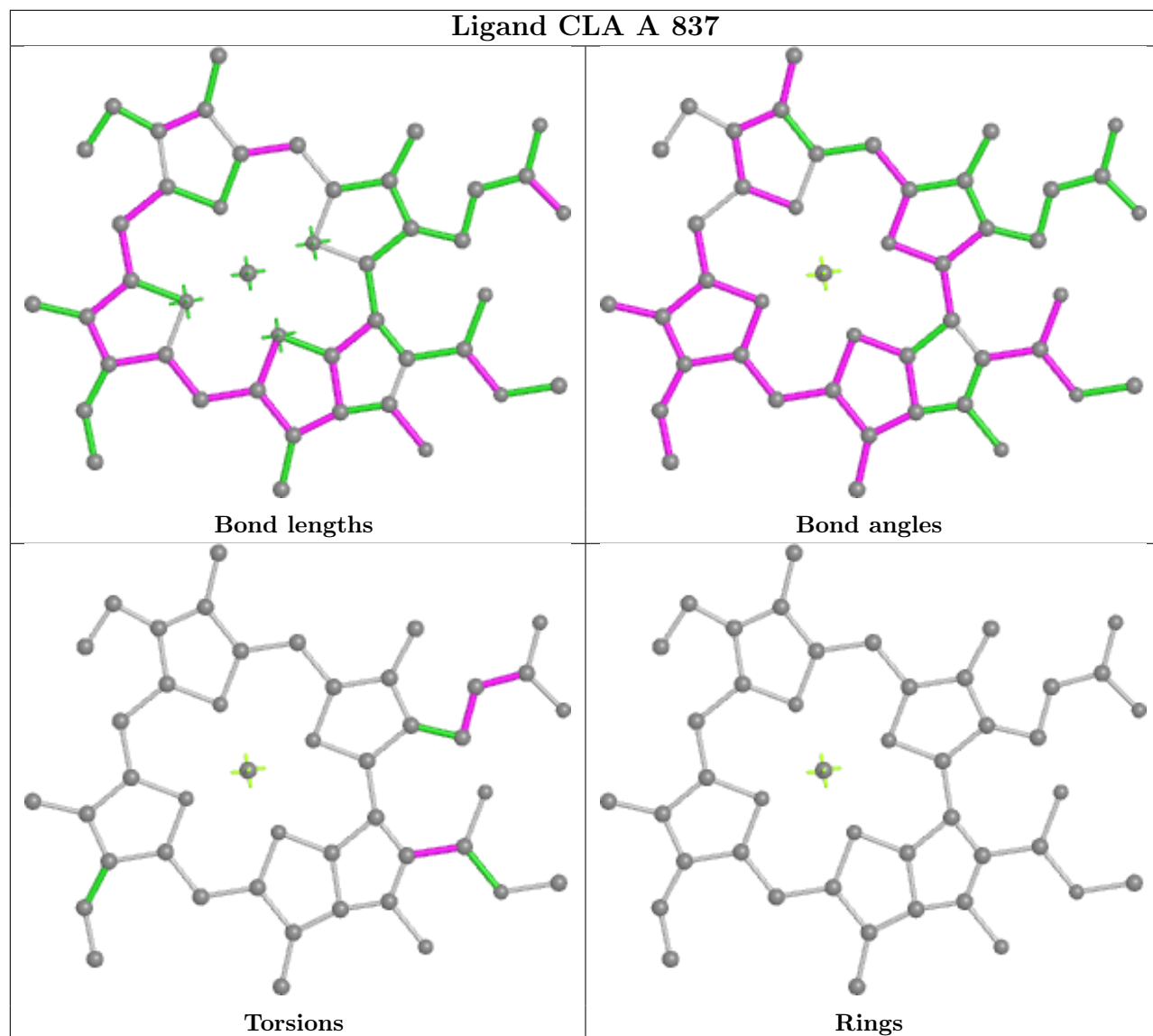


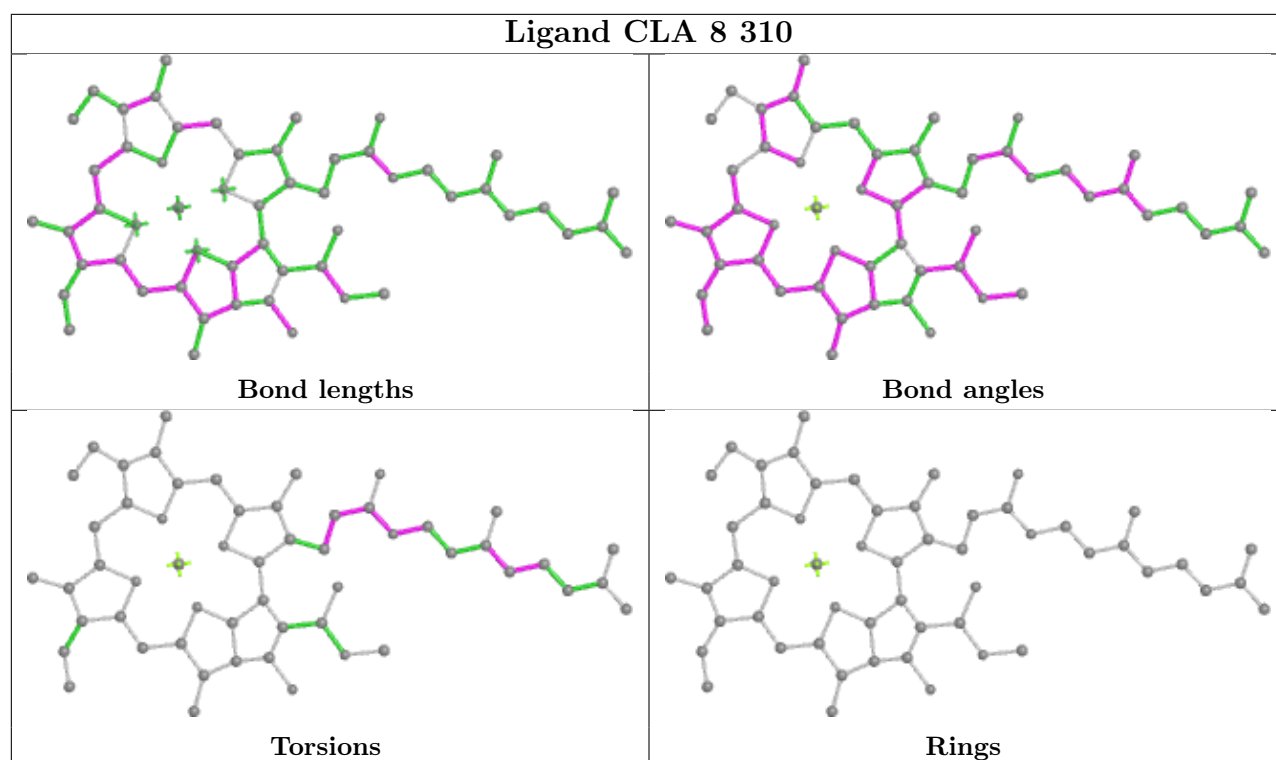
## Ligand BCR b 801



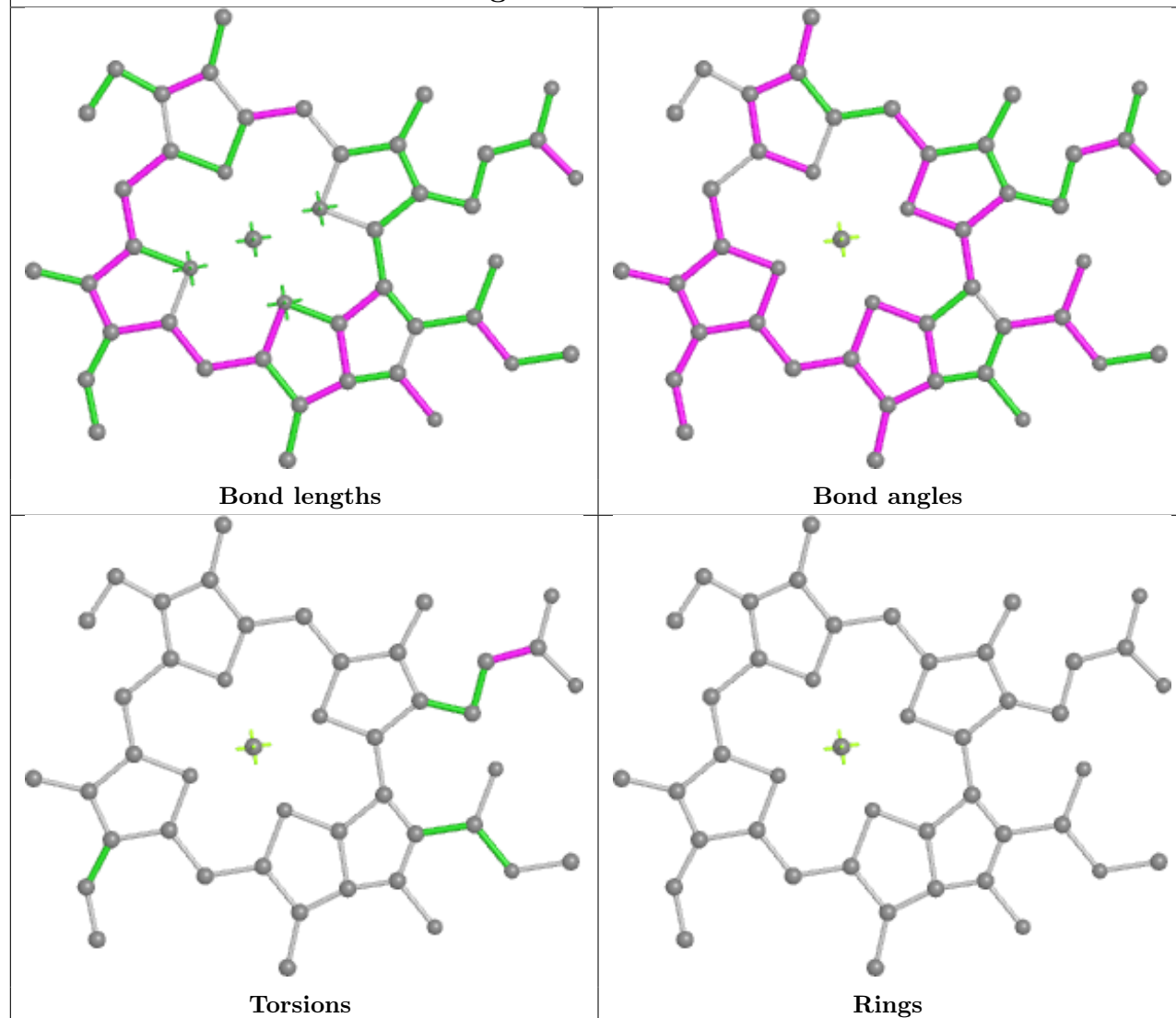


## Ligand CLA A 837

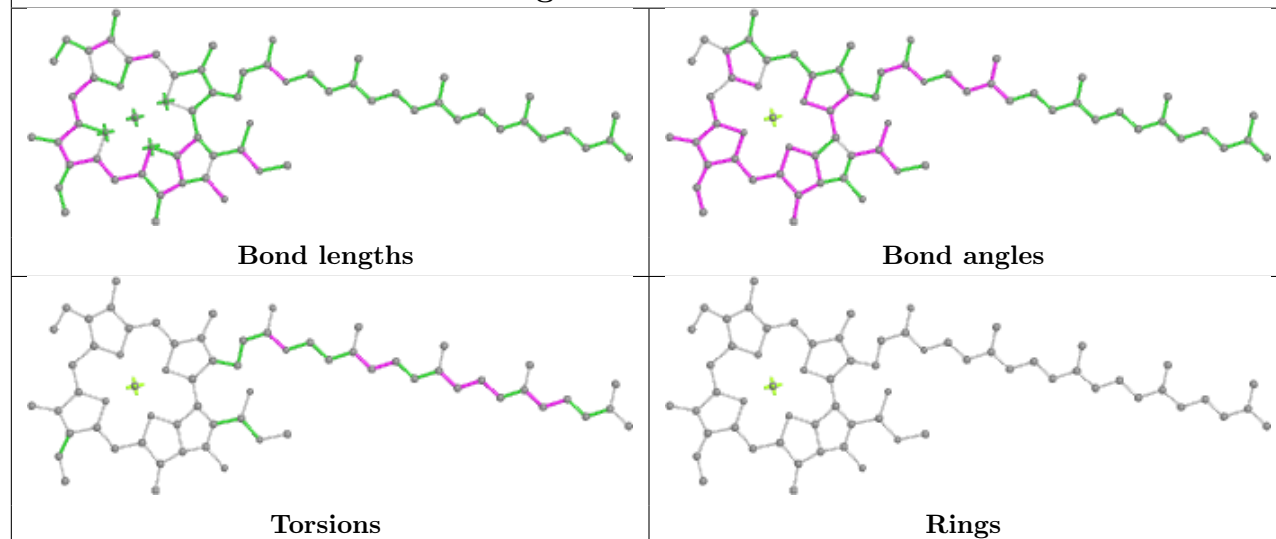


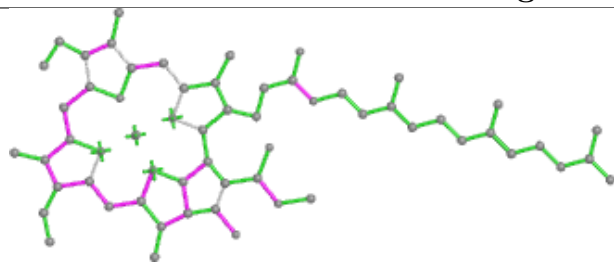


## Ligand CLA A 821

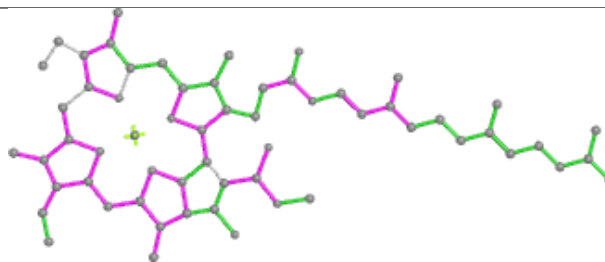


## Ligand CLA a 839

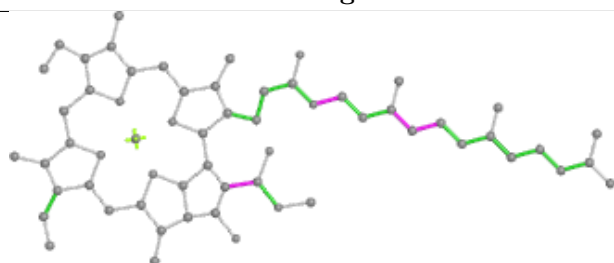


**Ligand CLA b 836**

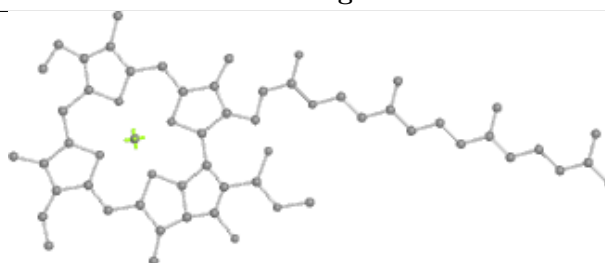
Bond lengths



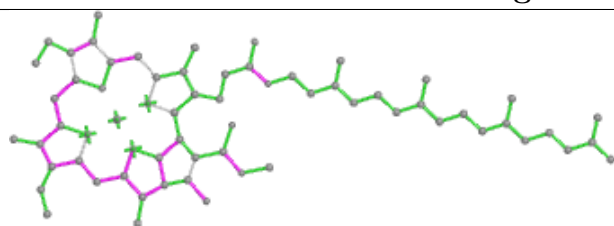
Bond angles



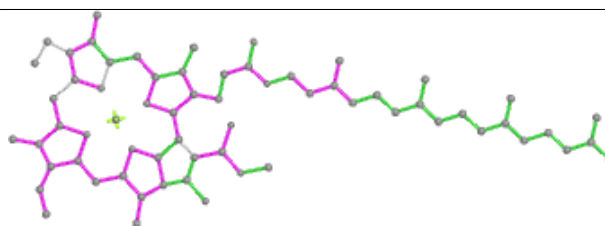
Torsions



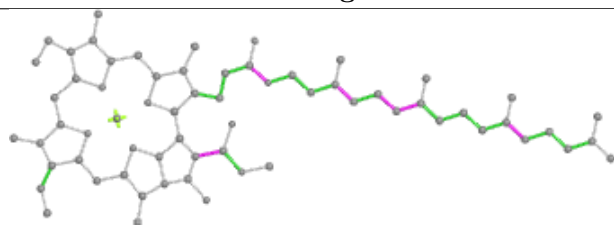
Rings

**Ligand CLA A 835**

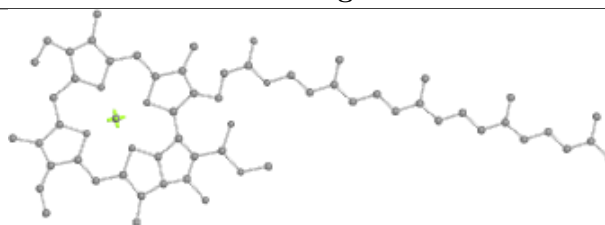
Bond lengths



Bond angles

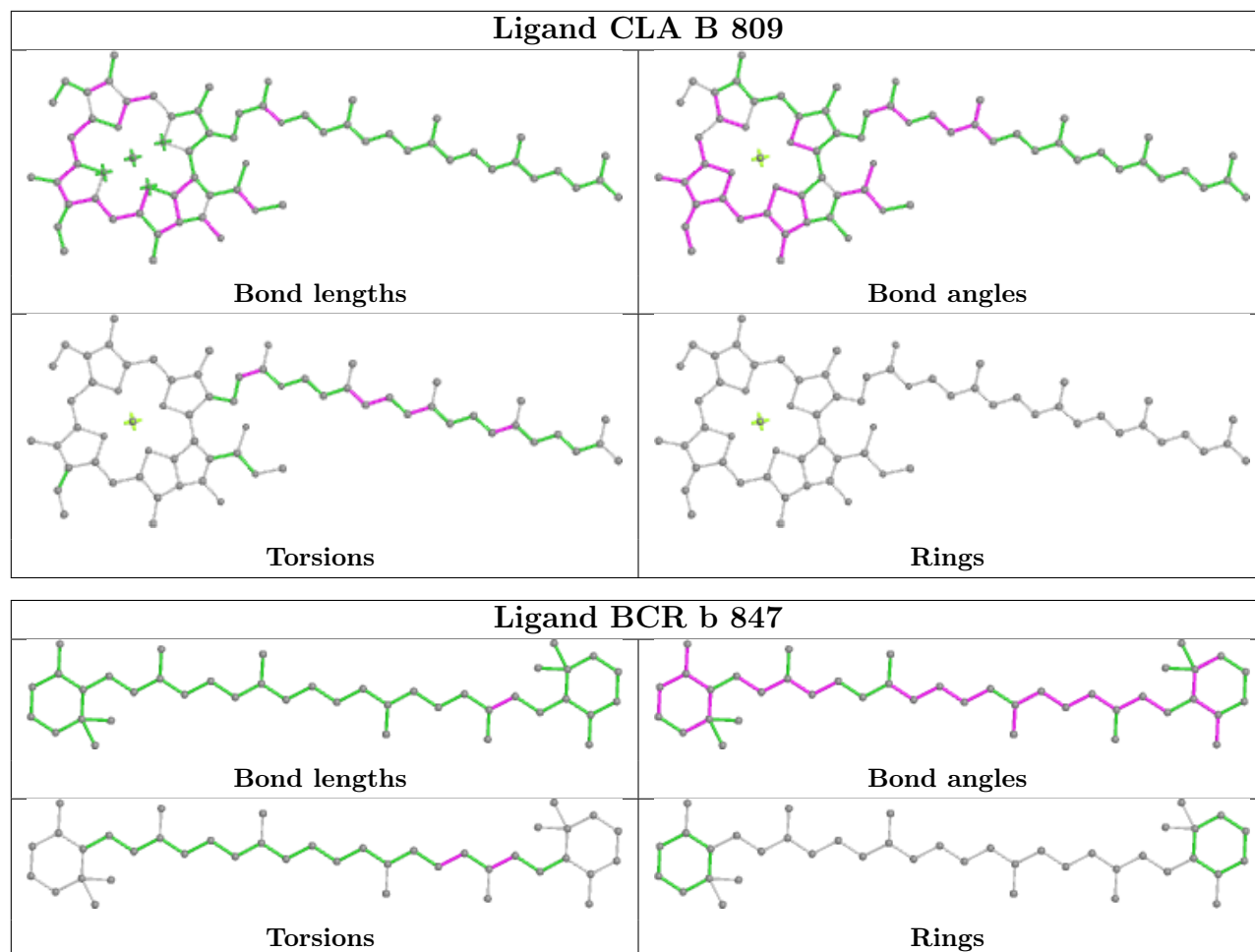


Torsions

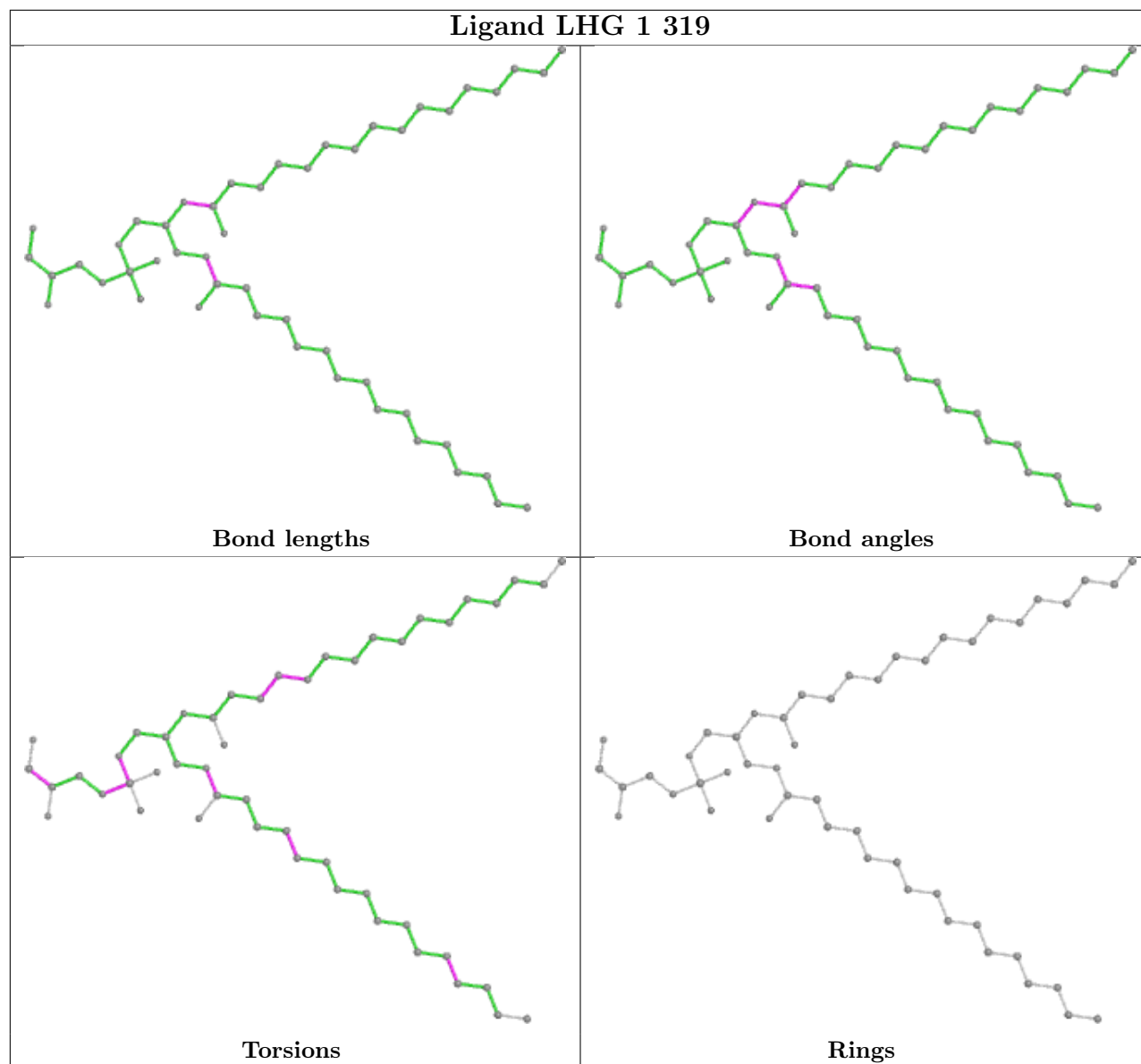


Rings

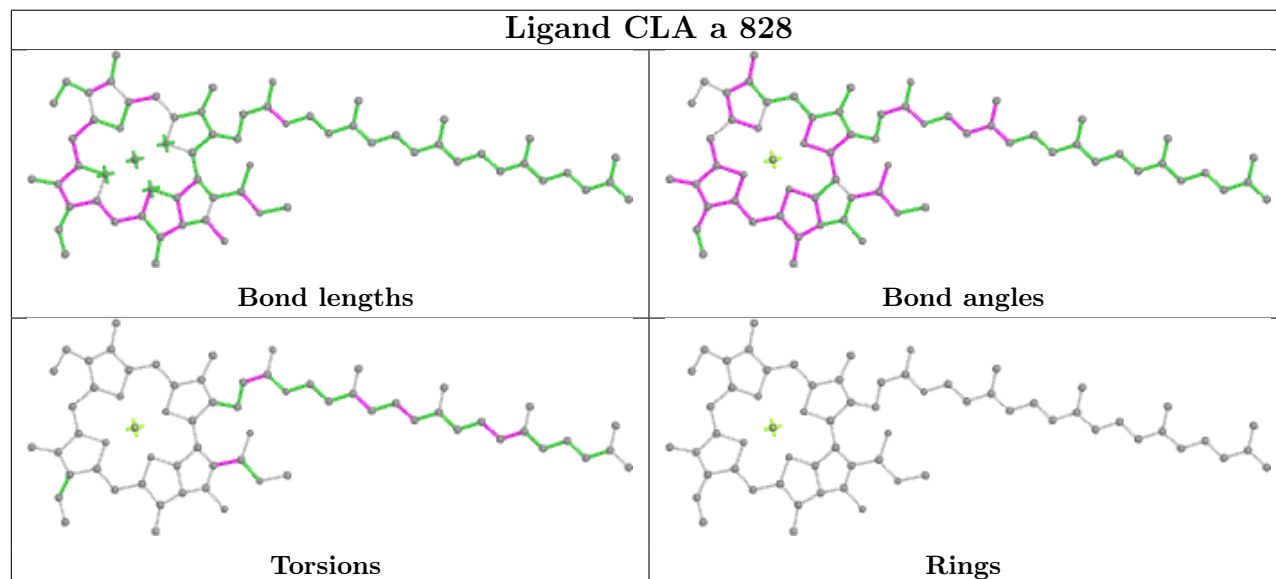




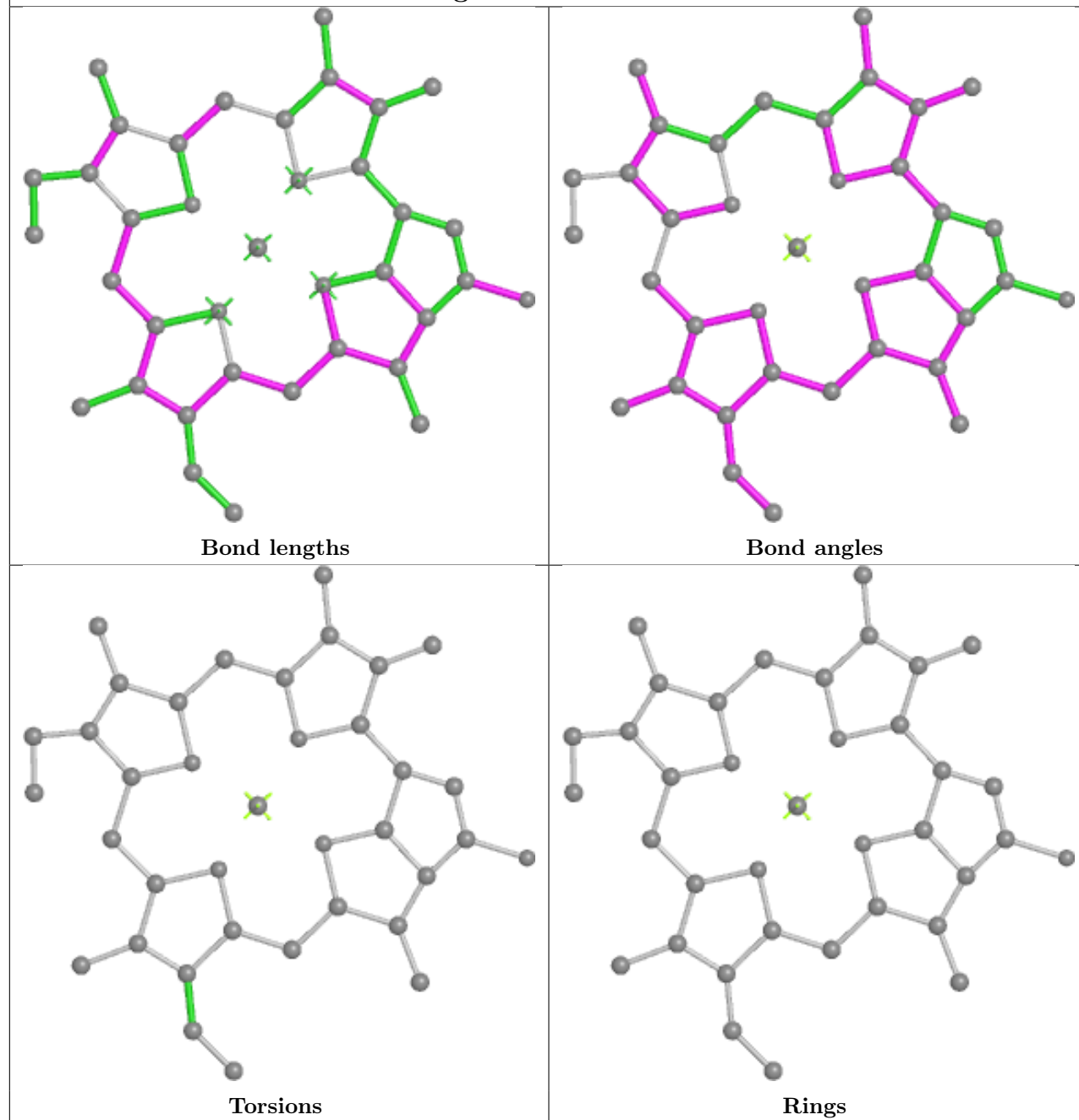
## Ligand LHG 1 319



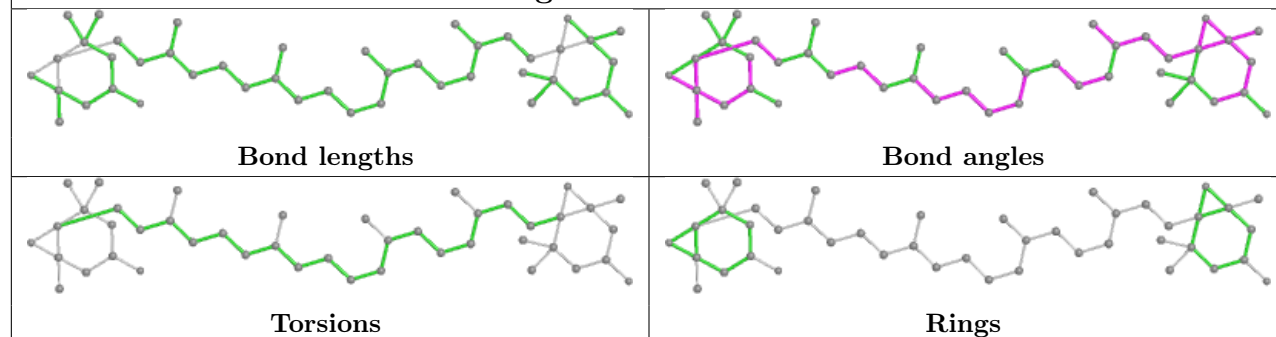
## Ligand CLA a 828



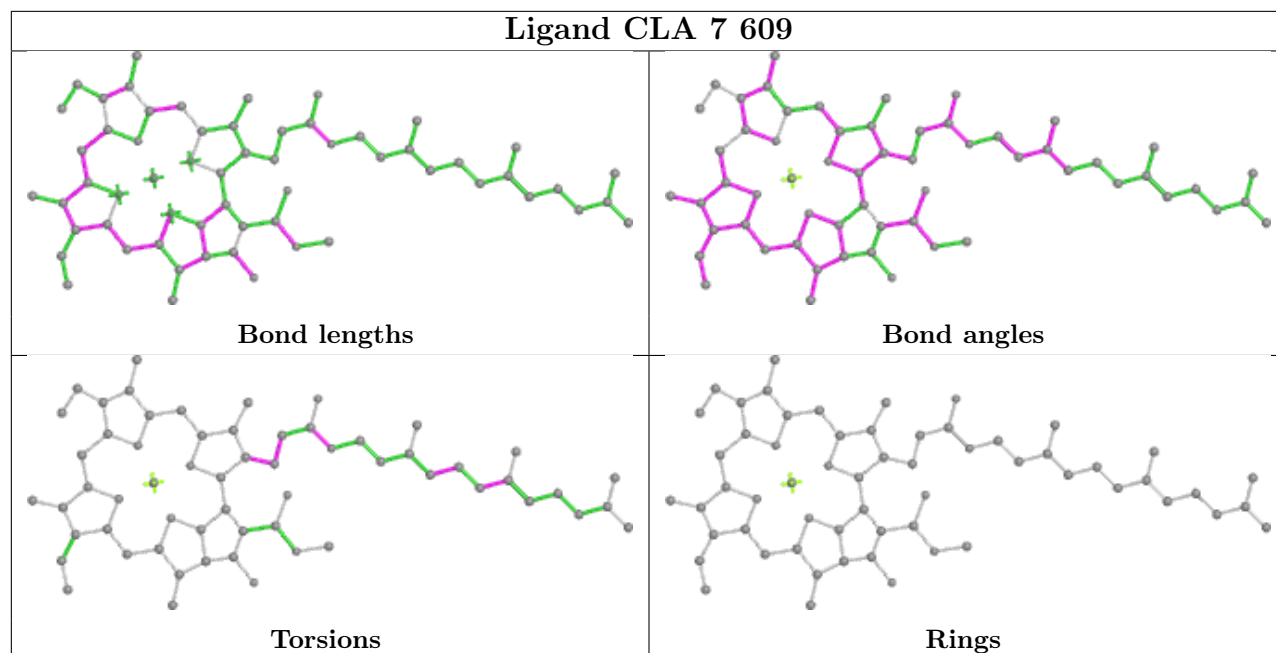
## Ligand CLA 3 310



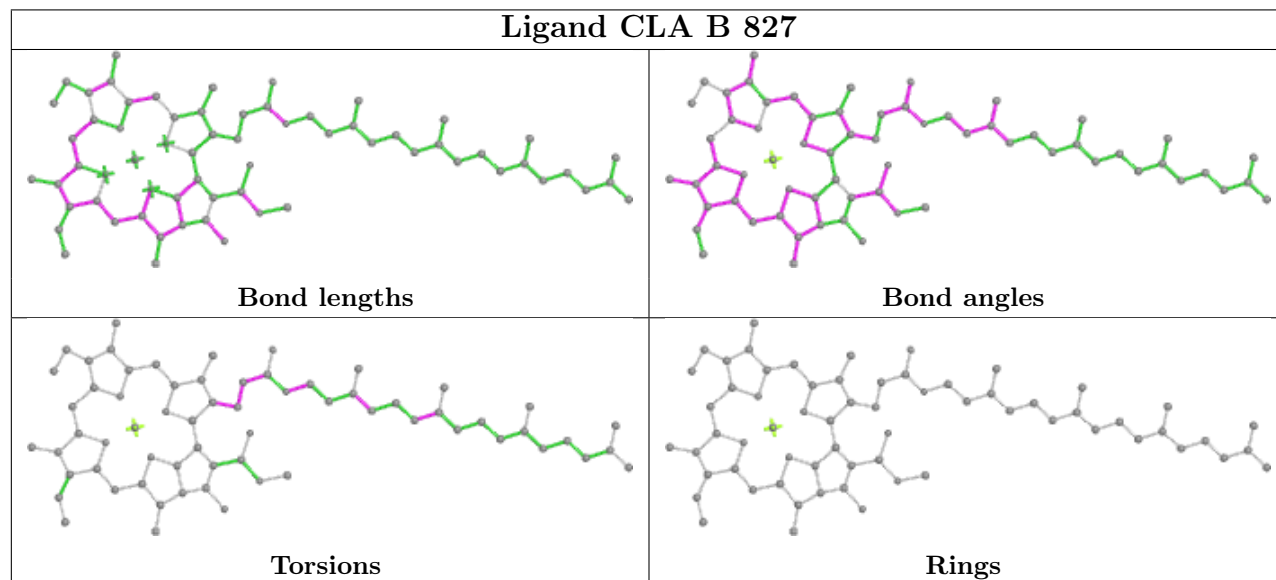
## Ligand XAT 2 616



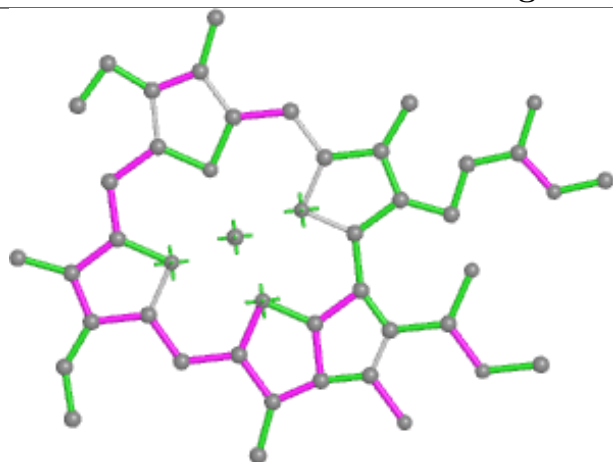
## Ligand CLA 7 609



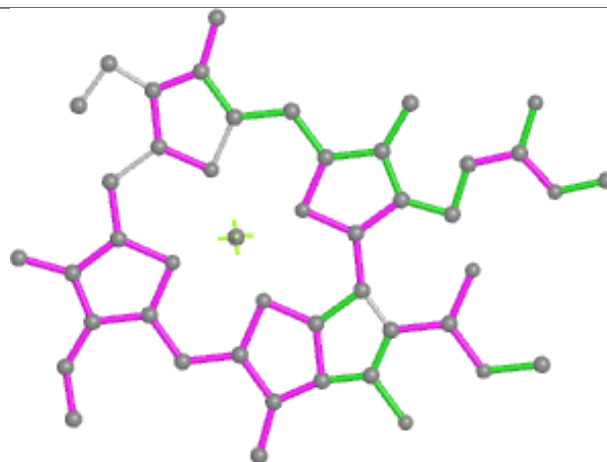
## Ligand CLA B 827



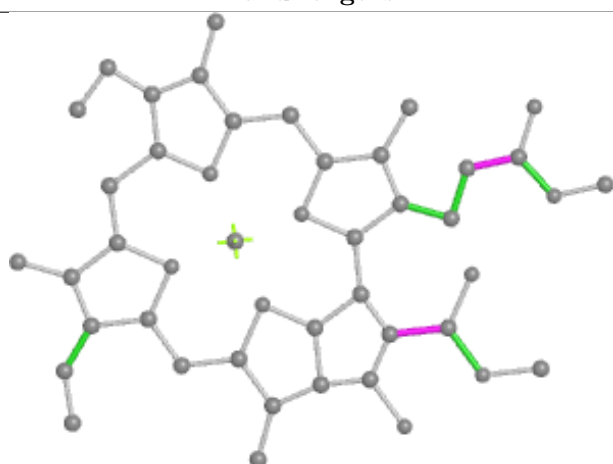
## Ligand CLA 9 603



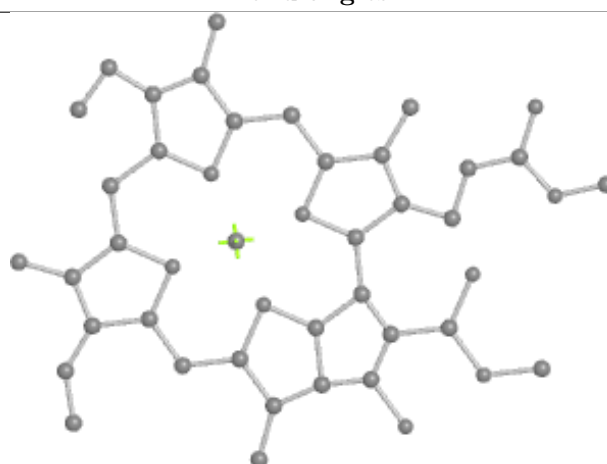
Bond lengths



Bond angles

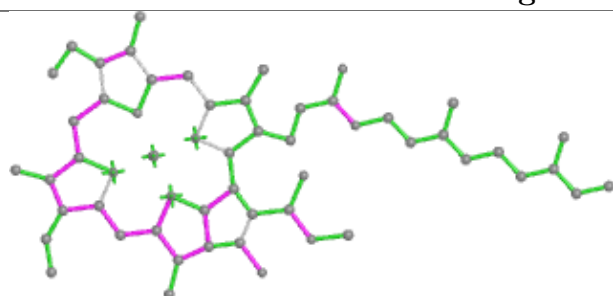


Torsions

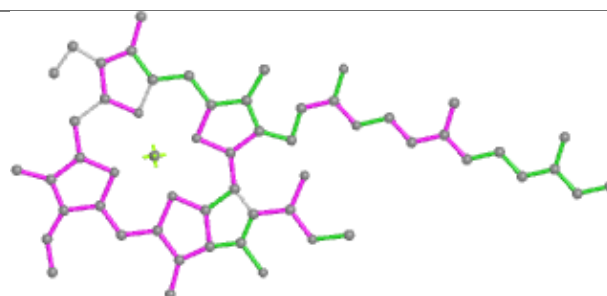


Rings

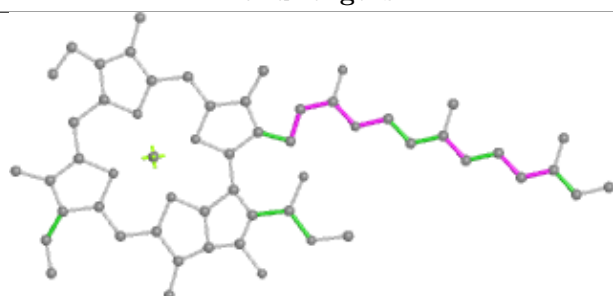
## Ligand CLA 9 612



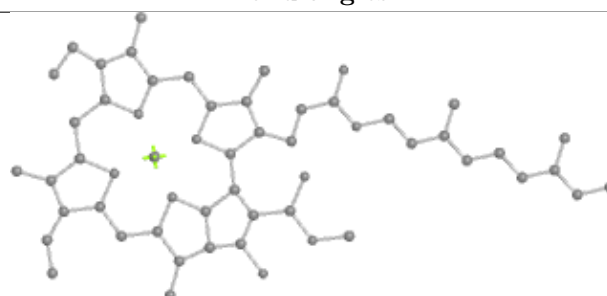
Bond lengths



Bond angles

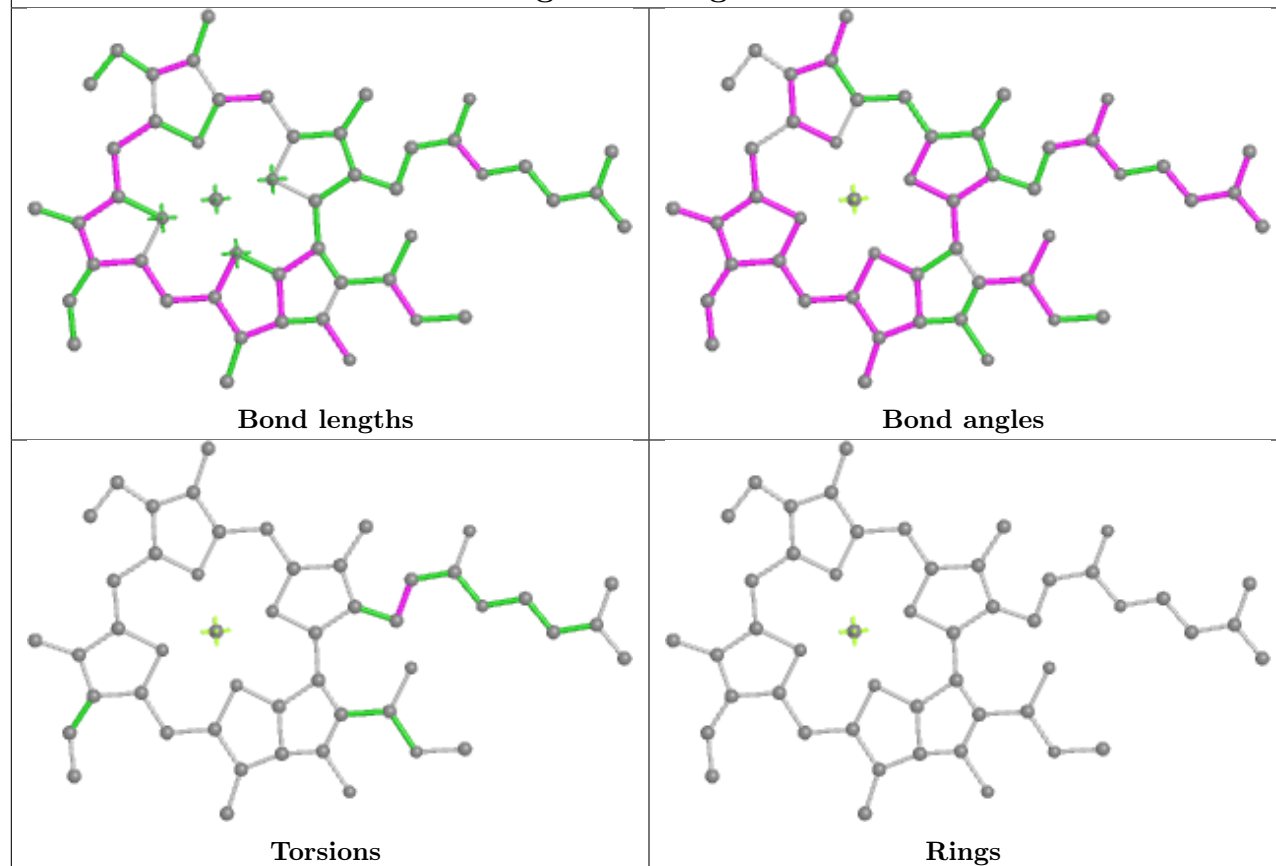


Torsions

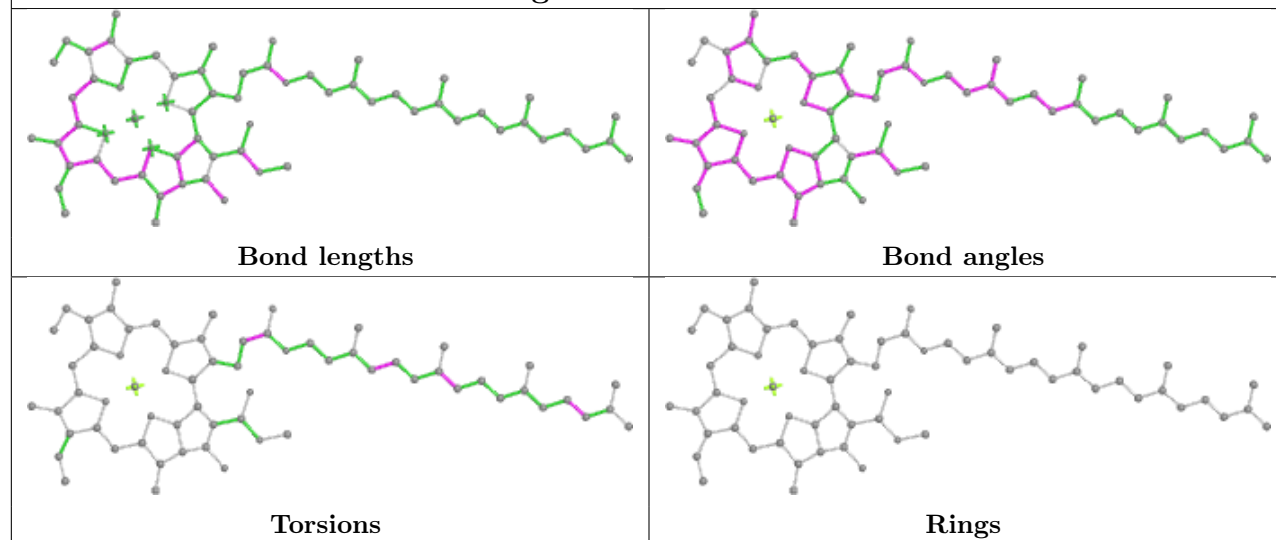


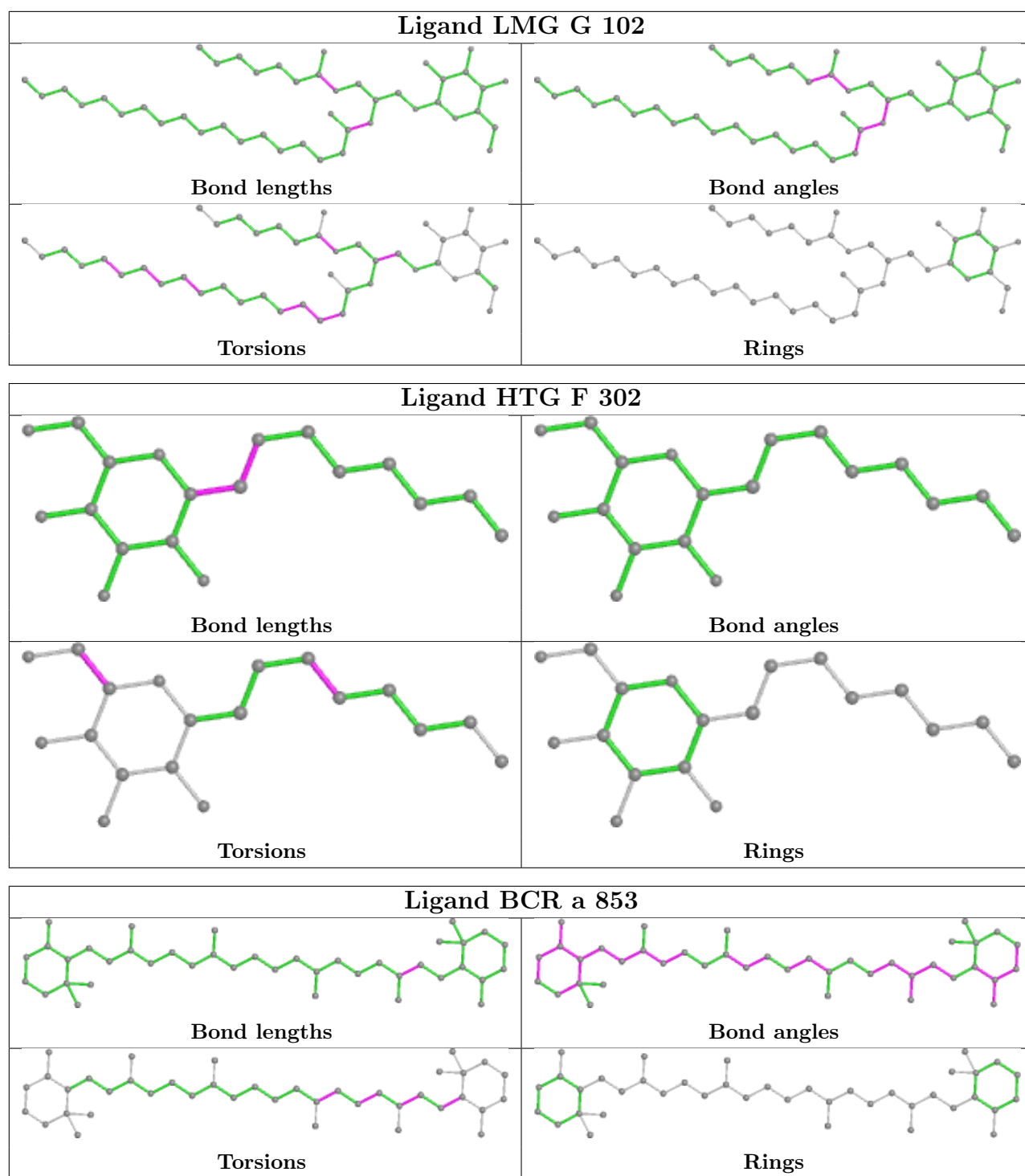
Rings

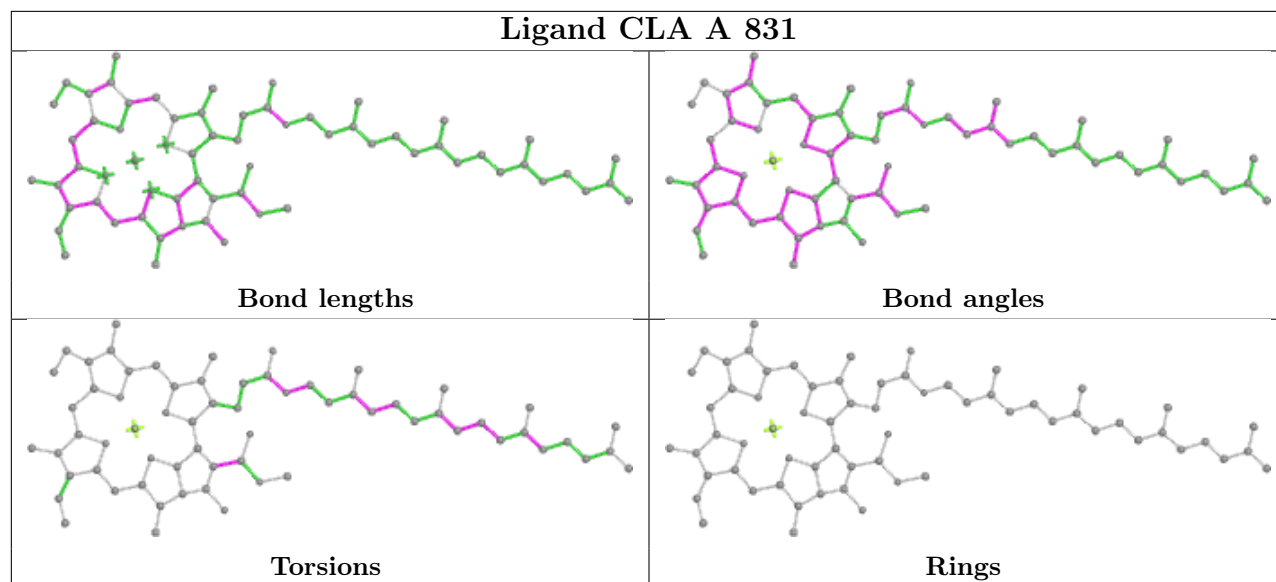
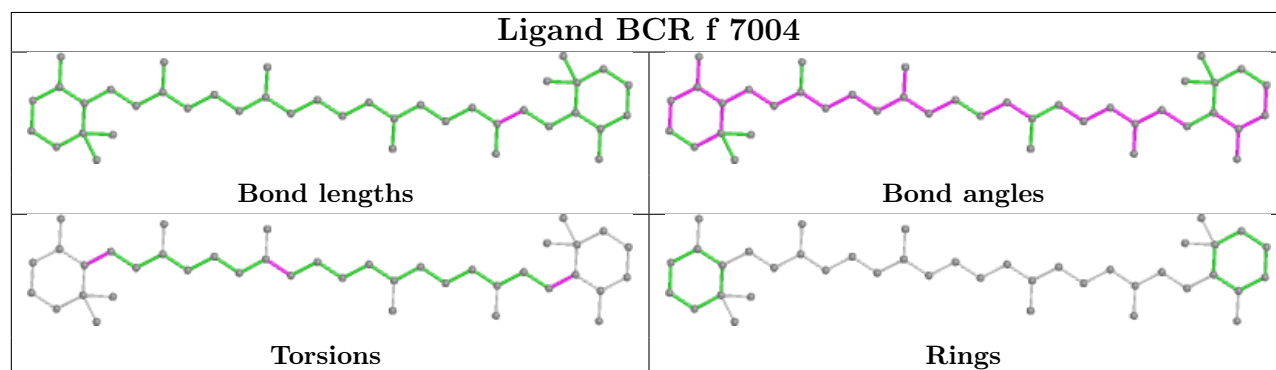
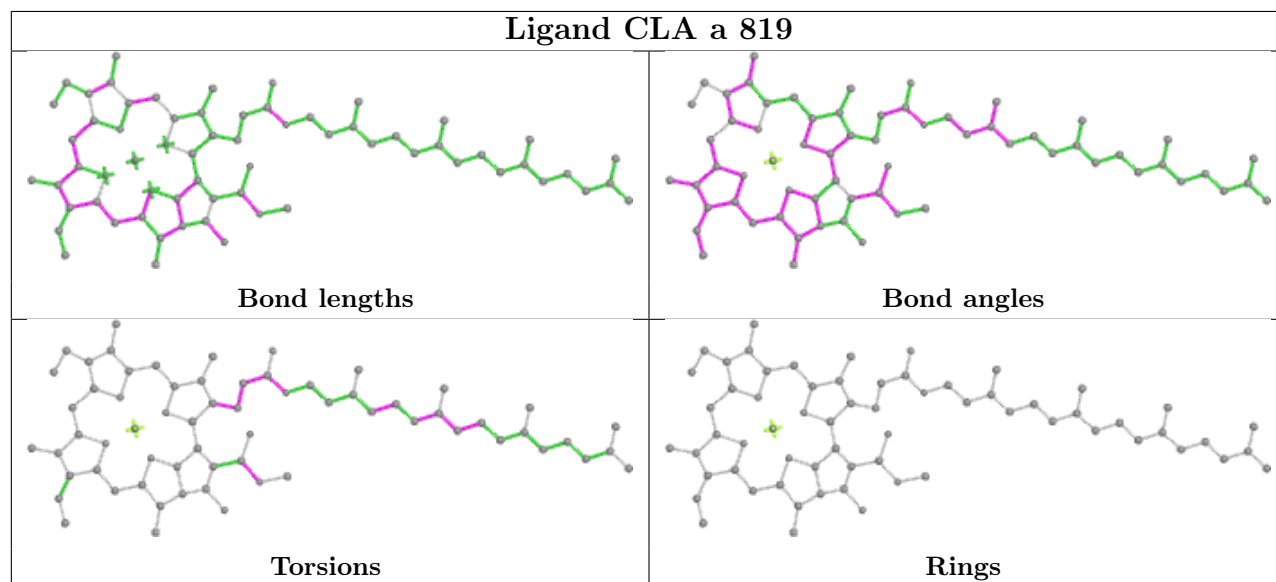
## Ligand CLA g 102



## Ligand CLA A 802

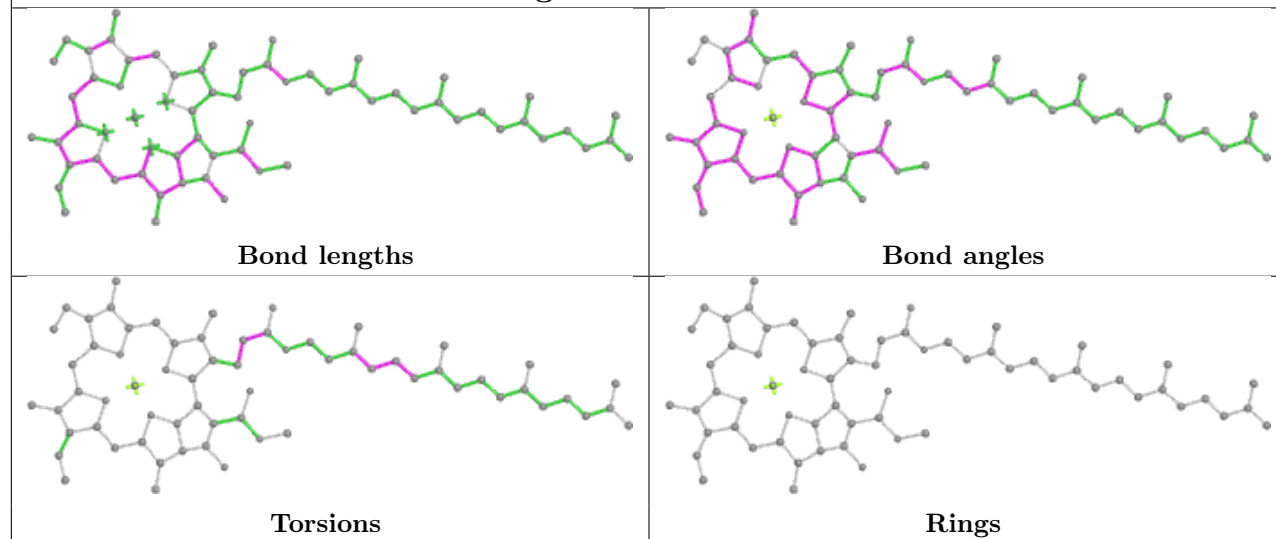




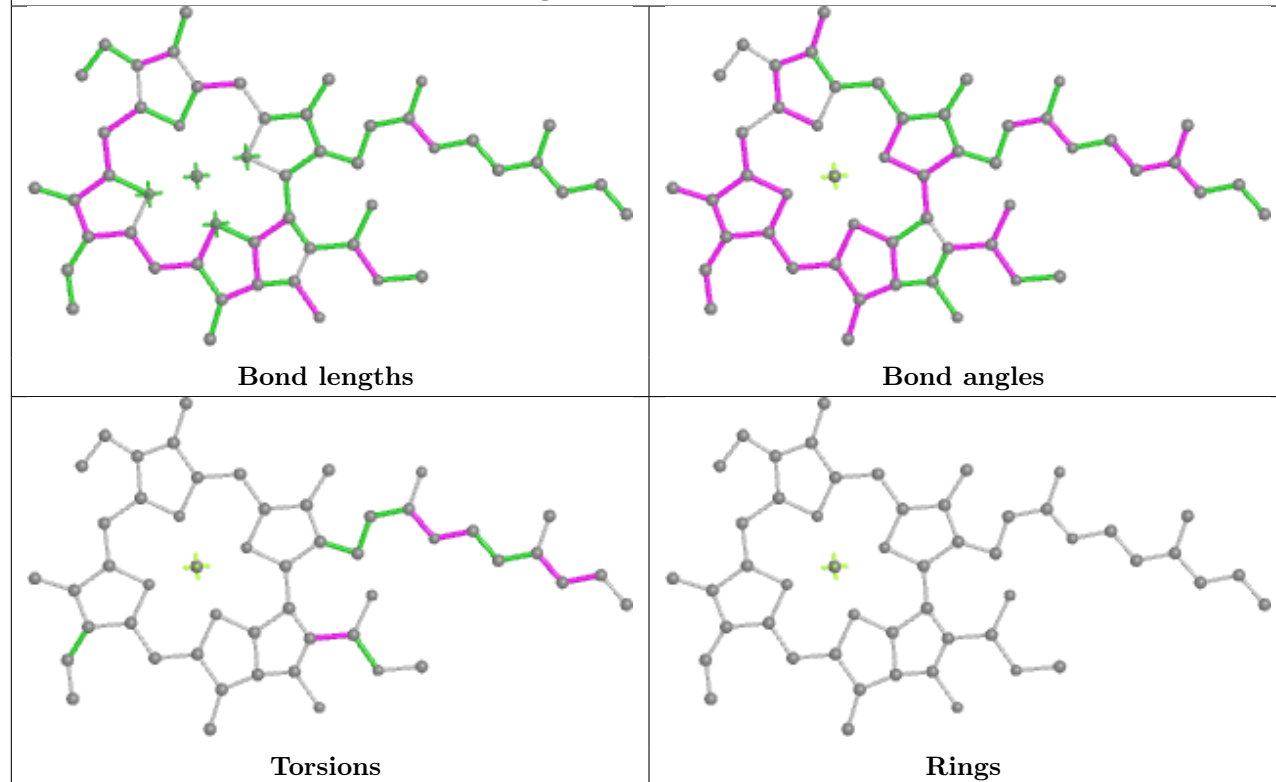
**Ligand CLA A 831****Ligand BCR f 7004****Ligand CLA a 819**



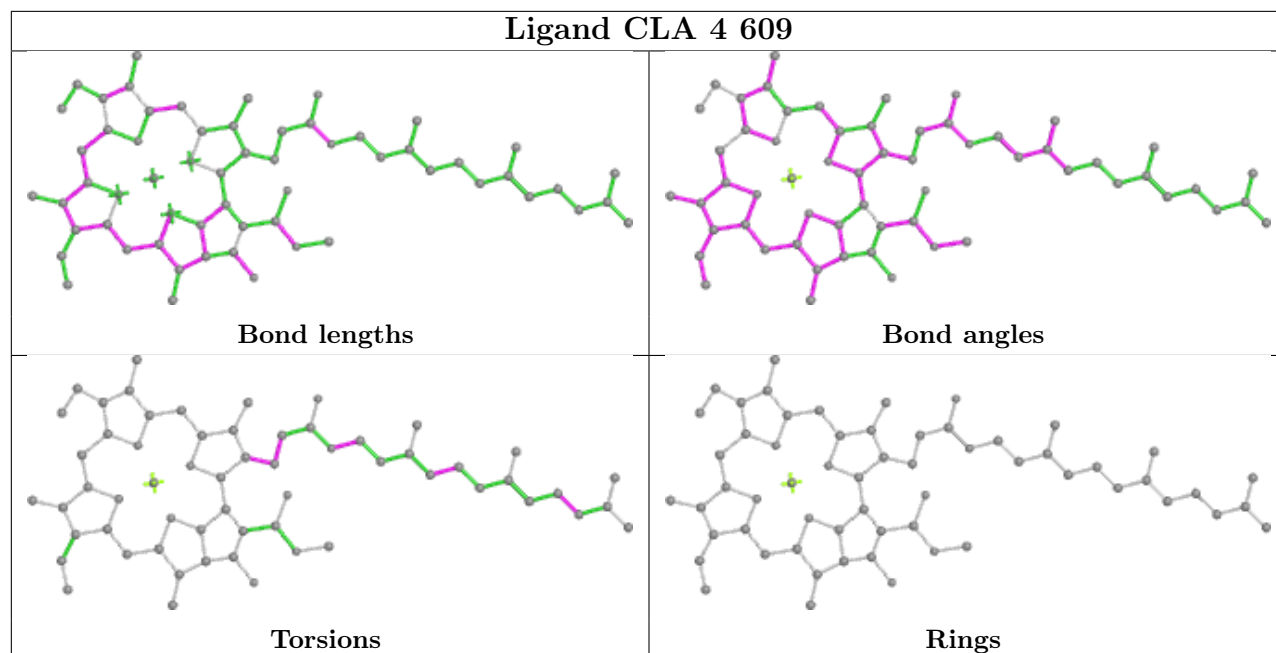
## Ligand CLA b 807



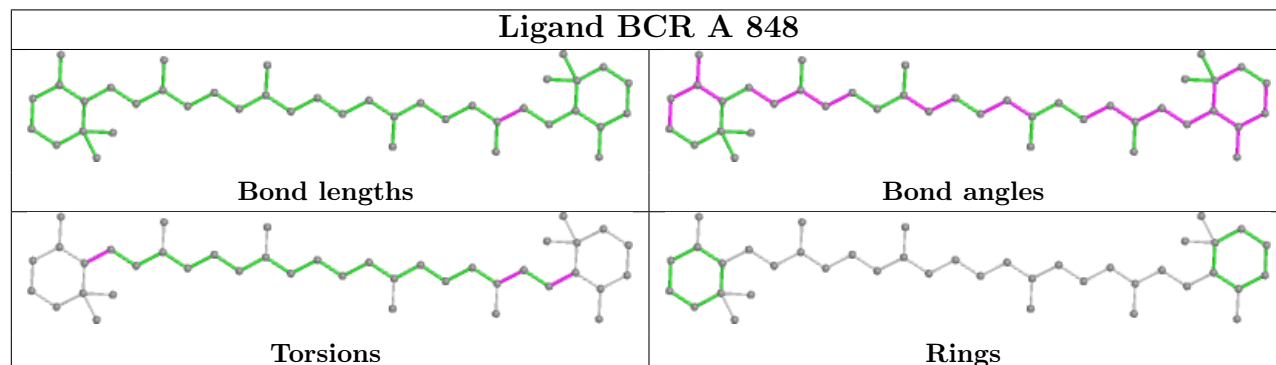
## Ligand CLA 4 611



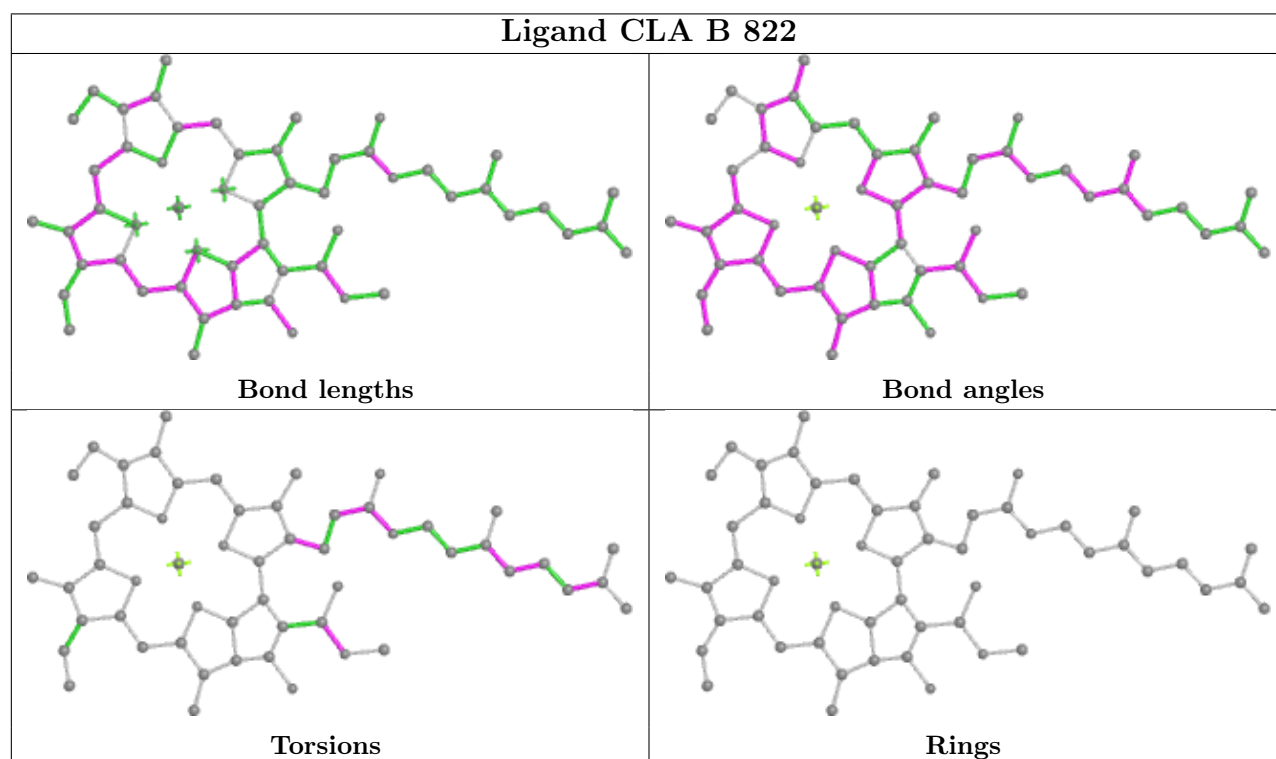
## Ligand CLA 4 609



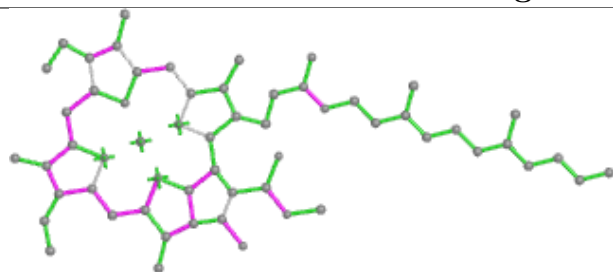
## Ligand BCR A 848



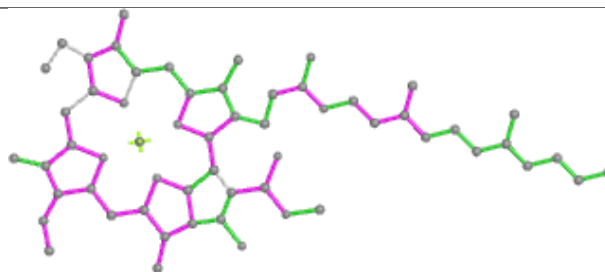
## Ligand CLA B 822



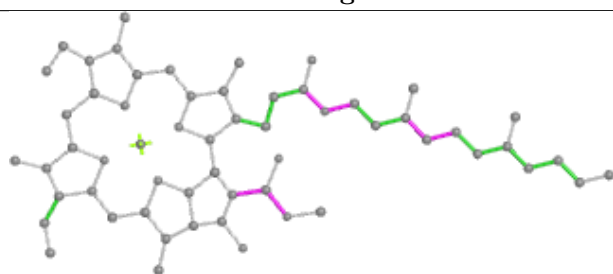
## Ligand CLA B 833



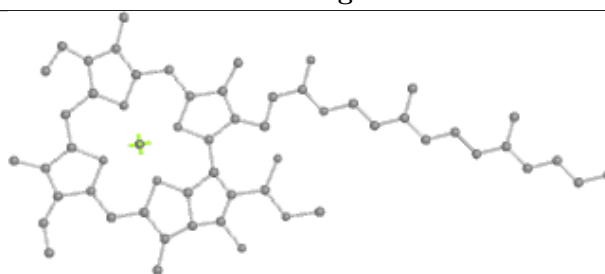
Bond lengths



Bond angles

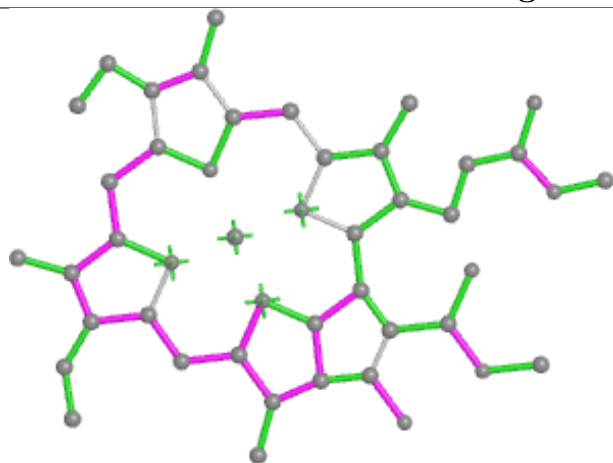


Torsions

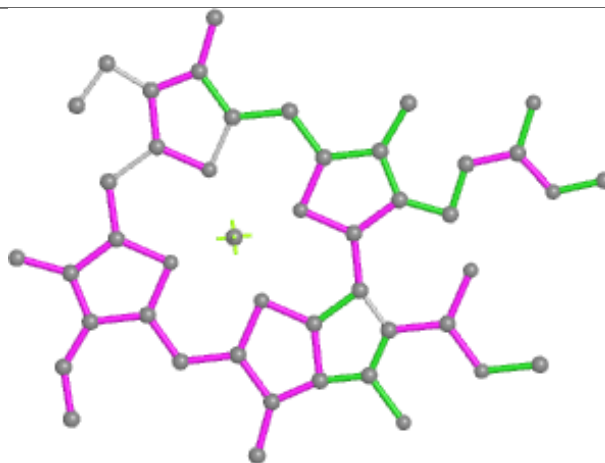


Rings

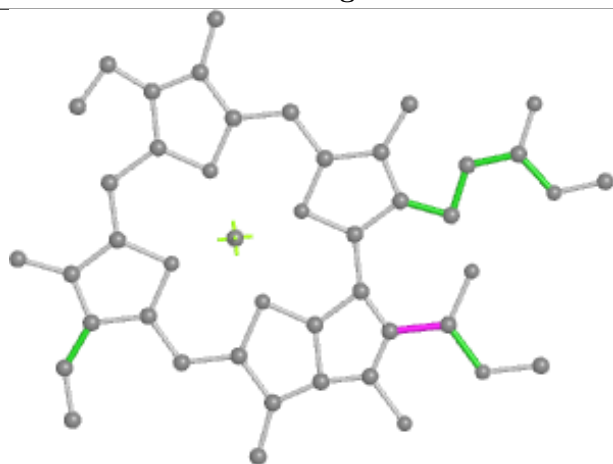
## Ligand CLA 3 301



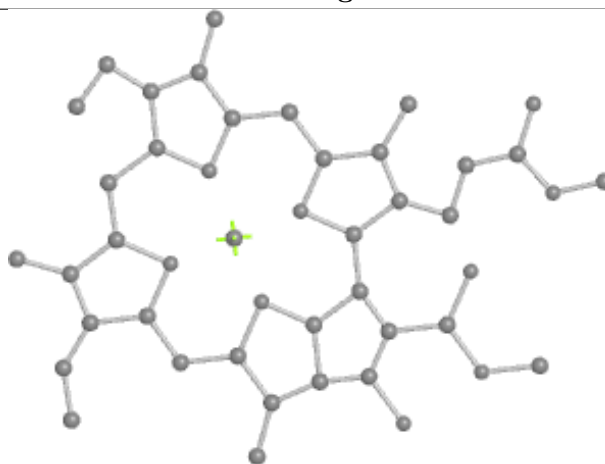
Bond lengths



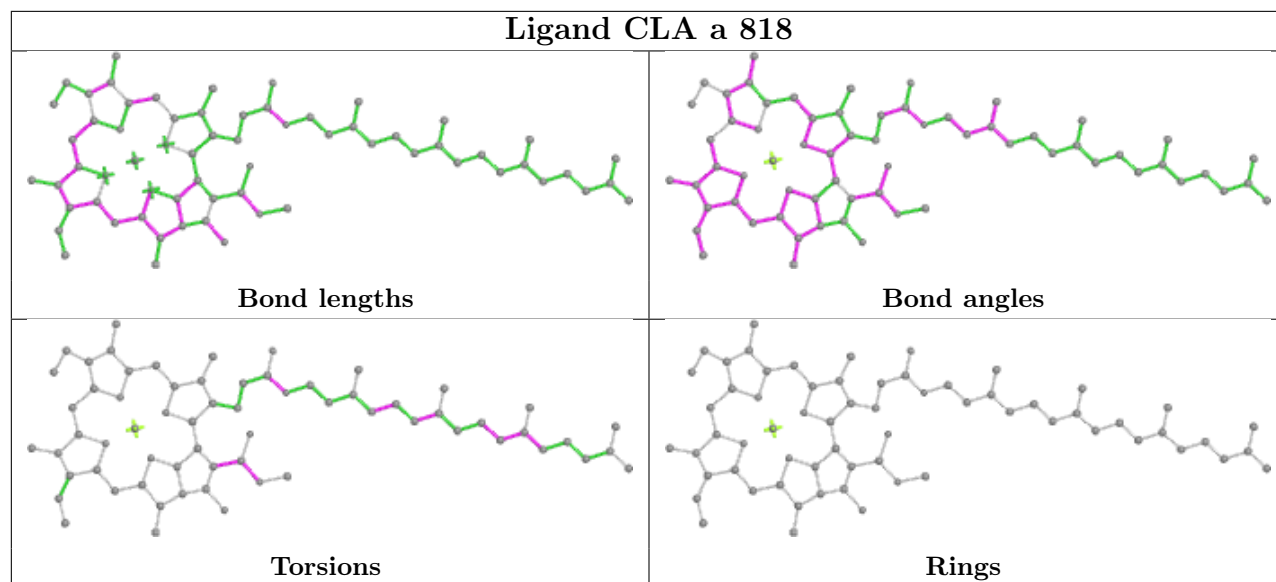
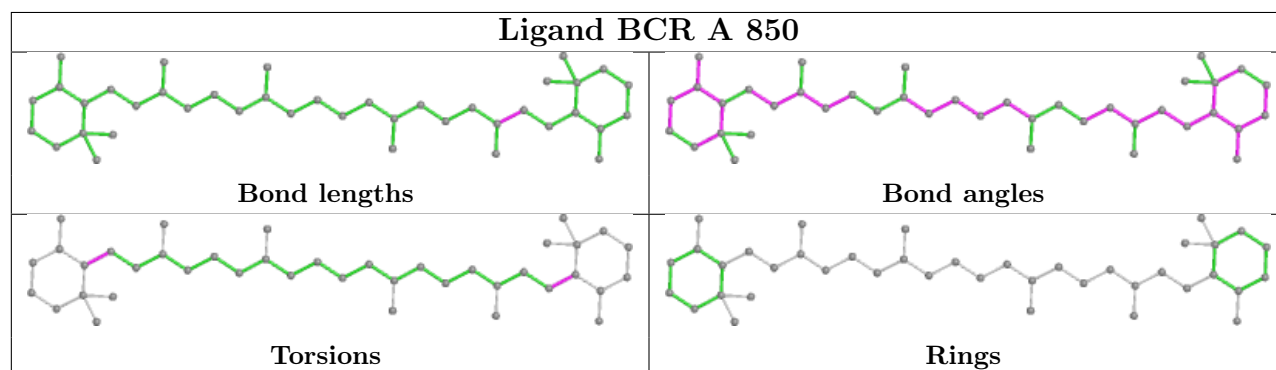
Bond angles



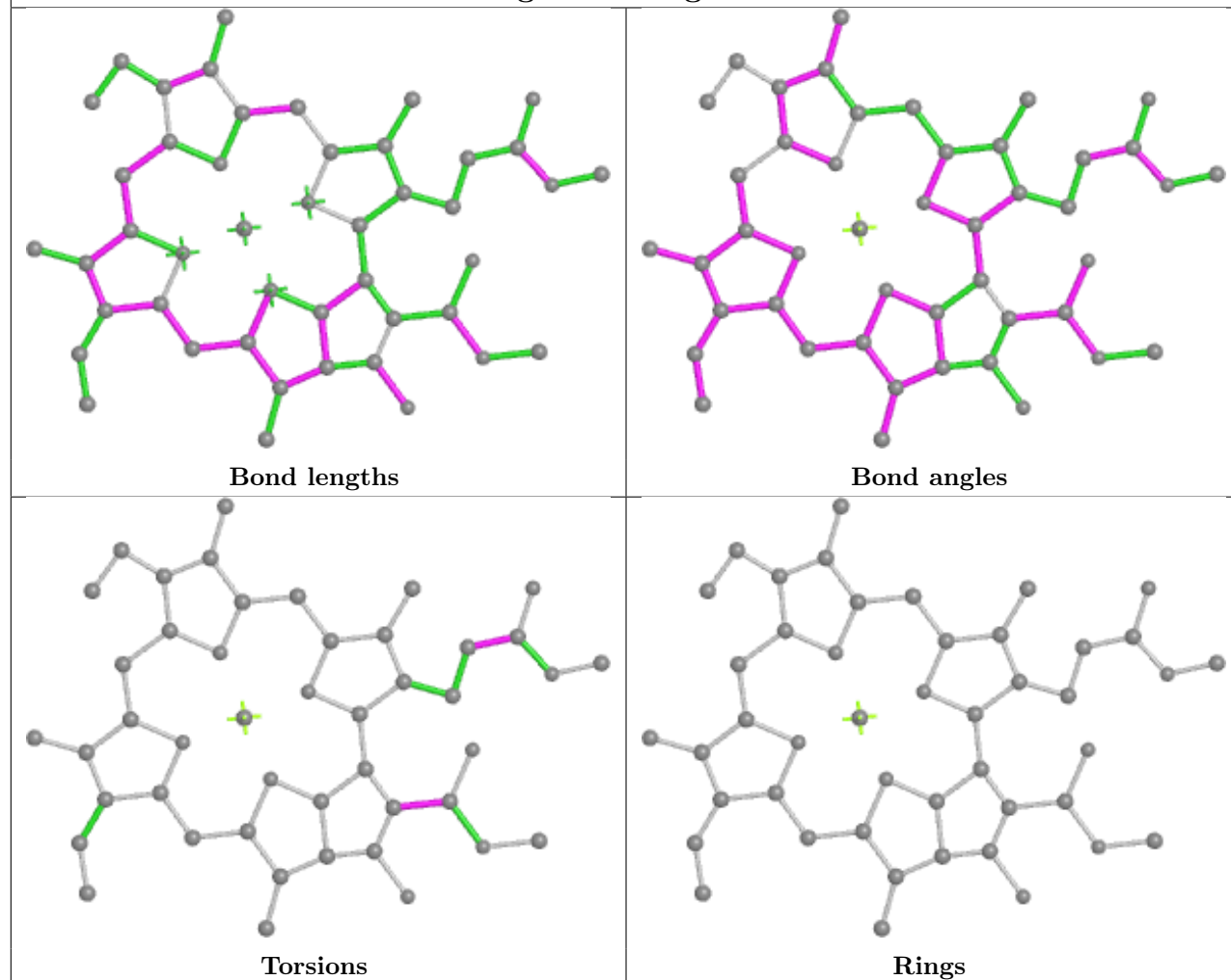
Torsions



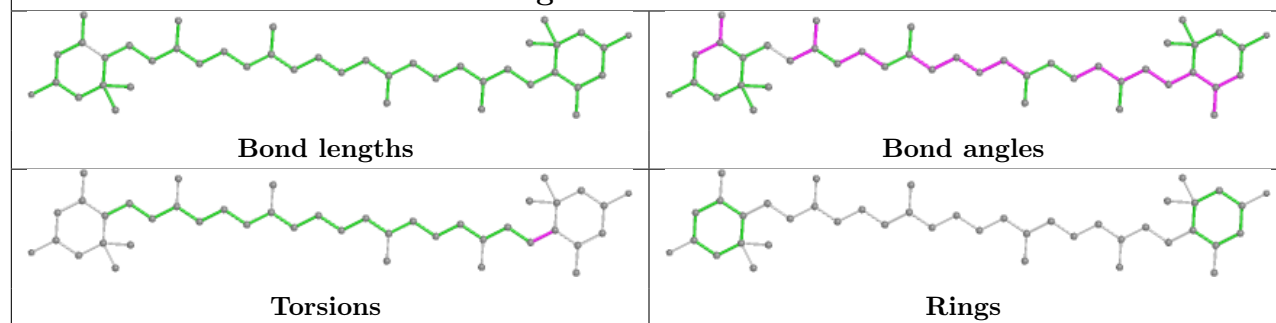
Rings

**Ligand CLA a 818****Ligand BCR A 850**

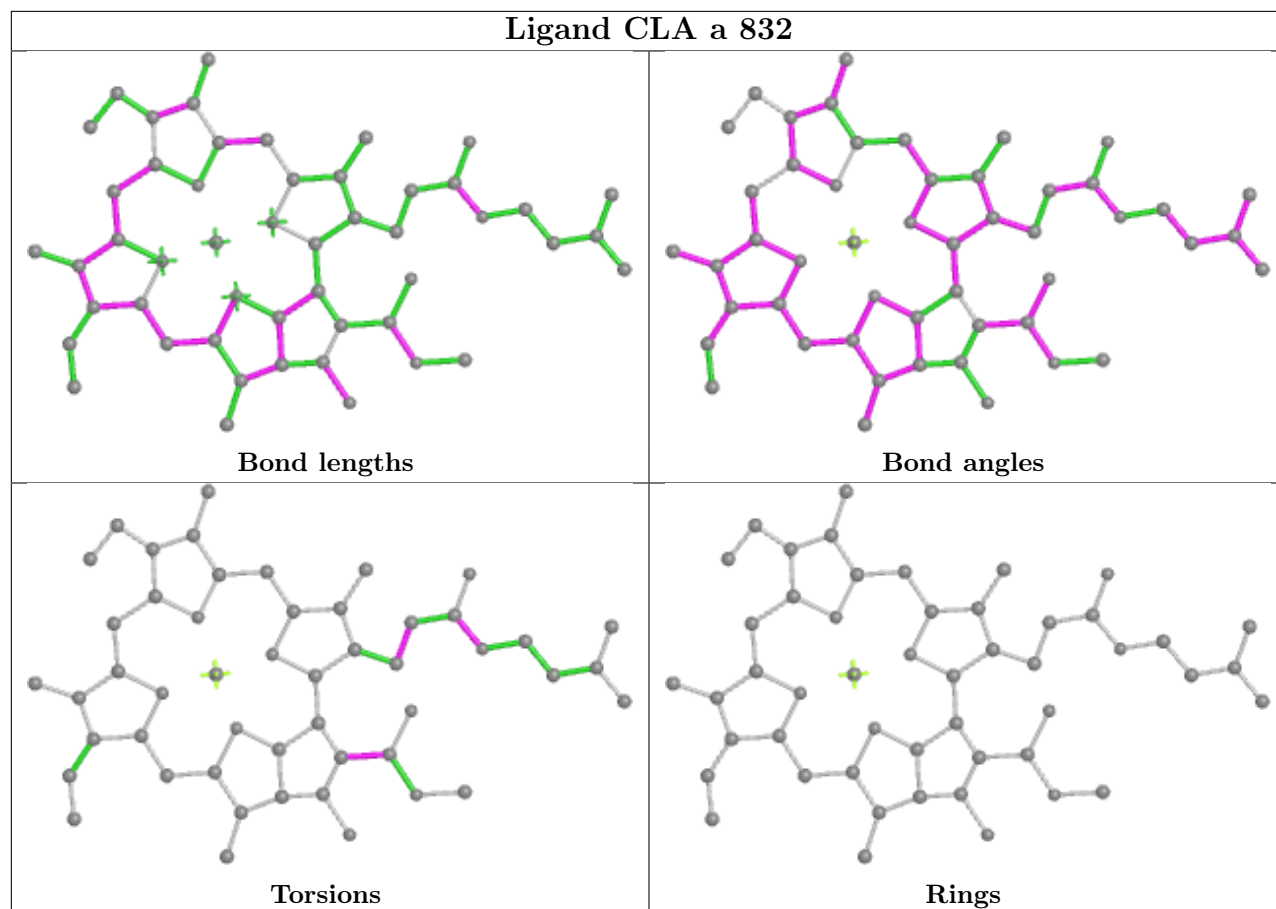
## Ligand CLA g 103



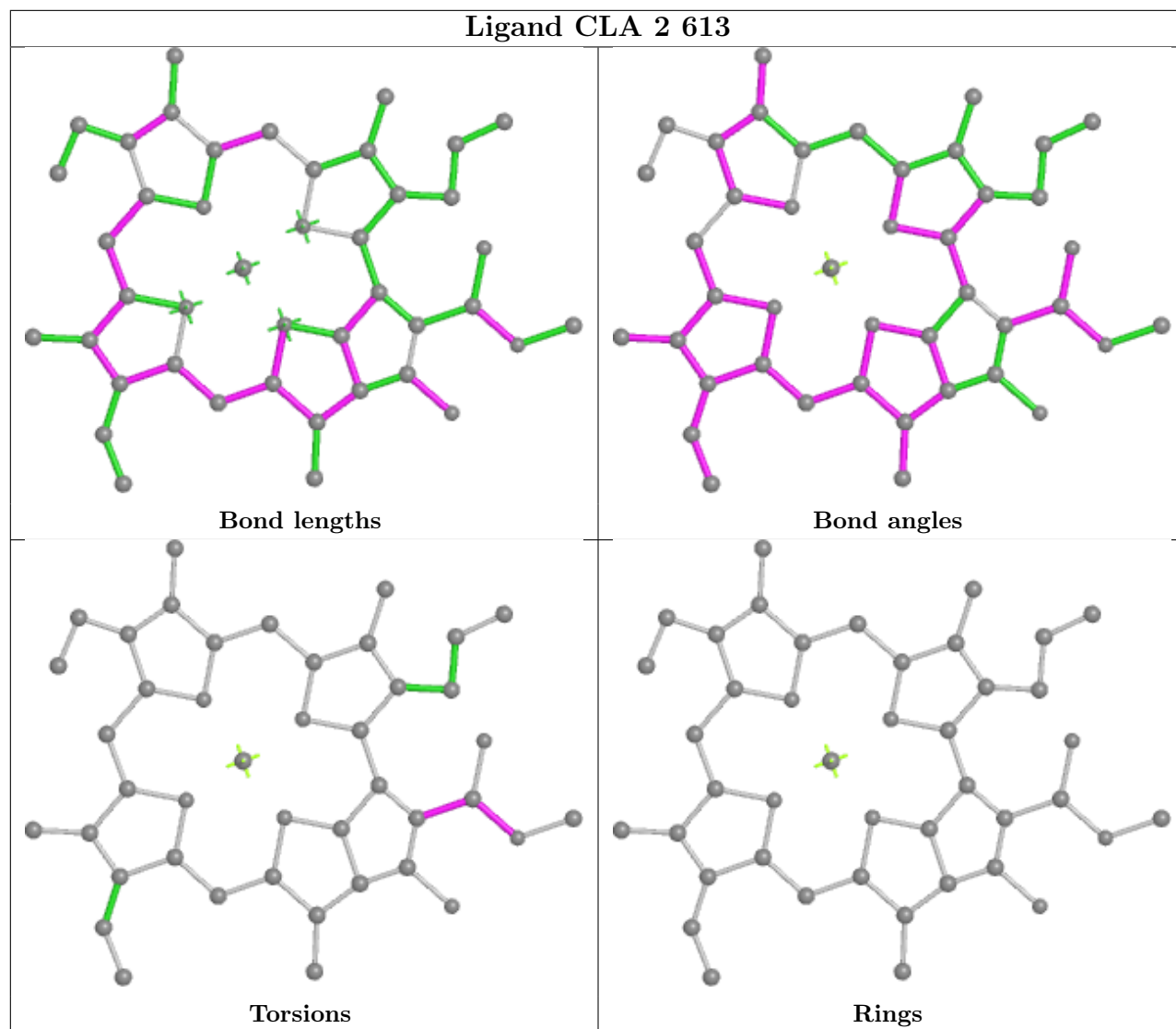
## Ligand LUT 1 320



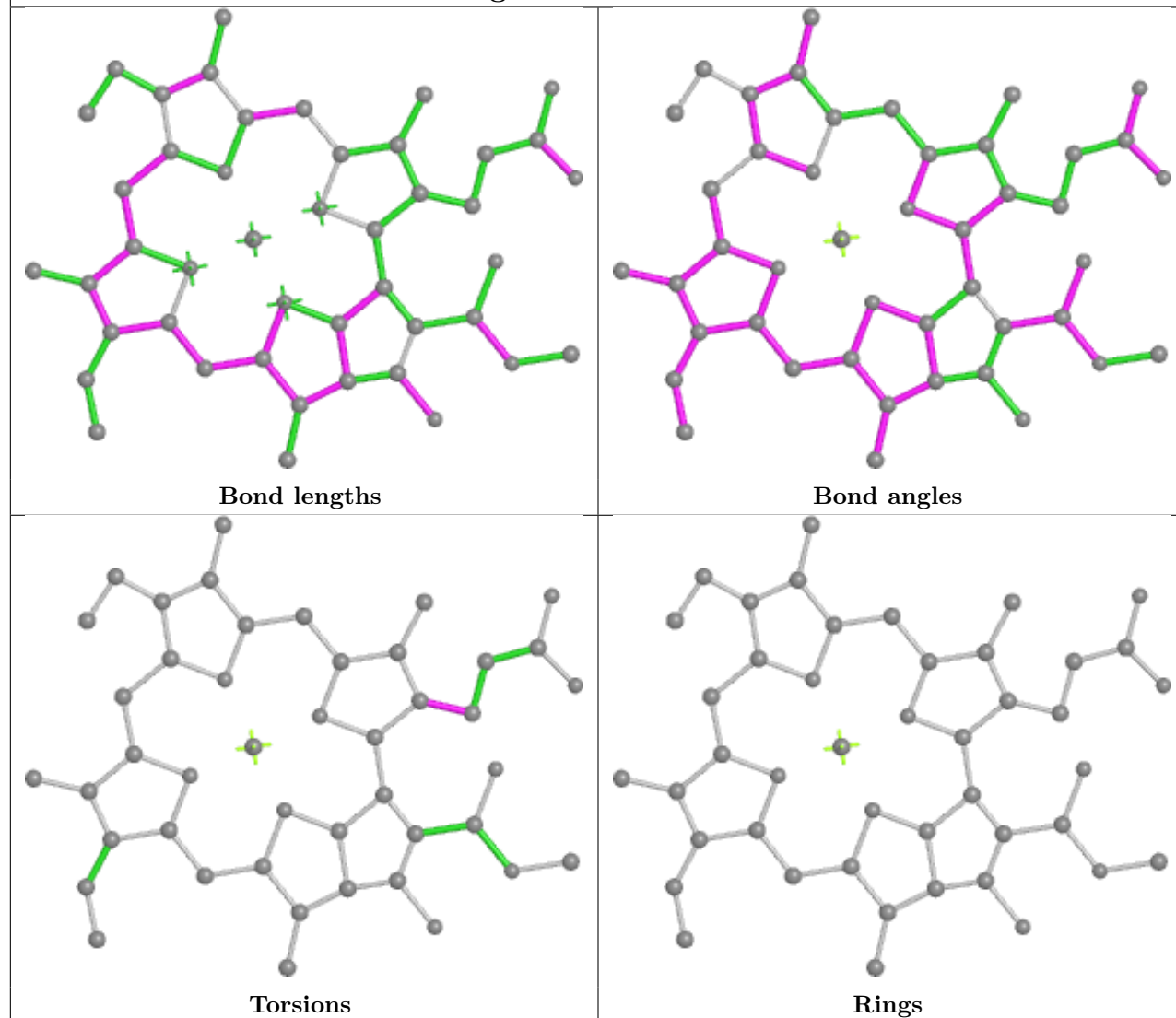
## Ligand CLA a 832



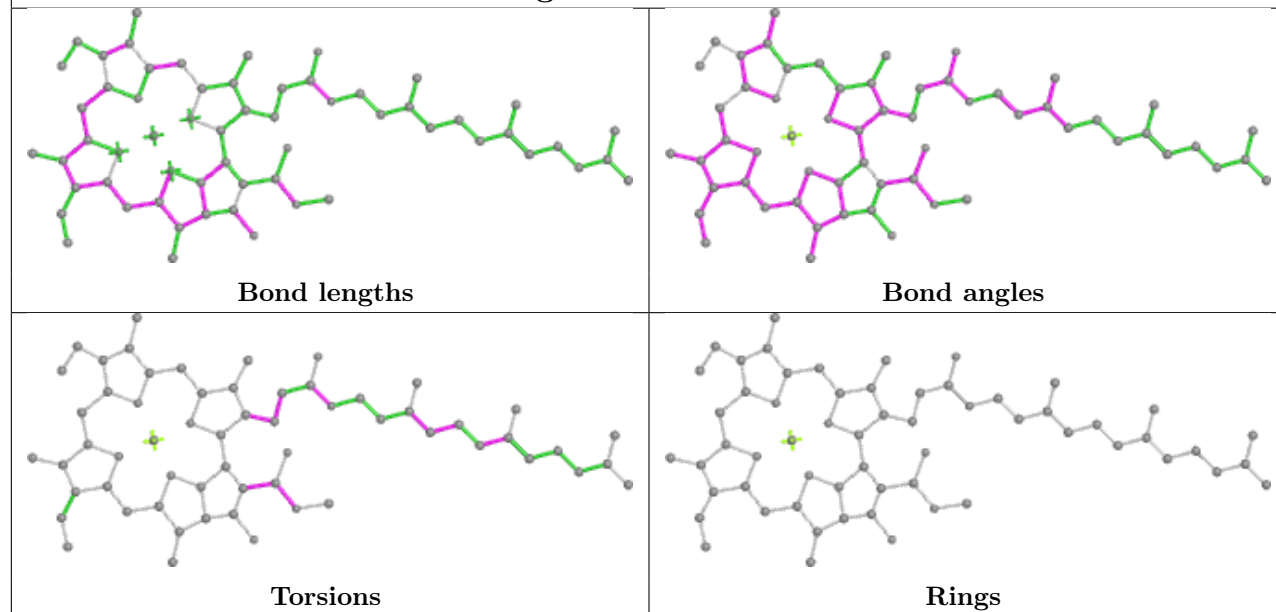
## Ligand CLA 2 613



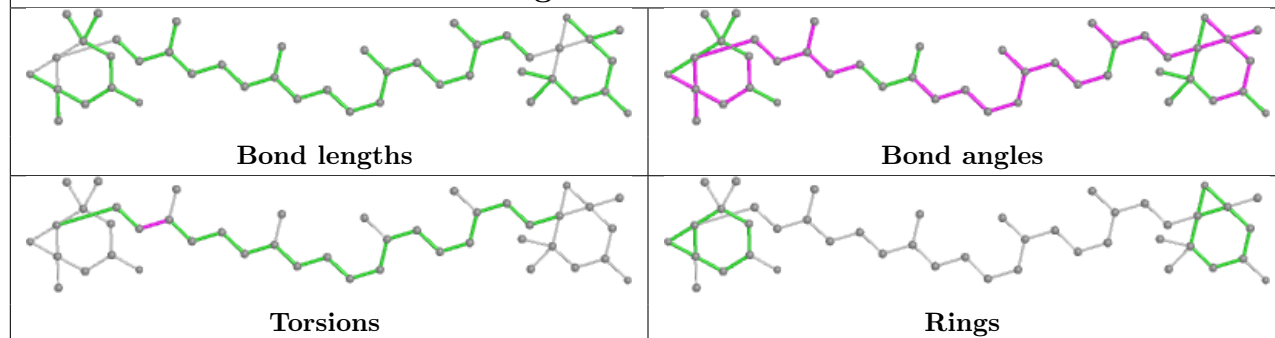
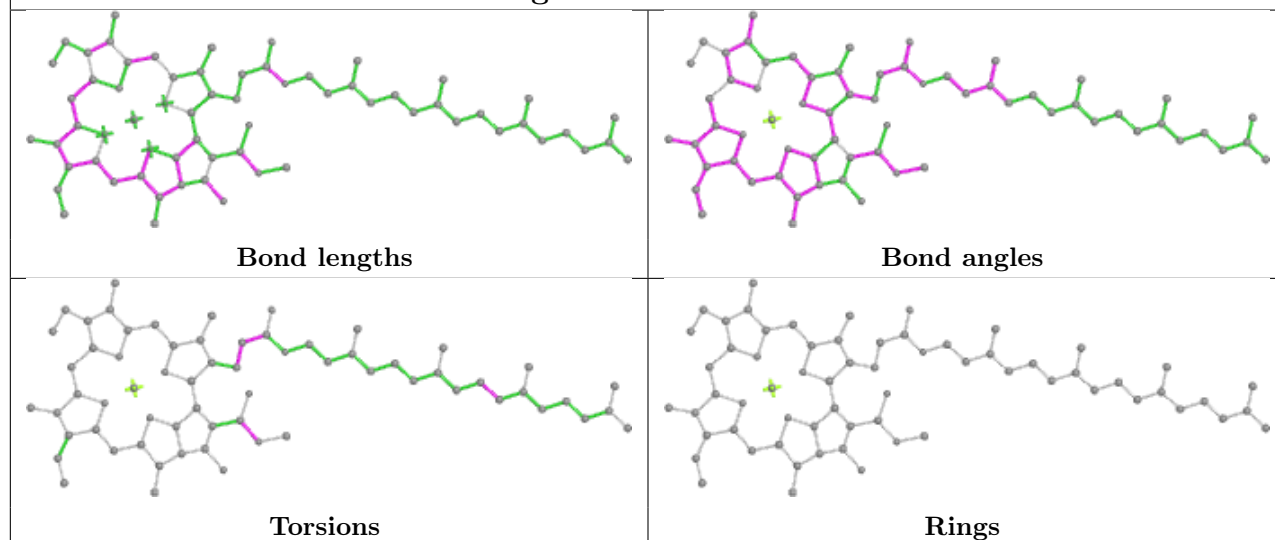
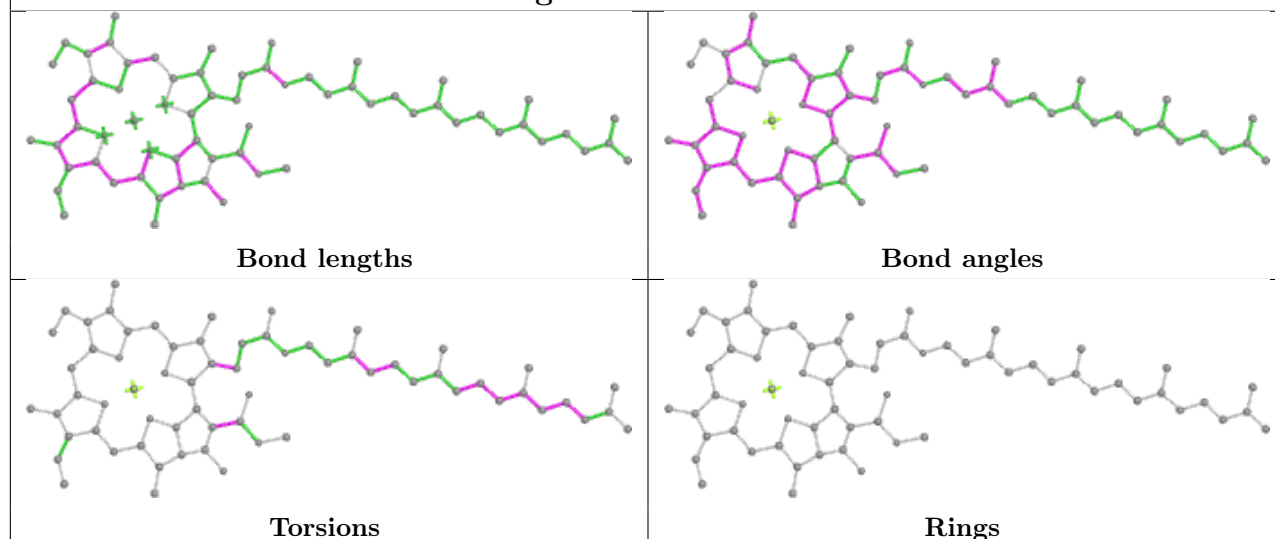
## Ligand CLA A 815

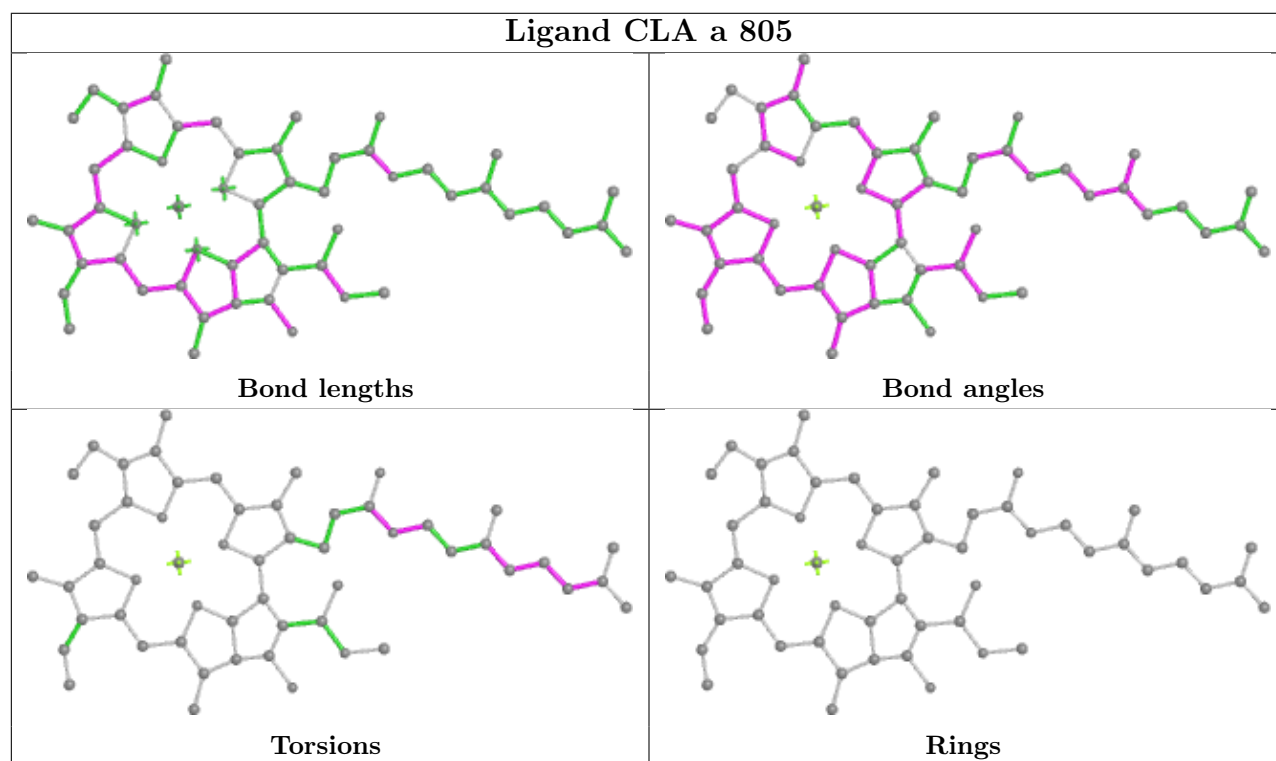
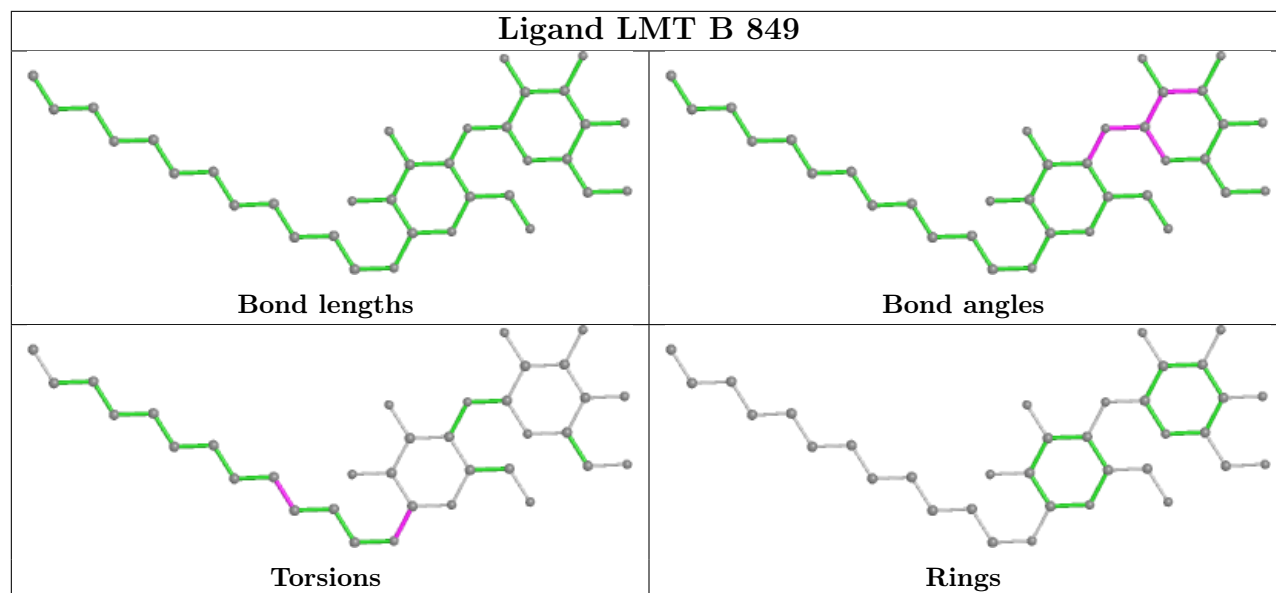


## Ligand CLA 8 301

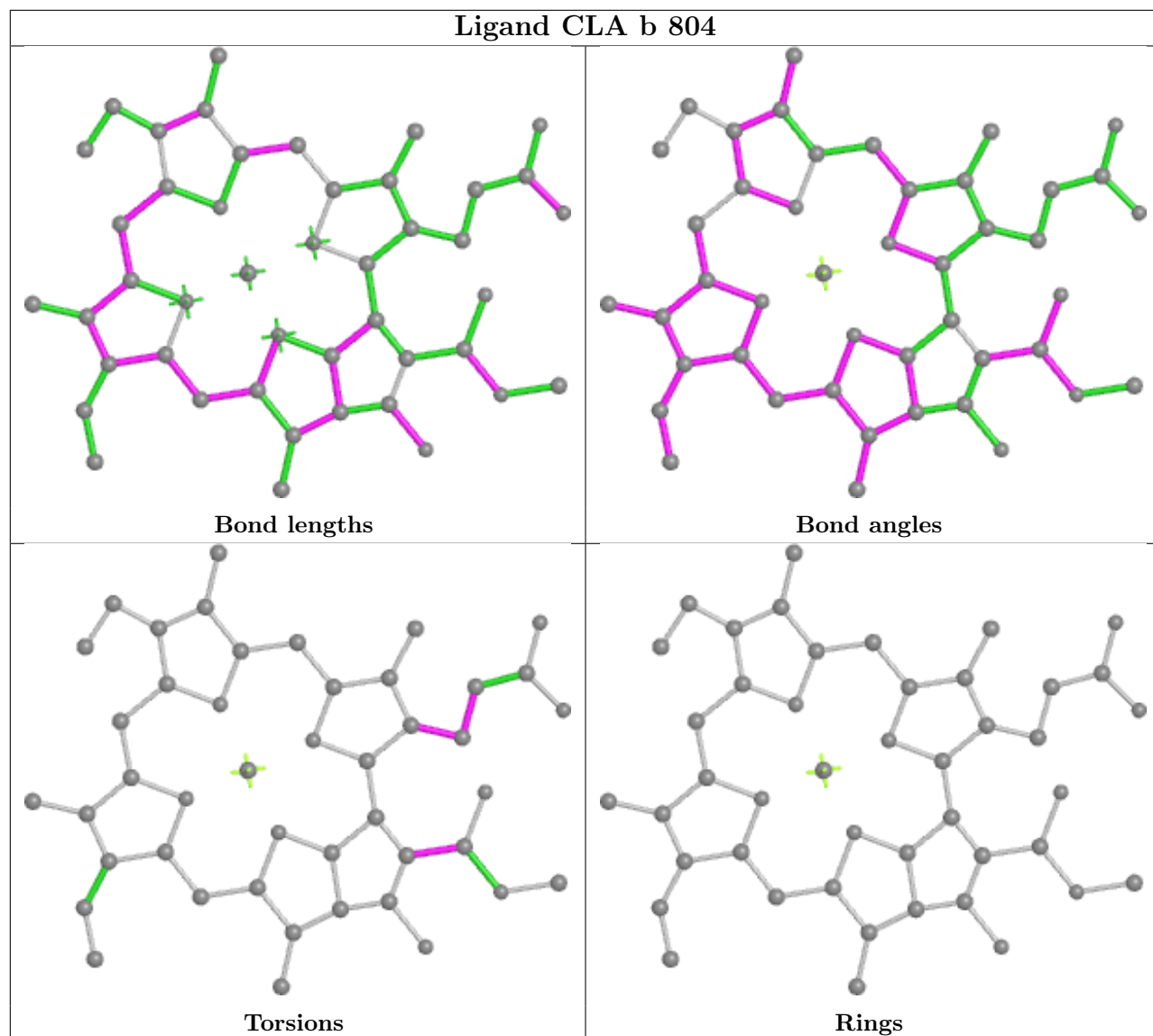




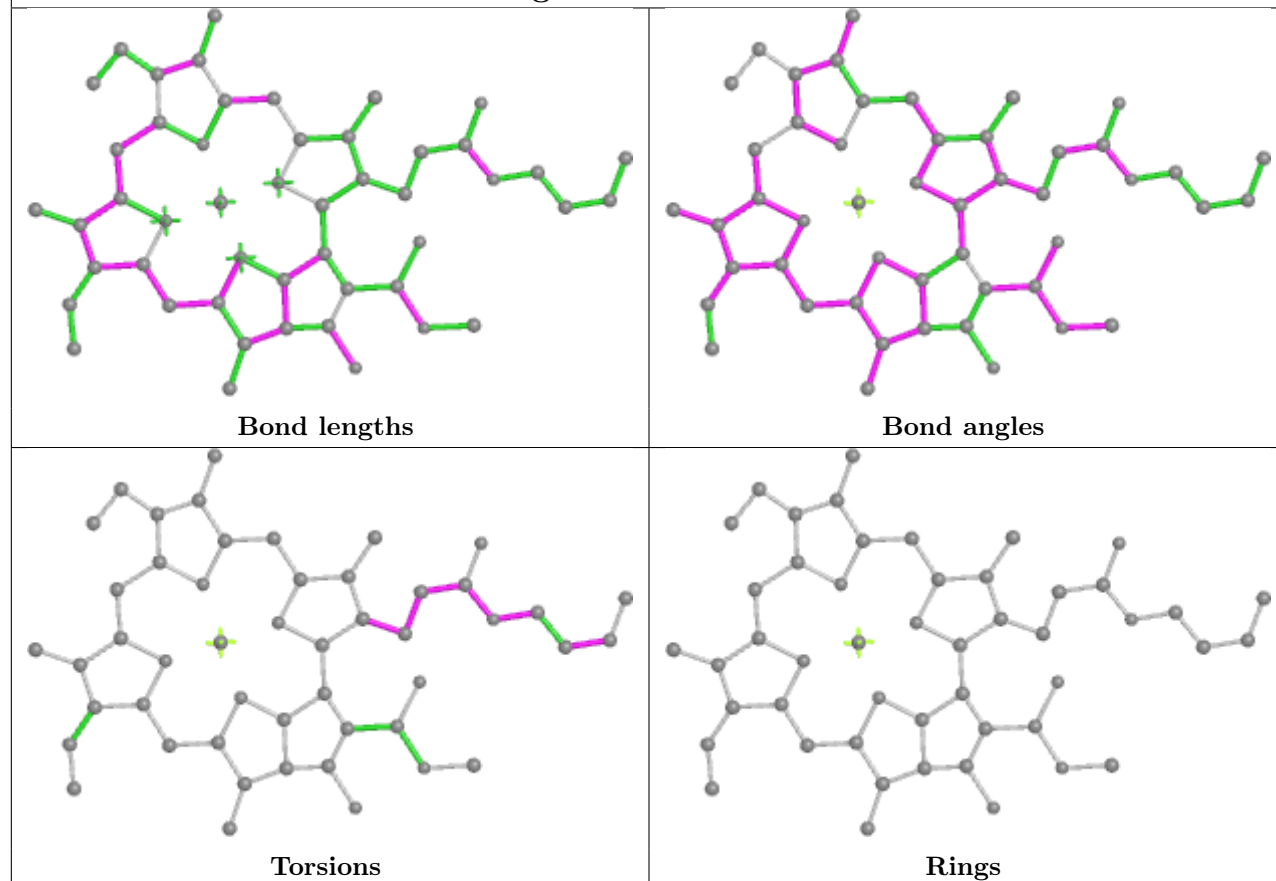
**Ligand XAT 3 317****Ligand CLA B 803****Ligand CLA a 806**



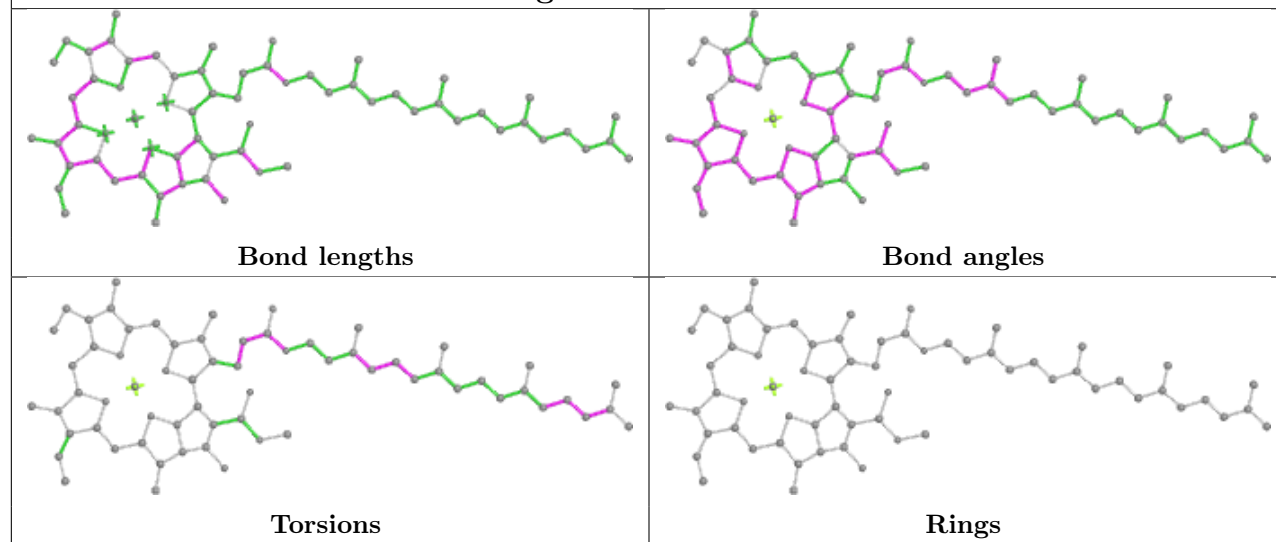
## Ligand CLA b 804

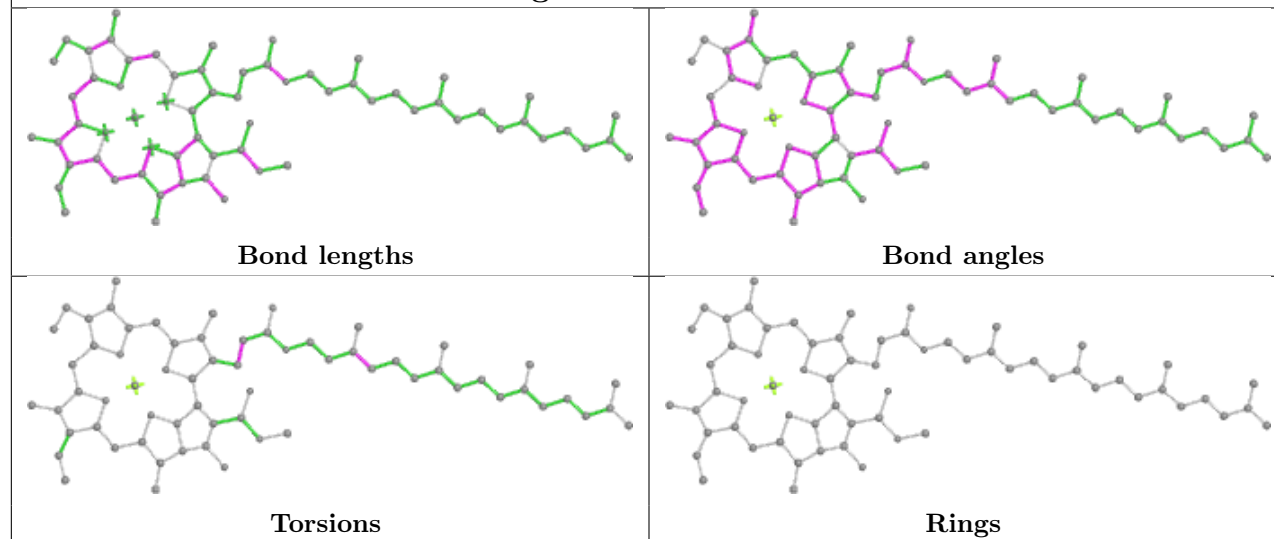
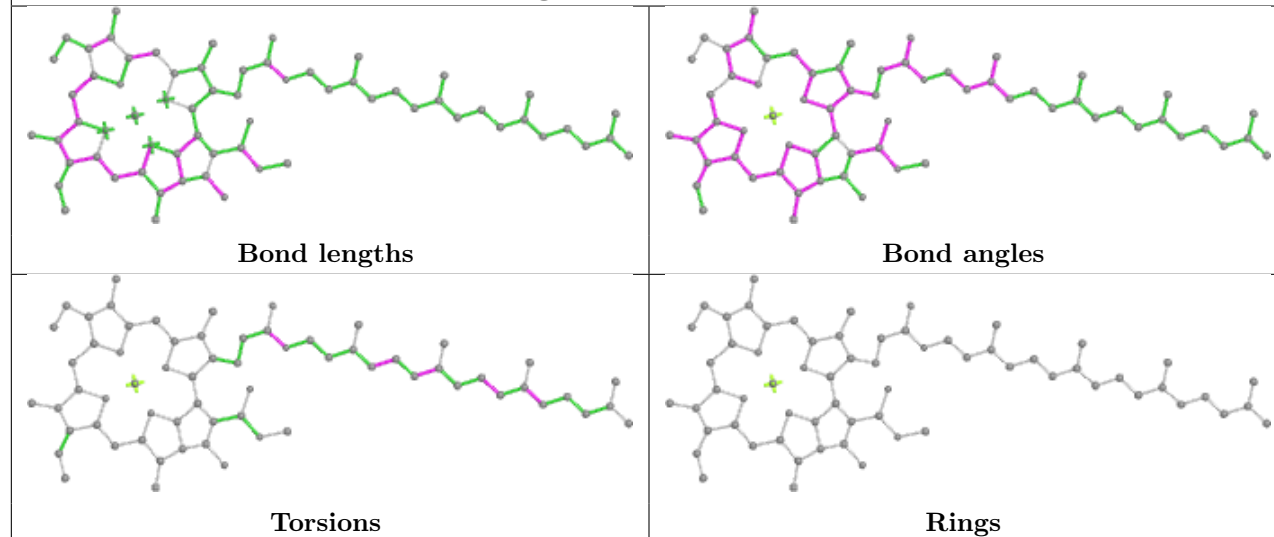


## Ligand CLA B 831

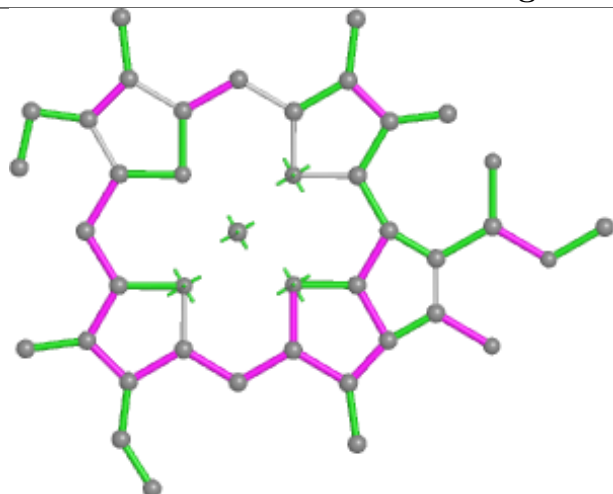


## Ligand CLA a 844

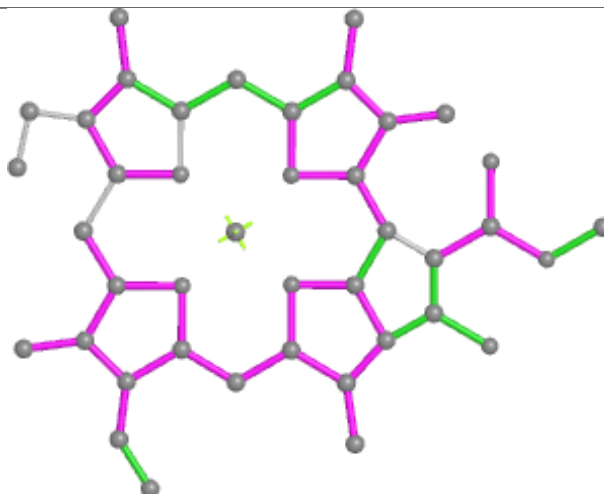


**Ligand CLA A 803****Ligand CLA b 825**

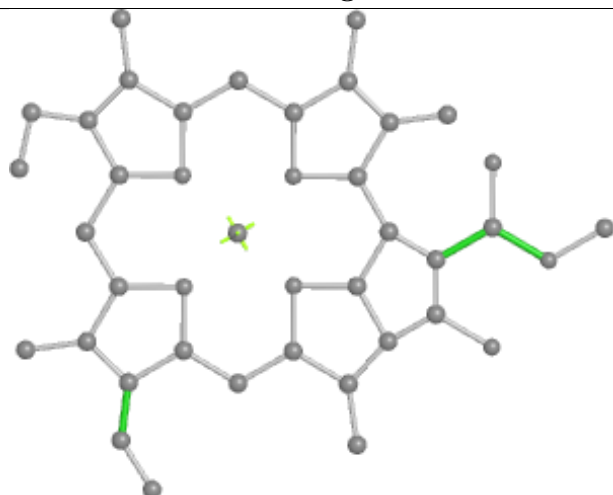
## Ligand CLA 7 610



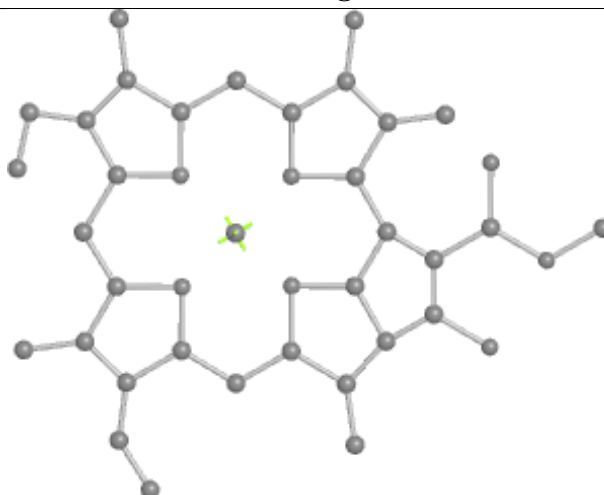
Bond lengths



Bond angles

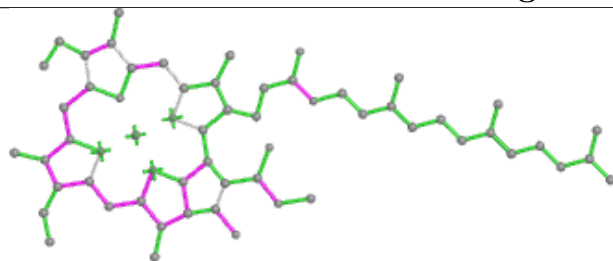


Torsions

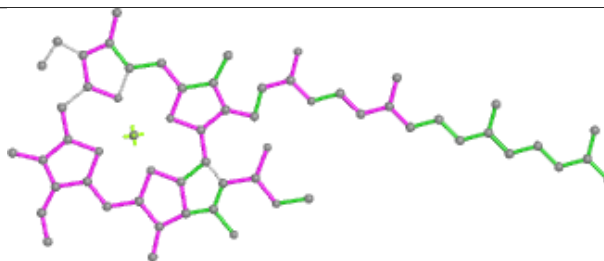


Rings

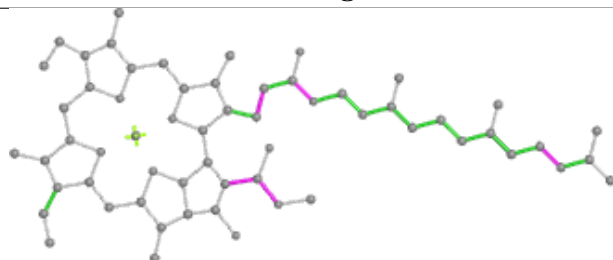
## Ligand CLA 4 602



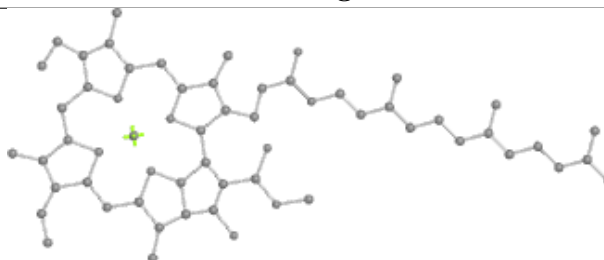
Bond lengths



Bond angles

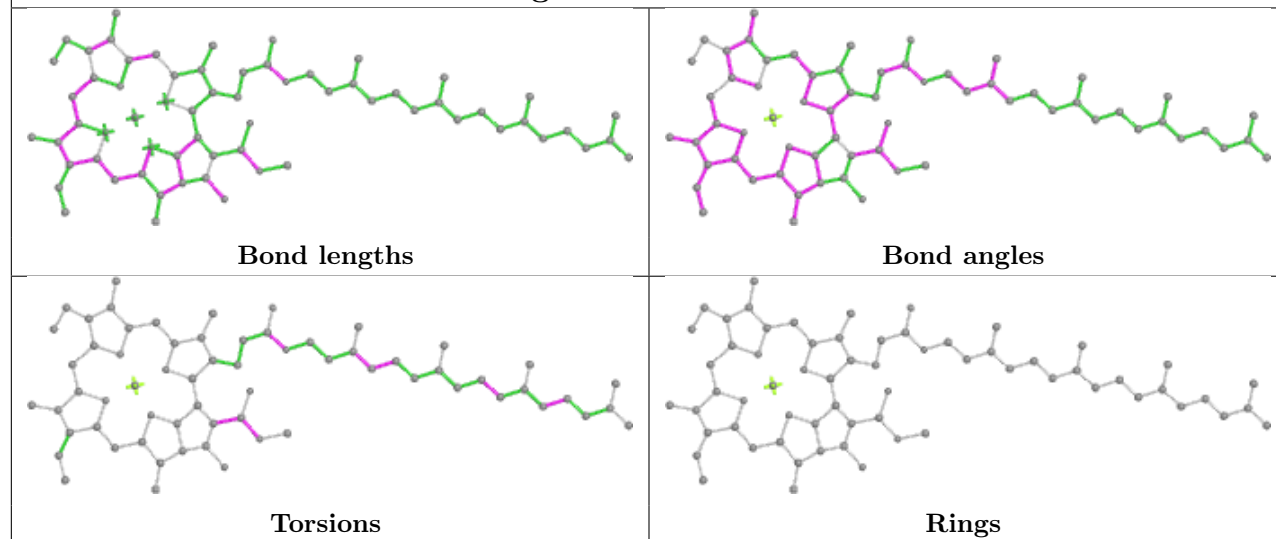


Torsions

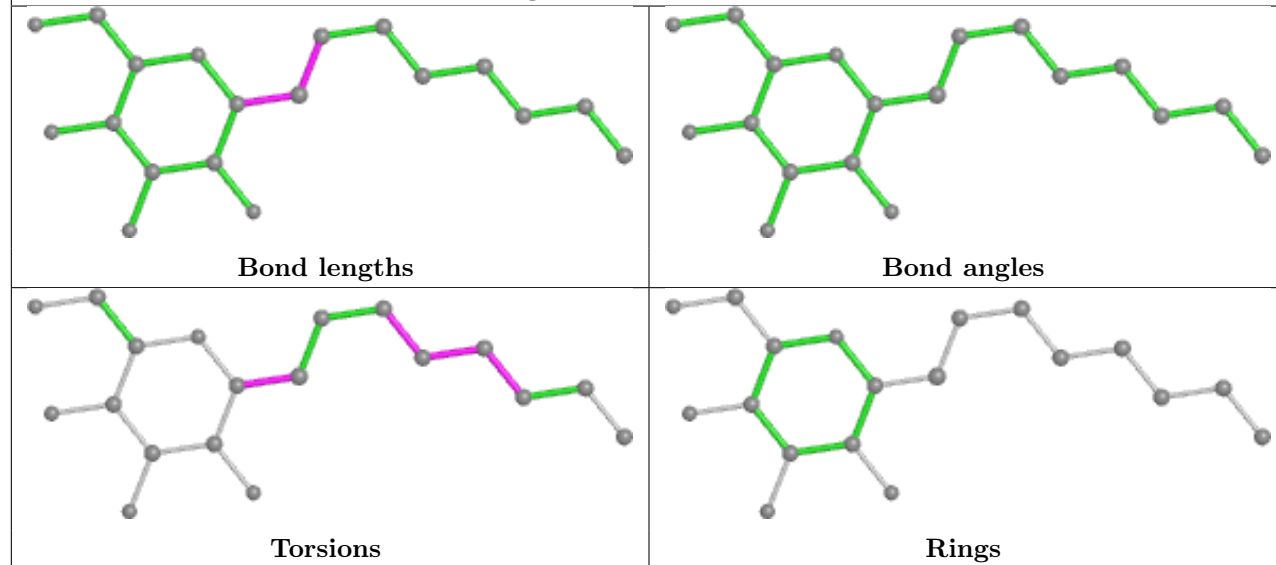


Rings

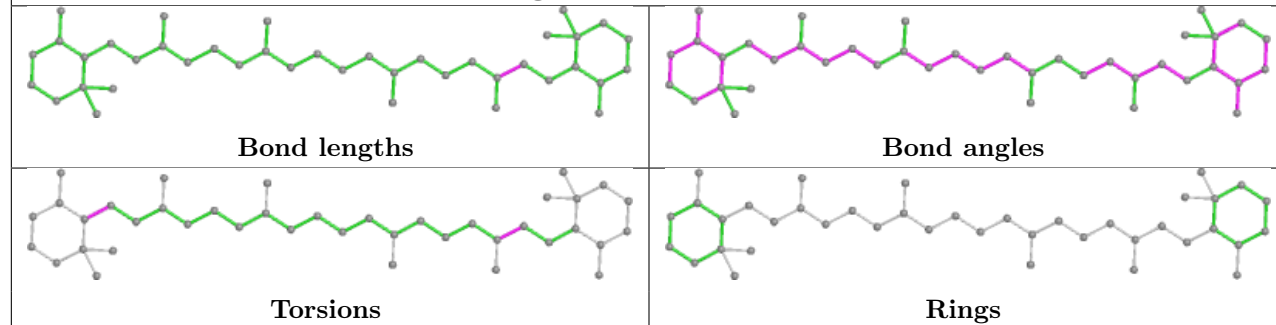
## Ligand CLA A 818



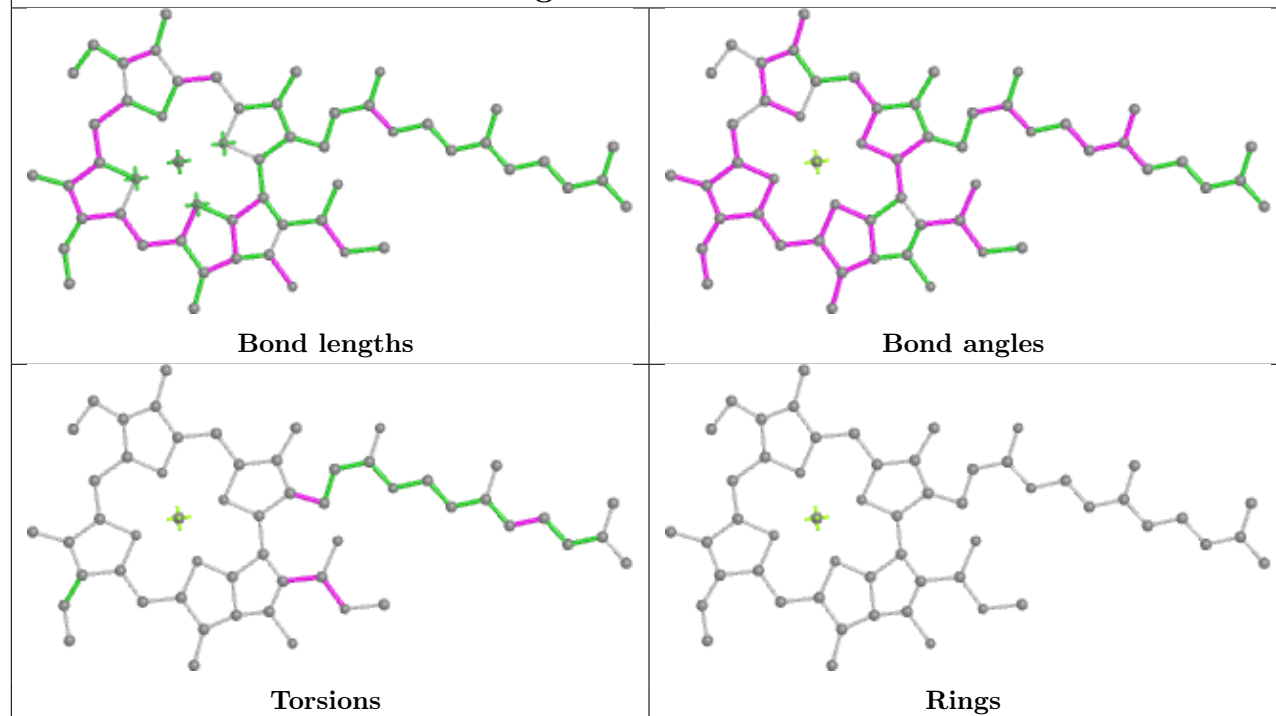
## Ligand HTG J 3001



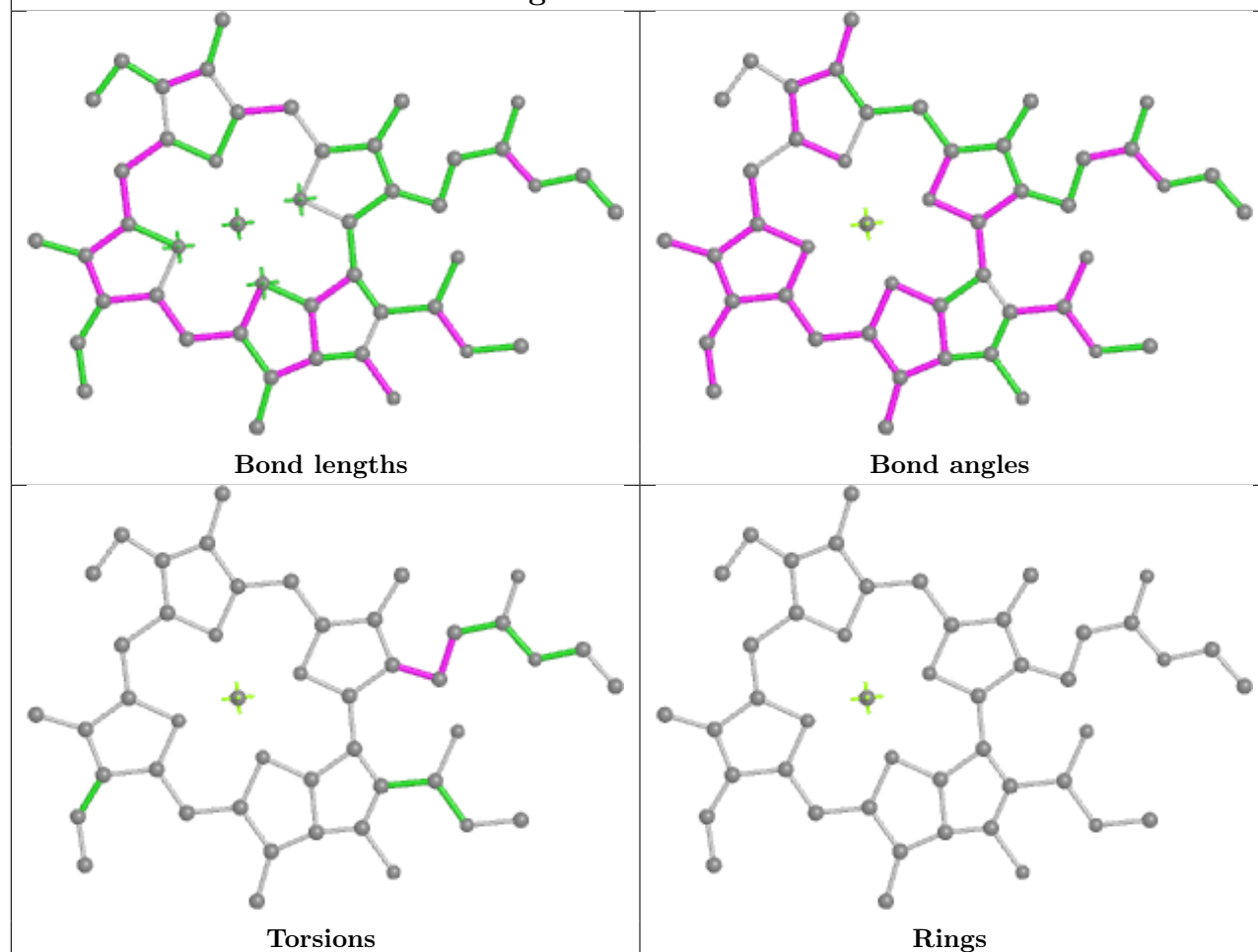
## Ligand BCR G 105



## Ligand CLA b 815

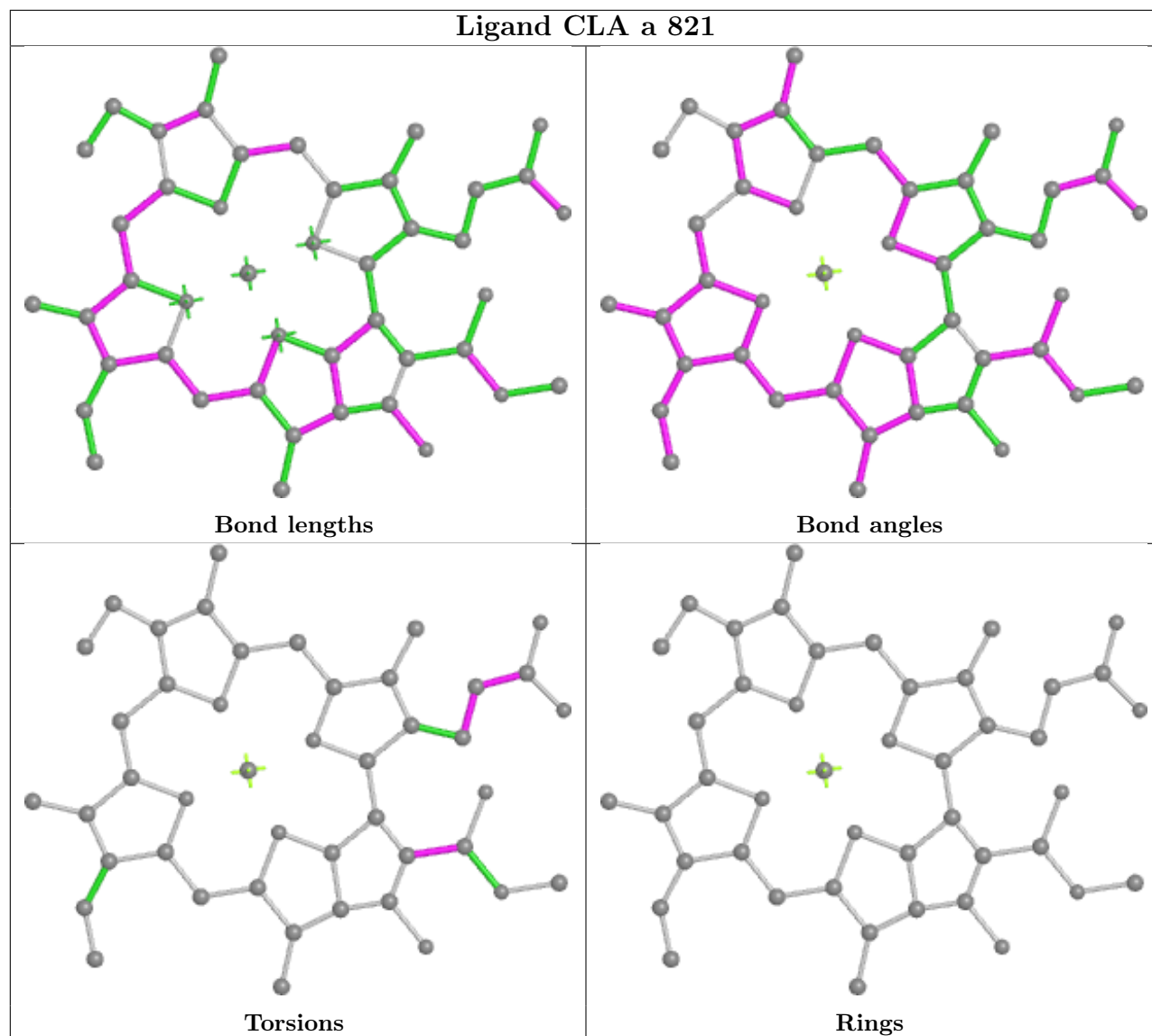


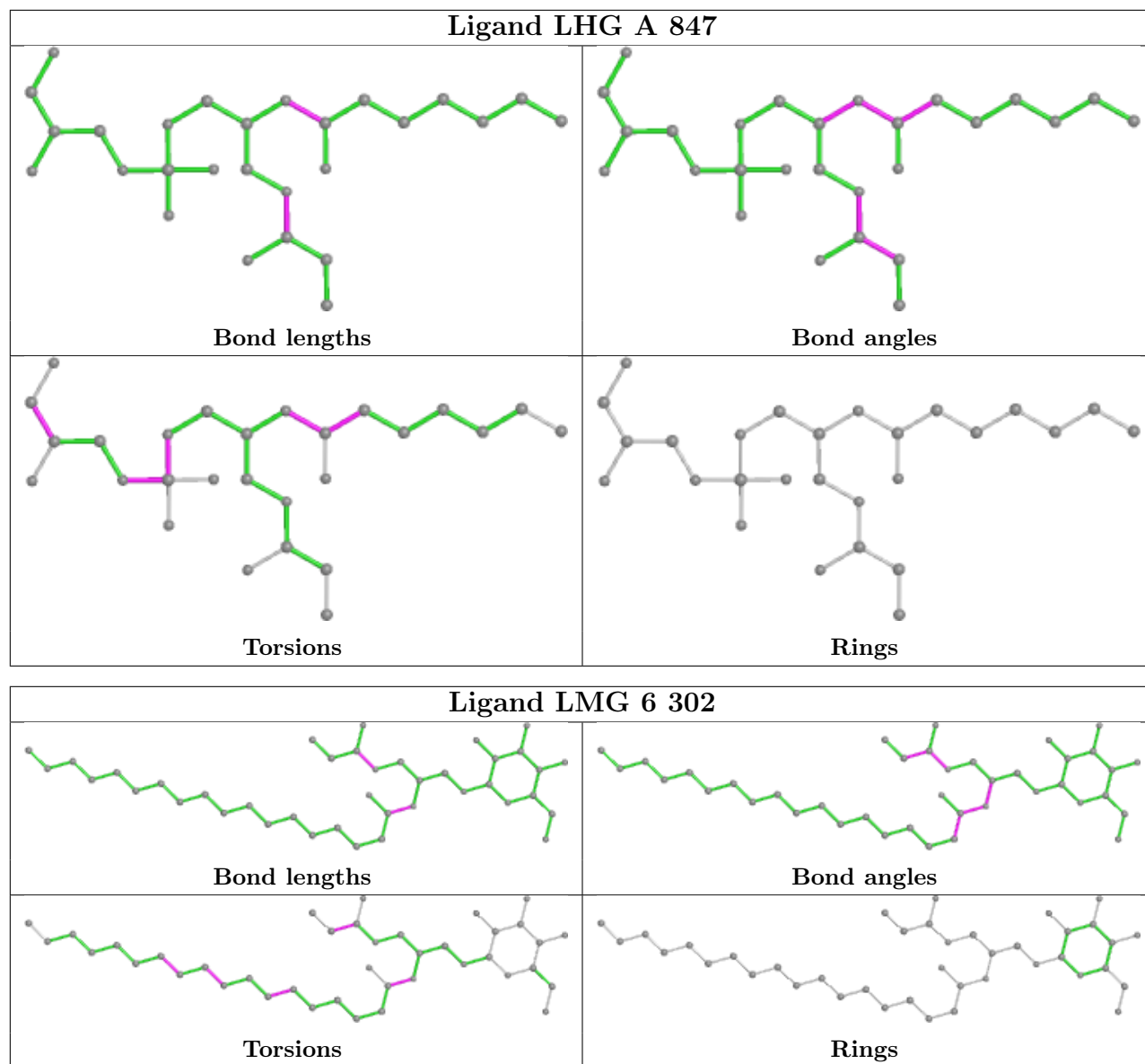
## Ligand CLA 3 306



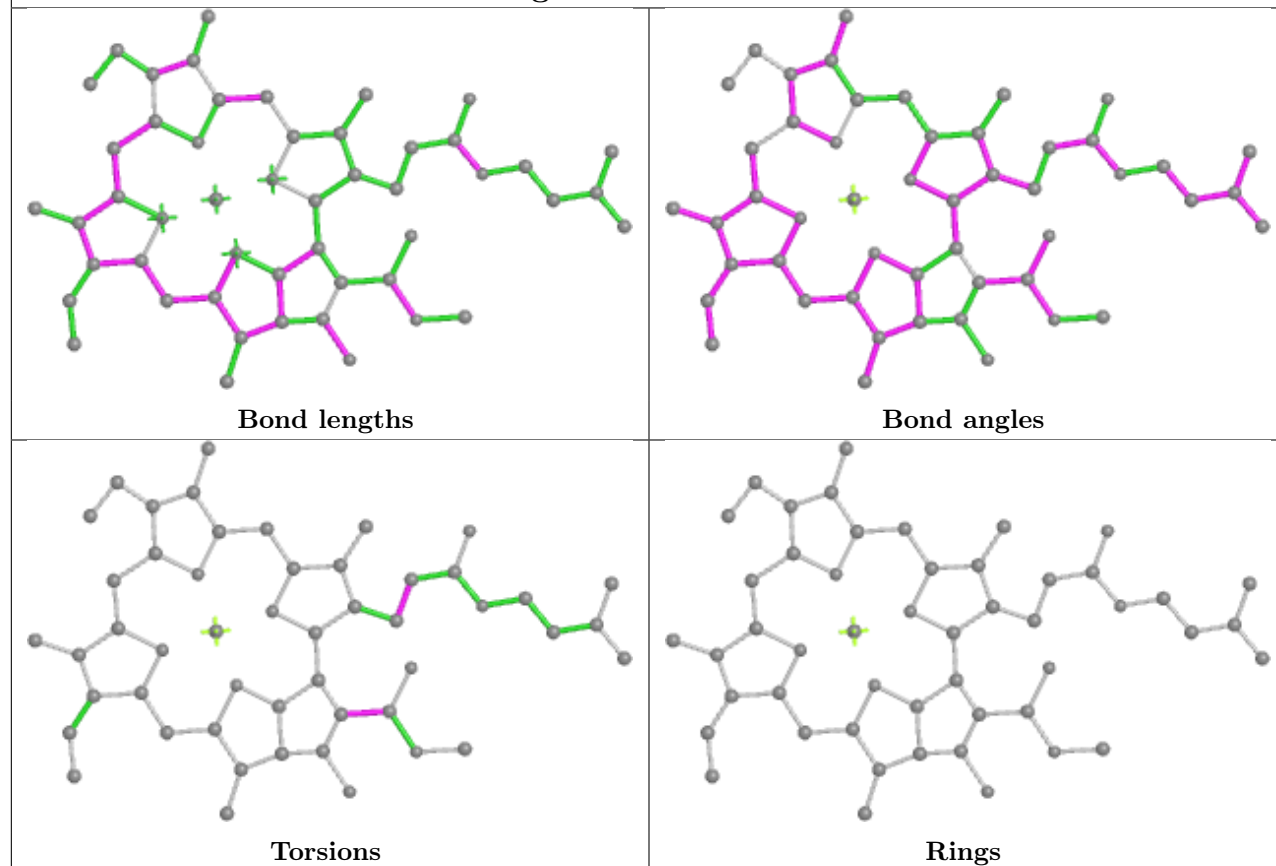


## Ligand CLA a 821

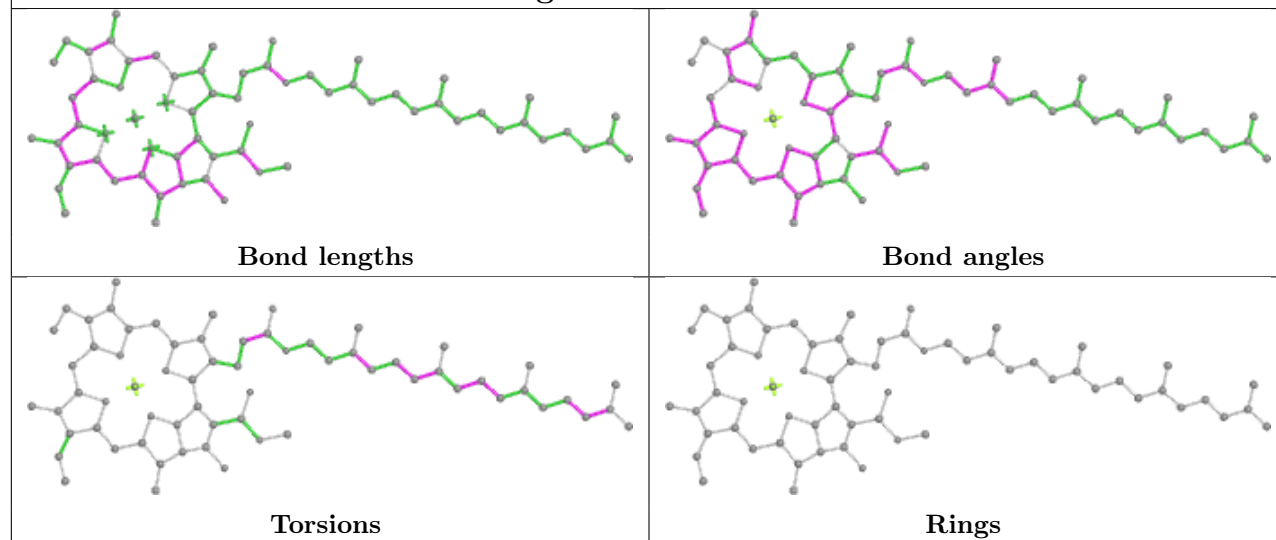




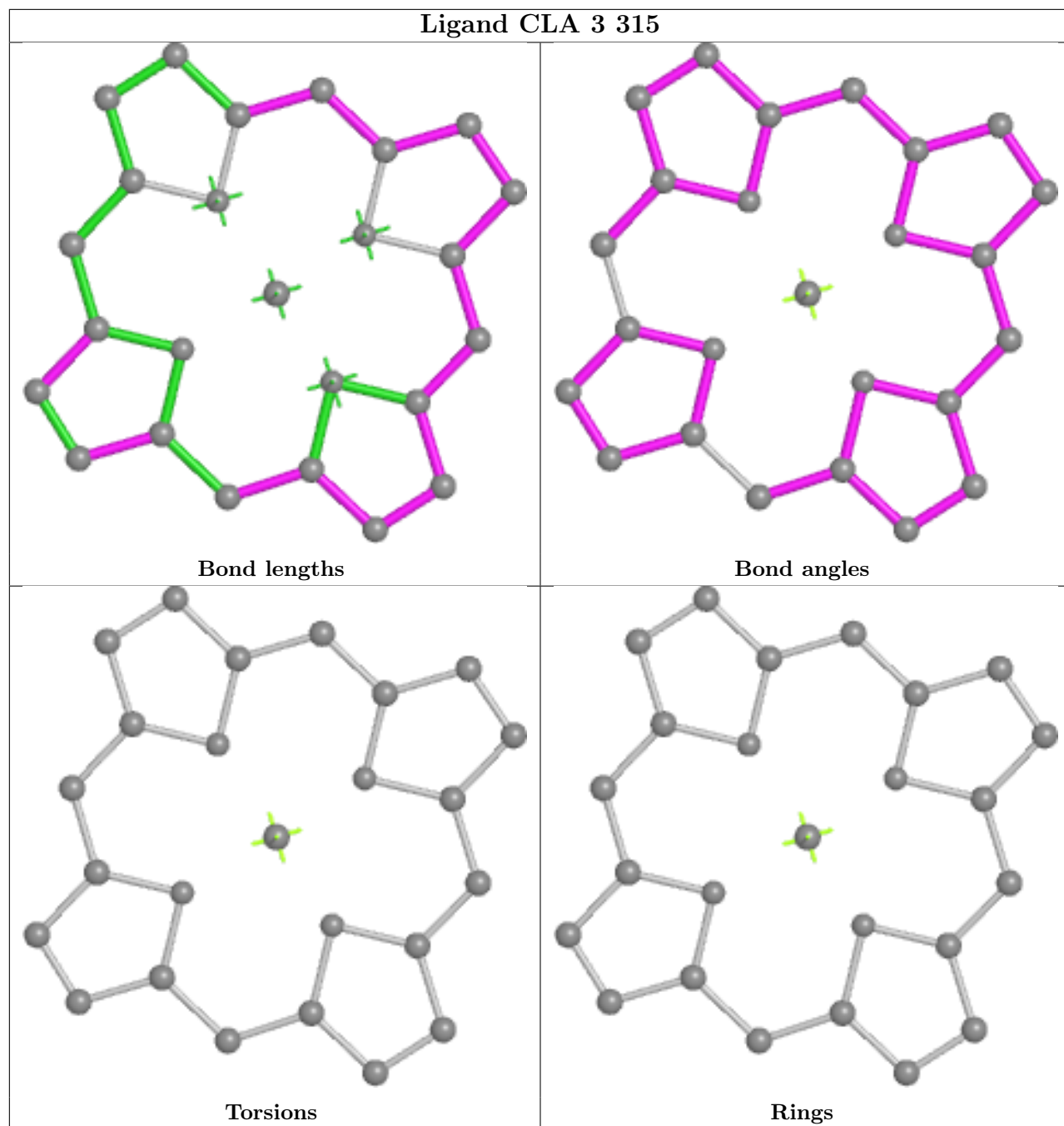
## Ligand CLA A 832



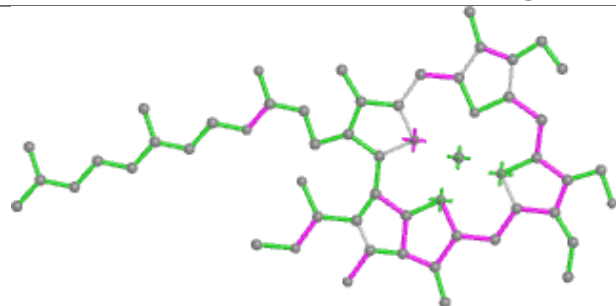
## Ligand CLA 1 304



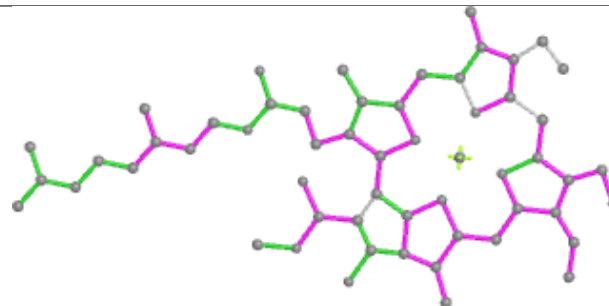
## Ligand CLA 3 315



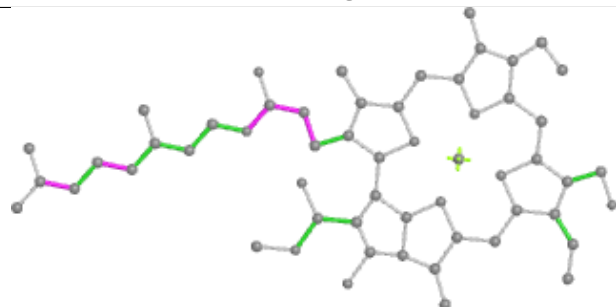
## Ligand CHL 9 605



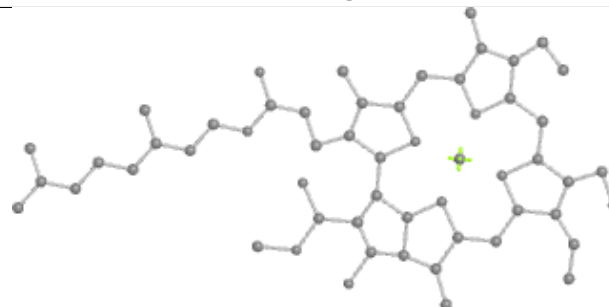
Bond lengths



Bond angles

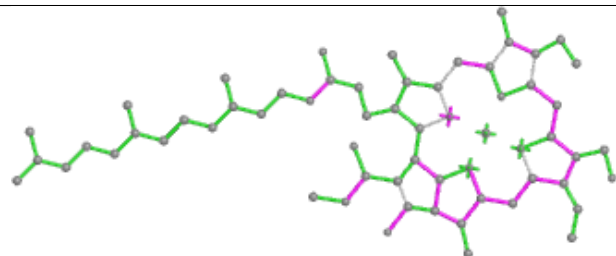


Torsions

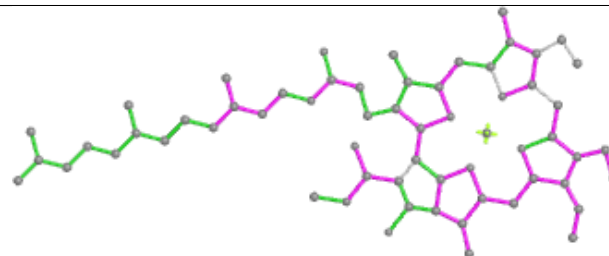


Rings

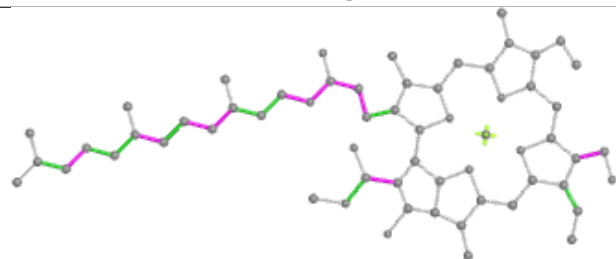
## Ligand CHL 6 303



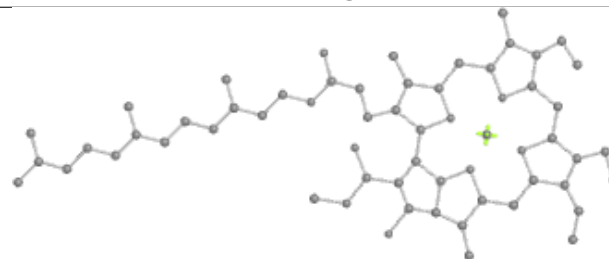
Bond lengths



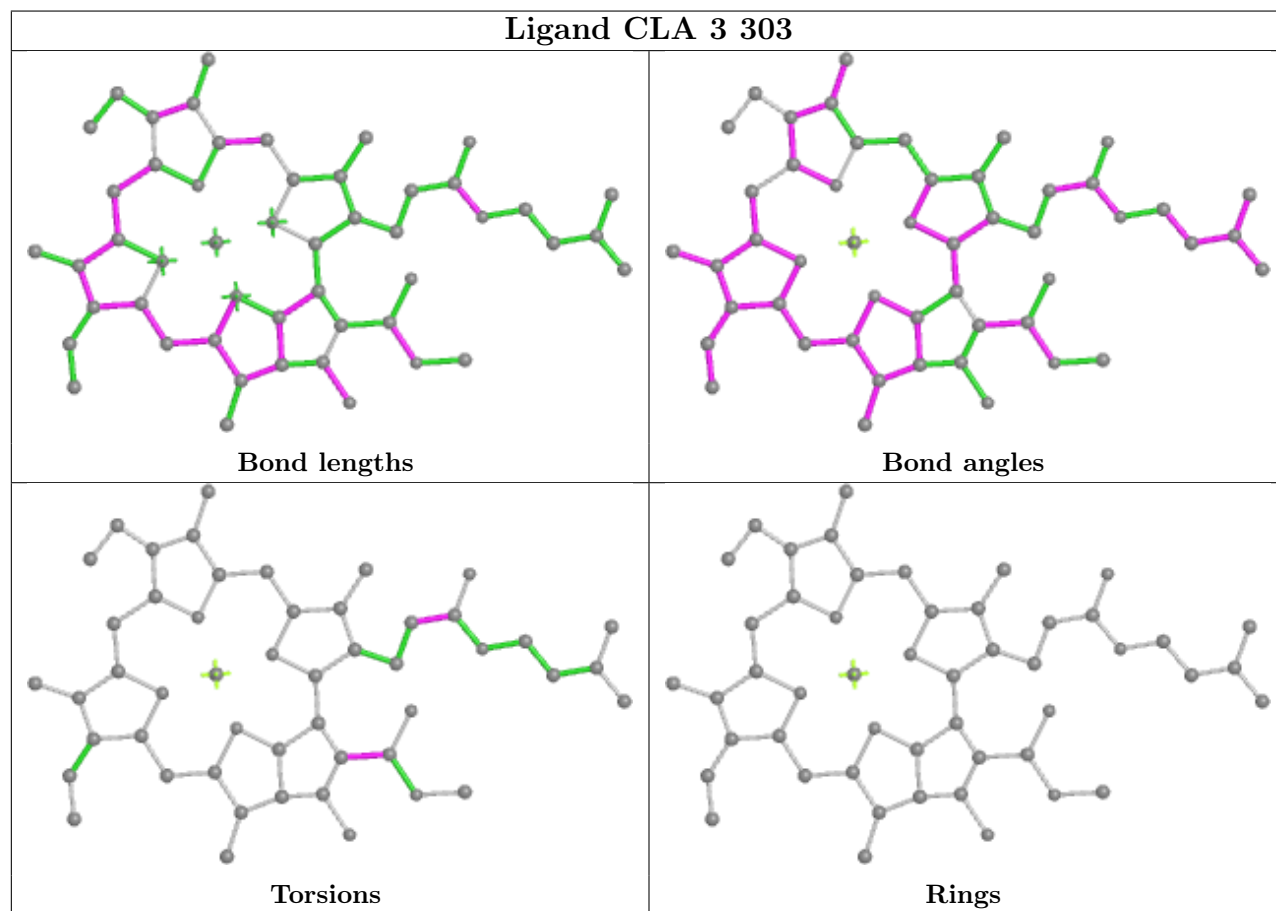
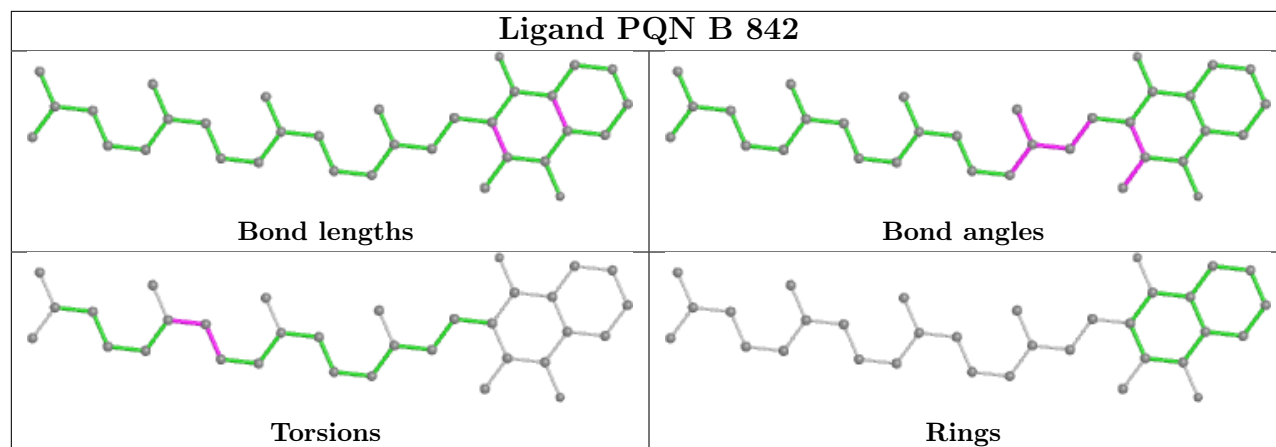
Bond angles



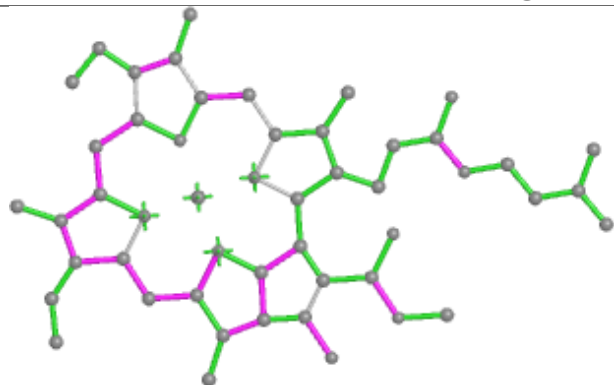
Torsions



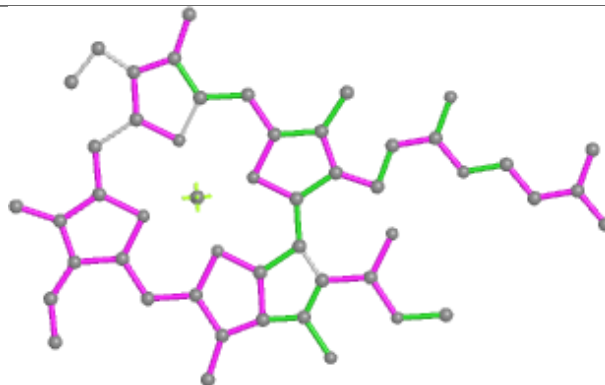
Rings



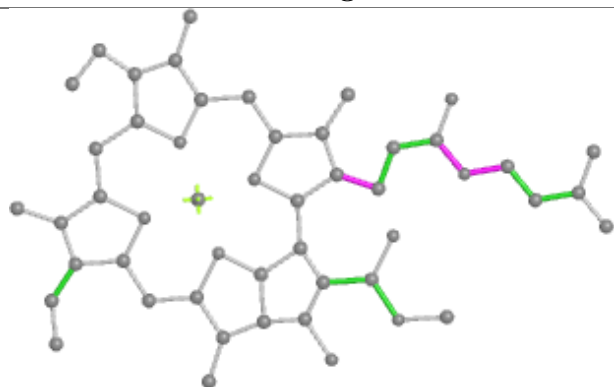
## Ligand CLA 8 307



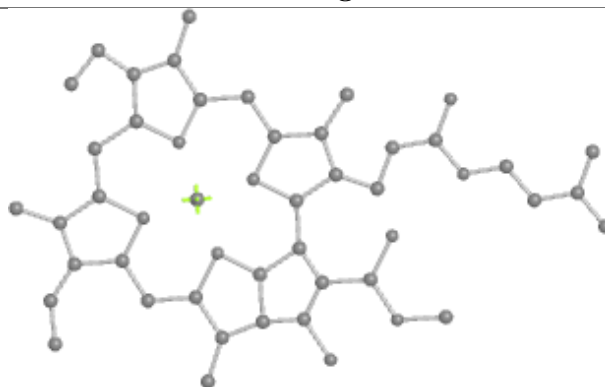
Bond lengths



Bond angles

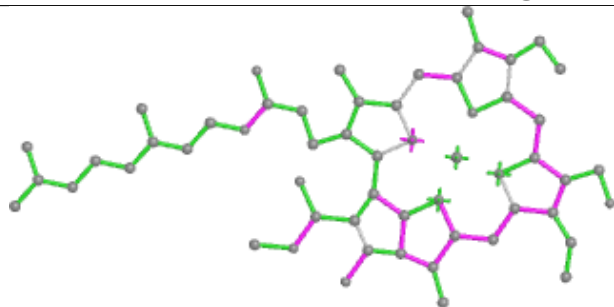


Torsions

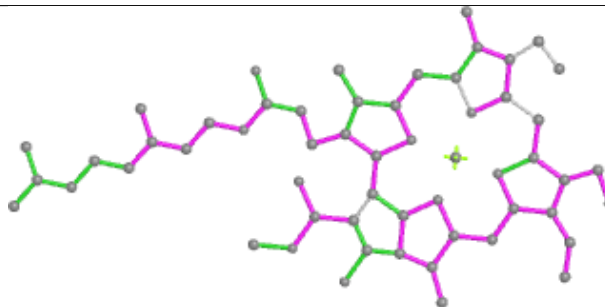


Rings

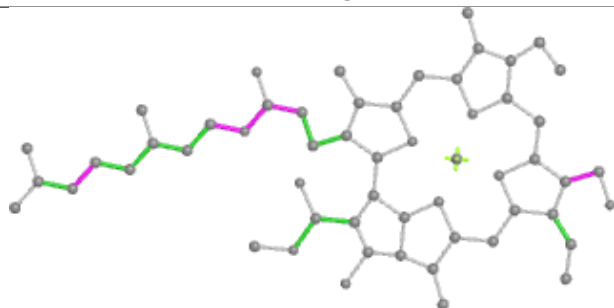
## Ligand CHL 4 605



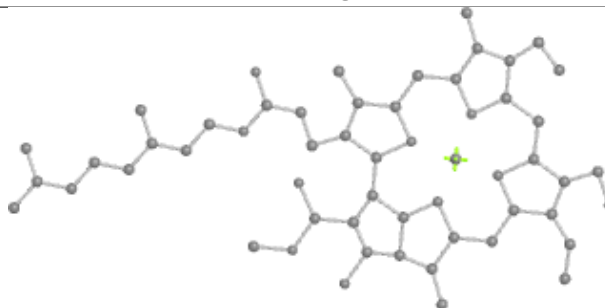
Bond lengths



Bond angles

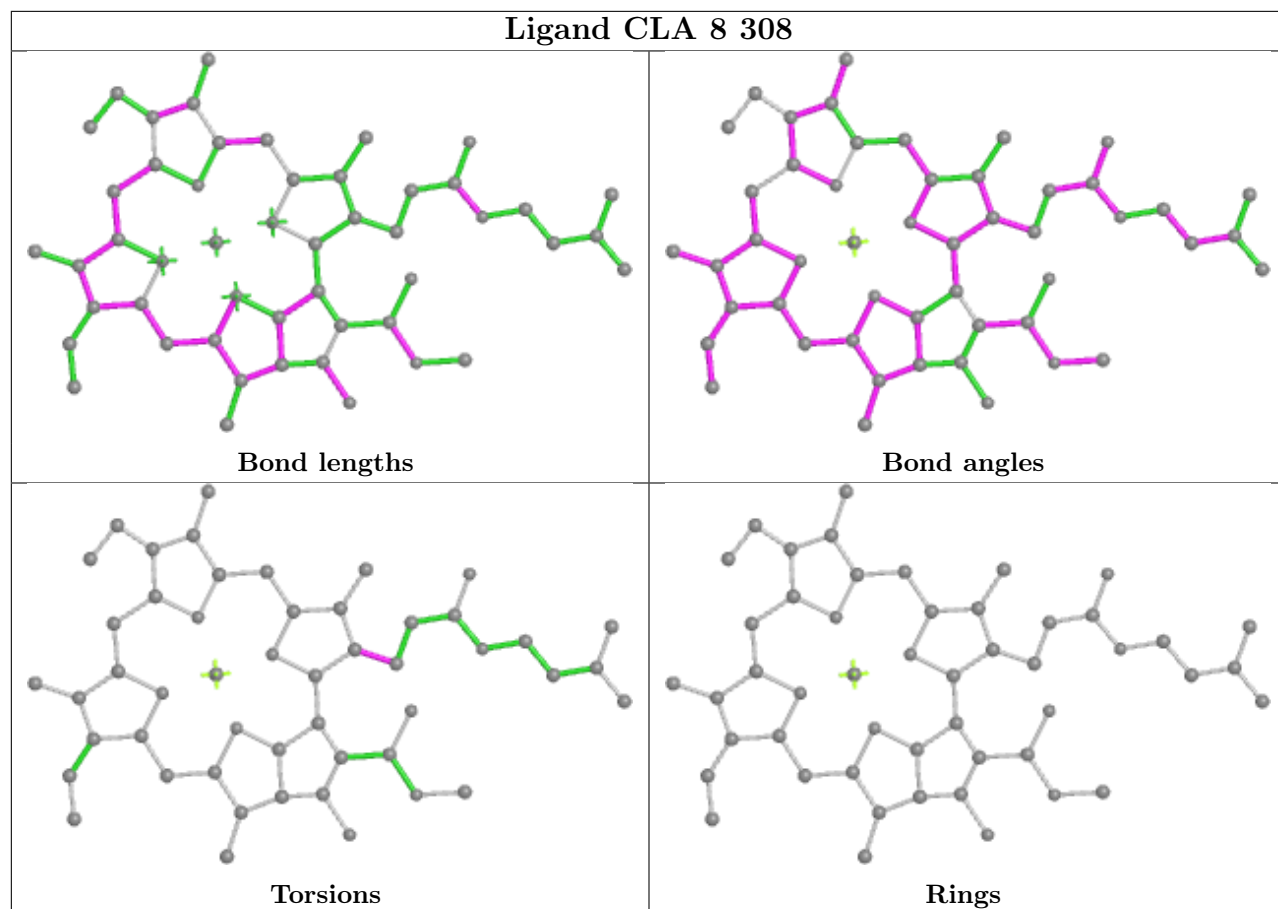


Torsions



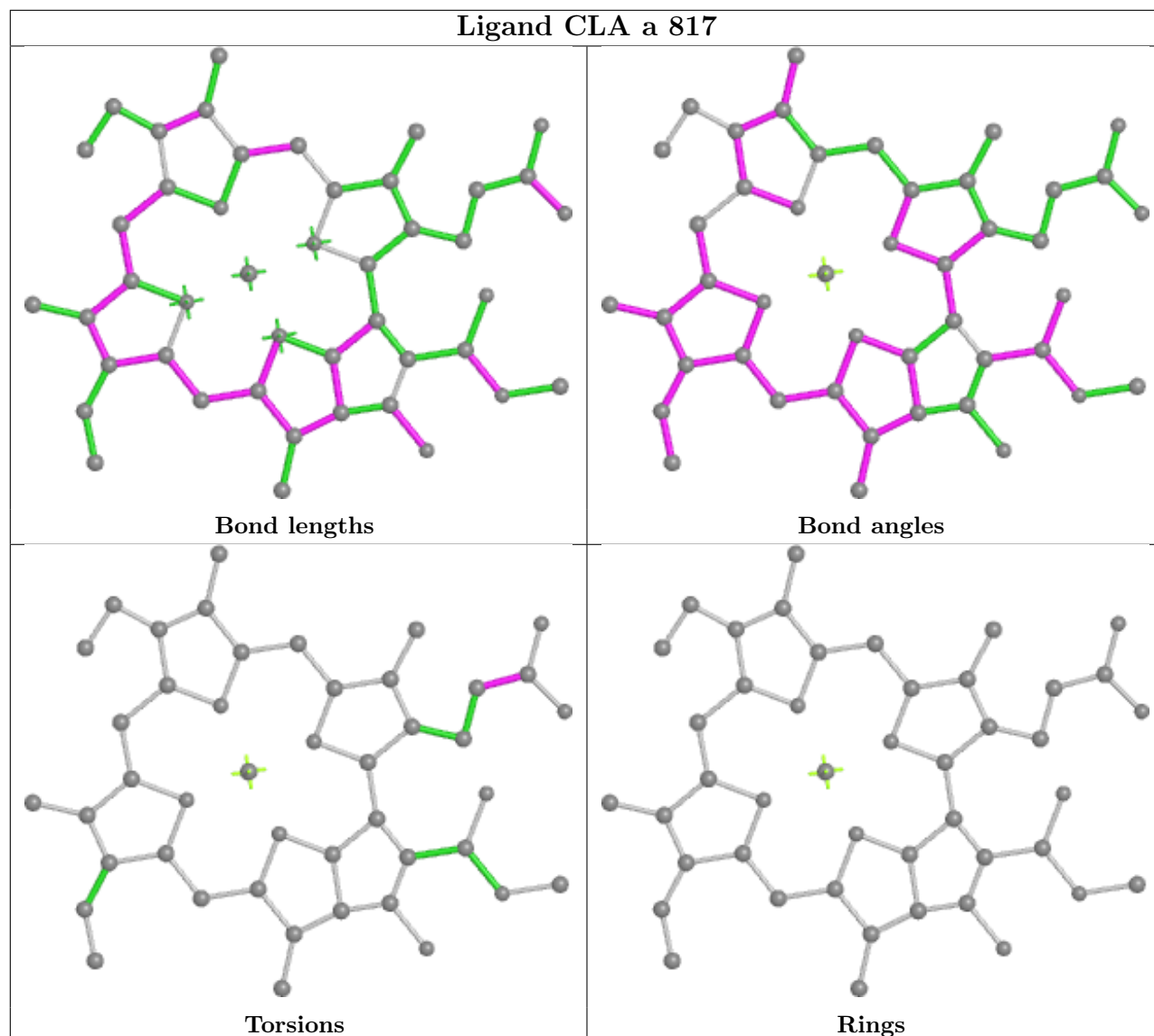
Rings

## Ligand CLA 8 308

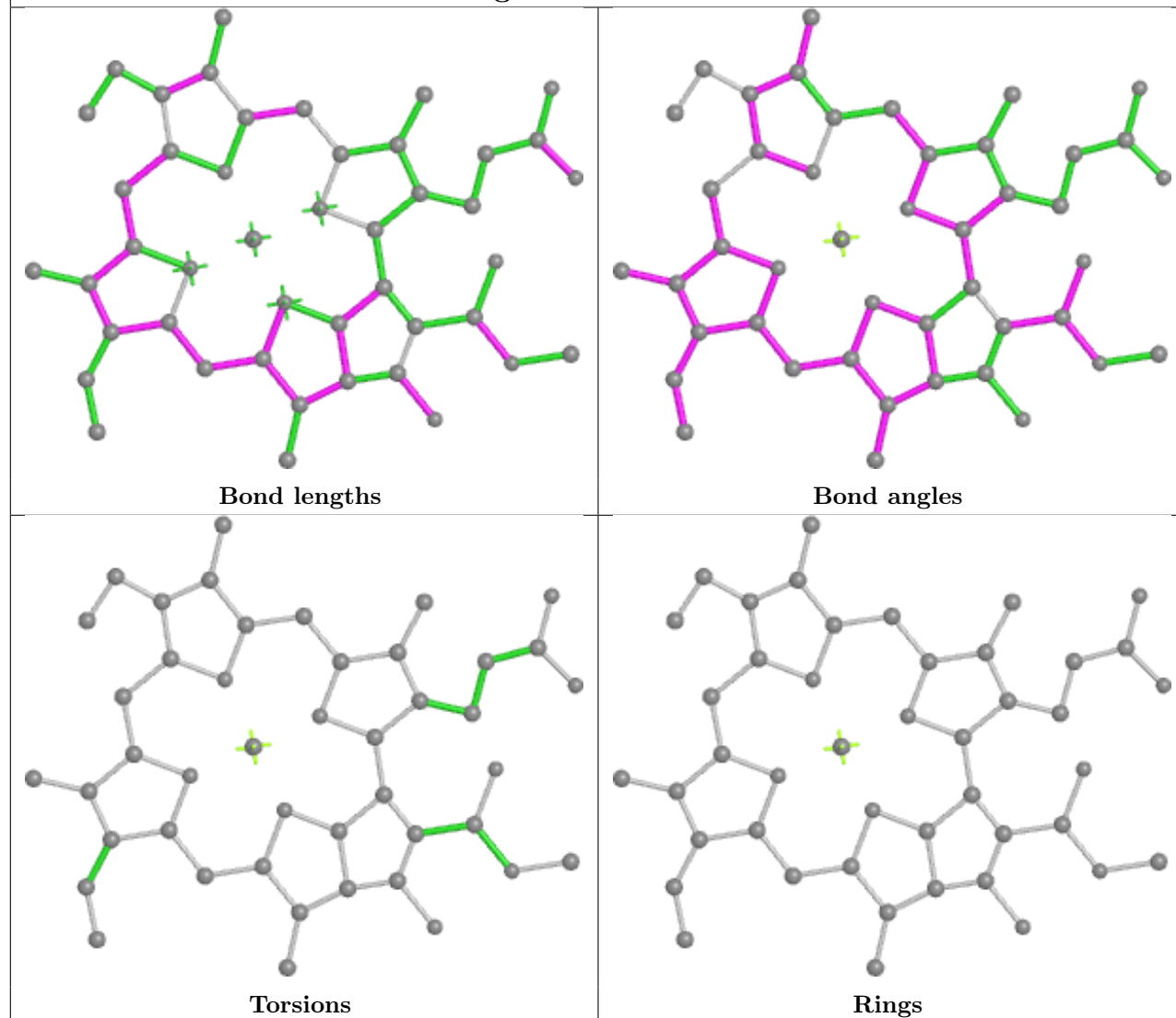




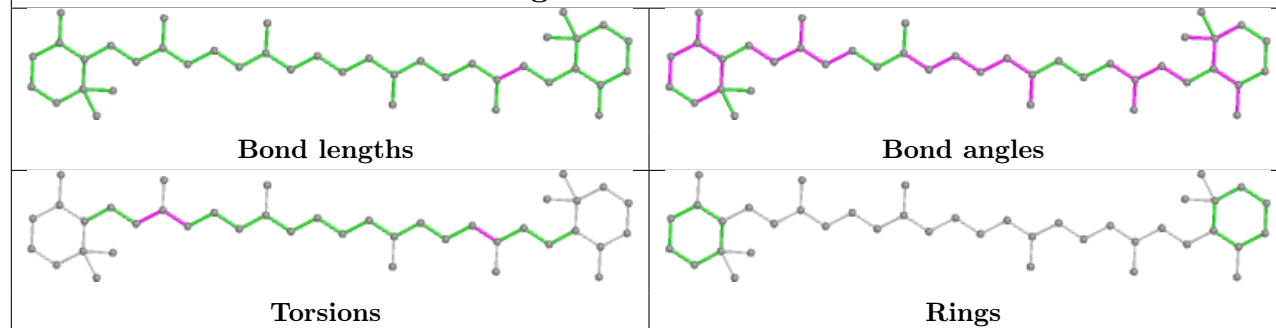
## Ligand CLA a 817

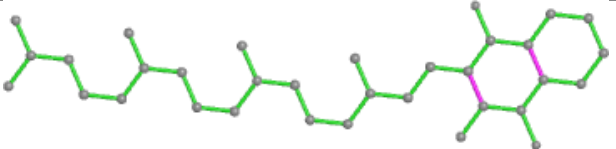
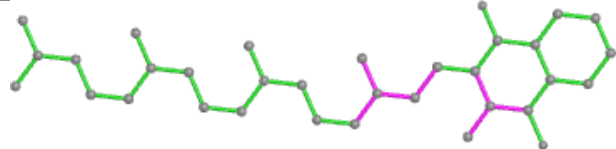
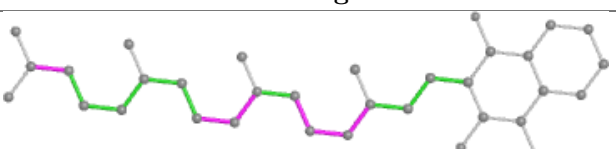
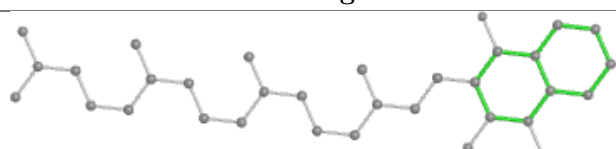


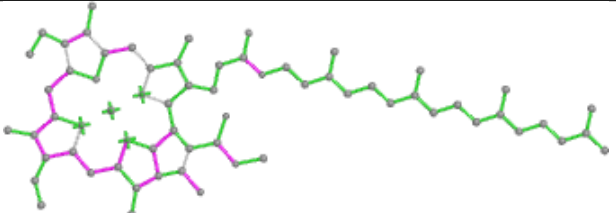
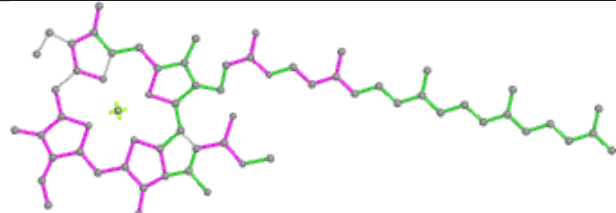
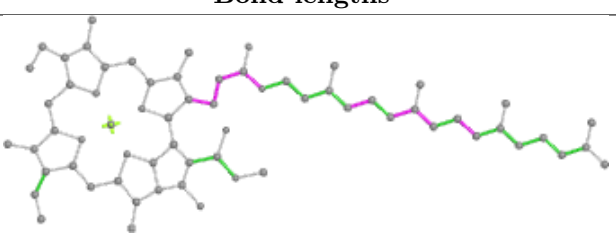
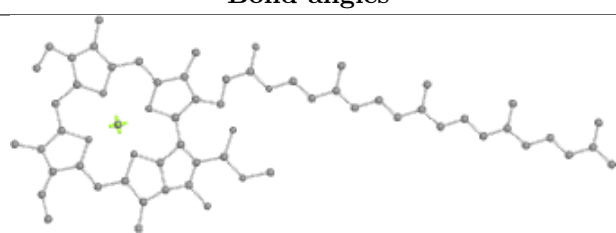
## Ligand CLA 9 613

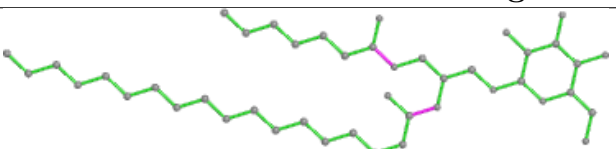
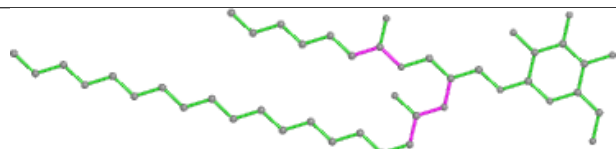
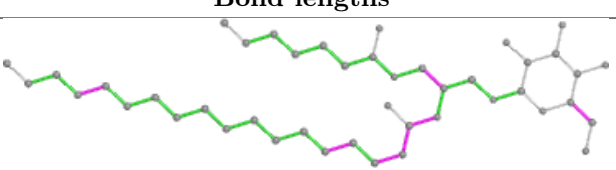
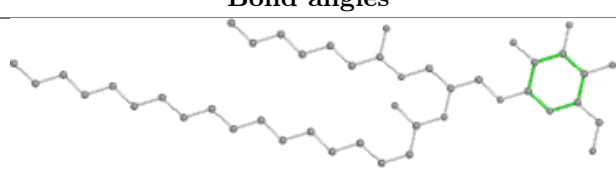


## Ligand BCR B 845

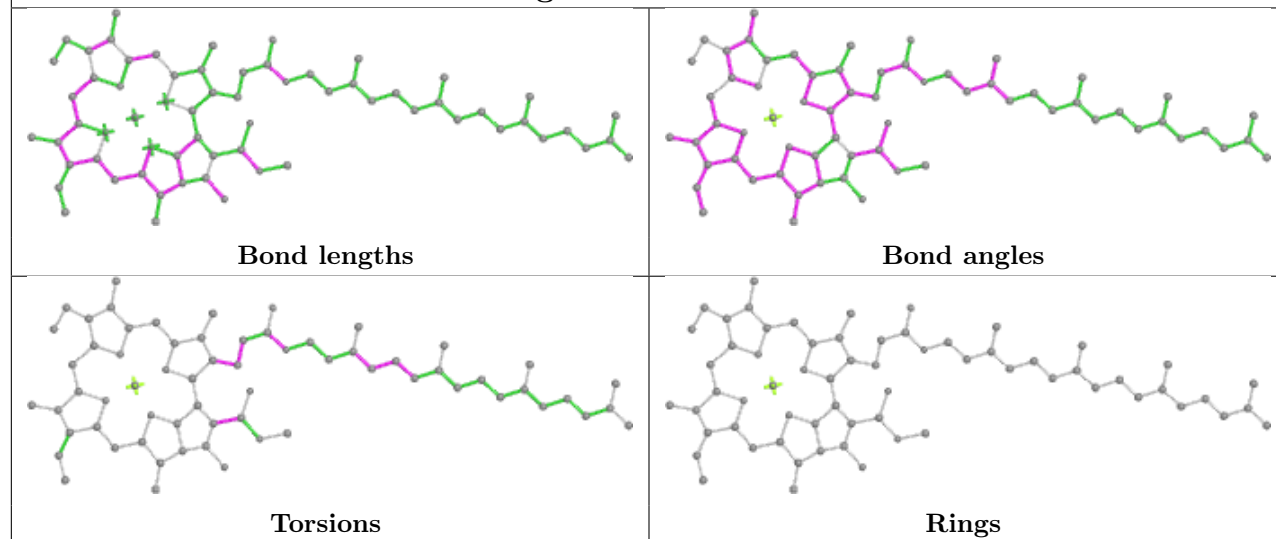


Ligand PQN A 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

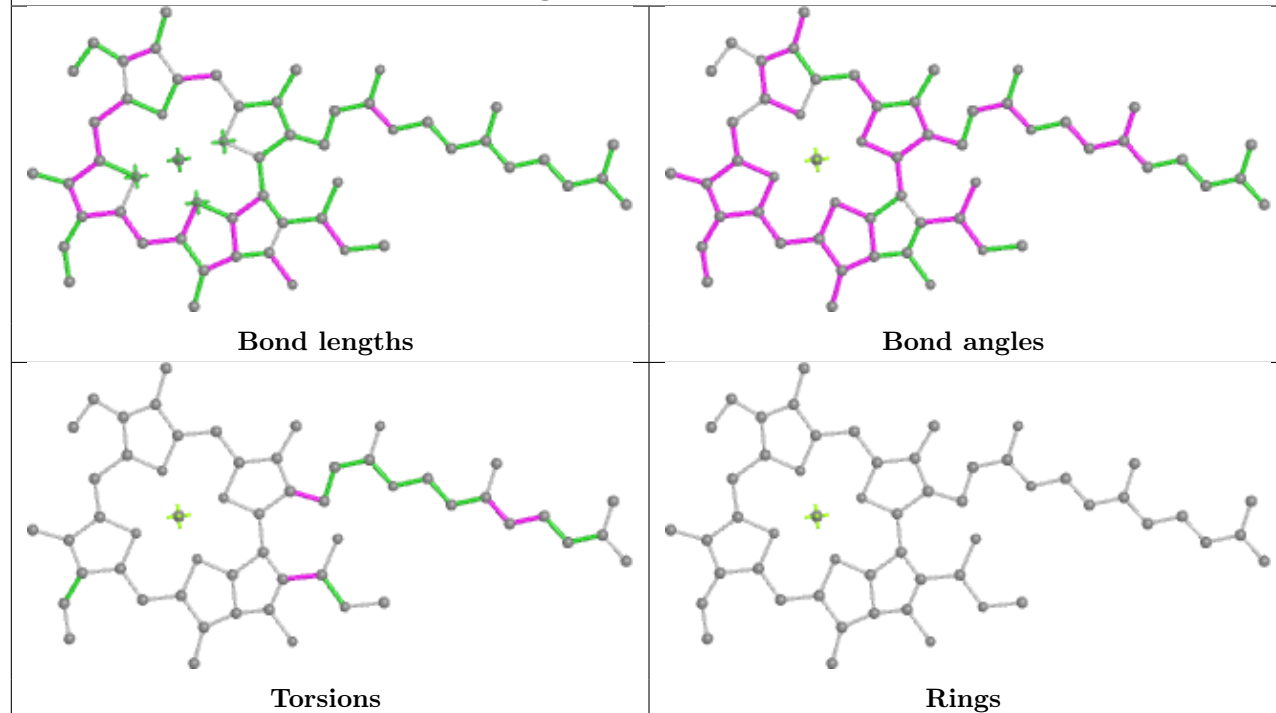
Ligand CLA A 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG 4 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

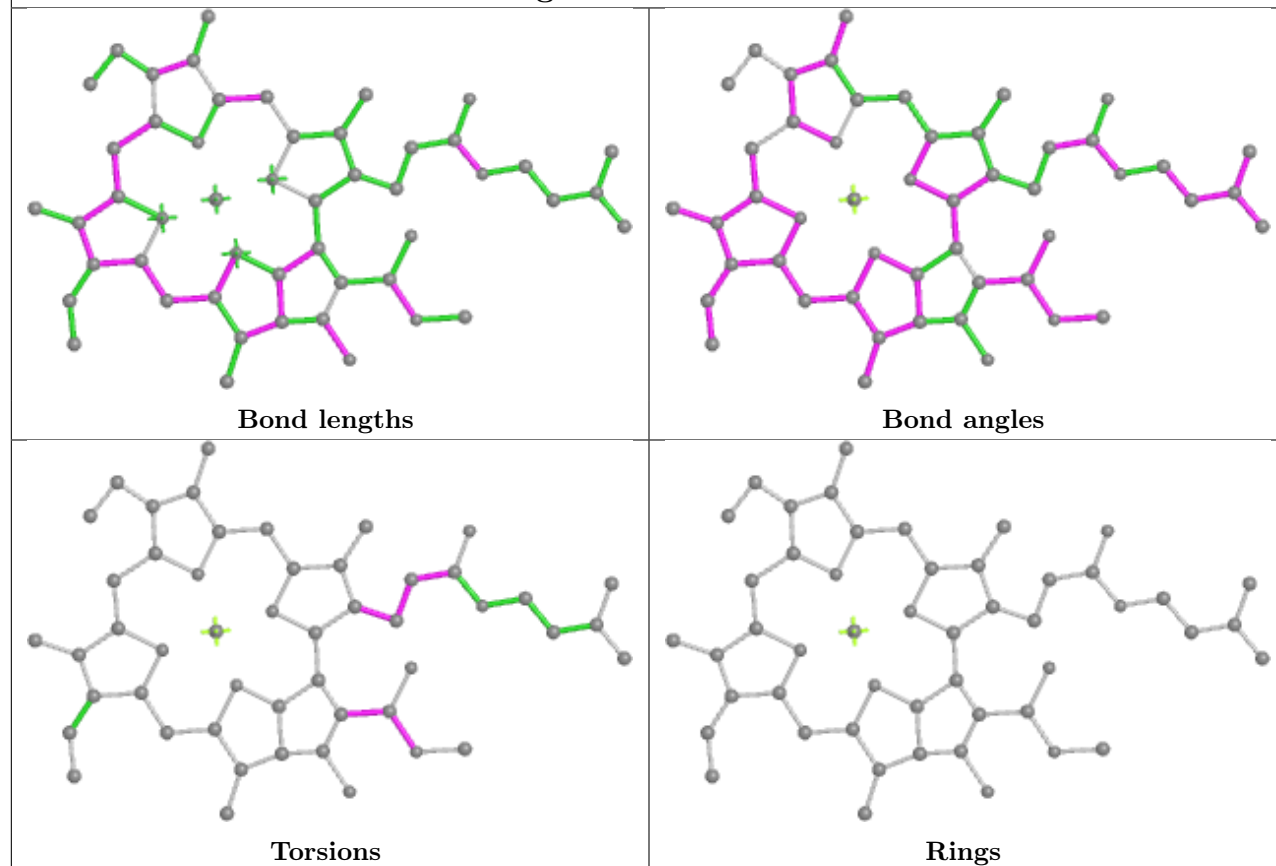
## Ligand CLA a 834



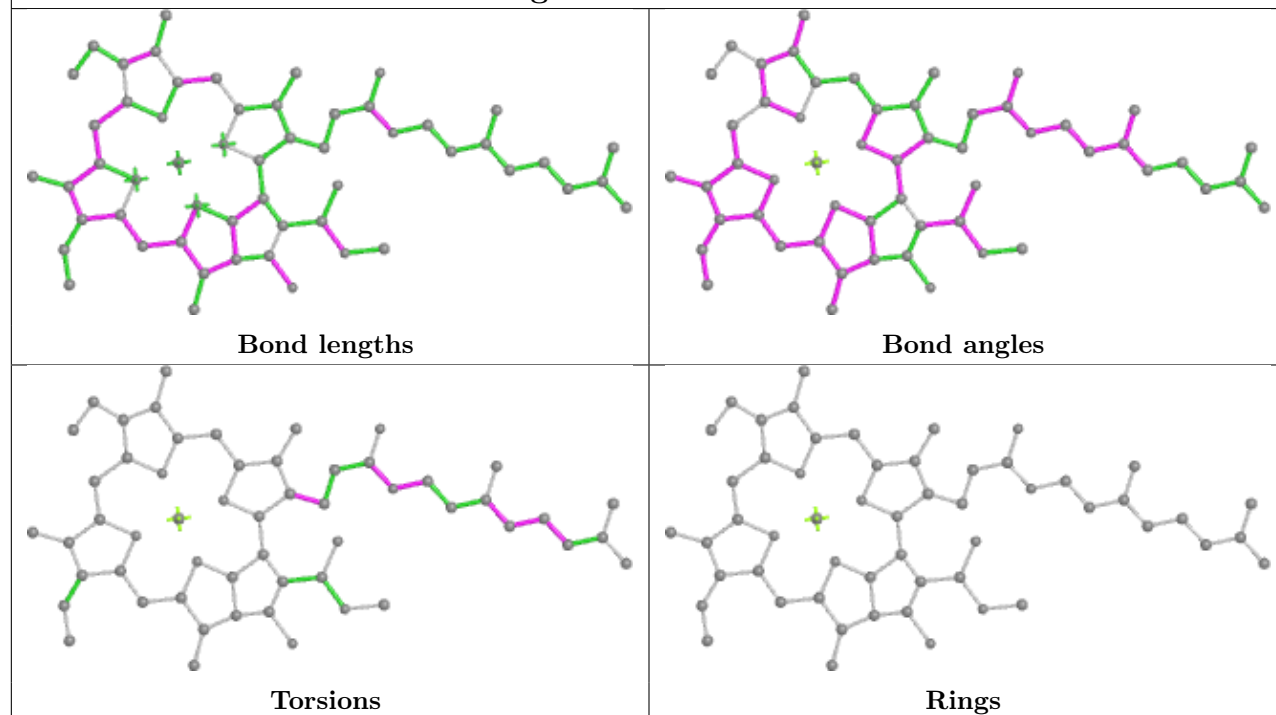
## Ligand CLA 4 610



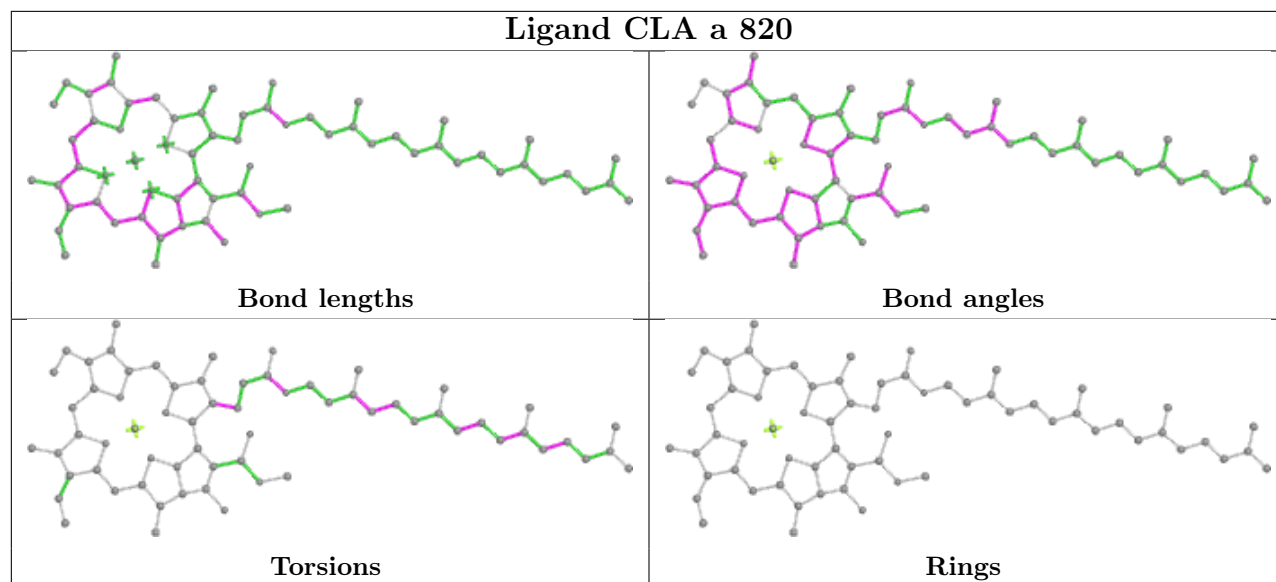
## Ligand CLA a 816



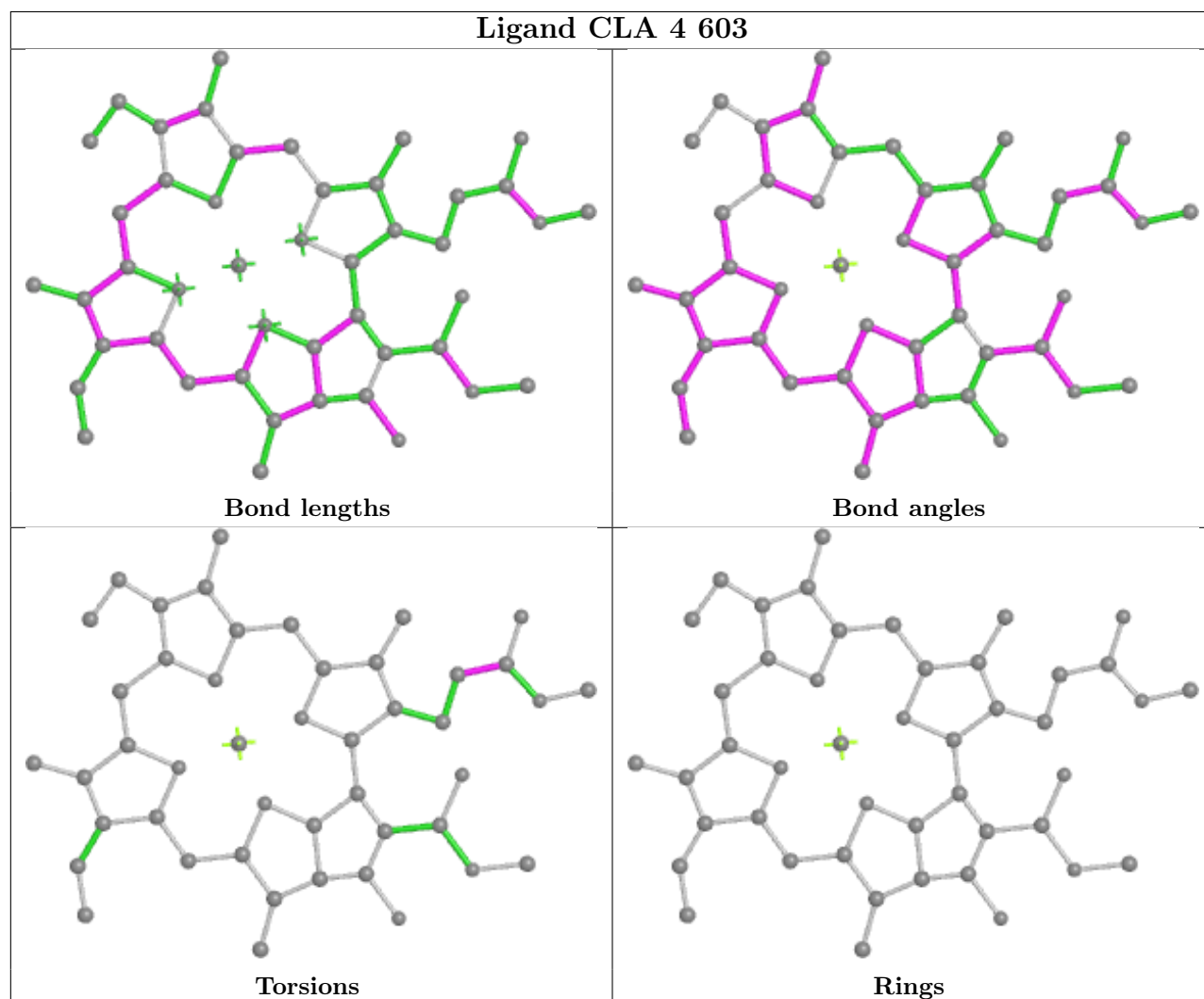
## Ligand CLA f 7003



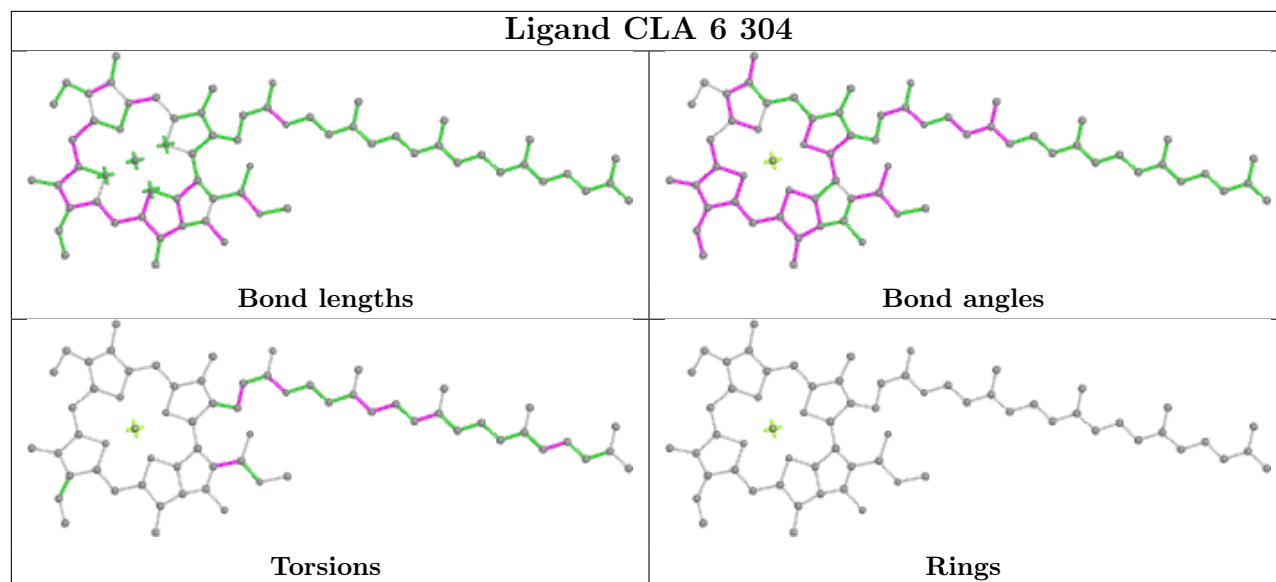
## Ligand CLA a 820



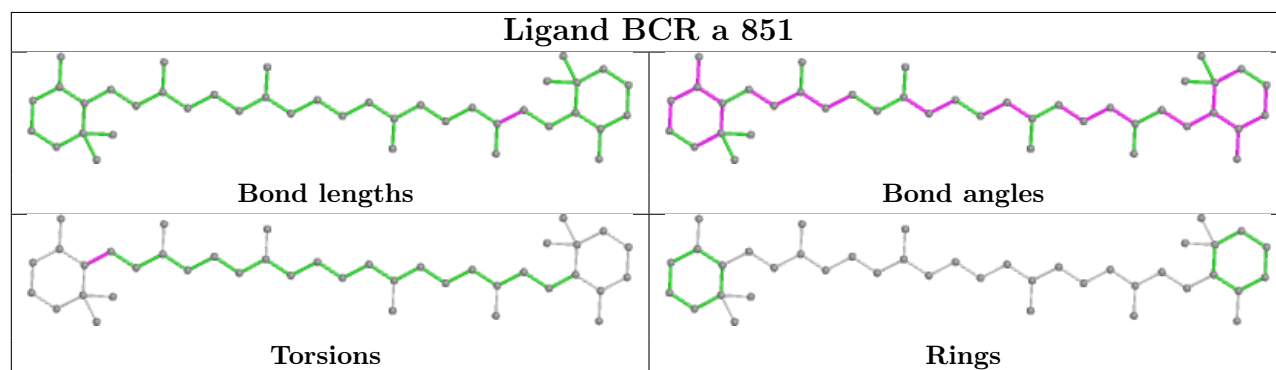
## Ligand CLA 4 603



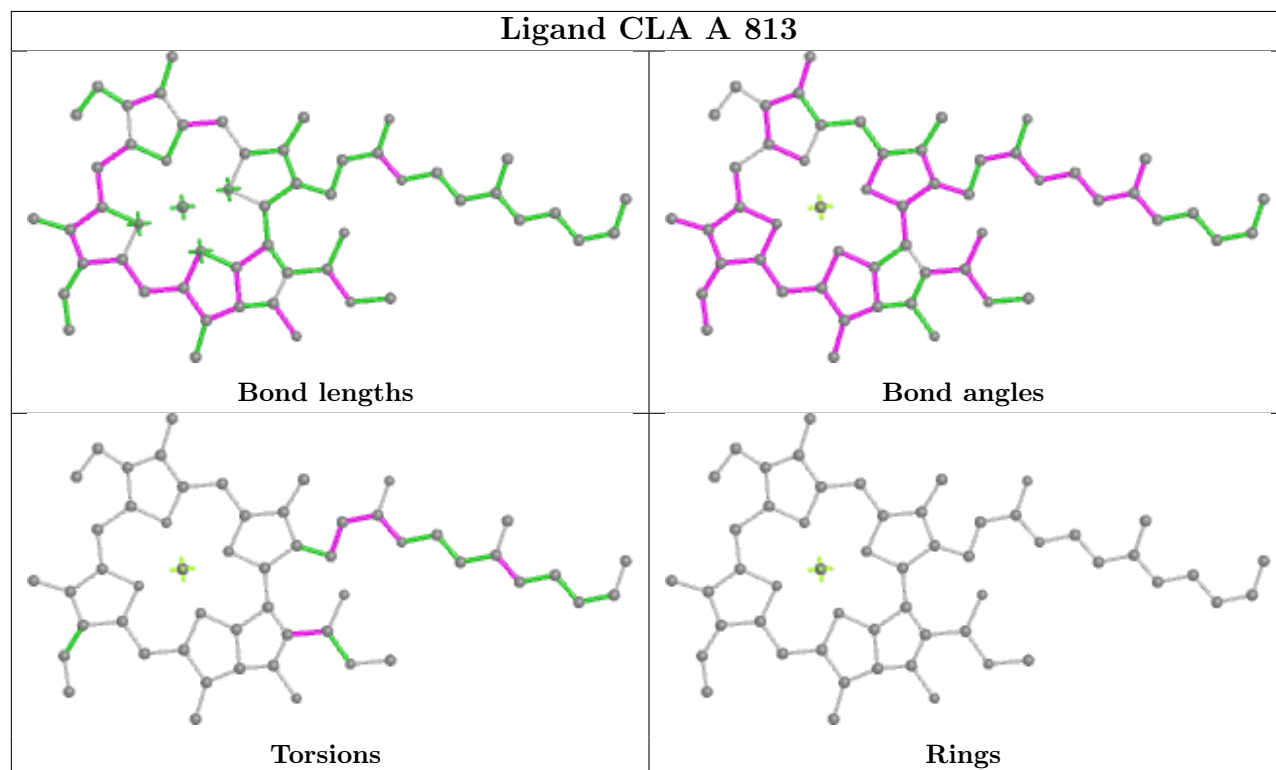
## Ligand CLA 6 304

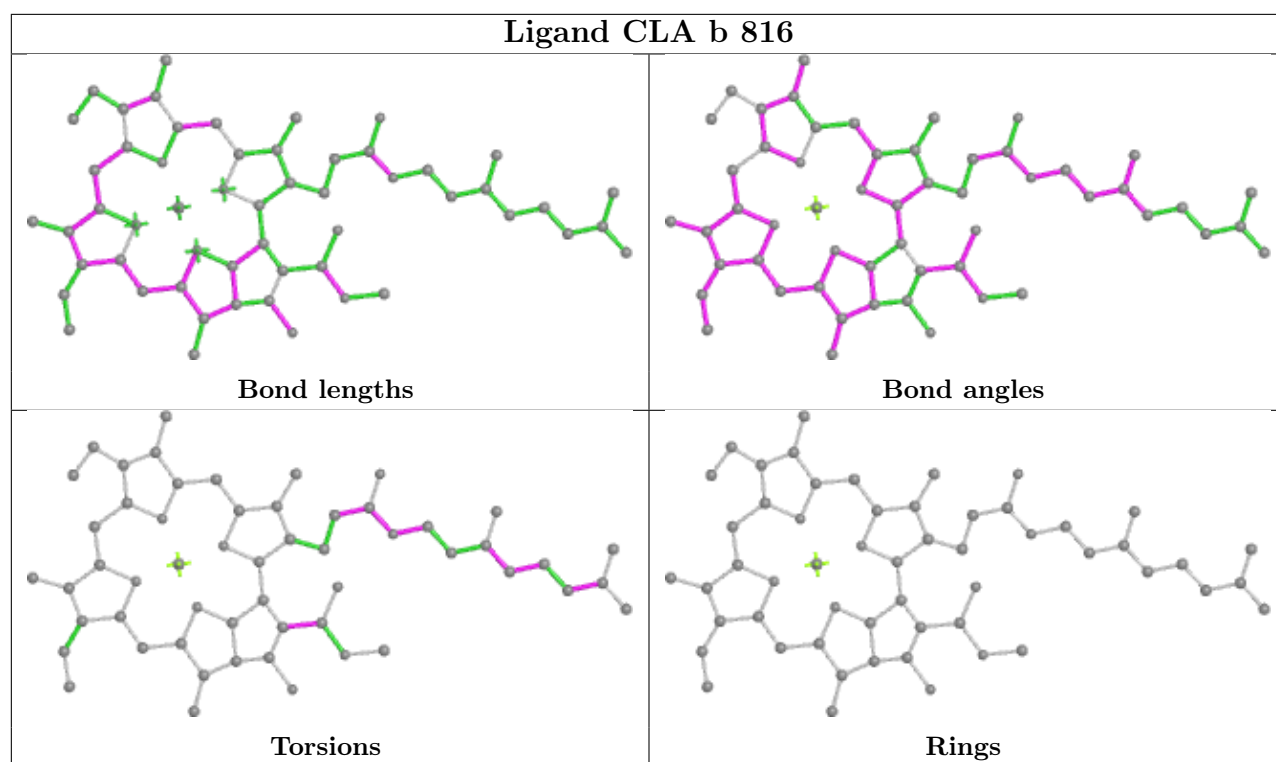


## Ligand BCR a 851



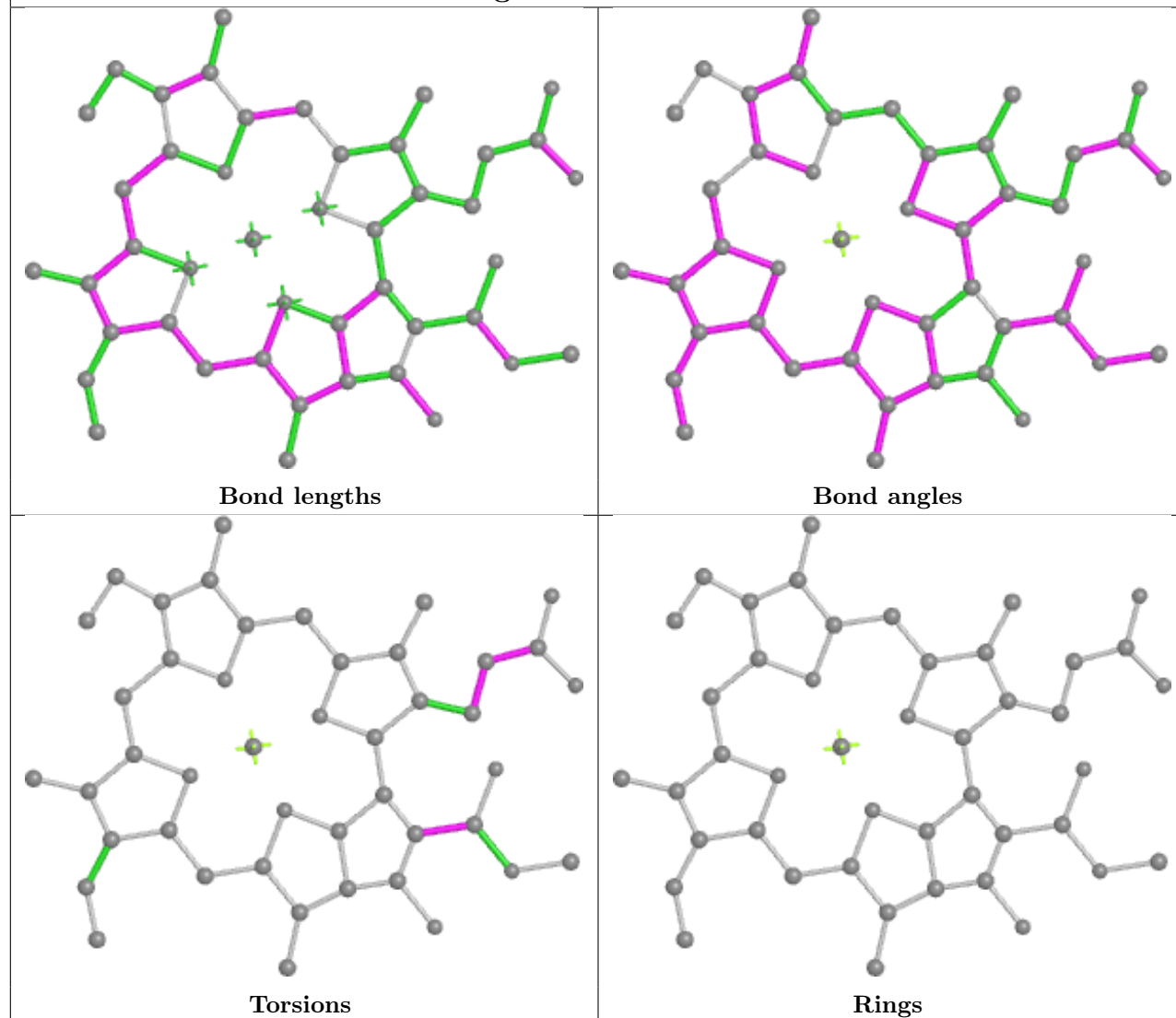
## Ligand CLA A 813



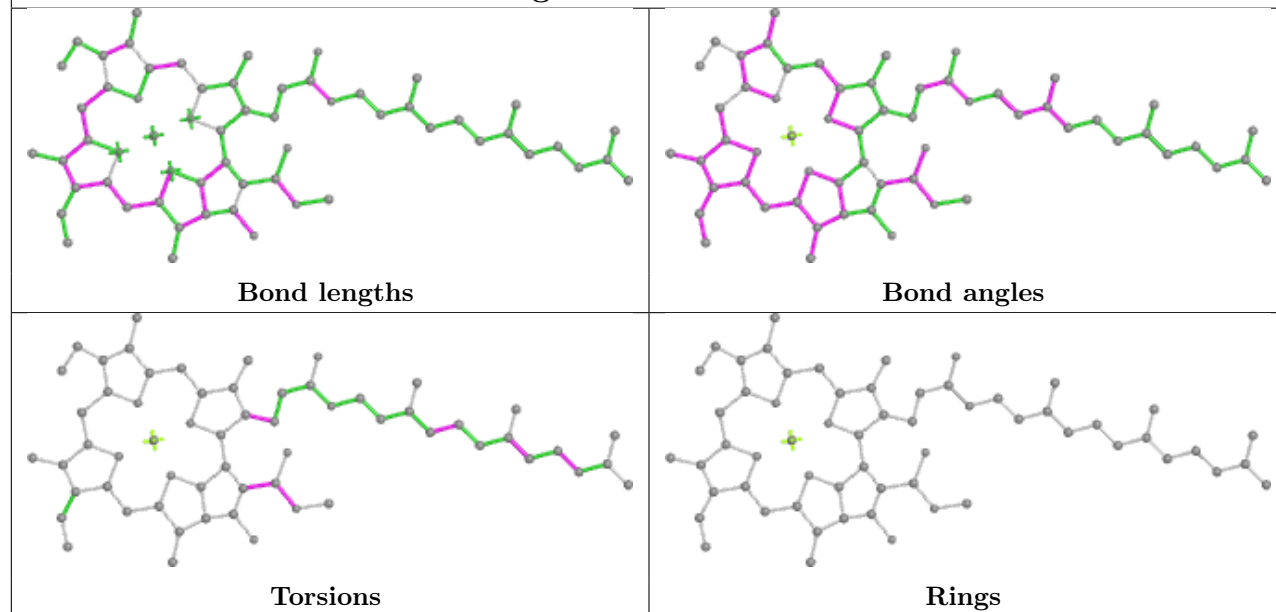




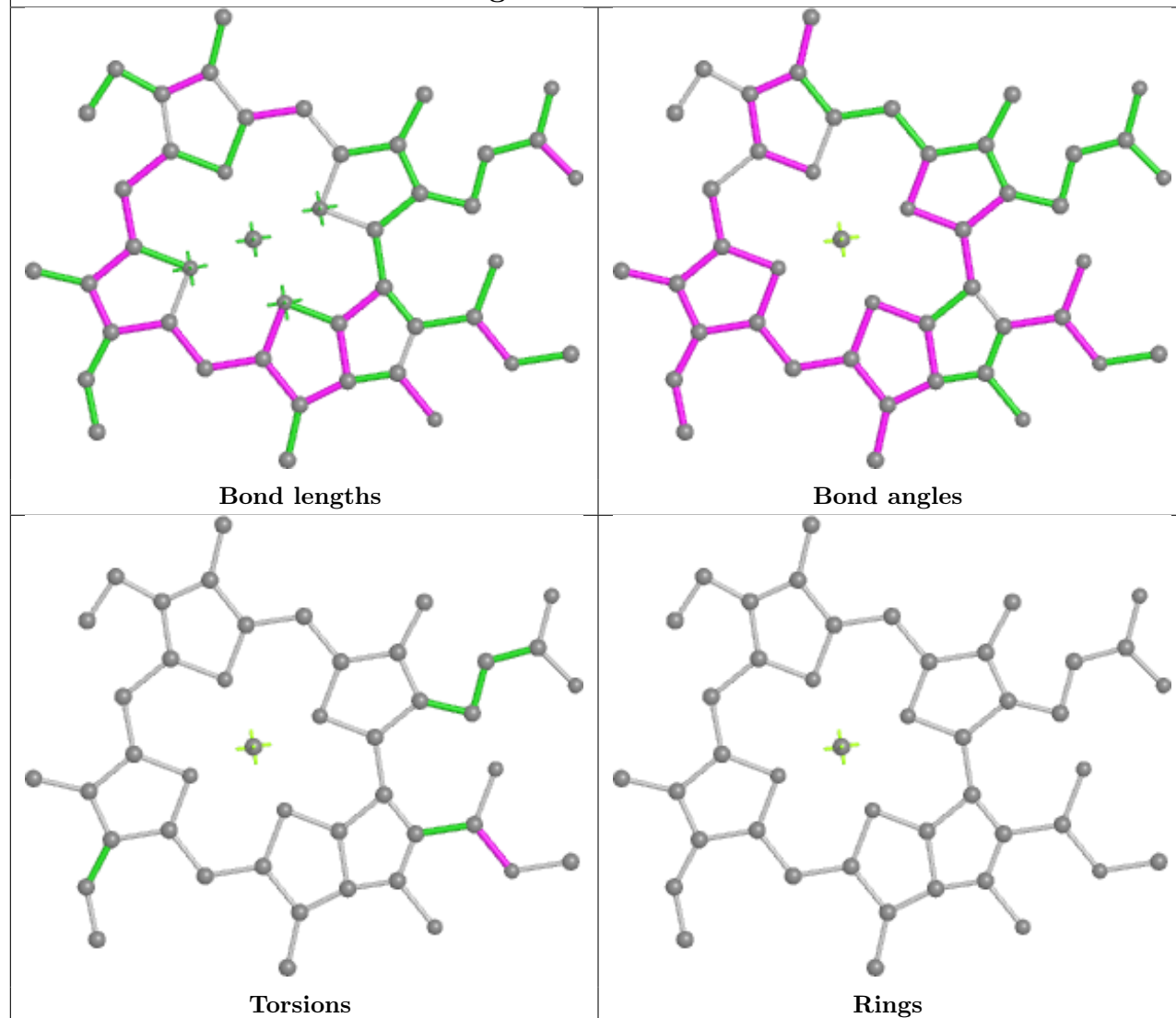
## Ligand CLA a 837



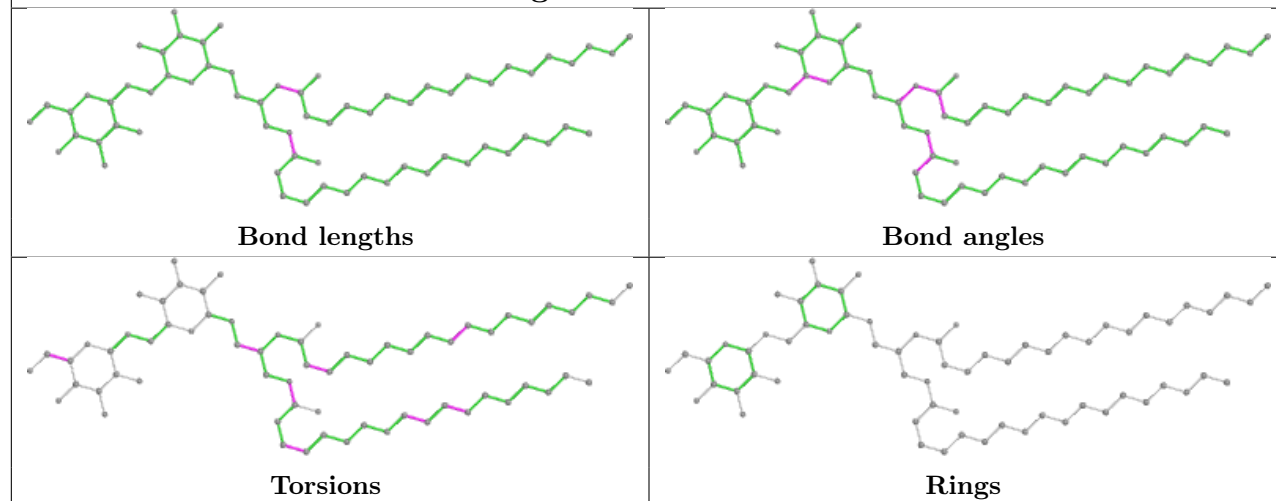
## Ligand CLA B 815



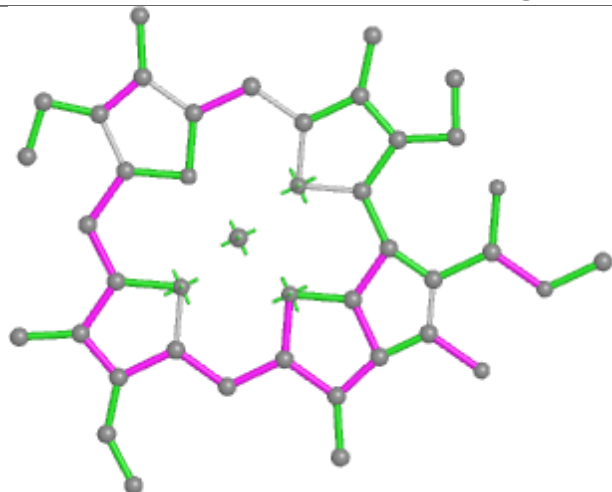
## Ligand CLA G 101



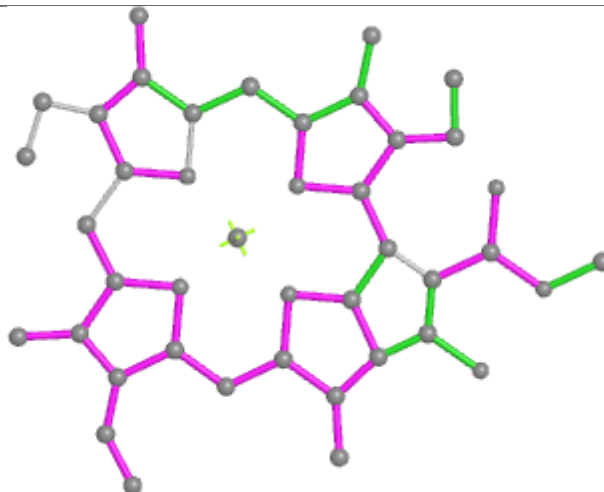
## Ligand DGD b 849



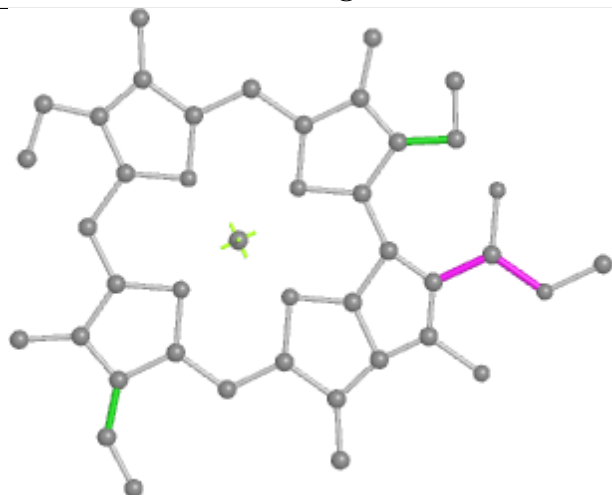
## Ligand CLA 6 307



Bond lengths



Bond angles

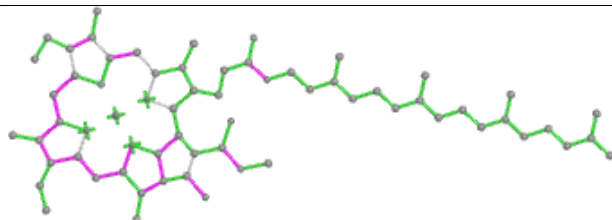


Torsions

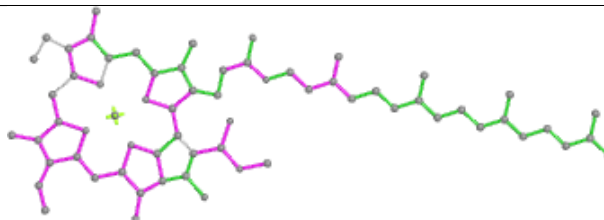


Rings

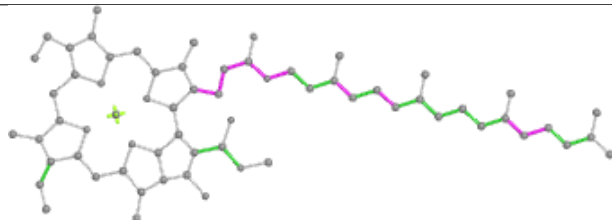
## Ligand CLA A 830



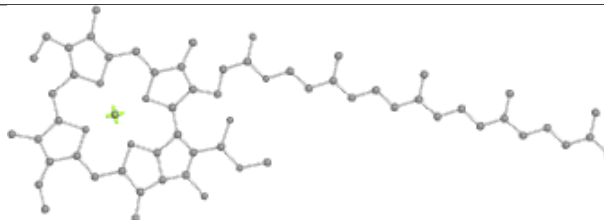
Bond lengths



Bond angles

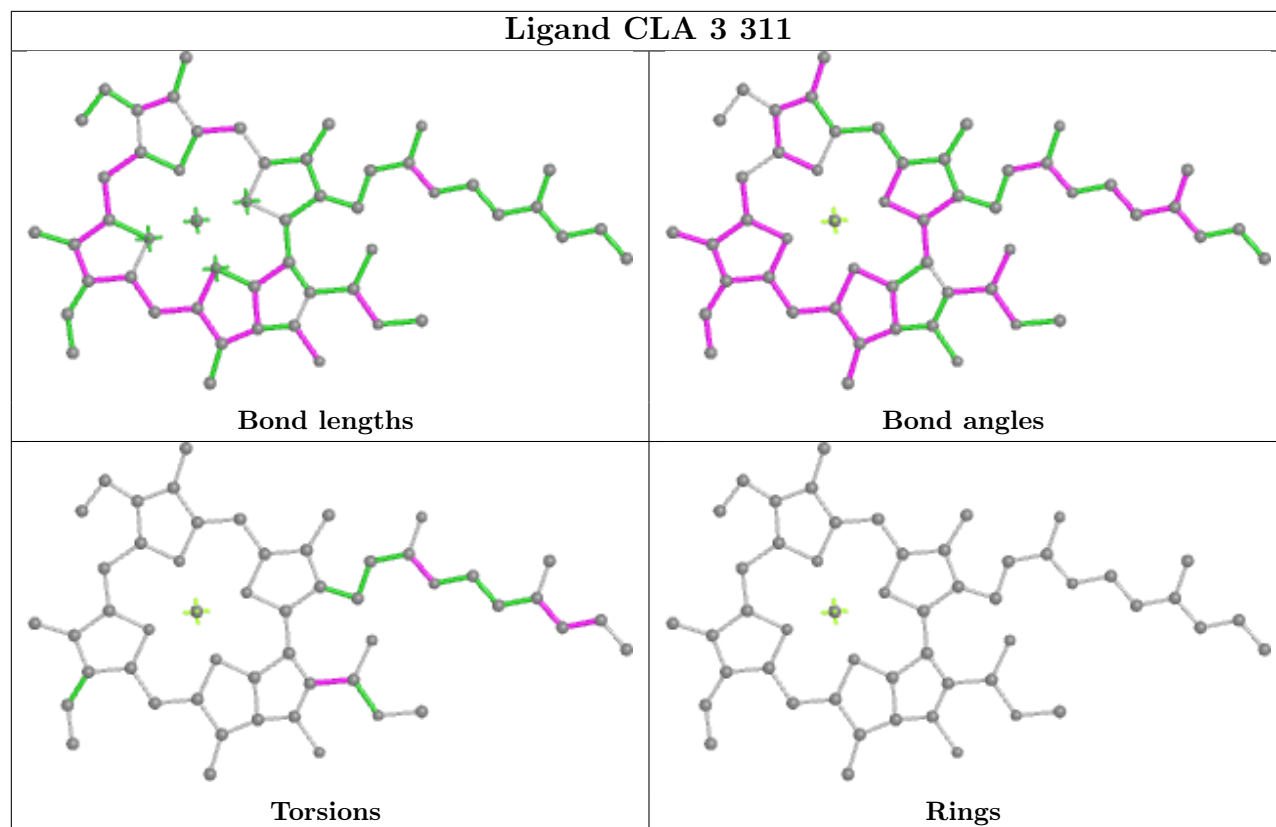


Torsions

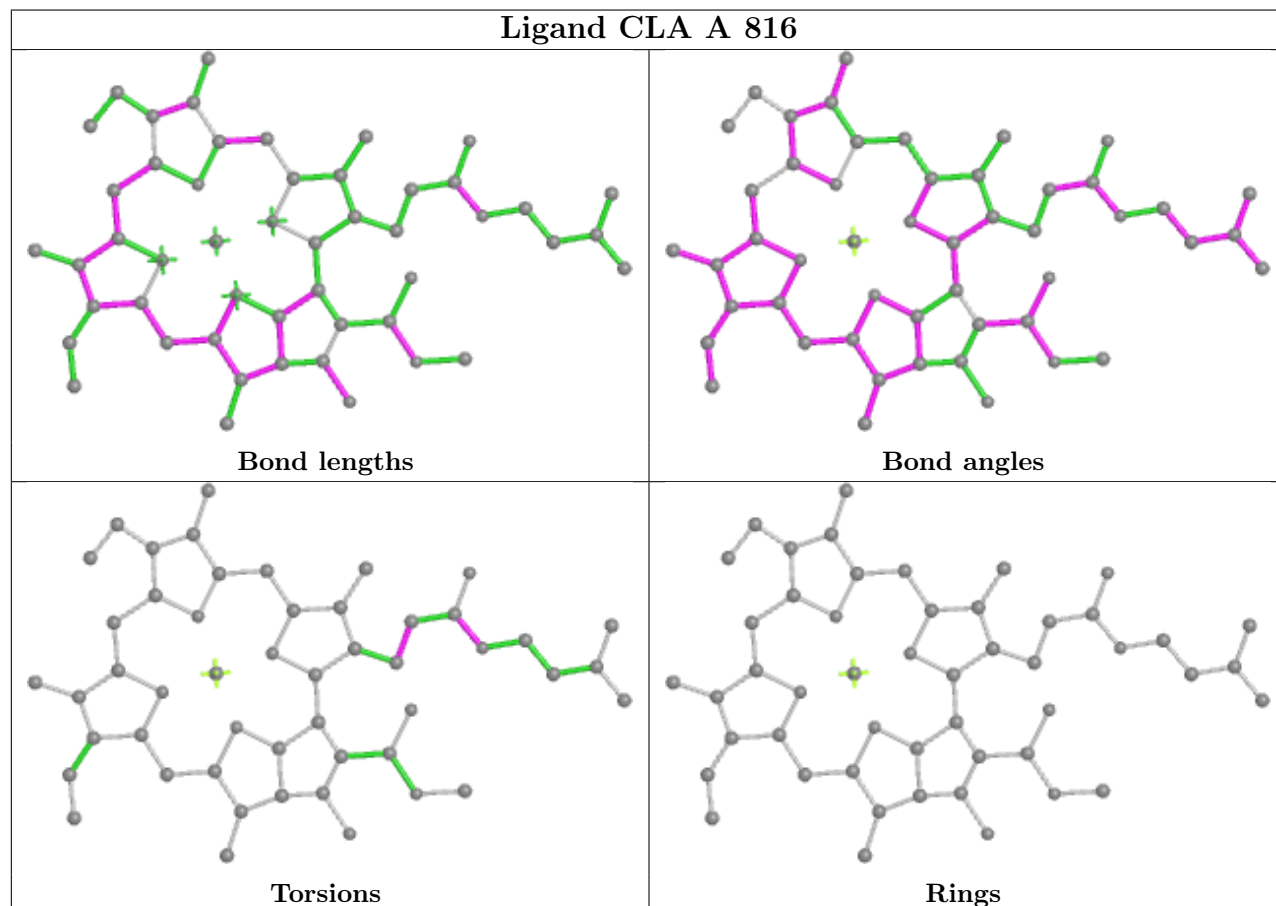


Rings

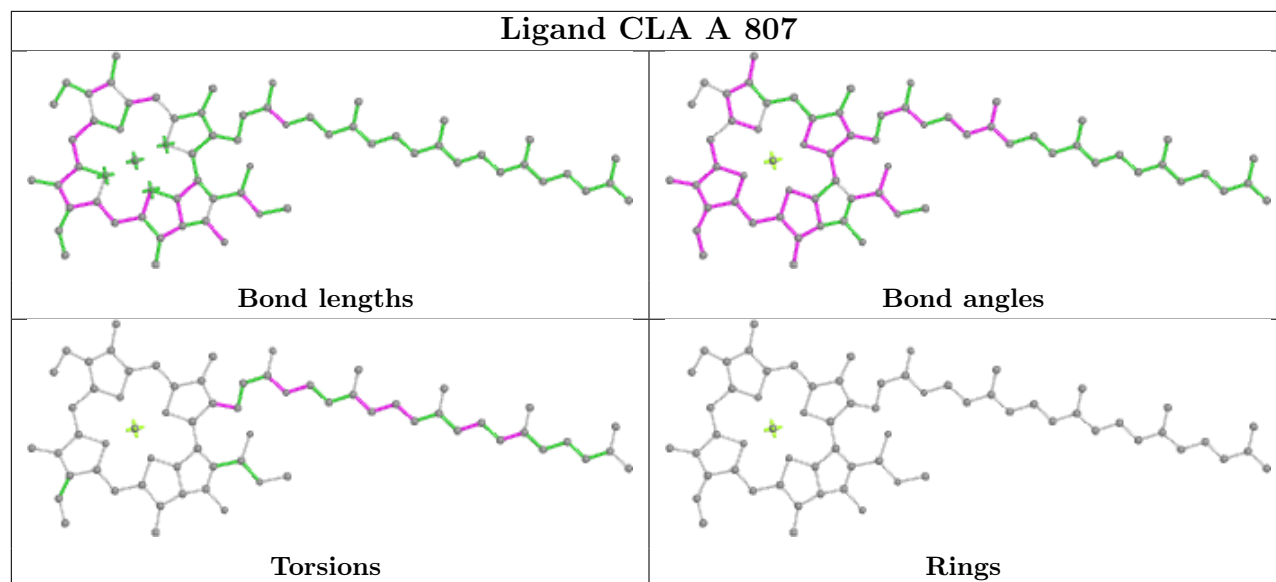
## Ligand CLA 3 311



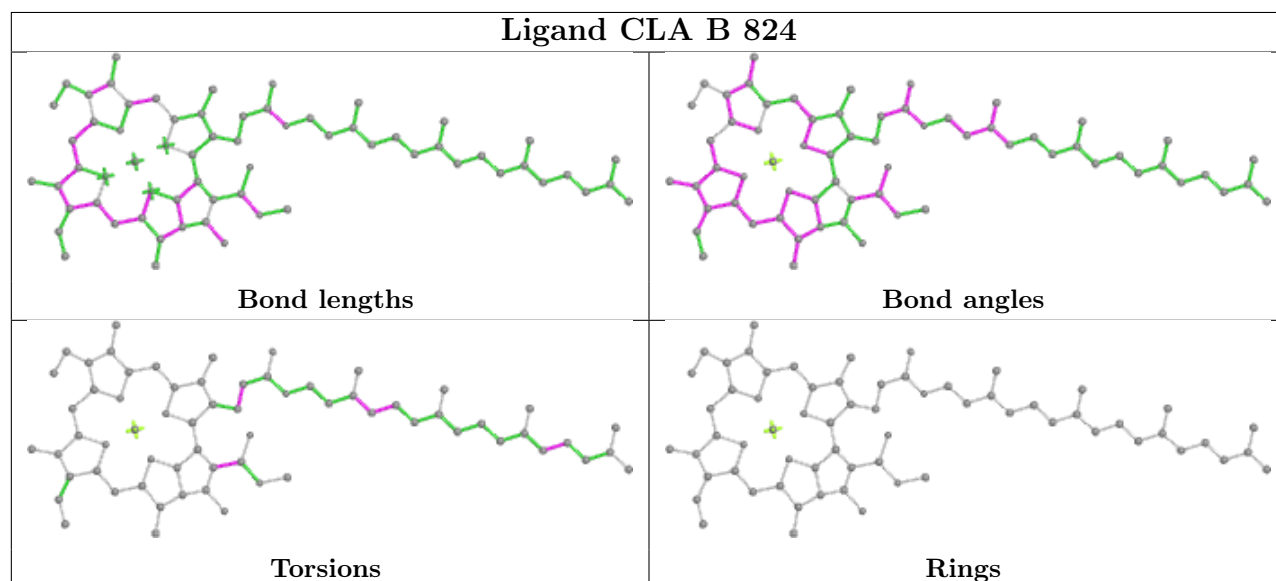
## Ligand CLA A 816



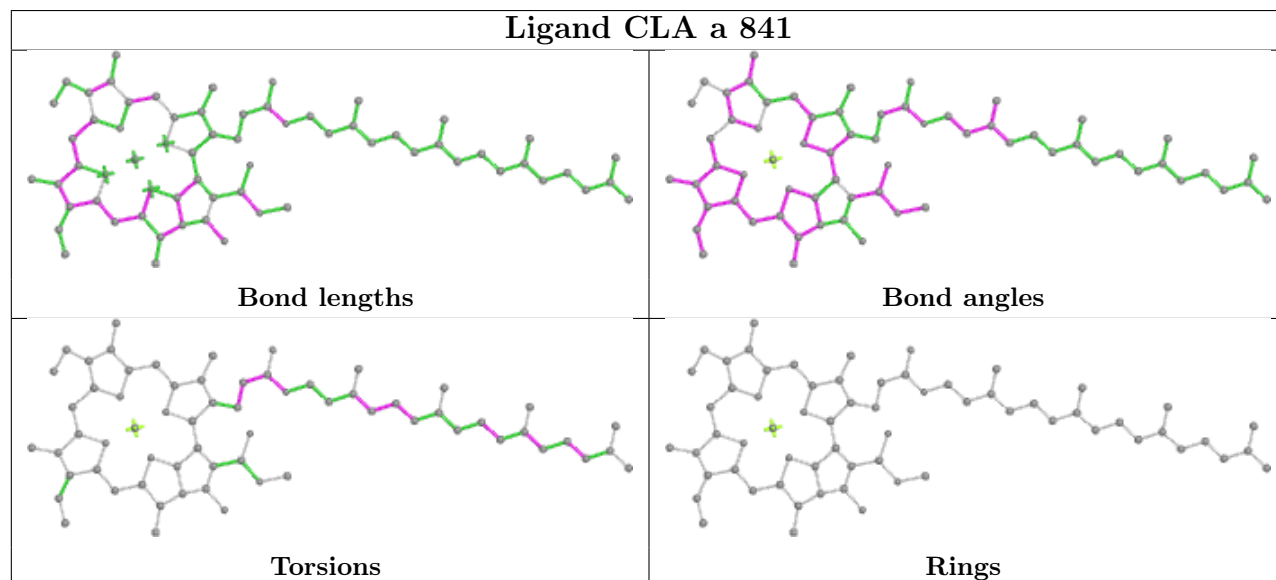
## Ligand CLA A 807



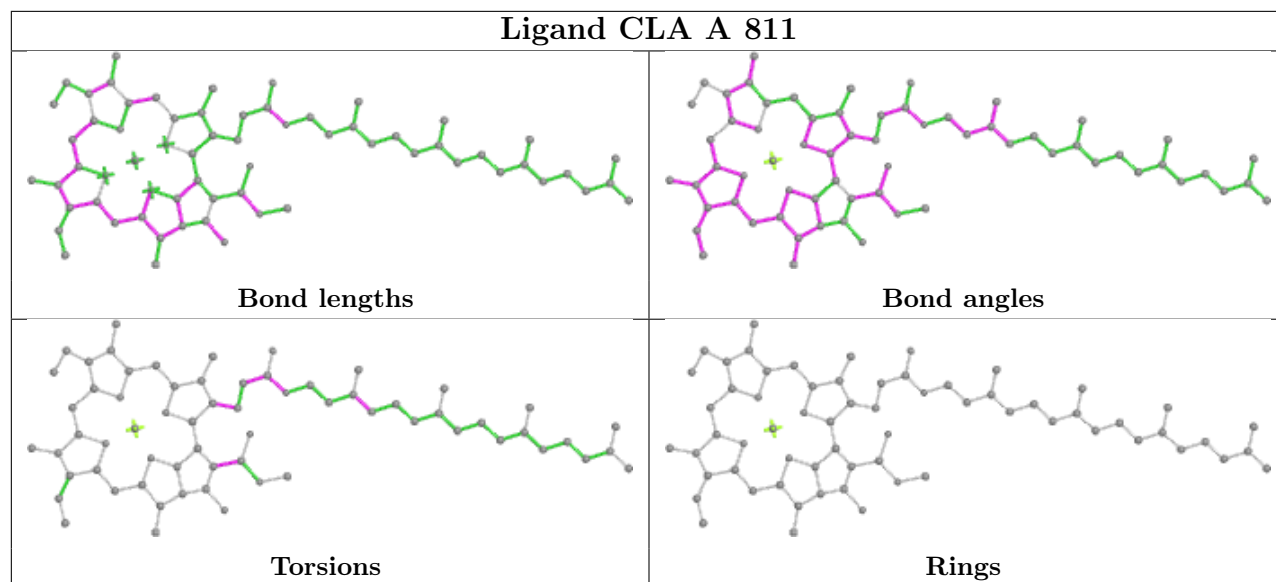
## Ligand CLA B 824



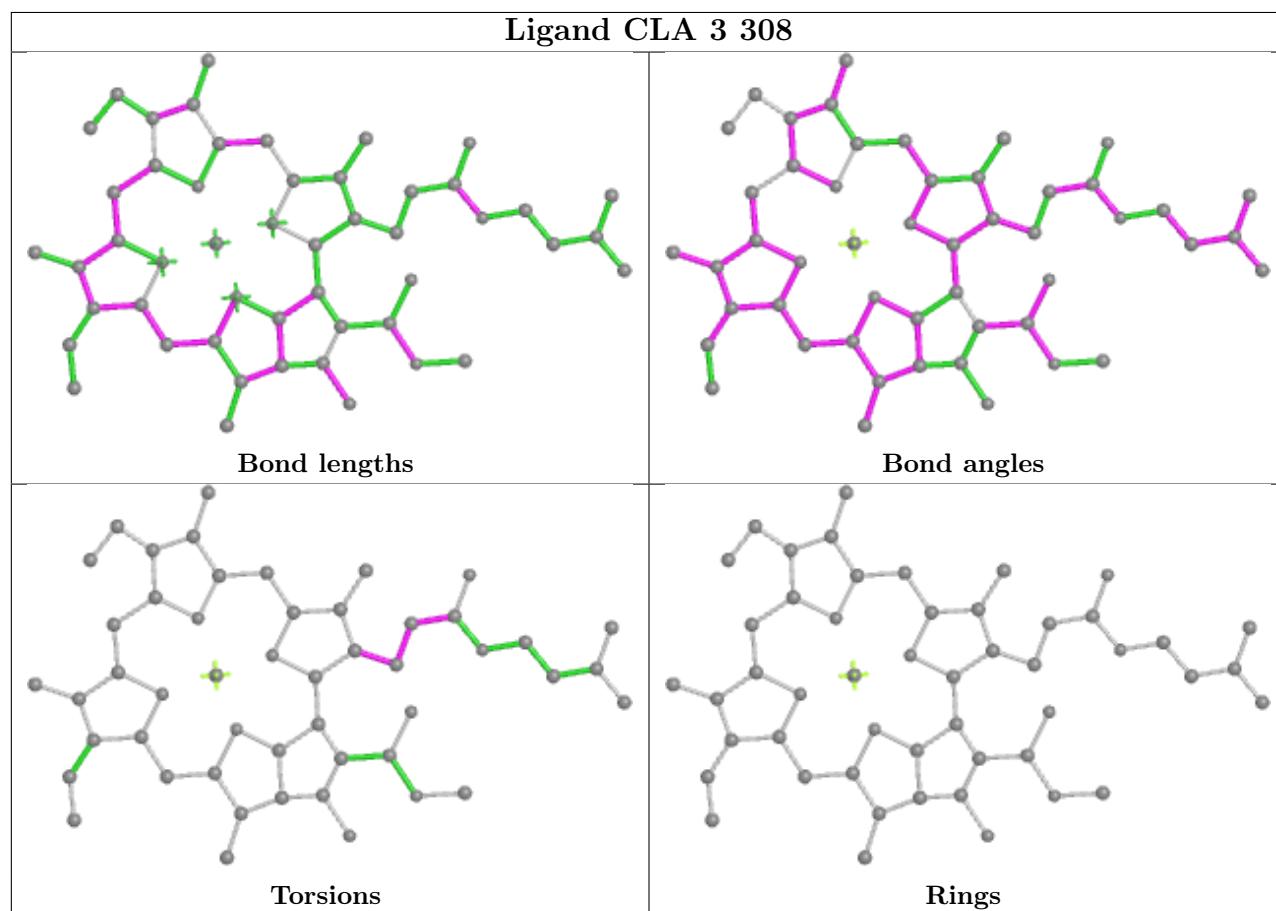
## Ligand CLA a 841

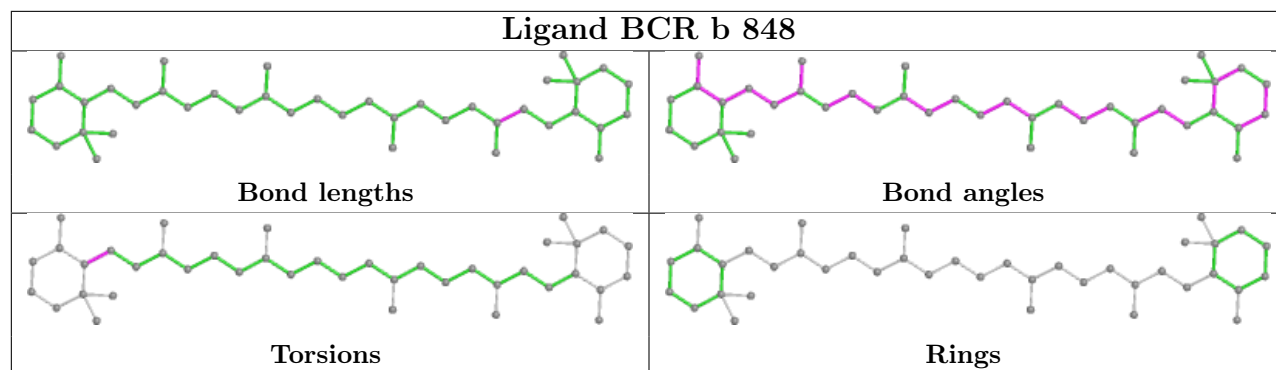
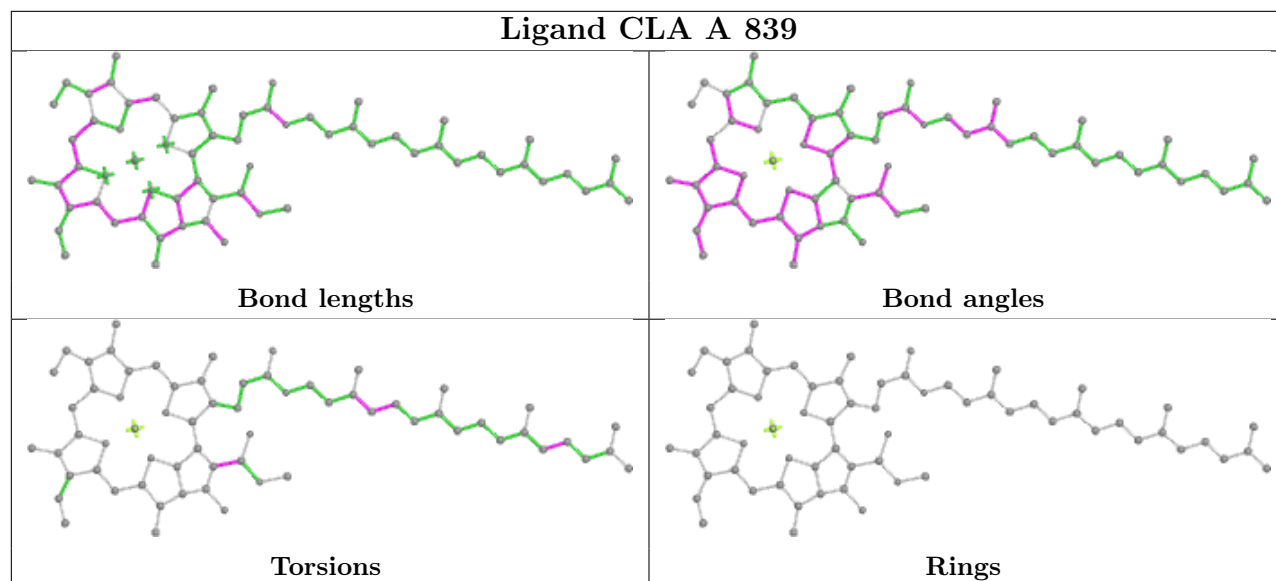
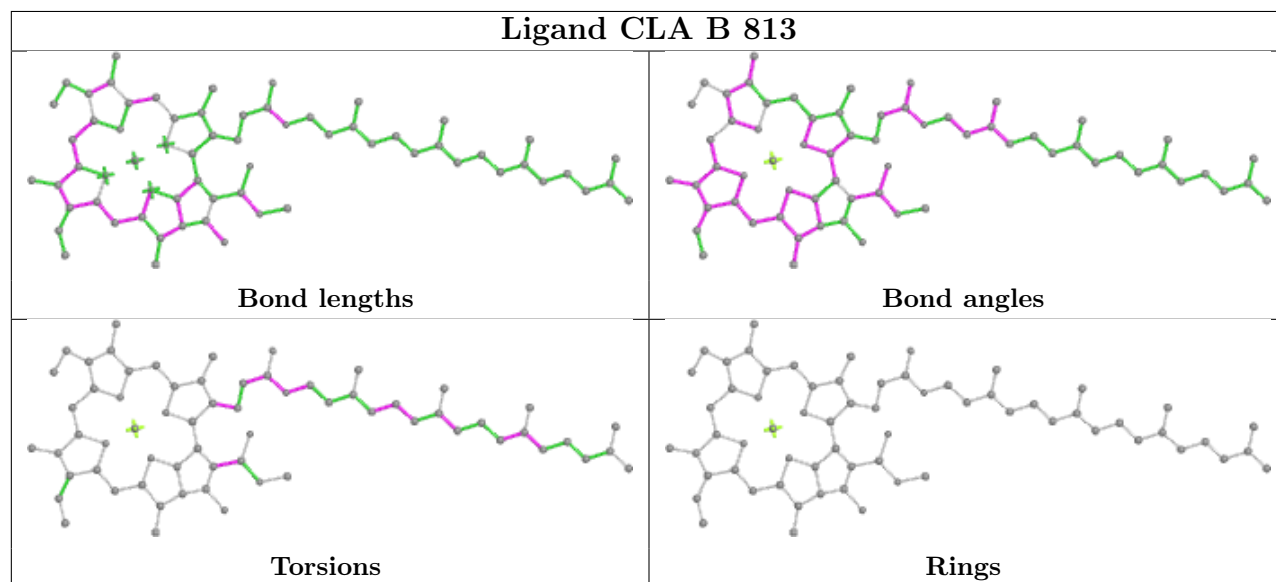


## Ligand CLA A 811

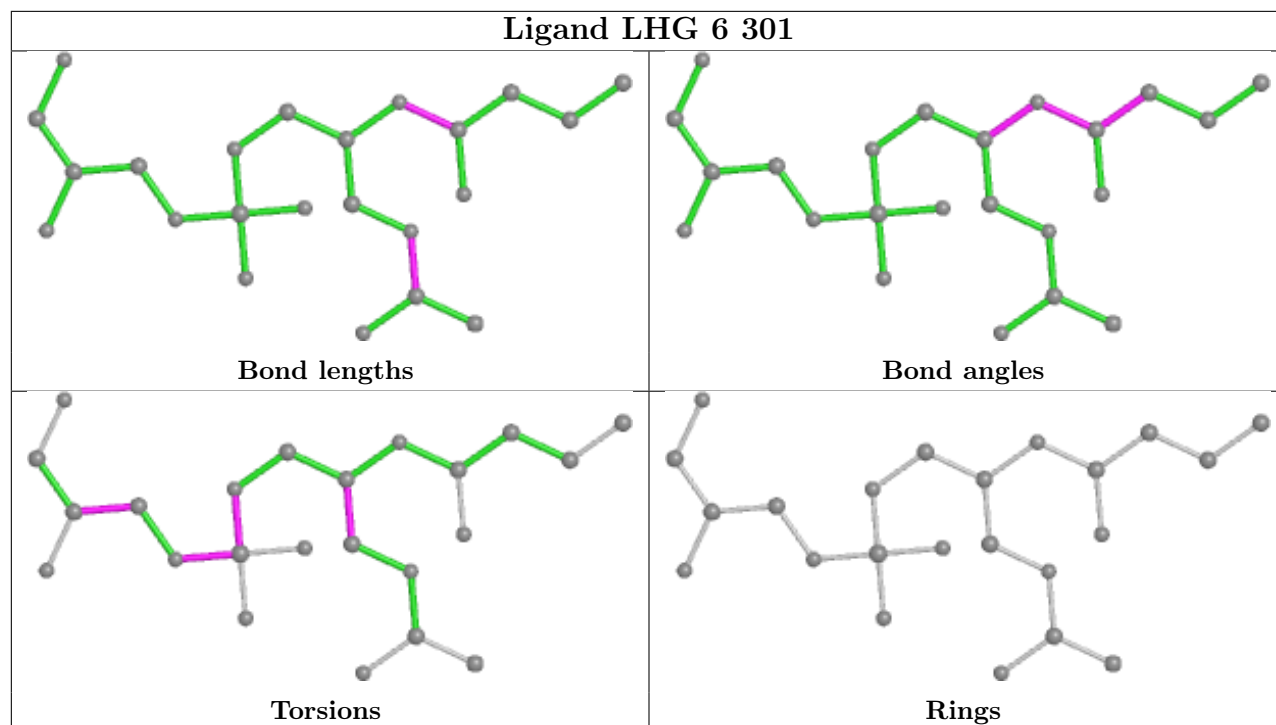


## Ligand CLA 3 308

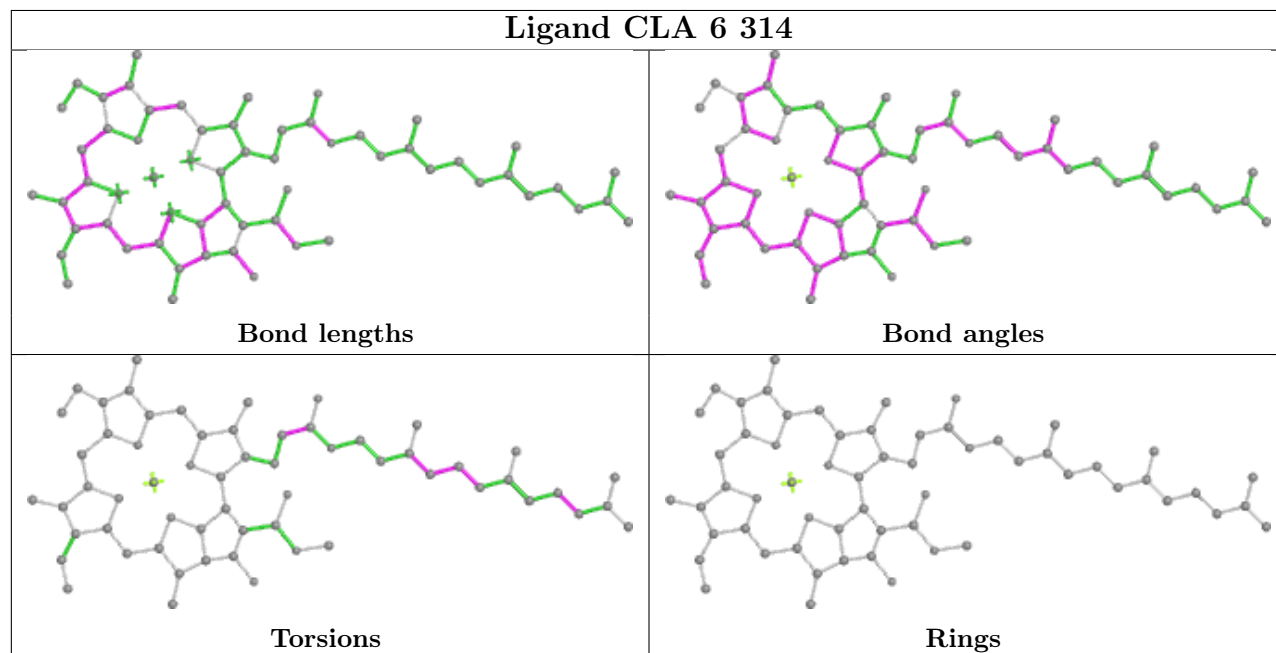


**Ligand BCR b 848****Ligand CLA A 839****Ligand CLA B 813**

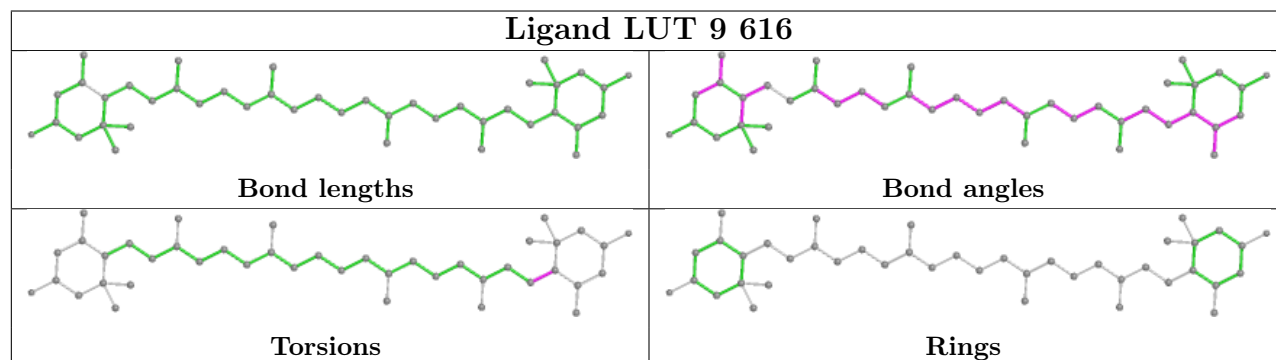
## Ligand LHG 6 301



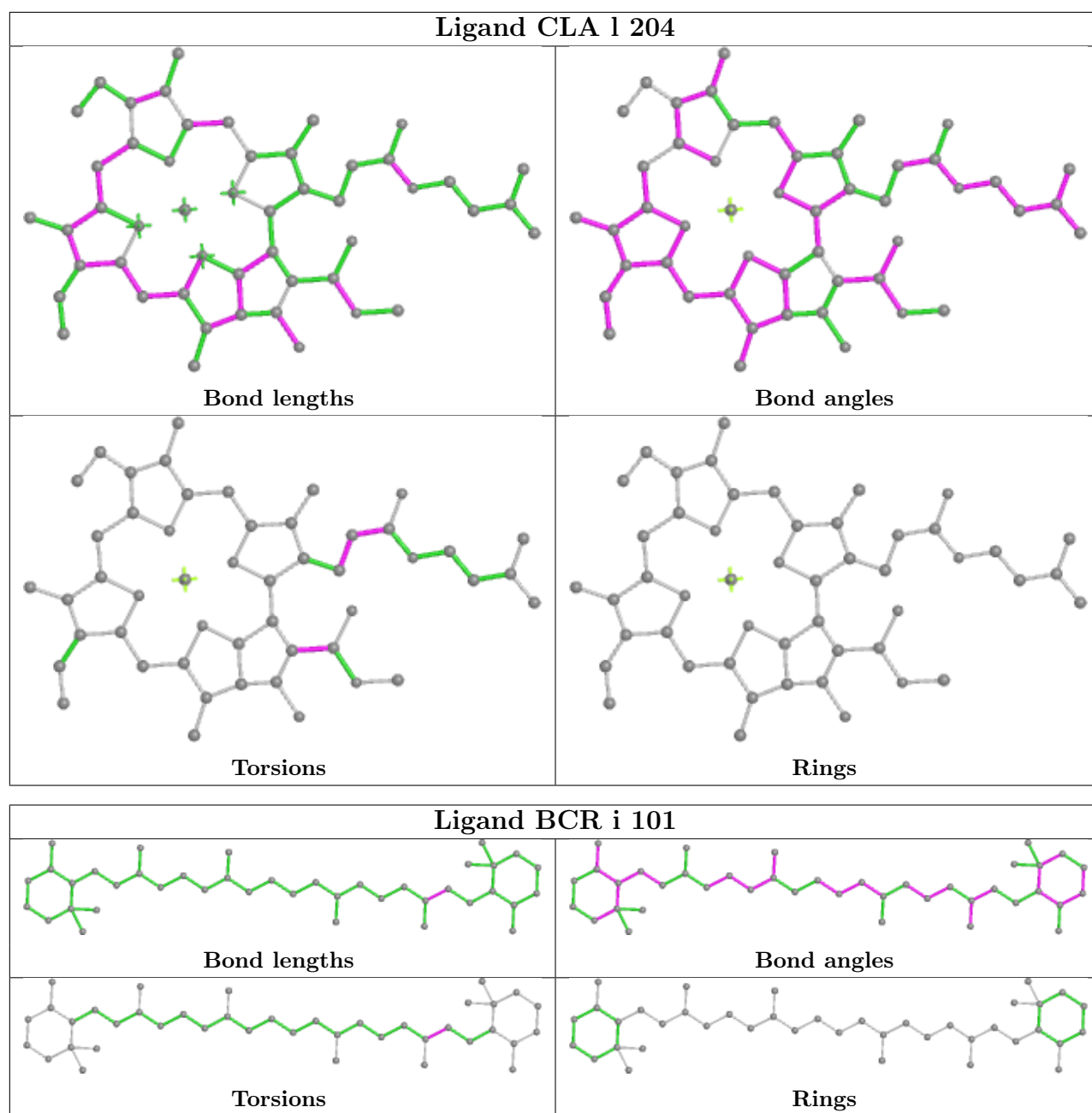
## Ligand CLA 6 314



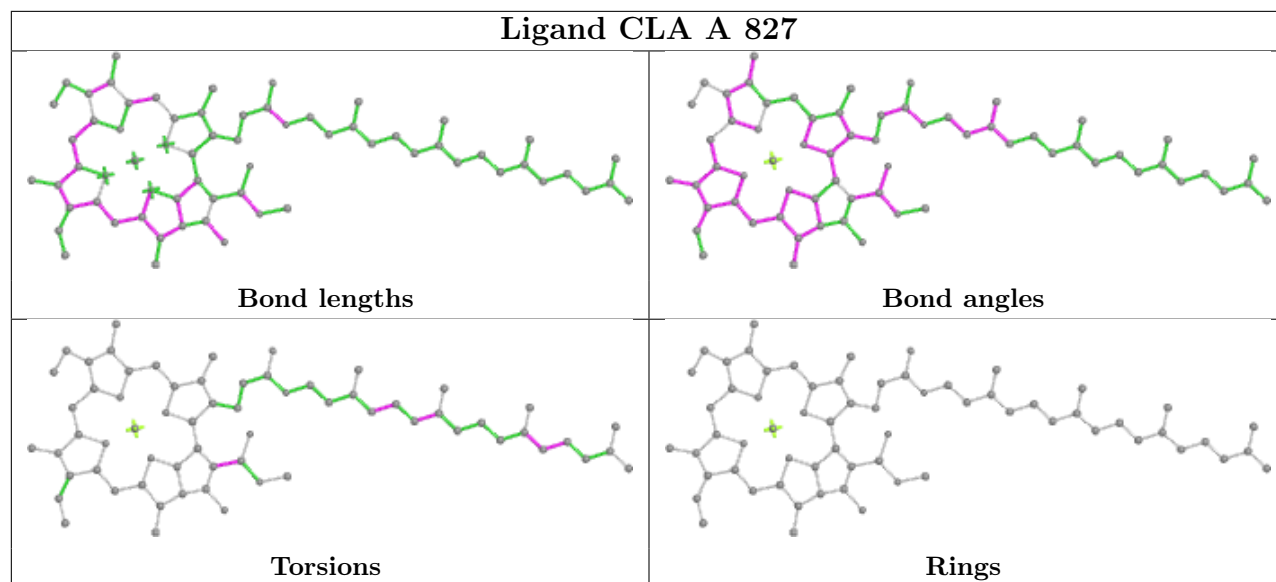
## Ligand LUT 9 616



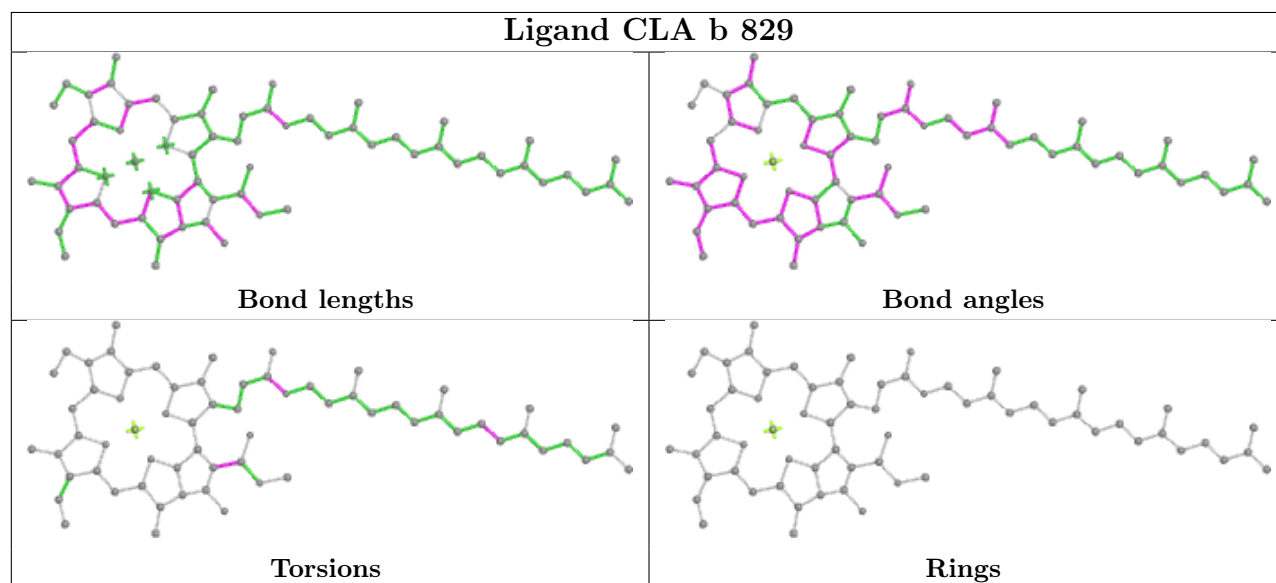




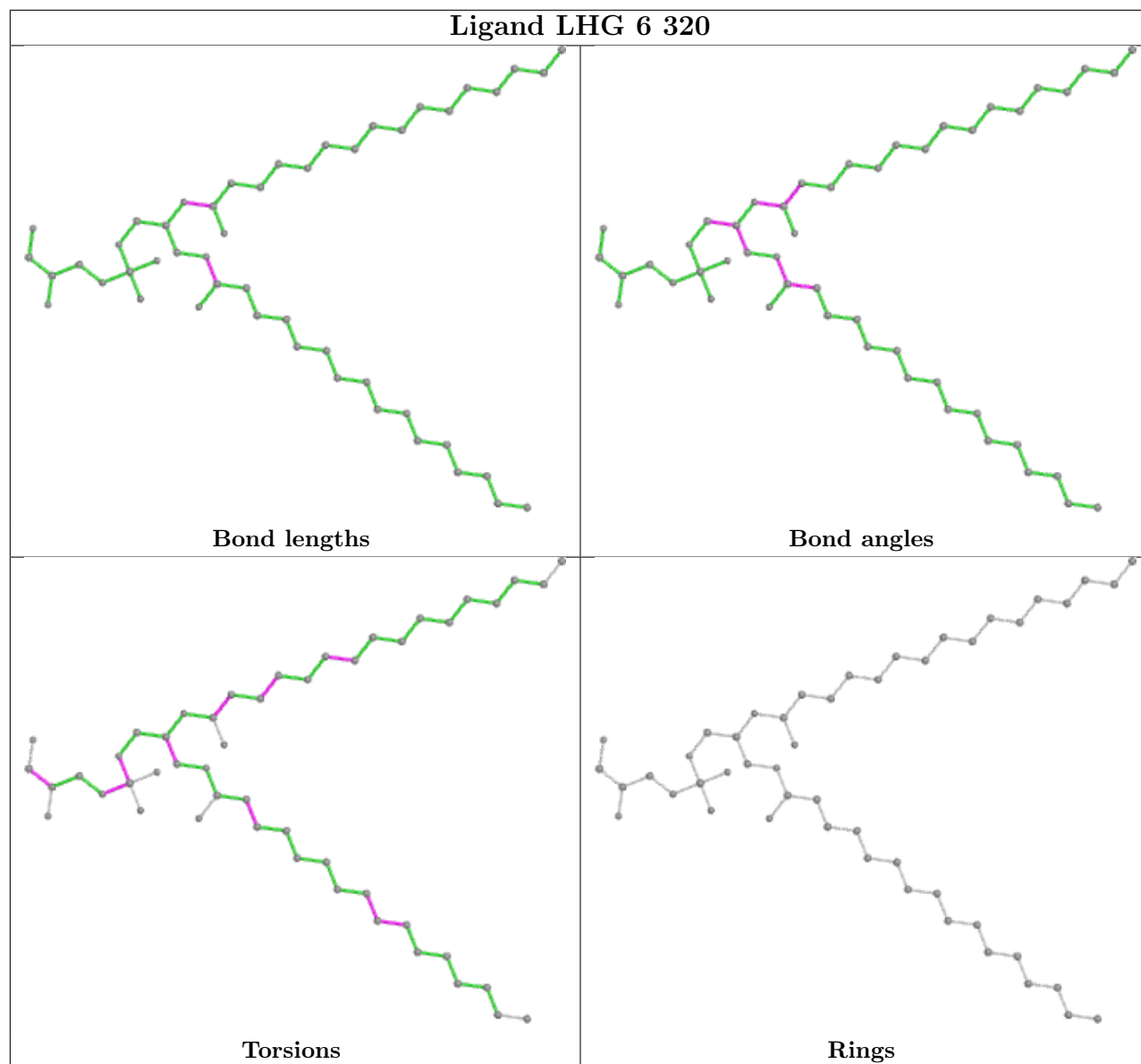
## Ligand CLA A 827



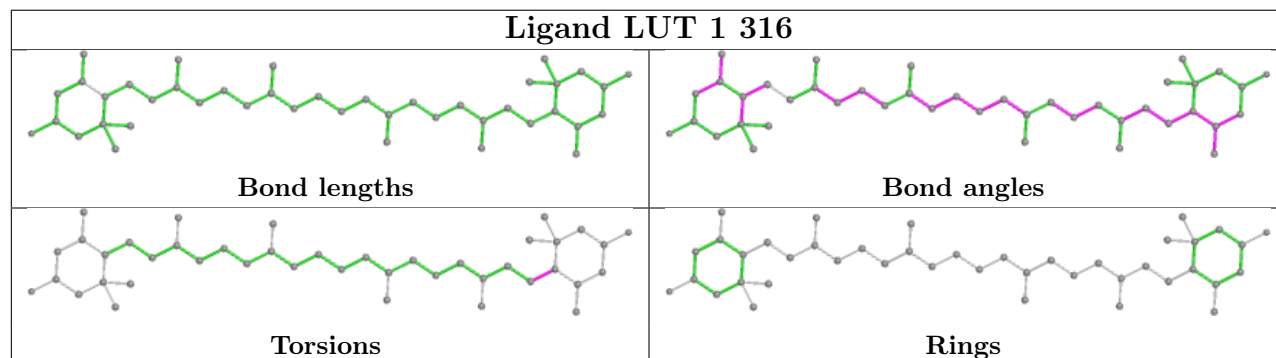
## Ligand CLA b 829



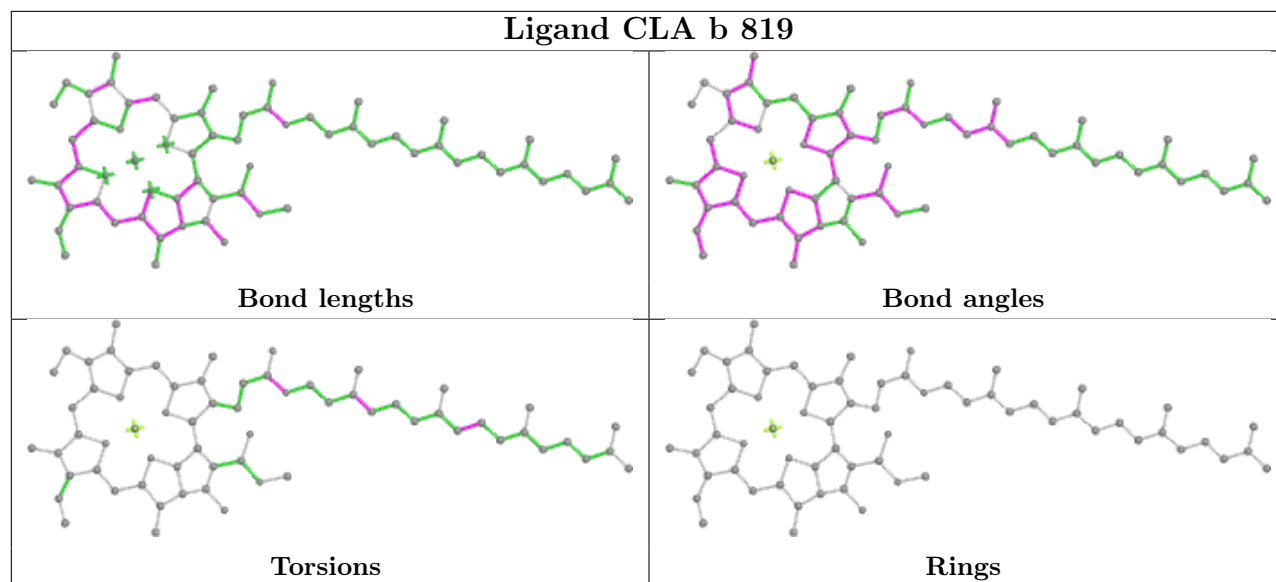
## Ligand LHG 6 320



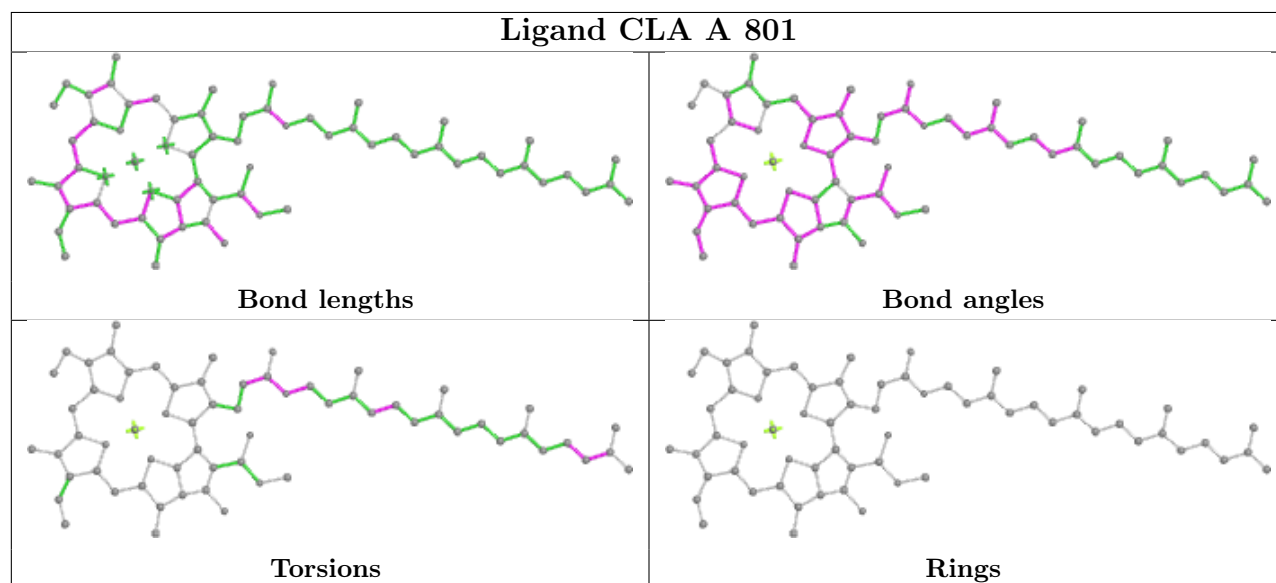
## Ligand LUT 1 316



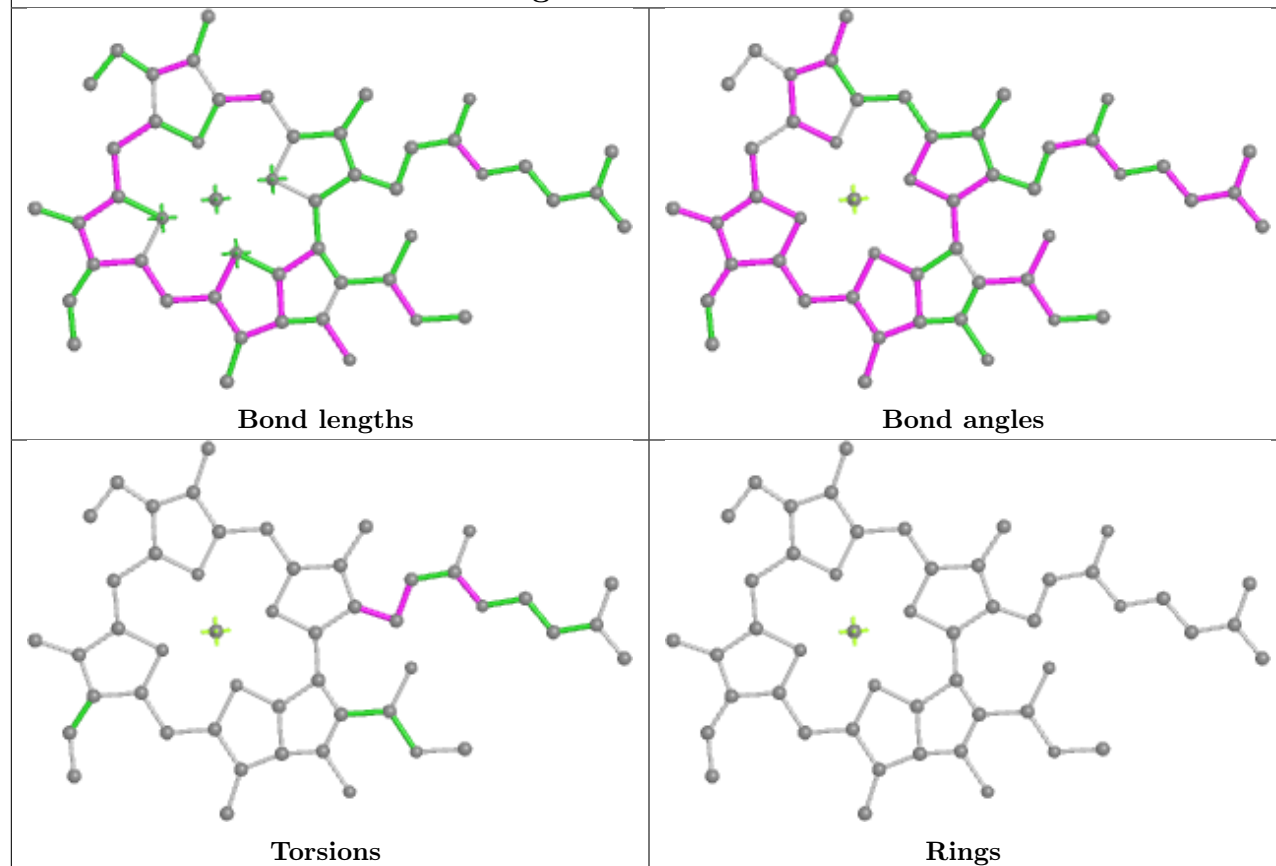
## Ligand CLA b 819



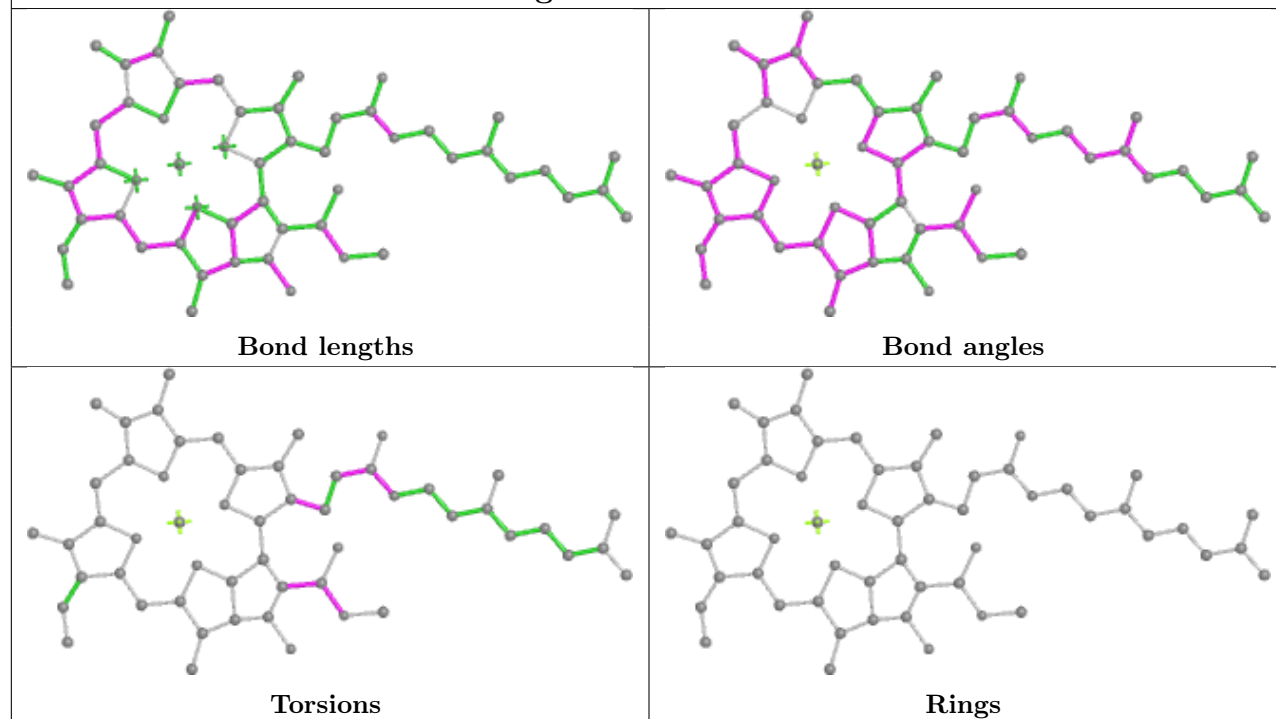
## Ligand CLA A 801



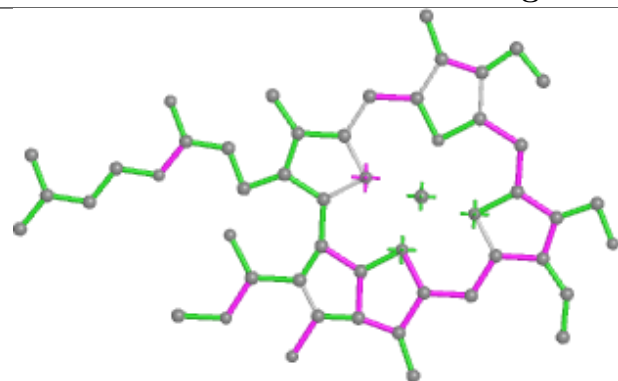
## Ligand CLA B 830



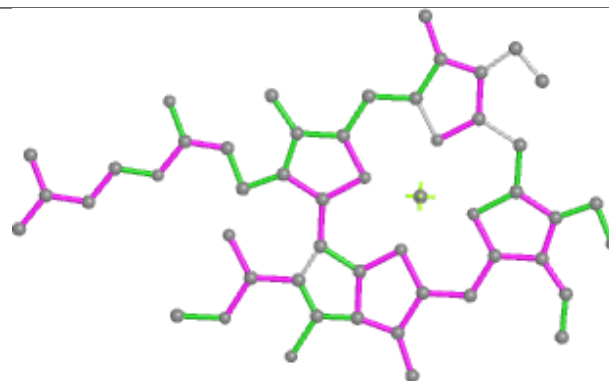
## Ligand CLA b 811



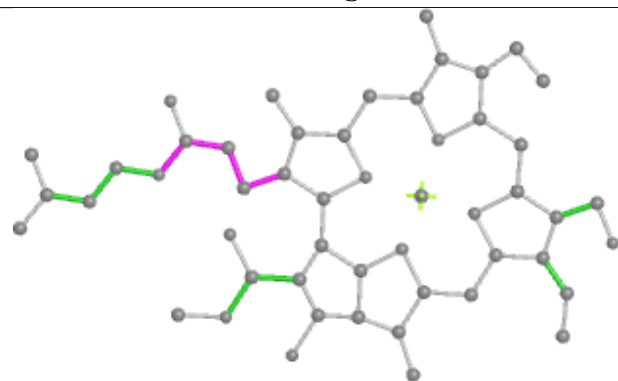
## Ligand CHL 4 606



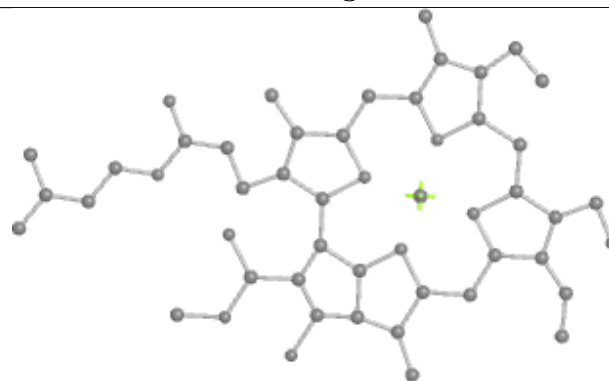
Bond lengths



Bond angles

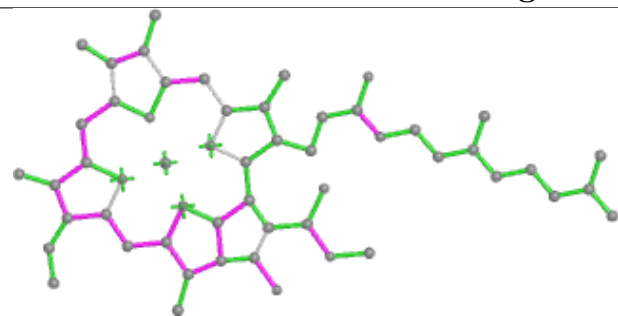


Torsions

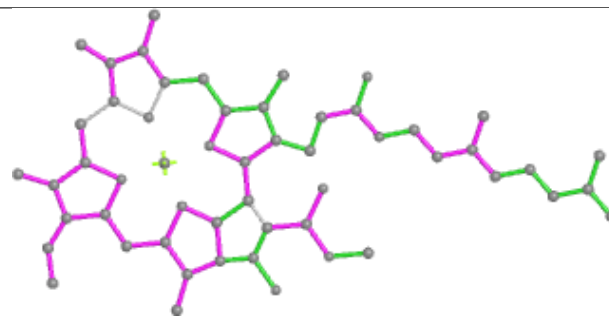


Rings

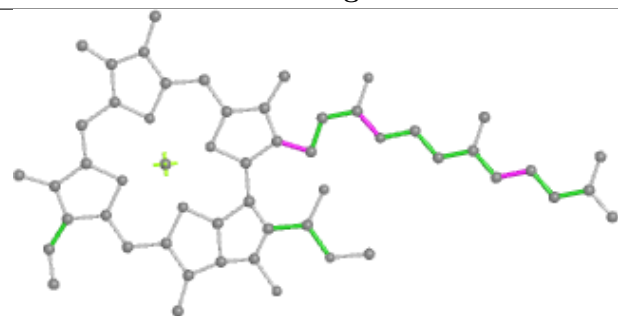
## Ligand CLA B 811



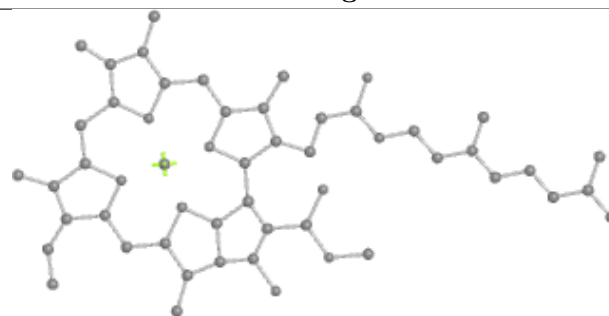
Bond lengths



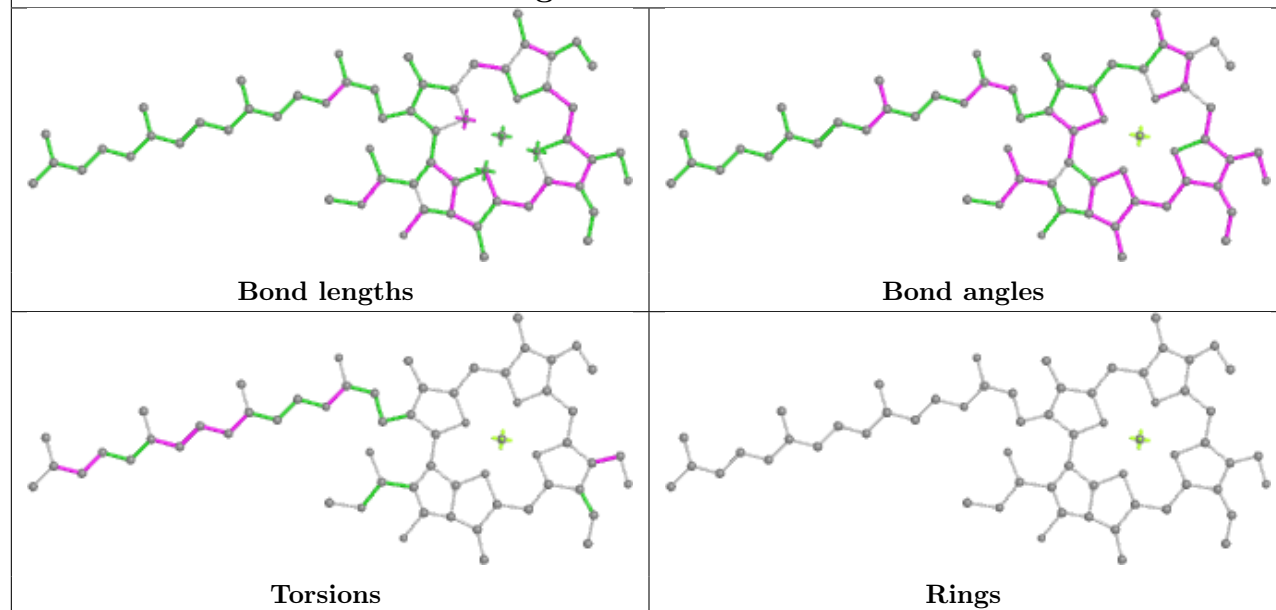
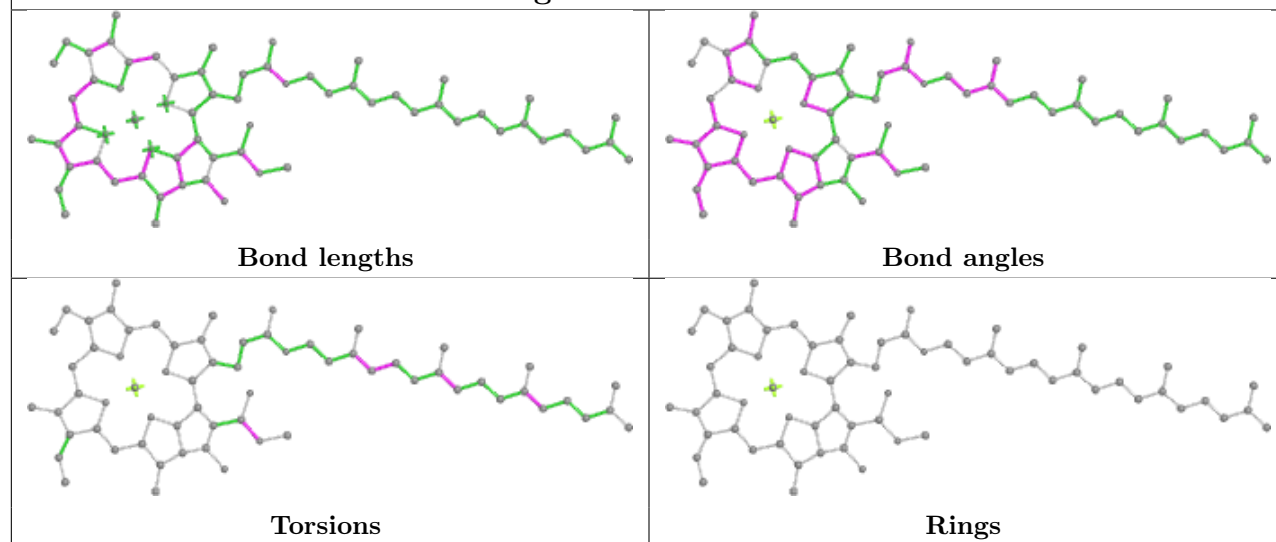
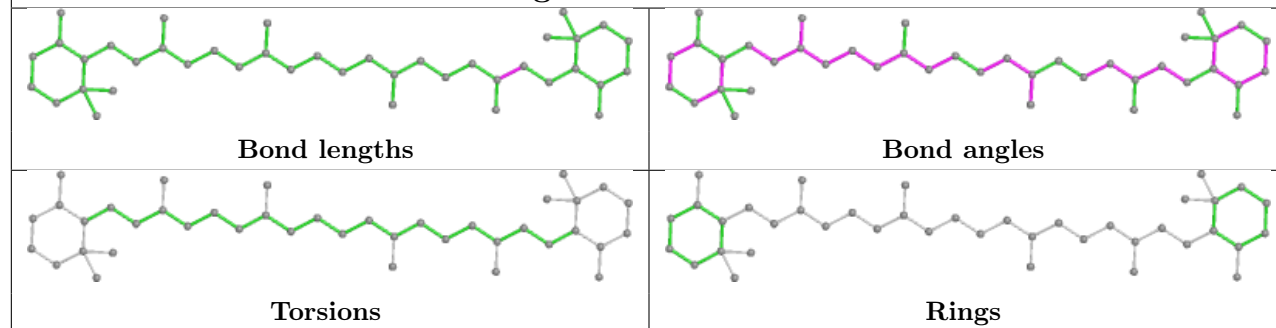
Bond angles



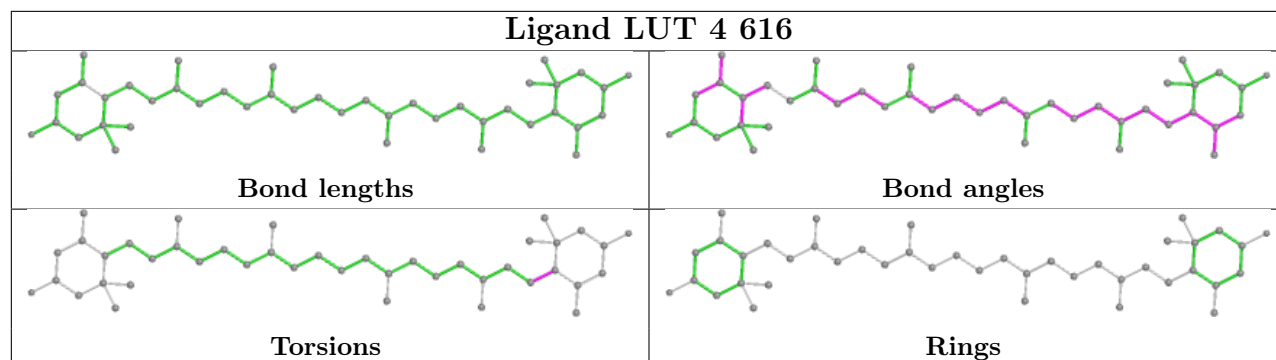
Torsions



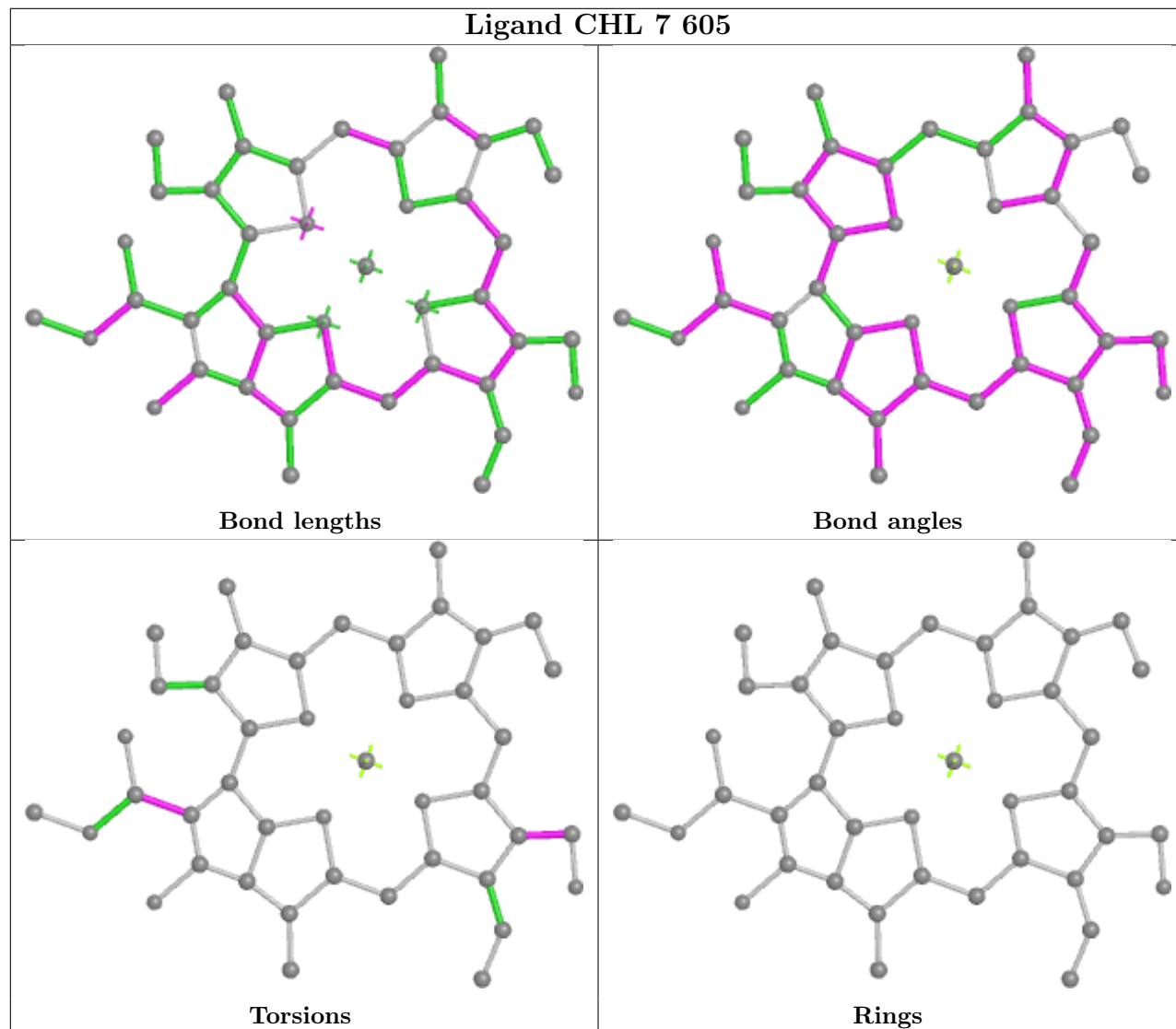
Rings

**Ligand CHL 2 601****Ligand CLA F 301****Ligand BCR b 843**

## Ligand LUT 4 616

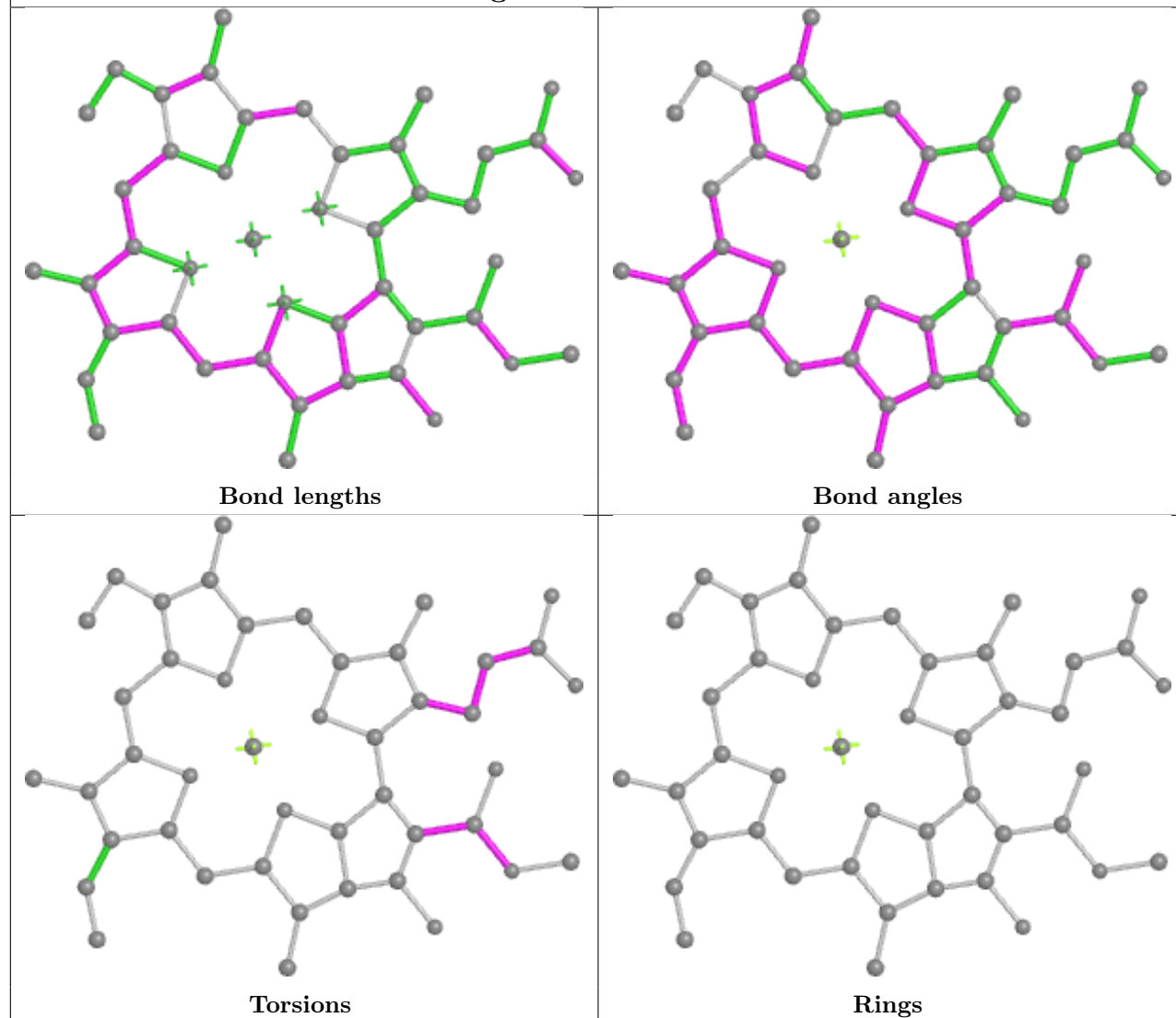


## Ligand CHL 7 605

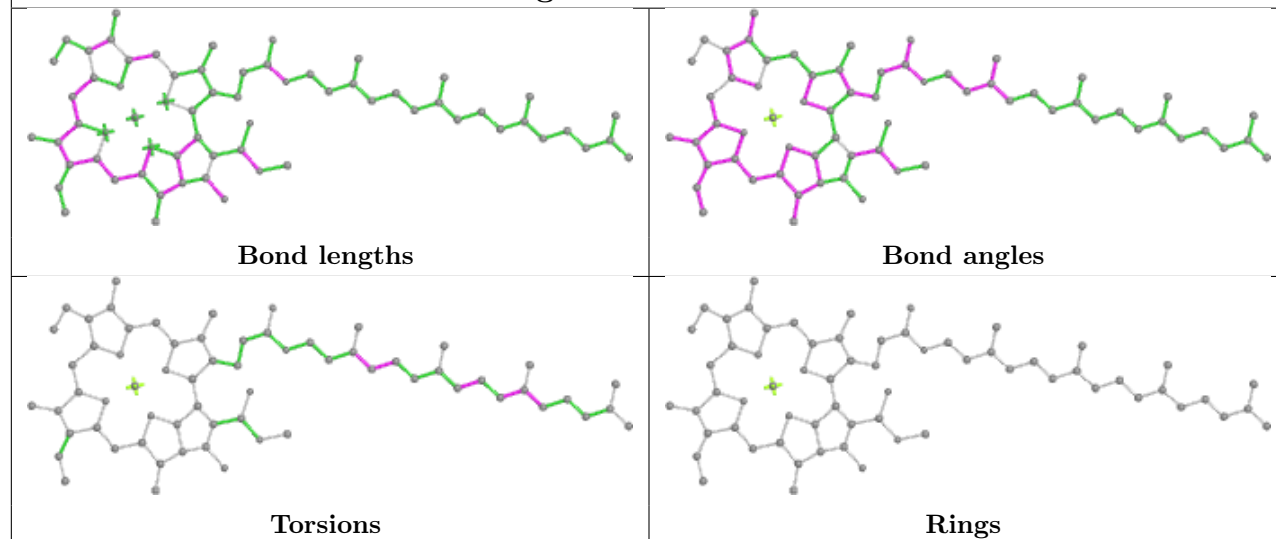




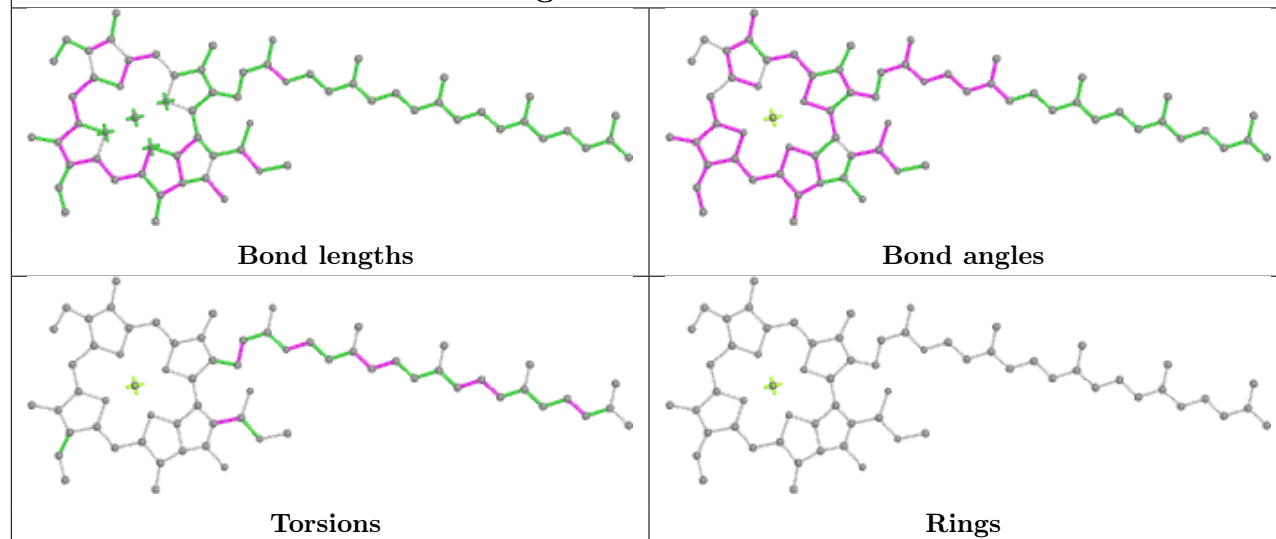
## Ligand CLA B 804



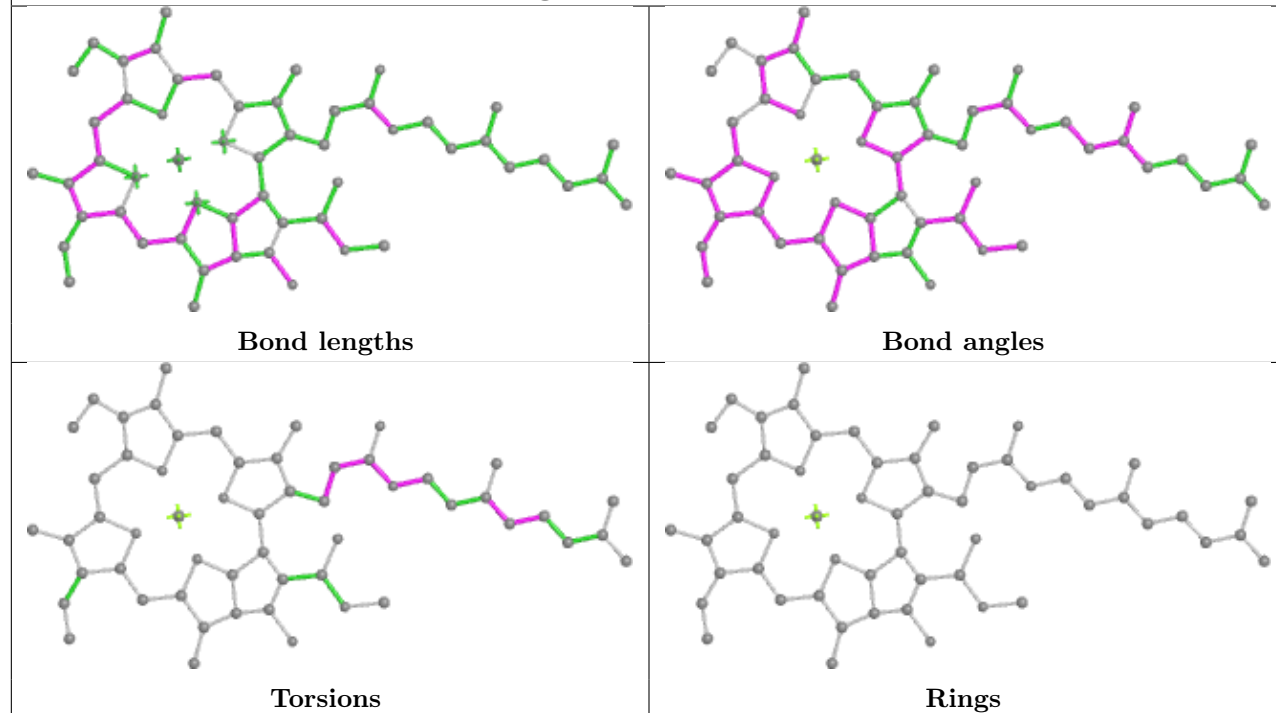
## Ligand CLA a 842



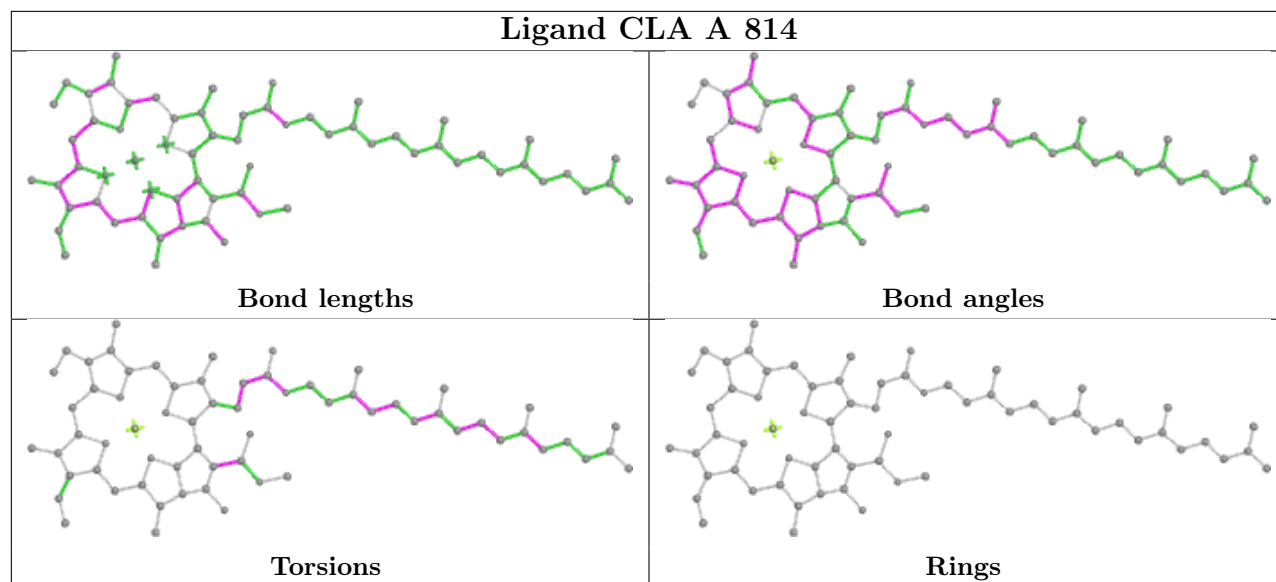
## Ligand CLA a 856



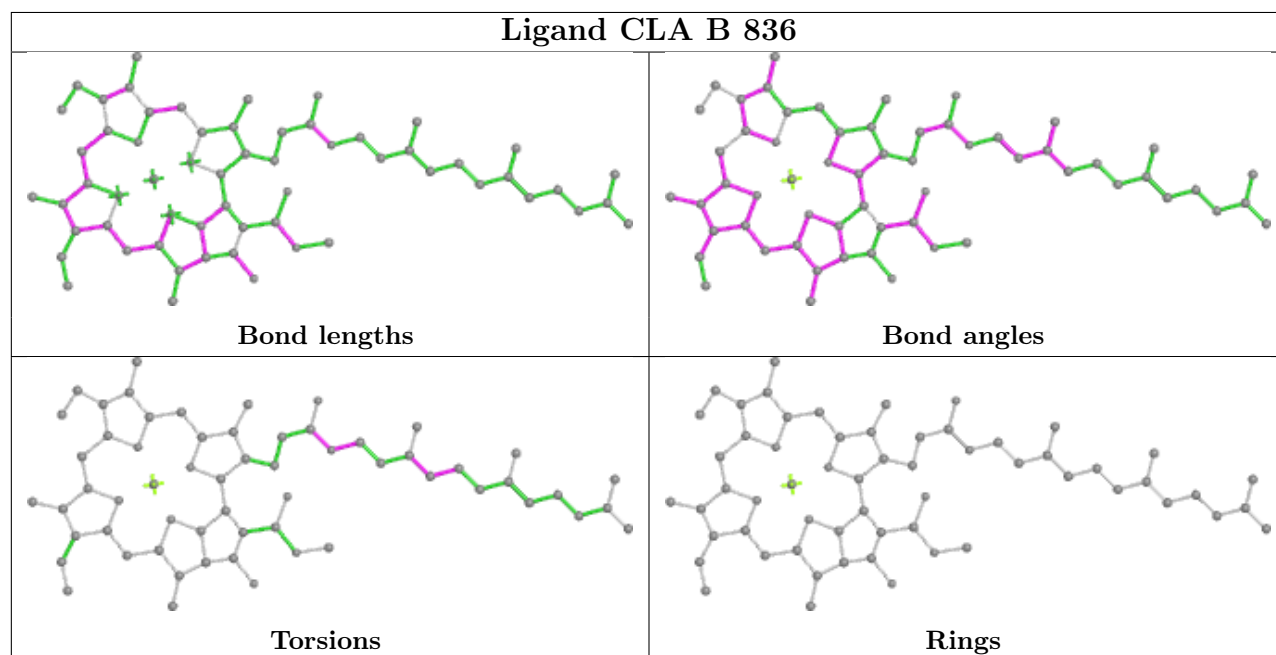
## Ligand CLA 3 312

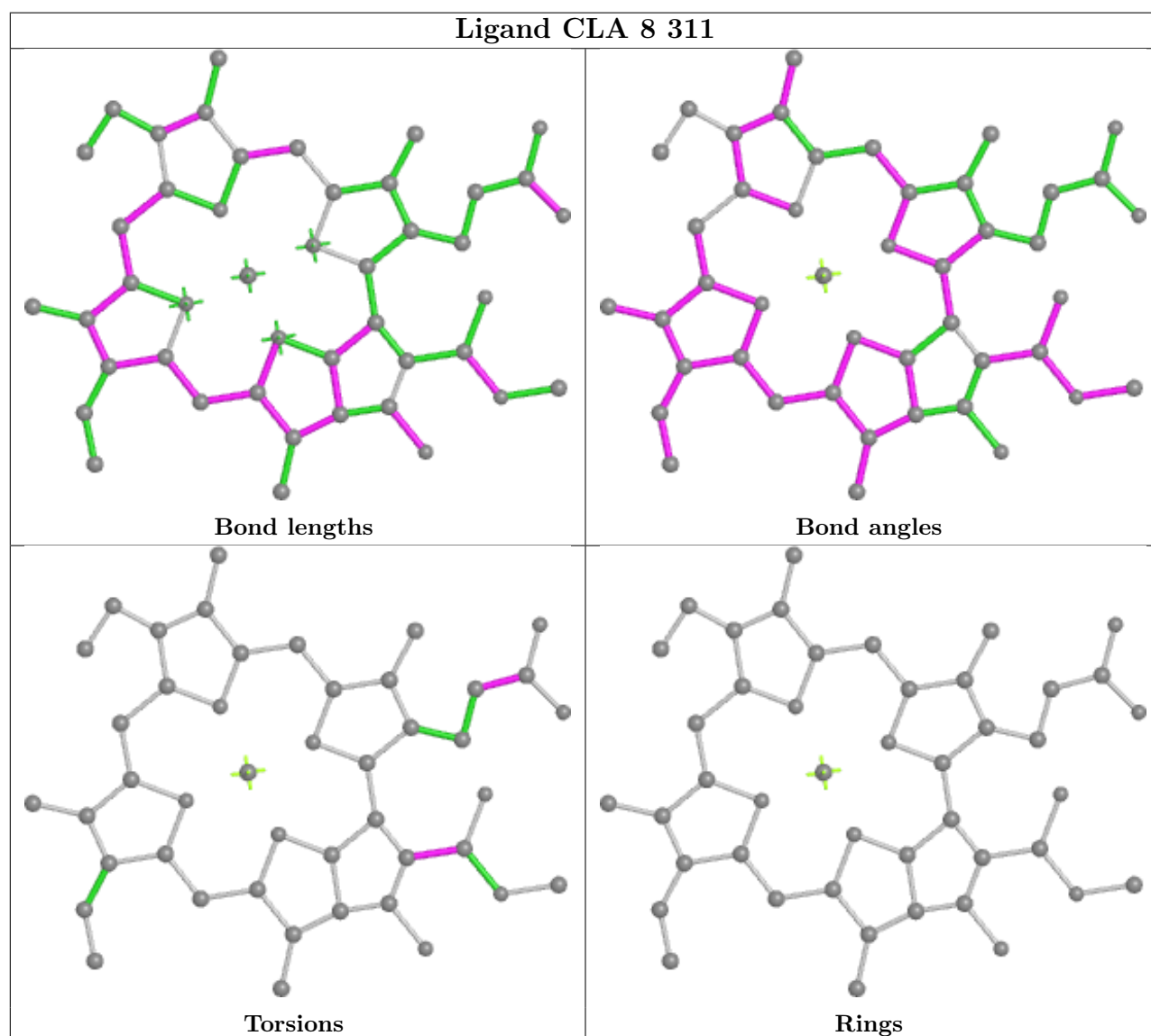
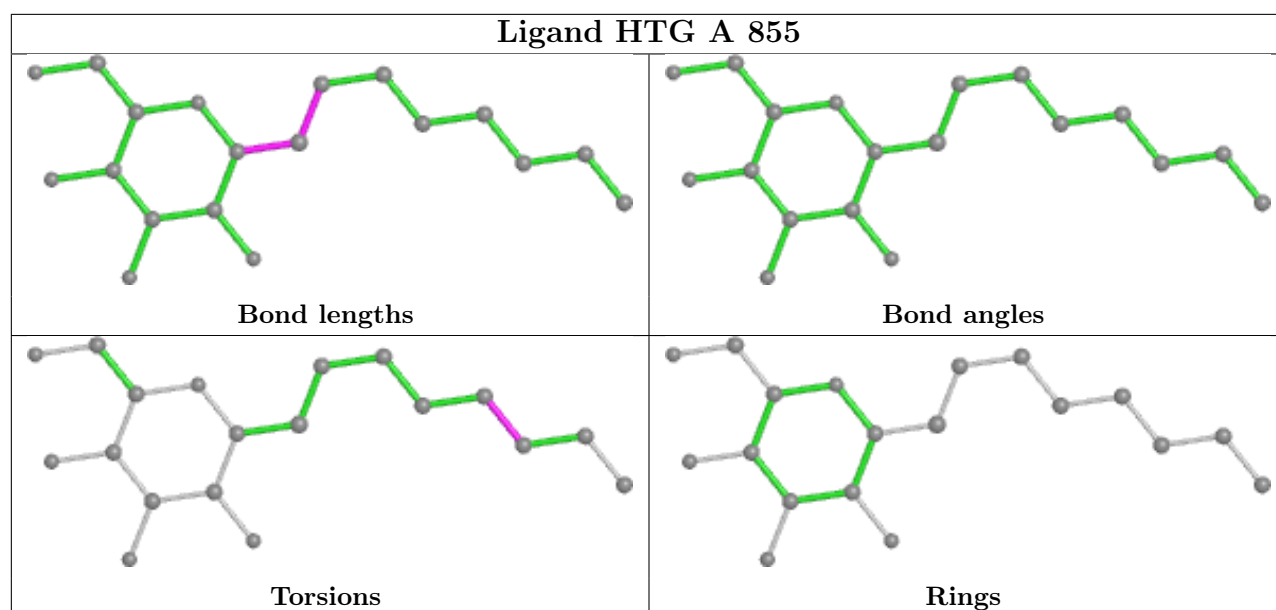


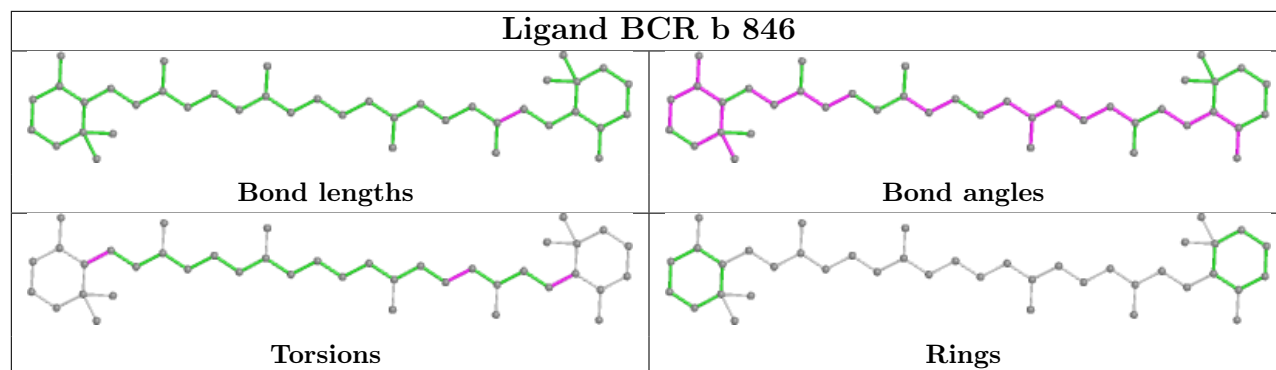
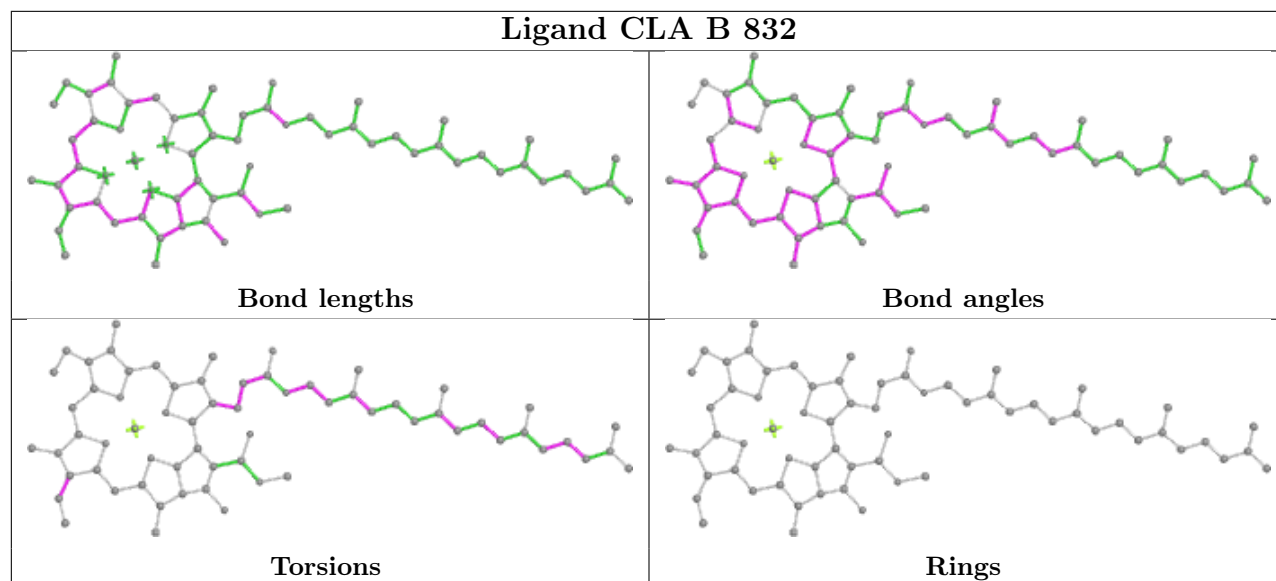
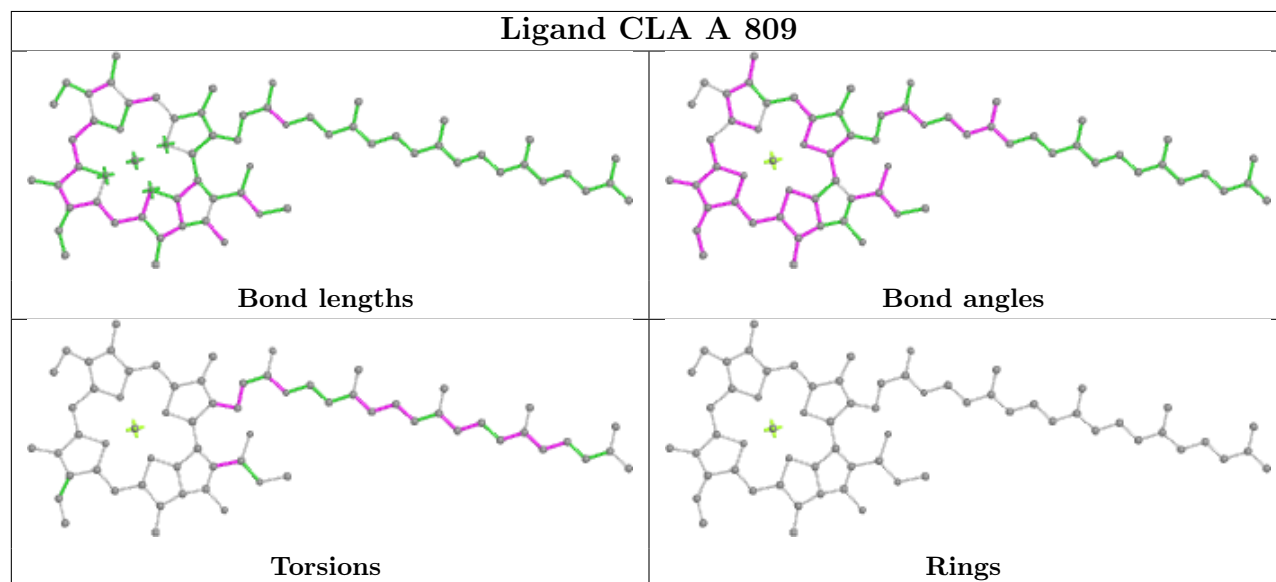
## Ligand CLA A 814



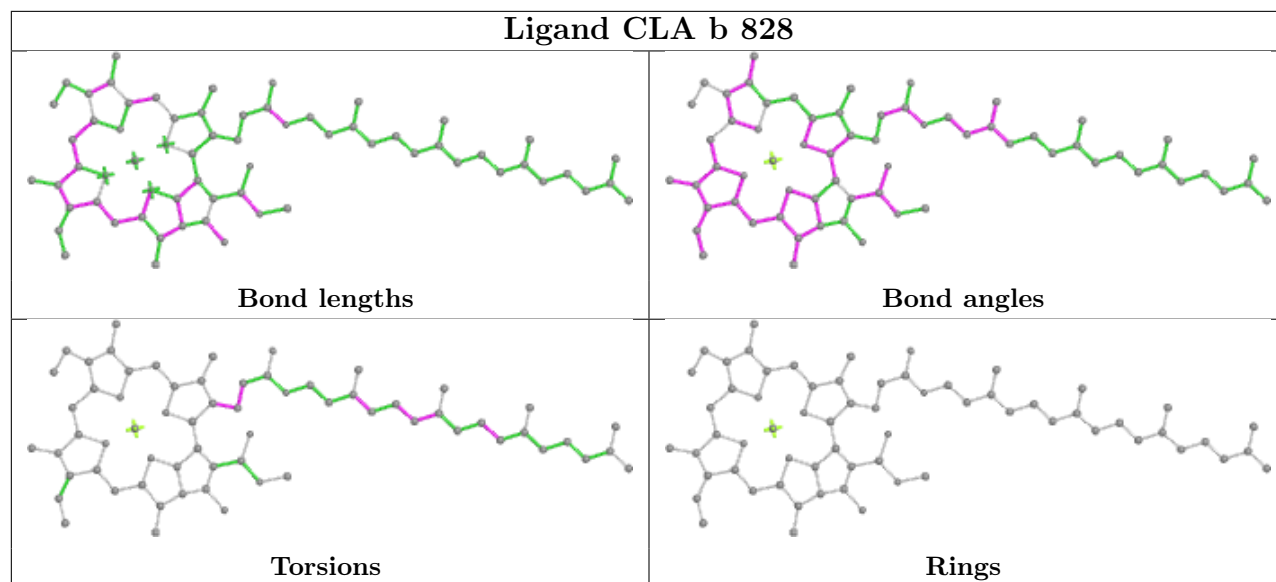
## Ligand CLA B 836



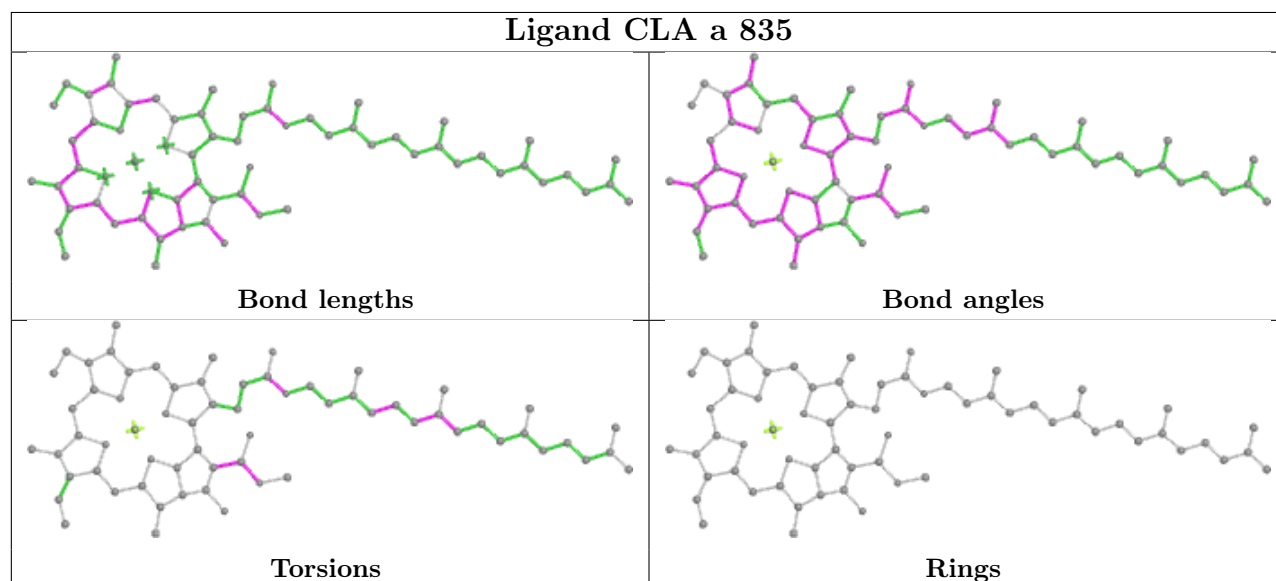


**Ligand BCR b 846****Ligand CLA B 832****Ligand CLA A 809**

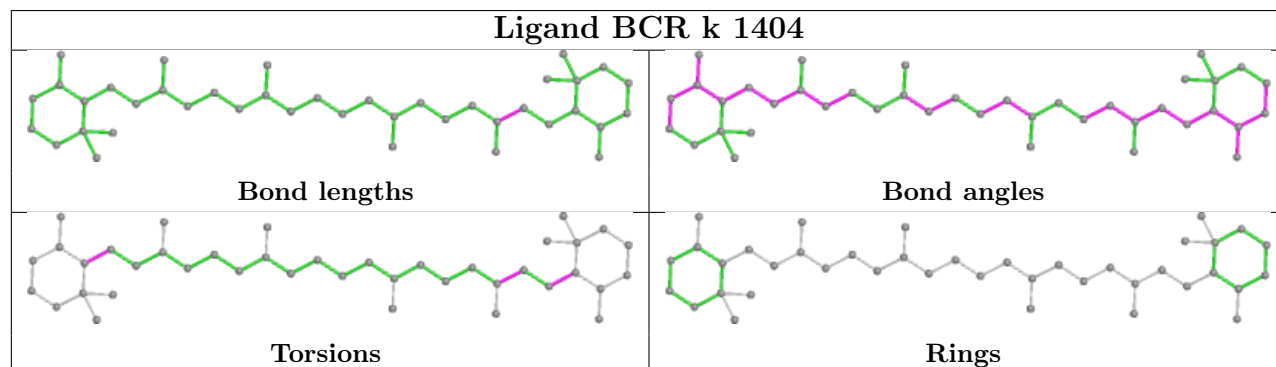
## Ligand CLA b 828



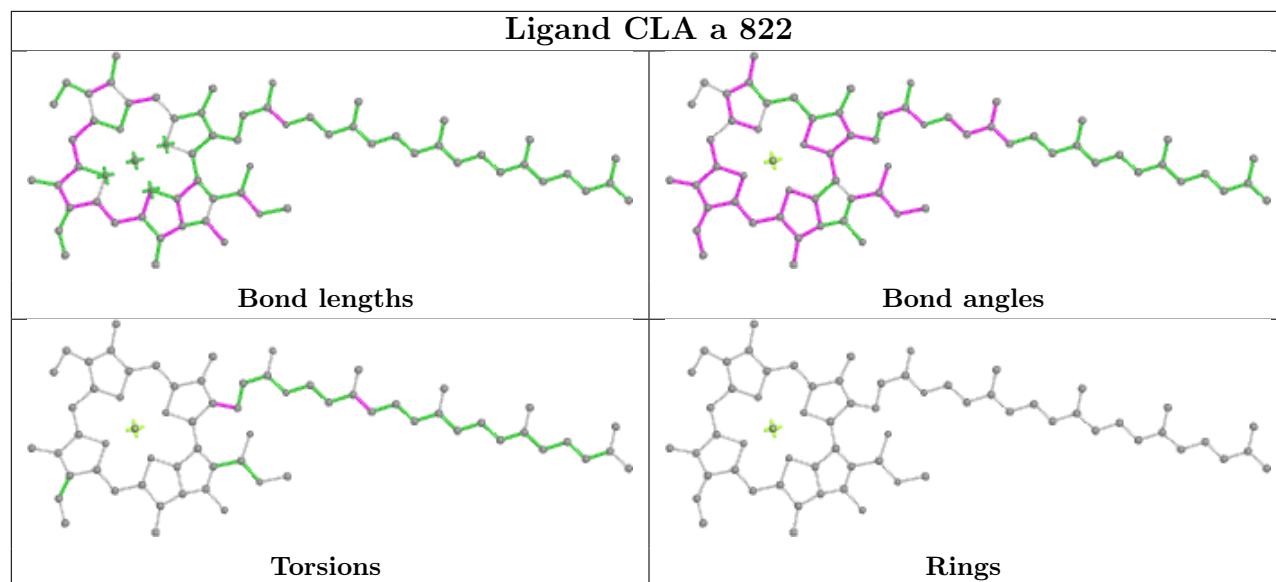
## Ligand CLA a 835



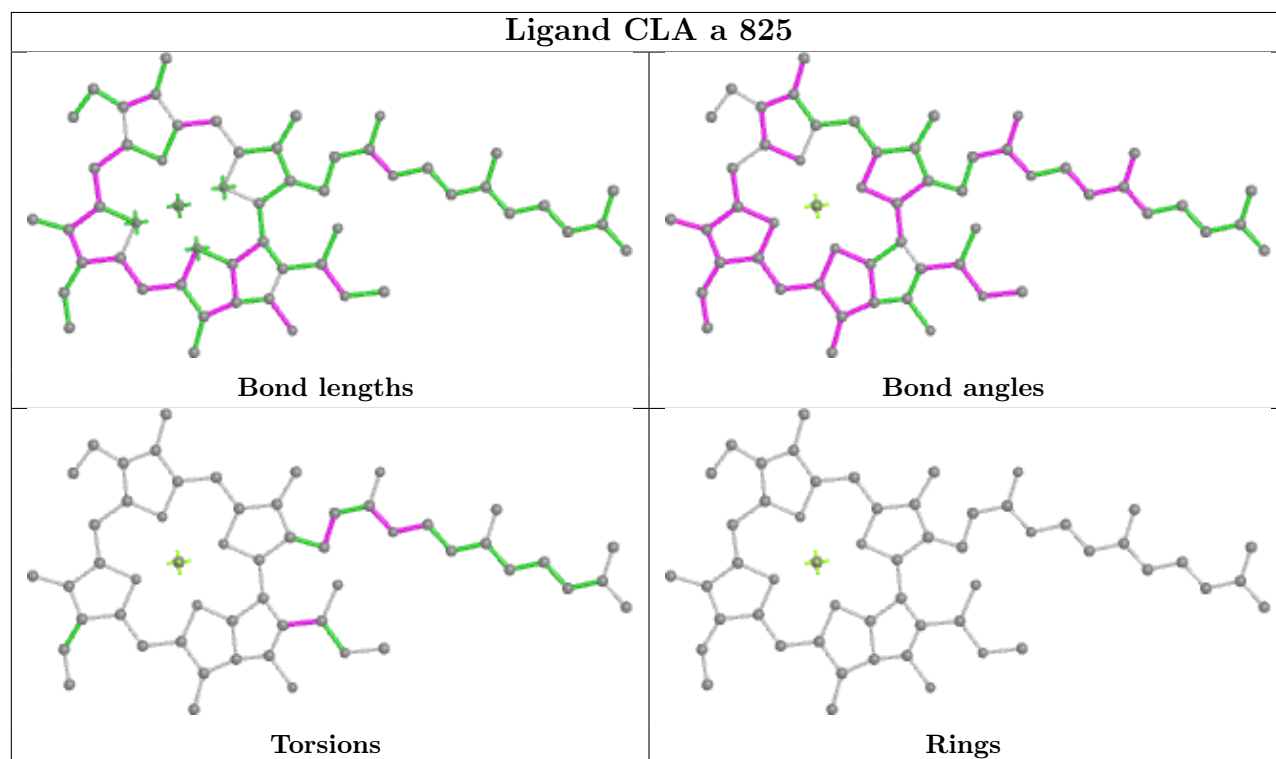
## Ligand BCR k 1404



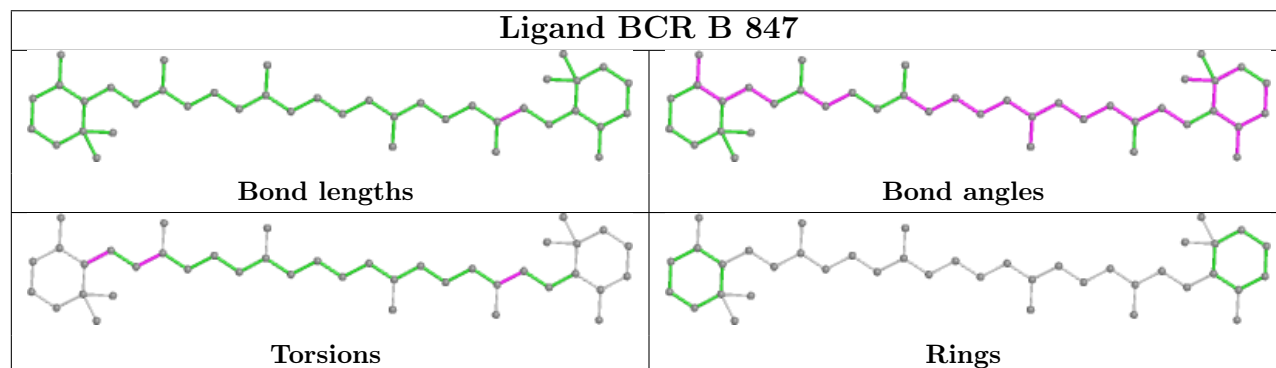
## Ligand CLA a 822



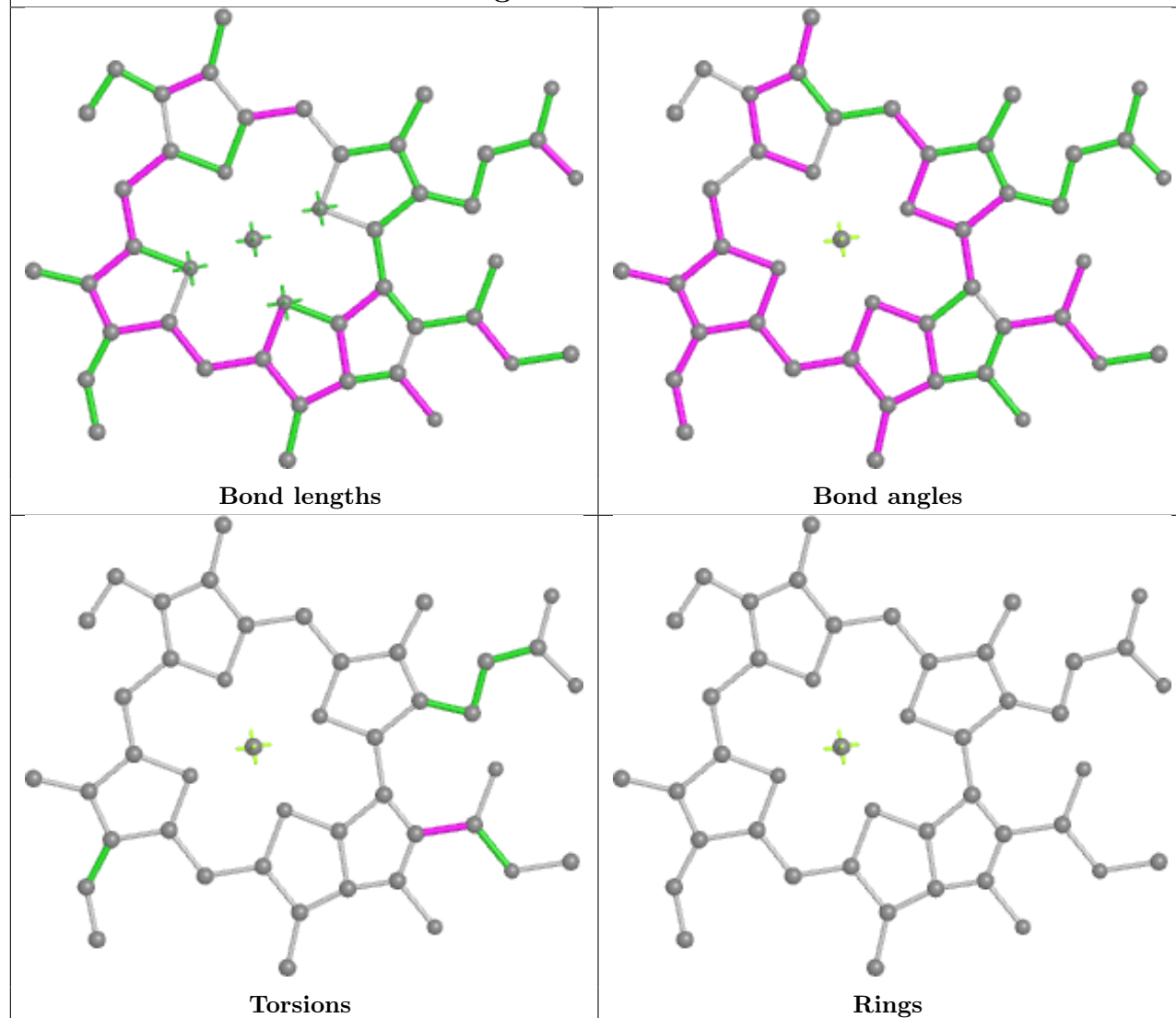
## Ligand CLA a 825



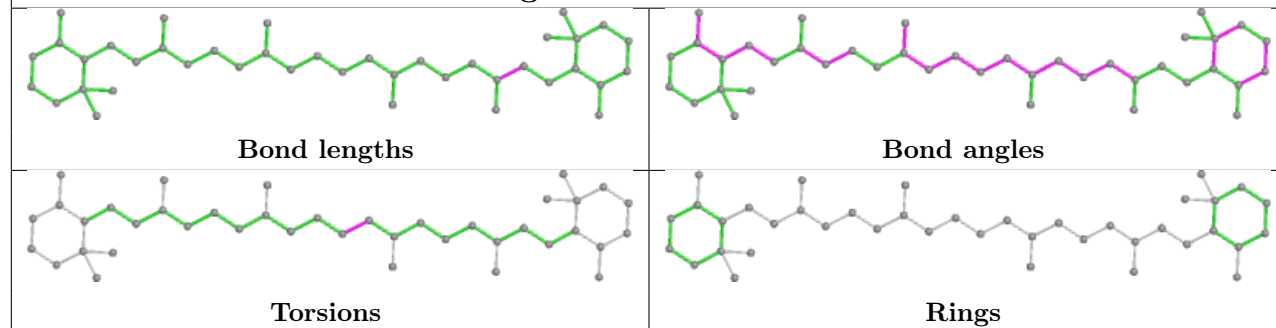
## Ligand BCR B 847



## Ligand CLA 8 303

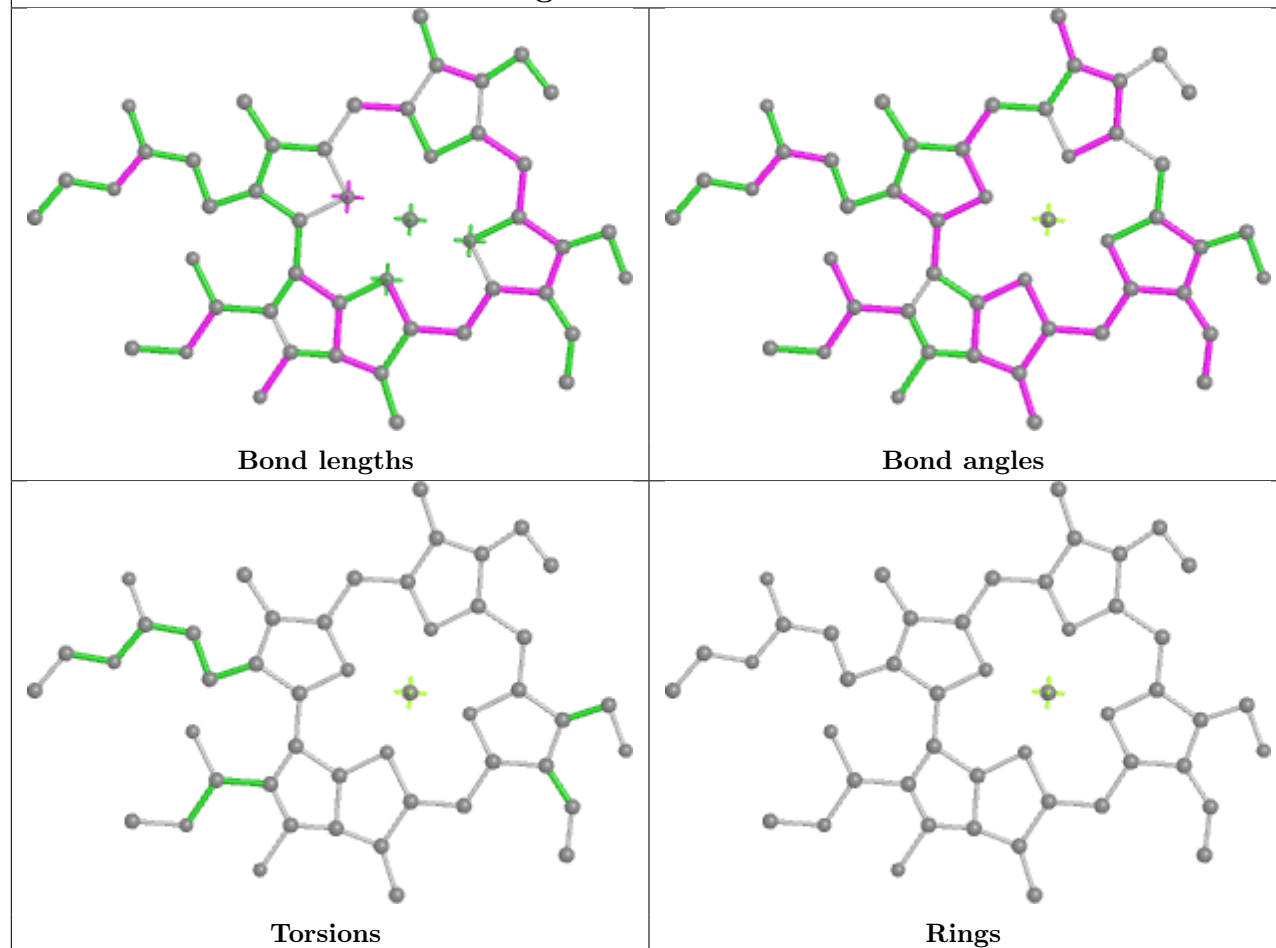


## Ligand BCR K 4001

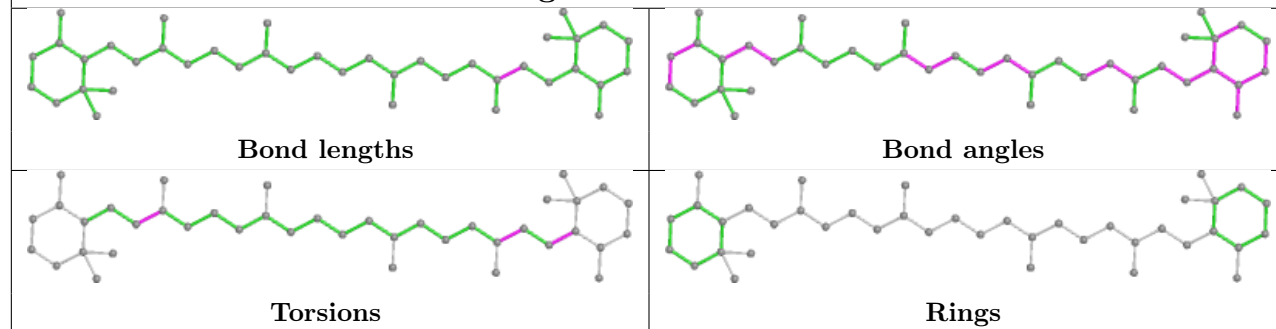




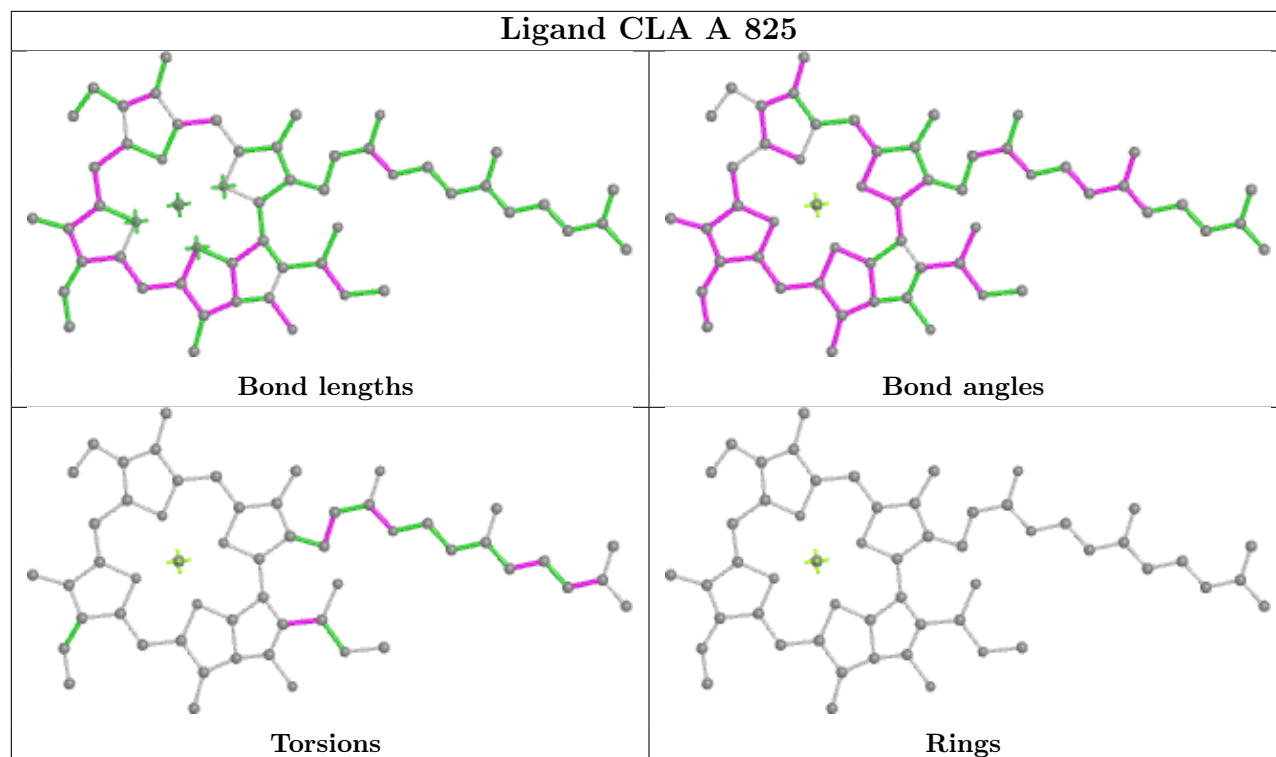
## Ligand CHL 7 606



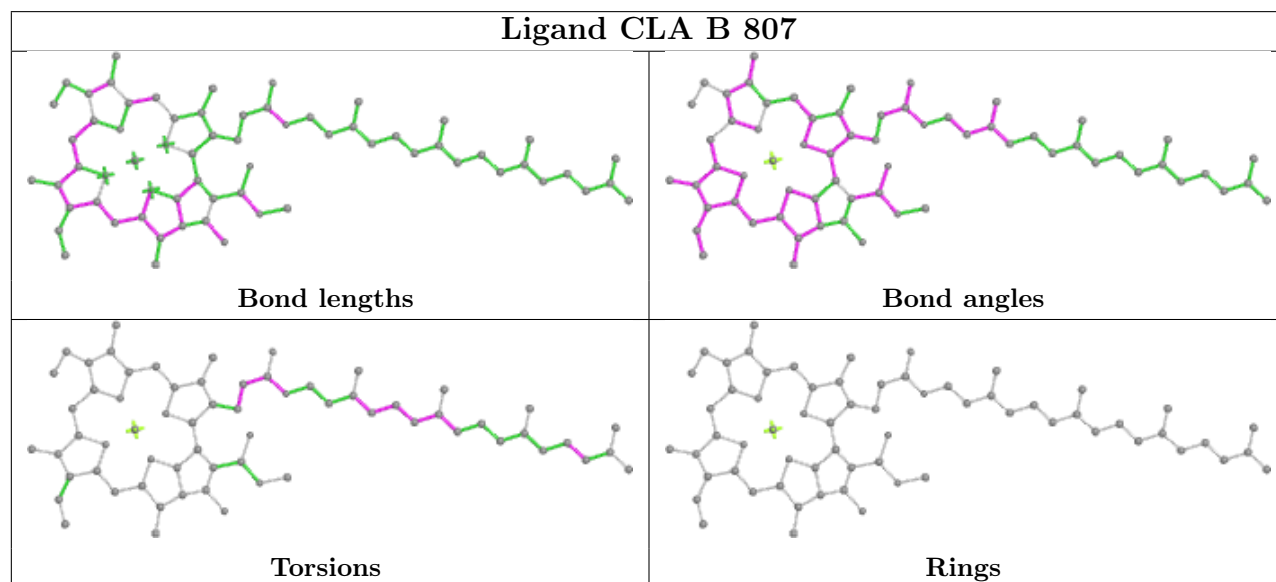
## Ligand BCR 1 205



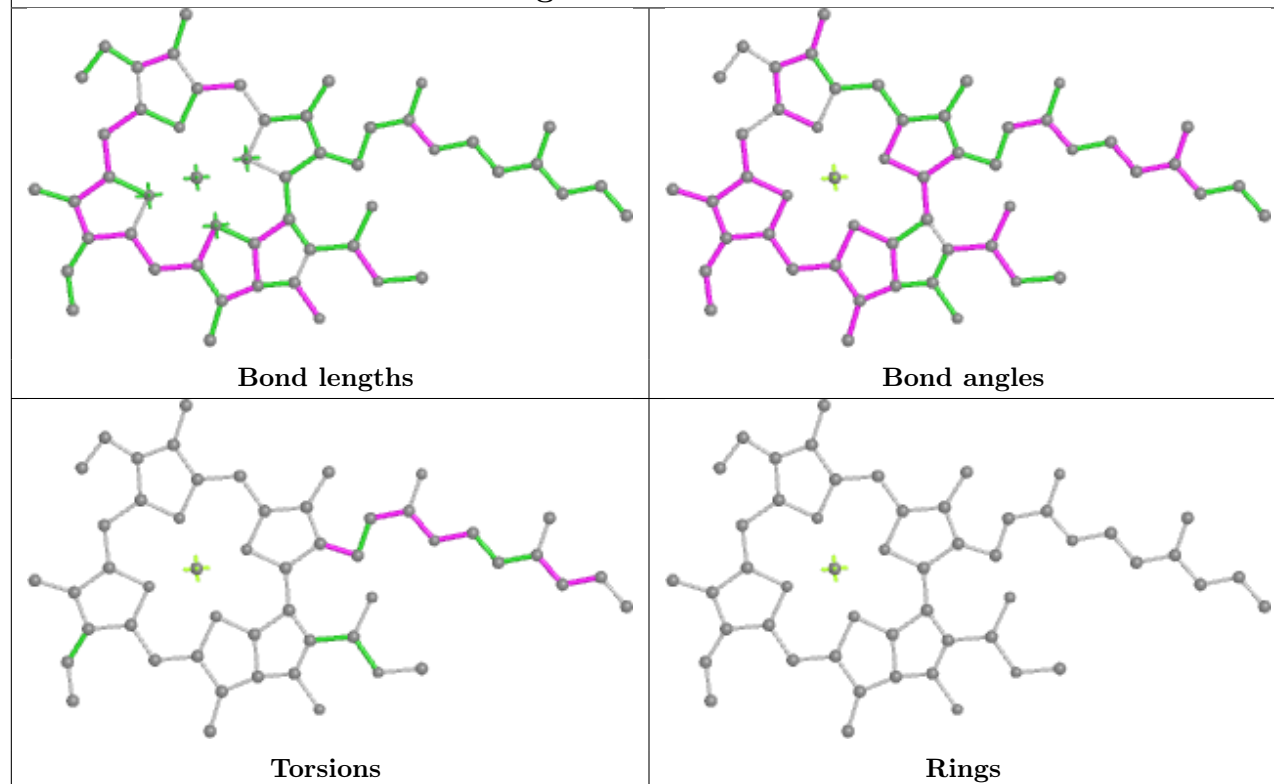
## Ligand CLA A 825



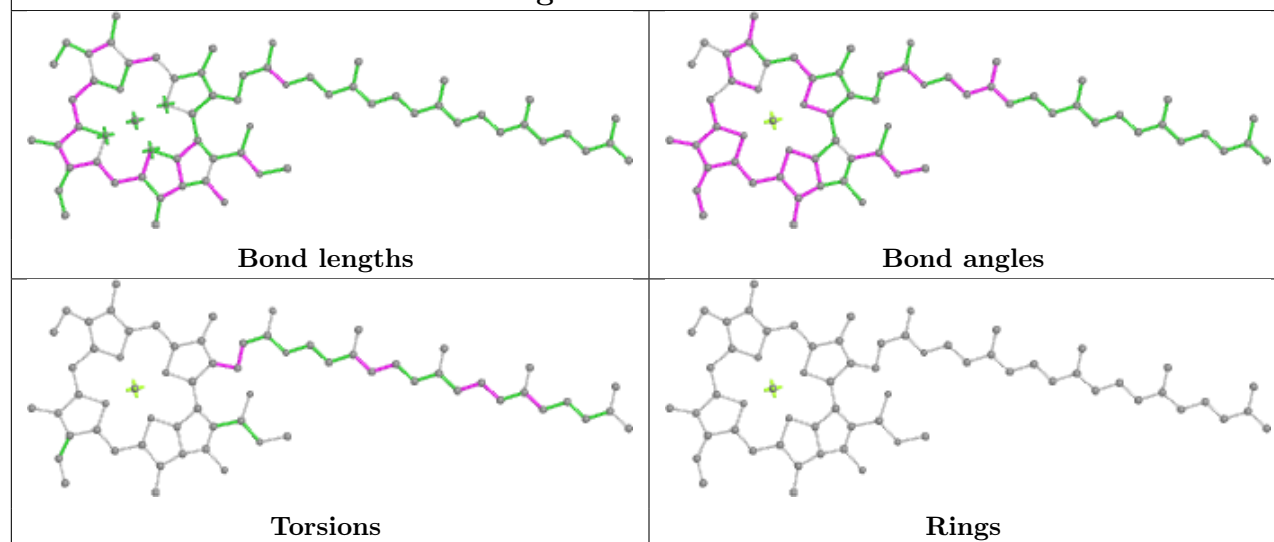
## Ligand CLA B 807



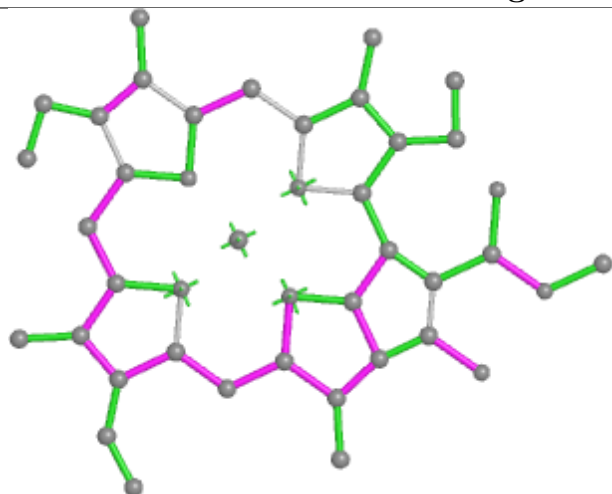
## Ligand CLA 6 313



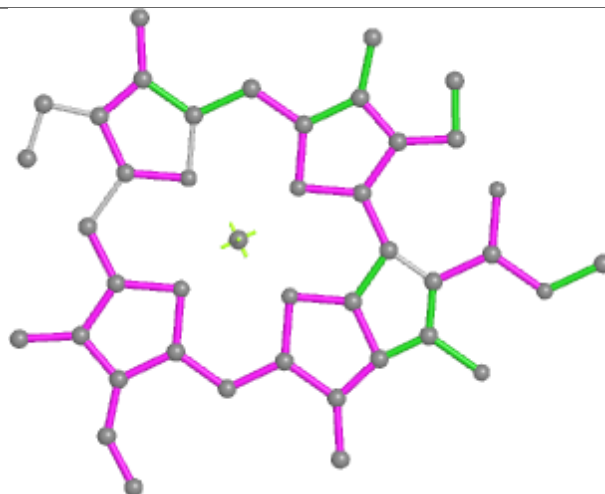
## Ligand CLA 1 309



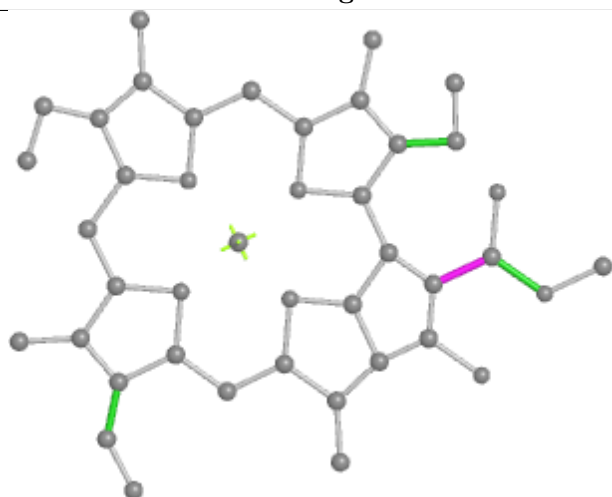
## Ligand CLA J 3002



Bond lengths



Bond angles

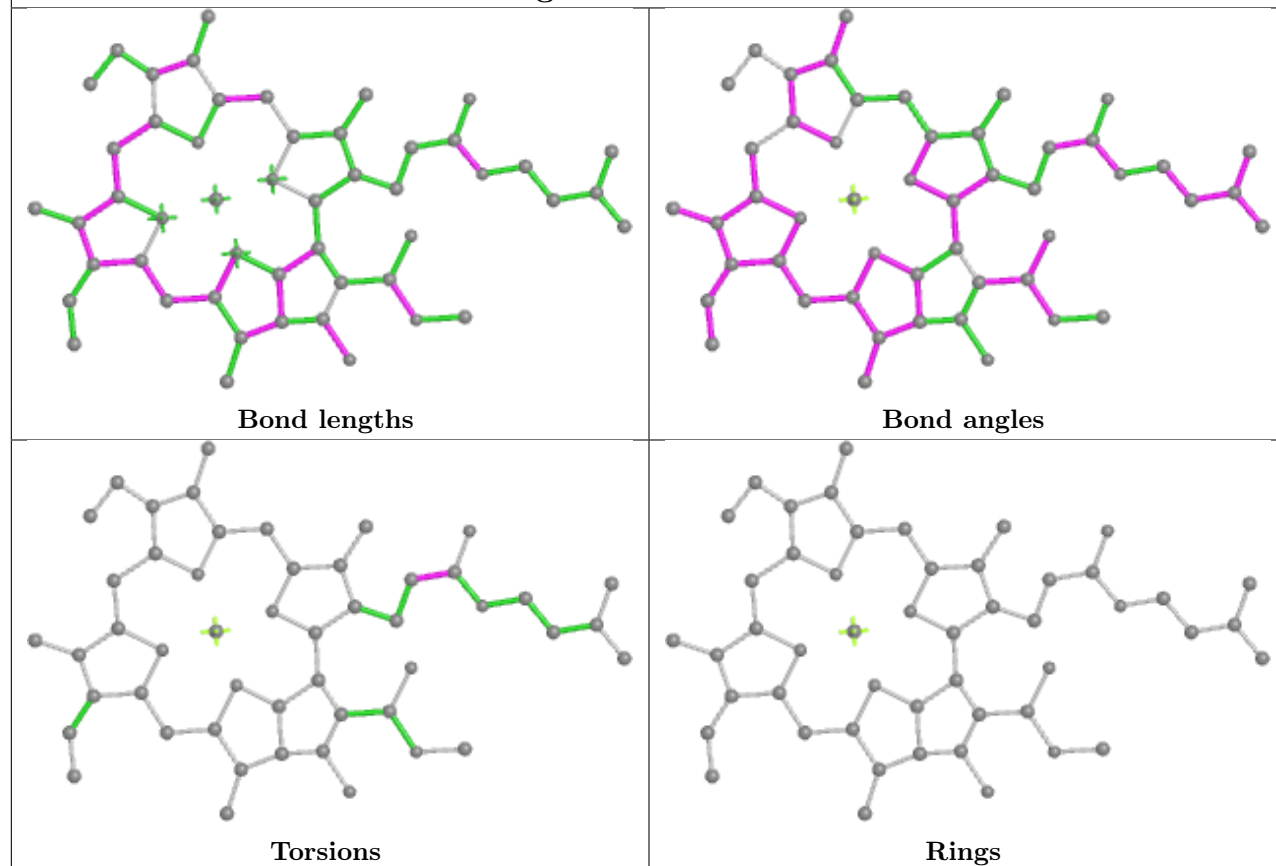


Torsions

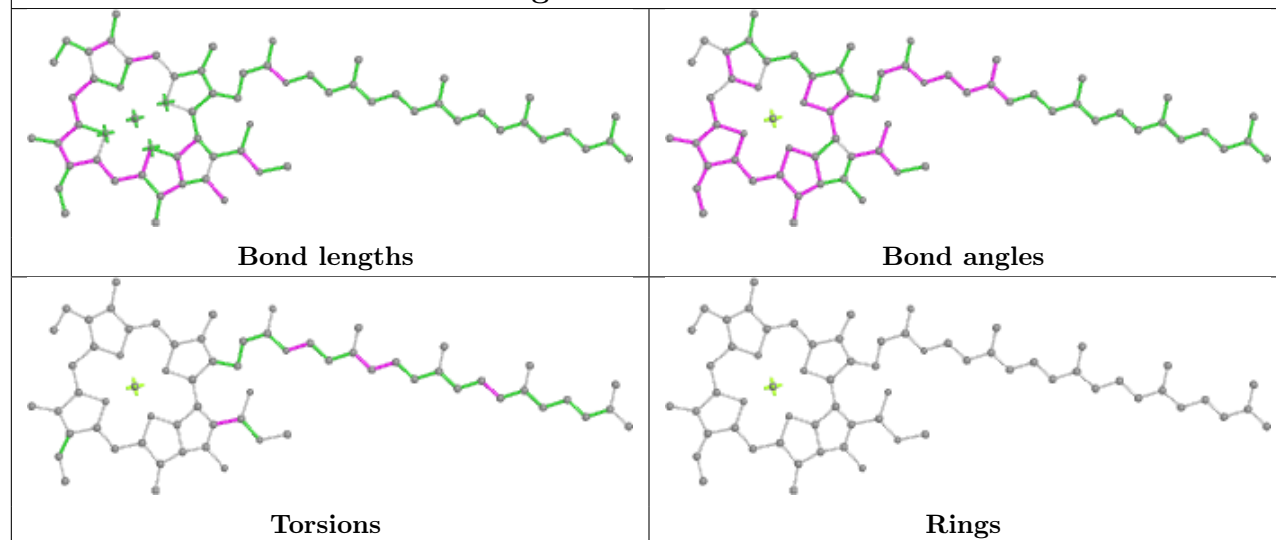


Rings

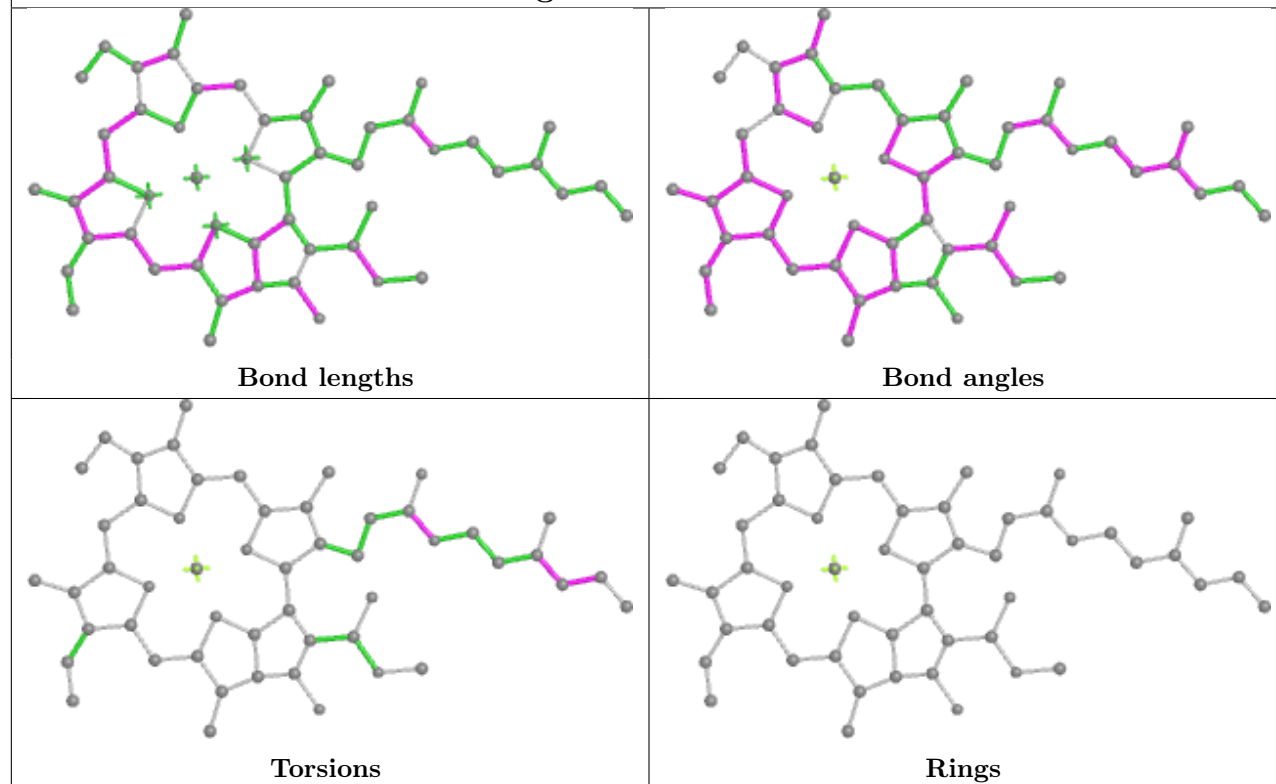
## Ligand CLA 8 302



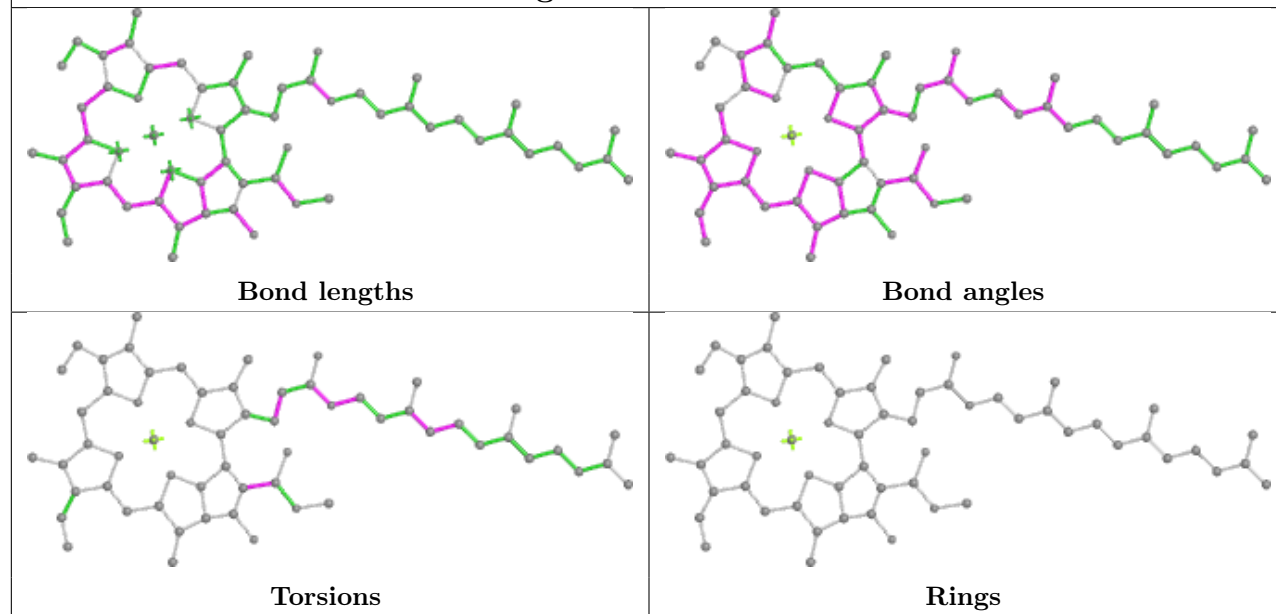
## Ligand CLA A 840



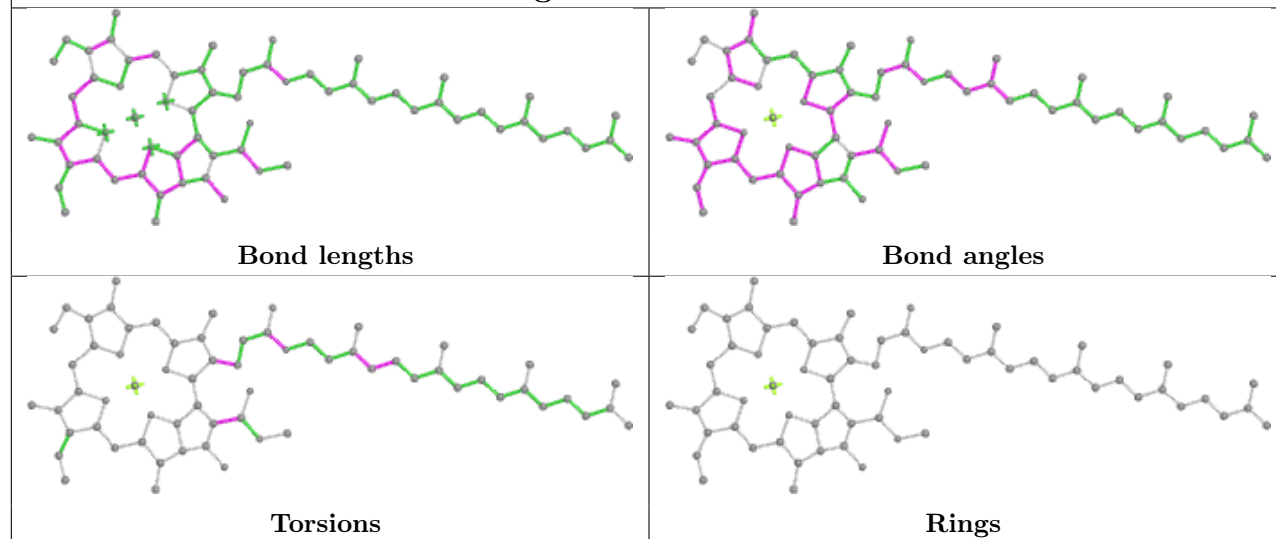
## Ligand CLA 7 611



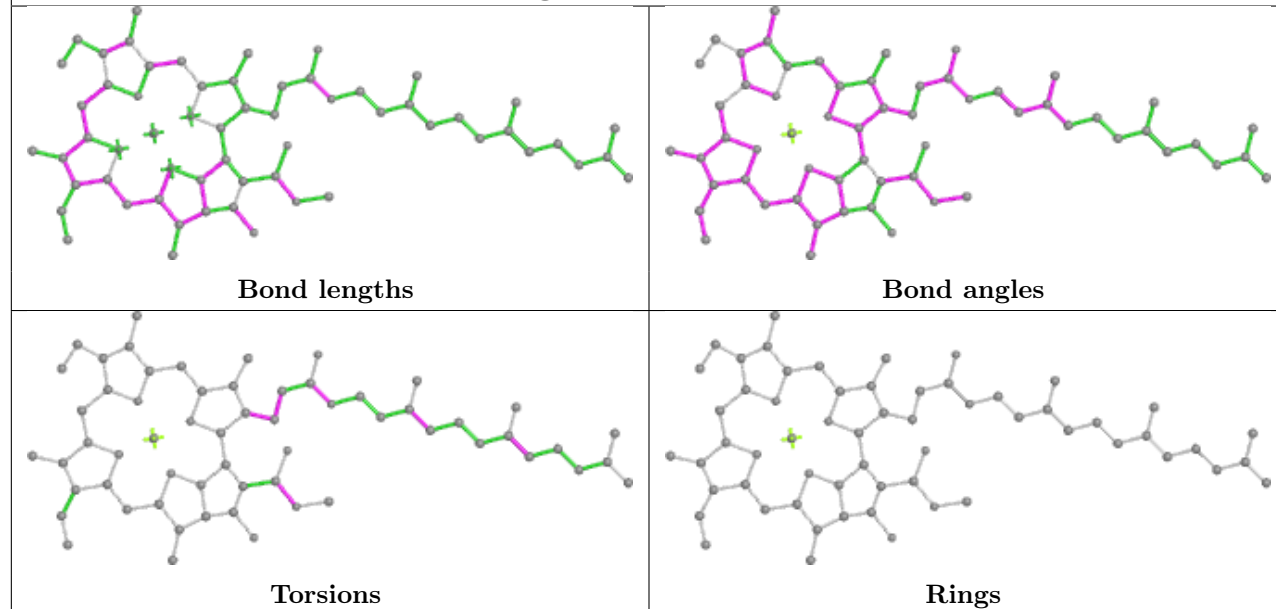
## Ligand CLA 3 302



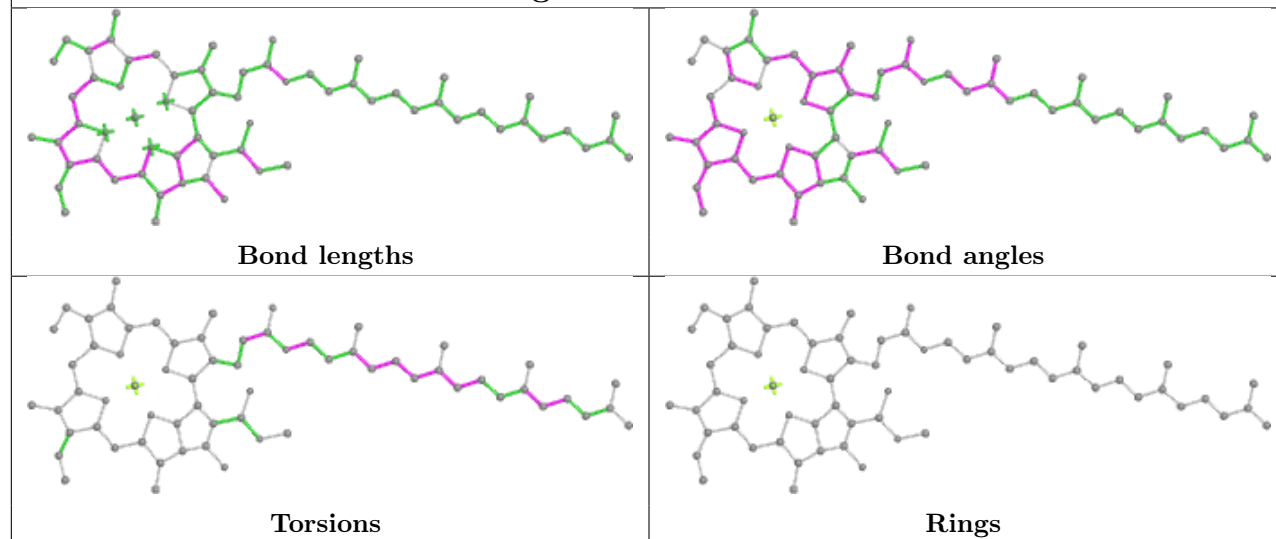
## Ligand CLA L 202



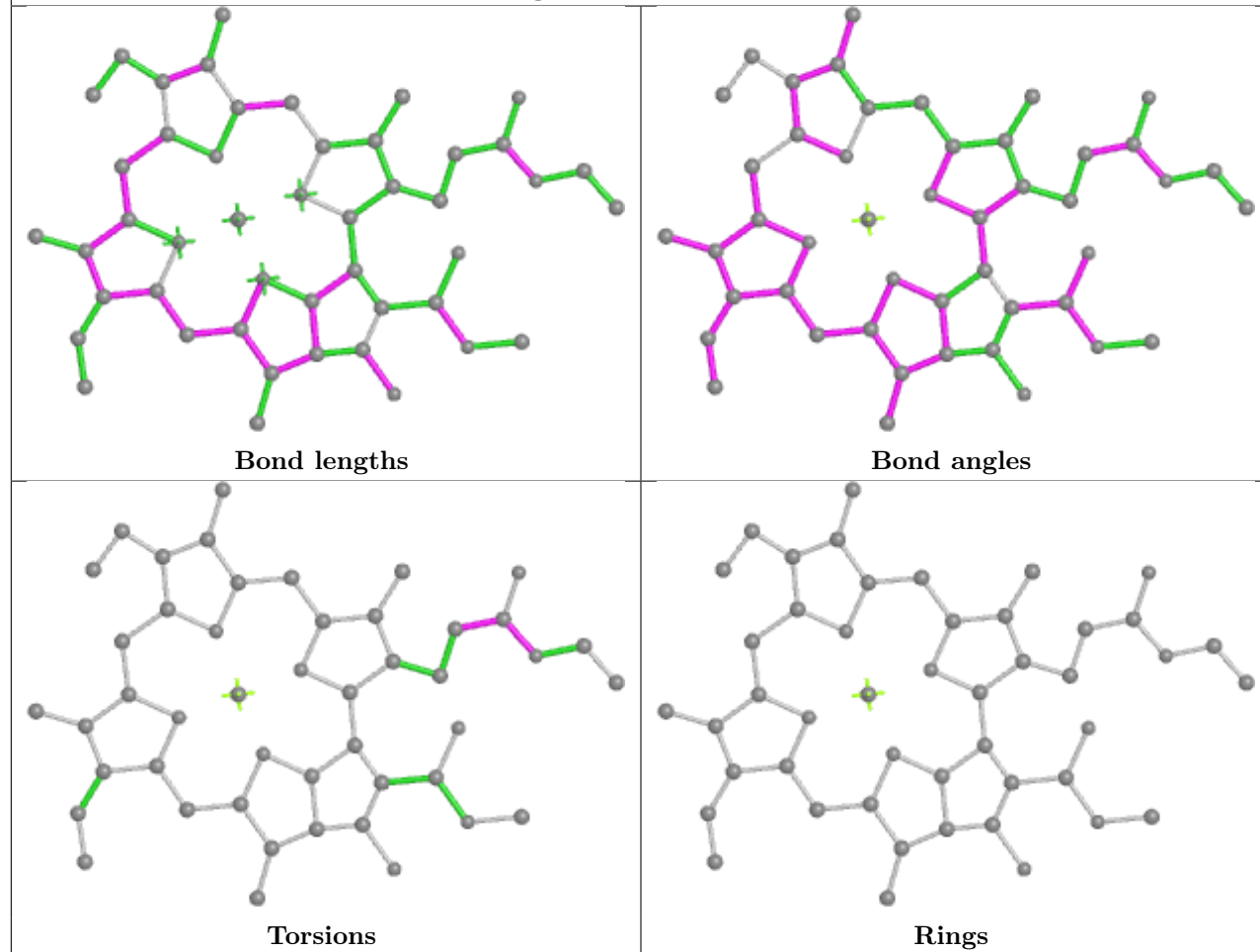
## Ligand CLA 6 311



## Ligand CLA B 802

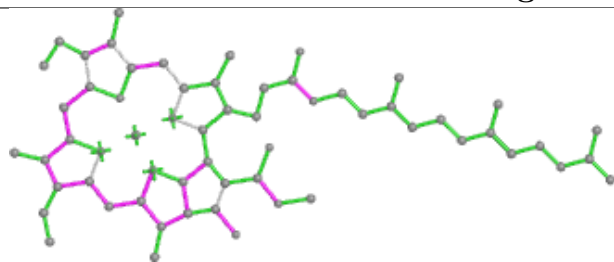


## Ligand CLA 9 614

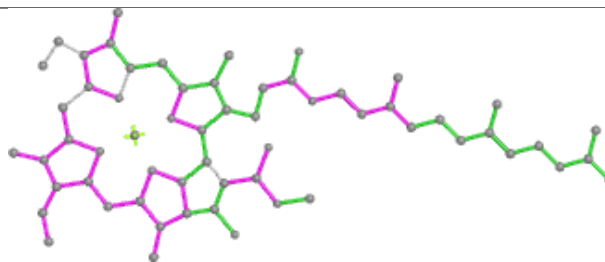




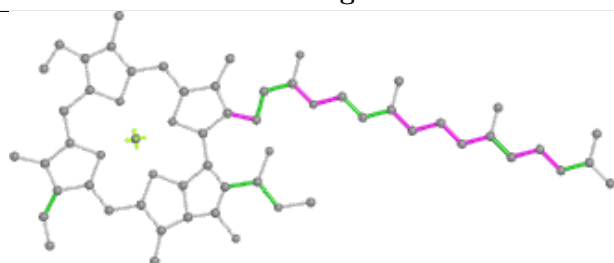
## Ligand CLA b 818



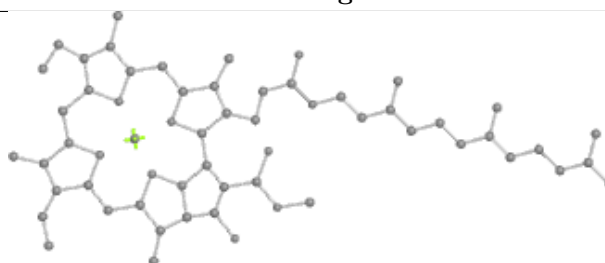
Bond lengths



Bond angles

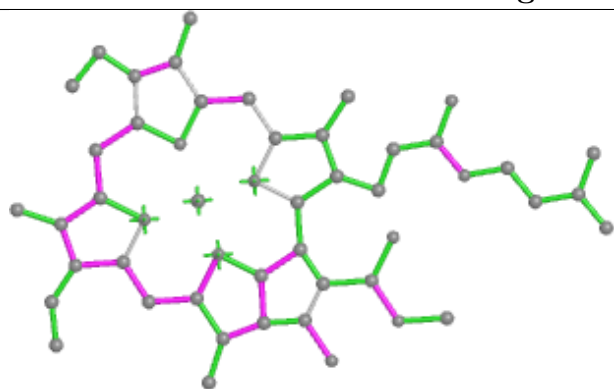


Torsions

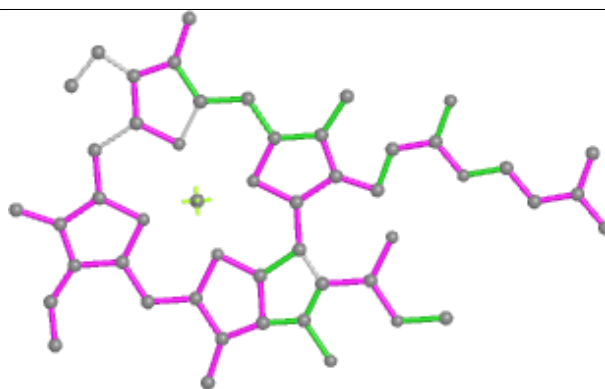


Rings

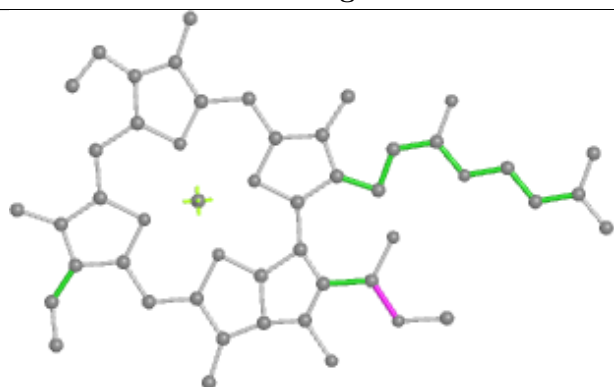
## Ligand CLA b 820



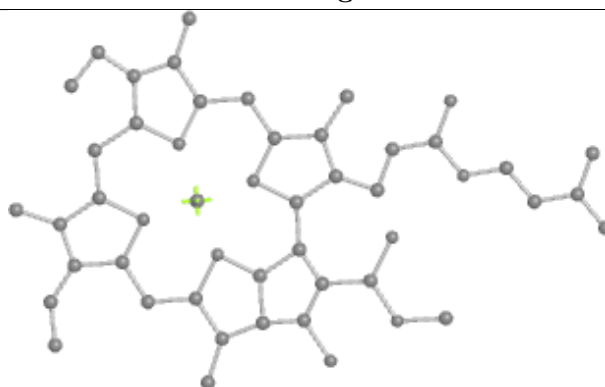
Bond lengths



Bond angles

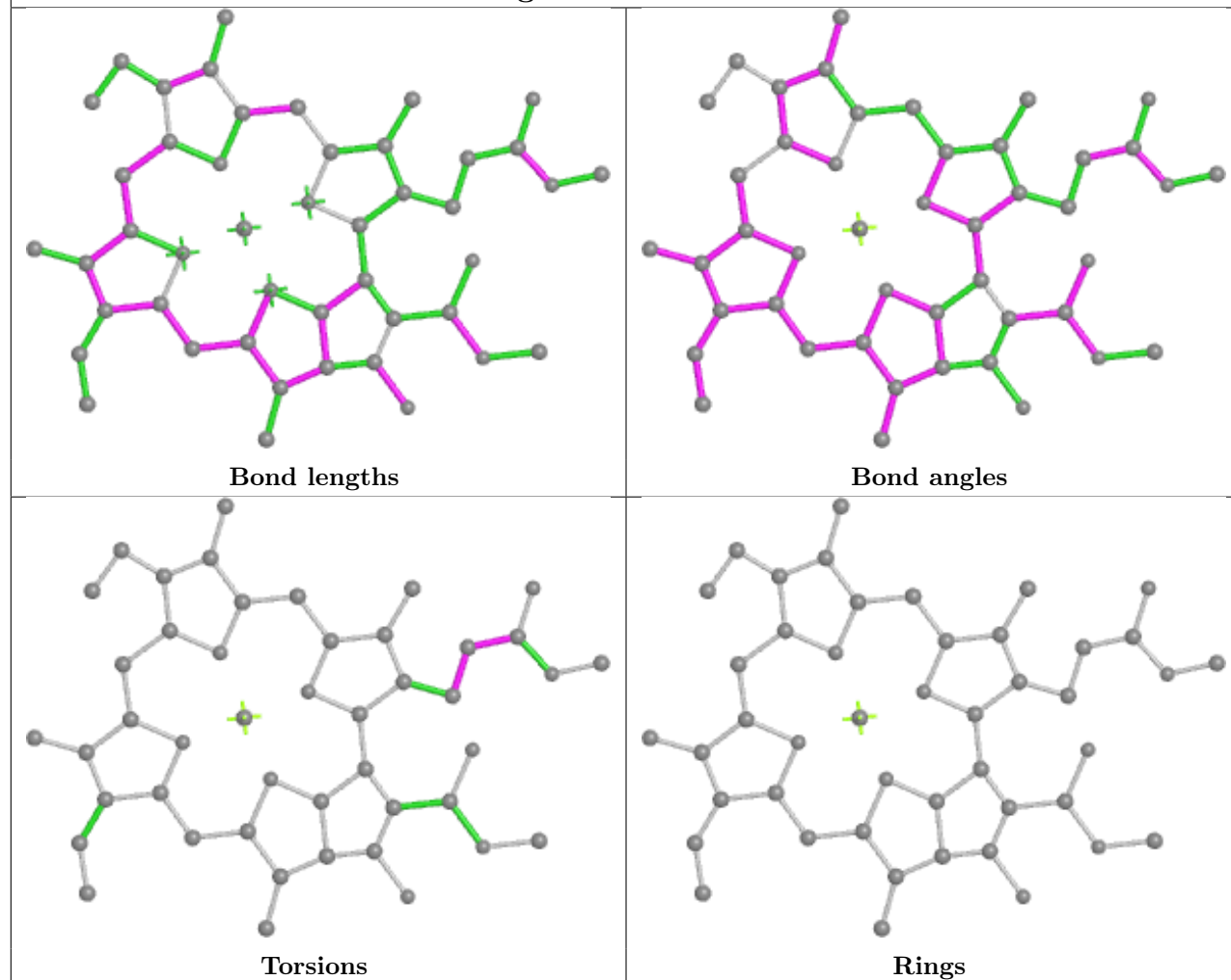


Torsions

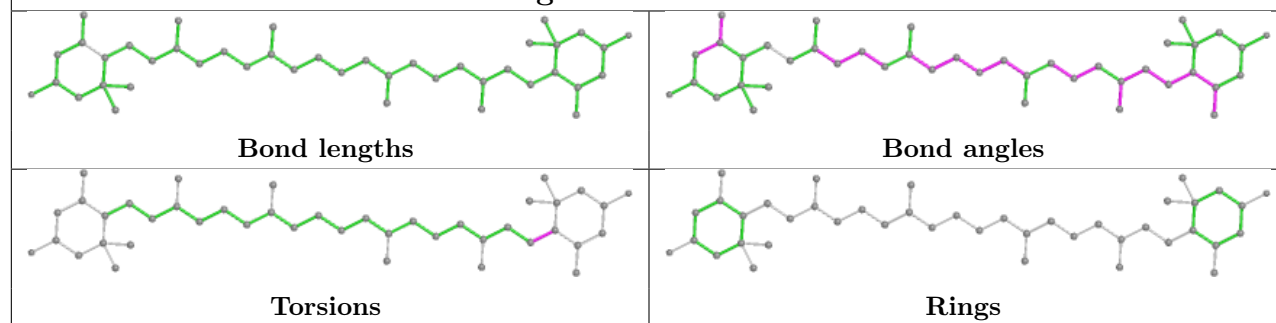


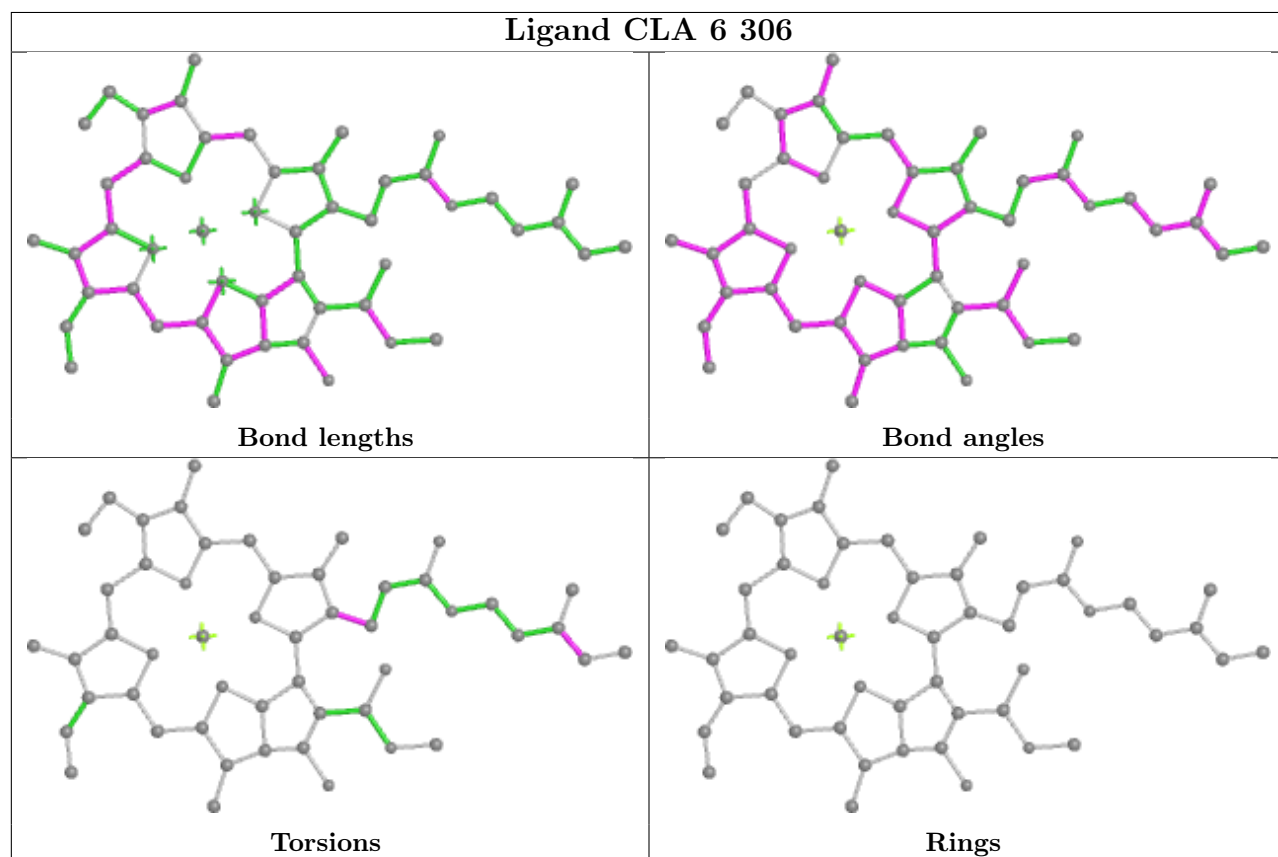
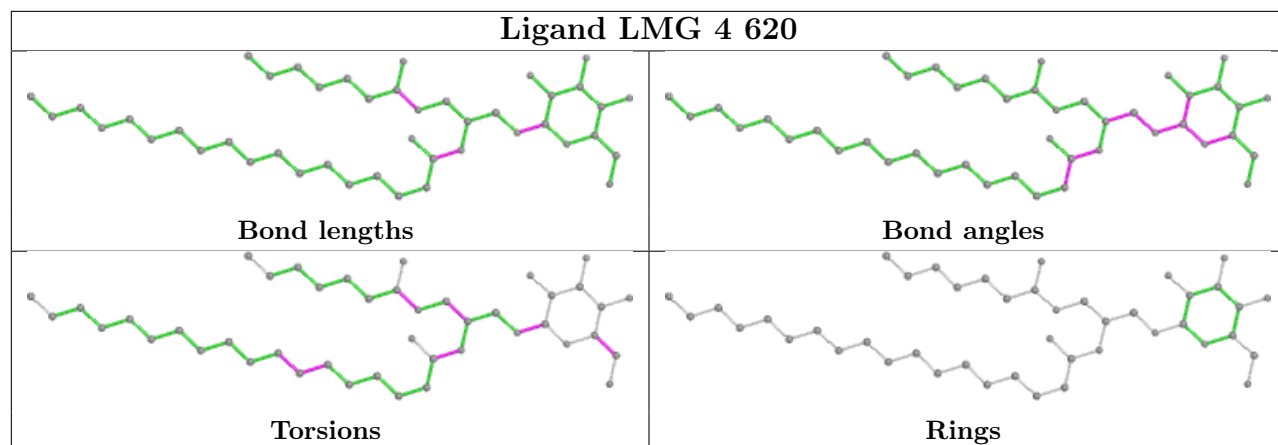
Rings

## Ligand CLA 6 316

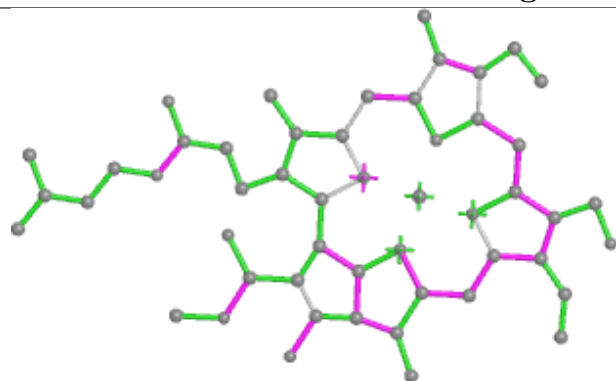


## Ligand LUT 8 314

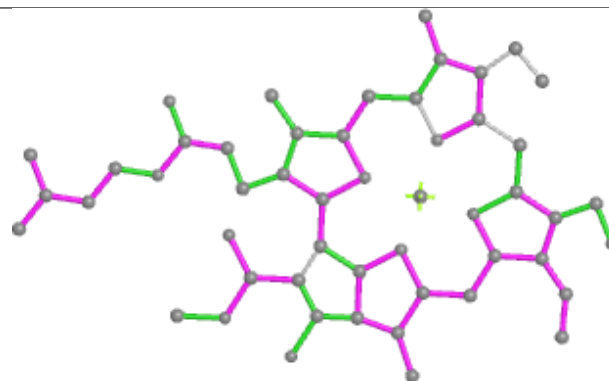




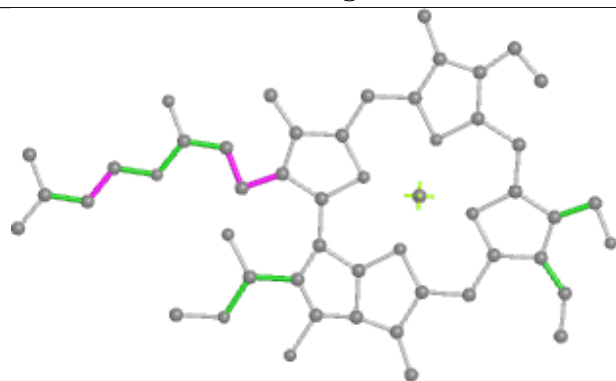
## Ligand CHL 9 606



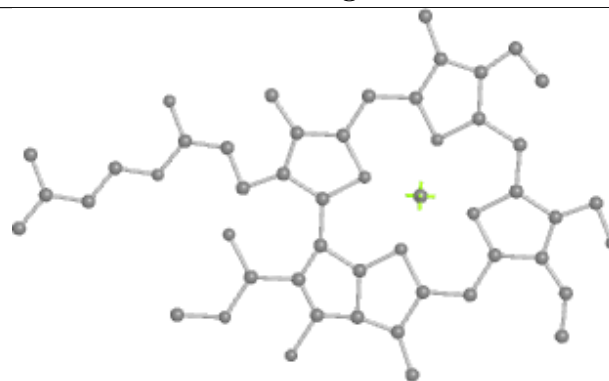
Bond lengths



Bond angles

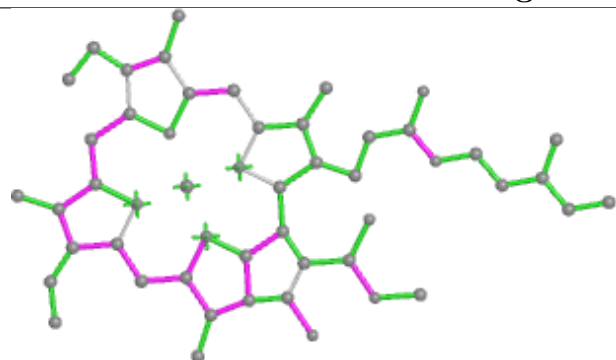


Torsions

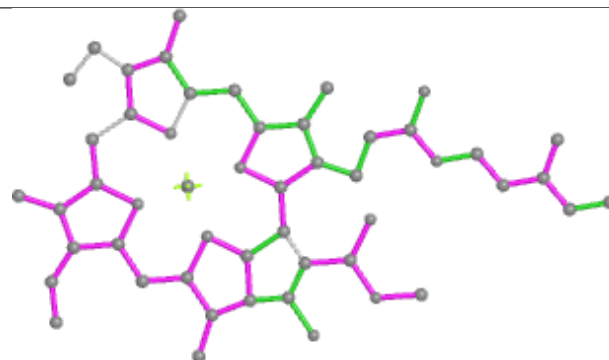


Rings

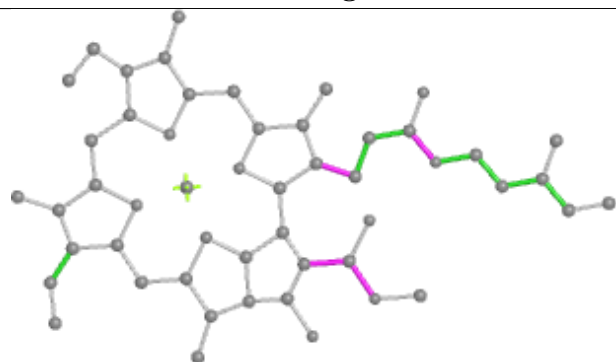
## Ligand CLA A 824



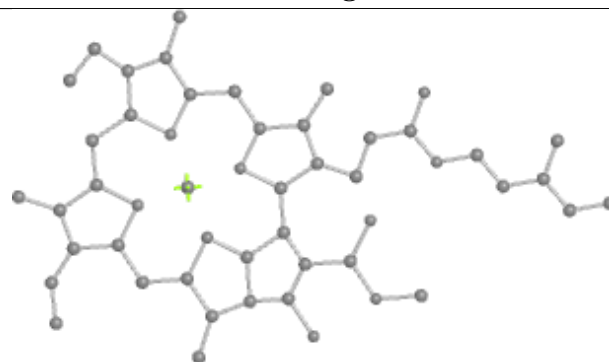
Bond lengths



Bond angles

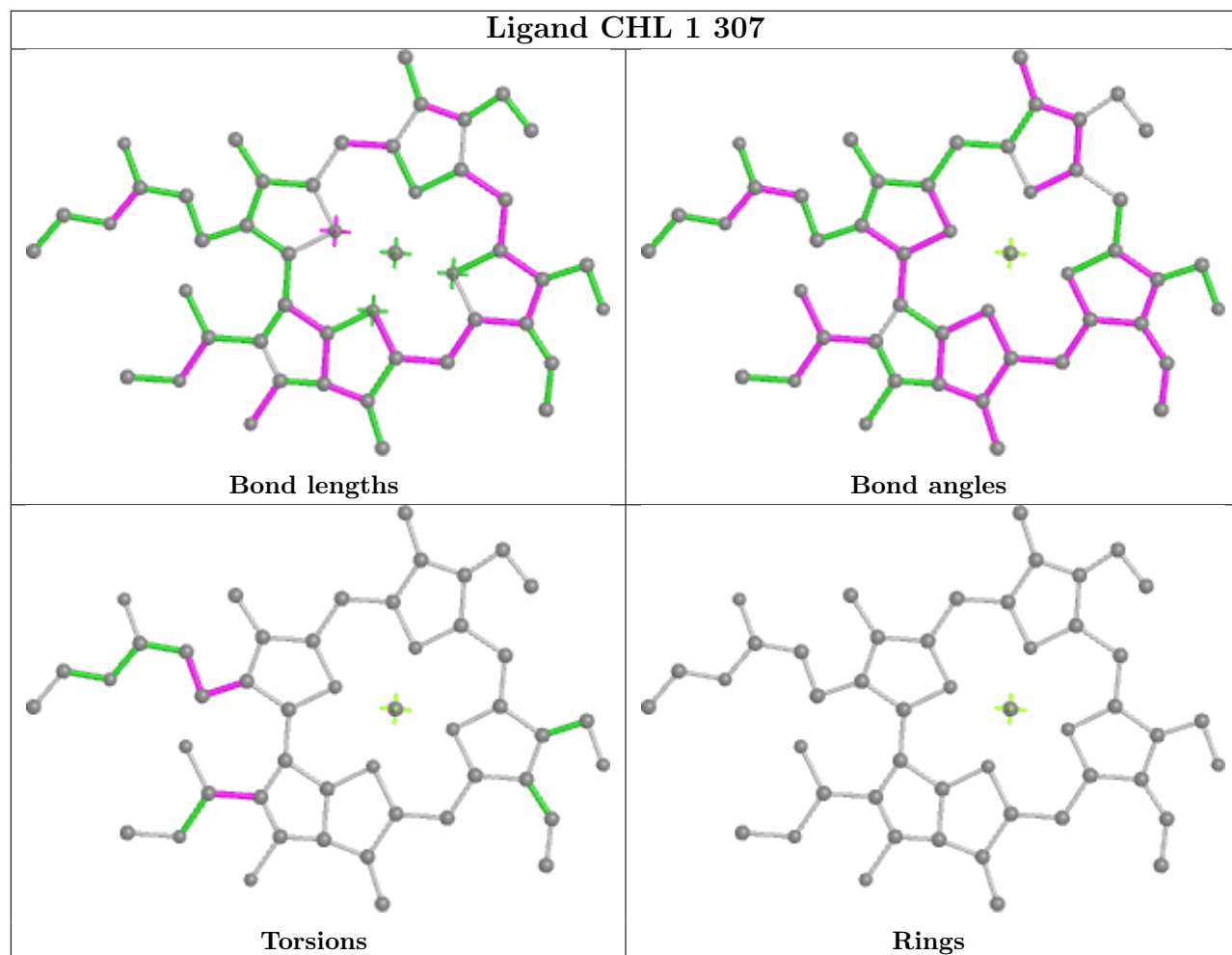


Torsions

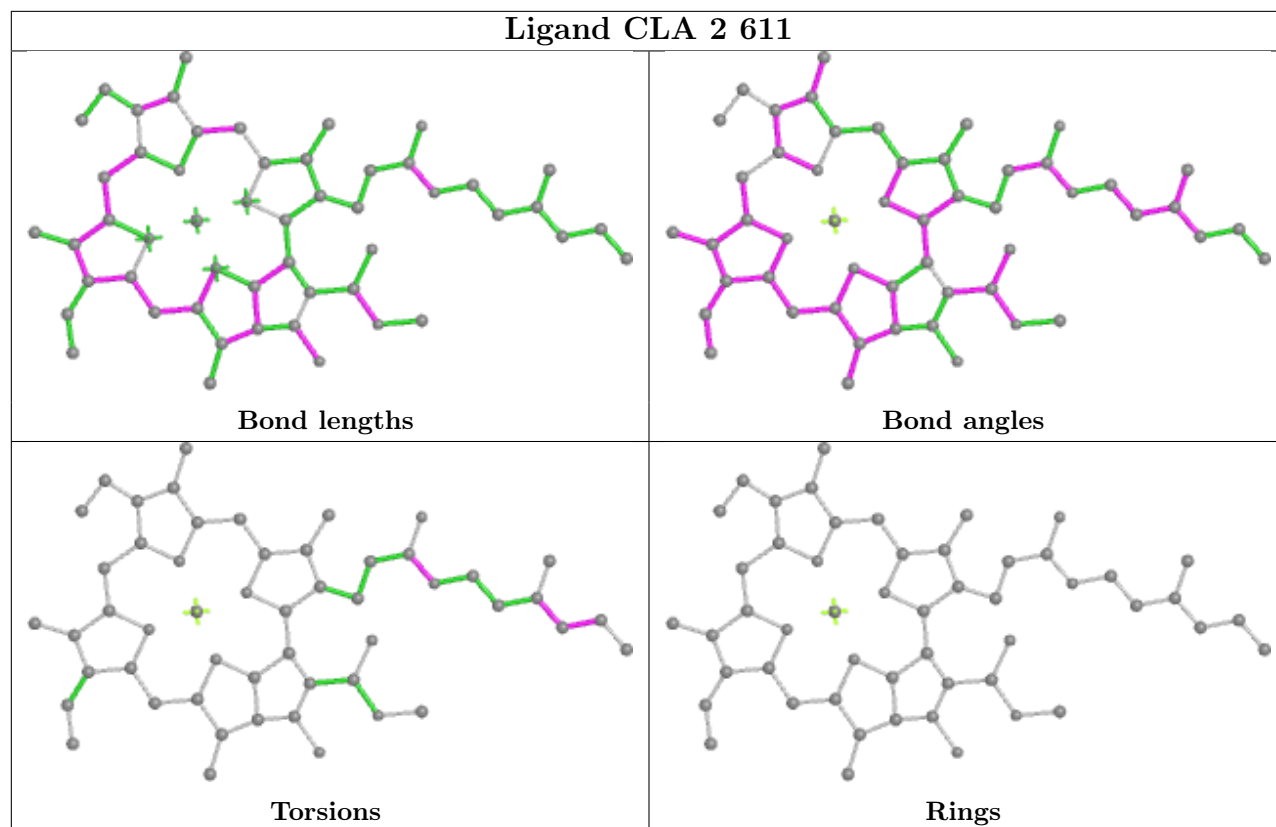


Rings

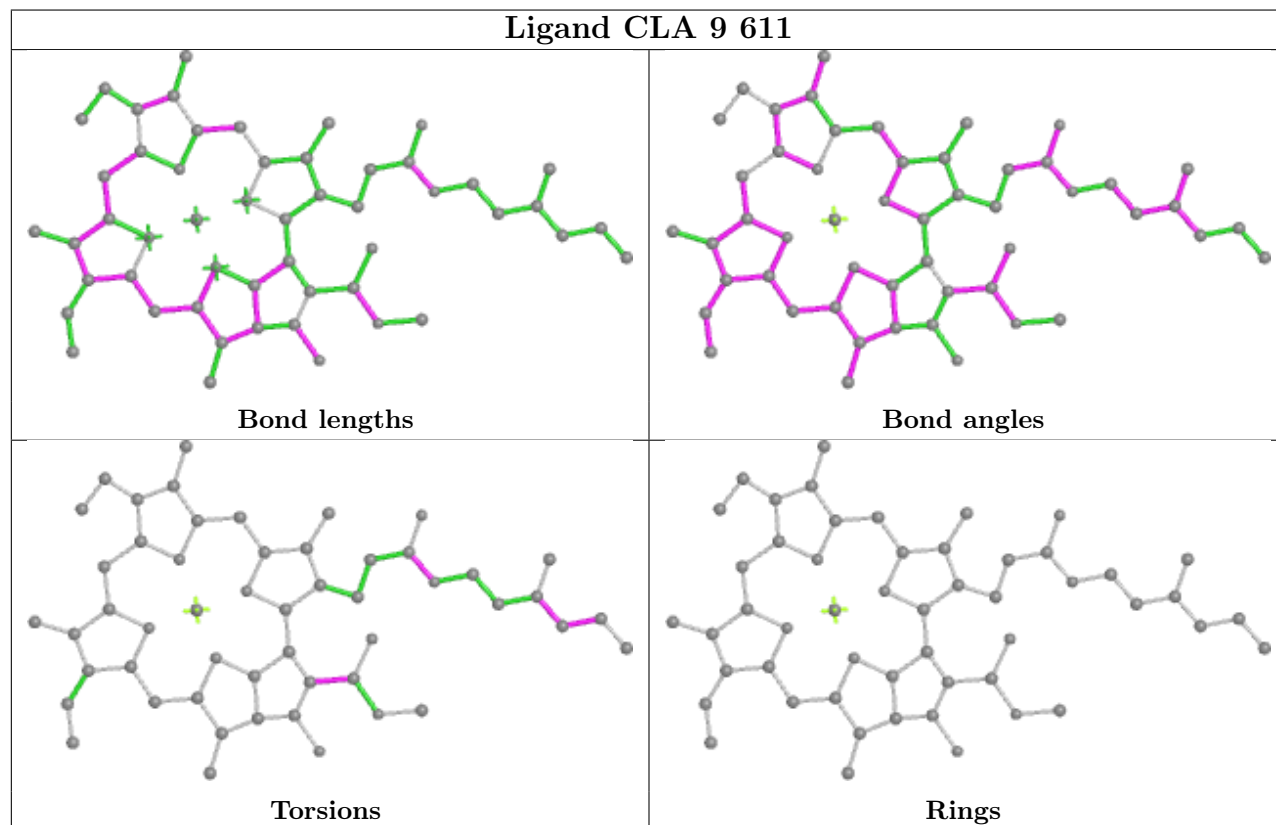
## Ligand CHL 1 307

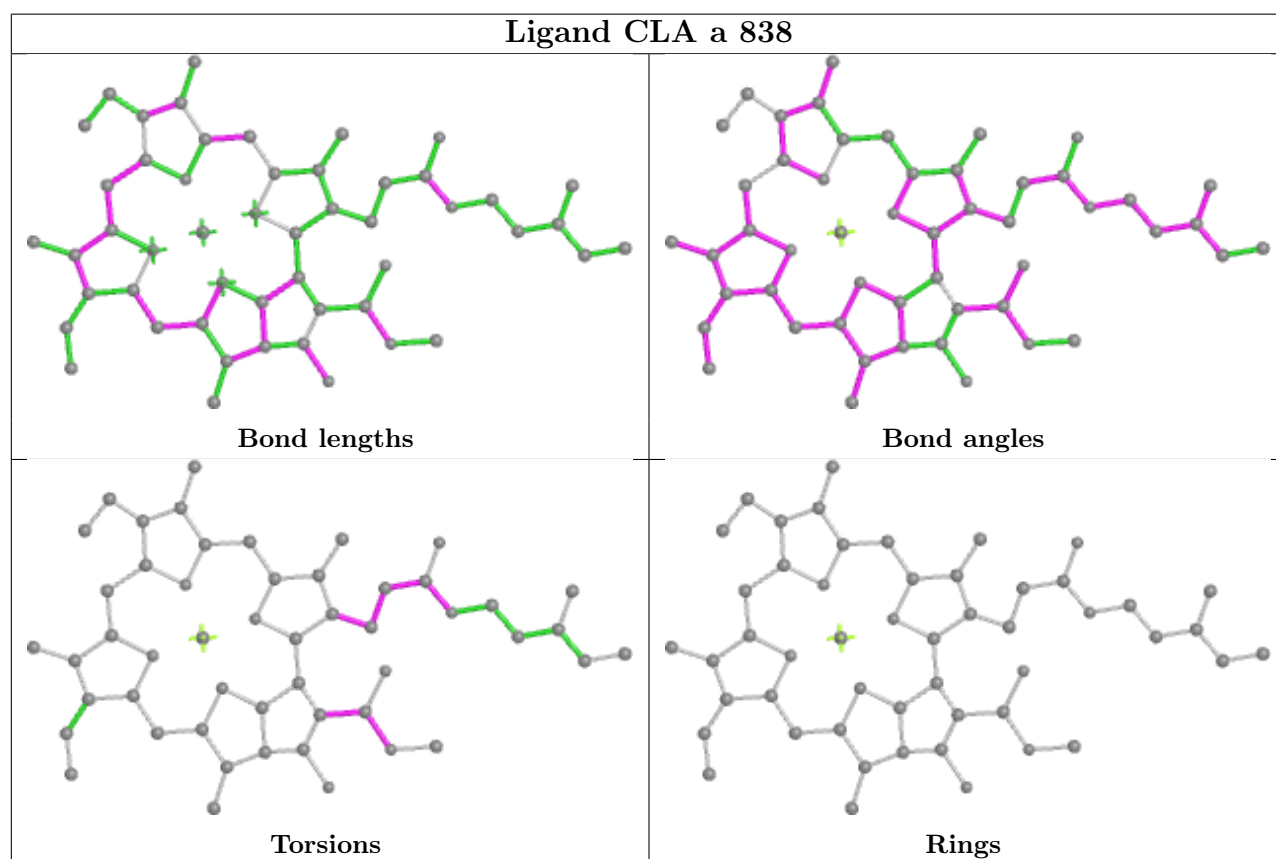
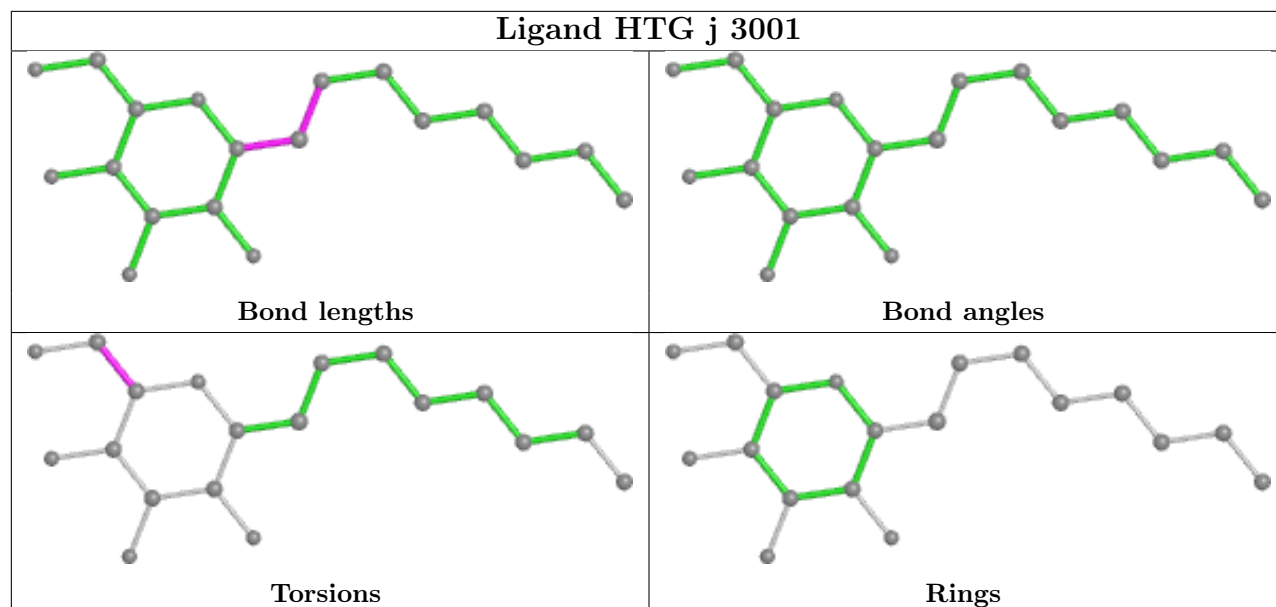


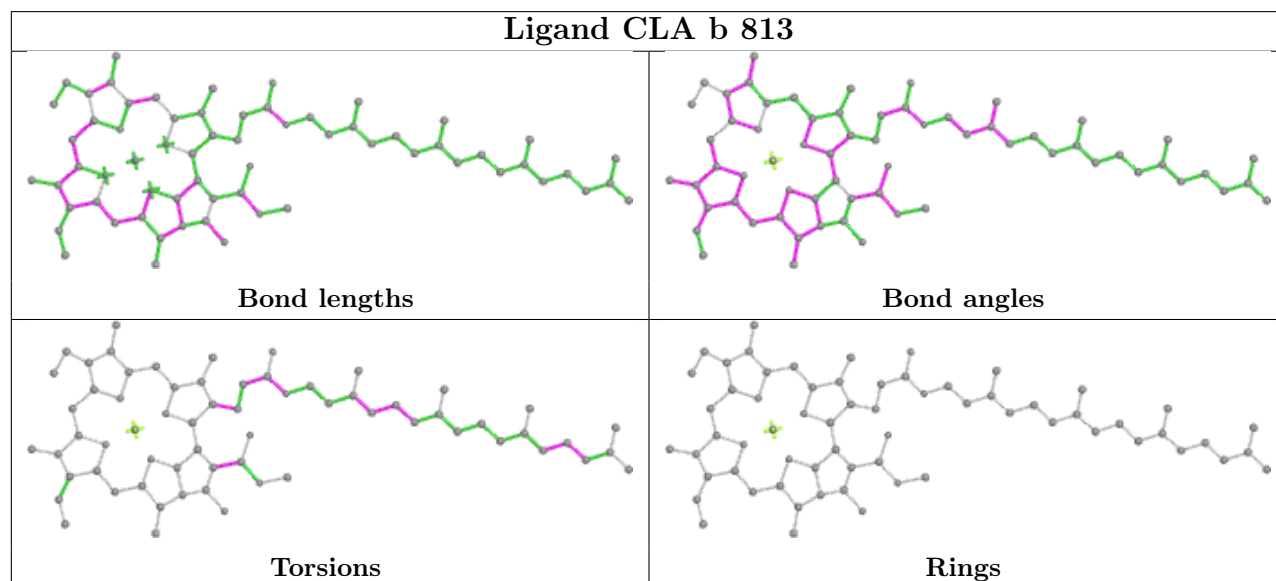
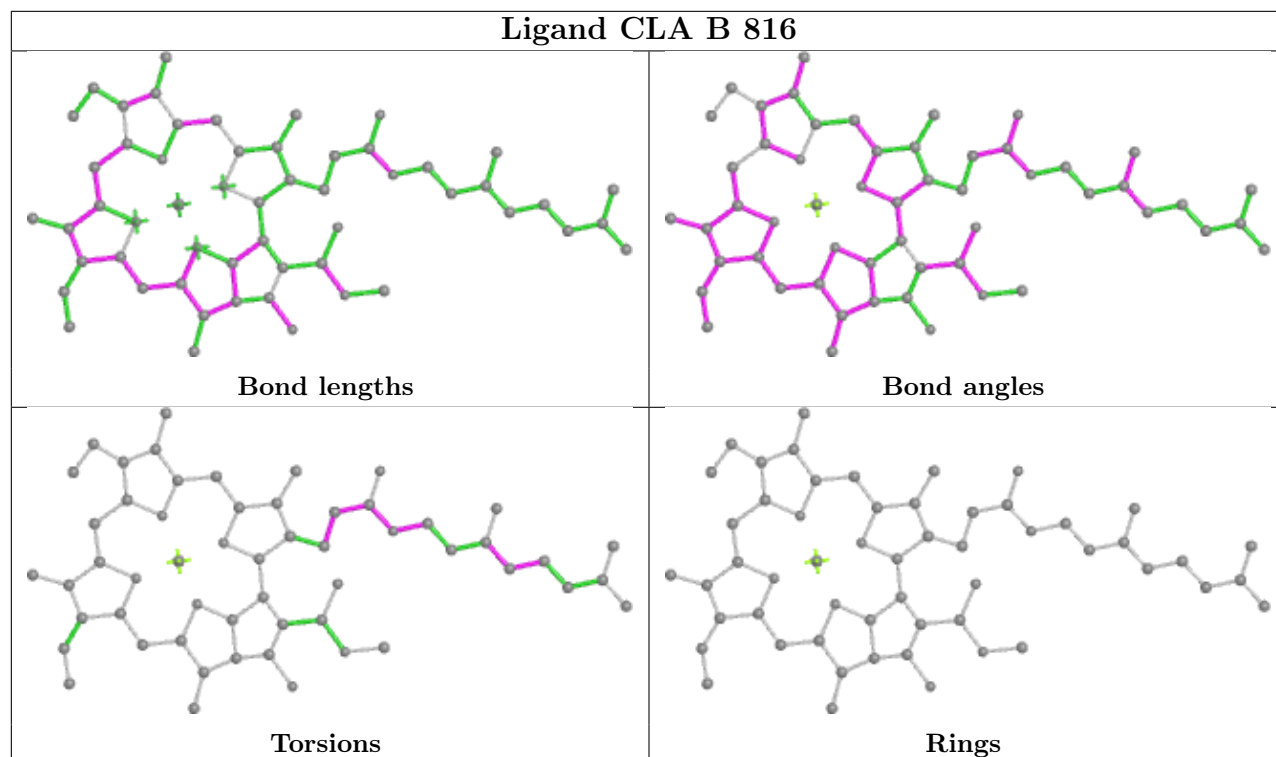
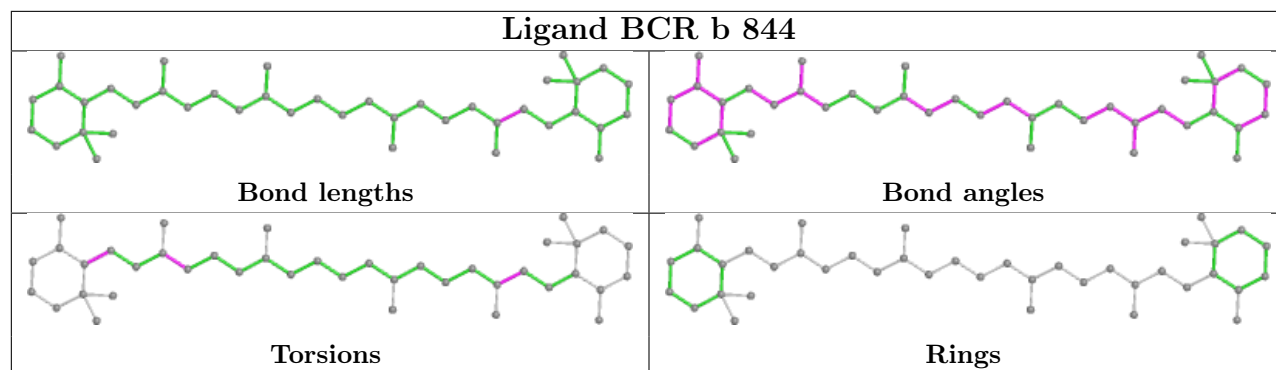
## Ligand CLA 2 611



## Ligand CLA 9 611

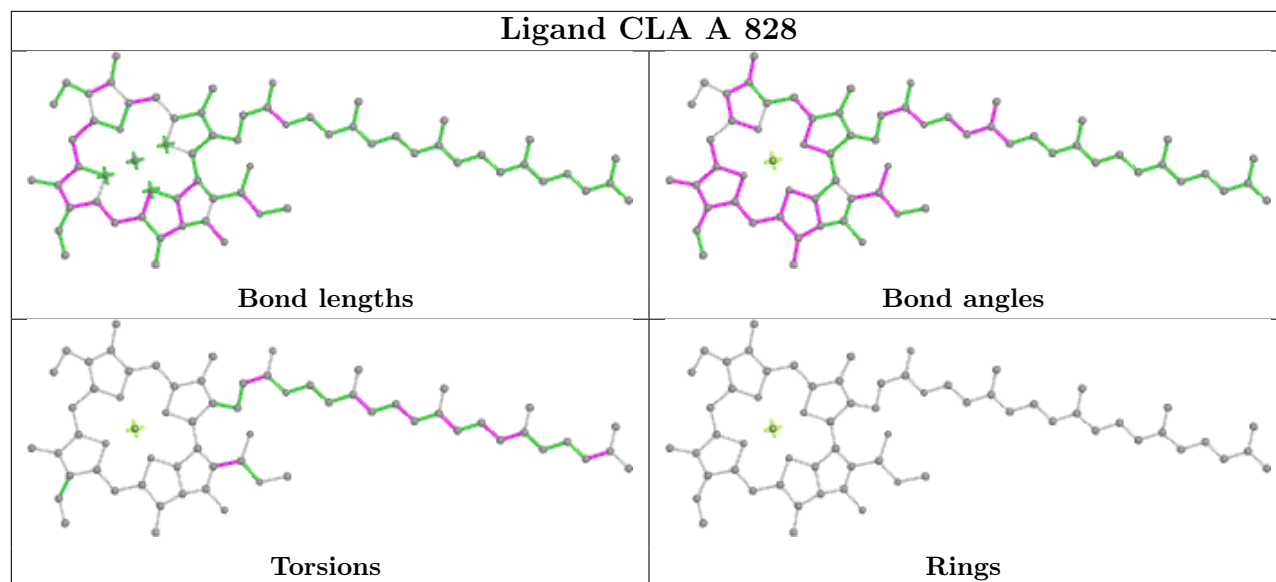




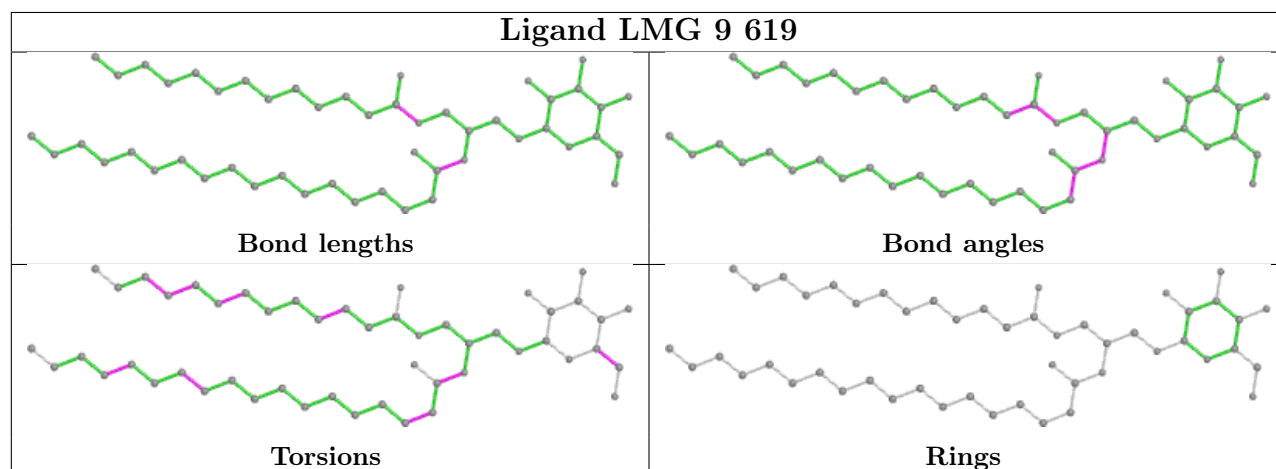




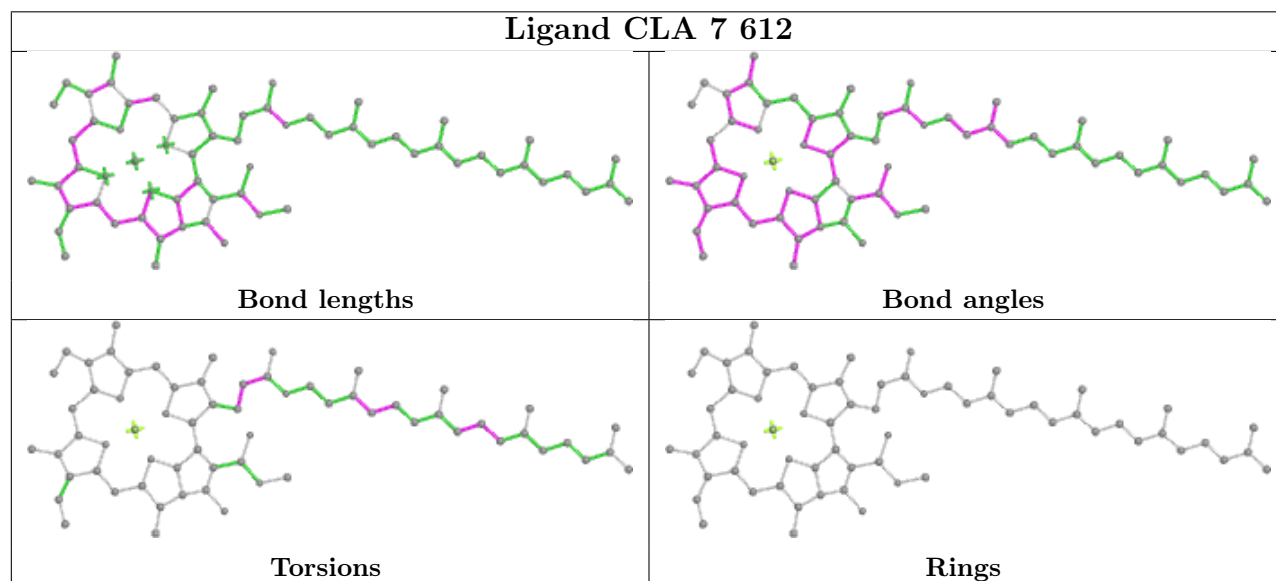
## Ligand CLA A 828

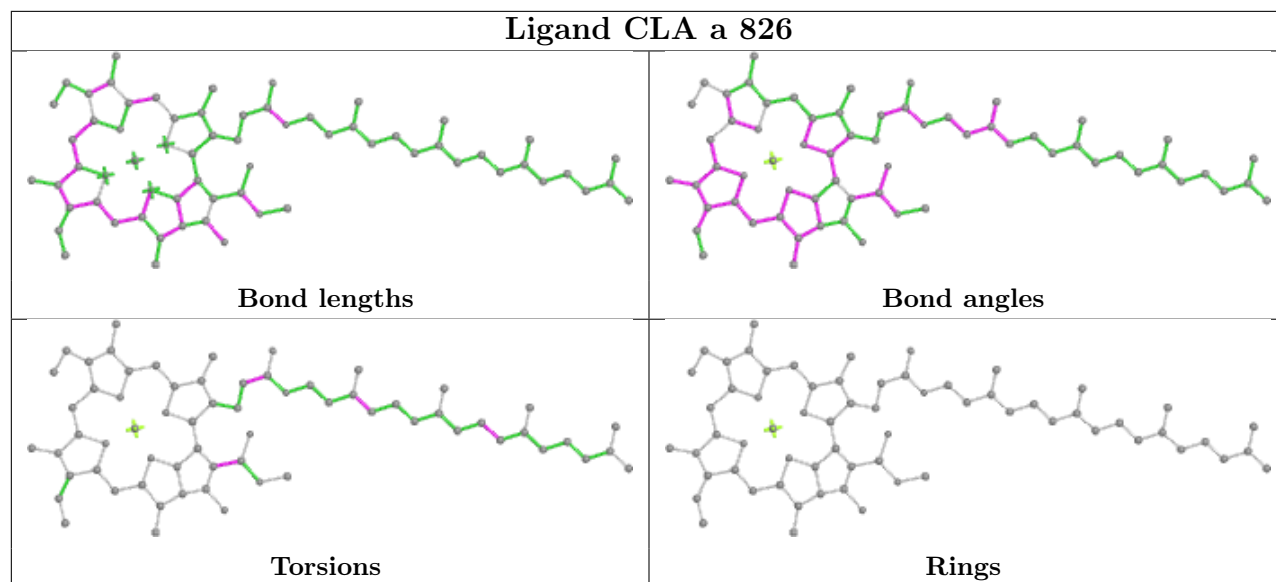
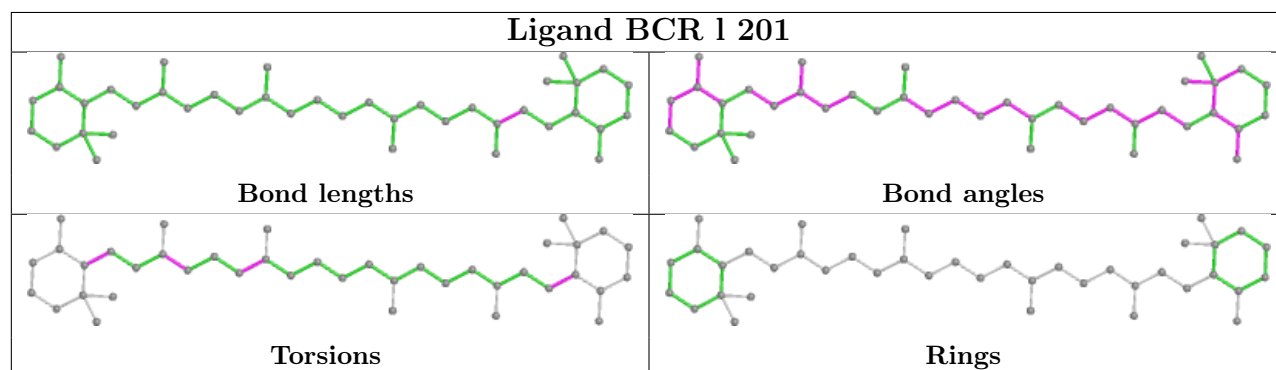
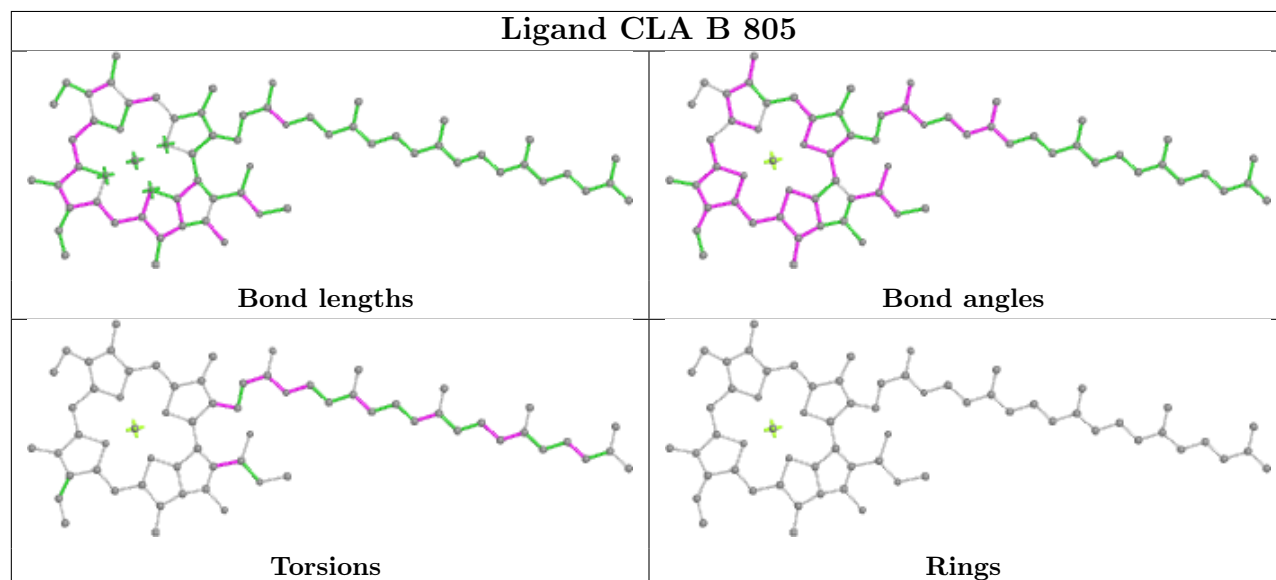


## Ligand LMG 9 619

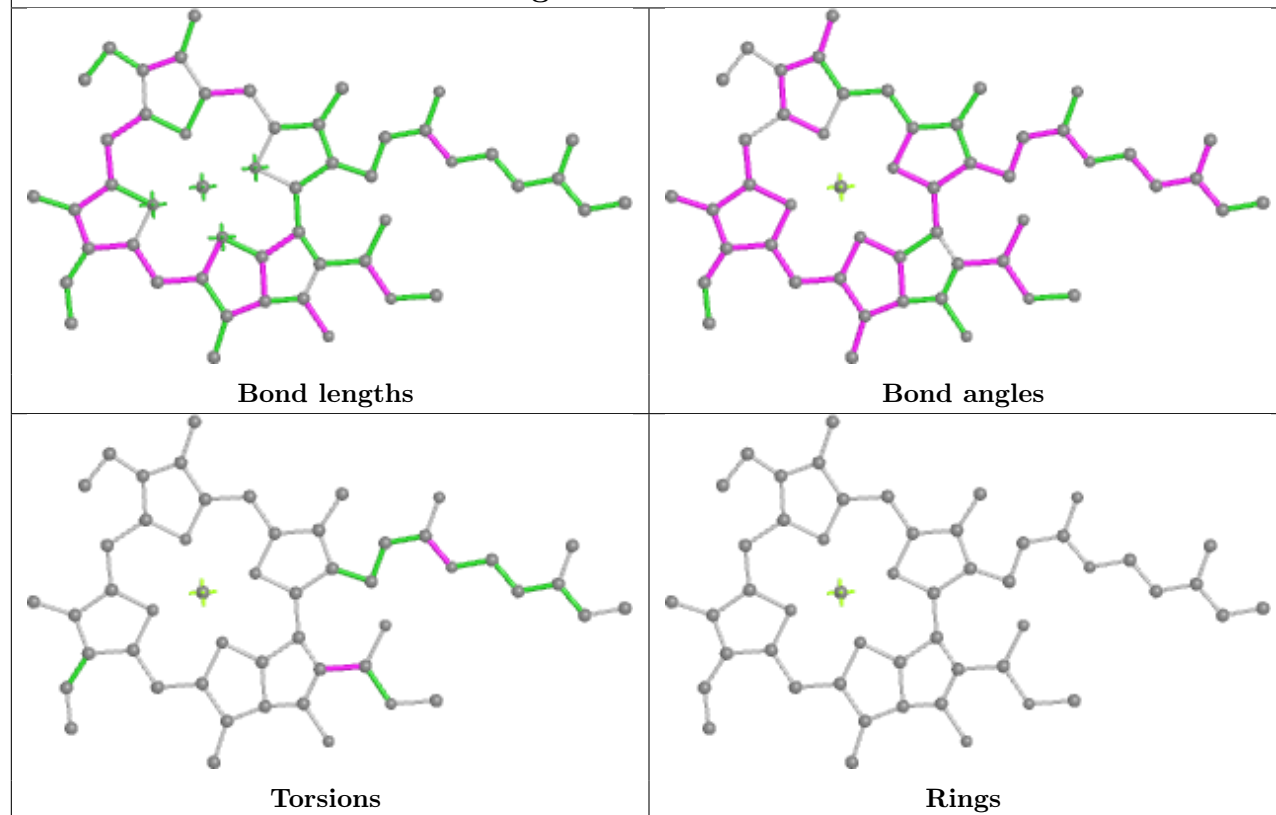


## Ligand CLA 7 612

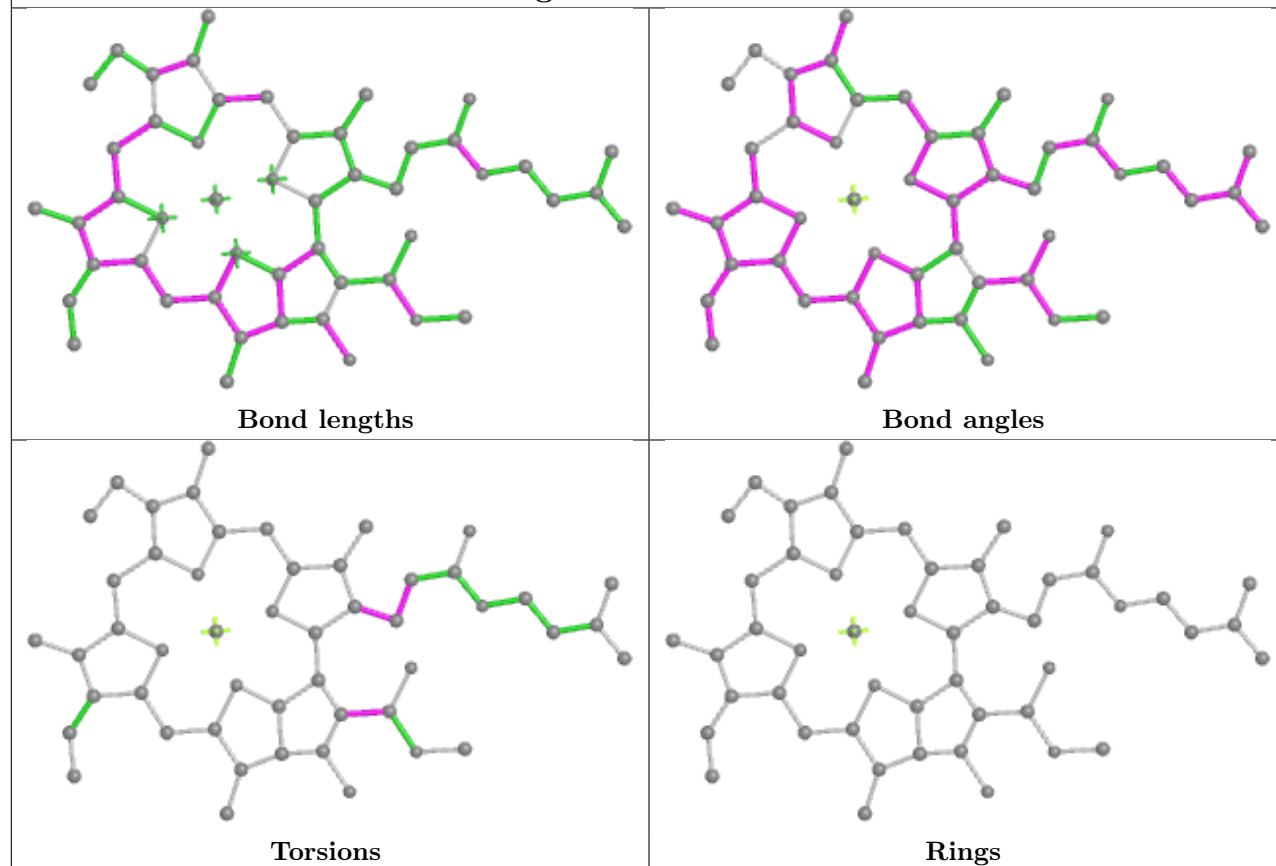


**Ligand CLA a 826****Ligand BCR 1 201****Ligand CLA B 805**

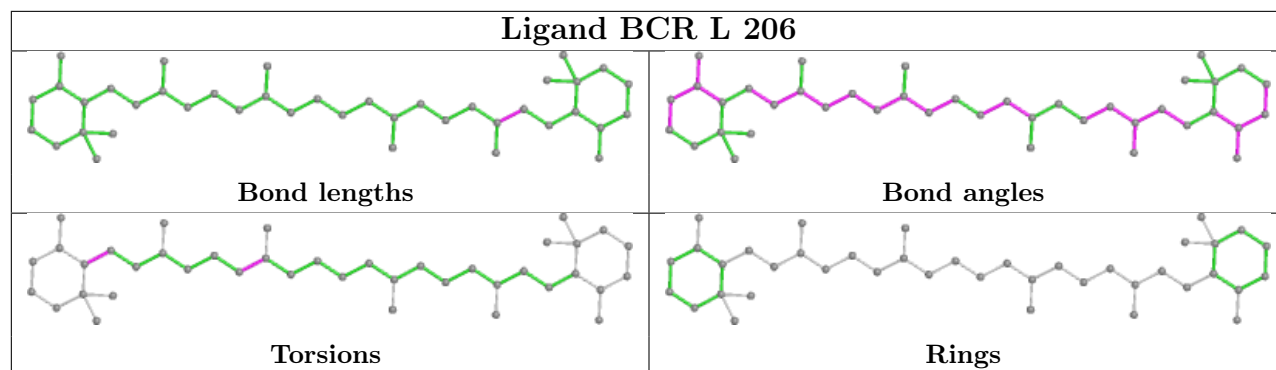
## Ligand CLA A 838



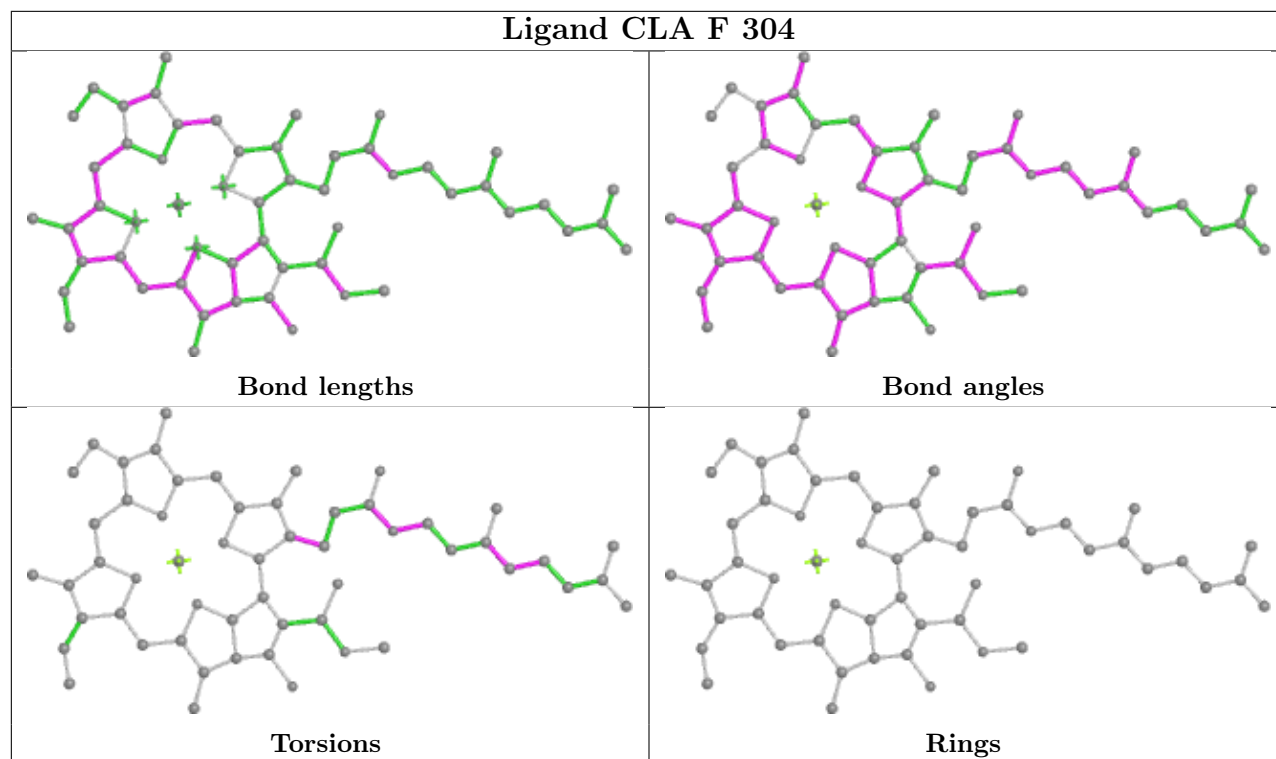
## Ligand CLA b 830



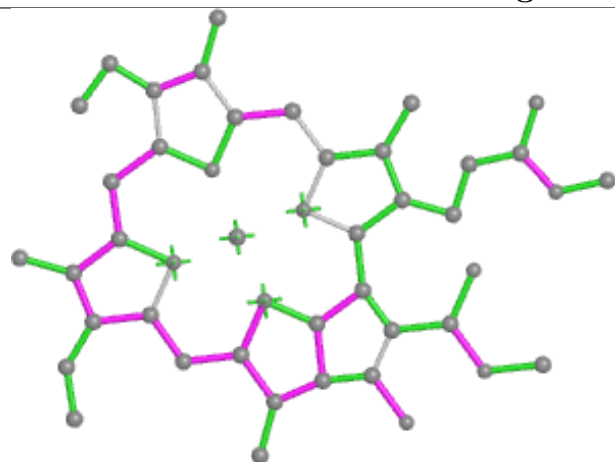
## Ligand BCR L 206



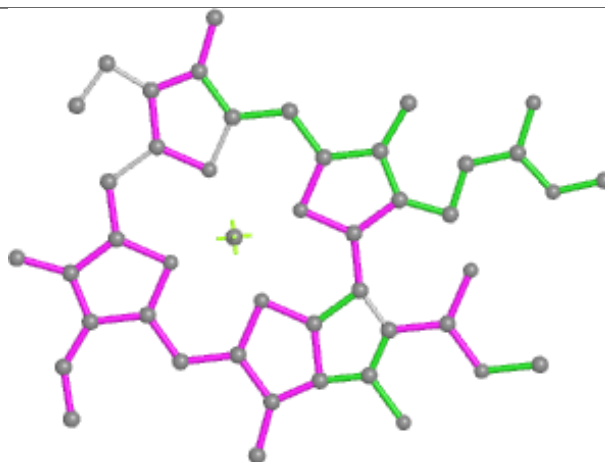
## Ligand CLA F 304



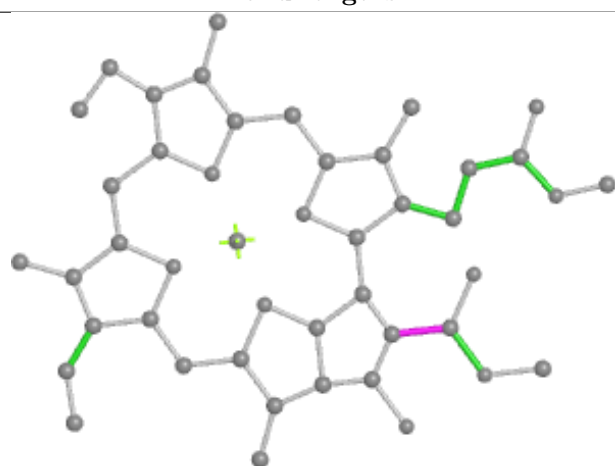
## Ligand CLA B 821



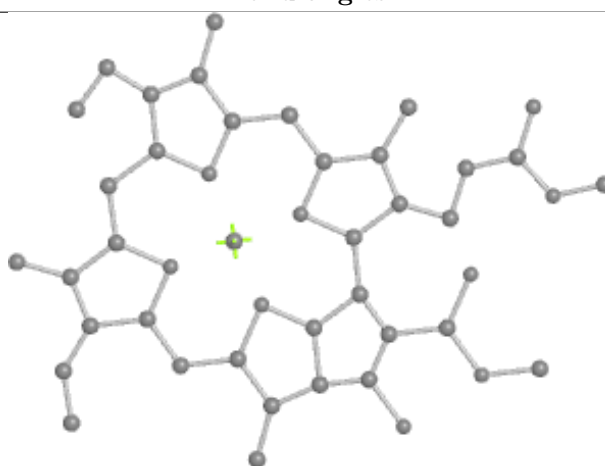
Bond lengths



Bond angles

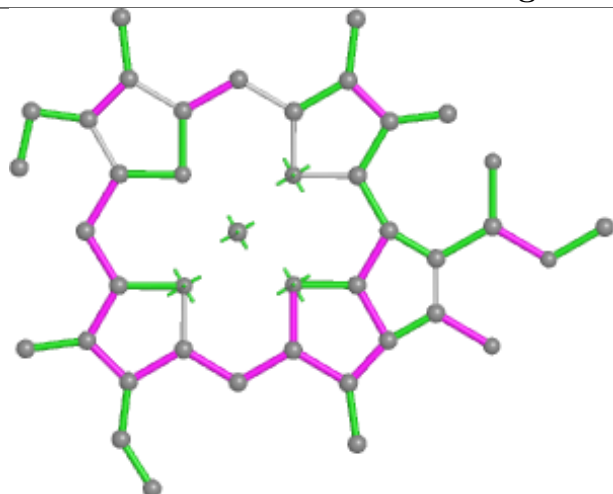


Torsions

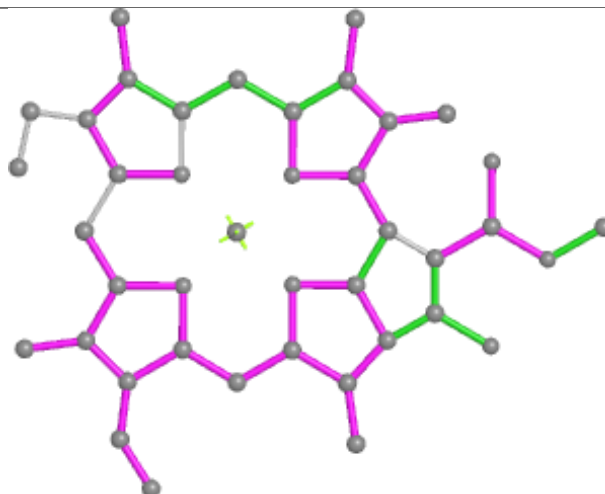


Rings

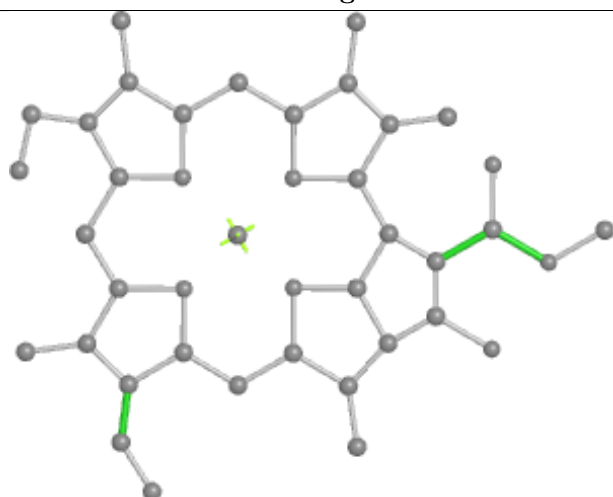
## Ligand CLA 2 610



Bond lengths



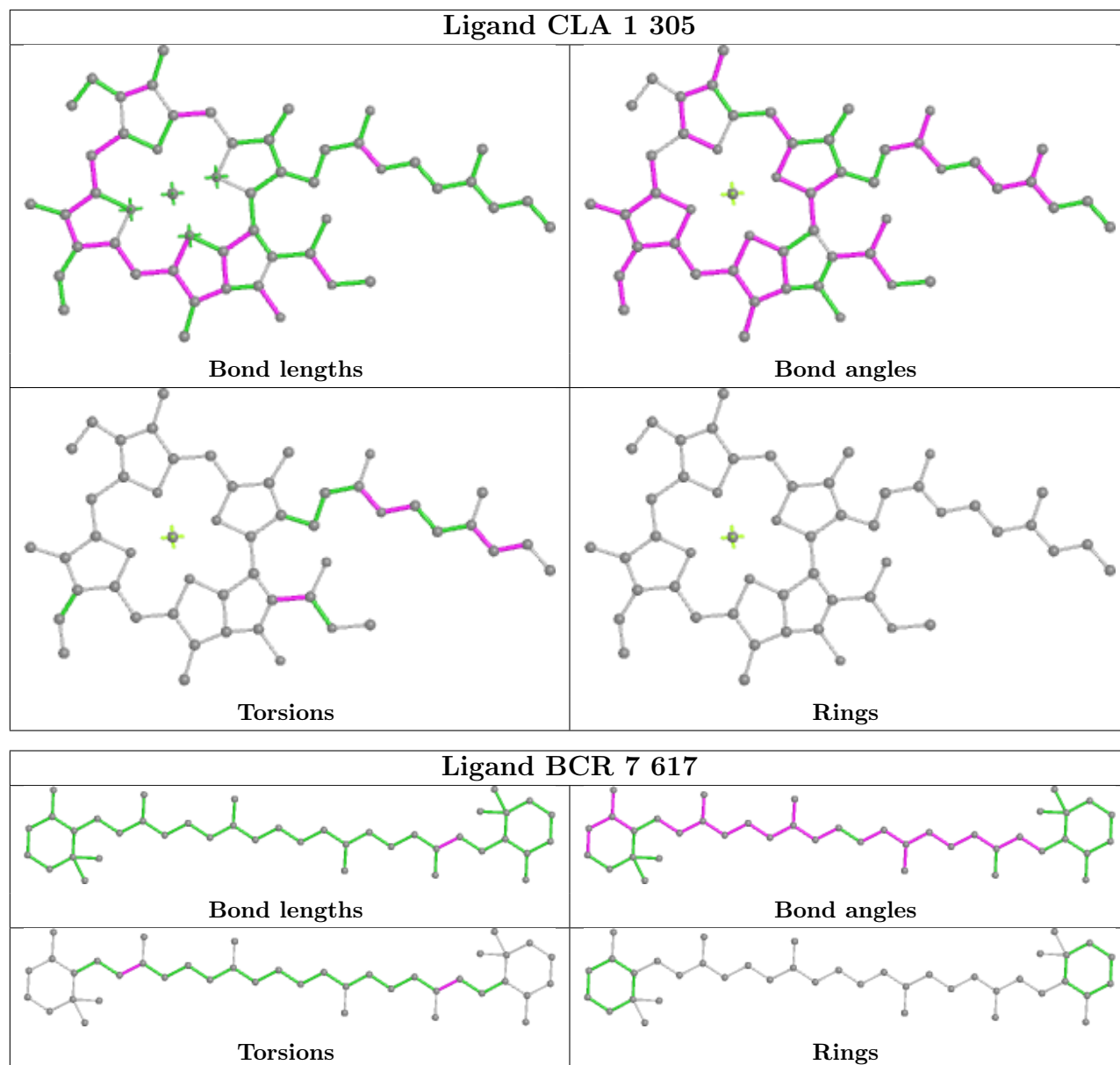
Bond angles



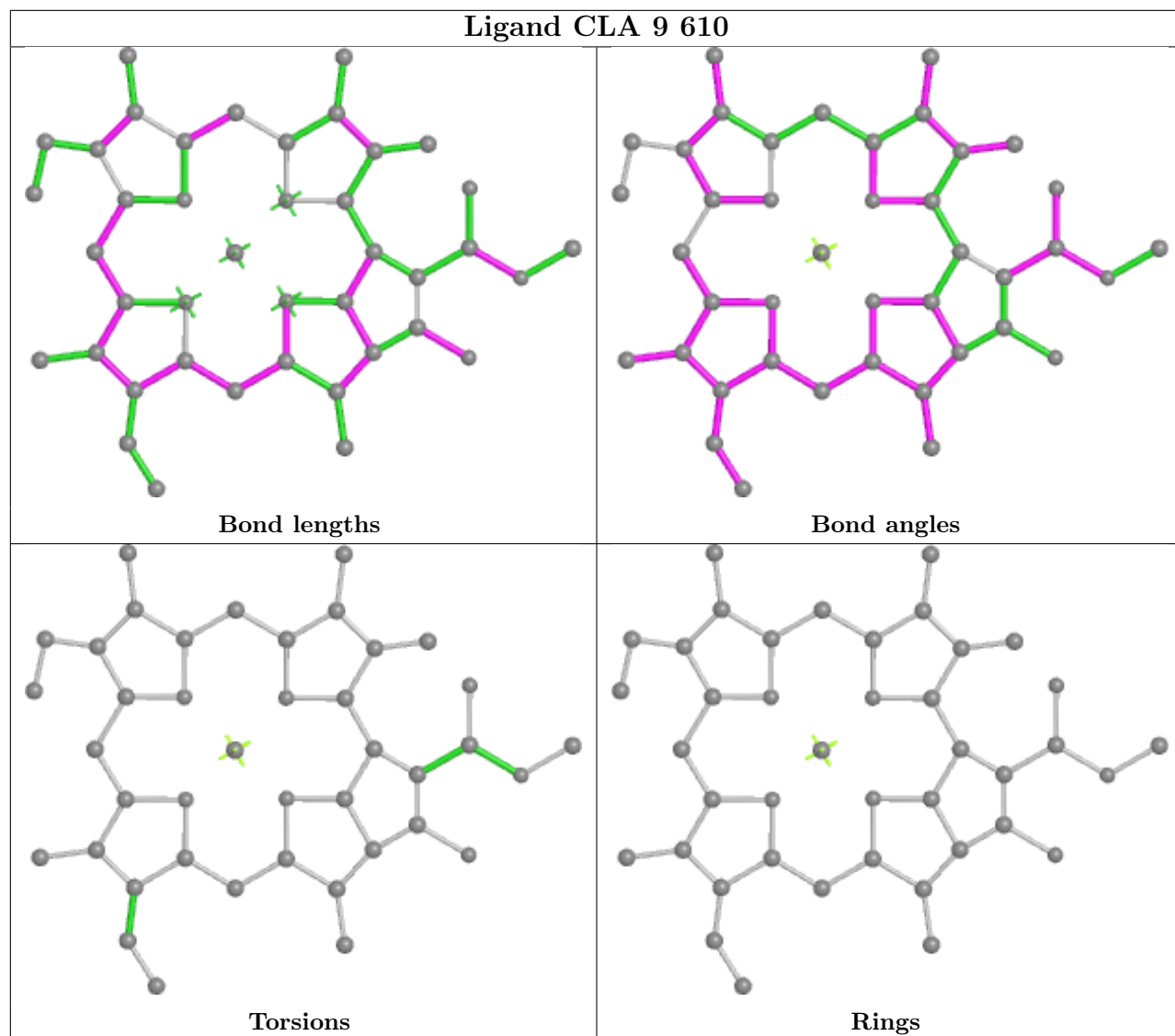
Torsions



Rings

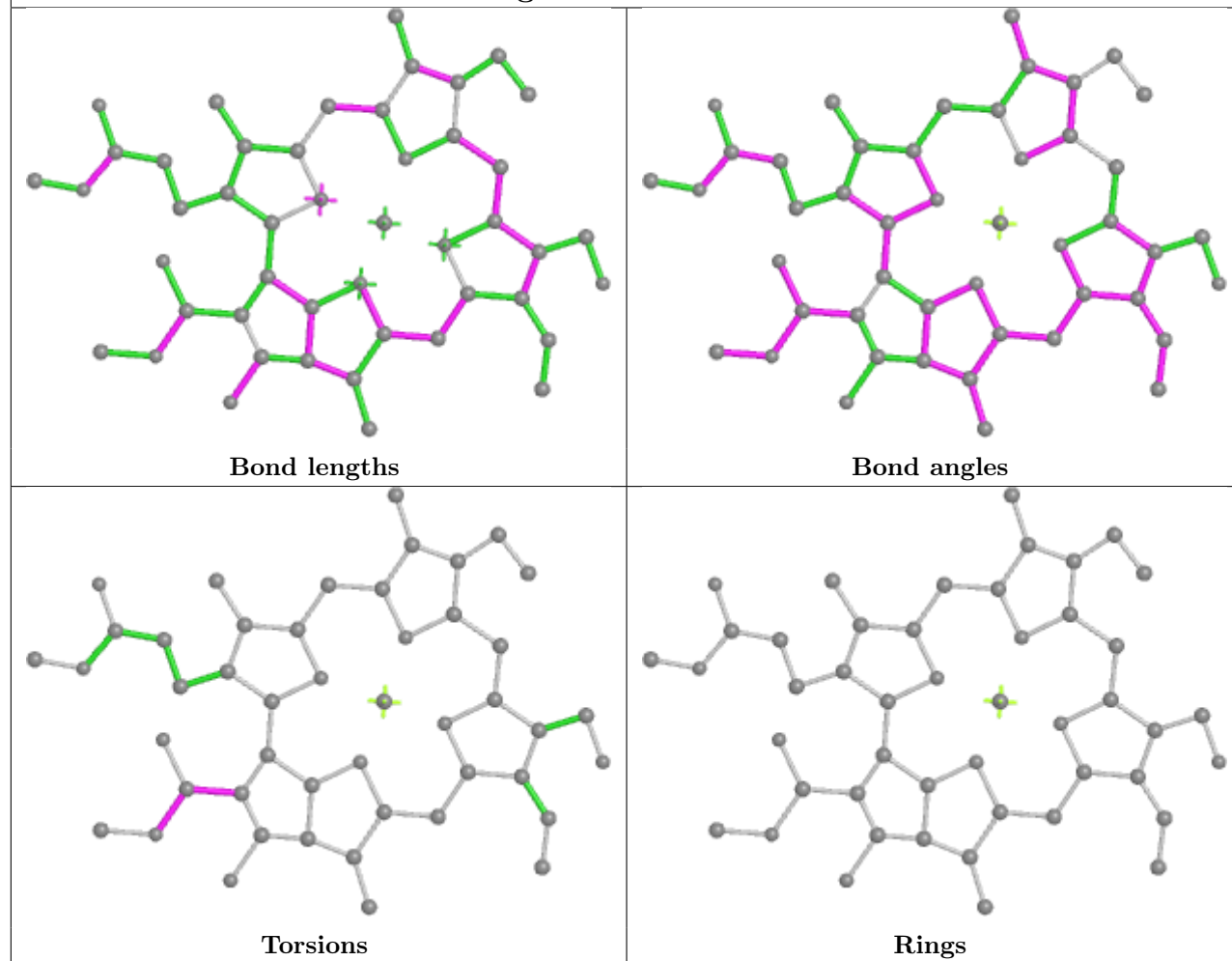


## Ligand CLA 9 610

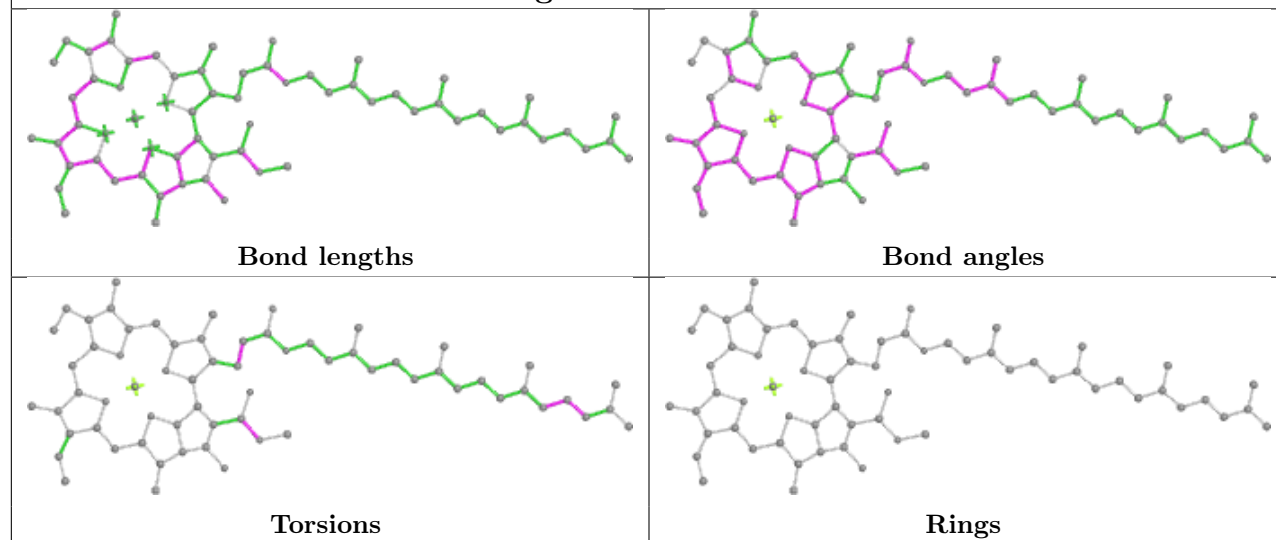




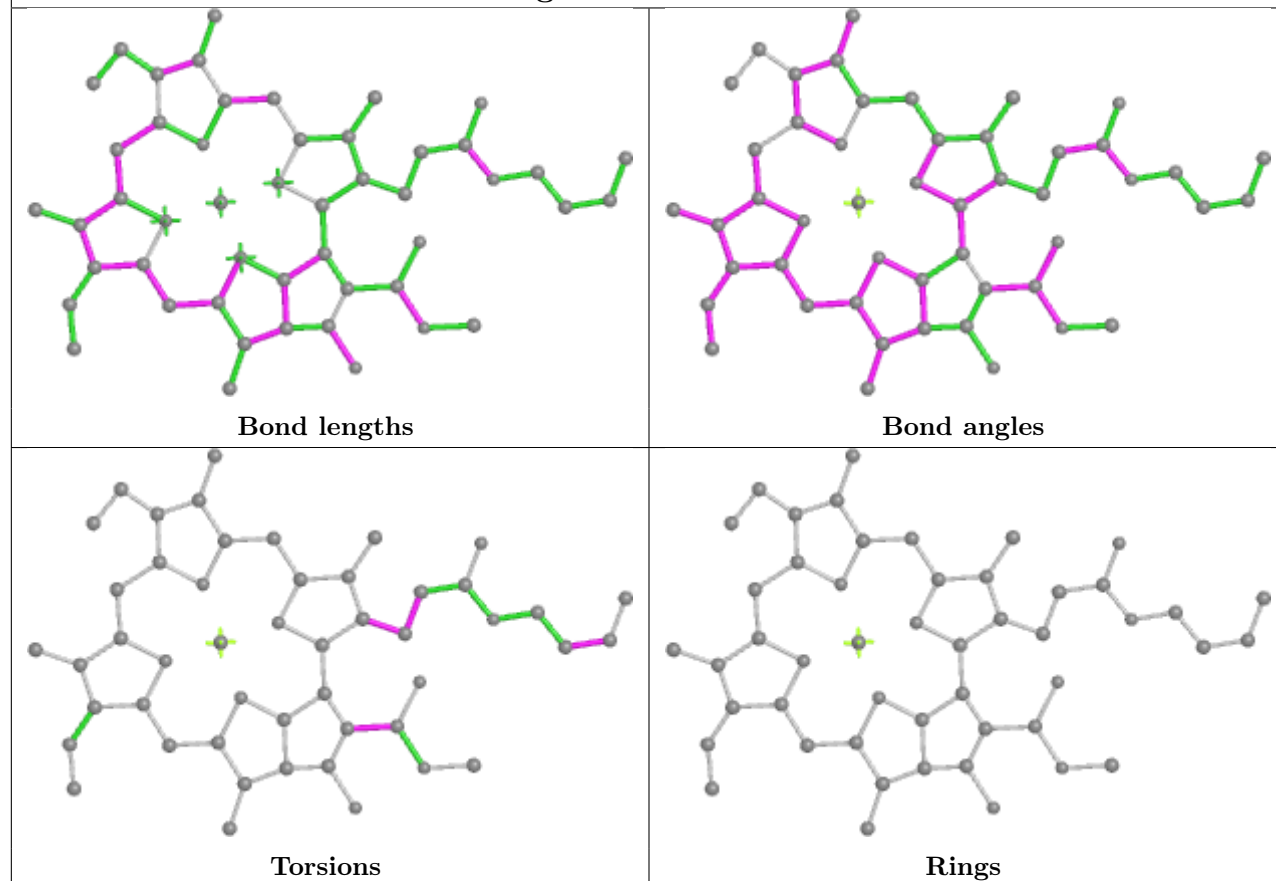
## Ligand CHL 8 306



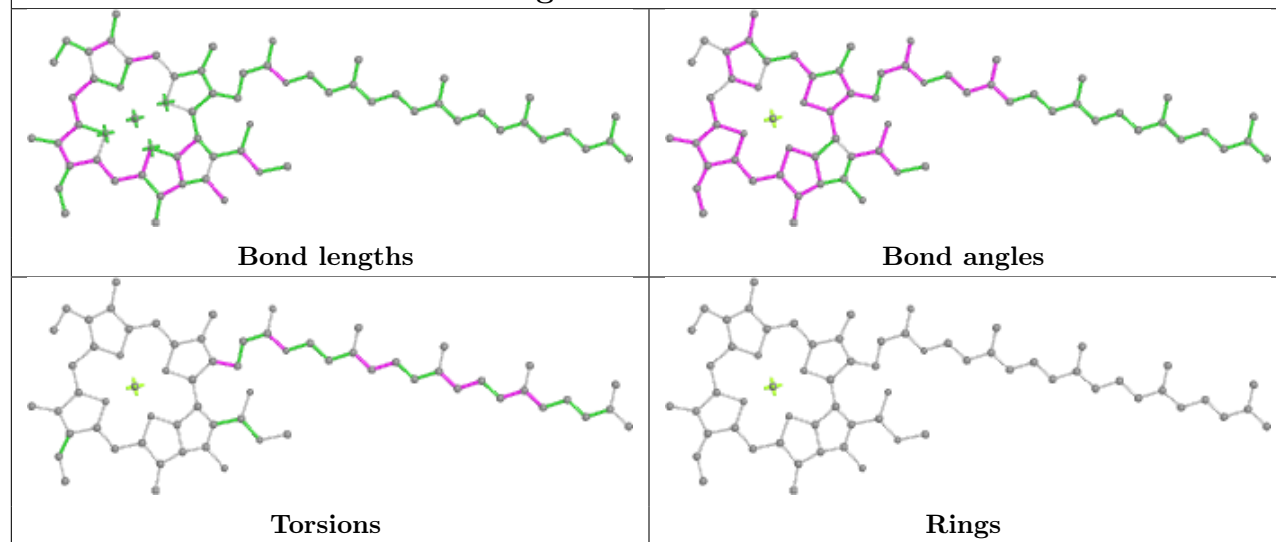
## Ligand CLA b 840

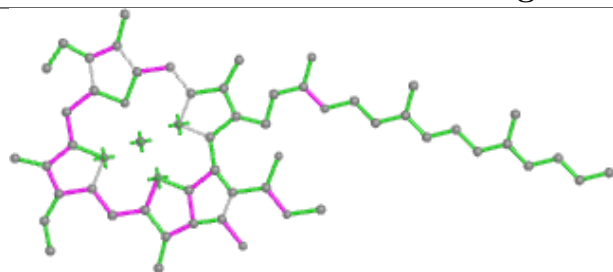
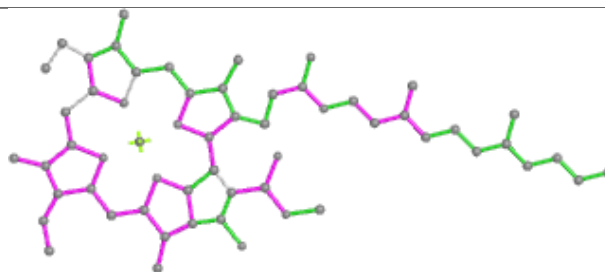
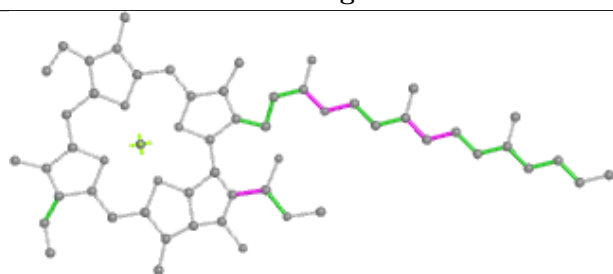
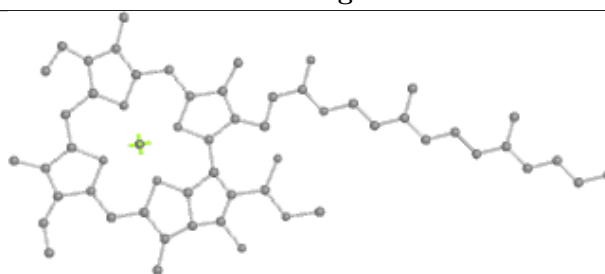
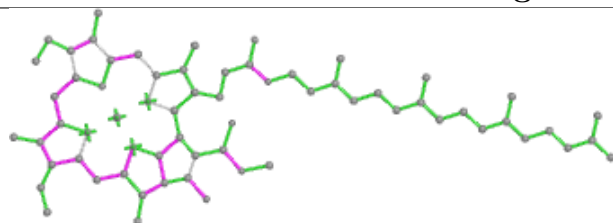
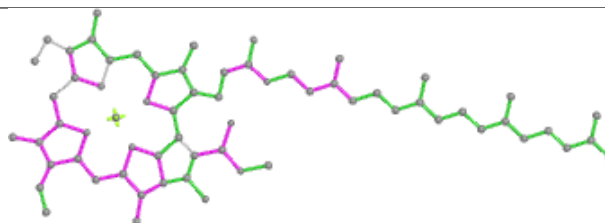
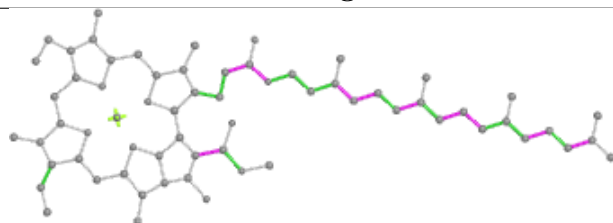
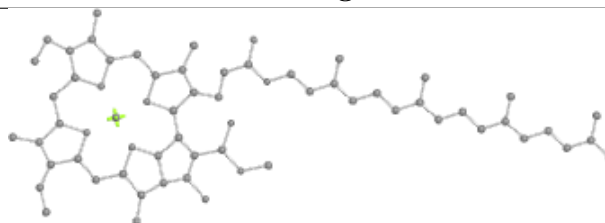


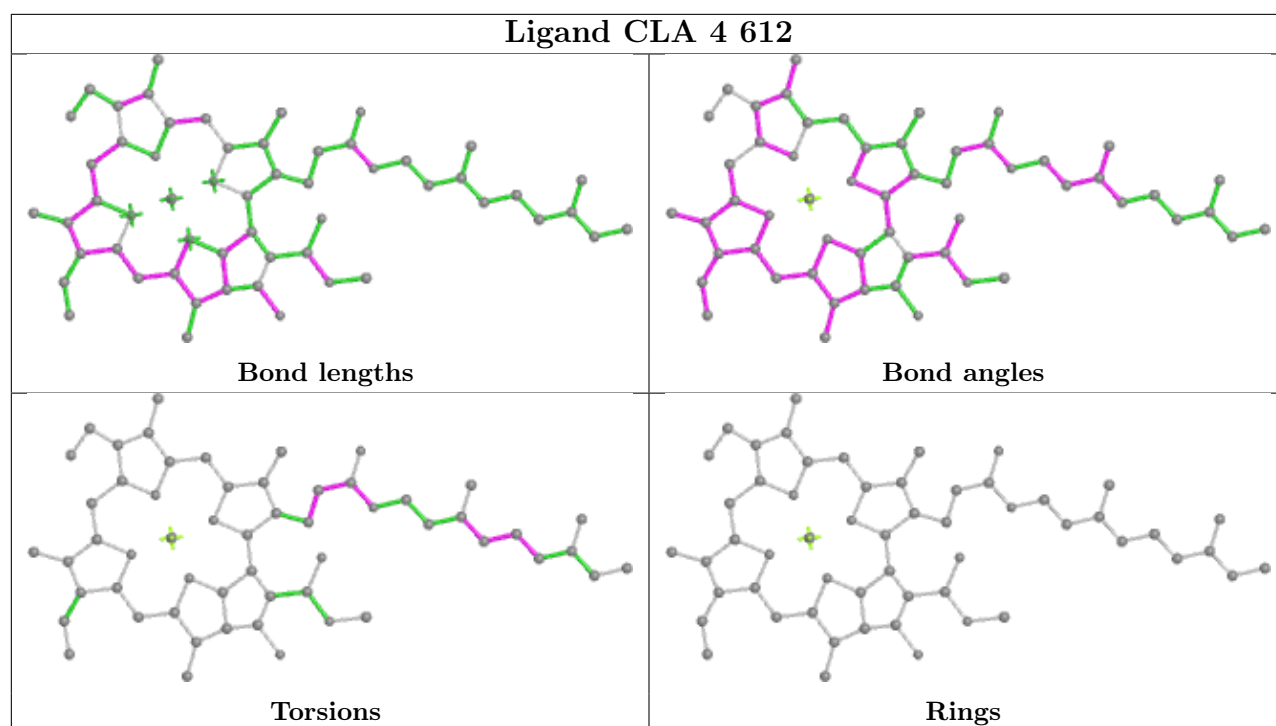
## Ligand CLA a 823



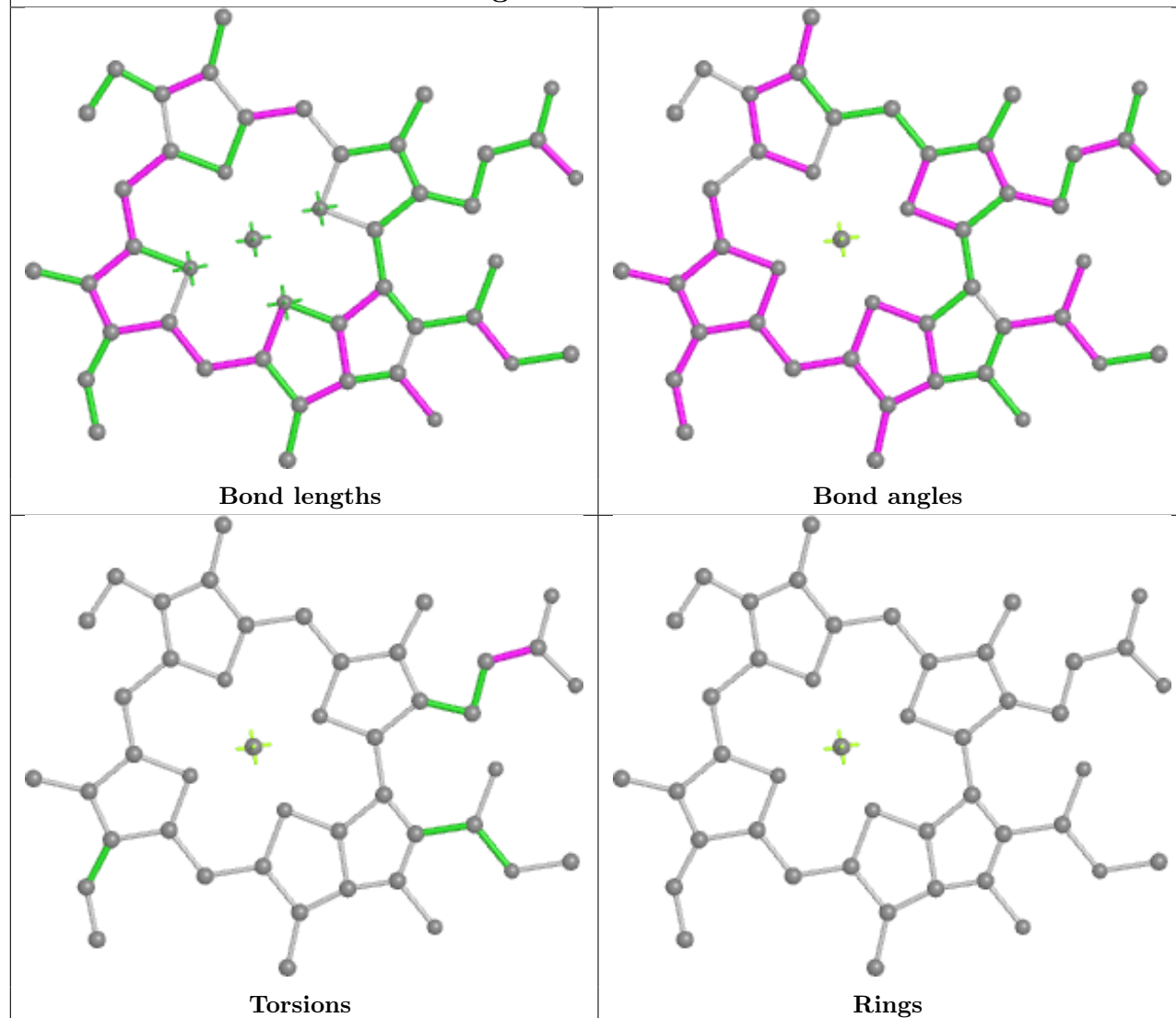
## Ligand CLA a 807



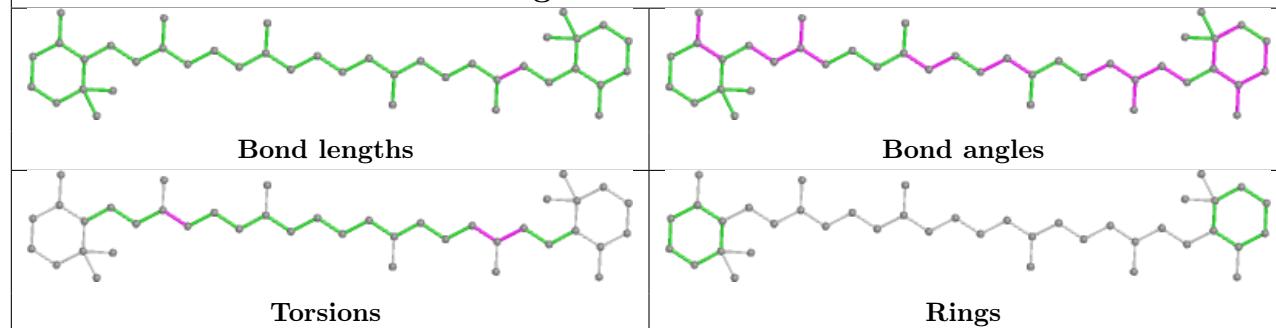
**Ligand CLA b 833****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 826****Bond lengths****Bond angles****Torsions****Rings**

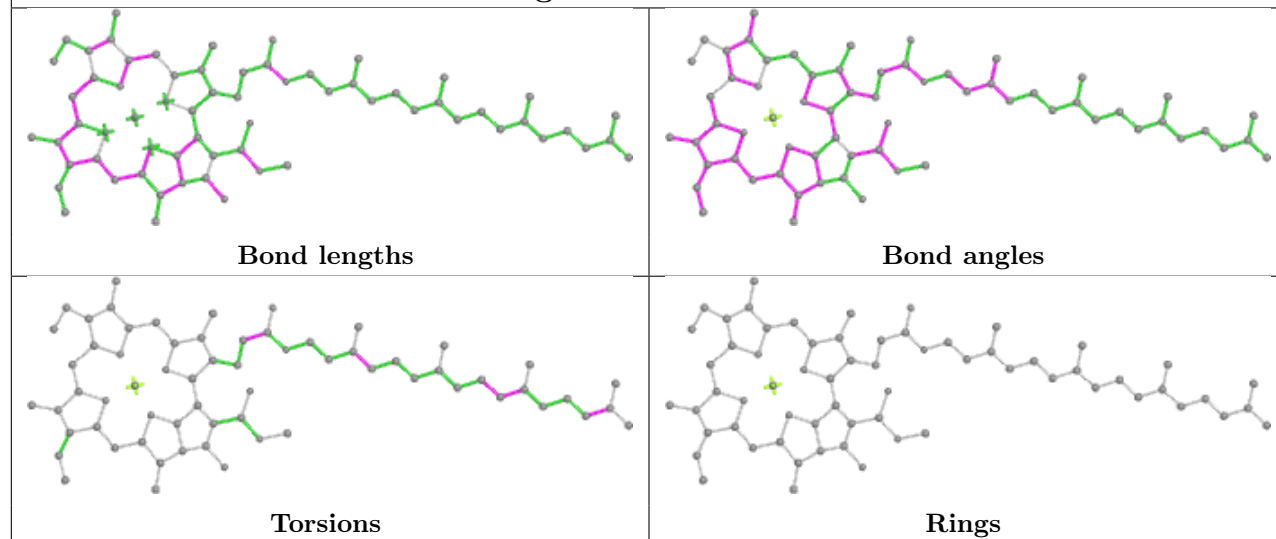
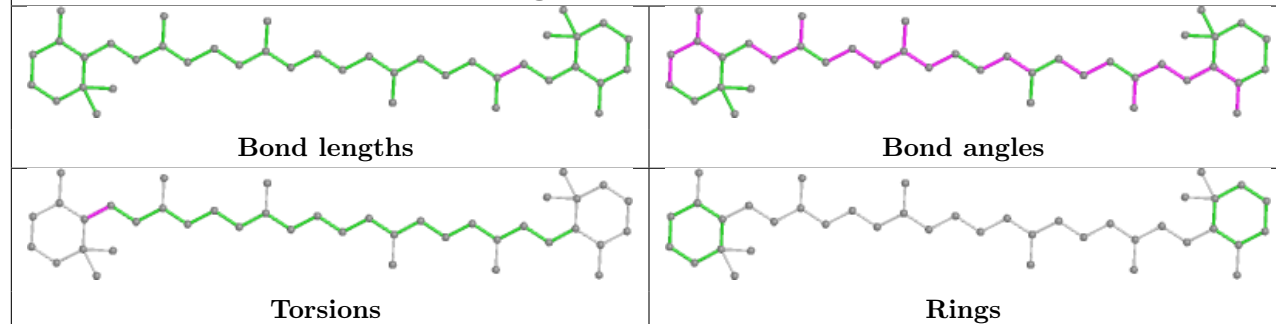


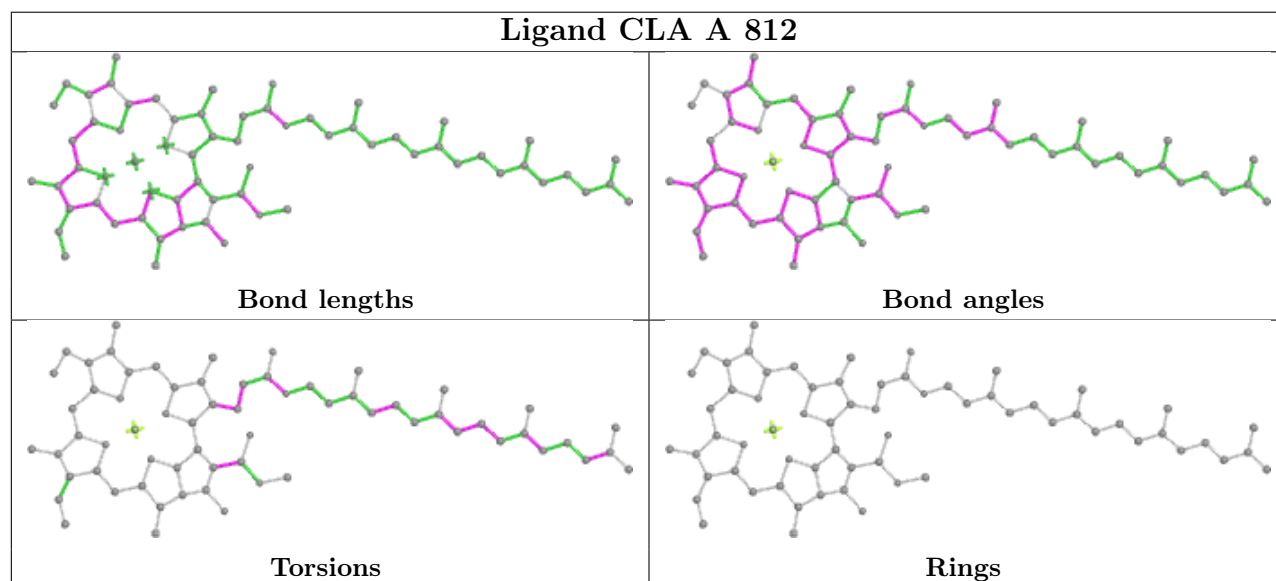
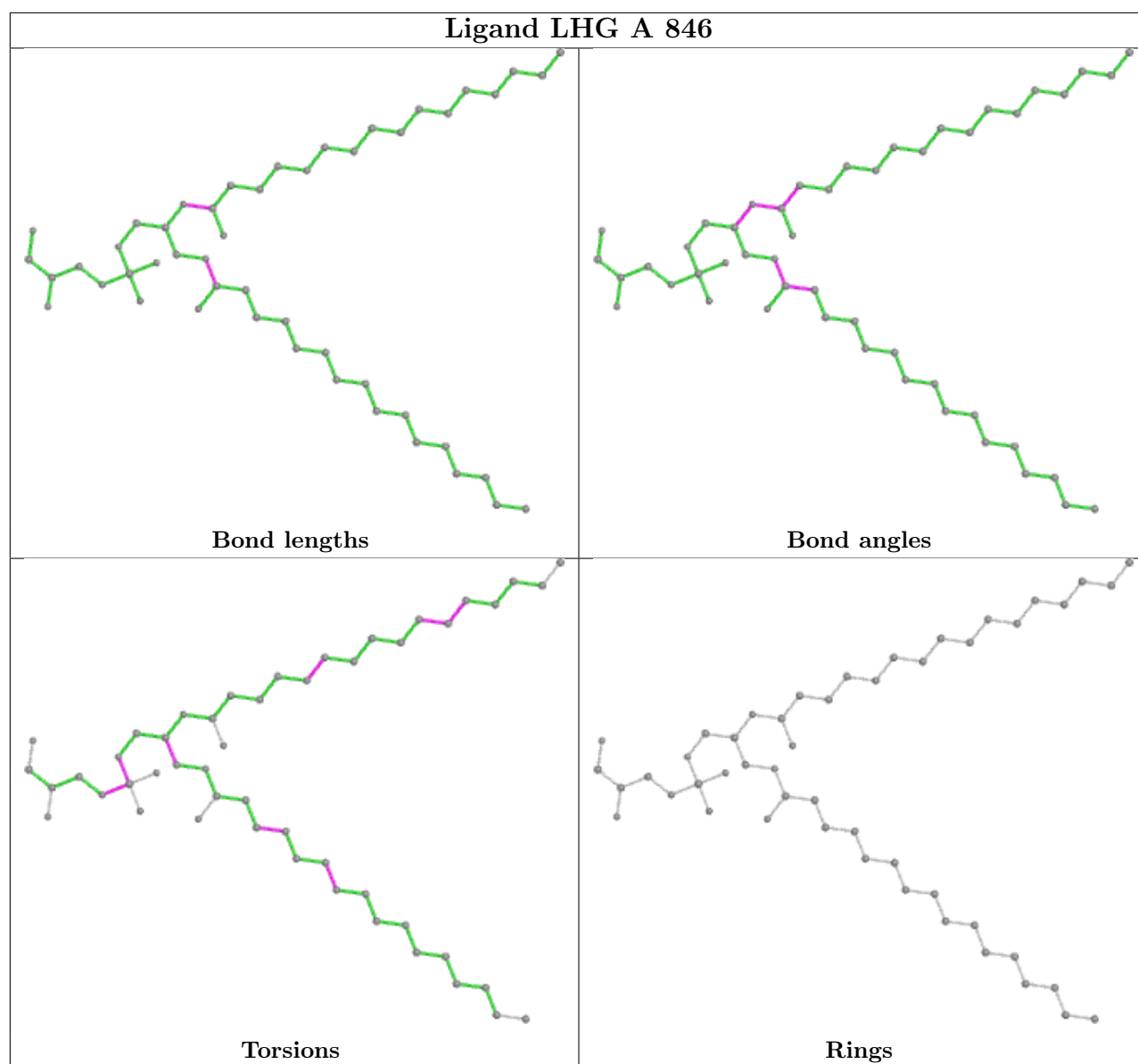
## Ligand CLA F 303



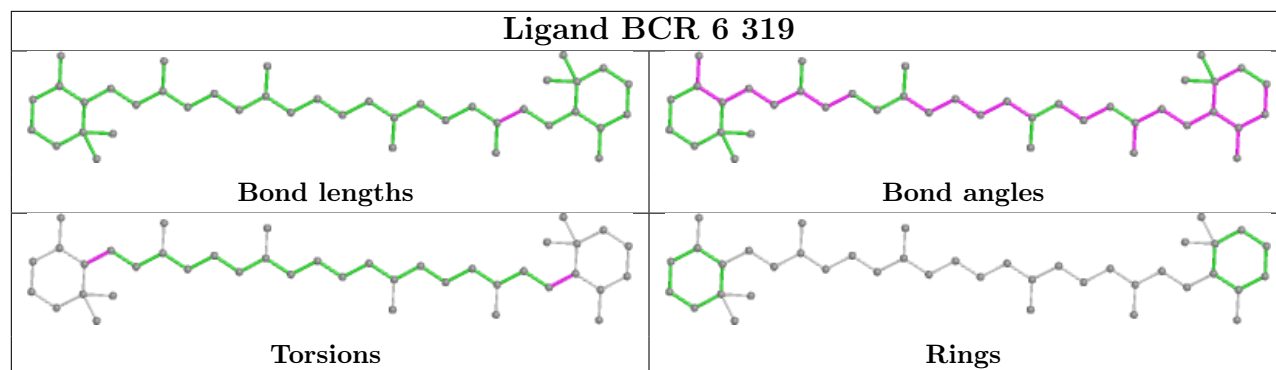
## Ligand BCR b 845



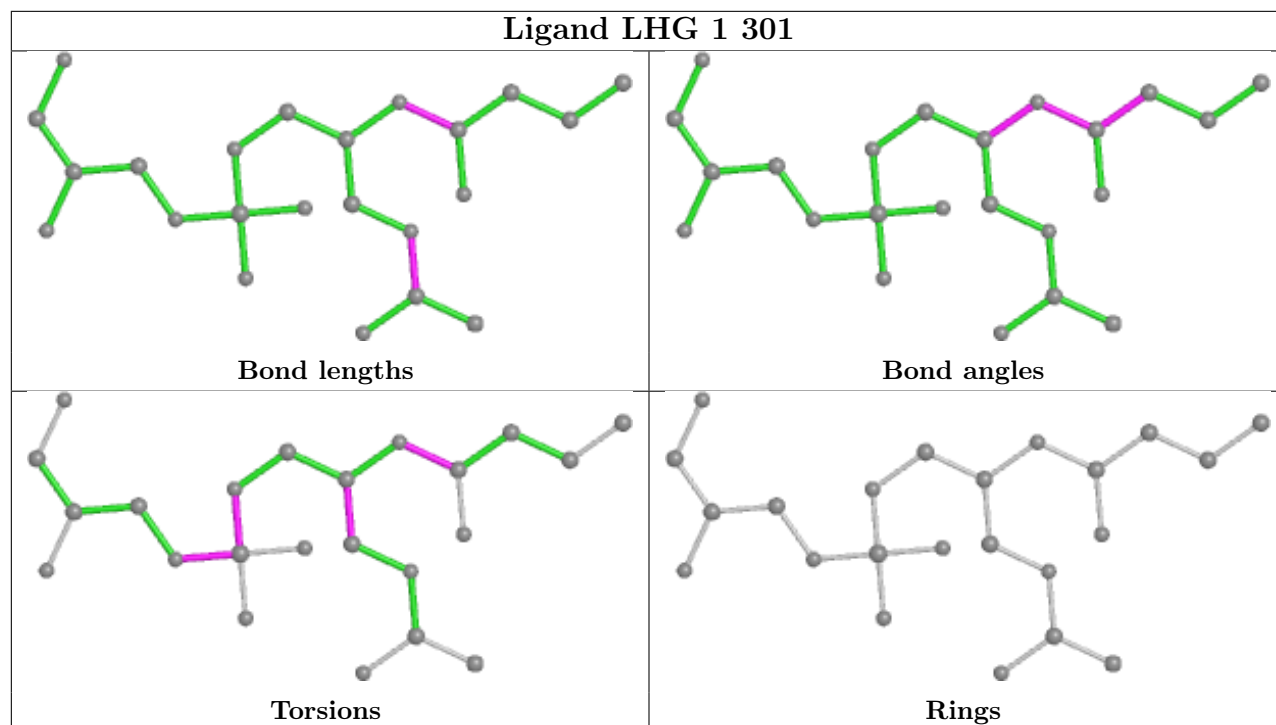
**Ligand CLA b 809****Ligand BCR B 848**



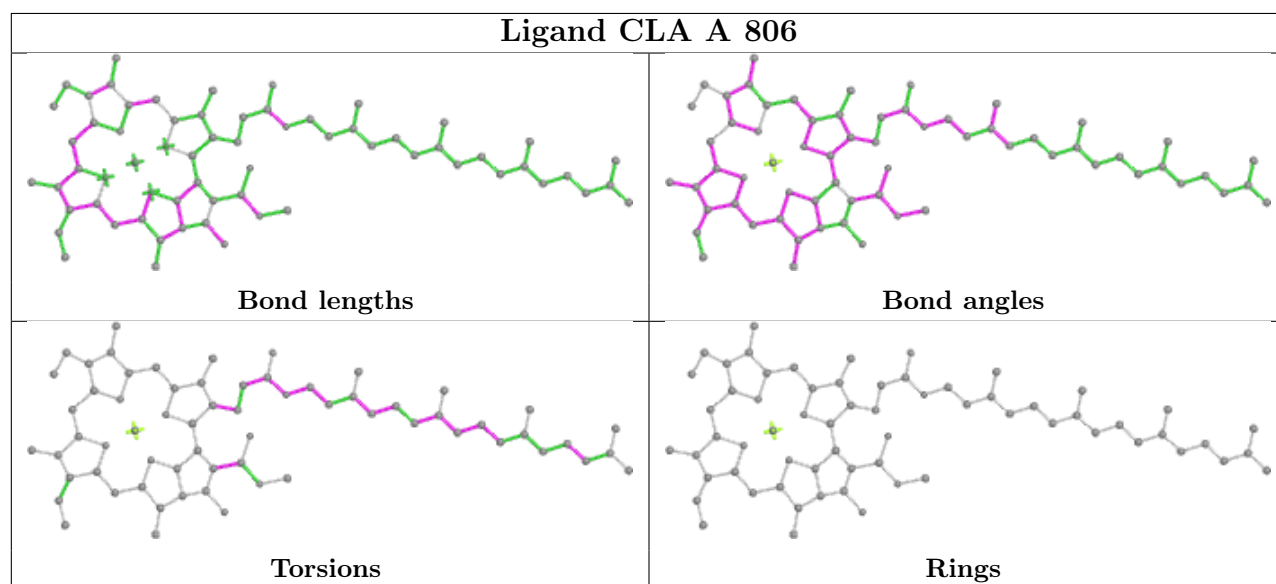
## Ligand BCR 6 319



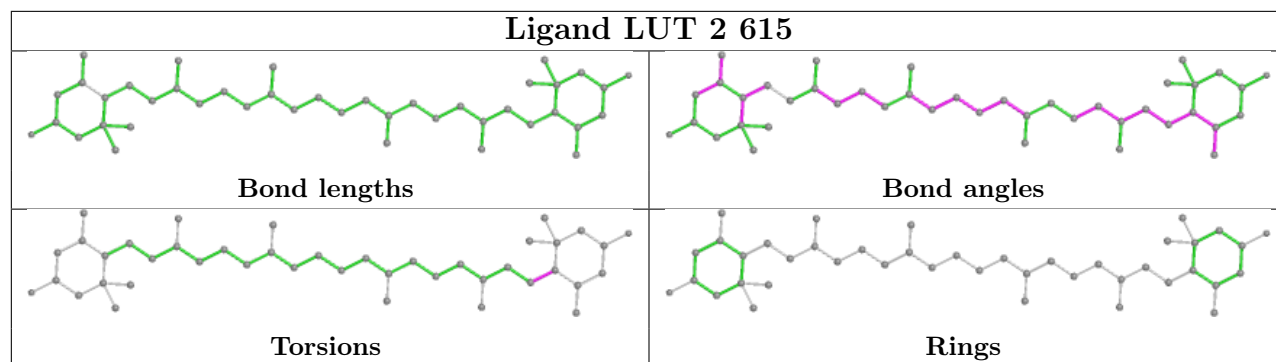
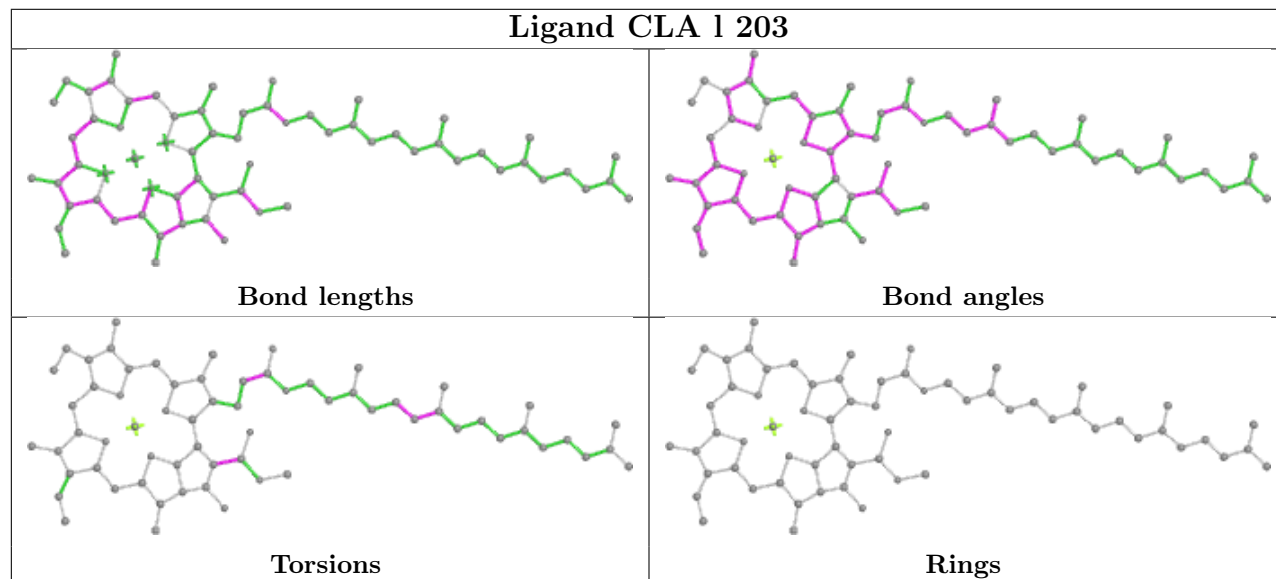
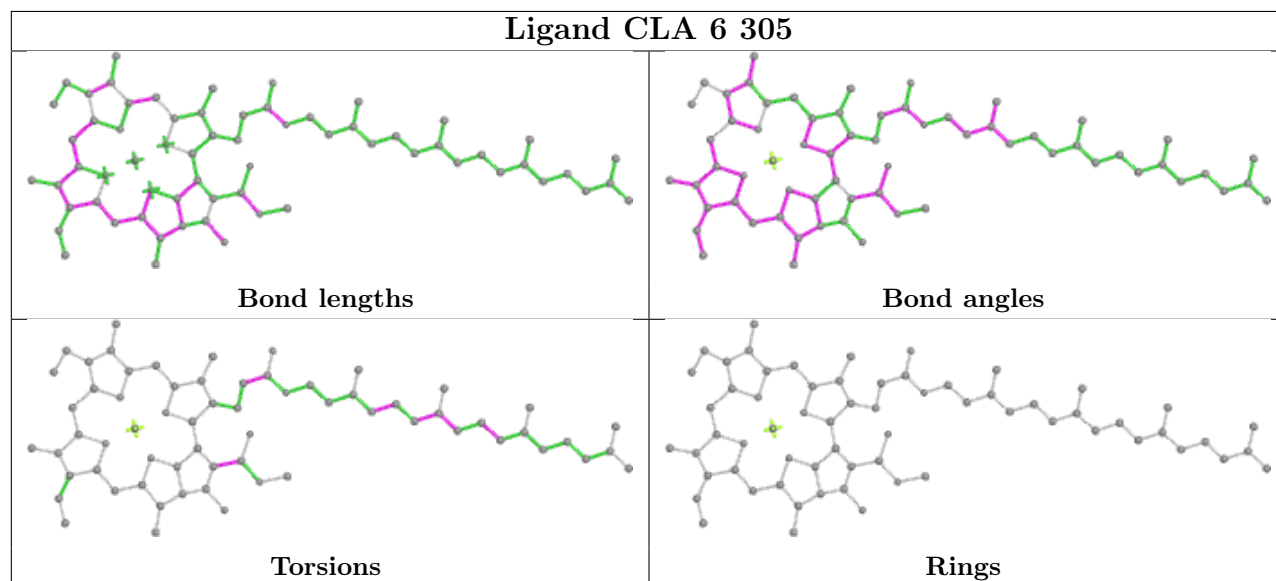
## Ligand LHG 1 301



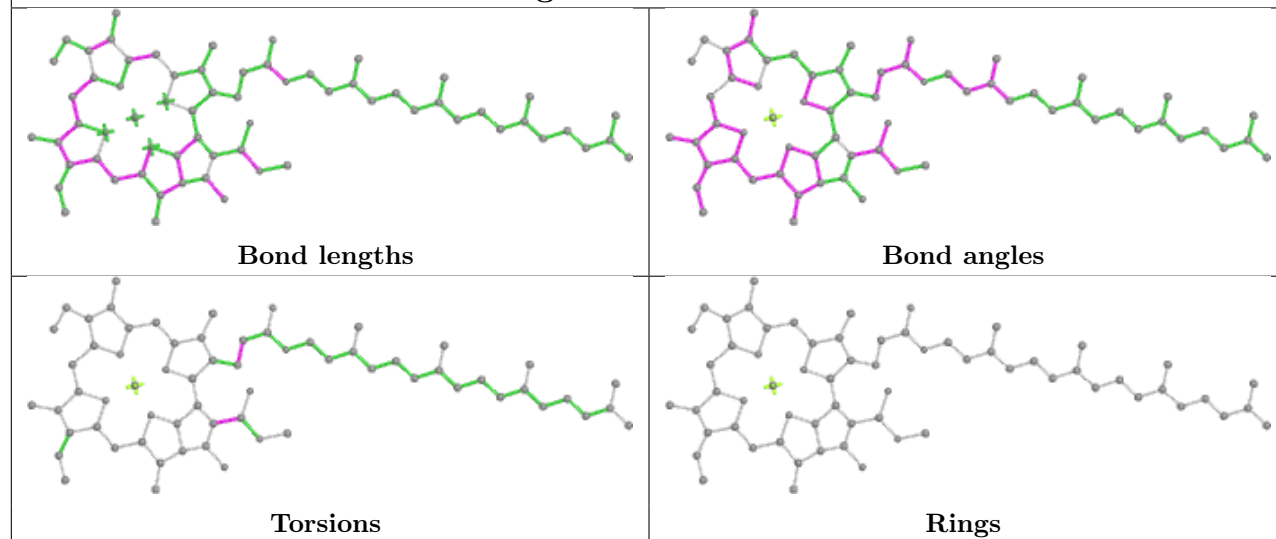
## Ligand CLA A 806



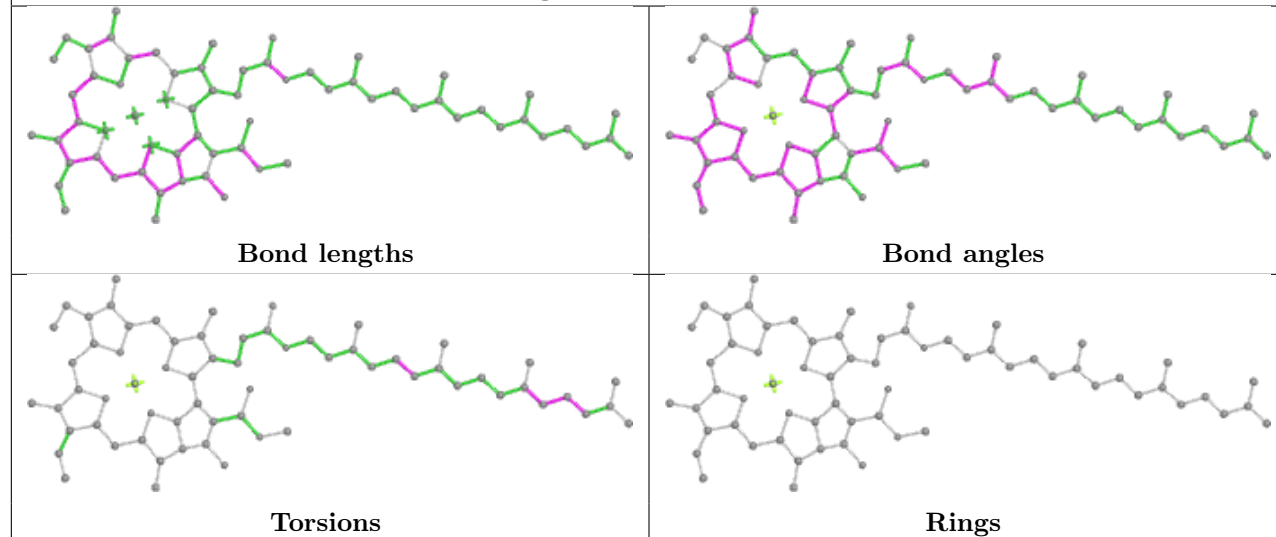


**Ligand LUT 2 615****Ligand CLA 1 203****Ligand CLA 6 305**

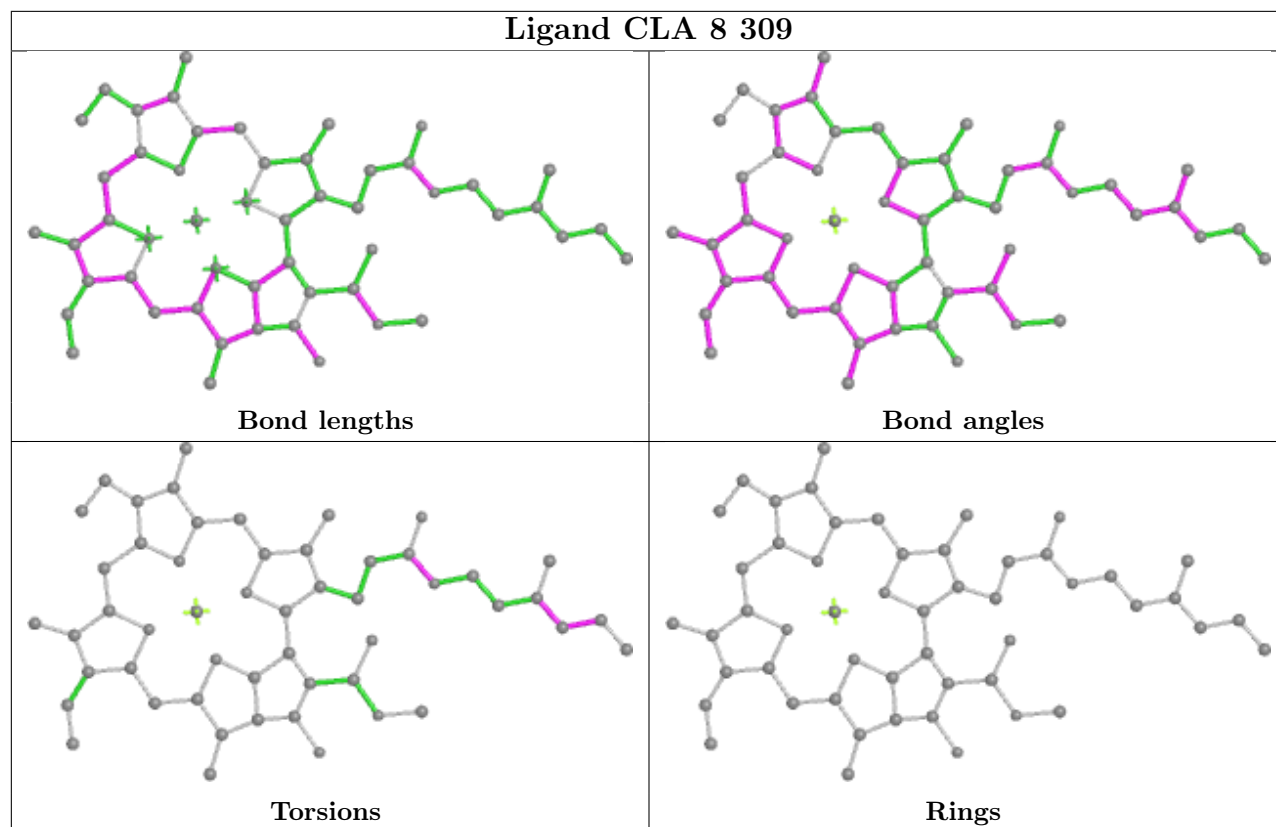
## Ligand CLA a 810



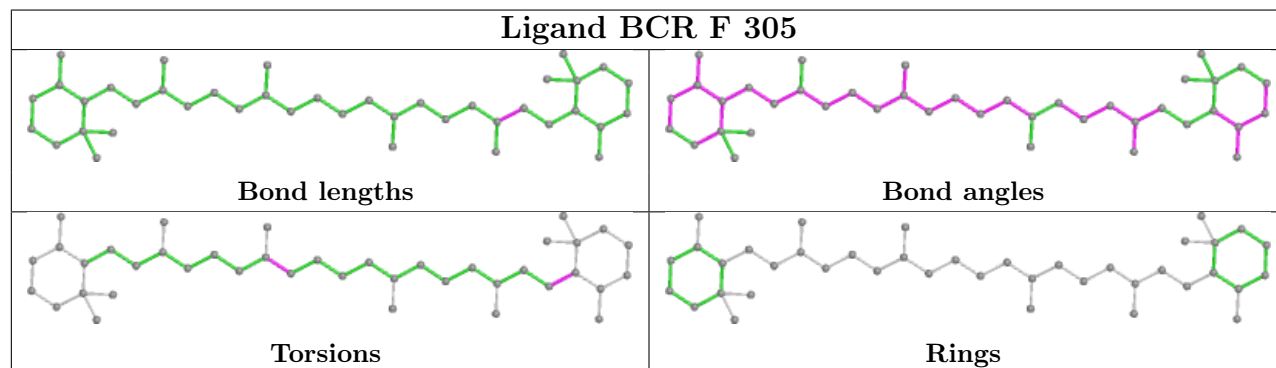
## Ligand CLA 1 308



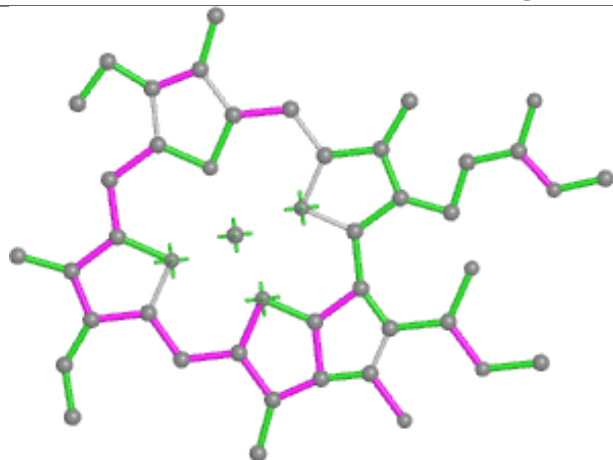
## Ligand CLA 8 309



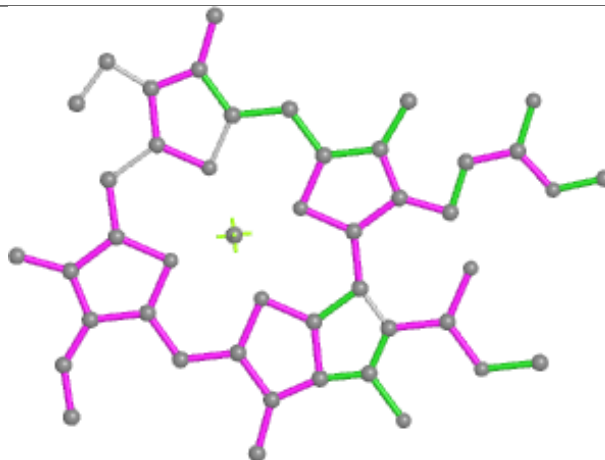
## Ligand BCR F 305



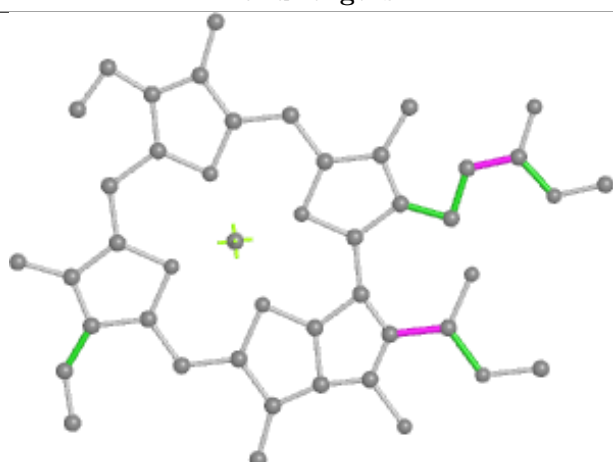
## Ligand CLA 9 601



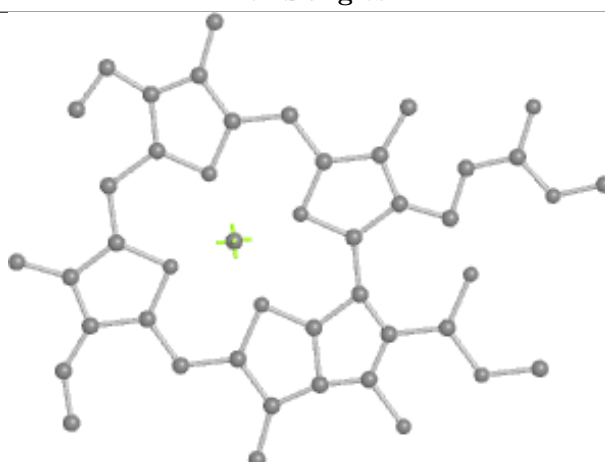
Bond lengths



Bond angles

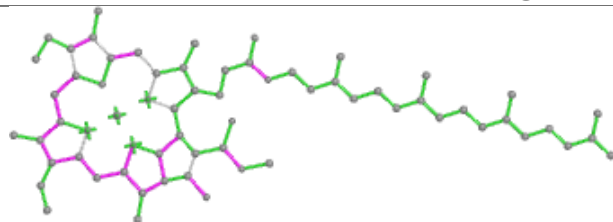


Torsions

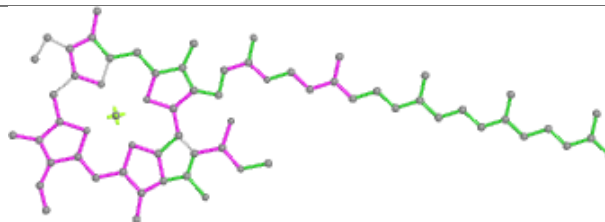


Rings

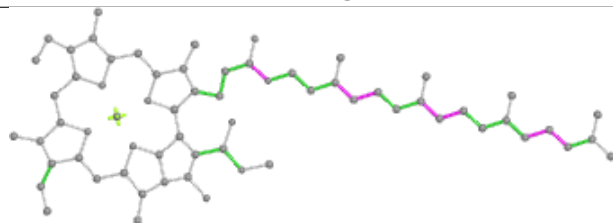
## Ligand CLA b 814



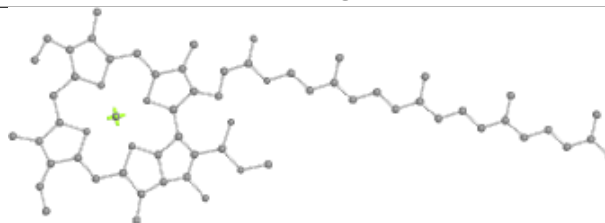
Bond lengths



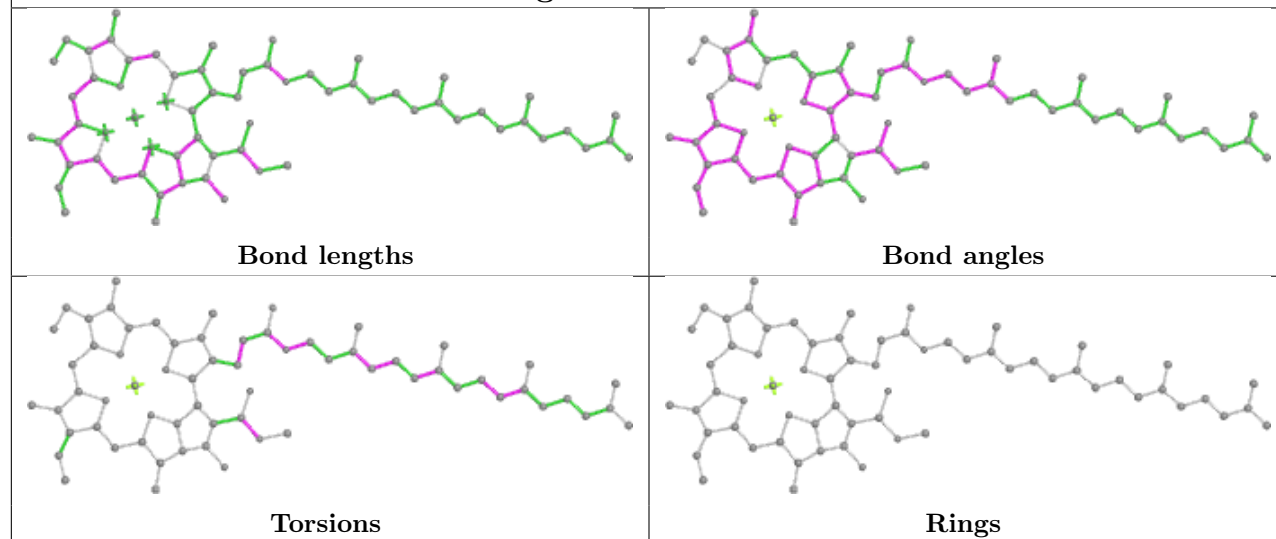
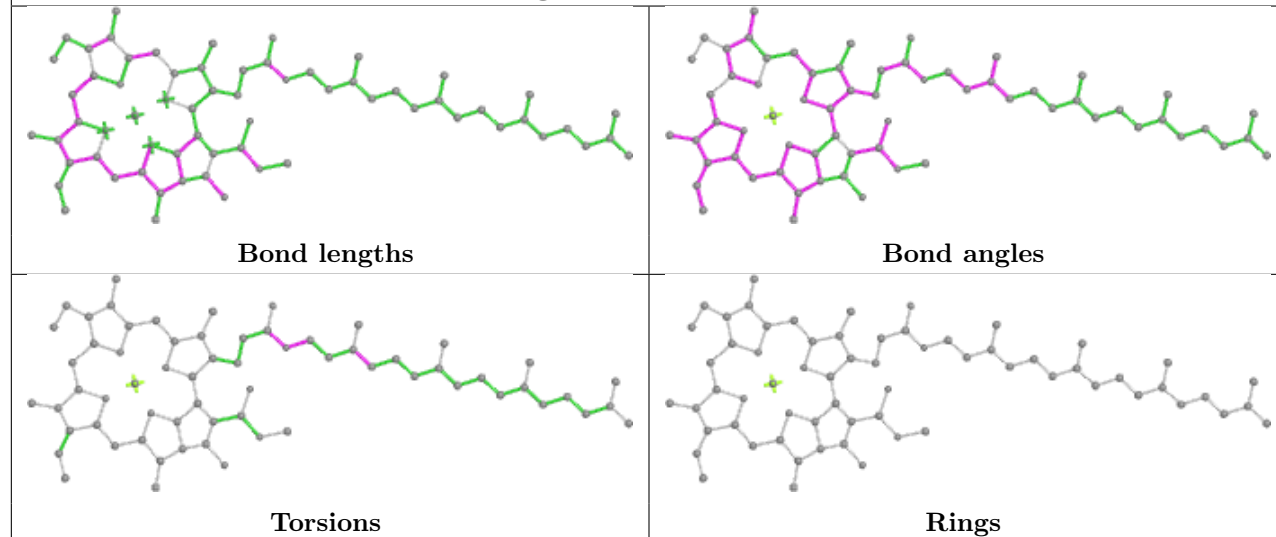
Bond angles



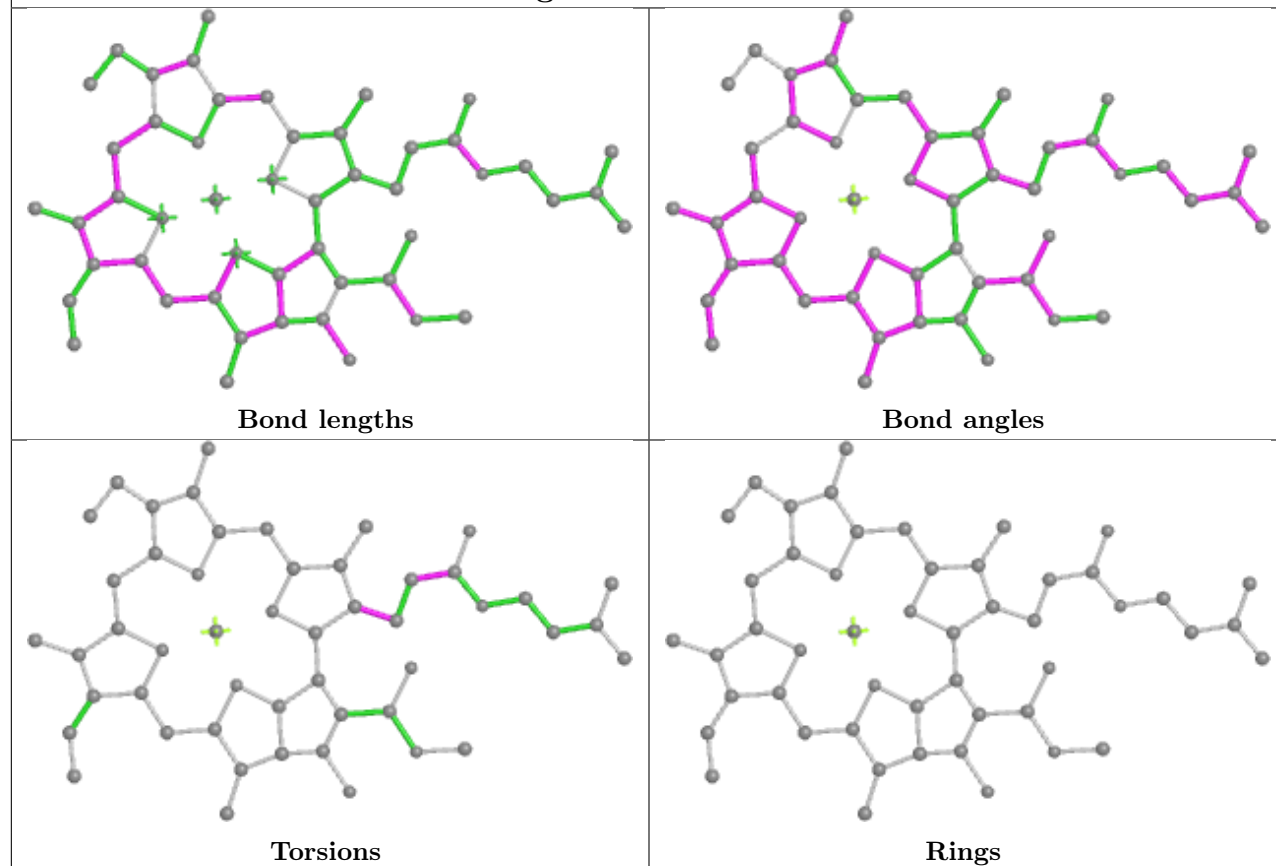
Torsions



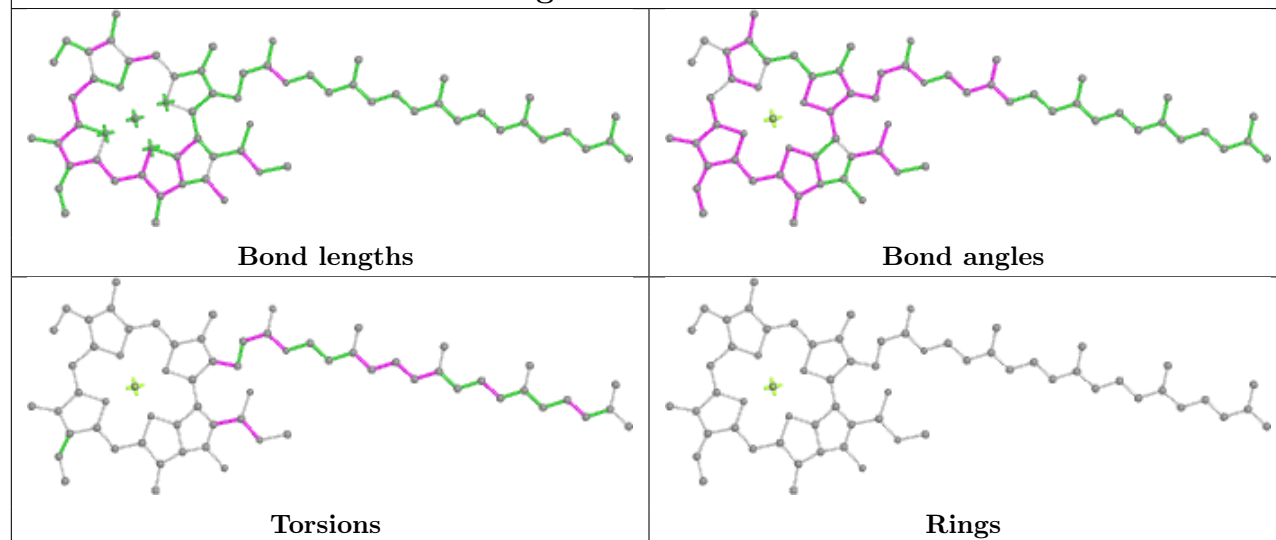
Rings

**Ligand CLA a 843****Ligand CLA L 203**

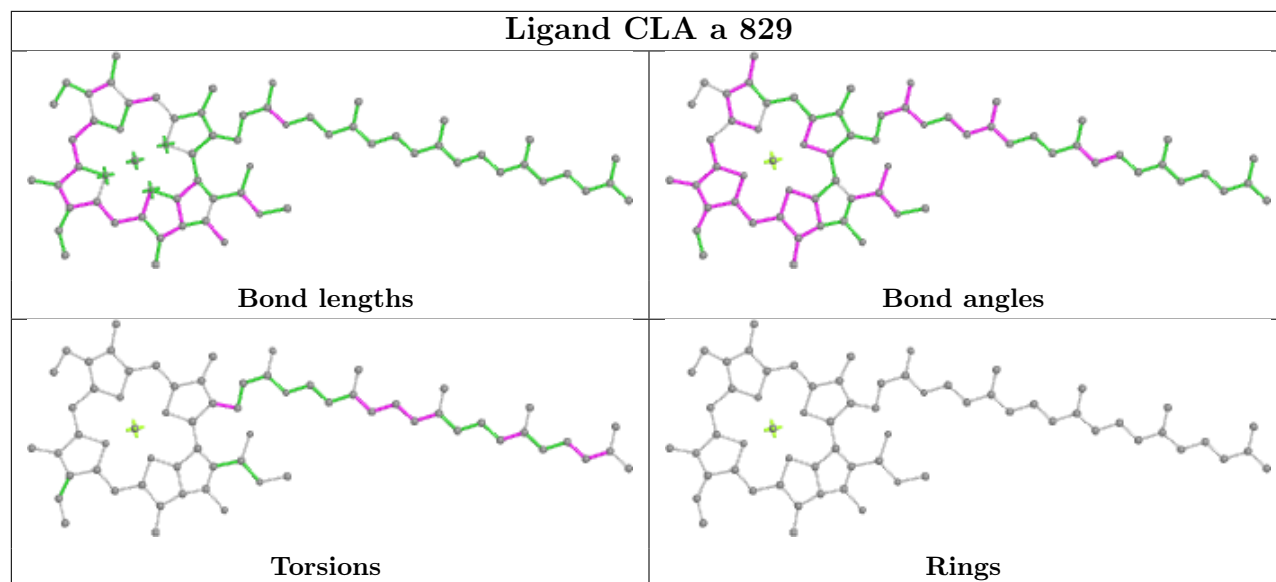
## Ligand CLA 4 608



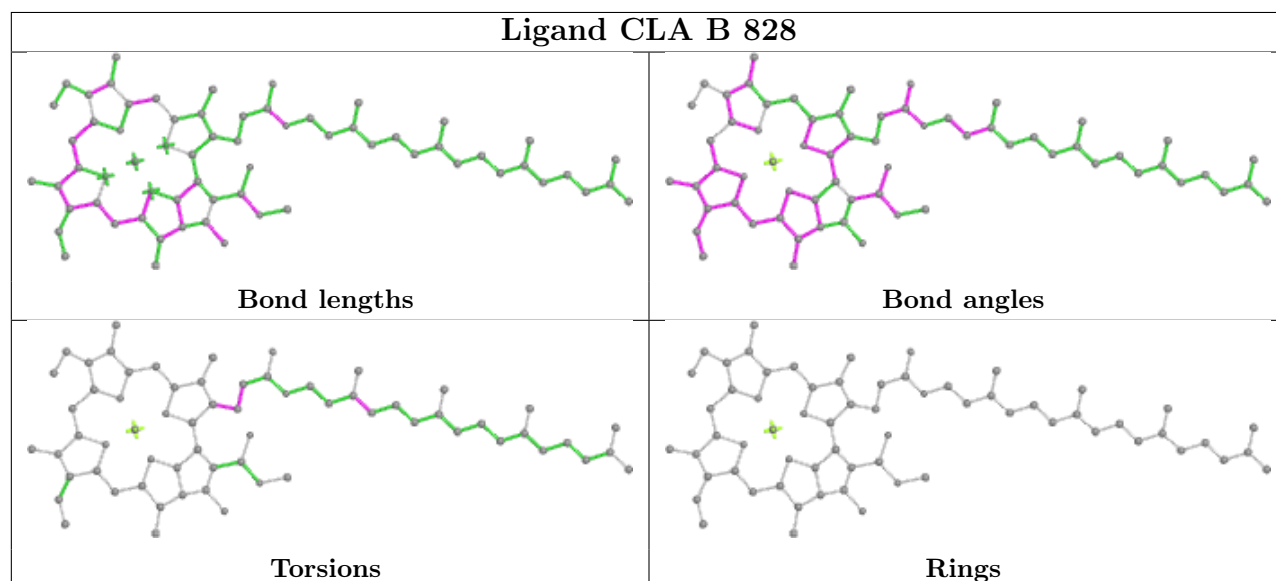
## Ligand CLA a 804



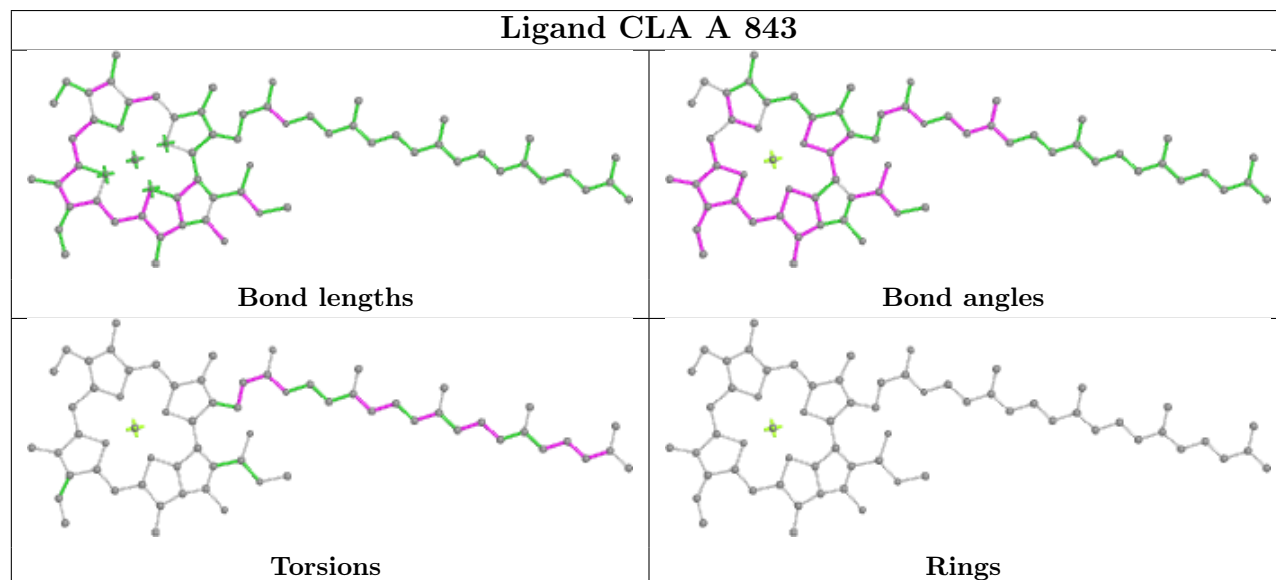
## Ligand CLA a 829



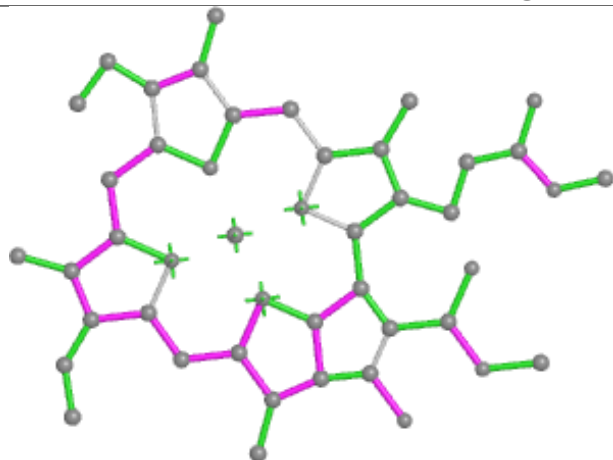
## Ligand CLA B 828



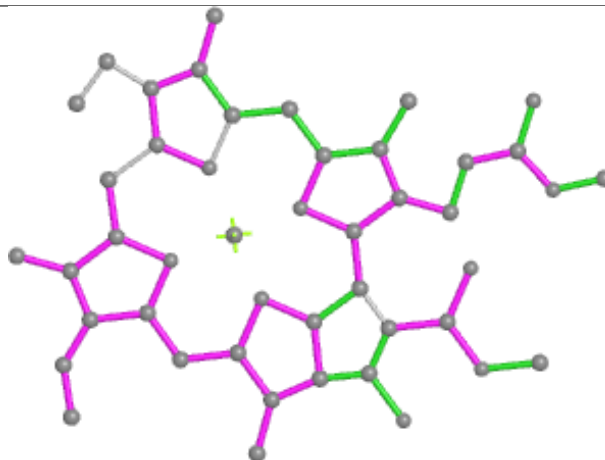
## Ligand CLA A 843



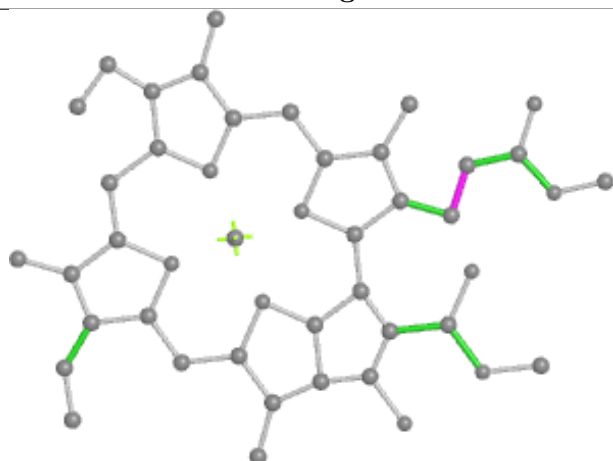
## Ligand CLA 8 312



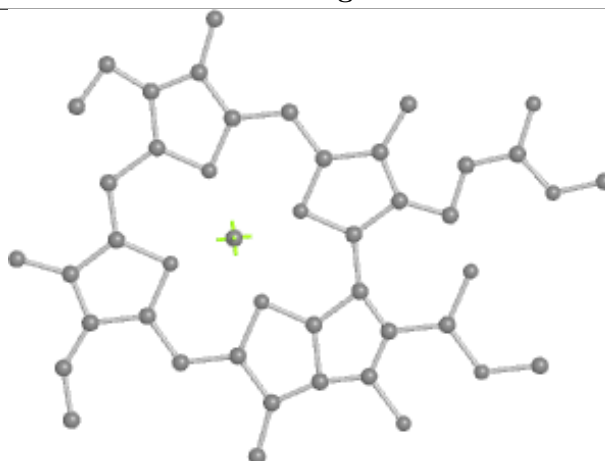
Bond lengths



Bond angles

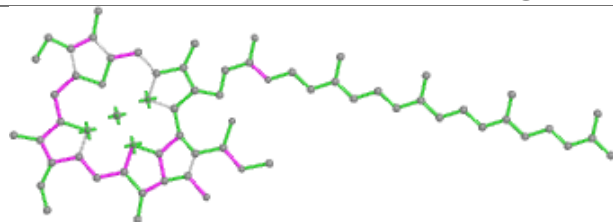


Torsions

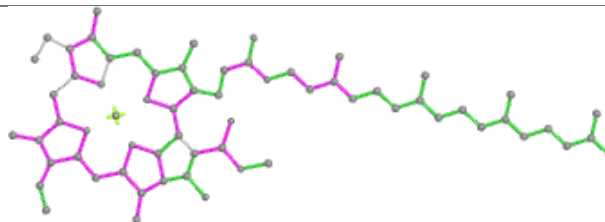


Rings

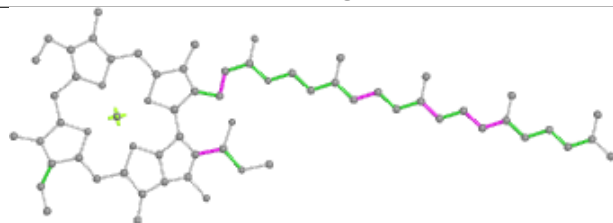
## Ligand CLA b 826



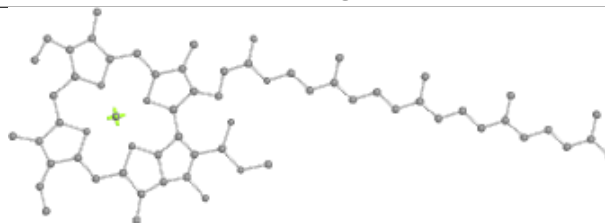
Bond lengths



Bond angles

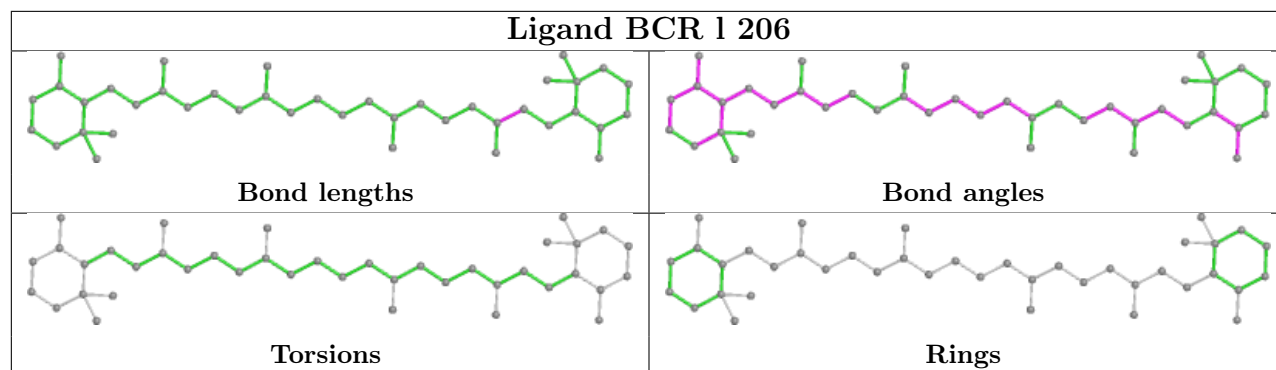
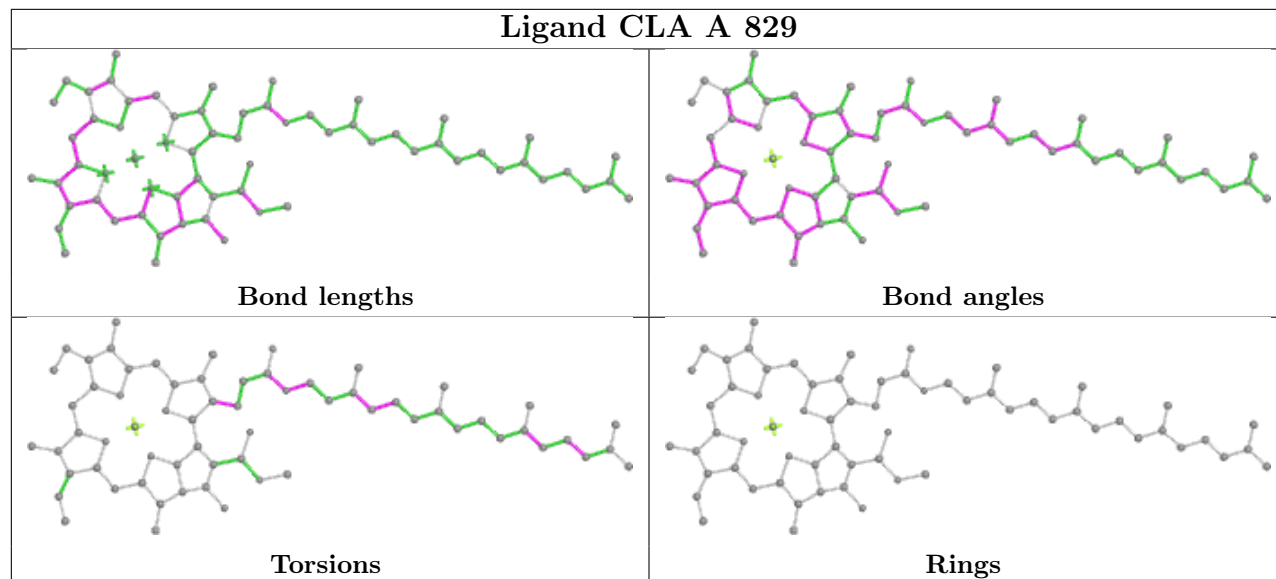
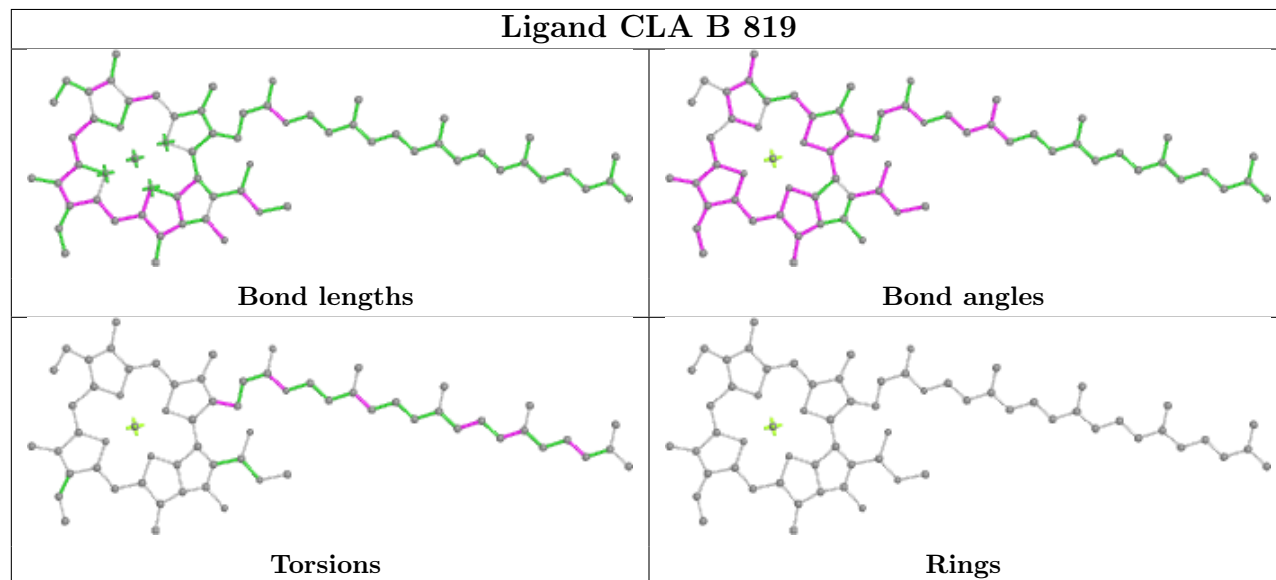


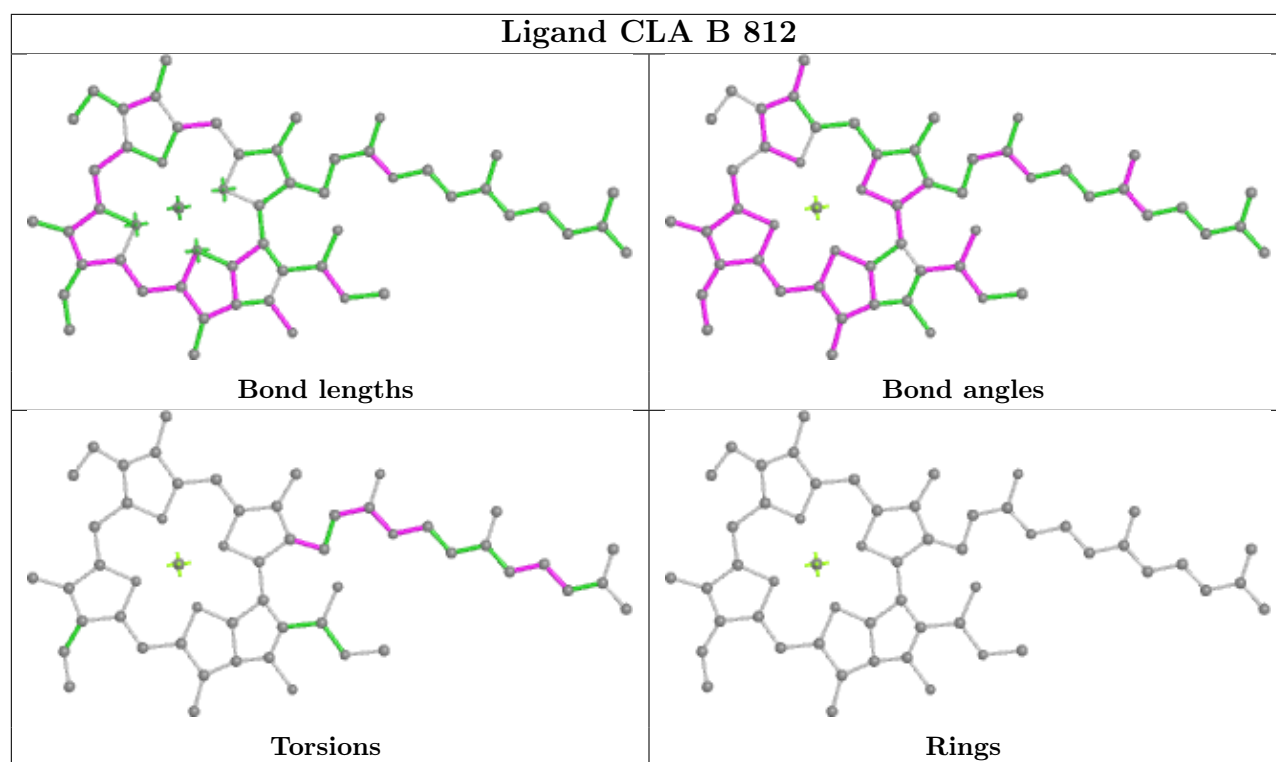
Torsions



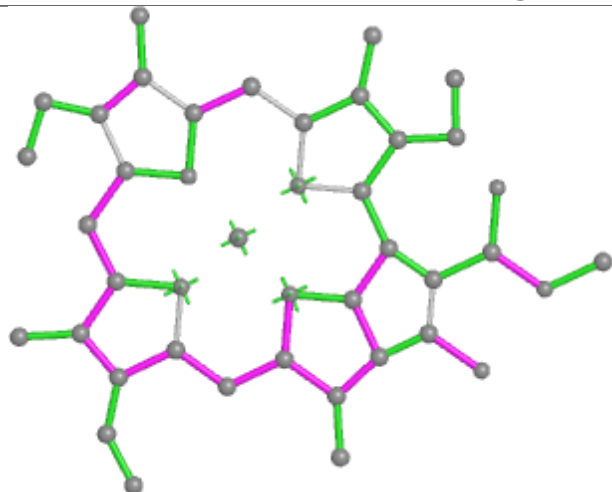
Rings



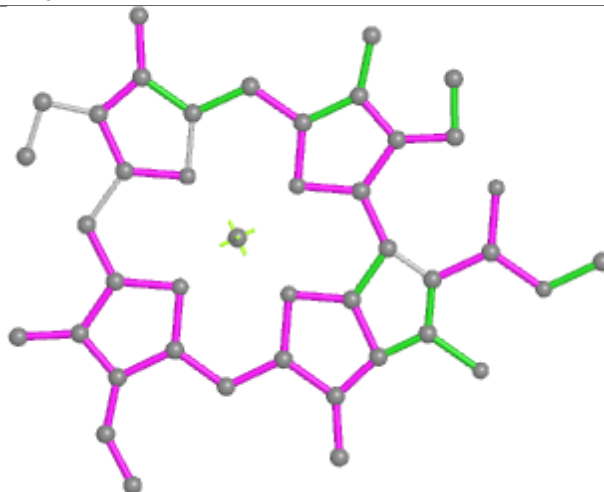
**Ligand BCR 1 206****Ligand CLA A 829****Ligand CLA B 819**



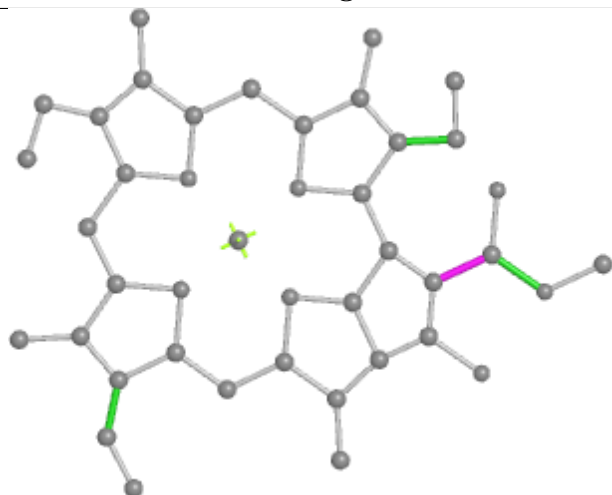
## Ligand CLA j 3002



Bond lengths



Bond angles

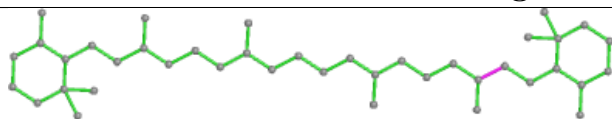


Torsions

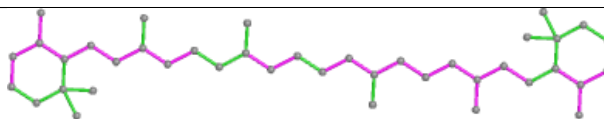


Rings

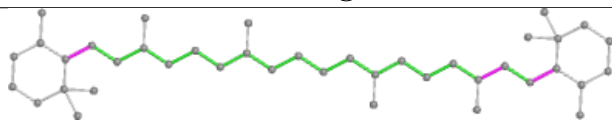
## Ligand BCR A 851



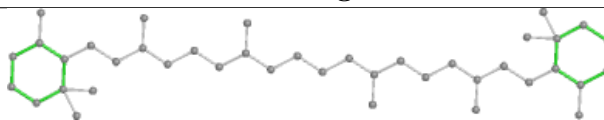
Bond lengths



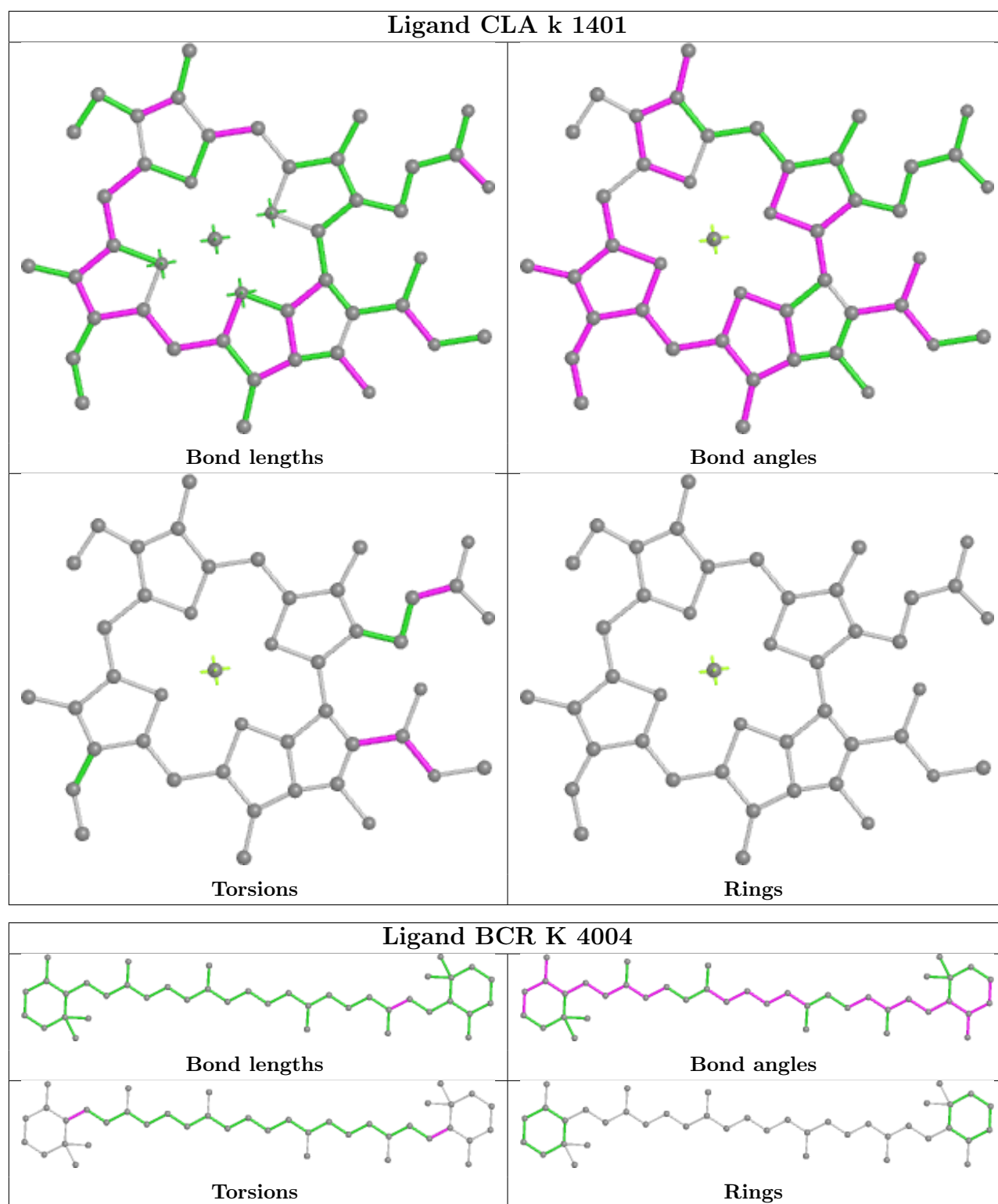
Bond angles

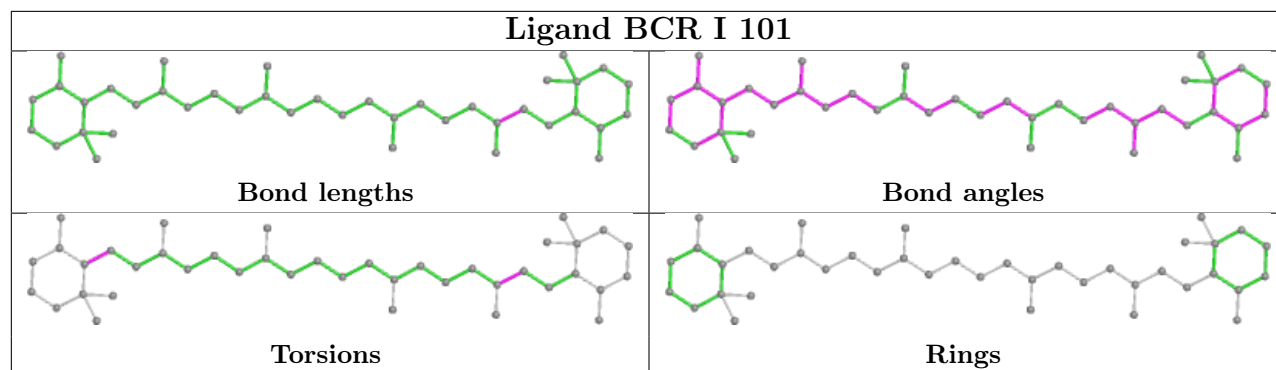
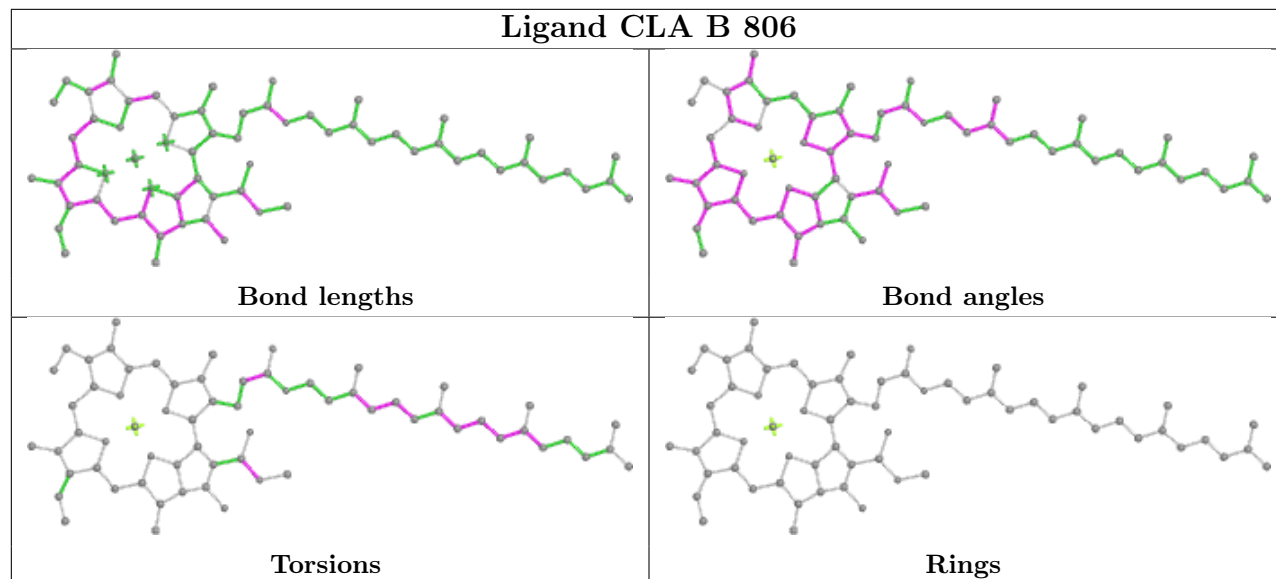


Torsions

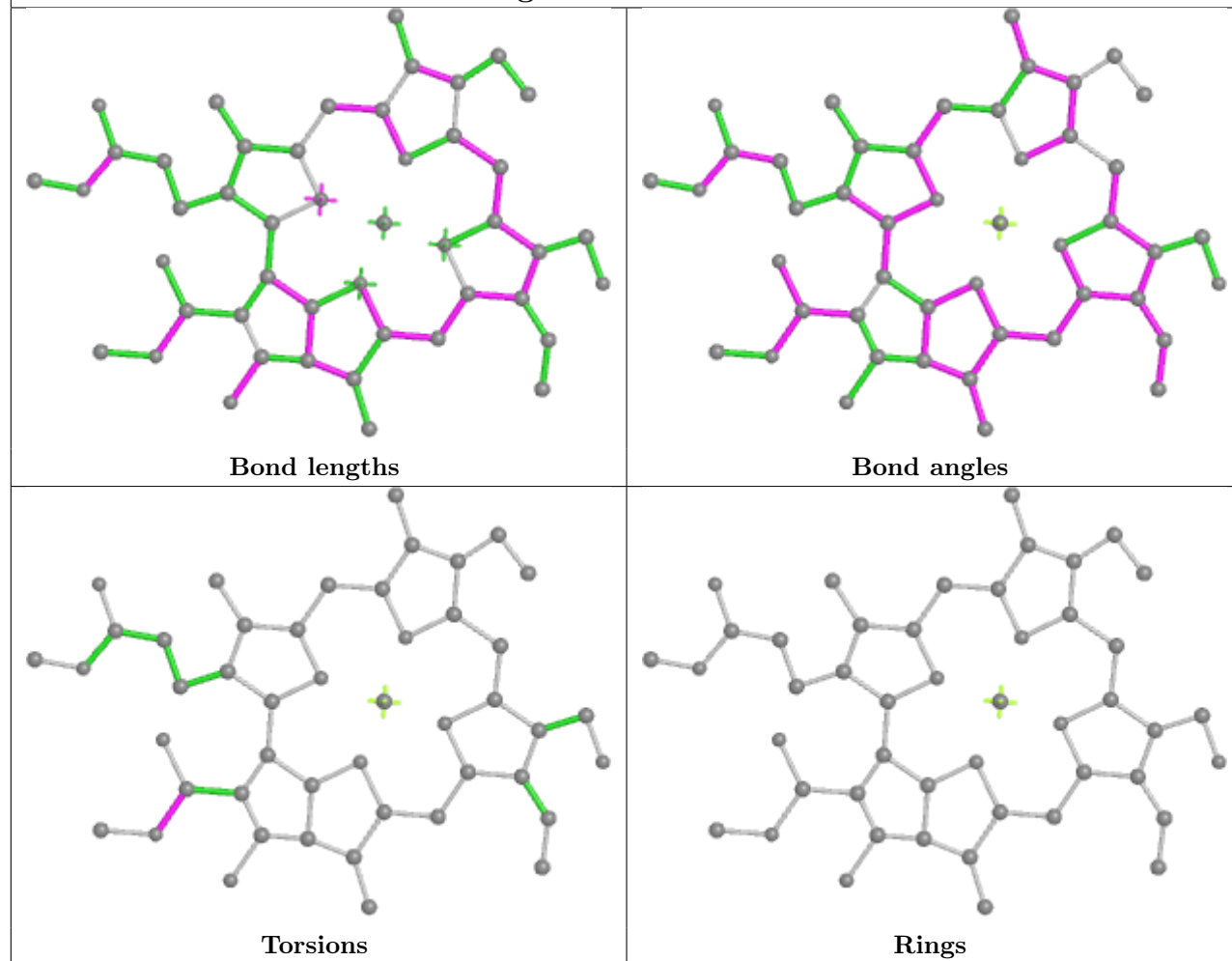


Rings

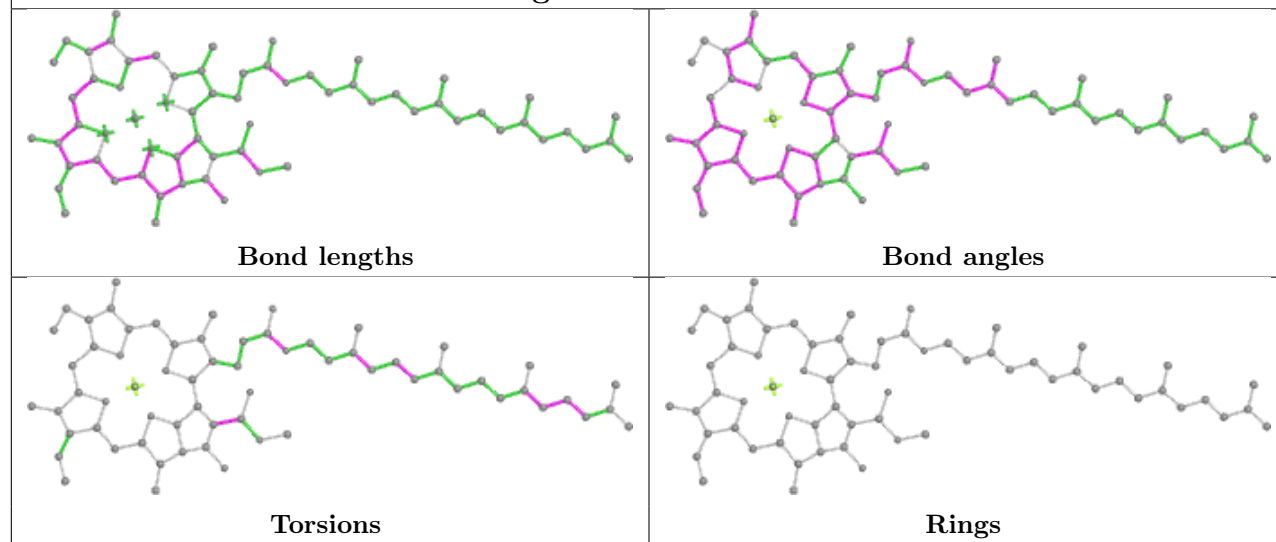


**Ligand BCR I 101****Ligand CLA B 806**

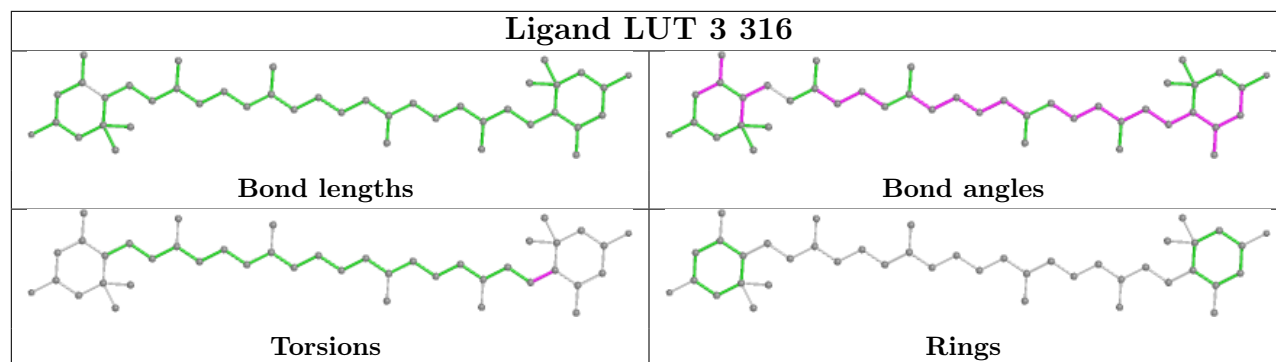
## Ligand CHL 3 307



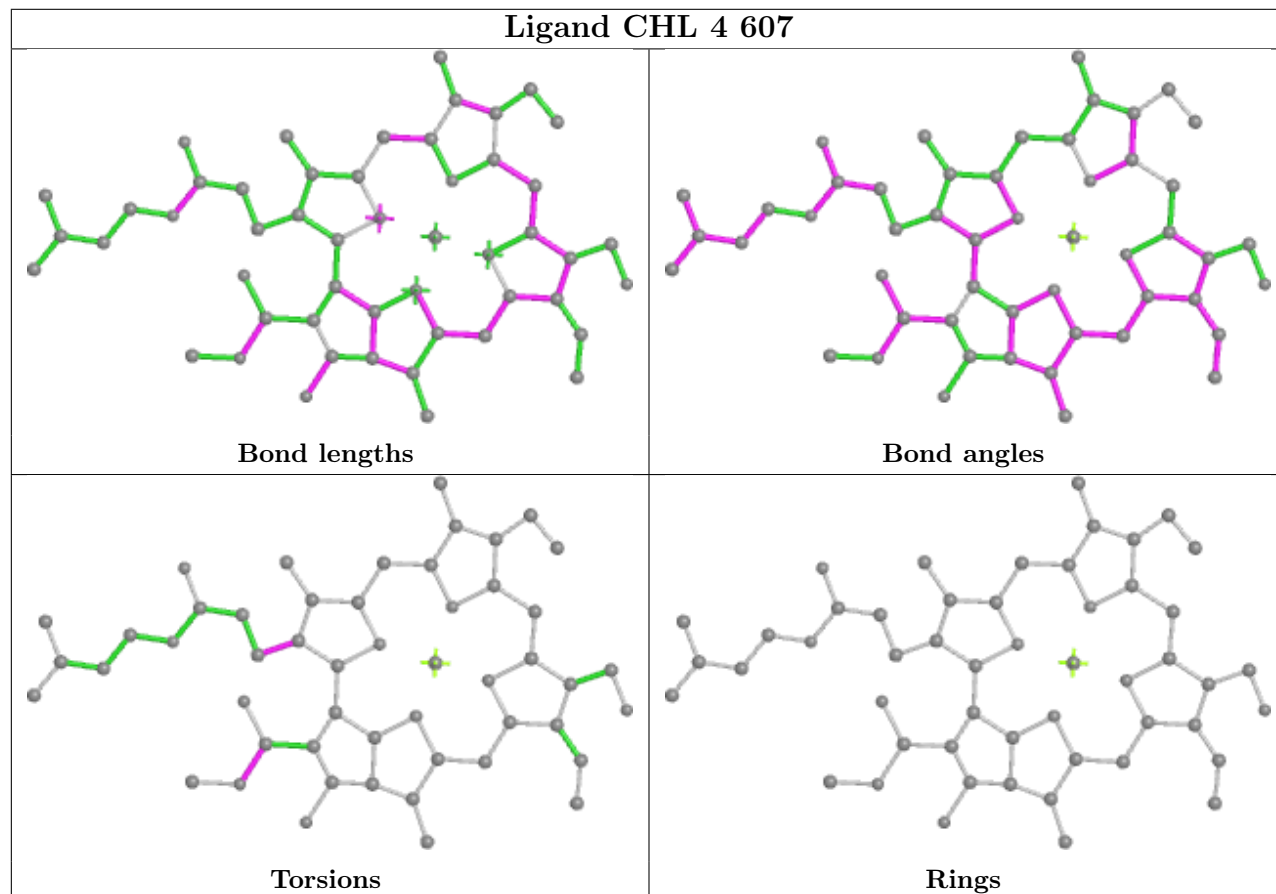
## Ligand CLA B 837



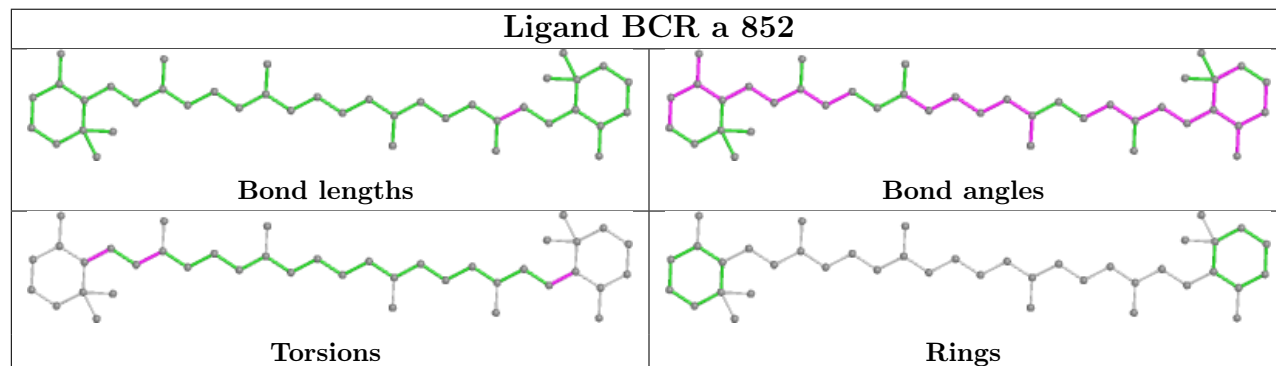
## Ligand LUT 3 316

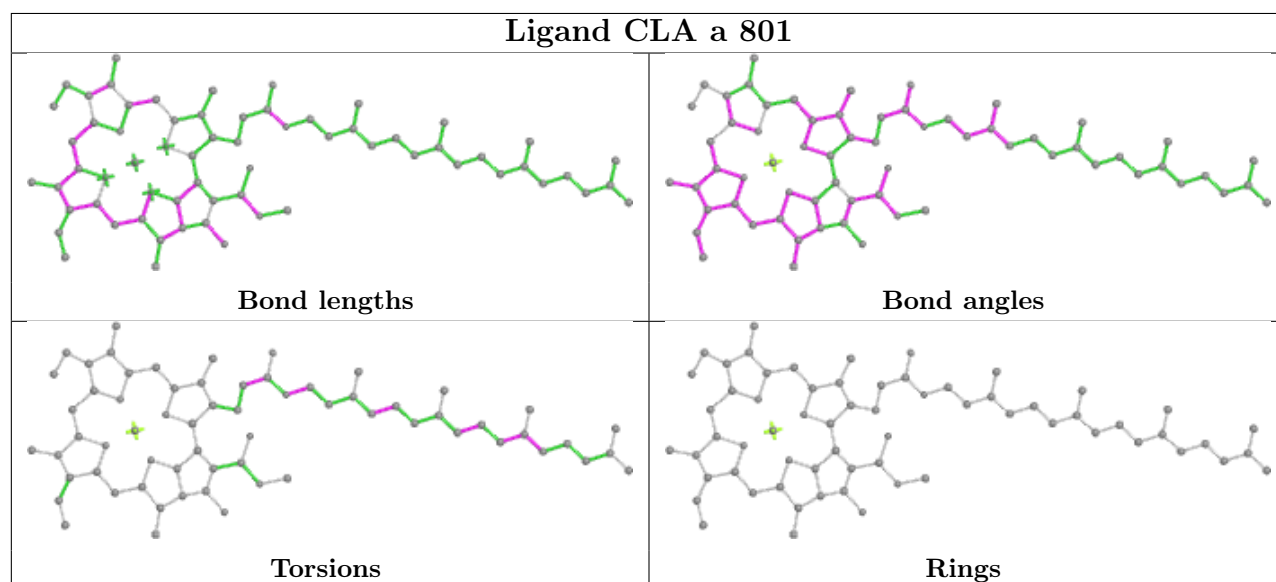
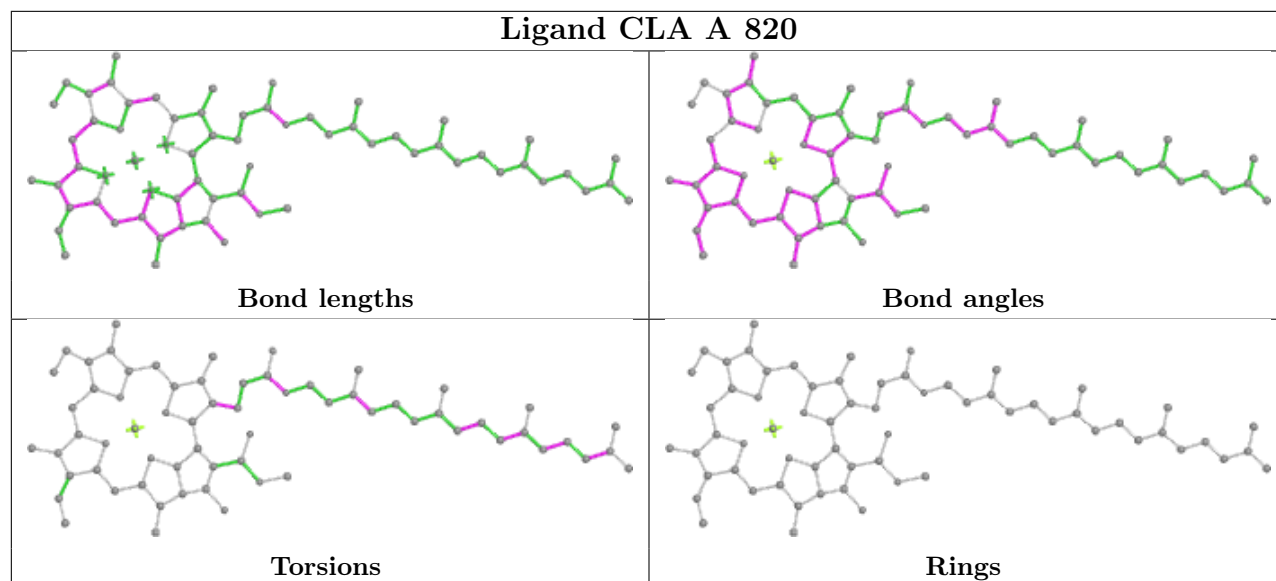
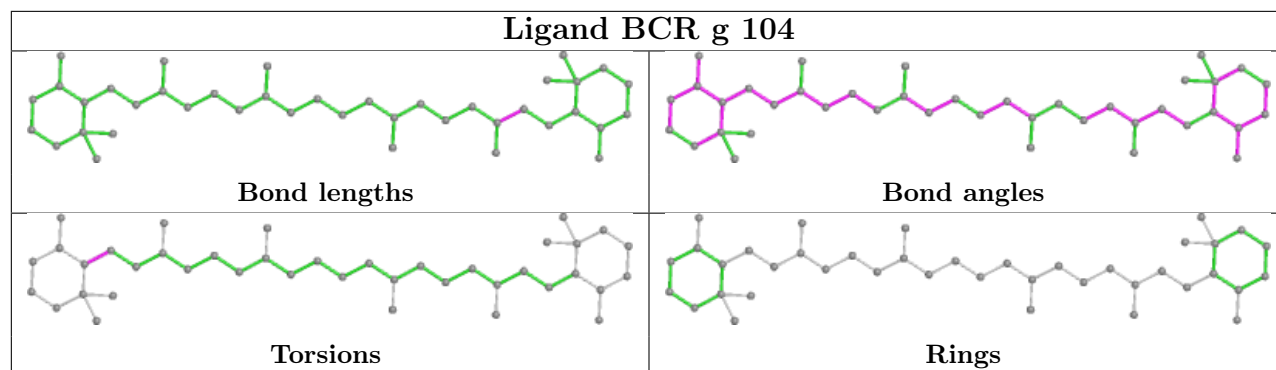


## Ligand CHL 4 607



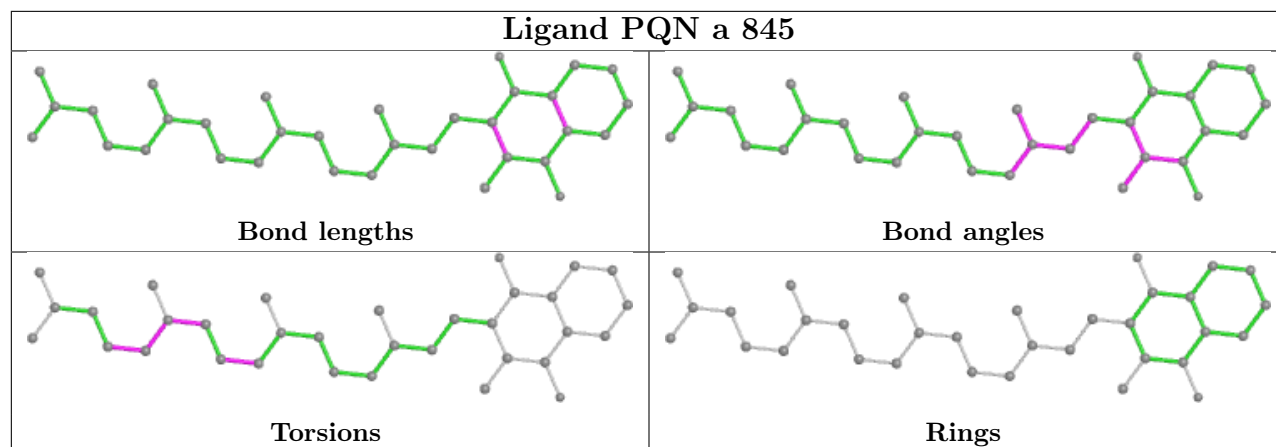
## Ligand BCR a 852



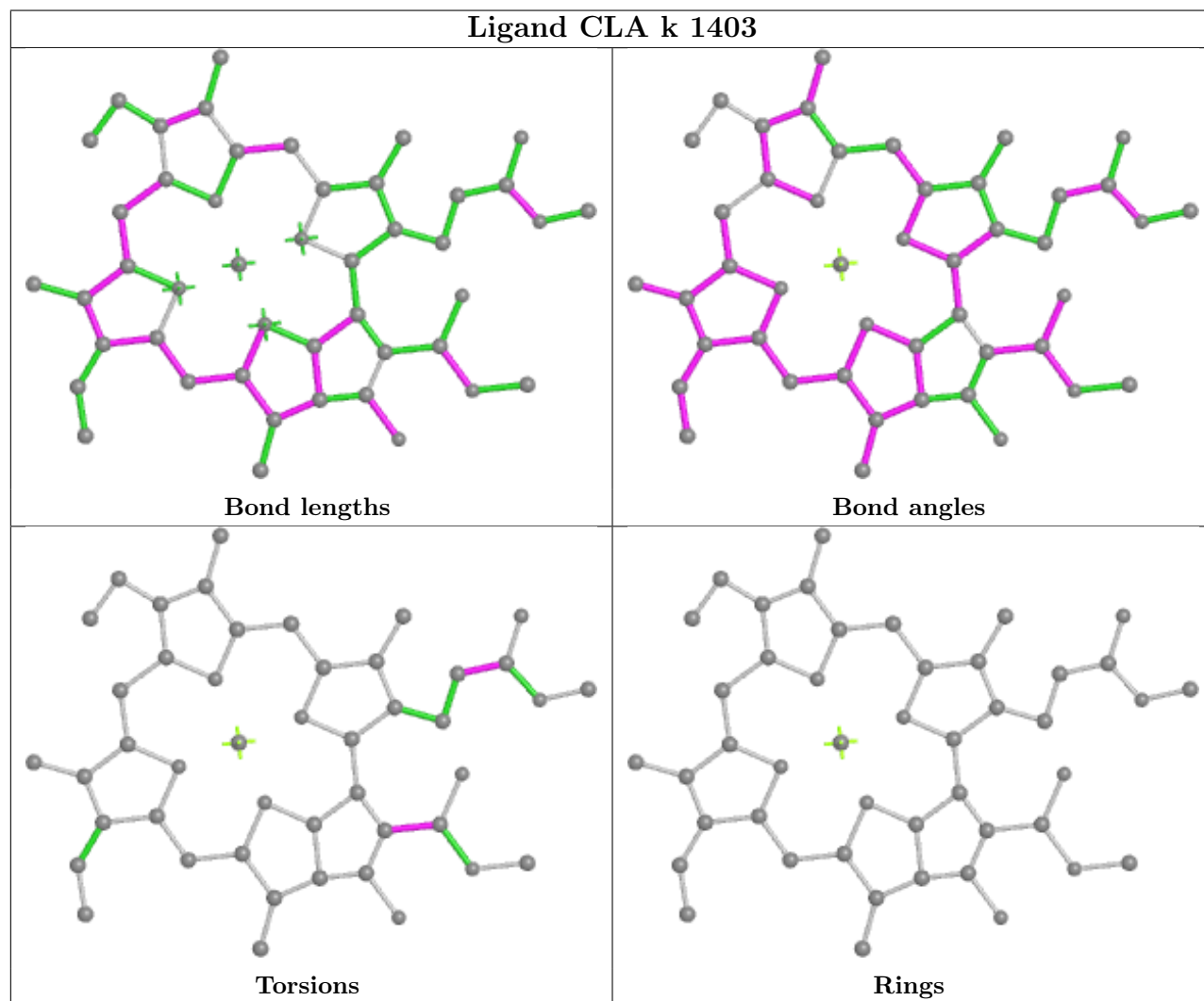




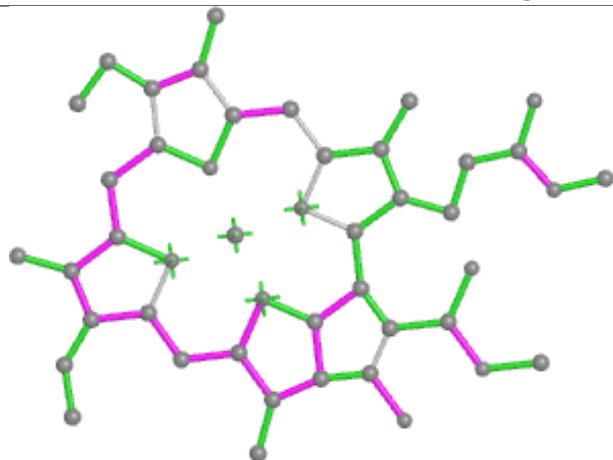
## Ligand PQN a 845



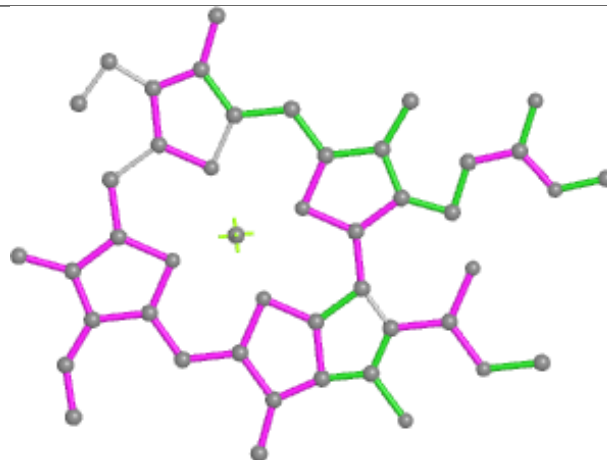
## Ligand CLA k 1403



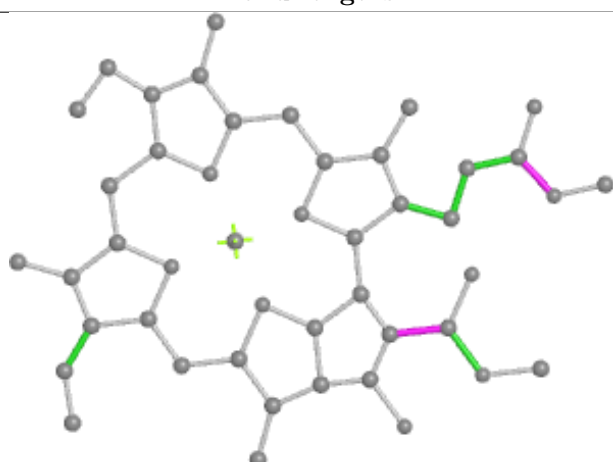
## Ligand CLA 6 309



Bond lengths



Bond angles

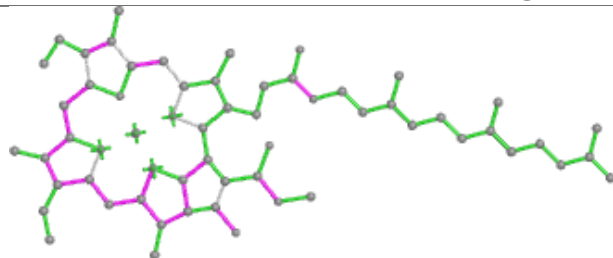


Torsions

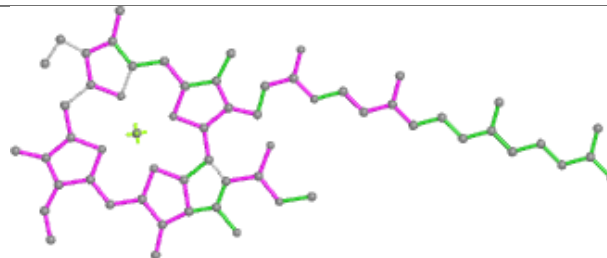


Rings

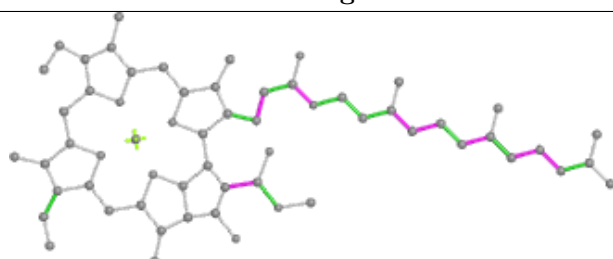
## Ligand CLA 9 602



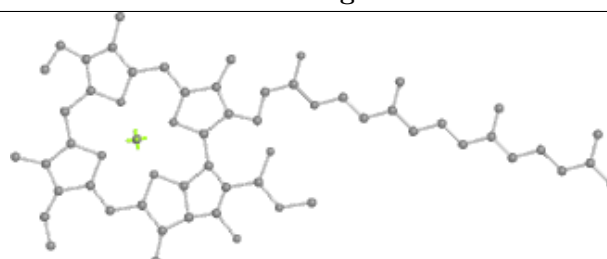
Bond lengths



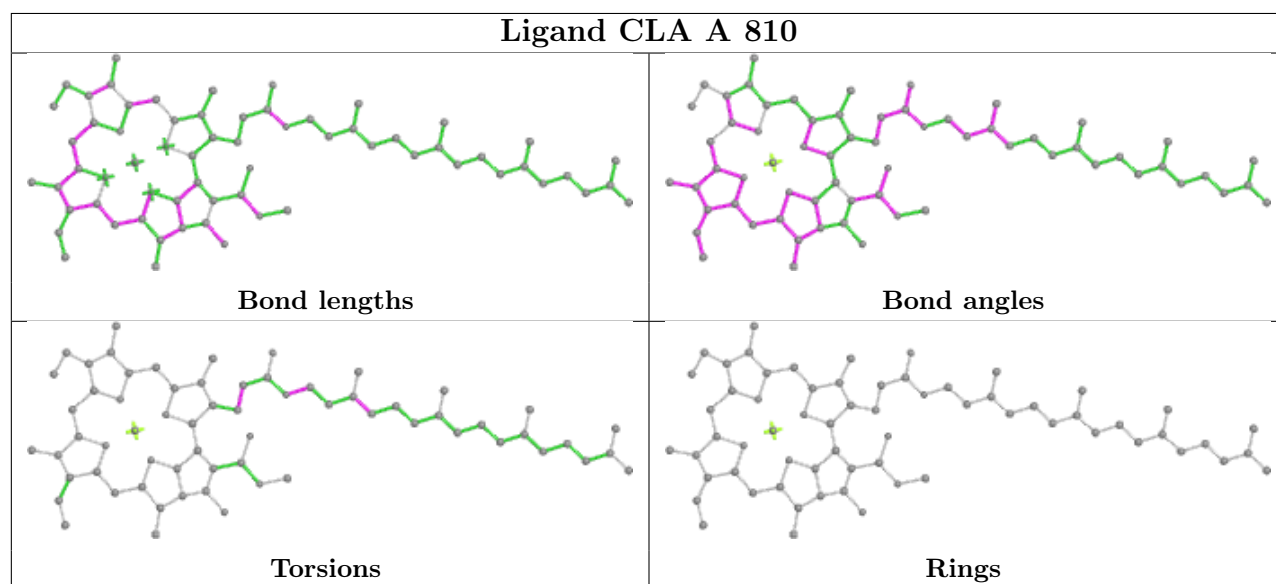
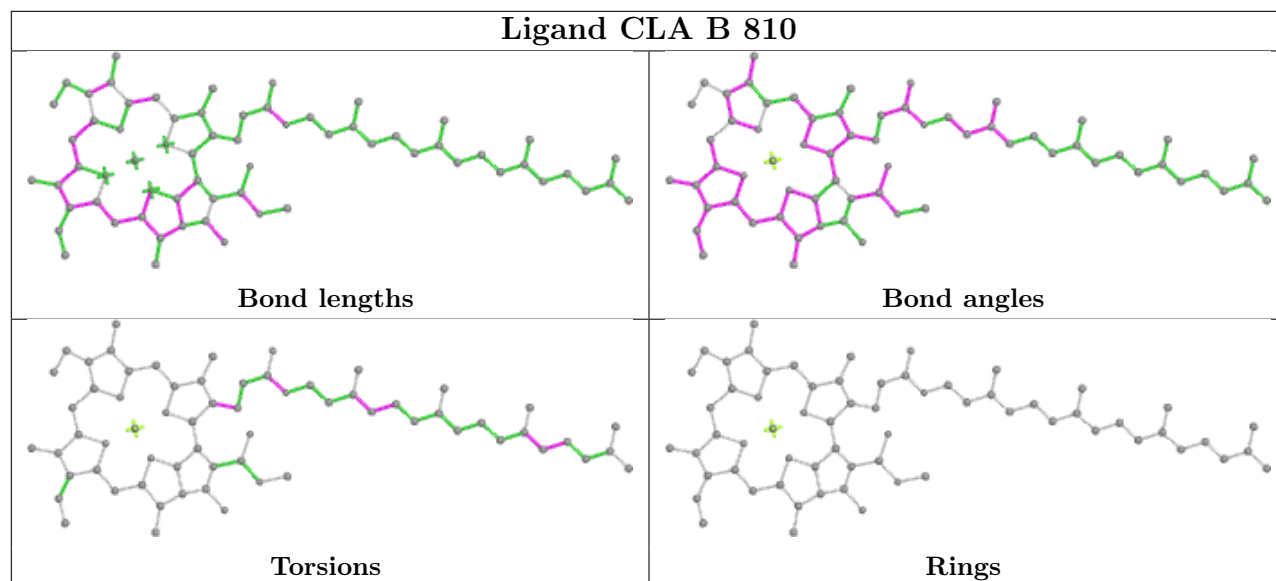
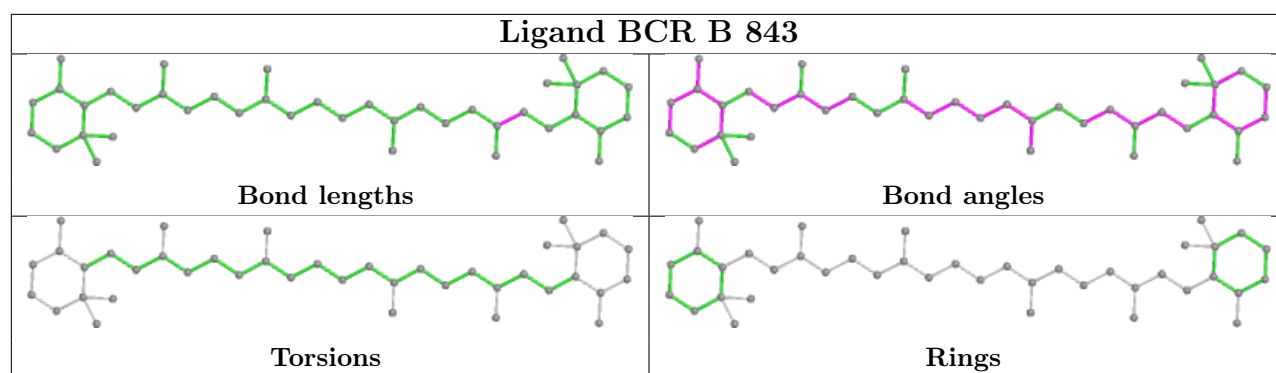
Bond angles



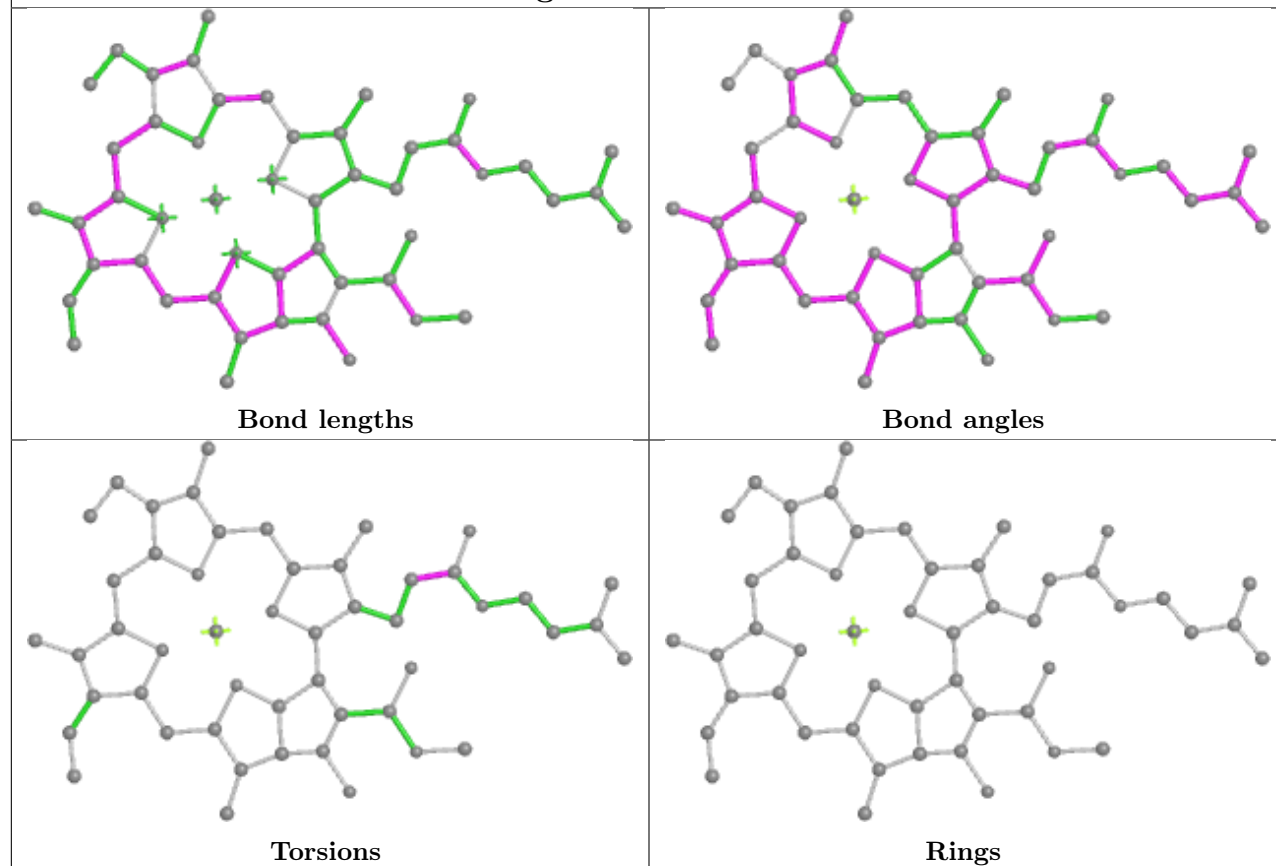
Torsions



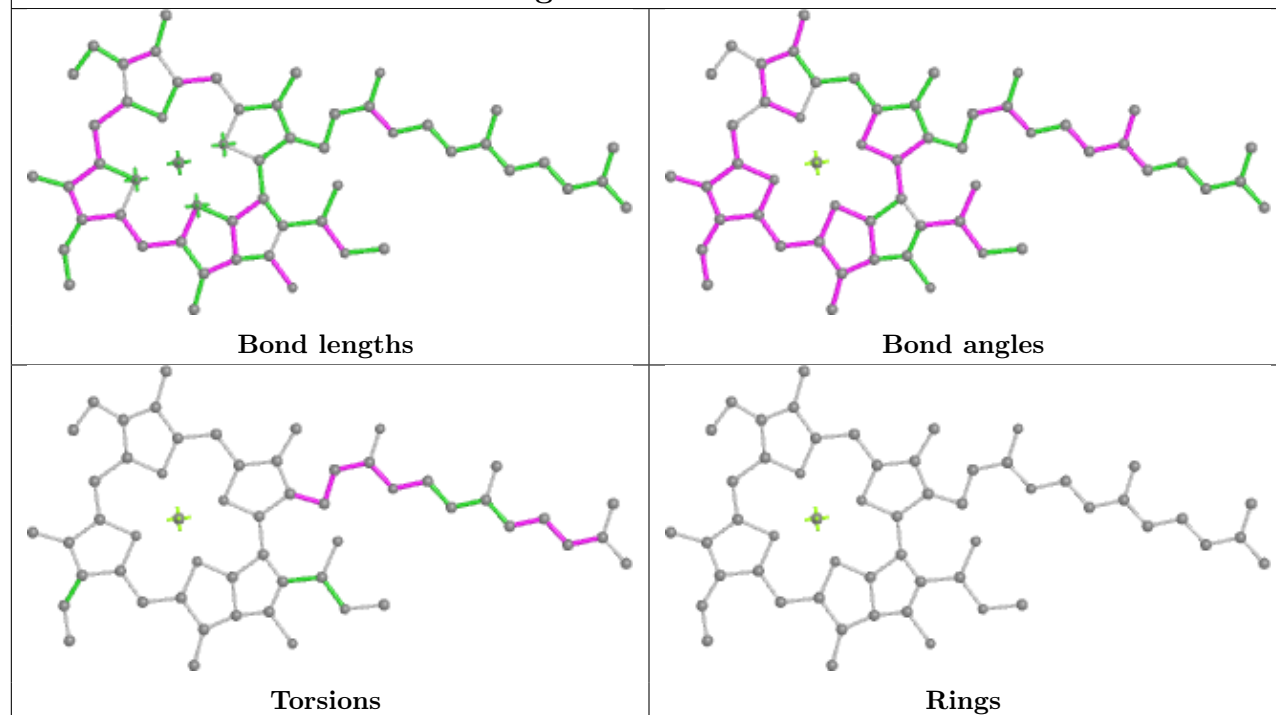
Rings

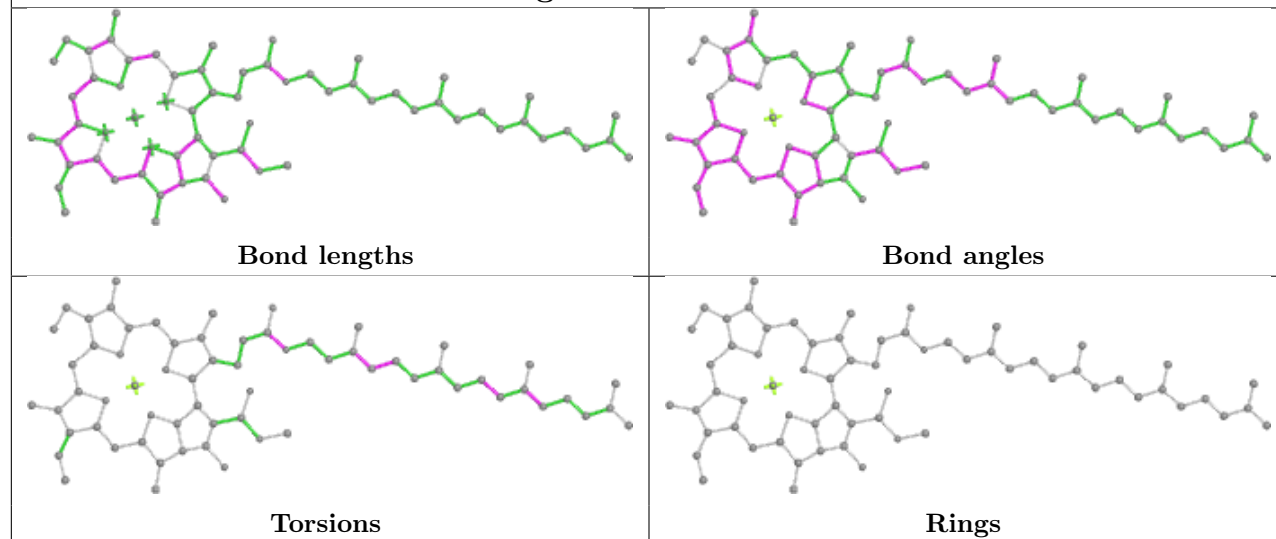
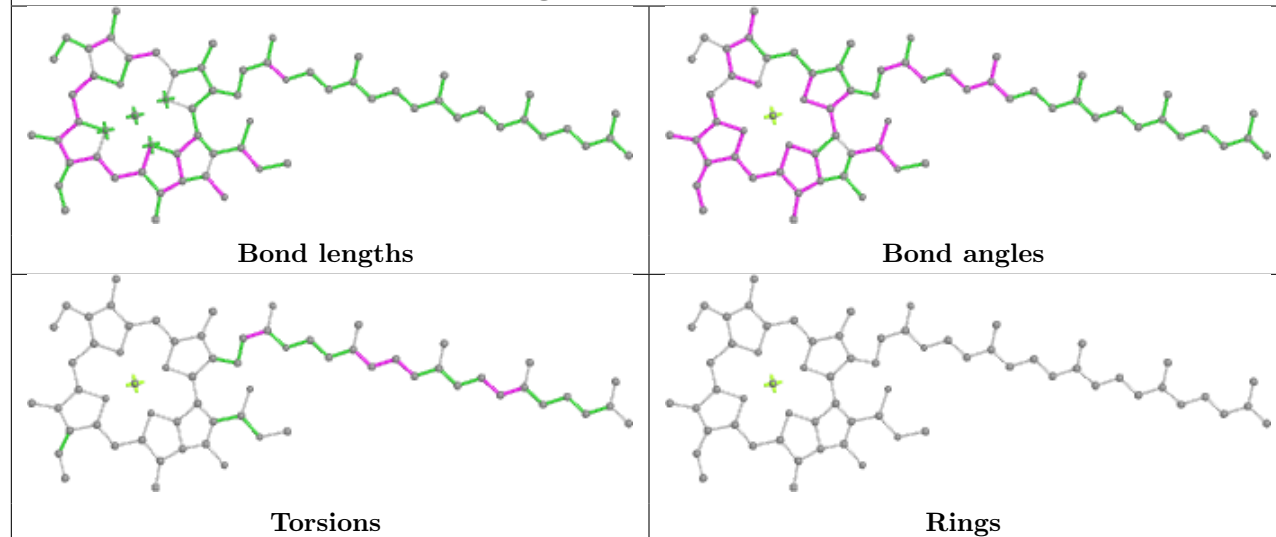


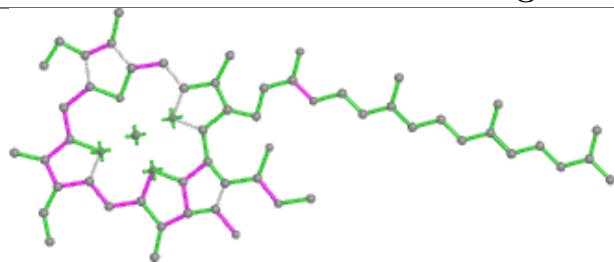
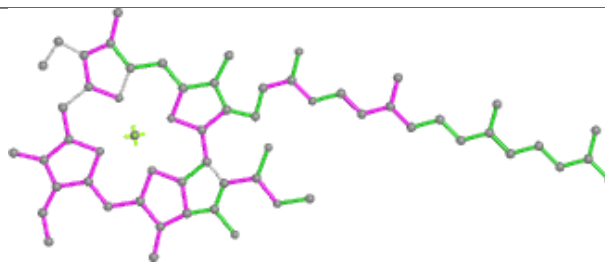
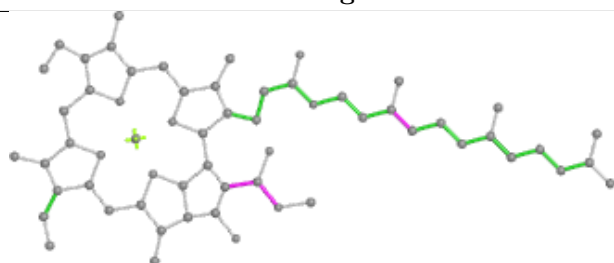
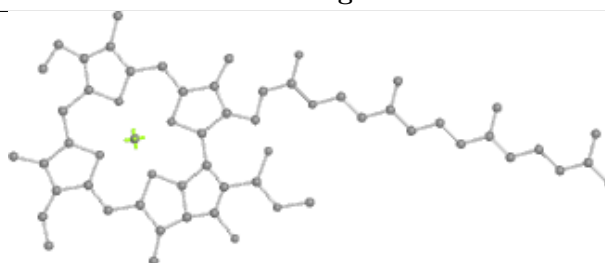
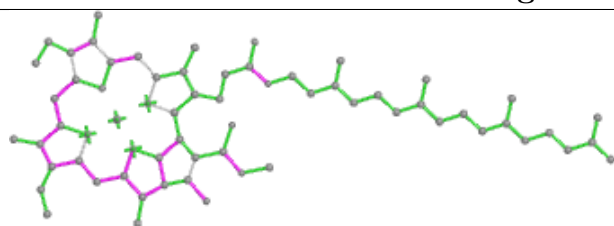
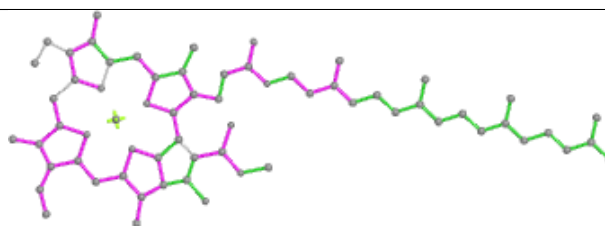
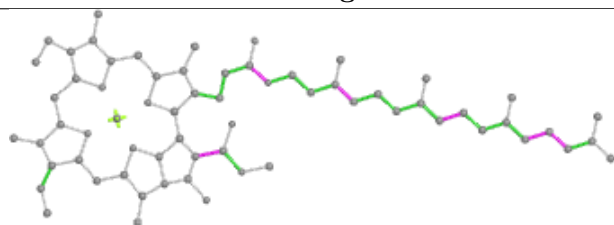
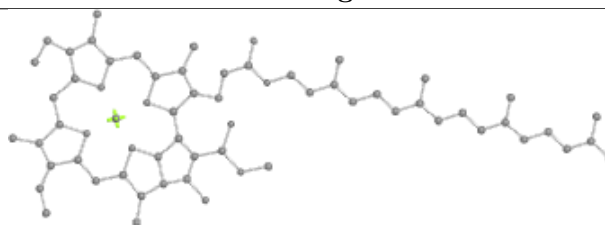
## Ligand CLA 4 614



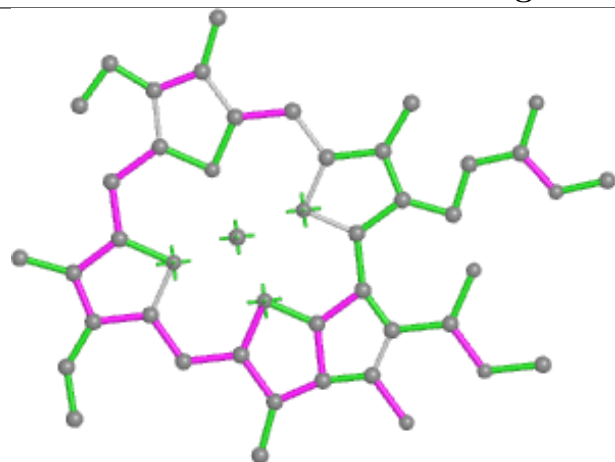
## Ligand CLA b 812



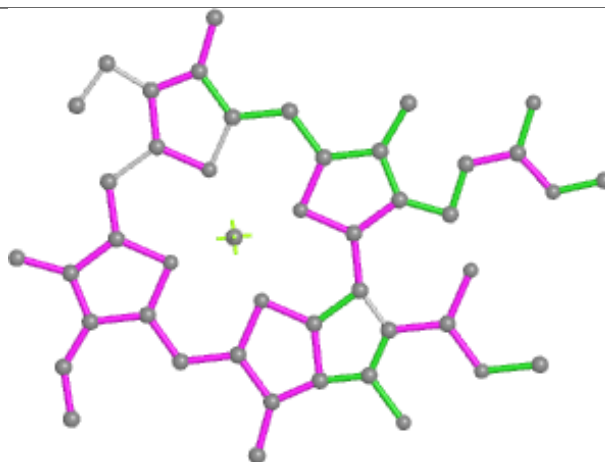
**Ligand CLA 6 310****Ligand CLA b 806**

**Ligand CLA b 823****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA b 837****Bond lengths****Bond angles****Torsions****Rings**

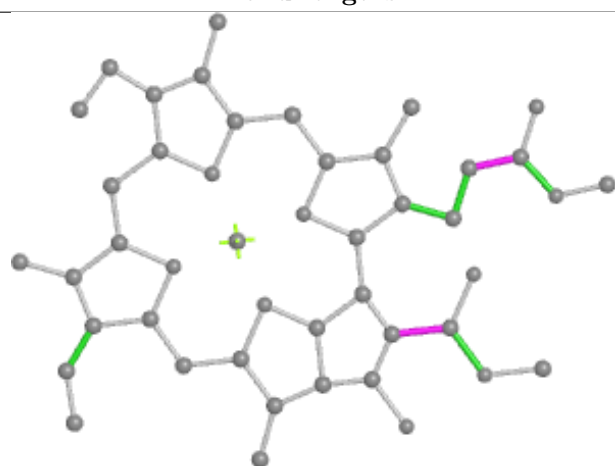
## Ligand CLA G 104



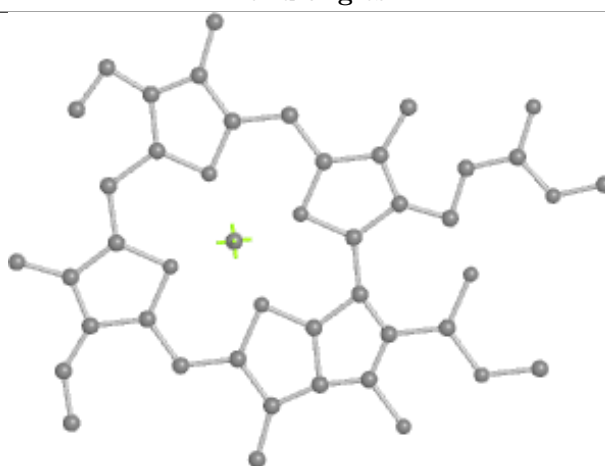
Bond lengths



Bond angles

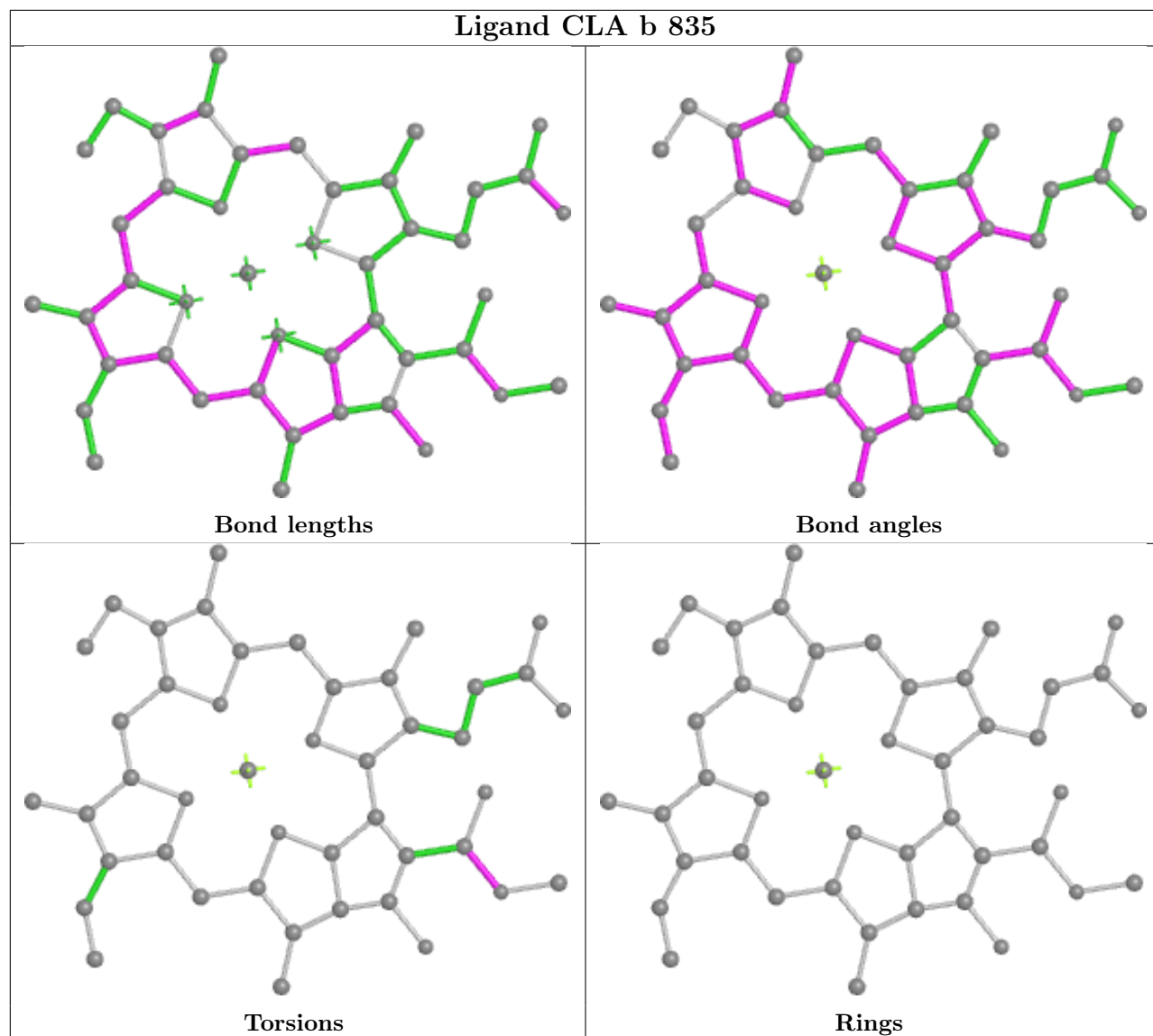


Torsions



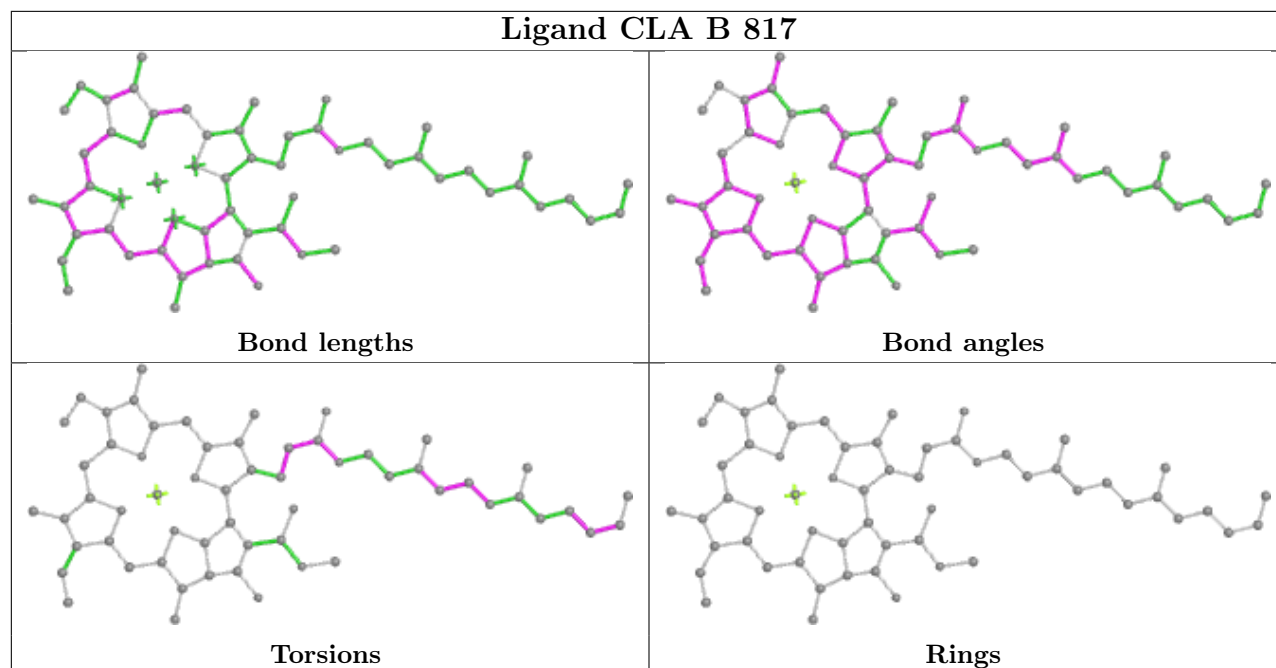
Rings

## Ligand CLA b 835

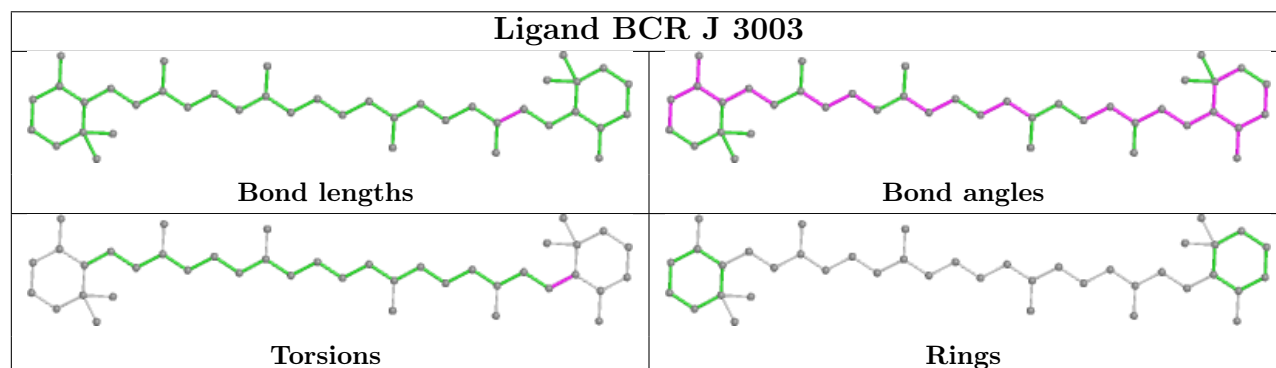




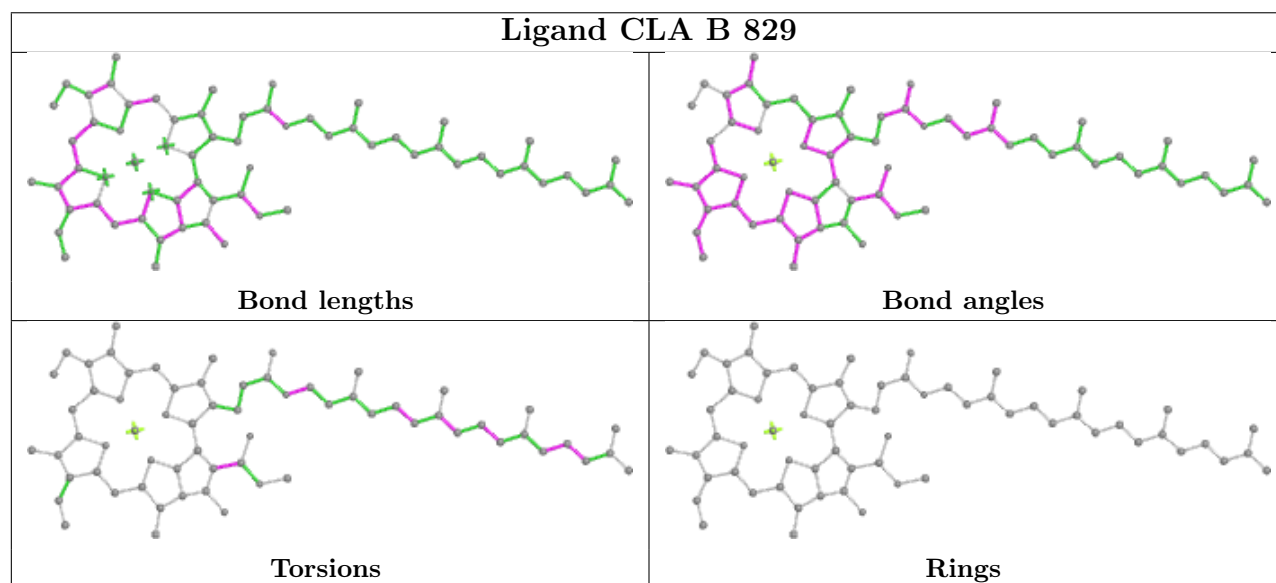
## Ligand CLA B 817

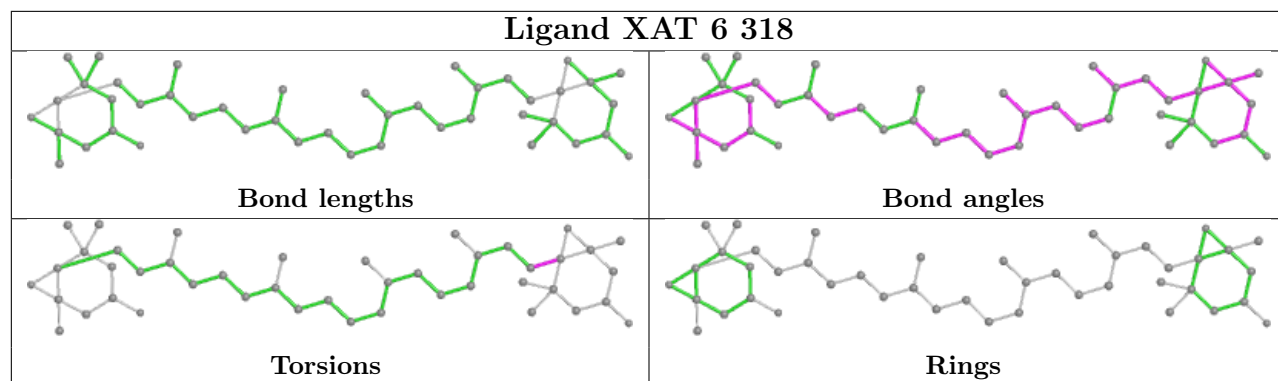
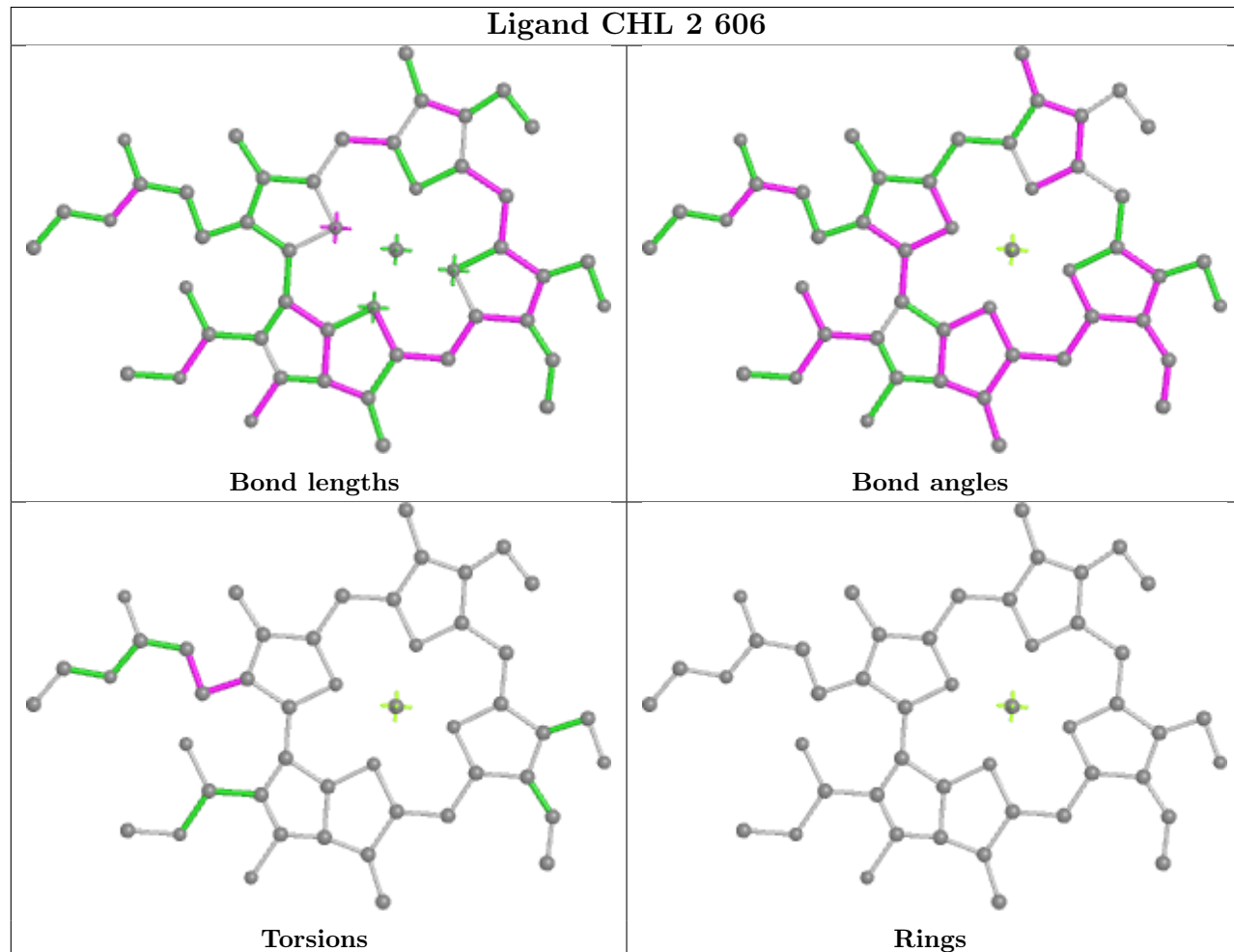


## Ligand BCR J 3003

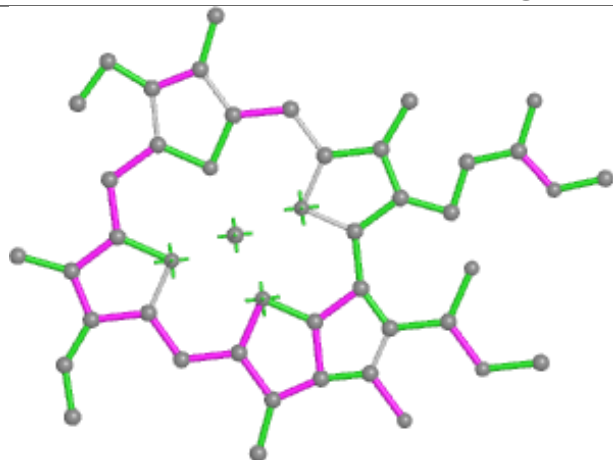


## Ligand CLA B 829

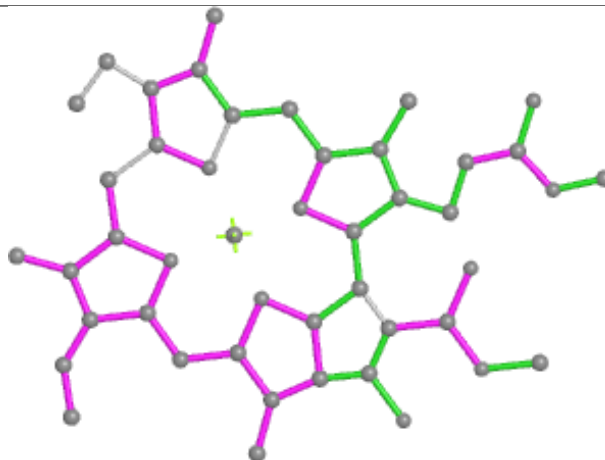


**Ligand XAT 6 318****Ligand CHL 2 606**

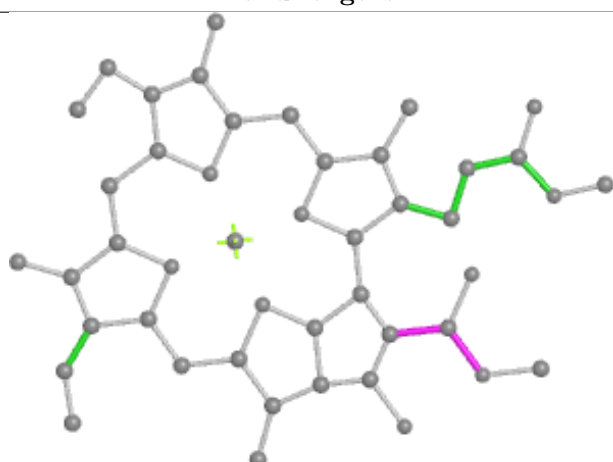
## Ligand CLA b 821



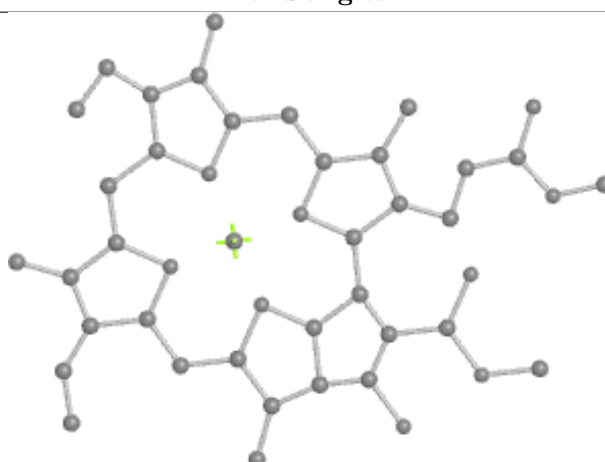
Bond lengths



Bond angles

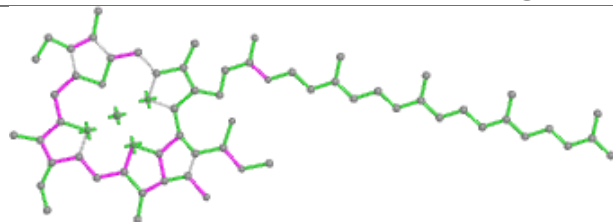


Torsions

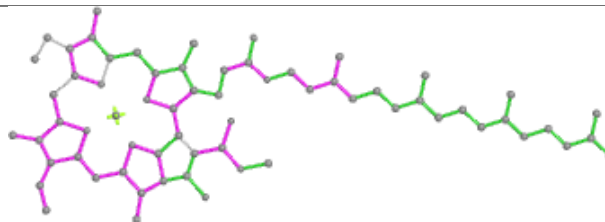


Rings

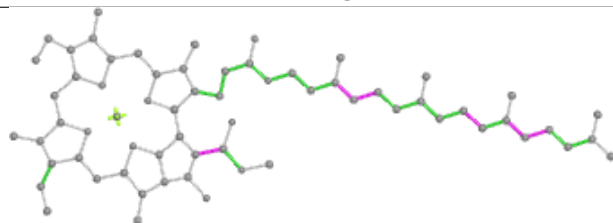
## Ligand CLA a 808



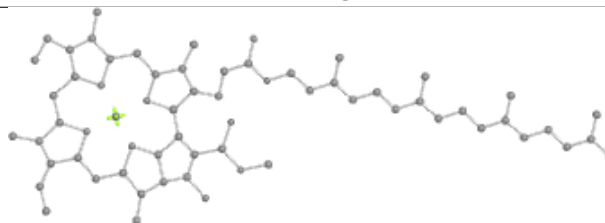
Bond lengths



Bond angles

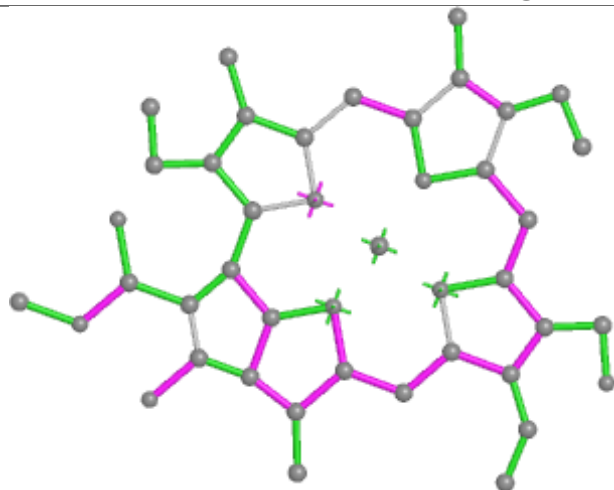


Torsions

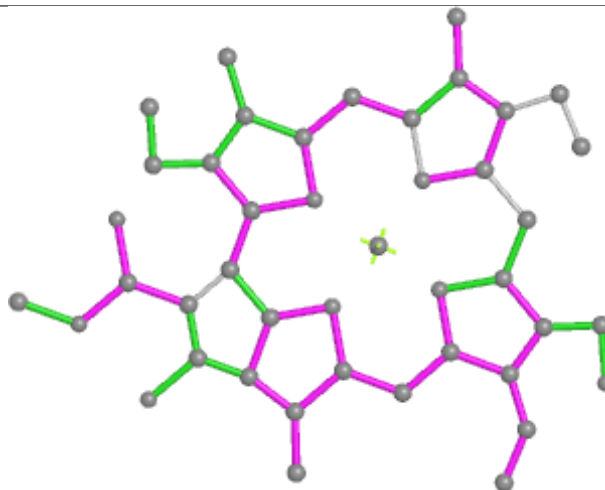


Rings

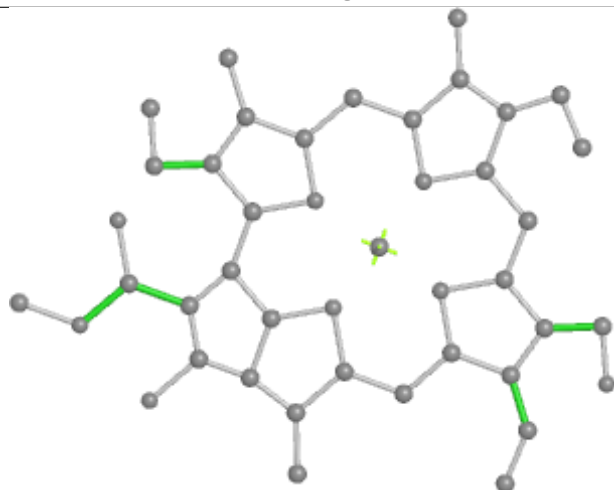
## Ligand CHL 9 615



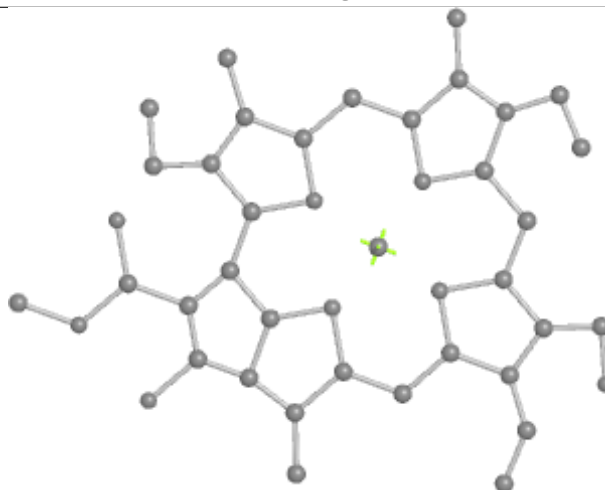
Bond lengths



Bond angles

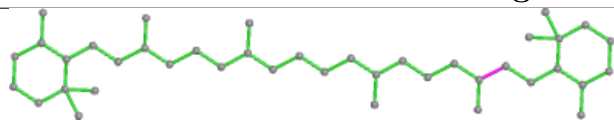


Torsions

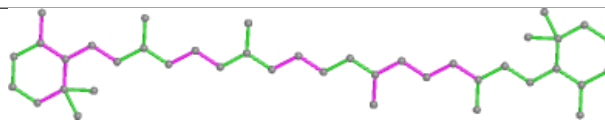


Rings

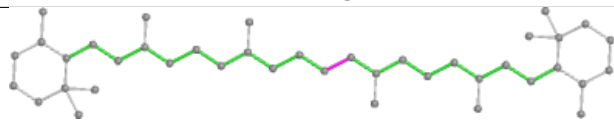
## Ligand BCR B 801



Bond lengths



Bond angles

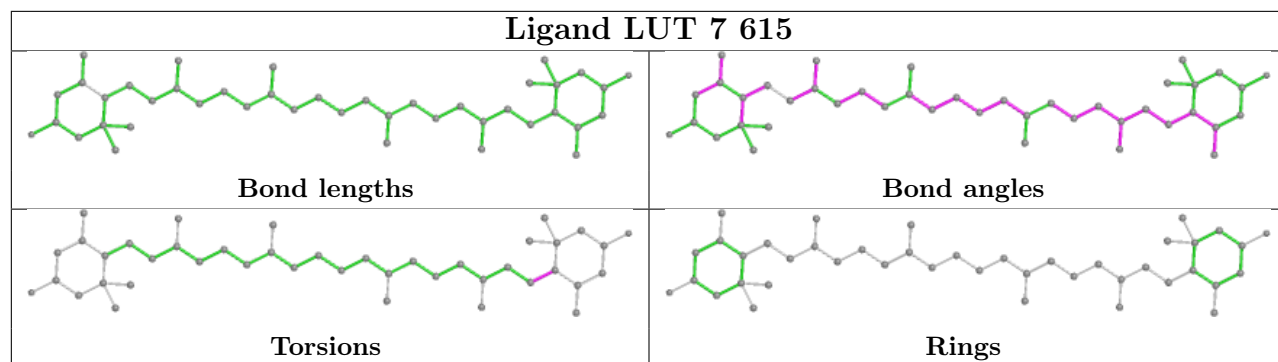


Torsions

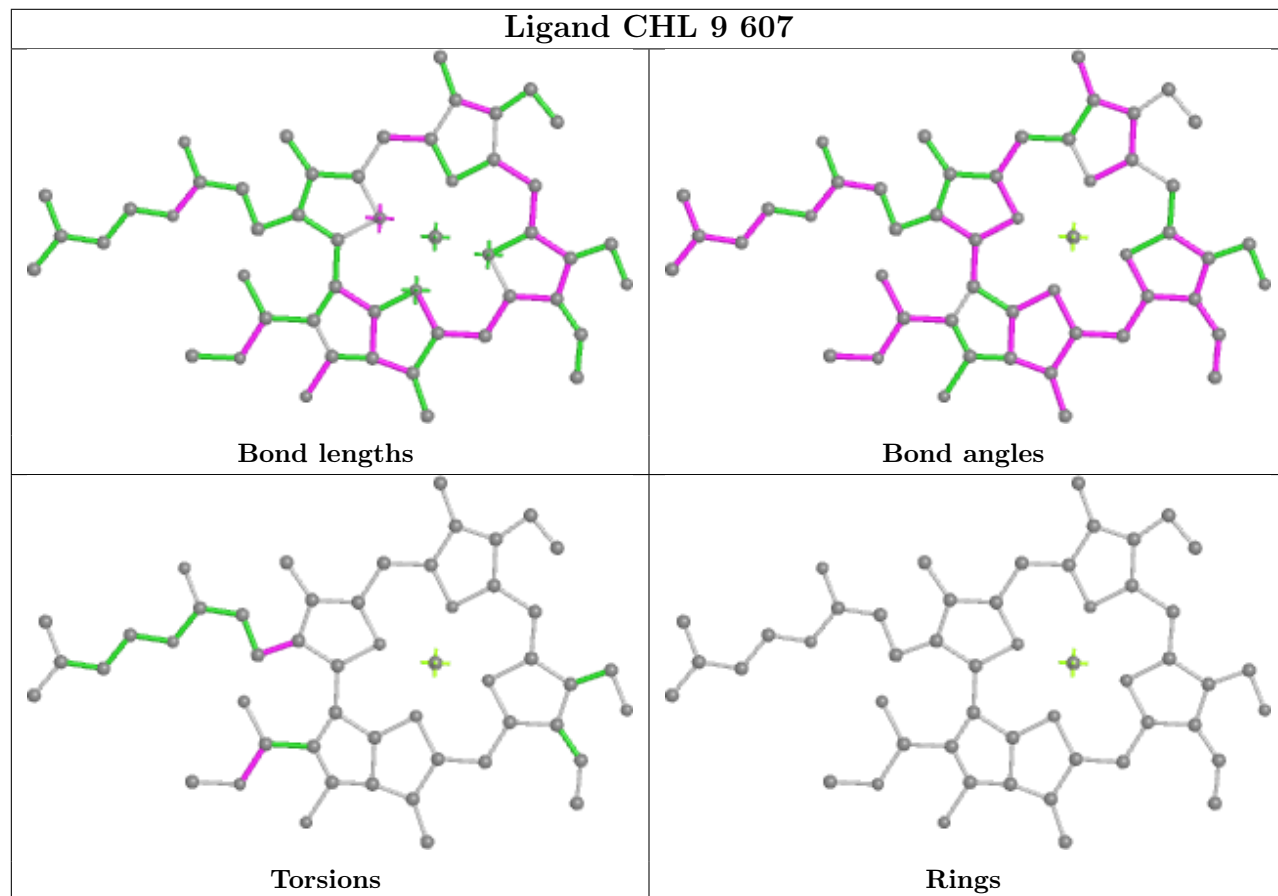


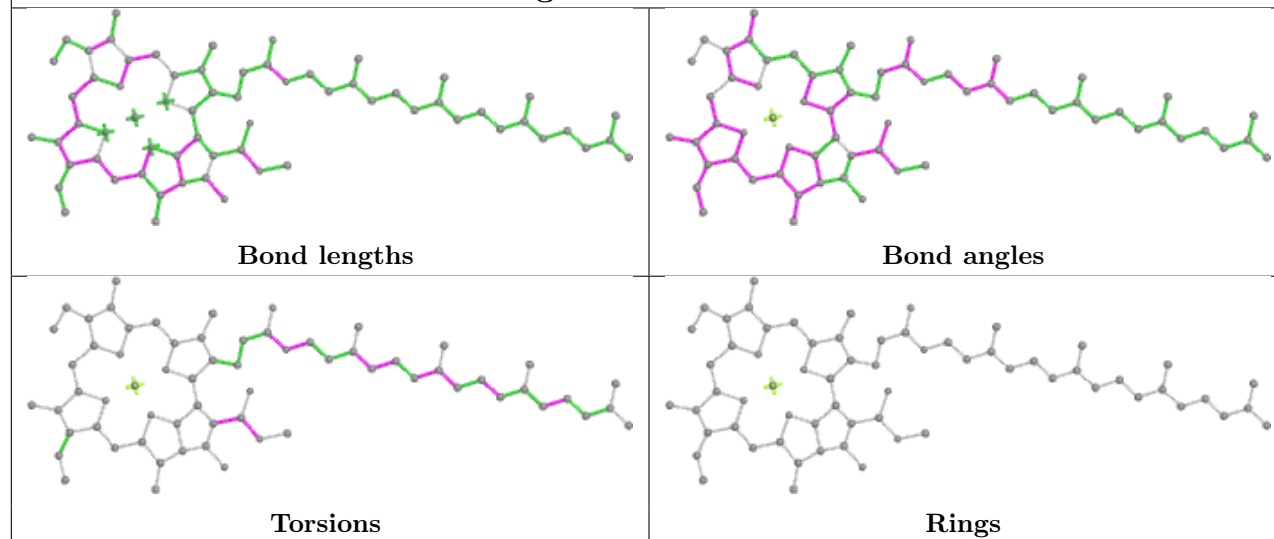
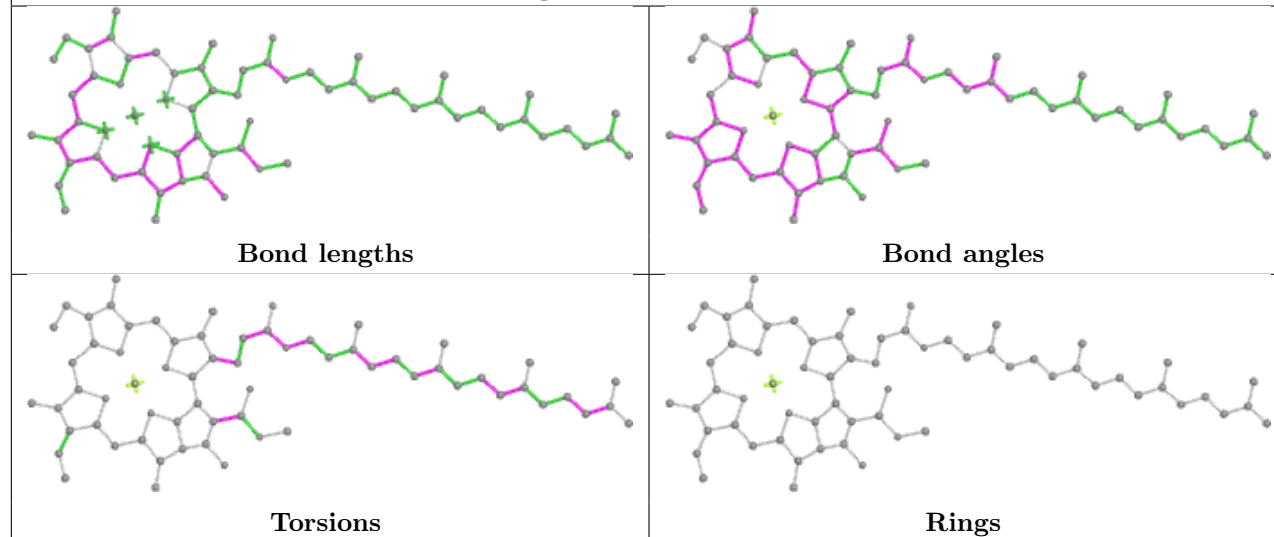
Rings

## Ligand LUT 7 615

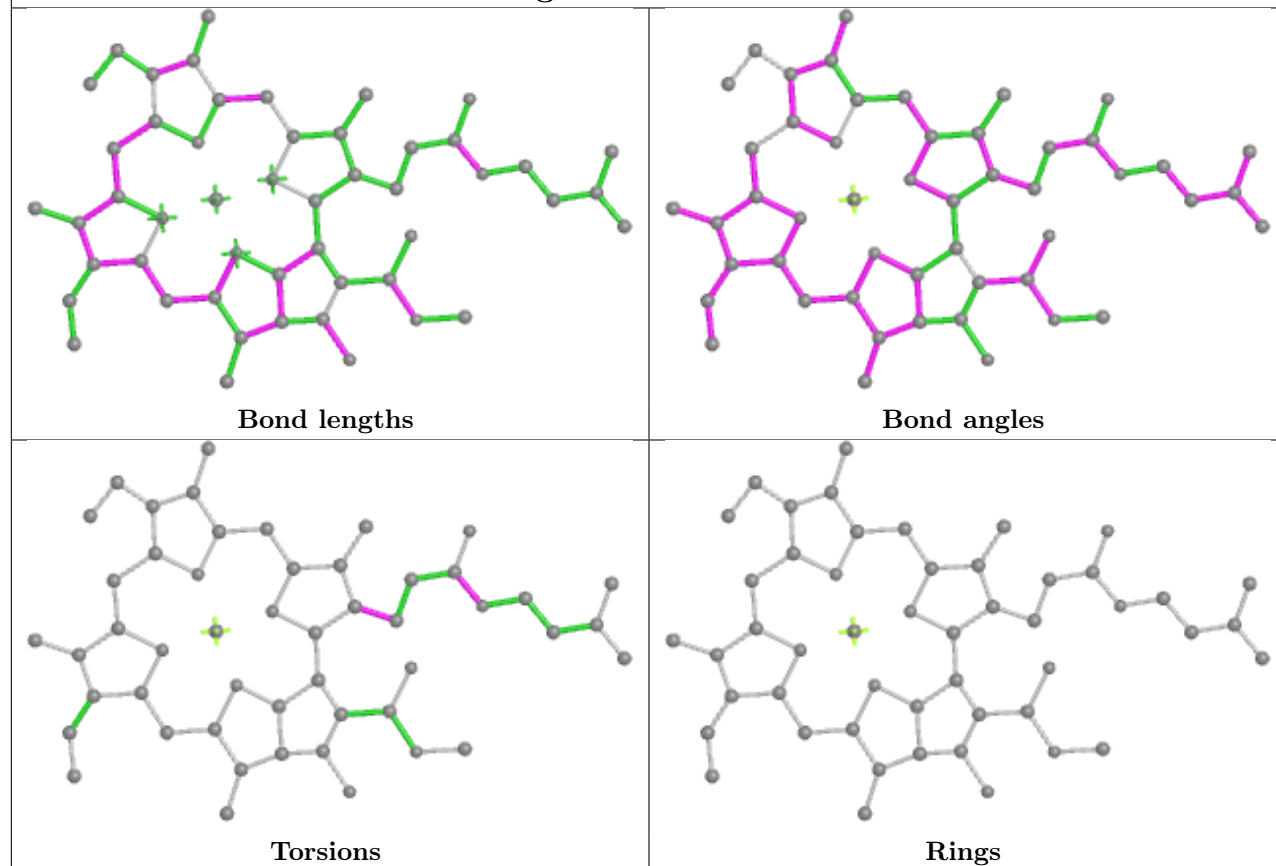


## Ligand CHL 9 607

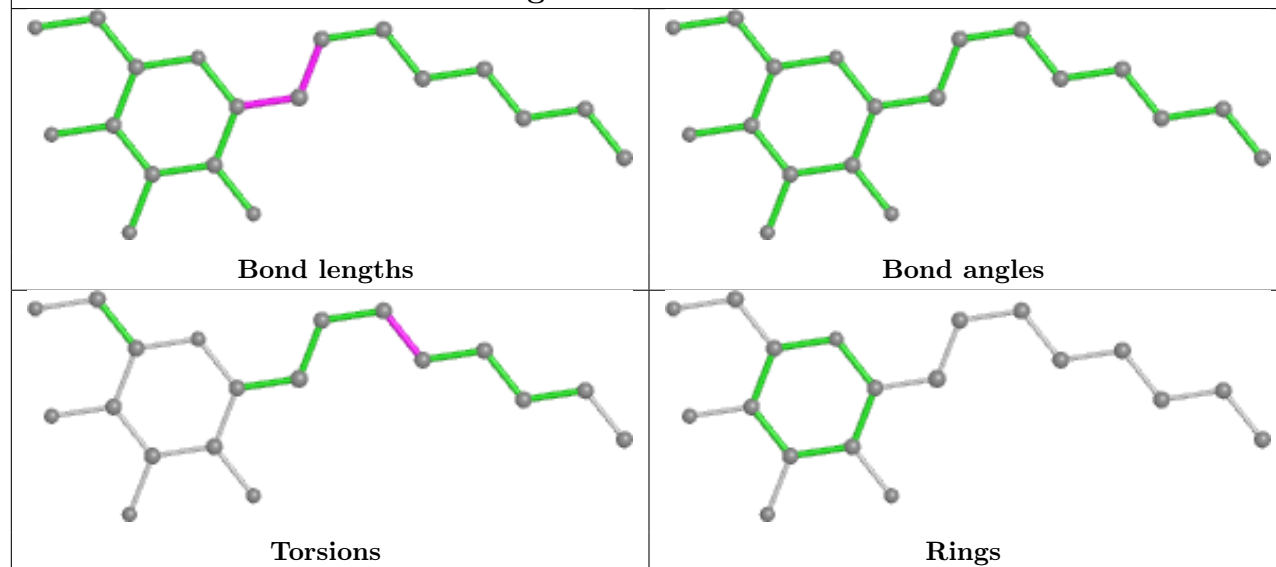


**Ligand CLA a 831****Ligand CLA b 805**

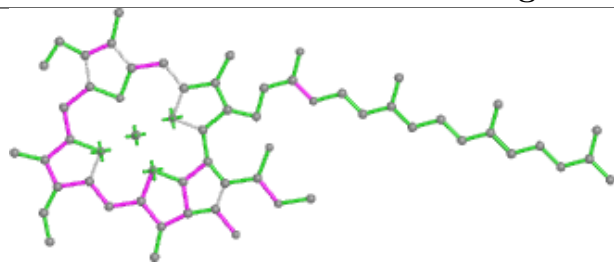
## Ligand CLA 9 608



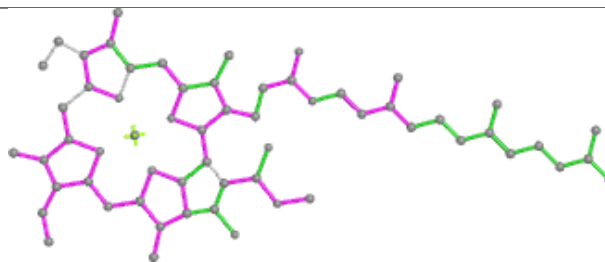
## Ligand HTG f 7001



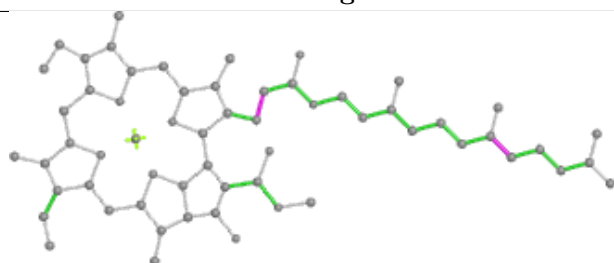
## Ligand CLA 1 310



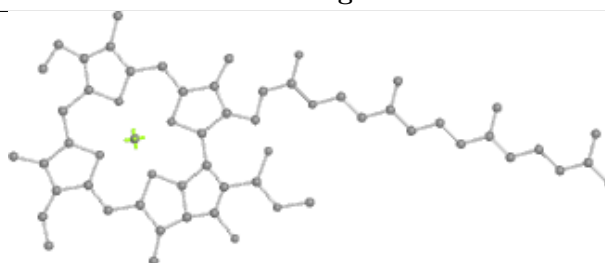
Bond lengths



Bond angles

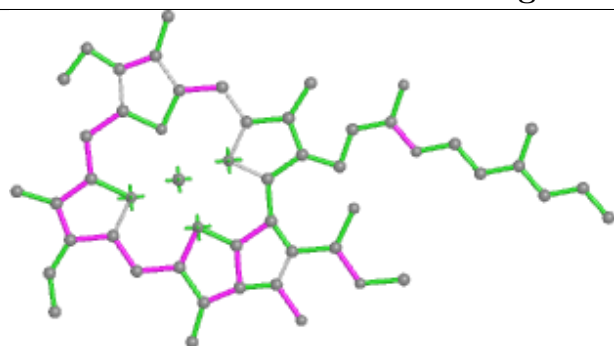


Torsions

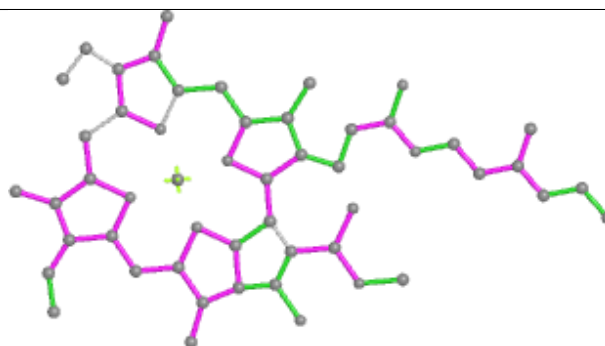


Rings

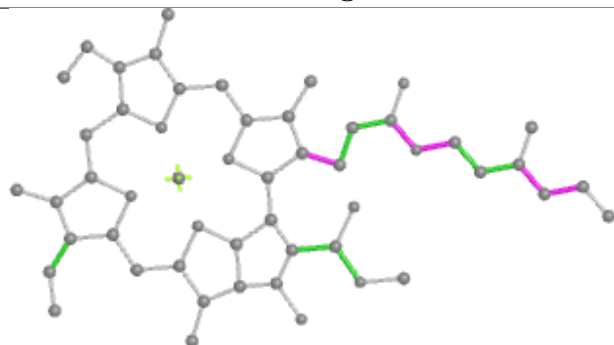
## Ligand CLA 1 312



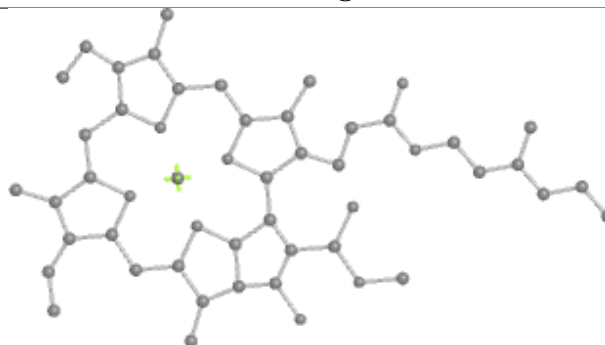
Bond lengths



Bond angles



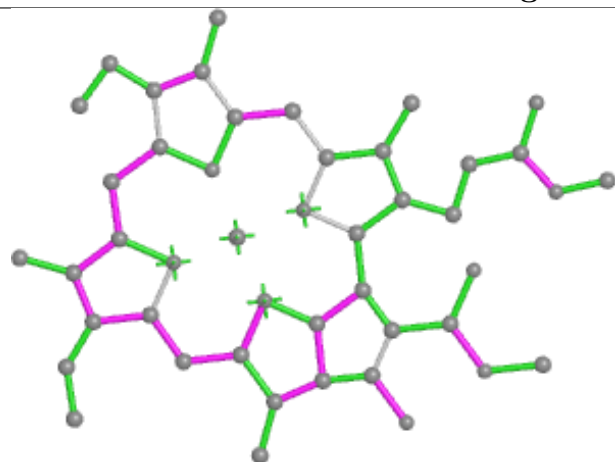
Torsions



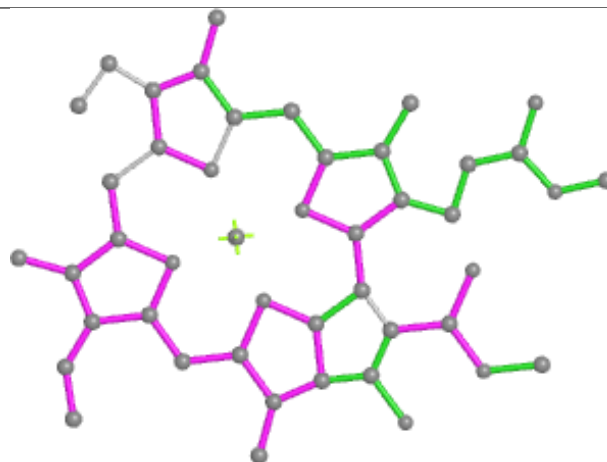
Rings



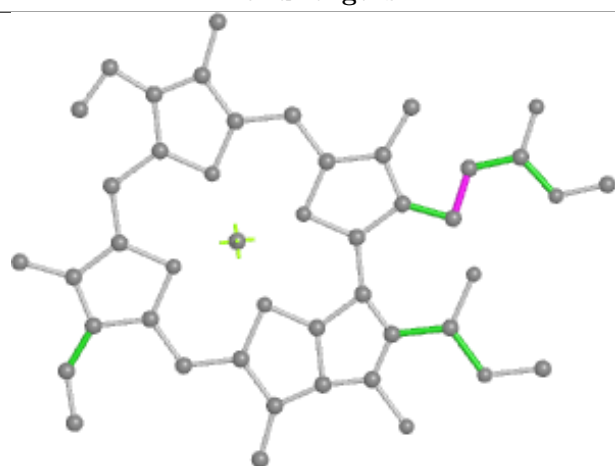
## Ligand CLA 3 314



Bond lengths



Bond angles

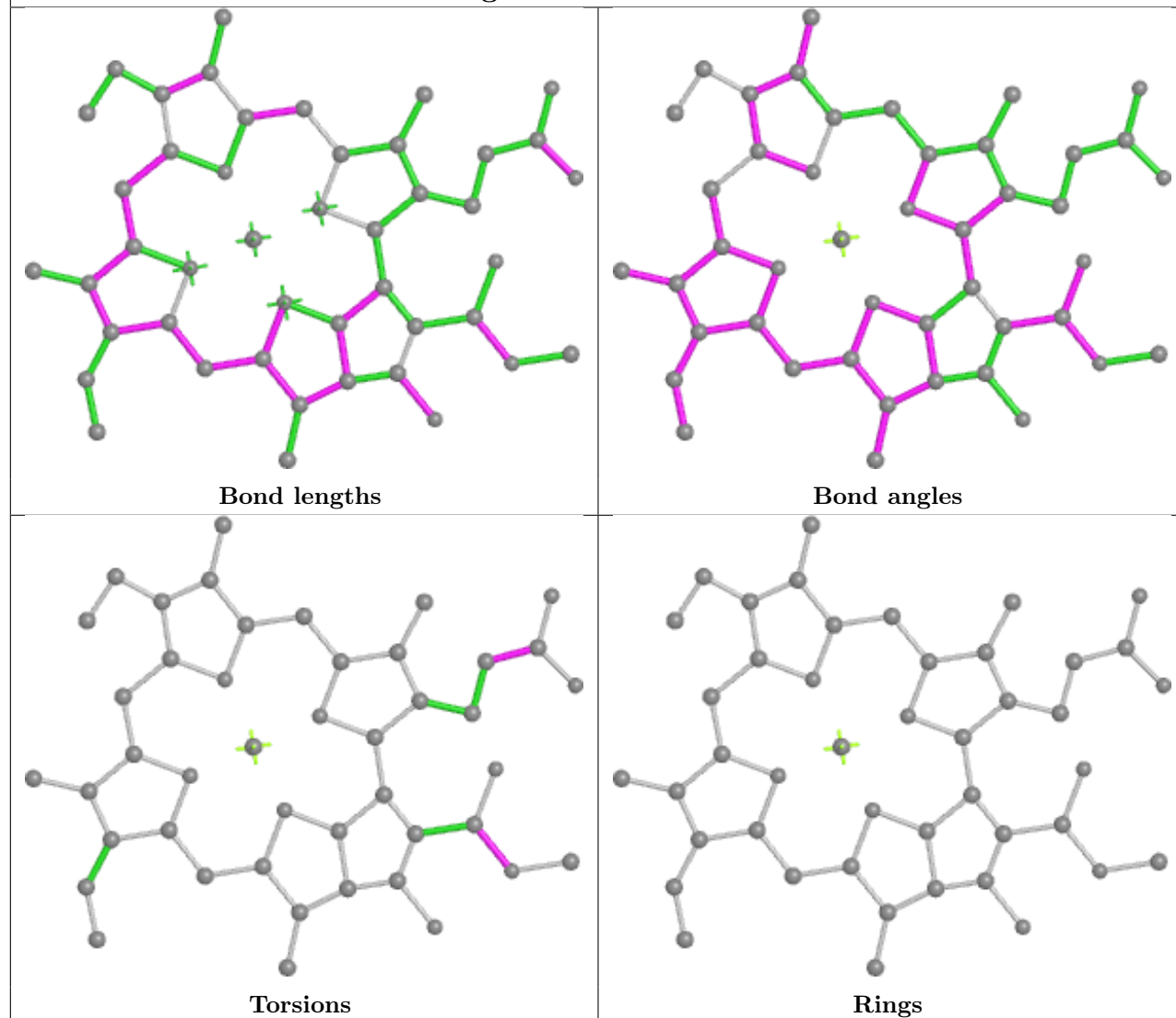


Torsions

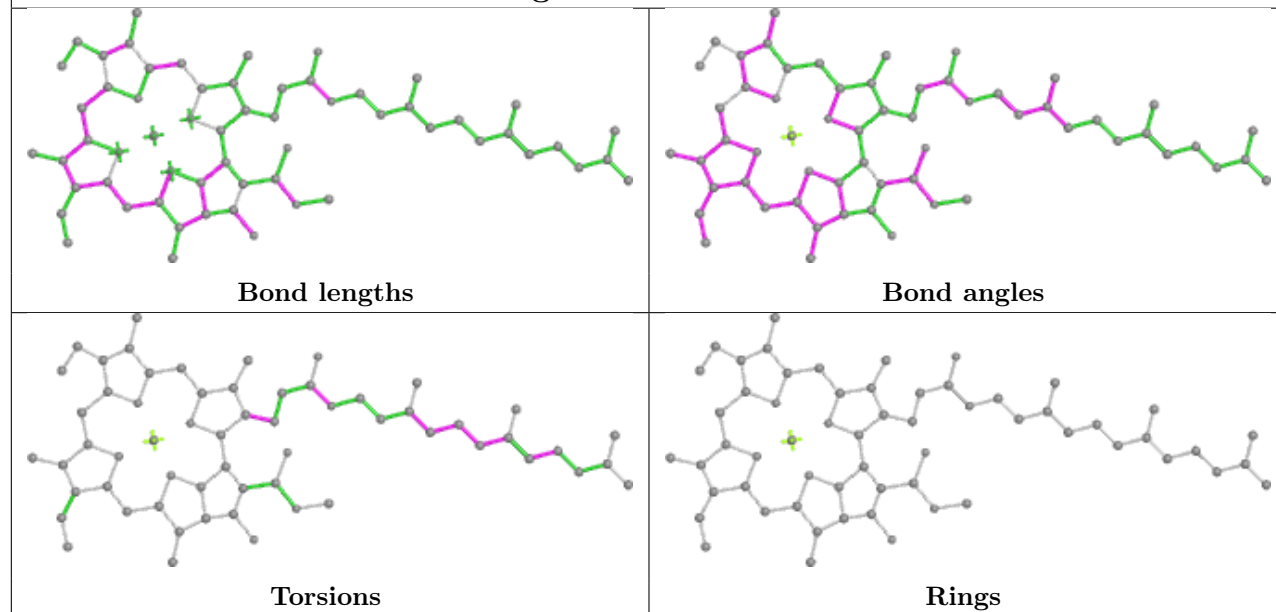


Rings

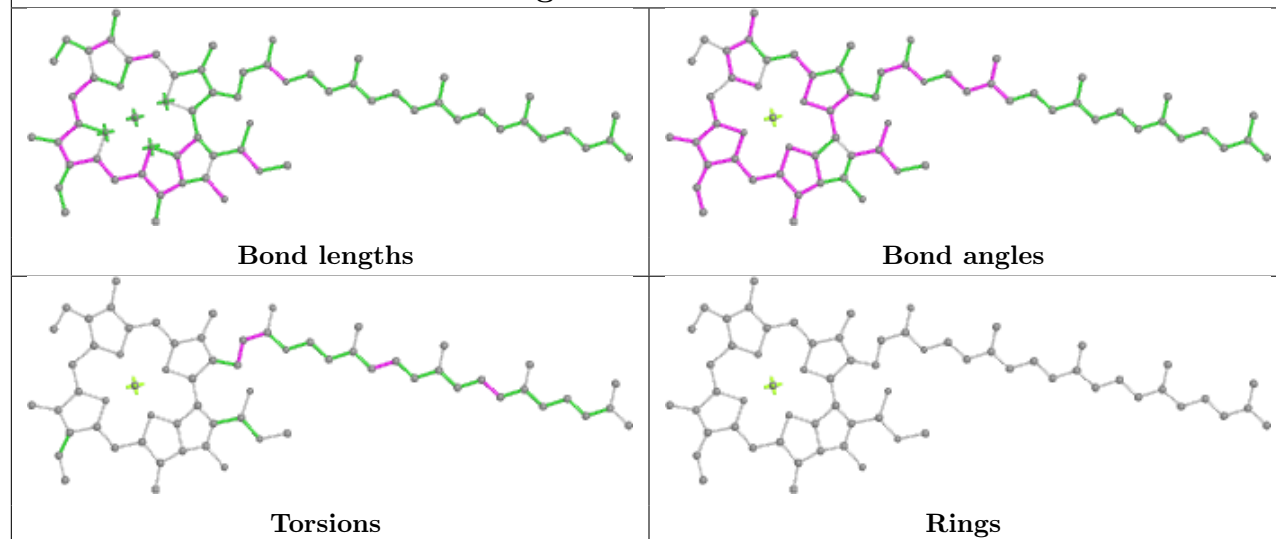
## Ligand CLA K 4002



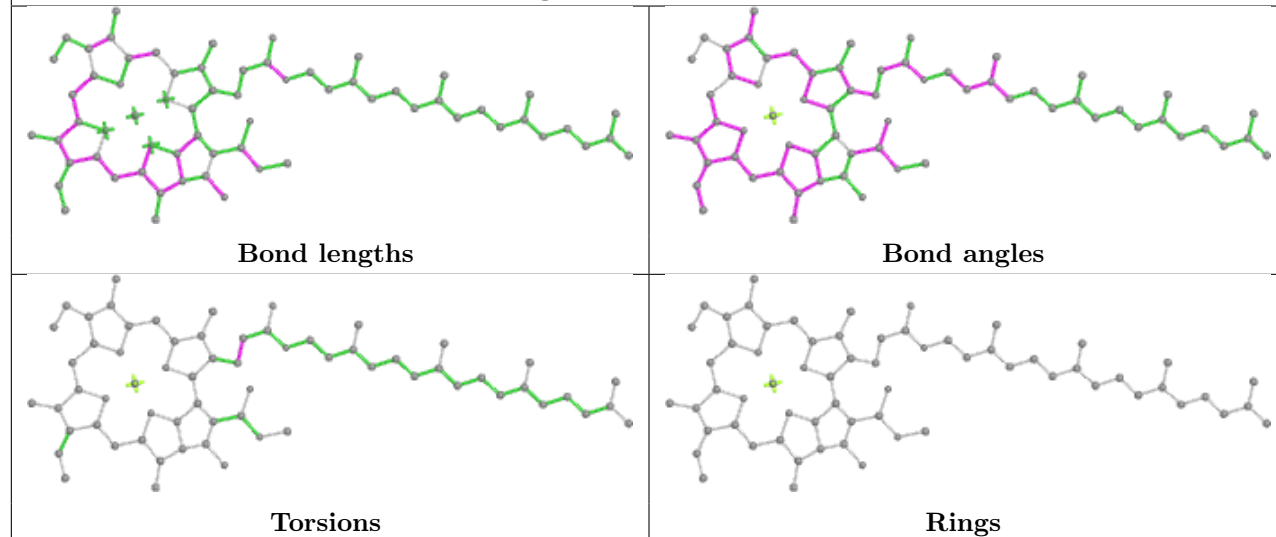
## Ligand CLA B 818



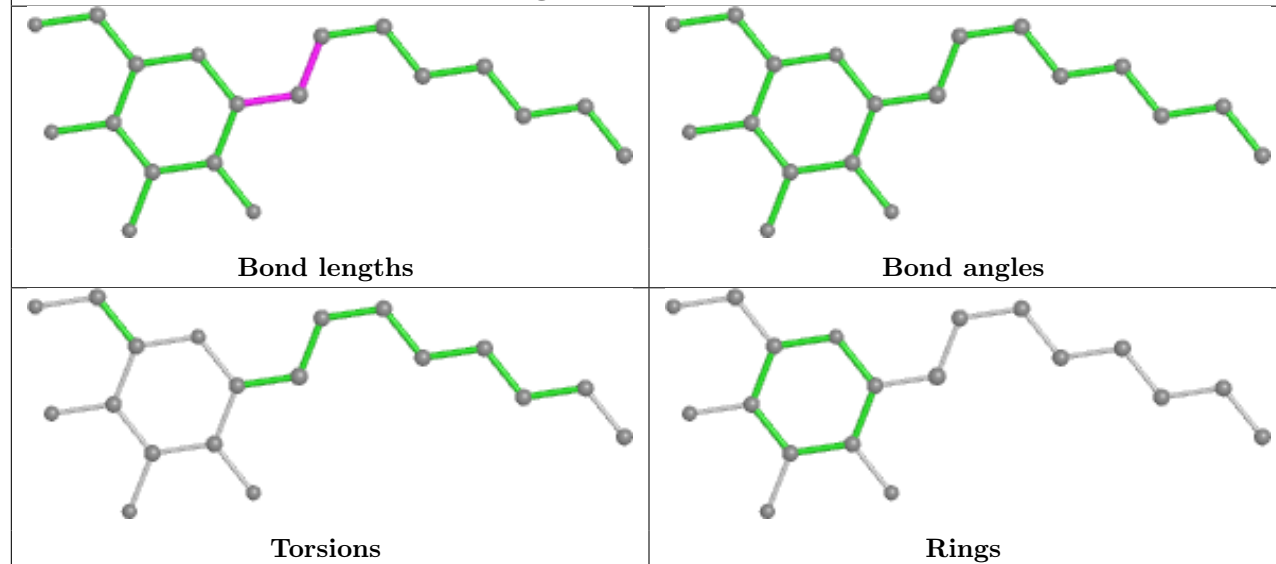
## Ligand CLA 1 313



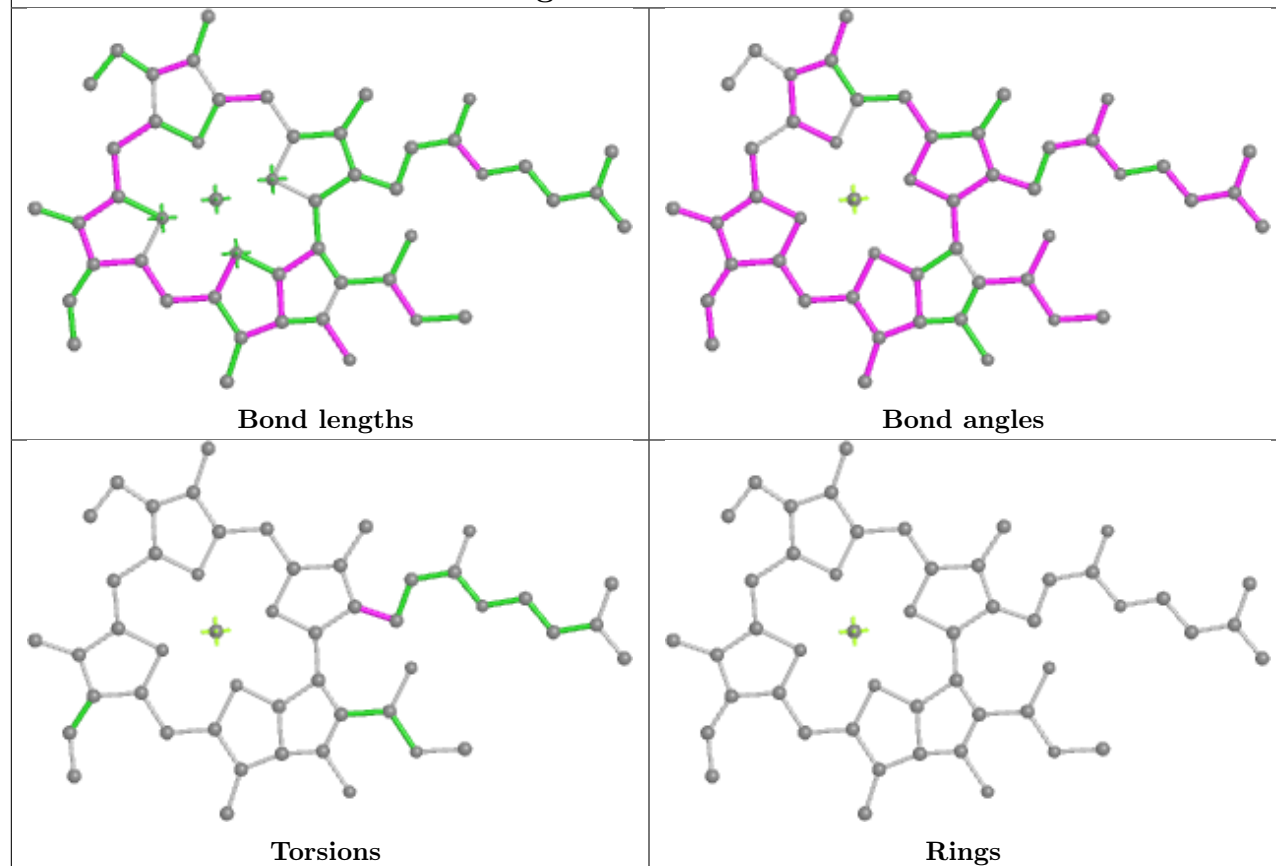
## Ligand CLA a 803



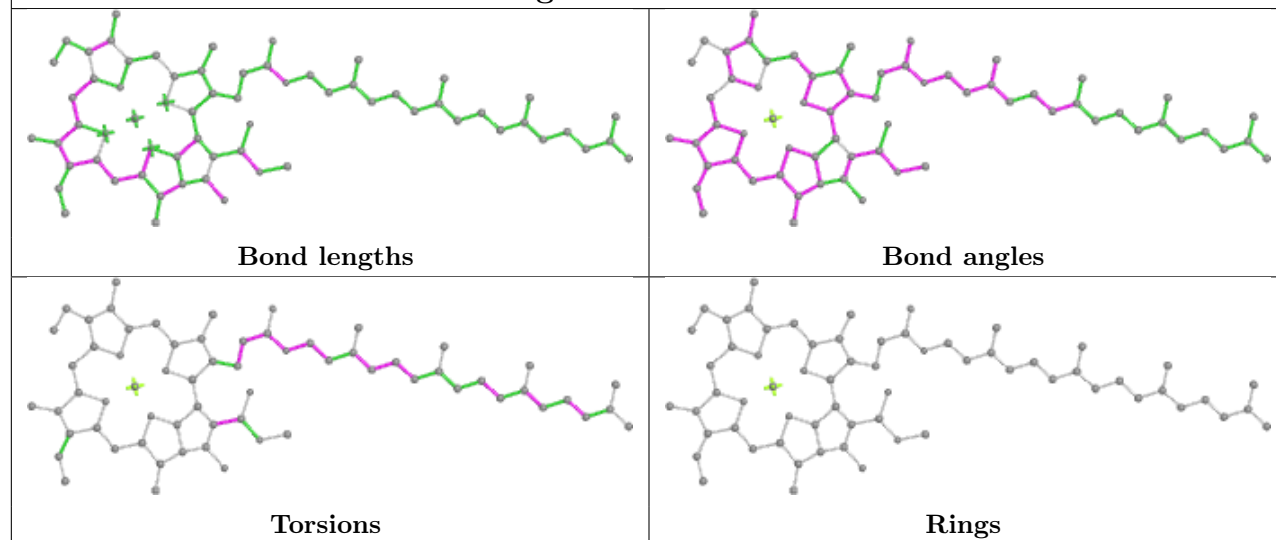
## Ligand HTG a 857



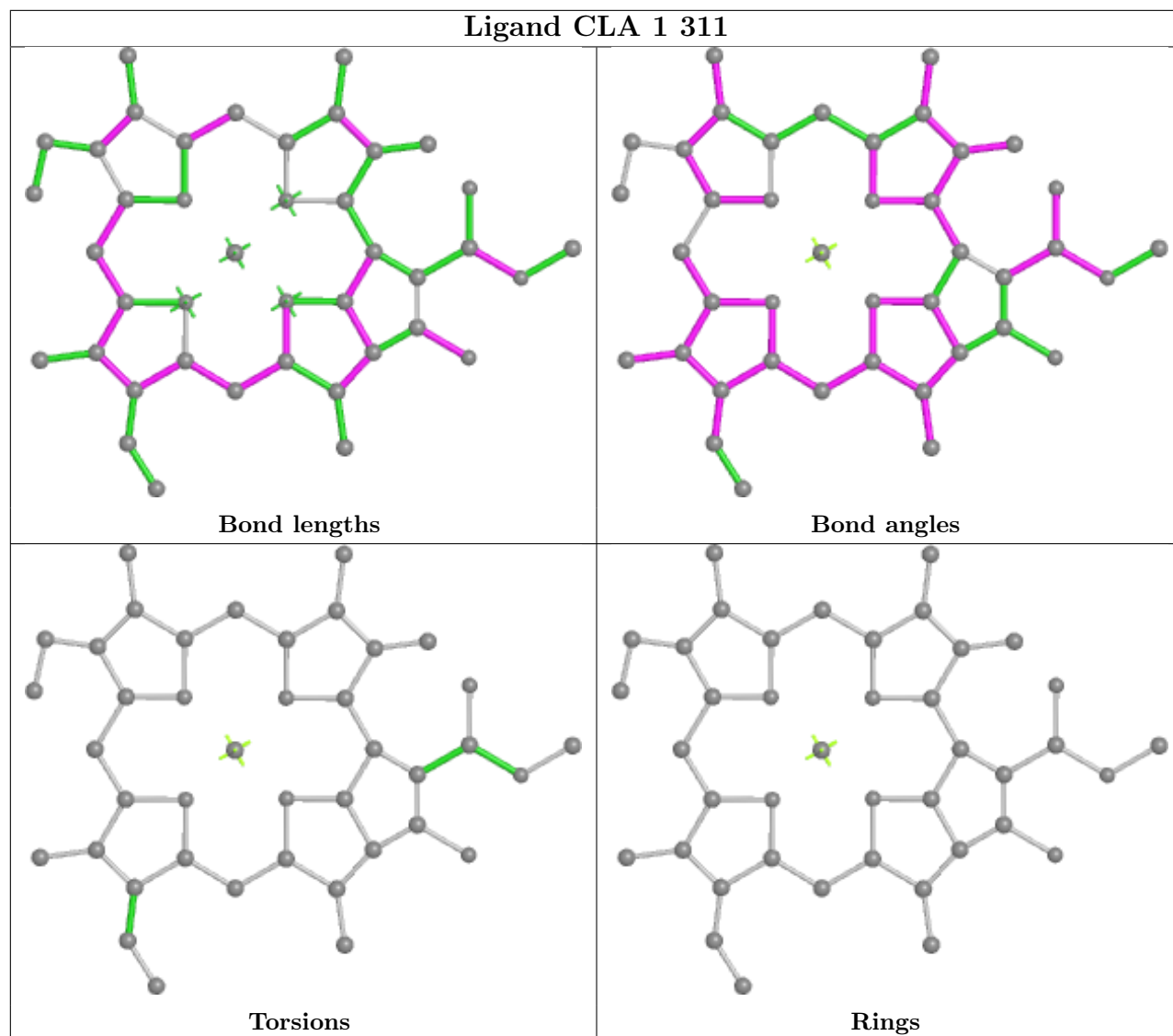
## Ligand CLA 3 309



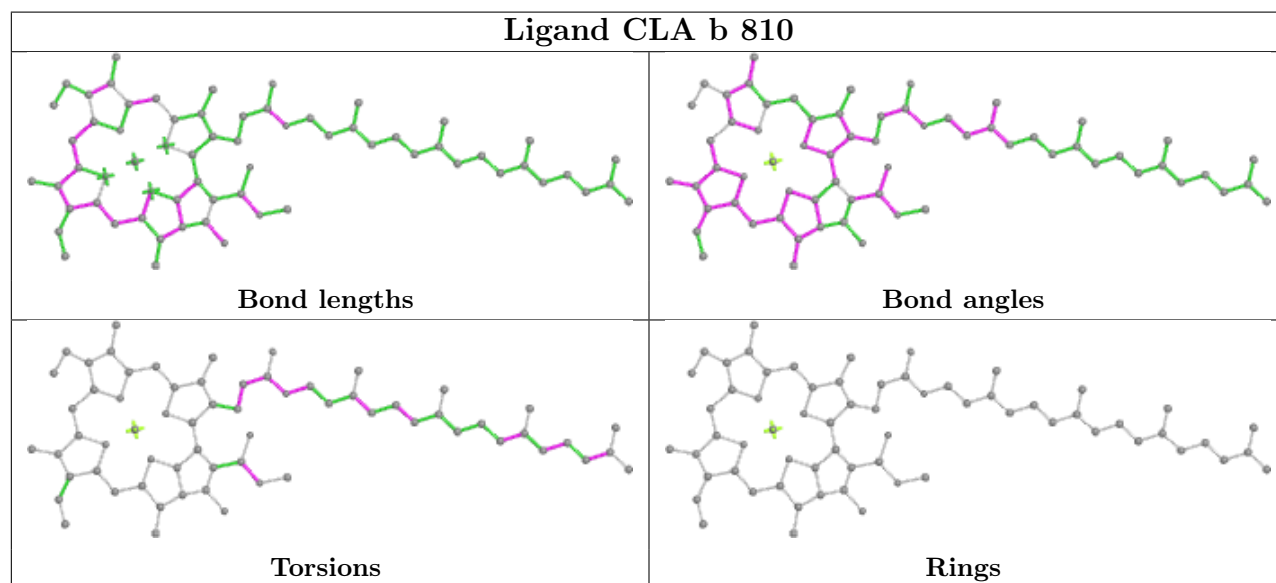
## Ligand CLA a 802



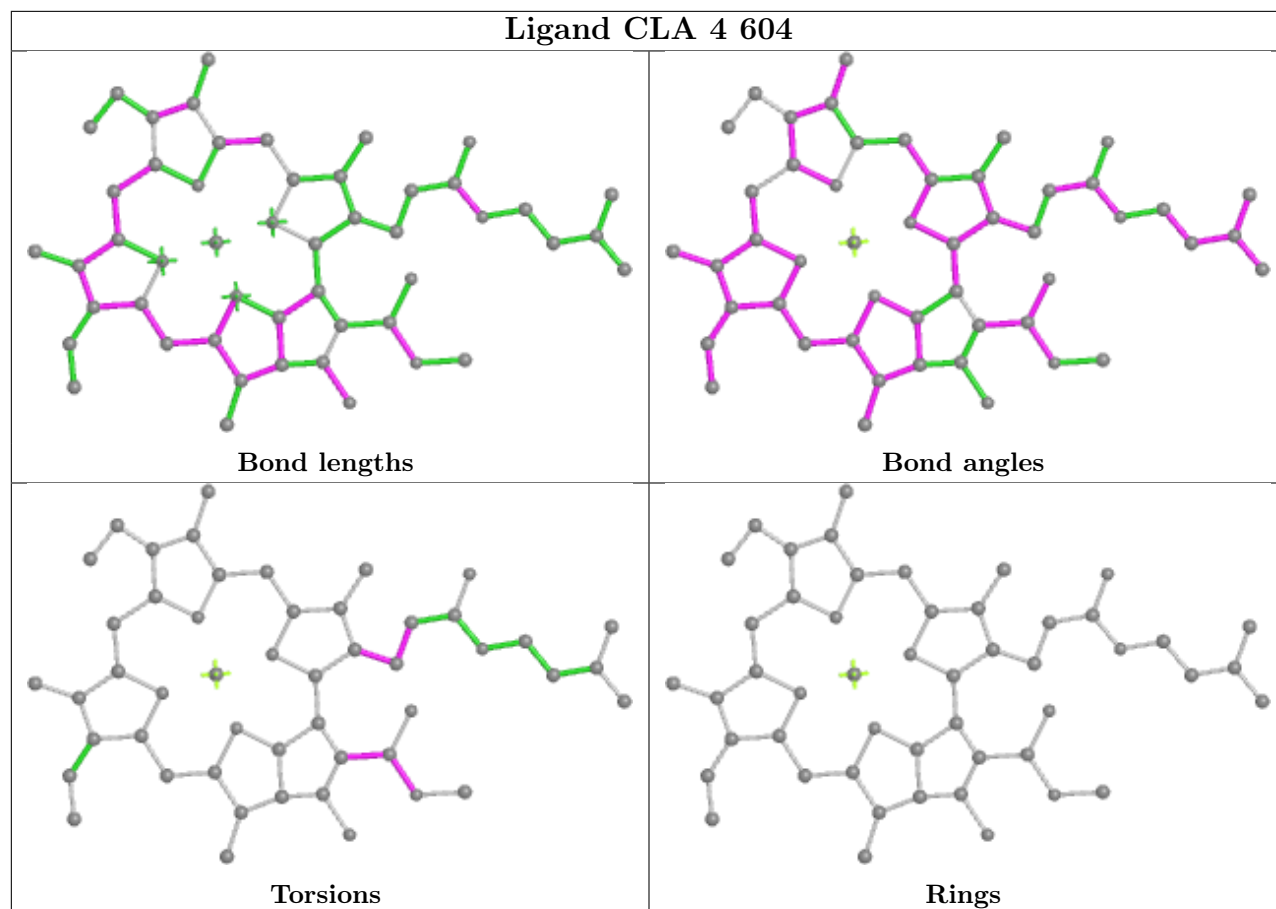
## Ligand CLA 1 311



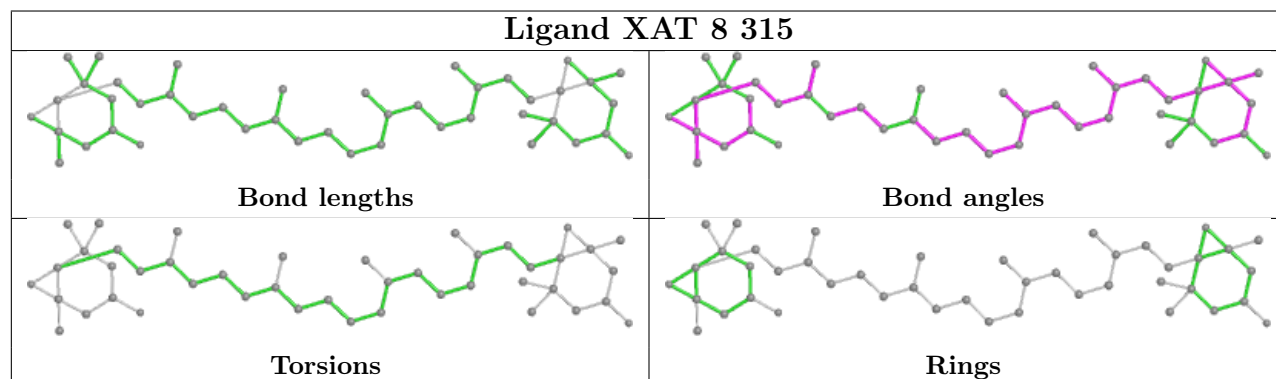
## Ligand CLA b 810



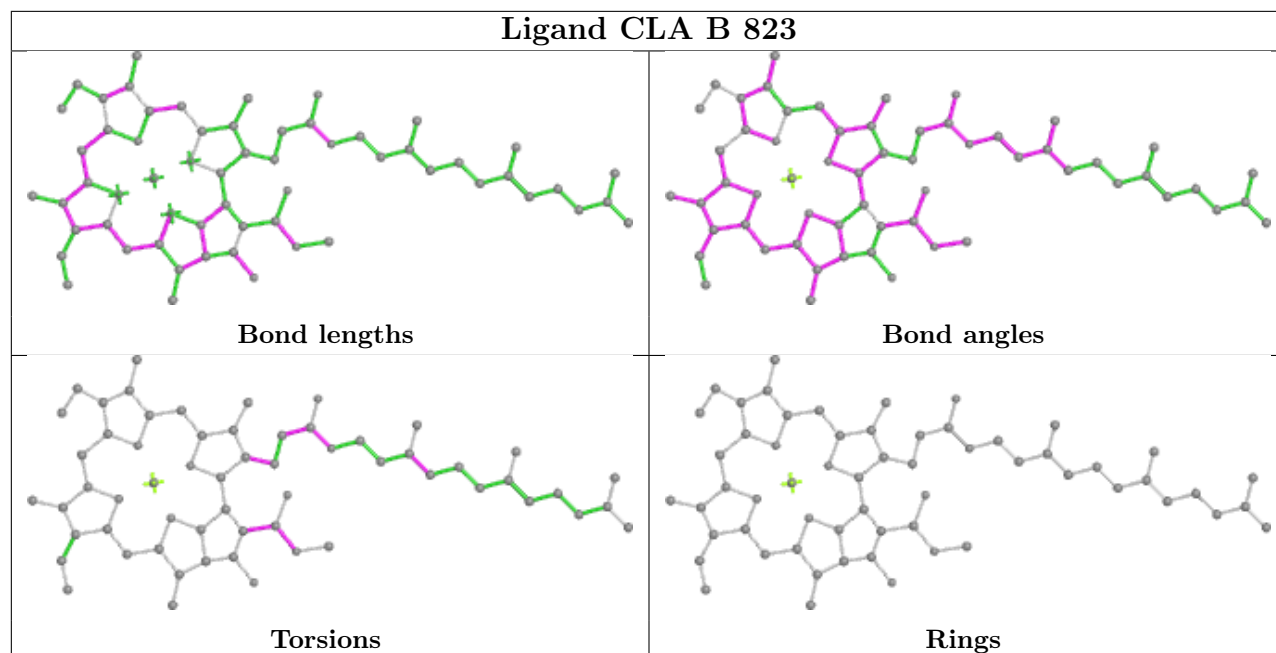
## Ligand CLA 4 604



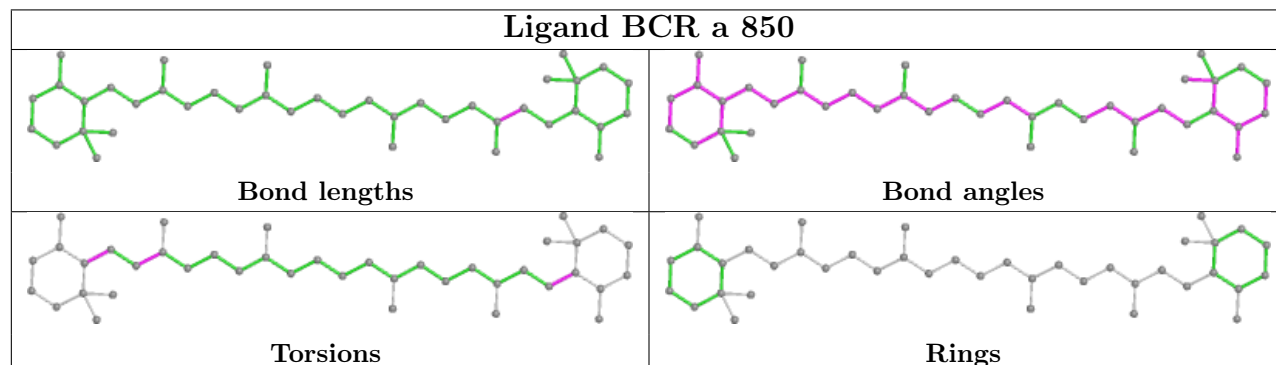
## Ligand XAT 8 315



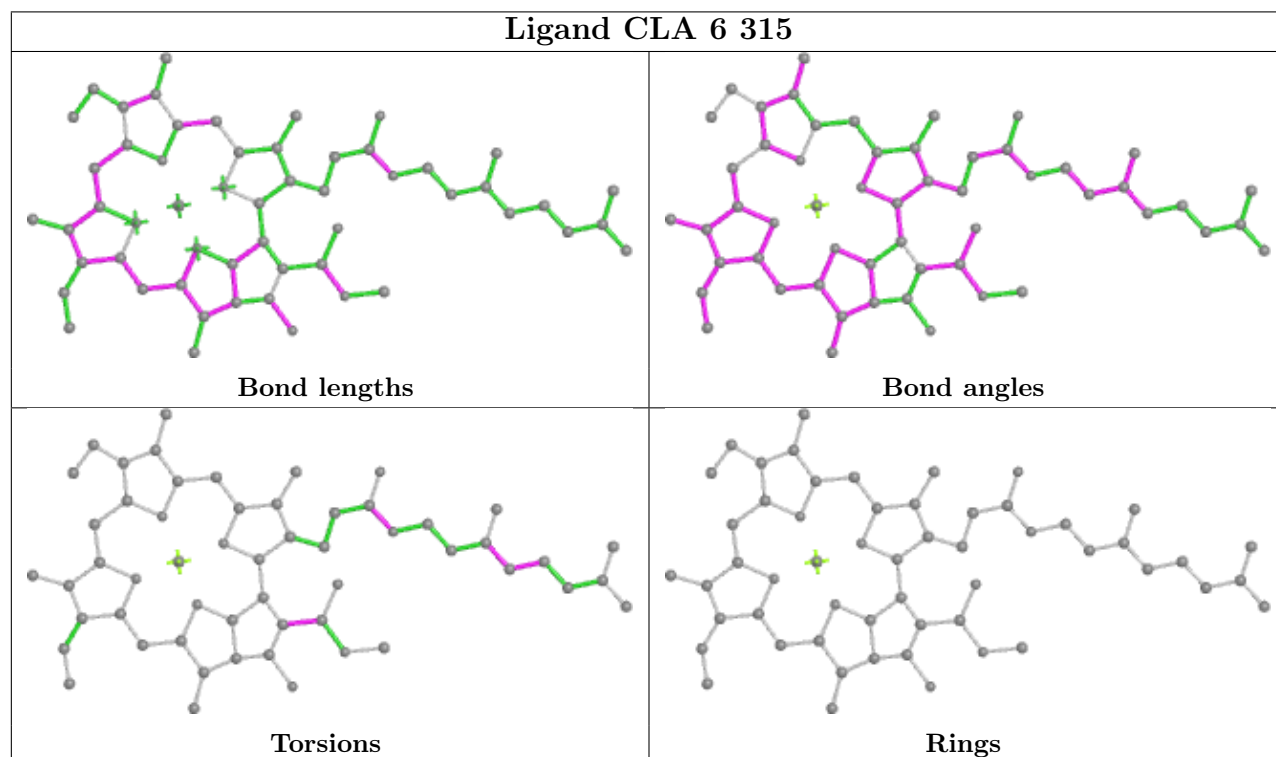
## Ligand CLA B 823



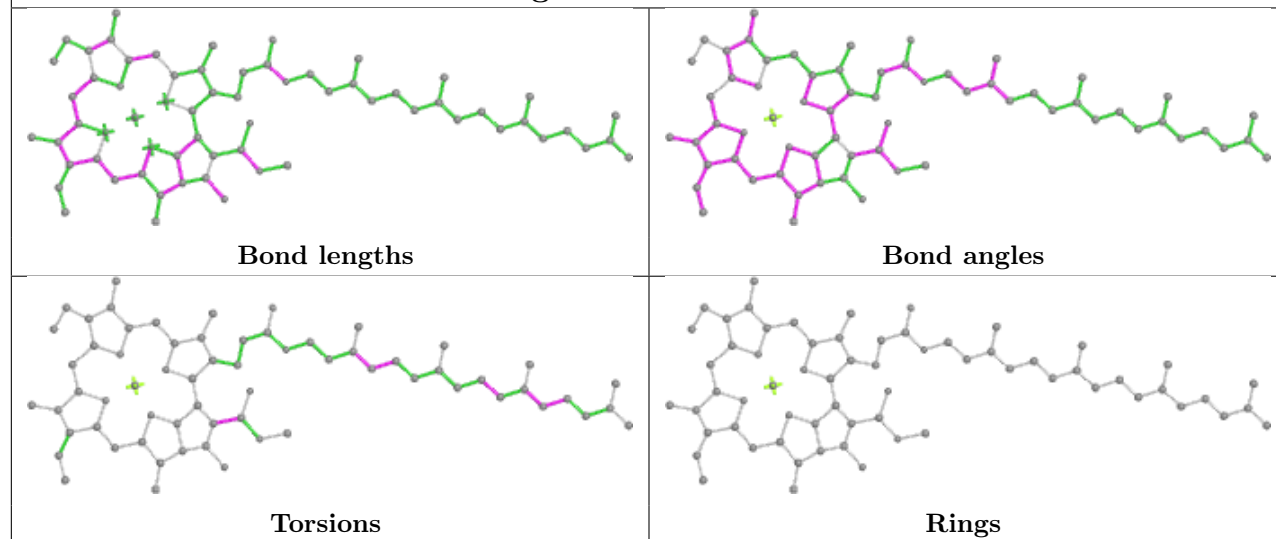
## Ligand BCR a 850



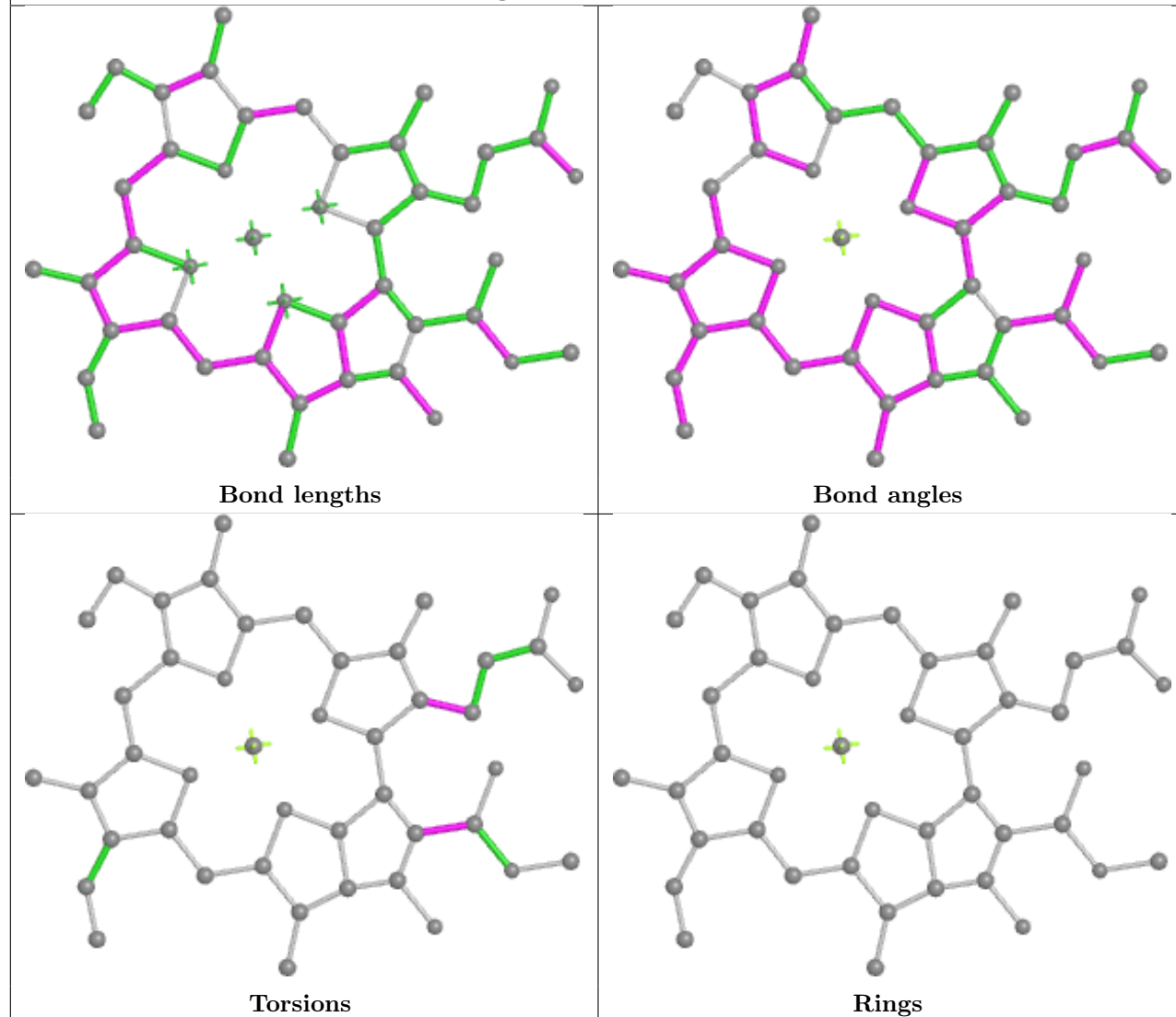
## Ligand CLA 6 315



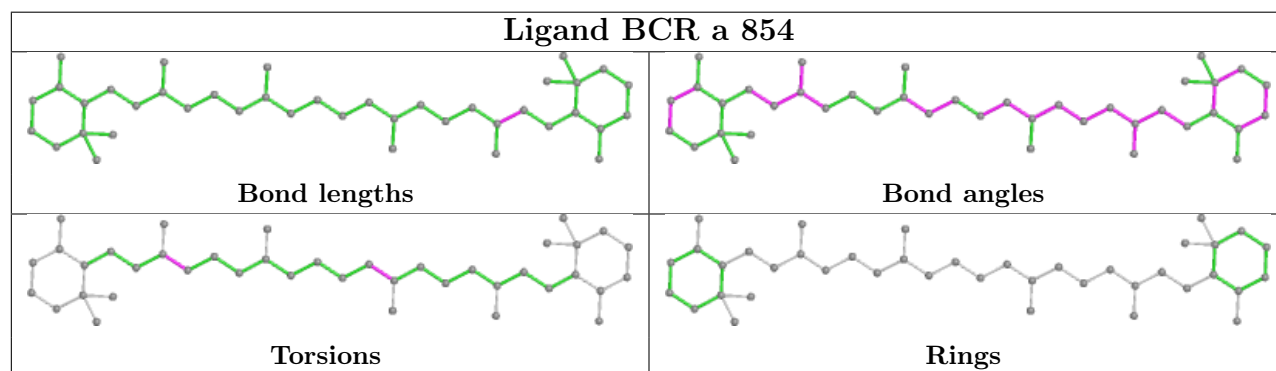
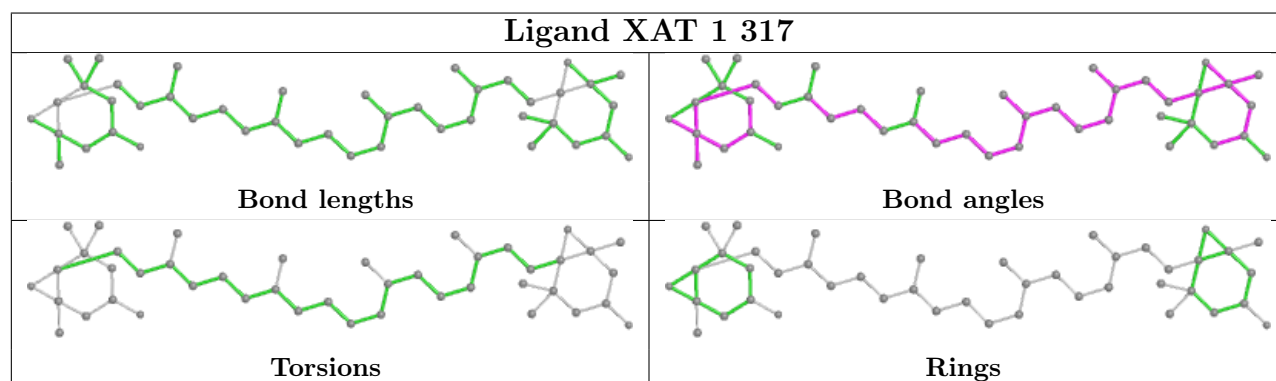
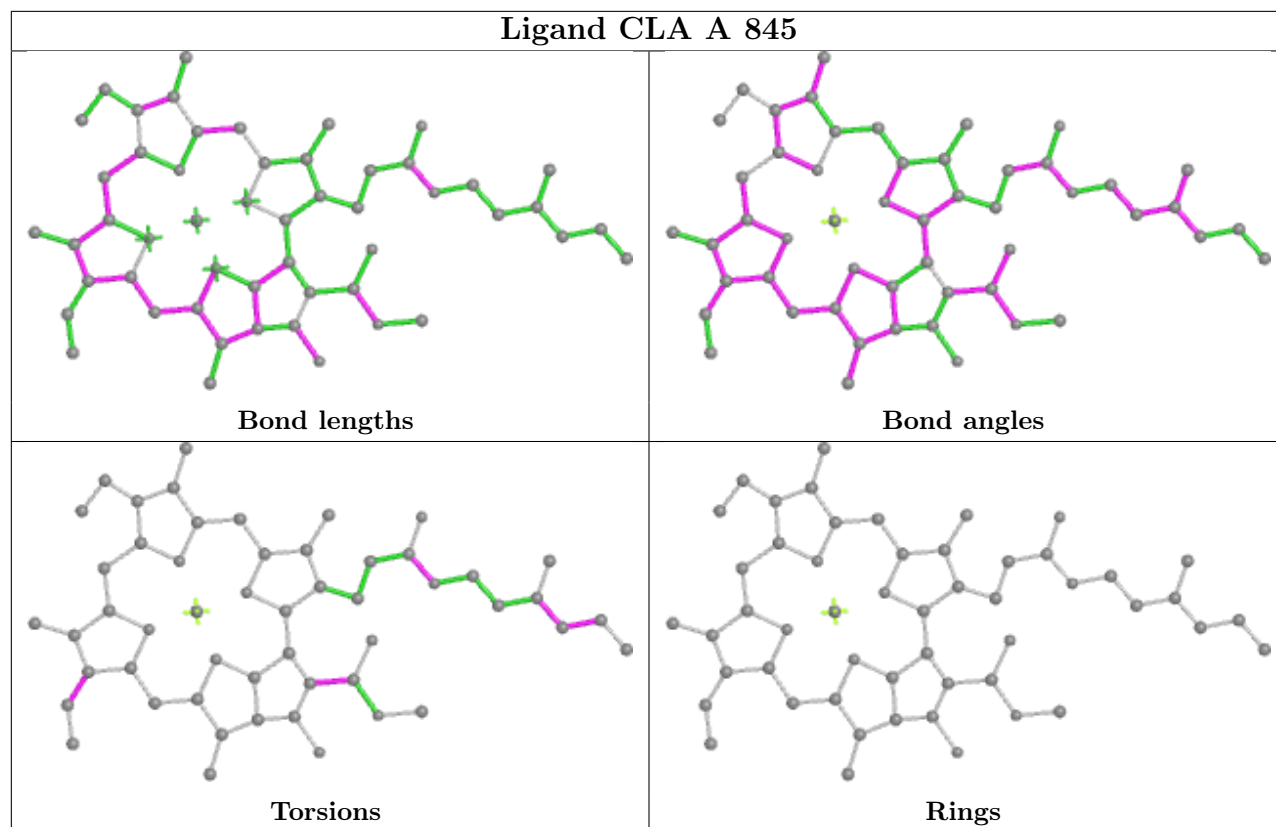
## Ligand CLA A 808



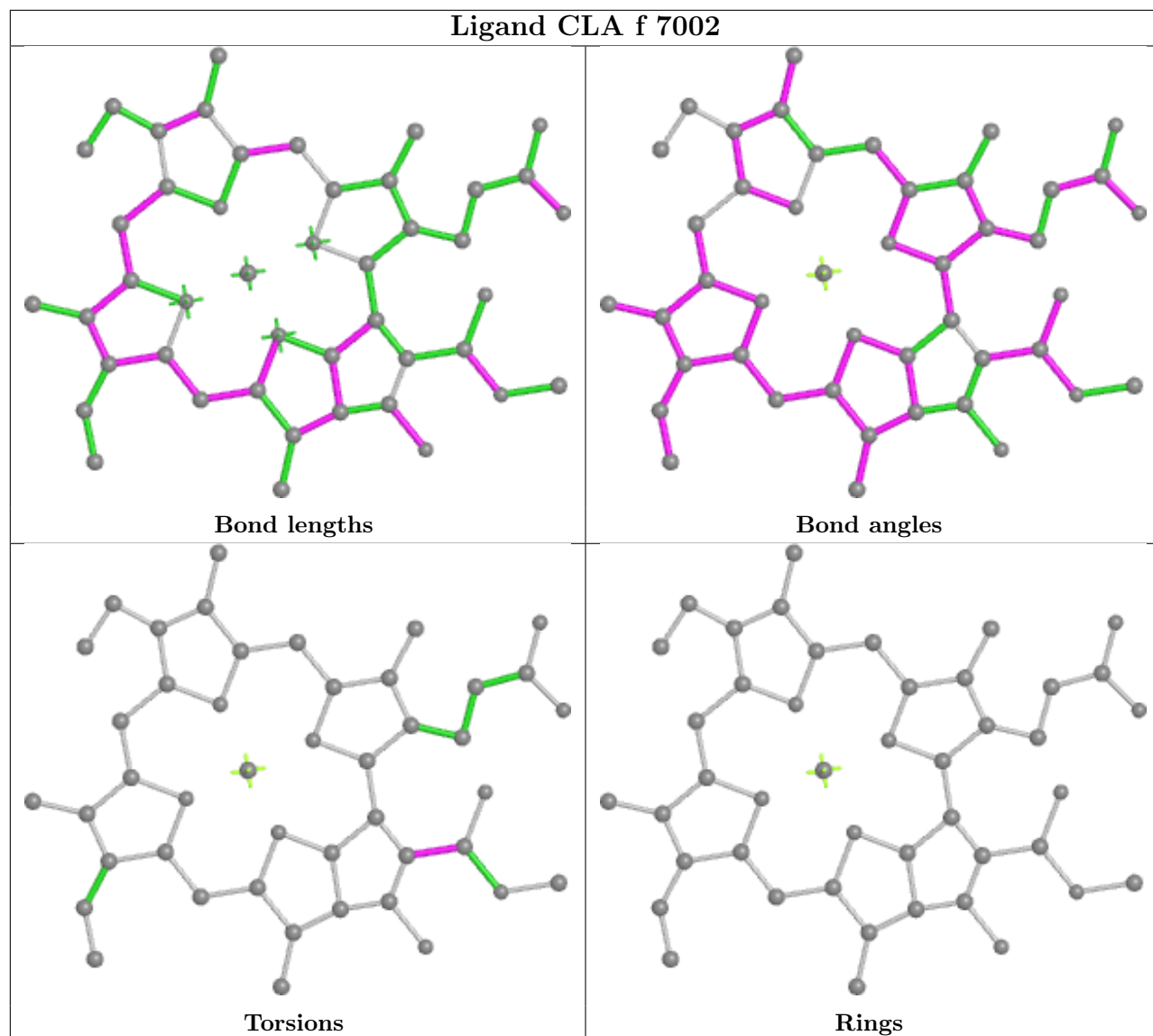
## Ligand CLA a 815



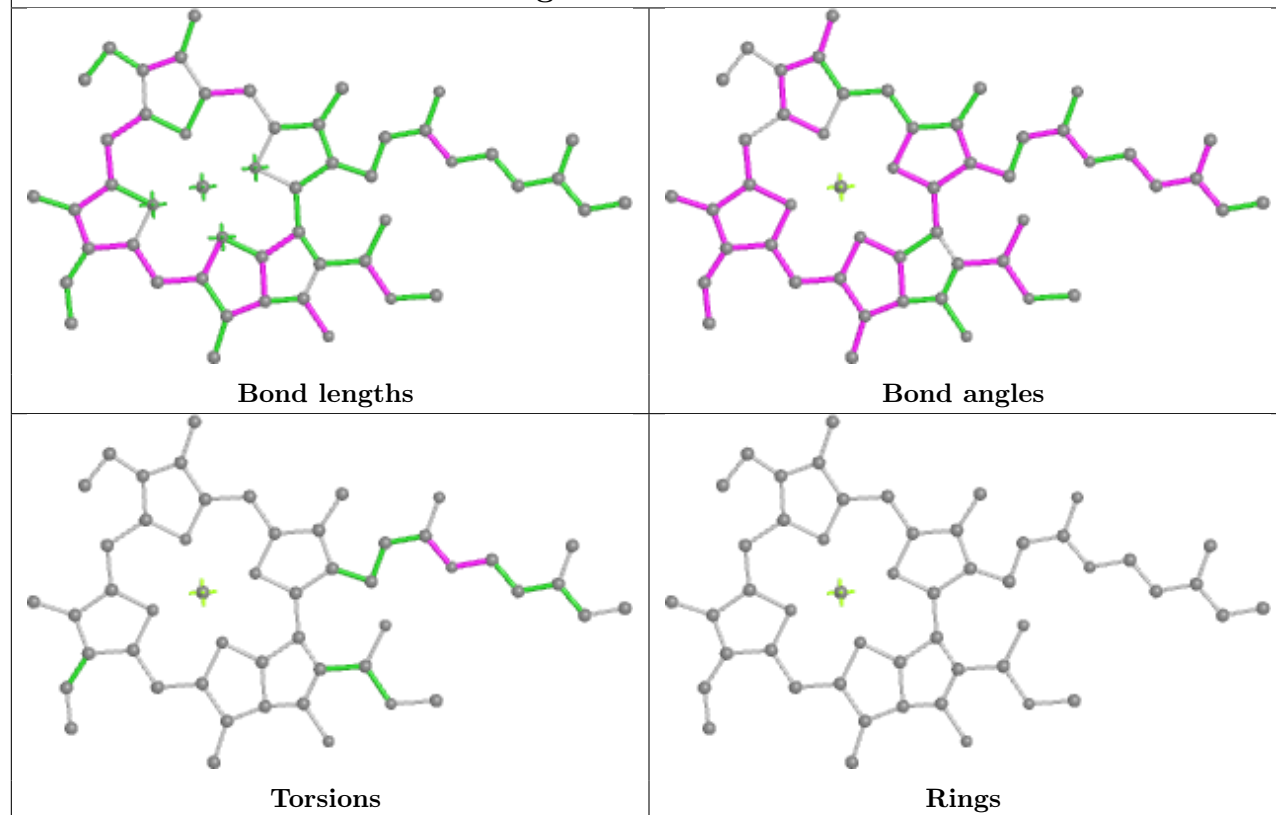




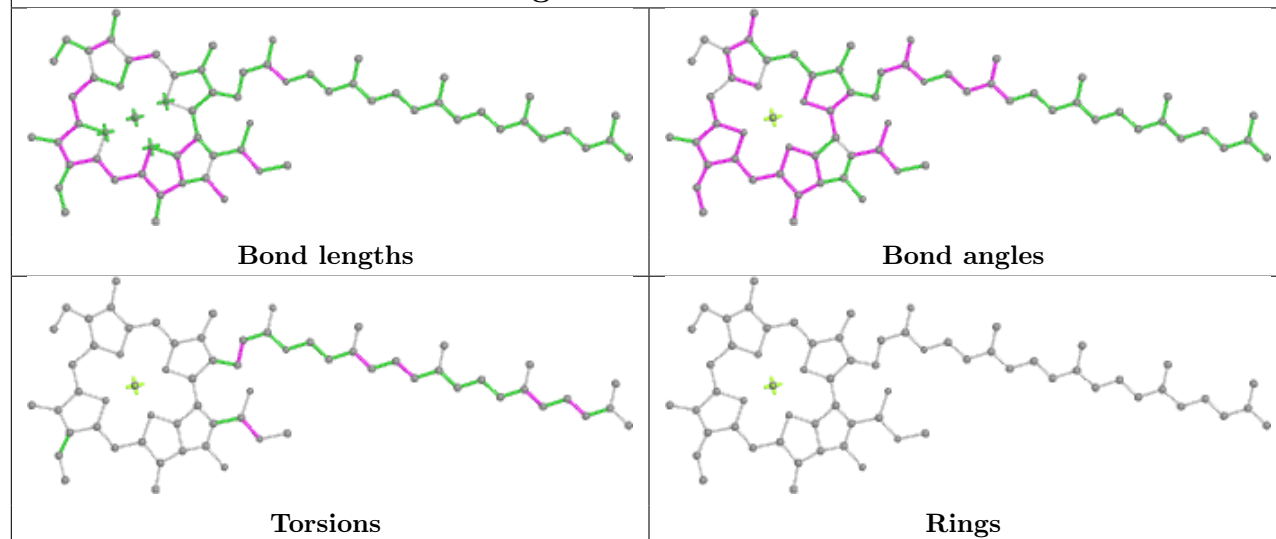
## Ligand CLA f 7002

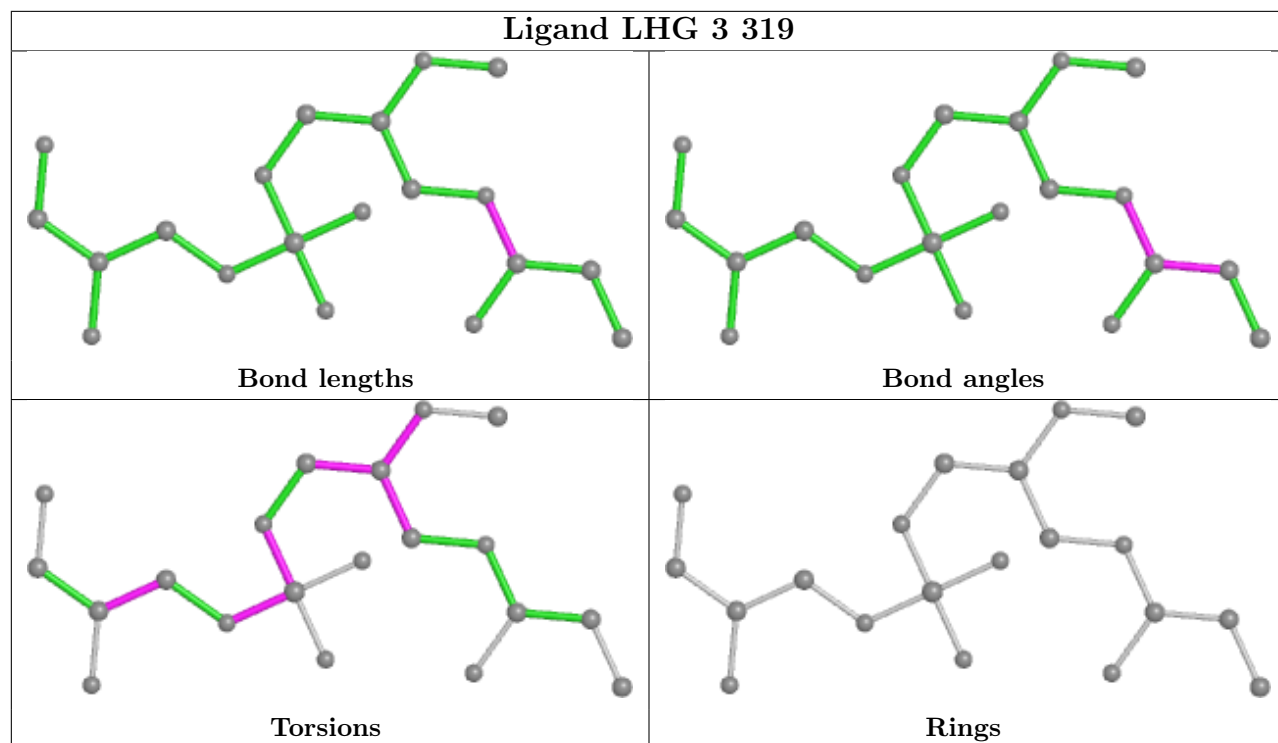


## Ligand CLA 7 603

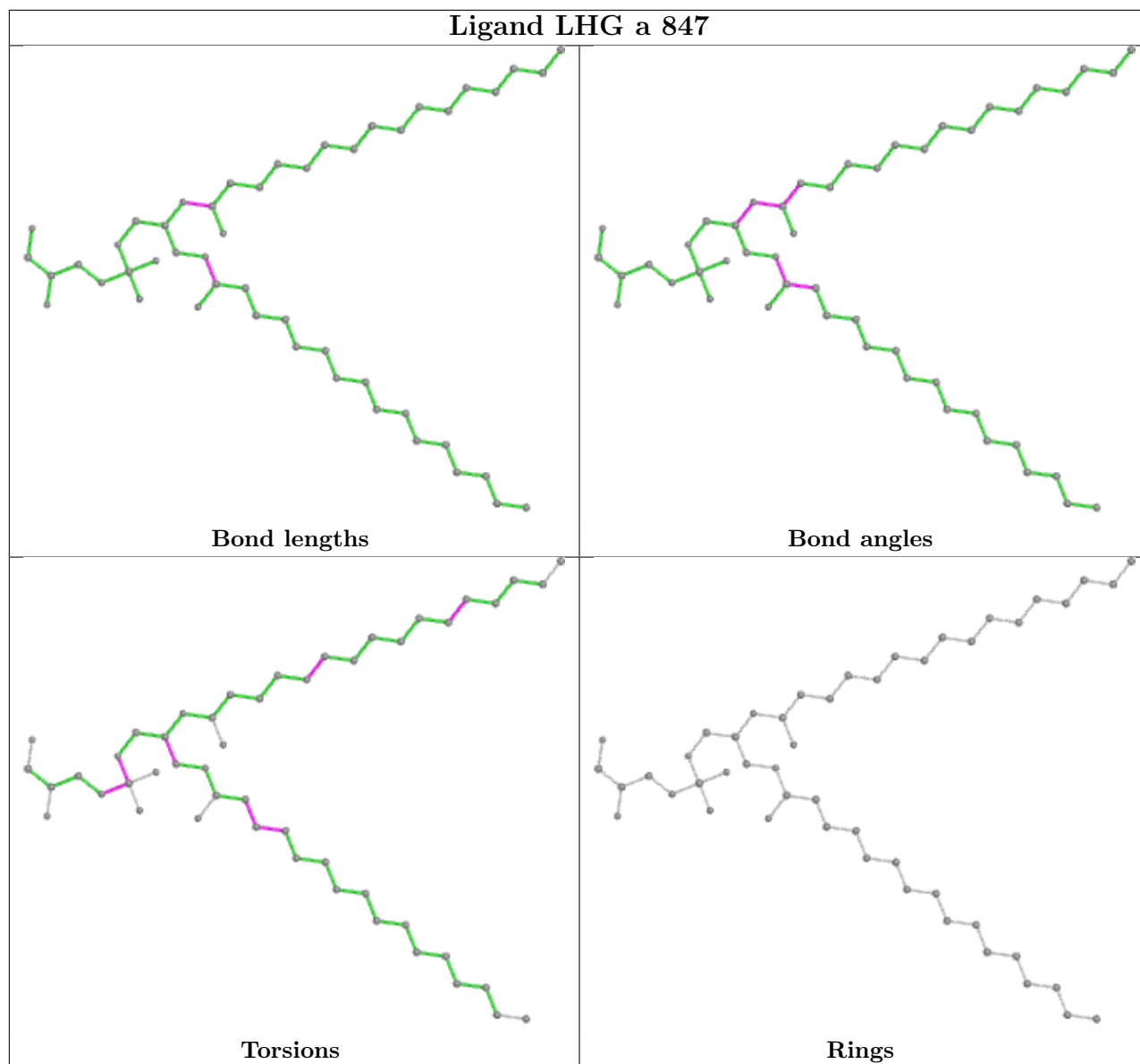


## Ligand CLA B 840

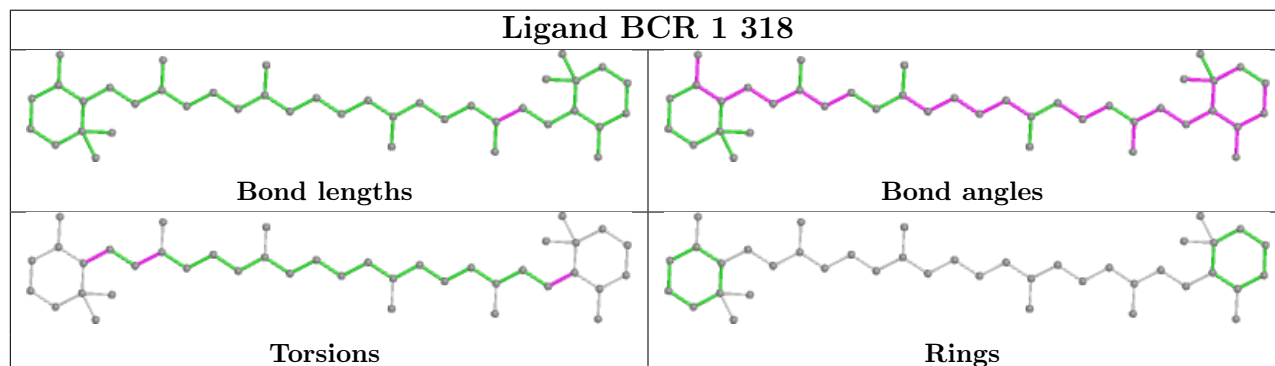




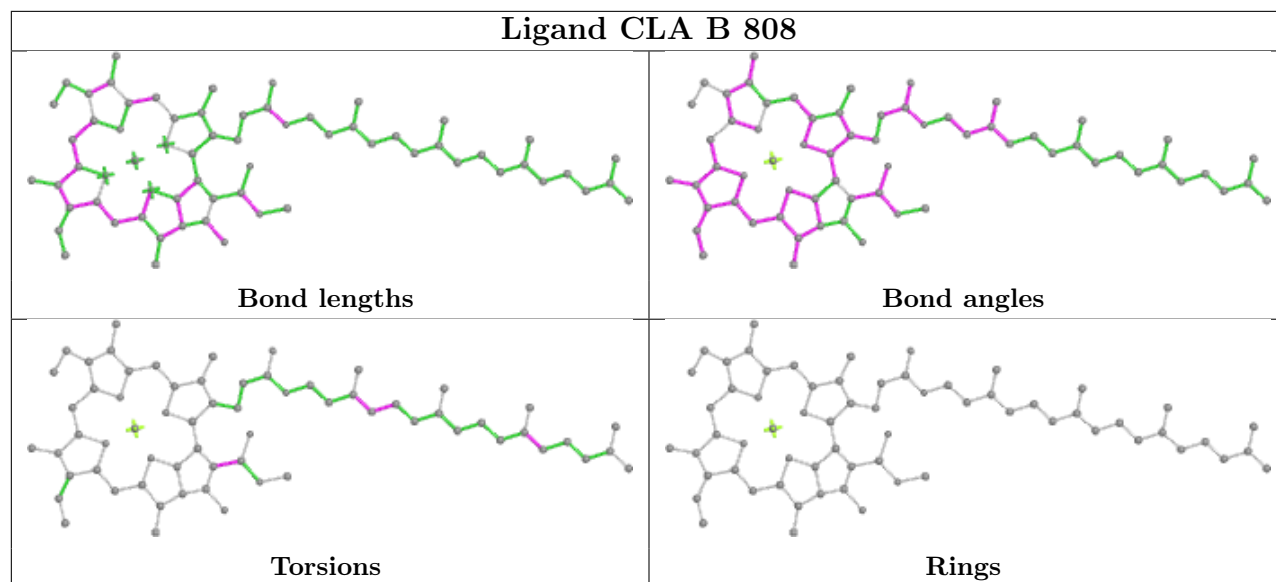
## Ligand LHG a 847



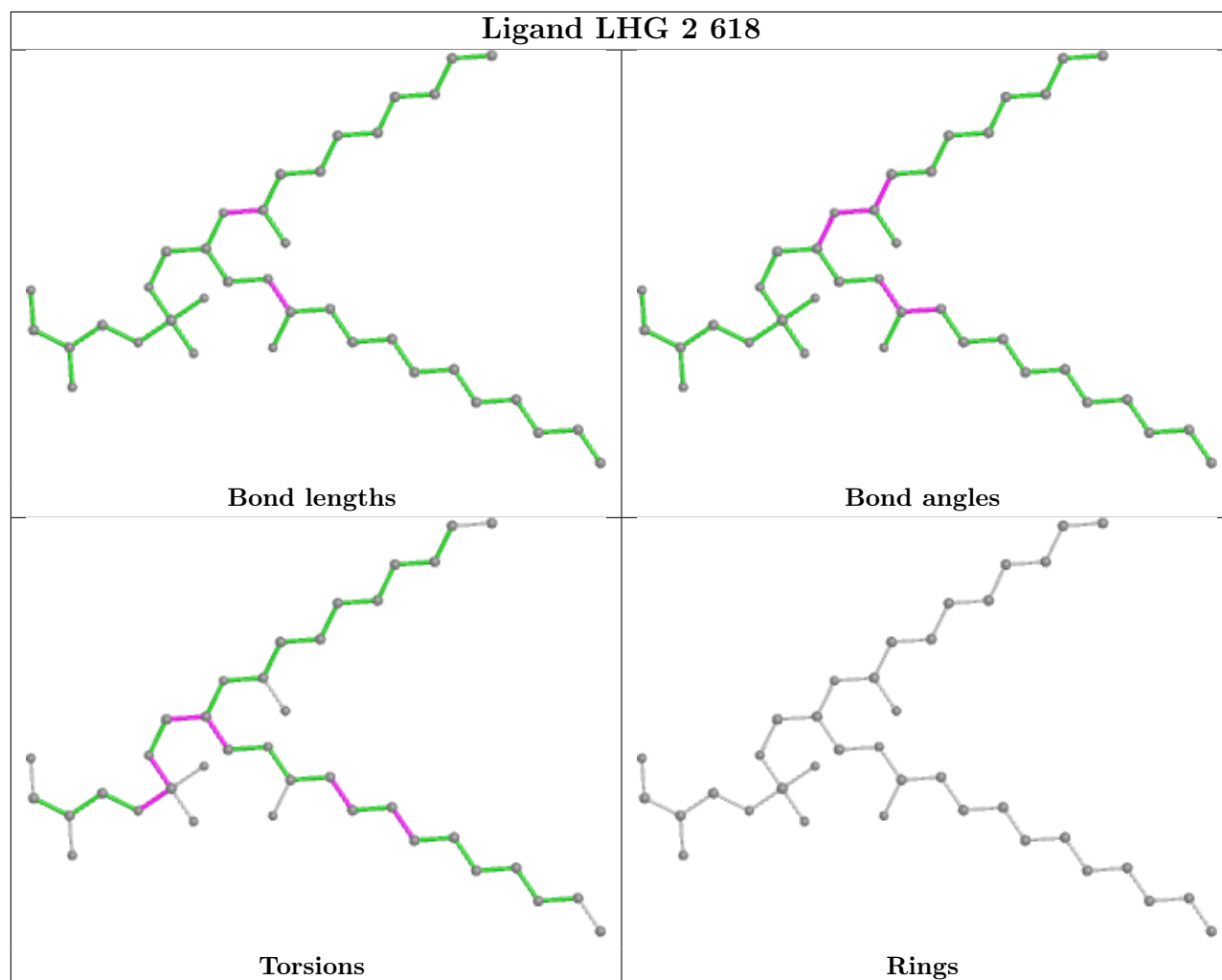
## Ligand BCR 1 318



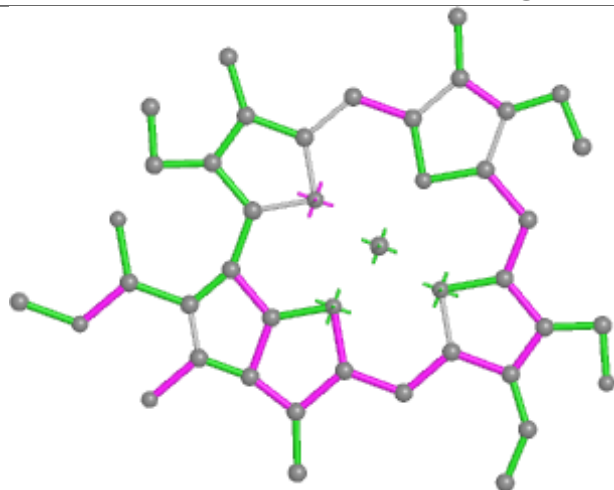
## Ligand CLA B 808



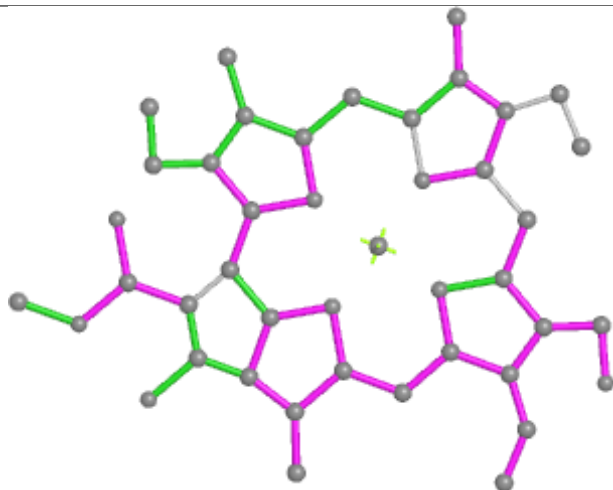
## Ligand LHG 2 618



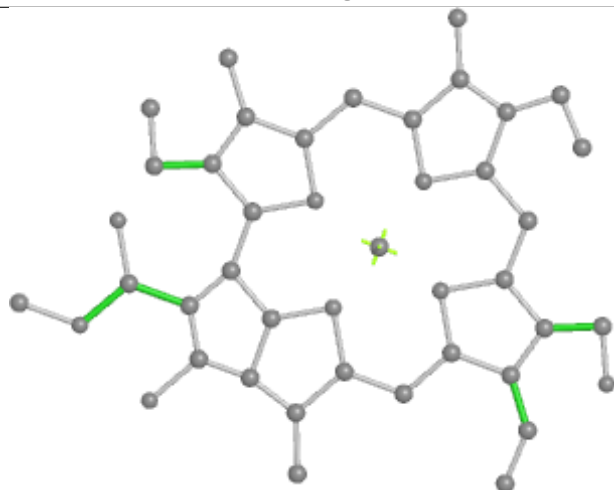
## Ligand CHL 2 605



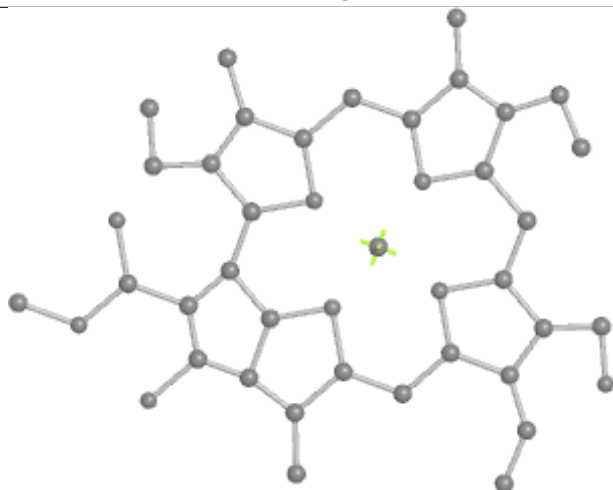
Bond lengths



Bond angles

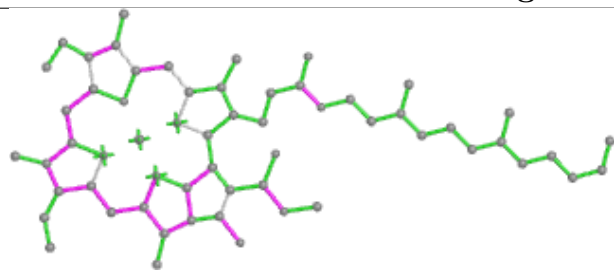


Torsions

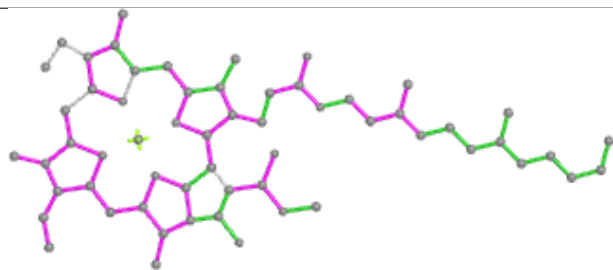


Rings

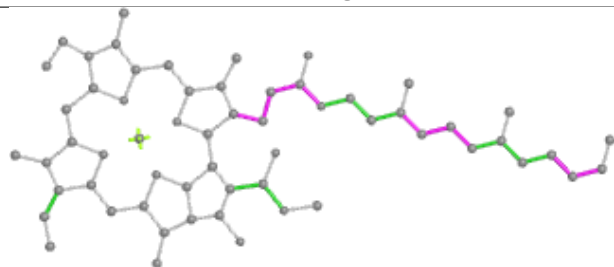
## Ligand CLA b 817



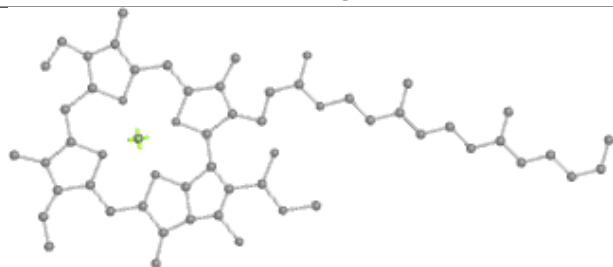
Bond lengths



Bond angles

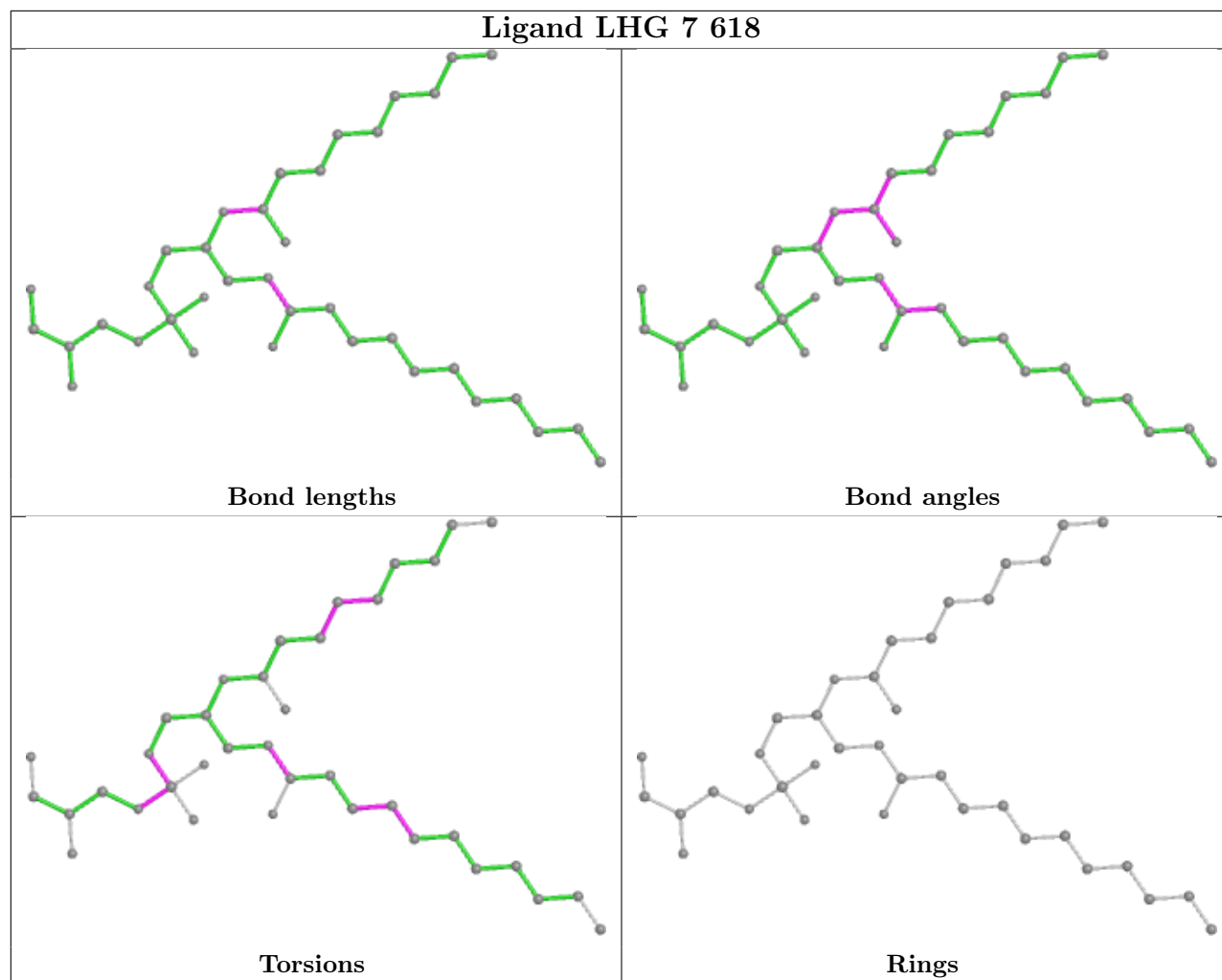


Torsions



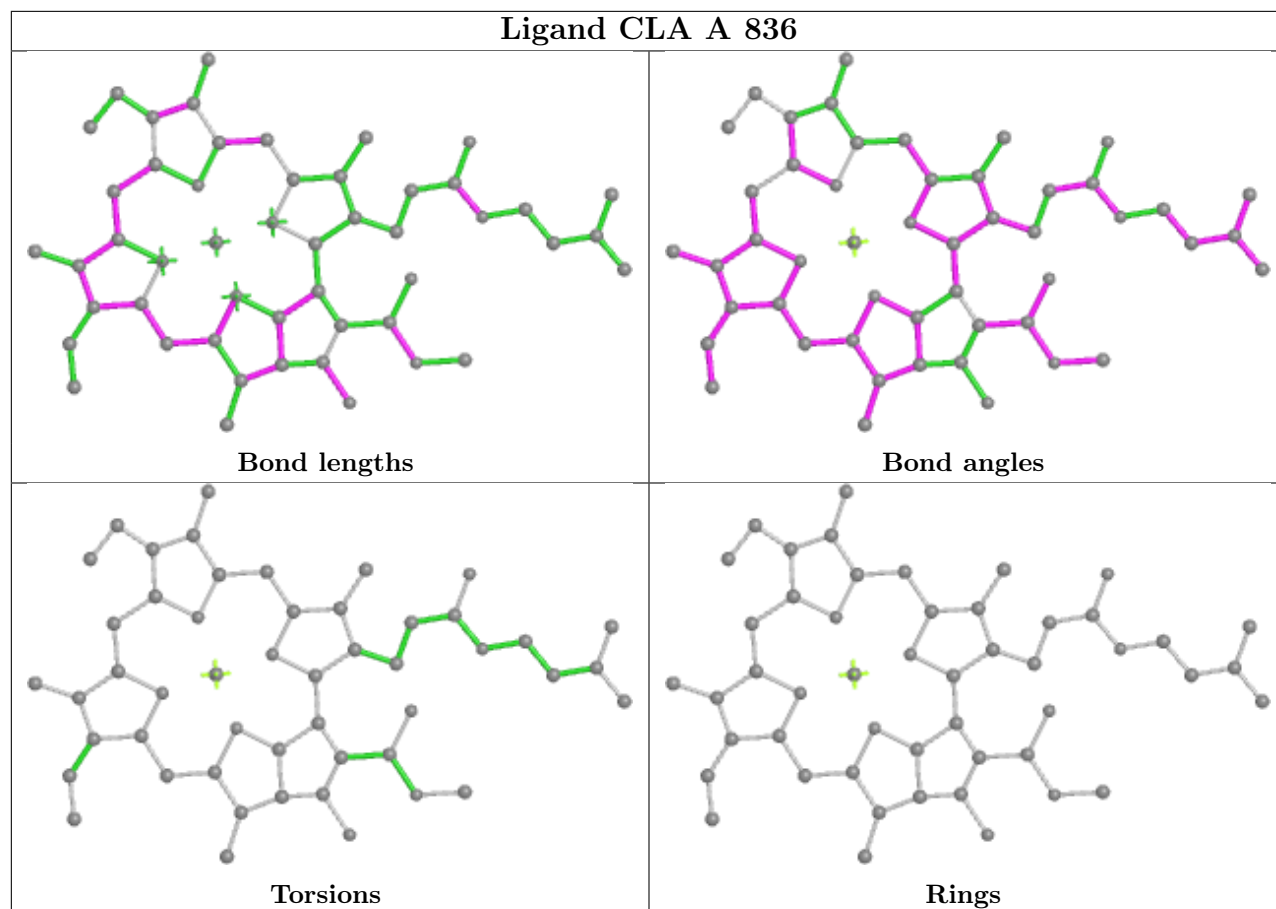
Rings

## Ligand LHG 7 618

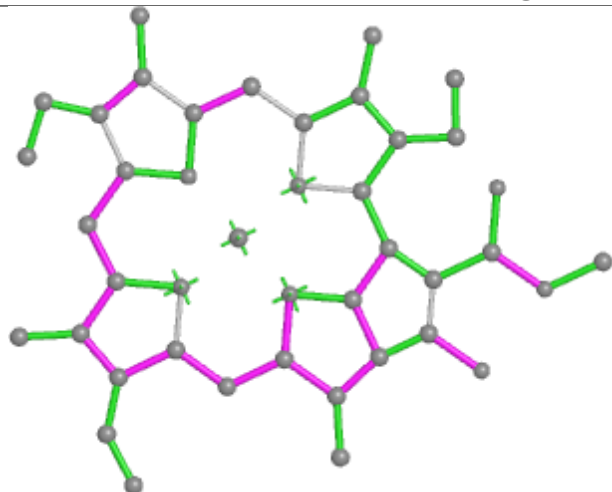




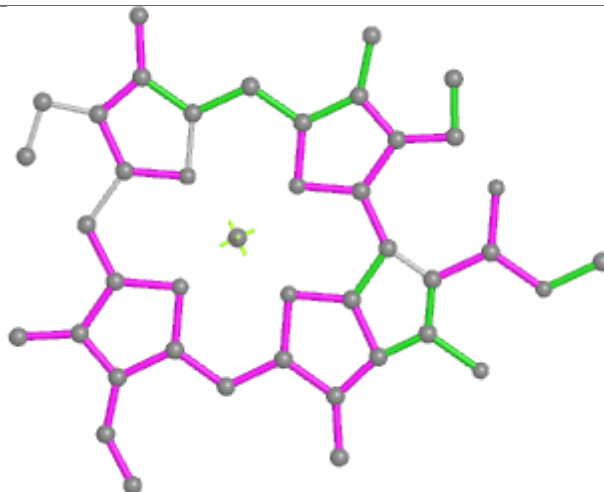
## Ligand CLA A 836



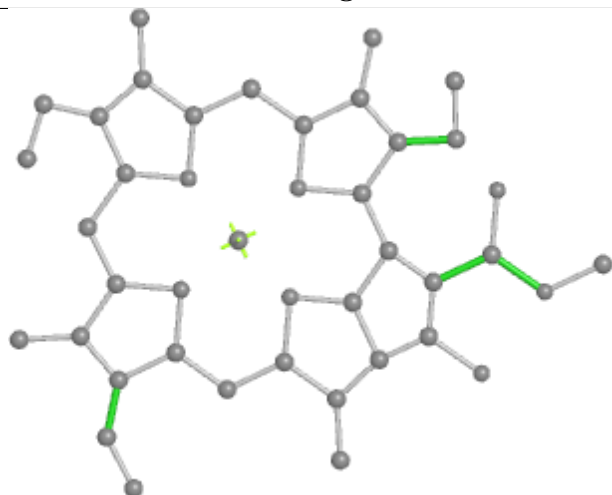
## Ligand CLA 8 304



Bond lengths



Bond angles

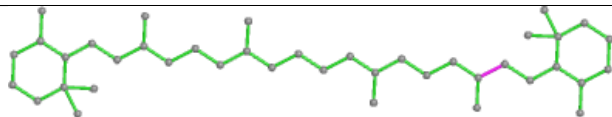


Torsions

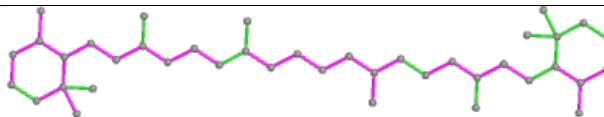


Rings

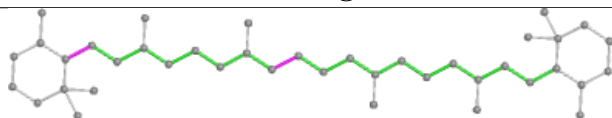
## Ligand BCR 2 617



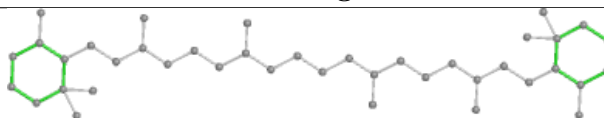
Bond lengths



Bond angles

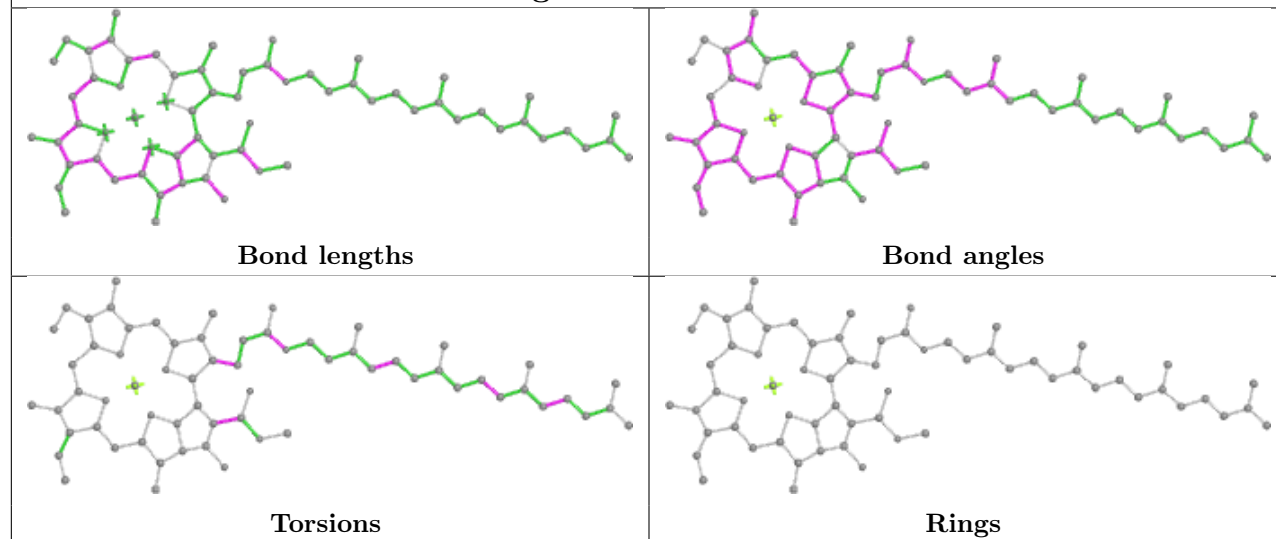


Torsions

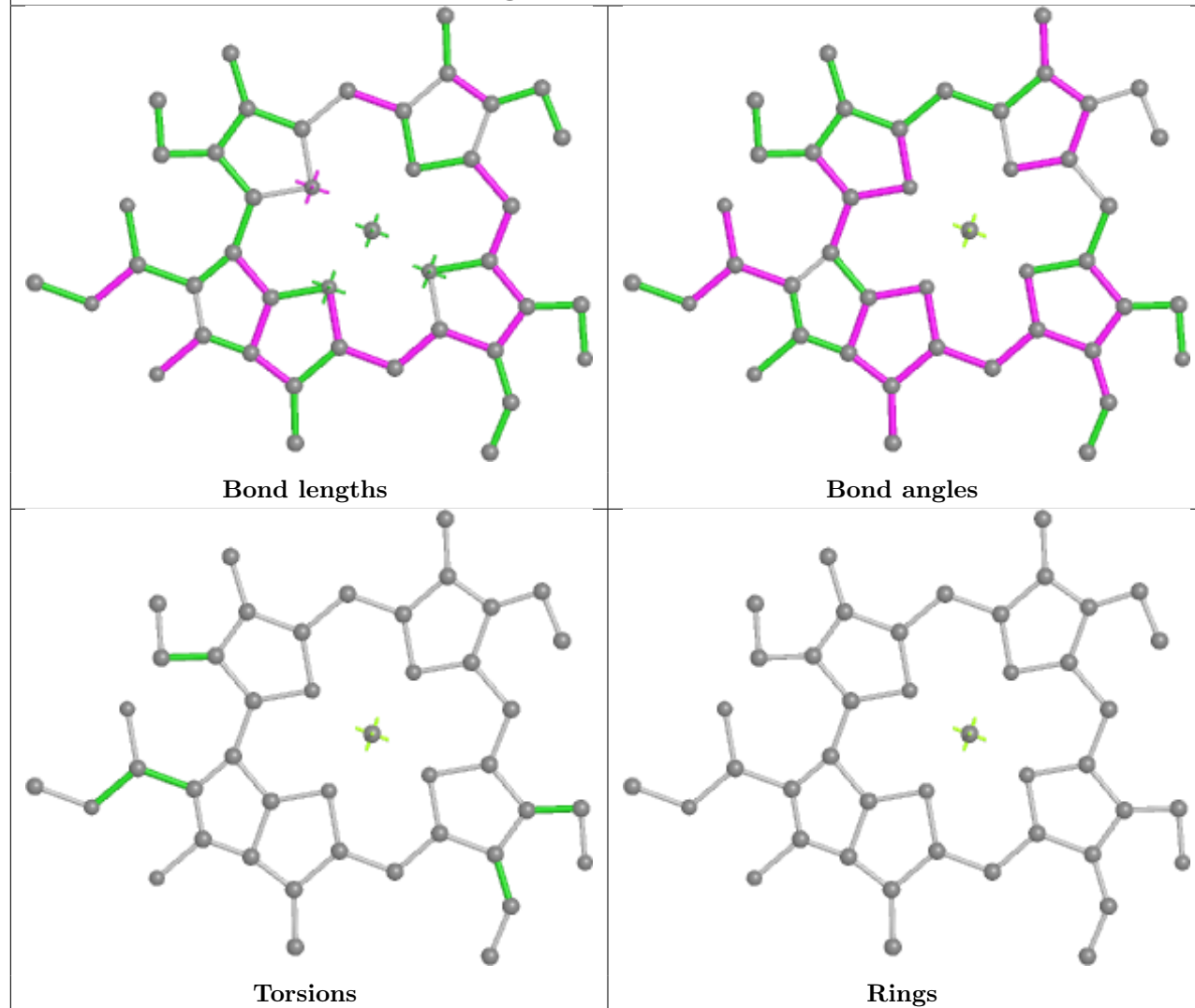


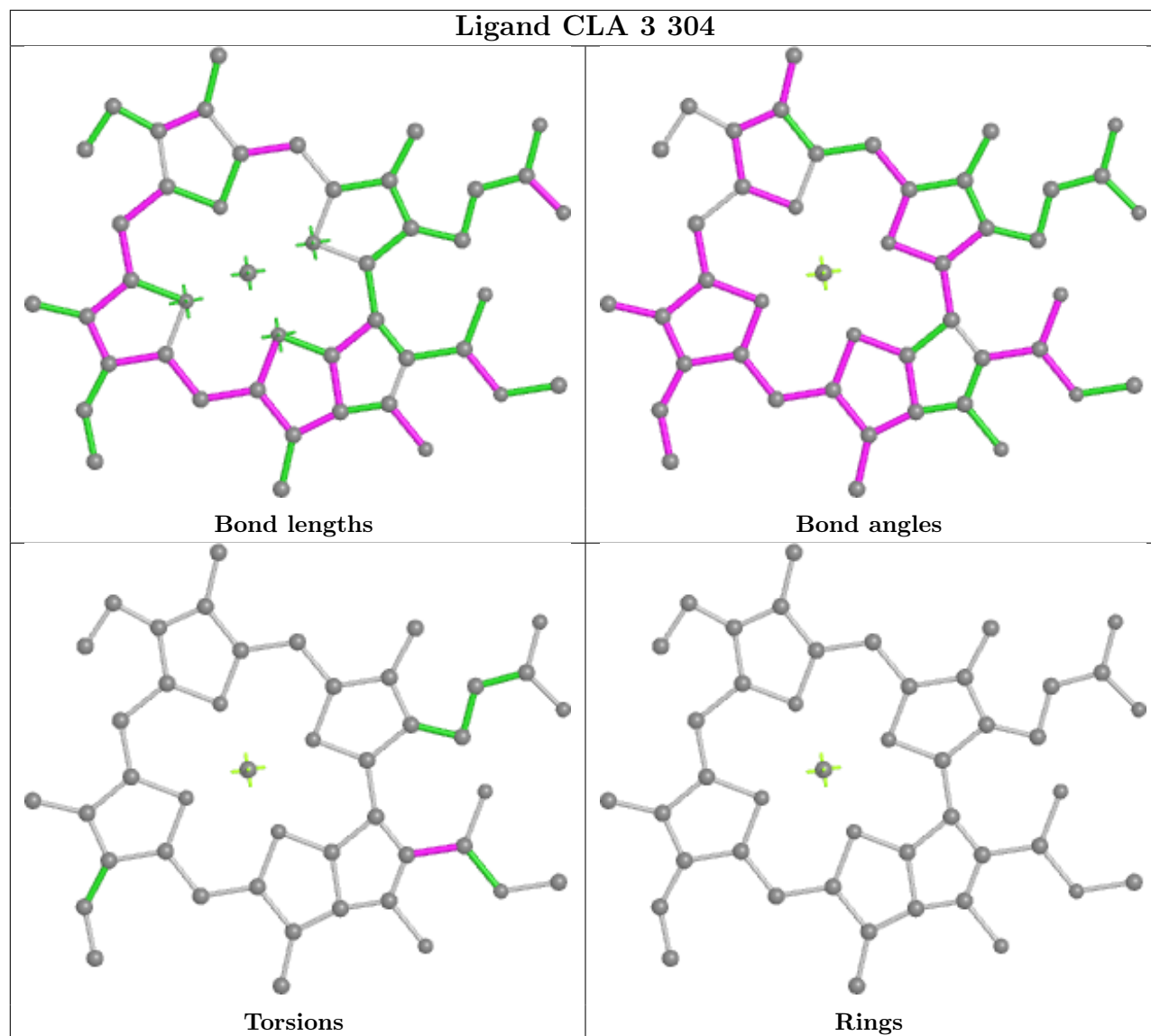
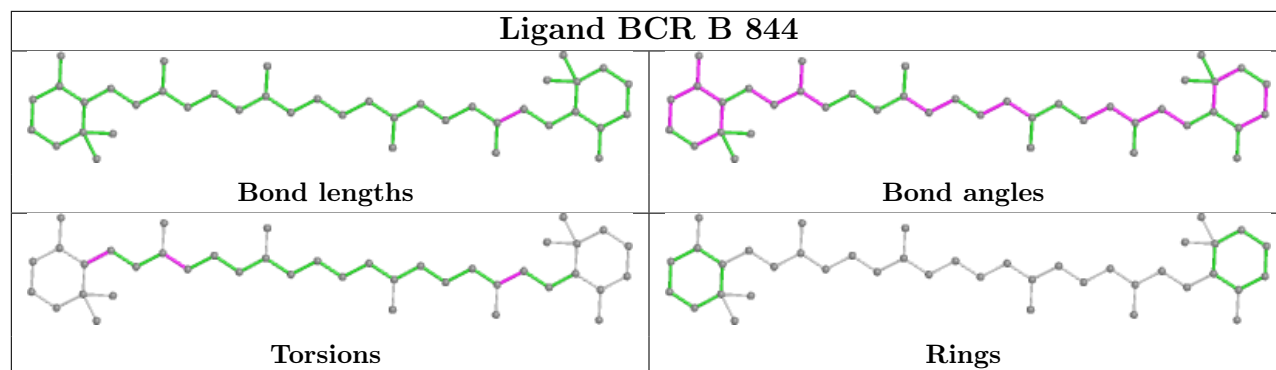
Rings

## Ligand CLA B 825

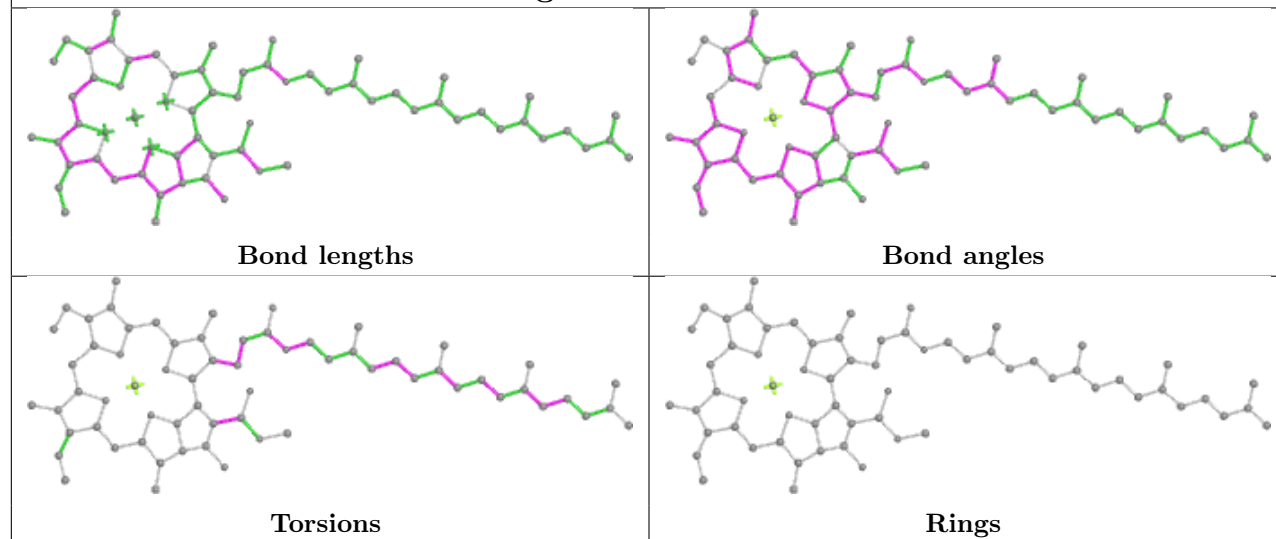


## Ligand CHL 4 615

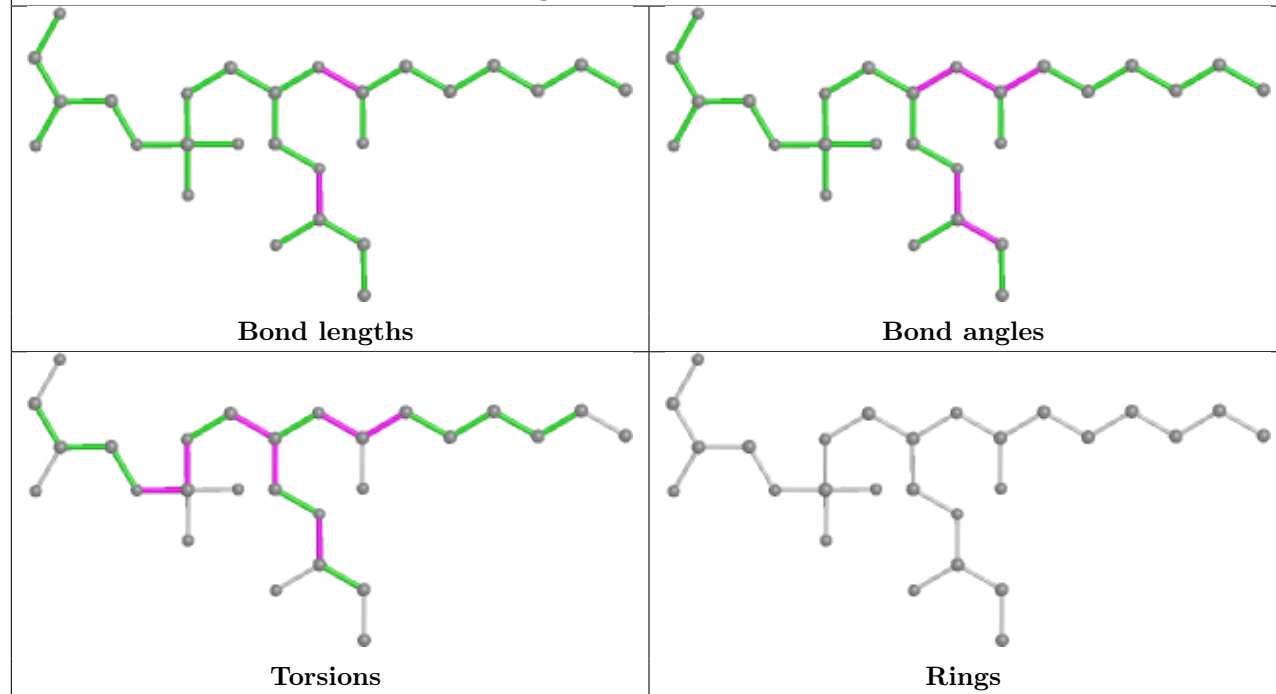




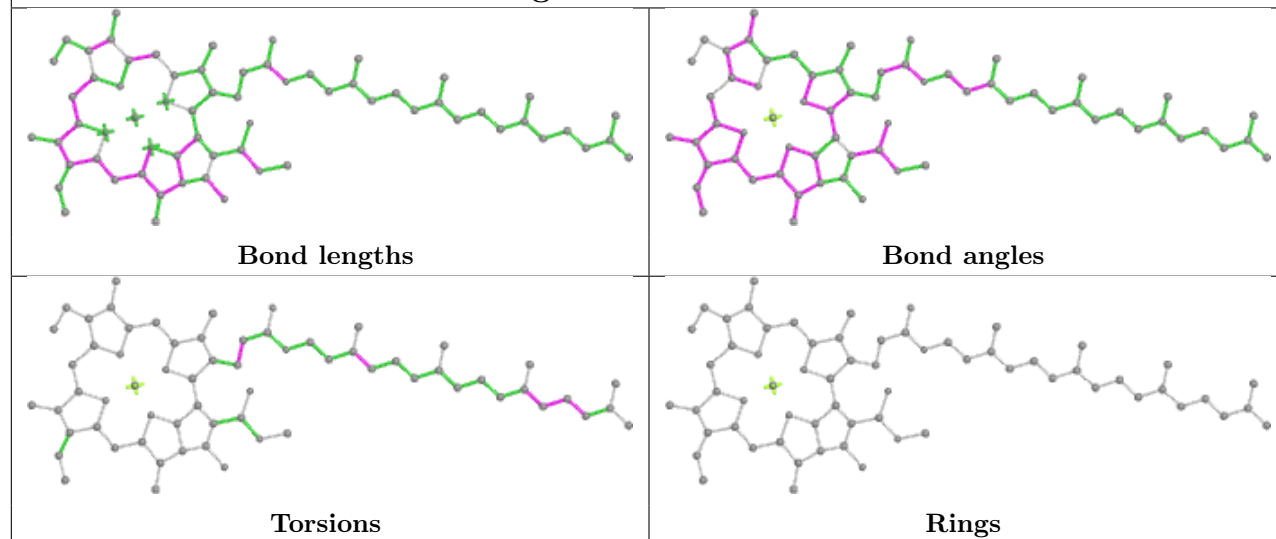
## Ligand CLA a 812



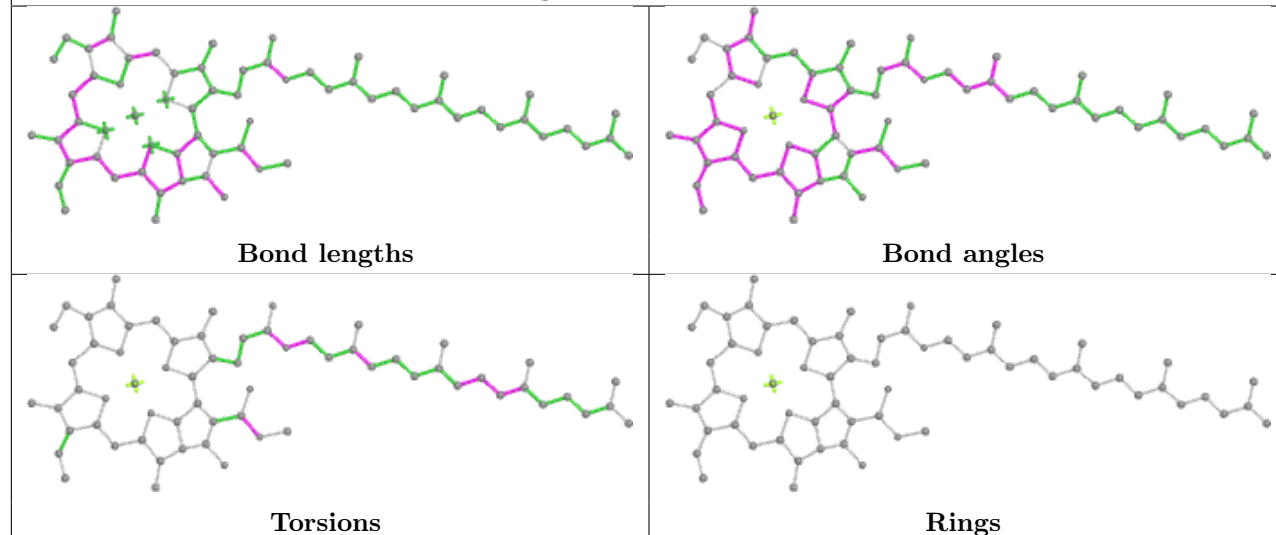
## Ligand LHG a 848



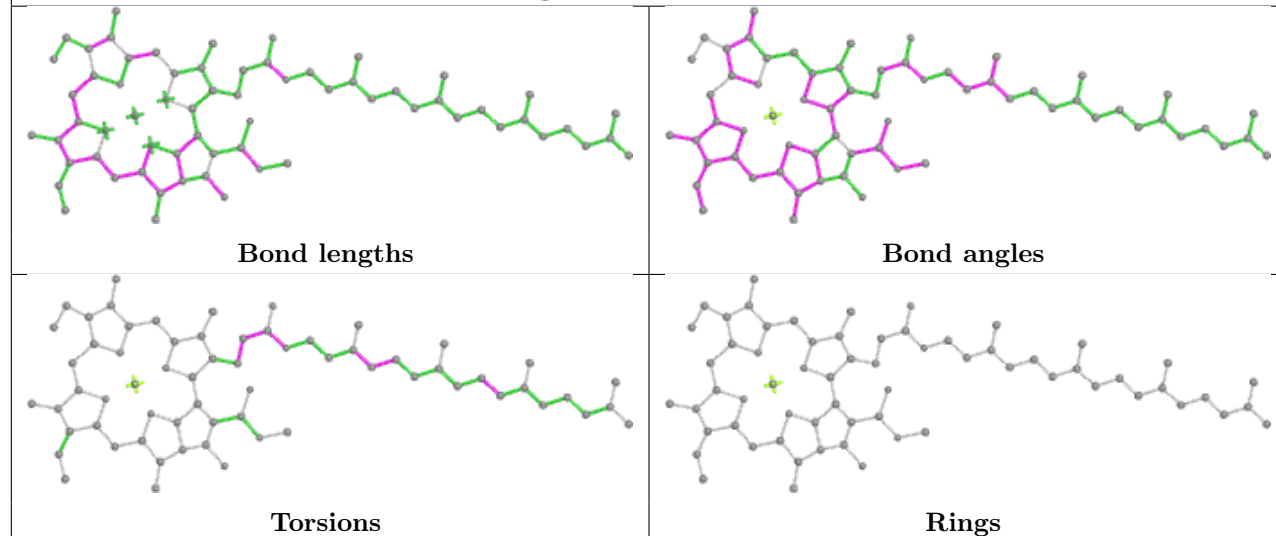
## Ligand CLA B 839



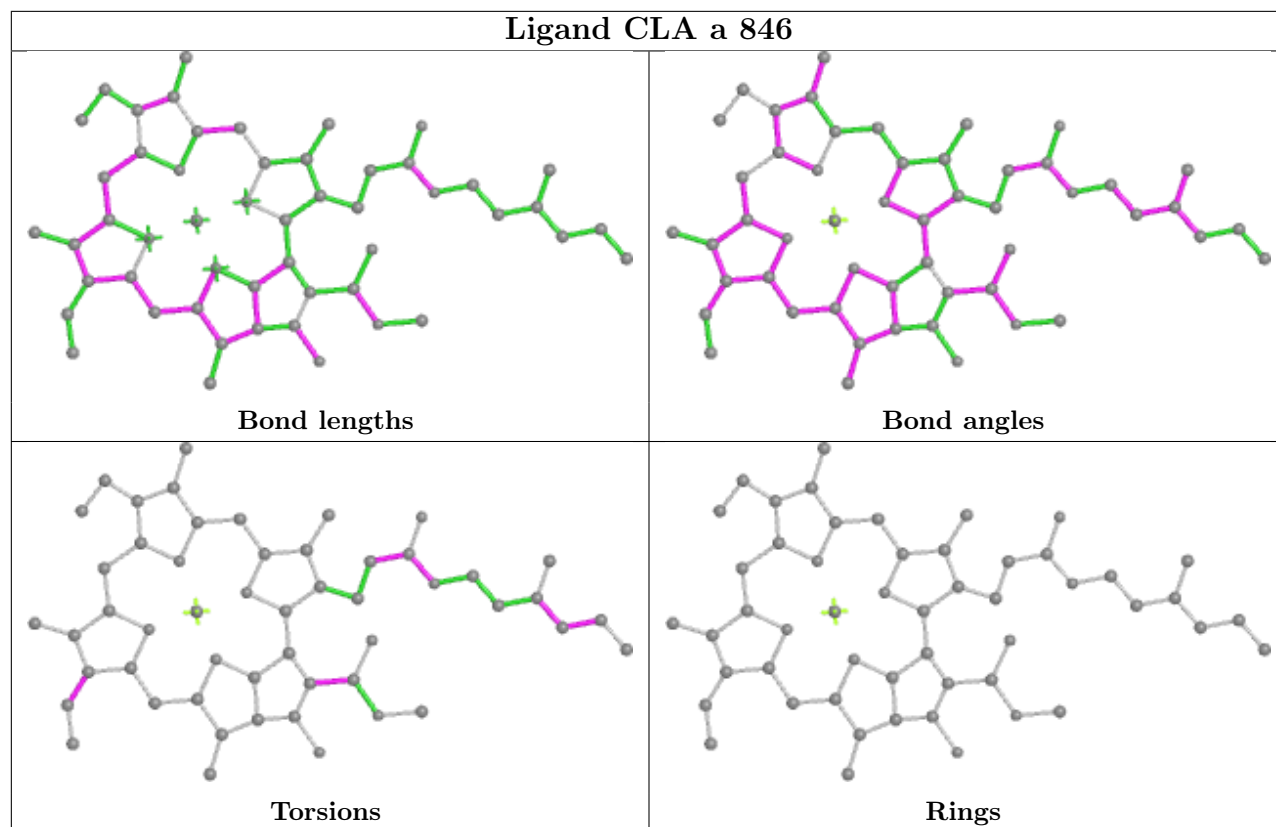
## Ligand CLA 2 603



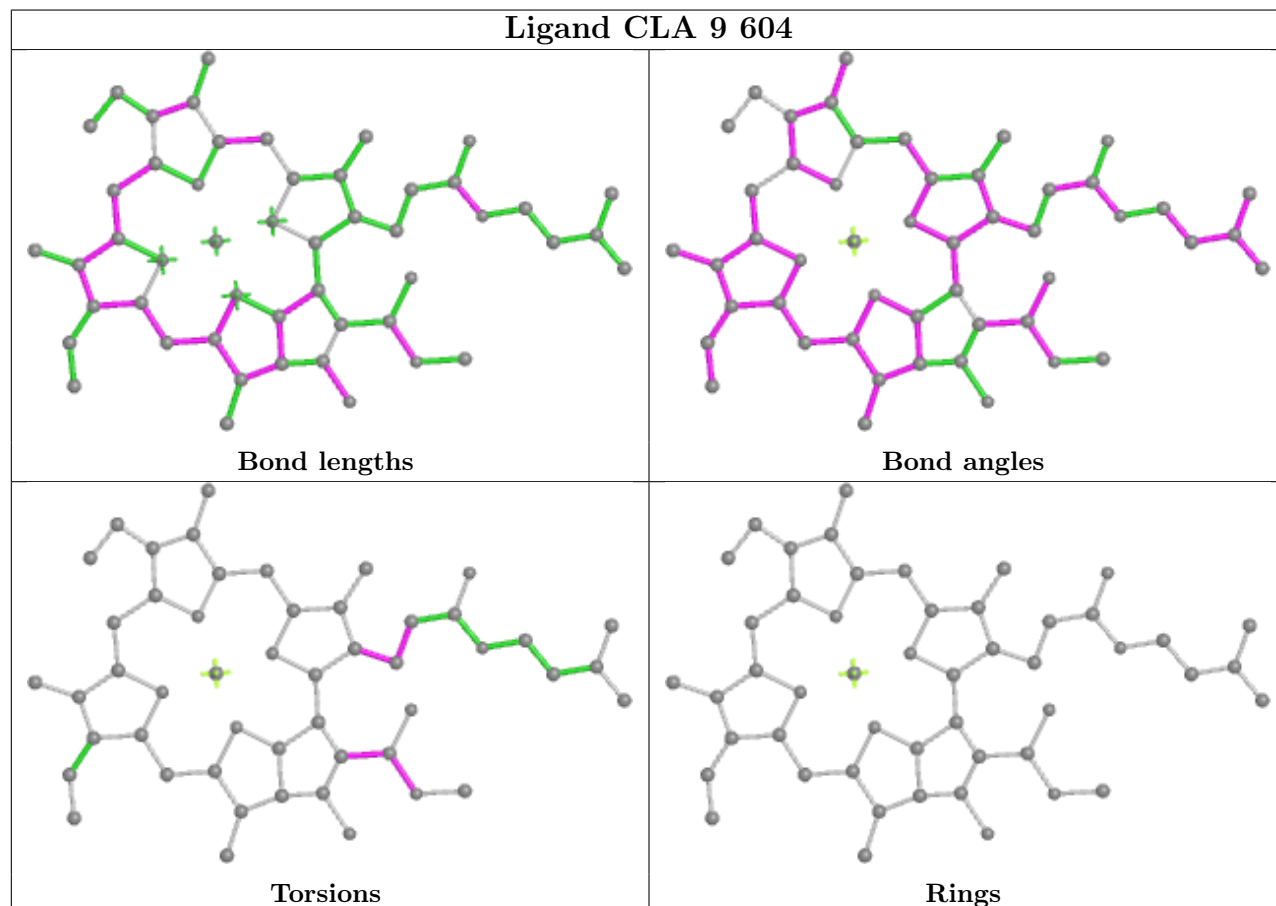
## Ligand CLA 2 612



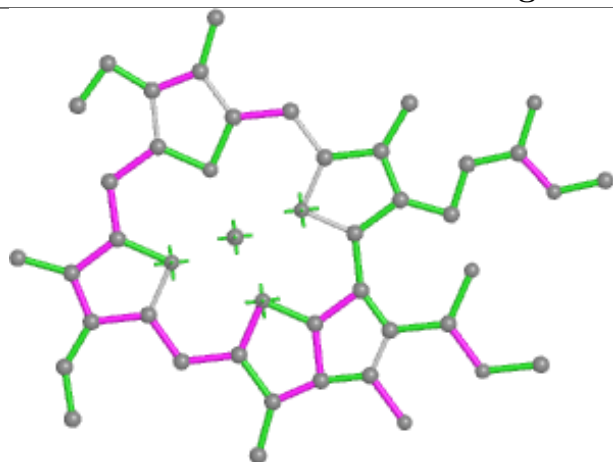
## Ligand CLA a 846



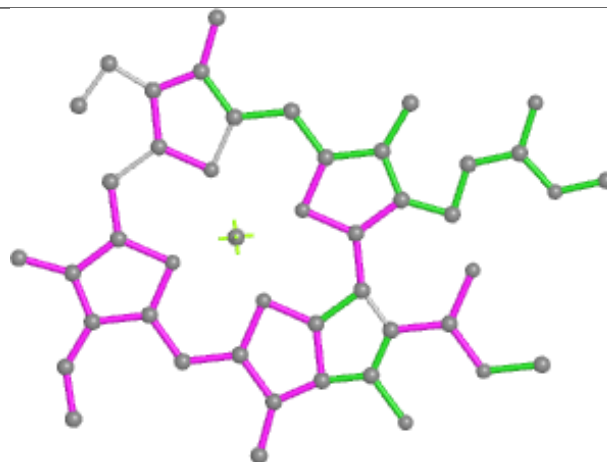
## Ligand CLA 9 604



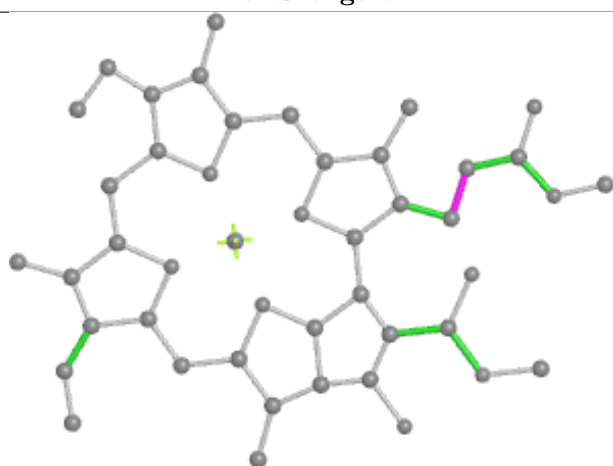
## Ligand CLA 1 315



Bond lengths



Bond angles

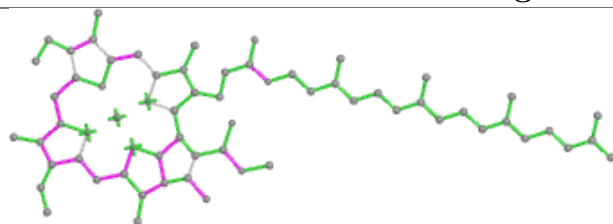


Torsions

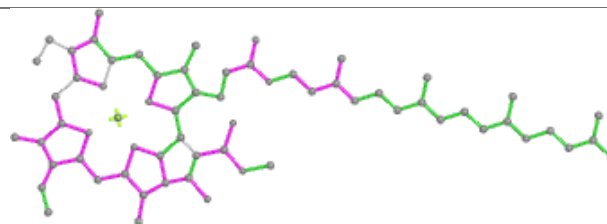


Rings

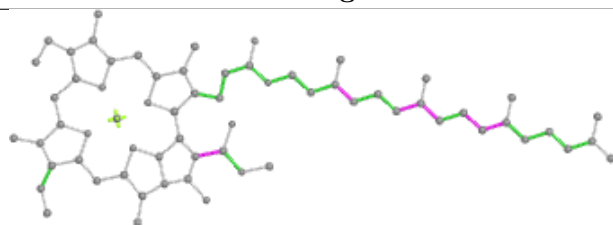
## Ligand CLA B 826



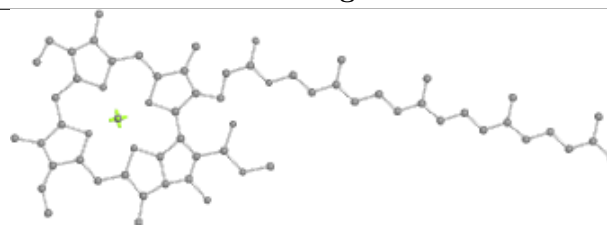
Bond lengths



Bond angles



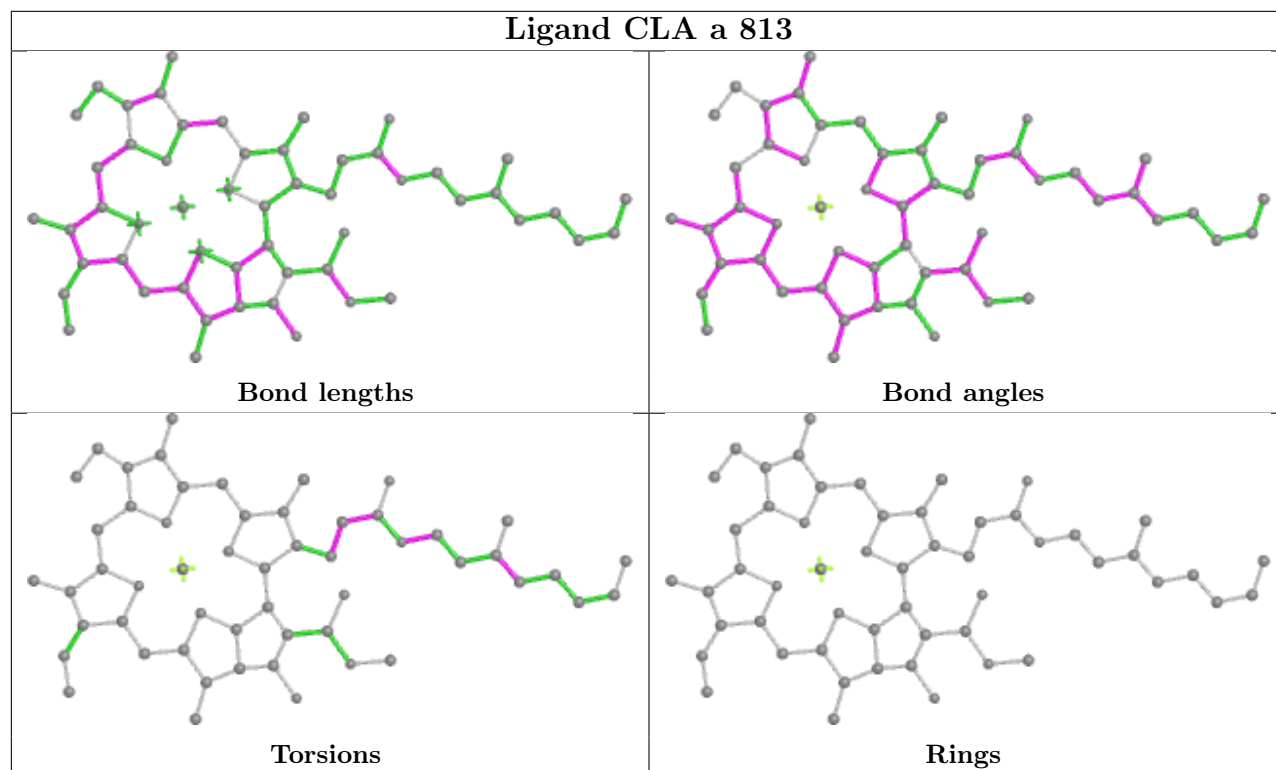
Torsions



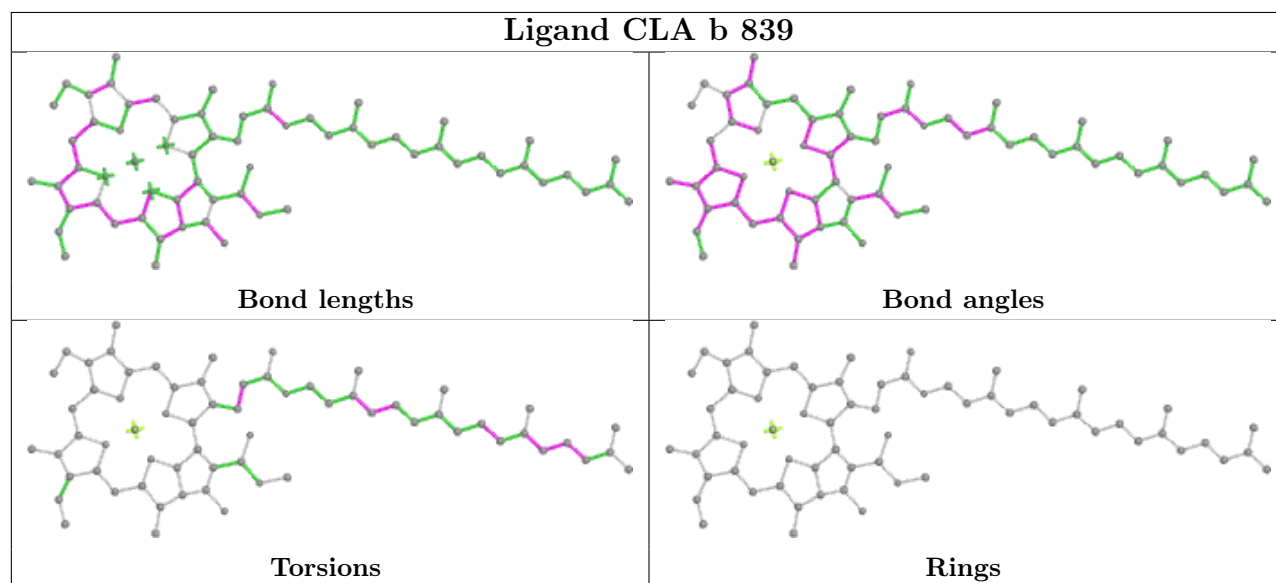
Rings



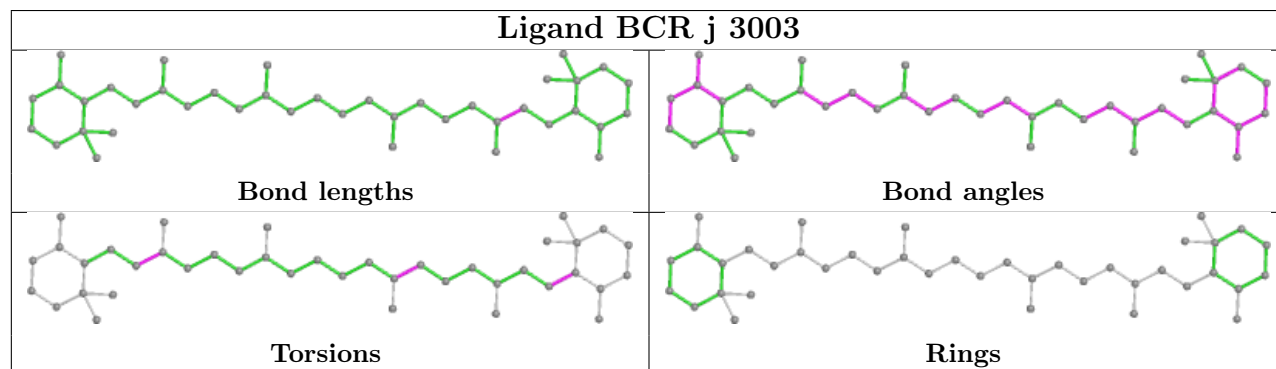
## Ligand CLA a 813



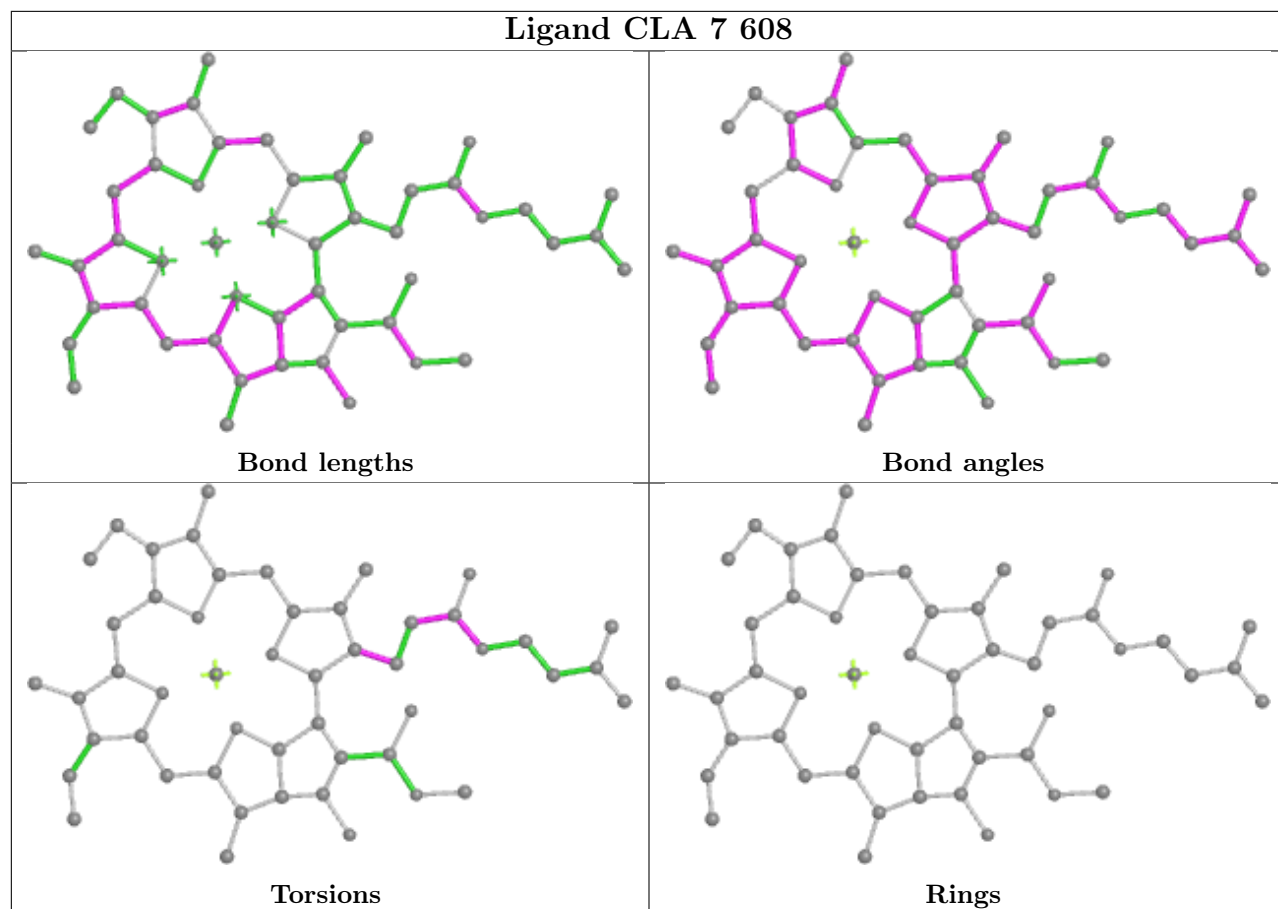
## Ligand CLA b 839



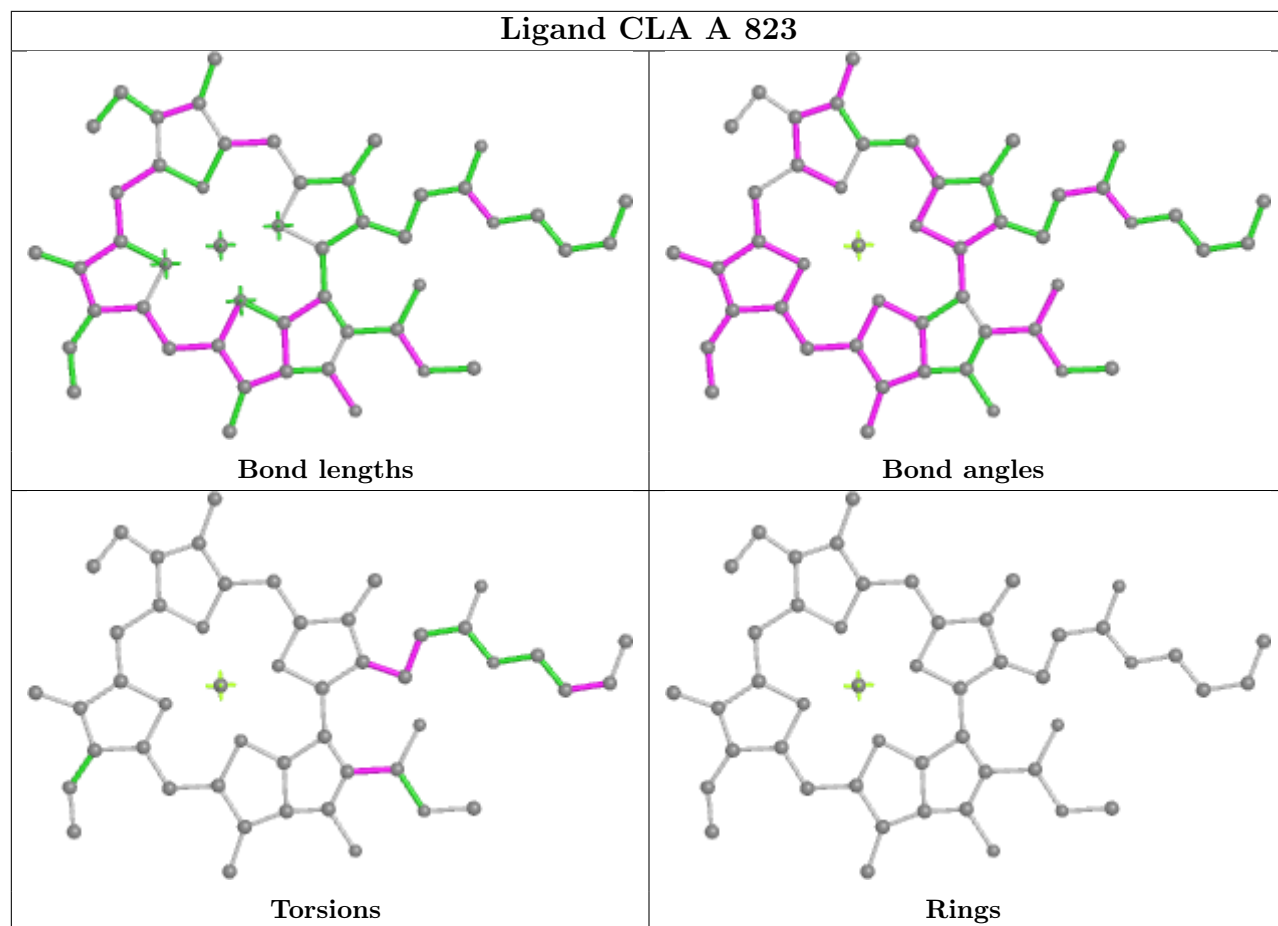
## Ligand BCR j 3003



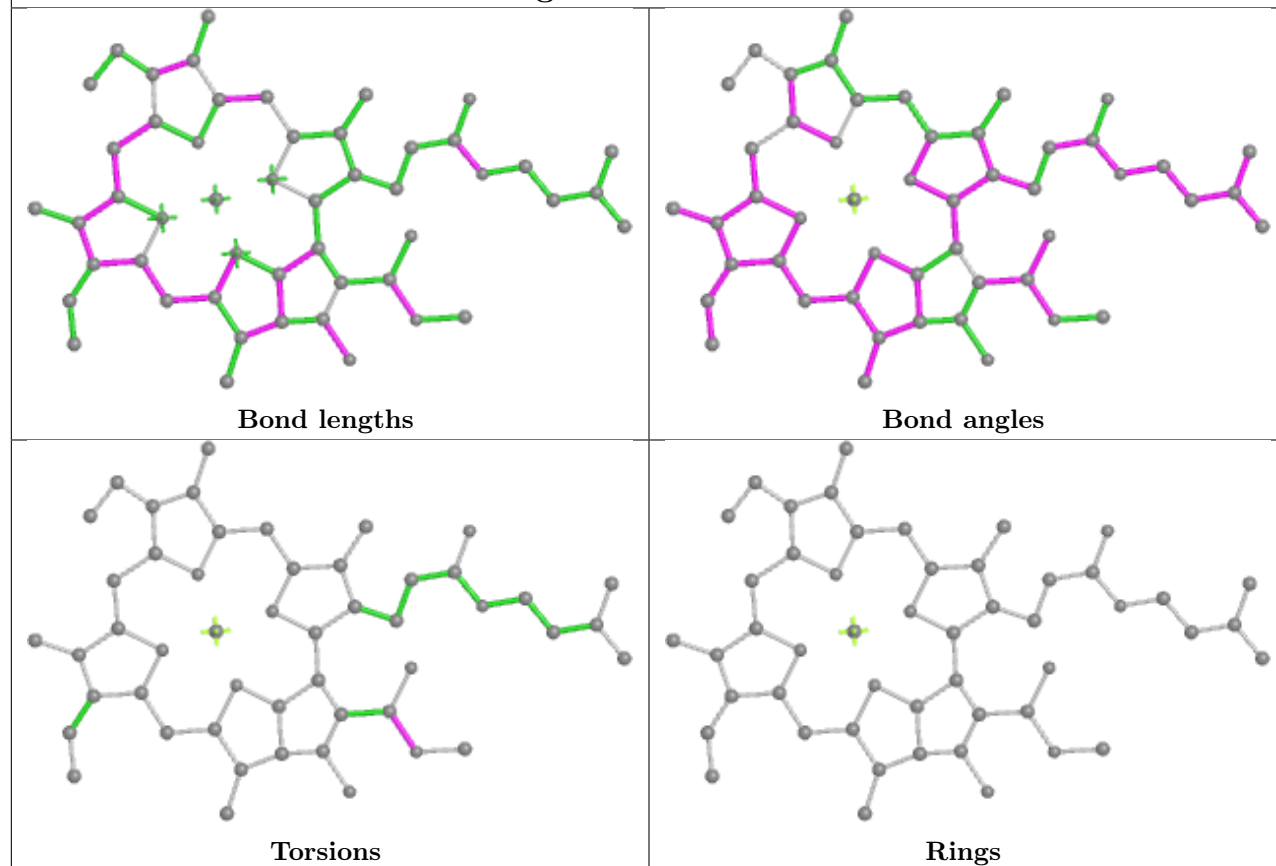
## Ligand CLA 7 608



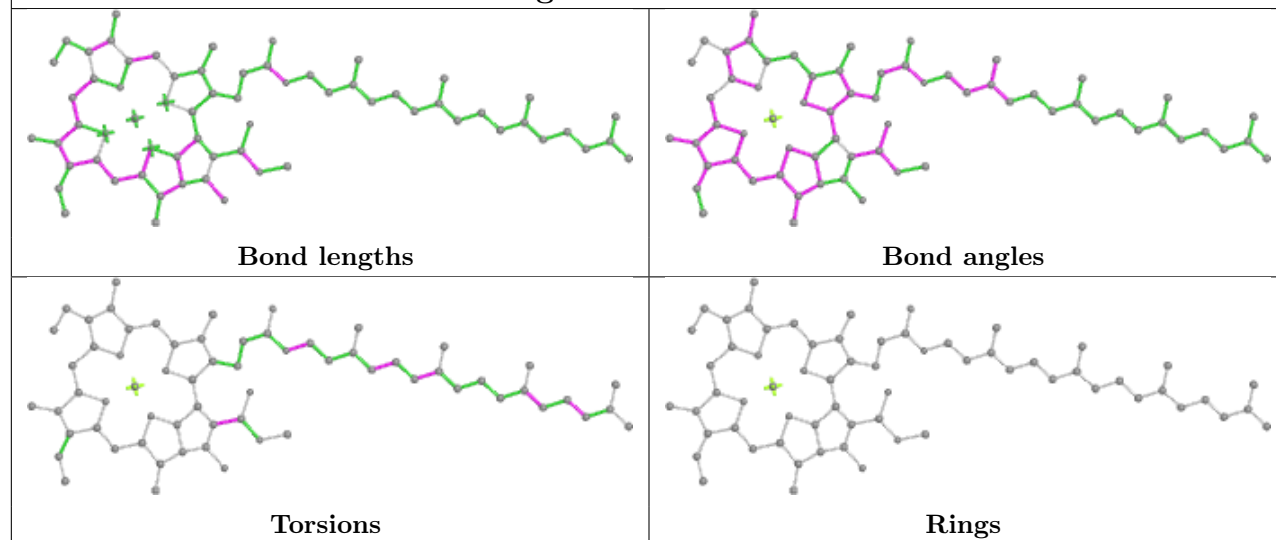
## Ligand CLA A 823



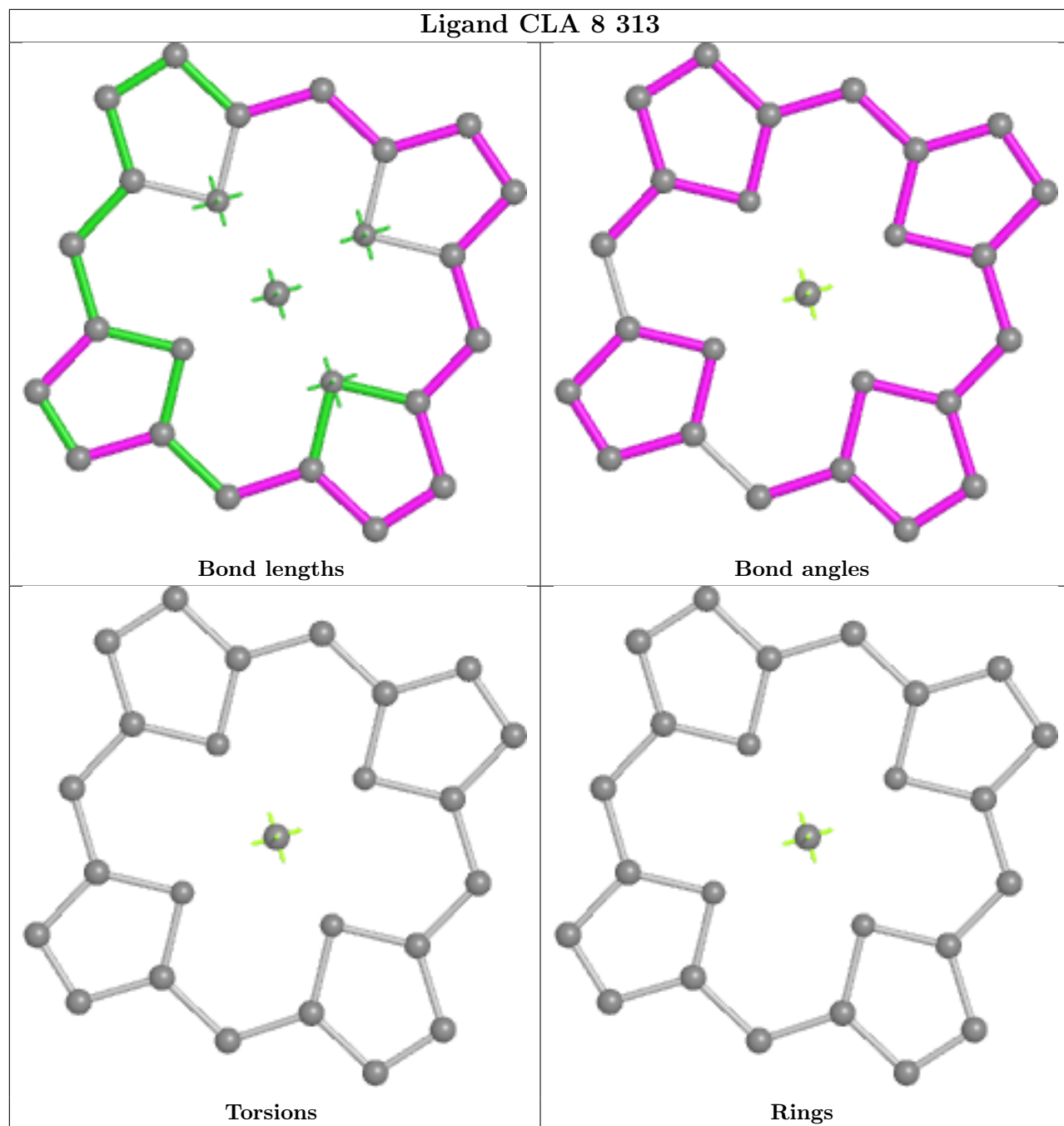
## Ligand CLA a 836



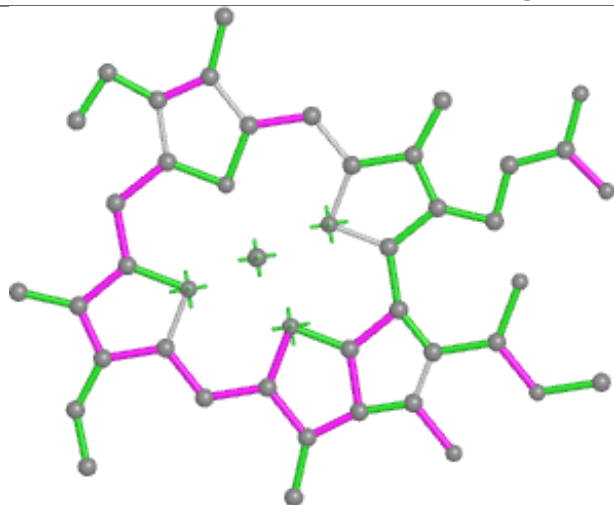
## Ligand CLA a 827



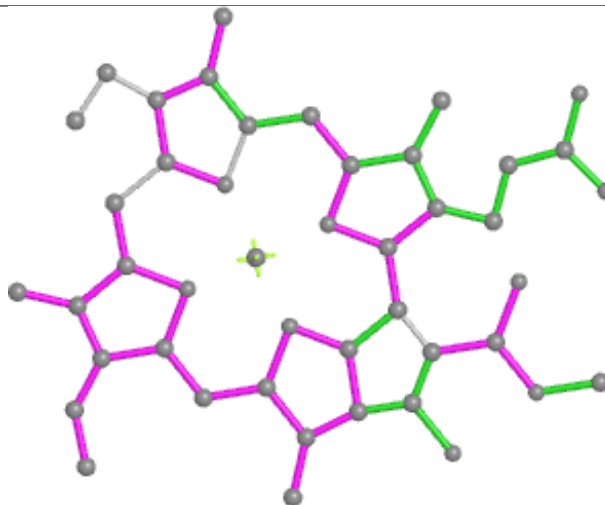
## Ligand CLA 8 313



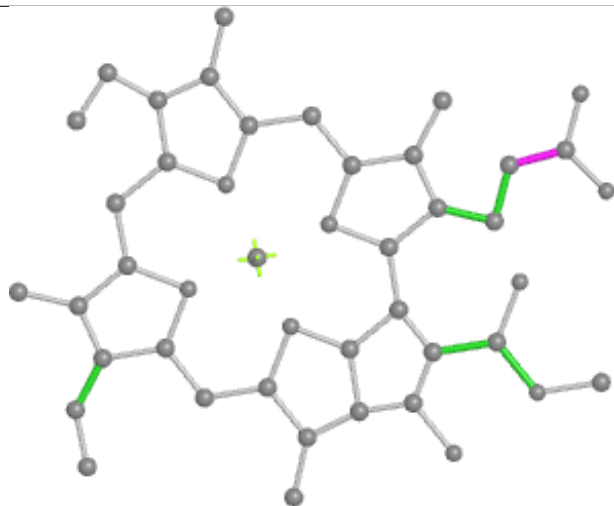
## Ligand CLA 4 613



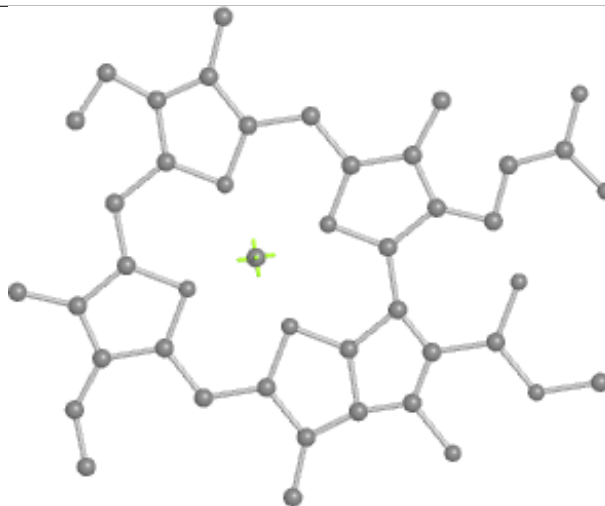
Bond lengths



Bond angles

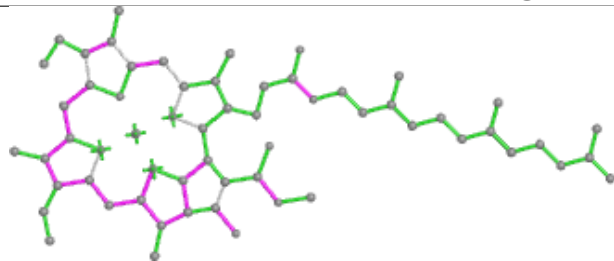


Torsions

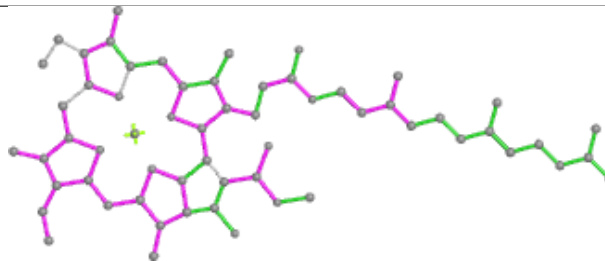


Rings

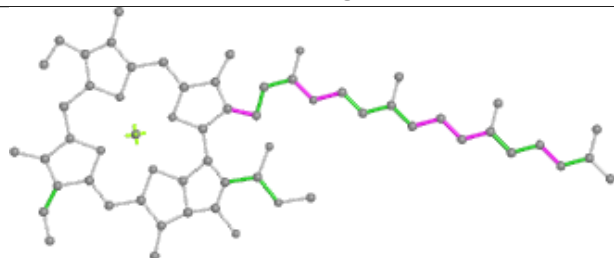
## Ligand CLA 2 604



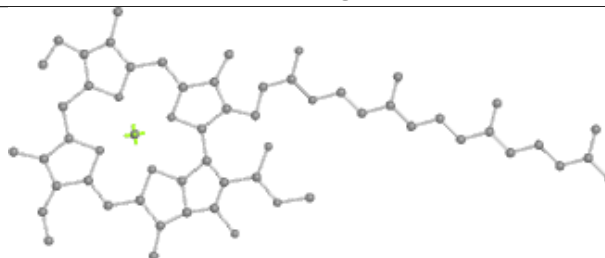
Bond lengths



Bond angles

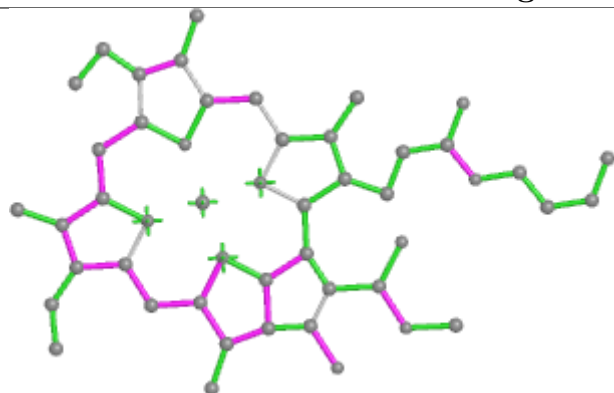


Torsions

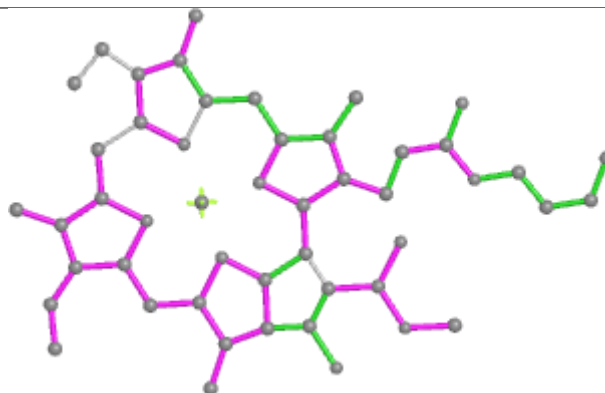


Rings

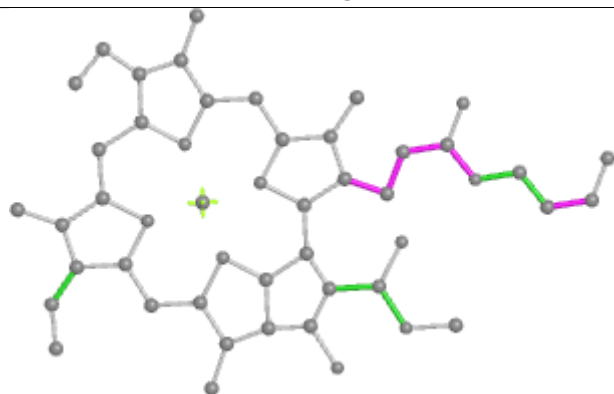
## Ligand CLA b 831



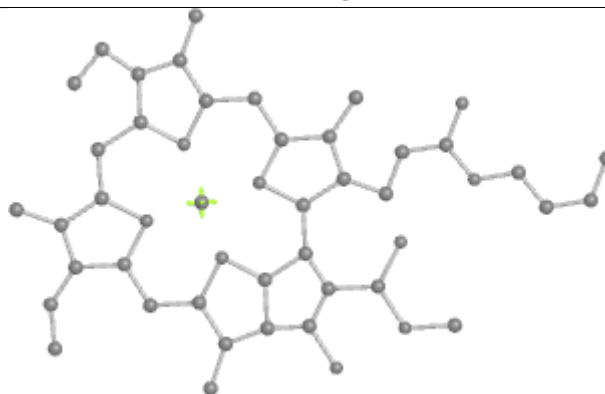
Bond lengths



Bond angles

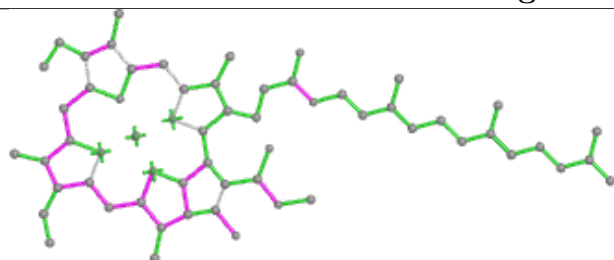


Torsions

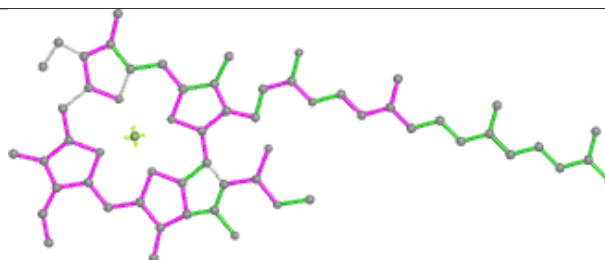


Rings

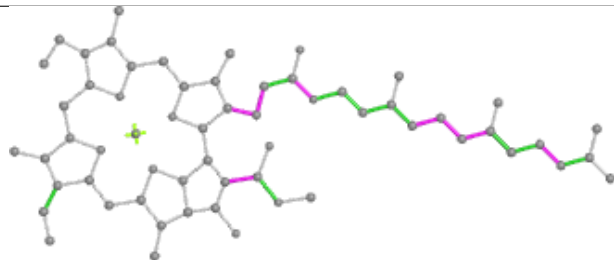
## Ligand CLA 7 604



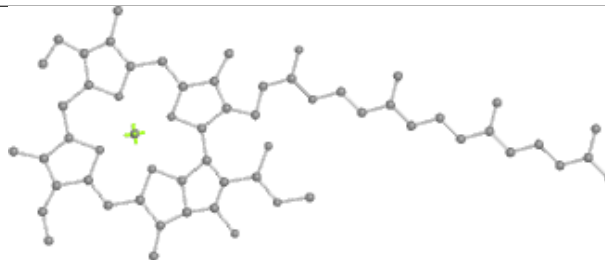
Bond lengths



Bond angles

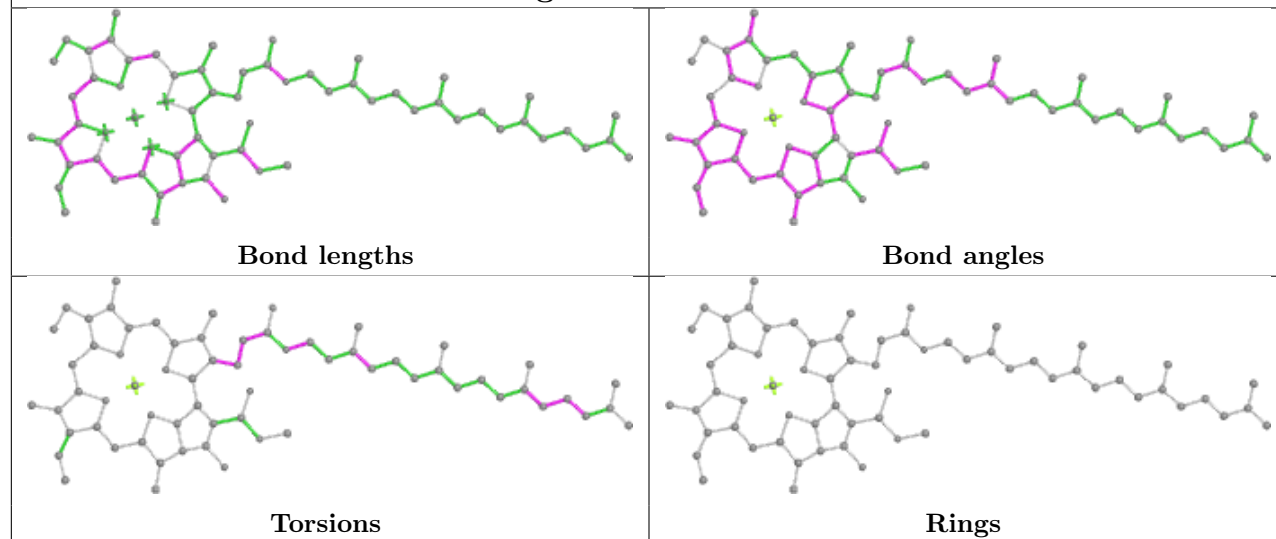


Torsions

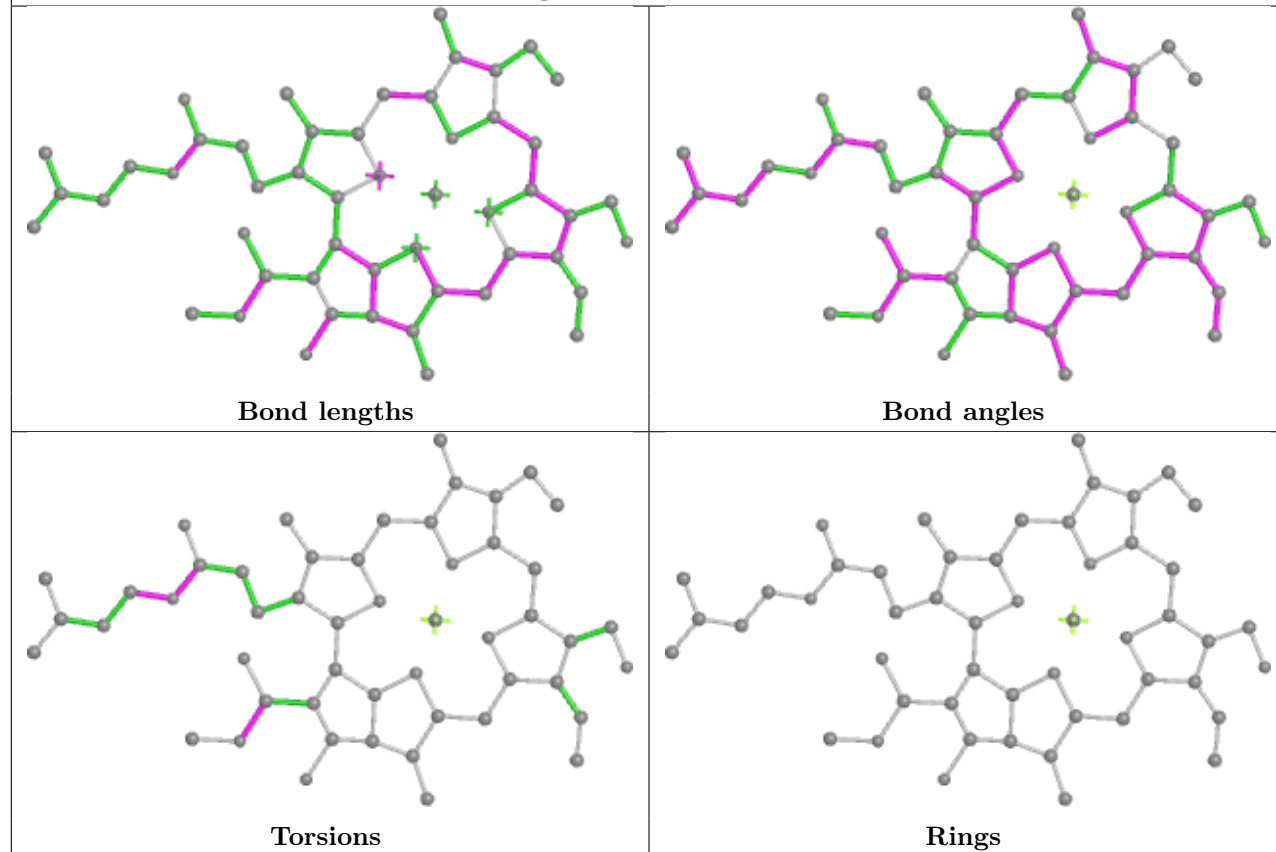


Rings

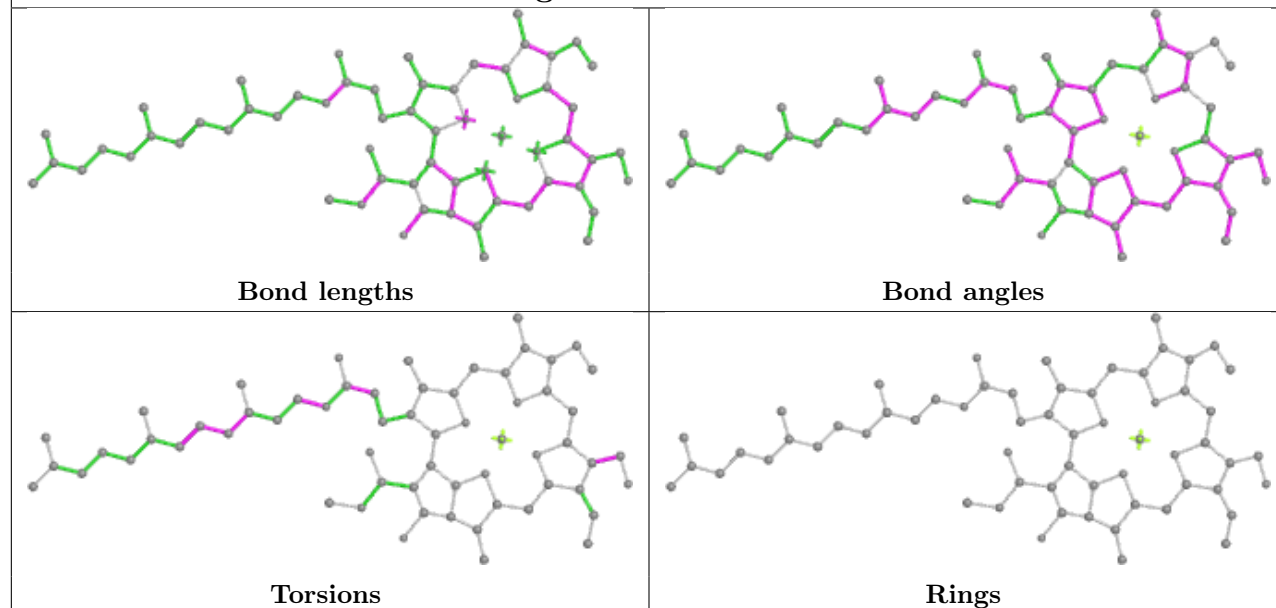
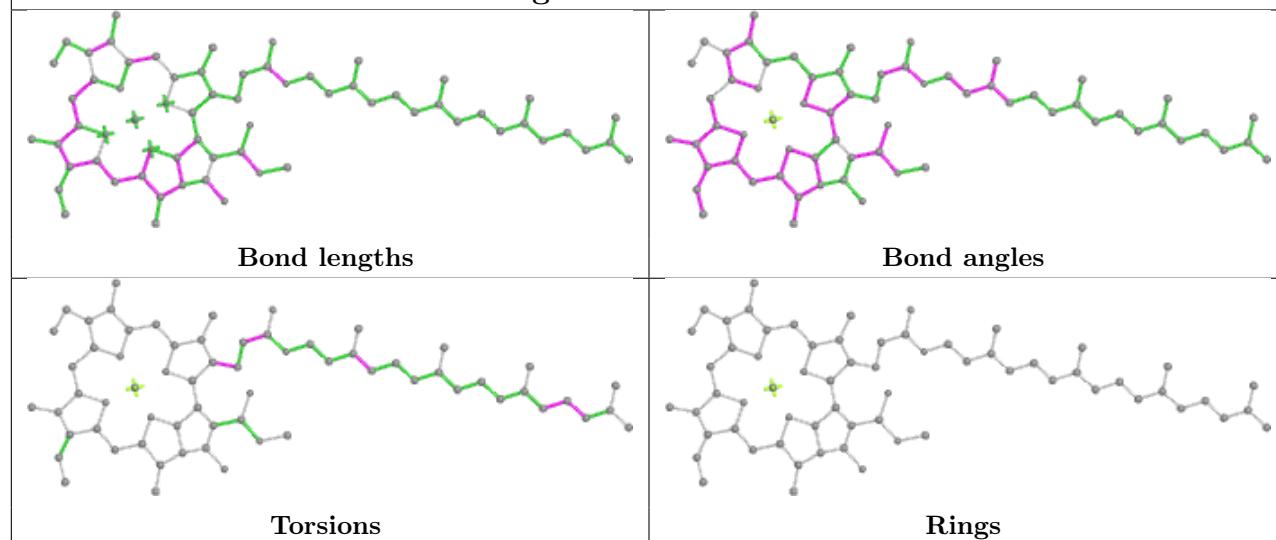
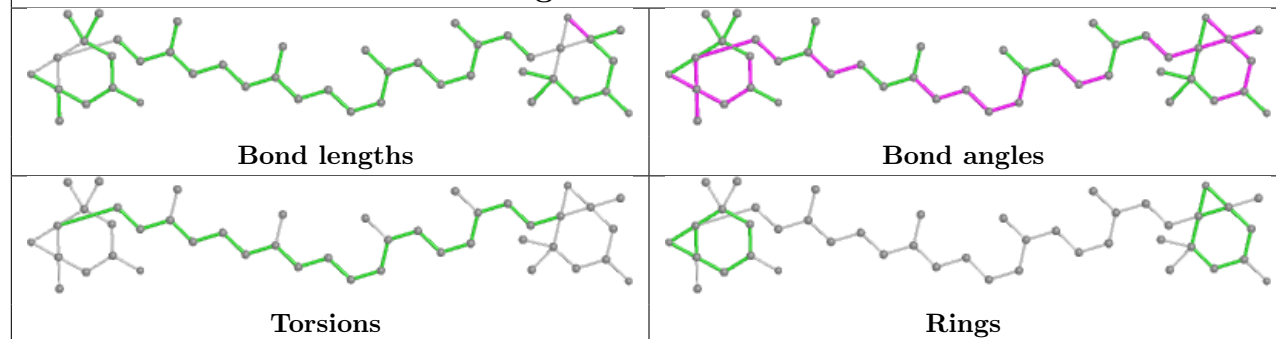
## Ligand CLA a 830

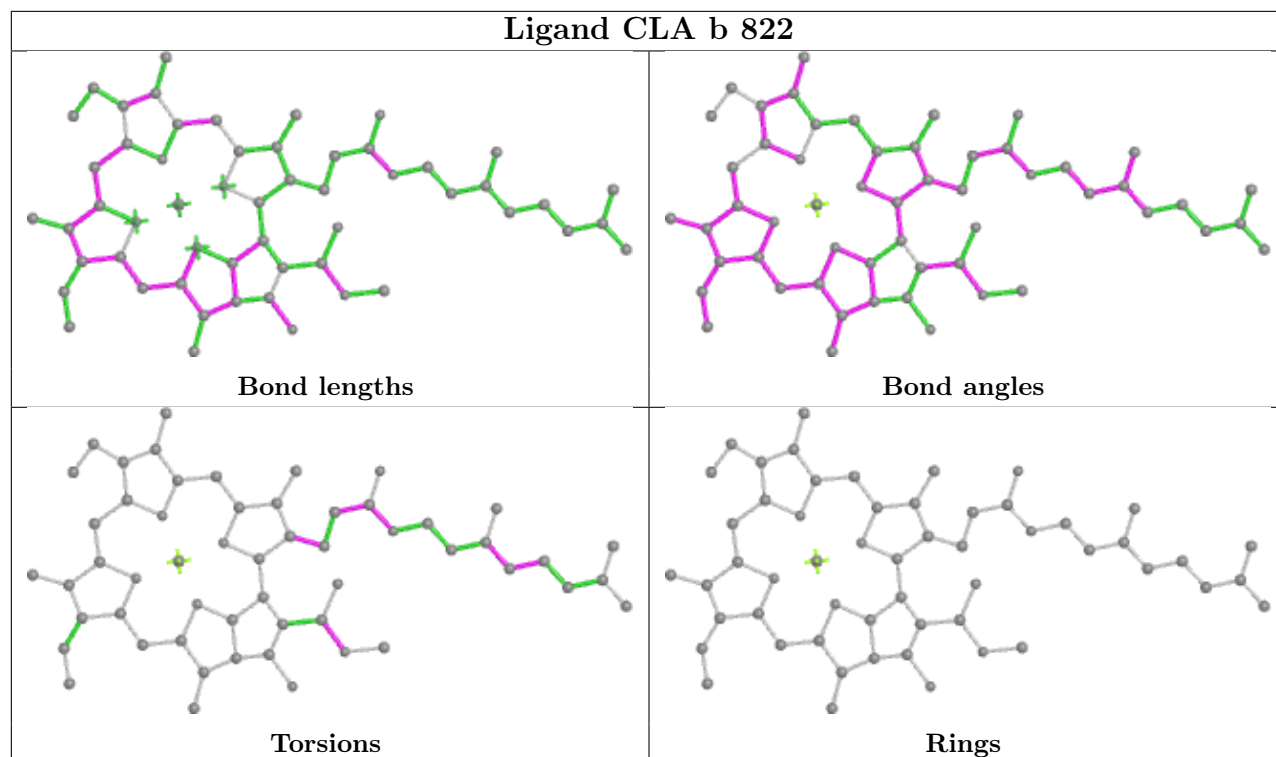
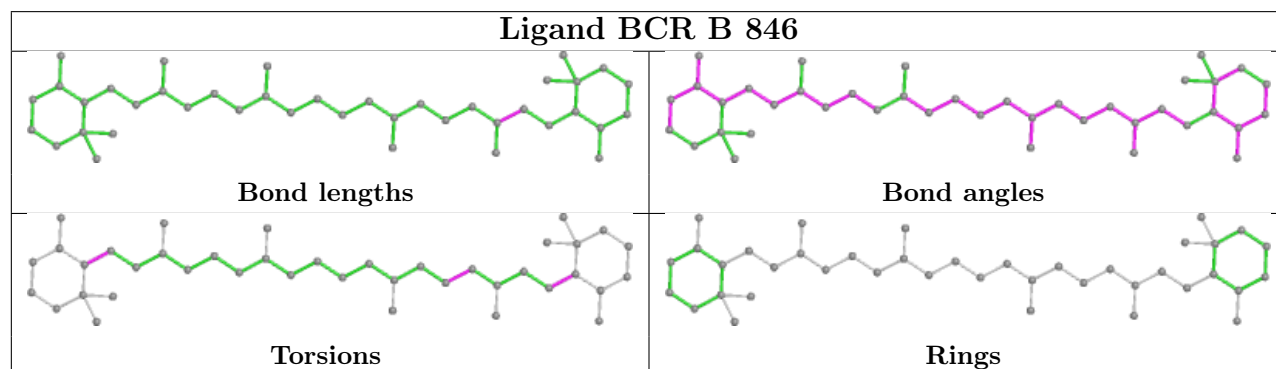


## Ligand CHL 2 607

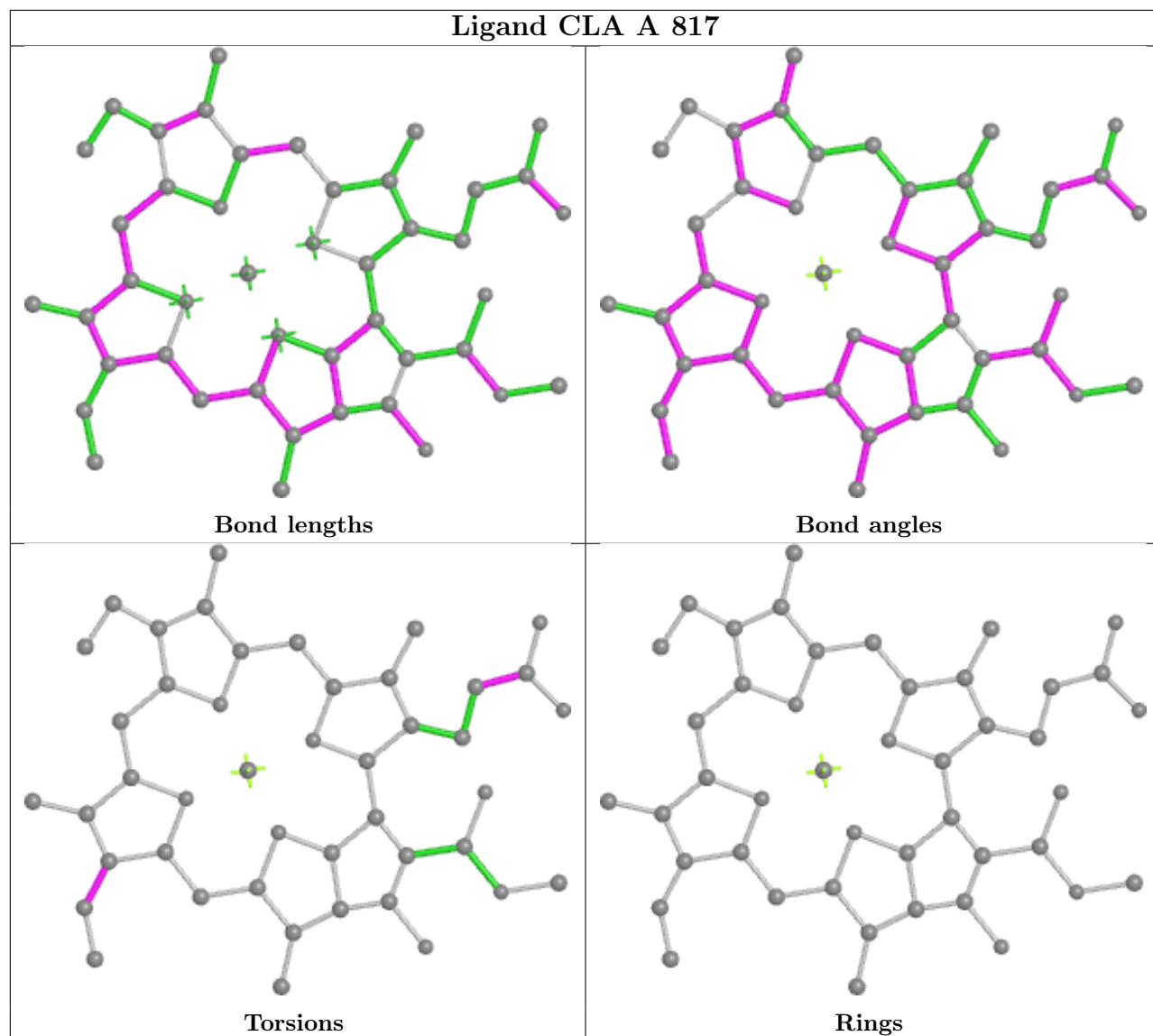




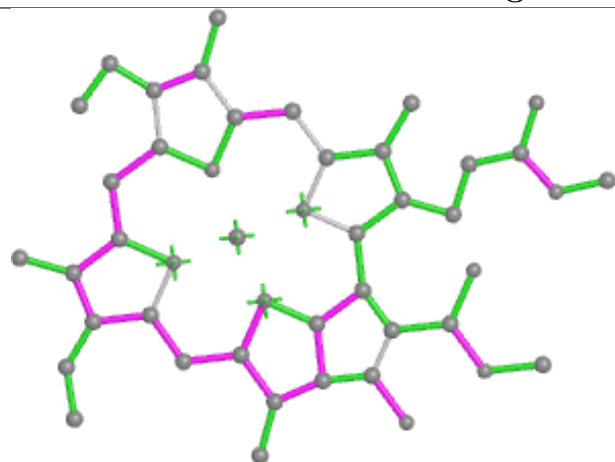
**Ligand CHL 7 601****Ligand CLA B 841****Ligand XAT 9 617**

**Ligand CLA b 822****Ligand BCR B 846**

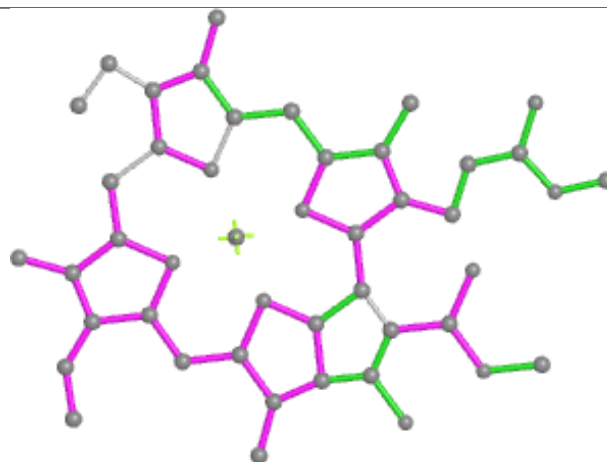
## Ligand CLA A 817



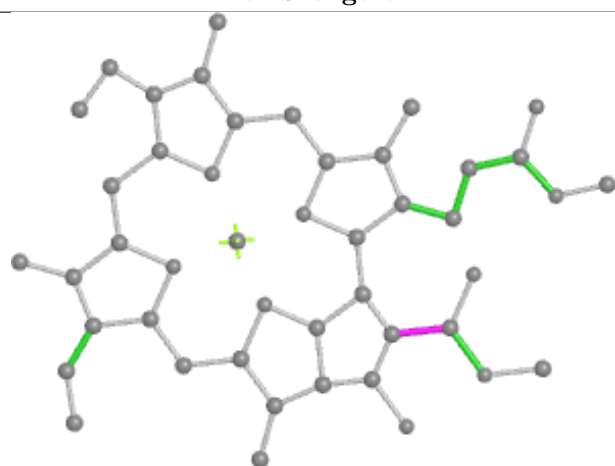
## Ligand CLA K 4003



Bond lengths



Bond angles

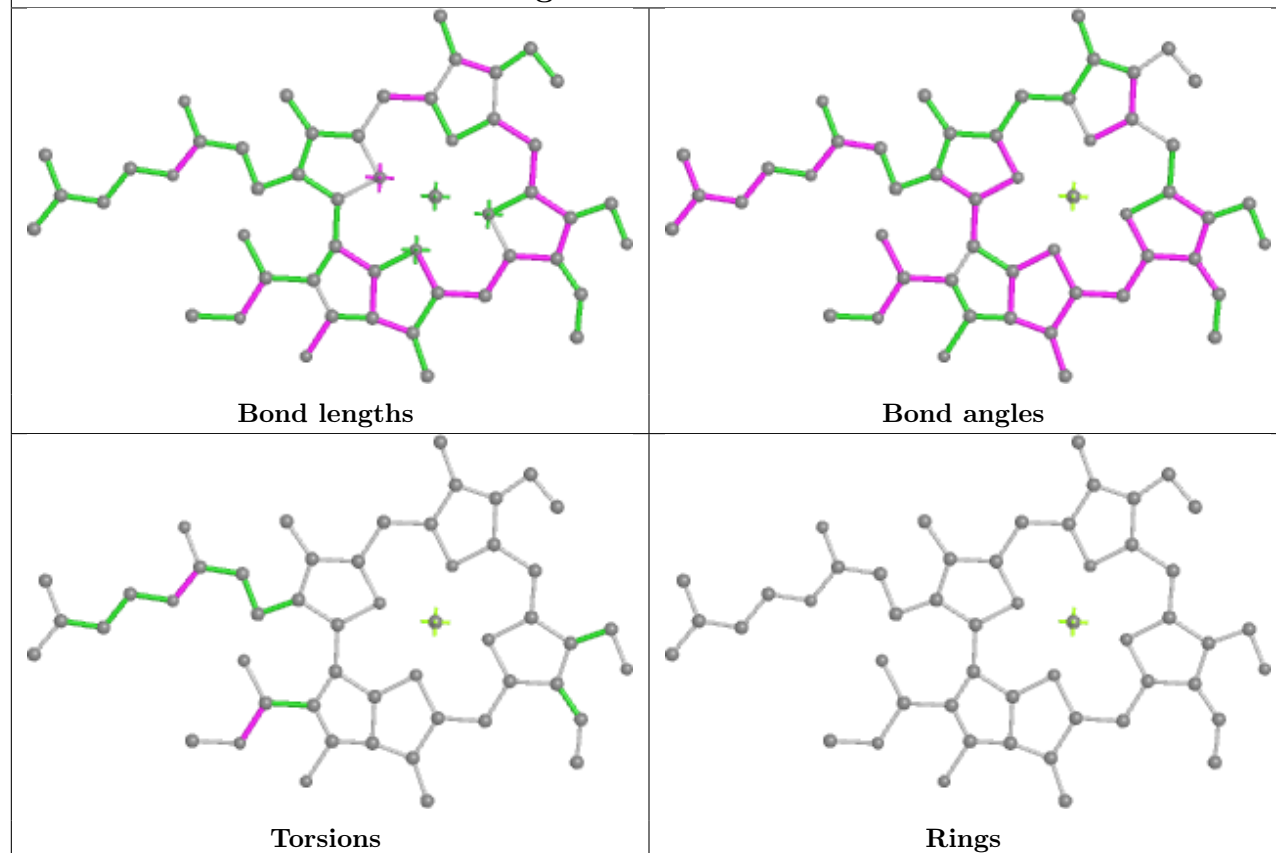


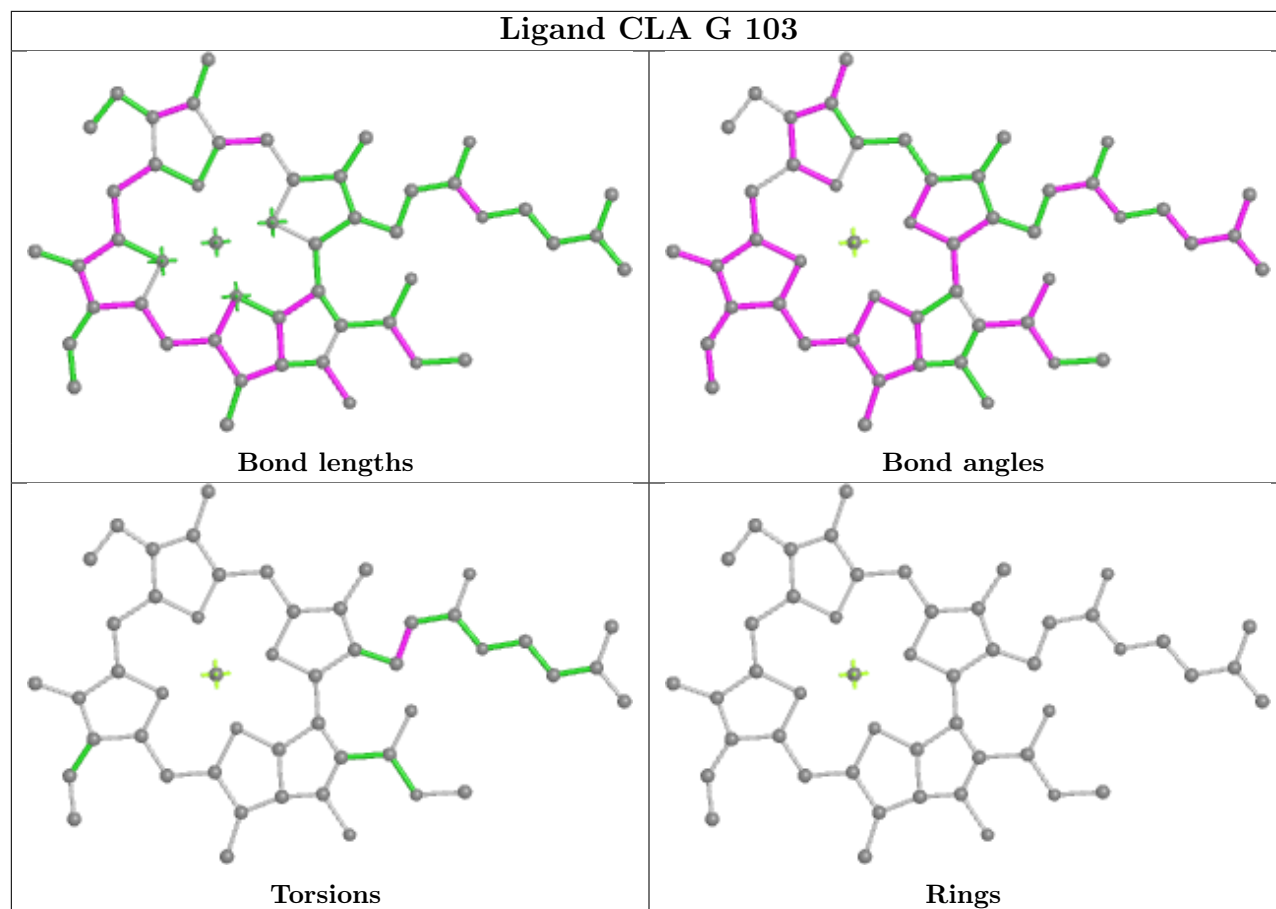
Torsions



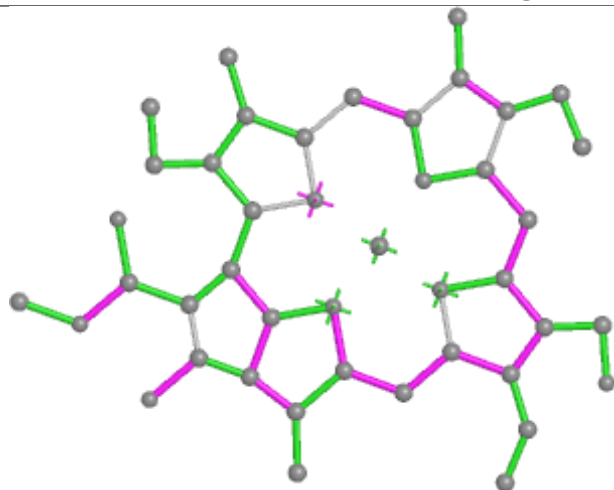
Rings

## Ligand CHL 7 607

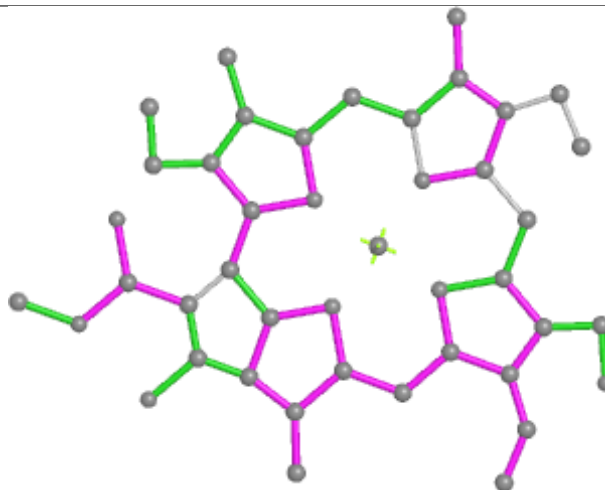




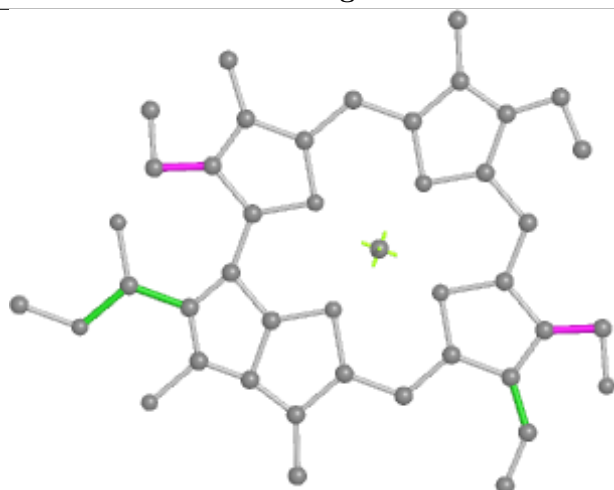
## Ligand CHL 7 614



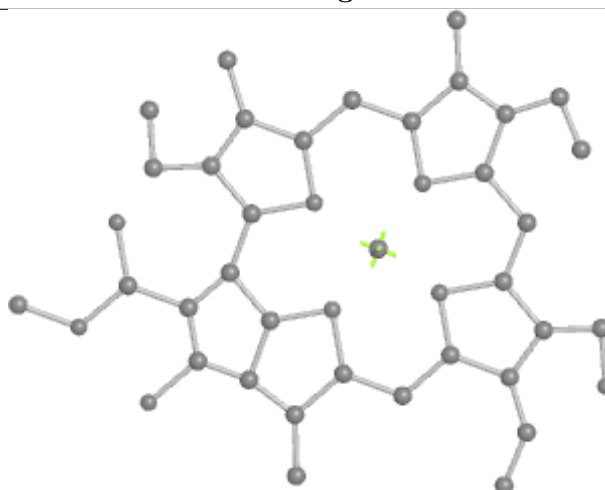
Bond lengths



Bond angles

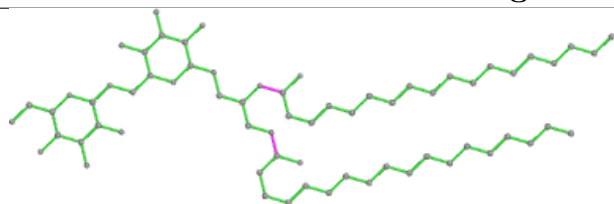


Torsions

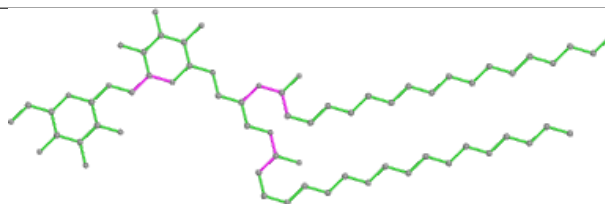


Rings

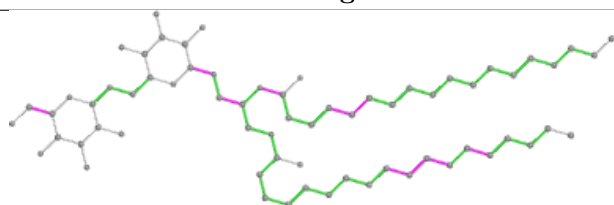
## Ligand DGD B 850



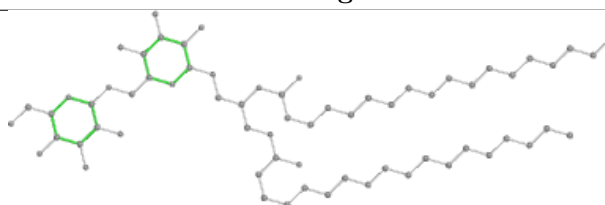
Bond lengths



Bond angles

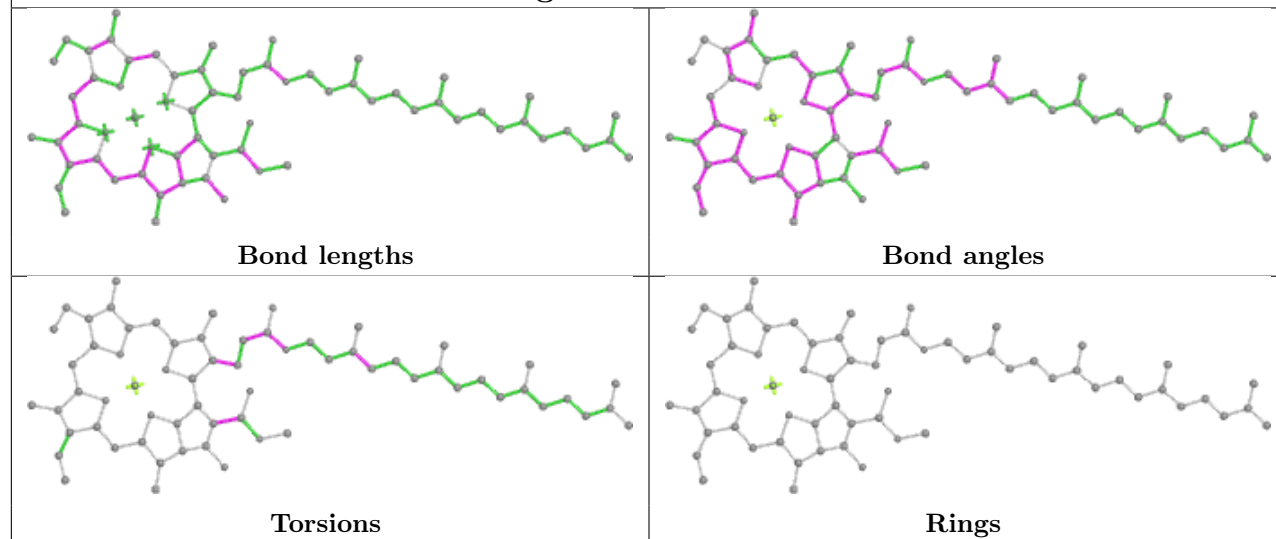


Torsions

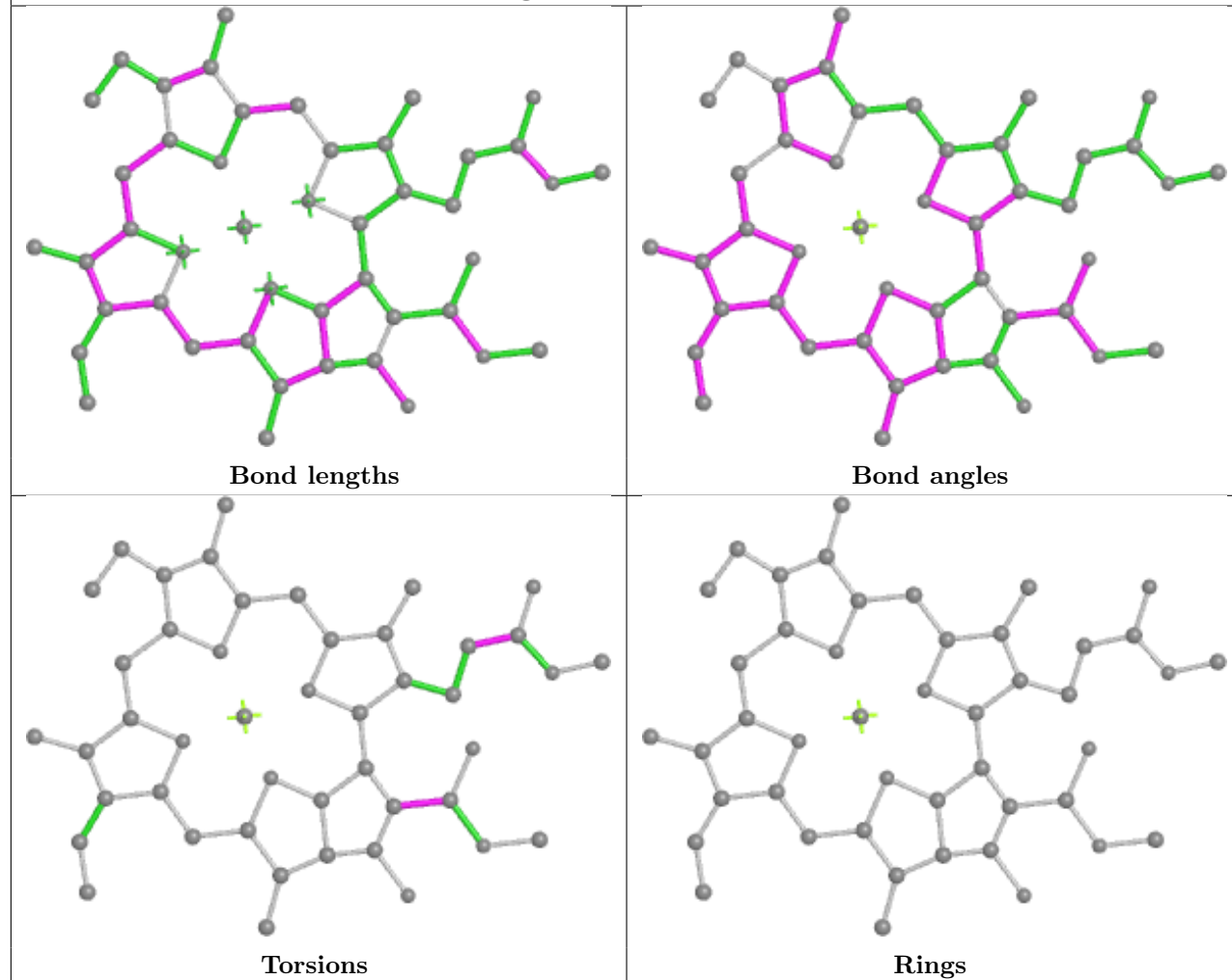


Rings

## Ligand CLA a 811

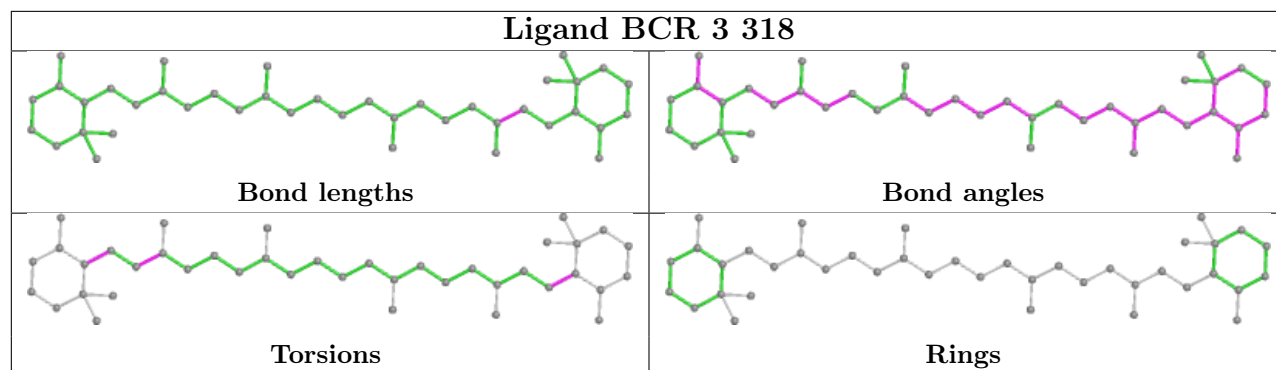


## Ligand CLA 4 601

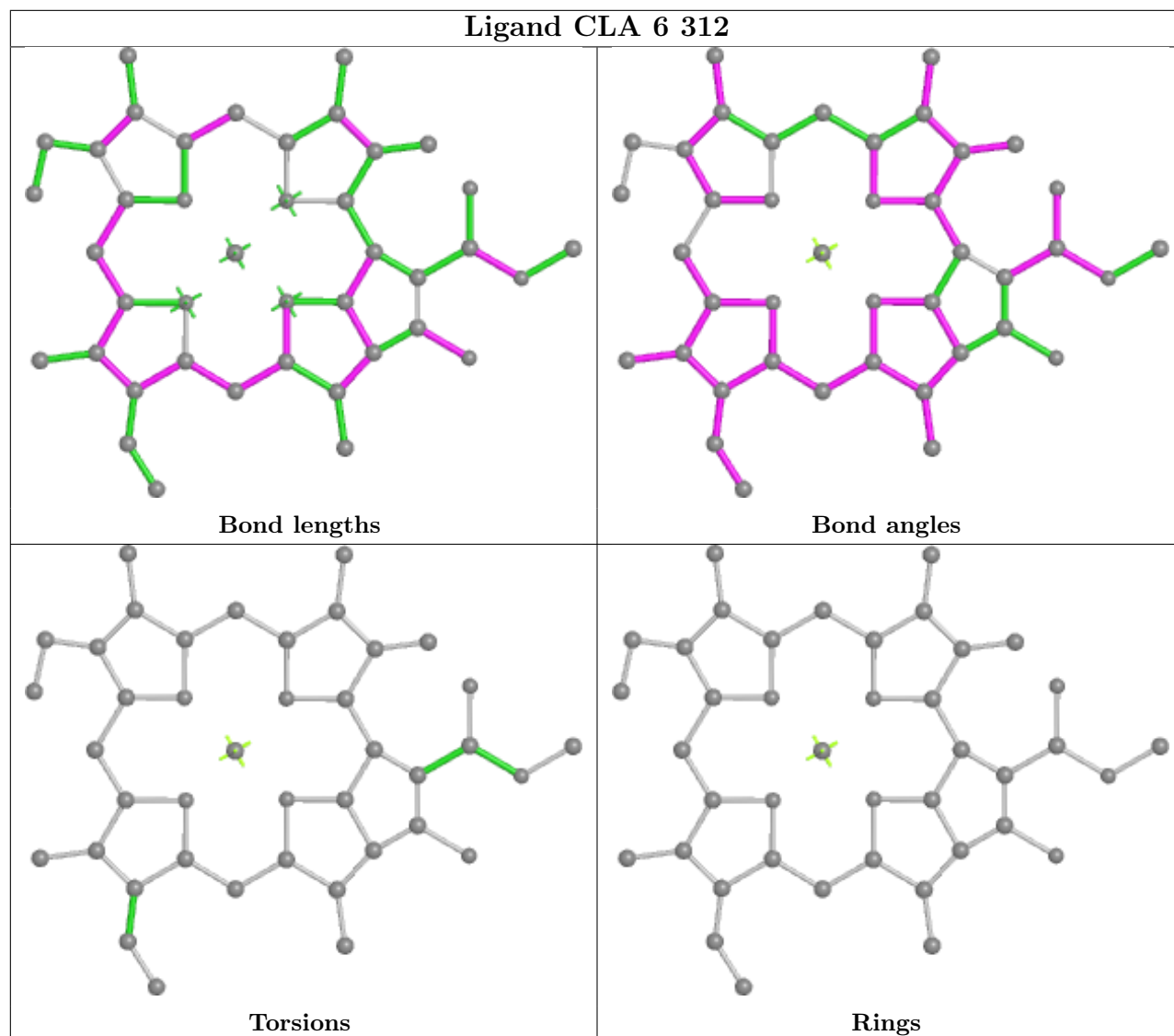


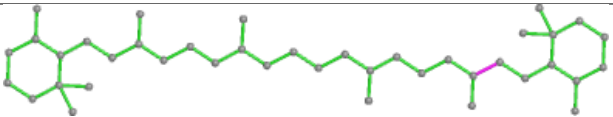
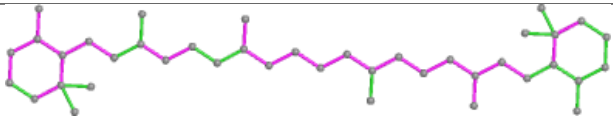
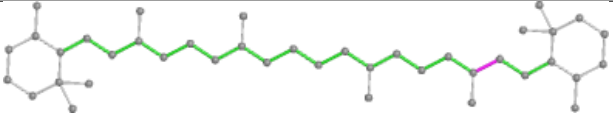
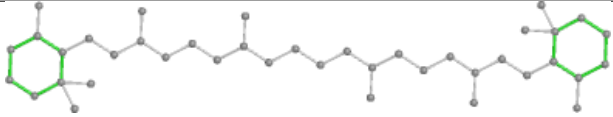


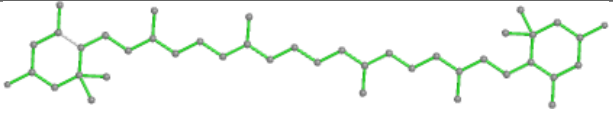
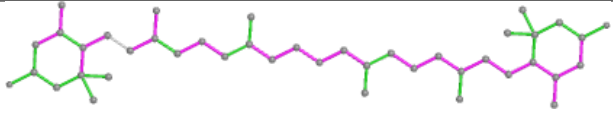
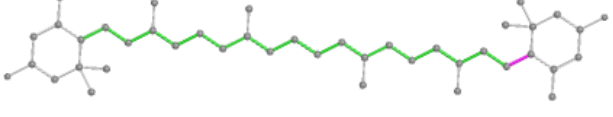
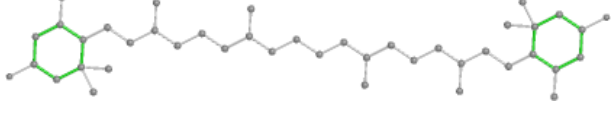
## Ligand BCR 3 318



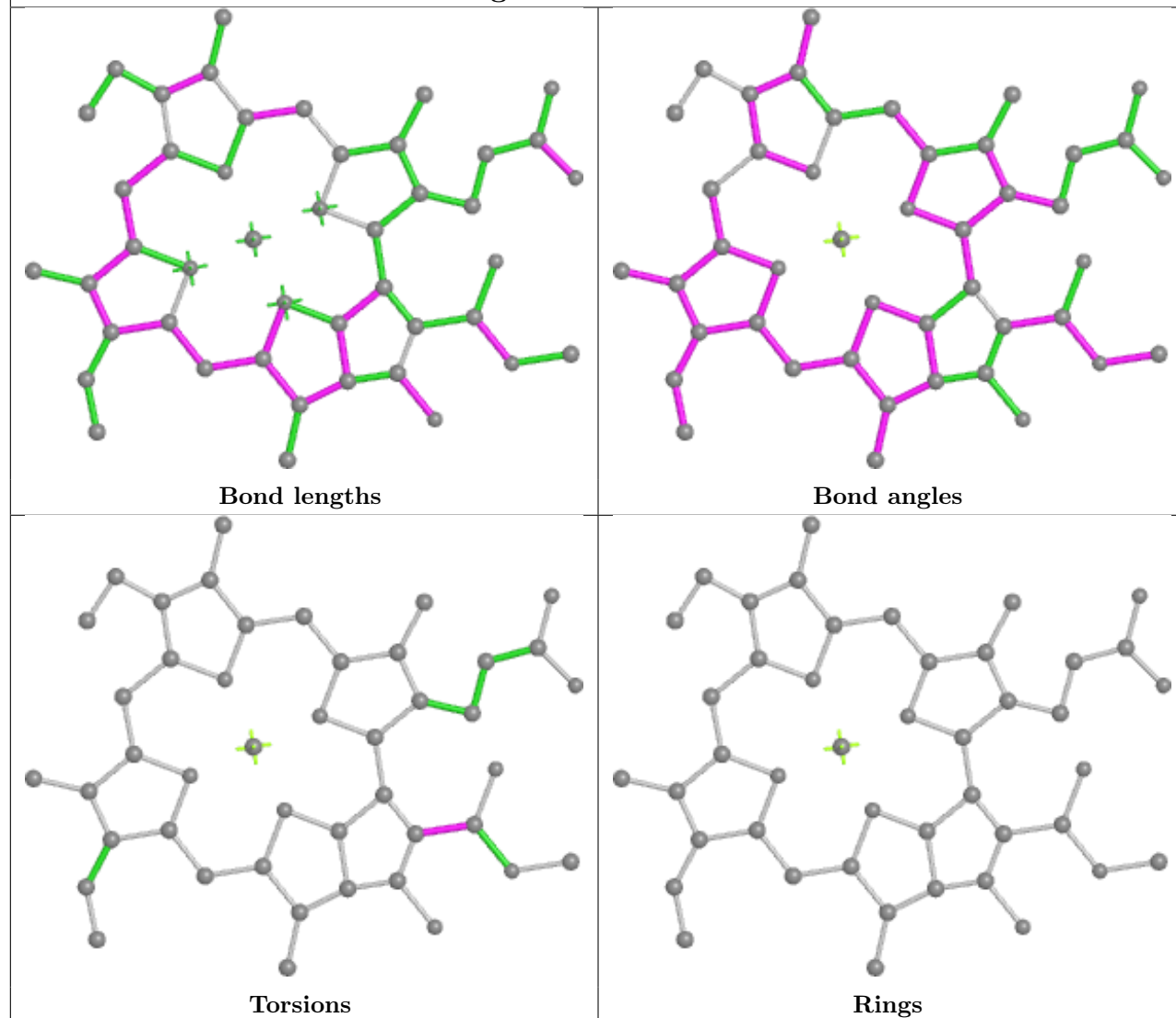
## Ligand CLA 6 312



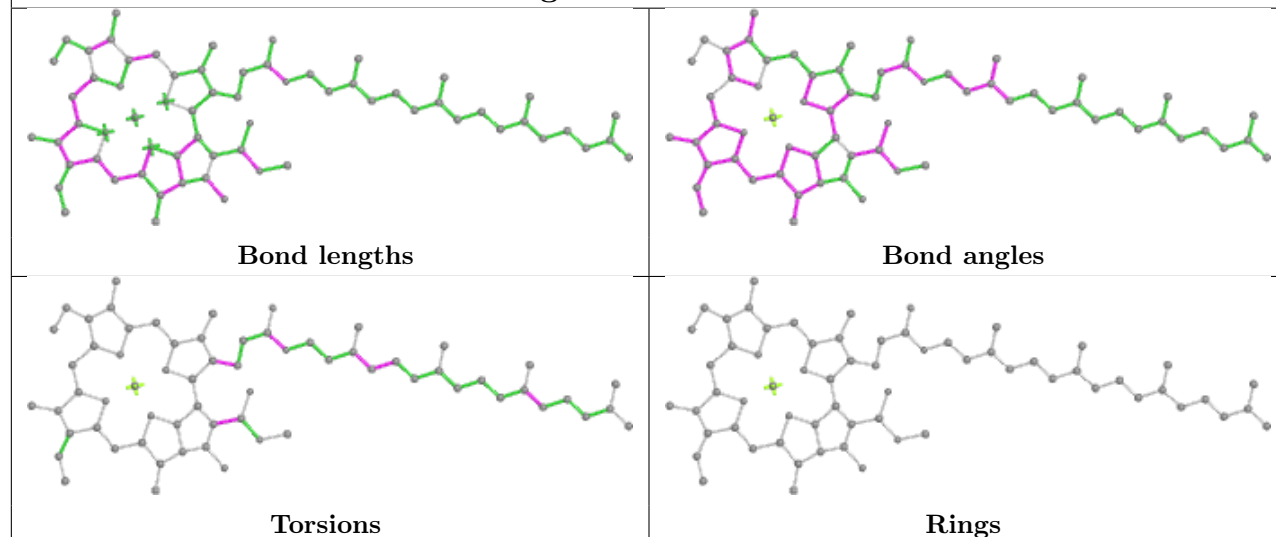
Ligand BCR a 849	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand LUT 6 317	
	Bond lengths
	Bond angles
	Torsions
	Rings

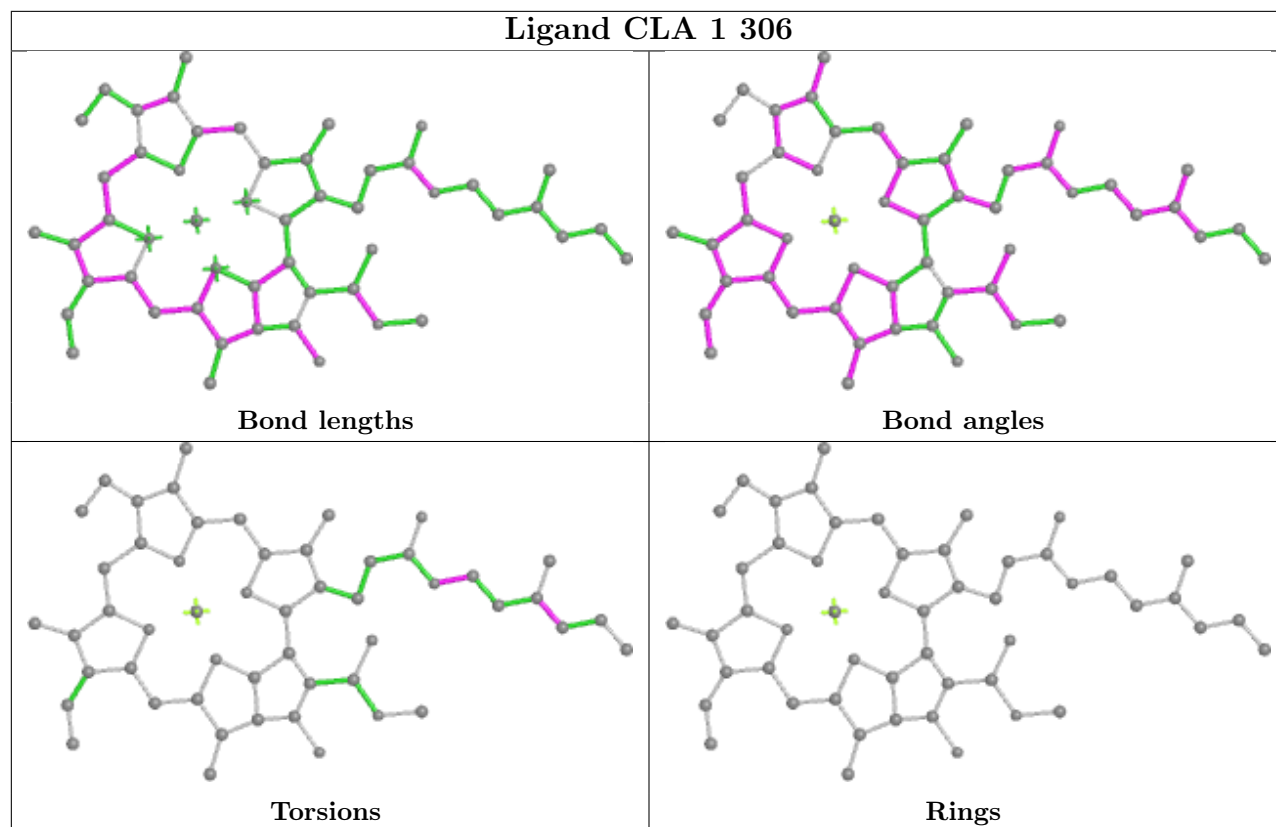
## Ligand CLA B 835



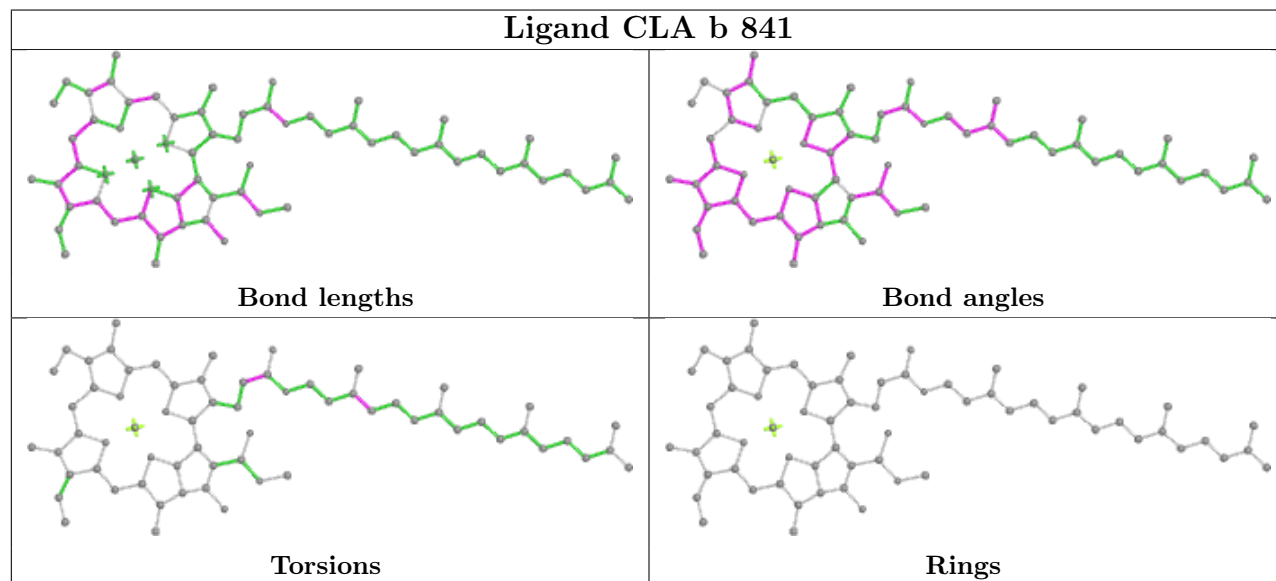
## Ligand CLA 1 202



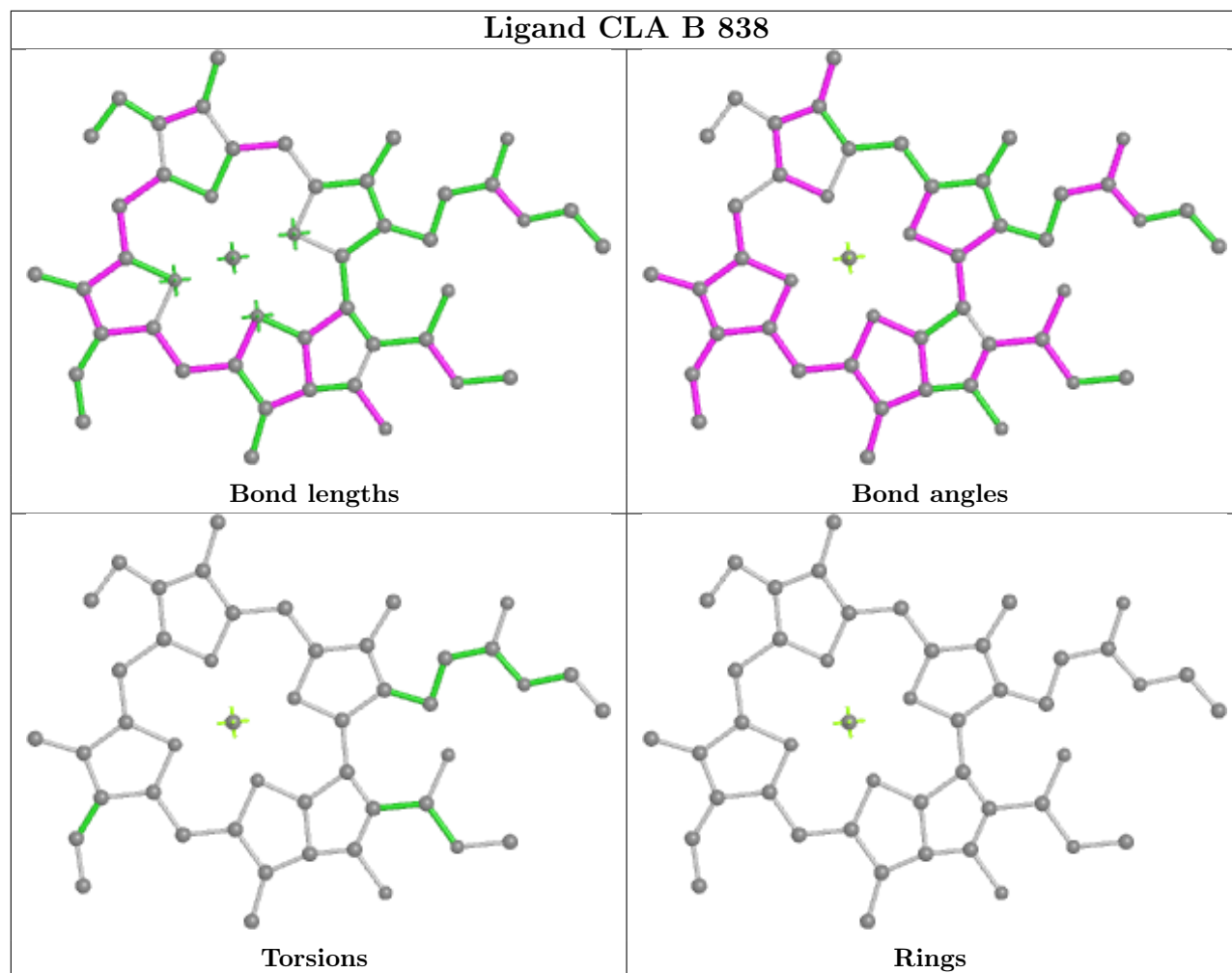
## Ligand CLA 1 306



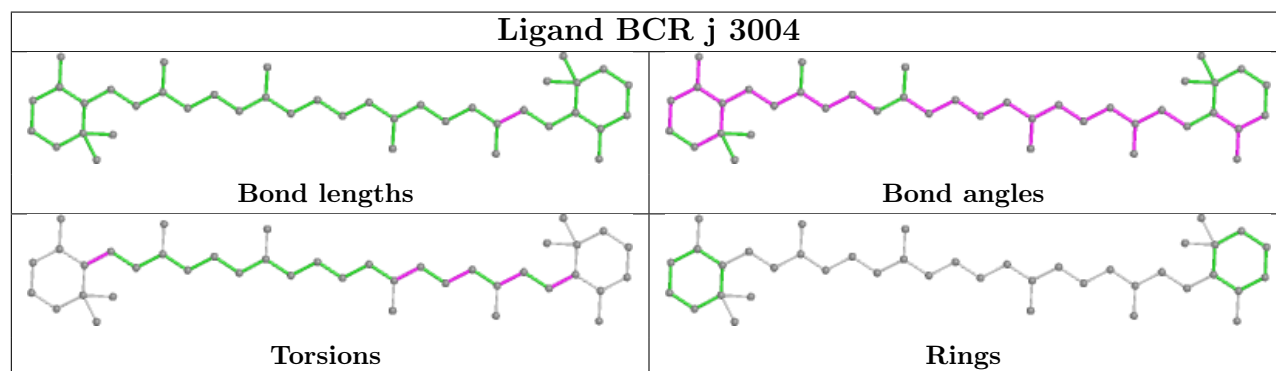
## Ligand CLA b 841



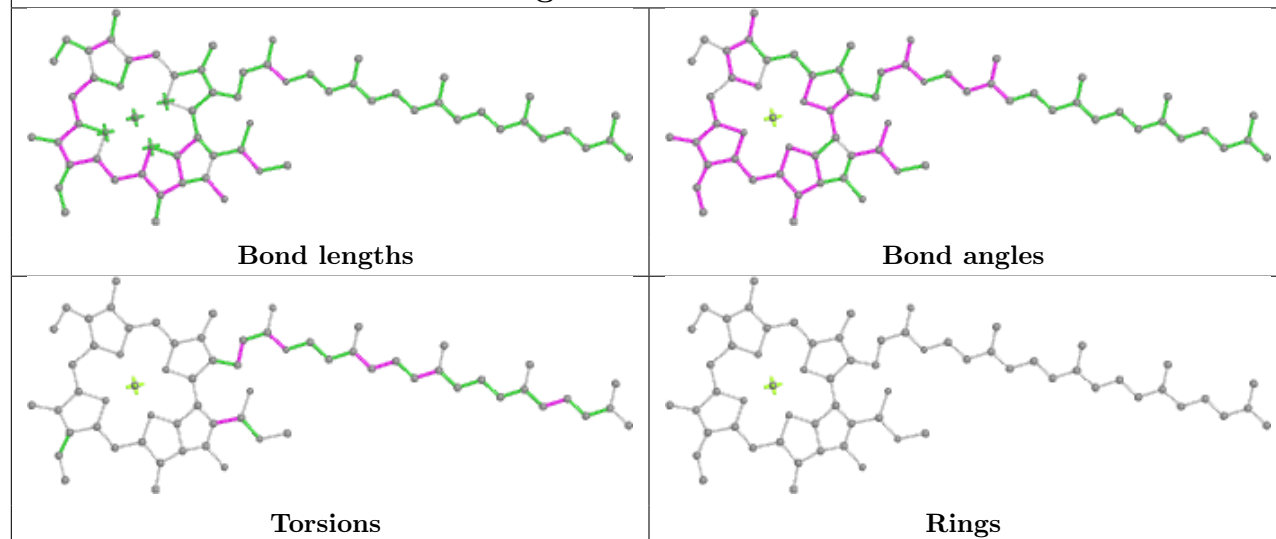
## Ligand CLA B 838



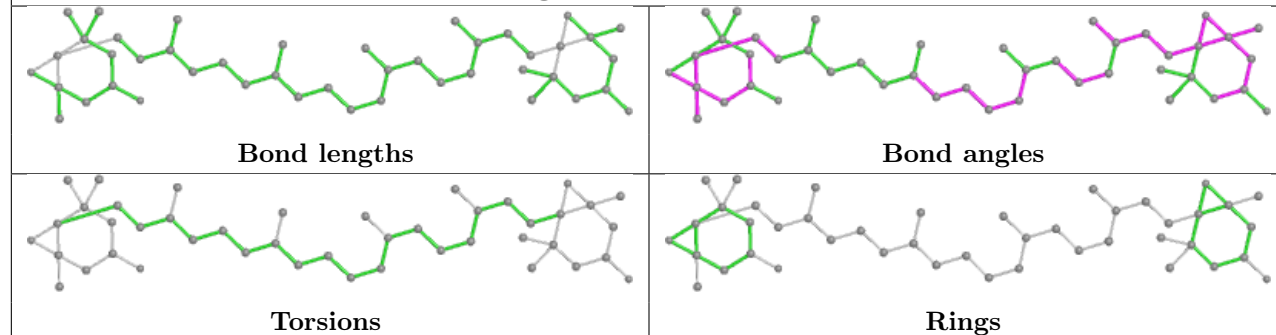
## Ligand BCR j 3004



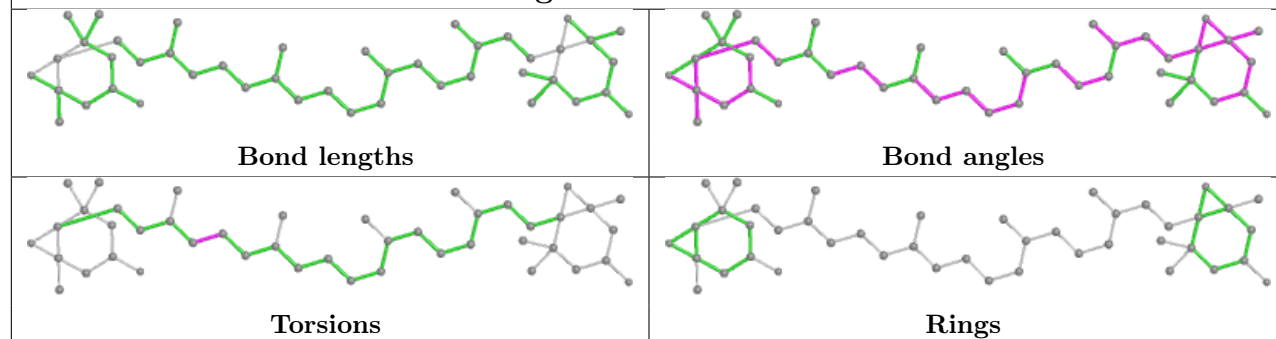
## Ligand CLA 1 303



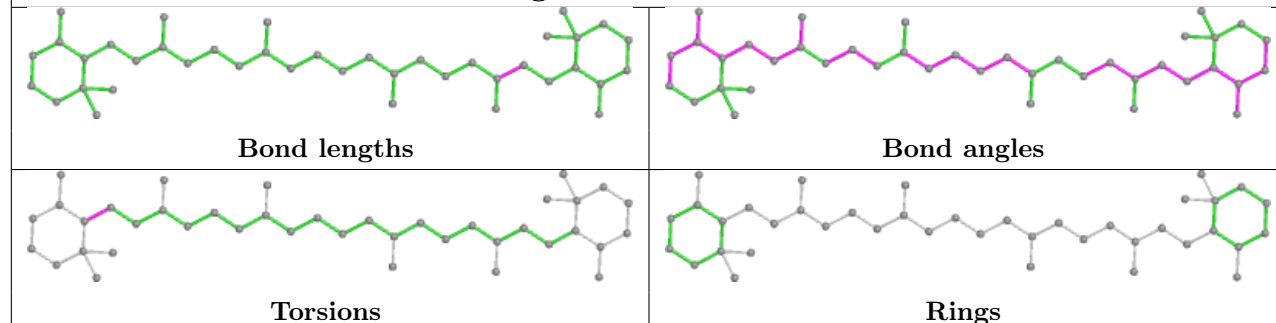
## Ligand XAT 4 617



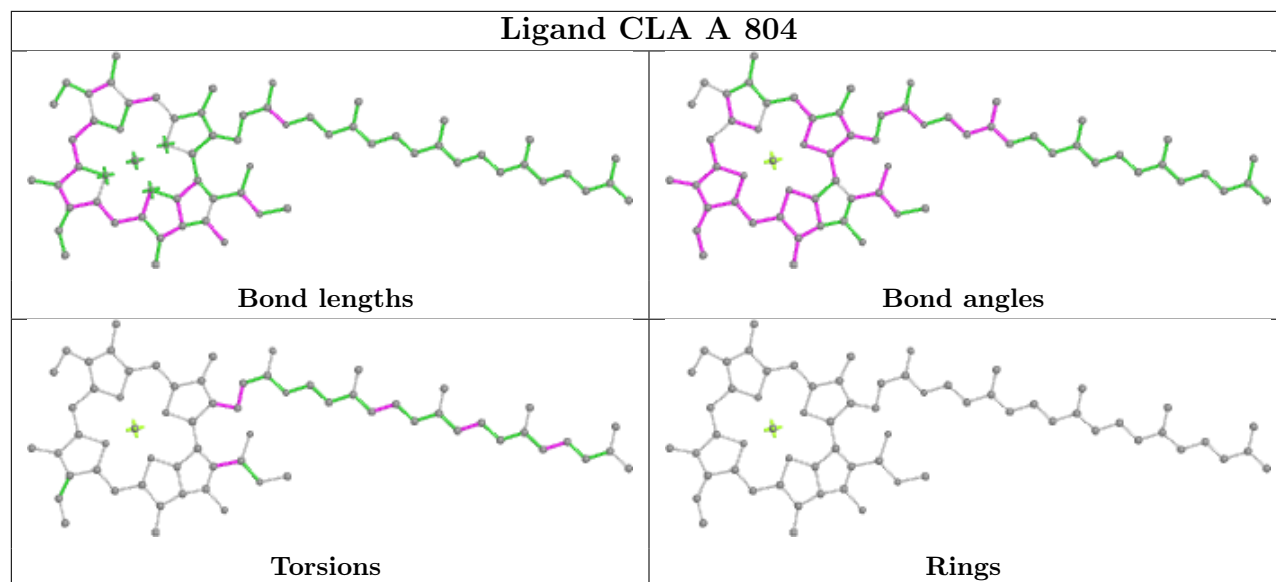
## Ligand XAT 7 616



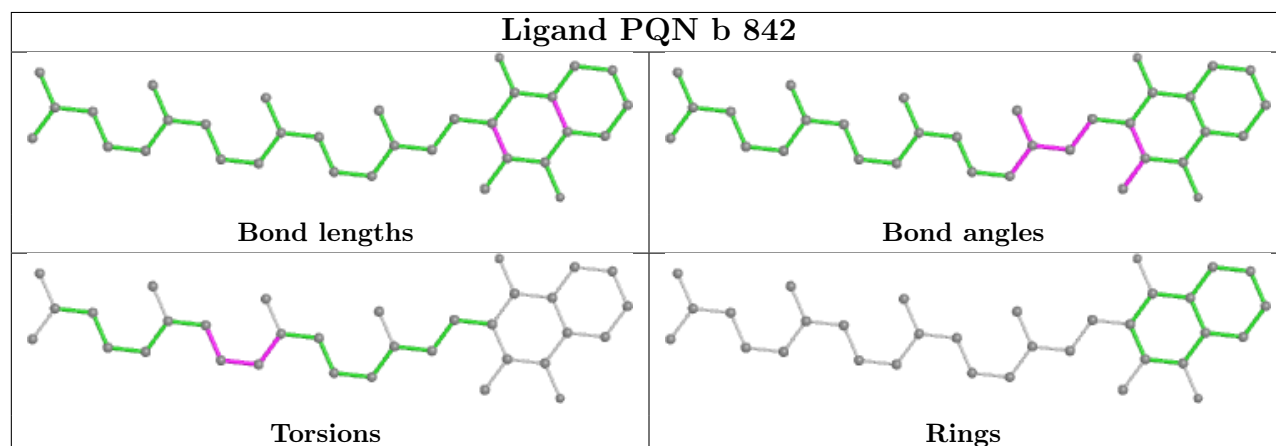
## Ligand BCR A 849



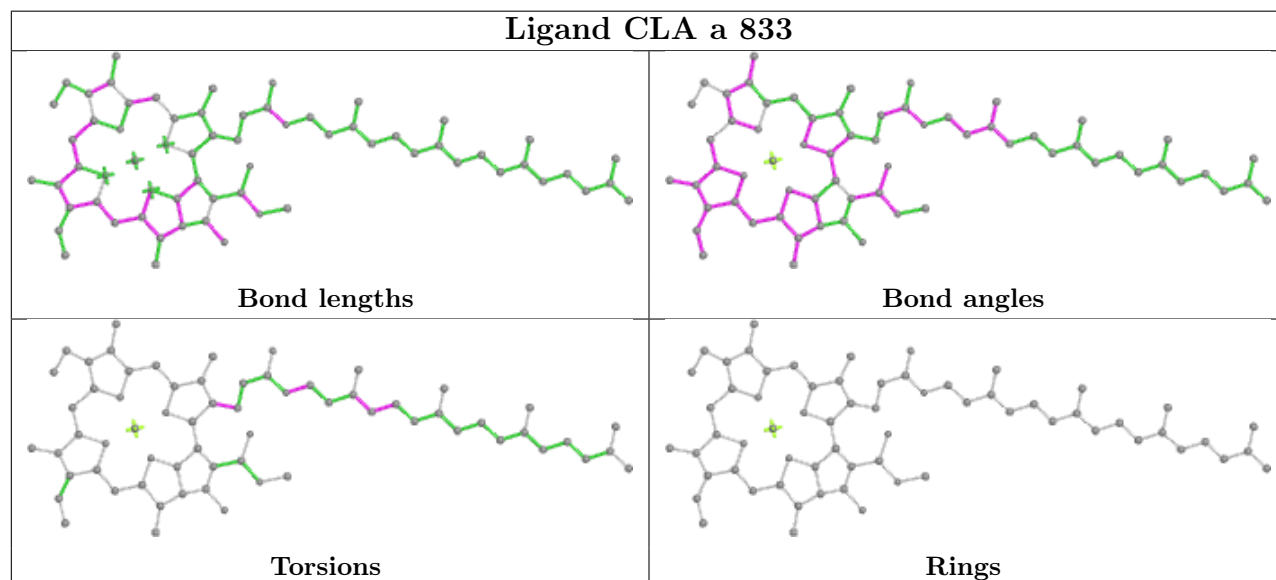
## Ligand CLA A 804

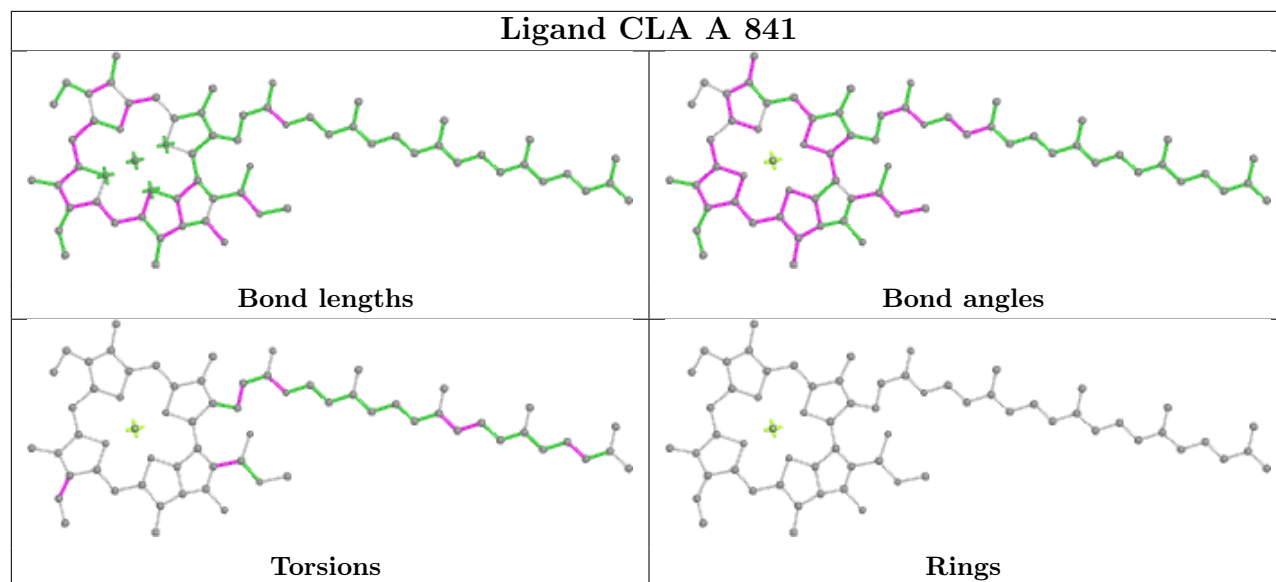


## Ligand PQN b 842



## Ligand CLA a 833





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	742/742 (100%)	-0.23	4 (0%) 87 83	42, 58, 91, 169	0
1	a	742/742 (100%)	-0.42	5 (0%) 84 79	36, 48, 81, 140	0
2	B	733/733 (100%)	-0.22	11 (1%) 71 64	42, 56, 80, 121	0
2	b	733/733 (100%)	-0.24	6 (0%) 82 77	36, 55, 86, 139	0
3	C	80/80 (100%)	-0.22	0 100 100	50, 62, 77, 96	0
3	c	80/80 (100%)	-0.12	0 100 100	44, 55, 72, 88	0
4	D	141/141 (100%)	-0.03	3 (2%) 63 55	53, 71, 103, 163	0
4	d	140/141 (99%)	-0.16	4 (2%) 54 45	45, 61, 92, 132	0
5	E	63/64 (98%)	-0.11	0 100 100	51, 77, 115, 127	0
5	e	63/64 (98%)	-0.09	0 100 100	51, 78, 96, 119	0
6	F	151/151 (100%)	-0.10	3 (1%) 64 56	50, 69, 98, 126	0
6	f	151/151 (100%)	-0.06	3 (1%) 64 56	49, 73, 101, 132	0
7	G	95/95 (100%)	-0.04	2 (2%) 63 55	60, 79, 103, 127	0
7	g	95/95 (100%)	0.30	6 (6%) 27 21	62, 83, 123, 171	0
8	H	90/90 (100%)	0.05	2 (2%) 62 53	61, 83, 116, 127	0
8	h	90/90 (100%)	0.01	4 (4%) 39 32	51, 70, 100, 111	0
9	I	29/30 (96%)	-0.18	1 (3%) 48 40	53, 65, 87, 117	0
9	i	30/30 (100%)	-0.40	2 (6%) 25 19	48, 56, 80, 129	0
10	J	39/39 (100%)	-0.31	1 (2%) 57 49	51, 62, 97, 100	0
10	j	39/39 (100%)	-0.06	1 (2%) 57 49	48, 65, 94, 100	0
11	K	45/84 (53%)	0.33	1 (2%) 62 53	92, 111, 131, 142	0
11	k	46/84 (54%)	0.36	2 (4%) 40 32	68, 86, 126, 134	0
12	L	153/153 (100%)	0.32	6 (3%) 44 36	56, 80, 120, 143	0
12	l	151/153 (98%)	-0.16	1 (0%) 84 79	42, 60, 87, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1	195/195 (100%)	0.16	8 (4%) 42 34	61, 87, 119, 136	0
13	6	195/195 (100%)	0.51	13 (6%) 25 19	74, 114, 164, 176	0
14	2	206/206 (100%)	0.37	9 (4%) 39 32	67, 97, 133, 188	0
14	7	206/206 (100%)	0.21	9 (4%) 39 32	61, 89, 122, 158	0
15	3	218/218 (100%)	0.20	4 (1%) 67 60	62, 96, 133, 154	0
15	8	217/218 (99%)	-0.03	3 (1%) 73 66	56, 81, 112, 142	0
16	4	196/196 (100%)	0.29	5 (2%) 57 49	61, 85, 115, 160	0
16	9	196/196 (100%)	0.39	11 (5%) 31 24	65, 97, 134, 155	0
All	All	6350/6434 (98%)	-0.07	130 (2%) 64 56	36, 68, 116, 188	0

The worst 5 of 130 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	2	87	GLU	6.2
16	9	164	GLY	5.4
16	9	122	ASN	5.3
7	g	35	VAL	4.5
7	G	35	VAL	4.5

## 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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
17	CLA	8	309	52/65	0.49	0.24	155,164,169,259	0
17	CLA	a	846	52/65	0.59	0.16	86,102,115,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
19	LHG	3	319	20/49	0.62	0.17	152,157,193,194	0
17	CLA	3	310	37/65	0.67	0.17	179,186,191,221	0
27	LUT	6	321	42/42	0.68	0.19	107,113,133,134	0
20	BCR	L	206	40/40	0.69	0.26	146,151,156,156	0
17	CLA	A	845	52/65	0.69	0.16	90,115,146,149	0
23	LMT	B	849	35/35	0.71	0.15	80,97,102,103	0
17	CLA	6	316	46/65	0.72	0.17	152,162,171,203	0
17	CLA	8	311	45/65	0.72	0.14	100,110,122,161	0
17	CLA	3	301	46/65	0.74	0.14	142,149,154,175	0
17	CLA	K	4002	45/65	0.75	0.15	115,123,125,154	0
17	CLA	8	313	25/65	0.75	0.15	102,110,116,146	0
25	LMG	6	302	40/55	0.76	0.19	116,148,163,164	0
25	LMG	4	620	44/55	0.76	0.16	89,97,111,113	0
17	CLA	3	311	52/65	0.78	0.14	129,142,154,157	0
17	CLA	L	202	65/65	0.78	0.18	83,111,131,132	0
17	CLA	l	202	65/65	0.81	0.17	57,88,111,113	0
17	CLA	6	309	46/65	0.81	0.16	92,99,106,137	0
17	CLA	6	310	65/65	0.81	0.14	80,90,121,126	0
17	CLA	k	1403	46/65	0.81	0.13	89,95,103,110	0
20	BCR	K	4004	40/40	0.81	0.17	94,115,138,138	0
20	BCR	2	617	40/40	0.82	0.23	125,133,163,164	0
20	BCR	6	319	40/40	0.82	0.18	104,124,138,140	0
20	BCR	7	617	40/40	0.82	0.22	112,119,127,128	0
17	CLA	9	611	52/65	0.82	0.12	76,89,102,103	0
17	CLA	J	3002	42/65	0.82	0.12	92,105,119,148	0
17	CLA	3	313	45/65	0.82	0.12	85,97,102,106	0
26	CHL	6	308	47/66	0.82	0.14	103,135,146,149	0
17	CLA	7	611	52/65	0.82	0.13	87,104,123,126	0
17	CLA	B	811	54/65	0.83	0.14	58,74,103,104	0
20	BCR	A	856	40/40	0.83	0.14	65,71,85,85	0
17	CLA	j	3002	42/65	0.83	0.11	91,94,96,97	0
26	CHL	9	615	43/66	0.83	0.15	90,144,147,148	0
17	CLA	3	315	25/65	0.83	0.13	112,115,121,157	0
17	CLA	2	604	60/65	0.84	0.14	100,111,118,119	0
17	CLA	b	811	54/65	0.84	0.13	50,74,114,114	0
25	LMG	G	102	44/55	0.84	0.13	72,95,110,113	0
25	LMG	4	619	44/55	0.84	0.16	82,92,103,104	0
20	BCR	1	318	40/40	0.84	0.18	94,105,126,127	0
17	CLA	g	101	41/65	0.84	0.16	146,164,166,167	0
26	CHL	2	606	48/66	0.84	0.12	89,97,105,107	0
20	BCR	k	1404	40/40	0.84	0.14	49,89,103,104	0
20	BCR	l	206	40/40	0.84	0.16	77,82,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
17	CLA	1	309	65/65	0.84	0.15	71,79,106,108	0
17	CLA	2	608	50/65	0.85	0.13	65,69,108,111	0
17	CLA	2	613	43/65	0.85	0.12	80,88,94,95	0
20	BCR	b	844	40/40	0.85	0.15	52,67,91,93	0
20	BCR	A	848	40/40	0.85	0.15	50,59,95,95	0
25	LMG	9	619	50/55	0.85	0.15	68,88,96,98	0
17	CLA	A	824	51/65	0.85	0.14	77,89,118,118	0
20	BCR	K	4001	40/40	0.85	0.18	91,94,96,96	0
17	CLA	6	312	41/65	0.85	0.14	90,102,109,129	0
27	LUT	4	616	42/42	0.85	0.16	71,90,94,95	0
17	CLA	6	313	52/65	0.85	0.14	83,94,119,120	0
28	XAT	9	617	44/44	0.85	0.14	72,81,97,98	0
17	CLA	K	4003	46/65	0.86	0.14	81,119,128,130	0
17	CLA	k	1401	45/65	0.86	0.11	75,83,94,96	0
17	CLA	2	609	60/65	0.86	0.13	73,87,98,101	0
19	LHG	A	847	27/49	0.86	0.12	68,88,113,113	0
20	BCR	b	843	40/40	0.86	0.14	54,60,68,69	0
26	CHL	2	605	43/66	0.86	0.11	77,89,100,106	0
17	CLA	2	610	41/65	0.86	0.12	80,94,108,110	0
26	CHL	2	614	43/66	0.86	0.14	116,134,143,145	0
19	LHG	a	848	27/49	0.86	0.16	74,95,125,127	0
26	CHL	7	605	43/66	0.86	0.12	85,89,93,99	0
26	CHL	7	606	48/66	0.86	0.11	71,87,104,105	0
26	CHL	7	614	43/66	0.86	0.14	105,120,127,139	0
17	CLA	7	604	60/65	0.86	0.14	92,101,106,109	0
17	CLA	l	204	50/65	0.86	0.13	46,59,100,104	0
27	LUT	6	317	42/42	0.86	0.16	86,93,118,120	0
20	BCR	I	101	40/40	0.86	0.12	54,60,65,65	0
17	CLA	A	837	45/65	0.86	0.11	84,95,103,165	0
17	CLA	k	1402	46/65	0.87	0.11	62,78,100,106	0
20	BCR	a	849	40/40	0.87	0.14	56,63,75,76	0
17	CLA	1	315	46/65	0.87	0.09	76,87,93,132	0
17	CLA	f	7003	55/65	0.87	0.12	68,87,121,122	0
20	BCR	j	3004	40/40	0.87	0.12	56,71,82,84	0
27	LUT	1	320	42/42	0.87	0.12	71,79,90,91	0
17	CLA	F	304	55/65	0.87	0.11	52,69,95,95	0
17	CLA	4	604	50/65	0.87	0.14	75,84,111,114	0
17	CLA	1	312	52/65	0.87	0.12	70,76,99,100	0
19	LHG	6	320	49/49	0.87	0.17	90,100,111,113	0
20	BCR	a	852	40/40	0.88	0.12	40,62,120,120	0
20	BCR	8	316	40/40	0.88	0.16	66,71,88,90	0
26	CHL	4	615	43/66	0.88	0.10	61,74,87,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
26	CHL	6	303	61/66	0.88	0.13	78,91,102,103	0
22	HTG	J	3001	19/19	0.88	0.11	73,76,78,82	0
22	HTG	f	7001	19/19	0.88	0.14	49,104,107,108	0
17	CLA	9	604	50/65	0.88	0.13	105,116,125,126	0
24	DGD	b	849	66/66	0.88	0.13	41,64,90,91	0
17	CLA	B	821	46/65	0.88	0.12	51,60,72,80	0
20	BCR	g	104	40/40	0.88	0.14	57,102,117,118	0
17	CLA	L	204	50/65	0.88	0.13	76,84,109,109	0
17	CLA	g	102	50/65	0.88	0.12	92,107,123,124	0
20	BCR	4	618	40/40	0.88	0.16	79,86,89,90	0
17	CLA	g	103	46/65	0.88	0.11	87,99,103,116	0
17	CLA	7	610	41/65	0.89	0.11	74,82,94,99	0
17	CLA	3	305	42/65	0.89	0.09	67,78,84,90	0
26	CHL	2	601	61/66	0.89	0.14	68,99,113,115	0
20	BCR	b	846	40/40	0.89	0.11	48,56,76,77	0
19	LHG	7	618	37/49	0.89	0.15	83,95,102,104	0
17	CLA	7	613	43/65	0.89	0.10	73,78,82,86	0
26	CHL	4	605	56/66	0.89	0.12	69,88,96,102	0
17	CLA	8	308	50/65	0.89	0.11	75,81,87,88	0
20	BCR	B	845	40/40	0.89	0.12	47,63,102,102	0
20	BCR	B	846	40/40	0.89	0.12	49,53,70,70	0
17	CLA	4	610	55/65	0.89	0.11	72,88,94,122	0
17	CLA	G	104	46/65	0.89	0.10	70,93,100,111	0
17	CLA	2	611	52/65	0.89	0.11	68,83,119,128	0
26	CHL	9	606	51/66	0.89	0.13	86,106,118,119	0
17	CLA	b	817	59/65	0.89	0.12	56,59,67,68	0
17	CLA	6	315	55/65	0.89	0.12	105,114,131,131	0
17	CLA	9	613	45/65	0.89	0.12	87,105,115,137	0
17	CLA	9	614	47/65	0.89	0.10	62,75,97,99	0
17	CLA	1	314	55/65	0.89	0.12	78,93,105,110	0
27	LUT	7	615	42/42	0.89	0.13	72,83,97,98	0
17	CLA	1	310	60/65	0.89	0.12	63,80,90,92	0
20	BCR	9	618	40/40	0.90	0.13	86,92,100,101	0
22	HTG	F	302	19/19	0.90	0.16	43,98,105,107	0
17	CLA	b	835	45/65	0.90	0.10	86,92,94,96	0
17	CLA	A	816	50/65	0.90	0.10	52,70,108,108	0
22	HTG	j	3001	19/19	0.90	0.10	61,71,80,84	0
17	CLA	A	823	49/65	0.90	0.10	66,79,104,105	0
20	BCR	A	850	40/40	0.90	0.12	53,72,112,112	0
17	CLA	1	311	41/65	0.90	0.11	67,74,81,82	0
17	CLA	7	608	50/65	0.90	0.13	60,65,93,96	0
17	CLA	7	609	60/65	0.90	0.12	64,86,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
17	CLA	B	812	55/65	0.90	0.11	53,62,106,107	0
17	CLA	B	817	59/65	0.90	0.11	46,53,59,64	0
17	CLA	4	609	60/65	0.90	0.12	69,86,106,111	0
17	CLA	8	303	45/65	0.90	0.12	75,92,99,133	0
17	CLA	A	805	55/65	0.90	0.11	45,54,89,89	0
17	CLA	4	611	52/65	0.90	0.10	71,88,123,125	0
17	CLA	a	824	51/65	0.90	0.10	61,74,91,93	0
26	CHL	4	606	51/66	0.90	0.11	71,81,109,110	0
17	CLA	3	304	45/65	0.90	0.13	109,122,133,162	0
17	CLA	9	603	46/65	0.90	0.10	62,64,77,78	0
17	CLA	6	305	65/65	0.90	0.14	83,87,104,110	0
17	CLA	6	306	51/65	0.90	0.13	118,123,130,131	0
20	BCR	b	845	40/40	0.90	0.13	46,67,106,106	0
17	CLA	9	612	56/65	0.90	0.10	68,77,89,92	0
26	CHL	9	605	56/66	0.90	0.12	80,94,97,126	0
17	CLA	6	307	42/65	0.90	0.12	112,126,137,139	0
26	CHL	9	607	51/66	0.90	0.12	67,77,98,99	0
20	BCR	j	3003	40/40	0.90	0.11	42,52,59,61	0
17	CLA	A	808	65/65	0.90	0.11	52,61,113,115	0
27	LUT	3	316	42/42	0.90	0.11	74,78,97,99	0
17	CLA	b	815	55/65	0.90	0.11	62,78,93,94	0
19	LHG	1	301	23/49	0.90	0.14	63,84,93,94	0
19	LHG	1	319	49/49	0.90	0.14	77,84,109,109	0
17	CLA	6	311	60/65	0.90	0.12	81,99,115,116	0
27	LUT	8	314	42/42	0.90	0.11	57,73,82,84	0
27	LUT	9	616	42/42	0.90	0.13	68,79,103,104	0
28	XAT	7	616	44/44	0.90	0.13	57,64,73,74	0
28	XAT	8	315	44/44	0.90	0.12	64,69,80,83	0
17	CLA	3	309	50/65	0.90	0.12	76,95,104,107	0
17	CLA	a	816	50/65	0.91	0.11	43,52,94,96	0
17	CLA	a	817	45/65	0.91	0.10	64,73,78,79	0
22	HTG	A	855	19/19	0.91	0.09	68,72,74,75	0
19	LHG	2	618	37/49	0.91	0.13	80,91,127,130	0
17	CLA	a	823	49/65	0.91	0.10	60,67,102,104	0
22	HTG	a	857	19/19	0.91	0.08	53,70,79,81	0
17	CLA	A	822	65/65	0.91	0.12	49,67,76,79	0
19	LHG	6	301	23/49	0.91	0.12	67,101,110,111	0
17	CLA	3	303	50/65	0.91	0.10	60,67,75,76	0
24	DGD	B	850	66/66	0.91	0.12	52,71,93,102	0
17	CLA	b	807	65/65	0.91	0.12	42,51,102,104	0
17	CLA	B	816	55/65	0.91	0.12	60,67,73,91	0
17	CLA	b	812	55/65	0.91	0.12	59,70,103,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	BCR	A	851	40/40	0.91	0.12	43,66,78,79	0
17	CLA	b	814	65/65	0.91	0.10	47,55,69,71	0
20	BCR	B	801	40/40	0.91	0.12	43,46,54,55	0
26	CHL	1	307	48/66	0.91	0.12	75,95,109,110	0
20	BCR	B	843	40/40	0.91	0.12	54,64,72,72	0
20	BCR	B	844	40/40	0.91	0.13	50,53,85,87	0
17	CLA	A	832	50/65	0.91	0.11	52,70,98,99	0
26	CHL	2	607	51/66	0.91	0.12	66,75,117,118	0
17	CLA	b	816	55/65	0.91	0.10	57,65,72,75	0
20	BCR	G	105	40/40	0.91	0.12	63,71,83,83	0
17	CLA	B	807	65/65	0.91	0.13	51,66,113,117	0
17	CLA	b	820	50/65	0.91	0.12	65,72,77,82	0
17	CLA	b	821	46/65	0.91	0.11	58,69,90,118	0
17	CLA	b	834	65/65	0.91	0.10	61,74,105,106	0
26	CHL	7	601	61/66	0.91	0.11	62,74,93,95	0
17	CLA	B	835	45/65	0.91	0.09	57,66,70,72	0
17	CLA	8	304	42/65	0.91	0.10	59,72,78,80	0
20	BCR	3	318	40/40	0.91	0.13	77,83,105,108	0
17	CLA	2	603	65/65	0.91	0.11	64,72,106,108	0
17	CLA	3	312	55/65	0.91	0.11	86,107,114,117	0
17	CLA	8	310	55/65	0.91	0.10	74,88,99,104	0
17	CLA	L	203	65/65	0.91	0.12	64,74,87,89	0
27	LUT	1	316	42/42	0.91	0.12	69,74,100,101	0
17	CLA	3	314	46/65	0.91	0.10	73,78,101,103	0
27	LUT	2	615	42/42	0.91	0.12	77,84,89,89	0
17	CLA	A	835	65/65	0.91	0.13	58,67,75,81	0
17	CLA	4	603	46/65	0.91	0.11	54,62,69,72	0
17	CLA	9	609	60/65	0.91	0.12	72,93,107,108	0
20	BCR	i	101	40/40	0.91	0.10	36,45,49,50	0
17	CLA	9	610	41/65	0.91	0.11	99,103,113,114	0
17	CLA	1	304	65/65	0.91	0.12	63,70,95,97	0
17	CLA	1	305	52/65	0.91	0.11	76,101,105,108	0
28	XAT	3	317	44/44	0.91	0.14	61,74,100,101	0
28	XAT	4	617	44/44	0.91	0.12	63,72,87,88	0
28	XAT	6	318	44/44	0.91	0.12	71,81,94,95	0
17	CLA	1	308	65/65	0.91	0.14	57,92,120,121	0
17	CLA	G	101	45/65	0.91	0.10	74,79,85,89	0
17	CLA	4	613	45/65	0.91	0.11	92,103,108,160	0
17	CLA	3	308	50/65	0.92	0.11	76,86,93,104	0
17	CLA	B	815	60/65	0.92	0.12	60,72,100,102	0
17	CLA	A	834	65/65	0.92	0.10	49,60,71,75	0
17	CLA	b	818	60/65	0.92	0.10	44,47,53,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
17	CLA	1	306	52/65	0.92	0.10	90,99,109,111	0
20	BCR	F	305	40/40	0.92	0.10	46,51,58,60	0
17	CLA	A	818	65/65	0.92	0.11	58,71,95,97	0
17	CLA	b	830	50/65	0.92	0.10	46,59,70,74	0
20	BCR	J	3003	40/40	0.92	0.10	45,54,67,68	0
26	CHL	1	302	61/66	0.92	0.11	64,74,101,105	0
17	CLA	b	831	49/65	0.92	0.10	51,55,71,71	0
17	CLA	b	832	65/65	0.92	0.11	36,55,70,79	0
20	BCR	L	201	40/40	0.92	0.11	51,59,72,73	0
17	CLA	B	818	60/65	0.92	0.10	45,50,57,61	0
17	CLA	A	836	50/65	0.92	0.10	60,73,80,86	0
17	CLA	b	841	65/65	0.92	0.12	64,80,92,94	0
26	CHL	3	307	47/66	0.92	0.10	72,77,94,97	0
17	CLA	9	601	46/65	0.92	0.11	81,91,95,110	0
17	CLA	B	822	55/65	0.92	0.10	48,58,82,83	0
26	CHL	4	607	51/66	0.92	0.12	57,73,82,85	0
17	CLA	4	601	46/65	0.92	0.10	84,92,95,111	0
20	BCR	a	850	40/40	0.92	0.10	39,48,79,81	0
20	BCR	a	851	40/40	0.92	0.09	37,53,66,67	0
17	CLA	B	823	60/65	0.92	0.10	46,57,84,84	0
20	BCR	a	853	40/40	0.92	0.12	44,48,66,67	0
17	CLA	B	834	65/65	0.92	0.11	46,58,90,90	0
26	CHL	7	607	51/66	0.92	0.12	64,70,92,98	0
17	CLA	A	810	65/65	0.92	0.10	43,51,85,89	0
26	CHL	8	306	47/66	0.92	0.10	60,64,79,84	0
17	CLA	F	301	65/65	0.92	0.12	48,55,83,87	0
17	CLA	A	839	65/65	0.92	0.11	54,60,80,83	0
20	BCR	b	847	40/40	0.92	0.09	40,49,69,70	0
20	BCR	f	7004	40/40	0.92	0.10	55,62,66,66	0
17	CLA	A	840	65/65	0.92	0.11	48,55,95,96	0
17	CLA	a	804	65/65	0.92	0.10	36,52,71,73	0
17	CLA	a	809	65/65	0.92	0.10	36,39,53,57	0
17	CLA	A	841	65/65	0.92	0.10	44,50,55,60	0
17	CLA	A	813	54/65	0.92	0.10	60,68,77,95	0
20	BCR	l	205	40/40	0.92	0.10	39,46,52,54	0
17	CLA	A	804	65/65	0.92	0.10	46,58,70,71	0
17	CLA	2	612	65/65	0.92	0.12	70,93,113,118	0
17	CLA	a	843	65/65	0.92	0.10	35,39,60,65	0
17	CLA	B	810	65/65	0.92	0.12	59,77,84,86	0
28	XAT	2	616	44/44	0.92	0.12	69,79,86,87	0
17	CLA	A	817	45/65	0.92	0.10	66,75,86,92	0
17	CLA	b	810	65/65	0.92	0.10	39,49,59,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	BCR	A	849	40/40	0.92	0.11	54,62,83,84	0
17	CLA	A	833	65/65	0.92	0.10	54,61,101,102	0
17	CLA	B	814	65/65	0.92	0.10	50,57,80,82	0
17	CLA	1	303	65/65	0.92	0.12	60,67,83,90	0
17	CLA	a	838	51/65	0.93	0.10	36,40,63,68	0
17	CLA	a	839	65/65	0.93	0.10	36,43,65,69	0
17	CLA	a	842	65/65	0.93	0.12	47,59,96,98	0
17	CLA	A	821	45/65	0.93	0.09	69,74,88,109	0
17	CLA	A	811	65/65	0.93	0.10	54,69,89,90	0
17	CLA	2	602	65/65	0.93	0.11	66,73,80,83	0
17	CLA	B	825	65/65	0.93	0.12	42,50,83,88	0
17	CLA	B	827	65/65	0.93	0.12	49,61,78,80	0
20	BCR	B	847	40/40	0.93	0.10	44,49,52,53	0
20	BCR	B	848	40/40	0.93	0.10	40,45,51,52	0
17	CLA	7	602	65/65	0.93	0.11	62,70,88,93	0
17	CLA	7	603	51/65	0.93	0.10	52,60,97,98	0
17	CLA	B	829	65/65	0.93	0.11	42,50,76,77	0
17	CLA	B	832	65/65	0.93	0.11	43,48,73,76	0
17	CLA	B	833	58/65	0.93	0.10	43,52,79,80	0
17	CLA	A	812	65/65	0.93	0.10	49,63,74,82	0
17	CLA	4	608	50/65	0.93	0.10	56,66,76,86	0
20	BCR	L	205	40/40	0.93	0.10	51,61,70,71	0
17	CLA	A	819	65/65	0.93	0.12	54,65,117,120	0
17	CLA	8	302	50/65	0.93	0.09	46,54,73,74	0
17	CLA	B	836	60/65	0.93	0.11	43,46,97,97	0
17	CLA	B	803	65/65	0.93	0.10	39,50,61,68	0
17	CLA	b	822	55/65	0.93	0.08	46,60,80,83	0
17	CLA	b	823	60/65	0.93	0.10	50,60,92,94	0
17	CLA	b	829	65/65	0.93	0.10	39,54,67,69	0
17	CLA	4	612	56/65	0.93	0.10	63,78,87,88	0
17	CLA	8	312	46/65	0.93	0.09	57,66,99,103	0
17	CLA	3	302	60/65	0.93	0.10	67,79,85,95	0
17	CLA	4	614	50/65	0.93	0.10	60,68,90,91	0
17	CLA	9	602	60/65	0.93	0.10	60,67,74,86	0
17	CLA	b	833	58/65	0.93	0.11	48,63,77,78	0
17	CLA	a	802	65/65	0.93	0.10	35,42,56,62	0
17	CLA	A	825	55/65	0.93	0.09	58,67,74,78	0
20	BCR	b	848	40/40	0.93	0.10	37,42,45,47	0
17	CLA	b	836	60/65	0.93	0.10	43,53,106,107	0
17	CLA	a	808	65/65	0.93	0.10	54,63,86,87	0
17	CLA	B	809	65/65	0.93	0.11	41,50,81,82	0
17	CLA	a	810	65/65	0.93	0.10	44,59,94,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
17	CLA	a	812	65/65	0.93	0.11	47,59,70,77	0
17	CLA	G	103	50/65	0.93	0.10	61,80,91,93	0
20	BCR	l	201	40/40	0.93	0.10	38,46,54,54	0
17	CLA	3	306	47/65	0.93	0.09	67,79,90,91	0
17	CLA	a	819	65/65	0.93	0.12	38,54,96,99	0
17	CLA	a	821	45/65	0.93	0.09	51,62,70,87	0
28	XAT	1	317	44/44	0.93	0.12	63,68,93,96	0
17	CLA	a	822	65/65	0.93	0.09	42,46,53,57	0
17	CLA	A	828	65/65	0.93	0.10	49,61,79,84	0
17	CLA	l	203	65/65	0.93	0.09	40,51,71,73	0
17	CLA	1	313	65/65	0.93	0.12	81,88,108,112	0
17	CLA	6	304	65/65	0.93	0.13	66,79,104,106	0
17	CLA	a	827	65/65	0.93	0.10	35,41,82,85	0
17	CLA	a	837	45/65	0.93	0.08	57,65,74,77	0
17	CLA	A	854	65/65	0.94	0.11	40,44,57,59	0
17	CLA	B	802	65/65	0.94	0.10	40,44,50,52	0
17	CLA	A	815	45/65	0.94	0.09	54,59,65,70	0
17	CLA	8	305	47/65	0.94	0.09	61,71,78,79	0
17	CLA	4	602	60/65	0.94	0.10	54,67,73,74	0
17	CLA	B	804	45/65	0.94	0.08	44,50,68,77	0
17	CLA	a	828	65/65	0.94	0.11	37,44,67,72	0
17	CLA	b	837	65/65	0.94	0.10	46,57,69,70	0
17	CLA	a	829	65/65	0.94	0.09	35,41,56,58	0
17	CLA	a	833	65/65	0.94	0.10	39,46,98,102	0
17	CLA	a	834	65/65	0.94	0.09	37,44,48,50	0
17	CLA	a	836	50/65	0.94	0.08	42,54,73,74	0
17	CLA	B	824	65/65	0.94	0.10	48,53,70,74	0
17	CLA	B	806	65/65	0.94	0.09	43,52,60,64	0
17	CLA	9	608	50/65	0.94	0.11	72,78,103,105	0
17	CLA	A	820	65/65	0.94	0.09	46,50,57,58	0
17	CLA	A	826	65/65	0.94	0.10	47,57,65,66	0
17	CLA	B	830	50/65	0.94	0.09	45,56,75,75	0
20	BCR	b	801	40/40	0.94	0.08	36,43,52,55	0
17	CLA	B	831	49/65	0.94	0.09	45,53,62,65	0
17	CLA	b	806	65/65	0.94	0.09	39,43,52,65	0
17	CLA	A	827	65/65	0.94	0.11	40,60,97,98	0
18	PQN	A	844	33/33	0.94	0.10	42,45,57,58	0
18	PQN	B	842	33/33	0.94	0.10	46,56,63,63	0
18	PQN	a	845	33/33	0.94	0.10	35,48,54,58	0
17	CLA	b	809	65/65	0.94	0.10	39,50,72,75	0
17	CLA	A	802	65/65	0.94	0.11	41,45,51,53	0
17	CLA	A	829	65/65	0.94	0.09	42,46,55,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
17	CLA	A	809	65/65	0.94	0.09	44,51,63,65	0
17	CLA	b	813	65/65	0.94	0.10	44,57,67,69	0
17	CLA	A	842	65/65	0.94	0.09	42,45,56,65	0
17	CLA	B	838	47/65	0.94	0.09	43,48,65,68	0
17	CLA	B	839	65/65	0.94	0.10	53,60,69,72	0
17	CLA	a	811	65/65	0.94	0.10	42,59,94,96	0
17	CLA	6	314	60/65	0.94	0.12	66,109,124,125	0
17	CLA	B	841	65/65	0.94	0.10	49,56,63,68	0
17	CLA	a	813	54/65	0.94	0.09	43,51,60,70	0
17	CLA	a	815	45/65	0.94	0.08	41,54,63,63	0
20	BCR	A	852	40/40	0.94	0.09	42,44,49,50	0
17	CLA	A	843	65/65	0.94	0.10	48,64,79,81	0
17	CLA	F	303	45/65	0.94	0.08	51,60,71,76	0
17	CLA	b	825	65/65	0.94	0.11	38,55,82,83	0
17	CLA	b	826	65/65	0.94	0.10	48,55,59,62	0
17	CLA	b	828	65/65	0.94	0.10	41,47,56,56	0
17	CLA	a	818	65/65	0.94	0.11	45,53,81,83	0
17	CLA	7	612	65/65	0.94	0.09	56,66,87,89	0
17	CLA	A	814	65/65	0.94	0.10	50,59,67,68	0
19	LHG	A	846	49/49	0.95	0.09	44,49,58,59	0
17	CLA	a	840	65/65	0.95	0.10	36,41,87,89	0
17	CLA	a	841	65/65	0.95	0.10	55,62,65,67	0
20	BCR	a	854	40/40	0.95	0.07	35,40,47,47	0
17	CLA	B	820	50/65	0.95	0.09	53,69,95,100	0
17	CLA	A	830	65/65	0.95	0.08	45,53,58,61	0
17	CLA	a	844	65/65	0.95	0.09	38,49,59,64	0
19	LHG	a	847	49/49	0.95	0.09	35,41,47,48	0
17	CLA	A	831	65/65	0.95	0.08	43,52,59,61	0
17	CLA	a	856	65/65	0.95	0.09	36,41,56,59	0
17	CLA	b	804	45/65	0.95	0.07	42,52,68,75	0
17	CLA	A	806	65/65	0.95	0.08	46,51,59,59	0
17	CLA	b	838	47/65	0.95	0.07	38,44,54,64	0
17	CLA	b	839	65/65	0.95	0.08	38,44,50,53	0
17	CLA	8	301	60/65	0.95	0.09	56,64,68,72	0
17	CLA	b	840	65/65	0.95	0.08	36,41,59,67	0
17	CLA	A	838	51/65	0.95	0.09	45,60,67,68	0
17	CLA	f	7002	45/65	0.95	0.07	54,59,76,77	0
17	CLA	b	808	65/65	0.95	0.09	39,47,53,59	0
17	CLA	8	307	50/65	0.95	0.10	52,65,91,93	0
17	CLA	B	808	65/65	0.95	0.09	41,45,70,73	0
17	CLA	a	805	55/65	0.95	0.09	38,43,76,78	0
17	CLA	a	806	65/65	0.95	0.08	37,39,49,51	0

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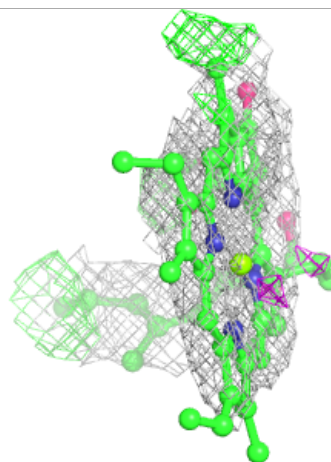
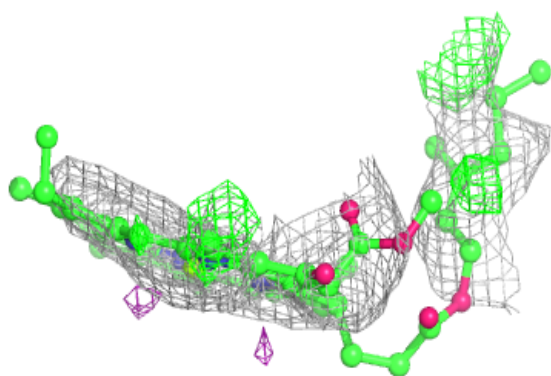
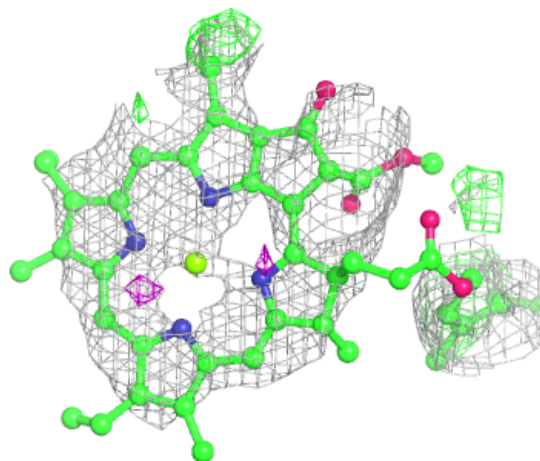
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
17	CLA	a	825	55/65	0.95	0.07	39,44,58,68	0
17	CLA	a	807	65/65	0.95	0.09	35,41,50,54	0
17	CLA	B	837	65/65	0.95	0.09	49,55,61,65	0
17	CLA	B	826	65/65	0.95	0.09	44,50,56,64	0
17	CLA	a	830	65/65	0.95	0.08	36,40,47,49	0
17	CLA	a	831	65/65	0.95	0.08	36,43,54,56	0
17	CLA	a	832	50/65	0.95	0.08	41,54,78,83	0
17	CLA	b	819	65/65	0.95	0.09	50,57,92,95	0
17	CLA	A	807	65/65	0.95	0.08	44,47,58,69	0
17	CLA	B	840	65/65	0.95	0.09	41,50,72,78	0
17	CLA	a	835	65/65	0.95	0.08	36,43,48,49	0
17	CLA	B	828	65/65	0.95	0.09	43,48,58,61	0
17	CLA	b	824	65/65	0.95	0.09	45,51,69,72	0
17	CLA	A	803	65/65	0.95	0.09	39,44,54,59	0
17	CLA	a	814	65/65	0.95	0.10	39,47,64,67	0
17	CLA	b	827	65/65	0.95	0.09	40,53,83,83	0
17	CLA	B	819	65/65	0.95	0.08	46,53,80,83	0
17	CLA	a	803	65/65	0.96	0.07	35,38,50,53	0
18	PQN	b	842	33/33	0.96	0.08	36,41,49,50	0
17	CLA	B	805	65/65	0.96	0.09	45,47,53,60	0
17	CLA	b	802	65/65	0.96	0.09	36,41,45,52	0
17	CLA	b	803	65/65	0.96	0.07	35,40,47,49	0
17	CLA	a	826	65/65	0.96	0.08	39,43,48,56	0
17	CLA	b	805	65/65	0.96	0.08	42,45,52,58	0
17	CLA	a	820	65/65	0.96	0.08	38,43,48,50	0
17	CLA	A	801	65/65	0.96	0.09	40,44,49,53	0
17	CLA	a	801	65/65	0.96	0.08	35,39,44,46	0
17	CLA	B	813	65/65	0.96	0.08	47,51,54,55	0
21	SF4	C	102	8/8	0.99	0.05	51,62,72,84	0
21	SF4	a	855	8/8	0.99	0.04	37,37,43,43	0
21	SF4	c	101	8/8	0.99	0.06	41,46,54,56	0
21	SF4	c	102	8/8	0.99	0.04	41,50,62,77	0
21	SF4	A	853	8/8	0.99	0.05	43,44,48,51	0
21	SF4	C	101	8/8	0.99	0.06	47,49,53,57	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.

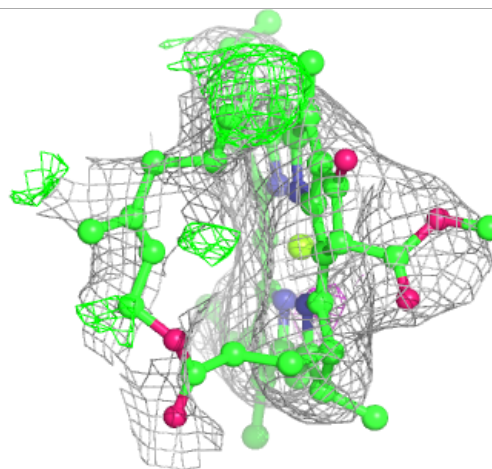
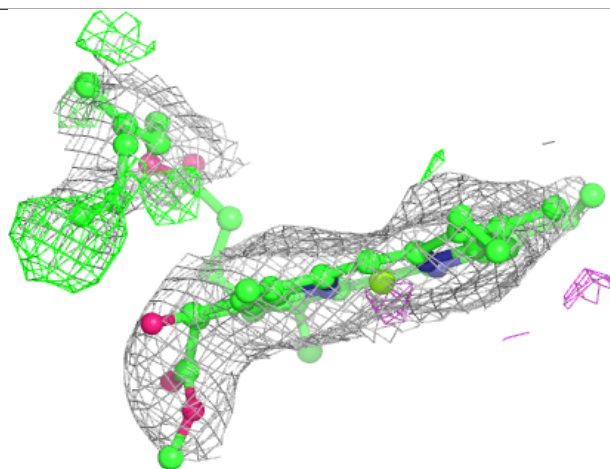
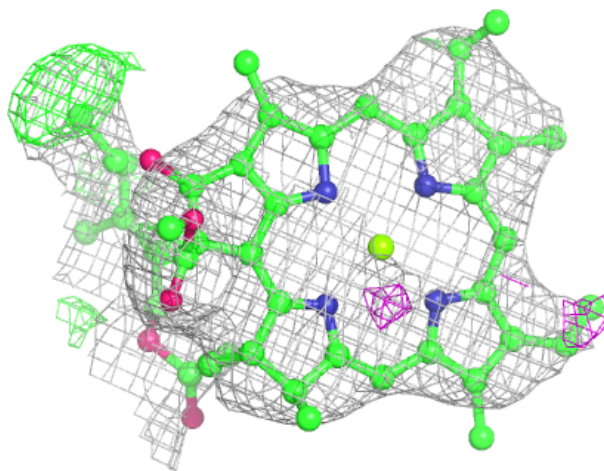
**Electron density around CLA 8 309:**

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



**Electron density around CLA a 846:**

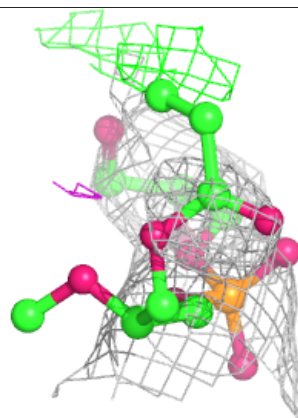
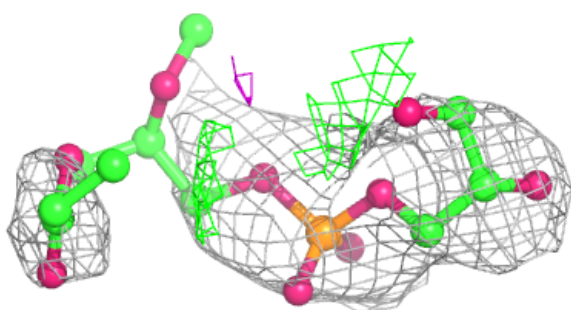
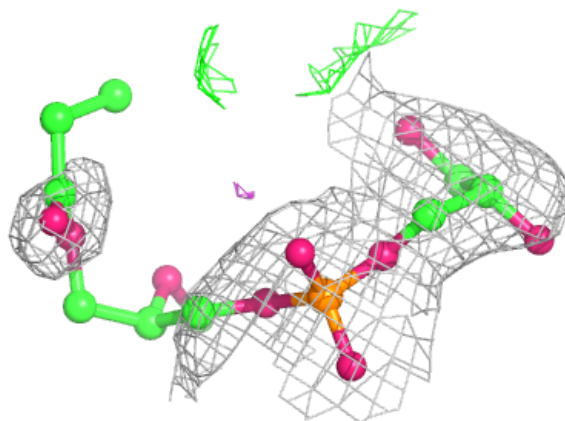
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





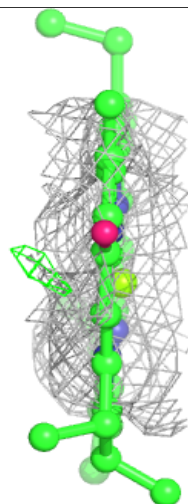
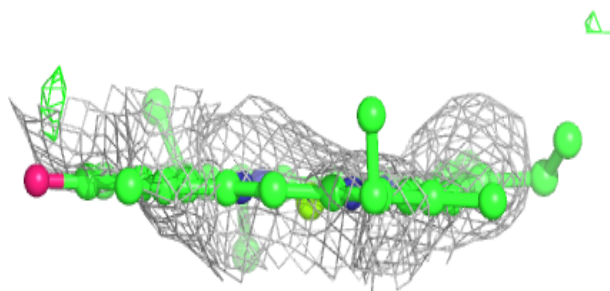
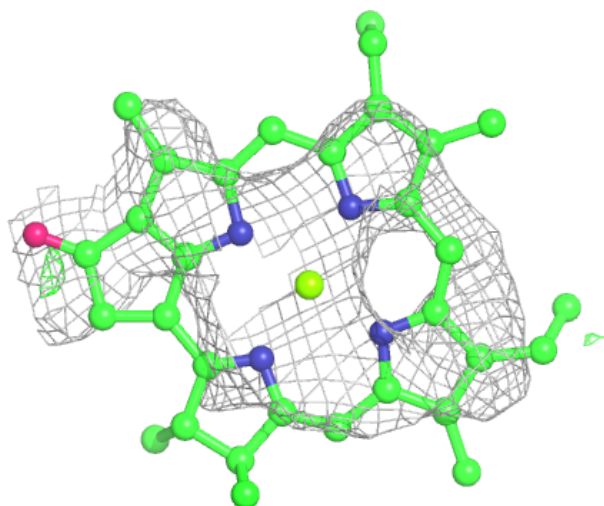
**Electron density around LHG 3 319:**

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



**Electron density around CLA 3 310:**

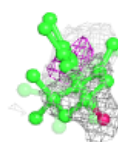
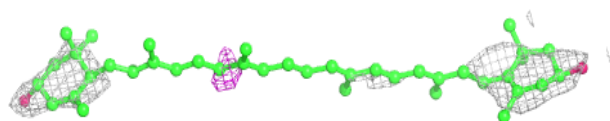
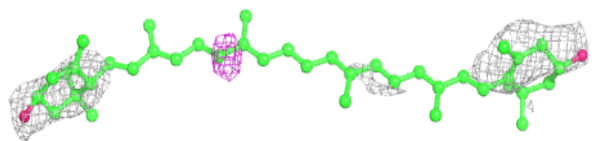
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



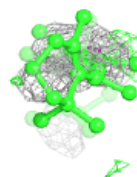
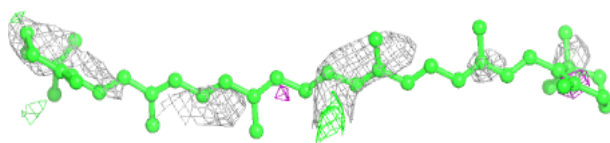
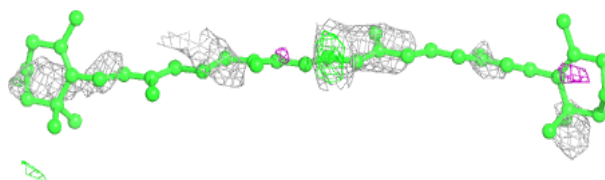


**Electron density around LUT 6 321:**

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

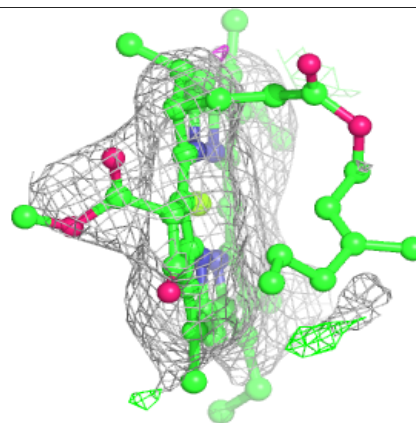
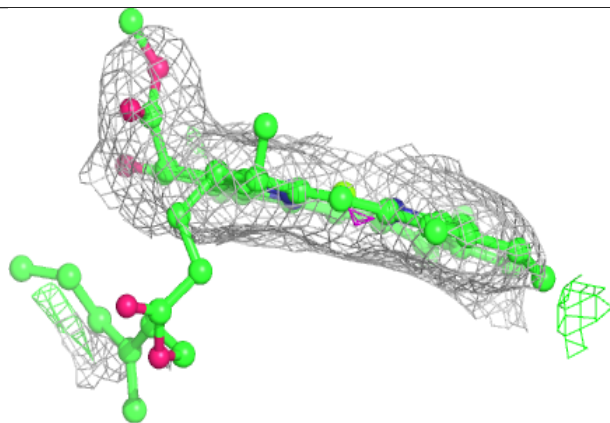
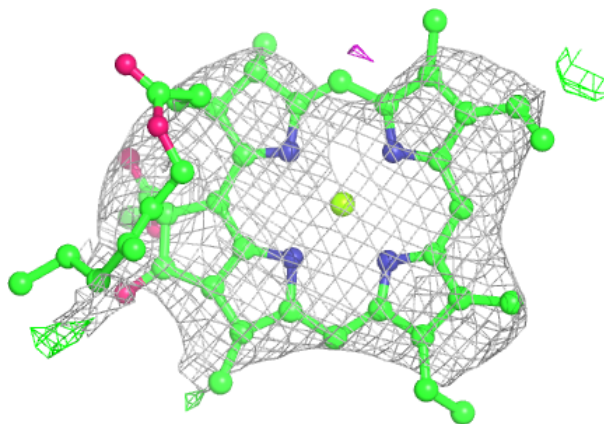
**Electron density around BCR L 206:**

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

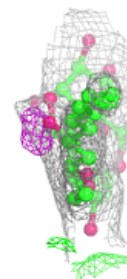
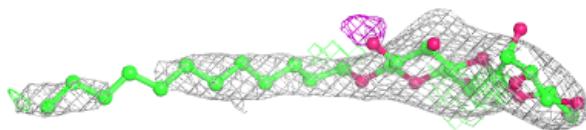
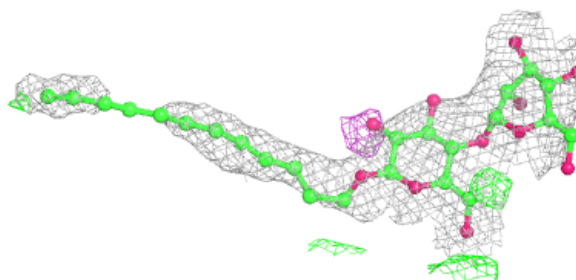


**Electron density around CLA A 845:**

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

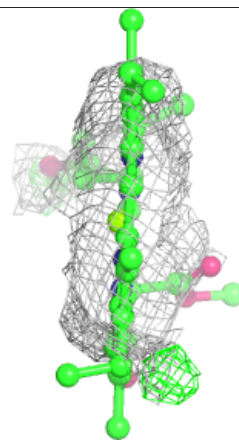
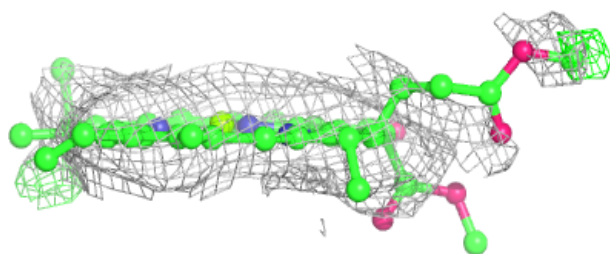
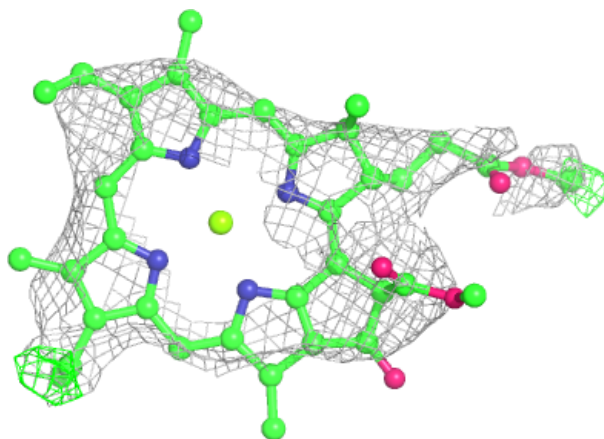
**Electron density around LMT B 849:**

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



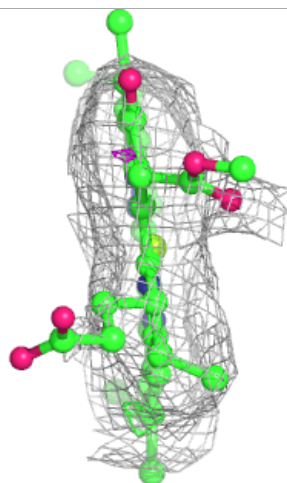
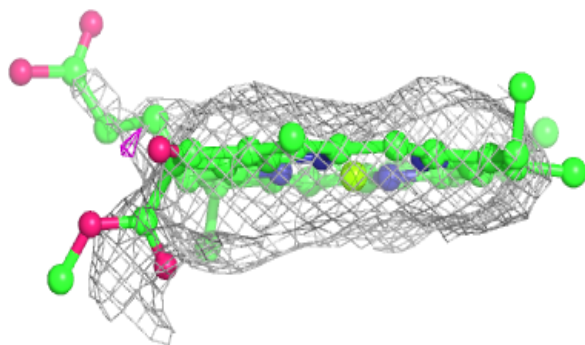
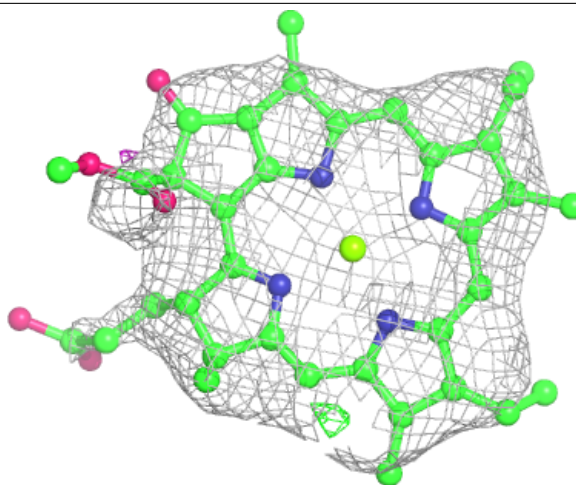
**Electron density around CLA 6 316:**

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



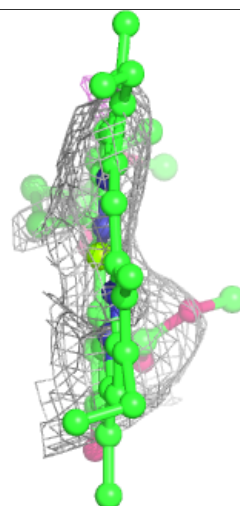
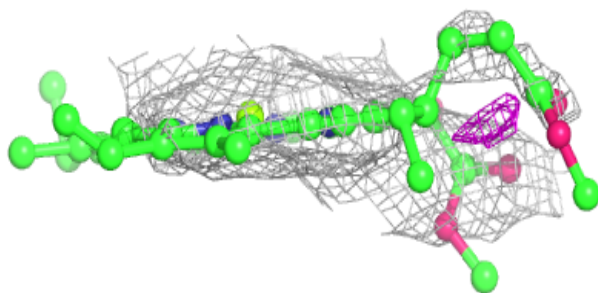
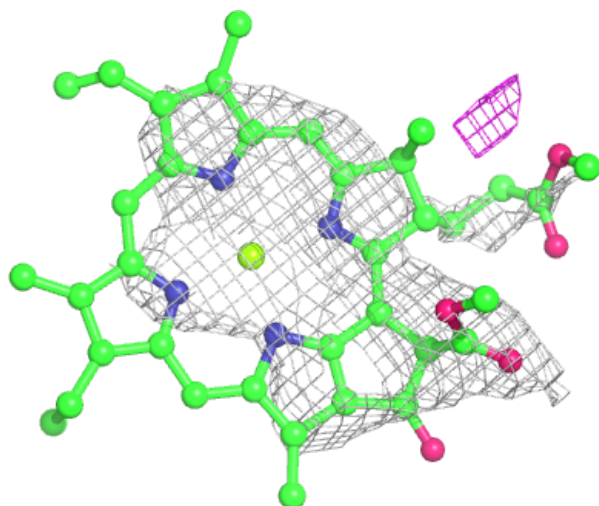
**Electron density around CLA 8 311:**

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



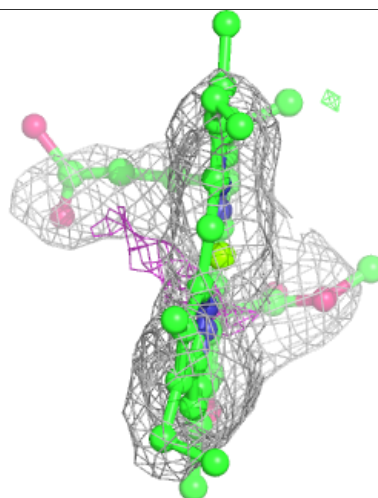
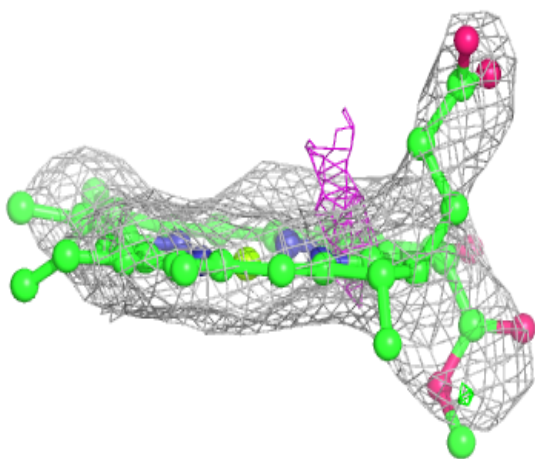
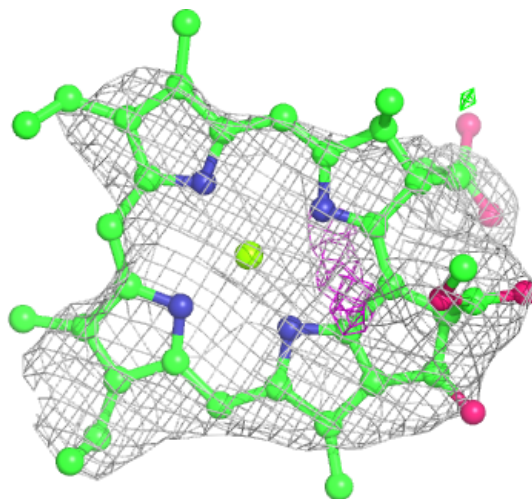
**Electron density around CLA 3 301:**

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



**Electron density around CLA K 4002:**

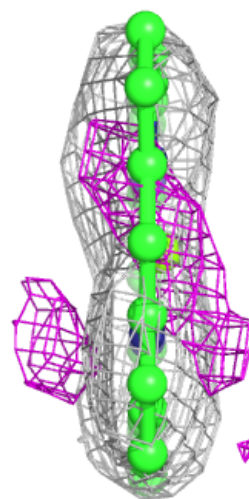
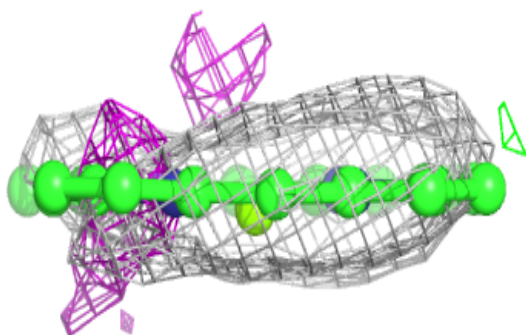
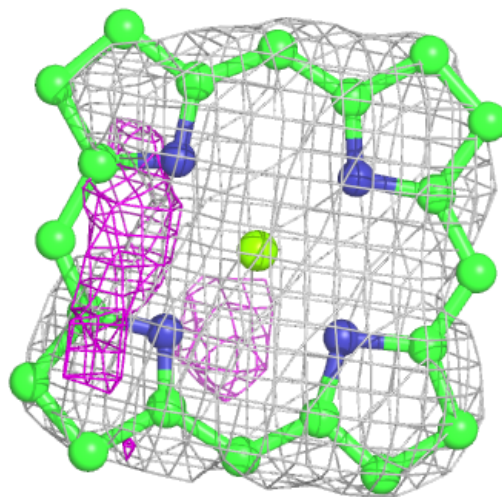
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





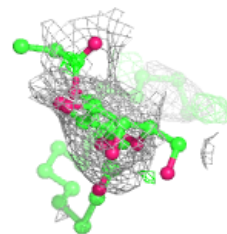
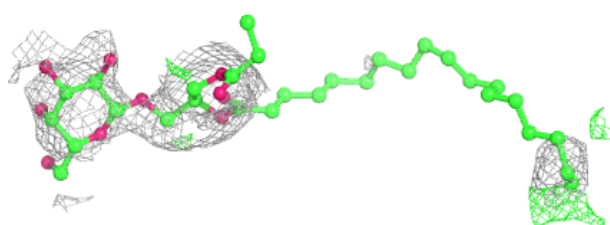
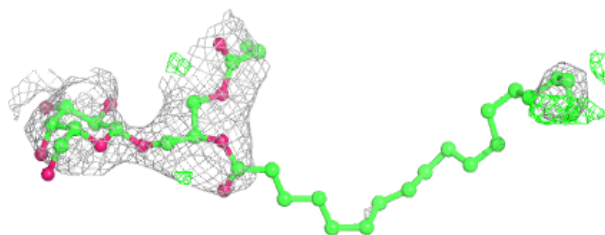
**Electron density around CLA 8 313:**

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

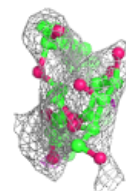
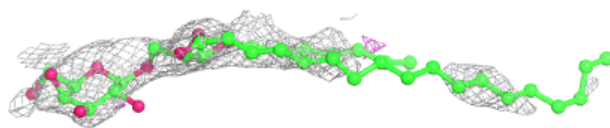
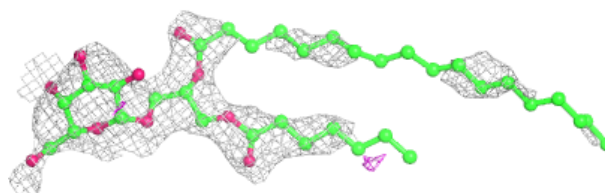


**Electron density around LMG 6 302:**

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

**Electron density around LMG 4 620:**

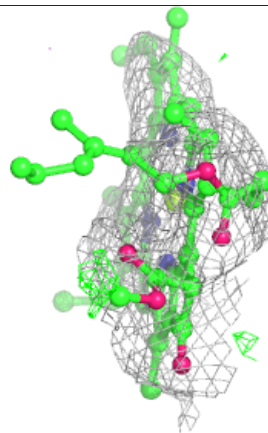
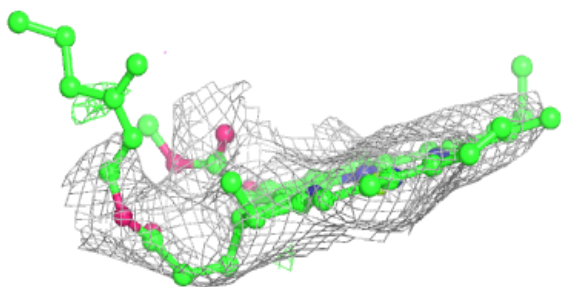
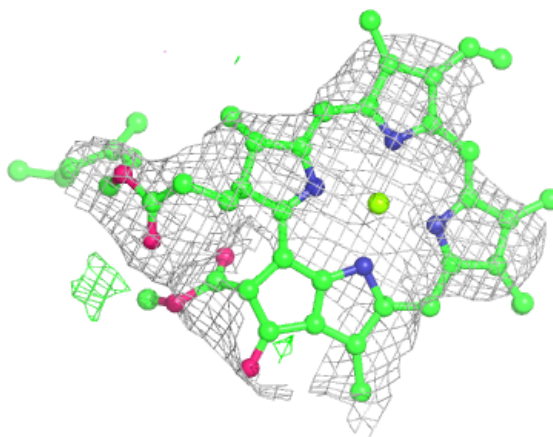
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





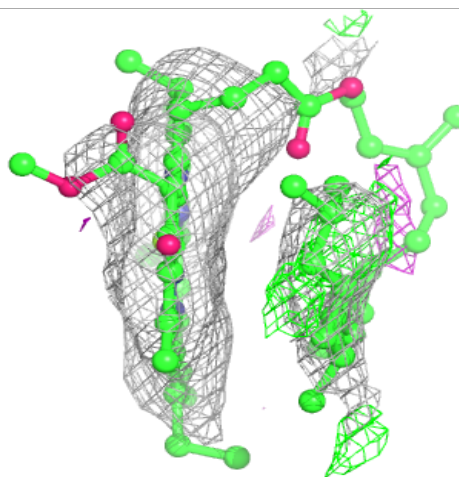
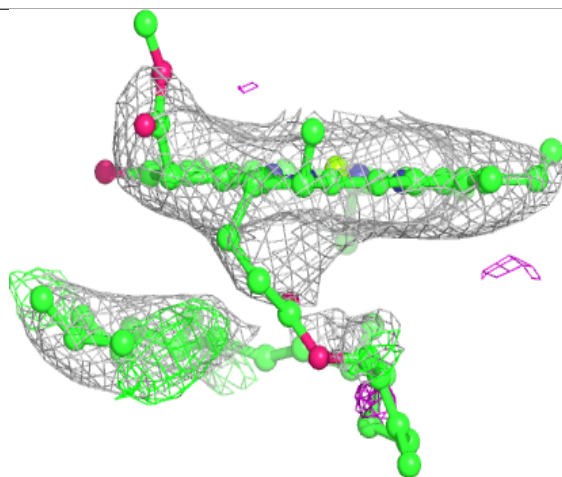
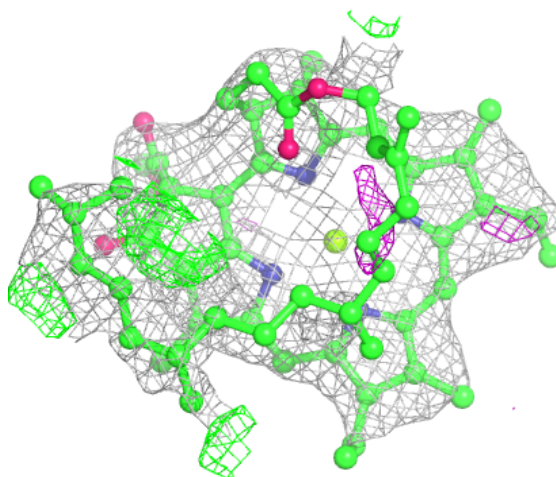
**Electron density around CLA 3 311:**

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



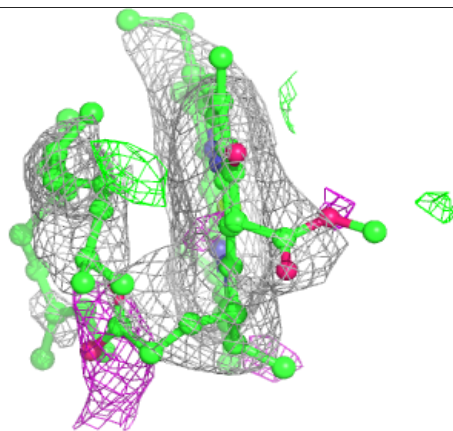
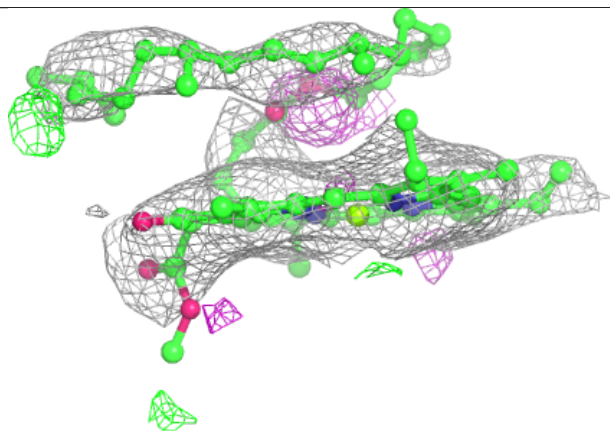
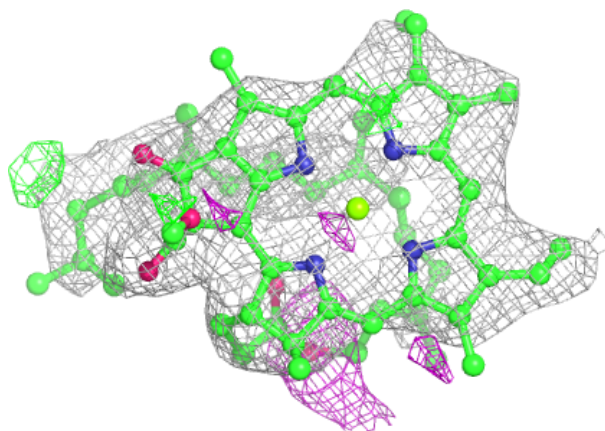
**Electron density around CLA L 202:**

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



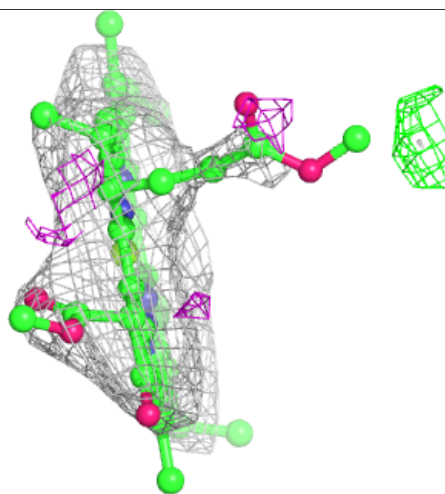
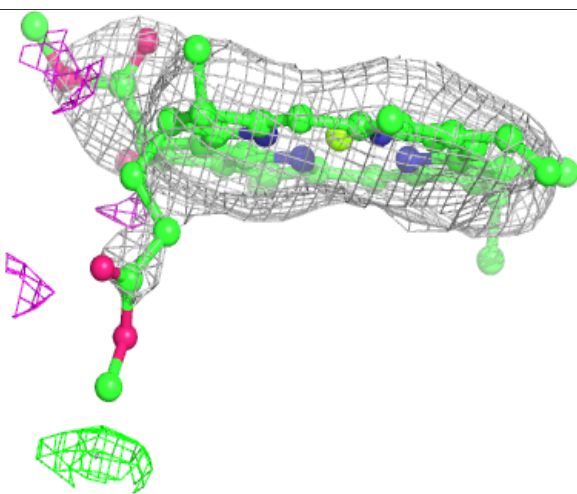
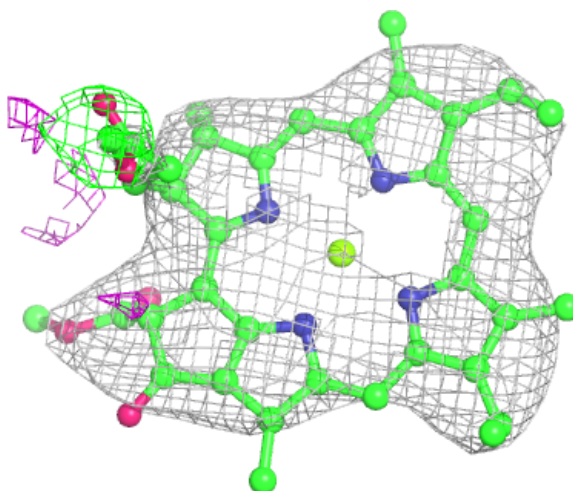
**Electron density around CLA 1 202:**

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



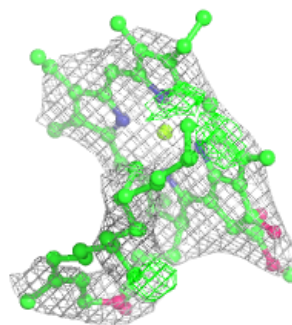
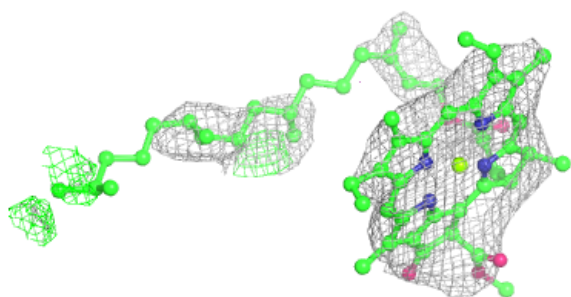
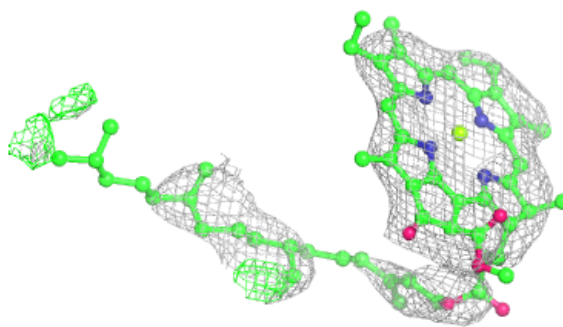
**Electron density around CLA 6 309:**

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



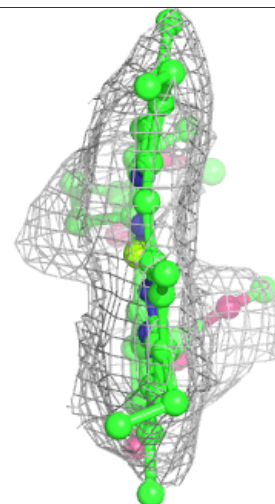
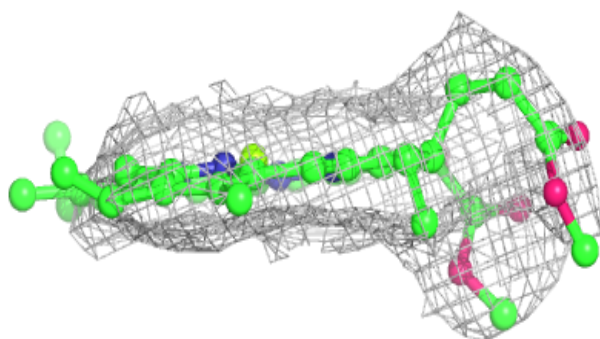
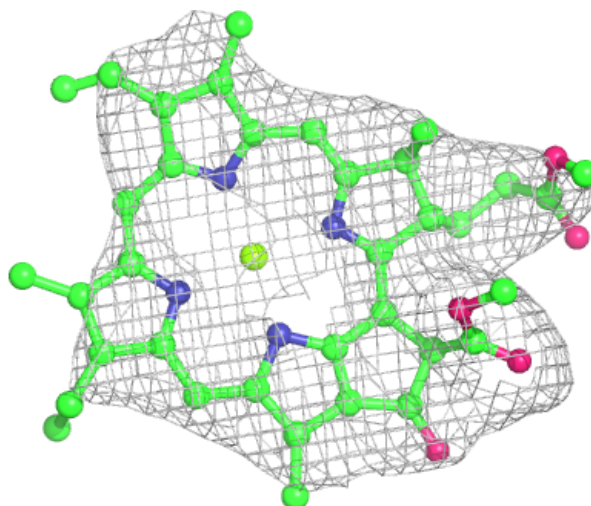
**Electron density around CLA 6 310:**

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



**Electron density around CLA k 1403:**

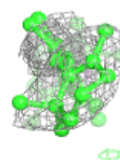
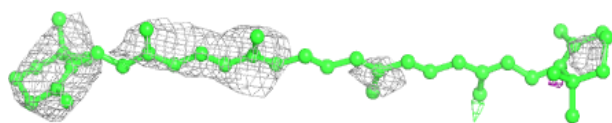
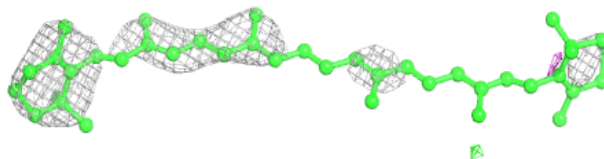
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



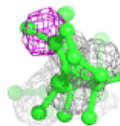
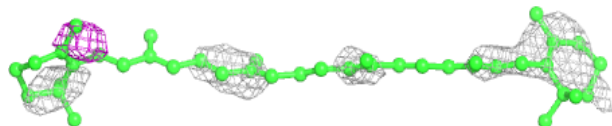
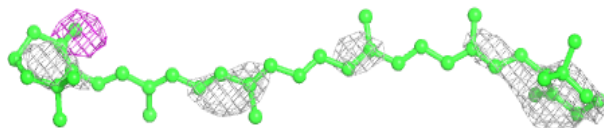


**Electron density around BCR K 4004:**

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

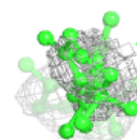
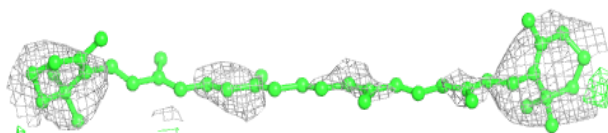
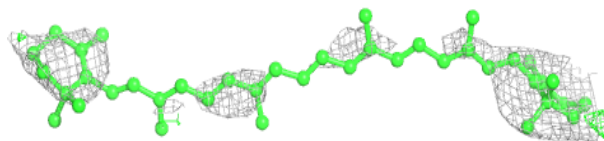
**Electron density around BCR 2 617:**

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

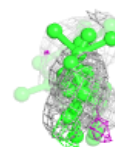
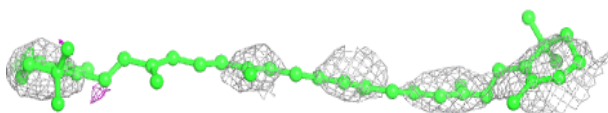
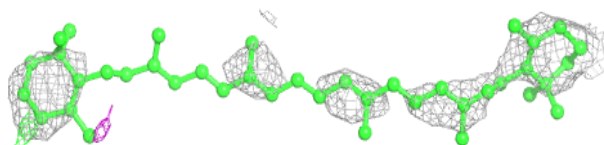


**Electron density around BCR 6 319:**

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

**Electron density around BCR 7 617:**

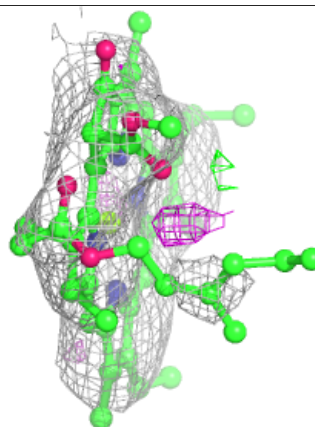
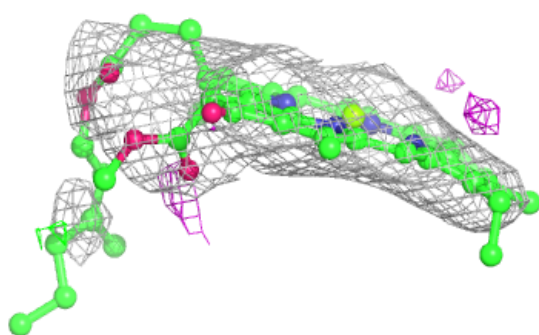
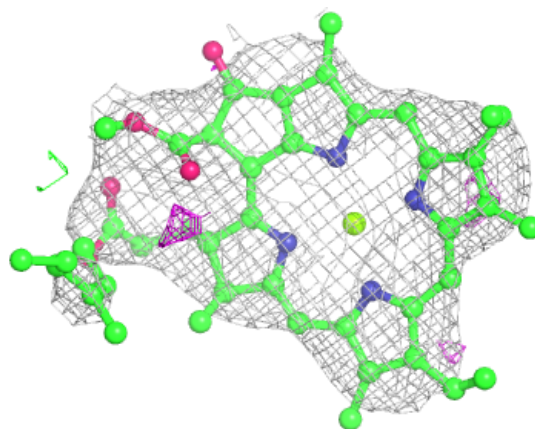
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





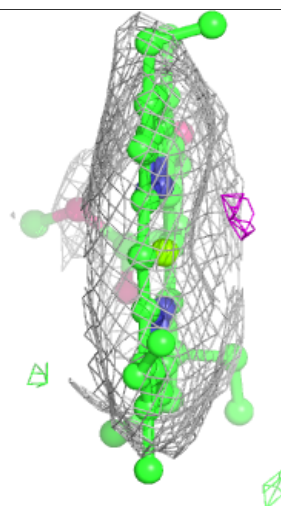
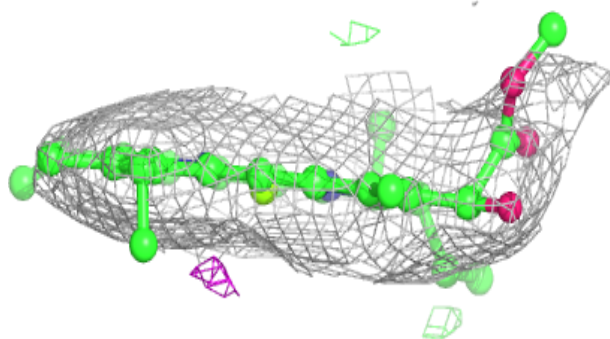
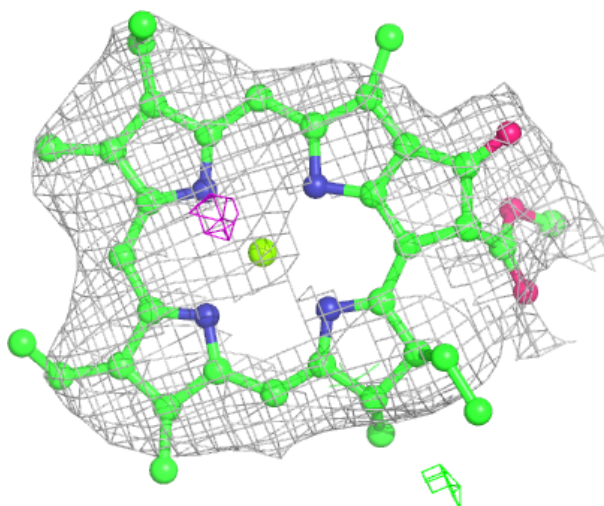
**Electron density around CLA 9 611:**

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



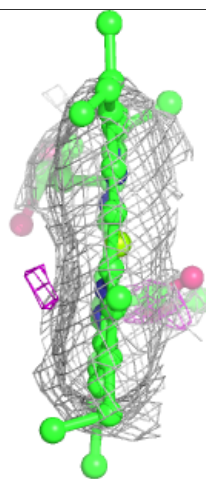
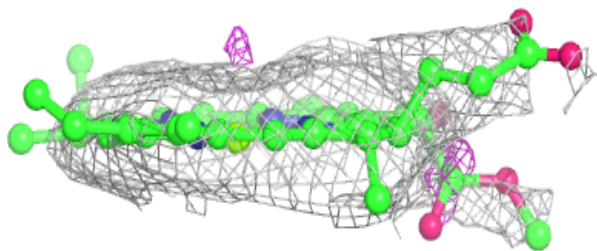
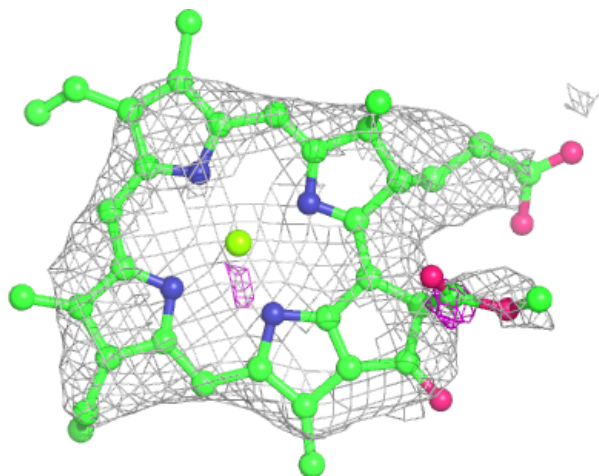
**Electron density around CLA J 3002:**

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



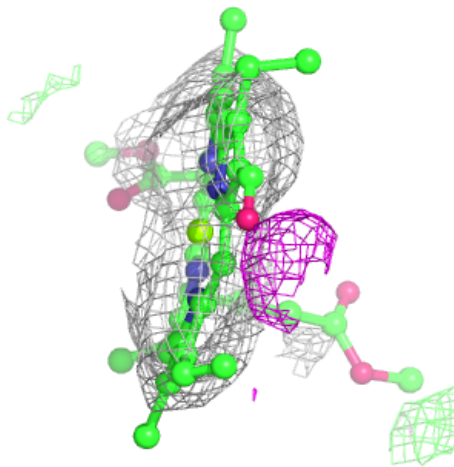
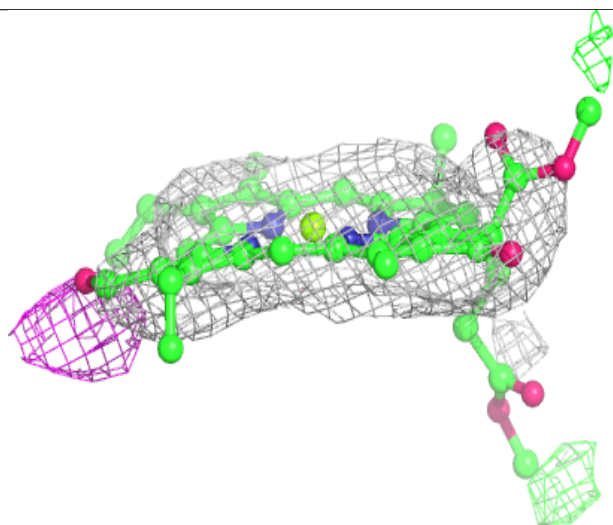
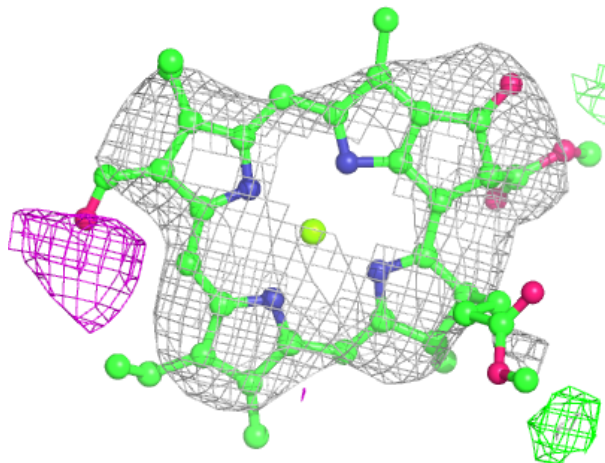
**Electron density around CLA 3 313:**

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



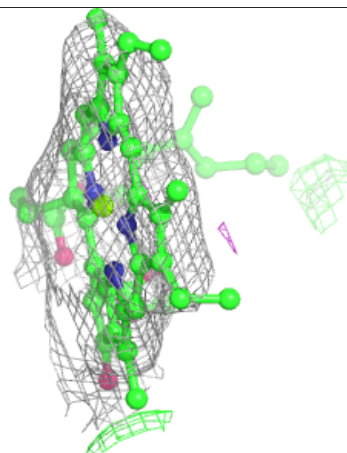
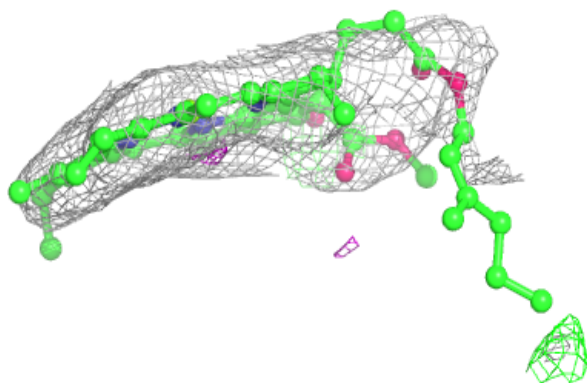
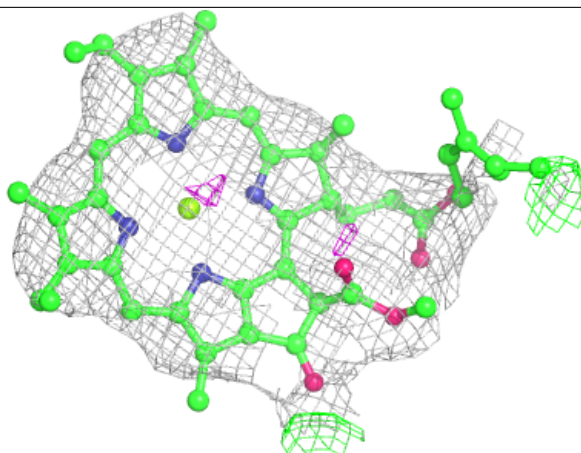
**Electron density around CHL 6 308:**

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



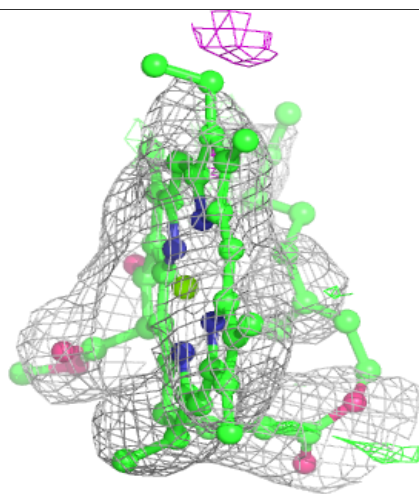
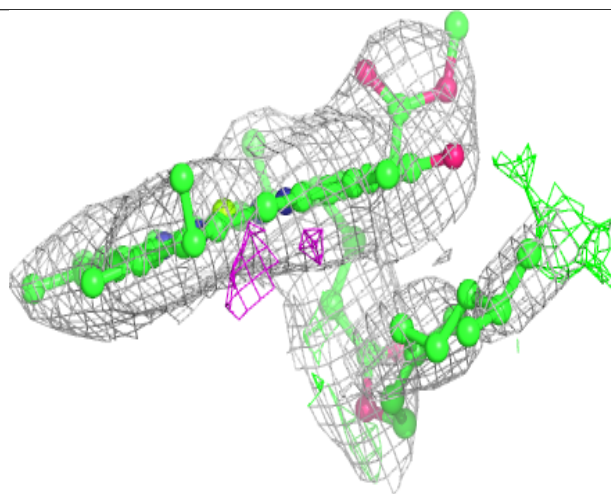
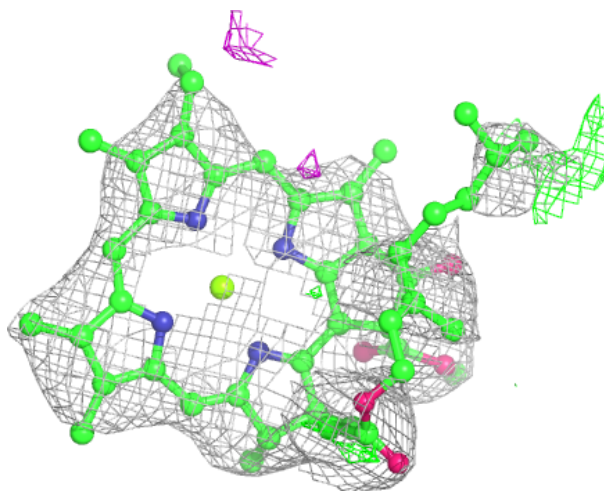
**Electron density around CLA 7 611:**

$2mF_o-DF_c$  (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:**

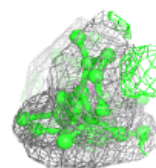
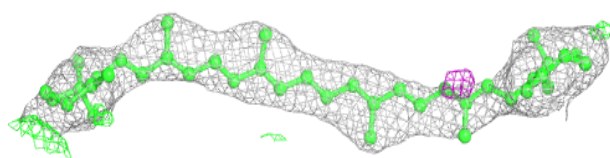
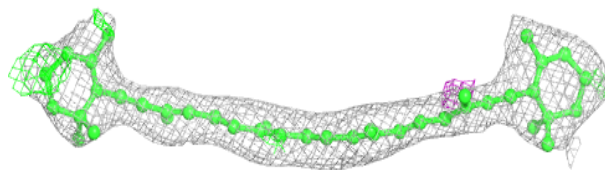
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





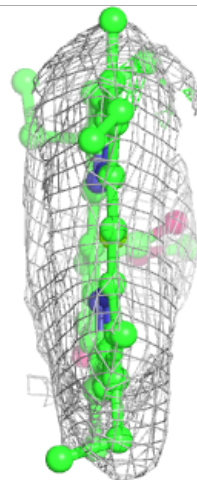
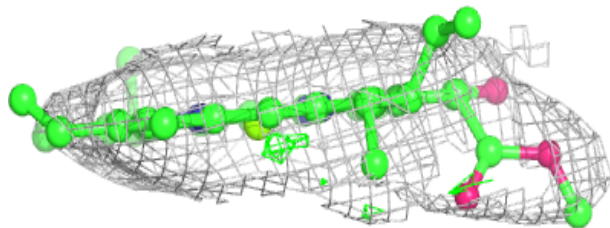
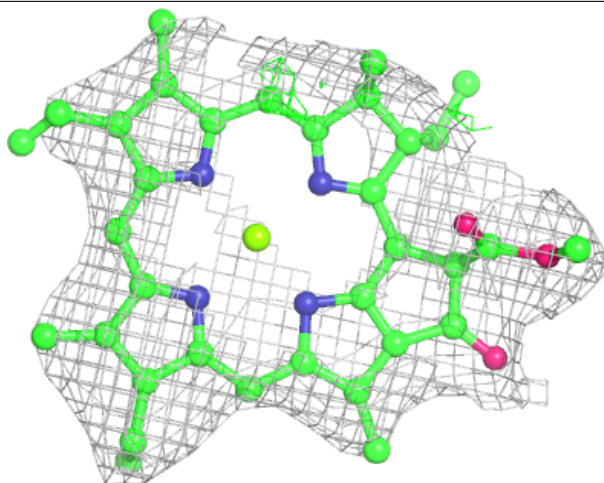
**Electron density around BCR A 856:**

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



**Electron density around CLA j 3002:**

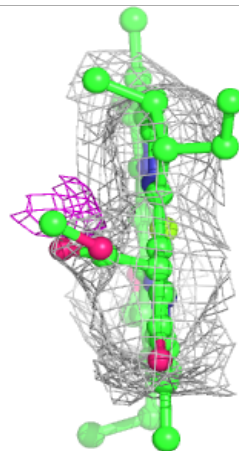
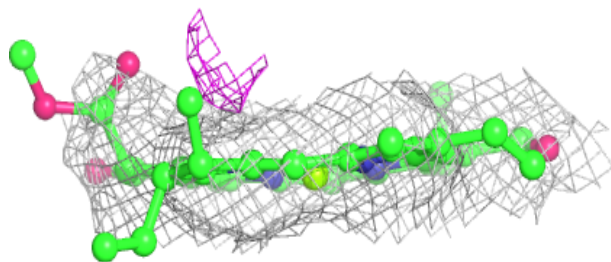
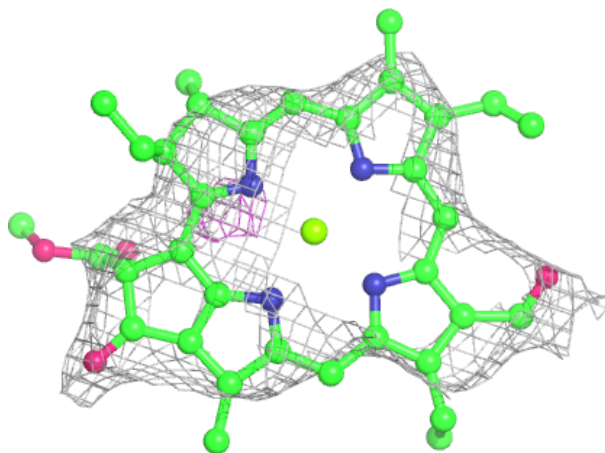
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





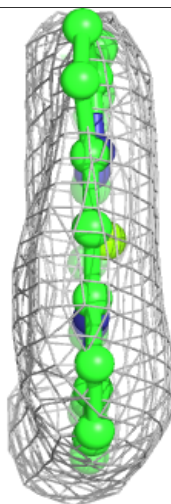
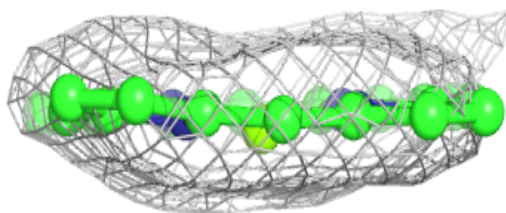
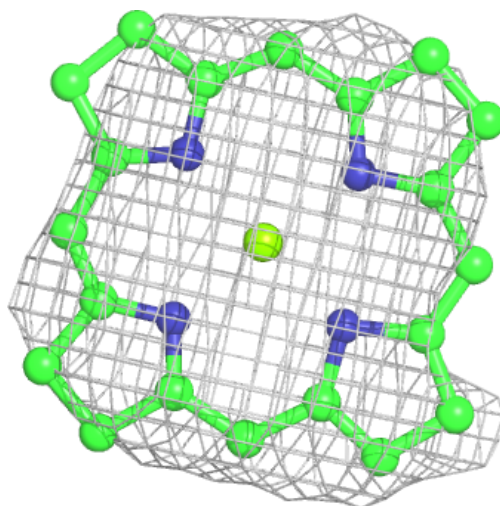
**Electron density around CHL 9 615:**

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



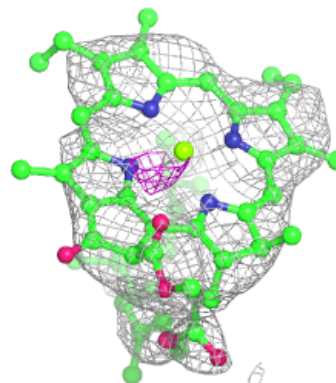
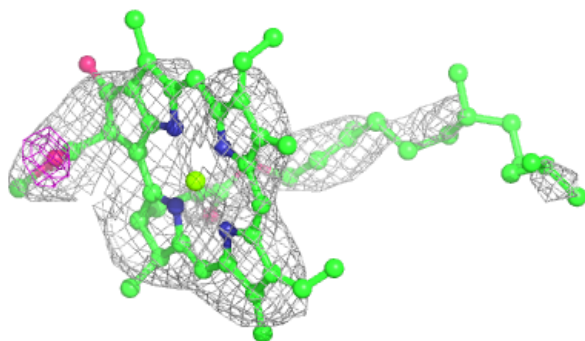
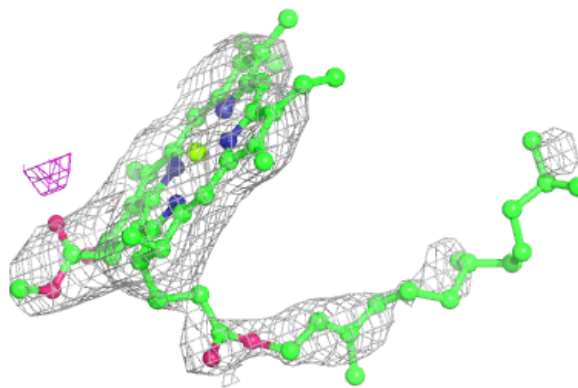
**Electron density around CLA 3 315:**

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



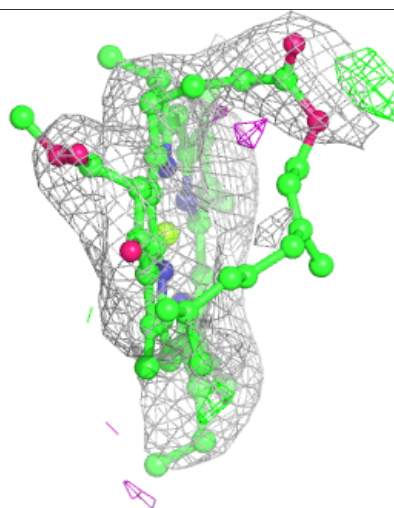
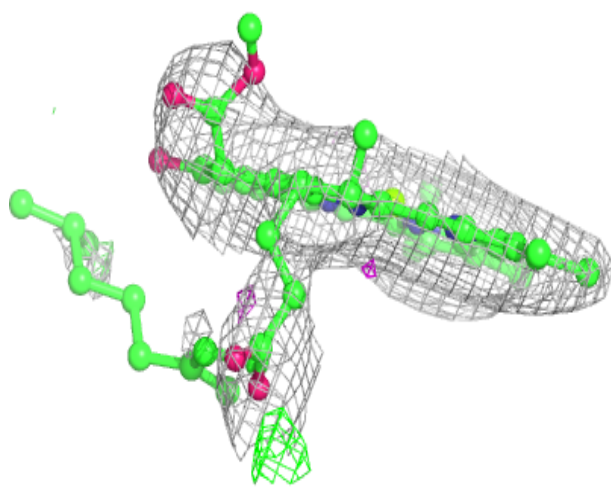
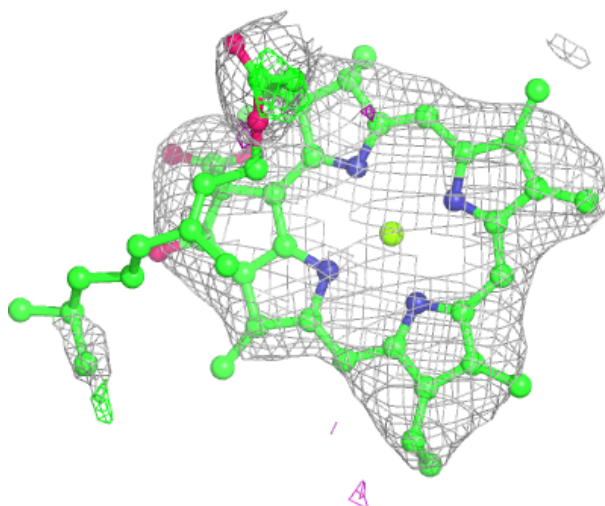
**Electron density around CLA 2 604:**

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



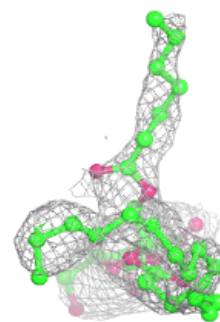
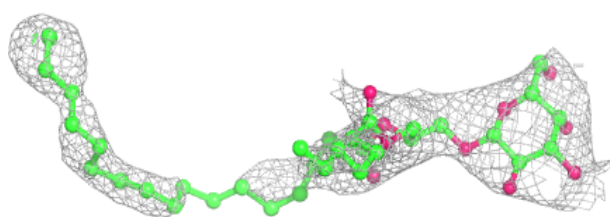
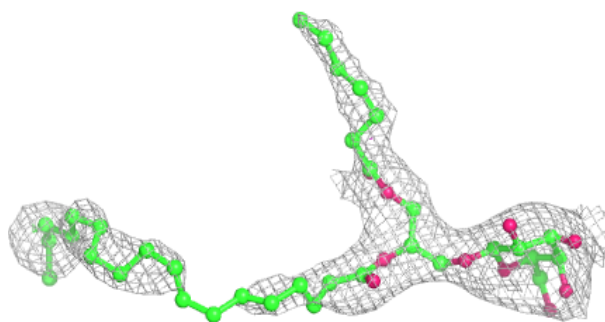
**Electron density around CLA b 811:**

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

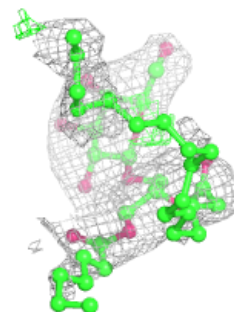
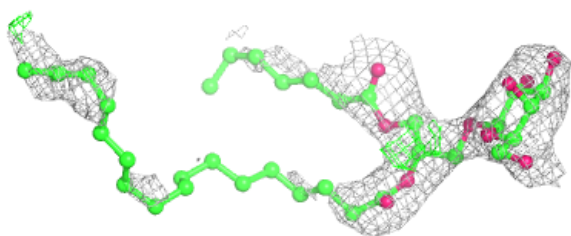
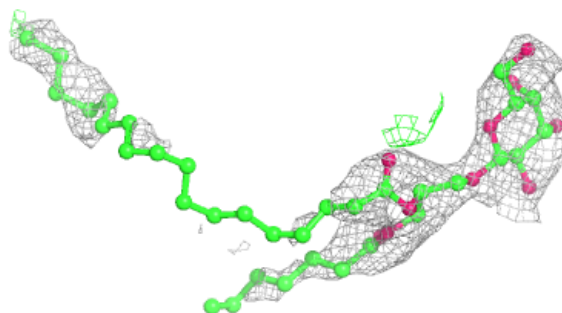


**Electron density around LMG G 102:**

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

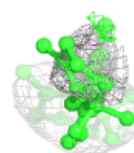
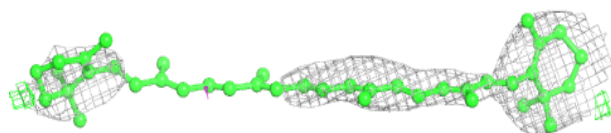
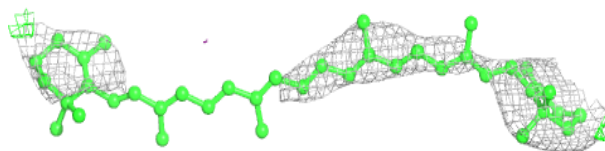
**Electron density around LMG 4 619:**

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



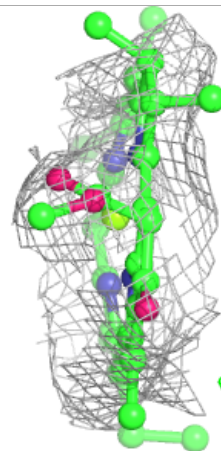
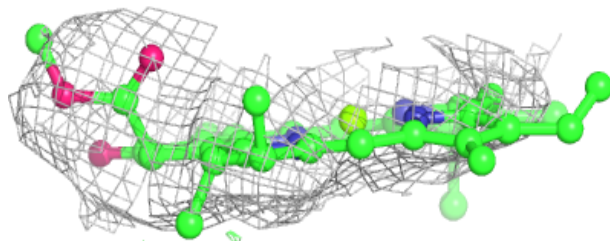
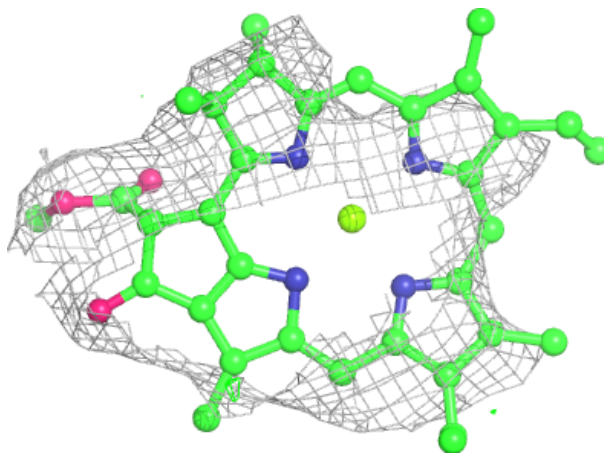
**Electron density around BCR 1 318:**

$2mF_o-DF_c$  (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:**

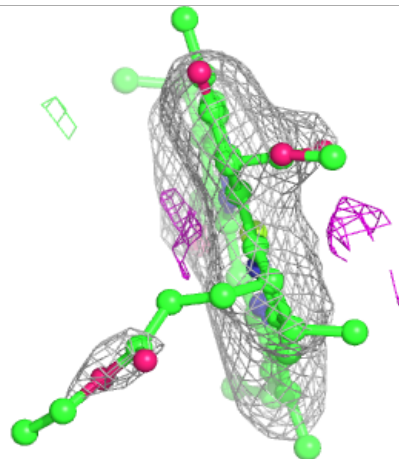
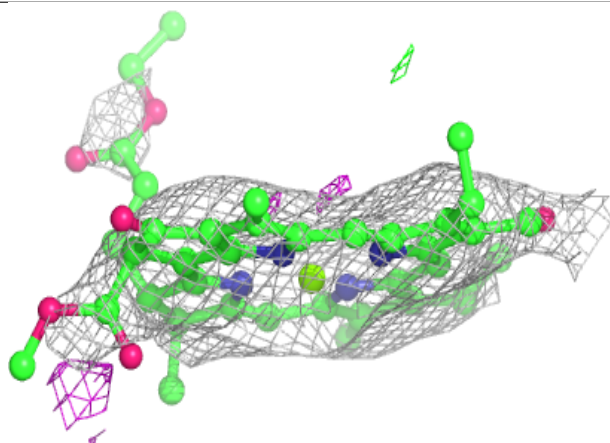
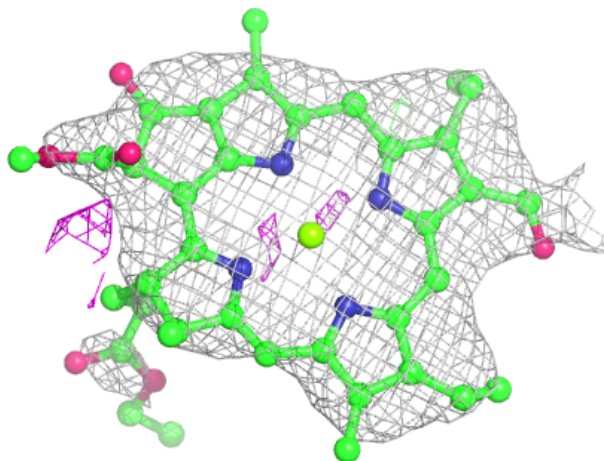
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CHL 2 606:**

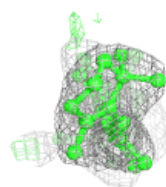
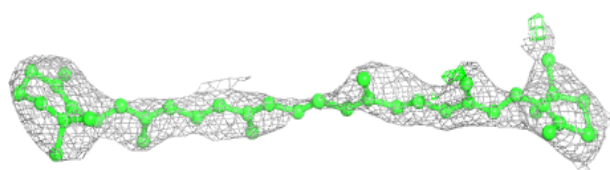
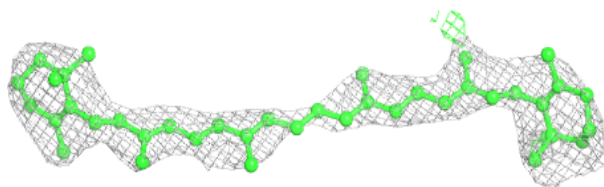
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



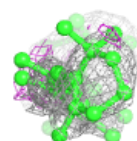
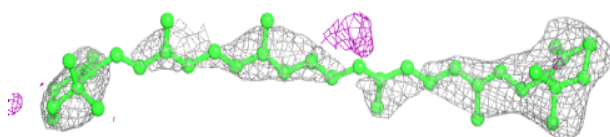
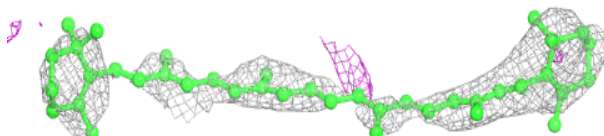


**Electron density around BCR k 1404:**

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

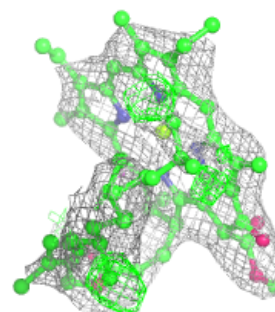
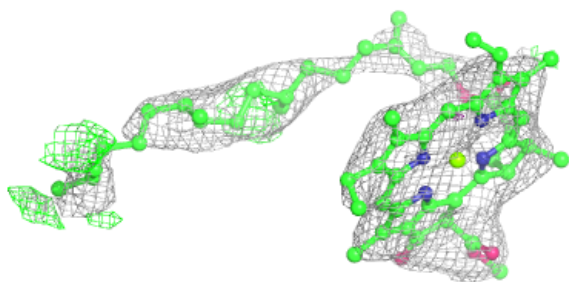
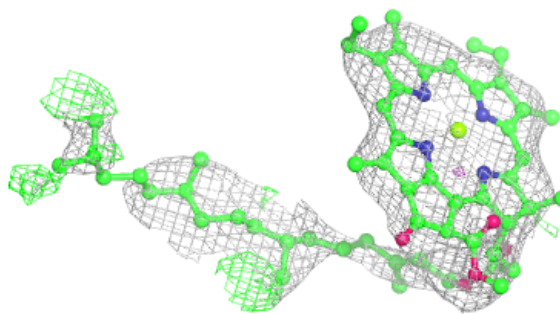
**Electron density around BCR l 206:**

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



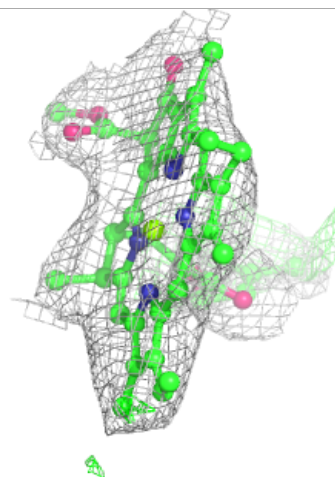
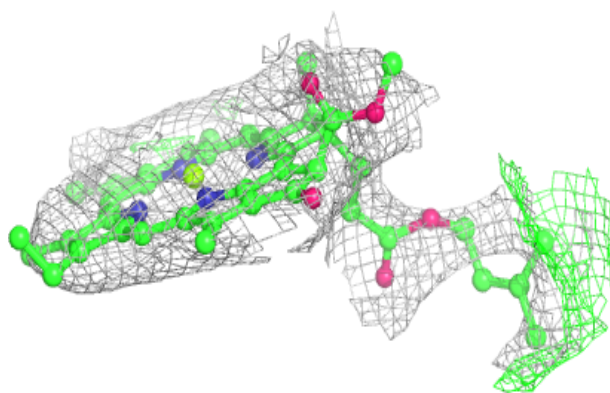
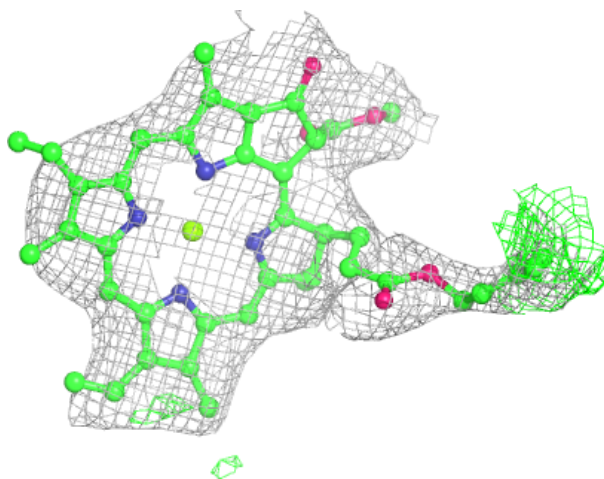
**Electron density around CLA 1 309:**

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



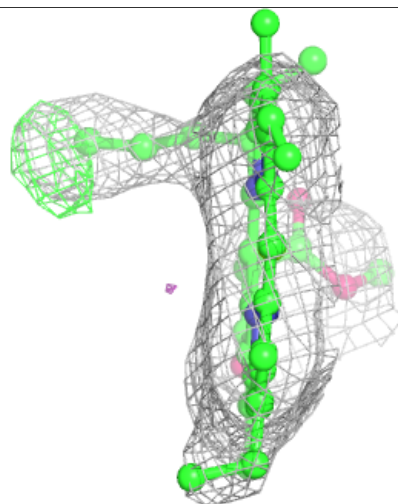
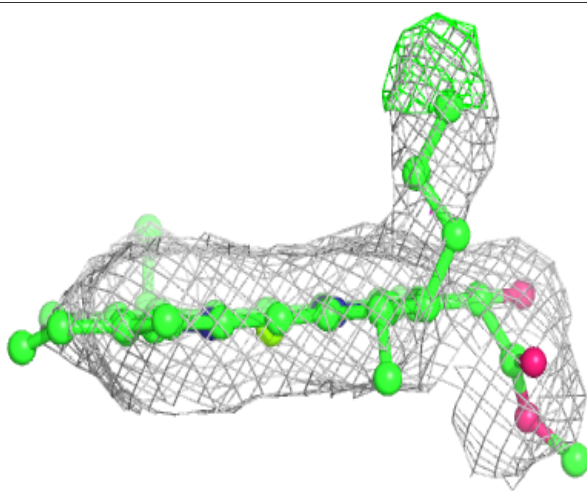
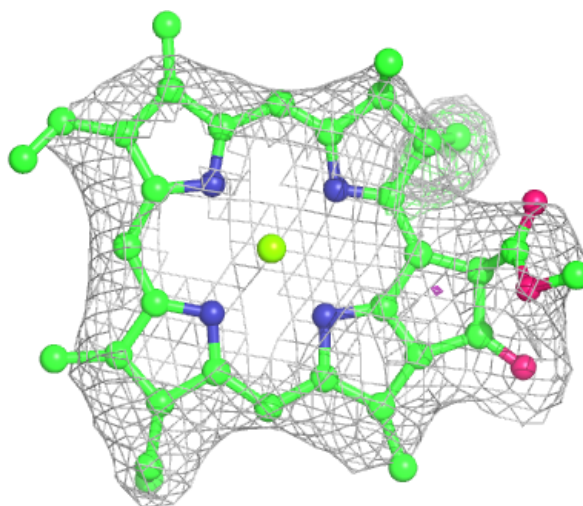
**Electron density around CLA 2 608:**

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



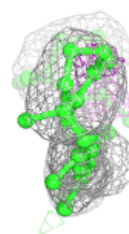
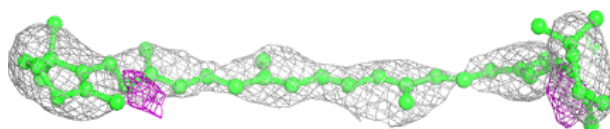
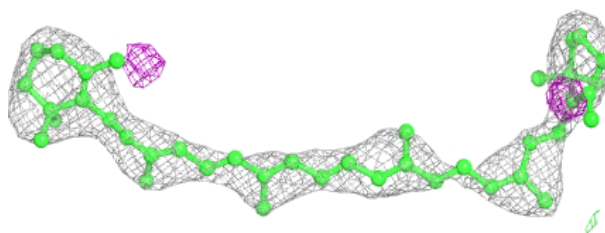
**Electron density around CLA 2 613:**

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

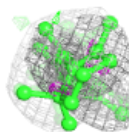
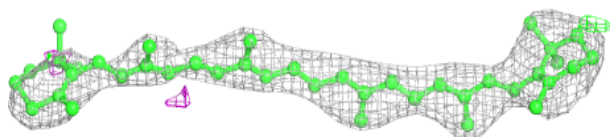
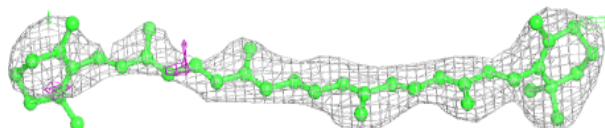


**Electron density around BCR b 844:**

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

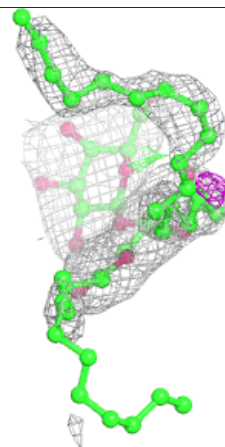
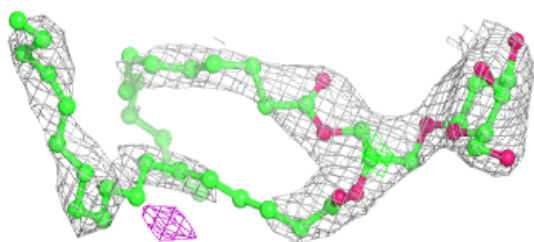
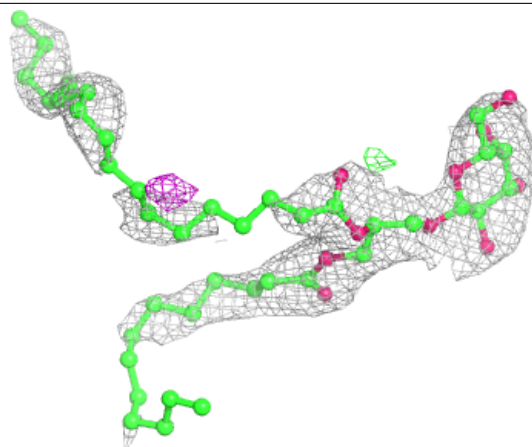
**Electron density around BCR A 848:**

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



**Electron density around LMG 9 619:**

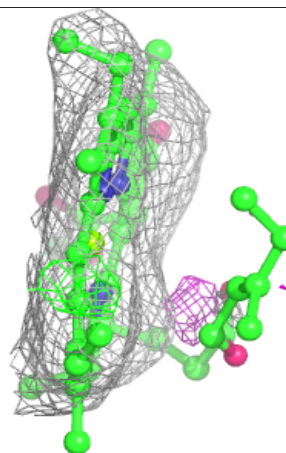
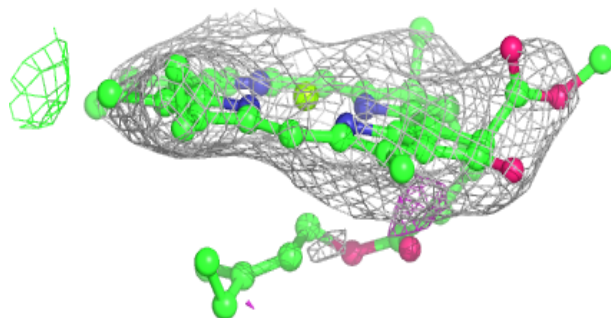
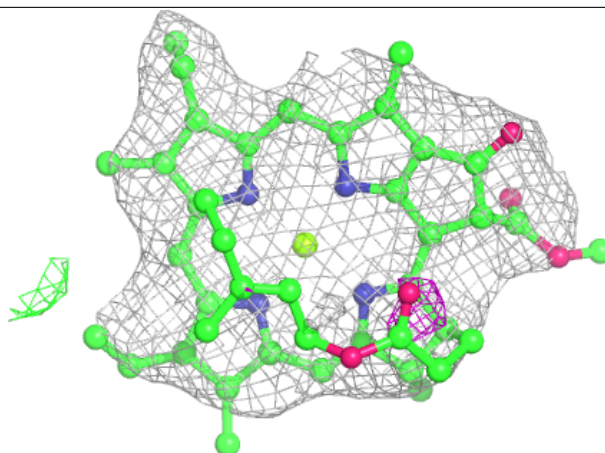
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



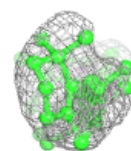
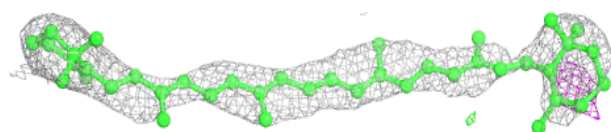
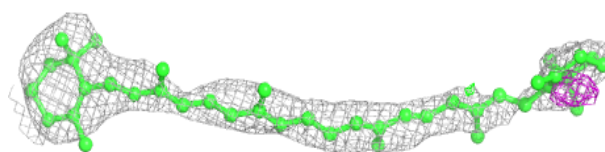


**Electron density around CLA A 824:**

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

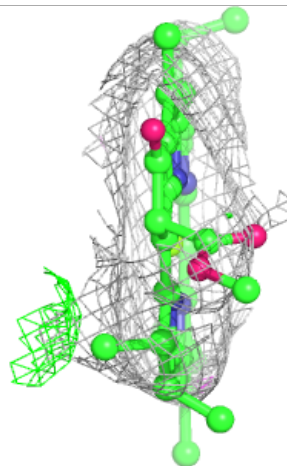
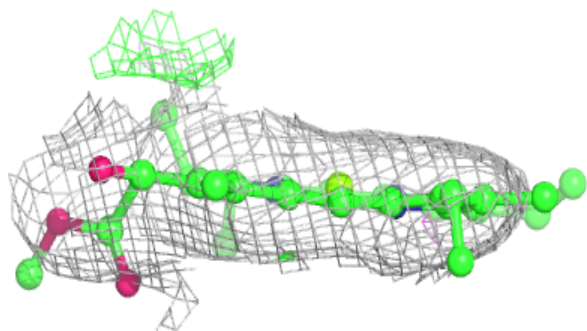
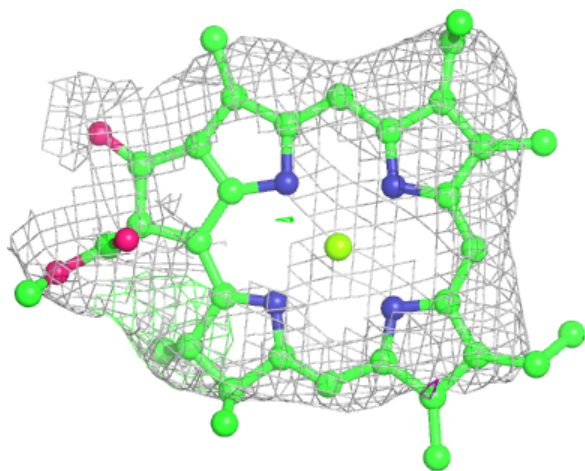
**Electron density around BCR K 4001:**

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



**Electron density around CLA 6 312:**

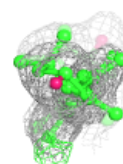
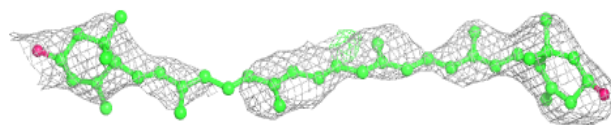
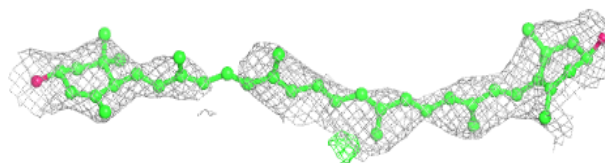
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





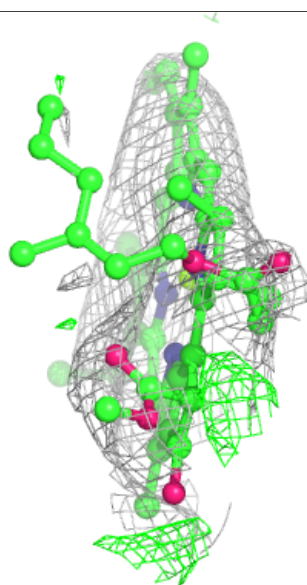
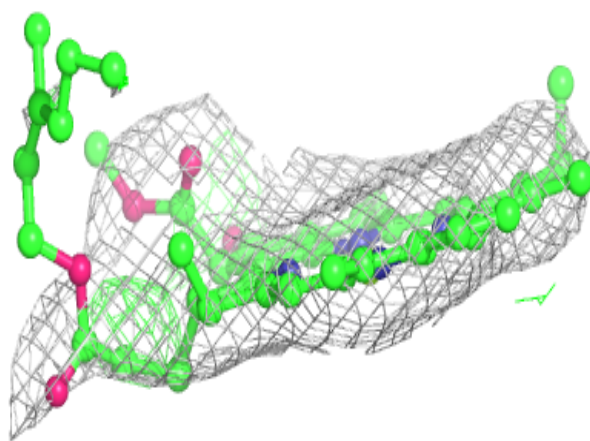
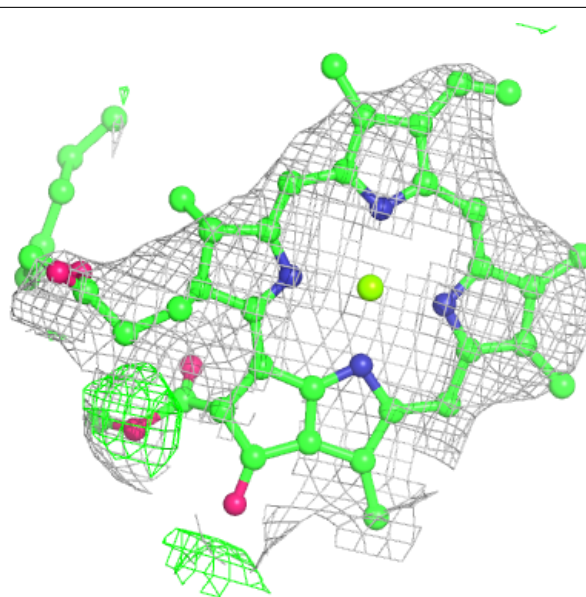
**Electron density around LUT 4 616:**

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



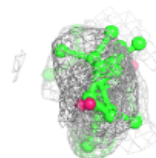
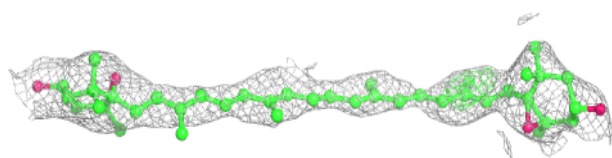
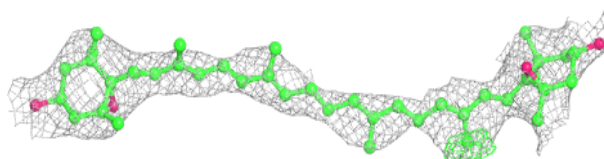
**Electron density around CLA 6 313:**

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



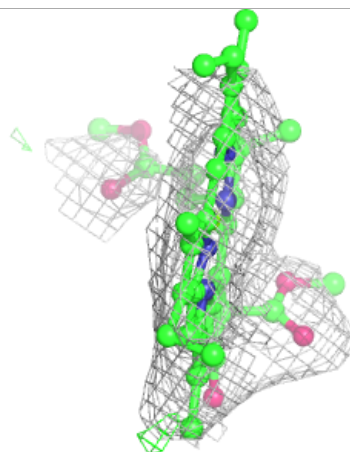
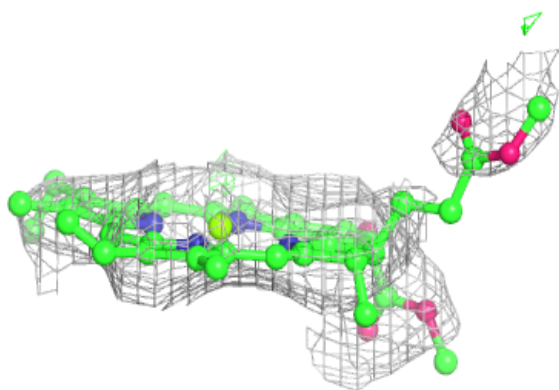
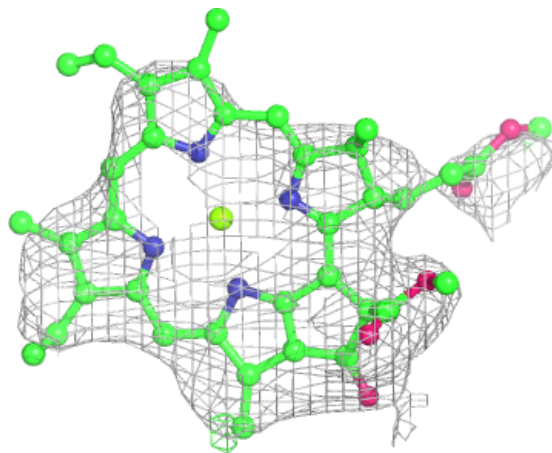
**Electron density around XAT 9 617:**

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



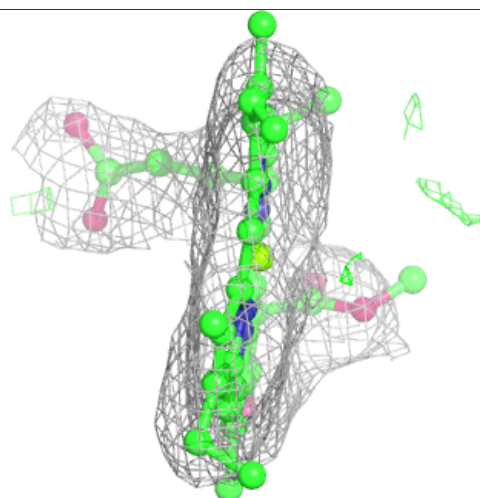
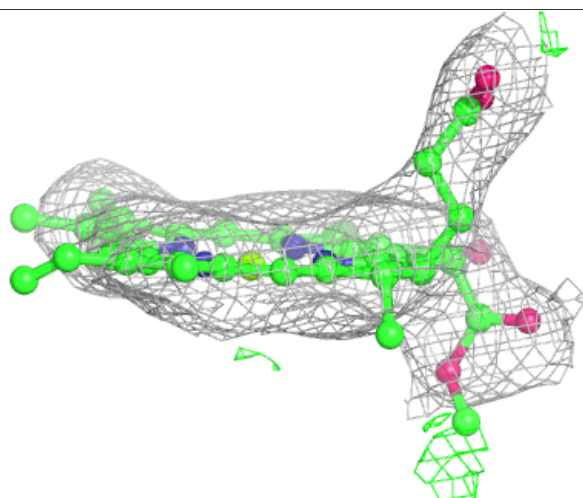
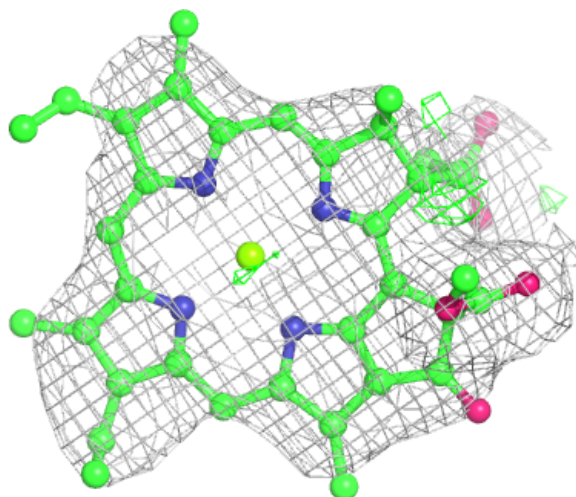
**Electron density around CLA K 4003:**

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



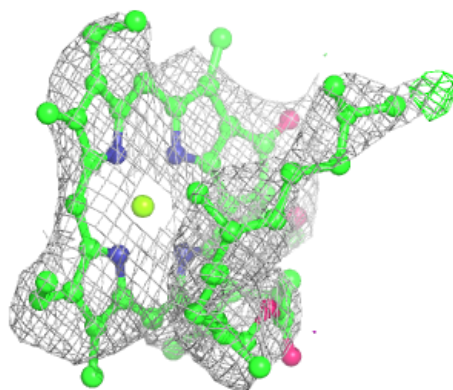
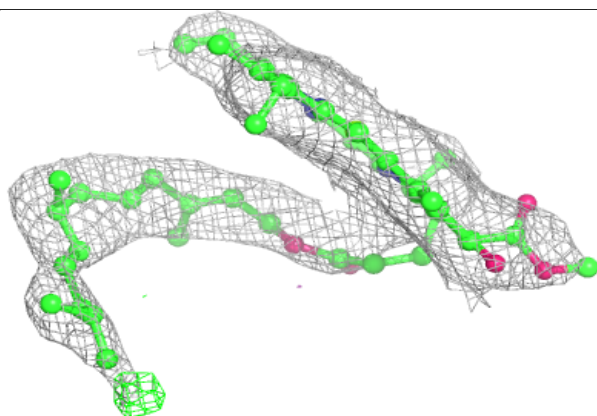
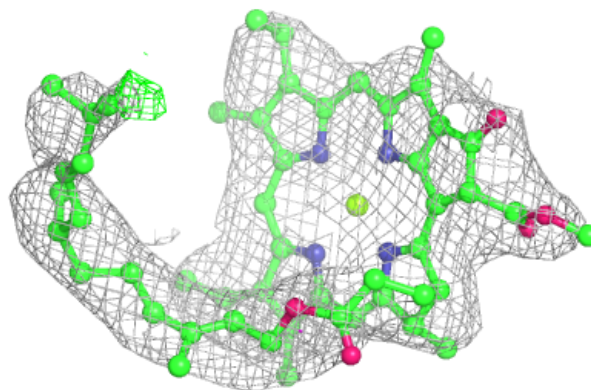
**Electron density around CLA k 1401:**

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

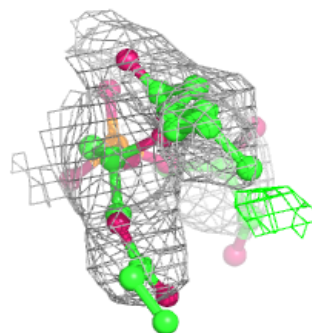
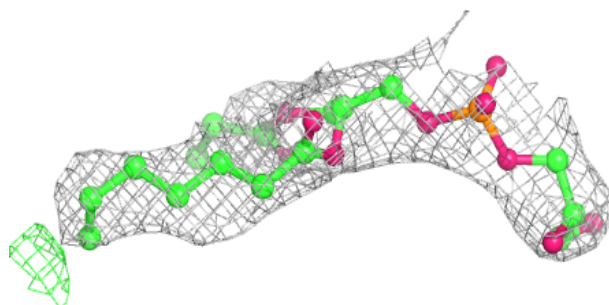
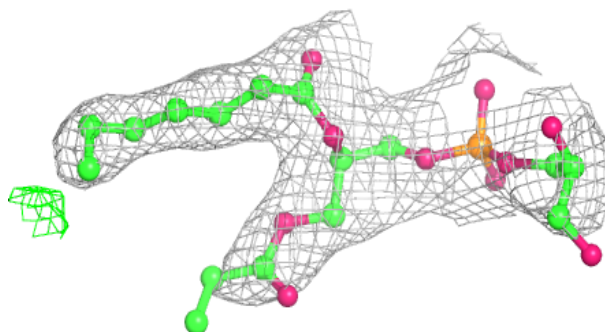


**Electron density around CLA 2 609:**

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

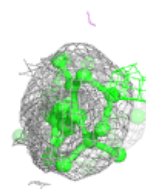
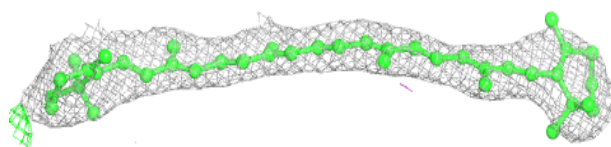
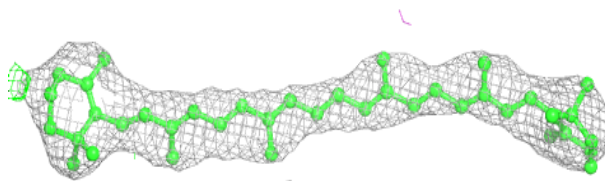
**Electron density around LHG A 847:**

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



**Electron density around BCR b 843:**

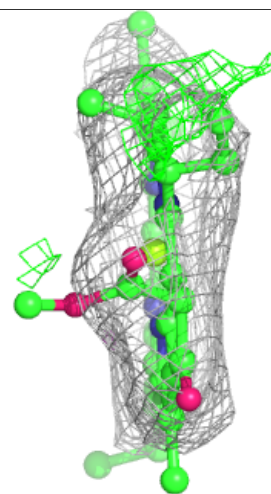
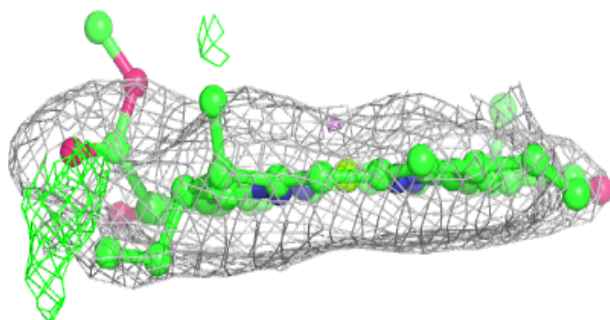
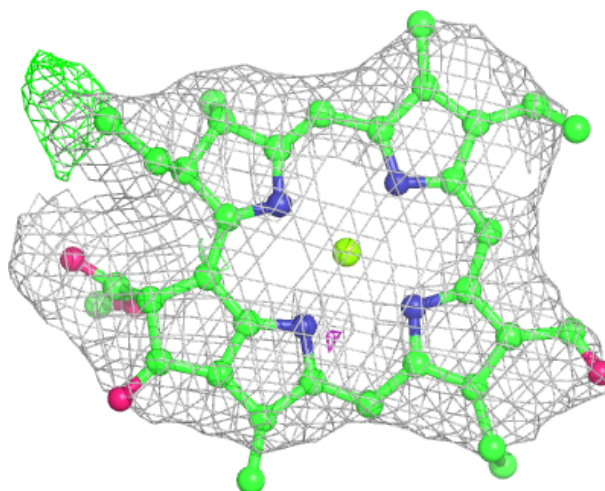
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CHL 2 605:**

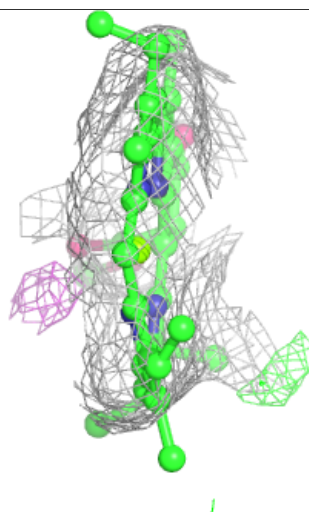
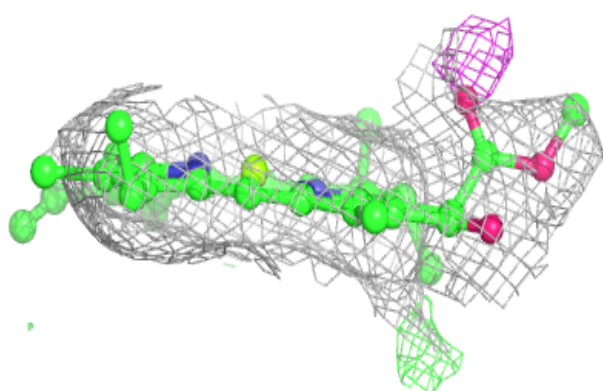
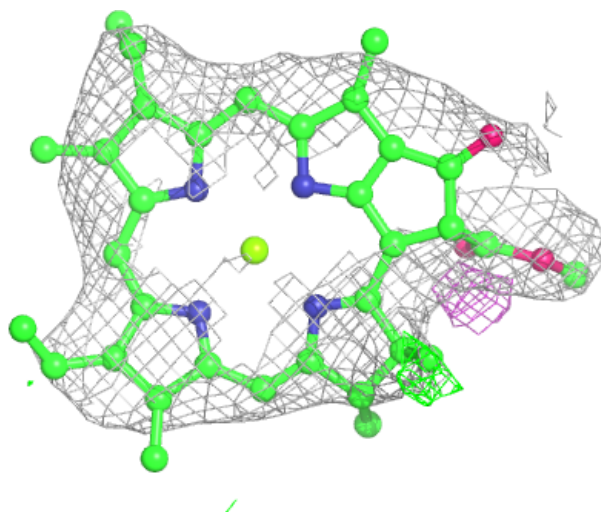
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





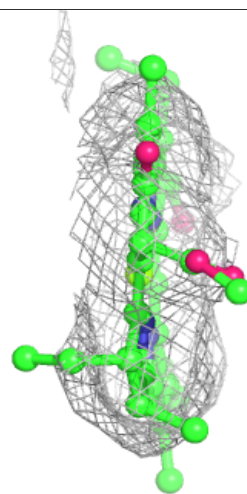
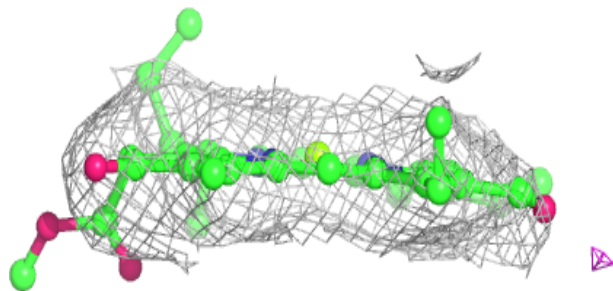
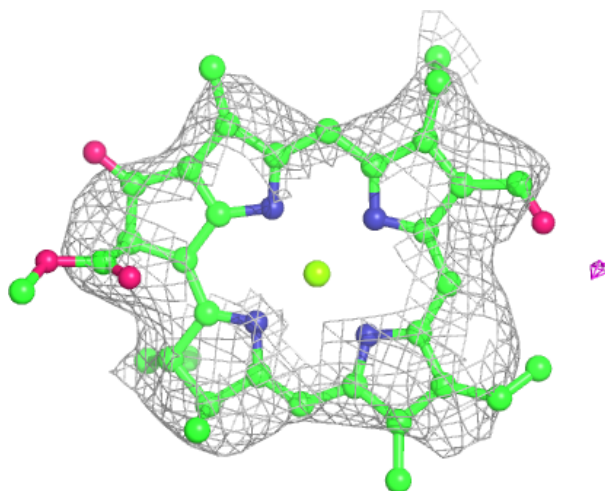
**Electron density around CLA 2 610:**

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



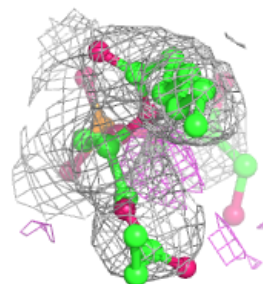
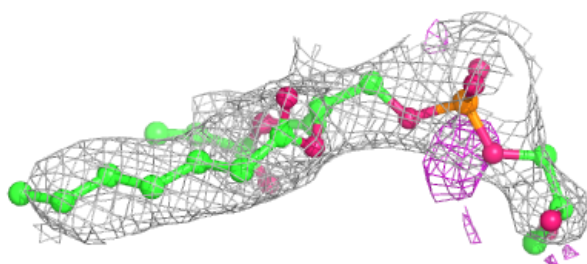
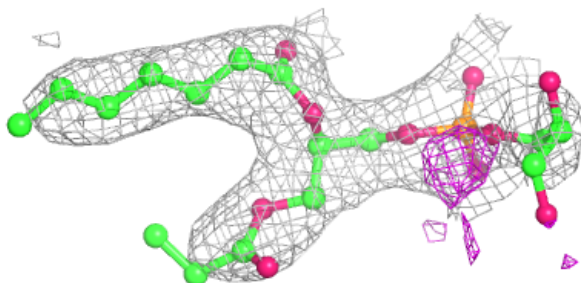
**Electron density around CHL 2 614:**

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



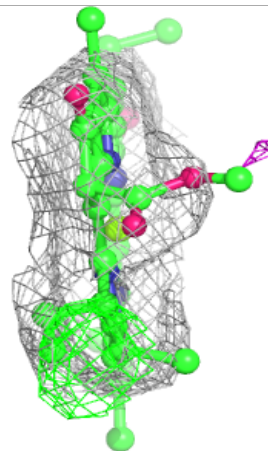
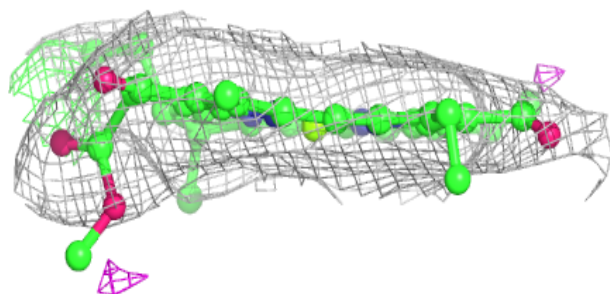
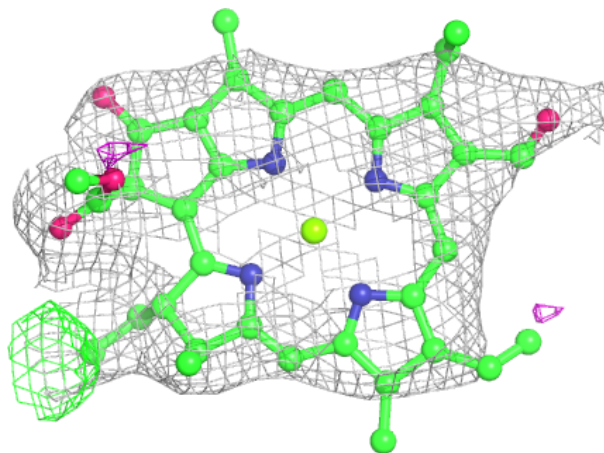
**Electron density around LHG a 848:**

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



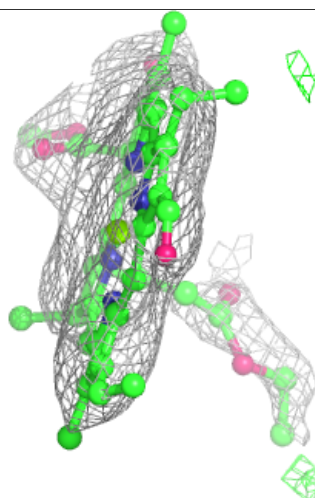
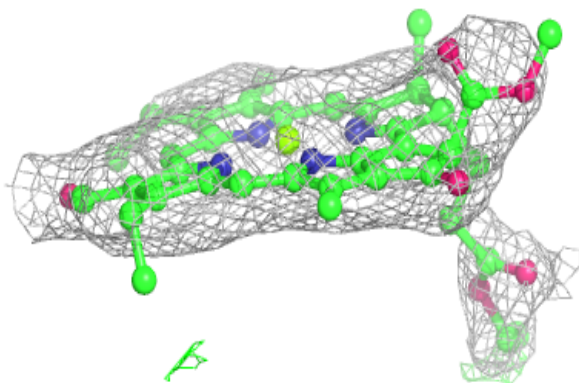
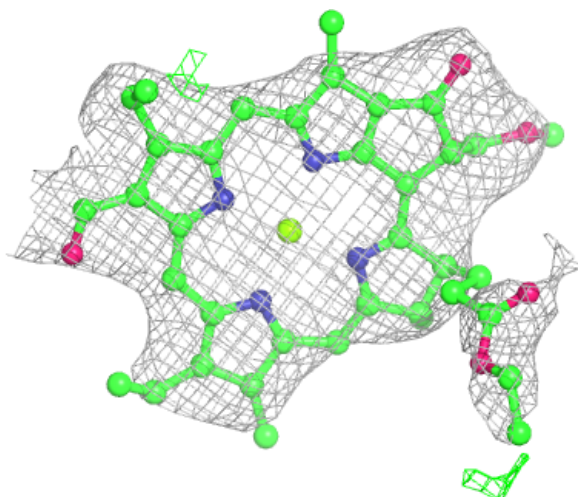
**Electron density around CHL 7 605:**

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



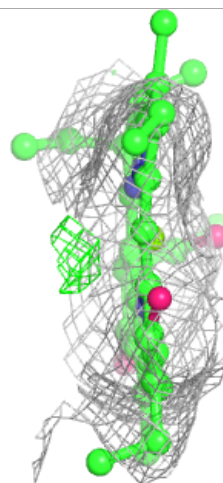
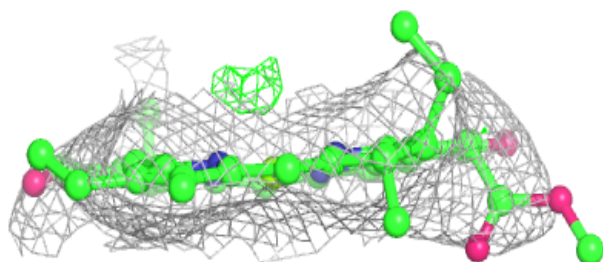
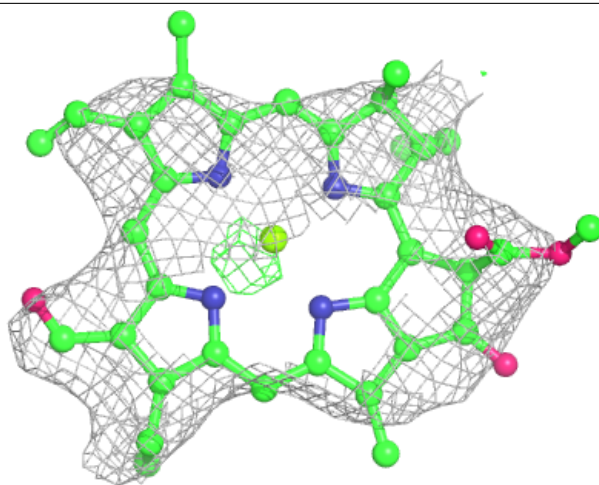
**Electron density around CHL 7 606:**

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



**Electron density around CHL 7 614:**

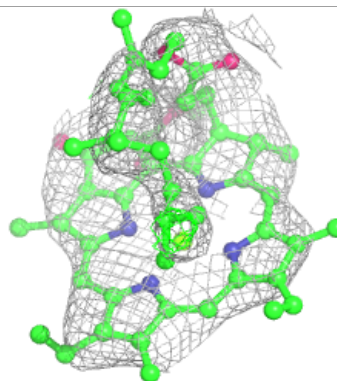
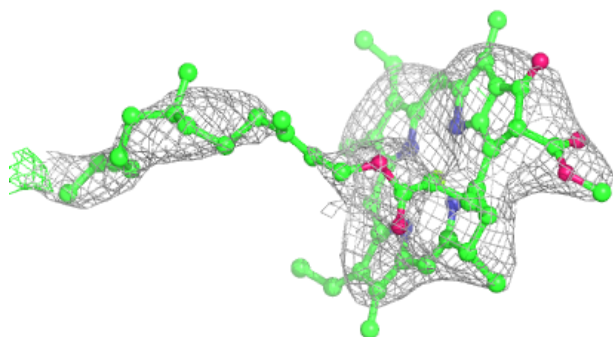
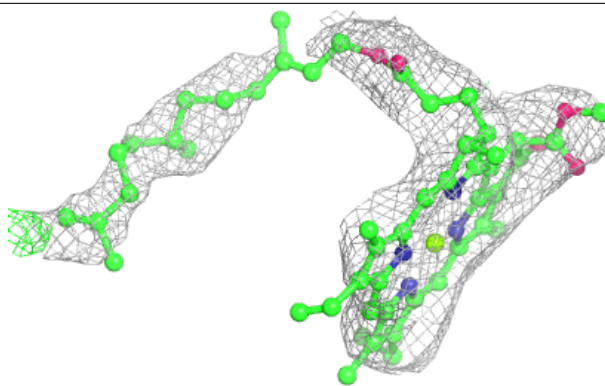
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



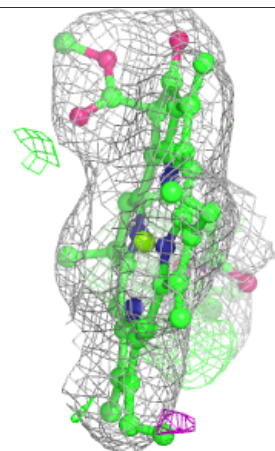
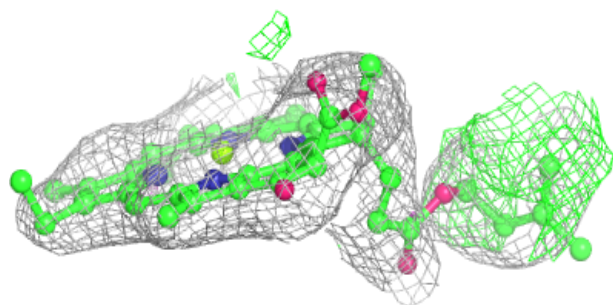
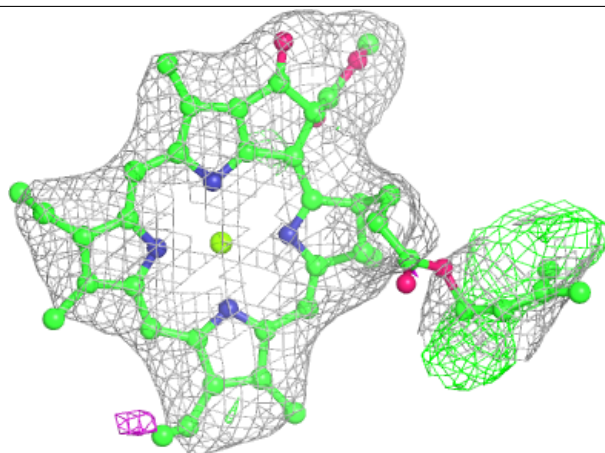


**Electron density around CLA 7 604:**

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

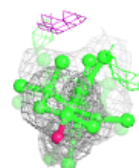
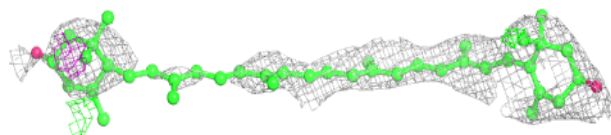
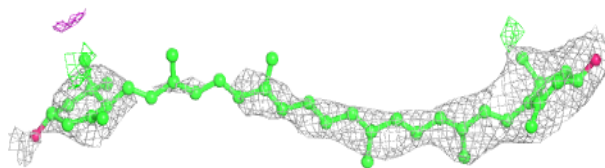
**Electron density around CLA 1 204:**

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

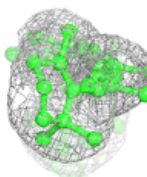
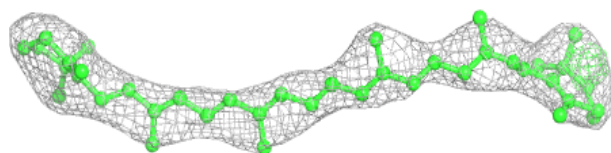
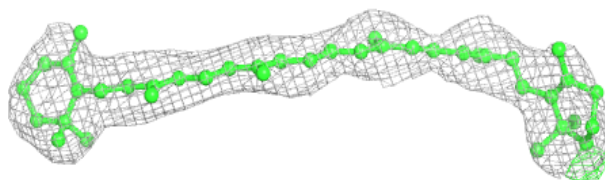


**Electron density around LUT 6 317:**

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

**Electron density around BCR I 101:**

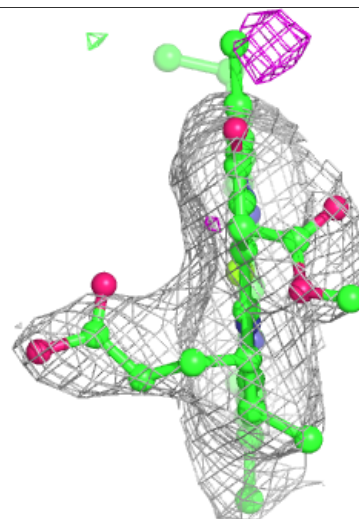
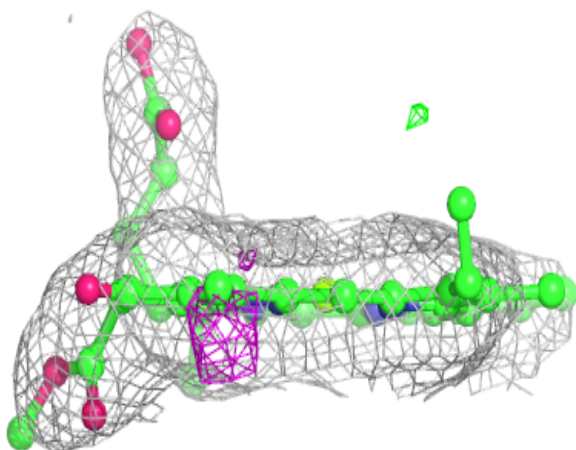
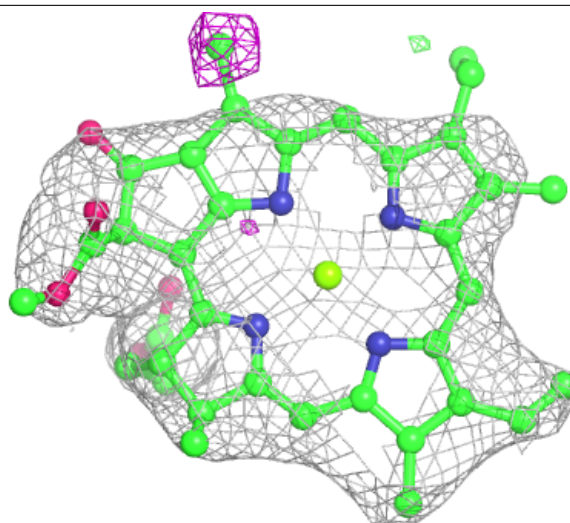
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





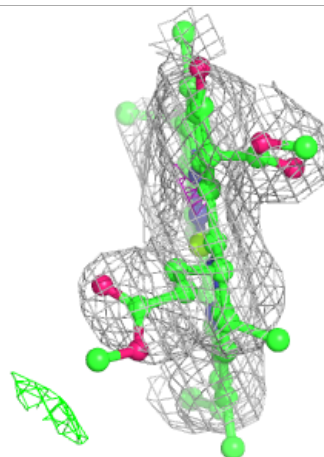
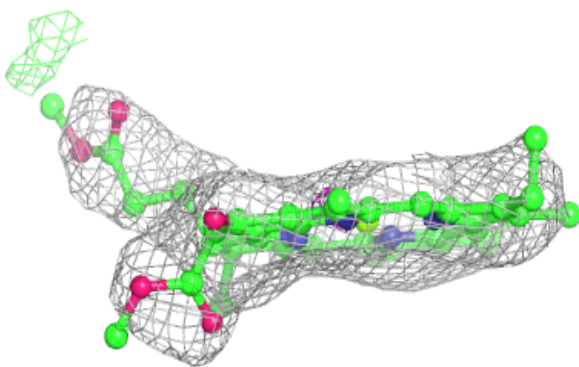
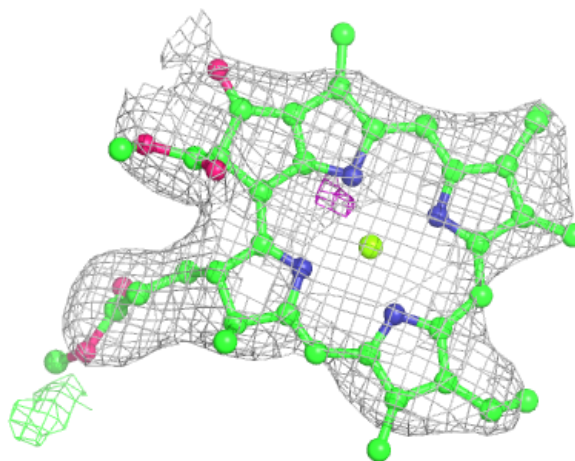
**Electron density around CLA A 837:**

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



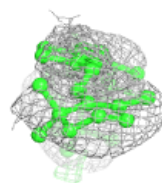
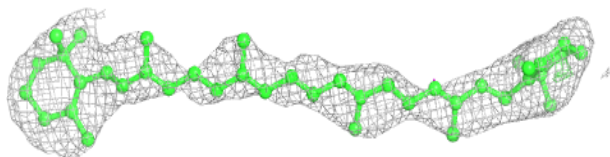
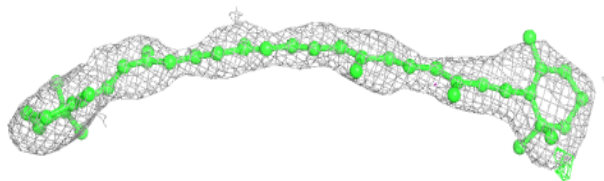
**Electron density around CLA k 1402:**

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

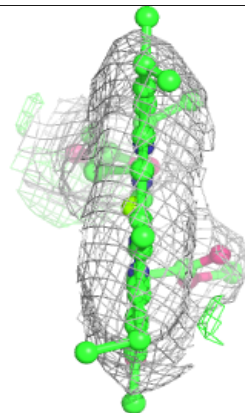
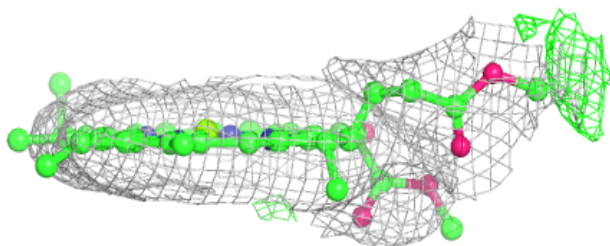
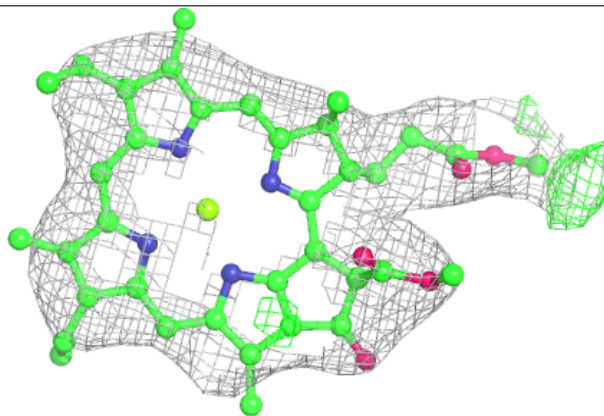


**Electron density around BCR a 849:**

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

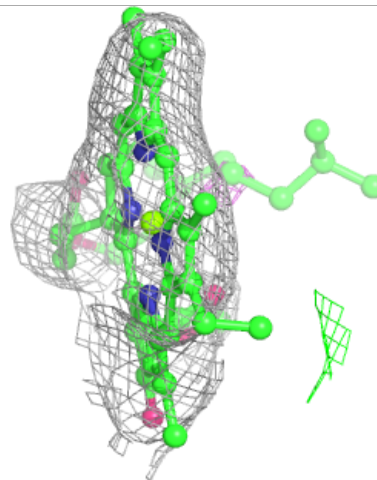
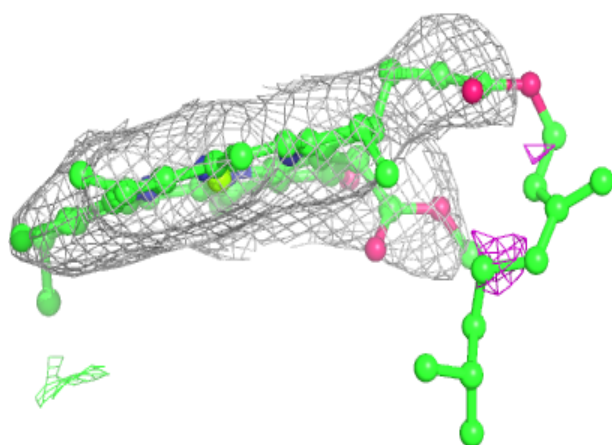
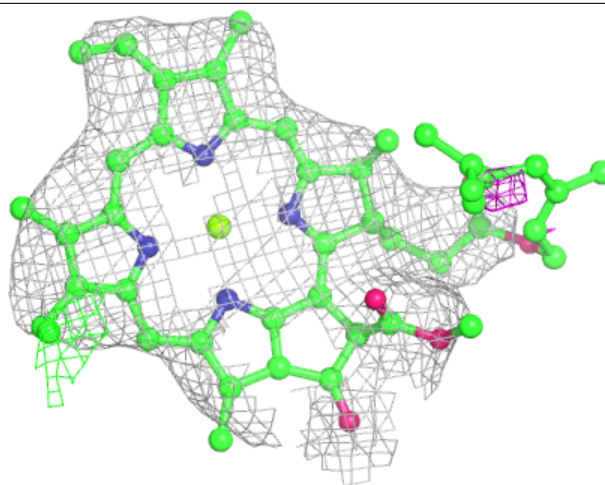
**Electron density around CLA 1 315:**

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



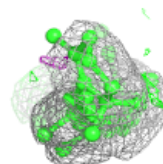
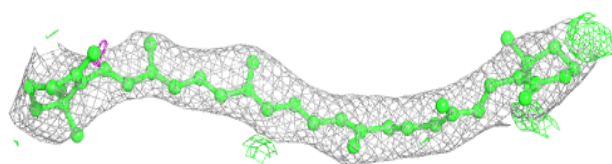
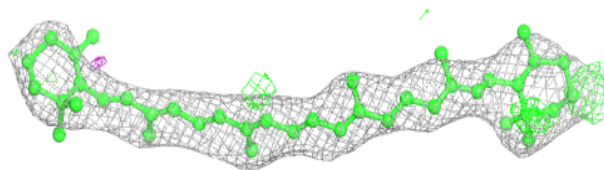
**Electron density around CLA f 7003:**

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

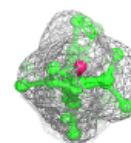
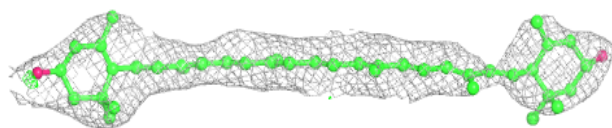
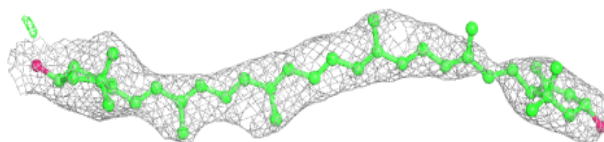


**Electron density around BCR j 3004:**

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

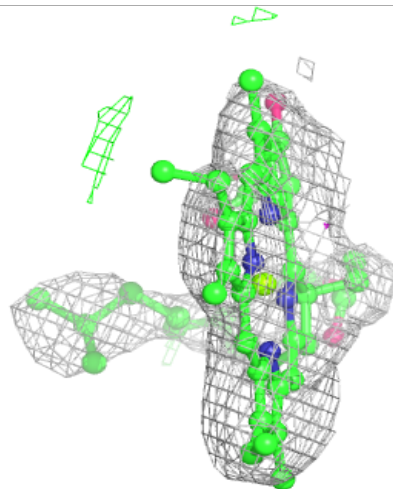
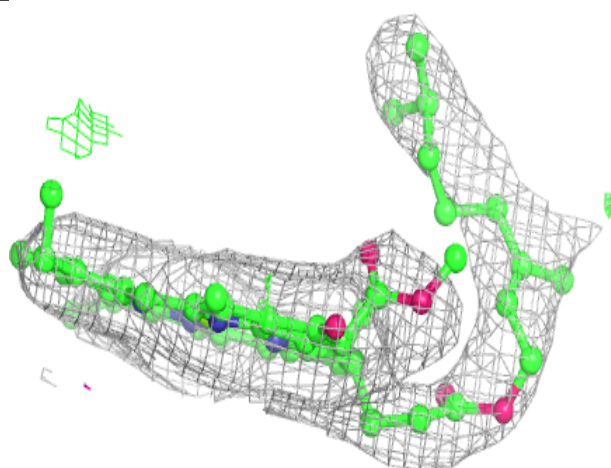
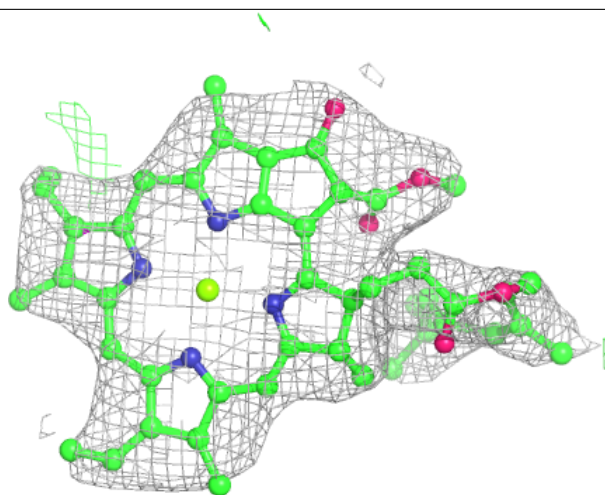
**Electron density around LUT 1 320:**

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



**Electron density around CLA F 304:**

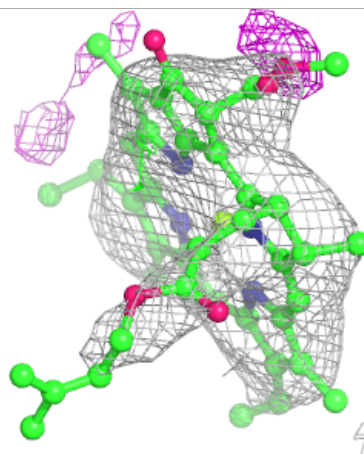
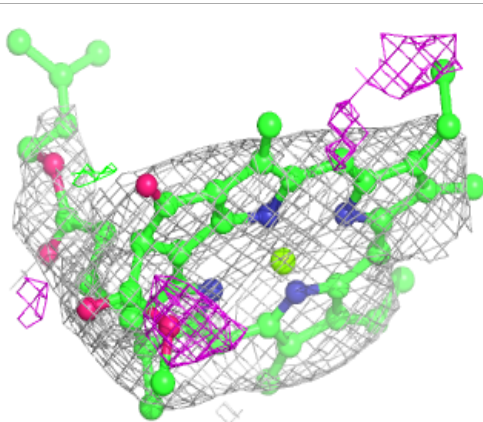
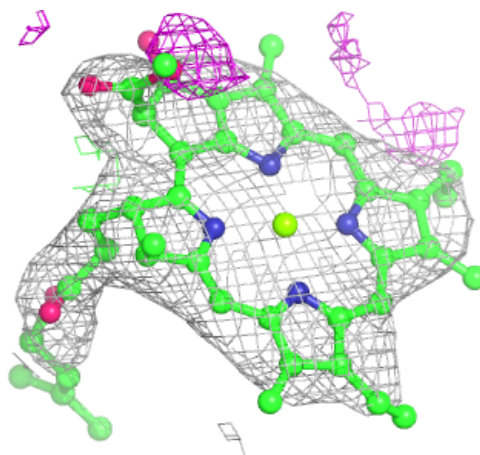
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





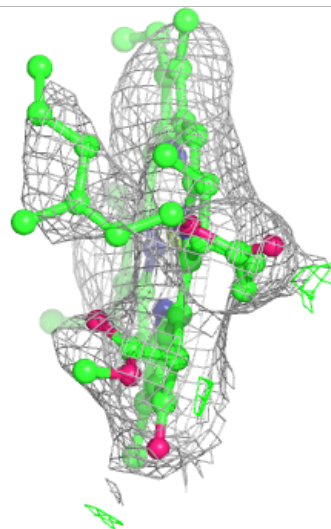
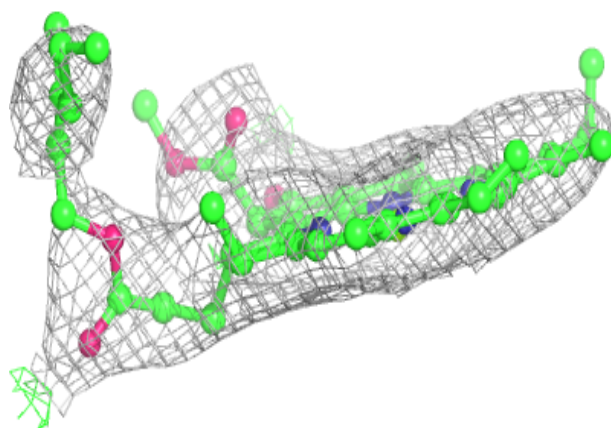
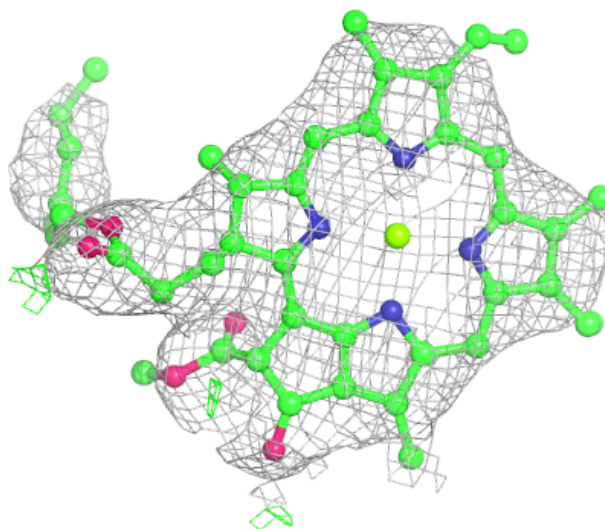
**Electron density around CLA 4 604:**

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



**Electron density around CLA 1 312:**

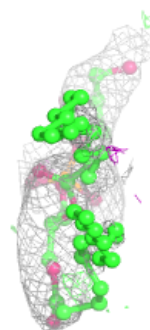
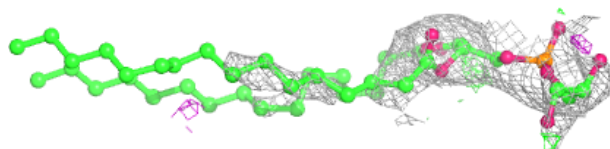
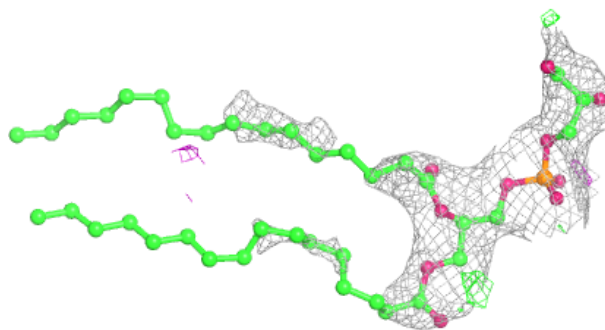
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



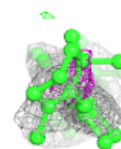
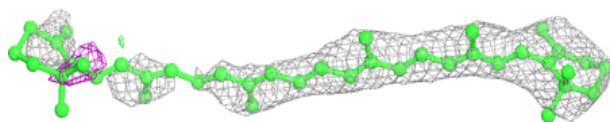
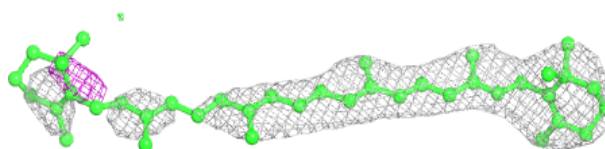


**Electron density around LHG 6 320:**

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

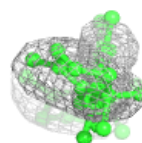
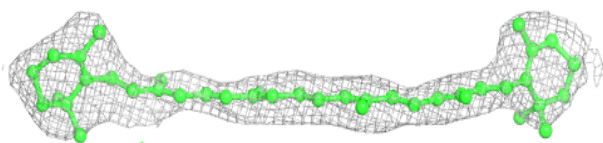
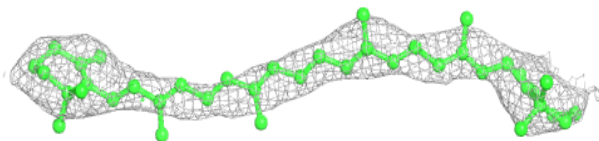
**Electron density around BCR a 852:**

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



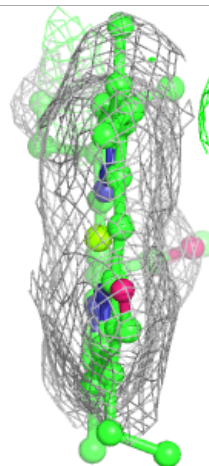
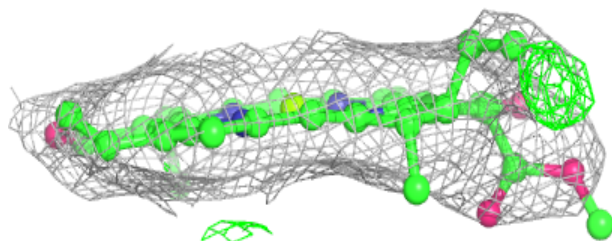
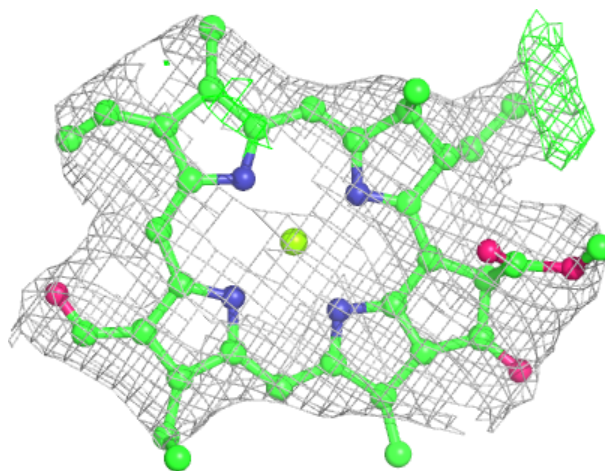
**Electron density around BCR 8 316:**

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



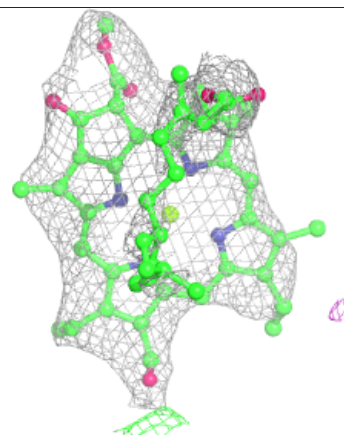
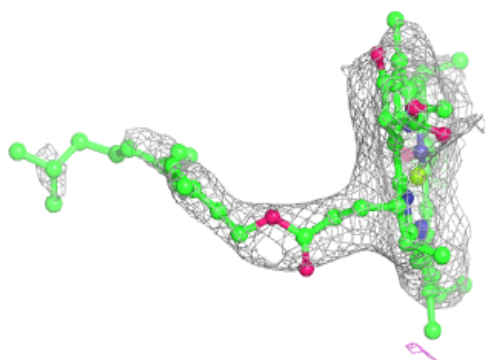
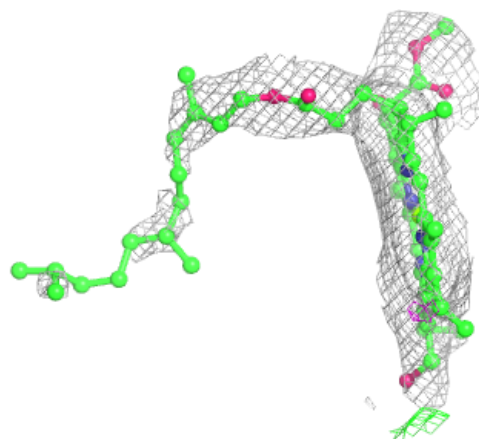
**Electron density around CHL 4 615:**

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



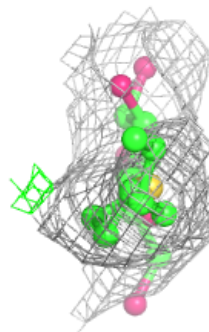
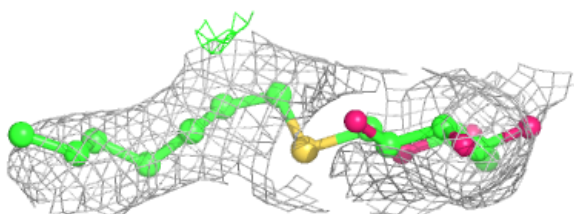
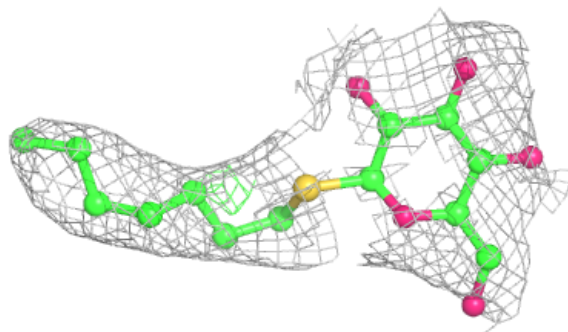
**Electron density around CHL 6 303:**

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

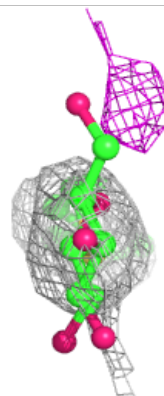
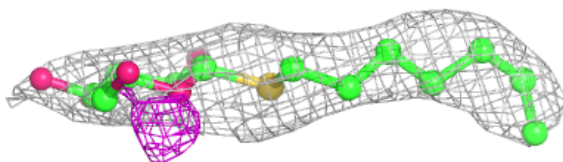
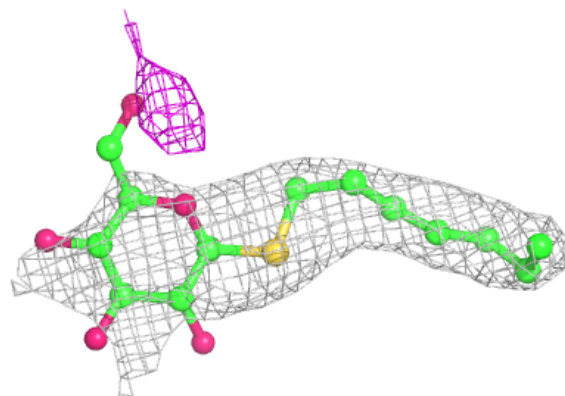


**Electron density around HTG J 3001:**

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

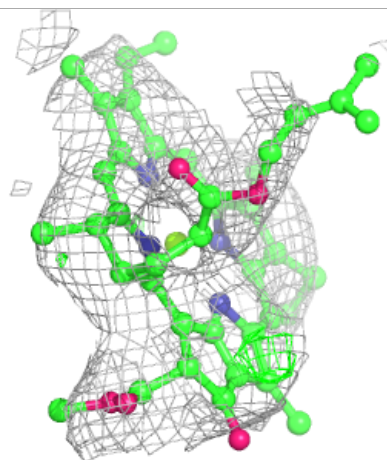
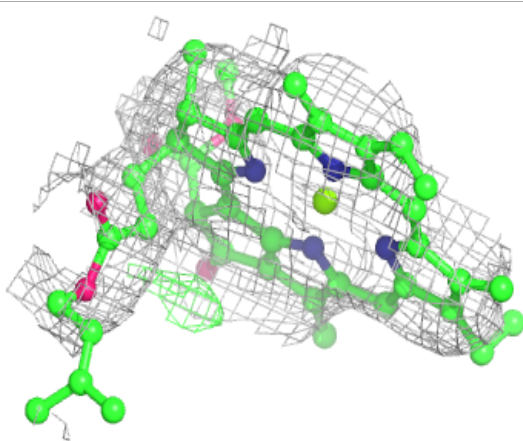
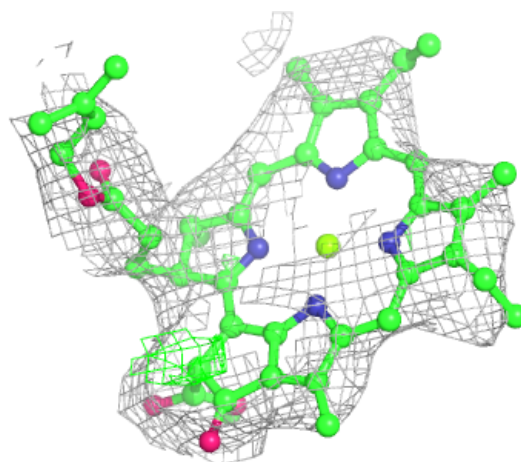
**Electron density around HTG f 7001:**

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



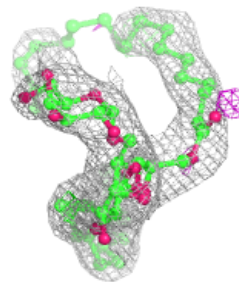
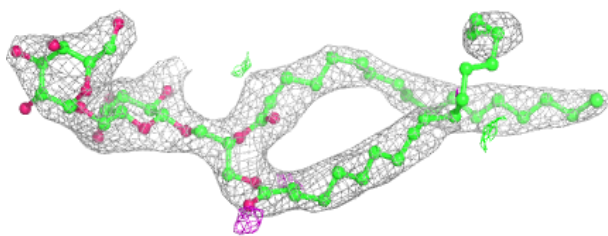
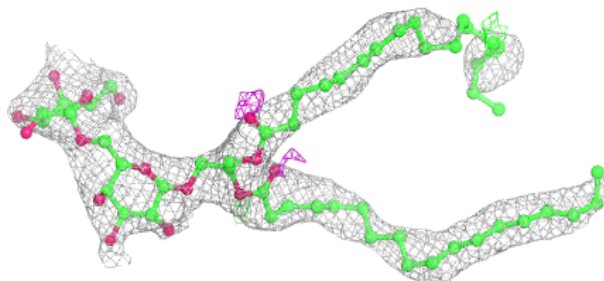
**Electron density around CLA 9 604:**

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



**Electron density around DGD b 849:**

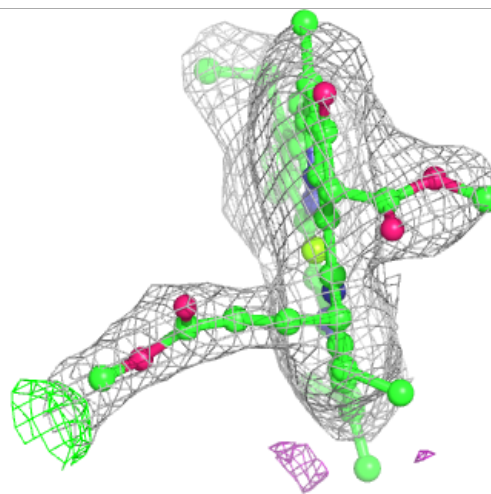
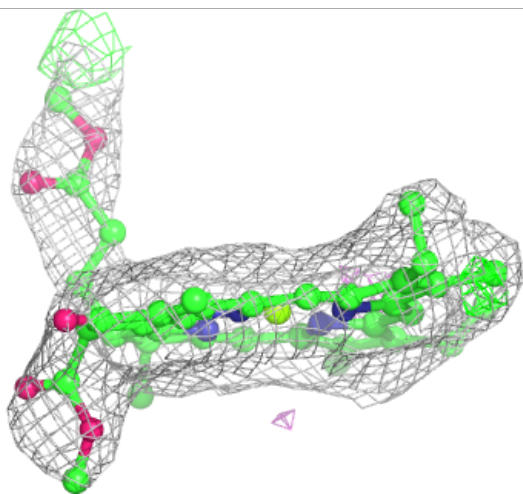
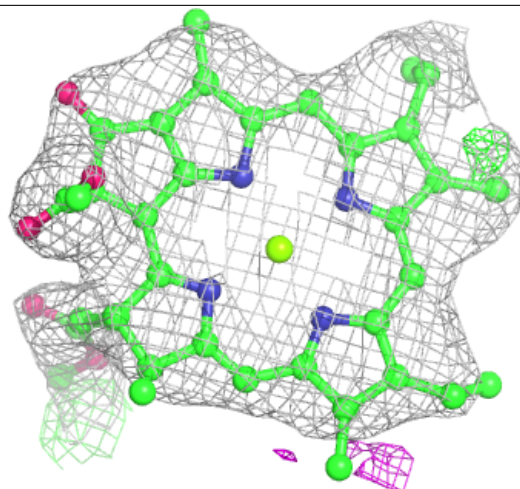
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA B 821:**

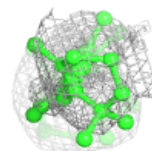
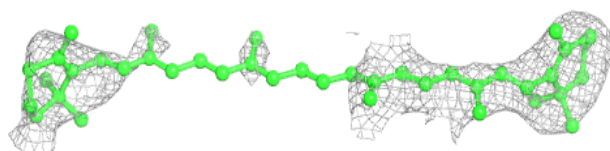
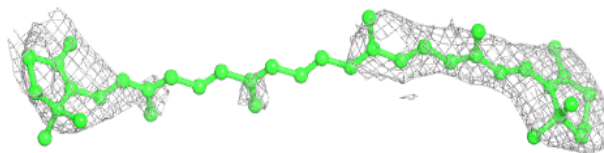
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





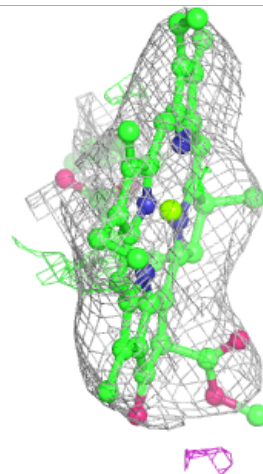
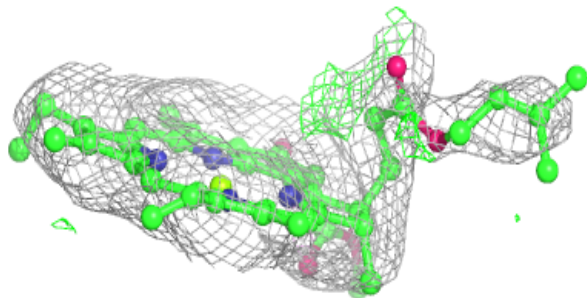
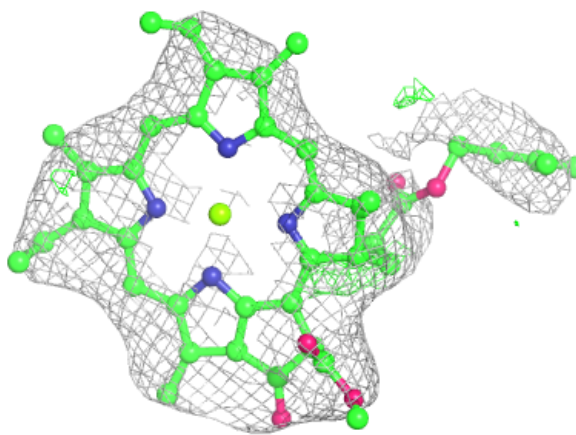
**Electron density around BCR g 104:**

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



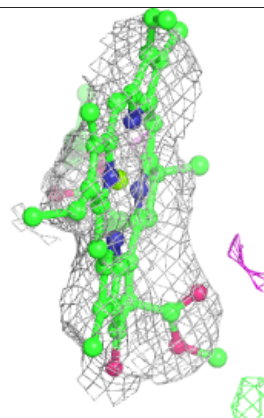
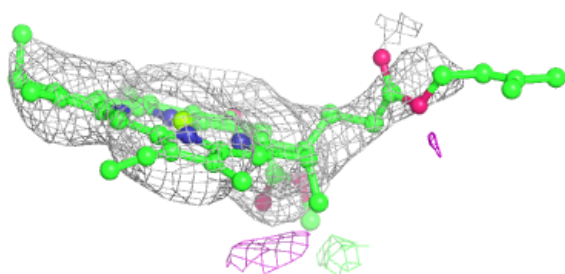
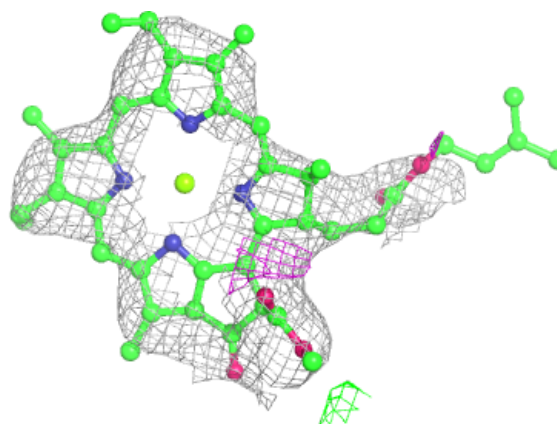
**Electron density around CLA L 204:**

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

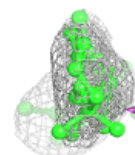
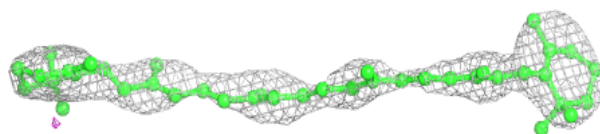
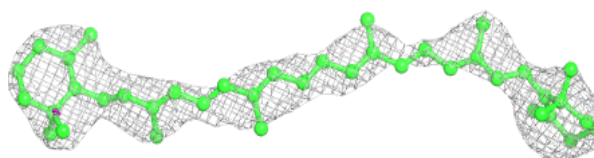


**Electron density around CLA g 102:**

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

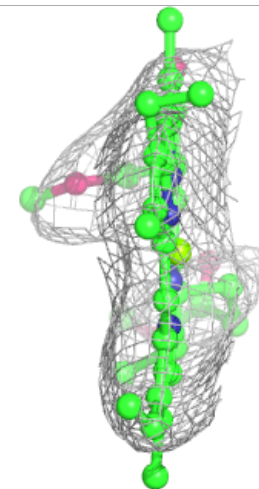
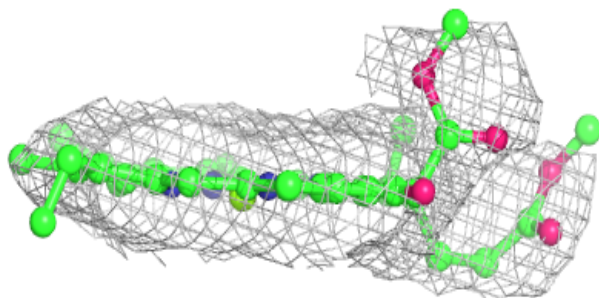
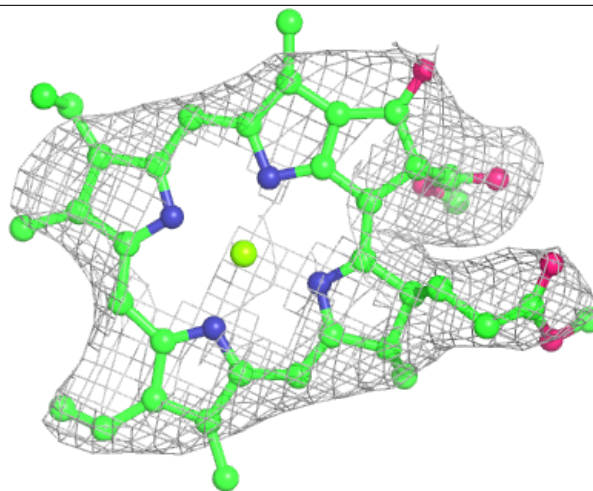
**Electron density around BCR 4 618:**

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



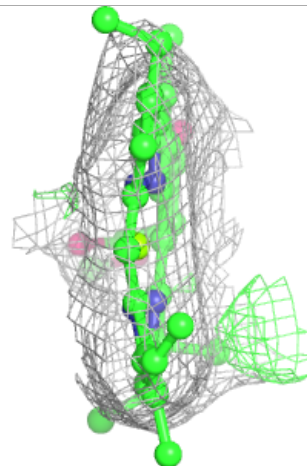
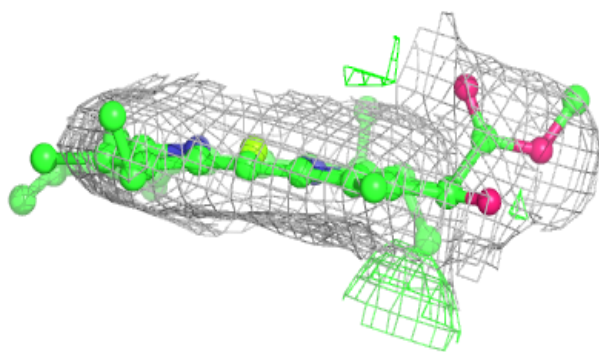
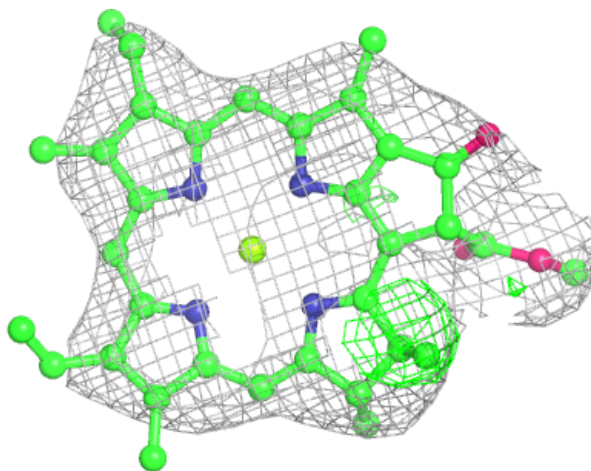
**Electron density around CLA g 103:**

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



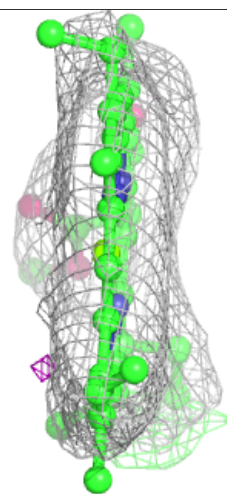
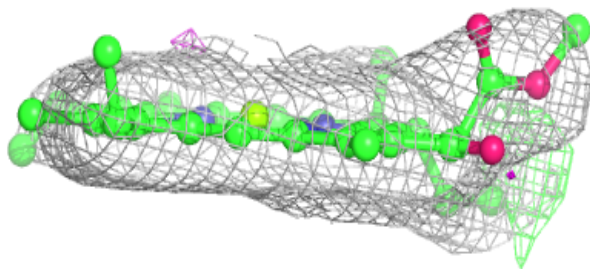
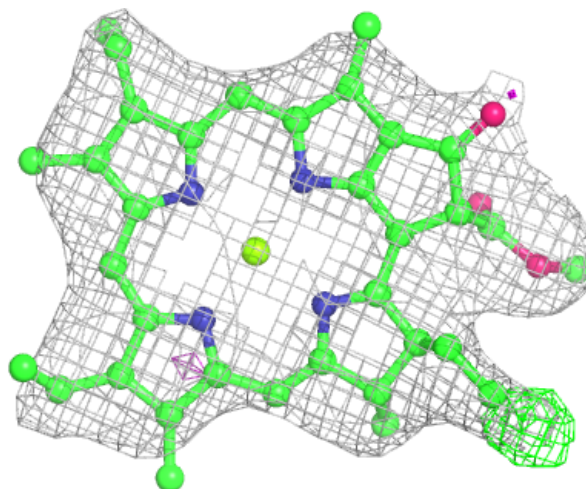
**Electron density around CLA 7 610:**

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



**Electron density around CLA 3 305:**

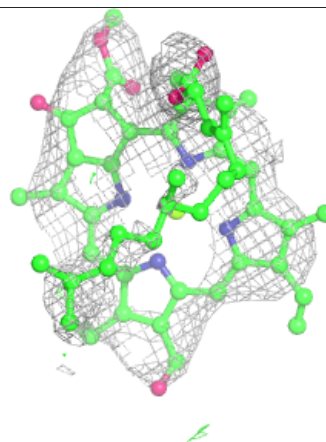
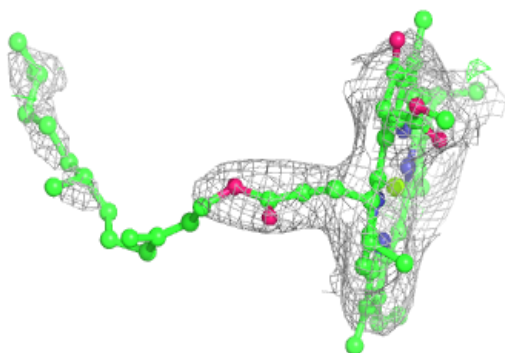
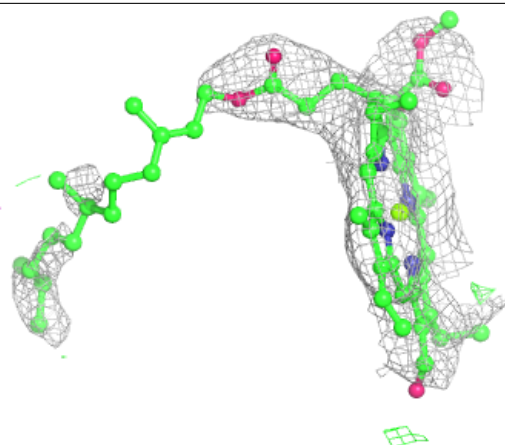
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



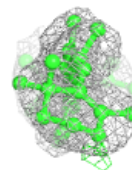
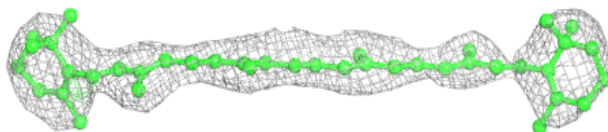
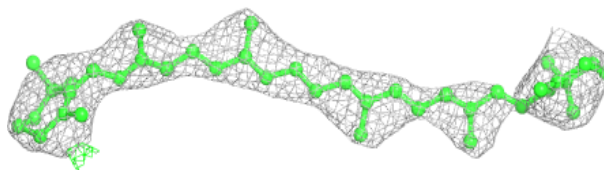


**Electron density around CHL 2 601:**

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

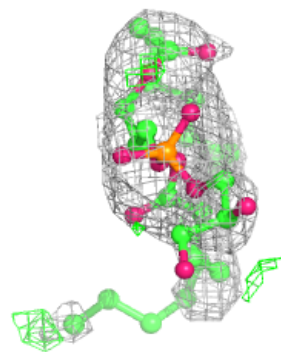
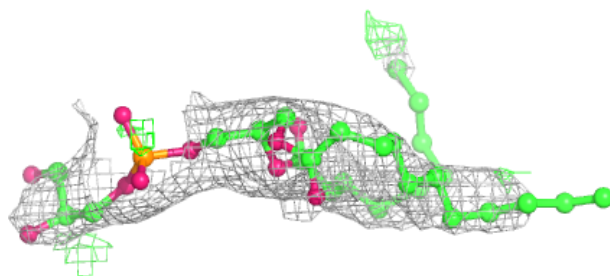
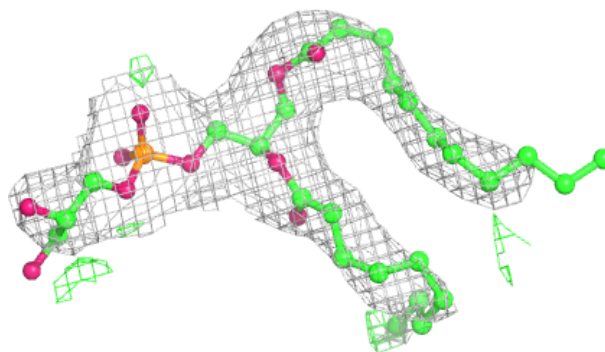
**Electron density around BCR b 846:**

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



**Electron density around LHG 7 618:**

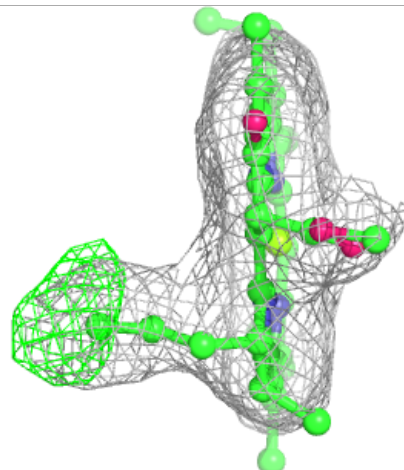
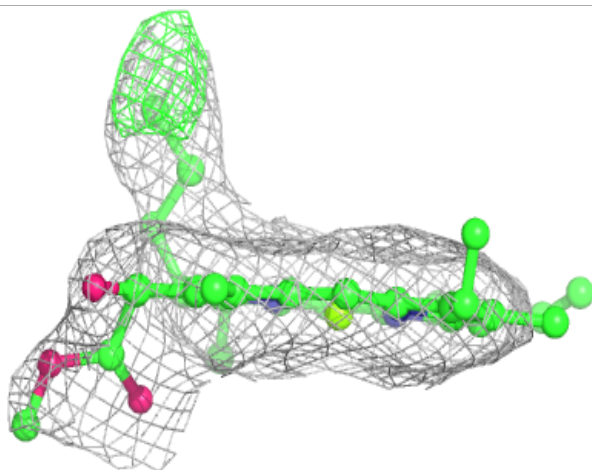
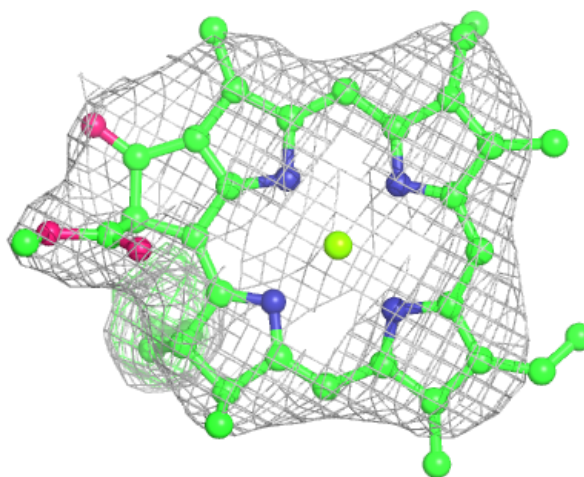
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





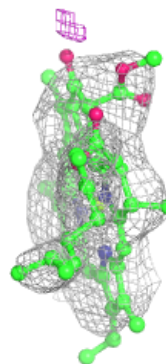
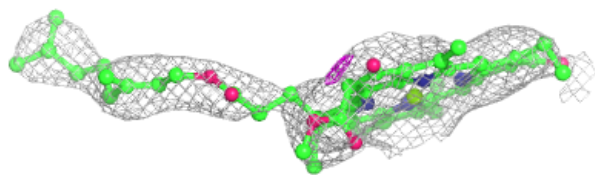
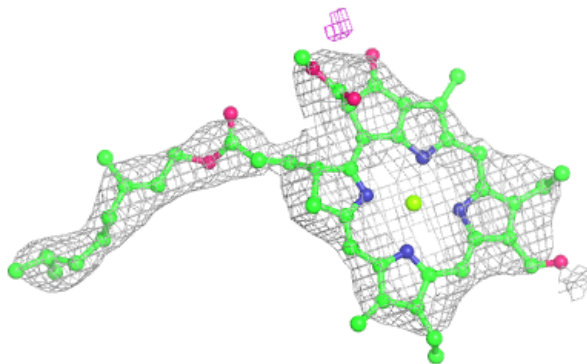
**Electron density around CLA 7 613:**

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



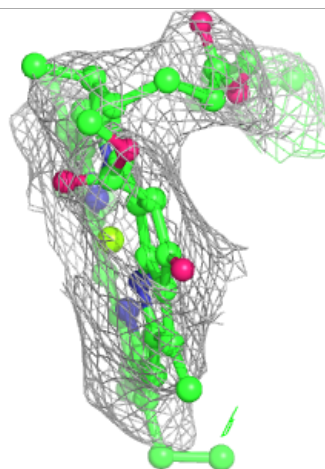
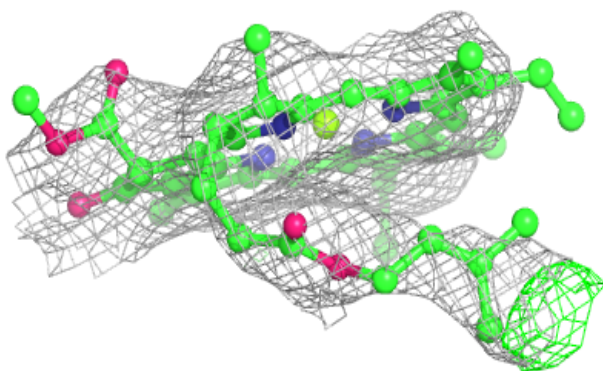
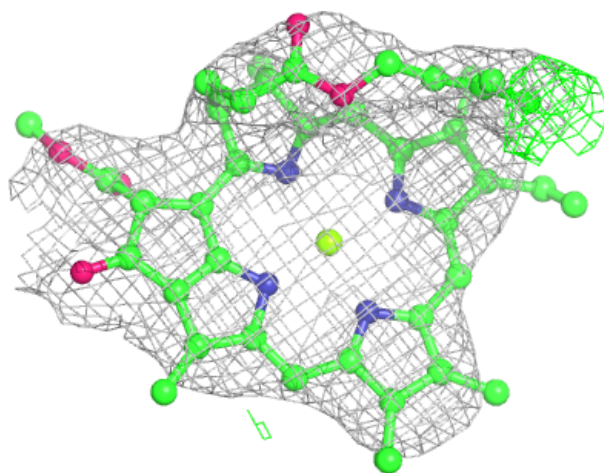
**Electron density around CHL 4 605:**

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



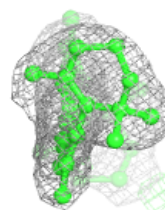
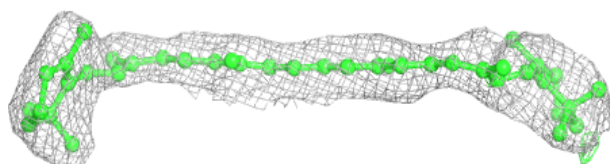
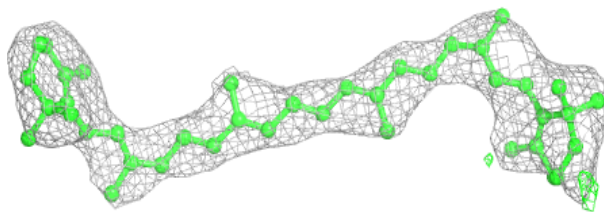
**Electron density around CLA 8 308:**

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

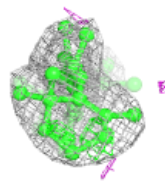
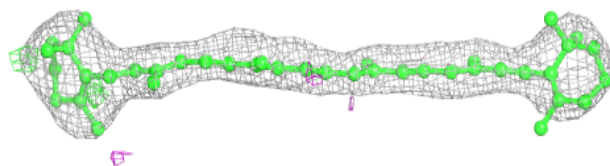
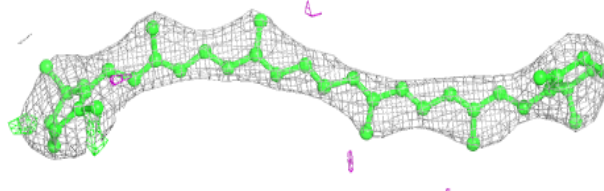


**Electron density around BCR B 845:**

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

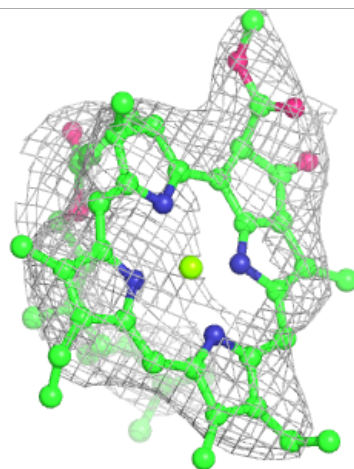
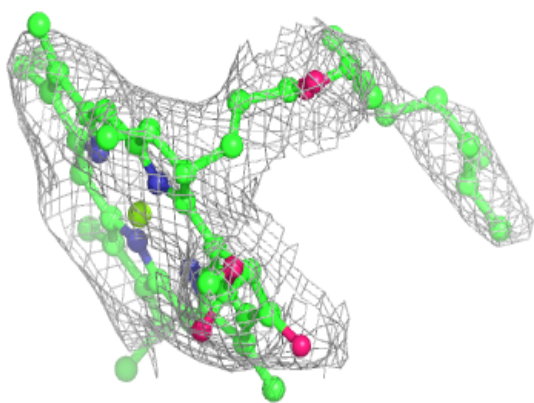
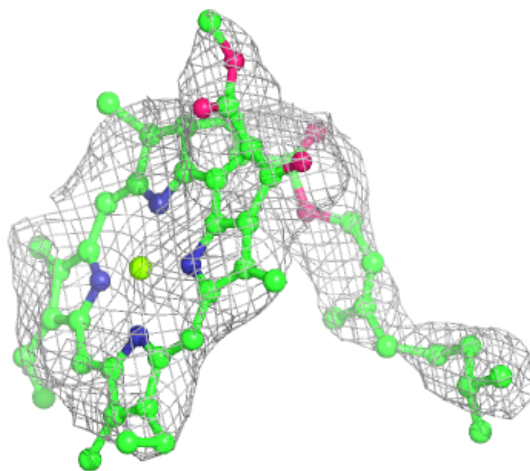
**Electron density around BCR B 846:**

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



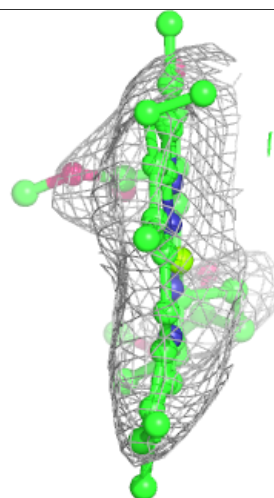
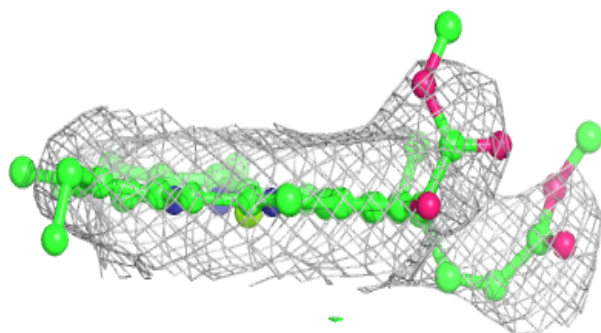
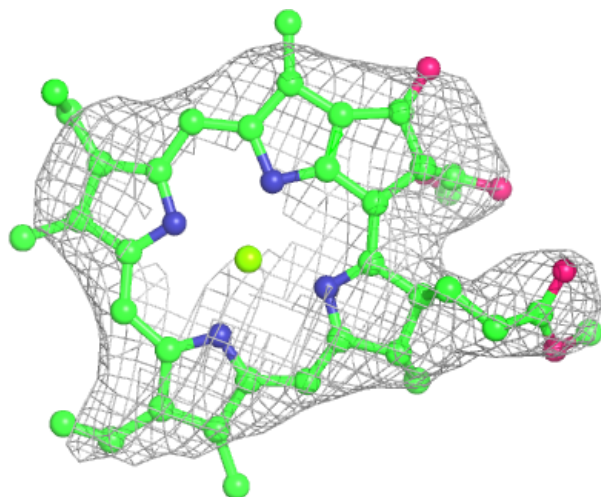
**Electron density around CLA 4 610:**

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



**Electron density around CLA G 104:**

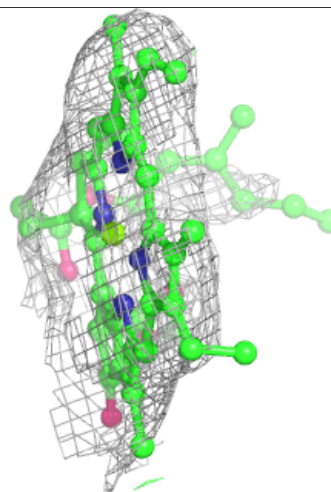
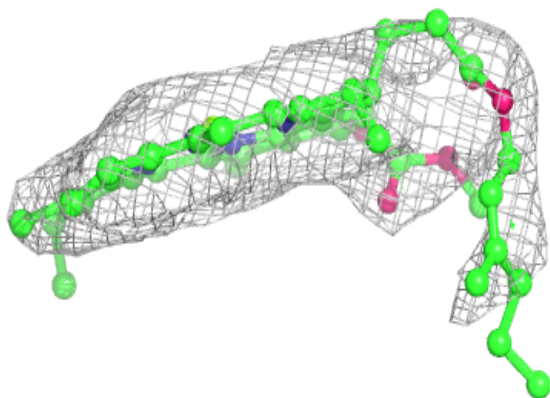
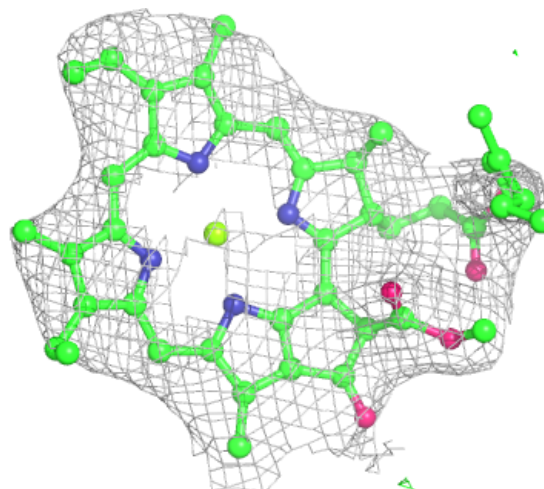
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





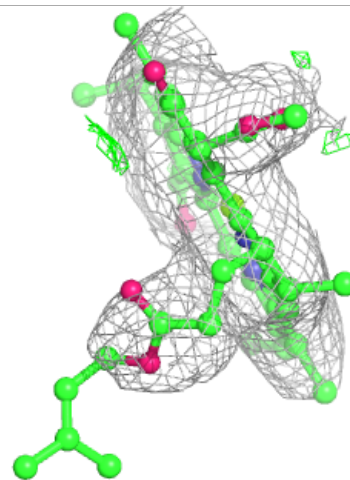
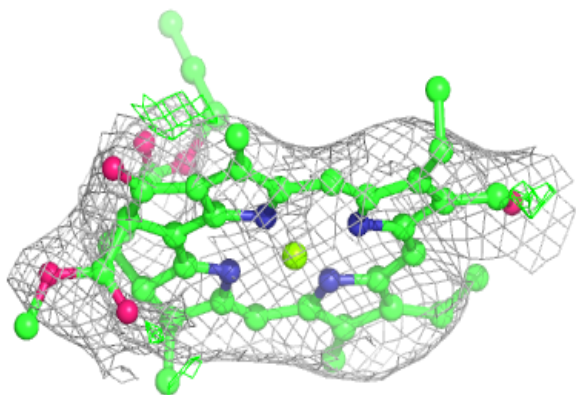
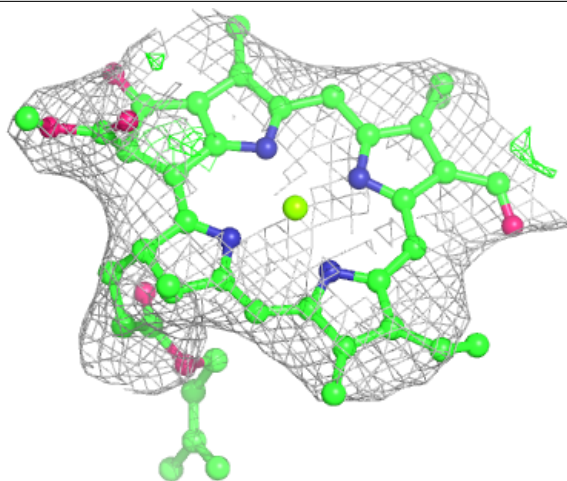
**Electron density around CLA 2 611:**

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



**Electron density around CHL 9 606:**

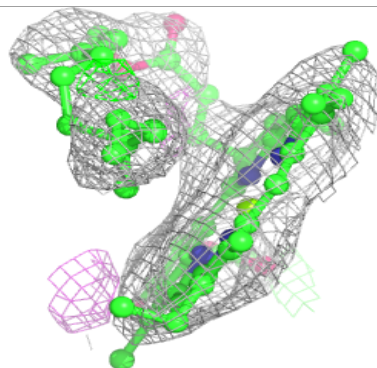
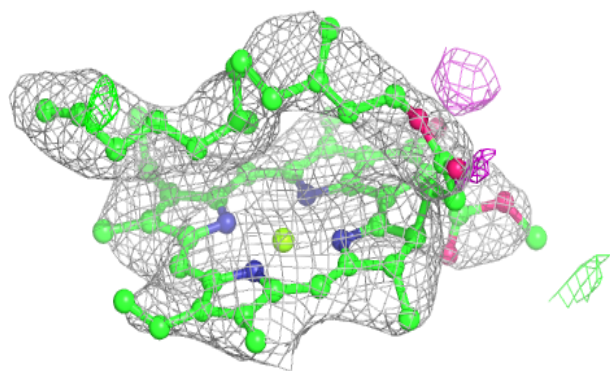
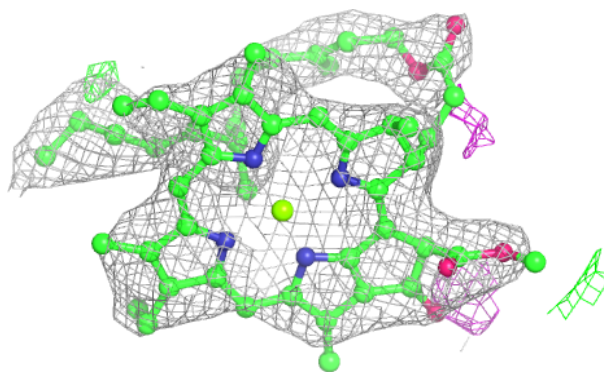
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





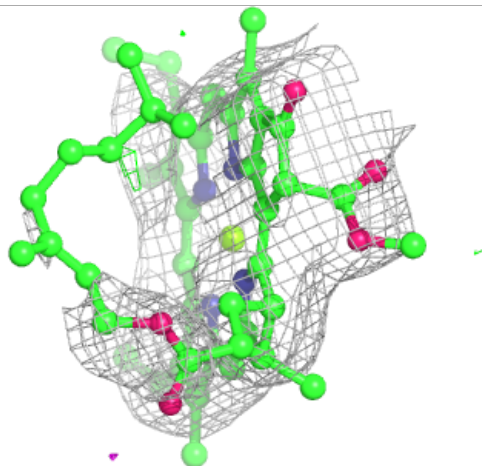
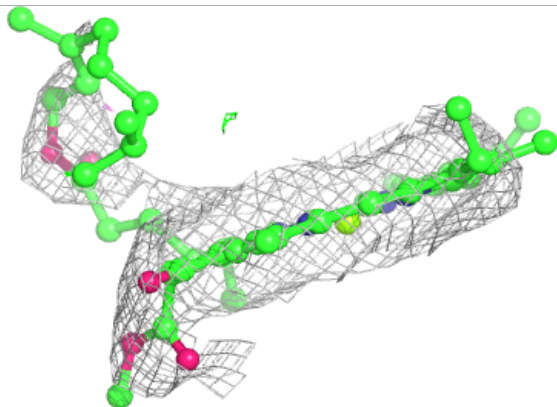
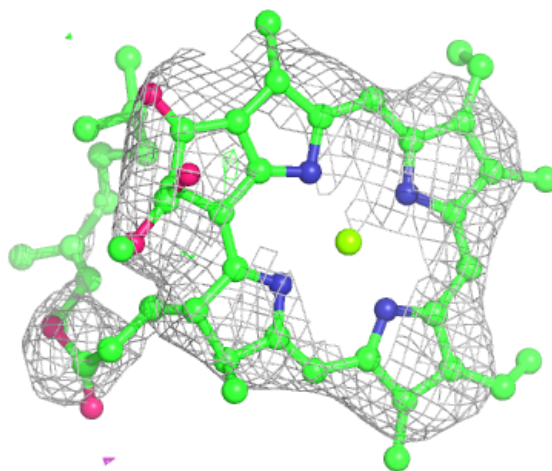
**Electron density around CLA b 817:**

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



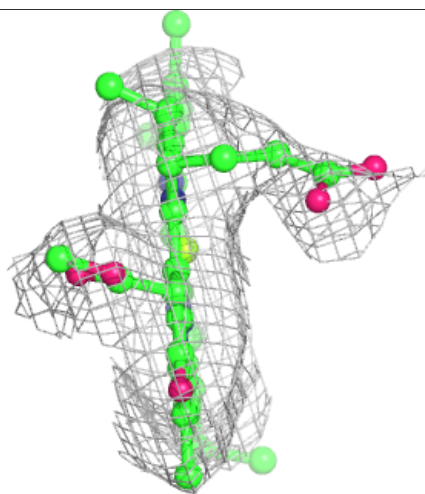
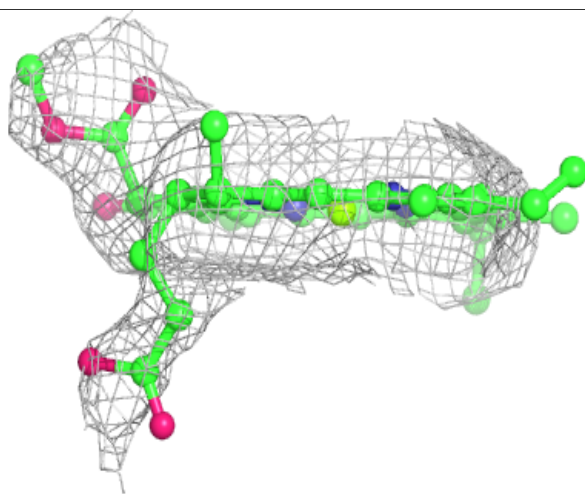
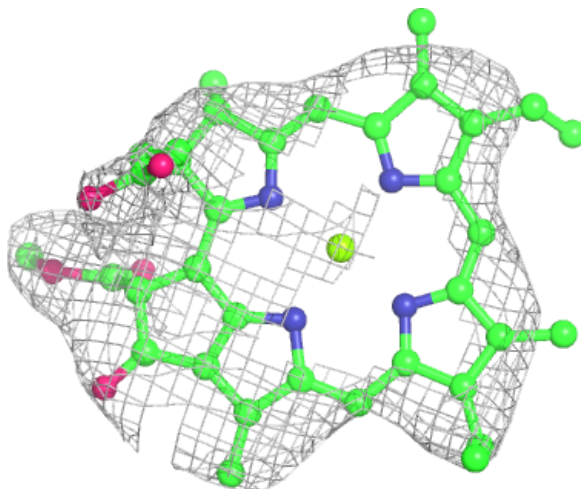
**Electron density around CLA 6 315:**

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



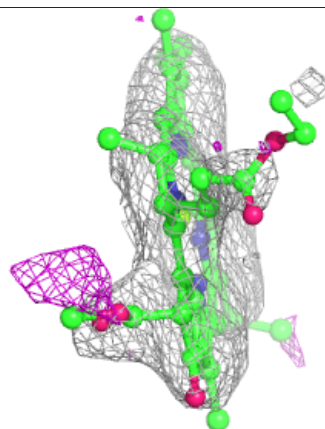
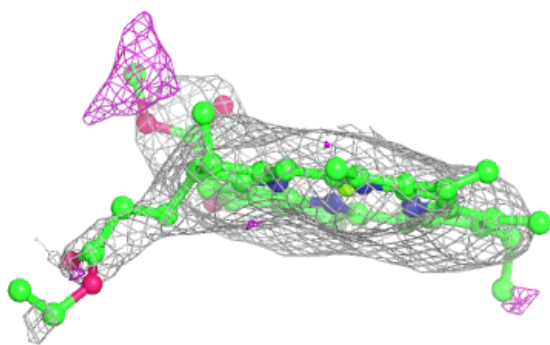
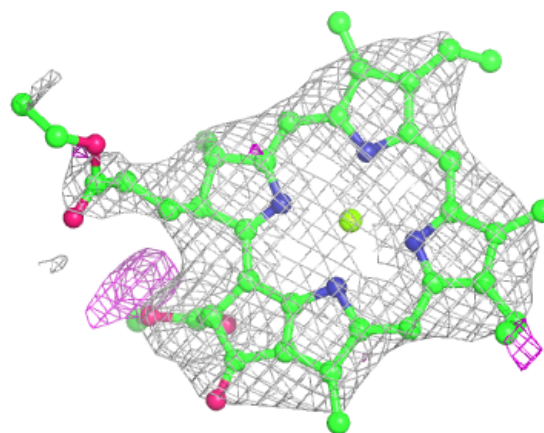
**Electron density around CLA 9 613:**

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



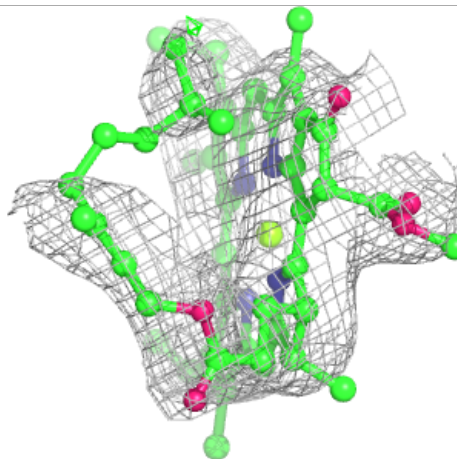
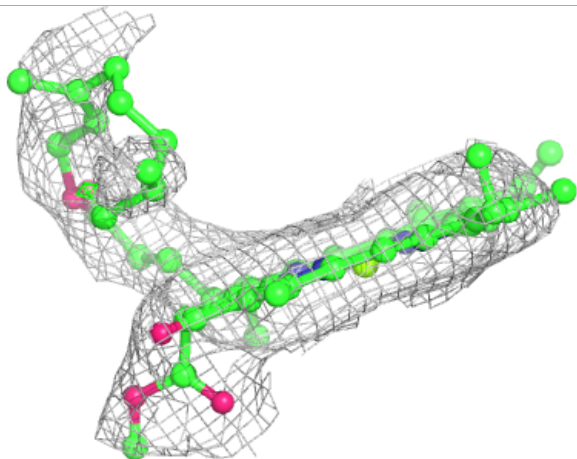
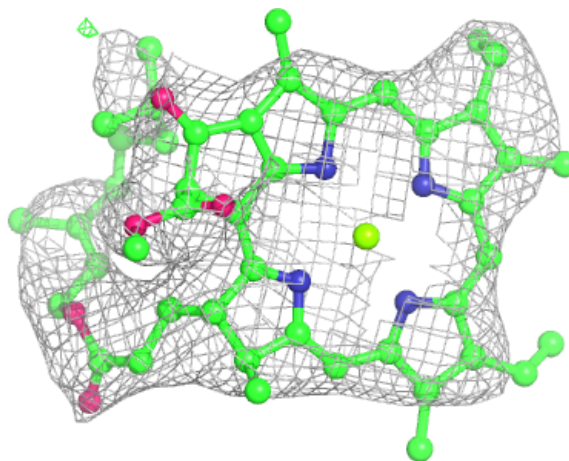
**Electron density around CLA 9 614:**

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



**Electron density around CLA 1 314:**

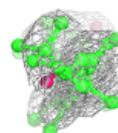
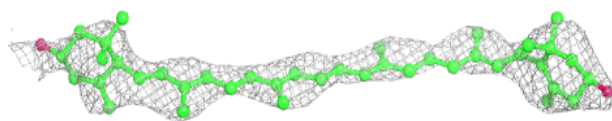
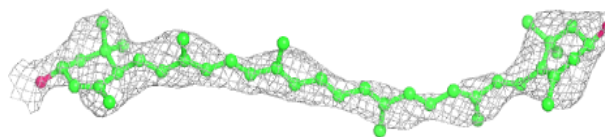
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



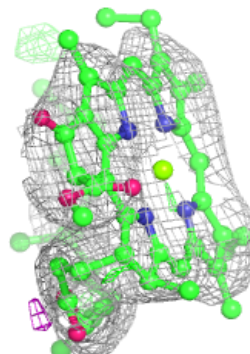
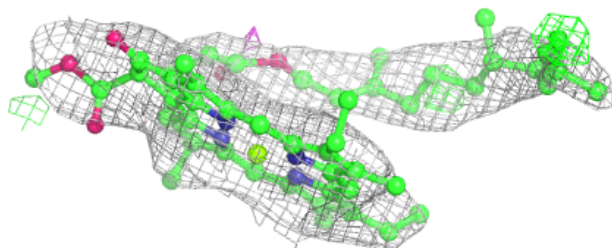
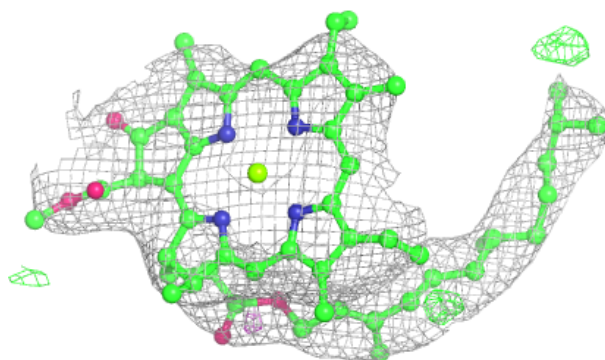


**Electron density around LUT 7 615:**

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

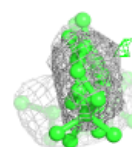
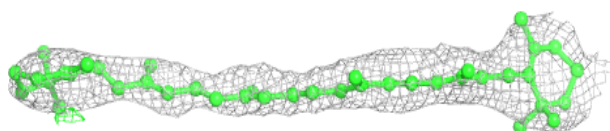
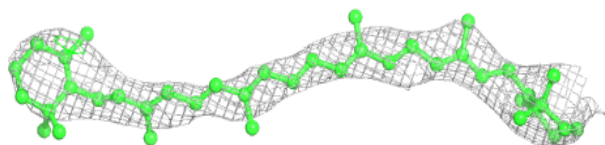
**Electron density around CLA 1 310:**

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

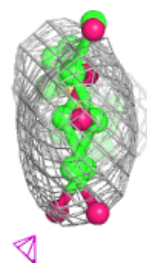
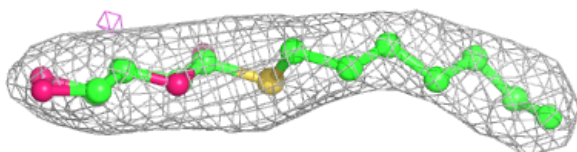
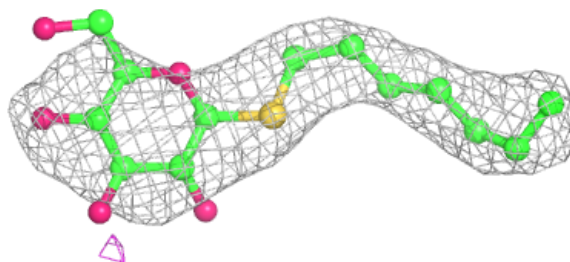


**Electron density around BCR 9 618:**

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

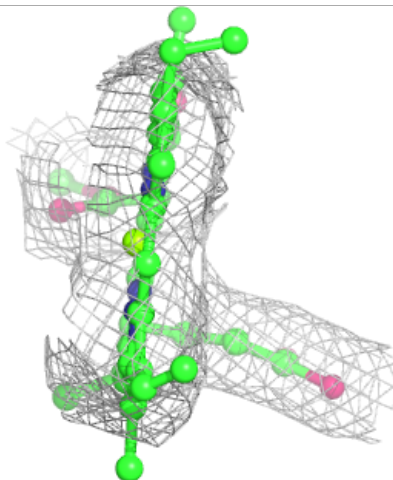
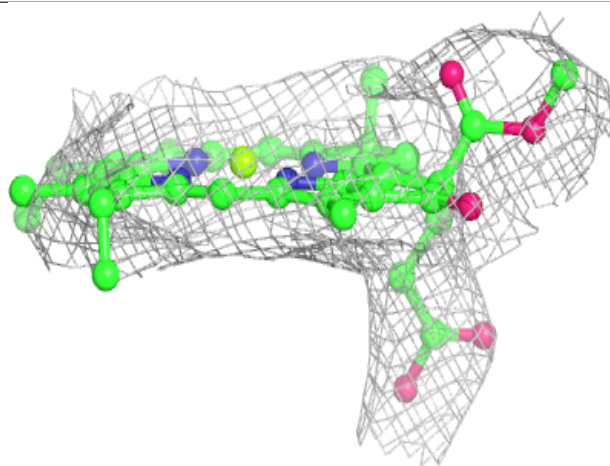
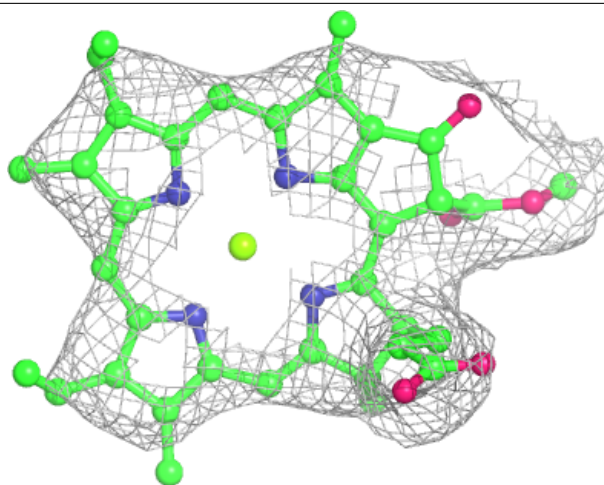
**Electron density around HTG F 302:**

$2mF_o-DF_c$  (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:**

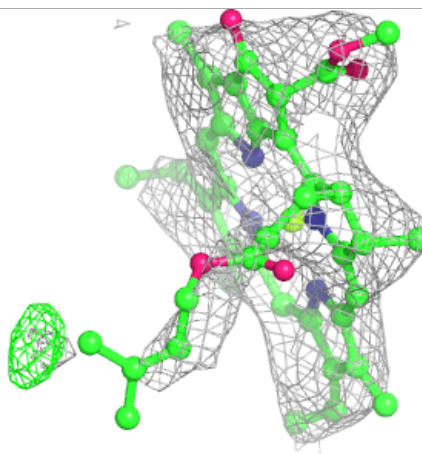
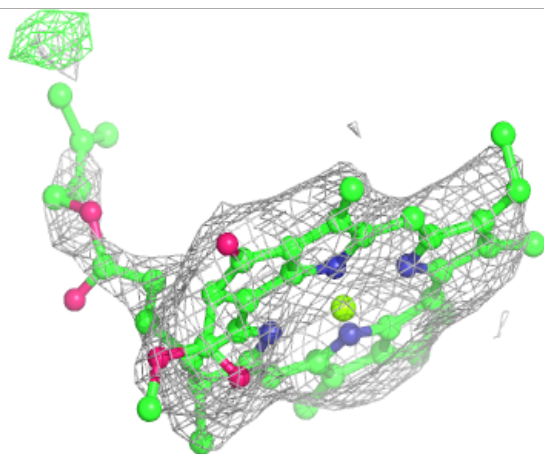
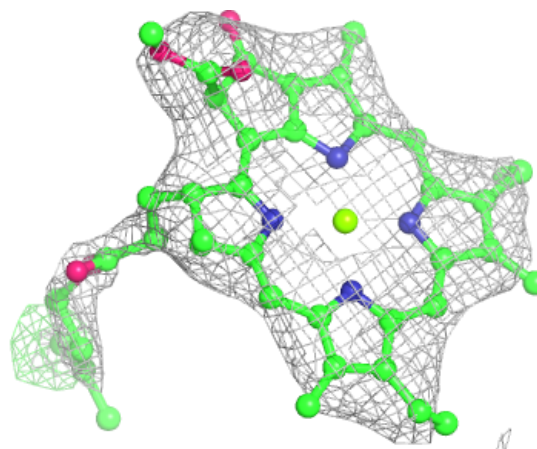
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





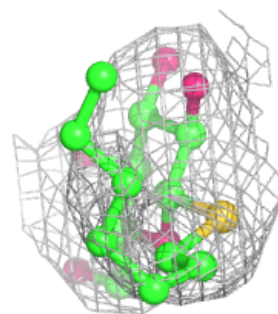
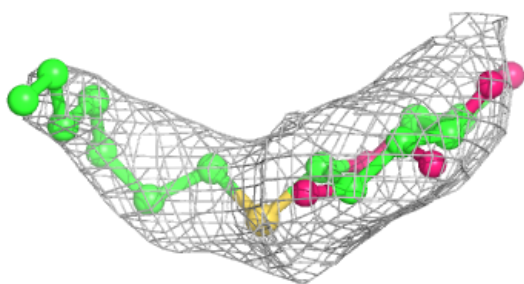
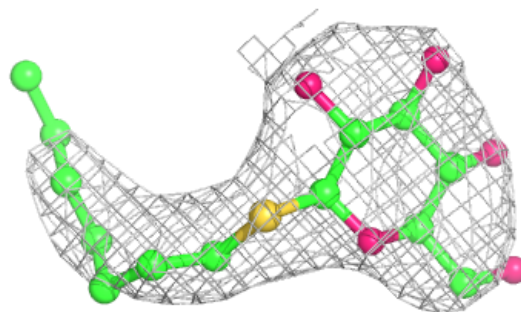
**Electron density around CLA A 816:**

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



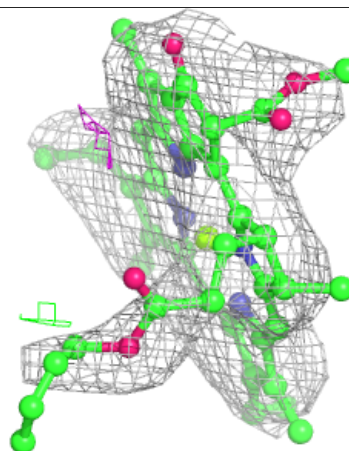
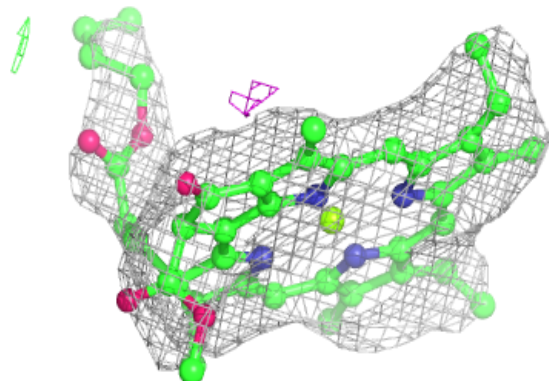
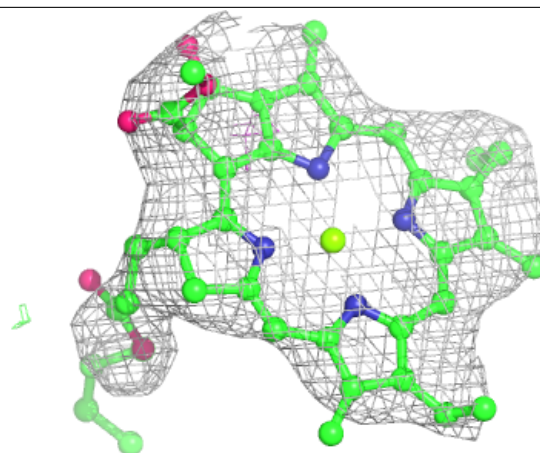
**Electron density around HTG j 3001:**

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

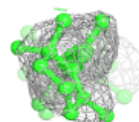
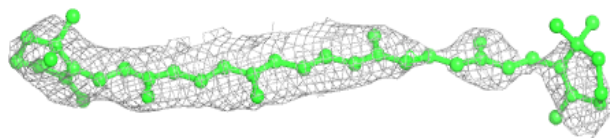
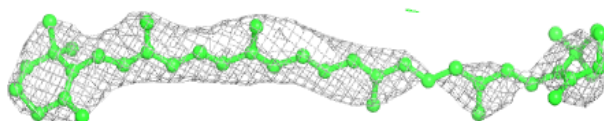


**Electron density around CLA A 823:**

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

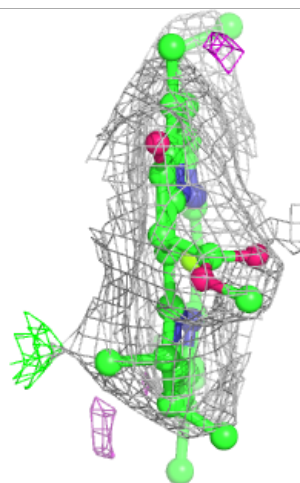
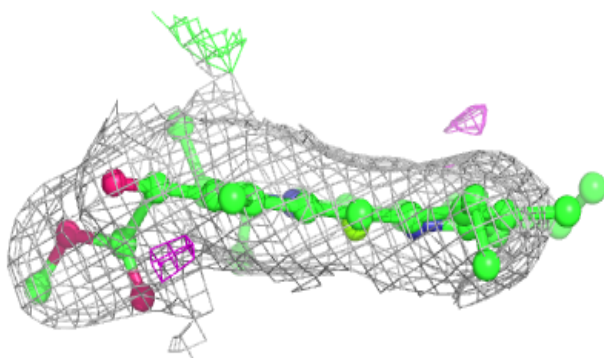
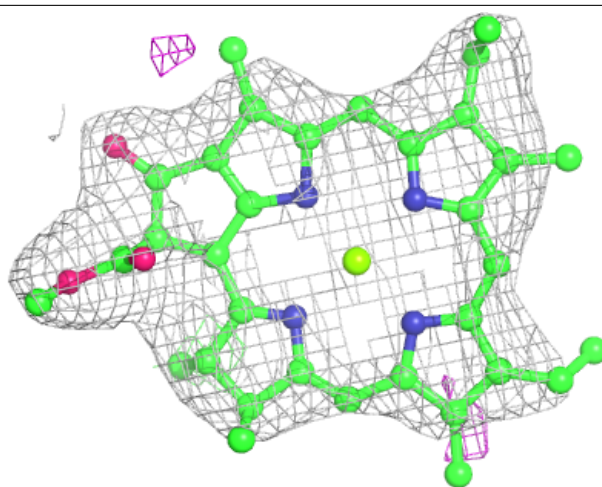
**Electron density around BCR A 850:**

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



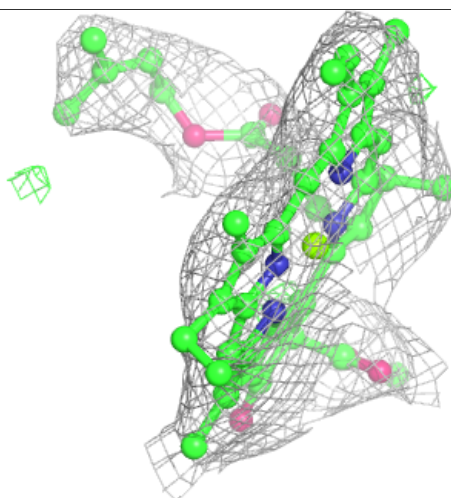
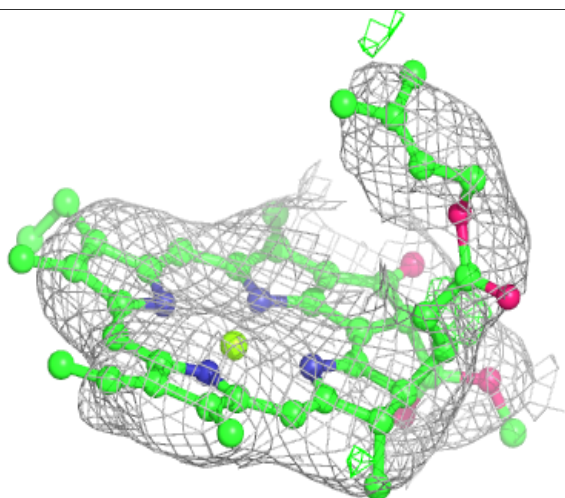
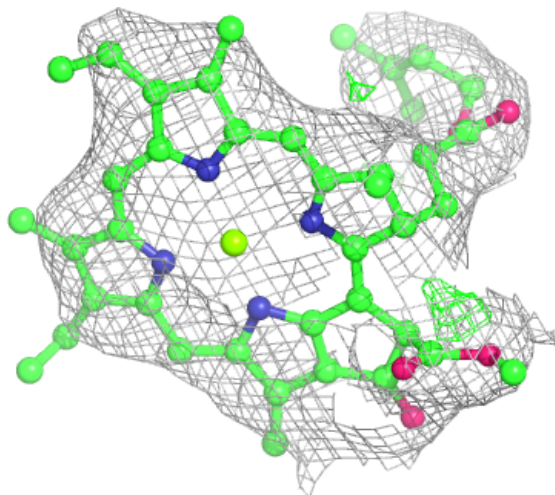
**Electron density around CLA 1 311:**

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



**Electron density around CLA 7 608:**

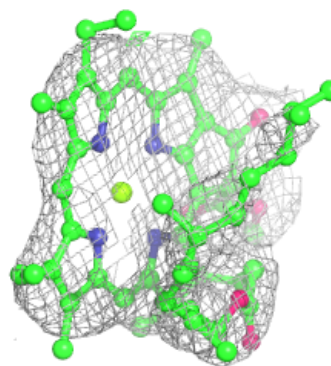
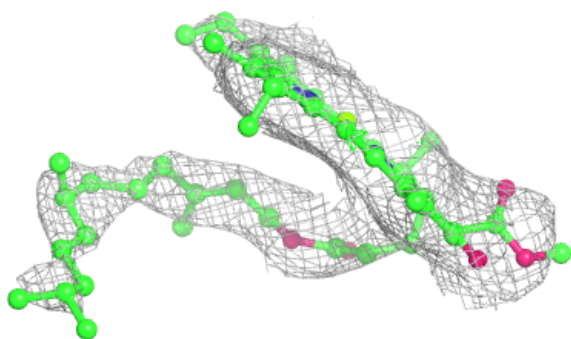
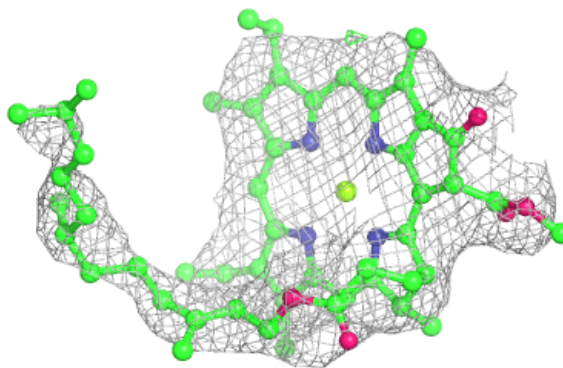
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





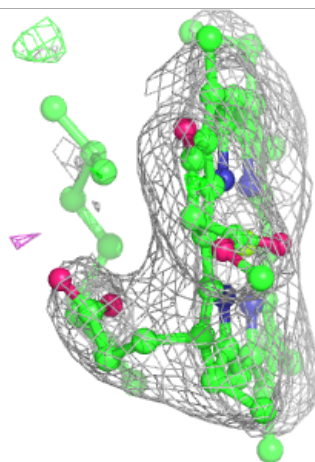
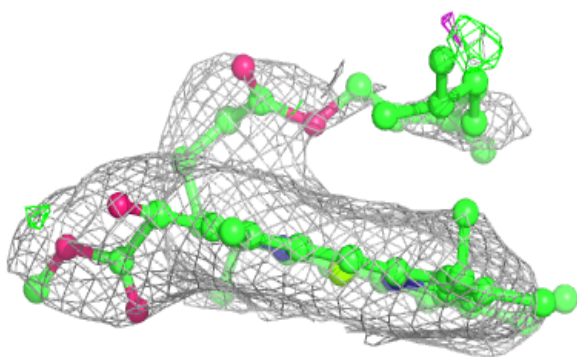
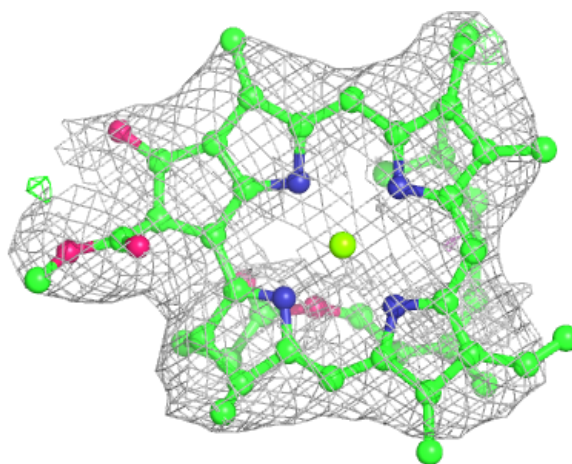
**Electron density around CLA 7 609:**

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



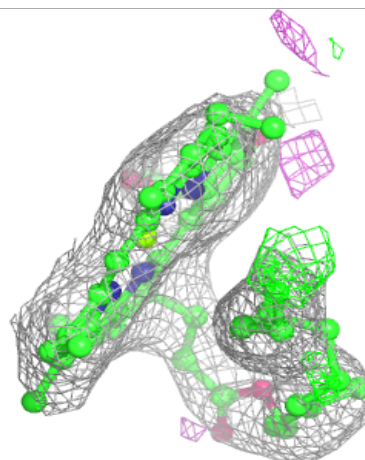
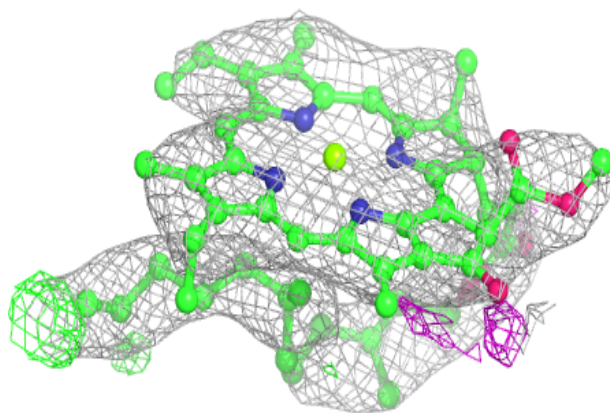
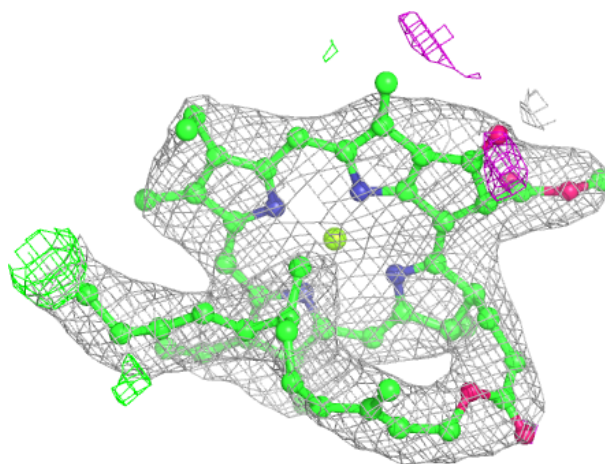
**Electron density around CLA B 812:**

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



**Electron density around CLA B 817:**

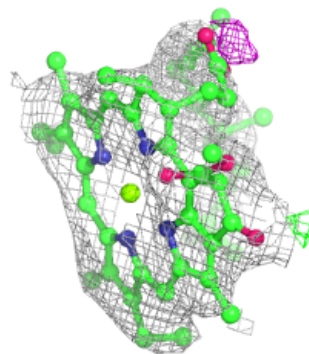
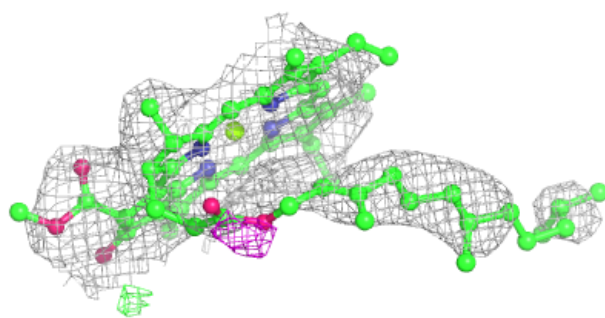
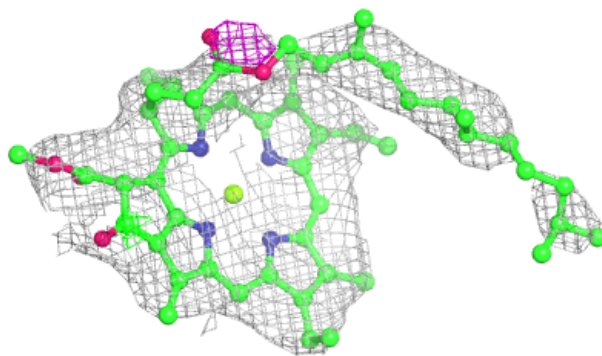
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





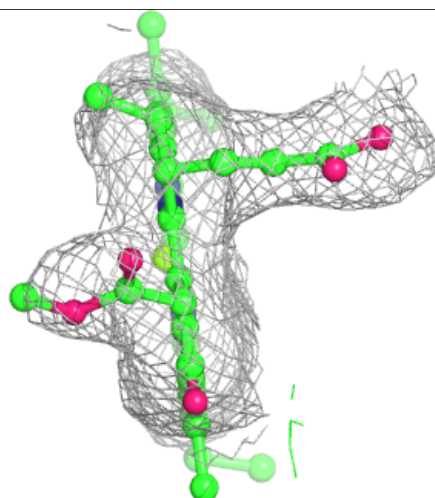
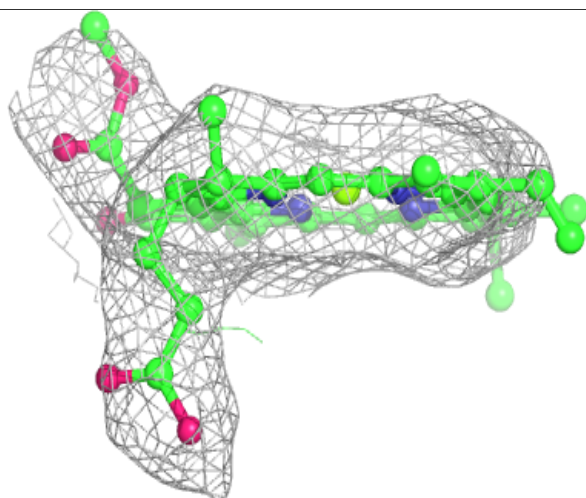
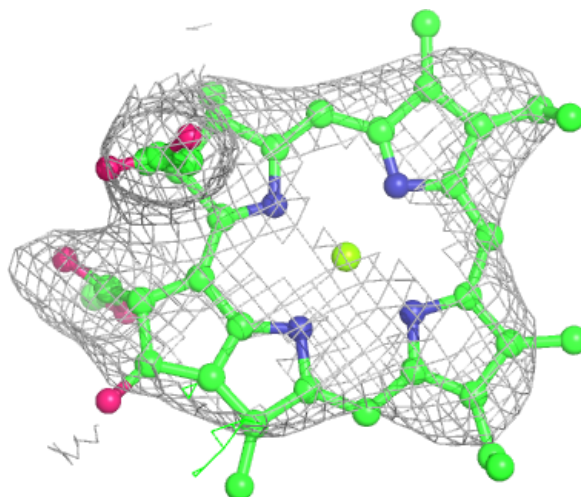
**Electron density around CLA 4 609:**

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



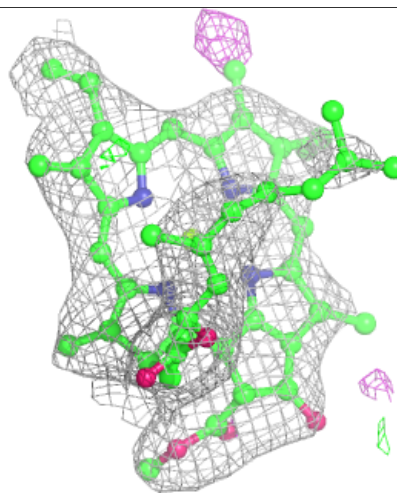
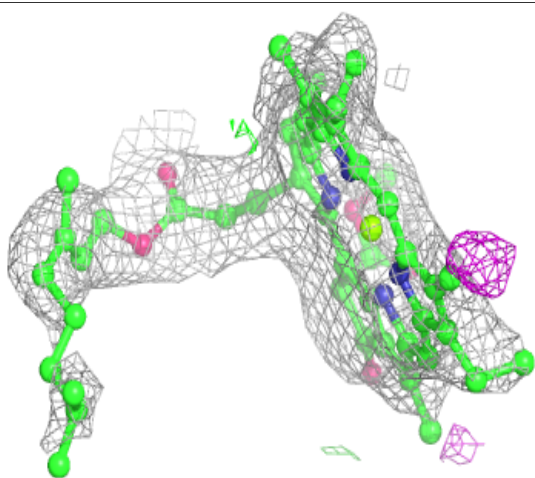
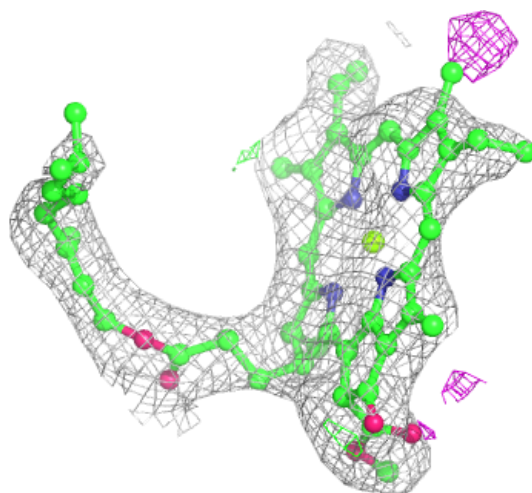
**Electron density around CLA 8 303:**

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



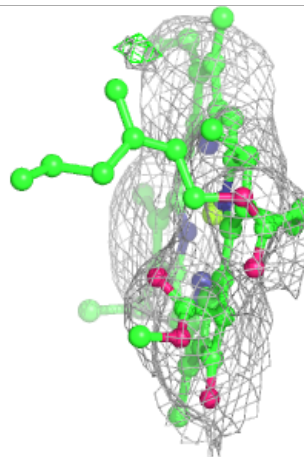
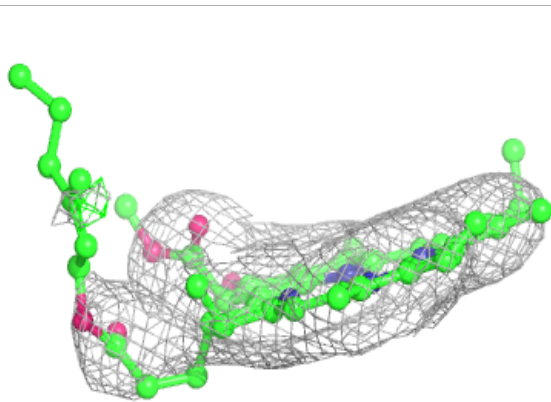
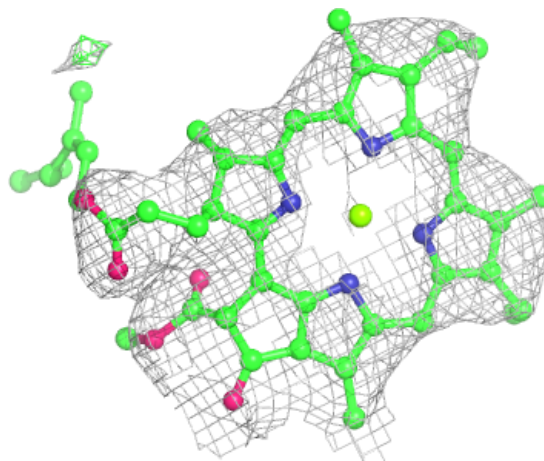
**Electron density around CLA A 805:**

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



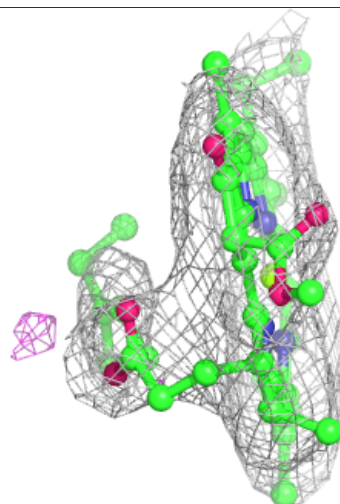
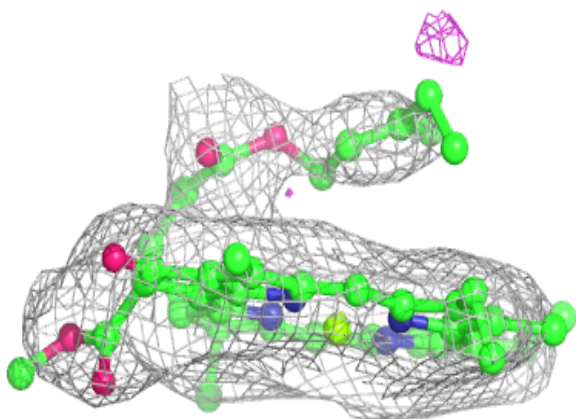
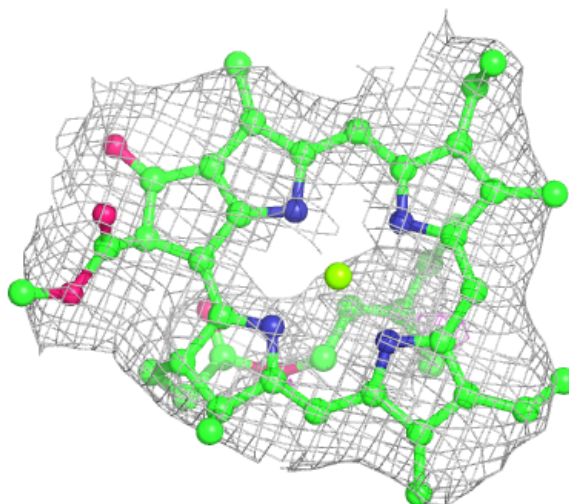
**Electron density around CLA 4 611:**

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



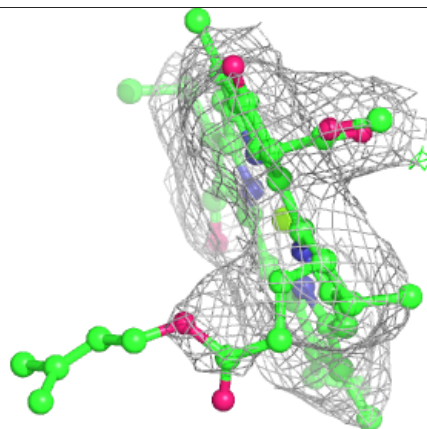
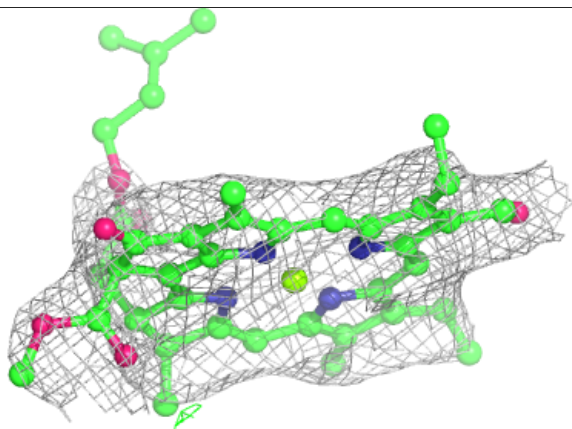
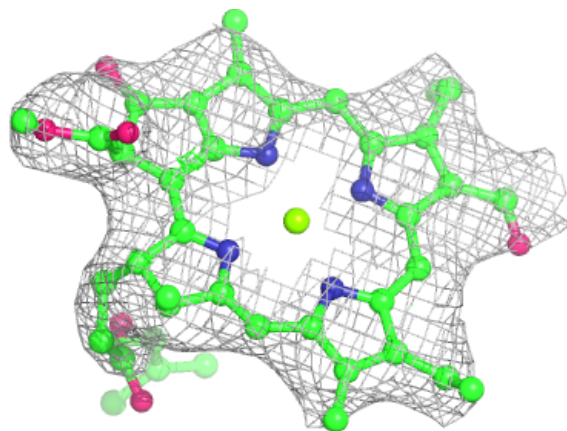
**Electron density around CLA a 824:**

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



**Electron density around CHL 4 606:**

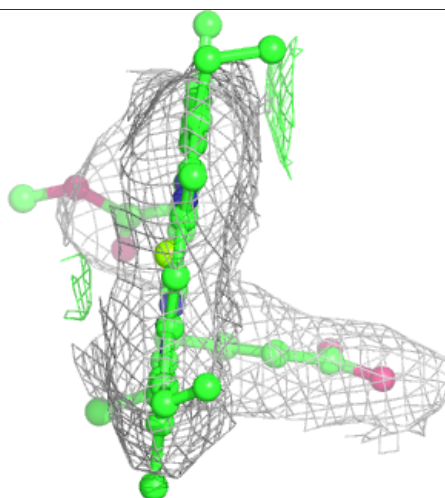
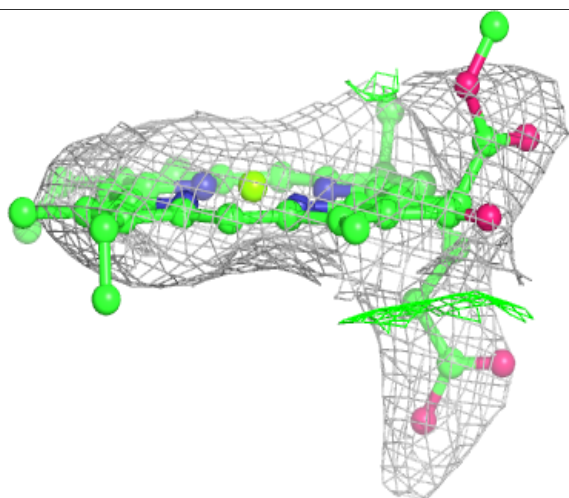
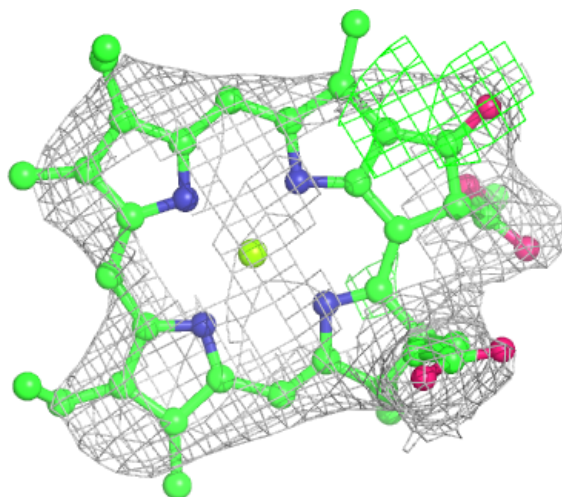
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





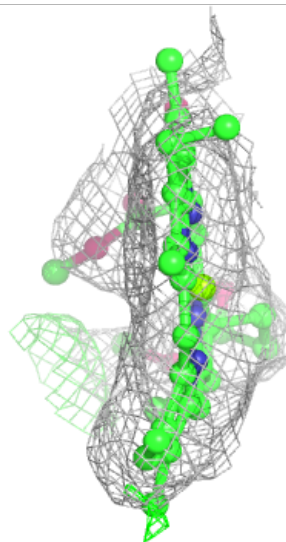
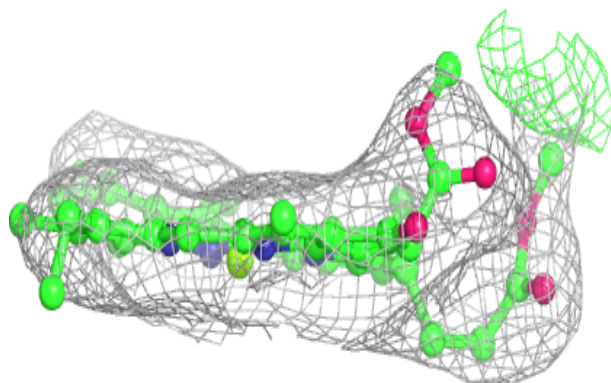
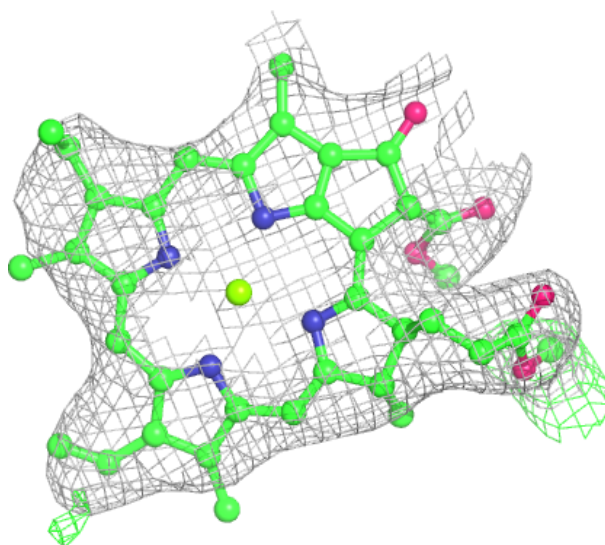
**Electron density around CLA 3 304:**

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



**Electron density around CLA 9 603:**

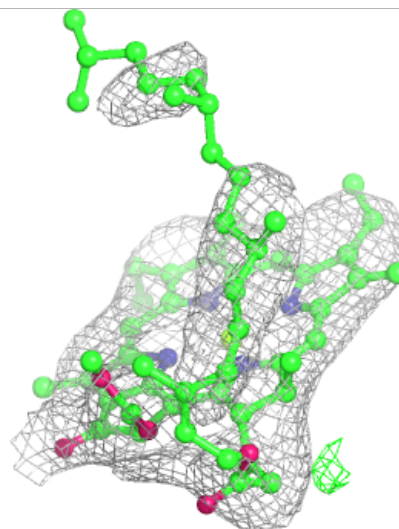
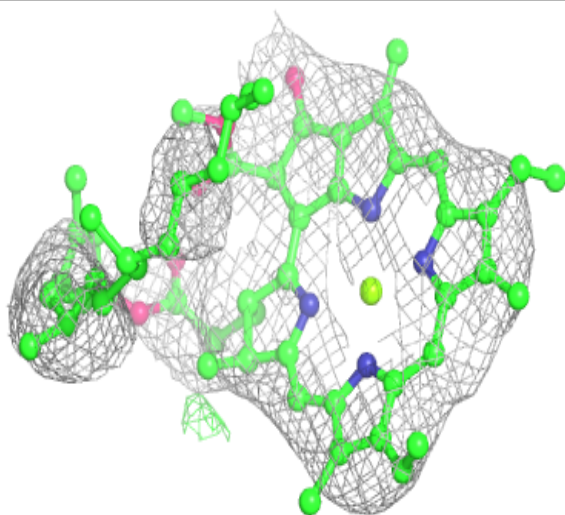
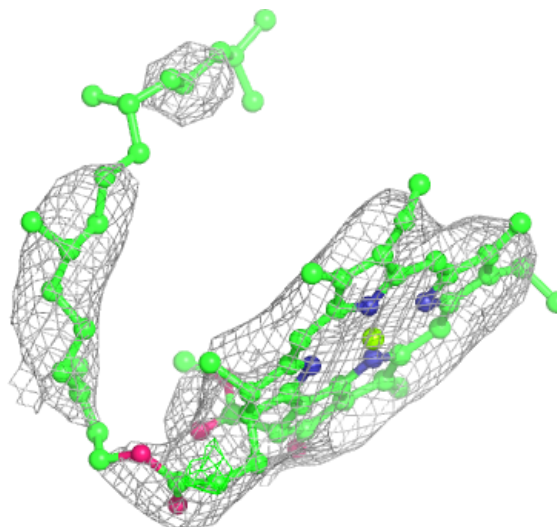
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





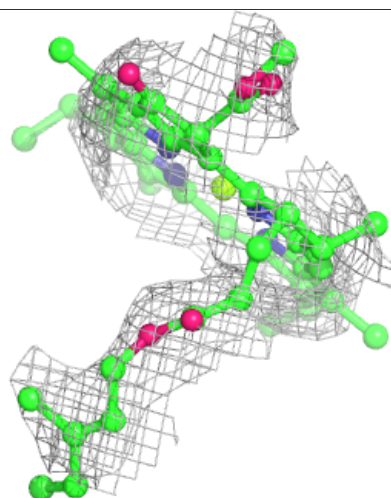
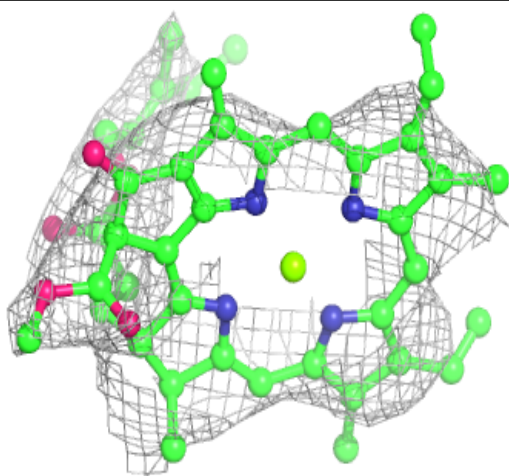
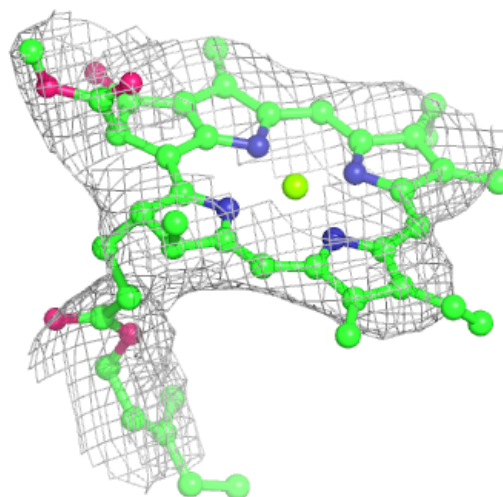
**Electron density around CLA 6 305:**

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



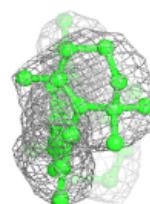
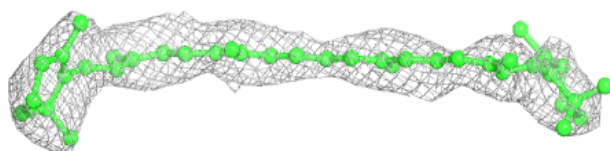
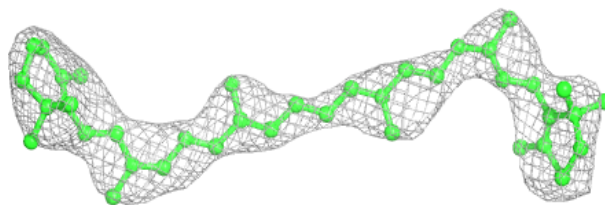
**Electron density around CLA 6 306:**

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

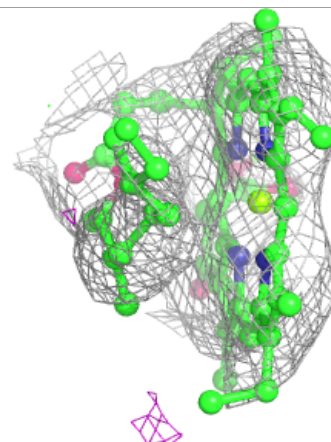
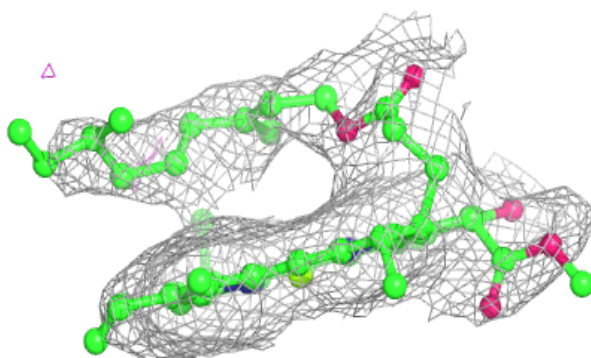
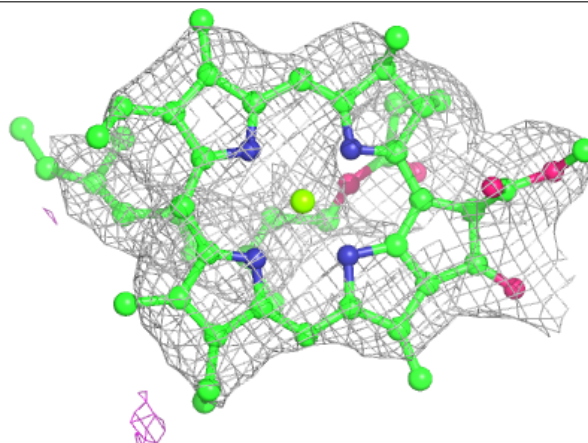


**Electron density around BCR b 845:**

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

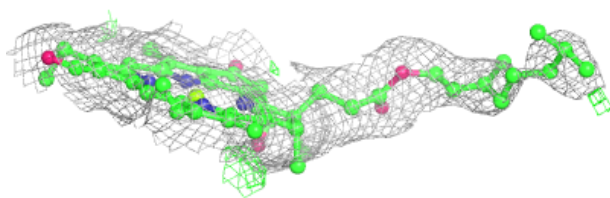
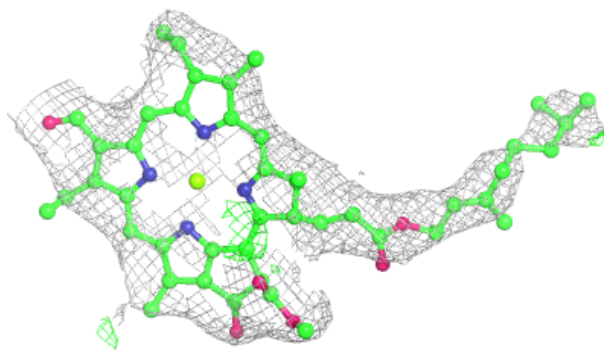
**Electron density around CLA 9 612:**

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



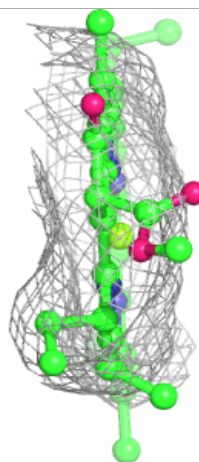
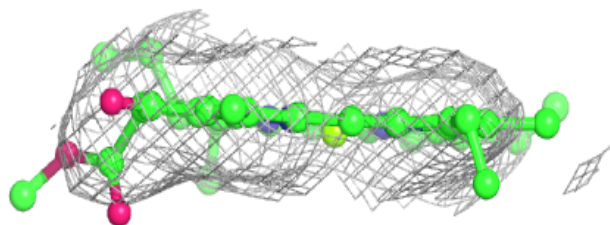
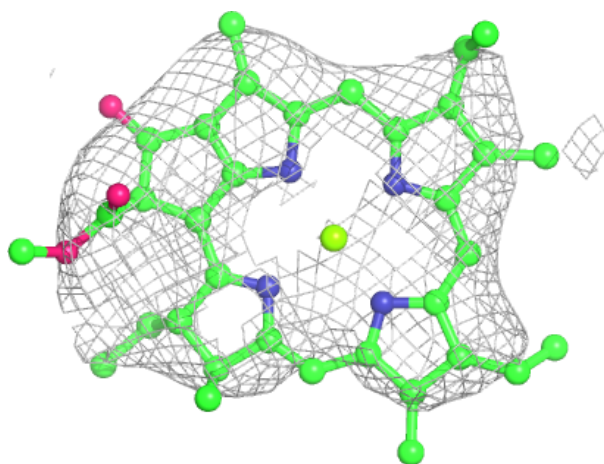
**Electron density around CHL 9 605:**

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



**Electron density around CLA 6 307:**

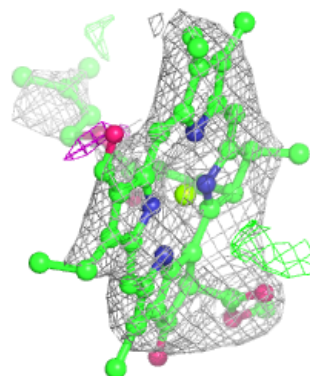
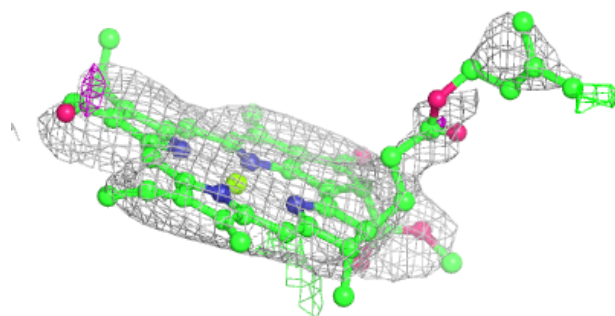
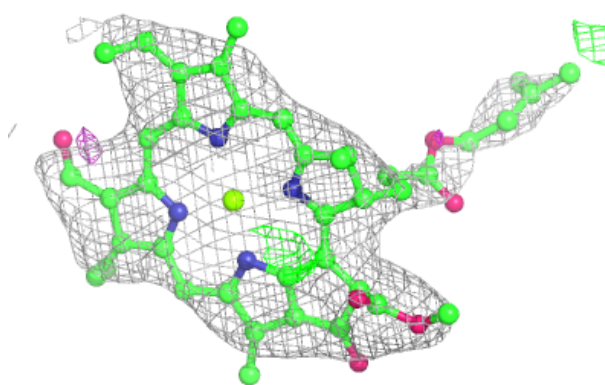
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



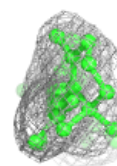
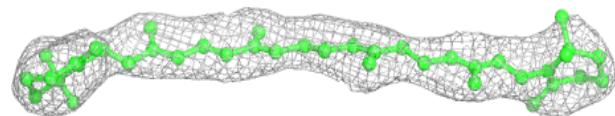
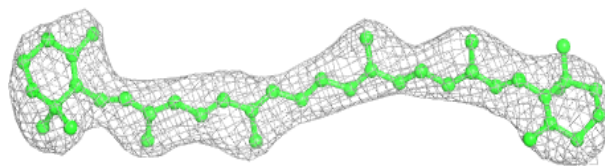


**Electron density around CHL 9 607:**

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

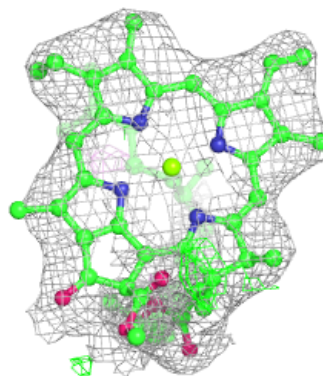
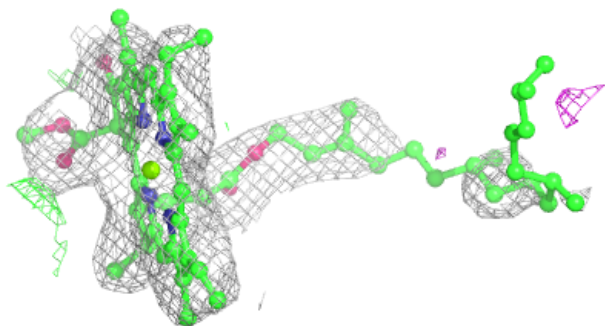
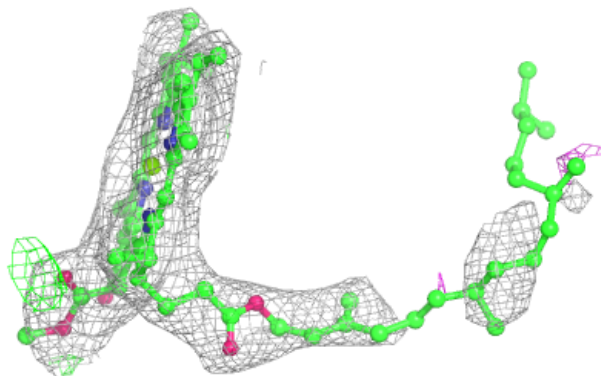
**Electron density around BCR j 3003:**

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

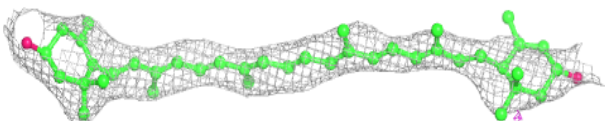
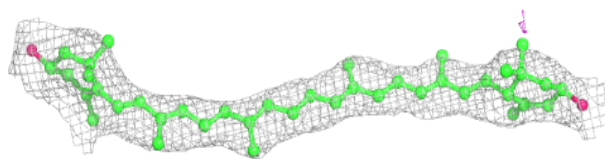


**Electron density around CLA A 808:**

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

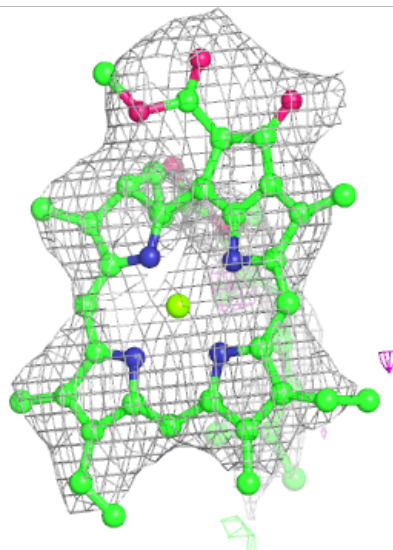
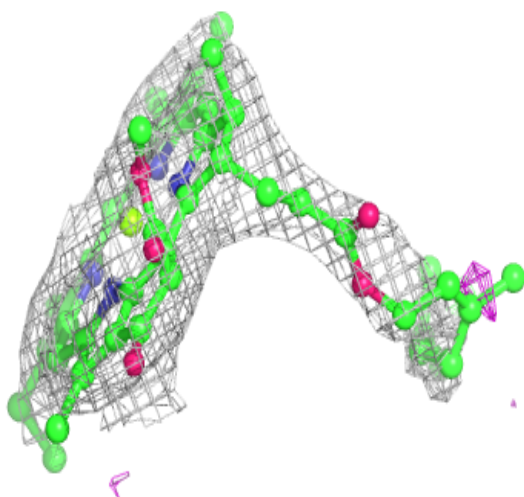
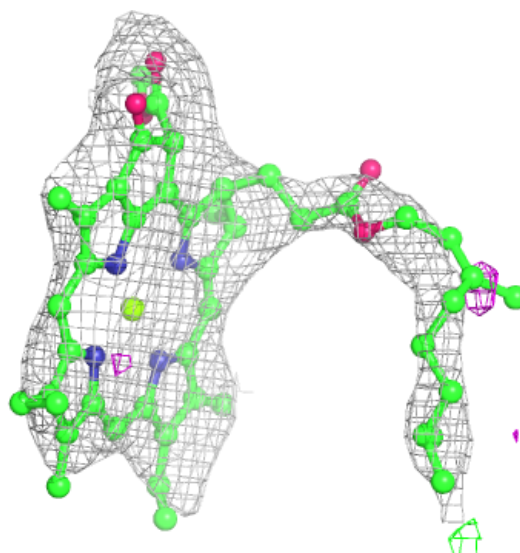
**Electron density around LUT 3 316:**

$2mF_o-DF_c$  (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:**

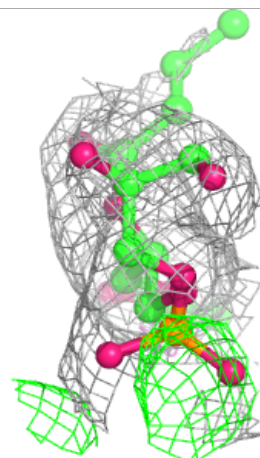
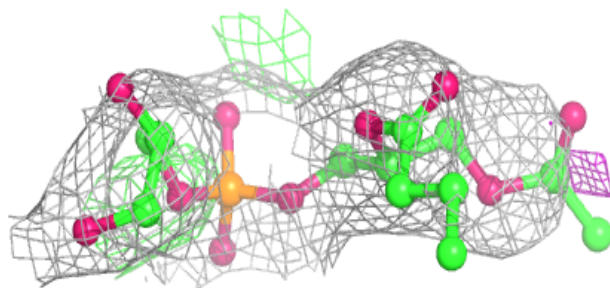
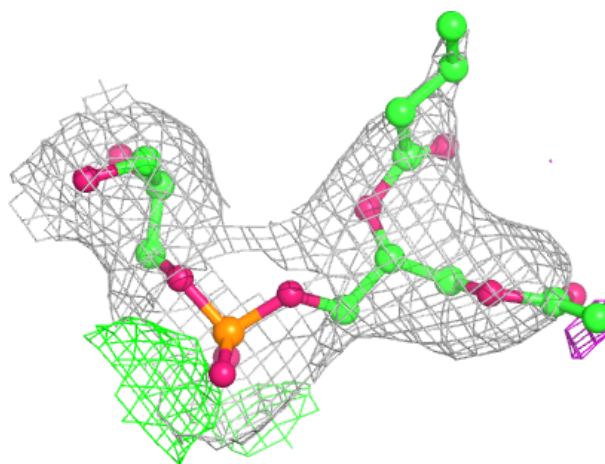
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





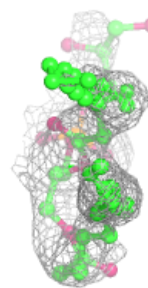
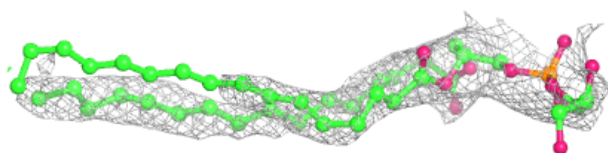
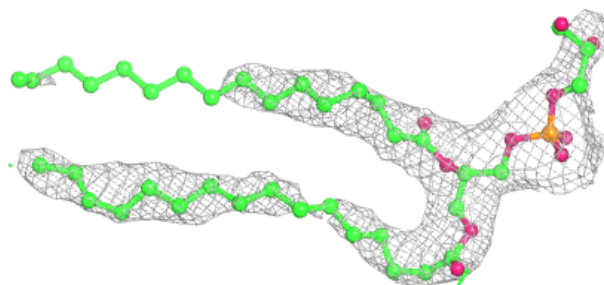
**Electron density around LHG 1 301:**

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

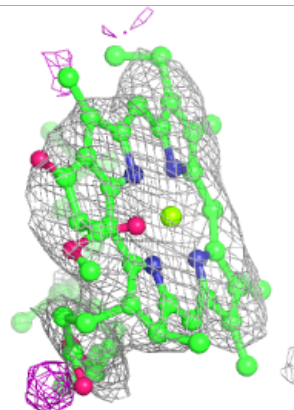
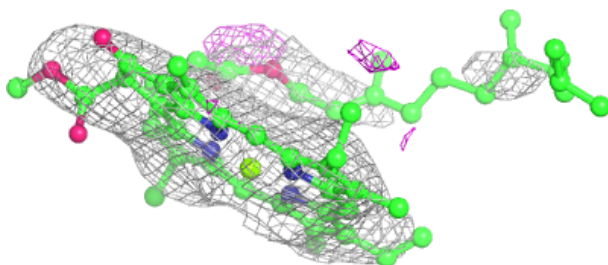
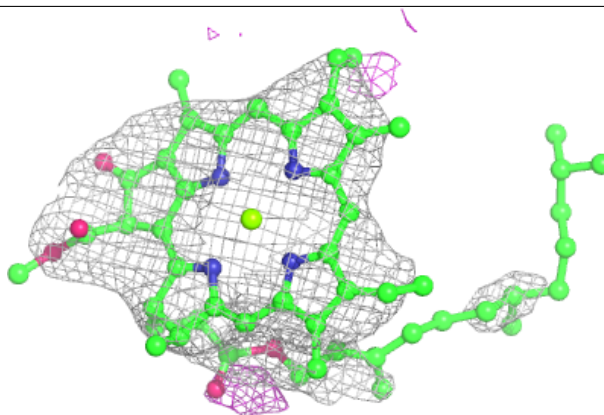


**Electron density around LHG 1 319:**

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

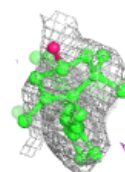
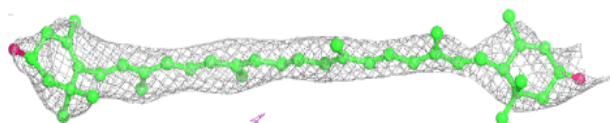
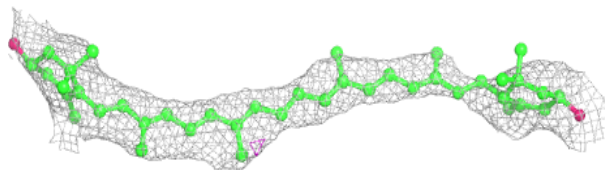
**Electron density around CLA 6 311:**

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

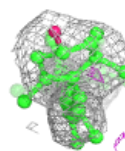
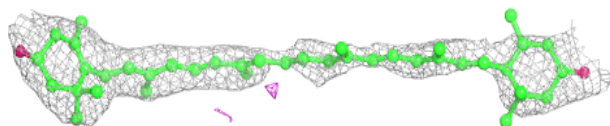
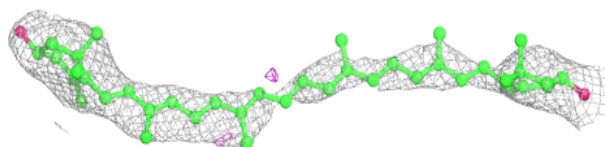


**Electron density around LUT 8 314:**

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

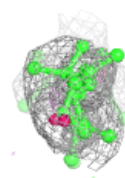
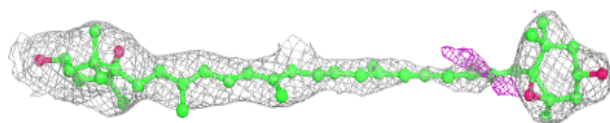
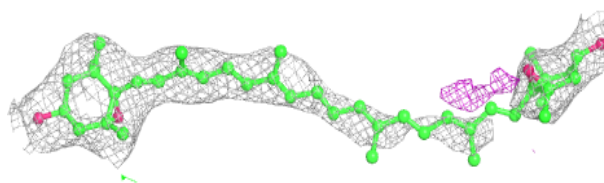
**Electron density around LUT 9 616:**

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

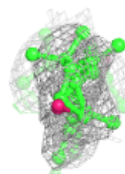
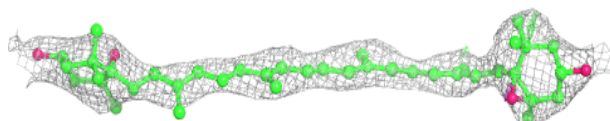
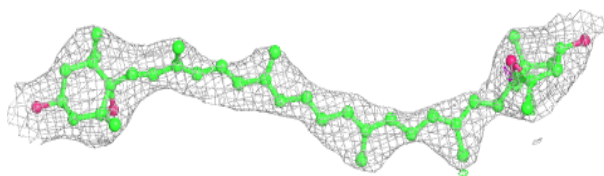


**Electron density around XAT 7 616:**

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

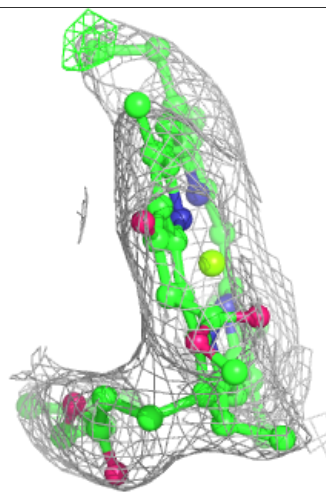
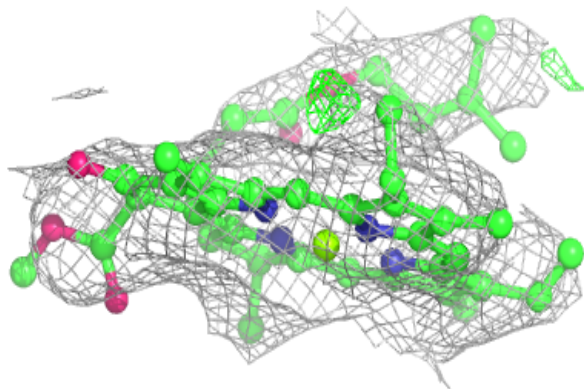
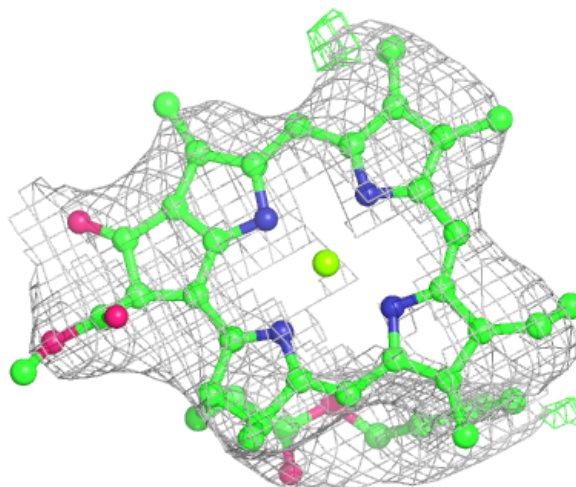
**Electron density around XAT 8 315:**

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



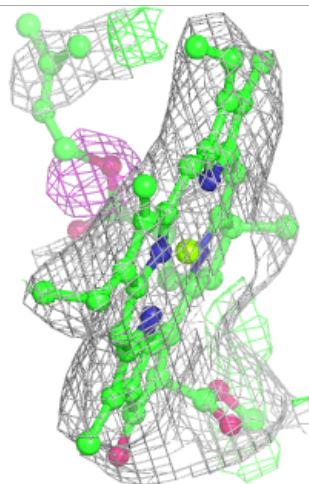
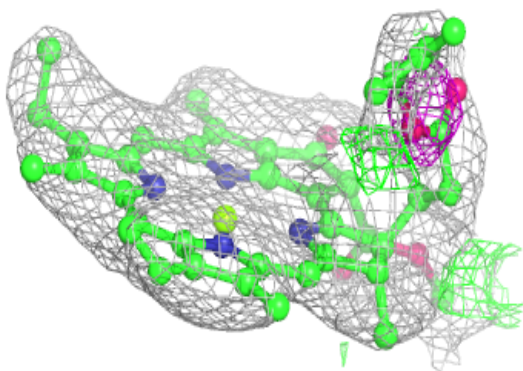
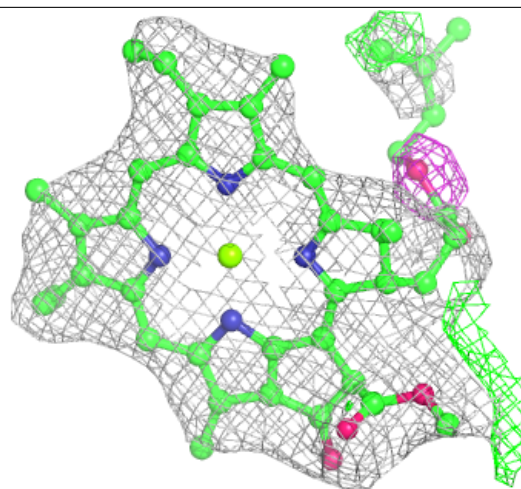
**Electron density around CLA 3 309:**

$2mF_o-DF_c$  (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:**

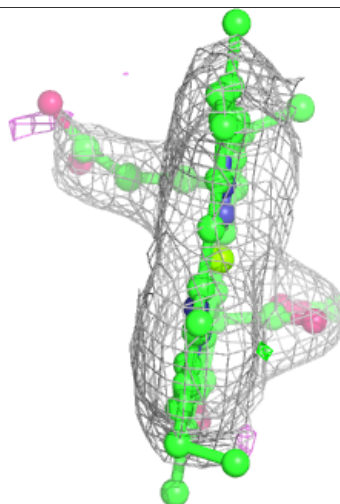
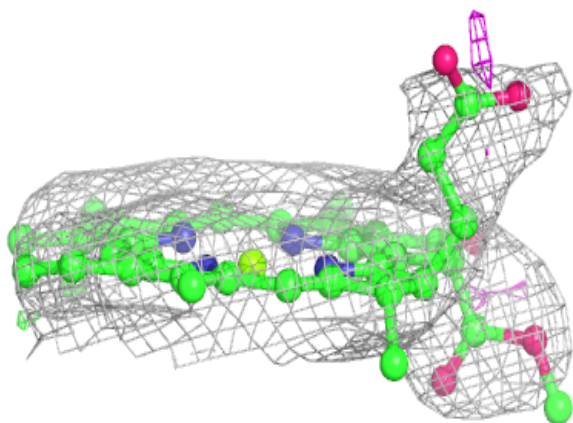
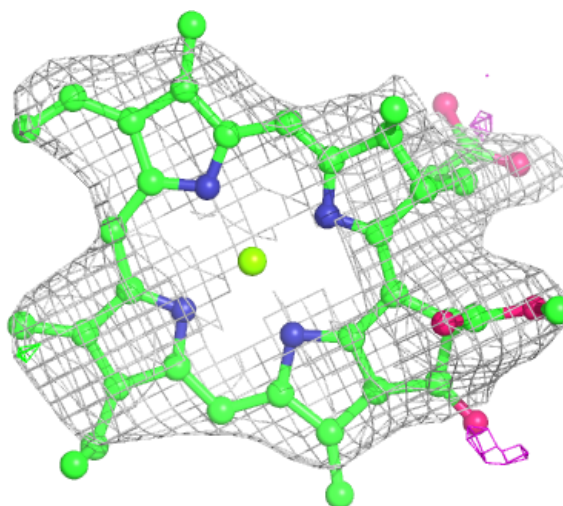
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





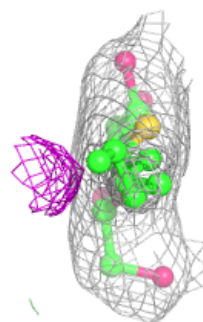
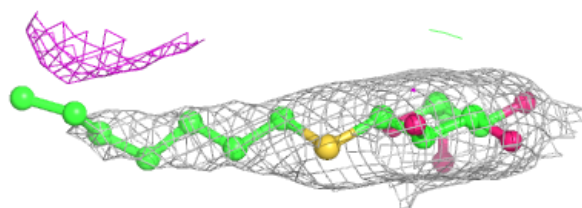
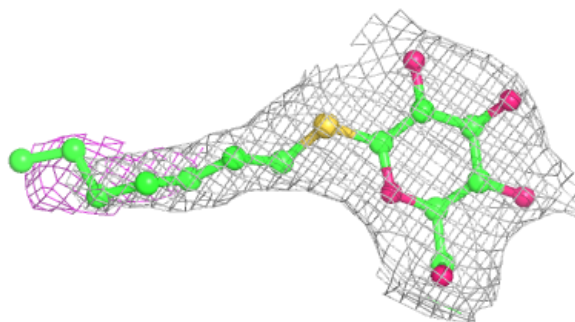
**Electron density around CLA a 817:**

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

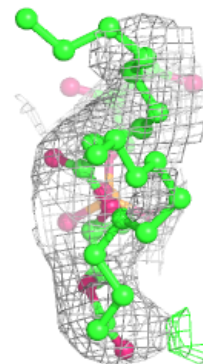
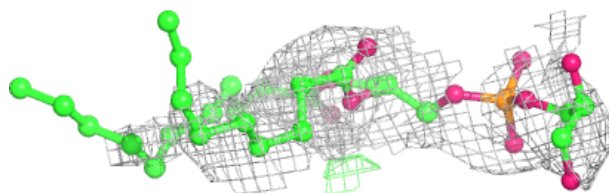
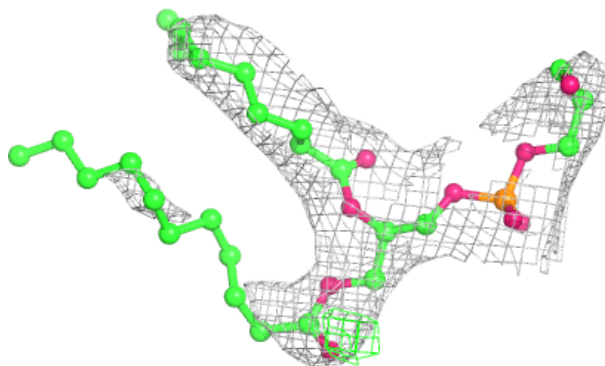


**Electron density around HTG A 855:**

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

**Electron density around LHG 2 618:**

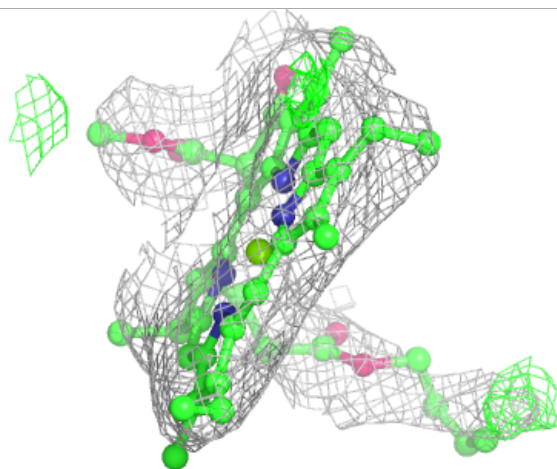
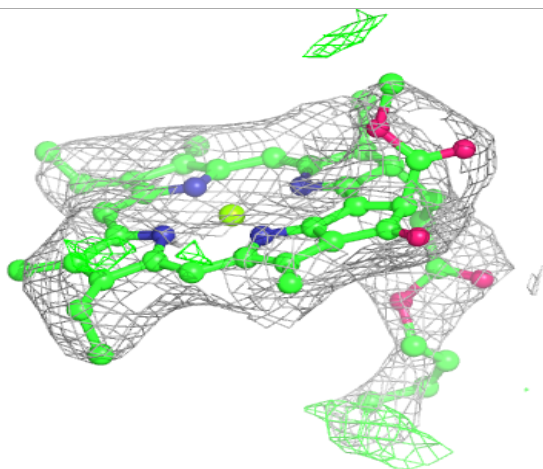
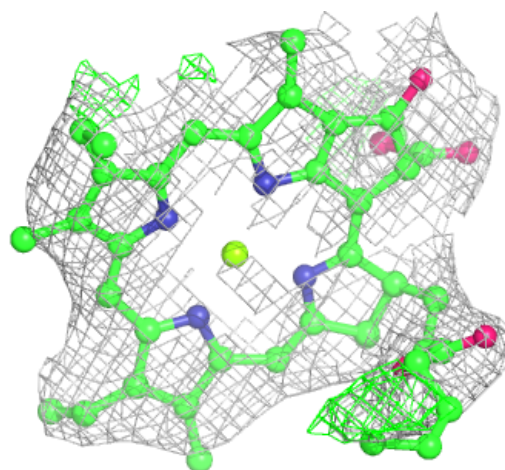
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





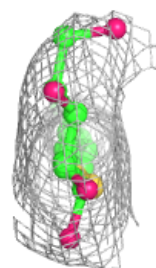
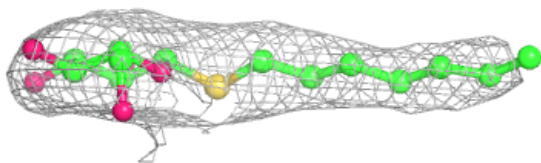
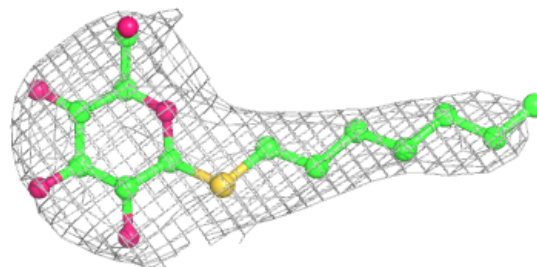
**Electron density around CLA a 823:**

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

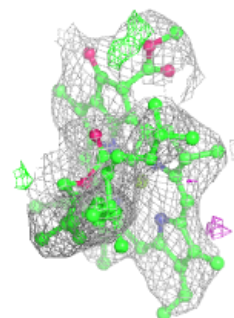
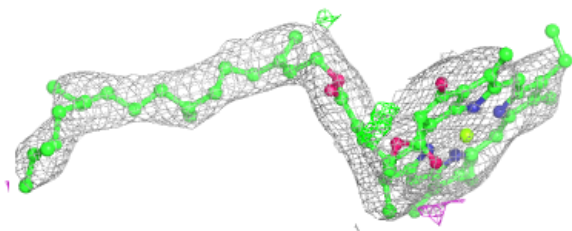
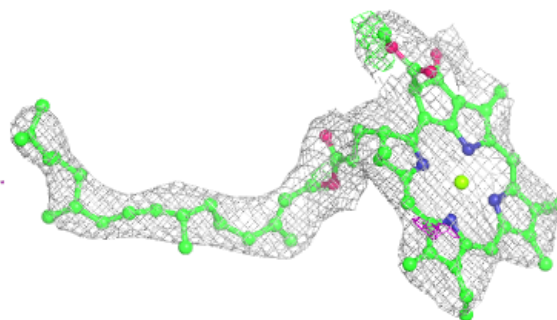


**Electron density around HTG a 857:**

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

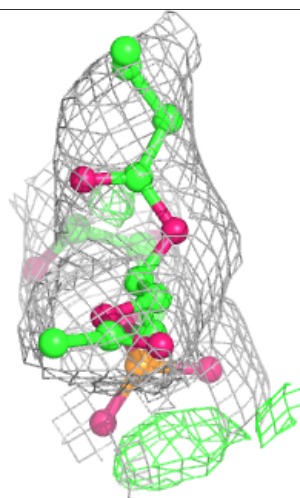
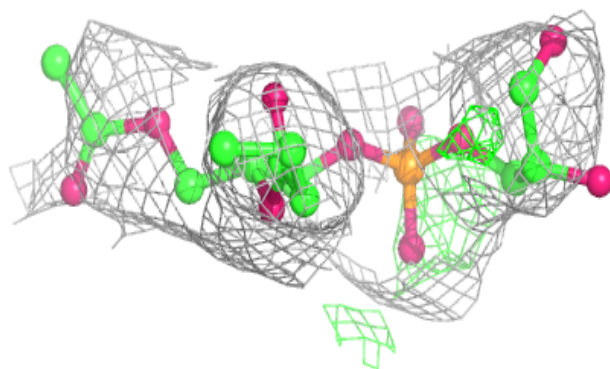
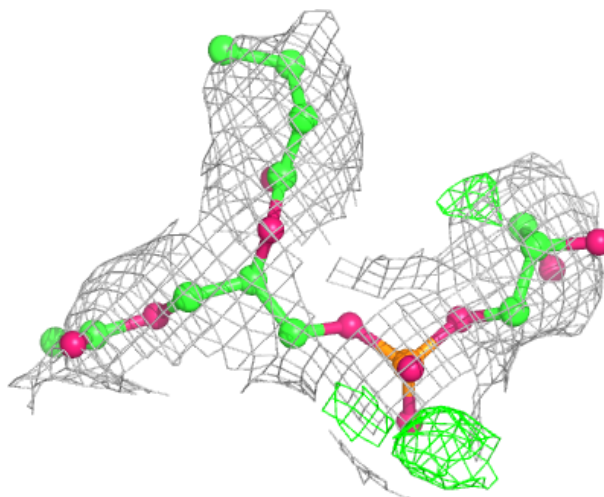
**Electron density around CLA A 822:**

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



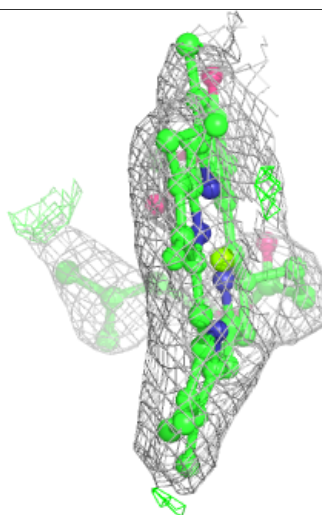
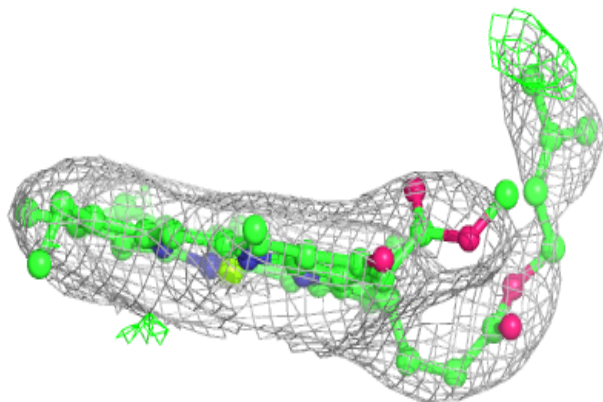
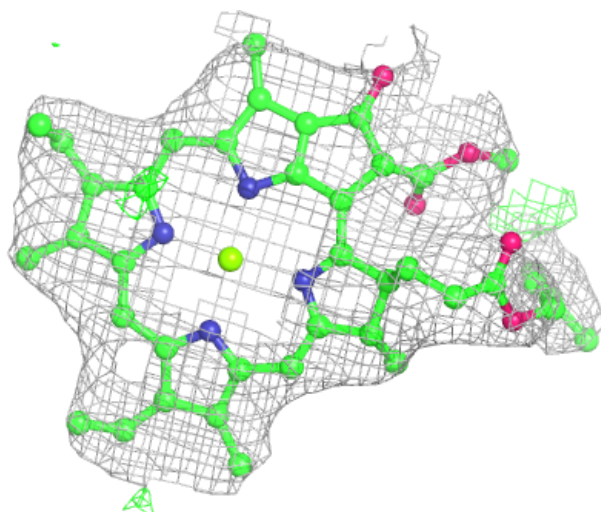
**Electron density around LHG 6 301:**

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



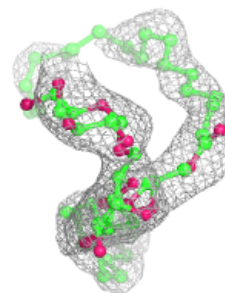
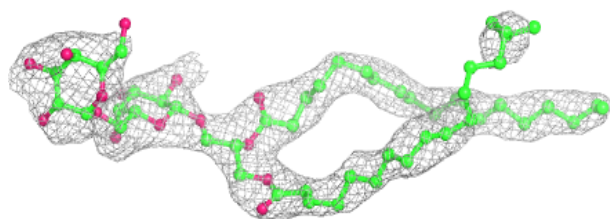
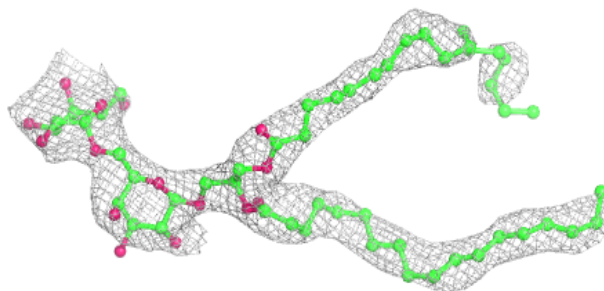
**Electron density around CLA 3 303:**

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

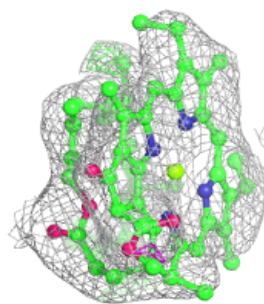
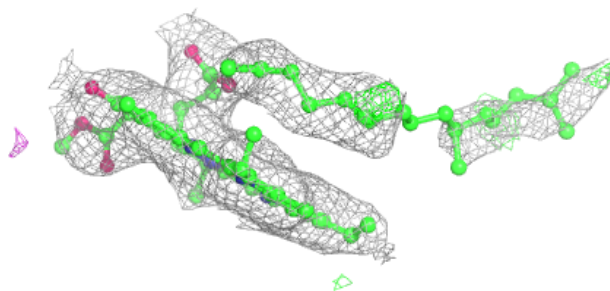
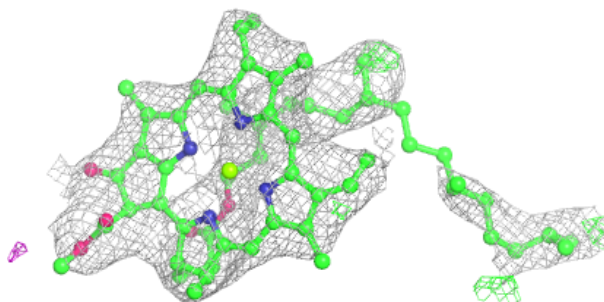


**Electron density around DGD B 850:**

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

**Electron density around CLA b 807:**

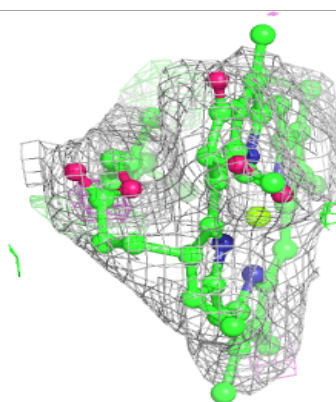
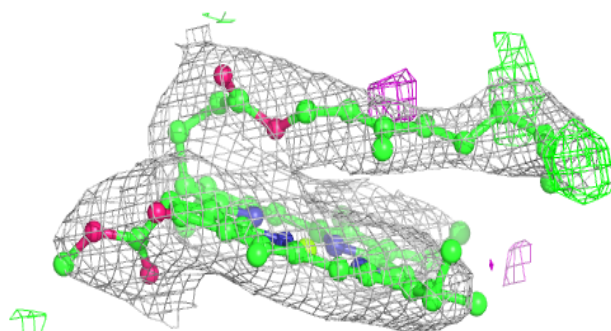
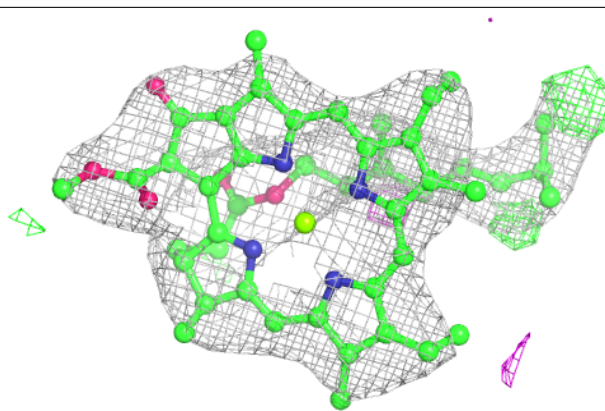
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





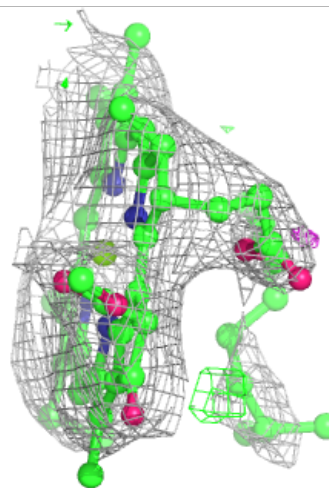
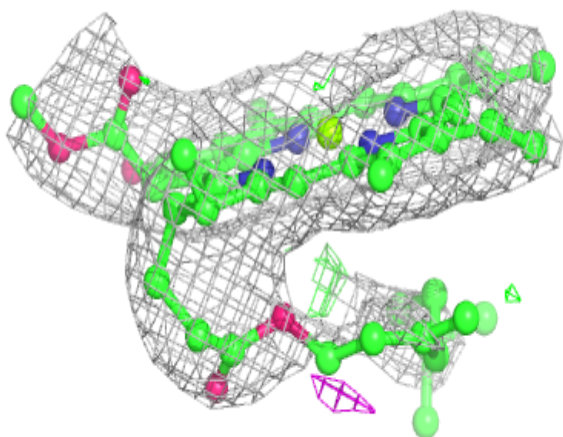
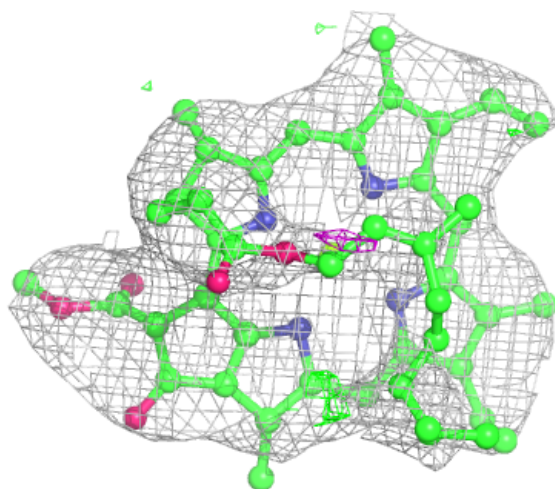
**Electron density around CLA B 816:**

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



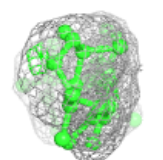
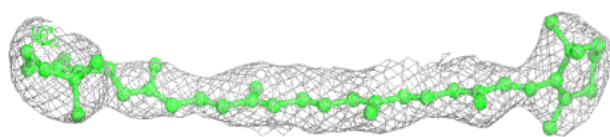
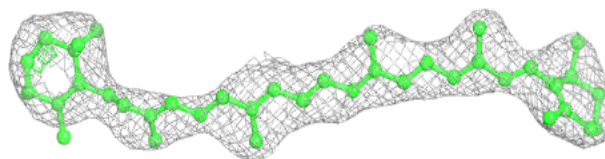
**Electron density around CLA b 812:**

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

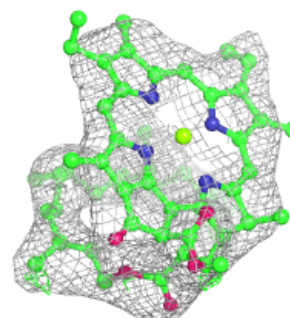
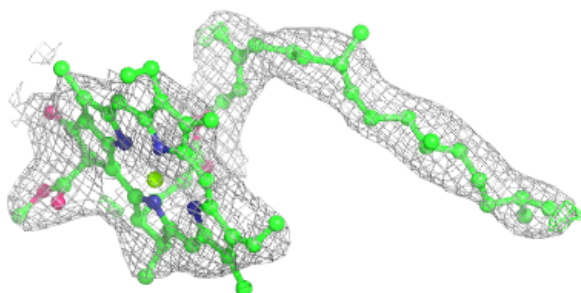
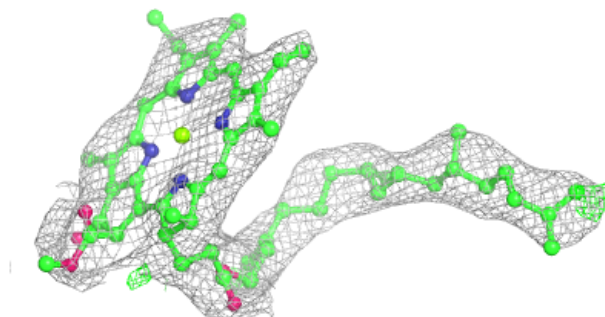


**Electron density around BCR A 851:**

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

**Electron density around CLA b 814:**

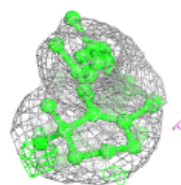
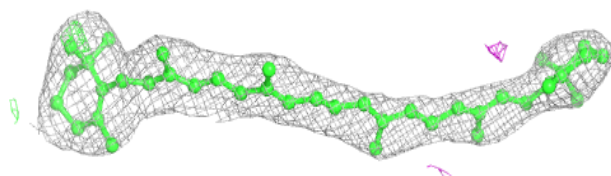
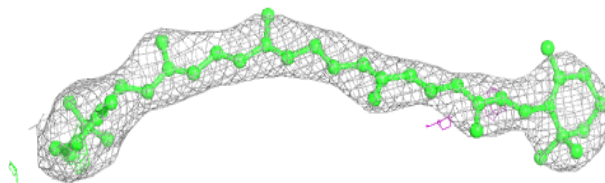
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





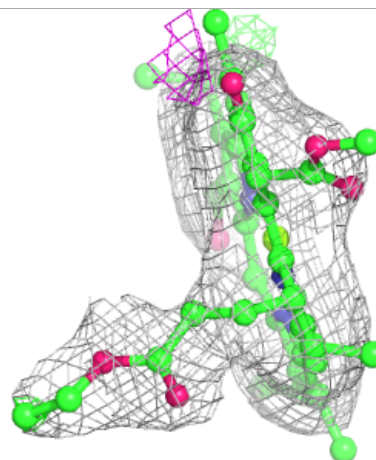
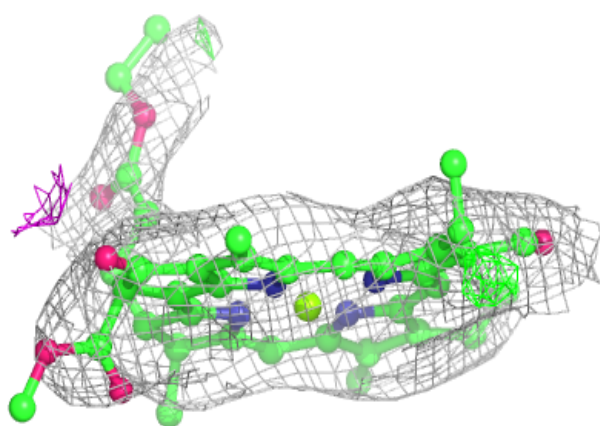
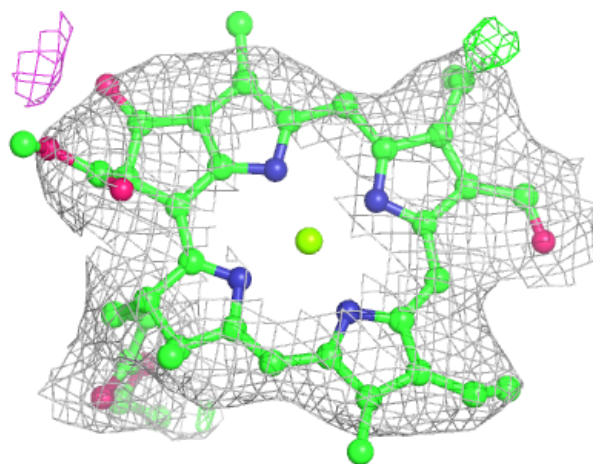
**Electron density around BCR B 801:**

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



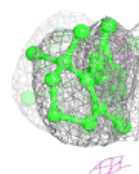
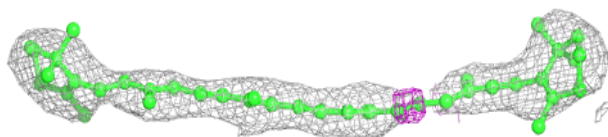
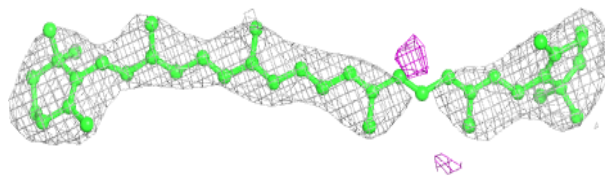
**Electron density around CHL 1 307:**

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

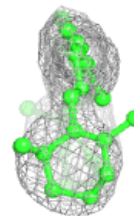
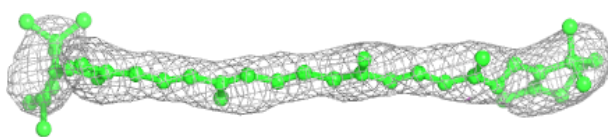
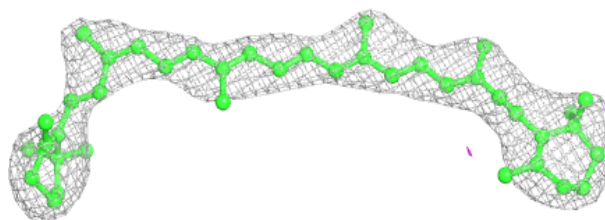


**Electron density around BCR B 843:**

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

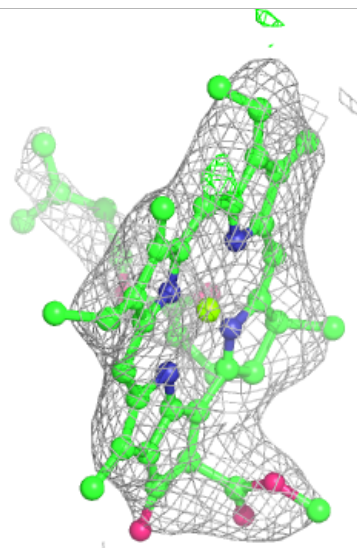
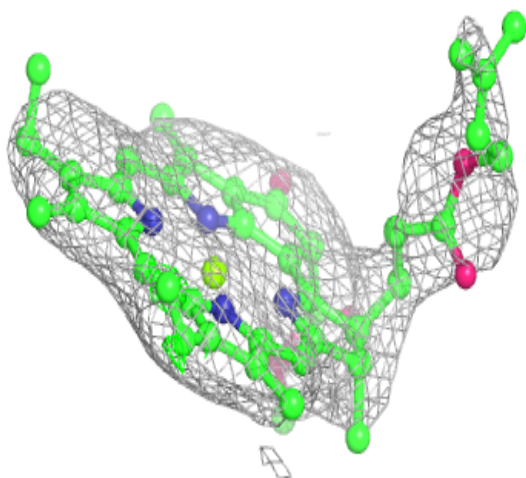
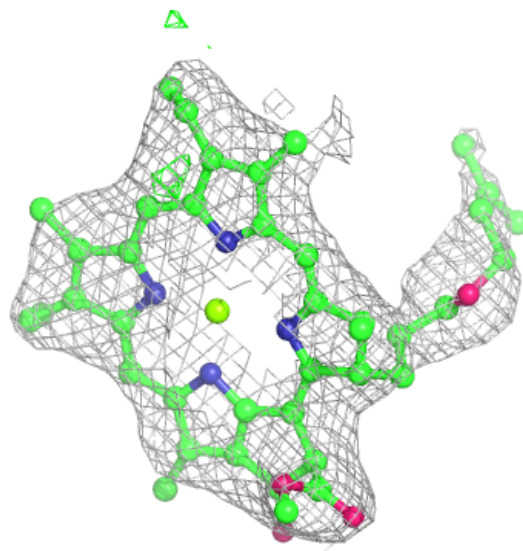
**Electron density around BCR B 844:**

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



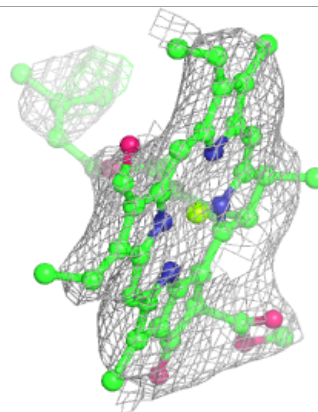
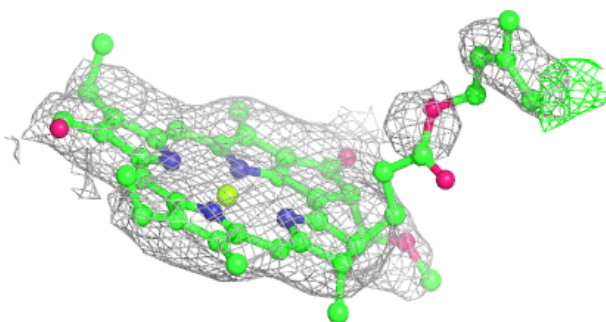
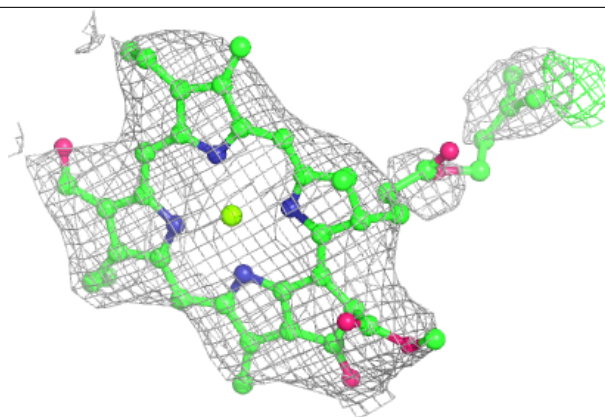
**Electron density around CLA A 832:**

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

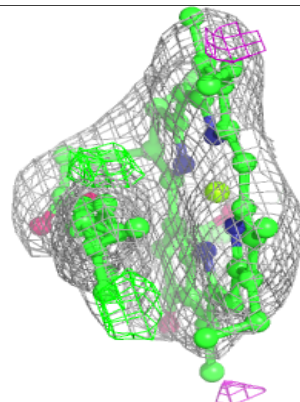
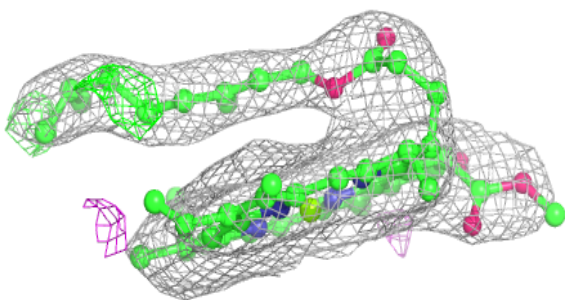
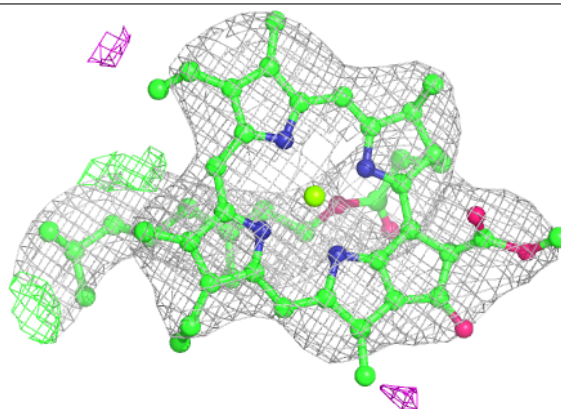


**Electron density around CHL 2 607:**

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

**Electron density around CLA b 816:**

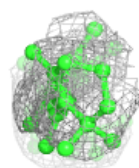
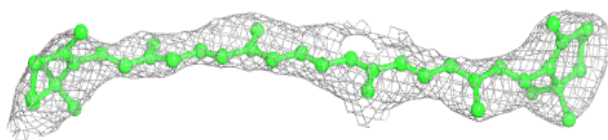
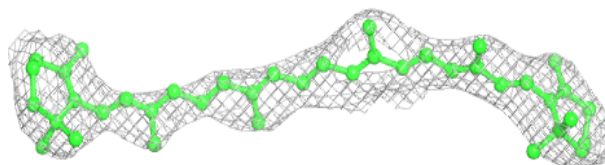
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



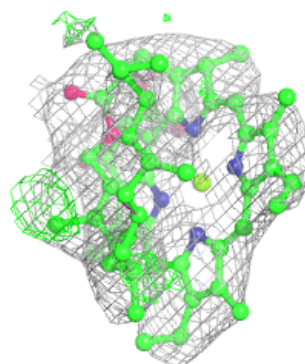
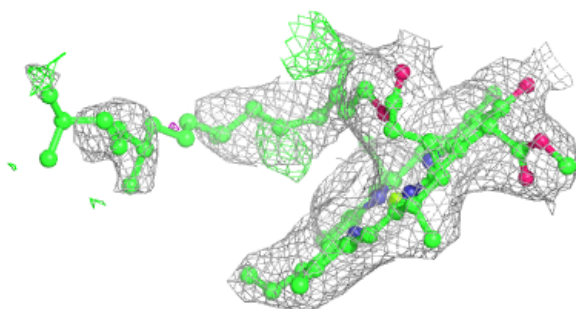
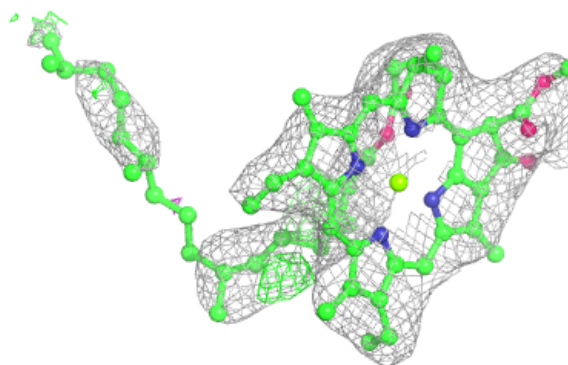


**Electron density around BCR G 105:**

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

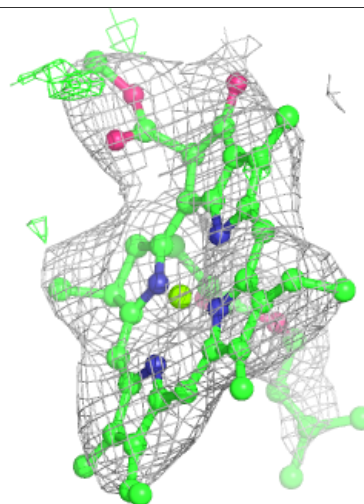
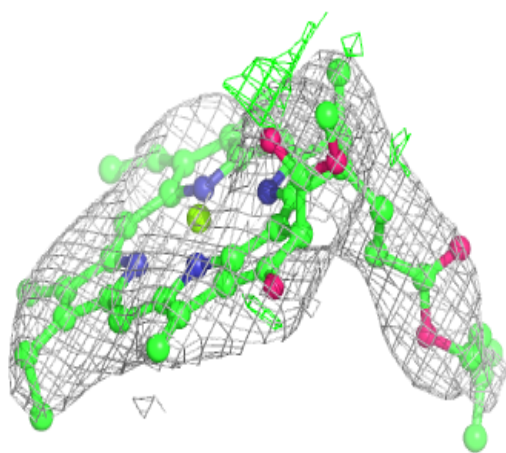
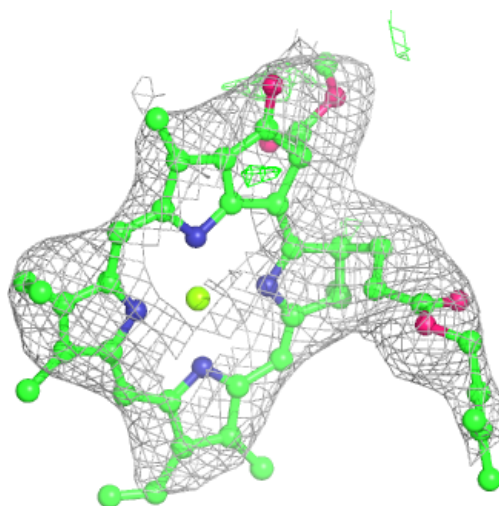
**Electron density around CLA B 807:**

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



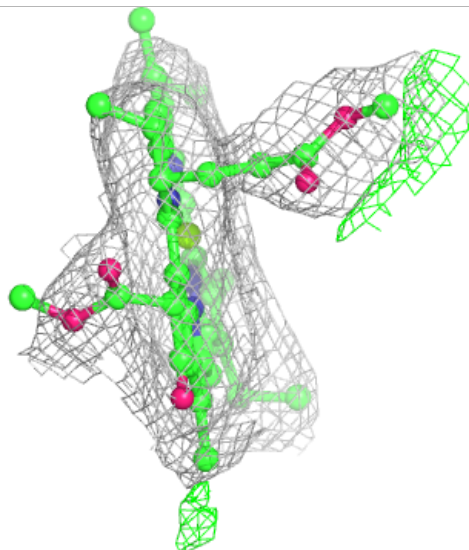
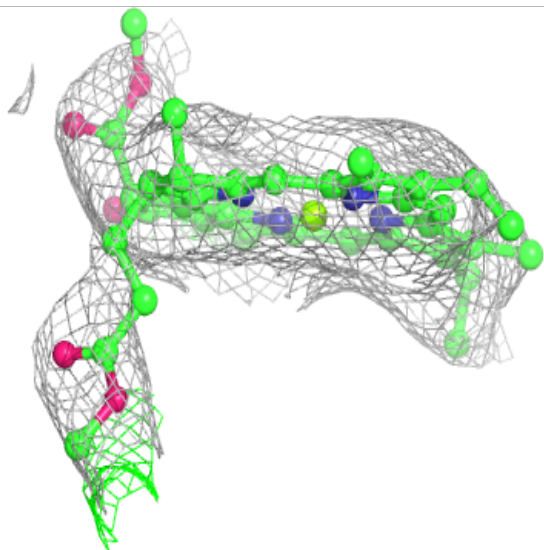
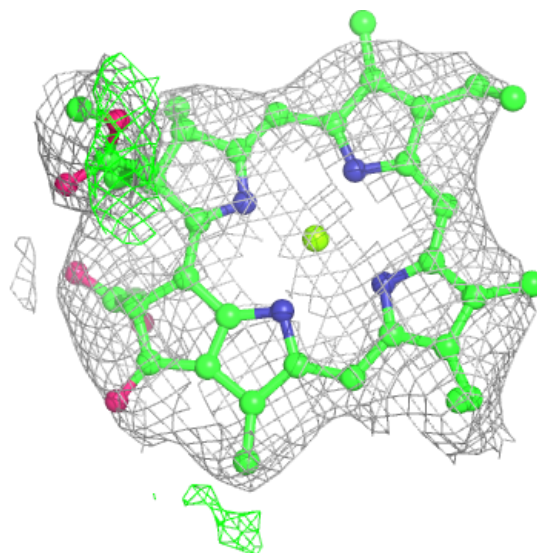
**Electron density around CLA b 820:**

$2mF_o-DF_c$  (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:**

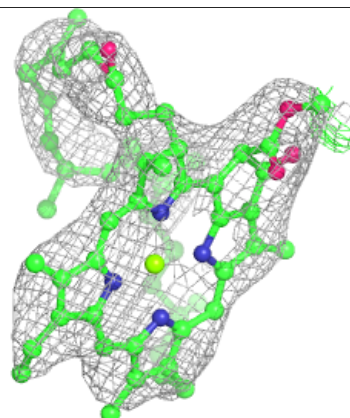
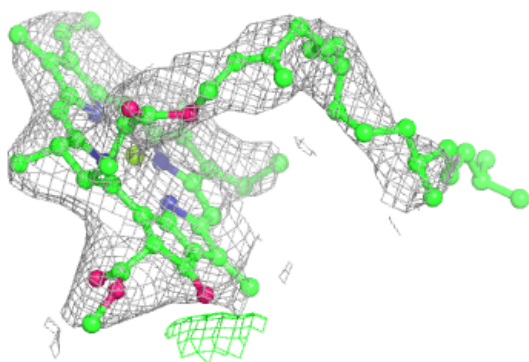
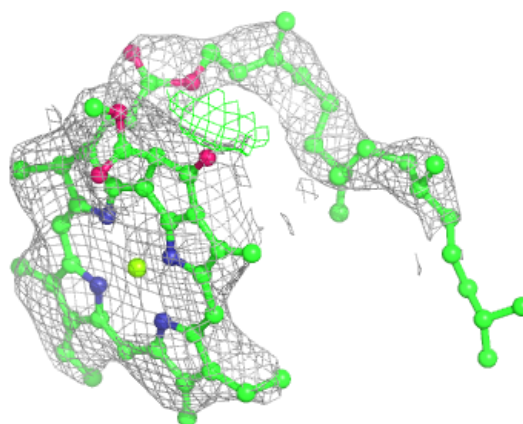
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



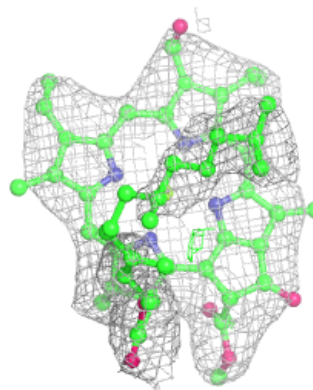
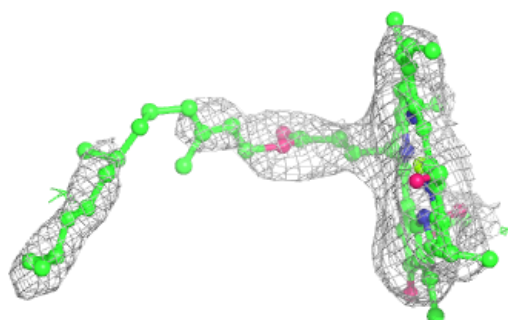
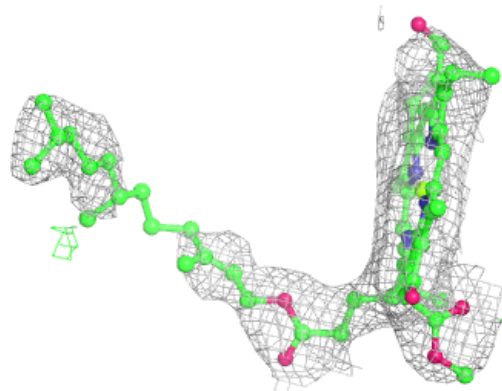


**Electron density around CLA b 834:**

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

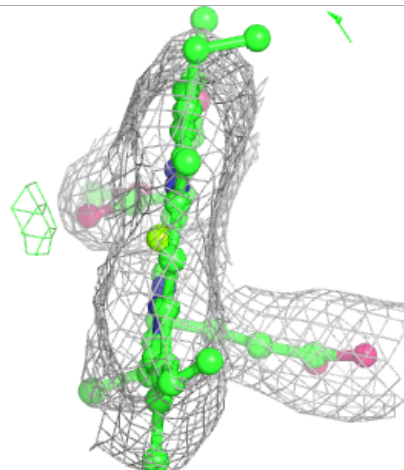
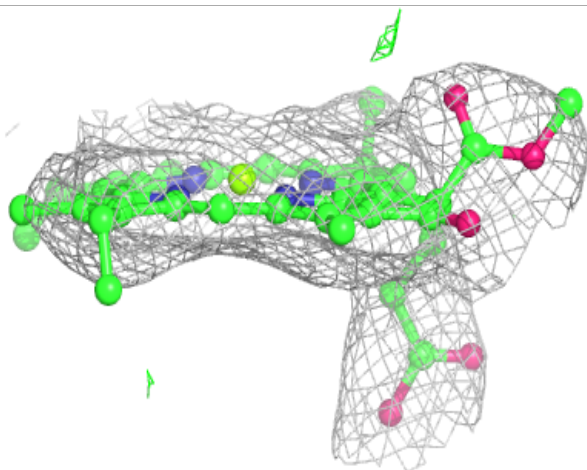
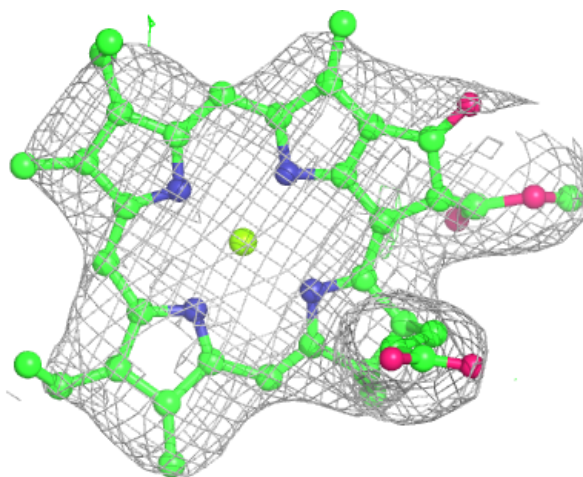
**Electron density around CHL 7 601:**

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



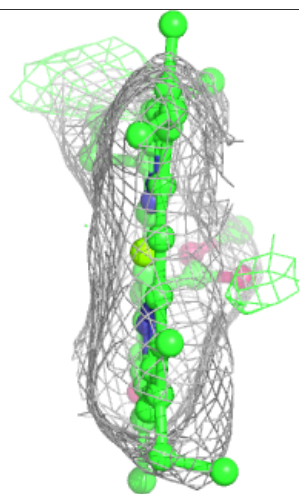
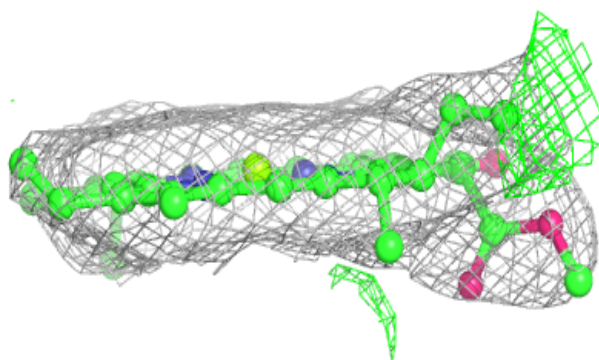
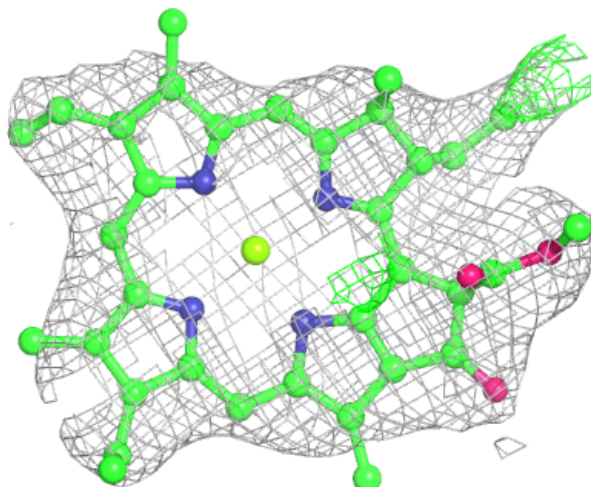
**Electron density around CLA B 835:**

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



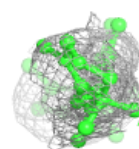
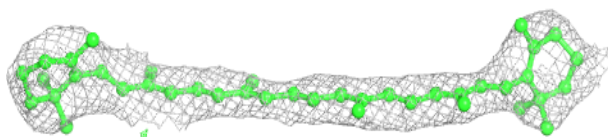
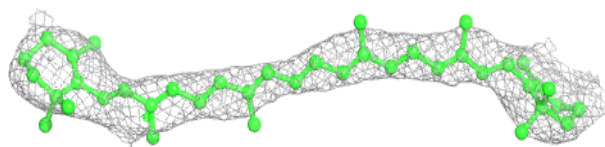
**Electron density around CLA 8 304:**

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



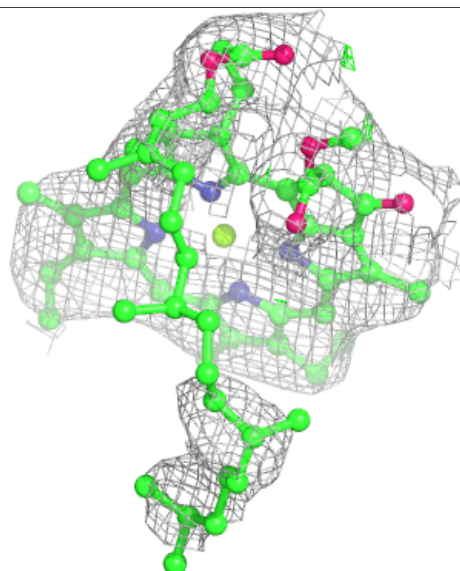
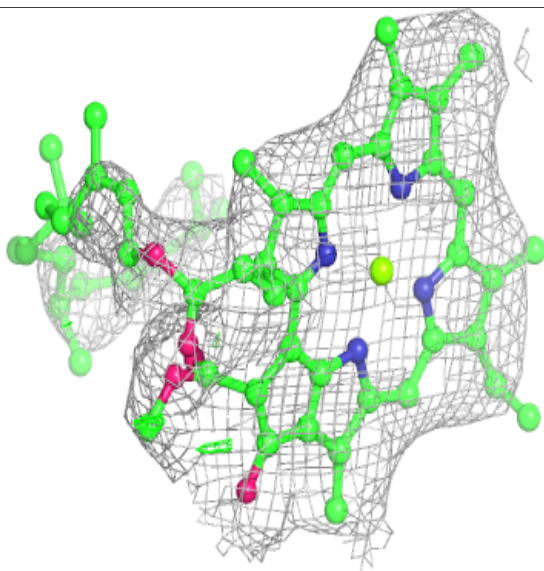
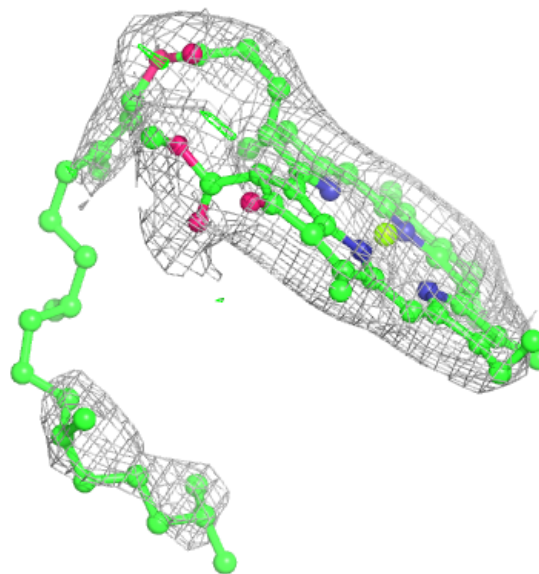
**Electron density around BCR 3 318:**

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



**Electron density around CLA 2 603:**

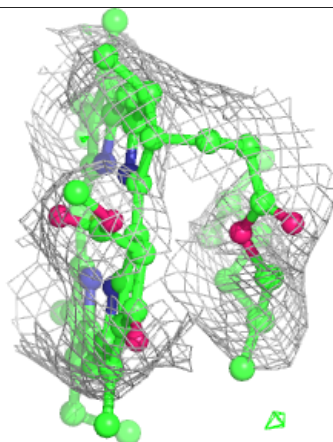
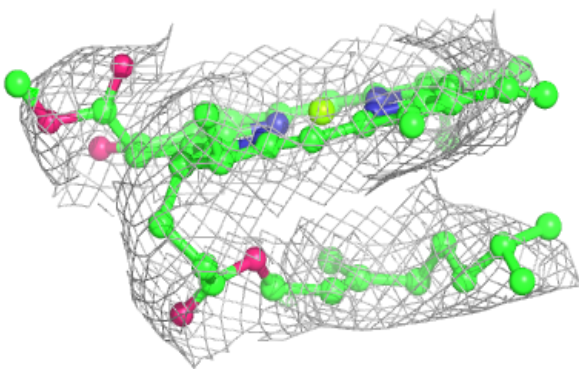
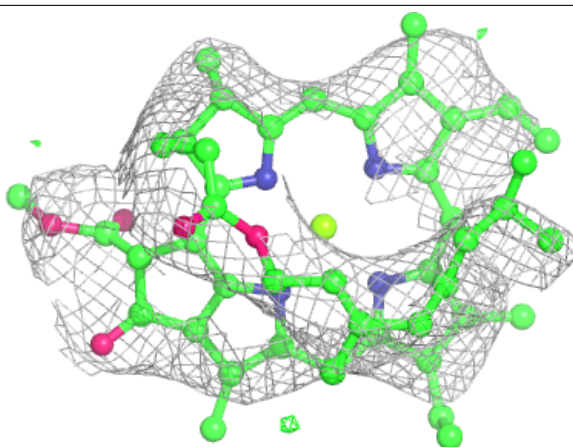
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





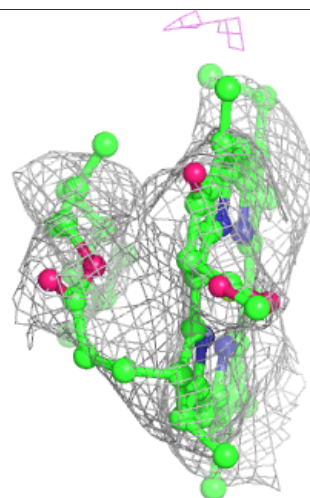
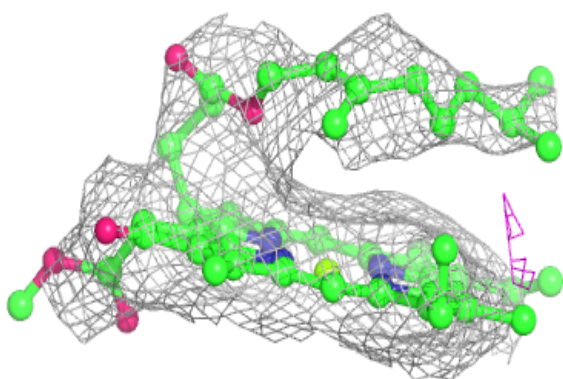
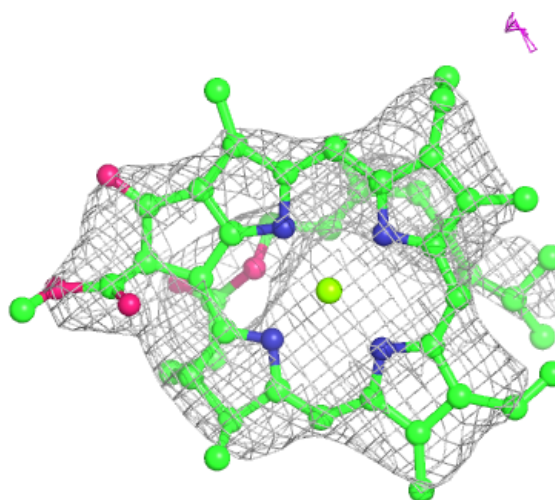
**Electron density around CLA 3 312:**

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



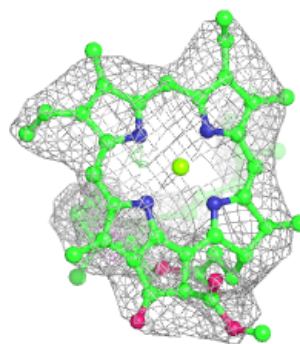
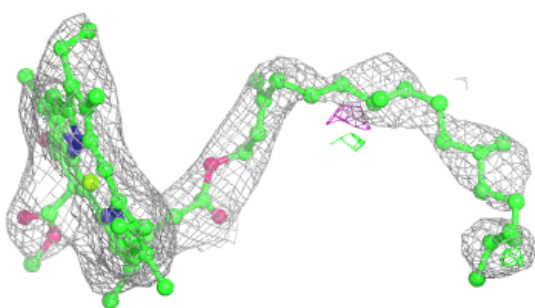
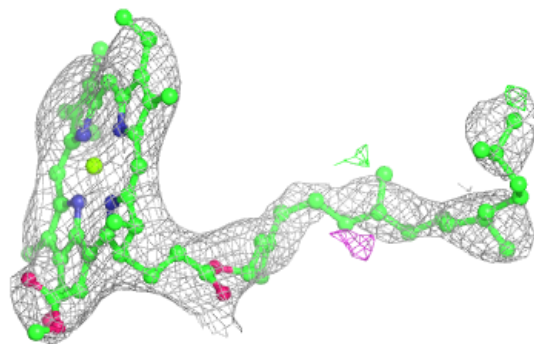
**Electron density around CLA 8 310:**

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

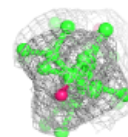
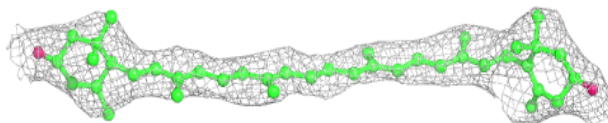
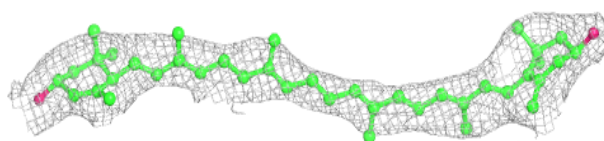


**Electron density around CLA L 203:**

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

**Electron density around LUT 1 316:**

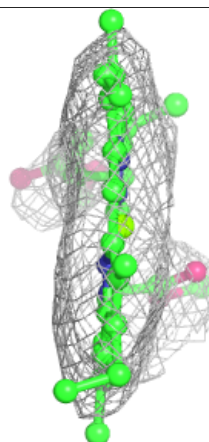
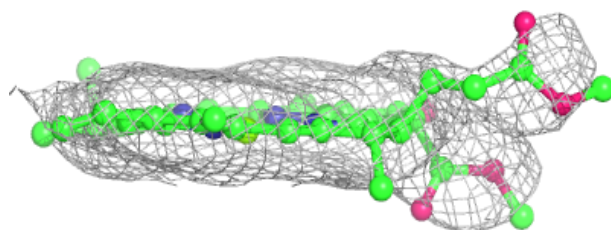
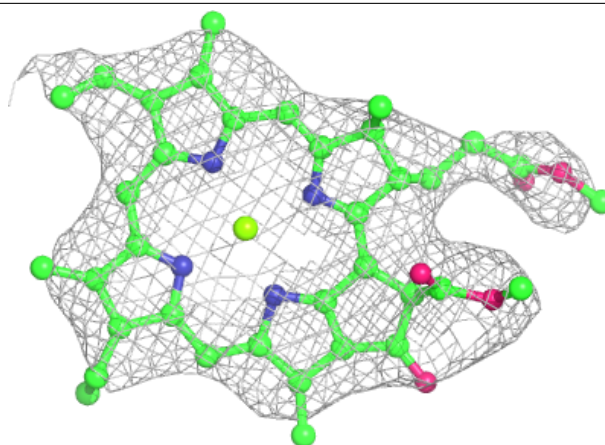
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



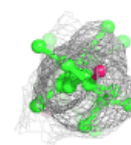
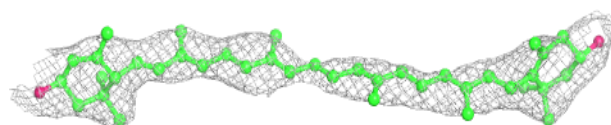
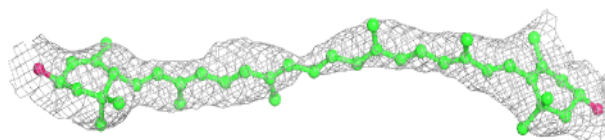


**Electron density around CLA 3 314:**

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

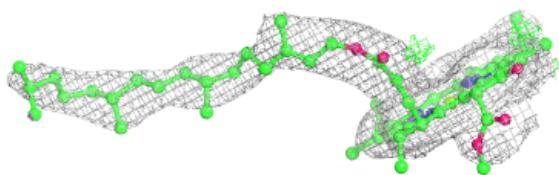
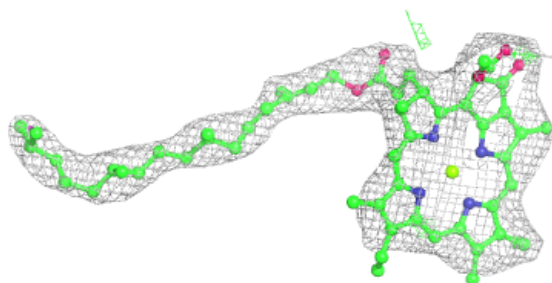
**Electron density around LUT 2 615:**

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



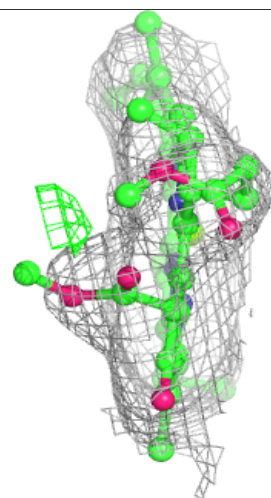
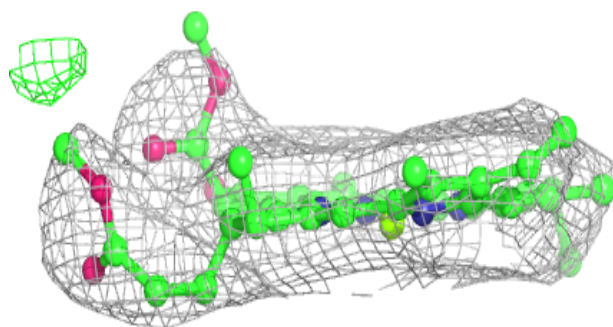
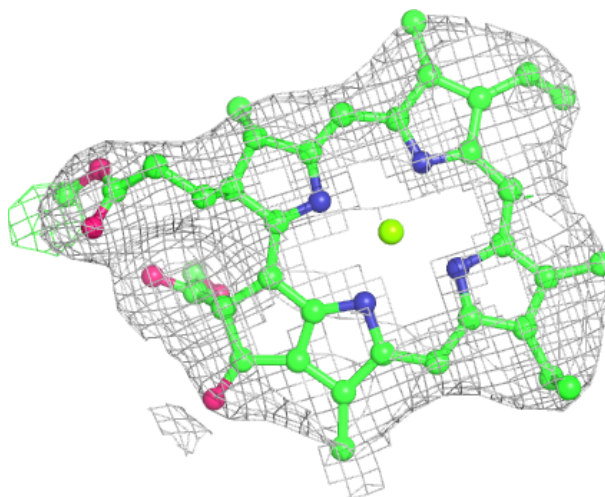
**Electron density around CLA A 835:**

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



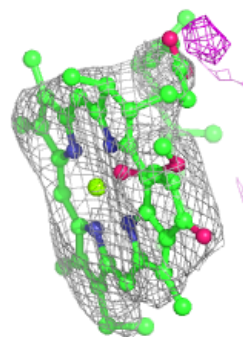
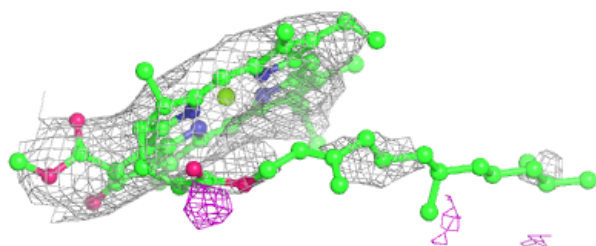
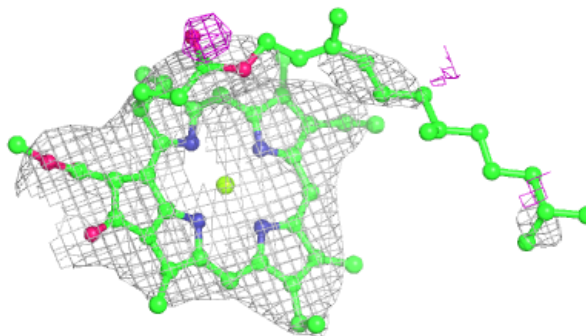
**Electron density around CLA 4 603:**

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

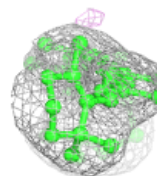
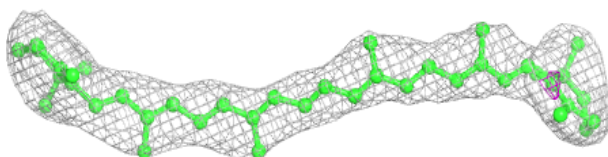
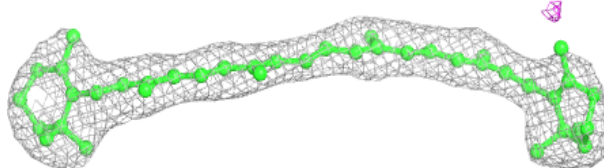


**Electron density around CLA 9 609:**

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

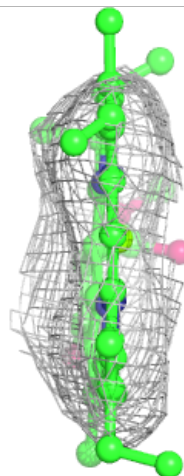
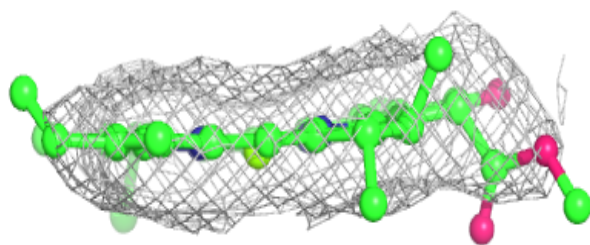
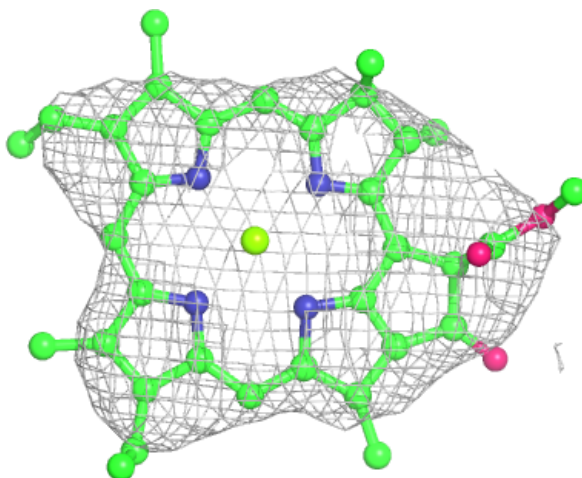
**Electron density around BCR i 101:**

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



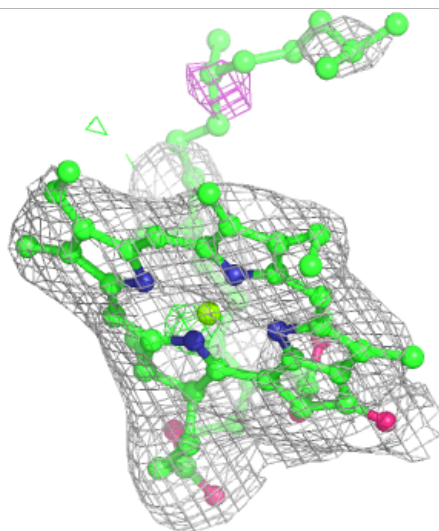
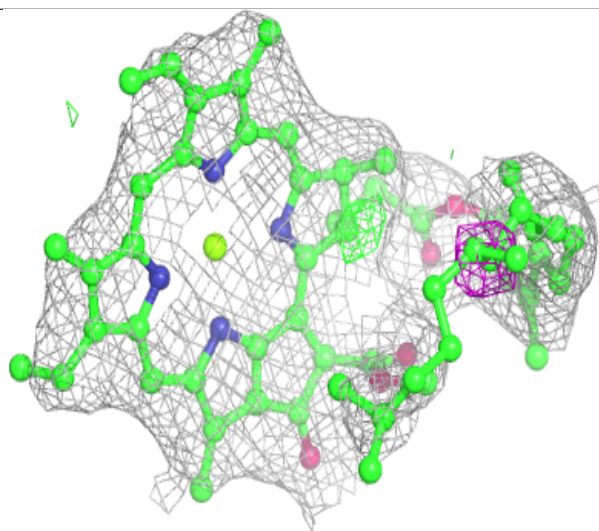
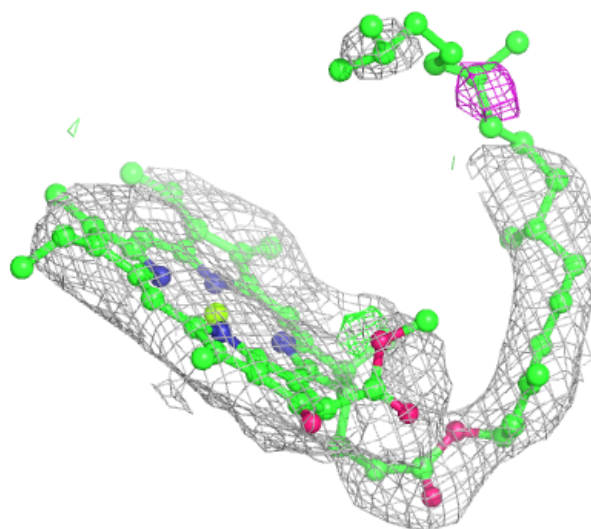
**Electron density around CLA 9 610:**

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



**Electron density around CLA 1 304:**

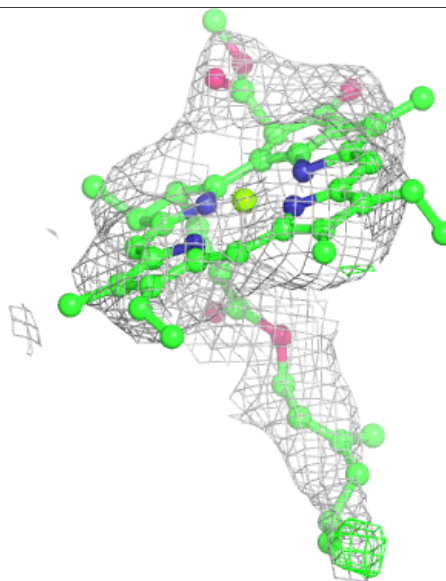
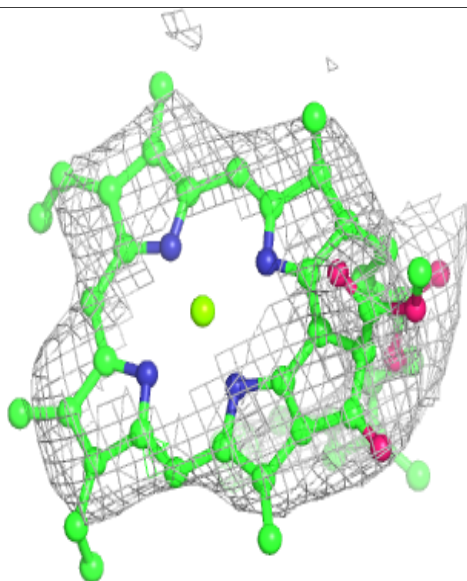
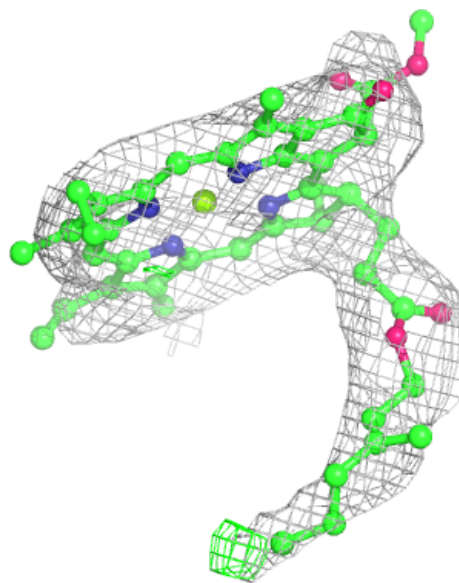
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





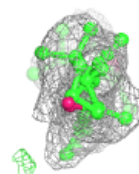
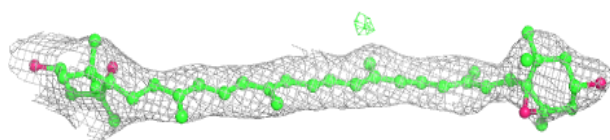
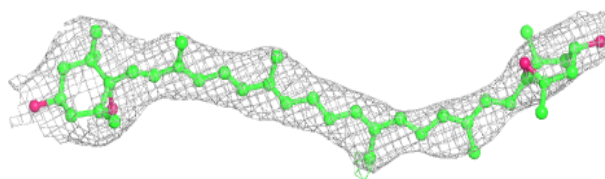
**Electron density around CLA 1 305:**

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

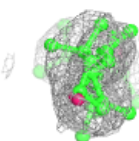
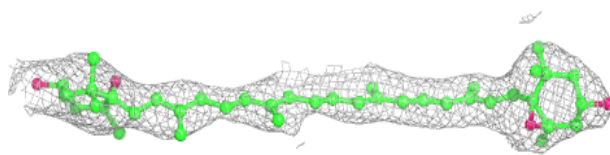
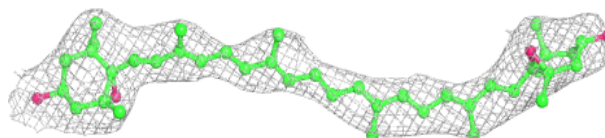


**Electron density around XAT 3 317:**

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

**Electron density around XAT 4 617:**

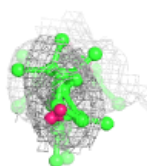
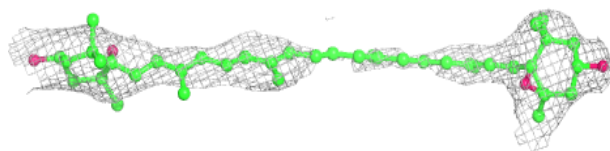
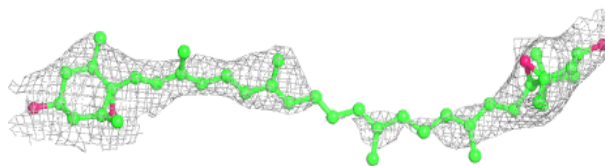
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





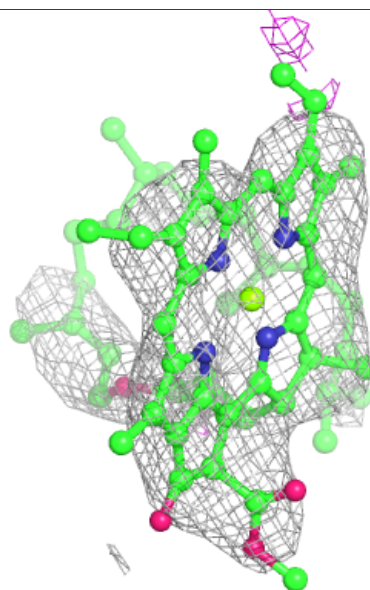
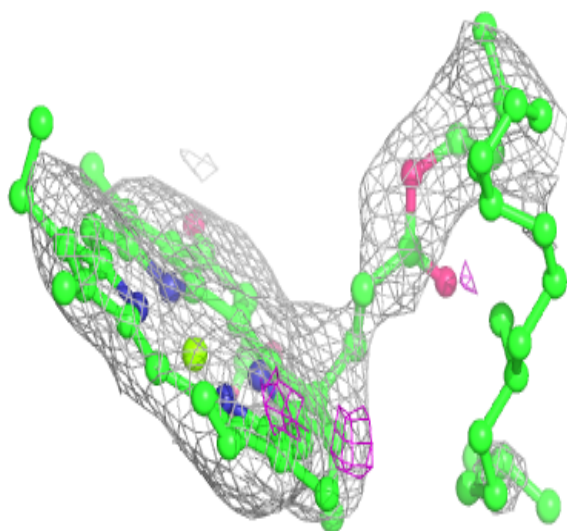
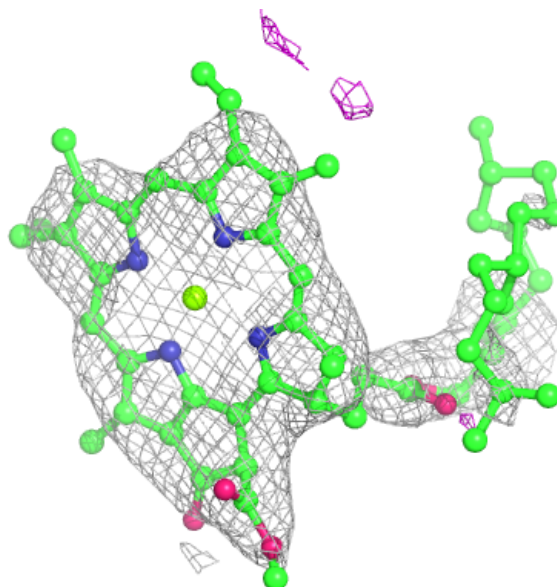
**Electron density around XAT 6 318:**

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



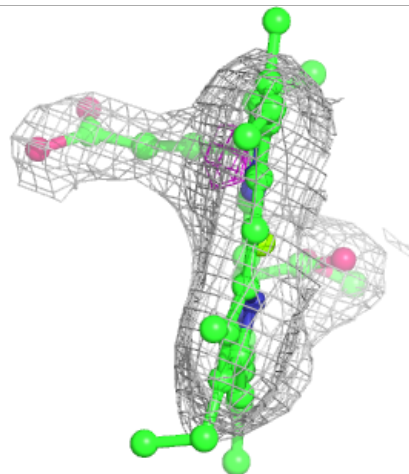
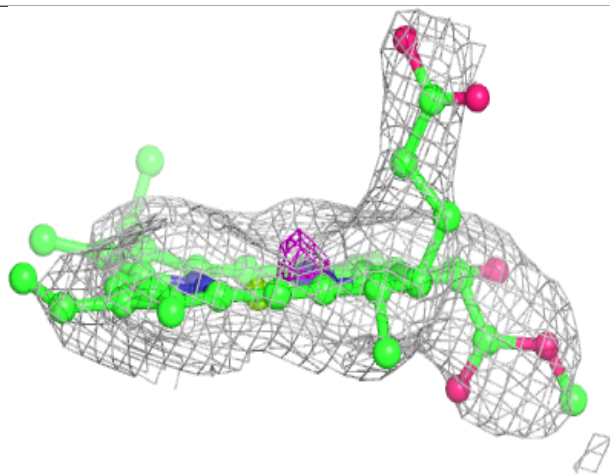
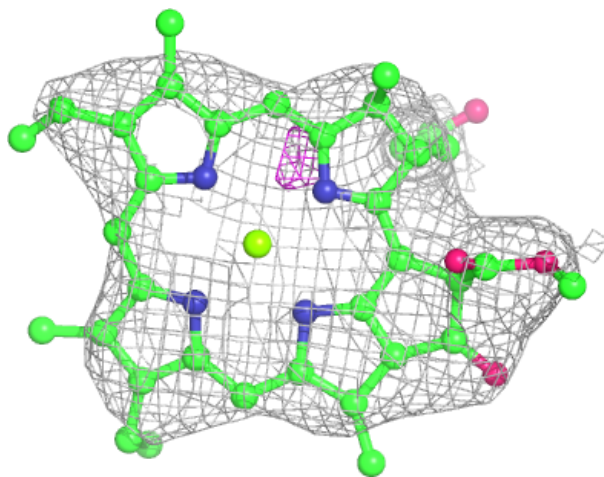
**Electron density around CLA 1 308:**

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



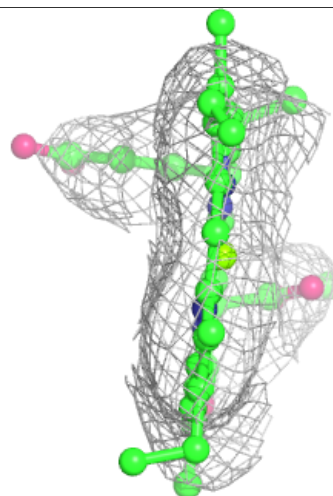
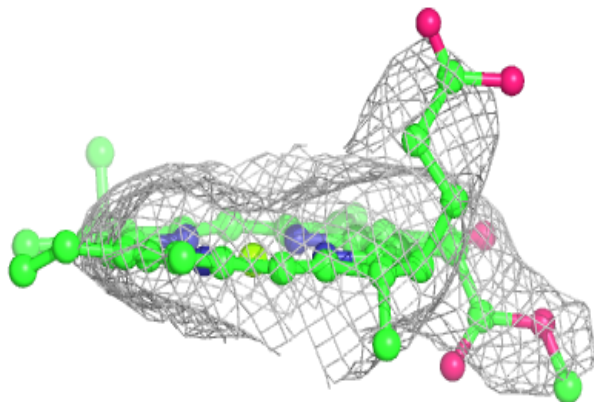
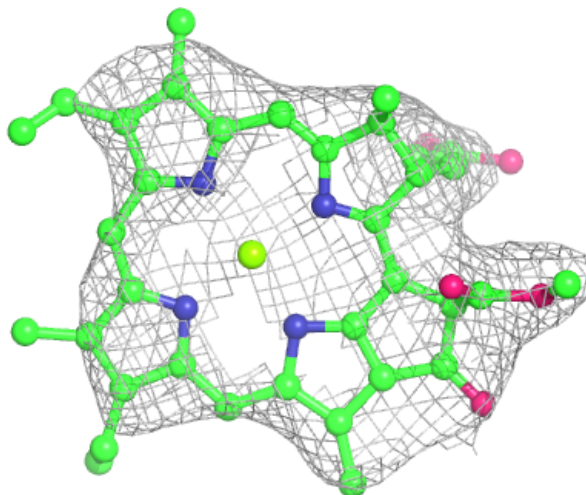
**Electron density around CLA G 101:**

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



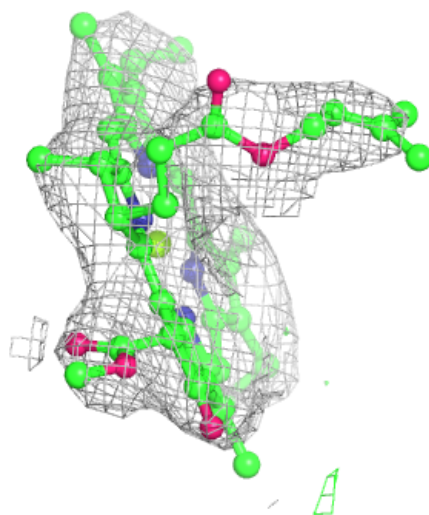
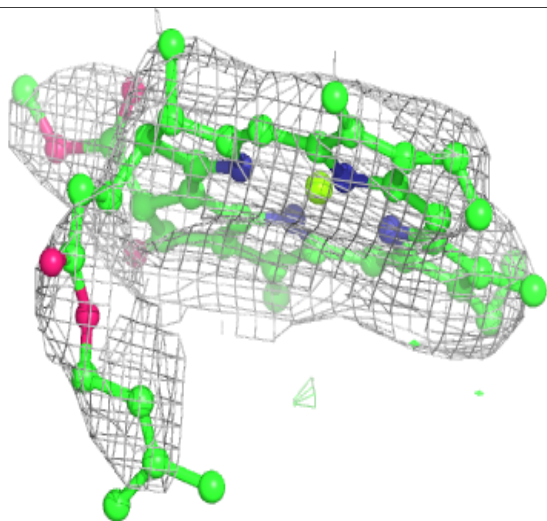
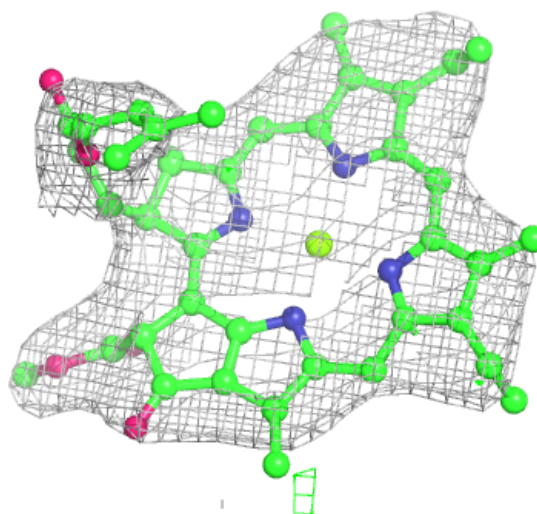
**Electron density around CLA 4 613:**

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



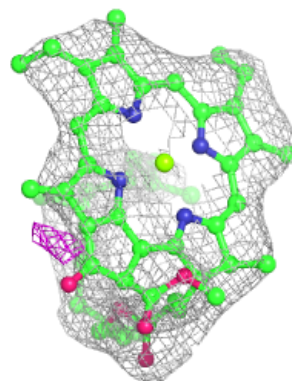
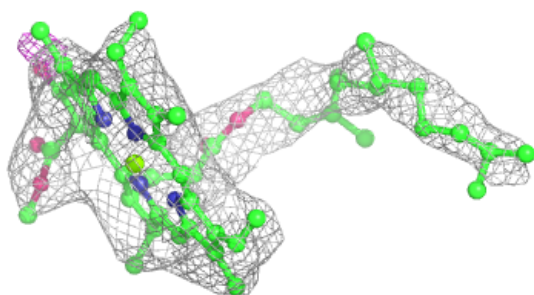
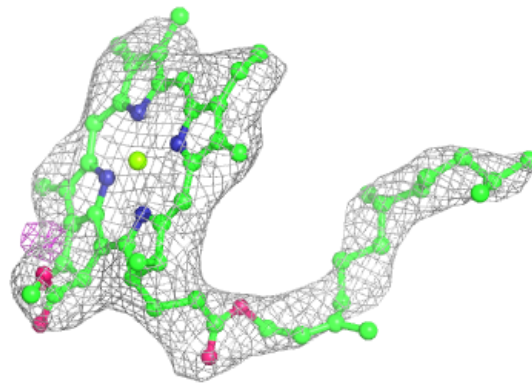
**Electron density around CLA 3 308:**

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

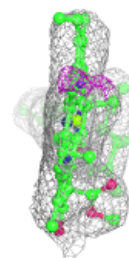
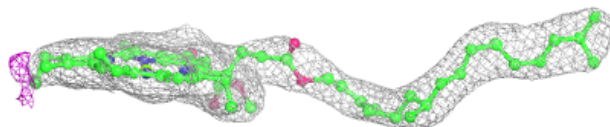
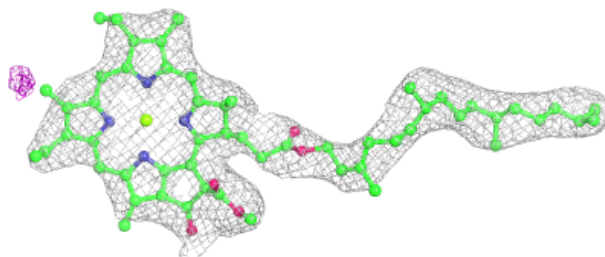


**Electron density around CLA B 815:**

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

**Electron density around CLA A 834:**

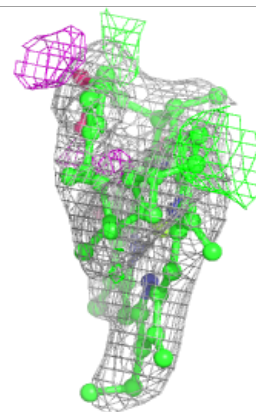
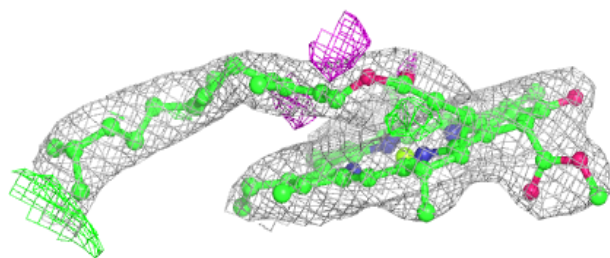
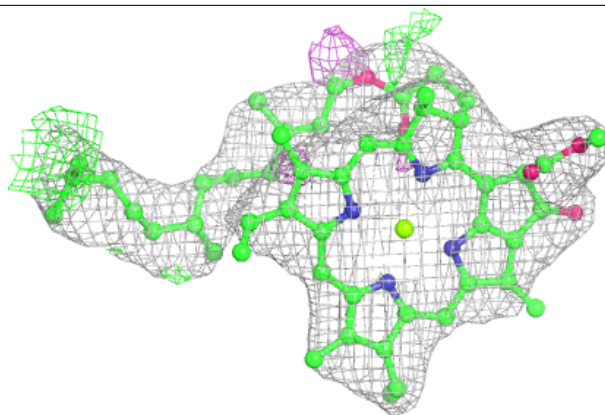
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



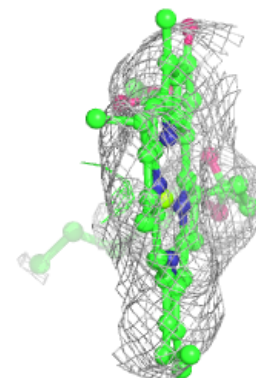
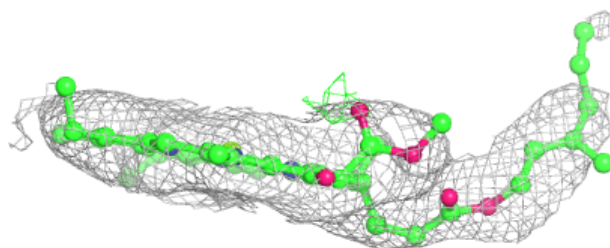
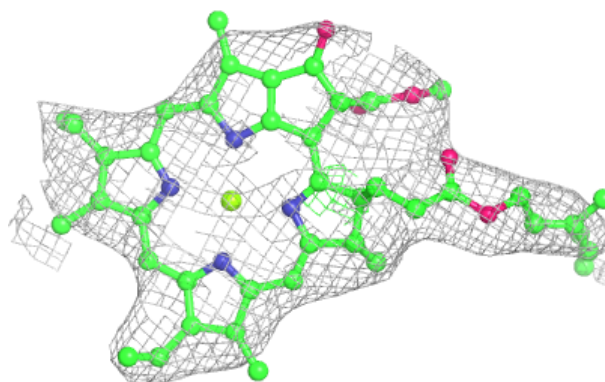


**Electron density around CLA b 818:**

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

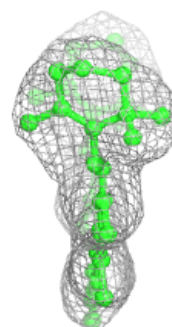
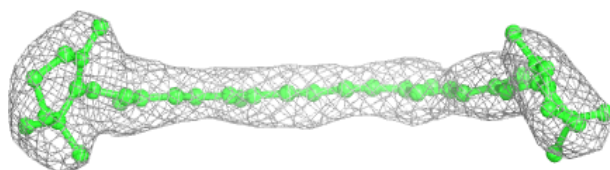
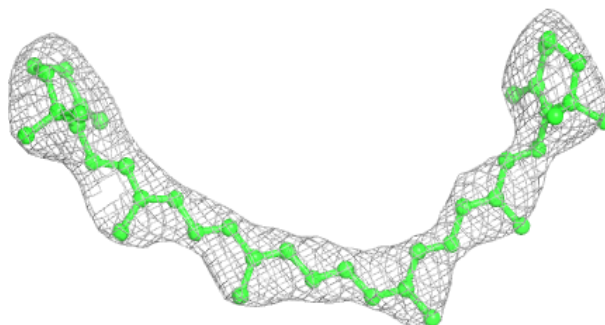
**Electron density around CLA 1 306:**

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

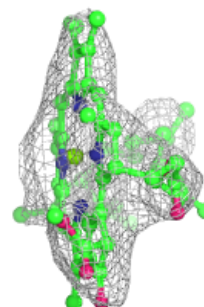
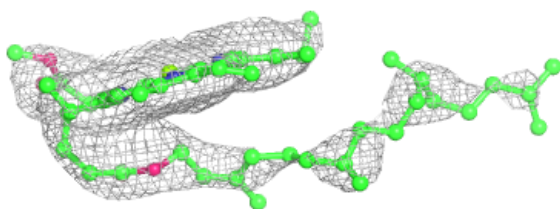
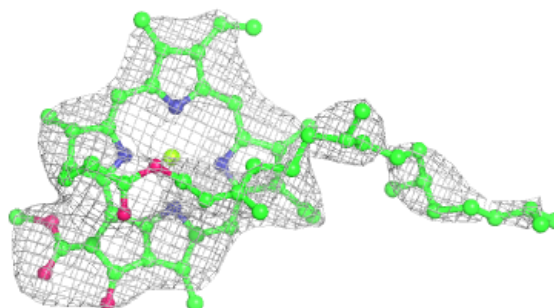


**Electron density around BCR F 305:**

$2mF_o-DF_c$  (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:**

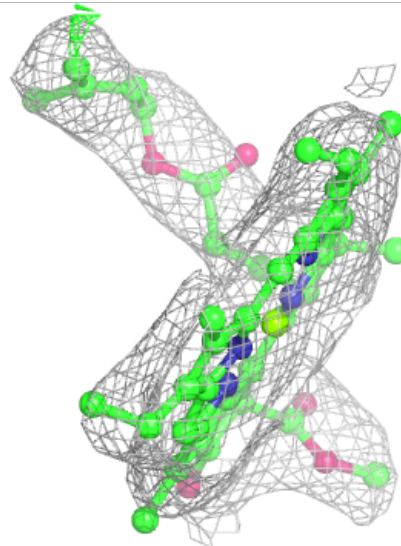
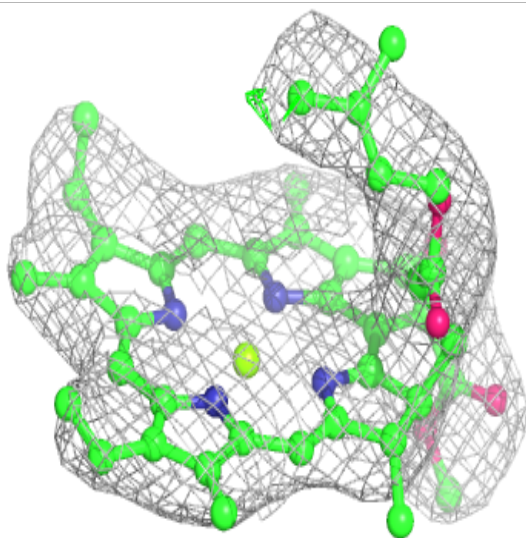
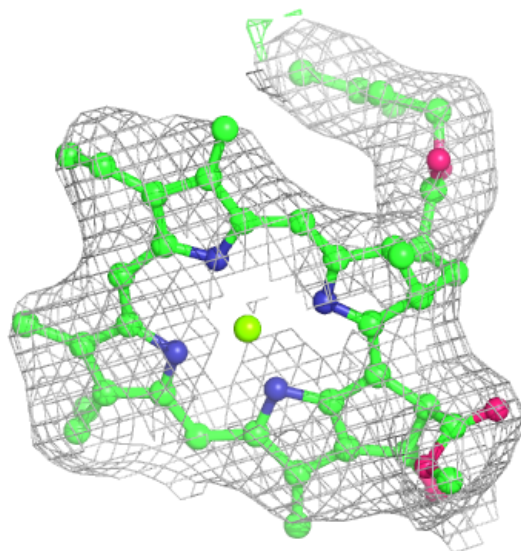
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





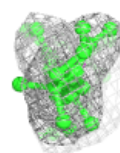
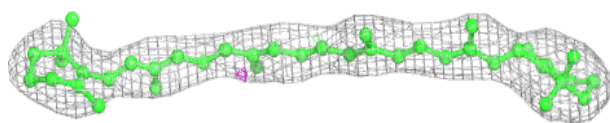
**Electron density around CLA b 830:**

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

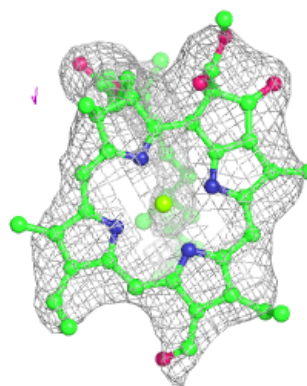
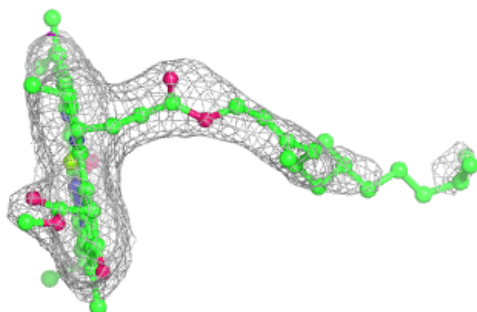
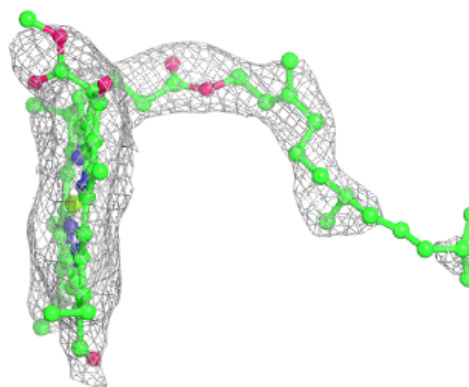


**Electron density around BCR J 3003:**

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

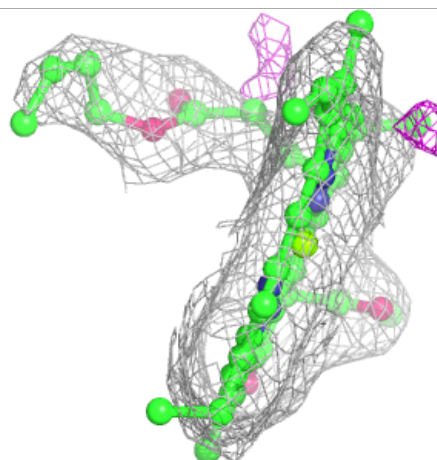
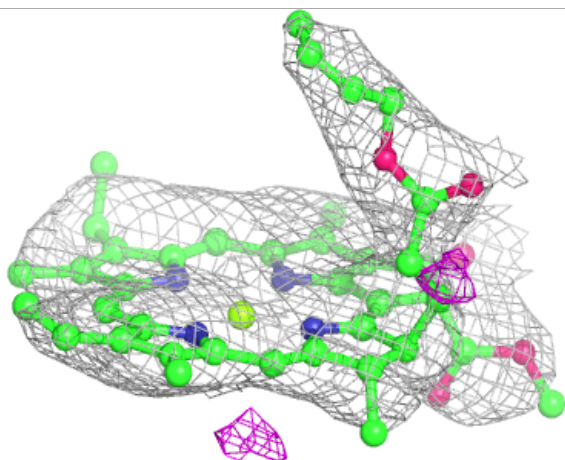
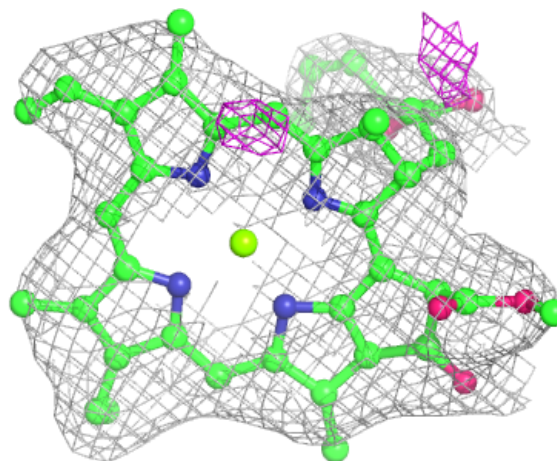
**Electron density around CHL 1 302:**

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



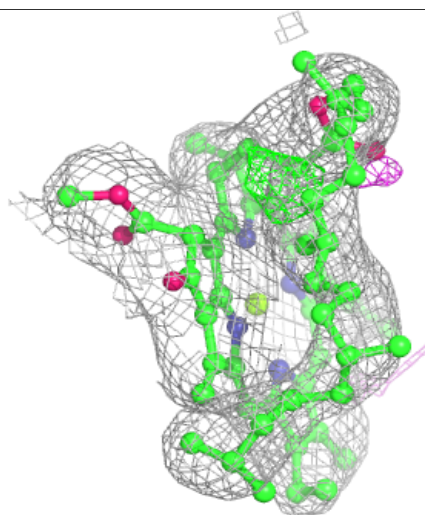
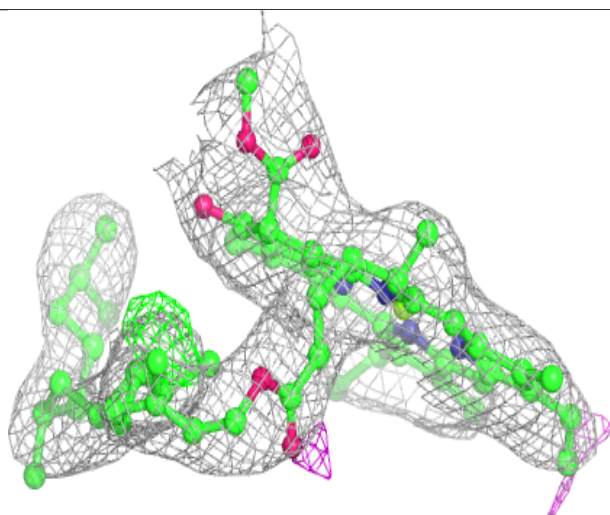
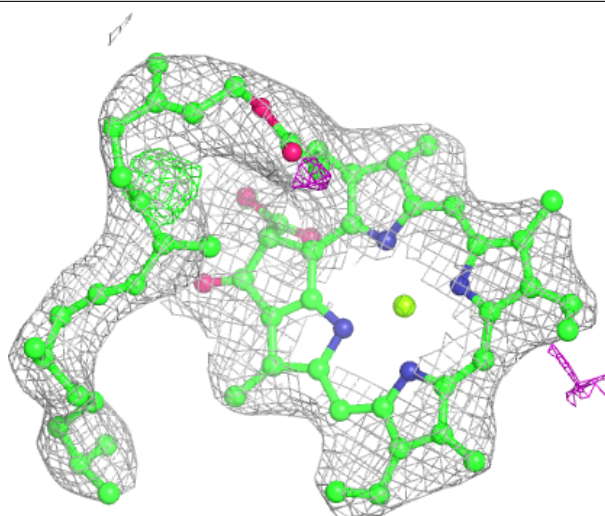
**Electron density around CLA b 831:**

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



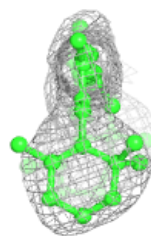
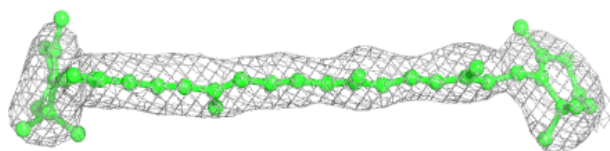
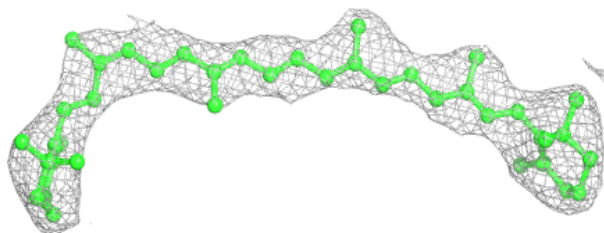
**Electron density around CLA b 832:**

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

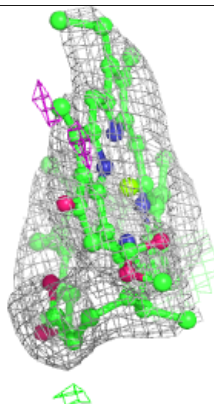
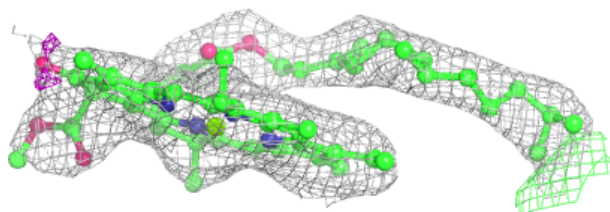
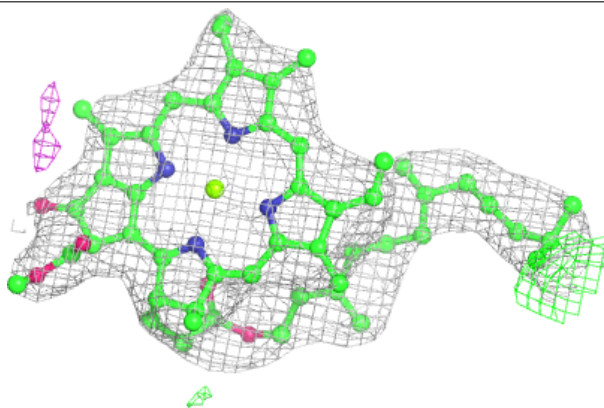


**Electron density around BCR L 201:**

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

**Electron density around CLA B 818:**

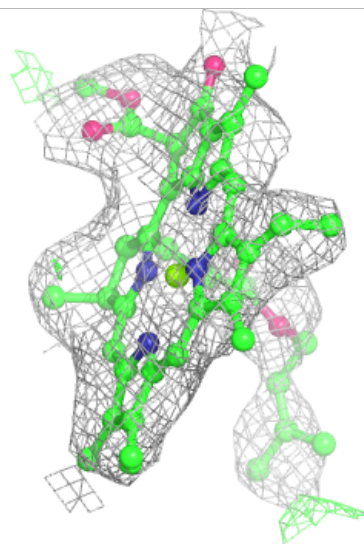
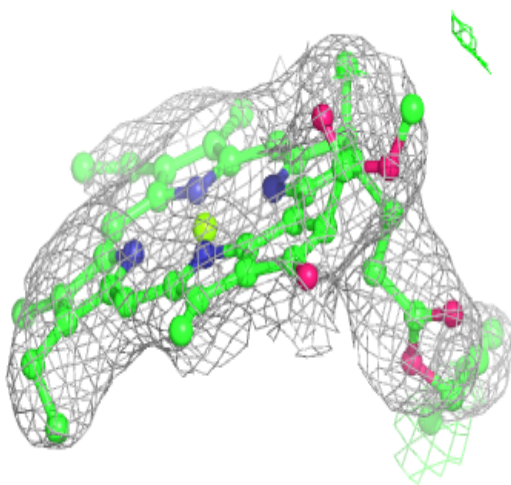
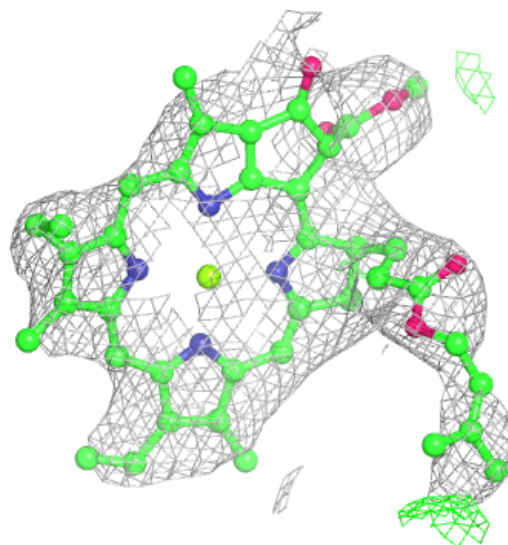
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





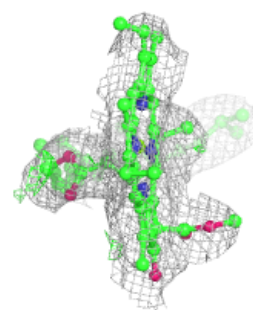
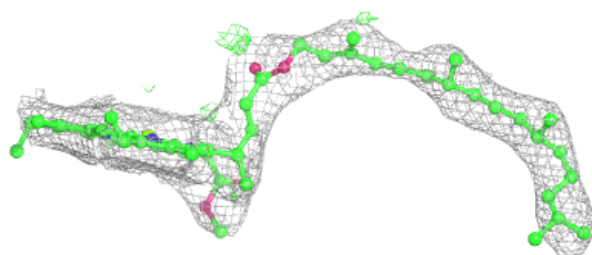
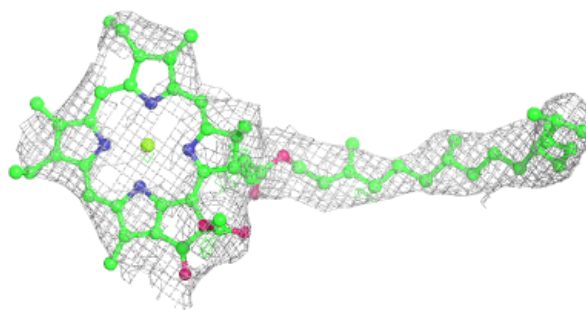
**Electron density around CLA A 836:**

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



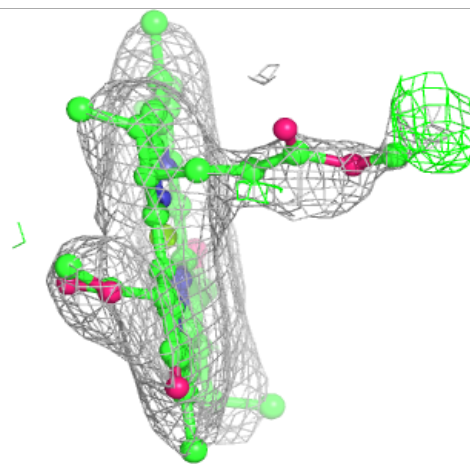
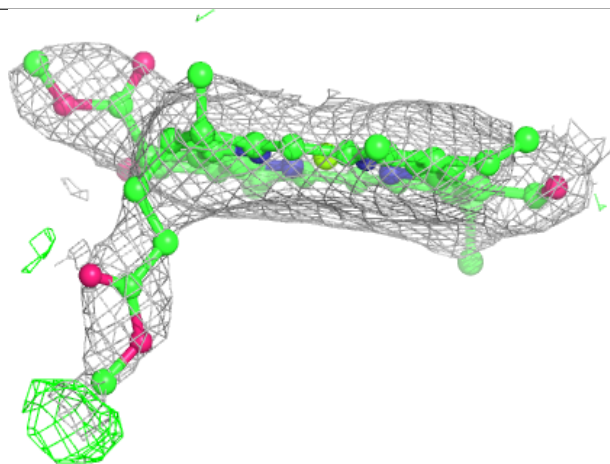
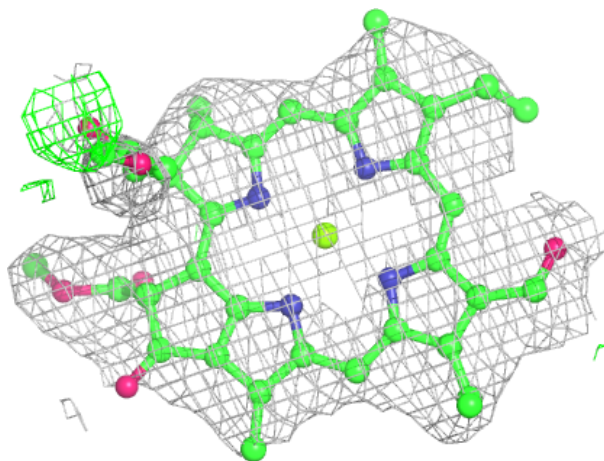
**Electron density around CLA b 841:**

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



**Electron density around CHL 3 307:**

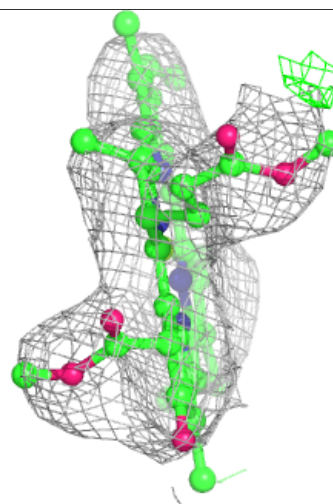
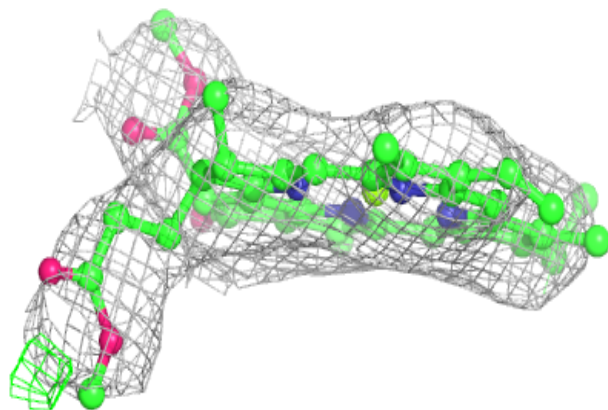
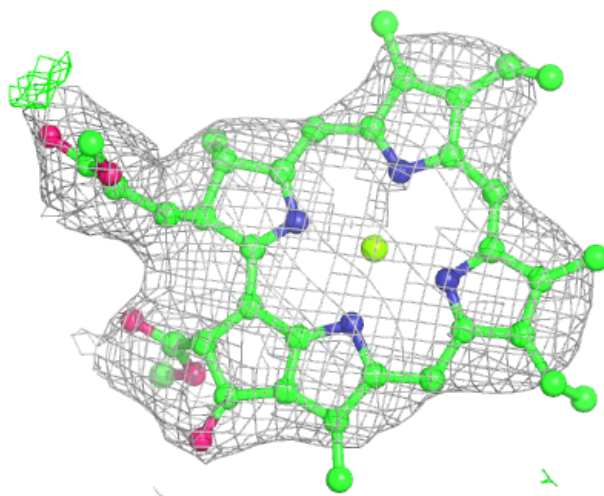
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





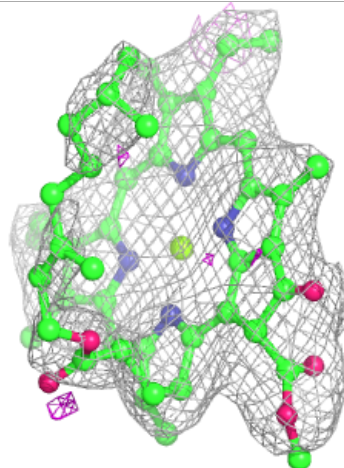
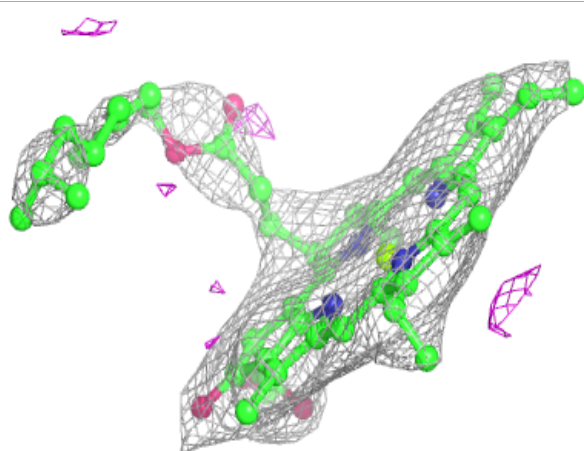
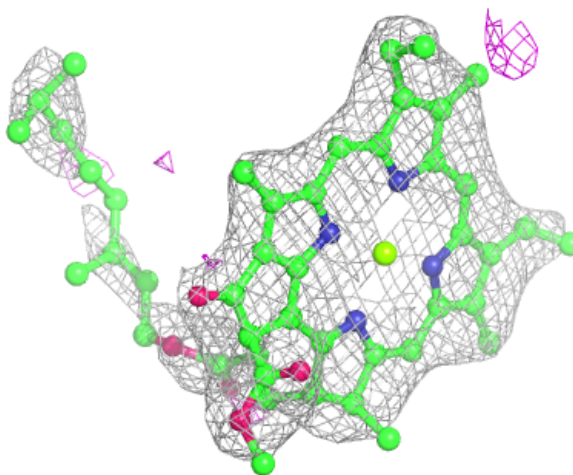
**Electron density around CLA 9 601:**

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



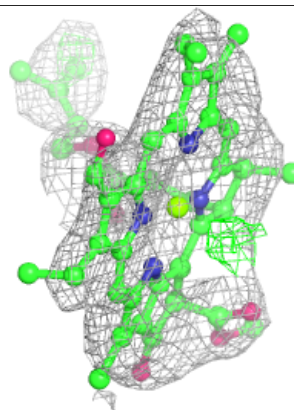
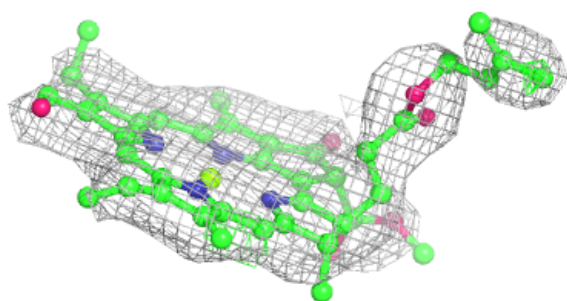
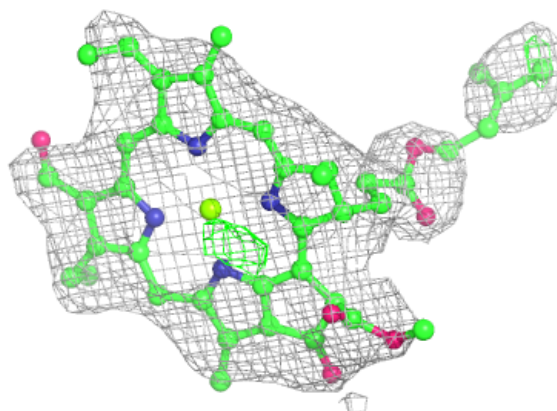
**Electron density around CLA B 822:**

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



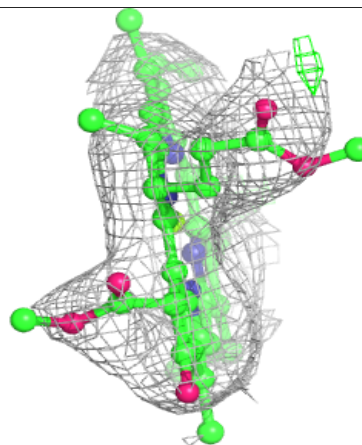
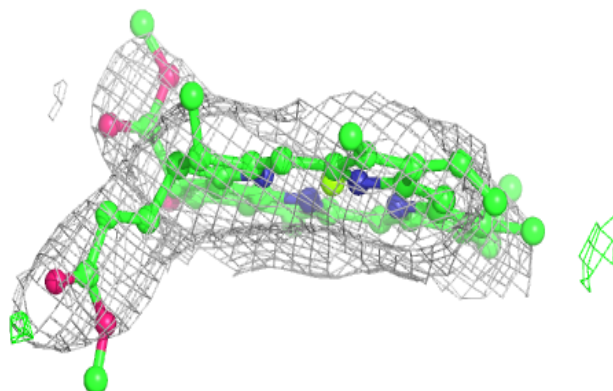
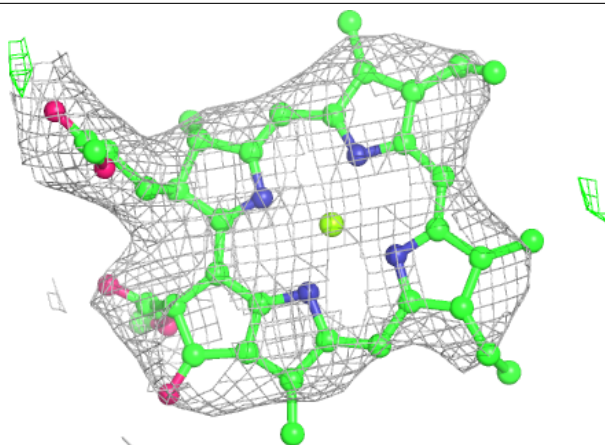
**Electron density around CHL 4 607:**

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

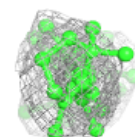
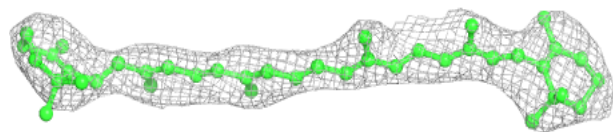
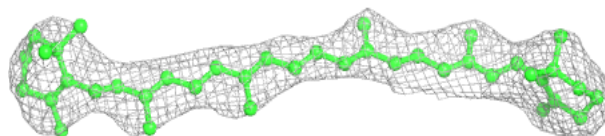


**Electron density around CLA 4 601:**

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

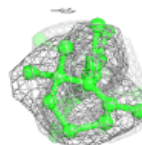
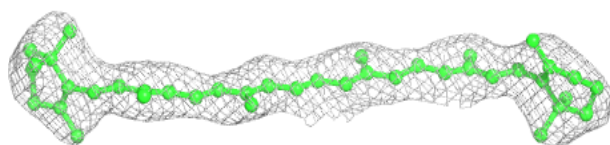
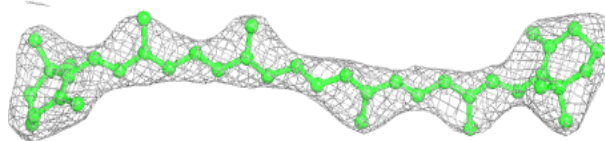
**Electron density around BCR a 850:**

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

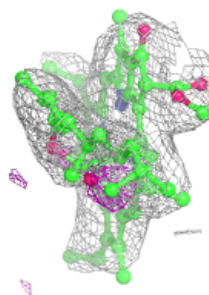
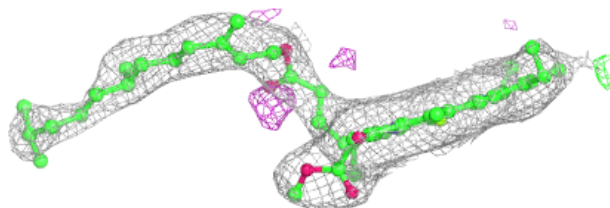
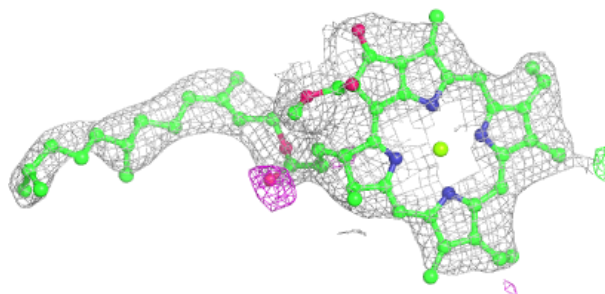


**Electron density around BCR a 851:**

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

**Electron density around CLA B 823:**

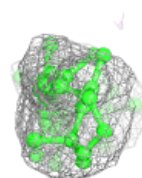
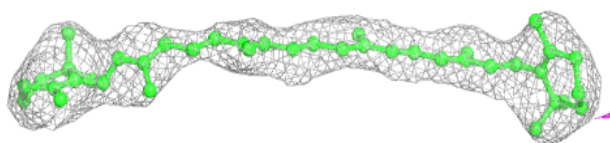
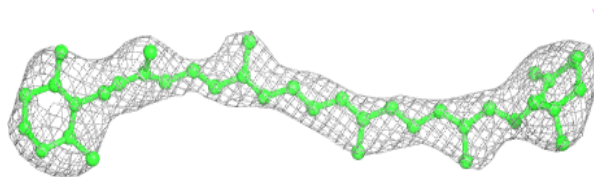
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



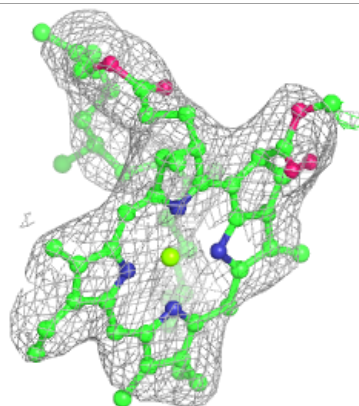
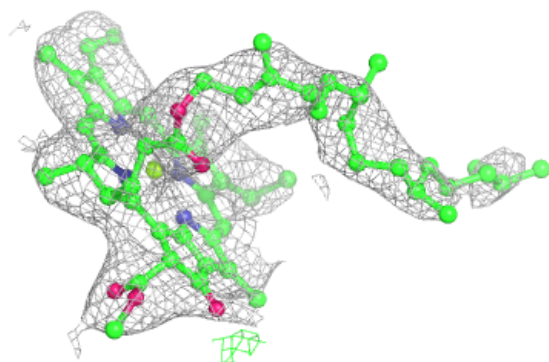
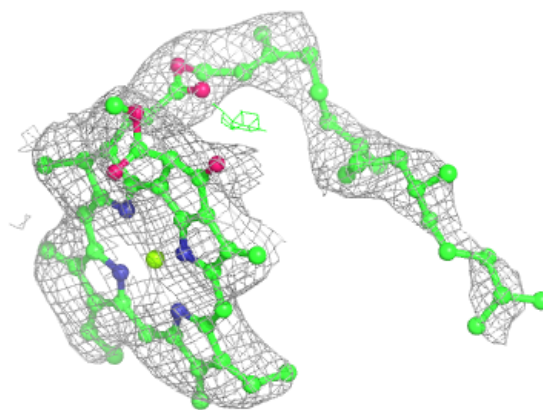


**Electron density around BCR a 853:**

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

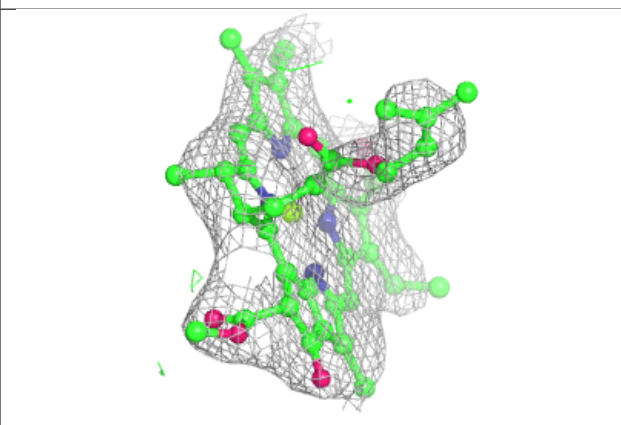
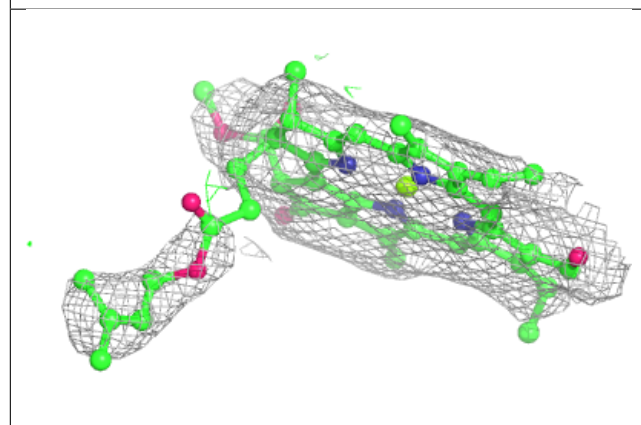
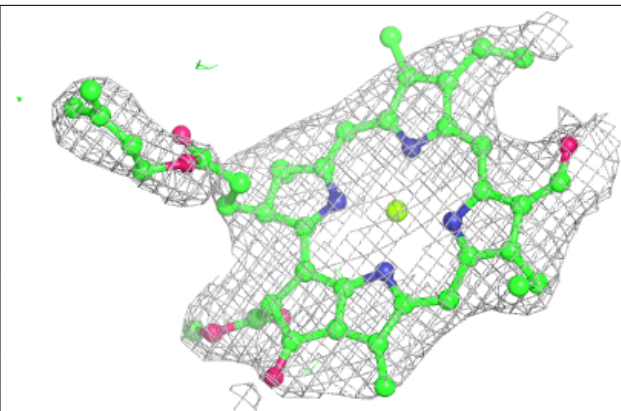
**Electron density around CLA B 834:**

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

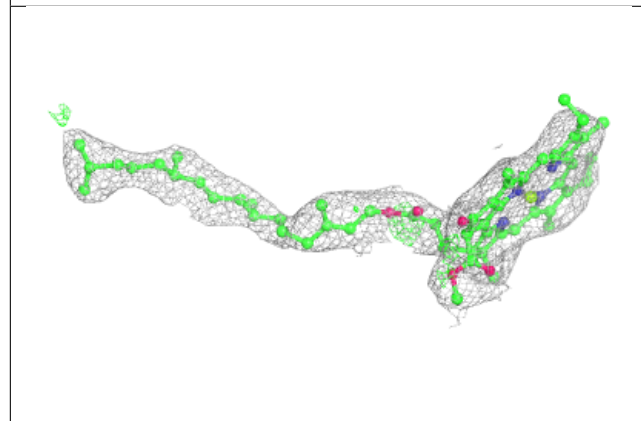
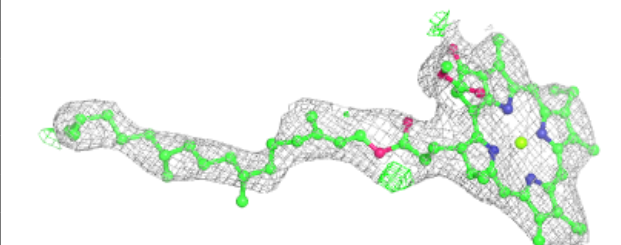


**Electron density around CHL 7 607:**

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

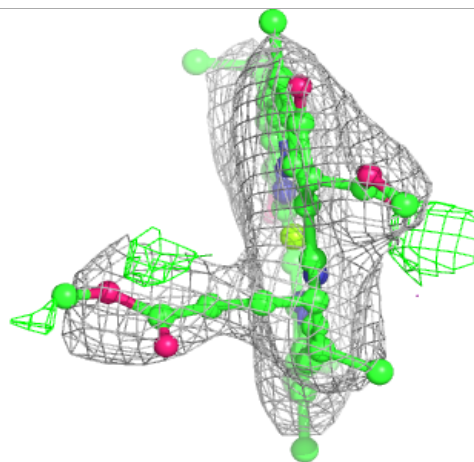
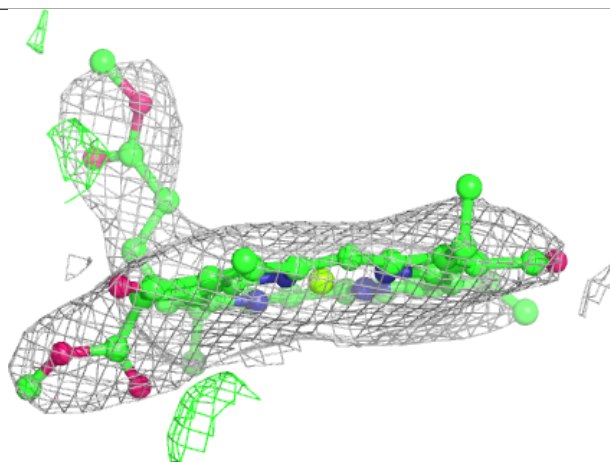
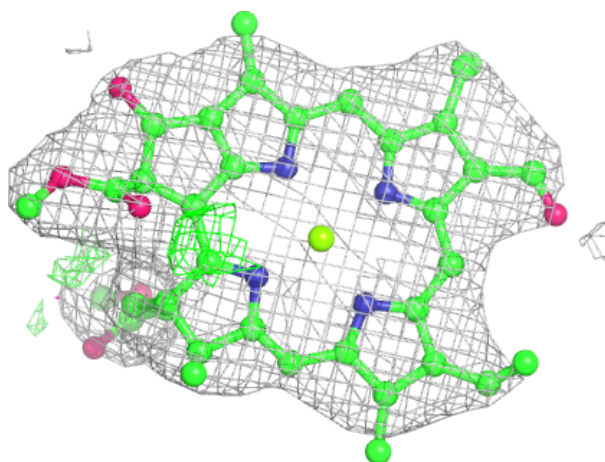
**Electron density around CLA A 810:**

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



**Electron density around CHL 8 306:**

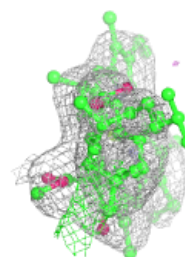
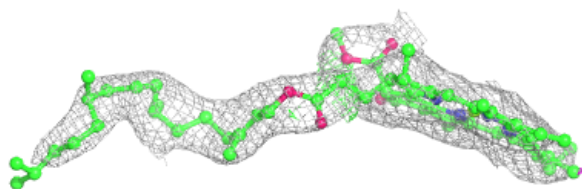
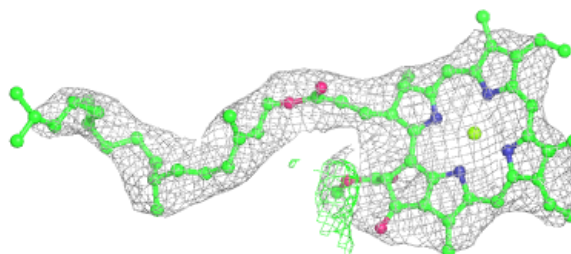
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



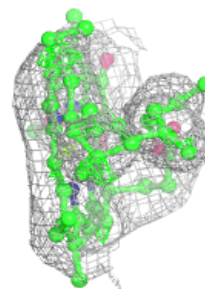
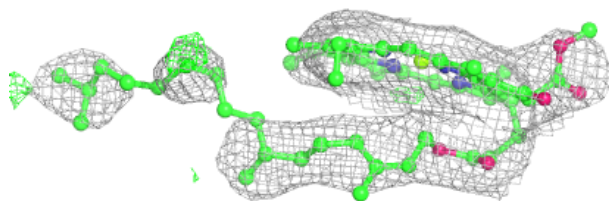
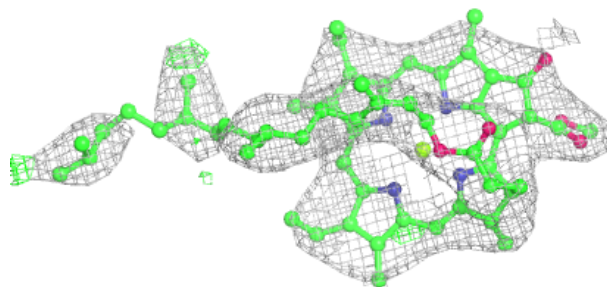


**Electron density around CLA F 301:**

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

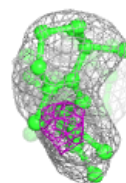
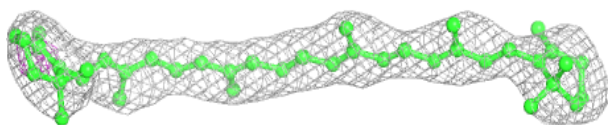
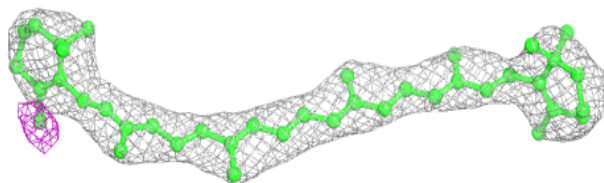
**Electron density around CLA A 839:**

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

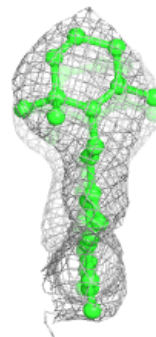
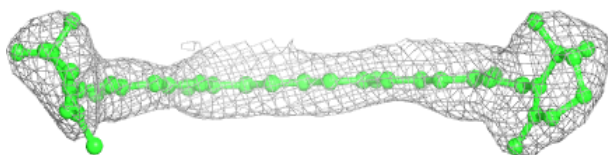
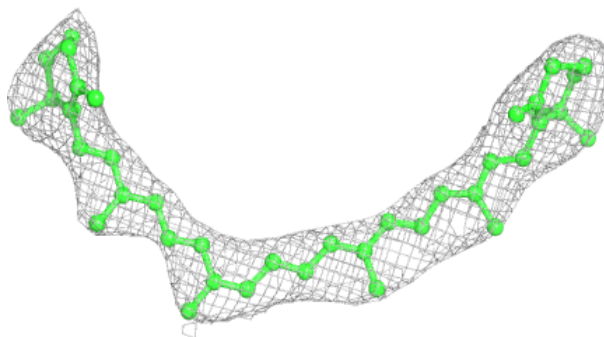


**Electron density around BCR b 847:**

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

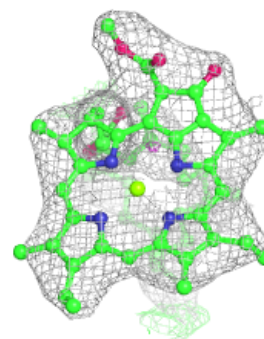
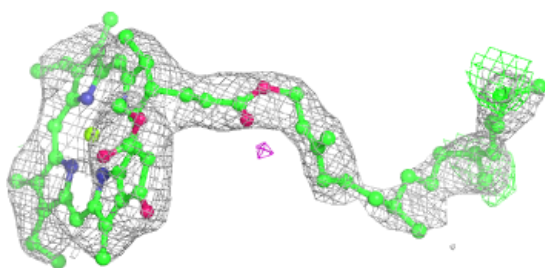
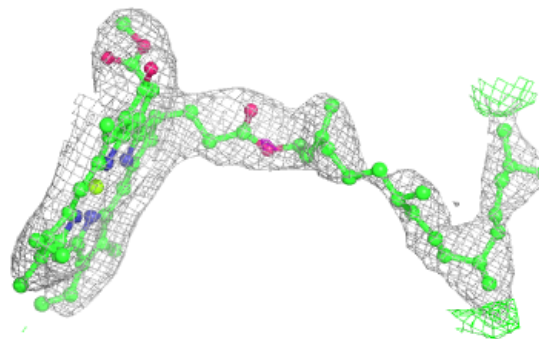
**Electron density around BCR f 7004:**

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

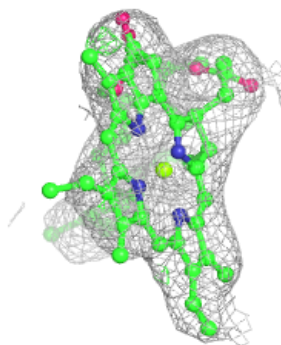
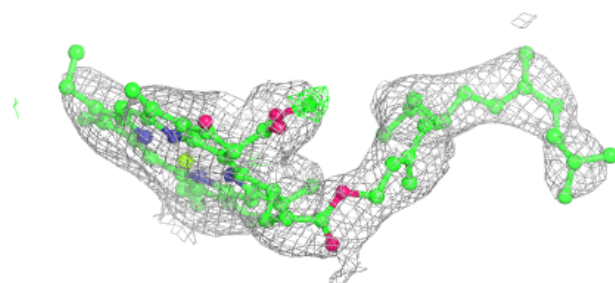
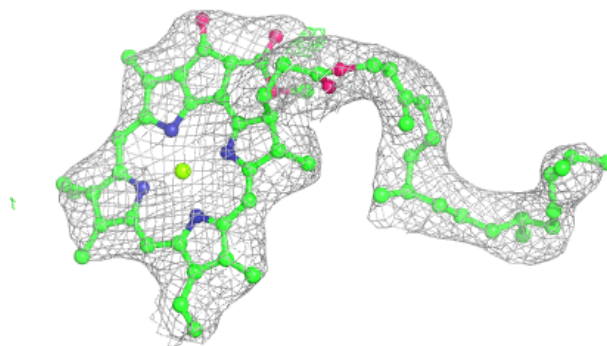


**Electron density around CLA A 840:**

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

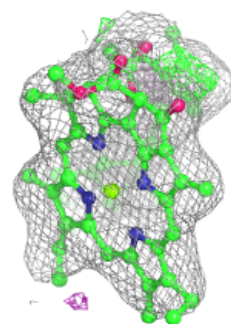
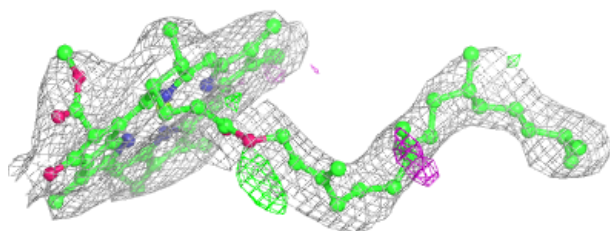
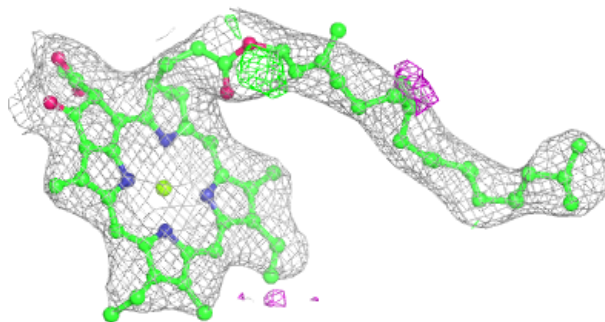
**Electron density around CLA a 804:**

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

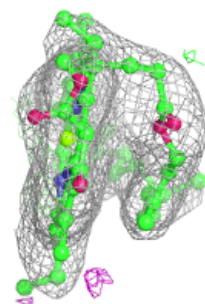
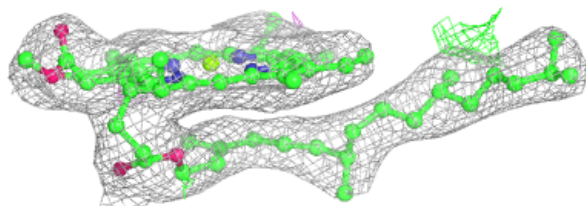
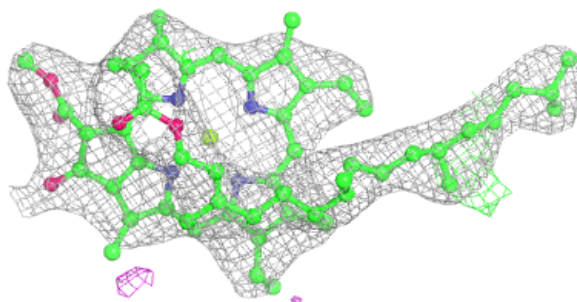


**Electron density around CLA a 809:**

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

**Electron density around CLA A 841:**

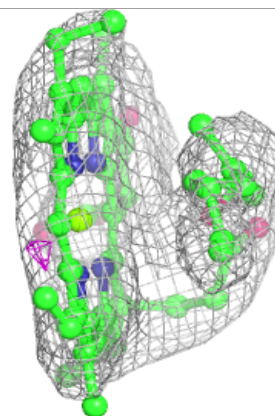
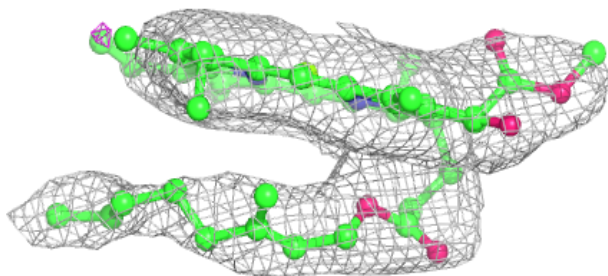
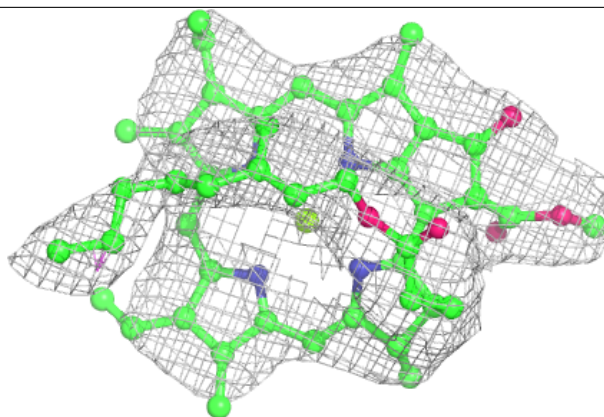
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



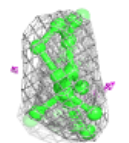
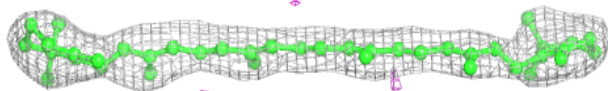
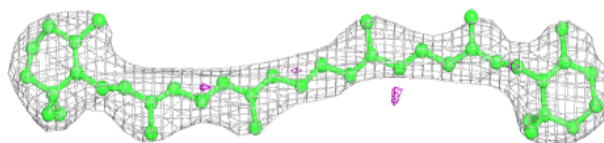


**Electron density around CLA A 813:**

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

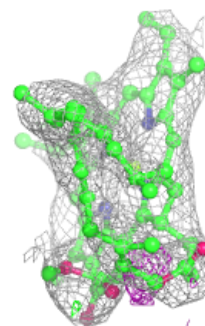
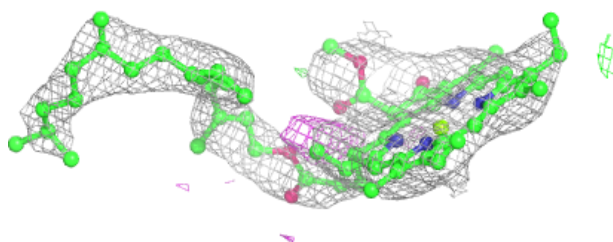
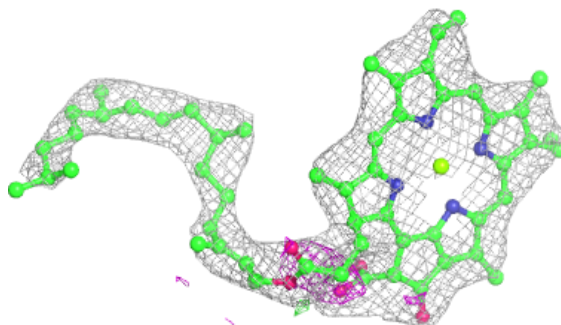
**Electron density around BCR 1 205:**

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

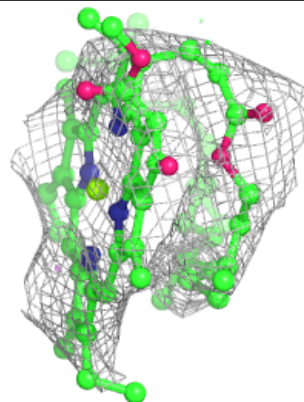
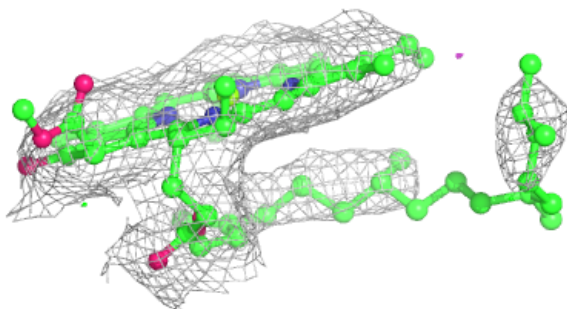
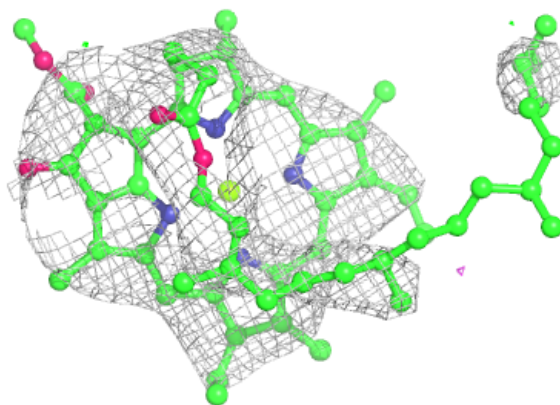


**Electron density around CLA A 804:**

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

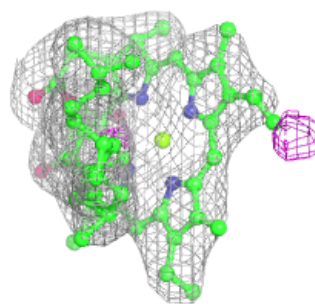
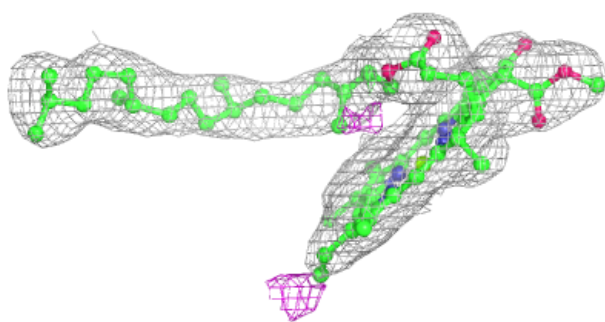
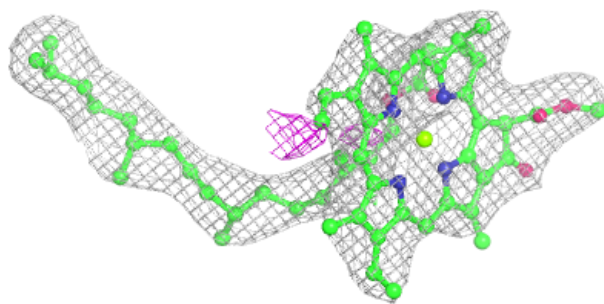
**Electron density around CLA 2 612:**

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



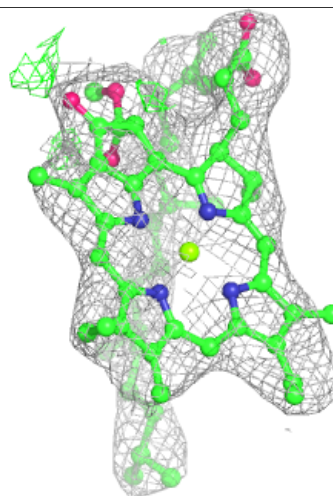
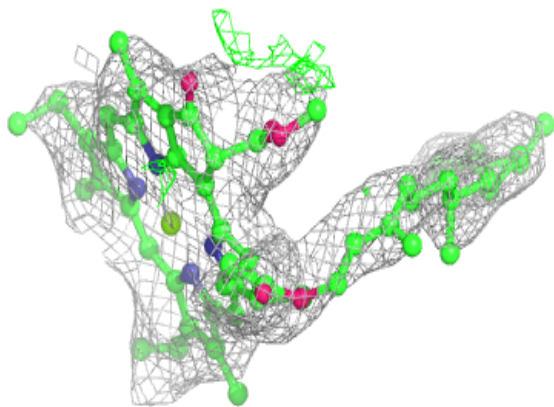
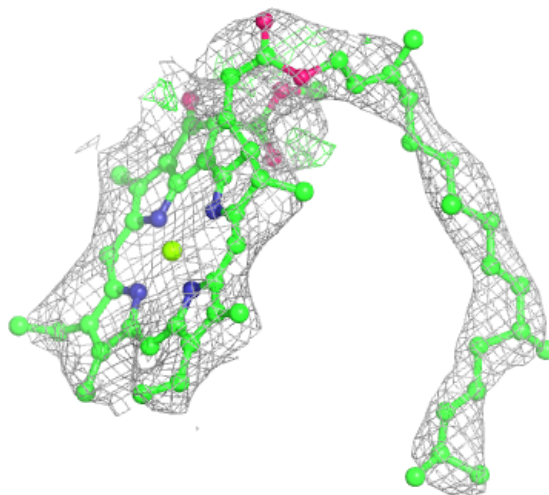
**Electron density around CLA a 843:**

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



**Electron density around CLA B 810:**

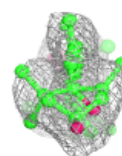
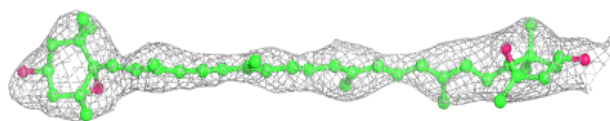
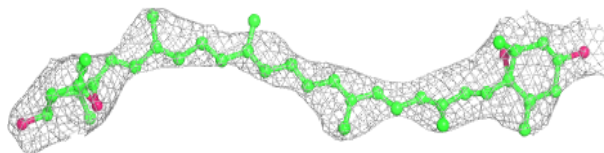
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





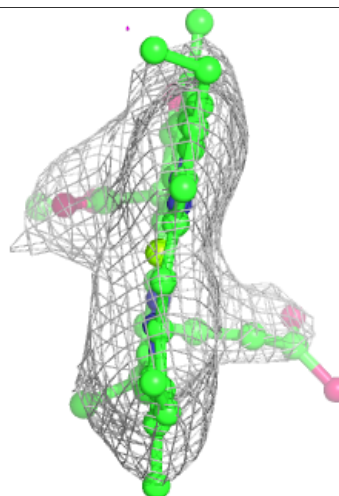
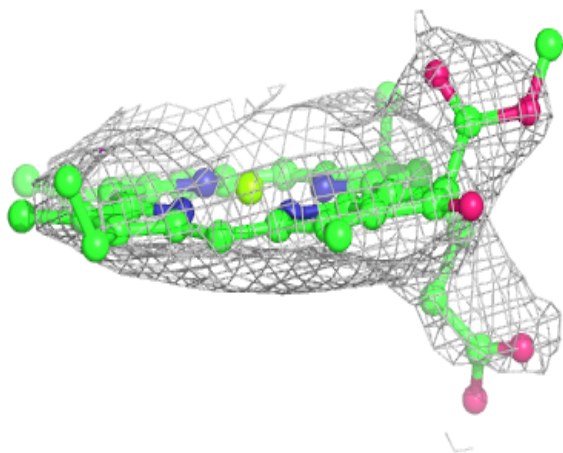
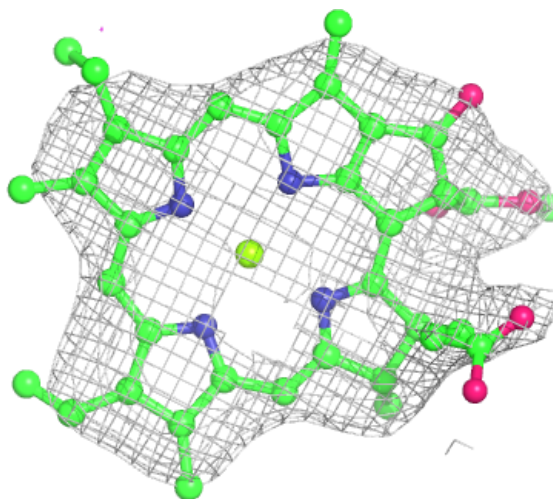
**Electron density around XAT 2 616:**

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



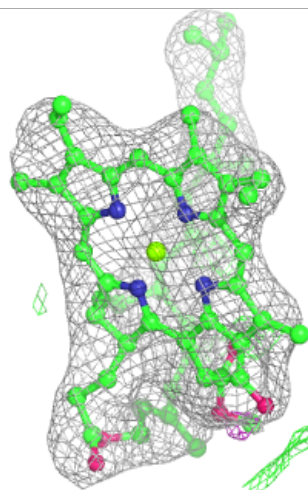
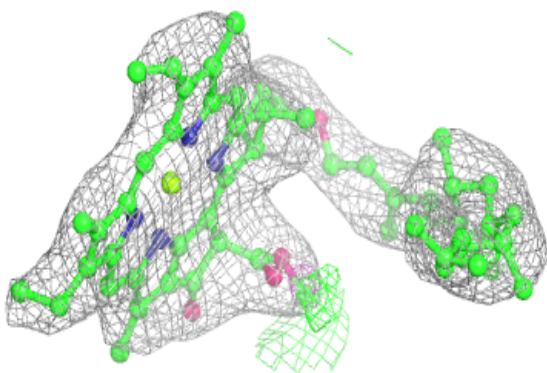
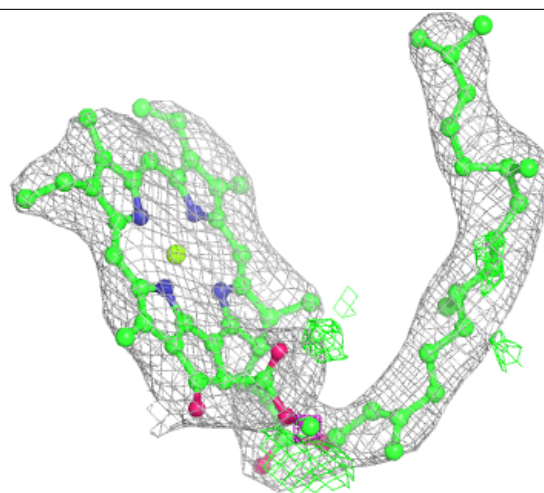
**Electron density around CLA A 817:**

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



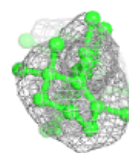
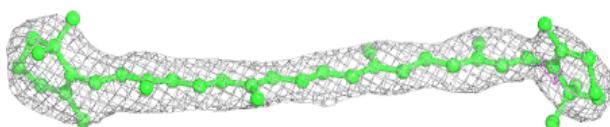
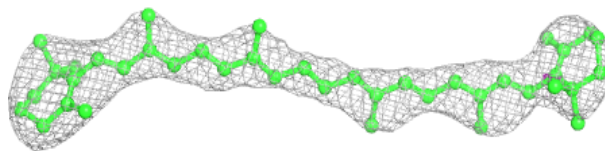
**Electron density around CLA b 810:**

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

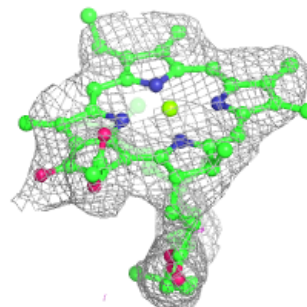
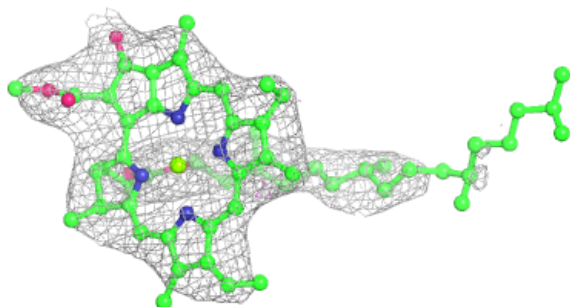
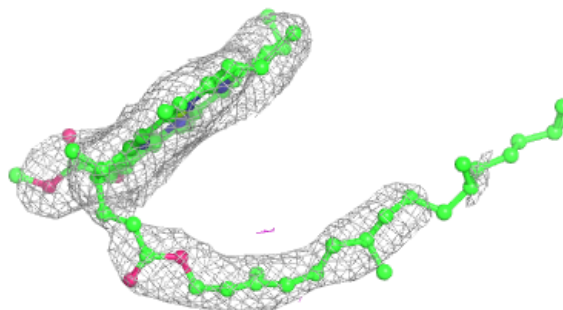


**Electron density around BCR A 849:**

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

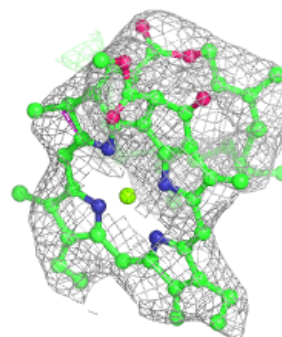
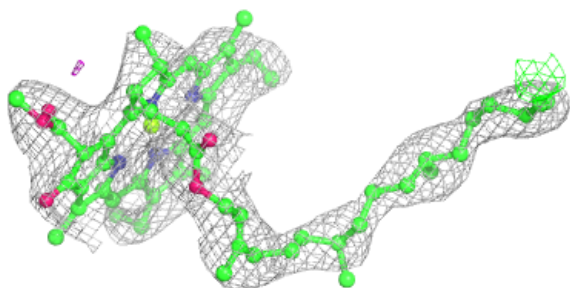
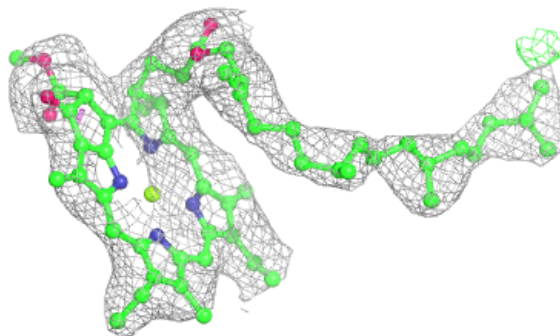
**Electron density around CLA A 833:**

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

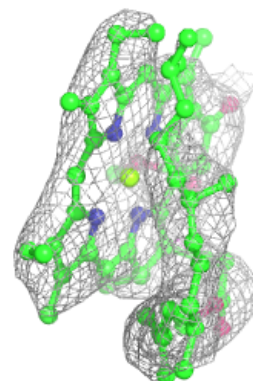
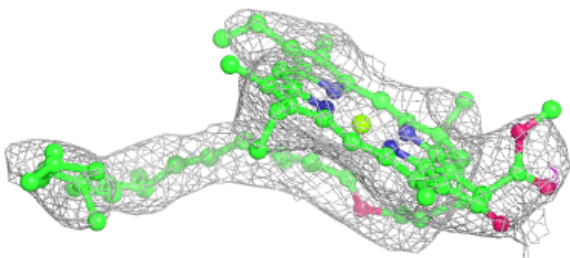
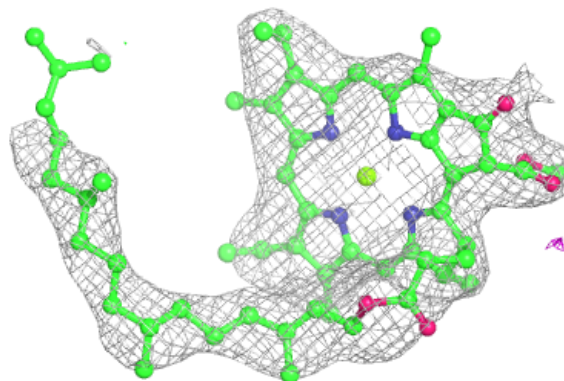


**Electron density around CLA B 814:**

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

**Electron density around CLA 1 303:**

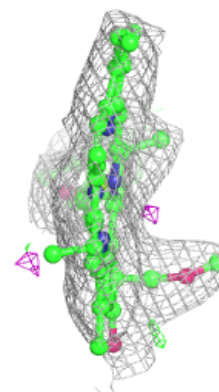
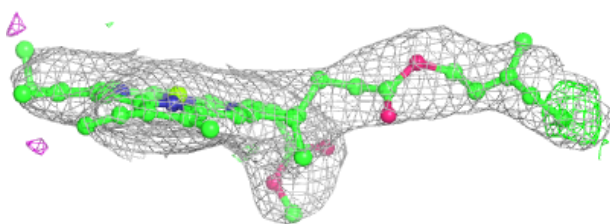
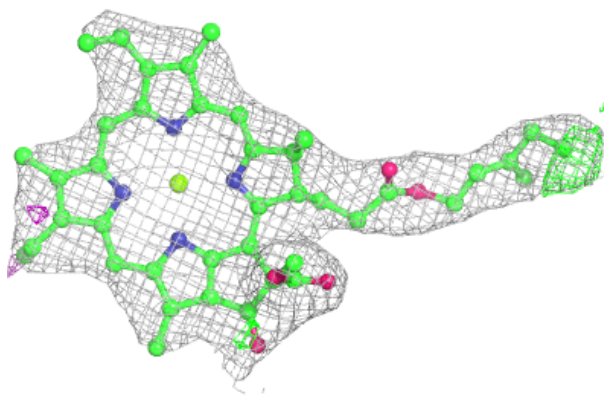
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



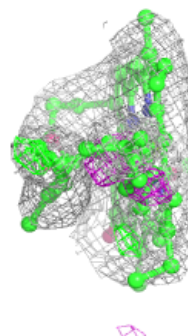
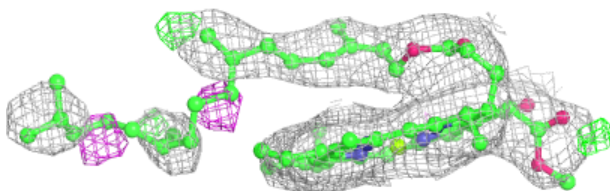
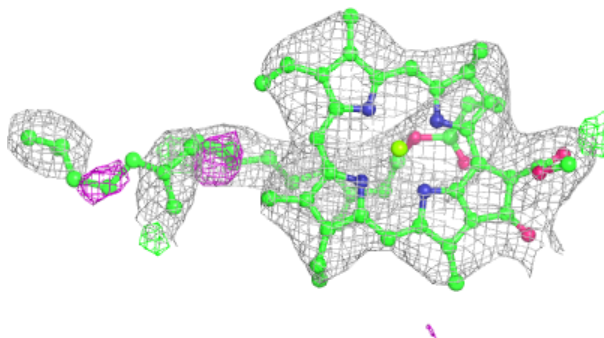


**Electron density around CLA a 838:**

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

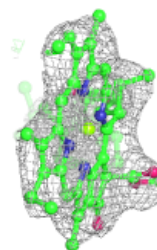
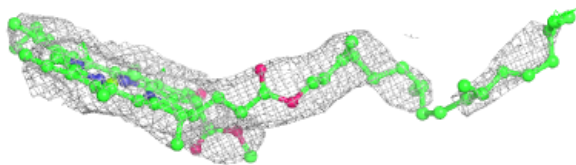
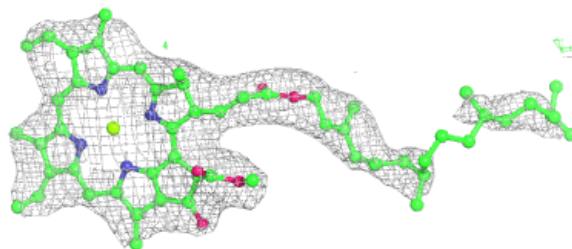
**Electron density around CLA a 839:**

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



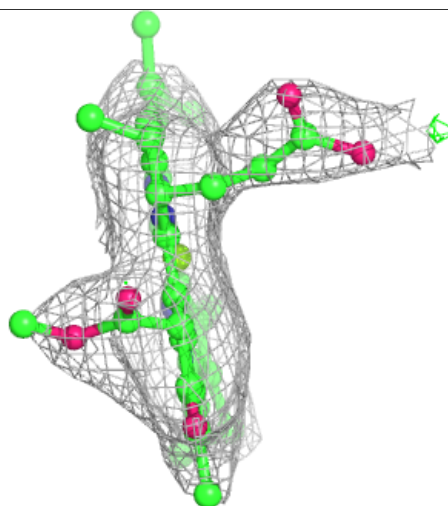
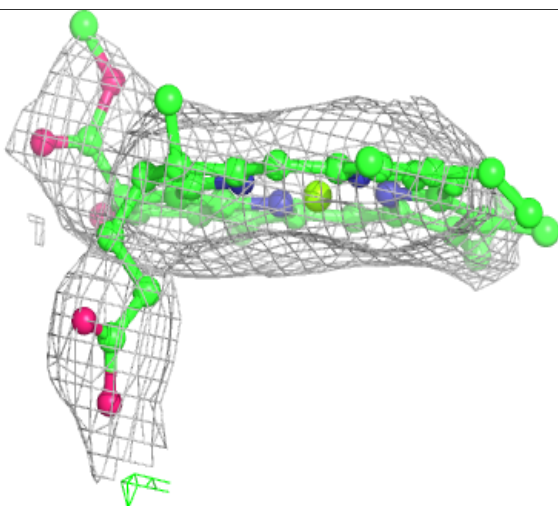
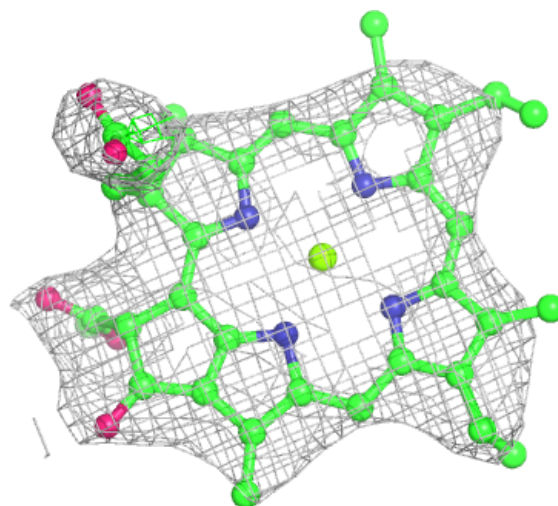
**Electron density around CLA a 842:**

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



**Electron density around CLA A 821:**

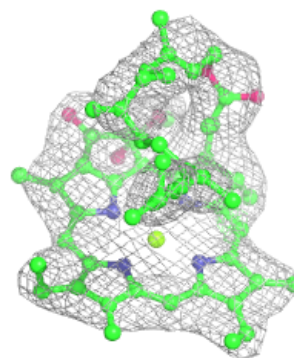
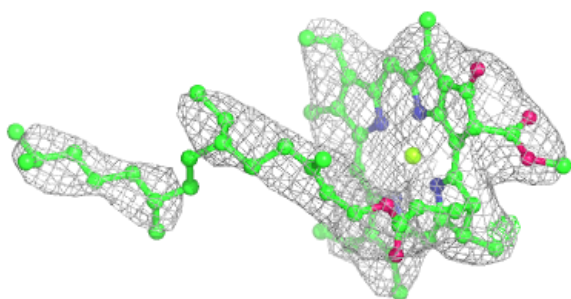
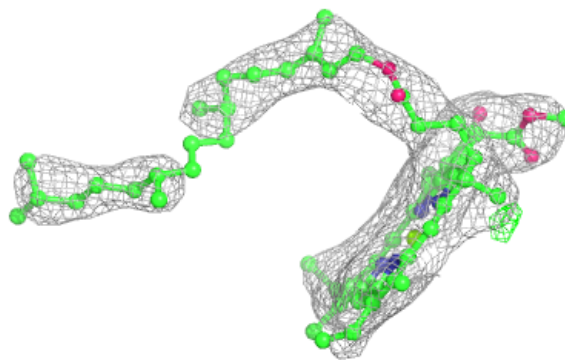
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



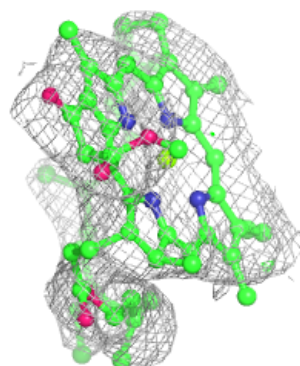
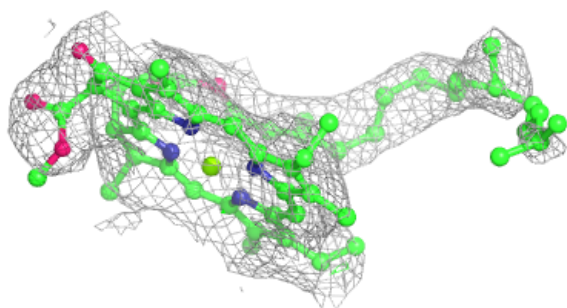
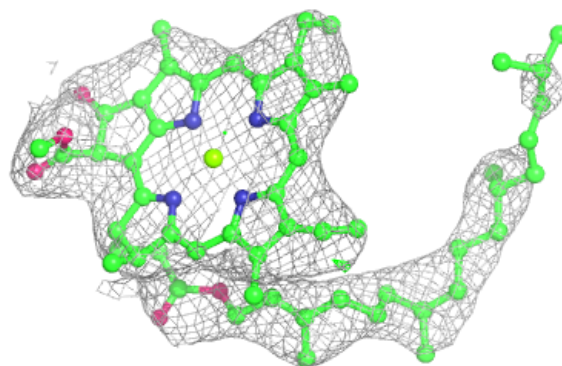


**Electron density around CLA A 811:**

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

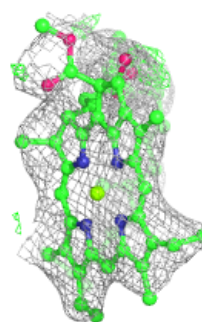
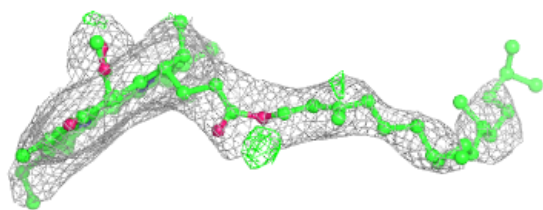
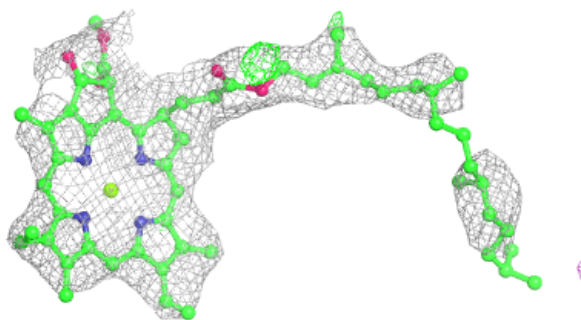
**Electron density around CLA 2 602:**

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

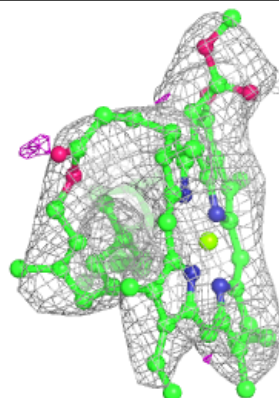
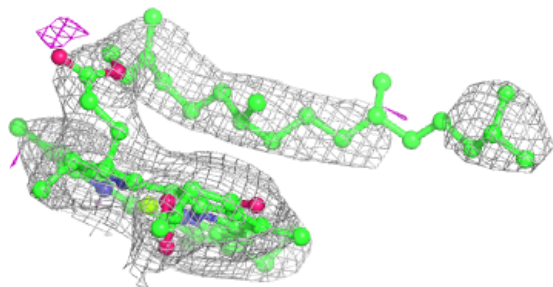
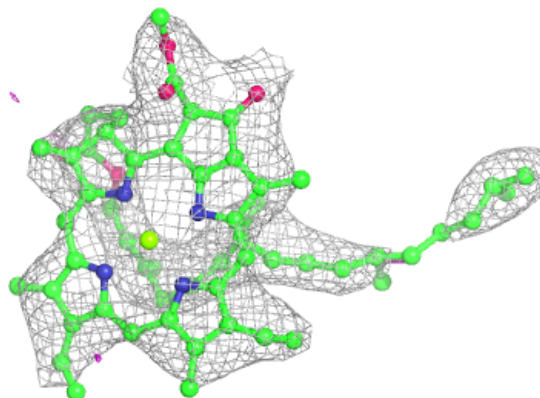


**Electron density around CLA B 825:**

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

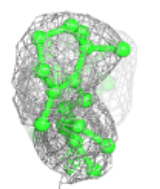
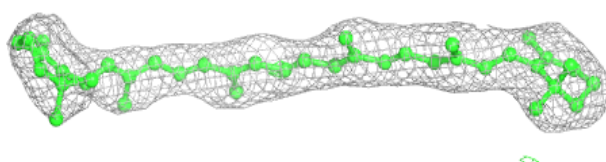
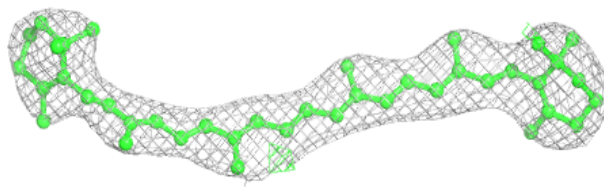
**Electron density around CLA B 827:**

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

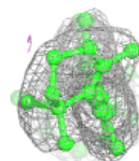
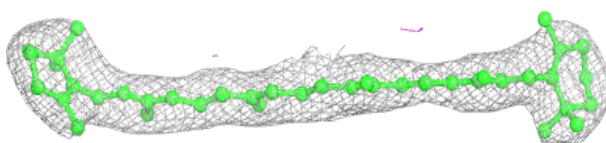
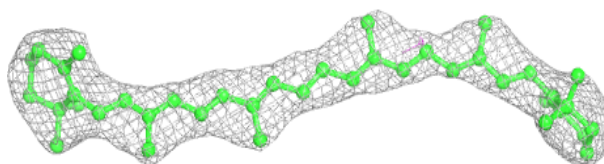


**Electron density around BCR B 847:**

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

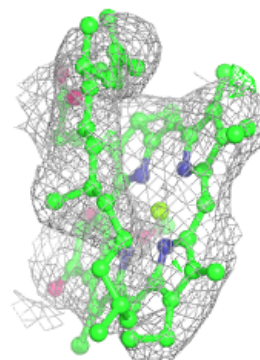
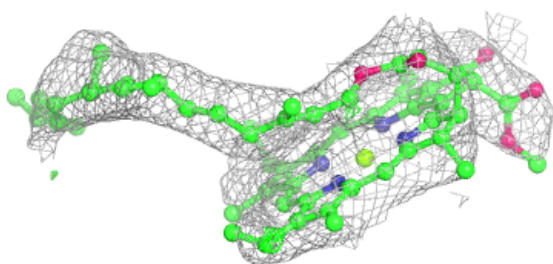
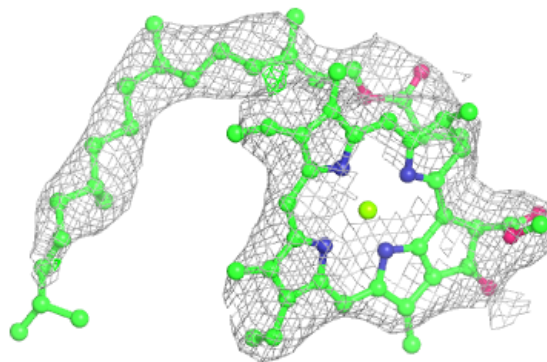
**Electron density around BCR B 848:**

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



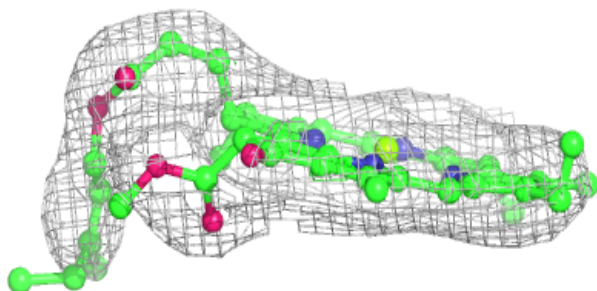
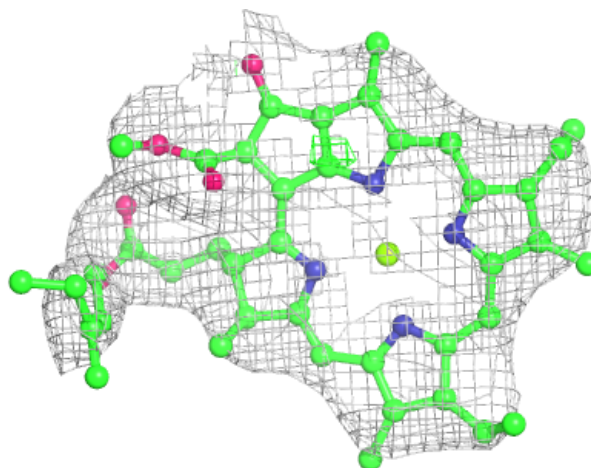
**Electron density around CLA 7 602:**

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



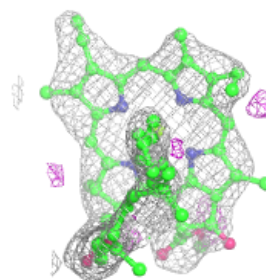
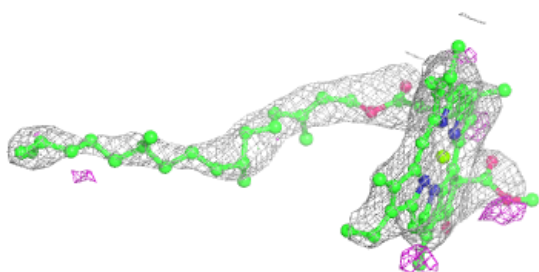
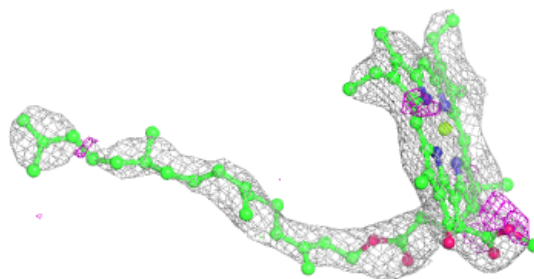
**Electron density around CLA 7 603:**

$2mF_o-DF_c$  (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:**

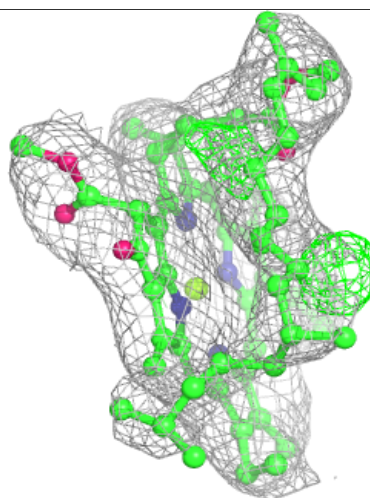
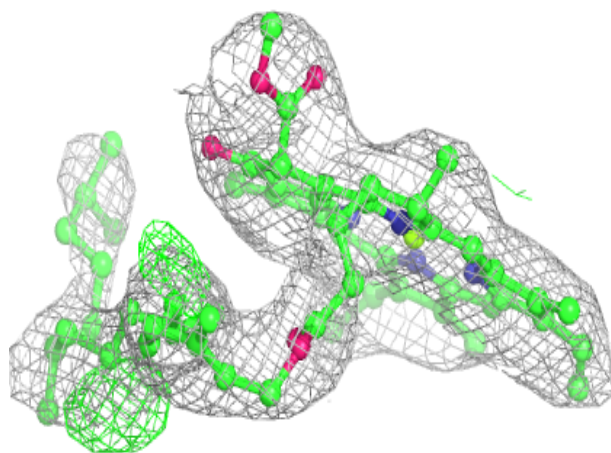
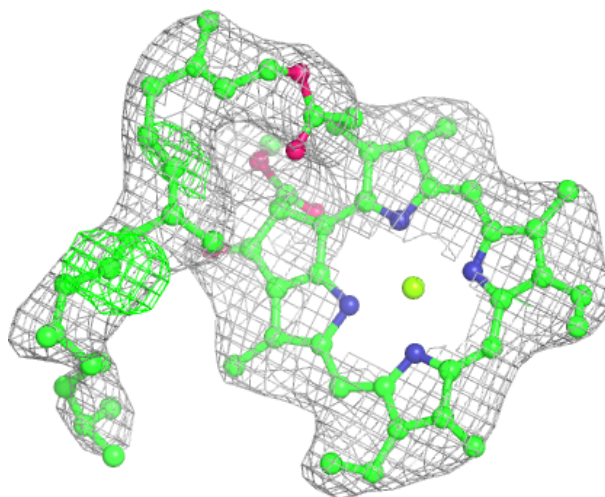
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





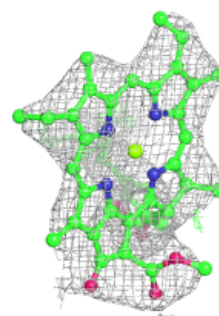
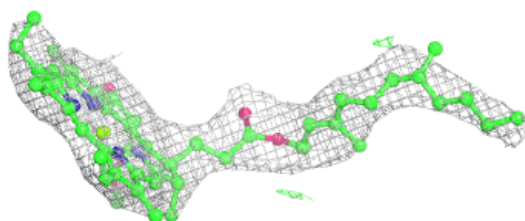
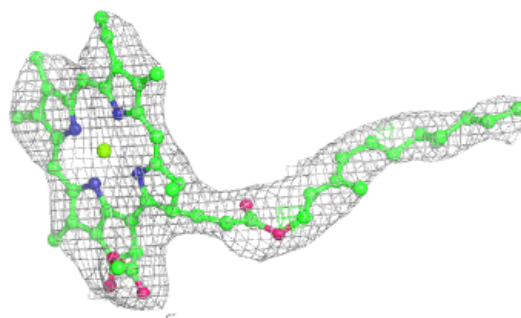
**Electron density around CLA B 832:**

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

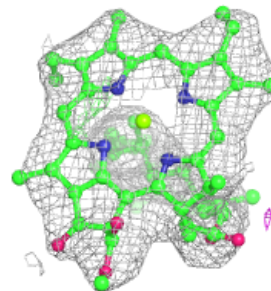
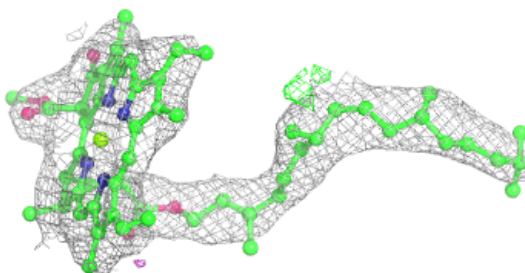
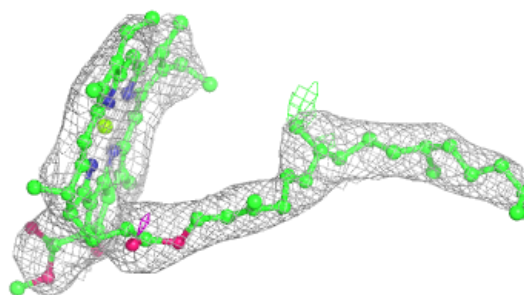


**Electron density around CLA B 833:**

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

**Electron density around CLA A 812:**

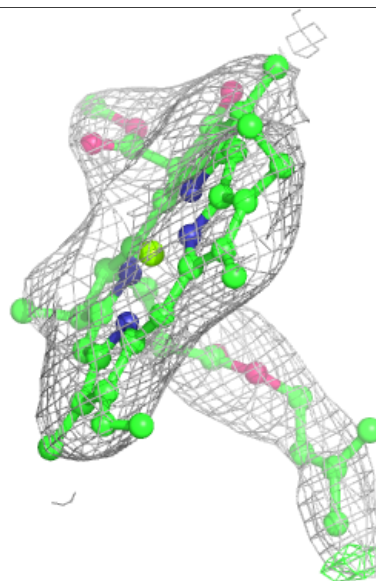
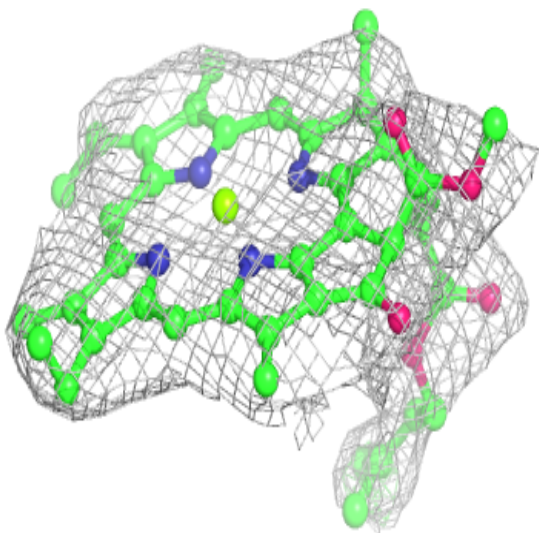
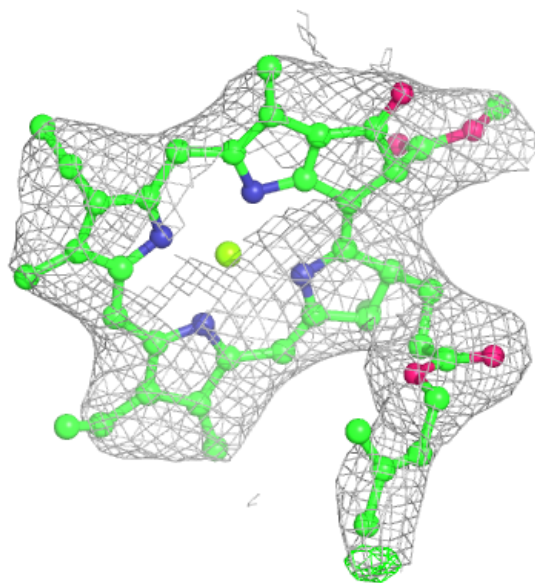
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





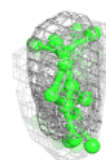
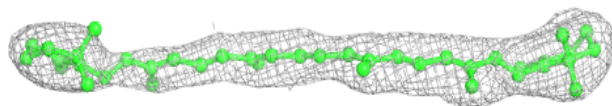
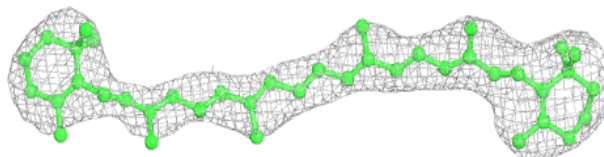
**Electron density around CLA 4 608:**

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

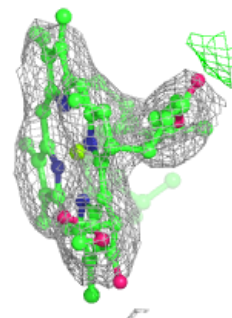
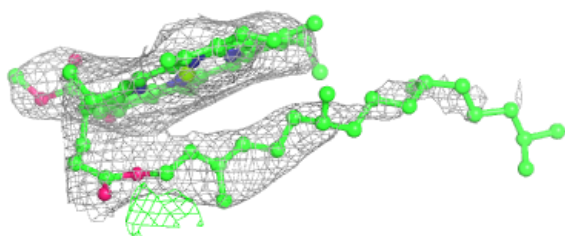
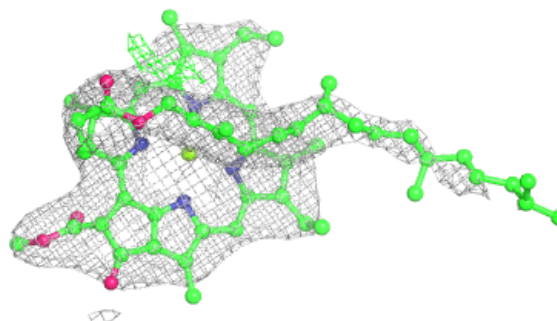


**Electron density around BCR L 205:**

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

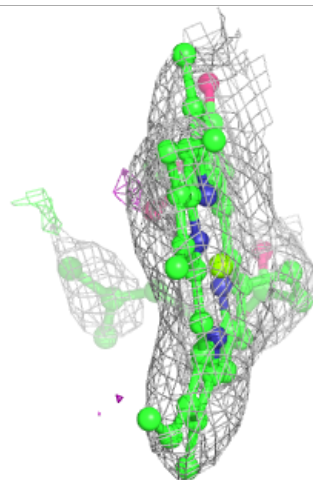
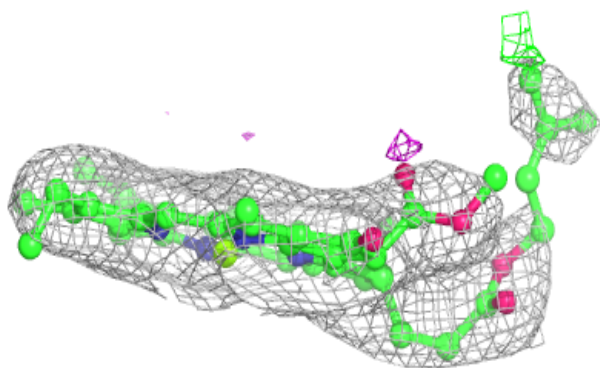
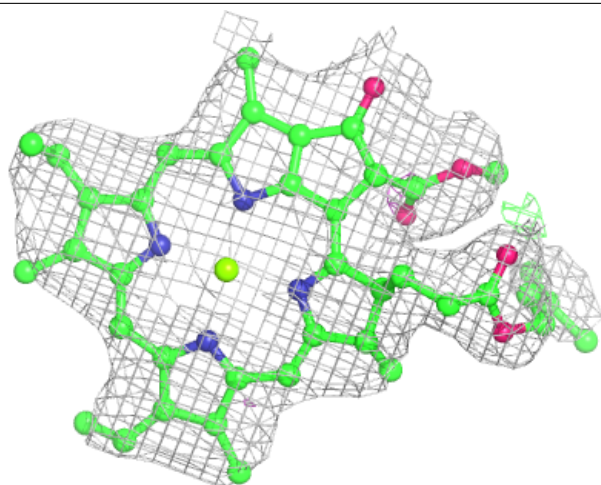
**Electron density around CLA A 819:**

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



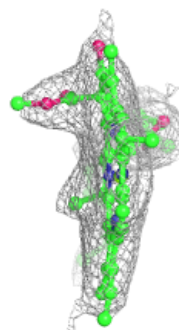
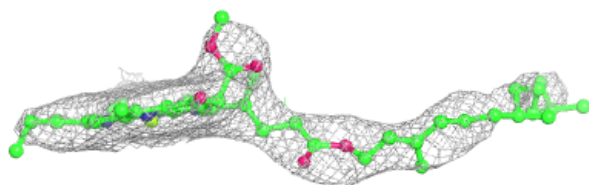
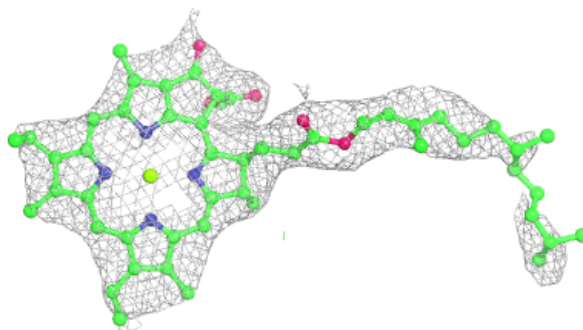
**Electron density around CLA 8 302:**

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

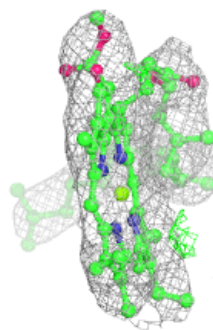
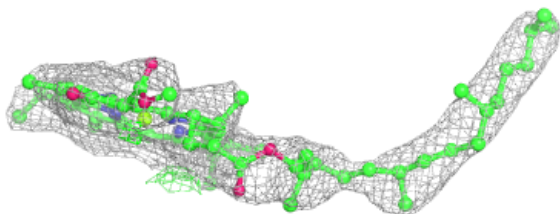
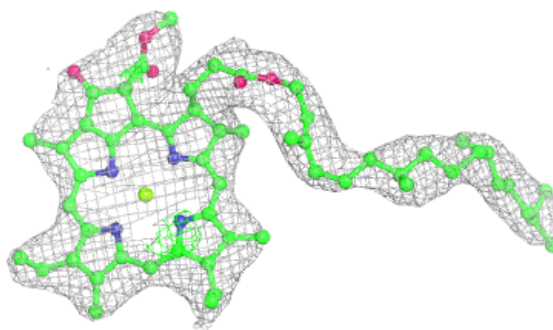


**Electron density around CLA B 836:**

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

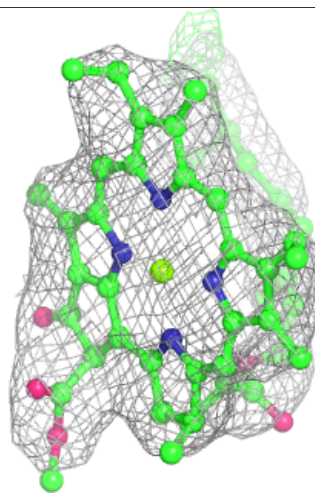
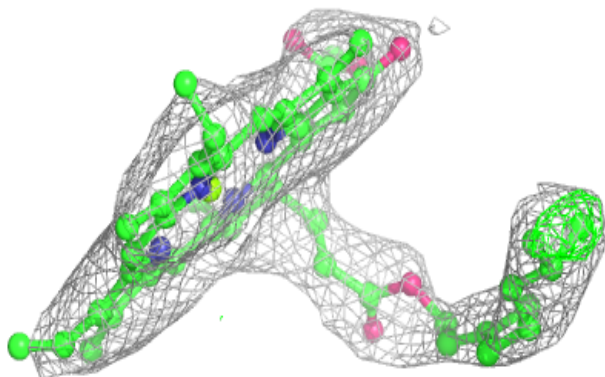
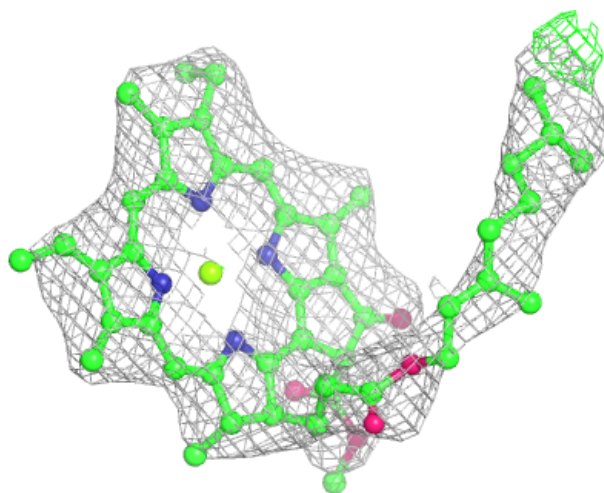
**Electron density around CLA B 803:**

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



**Electron density around CLA b 822:**

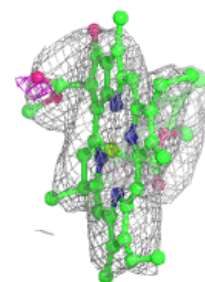
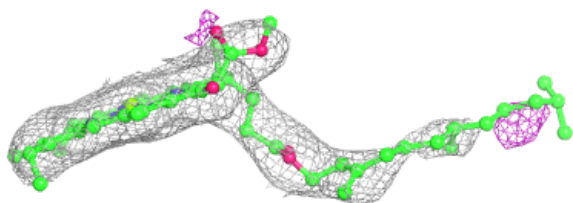
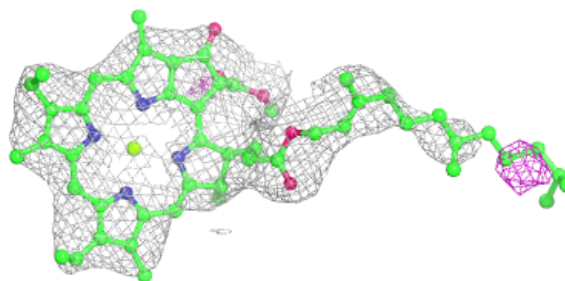
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



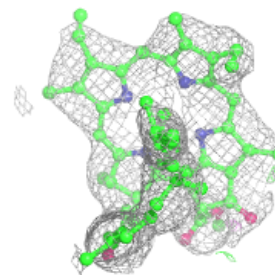
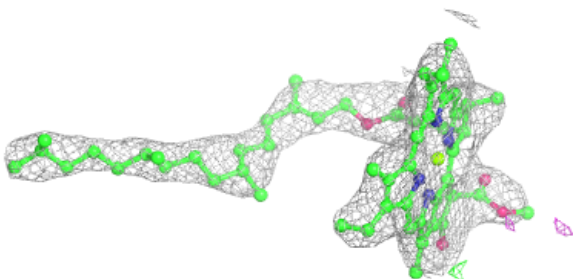
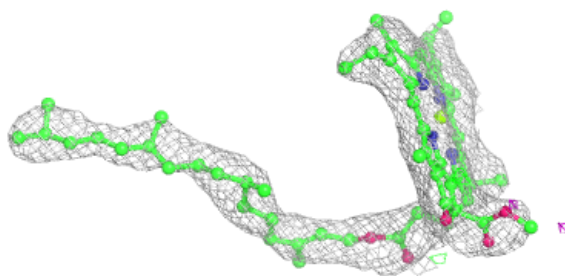


**Electron density around CLA b 823:**

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

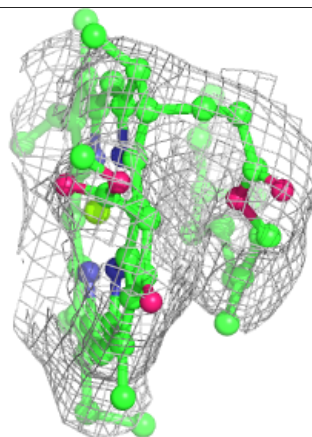
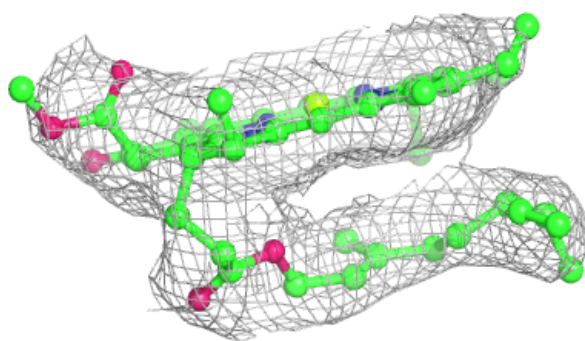
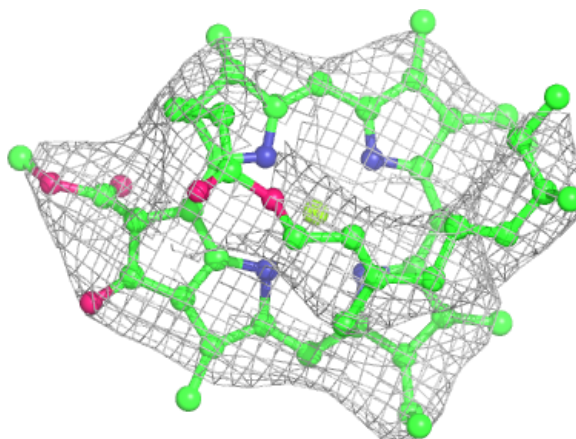
**Electron density around CLA b 829:**

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



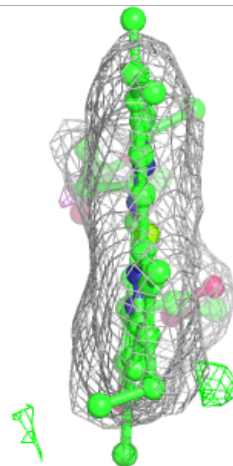
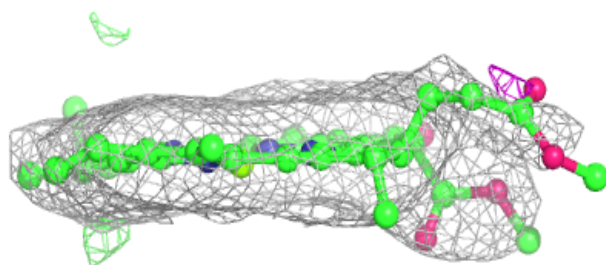
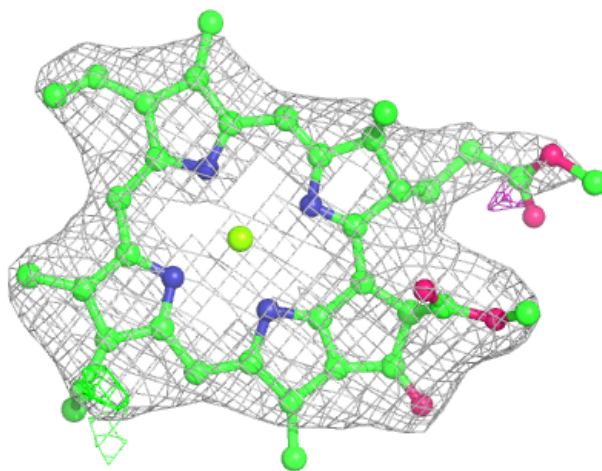
**Electron density around CLA 4 612:**

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



**Electron density around CLA 8 312:**

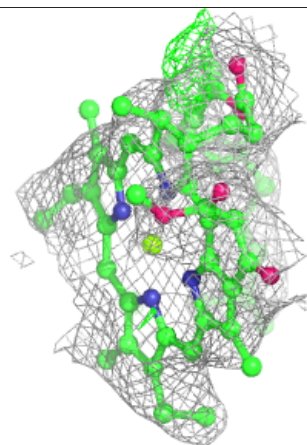
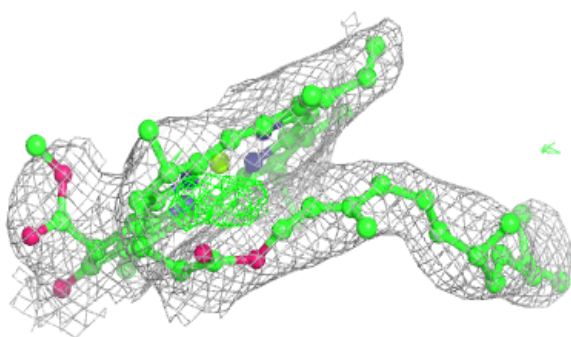
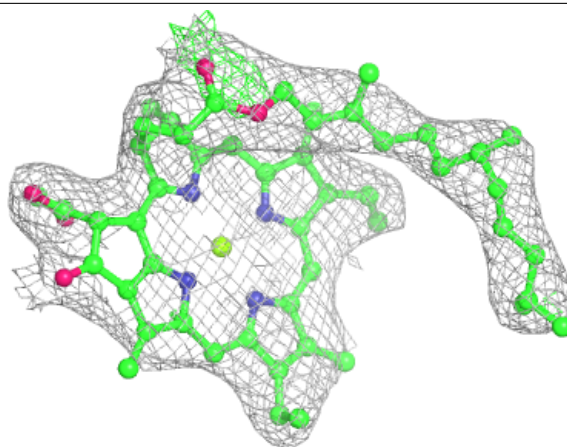
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





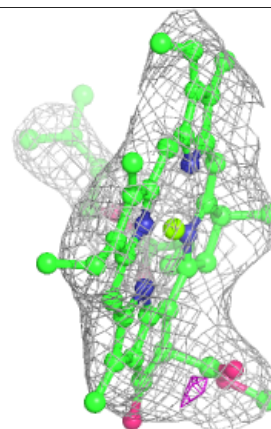
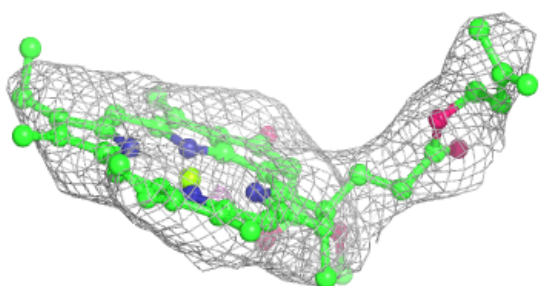
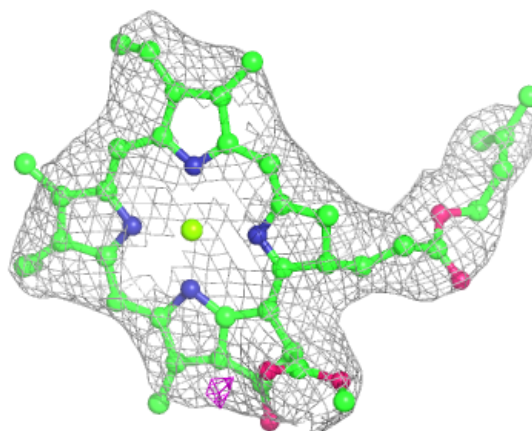
**Electron density around CLA 3 302:**

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

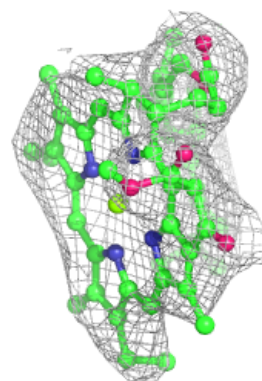
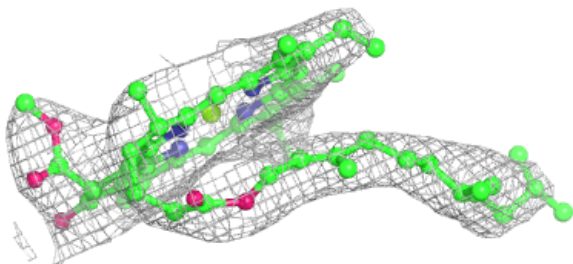
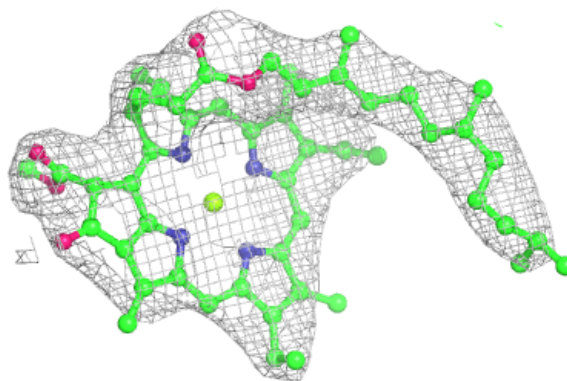


**Electron density around CLA 4 614:**

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

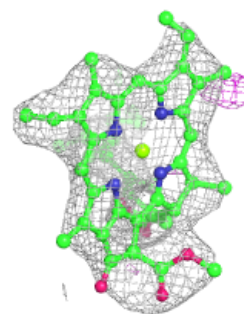
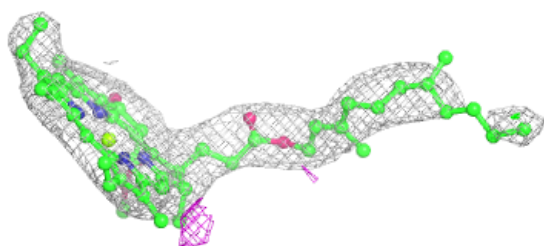
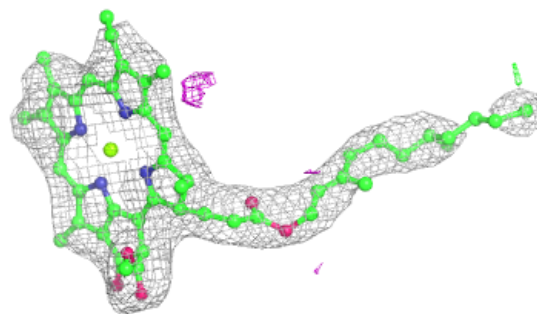
**Electron density around CLA 9 602:**

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

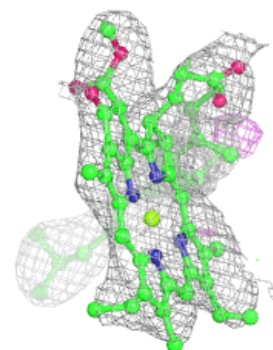
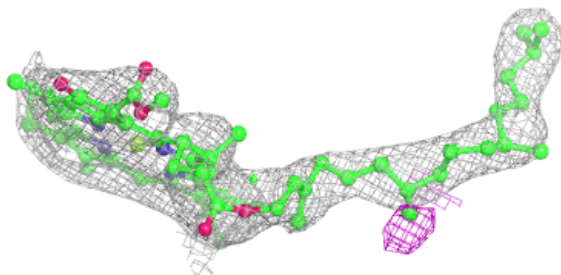
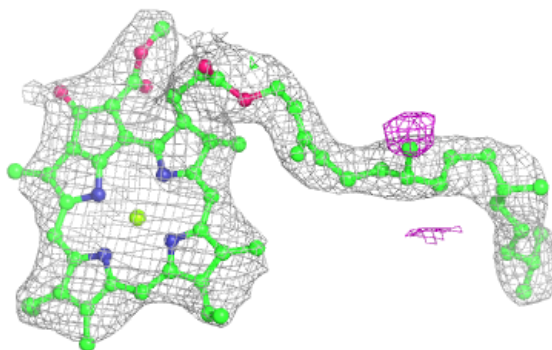


**Electron density around CLA b 833:**

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

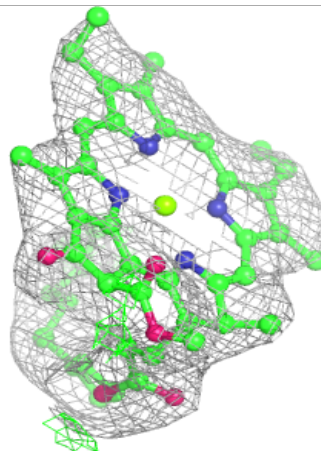
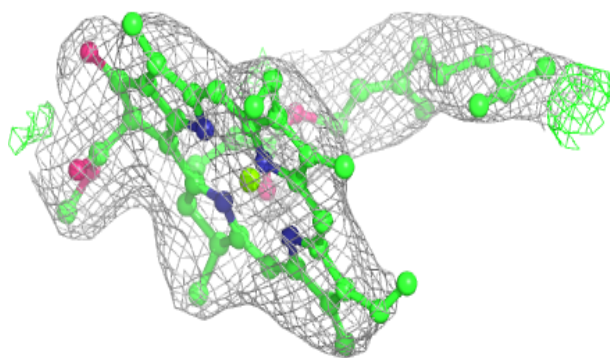
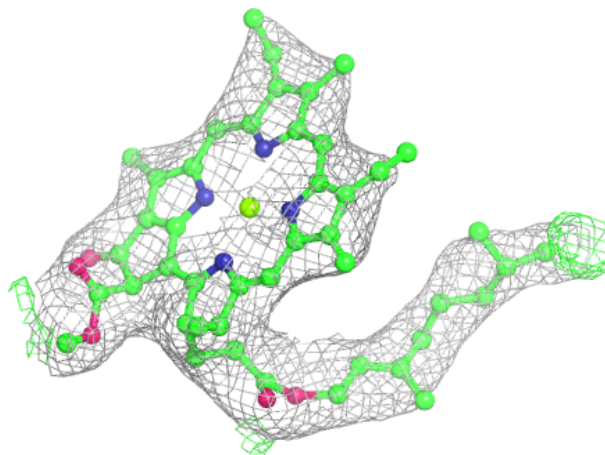
**Electron density around CLA a 802:**

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



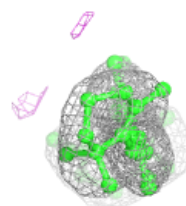
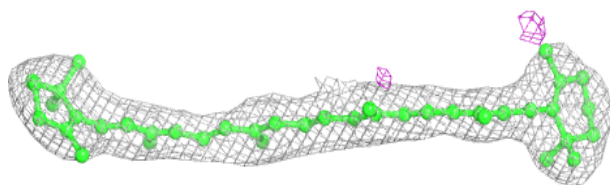
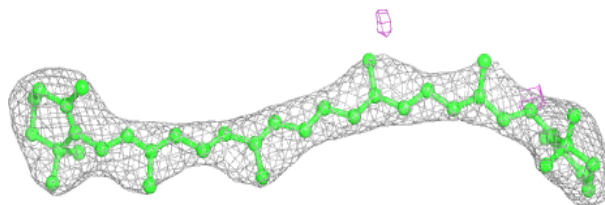
**Electron density around CLA A 825:**

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

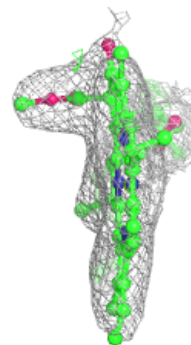
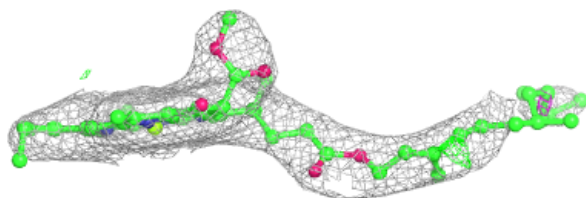
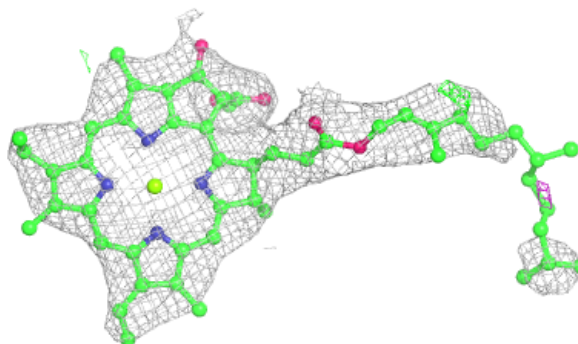


**Electron density around BCR b 848:**

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

**Electron density around CLA b 836:**

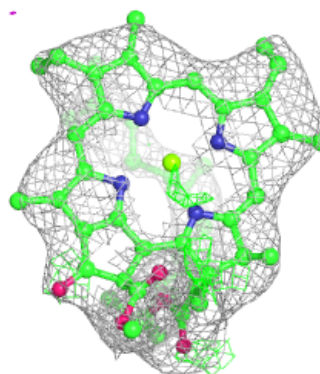
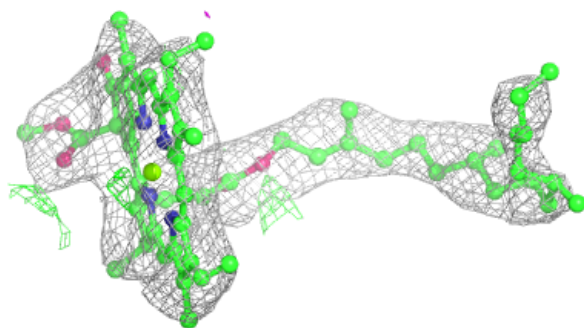
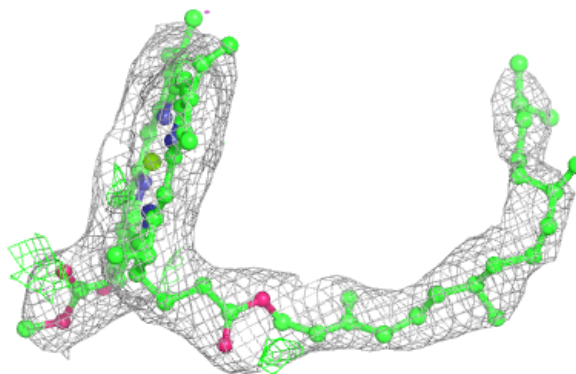
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



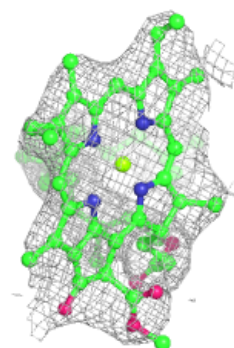
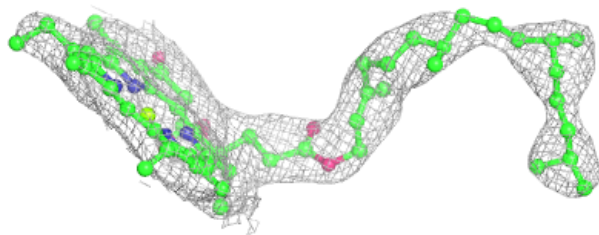
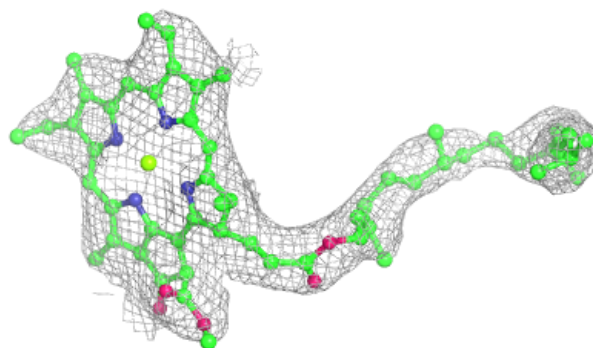


**Electron density around CLA a 808:**

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

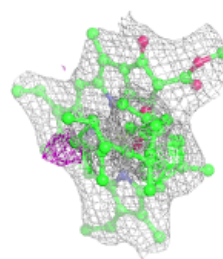
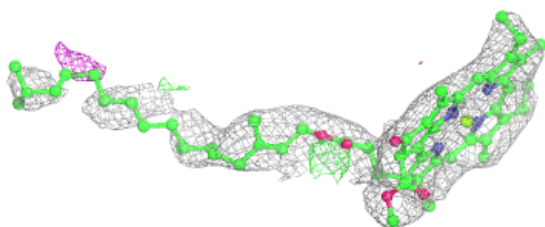
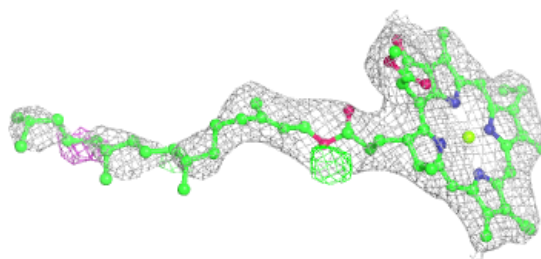
**Electron density around CLA B 809:**

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

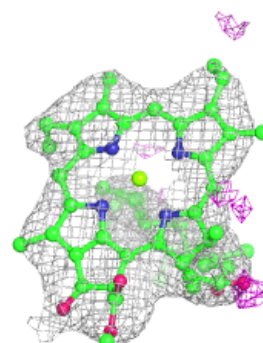
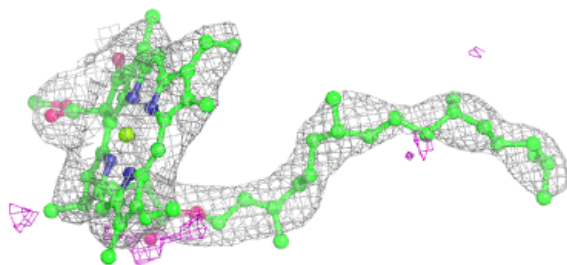
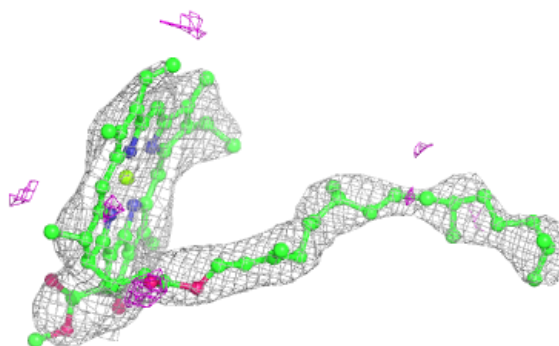


**Electron density around CLA a 810:**

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

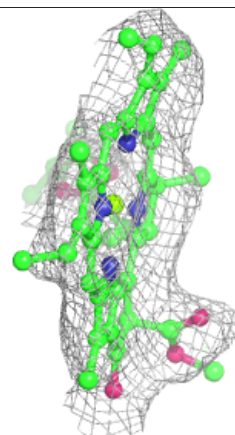
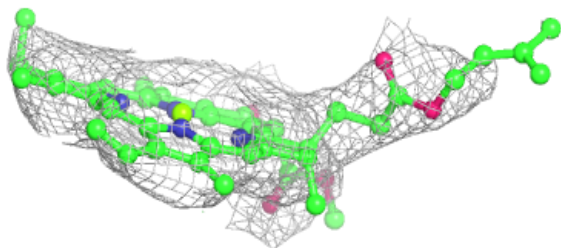
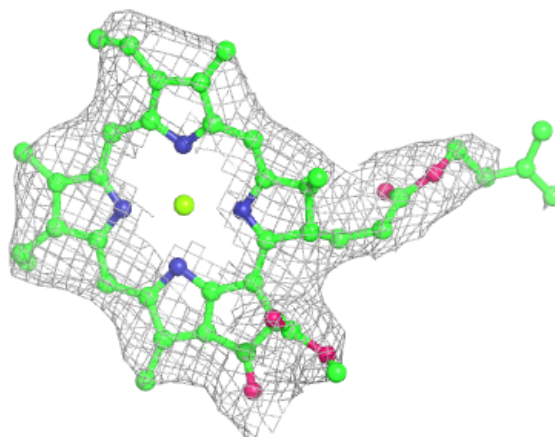
**Electron density around CLA a 812:**

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

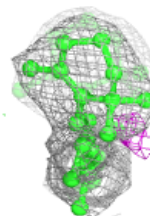
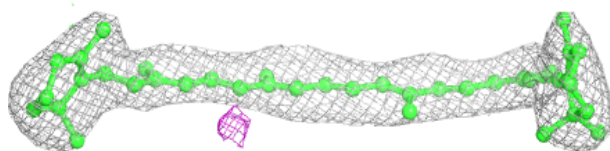
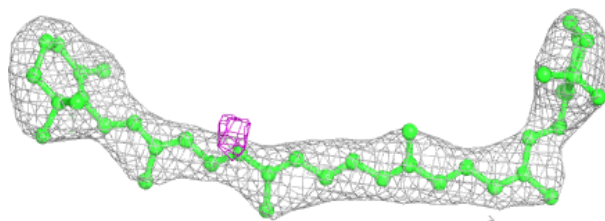


**Electron density around CLA G 103:**

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

**Electron density around BCR 1 201:**

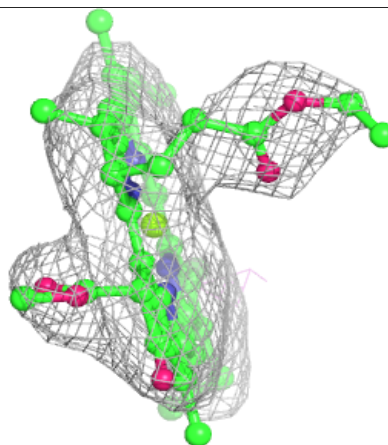
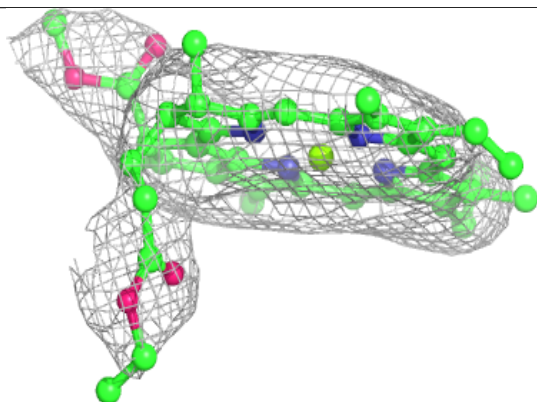
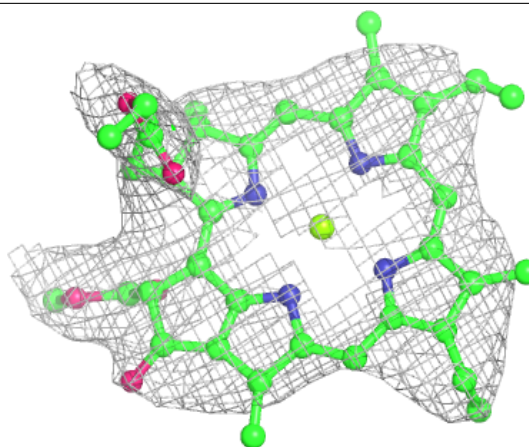
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





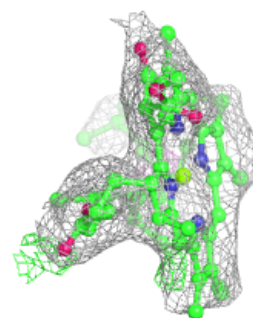
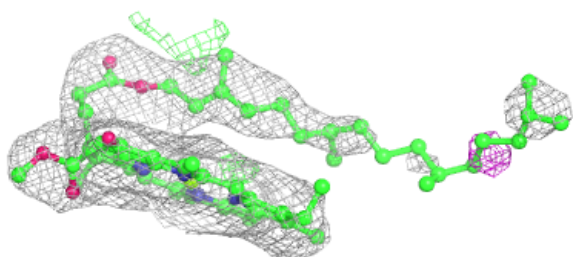
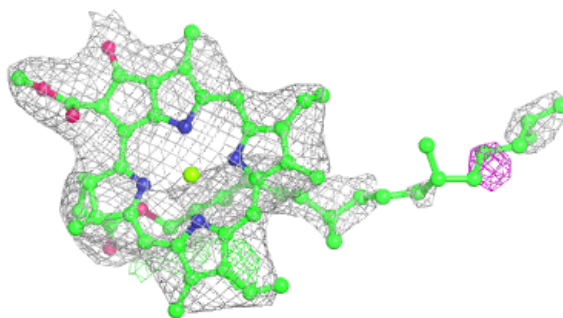
**Electron density around CLA 3 306:**

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



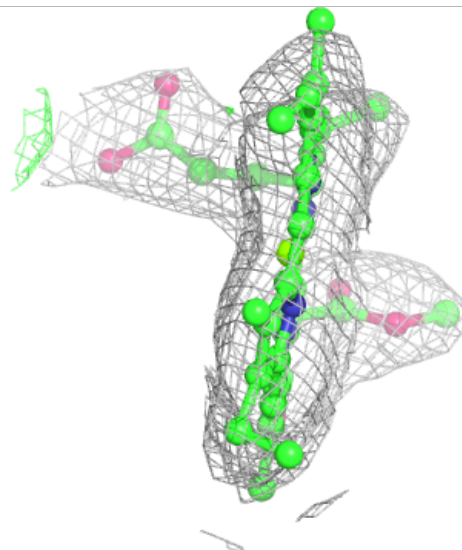
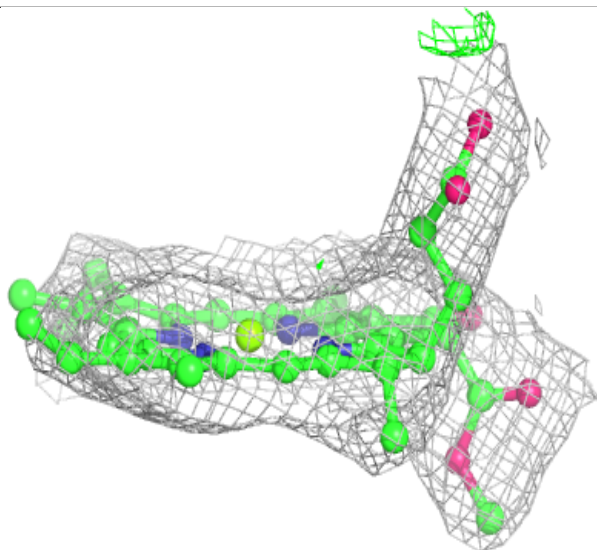
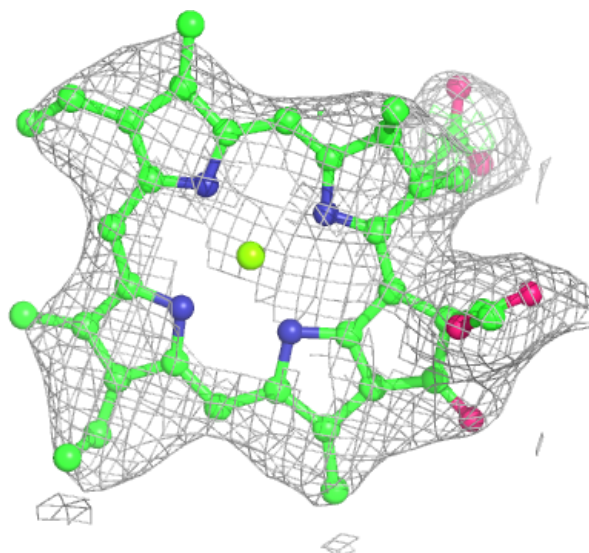
**Electron density around CLA a 819:**

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



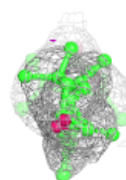
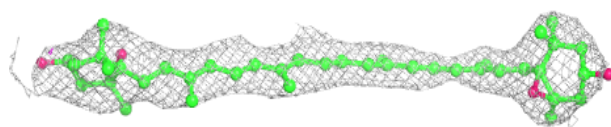
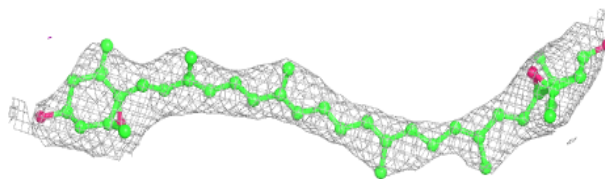
**Electron density around CLA a 821:**

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

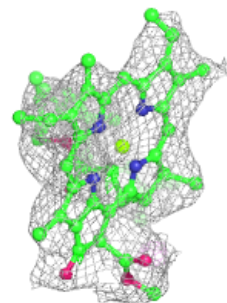
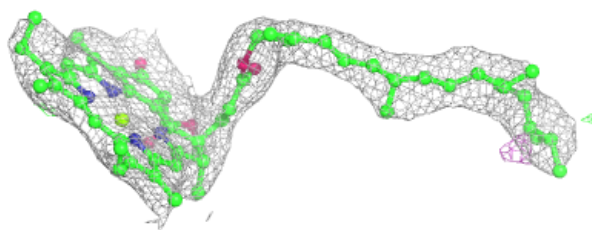
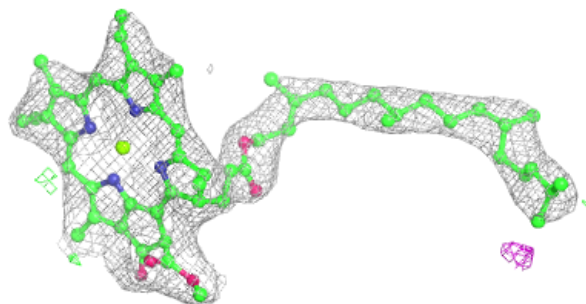


**Electron density around XAT 1 317:**

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

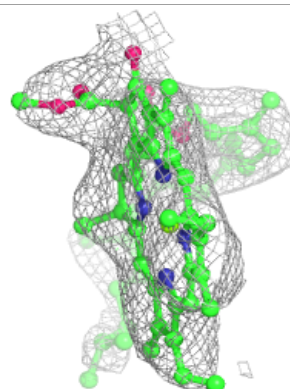
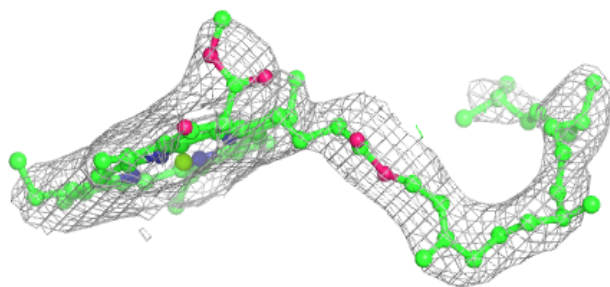
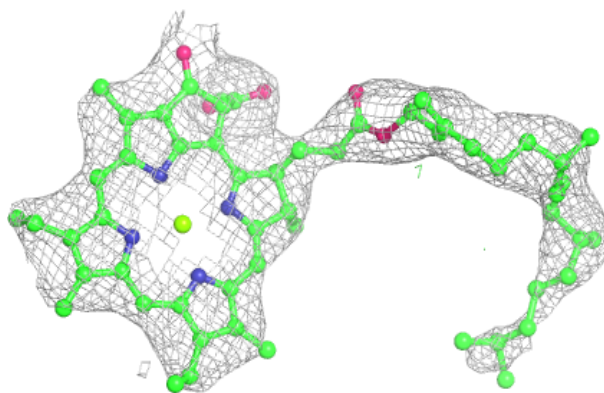
**Electron density around CLA a 822:**

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

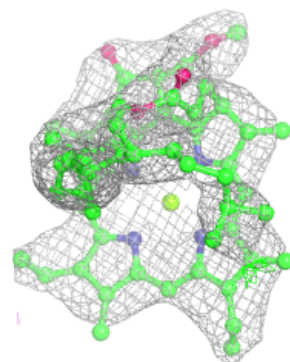
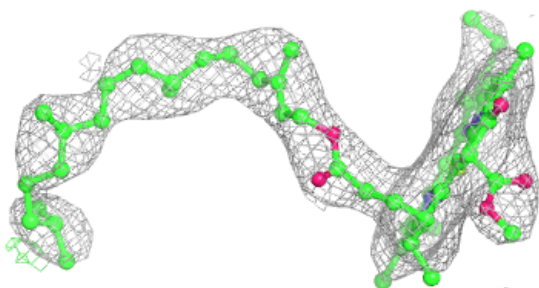
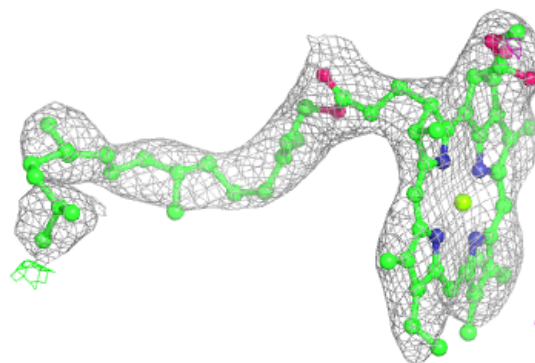


**Electron density around CLA A 828:**

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

**Electron density around CLA 1 203:**

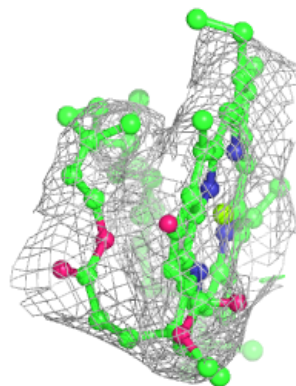
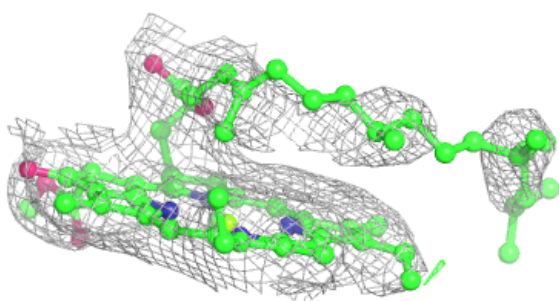
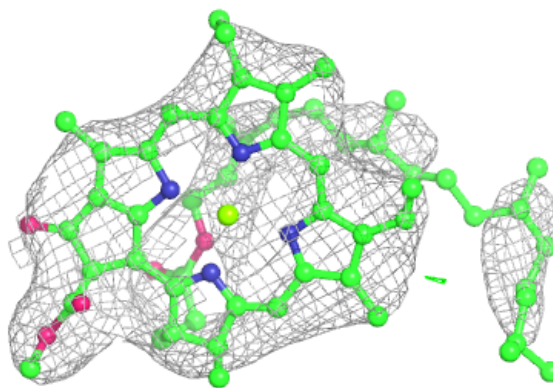
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



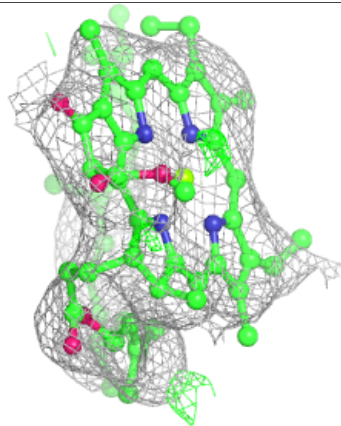
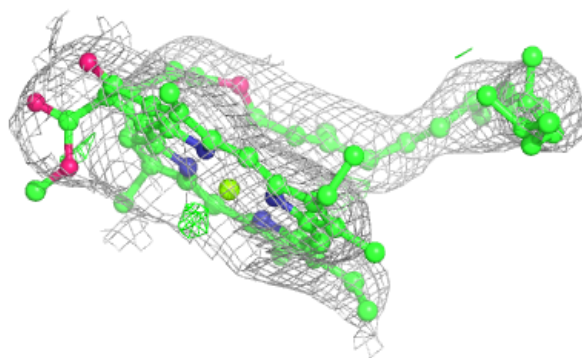
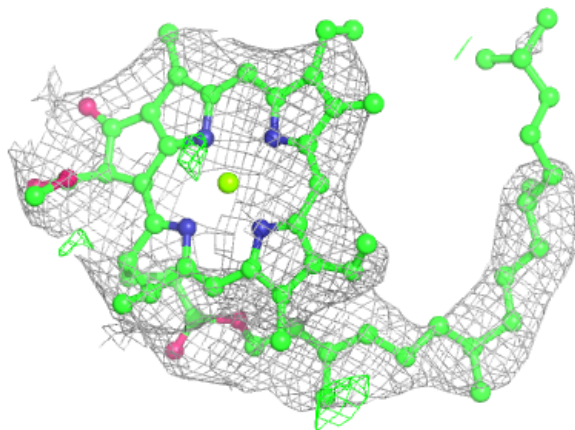


**Electron density around CLA 1 313:**

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

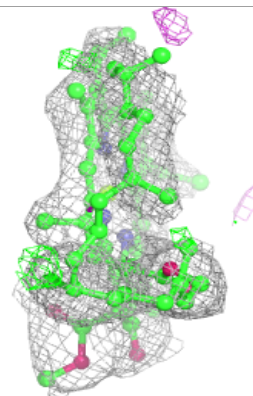
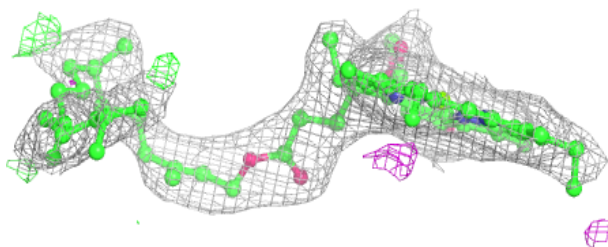
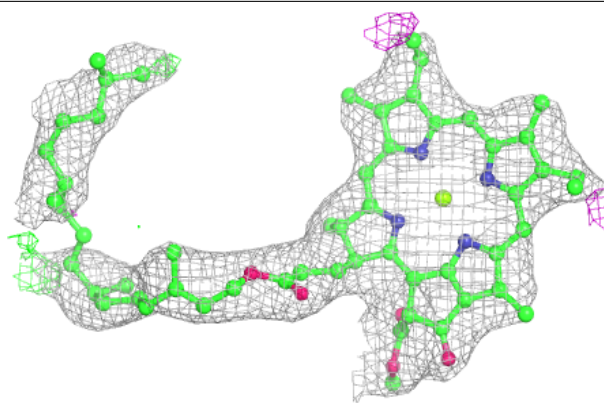
**Electron density around CLA 6 304:**

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



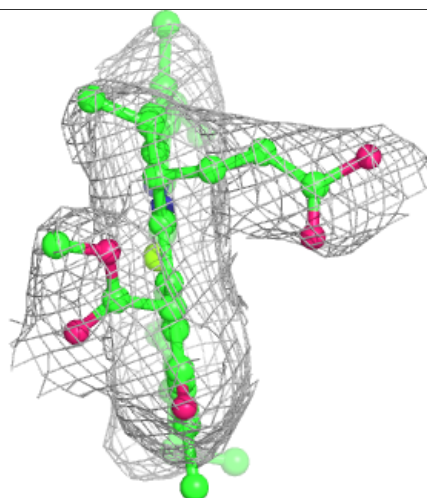
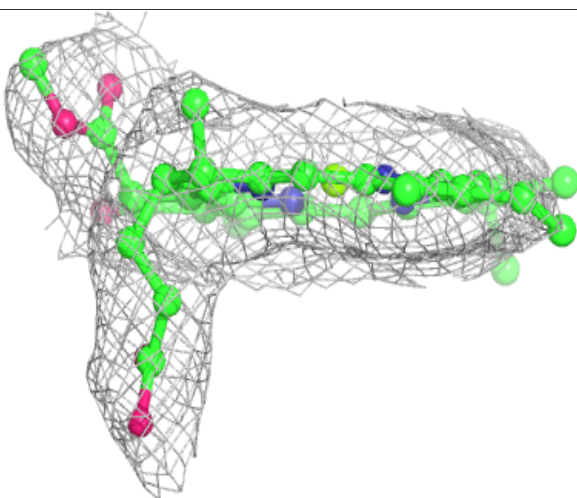
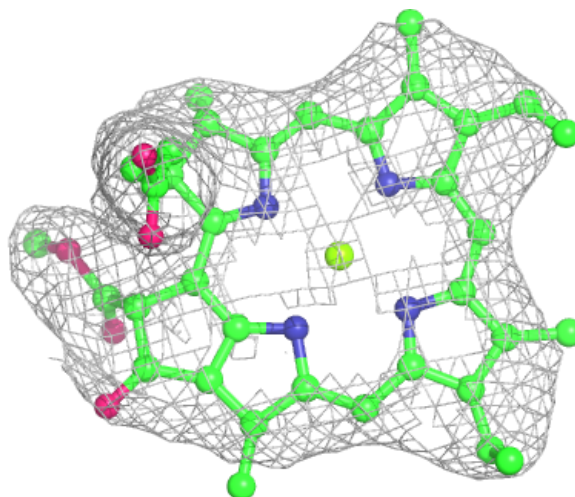
**Electron density around CLA a 827:**

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



**Electron density around CLA a 837:**

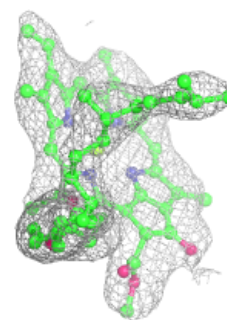
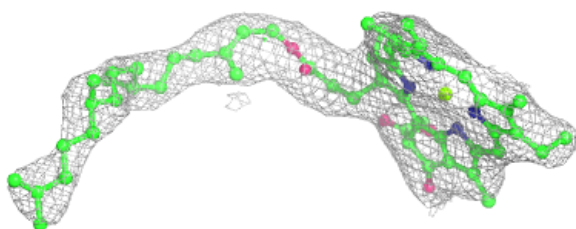
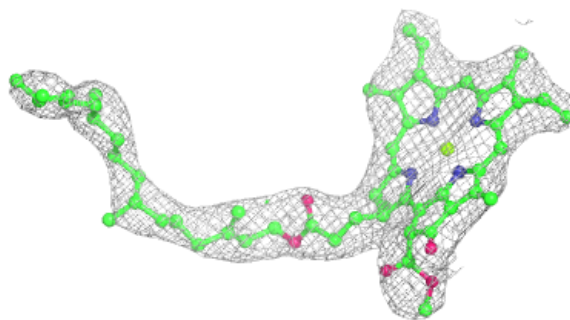
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



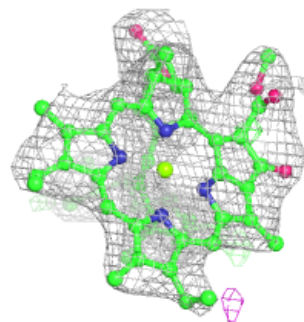
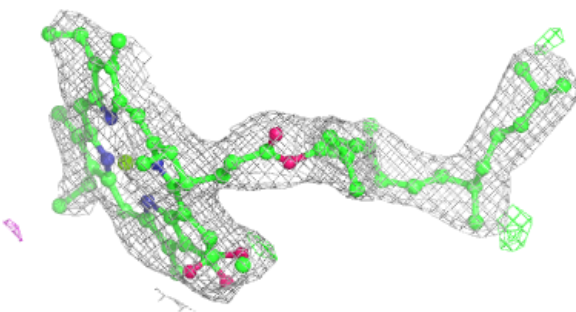
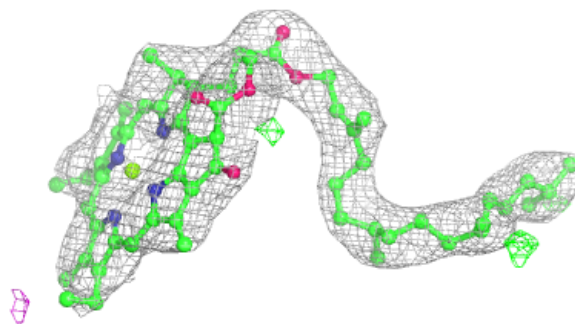


**Electron density around CLA A 854:**

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

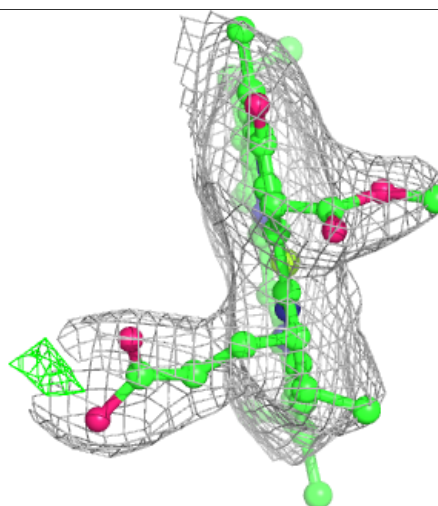
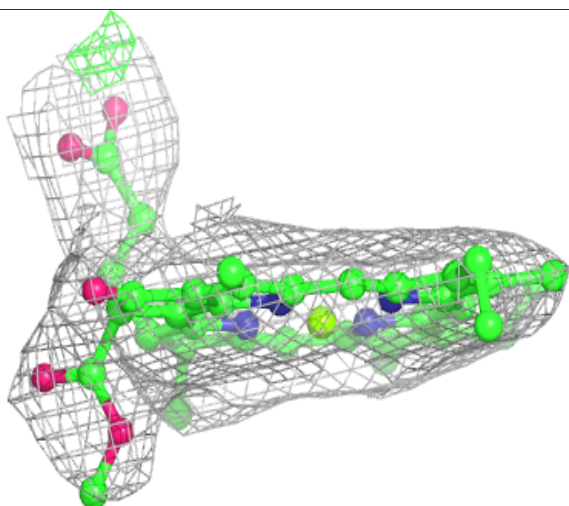
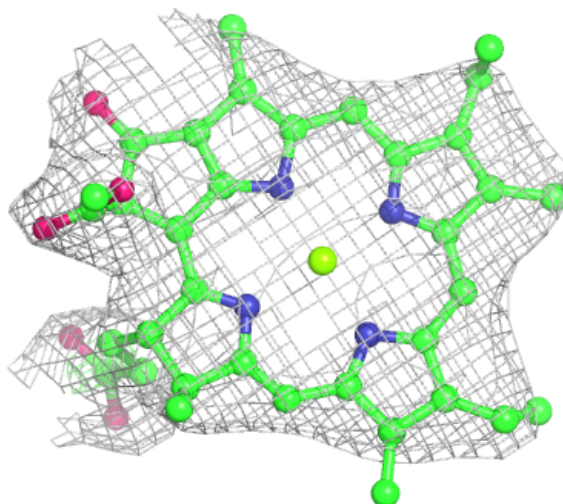
**Electron density around CLA B 802:**

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



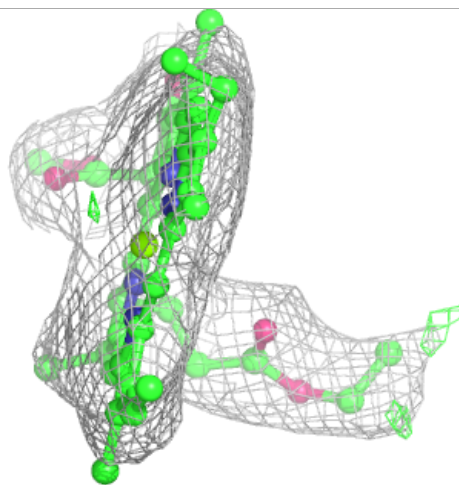
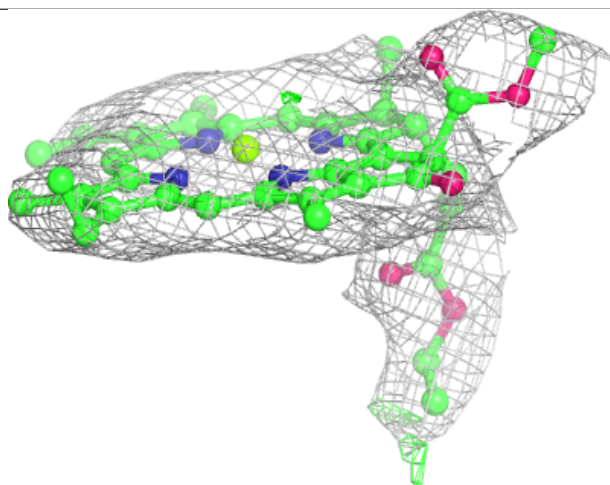
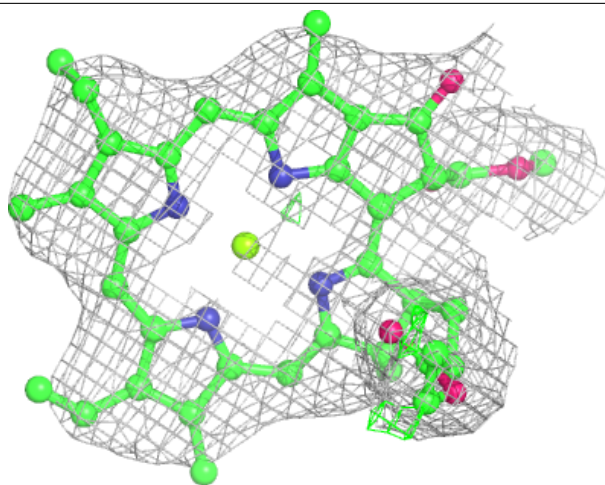
**Electron density around CLA A 815:**

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



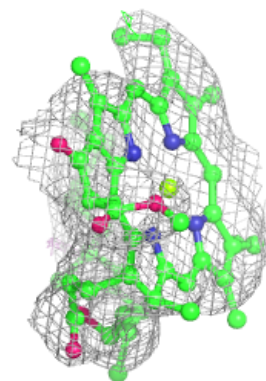
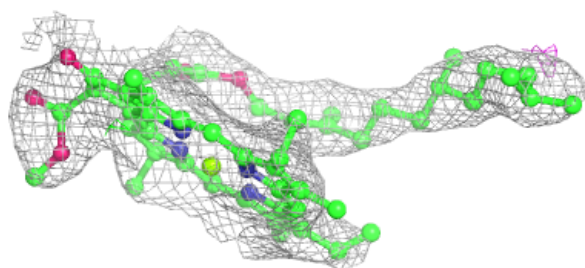
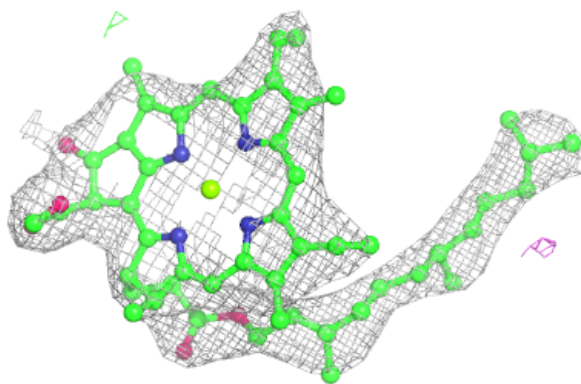
**Electron density around CLA 8 305:**

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



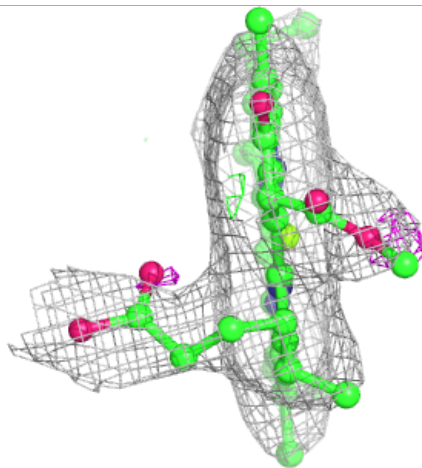
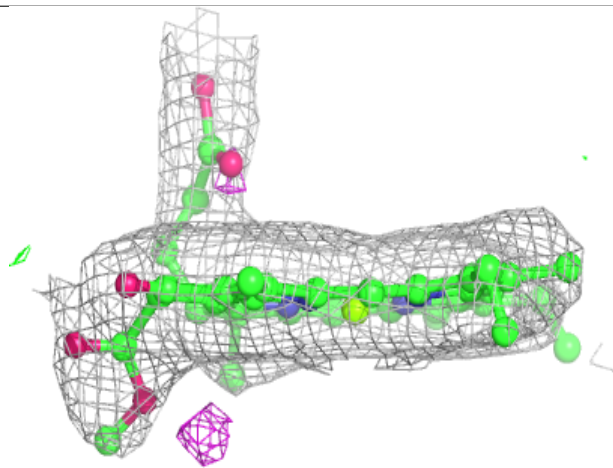
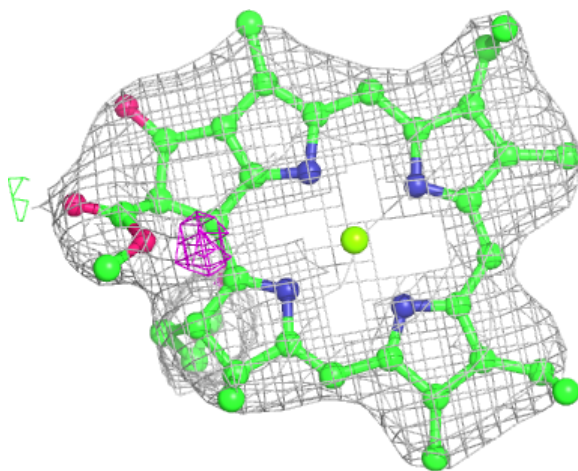
**Electron density around CLA 4 602:**

$2mF_o-DF_c$  (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:**

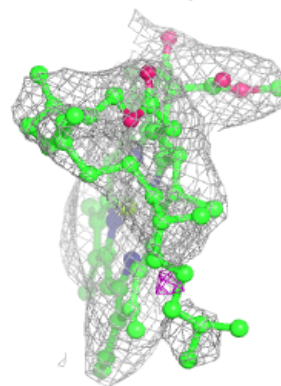
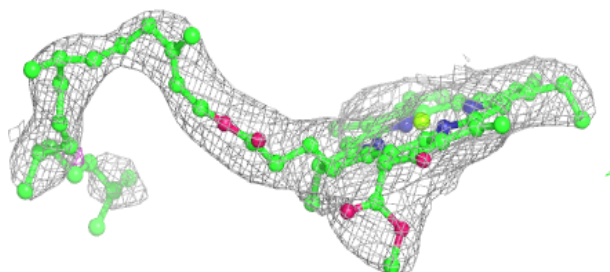
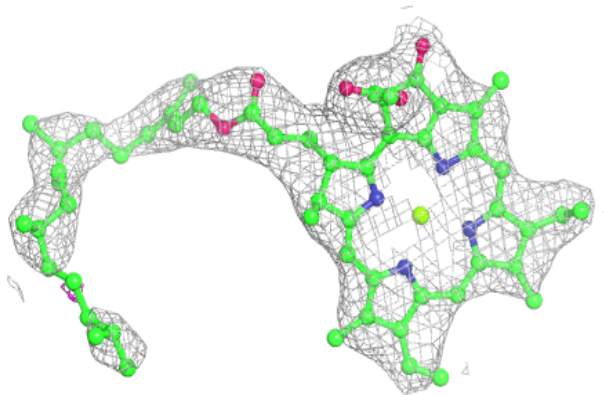
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



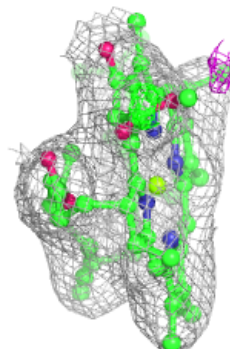
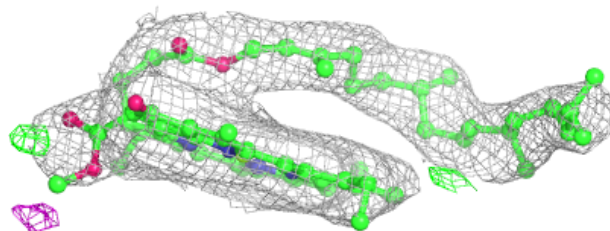
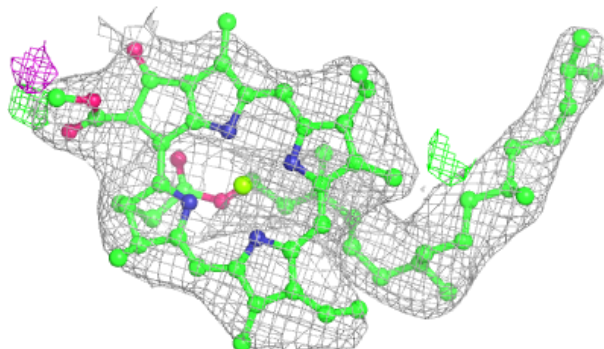


**Electron density around CLA a 828:**

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

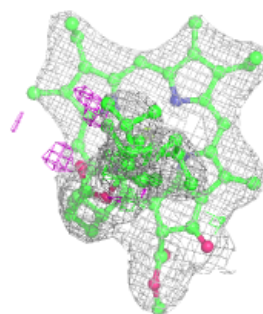
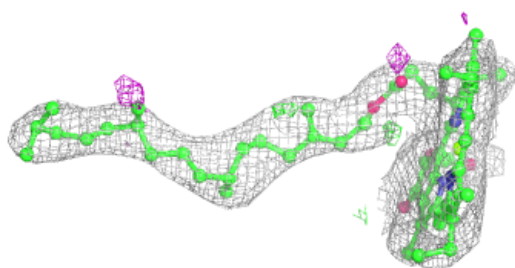
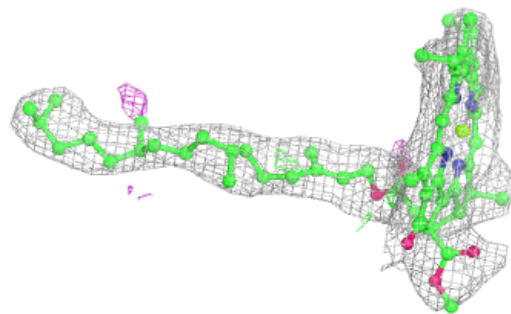
**Electron density around CLA b 837:**

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

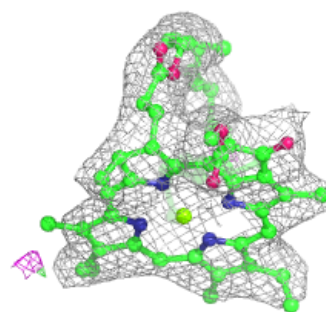
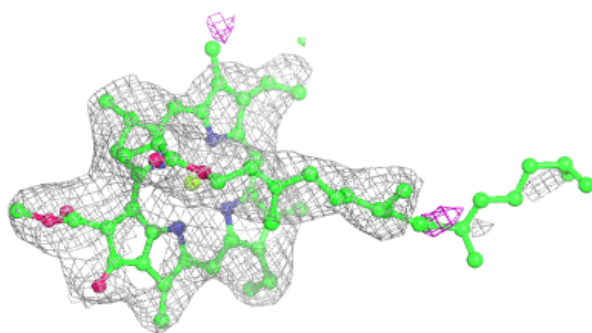
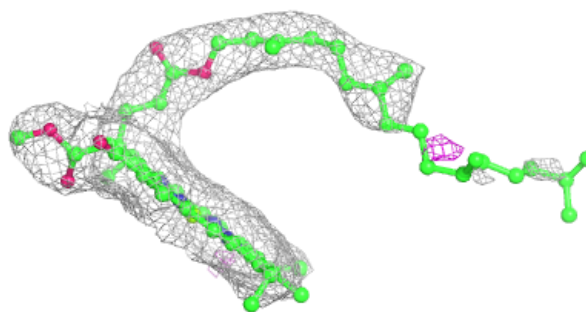


**Electron density around CLA a 829:**

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

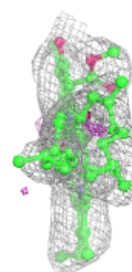
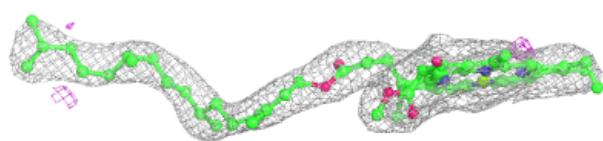
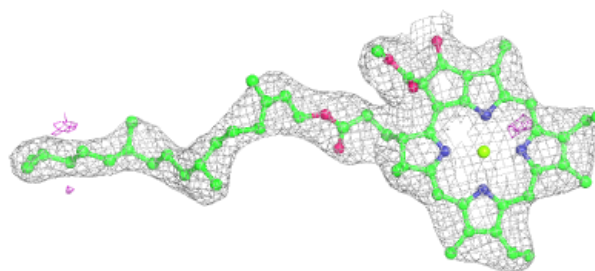
**Electron density around CLA a 833:**

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



**Electron density around CLA a 834:**

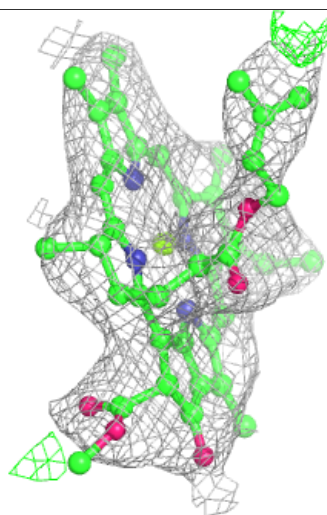
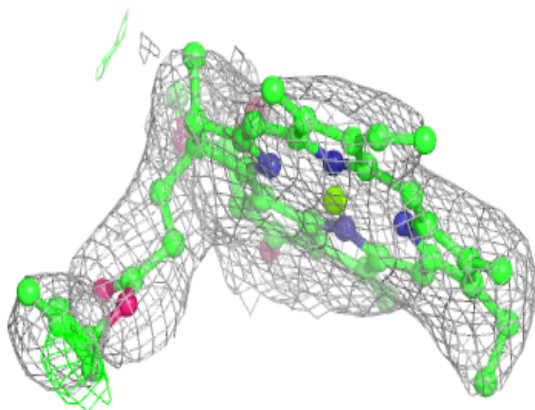
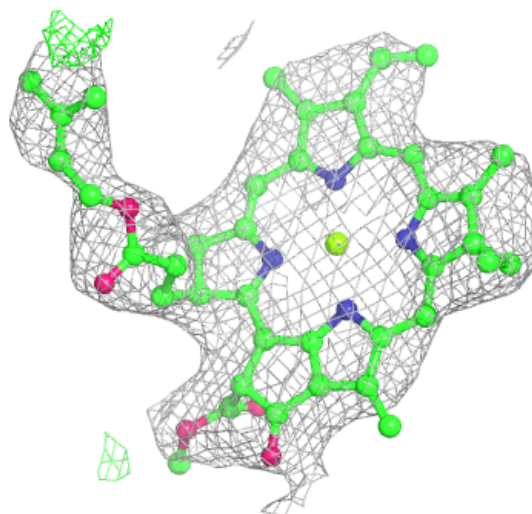
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





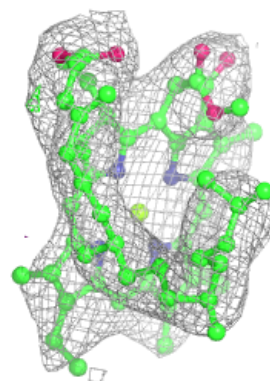
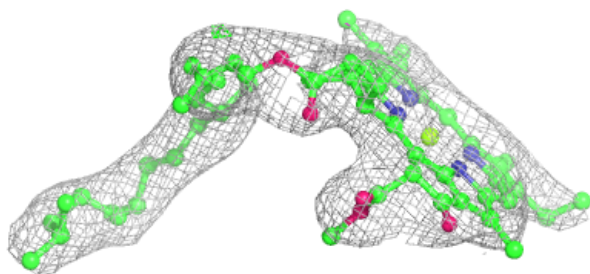
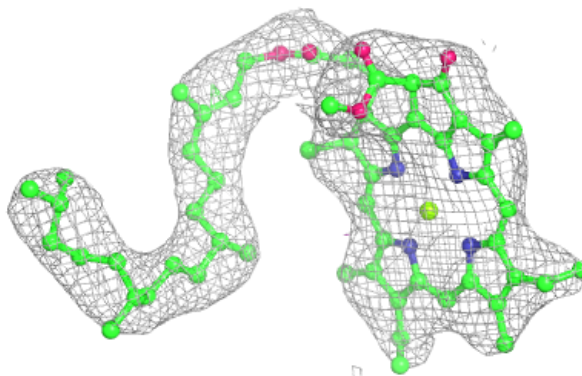
**Electron density around CLA a 836:**

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



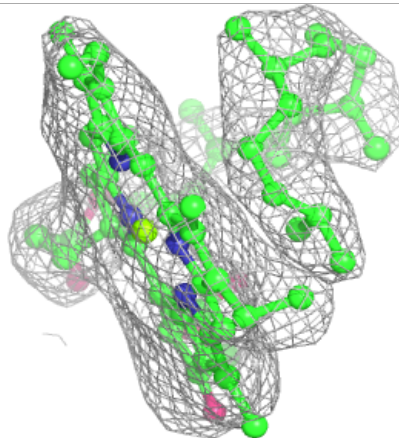
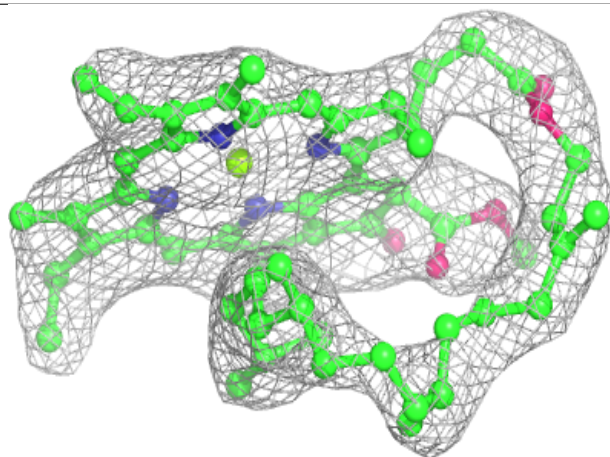
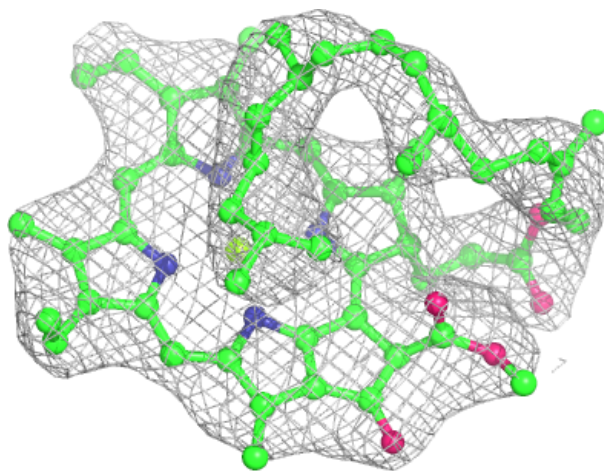
**Electron density around CLA B 824:**

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



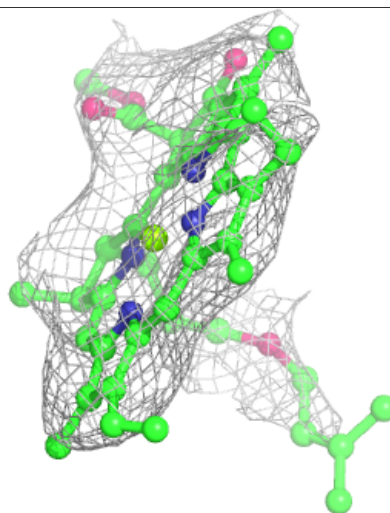
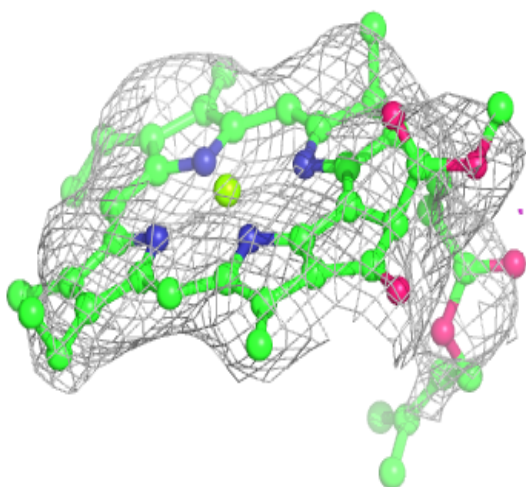
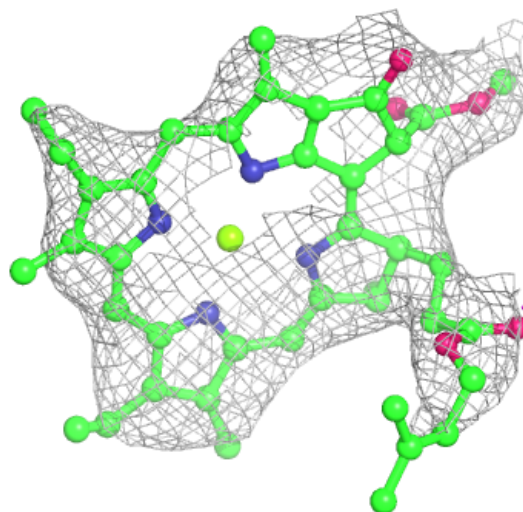
**Electron density around CLA B 806:**

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



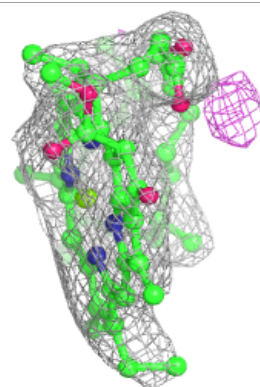
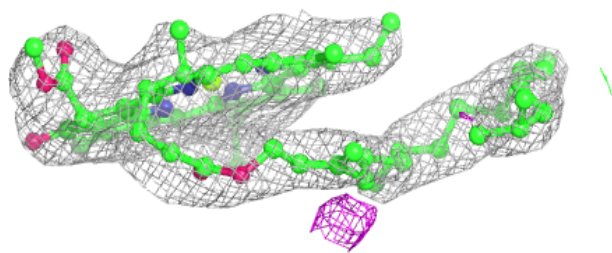
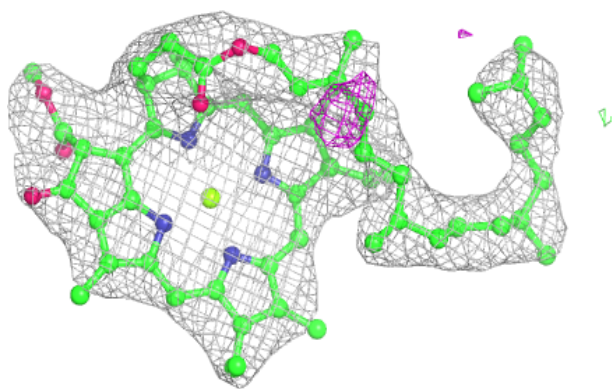
**Electron density around CLA 9 608:**

$2mF_o-DF_c$  (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:**

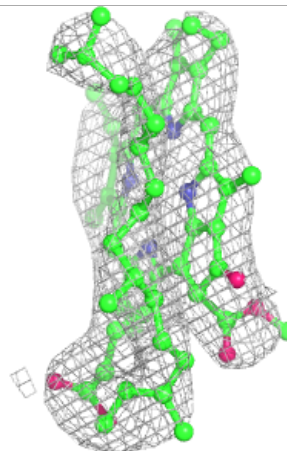
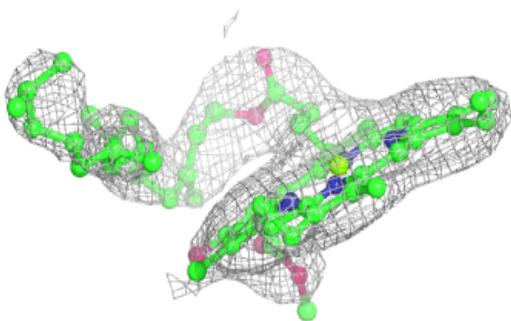
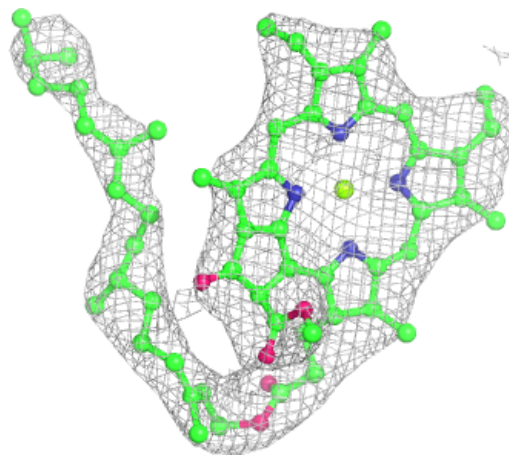
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





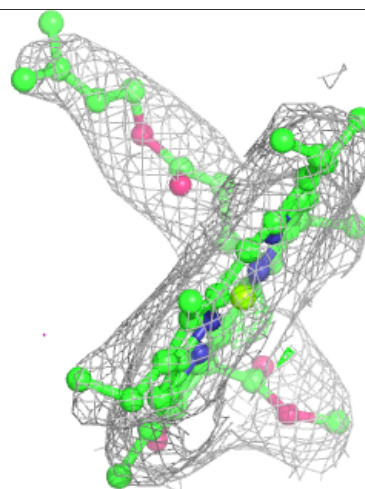
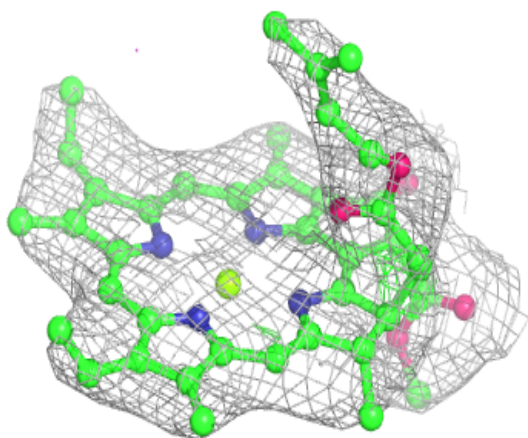
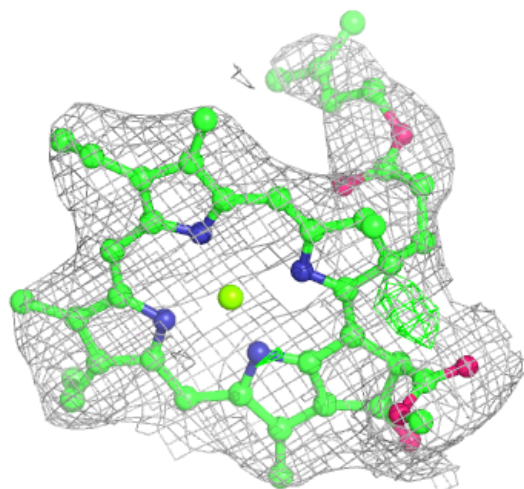
**Electron density around CLA A 826:**

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



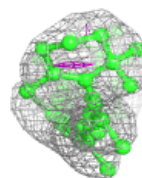
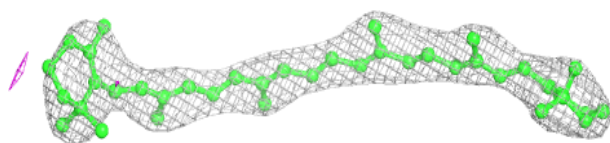
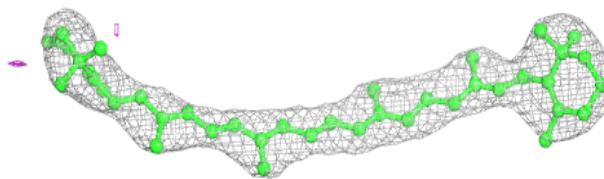
**Electron density around CLA B 830:**

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



**Electron density around BCR b 801:**

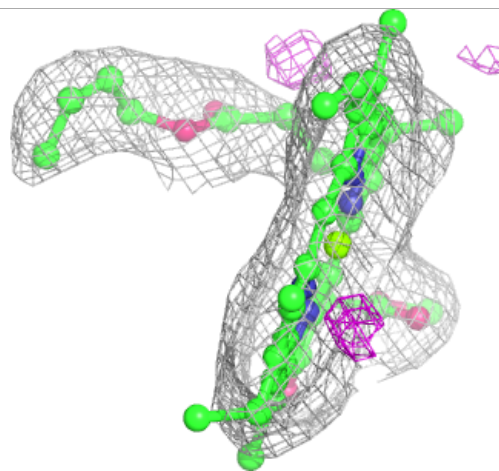
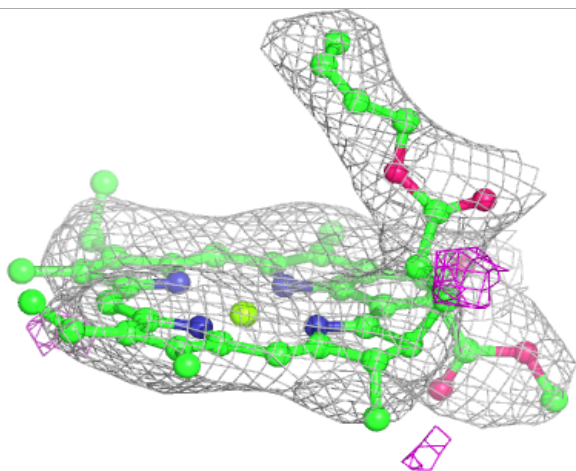
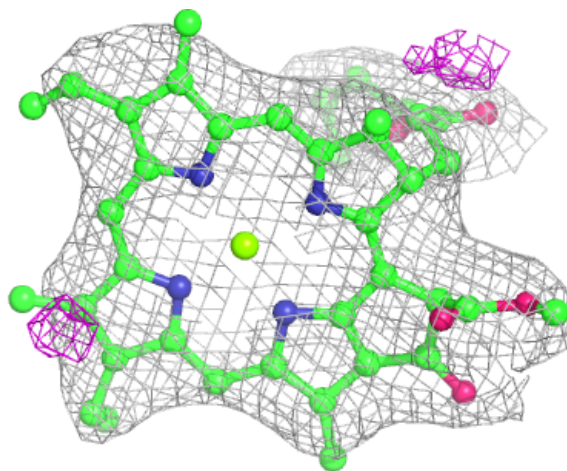
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





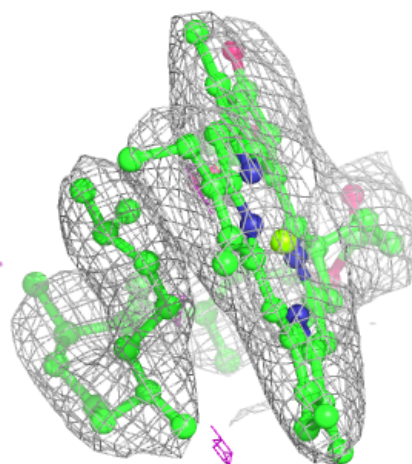
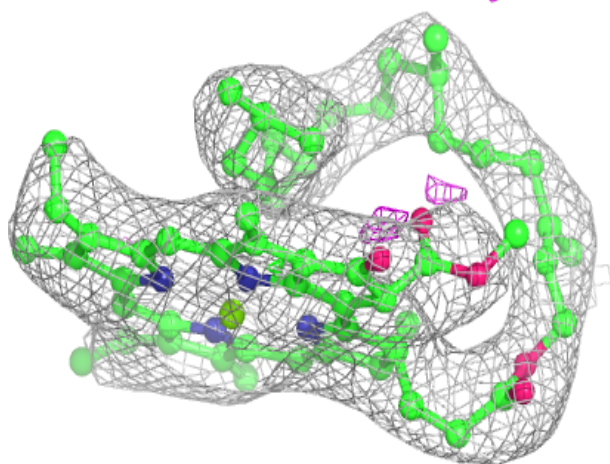
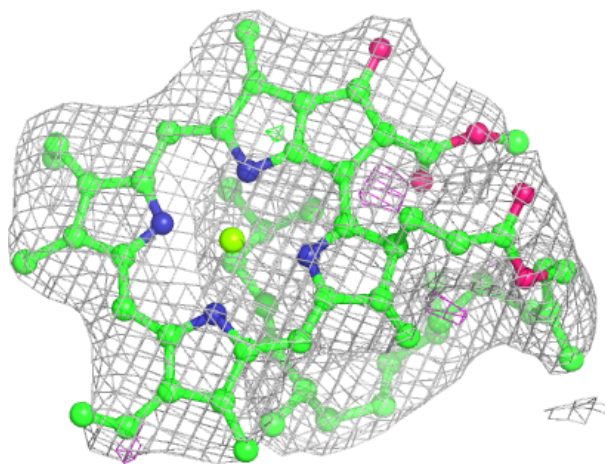
**Electron density around CLA B 831:**

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



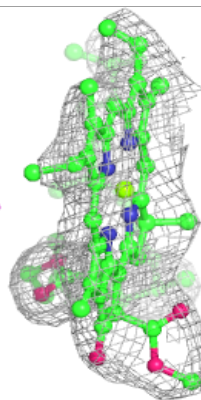
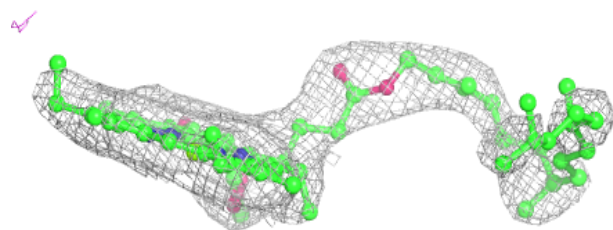
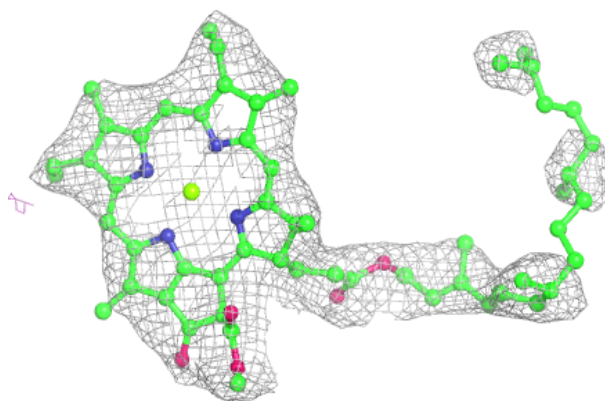
**Electron density around CLA b 806:**

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

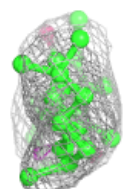
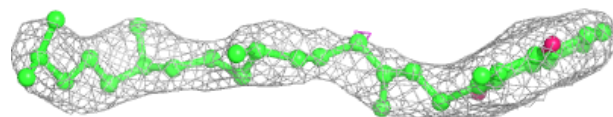
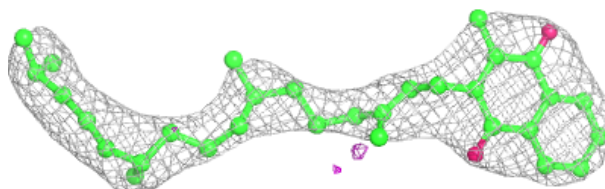


**Electron density around CLA A 827:**

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

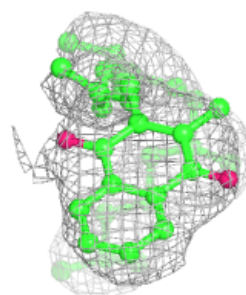
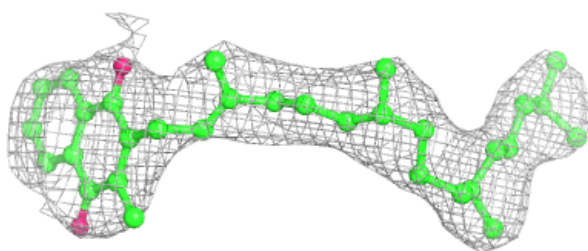
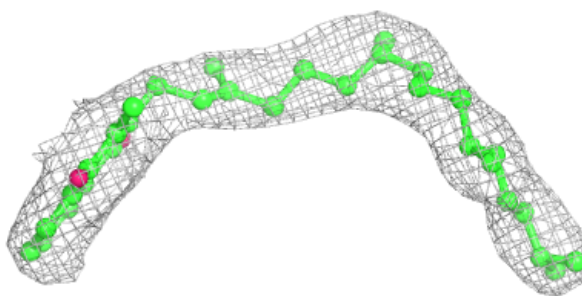
**Electron density around PQN A 844:**

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

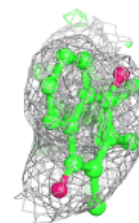
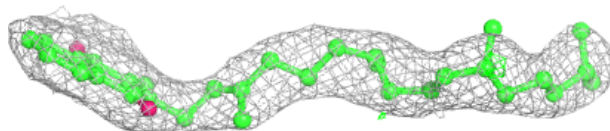
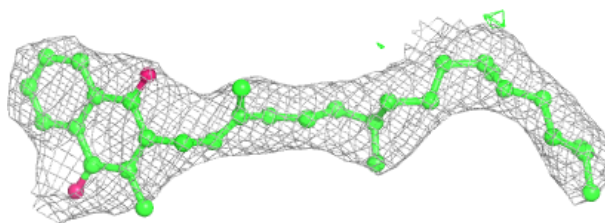


**Electron density around PQN B 842:**

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

**Electron density around PQN a 845:**

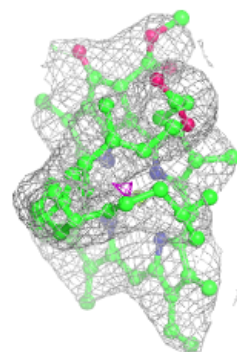
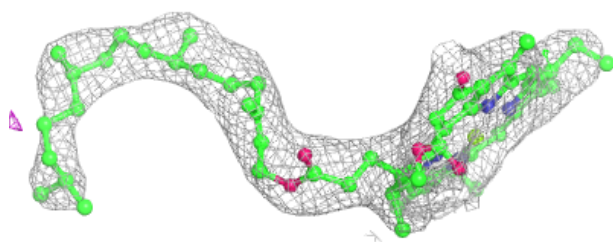
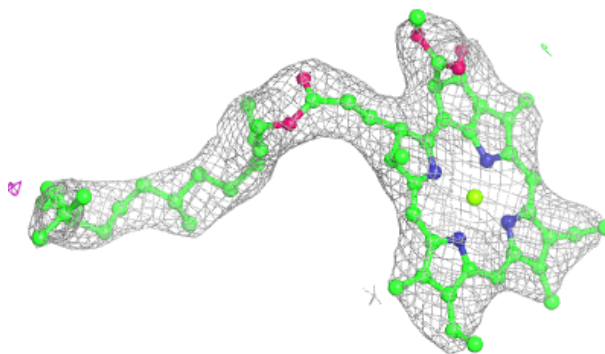
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



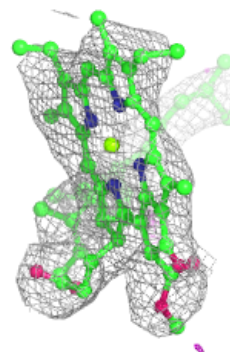
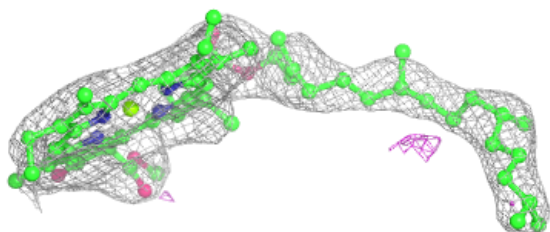
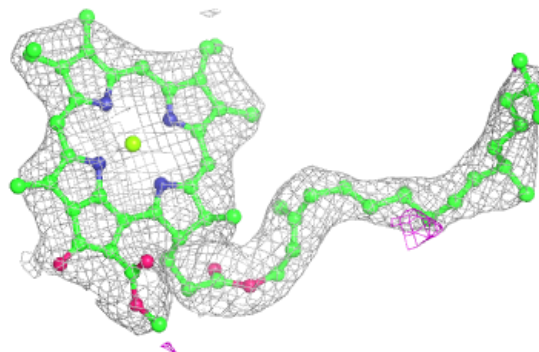


**Electron density around CLA b 809:**

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

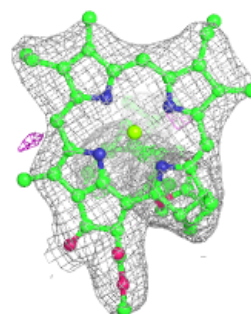
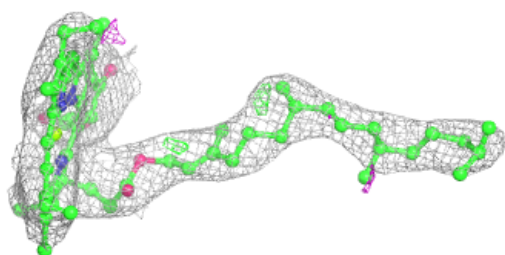
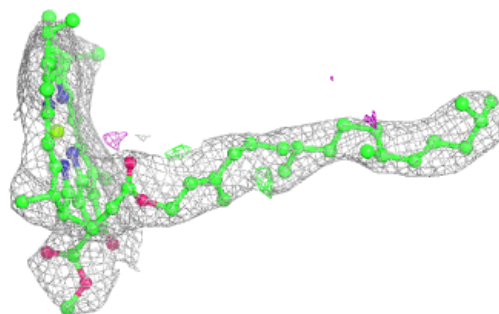
**Electron density around CLA A 802:**

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

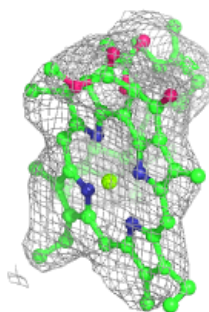
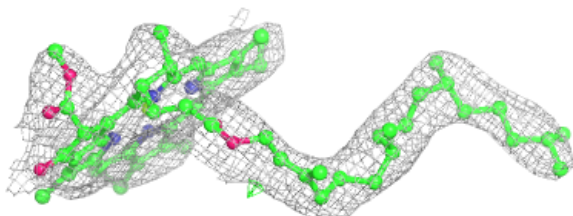
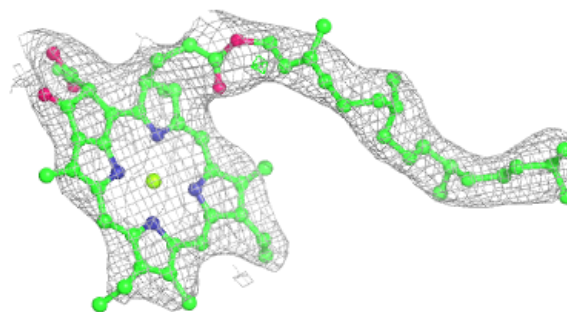


**Electron density around CLA A 829:**

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

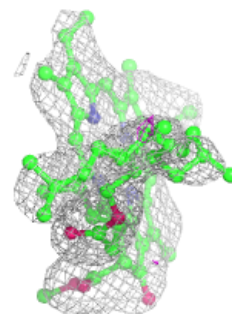
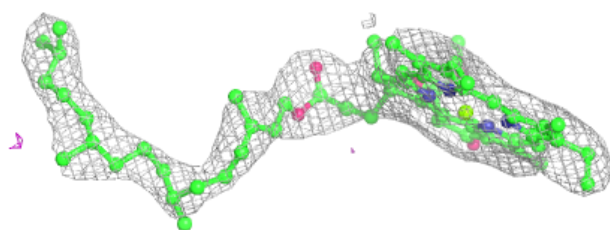
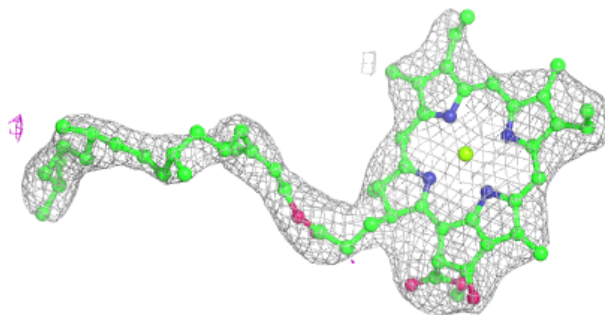
**Electron density around CLA A 809:**

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

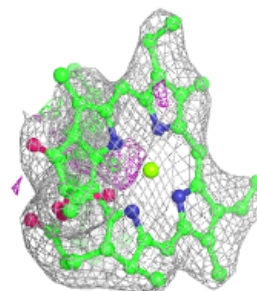
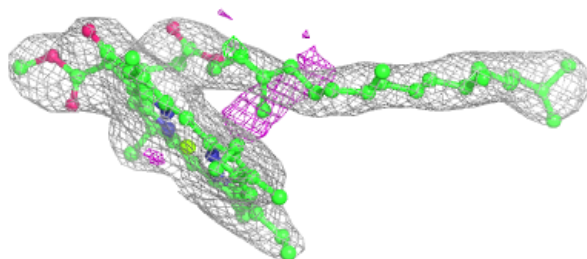
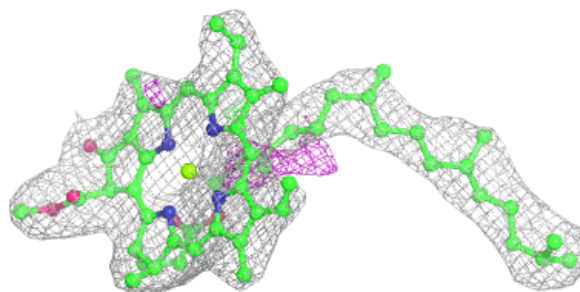


**Electron density around CLA b 813:**

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

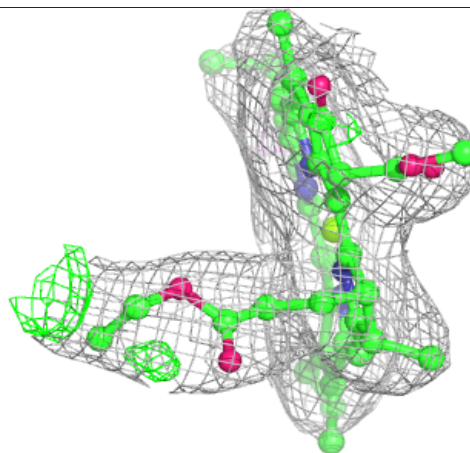
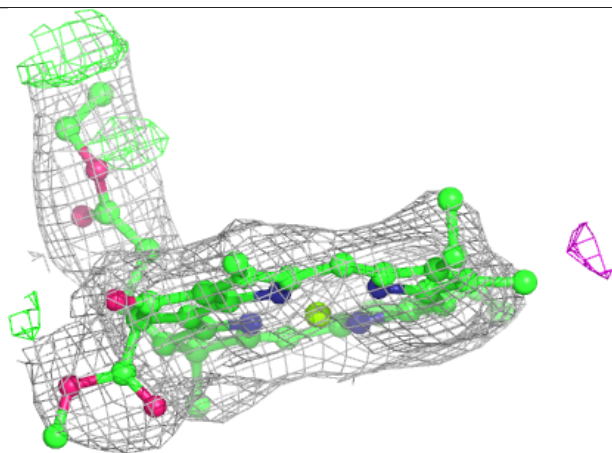
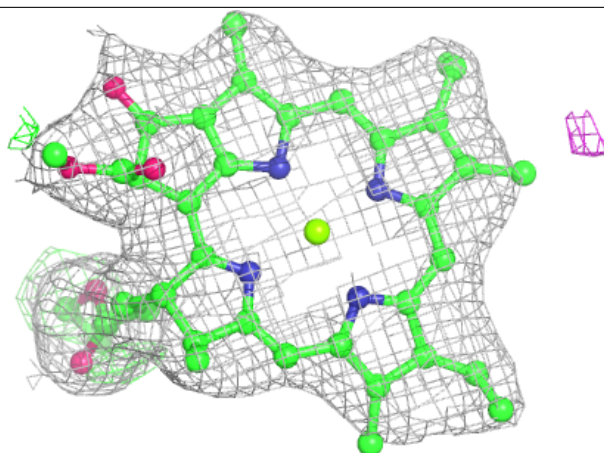
**Electron density around CLA A 842:**

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



**Electron density around CLA B 838:**

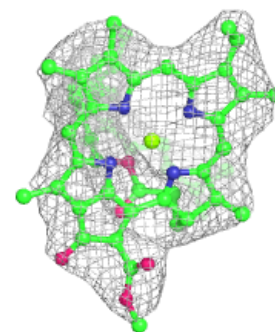
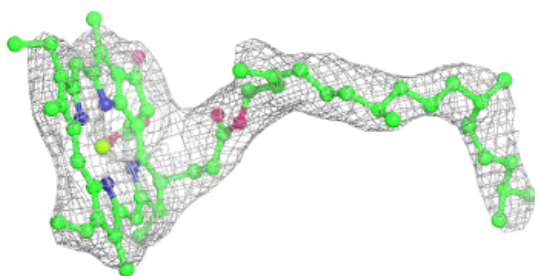
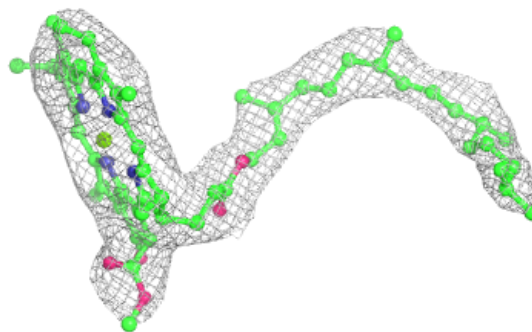
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



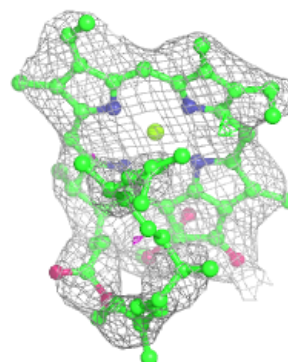
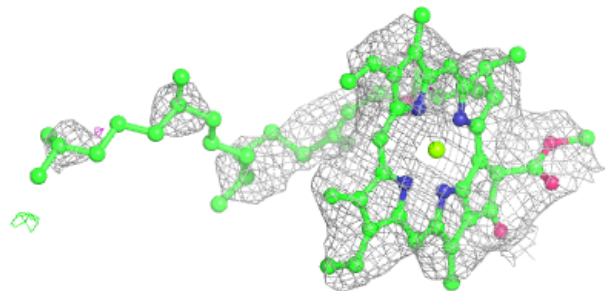
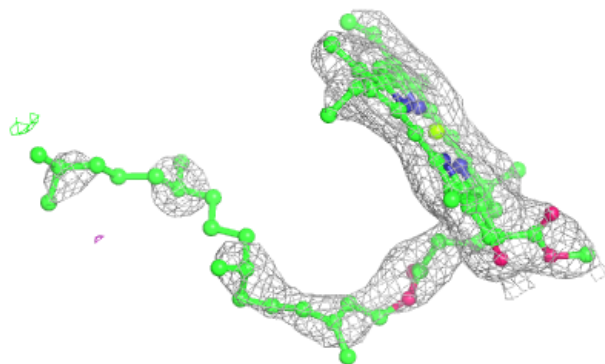


**Electron density around CLA B 839:**

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

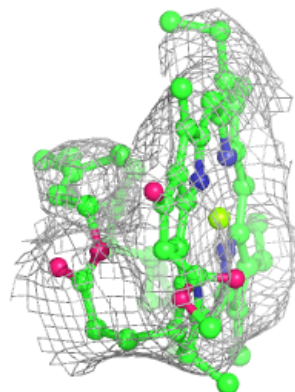
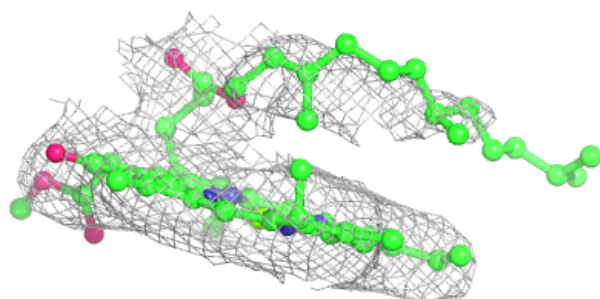
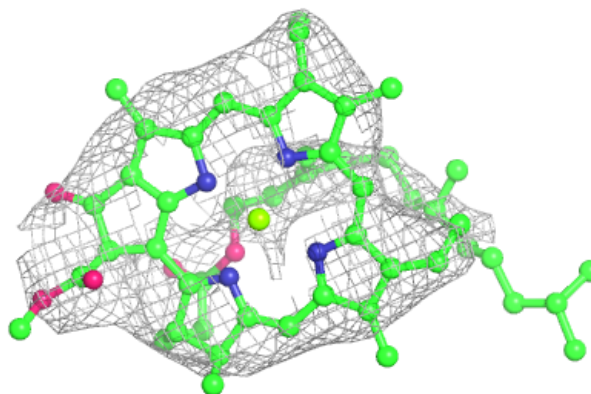
**Electron density around CLA a 811:**

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

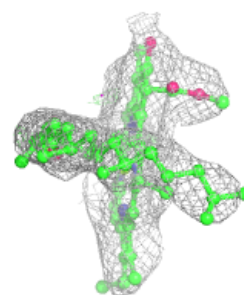
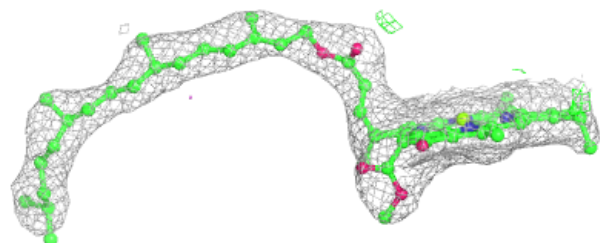
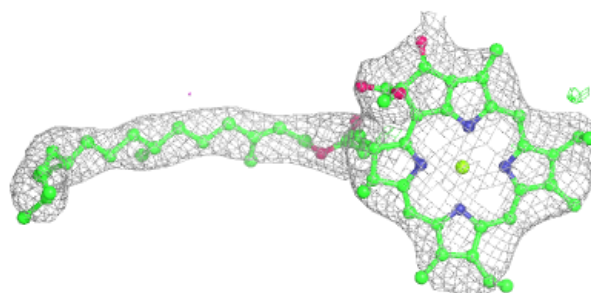


**Electron density around CLA 6 314:**

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

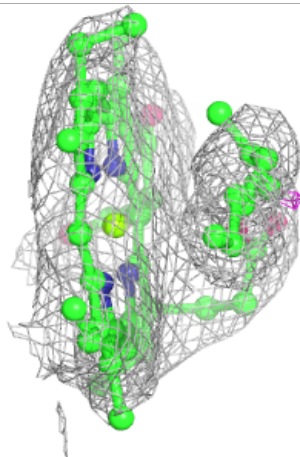
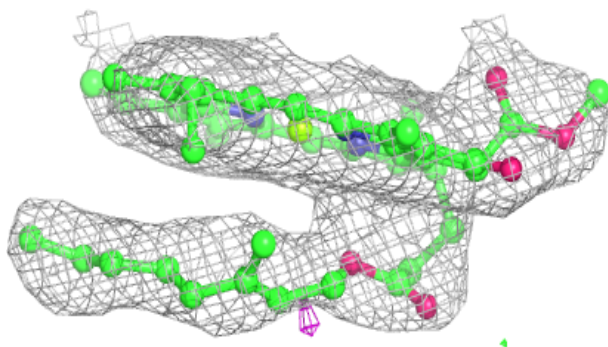
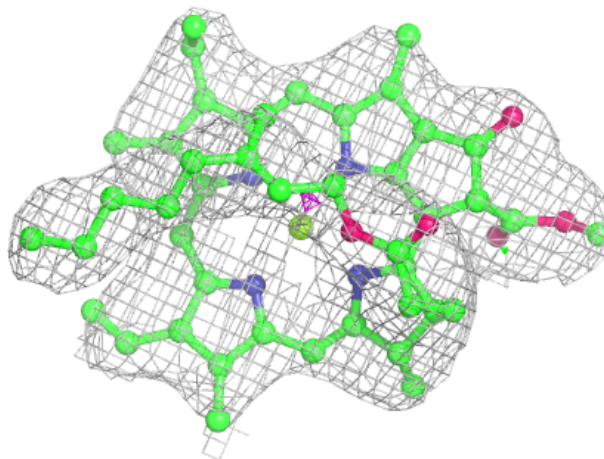
**Electron density around CLA B 841:**

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



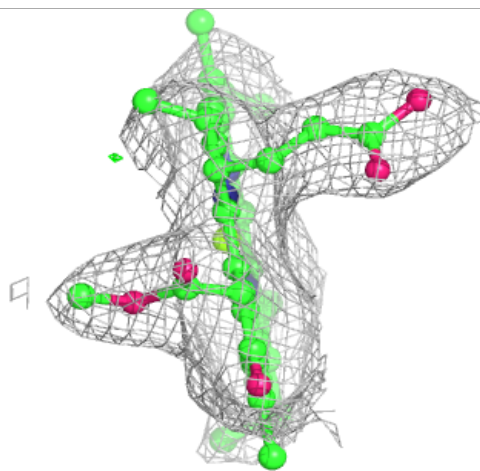
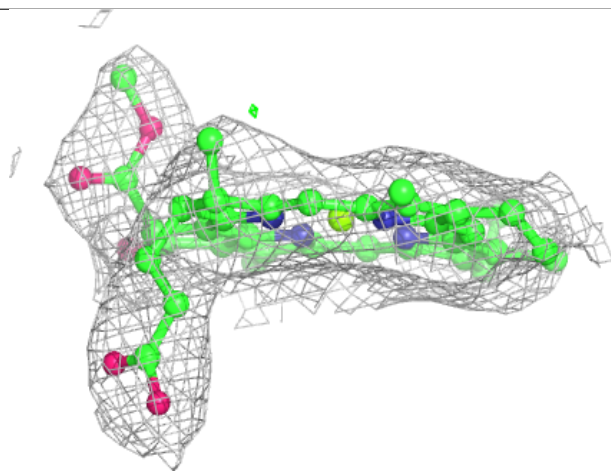
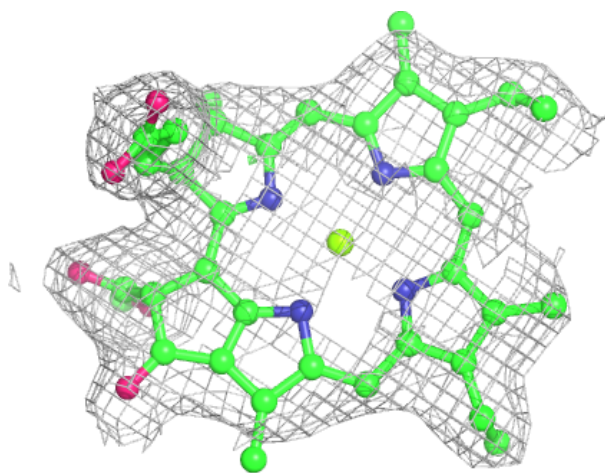
**Electron density around CLA a 813:**

$2mF_o-DF_c$  (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:**

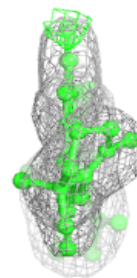
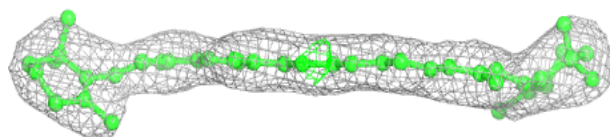
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



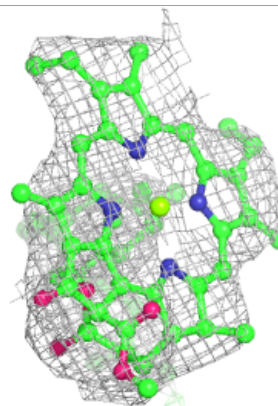
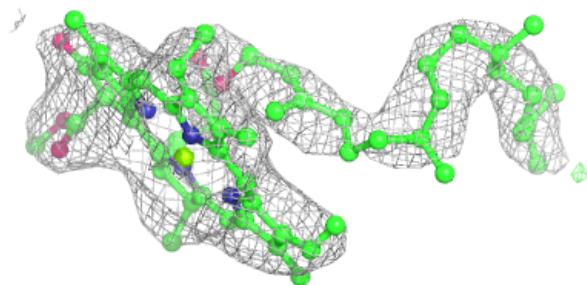
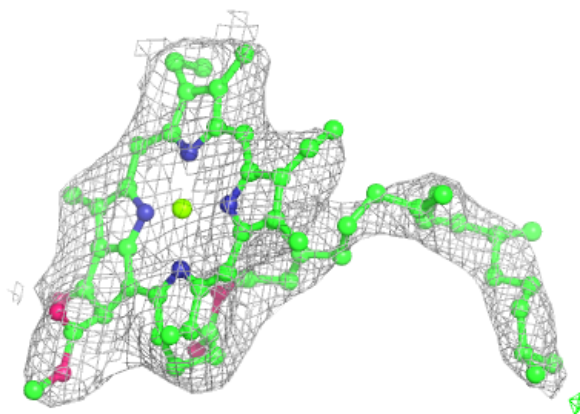


**Electron density around BCR A 852:**

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

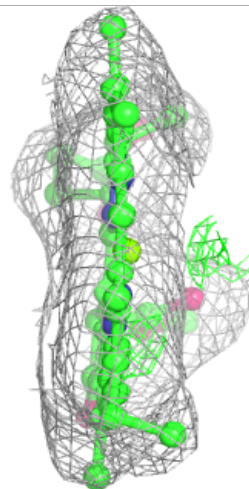
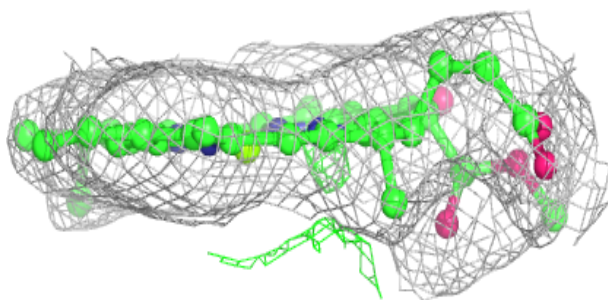
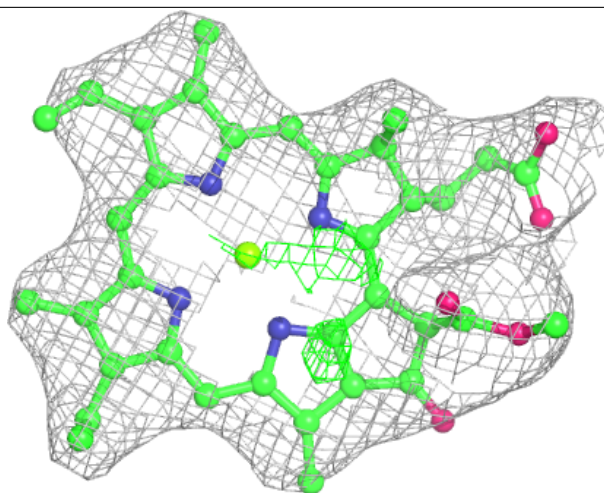
**Electron density around CLA A 843:**

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



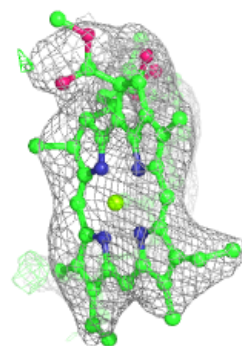
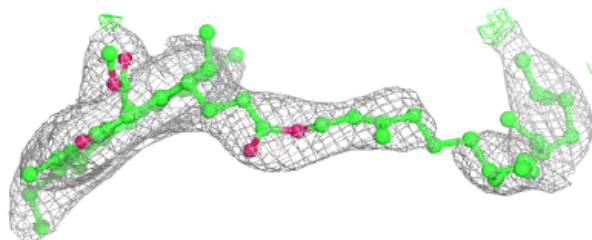
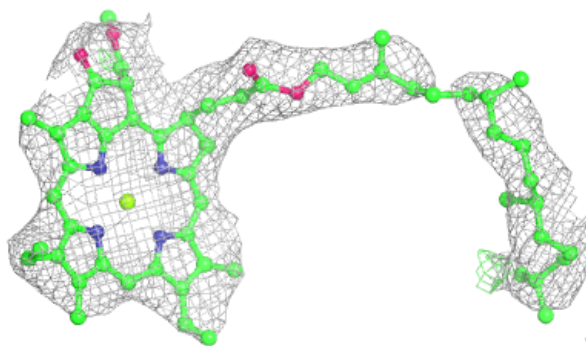
**Electron density around CLA F 303:**

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

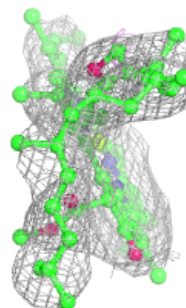
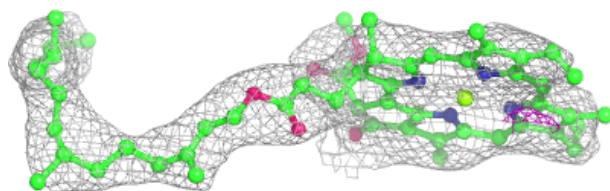
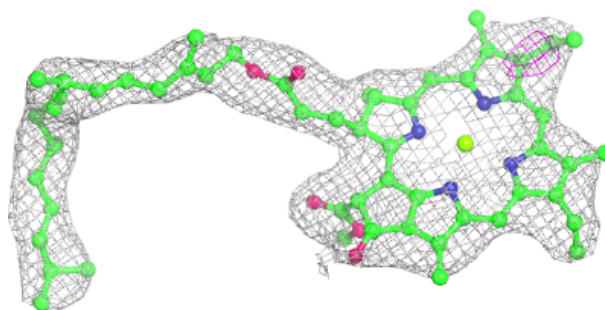


**Electron density around CLA b 825:**

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

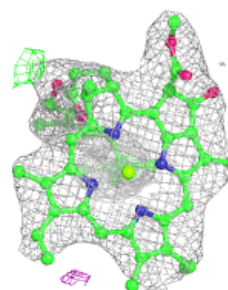
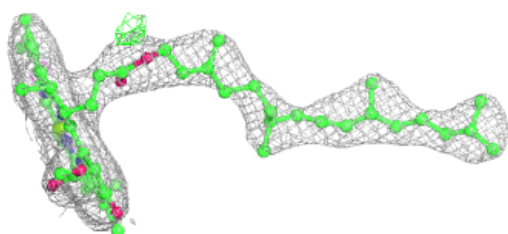
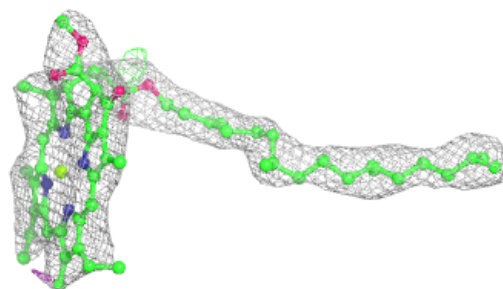
**Electron density around CLA b 826:**

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

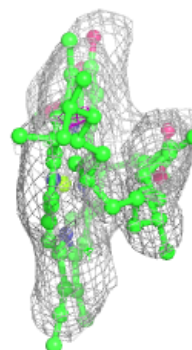
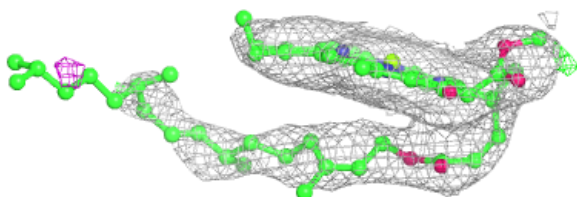
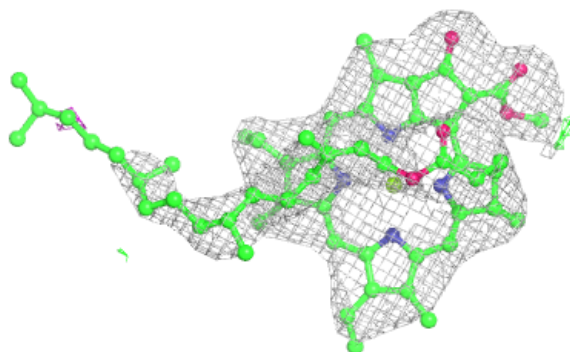


**Electron density around CLA b 828:**

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

**Electron density around CLA a 818:**

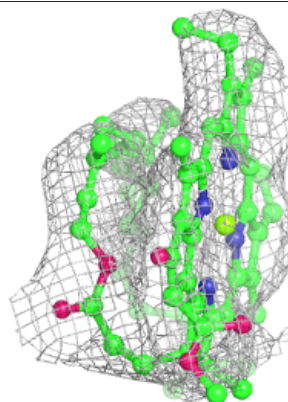
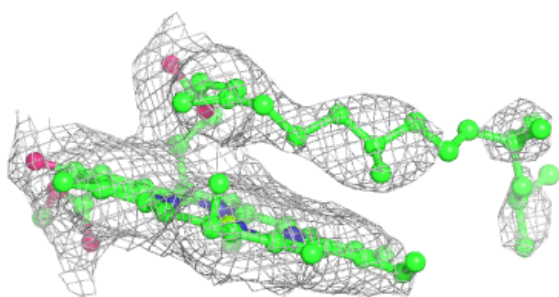
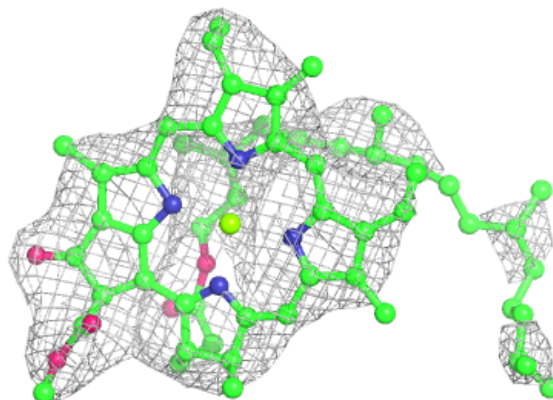
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





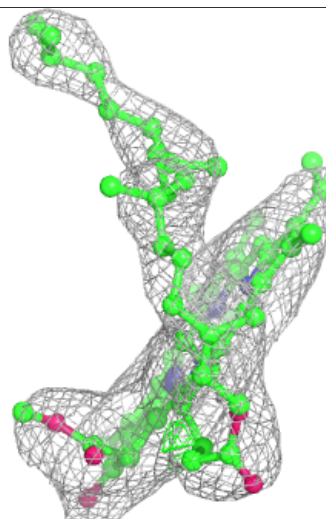
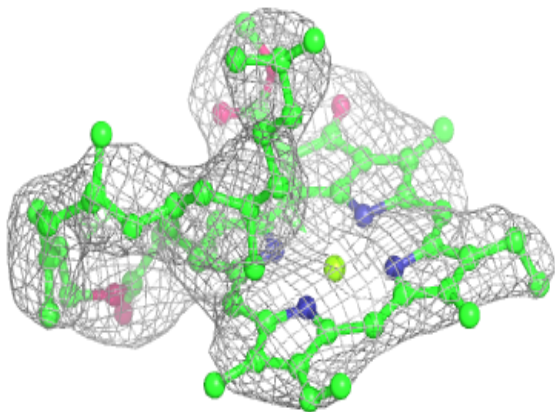
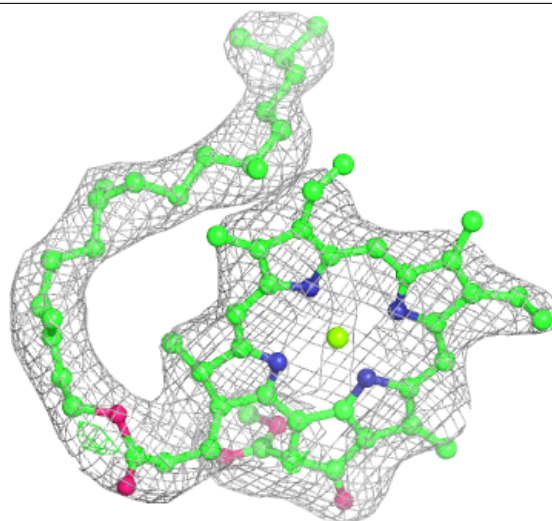
**Electron density around CLA 7 612:**

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



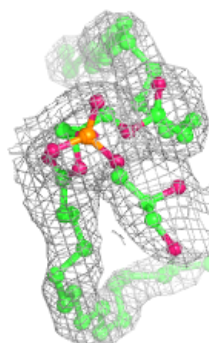
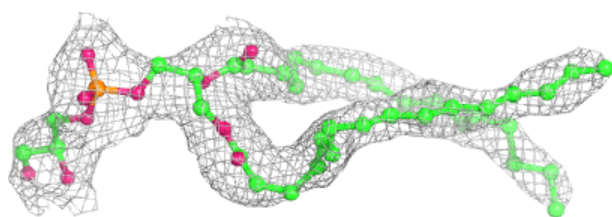
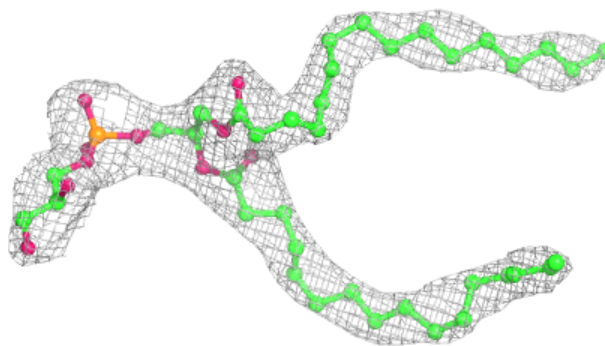
**Electron density around CLA A 814:**

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

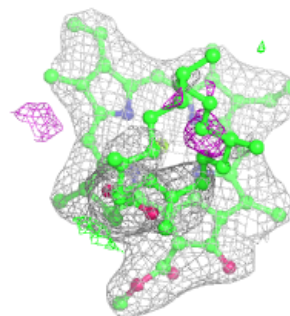
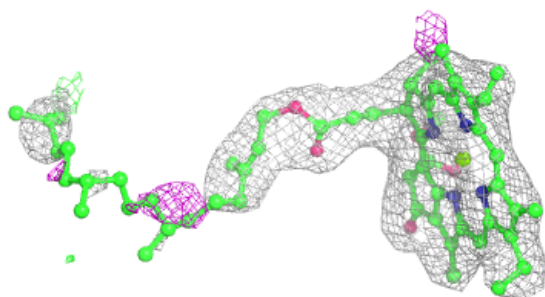
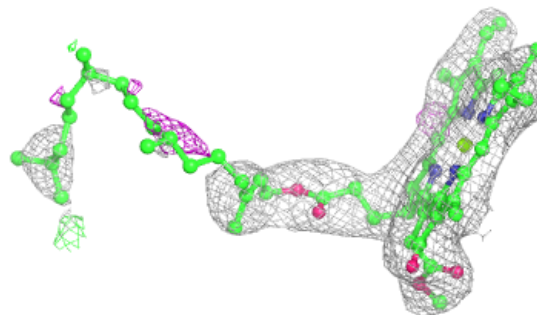


**Electron density around LHG A 846:**

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

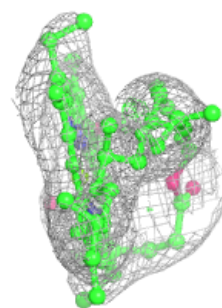
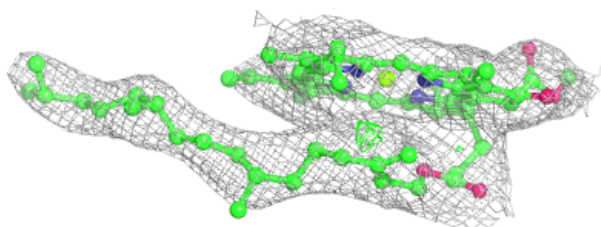
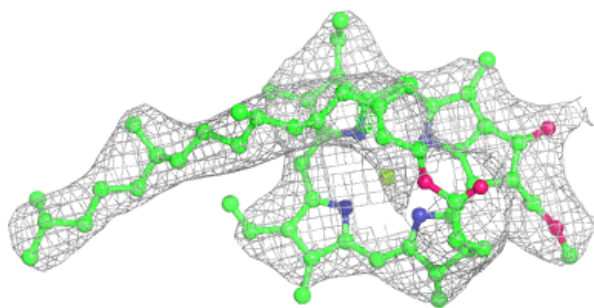
**Electron density around CLA a 840:**

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

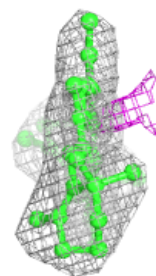
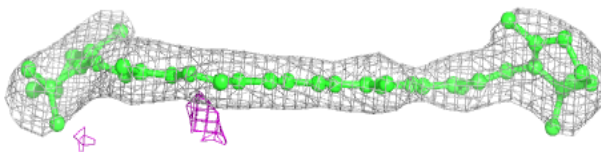
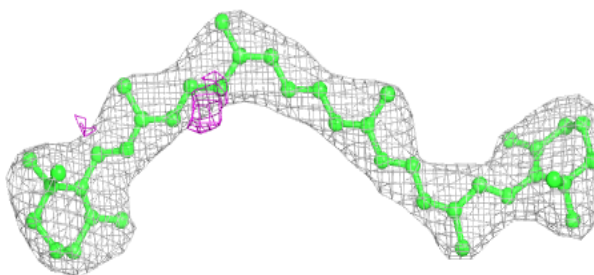


**Electron density around CLA a 841:**

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

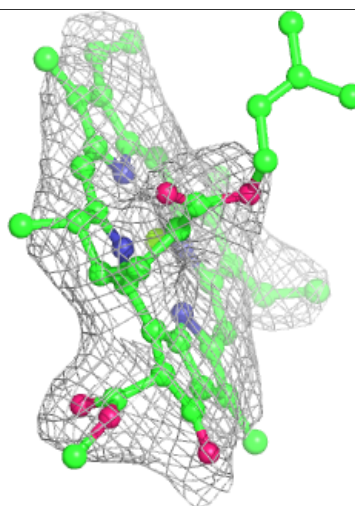
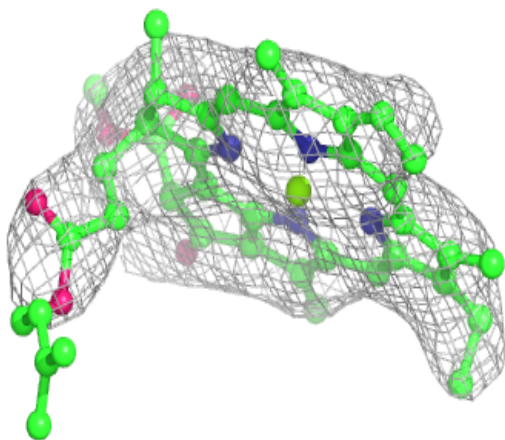
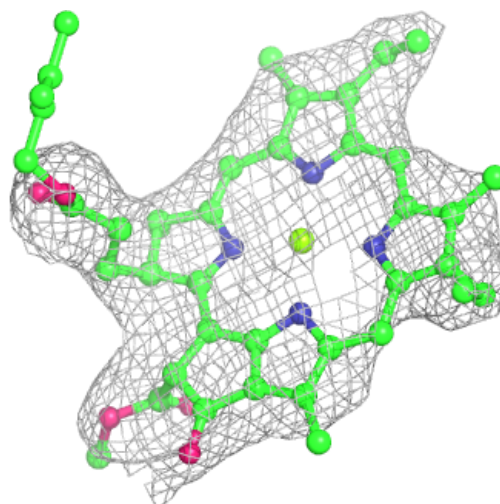
**Electron density around BCR a 854:**

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



**Electron density around CLA B 820:**

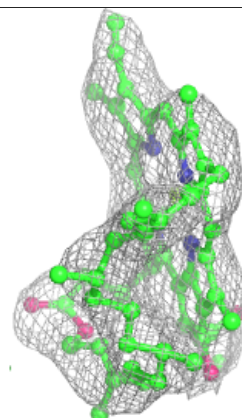
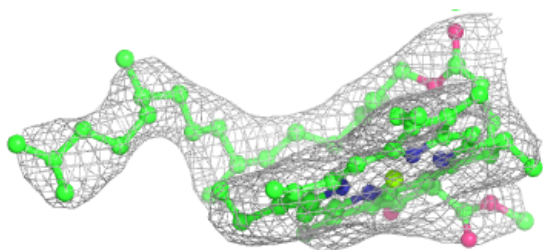
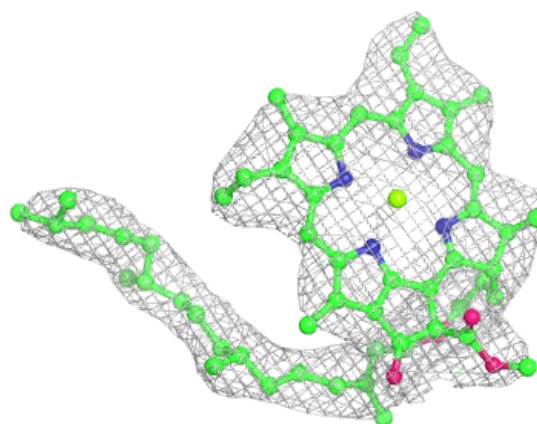
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



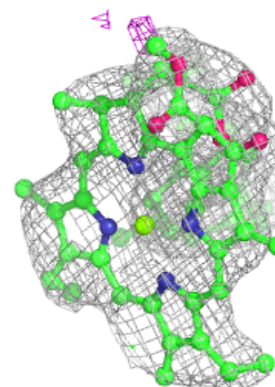
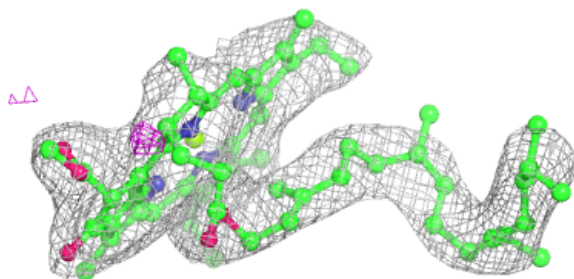
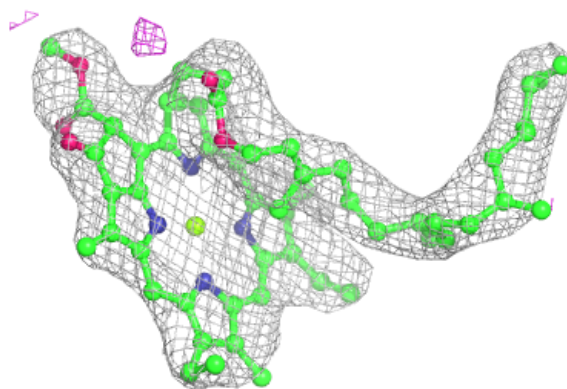


**Electron density around CLA A 830:**

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

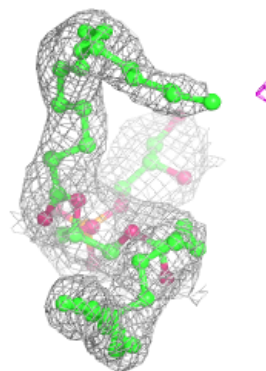
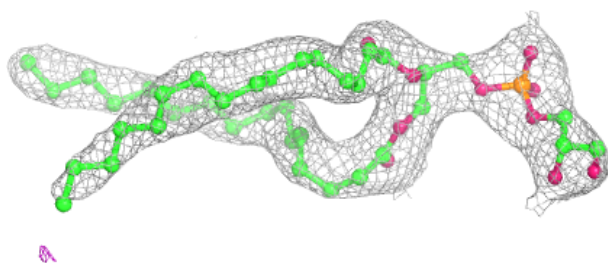
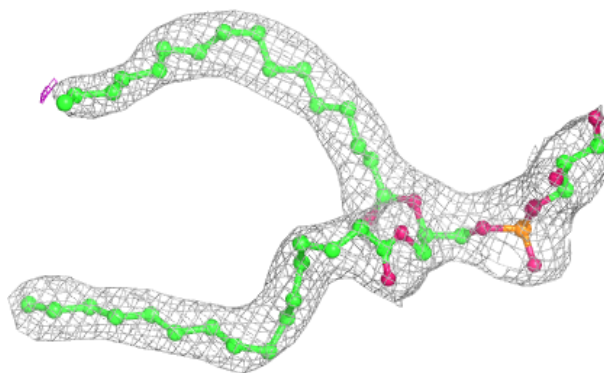
**Electron density around CLA a 844:**

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

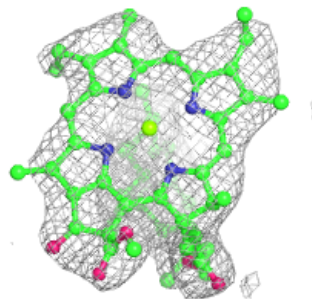
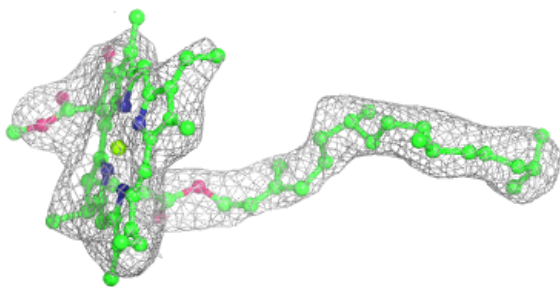
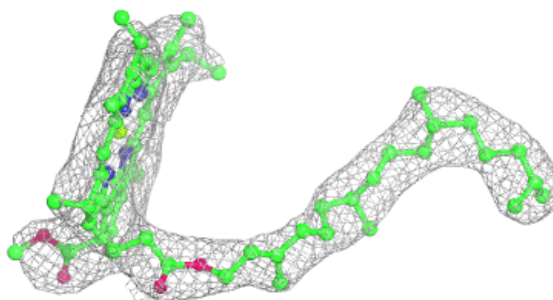


**Electron density around LHG a 847:**

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

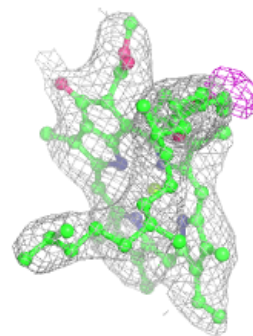
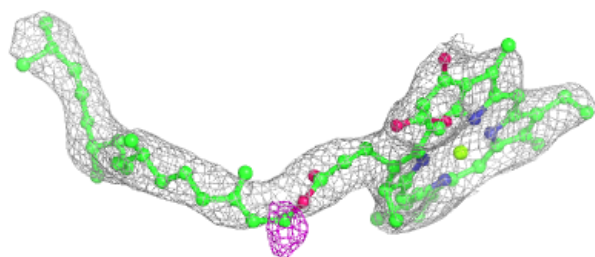
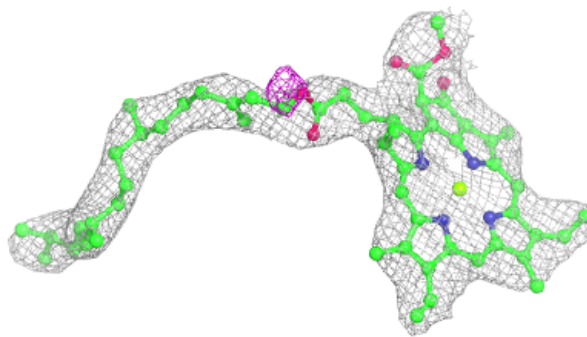
**Electron density around CLA A 831:**

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



**Electron density around CLA a 856:**

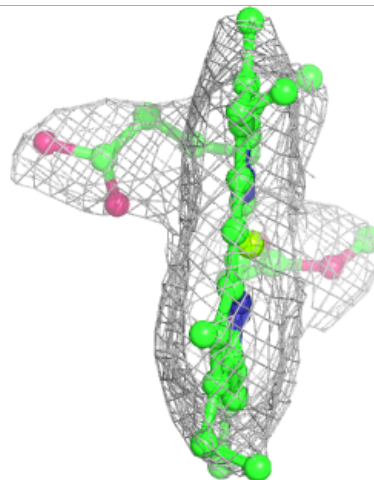
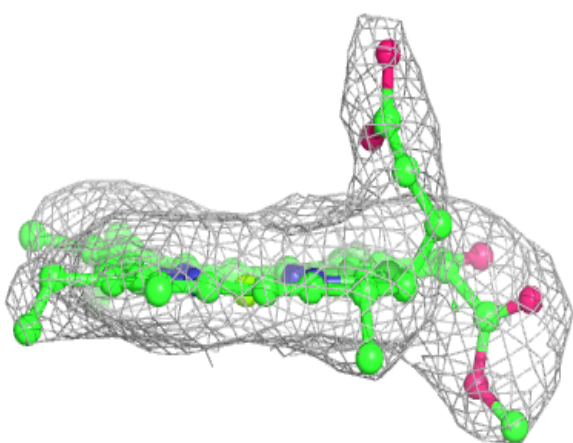
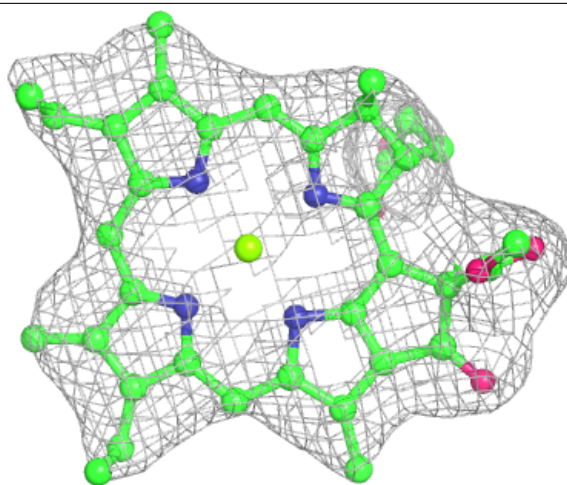
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





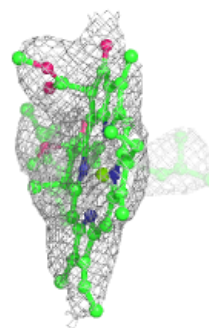
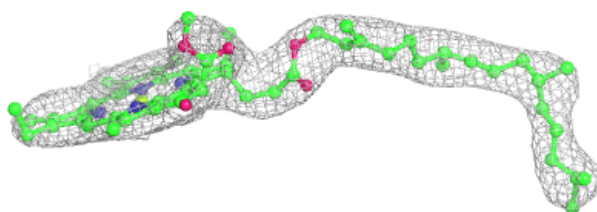
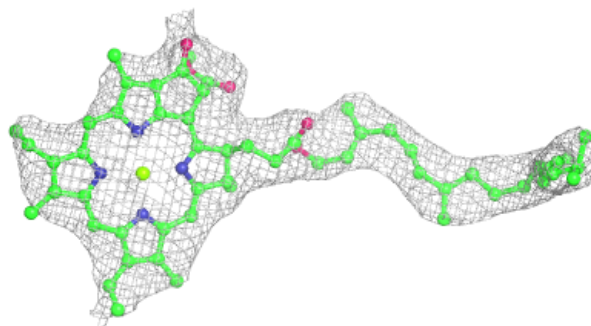
**Electron density around CLA b 804:**

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



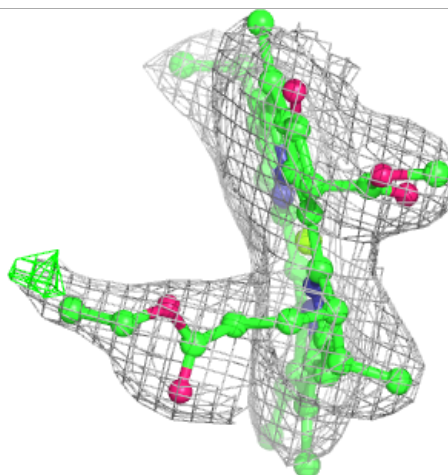
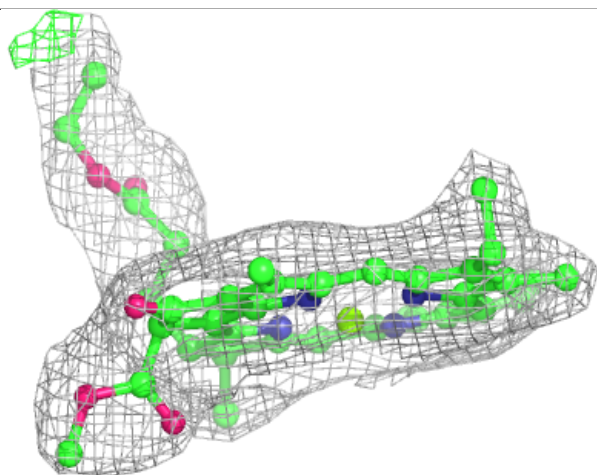
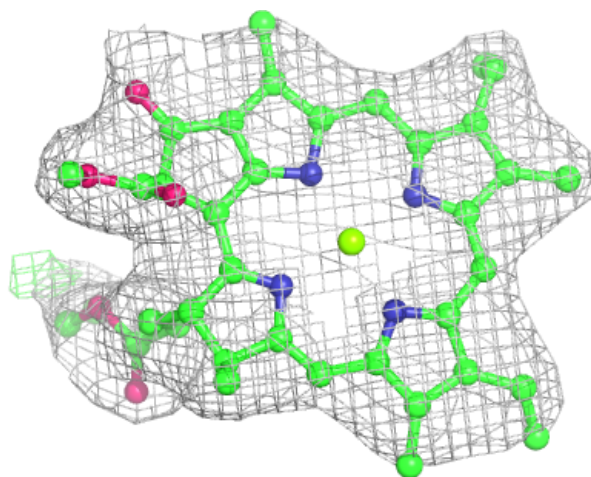
**Electron density around CLA A 806:**

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



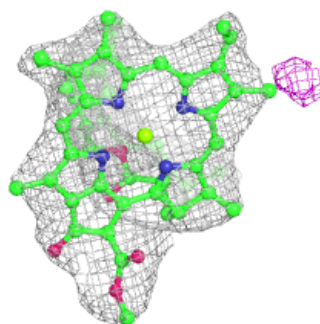
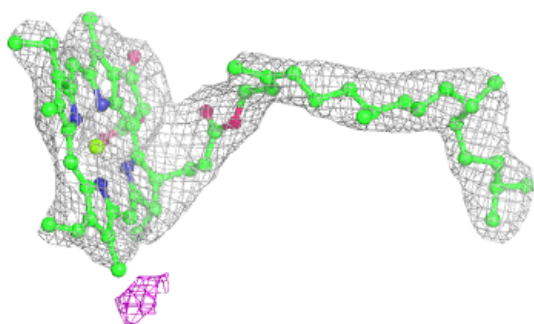
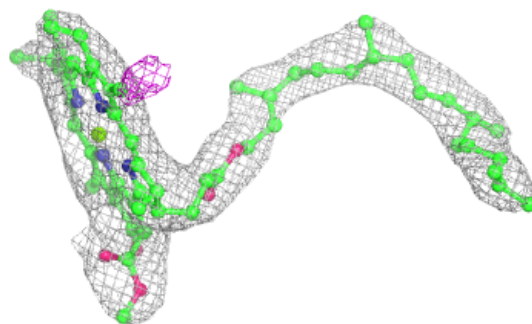
**Electron density around CLA b 838:**

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

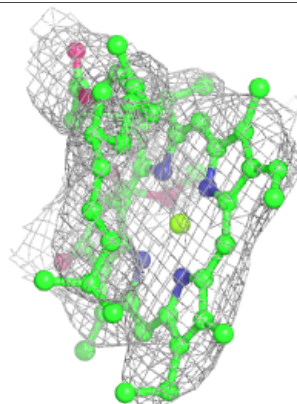
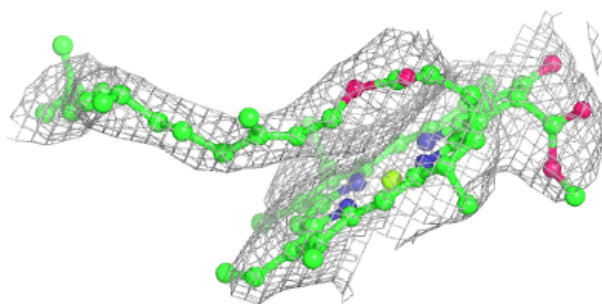
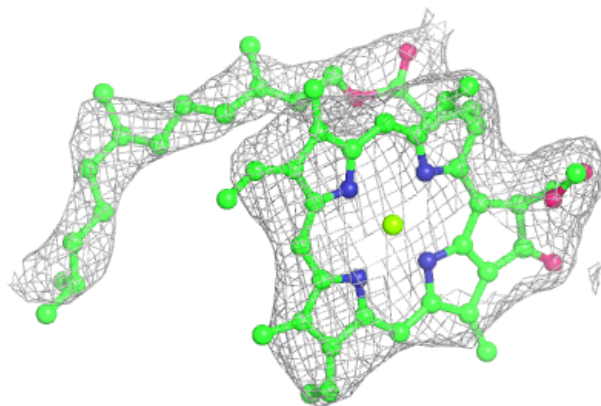


**Electron density around CLA b 839:**

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

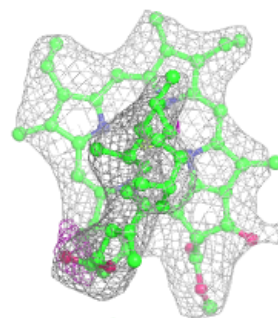
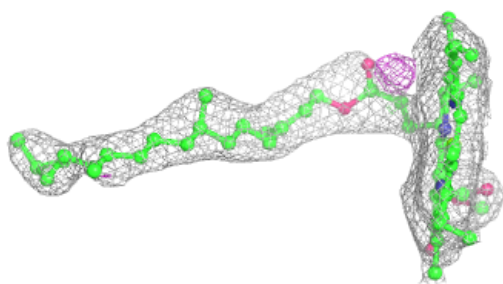
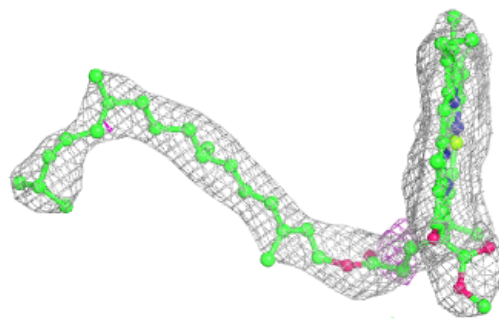
**Electron density around CLA 8 301:**

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

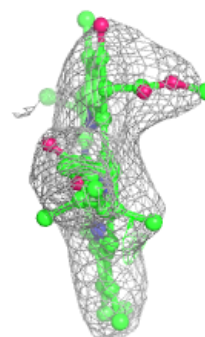
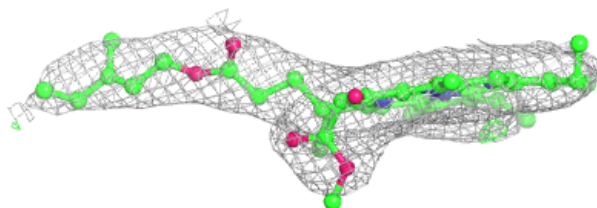
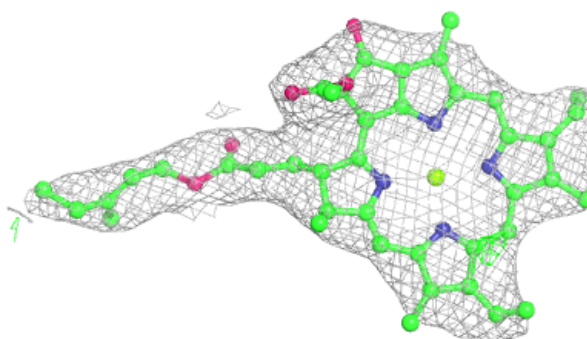


**Electron density around CLA b 840:**

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

**Electron density around CLA A 838:**

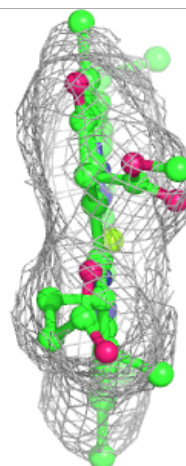
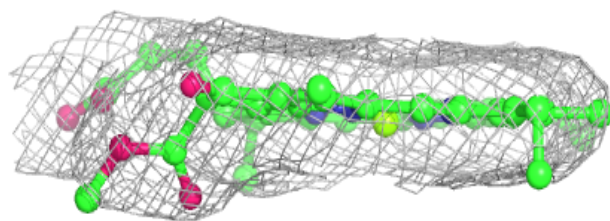
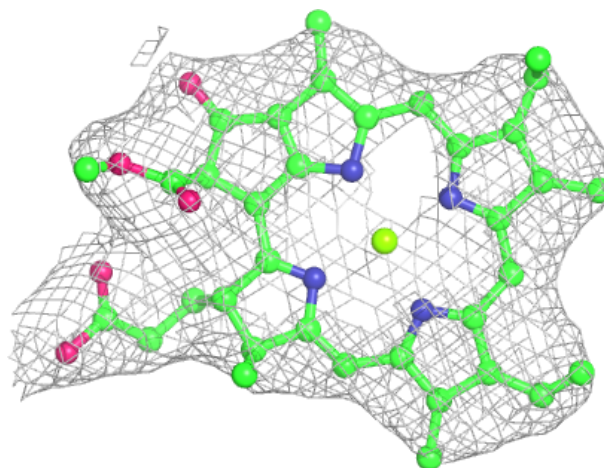
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





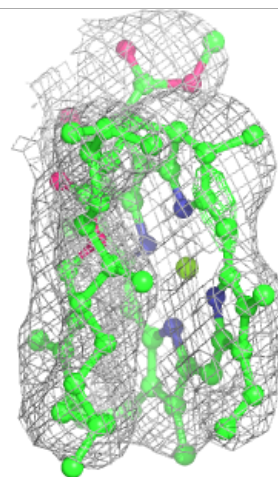
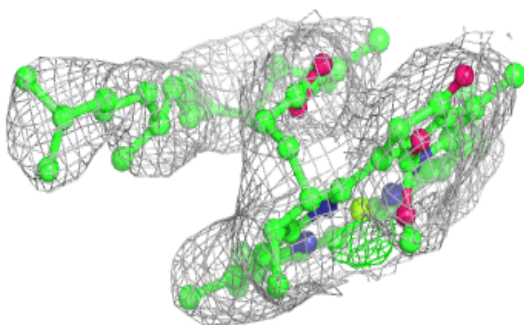
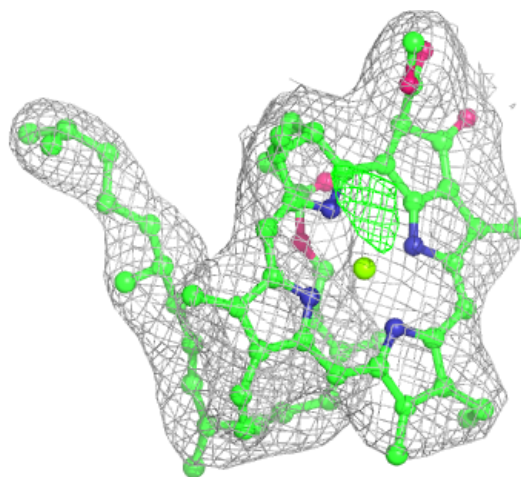
**Electron density around CLA f 7002:**

$2mF_o-DF_c$  (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:**

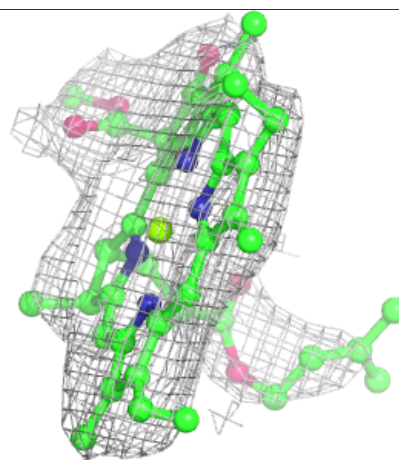
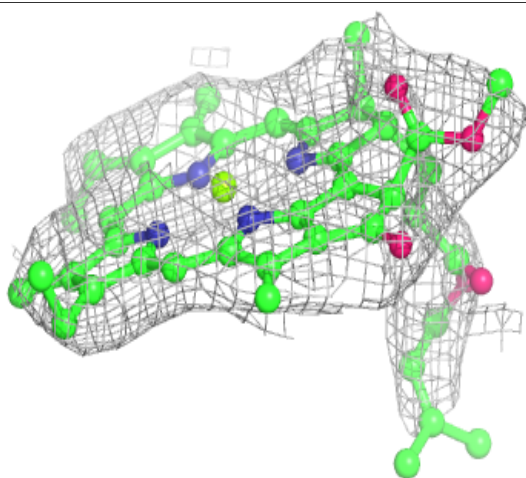
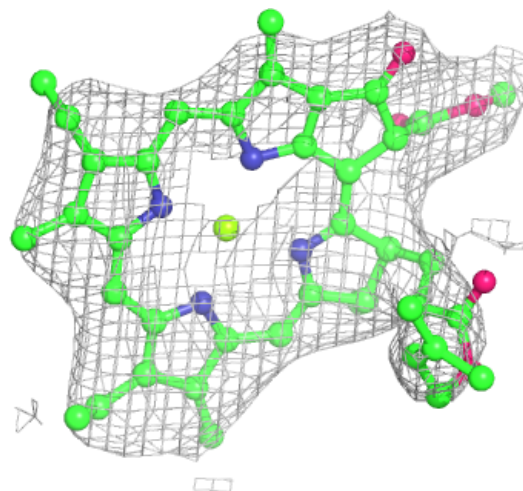
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





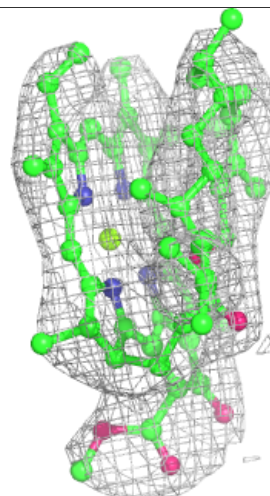
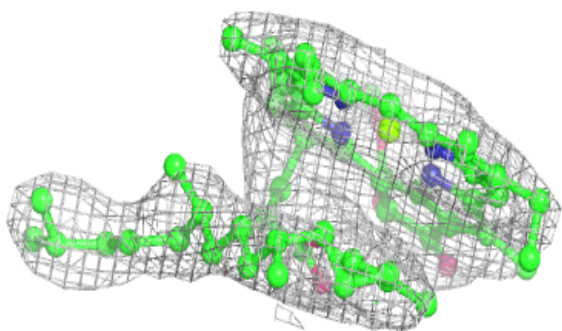
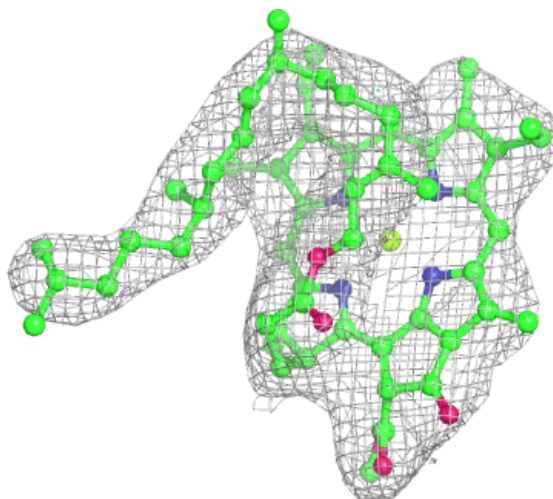
**Electron density around CLA 8 307:**

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



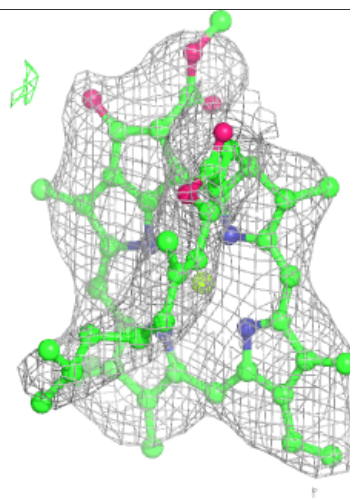
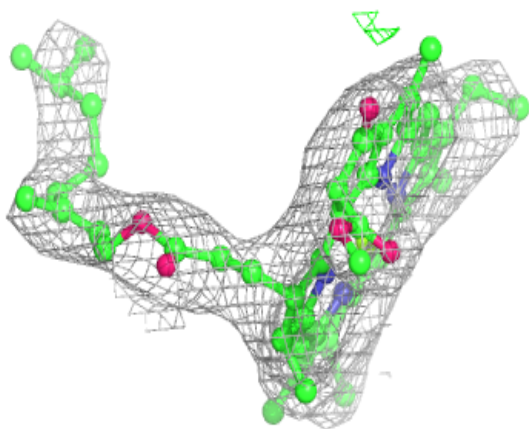
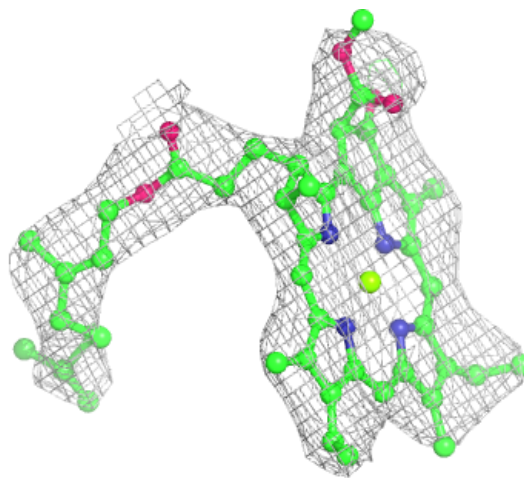
**Electron density around CLA B 808:**

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



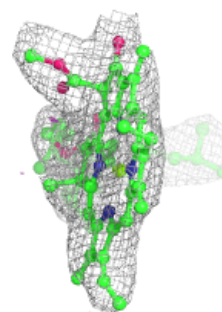
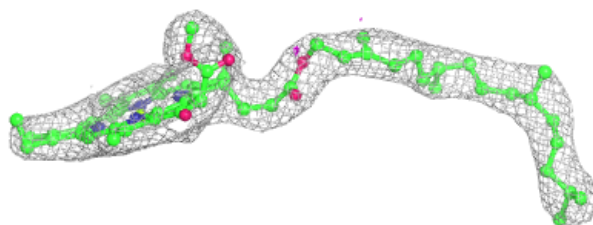
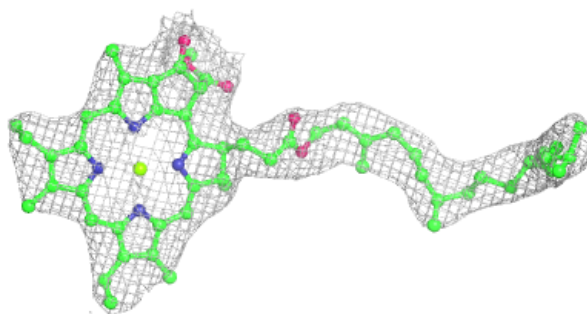
**Electron density around CLA a 805:**

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



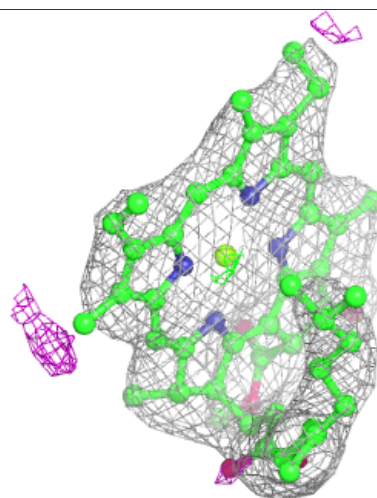
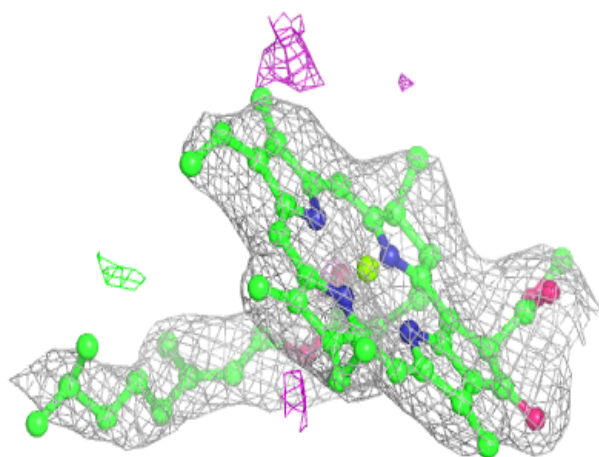
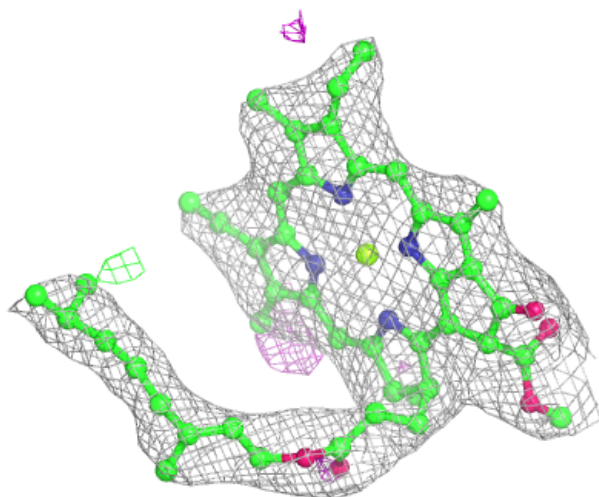
**Electron density around CLA a 806:**

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



**Electron density around CLA a 825:**

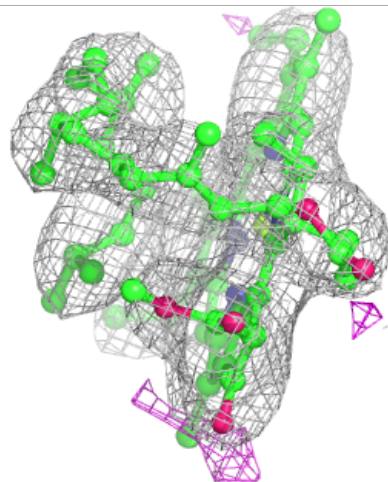
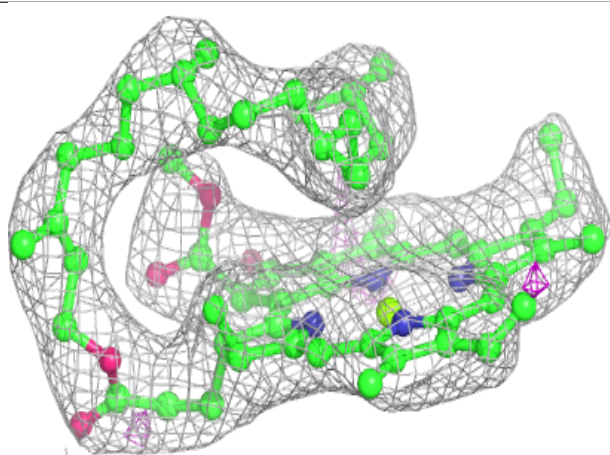
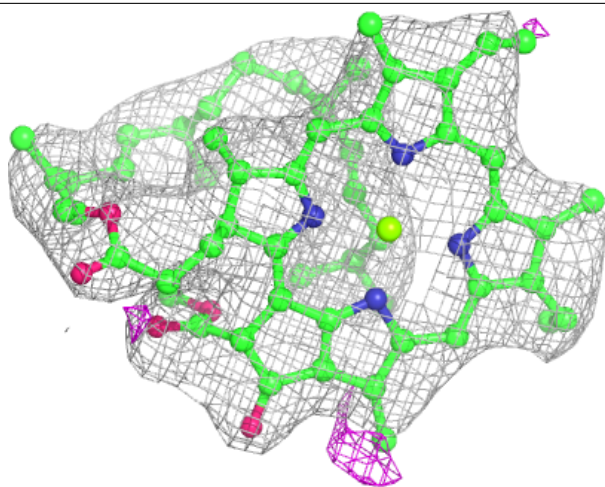
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





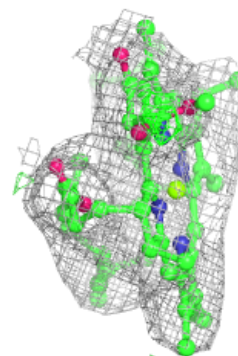
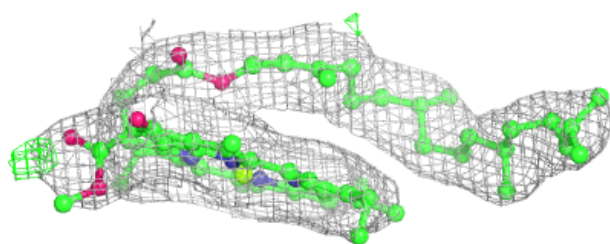
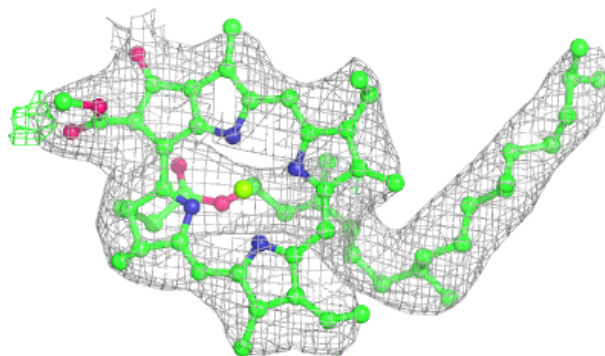
**Electron density around CLA a 807:**

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

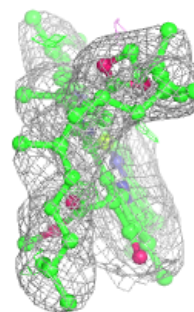
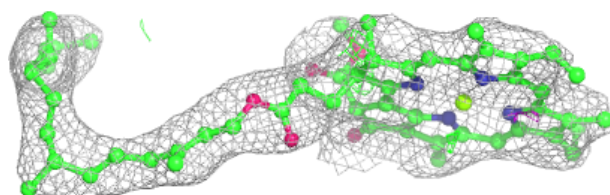
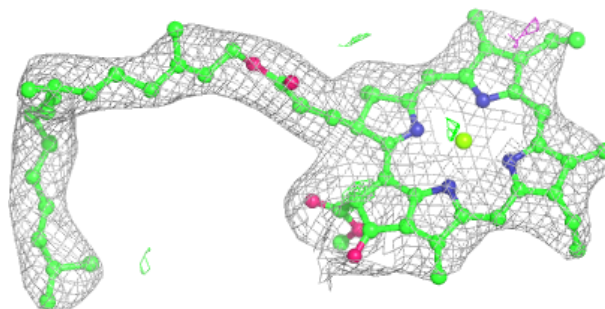


**Electron density around CLA B 837:**

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

**Electron density around CLA B 826:**

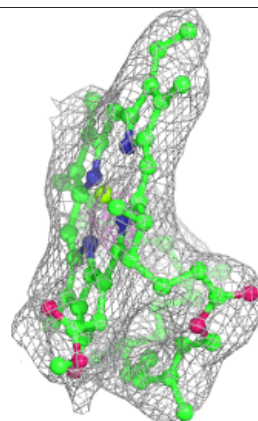
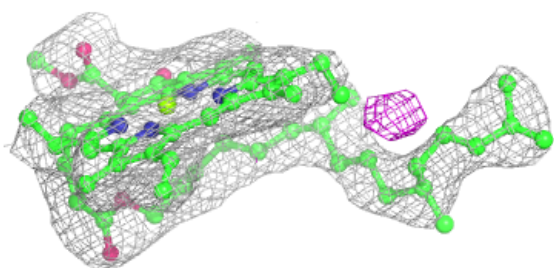
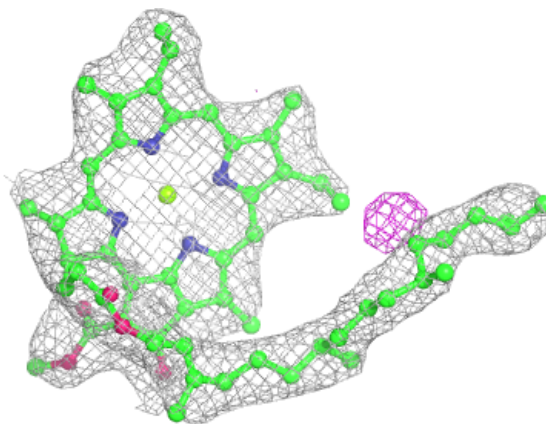
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



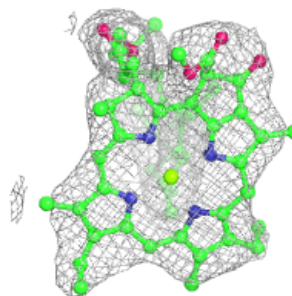
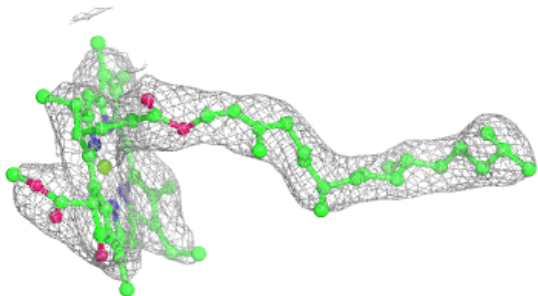
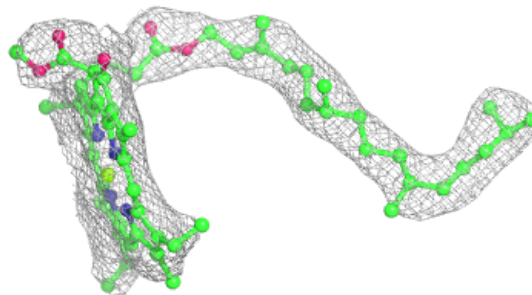


**Electron density around CLA a 830:**

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

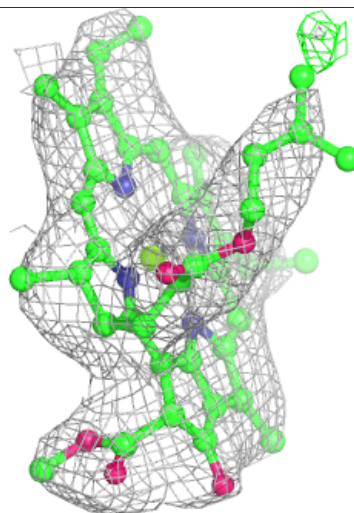
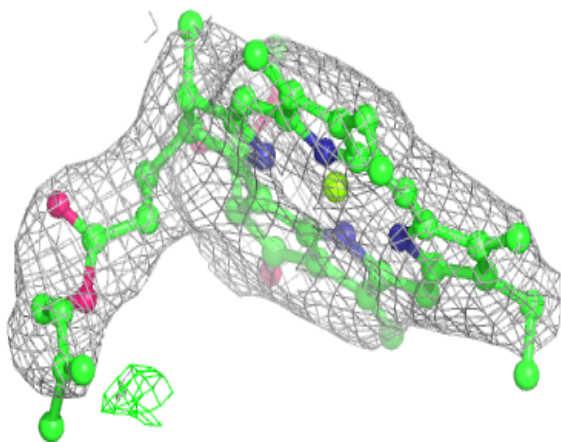
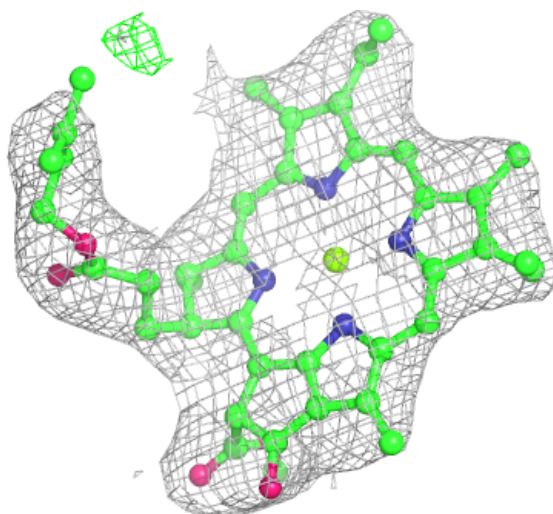
**Electron density around CLA a 831:**

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



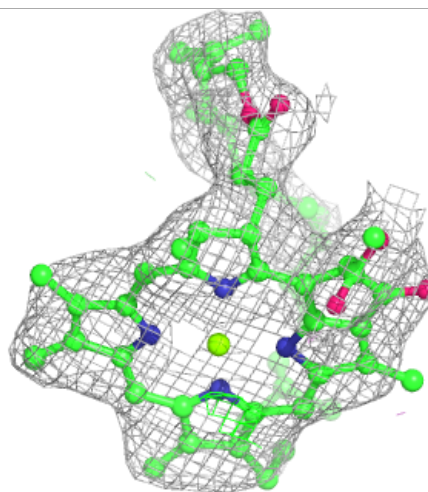
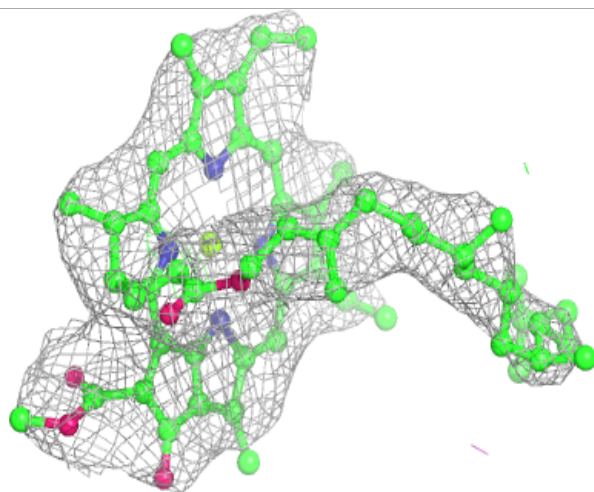
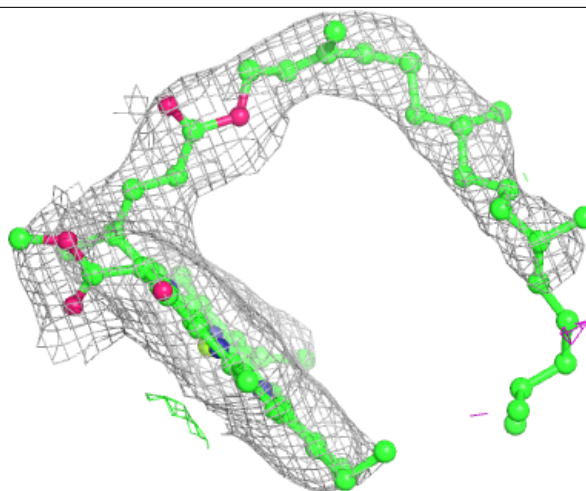
**Electron density around CLA a 832:**

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



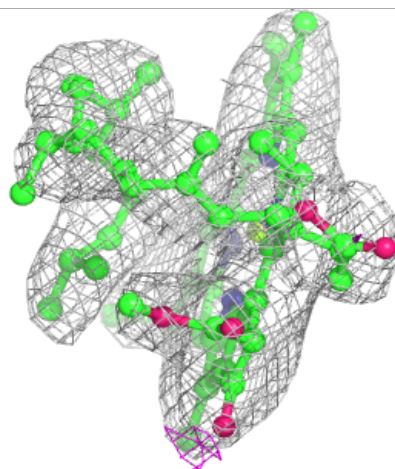
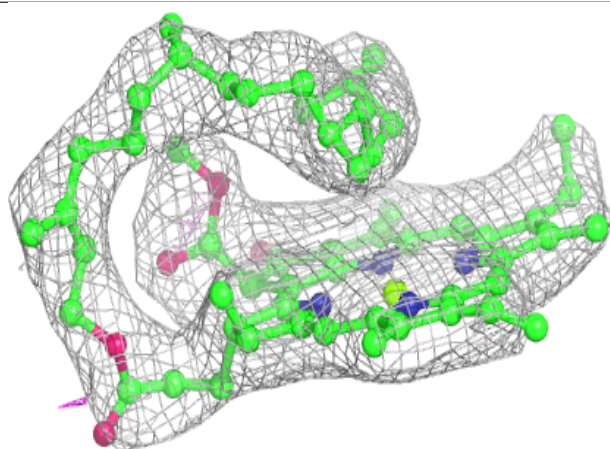
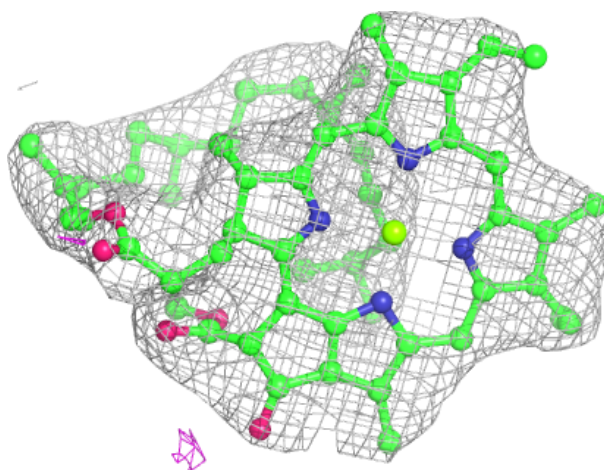
**Electron density around CLA b 819:**

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



**Electron density around CLA A 807:**

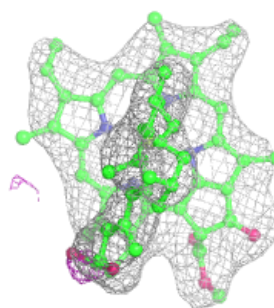
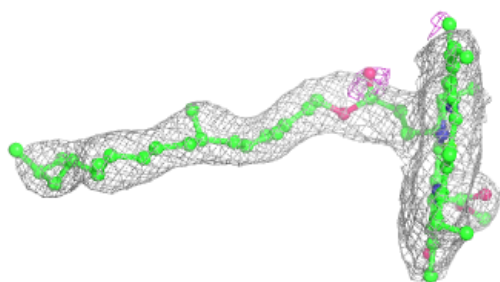
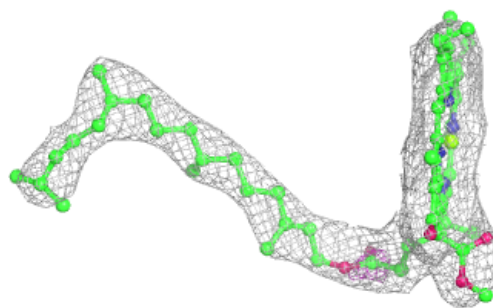
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



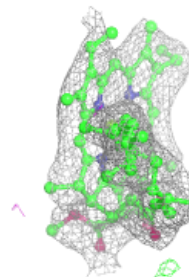
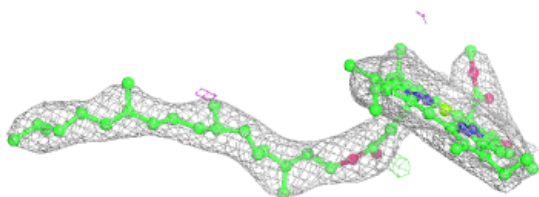
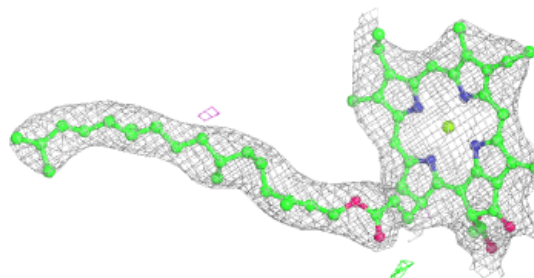


**Electron density around CLA B 840:**

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

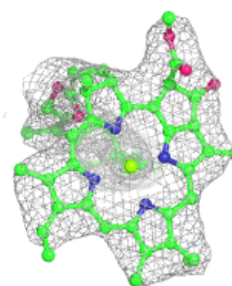
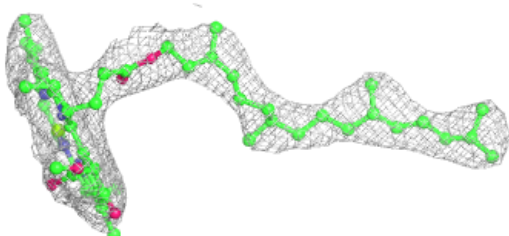
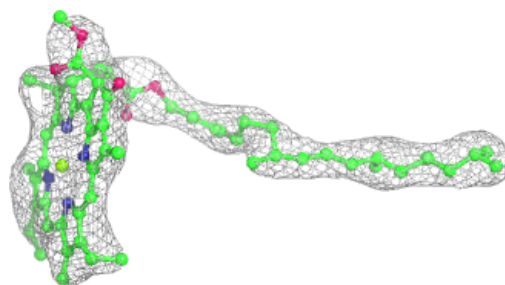
**Electron density around CLA a 835:**

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

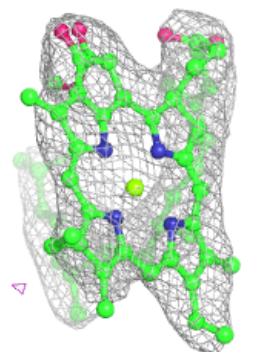
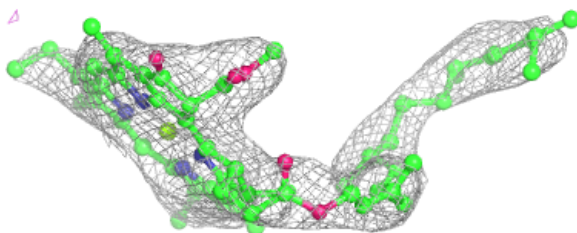
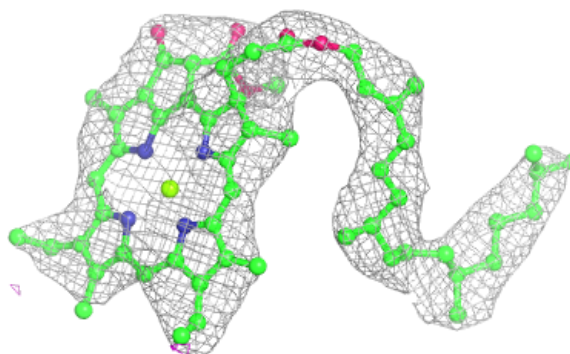


**Electron density around CLA B 828:**

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

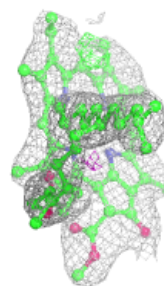
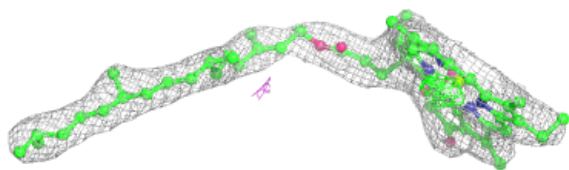
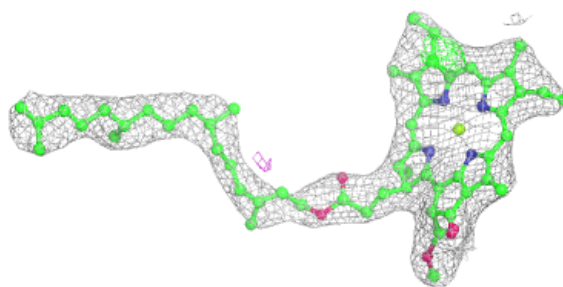
**Electron density around CLA b 824:**

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



**Electron density around CLA A 803:**

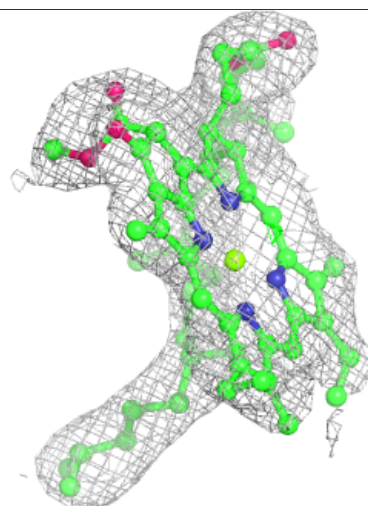
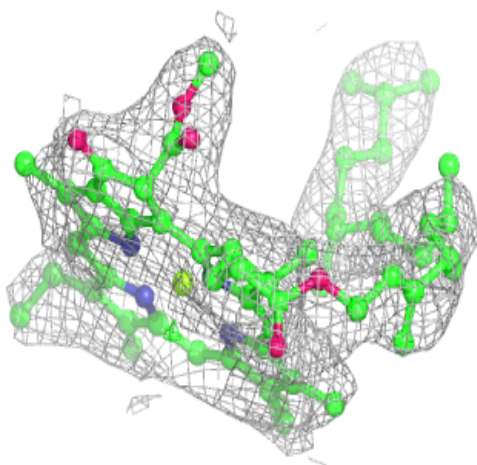
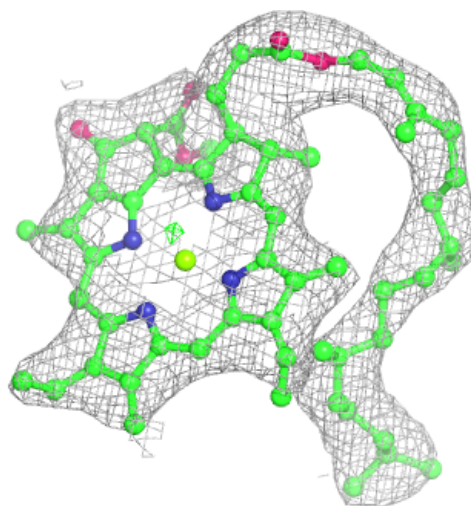
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





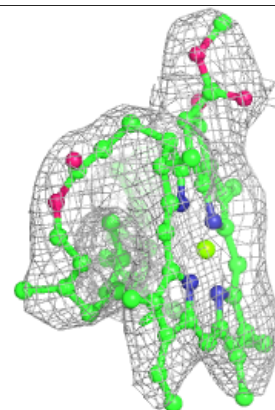
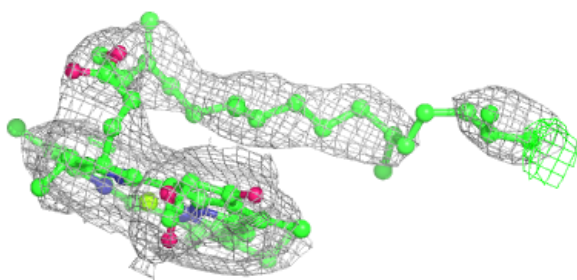
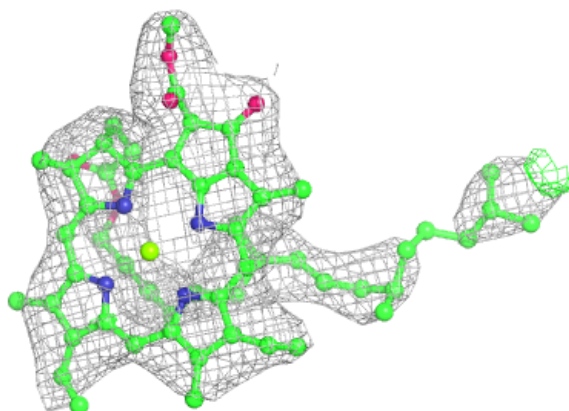
**Electron density around CLA a 814:**

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



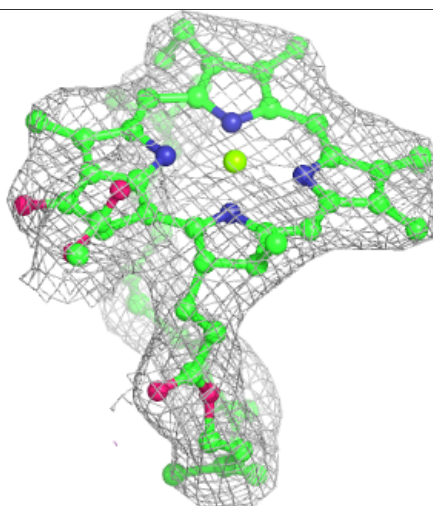
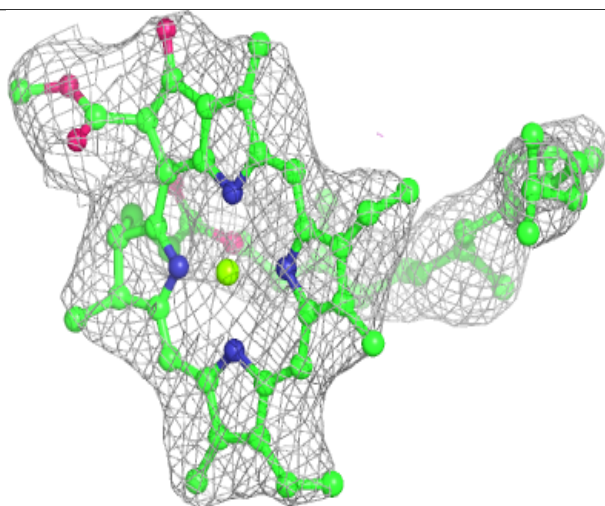
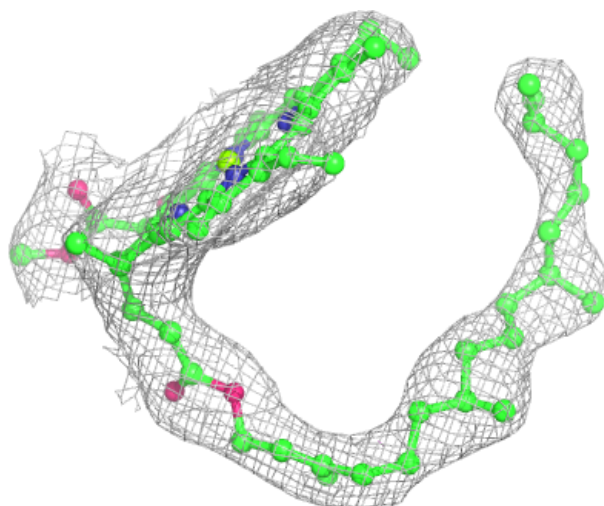
**Electron density around CLA b 827:**

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



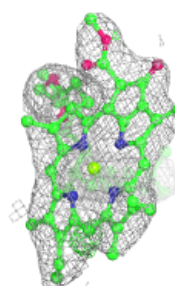
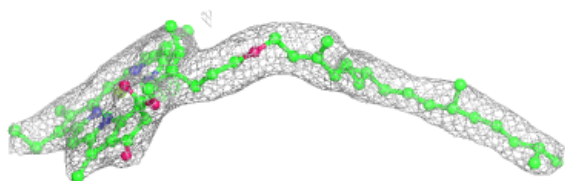
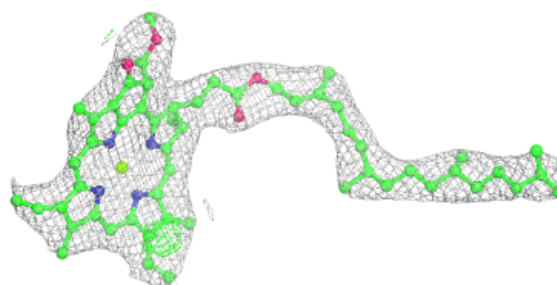
**Electron density around CLA B 819:**

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

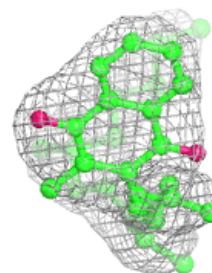
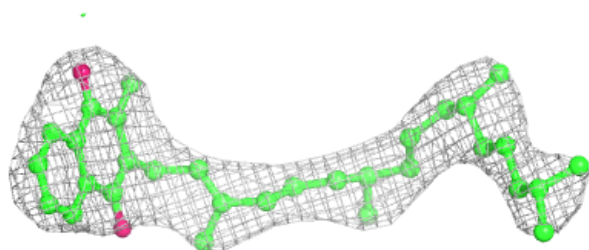
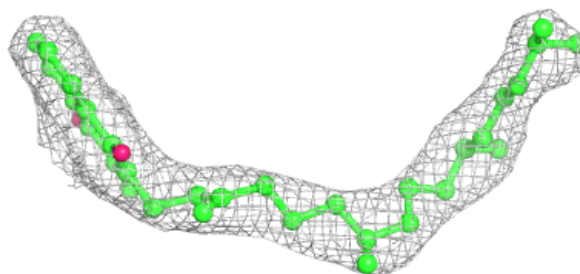


**Electron density around CLA a 803:**

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

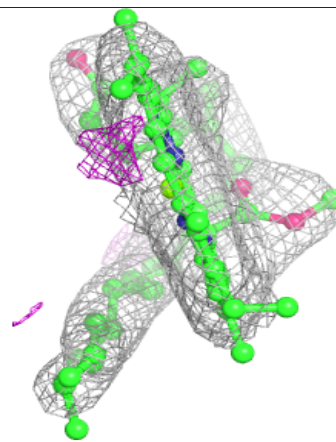
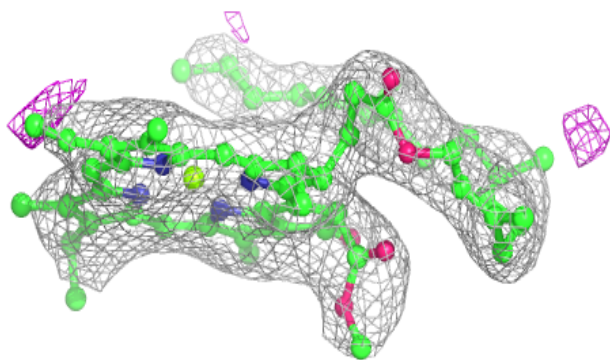
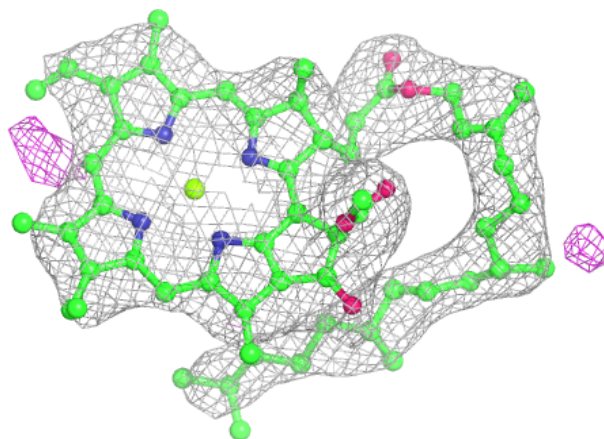
**Electron density around PQN b 842:**

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



**Electron density around CLA B 805:**

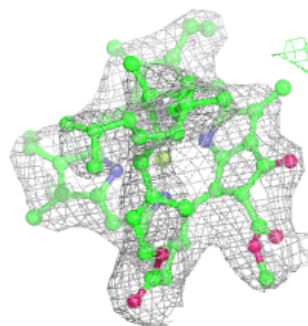
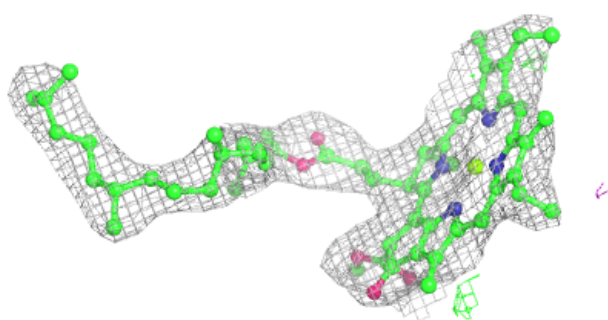
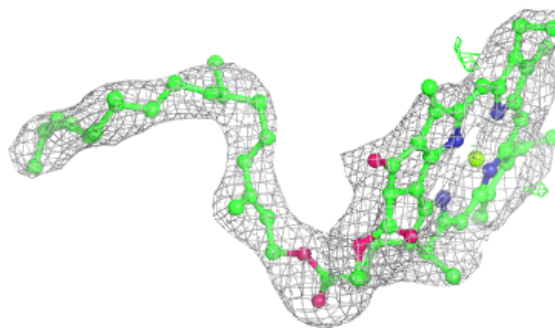
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



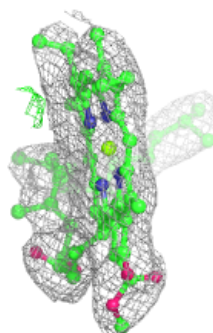
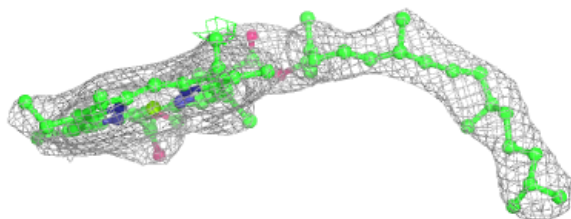
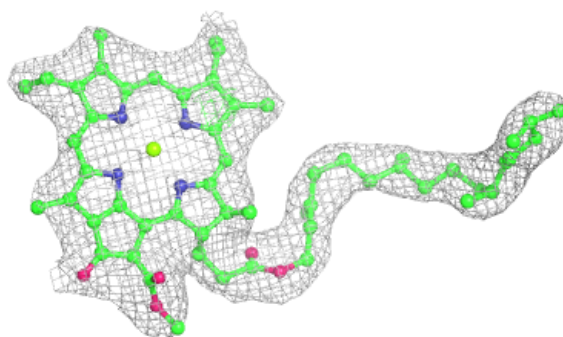


**Electron density around CLA b 802:**

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

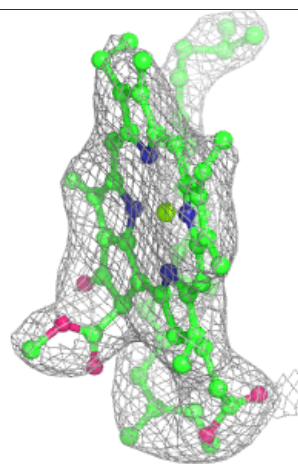
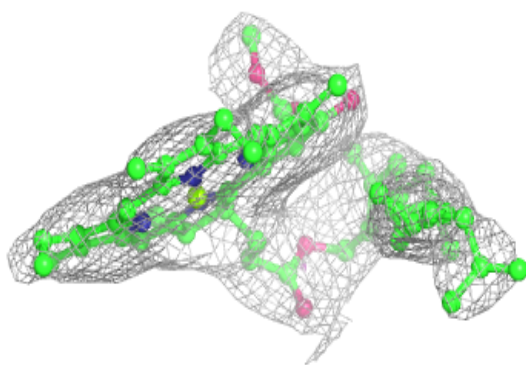
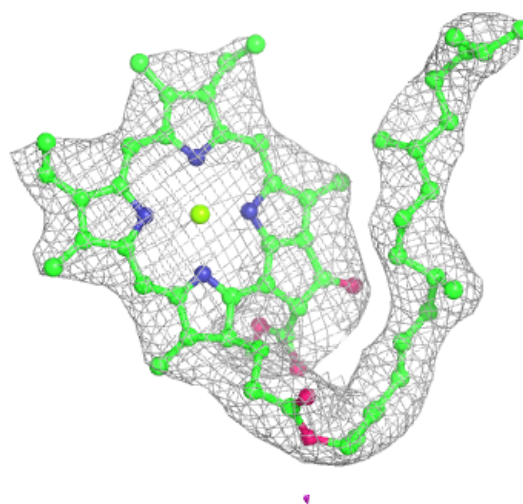
**Electron density around CLA b 803:**

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



**Electron density around CLA a 826:**

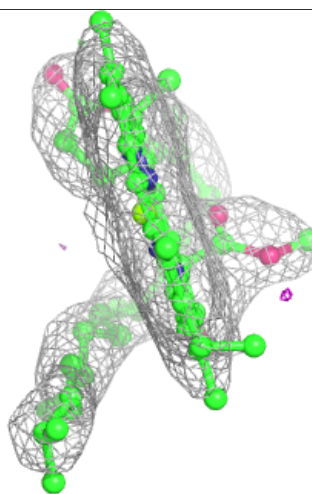
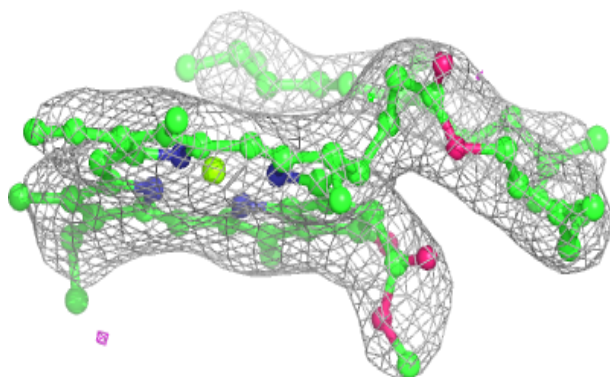
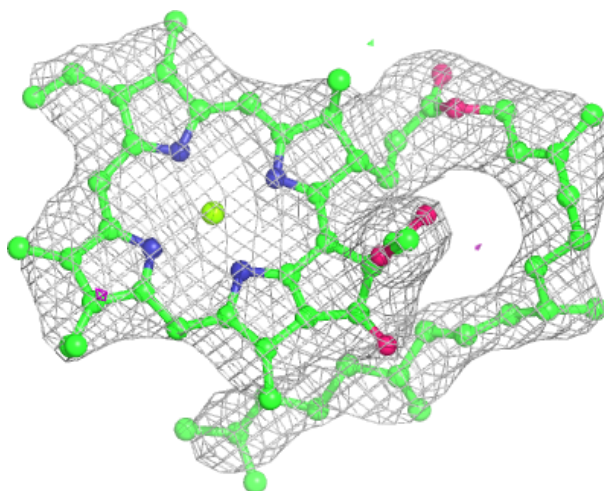
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





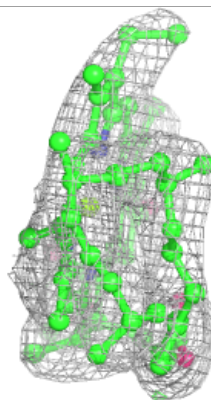
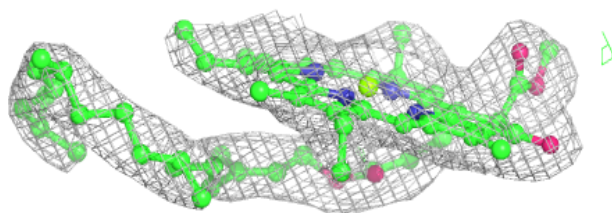
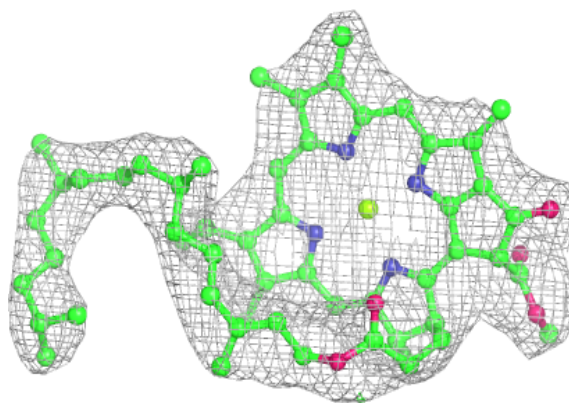
**Electron density around CLA b 805:**

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

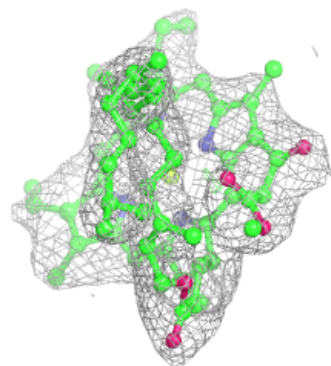
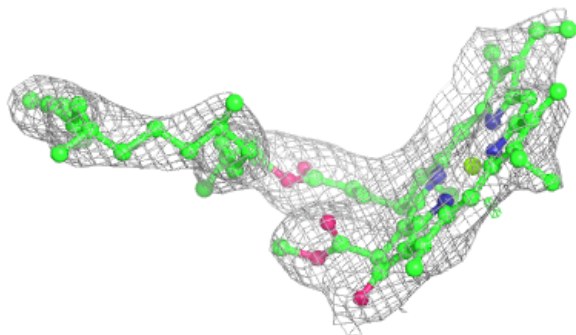
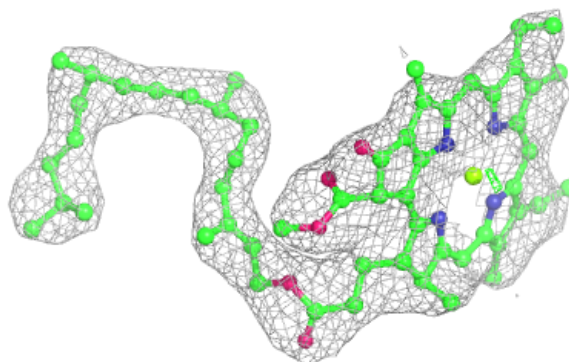


**Electron density around CLA a 820:**

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

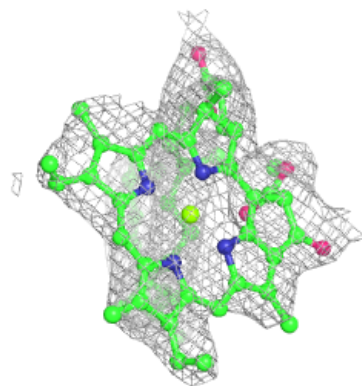
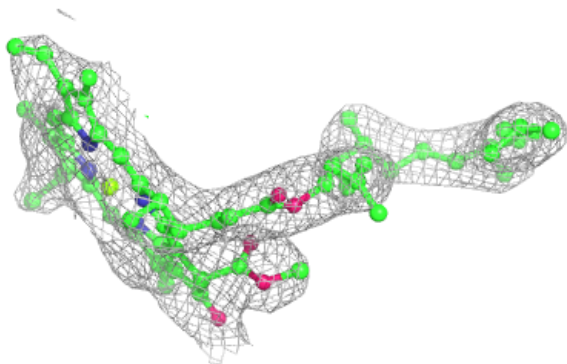
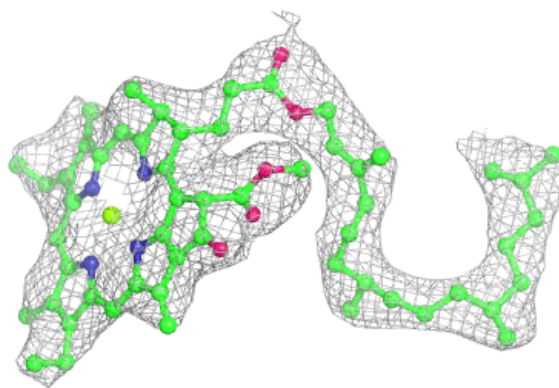
**Electron density around CLA A 801:**

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

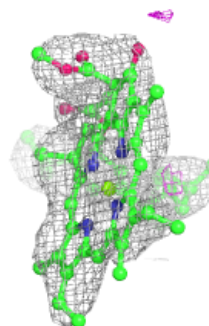
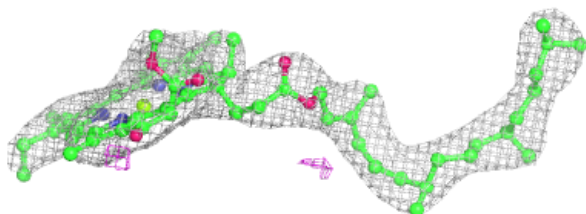
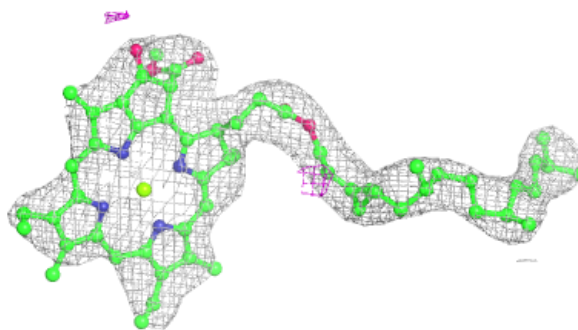


**Electron density around CLA a 801:**

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

**Electron density around CLA B 813:**

$2mF_o-DF_c$  (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.