



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 11, 2021 – 12:33 AM JST

PDB ID : 7DKZ
Title : Structure of plant photosystem I-light harvesting complex I supercomplex
Authors : Wang, J.; Yu, L.J.; Wang, W.
Deposited on : 2020-11-25
Resolution : 2.39 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.22
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.22

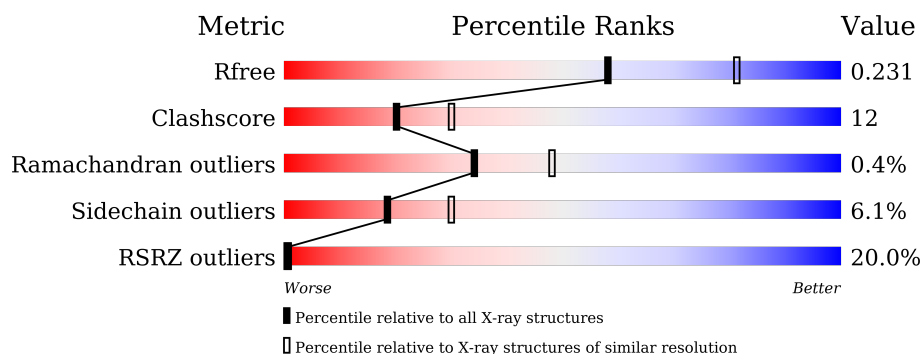
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	1	195	<div> <div>18%</div> <div> <div>75%</div> <div>22%</div> <div>..</div> </div> </div>
2	2	269	<div> <div>21%</div> <div> <div>54%</div> <div>19%</div> <div>•</div> <div>24%</div> </div> </div>
3	3	275	<div> <div>35%</div> <div> <div>65%</div> <div>13%</div> <div>•</div> <div>21%</div> </div> </div>
4	4	198	<div> <div>10%</div> <div> <div>78%</div> <div>18%</div> <div>•</div> <div>•</div> </div> </div>
5	A	758	<div> <div>24%</div> <div> <div>77%</div> <div>19%</div> <div>•</div> <div>•</div> </div> </div>
6	B	734	<div> <div>10%</div> <div> <div>81%</div> <div>17%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
7	C	81	
8	D	143	
9	E	66	
10	F	154	
11	G	97	
12	H	88	
13	I	40	
14	J	42	
15	L	157	
16	K	80	

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	301	X	-	-	-
17	CLA	1	302	X	-	-	-
17	CLA	1	303	X	-	-	-
17	CLA	1	304	X	-	-	-
17	CLA	1	306	X	-	-	-
17	CLA	1	307	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	2	301	X	-	-	-
17	CLA	2	302	X	-	-	-
17	CLA	2	303	X	-	-	-
17	CLA	2	307	X	-	-	-
17	CLA	2	308	X	-	-	-
17	CLA	2	309	X	-	-	-
17	CLA	2	310	X	-	-	-
17	CLA	2	311	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	2	312	X	-	-	-
17	CLA	2	319	X	-	-	-
17	CLA	3	602	X	-	-	-
17	CLA	3	603	X	-	-	-
17	CLA	3	604	X	-	-	-
17	CLA	3	605	X	-	-	-
17	CLA	3	606	X	-	-	-
17	CLA	3	608	X	-	-	-
17	CLA	3	609	X	-	-	-
17	CLA	3	610	X	-	-	-
17	CLA	3	611	X	-	-	-
17	CLA	3	612	X	-	-	-
17	CLA	3	613	X	-	-	-
17	CLA	4	302	X	-	-	-
17	CLA	4	304	X	-	-	-
17	CLA	4	308	X	-	-	-
17	CLA	4	309	X	-	-	-
17	CLA	4	310	X	-	-	-
17	CLA	4	312	X	-	-	-
17	CLA	4	313	X	-	-	-
17	CLA	4	314	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
17	CLA	A	838	X	-	-	-
17	CLA	A	839	X	-	-	-
17	CLA	A	840	X	-	-	-
17	CLA	A	841	X	-	-	-
17	CLA	A	843	X	-	-	-
17	CLA	A	853	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	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B	823	X	-	-	-
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	B	842	X	-	-	-
17	CLA	F	304	X	-	-	-
17	CLA	F	306	X	-	-	-
17	CLA	F	307	X	-	-	-
17	CLA	G	103	X	-	-	-
17	CLA	G	104	X	-	-	-
17	CLA	G	105	X	-	-	-
17	CLA	J	101	X	-	-	-
17	CLA	J	103	X	-	-	-
17	CLA	K	201	X	-	-	-
17	CLA	K	202	X	-	-	-
17	CLA	L	202	X	-	-	-
17	CLA	L	203	X	-	-	-
18	CHL	1	305	X	-	-	-
18	CHL	2	304	X	-	-	-
18	CHL	2	305	X	-	-	-
18	CHL	2	306	X	-	-	-
18	CHL	2	313	X	-	-	-
18	CHL	3	601	X	-	-	-
18	CHL	3	607	X	-	-	-
18	CHL	4	301	X	-	-	-
18	CHL	4	305	X	-	-	-
18	CHL	4	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CHL	4	307	X	-	-	-
18	CHL	4	315	X	-	-	-
19	LUT	4	316	-	X	-	-
20	XAT	4	317	X	-	-	-
21	BCR	2	316	-	-	-	X
21	BCR	3	616	-	-	-	X
21	BCR	K	203	-	-	-	X
22	LHG	G	102	-	-	-	X
24	LMG	G	101	-	-	-	X
26	DGD	4	323	-	-	X	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 36093 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 Lhca1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	195	Total	C	N	O	S	0	0	0
			1507	979	252	271	5			

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	204	Total	C	N	O	S	0	0	0
			1592	1042	261	285	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	216	Total	C	N	O	S	0	0	0
			1661	1088	268	300	5			

- Molecule 4 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	195	Total	C	N	O	S	0	0	0
			1535	1006	249	277	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	89	LYS	ARG	conflict	UNP Q9SQL2
4	128	ASP	ALA	conflict	UNP Q9SQL2
4	149	PHE	SER	conflict	UNP Q9SQL2

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	742	Total	C	N	O	S	0	0	0
			5852	3835	997	1002	18			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	ILE	VAL	conflict	UNP A0A0F6NFW5

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	733	Total	C	N	O	S	0	0	0
			5856	3848	998	996	14			

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	C	80	Total	C	N	O	S	0	0	0
			611	379	107	114	11			

- Molecule 8 is a protein called PsaD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	D	140	Total	C	N	O	S	0	0	0
			1110	716	191	200	3			

- Molecule 9 is a protein called PsaE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	E	63	Total	C	N	O	0	0	0
			505	320	89	96			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	PRO	-	expression tag	UNP E1C9K6
E	0	PRO	-	expression tag	UNP E1C9K6
E	14	GLN	LYS	conflict	UNP E1C9K6
E	60	VAL	-	expression tag	UNP E1C9K6
E	61	GLU	-	expression tag	UNP E1C9K6
E	62	GLU	-	expression tag	UNP E1C9K6
E	63	VAL	-	expression tag	UNP E1C9K6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	64	LYS	-	expression tag	UNP E1C9K6

- Molecule 10 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	F	152	Total	C	N	O	S	0	0	0
			1198	777	208	211	2			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	79	ALA	SER	conflict	UNP A0A0M3KL12
F	86	ASP	GLU	conflict	UNP A0A0M3KL12
F	107	LEU	ILE	conflict	UNP A0A0M3KL12
F	110	PRO	ALA	conflict	UNP A0A0M3KL12
F	133	GLY	ALA	conflict	UNP A0A0M3KL12
F	187	ASP	GLU	conflict	UNP A0A0M3KL12
F	203	THR	SER	conflict	UNP A0A0M3KL12

- Molecule 11 is a protein called PsaG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	G	95	Total	C	N	O		0	0	0
			737	477	122	138				

- Molecule 12 is a protein called PsaH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	H	88	Total	C	N	O		0	0	0
			673	442	106	125				

- Molecule 13 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	I	30	Total	C	N	O	S	0	0	0
			226	156	34	35	1			

- Molecule 14 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	J	39	Total	C	N	O	S	0	0	0
			309	208	48	52	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	32	PHE	LEU	conflict	UNP D5MAL3

- Molecule 15 is a protein called PsaL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	L	151	Total	C	N	O	S	0	0	0
			1122	737	182	202	1			

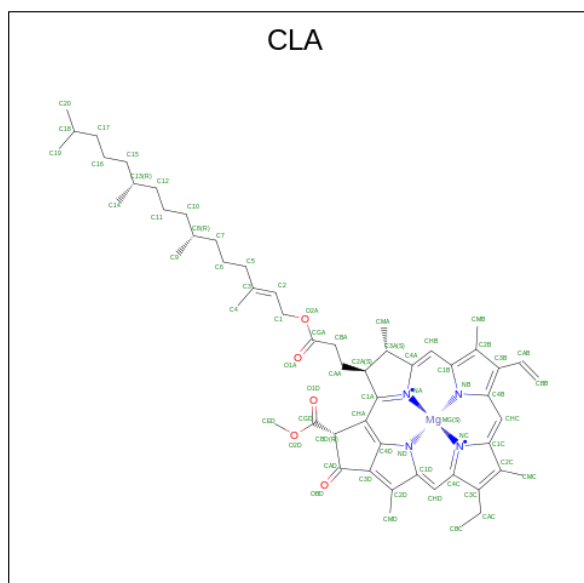
- Molecule 16 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	K	77	Total	C	N	O	S	0	0	0
			515	326	86	100	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	85	ALA	VAL	conflict	UNP E1C9L3

- Molecule 17 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	1	1	Total	C	Mg	N	O	0	0
			46	36	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
			51	41	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
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	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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
			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	4	1	Total	C	Mg	N	O	0	0
			60	50	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
			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
			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
			47	37	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
			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
			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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		
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
			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
			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		

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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	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	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
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	B	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
17	B	1	Total 55	C 45	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 55	C 45	Mg 1	N 4	O 5	0	0
17	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
17	B	1	Total 59	C 49	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

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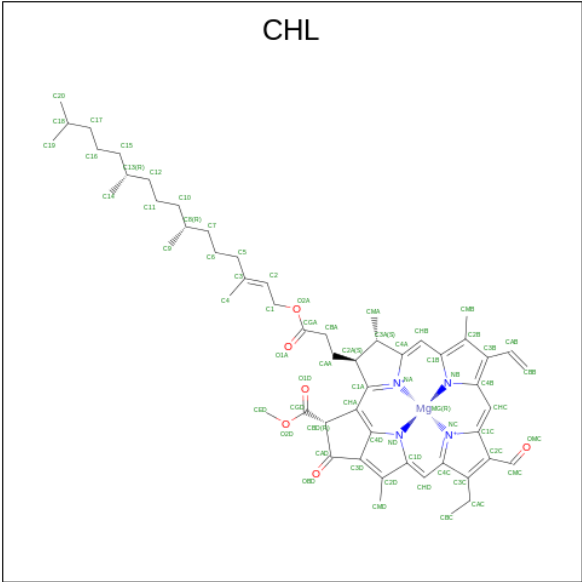
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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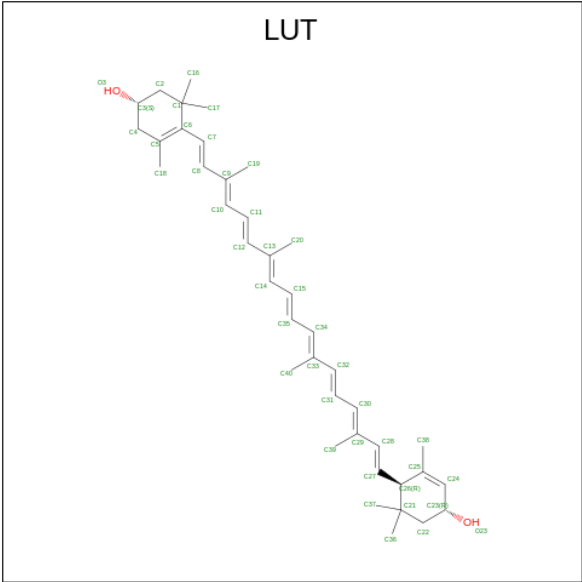
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	F	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	G	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	G	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	G	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	J	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	K	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		

- Molecule 18 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



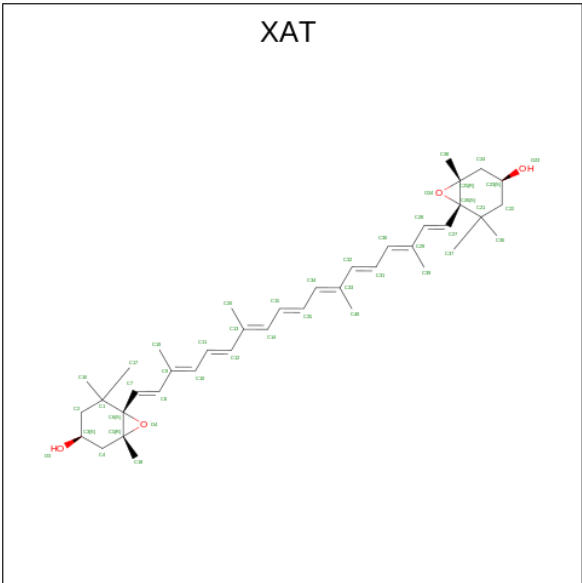
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	1	1	Total 48	C 37	Mg 1	N 4	O 6	0	0
18	2	1	Total 43	C 34	Mg 1	N 4	O 4	0	0
18	2	1	Total 48	C 37	Mg 1	N 4	O 6	0	0
18	2	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
18	2	1	Total 43	C 34	Mg 1	N 4	O 4	0	0
18	3	1	Total 56	C 45	Mg 1	N 4	O 6	0	0
18	3	1	Total 47	C 36	Mg 1	N 4	O 6	0	0
18	4	1	Total 61	C 50	Mg 1	N 4	O 6	0	0
18	4	1	Total 56	C 45	Mg 1	N 4	O 6	0	0
18	4	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
18	4	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
18	4	1	Total 43	C 34	Mg 1	N 4	O 4	0	0

- Molecule 19 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



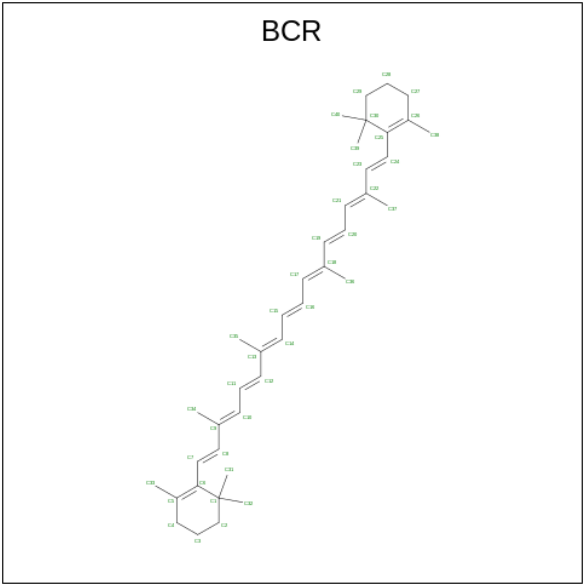
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	1	1	Total	C	O	0	0
			42	40	2		
19	2	1	Total	C	O	0	0
			42	40	2		
19	3	1	Total	C	O	0	0
			42	40	2		
19	4	1	Total	C	O	0	0
			42	40	2		

- Molecule 20 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: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	1	1	Total	C	O	0	0
			44	40	4		
20	2	1	Total	C	O	0	0
			44	40	4		
20	3	1	Total	C	O	0	0
			44	40	4		
20	4	1	Total	C	O	0	0
			44	40	4		

- Molecule 21 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



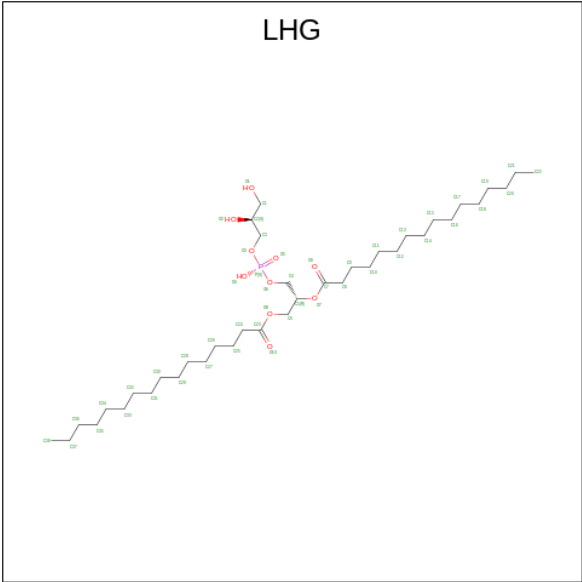
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	1	1	Total	C	0	0
			40	40		
21	2	1	Total	C	0	0
			40	40		
21	3	1	Total	C	0	0
			40	40		
21	4	1	Total	C	0	0
			40	40		
21	A	1	Total	C	0	0
			40	40		
21	A	1	Total	C	0	0
			40	40		
21	A	1	Total	C	0	0
			40	40		
21	A	1	Total	C	0	0
			40	40		

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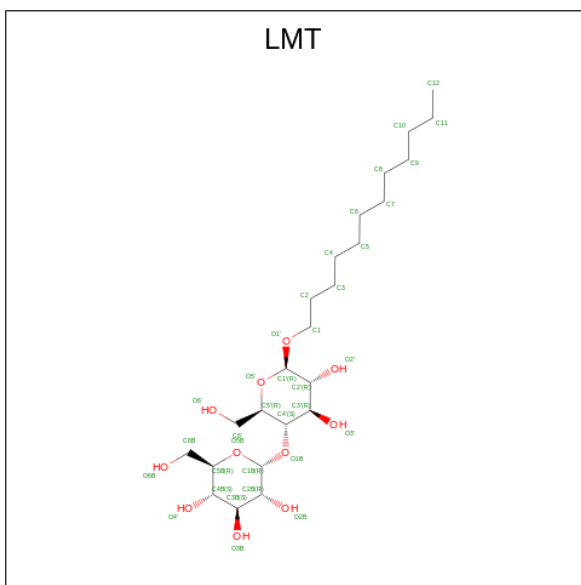
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	F	1	Total C 40 40	0	0
21	F	1	Total C 40 40	0	0
21	G	1	Total C 40 40	0	0
21	I	1	Total C 40 40	0	0
21	J	1	Total C 40 40	0	0
21	J	1	Total C 40 40	0	0
21	L	1	Total C 40 40	0	0
21	L	1	Total C 40 40	0	0
21	L	1	Total C 40 40	0	0
21	K	1	Total C 40 40	0	0

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



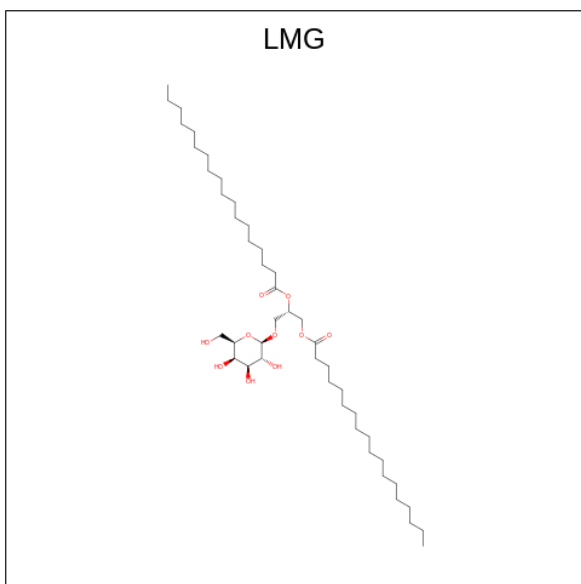
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	1	1	Total	C	O	P	0	0
			49	38	10	1		
22	2	1	Total	C	O	P	0	0
			37	26	10	1		
22	A	1	Total	C	O	P	0	0
			49	38	10	1		
22	A	1	Total	C	O	P	0	0
			27	16	10	1		
22	B	1	Total	C	O	P	0	0
			23	12	10	1		
22	F	1	Total	C	O	P	0	0
			40	29	10	1		
22	G	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 23 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	2	1	Total 35	C 24	O 11	0	0
23	A	1	Total 35	C 24	O 11	0	0

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



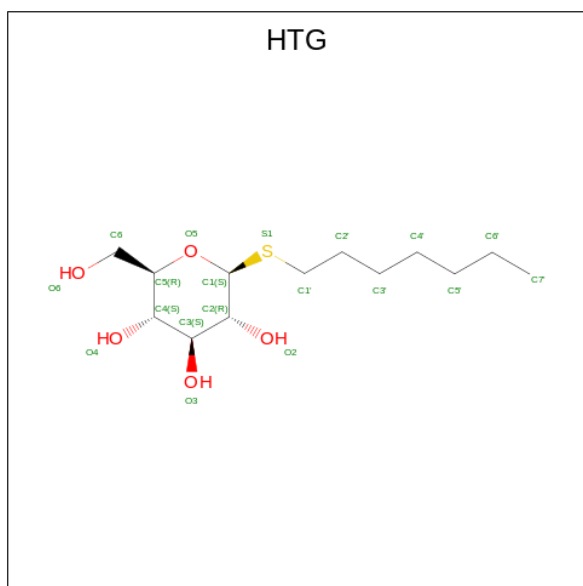
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	4	1	Total	C	O	0	0
			50	40	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	4	1	Total	C	O	0	0
			49	39	10		
24	B	1	Total	C	O	0	0
			52	42	10		
24	F	1	Total	C	O	0	0
			55	45	10		
24	G	1	Total	C	O	0	0
			40	30	10		

- Molecule 25 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



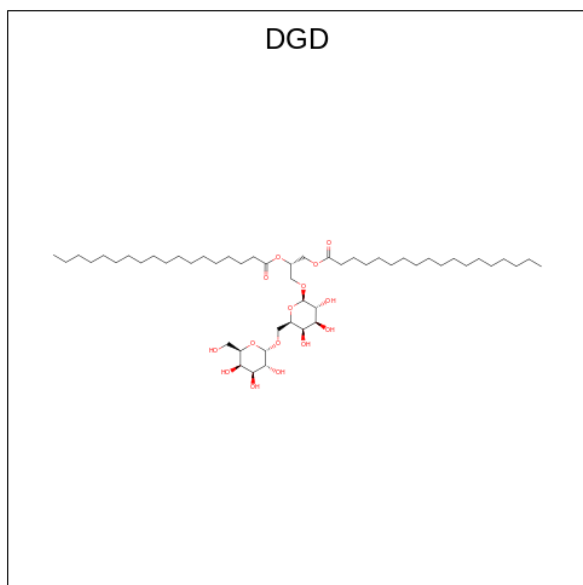
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	4	1	Total	C	O	S	0	0
			19	13	5	1		
25	4	1	Total	C	O	S	0	0
			19	13	5	1		
25	A	1	Total	C	O	S	0	0
			19	13	5	1		
25	B	1	Total	C	O	S	0	0
			19	13	5	1		
25	F	1	Total	C	O	S	0	0
			17	11	5	1		
25	F	1	Total	C	O	S	0	0
			19	13	5	1		
25	F	1	Total	C	O	S	0	0
			16	10	5	1		

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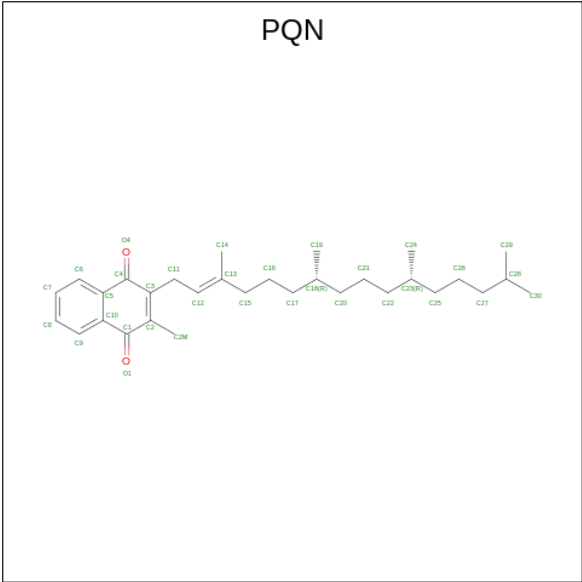
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	J	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



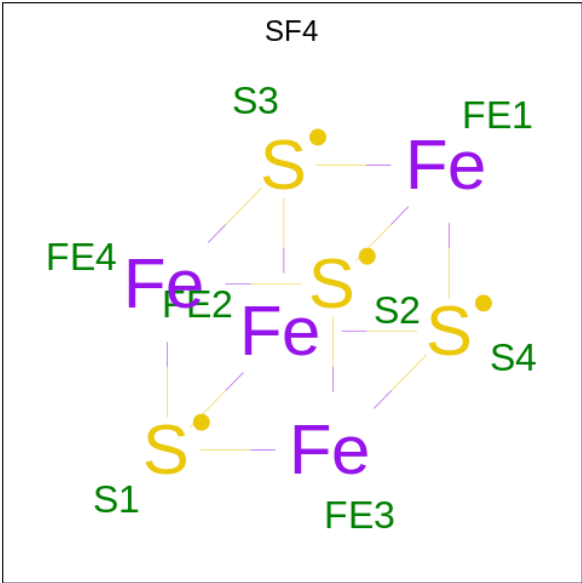
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	4	1	Total	C	O	0	0
			60	45	15		
26	B	1	Total	C	O	0	0
			66	51	15		

- Molecule 27 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 28 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	Fe	S	0	0
			8	4	4		
28	C	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	C	1	Total	Fe	S	0	0
			8	4	4		

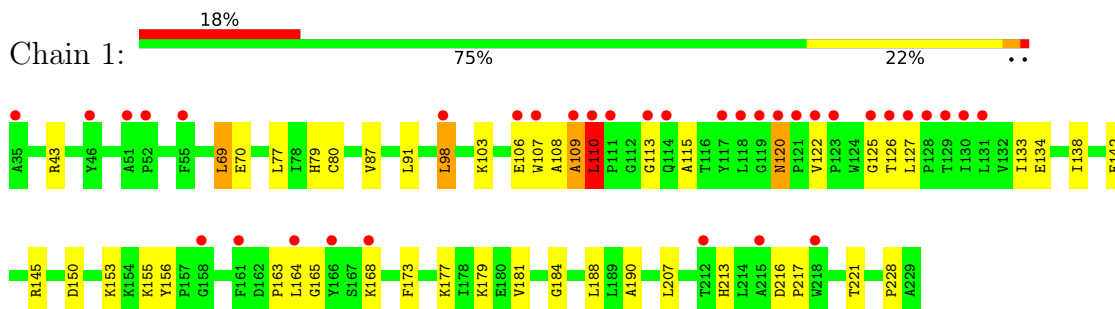
- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	1	3	Total	O	0	0
			3	3		
29	2	5	Total	O	0	0
			5	5		
29	3	3	Total	O	0	0
			3	3		
29	4	7	Total	O	0	0
			7	7		
29	A	25	Total	O	0	0
			25	25		
29	B	39	Total	O	0	0
			39	39		
29	C	3	Total	O	0	0
			3	3		
29	F	5	Total	O	0	0
			5	5		
29	G	1	Total	O	0	0
			1	1		
29	J	1	Total	O	0	0
			1	1		
29	L	1	Total	O	0	0
			1	1		

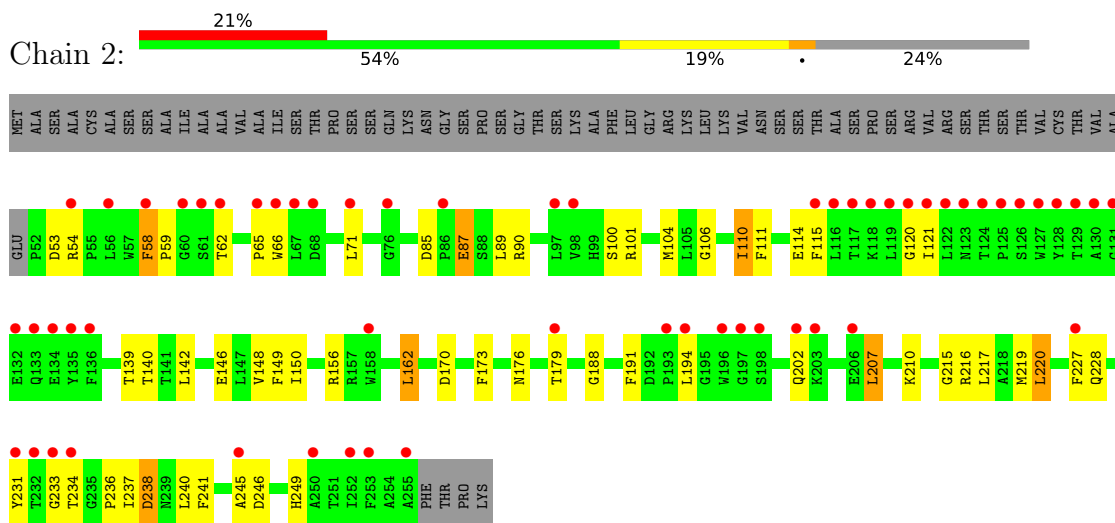
3 Residue-property plots

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

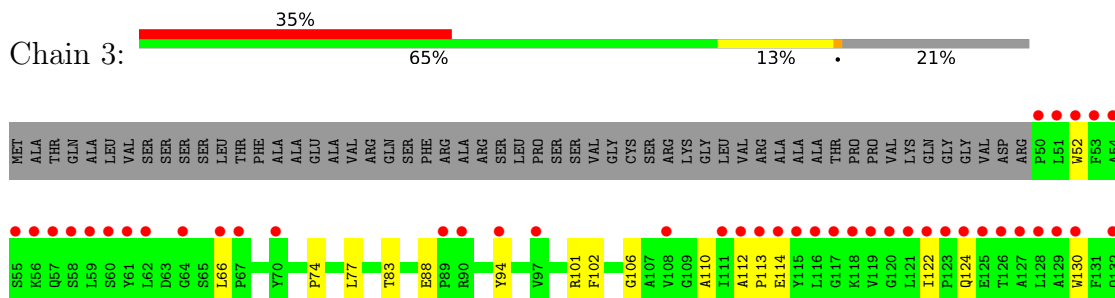
- Molecule 1: Lhca1

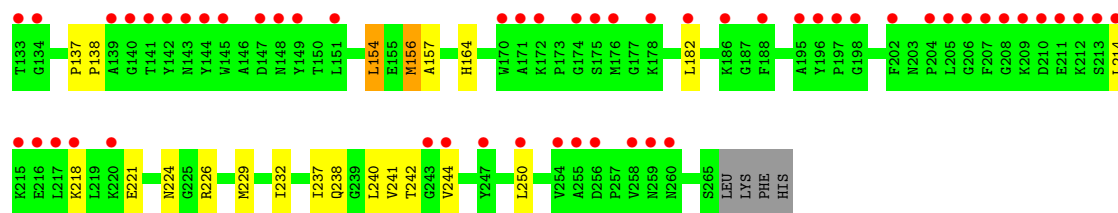


- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

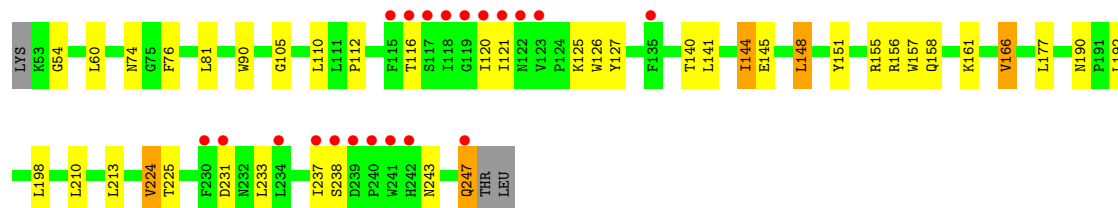
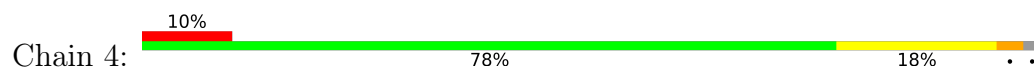


- Molecule 3: Chlorophyll a-b binding protein 3, chloroplastic

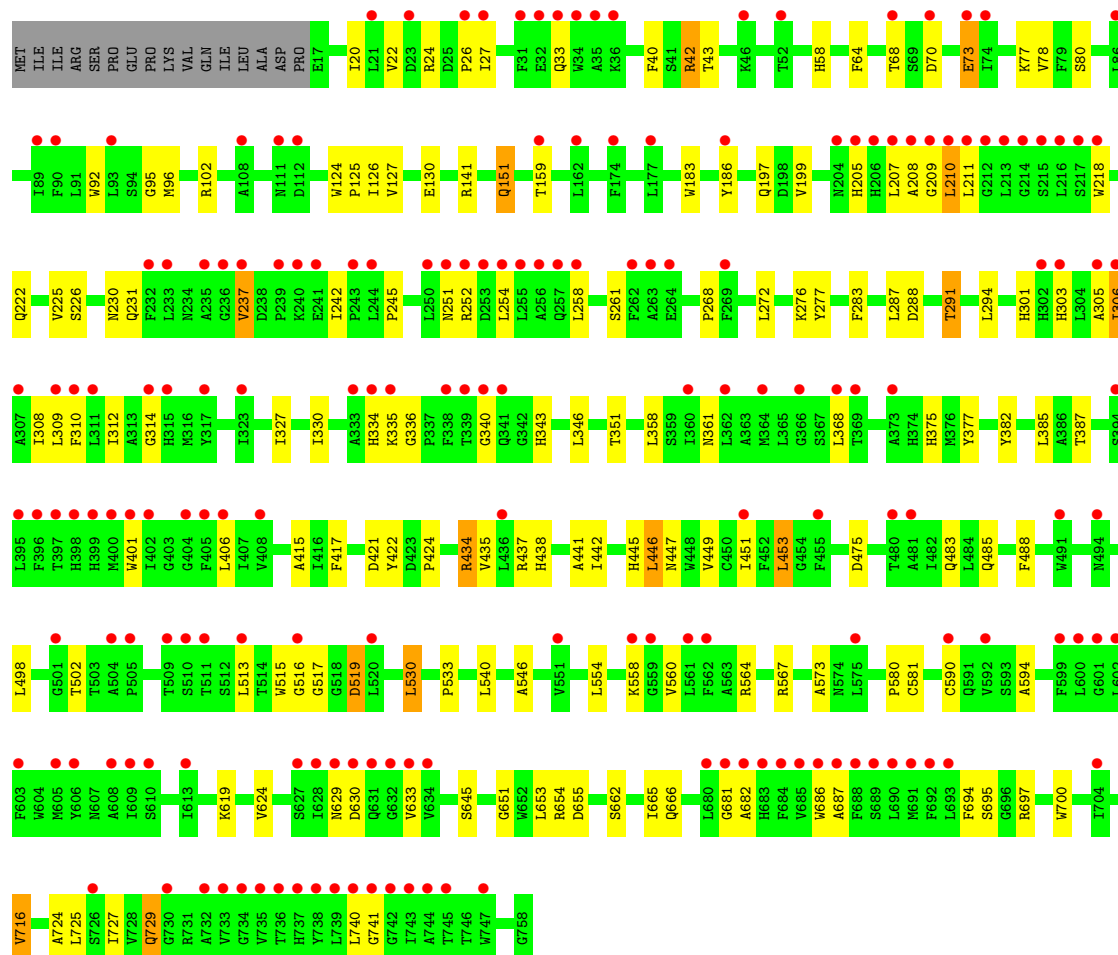
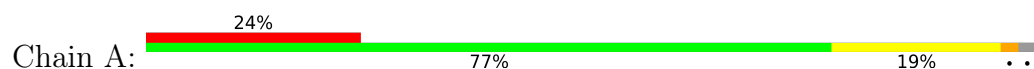




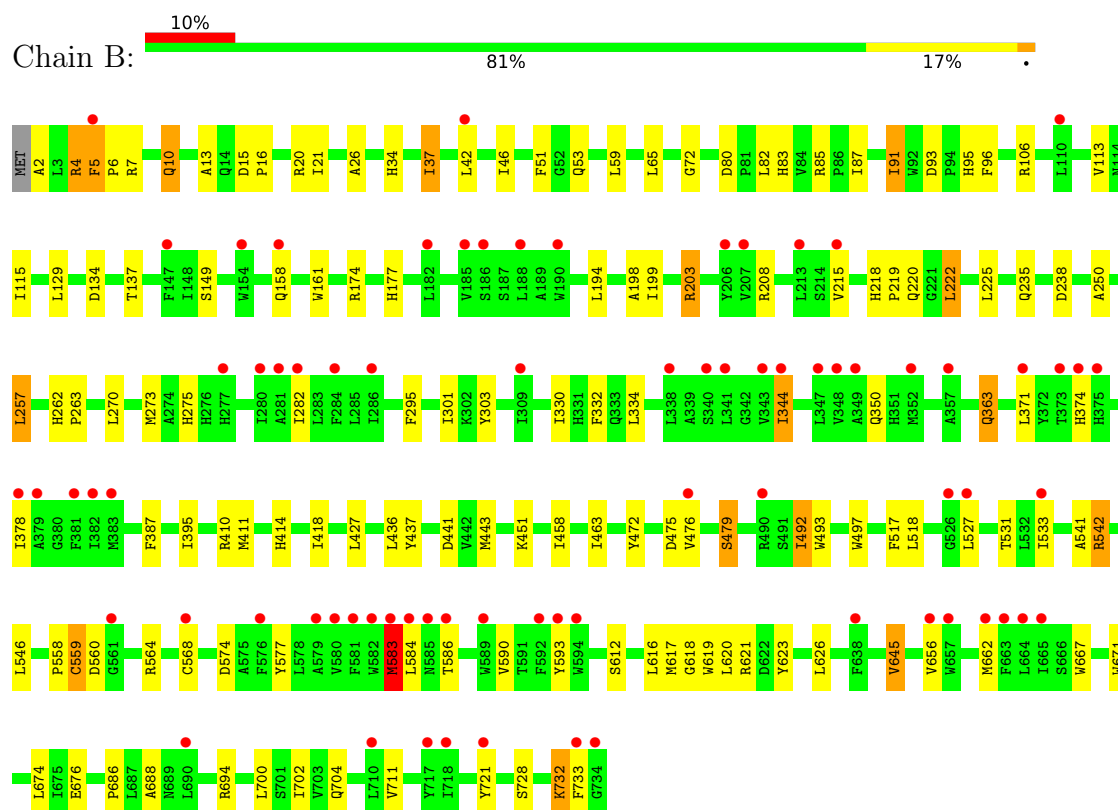
● Molecule 4: Chlorophyll a-b binding protein P4, chloroplastic



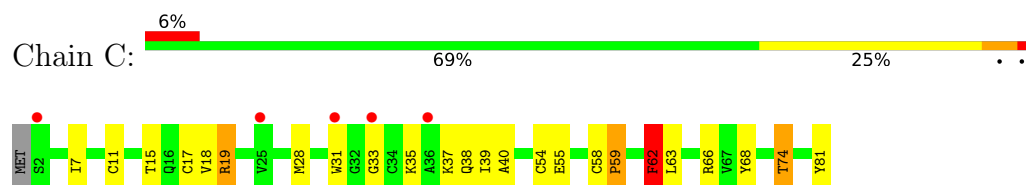
● Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1



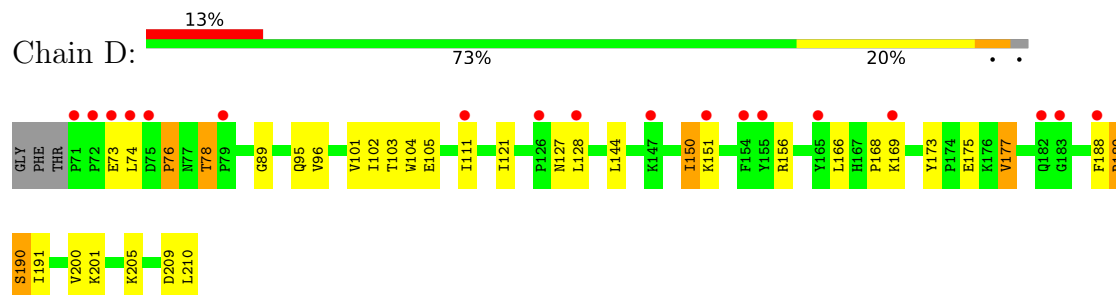
• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2



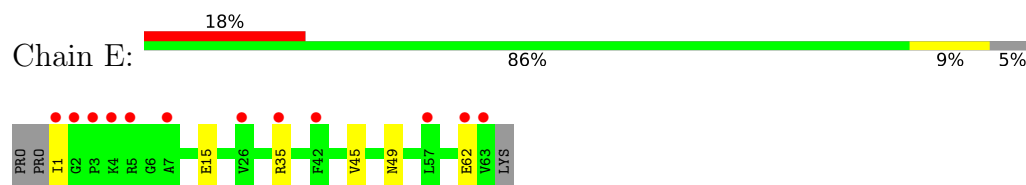
• Molecule 7: Photosystem I iron-sulfur center



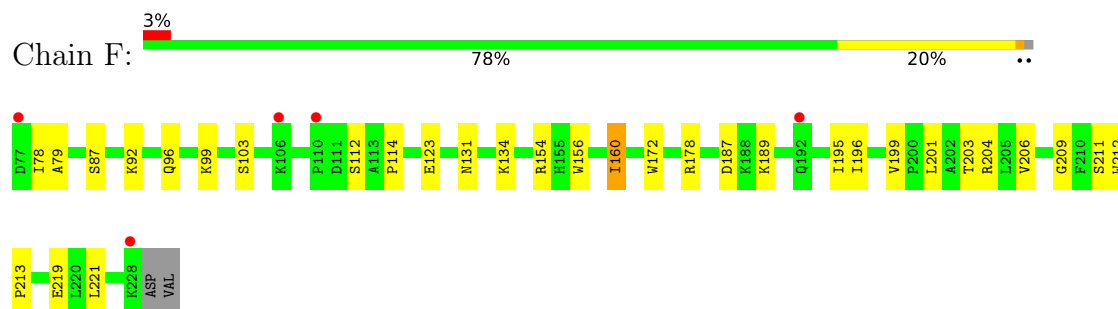
• Molecule 8: PsaD



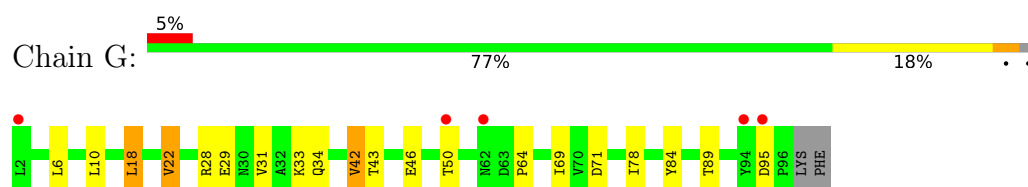
• Molecule 9: PsaE



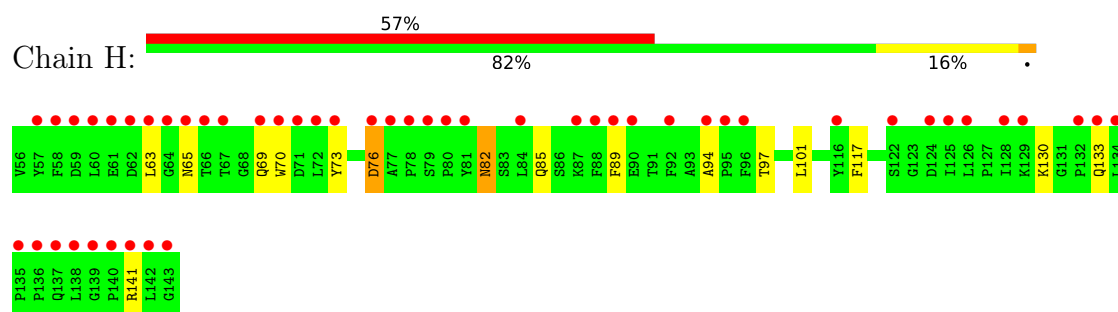
- Molecule 10: PSI-F



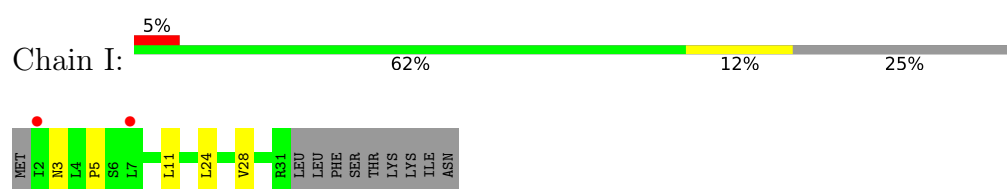
- Molecule 11: PsaG



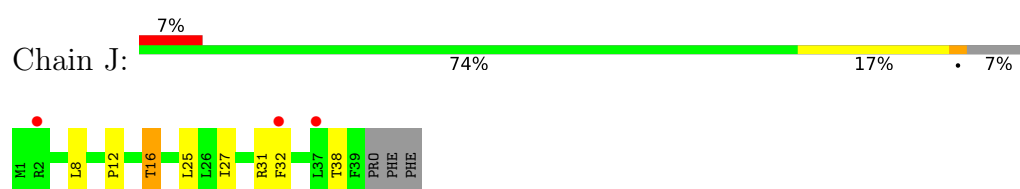
- Molecule 12: PsaH



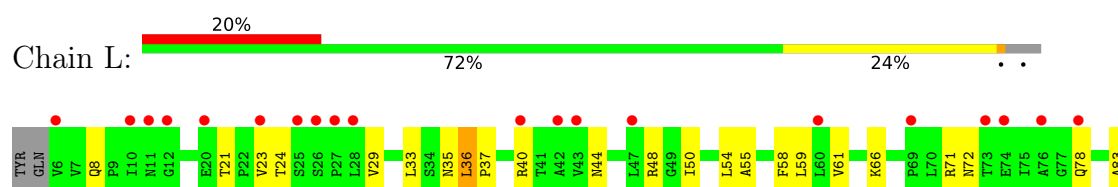
- Molecule 13: Photosystem I reaction center subunit VIII

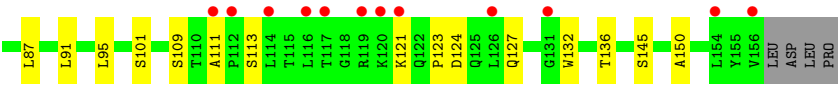


- Molecule 14: Photosystem I reaction center subunit IX

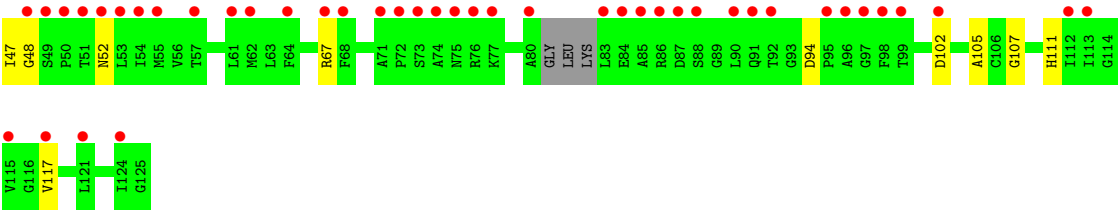
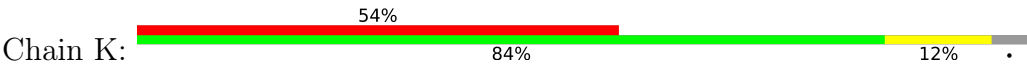


- Molecule 15: PsaL





● Molecule 16: PSI-K



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	225.65Å 168.95Å 185.22Å 90.00° 121.39° 90.00°	Depositor
Resolution (Å)	44.41 – 2.39 44.41 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.9 (44.41-2.39) 99.0 (44.41-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.189 , 0.227 0.194 , 0.231	Depositor DCC
R_{free} test set	11616 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	65.4	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 80.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	36093	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1	0.37	0/1557	0.53	1/2127 (0.0%)
2	2	0.30	0/1651	0.46	0/2262
3	3	0.28	0/1713	0.42	0/2326
4	4	0.49	0/1584	0.62	0/2159
5	A	0.37	0/6050	0.50	0/8254
6	B	0.50	0/6068	0.65	2/8286 (0.0%)
7	C	0.79	2/624 (0.3%)	0.91	3/846 (0.4%)
8	D	0.41	0/1140	0.58	0/1540
9	E	0.47	0/515	0.57	0/700
10	F	0.47	0/1226	0.66	0/1658
11	G	0.49	0/755	0.54	0/1027
12	H	0.30	0/693	0.43	0/942
13	I	0.33	0/232	0.47	0/317
14	J	0.43	0/317	0.58	0/432
15	L	0.30	0/1153	0.45	0/1576
16	K	0.26	0/520	0.45	0/707
All	All	0.42	2/25798 (0.0%)	0.56	6/35159 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	C	1	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	59	PRO	N-CA	13.00	1.69	1.47
7	C	58	CYS	C-N	5.11	1.44	1.34

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	62	PHE	CB-CA-C	11.16	132.72	110.40
6	B	542	ARG	NE-CZ-NH2	-7.77	116.42	120.30
6	B	583	MET	CG-SD-CE	7.34	111.94	100.20
1	1	110	LEU	CA-CB-CG	7.14	131.73	115.30
7	C	59	PRO	CA-N-CD	-6.16	102.88	111.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	C	62	PHE	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1507	0	1468	35	0
2	2	1592	0	1531	50	0
3	3	1661	0	1620	31	0
4	4	1535	0	1496	40	0
5	A	5852	0	5713	109	0
6	B	5856	0	5653	111	0
7	C	611	0	591	18	0
8	D	1110	0	1123	18	0
9	E	505	0	503	3	0
10	F	1198	0	1228	19	0
11	G	737	0	721	14	0
12	H	673	0	667	12	0
13	I	226	0	242	3	0
14	J	309	0	320	8	0
15	L	1122	0	1133	27	0
16	K	515	0	513	5	0
17	1	672	0	636	39	0
17	2	533	0	480	26	0
17	3	542	0	433	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	4	540	0	476	28	0
17	A	2582	0	2646	146	0
17	B	2493	0	2566	130	0
17	F	165	0	154	8	0
17	G	137	0	101	10	0
17	J	107	0	103	9	0
17	K	105	0	92	4	0
17	L	180	0	183	14	0
18	1	48	0	33	6	0
18	2	185	0	128	12	0
18	3	103	0	72	19	0
18	4	262	0	207	31	0
19	1	42	0	56	9	0
19	2	42	0	56	4	0
19	3	42	0	56	4	0
19	4	42	0	56	4	0
20	1	44	0	56	3	0
20	2	44	0	56	10	0
20	3	44	0	56	13	0
20	4	44	0	56	10	0
21	1	40	0	56	0	0
21	2	40	0	56	8	0
21	3	40	0	56	4	0
21	4	40	0	56	14	0
21	A	240	0	336	26	0
21	B	240	0	336	24	0
21	F	80	0	112	4	0
21	G	40	0	56	2	0
21	I	40	0	56	4	0
21	J	80	0	112	8	0
21	K	40	0	56	4	0
21	L	120	0	168	11	0
22	1	49	0	74	6	0
22	2	37	0	44	7	0
22	A	76	0	98	3	0
22	B	23	0	16	1	0
22	F	40	0	53	2	0
22	G	49	0	74	2	0
23	2	35	0	46	3	0
23	A	35	0	45	2	0
24	4	99	0	143	7	0
24	B	52	0	77	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	F	55	0	86	1	0
24	G	40	0	53	3	0
25	4	38	0	52	4	0
25	A	19	0	26	0	0
25	B	19	0	26	1	0
25	F	52	0	62	2	0
25	J	19	0	26	3	0
26	4	60	0	81	29	0
26	B	66	0	96	7	0
27	A	33	0	46	6	0
27	B	33	0	46	3	0
28	A	8	0	0	0	0
28	C	16	0	0	0	0
29	1	3	0	0	0	0
29	2	5	0	0	0	0
29	3	3	0	0	0	0
29	4	7	0	0	0	0
29	A	25	0	0	1	0
29	B	39	0	0	2	0
29	C	3	0	0	0	0
29	F	5	0	0	0	0
29	G	1	0	0	0	0
29	J	1	0	0	0	0
29	L	1	0	0	0	0
All	All	36093	0	36006	898	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 898 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:59:PRO:N	7:C:59:PRO:CA	1.69	1.32
6:B:303:TYR:CD2	11:G:34:GLN:HB3	1.94	1.03
3:3:74:PRO:HD2	20:3:615:XAT:O23	1.57	1.02
3:3:229:MET:HB3	20:3:615:XAT:H402	1.42	1.02
17:3:602:CLA:HAB	20:3:615:XAT:H32	1.44	0.99

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	193/195 (99%)	178 (92%)	12 (6%)	3 (2%)	9	13
2	2	202/269 (75%)	191 (95%)	9 (4%)	2 (1%)	15	23
3	3	214/275 (78%)	197 (92%)	17 (8%)	0	100	100
4	4	193/198 (98%)	179 (93%)	13 (7%)	1 (0%)	29	41
5	A	740/758 (98%)	707 (96%)	30 (4%)	3 (0%)	34	48
6	B	731/734 (100%)	709 (97%)	19 (3%)	3 (0%)	34	48
7	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
8	D	138/143 (96%)	127 (92%)	9 (6%)	2 (1%)	11	15
9	E	61/66 (92%)	59 (97%)	2 (3%)	0	100	100
10	F	150/154 (97%)	148 (99%)	2 (1%)	0	100	100
11	G	93/97 (96%)	88 (95%)	5 (5%)	0	100	100
12	H	86/88 (98%)	80 (93%)	6 (7%)	0	100	100
13	I	28/40 (70%)	26 (93%)	2 (7%)	0	100	100
14	J	37/42 (88%)	37 (100%)	0	0	100	100
15	L	149/157 (95%)	145 (97%)	4 (3%)	0	100	100
16	K	73/80 (91%)	67 (92%)	6 (8%)	0	100	100
All	All	3166/3377 (94%)	3012 (95%)	140 (4%)	14 (0%)	34	48

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	516	GLY
6	B	5	PHE
8	D	76	PRO
1	1	109	ALA
6	B	559	CYS

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	1	155/158 (98%)	147 (95%)	8 (5%)	23	38
2	2	164/216 (76%)	150 (92%)	14 (8%)	10	16
3	3	167/213 (78%)	158 (95%)	9 (5%)	22	36
4	4	161/164 (98%)	149 (92%)	12 (8%)	13	21
5	A	603/618 (98%)	573 (95%)	30 (5%)	24	40
6	B	598/599 (100%)	568 (95%)	30 (5%)	24	40
7	C	69/70 (99%)	65 (94%)	4 (6%)	20	32
8	D	120/122 (98%)	109 (91%)	11 (9%)	9	13
9	E	55/58 (95%)	53 (96%)	2 (4%)	35	54
10	F	124/127 (98%)	114 (92%)	10 (8%)	11	18
11	G	80/82 (98%)	70 (88%)	10 (12%)	4	5
12	H	71/71 (100%)	67 (94%)	4 (6%)	21	34
13	I	25/36 (69%)	23 (92%)	2 (8%)	12	18
14	J	32/35 (91%)	29 (91%)	3 (9%)	8	13
15	L	118/124 (95%)	111 (94%)	7 (6%)	19	32
16	K	51/58 (88%)	49 (96%)	2 (4%)	32	50
All	All	2593/2751 (94%)	2435 (94%)	158 (6%)	18	30

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	D	189	ARG
12	H	101	LEU
9	E	62	GLU
11	G	6	LEU
15	L	36	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	4	247	GLN
6	B	218	HIS
12	H	82	ASN
12	H	85	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

215 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	826	29	56,73,73	1.66	6 (10%)	55,113,113	1.66	11 (20%)
28	SF4	C	101	7	0,12,12	0.00	-	-		
17	CLA	B	819	-	50,67,73	1.67	6 (12%)	47,105,113	1.72	13 (27%)
21	BCR	1	316	-	41,41,41	1.07	2 (4%)	56,56,56	1.24	6 (10%)
17	CLA	4	310	-	51,68,73	1.57	5 (9%)	49,107,113	1.96	15 (30%)
17	CLA	A	806	-	56,73,73	1.59	5 (8%)	55,113,113	1.52	9 (16%)
17	CLA	A	831	-	56,73,73	1.58	4 (7%)	55,113,113	1.72	14 (25%)
18	CHL	1	305	1	42,56,74	2.32	13 (30%)	42,92,114	2.18	13 (30%)
17	CLA	L	203	-	56,73,73	1.57	5 (8%)	55,113,113	1.65	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LHG	B	801	17	22,22,48	1.09	2 (9%)	25,28,54	1.10	2 (8%)
17	CLA	K	202	-	51,68,73	1.69	6 (11%)	49,107,113	1.63	8 (16%)
24	LMG	4	319	-	50,50,55	0.88	3 (6%)	58,58,63	1.46	8 (13%)
25	HTG	4	322	-	19,19,19	1.07	2 (10%)	23,24,24	1.23	3 (13%)
26	DGD	4	323	-	61,61,67	0.89	2 (3%)	75,75,81	1.76	21 (28%)
17	CLA	B	833	-	51,68,73	1.54	8 (15%)	49,107,113	1.73	12 (24%)
17	CLA	3	613	-	37,54,73	1.93	5 (13%)	32,90,113	1.90	7 (21%)
17	CLA	4	311	4	43,60,73	1.82	4 (9%)	39,97,113	1.73	8 (20%)
17	CLA	B	830	-	56,73,73	1.66	8 (14%)	55,113,113	1.69	13 (23%)
17	CLA	A	853	29	56,73,73	1.54	6 (10%)	55,113,113	2.33	21 (38%)
17	CLA	A	829	-	56,73,73	1.55	8 (14%)	55,113,113	1.71	8 (14%)
17	CLA	A	822	-	42,59,73	1.83	5 (11%)	38,96,113	1.78	9 (23%)
17	CLA	B	836	29	33,53,73	1.94	4 (12%)	27,89,113	2.33	14 (51%)
17	CLA	B	842	22	56,73,73	1.52	5 (8%)	55,113,113	1.78	15 (27%)
17	CLA	A	810	17	56,73,73	1.56	5 (8%)	55,113,113	1.63	11 (20%)
23	LMT	A	855	-	36,36,36	1.11	4 (11%)	47,47,47	0.92	1 (2%)
18	CHL	4	306	29	45,59,74	2.23	13 (28%)	46,96,114	2.41	15 (32%)
21	BCR	A	851	-	41,41,41	0.89	2 (4%)	56,56,56	1.21	6 (10%)
17	CLA	2	308	2	51,68,73	1.65	6 (11%)	49,107,113	1.56	7 (14%)
19	LUT	3	614	-	42,43,43	5.66	20 (47%)	51,60,60	5.51	31 (60%)
17	CLA	B	816	-	56,73,73	1.58	6 (10%)	55,113,113	1.62	9 (16%)
17	CLA	B	841	-	56,73,73	1.69	6 (10%)	55,113,113	1.54	10 (18%)
17	CLA	A	826	-	56,73,73	1.51	5 (8%)	55,113,113	1.55	8 (14%)
17	CLA	A	840	-	56,73,73	1.57	8 (14%)	55,113,113	1.68	14 (25%)
17	CLA	1	310	1	43,60,73	1.82	7 (16%)	39,97,113	1.65	10 (25%)
20	XAT	2	315	-	39,47,47	4.99	17 (43%)	54,74,74	5.48	32 (59%)
17	CLA	A	839	29	56,73,73	1.71	8 (14%)	55,113,113	1.36	7 (12%)
21	BCR	G	106	-	41,41,41	1.06	2 (4%)	56,56,56	1.13	5 (8%)
21	BCR	A	847	-	41,41,41	1.08	3 (7%)	56,56,56	1.22	5 (8%)
20	XAT	4	317	-	39,47,47	5.05	17 (43%)	54,74,74	5.30	32 (59%)
17	CLA	J	101	-	56,73,73	1.59	6 (10%)	55,113,113	1.69	11 (20%)
17	CLA	2	307	2	41,58,73	1.86	5 (12%)	37,95,113	1.88	10 (27%)
17	CLA	4	302	4	51,68,73	1.72	8 (15%)	49,107,113	1.61	9 (18%)
17	CLA	A	814	-	41,58,73	1.83	5 (12%)	37,95,113	1.82	9 (24%)
18	CHL	4	301	1	55,69,74	1.69	14 (25%)	58,108,114	2.32	20 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	B	840	29	56,73,73	1.50	4 (7%)	55,113,113	1.63	9 (16%)
21	BCR	L	206	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	7 (12%)
17	CLA	1	311	1	51,68,73	1.57	6 (11%)	49,107,113	1.65	11 (22%)
17	CLA	B	827	29	56,73,73	1.49	6 (10%)	55,113,113	1.73	12 (21%)
26	DGD	B	850	-	67,67,67	1.13	6 (8%)	81,81,81	1.50	10 (12%)
18	CHL	4	315	4	37,51,74	2.22	10 (27%)	36,86,114	2.24	9 (25%)
24	LMG	B	852	-	52,52,55	1.09	4 (7%)	60,60,63	1.49	7 (11%)
21	BCR	K	203	-	41,41,41	1.08	2 (4%)	56,56,56	1.21	6 (10%)
23	LMT	2	318	-	36,36,36	1.09	5 (13%)	47,47,47	1.11	3 (6%)
21	BCR	B	847	-	41,41,41	1.10	2 (4%)	56,56,56	1.45	10 (17%)
17	CLA	B	805	-	56,73,73	1.50	4 (7%)	55,113,113	1.58	10 (18%)
17	CLA	2	301	2	56,73,73	1.62	7 (12%)	55,113,113	1.63	10 (18%)
18	CHL	2	305	29	42,56,74	2.25	13 (30%)	42,92,114	2.33	13 (30%)
17	CLA	A	825	29	56,73,73	1.59	5 (8%)	55,113,113	1.56	9 (16%)
17	CLA	A	820	29	56,73,73	1.61	5 (8%)	55,113,113	1.52	10 (18%)
17	CLA	L	204	-	41,58,73	1.91	5 (12%)	37,95,113	1.78	11 (29%)
20	XAT	1	315	-	39,47,47	5.00	17 (43%)	54,74,74	5.48	32 (59%)
25	HTG	F	305	-	19,19,19	1.05	2 (10%)	23,24,24	1.73	4 (17%)
17	CLA	B	811	6	56,73,73	1.58	4 (7%)	55,113,113	1.73	11 (20%)
20	XAT	3	615	-	39,47,47	4.99	17 (43%)	54,74,74	5.48	32 (59%)
17	CLA	1	309	22	56,73,73	1.67	4 (7%)	55,113,113	1.52	12 (21%)
17	CLA	B	808	6	56,73,73	1.41	8 (14%)	55,113,113	1.67	11 (20%)
21	BCR	I	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.21	4 (7%)
17	CLA	A	811	-	45,62,73	1.78	5 (11%)	41,99,113	1.64	7 (17%)
17	CLA	4	313	-	33,53,73	2.02	5 (15%)	27,89,113	2.21	12 (44%)
17	CLA	A	809	-	56,73,73	1.56	5 (8%)	55,113,113	1.59	9 (16%)
17	CLA	2	302	-	42,59,73	1.80	6 (14%)	38,96,113	1.88	10 (26%)
17	CLA	B	809	-	56,73,73	1.62	6 (10%)	55,113,113	1.54	10 (18%)
22	LHG	2	317	-	36,36,48	0.71	1 (2%)	39,42,54	1.23	4 (10%)
17	CLA	A	801	-	56,73,73	1.44	3 (5%)	55,113,113	2.27	15 (27%)
17	CLA	A	824	29	56,73,73	1.63	5 (8%)	55,113,113	1.58	9 (16%)
17	CLA	B	839	-	38,55,73	1.77	4 (10%)	33,91,113	2.56	18 (54%)
21	BCR	F	303	-	41,41,41	0.92	2 (4%)	56,56,56	1.43	11 (19%)
22	LHG	G	102	-	48,48,48	0.67	1 (2%)	51,54,54	1.23	6 (11%)
24	LMG	F	309	-	55,55,55	0.85	2 (3%)	63,63,63	1.45	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	828	-	56,73,73	1.56	5 (8%)	55,113,113	1.63	11 (20%)
17	CLA	1	303	29	42,59,73	1.78	5 (11%)	38,96,113	1.81	10 (26%)
17	CLA	B	820	-	51,68,73	1.57	5 (9%)	49,107,113	1.76	14 (28%)
18	CHL	3	607	29	41,55,74	2.25	11 (26%)	41,91,114	2.24	12 (29%)
25	HTG	4	321	-	19,19,19	1.14	2 (10%)	23,24,24	1.14	1 (4%)
17	CLA	A	823	-	46,63,73	1.78	5 (10%)	43,101,113	1.70	8 (18%)
17	CLA	4	312	4	47,64,73	1.68	7 (14%)	44,102,113	1.72	7 (15%)
17	CLA	B	804	-	56,73,73	1.68	5 (8%)	55,113,113	1.47	9 (16%)
17	CLA	B	806	-	33,53,73	1.85	4 (12%)	27,89,113	2.49	10 (37%)
17	CLA	G	103	29	32,49,73	2.13	6 (18%)	26,84,113	2.07	6 (23%)
21	BCR	A	846	-	41,41,41	1.05	2 (4%)	56,56,56	1.33	8 (14%)
17	CLA	1	301	1	56,73,73	1.71	5 (8%)	55,113,113	1.36	8 (14%)
17	CLA	1	313	1	37,54,73	1.86	7 (18%)	32,90,113	1.92	8 (25%)
21	BCR	L	205	-	41,41,41	0.98	1 (2%)	56,56,56	1.10	4 (7%)
17	CLA	3	602	3	51,68,73	1.69	6 (11%)	49,107,113	1.59	9 (18%)
17	CLA	B	807	-	56,73,73	1.54	7 (12%)	55,113,113	1.62	8 (14%)
17	CLA	A	815	29	33,53,73	2.07	6 (18%)	27,89,113	2.05	9 (33%)
17	CLA	A	841	29	56,73,73	1.54	5 (8%)	55,113,113	1.63	12 (21%)
21	BCR	A	850	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	8 (14%)
25	HTG	A	854	-	19,19,19	0.84	1 (5%)	23,24,24	0.92	0
17	CLA	3	608	3	41,58,73	1.86	5 (12%)	37,95,113	1.82	9 (24%)
17	CLA	2	319	4	37,54,73	1.94	5 (13%)	32,90,113	1.95	11 (34%)
17	CLA	B	838	-	56,73,73	1.50	6 (10%)	55,113,113	1.82	12 (21%)
19	LUT	1	314	-	42,43,43	5.53	20 (47%)	51,60,60	5.67	33 (64%)
17	CLA	4	309	4	51,68,73	1.69	4 (7%)	49,107,113	1.55	11 (22%)
17	CLA	B	814	-	46,63,73	1.69	8 (17%)	43,101,113	1.89	10 (23%)
17	CLA	A	802	29	56,73,73	1.53	7 (12%)	55,113,113	1.90	12 (21%)
17	CLA	A	816	-	56,73,73	1.59	6 (10%)	55,113,113	1.53	10 (18%)
17	CLA	A	812	-	56,73,73	1.66	5 (8%)	55,113,113	1.57	11 (20%)
17	CLA	A	838	-	56,73,73	1.65	5 (8%)	55,113,113	1.81	15 (27%)
21	BCR	B	844	-	41,41,41	0.99	2 (4%)	56,56,56	1.28	7 (12%)
17	CLA	B	823	-	56,73,73	1.41	5 (8%)	55,113,113	1.83	10 (18%)
21	BCR	A	849	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	7 (12%)
17	CLA	1	304	-	33,50,73	2.05	6 (18%)	27,85,113	2.03	8 (29%)
21	BCR	L	201	-	41,41,41	1.02	2 (4%)	56,56,56	1.20	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	J	103	14	33,50,73	1.90	5 (15%)	27,85,113	2.17	8 (29%)
17	CLA	B	810	-	56,73,73	1.62	6 (10%)	55,113,113	1.49	11 (20%)
17	CLA	B	822	-	41,58,73	1.77	4 (9%)	37,95,113	2.05	13 (35%)
17	CLA	3	612	-	33,53,73	2.04	6 (18%)	27,89,113	2.10	7 (25%)
21	BCR	3	616	-	41,41,41	1.09	2 (4%)	56,56,56	1.30	5 (8%)
17	CLA	1	302	-	56,73,73	1.60	4 (7%)	55,113,113	1.62	9 (16%)
22	LHG	A	845	17	26,26,48	0.87	1 (3%)	29,32,54	1.32	3 (10%)
21	BCR	2	316	-	41,41,41	1.18	3 (7%)	56,56,56	1.25	8 (14%)
17	CLA	B	802	-	56,73,73	1.52	6 (10%)	55,113,113	1.53	13 (23%)
17	CLA	A	821	-	40,57,73	1.81	5 (12%)	34,93,113	2.04	10 (29%)
17	CLA	B	834	-	49,66,73	1.62	9 (18%)	46,104,113	1.91	16 (34%)
17	CLA	B	812	-	56,73,73	1.61	6 (10%)	55,113,113	1.41	10 (18%)
18	CHL	2	304	29	37,51,74	2.22	11 (29%)	36,86,114	2.47	13 (36%)
21	BCR	J	104	-	41,41,41	1.00	3 (7%)	56,56,56	1.23	4 (7%)
17	CLA	2	312	-	34,51,73	2.07	5 (14%)	28,86,113	2.02	8 (28%)
18	CHL	4	305	29	50,64,74	1.90	11 (22%)	52,102,114	2.31	13 (25%)
19	LUT	4	316	-	42,43,43	5.53	22 (52%)	51,60,60	5.74	35 (68%)
17	CLA	3	609	3	41,58,73	1.82	4 (9%)	37,95,113	1.86	11 (29%)
17	CLA	B	818	-	46,63,73	1.75	4 (8%)	43,101,113	1.87	10 (23%)
21	BCR	B	848	-	41,41,41	1.06	2 (4%)	56,56,56	1.20	7 (12%)
21	BCR	B	845	-	41,41,41	0.92	1 (2%)	56,56,56	1.36	9 (16%)
17	CLA	4	304	29	41,58,73	1.64	7 (17%)	37,95,113	2.15	14 (37%)
17	CLA	G	105	11	37,54,73	1.97	7 (18%)	32,90,113	1.99	11 (34%)
17	CLA	2	309	-	32,49,73	2.09	5 (15%)	26,84,113	2.19	9 (34%)
17	CLA	A	808	5	56,73,73	1.42	7 (12%)	55,113,113	1.85	12 (21%)
18	CHL	4	307	29	45,59,74	2.21	12 (26%)	46,96,114	2.18	14 (30%)
17	CLA	1	308	1	51,68,73	1.66	6 (11%)	49,107,113	1.57	8 (16%)
17	CLA	A	813	-	33,53,73	2.05	7 (21%)	27,89,113	1.88	9 (33%)
17	CLA	B	821	29	56,73,73	1.45	6 (10%)	55,113,113	1.72	10 (18%)
17	CLA	K	201	-	33,53,73	2.01	5 (15%)	27,89,113	2.14	7 (25%)
17	CLA	F	307	10	46,63,73	1.65	6 (13%)	43,101,113	1.65	9 (20%)
21	BCR	B	846	-	41,41,41	1.02	2 (4%)	56,56,56	1.24	8 (14%)
17	CLA	F	306	29	33,53,73	2.02	5 (15%)	27,89,113	2.10	9 (33%)
27	PQN	A	842	-	34,34,34	4.59	16 (47%)	42,45,45	4.02	17 (40%)
17	CLA	B	831	-	56,73,73	1.48	8 (14%)	55,113,113	1.92	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	4	303	4	51,68,73	1.86	6 (11%)	49,107,113	1.74	10 (20%)
17	CLA	A	832	-	56,73,73	1.66	4 (7%)	55,113,113	1.61	9 (16%)
17	CLA	B	825	-	51,68,73	1.51	5 (9%)	49,107,113	1.95	11 (22%)
17	CLA	B	835	-	56,73,73	1.67	6 (10%)	55,113,113	1.42	10 (18%)
28	SF4	C	102	7	0,12,12	0.00	-	-		
25	HTG	F	310	-	16,16,19	1.15	2 (12%)	20,21,24	1.41	4 (20%)
17	CLA	A	807	5	56,73,73	1.56	7 (12%)	55,113,113	1.46	6 (10%)
17	CLA	3	611	3	46,63,73	1.76	5 (10%)	43,101,113	1.72	7 (16%)
17	CLA	1	312	-	46,63,73	1.79	4 (8%)	43,101,113	1.73	11 (25%)
17	CLA	A	830	-	41,58,73	1.87	5 (12%)	37,95,113	1.89	9 (24%)
17	CLA	L	202	15	56,73,73	1.58	5 (8%)	55,113,113	1.60	10 (18%)
18	CHL	2	306	29	45,59,74	2.15	14 (31%)	46,96,114	2.26	13 (28%)
21	BCR	4	318	-	41,41,41	0.97	1 (2%)	56,56,56	1.26	8 (14%)
24	LMG	4	320	-	49,49,55	1.04	4 (8%)	57,57,63	1.46	5 (8%)
17	CLA	4	308	4	41,58,73	1.73	5 (12%)	37,95,113	2.12	11 (29%)
17	CLA	A	805	5	56,73,73	1.54	7 (12%)	55,113,113	1.63	13 (23%)
17	CLA	B	824	-	46,63,73	1.60	5 (10%)	43,101,113	1.78	8 (18%)
27	PQN	B	843	-	34,34,34	4.45	14 (41%)	42,45,45	4.44	23 (54%)
17	CLA	B	837	-	51,68,73	1.38	4 (7%)	49,107,113	2.04	12 (24%)
17	CLA	A	803	17	46,63,73	1.76	6 (13%)	43,101,113	1.63	8 (18%)
17	CLA	2	311	2	56,73,73	1.62	5 (8%)	55,113,113	1.63	9 (16%)
17	CLA	3	606	3	38,55,73	1.96	5 (13%)	33,91,113	1.96	11 (33%)
17	CLA	B	832	-	41,58,73	1.70	6 (14%)	37,95,113	1.88	10 (27%)
22	LHG	A	844	-	48,48,48	0.67	1 (2%)	51,54,54	1.29	6 (11%)
17	CLA	A	836	-	56,73,73	1.53	5 (8%)	55,113,113	1.77	11 (20%)
17	CLA	A	818	-	56,73,73	1.58	5 (8%)	55,113,113	1.66	10 (18%)
17	CLA	F	304	-	56,73,73	1.60	7 (12%)	55,113,113	1.66	9 (16%)
17	CLA	3	603	3	41,58,73	1.86	7 (17%)	37,95,113	1.85	9 (24%)
25	HTG	J	102	-	19,19,19	1.20	2 (10%)	23,24,24	1.30	3 (13%)
28	SF4	A	852	6,5	0,12,12	0.00	-	-		
17	CLA	A	834	5	33,53,73	2.03	5 (15%)	27,89,113	2.06	7 (25%)
17	CLA	B	817	-	46,63,73	1.66	6 (13%)	43,101,113	1.92	10 (23%)
19	LUT	2	314	-	42,43,43	5.62	20 (47%)	51,60,60	5.61	32 (62%)
17	CLA	A	804	-	56,73,73	1.59	6 (10%)	55,113,113	1.54	8 (14%)
17	CLA	B	803	-	56,73,73	1.60	7 (12%)	55,113,113	1.51	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	827	-	56,73,73	1.57	5 (8%)	55,113,113	1.79	12 (21%)
24	LMG	G	101	-	40,40,55	0.87	2 (5%)	48,48,63	1.28	3 (6%)
17	CLA	B	813	-	45,62,73	1.68	7 (15%)	46,100,113	1.77	8 (17%)
18	CHL	2	313	2	37,51,74	2.28	11 (29%)	36,86,114	2.51	13 (36%)
17	CLA	A	833	-	41,58,73	1.83	6 (14%)	37,95,113	1.86	10 (27%)
17	CLA	B	829	-	56,73,73	1.60	7 (12%)	55,113,113	1.55	11 (20%)
18	CHL	3	601	2	47,61,74	2.10	12 (25%)	48,98,114	2.52	17 (35%)
17	CLA	A	835	-	42,59,73	1.85	5 (11%)	38,96,113	1.83	10 (26%)
17	CLA	3	604	-	33,53,73	2.08	5 (15%)	27,89,113	2.07	10 (37%)
17	CLA	B	828	-	56,73,73	1.65	5 (8%)	55,113,113	1.68	11 (20%)
17	CLA	2	310	2	43,60,73	1.96	6 (13%)	39,97,113	1.67	7 (17%)
17	CLA	A	817	-	56,73,73	1.64	8 (14%)	55,113,113	1.60	11 (20%)
17	CLA	A	837	-	56,73,73	1.61	4 (7%)	55,113,113	1.63	10 (18%)
22	LHG	1	317	17	48,48,48	0.68	1 (2%)	51,54,54	1.23	6 (11%)
21	BCR	A	848	-	41,41,41	1.05	2 (4%)	56,56,56	1.22	6 (10%)
17	CLA	4	314	-	38,55,73	1.94	4 (10%)	33,91,113	2.21	14 (42%)
17	CLA	B	815	-	56,73,73	1.54	4 (7%)	55,113,113	1.55	11 (20%)
25	HTG	F	301	-	17,17,19	0.96	2 (11%)	21,22,24	0.69	0
17	CLA	G	104	-	41,58,73	1.96	5 (12%)	37,95,113	1.90	9 (24%)
17	CLA	2	303	-	51,68,73	1.67	5 (9%)	49,107,113	1.63	10 (20%)
25	HTG	B	851	-	19,19,19	1.06	1 (5%)	23,24,24	1.87	7 (30%)
17	CLA	A	819	-	33,53,73	2.03	5 (15%)	27,89,113	2.09	9 (33%)
17	CLA	A	843	22	43,60,73	1.88	6 (13%)	39,97,113	1.85	10 (25%)
21	BCR	F	308	-	41,41,41	1.05	2 (4%)	56,56,56	1.27	8 (14%)
21	BCR	B	849	-	41,41,41	0.96	2 (4%)	56,56,56	1.19	3 (5%)
17	CLA	1	307	1	56,73,73	1.64	5 (8%)	55,113,113	1.57	10 (18%)
22	LHG	F	302	-	39,39,48	0.65	0	42,45,54	1.25	6 (14%)
17	CLA	3	605	-	33,50,73	2.17	6 (18%)	27,85,113	1.86	8 (29%)
21	BCR	J	105	-	41,41,41	1.16	2 (4%)	56,56,56	1.43	9 (16%)
17	CLA	3	610	-	43,60,73	1.86	6 (13%)	39,97,113	1.92	10 (25%)
17	CLA	1	306	29	37,54,73	1.99	5 (13%)	32,90,113	1.89	9 (28%)

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	826	29	1/1/15/20	16/37/115/115	-
28	SF4	C	101	7	-	-	0/6/5/5
17	CLA	B	819	-	1/1/13/20	5/30/108/115	-
21	BCR	1	316	-	-	12/29/63/63	0/2/2/2
17	CLA	4	310	-	1/1/14/20	15/31/109/115	-
17	CLA	A	806	-	1/1/15/20	10/37/115/115	-
17	CLA	A	831	-	1/1/15/20	16/37/115/115	-
18	CHL	1	305	1	3/3/16/26	7/18/116/137	-
17	CLA	L	203	-	1/1/15/20	10/37/115/115	-
22	LHG	B	801	17	-	10/26/26/53	-
17	CLA	K	202	-	1/1/14/20	16/31/109/115	-
24	LMG	4	319	-	-	15/45/65/70	0/1/1/1
25	HTG	4	322	-	-	1/10/30/30	0/1/1/1
26	DGD	4	323	-	-	27/49/89/95	0/2/2/2
17	CLA	B	833	-	1/1/14/20	6/31/109/115	-
17	CLA	3	613	-	1/1/11/20	2/15/93/115	-
17	CLA	B	830	-	1/1/15/20	5/37/115/115	-
17	CLA	4	311	4	-	4/22/100/115	-
17	CLA	A	853	29	1/1/15/20	16/37/115/115	-
17	CLA	A	829	-	1/1/15/20	14/37/115/115	-
17	CLA	A	822	-	1/1/12/20	11/21/99/115	-
17	CLA	B	836	29	1/1/11/20	2/11/91/115	-
17	CLA	B	842	22	1/1/15/20	7/37/115/115	-
17	CLA	A	810	17	1/1/15/20	13/37/115/115	-
23	LMT	A	855	-	-	14/21/61/61	0/2/2/2
18	CHL	4	306	29	3/3/17/26	7/21/119/137	-
21	BCR	A	851	-	-	7/29/63/63	0/2/2/2
17	CLA	2	308	2	1/1/14/20	11/31/109/115	-
19	LUT	3	614	-	-	12/29/67/67	0/2/2/2
17	CLA	B	816	-	1/1/15/20	9/37/115/115	-
17	CLA	B	841	-	1/1/15/20	11/37/115/115	-
17	CLA	A	826	-	1/1/15/20	11/37/115/115	-
17	CLA	A	840	-	1/1/15/20	14/37/115/115	-
17	CLA	1	310	1	1/1/12/20	8/22/100/115	-
20	XAT	2	315	-	-	13/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	839	29	1/1/15/20	16/37/115/115	-
21	BCR	G	106	-	-	6/29/63/63	0/2/2/2
21	BCR	A	847	-	-	6/29/63/63	0/2/2/2
20	XAT	4	317	-	3/3/12/26	11/31/93/93	0/4/4/4
17	CLA	J	101	-	1/1/15/20	8/37/115/115	-
17	CLA	2	307	2	1/1/12/20	1/19/97/115	-
17	CLA	4	302	4	1/1/14/20	4/31/109/115	-
17	CLA	A	814	-	1/1/12/20	9/19/97/115	-
18	CHL	4	301	1	4/4/19/26	15/33/131/137	-
17	CLA	B	840	29	1/1/15/20	13/37/115/115	-
21	BCR	L	206	-	-	4/29/63/63	0/2/2/2
17	CLA	1	311	1	1/1/14/20	6/31/109/115	-
17	CLA	B	827	29	1/1/15/20	11/37/115/115	-
26	DGD	B	850	-	-	24/55/95/95	0/2/2/2
18	CHL	4	315	4	3/3/15/26	2/12/110/137	-
24	LMG	B	852	-	-	21/47/67/70	0/1/1/1
21	BCR	K	203	-	-	15/29/63/63	0/2/2/2
23	LMT	2	318	-	-	11/21/61/61	0/2/2/2
21	BCR	B	847	-	-	3/29/63/63	0/2/2/2
17	CLA	B	805	-	1/1/15/20	11/37/115/115	-
17	CLA	2	301	2	1/1/15/20	5/37/115/115	-
18	CHL	2	305	29	3/3/16/26	2/18/116/137	-
17	CLA	A	825	29	1/1/15/20	8/37/115/115	-
17	CLA	A	820	29	1/1/15/20	8/37/115/115	-
17	CLA	L	204	-	-	6/19/97/115	-
20	XAT	1	315	-	-	13/31/93/93	0/4/4/4
25	HTG	F	305	-	-	3/10/30/30	0/1/1/1
17	CLA	B	811	6	1/1/15/20	9/37/115/115	-
20	XAT	3	615	-	-	13/31/93/93	0/4/4/4
17	CLA	1	309	22	1/1/15/20	17/37/115/115	-
17	CLA	B	808	6	1/1/15/20	15/37/115/115	-
21	BCR	I	101	-	-	5/29/63/63	0/2/2/2
17	CLA	A	811	-	1/1/12/20	5/24/102/115	-
17	CLA	4	313	-	1/1/11/20	7/11/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	809	-	1/1/15/20	16/37/115/115	-
17	CLA	2	302	-	1/1/12/20	2/21/99/115	-
17	CLA	B	809	-	1/1/15/20	14/37/115/115	-
22	LHG	2	317	-	-	19/41/41/53	-
17	CLA	A	801	-	2/2/15/20	9/37/115/115	-
17	CLA	A	824	29	1/1/15/20	11/37/115/115	-
17	CLA	B	839	-	1/1/11/20	4/16/94/115	-
21	BCR	F	303	-	-	5/29/63/63	0/2/2/2
22	LHG	G	102	-	-	26/53/53/53	-
24	LMG	F	309	-	-	20/50/70/70	0/1/1/1
17	CLA	A	828	-	1/1/15/20	8/37/115/115	-
17	CLA	1	303	29	1/1/12/20	8/21/99/115	-
17	CLA	B	820	-	1/1/14/20	14/31/109/115	-
18	CHL	3	607	29	3/3/16/26	4/17/115/137	-
17	CLA	A	823	-	1/1/13/20	6/25/103/115	-
17	CLA	4	312	4	1/1/13/20	5/27/105/115	-
17	CLA	B	804	-	1/1/15/20	6/37/115/115	-
17	CLA	B	806	-	1/1/11/20	2/11/91/115	-
17	CLA	G	103	29	1/1/10/20	2/8/86/115	-
21	BCR	A	846	-	-	2/29/63/63	0/2/2/2
17	CLA	1	301	1	1/1/15/20	9/37/115/115	-
17	CLA	1	313	1	1/1/11/20	4/15/93/115	-
21	BCR	L	205	-	-	10/29/63/63	0/2/2/2
17	CLA	3	602	3	1/1/14/20	5/31/109/115	-
17	CLA	B	807	-	1/1/15/20	13/37/115/115	-
17	CLA	A	815	29	1/1/11/20	2/11/91/115	-
17	CLA	A	841	29	1/1/15/20	13/37/115/115	-
21	BCR	A	850	-	-	8/29/63/63	0/2/2/2
25	HTG	A	854	-	-	2/10/30/30	0/1/1/1
17	CLA	3	608	3	1/1/12/20	4/19/97/115	-
17	CLA	2	319	4	1/1/11/20	3/15/93/115	-
17	CLA	B	838	-	1/1/15/20	11/37/115/115	-
19	LUT	1	314	-	-	12/29/67/67	0/2/2/2
17	CLA	4	309	4	1/1/14/20	8/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	814	-	1/1/13/20	7/25/103/115	-
17	CLA	A	802	29	1/1/15/20	6/37/115/115	-
17	CLA	A	816	-	1/1/15/20	15/37/115/115	-
17	CLA	A	812	-	1/1/15/20	11/37/115/115	-
17	CLA	A	838	-	1/1/15/20	15/37/115/115	-
21	BCR	B	844	-	-	7/29/63/63	0/2/2/2
17	CLA	B	823	-	1/1/15/20	13/37/115/115	-
21	BCR	A	849	-	-	7/29/63/63	0/2/2/2
17	CLA	1	304	-	1/1/10/20	5/10/88/115	-
21	BCR	L	201	-	-	11/29/63/63	0/2/2/2
17	CLA	J	103	14	1/1/10/20	5/10/88/115	-
17	CLA	B	810	-	1/1/15/20	8/37/115/115	-
17	CLA	B	822	-	1/1/12/20	6/19/97/115	-
17	CLA	3	612	-	1/1/11/20	3/11/91/115	-
21	BCR	3	616	-	-	8/29/63/63	0/2/2/2
17	CLA	1	302	-	1/1/15/20	18/37/115/115	-
22	LHG	A	845	17	-	14/31/31/53	-
21	BCR	2	316	-	-	17/29/63/63	0/2/2/2
17	CLA	B	802	-	1/1/15/20	2/37/115/115	-
17	CLA	A	821	-	1/1/11/20	8/18/96/115	-
17	CLA	B	834	-	1/1/13/20	11/29/107/115	-
17	CLA	B	812	-	-	16/37/115/115	-
18	CHL	2	304	29	3/3/15/26	5/12/110/137	-
21	BCR	J	104	-	-	2/29/63/63	0/2/2/2
17	CLA	2	312	-	1/1/10/20	0/11/89/115	-
18	CHL	4	305	29	4/4/18/26	10/27/125/137	-
19	LUT	4	316	-	-	13/29/67/67	0/2/2/2
17	CLA	3	609	3	1/1/12/20	4/19/97/115	-
17	CLA	B	818	-	1/1/13/20	5/25/103/115	-
21	BCR	B	848	-	-	3/29/63/63	0/2/2/2
21	BCR	B	845	-	-	5/29/63/63	0/2/2/2
17	CLA	4	304	29	1/1/12/20	7/19/97/115	-
17	CLA	G	105	11	1/1/11/20	5/15/93/115	-
17	CLA	2	309	-	1/1/10/20	2/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	808	5	1/1/15/20	8/37/115/115	-
18	CHL	4	307	29	3/3/17/26	2/21/119/137	-
17	CLA	1	308	1	1/1/14/20	9/31/109/115	-
17	CLA	A	813	-	1/1/11/20	1/11/91/115	-
17	CLA	B	821	29	1/1/15/20	3/37/115/115	-
17	CLA	K	201	-	1/1/11/20	4/11/91/115	-
17	CLA	F	307	10	1/1/13/20	9/25/103/115	-
21	BCR	B	846	-	-	7/29/63/63	0/2/2/2
17	CLA	F	306	29	1/1/11/20	0/11/91/115	-
27	PQN	A	842	-	-	6/23/43/43	0/2/2/2
17	CLA	B	831	-	1/1/15/20	12/37/115/115	-
17	CLA	4	303	4	-	13/31/109/115	-
17	CLA	A	832	-	1/1/15/20	13/37/115/115	-
17	CLA	B	825	-	1/1/14/20	10/31/109/115	-
17	CLA	B	835	-	1/1/15/20	11/37/115/115	-
28	SF4	C	102	7	-	-	0/6/5/5
25	HTG	F	310	-	-	3/7/27/30	0/1/1/1
17	CLA	A	807	5	1/1/15/20	19/37/115/115	-
17	CLA	3	611	3	1/1/13/20	9/25/103/115	-
17	CLA	1	312	-	1/1/13/20	9/25/103/115	-
17	CLA	A	830	-	1/1/12/20	5/19/97/115	-
17	CLA	L	202	15	1/1/15/20	15/37/115/115	-
18	CHL	2	306	29	3/3/17/26	5/21/119/137	-
21	BCR	4	318	-	-	7/29/63/63	0/2/2/2
24	LMG	4	320	-	-	20/44/64/70	0/1/1/1
17	CLA	4	308	4	1/1/12/20	3/19/97/115	-
17	CLA	A	805	5	1/1/15/20	19/37/115/115	-
17	CLA	B	824	-	1/1/13/20	10/25/103/115	-
27	PQN	B	843	-	-	3/23/43/43	0/2/2/2
17	CLA	B	837	-	1/1/14/20	11/31/109/115	-
17	CLA	A	803	17	1/1/13/20	10/25/103/115	-
17	CLA	2	311	2	1/1/15/20	16/37/115/115	-
17	CLA	3	606	3	1/1/11/20	7/16/94/115	-
17	CLA	B	832	-	1/1/12/20	3/19/97/115	-
22	LHG	A	844	-	-	26/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	836	-	1/1/15/20	14/37/115/115	-
17	CLA	A	818	-	1/1/15/20	16/37/115/115	-
17	CLA	F	304	-	1/1/15/20	7/37/115/115	-
17	CLA	3	603	3	1/1/12/20	2/19/97/115	-
25	HTG	J	102	-	-	6/10/30/30	0/1/1/1
28	SF4	A	852	6,5	-	-	0/6/5/5
17	CLA	A	834	5	1/1/11/20	7/11/91/115	-
17	CLA	B	817	-	1/1/13/20	10/25/103/115	-
19	LUT	2	314	-	-	12/29/67/67	0/2/2/2
17	CLA	A	804	-	1/1/15/20	13/37/115/115	-
17	CLA	B	803	-	1/1/15/20	14/37/115/115	-
17	CLA	A	827	-	1/1/15/20	9/37/115/115	-
24	LMG	G	101	-	-	15/35/55/70	0/1/1/1
17	CLA	B	813	-	1/1/13/20	11/25/101/115	-
18	CHL	2	313	2	3/3/15/26	5/12/110/137	-
17	CLA	A	833	-	1/1/12/20	3/19/97/115	-
17	CLA	B	829	-	1/1/15/20	14/37/115/115	-
18	CHL	3	601	2	3/3/17/26	3/24/122/137	-
17	CLA	A	835	-	1/1/12/20	9/21/99/115	-
17	CLA	3	604	-	1/1/11/20	3/11/91/115	-
17	CLA	B	828	-	1/1/15/20	8/37/115/115	-
17	CLA	2	310	2	1/1/12/20	7/22/100/115	-
17	CLA	A	817	-	1/1/15/20	11/37/115/115	-
17	CLA	A	837	-	1/1/15/20	15/37/115/115	-
22	LHG	1	317	17	-	23/53/53/53	-
21	BCR	A	848	-	-	7/29/63/63	0/2/2/2
17	CLA	4	314	-	1/1/11/20	2/16/94/115	-
17	CLA	B	815	-	1/1/15/20	16/37/115/115	-
25	HTG	F	301	-	-	4/8/28/30	0/1/1/1
17	CLA	G	104	-	1/1/12/20	4/19/97/115	-
17	CLA	2	303	-	1/1/14/20	17/31/109/115	-
25	HTG	B	851	-	-	7/10/30/30	0/1/1/1
17	CLA	A	819	-	1/1/11/20	3/11/91/115	-
17	CLA	A	843	22	1/1/12/20	9/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	F	308	-	-	3/29/63/63	0/2/2/2
21	BCR	B	849	-	-	8/29/63/63	0/2/2/2
17	CLA	1	307	1	1/1/15/20	13/37/115/115	-
22	LHG	F	302	-	-	30/44/44/53	-
17	CLA	3	605	-	1/1/10/20	3/10/88/115	-
21	BCR	J	105	-	-	7/29/63/63	0/2/2/2
17	CLA	3	610	-	1/1/12/20	8/22/100/115	-
17	CLA	1	306	29	1/1/11/20	1/15/93/115	-

The worst 5 of 1212 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	314	LUT	C24-C25	15.75	1.52	1.33
19	2	314	LUT	C24-C25	15.50	1.52	1.33
19	3	614	LUT	C24-C25	15.40	1.52	1.33
19	4	316	LUT	C24-C25	15.00	1.51	1.33
19	3	614	LUT	C14-C13	12.92	1.52	1.35

The worst 5 of 2188 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	842	PQN	C6-C5-C10	-13.60	104.14	119.26
27	A	842	PQN	C9-C10-C5	-12.36	105.51	119.26
19	4	316	LUT	C31-C30-C29	-11.83	110.43	127.31
19	4	316	LUT	C11-C10-C9	-11.79	110.48	127.31
19	2	314	LUT	C35-C34-C33	-11.70	110.62	127.31

5 of 178 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	1	301	CLA	ND
17	1	302	CLA	ND
17	1	303	CLA	ND
17	1	304	CLA	ND
17	1	306	CLA	ND

5 of 1918 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	1	304	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	1	307	CLA	CBA-CGA-O2A-C1
17	1	307	CLA	O1A-CGA-O2A-C1
17	1	309	CLA	C1A-C2A-CAA-CBA
17	1	311	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

197 monomers are involved in 630 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	826	CLA	8	0
17	B	819	CLA	4	0
17	4	310	CLA	1	0
17	A	806	CLA	2	0
17	A	831	CLA	6	0
18	1	305	CHL	6	0
17	L	203	CLA	6	0
22	B	801	LHG	1	0
17	K	202	CLA	2	0
25	4	322	HTG	2	0
26	4	323	DGD	29	0
17	B	833	CLA	2	0
17	3	613	CLA	3	0
17	4	311	CLA	3	0
17	B	830	CLA	3	0
17	A	853	CLA	9	0
17	A	829	CLA	2	0
17	A	822	CLA	1	0
17	B	836	CLA	5	0
17	B	842	CLA	5	0
17	A	810	CLA	8	0
23	A	855	LMT	2	0
18	4	306	CHL	7	0
21	A	851	BCR	5	0
17	2	308	CLA	5	0
19	3	614	LUT	4	0
17	B	816	CLA	3	0
17	B	841	CLA	2	0
17	A	826	CLA	2	0
17	A	840	CLA	4	0
17	1	310	CLA	6	0
20	2	315	XAT	10	0
17	A	839	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	G	106	BCR	2	0
21	A	847	BCR	1	0
20	4	317	XAT	10	0
17	J	101	CLA	6	0
17	2	307	CLA	4	0
17	4	302	CLA	7	0
17	A	814	CLA	4	0
18	4	301	CHL	11	0
17	B	840	CLA	1	0
21	L	206	BCR	4	0
17	1	311	CLA	6	0
17	B	827	CLA	11	0
26	B	850	DGD	7	0
18	4	315	CHL	4	0
24	B	852	LMG	6	0
21	K	203	BCR	4	0
23	2	318	LMT	3	0
21	B	847	BCR	8	0
17	B	805	CLA	3	0
17	2	301	CLA	4	0
18	2	305	CHL	2	0
17	A	825	CLA	5	0
17	A	820	CLA	8	0
17	L	204	CLA	4	0
20	1	315	XAT	3	0
25	F	305	HTG	1	0
17	B	811	CLA	6	0
20	3	615	XAT	13	0
17	1	309	CLA	6	0
17	B	808	CLA	1	0
21	I	101	BCR	4	0
17	A	811	CLA	3	0
17	A	809	CLA	3	0
17	2	302	CLA	4	0
17	B	809	CLA	6	0
22	2	317	LHG	7	0
17	A	801	CLA	1	0
17	A	824	CLA	4	0
17	B	839	CLA	4	0
21	F	303	BCR	1	0
22	G	102	LHG	2	0
24	F	309	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	828	CLA	6	0
17	1	303	CLA	2	0
17	B	820	CLA	1	0
18	3	607	CHL	2	0
25	4	321	HTG	2	0
17	A	823	CLA	5	0
17	B	804	CLA	3	0
17	B	806	CLA	2	0
17	G	103	CLA	4	0
21	A	846	BCR	11	0
17	1	301	CLA	2	0
21	L	205	BCR	4	0
17	3	602	CLA	6	0
17	B	807	CLA	4	0
17	A	815	CLA	1	0
17	A	841	CLA	5	0
21	A	850	BCR	3	0
17	3	608	CLA	7	0
17	B	838	CLA	5	0
19	1	314	LUT	9	0
17	4	309	CLA	2	0
17	A	802	CLA	2	0
17	A	816	CLA	4	0
17	A	812	CLA	3	0
17	A	838	CLA	4	0
21	B	844	BCR	4	0
17	B	823	CLA	5	0
21	A	849	BCR	3	0
17	1	304	CLA	6	0
21	L	201	BCR	3	0
17	J	103	CLA	3	0
17	B	810	CLA	7	0
17	B	822	CLA	3	0
17	3	612	CLA	1	0
21	3	616	BCR	4	0
17	1	302	CLA	5	0
22	A	845	LHG	1	0
21	2	316	BCR	8	0
17	B	802	CLA	3	0
17	A	821	CLA	1	0
17	B	834	CLA	3	0
17	B	812	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	2	304	CHL	1	0
21	J	104	BCR	2	0
17	2	312	CLA	3	0
18	4	305	CHL	7	0
19	4	316	LUT	4	0
17	3	609	CLA	2	0
17	B	818	CLA	2	0
21	B	848	BCR	4	0
21	B	845	BCR	4	0
17	4	304	CLA	6	0
17	G	105	CLA	1	0
17	2	309	CLA	3	0
17	A	808	CLA	6	0
18	4	307	CHL	5	0
17	1	308	CLA	6	0
17	A	813	CLA	1	0
17	B	821	CLA	3	0
17	K	201	CLA	2	0
17	F	307	CLA	2	0
21	B	846	BCR	2	0
17	F	306	CLA	4	0
27	A	842	PQN	6	0
17	B	831	CLA	2	0
17	4	303	CLA	5	0
17	A	832	CLA	4	0
17	B	825	CLA	4	0
17	B	835	CLA	3	0
25	F	310	HTG	1	0
17	A	807	CLA	2	0
17	3	611	CLA	1	0
17	1	312	CLA	2	0
17	A	830	CLA	1	0
17	L	202	CLA	5	0
18	2	306	CHL	5	0
21	4	318	BCR	14	0
24	4	320	LMG	7	0
17	4	308	CLA	3	0
17	A	805	CLA	5	0
17	B	824	CLA	4	0
27	B	843	PQN	3	0
17	B	837	CLA	7	0
17	A	803	CLA	7	0

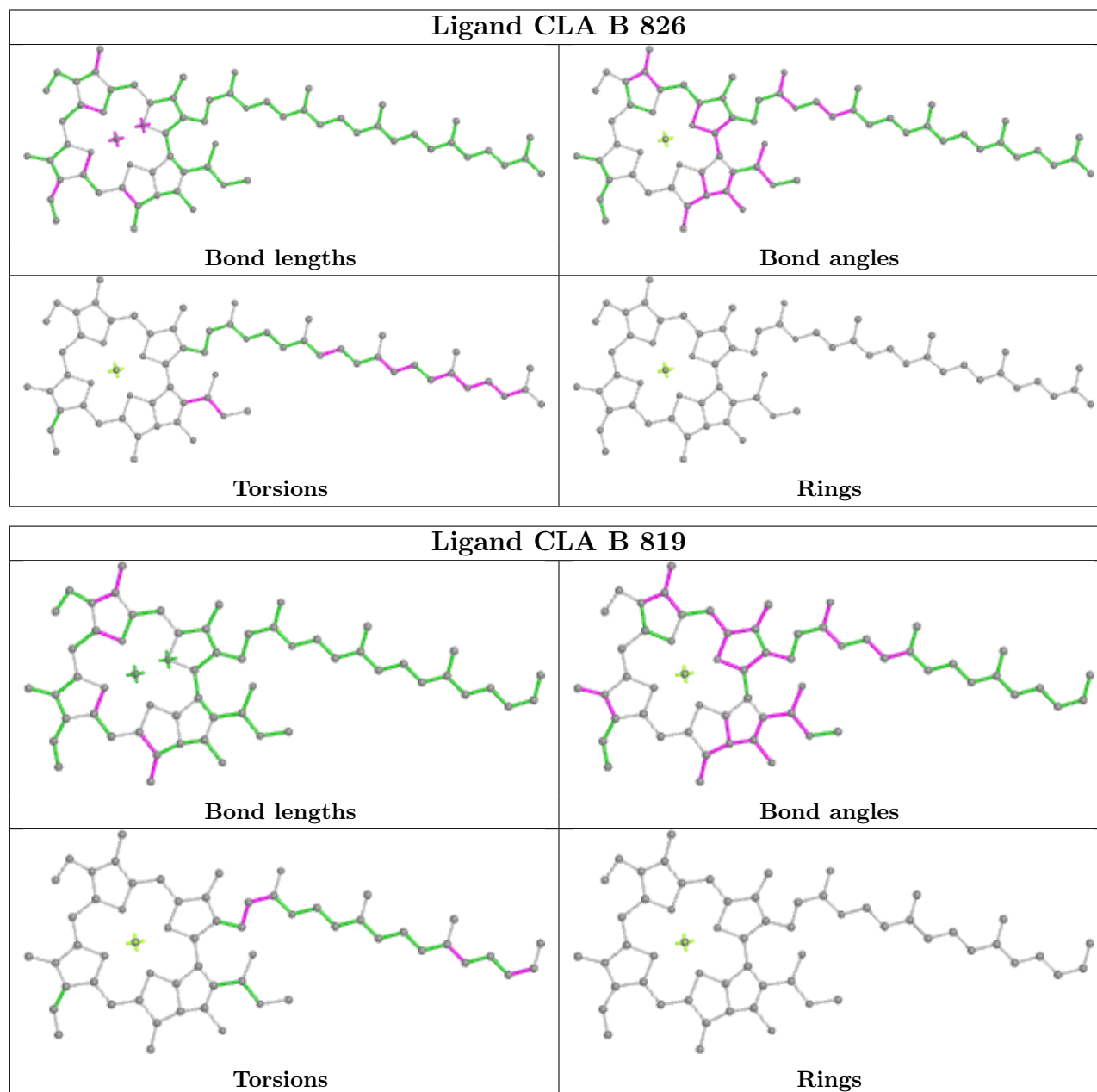
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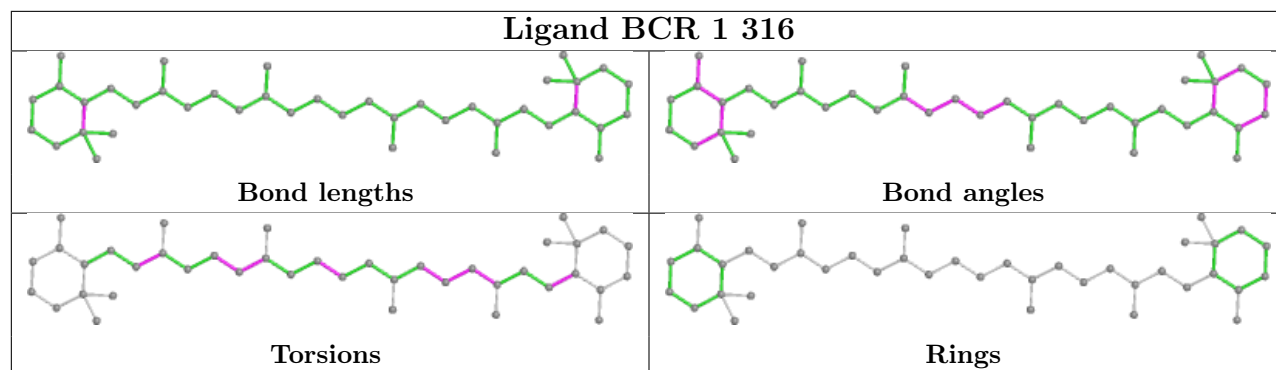
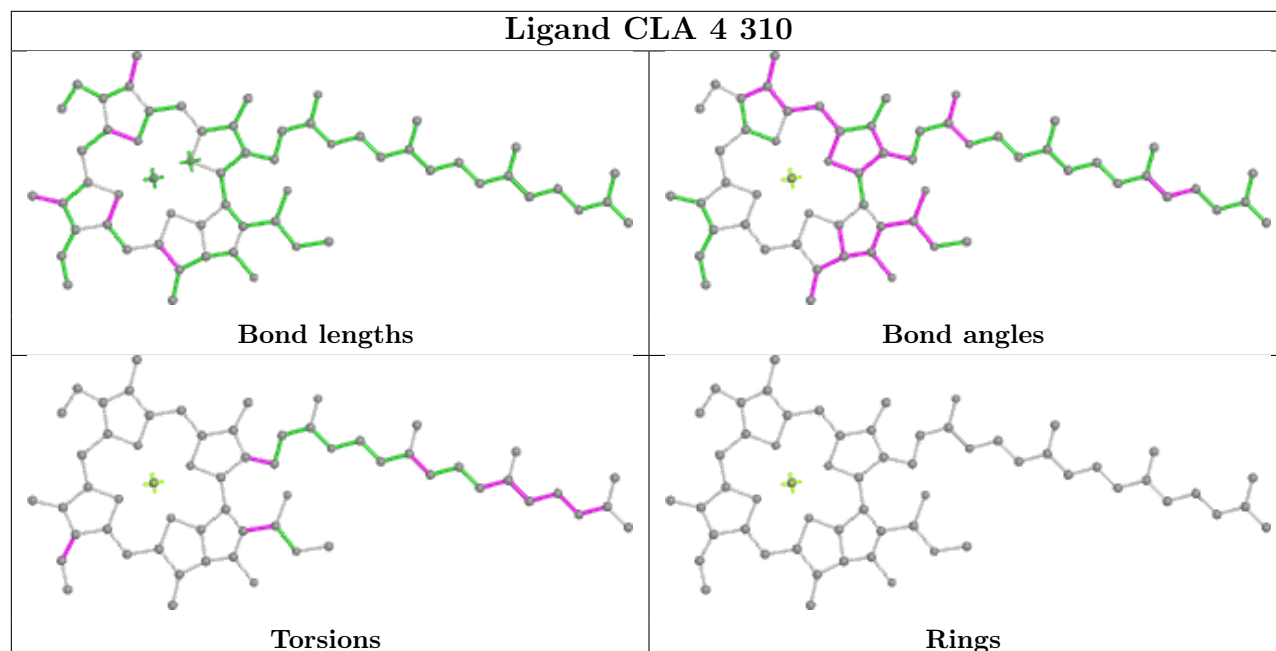
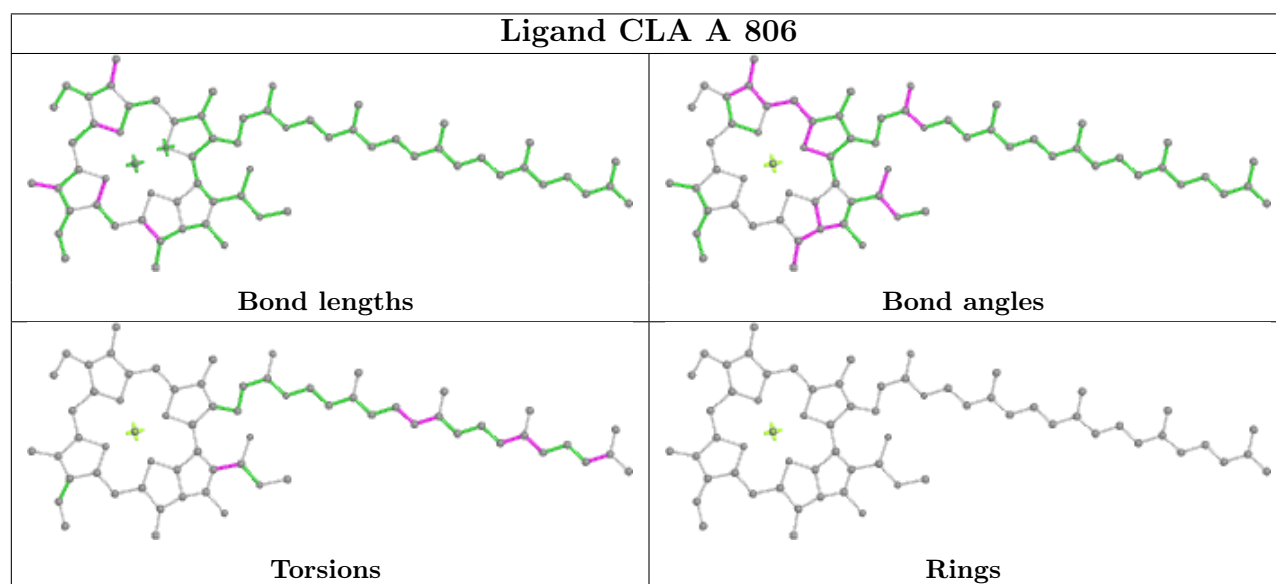
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	2	311	CLA	4	0
17	B	832	CLA	5	0
22	A	844	LHG	2	0
17	A	836	CLA	4	0
17	A	818	CLA	4	0
17	F	304	CLA	2	0
17	3	603	CLA	5	0
25	J	102	HTG	3	0
17	A	834	CLA	2	0
19	2	314	LUT	4	0
17	A	804	CLA	8	0
17	B	803	CLA	6	0
17	A	827	CLA	3	0
24	G	101	LMG	3	0
18	2	313	CHL	5	0
17	B	829	CLA	6	0
18	3	601	CHL	17	0
17	A	835	CLA	3	0
17	B	828	CLA	3	0
17	2	310	CLA	2	0
17	A	817	CLA	5	0
17	A	837	CLA	7	0
22	1	317	LHG	6	0
21	A	848	BCR	3	0
17	4	314	CLA	2	0
17	B	815	CLA	5	0
17	G	104	CLA	5	0
17	2	303	CLA	1	0
25	B	851	HTG	1	0
17	A	819	CLA	5	0
17	A	843	CLA	6	0
21	F	308	BCR	3	0
21	B	849	BCR	3	0
17	1	307	CLA	5	0
22	F	302	LHG	2	0
17	3	605	CLA	2	0
21	J	105	BCR	6	0
17	3	610	CLA	1	0

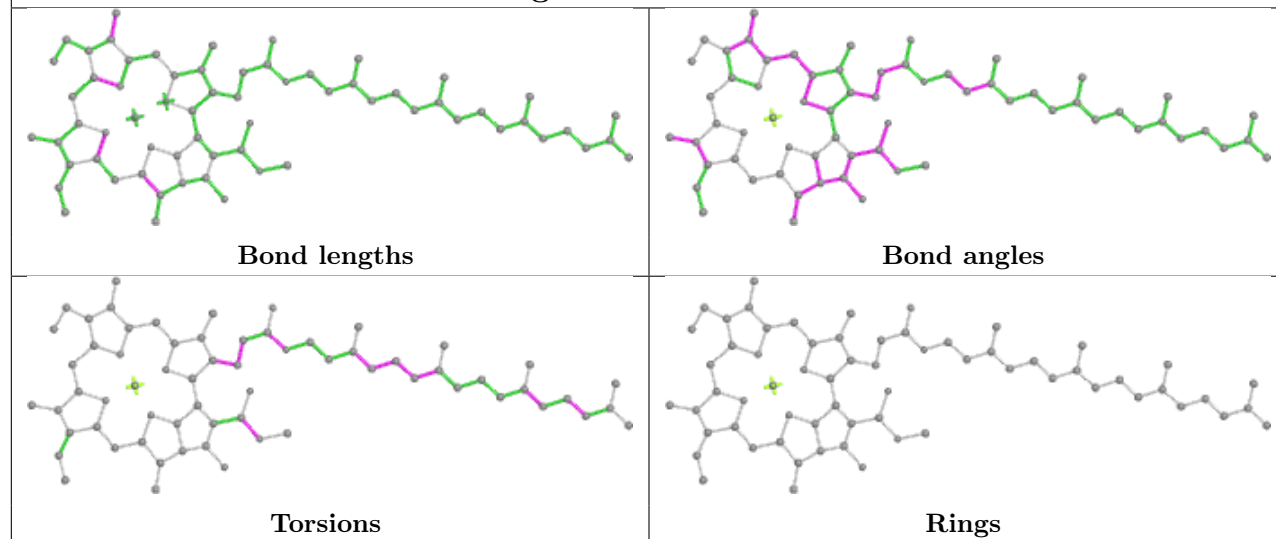
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

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

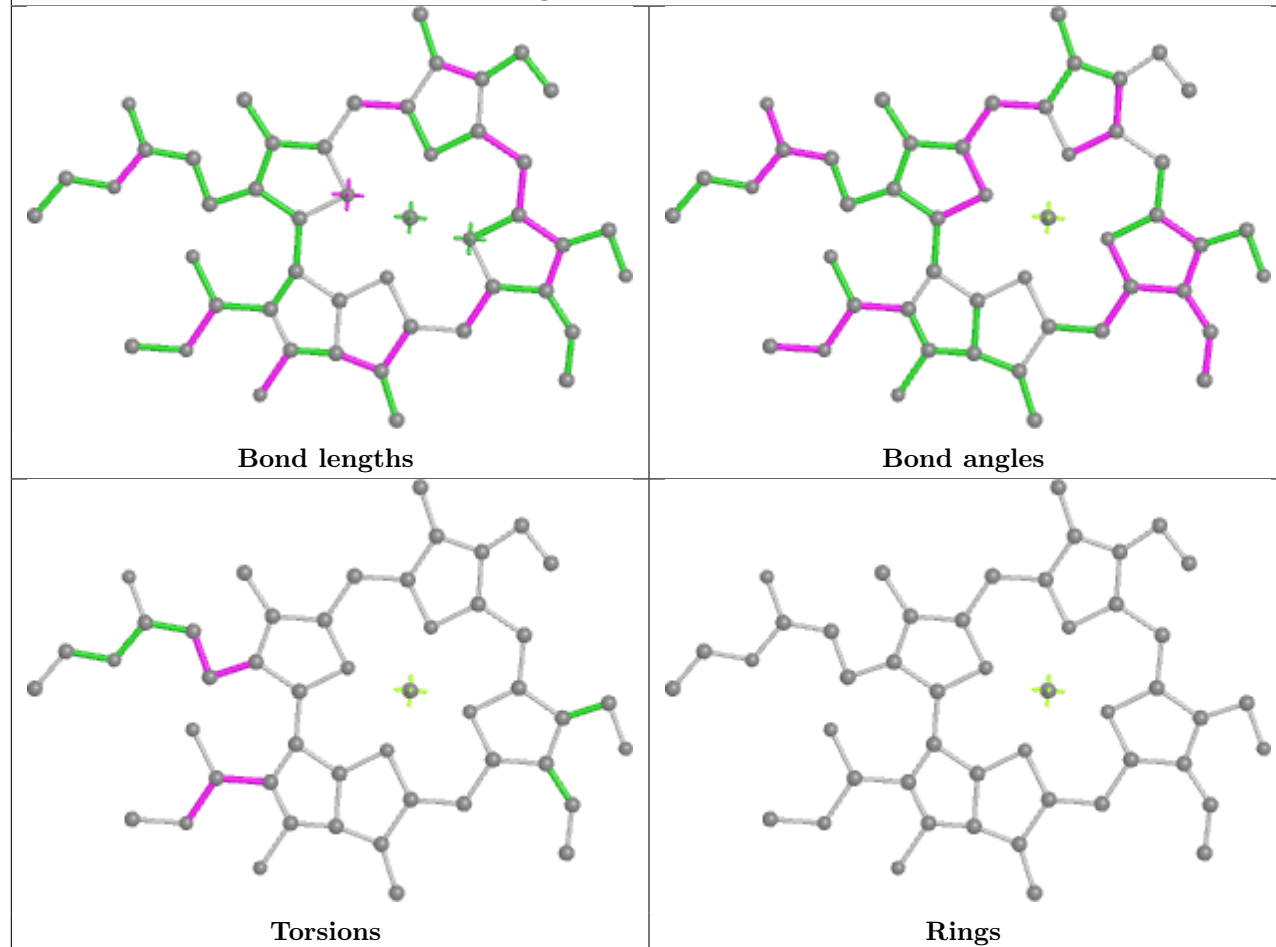


Ligand BCR 1 316**Ligand CLA 4 310****Ligand CLA A 806**

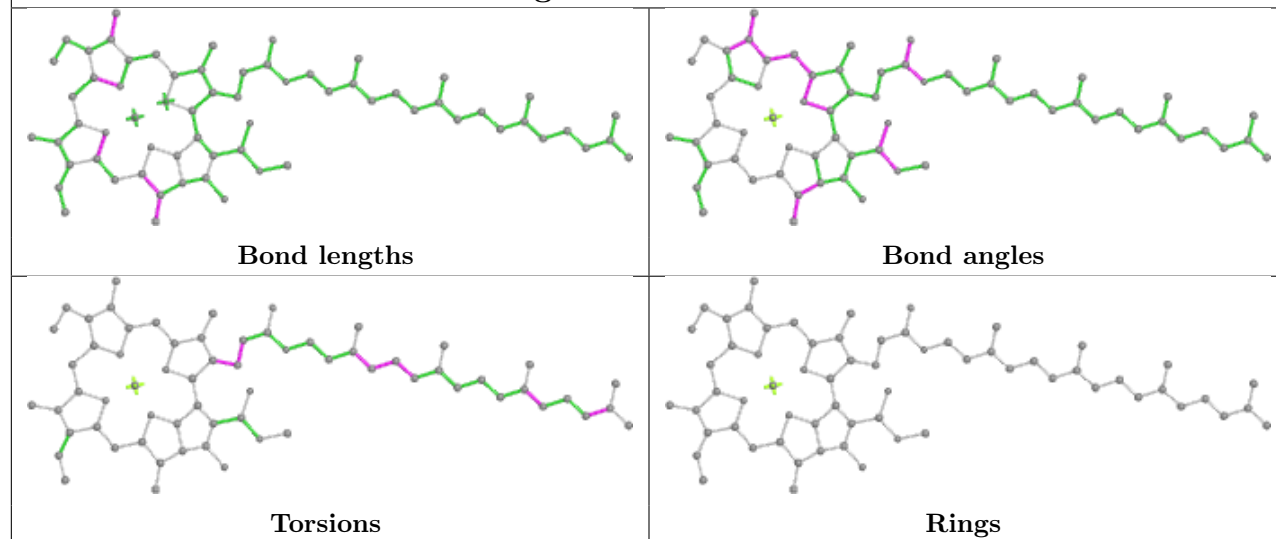
Ligand CLA A 831



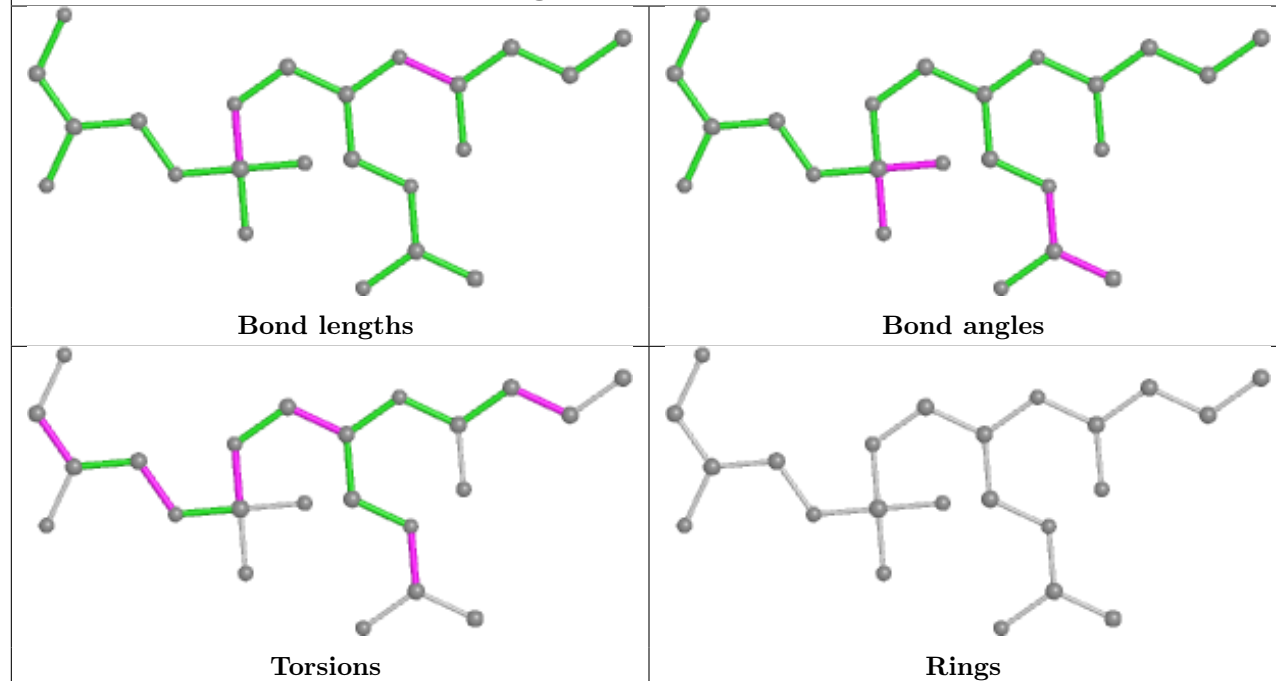
Ligand CHL 1 305



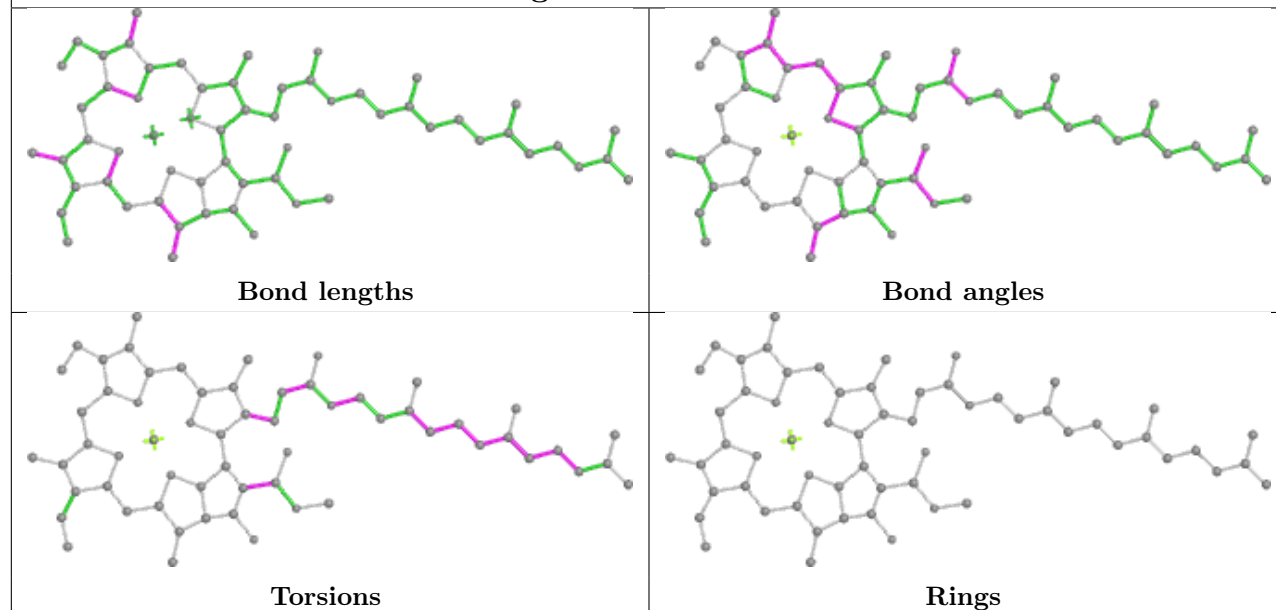
Ligand CLA L 203



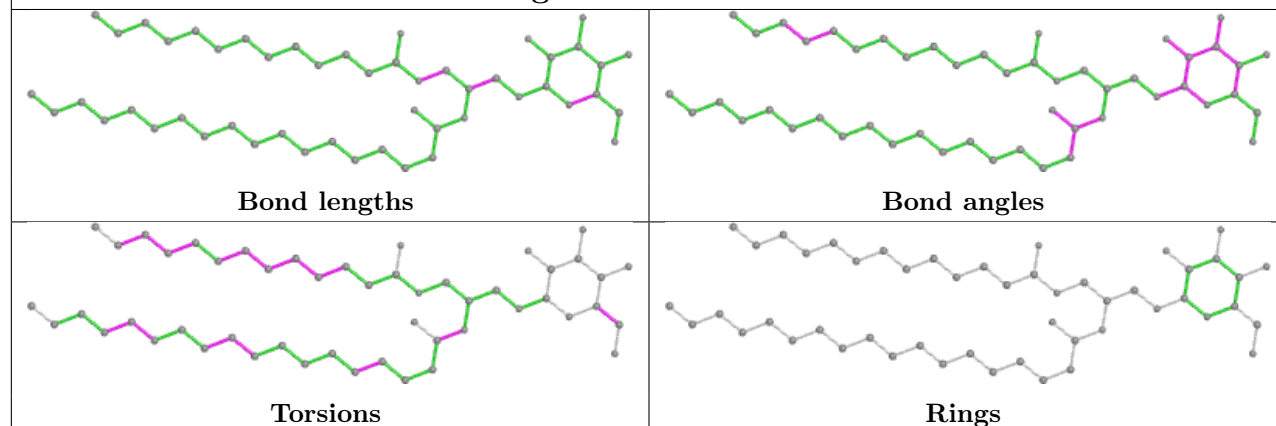
Ligand LHG B 801



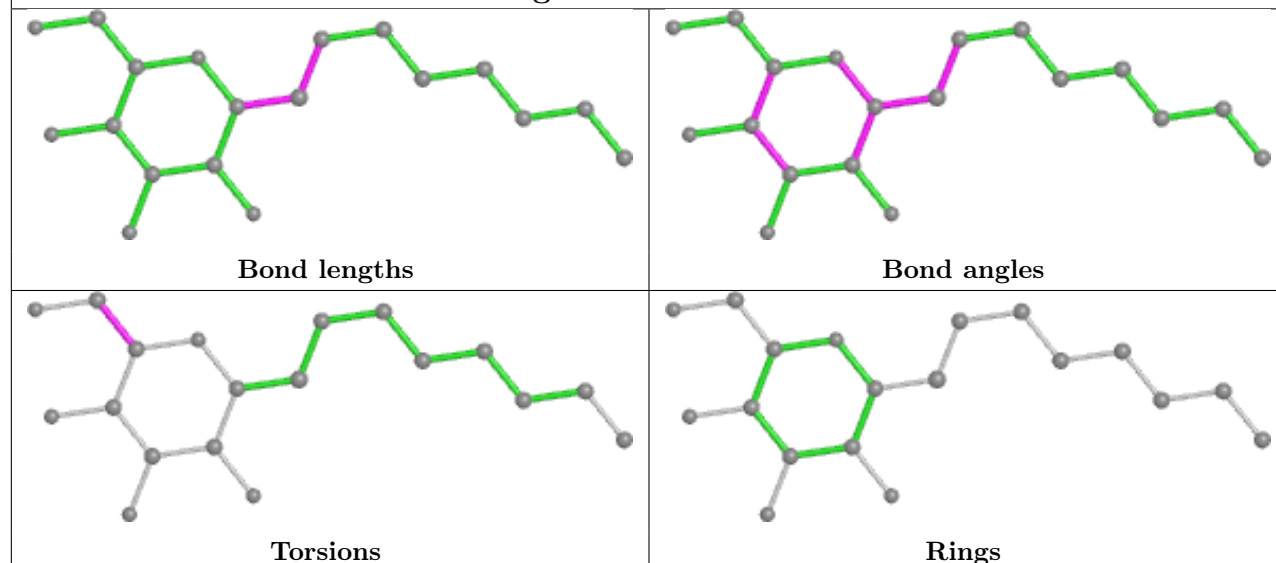
Ligand CLA K 202

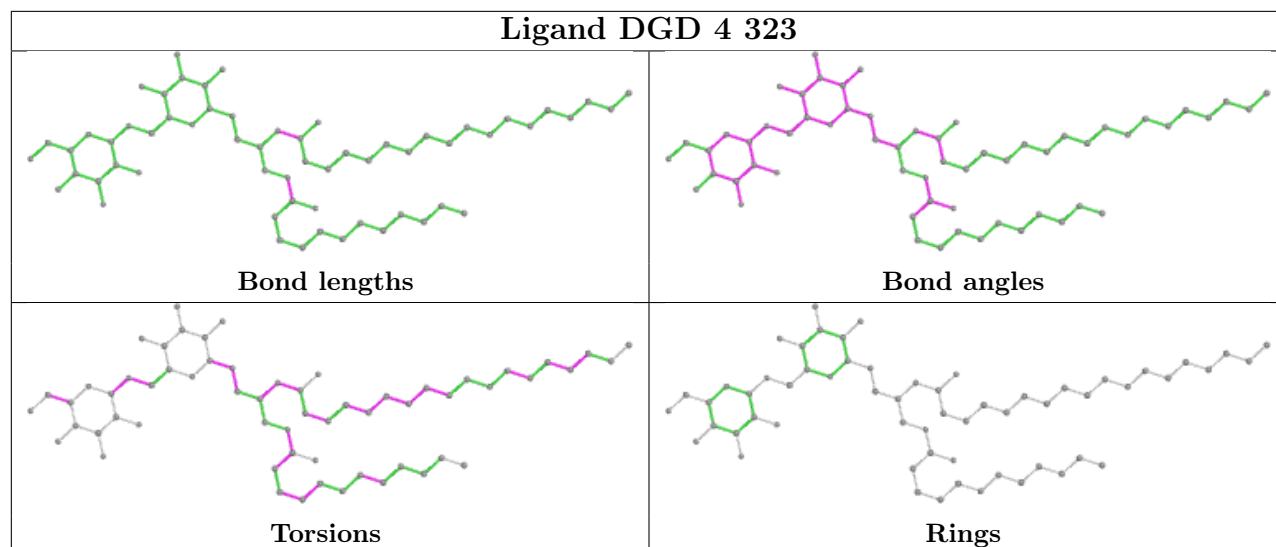
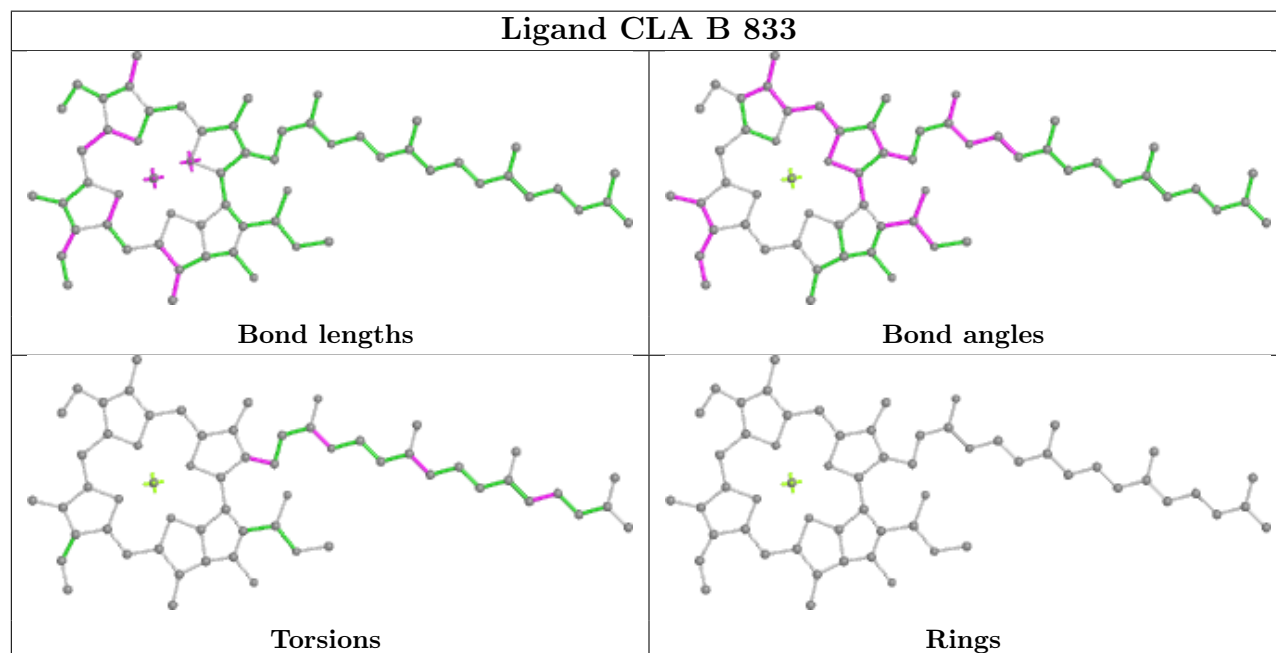


Ligand LMG 4 319

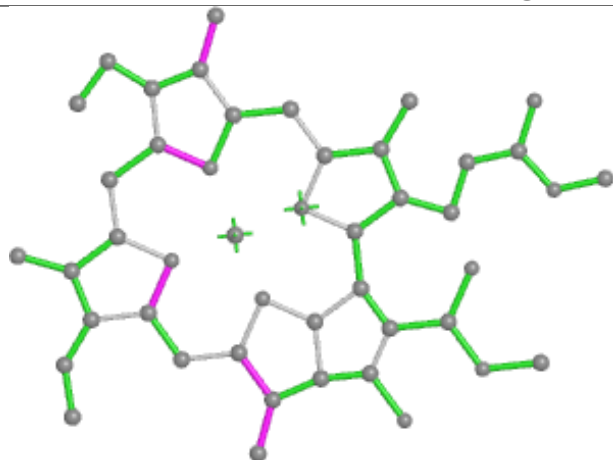


Ligand HTG 4 322

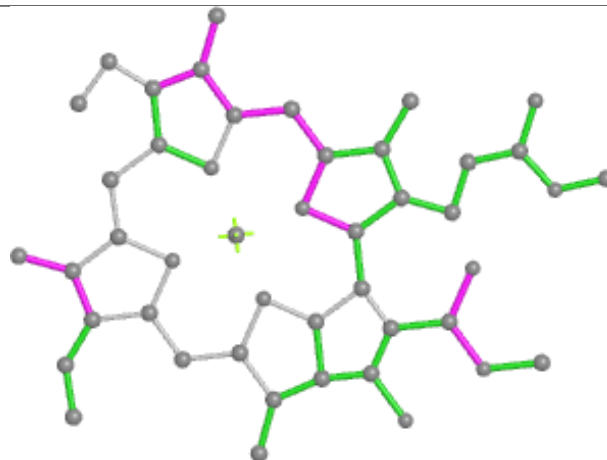


Ligand DGD 4 323**Ligand CLA B 833**

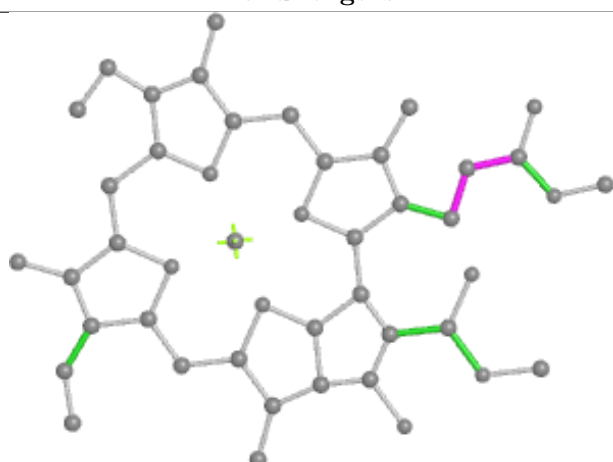
Ligand CLA 3 613



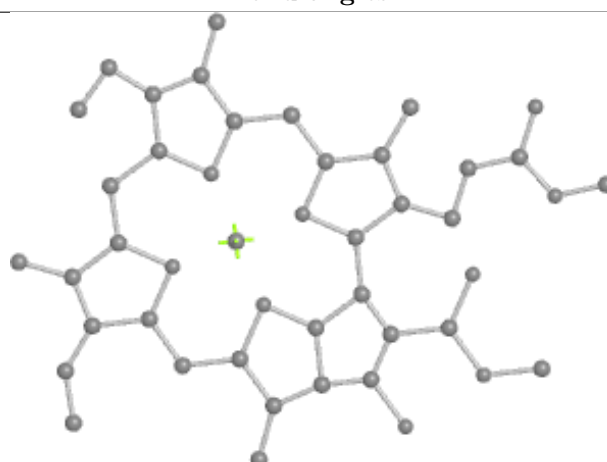
Bond lengths



Bond angles

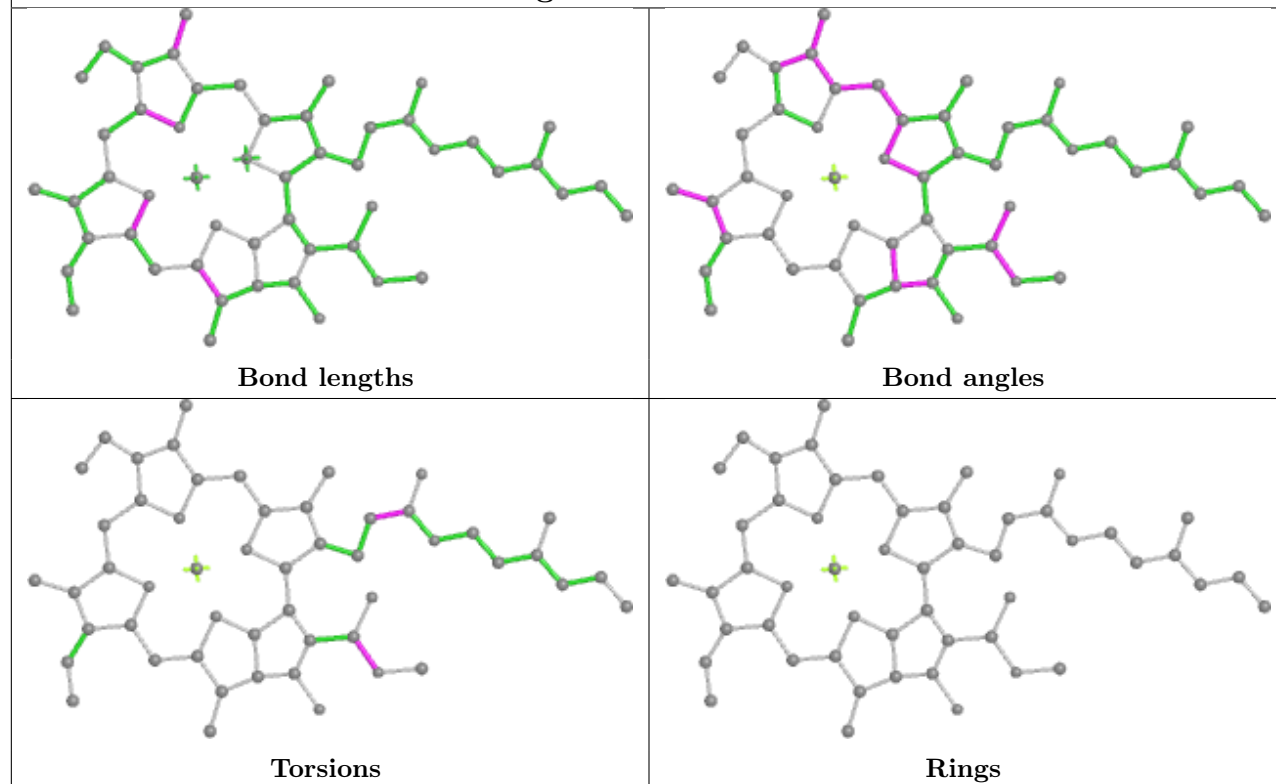


Torsions

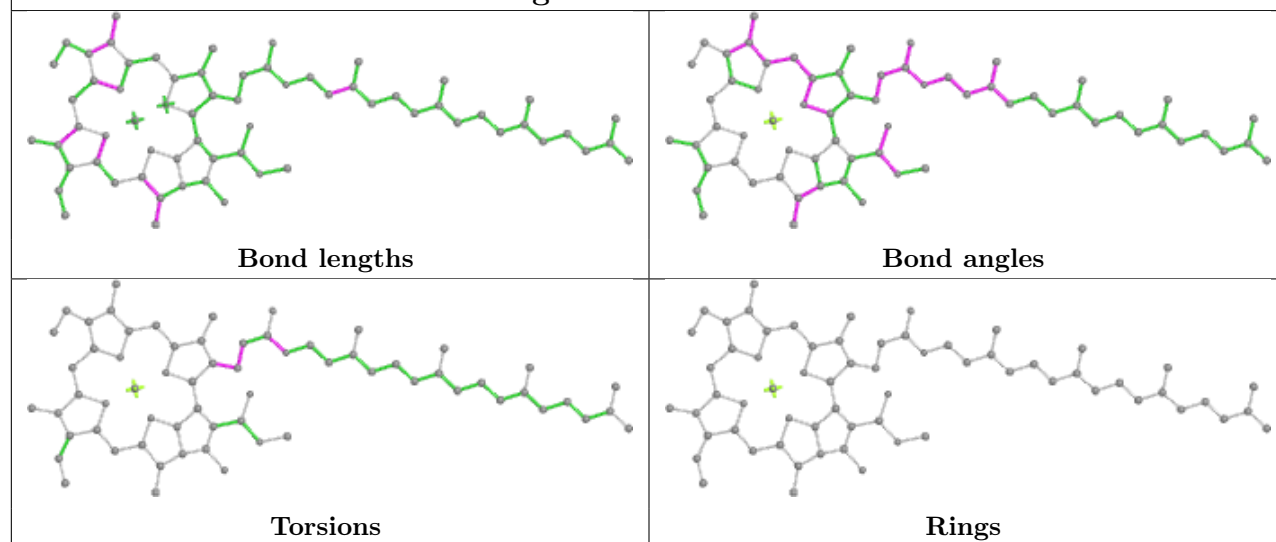


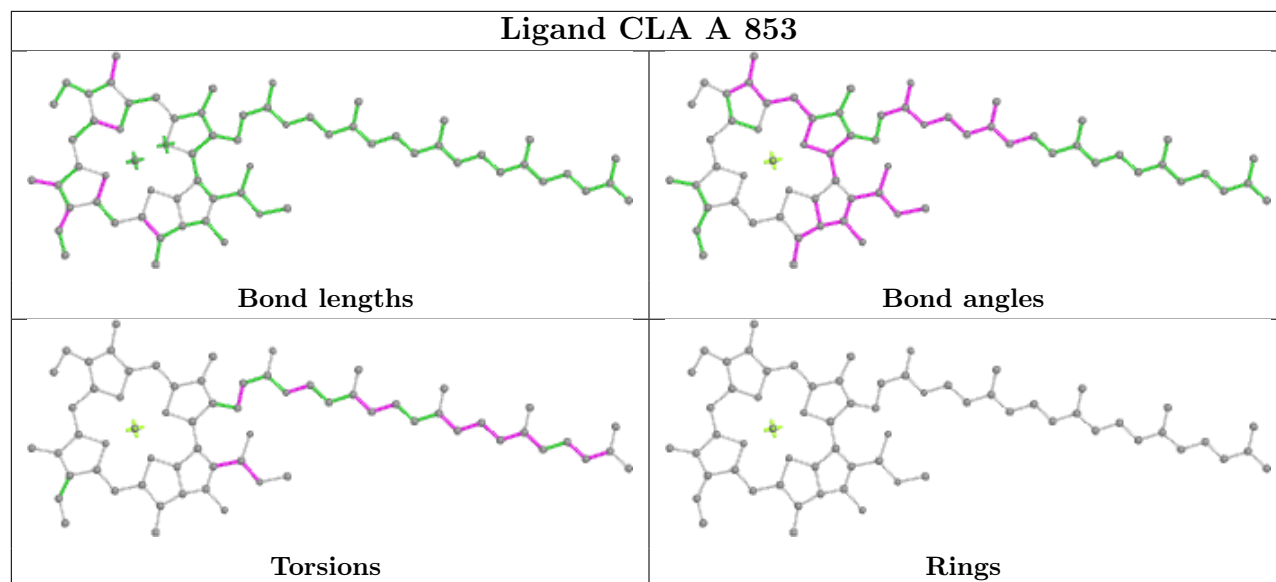
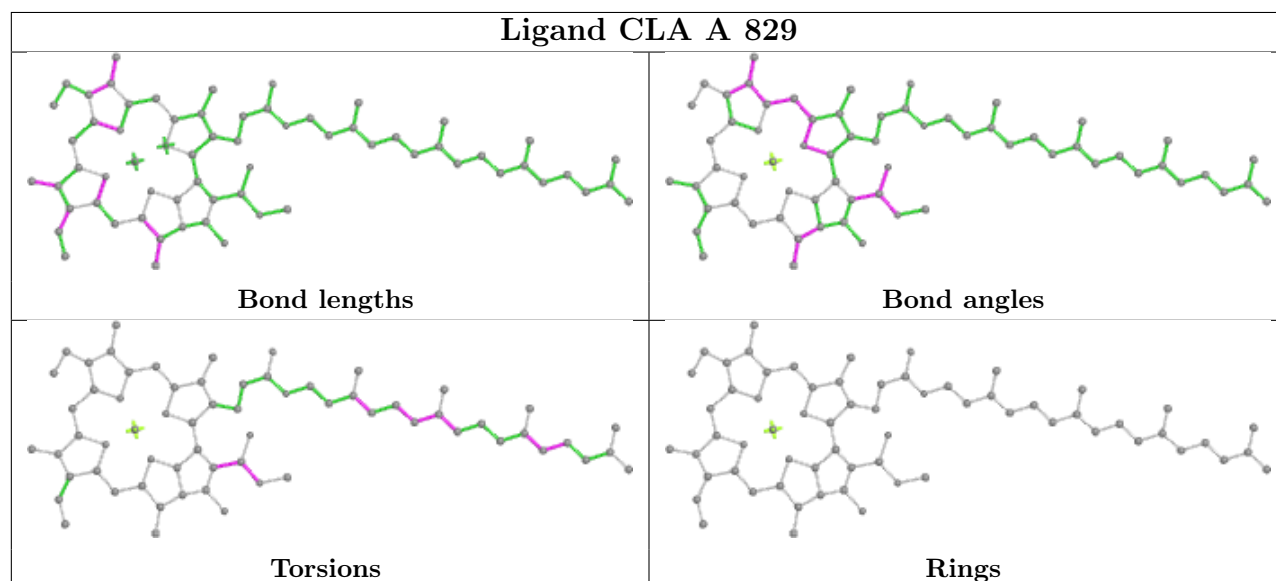
Rings

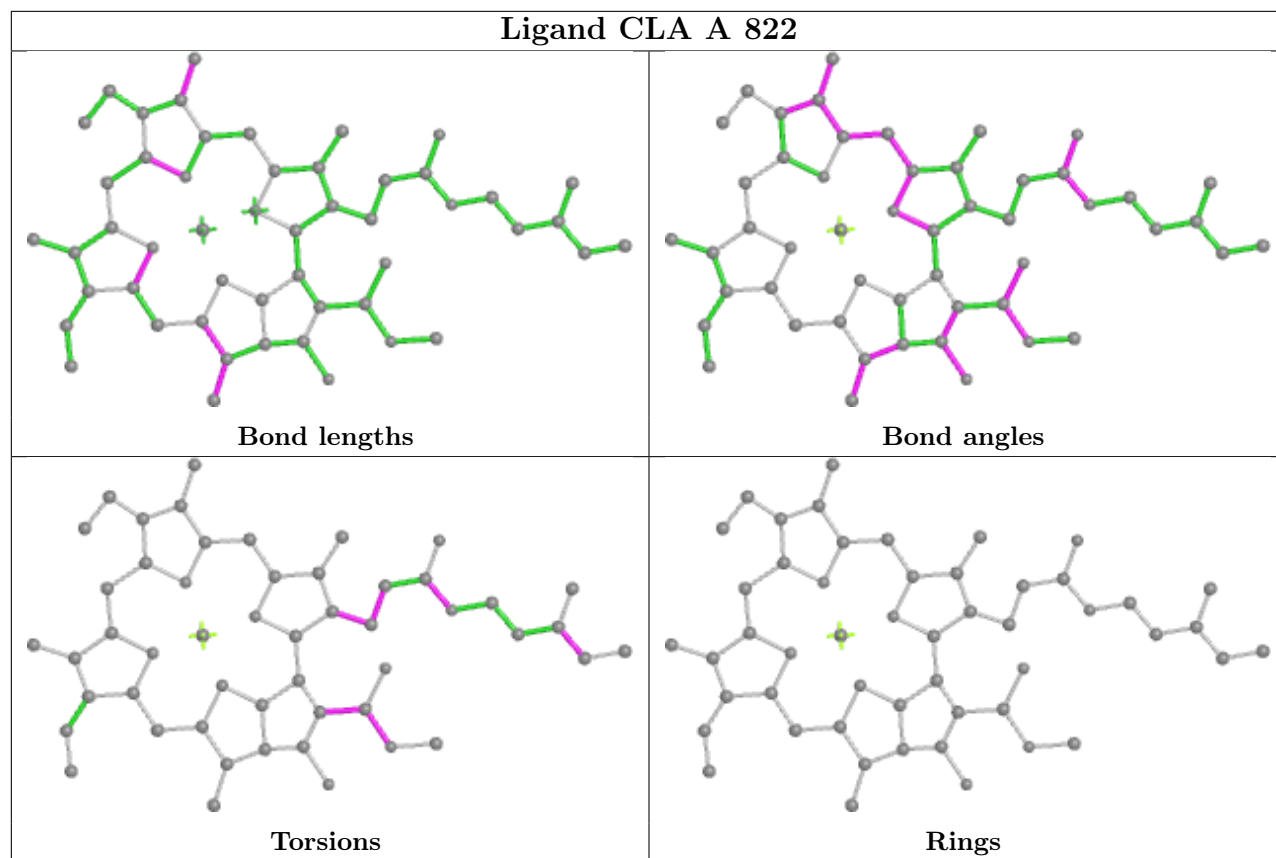
Ligand CLA 4 311



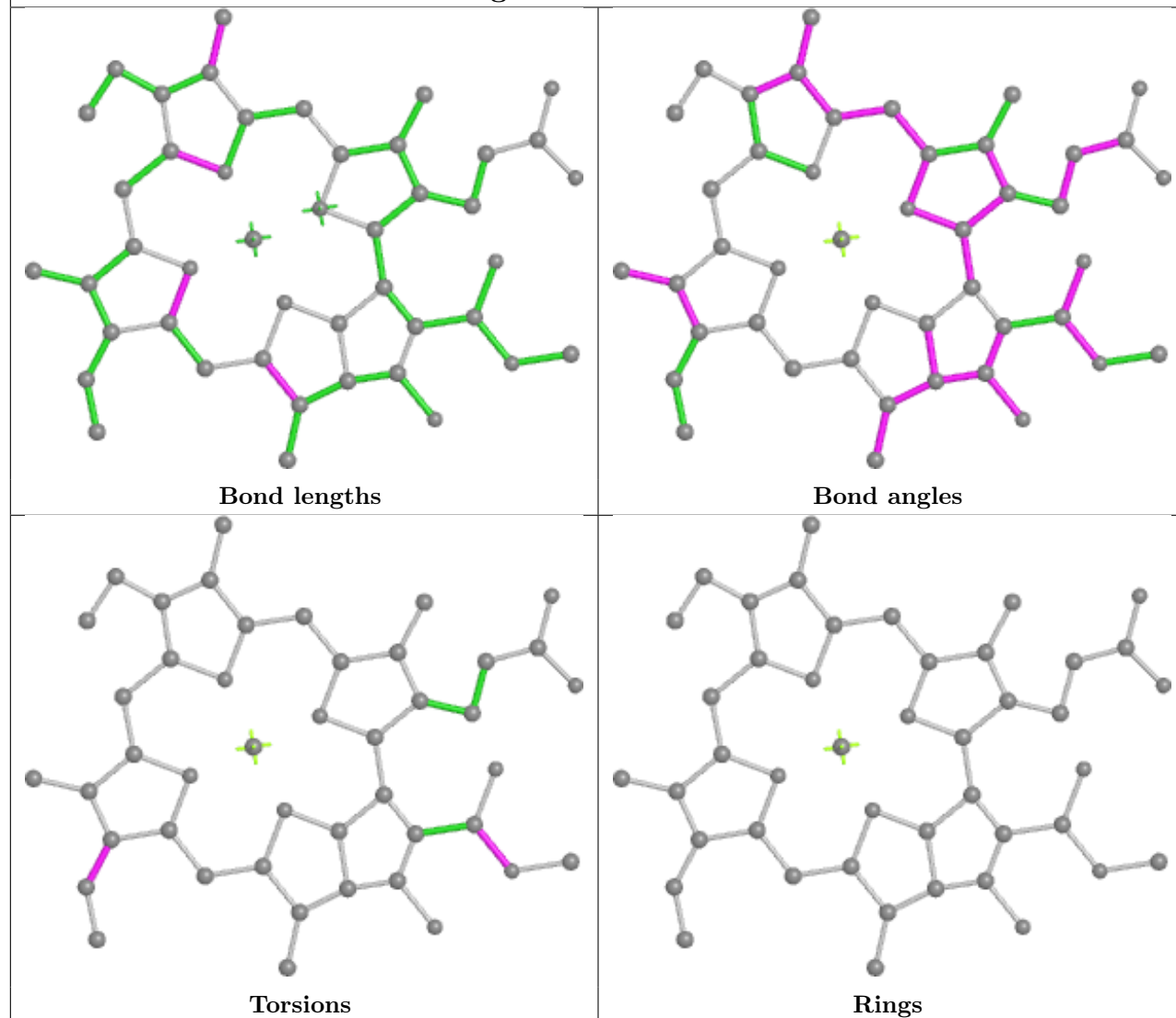
Ligand CLA B 830



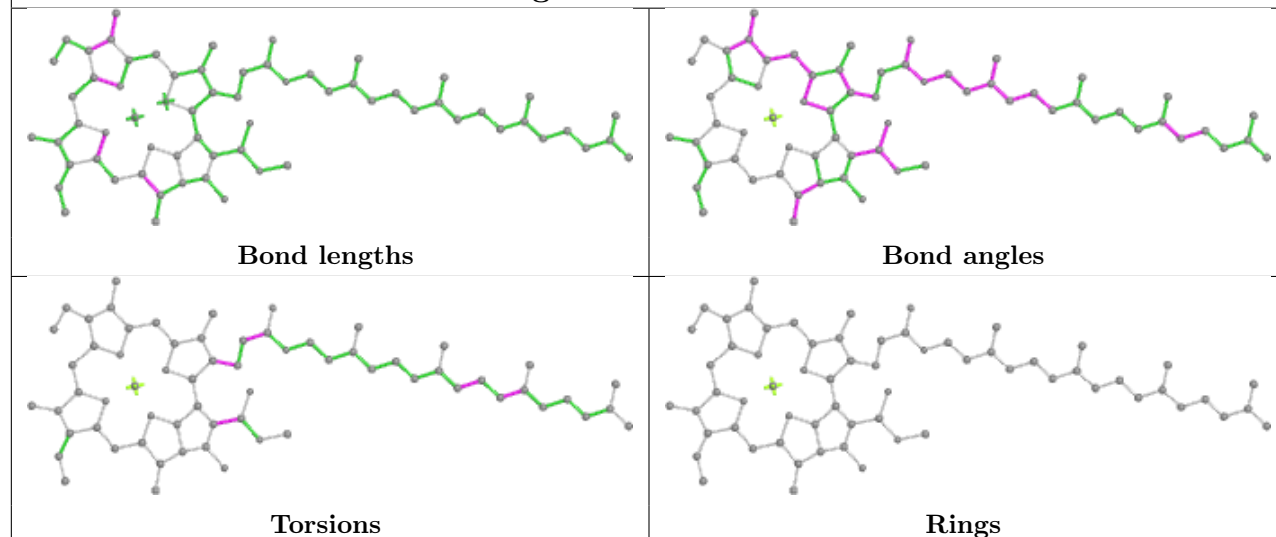
Ligand CLA A 853**Ligand CLA A 829**



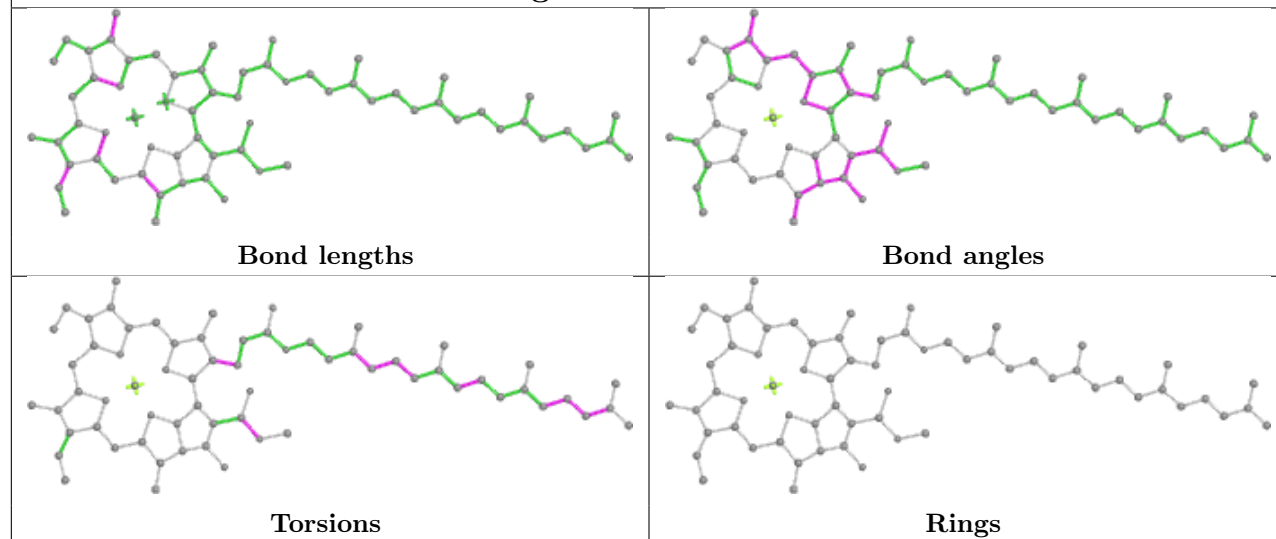
Ligand CLA B 836



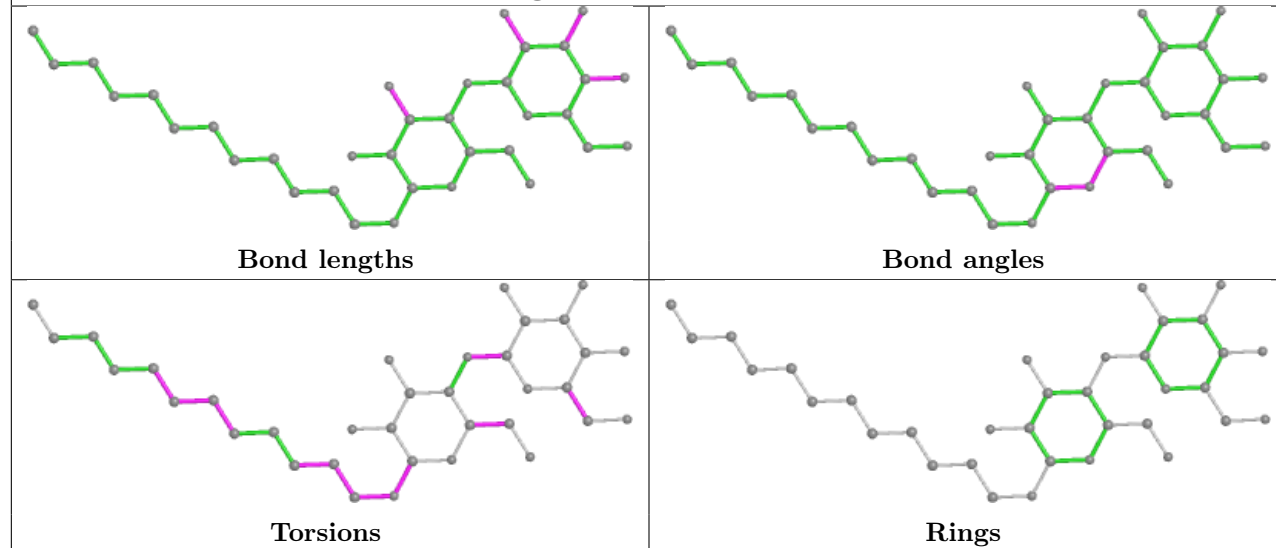
Ligand CLA B 842



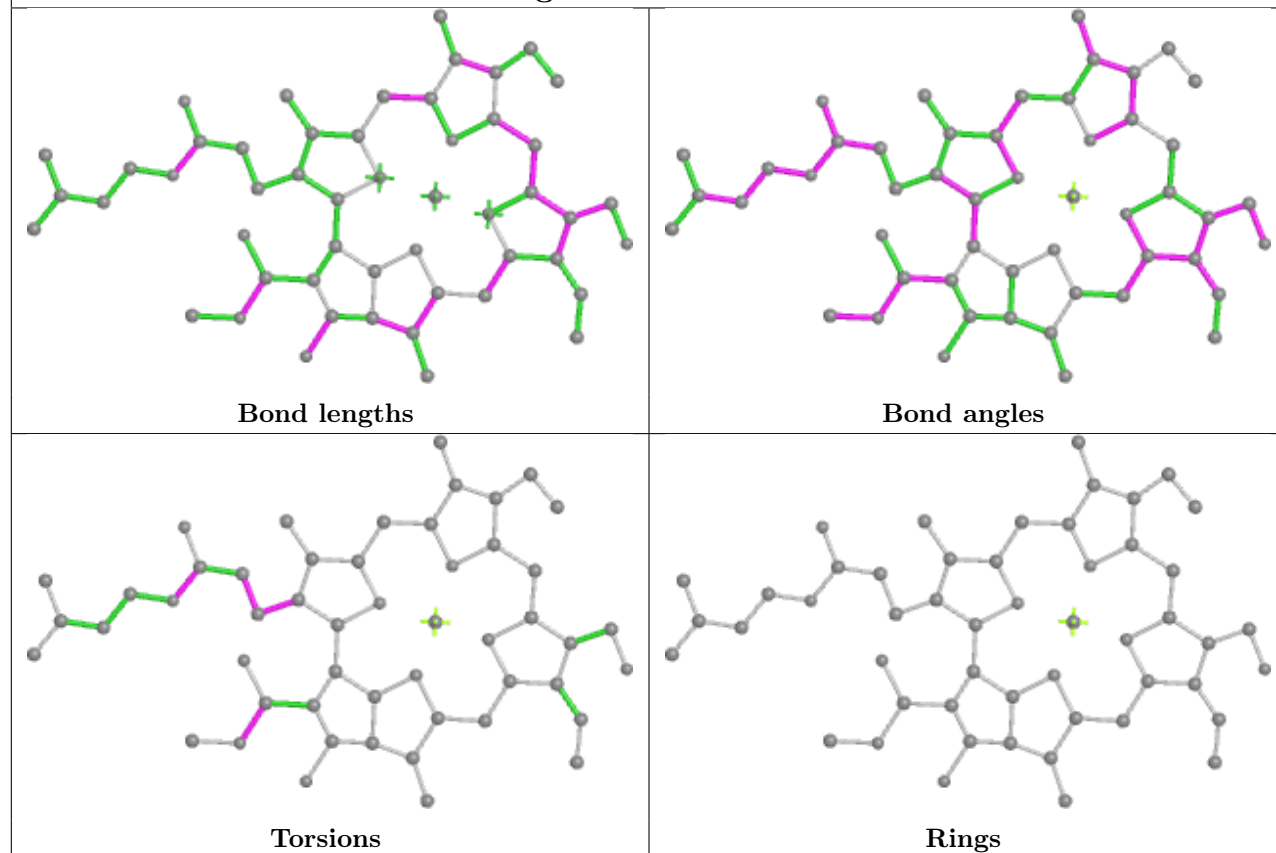
Ligand CLA A 810



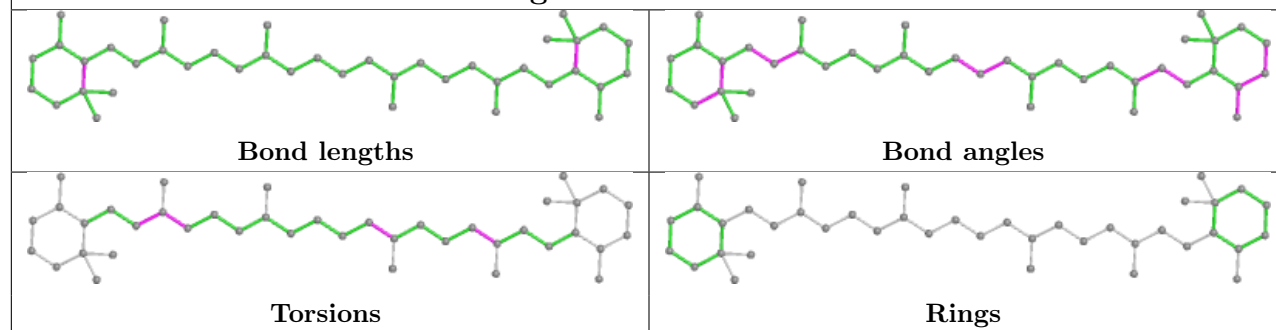
Ligand LMT A 855

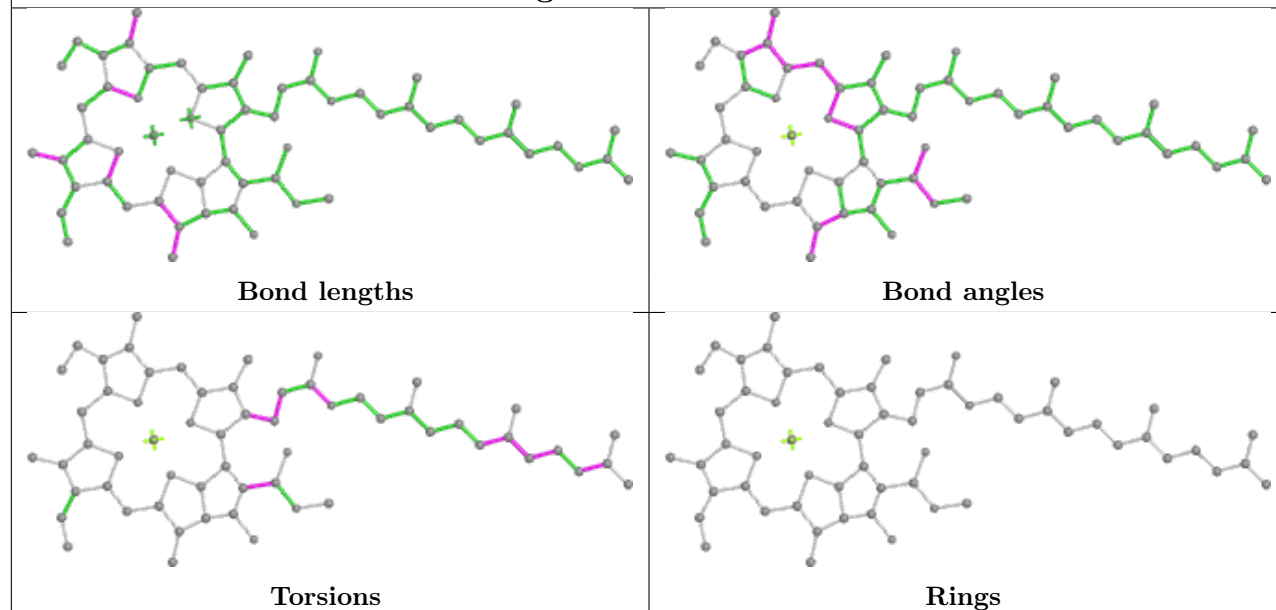
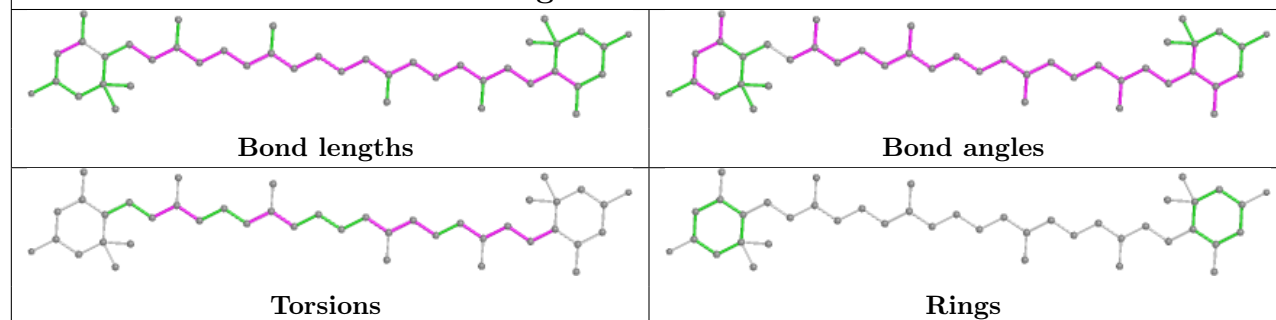
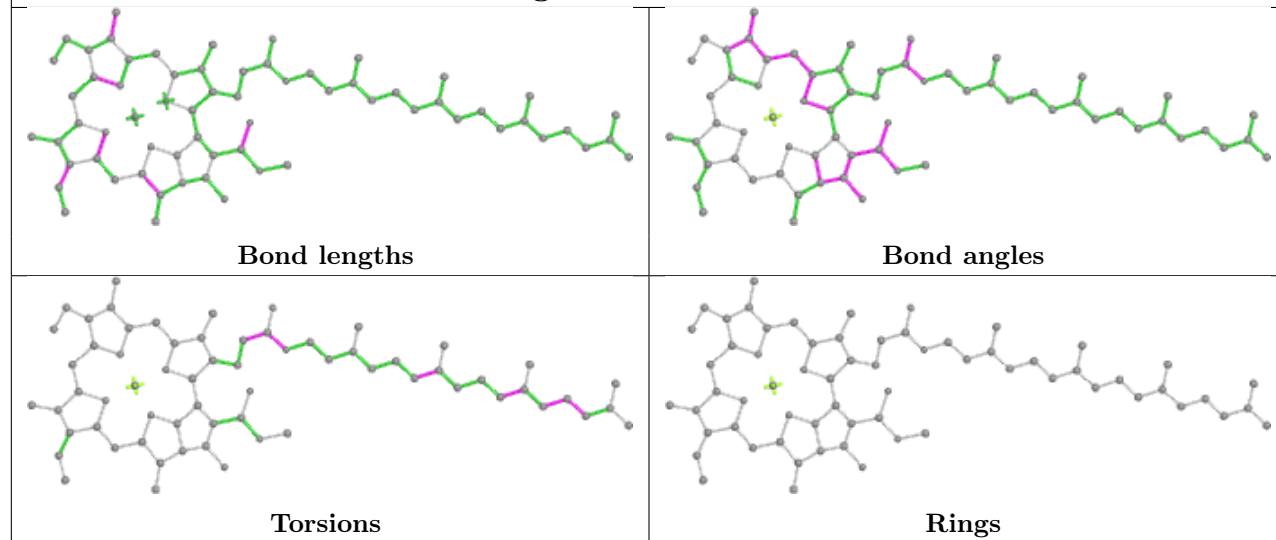


Ligand CHL 4 306

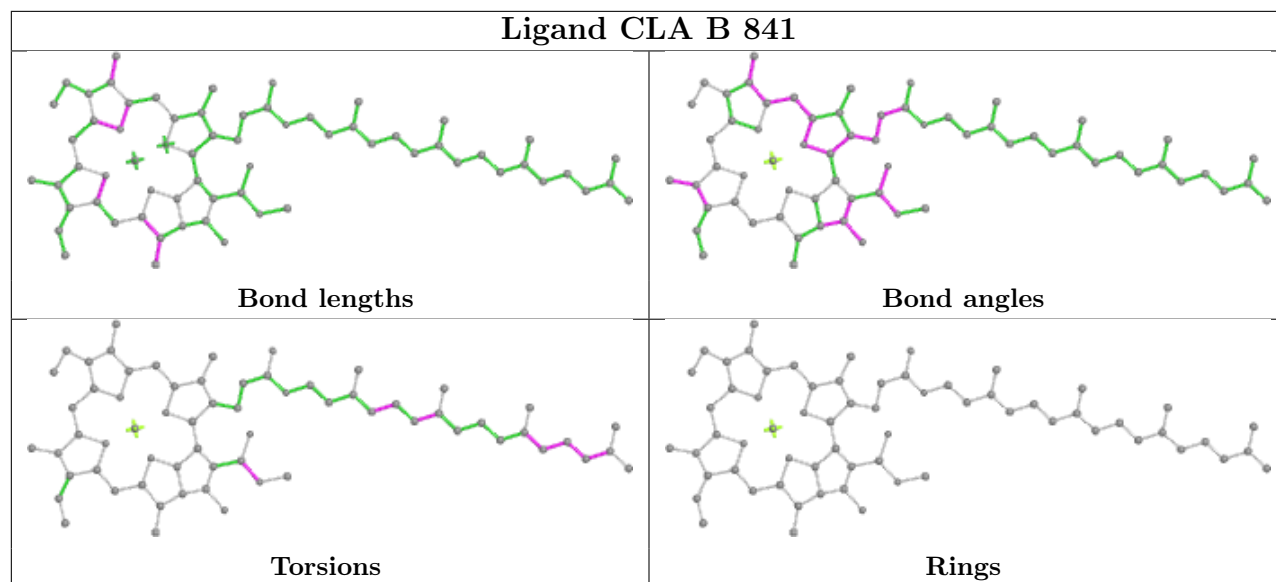


Ligand BCR A 851

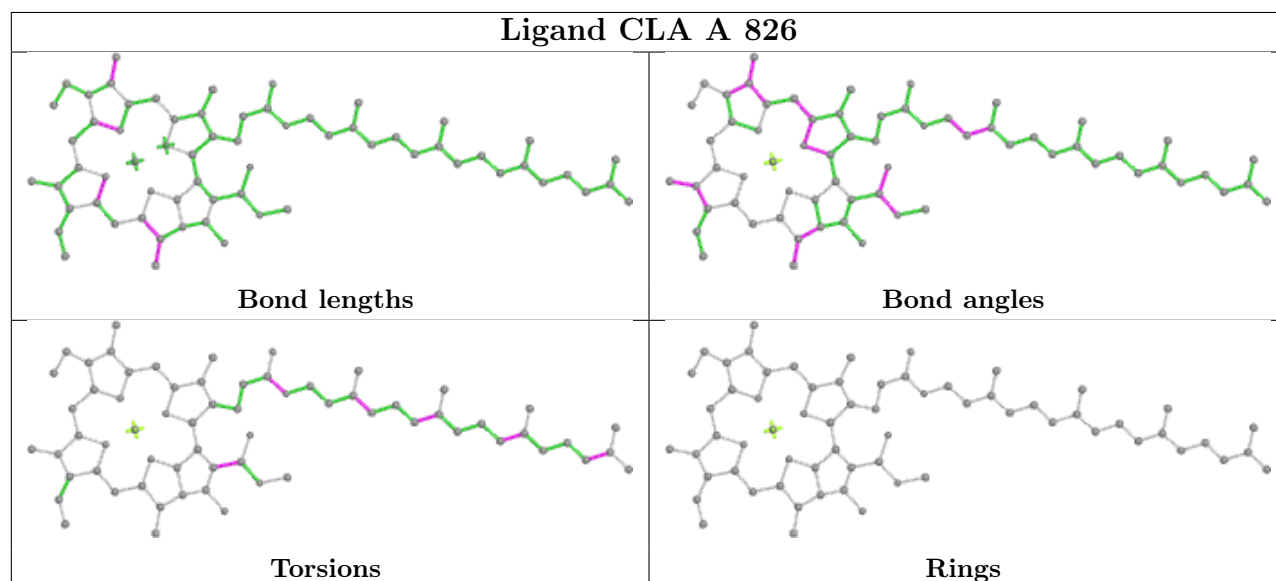


Ligand CLA 2 308**Ligand LUT 3 614****Ligand CLA B 816**

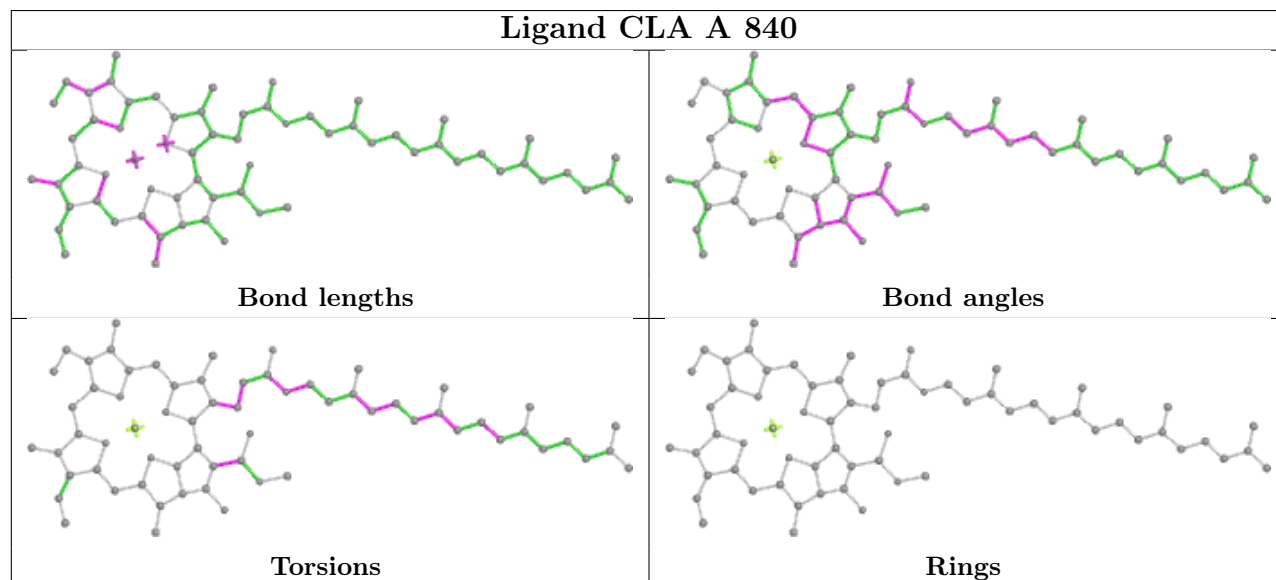
Ligand CLA B 841

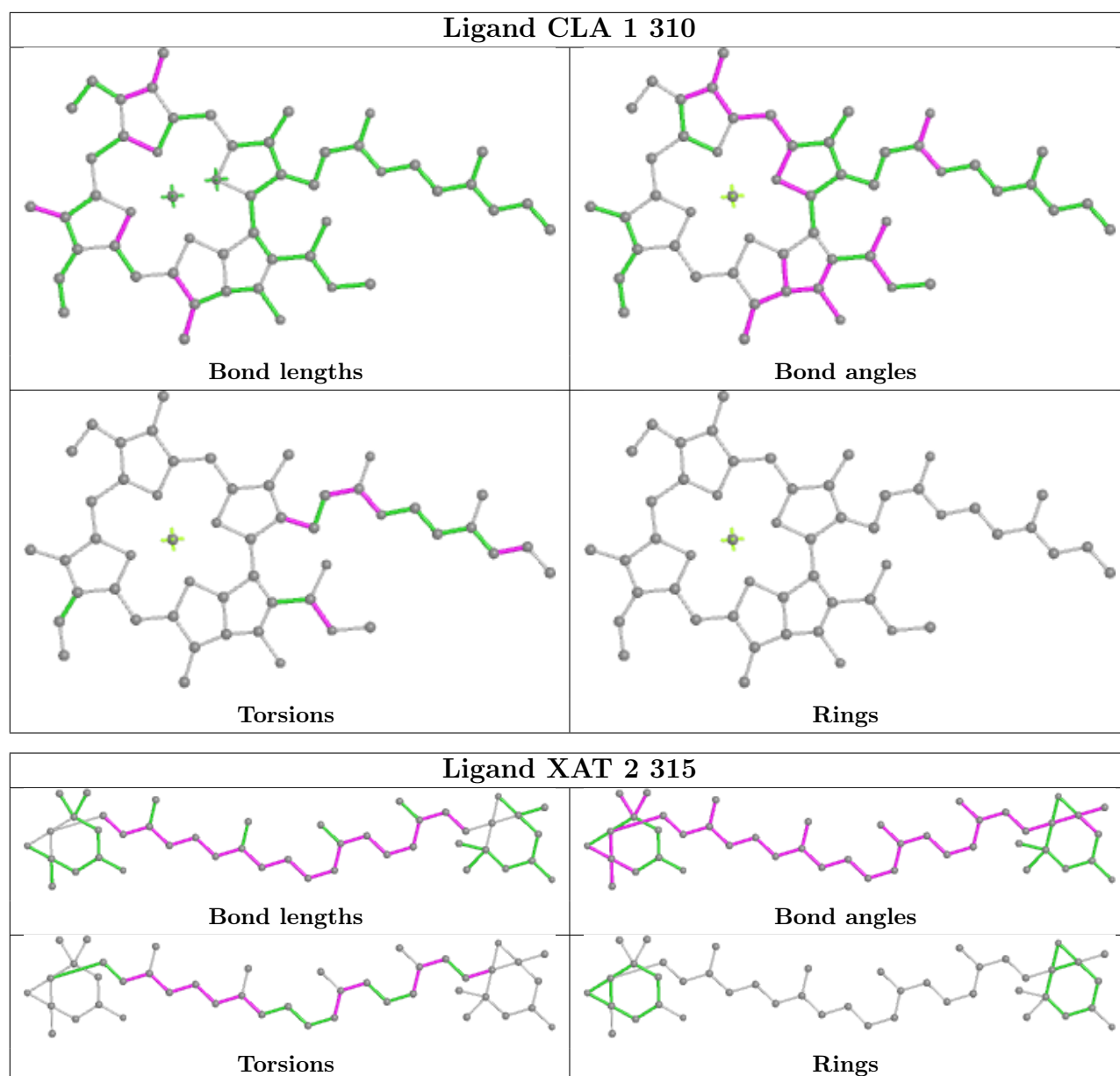


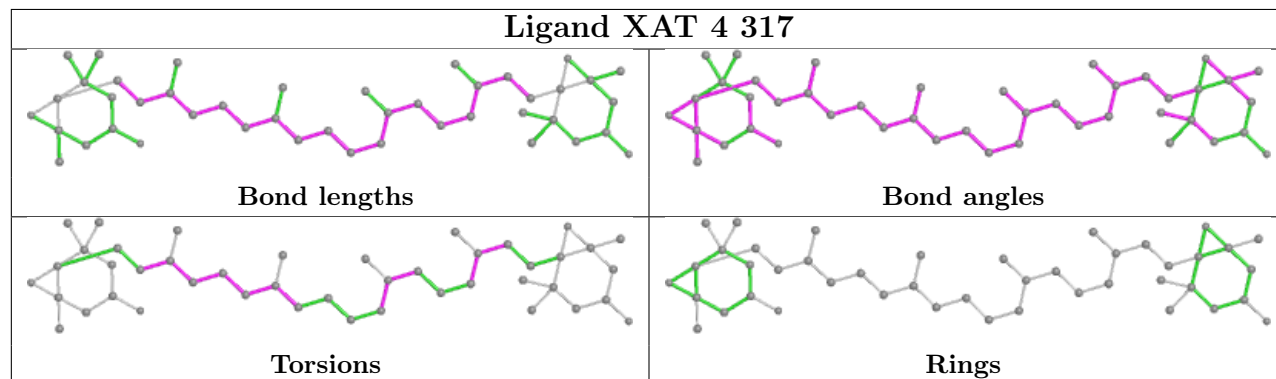
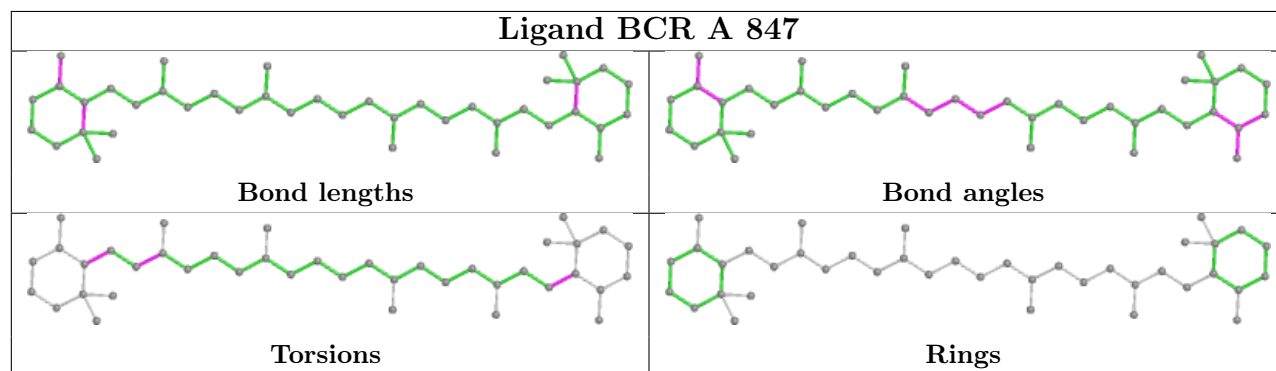
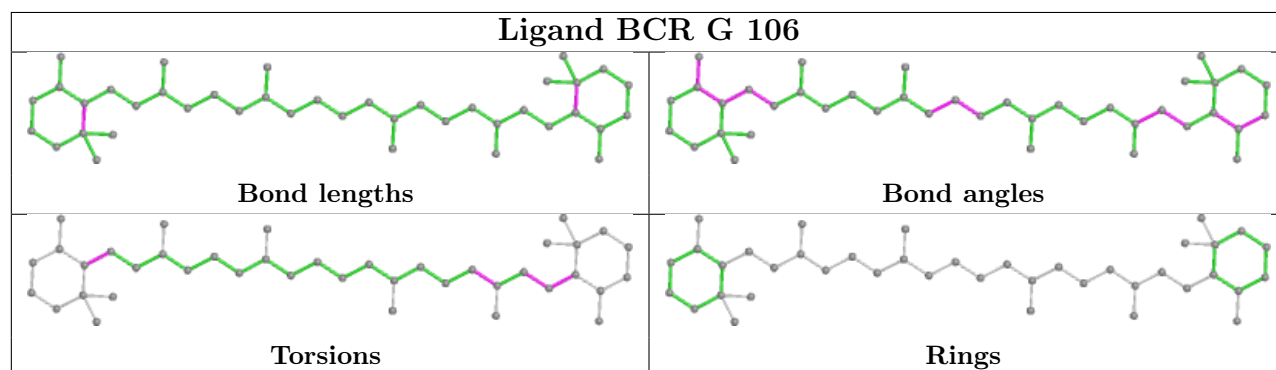
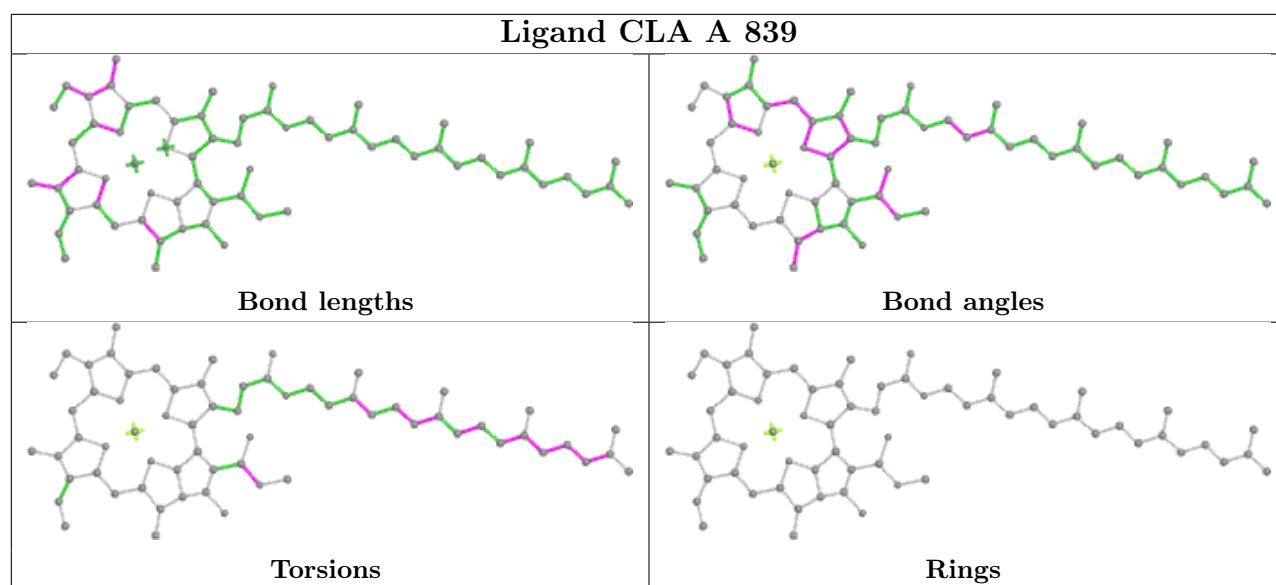
Ligand CLA A 826



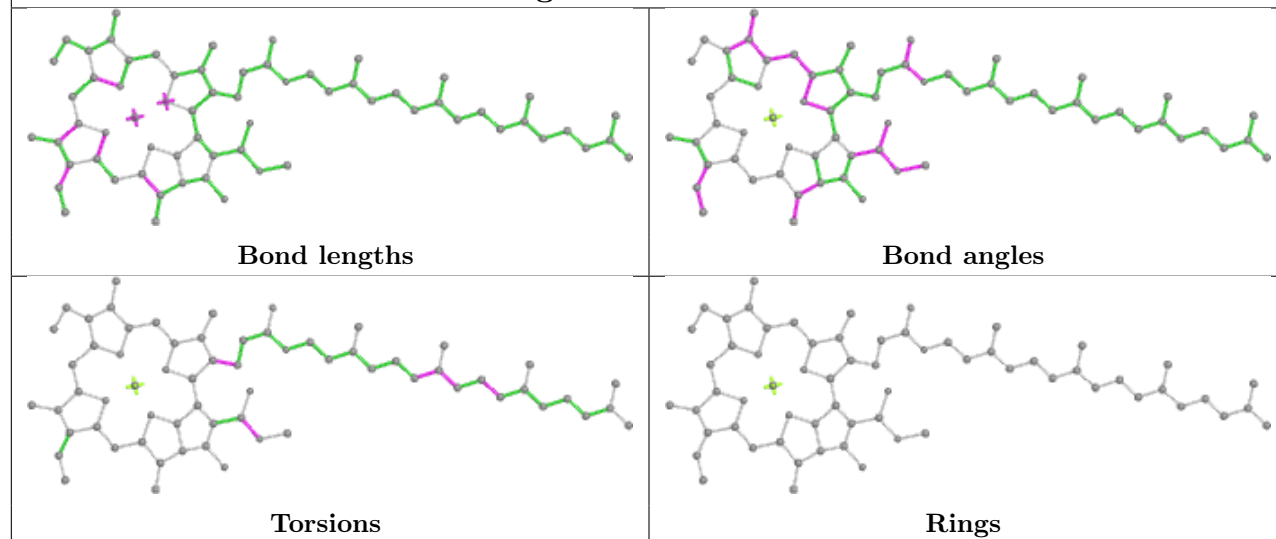
Ligand CLA A 840



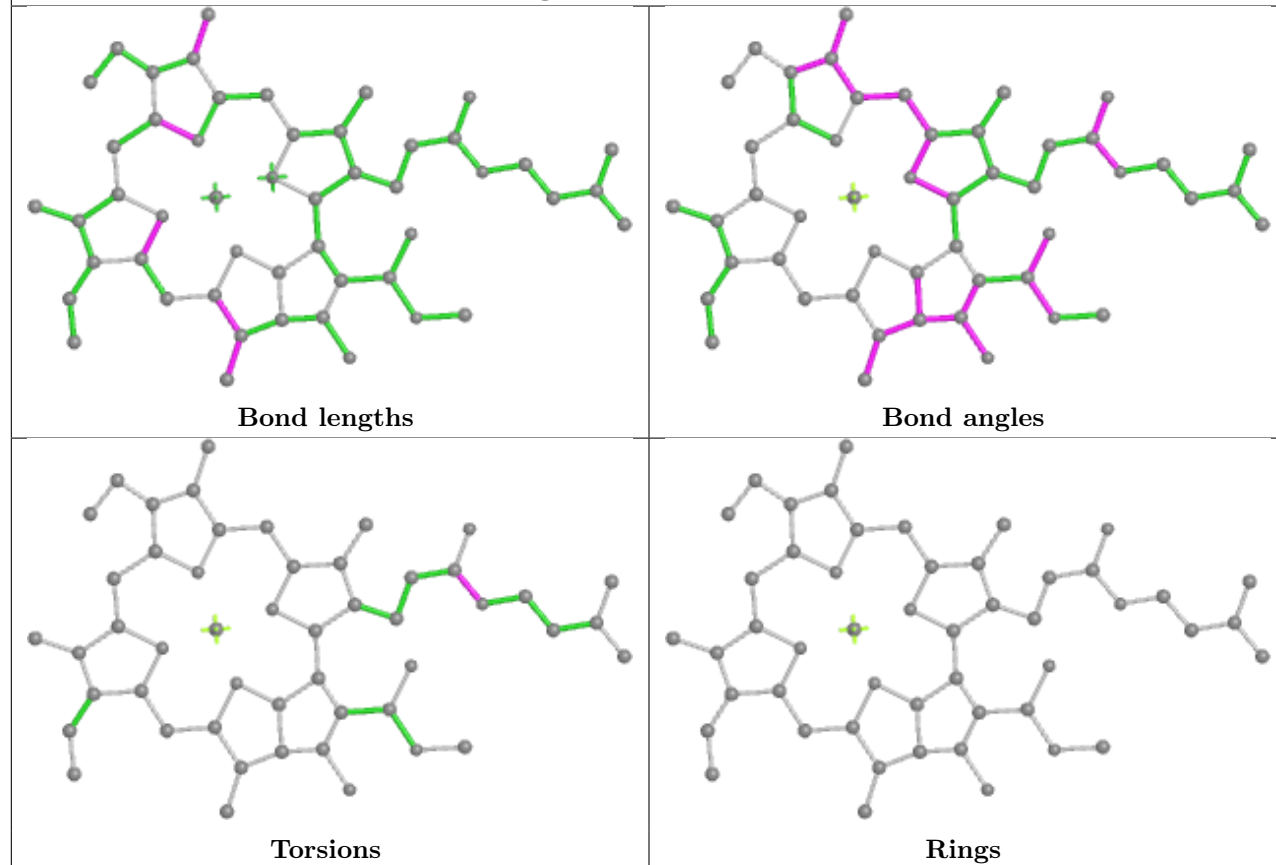




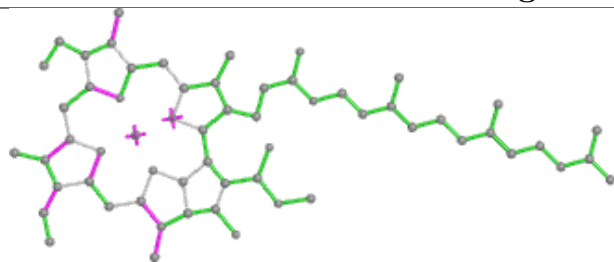
Ligand CLA J 101



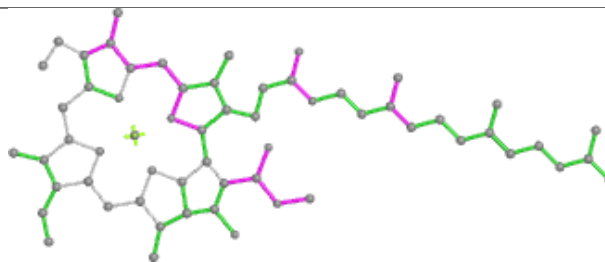
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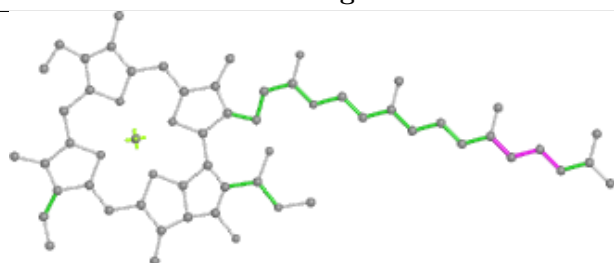
Ligand CLA 4 302



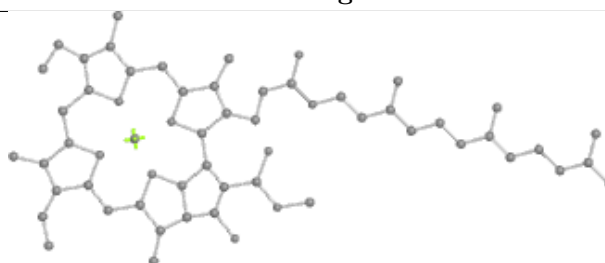
Bond lengths



Bond angles

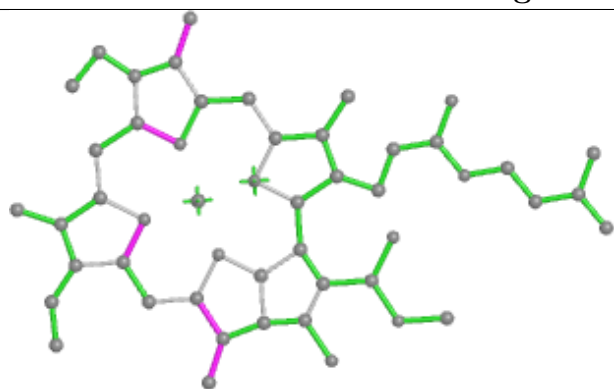


Torsions

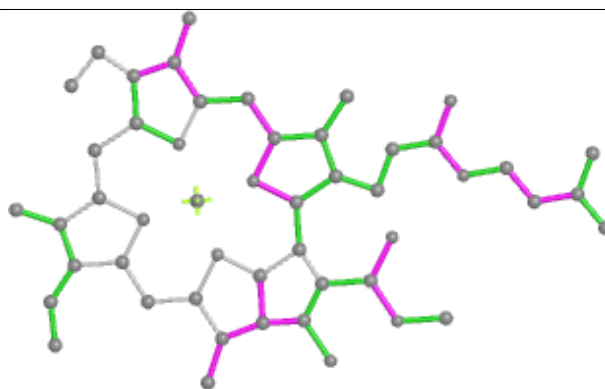


Rings

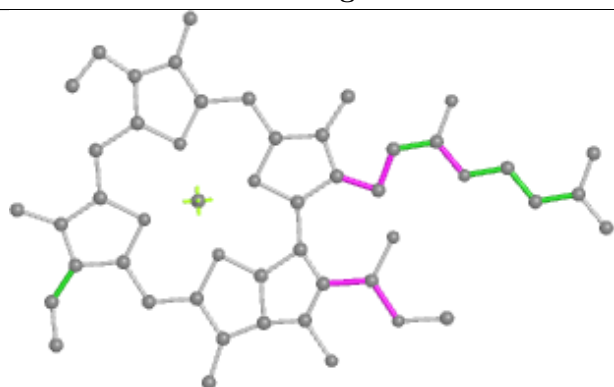
Ligand CLA A 814



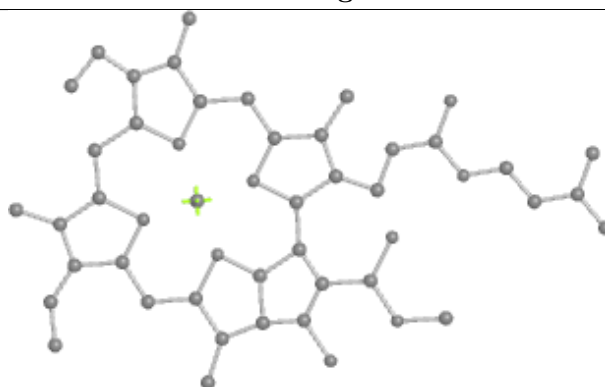
Bond lengths



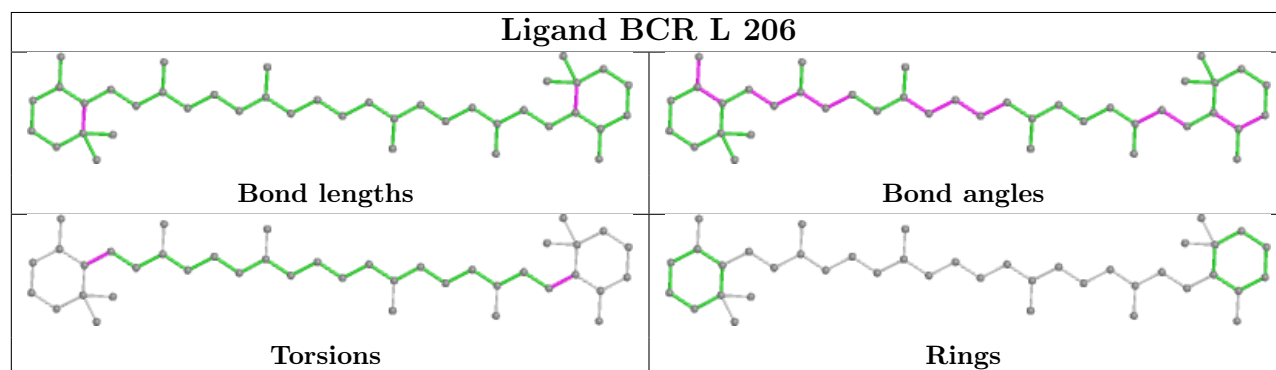
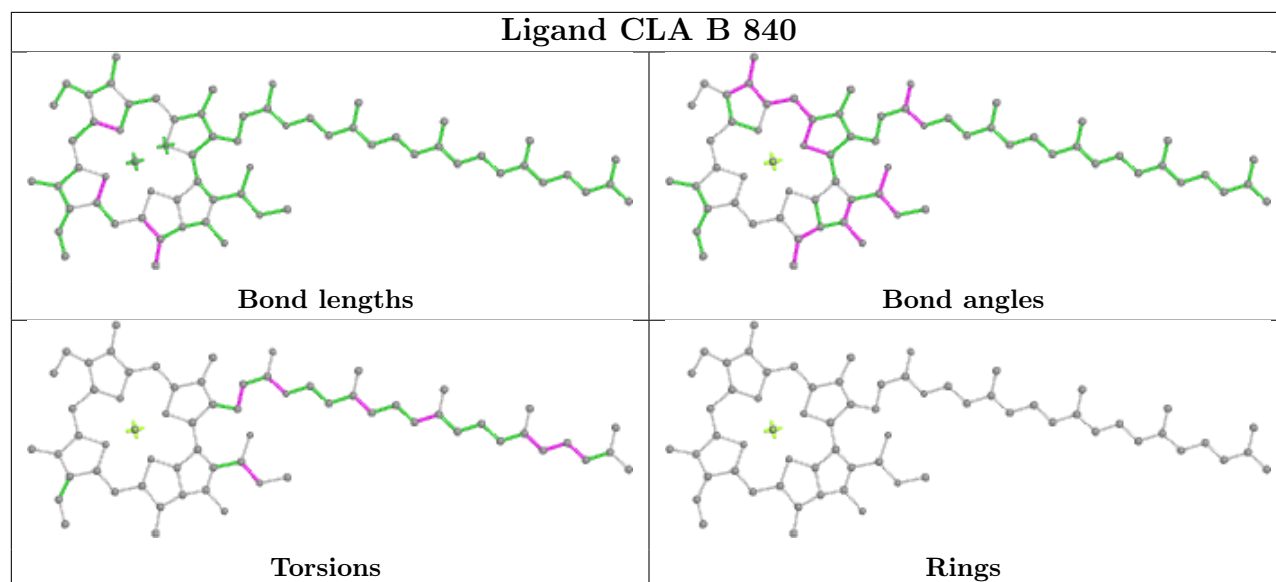
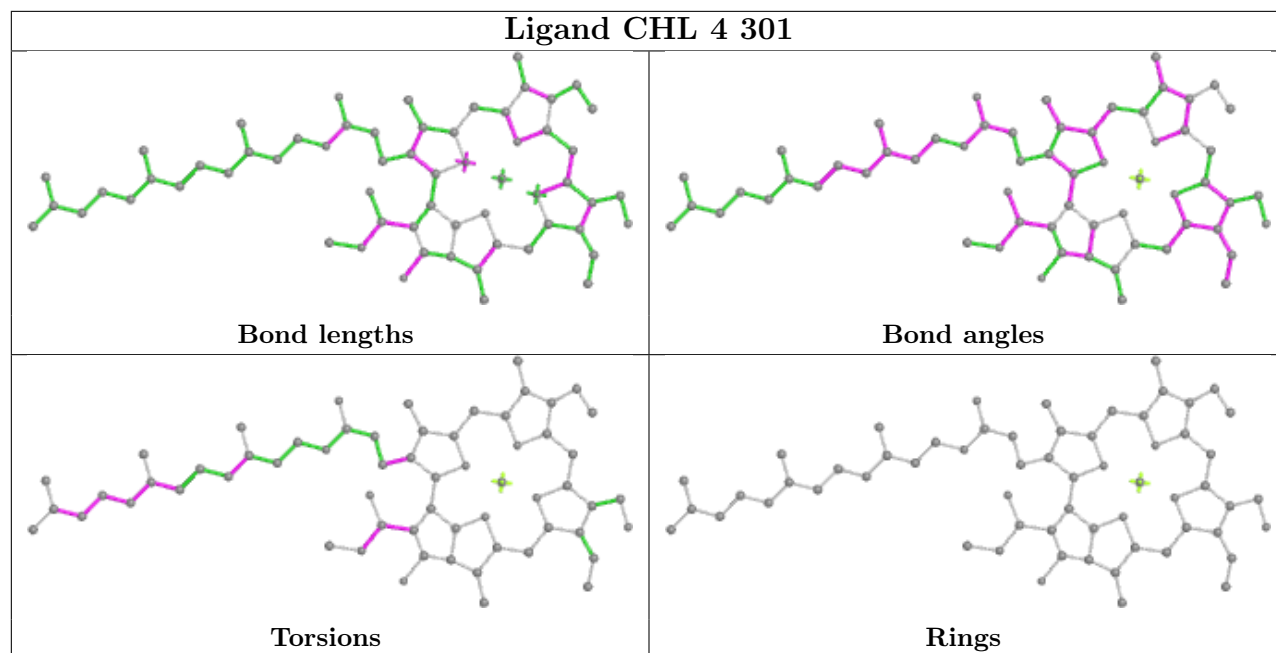
Bond angles



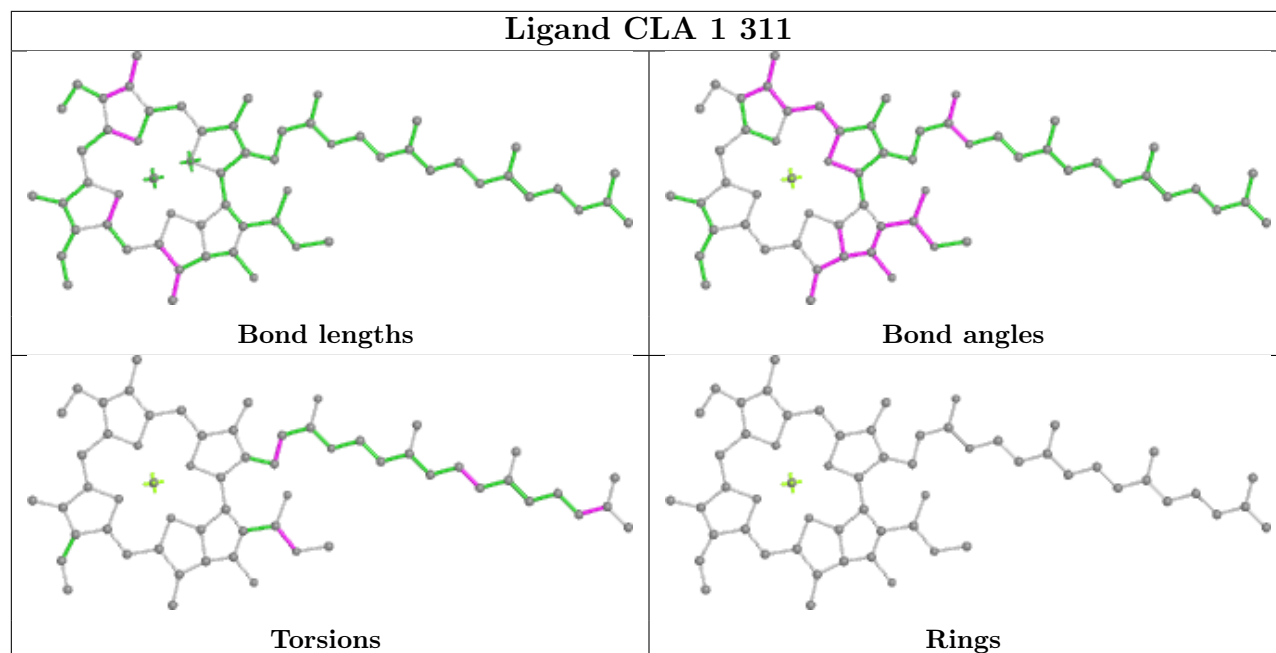
Torsions



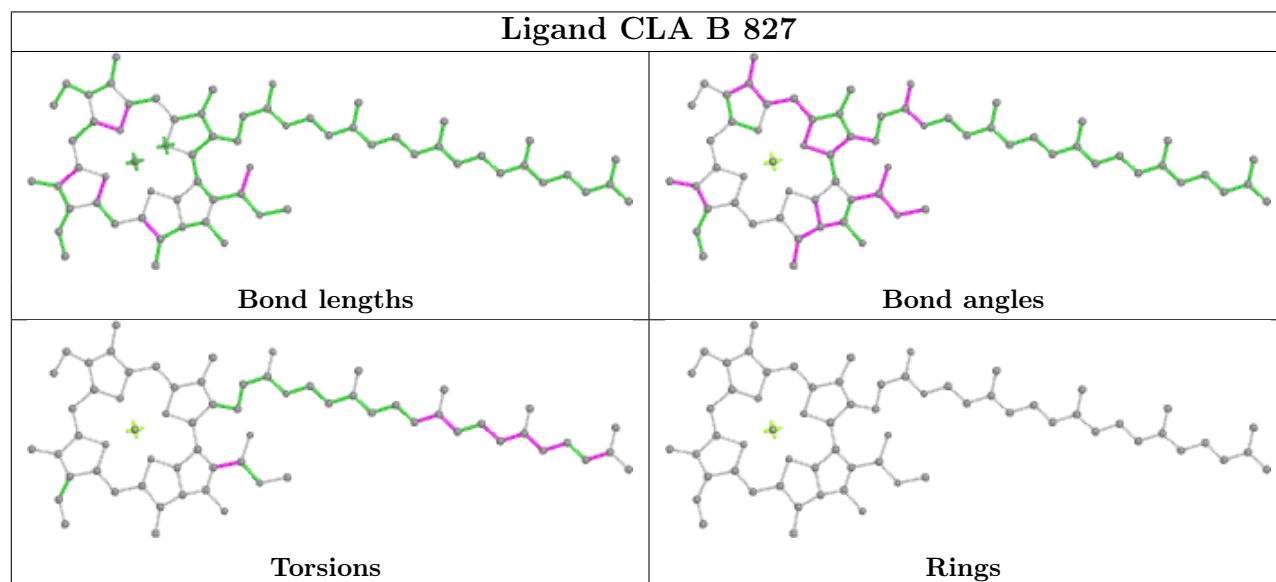
Rings



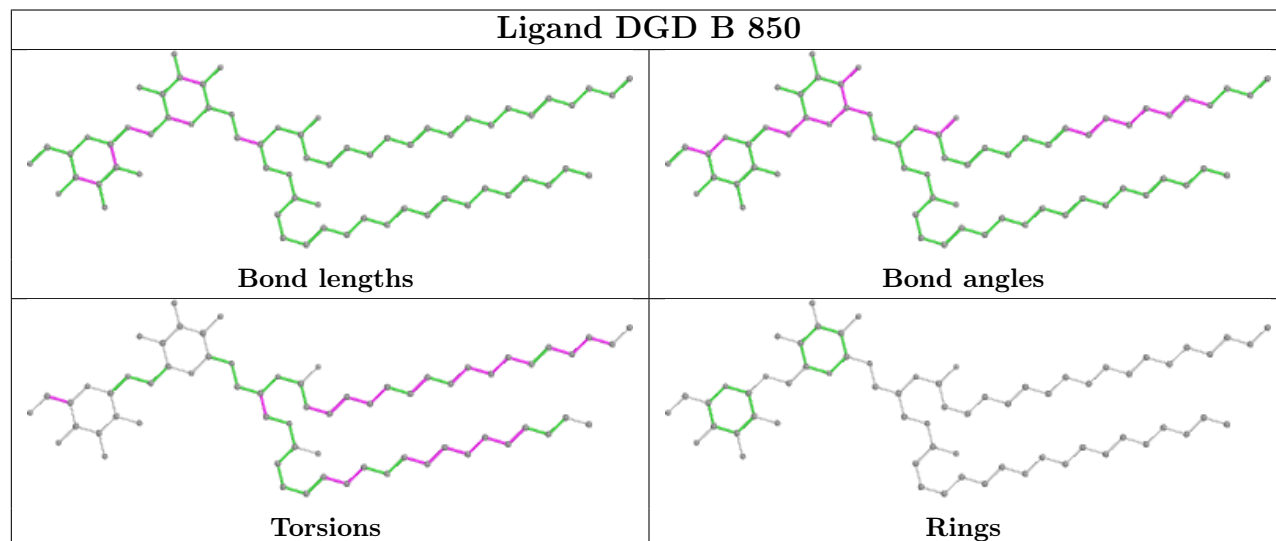
Ligand CLA 1 311



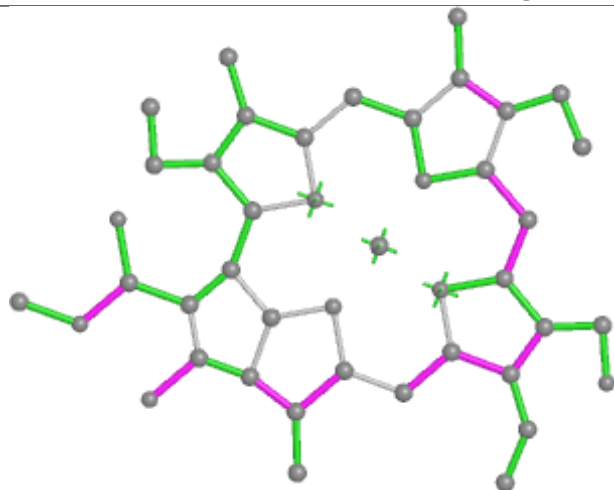
Ligand CLA B 827



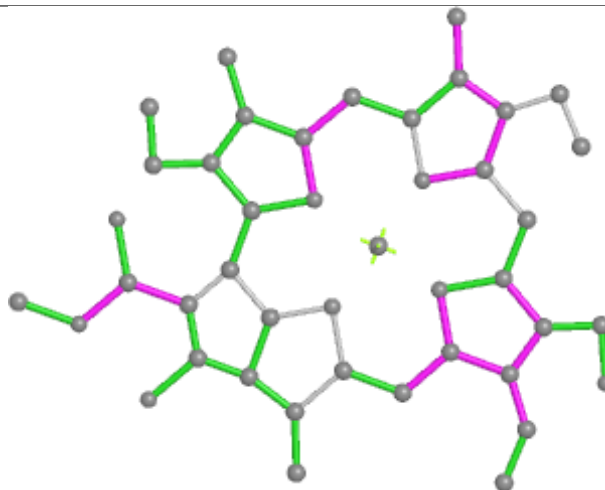
Ligand DGD B 850



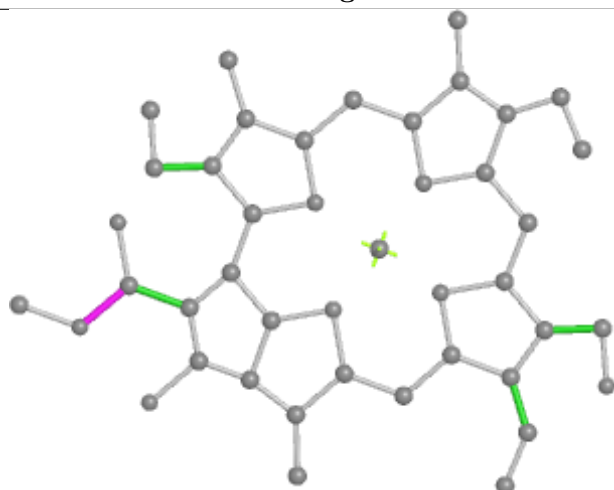
Ligand CHL 4 315



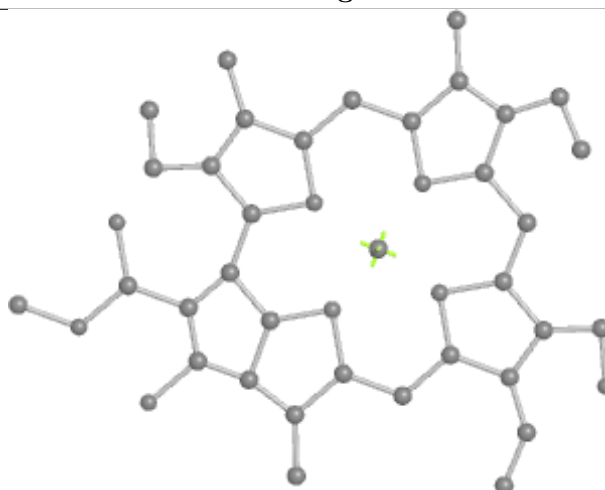
Bond lengths



Bond angles

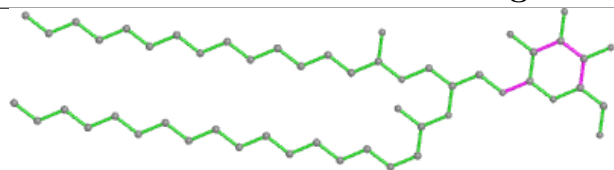


Torsions

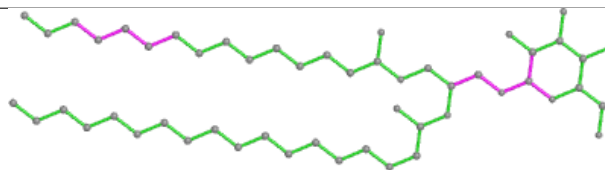


Rings

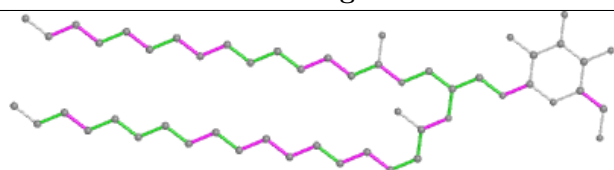
Ligand LMG B 852



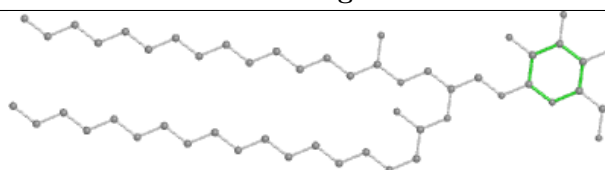
Bond lengths



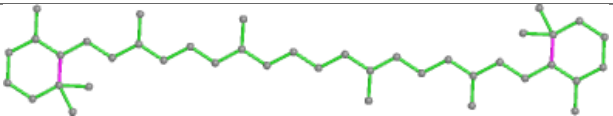
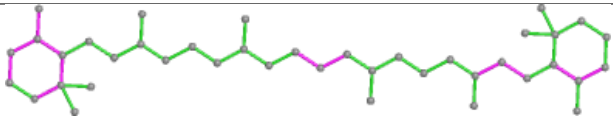
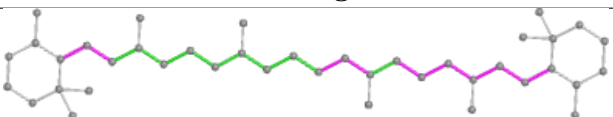
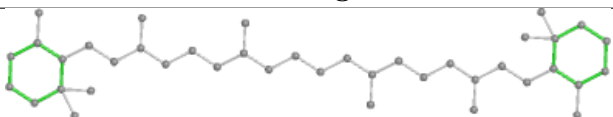
Bond angles

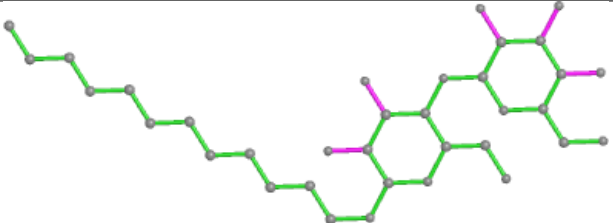
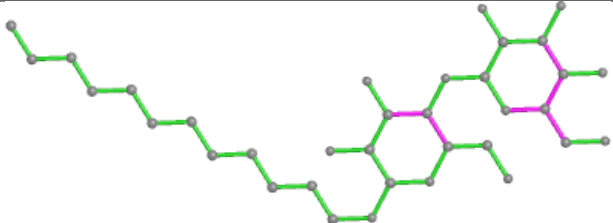
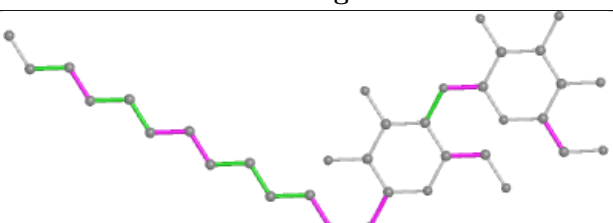
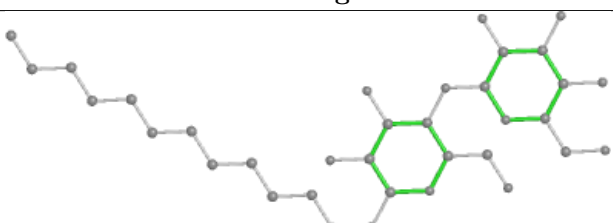


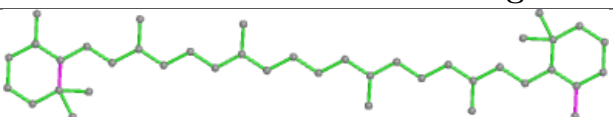
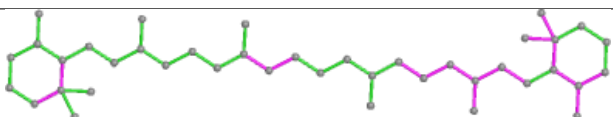
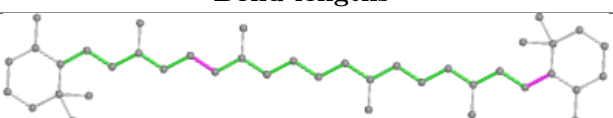
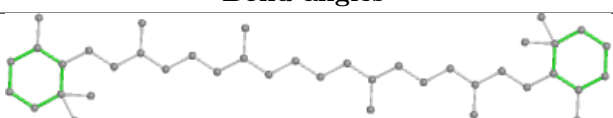
Torsions

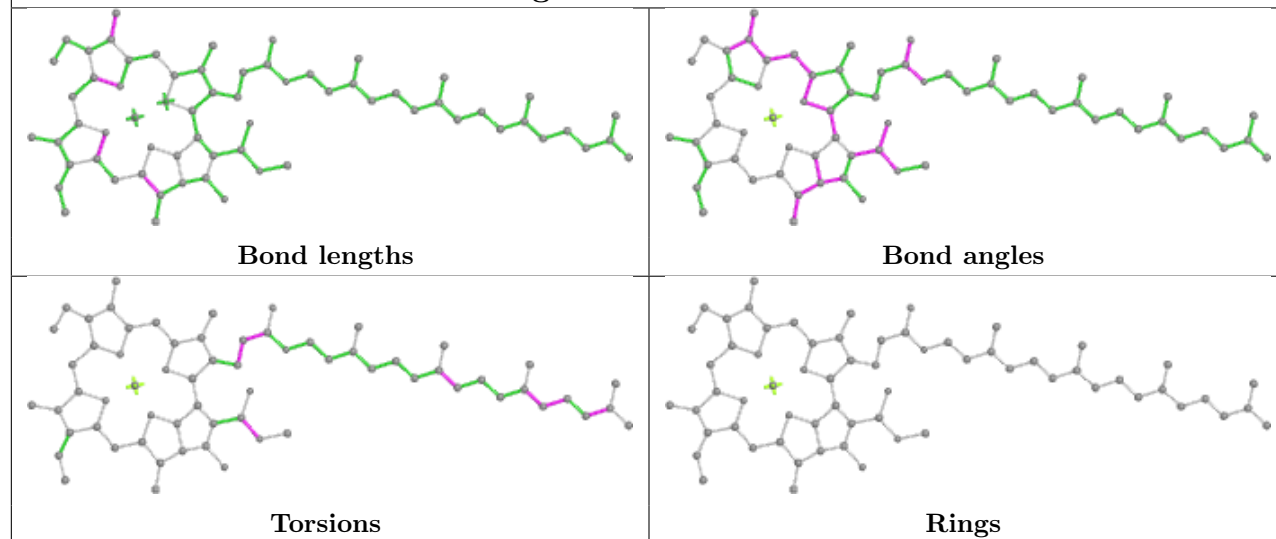
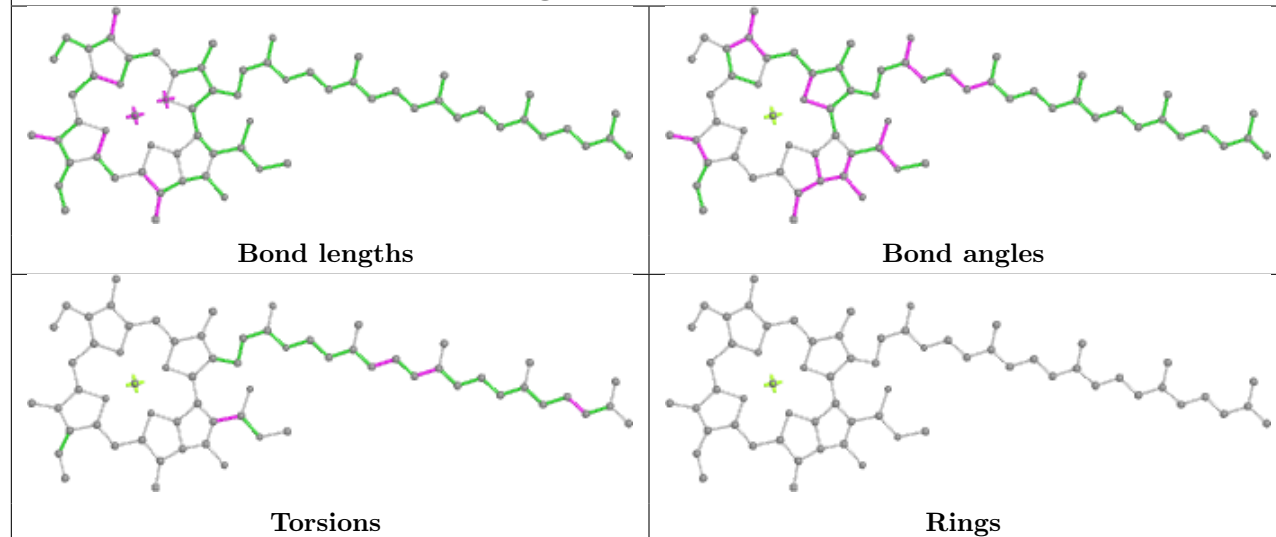


Rings

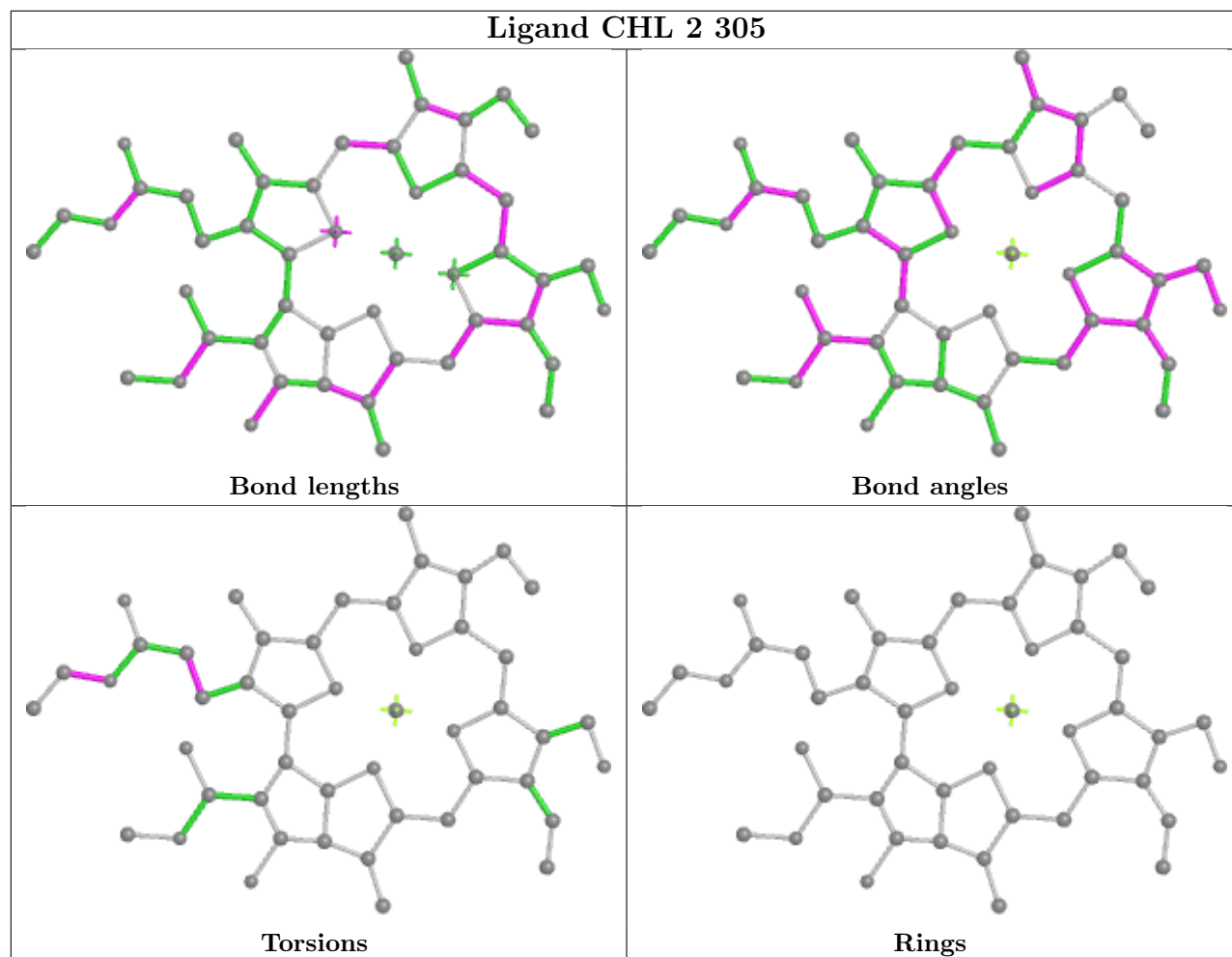
Ligand BCR K 203	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand LMT 2 318	
	Bond lengths
	Bond angles
	Torsions
	Rings

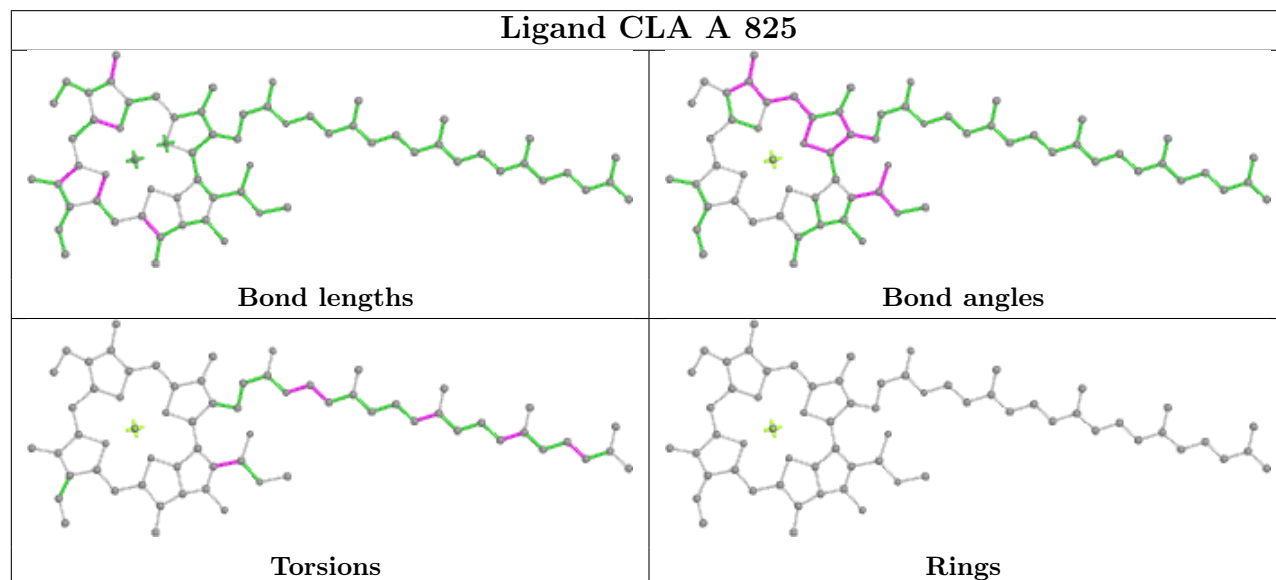
Ligand BCR B 847	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand CLA B 805**Ligand CLA 2 301**

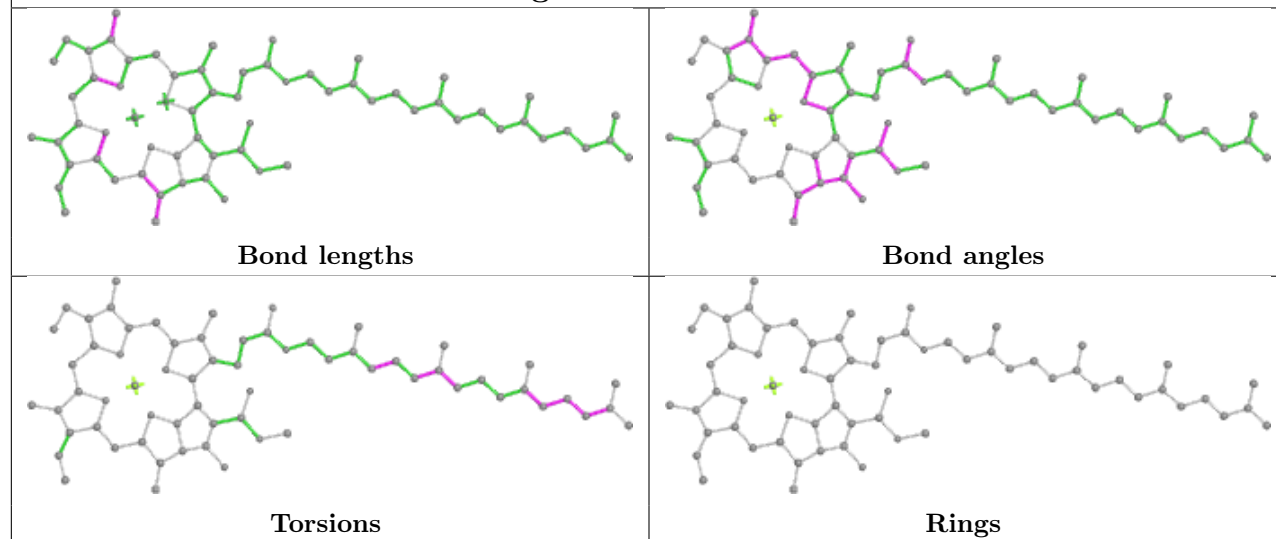
Ligand CHL 2 305



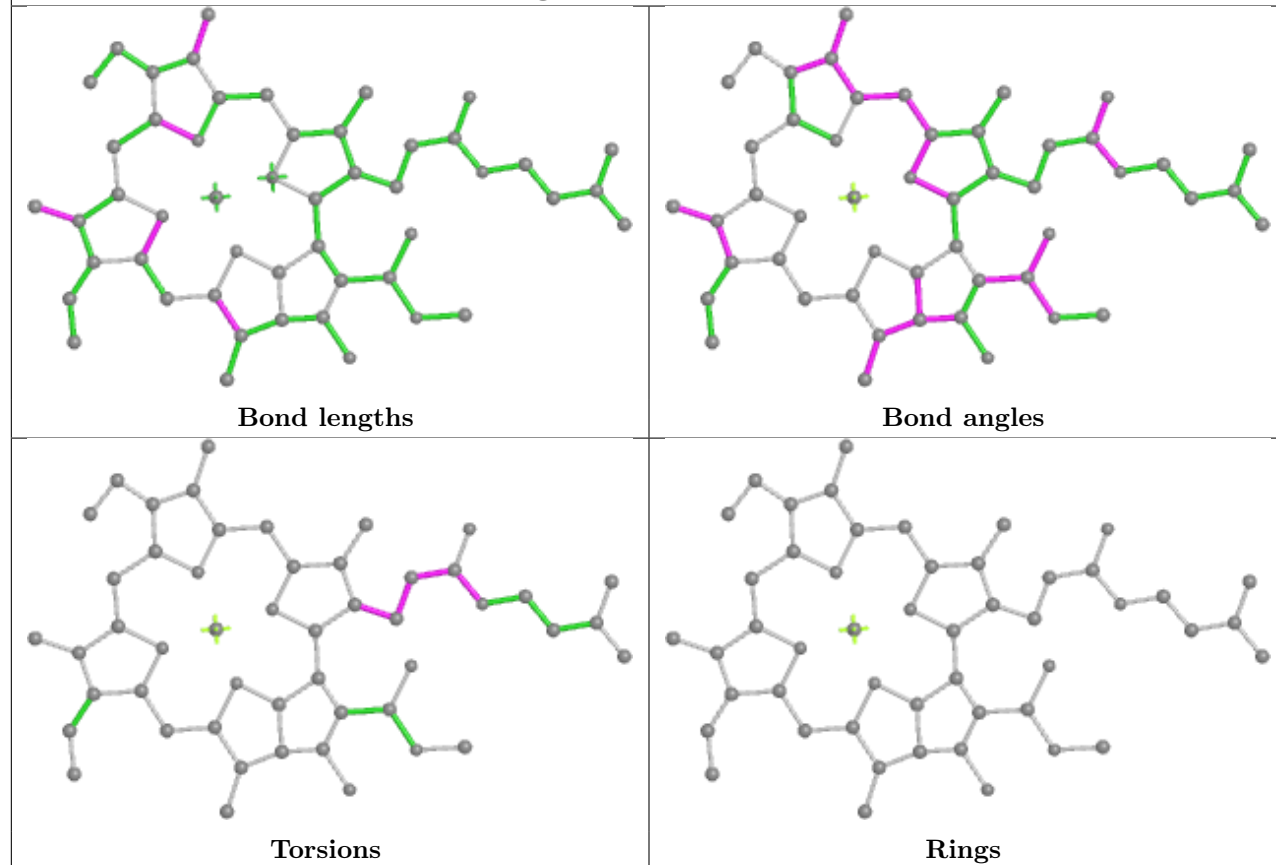
Ligand CLA A 825



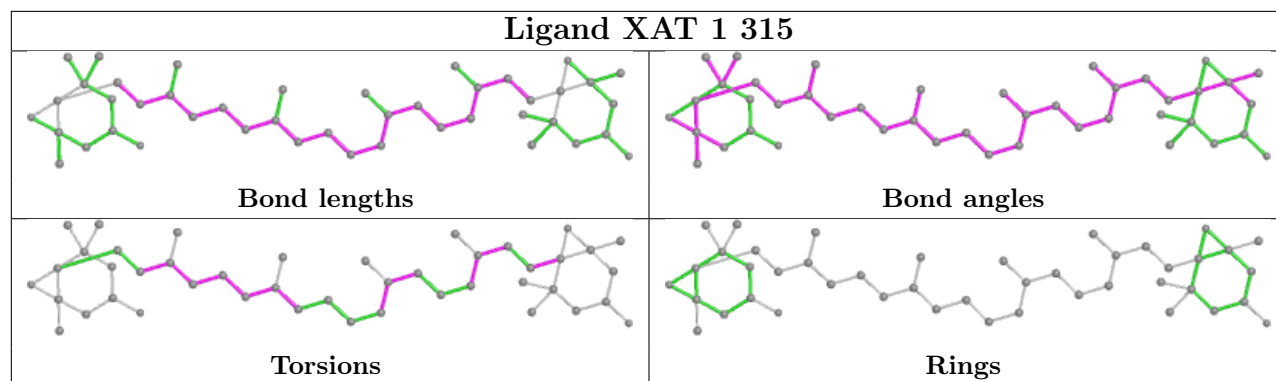
Ligand CLA A 820



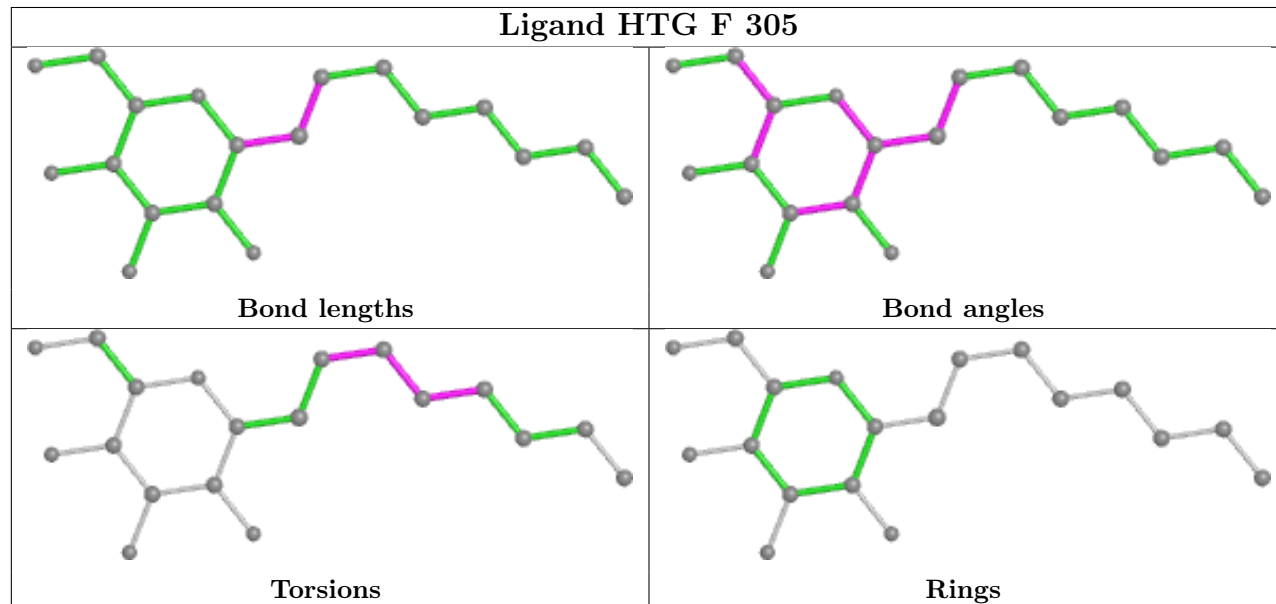
Ligand CLA L 204



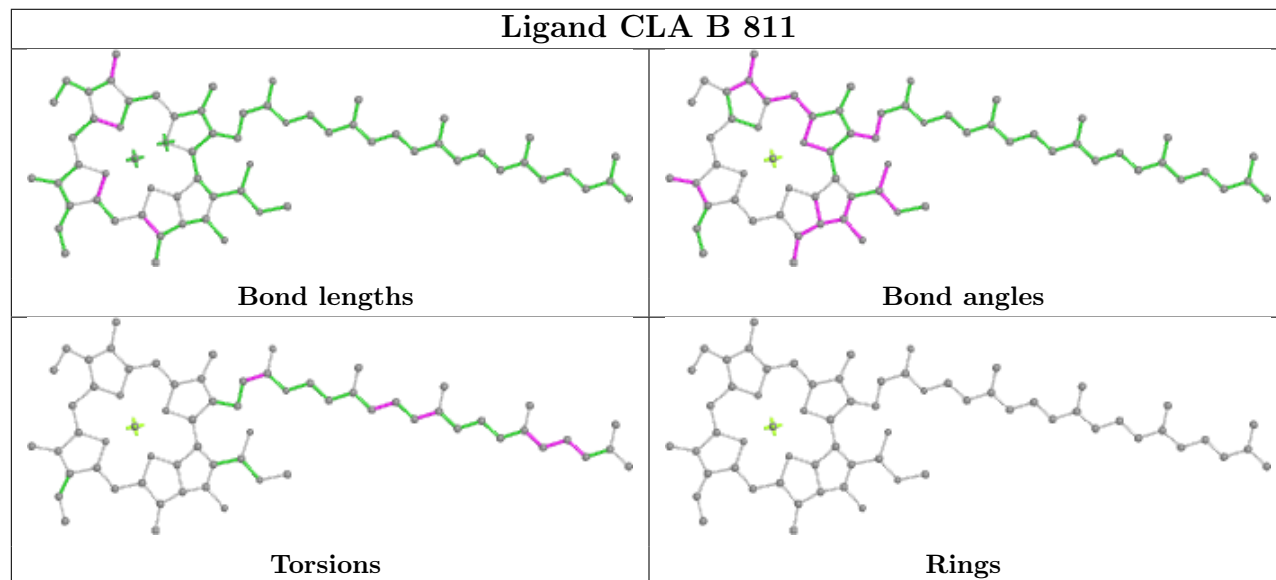
Ligand XAT 1 315

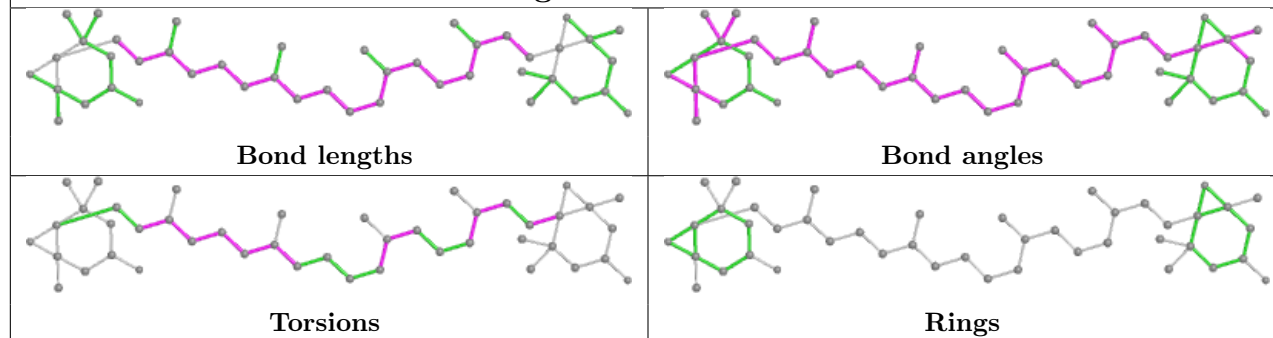
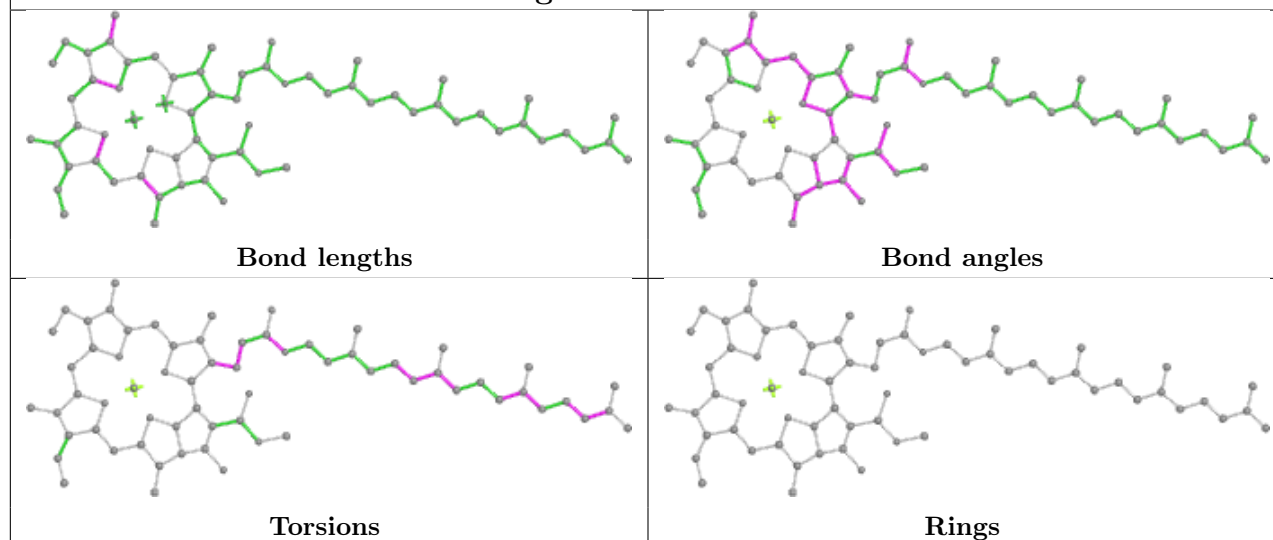
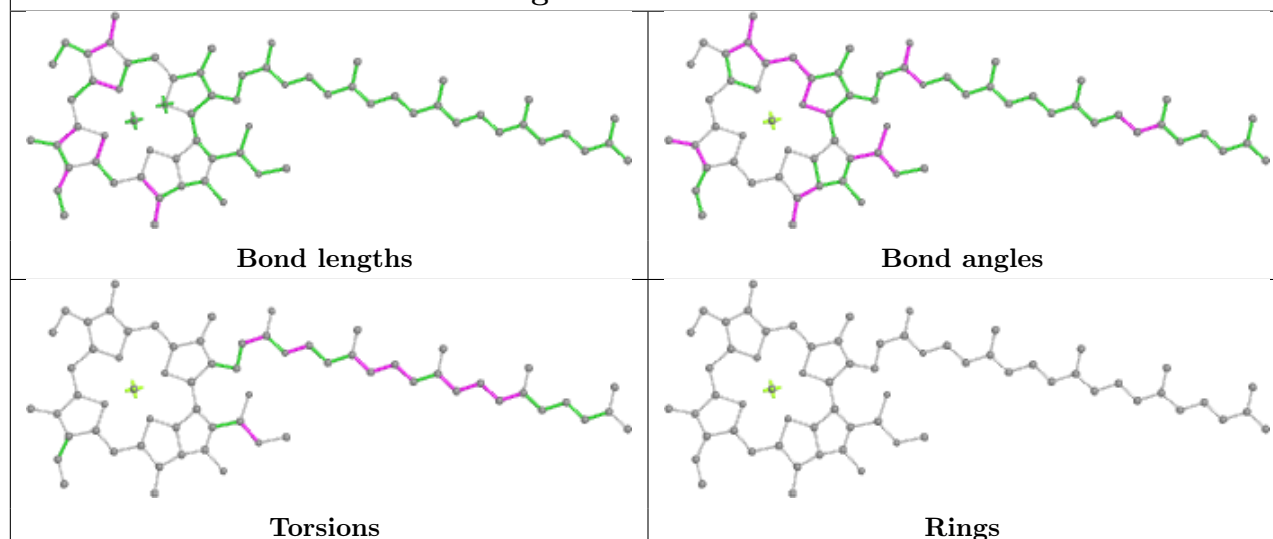


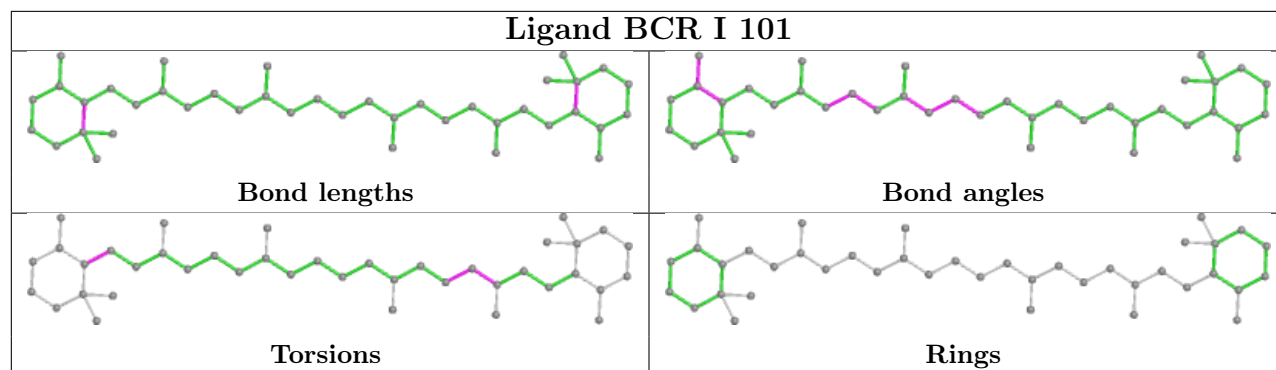
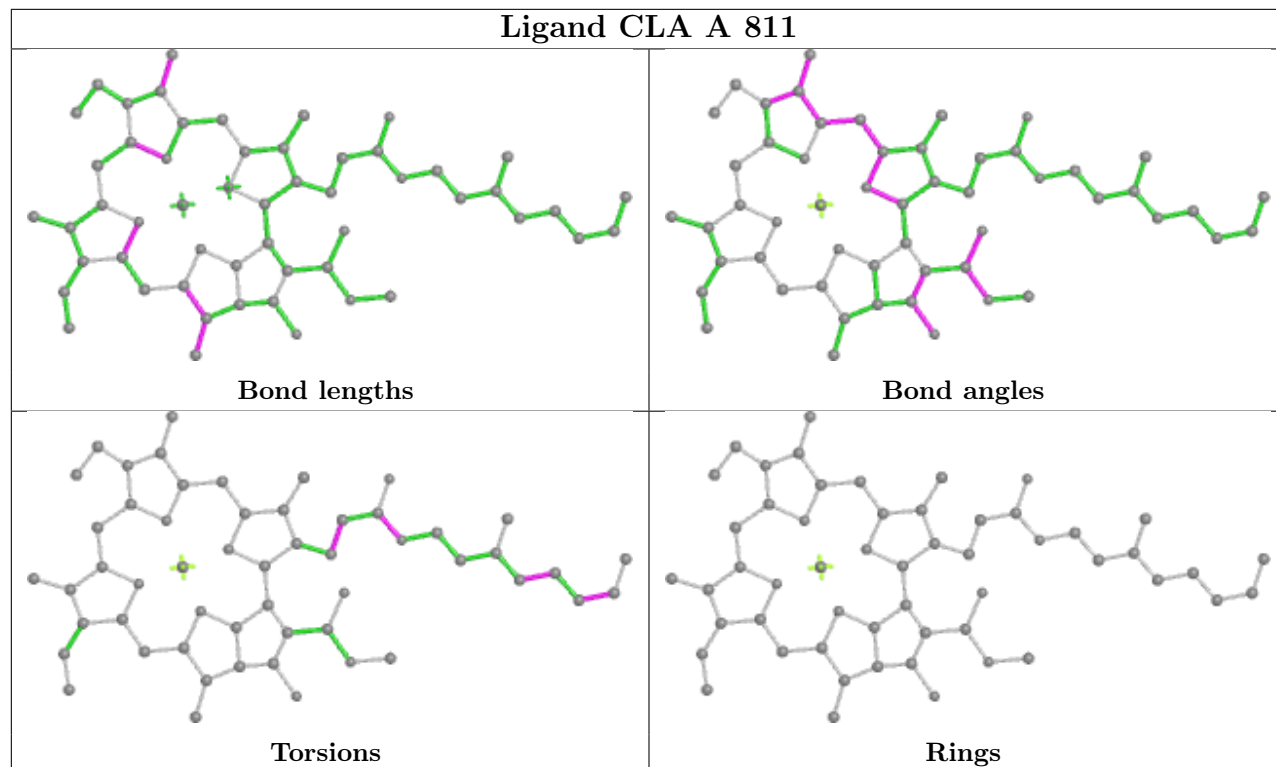
Ligand HTG F 305



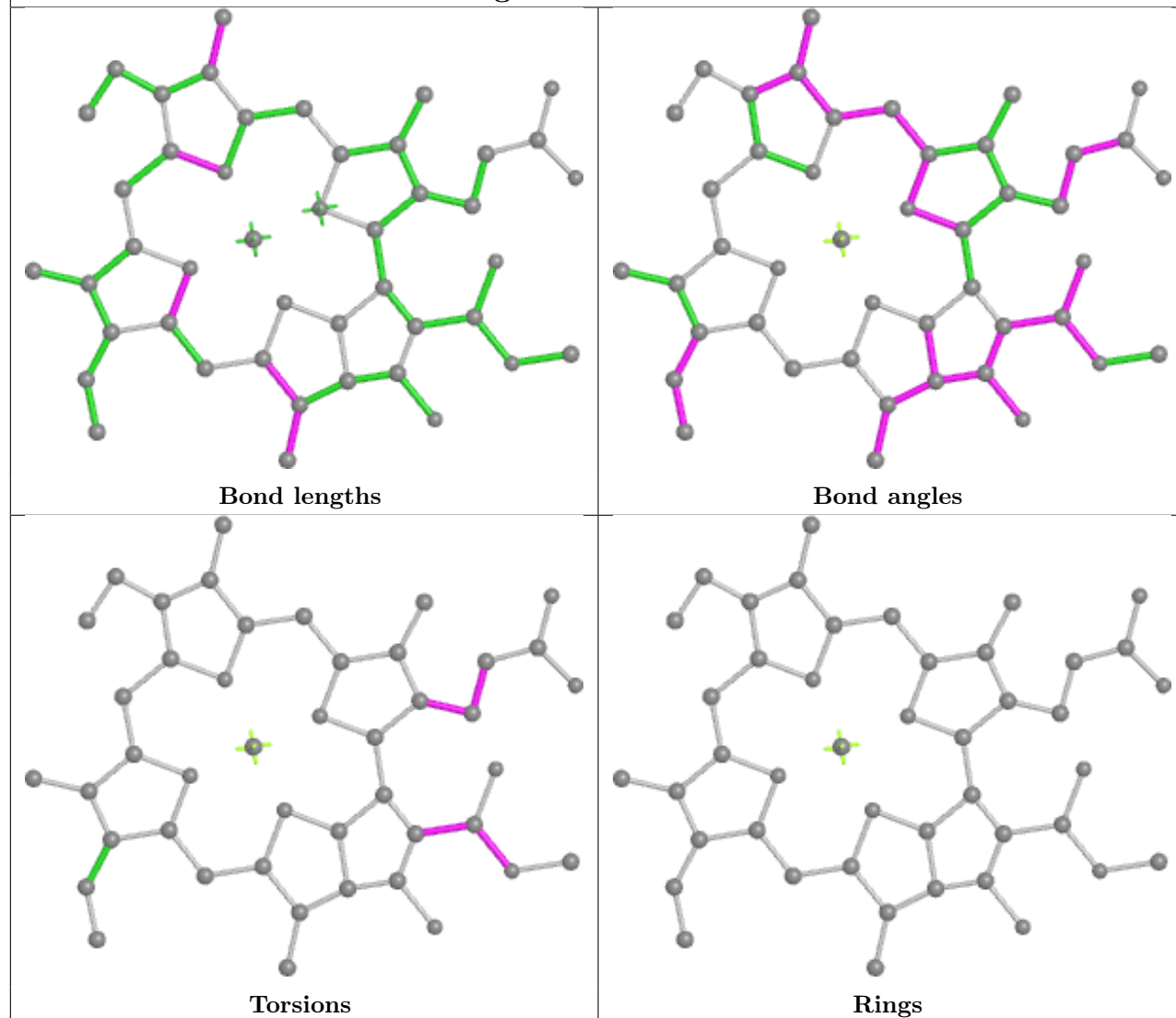
Ligand CLA B 811



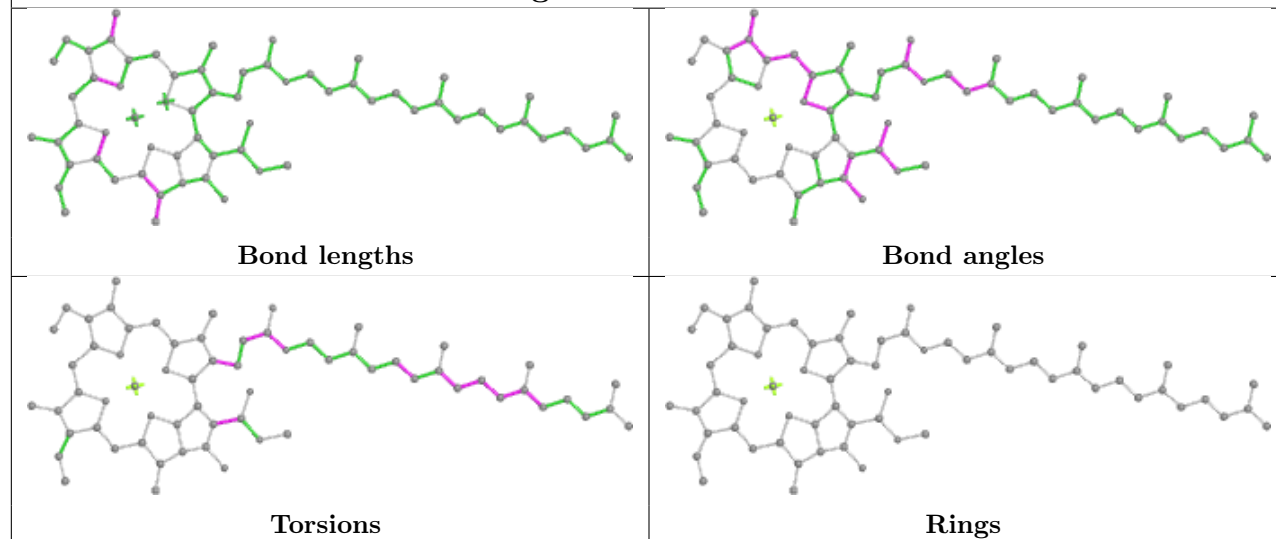
Ligand XAT 3 615**Ligand CLA 1 309****Ligand CLA B 808**

Ligand BCR I 101**Ligand CLA A 811**

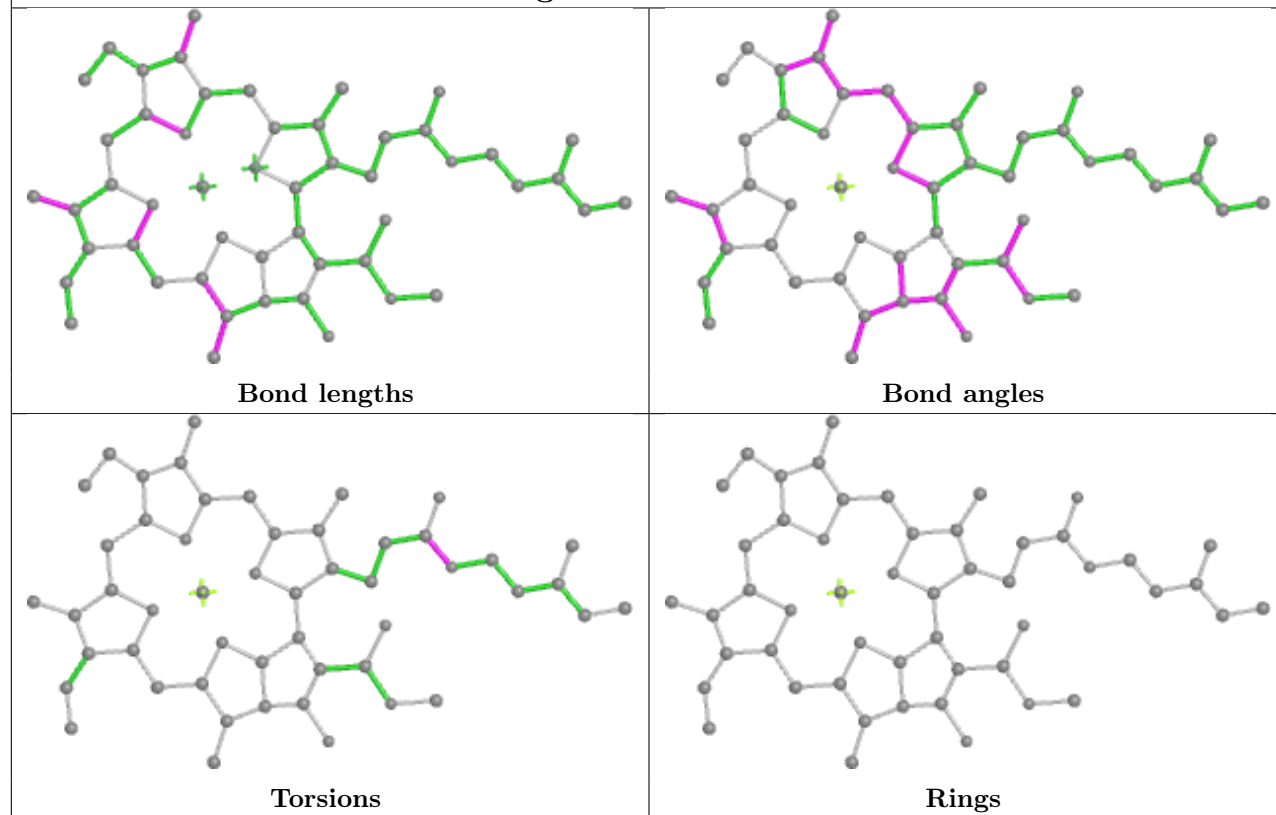
Ligand CLA 4 313



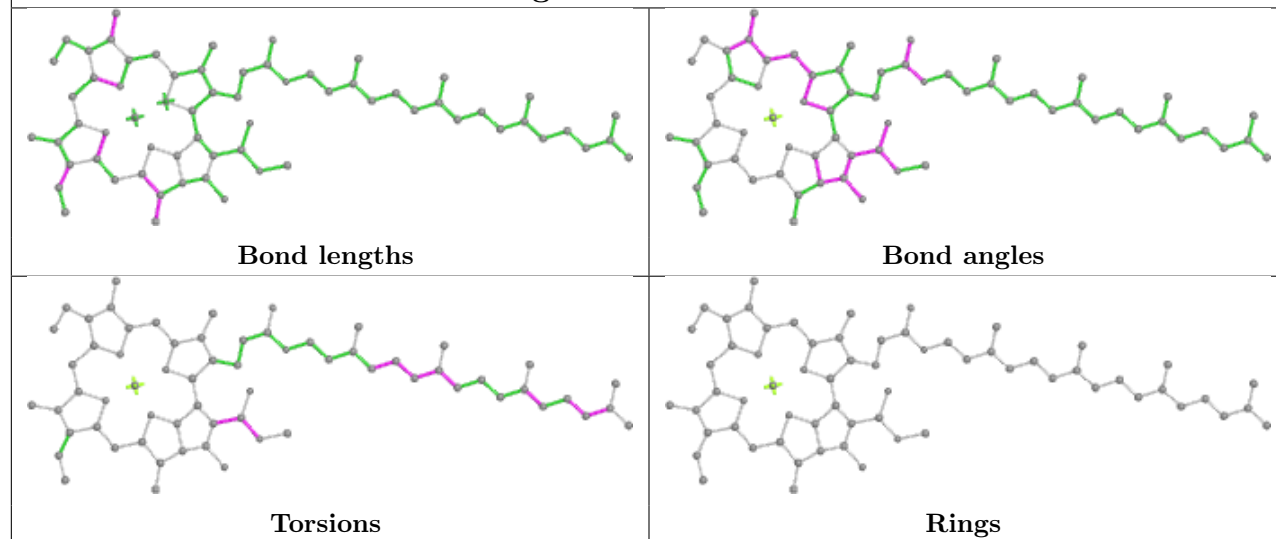
Ligand CLA A 809



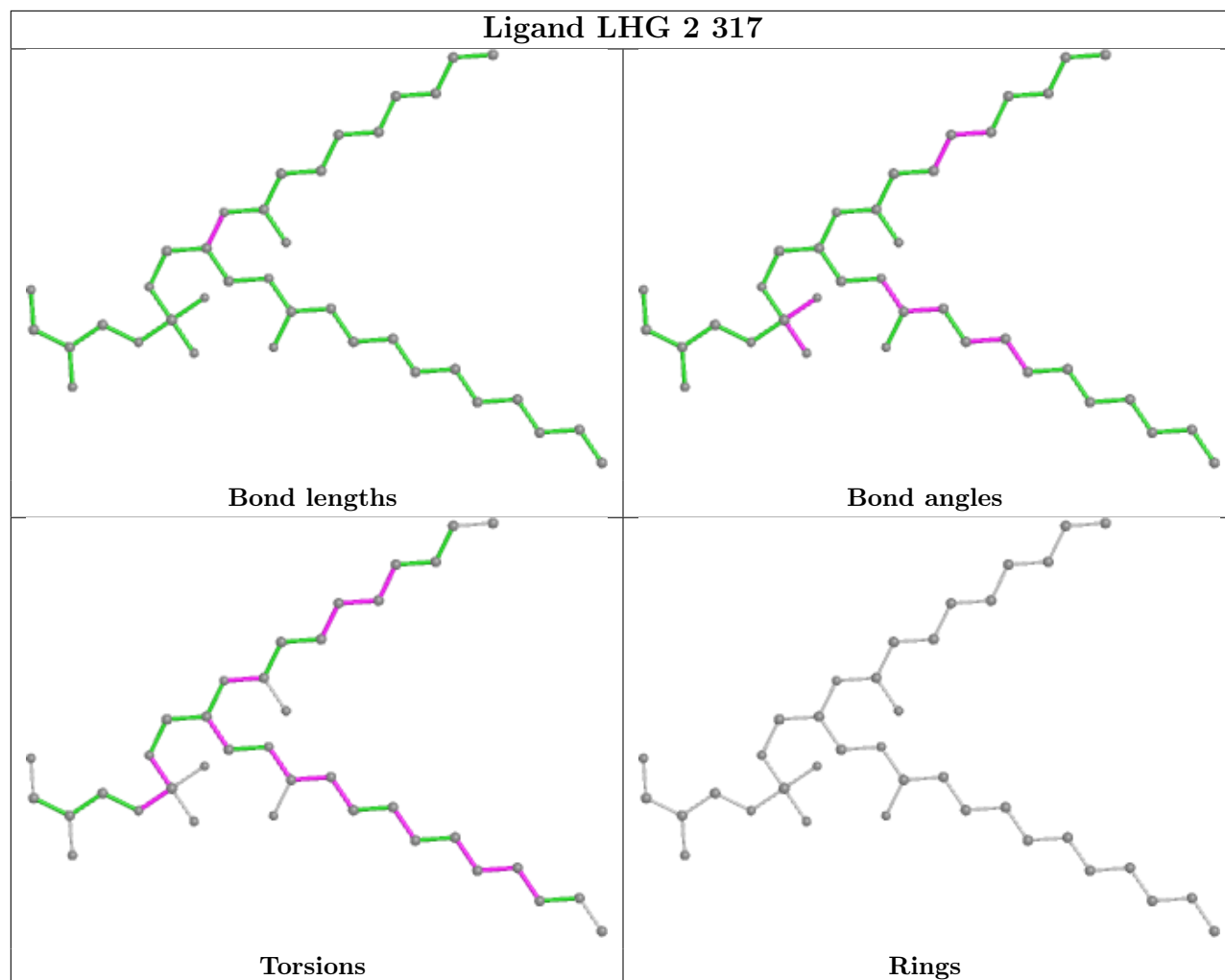
Ligand CLA 2 302



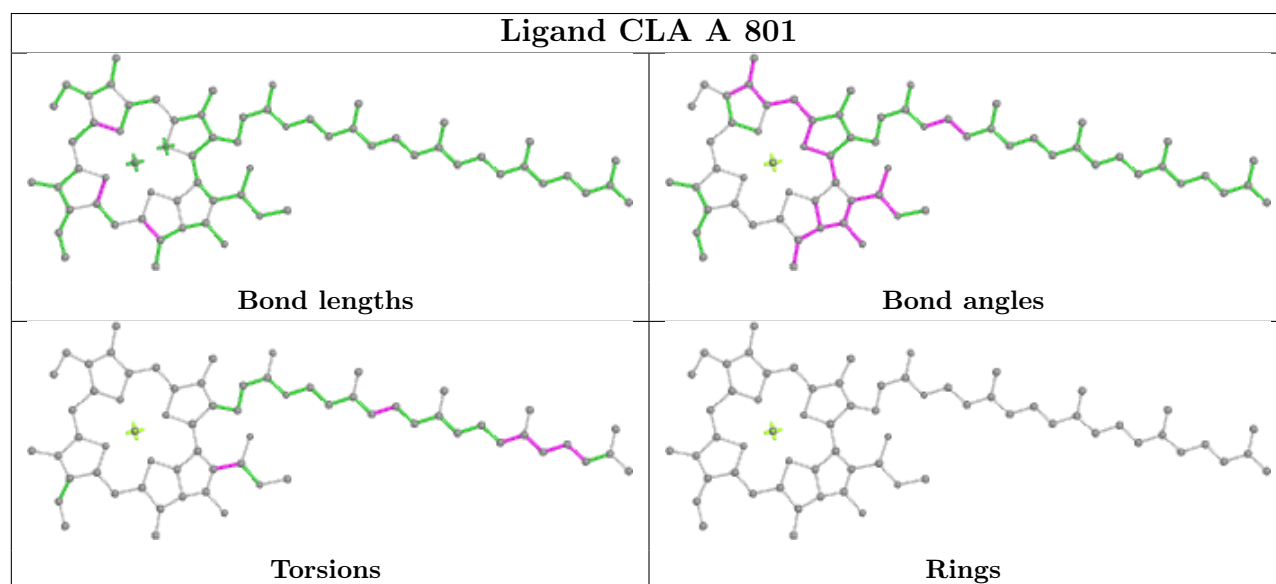
Ligand CLA B 809



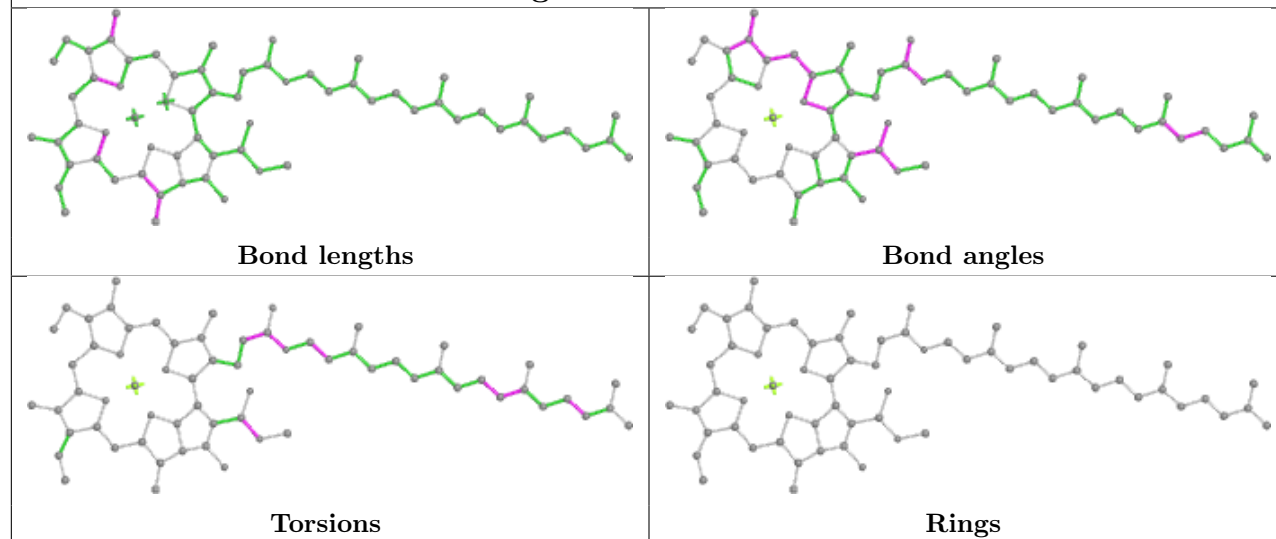
Ligand LHG 2 317



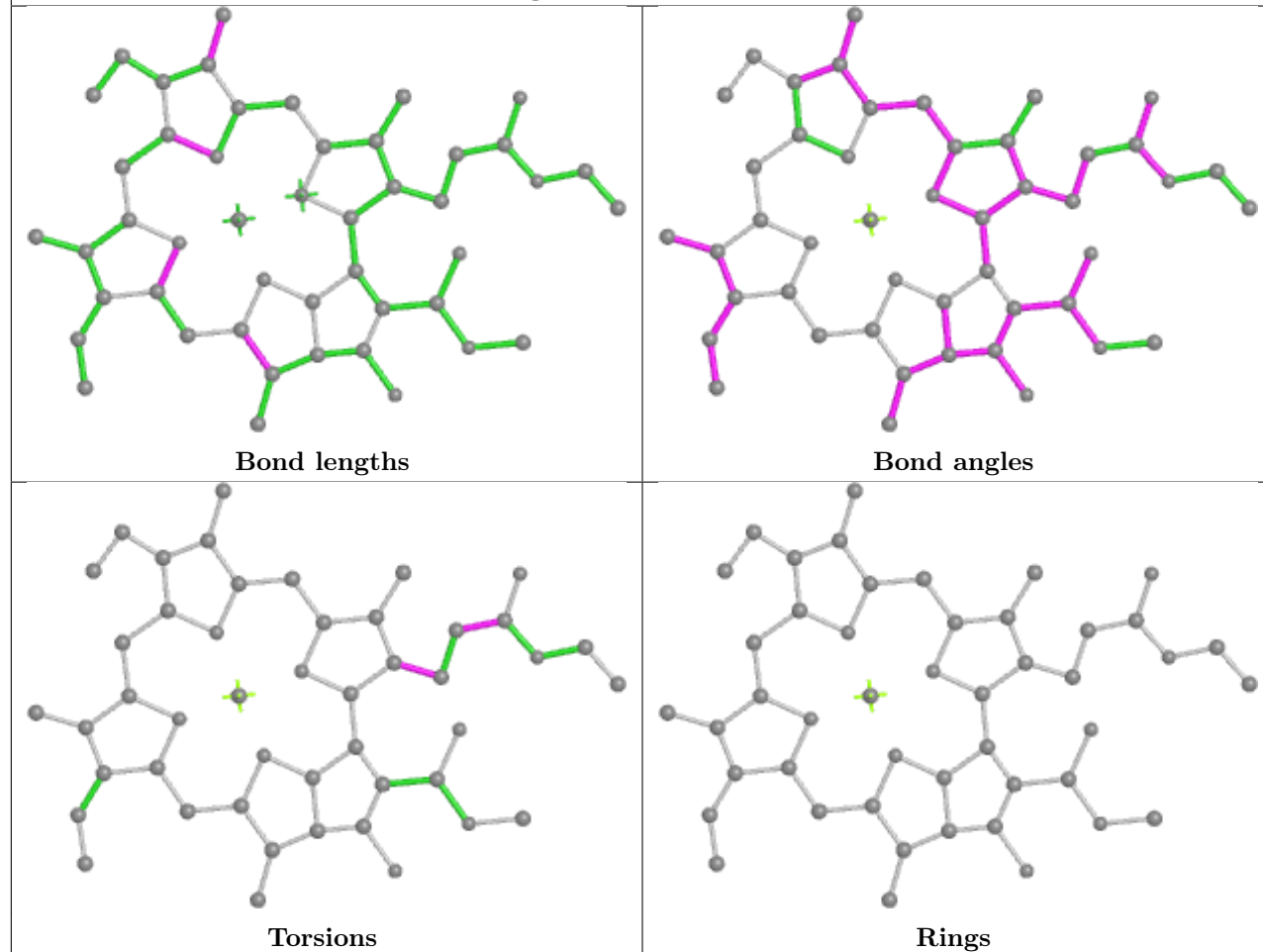
Ligand CLA A 801

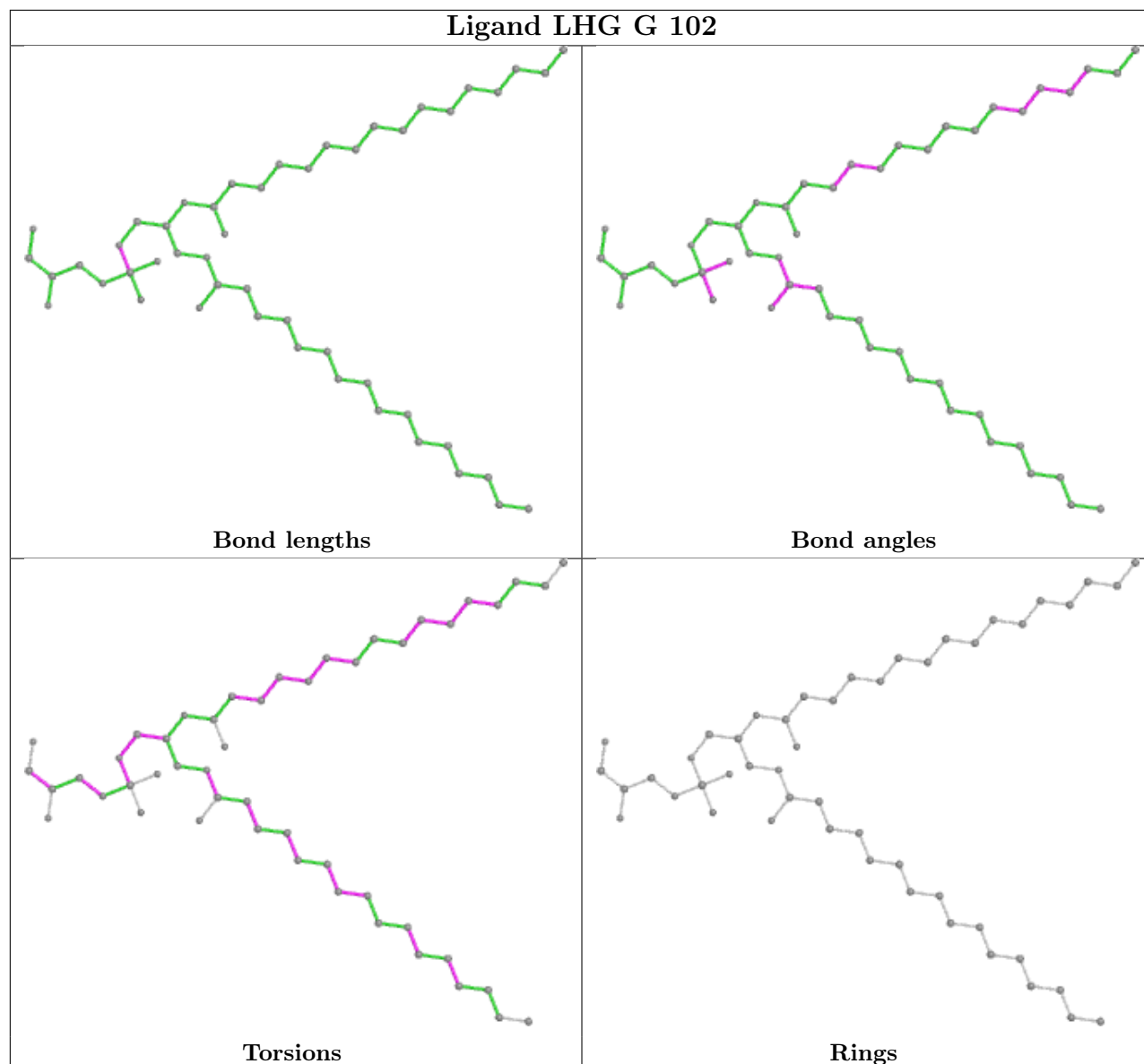
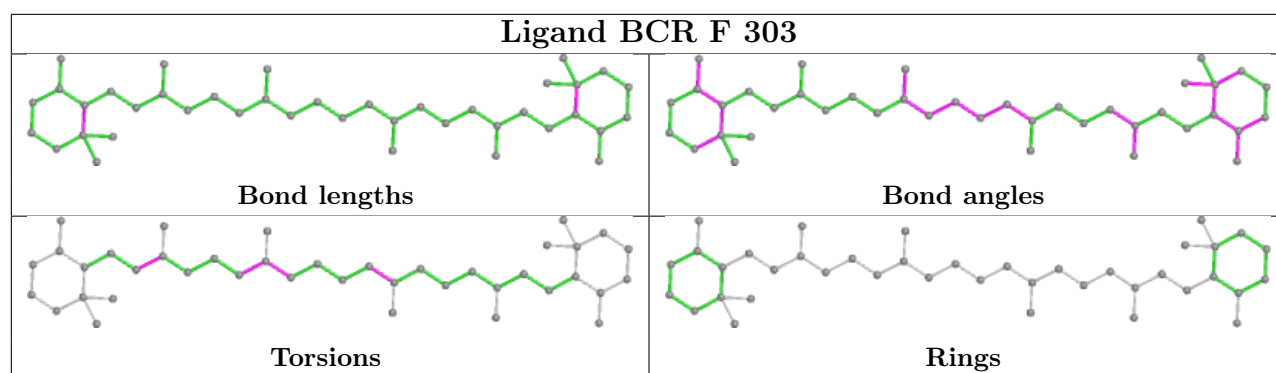


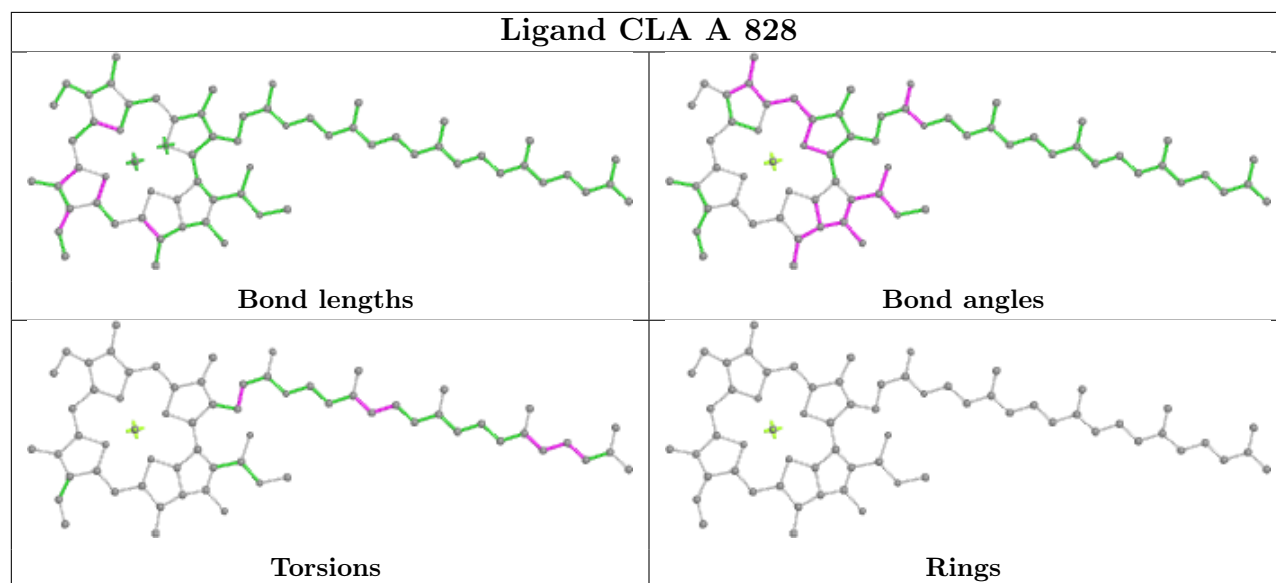
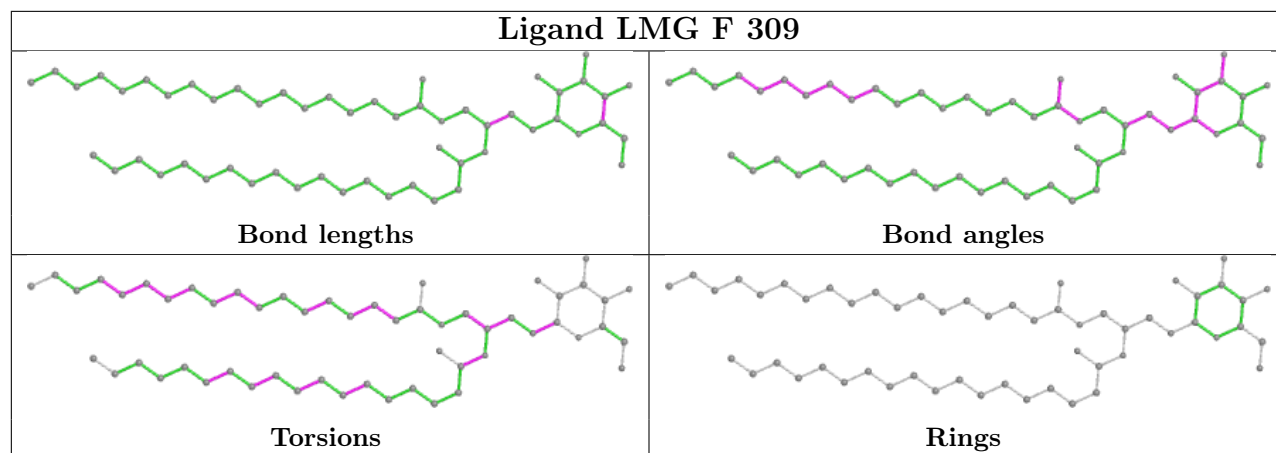
Ligand CLA A 824



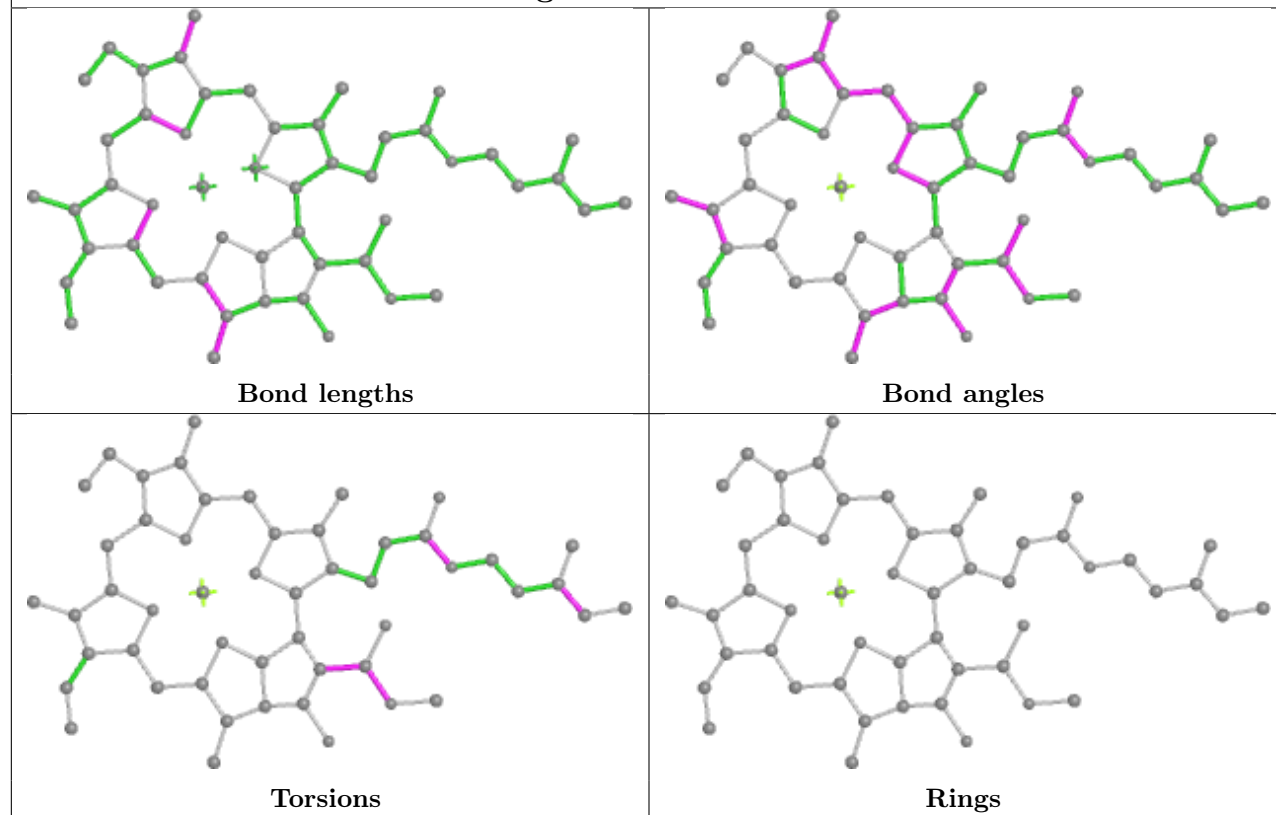
Ligand CLA B 839



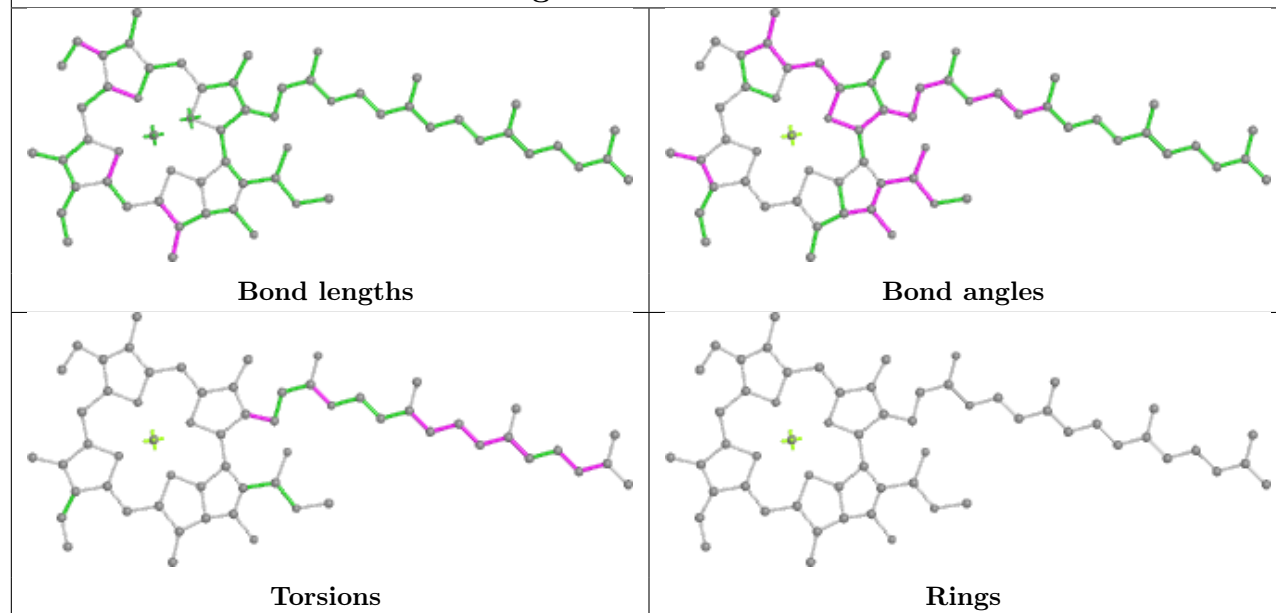




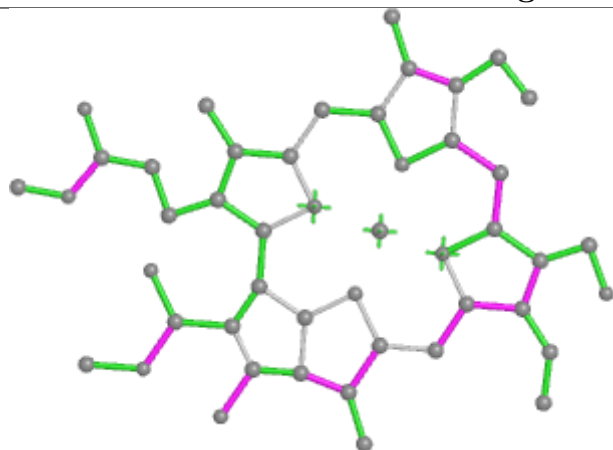
Ligand CLA 1 303



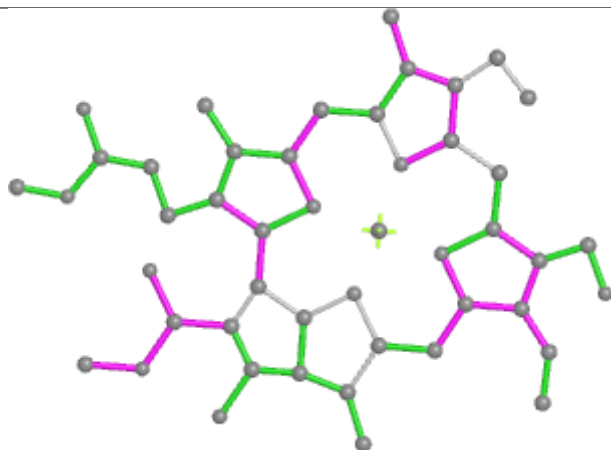
Ligand CLA B 820



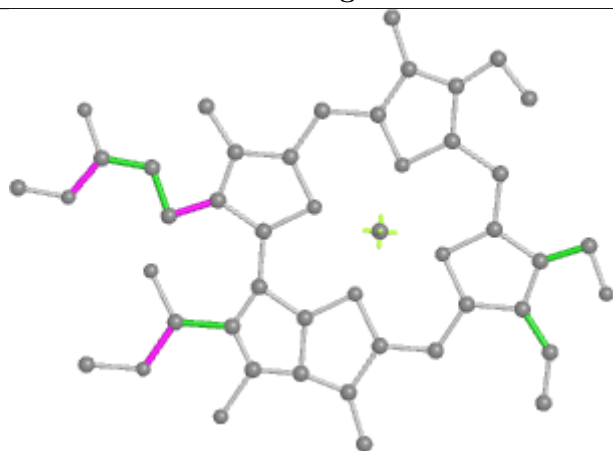
Ligand CHL 3 607



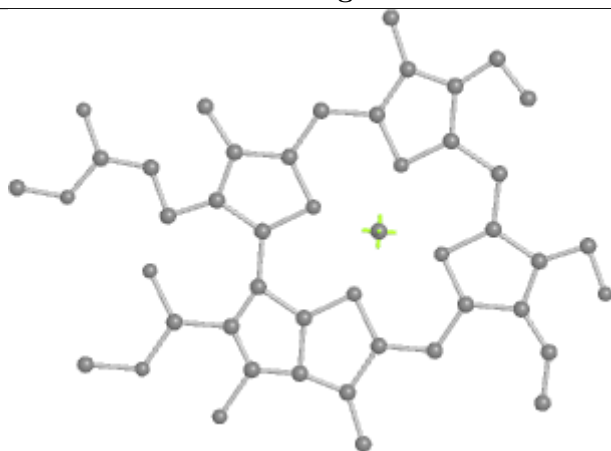
Bond lengths



Bond angles

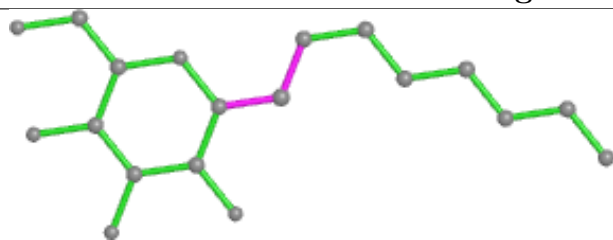


Torsions

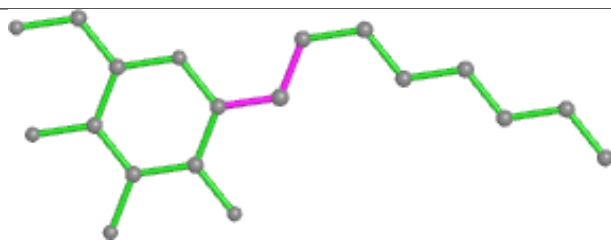


Rings

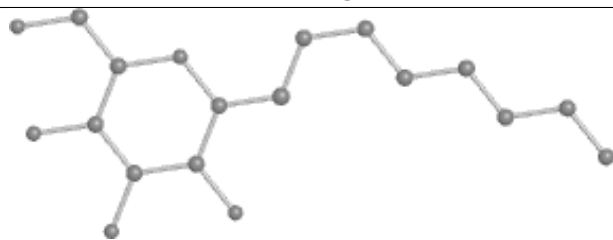
Ligand HTG 4 321



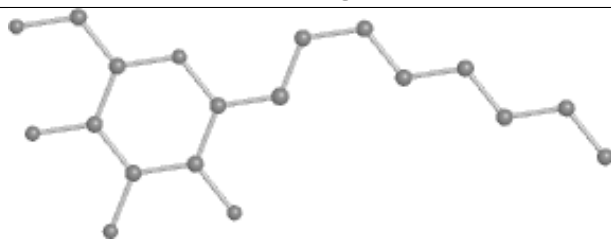
Bond lengths



Bond angles

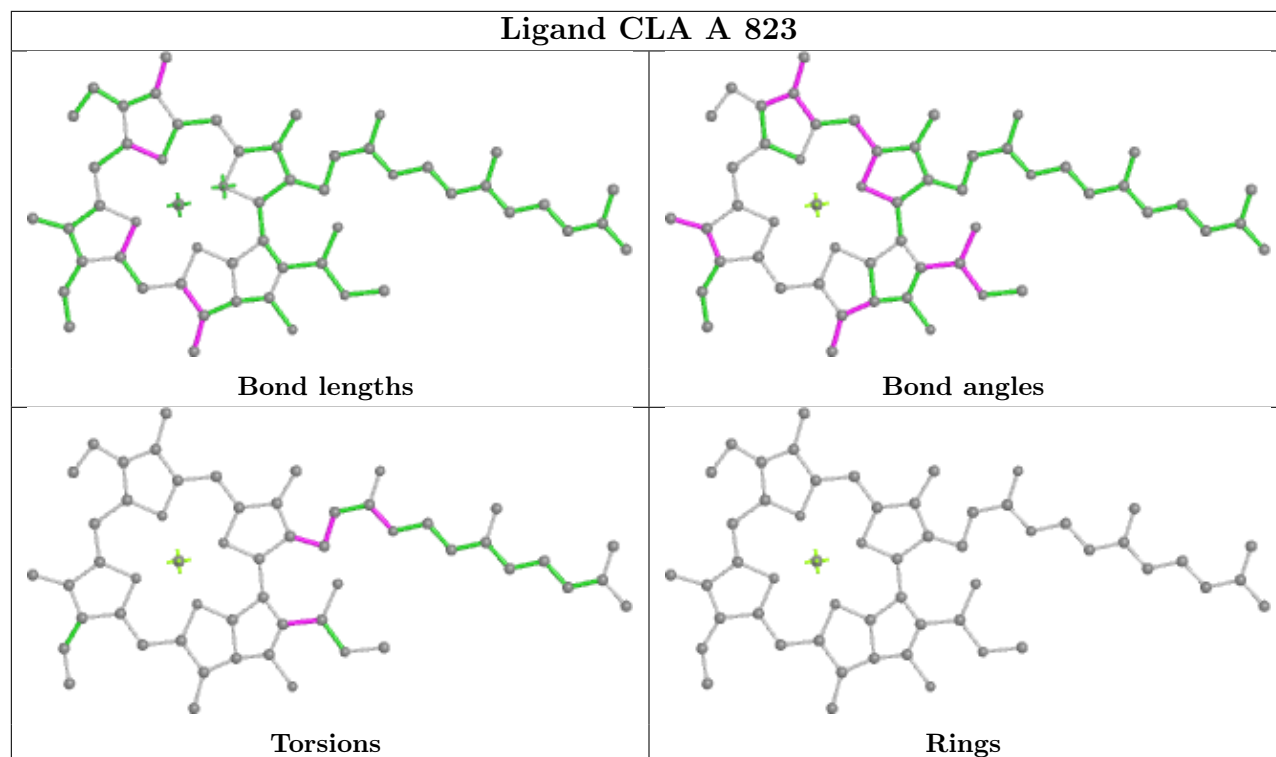


Torsions

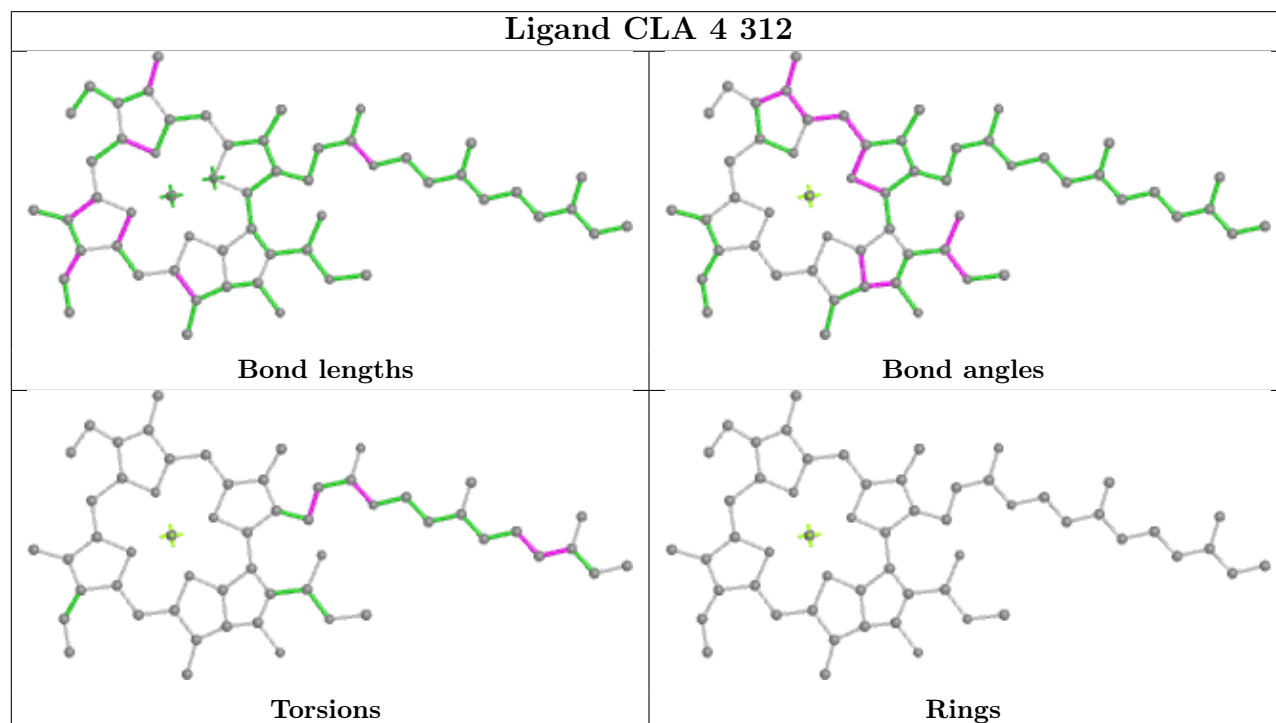


Rings

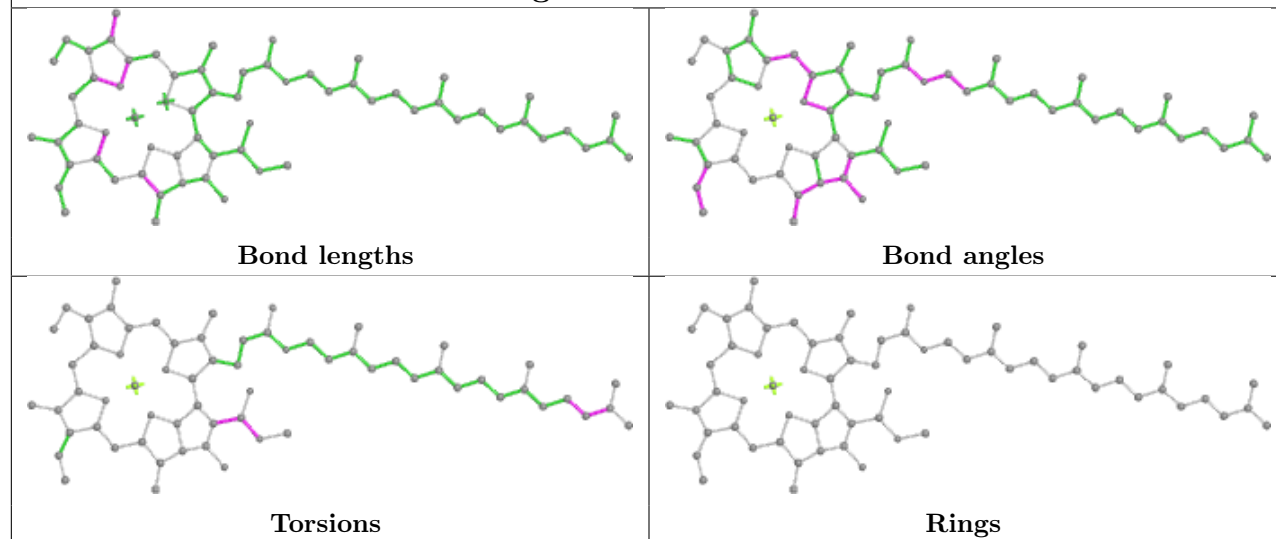
Ligand CLA A 823



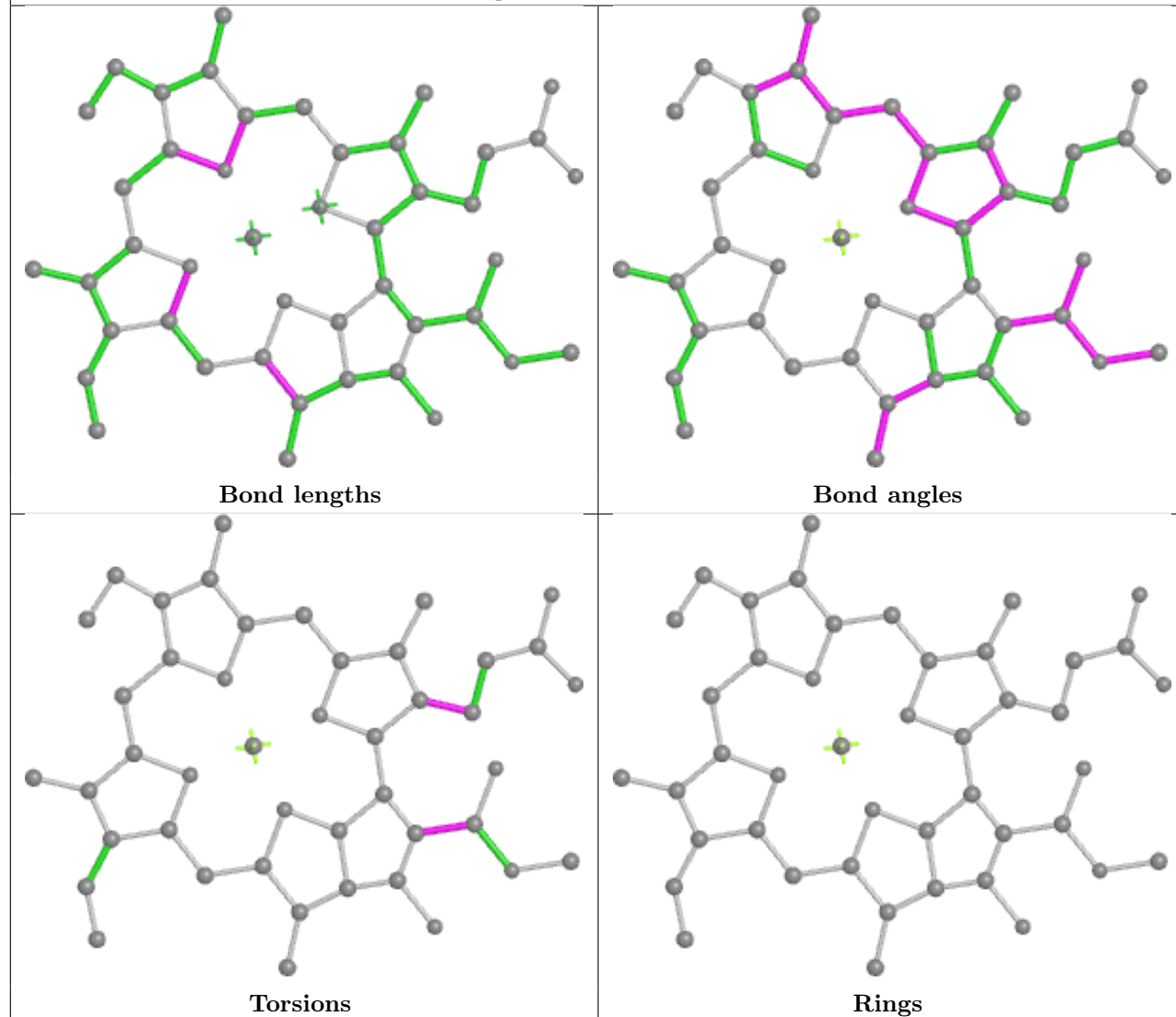
Ligand CLA 4 312



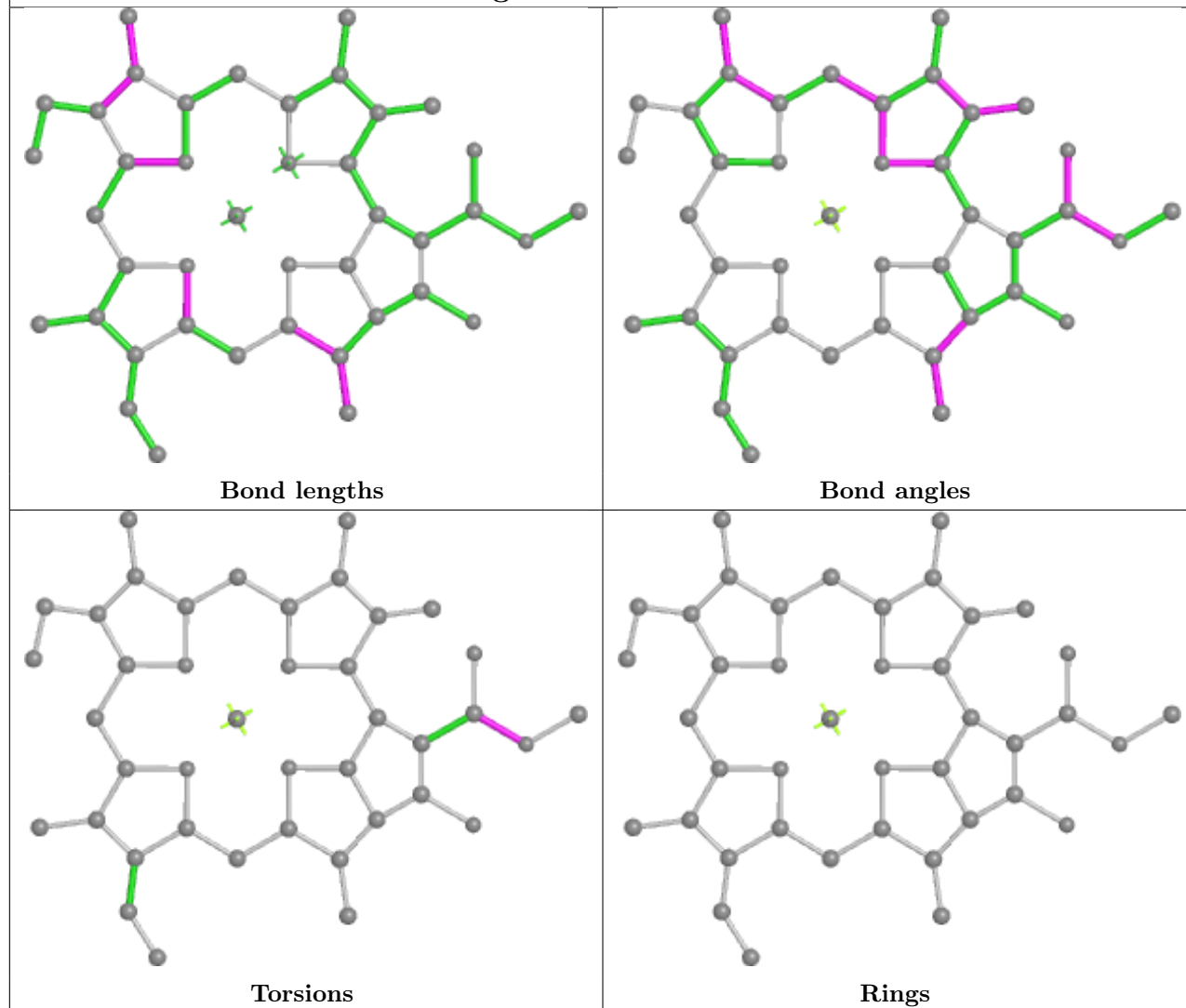
Ligand CLA B 804



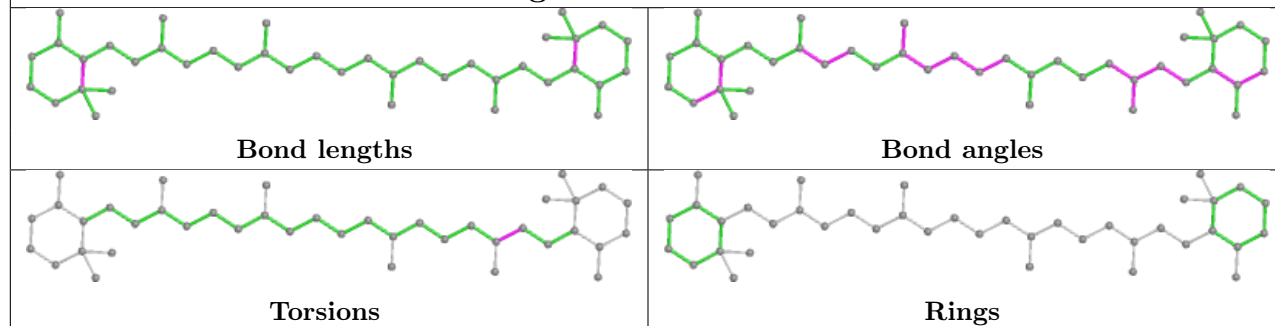
Ligand CLA B 806



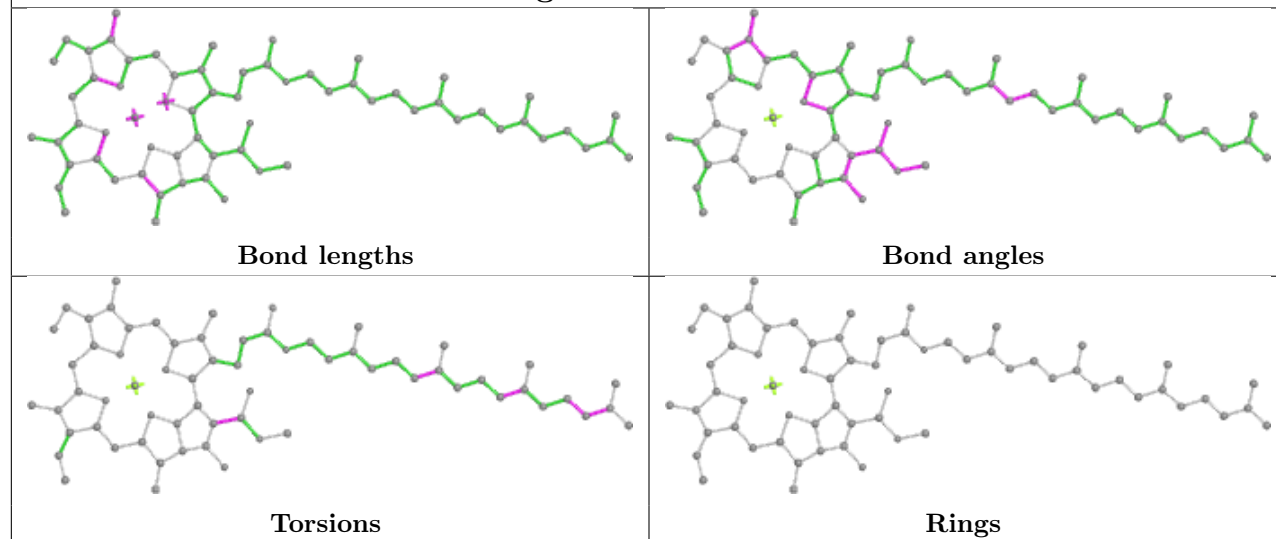
Ligand CLA G 103



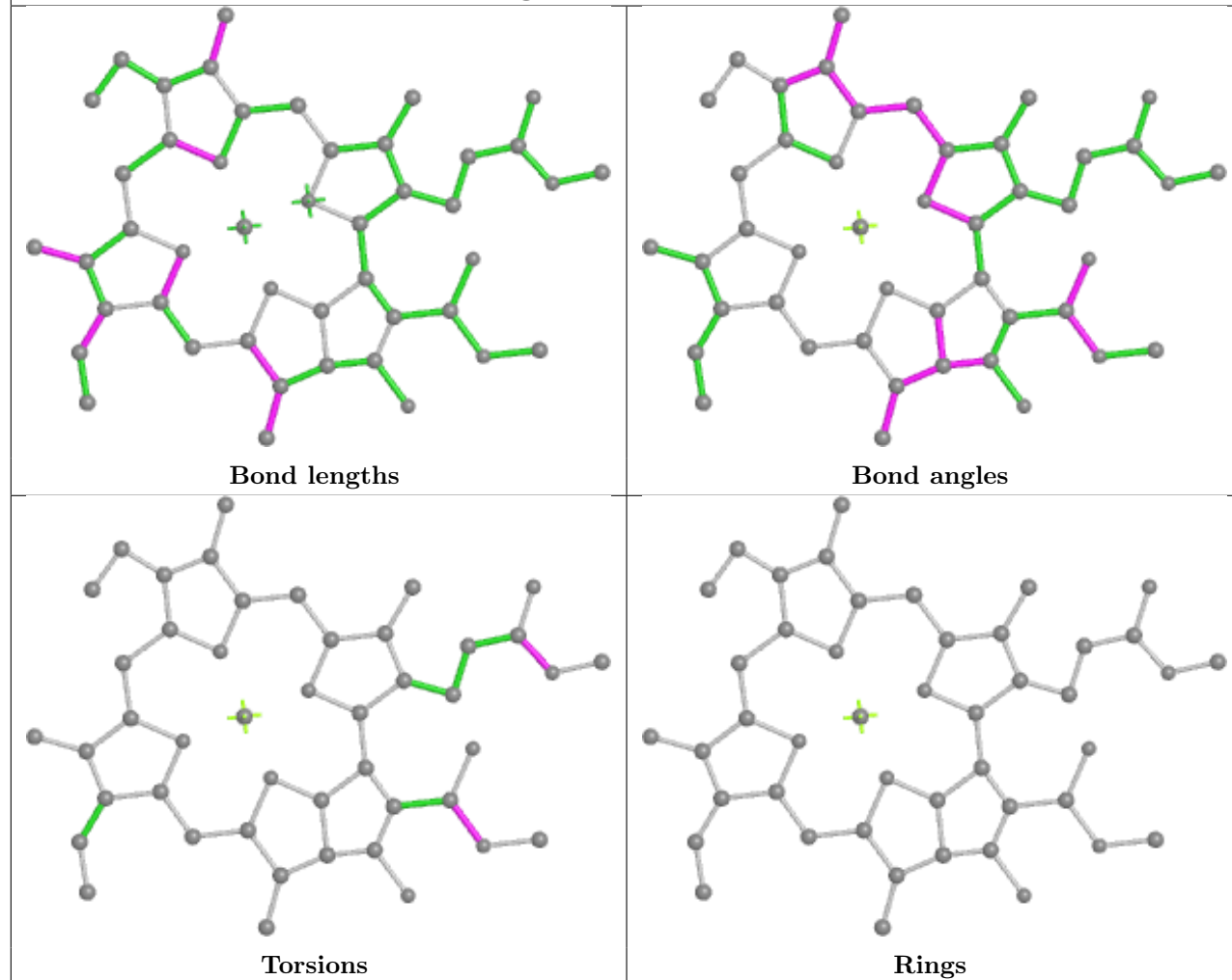
Ligand BCR A 846

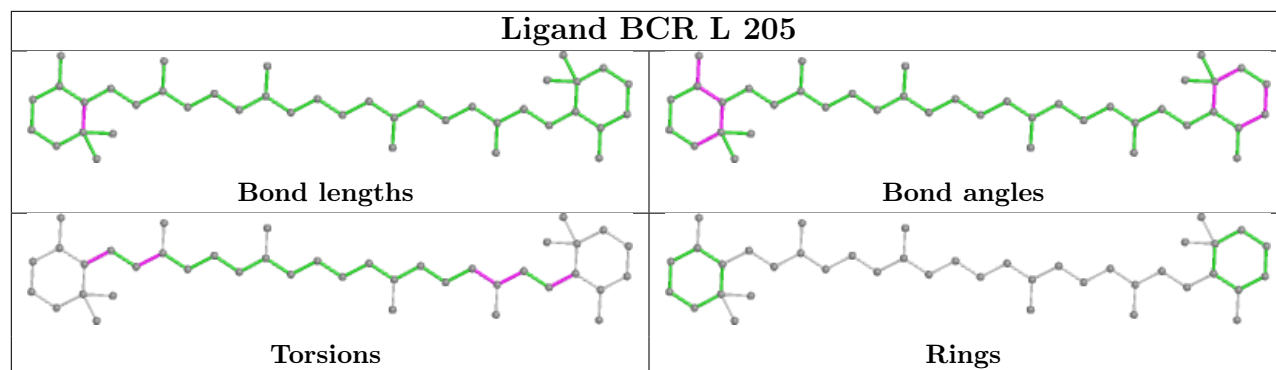
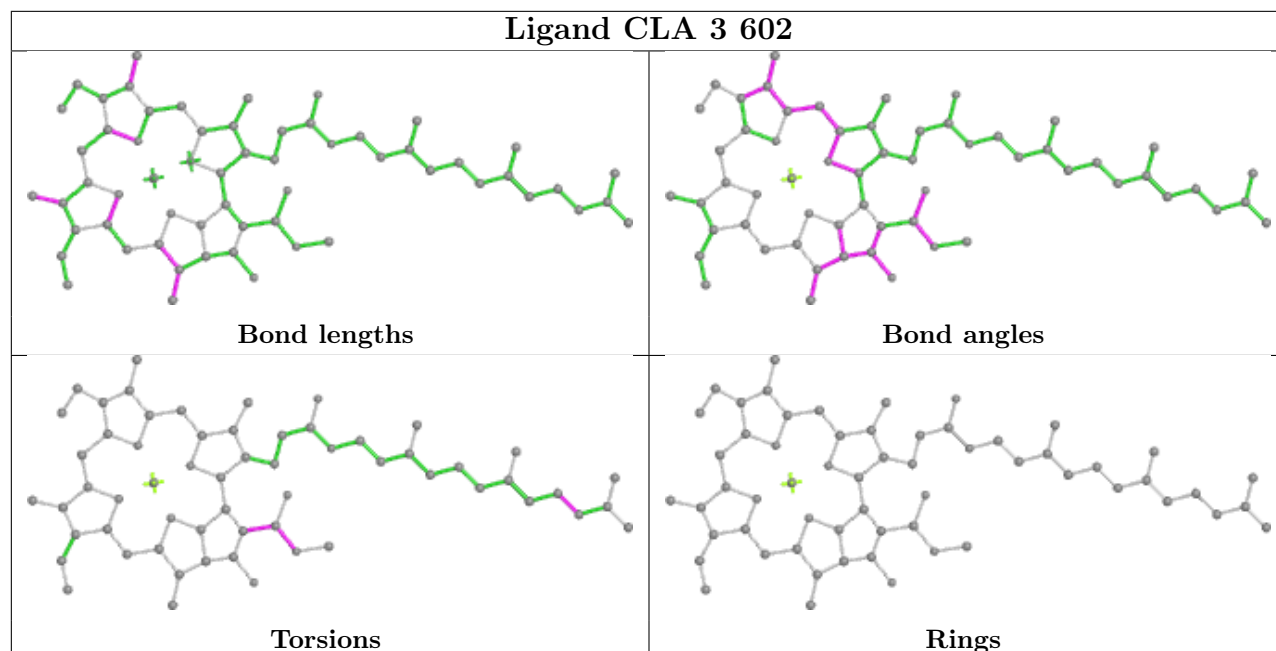
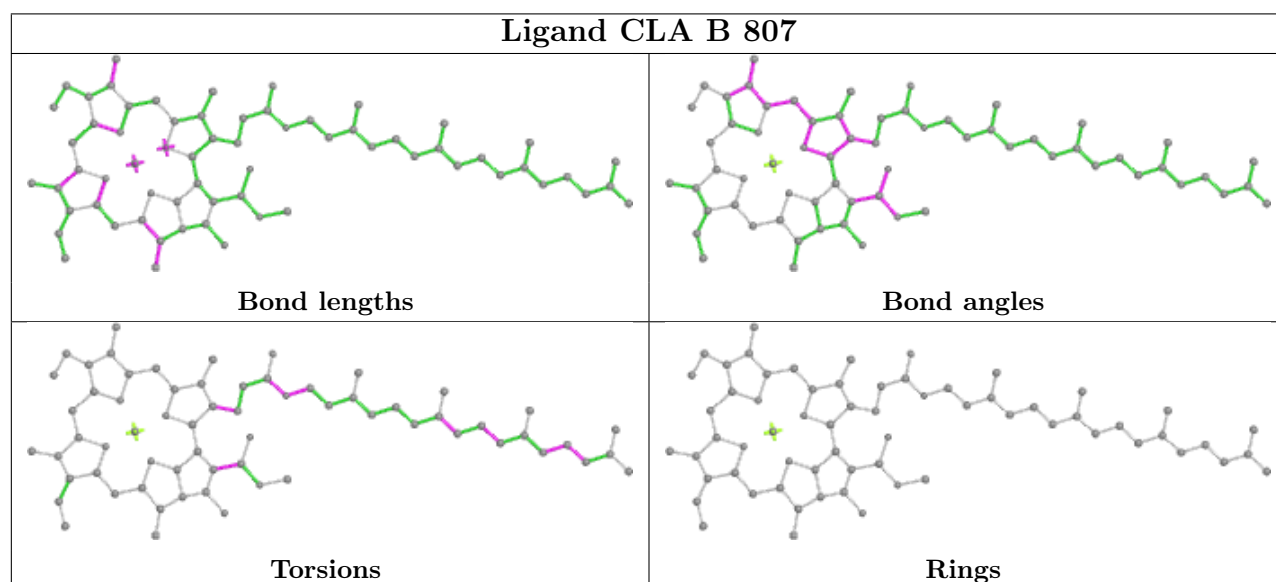


Ligand CLA 1 301

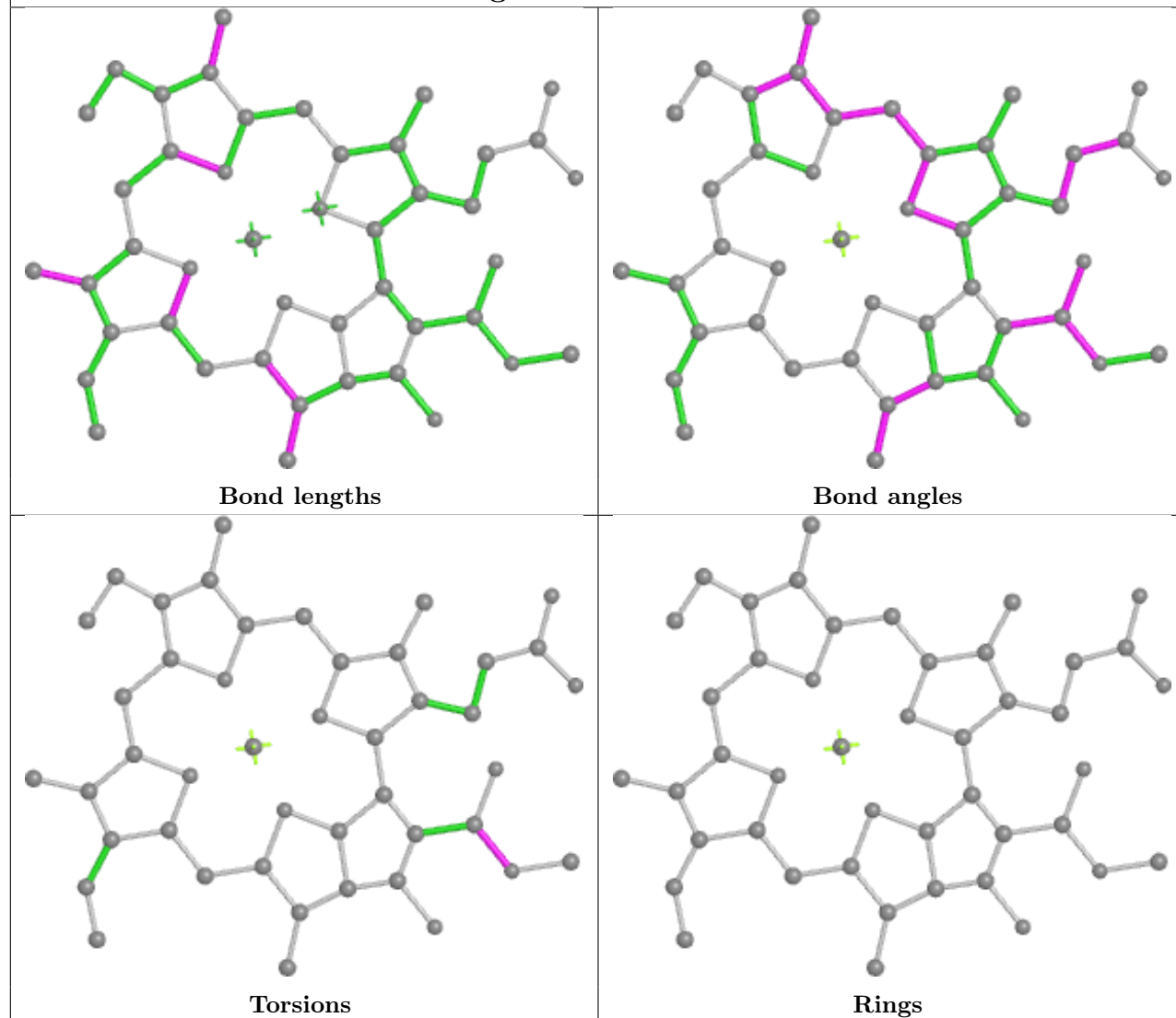


Ligand CLA 1 313

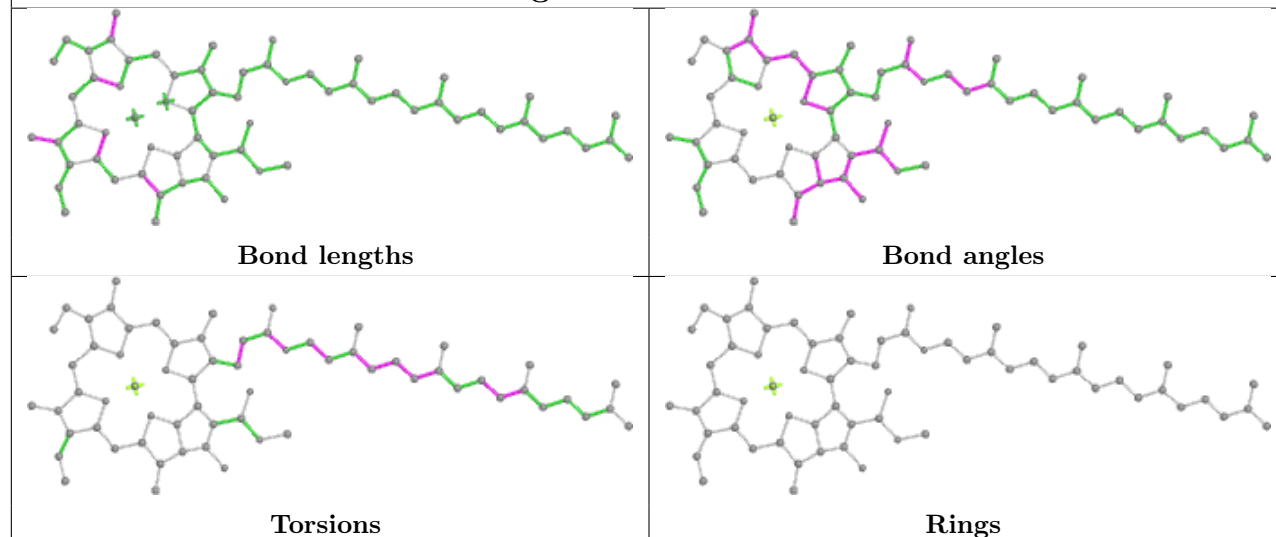


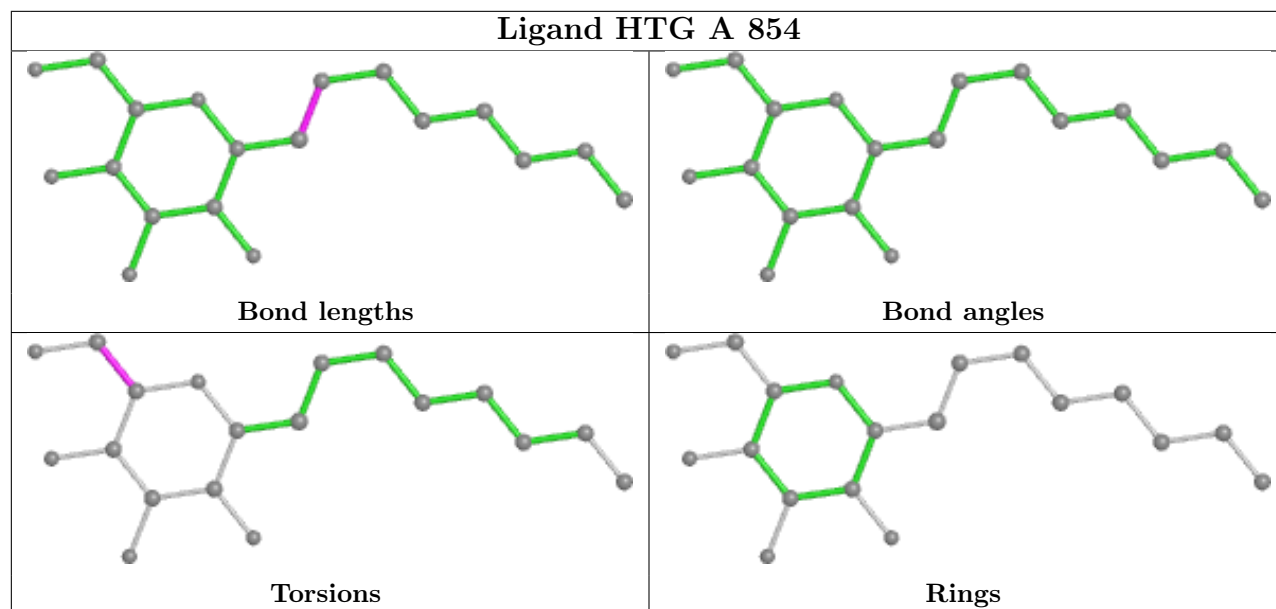
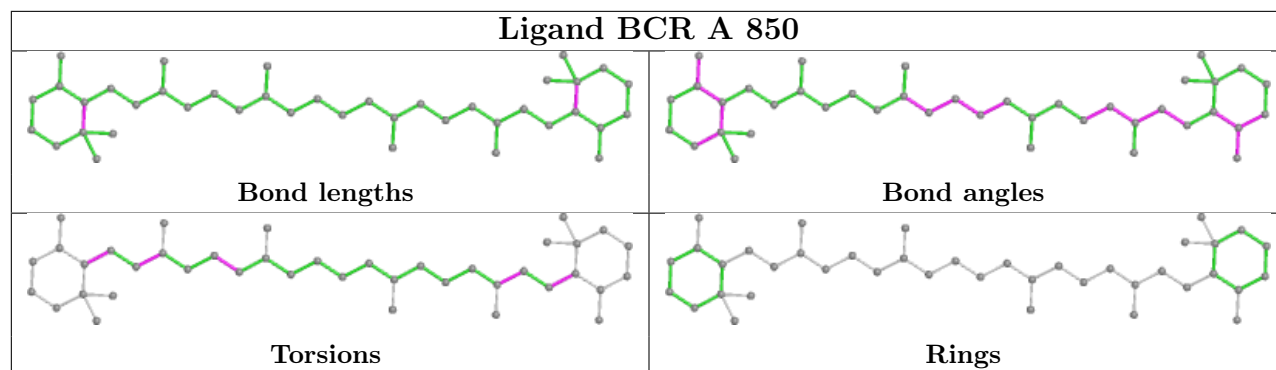
Ligand BCR L 205**Ligand CLA 3 602****Ligand CLA B 807**

Ligand CLA A 815

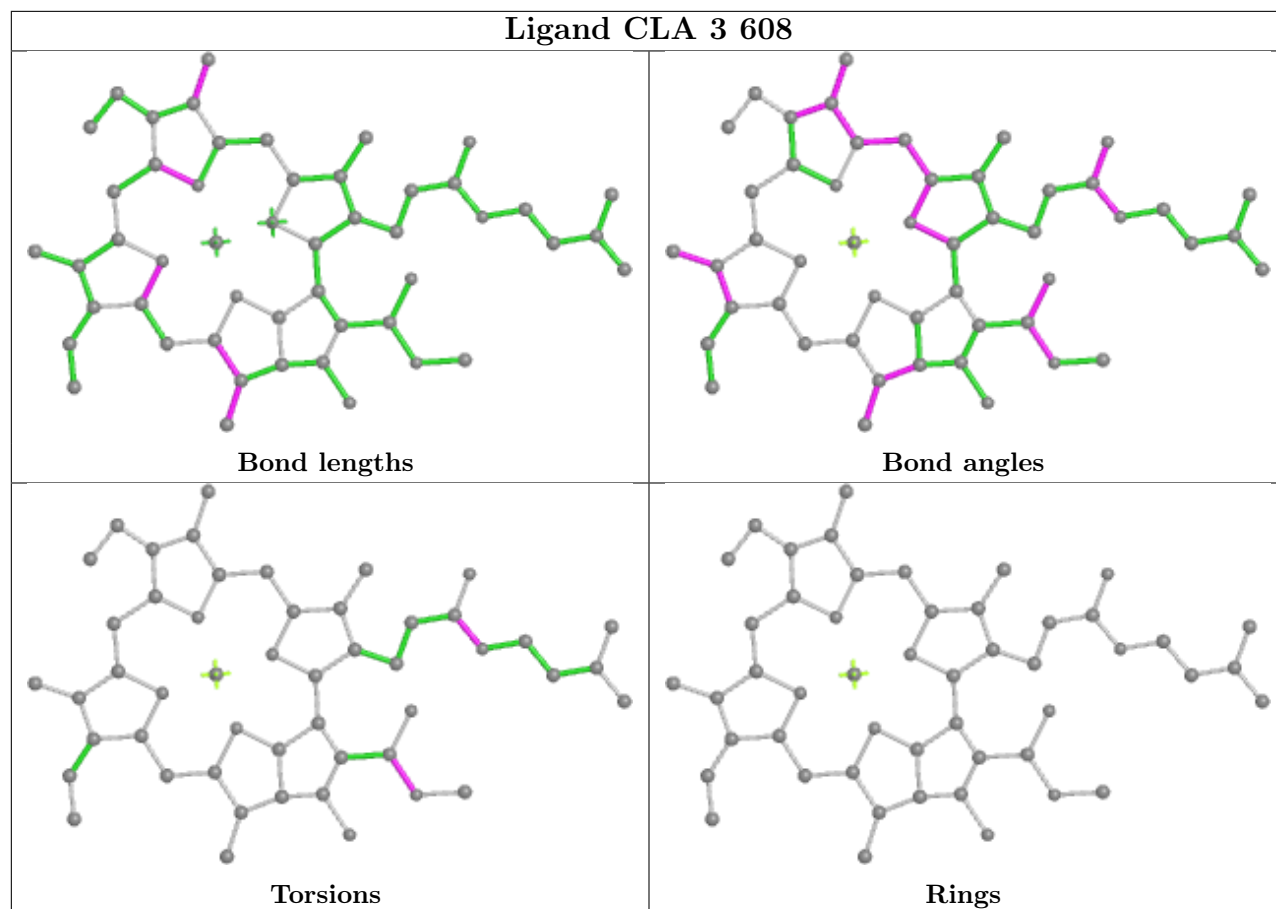


Ligand CLA A 841

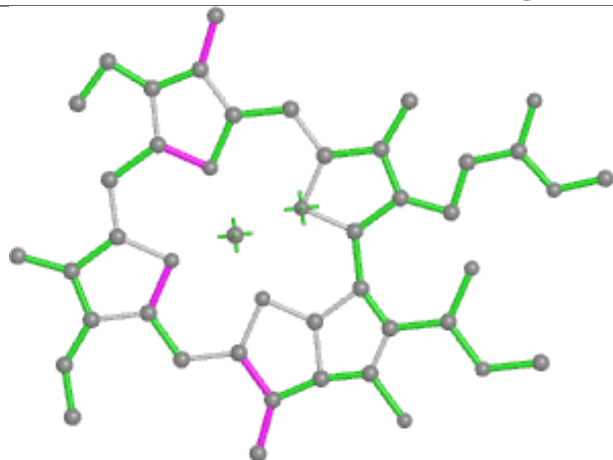




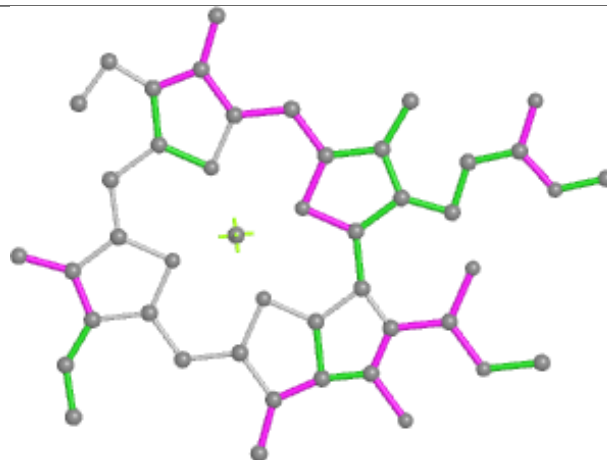
Ligand CLA 3 608



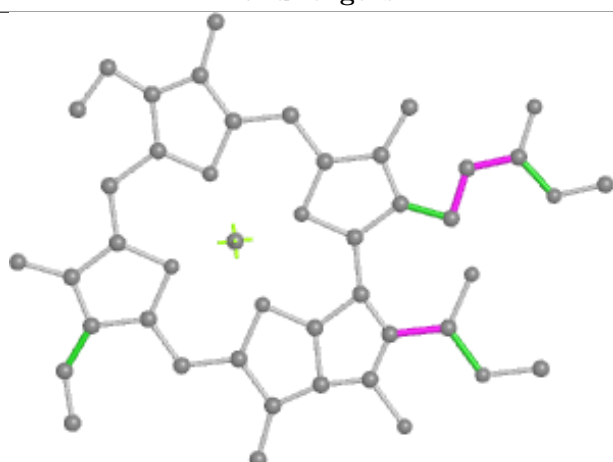
Ligand CLA 2 319



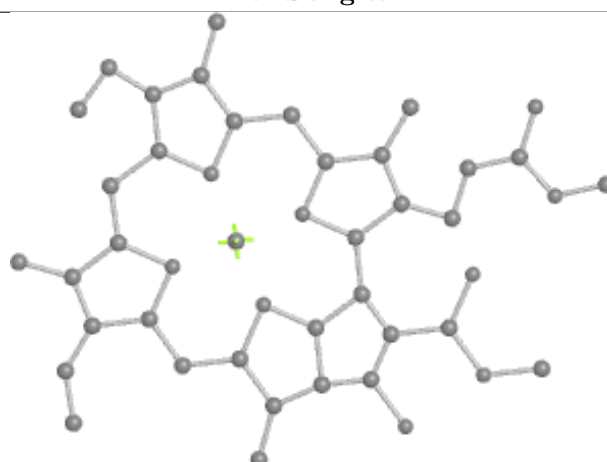
Bond lengths



Bond angles

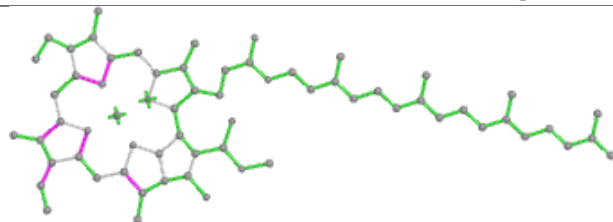


Torsions

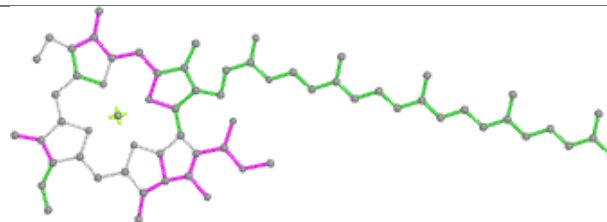


Rings

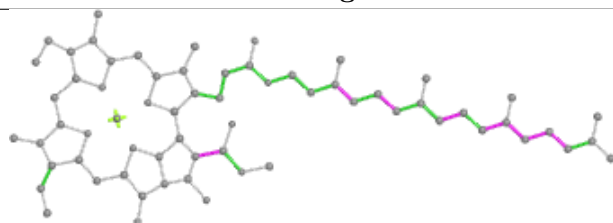
Ligand CLA B 838



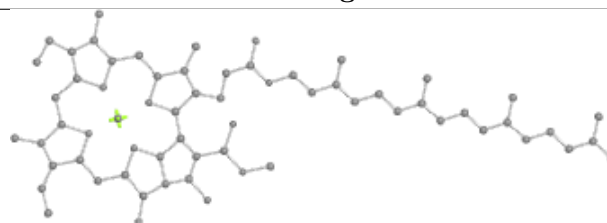
Bond lengths



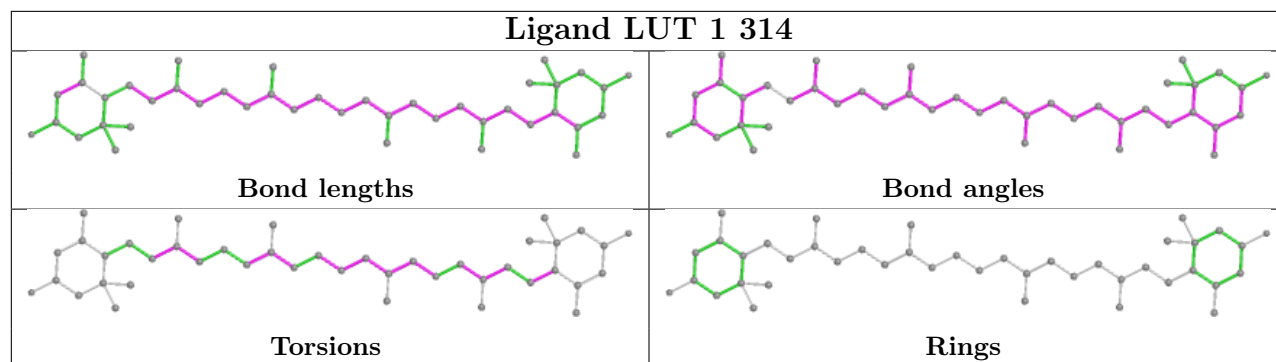
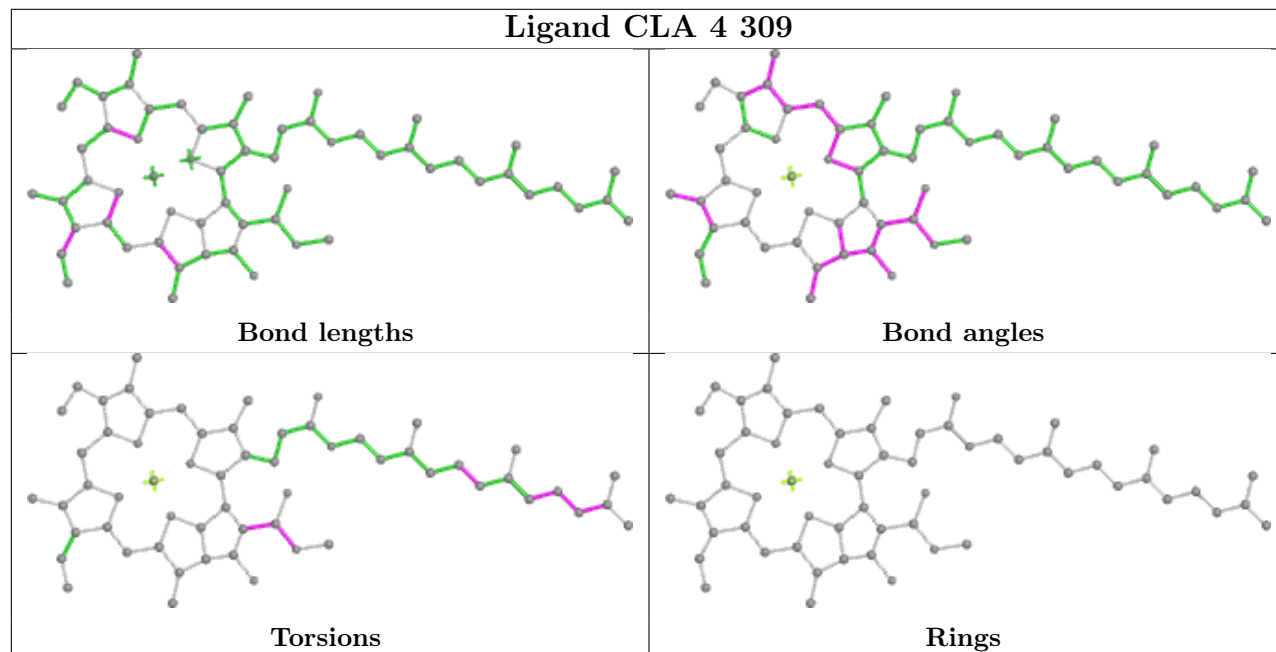
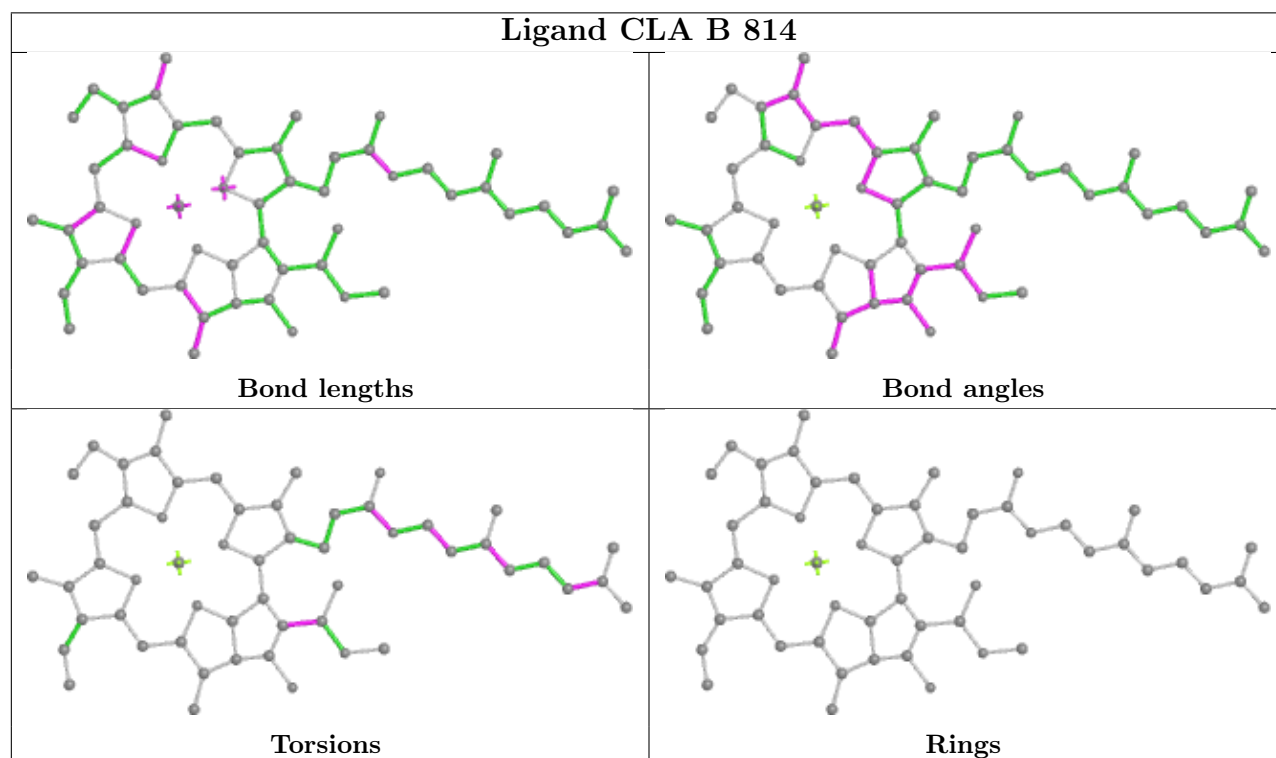
Bond angles



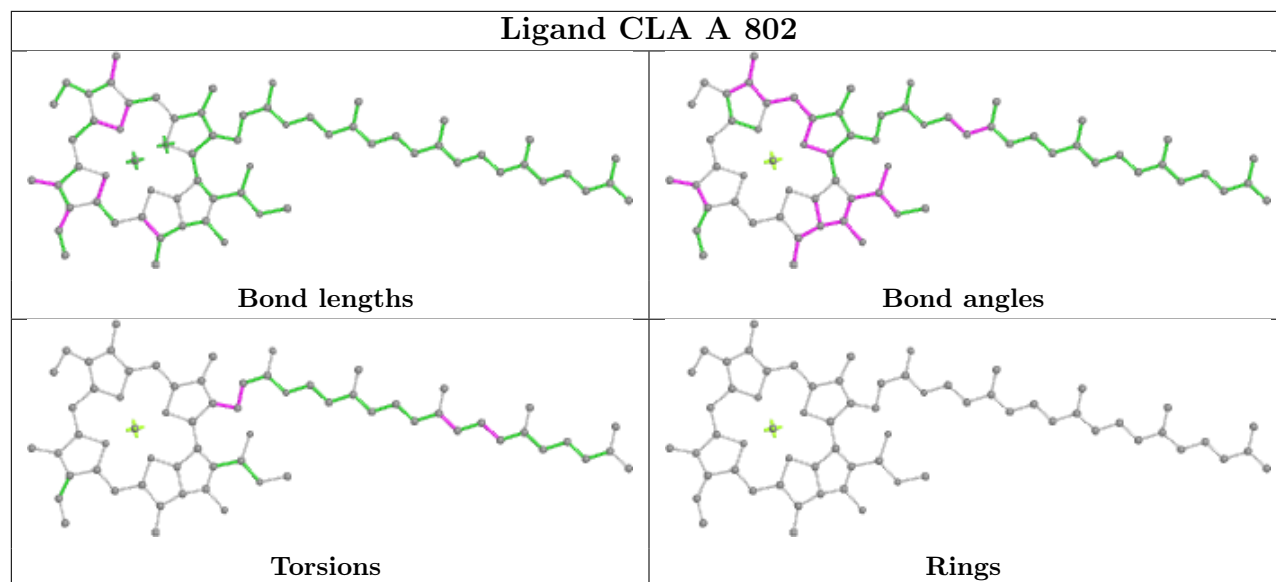
Torsions



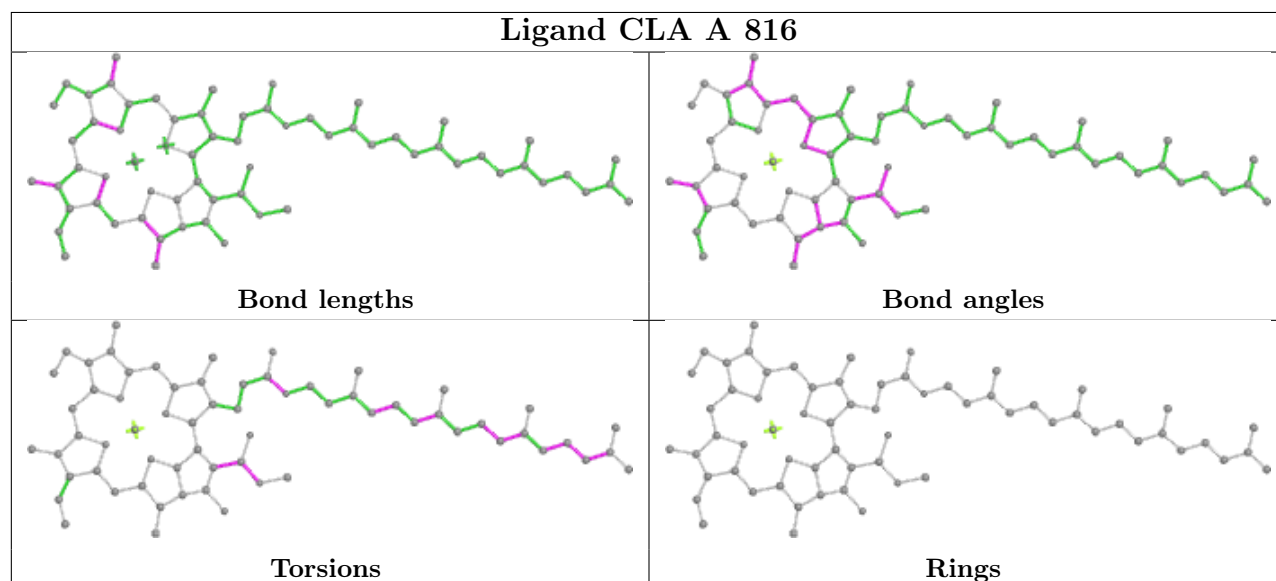
Rings

Ligand LUT 1 314**Ligand CLA 4 309****Ligand CLA B 814**

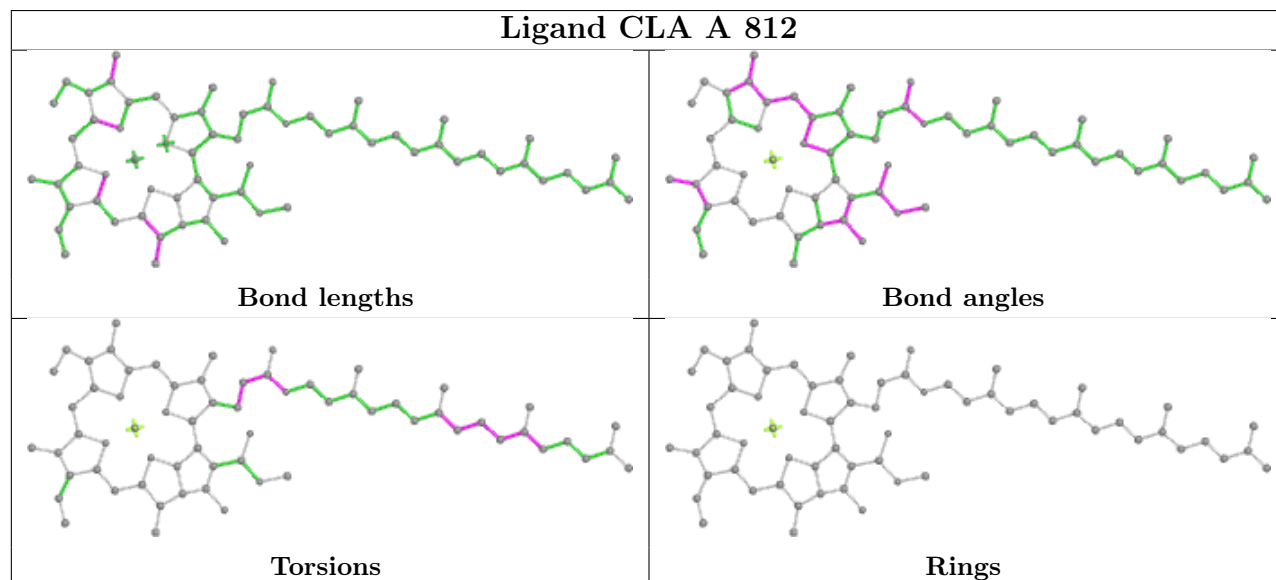
Ligand CLA A 802

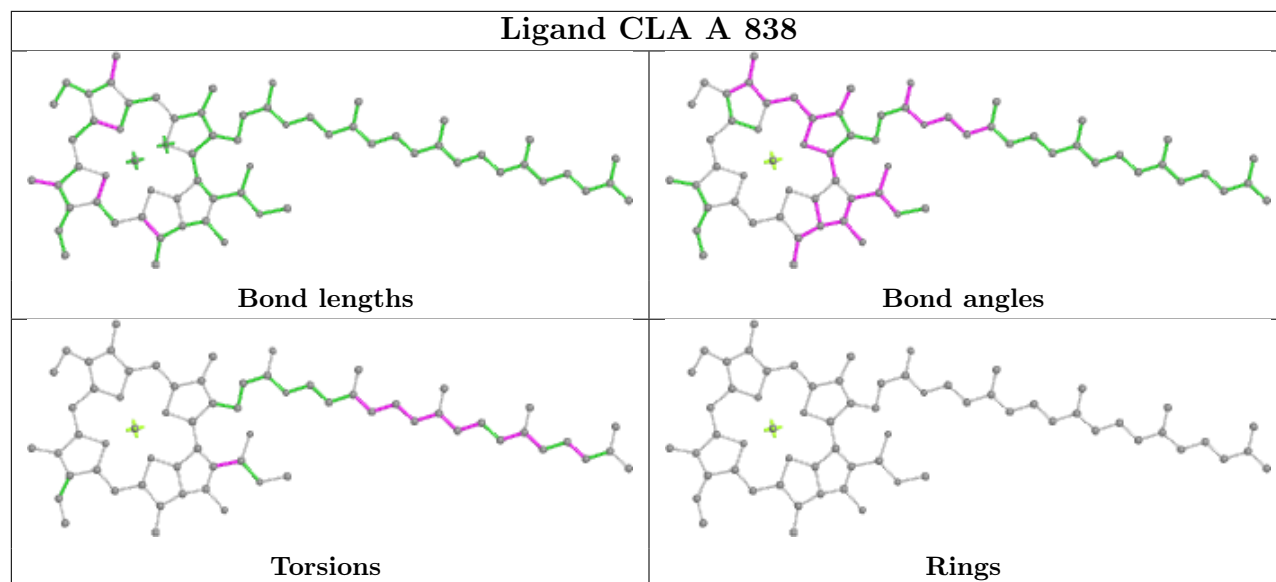
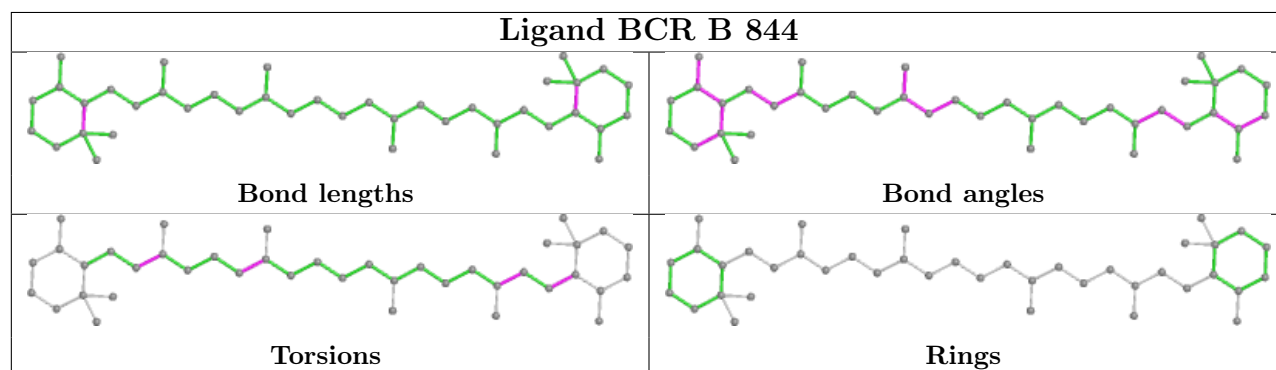
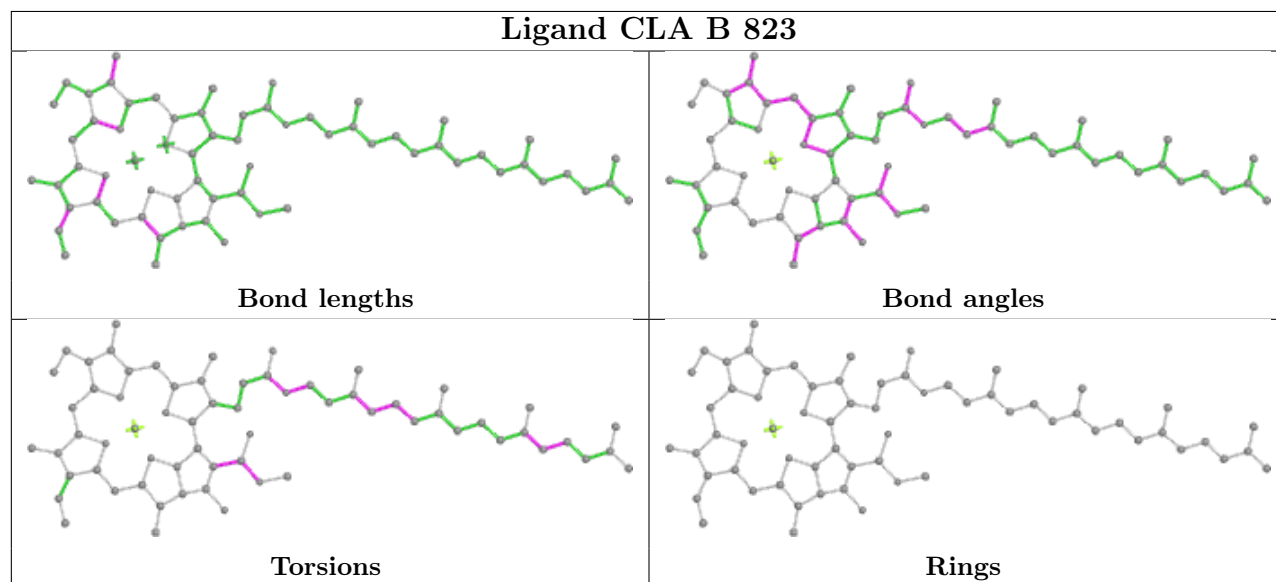


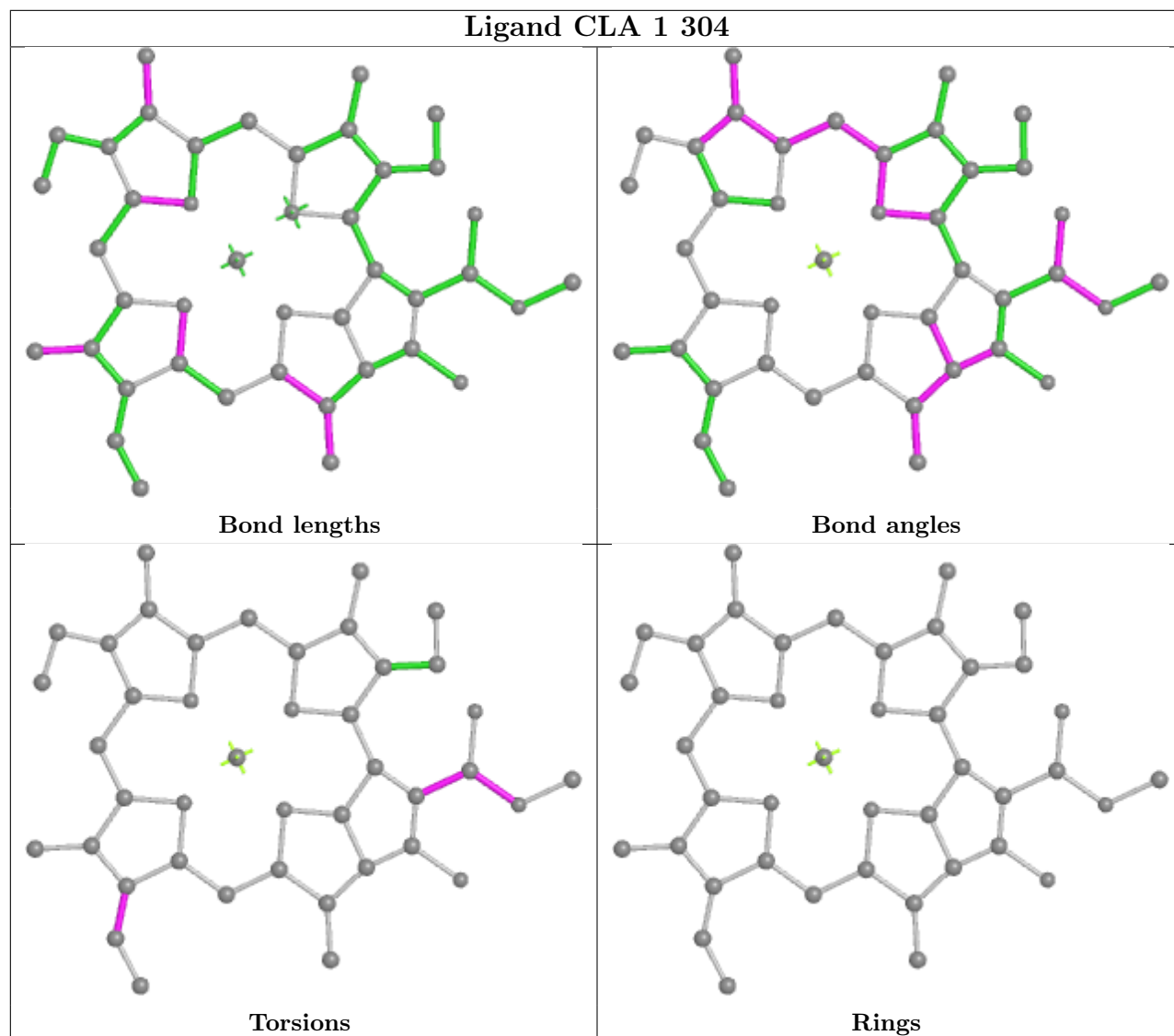
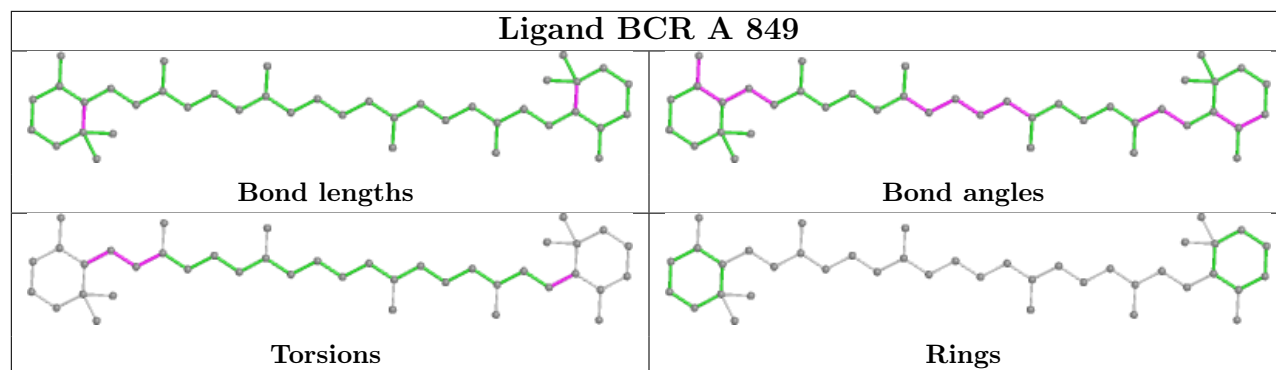
Ligand CLA A 816



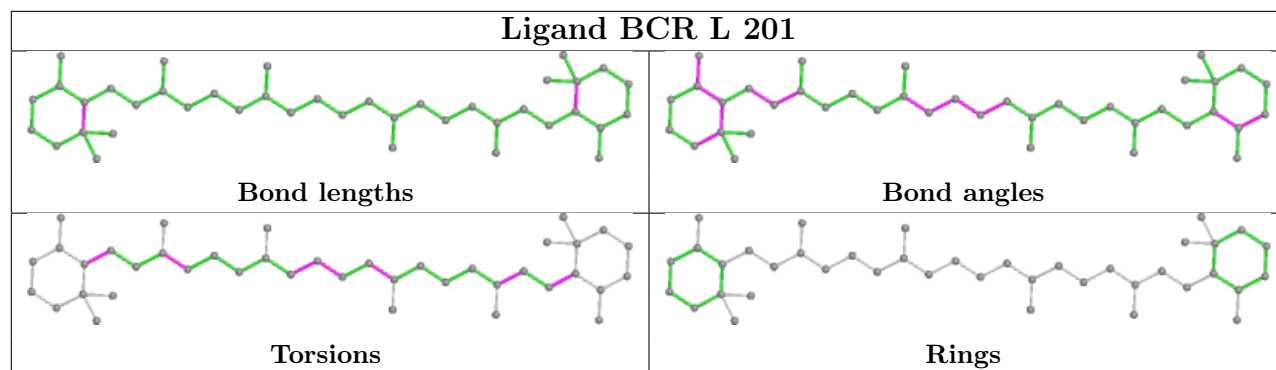
Ligand CLA A 812



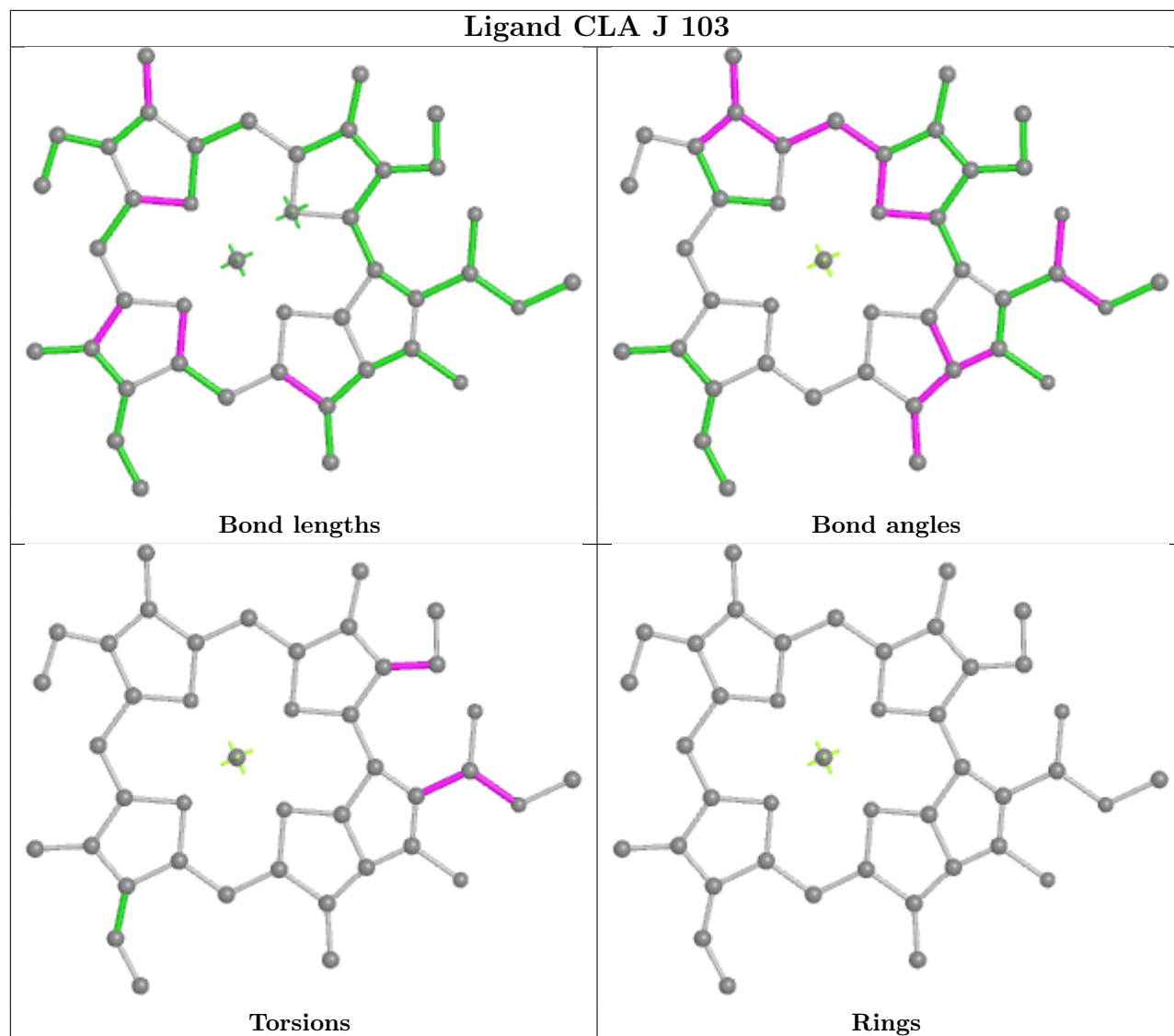
Ligand CLA A 838**Ligand BCR B 844****Ligand CLA B 823**



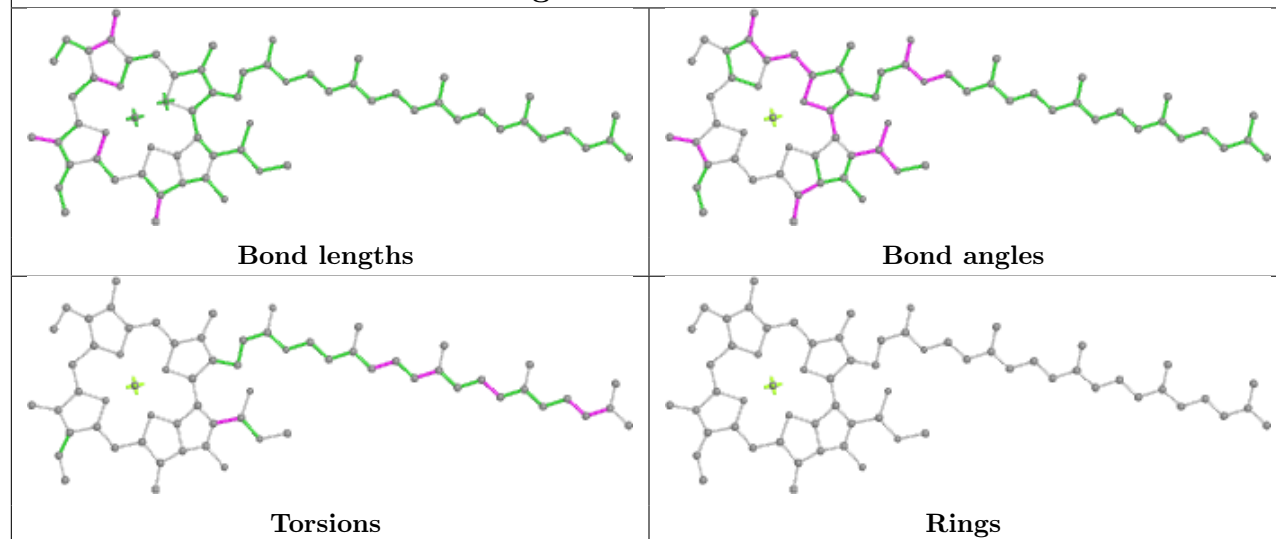
Ligand BCR L 201



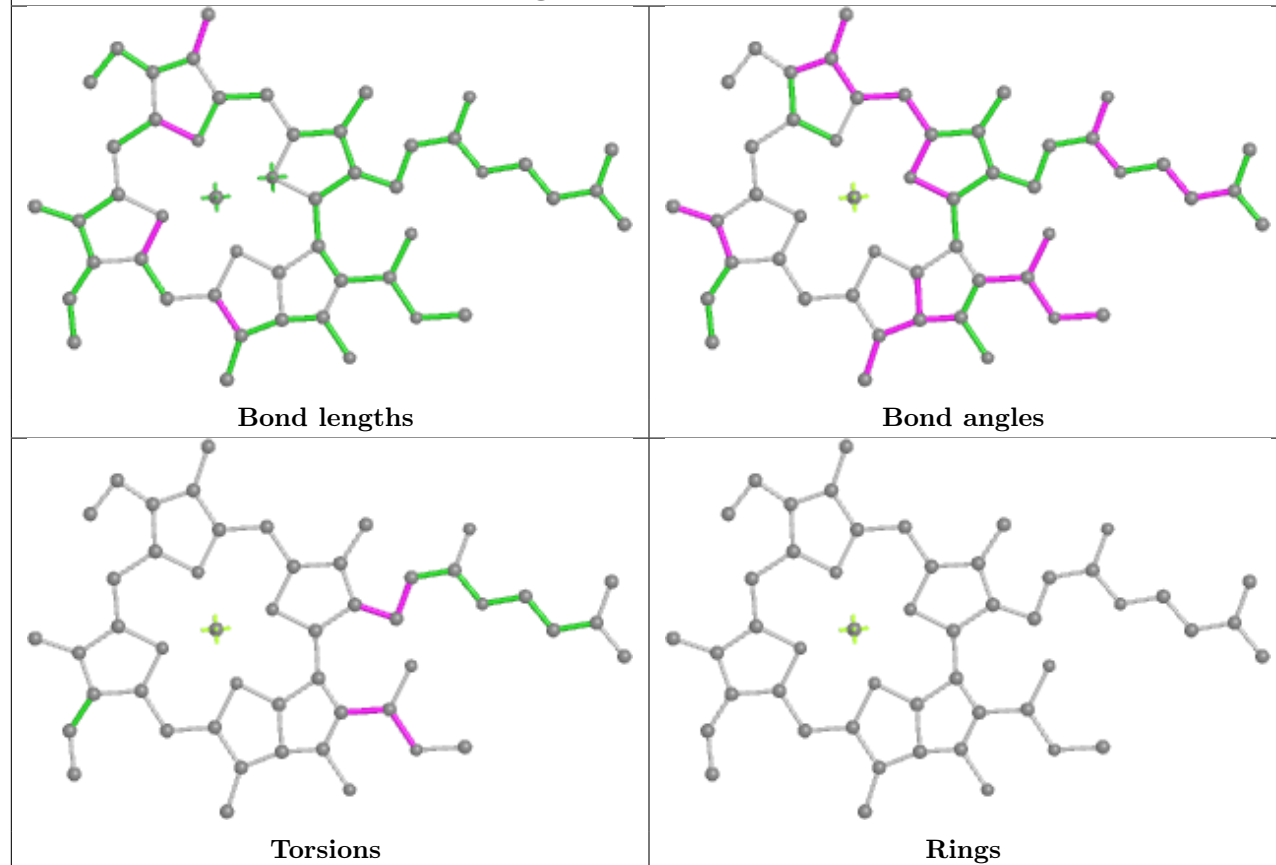
Ligand CLA J 103



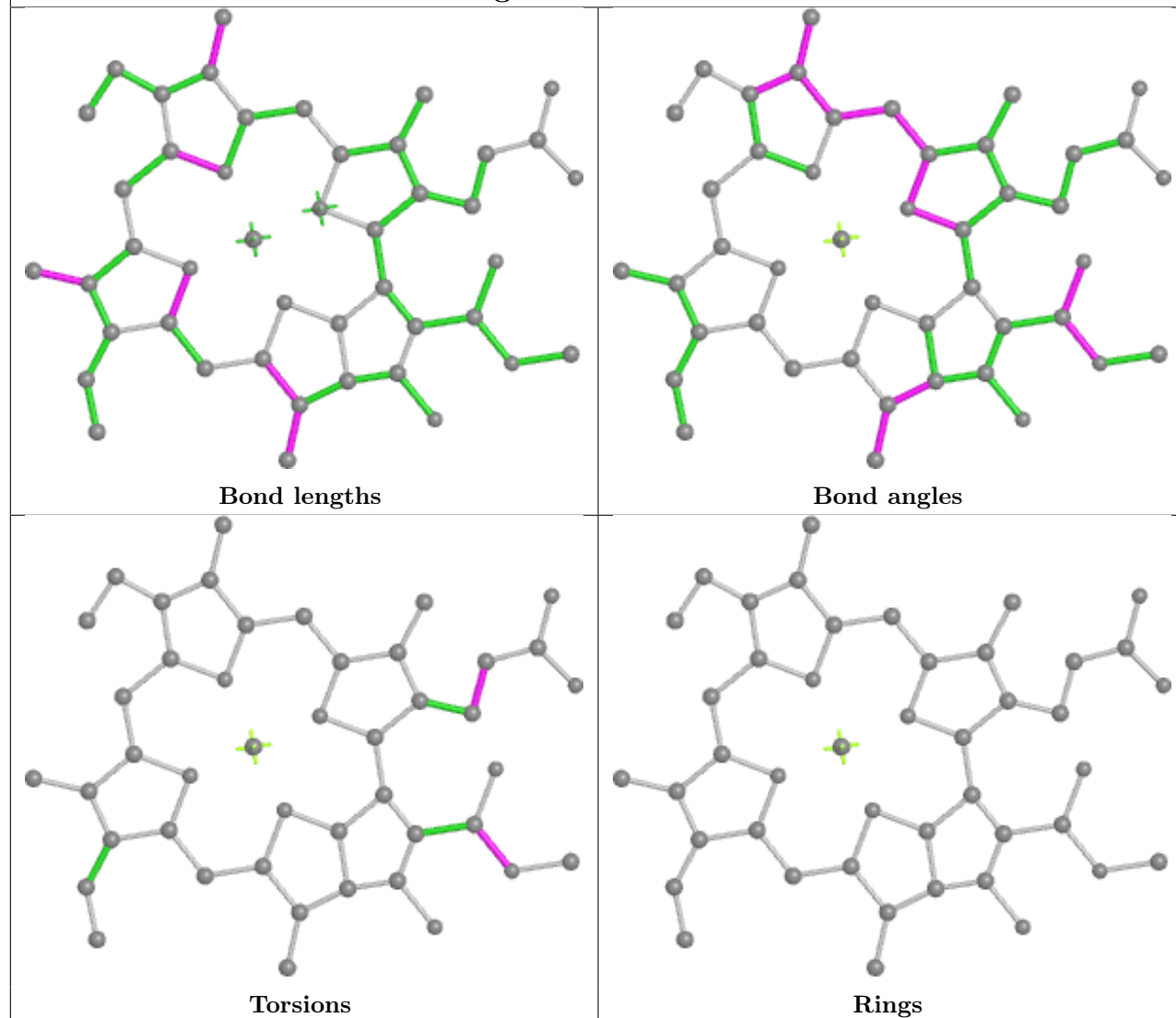
Ligand CLA B 810



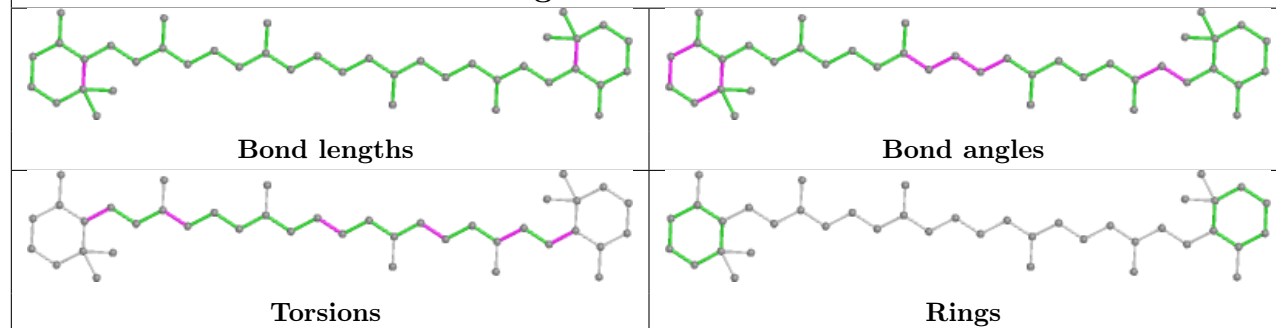
Ligand CLA B 822



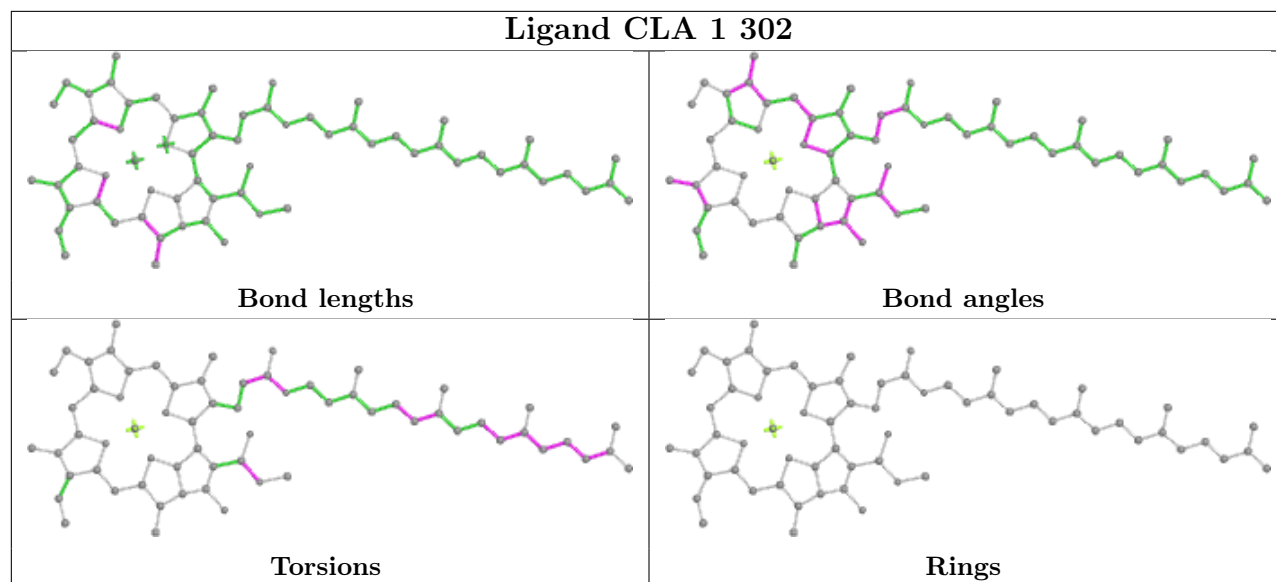
Ligand CLA 3 612



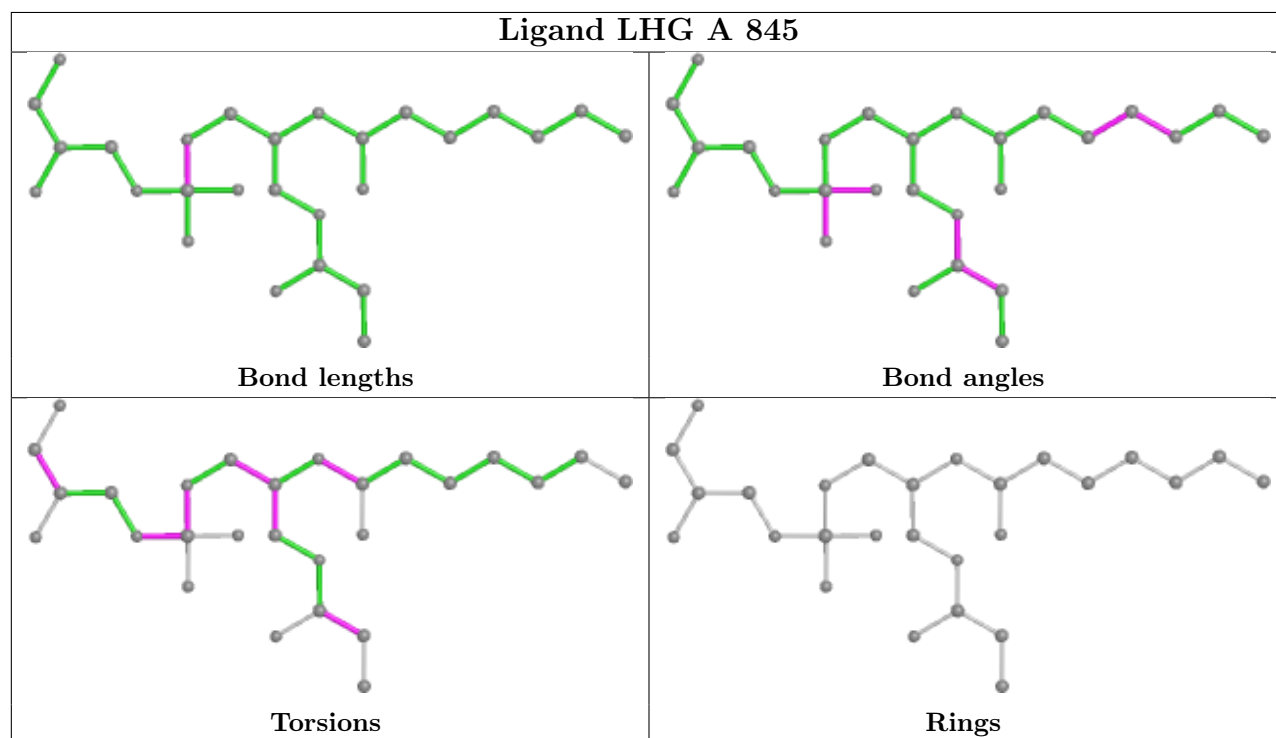
Ligand BCR 3 616



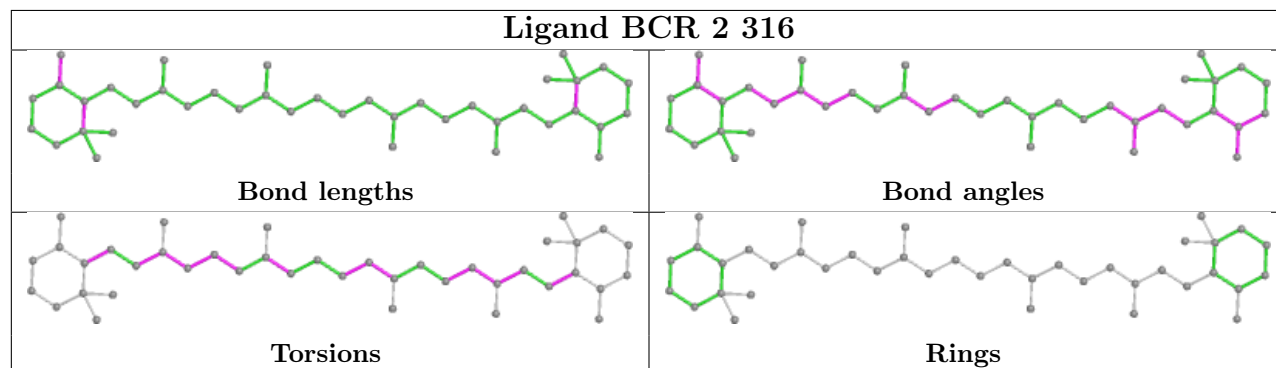
Ligand CLA 1 302



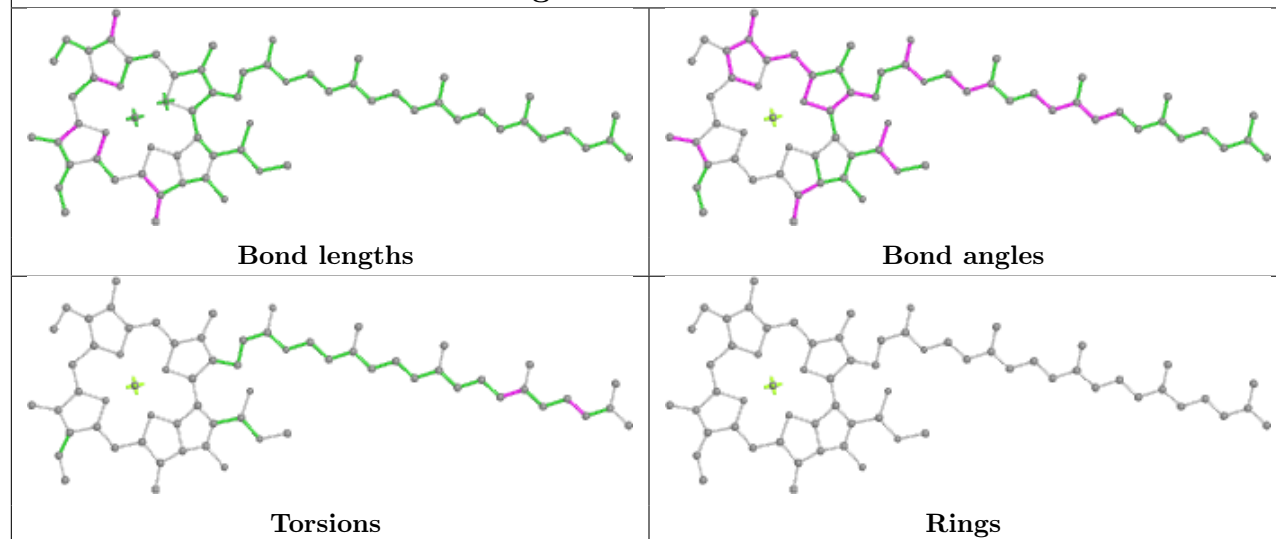
Ligand LHG A 845



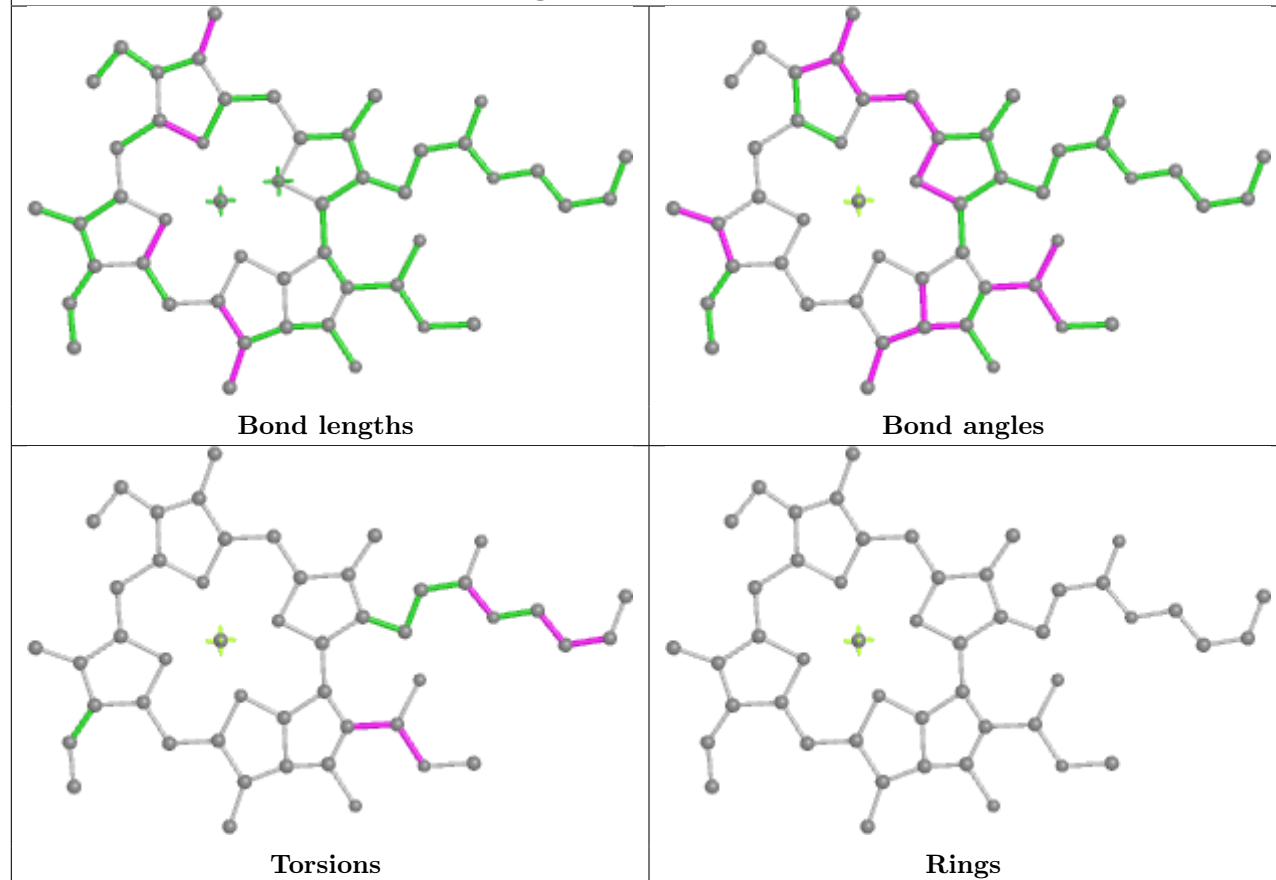
Ligand BCR 2 316



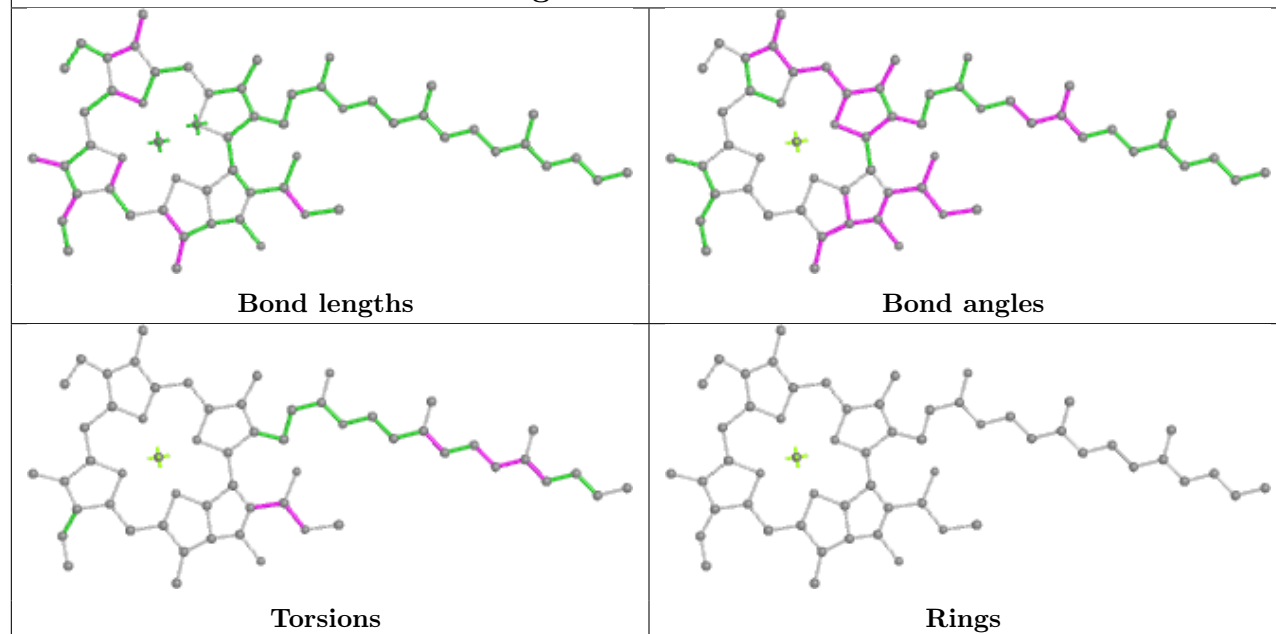
Ligand CLA B 802



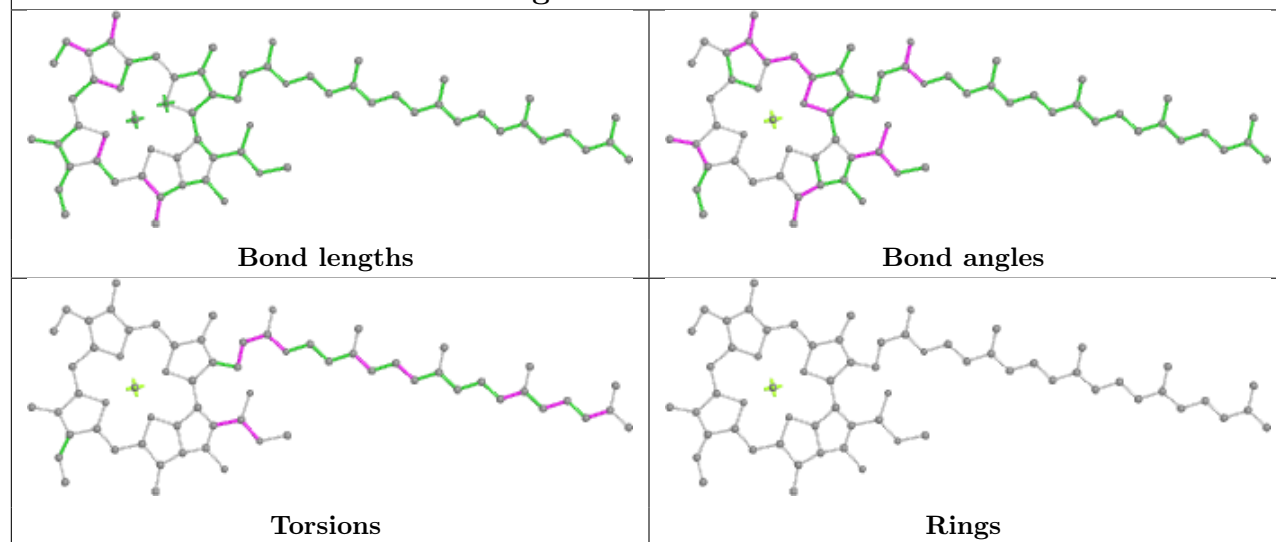
Ligand CLA A 821



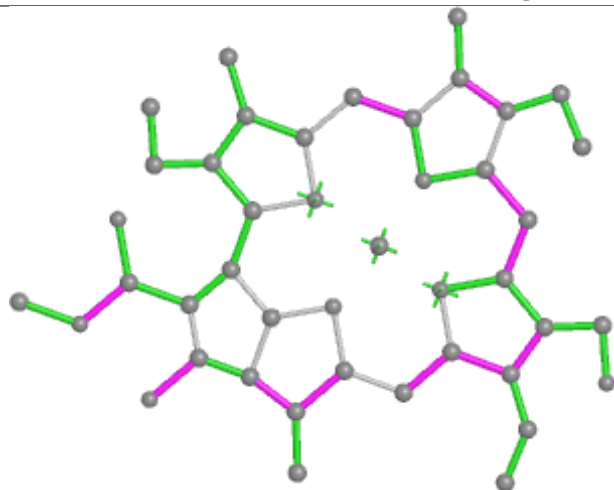
Ligand CLA B 834



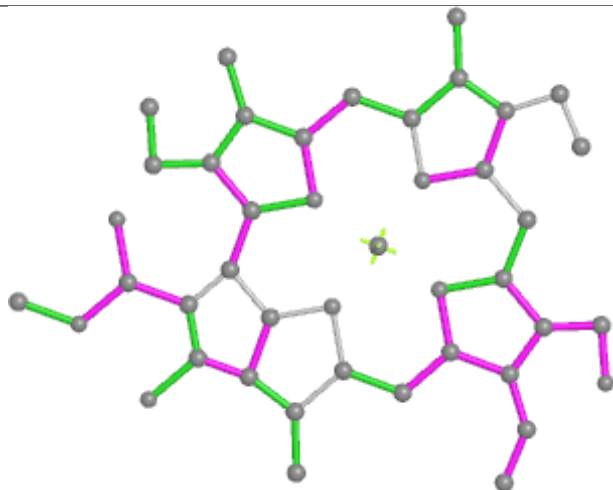
Ligand CLA B 812



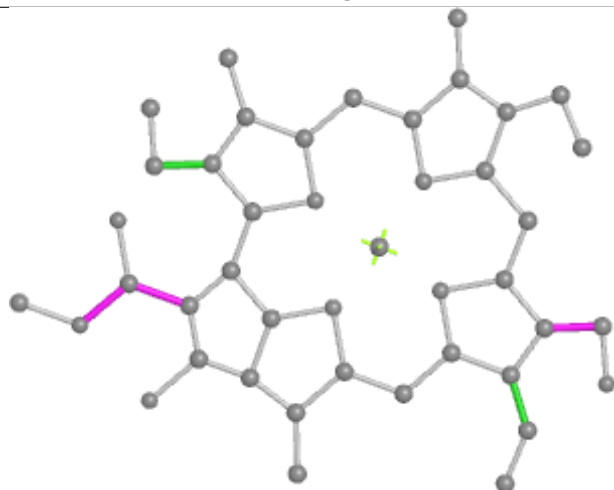
Ligand CHL 2 304



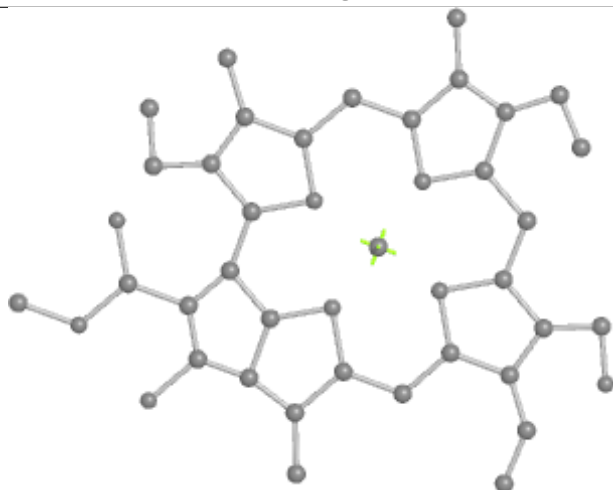
Bond lengths



Bond angles

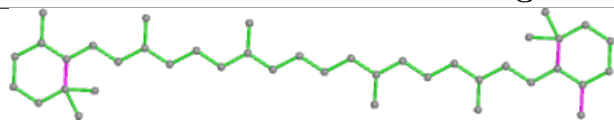


Torsions

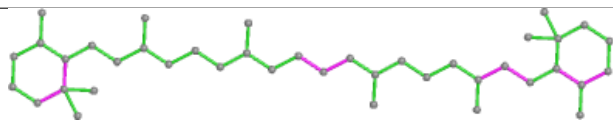


Rings

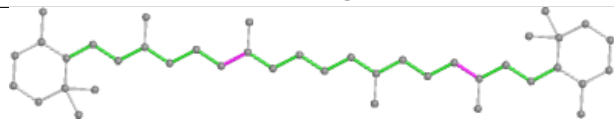
Ligand BCR J 104



Bond lengths



Bond angles

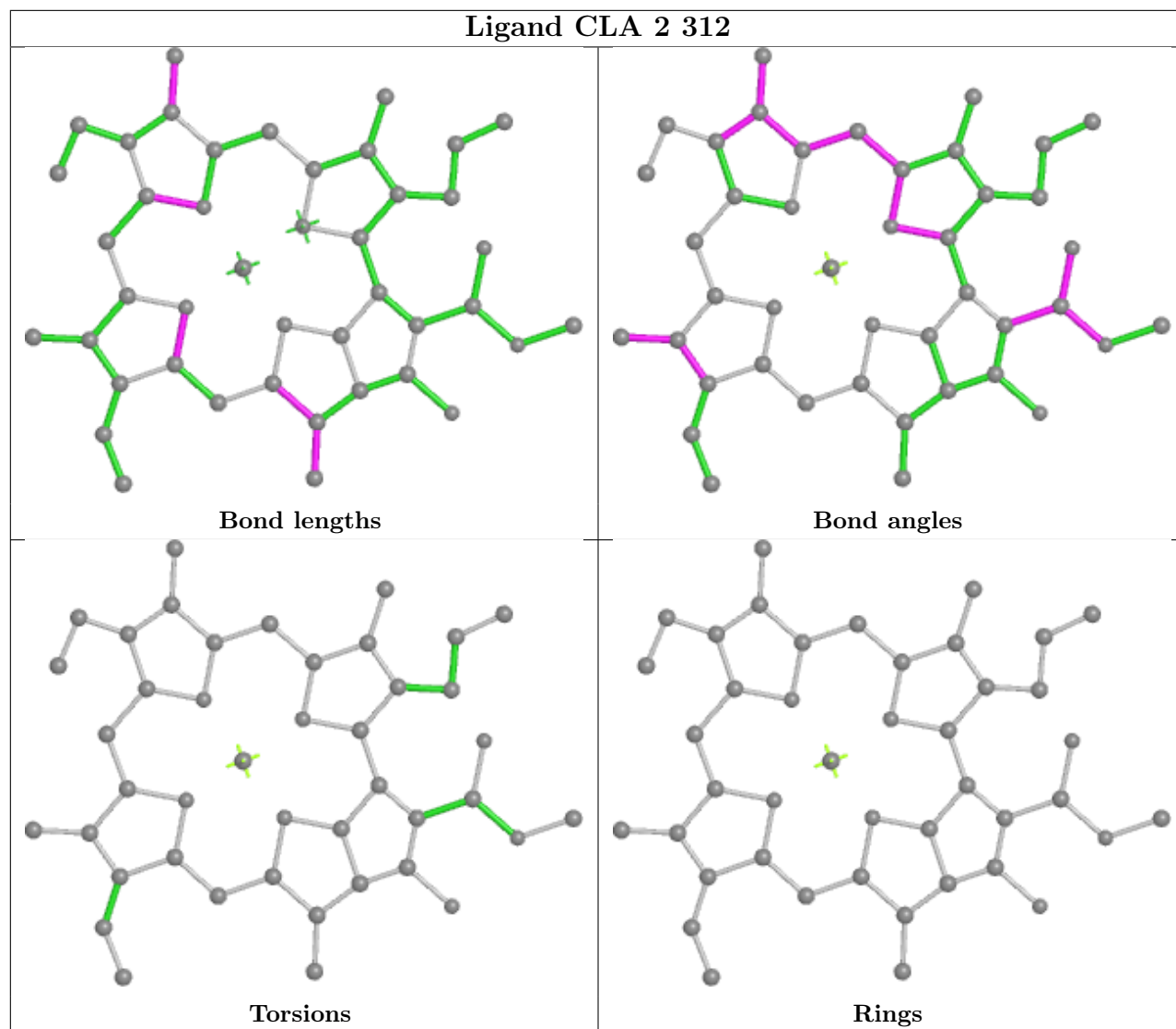


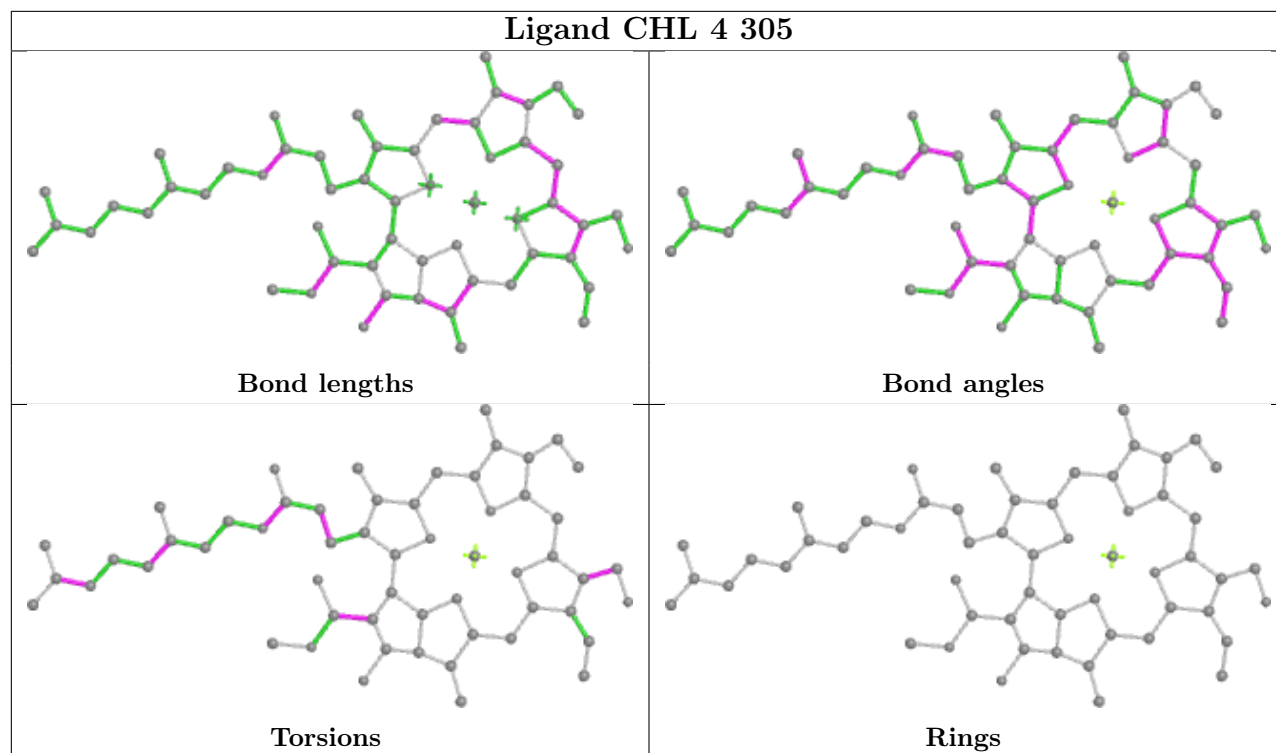
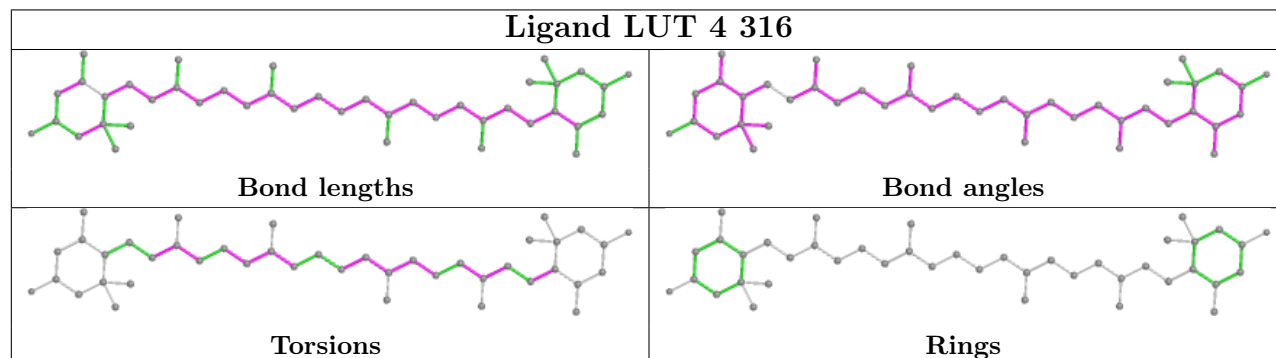
Torsions



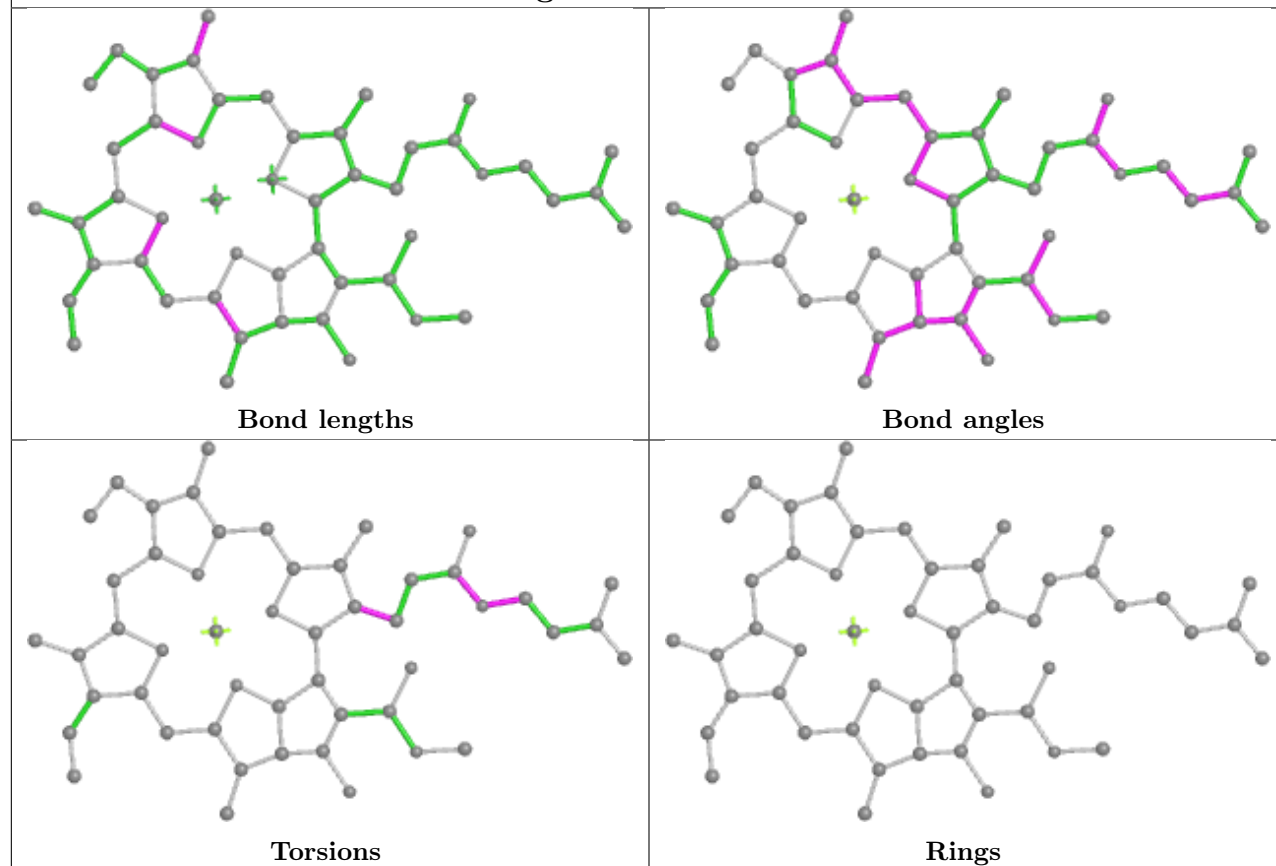
Rings

Ligand CLA 2 312

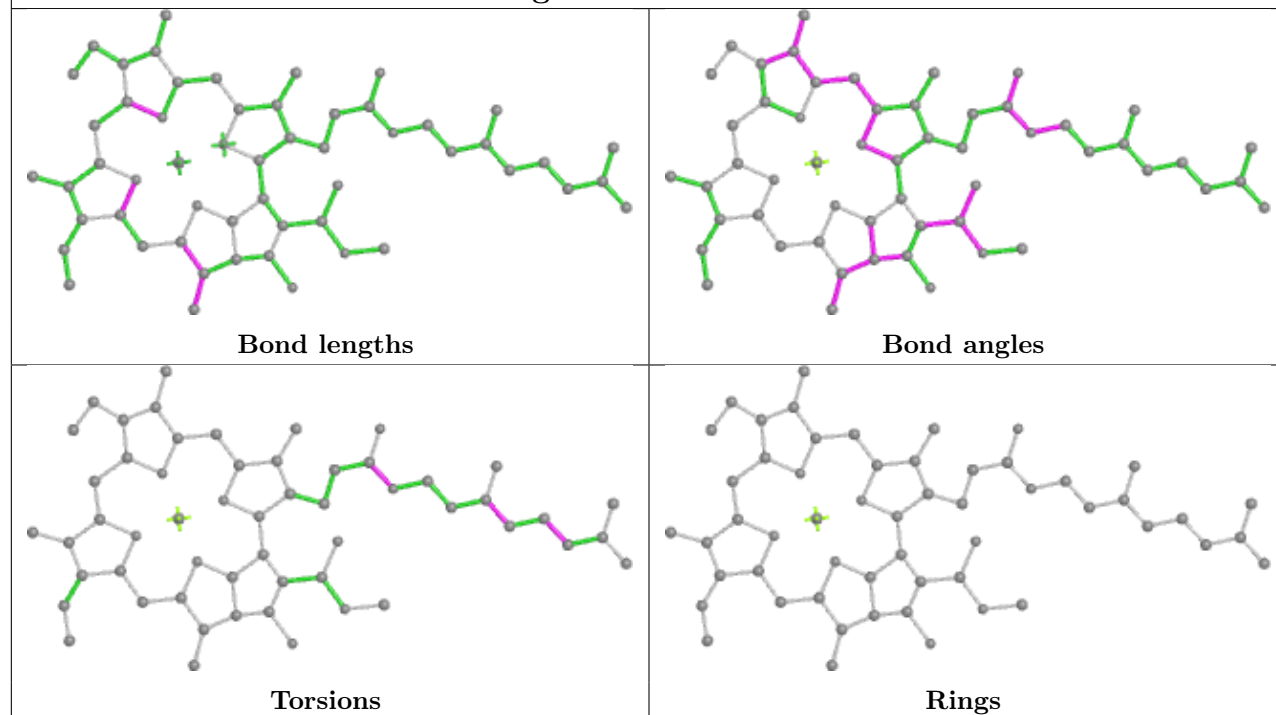


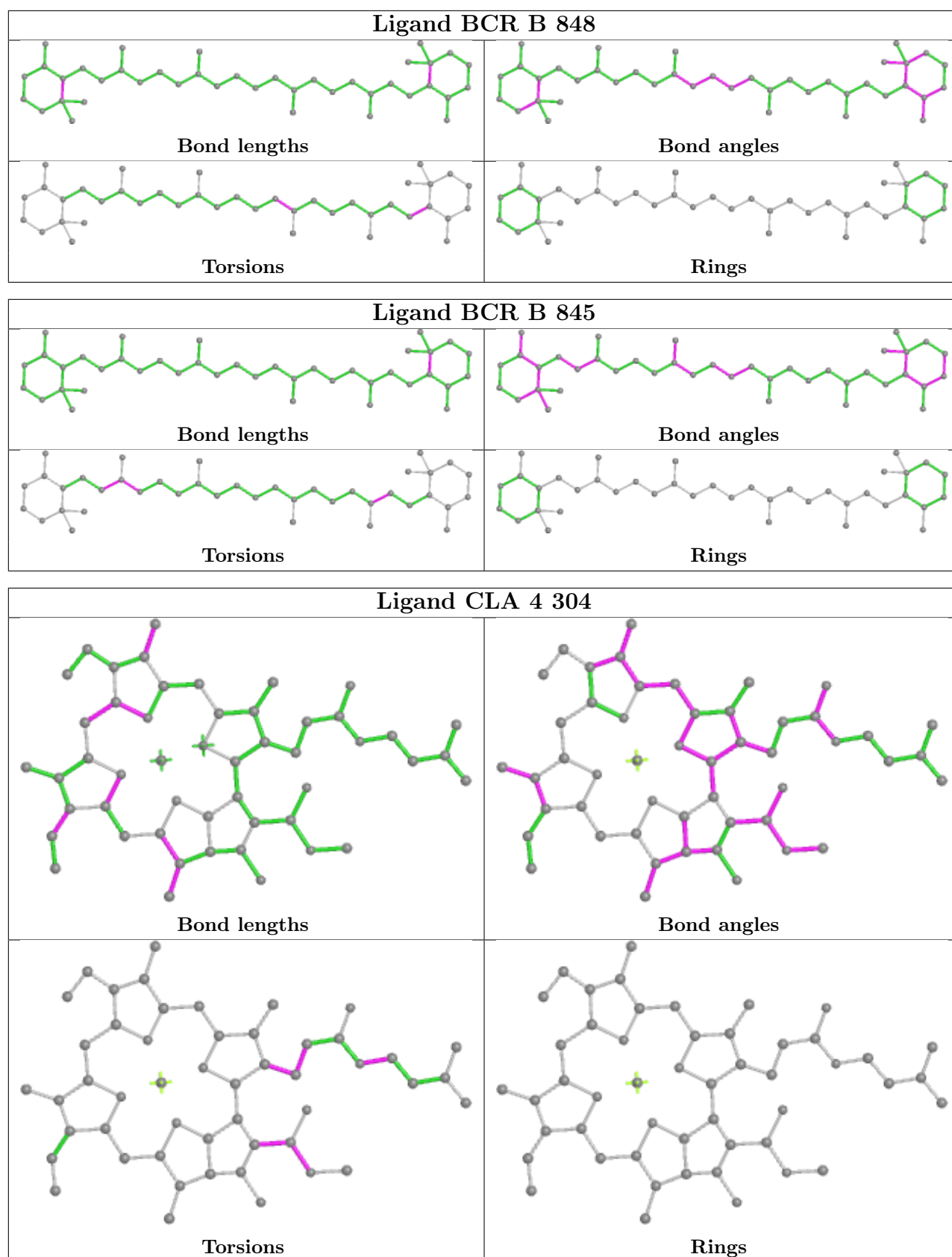
Ligand CHL 4 305**Ligand LUT 4 316**

Ligand CLA 3 609

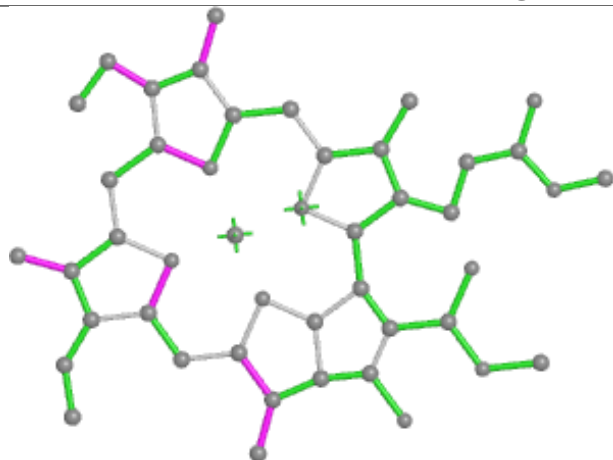


Ligand CLA B 818

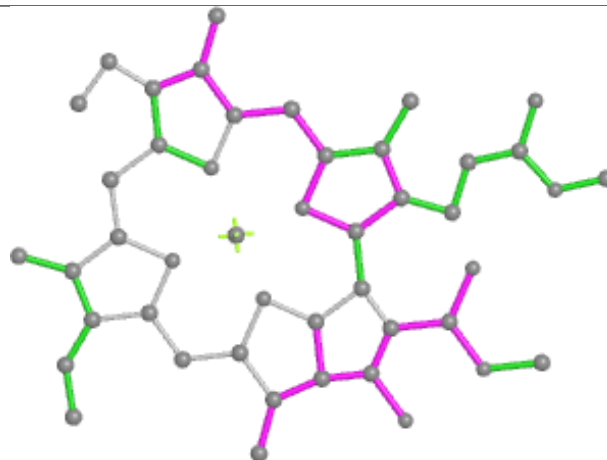




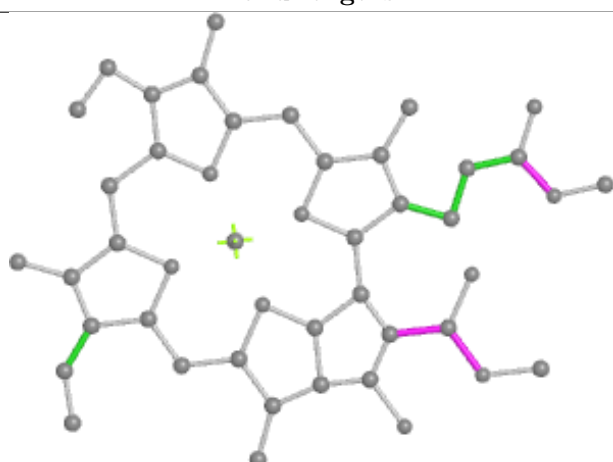
Ligand CLA G 105



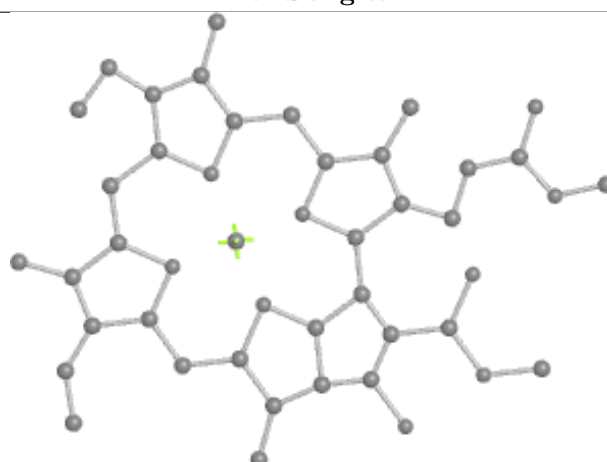
Bond lengths



Bond angles

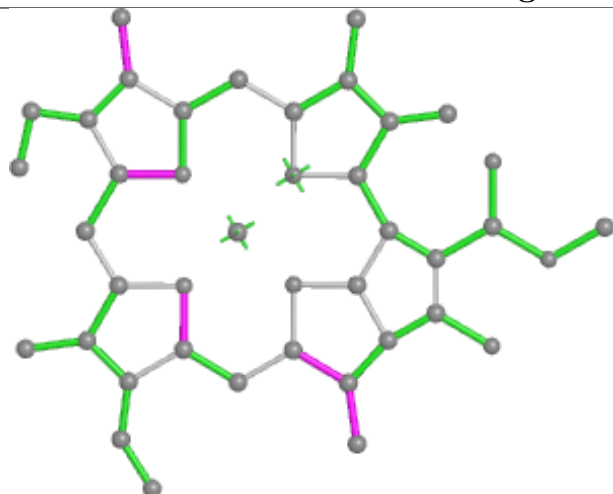


Torsions

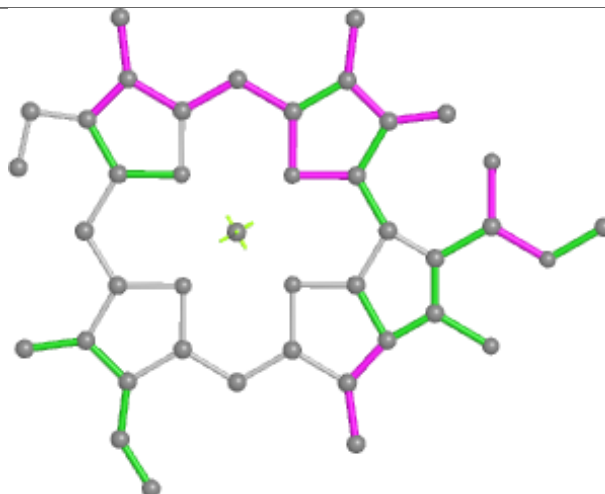


Rings

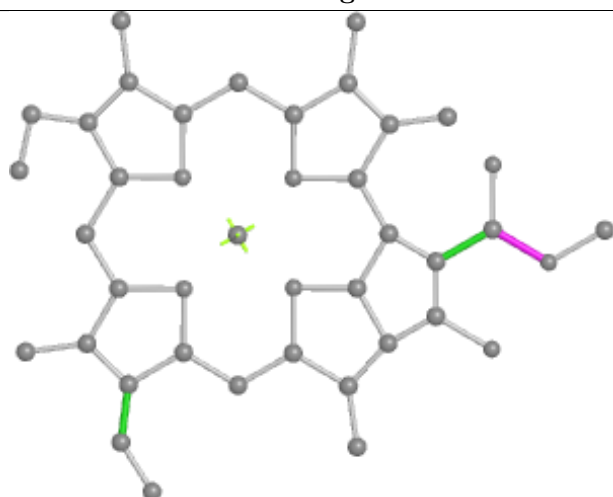
Ligand CLA 2 309



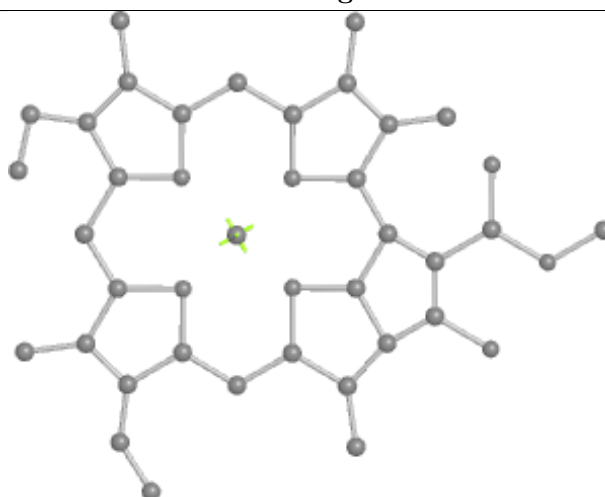
Bond lengths



Bond angles

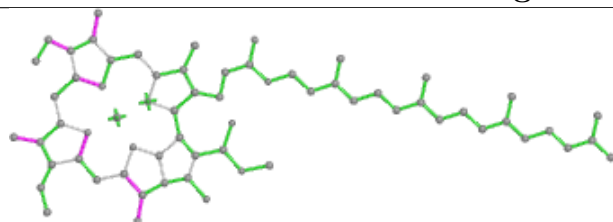


Torsions

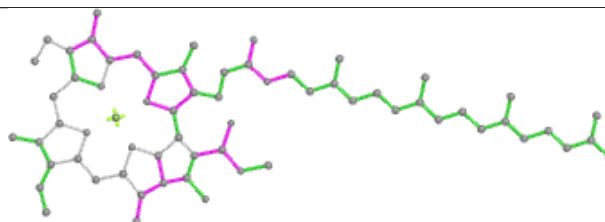


Rings

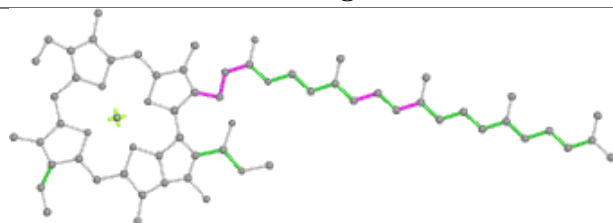
Ligand CLA A 808



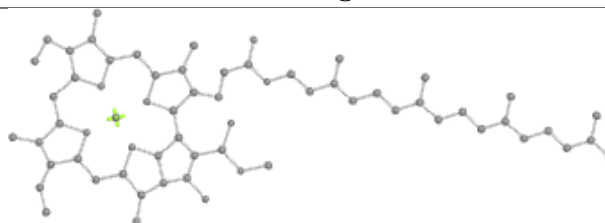
Bond lengths



Bond angles

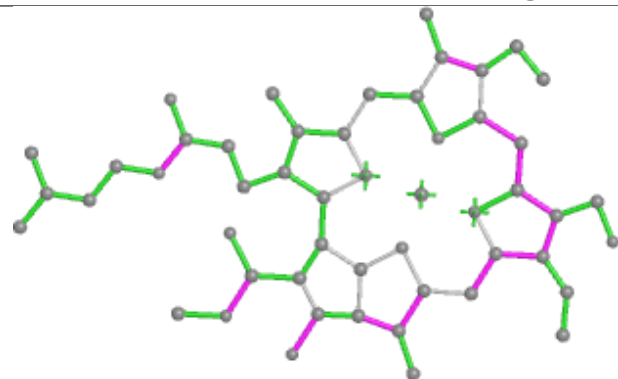


Torsions

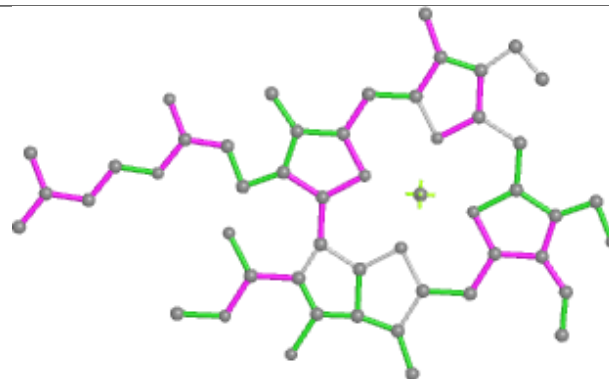


Rings

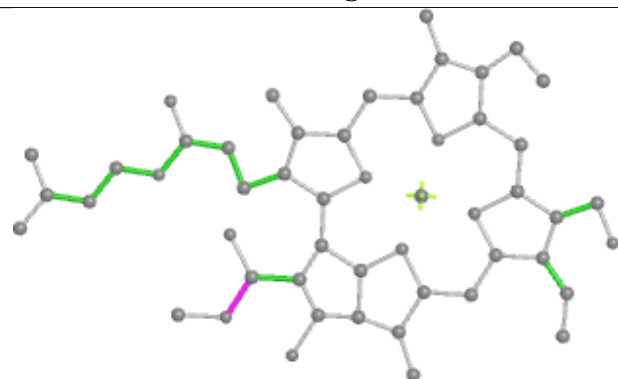
Ligand CHL 4 307



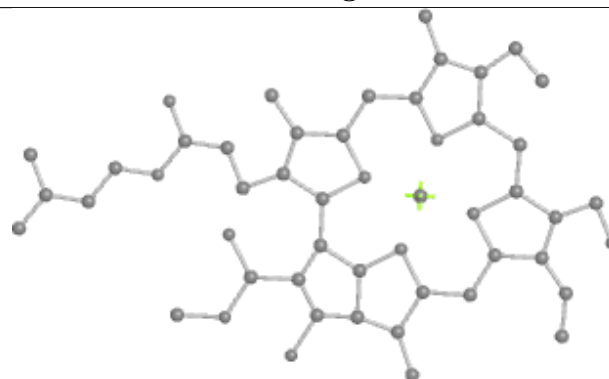
Bond lengths



Bond angles

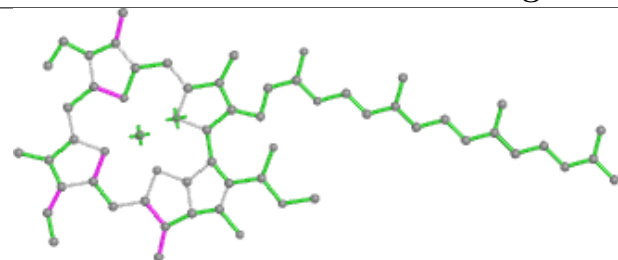


Torsions

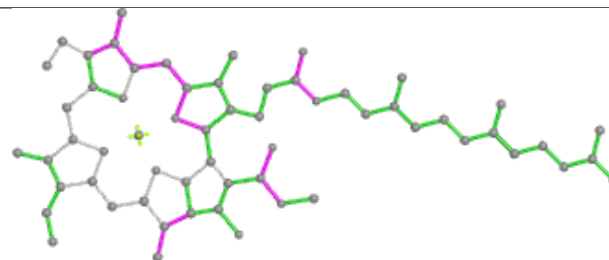


Rings

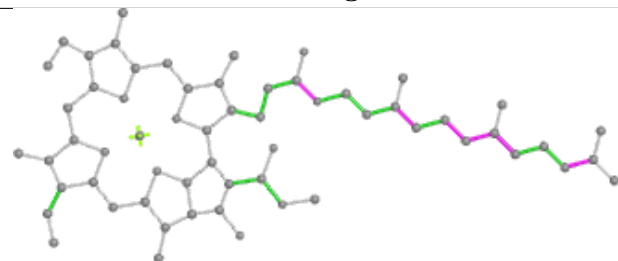
Ligand CLA 1 308



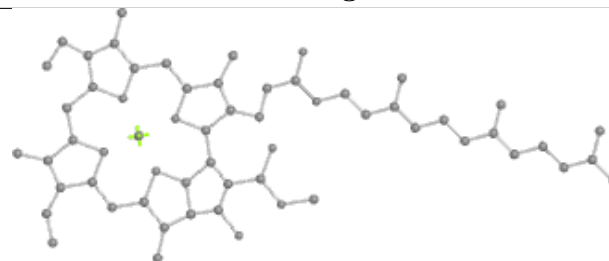
Bond lengths



Bond angles

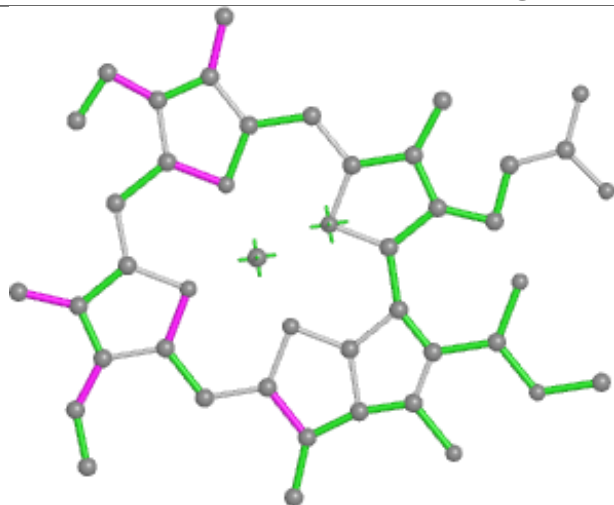


Torsions

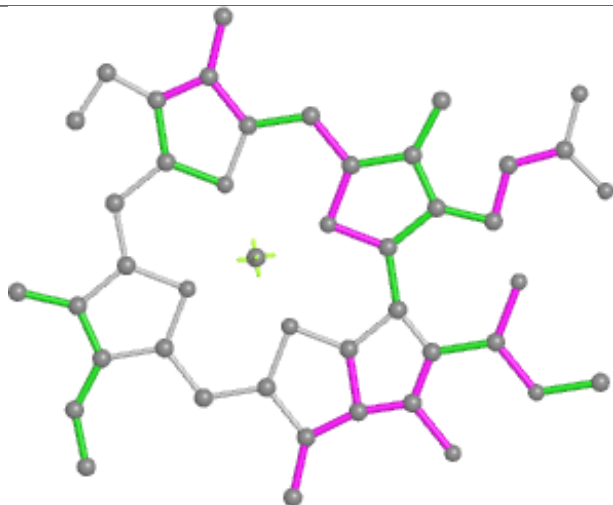


Rings

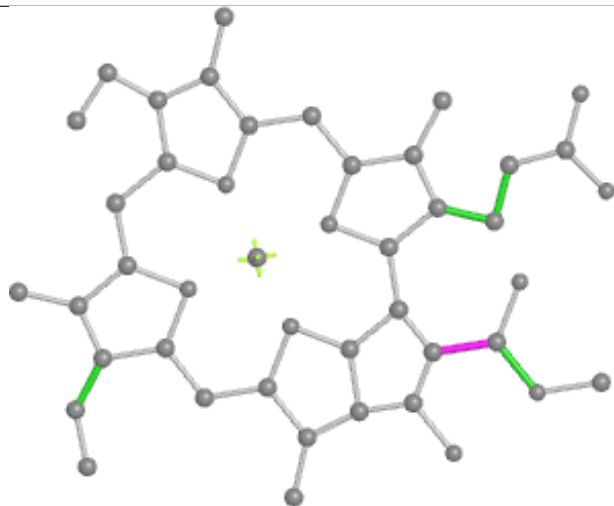
Ligand CLA A 813



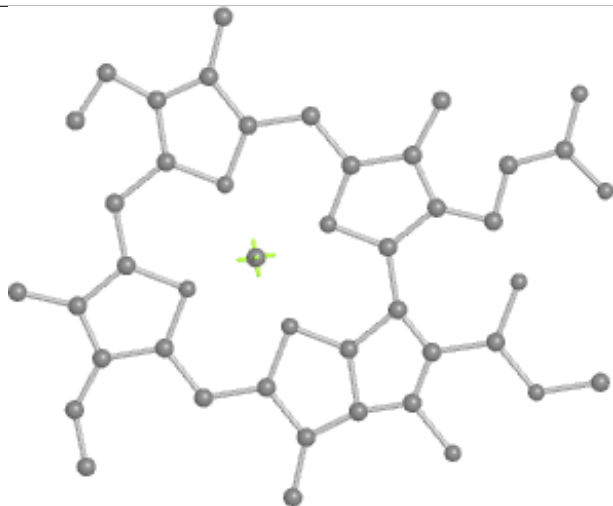
Bond lengths



Bond angles

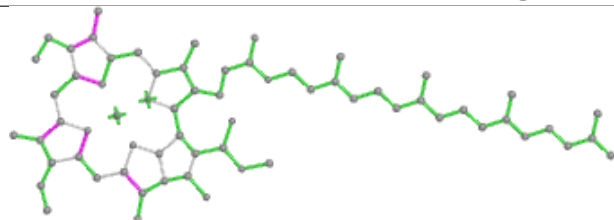


Torsions

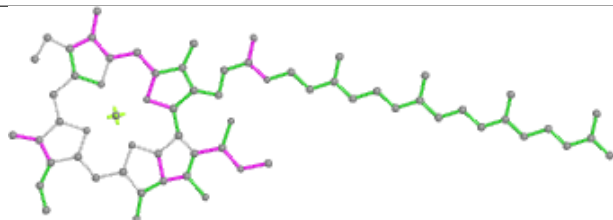


Rings

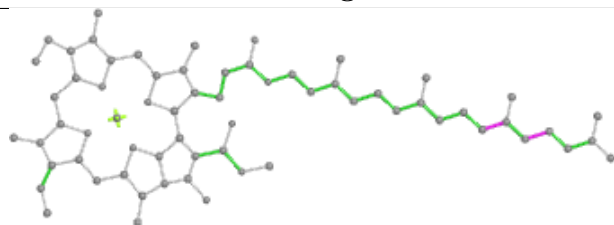
Ligand CLA B 821



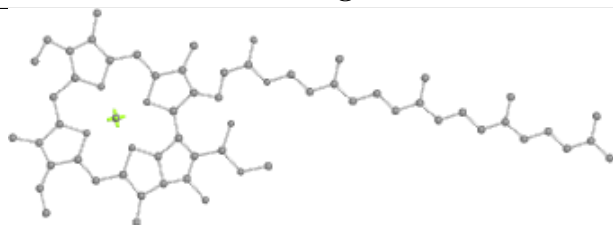
Bond lengths



Bond angles

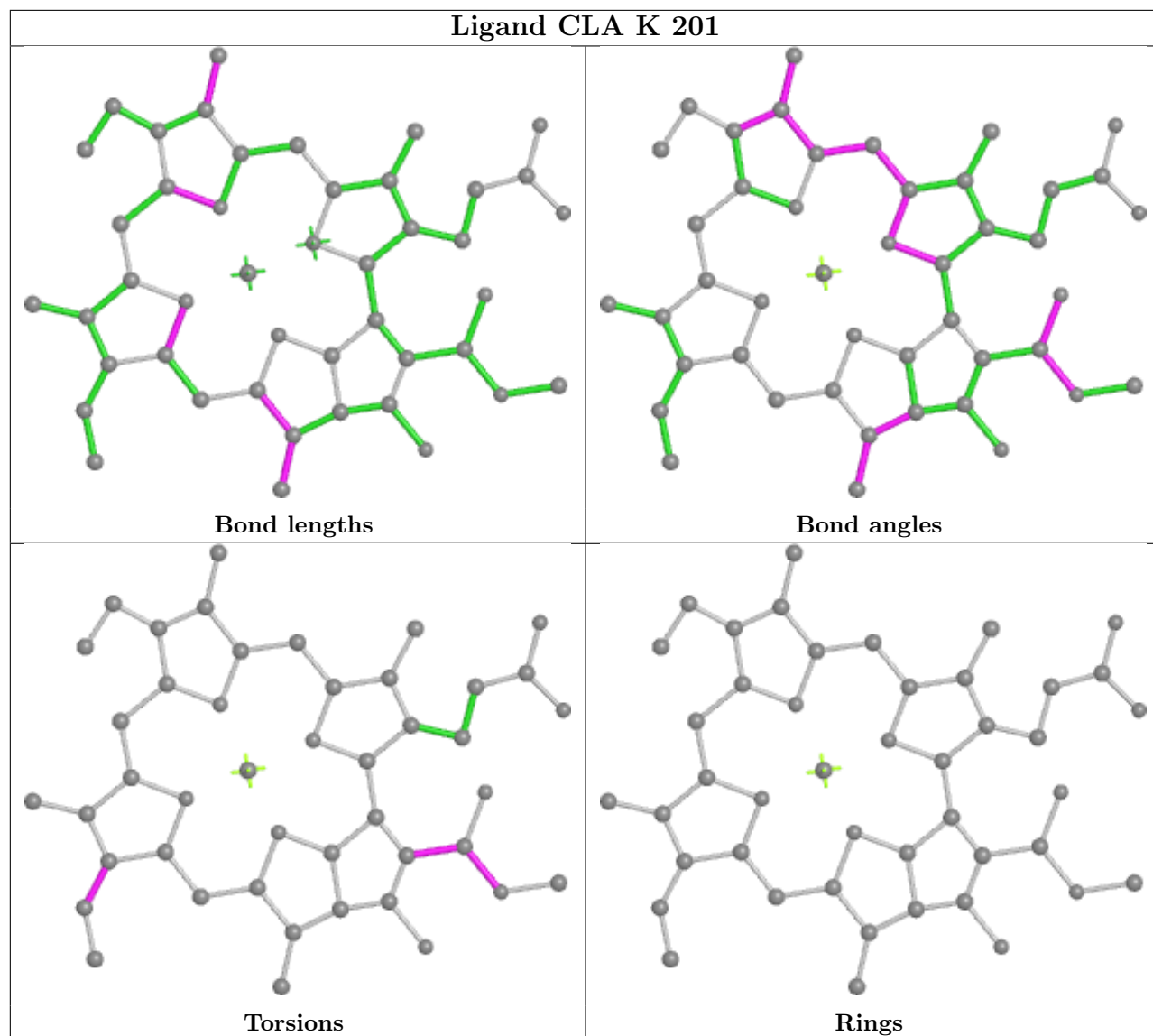


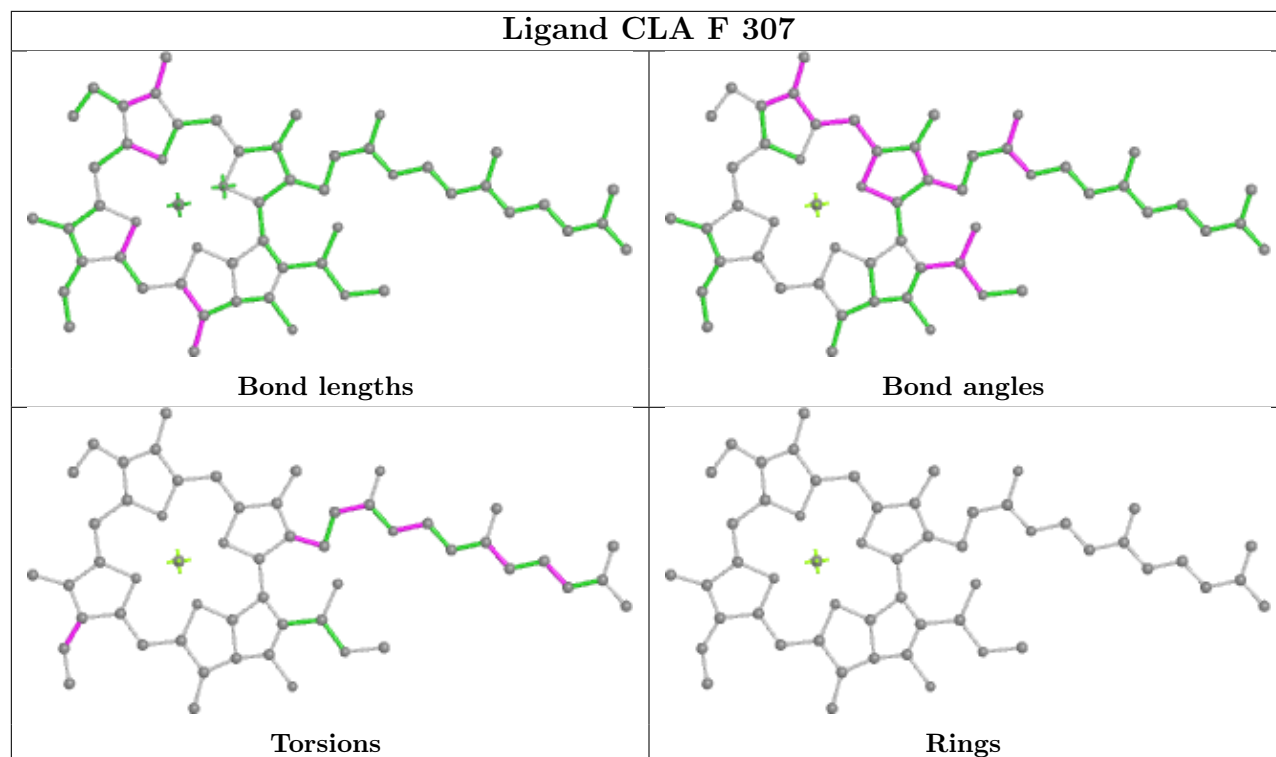
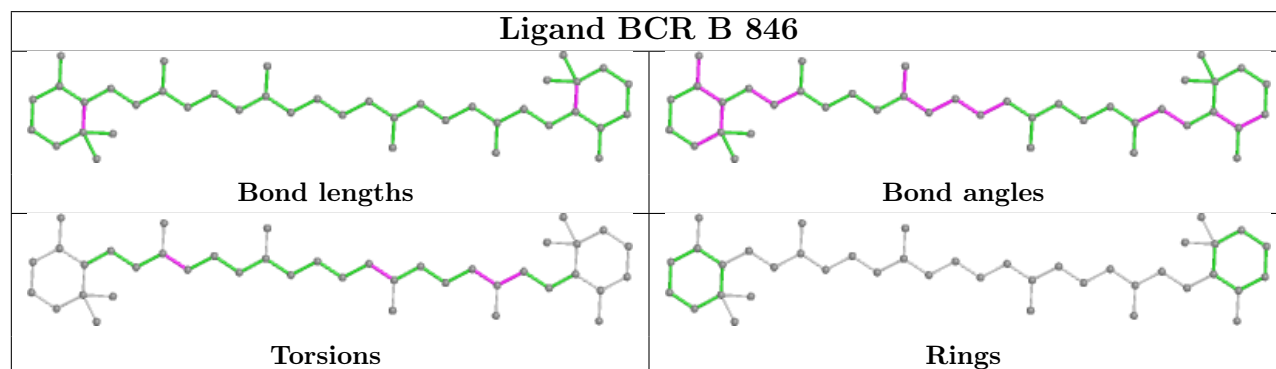
Torsions



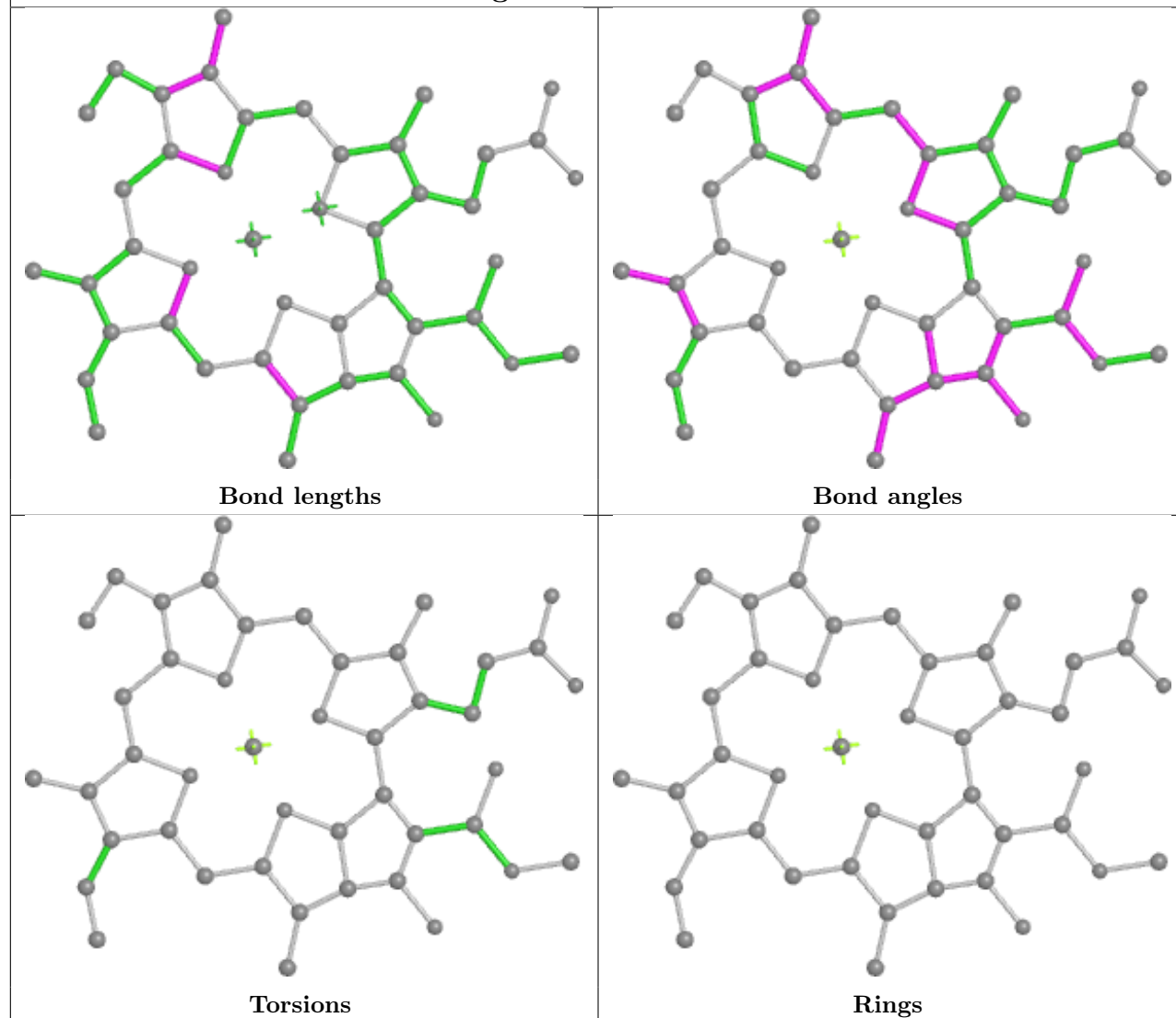
Rings

Ligand CLA K 201

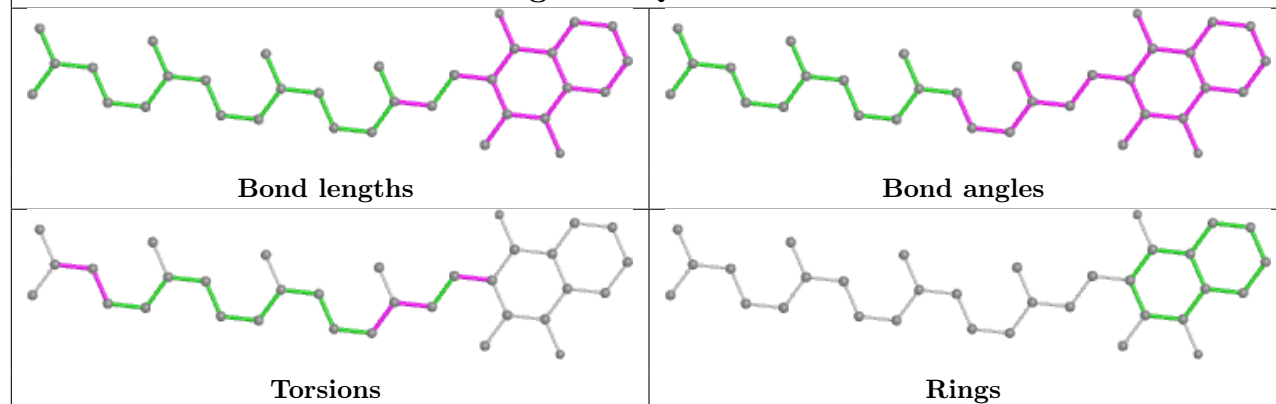


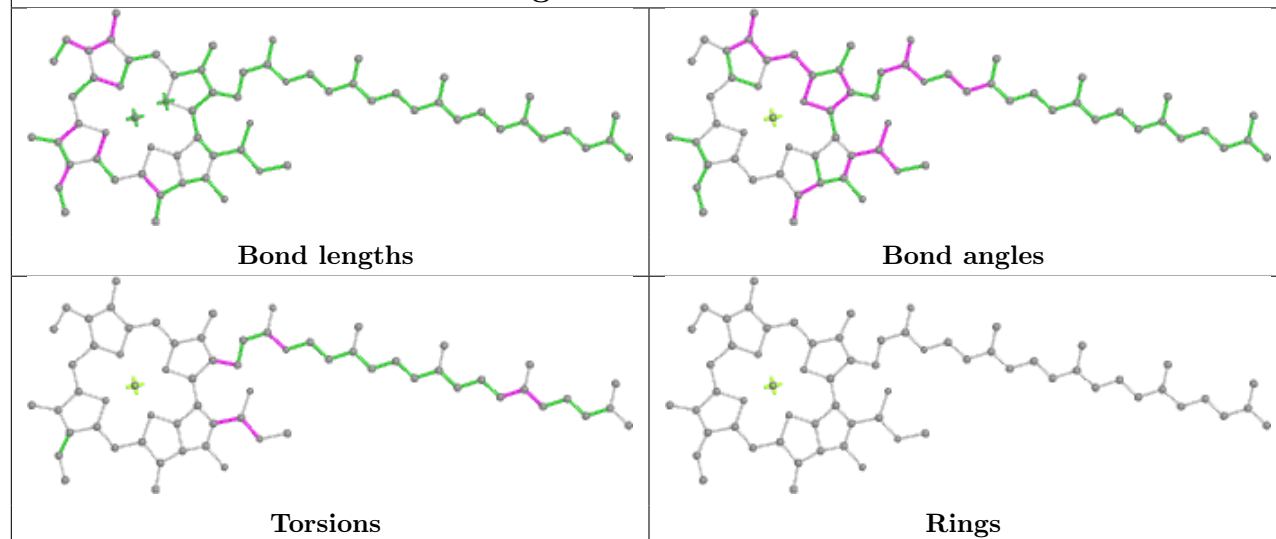
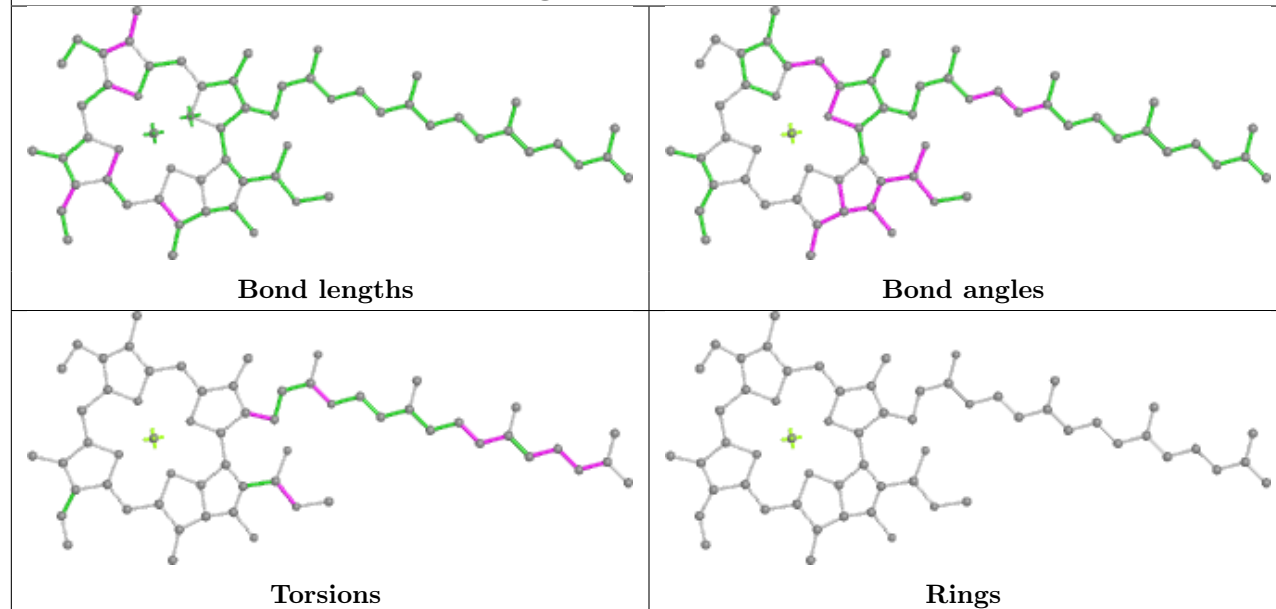
Ligand CLA F 307**Ligand BCR B 846**

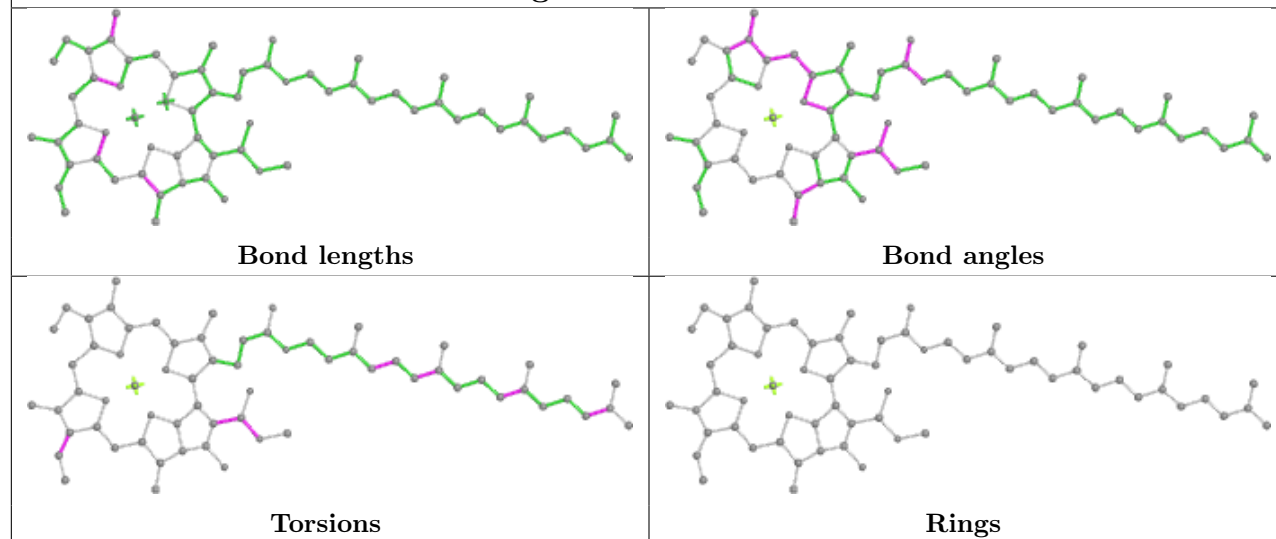
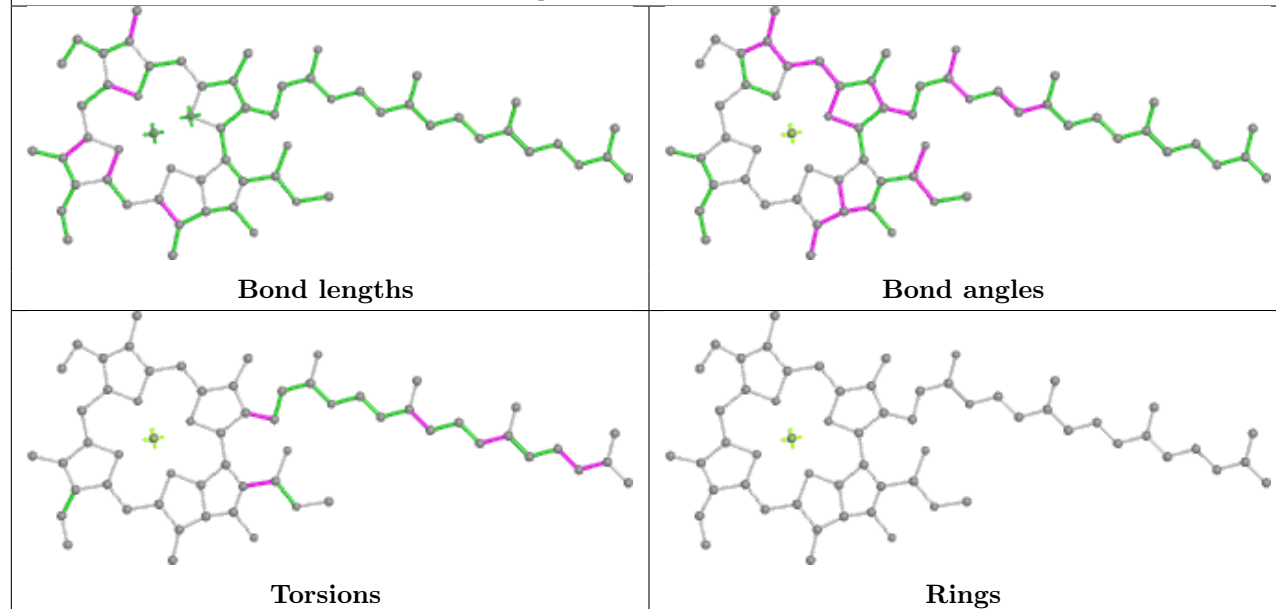
Ligand CLA F 306



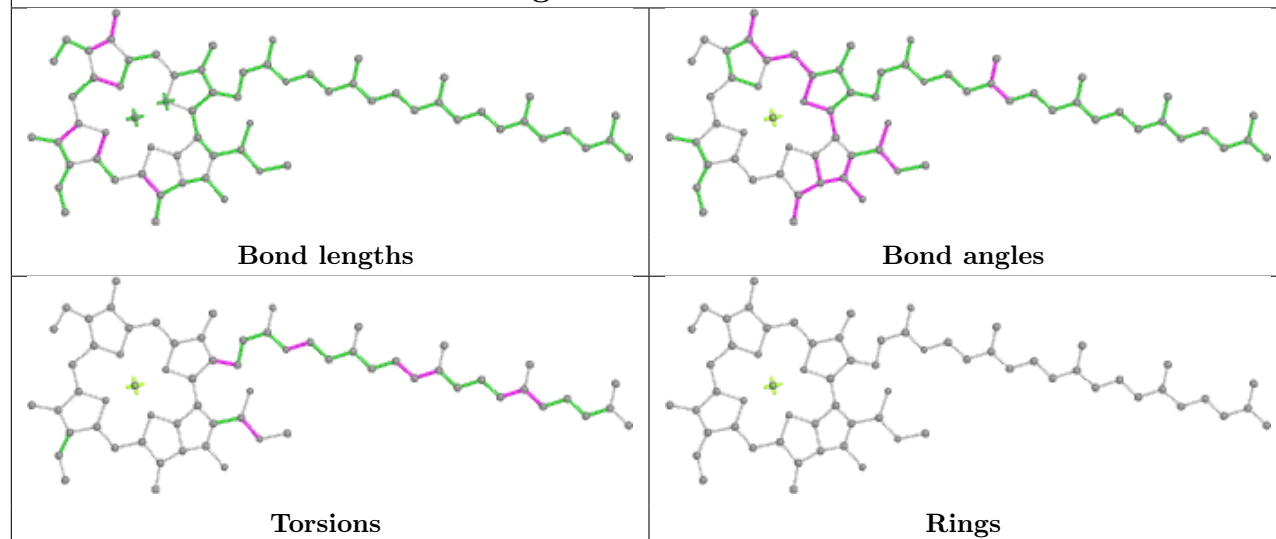
Ligand PQN A 842



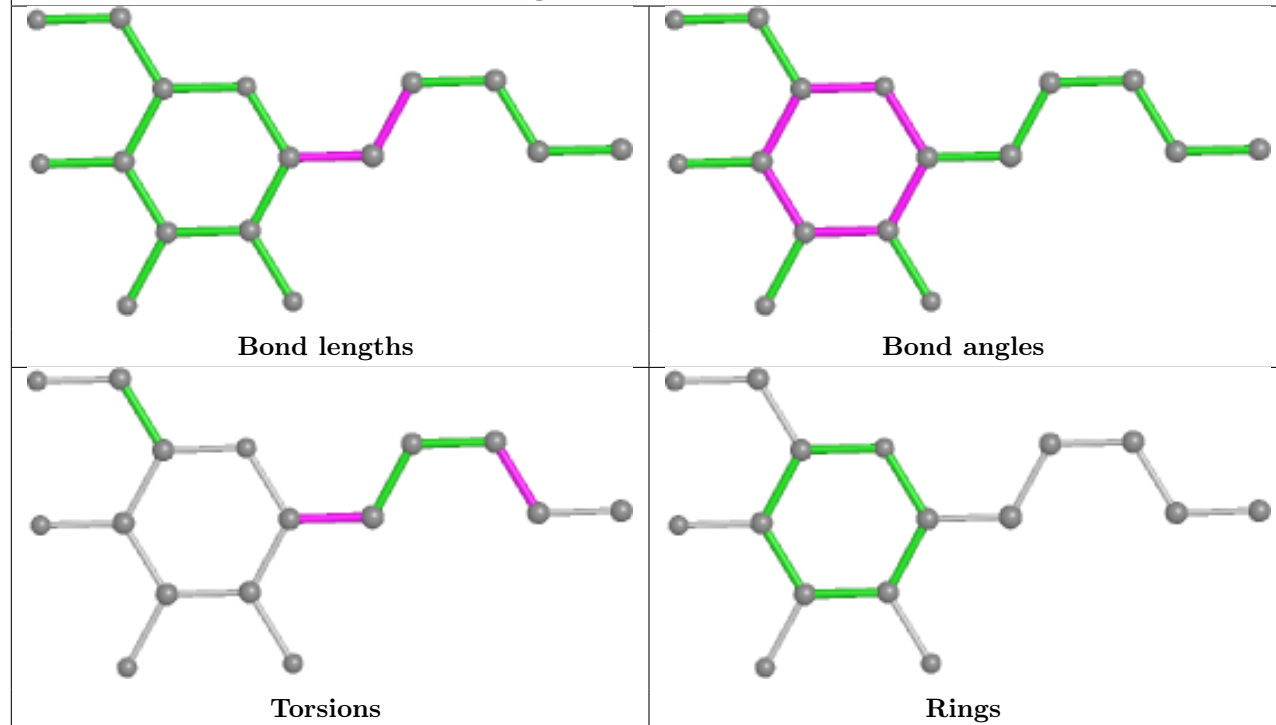
Ligand CLA B 831**Ligand CLA 4 303**

Ligand CLA A 832**Ligand CLA B 825**

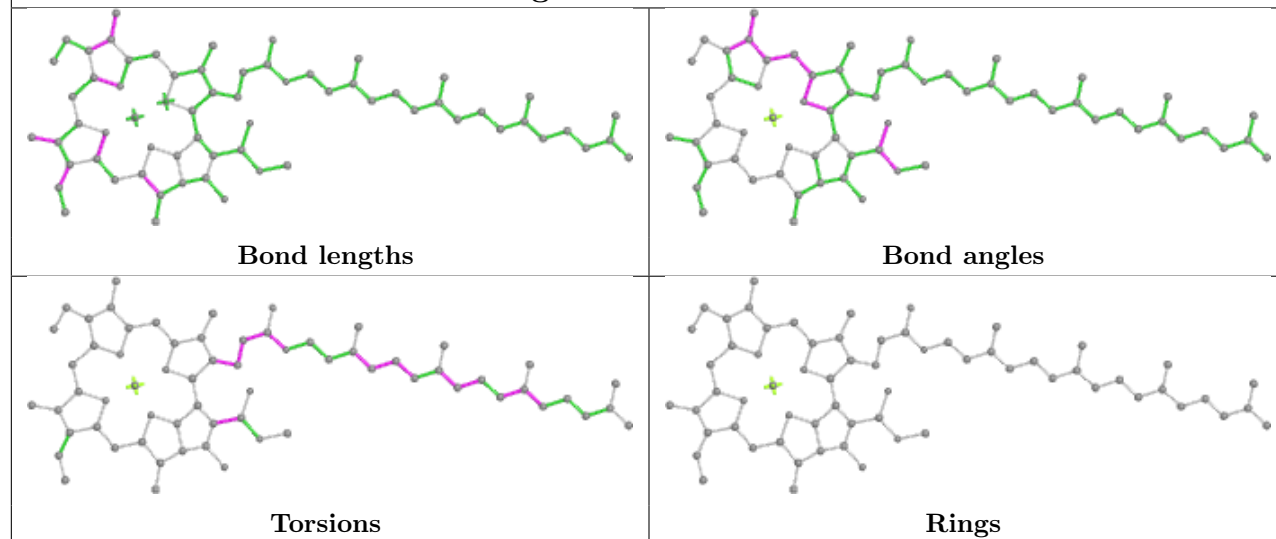
Ligand CLA B 835



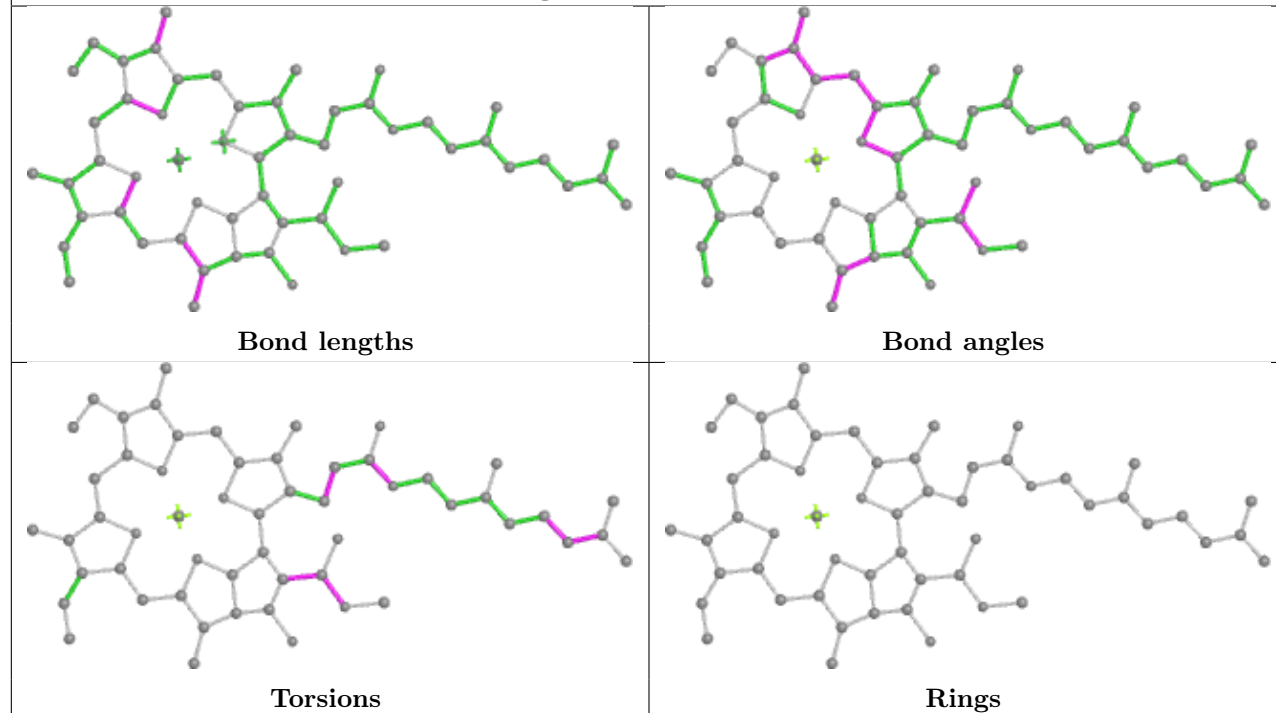
Ligand HTG F 310



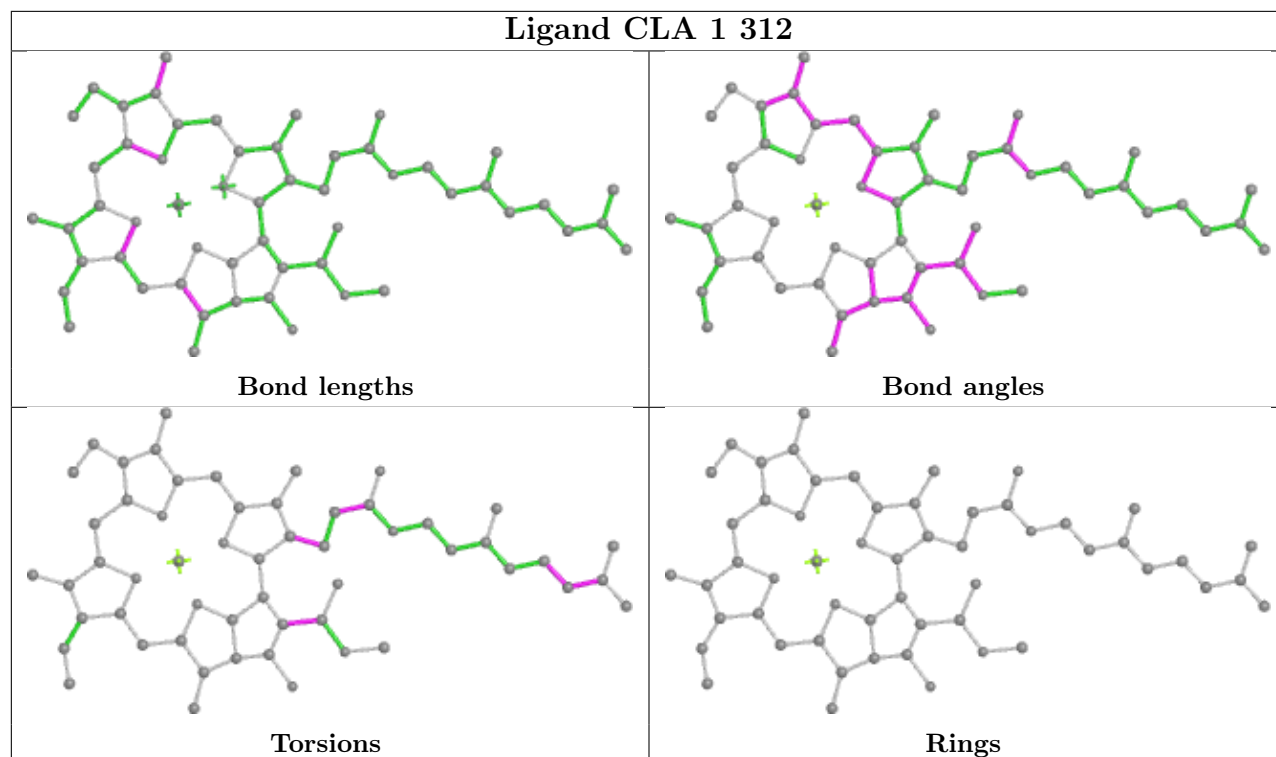
Ligand CLA A 807



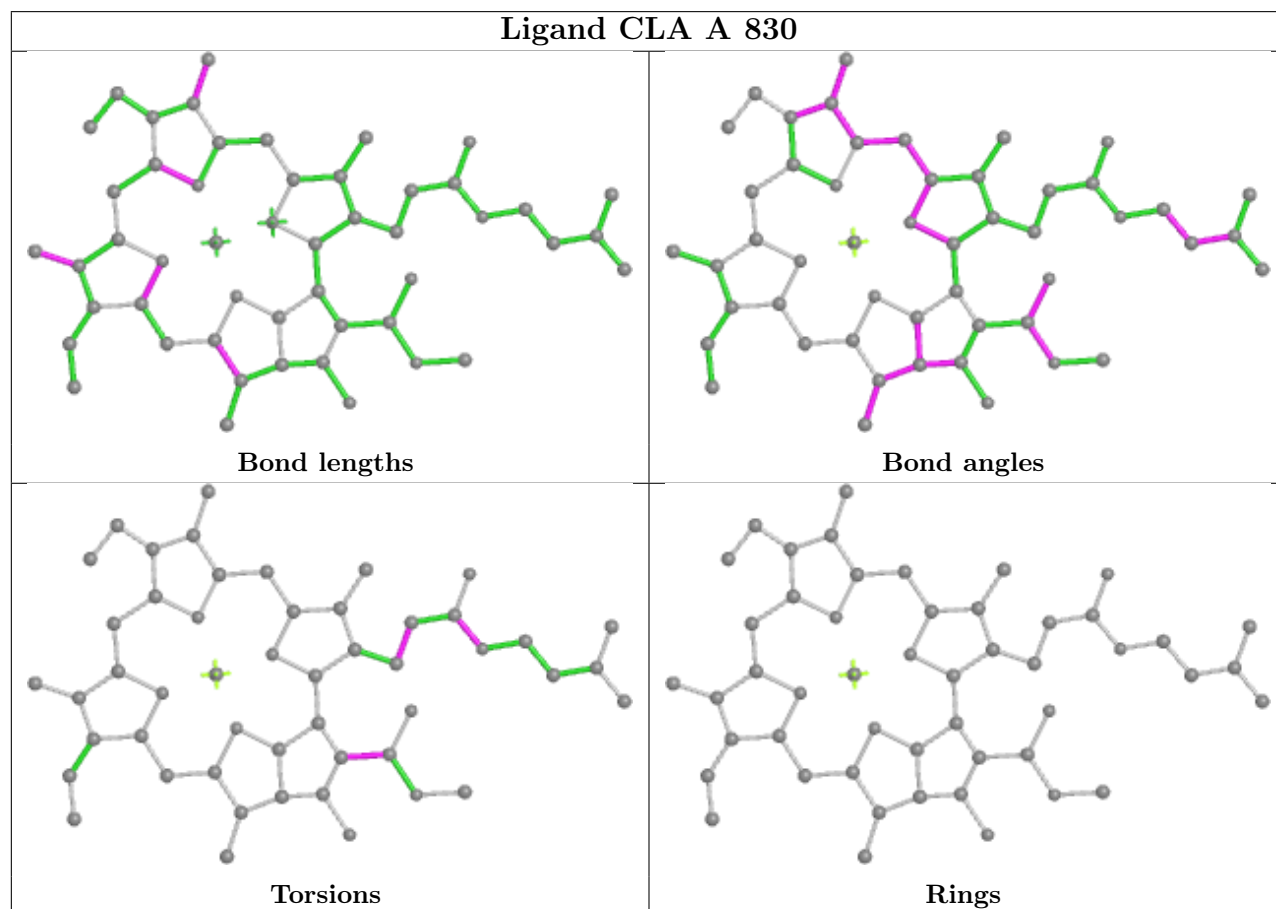
Ligand CLA 3 611



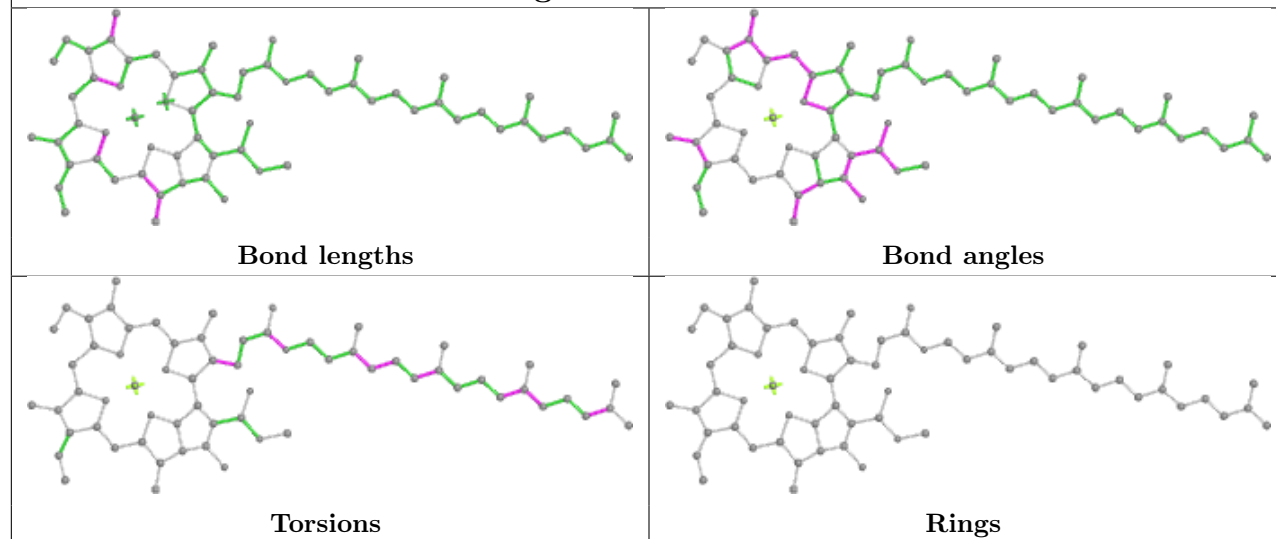
Ligand CLA 1 312



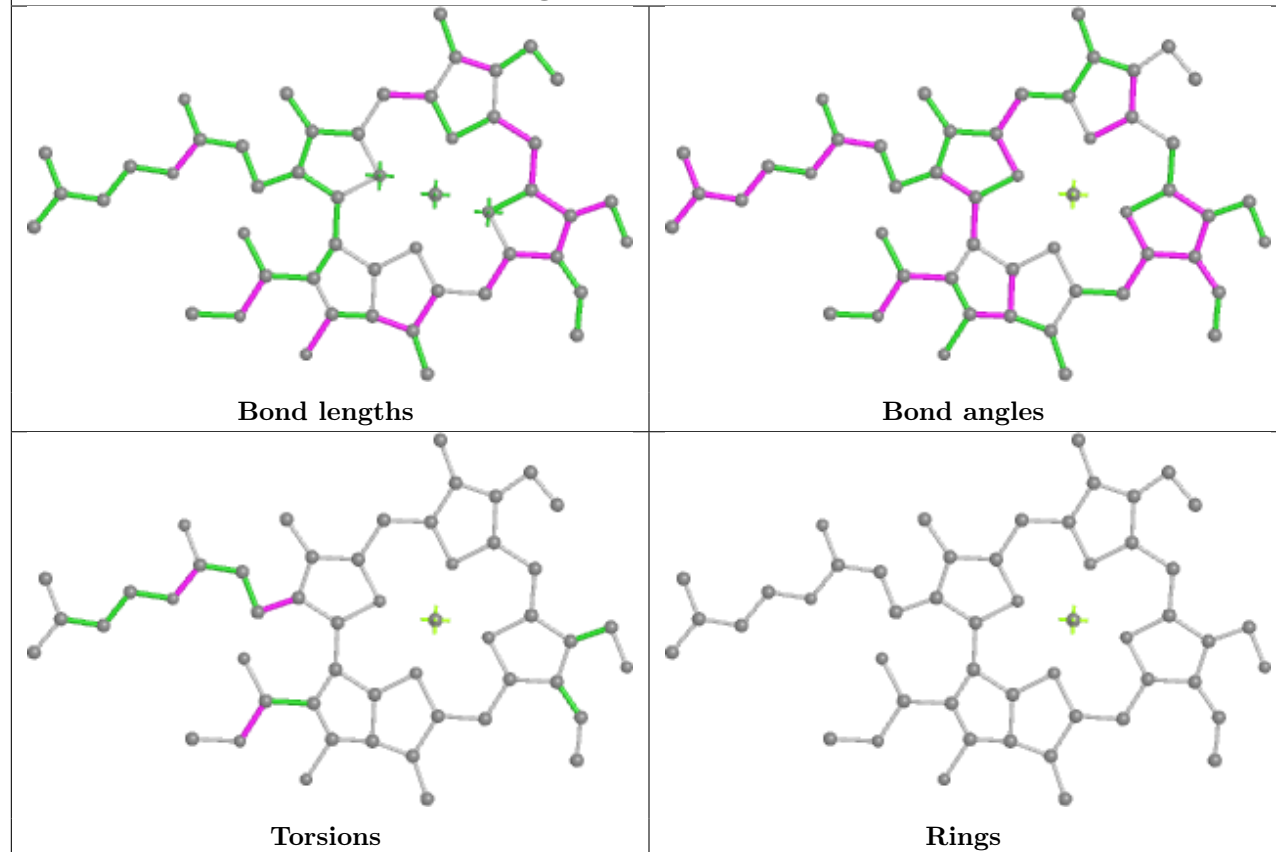
Ligand CLA A 830

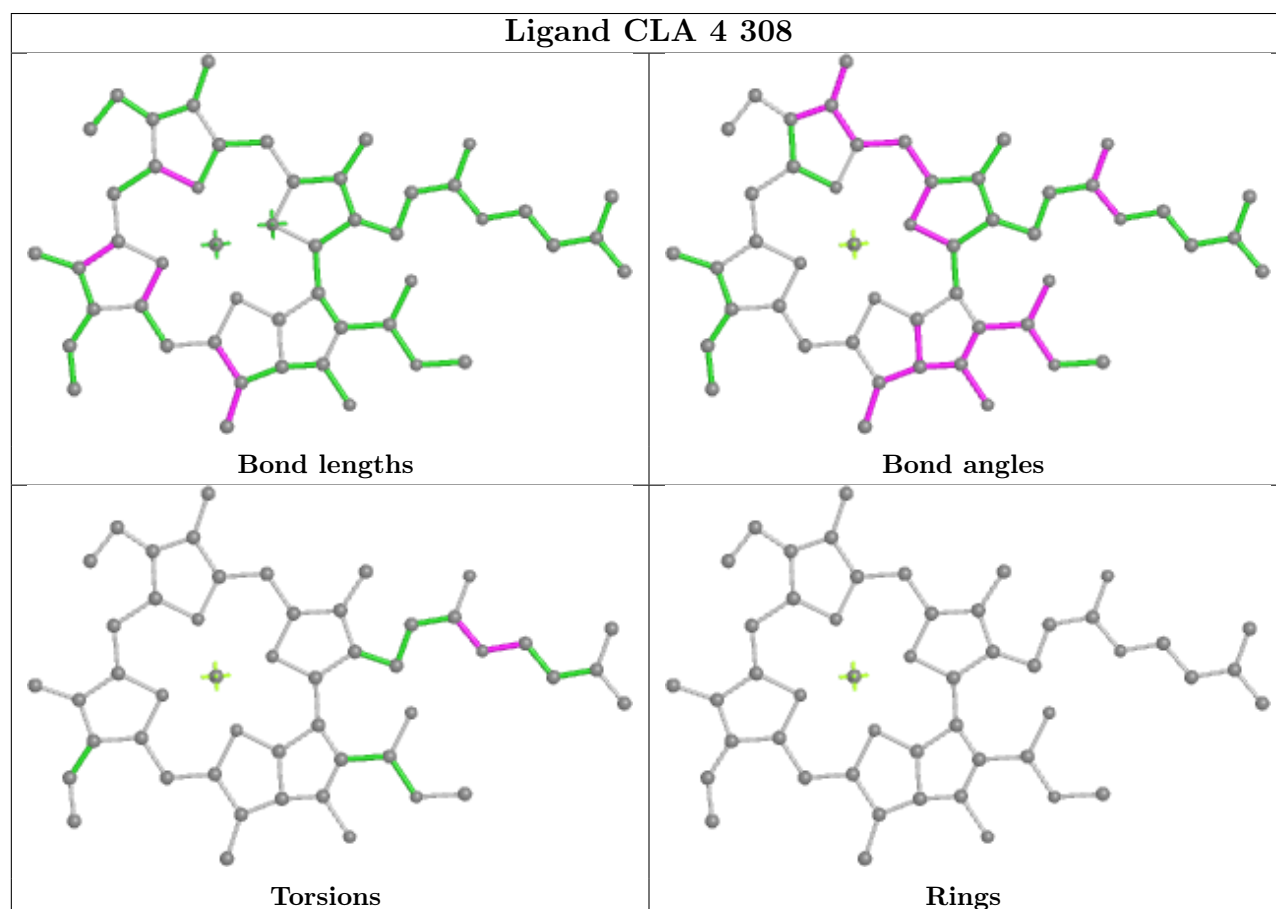
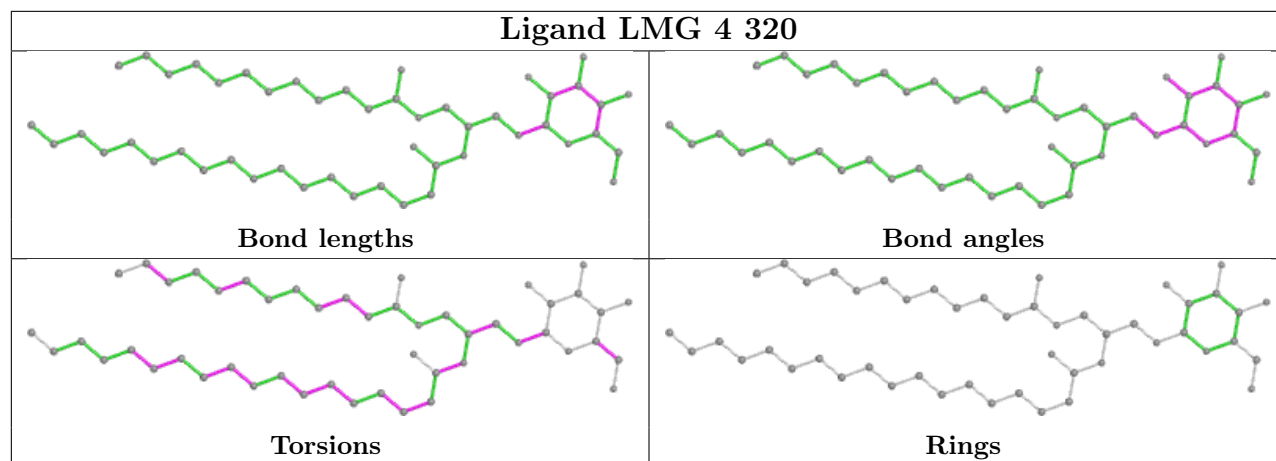
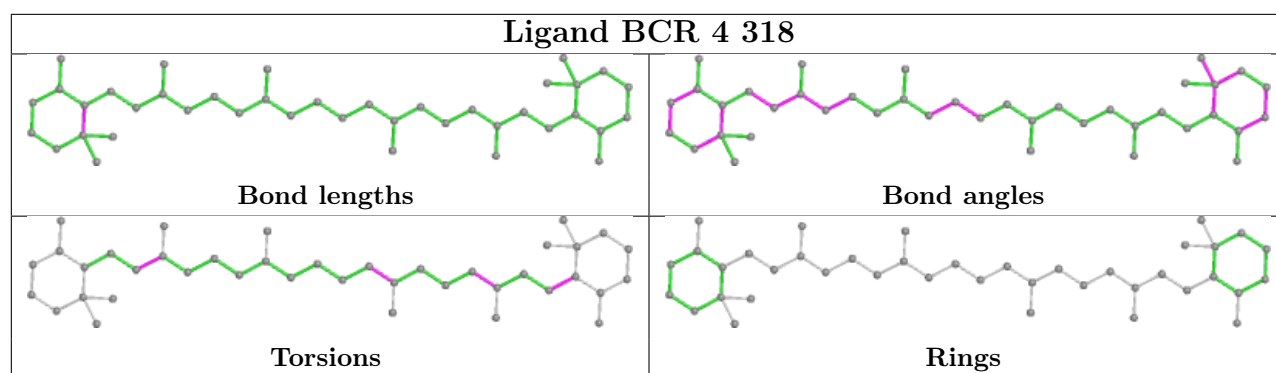


Ligand CLA L 202

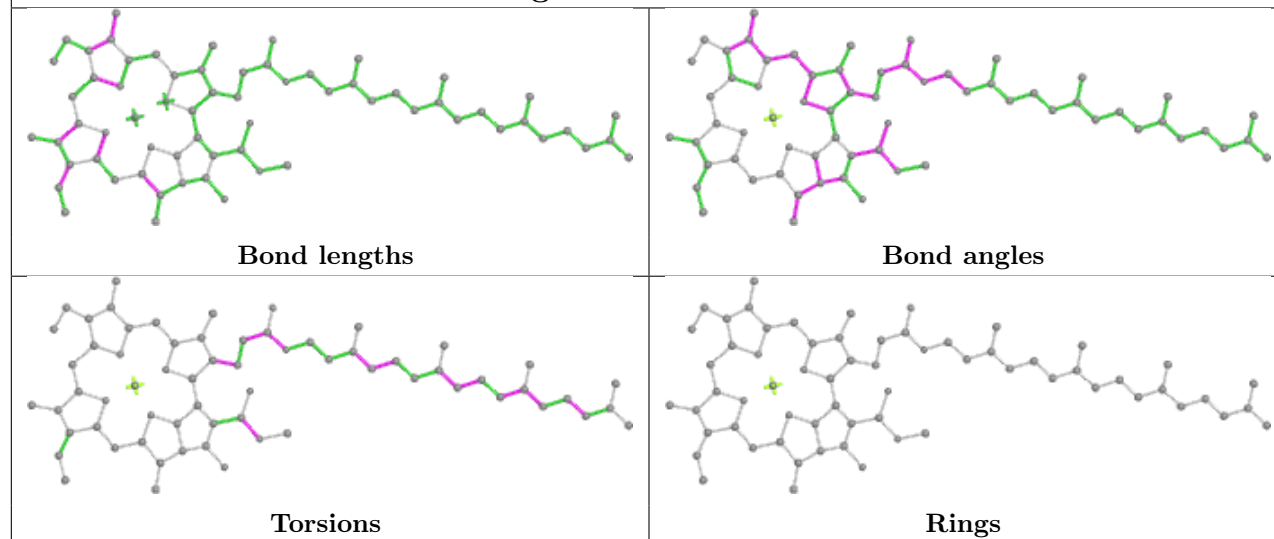


Ligand CHL 2 306

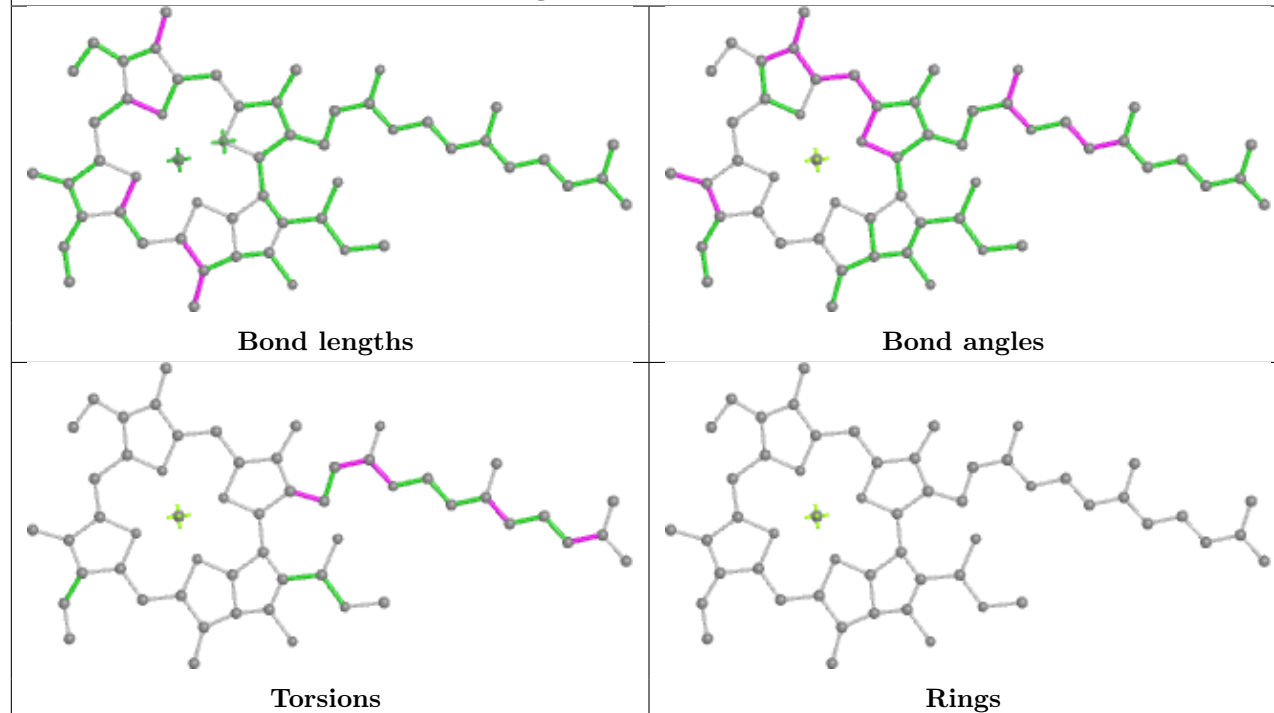


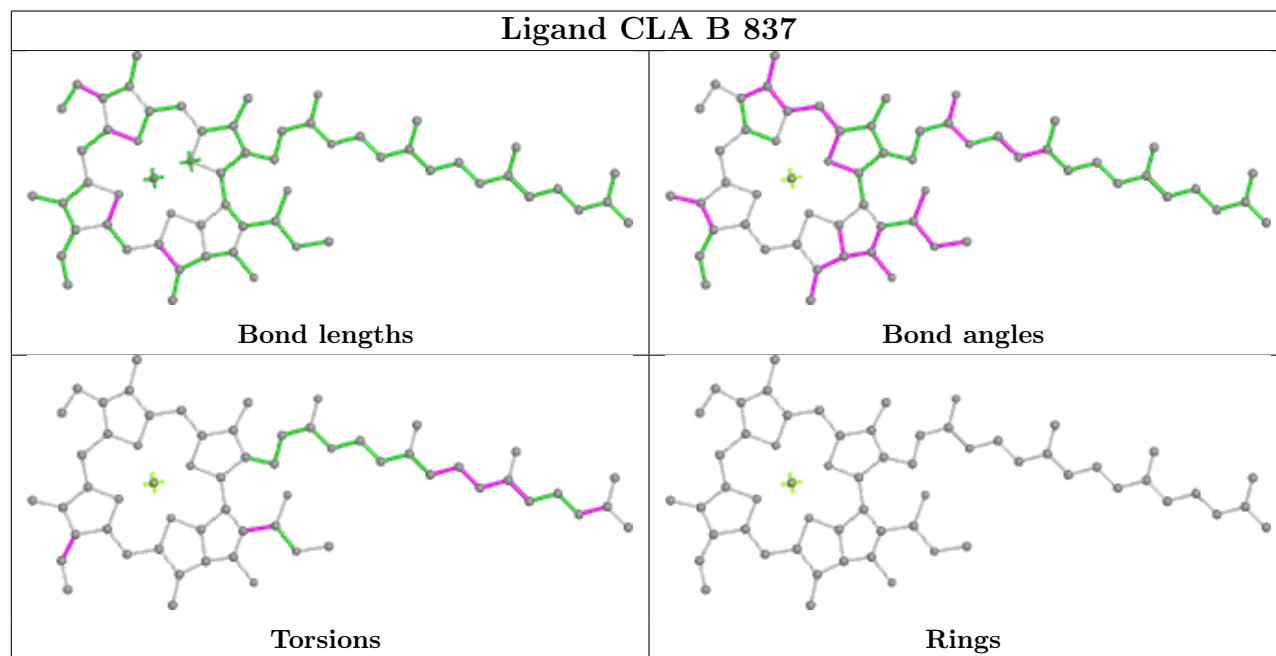
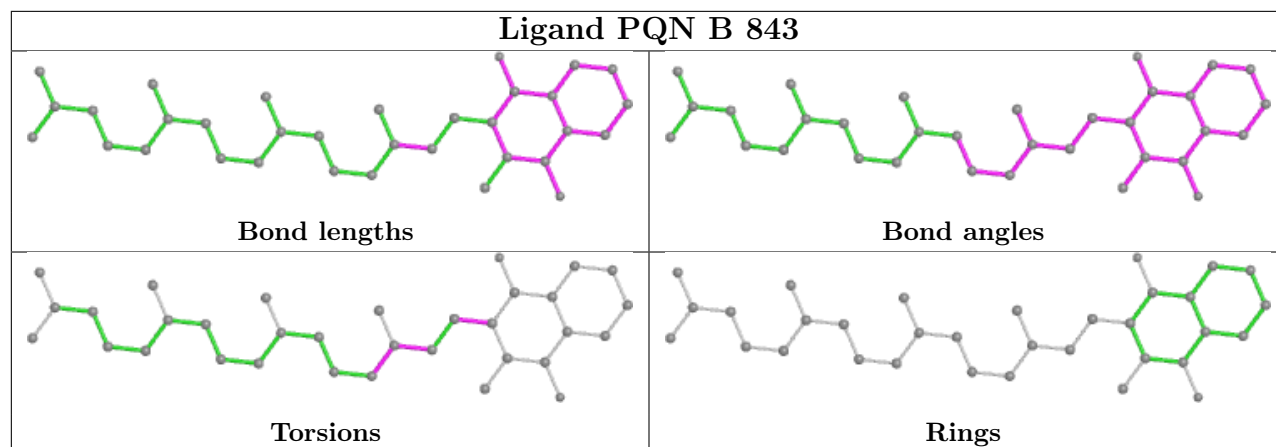


Ligand CLA A 805

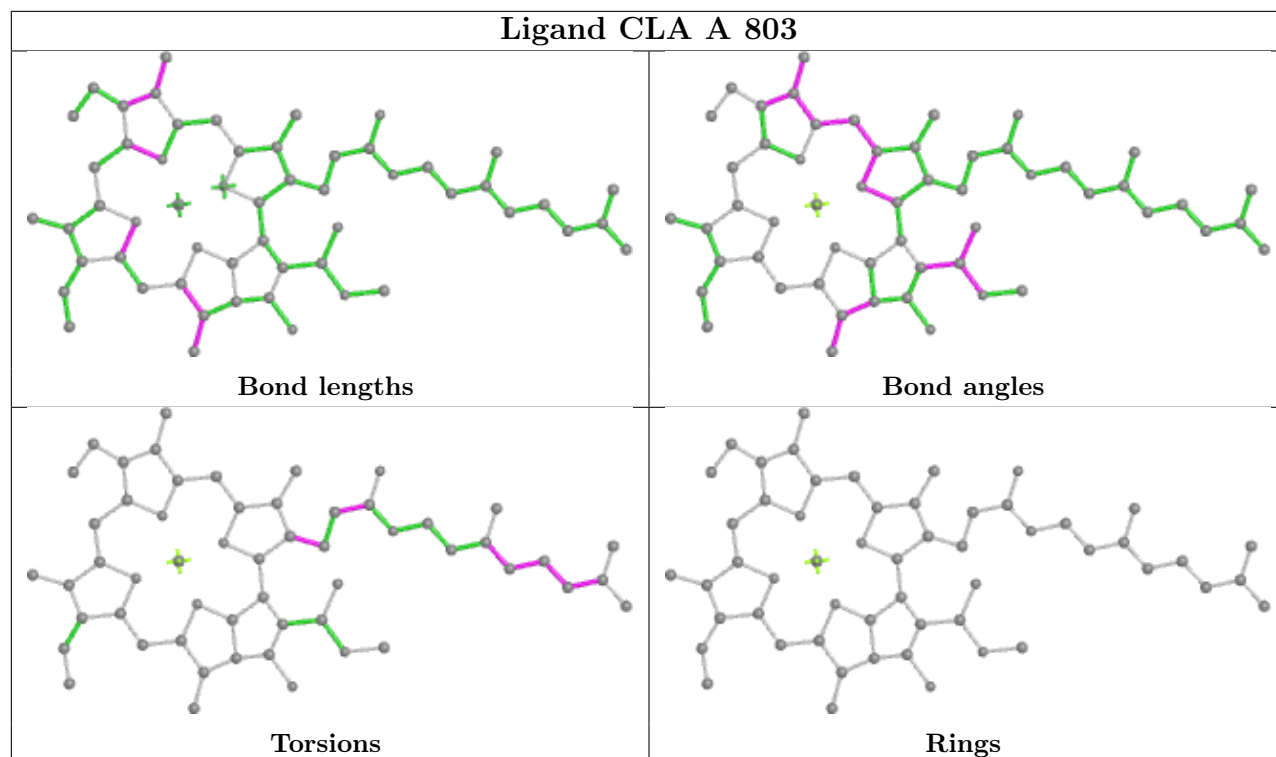


Ligand CLA B 824

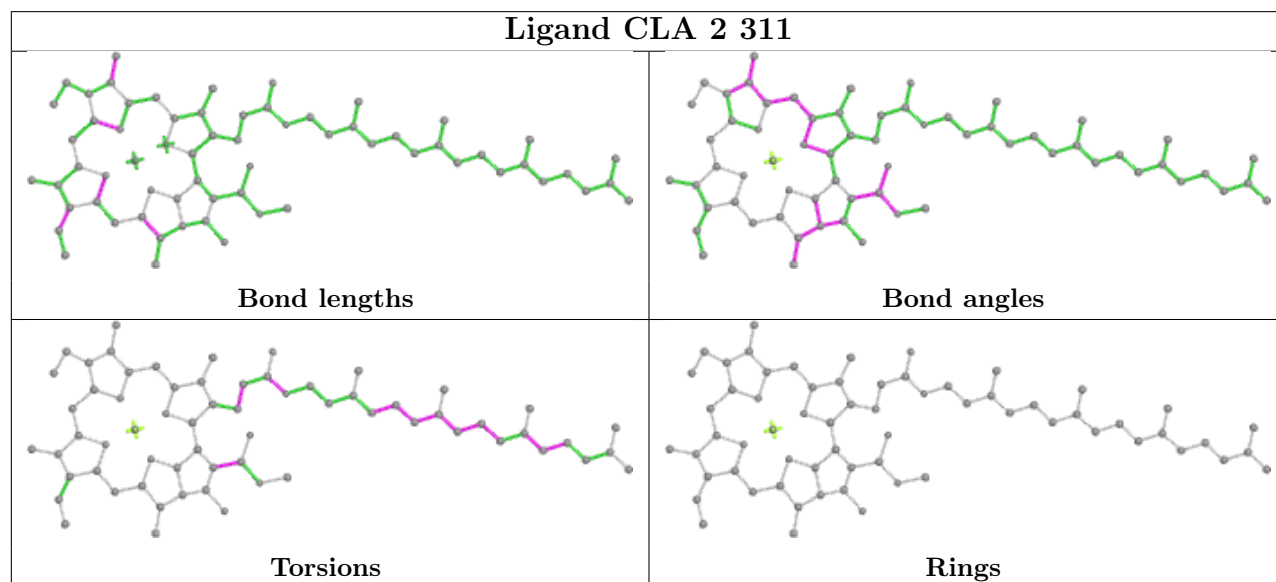




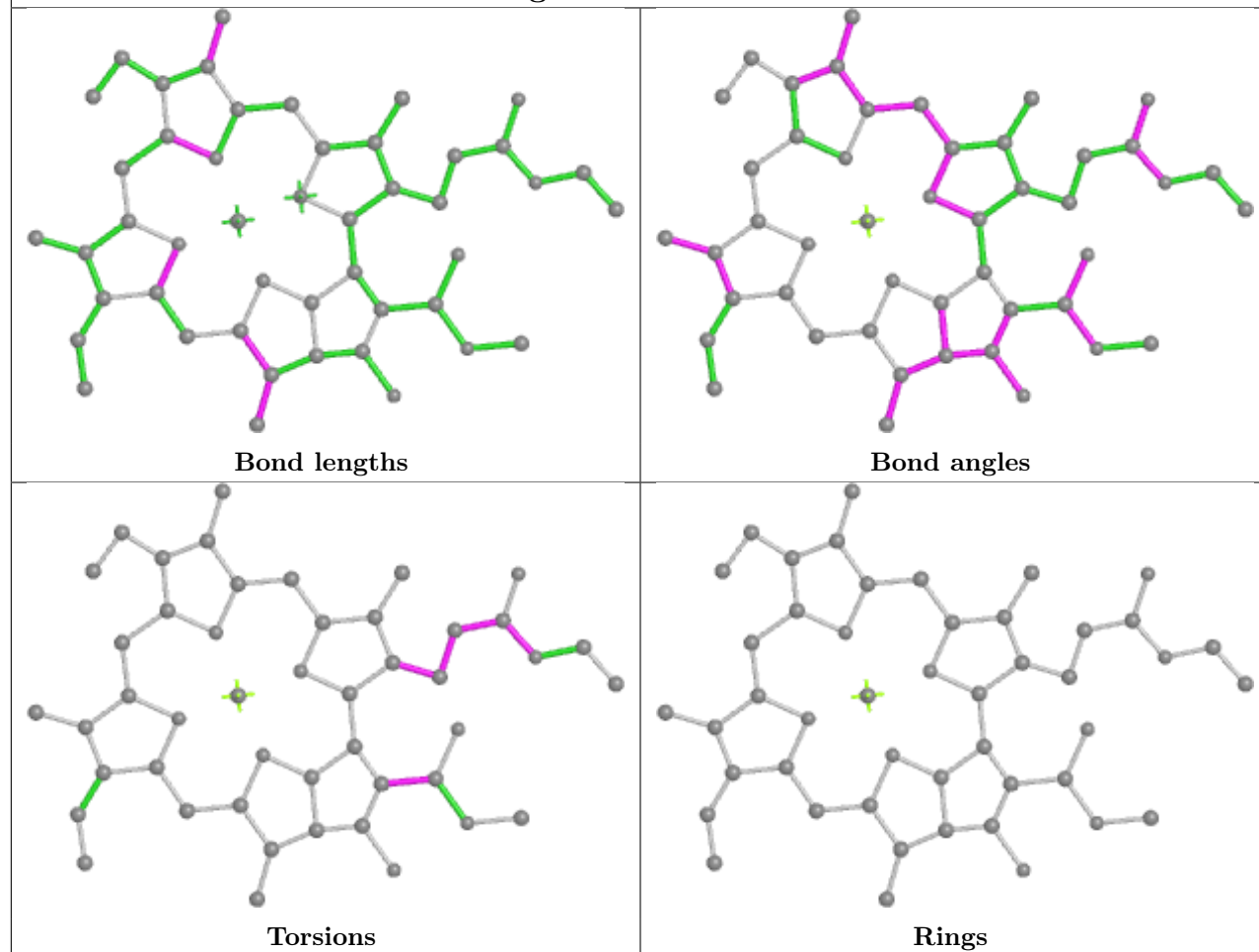
Ligand CLA A 803

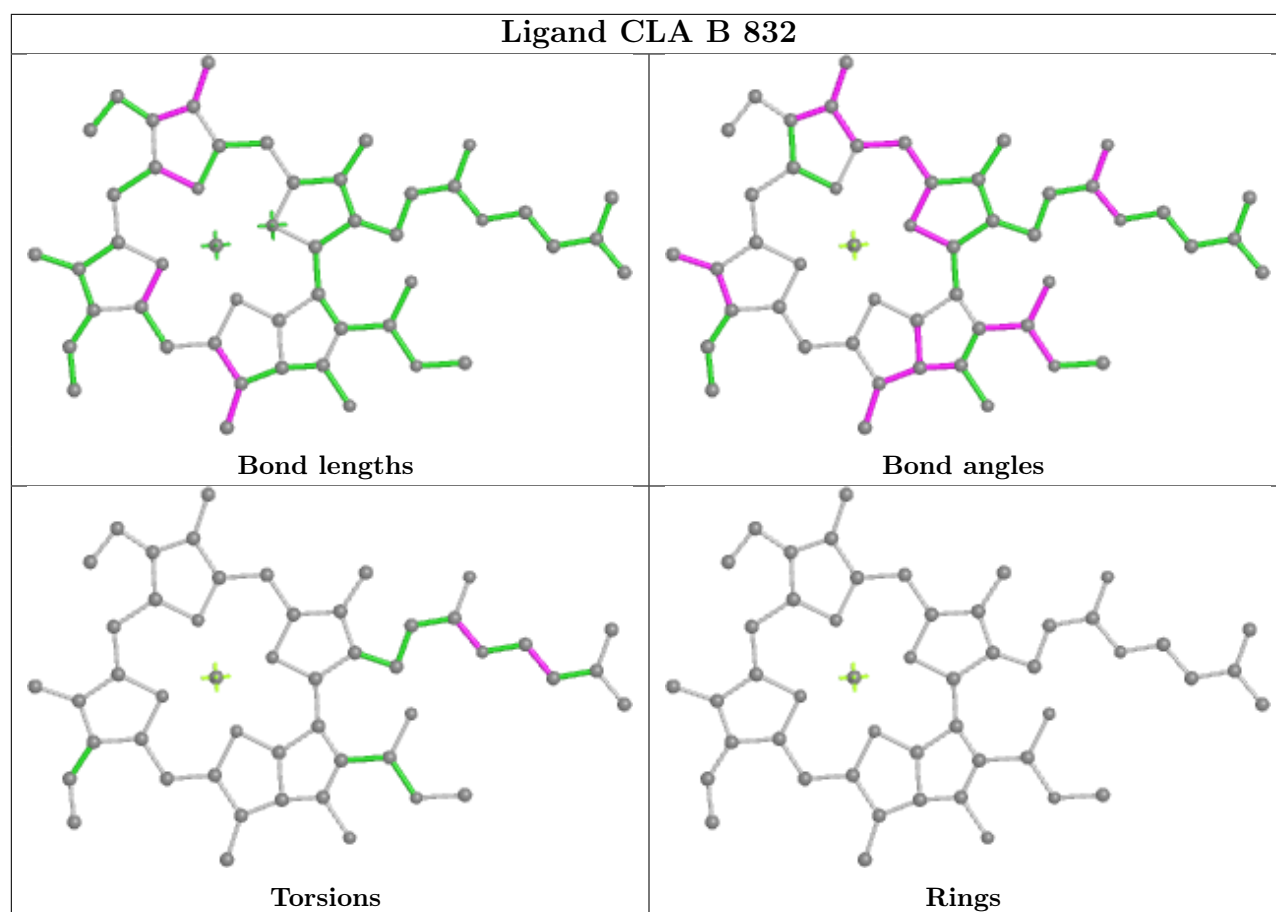


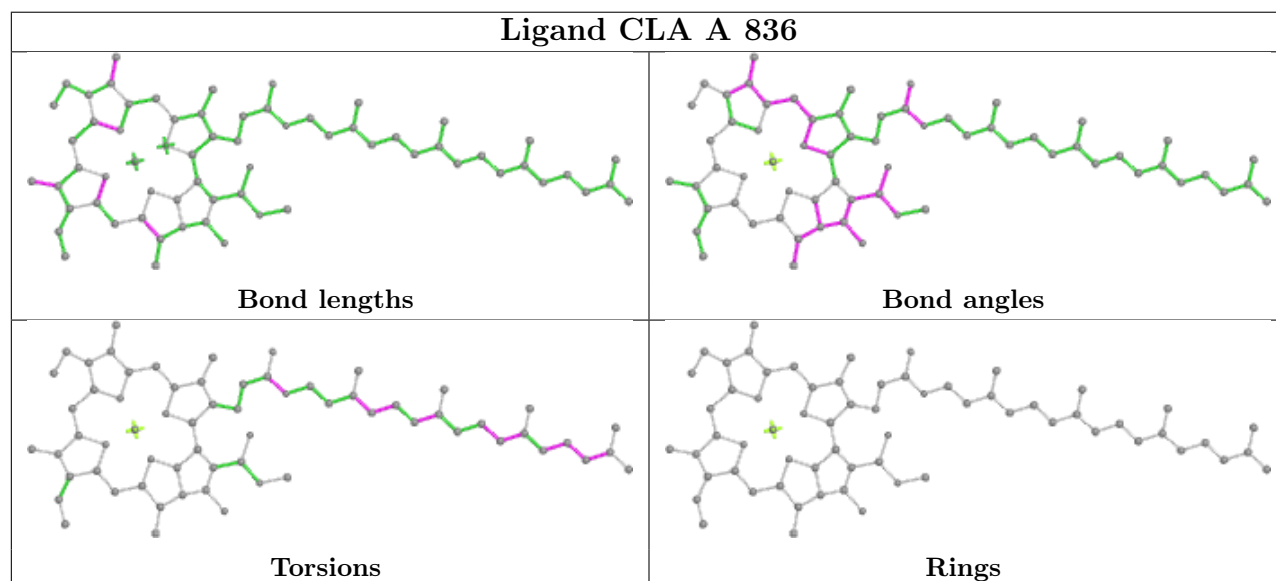
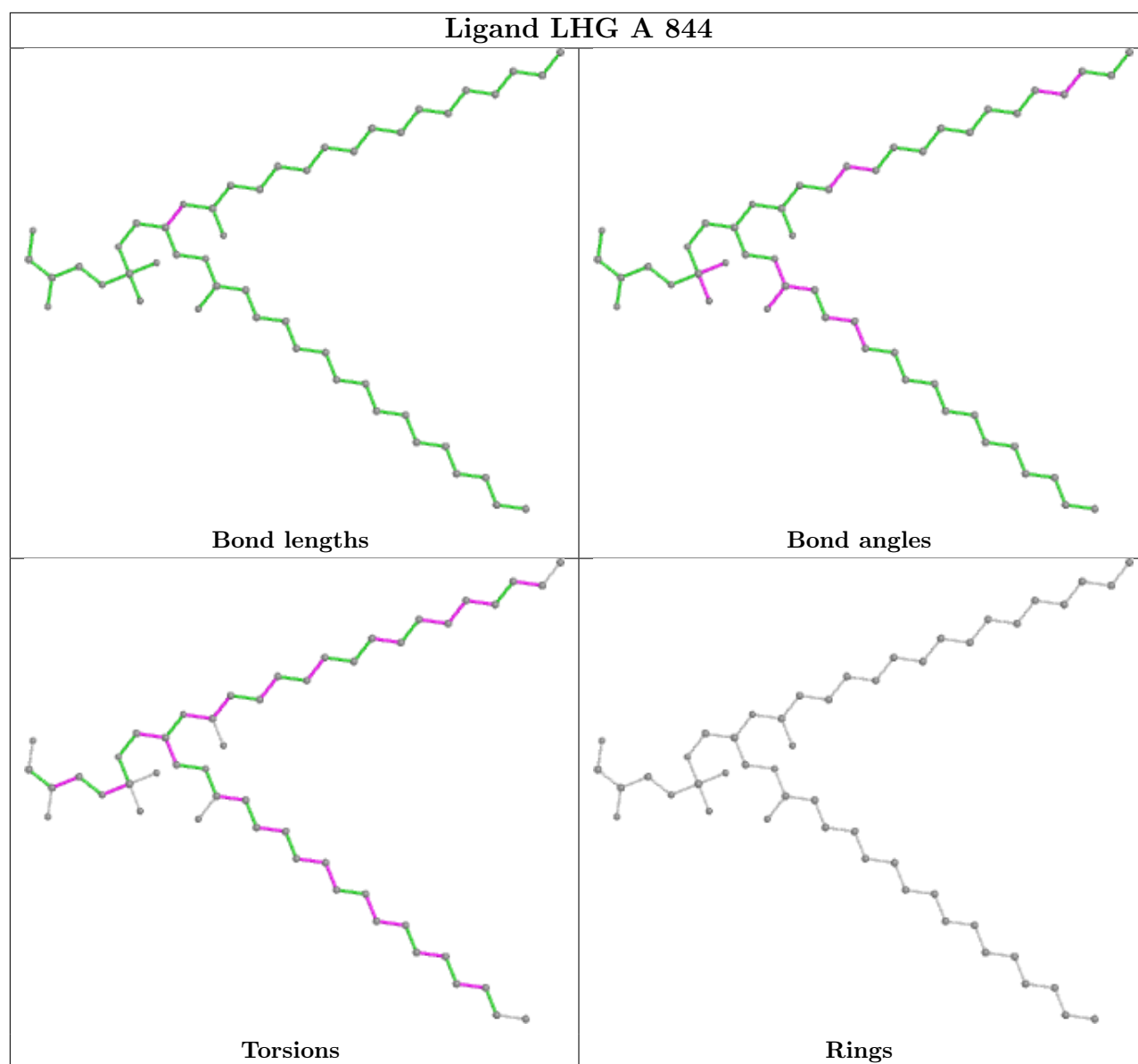
Ligand CLA 2 311

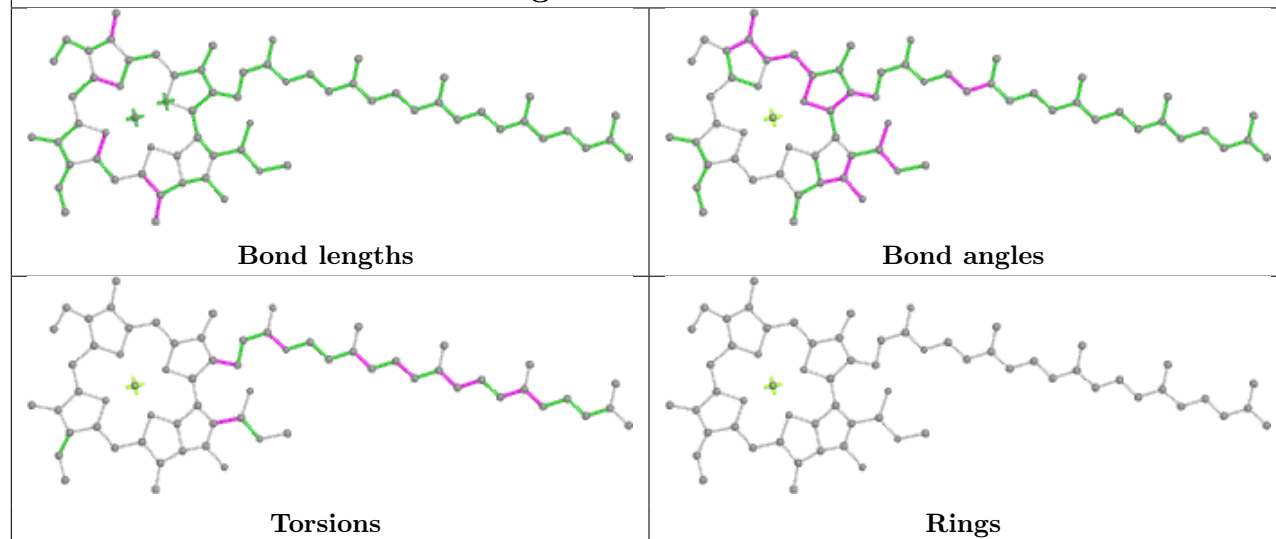
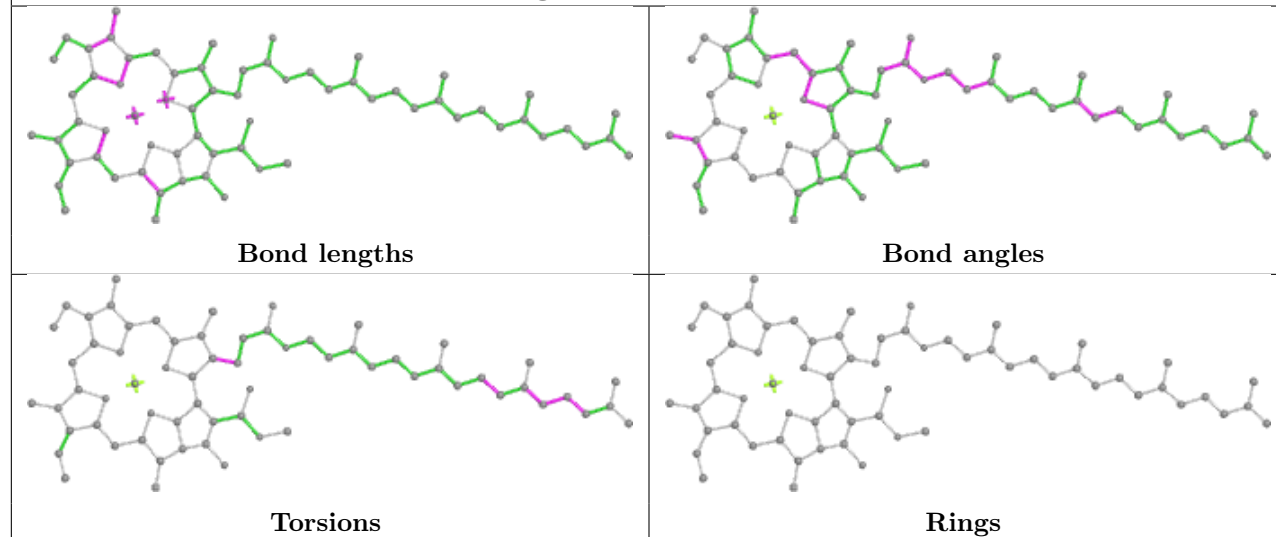


Ligand CLA 3 606

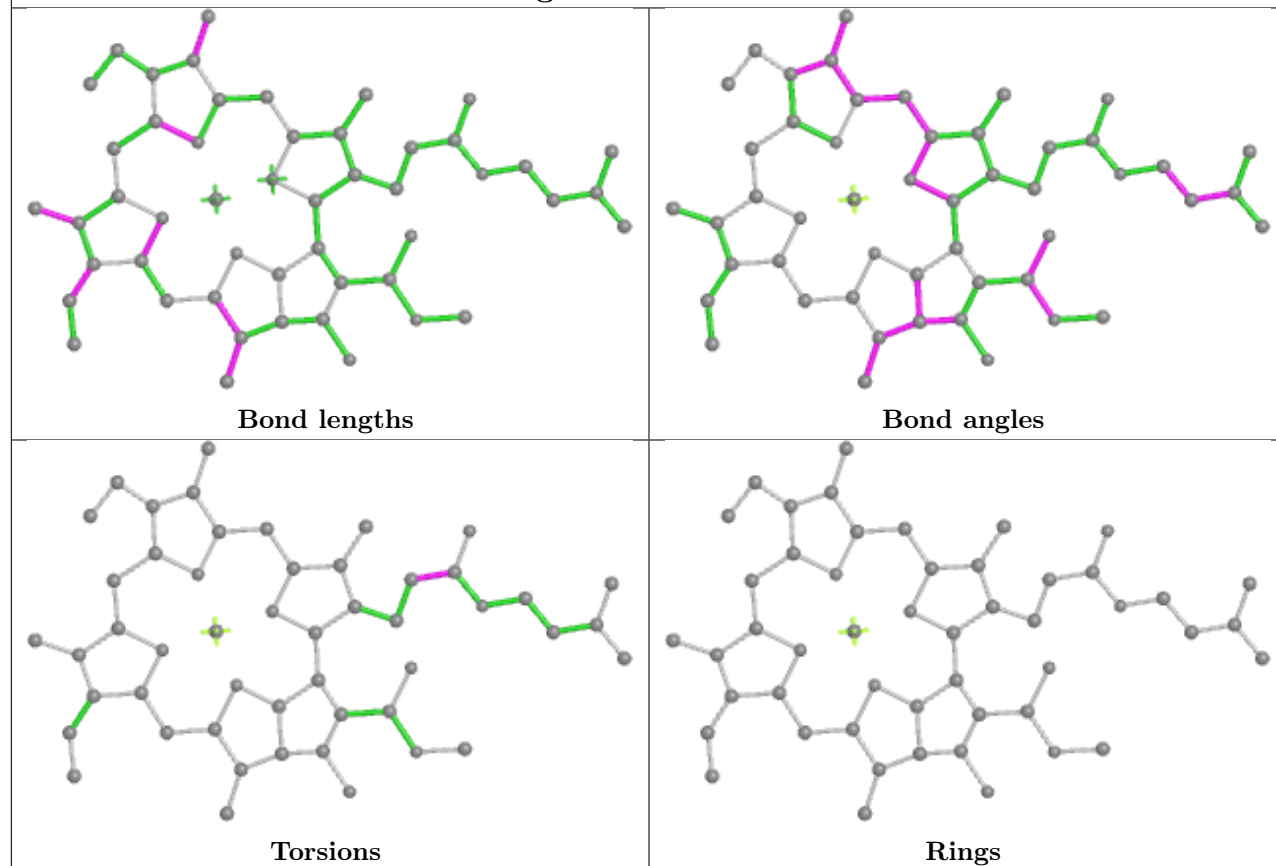




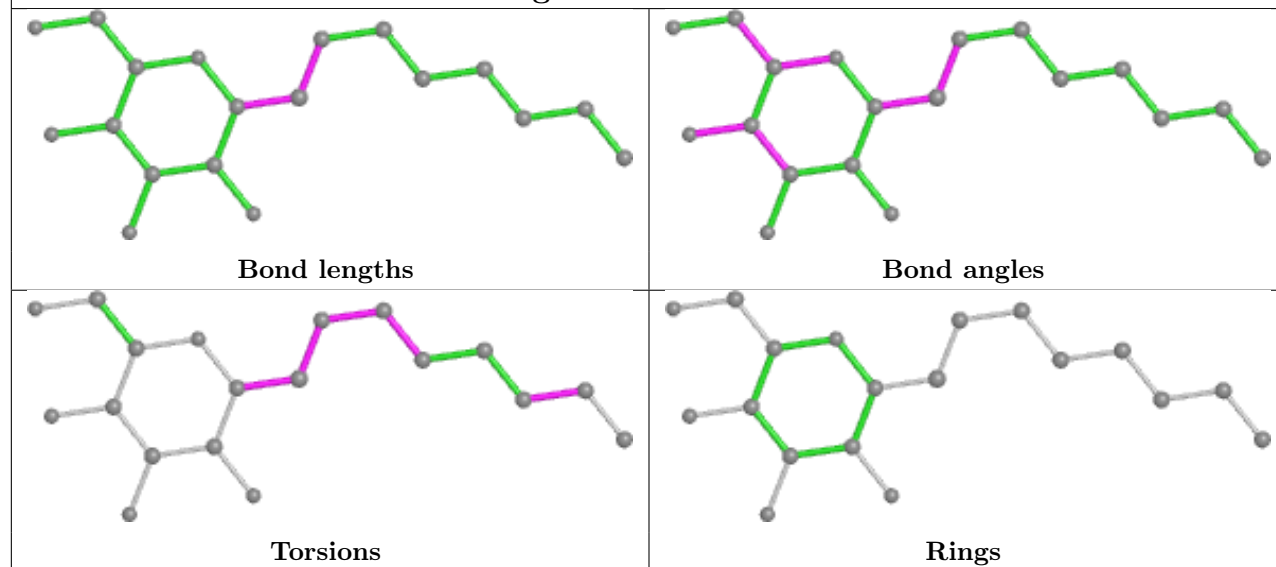


Ligand CLA A 818**Ligand CLA F 304**

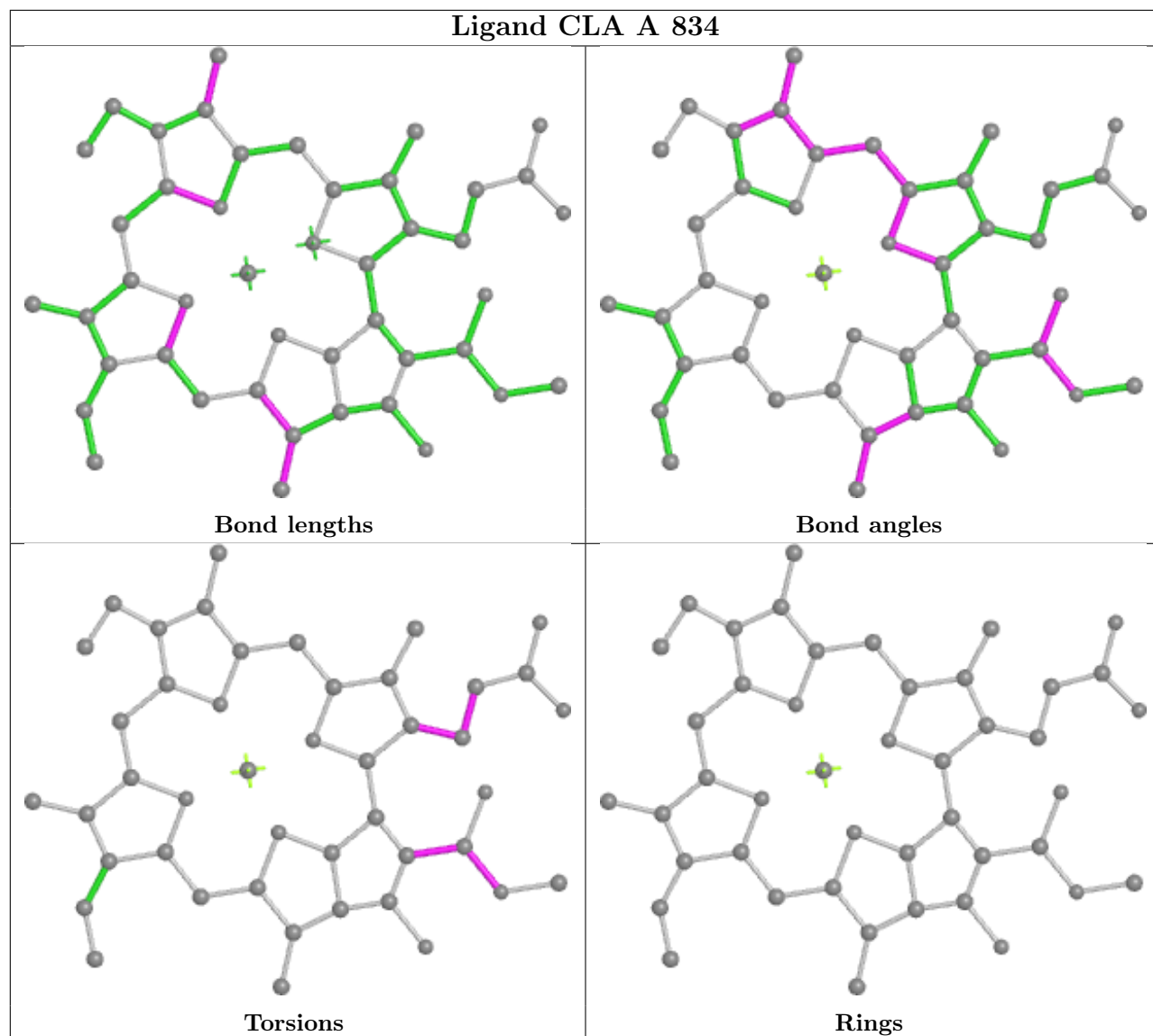
Ligand CLA 3 603



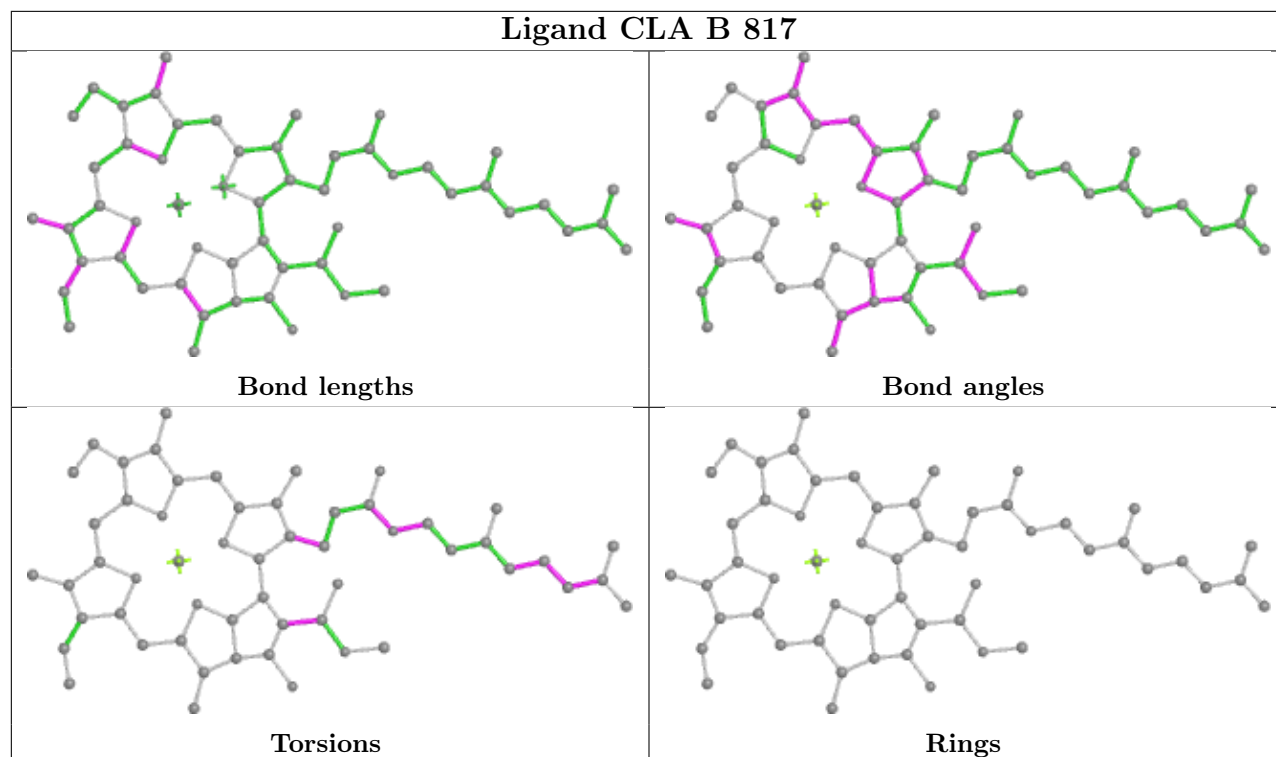
Ligand HTG J 102



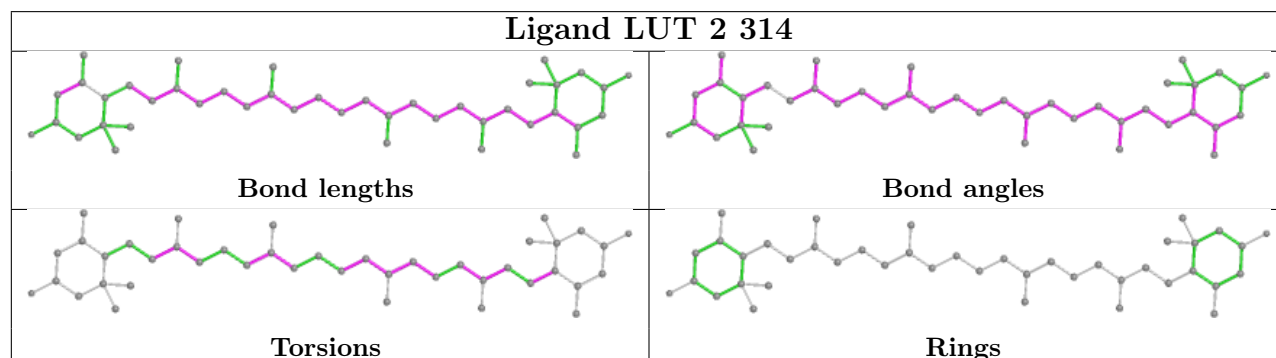
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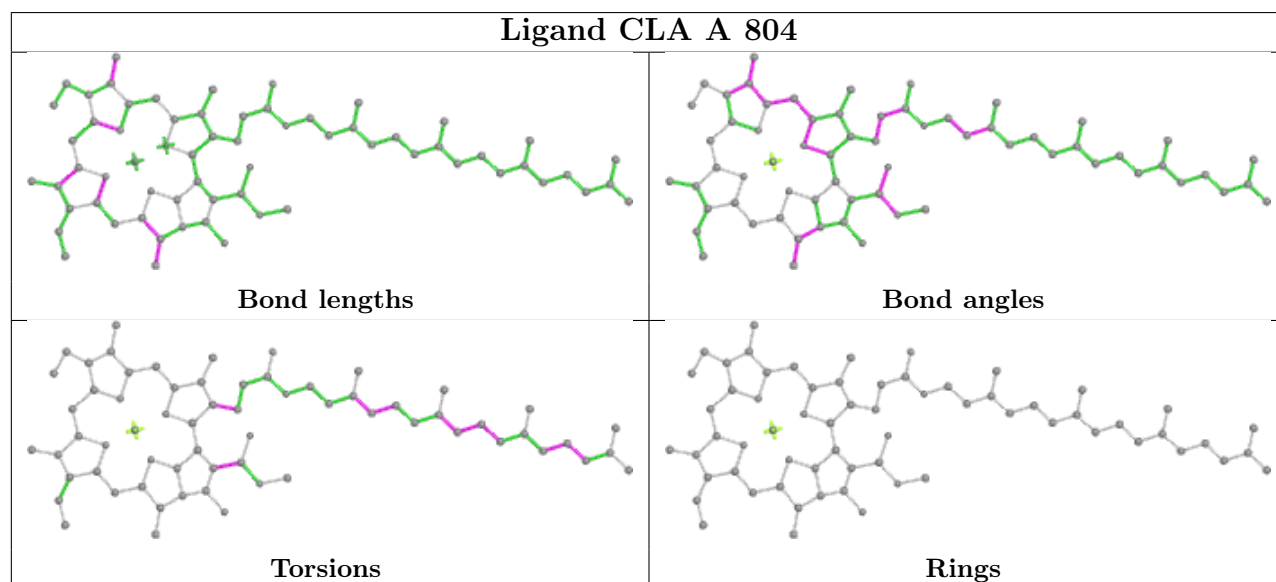
Ligand CLA B 817

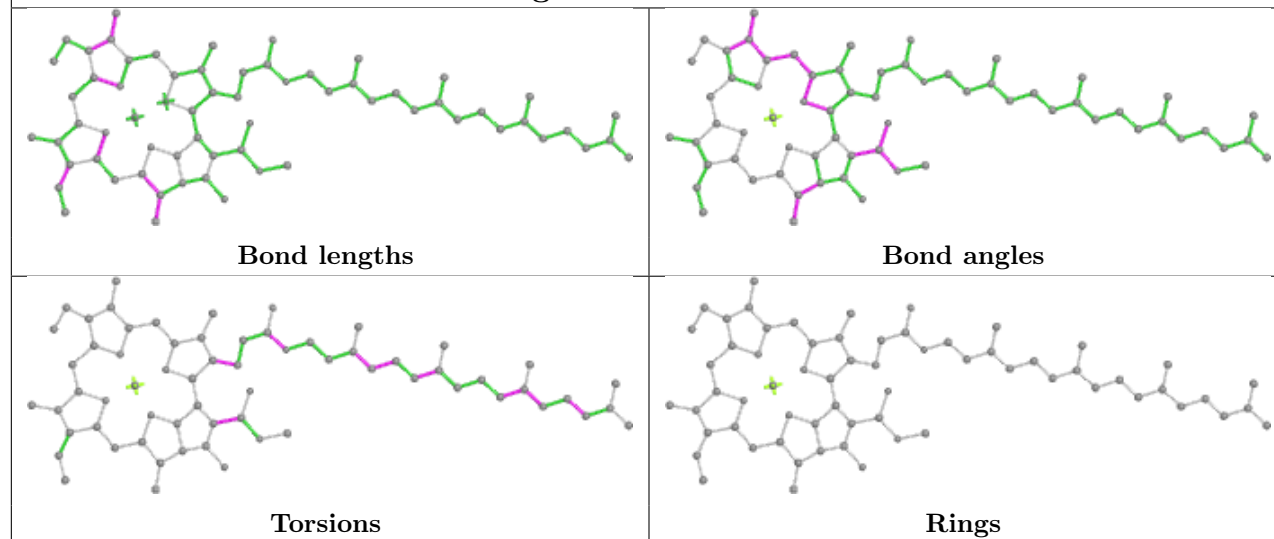
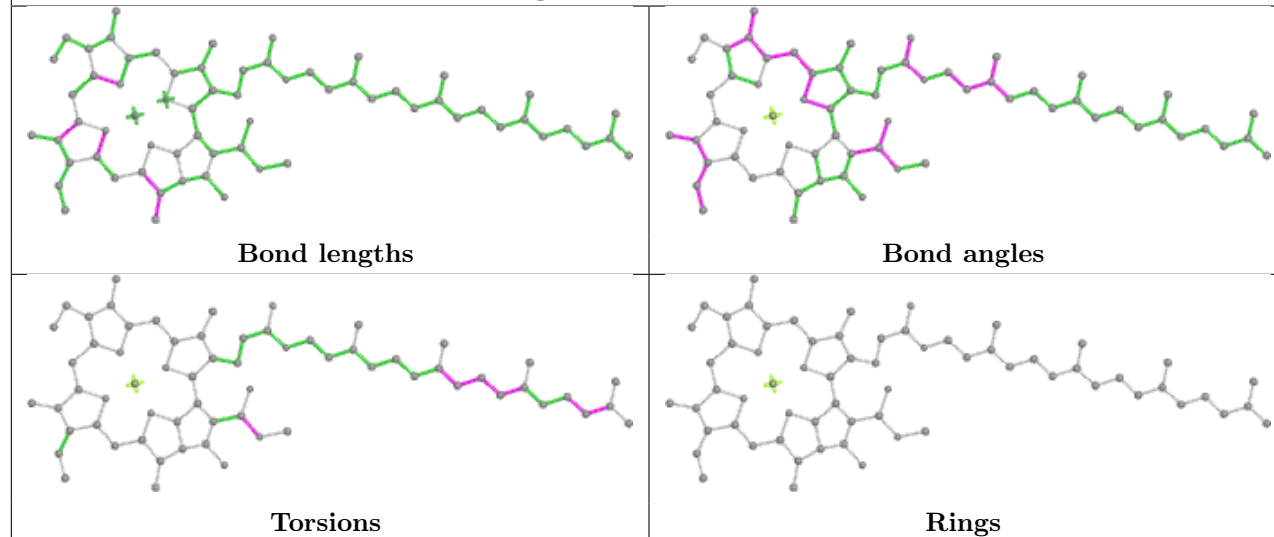
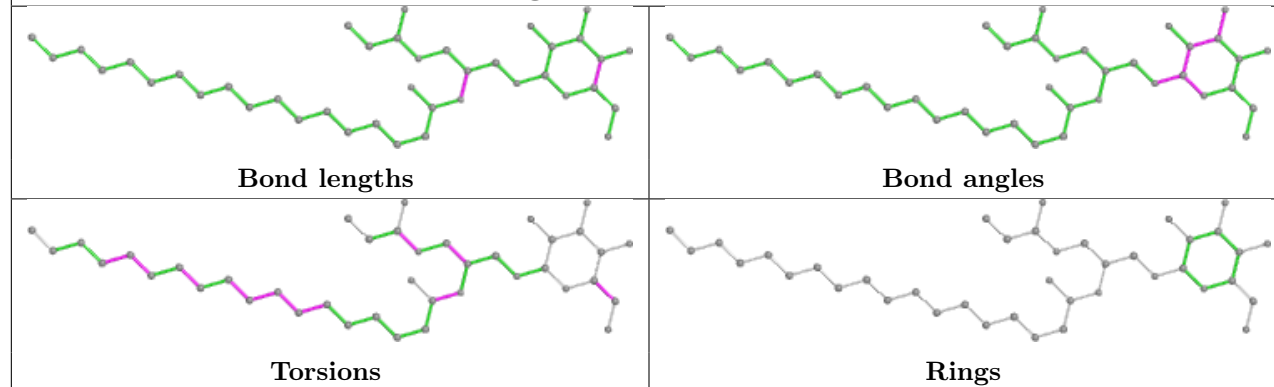


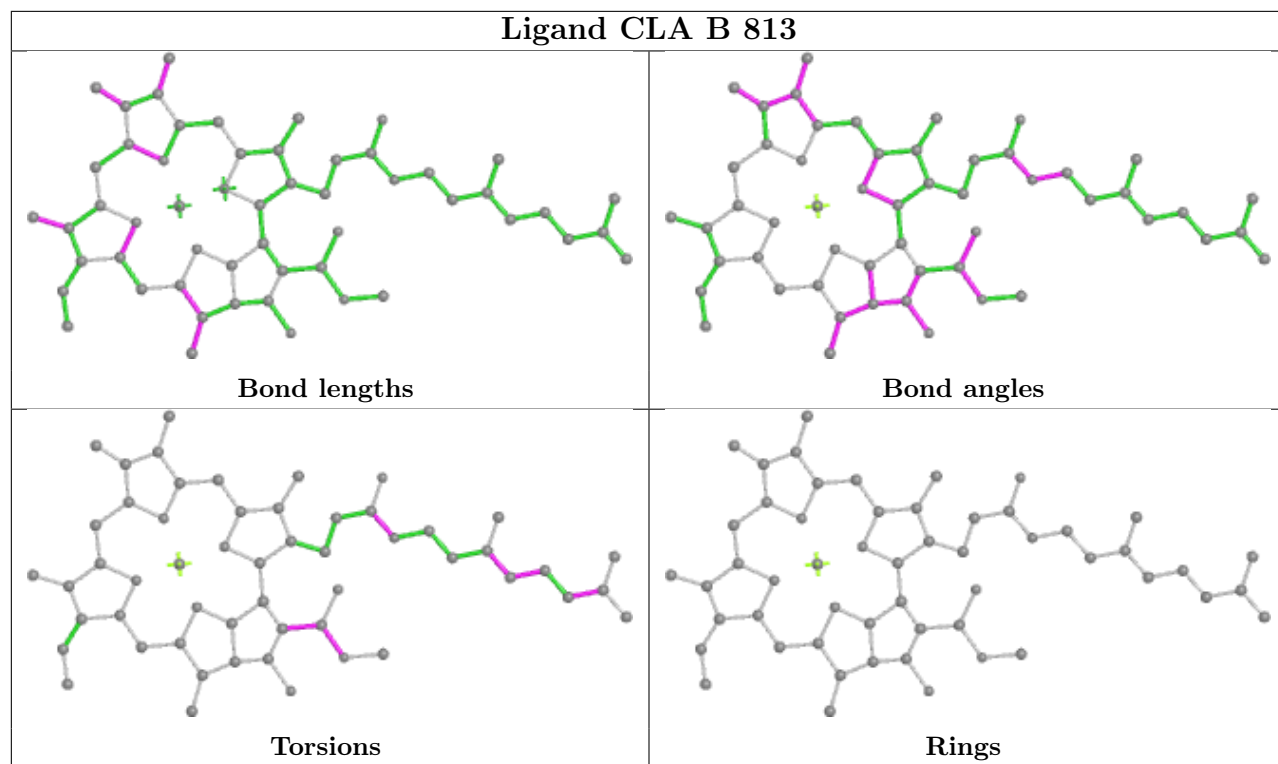
Ligand LUT 2 314



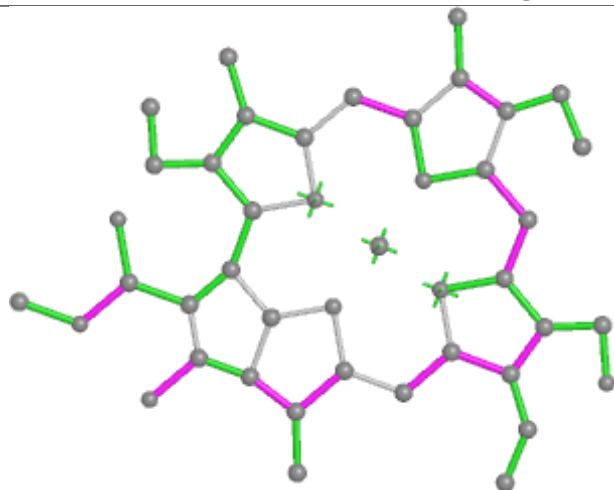
Ligand CLA A 804



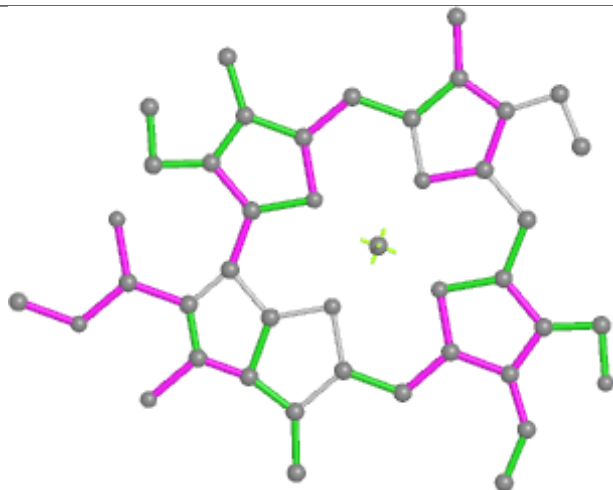
Ligand CLA B 803**Ligand CLA A 827****Ligand LMG G 101**



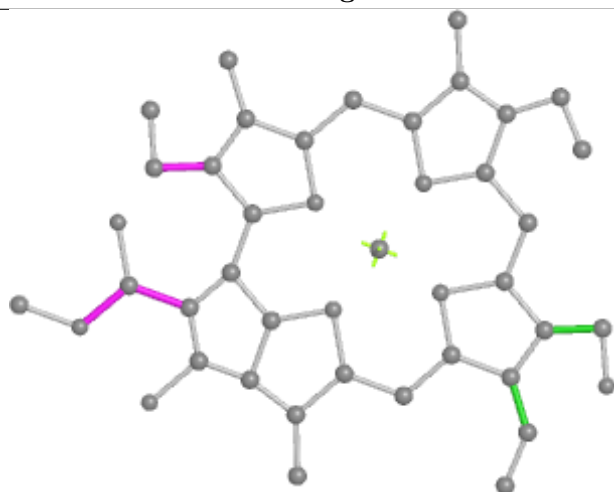
Ligand CHL 2 313



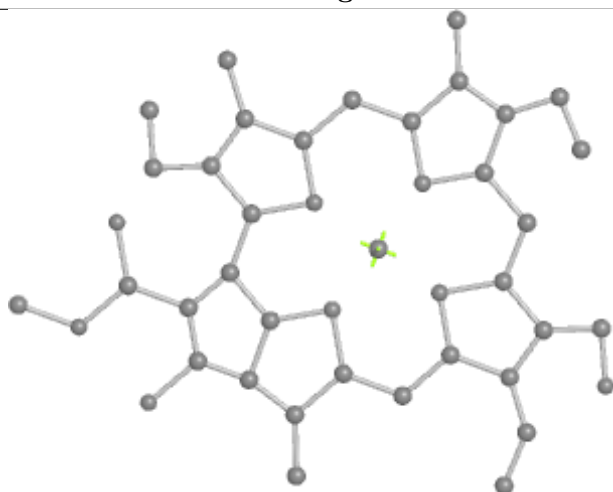
Bond lengths



Bond angles

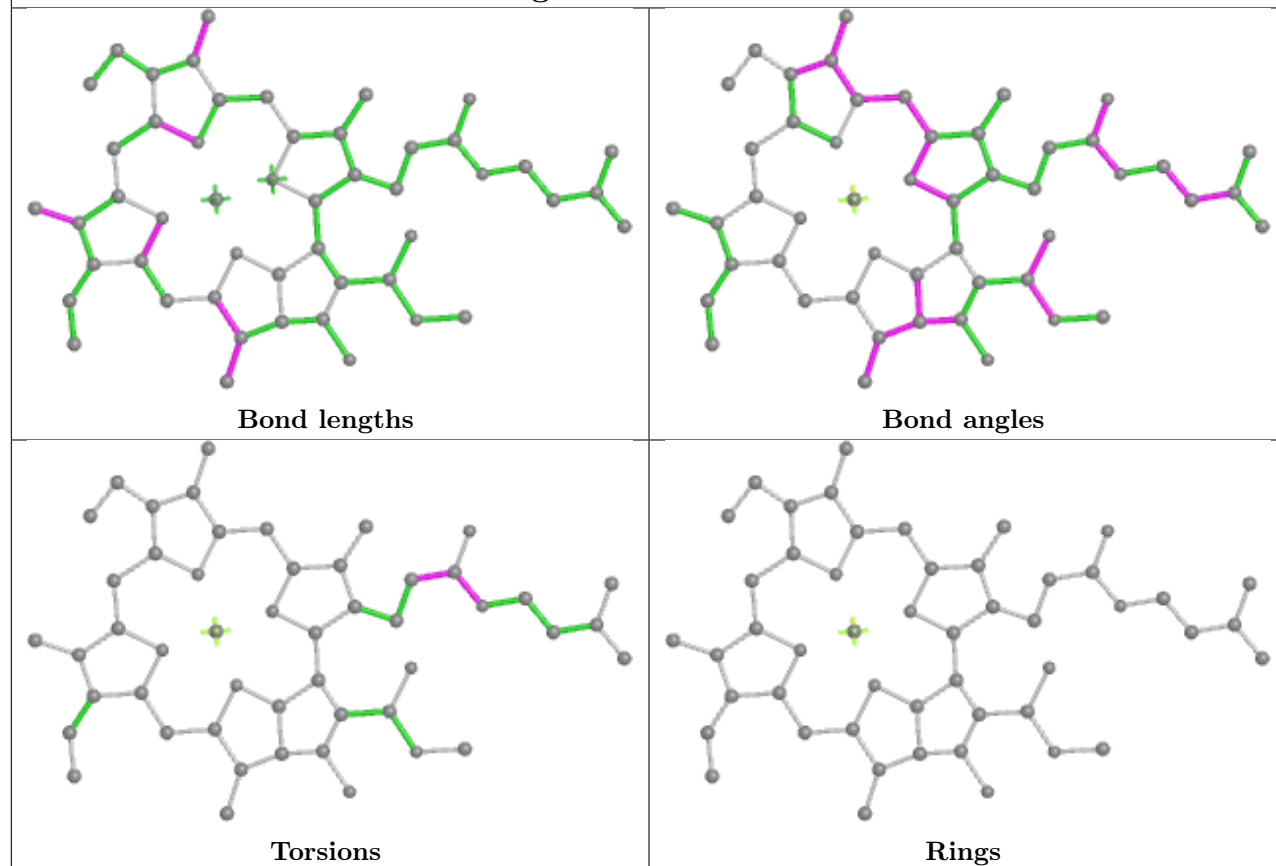


Torsions

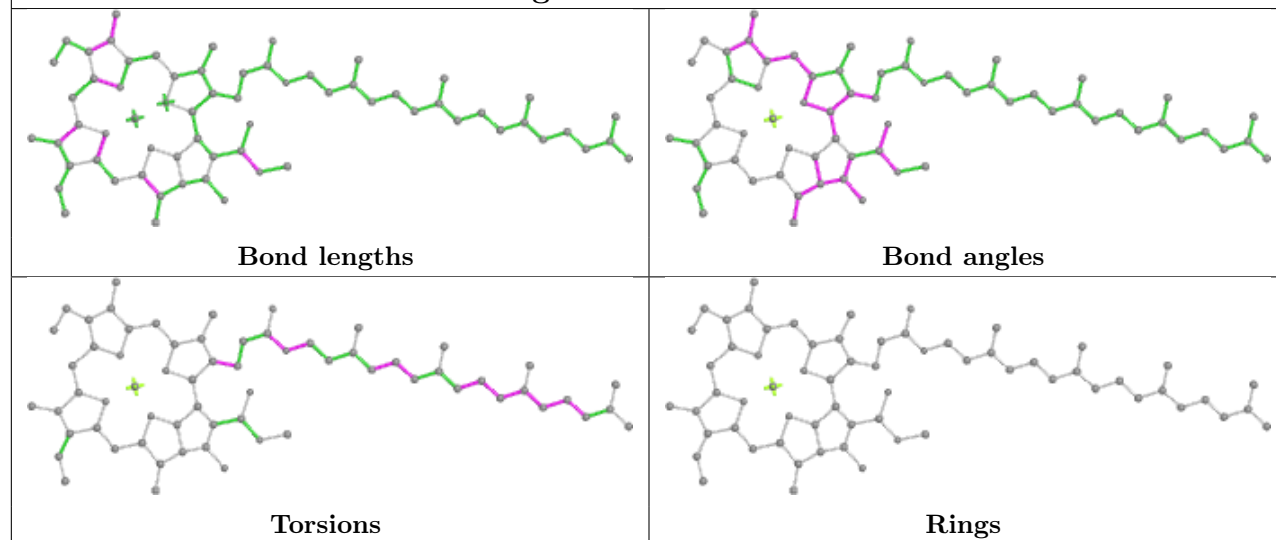


Rings

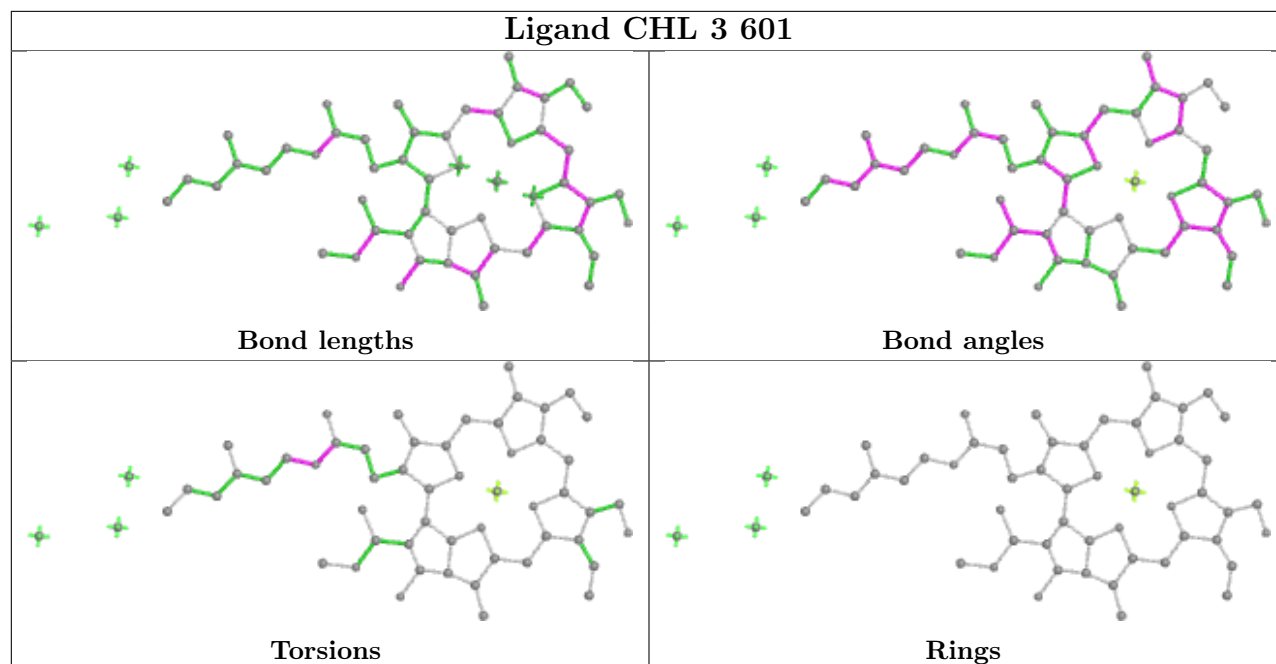
Ligand CLA A 833



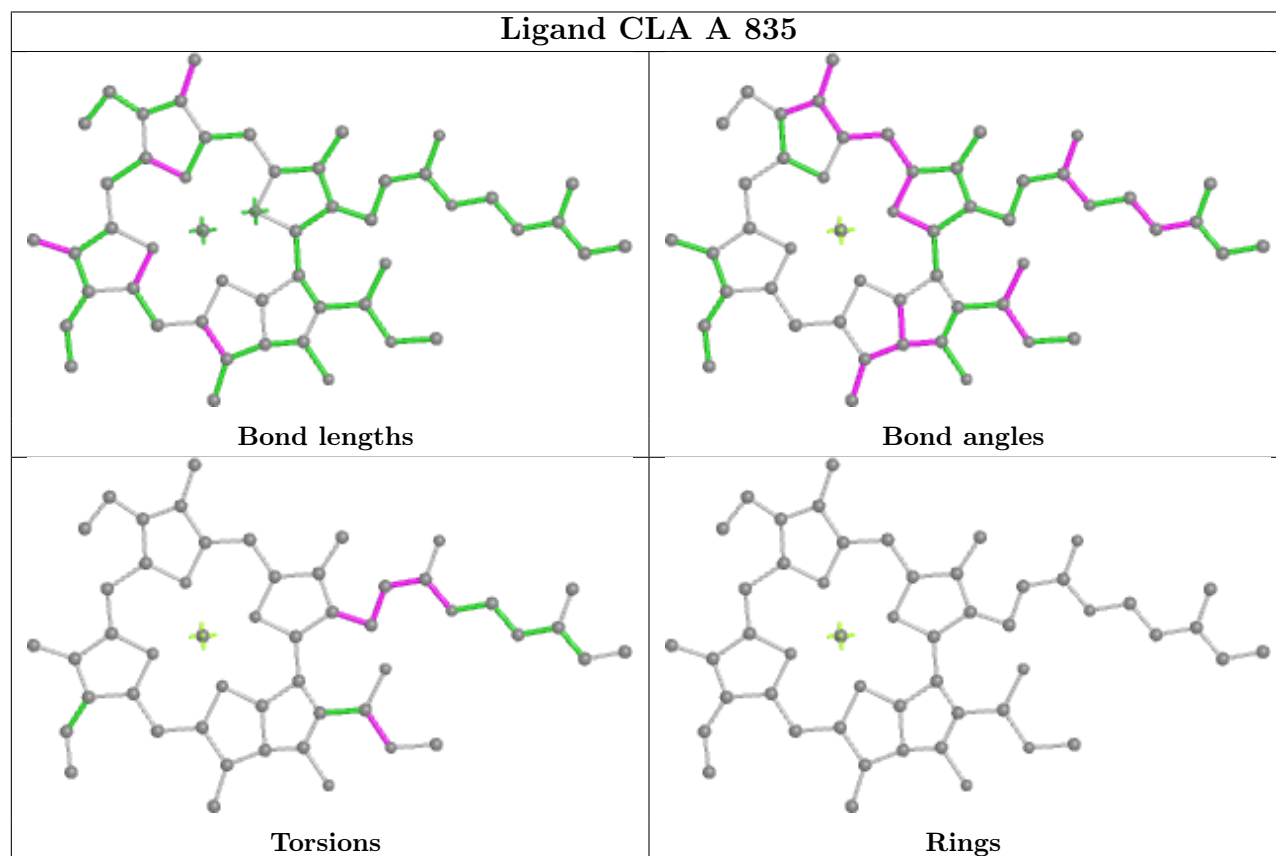
Ligand CLA B 829



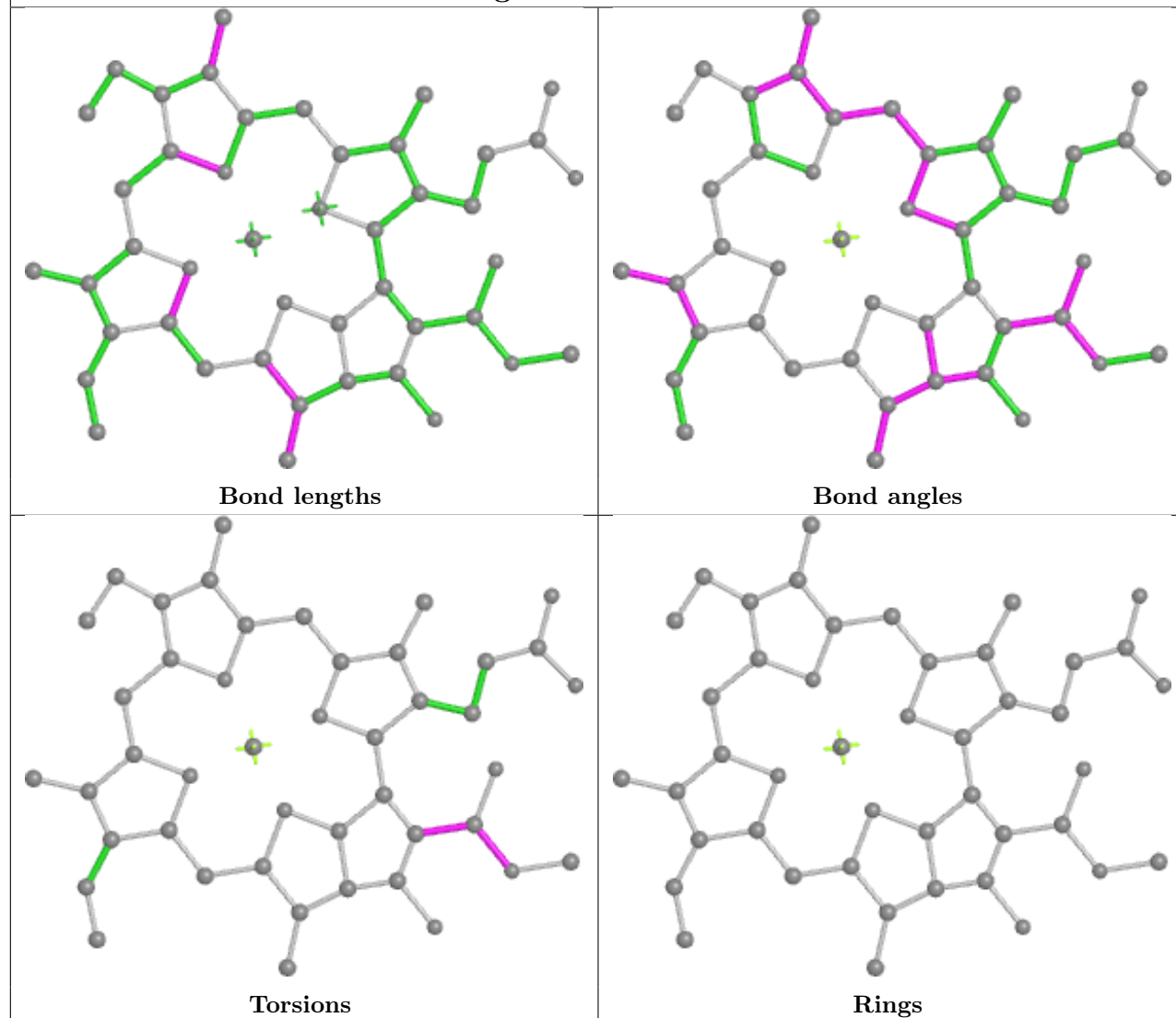
Ligand CHL 3 601



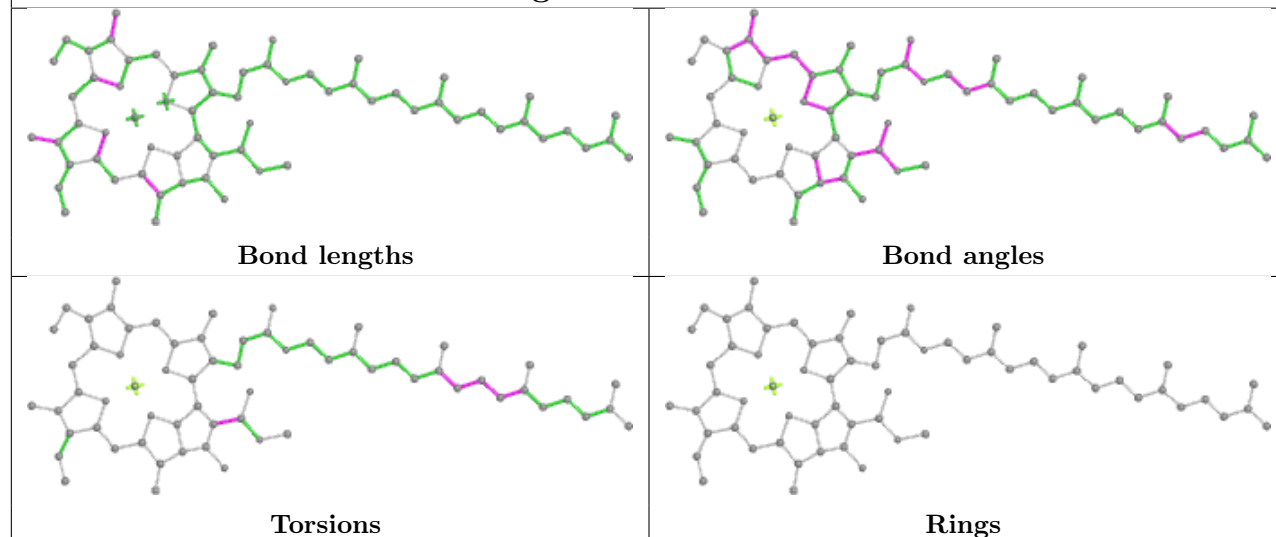
Ligand CLA A 835



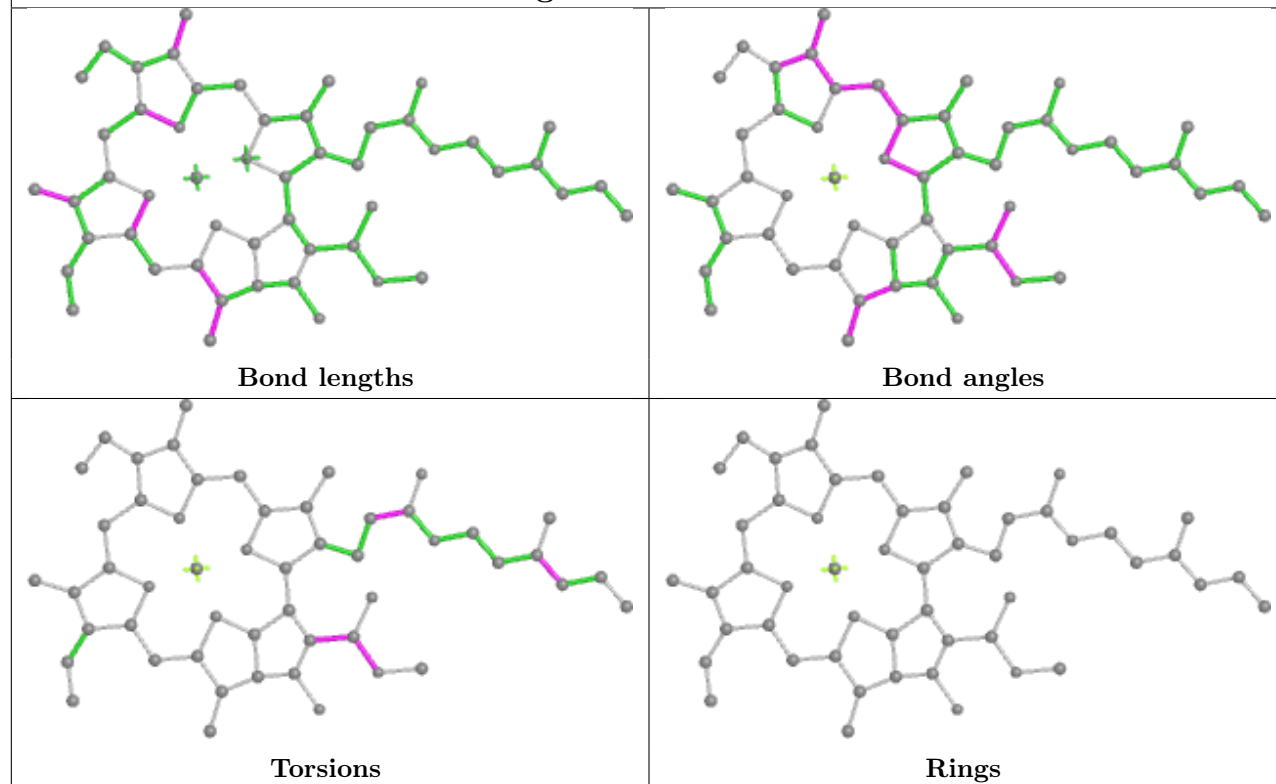
Ligand CLA 3 604



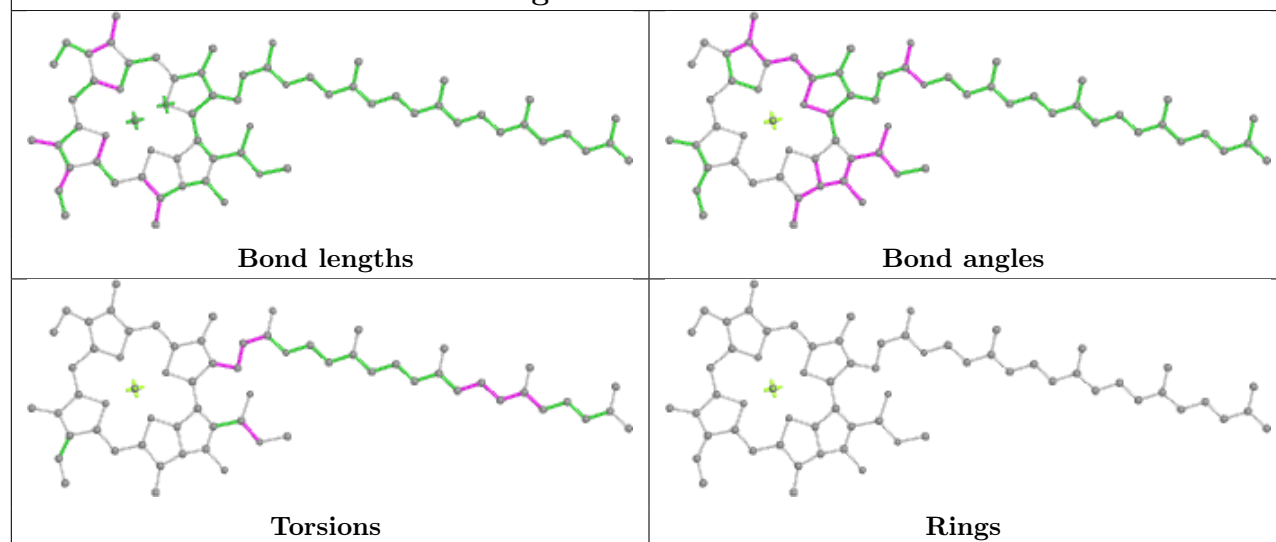
Ligand CLA B 828



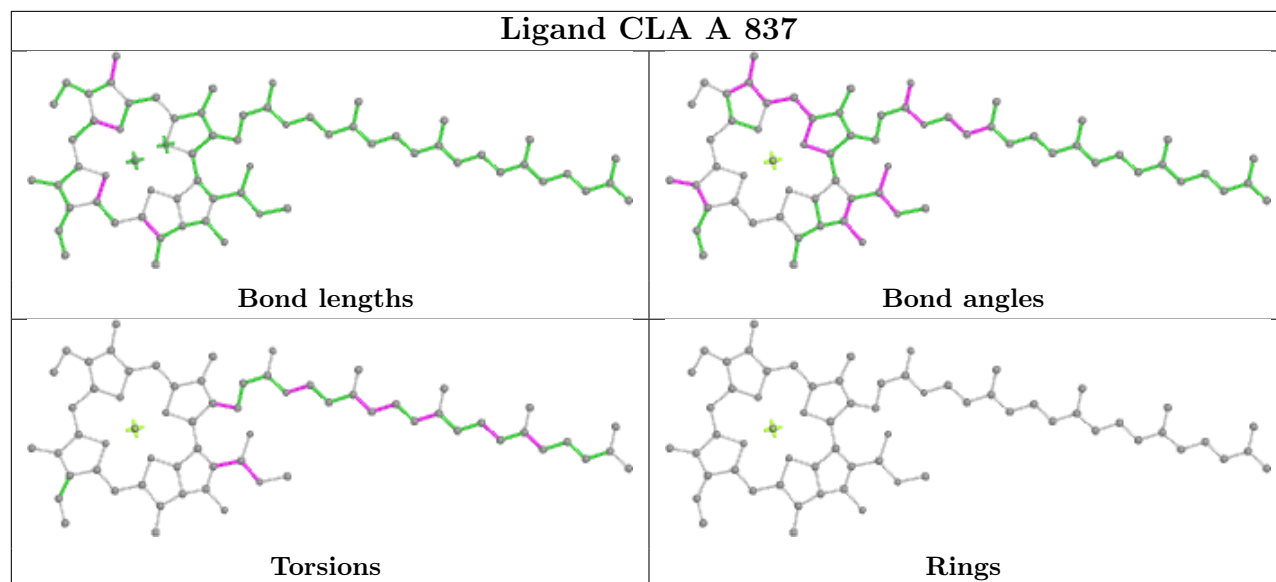
Ligand CLA 2 310



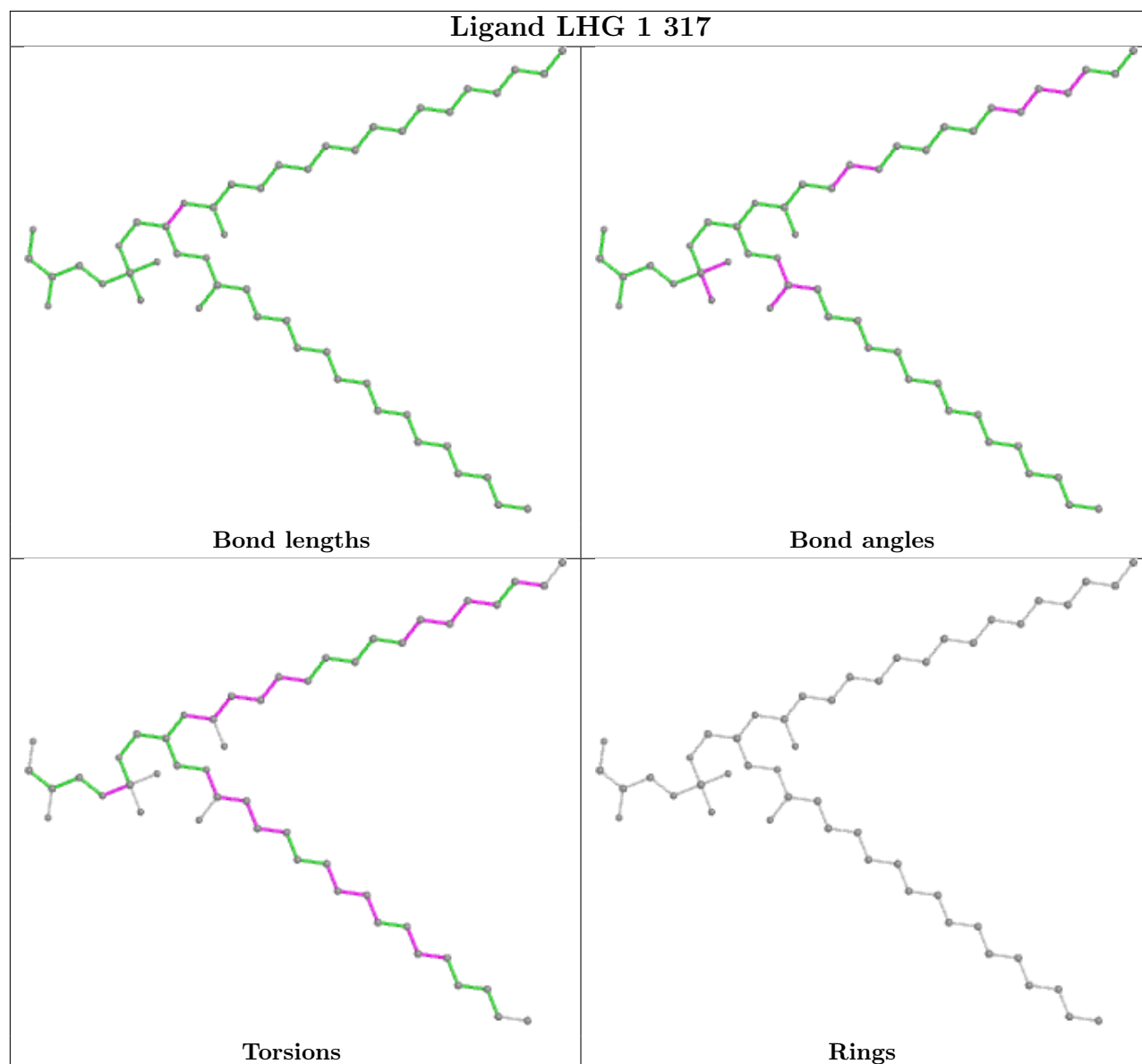
Ligand CLA A 817

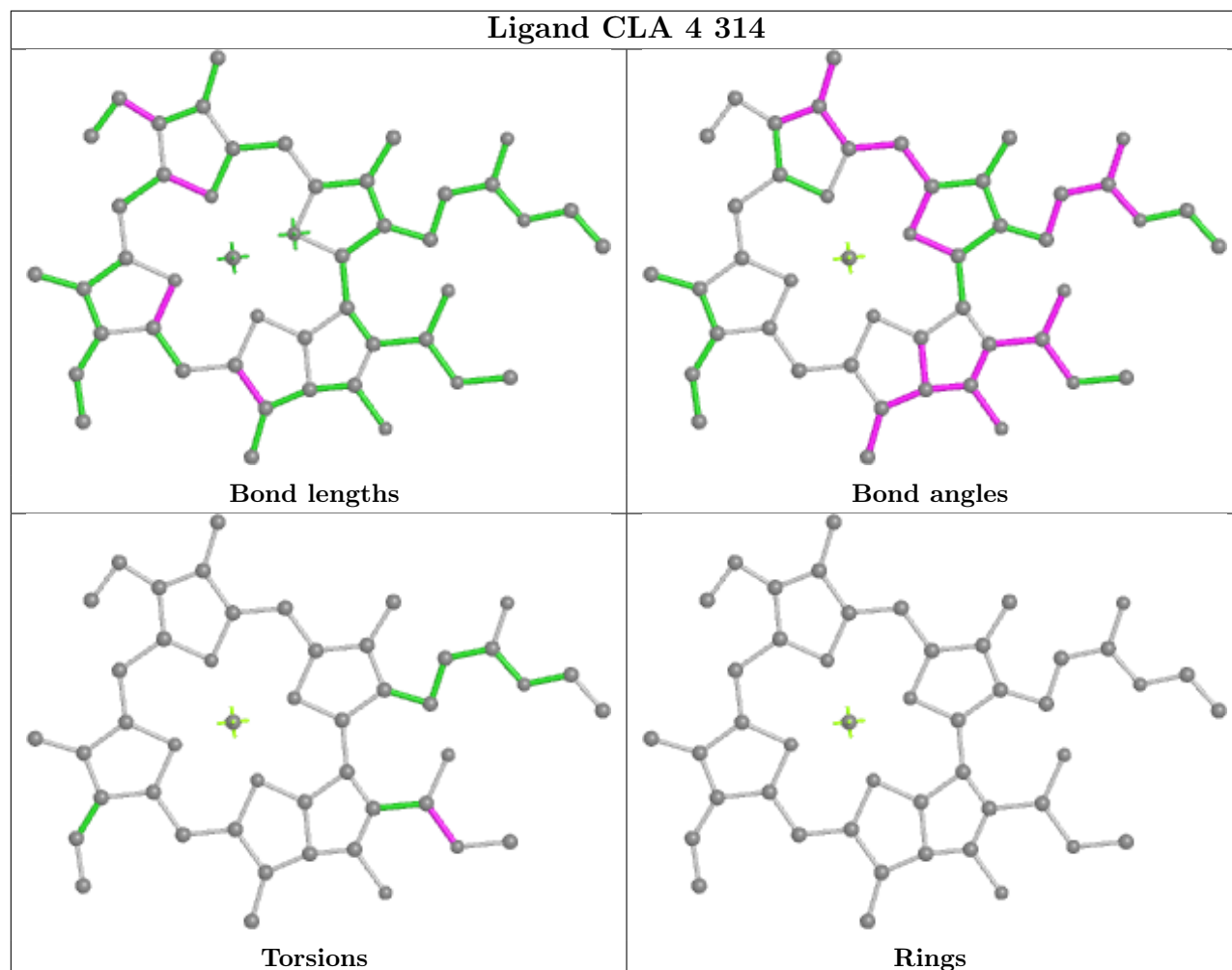
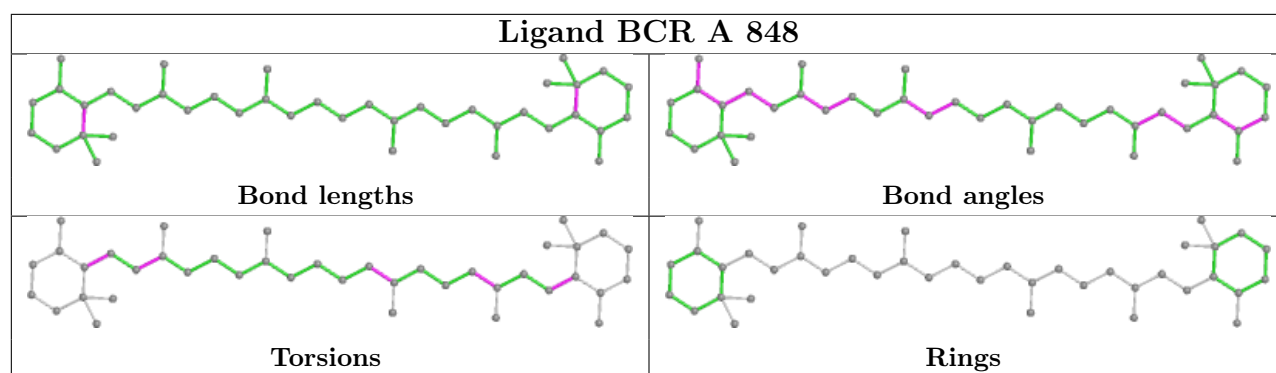


Ligand CLA A 837

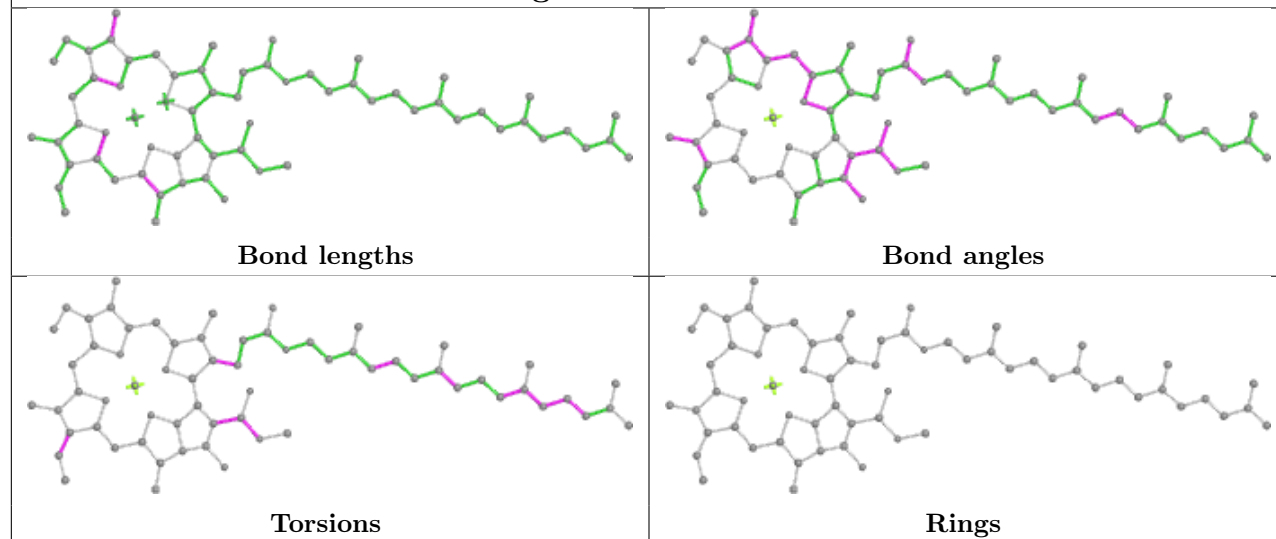


Ligand LHG 1 317

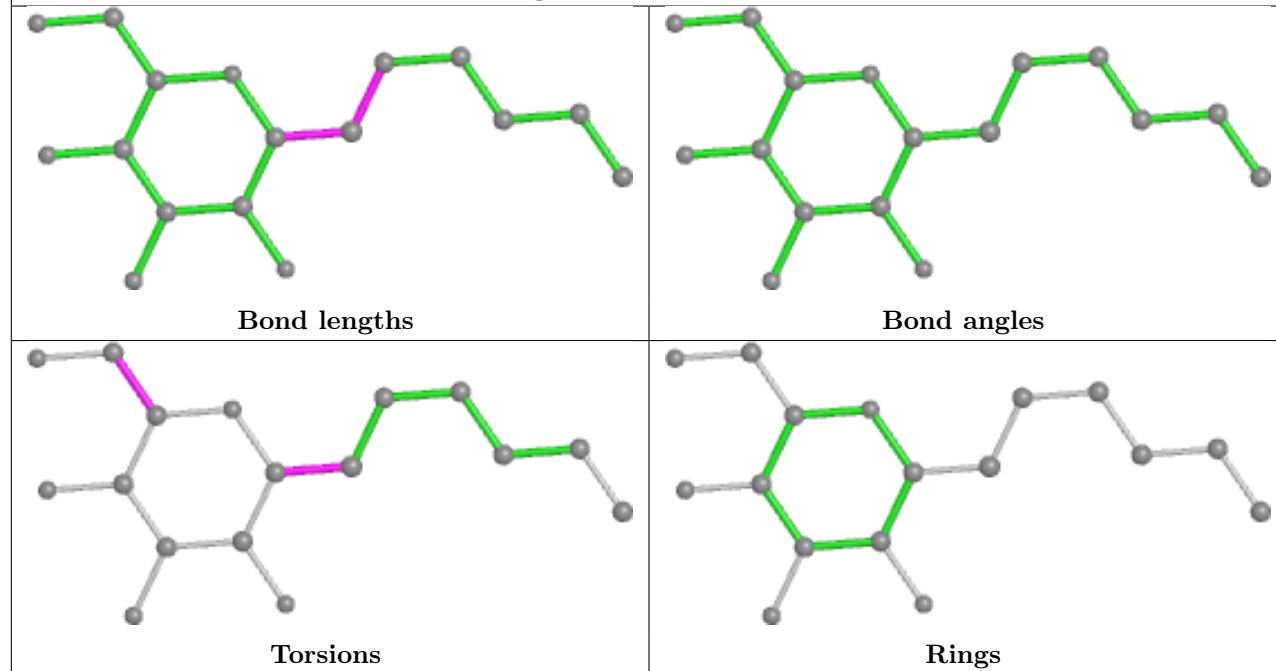




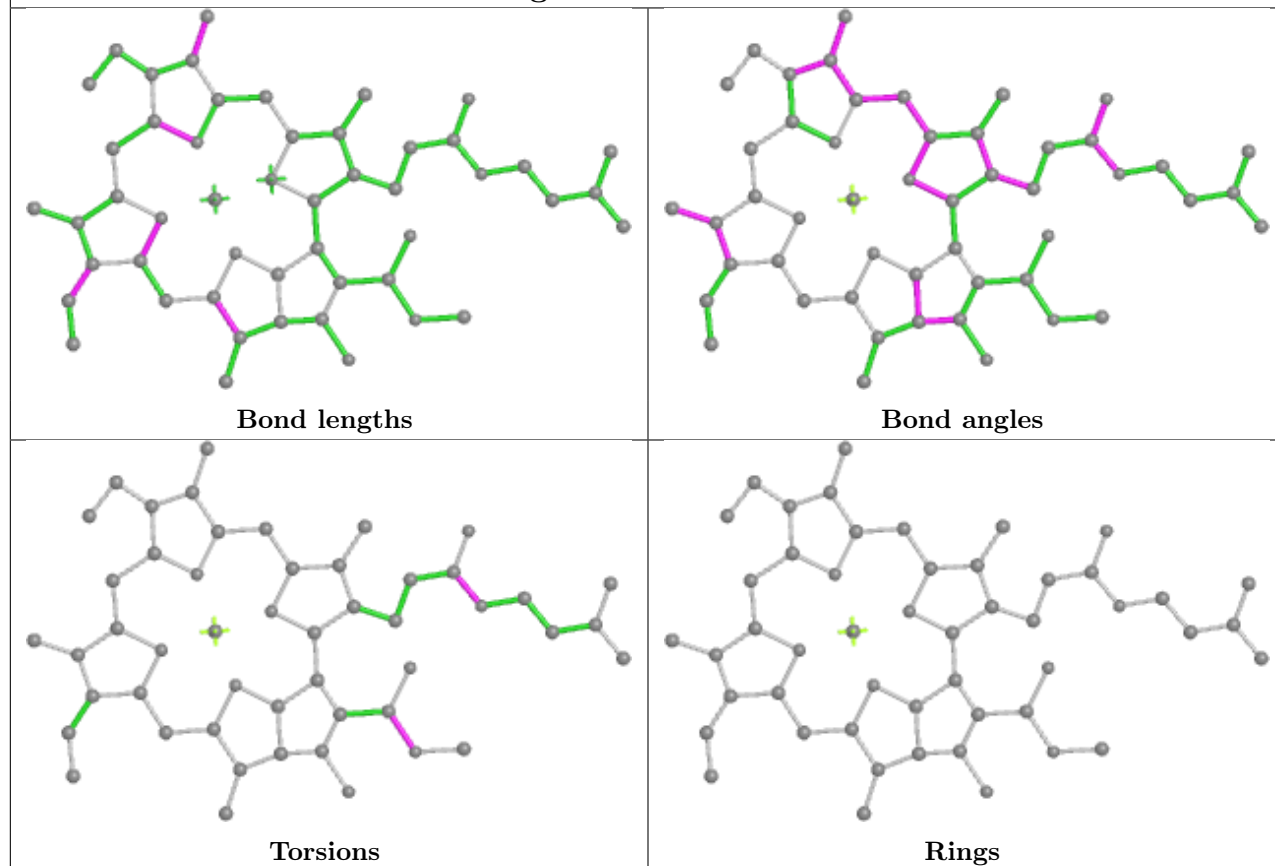
Ligand CLA B 815



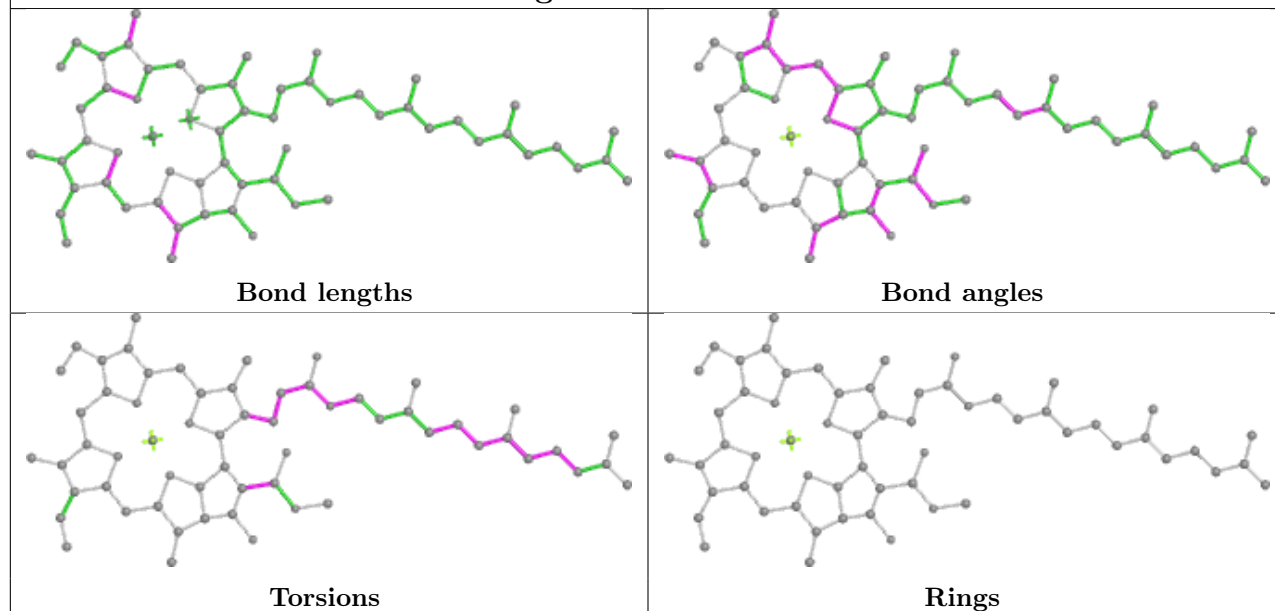
Ligand HTG F 301

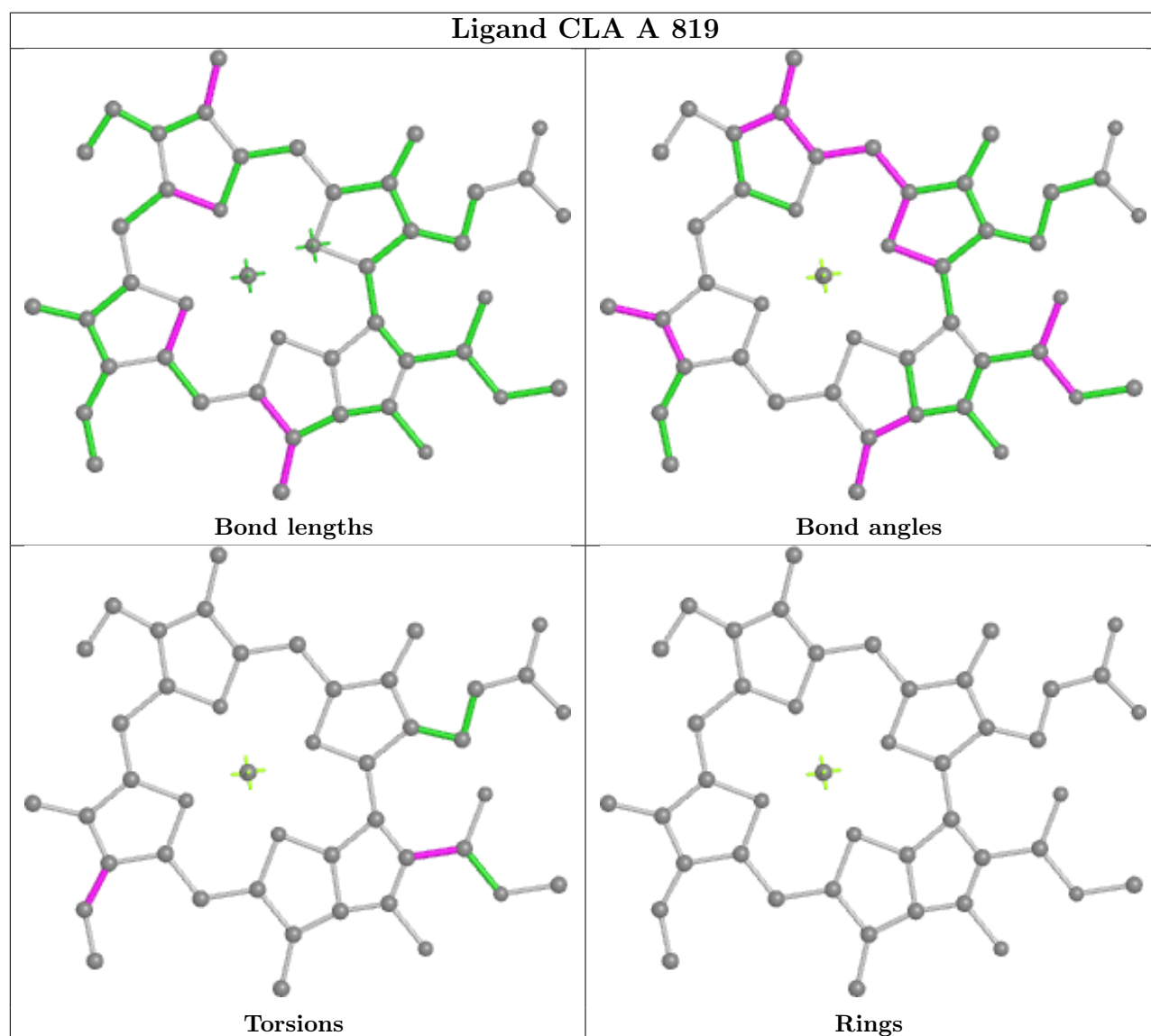
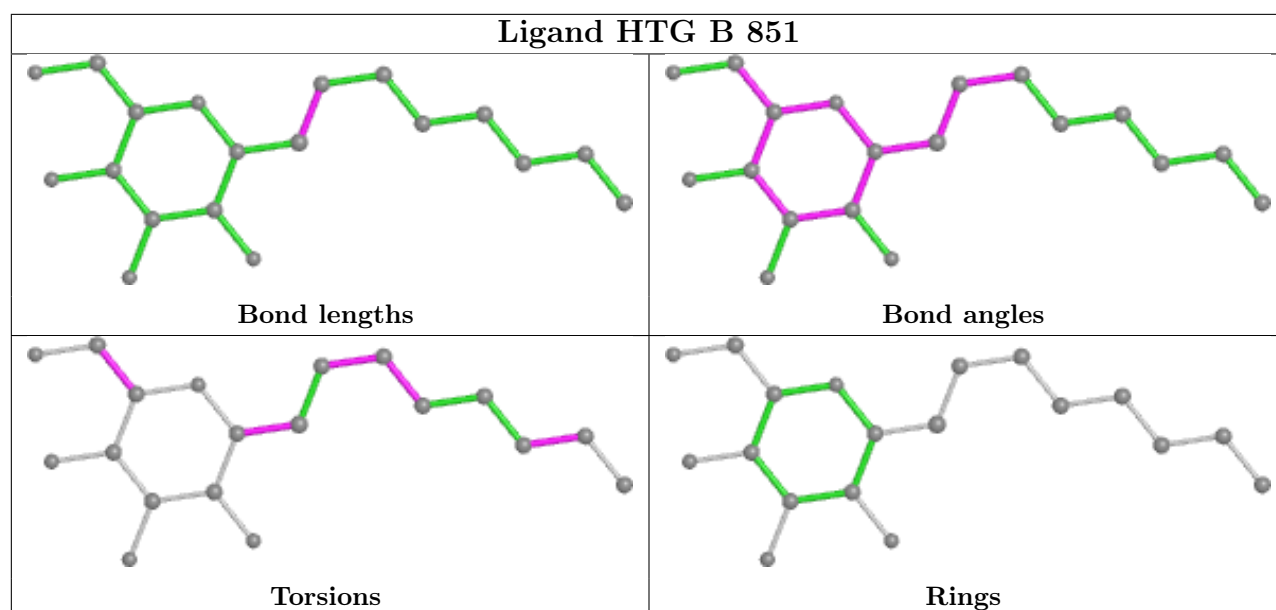


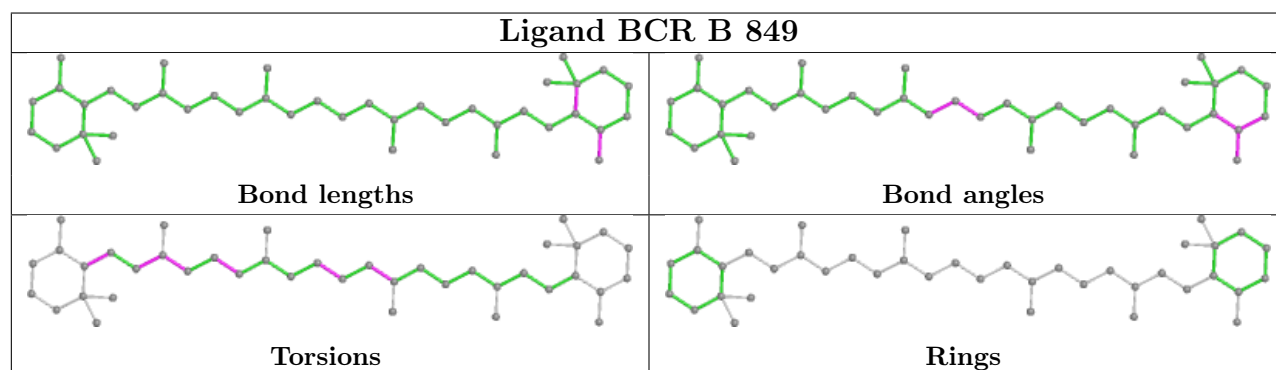
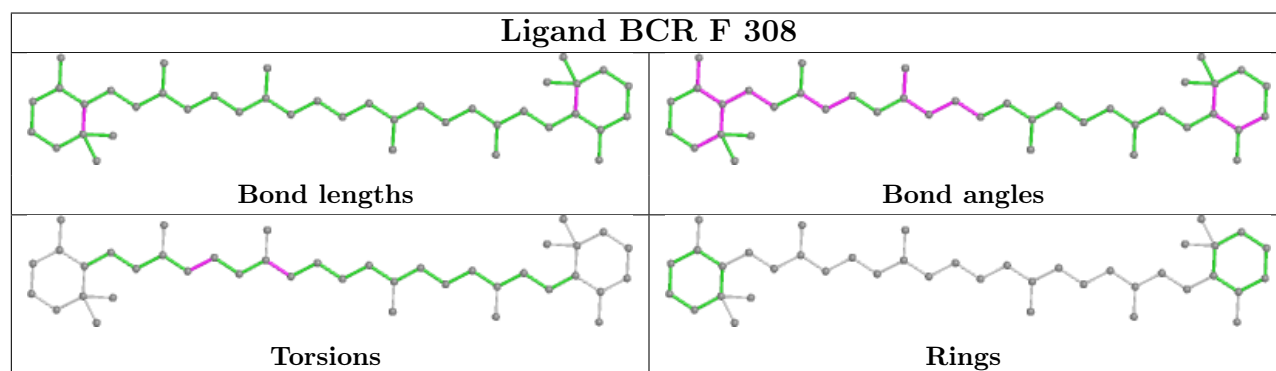
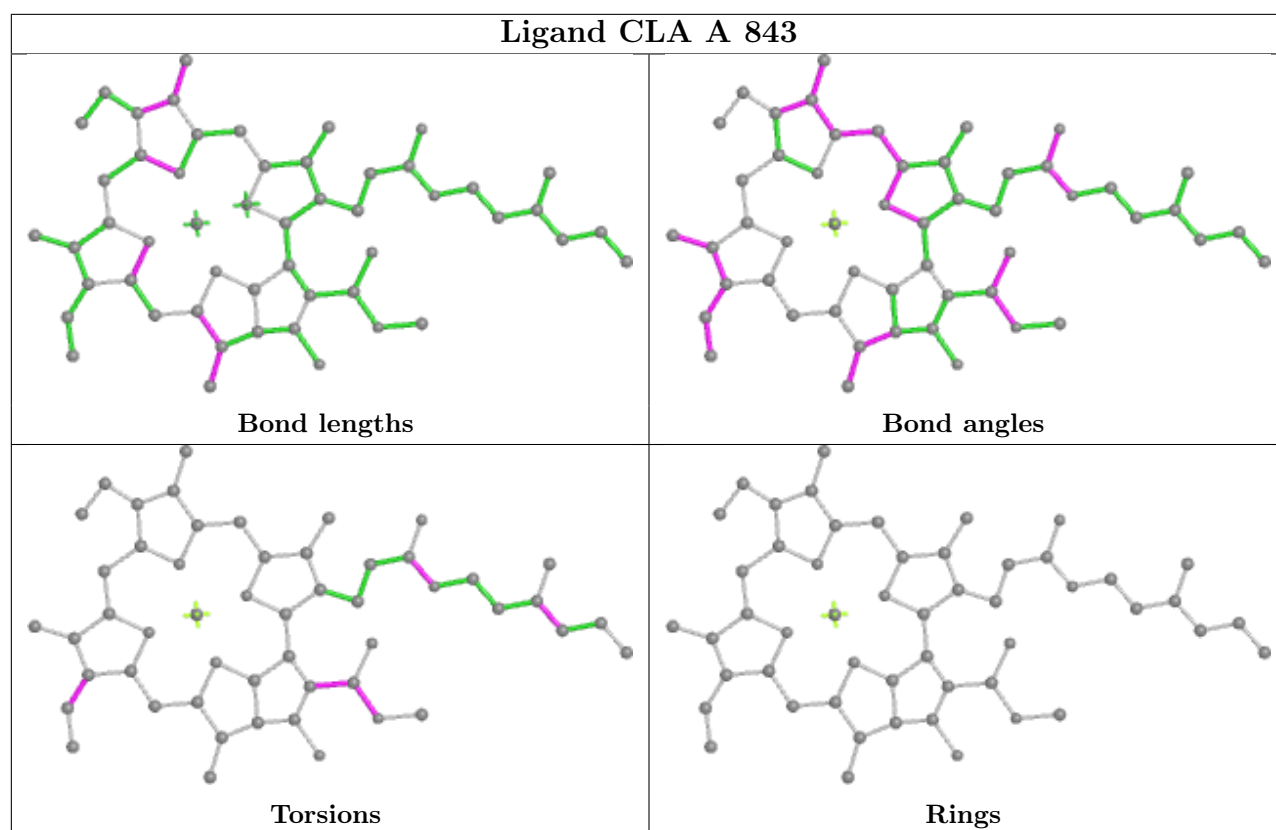
Ligand CLA G 104



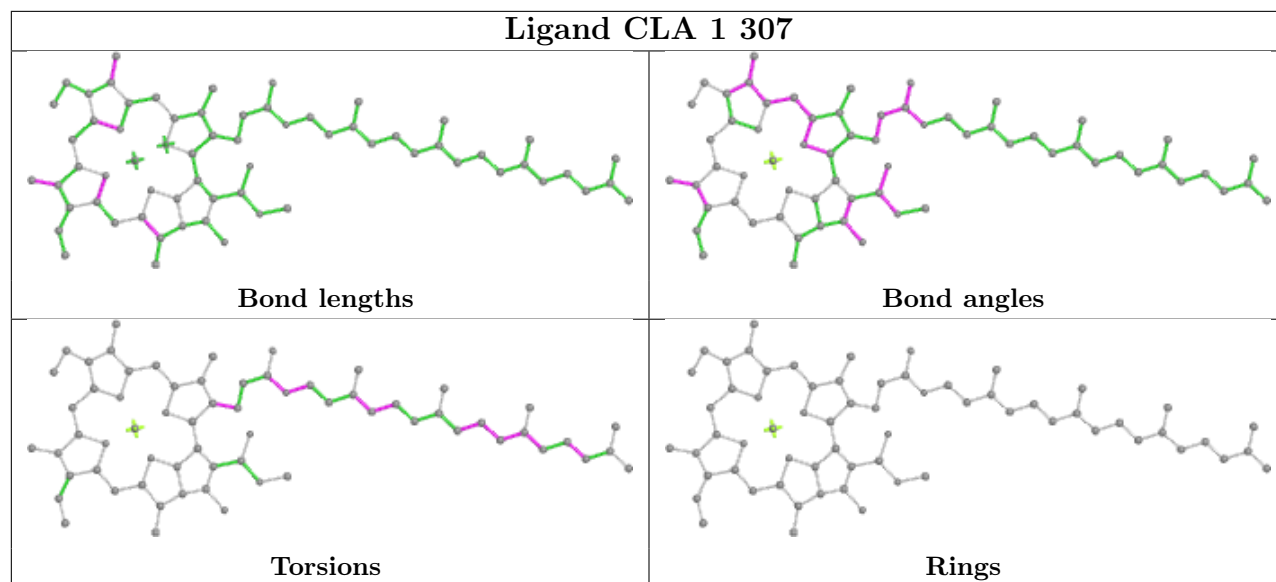
Ligand CLA 2 303



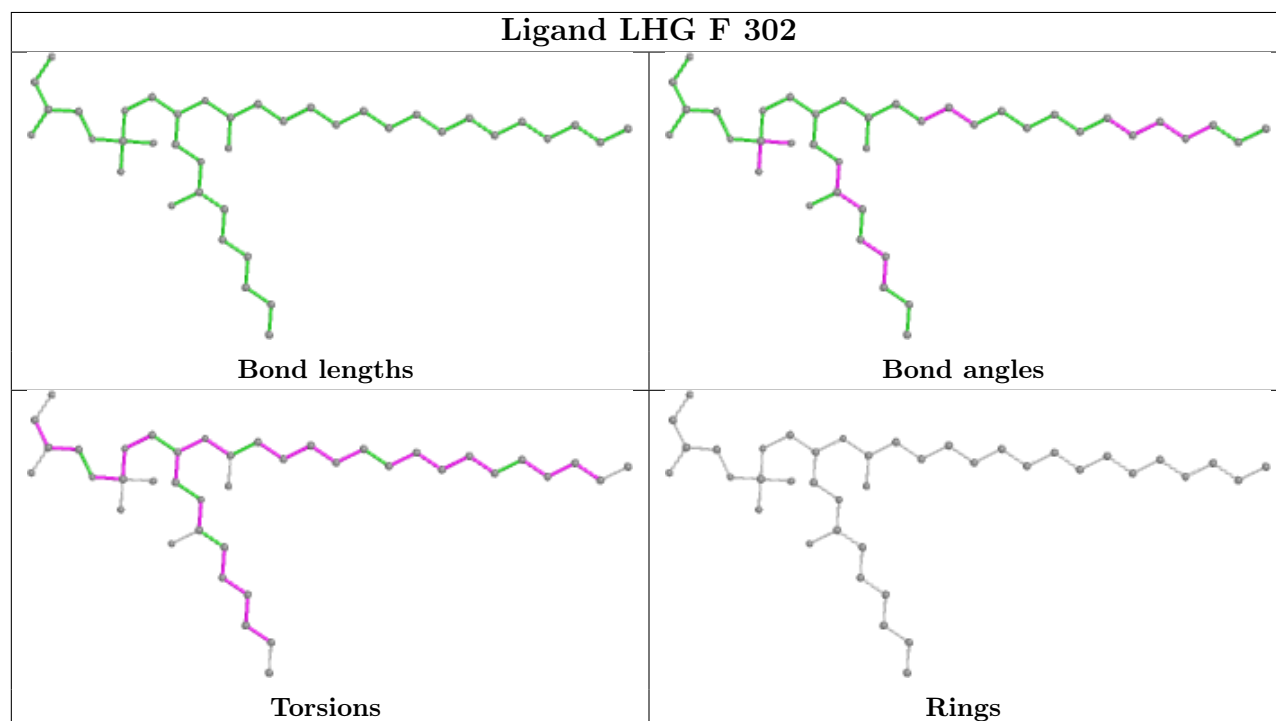




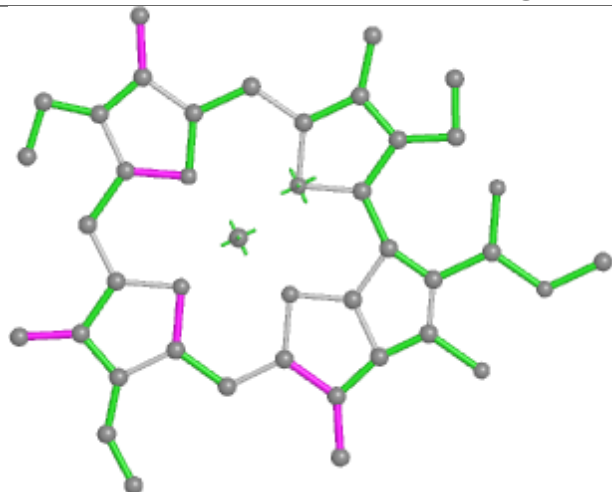
Ligand CLA 1 307



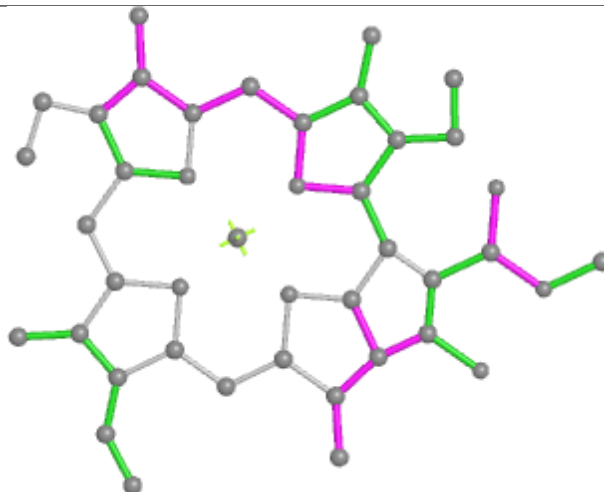
Ligand LHG F 302



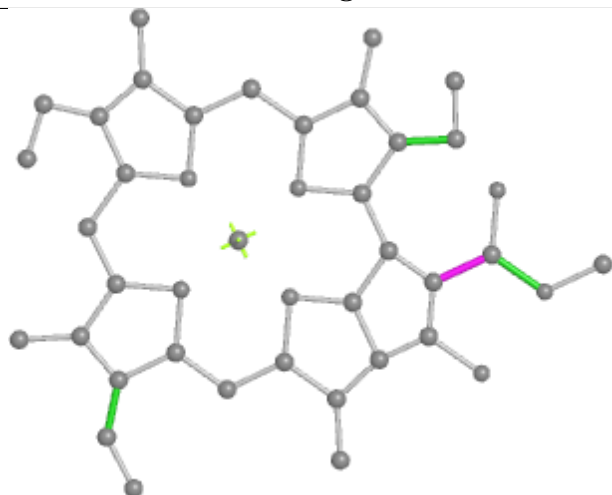
Ligand CLA 3 605



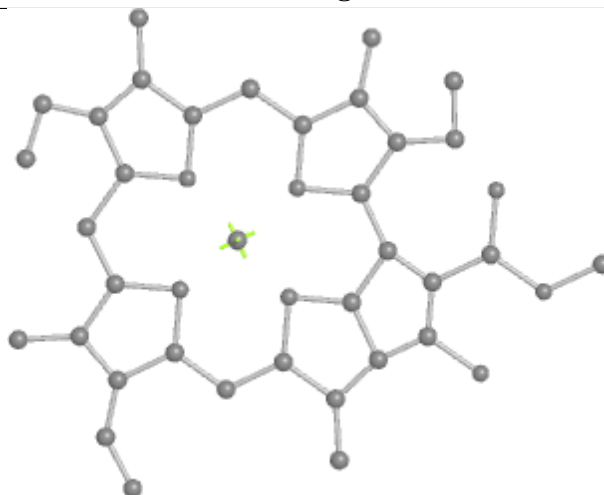
Bond lengths



Bond angles

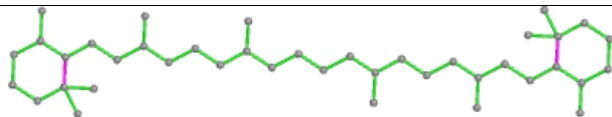


Torsions

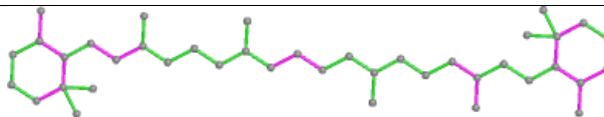


Rings

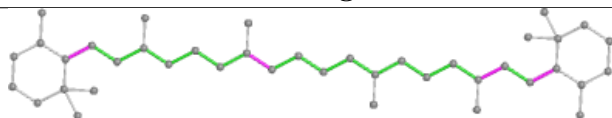
Ligand BCR J 105



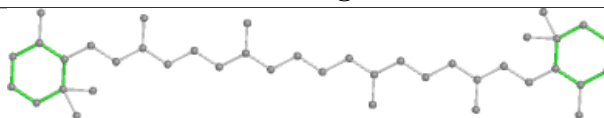
Bond lengths



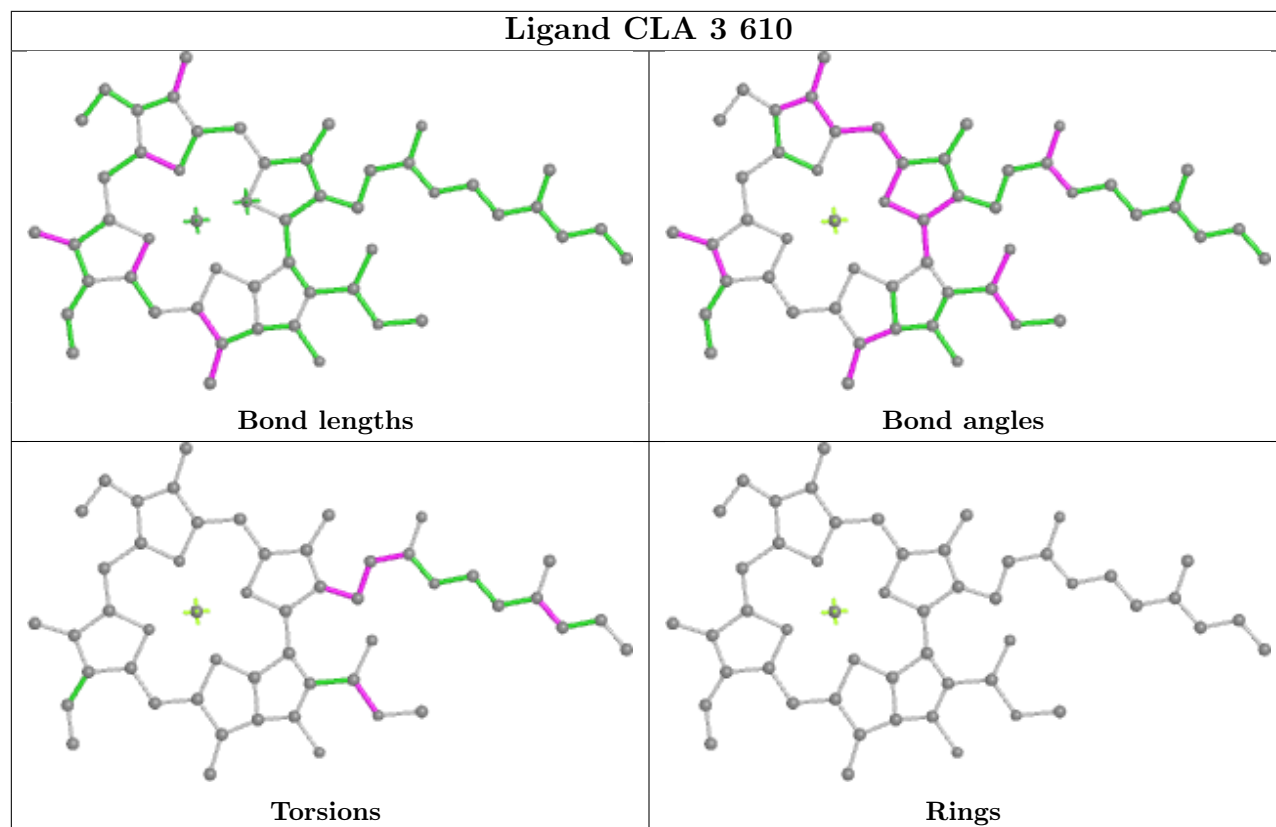
Bond angles

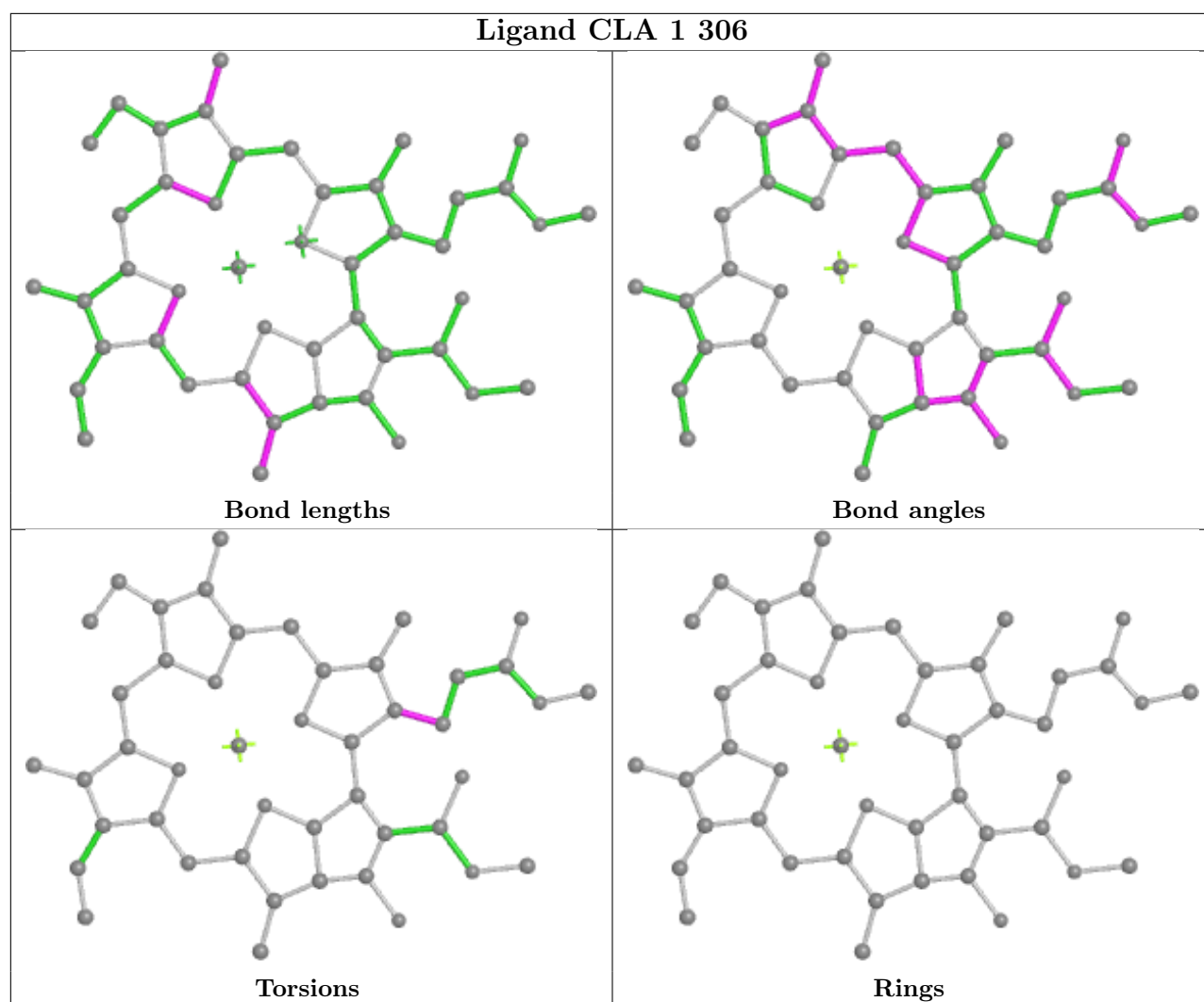


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	1	195/195 (100%)	0.83	35 (17%) 1 1	66, 95, 152, 193	0
2	2	204/269 (75%)	1.33	57 (27%) 0 0	87, 121, 159, 212	0
3	3	216/275 (78%)	2.37	97 (44%) 0 0	114, 161, 229, 257	0
4	4	195/198 (98%)	0.27	20 (10%) 6 6	60, 74, 111, 143	0
5	A	742/758 (97%)	1.08	180 (24%) 0 0	52, 94, 150, 233	0
6	B	733/734 (99%)	0.54	75 (10%) 6 6	30, 69, 98, 132	0
7	C	80/81 (98%)	0.37	5 (6%) 20 18	30, 78, 94, 120	0
8	D	140/143 (97%)	0.61	18 (12%) 3 3	66, 101, 137, 158	0
9	E	63/66 (95%)	1.32	12 (19%) 1 1	65, 84, 111, 129	0
10	F	152/154 (98%)	0.09	5 (3%) 46 45	30, 70, 96, 138	0
11	G	95/97 (97%)	0.13	5 (5%) 26 25	30, 91, 125, 156	0
12	H	88/88 (100%)	2.26	50 (56%) 0 0	96, 132, 182, 259	0
13	I	30/40 (75%)	0.61	2 (6%) 17 16	92, 108, 146, 208	0
14	J	39/42 (92%)	0.11	3 (7%) 13 12	60, 73, 101, 112	0
15	L	151/157 (96%)	0.89	32 (21%) 0 0	102, 137, 165, 192	0
16	K	77/80 (96%)	3.11	43 (55%) 0 0	137, 198, 248, 302	0
All	All	3200/3377 (94%)	0.94	639 (19%) 1 0	30, 91, 178, 302	0

The worst 5 of 639 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	I	2	ILE	16.1
3	3	121	LEU	15.9
3	3	128	LEU	14.4
16	K	85	ALA	12.5
3	3	122	ILE	12.4

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	LHG	G	102	49/49	0.50	0.45	92,119,171,174	0
24	LMG	G	101	40/55	0.59	0.42	110,157,180,181	0
21	BCR	K	203	40/40	0.67	0.42	142,185,227,229	0
20	XAT	3	615	44/44	0.70	0.33	62,89,98,100	0
25	HTG	B	851	19/19	0.70	0.37	107,134,142,143	0
25	HTG	F	301	17/19	0.72	0.32	124,149,155,159	0
25	HTG	F	310	16/19	0.72	0.38	114,141,144,146	0
23	LMT	A	855	35/35	0.73	0.23	97,154,171,172	0
24	LMG	4	320	49/55	0.74	0.33	96,119,174,176	0
21	BCR	2	316	40/40	0.77	0.60	148,157,172,173	0
21	BCR	A	846	40/40	0.77	0.32	116,137,151,153	0
25	HTG	4	322	19/19	0.78	0.25	107,129,140,145	0
21	BCR	G	106	40/40	0.78	0.26	71,90,129,130	0
21	BCR	3	616	40/40	0.78	0.44	156,164,187,189	0
21	BCR	A	849	40/40	0.78	0.38	100,137,196,199	0
26	DGD	4	323	60/66	0.78	0.24	90,115,130,138	0
22	LHG	F	302	40/49	0.79	0.28	111,140,164,167	0
17	CLA	K	201	45/65	0.82	0.24	172,184,191,193	0
17	CLA	2	303	60/65	0.82	0.31	120,132,139,142	0
26	DGD	B	850	66/66	0.82	0.25	80,94,119,120	0
24	LMG	F	309	55/55	0.83	0.23	91,108,120,124	0
17	CLA	3	604	45/65	0.84	0.30	137,162,170,173	0
22	LHG	2	317	37/49	0.84	0.32	155,163,179,187	0
19	LUT	3	614	42/42	0.84	0.30	127,146,163,166	0
24	LMG	B	852	52/55	0.84	0.23	100,127,143,148	0
17	CLA	A	814	50/65	0.85	0.24	119,141,161,164	0
17	CLA	3	610	52/65	0.85	0.30	177,188,210,215	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	HTG	4	321	19/19	0.85	0.30	125,139,147,147	0
17	CLA	A	843	52/65	0.86	0.38	173,188,196,199	0
17	CLA	G	103	41/65	0.86	0.19	105,122,131,136	0
20	XAT	2	315	44/44	0.86	0.30	62,89,98,100	0
17	CLA	L	203	65/65	0.86	0.25	119,143,157,167	0
21	BCR	B	846	40/40	0.86	0.21	62,77,125,126	0
23	LMT	2	318	35/35	0.86	0.15	120,133,143,146	0
21	BCR	A	850	40/40	0.87	0.24	72,108,147,148	0
17	CLA	L	204	50/65	0.87	0.33	122,147,157,163	0
17	CLA	A	817	65/65	0.87	0.26	103,129,169,173	0
17	CLA	A	813	45/65	0.87	0.18	89,111,120,126	0
21	BCR	1	316	40/40	0.88	0.39	98,125,149,151	0
17	CLA	3	602	60/65	0.88	0.20	132,157,174,178	0
17	CLA	3	609	50/65	0.88	0.26	147,163,173,175	0
17	CLA	A	824	65/65	0.88	0.23	90,102,108,111	0
17	CLA	A	833	50/65	0.88	0.22	120,135,146,157	0
17	CLA	K	202	60/65	0.89	0.28	146,176,193,196	0
21	BCR	B	847	40/40	0.89	0.23	49,65,85,92	0
17	CLA	L	202	65/65	0.89	0.29	142,154,170,175	0
21	BCR	L	206	40/40	0.89	0.27	156,168,177,178	0
17	CLA	A	815	45/65	0.89	0.20	114,125,135,140	0
17	CLA	B	817	55/65	0.89	0.19	72,86,123,134	0
17	CLA	A	820	65/65	0.89	0.20	103,126,143,144	0
19	LUT	2	314	42/42	0.90	0.18	97,114,124,130	0
21	BCR	J	105	40/40	0.90	0.17	73,85,100,101	0
21	BCR	L	205	40/40	0.90	0.22	101,116,137,137	0
17	CLA	A	825	65/65	0.90	0.20	76,98,163,165	0
21	BCR	A	847	40/40	0.90	0.45	87,120,171,173	0
22	LHG	1	317	49/49	0.90	0.21	85,100,127,130	0
17	CLA	3	612	45/65	0.90	0.33	197,212,229,235	0
17	CLA	A	811	54/65	0.90	0.24	107,127,140,140	0
25	HTG	F	305	19/19	0.90	0.20	62,83,100,104	0
17	CLA	2	312	43/65	0.90	0.16	122,142,146,147	0
17	CLA	3	611	55/65	0.90	0.14	143,177,193,195	0
21	BCR	F	303	40/40	0.90	0.23	48,60,65,66	0
18	CHL	2	305	48/66	0.91	0.25	105,129,162,162	0
22	LHG	A	845	27/49	0.91	0.41	128,174,191,196	0
19	LUT	1	314	42/42	0.91	0.15	67,95,116,120	0
17	CLA	A	803	55/65	0.91	0.19	64,82,119,124	0
17	CLA	A	809	65/65	0.91	0.24	100,120,149,151	0
21	BCR	A	848	40/40	0.91	0.56	92,116,163,164	0
17	CLA	J	103	42/65	0.91	0.21	83,101,120,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
17	CLA	1	304	42/65	0.91	0.13	80,107,125,133	0
18	CHL	1	305	48/66	0.91	0.16	102,114,132,134	0
21	BCR	L	201	40/40	0.92	0.27	95,107,120,123	0
17	CLA	4	304	50/65	0.92	0.15	55,78,112,117	0
17	CLA	1	303	51/65	0.92	0.17	112,124,138,143	0
17	CLA	A	837	65/65	0.92	0.24	92,103,174,177	0
17	CLA	A	821	49/65	0.92	0.18	130,142,169,175	0
21	BCR	B	845	40/40	0.92	0.24	62,73,118,122	0
17	CLA	B	816	65/65	0.92	0.19	65,78,97,99	0
17	CLA	A	822	51/65	0.92	0.20	137,148,164,169	0
17	CLA	B	824	55/65	0.92	0.18	63,74,104,112	0
17	CLA	A	812	65/65	0.92	0.29	88,112,121,122	0
18	CHL	3	601	56/66	0.92	0.17	108,134,146,147	0
24	LMG	4	319	50/55	0.92	0.20	68,89,131,132	0
17	CLA	A	804	65/65	0.93	0.20	77,91,115,117	0
17	CLA	2	310	52/65	0.93	0.17	106,113,156,164	0
17	CLA	1	307	65/65	0.93	0.18	74,93,123,129	0
17	CLA	1	312	55/65	0.93	0.17	74,88,119,123	0
17	CLA	1	301	65/65	0.93	0.14	60,72,107,115	0
18	CHL	2	313	43/66	0.93	0.10	99,119,137,139	0
17	CLA	A	801	65/65	0.93	0.23	52,67,83,87	0
17	CLA	2	308	60/65	0.93	0.19	111,122,145,151	0
17	CLA	A	834	45/65	0.93	0.36	156,170,177,185	0
17	CLA	A	835	51/65	0.93	0.19	78,102,129,135	0
17	CLA	A	829	65/65	0.94	0.20	68,82,94,98	0
17	CLA	A	830	50/65	0.94	0.20	102,117,152,156	0
17	CLA	A	831	65/65	0.94	0.25	84,103,108,110	0
21	BCR	I	101	40/40	0.94	0.21	92,99,112,114	0
17	CLA	4	312	56/65	0.94	0.14	70,84,109,112	0
17	CLA	3	606	47/65	0.94	0.15	113,124,135,138	0
17	CLA	A	816	65/65	0.94	0.19	116,134,152,155	0
18	CHL	2	304	43/66	0.94	0.18	101,117,129,137	0
17	CLA	3	608	50/65	0.94	0.17	120,130,136,139	0
18	CHL	2	306	51/66	0.94	0.17	84,101,141,144	0
17	CLA	A	840	65/65	0.94	0.28	52,63,76,90	0
17	CLA	A	819	45/65	0.94	0.19	126,138,151,155	0
22	LHG	B	801	23/49	0.94	0.13	67,88,119,120	0
17	CLA	B	803	65/65	0.94	0.22	106,119,153,161	0
17	CLA	B	804	65/65	0.94	0.23	50,60,68,74	0
17	CLA	B	813	54/65	0.94	0.12	61,90,114,117	0
17	CLA	B	814	55/65	0.94	0.15	61,75,121,123	0
17	CLA	B	815	65/65	0.94	0.17	57,67,75,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
17	CLA	1	310	52/65	0.94	0.15	88,103,145,147	0
17	CLA	1	306	46/65	0.94	0.17	91,101,117,120	0
17	CLA	B	818	55/65	0.94	0.14	63,73,95,102	0
21	BCR	4	318	40/40	0.94	0.16	61,90,99,104	0
17	CLA	B	823	65/65	0.94	0.18	62,75,131,140	0
17	CLA	1	302	65/65	0.94	0.16	70,87,125,128	0
17	CLA	B	842	65/65	0.94	0.16	57,69,84,94	0
17	CLA	3	603	50/65	0.94	0.23	116,128,132,135	0
17	CLA	G	104	50/65	0.94	0.14	76,95,125,133	0
21	BCR	B	844	40/40	0.94	0.19	69,83,97,102	0
17	CLA	G	105	46/65	0.94	0.21	92,122,136,144	0
17	CLA	1	308	60/65	0.94	0.15	89,100,129,133	0
27	PQN	B	843	33/33	0.94	0.26	65,84,91,97	0
17	CLA	1	311	60/65	0.95	0.14	64,75,111,113	0
17	CLA	B	807	65/65	0.95	0.17	57,69,79,82	0
17	CLA	B	812	65/65	0.95	0.20	76,107,137,144	0
17	CLA	A	805	65/65	0.95	0.25	69,82,91,93	0
17	CLA	A	806	65/65	0.95	0.17	72,81,131,134	0
17	CLA	2	307	50/65	0.95	0.16	90,95,110,113	0
17	CLA	A	826	65/65	0.95	0.20	90,119,149,154	0
18	CHL	4	301	61/66	0.95	0.13	66,78,116,118	0
17	CLA	A	828	65/65	0.95	0.29	73,89,106,107	0
17	CLA	A	810	65/65	0.95	0.19	80,88,102,113	0
17	CLA	B	820	60/65	0.95	0.29	46,66,85,87	0
19	LUT	4	316	42/42	0.95	0.14	63,72,86,91	0
20	XAT	1	315	44/44	0.95	0.15	62,89,98,100	0
17	CLA	1	309	65/65	0.95	0.23	84,105,142,147	0
17	CLA	3	605	42/65	0.95	0.13	125,135,143,147	0
17	CLA	B	826	65/65	0.95	0.21	50,67,87,92	0
17	CLA	B	831	65/65	0.95	0.19	48,63,105,107	0
17	CLA	B	838	65/65	0.95	0.16	43,58,72,81	0
17	CLA	B	839	47/65	0.95	0.17	52,58,84,93	0
17	CLA	A	832	65/65	0.95	0.19	89,101,142,149	0
17	CLA	4	309	60/65	0.95	0.13	61,72,98,100	0
17	CLA	4	310	60/65	0.95	0.19	68,89,116,121	0
25	HTG	A	854	19/19	0.95	0.10	63,78,85,96	0
17	CLA	4	311	52/65	0.95	0.14	72,83,118,119	0
17	CLA	J	101	65/65	0.95	0.17	62,76,93,101	0
17	CLA	2	309	41/65	0.95	0.15	126,134,143,146	0
17	CLA	A	839	65/65	0.95	0.19	47,59,97,101	0
25	HTG	J	102	19/19	0.95	0.24	75,82,115,120	0
17	CLA	4	313	45/65	0.95	0.14	73,98,120,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
17	CLA	2	301	65/65	0.95	0.15	86,105,122,135	0
27	PQN	A	842	33/33	0.95	0.30	49,61,85,91	0
17	CLA	2	302	51/65	0.95	0.12	89,102,120,127	0
17	CLA	4	308	50/65	0.96	0.15	52,64,103,109	0
21	BCR	B	848	40/40	0.96	0.20	48,58,74,79	0
21	BCR	B	849	40/40	0.96	0.21	60,75,82,83	0
17	CLA	2	319	46/65	0.96	0.15	68,80,109,111	0
21	BCR	F	308	40/40	0.96	0.15	53,62,72,78	0
17	CLA	A	827	65/65	0.96	0.26	64,76,89,94	0
17	CLA	B	822	50/65	0.96	0.17	70,80,109,113	0
21	BCR	J	104	40/40	0.96	0.17	63,73,87,91	0
17	CLA	A	841	65/65	0.96	0.23	82,100,138,149	0
17	CLA	2	311	65/65	0.96	0.16	109,127,142,147	0
17	CLA	B	825	60/65	0.96	0.19	51,60,107,115	0
17	CLA	A	853	65/65	0.96	0.31	48,61,88,96	0
18	CHL	3	607	47/66	0.96	0.17	124,135,160,166	0
17	CLA	B	829	65/65	0.96	0.22	54,65,124,133	0
18	CHL	4	305	56/66	0.96	0.15	68,77,116,118	0
22	LHG	A	844	49/49	0.96	0.27	69,83,92,96	0
18	CHL	4	306	51/66	0.96	0.16	66,79,130,133	0
18	CHL	4	315	43/66	0.96	0.12	67,88,102,117	0
17	CLA	3	613	46/65	0.96	0.13	106,121,156,159	0
17	CLA	B	832	50/65	0.96	0.13	53,62,96,105	0
17	CLA	B	833	60/65	0.96	0.13	44,58,104,110	0
17	CLA	B	834	58/65	0.96	0.13	46,59,102,105	0
17	CLA	B	835	65/65	0.96	0.19	53,67,106,116	0
17	CLA	B	836	45/65	0.96	0.12	62,71,94,97	0
17	CLA	4	302	60/65	0.96	0.12	50,62,94,97	0
20	XAT	4	317	44/44	0.96	0.15	58,67,81,88	0
17	CLA	B	805	65/65	0.96	0.27	62,78,101,112	0
17	CLA	B	806	45/65	0.96	0.13	62,71,90,114	0
17	CLA	F	304	65/65	0.96	0.17	44,58,76,84	0
17	CLA	F	307	55/65	0.96	0.13	49,67,123,125	0
17	CLA	4	303	60/65	0.96	0.16	52,67,108,113	0
17	CLA	B	809	65/65	0.96	0.17	71,88,138,144	0
17	CLA	B	811	65/65	0.96	0.21	70,83,118,125	0
17	CLA	4	314	47/65	0.96	0.14	57,70,104,106	0
17	CLA	1	313	46/65	0.96	0.13	73,84,105,117	0
21	BCR	A	851	40/40	0.96	0.27	45,63,77,79	0
17	CLA	A	823	55/65	0.96	0.14	105,121,137,143	0
17	CLA	A	802	65/65	0.96	0.19	59,73,82,90	0
17	CLA	A	836	65/65	0.96	0.14	86,106,146,154	0

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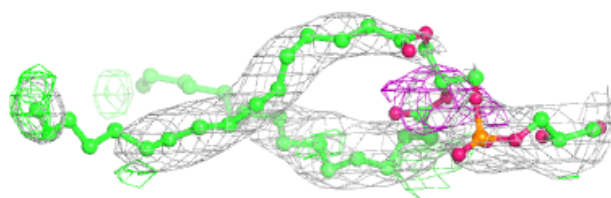
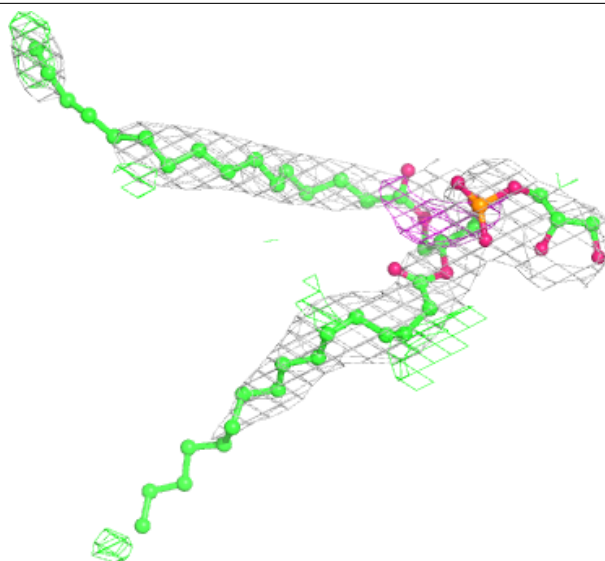
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
17	CLA	B	830	65/65	0.97	0.27	48,68,83,97	0
17	CLA	B	821	65/65	0.97	0.24	56,67,98,103	0
17	CLA	B	810	65/65	0.97	0.23	63,73,95,101	0
17	CLA	A	838	65/65	0.97	0.21	45,55,71,78	0
17	CLA	A	818	65/65	0.97	0.27	91,103,125,130	0
17	CLA	B	808	65/65	0.97	0.19	49,70,88,92	0
17	CLA	B	819	59/65	0.97	0.22	55,66,81,85	0
17	CLA	B	837	60/65	0.97	0.19	46,57,105,106	0
17	CLA	B	827	65/65	0.97	0.23	43,58,106,109	0
17	CLA	B	802	65/65	0.97	0.30	48,60,81,93	0
17	CLA	B	840	65/65	0.97	0.18	70,91,118,124	0
17	CLA	B	841	65/65	0.97	0.20	57,72,127,136	0
17	CLA	B	828	65/65	0.98	0.23	45,58,72,78	0
17	CLA	F	306	45/65	0.98	0.11	55,66,75,85	0
17	CLA	A	808	65/65	0.98	0.15	54,69,114,118	0
18	CHL	4	307	51/66	0.98	0.11	60,73,90,101	0
17	CLA	A	807	65/65	0.98	0.19	59,73,104,120	0
28	SF4	A	852	8/8	0.99	0.21	55,67,73,74	0
28	SF4	C	101	8/8	0.99	0.19	69,76,84,85	0
28	SF4	C	102	8/8	0.99	0.14	75,76,85,89	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.

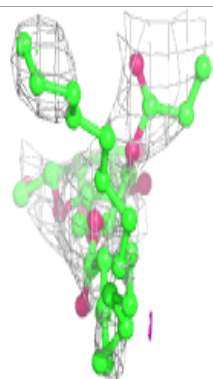
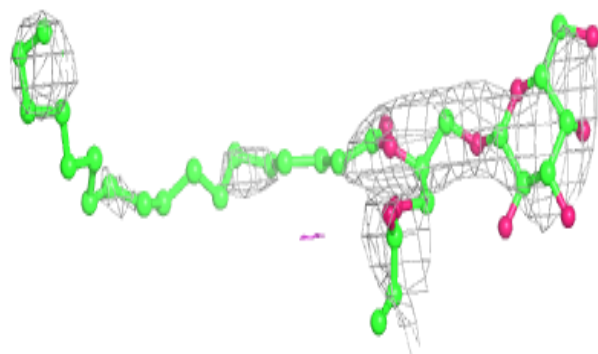
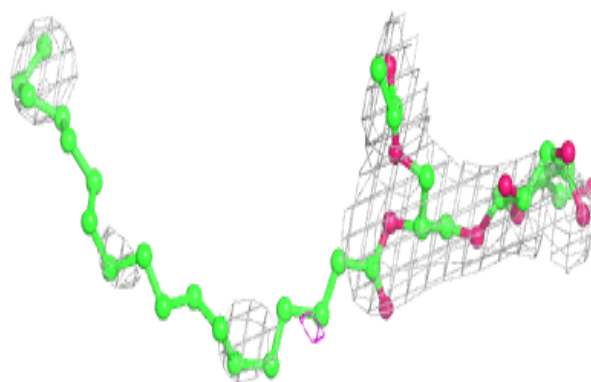
Electron density around LHG G 102:

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

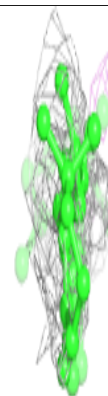
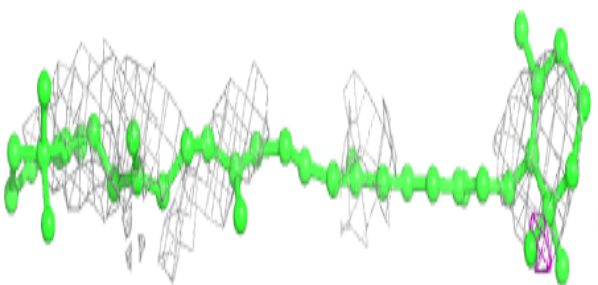
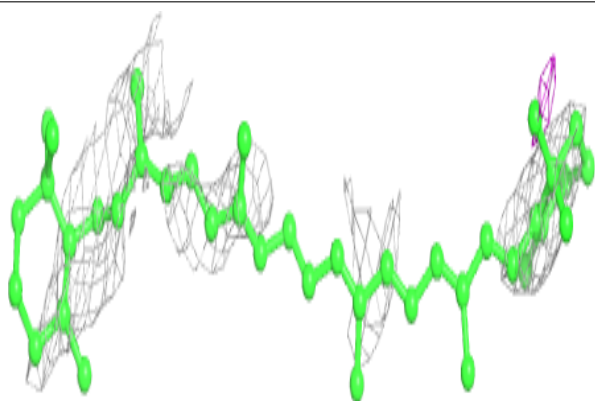


Electron density around LMG G 101:

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

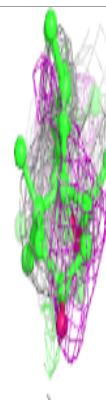
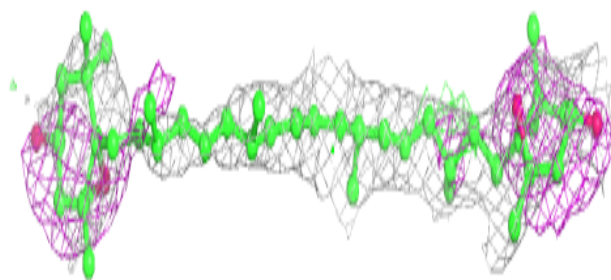
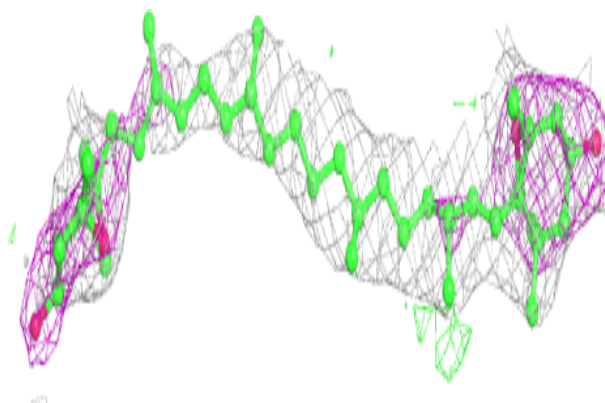
**Electron density around BCR K 203:**

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

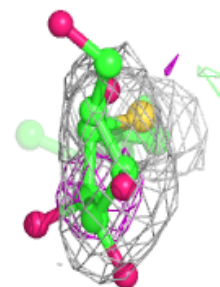
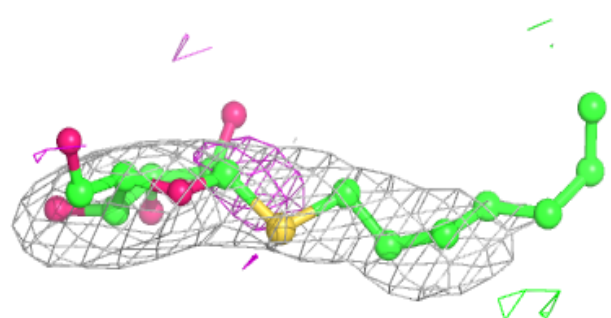
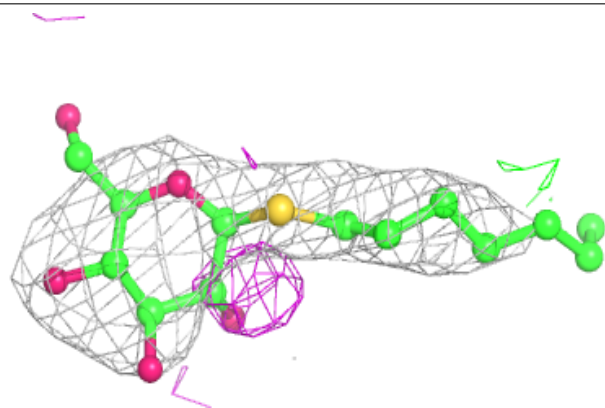


Electron density around XAT 3 615:

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

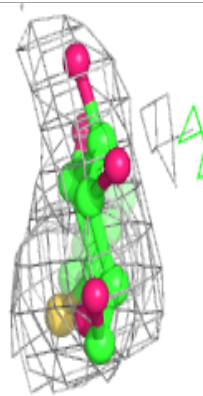
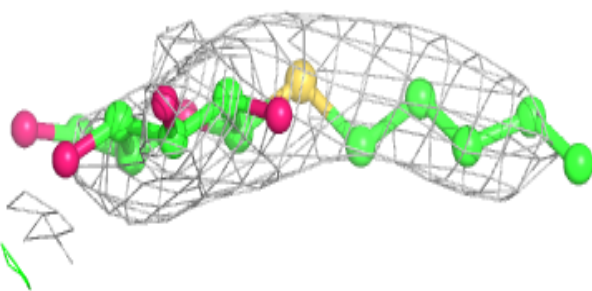
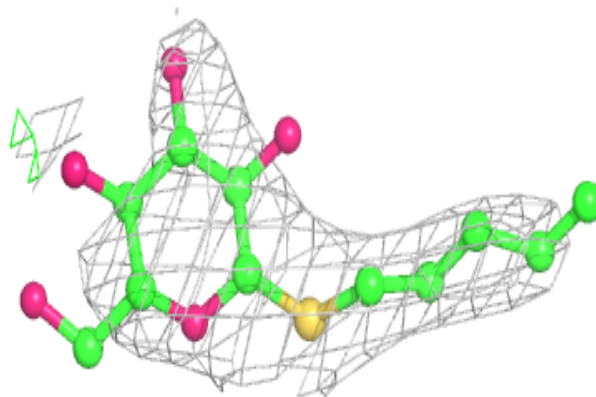
**Electron density around HTG B 851:**

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



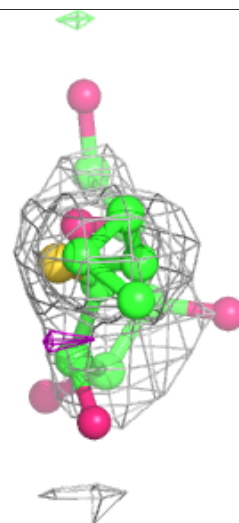
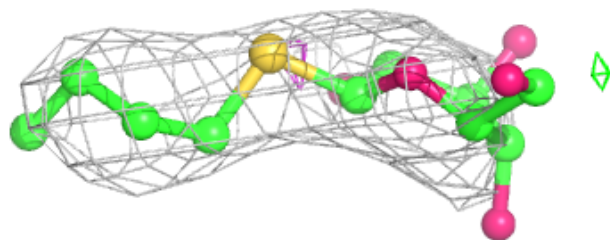
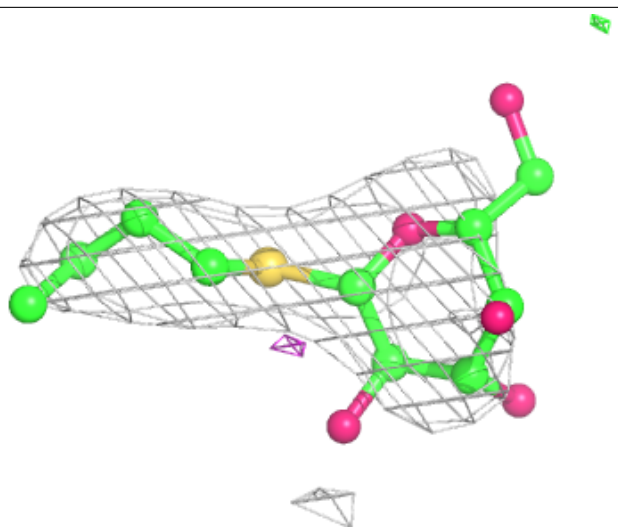
Electron density around HTG F 301:

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



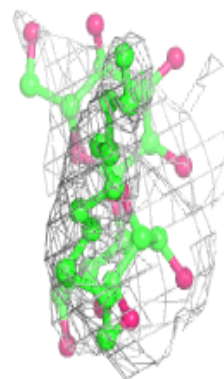
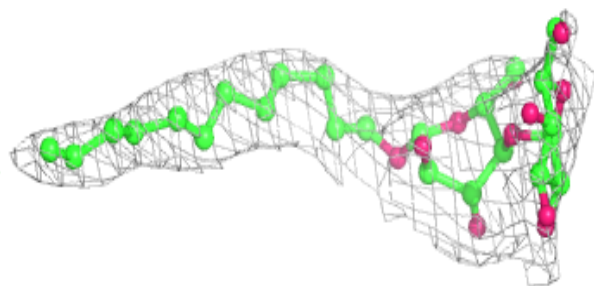
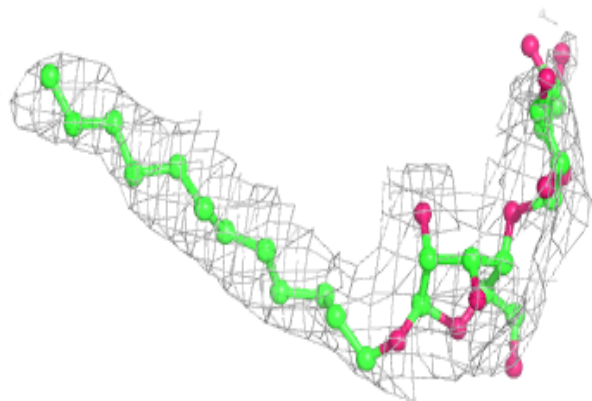
Electron density around HTG F 310:

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

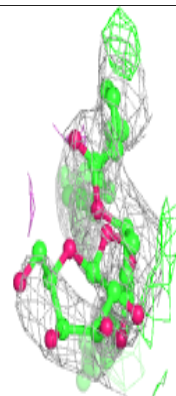
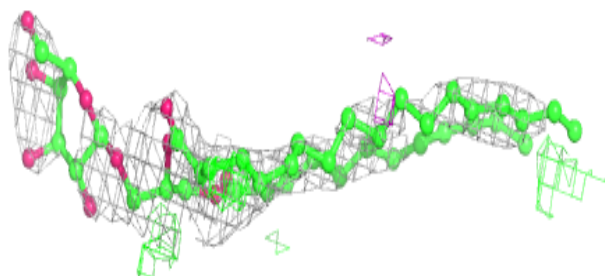
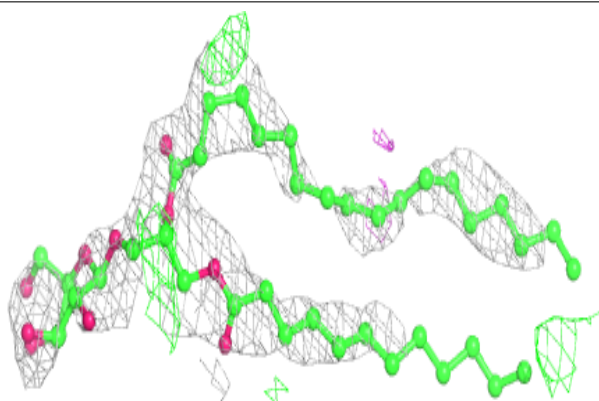


Electron density around LMT A 855:

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

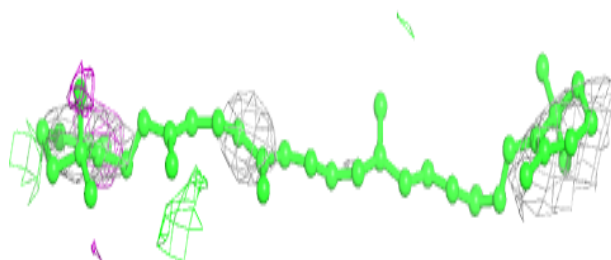
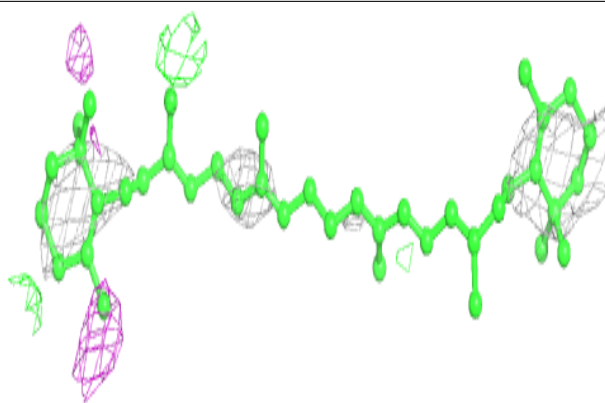
**Electron density around LMG 4 320:**

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

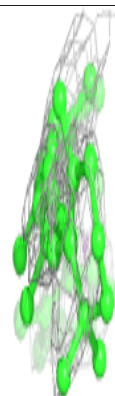
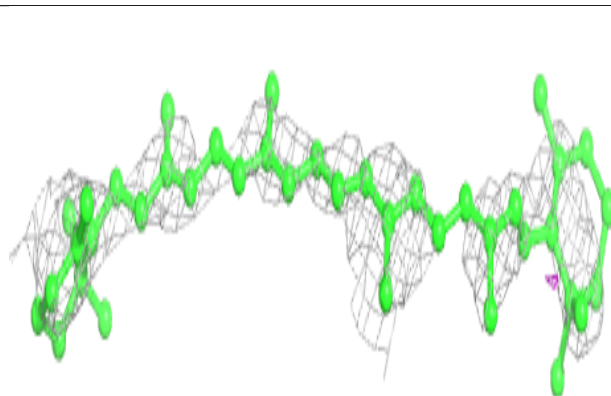
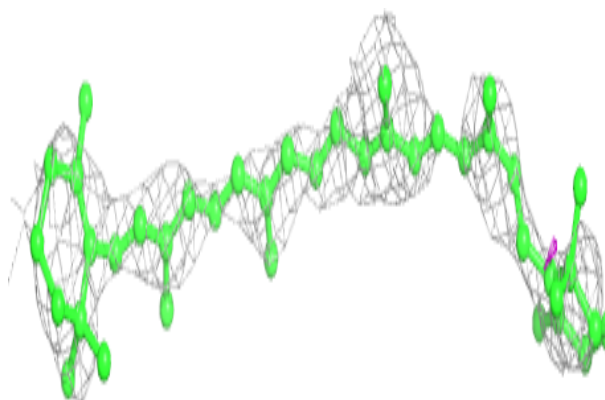


Electron density around BCR 2 316:

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

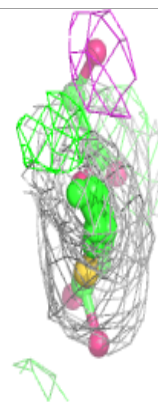
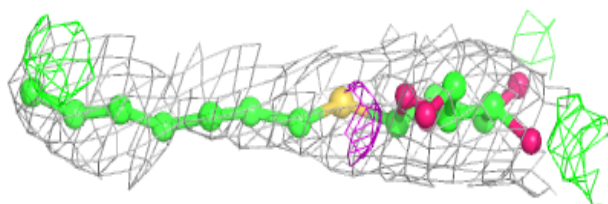
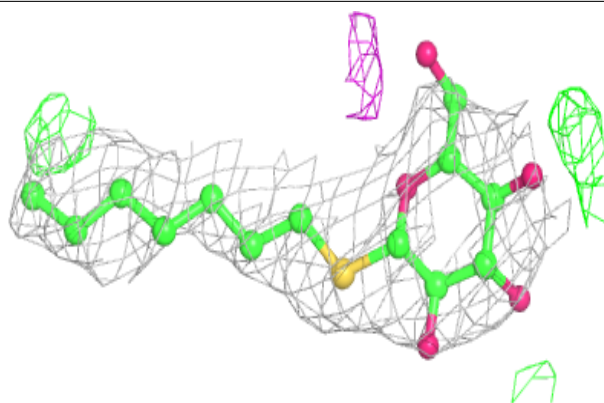
**Electron density around BCR A 846:**

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

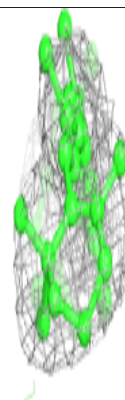
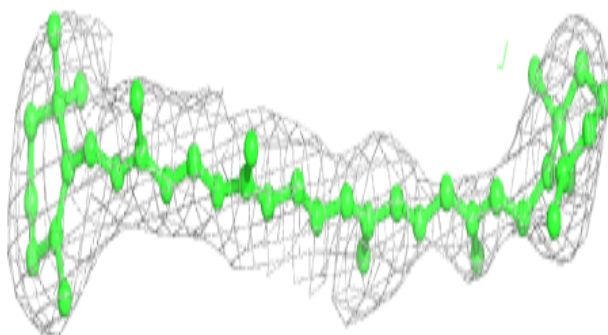
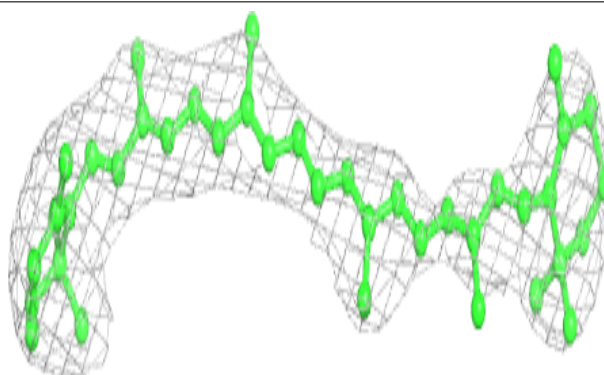


Electron density around HTG 4 322:

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

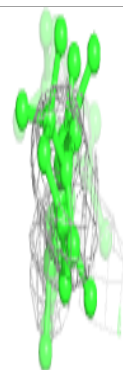
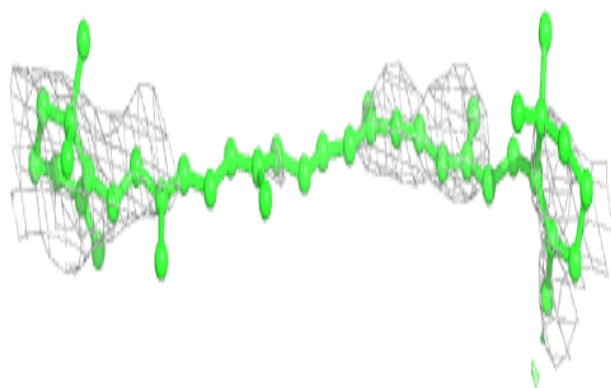
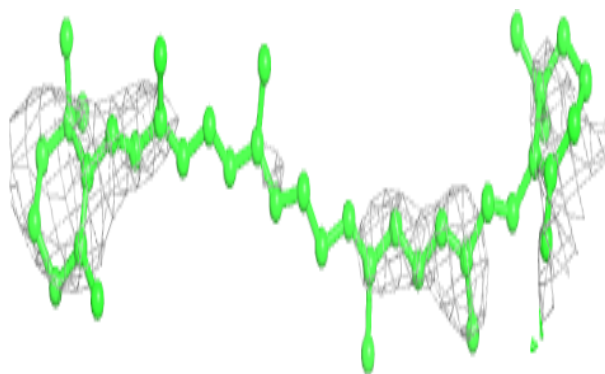
**Electron density around BCR G 106:**

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

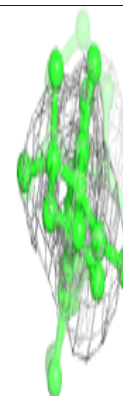
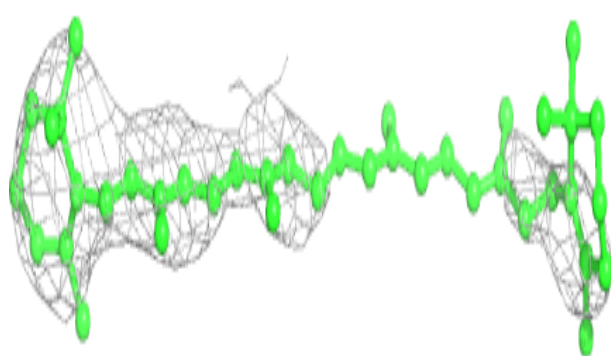
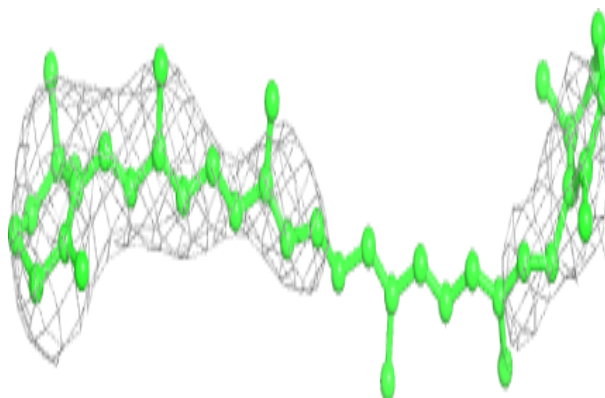


Electron density around BCR 3 616:

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

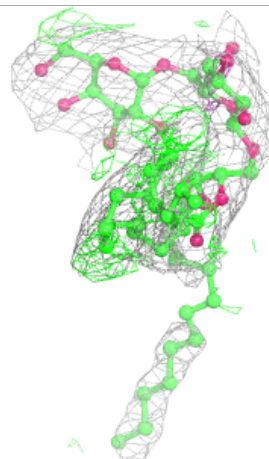
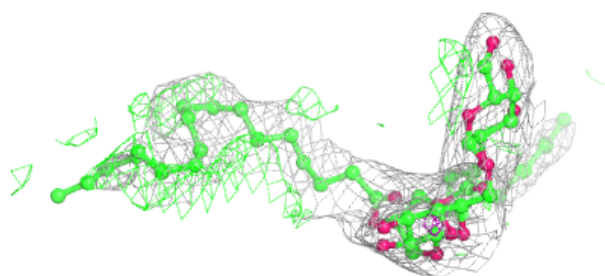
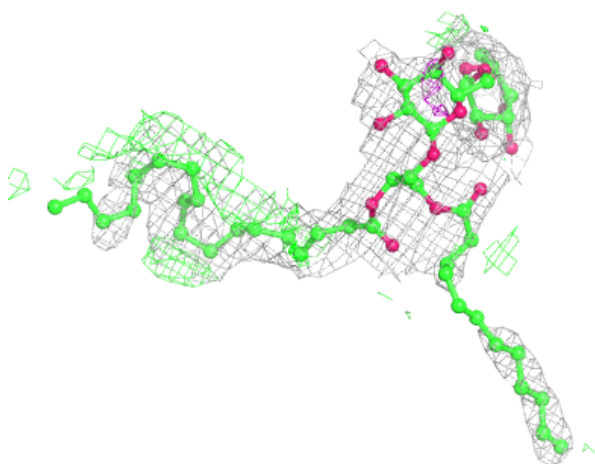
**Electron density around BCR A 849:**

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



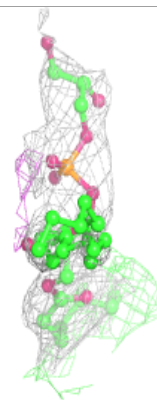
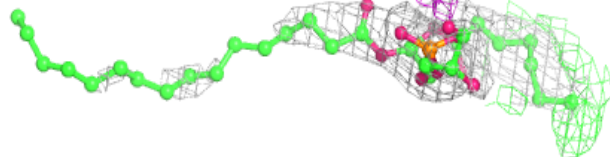
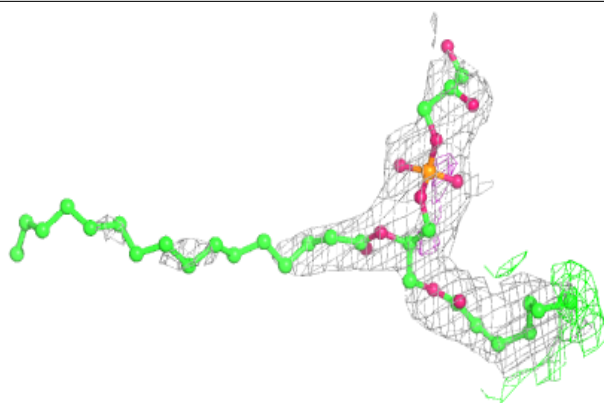
Electron density around DGD 4 323:

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



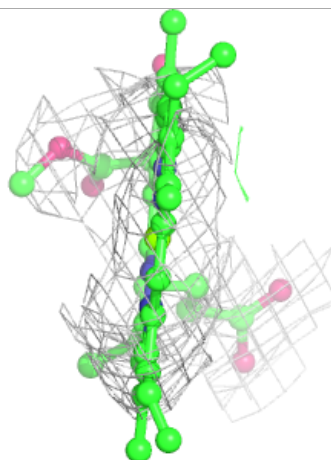
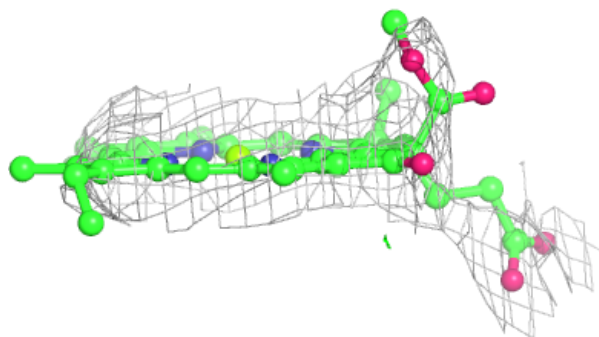
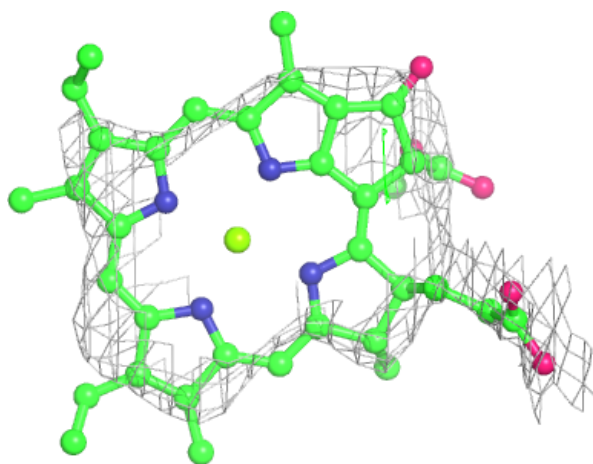
Electron density around LHG F 302:

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



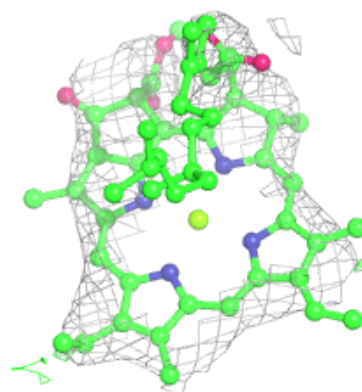
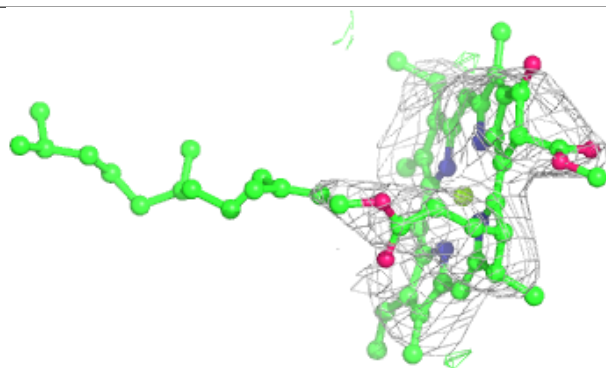
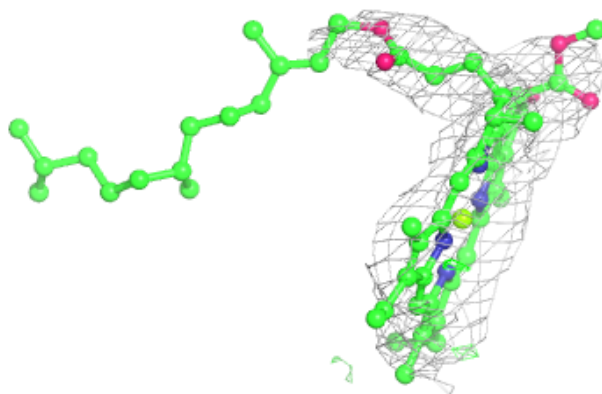
Electron density around CLA K 201:

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

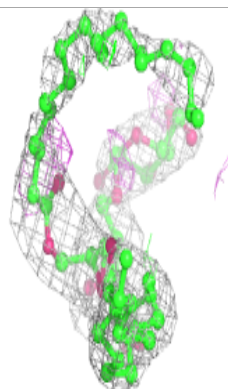
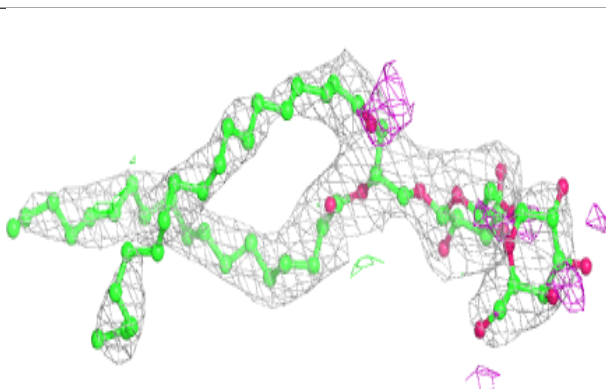
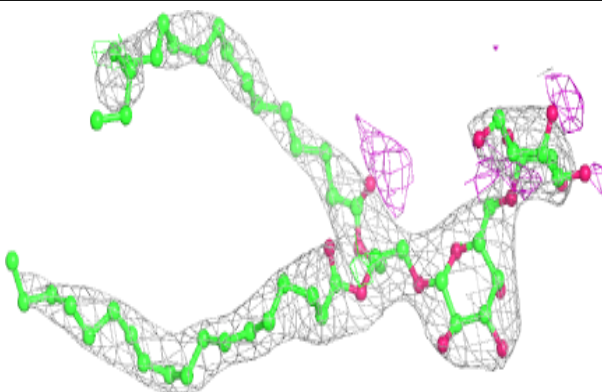


Electron density around CLA 2 303:

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

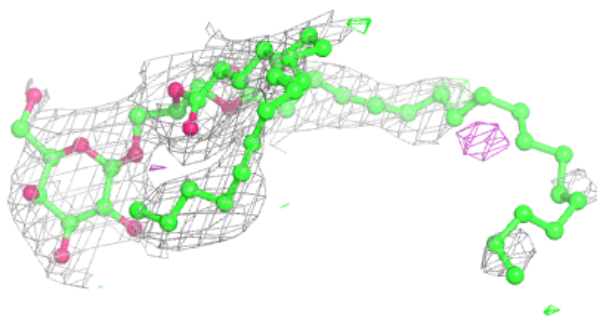
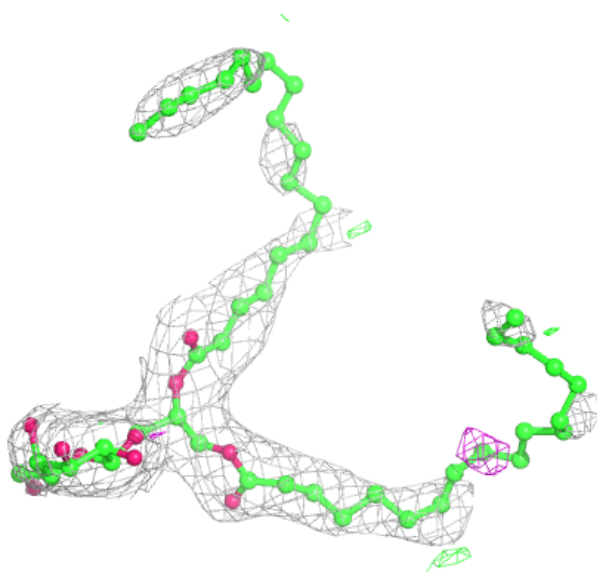
**Electron density around DGD B 850:**

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



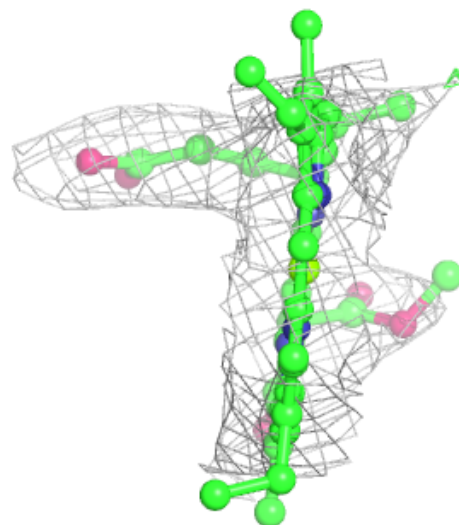
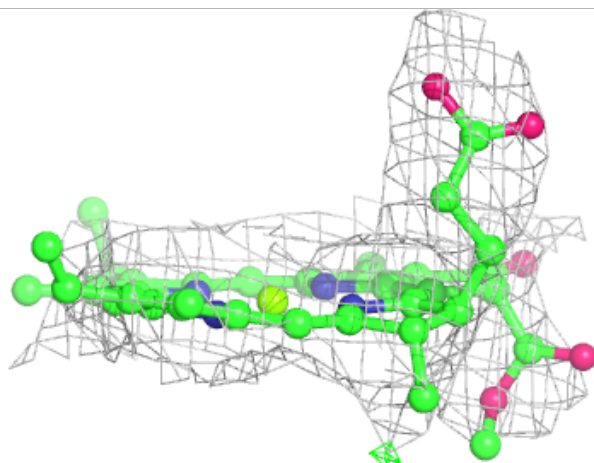
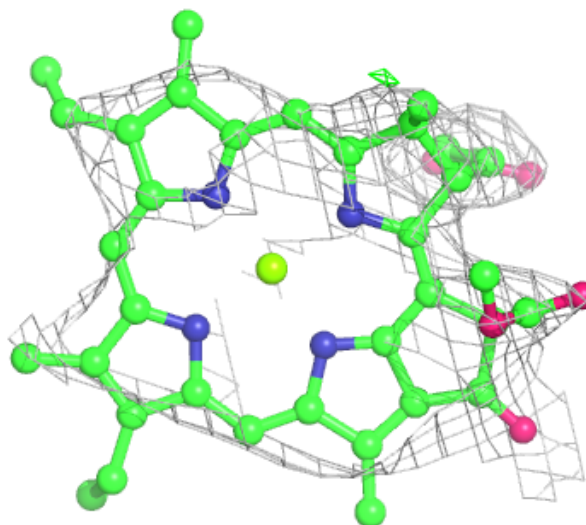
Electron density around LMG F 309:

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



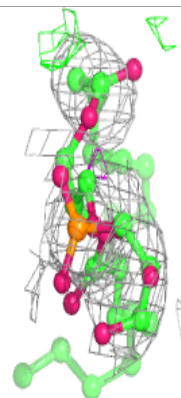
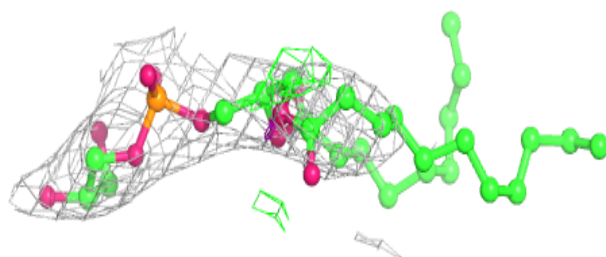
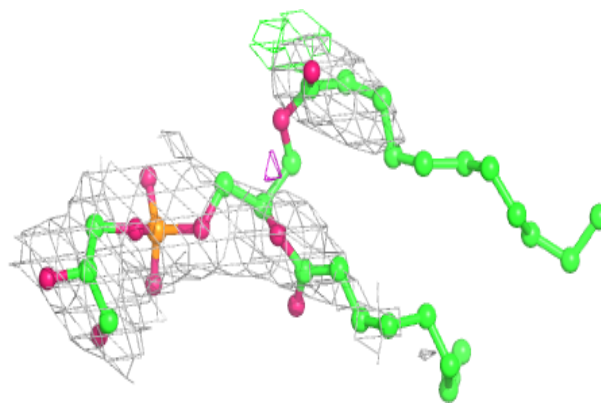
Electron density around CLA 3 604:

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

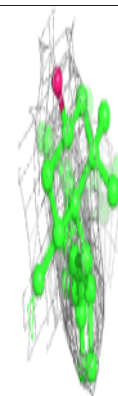
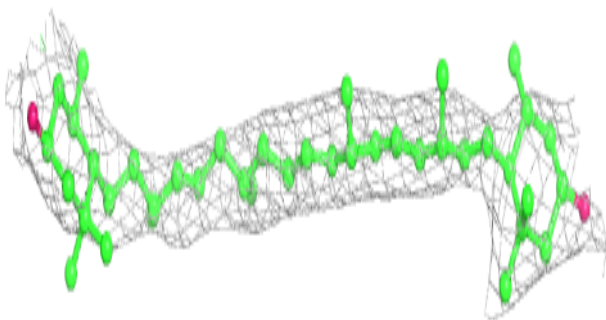
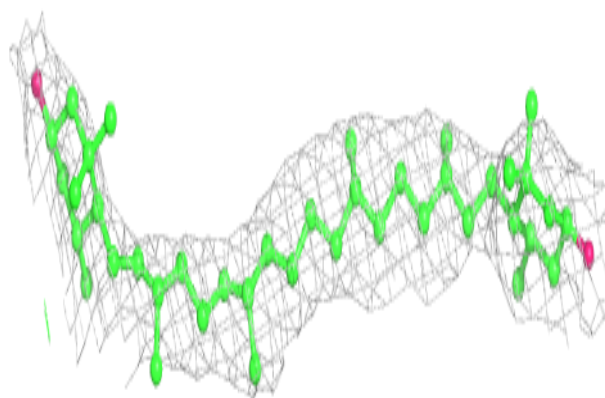


Electron density around LHG 2 317:

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

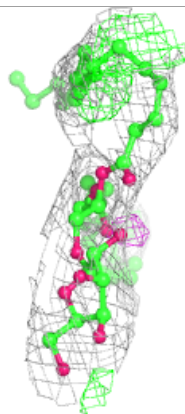
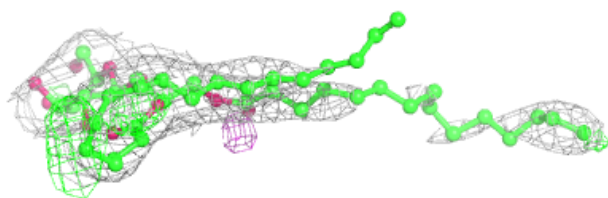
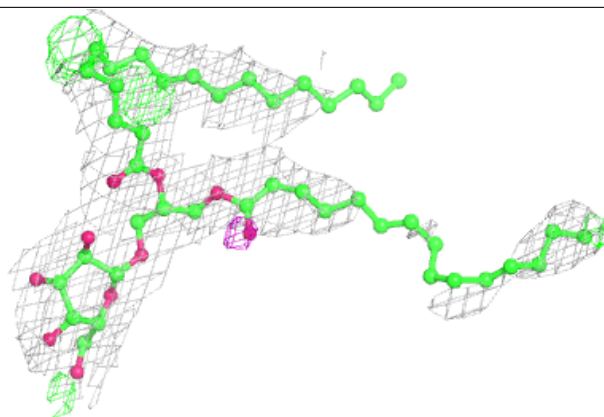
**Electron density around LUT 3 614:**

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



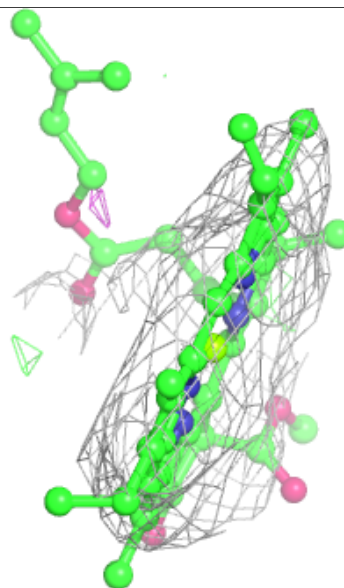
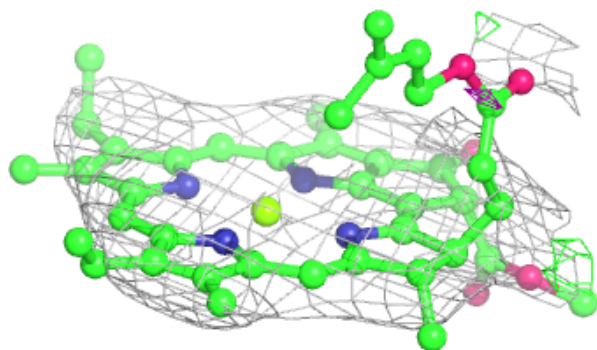
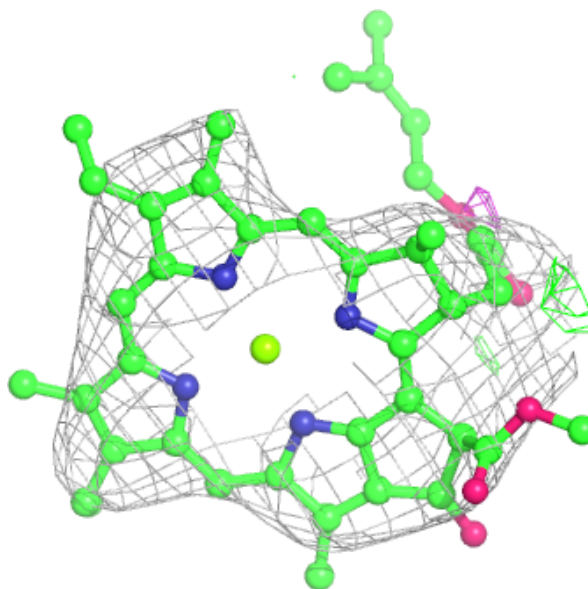
Electron density around LMG B 852:

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



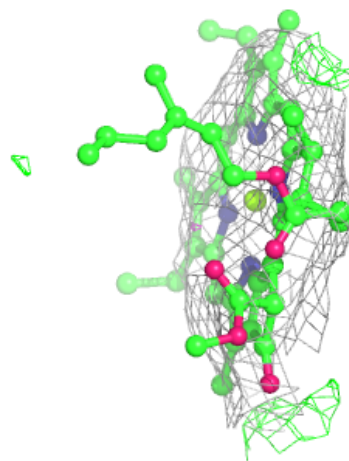
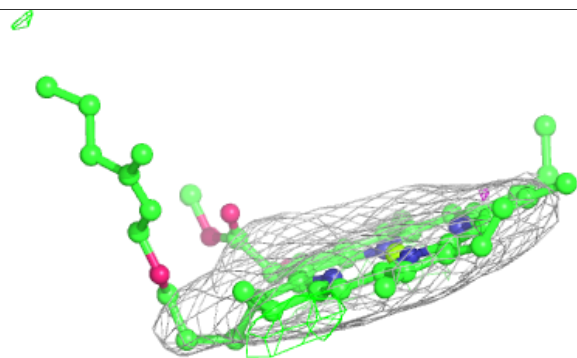
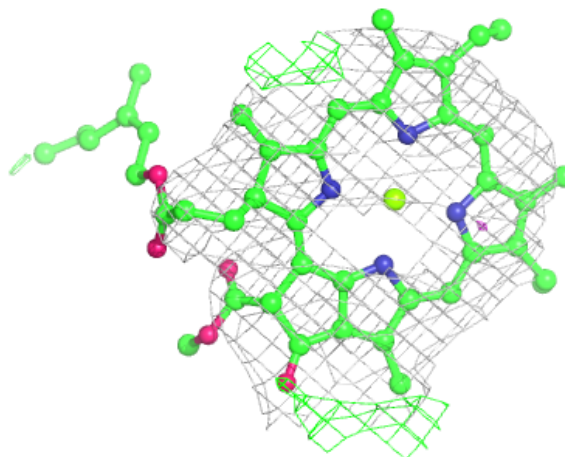
Electron density around CLA A 814:

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



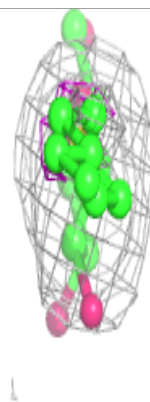
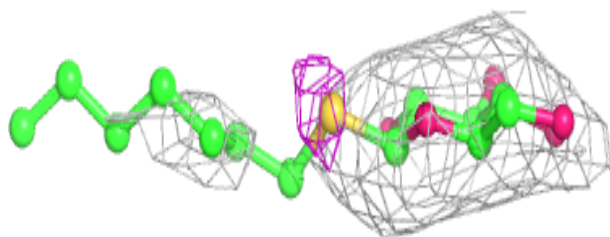
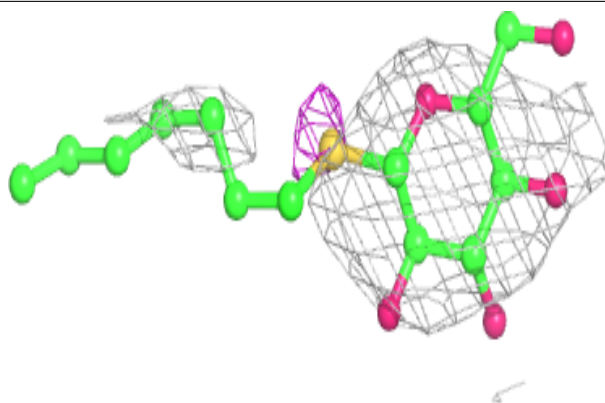
Electron density around CLA 3 610:

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



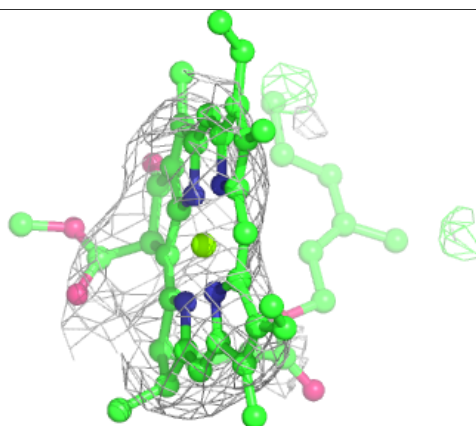
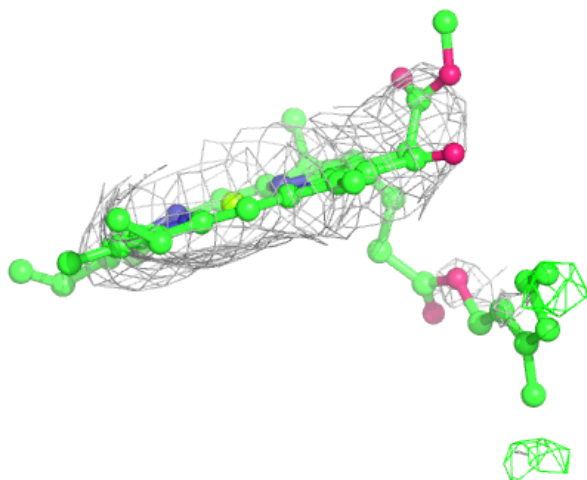
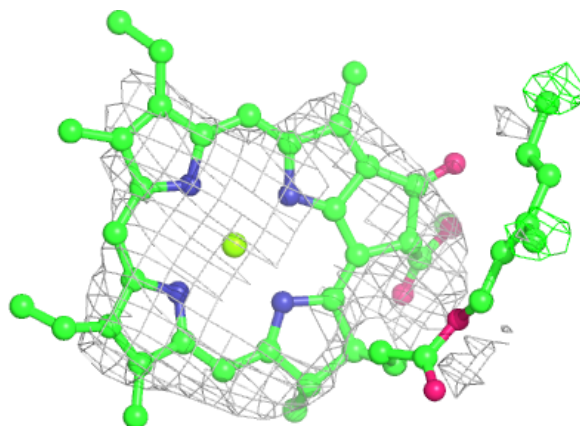
Electron density around HTG 4 321:

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



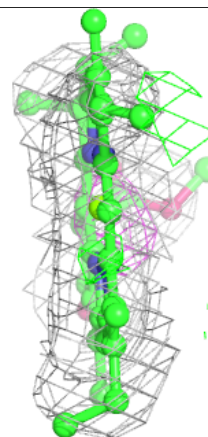
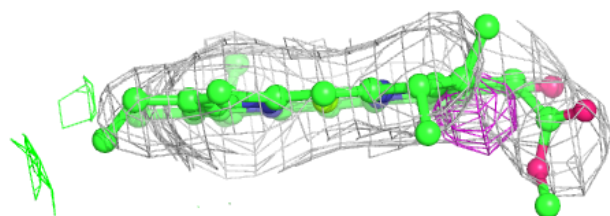
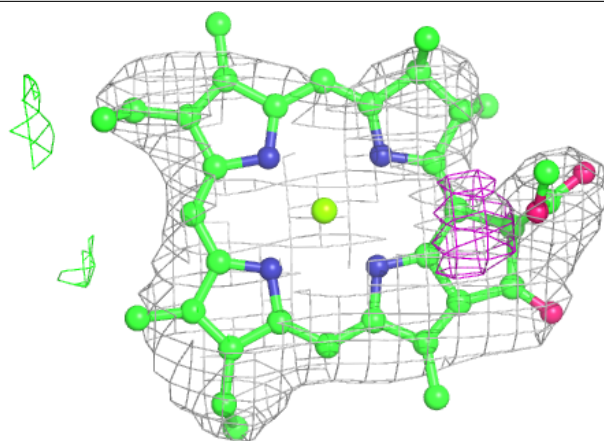
Electron density around CLA A 843:

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

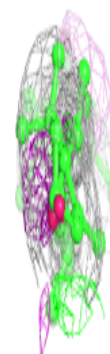
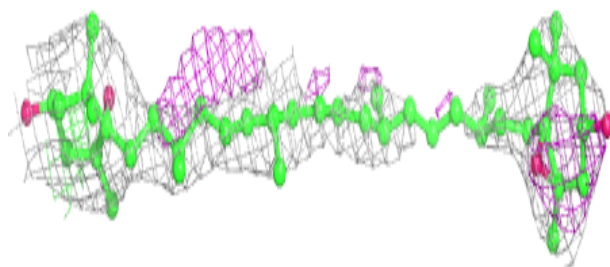
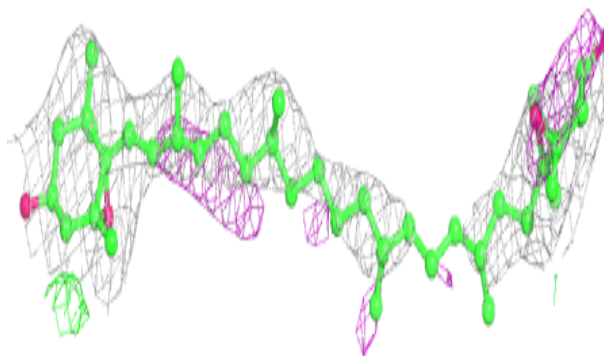


Electron density around CLA G 103:

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

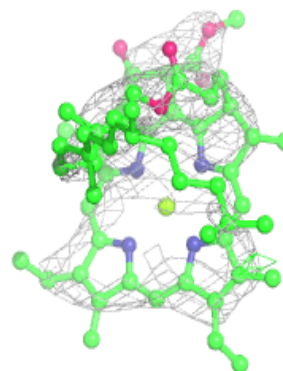
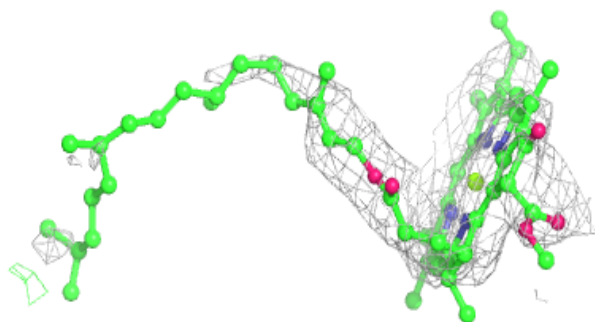
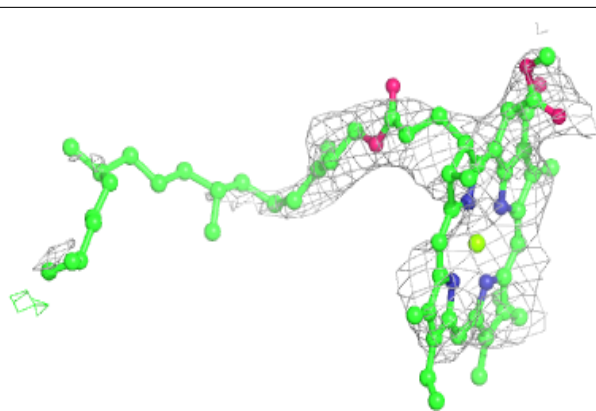
**Electron density around XAT 2 315:**

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

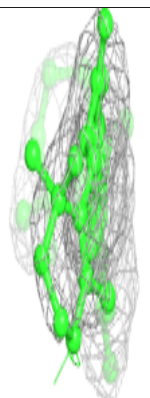
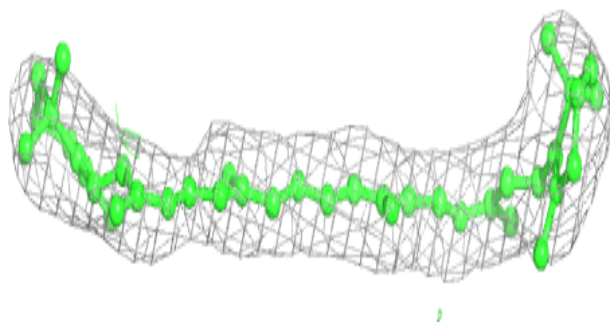
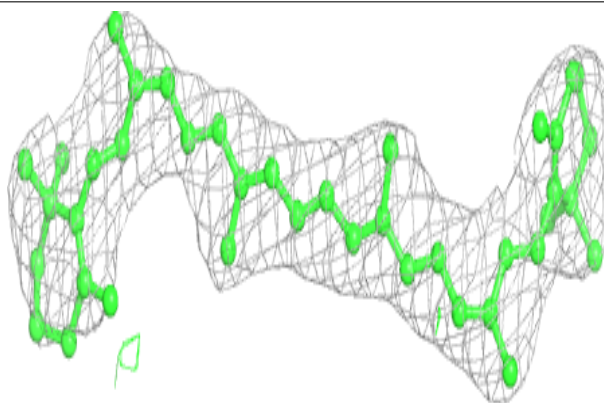


Electron density around CLA L 203:

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

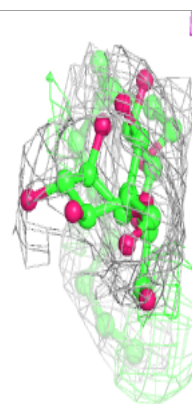
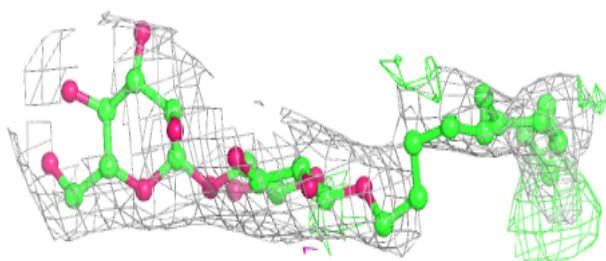
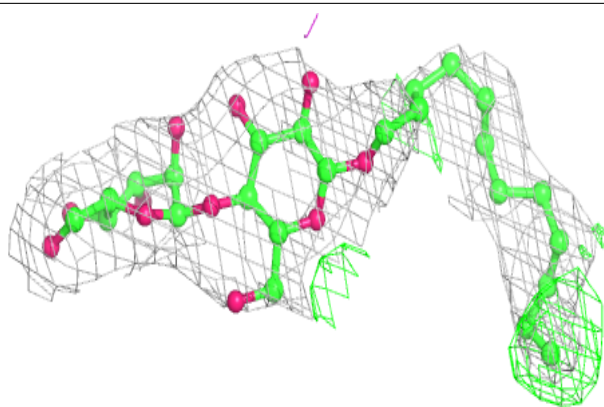
**Electron density around BCR B 846:**

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

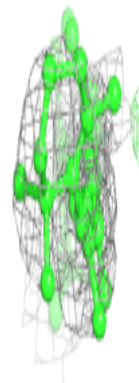
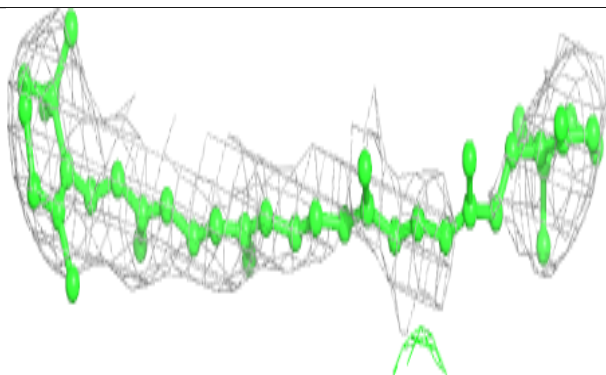
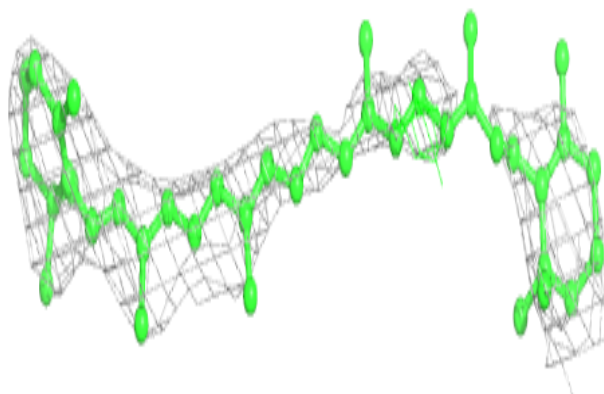


Electron density around LMT 2 318:

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

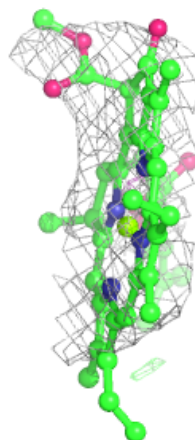
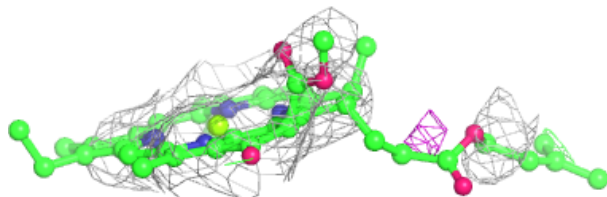
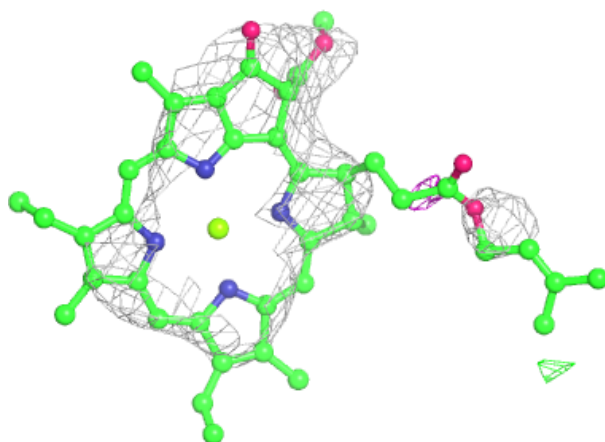
**Electron density around BCR A 850:**

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



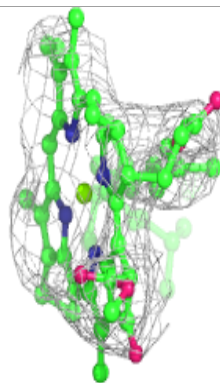
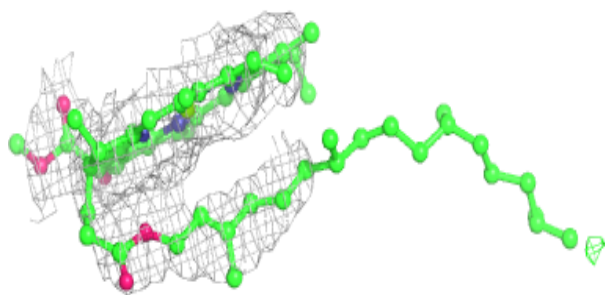
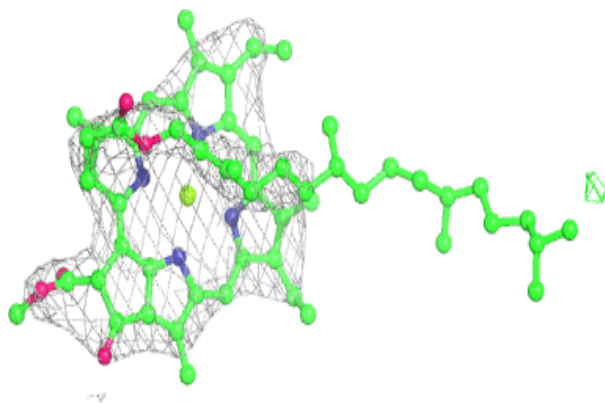
Electron density around CLA L 204:

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



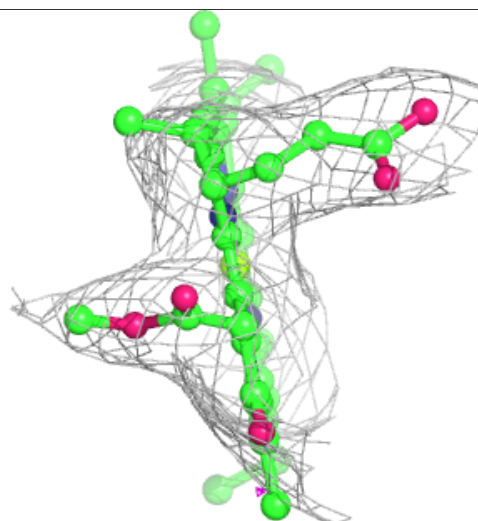
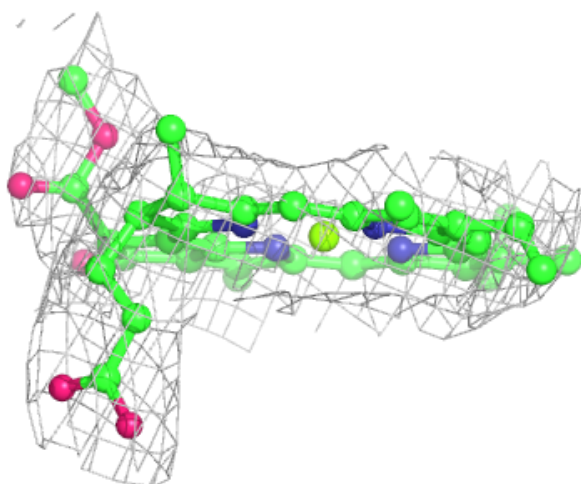
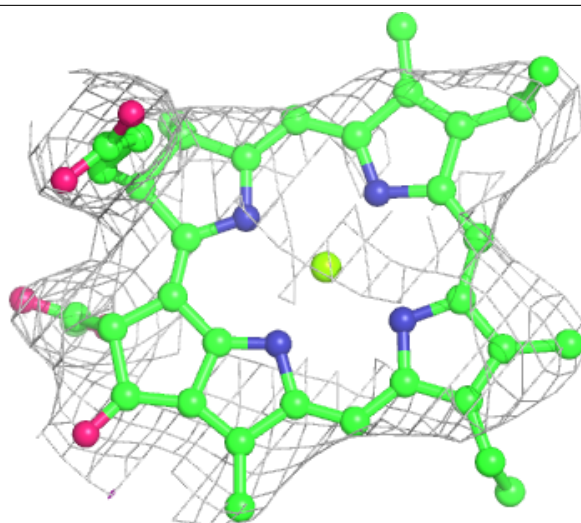
Electron density around CLA A 817:

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



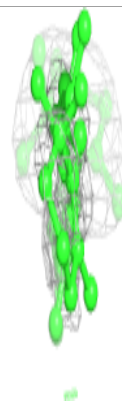
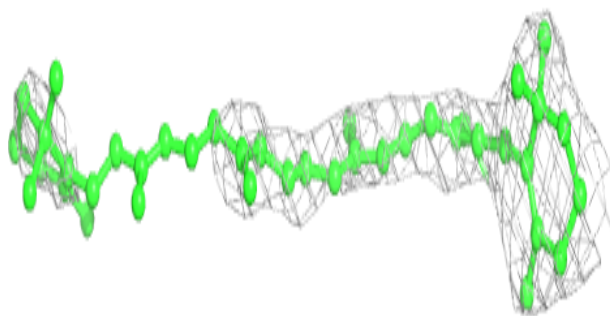
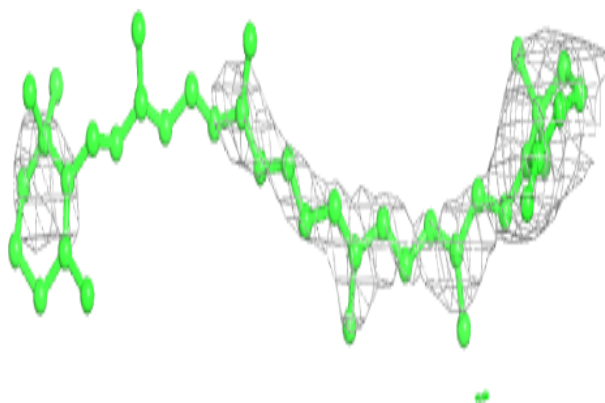
Electron density around CLA A 813:

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

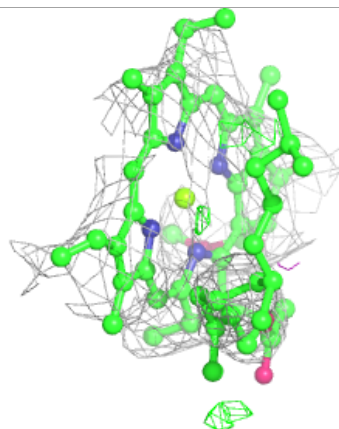
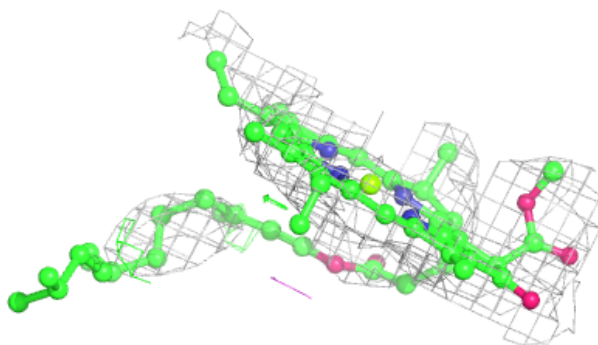
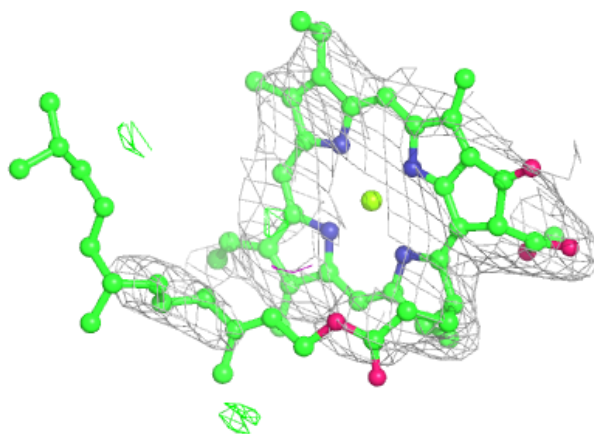


Electron density around BCR 1 316:

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

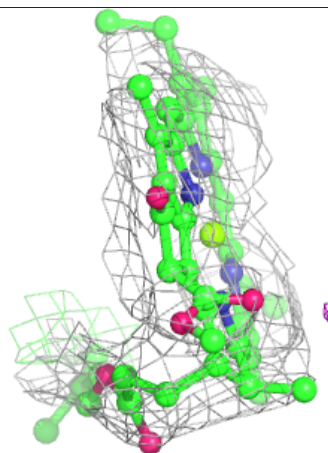
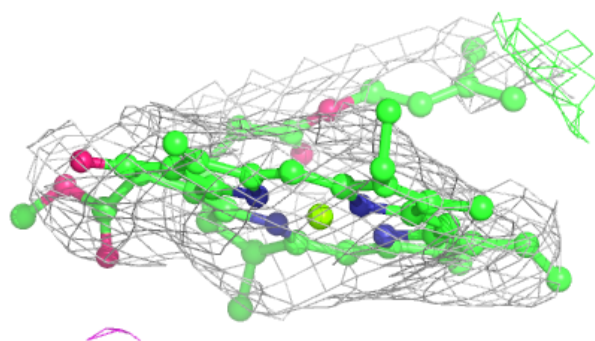
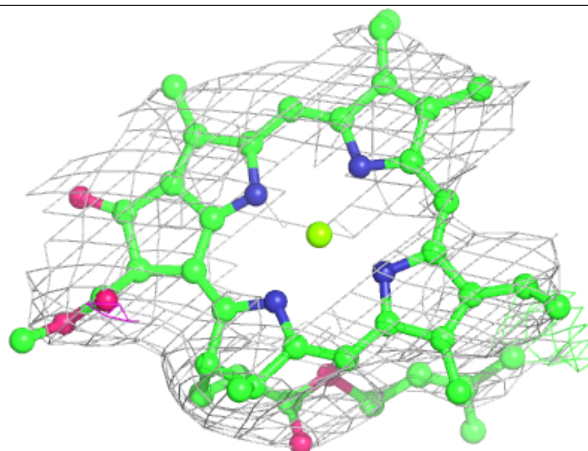
**Electron density around CLA 3 602:**

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



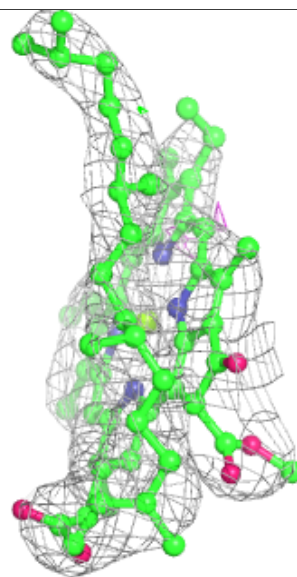
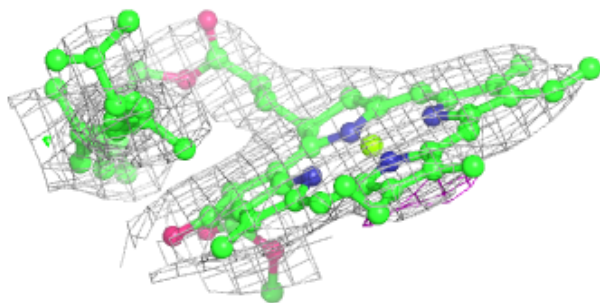
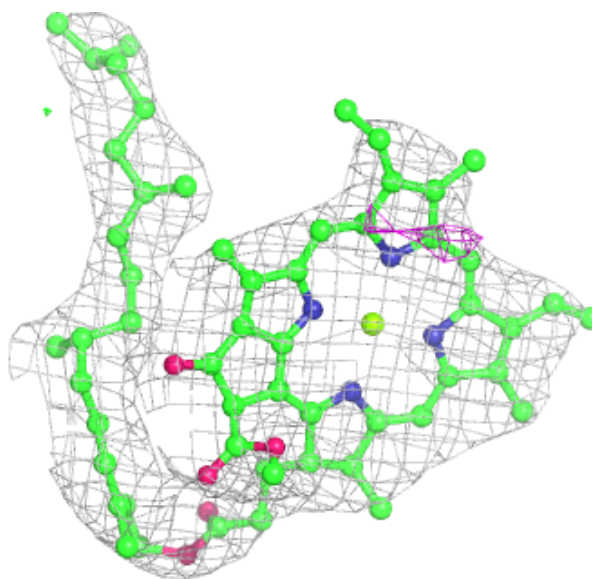
Electron density around CLA 3 609:

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



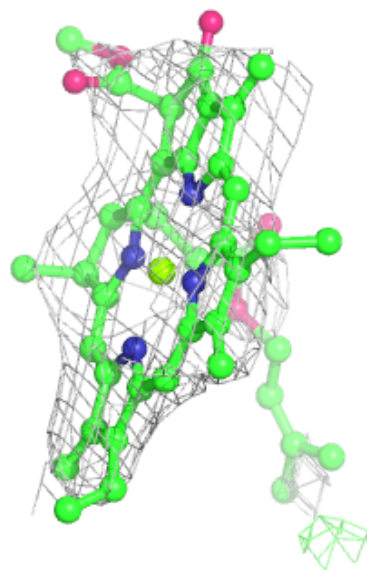
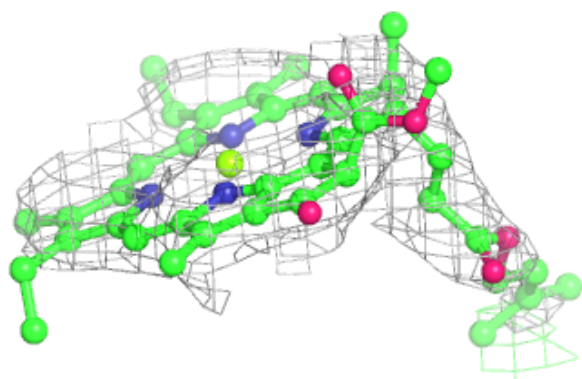
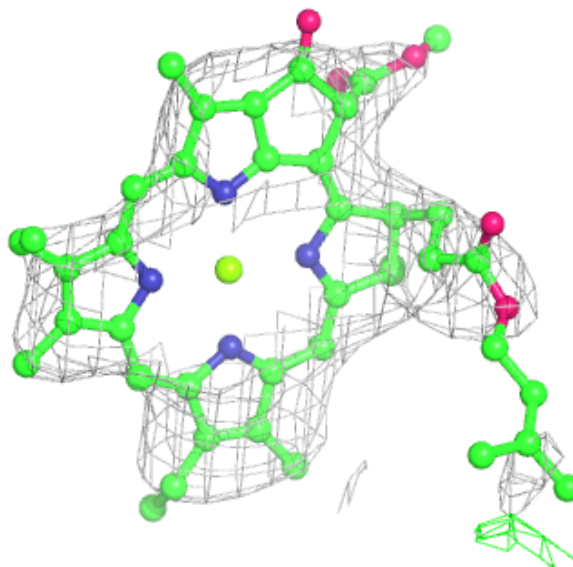
Electron density around CLA A 824:

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



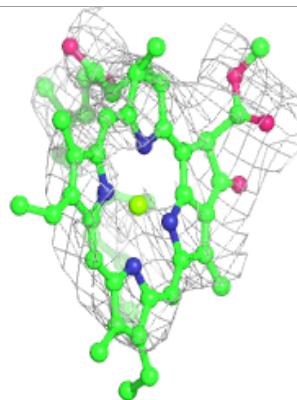
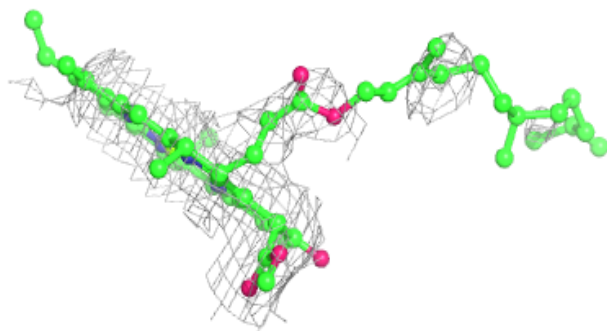
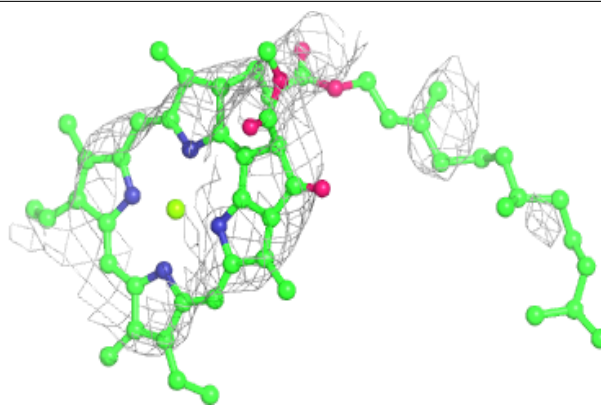
Electron density around CLA A 833:

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

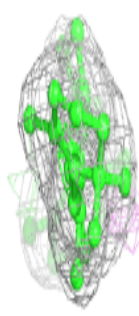
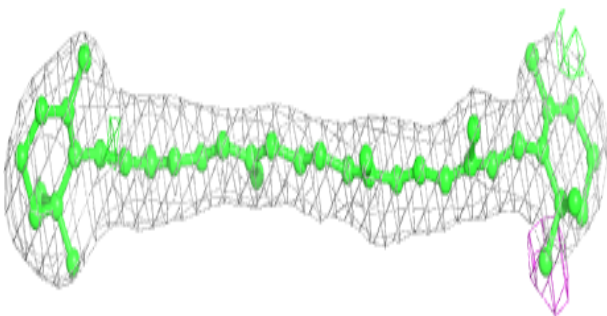
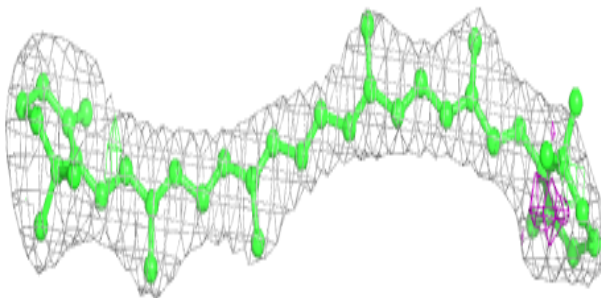


Electron density around CLA K 202:

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

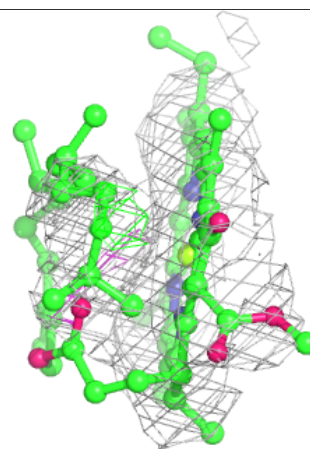
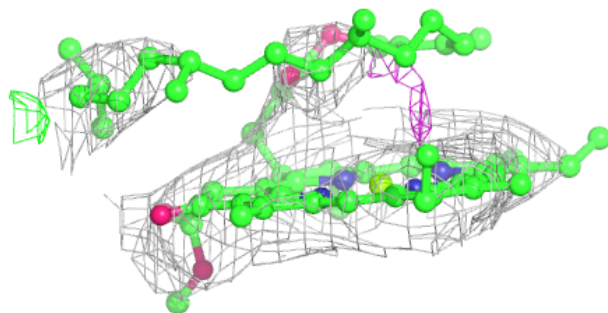
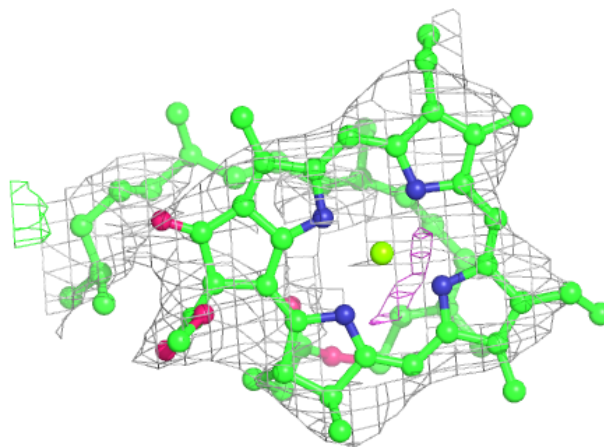
**Electron density around BCR B 847:**

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



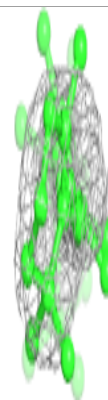
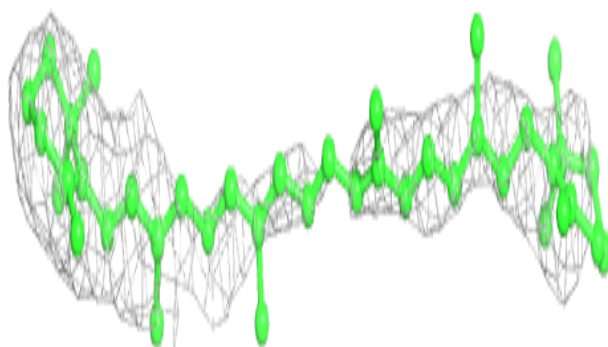
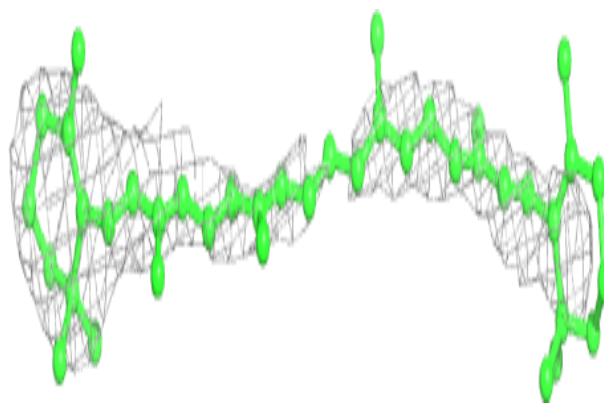
Electron density around CLA L 202:

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

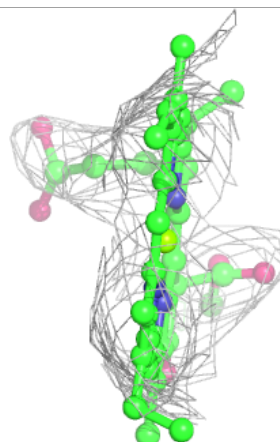
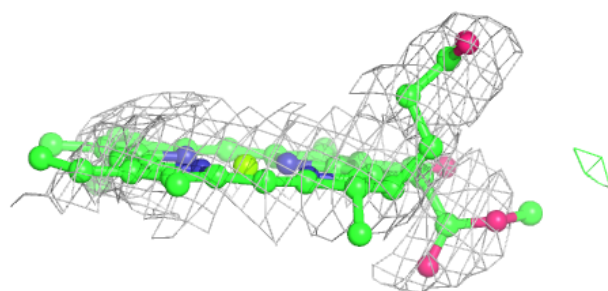
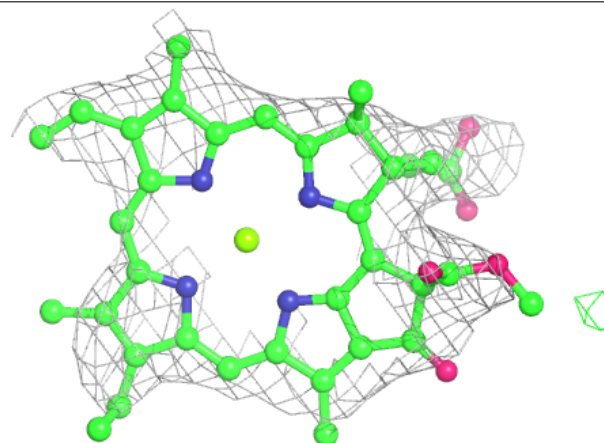


Electron density around BCR L 206:

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

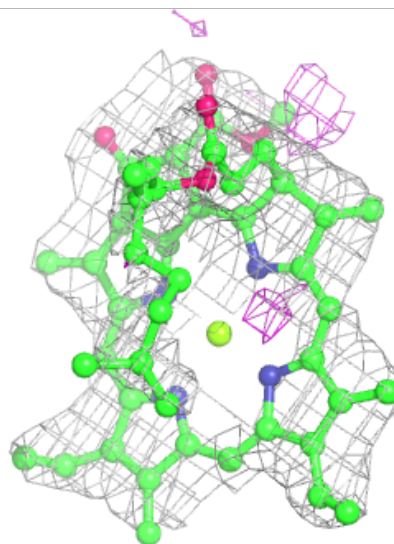
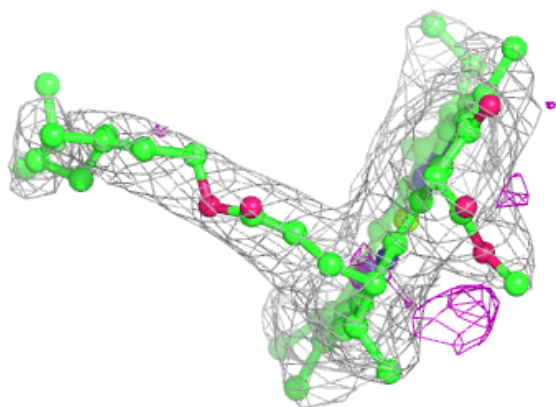
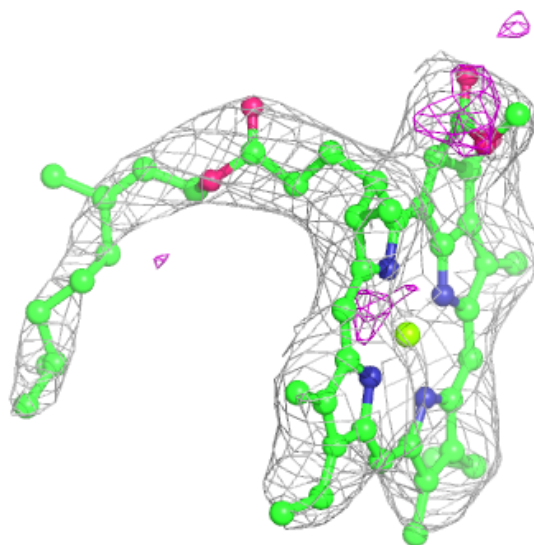
**Electron density around CLA A 815:**

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



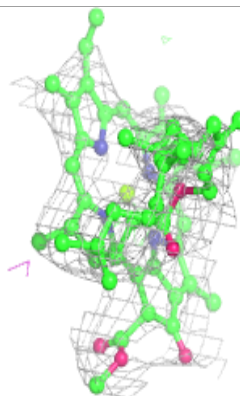
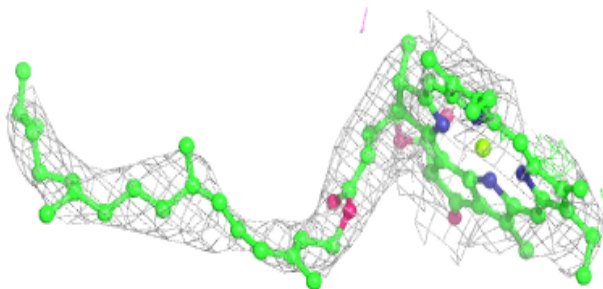
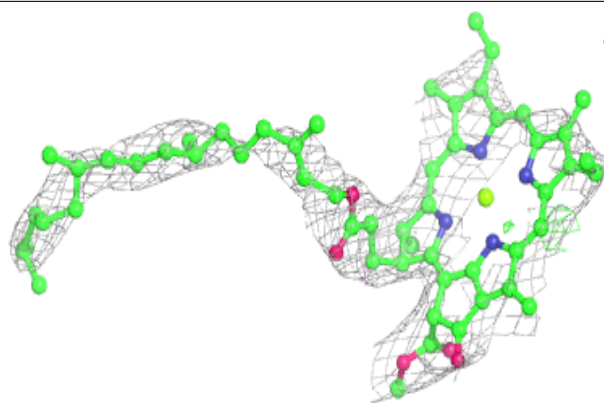
Electron density around CLA B 817:

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

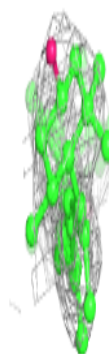
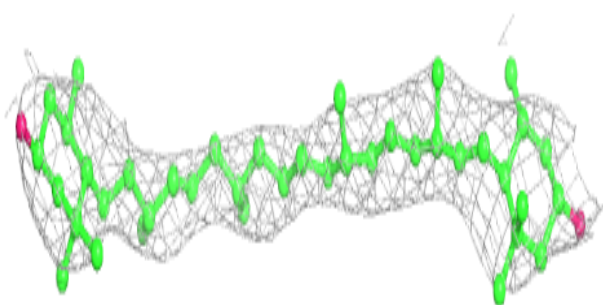
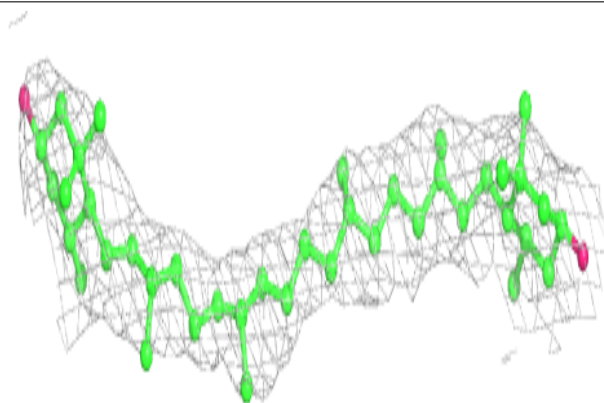


Electron density around CLA A 820:

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

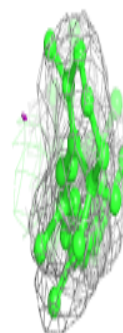
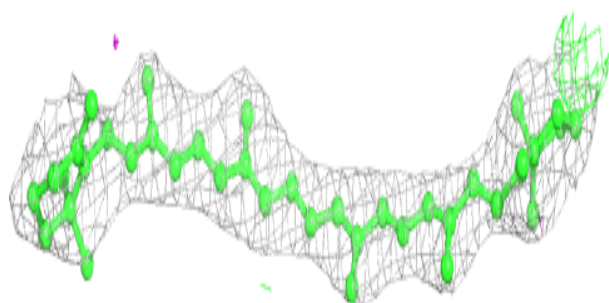
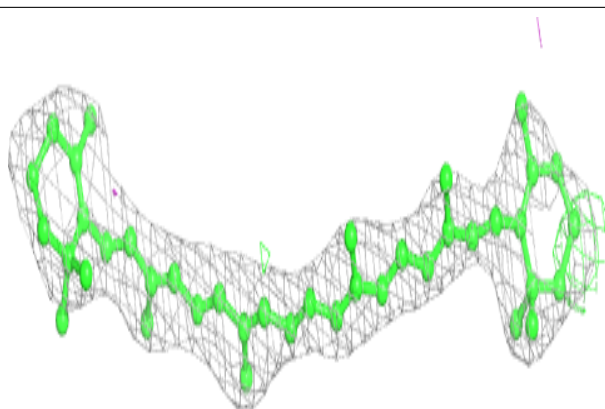
**Electron density around LUT 2 314:**

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

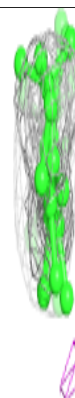
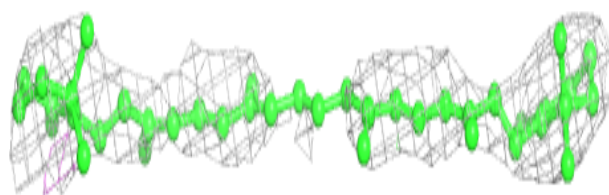
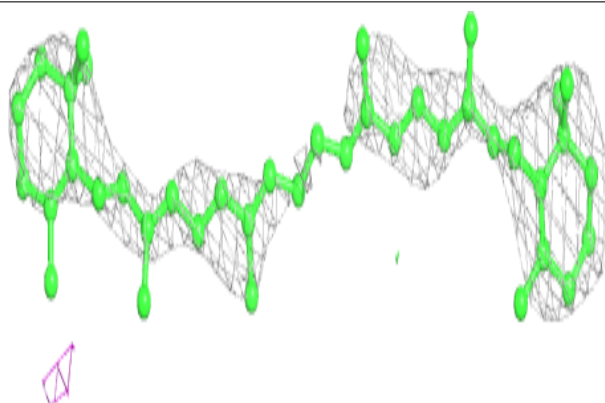


Electron density around BCR J 105:

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

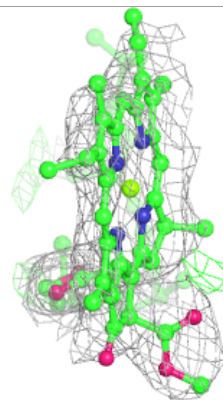
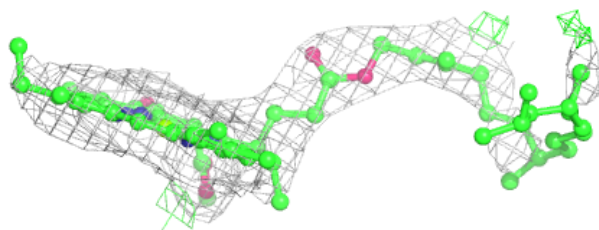
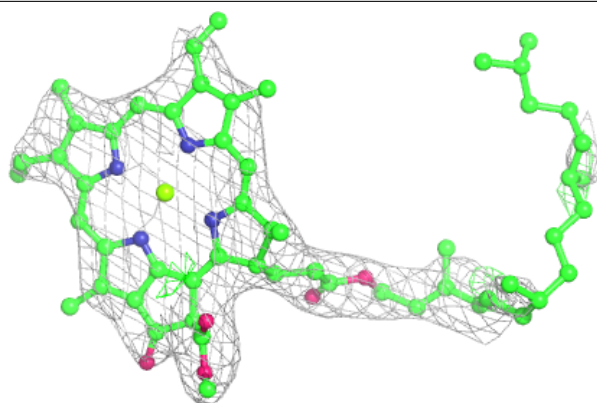
**Electron density around BCR L 205:**

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

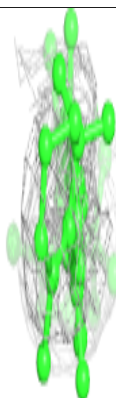
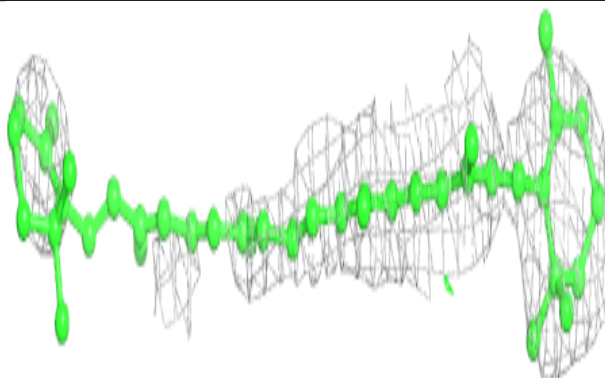
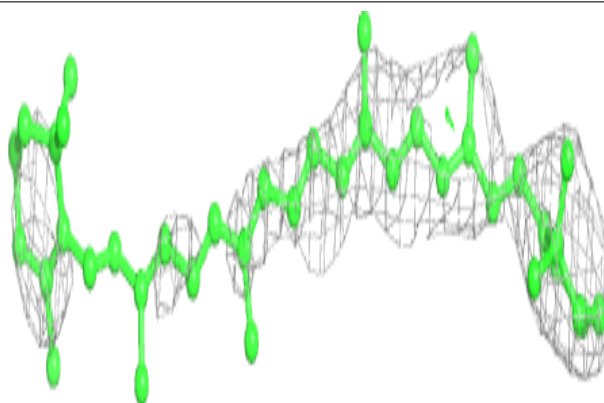


Electron density around CLA A 825:

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

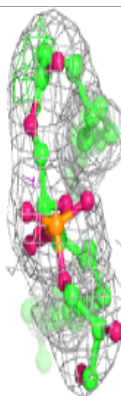
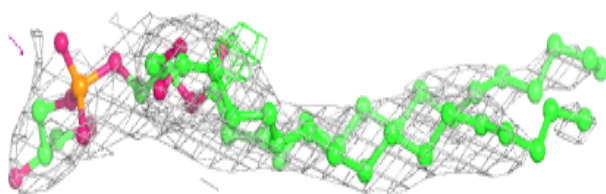
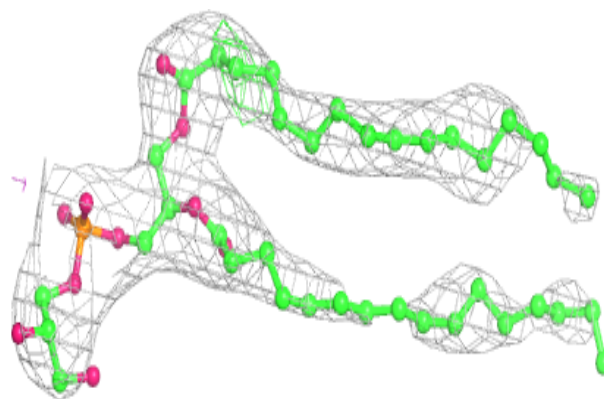
**Electron density around BCR A 847:**

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

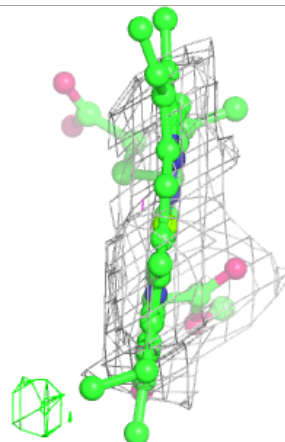
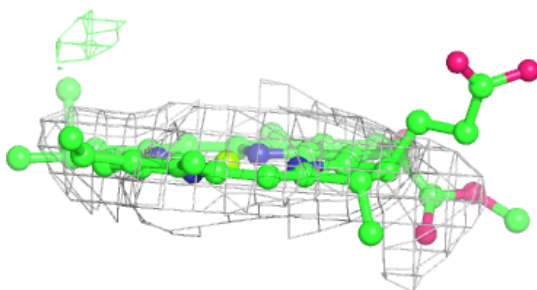
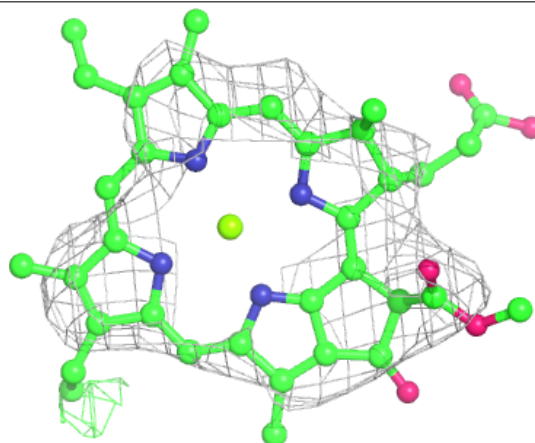


Electron density around LHG 1 317:

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

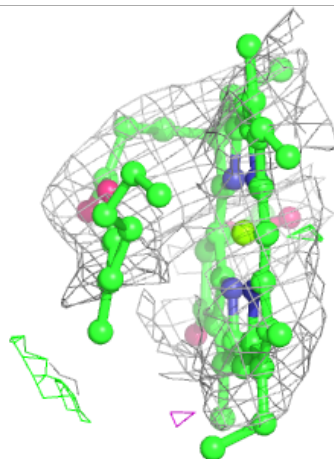
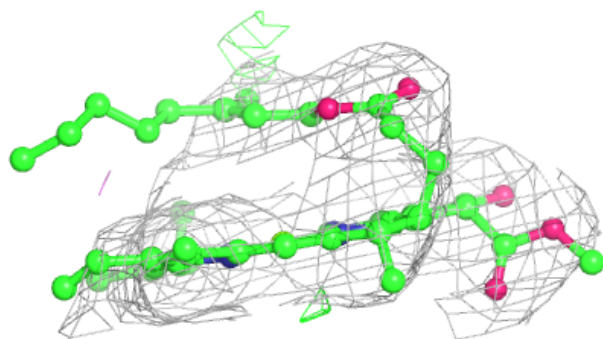
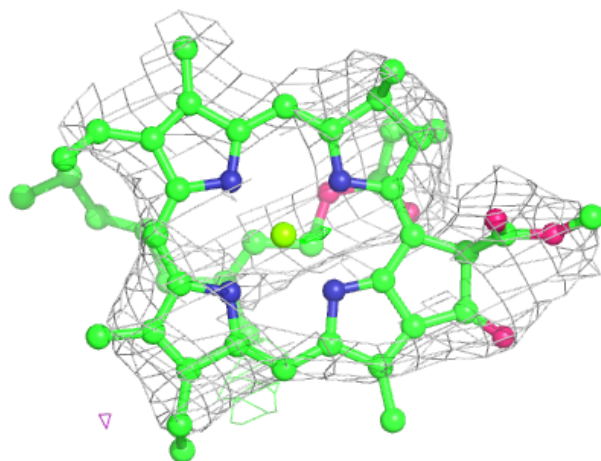
**Electron density around CLA 3 612:**

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



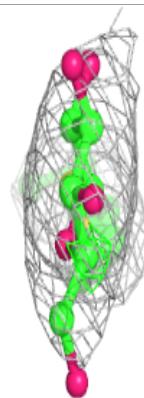
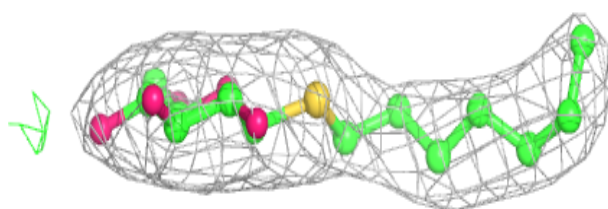
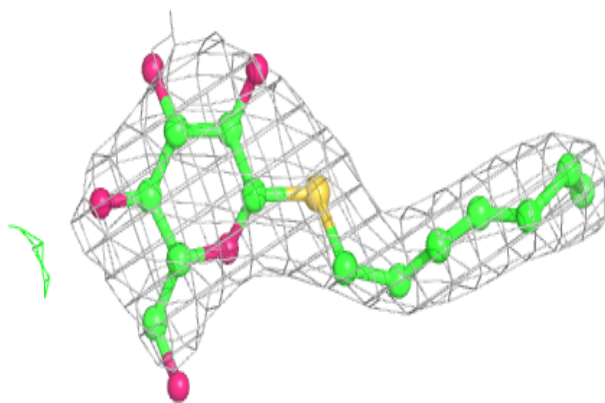
Electron density around CLA A 811:

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



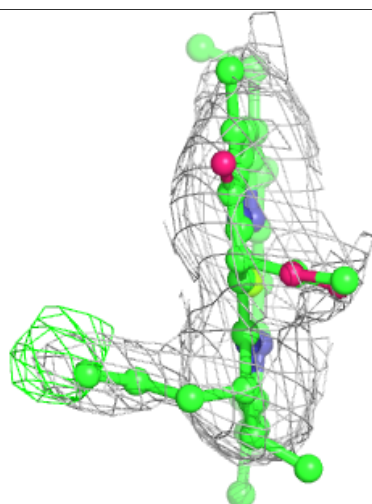
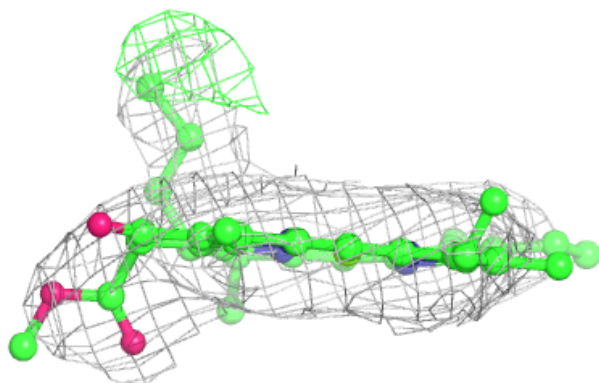
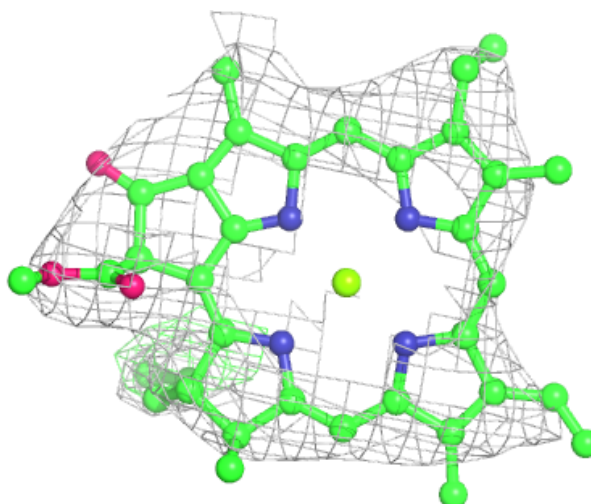
Electron density around HTG F 305:

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



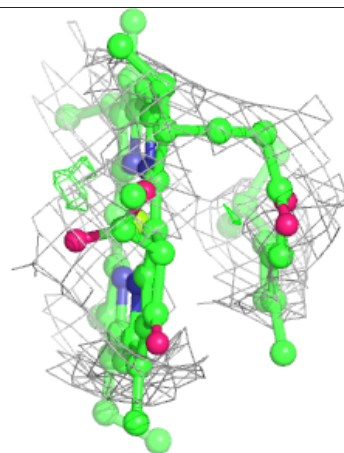
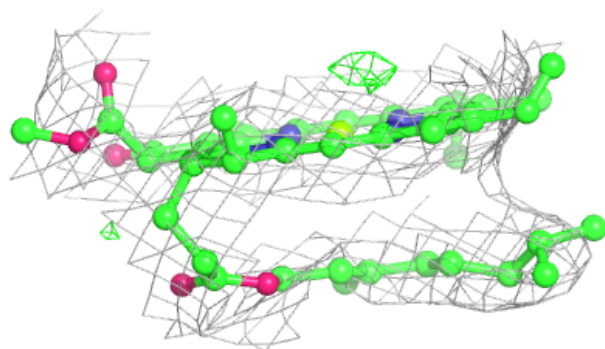
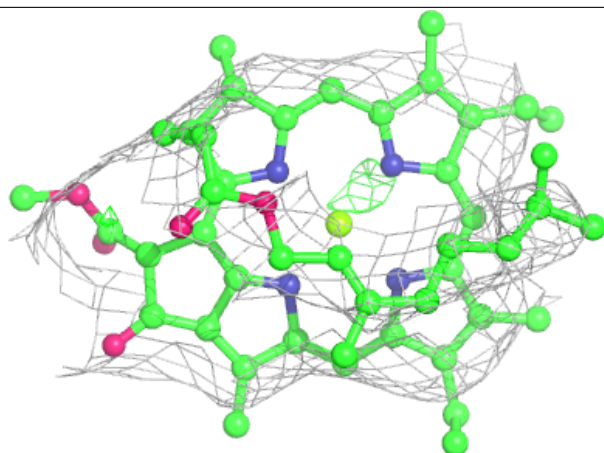
Electron density around CLA 2 312:

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

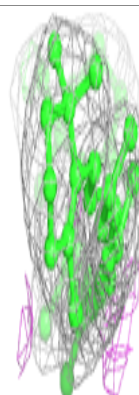
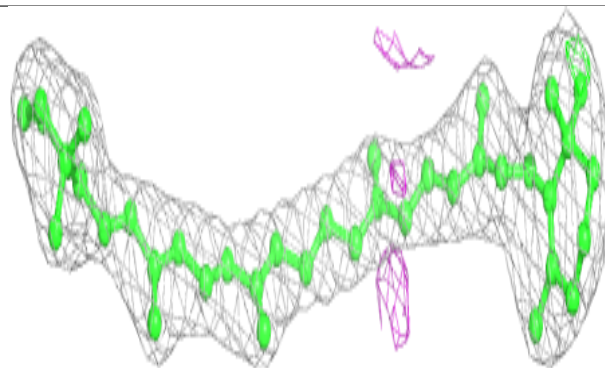
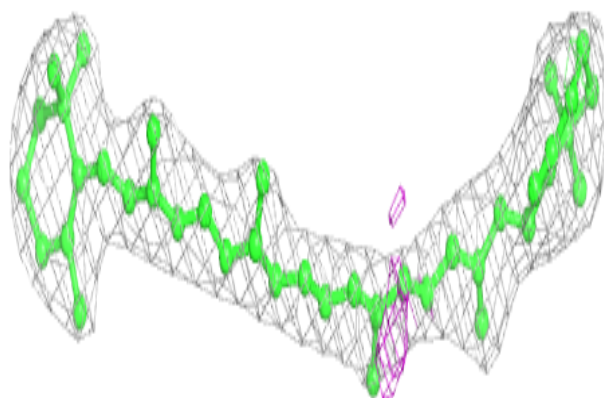


Electron density around CLA 3 611:

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

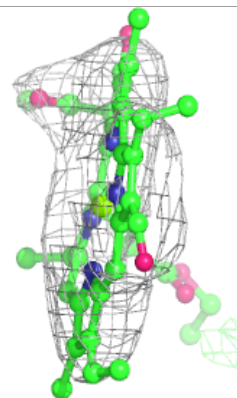
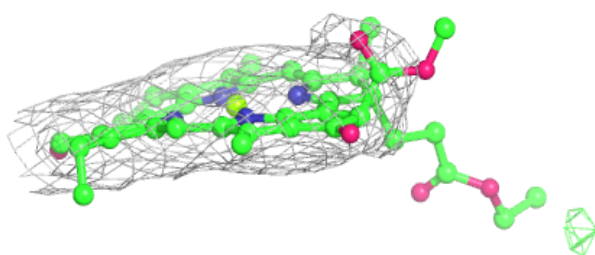
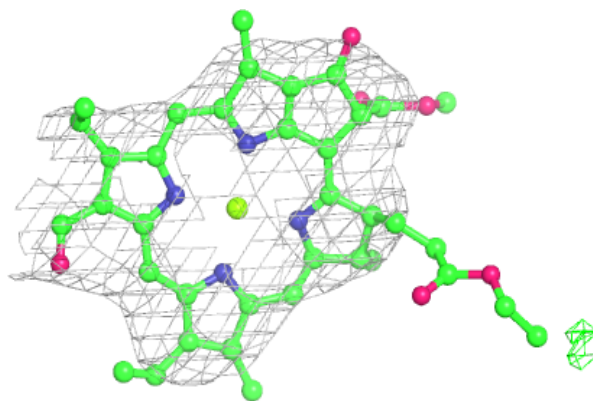
**Electron density around BCR F 303:**

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

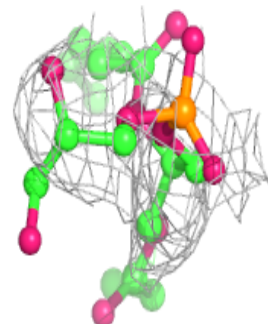
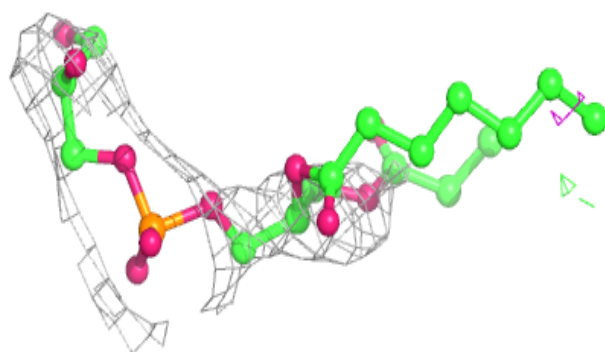
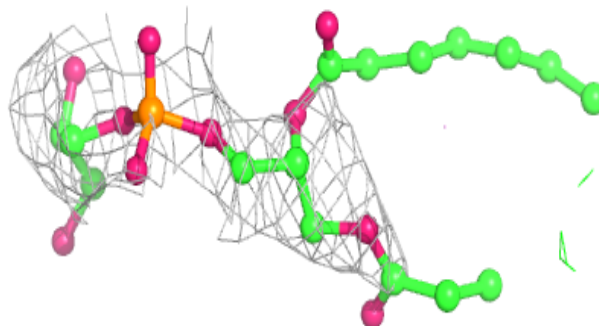


Electron density around CHL 2 305:

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

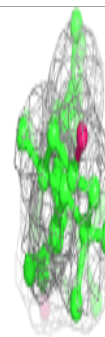
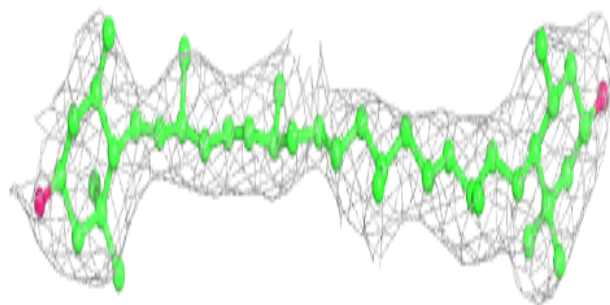
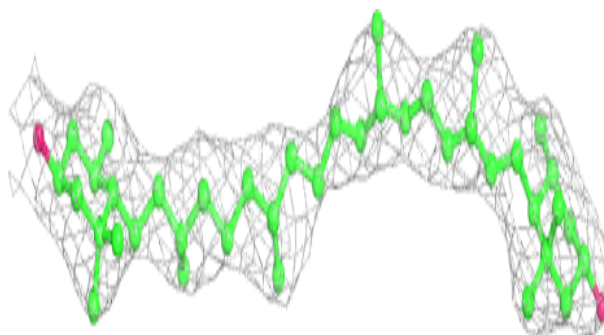
**Electron density around LHG A 845:**

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



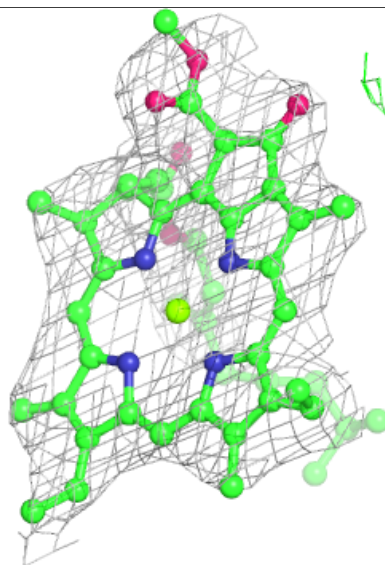
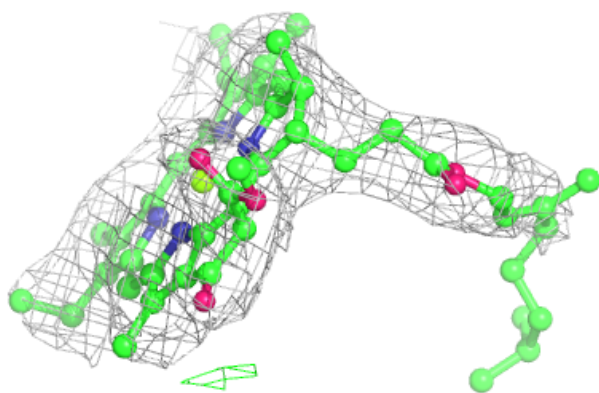
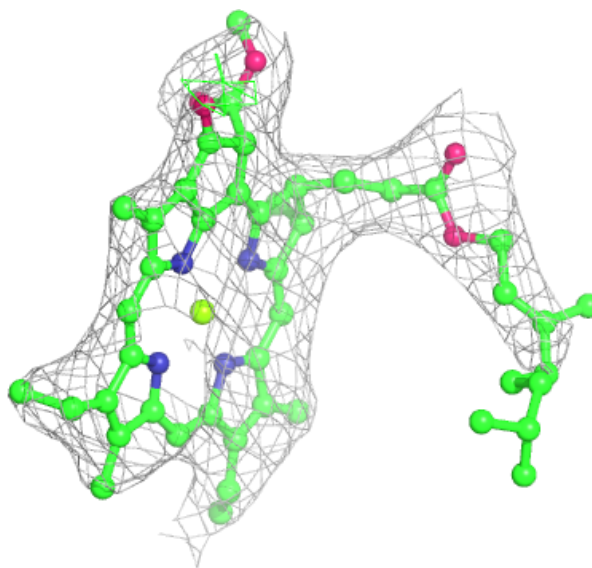
Electron density around LUT 1 314:

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



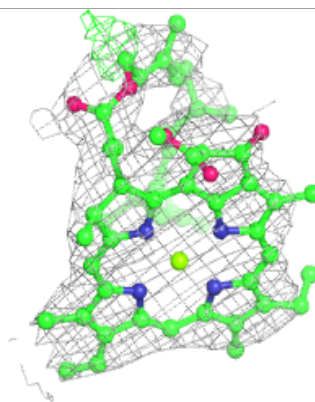
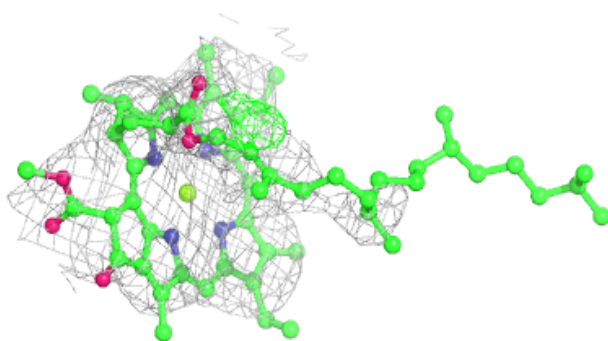
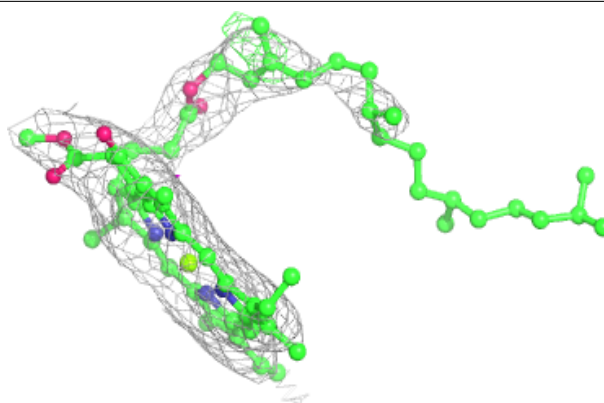
Electron density around CLA A 803:

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

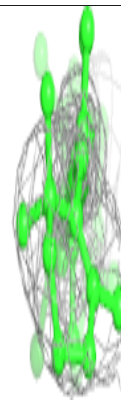
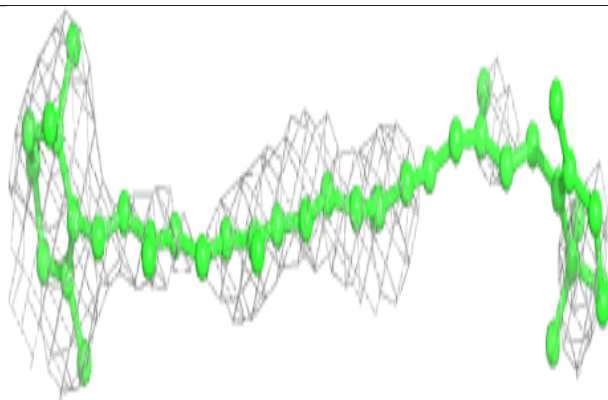
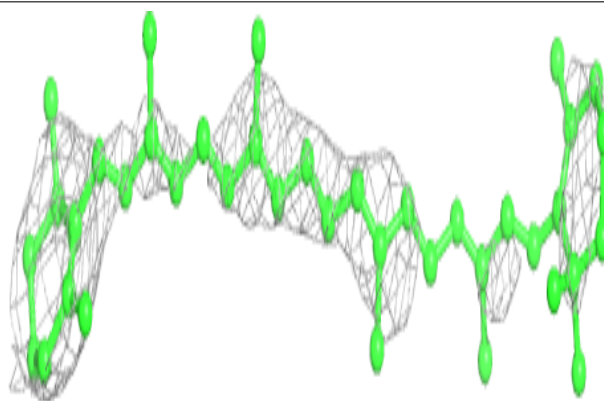


Electron density around CLA A 809:

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

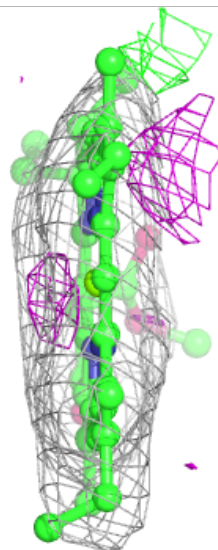
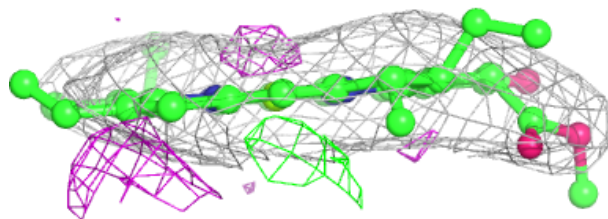
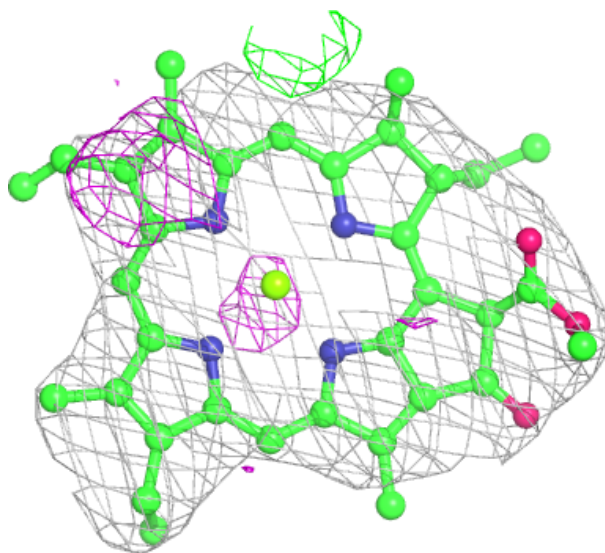
**Electron density around BCR A 848:**

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



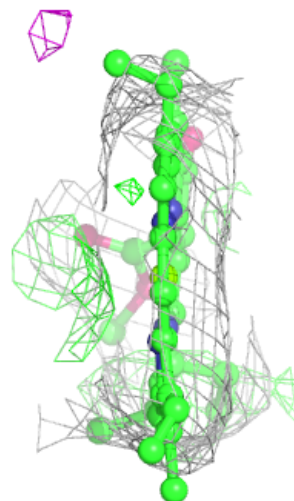
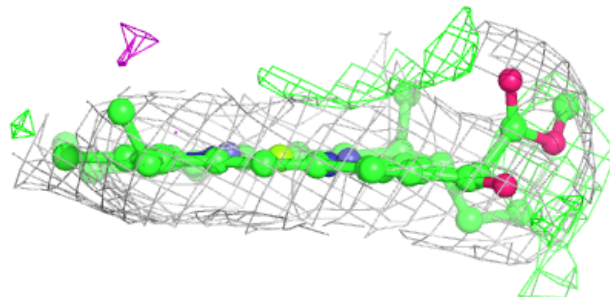
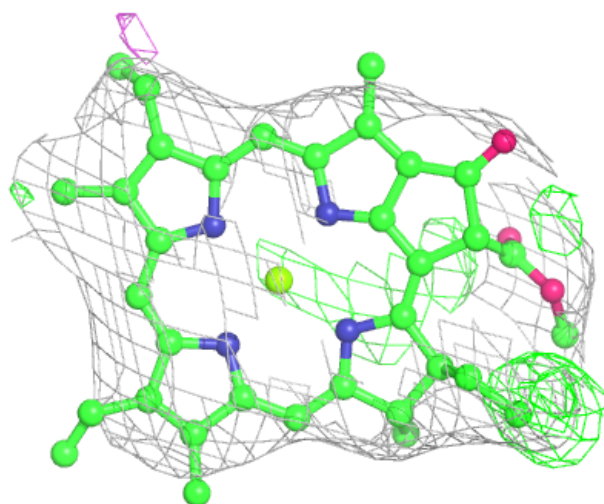
Electron density around CLA J 103:

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



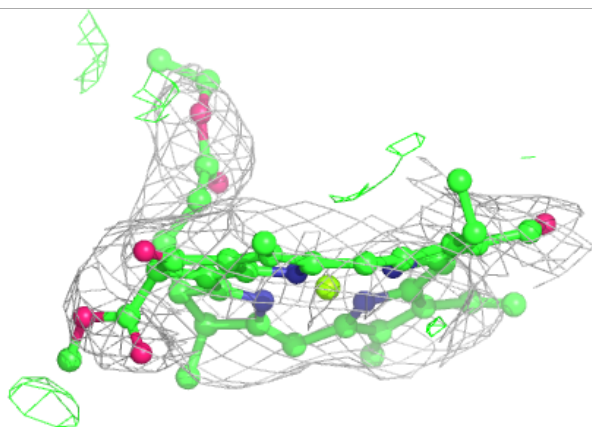
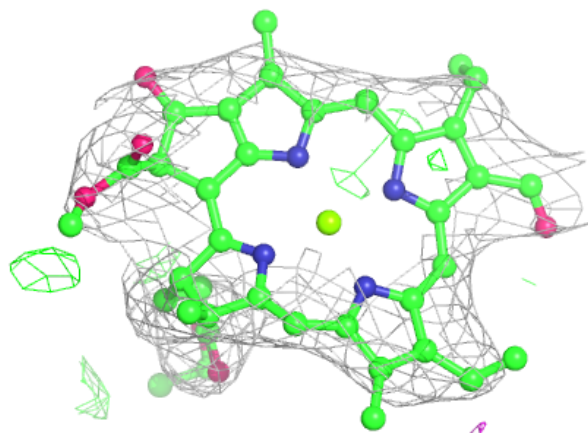
Electron density around CLA 1 304:

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



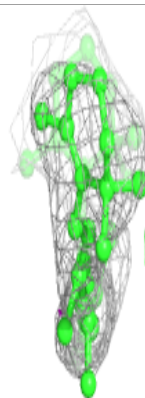
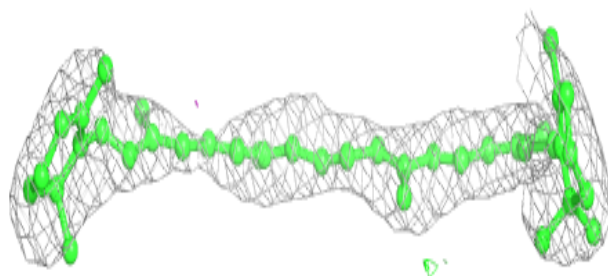
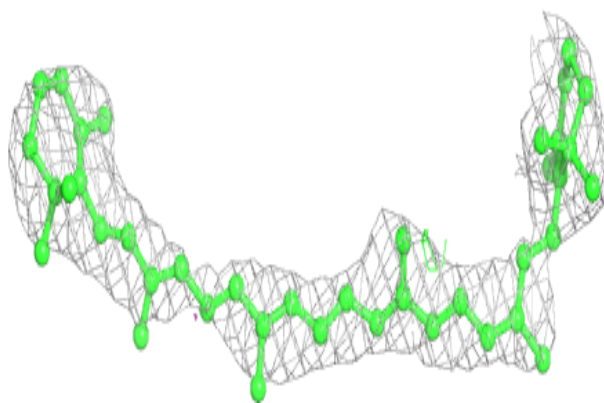
Electron density around CHL 1 305:

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



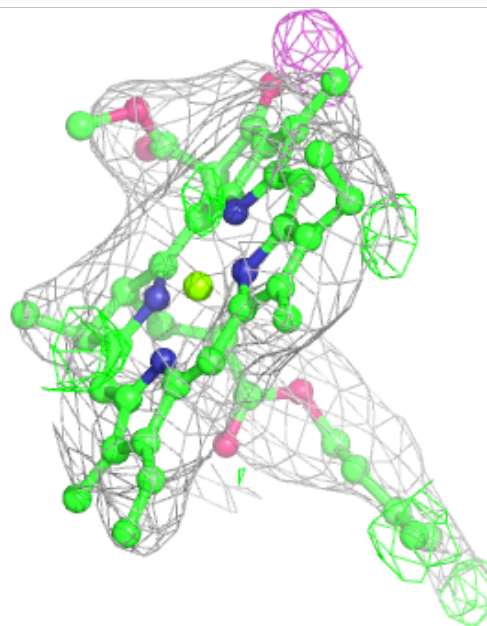
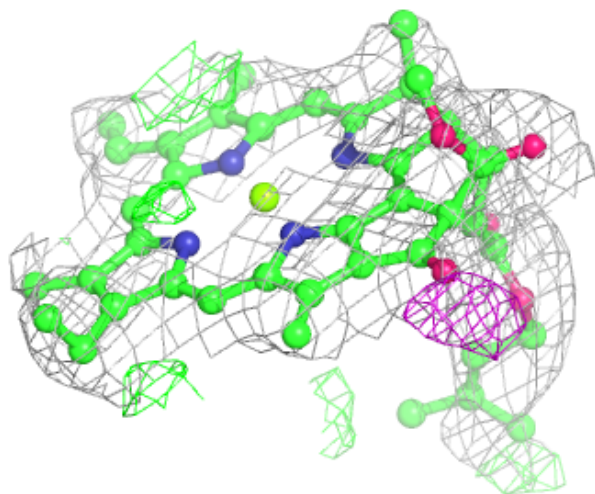
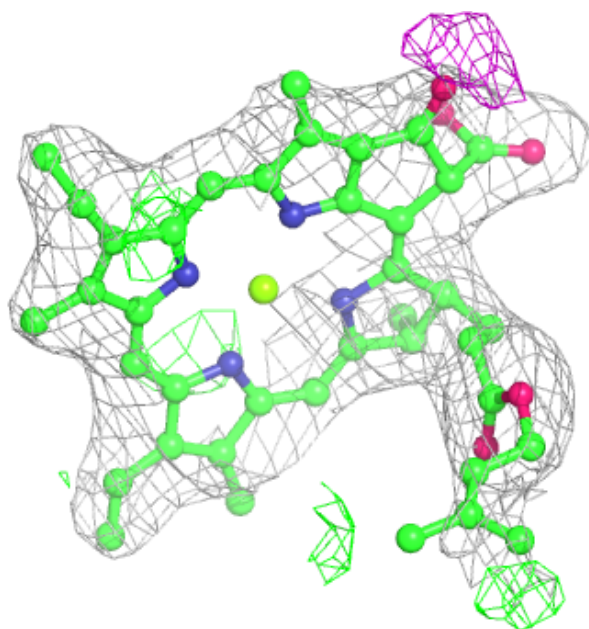
Electron density around BCR L 201:

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



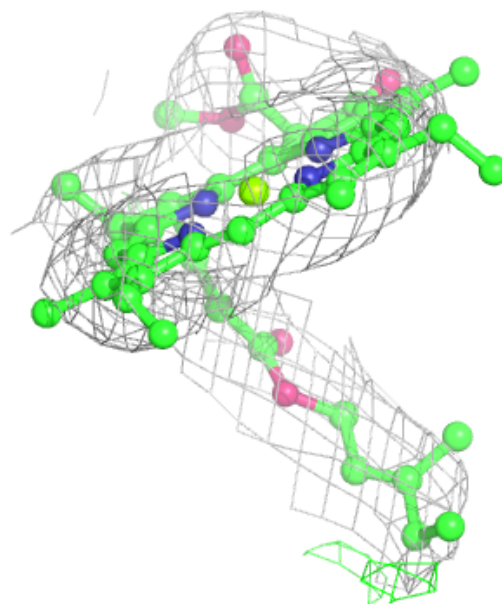
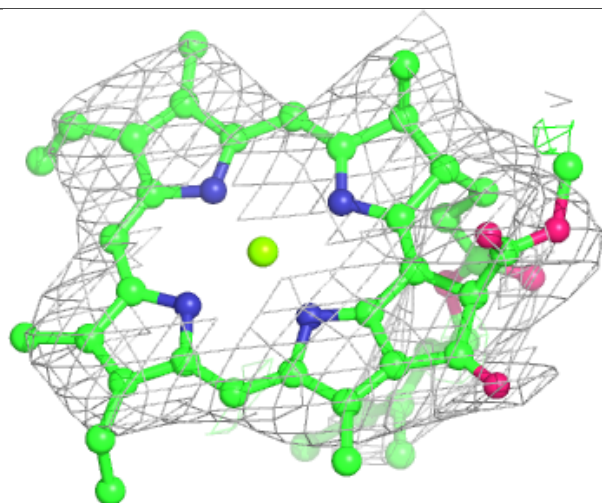
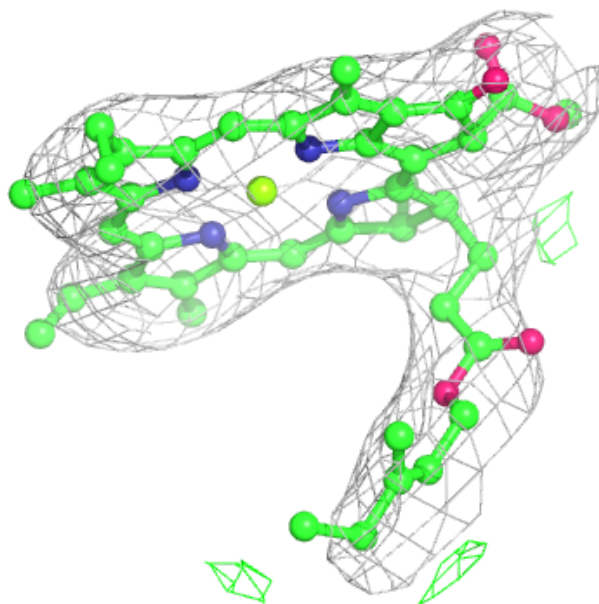
Electron density around CLA 4 304:

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



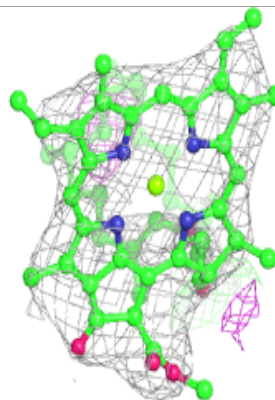
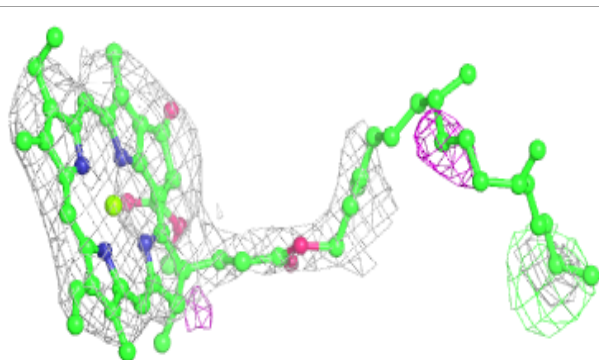
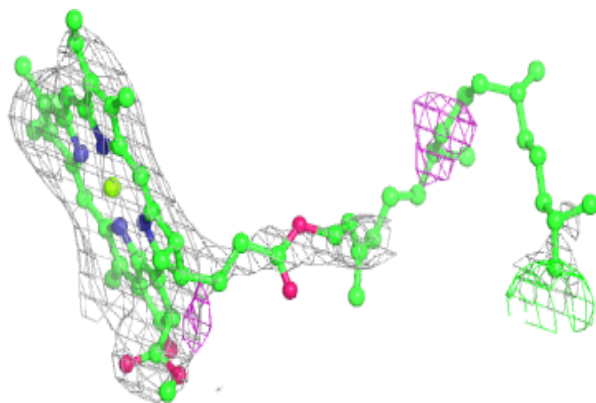
Electron density around CLA 1 303:

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



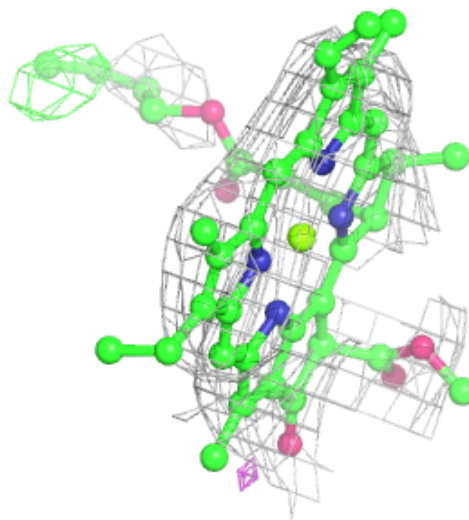
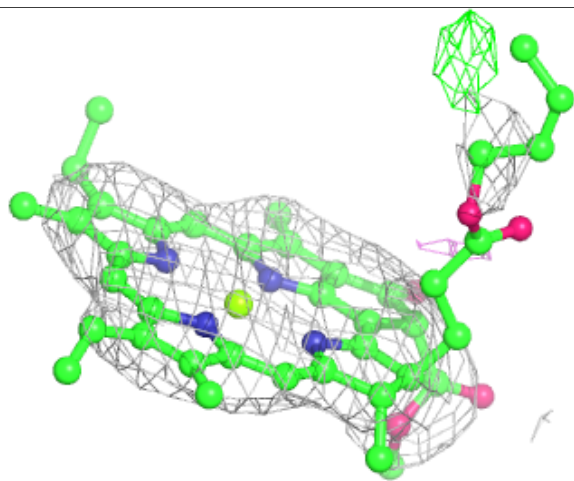
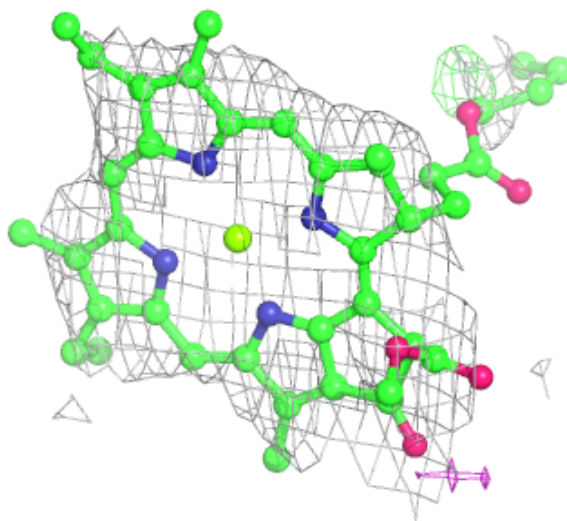
Electron density around CLA A 837:

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



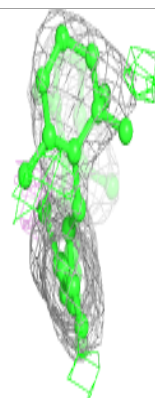
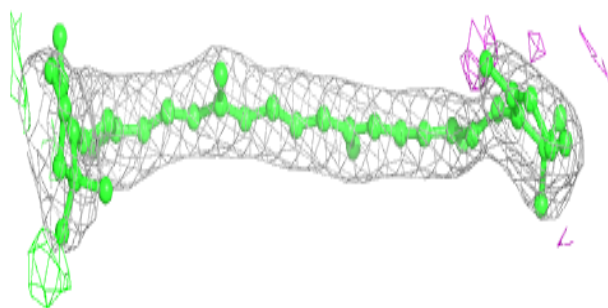
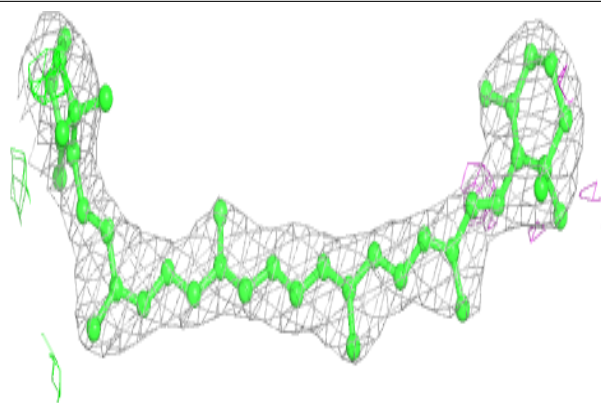
Electron density around CLA A 821:

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

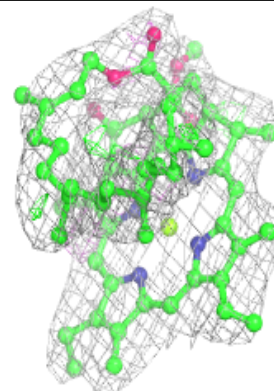
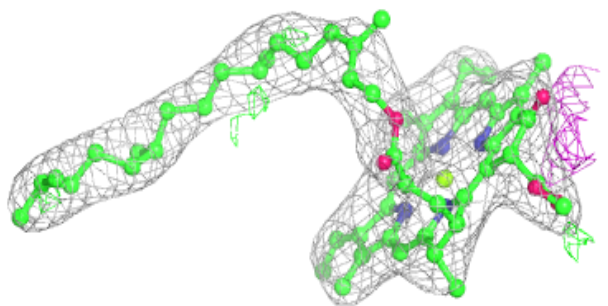
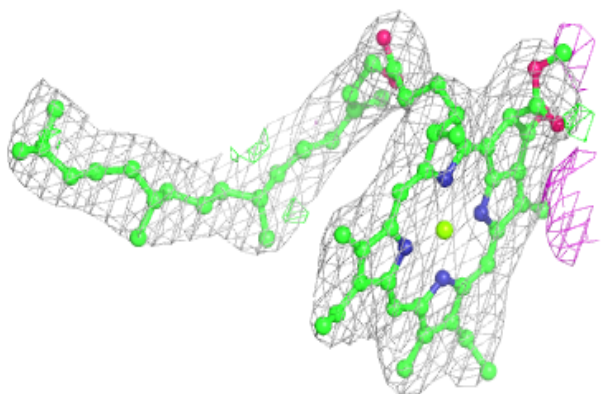


Electron density around BCR B 845:

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

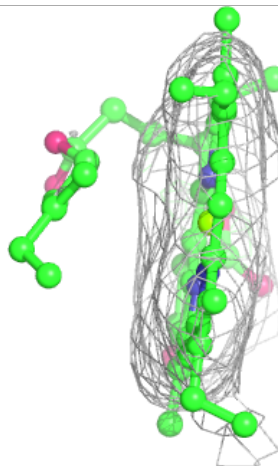
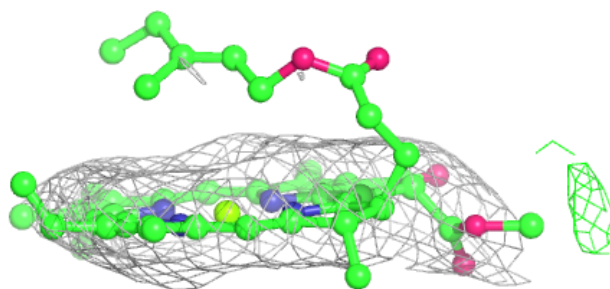
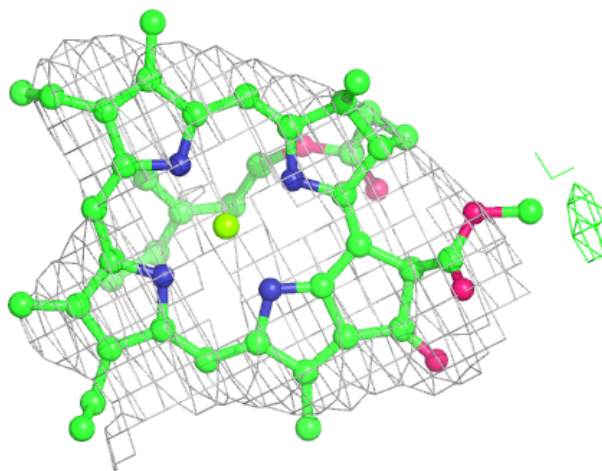
**Electron density around CLA B 816:**

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



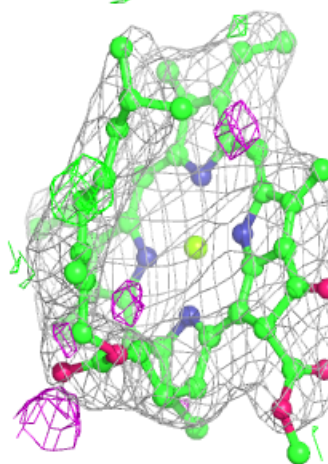
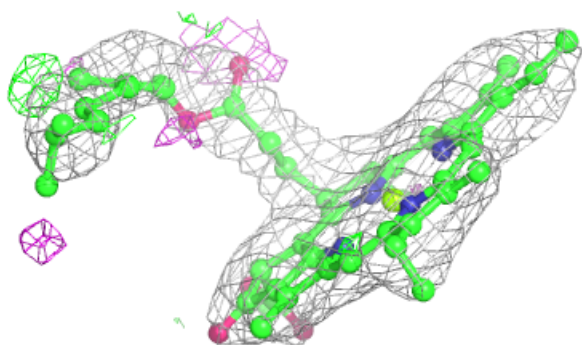
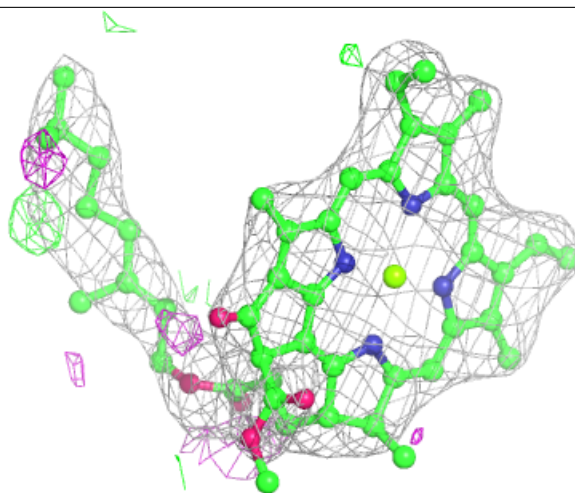
Electron density around CLA A 822:

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



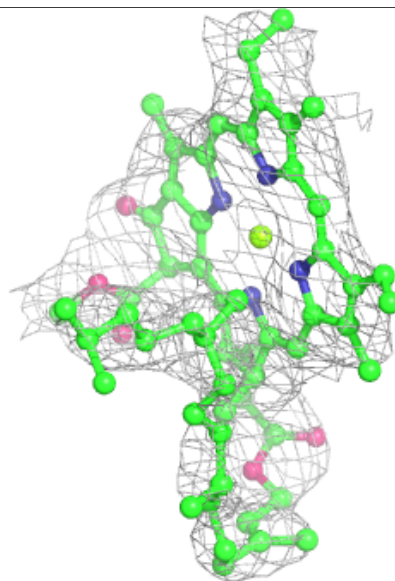
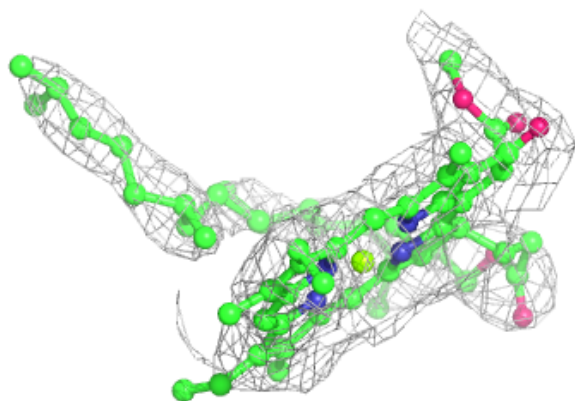
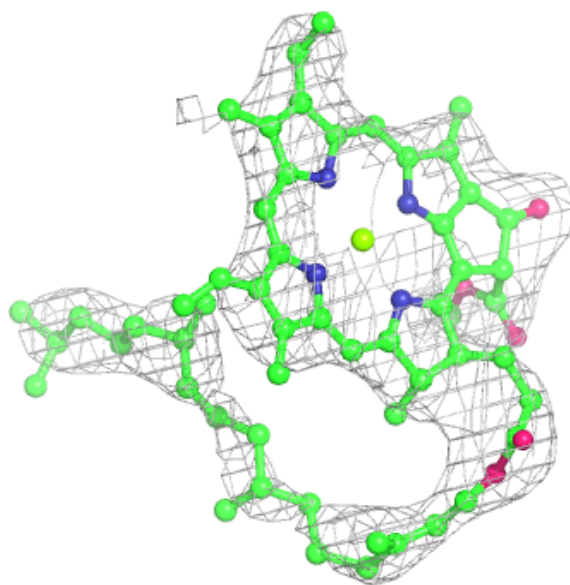
Electron density around CLA B 824:

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



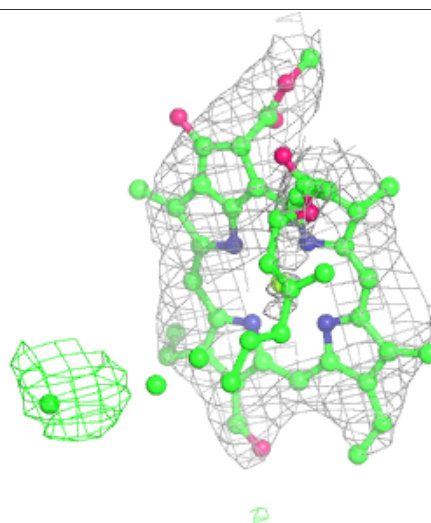
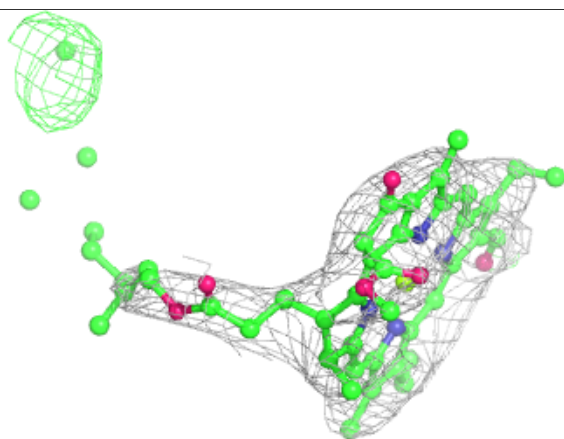
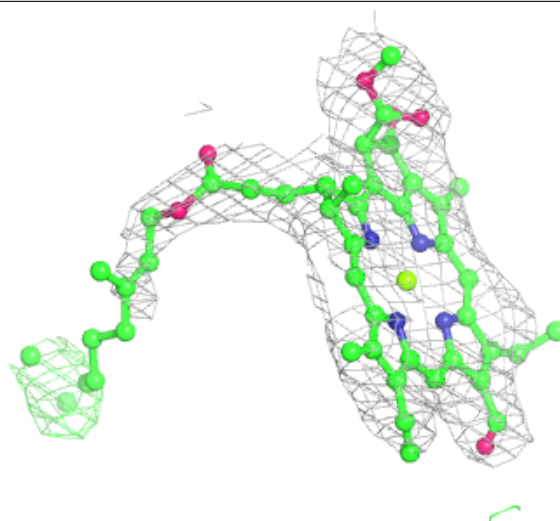
Electron density around CLA A 812:

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



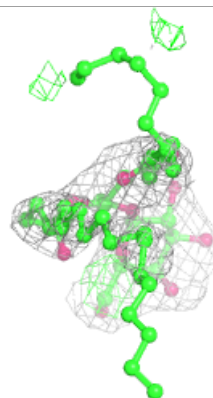
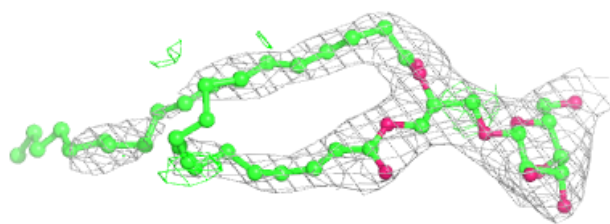
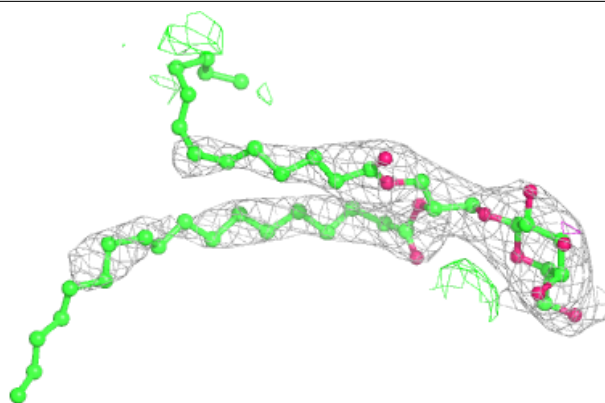
Electron density around CHL 3 601:

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

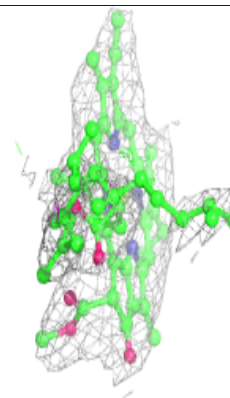
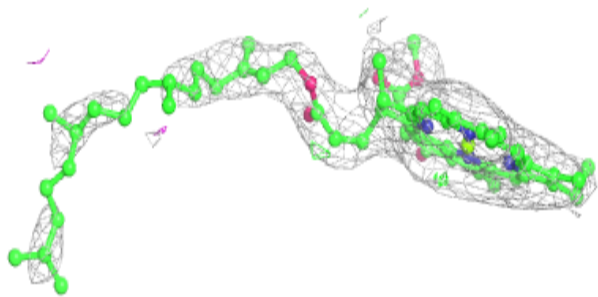
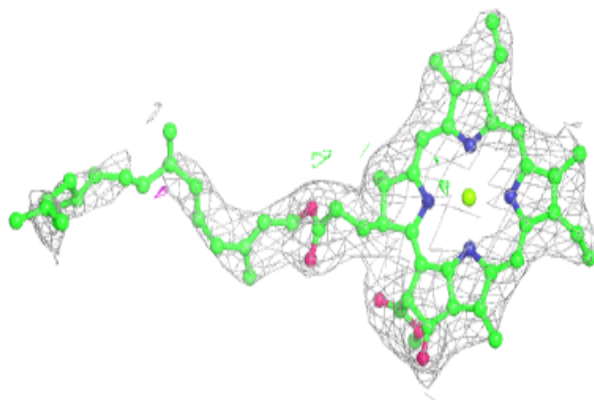


Electron density around LMG 4 319:

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

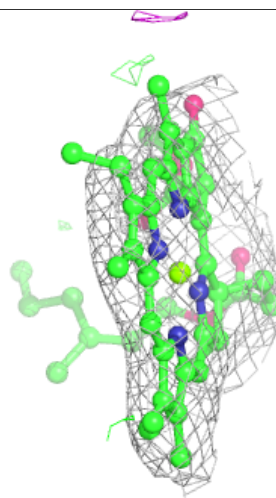
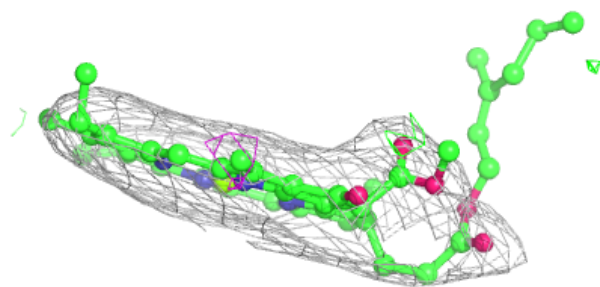
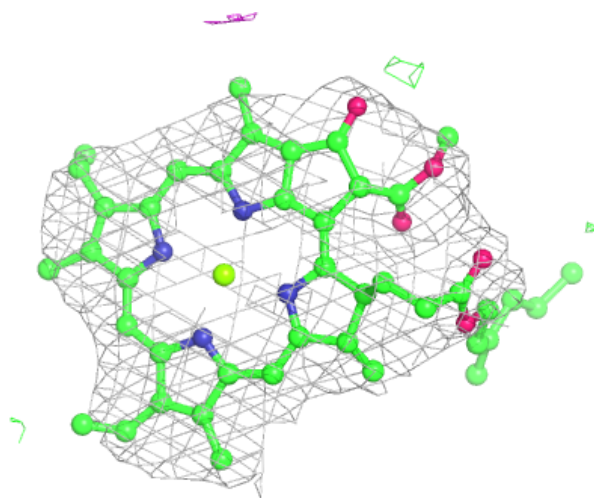
**Electron density around CLA A 804:**

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



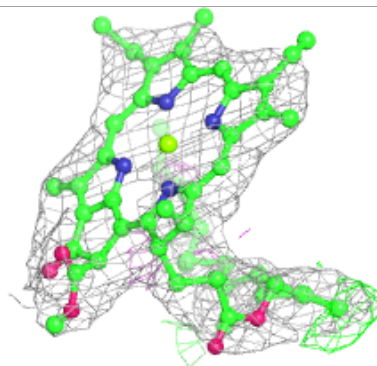
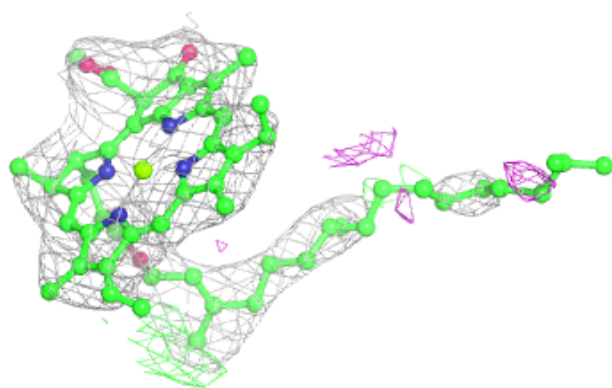
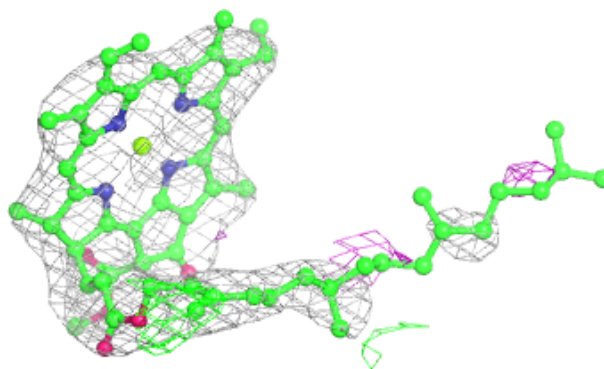
Electron density around CLA 2 310:

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



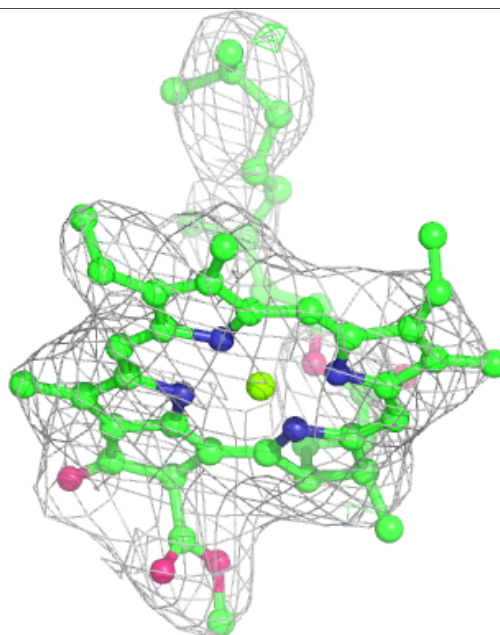
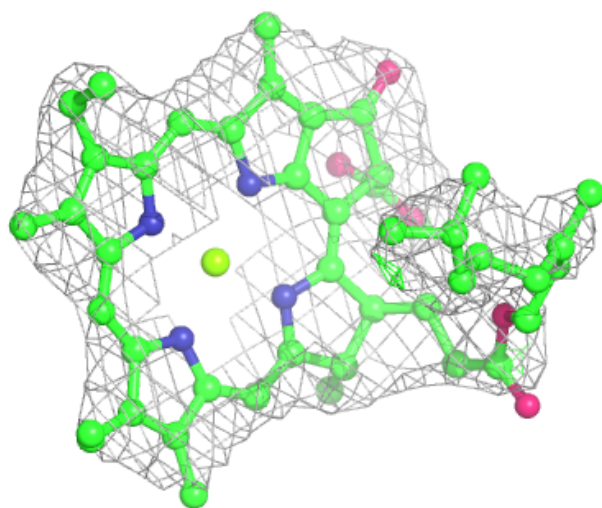
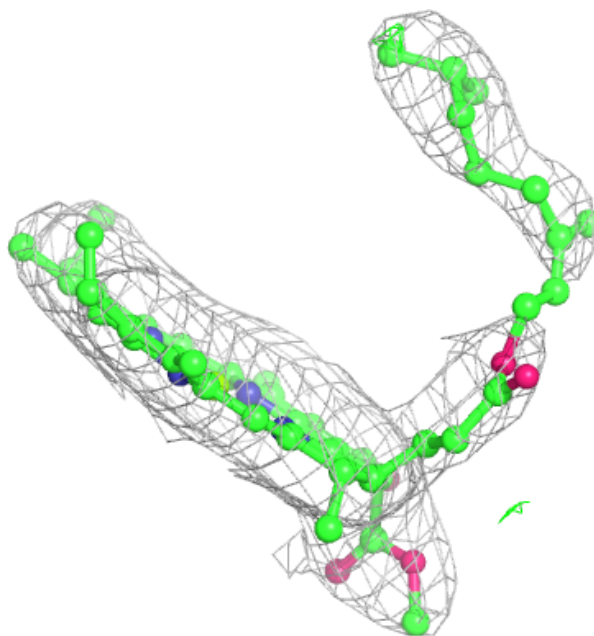
Electron density around CLA 1 307:

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



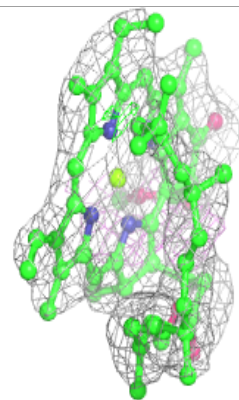
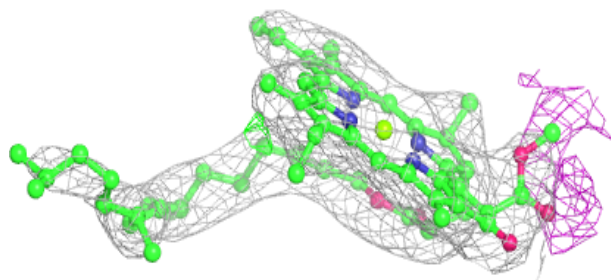
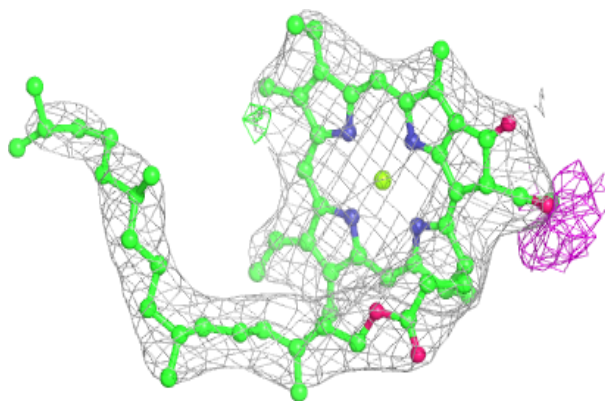
Electron density around CLA 1 312:

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



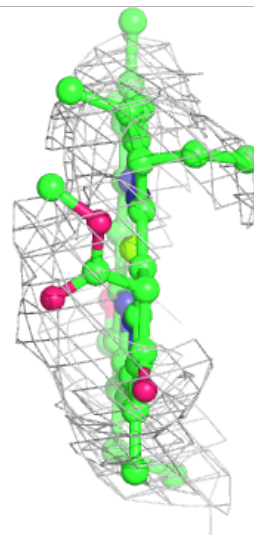
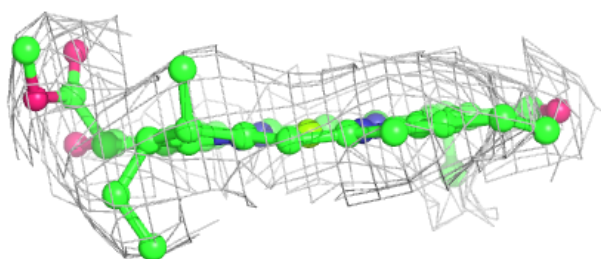
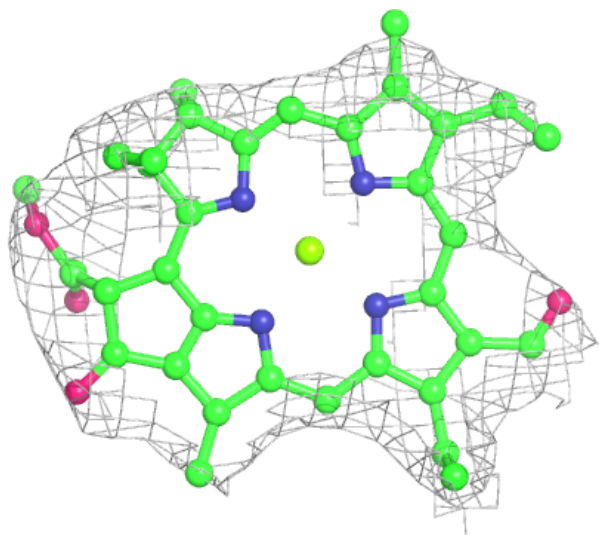
Electron density around CLA 1 301:

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



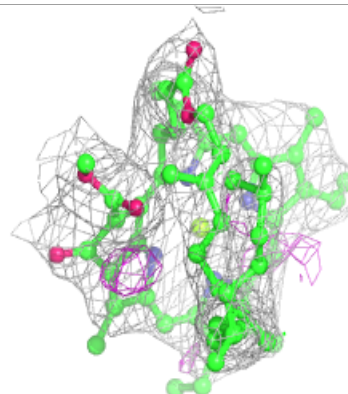
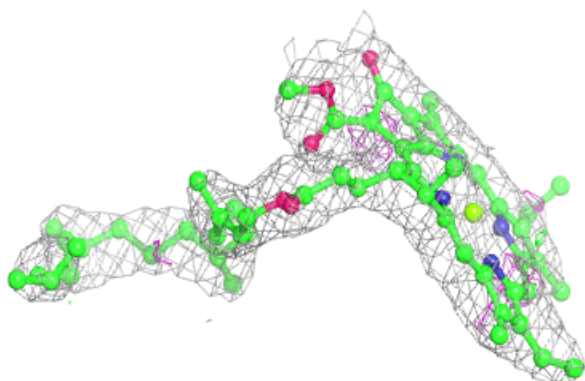
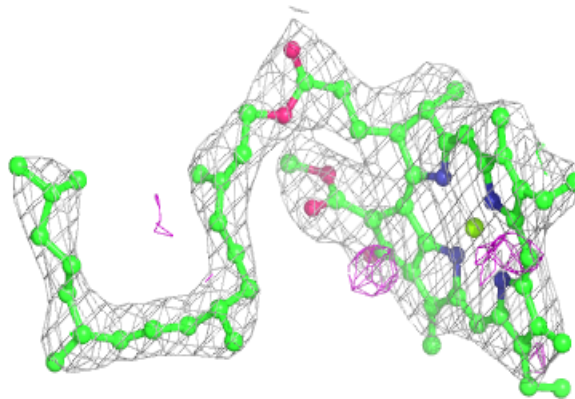
Electron density around CHL 2 313:

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

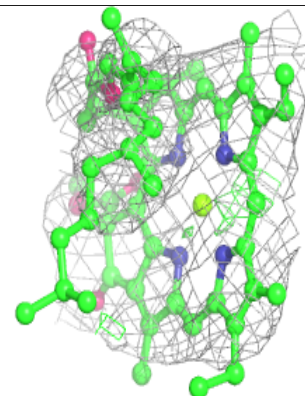
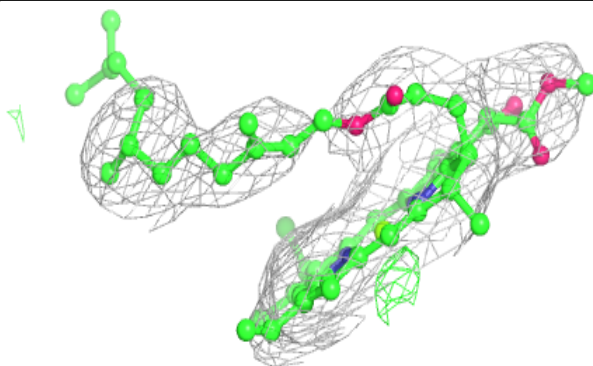
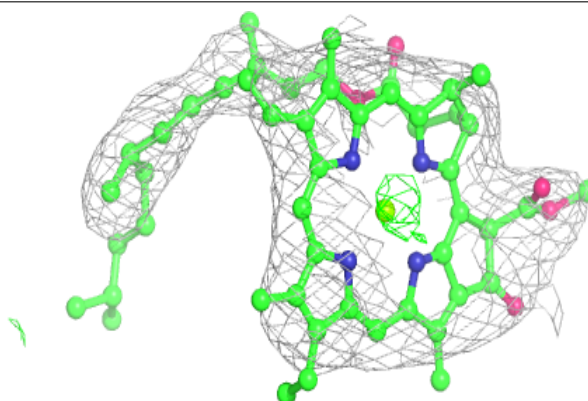


Electron density around CLA A 801:

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

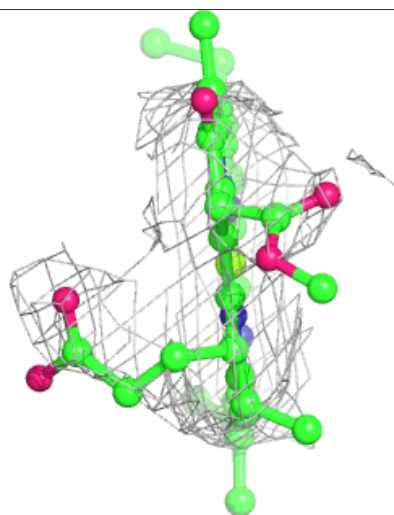
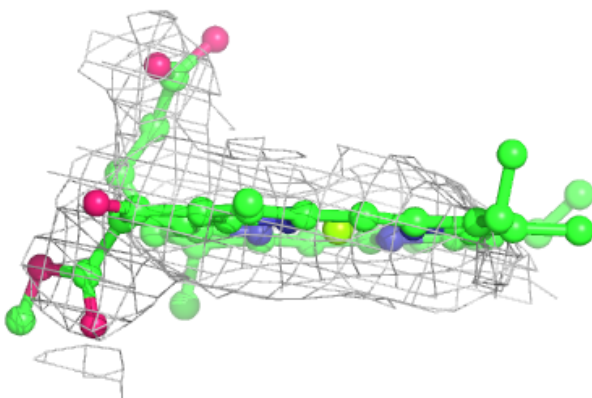
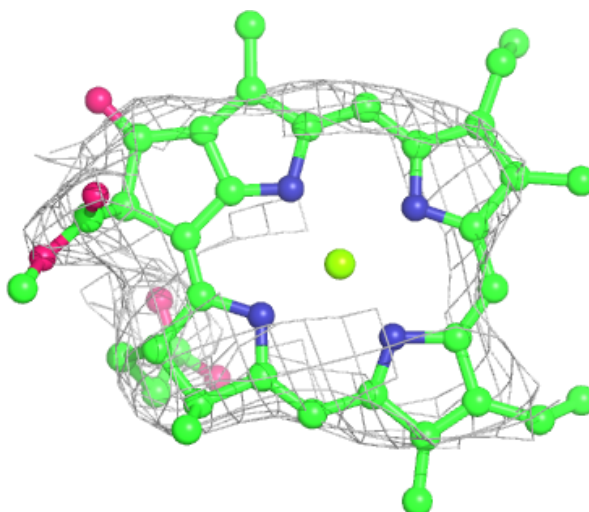
**Electron density around CLA 2 308:**

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



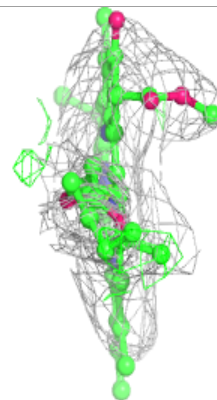
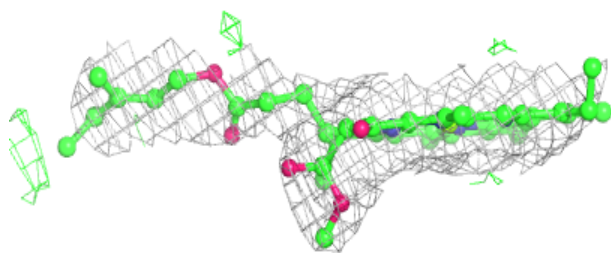
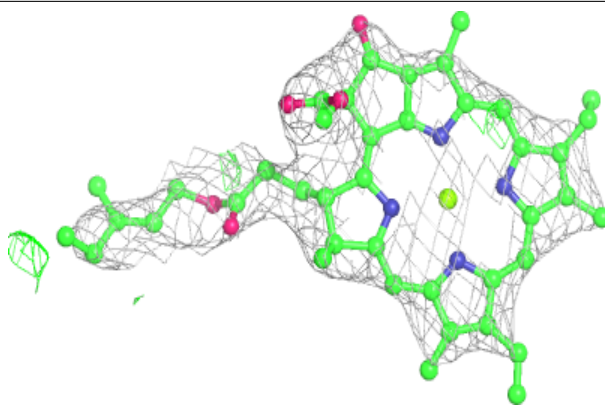
Electron density around CLA A 834:

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

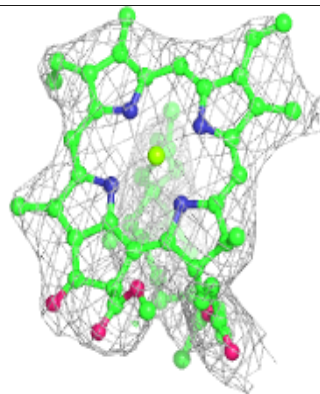
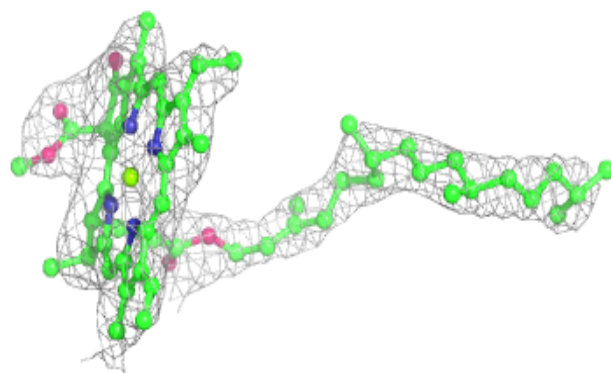
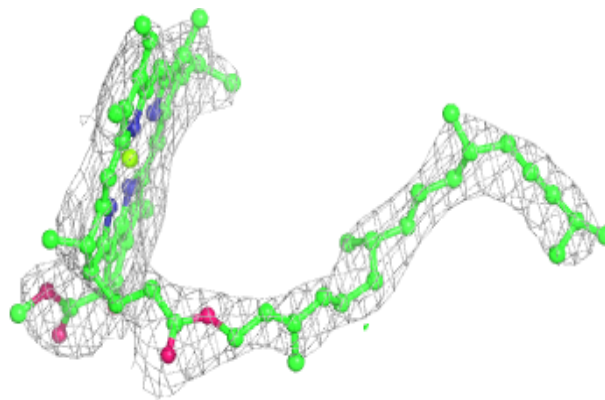


Electron density around CLA A 835:

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

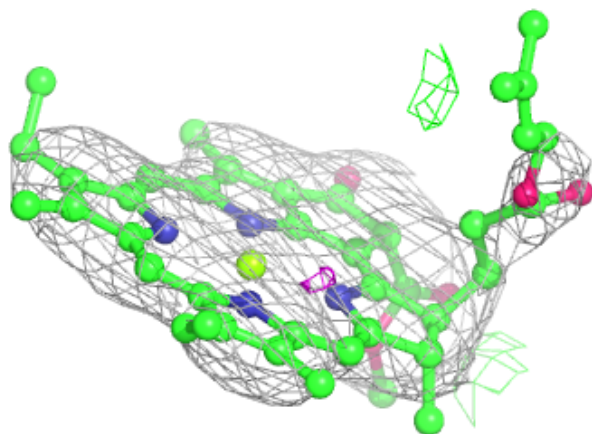
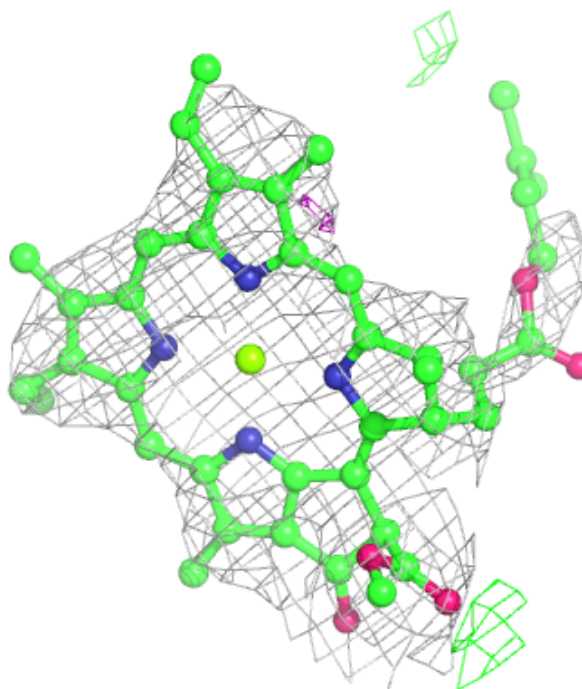
**Electron density around CLA A 829:**

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



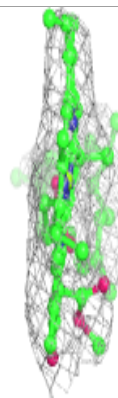
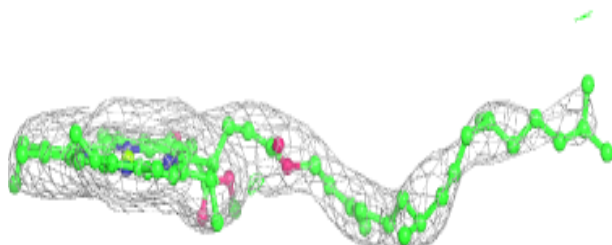
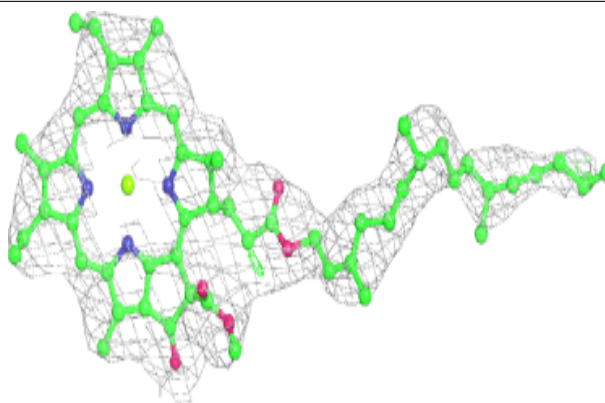
Electron density around CLA A 830:

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

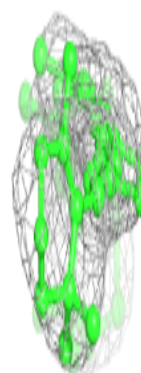
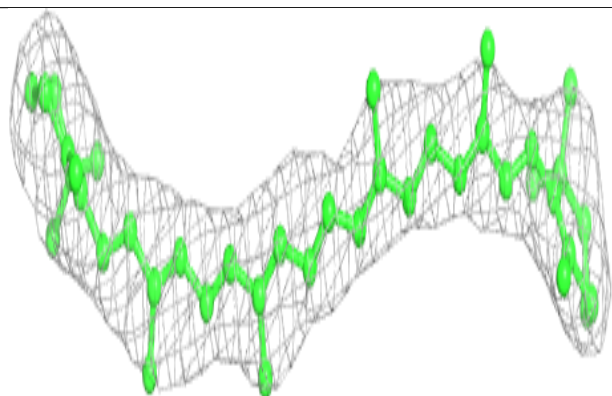
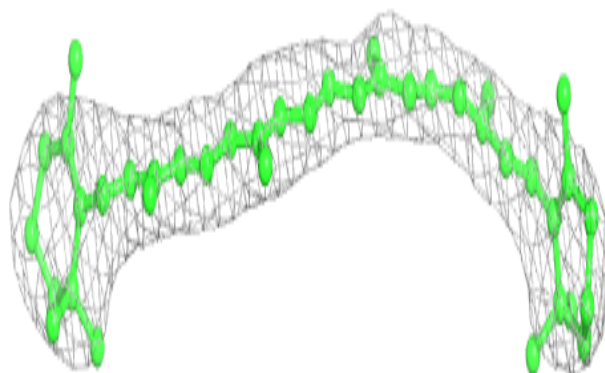


Electron density around CLA A 831:

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

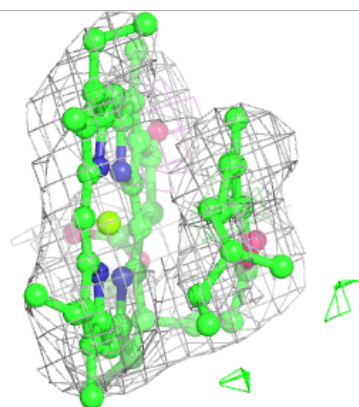
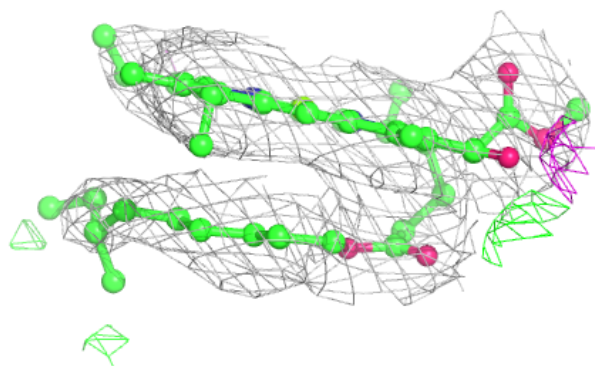
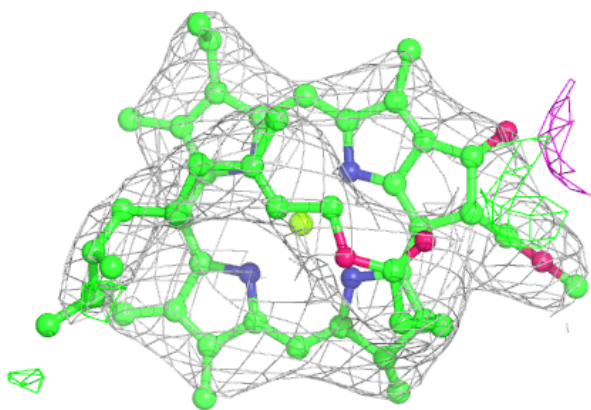
**Electron density around BCR I 101:**

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



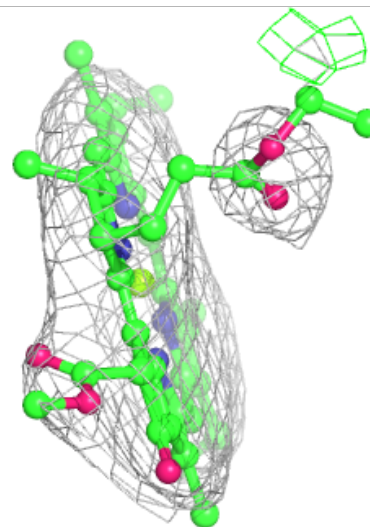
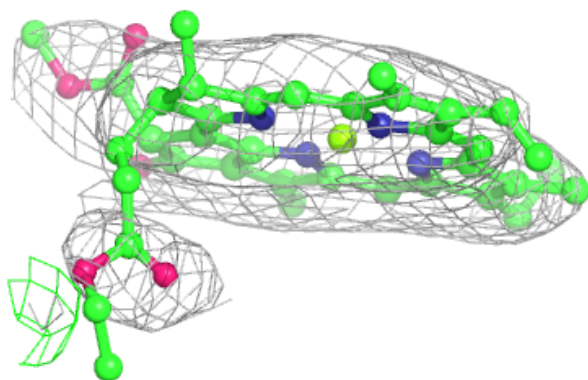
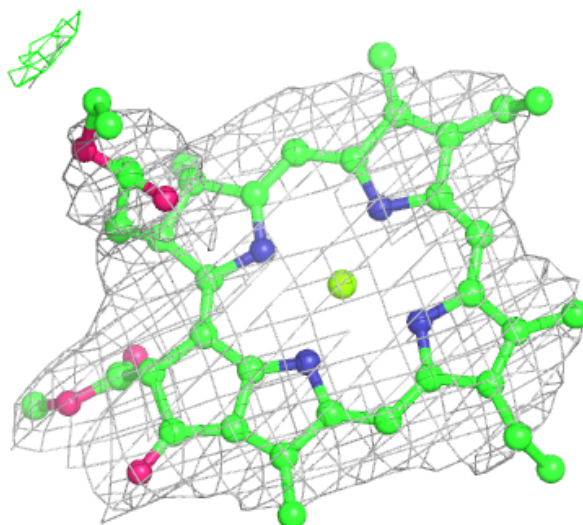
Electron density around CLA 4 312:

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



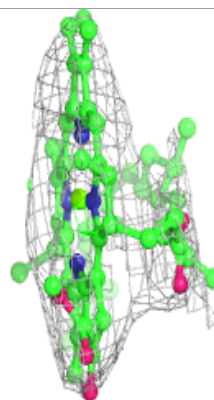
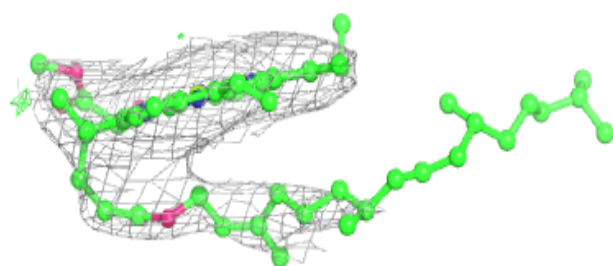
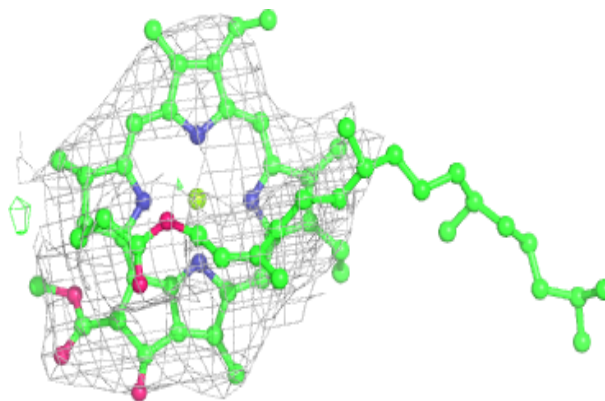
Electron density around CLA 3 606:

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



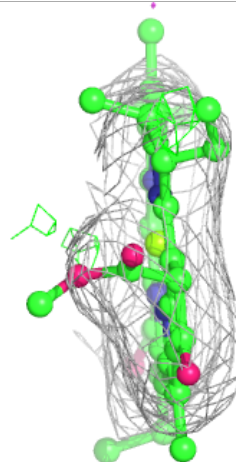
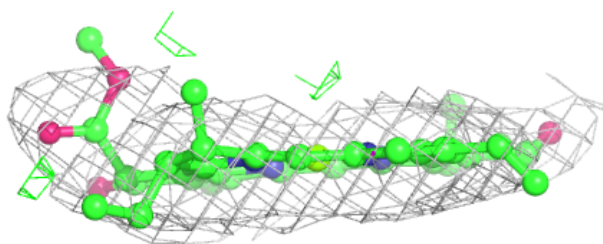
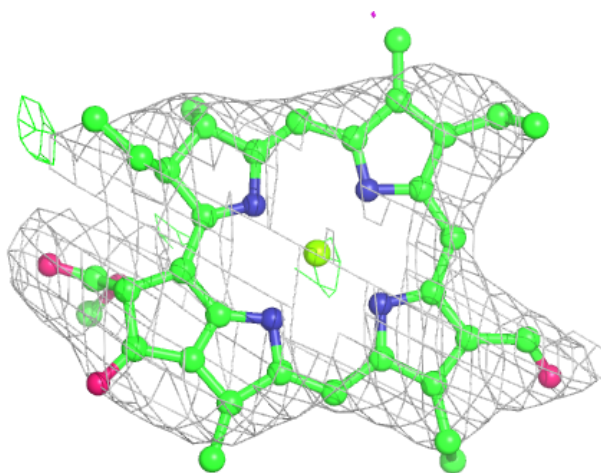
Electron density around CLA A 816:

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



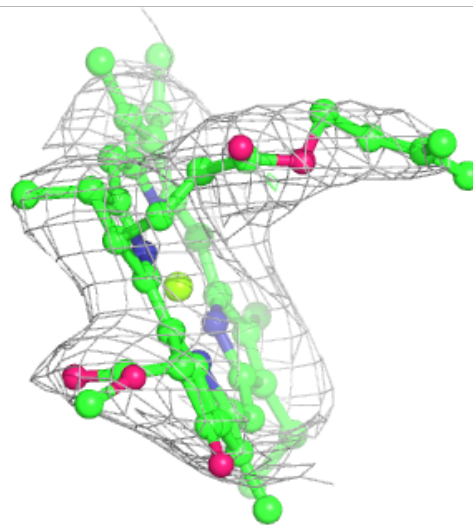
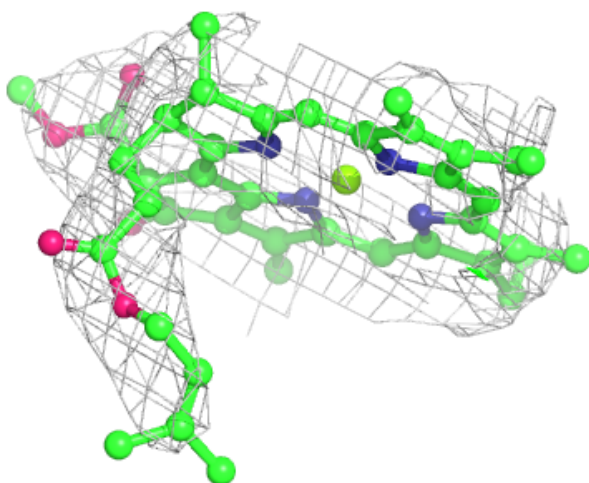
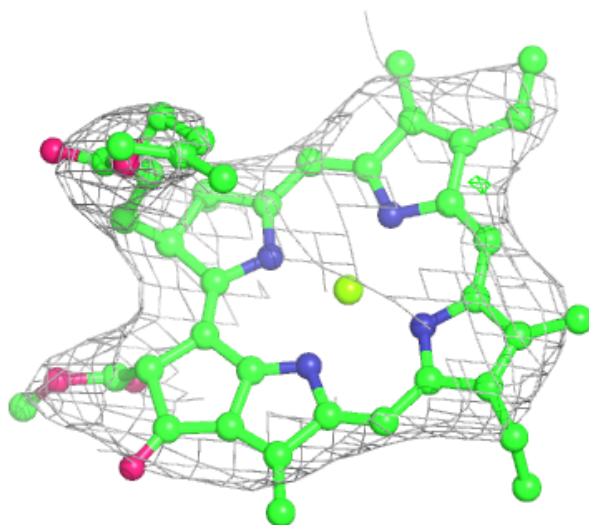
Electron density around CHL 2 304:

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



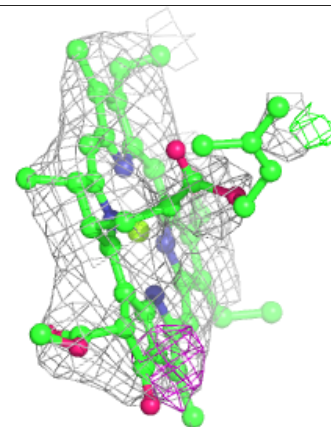
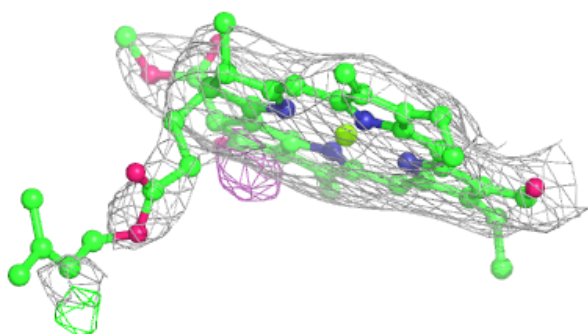
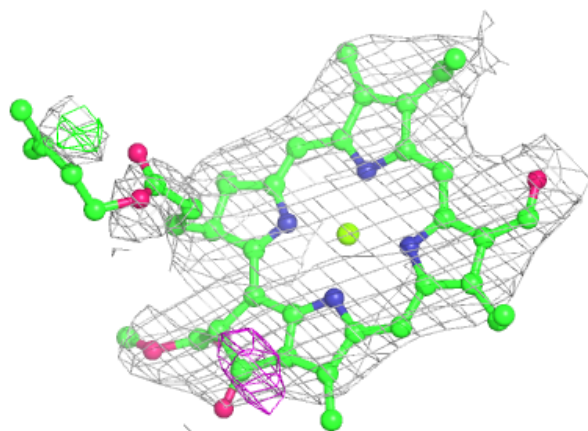
Electron density around CLA 3 608:

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

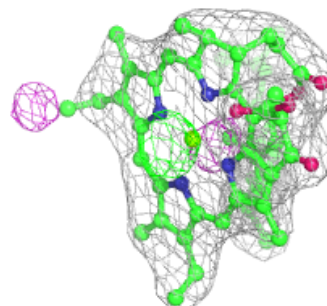
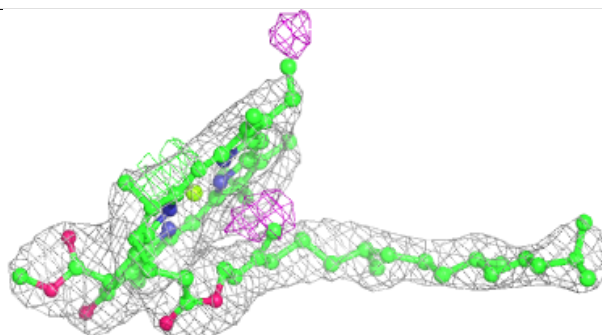
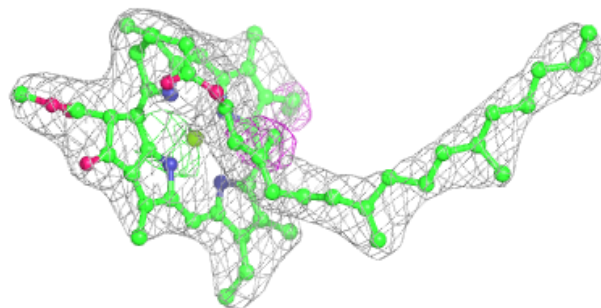


Electron density around CHL 2 306:

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

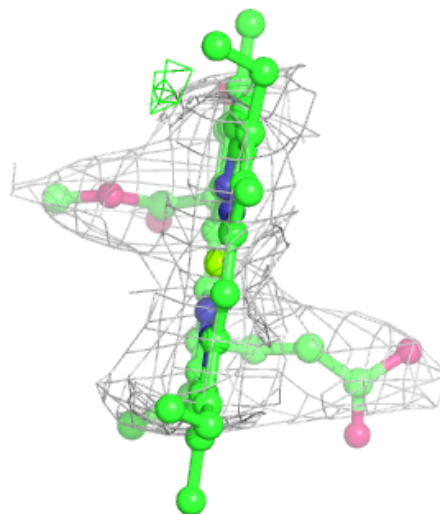
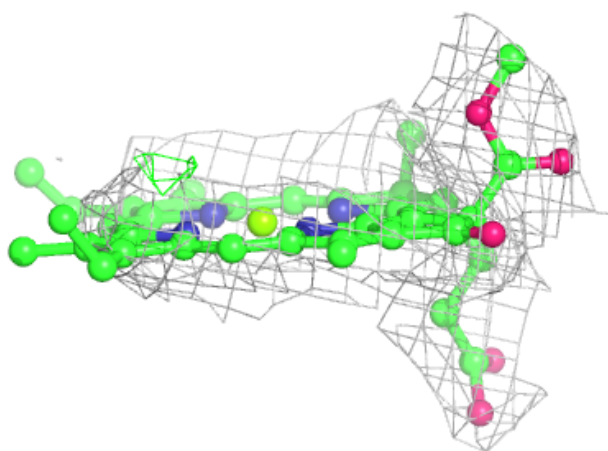
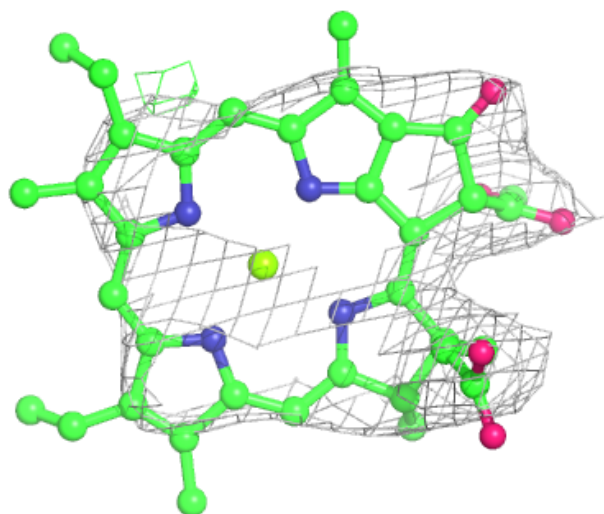
**Electron density around CLA A 840:**

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



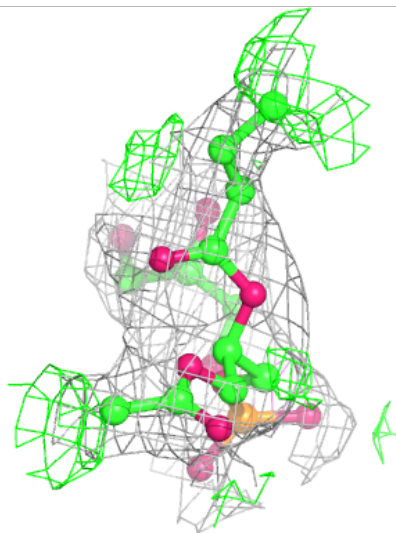
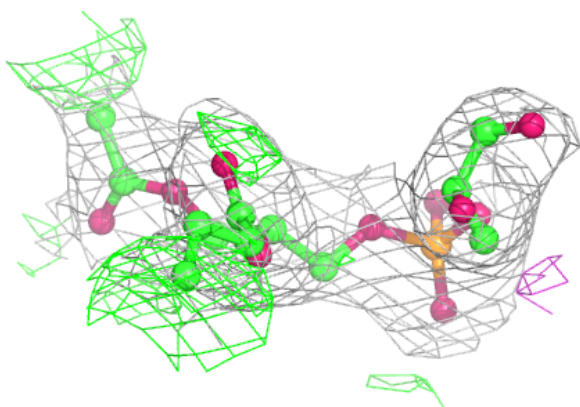
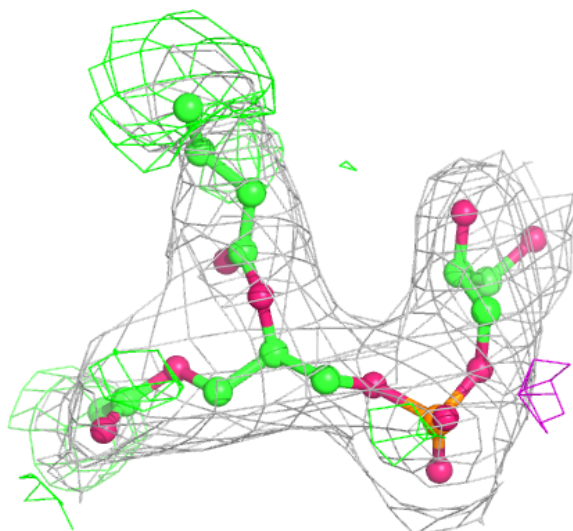
Electron density around CLA A 819:

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



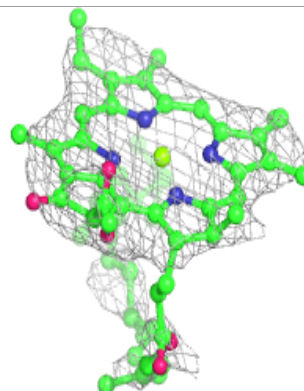
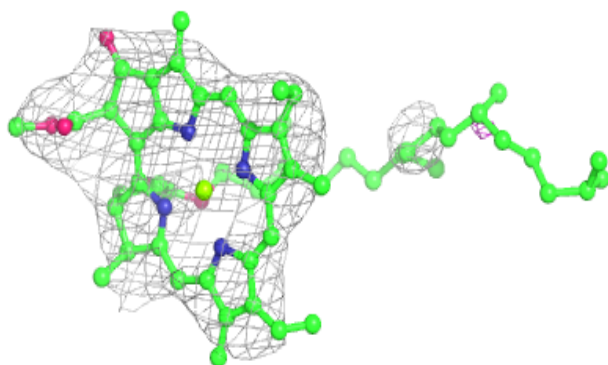
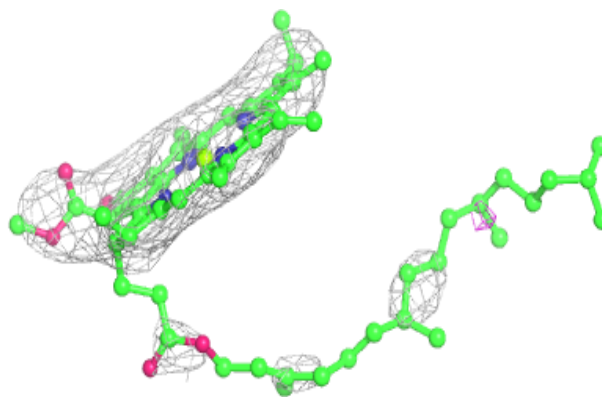
Electron density around LHG B 801:

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

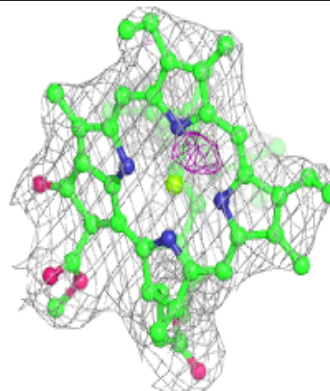
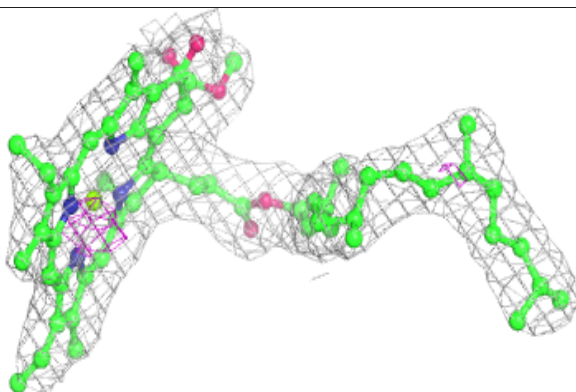
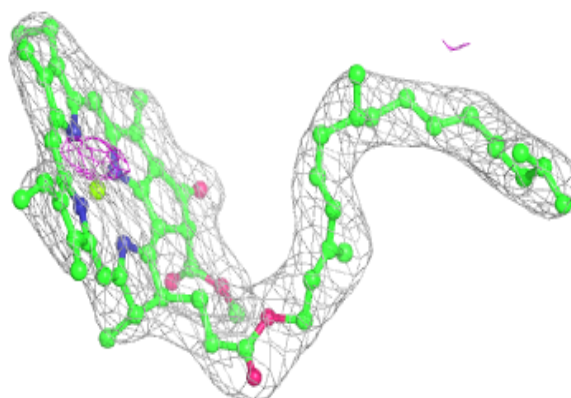


Electron density around CLA B 803:

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

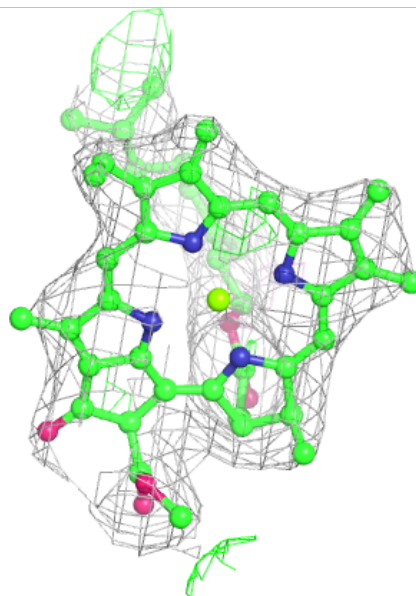
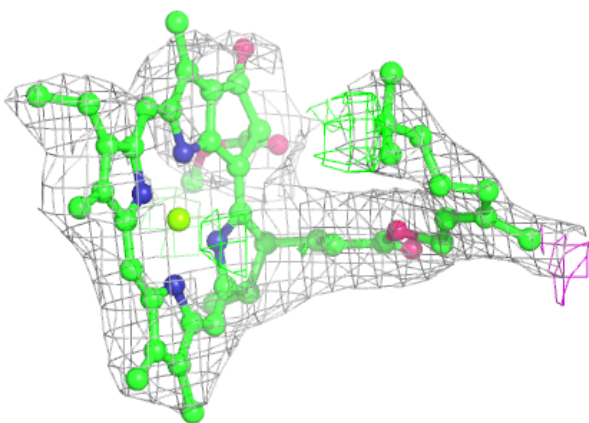
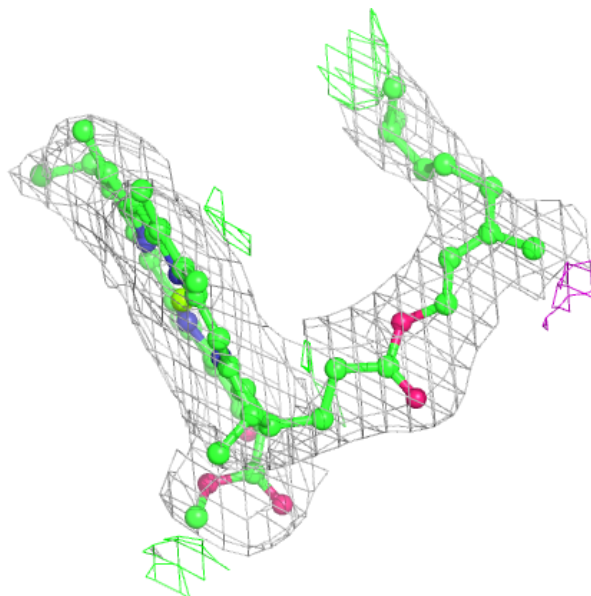
**Electron density around CLA B 804:**

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



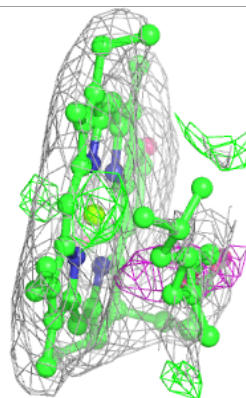
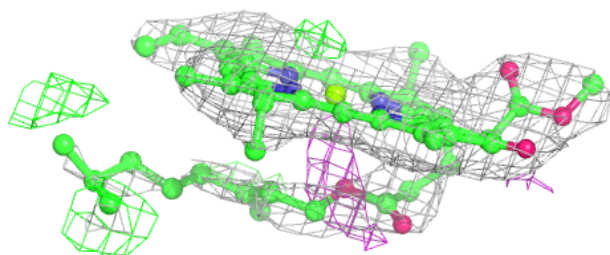
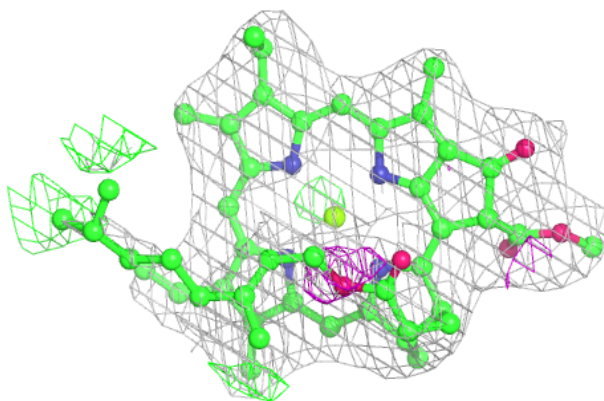
Electron density around CLA B 813:

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

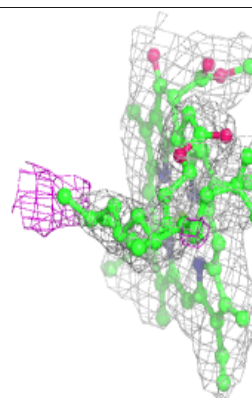
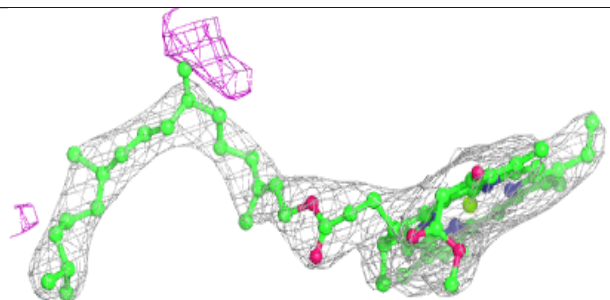
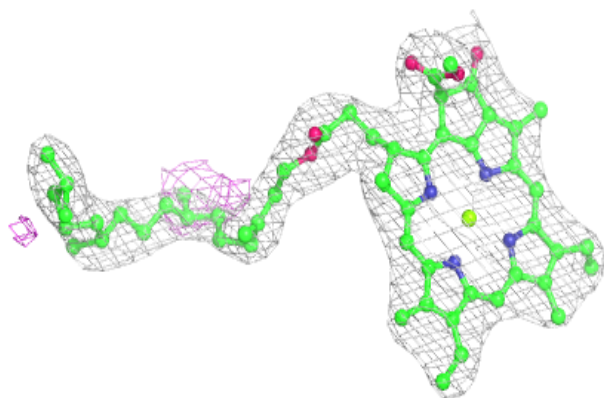


Electron density around CLA B 814:

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

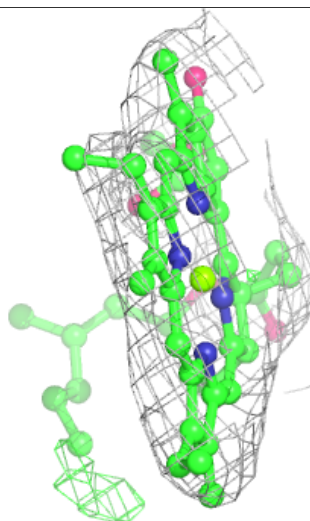
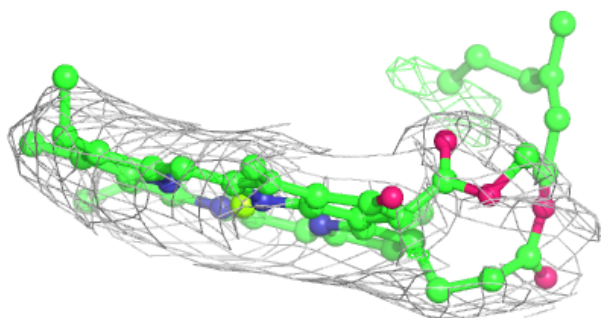
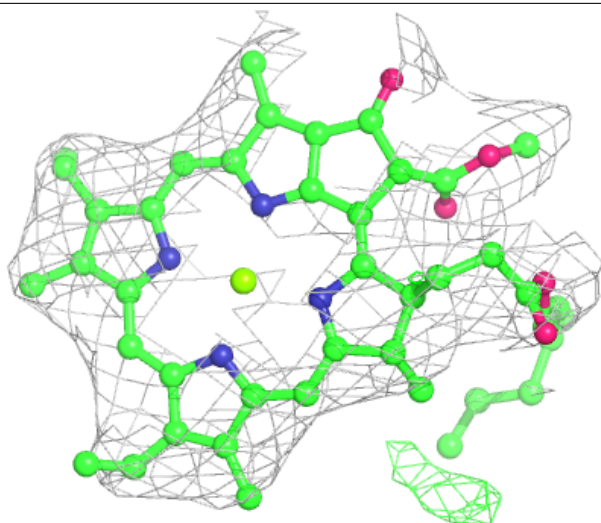
**Electron density around CLA B 815:**

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



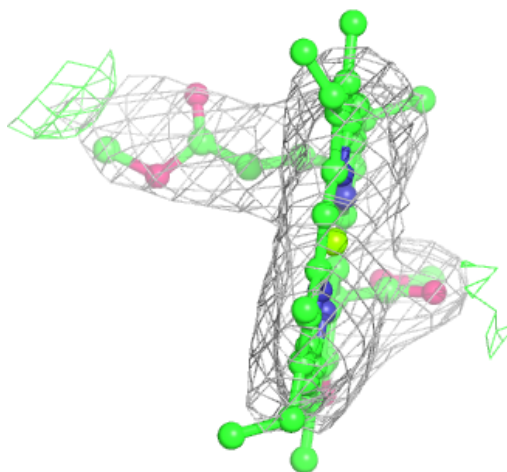
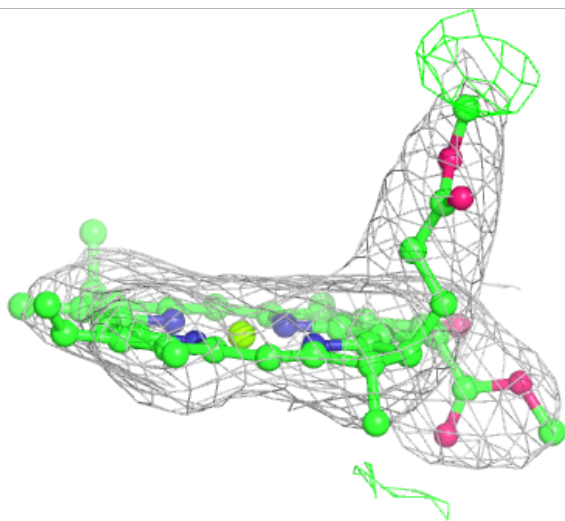
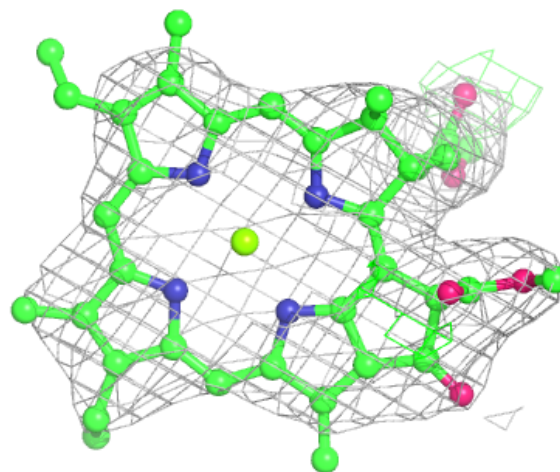
Electron density around CLA 1 310:

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



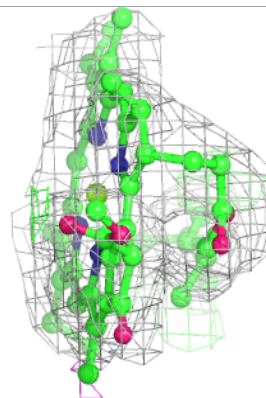
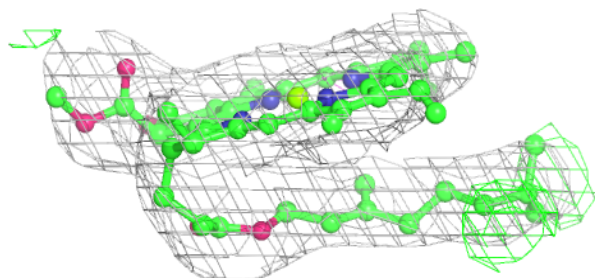
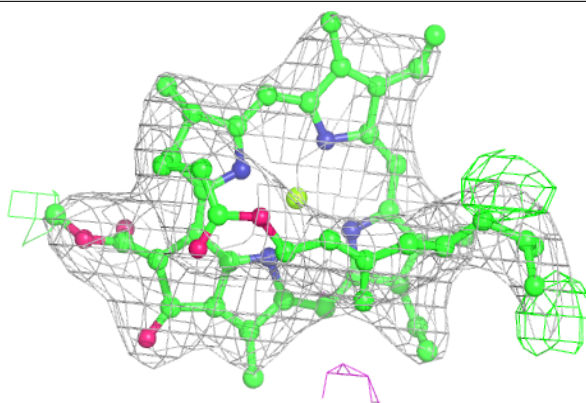
Electron density around CLA 1 306:

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

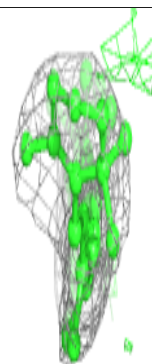
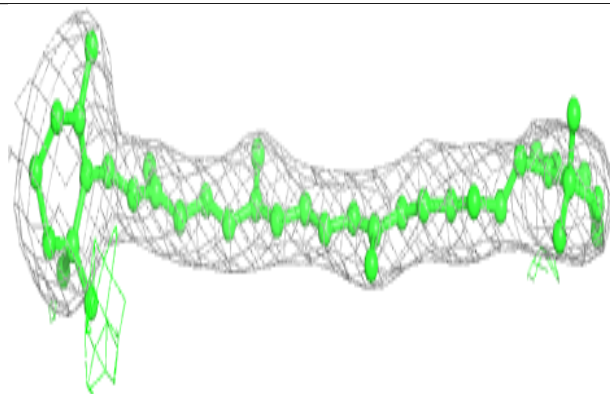
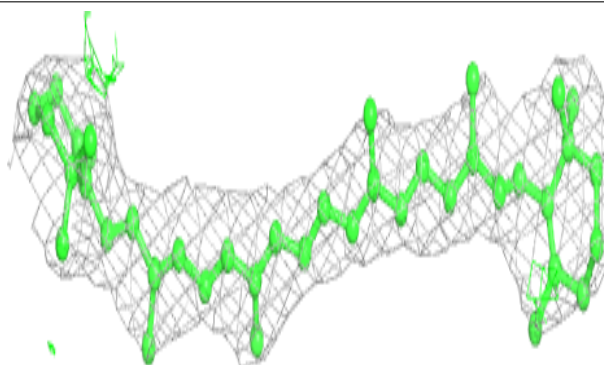


Electron density around CLA B 818:

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

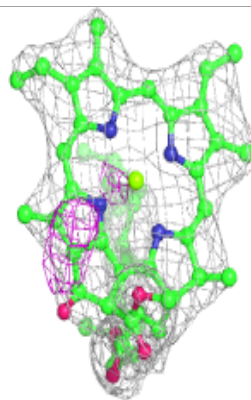
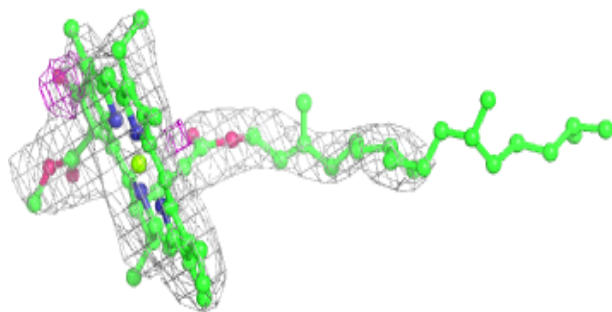
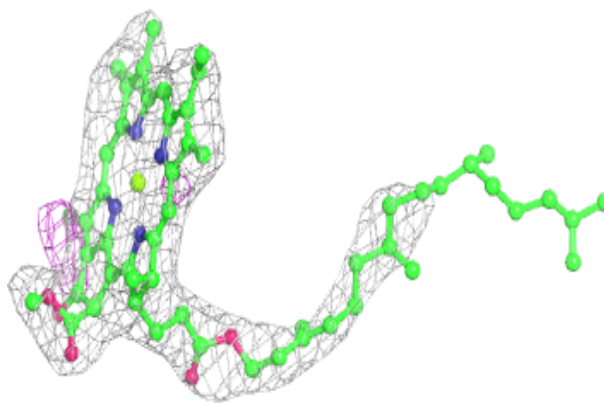
**Electron density around BCR 4 318:**

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



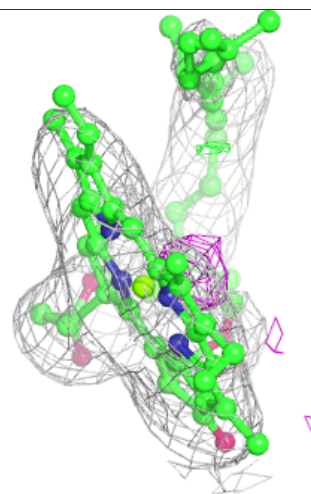
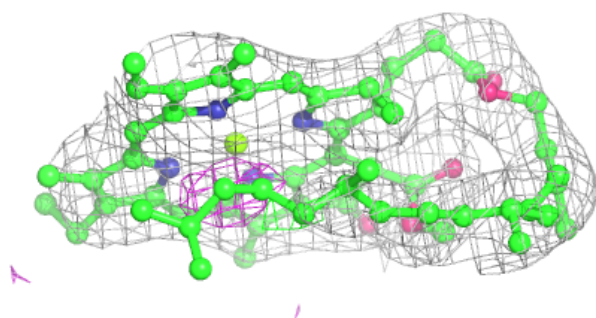
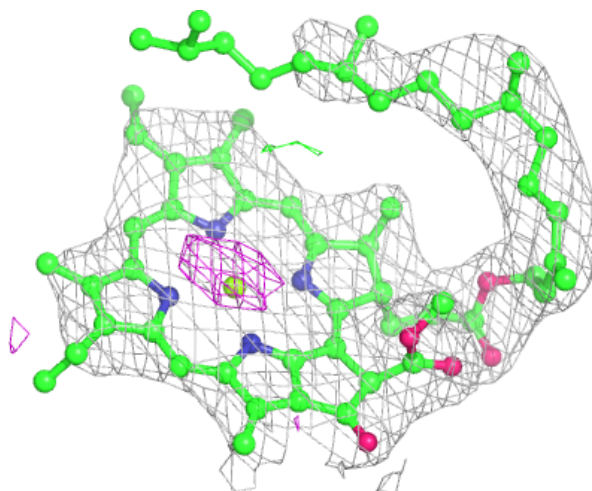
Electron density around CLA B 823:

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



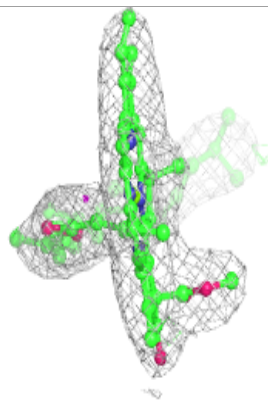
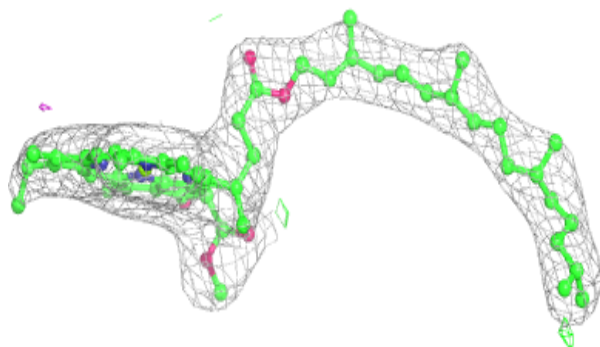
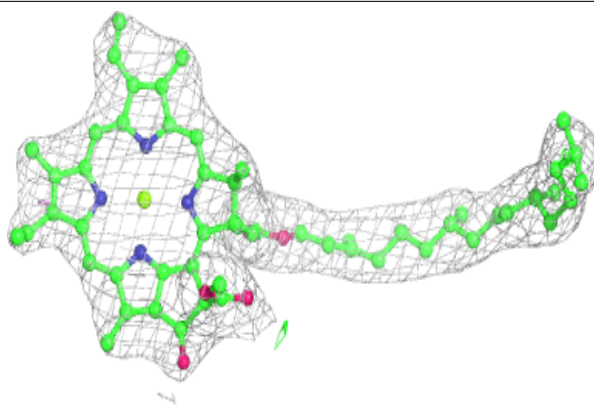
Electron density around CLA 1 302:

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



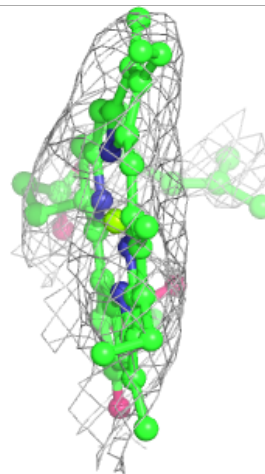
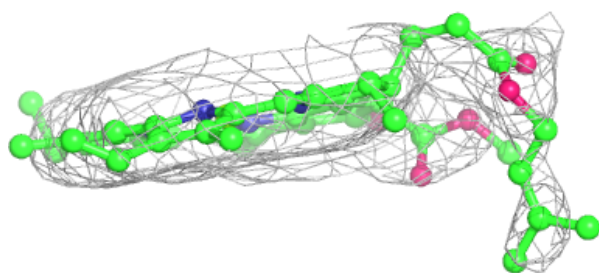
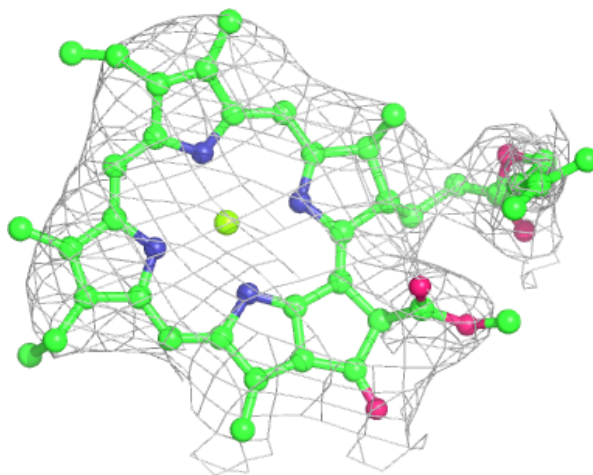
Electron density around CLA B 842:

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



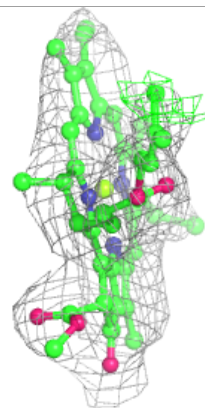
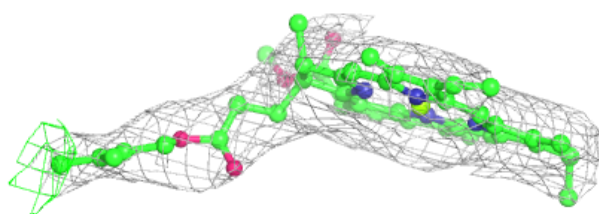
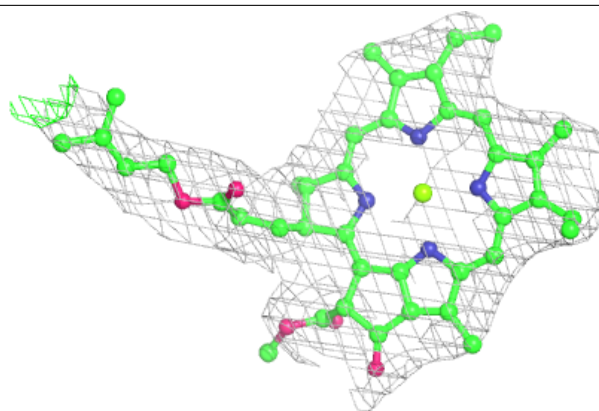
Electron density around CLA 3 603:

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

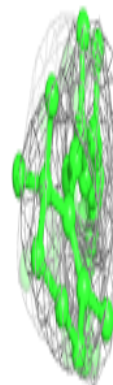
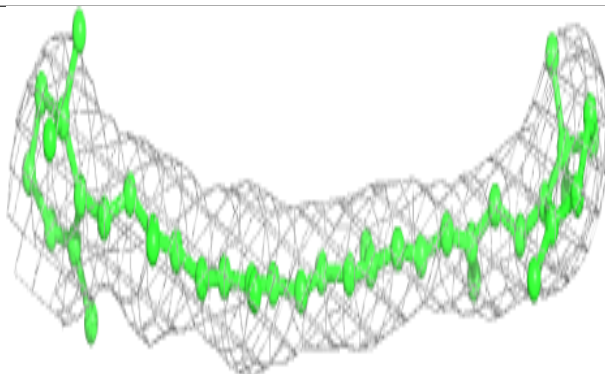
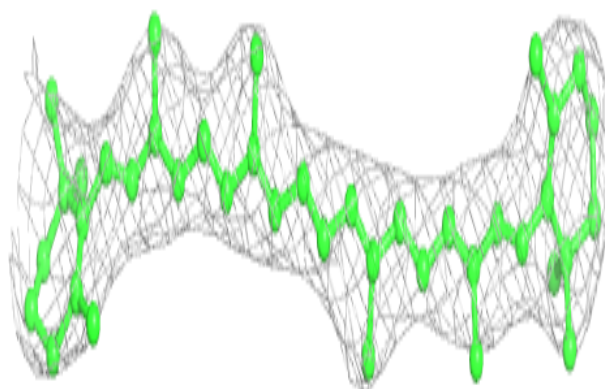


Electron density around CLA G 104:

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

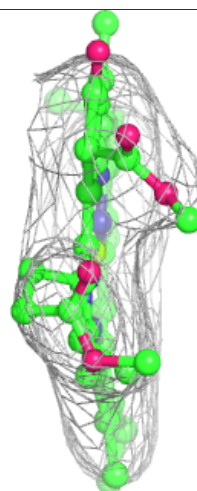
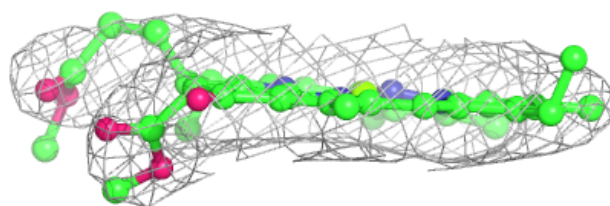
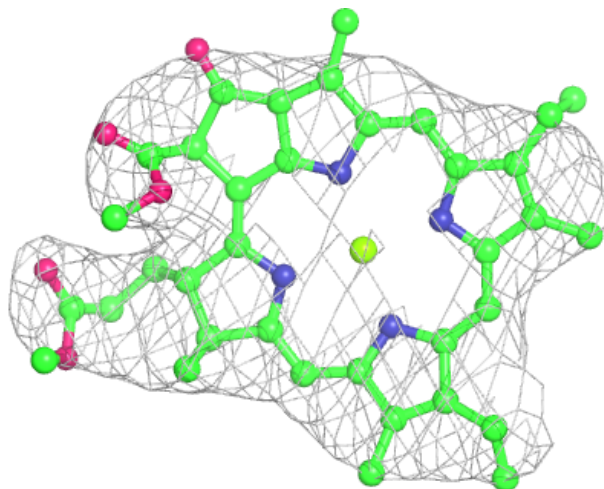
**Electron density around BCR B 844:**

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



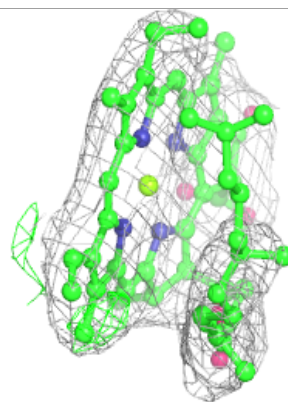
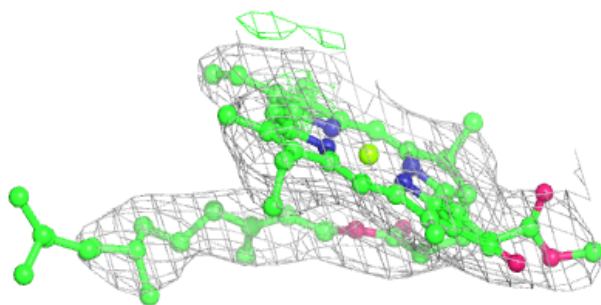
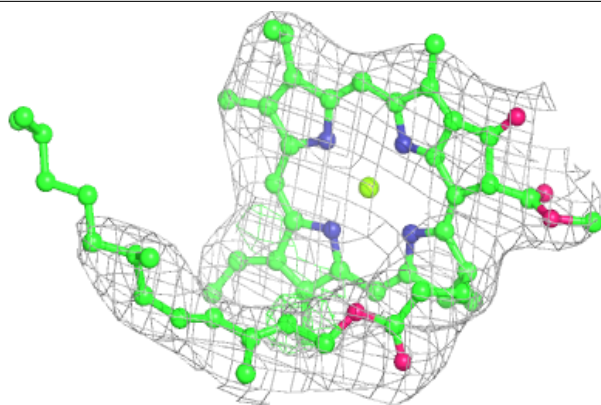
Electron density around CLA G 105:

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

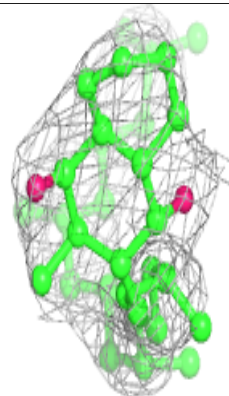
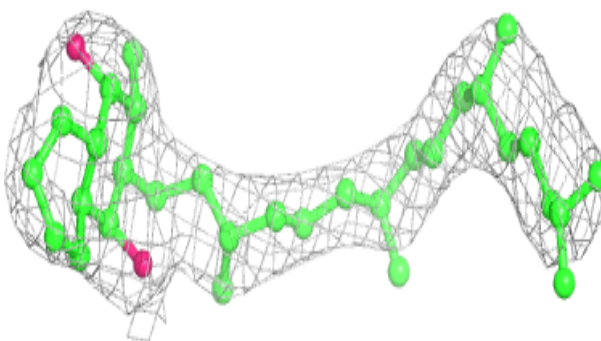
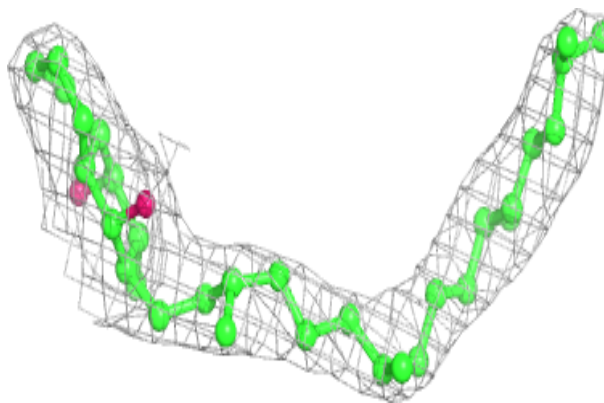


Electron density around CLA 1 308:

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

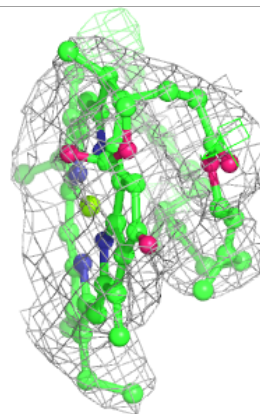
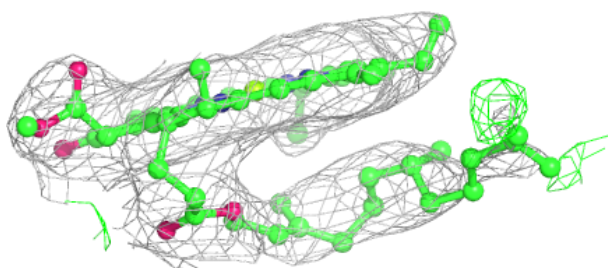
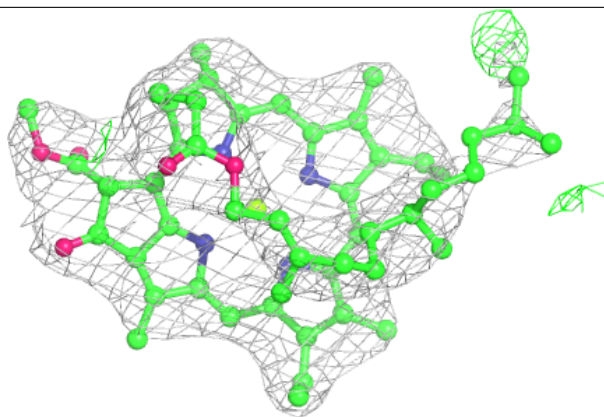
**Electron density around PQN B 843:**

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



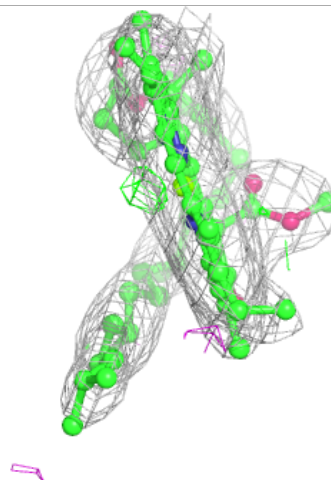
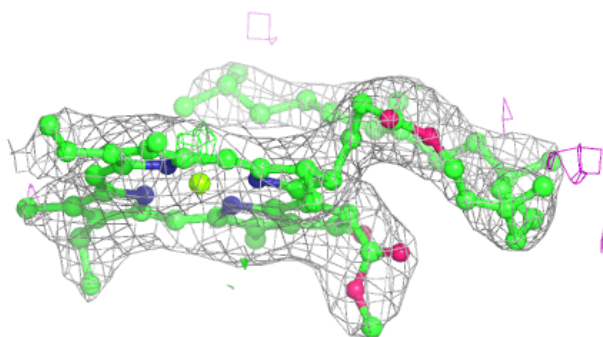
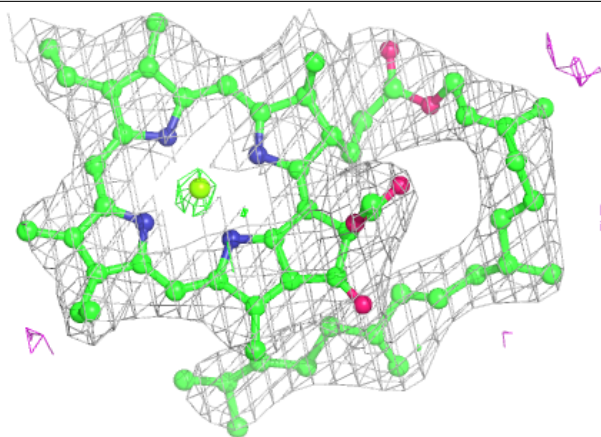
Electron density around CLA 1 311:

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



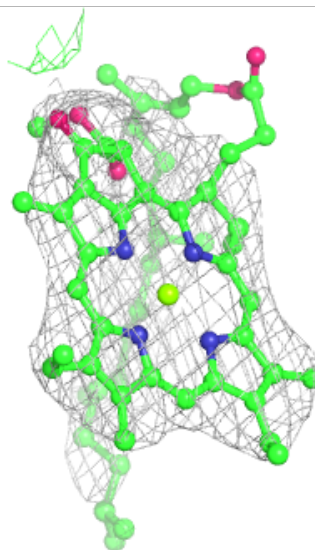
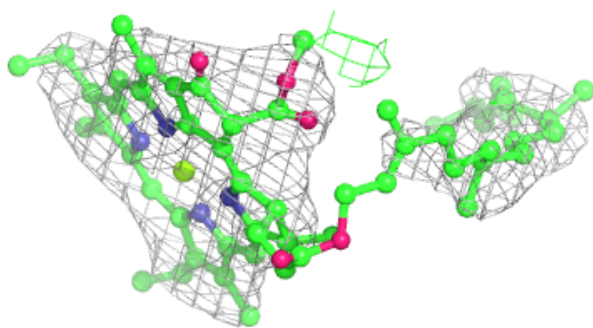
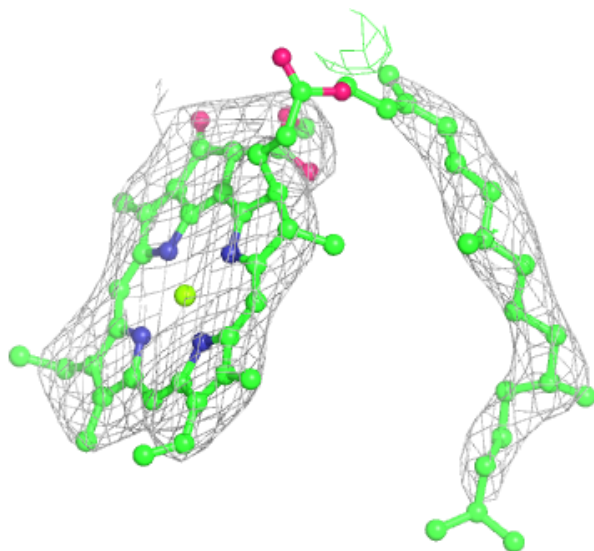
Electron density around CLA B 807:

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



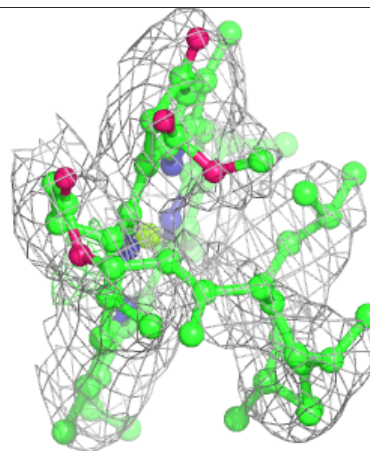
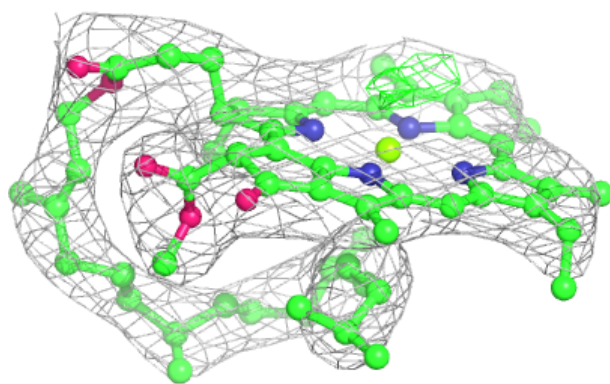
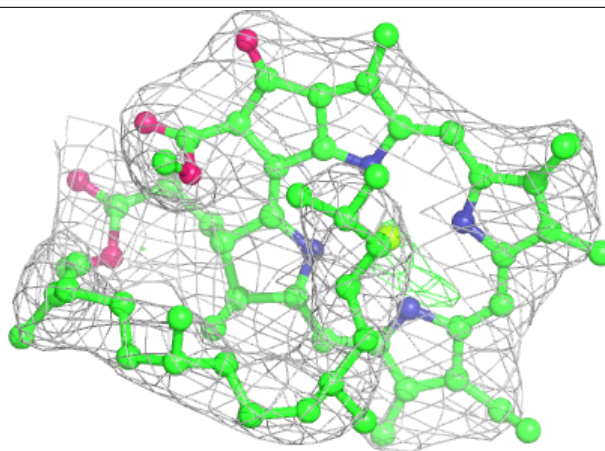
Electron density around CLA B 812:

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

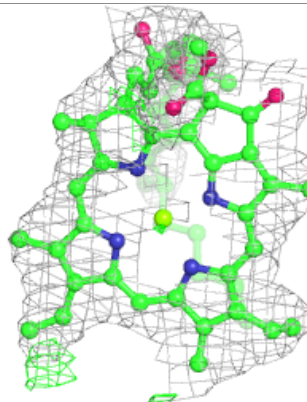
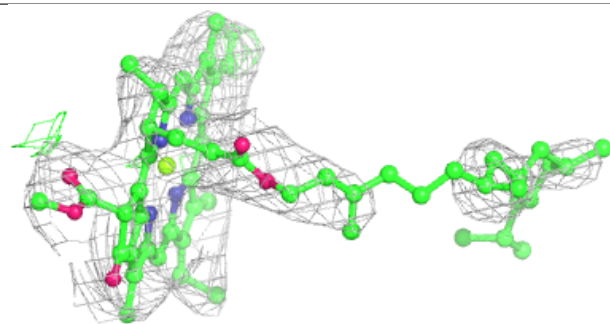
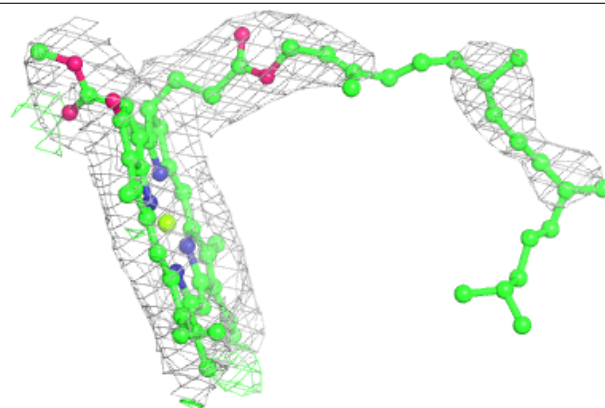


Electron density around CLA A 805:

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

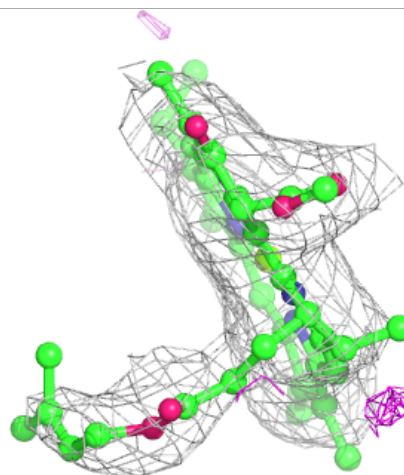
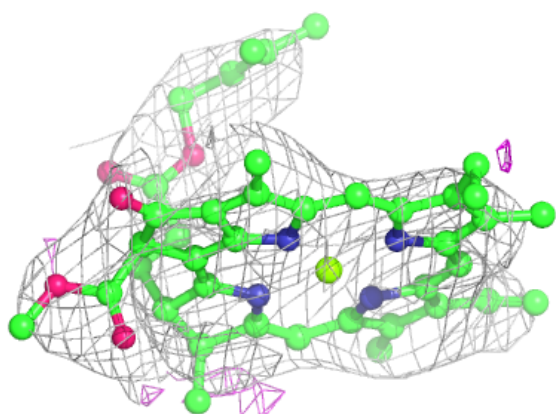
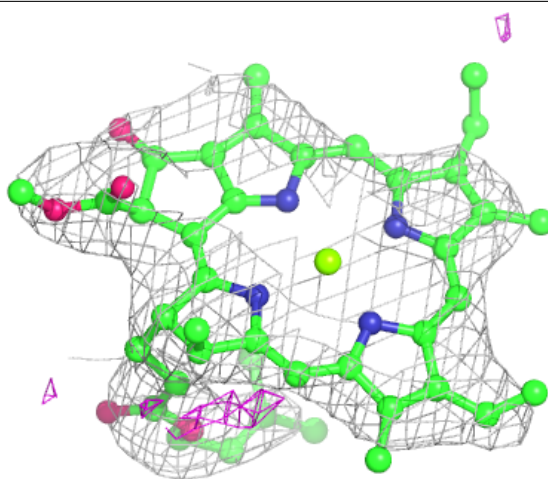
**Electron density around CLA A 806:**

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



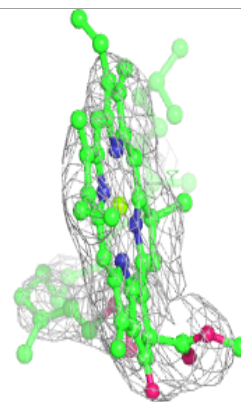
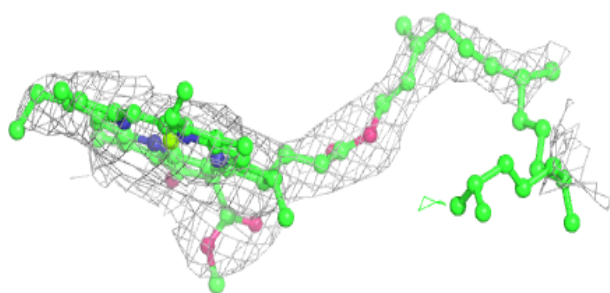
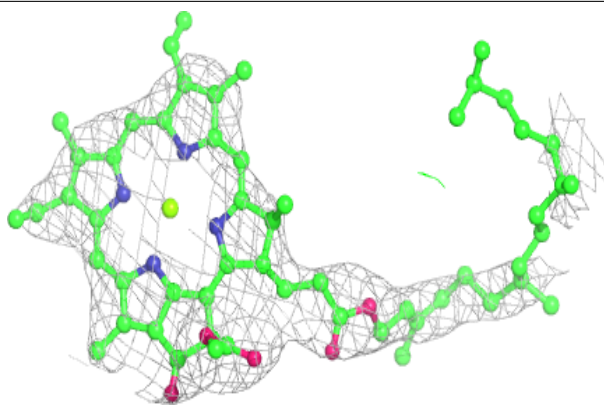
Electron density around CLA 2 307:

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



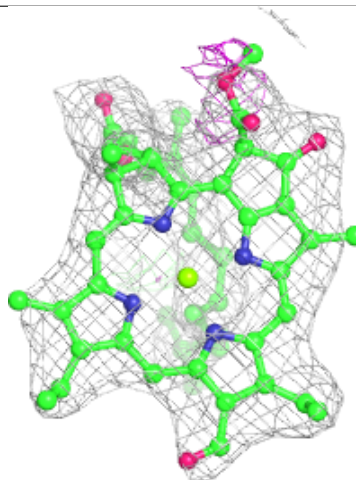
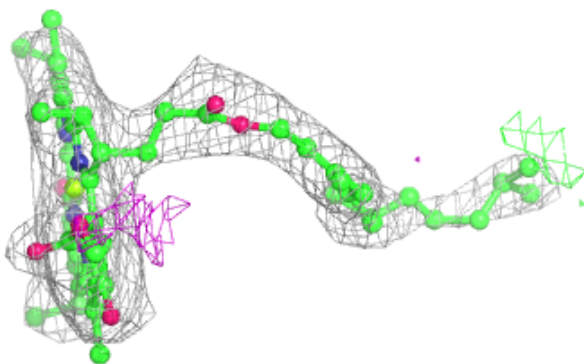
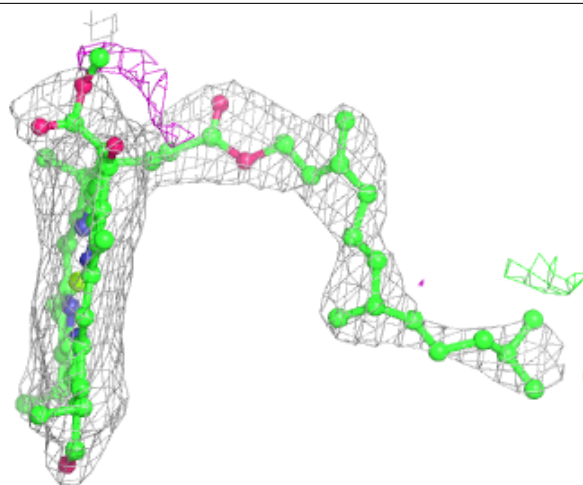
Electron density around CLA A 826:

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



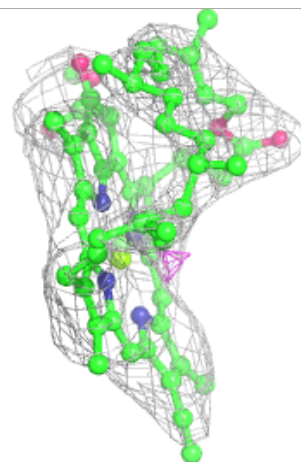
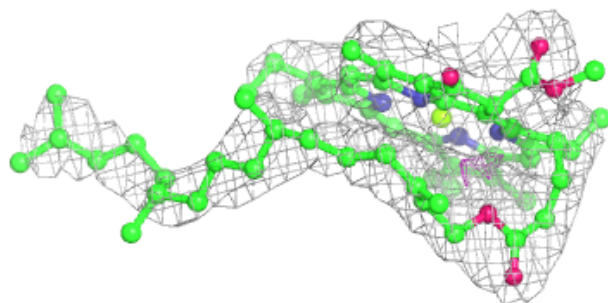
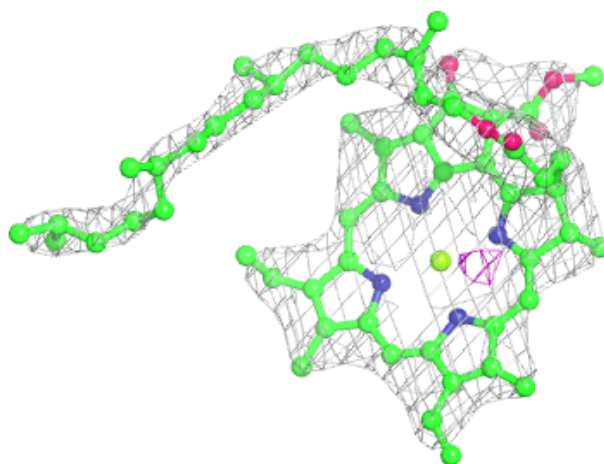
Electron density around CHL 4 301:

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



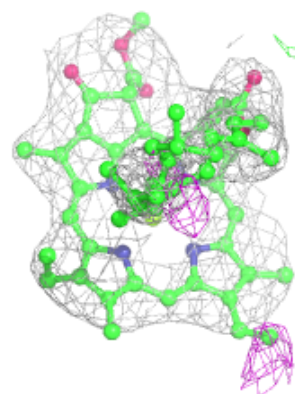
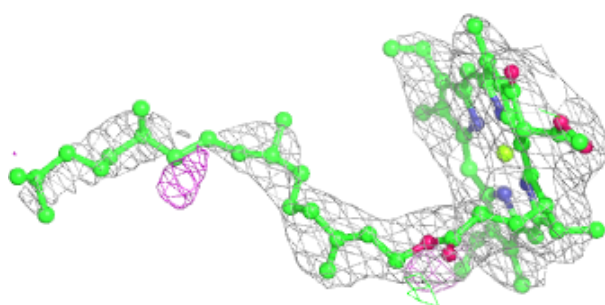
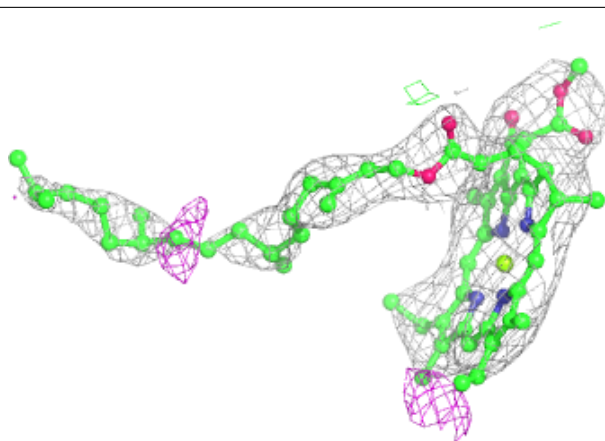
Electron density around CLA A 828:

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

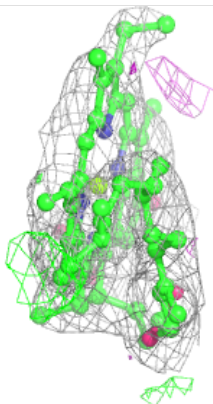
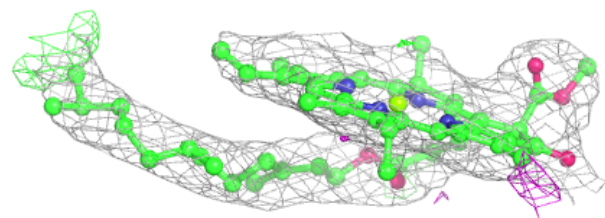
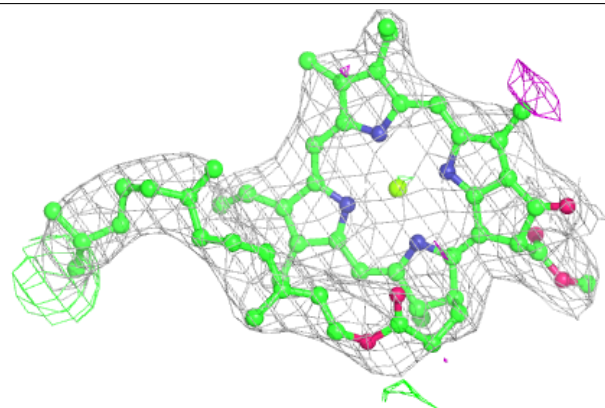


Electron density around CLA A 810:

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

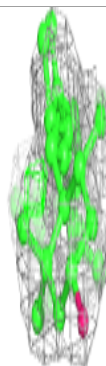
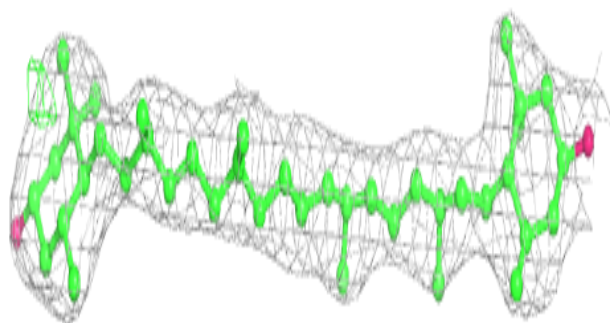
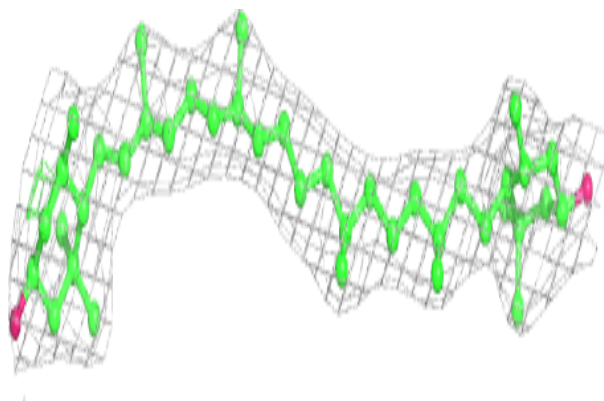
**Electron density around CLA B 820:**

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

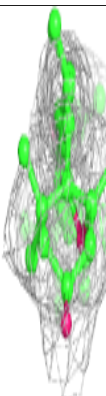
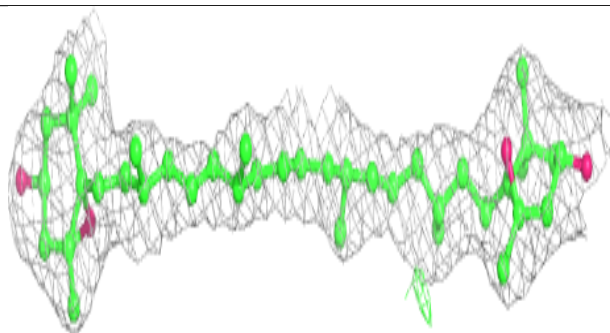
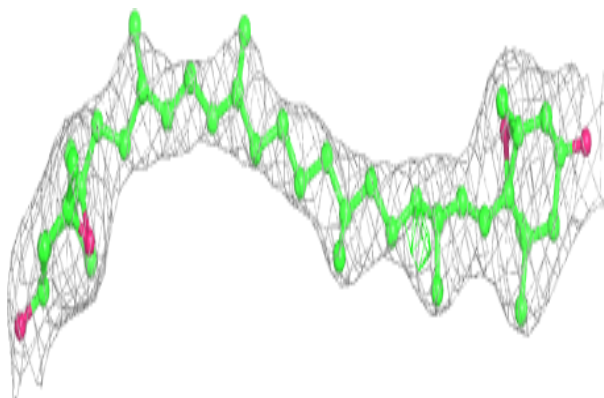


Electron density around LUT 4 316:

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

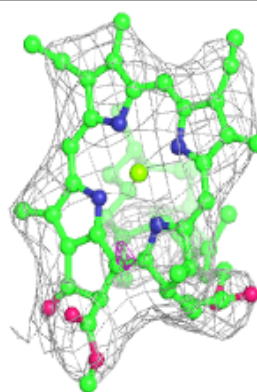
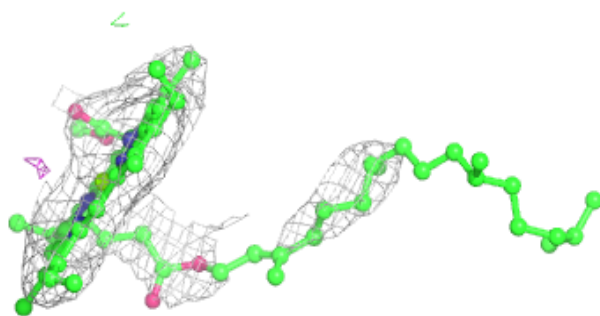
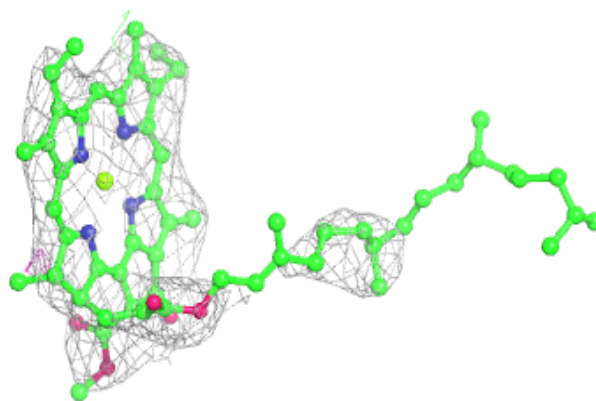
**Electron density around XAT 1 315:**

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



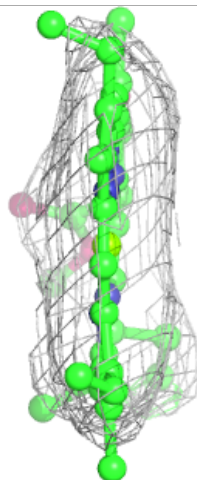
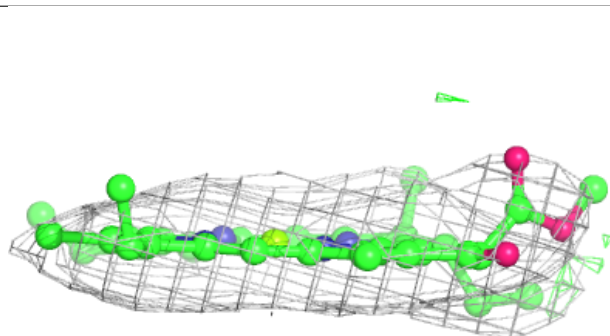
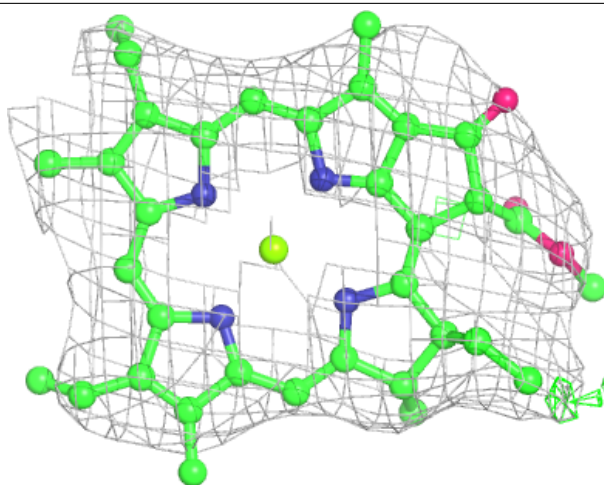
Electron density around CLA 1 309:

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



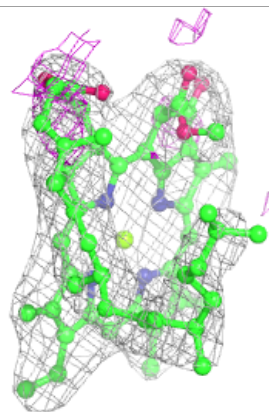
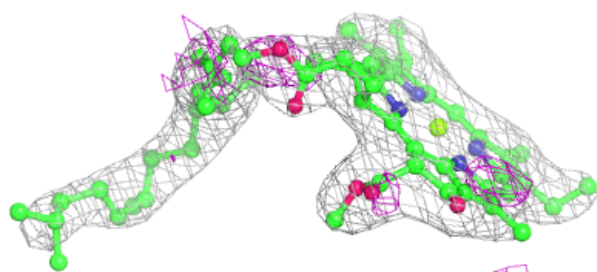
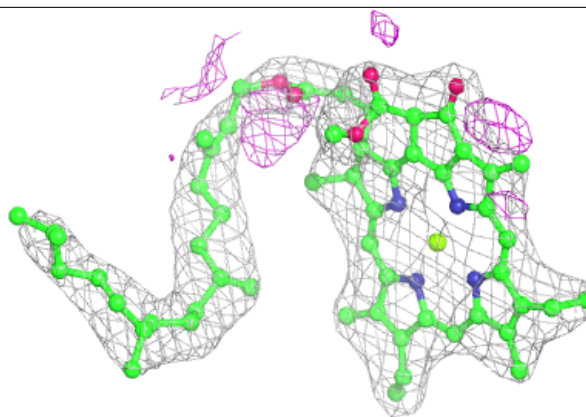
Electron density around CLA 3 605:

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

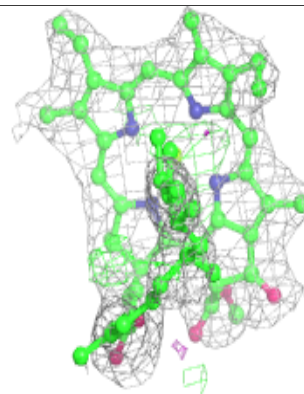
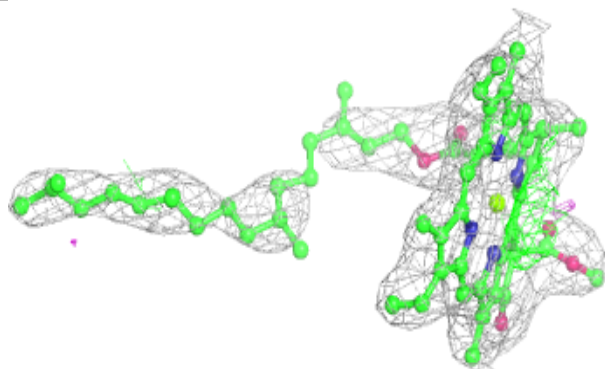
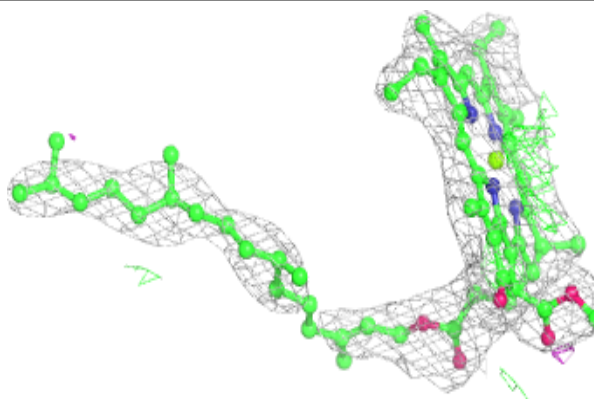


Electron density around CLA B 826:

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

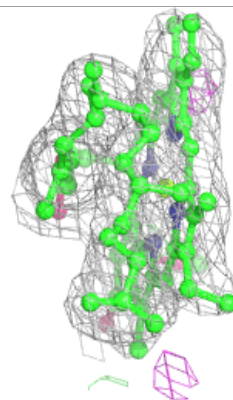
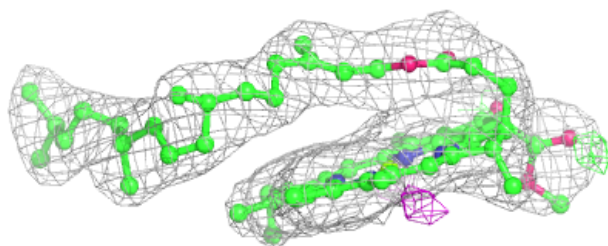
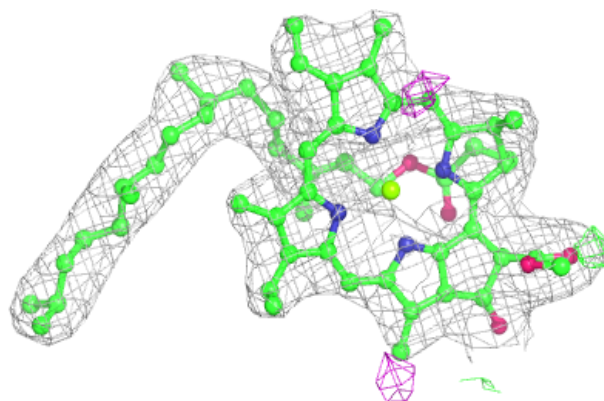
**Electron density around CLA B 831:**

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



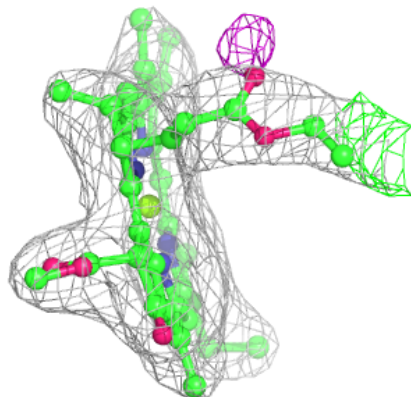
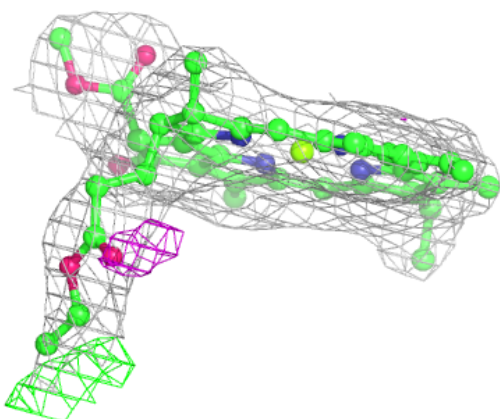
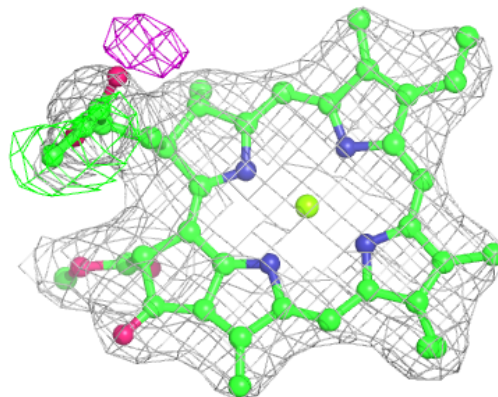
Electron density around CLA B 838:

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



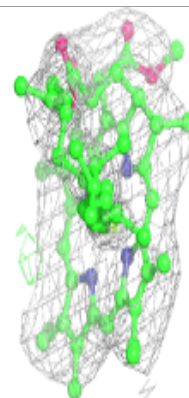
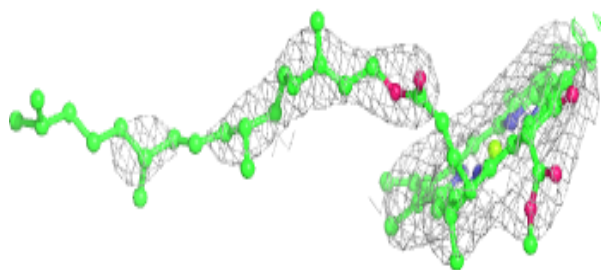
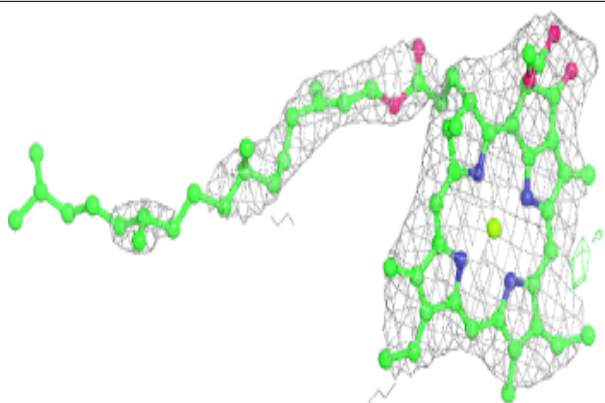
Electron density around CLA B 839:

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

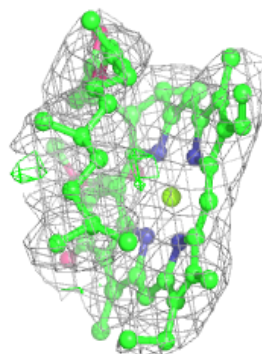
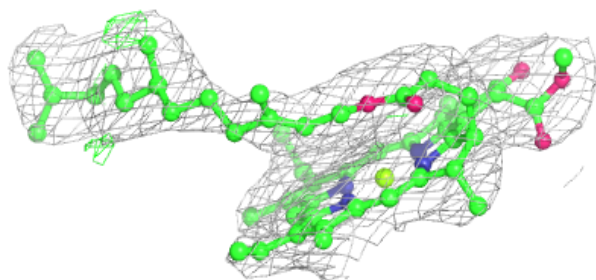
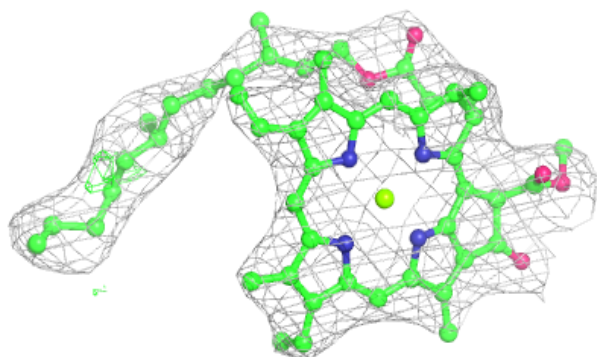


Electron density around CLA A 832:

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

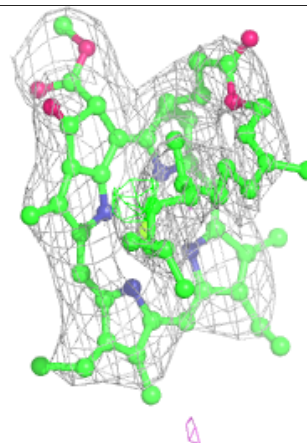
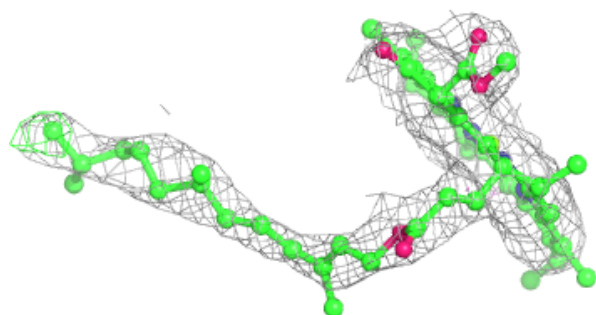
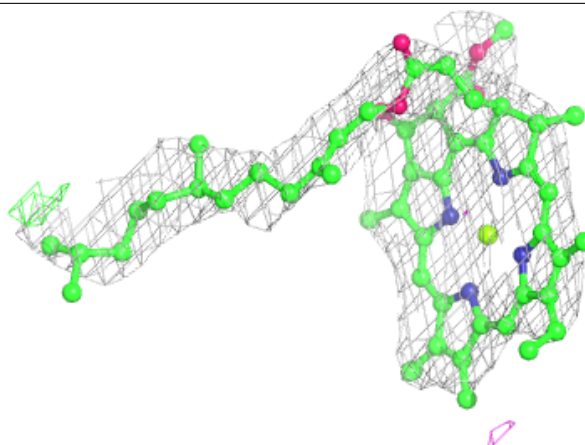
**Electron density around CLA 4 309:**

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

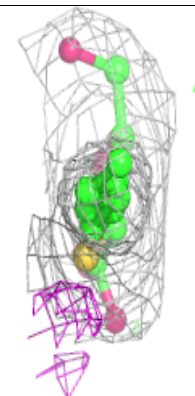
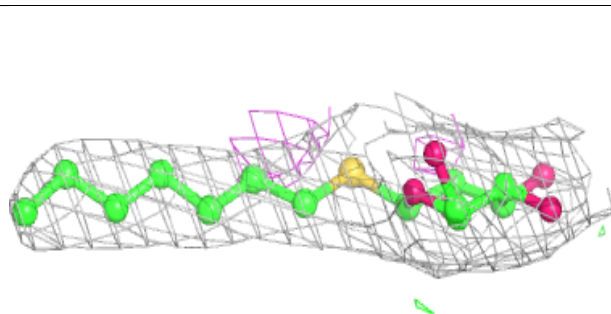
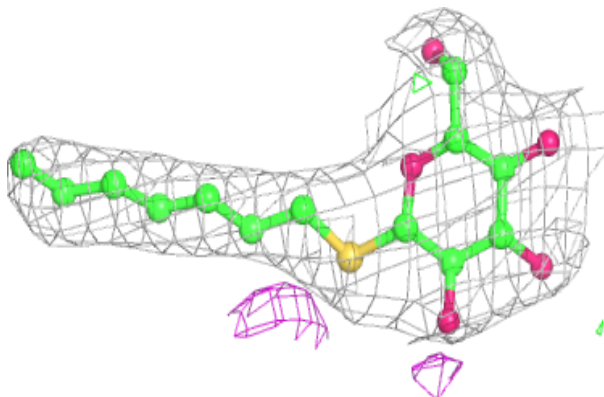


Electron density around CLA 4 310:

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

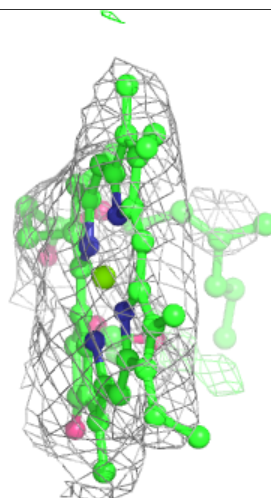
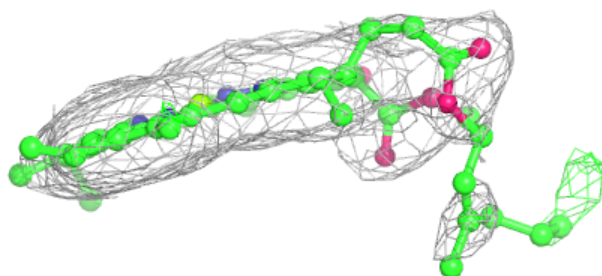
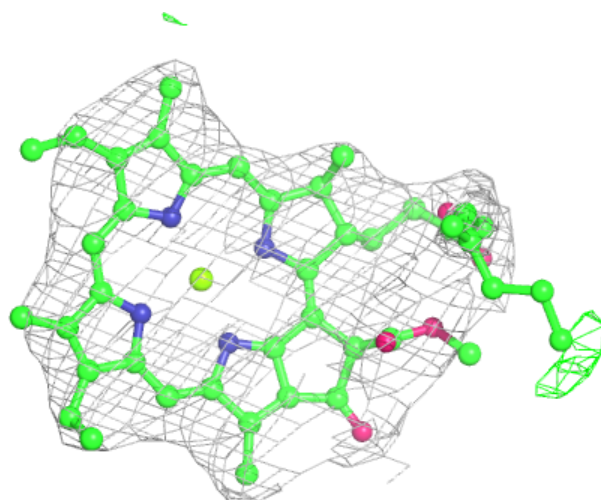
**Electron density around HTG A 854:**

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



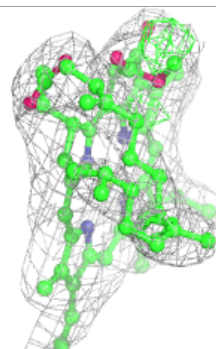
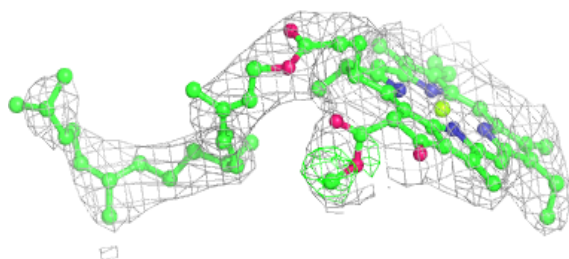
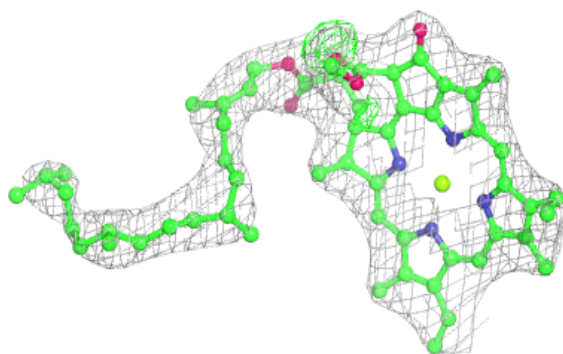
Electron density around CLA 4 311:

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



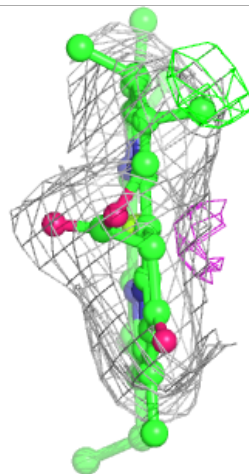
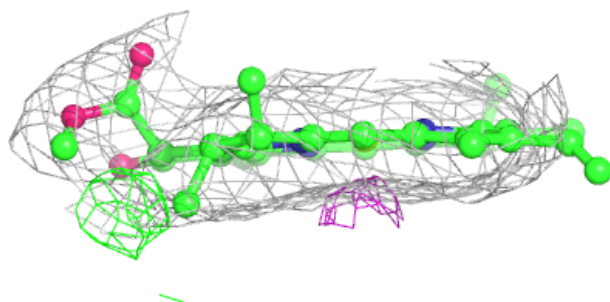
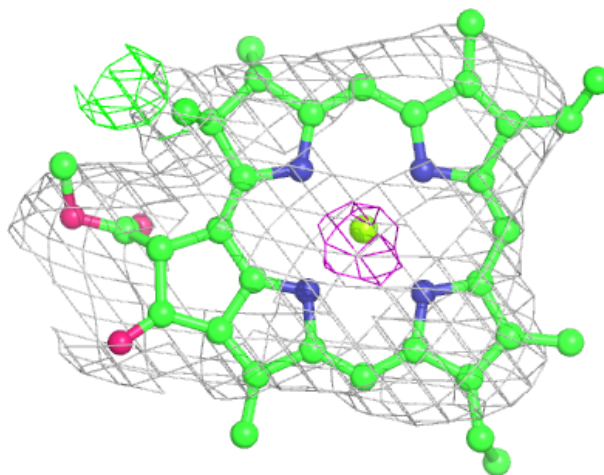
Electron density around CLA J 101:

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



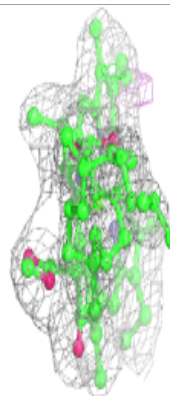
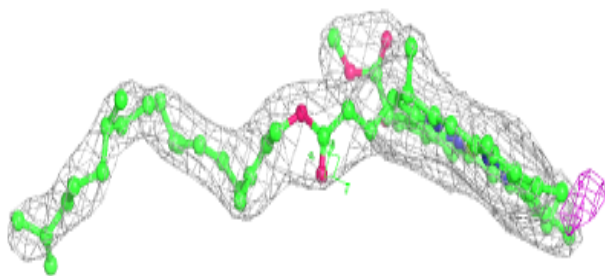
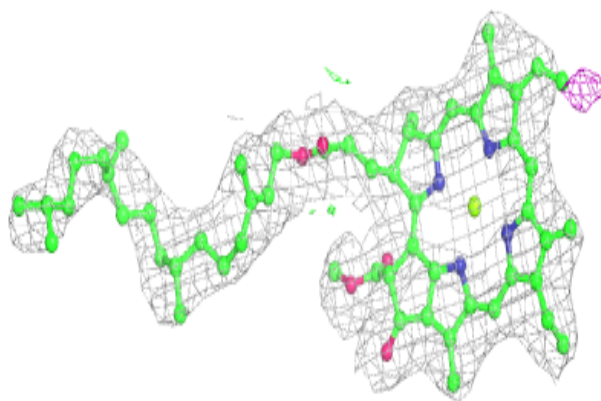
Electron density around CLA 2 309:

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

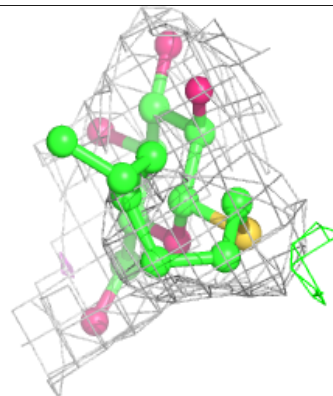
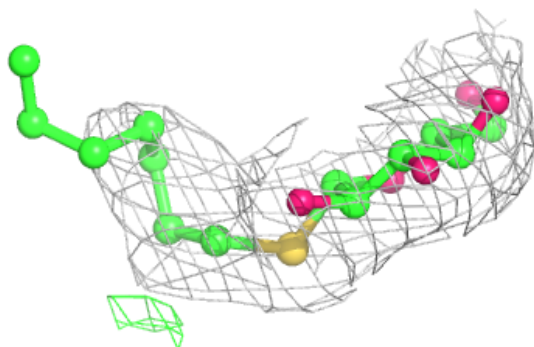
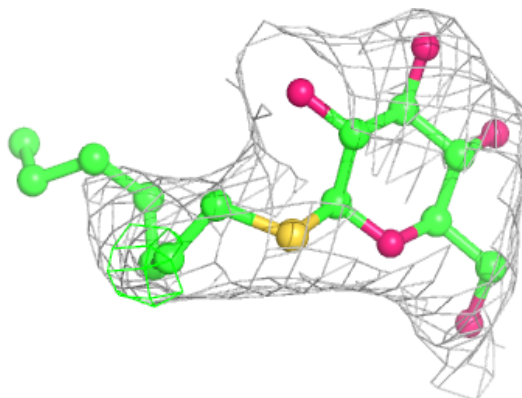


Electron density around CLA A 839:

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

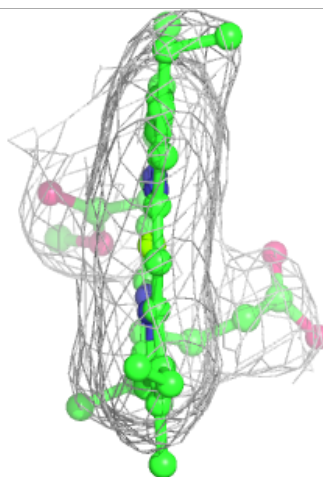
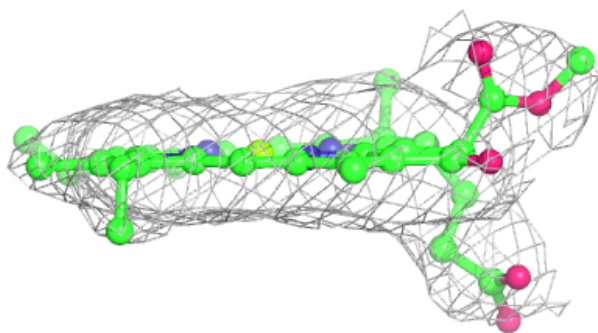
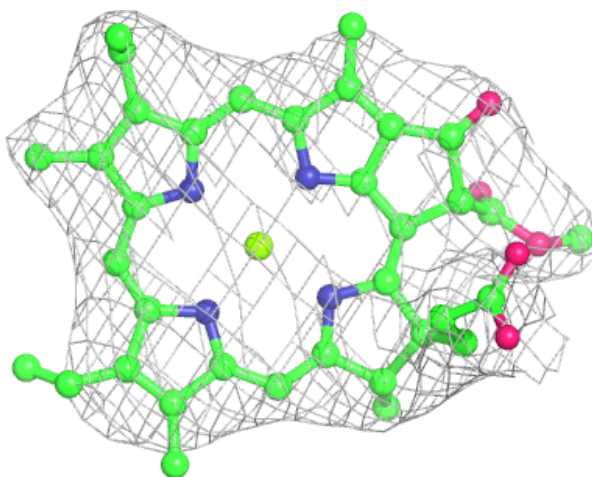
**Electron density around HTG J 102:**

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



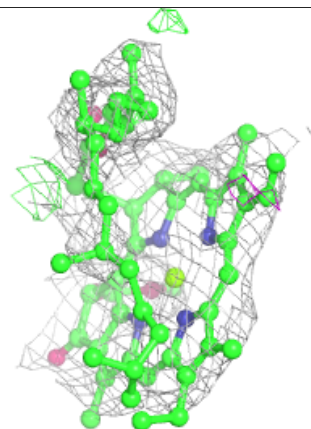
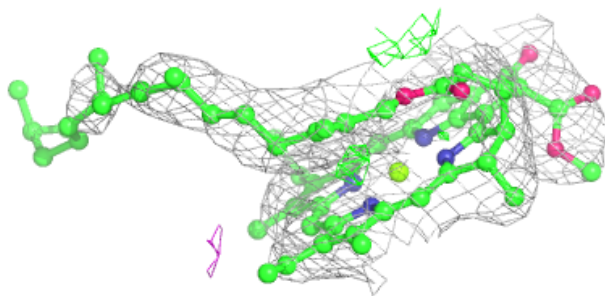
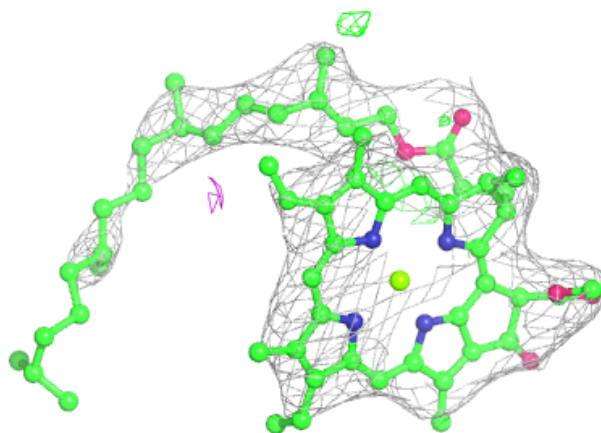
Electron density around CLA 4 313:

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

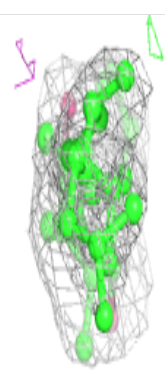
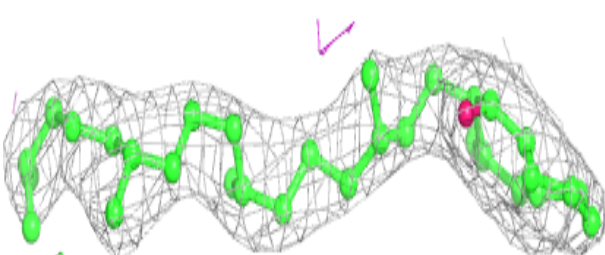
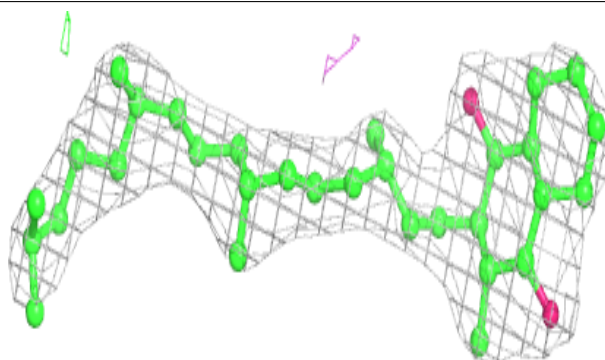


Electron density around CLA 2 301:

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

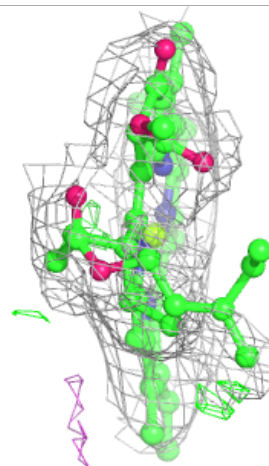
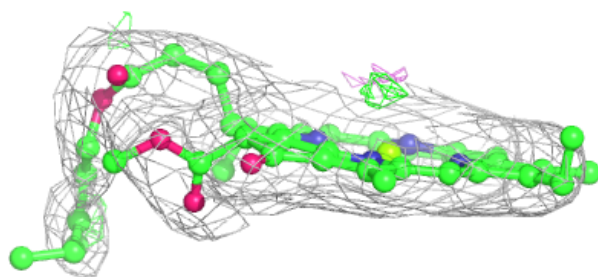
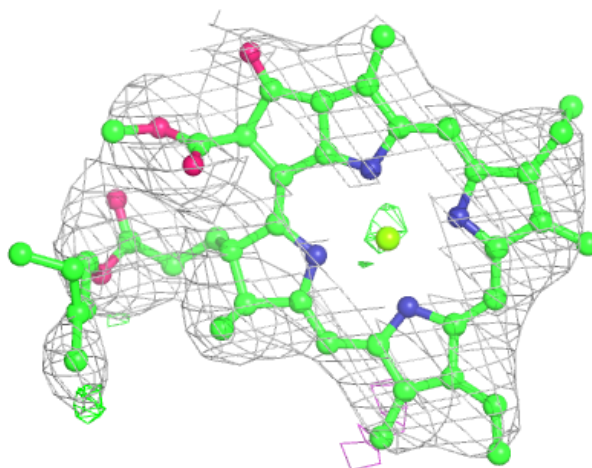
**Electron density around PQN A 842:**

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



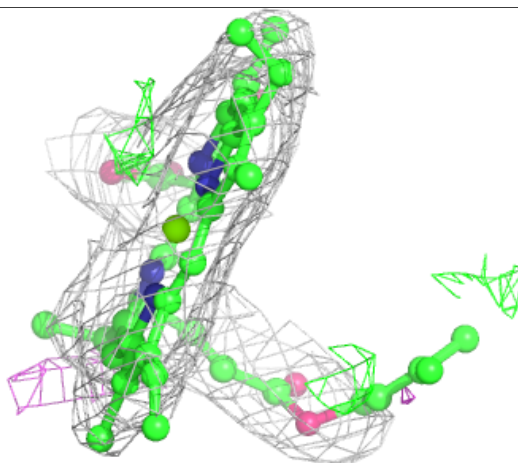
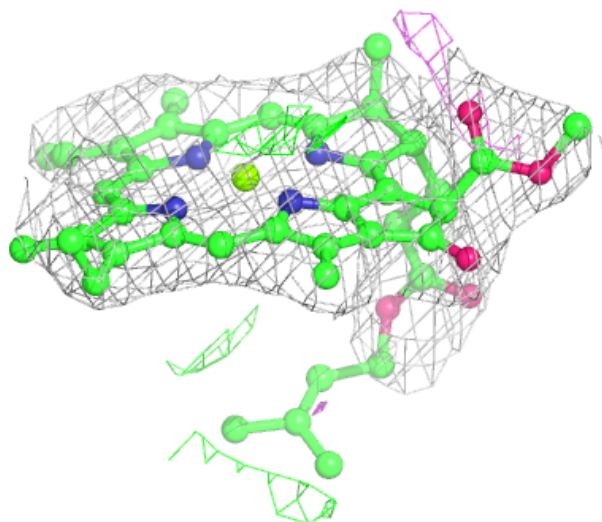
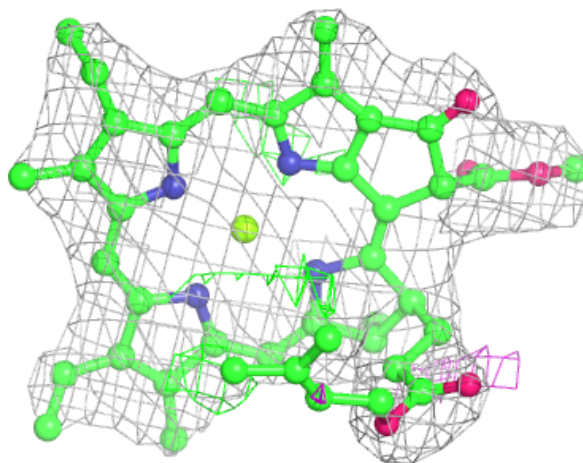
Electron density around CLA 2 302:

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



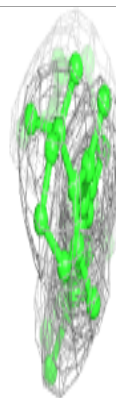
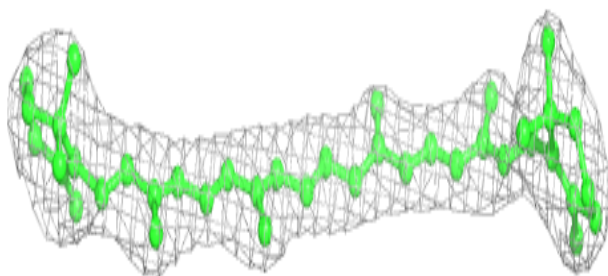
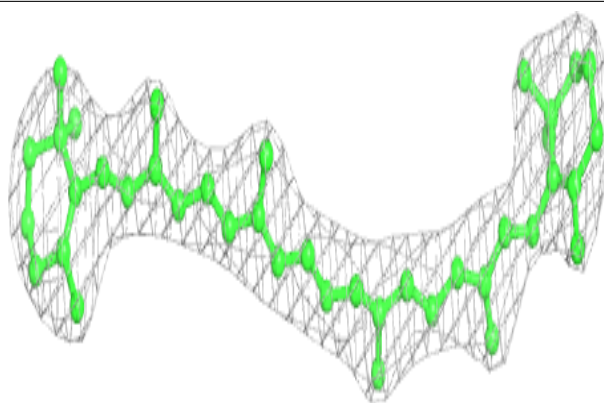
Electron density around CLA 4 308:

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

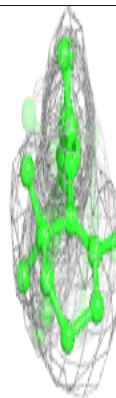
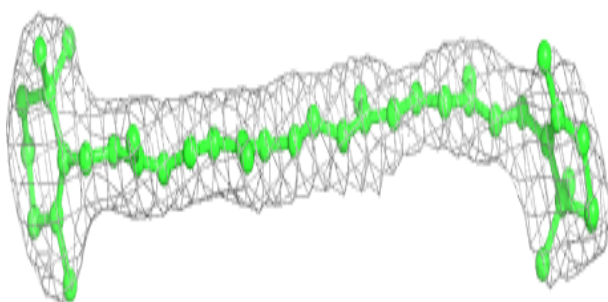
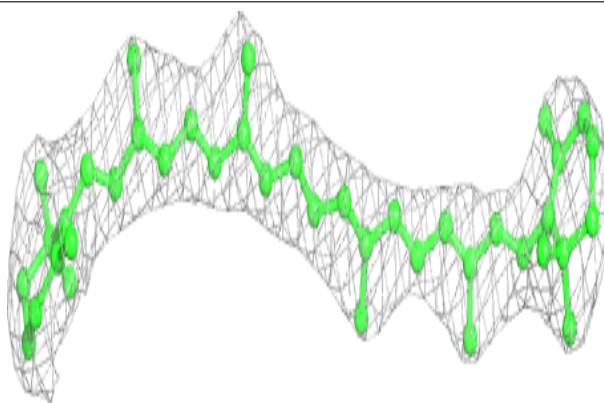


Electron density around BCR B 848:

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

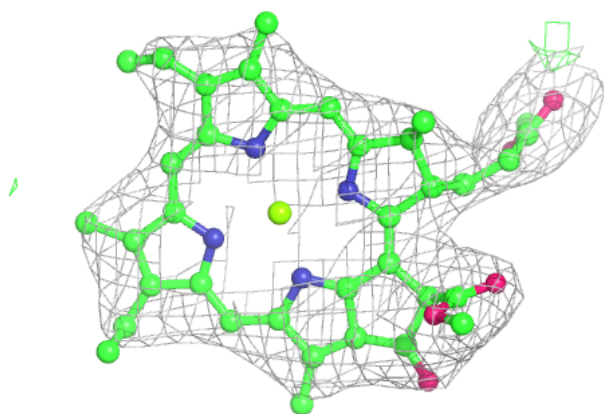
**Electron density around BCR B 849:**

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

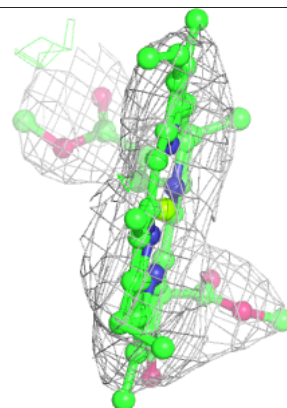
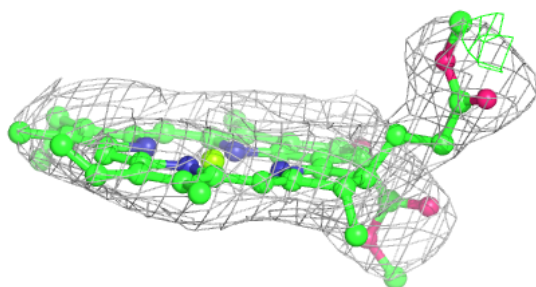


Electron density around CLA 2 319:

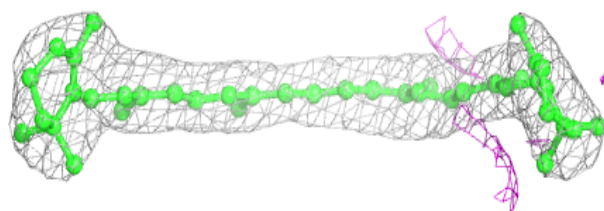
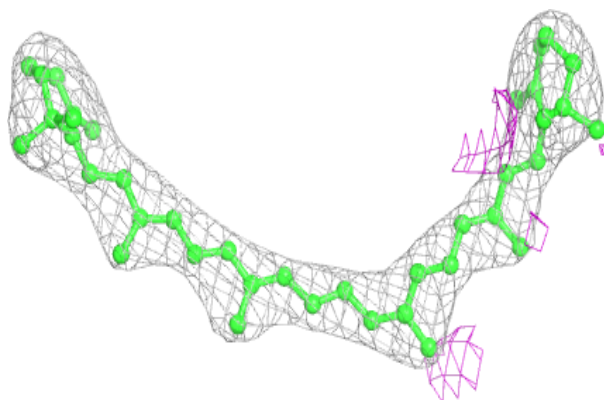
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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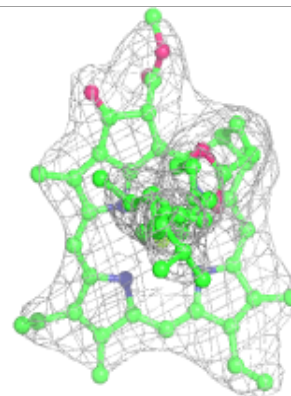
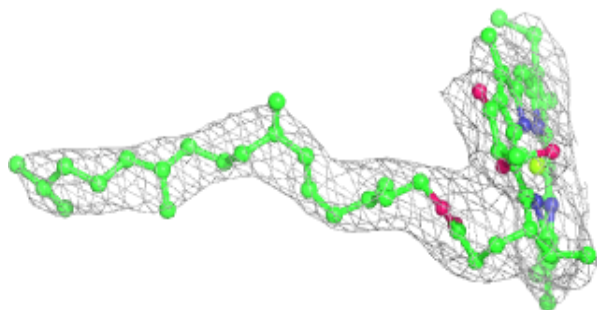
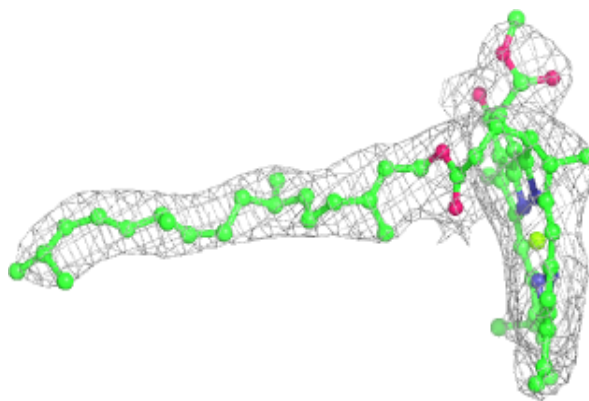
**Electron density around BCR F 308:**

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



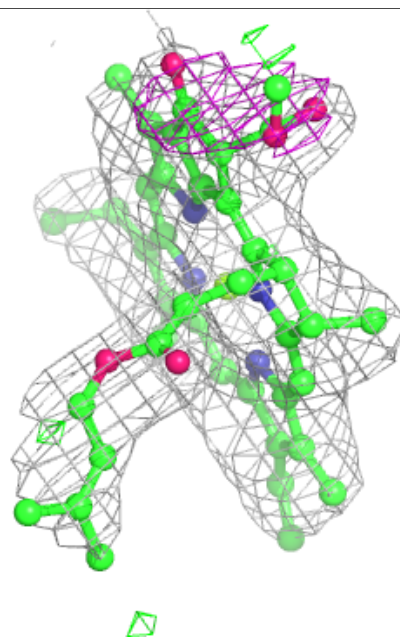
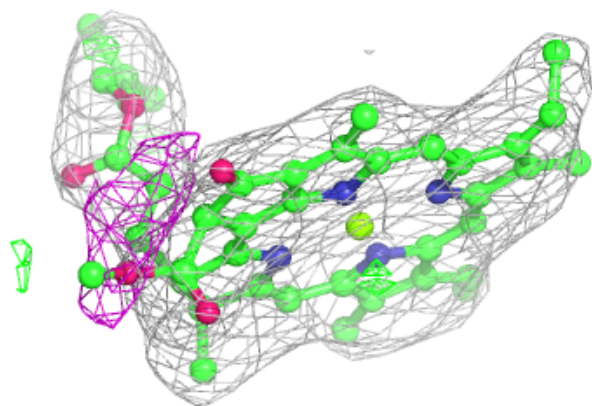
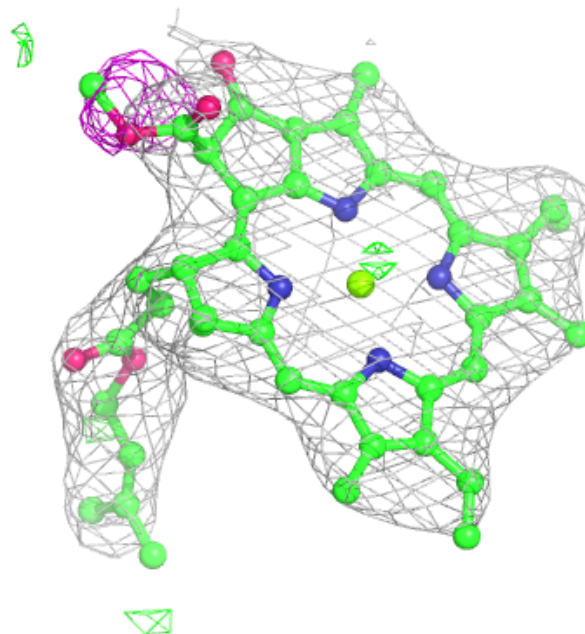
Electron density around CLA A 827:

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



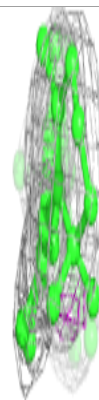
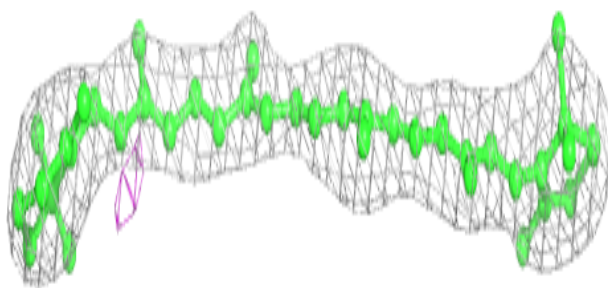
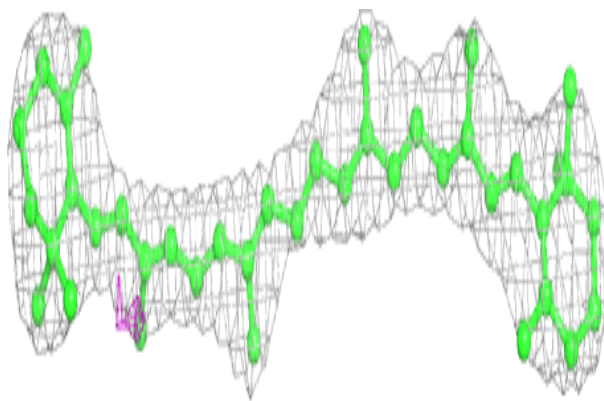
Electron density around CLA B 822:

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

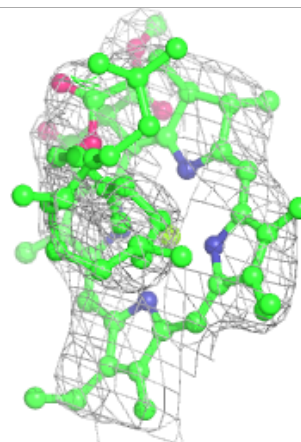
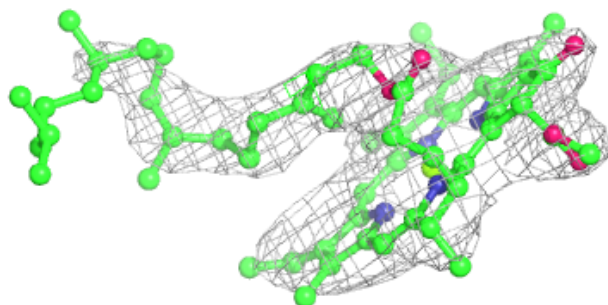
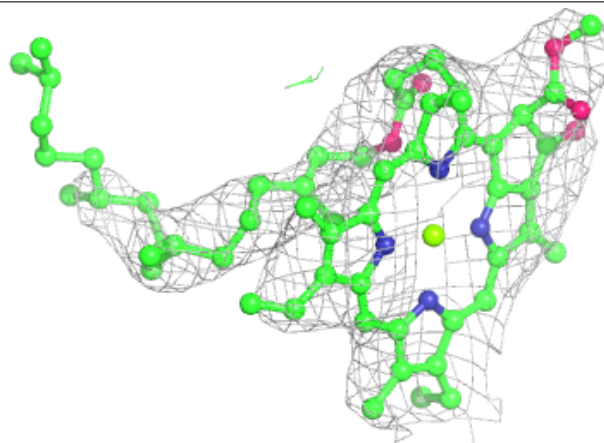


Electron density around BCR J 104:

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

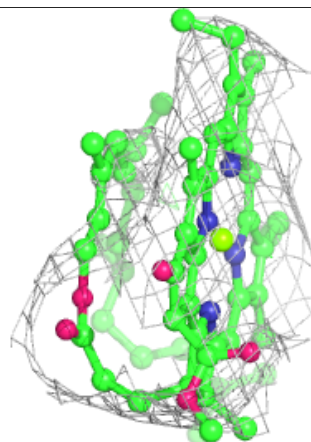
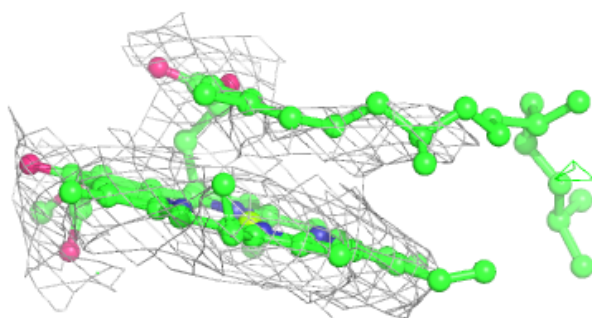
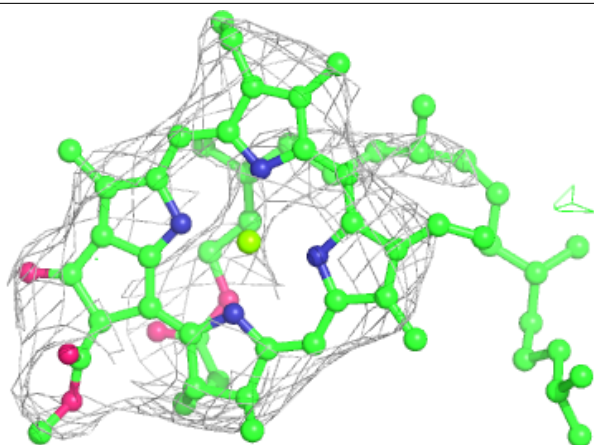
**Electron density around CLA A 841:**

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

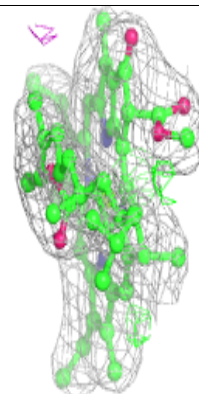
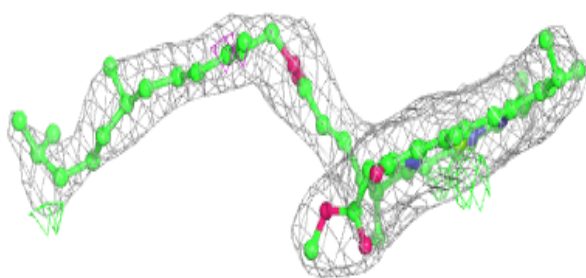
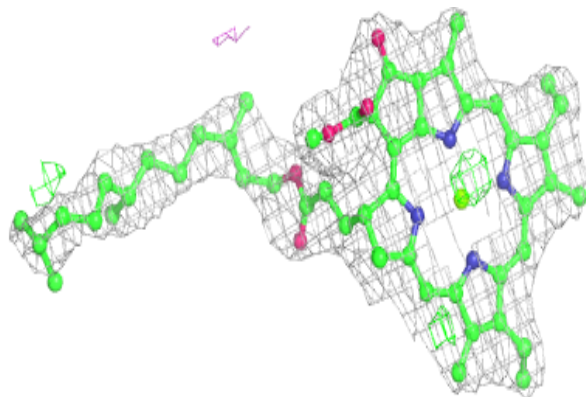


Electron density around CLA 2 311:

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

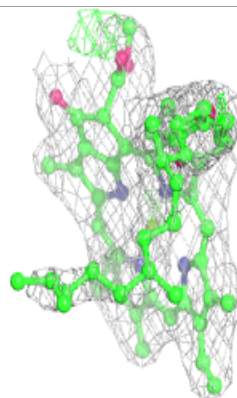
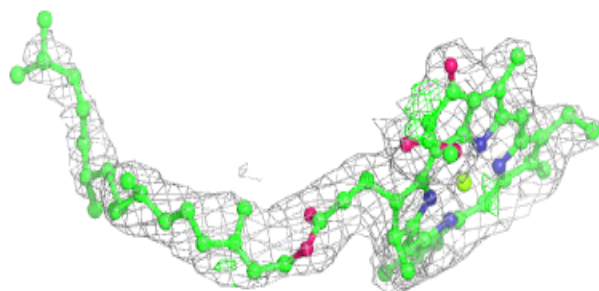
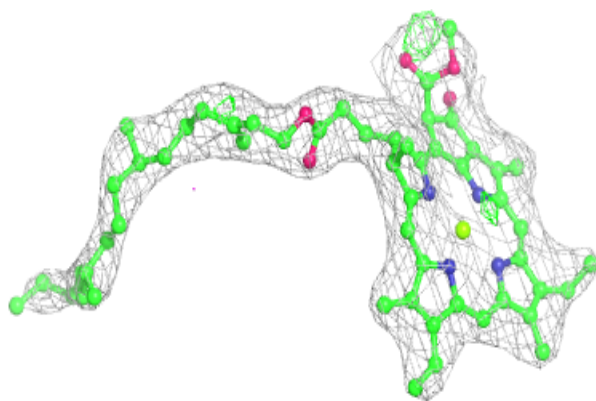
**Electron density around CLA B 825:**

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



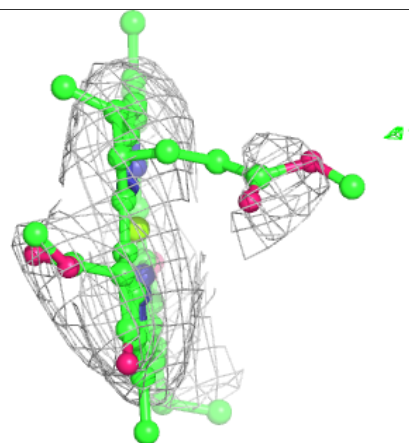
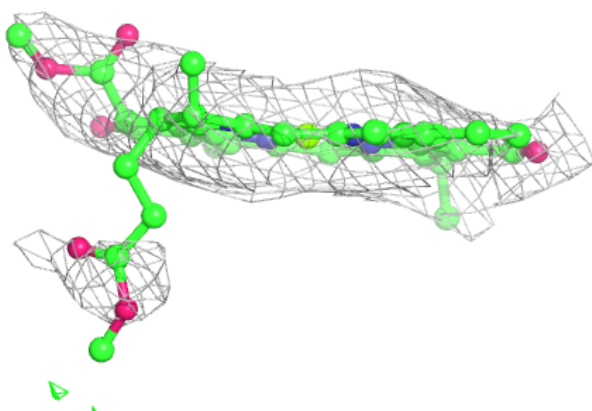
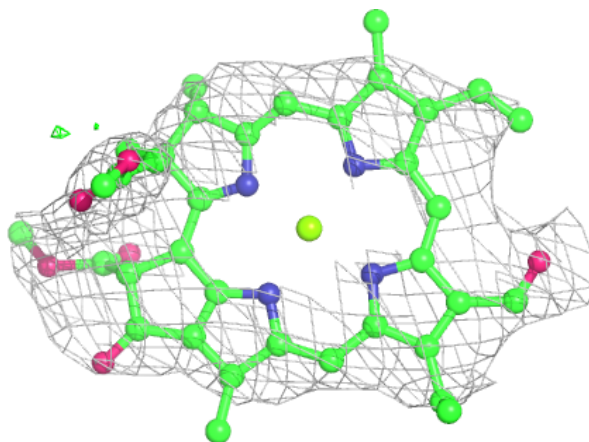
Electron density around CLA A 853:

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



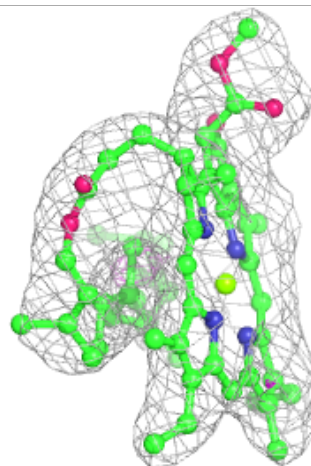
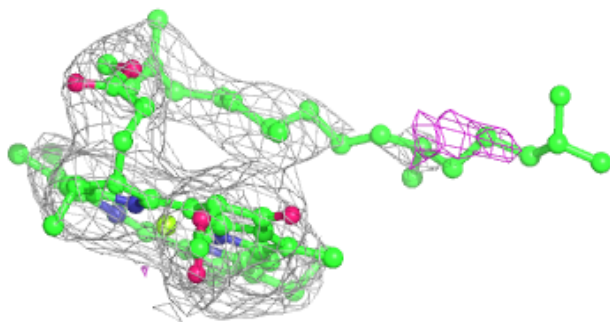
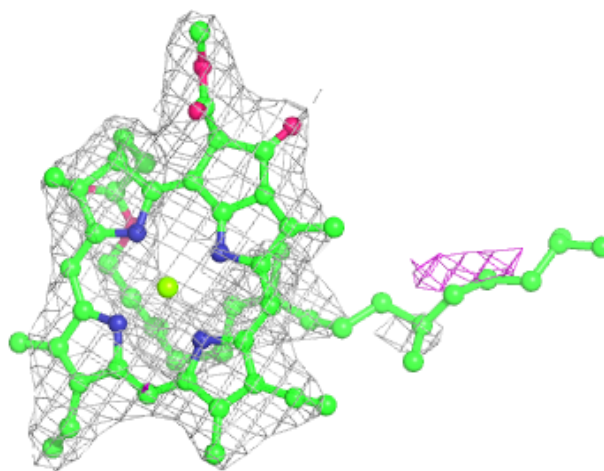
Electron density around CHL 3 607:

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



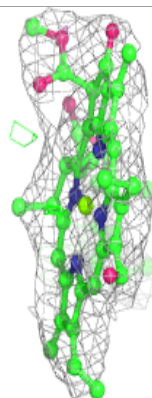
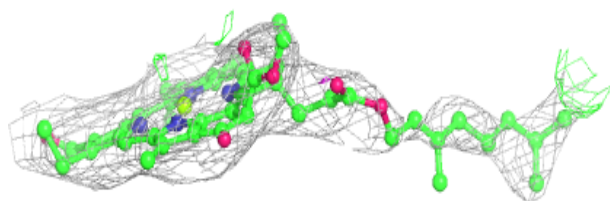
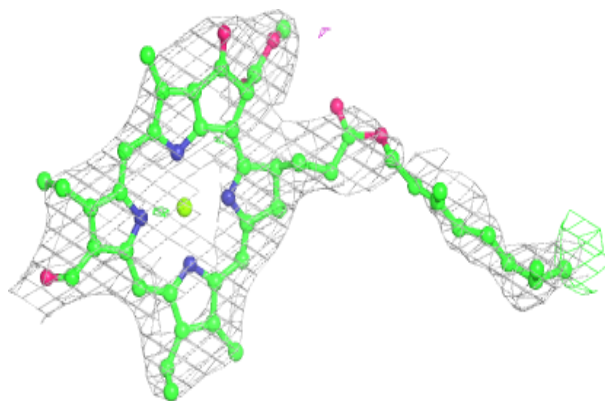
Electron density around CLA B 829:

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

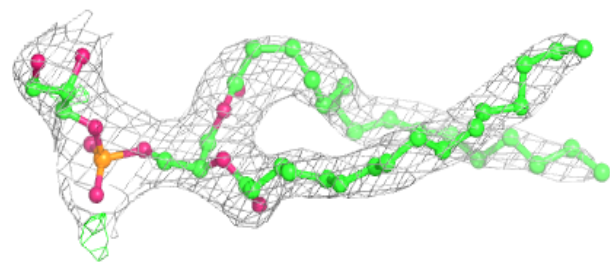
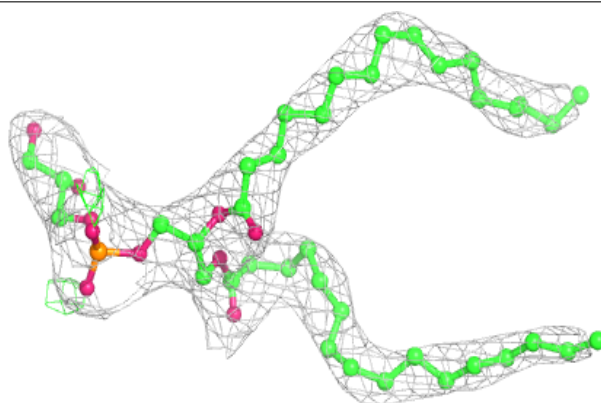


Electron density around CHL 4 305:

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

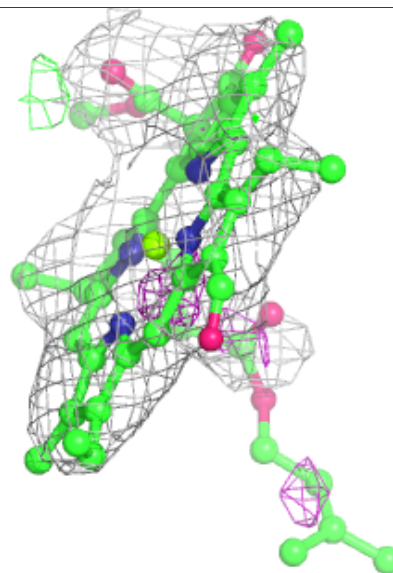
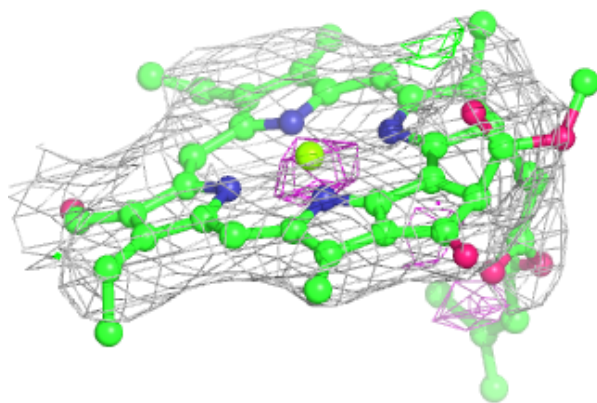
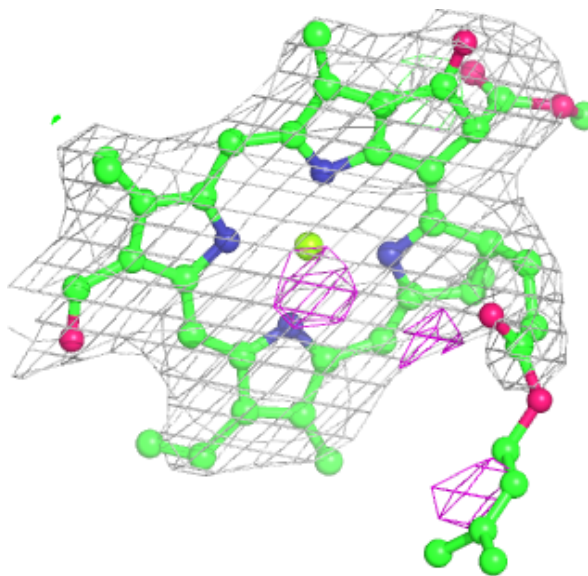
**Electron density around LHG A 844:**

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



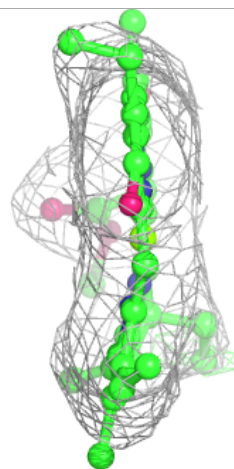
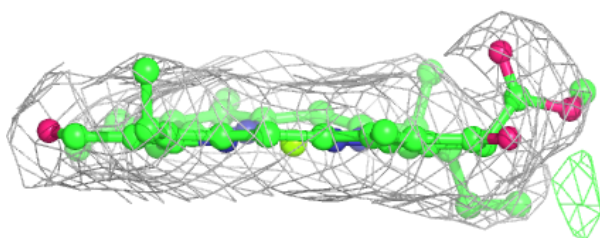
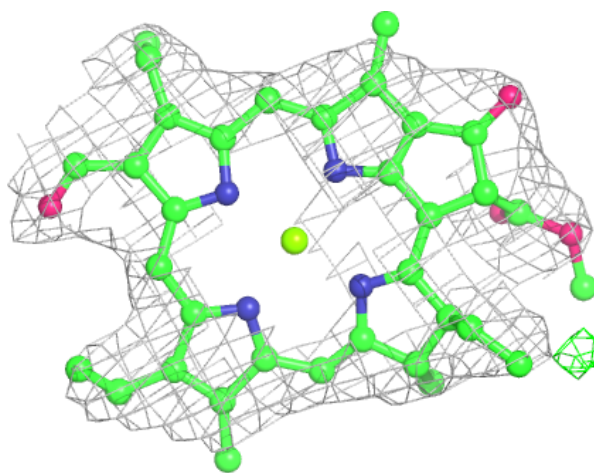
Electron density around CHL 4 306:

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



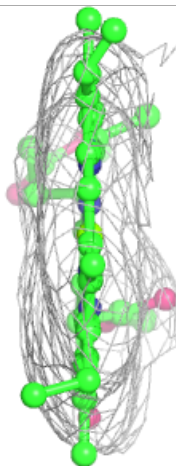
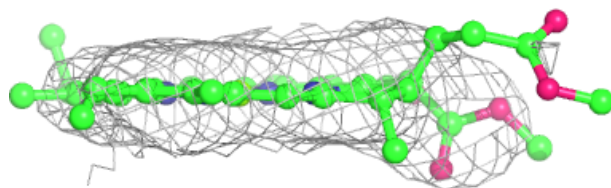
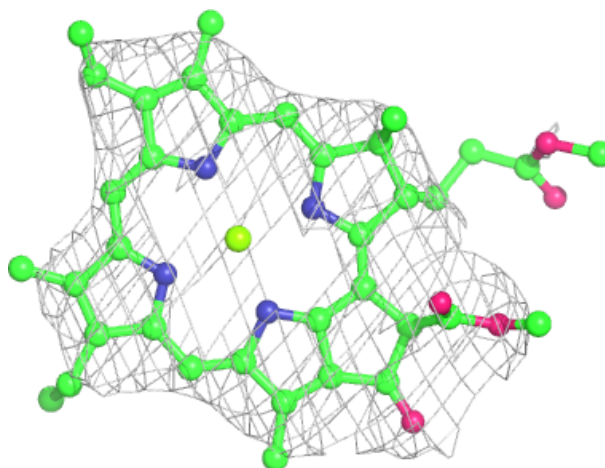
Electron density around CHL 4 315:

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



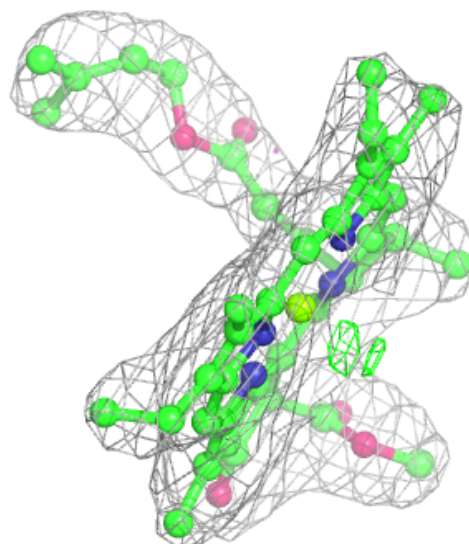
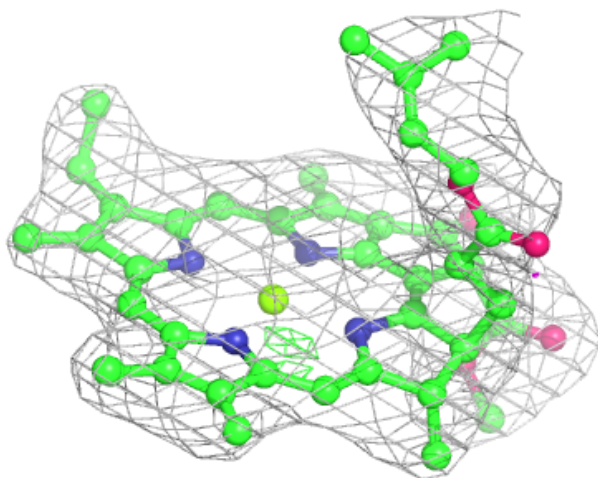
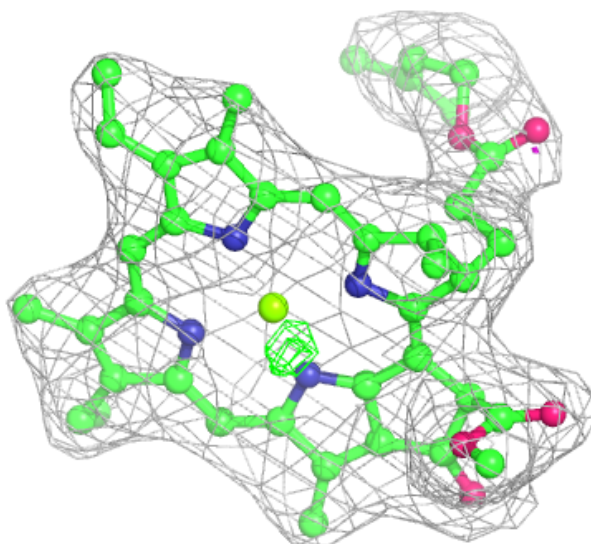
Electron density around CLA 3 613:

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



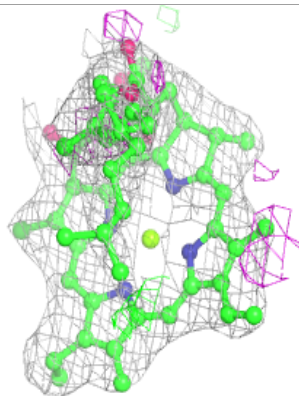
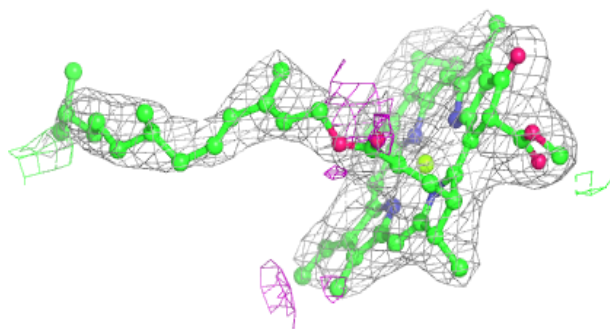
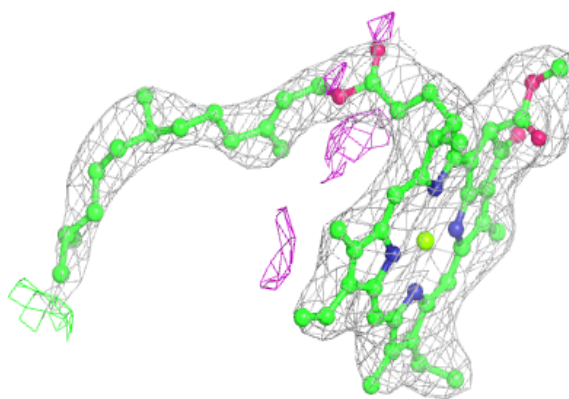
Electron density around CLA B 832:

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

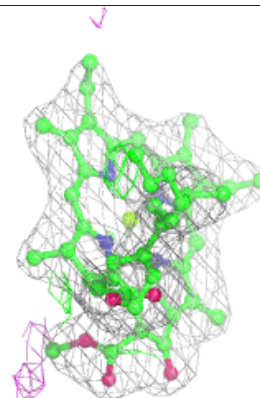
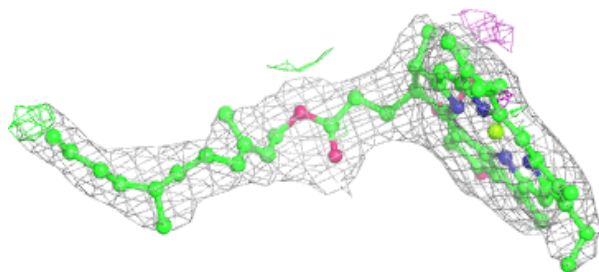
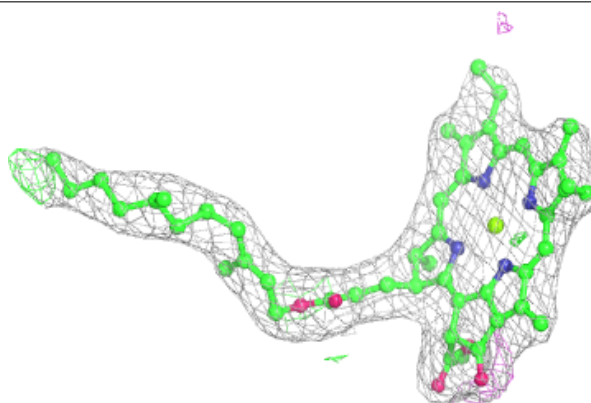


Electron density around CLA B 833:

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

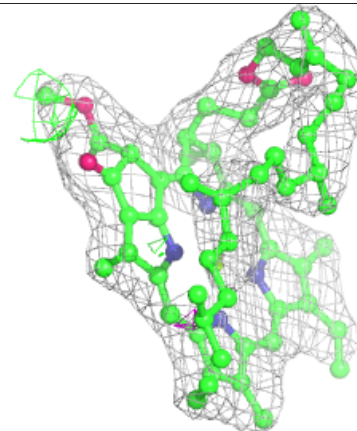
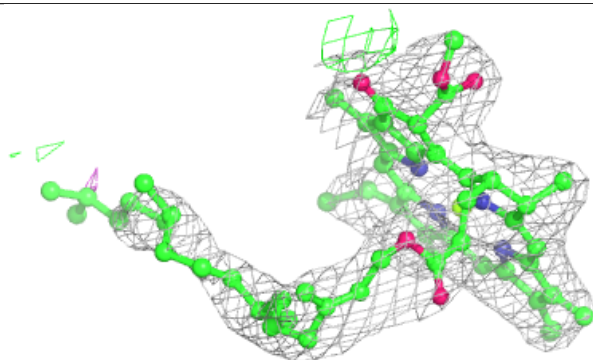
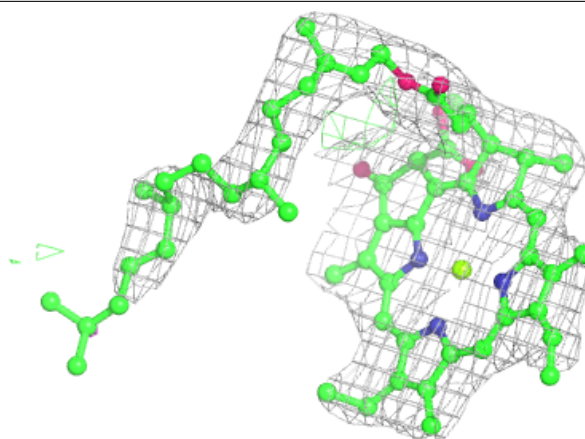
**Electron density around CLA B 834:**

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



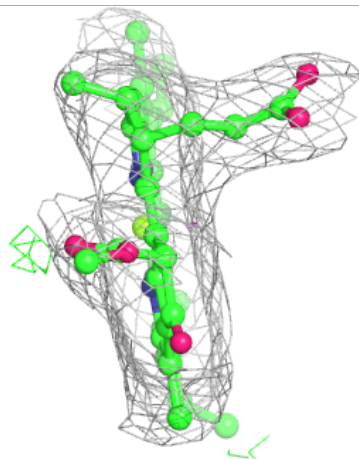
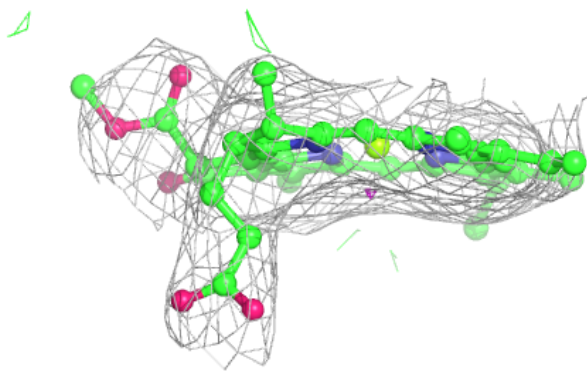
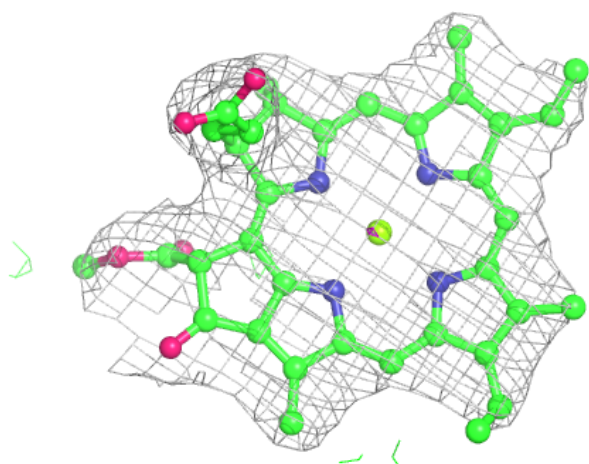
Electron density around CLA B 835:

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



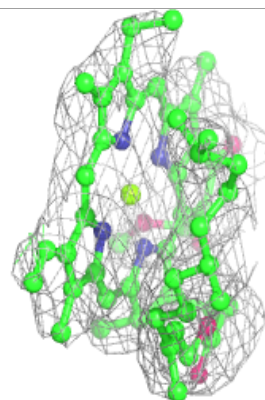
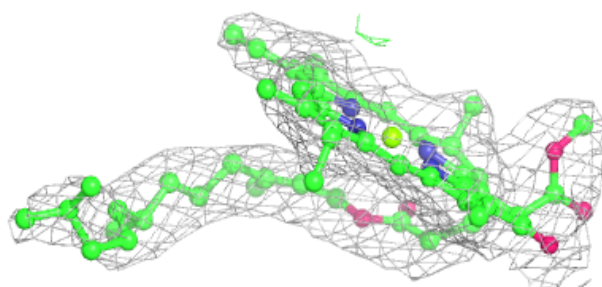
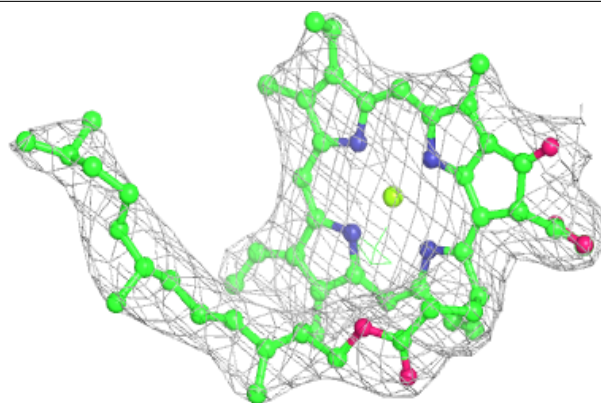
Electron density around CLA B 836:

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

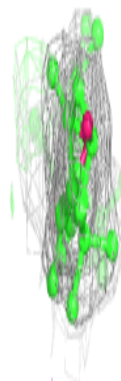
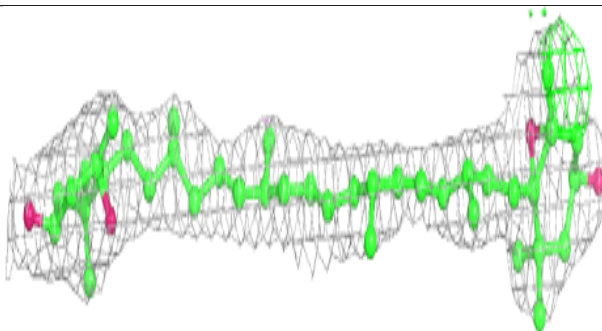
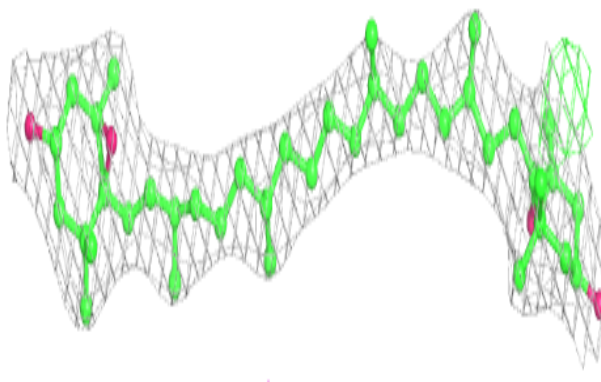


Electron density around CLA 4 302:

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

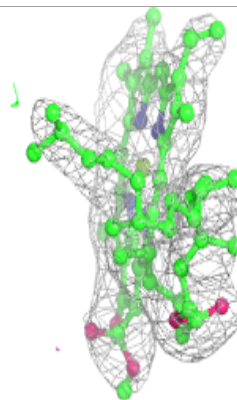
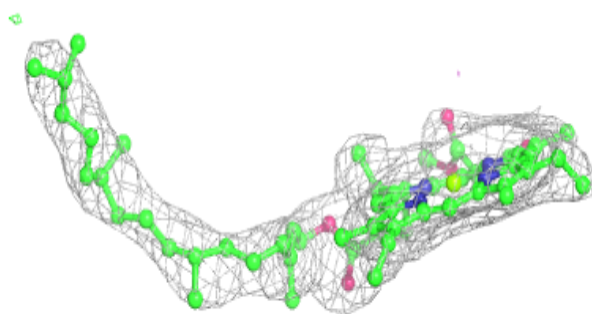
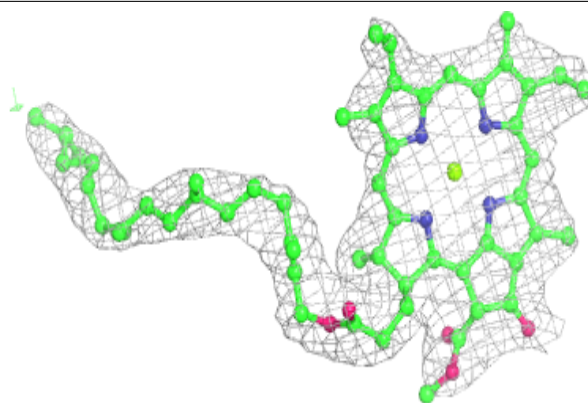
**Electron density around XAT 4 317:**

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



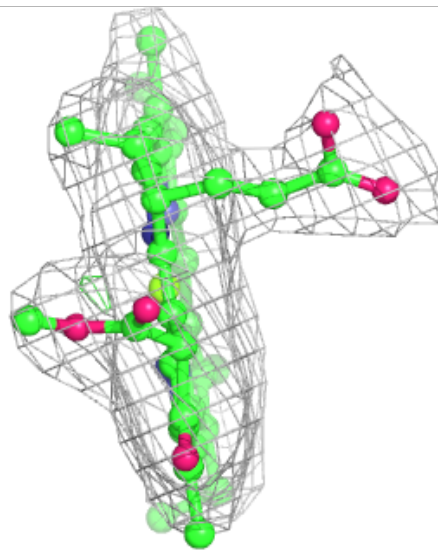
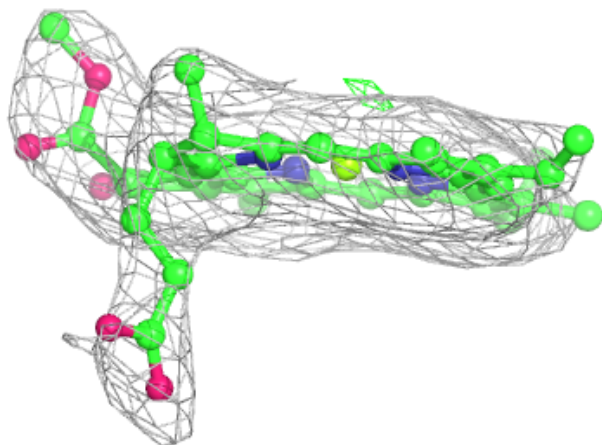
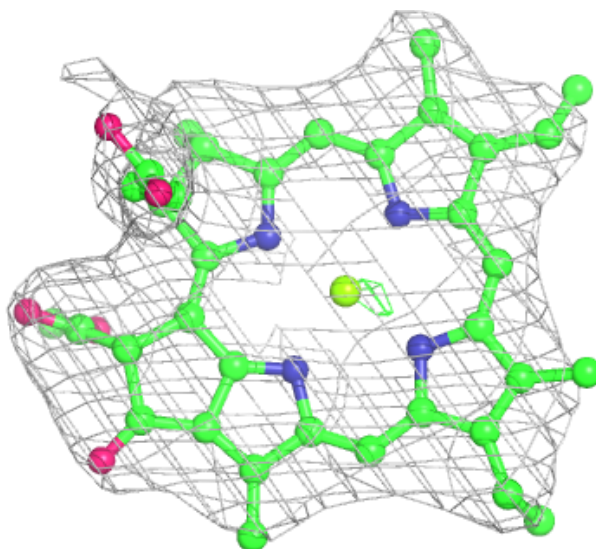
Electron density around CLA B 805:

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



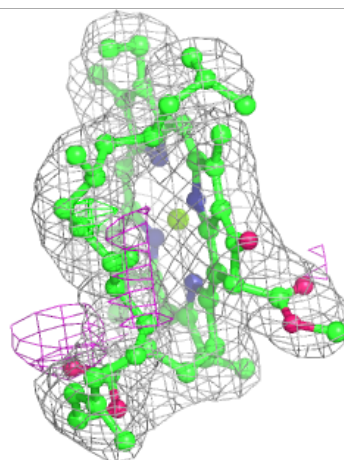
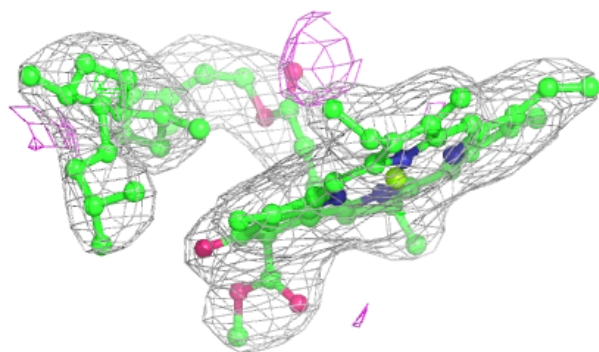
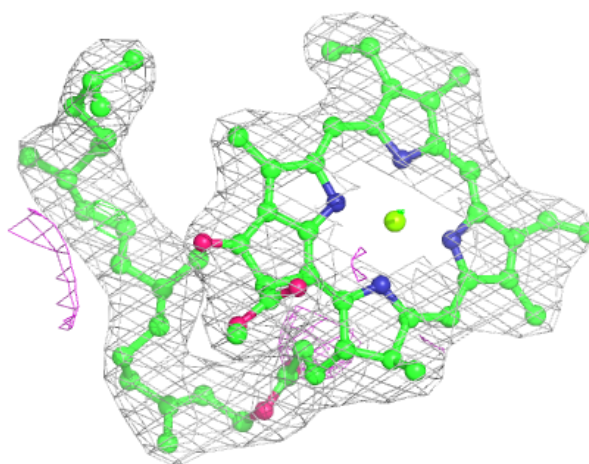
Electron density around CLA B 806:

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



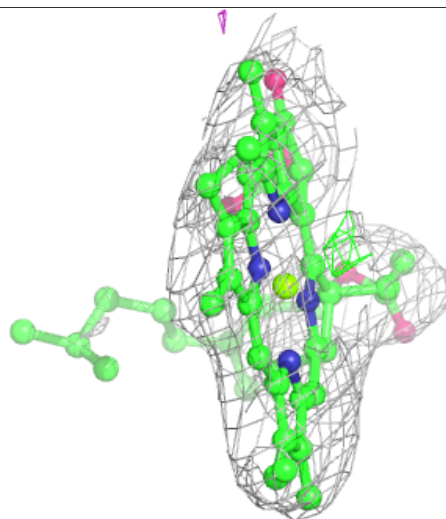
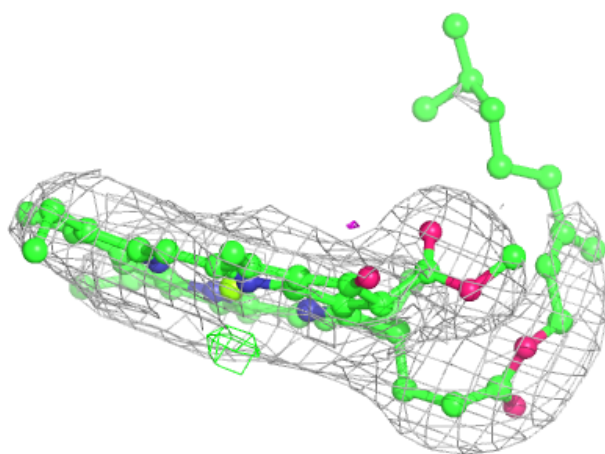
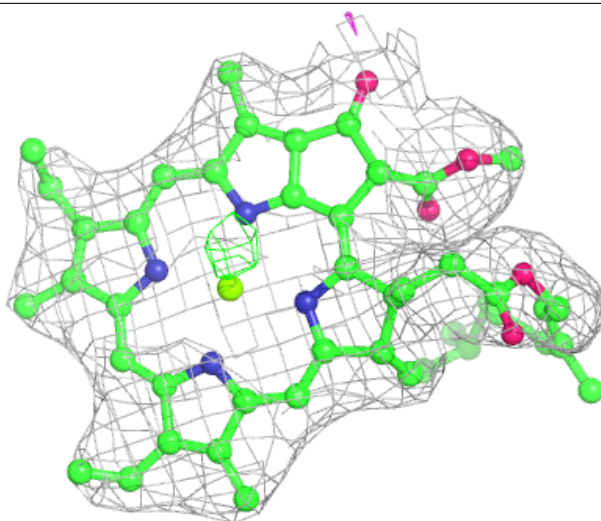
Electron density around CLA F 304:

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



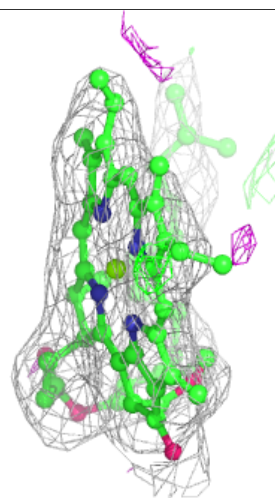
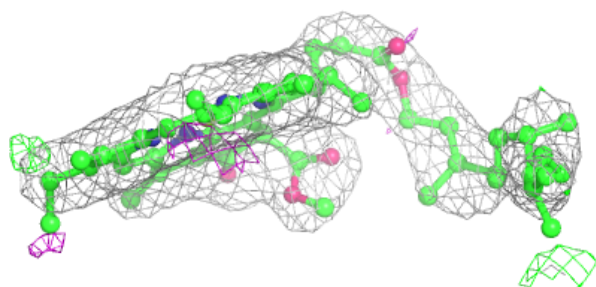
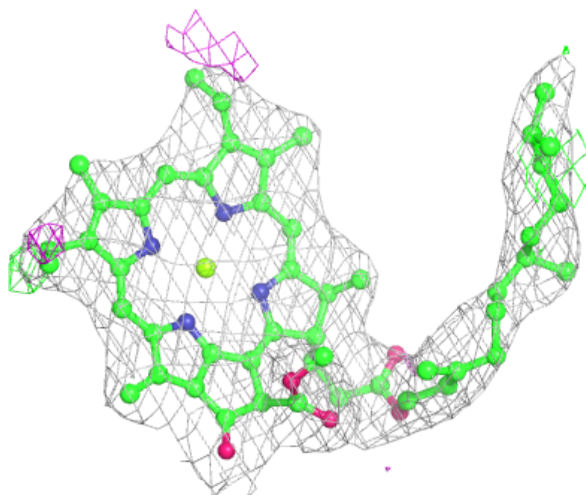
Electron density around CLA F 307:

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



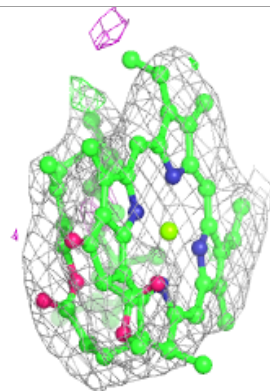
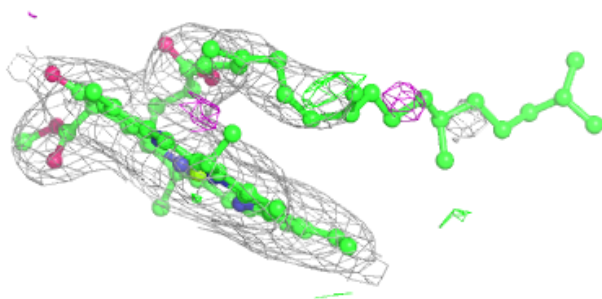
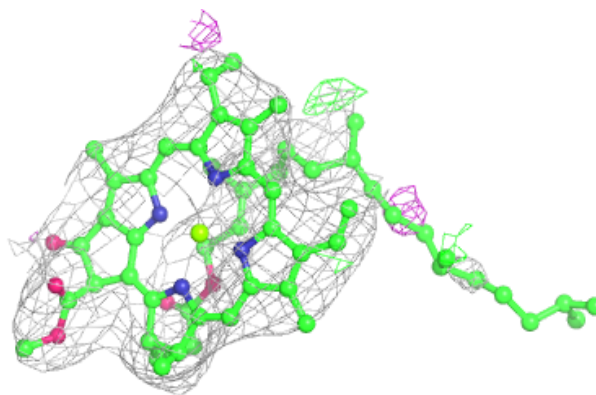
Electron density around CLA 4 303:

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

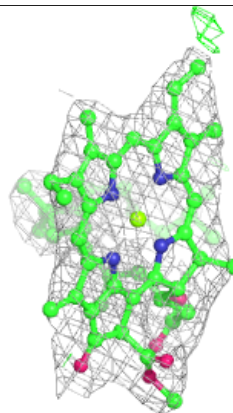
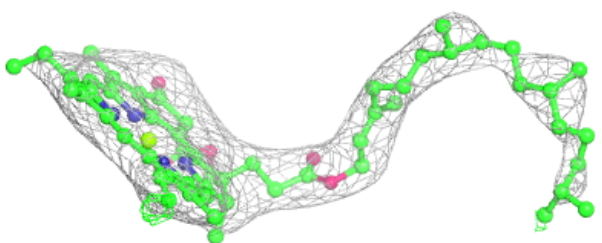
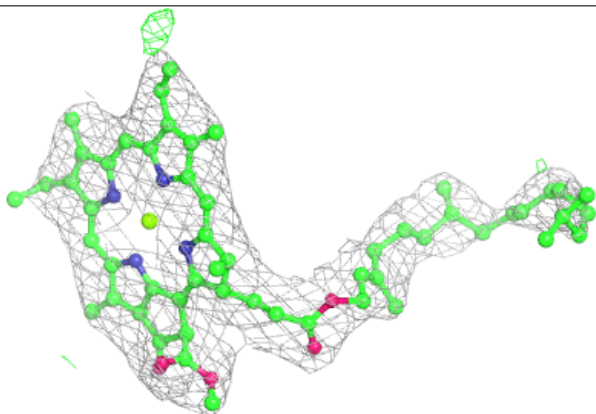


Electron density around CLA B 809:

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

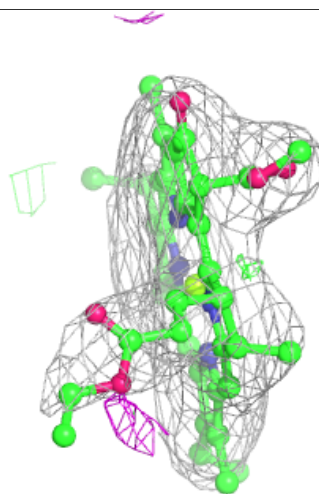
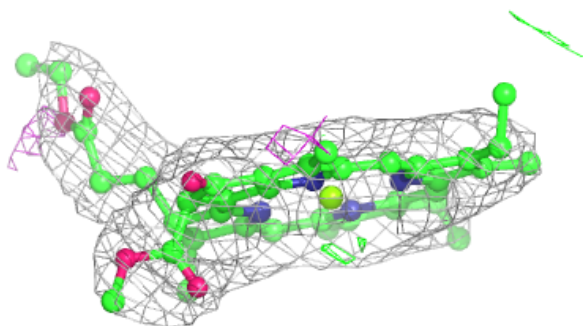
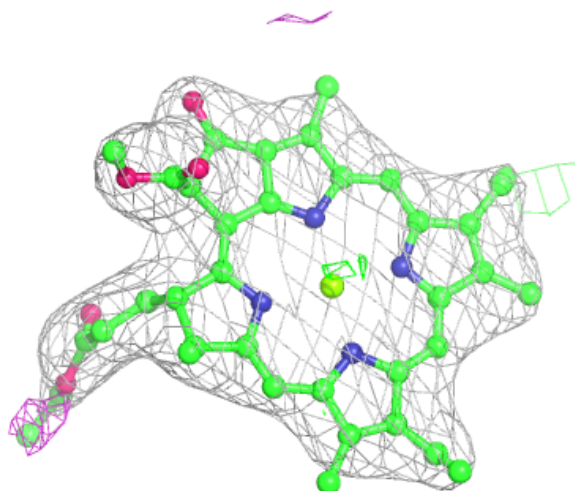
**Electron density around CLA B 811:**

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



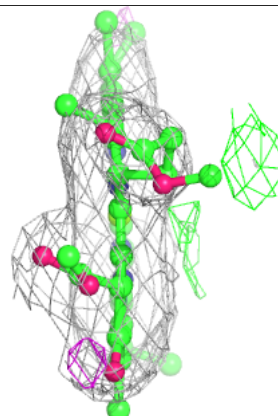
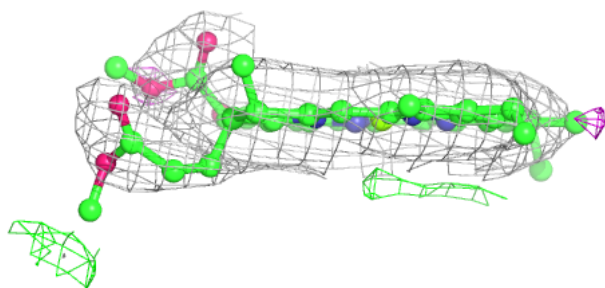
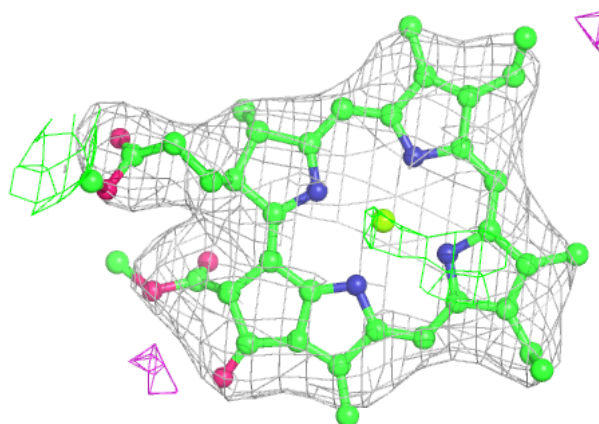
Electron density around CLA 4 314:

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

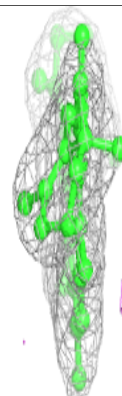
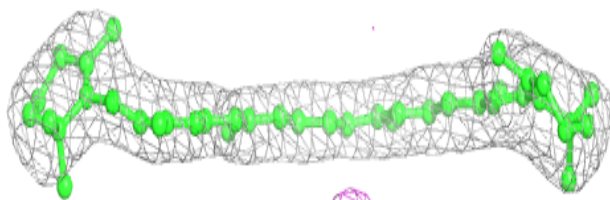
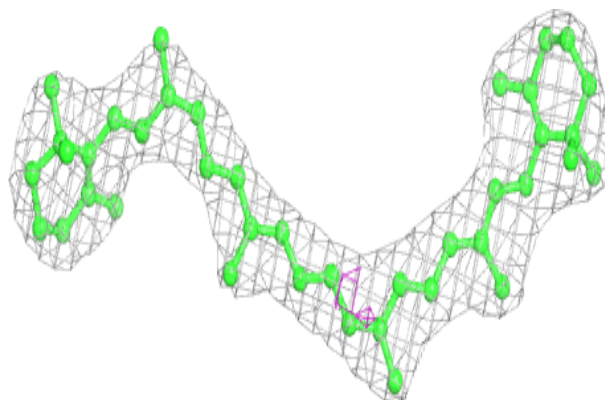


Electron density around CLA 1 313:

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

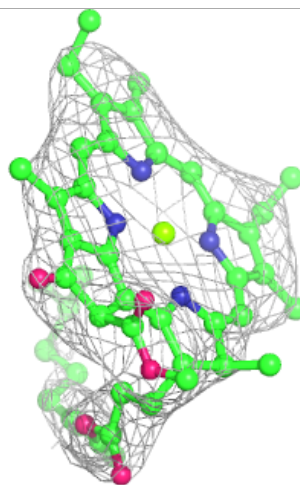
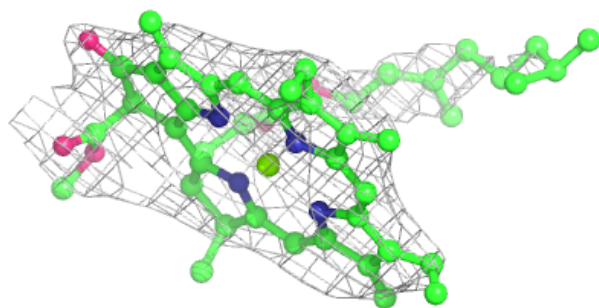
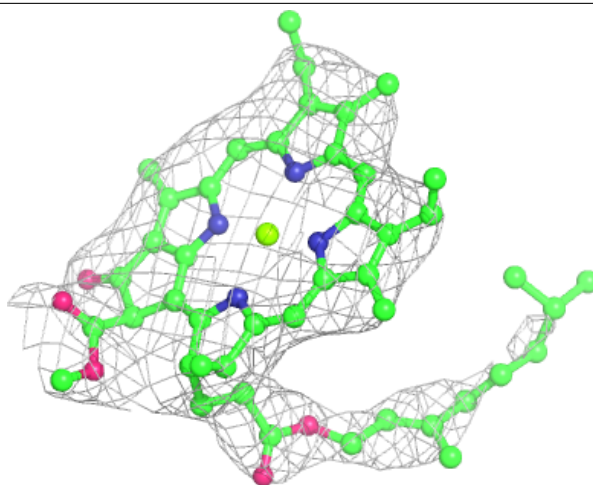
**Electron density around BCR A 851:**

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



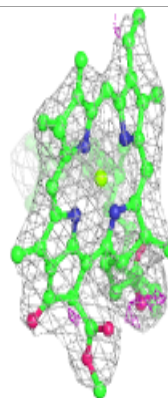
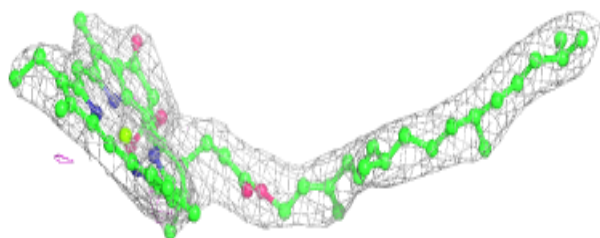
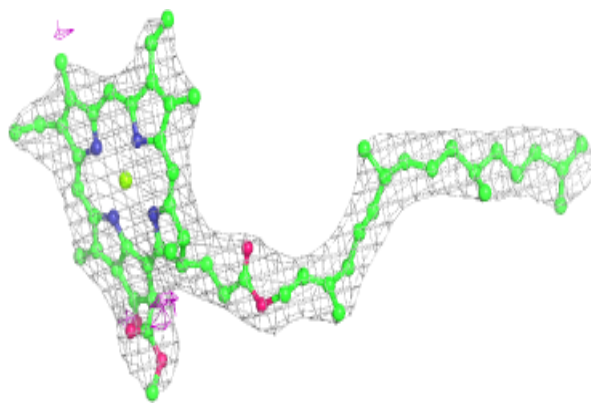
Electron density around CLA A 823:

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

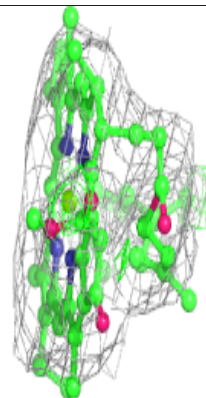
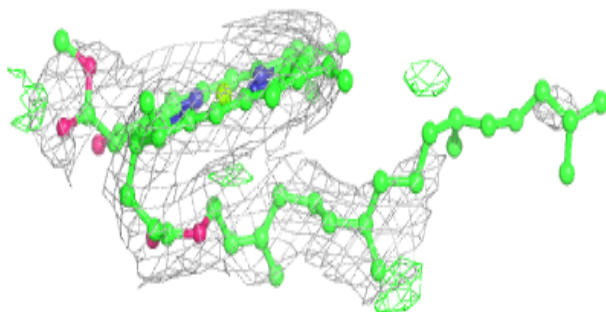
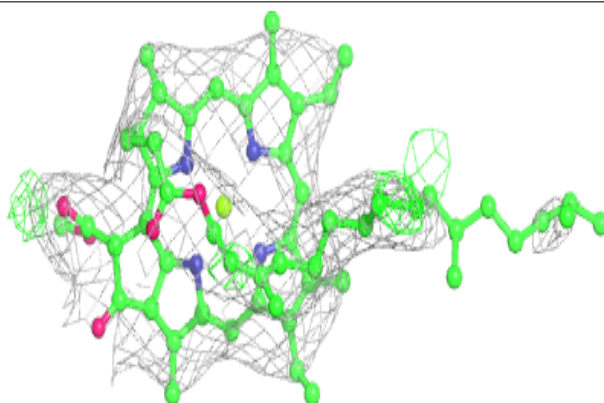


Electron density around CLA A 802:

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

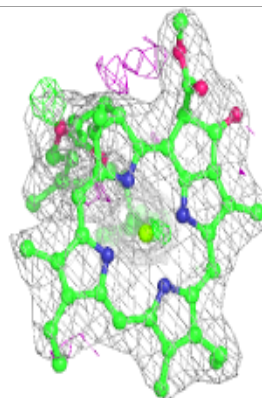
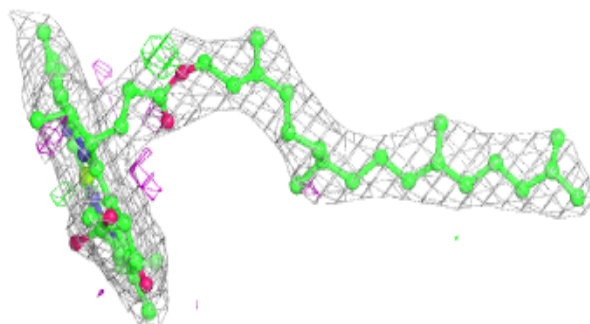
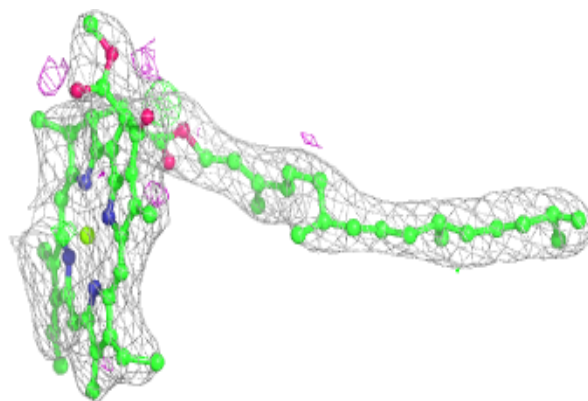
**Electron density around CLA A 836:**

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



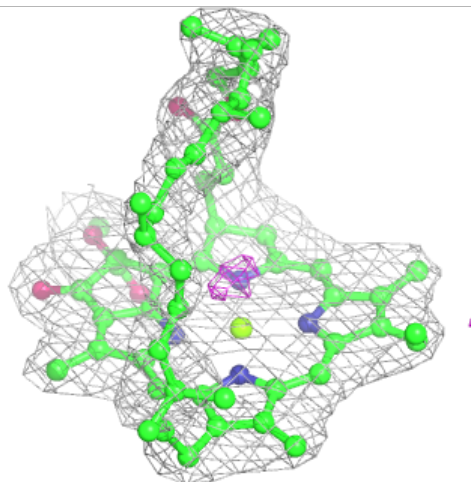
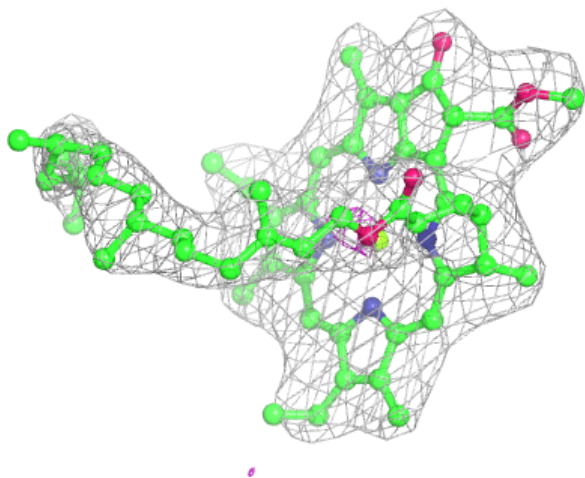
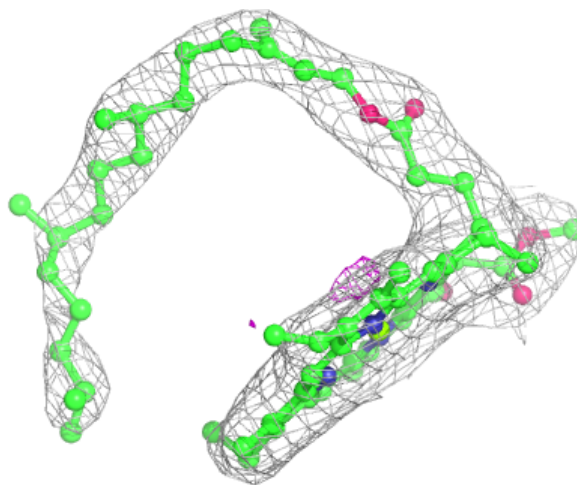
Electron density around CLA B 830:

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



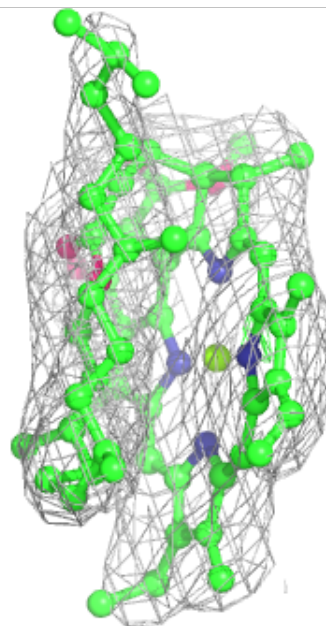
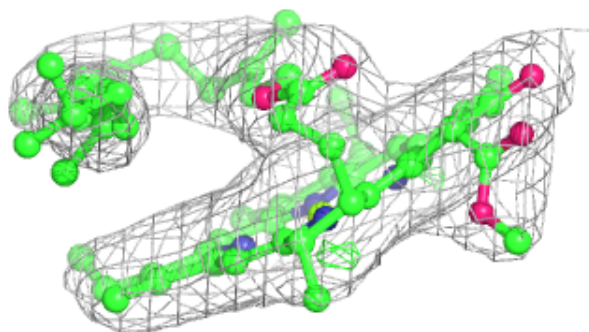
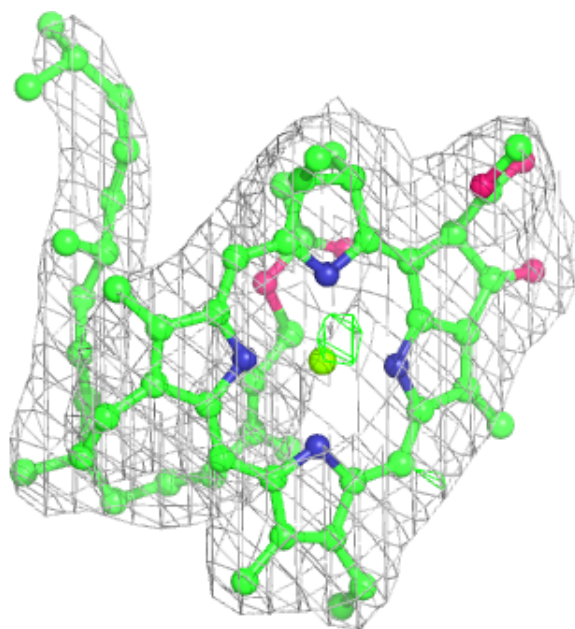
Electron density around CLA B 821:

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



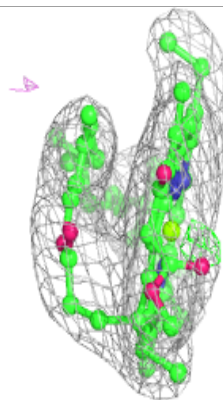
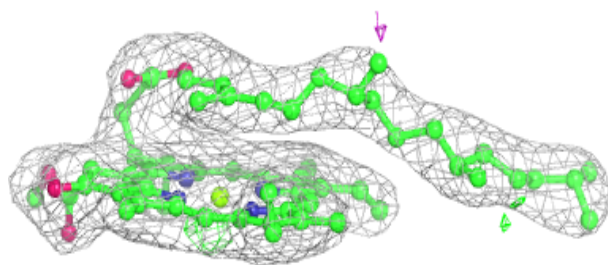
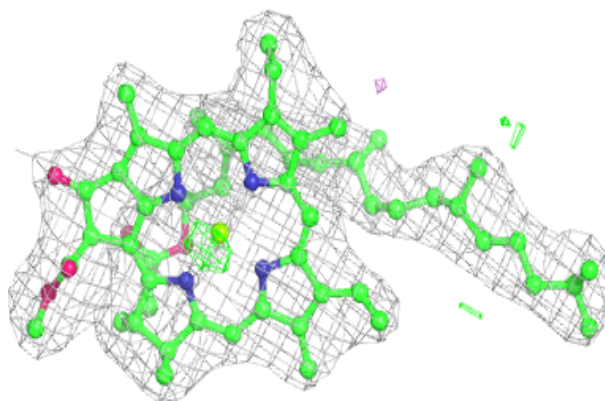
Electron density around CLA B 810:

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

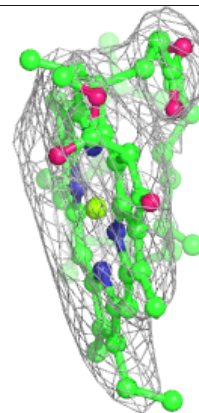
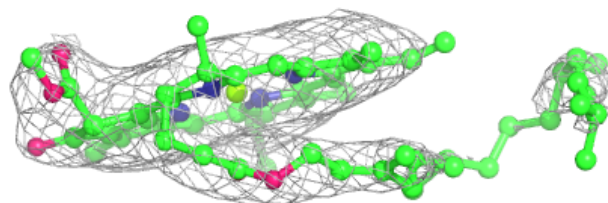
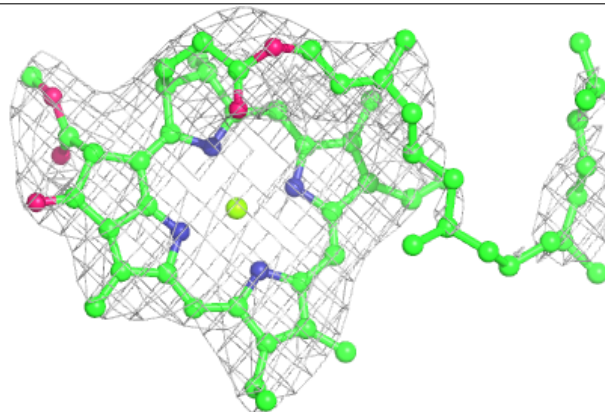


Electron density around CLA A 838:

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

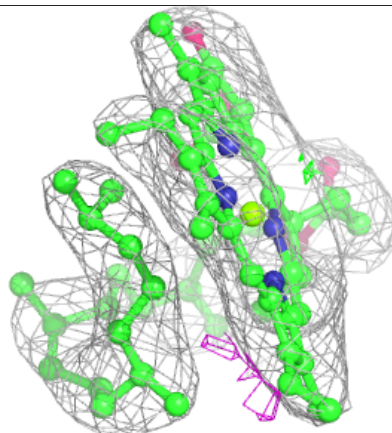
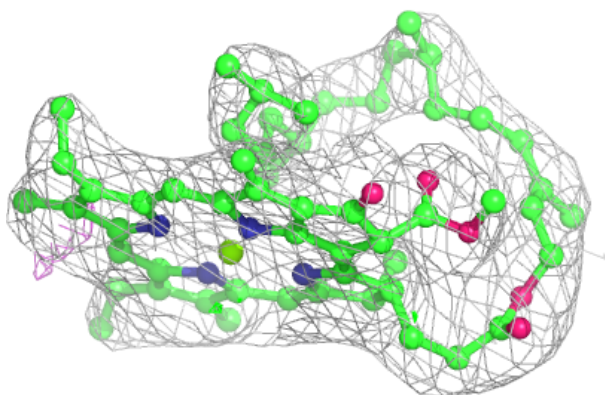
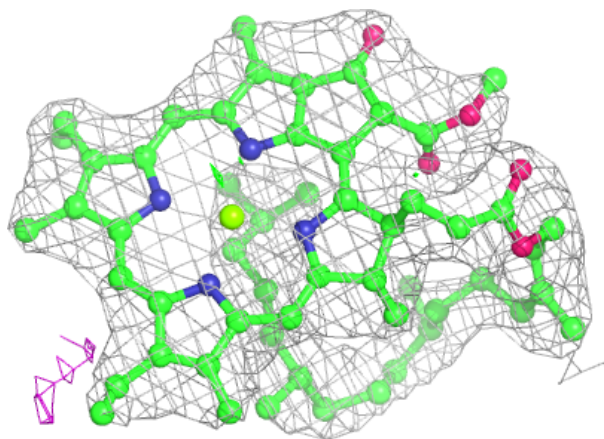
**Electron density around CLA A 818:**

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

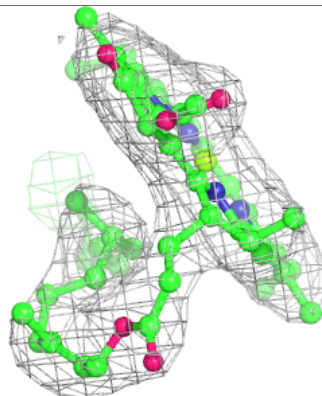
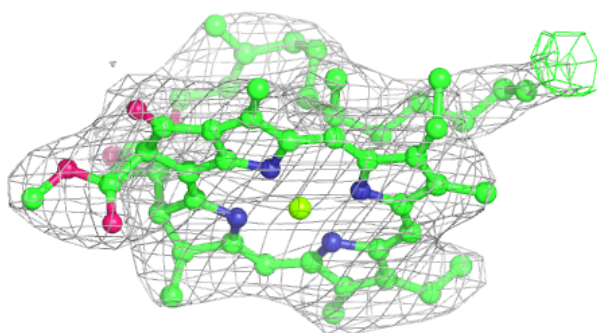
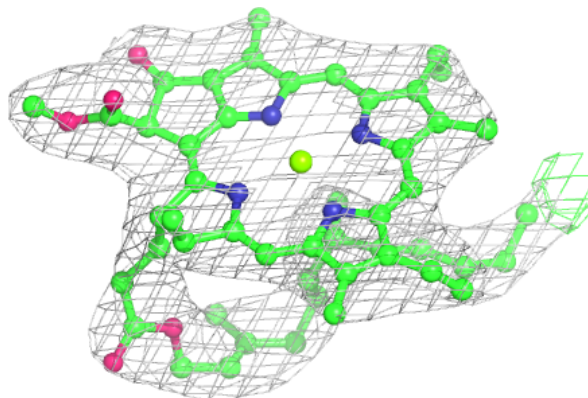


Electron density around CLA B 808:

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

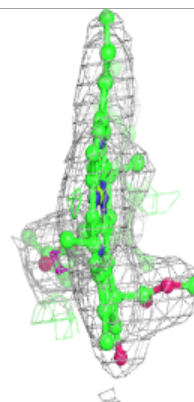
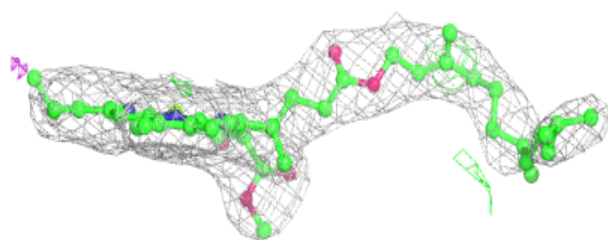
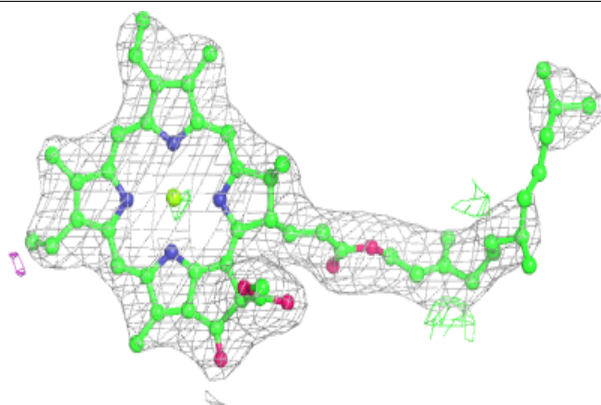
**Electron density around CLA B 819:**

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

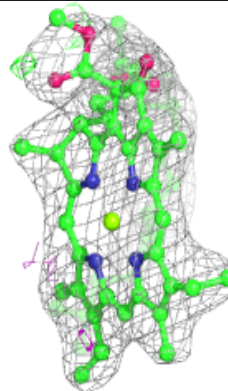
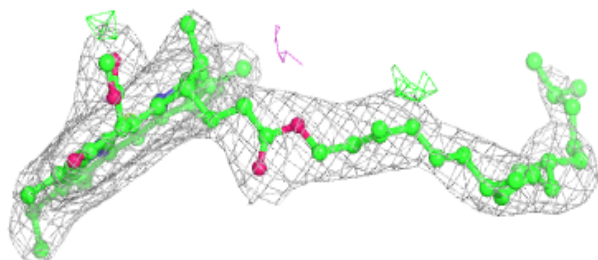
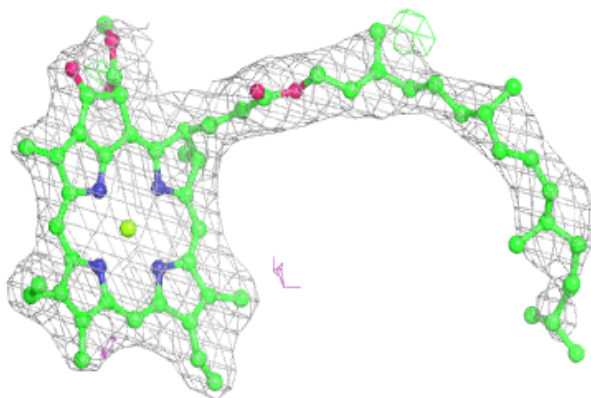


Electron density around CLA B 837:

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

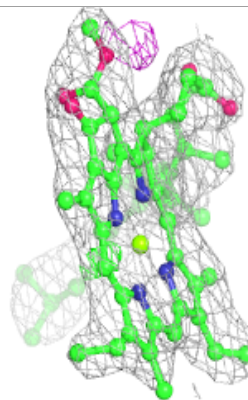
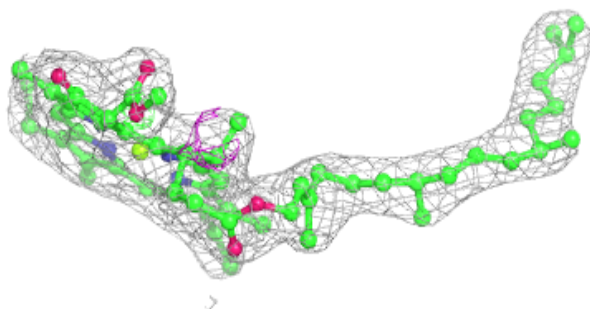
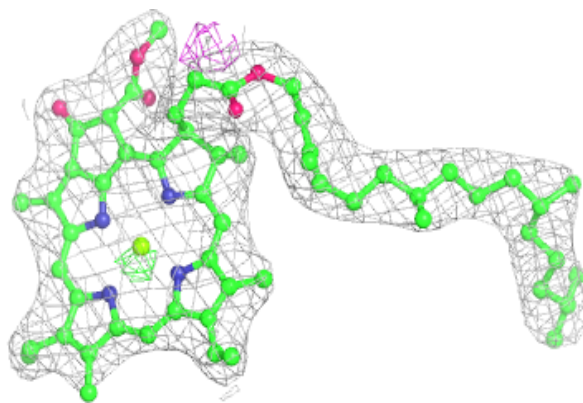
**Electron density around CLA B 827:**

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

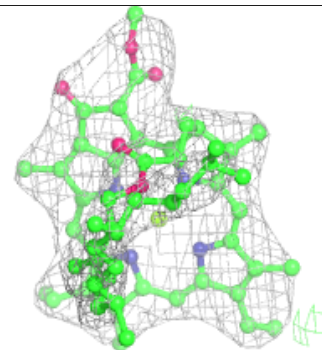
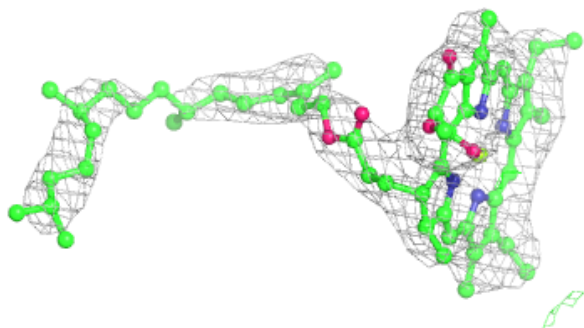
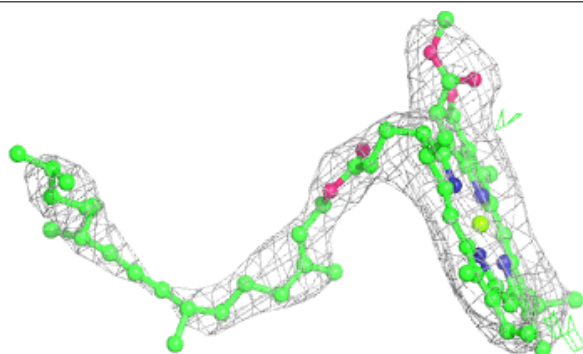


Electron density around CLA B 802:

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

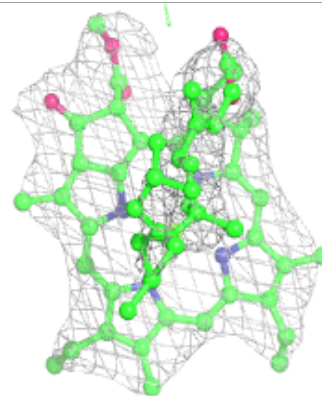
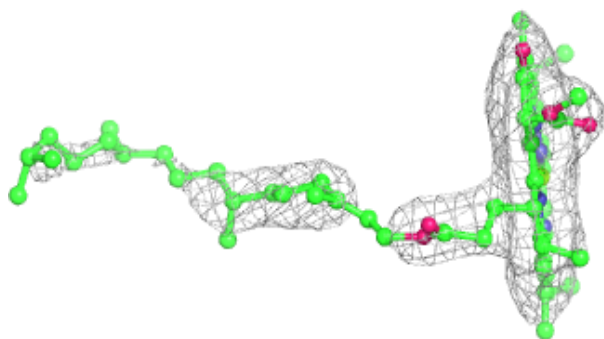
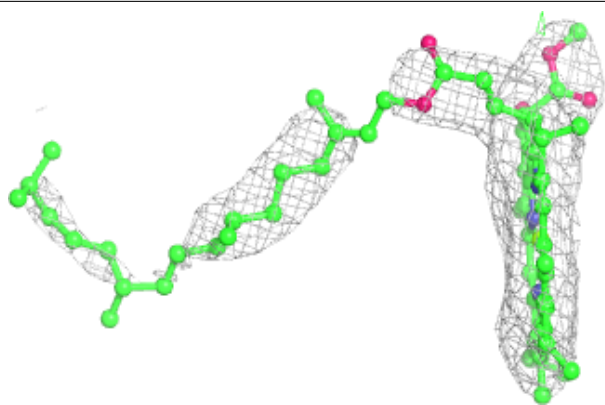
**Electron density around CLA B 840:**

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

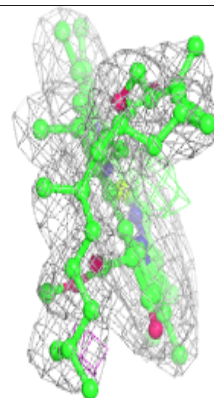
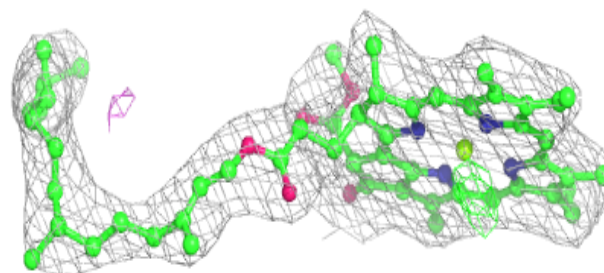
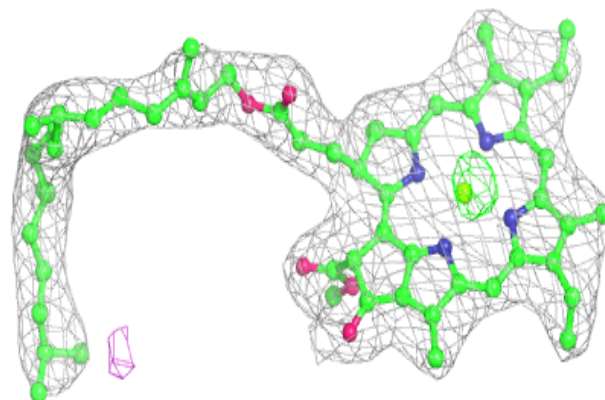


Electron density around CLA B 841:

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

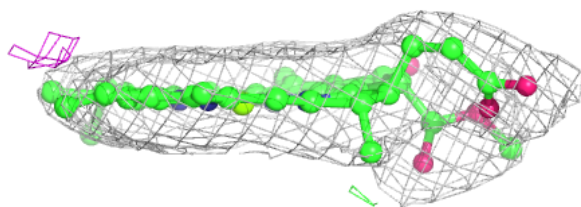
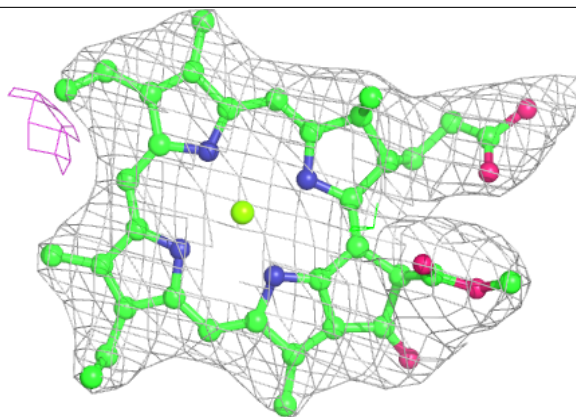
**Electron density around CLA B 828:**

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

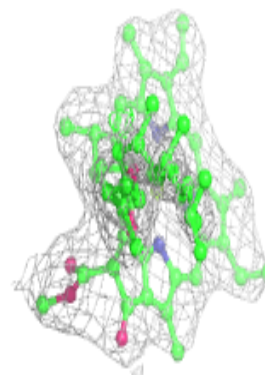
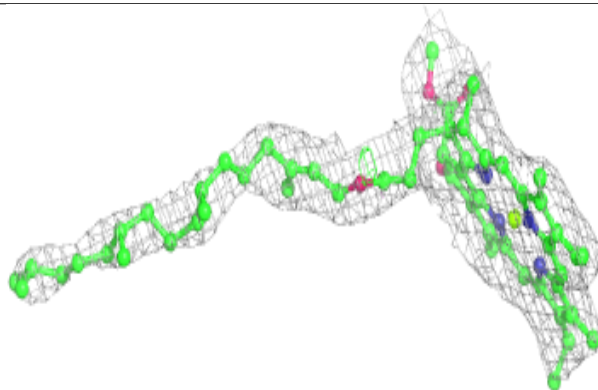
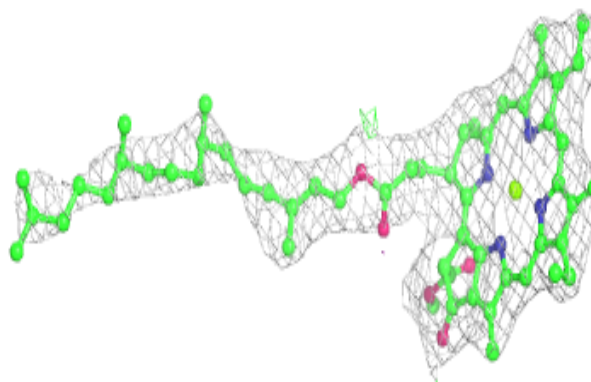


Electron density around CLA F 306:

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

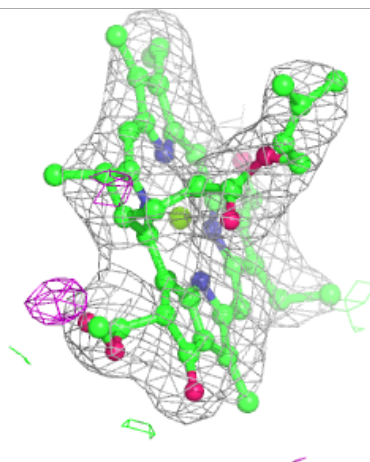
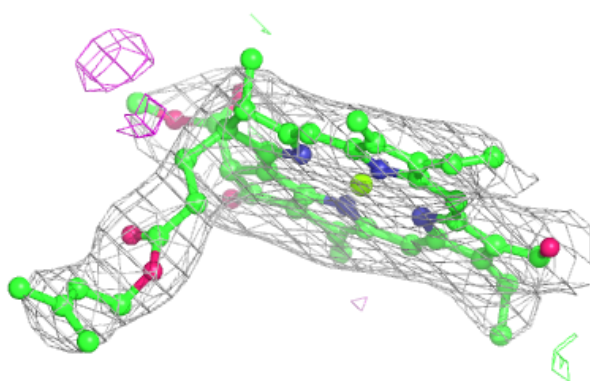
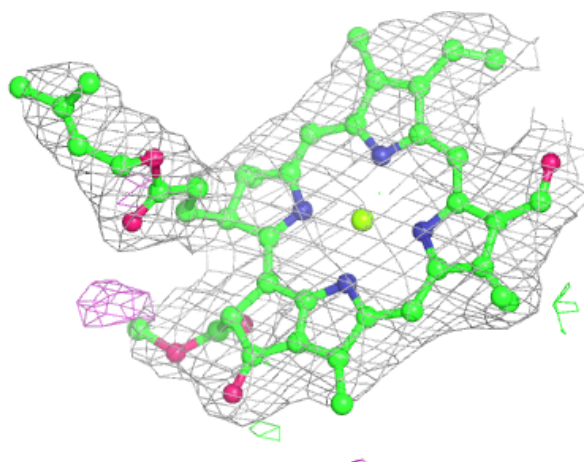
**Electron density around CLA A 808:**

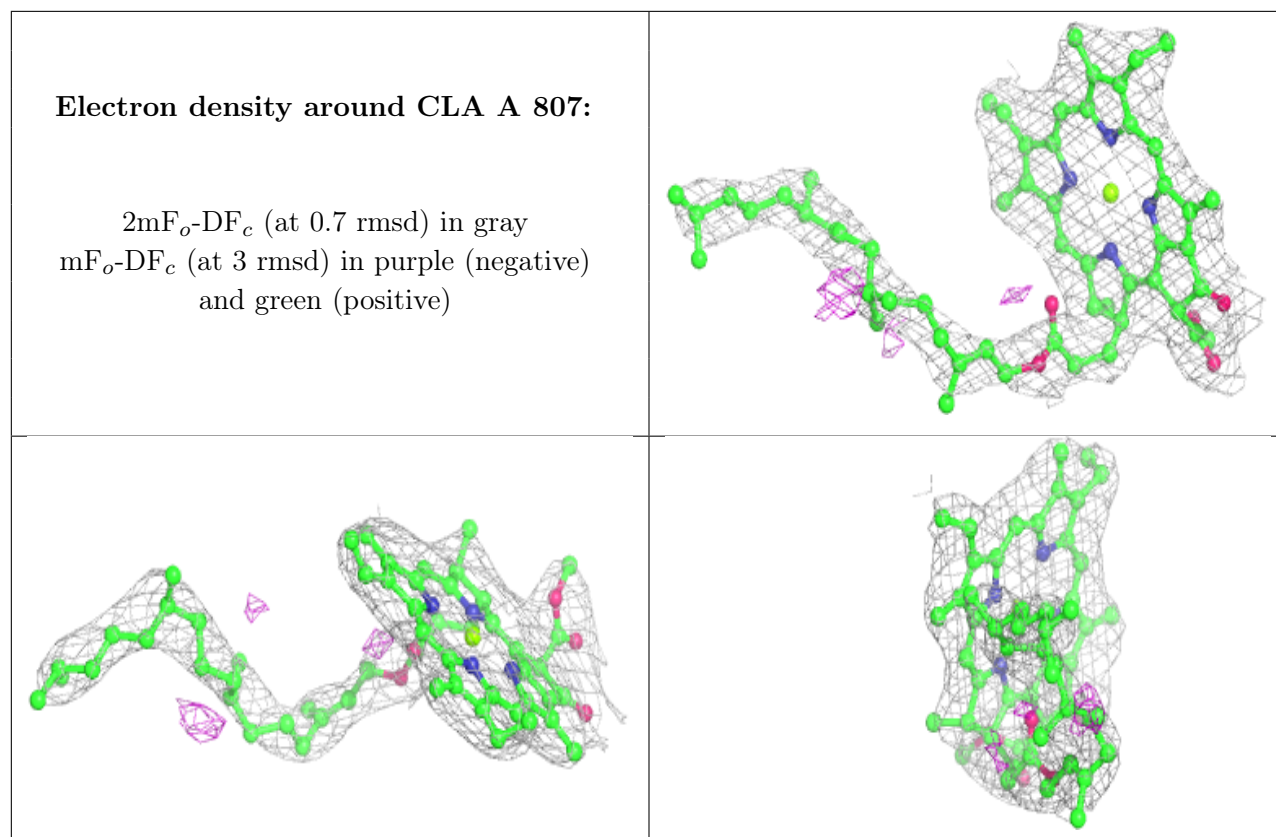
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CHL 4 307:

$2mF_o-DF_c$ (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.