



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 06:29 AM UTC

PDB ID : 6ZXS / pdb_00006zxs
Title : Cold grown Pea Photosystem I
Authors : Caspy, I.; Borovikova-Sheinker, A.; Subramanyam, R.; Nelson, N.
Deposited on : 2020-07-30
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

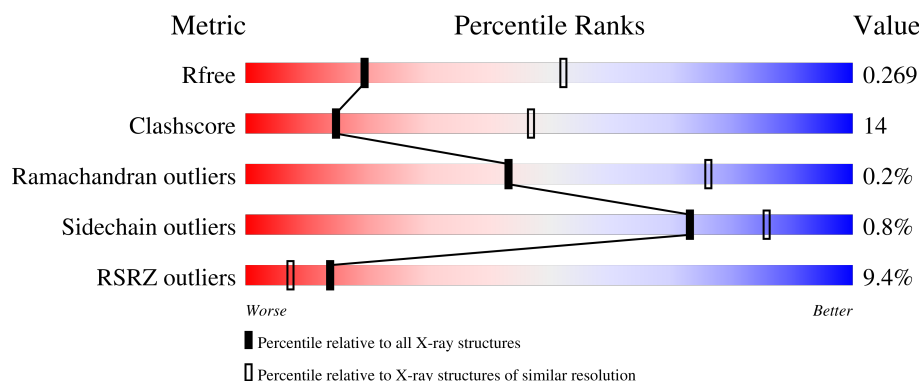
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	743	6% 78% 22%
2	B	733	9% 76% 23%
3	C	80	9% 81% 19%
4	D	143	12% 77% 23%
5	E	66	11% 91% 9%

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Mol	Chain	Length	Quality of chain
6	F	154	
7	G	97	
8	H	88	
9	I	30	
10	J	42	
11	K	80	
12	L	157	
13	1	193	
14	2	208	
15	3	221	
16	4	198	

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	CL0	A	801	X	-	-	-
18	CLA	1	5006	X	-	-	-
18	CLA	1	5007	X	-	-	-
18	CLA	1	5008	X	-	-	-
18	CLA	1	5009	X	-	-	-
18	CLA	1	5010	X	-	-	-
18	CLA	1	5011	X	-	-	-
18	CLA	1	5012	X	-	-	-
18	CLA	1	5013	X	-	-	-
18	CLA	1	5015	X	-	-	-
18	CLA	1	5017	X	-	-	-
18	CLA	1	5018	X	-	-	-
18	CLA	2	306	X	-	-	-
18	CLA	2	307	X	-	-	-
18	CLA	2	308	X	-	-	-
18	CLA	2	309	X	-	-	-
18	CLA	2	310	X	-	-	-
18	CLA	2	311	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	2	312	X	-	-	-
18	CLA	2	313	X	-	-	-
18	CLA	2	317	X	-	-	-
18	CLA	2	326	X	-	-	-
18	CLA	3	301	X	-	-	-
18	CLA	3	307	X	-	-	-
18	CLA	3	308	X	-	-	-
18	CLA	3	309	X	-	-	-
18	CLA	3	311	X	-	-	-
18	CLA	3	314	X	-	-	-
18	CLA	3	315	X	-	-	-
18	CLA	3	317	X	-	-	-
18	CLA	3	318	X	-	-	-
18	CLA	3	319	X	-	-	-
18	CLA	4	305	X	-	-	-
18	CLA	4	306	X	-	-	-
18	CLA	4	307	X	-	-	-
18	CLA	4	308	X	-	-	-
18	CLA	4	309	X	-	-	-
18	CLA	4	310	X	-	-	-
18	CLA	4	311	X	-	-	-
18	CLA	4	312	X	-	-	-
18	CLA	4	315	X	-	-	-
18	CLA	A	802	X	-	-	-
18	CLA	A	803	X	-	-	-
18	CLA	A	804	X	-	-	-
18	CLA	A	805	X	-	-	-
18	CLA	A	806	X	-	-	-
18	CLA	A	807	X	-	-	-
18	CLA	A	808	X	-	-	-
18	CLA	A	809	X	-	-	-
18	CLA	A	810	X	-	-	-
18	CLA	A	811	X	-	-	-
18	CLA	A	812	X	-	-	-
18	CLA	A	813	X	-	-	-
18	CLA	A	814	X	-	-	-
18	CLA	A	815	X	-	-	-
18	CLA	A	816	X	-	-	-
18	CLA	A	817	X	-	-	-
18	CLA	A	818	X	-	-	-
18	CLA	A	819	X	-	-	-
18	CLA	A	820	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	821	X	-	-	-
18	CLA	A	822	X	-	-	-
18	CLA	A	823	X	-	-	-
18	CLA	A	824	X	-	-	-
18	CLA	A	825	X	-	-	-
18	CLA	A	826	X	-	-	-
18	CLA	A	827	X	-	-	-
18	CLA	A	828	X	-	-	-
18	CLA	A	829	X	-	-	-
18	CLA	A	830	X	-	-	-
18	CLA	A	831	X	-	-	-
18	CLA	A	832	X	-	-	-
18	CLA	A	833	X	-	-	-
18	CLA	A	834	X	-	-	-
18	CLA	A	835	X	-	-	-
18	CLA	A	836	X	-	-	-
18	CLA	A	837	X	-	-	-
18	CLA	A	838	X	-	-	-
18	CLA	A	839	X	-	-	-
18	CLA	A	840	X	-	-	-
18	CLA	A	852	X	-	-	-
18	CLA	A	853	X	-	-	-
18	CLA	B	801	X	-	-	-
18	CLA	B	803	X	-	-	-
18	CLA	B	804	X	-	-	-
18	CLA	B	805	X	-	-	-
18	CLA	B	806	X	-	-	-
18	CLA	B	807	X	-	-	-
18	CLA	B	808	X	-	-	-
18	CLA	B	809	X	-	-	-
18	CLA	B	810	X	-	-	-
18	CLA	B	811	X	-	-	-
18	CLA	B	812	X	-	-	-
18	CLA	B	813	X	-	-	-
18	CLA	B	814	X	-	-	-
18	CLA	B	815	X	-	-	-
18	CLA	B	816	X	-	-	-
18	CLA	B	817	X	-	-	-
18	CLA	B	818	X	-	-	-
18	CLA	B	819	X	-	-	-
18	CLA	B	820	X	-	-	-
18	CLA	B	821	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	822	X	-	-	-
18	CLA	B	823	X	-	-	-
18	CLA	B	824	X	-	-	-
18	CLA	B	825	X	-	-	-
18	CLA	B	826	X	-	-	-
18	CLA	B	827	X	-	-	-
18	CLA	B	828	X	-	-	-
18	CLA	B	829	X	-	-	-
18	CLA	B	830	X	-	-	-
18	CLA	B	831	X	-	-	-
18	CLA	B	832	X	-	-	-
18	CLA	B	833	X	-	-	-
18	CLA	B	834	X	-	-	-
18	CLA	B	835	X	-	-	-
18	CLA	B	836	X	-	-	-
18	CLA	B	837	X	-	-	-
18	CLA	B	838	X	-	-	-
18	CLA	B	839	X	-	-	-
18	CLA	B	840	X	-	-	-
18	CLA	B	841	X	-	-	-
18	CLA	F	301	X	-	-	-
18	CLA	F	302	X	-	-	-
18	CLA	F	303	X	-	-	-
18	CLA	G	1601	X	-	-	-
18	CLA	G	1602	X	-	-	-
18	CLA	G	1603	X	-	-	-
18	CLA	H	1701	X	-	-	-
18	CLA	J	1101	X	-	-	-
18	CLA	J	1103	X	-	-	-
18	CLA	K	1401	X	-	-	-
18	CLA	K	1402	X	-	-	-
18	CLA	K	1403	X	-	-	-
18	CLA	K	1404	X	-	-	-
18	CLA	L	301	X	-	-	-
18	CLA	L	304	X	-	-	-
18	CLA	L	305	X	-	-	-
18	CLA	L	306	X	-	-	-
29	LUT	1	5004	X	-	-	-
29	LUT	2	303	X	-	-	-
29	LUT	3	304	X	-	-	-
29	LUT	J	1105	X	-	-	-
30	CHL	1	5014	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CHL	1	5016	X	-	-	-
30	CHL	2	314	X	-	-	-
30	CHL	2	315	X	-	-	-
30	CHL	2	316	X	-	-	-
30	CHL	2	318	X	-	-	-
30	CHL	2	319	X	-	-	-
30	CHL	3	310	X	-	-	-
30	CHL	3	312	X	-	-	-
30	CHL	3	313	X	-	-	-
30	CHL	3	316	X	-	-	-
30	CHL	4	302	X	-	-	-
30	CHL	4	313	X	-	-	-
30	CHL	4	314	X	-	-	-
30	CHL	4	316	X	-	-	-
30	CHL	4	317	X	-	-	-
30	CHL	4	318	X	-	-	-
31	XAT	2	304	X	-	-	-
31	XAT	4	304	X	-	-	-

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 37423 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	743	Total	C	N	O	S	0	0	0
			5858	3839	998	1003	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	733	Total	C	N	O	S	0	0	0
			5857	3848	998	997	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			612	379	107	115	11			

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	143	Total	C	N	O	S	0	0	0
			1132	731	194	204	3			

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	66	Total	C	N	O	0	0	0
			528	336	93	99			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	154	Total	C	N	O	S	0	0	0
			1206	782	207	215	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	80	ALA	SER	conflict	UNP A0A0M3KL12
F	87	ASP	GLU	conflict	UNP A0A0M3KL12
F	108	LEU	ILE	conflict	UNP A0A0M3KL12
F	111	PRO	ALA	conflict	UNP A0A0M3KL12
F	134	GLY	ALA	conflict	UNP A0A0M3KL12
F	188	ASP	GLU	conflict	UNP A0A0M3KL12
F	204	THR	SER	conflict	UNP A0A0M3KL12
F	205	GLY	ARG	conflict	UNP A0A0M3KL12

- Molecule 7 is a protein called PsaG.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	97	Total	C	N	O	0	0	0
			757	492	125	140			

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

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	60	LEU	ILE	conflict	UNP A0A0M3KL10
H	79	ASN	SER	conflict	UNP A0A0M3KL10
H	80	SER	PRO	conflict	UNP A0A0M3KL10
H	116	ALA	THR	conflict	UNP A0A0M3KL10
H	126	LYS	VAL	conflict	UNP A0A0M3KL10
H	134	GLN	LYS	conflict	UNP A0A0M3KL10
H	139	LEU	-	insertion	UNP A0A0M3KL10
H	?	-	LYS	deletion	UNP A0A0M3KL10

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	30	Total	C	N	O	S	0	0	0
			232	159	37	35	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	42	Total	C	N	O	S	0	0	0
			338	231	51	55	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 11 is a protein called Photosystem I reaction center subunit X psaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	80	Total	C	N	O	S	0	0	0
			558	353	98	104	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	86	ALA	VAL	conflict	UNP E1C9L3

- Molecule 12 is a protein called PsaL domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	157	Total	C	N	O	S	0	0	0
			1174	772	189	212	1			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	57	VAL	ILE	conflict	UNP E1C9L1
L	79	VAL	ILE	conflict	UNP E1C9L1
L	88	GLY	ALA	conflict	UNP E1C9L1
L	94	ASN	SER	conflict	UNP E1C9L1
L	108	PHE	TYR	conflict	UNP E1C9L1
L	143	ILE	LEU	conflict	UNP E1C9L1
L	157	ASP	ALA	conflict	UNP E1C9L1
L	172	GLN	GLU	conflict	UNP E1C9L1
L	201	PHE	TYR	conflict	UNP E1C9L1

- Molecule 13 is a protein called Lhca1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1	193	Total	C	N	O	S	0	0	0
			1508	982	252	269	5			

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	2	208	Total	C	N	O	S	0	0	0
			1620	1059	265	292	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	3	221	Total	C	N	O	S	0	0	0
			1706	1118	278	305	5			

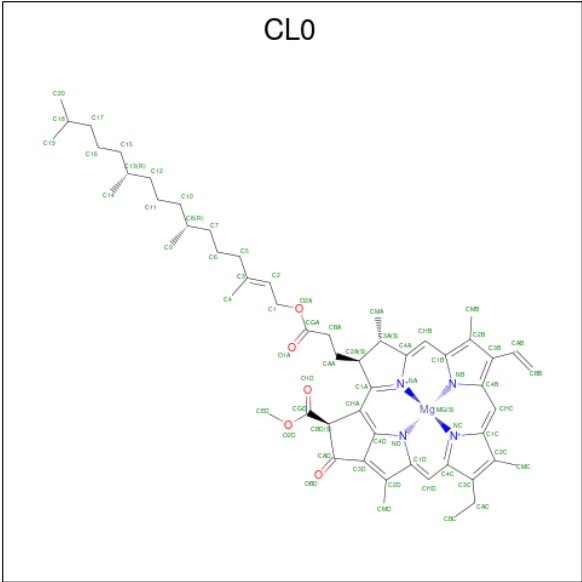
- Molecule 16 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	4	198	Total	C	N	O	S	0	0	0
			1559	1022	253	281	3			

There are 3 discrepancies between the modelled and reference sequences:

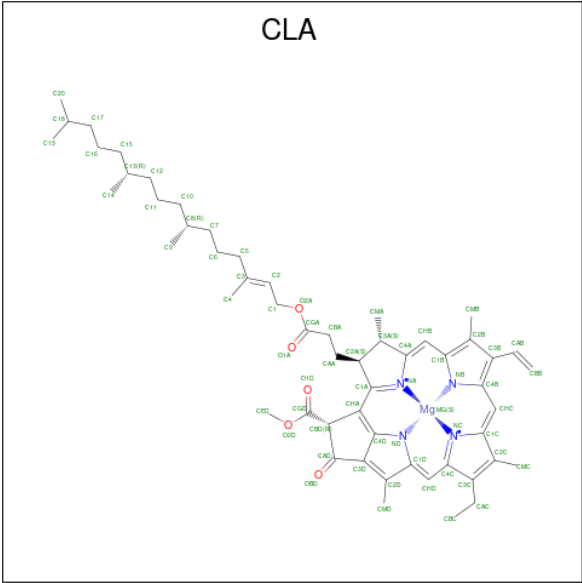
Chain	Residue	Modelled	Actual	Comment	Reference
4	89	LYS	ARG	conflict	UNP Q9SQL2
4	128	ASP	ALA	conflict	UNP Q9SQL2
4	149	PHE	SER	conflict	UNP Q9SQL2

- Molecule 17 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	A	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
18	B	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
18	B	1	Total 58	C 48	Mg 1	N 4	O 5	0	0
18	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	F	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	F	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	F	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	G	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	G	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
18	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	H	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	J	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
18	K	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	K	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
18	K	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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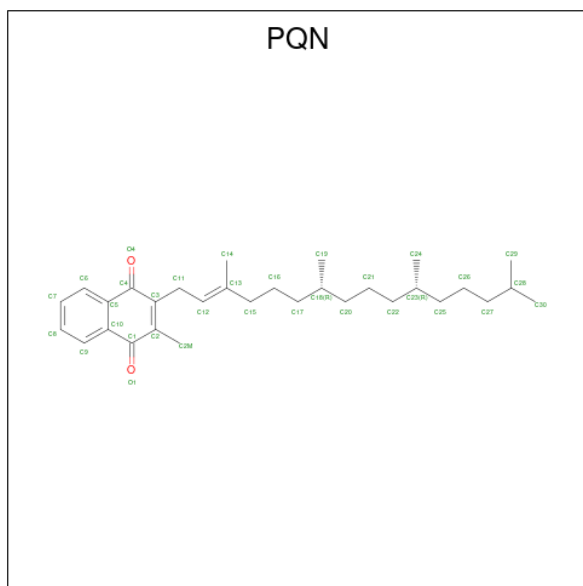
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	1	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
18	2	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
18	2	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
18	2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	2	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
18	2	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
18	2	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
18	2	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	2	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
18	3	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
18	3	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	3	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
18	3	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	3	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	3	1	Total 48	C 38	Mg 1	N 4	O 5	0	0
18	3	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	3	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
18	3	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
18	3	1	Total 60	C 50	Mg 1	N 4	O 5	0	0

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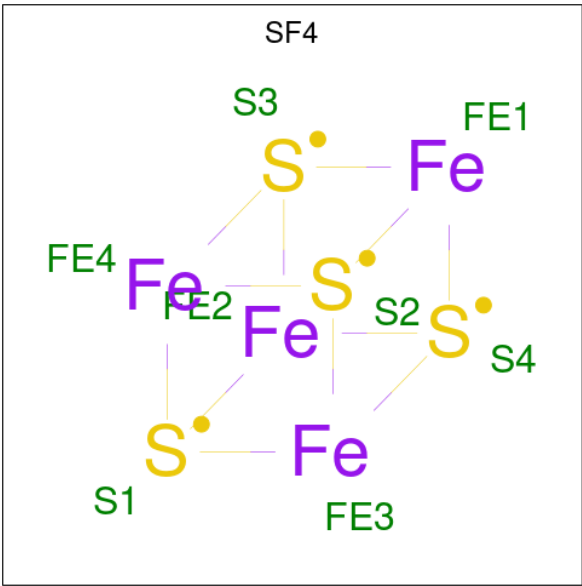
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 19 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



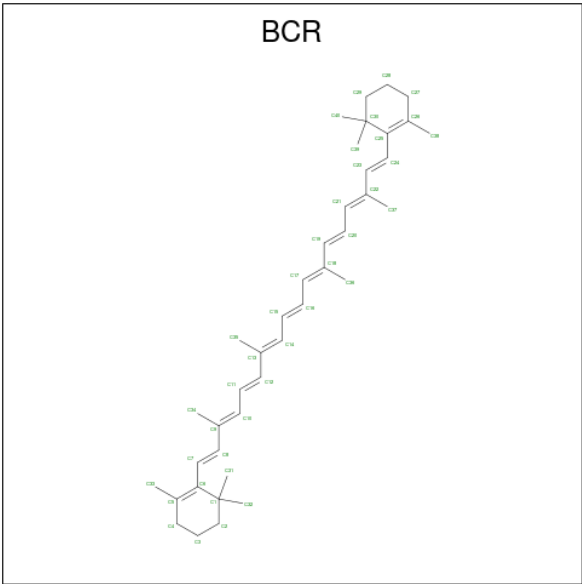
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			33	31	2		
19	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 20 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



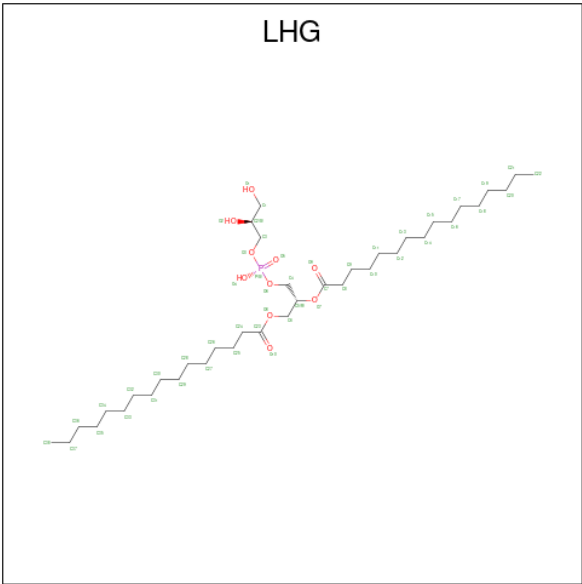
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total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

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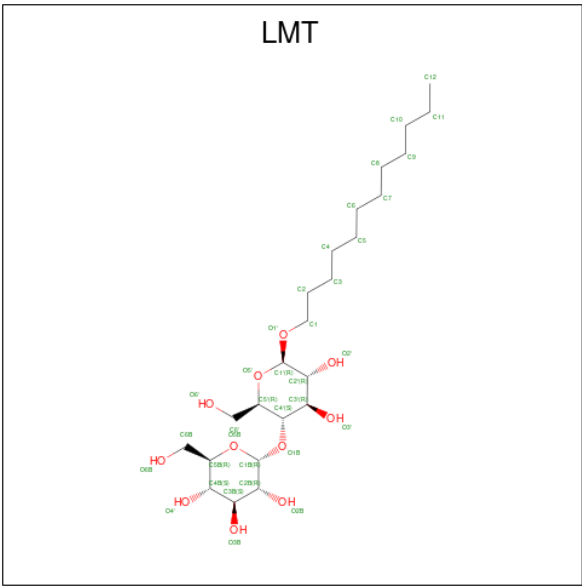
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	1	1	Total C 40 40	0	0
21	2	1	Total C 40 40	0	0
21	3	1	Total C 40 40	0	0
21	3	1	Total C 40 40	0	0
21	4	1	Total C 40 40	0	0

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



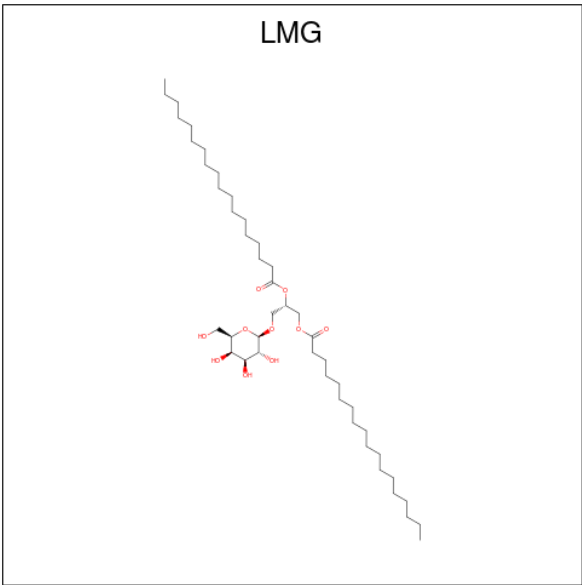
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C O P 49 38 10 1	0	0
22	A	1	Total C O P 40 29 10 1	0	0
22	B	1	Total C O P 21 10 10 1	0	0
22	B	1	Total C O P 49 38 10 1	0	0
22	1	1	Total C O P 49 38 10 1	0	0
22	2	1	Total C O P 35 24 10 1	0	0

- Molecule 23 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			35	24	11		
23	B	1	Total	C	O	0	0
			35	24	11		
23	B	1	Total	C	O	0	0
			32	21	11		
23	B	1	Total	C	O	0	0
			31	20	11		
23	G	1	Total	C	O	0	0
			35	24	11		
23	G	1	Total	C	O	0	0
			31	20	11		
23	J	1	Total	C	O	0	0
			25	14	11		
23	2	1	Total	C	O	0	0
			35	24	11		
23	4	1	Total	C	O	0	0
			35	24	11		

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



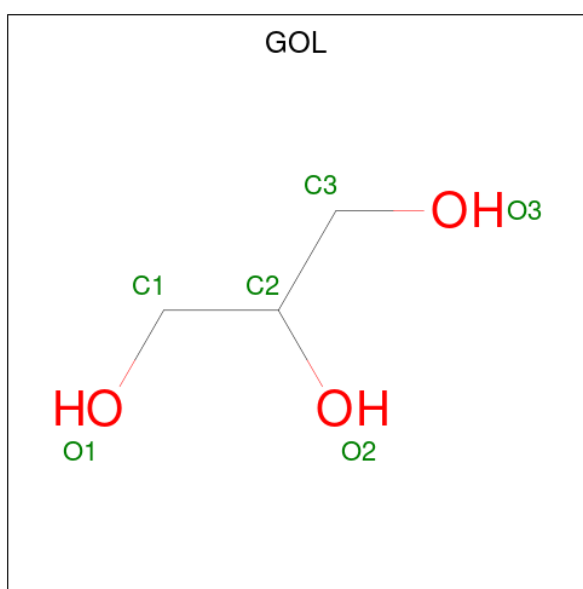
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	1	Total	C	O	0	0
			50	40	10		
24	B	1	Total	C	O	0	0
			35	25	10		
24	B	1	Total	C	O	0	0
			33	23	10		
24	B	1	Total	C	O	0	0
			13	7	6		
24	F	1	Total	C	O	0	0
			47	37	10		
24	F	1	Total	C	O	0	0
			36	26	10		
24	F	1	Total	C	O	0	0
			34	24	10		
24	G	1	Total	C	O	0	0
			25	15	10		
24	J	1	Total	C	O	0	0
			30	20	10		
24	1	1	Total	C	O	0	0
			49	39	10		
24	1	1	Total	C	O	0	0
			46	36	10		
24	2	1	Total	C	O	0	0
			13	7	6		
24	2	1	Total	C	O	0	0
			13	7	6		
24	2	1	Total	C	O	0	0
			25	15	10		

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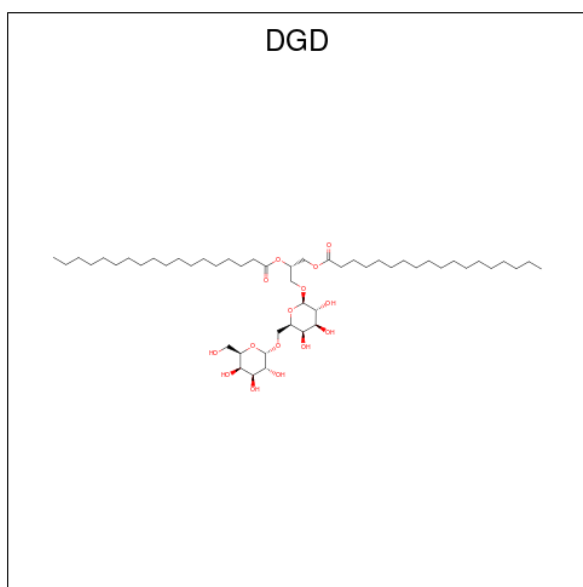
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	2	1	Total	C	O	0	0
			36	26	10		
24	2	1	Total	C	O	0	0
			13	7	6		
24	2	1	Total	C	O	0	0
			13	7	6		
24	4	1	Total	C	O	0	0
			13	7	6		

- Molecule 25 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	O	0	0
			6	3	3		
25	4	1	Total	C	O	0	0
			6	3	3		

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

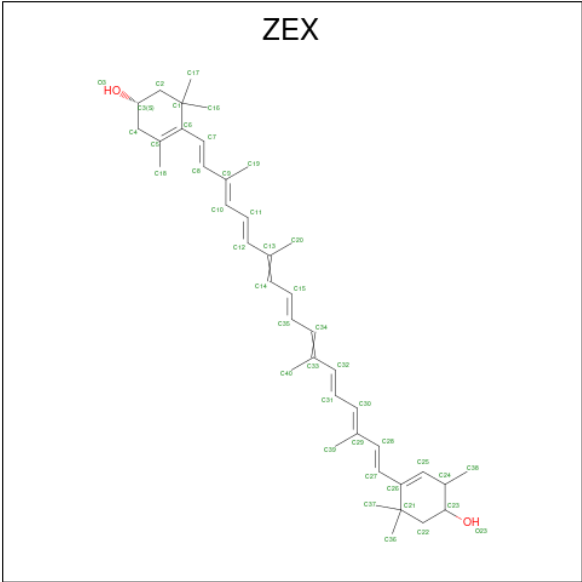


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	B	1	Total	C	O	0	0
			61	46	15		
26	F	1	Total	C	O	0	0
			57	42	15		
26	J	1	Total	C	O	0	0
			58	43	15		
26	1	1	Total	C	O	0	0
			35	26	9		
26	2	1	Total	C	O	0	0
			51	36	15		

- Molecule 27 is CALCIUM ION (CCD ID: CA) (formula: Ca).

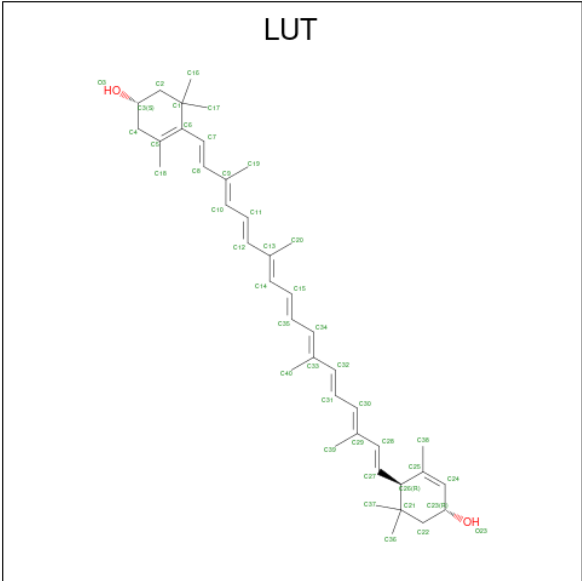
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	B	1	Total	Ca	0	0
			1	1		
27	3	1	Total	Ca	0	0
			1	1		

- Molecule 28 is (1R,2S)-4-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl]-2,5,5-trimethylcyclohex-3-en-1-ol (CCD ID: ZEX) (formula: C₄₀H₅₆O₂).



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

- Molecule 29 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



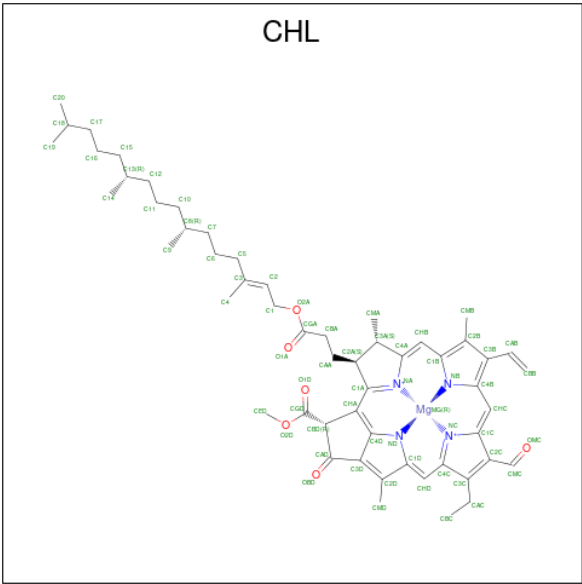
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	J	1	Total	C	O	0	0
			42	40	2		
29	1	1	Total	C	O	0	0
			42	40	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	1	1	Total	C	O	0	0
			42	40	2		
29	2	1	Total	C	O	0	0
			42	40	2		
29	3	1	Total	C	O	0	0
			42	40	2		
29	3	1	Total	C	O	0	0
			42	40	2		
29	4	1	Total	C	O	0	0
			42	40	2		

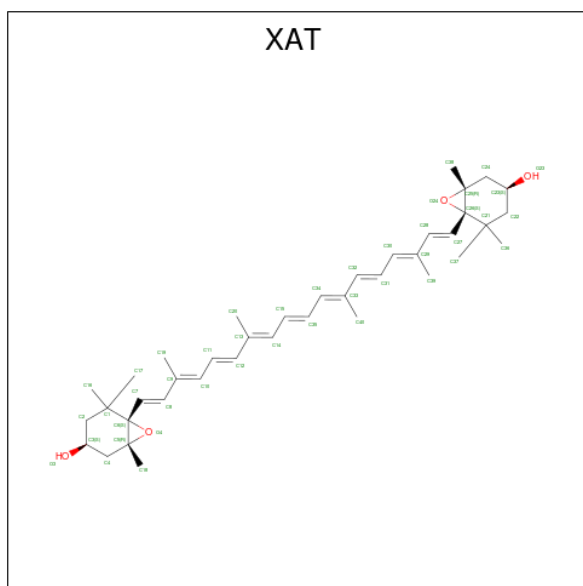
- Molecule 30 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	2	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
30	3	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
30	3	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
30	3	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
30	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
30	4	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
30	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
30	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
30	4	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
30	4	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
30	4	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		

- Molecule 31 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 (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	2	1	Total	C	O	0	0
			44	40	4		
31	4	1	Total	C	O	0	0
			44	40	4		

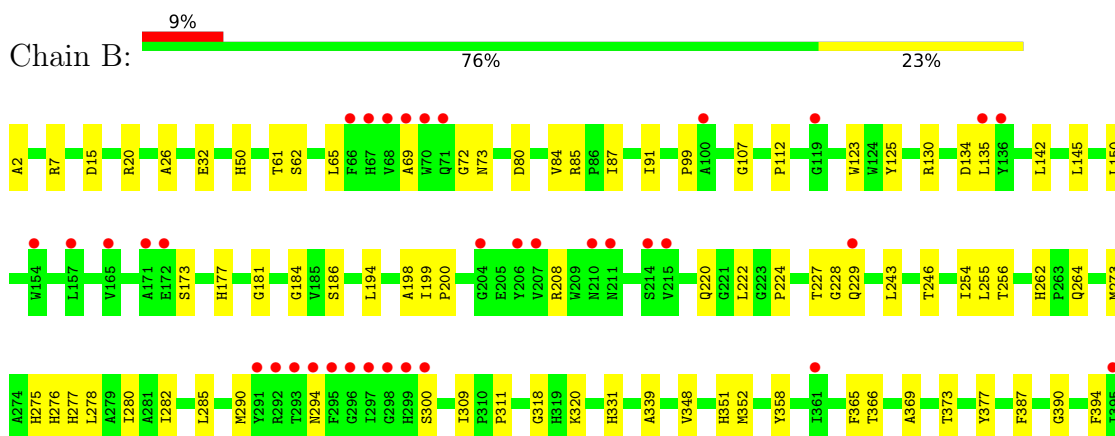
3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

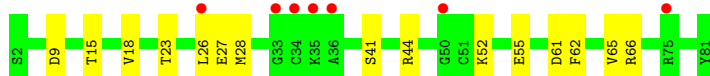
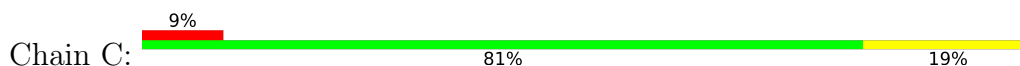


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

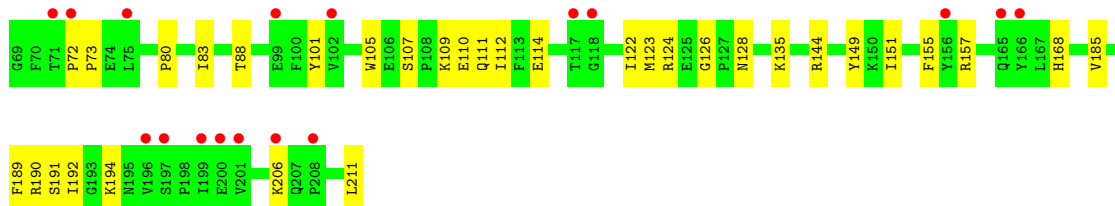
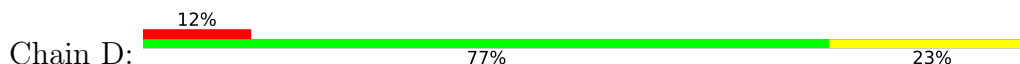




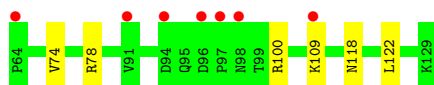
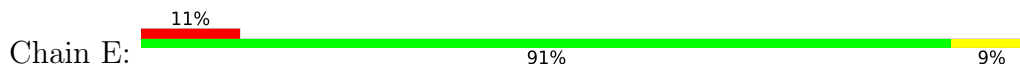
● Molecule 3: Photosystem I iron-sulfur center



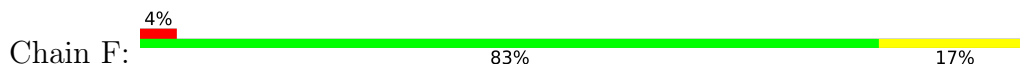
● Molecule 4: PsadD



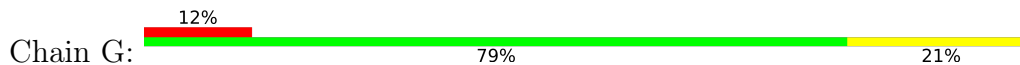
● Molecule 5: PsaeE



● Molecule 6: Photosystem I reaction center subunit III

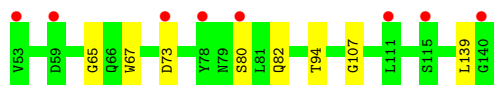


● Molecule 7: PsagG

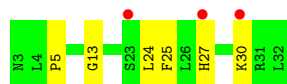




- Molecule 8: Photosystem I reaction center subunit VI



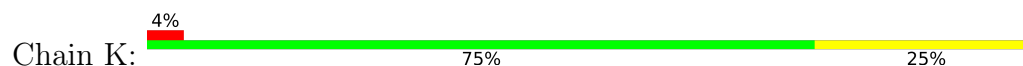
- Molecule 9: Photosystem I reaction center subunit VIII



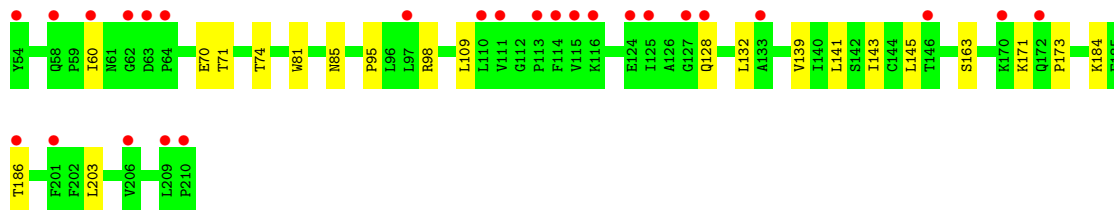
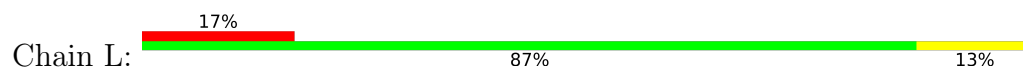
- Molecule 10: Photosystem I reaction center subunit IX



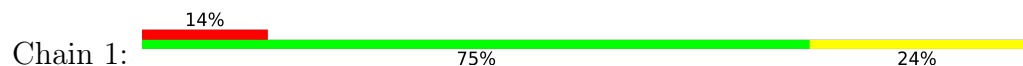
- Molecule 11: Photosystem I reaction center subunit X psaK

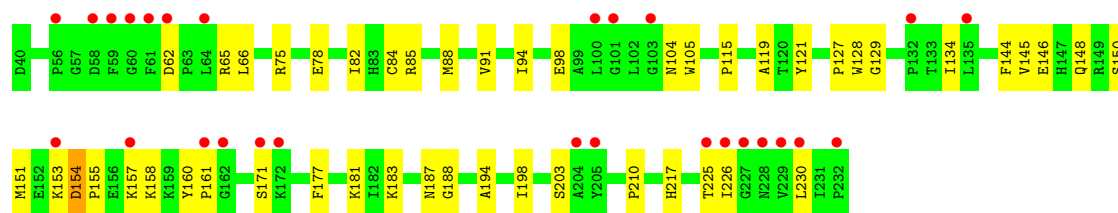


- Molecule 12: PsaL domain-containing protein

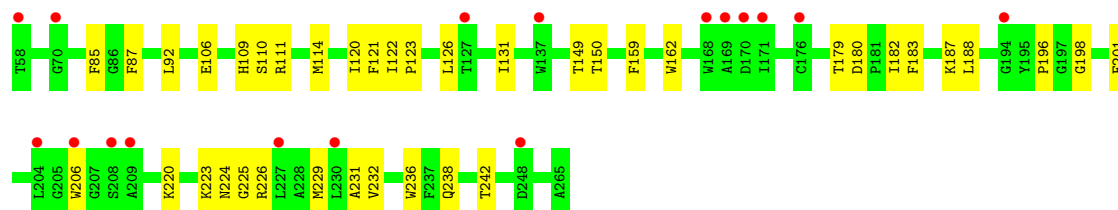
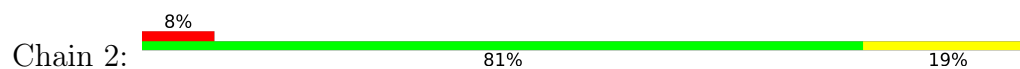


- Molecule 13: Lhca1

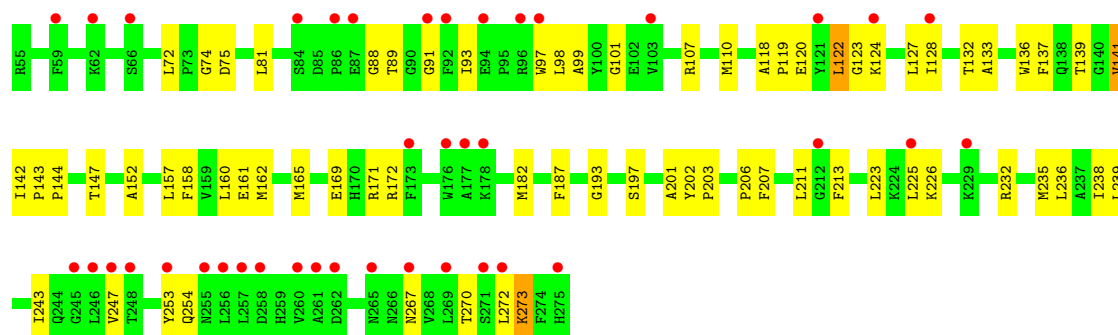




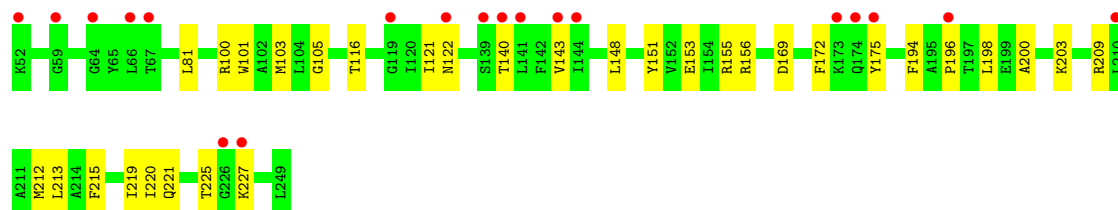
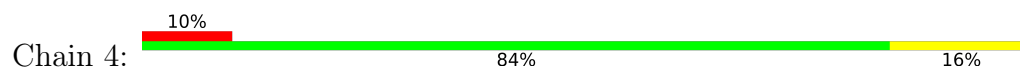
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	190.20Å 201.79Å 213.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 3.00 49.63 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.7 (49.63-3.00) 91.6 (49.63-3.00)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.239 , 0.270 0.239 , 0.269	Depositor DCC
R_{free} test set	3337 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	96.1	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	37423	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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: LMG, CHL, DGD, BCR, LHG, CA, CL0, PQN, GOL, CLA, ZEX, XAT, SF4, LMT, LUT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.12	0/6057	0.29	0/8264
2	B	0.10	0/6069	0.27	0/8286
3	C	0.11	0/625	0.32	0/846
4	D	0.10	0/1163	0.31	0/1572
5	E	0.10	0/540	0.32	0/734
6	F	0.10	0/1234	0.27	0/1670
7	G	0.08	0/776	0.23	0/1054
8	H	0.09	0/693	0.26	0/942
9	I	0.10	0/238	0.26	0/324
10	J	0.10	0/349	0.27	0/476
11	K	0.09	0/564	0.29	0/763
12	L	0.09	0/1207	0.26	0/1651
13	1	0.10	0/1558	0.27	0/2125
14	2	0.10	0/1679	0.26	0/2302
15	3	0.10	0/1760	0.29	0/2390
16	4	0.09	0/1608	0.25	0/2191
All	All	0.10	0/26120	0.28	0/35590

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5858	0	5717	143	0
2	B	5857	0	5653	141	0
3	C	612	0	591	13	0
4	D	1132	0	1141	19	0
5	E	528	0	528	6	0
6	F	1206	0	1231	20	0
7	G	757	0	743	16	0
8	H	673	0	667	7	0
9	I	232	0	253	5	0
10	J	338	0	345	13	0
11	K	558	0	587	18	0
12	L	1174	0	1183	17	0
13	1	1508	0	1489	43	0
14	2	1620	0	1554	33	0
15	3	1706	0	1659	62	0
16	4	1559	0	1524	28	0
17	A	65	0	72	7	0
18	1	608	0	562	37	0
18	2	572	0	538	34	0
18	3	531	0	456	29	0
18	4	516	0	488	19	0
18	A	2543	0	2661	203	0
18	B	2480	0	2602	191	0
18	F	195	0	215	12	0
18	G	166	0	152	5	0
18	H	60	0	59	6	0
18	J	115	0	110	8	0
18	K	199	0	158	16	0
18	L	215	0	183	7	0
19	A	33	0	46	5	0
19	B	33	0	46	2	0
20	A	8	0	0	0	0
20	C	16	0	0	1	0
21	1	40	0	53	3	0
21	2	40	0	53	10	0
21	3	80	0	106	6	0
21	4	40	0	52	7	0
21	A	240	0	317	33	0
21	B	240	0	317	27	0
21	F	80	0	105	11	0
21	G	40	0	53	4	0
21	I	80	0	105	4	0
21	J	40	0	53	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	K	40	0	53	2	0
21	L	120	0	159	7	0
22	1	49	0	74	3	0
22	2	35	0	40	1	0
22	A	89	0	127	16	0
22	B	70	0	86	8	0
23	2	35	0	46	1	0
23	4	35	0	46	0	0
23	A	35	0	45	0	0
23	B	98	0	118	3	0
23	G	66	0	80	3	0
23	J	25	0	22	0	0
24	1	95	0	136	9	0
24	2	113	0	106	5	0
24	4	13	0	11	0	0
24	A	50	0	73	6	0
24	B	81	0	87	2	0
24	F	117	0	147	5	0
24	G	25	0	20	1	0
24	J	30	0	30	0	0
25	4	6	0	8	0	0
25	A	6	0	8	1	0
26	1	35	0	39	0	0
26	2	51	0	60	5	0
26	B	61	0	83	8	0
26	F	57	0	75	0	0
26	J	58	0	77	4	0
27	3	1	0	0	0	0
27	B	1	0	0	0	0
28	F	42	0	56	3	0
29	1	84	0	110	14	0
29	2	42	0	55	5	0
29	3	84	0	110	12	0
29	4	42	0	55	2	0
29	J	42	0	55	9	0
30	1	108	0	87	10	0
30	2	272	0	224	19	0
30	3	215	0	172	23	0
30	4	314	0	243	20	0
31	2	44	0	56	7	0
31	4	44	0	56	6	0
All	All	37423	0	37562	1032	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 14.

The worst 5 of 1032 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)
11:K:61:LEU:HB3	18:K:1403:CLA:HAB	1.45	0.97
31:2:304:XAT:H8	18:2:311:CLA:HBB1	1.50	0.94
1:A:401:TRP:CD1	18:A:826:CLA:HAB	2.10	0.87
18:B:807:CLA:H152	18:B:829:CLA:HBB2	1.58	0.85
24:1:5001:LMG:H122	30:1:5016:CHL:HBA1	1.61	0.83

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	741/743 (100%)	700 (94%)	40 (5%)	1 (0%)	48	80
2	B	731/733 (100%)	707 (97%)	23 (3%)	1 (0%)	48	80
3	C	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
4	D	141/143 (99%)	131 (93%)	9 (6%)	1 (1%)	18	53
5	E	64/66 (97%)	59 (92%)	5 (8%)	0	100	100
6	F	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
7	G	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
8	H	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
9	I	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
10	J	40/42 (95%)	38 (95%)	2 (5%)	0	100	100
11	K	78/80 (98%)	70 (90%)	8 (10%)	0	100	100
12	L	155/157 (99%)	147 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	1	191/193 (99%)	181 (95%)	7 (4%)	3 (2%)	7	34
14	2	206/208 (99%)	189 (92%)	17 (8%)	0	100	100
15	3	219/221 (99%)	201 (92%)	18 (8%)	0	100	100
16	4	196/198 (99%)	188 (96%)	8 (4%)	0	100	100
All	All	3201/3233 (99%)	3034 (95%)	161 (5%)	6 (0%)	43	76

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	1	161	PRO
1	A	720	THR
2	B	492	ILE
13	1	115	PRO
13	1	154	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	604/604 (100%)	599 (99%)	5 (1%)	73	86
2	B	598/598 (100%)	591 (99%)	7 (1%)	63	82
3	C	69/69 (100%)	69 (100%)	0	100	100
4	D	122/122 (100%)	122 (100%)	0	100	100
5	E	58/58 (100%)	57 (98%)	1 (2%)	53	78
6	F	125/126 (99%)	125 (100%)	0	100	100
7	G	82/82 (100%)	82 (100%)	0	100	100
8	H	71/71 (100%)	71 (100%)	0	100	100
9	I	26/26 (100%)	26 (100%)	0	100	100
10	J	35/35 (100%)	35 (100%)	0	100	100
11	K	58/58 (100%)	58 (100%)	0	100	100
12	L	124/124 (100%)	123 (99%)	1 (1%)	73	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	1	158/158 (100%)	158 (100%)	0	100	100
14	2	167/167 (100%)	166 (99%)	1 (1%)	78	88
15	3	171/172 (99%)	166 (97%)	5 (3%)	37	70
16	4	164/164 (100%)	164 (100%)	0	100	100
All	All	2632/2634 (100%)	2612 (99%)	20 (1%)	73	86

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	2	242	THR
15	3	141	VAL
15	3	273	LYS
15	3	147	THR
2	B	256	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	608	GLN
15	3	244	GLN
7	G	90	GLN
16	4	222	HIS
13	1	228	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 240 ligands modelled in this entry, 2 are monoatomic - leaving 238 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
18	CLA	2	312	22	64,68,73	1.41	8 (12%)	76,107,113	1.91	16 (21%)
18	CLA	2	326	16	54,58,73	1.53	8 (14%)	64,95,113	2.04	16 (25%)
18	CLA	3	309	-	59,63,73	1.47	8 (13%)	70,101,113	2.07	22 (31%)
23	LMT	J	1107	-	26,26,36	1.29	4 (15%)	37,37,47	1.07	2 (5%)
18	CLA	B	829	-	69,73,73	1.36	8 (11%)	82,113,113	1.81	17 (20%)
18	CLA	A	806	-	64,68,73	1.42	7 (10%)	76,107,113	1.90	17 (22%)
18	CLA	A	839	-	69,73,73	1.36	8 (11%)	82,113,113	1.80	16 (19%)
24	LMG	1	5020	-	46,46,55	1.04	3 (6%)	54,54,63	1.08	4 (7%)
24	LMG	2	324	-	13,13,55	0.58	0	18,18,63	0.68	0
22	LHG	A	848	-	48,48,48	0.38	0	51,54,54	1.05	3 (5%)
18	CLA	A	840	22	64,68,73	1.41	7 (10%)	76,107,113	1.93	17 (22%)
18	CLA	B	817	-	64,68,73	1.40	7 (10%)	76,107,113	1.90	19 (25%)
18	CLA	A	814	-	50,54,73	1.59	7 (14%)	59,90,113	2.03	15 (25%)
19	PQN	B	842	-	34,34,34	0.42	0	43,45,45	1.10	3 (6%)
30	CHL	2	316	-	42,56,74	1.56	9 (21%)	36,92,114	2.01	12 (33%)
18	CLA	J	1101	-	69,73,73	1.35	6 (8%)	82,113,113	1.91	19 (23%)
18	CLA	K	1401	-	49,53,73	1.61	8 (16%)	58,89,113	2.03	15 (25%)
18	CLA	1	5012	-	50,54,73	1.58	7 (14%)	59,90,113	2.03	15 (25%)
21	BCR	B	846	-	41,41,41	1.60	4 (9%)	56,56,56	4.40	13 (23%)
18	CLA	2	317	-	59,63,73	1.46	7 (11%)	70,101,113	1.96	16 (22%)
21	BCR	A	846	-	41,41,41	1.60	4 (9%)	56,56,56	4.41	14 (25%)
18	CLA	4	315	-	69,73,73	1.35	7 (10%)	82,113,113	1.88	17 (20%)
18	CLA	G	1603	-	69,73,73	1.36	8 (11%)	82,113,113	1.86	19 (23%)
18	CLA	A	812	-	69,73,73	1.34	7 (10%)	82,113,113	1.89	20 (24%)
18	CLA	B	809	-	69,73,73	1.35	6 (8%)	82,113,113	1.84	15 (18%)
18	CLA	1	5011	-	54,58,73	1.53	7 (12%)	64,95,113	2.05	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	805	-	69,73,73	1.35	7 (10%)	82,113,113	1.83	17 (20%)
18	CLA	4	307	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	19 (23%)
20	SF4	C	101	3	0,12,12	-	-	-		
18	CLA	A	810	-	69,73,73	1.35	7 (10%)	82,113,113	1.83	15 (18%)
21	BCR	I	101	-	41,41,41	1.64	4 (9%)	56,56,56	4.46	18 (32%)
24	LMG	2	301	-	13,13,55	0.57	0	18,18,63	0.59	0
23	LMT	2	325	-	36,36,36	1.13	4 (11%)	47,47,47	1.10	3 (6%)
18	CLA	1	5007	13	50,54,73	1.58	7 (14%)	59,90,113	2.02	17 (28%)
30	CHL	3	312	-	45,59,74	1.46	7 (15%)	40,96,114	1.97	11 (27%)
21	BCR	B	802	-	41,41,41	1.60	4 (9%)	56,56,56	4.86	18 (32%)
21	BCR	A	843	-	41,41,41	1.59	4 (9%)	56,56,56	4.48	19 (33%)
18	CLA	B	807	2	69,73,73	1.35	7 (10%)	82,113,113	1.83	16 (19%)
18	CLA	1	5018	13	64,68,73	1.42	8 (12%)	76,107,113	1.89	20 (26%)
18	CLA	4	311	-	64,68,73	1.40	7 (10%)	76,107,113	1.92	19 (25%)
21	BCR	3	306	-	41,41,41	1.62	4 (9%)	56,56,56	4.21	19 (33%)
18	CLA	1	5008	-	59,63,73	1.46	7 (11%)	70,101,113	2.02	17 (24%)
24	LMG	F	306	-	47,47,55	1.09	4 (8%)	55,55,63	1.12	4 (7%)
18	CLA	A	853	-	69,73,73	1.35	5 (7%)	82,113,113	1.91	16 (19%)
24	LMG	B	850	-	35,35,55	0.79	1 (2%)	43,43,63	1.15	5 (11%)
18	CLA	1	5010	-	69,73,73	1.36	6 (8%)	82,113,113	1.90	19 (23%)
21	BCR	L	302	-	41,41,41	1.59	4 (9%)	56,56,56	4.61	20 (35%)
18	CLA	B	835	-	59,63,73	1.47	7 (11%)	70,101,113	1.99	20 (28%)
18	CLA	A	804	-	69,73,73	1.35	7 (10%)	82,113,113	1.90	18 (21%)
22	LHG	1	5019	-	48,48,48	0.40	0	51,54,54	1.06	3 (5%)
21	BCR	L	307	-	41,41,41	1.60	4 (9%)	56,56,56	4.50	15 (26%)
24	LMG	A	851	-	50,50,55	1.18	5 (10%)	58,58,63	1.07	3 (5%)
18	CLA	B	801	-	69,73,73	1.36	8 (11%)	82,113,113	1.90	18 (21%)
24	LMG	F	308	-	34,34,55	0.51	0	42,42,63	1.10	2 (4%)
25	GOL	4	321	-	5,5,5	0.56	0	5,5,5	0.29	0
17	CL0	A	801	-	58,73,73	3.28	17 (29%)	60,113,113	2.79	16 (26%)
18	CLA	A	852	-	69,73,73	1.36	8 (11%)	82,113,113	1.85	18 (21%)
18	CLA	B	838	-	54,58,73	1.53	7 (12%)	64,95,113	2.07	20 (31%)
29	LUT	3	303	-	42,43,43	2.47	1 (2%)	51,60,60	1.82	15 (29%)
18	CLA	L	305	-	64,68,73	1.40	7 (10%)	76,107,113	1.95	19 (25%)
18	CLA	4	312	-	50,54,73	1.58	7 (14%)	59,90,113	2.06	15 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	2	307	14	56,60,73	1.51	8 (14%)	65,97,113	2.04	19 (29%)
18	CLA	A	828	-	69,73,73	1.36	7 (10%)	82,113,113	1.90	16 (19%)
21	BCR	B	847	-	41,41,41	1.60	4 (9%)	56,56,56	4.54	14 (25%)
24	LMG	B	854	-	13,13,55	0.56	0	18,18,63	0.73	0
26	DGD	F	309	-	58,58,67	1.12	4 (6%)	72,72,81	1.07	2 (2%)
30	CHL	2	319	-	50,64,74	1.36	8 (16%)	46,102,114	1.86	12 (26%)
18	CLA	B	834	-	64,68,73	1.41	8 (12%)	76,107,113	1.88	14 (18%)
29	LUT	4	303	-	42,43,43	2.48	1 (2%)	51,60,60	1.81	13 (25%)
24	LMG	F	307	-	36,36,55	0.79	1 (2%)	44,44,63	1.05	2 (4%)
18	CLA	B	841	22	69,73,73	1.36	7 (10%)	82,113,113	1.82	20 (24%)
18	CLA	A	813	-	69,73,73	1.35	6 (8%)	82,113,113	1.91	18 (21%)
18	CLA	B	804	-	69,73,73	1.35	6 (8%)	82,113,113	1.82	19 (23%)
28	ZEX	F	310	-	43,43,43	0.74	1 (2%)	51,60,60	2.01	13 (25%)
21	BCR	B	844	-	41,41,41	1.59	4 (9%)	56,56,56	4.51	17 (30%)
18	CLA	1	5015	-	69,73,73	1.35	7 (10%)	82,113,113	1.85	16 (19%)
18	CLA	1	5009	-	69,73,73	1.36	6 (8%)	82,113,113	1.89	18 (21%)
18	CLA	2	308	-	69,73,73	1.35	7 (10%)	82,113,113	1.96	18 (21%)
18	CLA	A	816	-	60,64,73	1.45	7 (11%)	71,102,113	1.96	19 (26%)
30	CHL	4	317	-	37,51,74	1.58	9 (24%)	30,86,114	2.27	10 (33%)
18	CLA	B	831	-	69,73,73	1.36	7 (10%)	82,113,113	1.89	19 (23%)
18	CLA	A	837	-	69,73,73	1.36	7 (10%)	82,113,113	1.84	15 (18%)
18	CLA	H	1701	-	64,68,73	1.41	6 (9%)	76,107,113	1.93	18 (23%)
18	CLA	F	302	-	69,73,73	1.36	8 (11%)	82,113,113	1.82	18 (21%)
18	CLA	B	839	-	69,73,73	1.36	7 (10%)	82,113,113	1.86	17 (20%)
18	CLA	B	819	-	69,73,73	1.34	7 (10%)	82,113,113	1.92	19 (23%)
18	CLA	2	313	-	54,58,73	1.53	7 (12%)	64,95,113	2.12	19 (29%)
24	LMG	2	322	-	36,36,55	0.69	1 (2%)	44,44,63	1.07	2 (4%)
18	CLA	B	830	-	69,73,73	1.38	8 (11%)	82,113,113	1.91	16 (19%)
18	CLA	G	1601	-	59,63,73	1.47	7 (11%)	70,101,113	1.98	17 (24%)
20	SF4	C	102	3	0,12,12	-	-	-	-	-
21	BCR	F	304	-	41,41,41	1.60	4 (9%)	56,56,56	4.50	16 (28%)
18	CLA	1	5017	-	49,53,73	1.61	7 (14%)	58,89,113	2.03	14 (24%)
21	BCR	A	855	-	41,41,41	1.60	4 (9%)	56,56,56	4.56	17 (30%)
18	CLA	3	308	-	56,60,73	1.50	7 (12%)	65,97,113	2.04	18 (27%)
18	CLA	4	309	-	64,68,73	1.41	7 (10%)	76,107,113	1.94	20 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LHG	2	320	18	34,34,48	0.45	0	37,40,54	1.16	3 (8%)
18	CLA	A	805	-	69,73,73	1.36	7 (10%)	82,113,113	1.82	18 (21%)
18	CLA	B	816	-	59,63,73	1.46	7 (11%)	70,101,113	2.05	21 (30%)
18	CLA	B	820	-	69,73,73	1.34	7 (10%)	82,113,113	1.81	17 (20%)
18	CLA	A	823	-	69,73,73	1.36	8 (11%)	82,113,113	1.94	19 (23%)
26	DGD	2	327	-	52,52,67	0.98	3 (5%)	66,66,81	1.10	5 (7%)
30	CHL	2	318	-	40,54,74	1.52	9 (22%)	34,90,114	2.11	10 (29%)
21	BCR	K	1405	-	41,41,41	1.61	4 (9%)	56,56,56	4.45	18 (32%)
30	CHL	2	314	14	60,74,74	1.34	8 (13%)	58,114,114	1.70	12 (20%)
24	LMG	G	1607	-	25,25,55	0.69	1 (4%)	33,33,63	1.29	5 (15%)
18	CLA	A	807	1	69,73,73	1.35	7 (10%)	82,113,113	1.89	18 (21%)
21	BCR	1	5005	-	41,41,41	1.59	4 (9%)	56,56,56	4.51	15 (26%)
25	GOL	A	854	-	5,5,5	0.56	0	5,5,5	0.30	0
30	CHL	4	316	-	55,69,74	1.35	10 (18%)	52,108,114	1.76	12 (23%)
18	CLA	B	822	-	69,73,73	1.36	7 (10%)	82,113,113	1.89	18 (21%)
24	LMG	1	5001	-	49,49,55	1.14	5 (10%)	57,57,63	1.13	4 (7%)
18	CLA	3	315	15	69,73,73	1.35	7 (10%)	82,113,113	1.81	17 (20%)
18	CLA	2	311	-	54,58,73	1.51	7 (12%)	64,95,113	2.09	18 (28%)
18	CLA	3	307	-	59,63,73	1.48	7 (11%)	70,101,113	1.97	20 (28%)
18	CLA	A	824	-	59,63,73	1.48	8 (13%)	70,101,113	1.95	16 (22%)
30	CHL	3	313	-	45,59,74	1.42	7 (15%)	40,96,114	2.02	11 (27%)
18	CLA	B	811	-	69,73,73	1.36	8 (11%)	82,113,113	1.83	18 (21%)
18	CLA	A	831	-	69,73,73	1.35	7 (10%)	82,113,113	1.88	21 (25%)
24	LMG	2	323	-	13,13,55	0.63	0	18,18,63	0.93	1 (5%)
31	XAT	2	304	-	41,47,47	0.71	1 (2%)	54,74,74	1.82	10 (18%)
18	CLA	B	810	2	69,73,73	1.36	7 (10%)	82,113,113	1.81	17 (20%)
18	CLA	K	1403	-	52,56,73	1.56	6 (11%)	61,92,113	2.19	17 (27%)
30	CHL	4	318	-	50,64,74	1.35	7 (14%)	46,102,114	1.86	12 (26%)
18	CLA	4	308	-	64,68,73	1.41	7 (10%)	76,107,113	1.97	18 (23%)
20	SF4	A	842	2,1	0,12,12	-	-	-	-	-
18	CLA	A	836	-	69,73,73	1.35	7 (10%)	82,113,113	1.85	20 (24%)
18	CLA	B	803	-	69,73,73	1.37	6 (8%)	82,113,113	1.78	13 (15%)
18	CLA	B	837	-	69,73,73	1.34	7 (10%)	82,113,113	1.90	18 (21%)
18	CLA	A	803	-	69,73,73	1.34	7 (10%)	82,113,113	1.90	21 (25%)
18	CLA	2	306	-	64,68,73	1.40	7 (10%)	76,107,113	1.93	19 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	1	5013	-	50,54,73	1.58	6 (12%)	59,90,113	2.10	13 (22%)
22	LHG	B	849	-	48,48,48	0.40	0	51,54,54	1.03	2 (3%)
30	CHL	1	5014	-	41,55,74	1.43	7 (17%)	35,91,114	2.10	11 (31%)
18	CLA	B	821	-	50,54,73	1.59	7 (14%)	59,90,113	2.04	14 (23%)
23	LMT	B	852	-	36,36,36	1.12	4 (11%)	47,47,47	1.08	2 (4%)
18	CLA	A	829	-	69,73,73	1.35	8 (11%)	82,113,113	1.91	18 (21%)
18	CLA	3	318	-	50,54,73	1.59	6 (12%)	59,90,113	1.99	14 (23%)
18	CLA	3	314	-	52,56,73	1.56	8 (15%)	61,92,113	2.09	18 (29%)
18	CLA	B	828	-	69,73,73	1.36	6 (8%)	82,113,113	1.88	16 (19%)
18	CLA	A	815	-	69,73,73	1.35	7 (10%)	82,113,113	1.84	18 (21%)
18	CLA	4	305	-	64,68,73	1.41	7 (10%)	76,107,113	1.90	21 (27%)
18	CLA	B	827	-	69,73,73	1.37	7 (10%)	82,113,113	1.92	19 (23%)
19	PQN	A	841	-	34,34,34	0.43	0	43,45,45	1.15	4 (9%)
30	CHL	4	313	-	41,55,74	1.51	8 (19%)	35,91,114	2.14	11 (31%)
18	CLA	4	310	-	54,58,73	1.52	7 (12%)	64,95,113	2.03	15 (23%)
18	CLA	3	317	-	54,58,73	1.51	7 (12%)	64,95,113	2.14	19 (29%)
21	BCR	4	301	-	41,41,41	1.62	4 (9%)	56,56,56	4.45	17 (30%)
30	CHL	1	5016	-	55,69,74	1.39	8 (14%)	52,108,114	1.72	11 (21%)
18	CLA	B	815	-	69,73,73	1.35	7 (10%)	82,113,113	1.90	16 (19%)
18	CLA	B	833	-	62,66,73	1.43	6 (9%)	73,104,113	2.03	19 (26%)
18	CLA	J	1103	-	54,58,73	1.54	8 (14%)	64,95,113	2.08	19 (29%)
21	BCR	F	305	-	41,41,41	1.60	4 (9%)	56,56,56	4.61	19 (33%)
24	LMG	2	321	-	25,25,55	0.56	0	33,33,63	1.07	3 (9%)
24	LMG	4	320	-	13,13,55	0.56	0	18,18,63	0.68	0
18	CLA	A	802	-	69,73,73	1.35	7 (10%)	82,113,113	1.75	16 (19%)
18	CLA	A	827	-	69,73,73	1.36	7 (10%)	82,113,113	1.83	15 (18%)
18	CLA	A	809	-	54,58,73	1.52	7 (12%)	64,95,113	2.04	18 (28%)
21	BCR	A	847	-	41,41,41	1.60	4 (9%)	56,56,56	4.48	19 (33%)
29	LUT	2	303	-	42,43,43	2.43	1 (2%)	51,60,60	1.94	13 (25%)
30	CHL	4	314	-	45,59,74	1.59	8 (17%)	40,96,114	2.05	12 (30%)
18	CLA	3	301	-	49,53,73	1.60	7 (14%)	58,89,113	1.97	14 (24%)
18	CLA	L	306	-	54,58,73	1.53	7 (12%)	64,95,113	2.05	18 (28%)
18	CLA	B	812	-	64,68,73	1.41	6 (9%)	76,107,113	1.86	18 (23%)
18	CLA	L	304	12	54,58,73	1.52	6 (11%)	64,95,113	2.09	17 (26%)
18	CLA	B	826	-	69,73,73	1.35	7 (10%)	82,113,113	1.93	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	L	301	-	59,63,73	1.47	7 (11%)	70,101,113	1.94	19 (27%)
18	CLA	B	836	-	59,63,73	1.48	8 (13%)	70,101,113	1.98	18 (25%)
18	CLA	1	5006	13	69,73,73	1.37	7 (10%)	82,113,113	1.85	19 (23%)
21	BCR	B	843	-	41,41,41	1.61	4 (9%)	56,56,56	4.79	19 (33%)
18	CLA	B	825	-	69,73,73	1.36	7 (10%)	82,113,113	1.92	16 (19%)
18	CLA	B	813	-	50,54,73	1.59	6 (12%)	59,90,113	2.03	12 (20%)
21	BCR	L	303	-	41,41,41	1.61	4 (9%)	56,56,56	4.52	14 (25%)
18	CLA	A	825	-	69,73,73	1.37	8 (11%)	82,113,113	1.91	20 (24%)
23	LMT	4	319	-	36,36,36	1.12	4 (11%)	47,47,47	0.98	2 (4%)
18	CLA	A	835	-	69,73,73	1.35	7 (10%)	82,113,113	1.87	17 (20%)
18	CLA	G	1602	7	50,54,73	1.60	8 (16%)	59,90,113	2.02	12 (20%)
18	CLA	4	306	-	54,58,73	1.53	8 (14%)	64,95,113	2.12	20 (31%)
21	BCR	3	305	-	41,41,41	1.59	4 (9%)	56,56,56	4.51	14 (25%)
26	DGD	1	5002	-	35,35,67	0.98	2 (5%)	43,43,81	1.11	3 (6%)
18	CLA	K	1404	-	50,54,73	1.60	8 (16%)	59,90,113	2.03	13 (22%)
30	CHL	2	315	-	50,64,74	1.31	8 (16%)	46,102,114	1.85	12 (26%)
22	LHG	B	848	18	20,20,48	0.59	0	23,26,54	1.56	2 (8%)
18	CLA	A	817	-	69,73,73	1.36	7 (10%)	82,113,113	1.82	18 (21%)
18	CLA	A	834	-	55,59,73	1.52	7 (12%)	64,96,113	2.06	17 (26%)
18	CLA	B	840	-	69,73,73	1.35	6 (8%)	82,113,113	1.88	19 (23%)
18	CLA	A	821	-	64,68,73	1.41	7 (10%)	76,107,113	1.93	17 (22%)
21	BCR	B	845	-	41,41,41	1.59	4 (9%)	56,56,56	4.23	19 (33%)
21	BCR	J	1104	-	41,41,41	1.60	4 (9%)	56,56,56	4.45	14 (25%)
23	LMT	A	850	-	36,36,36	1.09	3 (8%)	47,47,47	1.17	1 (2%)
29	LUT	J	1105	-	42,43,43	2.45	1 (2%)	51,60,60	2.17	11 (21%)
18	CLA	A	838	-	69,73,73	1.37	8 (11%)	82,113,113	1.83	15 (18%)
18	CLA	A	830	-	69,73,73	1.35	7 (10%)	82,113,113	1.83	17 (20%)
26	DGD	B	855	-	62,62,67	1.21	6 (9%)	76,76,81	0.99	3 (3%)
30	CHL	4	302	13	50,64,74	1.34	8 (16%)	46,102,114	1.94	12 (26%)
30	CHL	3	316	-	41,55,74	1.58	9 (21%)	35,91,114	2.09	9 (25%)
18	CLA	B	814	-	69,73,73	1.36	6 (8%)	82,113,113	1.92	18 (21%)
18	CLA	B	832	-	64,68,73	1.41	6 (9%)	76,107,113	1.90	18 (23%)
18	CLA	B	818	-	69,73,73	1.35	6 (8%)	82,113,113	1.83	18 (21%)
18	CLA	2	309	14	69,73,73	1.36	7 (10%)	82,113,113	1.90	17 (20%)
18	CLA	A	818	-	54,58,73	1.54	7 (12%)	64,95,113	2.06	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	F	303	6	69,73,73	1.36	7 (10%)	82,113,113	1.84	19 (23%)
18	CLA	A	808	1	69,73,73	1.37	7 (10%)	82,113,113	1.85	18 (21%)
18	CLA	3	319	-	64,68,73	1.40	7 (10%)	76,107,113	1.92	17 (22%)
30	CHL	3	310	-	60,74,74	1.26	7 (11%)	58,114,114	1.80	11 (18%)
24	LMG	2	302	-	13,13,55	0.57	0	18,18,63	0.62	0
21	BCR	A	845	-	41,41,41	1.63	4 (9%)	56,56,56	4.49	18 (32%)
18	CLA	B	806	-	69,73,73	1.33	7 (10%)	82,113,113	1.91	18 (21%)
18	CLA	A	822	-	69,73,73	1.36	7 (10%)	82,113,113	1.83	18 (21%)
23	LMT	G	1606	-	32,32,36	1.18	4 (12%)	43,43,47	1.01	1 (2%)
23	LMT	B	853	-	33,33,36	1.19	5 (15%)	44,44,47	1.13	2 (4%)
18	CLA	F	301	-	69,73,73	1.36	7 (10%)	82,113,113	1.84	20 (24%)
31	XAT	4	304	-	41,47,47	0.69	1 (2%)	54,74,74	1.93	12 (22%)
18	CLA	3	311	-	59,63,73	1.48	8 (13%)	70,101,113	1.96	19 (27%)
18	CLA	A	833	1	59,63,73	1.47	8 (13%)	70,101,113	1.98	17 (24%)
21	BCR	G	1604	-	41,41,41	1.60	4 (9%)	56,56,56	4.52	14 (25%)
18	CLA	B	808	-	69,73,73	1.36	7 (10%)	82,113,113	1.82	17 (20%)
29	LUT	1	5004	-	42,43,43	2.48	1 (2%)	51,60,60	1.97	12 (23%)
18	CLA	A	811	-	59,63,73	1.46	6 (10%)	70,101,113	1.99	19 (27%)
23	LMT	B	856	-	32,32,36	1.19	5 (15%)	43,43,47	1.04	3 (6%)
21	BCR	A	844	-	41,41,41	1.59	4 (9%)	56,56,56	4.46	16 (28%)
18	CLA	2	310	-	69,73,73	1.34	7 (10%)	82,113,113	2.04	20 (24%)
18	CLA	A	820	-	64,68,73	1.41	7 (10%)	76,107,113	1.91	16 (21%)
26	DGD	J	1106	-	59,59,67	1.16	6 (10%)	73,73,81	1.21	5 (6%)
29	LUT	1	5003	-	42,43,43	2.50	1 (2%)	51,60,60	1.87	13 (25%)
21	BCR	I	102	-	41,41,41	1.59	4 (9%)	56,56,56	4.42	14 (25%)
21	BCR	2	305	-	41,41,41	1.63	4 (9%)	56,56,56	5.13	27 (48%)
18	CLA	K	1402	-	64,68,73	1.42	8 (12%)	76,107,113	1.90	17 (22%)
18	CLA	B	824	-	59,63,73	1.47	7 (11%)	70,101,113	1.92	17 (24%)
29	LUT	3	304	-	42,43,43	2.45	1 (2%)	51,60,60	1.92	10 (19%)
22	LHG	A	849	18	39,39,48	0.42	0	42,45,54	1.26	5 (11%)
23	LMT	G	1605	-	36,36,36	1.12	4 (11%)	47,47,47	1.01	1 (2%)
18	CLA	A	826	-	69,73,73	1.35	6 (8%)	82,113,113	1.86	17 (20%)
18	CLA	A	819	-	69,73,73	1.35	7 (10%)	82,113,113	1.74	16 (19%)
24	LMG	J	1102	-	30,30,55	0.55	0	38,38,63	1.11	3 (7%)
18	CLA	A	832	-	69,73,73	1.35	7 (10%)	82,113,113	1.81	21 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LMG	B	851	-	33,33,55	0.58	1 (3%)	41,41,63	1.45	7 (17%)
18	CLA	B	823	-	69,73,73	1.35	7 (10%)	82,113,113	1.85	18 (21%)

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
18	CLA	2	312	22	1/1/14/20	17/33/109/115	-
18	CLA	2	326	16	1/1/12/20	9/21/97/115	-
18	CLA	3	309	-	1/1/13/20	11/27/103/115	-
23	LMT	J	1107	-	-	5/11/51/61	0/2/2/2
18	CLA	B	829	-	1/1/15/20	18/39/115/115	-
18	CLA	A	806	-	1/1/14/20	16/33/109/115	-
18	CLA	A	839	-	1/1/15/20	5/39/115/115	-
24	LMG	1	5020	-	-	10/41/61/70	0/1/1/1
24	LMG	2	324	-	-	4/4/24/70	0/1/1/1
22	LHG	A	848	-	-	31/53/53/53	-
18	CLA	A	840	22	1/1/14/20	10/33/109/115	-
18	CLA	B	817	-	1/1/14/20	9/33/109/115	-
18	CLA	A	814	-	1/1/11/20	8/17/93/115	-
30	CHL	2	316	-	3/3/16/26	2/18/116/137	-
19	PQN	B	842	-	-	8/23/43/43	0/2/2/2
18	CLA	J	1101	-	1/1/15/20	14/39/115/115	-
18	CLA	K	1401	-	1/1/11/20	5/15/91/115	-
18	CLA	1	5012	-	1/1/11/20	5/17/93/115	-
21	BCR	B	846	-	-	8/29/63/63	0/2/2/2
18	CLA	2	317	-	1/1/13/20	8/27/103/115	-
21	BCR	A	846	-	-	14/29/63/63	0/2/2/2
18	CLA	4	315	-	1/1/15/20	19/39/115/115	-
18	CLA	G	1603	-	1/1/15/20	18/39/115/115	-
18	CLA	A	812	-	1/1/15/20	17/39/115/115	-
18	CLA	B	809	-	1/1/15/20	8/39/115/115	-
18	CLA	1	5011	-	1/1/12/20	5/21/97/115	-
18	CLA	B	805	-	1/1/15/20	20/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	4	307	-	1/1/15/20	15/39/115/115	-
21	BCR	I	101	-	-	15/29/63/63	0/2/2/2
18	CLA	A	810	-	1/1/15/20	19/39/115/115	-
24	LMG	2	301	-	-	3/4/24/70	0/1/1/1
20	SF4	C	101	3	-	-	0/6/5/5
23	LMT	2	325	-	-	9/21/61/61	0/2/2/2
18	CLA	1	5007	13	1/1/11/20	7/17/93/115	-
30	CHL	3	312	-	3/3/17/26	2/21/119/137	-
21	BCR	B	802	-	-	7/29/63/63	0/2/2/2
21	BCR	A	843	-	-	14/29/63/63	0/2/2/2
18	CLA	B	807	2	1/1/15/20	13/39/115/115	-
18	CLA	1	5018	13	1/1/14/20	18/33/109/115	-
18	CLA	4	311	-	1/1/14/20	12/33/109/115	-
21	BCR	3	306	-	-	14/29/63/63	0/2/2/2
18	CLA	1	5008	-	1/1/13/20	7/27/103/115	-
24	LMG	F	306	-	-	7/42/62/70	0/1/1/1
18	CLA	A	853	-	1/1/15/20	17/39/115/115	-
24	LMG	B	850	-	-	9/30/50/70	0/1/1/1
18	CLA	1	5010	-	1/1/15/20	12/39/115/115	-
21	BCR	L	302	-	-	12/29/63/63	0/2/2/2
18	CLA	B	835	-	1/1/13/20	9/27/103/115	-
18	CLA	A	804	-	1/1/15/20	23/39/115/115	-
22	LHG	1	5019	-	-	22/53/53/53	-
21	BCR	L	307	-	-	14/29/63/63	0/2/2/2
24	LMG	A	851	-	-	18/45/65/70	0/1/1/1
18	CLA	B	801	-	1/1/15/20	15/39/115/115	-
24	LMG	F	308	-	-	12/29/49/70	0/1/1/1
25	GOL	4	321	-	-	0/4/4/4	-
17	CL0	A	801	-	3/3/20/25	7/37/135/135	-
18	CLA	A	852	-	1/1/15/20	16/39/115/115	-
18	CLA	B	838	-	1/1/12/20	5/21/97/115	-
29	LUT	3	303	-	-	3/29/67/67	0/2/2/2
18	CLA	L	305	-	1/1/14/20	17/33/109/115	-
18	CLA	4	312	-	1/1/11/20	7/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	2	307	14	1/1/12/20	8/24/100/115	-
18	CLA	A	828	-	1/1/15/20	15/39/115/115	-
21	BCR	B	847	-	-	14/29/63/63	0/2/2/2
30	CHL	2	319	-	4/4/18/26	7/27/125/137	-
24	LMG	B	851	-	-	10/28/48/70	0/1/1/1
24	LMG	B	854	-	-	1/4/24/70	0/1/1/1
26	DGD	F	309	-	-	17/46/86/95	0/2/2/2
18	CLA	B	834	-	1/1/14/20	12/33/109/115	-
29	LUT	4	303	-	-	4/29/67/67	0/2/2/2
24	LMG	F	307	-	-	9/31/51/70	0/1/1/1
18	CLA	B	841	22	1/1/15/20	15/39/115/115	-
18	CLA	A	813	-	1/1/15/20	15/39/115/115	-
18	CLA	B	804	-	1/1/15/20	14/39/115/115	-
28	ZEX	F	310	-	-	3/29/67/67	0/2/2/2
21	BCR	B	844	-	-	10/29/63/63	0/2/2/2
18	CLA	1	5015	-	1/1/15/20	18/39/115/115	-
18	CLA	1	5009	-	1/1/15/20	15/39/115/115	-
18	CLA	2	308	-	1/1/15/20	17/39/115/115	-
18	CLA	A	816	-	1/1/13/20	16/29/105/115	-
18	CLA	B	831	-	1/1/15/20	15/39/115/115	-
18	CLA	A	837	-	1/1/15/20	7/39/115/115	-
18	CLA	H	1701	-	1/1/14/20	11/33/109/115	-
18	CLA	F	302	-	1/1/15/20	19/39/115/115	-
18	CLA	B	839	-	1/1/15/20	18/39/115/115	-
18	CLA	B	819	-	1/1/15/20	18/39/115/115	-
18	CLA	2	313	-	1/1/12/20	12/21/97/115	-
24	LMG	2	322	-	-	17/31/51/70	0/1/1/1
18	CLA	B	830	-	1/1/15/20	14/39/115/115	-
18	CLA	G	1601	-	1/1/13/20	9/27/103/115	-
20	SF4	C	102	3	-	-	0/6/5/5
21	BCR	F	304	-	-	8/29/63/63	0/2/2/2
18	CLA	1	5017	-	1/1/11/20	6/15/91/115	-
21	BCR	A	855	-	-	9/29/63/63	0/2/2/2
18	CLA	3	308	-	1/1/12/20	9/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	4	309	-	1/1/14/20	14/33/109/115	-
22	LHG	2	320	18	-	17/39/39/53	-
18	CLA	A	805	-	1/1/15/20	17/39/115/115	-
18	CLA	B	816	-	1/1/13/20	5/27/103/115	-
18	CLA	B	820	-	1/1/15/20	13/39/115/115	-
18	CLA	A	823	-	1/1/15/20	18/39/115/115	-
30	CHL	2	318	-	3/3/16/26	4/15/113/137	-
26	DGD	2	327	-	-	15/40/80/95	0/2/2/2
21	BCR	K	1405	-	-	13/29/63/63	0/2/2/2
30	CHL	2	314	14	4/4/20/26	9/39/137/137	-
24	LMG	G	1607	-	-	8/20/40/70	0/1/1/1
18	CLA	A	807	1	1/1/15/20	15/39/115/115	-
21	BCR	1	5005	-	-	9/29/63/63	0/2/2/2
25	GOL	A	854	-	-	1/4/4/4	-
30	CHL	4	316	-	4/4/19/26	7/33/131/137	-
18	CLA	B	822	-	1/1/15/20	14/39/115/115	-
24	LMG	1	5001	-	-	15/44/64/70	0/1/1/1
18	CLA	3	315	15	1/1/15/20	23/39/115/115	-
18	CLA	2	311	-	1/1/12/20	9/21/97/115	-
18	CLA	3	307	-	1/1/13/20	9/27/103/115	-
18	CLA	A	824	-	1/1/13/20	15/27/103/115	-
30	CHL	3	313	-	3/3/17/26	3/21/119/137	-
18	CLA	B	811	-	1/1/15/20	16/39/115/115	-
18	CLA	A	831	-	1/1/15/20	23/39/115/115	-
31	XAT	2	304	-	1/1/12/26	4/31/93/93	0/4/4/4
24	LMG	2	323	-	-	0/4/24/70	0/1/1/1
18	CLA	B	810	2	1/1/15/20	14/39/115/115	-
18	CLA	K	1403	-	1/1/11/20	10/19/95/115	-
30	CHL	4	318	-	4/4/18/26	6/27/125/137	-
18	CLA	4	308	-	1/1/14/20	19/33/109/115	-
20	SF4	A	842	2,1	-	-	0/6/5/5
18	CLA	A	836	-	1/1/15/20	15/39/115/115	-
18	CLA	B	803	-	1/1/15/20	11/39/115/115	-
18	CLA	B	837	-	1/1/15/20	20/39/115/115	-
18	CLA	A	803	-	1/1/15/20	21/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	2	306	-	1/1/14/20	9/33/109/115	-
18	CLA	1	5013	-	1/1/11/20	8/17/93/115	-
22	LHG	B	849	-	-	34/53/53/53	-
30	CHL	1	5014	-	3/3/16/26	3/17/115/137	-
18	CLA	B	821	-	1/1/11/20	7/17/93/115	-
23	LMT	B	852	-	-	13/21/61/61	0/2/2/2
18	CLA	A	829	-	1/1/15/20	15/39/115/115	-
18	CLA	3	318	-	1/1/11/20	6/17/93/115	-
18	CLA	3	314	-	1/1/11/20	7/19/95/115	-
18	CLA	B	828	-	1/1/15/20	22/39/115/115	-
18	CLA	A	815	-	1/1/15/20	11/39/115/115	-
18	CLA	4	305	-	1/1/14/20	9/33/109/115	-
18	CLA	B	827	-	1/1/15/20	9/39/115/115	-
30	CHL	4	313	-	3/3/16/26	1/17/115/137	-
19	PQN	A	841	-	-	6/23/43/43	0/2/2/2
18	CLA	4	310	-	1/1/12/20	8/21/97/115	-
18	CLA	3	317	-	1/1/12/20	7/21/97/115	-
21	BCR	4	301	-	-	13/29/63/63	0/2/2/2
30	CHL	1	5016	-	4/4/19/26	7/33/131/137	-
18	CLA	B	815	-	1/1/15/20	16/39/115/115	-
18	CLA	B	833	-	1/1/13/20	14/31/107/115	-
18	CLA	J	1103	-	1/1/12/20	7/21/97/115	-
21	BCR	F	305	-	-	14/29/63/63	0/2/2/2
24	LMG	2	321	-	-	5/20/40/70	0/1/1/1
24	LMG	4	320	-	-	0/4/24/70	0/1/1/1
18	CLA	A	802	-	1/1/15/20	20/39/115/115	-
18	CLA	A	827	-	1/1/15/20	15/39/115/115	-
18	CLA	A	809	-	1/1/12/20	8/21/97/115	-
21	BCR	A	847	-	-	13/29/63/63	0/2/2/2
29	LUT	2	303	-	1/1/12/27	3/29/67/67	0/2/2/2
30	CHL	4	314	-	3/3/17/26	2/21/119/137	-
18	CLA	3	301	-	1/1/11/20	4/15/91/115	-
18	CLA	L	306	-	1/1/12/20	8/21/97/115	-
18	CLA	B	812	-	1/1/14/20	9/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	L	304	12	1/1/12/20	7/21/97/115	-
18	CLA	B	826	-	1/1/15/20	18/39/115/115	-
18	CLA	L	301	-	1/1/13/20	10/27/103/115	-
18	CLA	B	836	-	1/1/13/20	9/27/103/115	-
18	CLA	1	5006	13	1/1/15/20	15/39/115/115	-
21	BCR	B	843	-	-	10/29/63/63	0/2/2/2
18	CLA	B	825	-	1/1/15/20	13/39/115/115	-
18	CLA	B	813	-	1/1/11/20	4/17/93/115	-
21	BCR	L	303	-	-	12/29/63/63	0/2/2/2
18	CLA	A	825	-	1/1/15/20	16/39/115/115	-
23	LMT	4	319	-	-	4/21/61/61	0/2/2/2
18	CLA	A	835	-	1/1/15/20	11/39/115/115	-
18	CLA	G	1602	7	1/1/11/20	6/17/93/115	-
18	CLA	4	306	-	1/1/12/20	9/21/97/115	-
21	BCR	3	305	-	-	12/29/63/63	0/2/2/2
26	DGD	1	5002	-	-	11/29/49/95	0/1/1/2
18	CLA	K	1404	-	1/1/11/20	8/17/93/115	-
30	CHL	2	315	-	4/4/18/26	7/27/125/137	-
22	LHG	B	848	18	-	9/23/23/53	-
18	CLA	A	817	-	1/1/15/20	16/39/115/115	-
18	CLA	A	834	-	1/1/12/20	9/23/99/115	-
18	CLA	B	840	-	1/1/15/20	18/39/115/115	-
18	CLA	A	821	-	1/1/14/20	9/33/109/115	-
29	LUT	J	1105	-	1/1/12/27	4/29/67/67	0/2/2/2
21	BCR	B	845	-	-	14/29/63/63	0/2/2/2
21	BCR	J	1104	-	-	15/29/63/63	0/2/2/2
23	LMT	A	850	-	-	11/21/61/61	0/2/2/2
18	CLA	A	838	-	1/1/15/20	15/39/115/115	-
18	CLA	A	830	-	1/1/15/20	12/39/115/115	-
30	CHL	4	302	13	4/4/18/26	4/27/125/137	-
26	DGD	B	855	-	-	19/50/90/95	0/2/2/2
30	CHL	3	316	-	3/3/16/26	4/17/115/137	-
18	CLA	B	814	-	1/1/15/20	13/39/115/115	-
18	CLA	B	832	-	1/1/14/20	18/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	818	-	1/1/15/20	15/39/115/115	-
18	CLA	2	309	14	1/1/15/20	19/39/115/115	-
18	CLA	A	818	-	1/1/12/20	7/21/97/115	-
18	CLA	F	303	6	1/1/15/20	18/39/115/115	-
18	CLA	A	808	1	1/1/15/20	19/39/115/115	-
18	CLA	3	319	-	1/1/14/20	20/33/109/115	-
30	CHL	3	310	-	4/4/20/26	12/39/137/137	-
24	LMG	2	302	-	-	0/4/24/70	0/1/1/1
21	BCR	A	845	-	-	11/29/63/63	0/2/2/2
18	CLA	B	806	-	1/1/15/20	16/39/115/115	-
18	CLA	A	822	-	1/1/15/20	15/39/115/115	-
23	LMT	G	1606	-	-	13/17/57/61	0/2/2/2
23	LMT	B	853	-	-	9/18/58/61	0/2/2/2
18	CLA	F	301	-	1/1/15/20	18/39/115/115	-
31	XAT	4	304	-	1/1/12/26	0/31/93/93	0/4/4/4
18	CLA	3	311	-	1/1/13/20	7/27/103/115	-
18	CLA	A	833	1	1/1/13/20	9/27/103/115	-
29	LUT	1	5004	-	1/1/12/27	4/29/67/67	0/2/2/2
18	CLA	B	808	-	1/1/15/20	13/39/115/115	-
21	BCR	G	1604	-	-	8/29/63/63	0/2/2/2
18	CLA	A	811	-	1/1/13/20	7/27/103/115	-
23	LMT	B	856	-	-	3/17/57/61	0/2/2/2
21	BCR	A	844	-	-	10/29/63/63	0/2/2/2
18	CLA	2	310	-	1/1/15/20	12/39/115/115	-
18	CLA	A	820	-	1/1/14/20	14/33/109/115	-
26	DGD	J	1106	-	-	14/47/87/95	0/2/2/2
29	LUT	1	5003	-	-	5/29/67/67	0/2/2/2
21	BCR	I	102	-	-	16/29/63/63	0/2/2/2
21	BCR	2	305	-	-	10/29/63/63	0/2/2/2
18	CLA	K	1402	-	1/1/14/20	18/33/109/115	-
18	CLA	B	824	-	1/1/13/20	13/27/103/115	-
29	LUT	3	304	-	1/1/12/27	7/29/67/67	0/2/2/2
22	LHG	A	849	18	-	22/44/44/53	-
23	LMT	G	1605	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	826	-	1/1/15/20	21/39/115/115	-
18	CLA	A	819	-	1/1/15/20	18/39/115/115	-
24	LMG	J	1102	-	-	6/25/45/70	0/1/1/1
18	CLA	A	832	-	1/1/15/20	19/39/115/115	-
30	CHL	4	317	-	3/3/15/26	0/12/110/137	-
18	CLA	B	823	-	1/1/15/20	14/39/115/115	-

The worst 5 of 1323 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	5003	LUT	C24-C25	15.43	1.51	1.33
29	4	303	LUT	C24-C25	15.33	1.51	1.33
29	3	303	LUT	C24-C25	15.29	1.51	1.33
29	1	5004	LUT	C24-C25	15.27	1.51	1.33
29	J	1105	LUT	C24-C25	15.12	1.51	1.33

The worst 5 of 3306 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	I	101	BCR	C10-C11-C12	19.60	180.00	123.20
21	G	1604	BCR	C10-C11-C12	19.21	178.87	123.20
21	K	1405	BCR	C10-C11-C12	19.06	178.43	123.20
21	F	304	BCR	C10-C11-C12	18.93	178.06	123.20
21	A	855	BCR	C10-C11-C12	18.90	177.97	123.20

5 of 206 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	801	CL0	NC
17	A	801	CL0	NA
17	A	801	CL0	ND
18	A	802	CLA	ND
18	A	803	CLA	ND

5 of 2665 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	802	CLA	C2-C1-O2A-CGA
18	A	802	CLA	C4-C3-C5-C6
18	A	803	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	A	803	CLA	C3A-C2A-CAA-CBA
18	A	803	CLA	C2B-C3B-CAB-CBB

There are no ring outliers.

218 monomers are involved in 749 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	2	312	CLA	7	0
18	2	326	CLA	3	0
18	3	309	CLA	3	0
18	B	829	CLA	6	0
18	A	806	CLA	6	0
18	A	839	CLA	5	0
24	1	5020	LMG	3	0
22	A	848	LHG	8	0
18	A	840	CLA	7	0
18	A	814	CLA	1	0
19	B	842	PQN	2	0
30	2	316	CHL	4	0
18	J	1101	CLA	8	0
18	K	1401	CLA	3	0
18	1	5012	CLA	3	0
21	B	846	BCR	3	0
18	2	317	CLA	2	0
21	A	846	BCR	7	0
18	4	315	CLA	3	0
18	G	1603	CLA	3	0
18	A	812	CLA	5	0
18	B	809	CLA	4	0
18	1	5011	CLA	2	0
18	B	805	CLA	8	0
18	4	307	CLA	2	0
18	A	810	CLA	7	0
21	I	101	BCR	2	0
24	2	301	LMG	1	0
23	2	325	LMT	1	0
18	1	5007	CLA	2	0
30	3	312	CHL	6	0
21	B	802	BCR	4	0
21	A	843	BCR	6	0
18	B	807	CLA	5	0
18	1	5018	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	4	311	CLA	3	0
21	3	306	BCR	3	0
18	1	5008	CLA	1	0
24	F	306	LMG	4	0
18	A	853	CLA	7	0
24	B	850	LMG	2	0
18	1	5010	CLA	5	0
21	L	302	BCR	1	0
18	B	835	CLA	4	0
18	A	804	CLA	6	0
22	1	5019	LHG	3	0
21	L	307	BCR	3	0
24	A	851	LMG	6	0
18	B	801	CLA	10	0
17	A	801	CL0	7	0
18	A	852	CLA	6	0
18	B	838	CLA	7	0
29	3	303	LUT	3	0
18	L	305	CLA	1	0
18	2	307	CLA	3	0
18	A	828	CLA	7	0
21	B	847	BCR	2	0
30	2	319	CHL	1	0
18	B	834	CLA	5	0
29	4	303	LUT	2	0
24	F	307	LMG	1	0
18	B	841	CLA	8	0
18	A	813	CLA	6	0
18	B	804	CLA	7	0
28	F	310	ZEX	3	0
21	B	844	BCR	4	0
18	1	5015	CLA	3	0
18	1	5009	CLA	5	0
18	2	308	CLA	3	0
18	A	816	CLA	8	0
30	4	317	CHL	3	0
18	B	831	CLA	5	0
18	A	837	CLA	9	0
18	H	1701	CLA	6	0
18	F	302	CLA	4	0
18	B	839	CLA	6	0
18	B	819	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	2	313	CLA	4	0
24	2	322	LMG	2	0
18	B	830	CLA	6	0
18	G	1601	CLA	1	0
20	C	102	SF4	1	0
21	F	304	BCR	6	0
18	1	5017	CLA	2	0
21	A	855	BCR	5	0
18	4	309	CLA	1	0
22	2	320	LHG	1	0
18	A	805	CLA	5	0
18	B	816	CLA	4	0
18	B	820	CLA	4	0
18	A	823	CLA	10	0
26	2	327	DGD	5	0
30	2	318	CHL	5	0
21	K	1405	BCR	2	0
30	2	314	CHL	5	0
24	G	1607	LMG	1	0
18	A	807	CLA	5	0
21	1	5005	BCR	3	0
25	A	854	GOL	1	0
30	4	316	CHL	5	0
18	B	822	CLA	3	0
24	1	5001	LMG	6	0
18	3	315	CLA	2	0
18	2	311	CLA	2	0
18	3	307	CLA	7	0
18	A	824	CLA	4	0
30	3	313	CHL	1	0
18	B	811	CLA	7	0
18	A	831	CLA	4	0
31	2	304	XAT	7	0
18	B	810	CLA	4	0
18	K	1403	CLA	4	0
30	4	318	CHL	5	0
18	4	308	CLA	2	0
18	A	836	CLA	6	0
18	B	803	CLA	7	0
18	B	837	CLA	8	0
18	A	803	CLA	9	0
18	2	306	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	1	5013	CLA	2	0
22	B	849	LHG	4	0
30	1	5014	CHL	4	0
18	B	821	CLA	2	0
18	A	829	CLA	3	0
18	3	318	CLA	2	0
18	3	314	CLA	2	0
18	B	828	CLA	8	0
18	A	815	CLA	3	0
18	4	305	CLA	3	0
18	B	827	CLA	5	0
19	A	841	PQN	5	0
30	4	313	CHL	1	0
18	4	310	CLA	3	0
18	3	317	CLA	8	0
21	4	301	BCR	7	0
30	1	5016	CHL	6	0
18	B	815	CLA	5	0
18	B	833	CLA	5	0
21	F	305	BCR	5	0
24	2	321	LMG	2	0
18	A	802	CLA	11	0
18	A	827	CLA	2	0
18	A	809	CLA	3	0
21	A	847	BCR	6	0
29	2	303	LUT	5	0
30	4	314	CHL	1	0
18	3	301	CLA	1	0
18	L	306	CLA	1	0
18	B	812	CLA	4	0
18	L	304	CLA	3	0
18	B	826	CLA	10	0
18	L	301	CLA	2	0
18	B	836	CLA	6	0
18	1	5006	CLA	12	0
21	B	843	BCR	7	0
18	B	825	CLA	6	0
18	B	813	CLA	2	0
21	L	303	BCR	3	0
18	A	825	CLA	8	0
18	A	835	CLA	7	0
18	G	1602	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	4	306	CLA	2	0
21	3	305	BCR	3	0
18	K	1404	CLA	3	0
30	2	315	CHL	6	0
22	B	848	LHG	4	0
18	A	817	CLA	5	0
18	A	834	CLA	2	0
18	B	840	CLA	4	0
18	A	821	CLA	2	0
21	B	845	BCR	9	0
21	J	1104	BCR	5	0
29	J	1105	LUT	9	0
18	A	838	CLA	4	0
18	A	830	CLA	3	0
26	B	855	DGD	8	0
30	4	302	CHL	5	0
30	3	316	CHL	6	0
18	B	814	CLA	5	0
18	B	832	CLA	4	0
18	B	818	CLA	9	0
18	2	309	CLA	5	0
18	A	818	CLA	1	0
18	F	303	CLA	6	0
18	A	808	CLA	8	0
18	3	319	CLA	5	0
30	3	310	CHL	10	0
24	2	302	LMG	1	0
21	A	845	BCR	7	0
18	B	806	CLA	9	0
18	A	822	CLA	13	0
23	G	1606	LMT	1	0
23	B	853	LMT	1	0
18	F	301	CLA	2	0
31	4	304	XAT	6	0
18	3	311	CLA	4	0
18	A	833	CLA	3	0
21	G	1604	BCR	4	0
18	B	808	CLA	5	0
29	1	5004	LUT	6	0
18	A	811	CLA	10	0
23	B	856	LMT	2	0
21	A	844	BCR	2	0

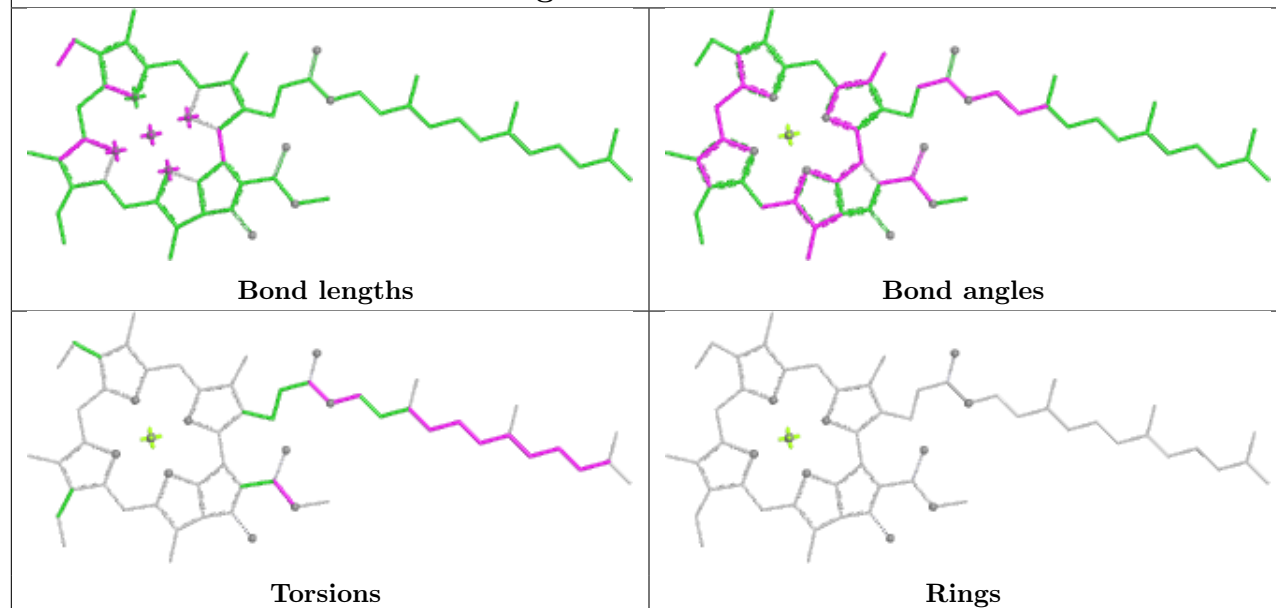
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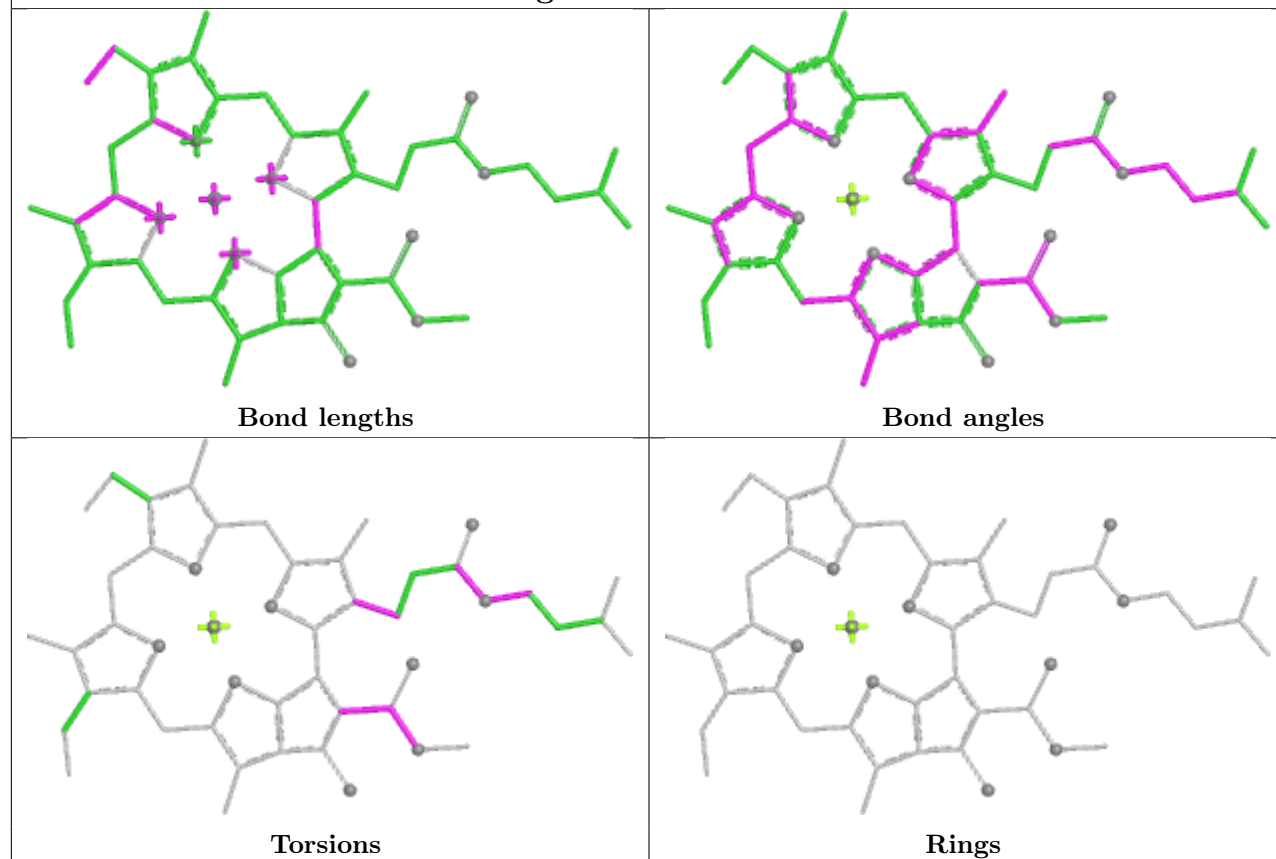
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	2	310	CLA	4	0
18	A	820	CLA	3	0
26	J	1106	DGD	4	0
29	1	5003	LUT	8	0
21	I	102	BCR	2	0
21	2	305	BCR	10	0
18	K	1402	CLA	6	0
18	B	824	CLA	8	0
29	3	304	LUT	9	0
22	A	849	LHG	8	0
23	G	1605	LMT	2	0
18	A	826	CLA	6	0
18	A	819	CLA	12	0
18	A	832	CLA	7	0
18	B	823	CLA	7	0

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

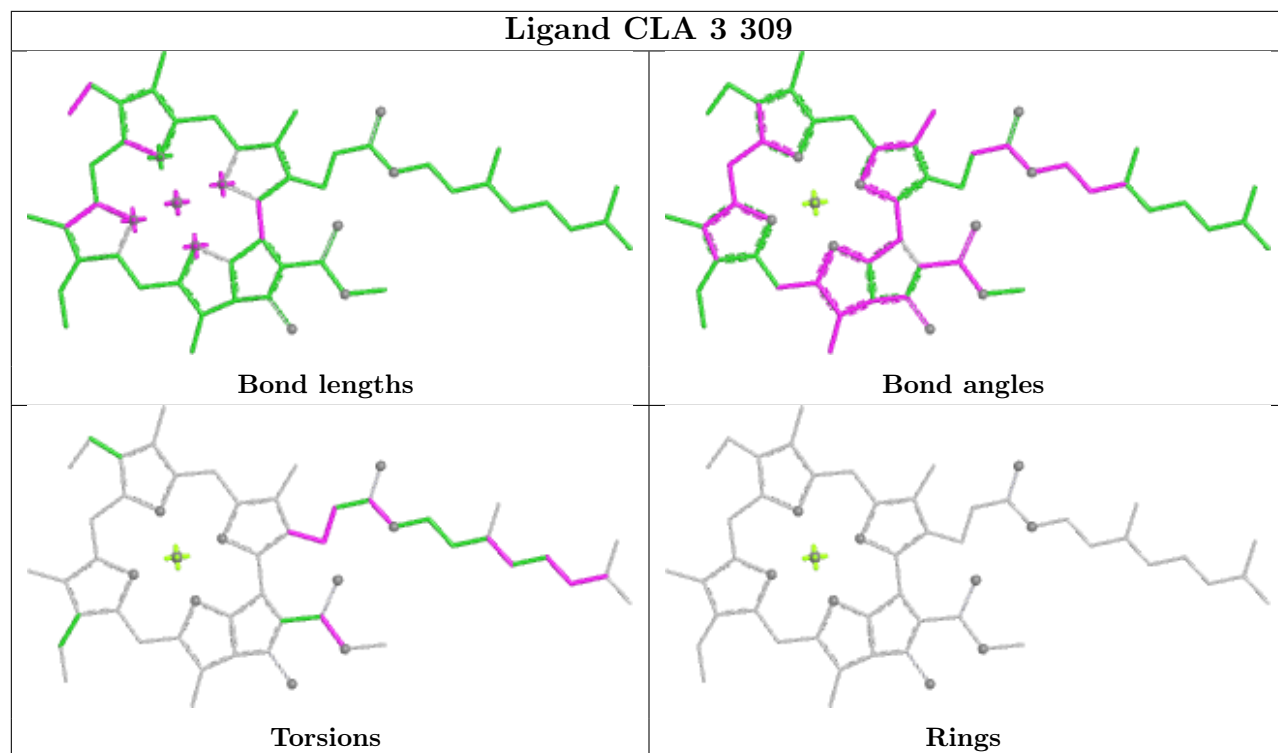
Ligand CLA 2 312



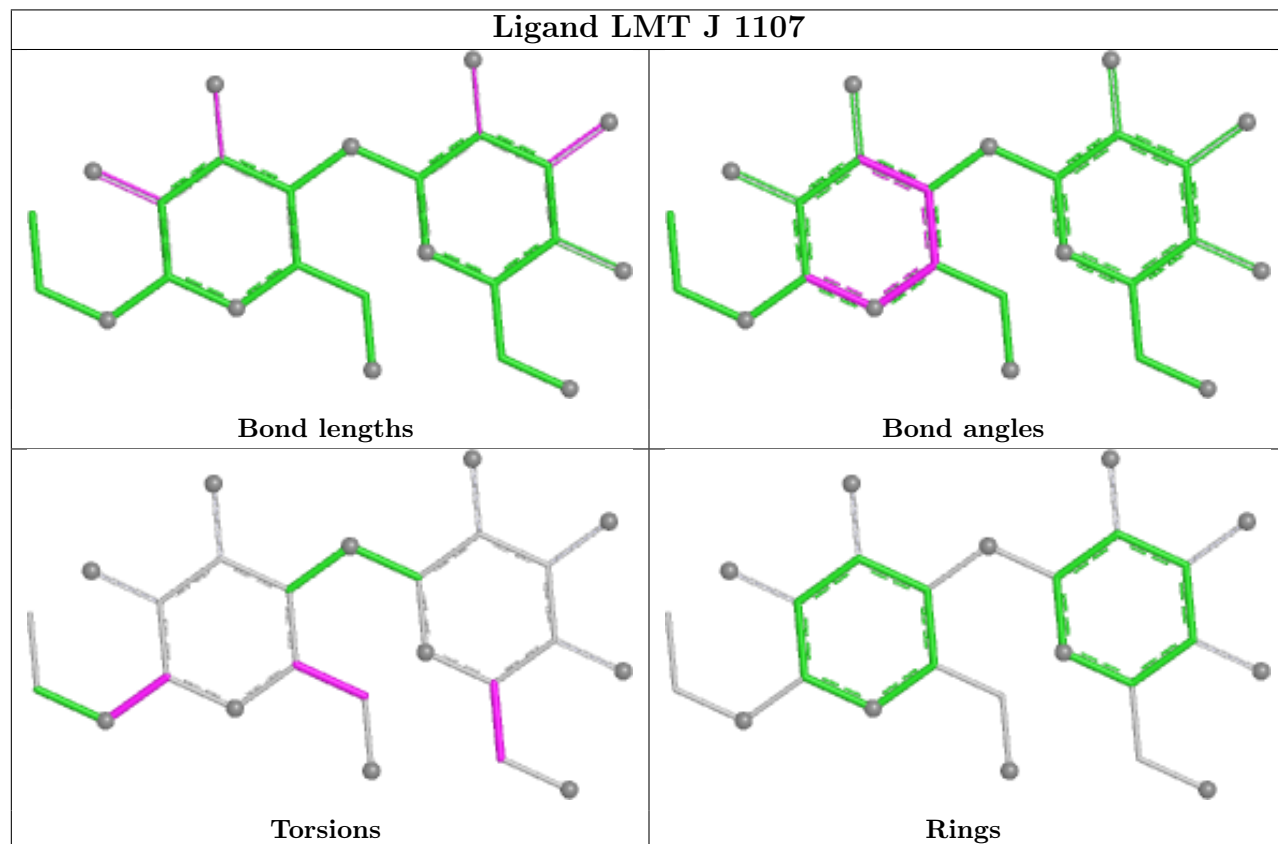
Ligand CLA 2 326



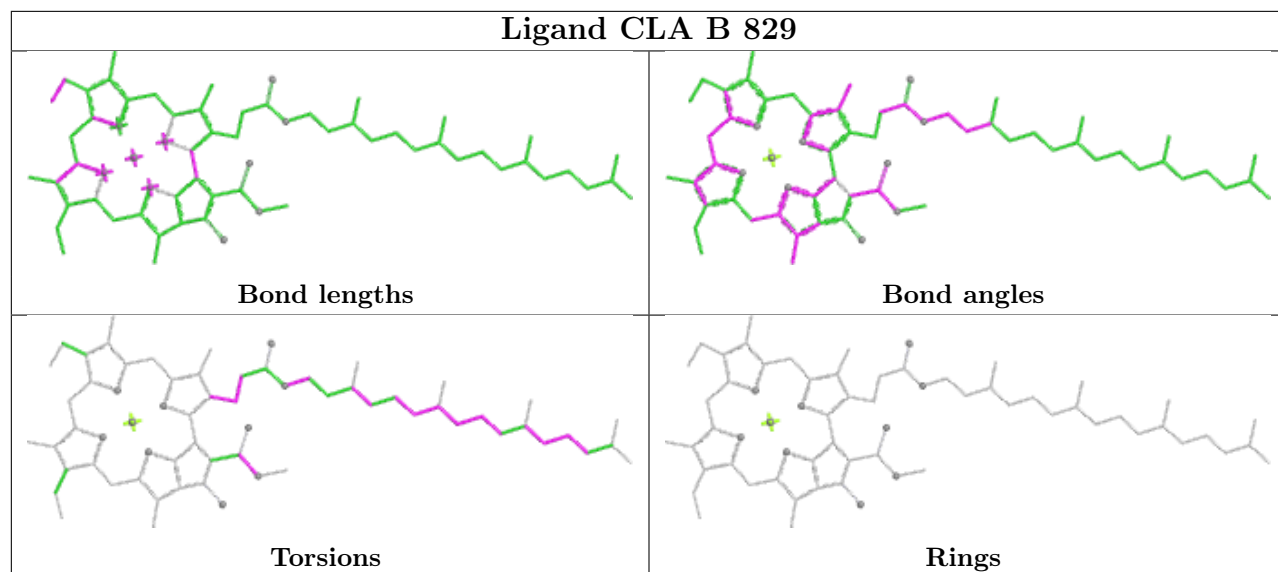
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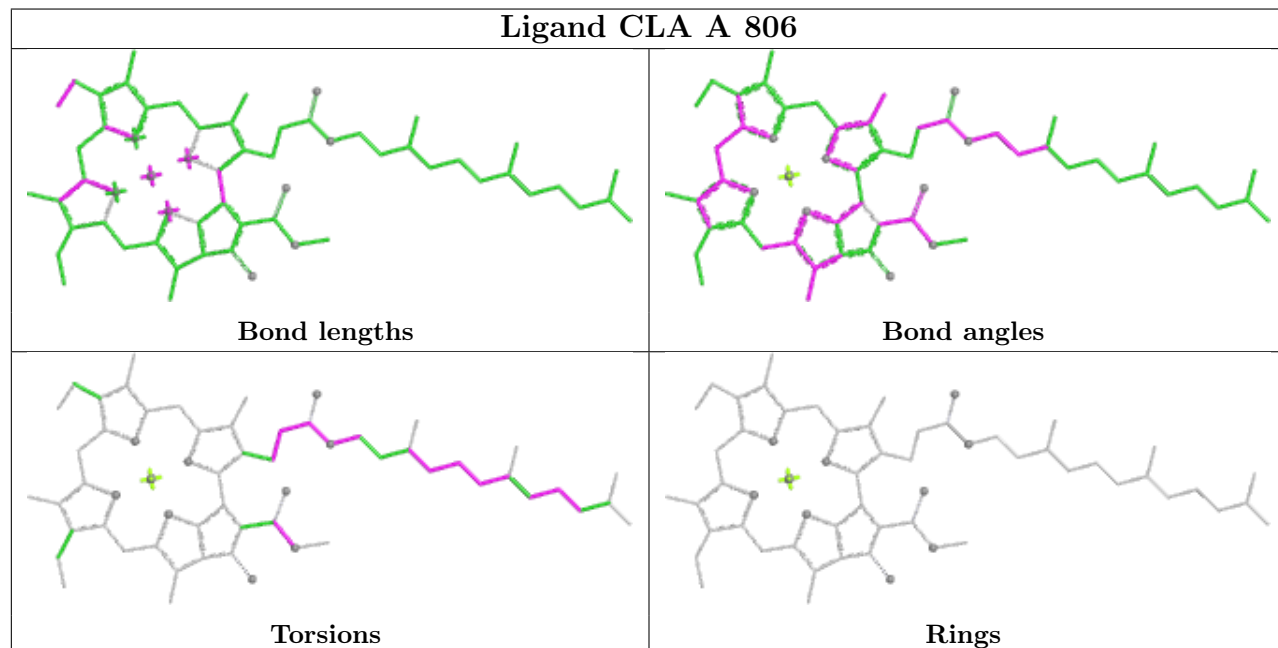
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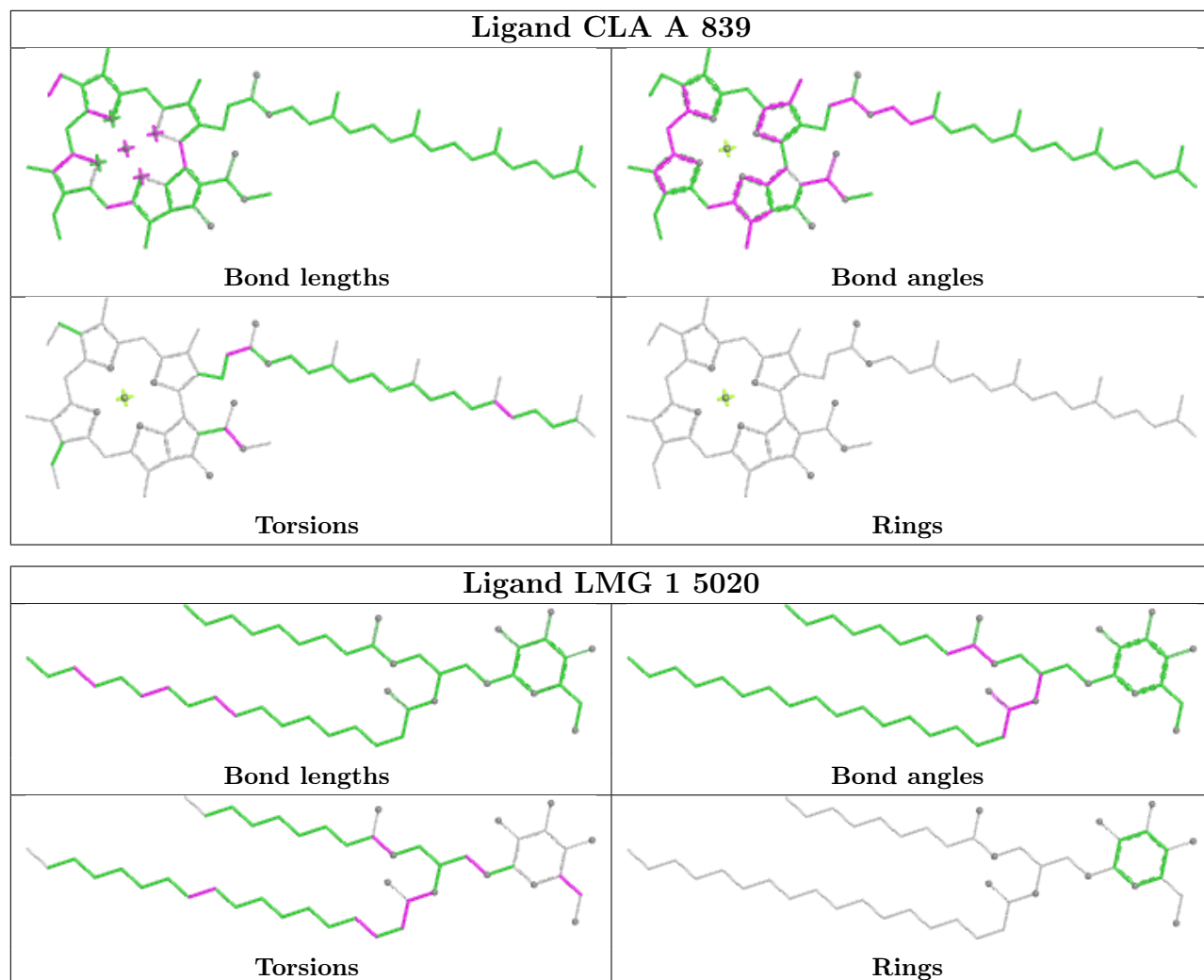


Ligand CLA B 829

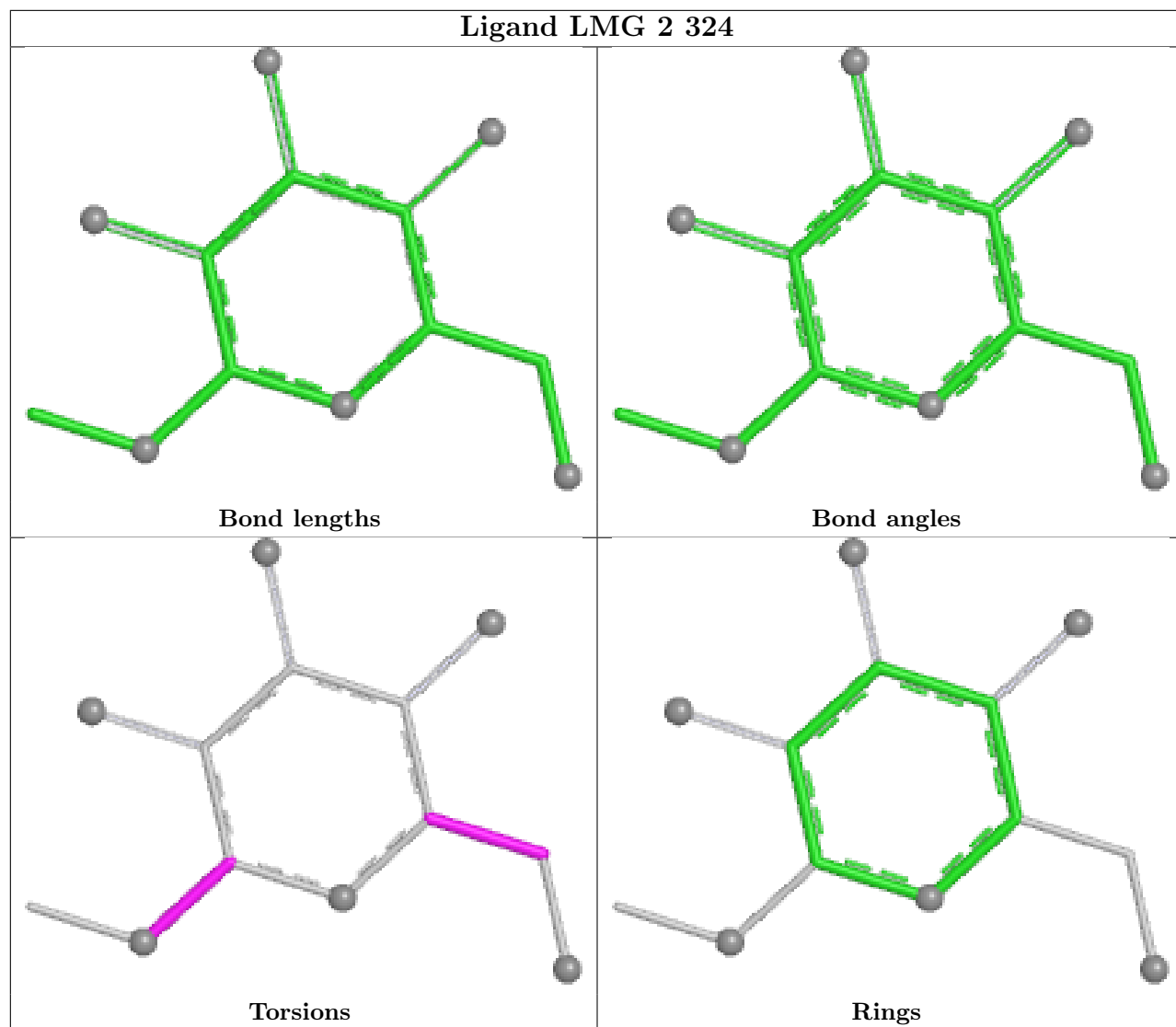


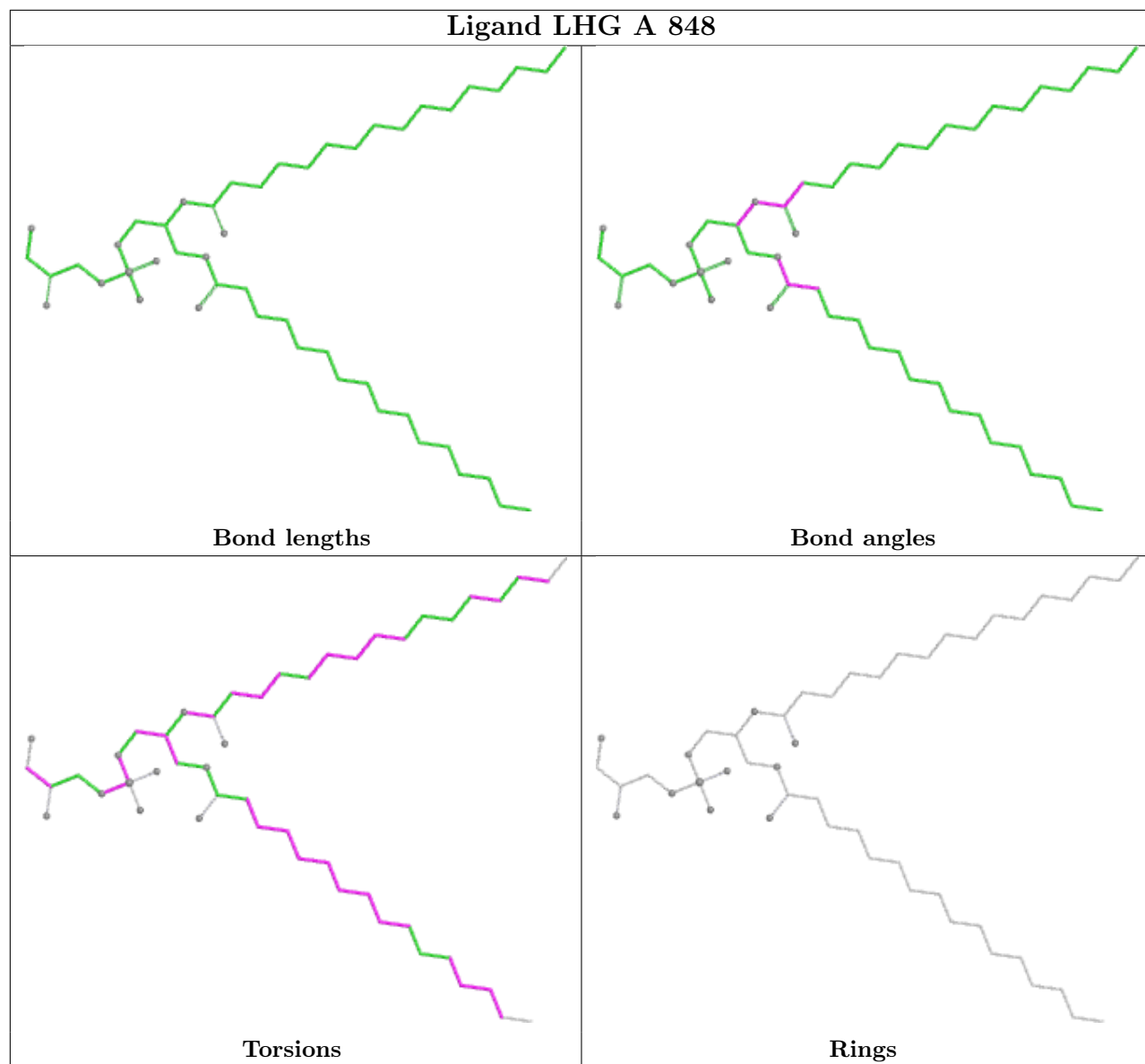
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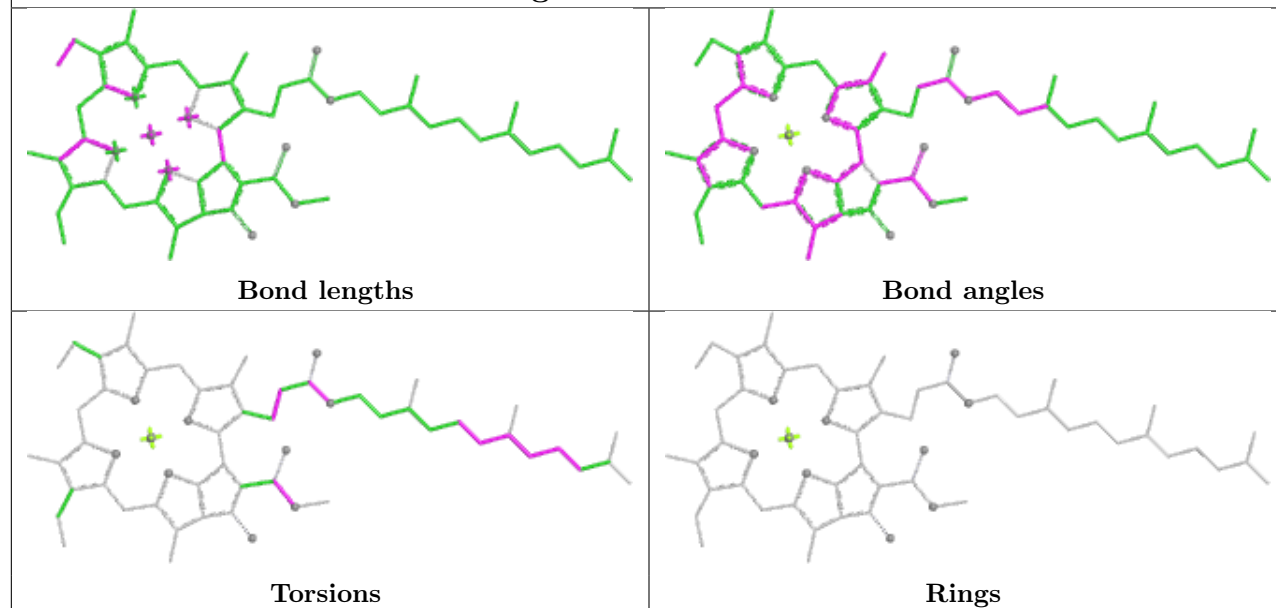


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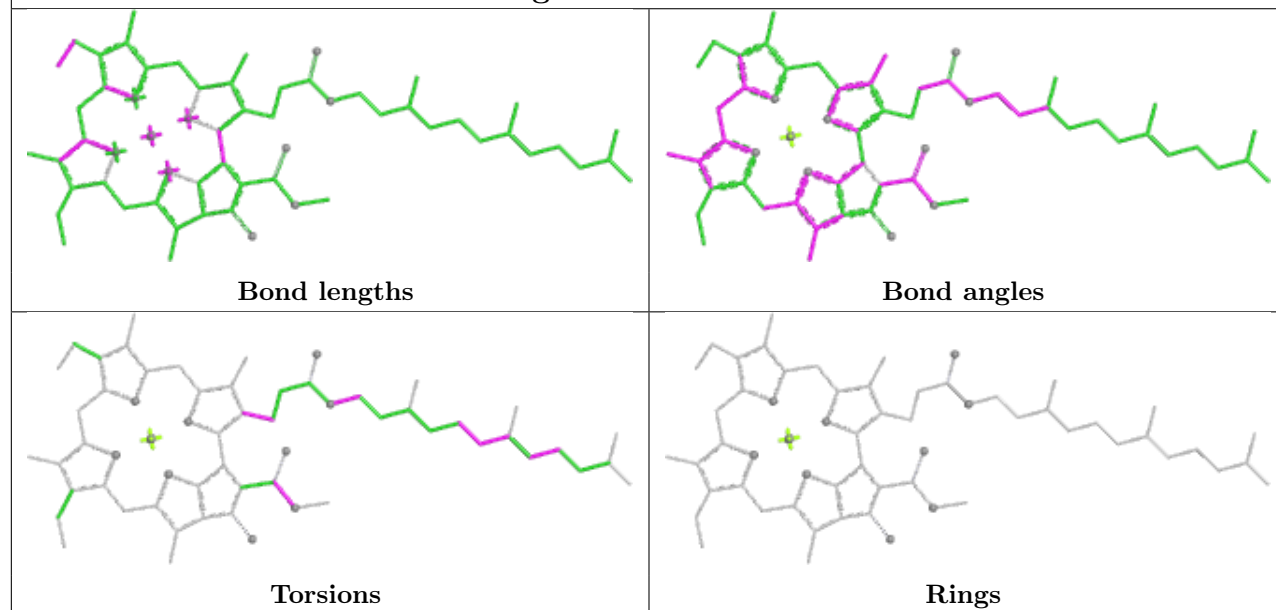




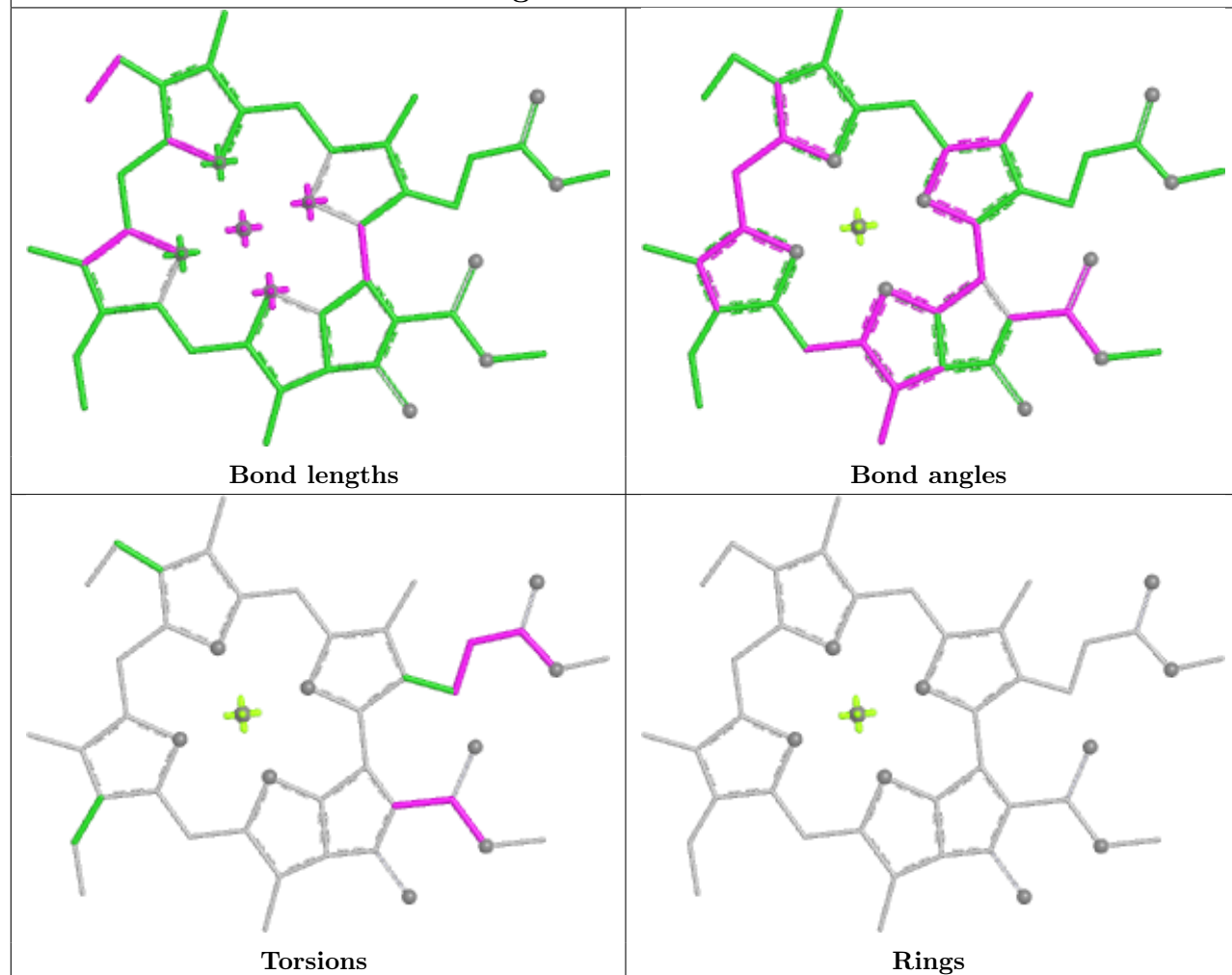
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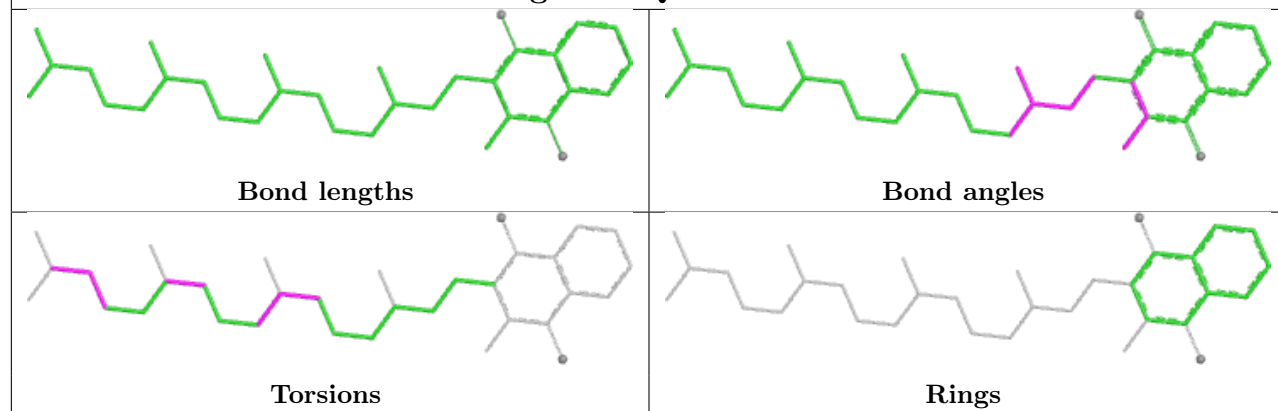
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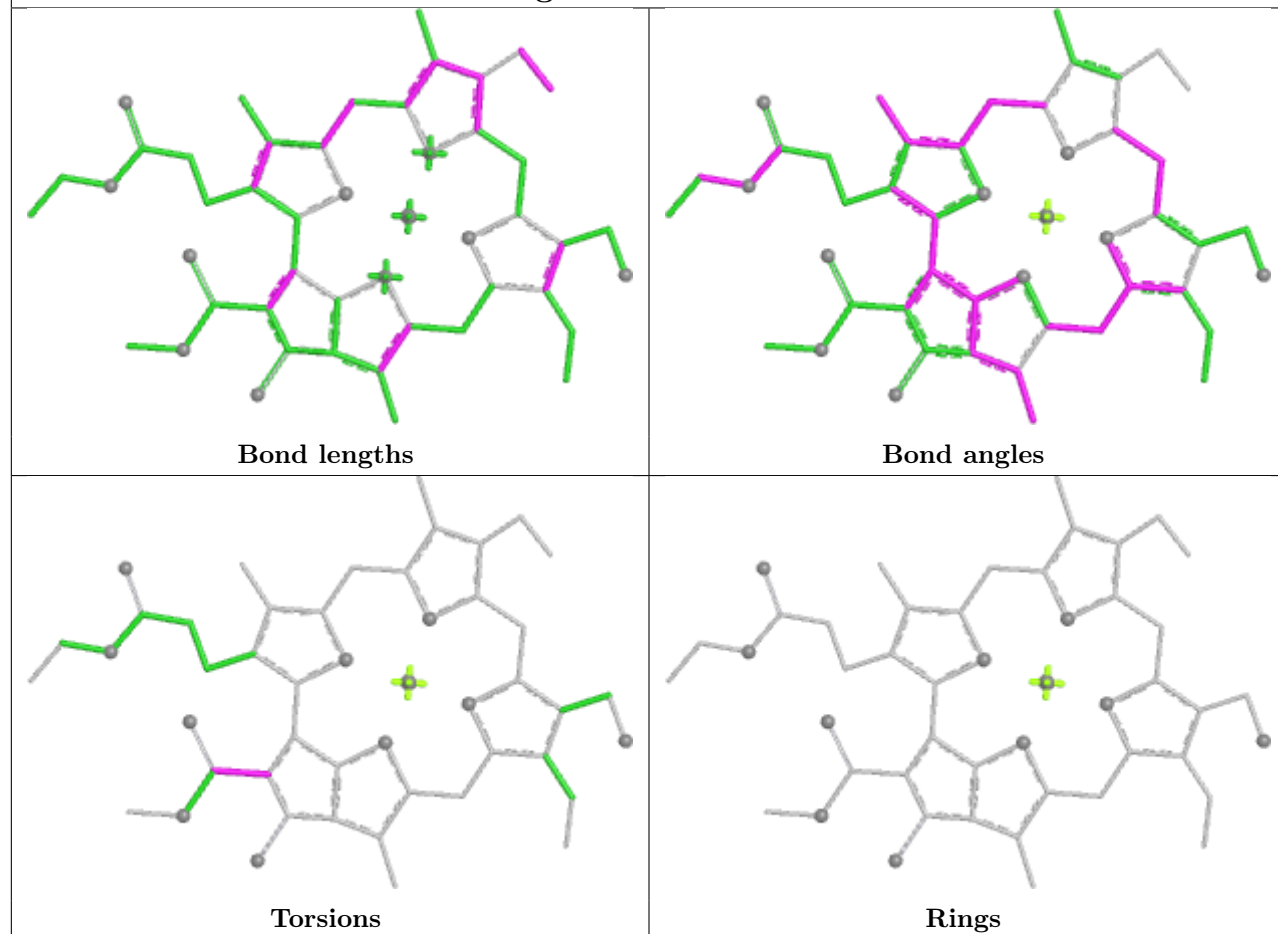
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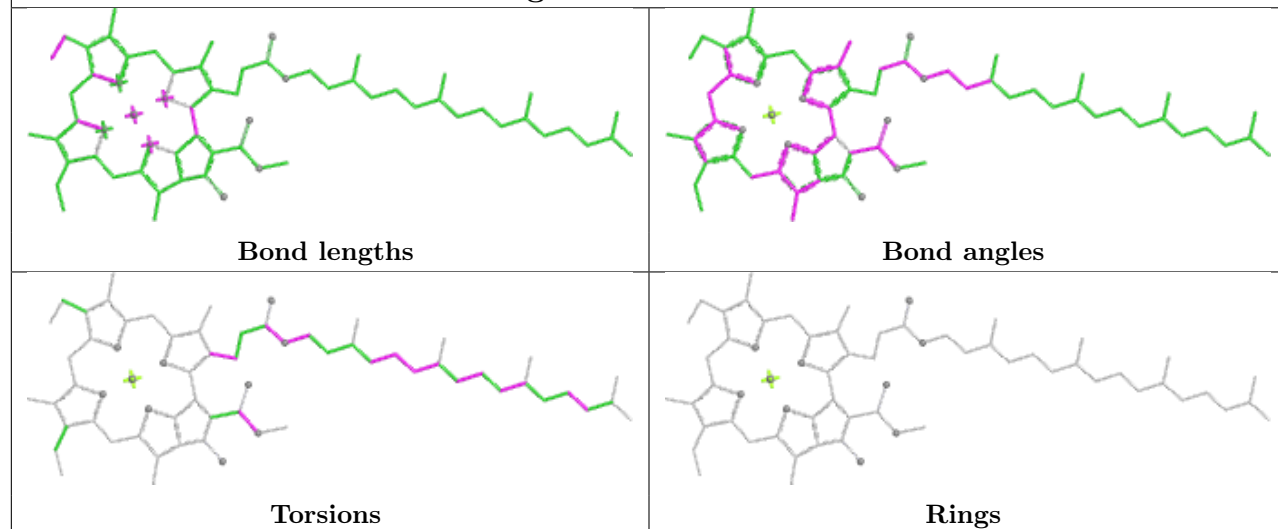
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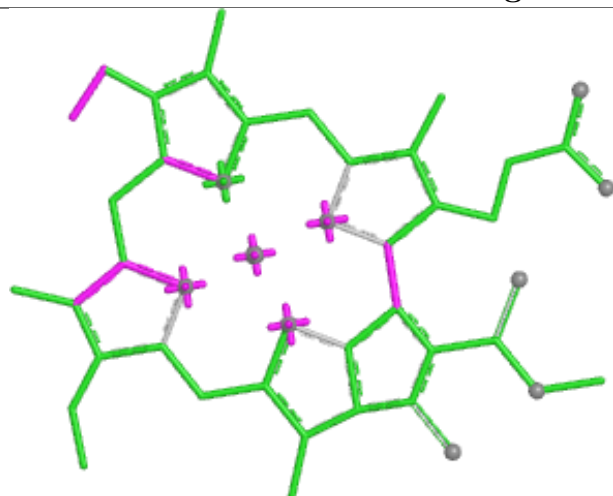
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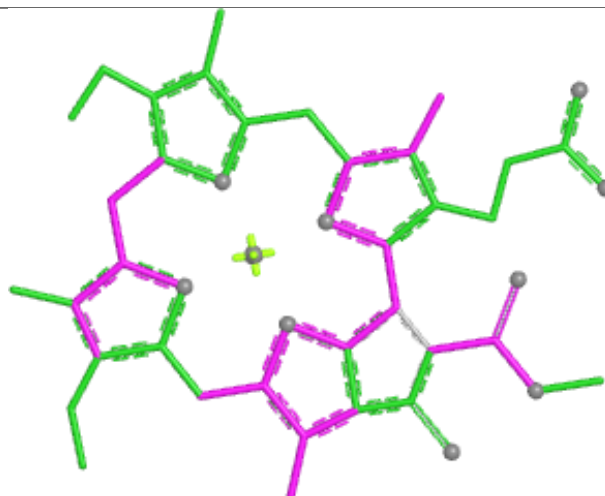
Ligand CLA J 1101



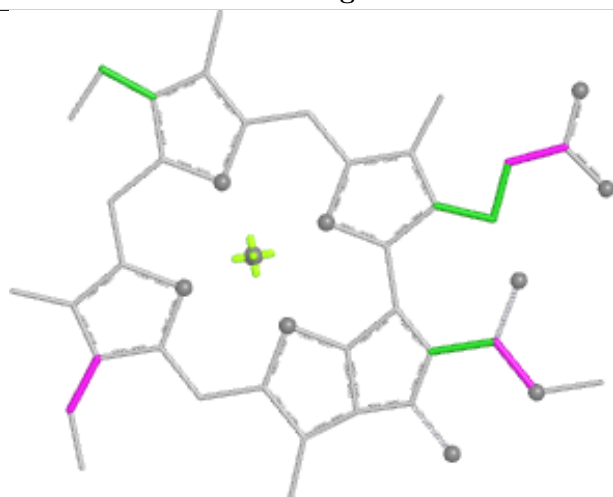
Ligand CLA K 1401



Bond lengths



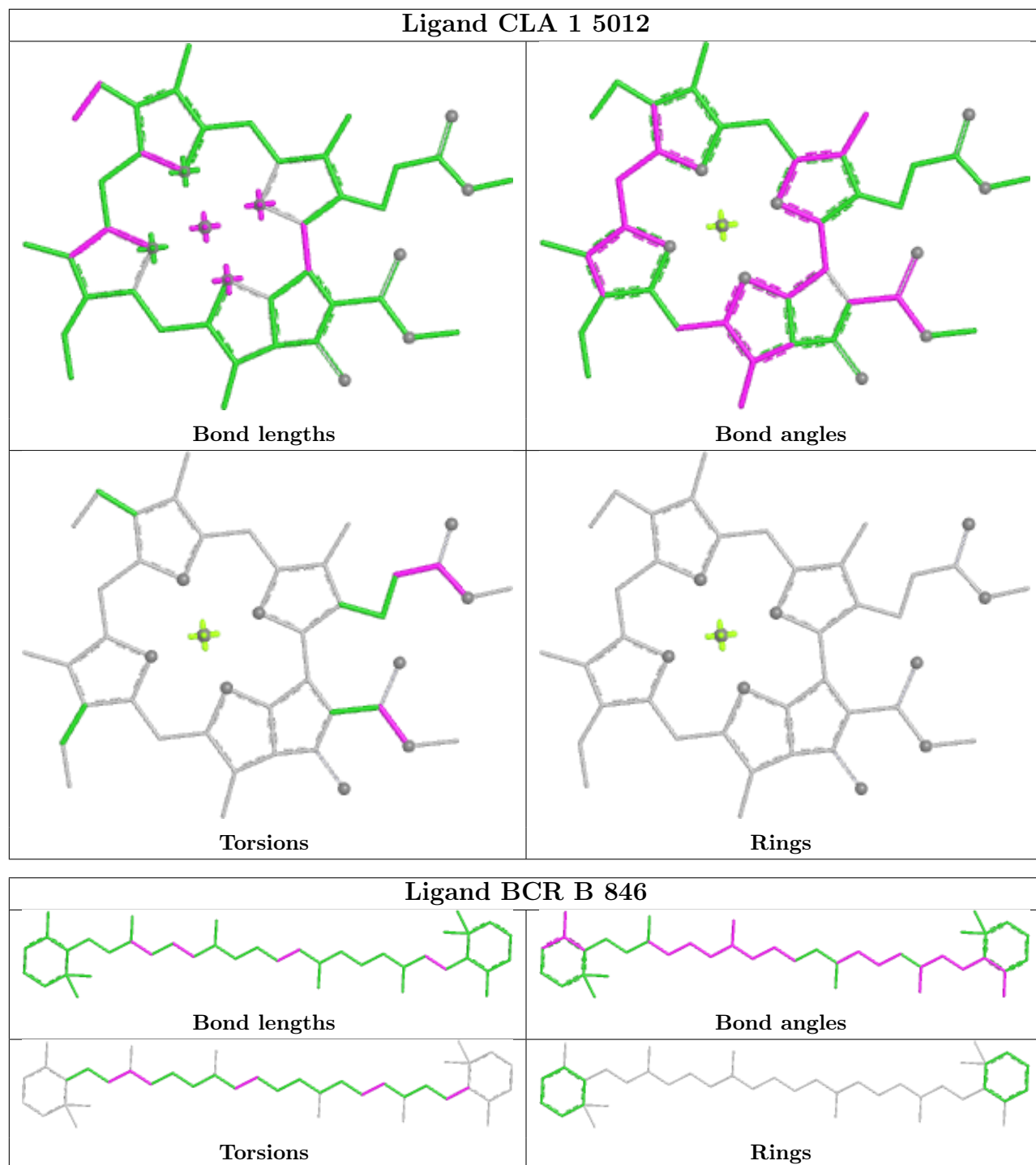
Bond angles

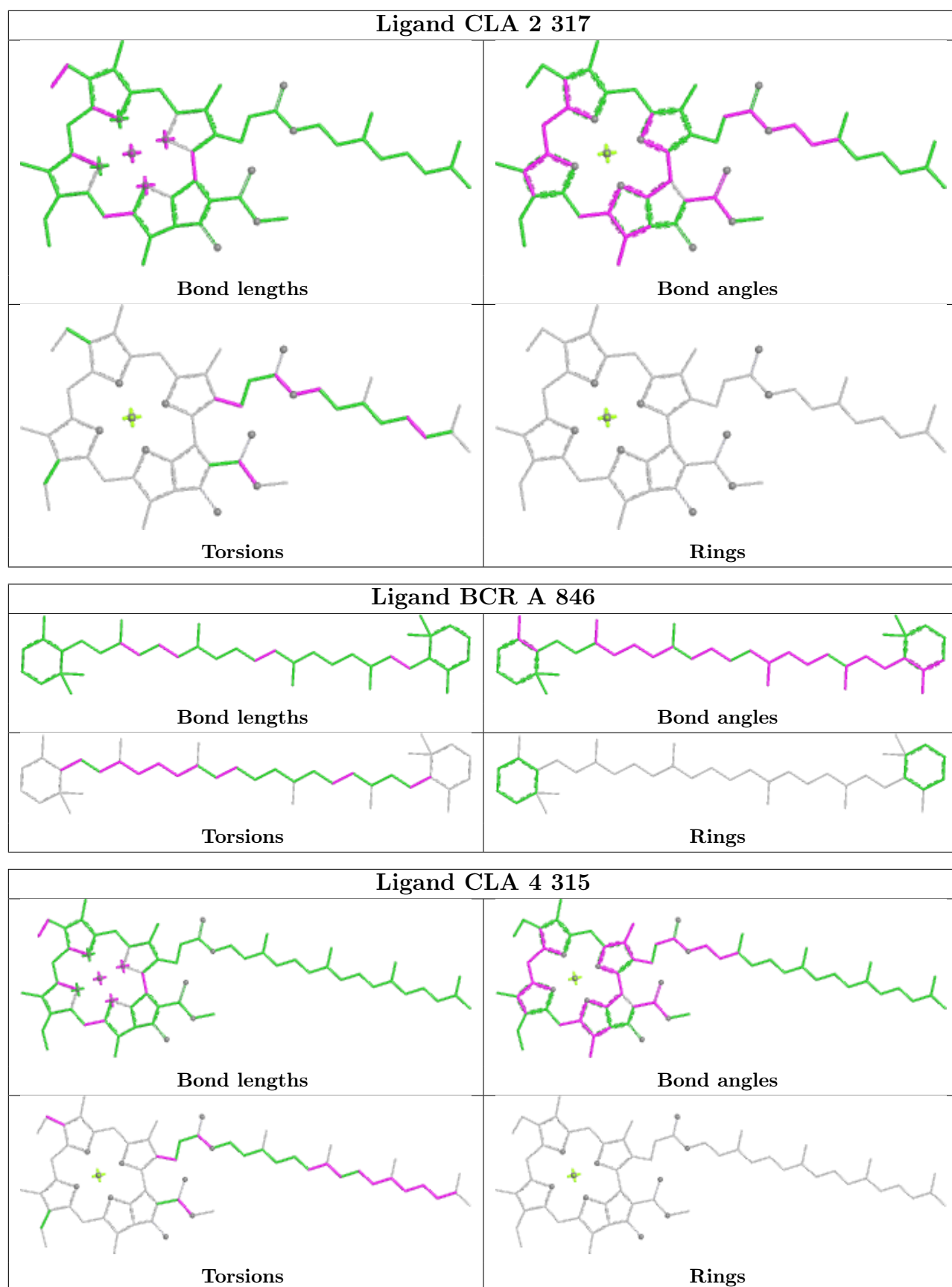


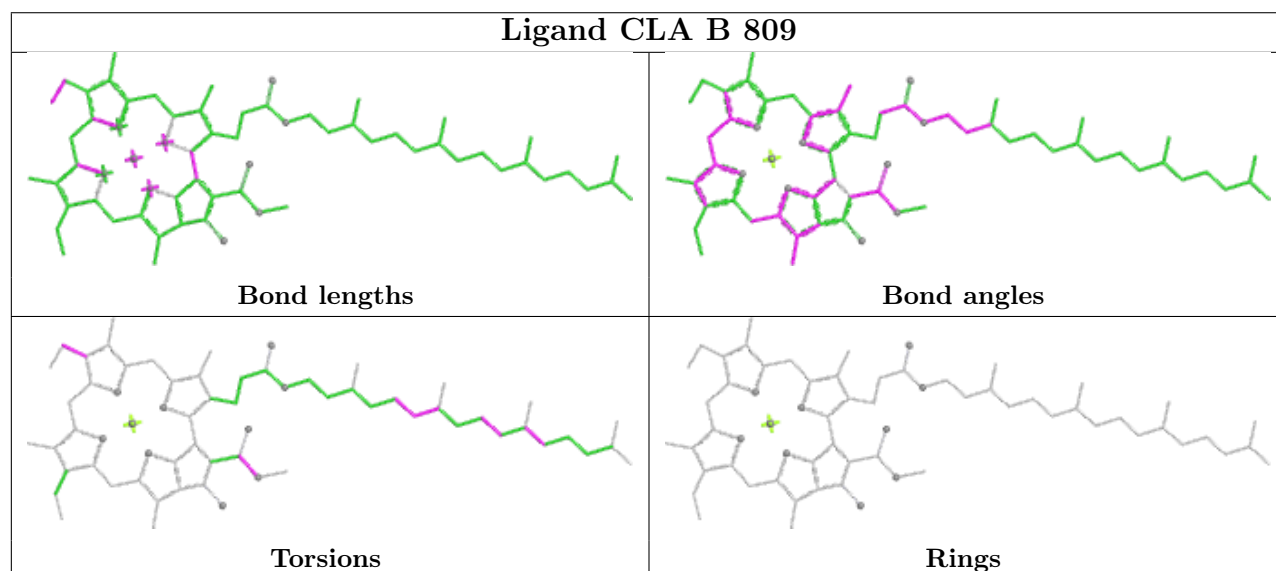
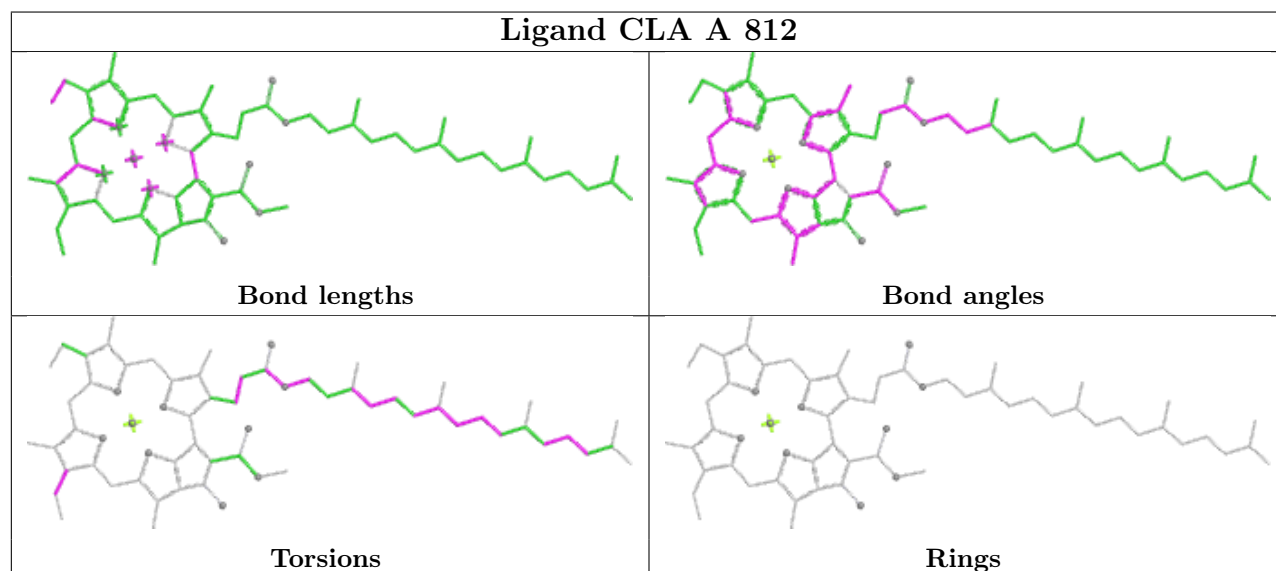
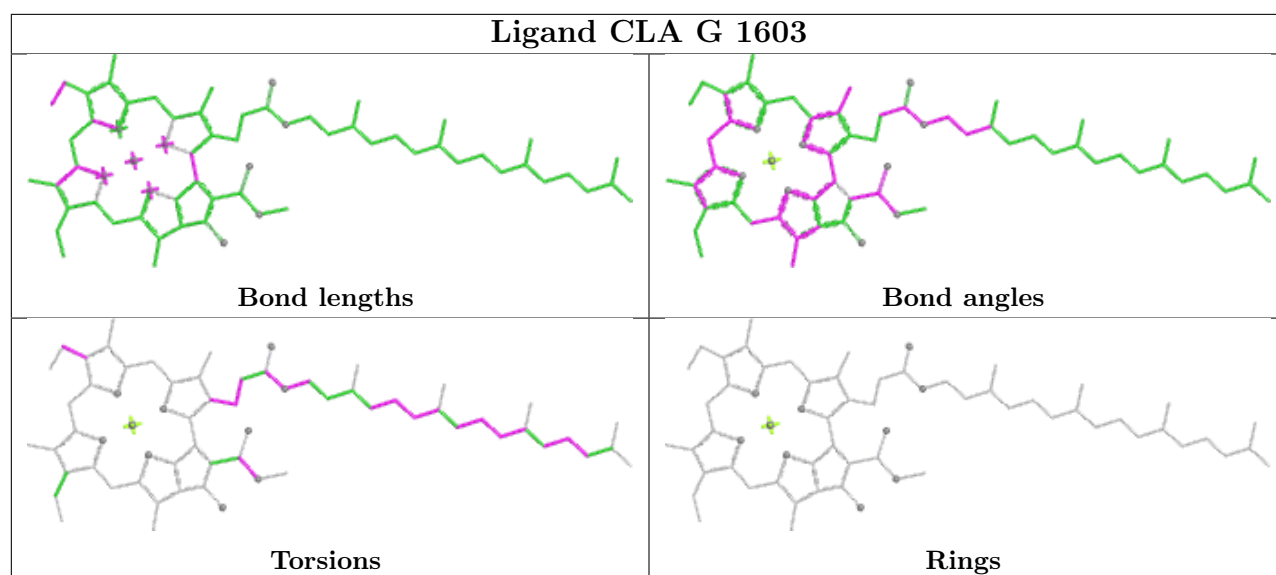
Torsions

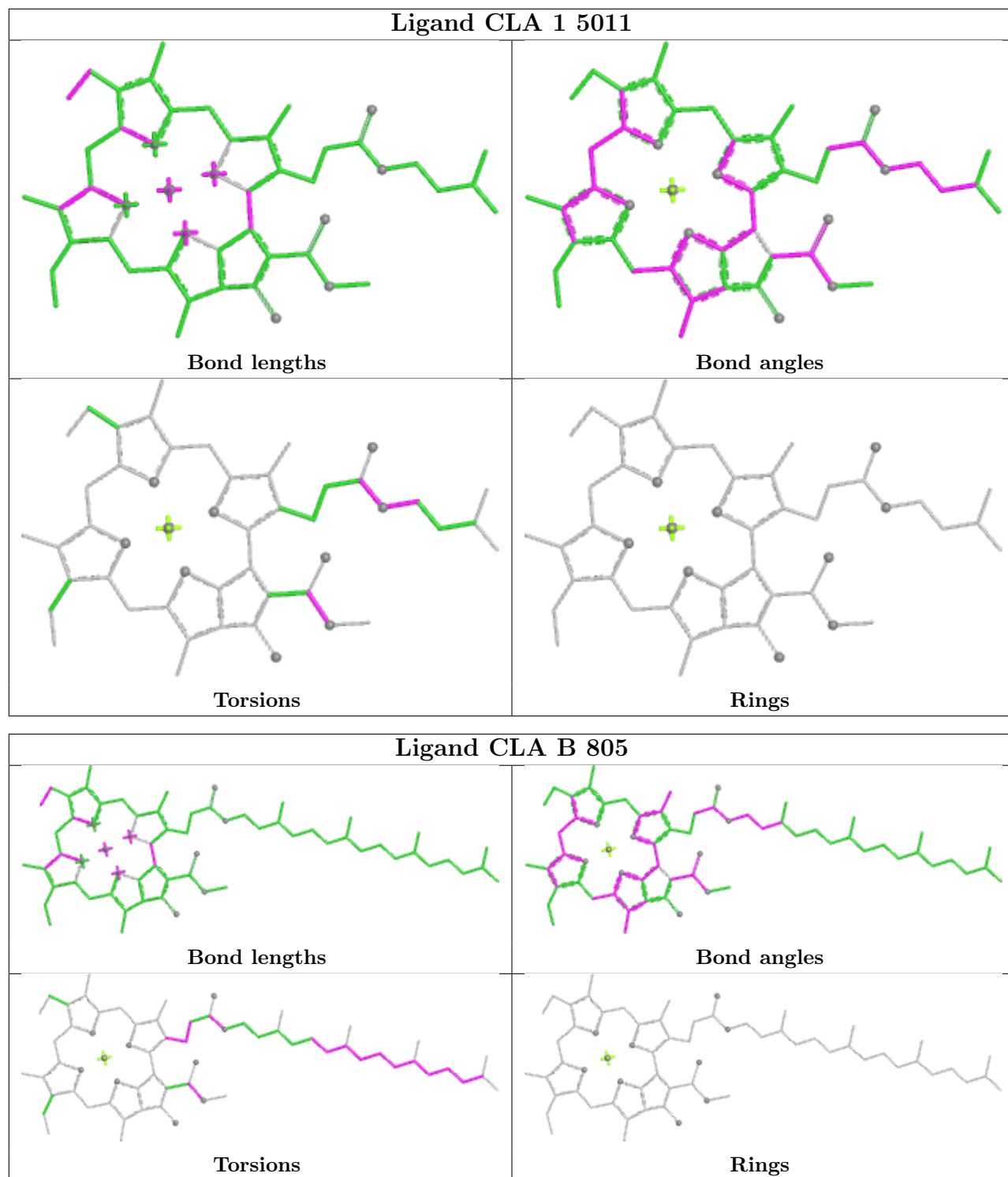


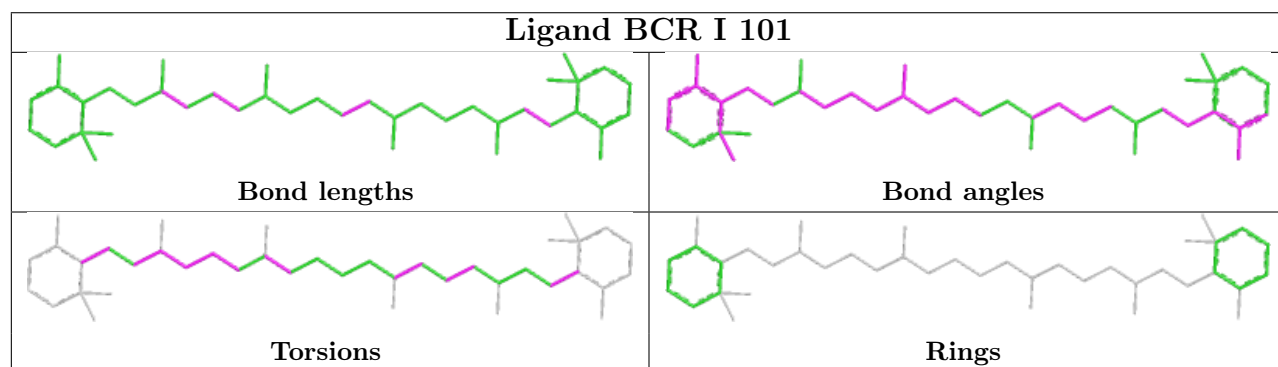
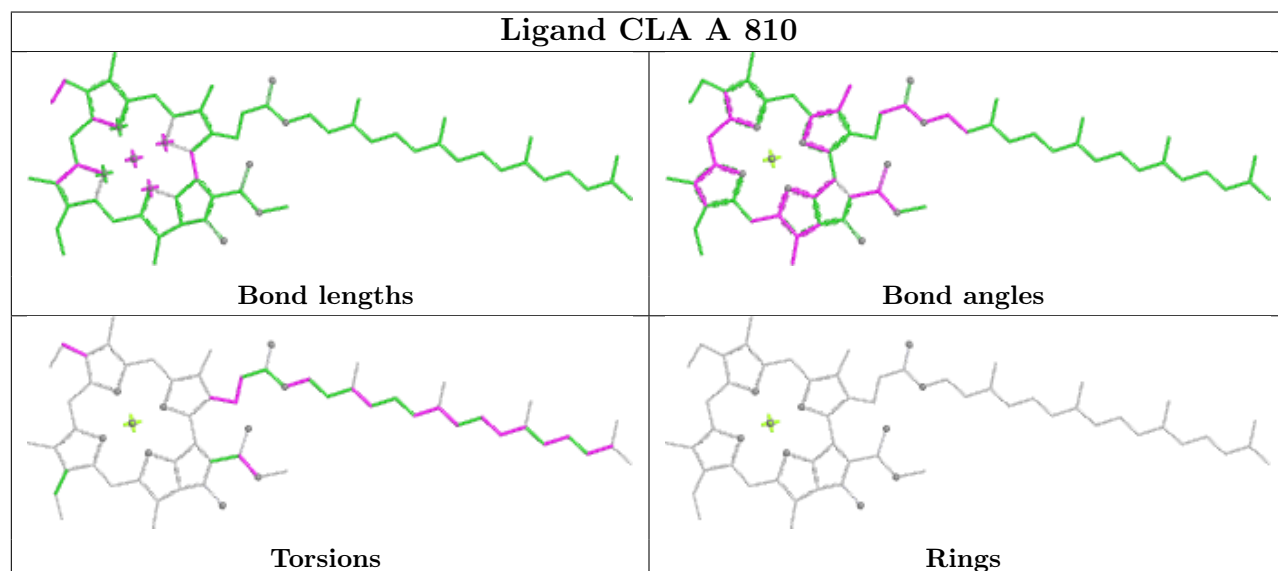
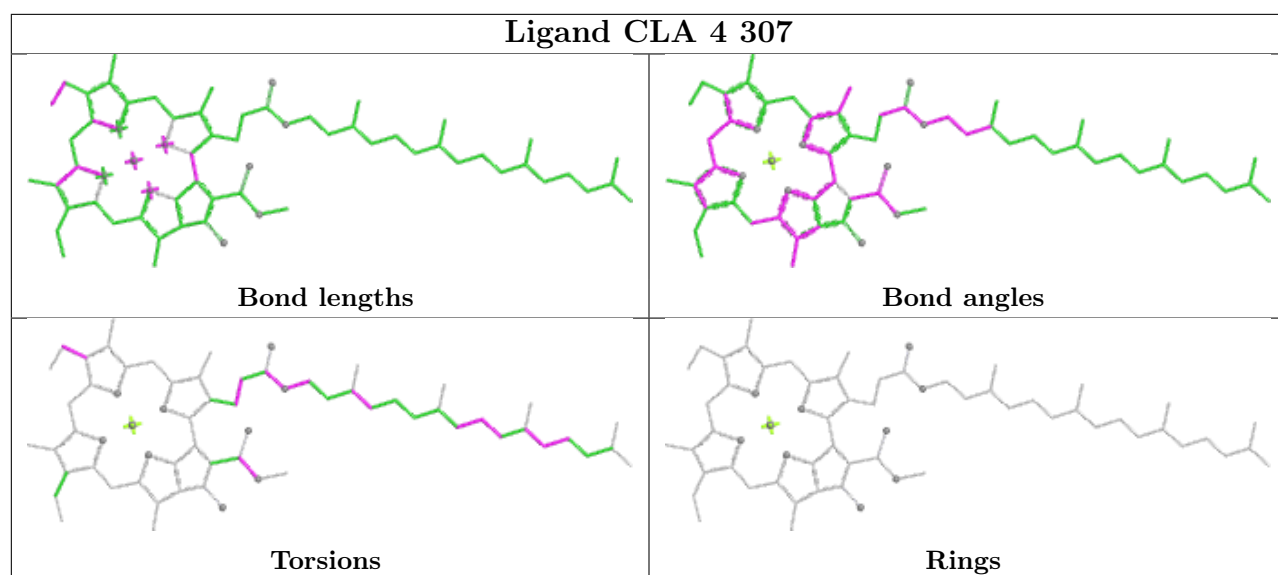
Rings

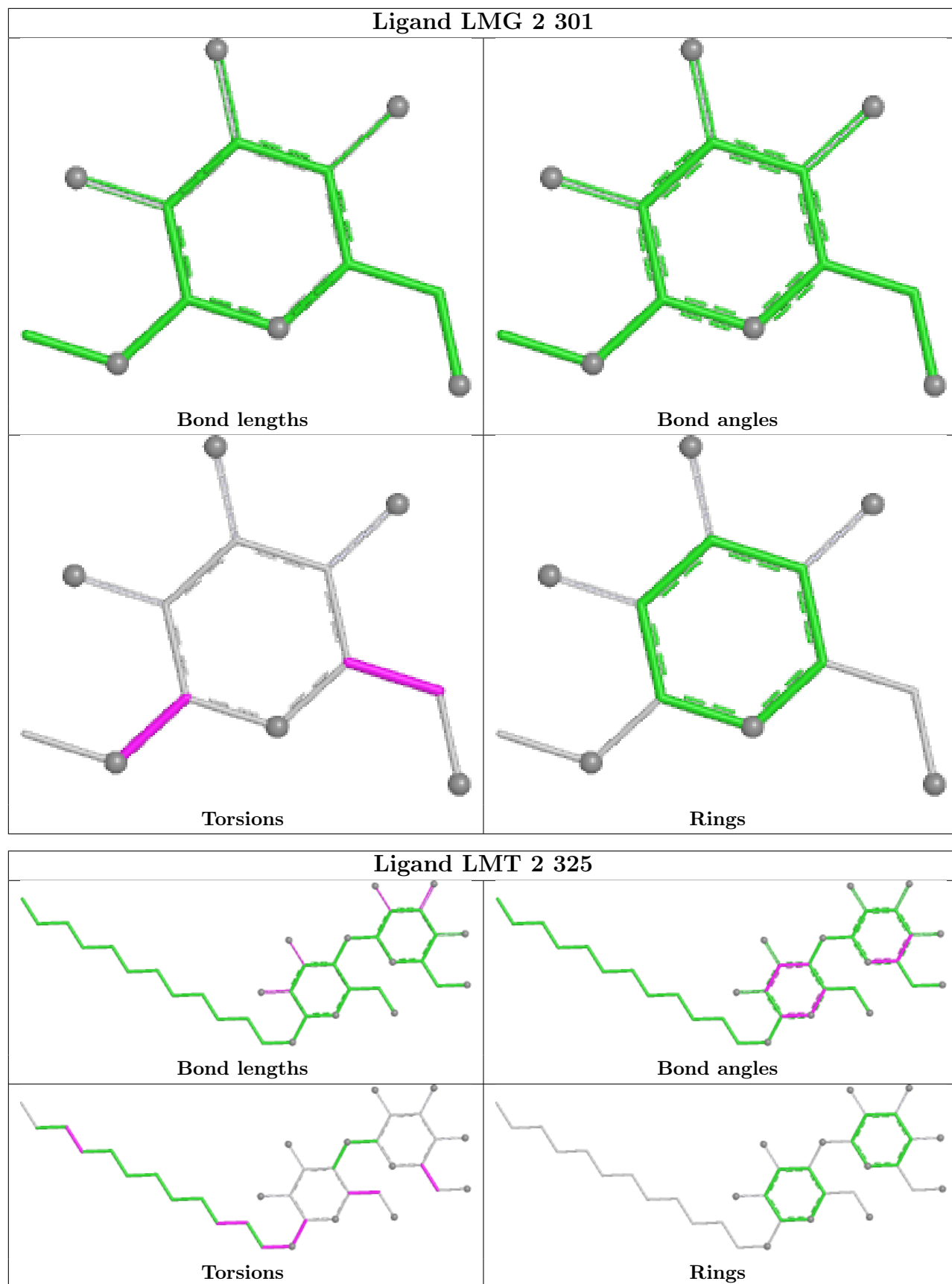


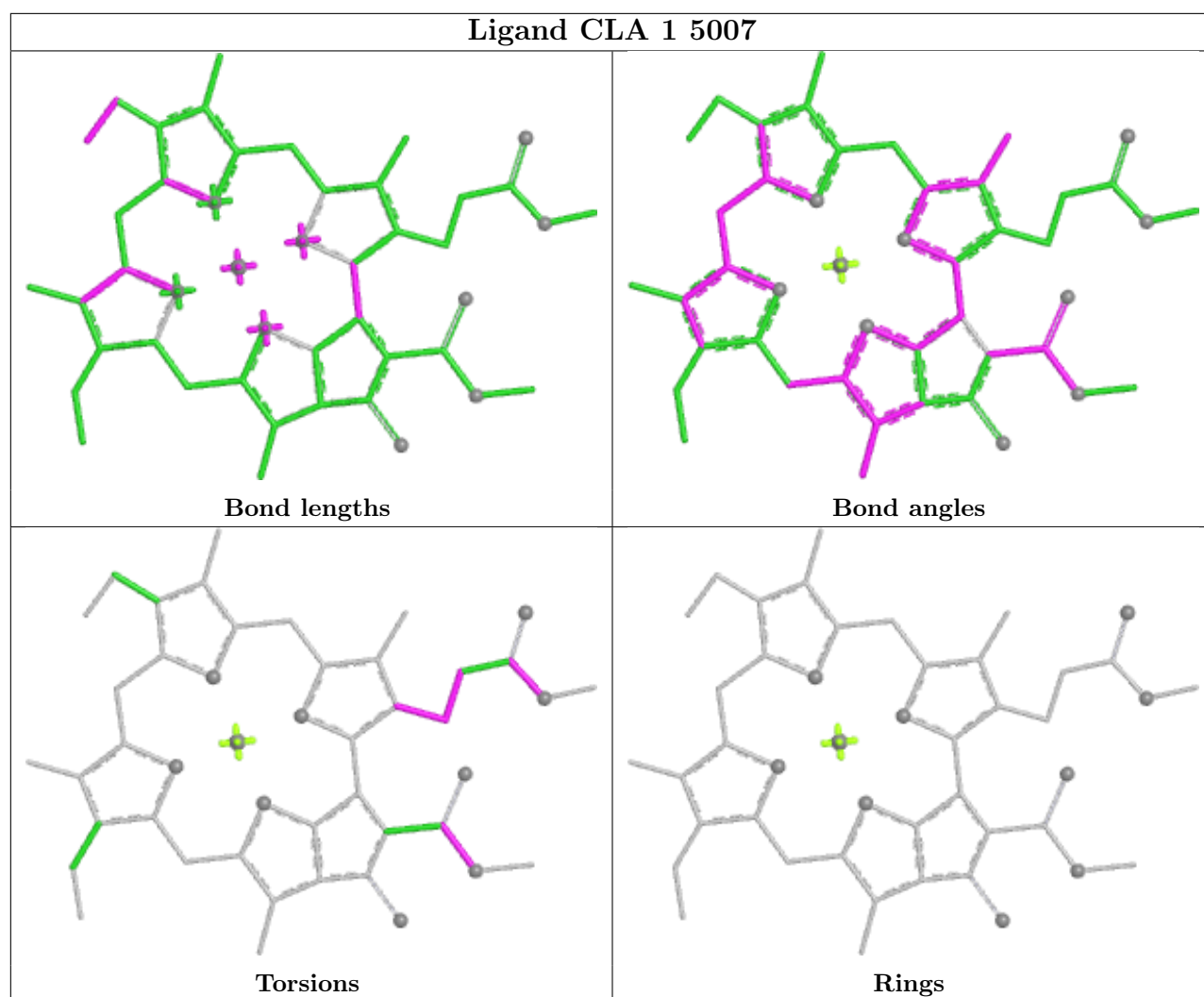


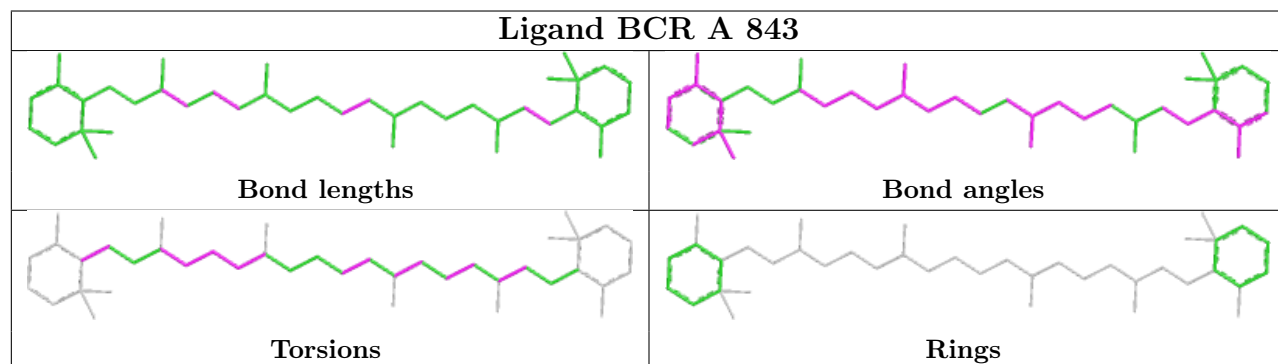
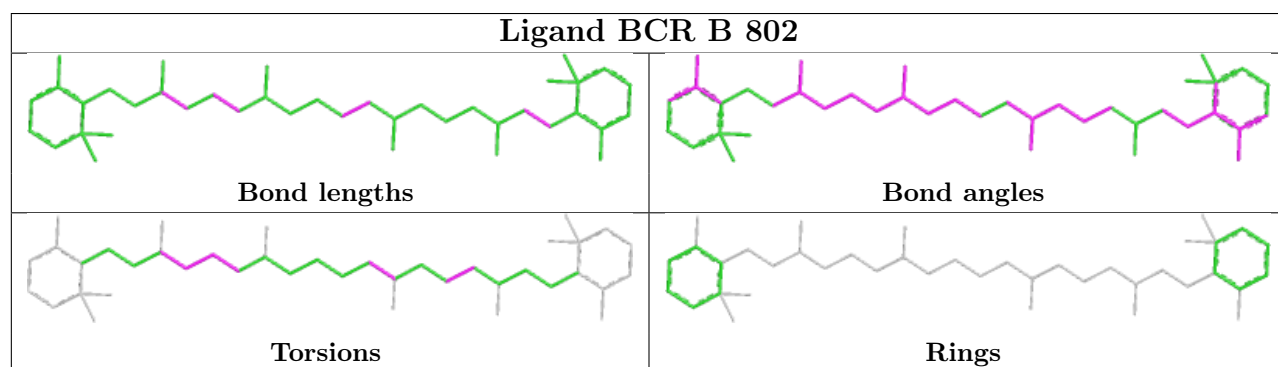
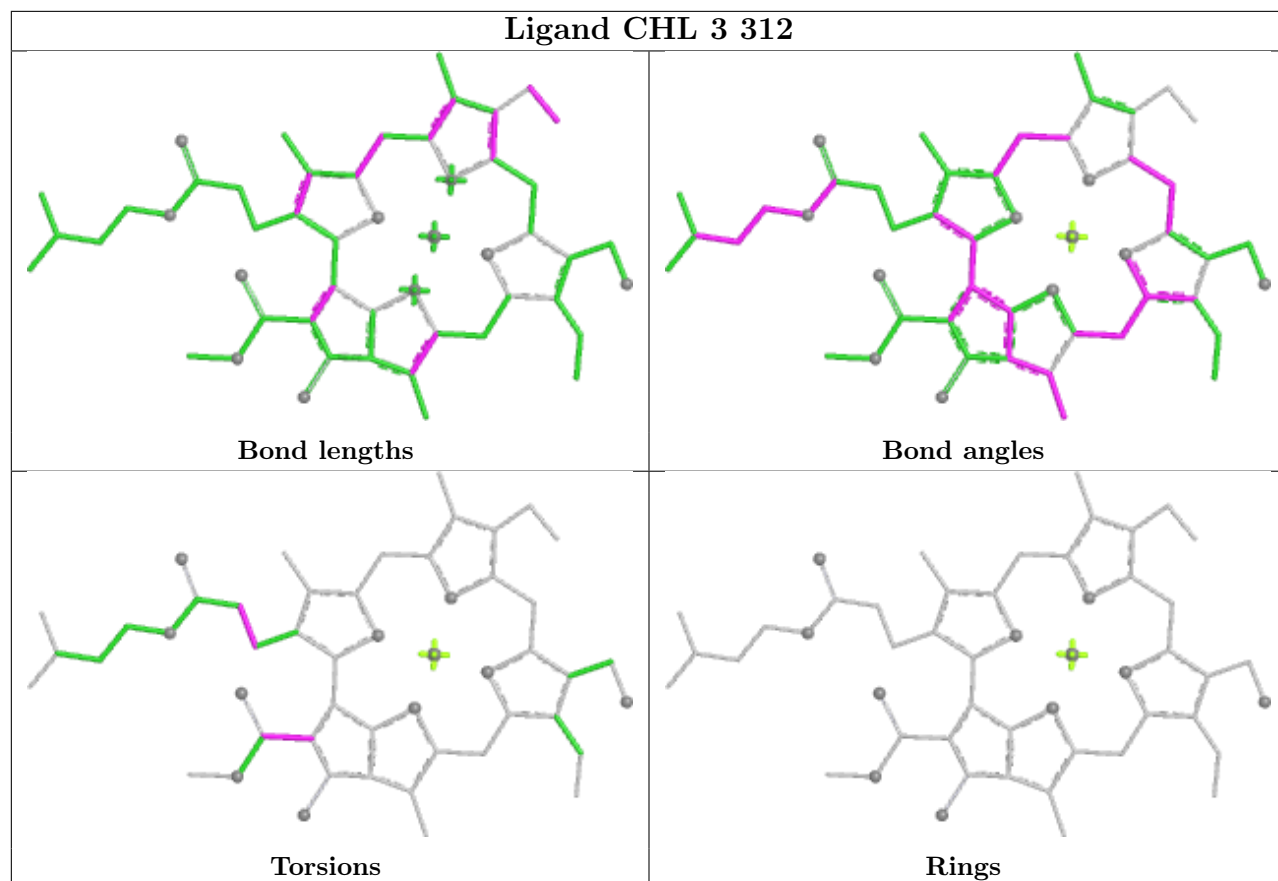


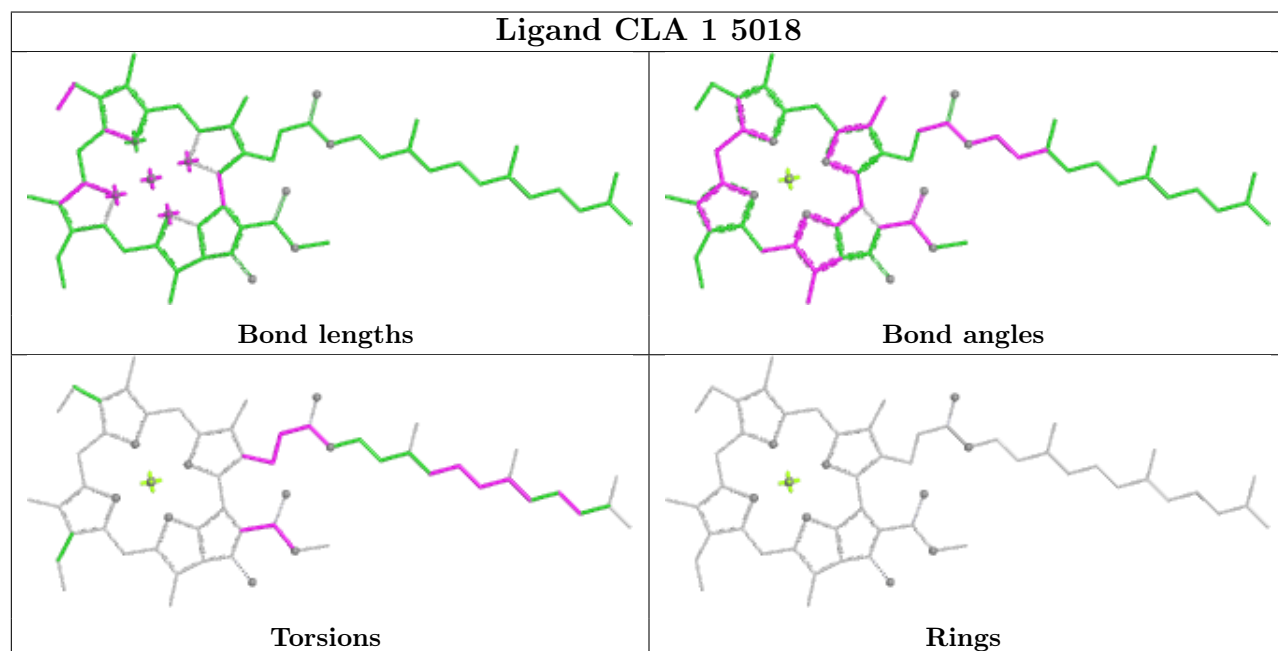
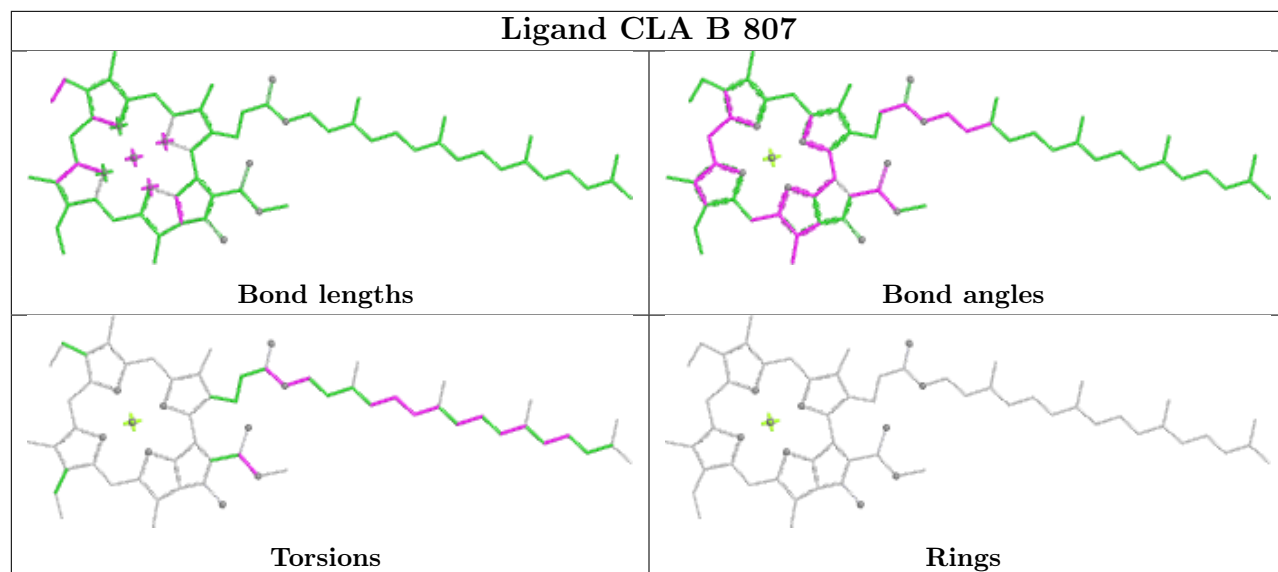


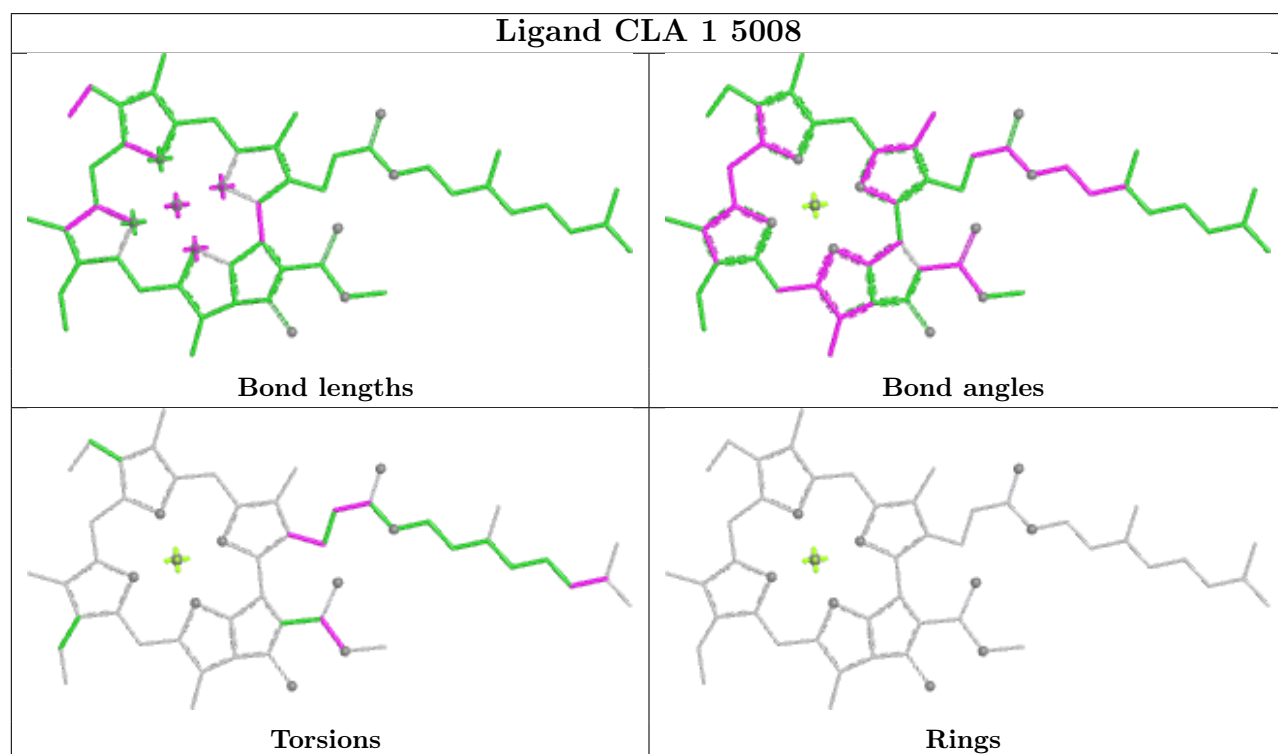
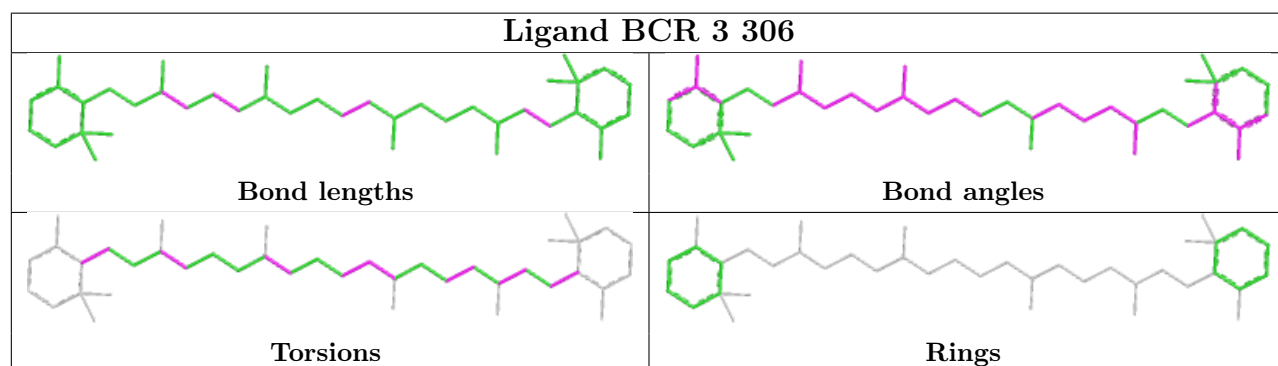
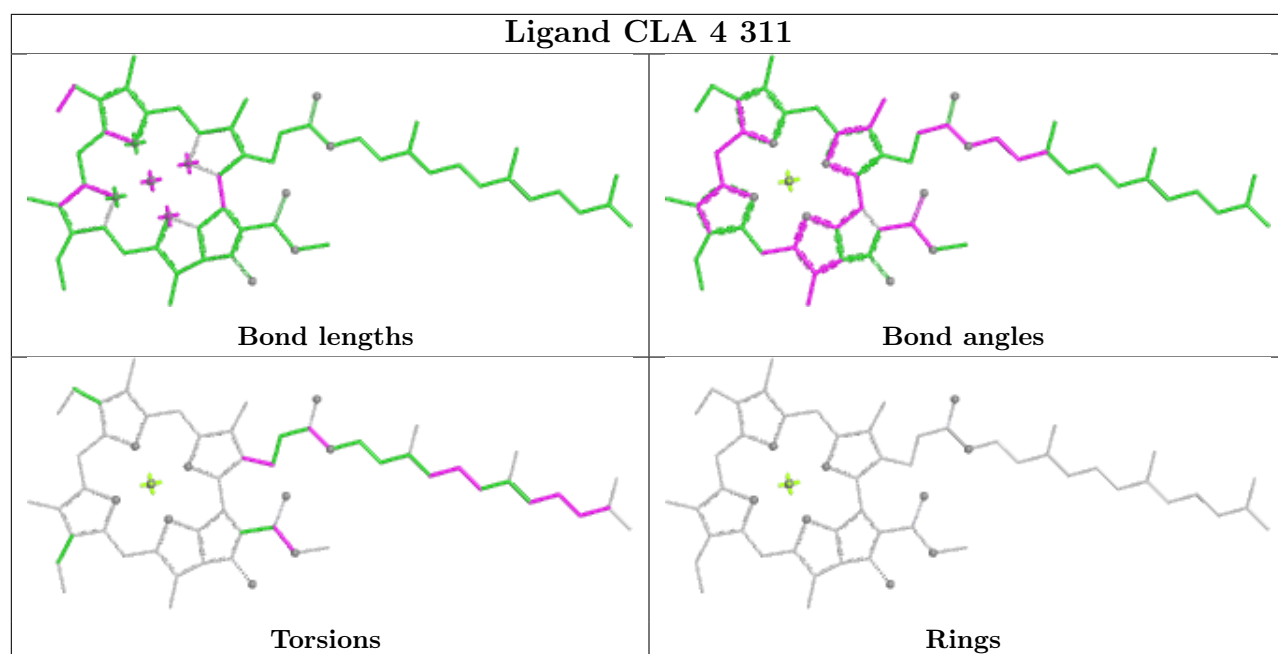


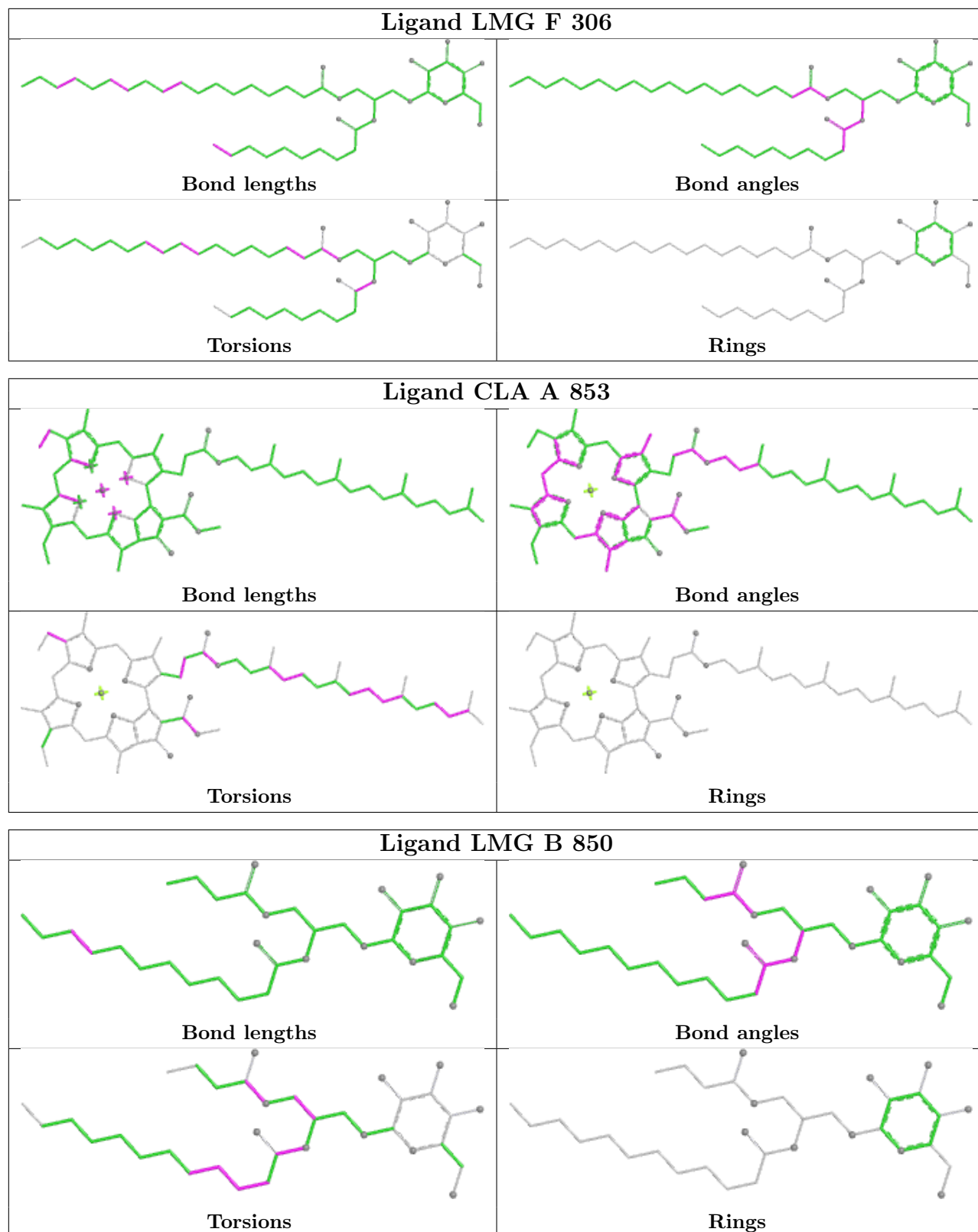


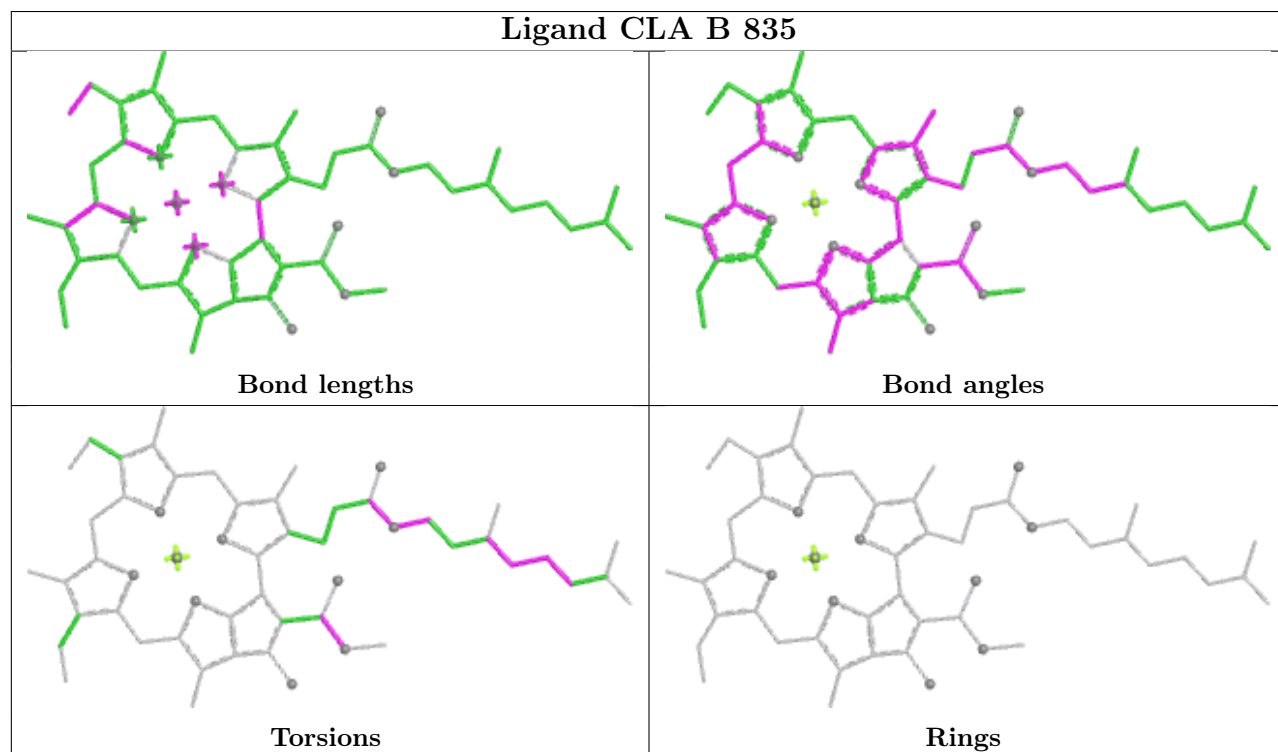
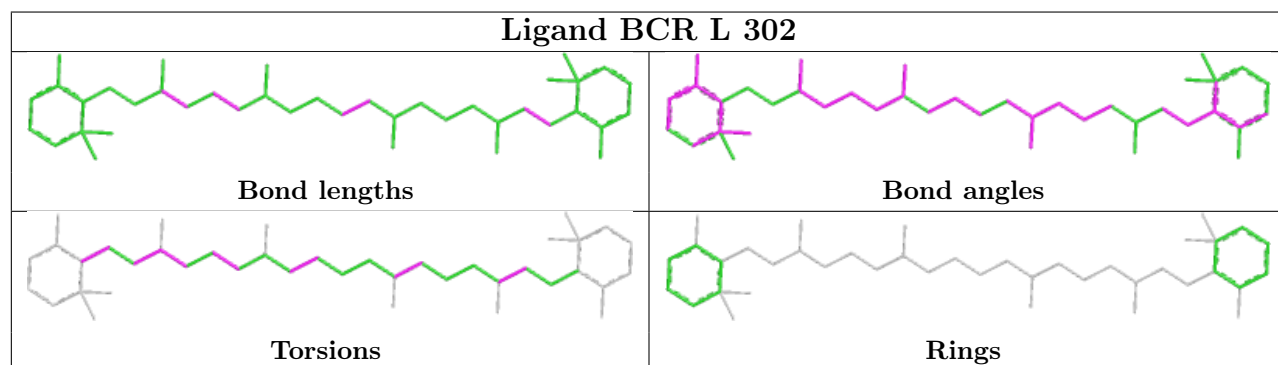
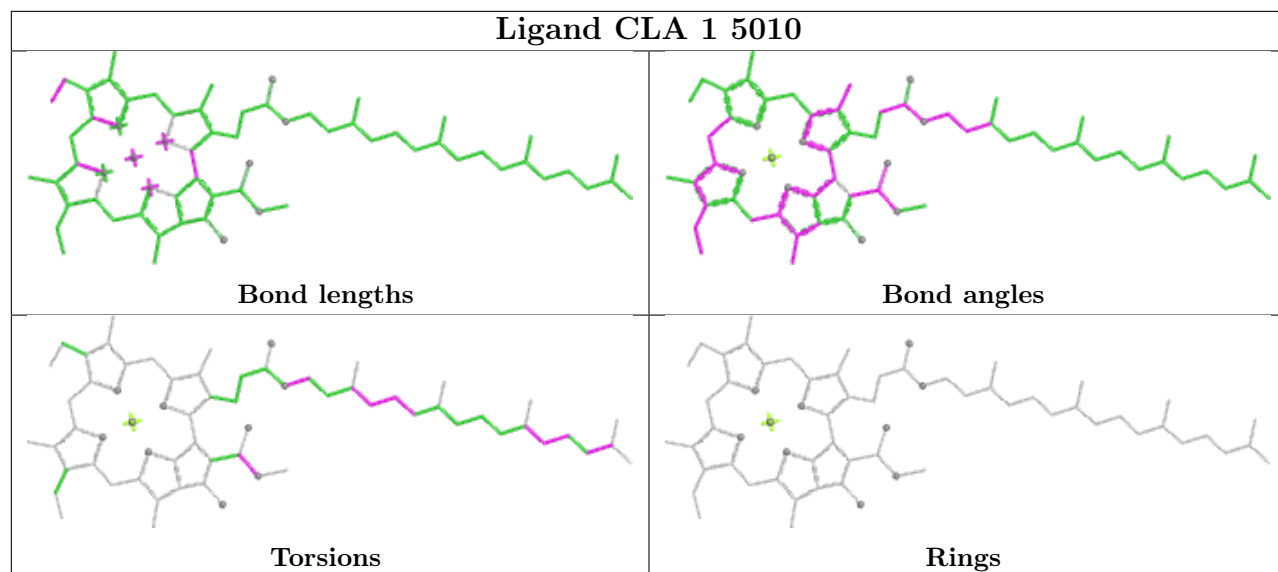


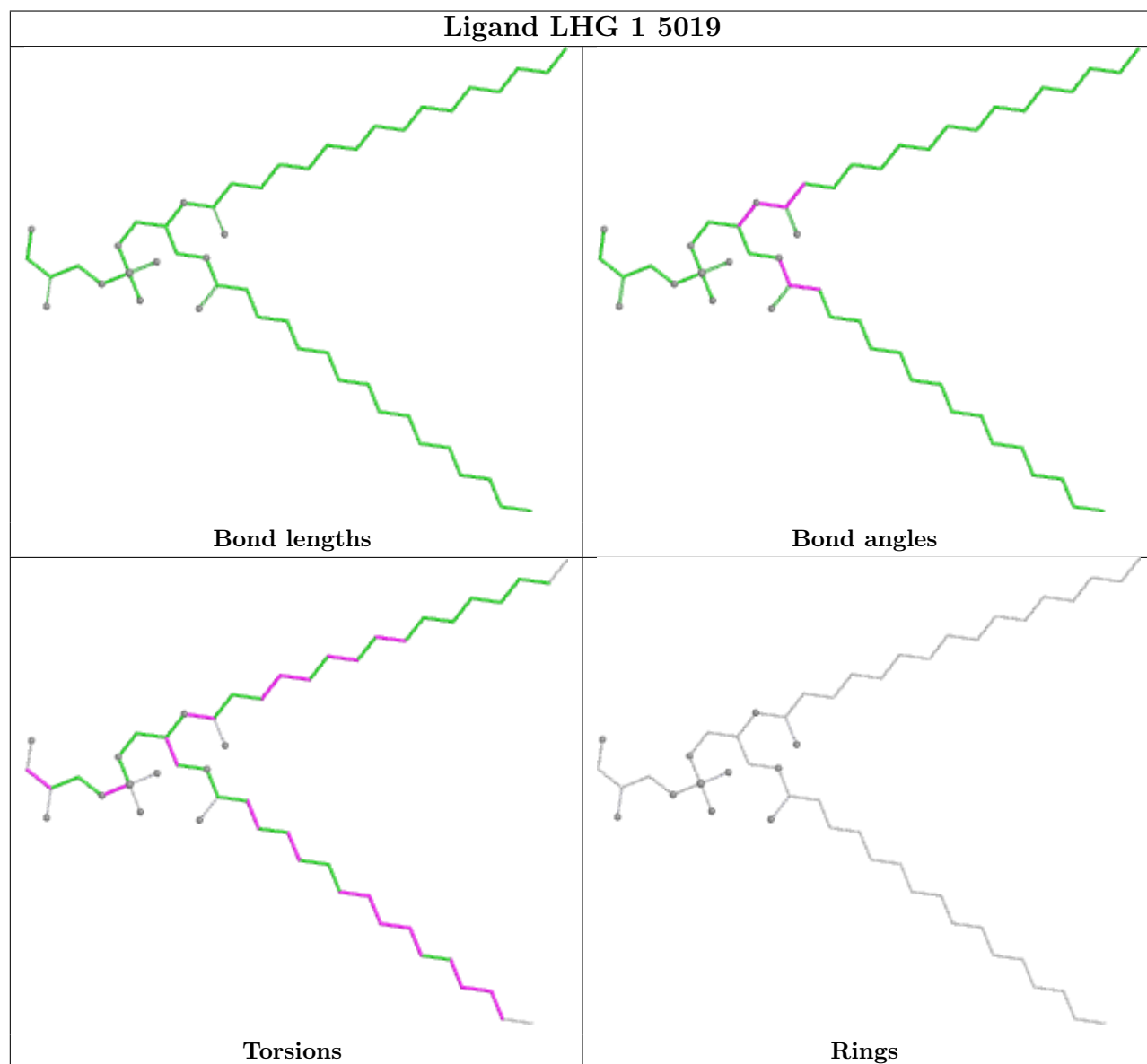
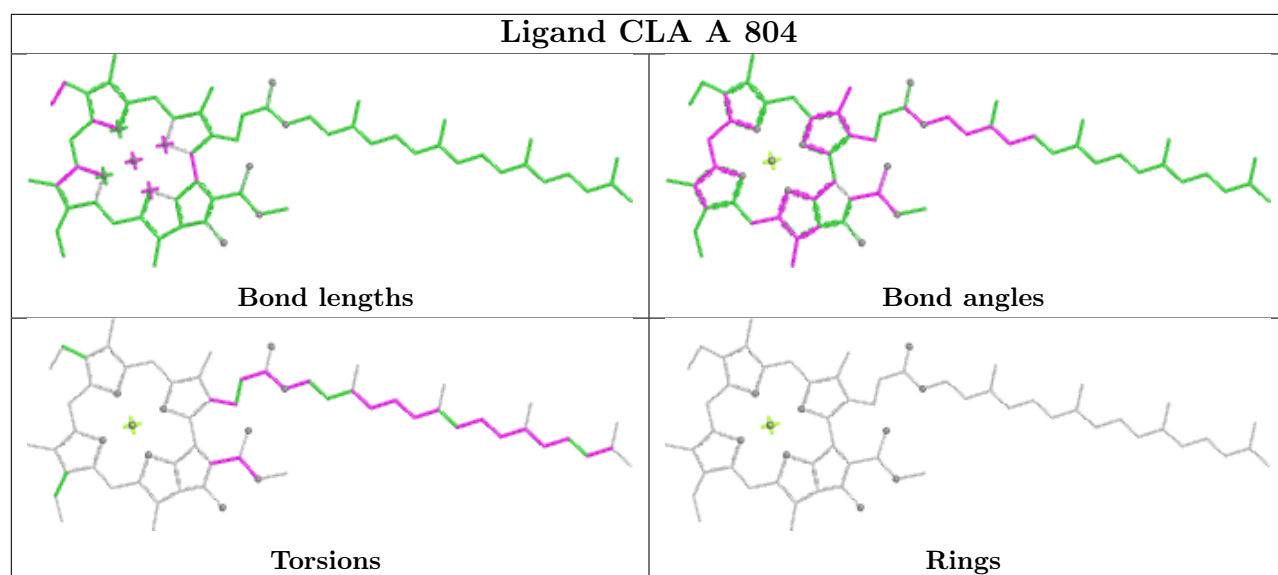


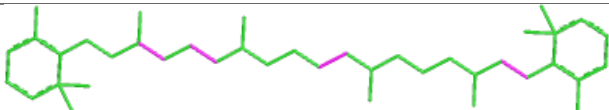
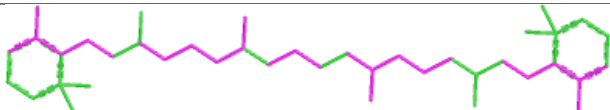
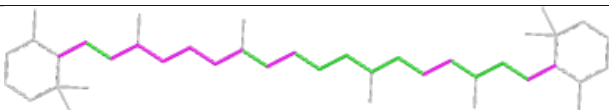
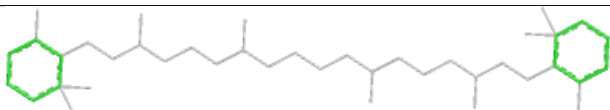


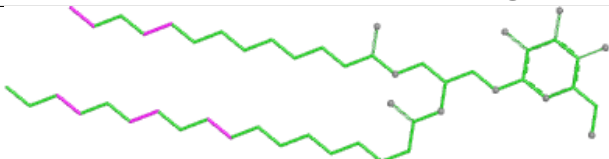
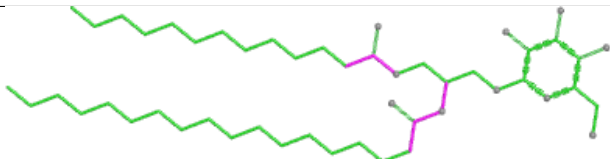
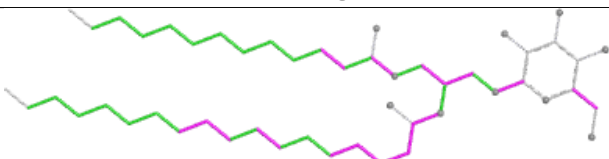
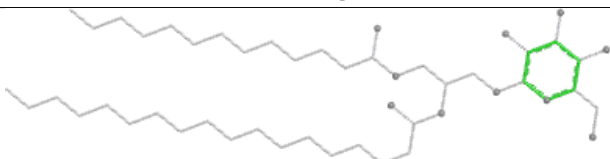


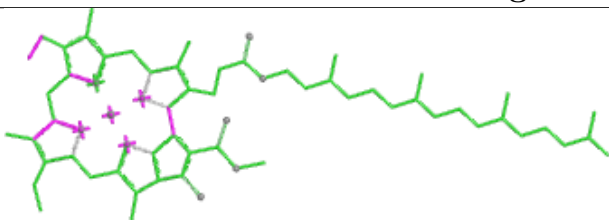
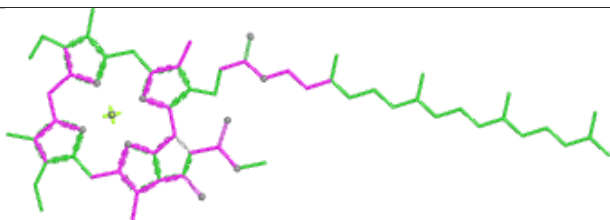
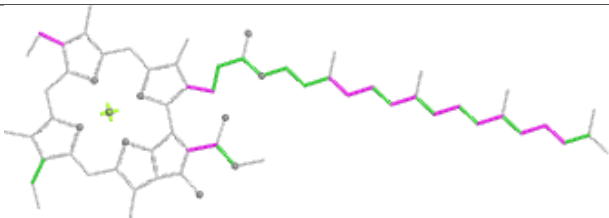
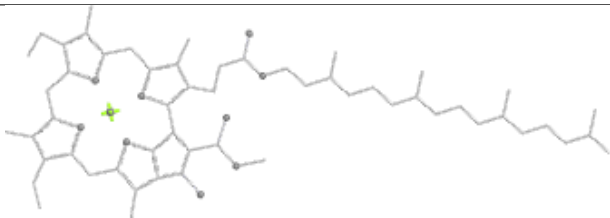


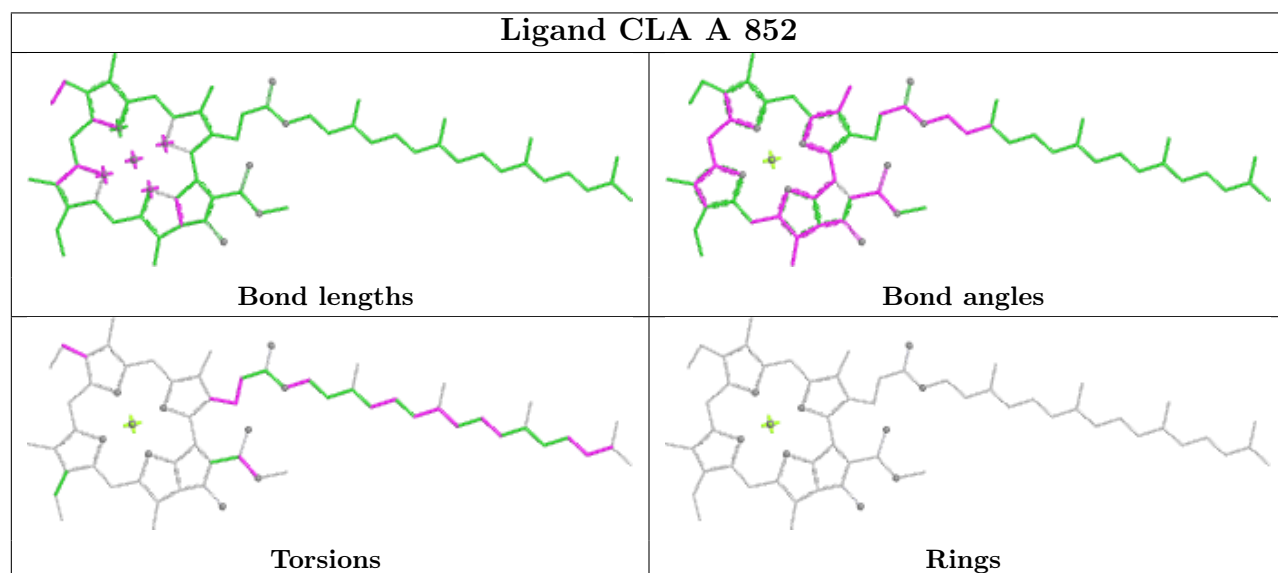
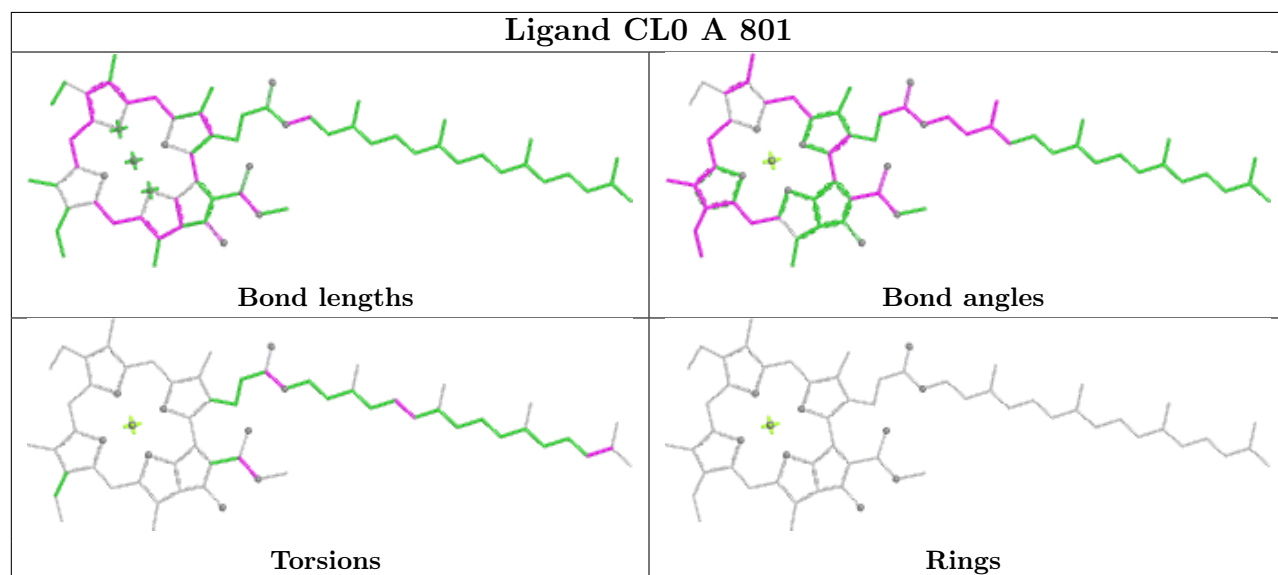
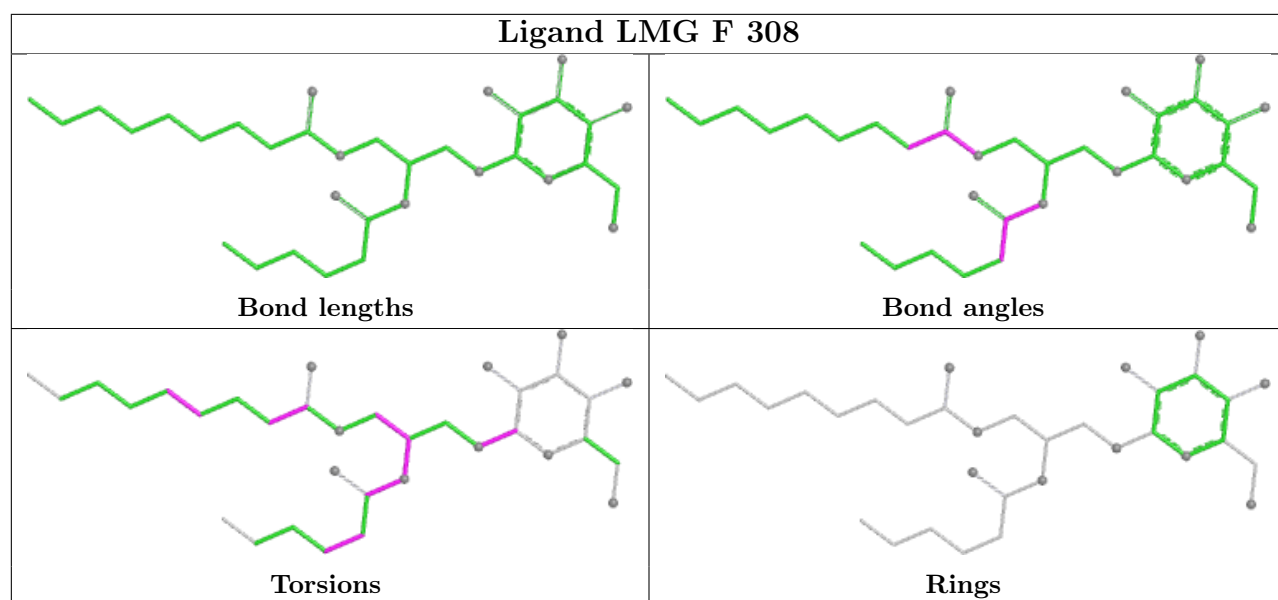


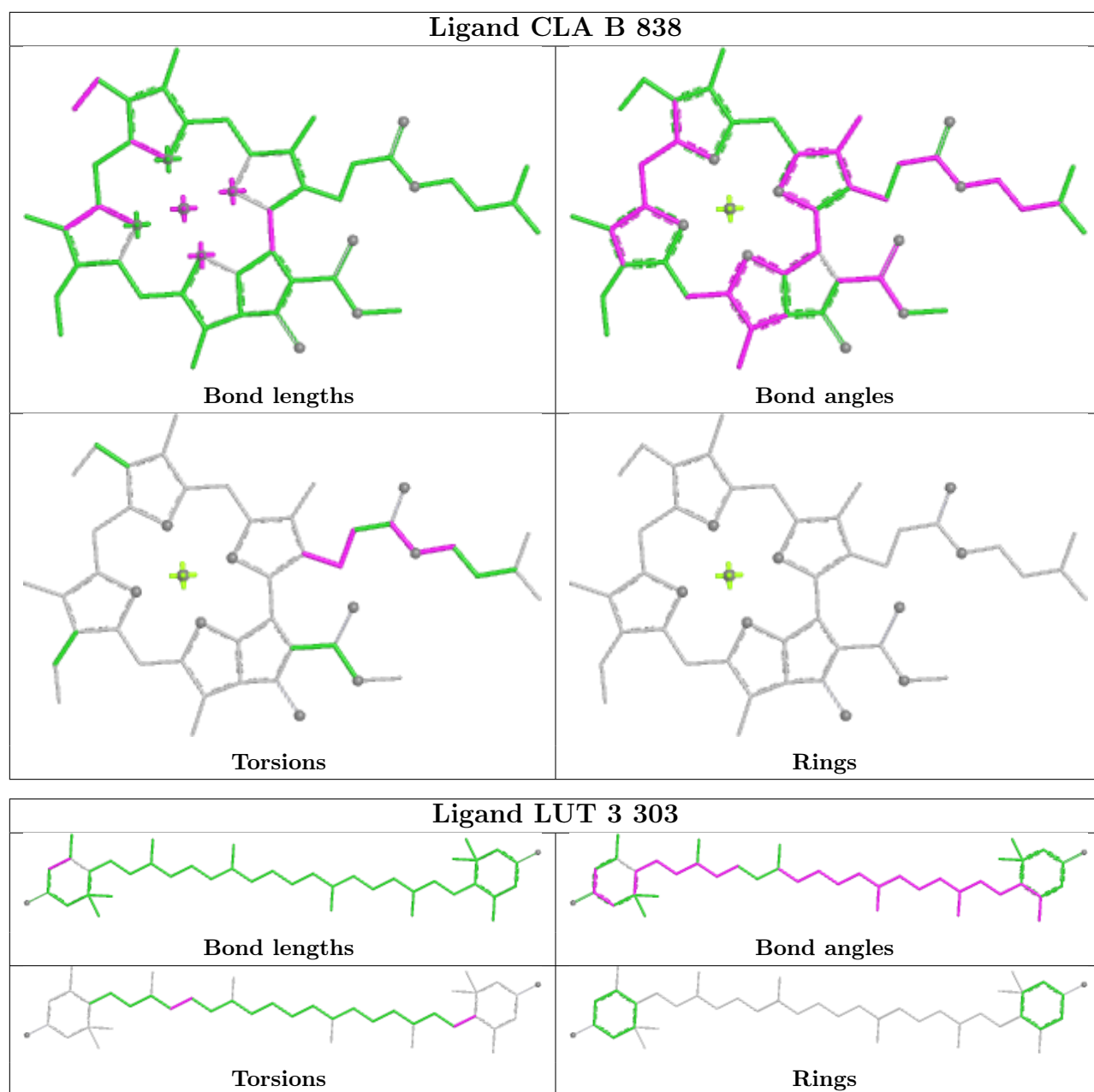


Ligand BCR L 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

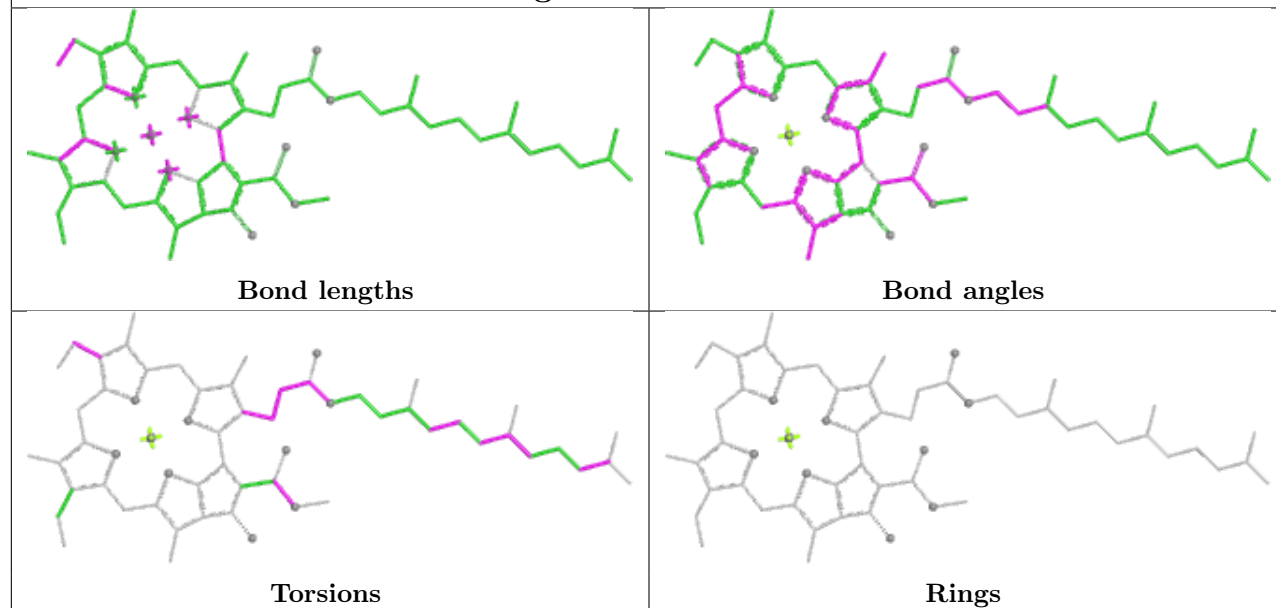
Ligand LMG A 851	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

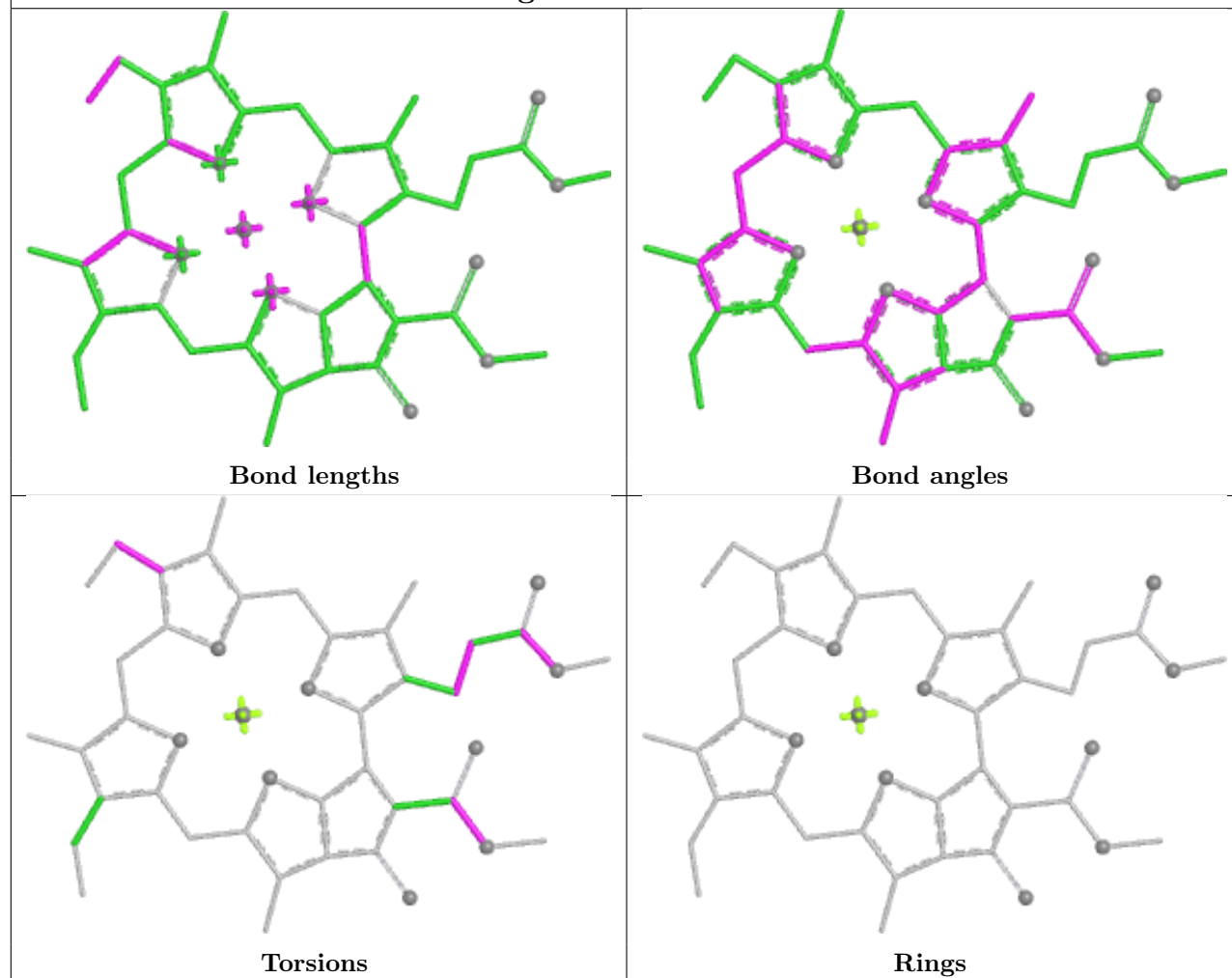




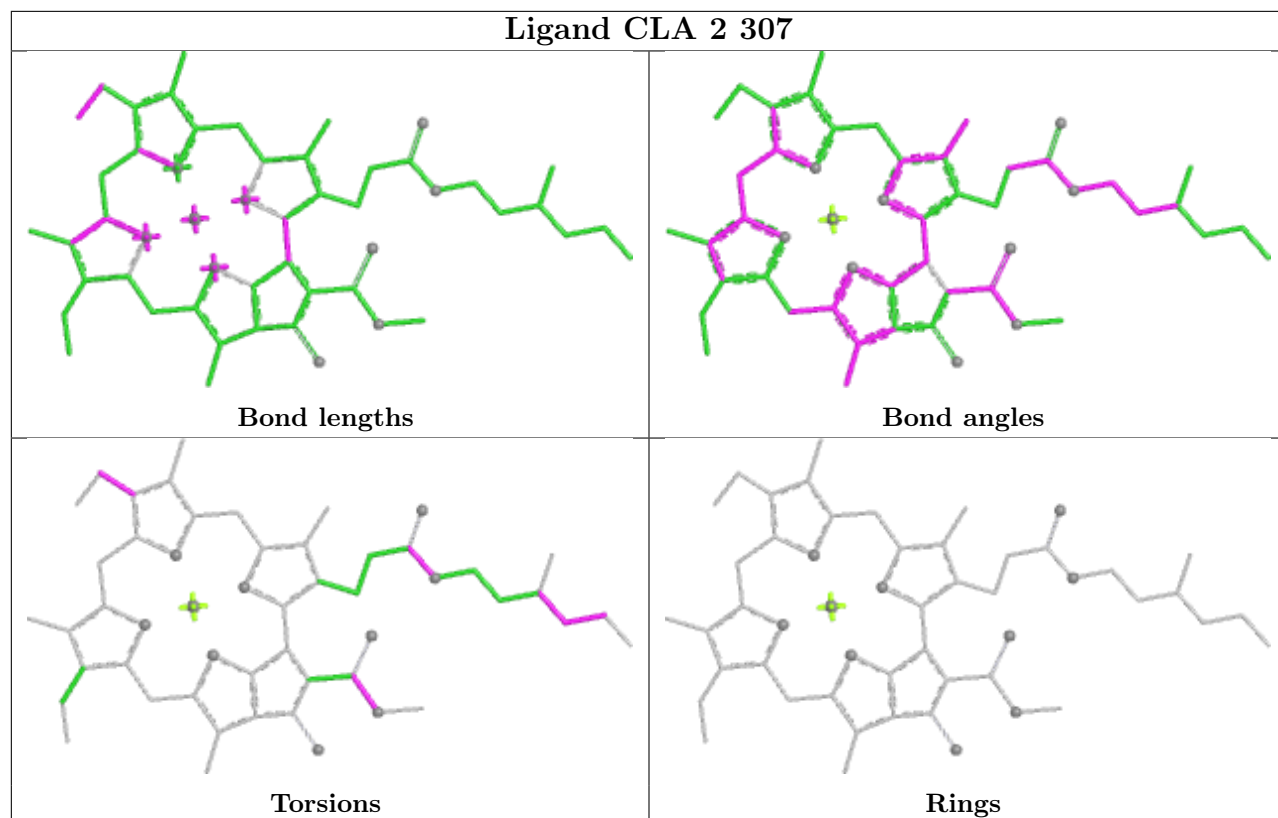
Ligand CLA L 305



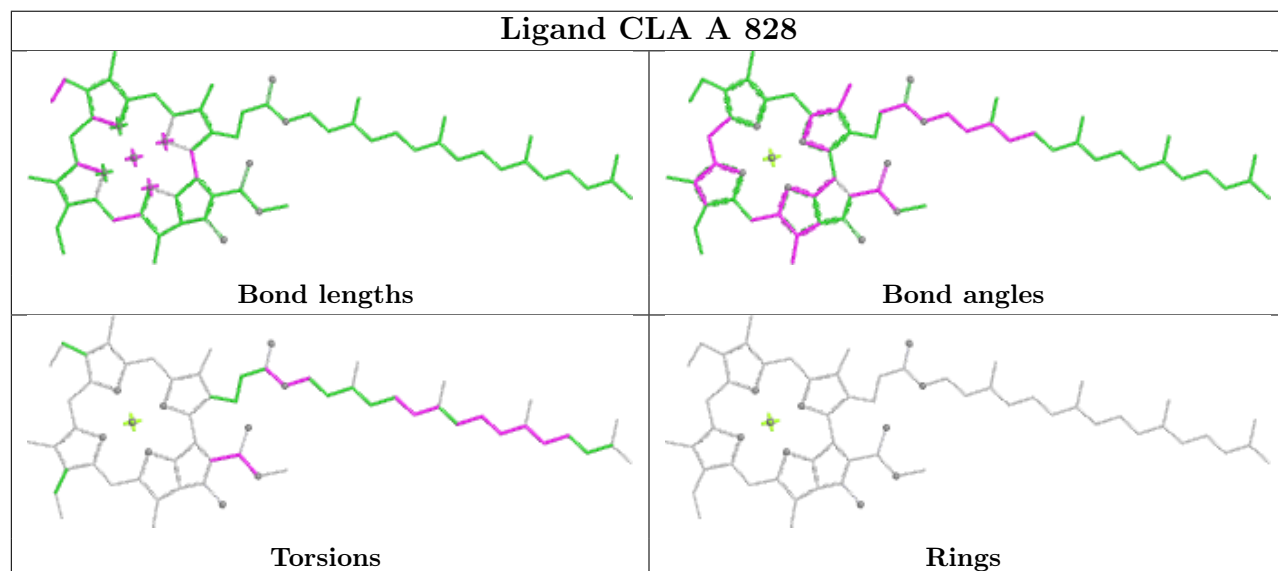
Ligand CLA 4 312



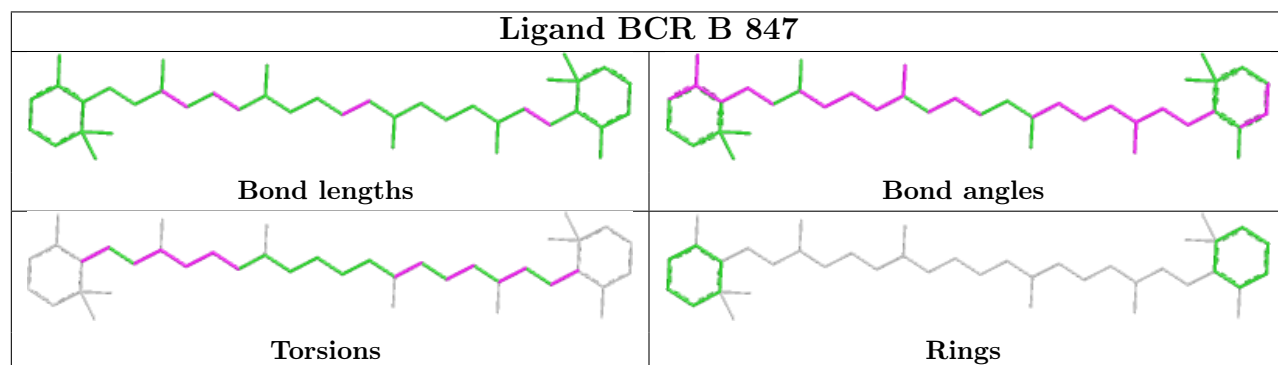
Ligand CLA 2 307

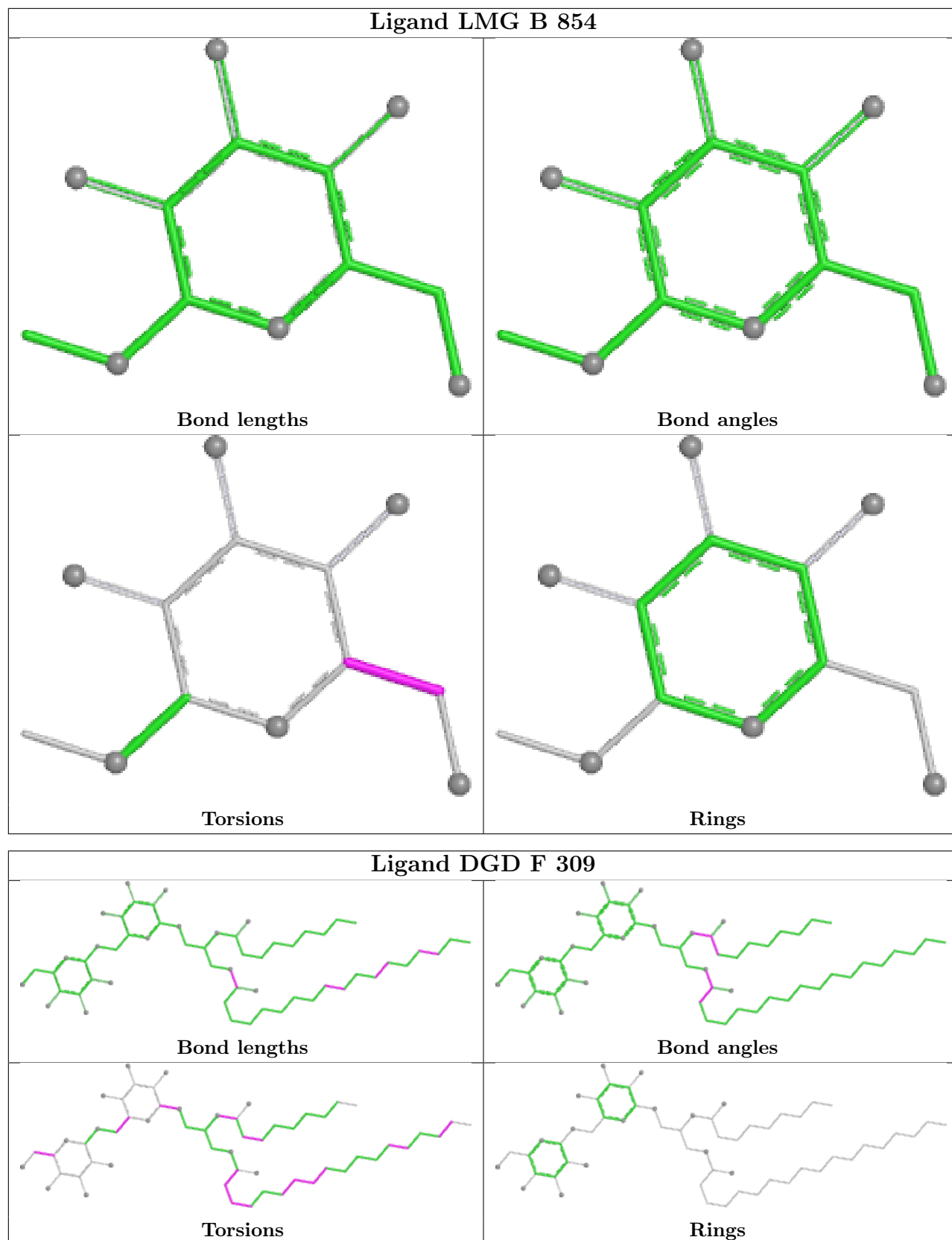


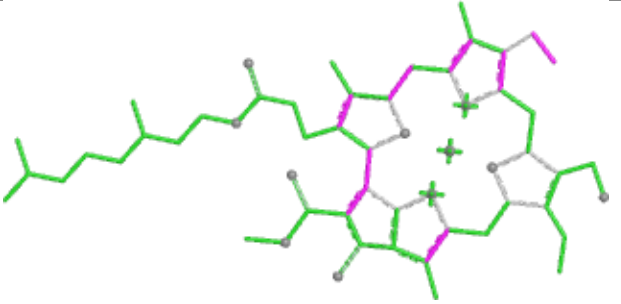
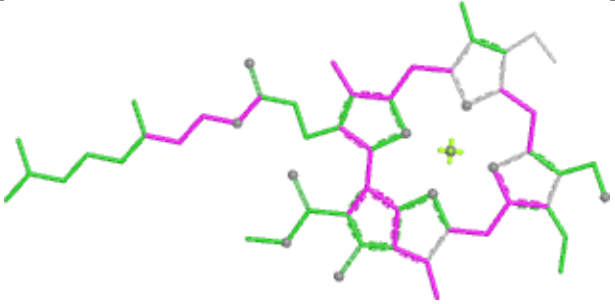
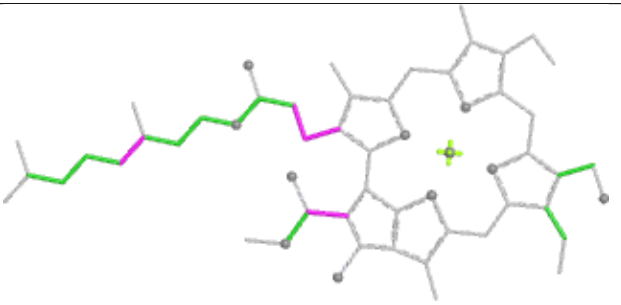
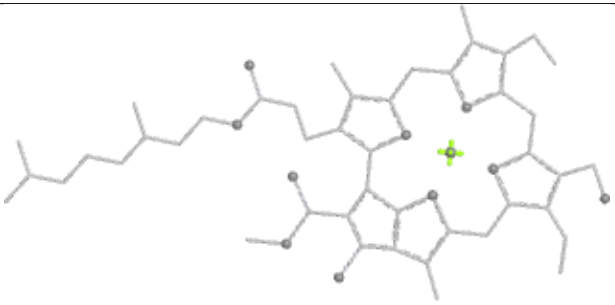
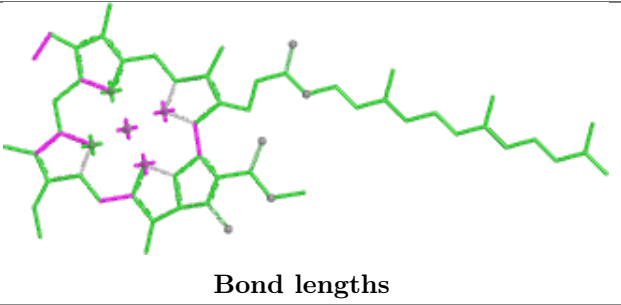
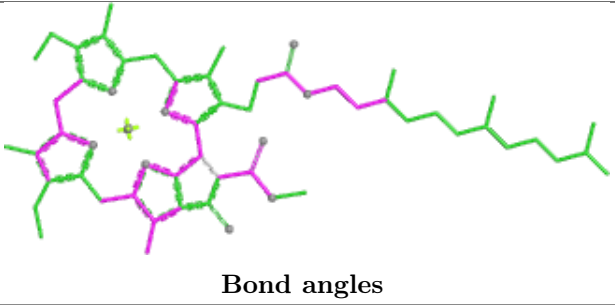
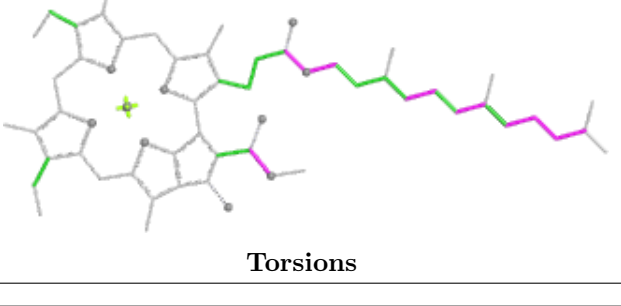
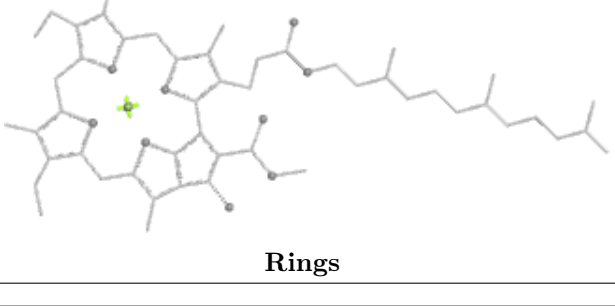
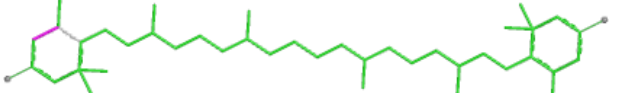
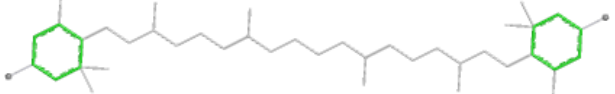
Ligand CLA A 828

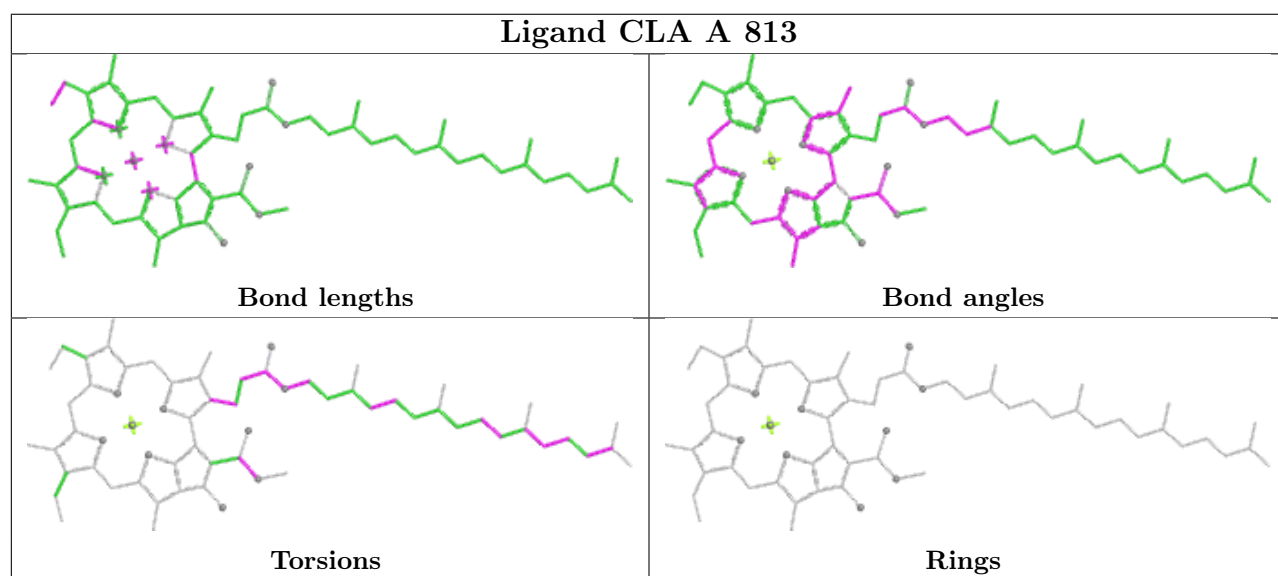
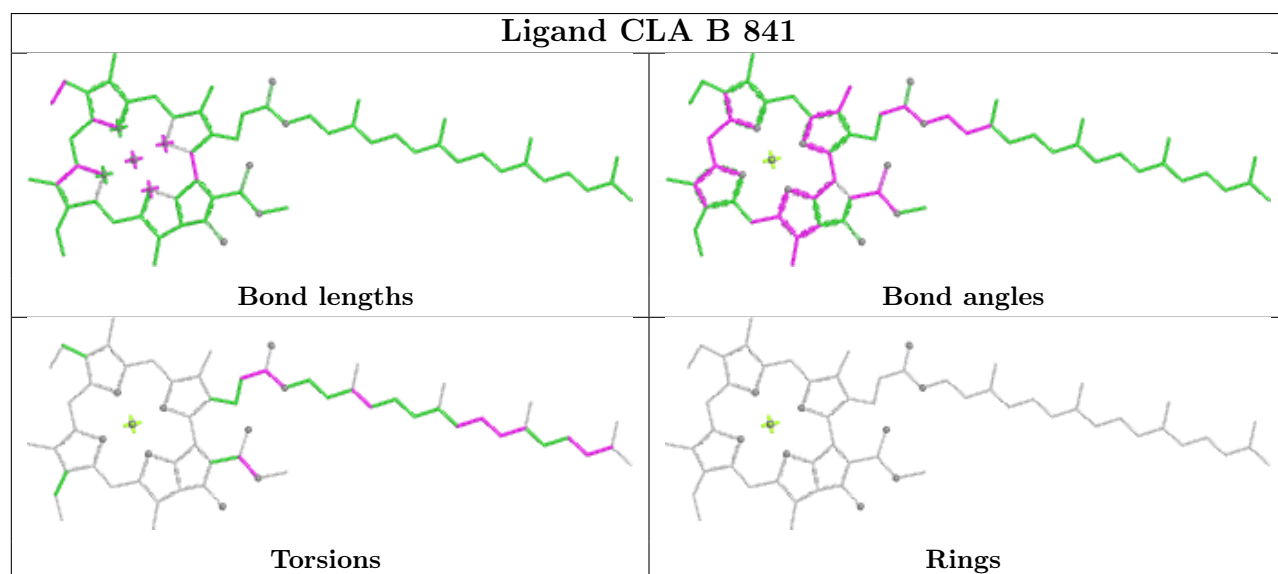
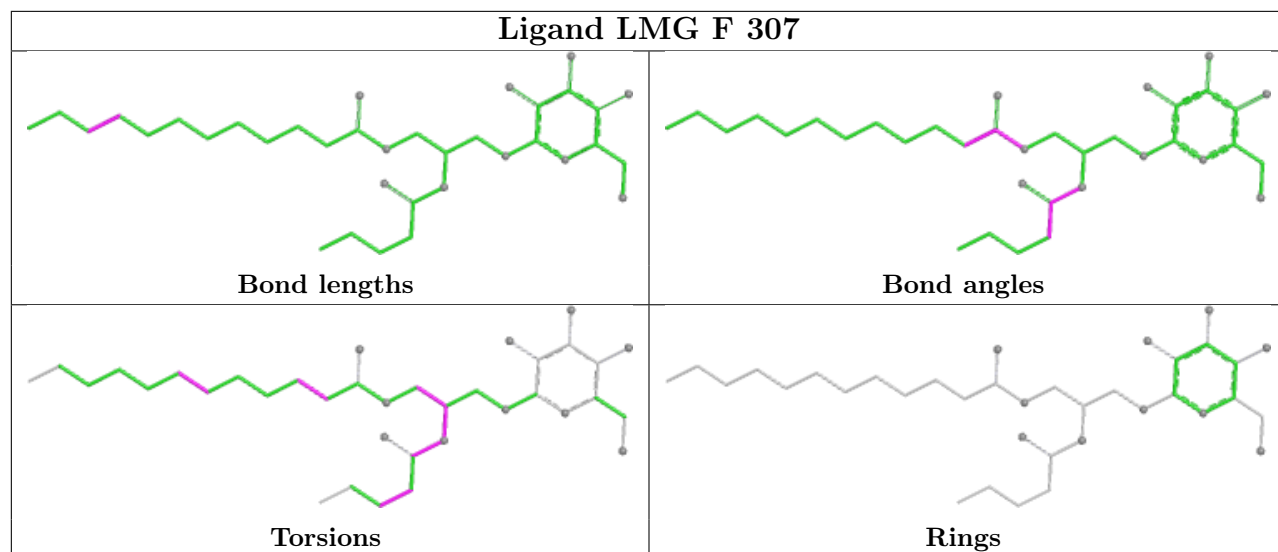


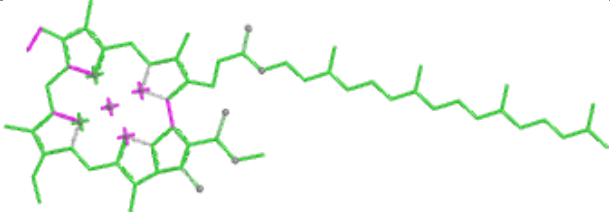
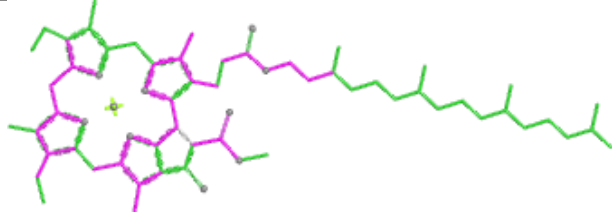
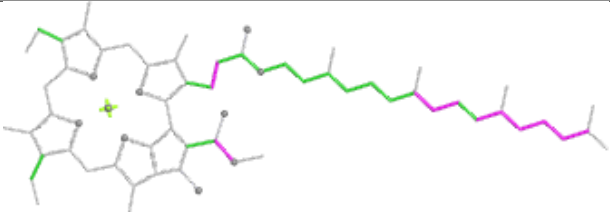
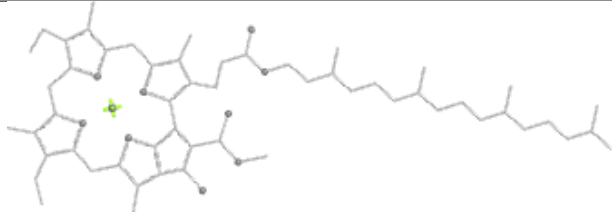
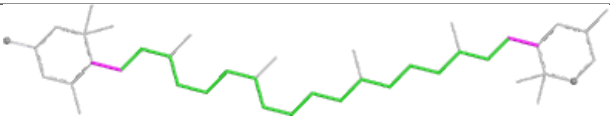
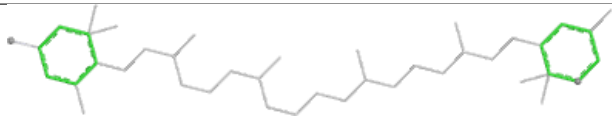
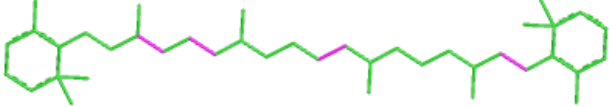
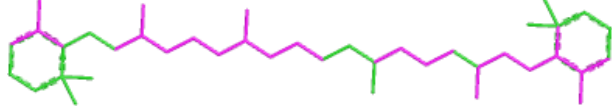
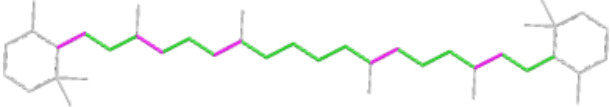
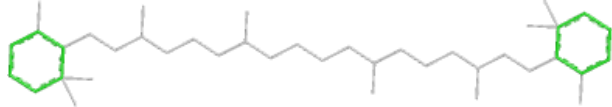
Ligand BCR B 847

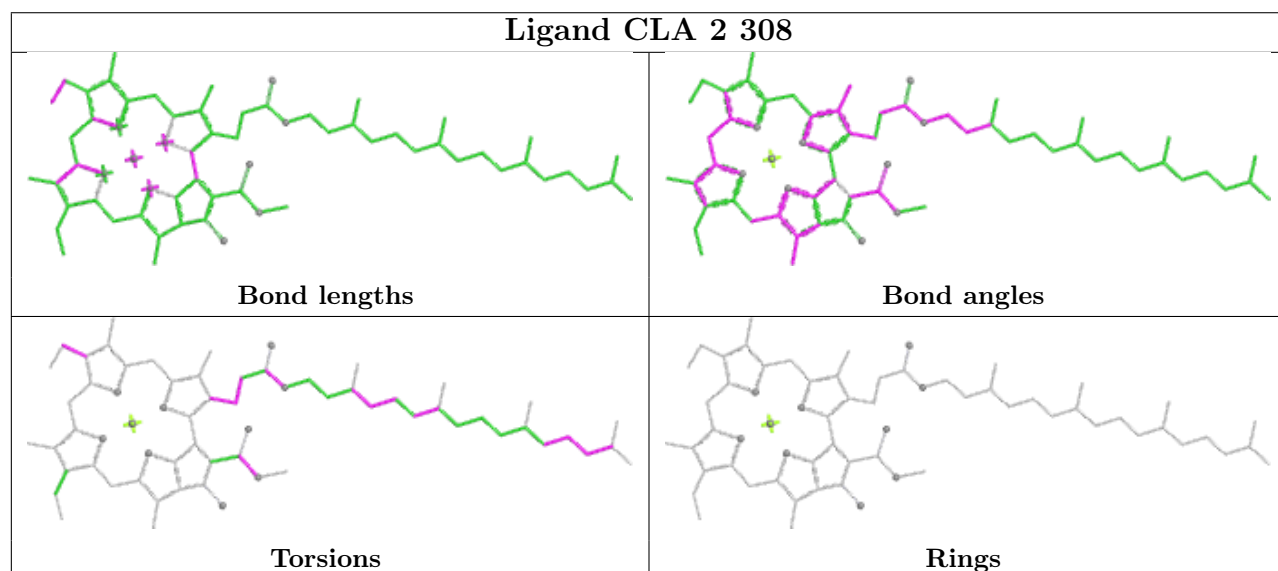
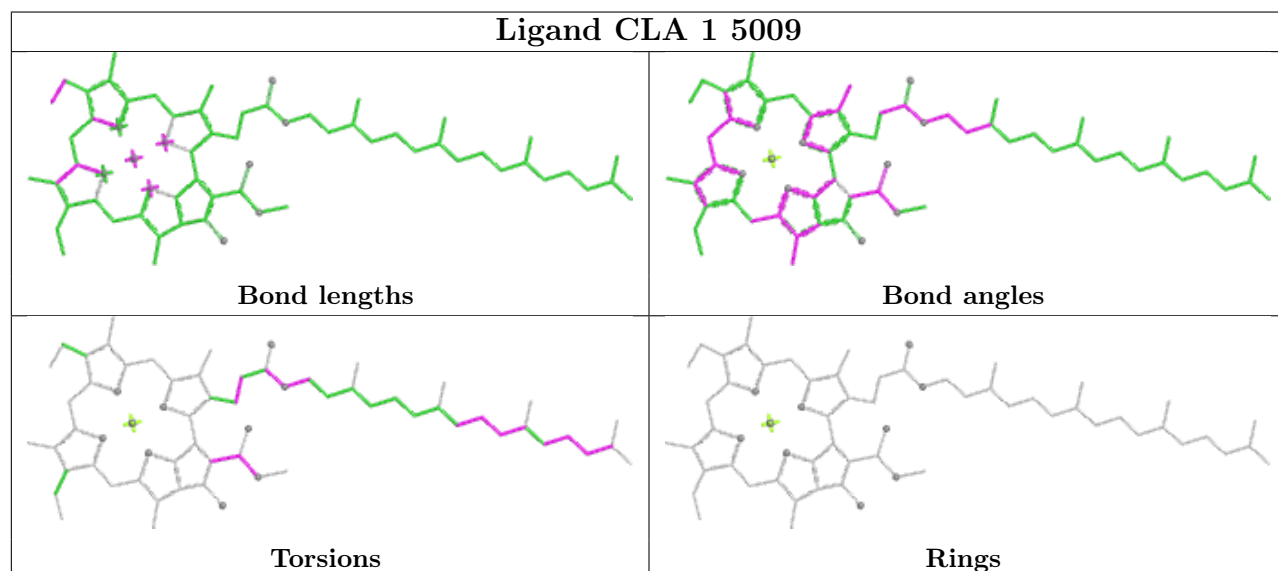
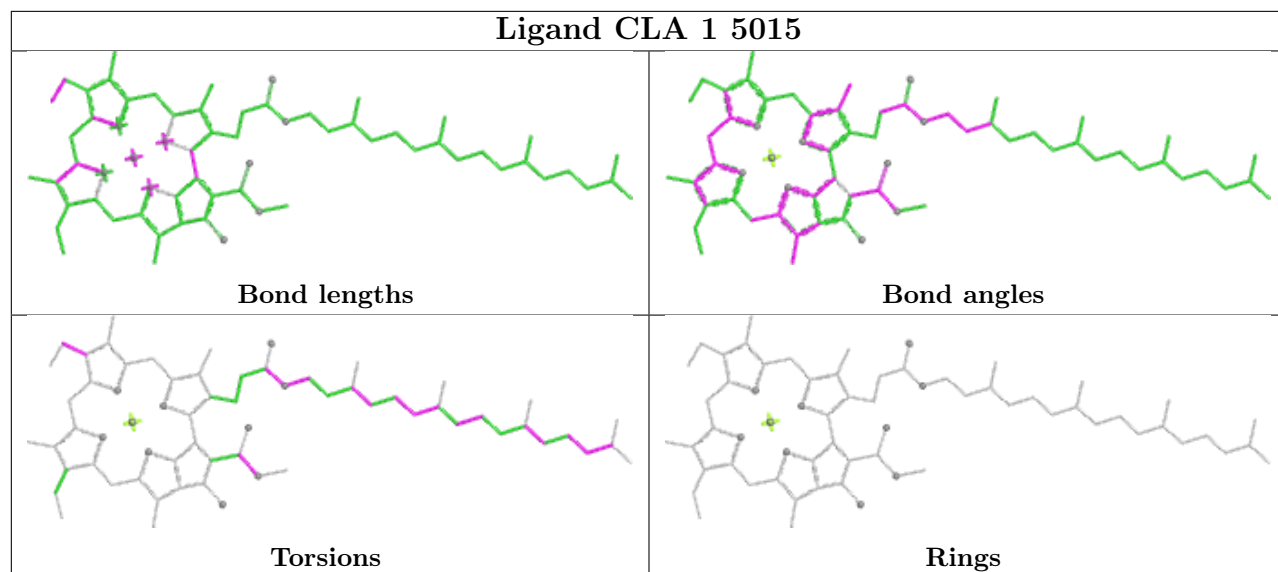


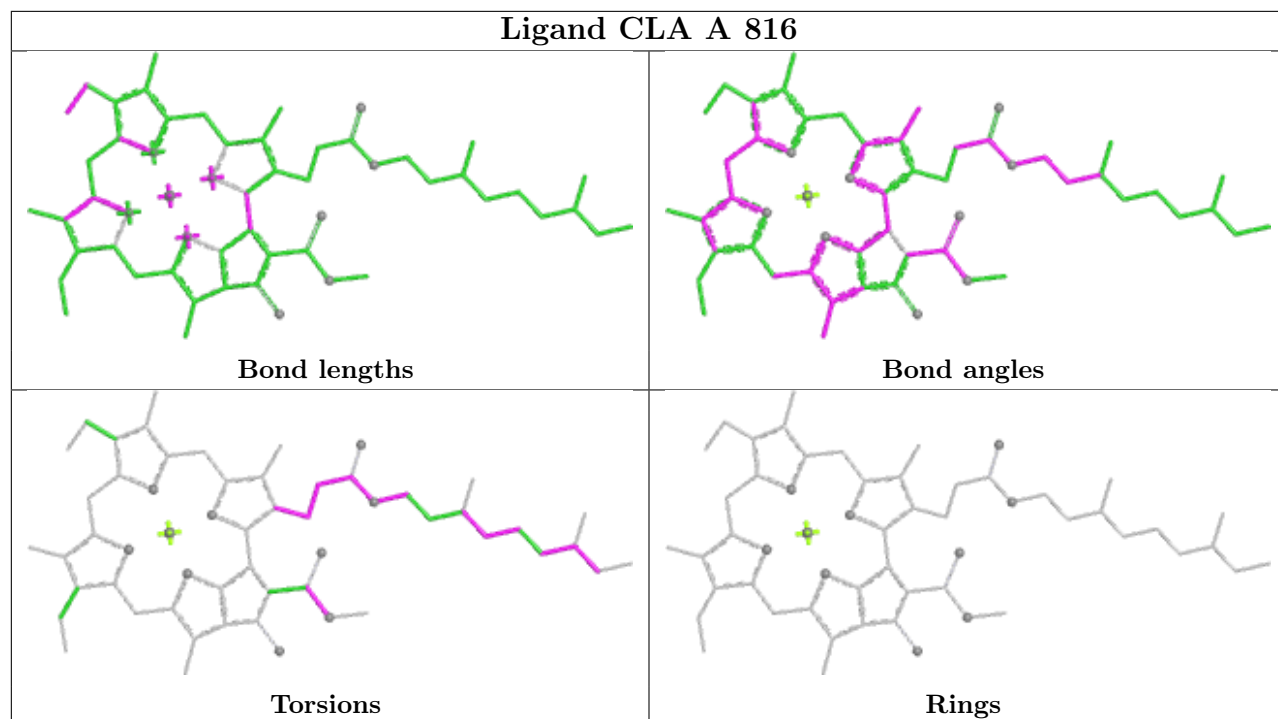


Ligand CHL 2 319	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 834	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT 4 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

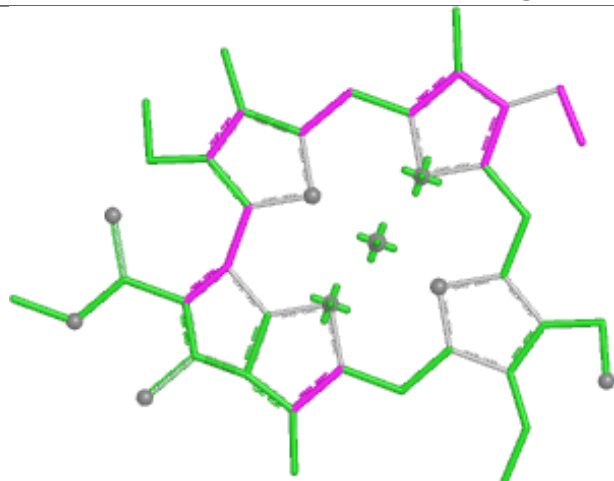


Ligand CLA B 804	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand ZEX F 310	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 844	
 Bond lengths	 Bond angles
 Torsions	 Rings

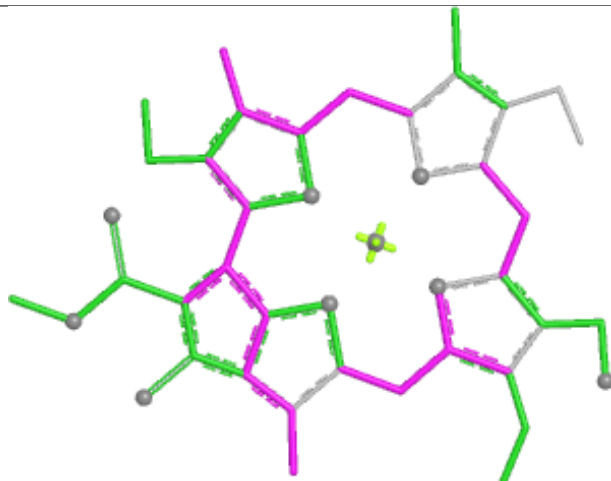




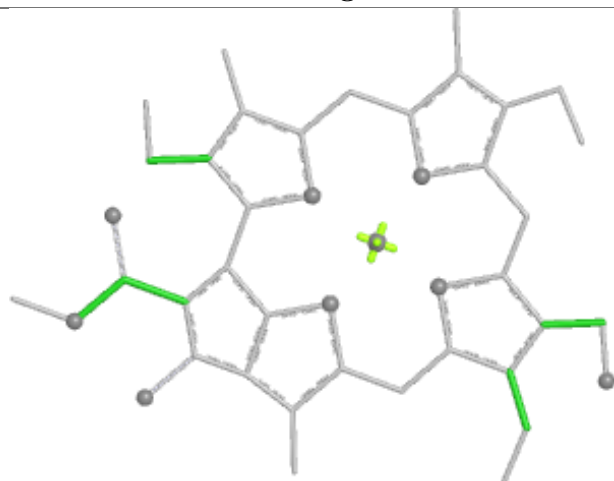
Ligand CHL 4 317



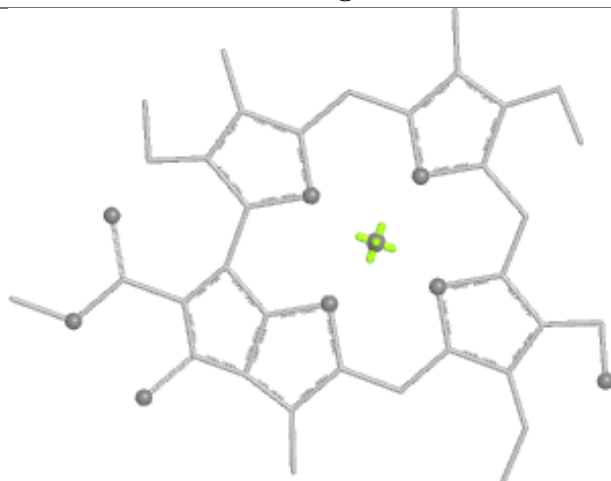
Bond lengths



Bond angles

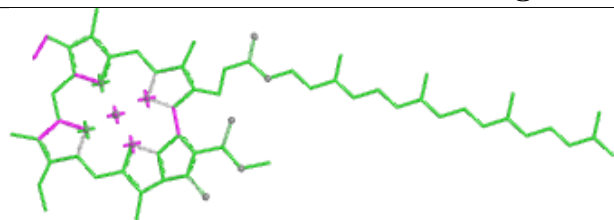


Torsions

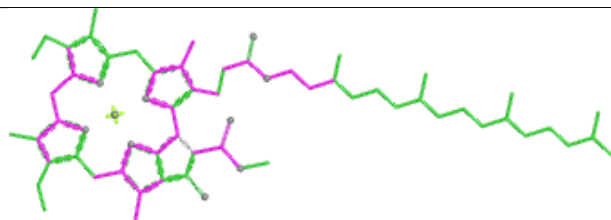


Rings

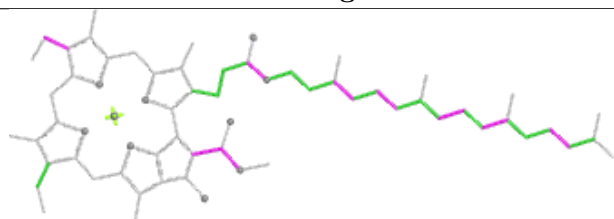
Ligand CLA B 831



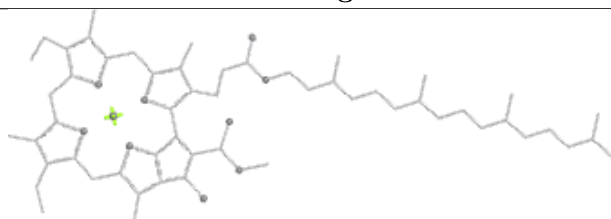
Bond lengths



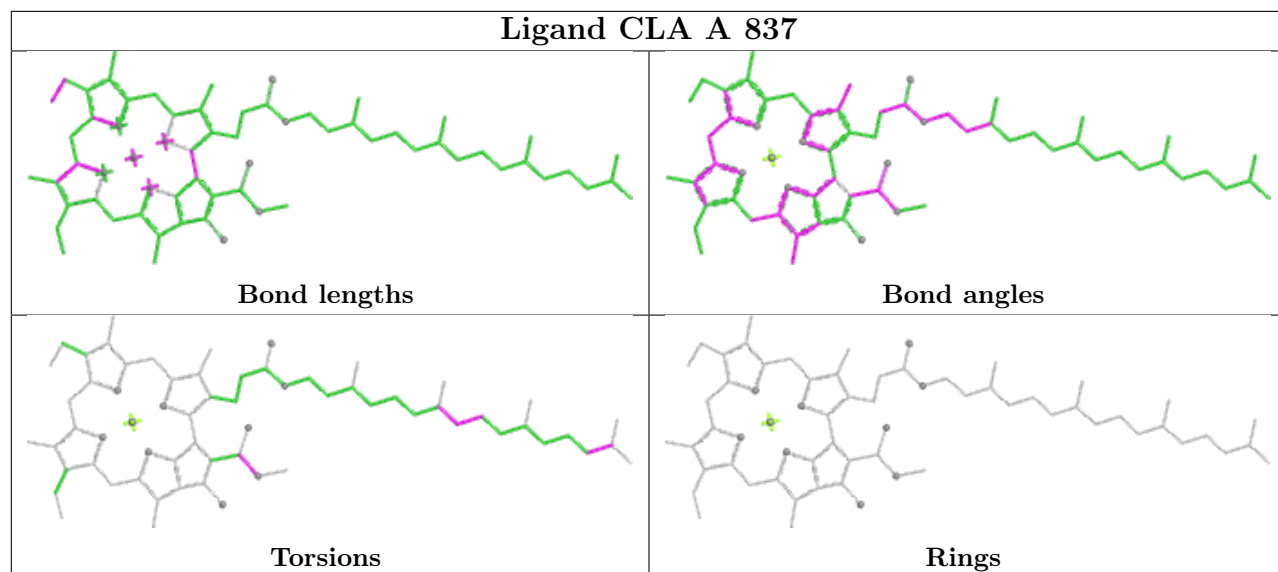
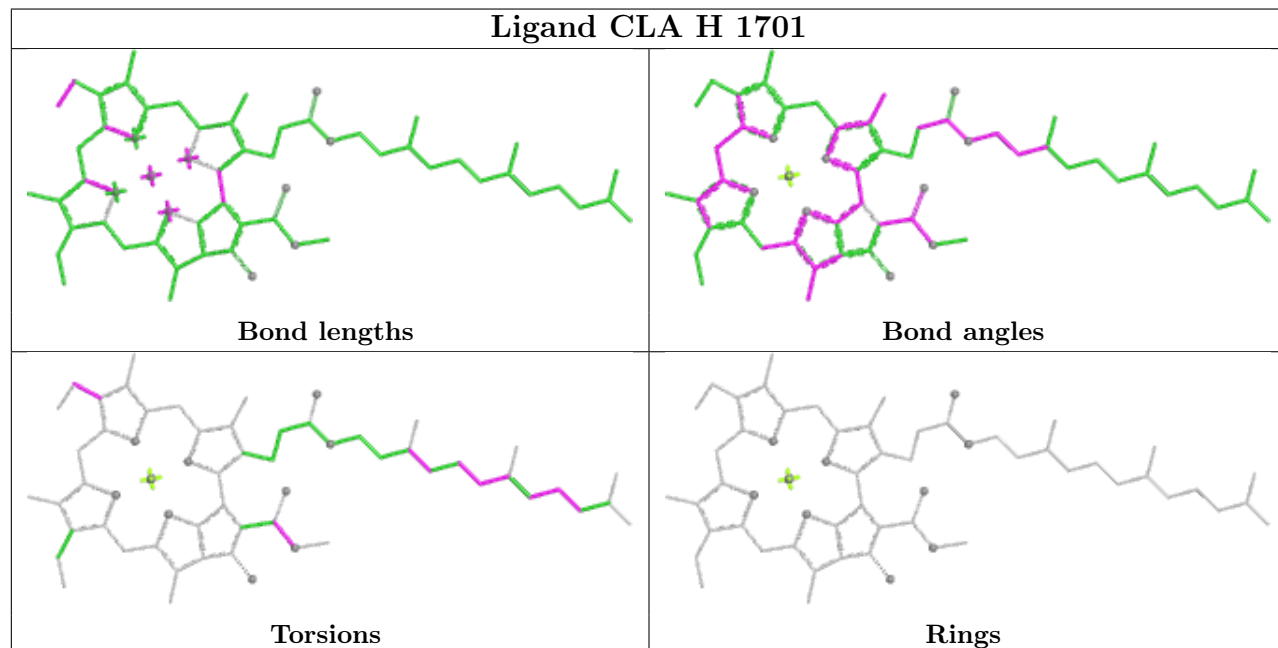
Bond angles



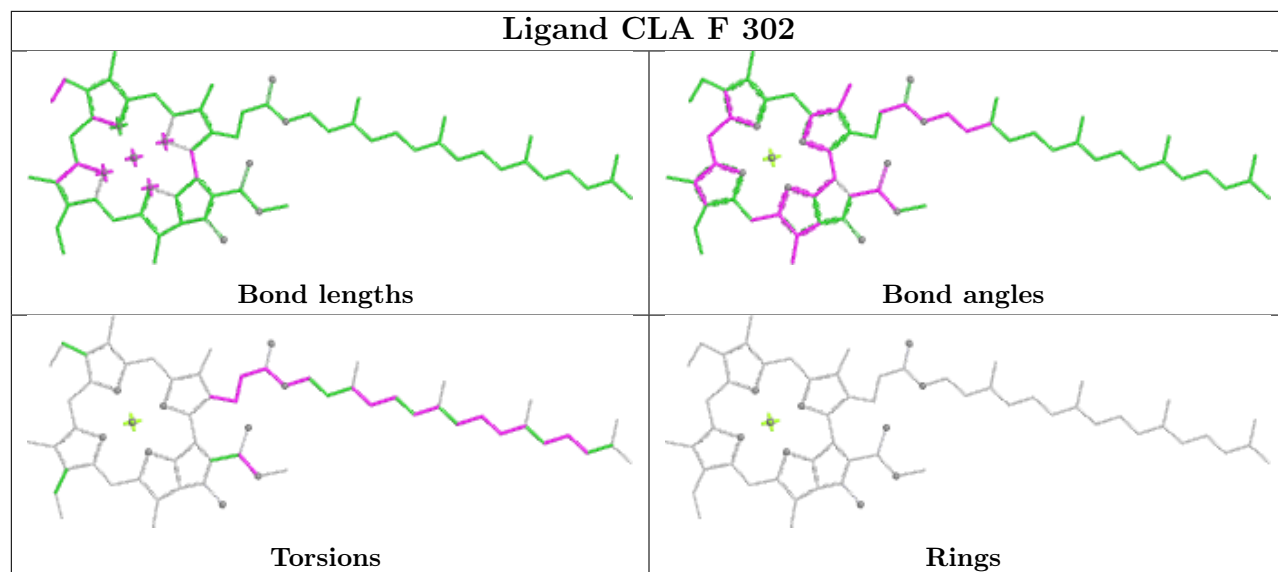
Torsions



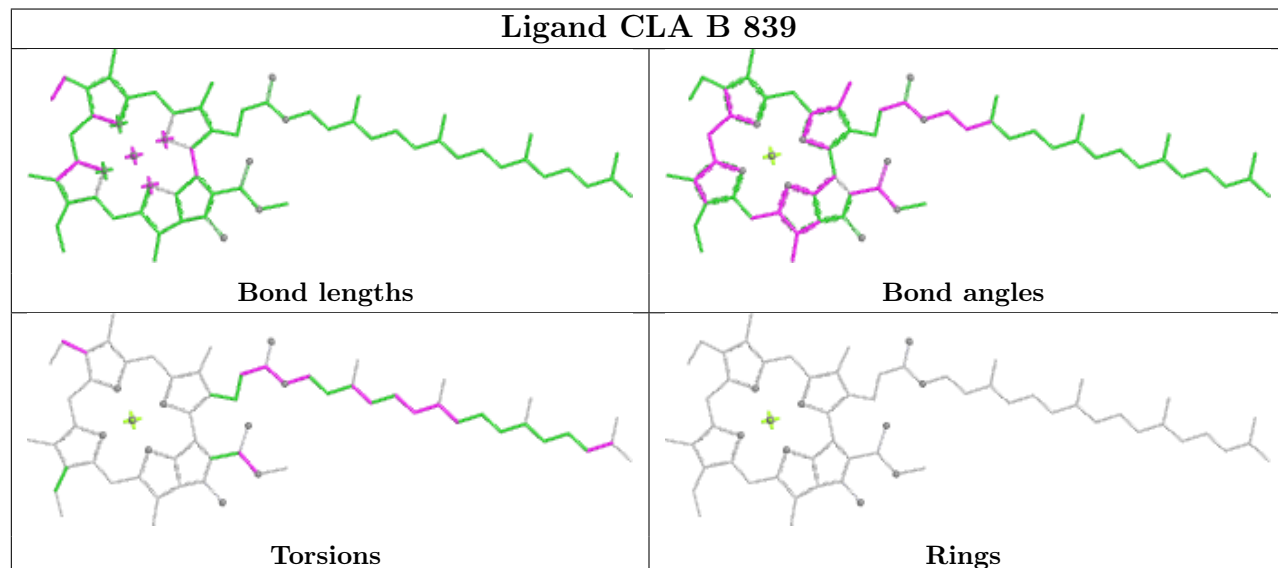
Rings

Ligand CLA A 837**Ligand CLA H 1701**

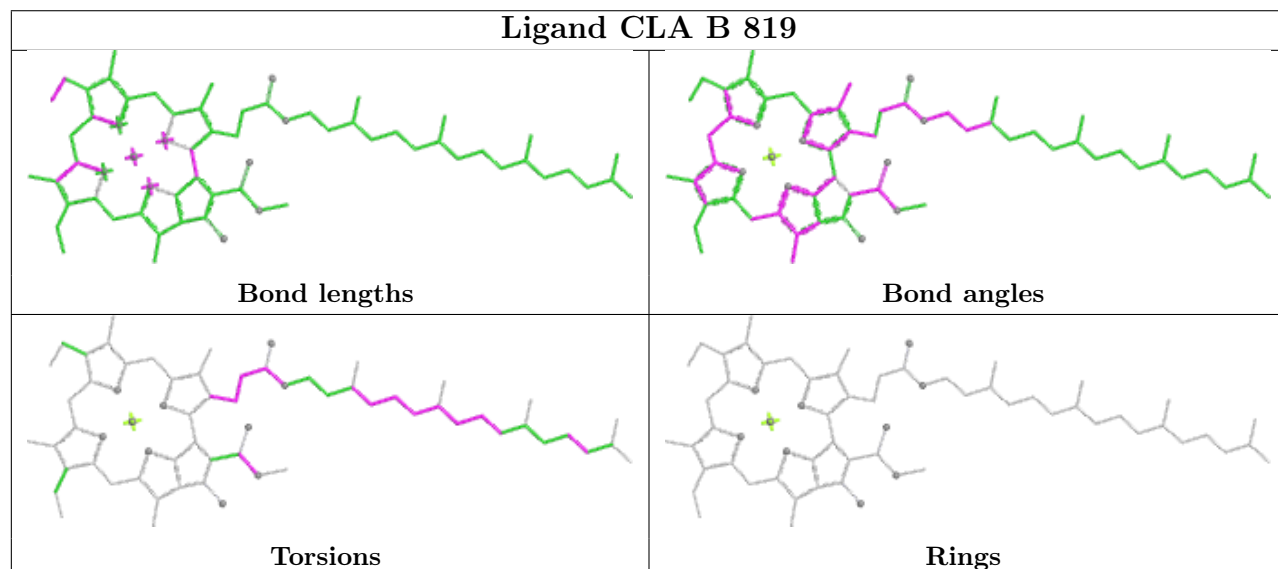
Ligand CLA F 302



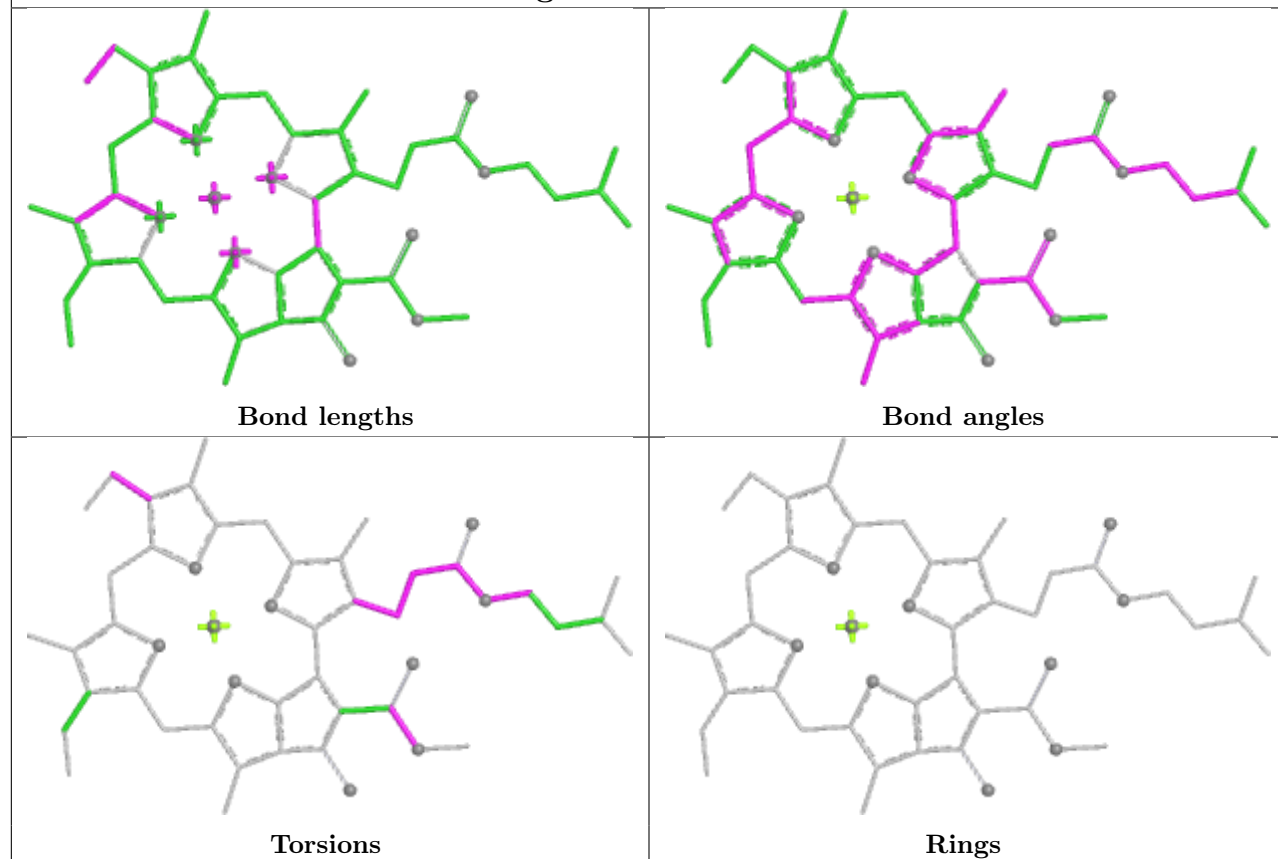
Ligand CLA B 839



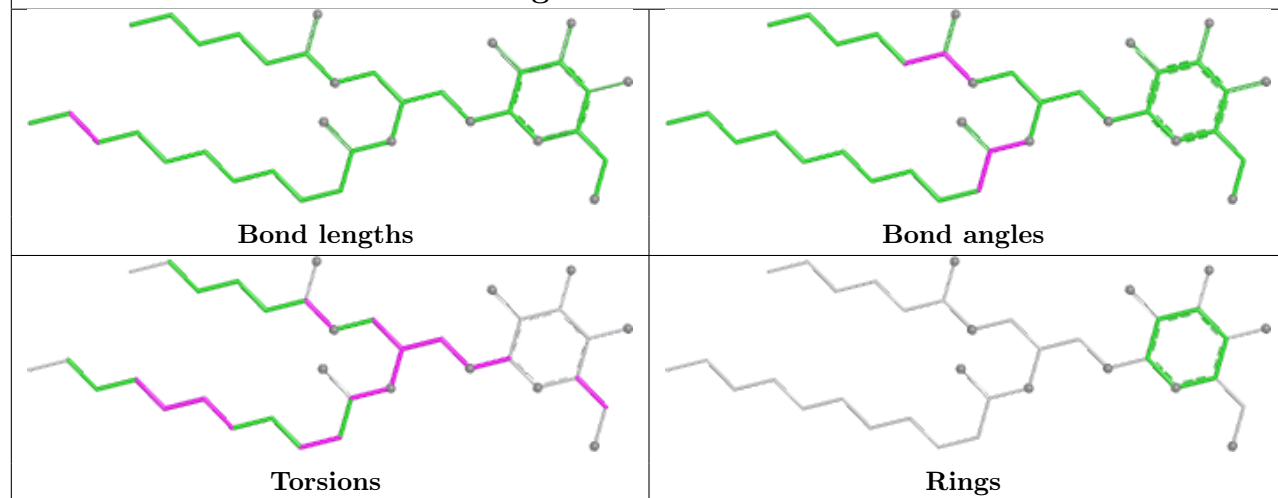
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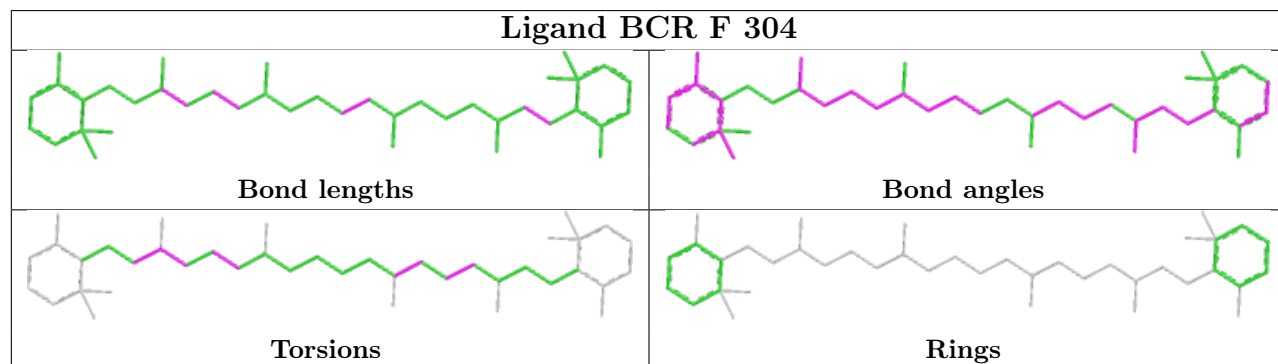
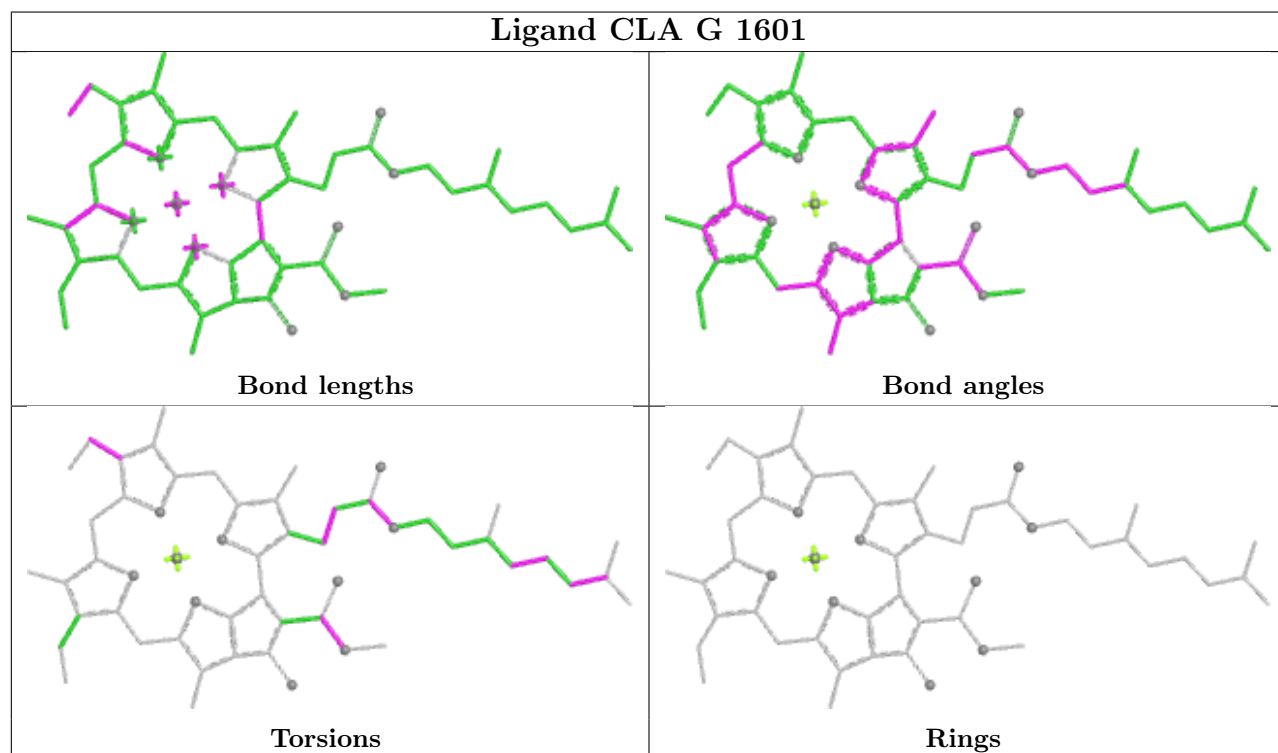
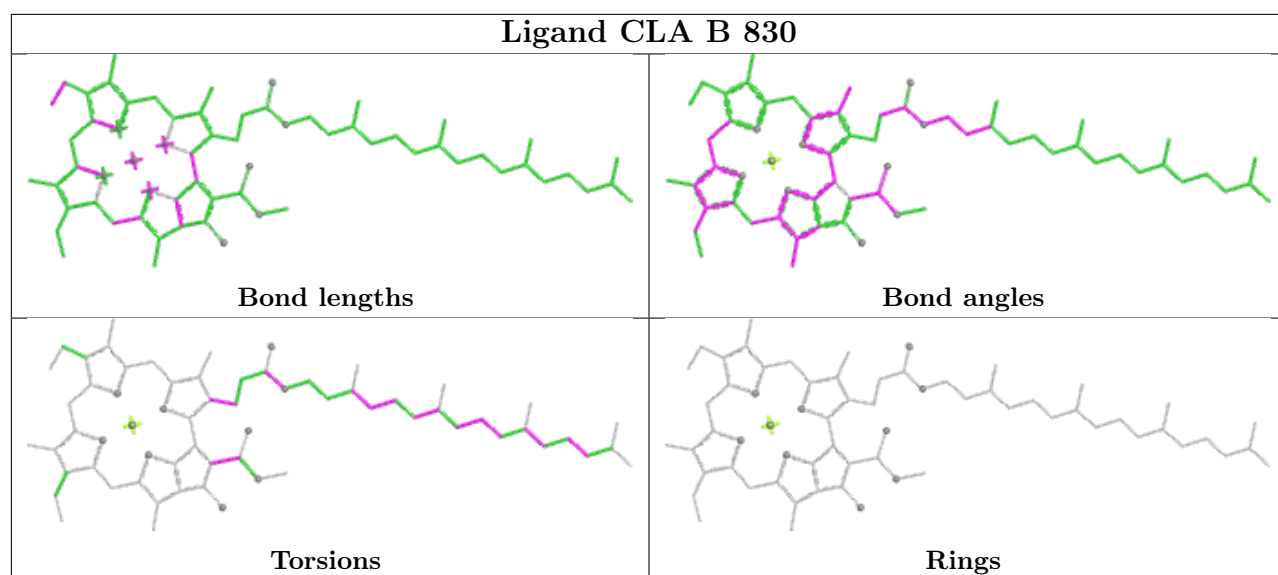


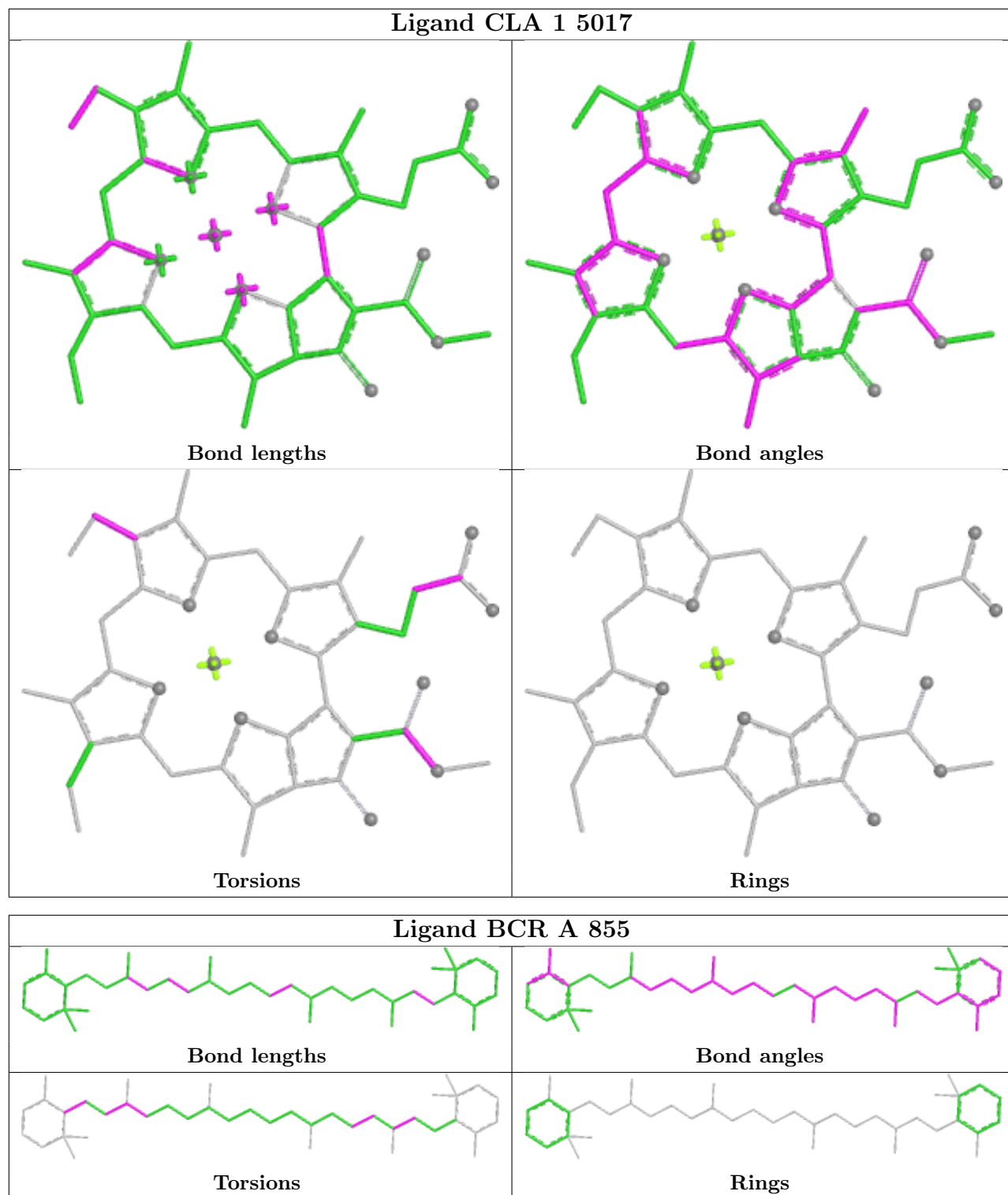
Ligand CLA 2 313



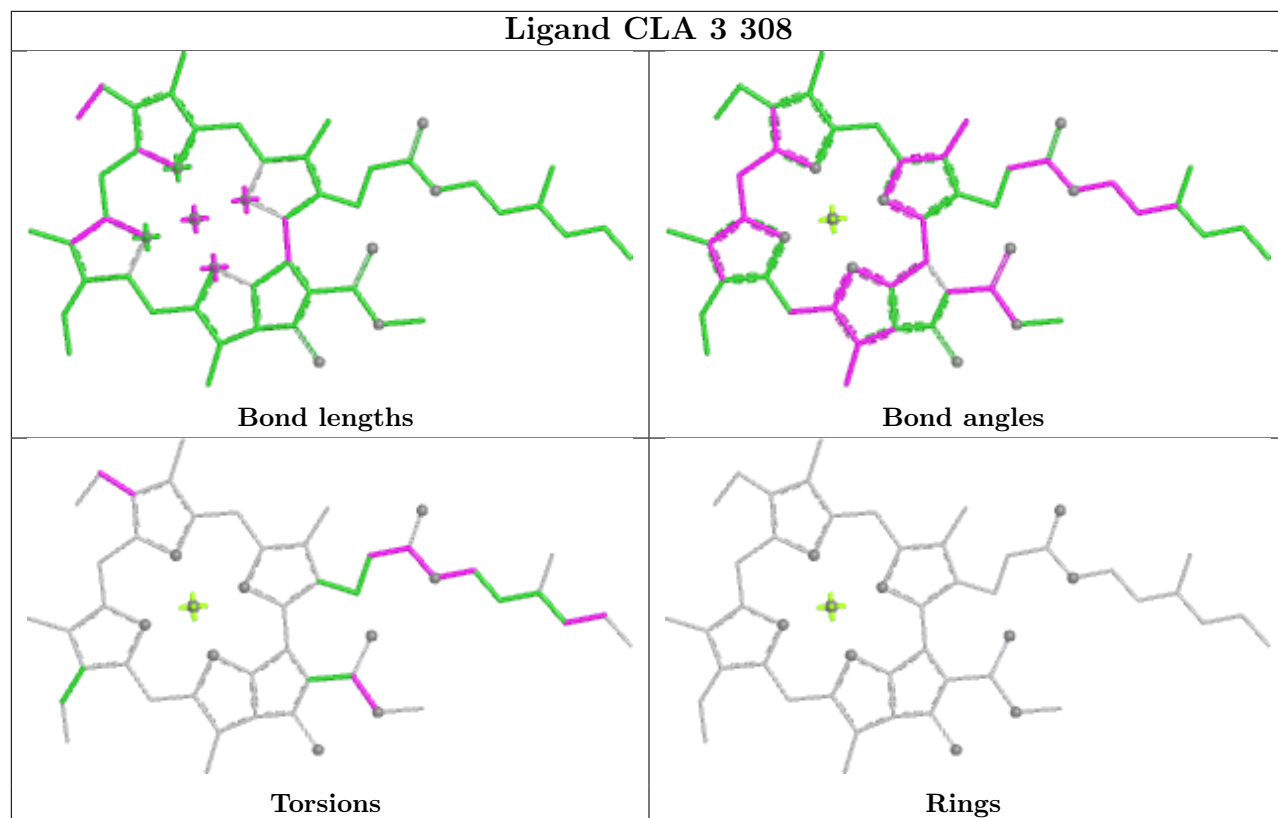
Ligand LMG 2 322



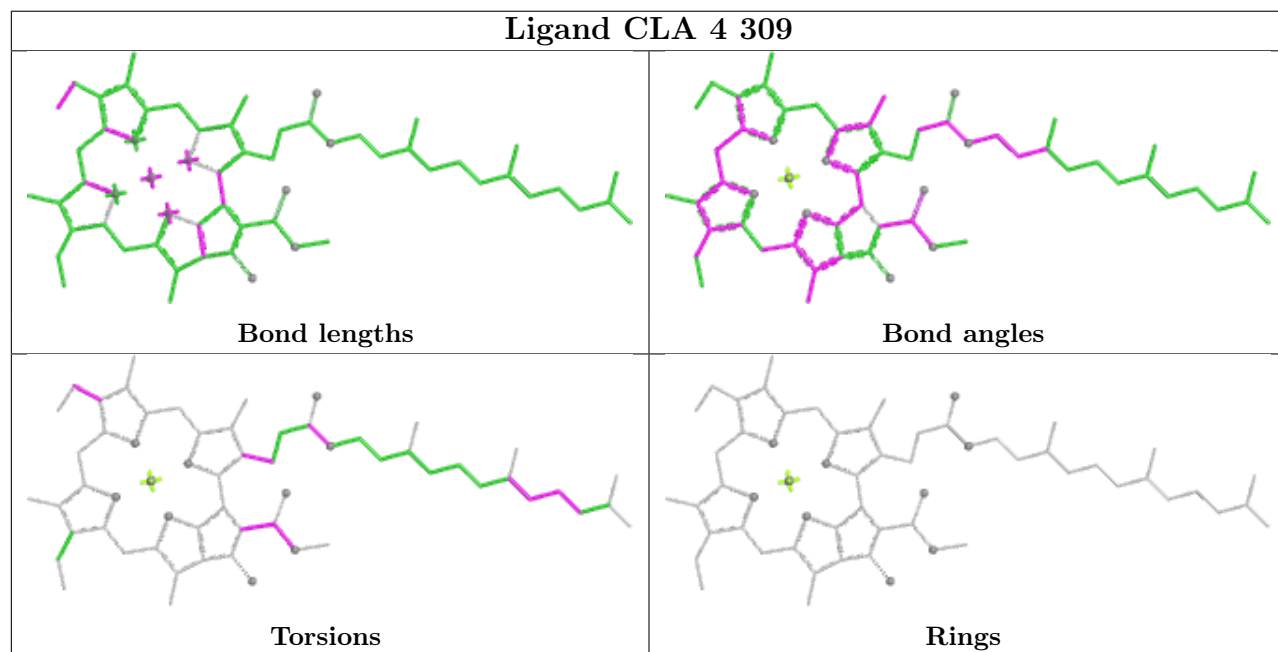




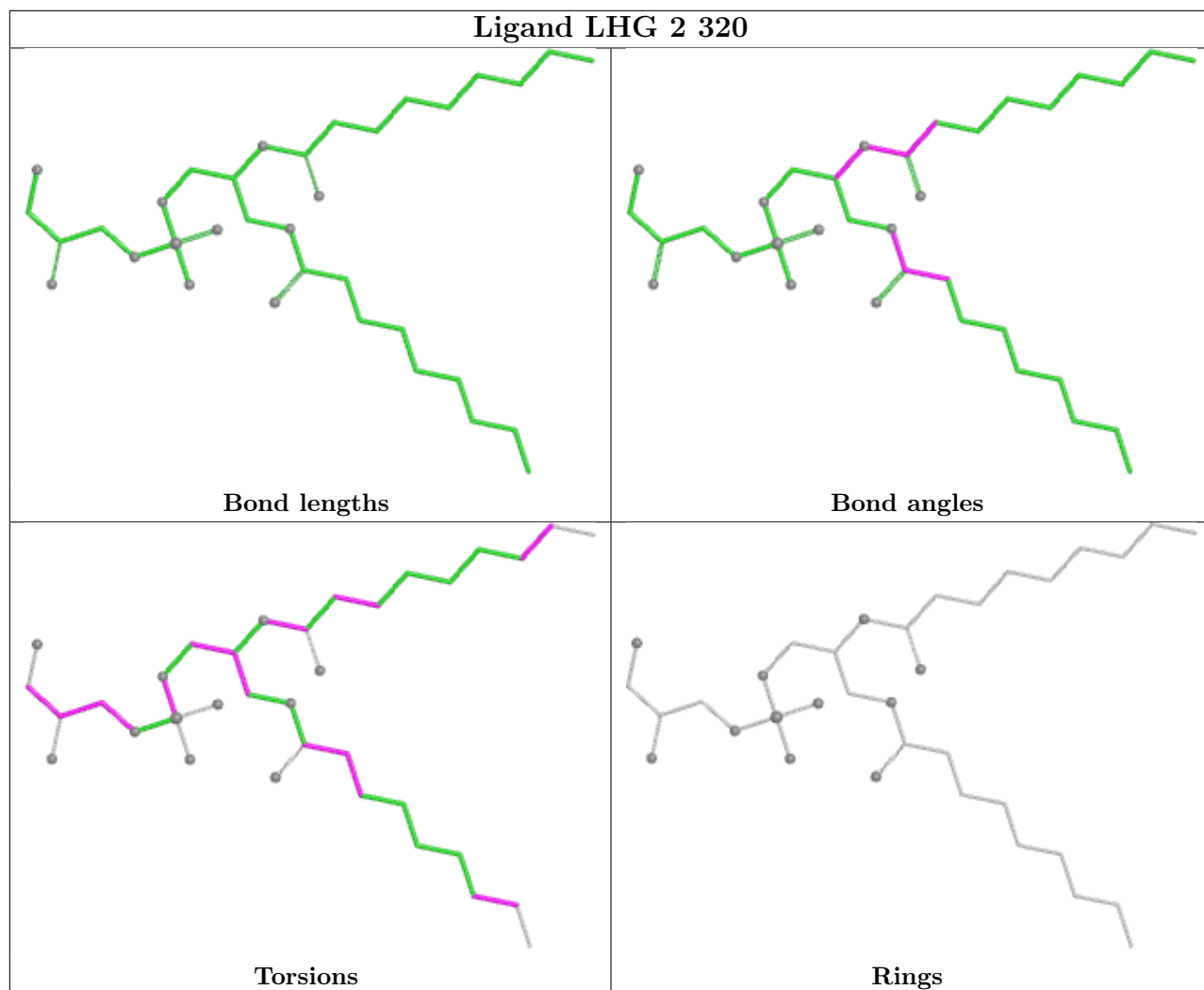
Ligand CLA 3 308



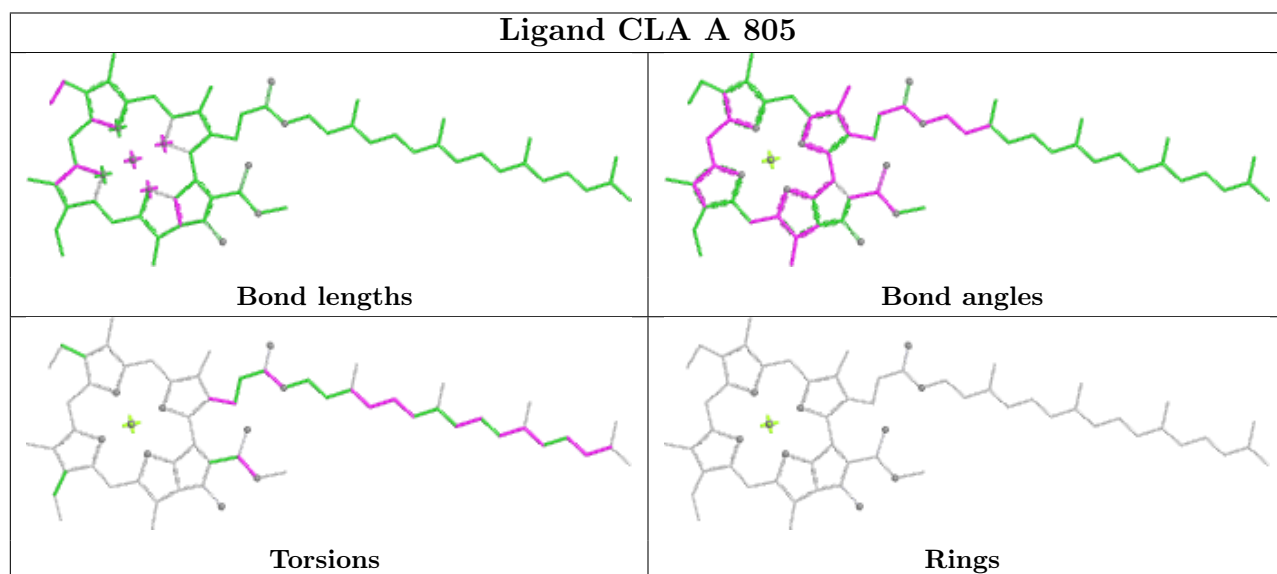
Ligand CLA 4 309

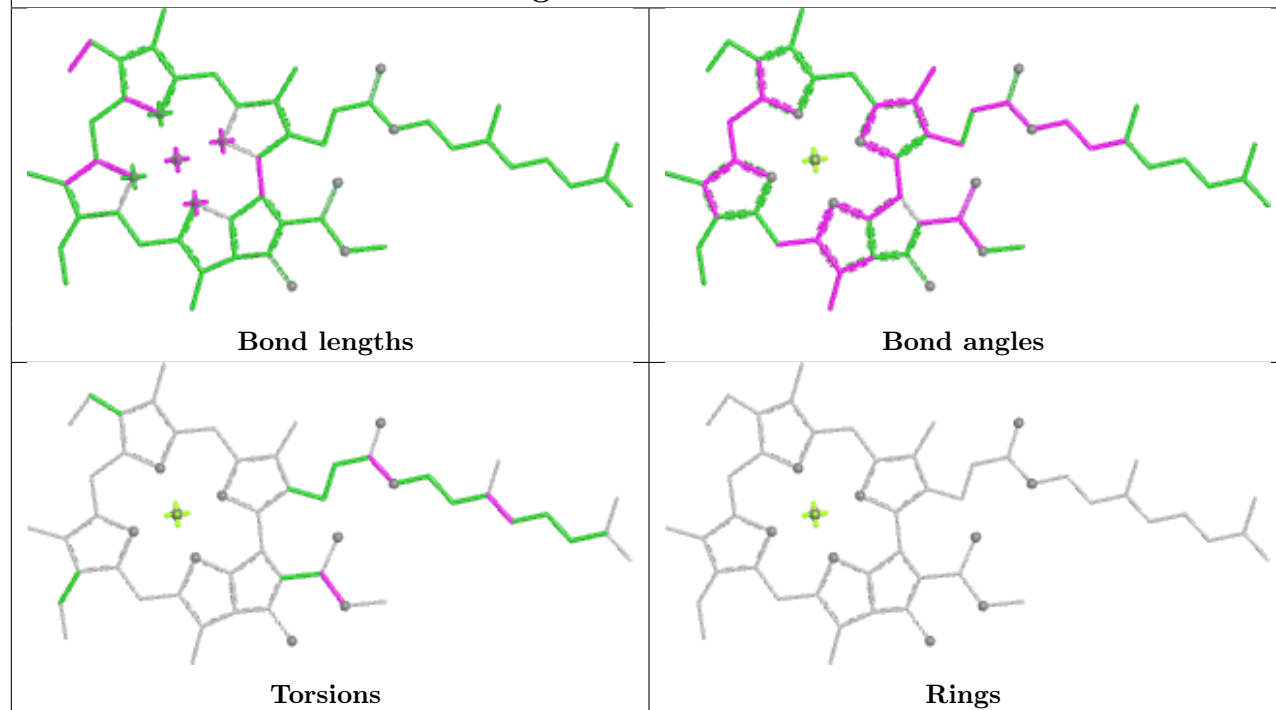
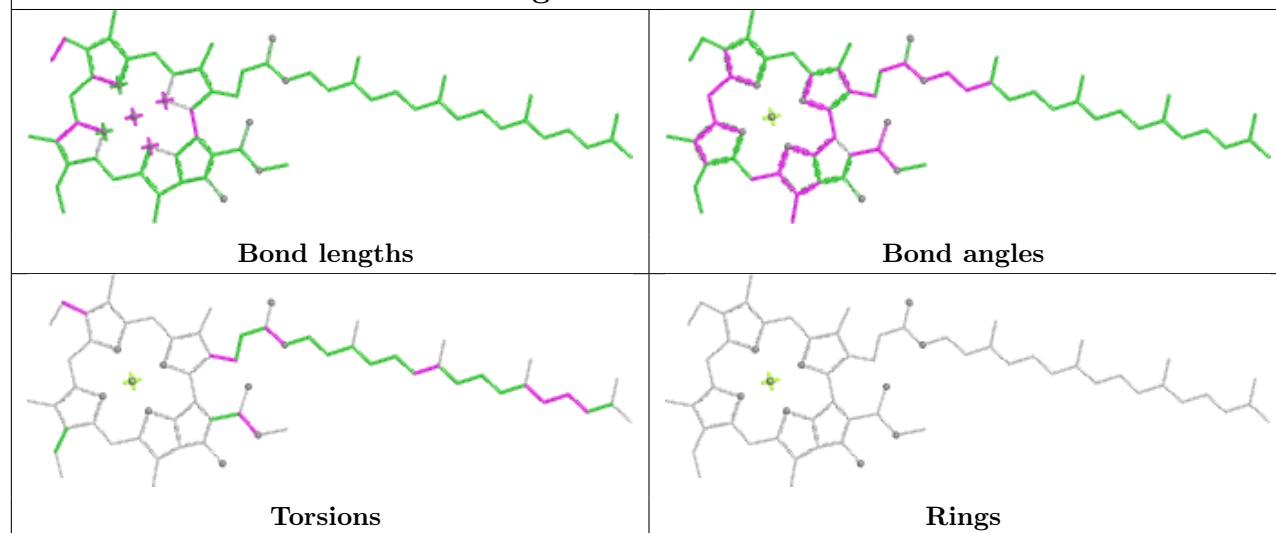


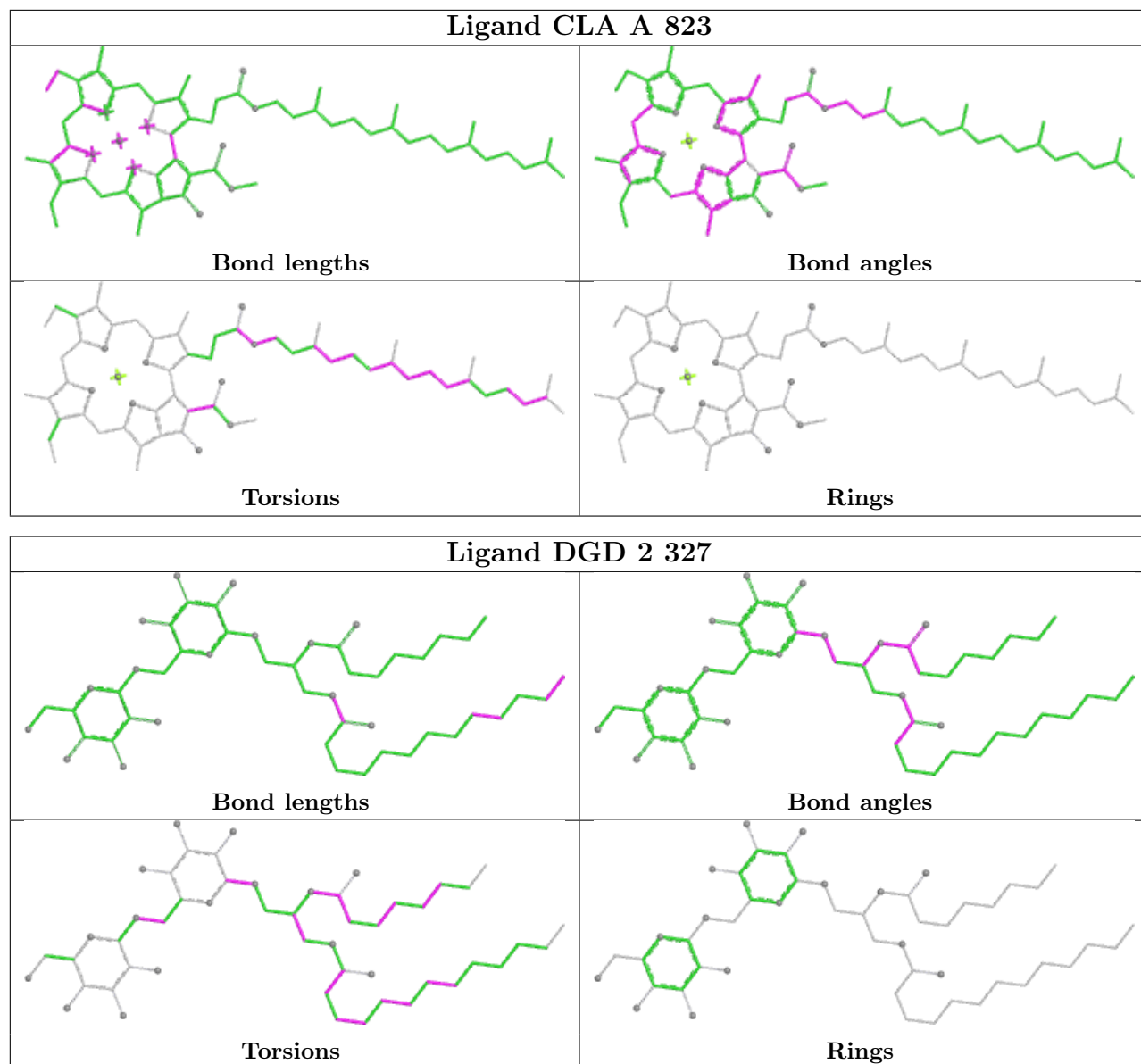
Ligand LHG 2 320



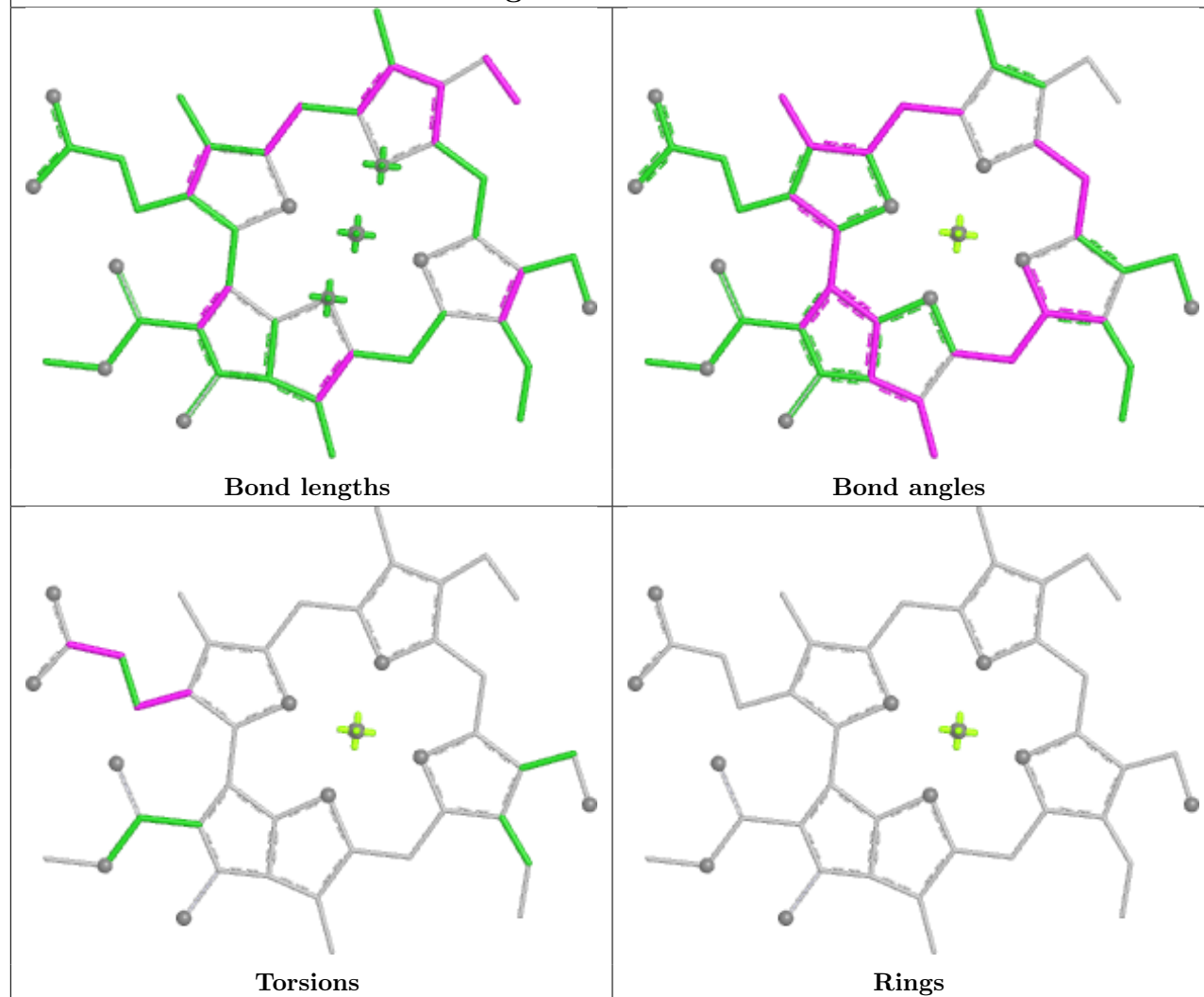
Ligand CLA A 805



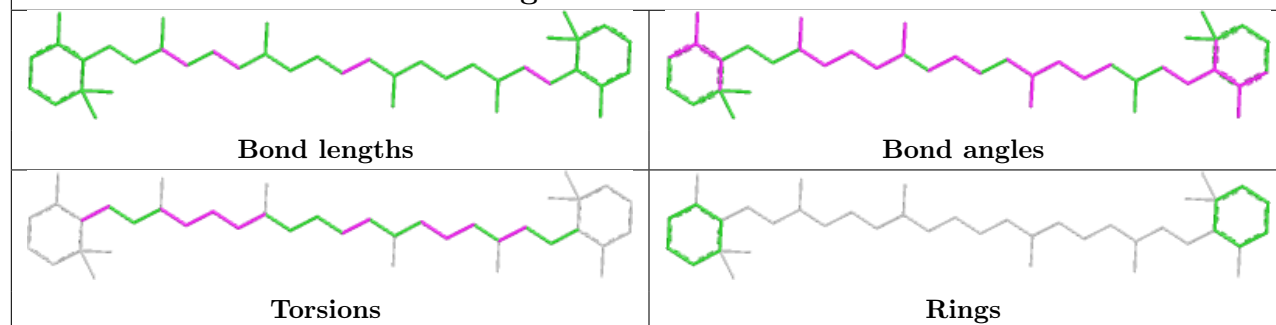
Ligand CLA B 816**Ligand CLA B 820**

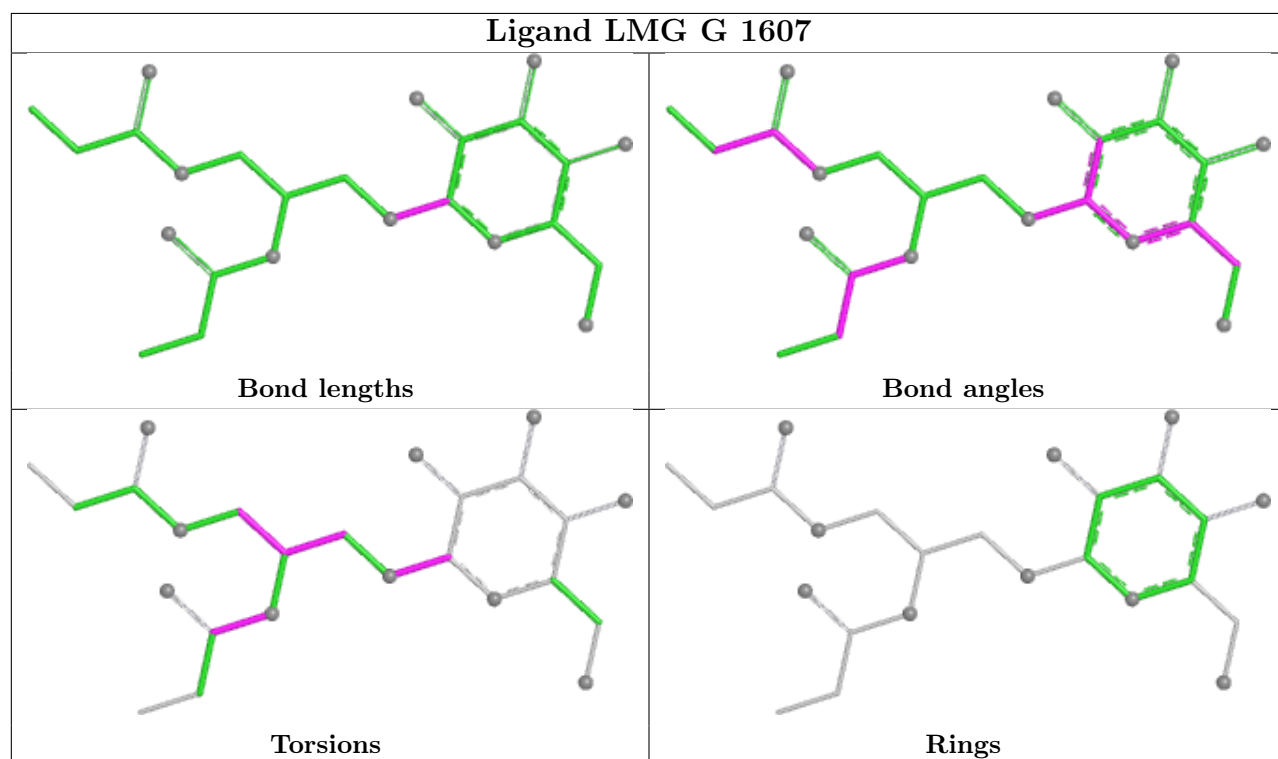
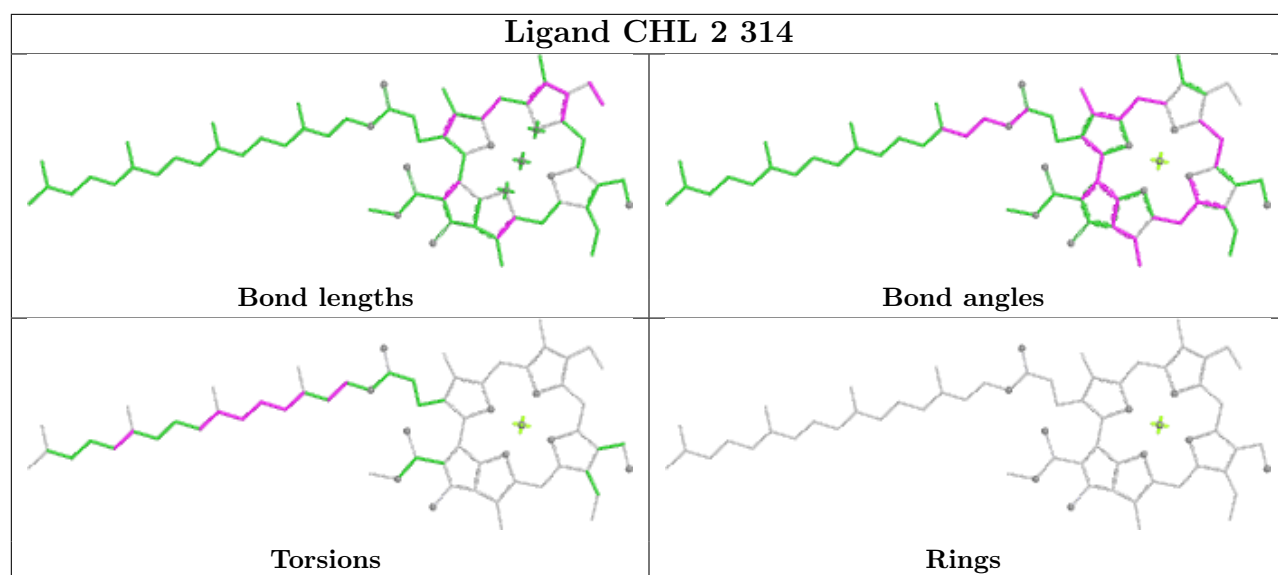


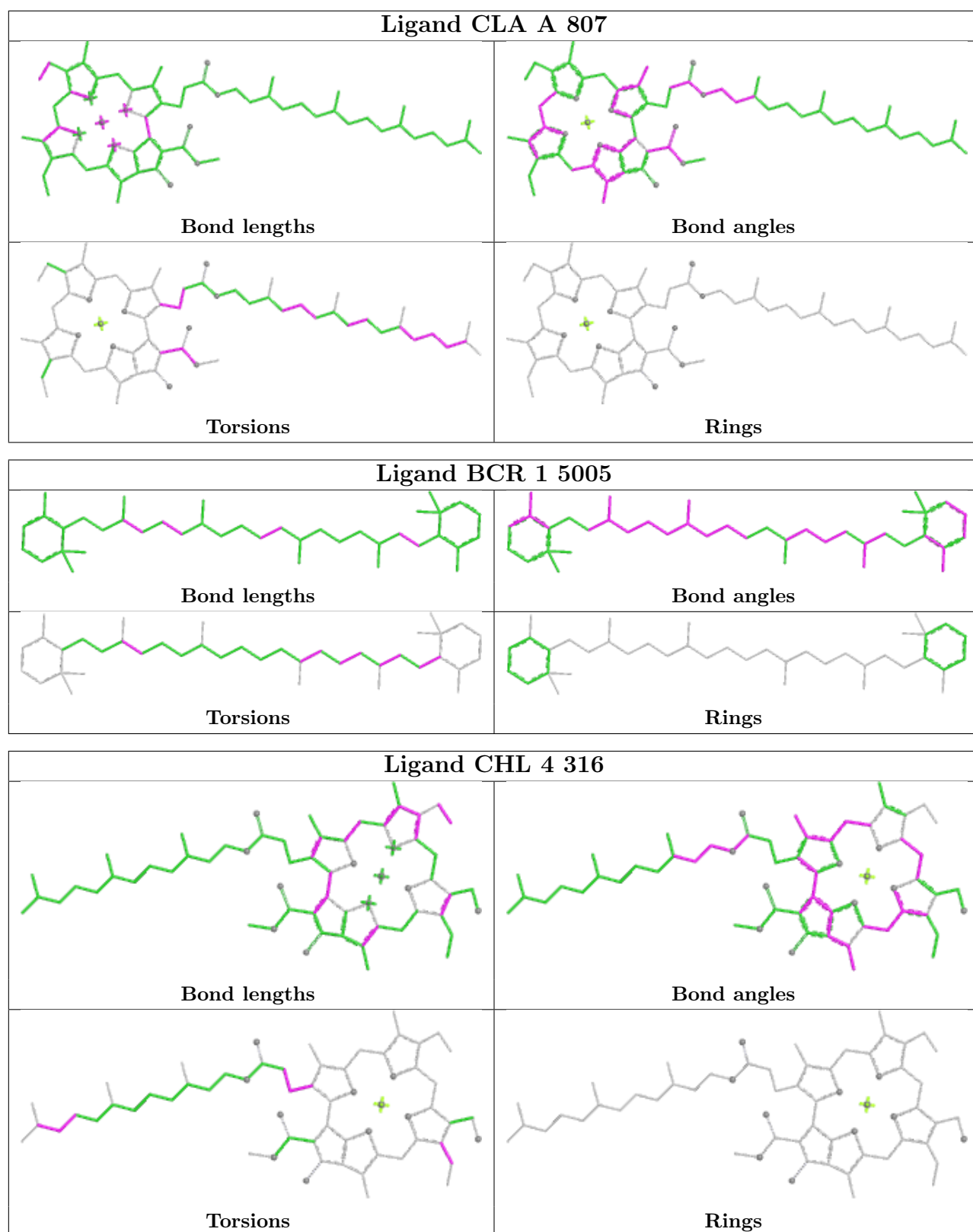
Ligand CHL 2 318

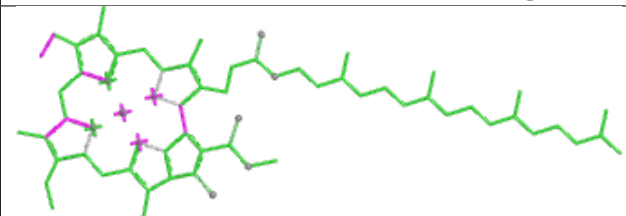
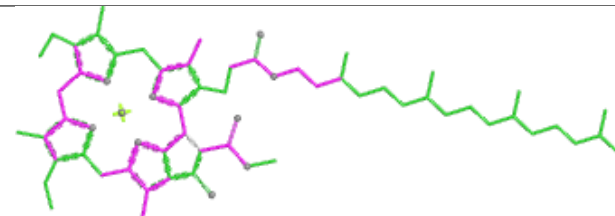
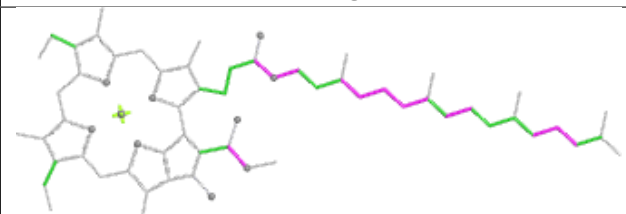
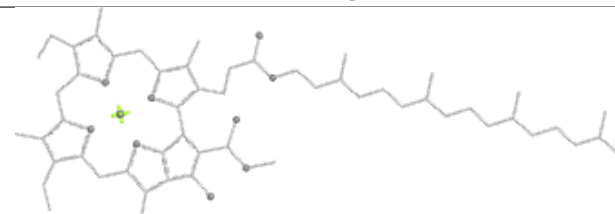


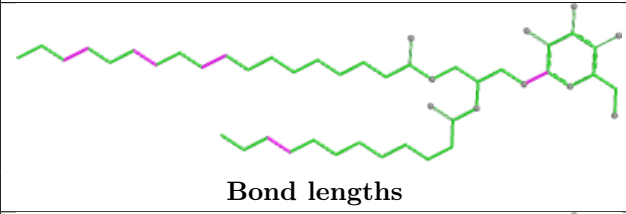
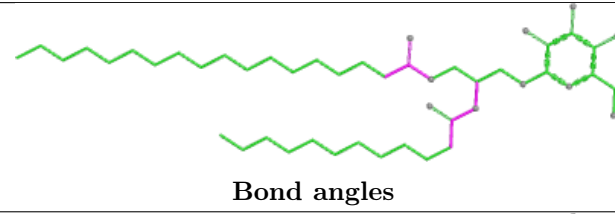
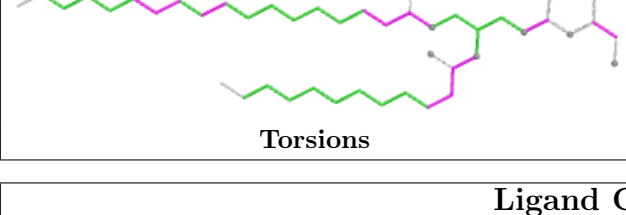
Ligand BCR K 1405

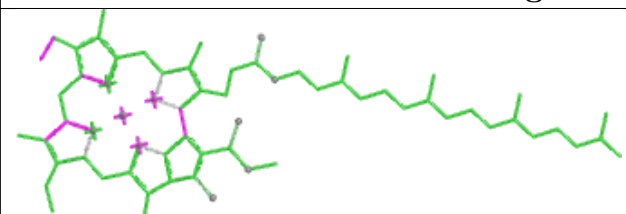
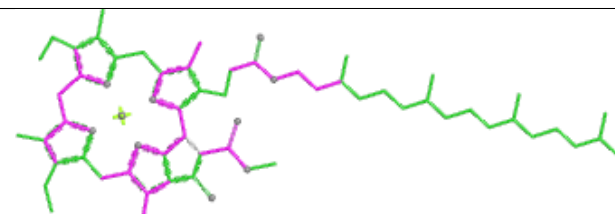
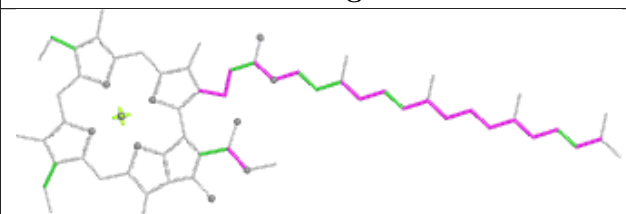
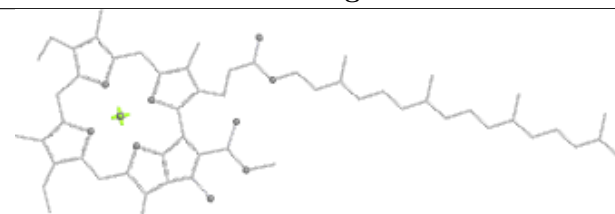




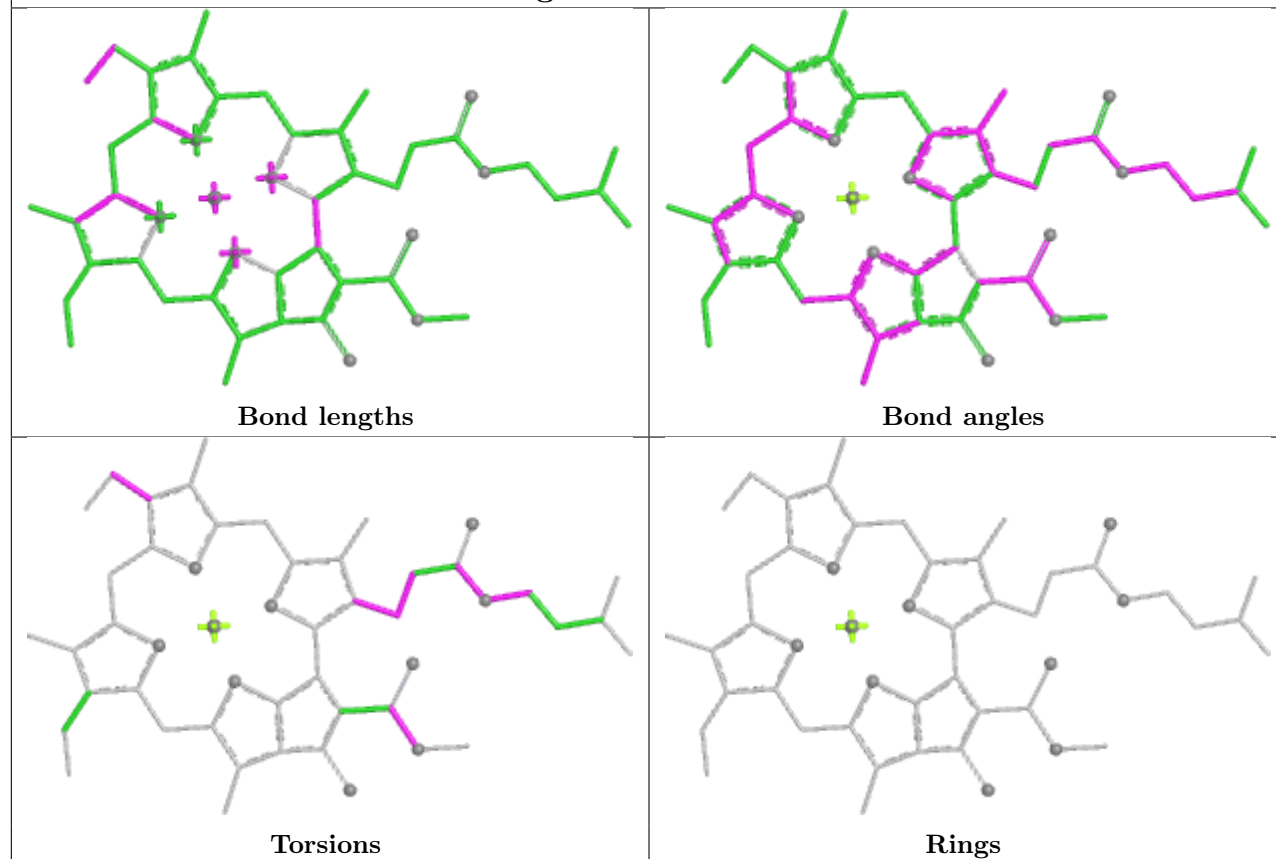


Ligand CLA B 822	
	
Bond lengths	Bond angles
	
Torsions	Rings

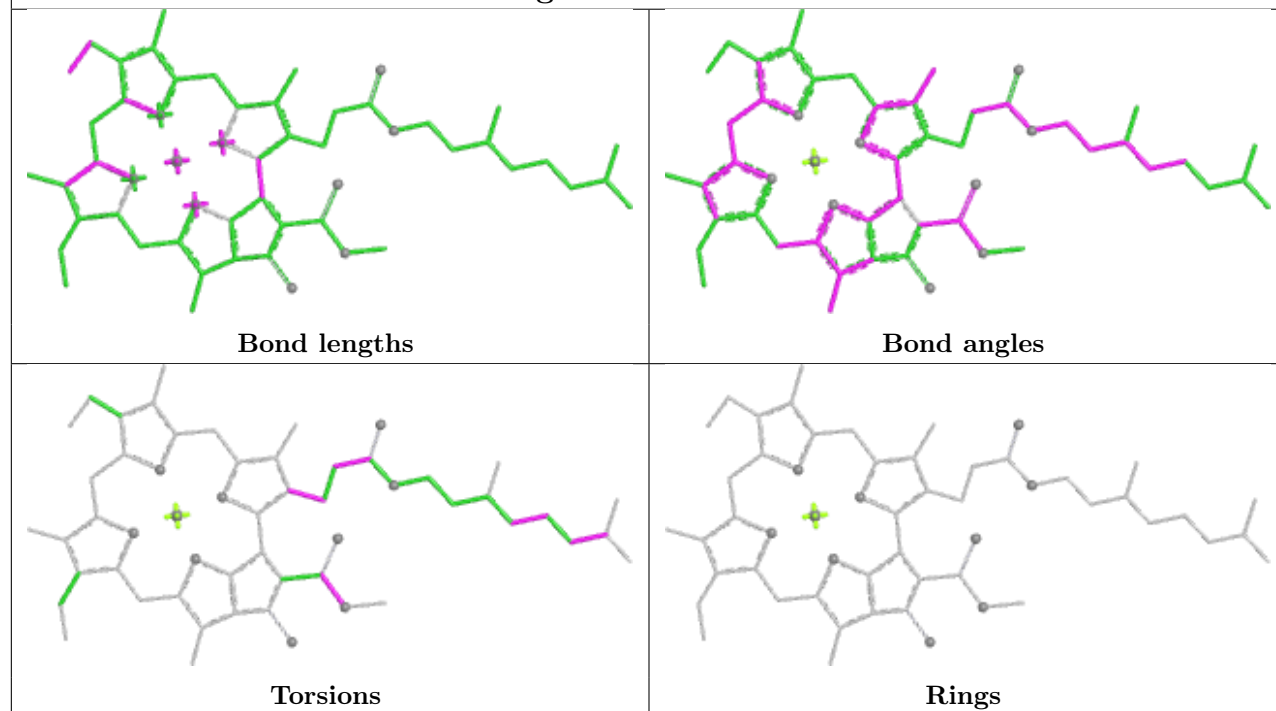
Ligand LMG 1 5001	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

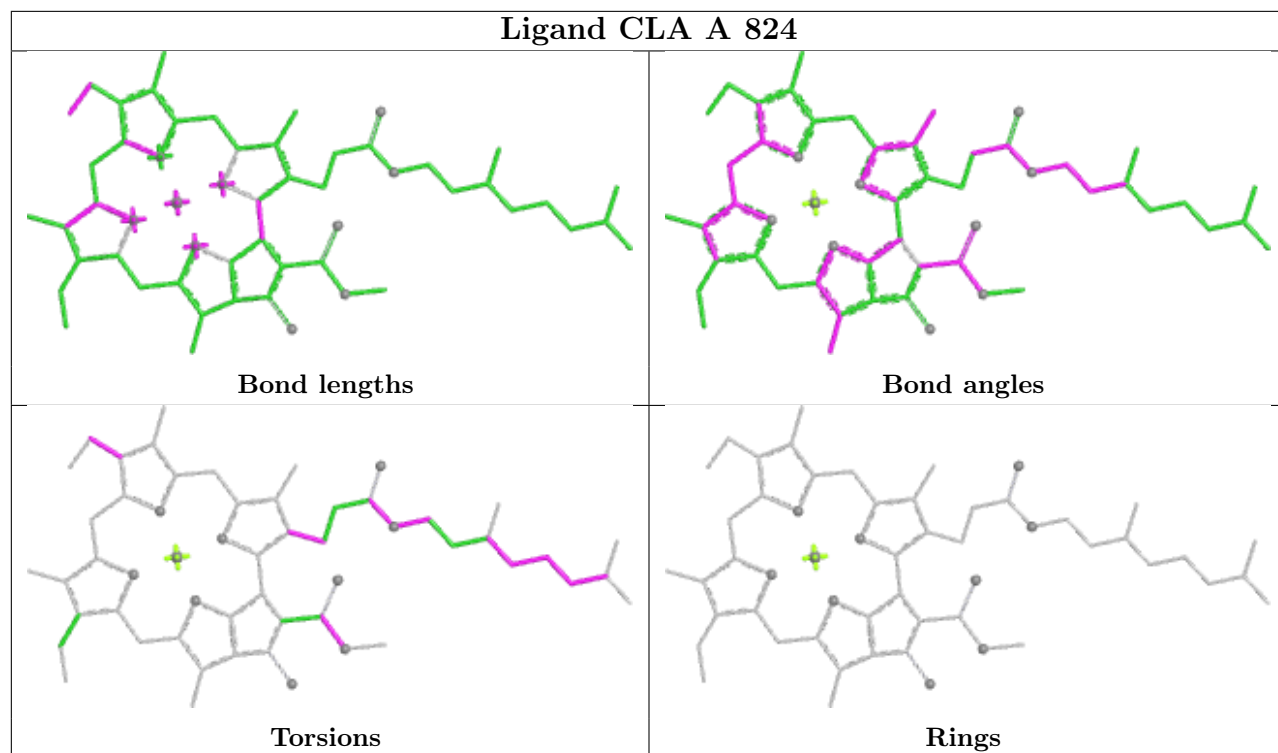
Ligand CLA 2 311



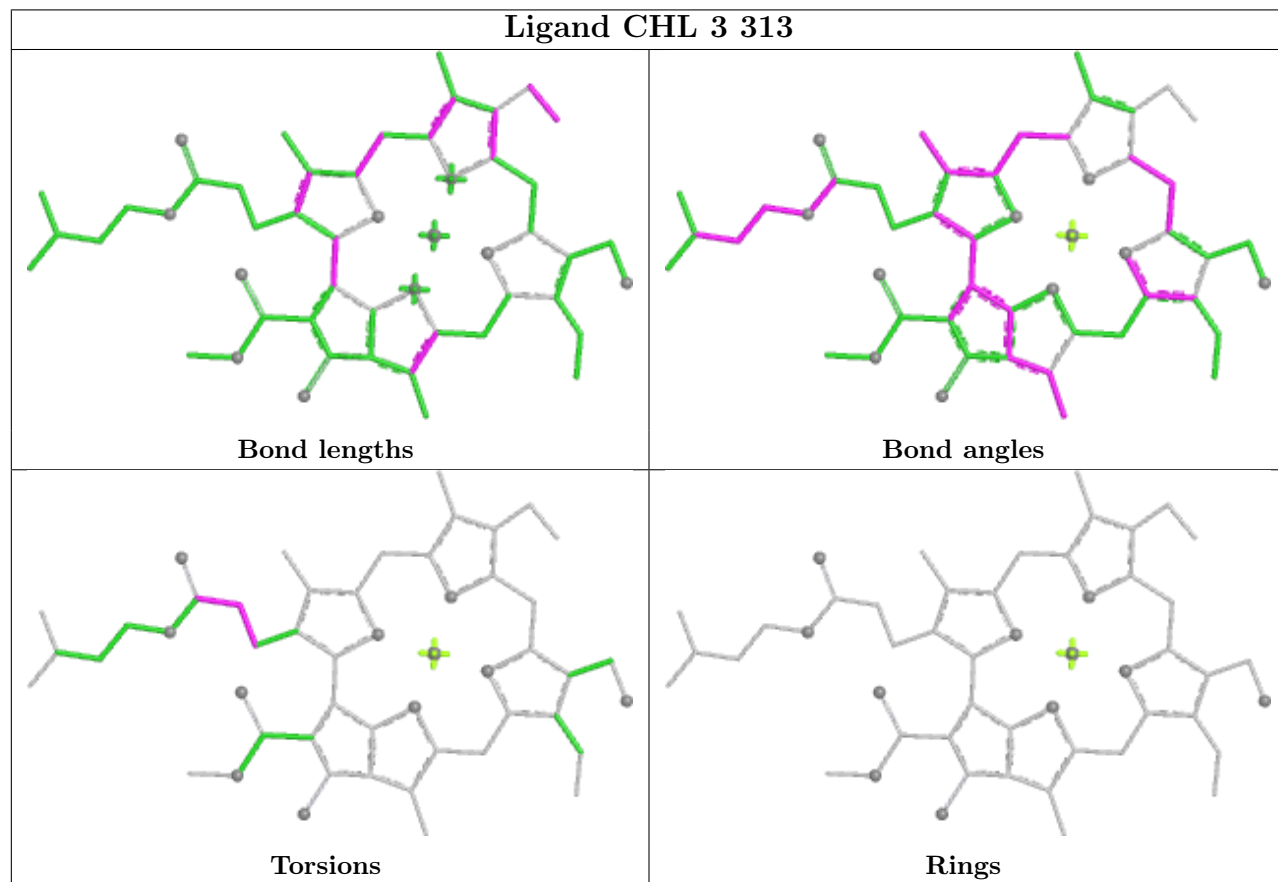
Ligand CLA 3 307



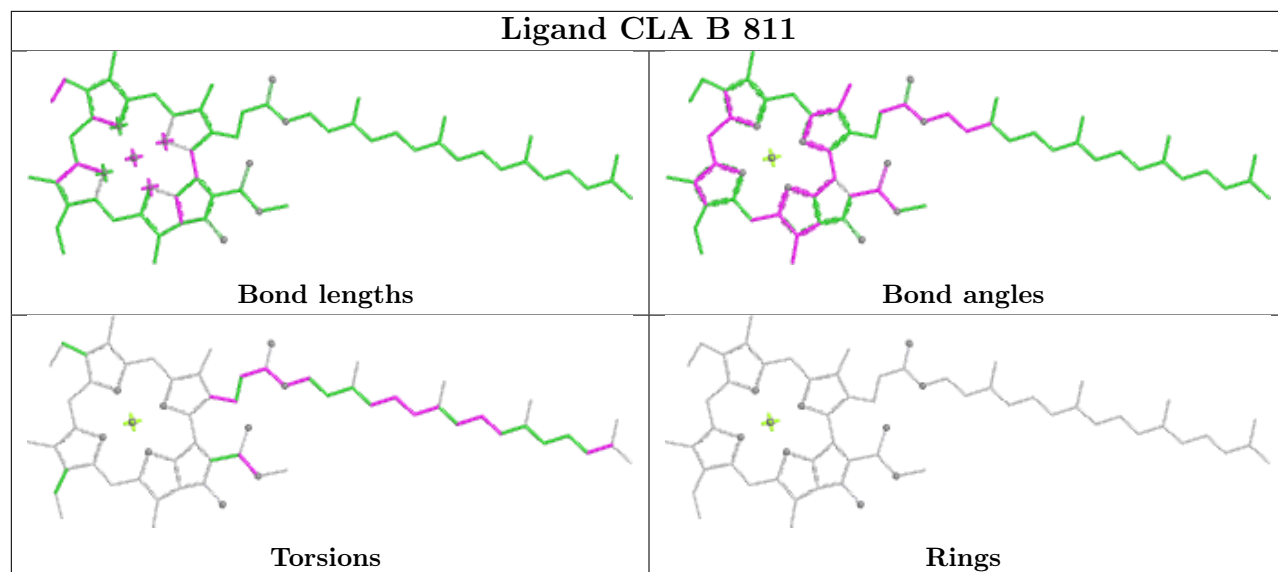
Ligand CLA A 824



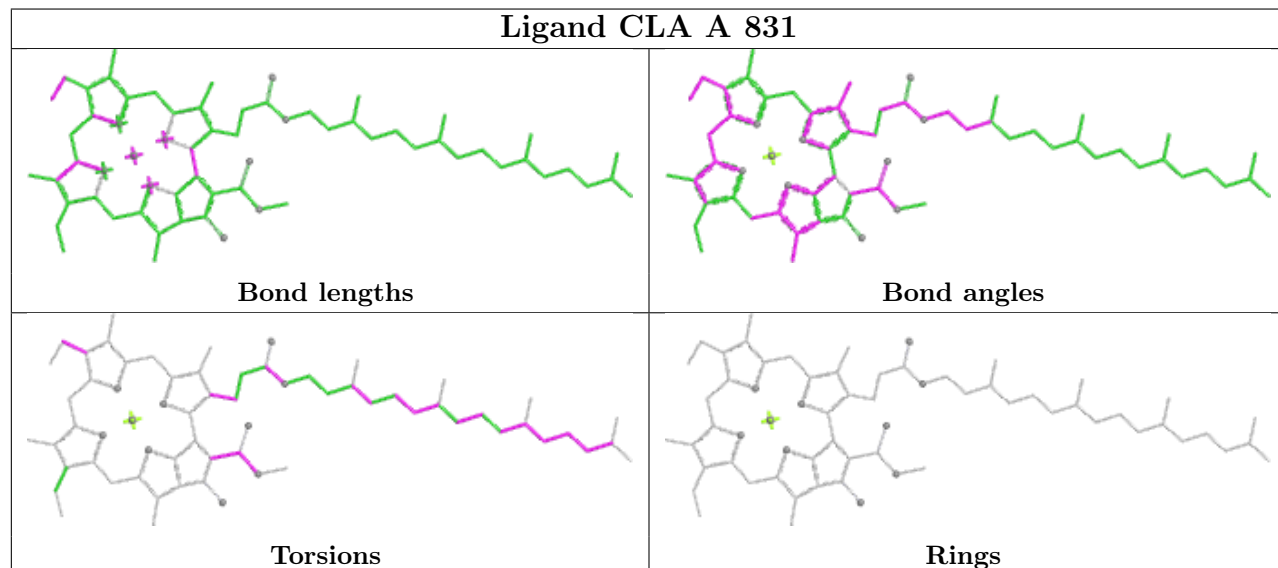
Ligand CHL 3 313



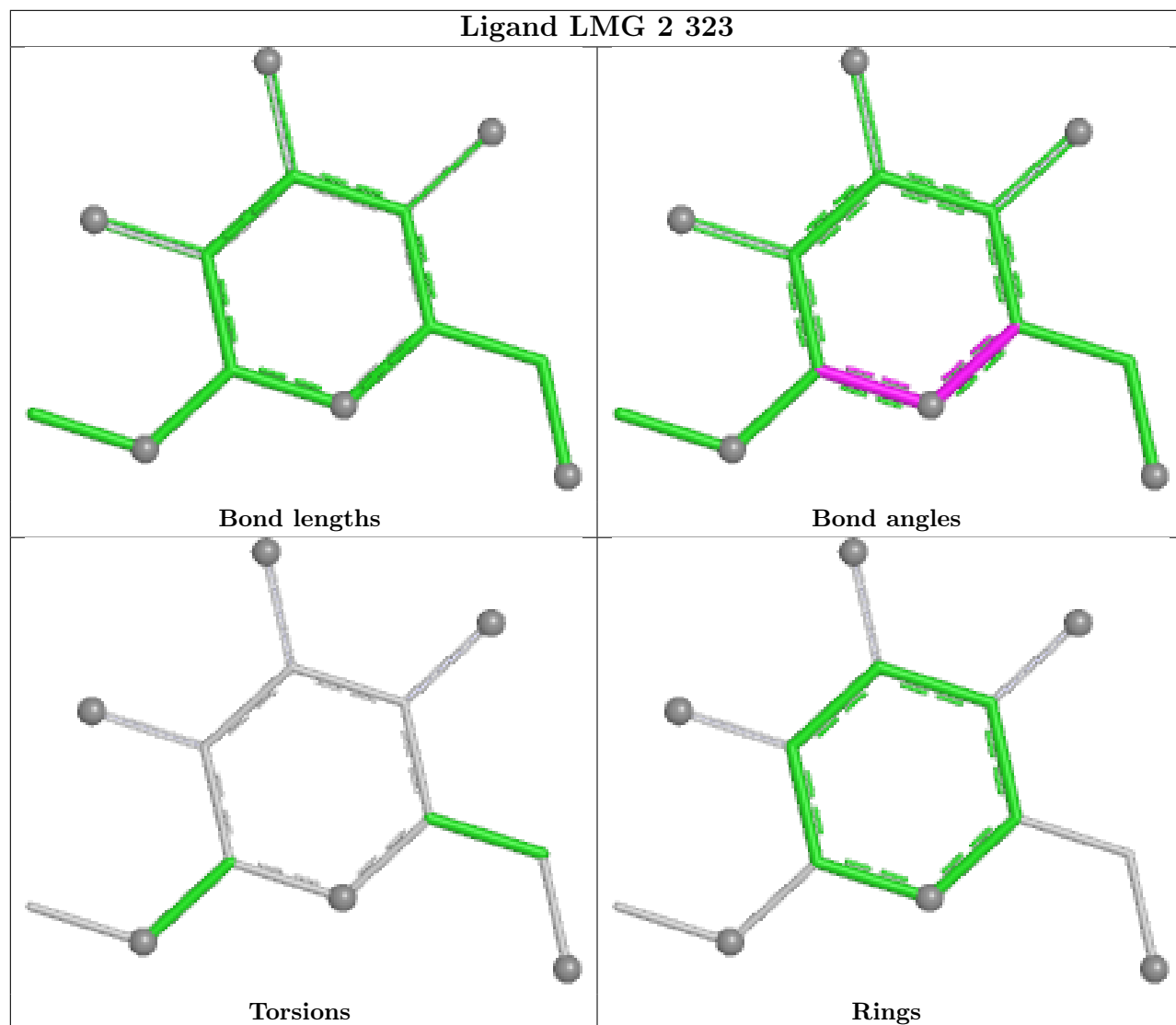
Ligand CLA B 811



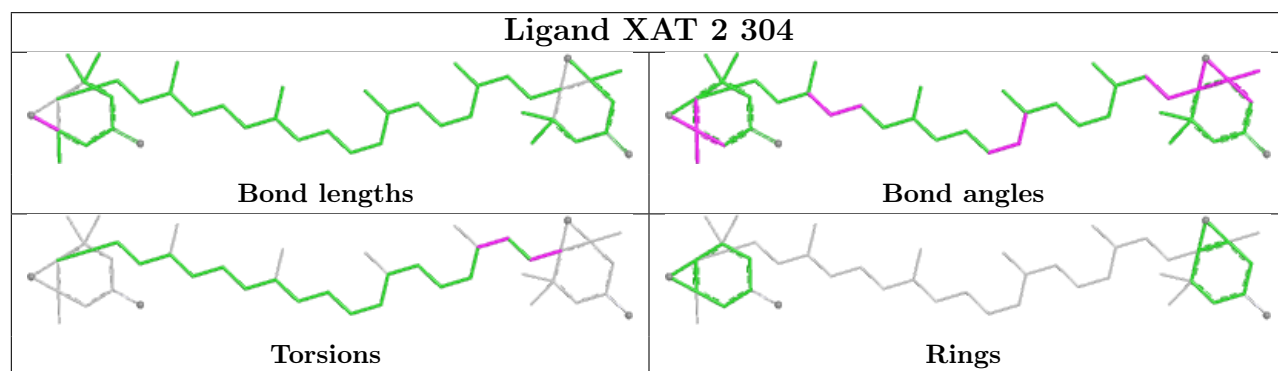
Ligand CLA A 831



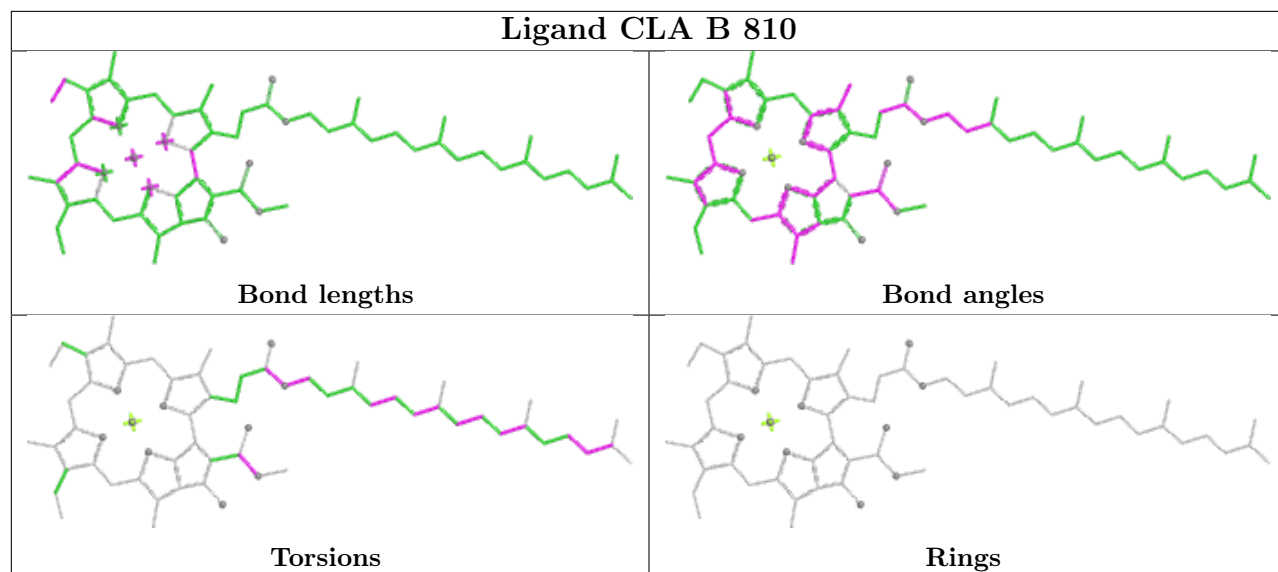
Ligand LMG 2 323



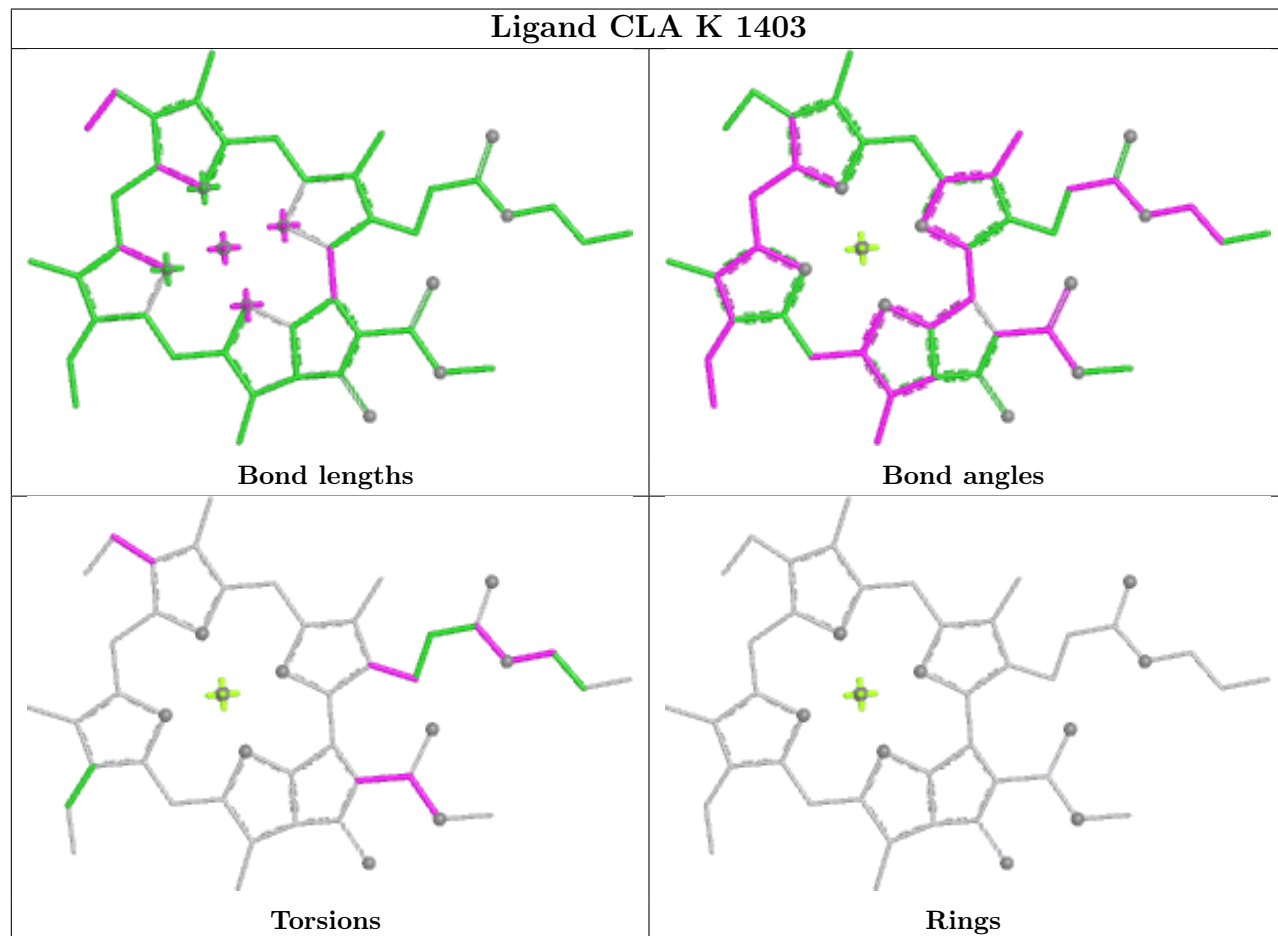
Ligand XAT 2 304



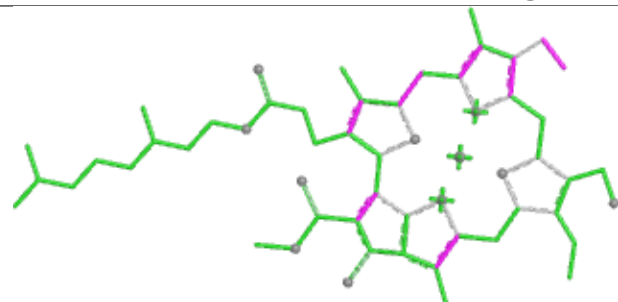
Ligand CLA B 810



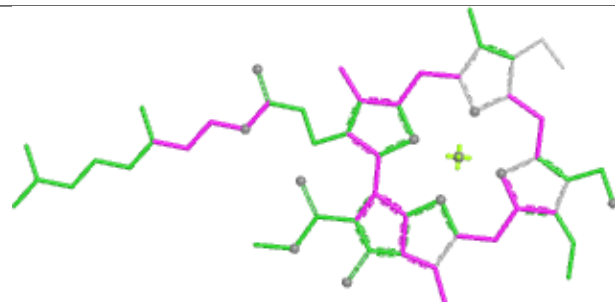
Ligand CLA K 1403



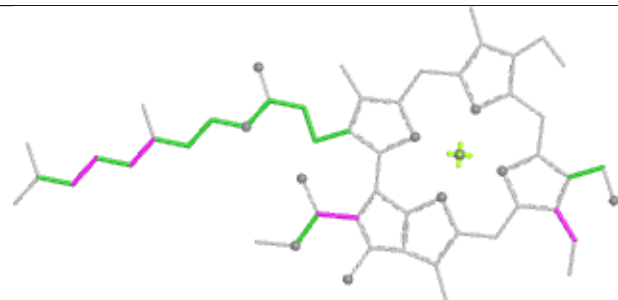
Ligand CHL 4 318



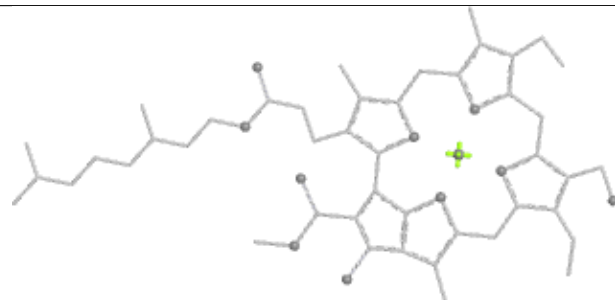
Bond lengths



Bond angles

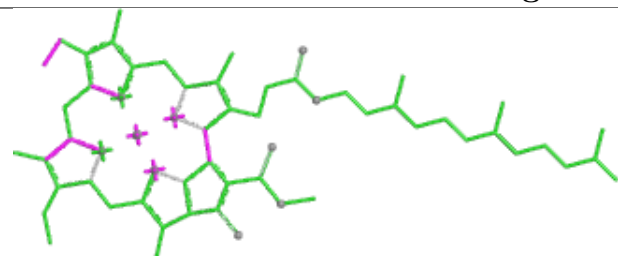


Torsions

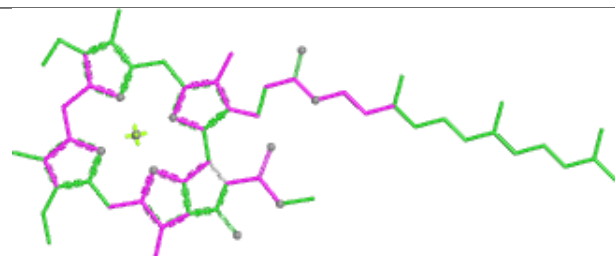


Rings

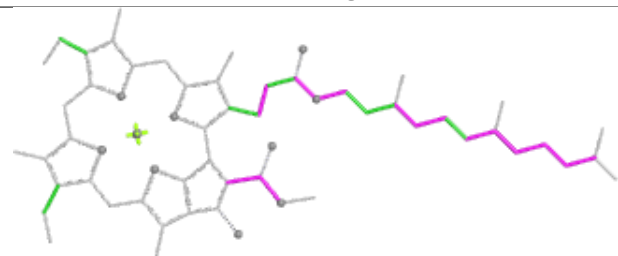
Ligand CLA 4 308



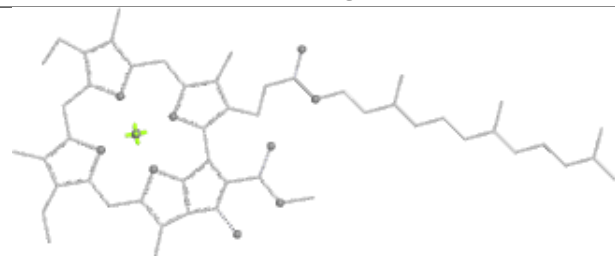
Bond lengths



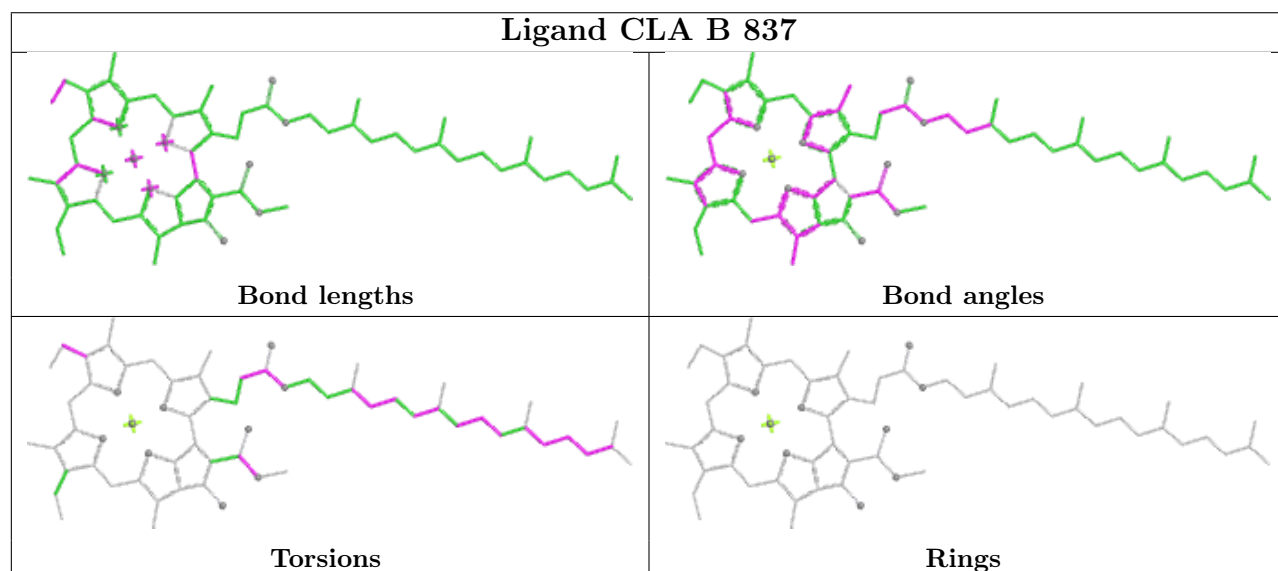
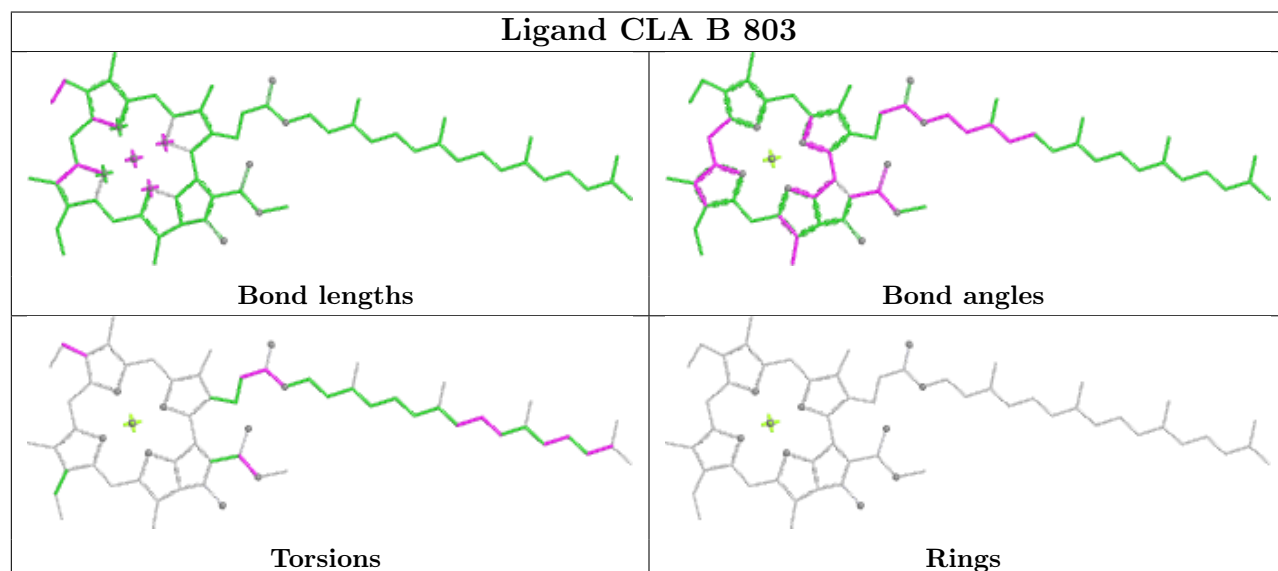
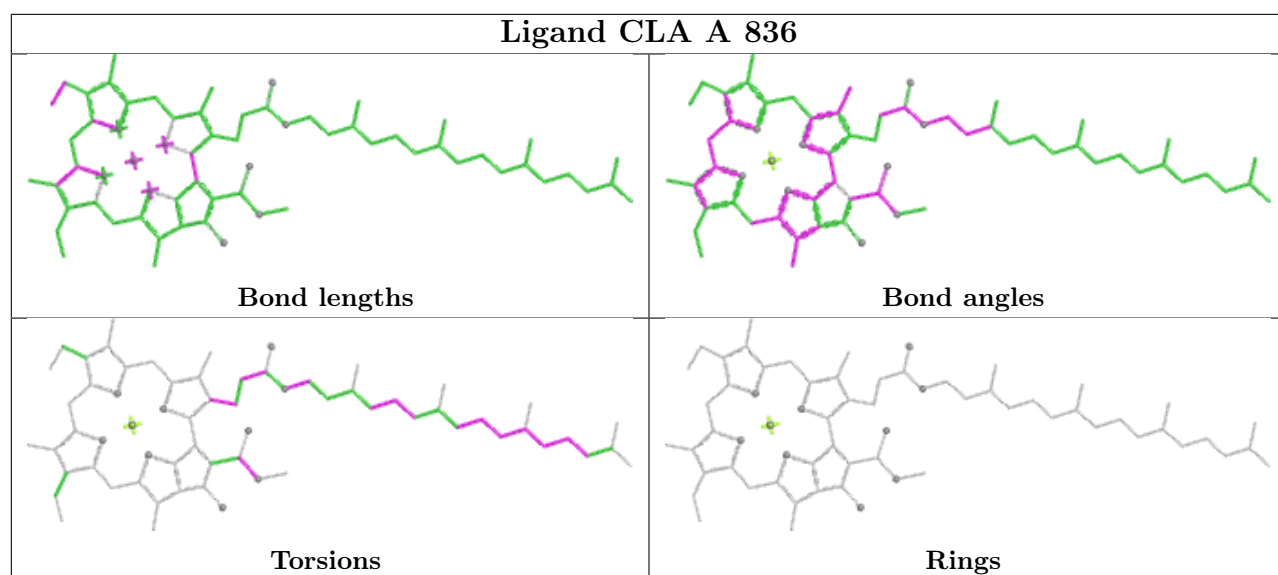
Bond angles

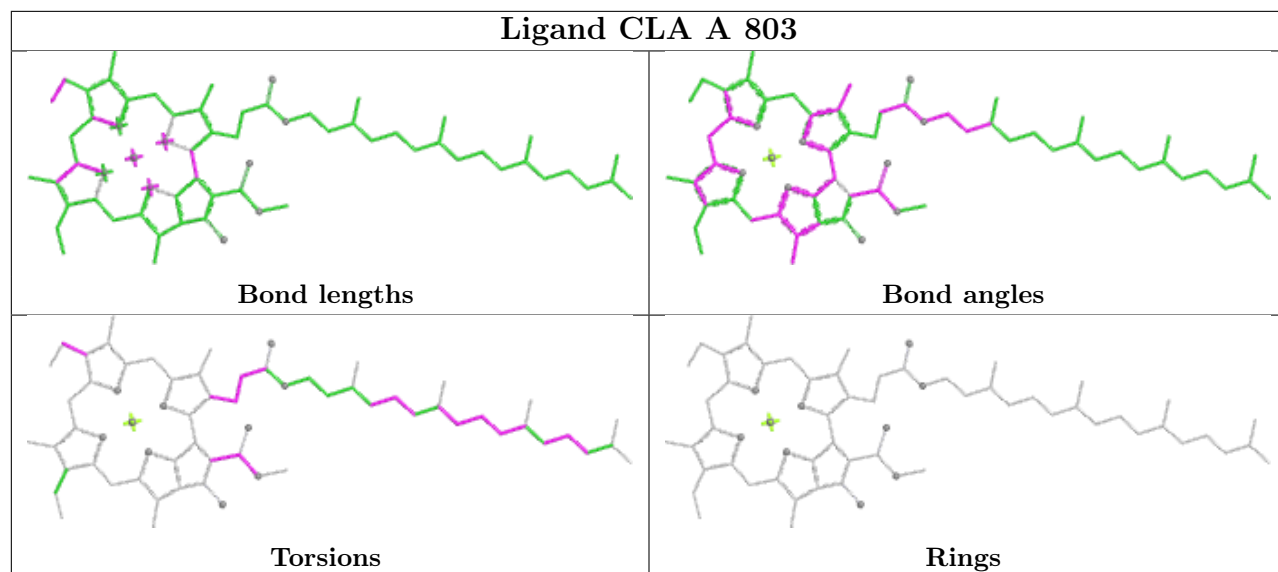
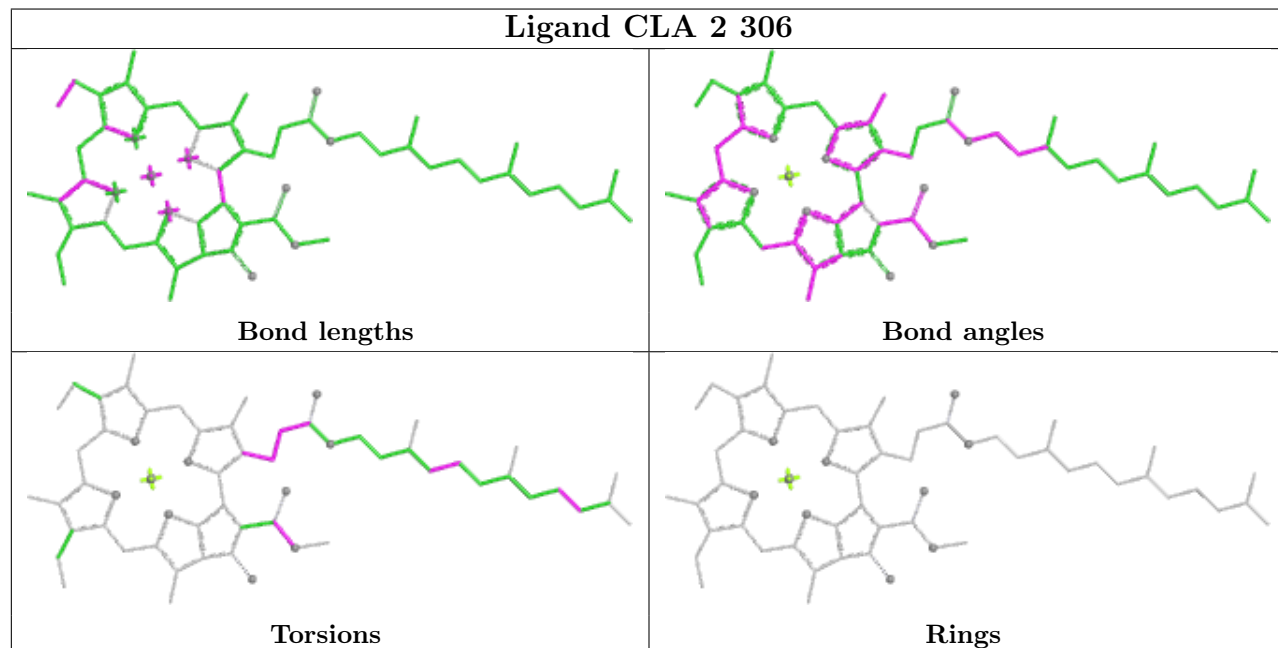


Torsions

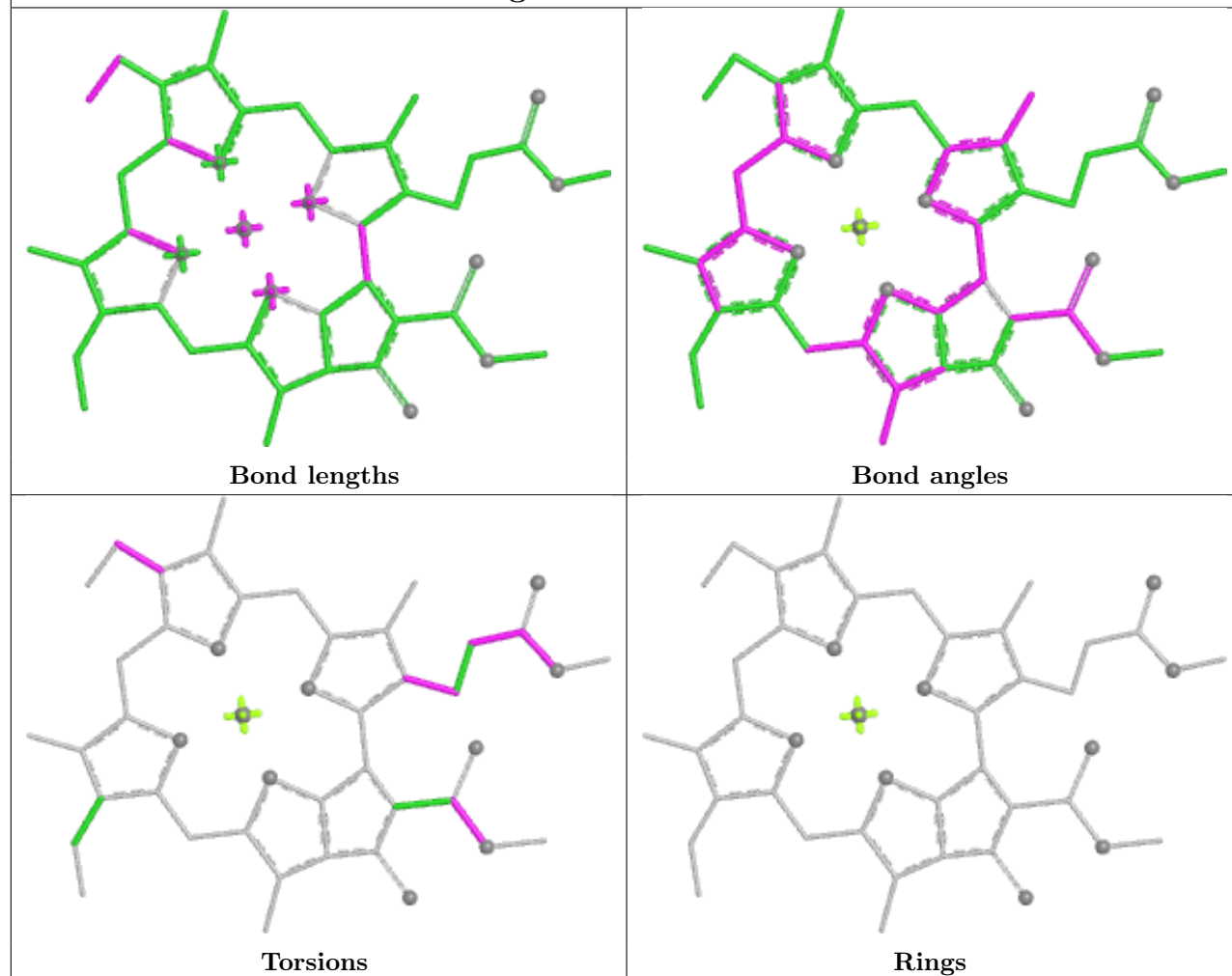


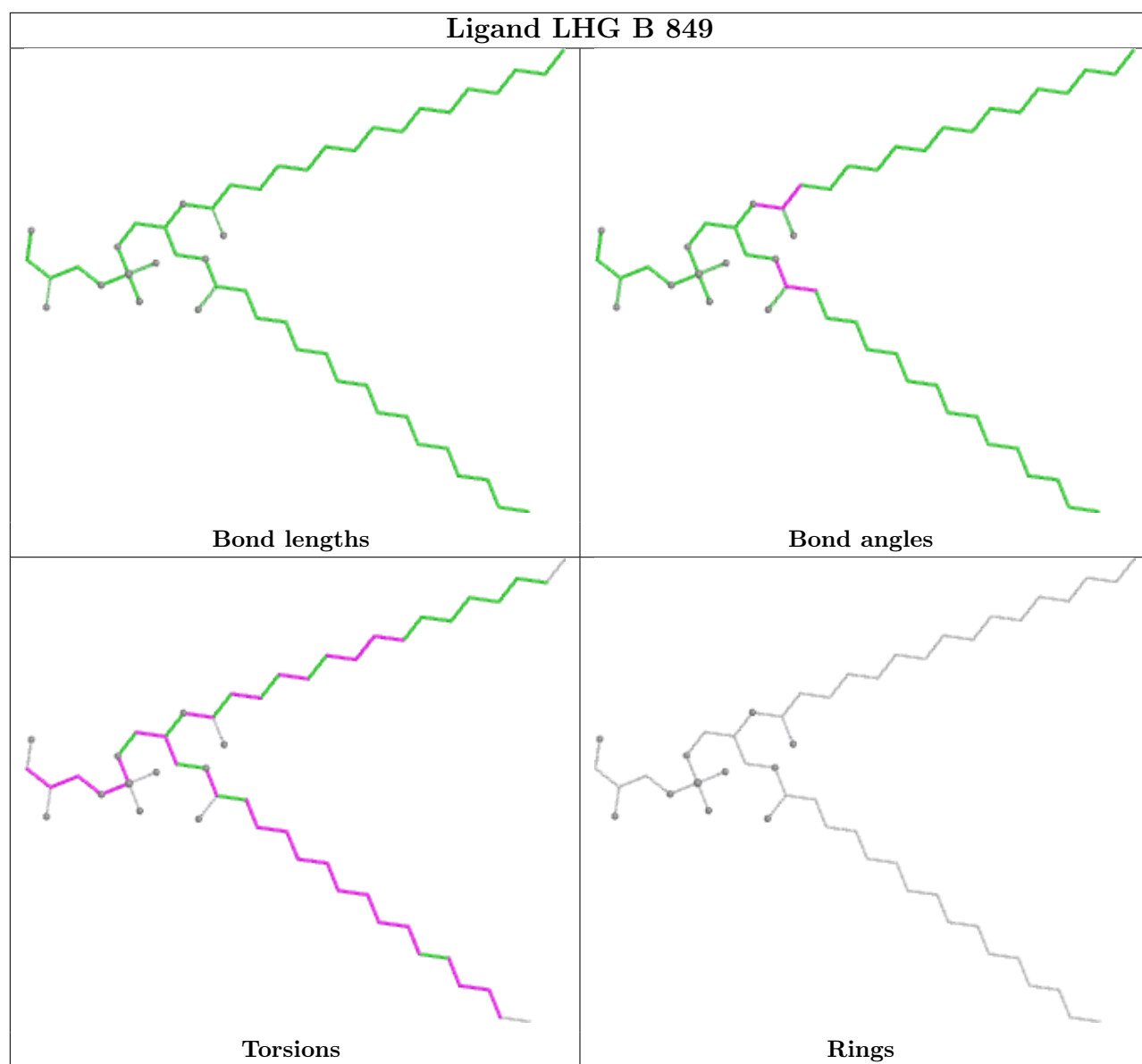
Rings

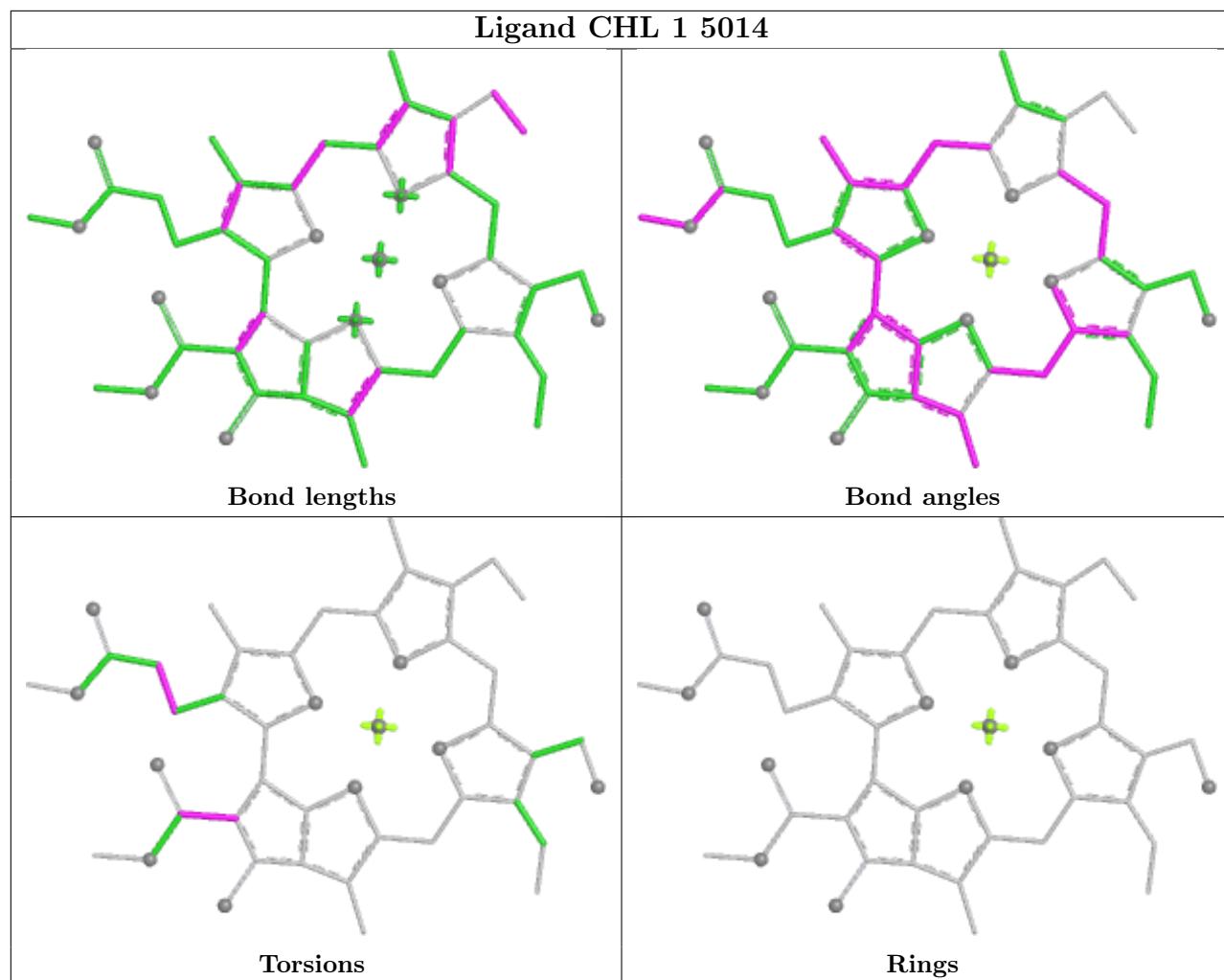


Ligand CLA A 803**Ligand CLA 2 306**

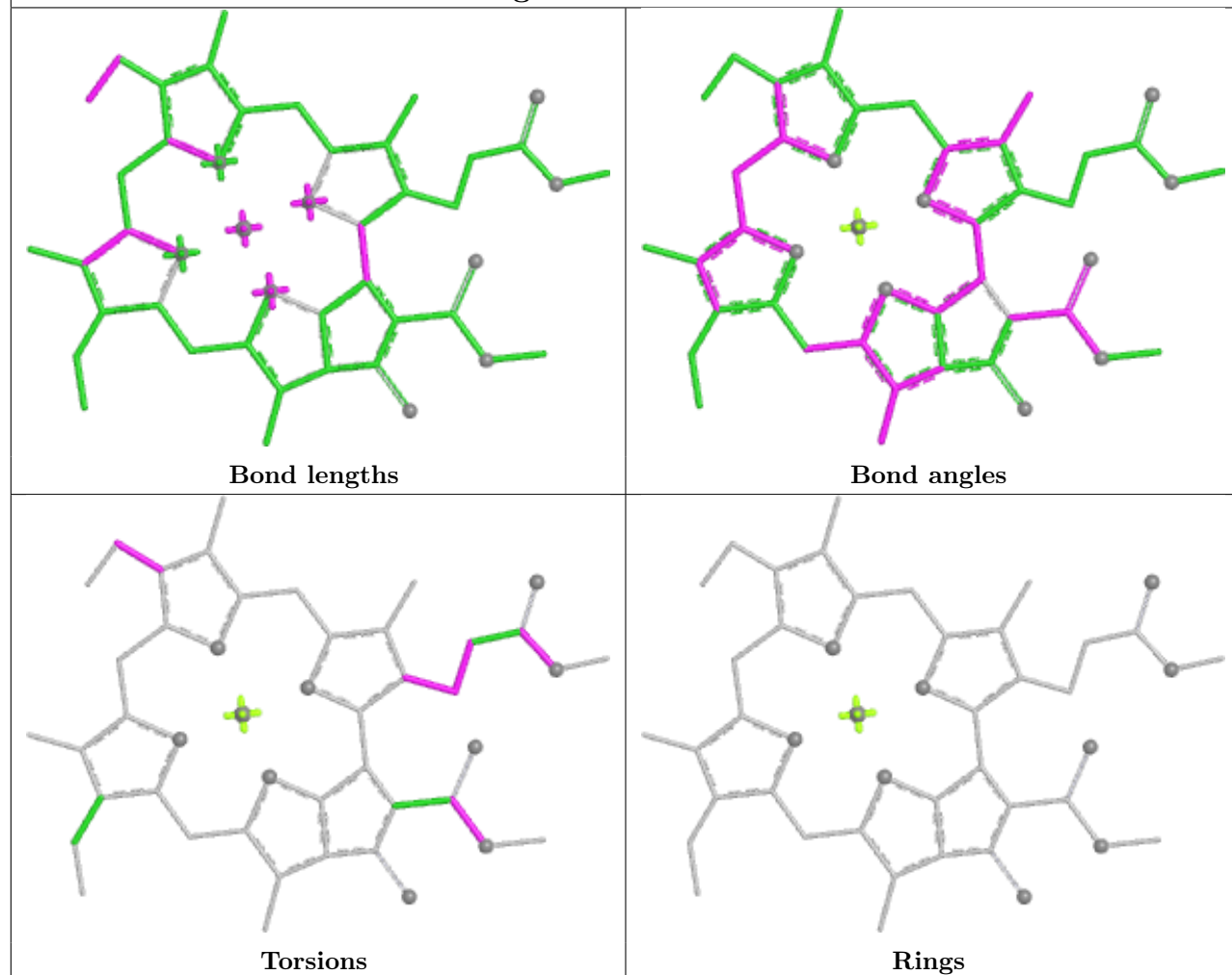
Ligand CLA 1 5013



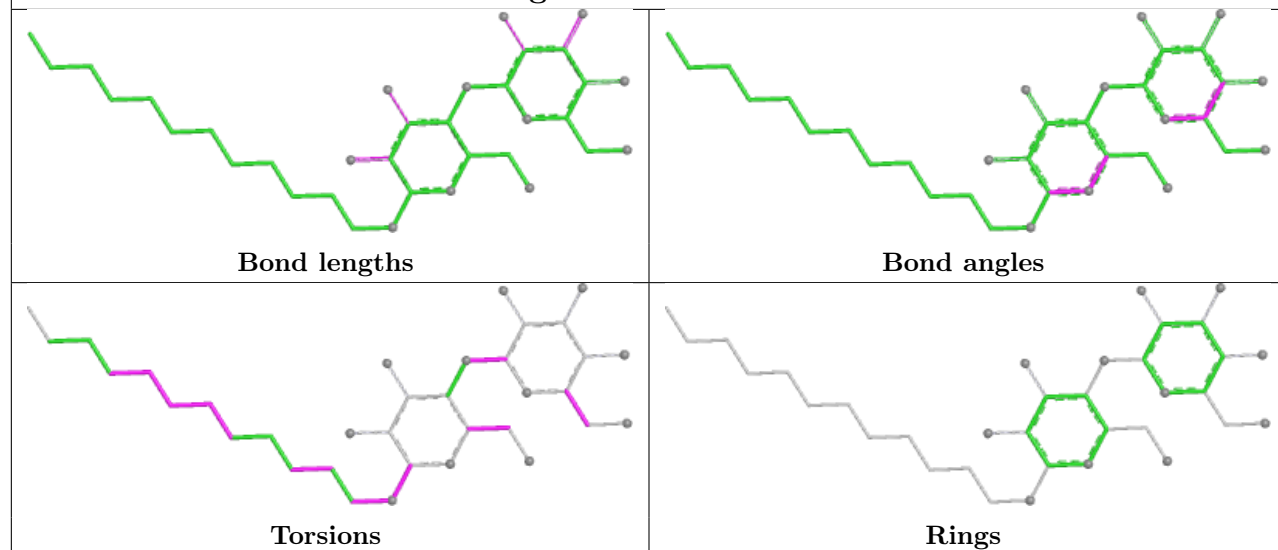




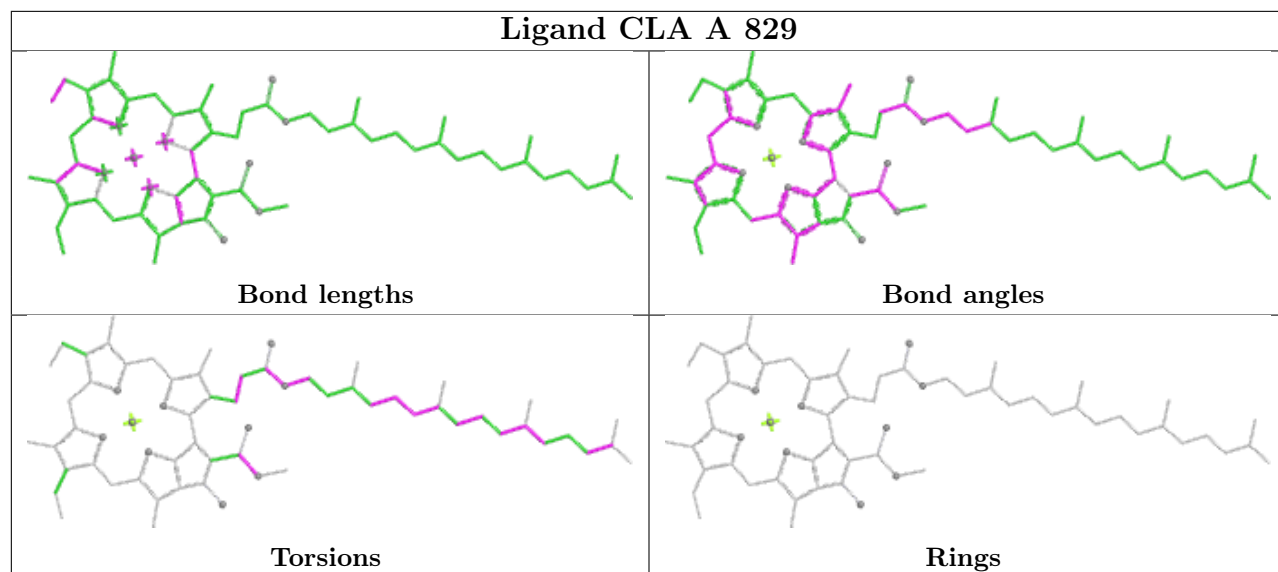
Ligand CLA B 821



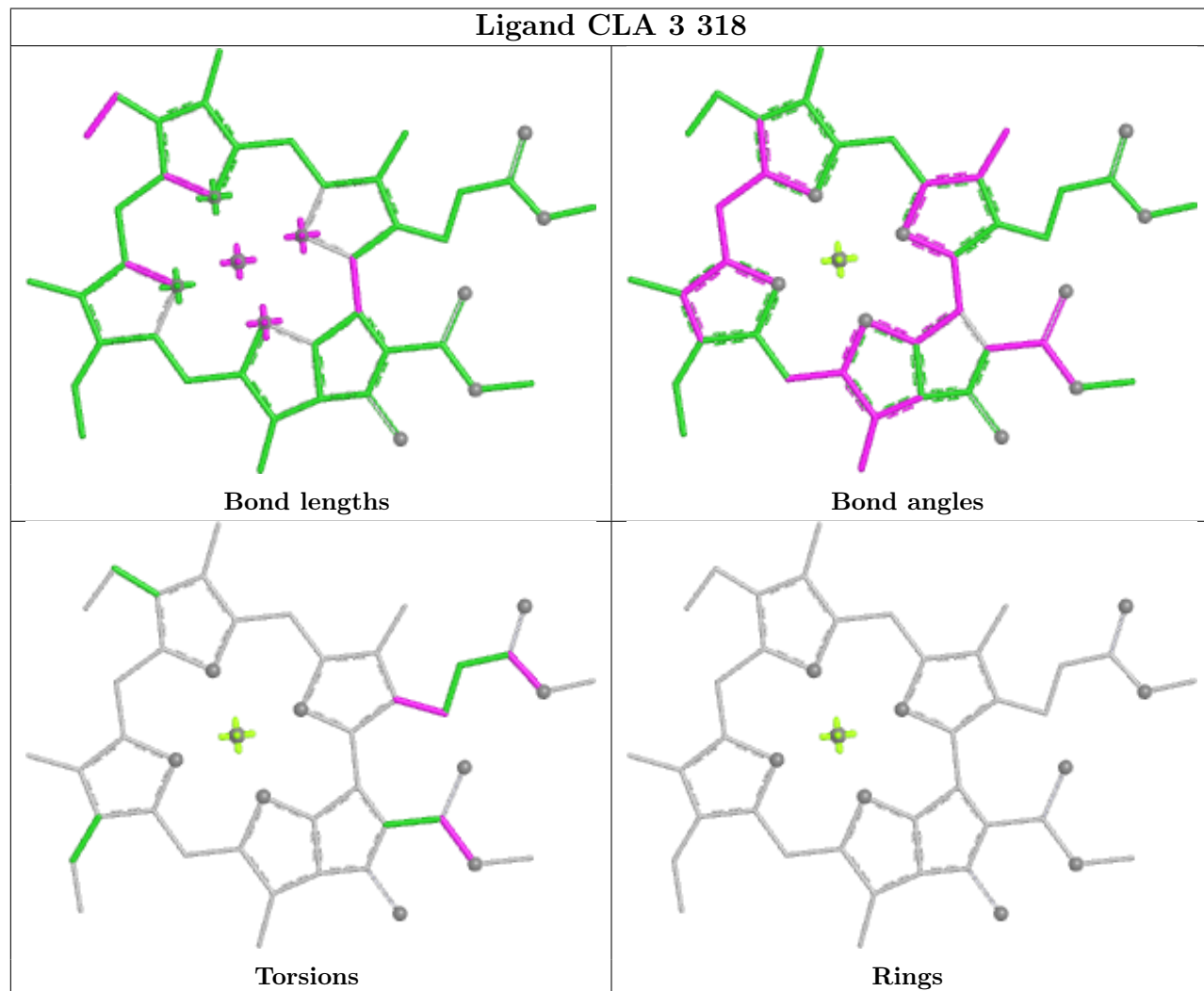
Ligand LMT B 852



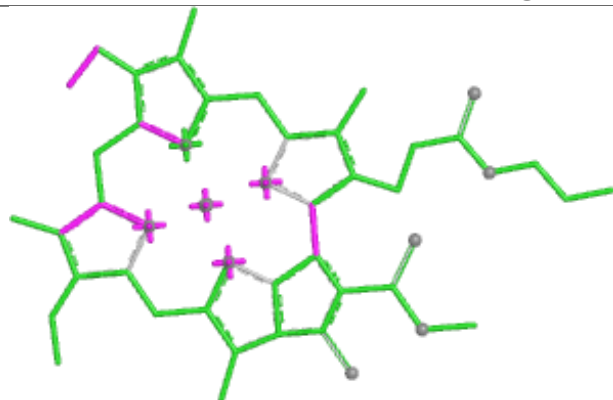
Ligand CLA A 829



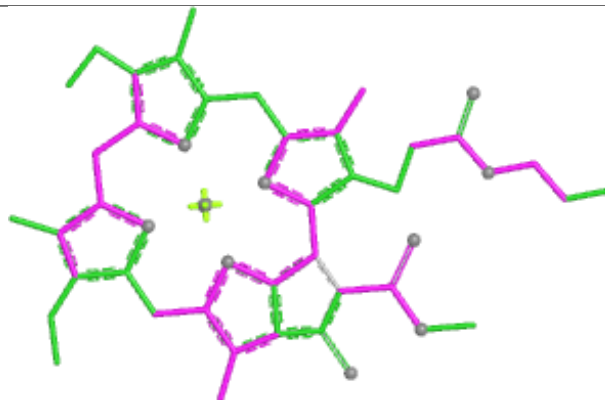
Ligand CLA 3 318



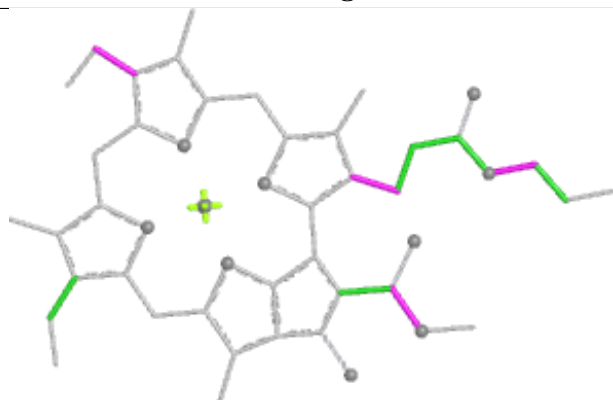
Ligand CLA 3 314



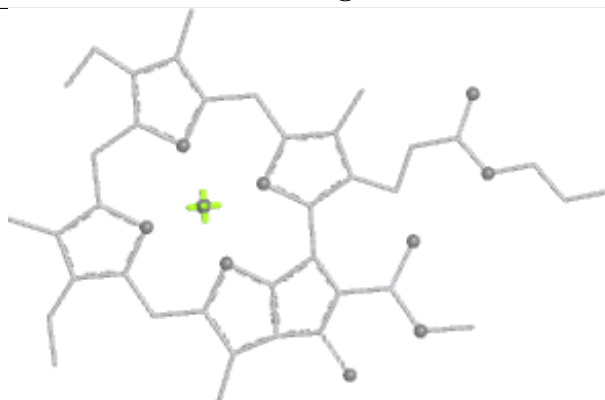
Bond lengths



Bond angles

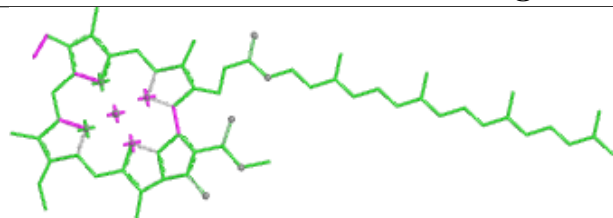


Torsions

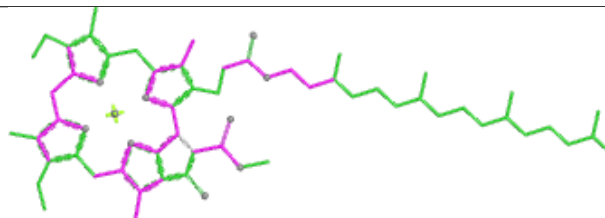


Rings

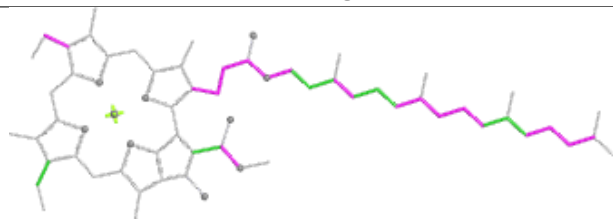
Ligand CLA B 828



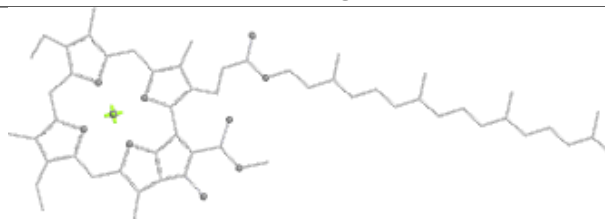
Bond lengths



Bond angles

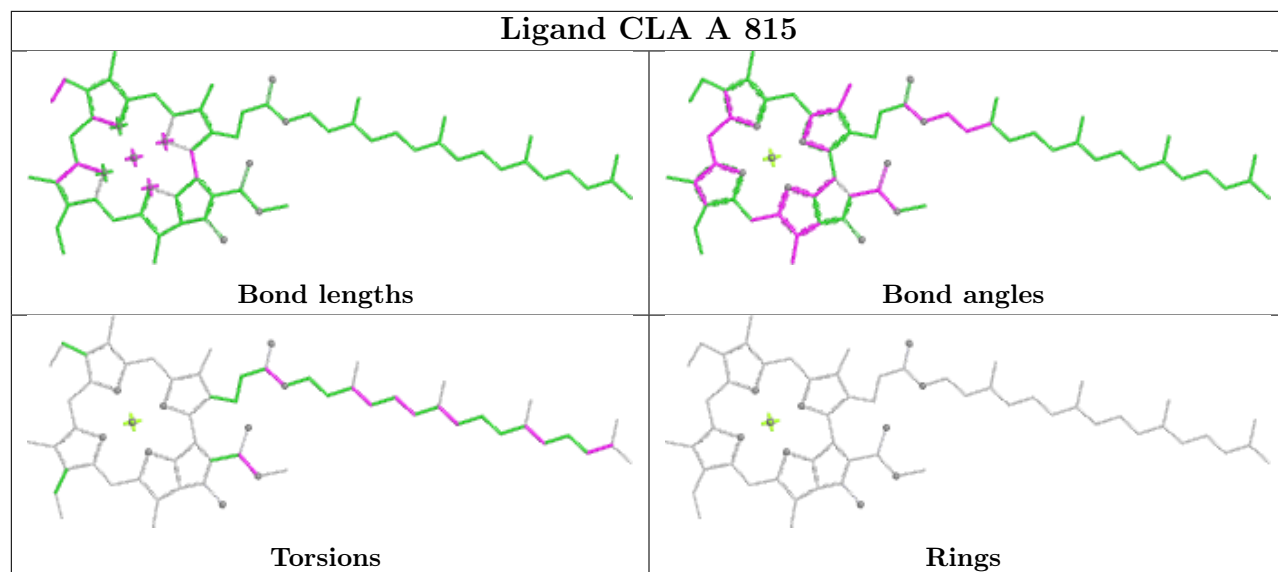


Torsions

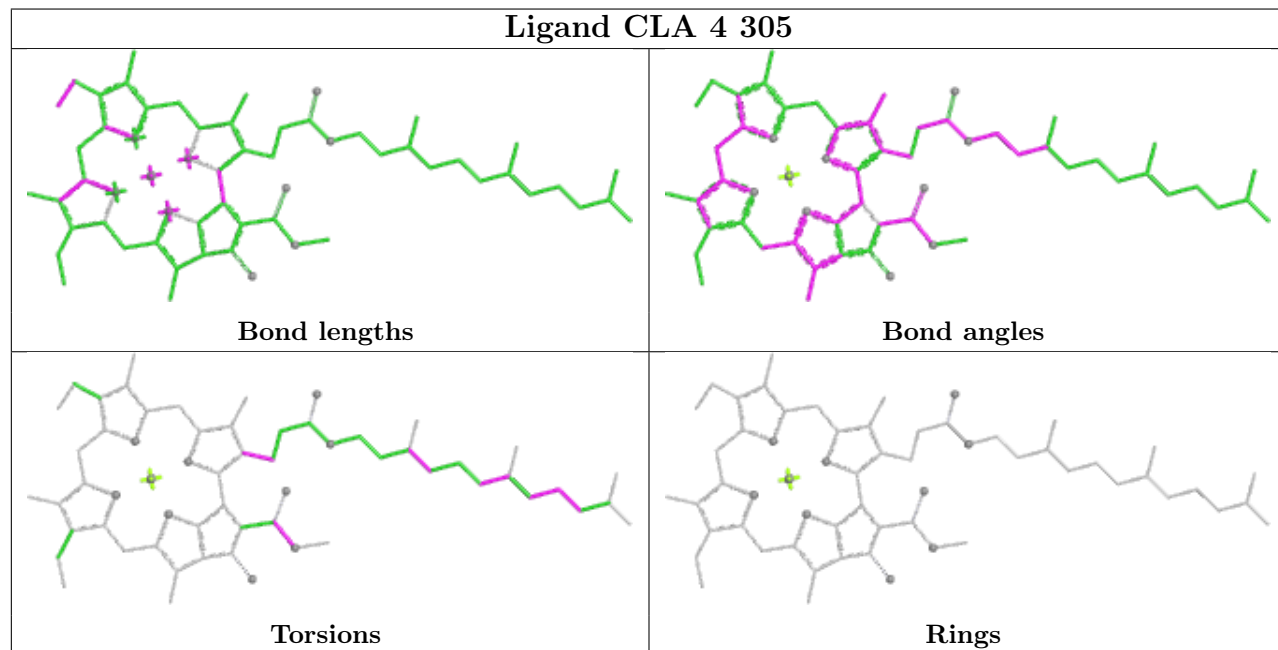


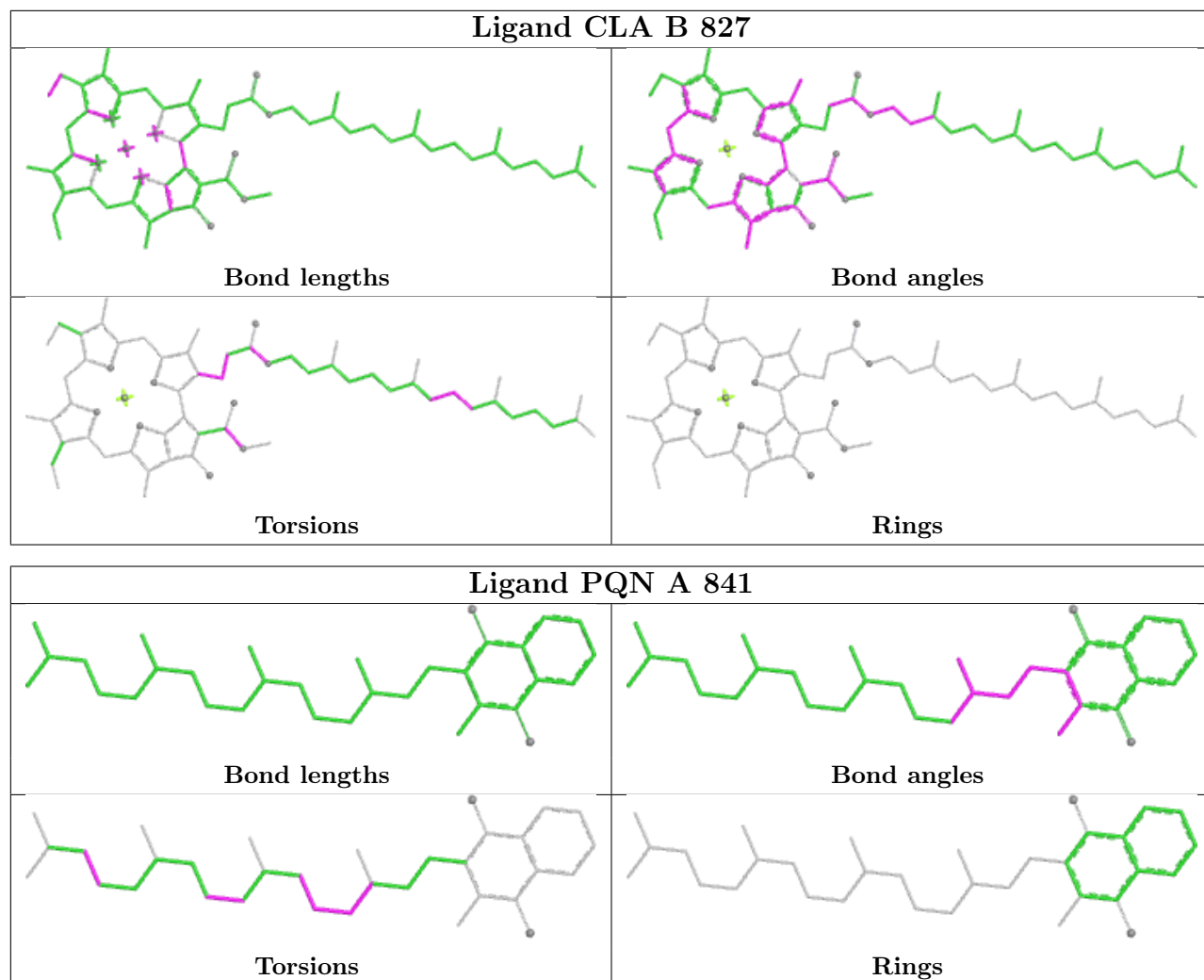
Rings

Ligand CLA A 815

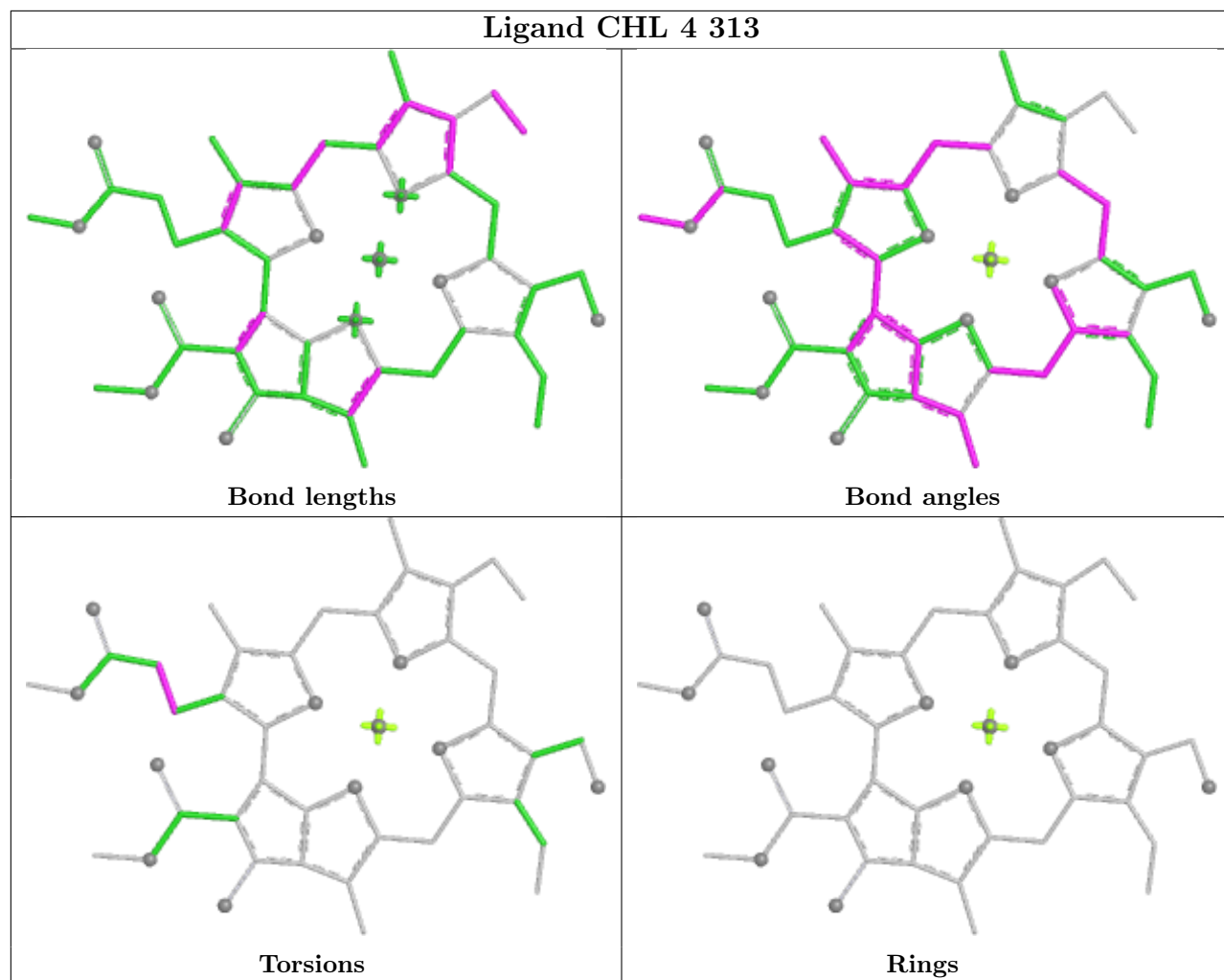


Ligand CLA 4 305

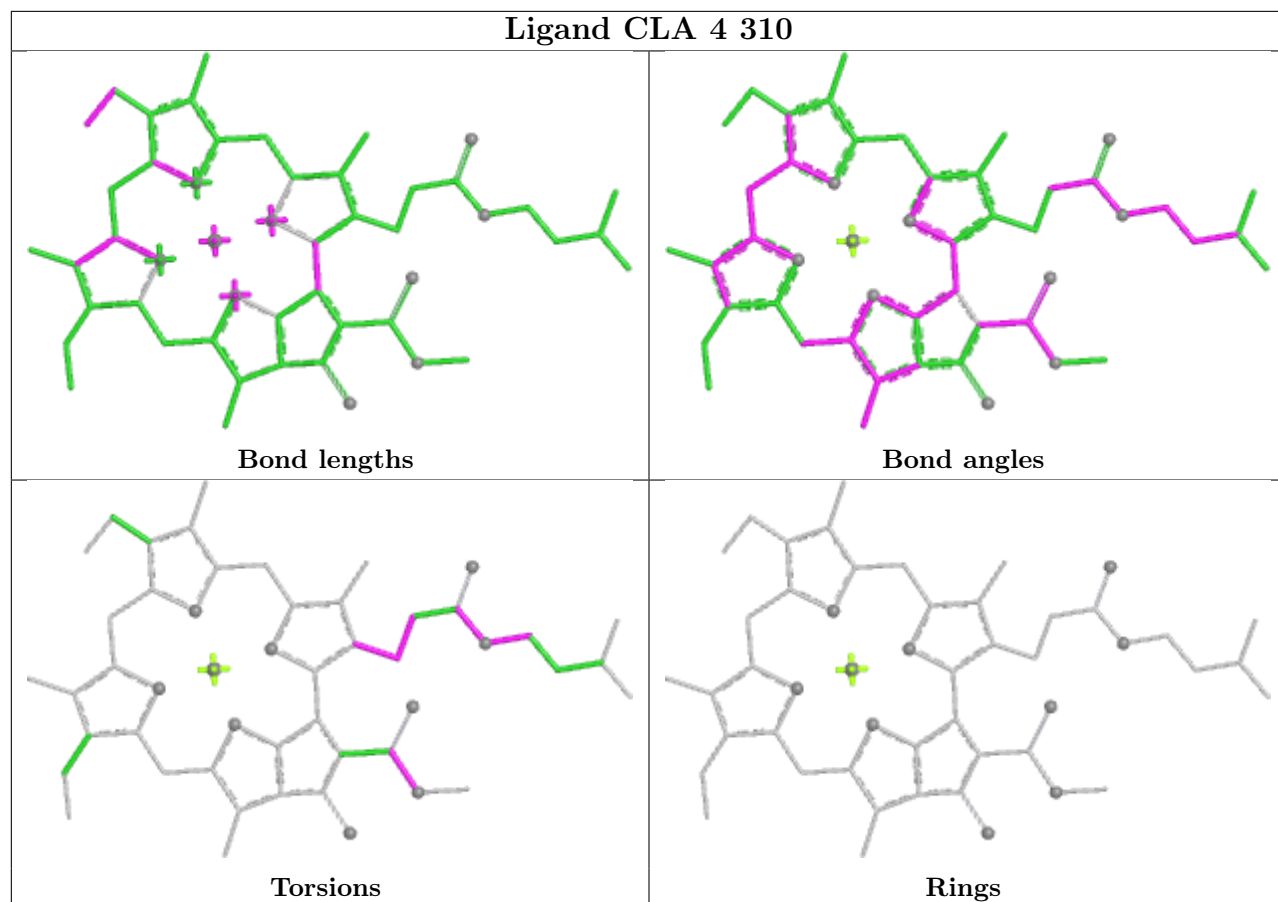




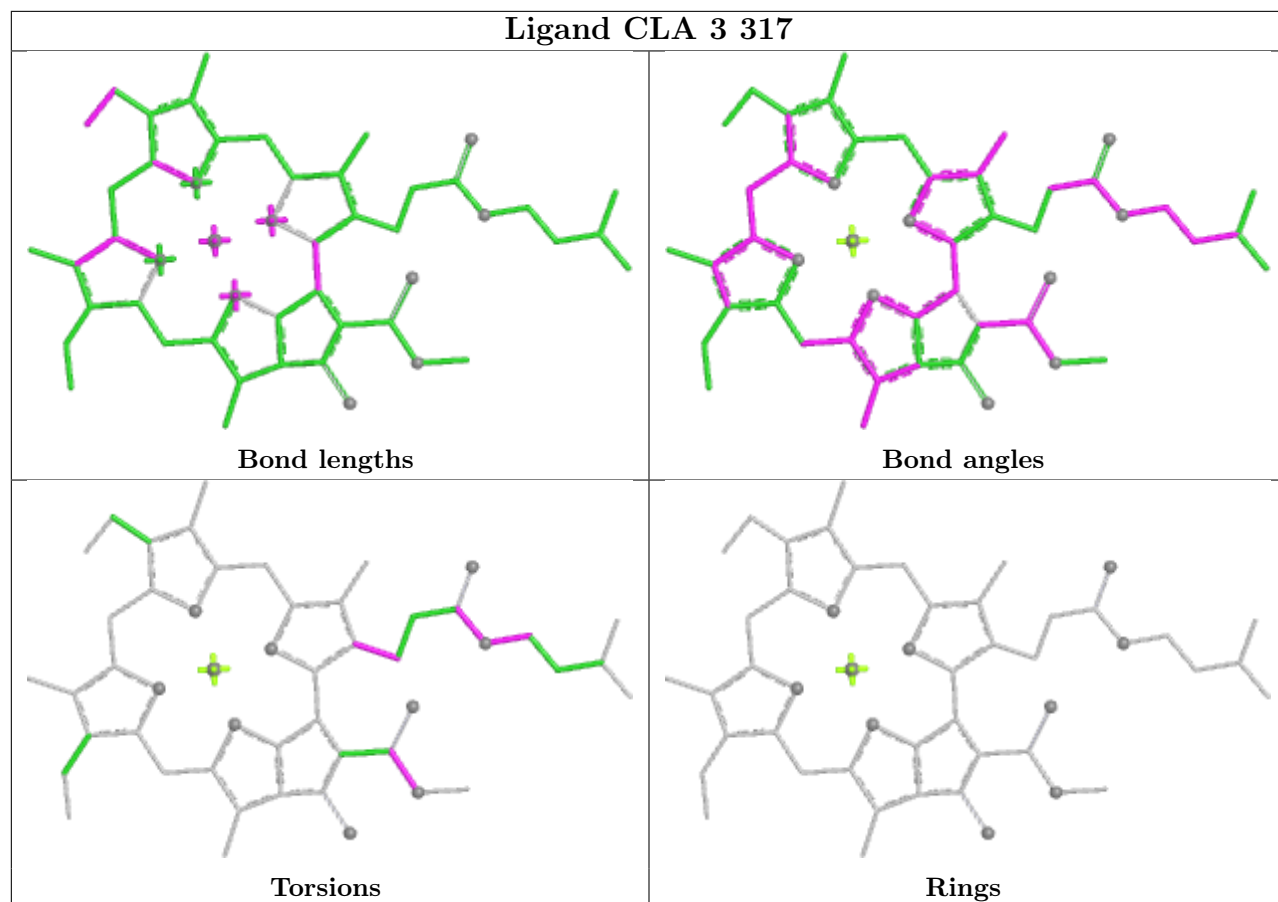
Ligand CHL 4 313



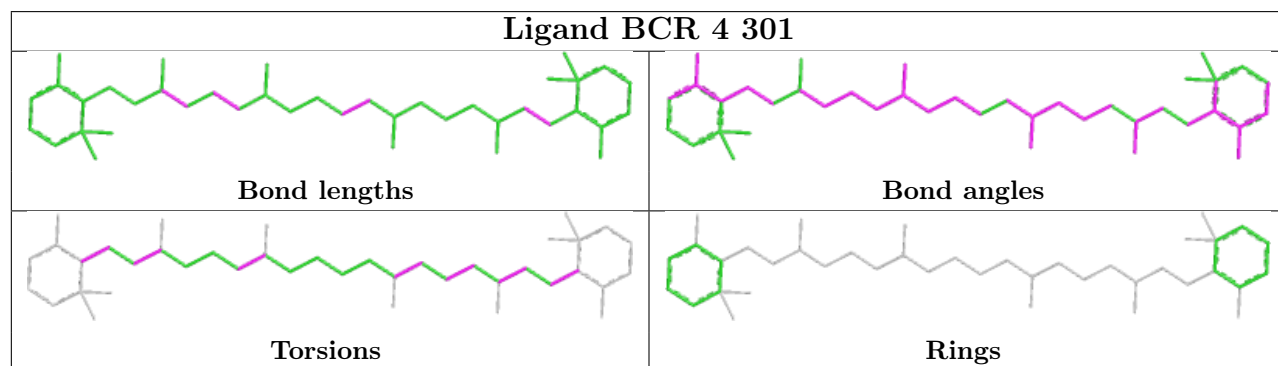
Ligand CLA 4 310

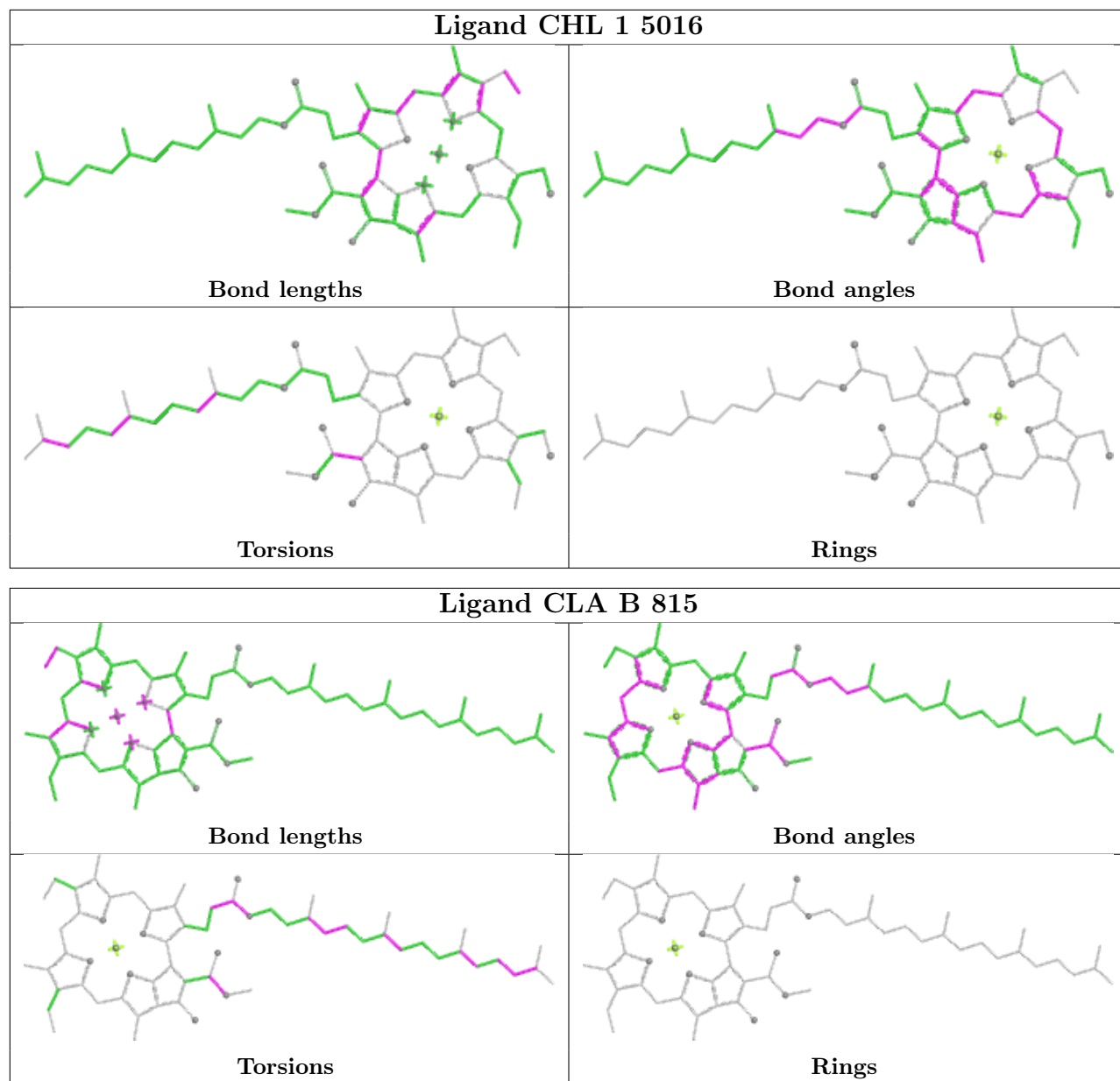


Ligand CLA 3 317

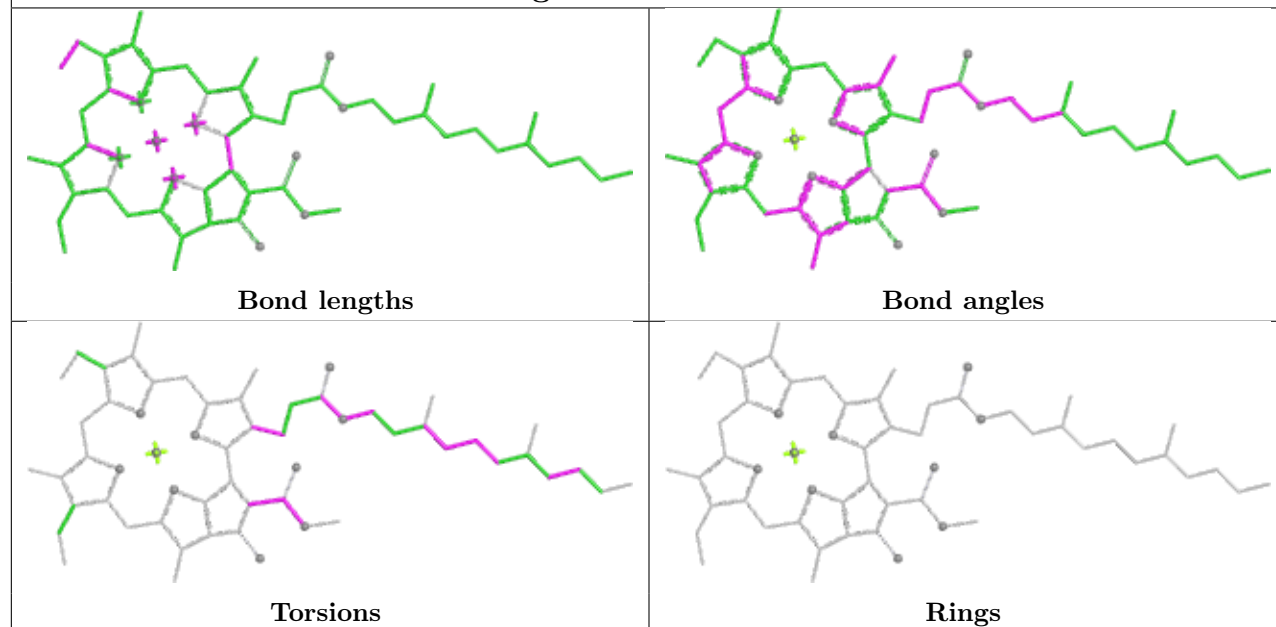


Ligand BCR 4 301

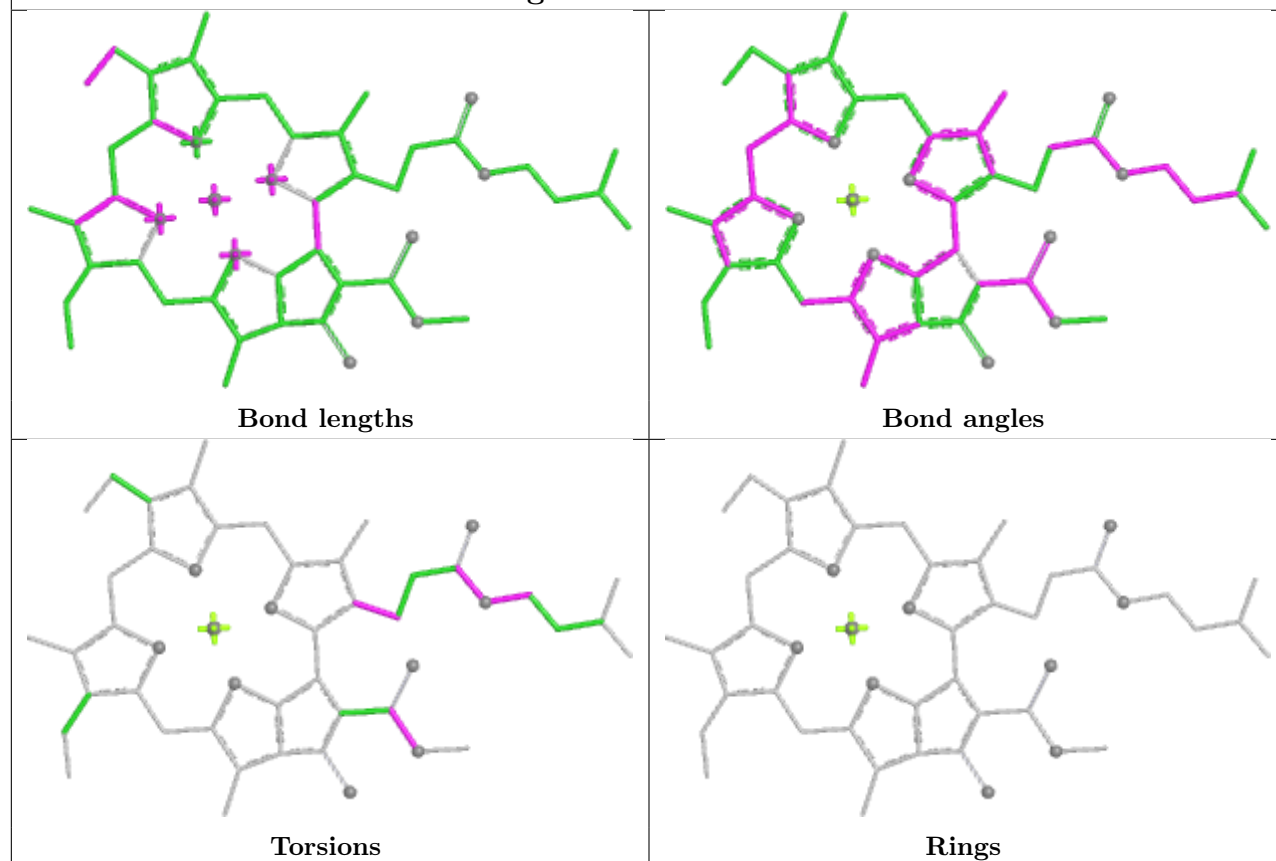


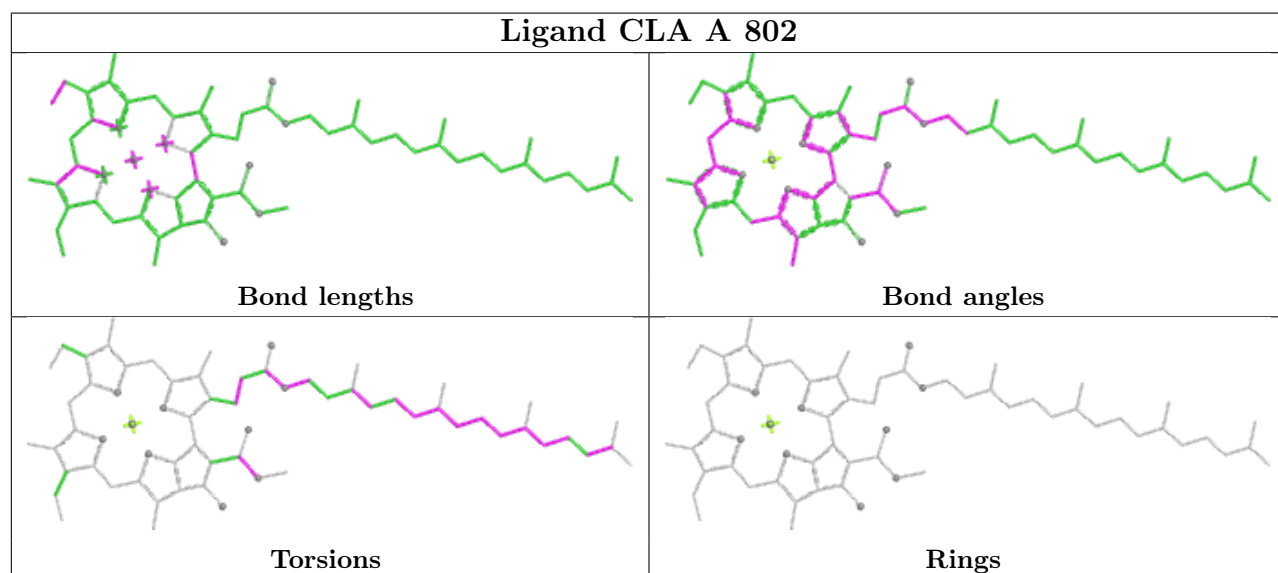
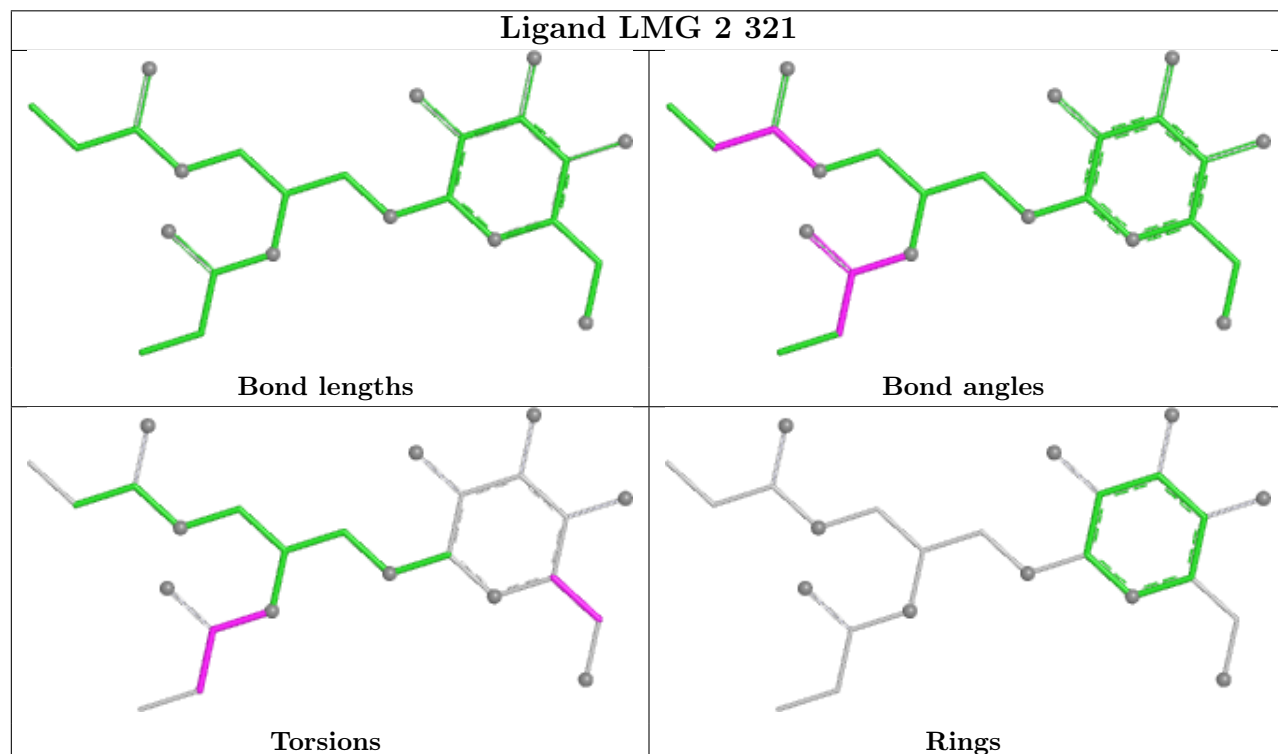
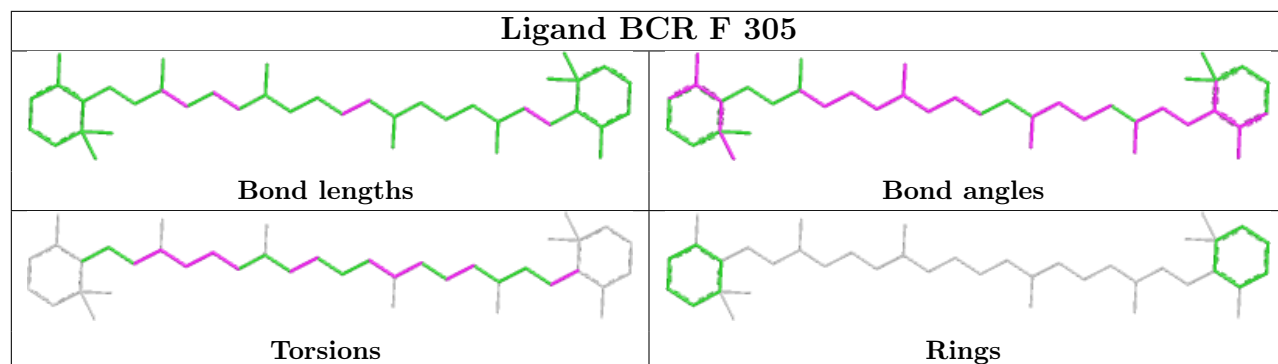


Ligand CLA B 833

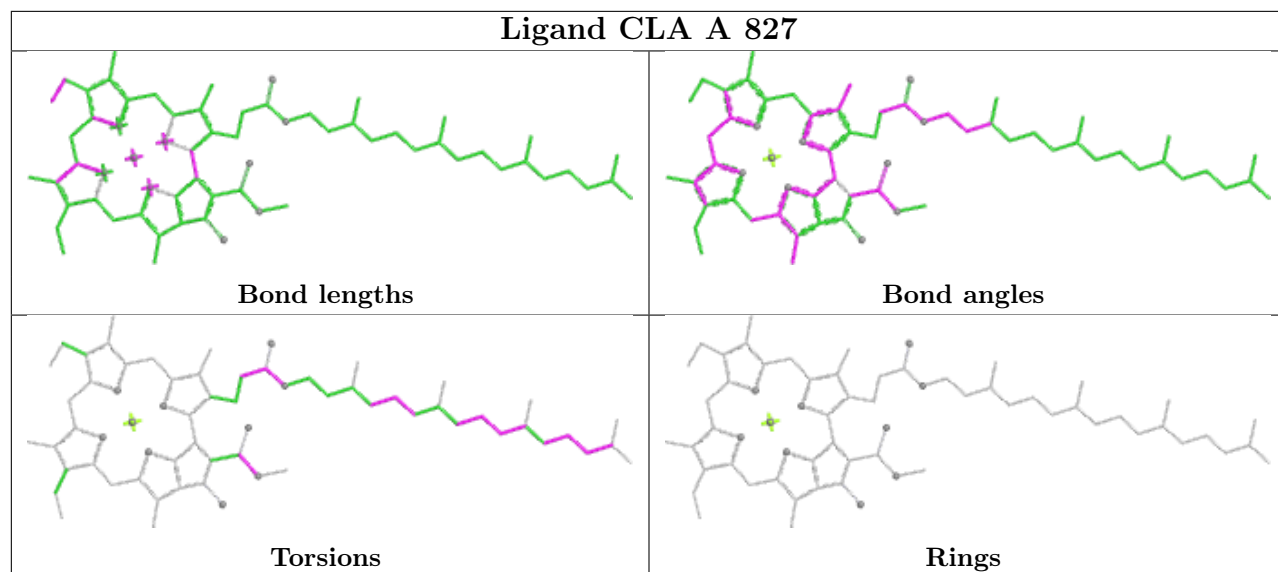


Ligand CLA J 1103

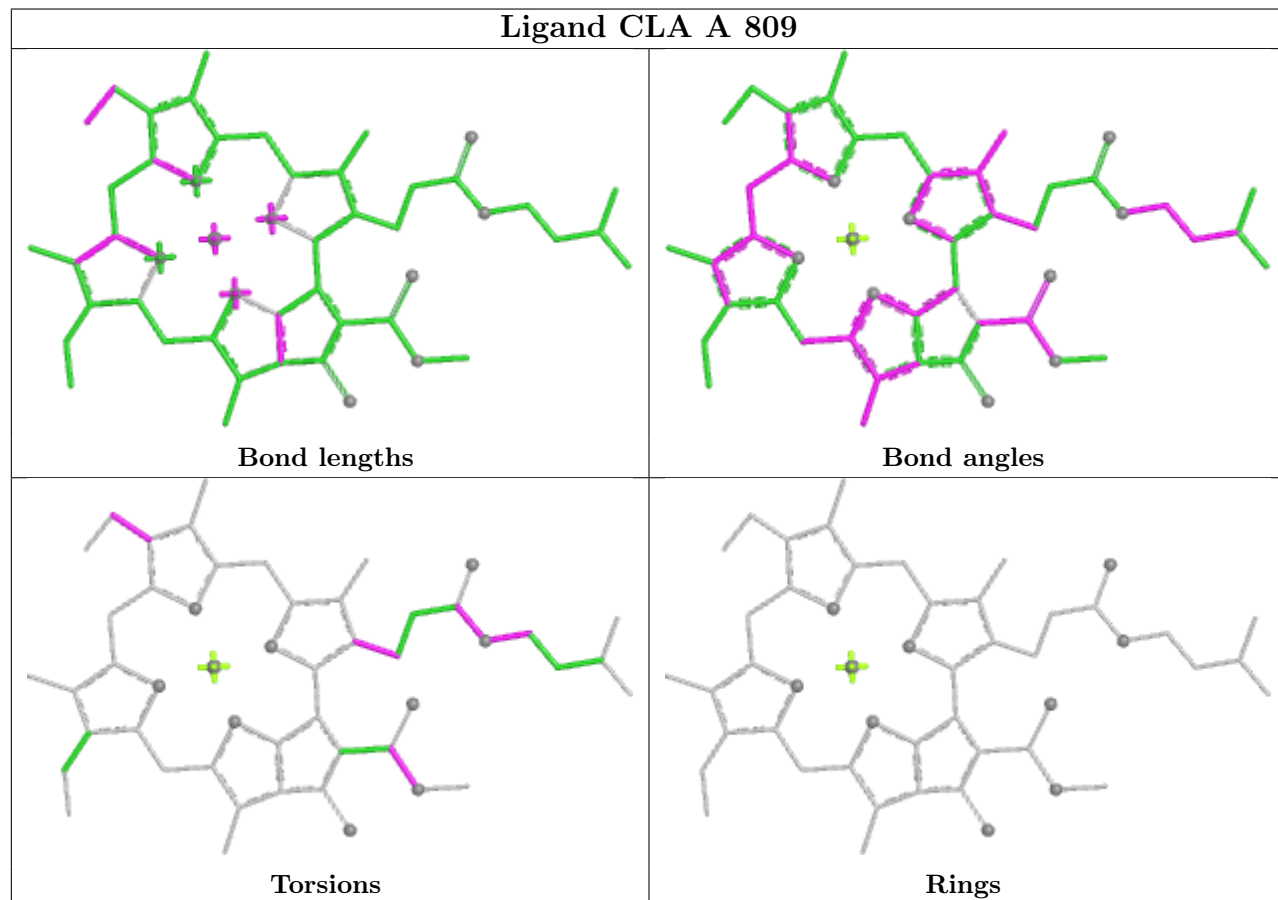


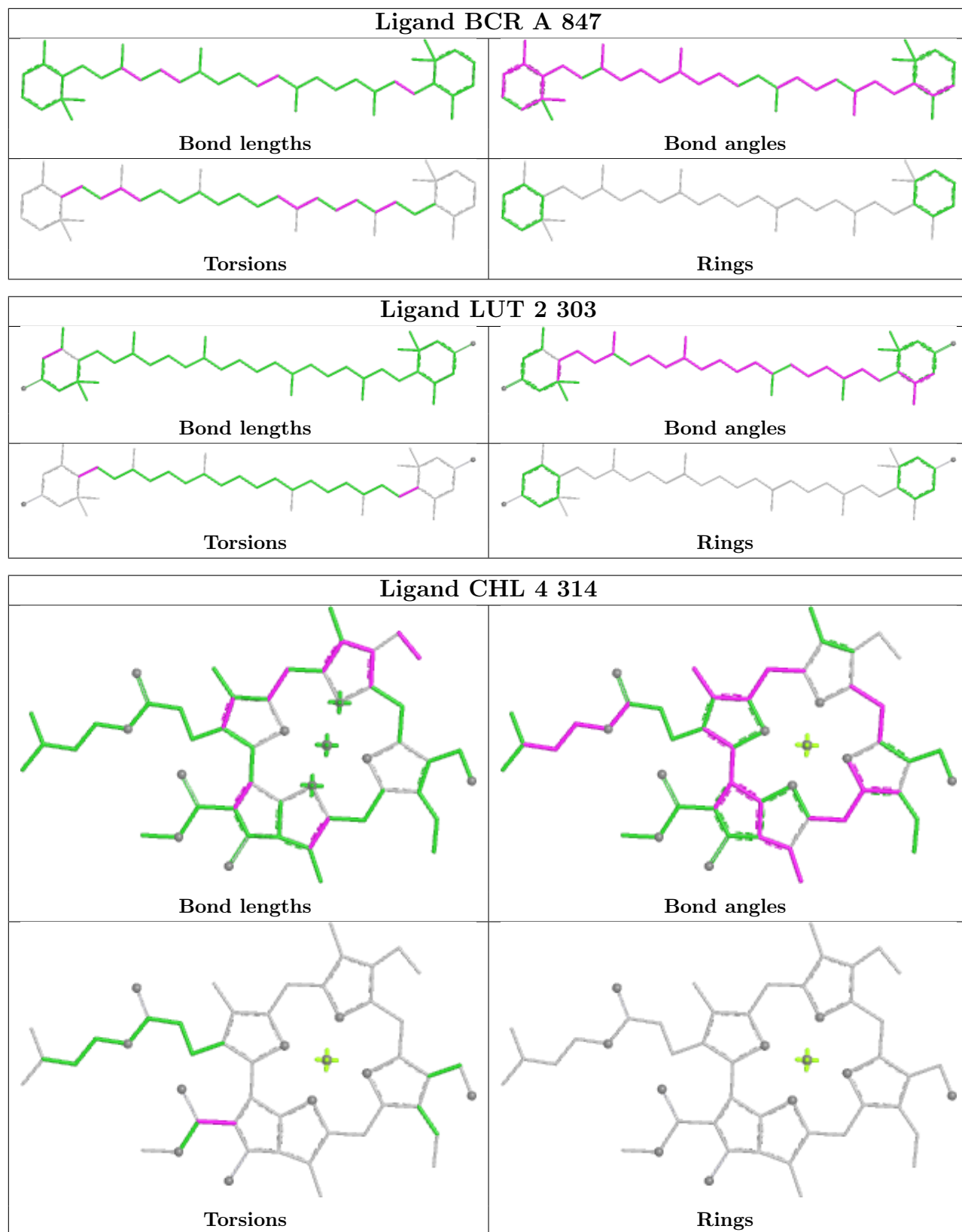


Ligand CLA A 827

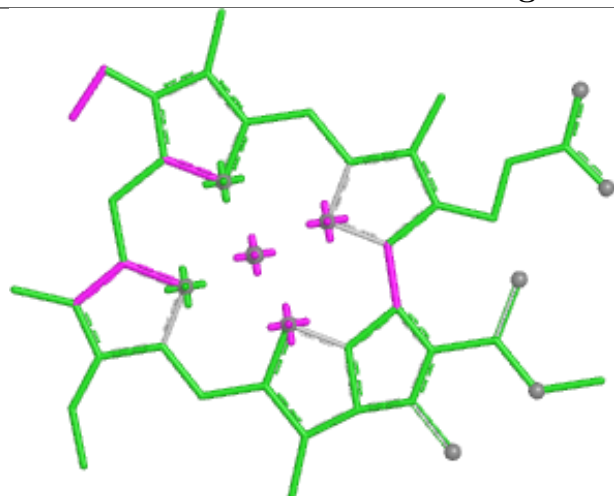


Ligand CLA A 809

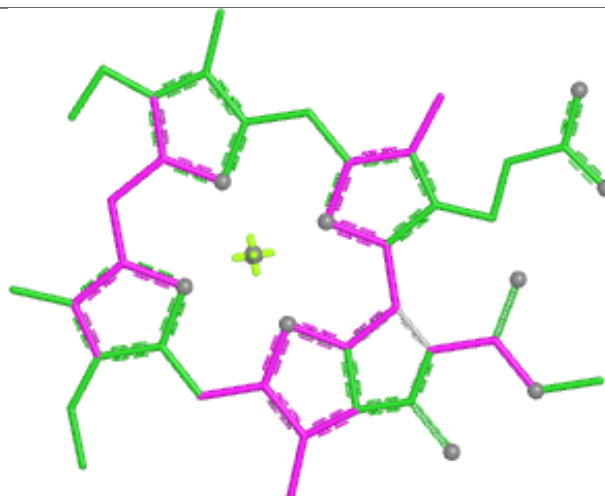




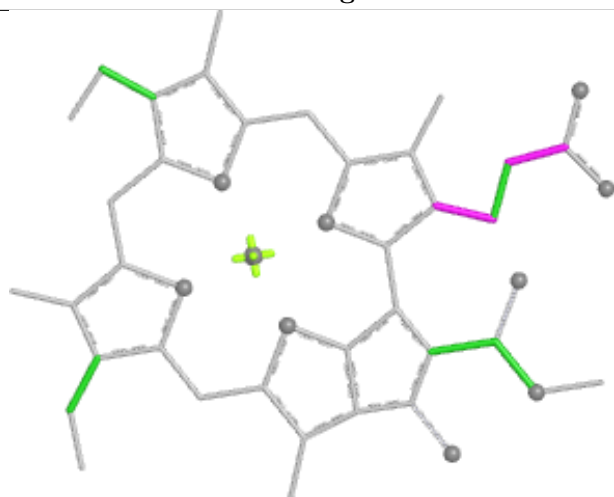
Ligand CLA 3 301



Bond lengths



Bond angles

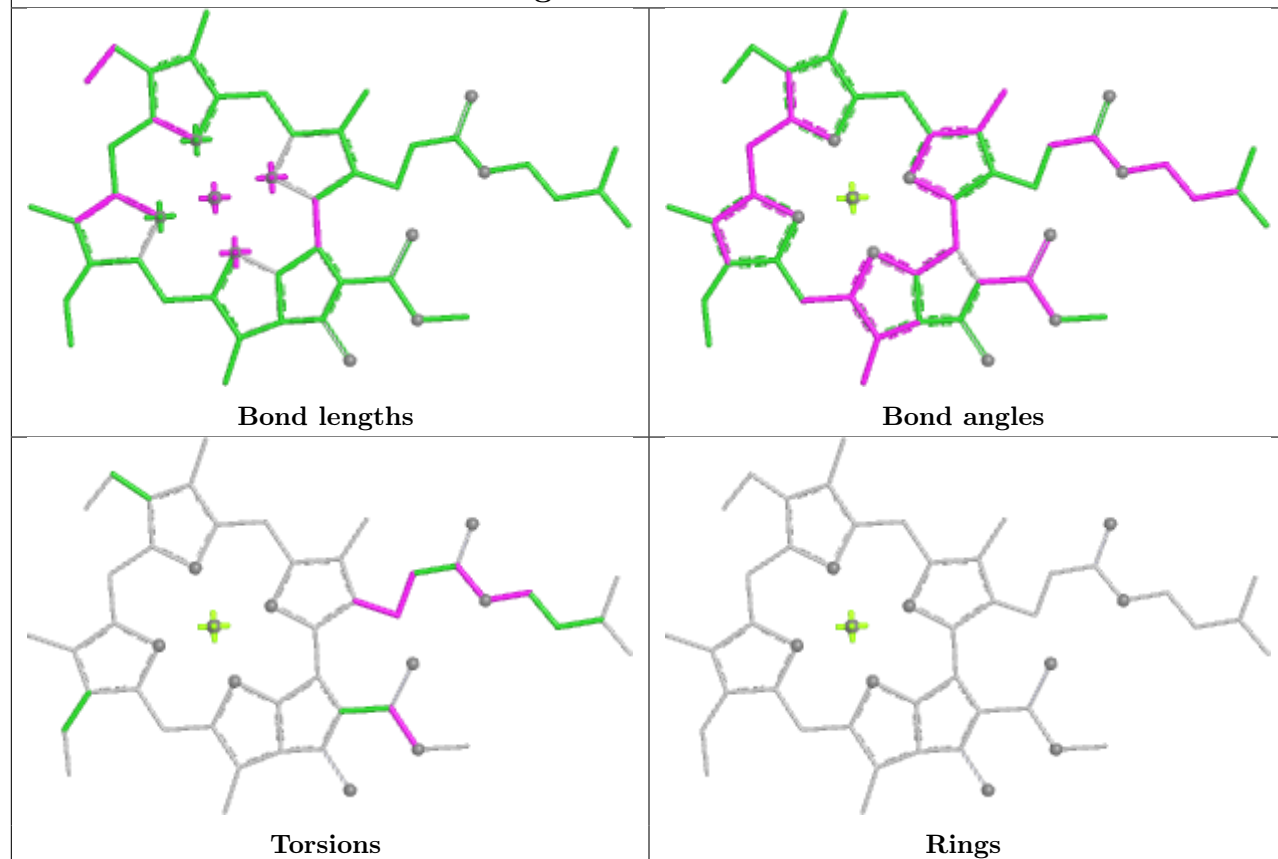


Torsions

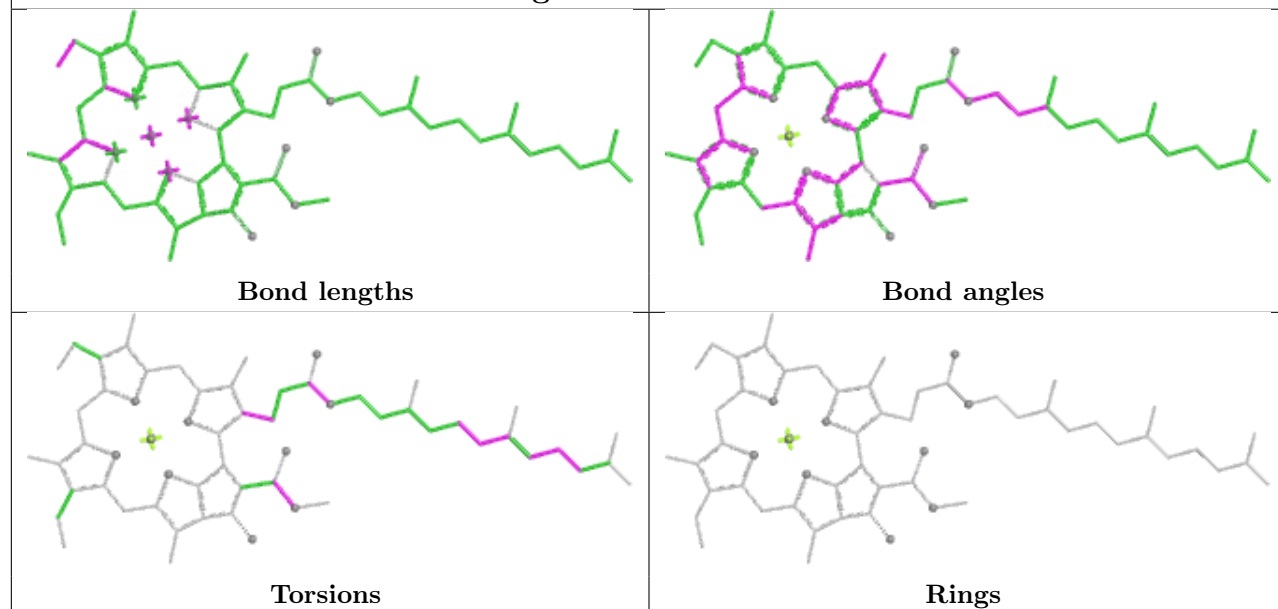


Rings

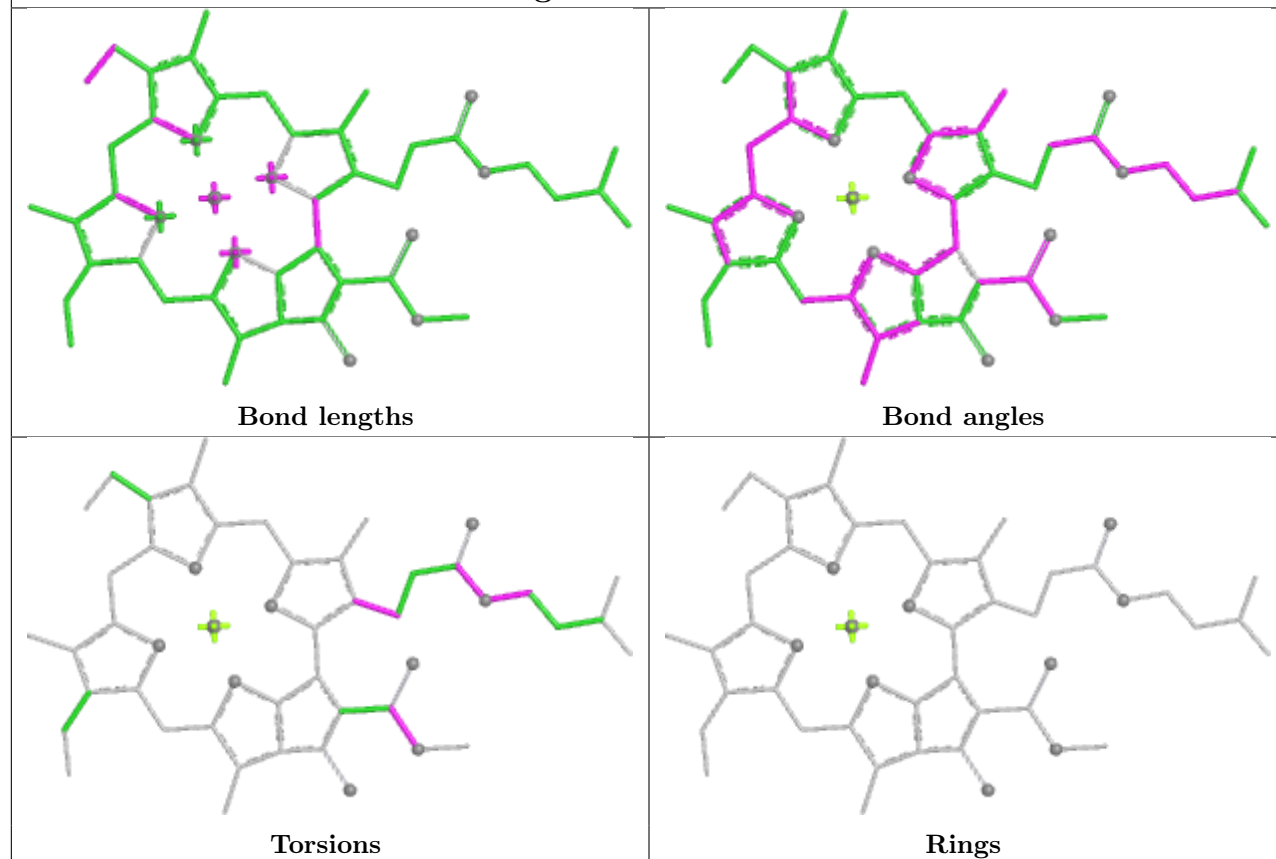
Ligand CLA L 306



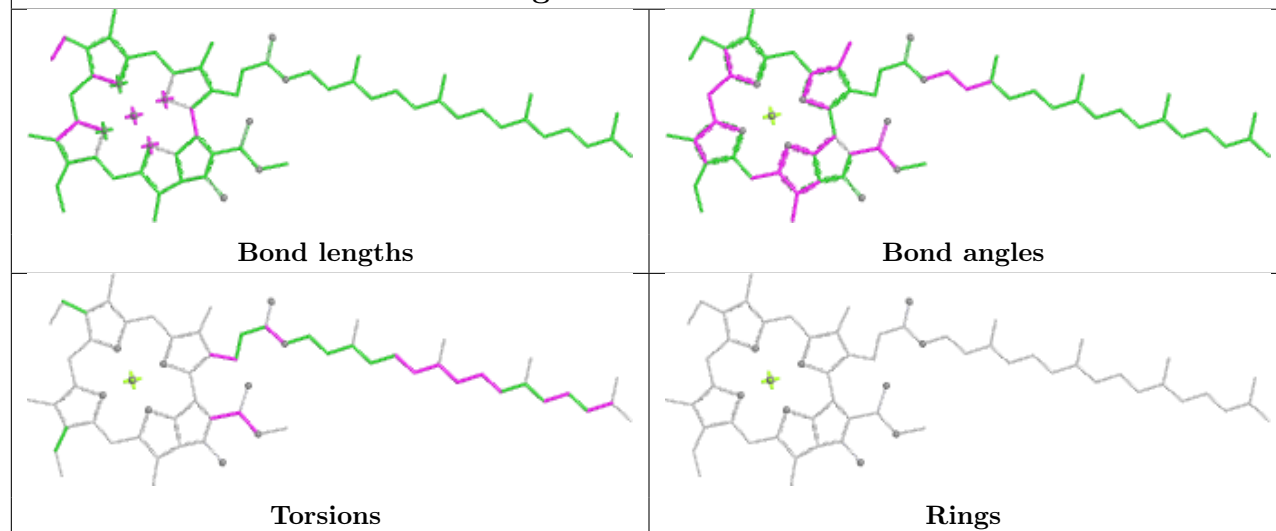
Ligand CLA B 812



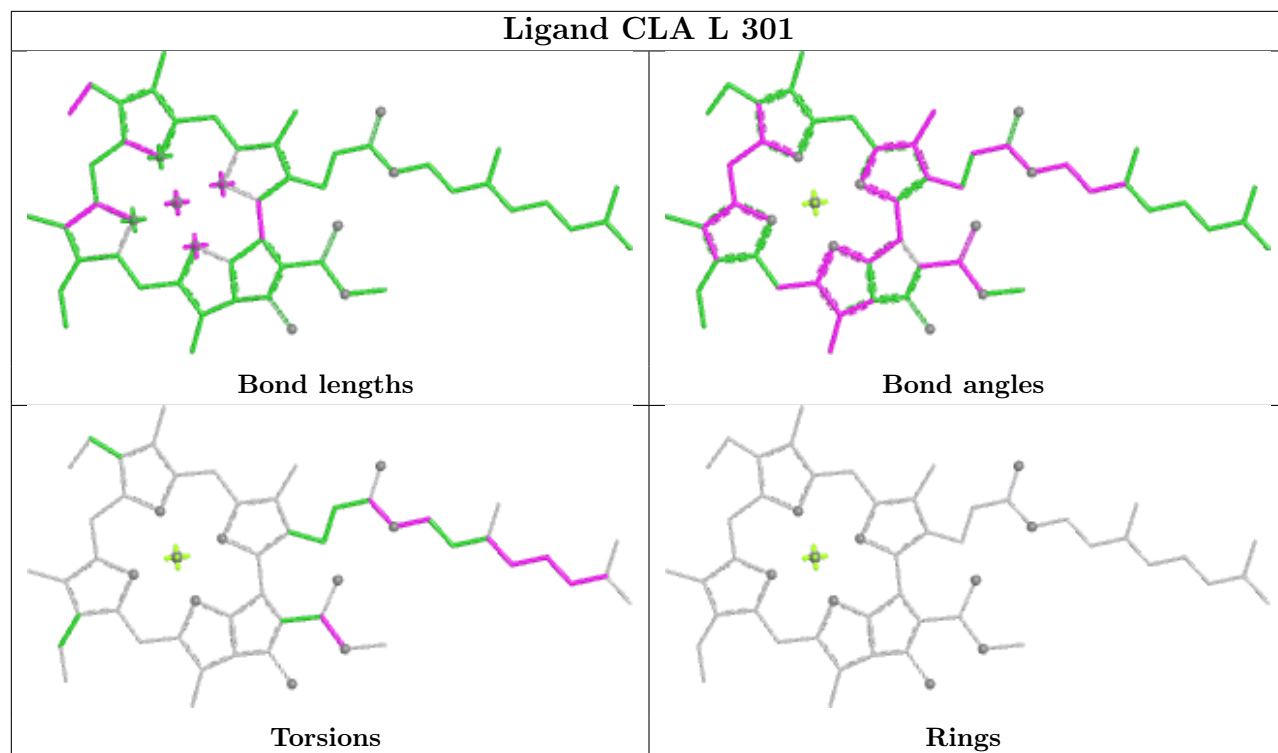
Ligand CLA L 304



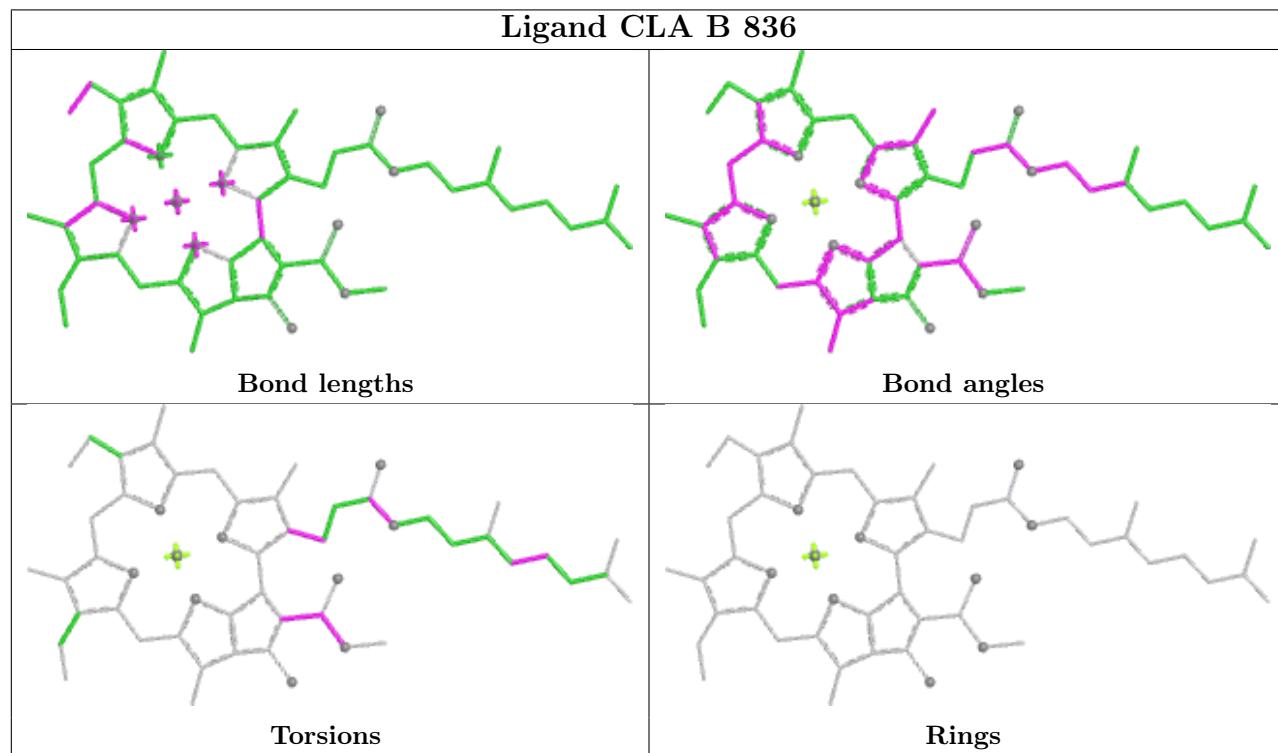
Ligand CLA B 826

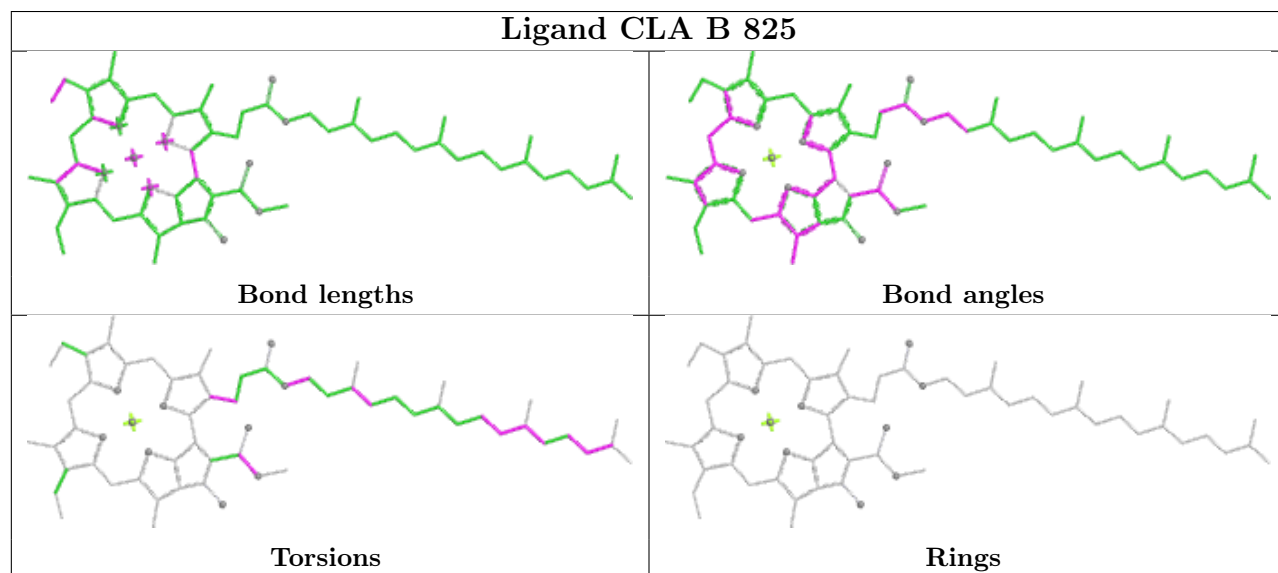
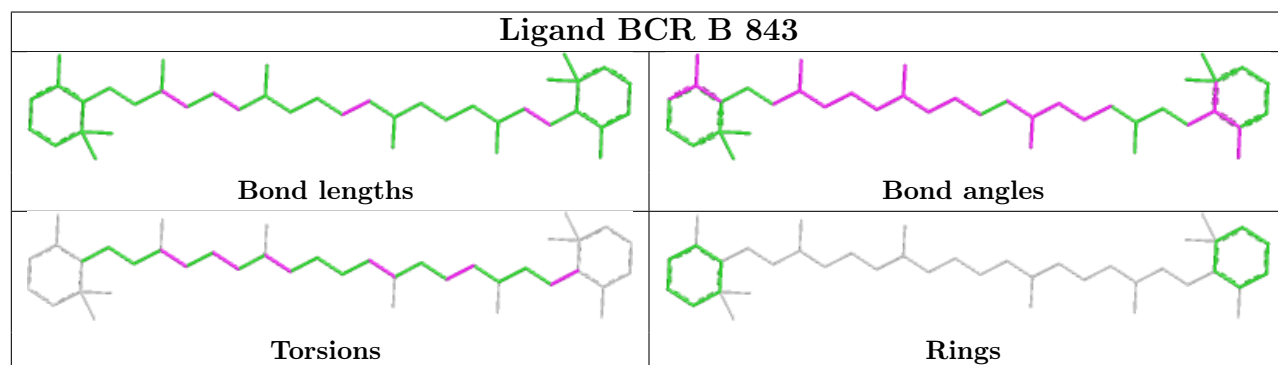
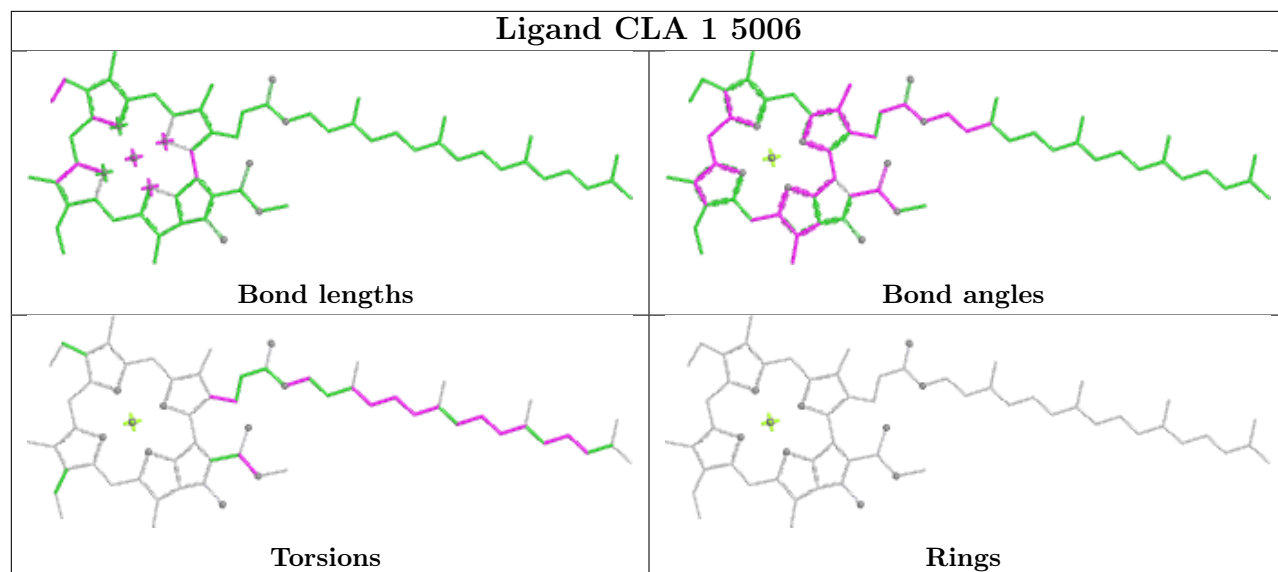


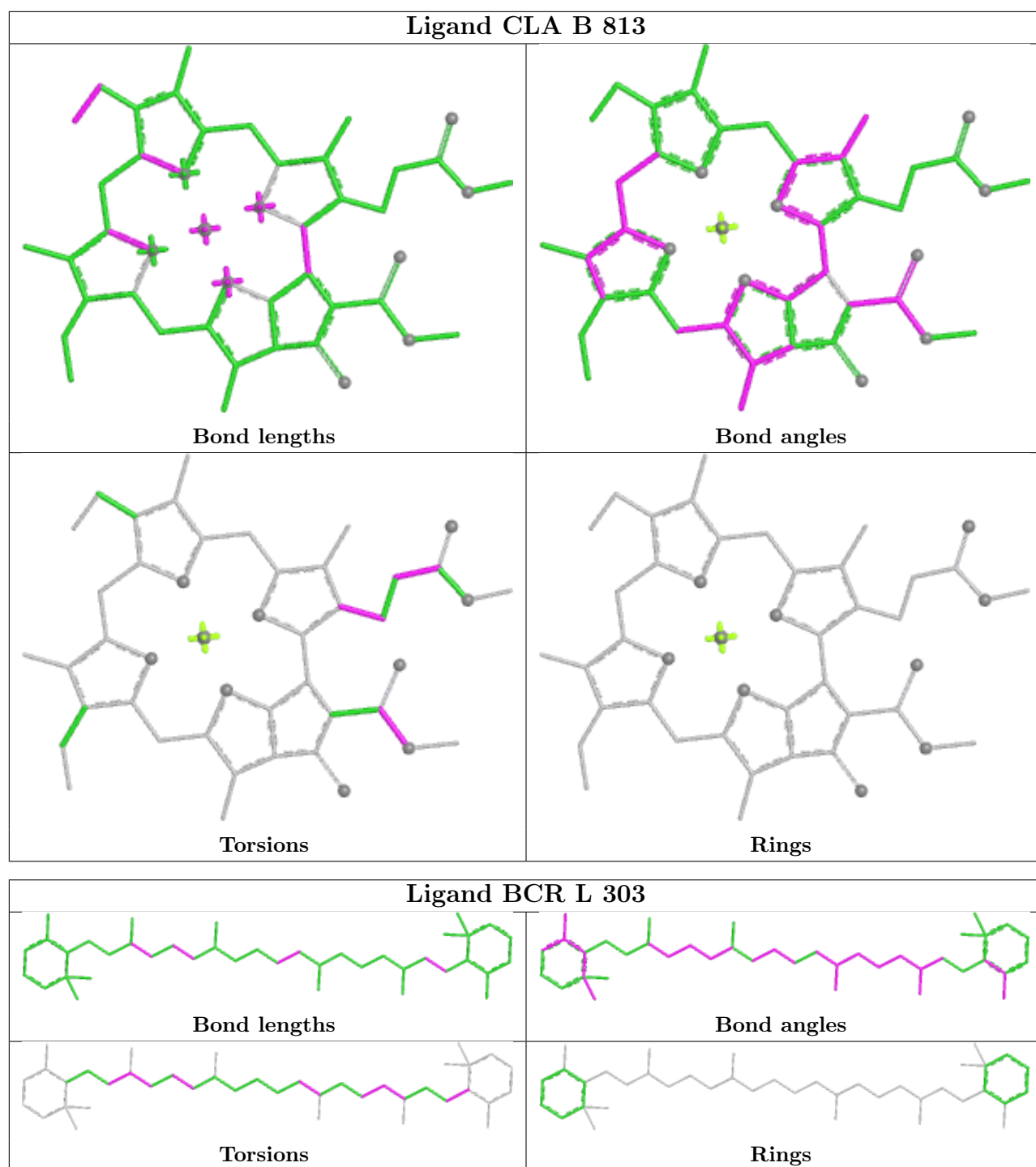
Ligand CLA L 301

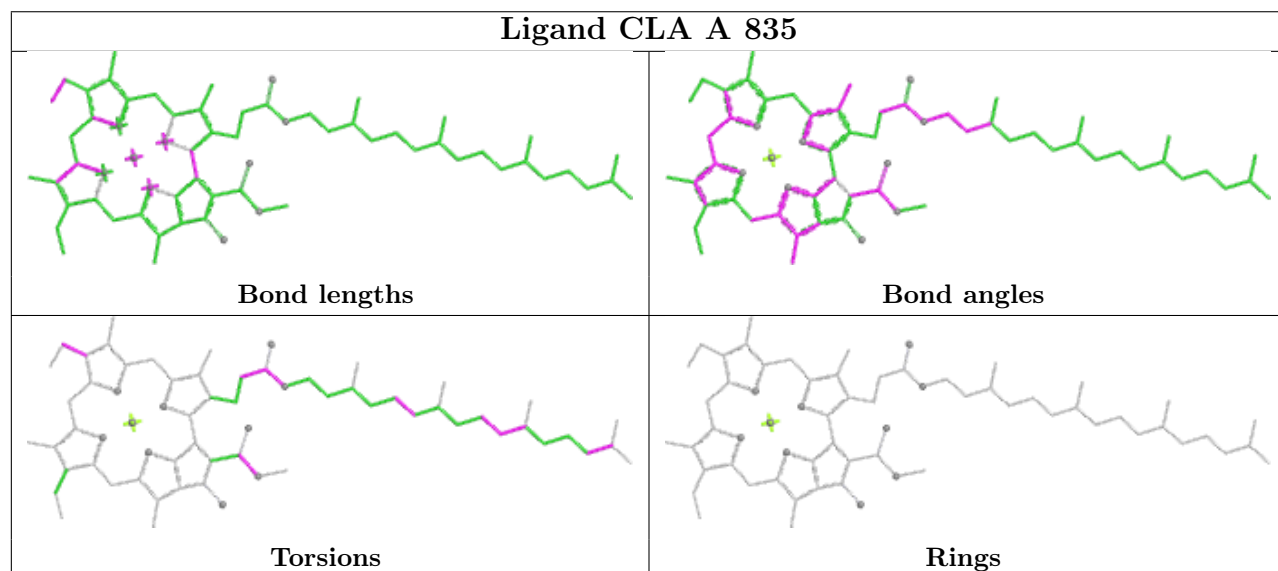
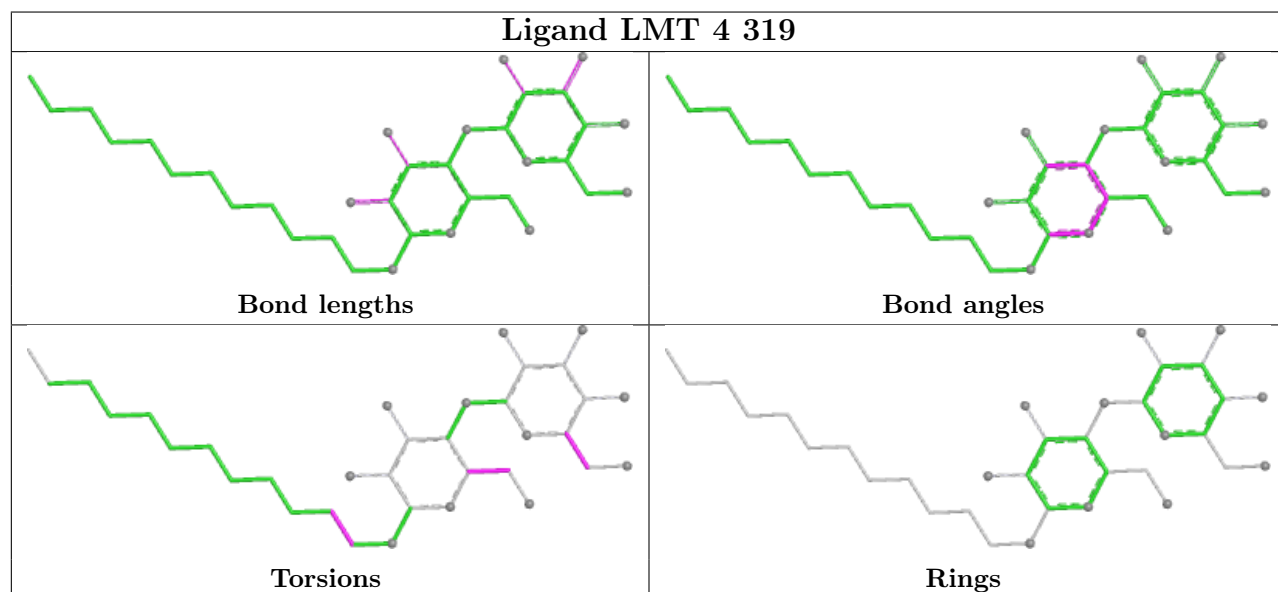
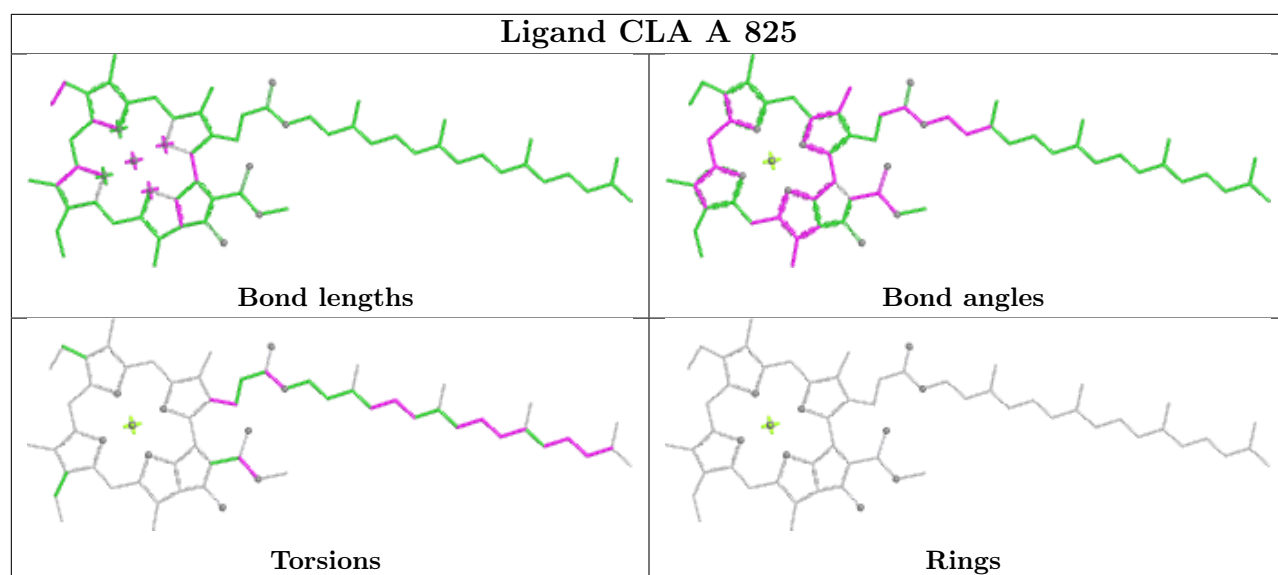


Ligand CLA B 836

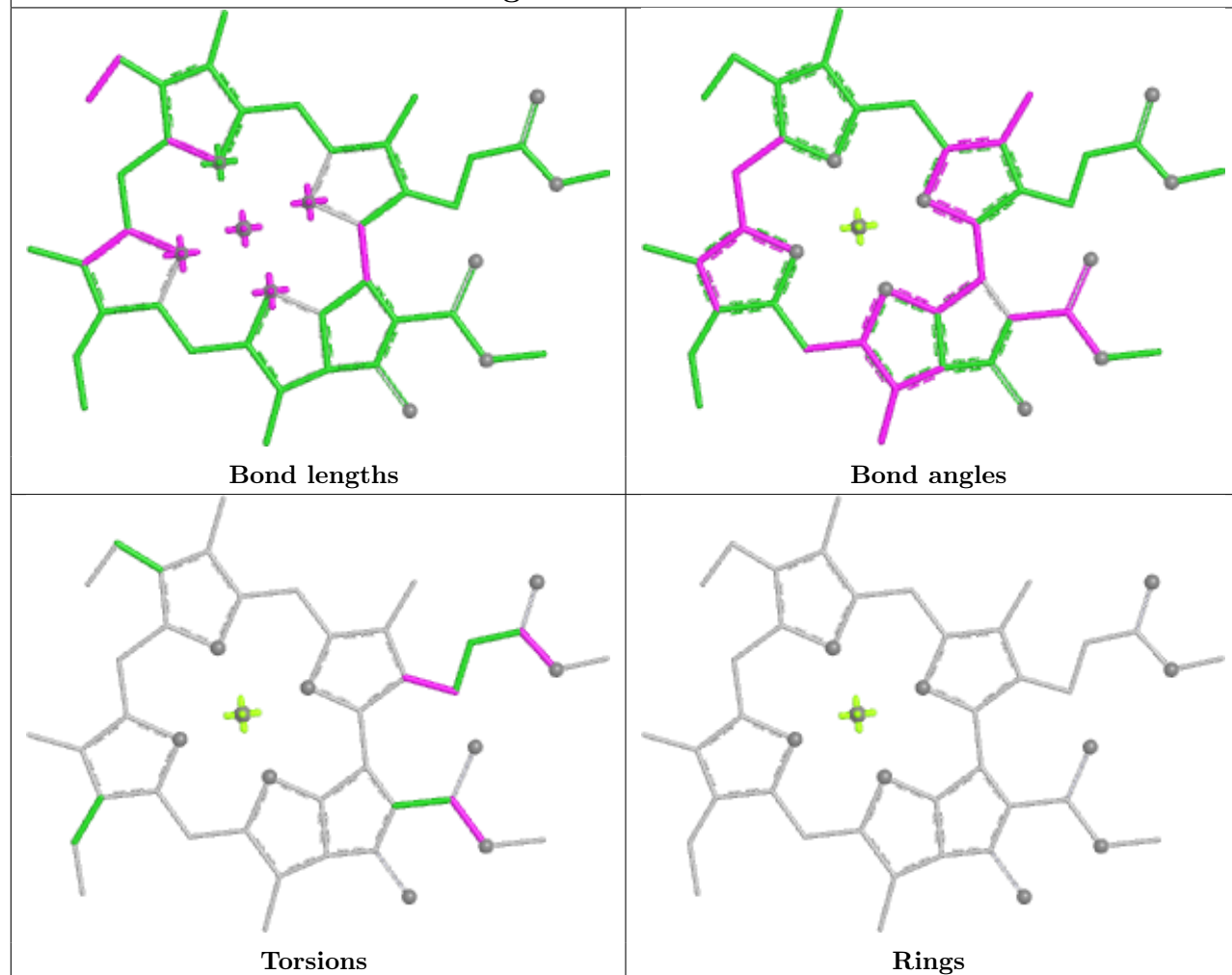




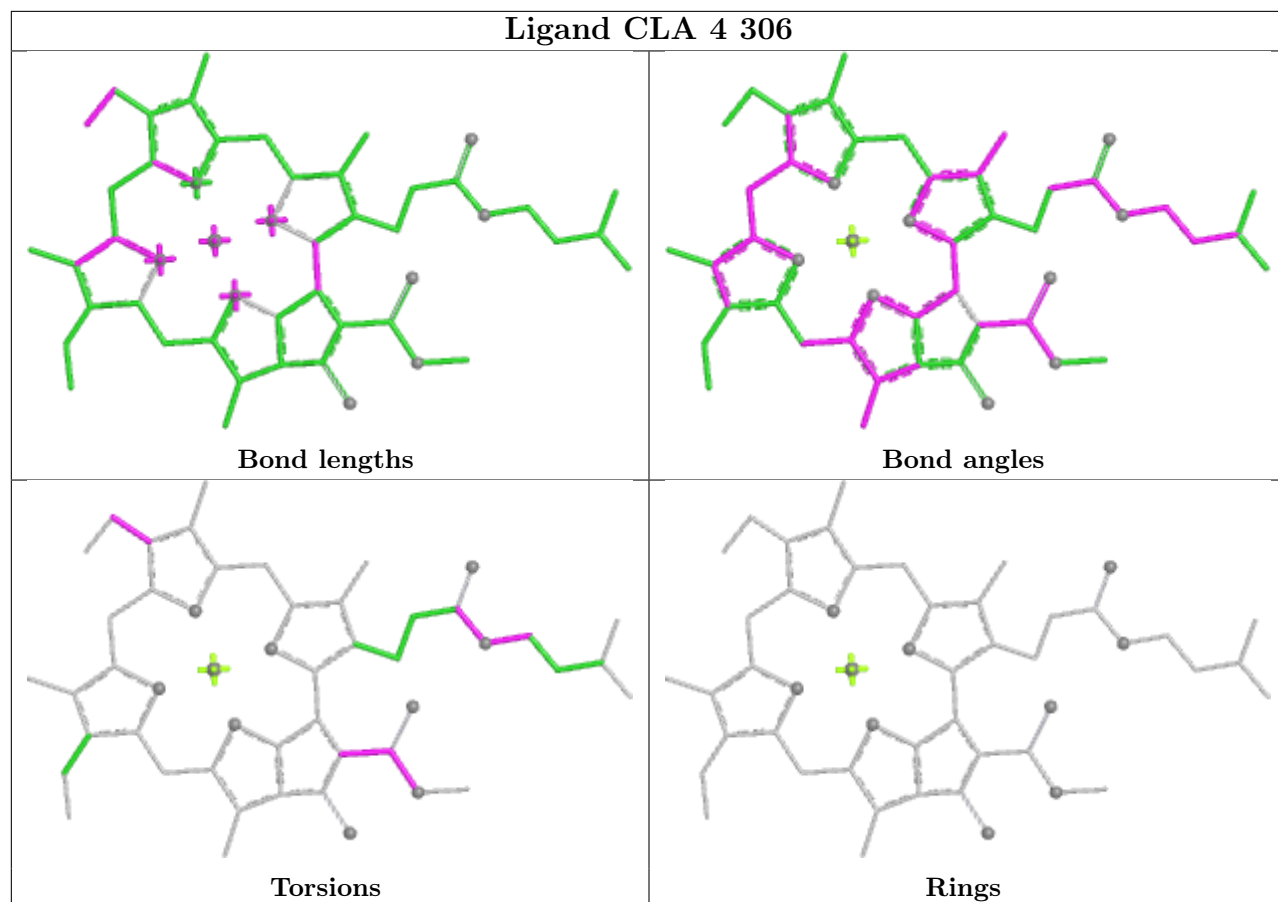




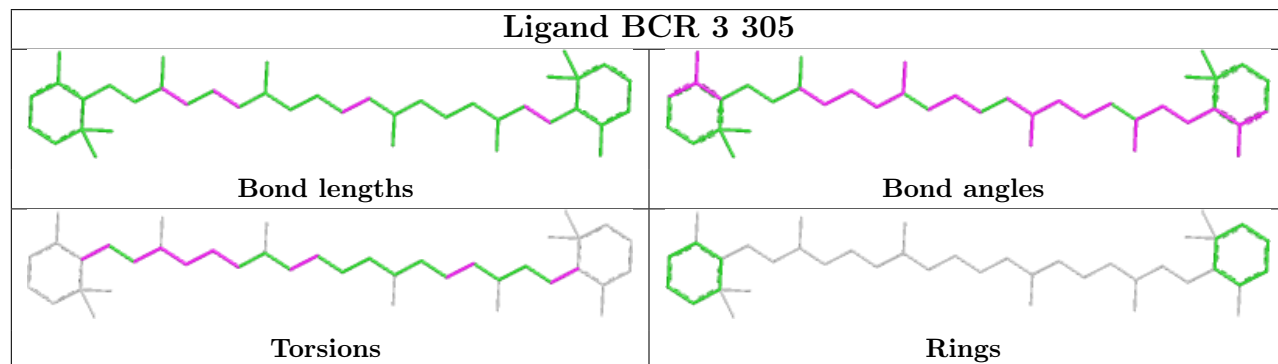
Ligand CLA G 1602

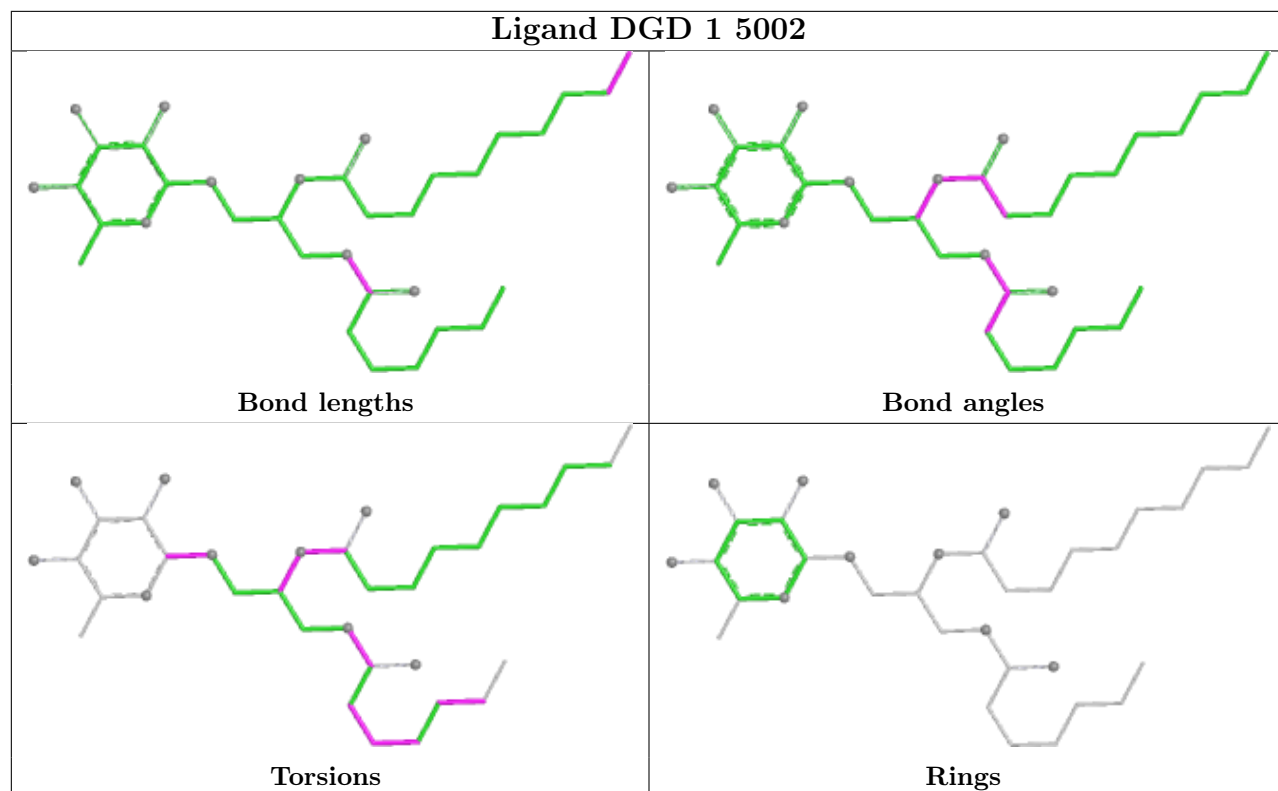


Ligand CLA 4 306

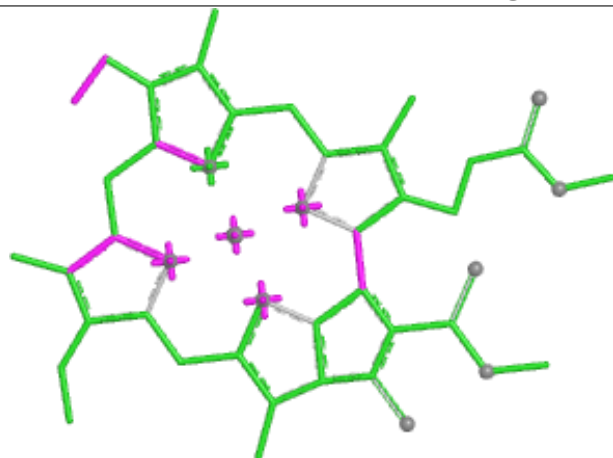


Ligand BCR 3 305

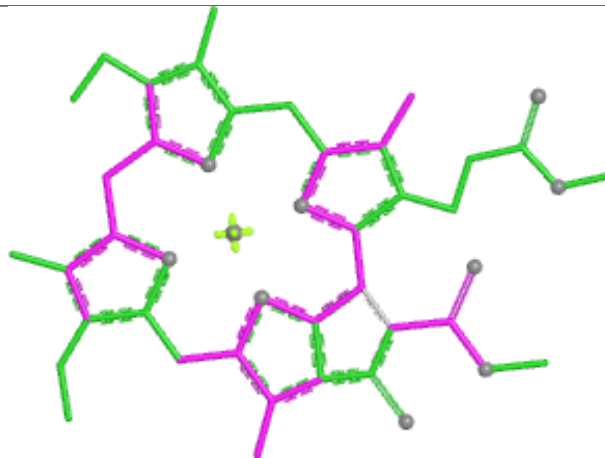




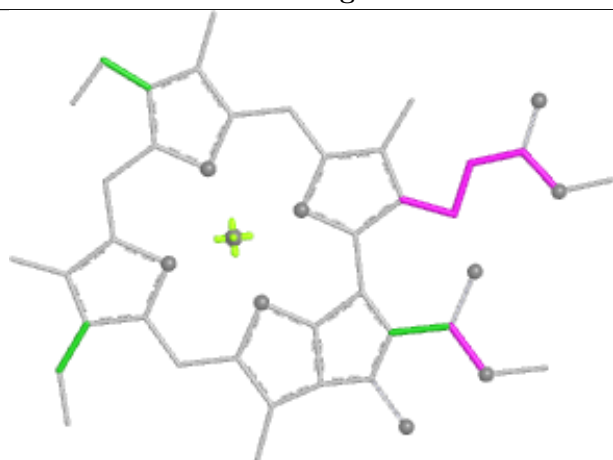
Ligand CLA K 1404



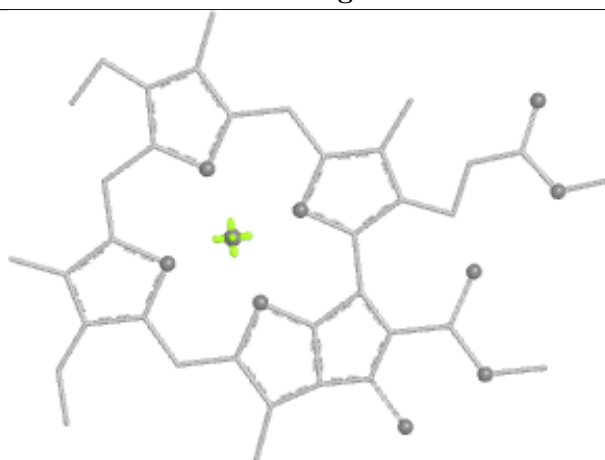
Bond lengths



Bond angles

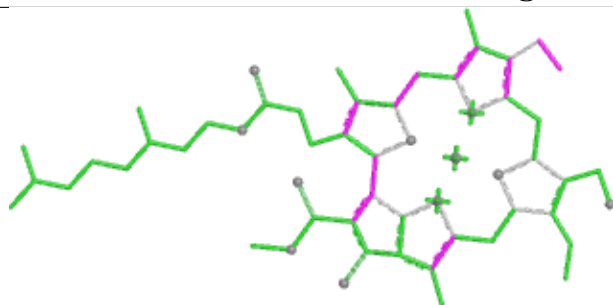


Torsions

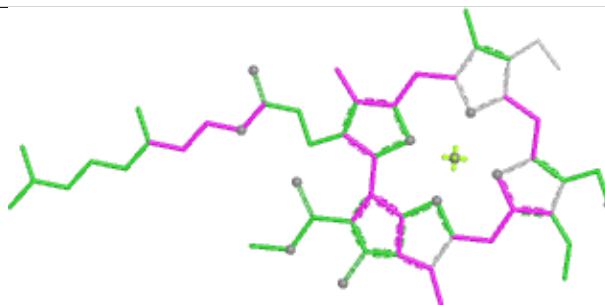


Rings

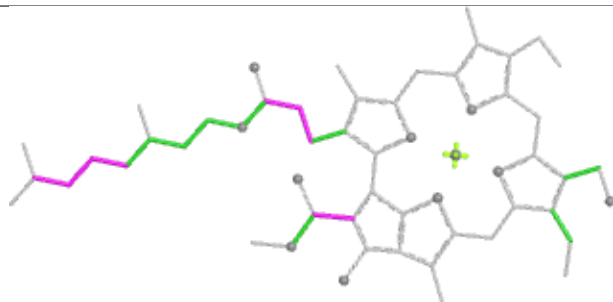
Ligand CHL 2 315



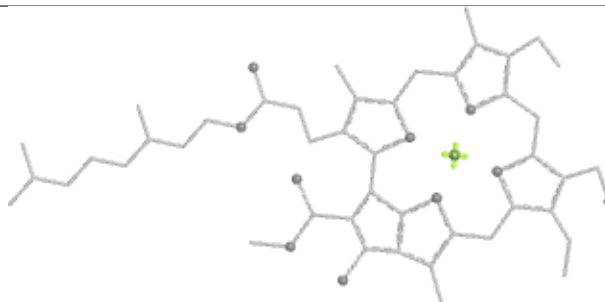
Bond lengths



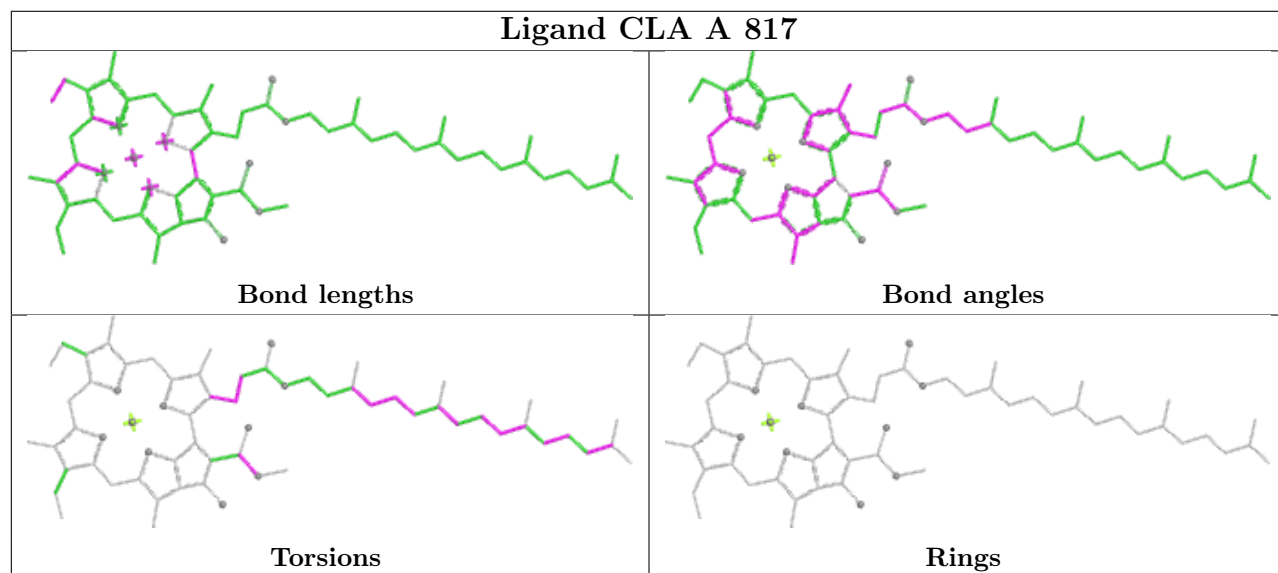
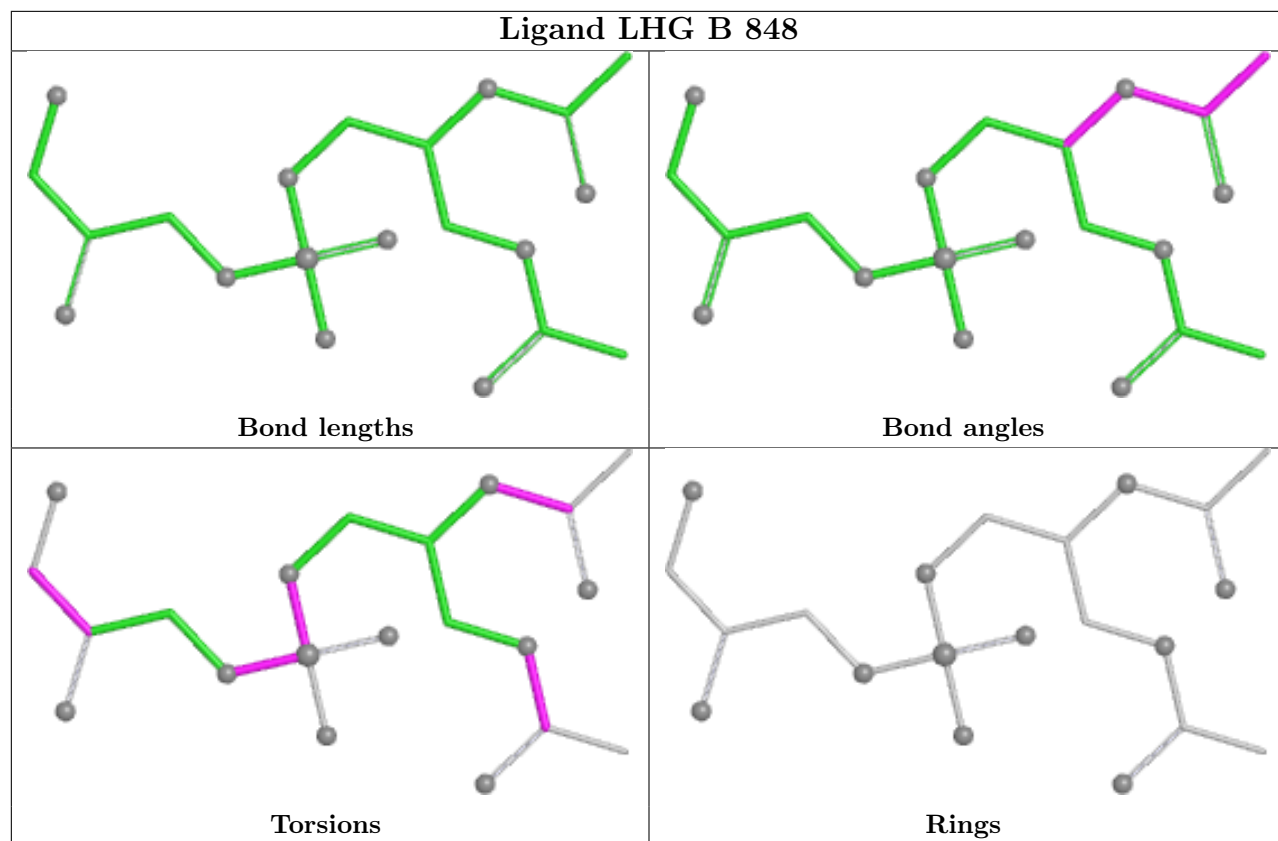
Bond angles



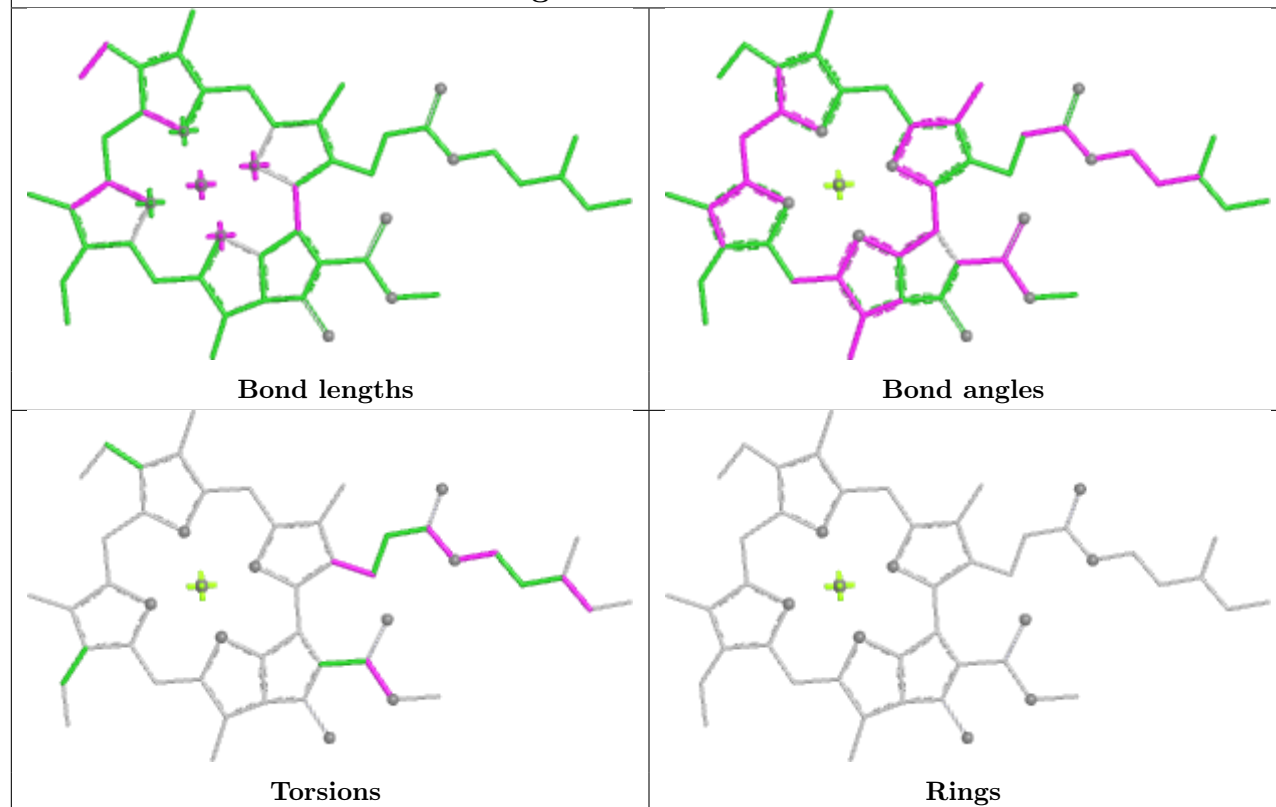
Torsions



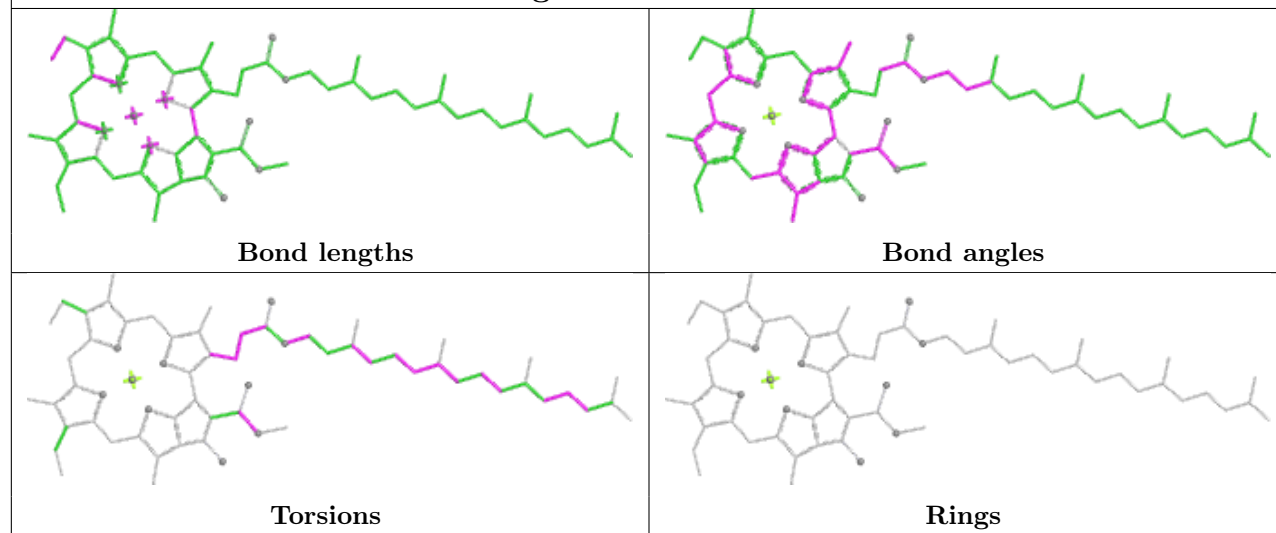
Rings

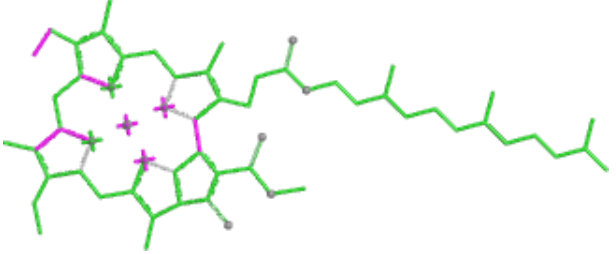
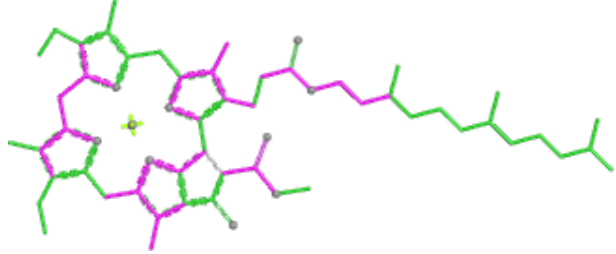
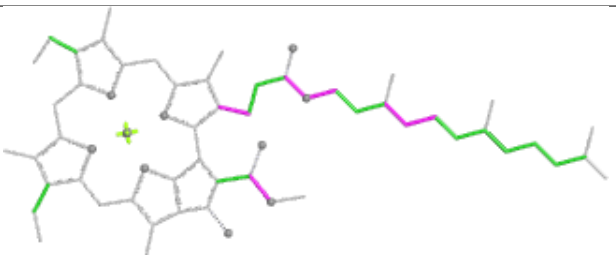
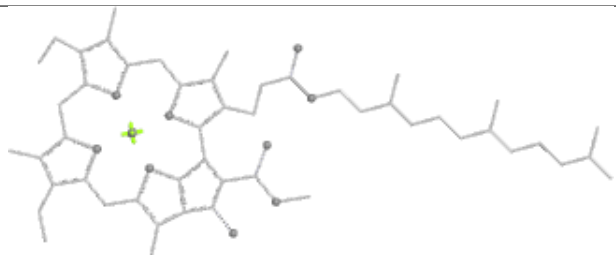
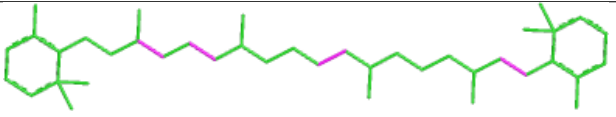
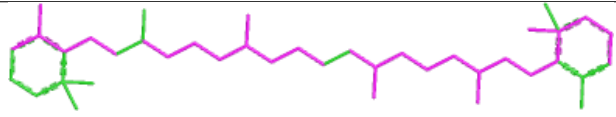
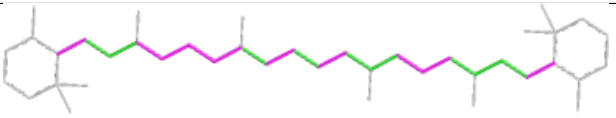
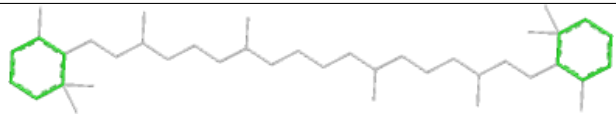
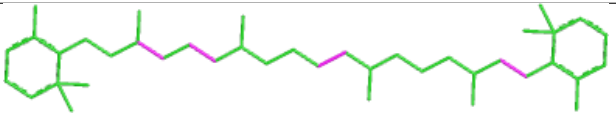
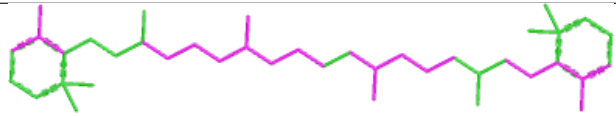
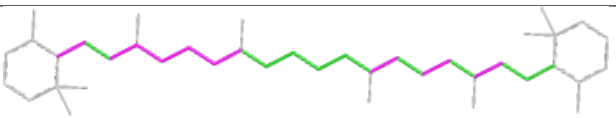
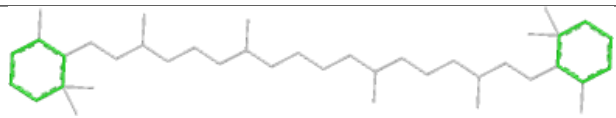


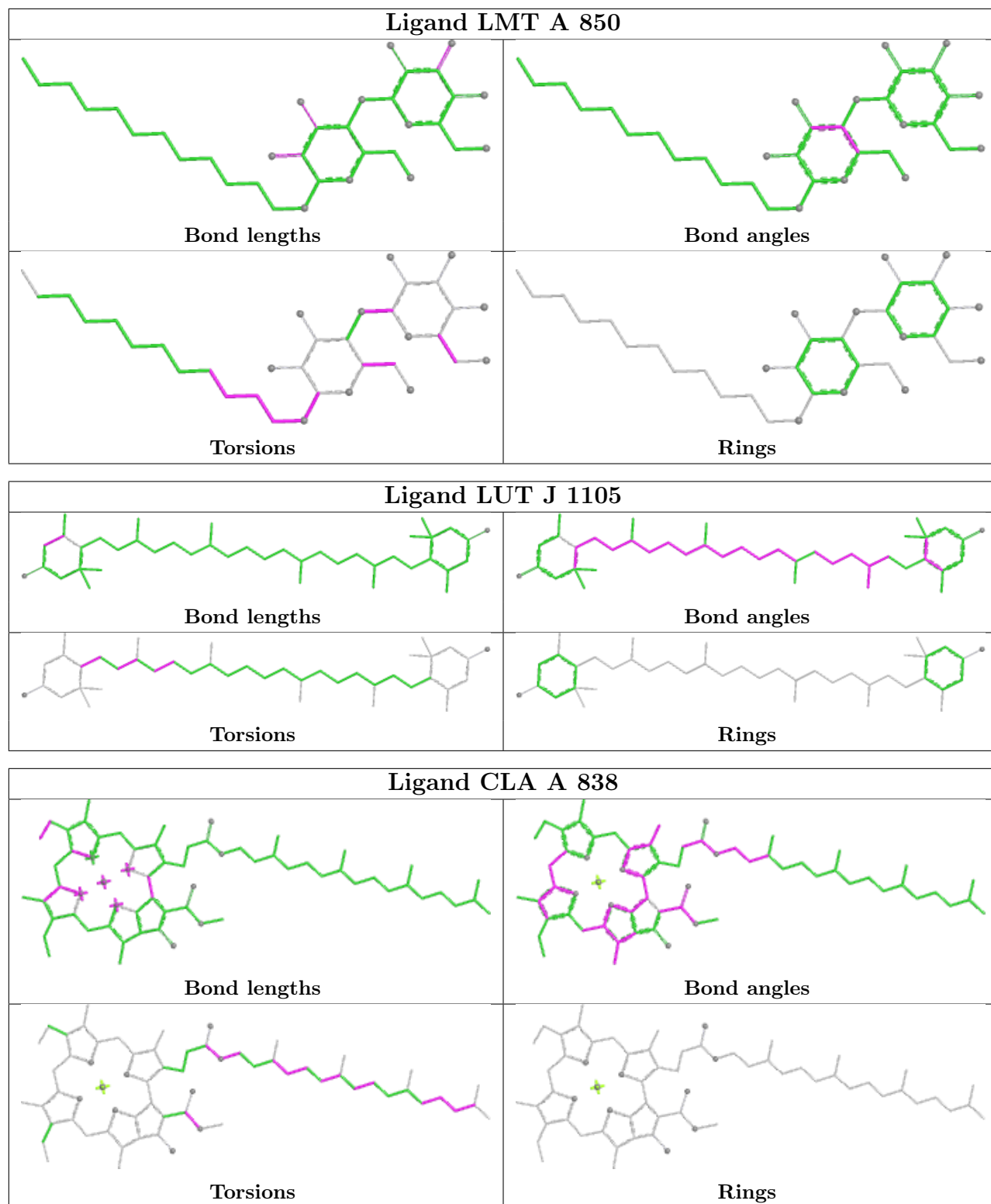
Ligand CLA A 834

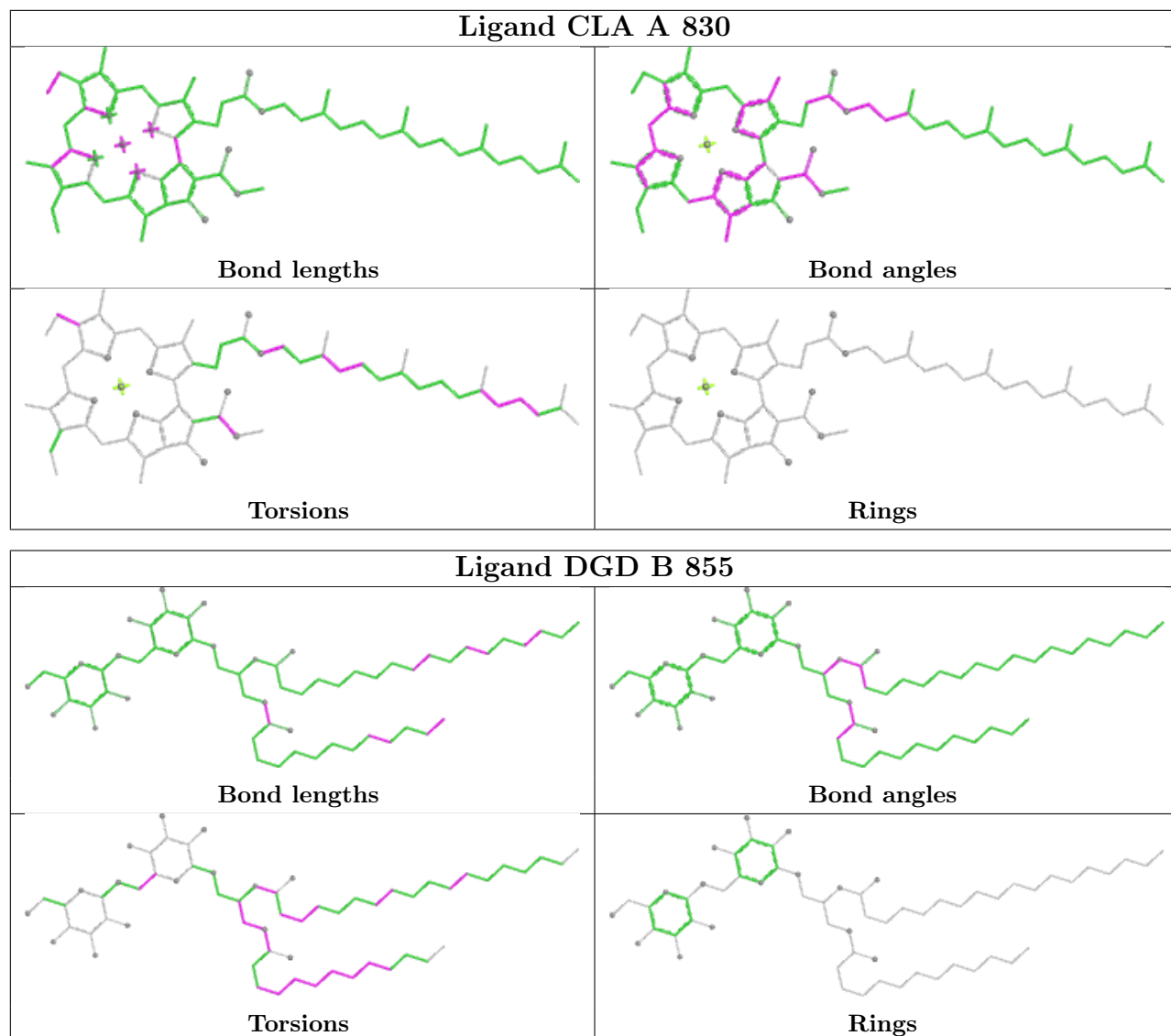


Ligand CLA B 840

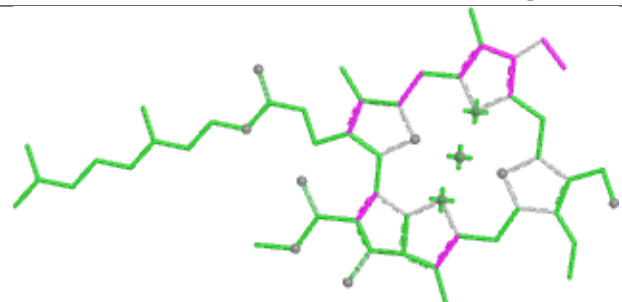


Ligand CLA A 821	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 845	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR J 1104	
 Bond lengths	 Bond angles
 Torsions	 Rings

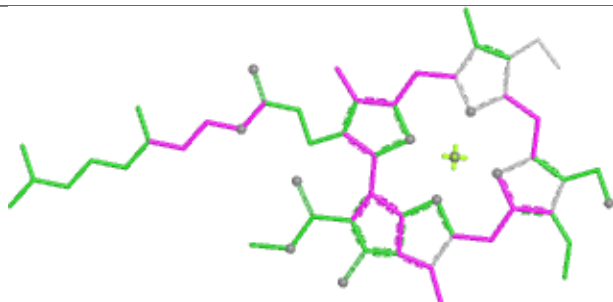




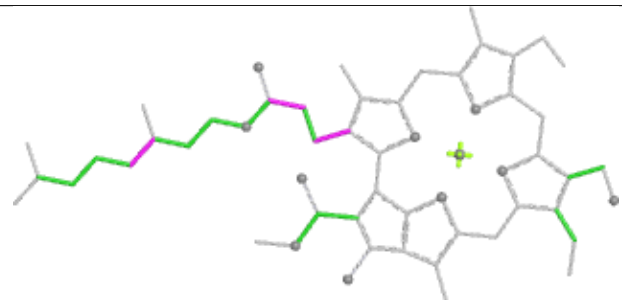
Ligand CHL 4 302



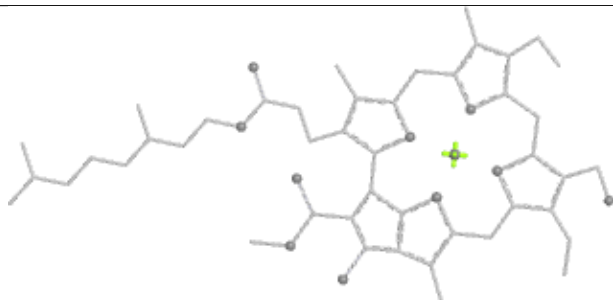
Bond lengths



Bond angles

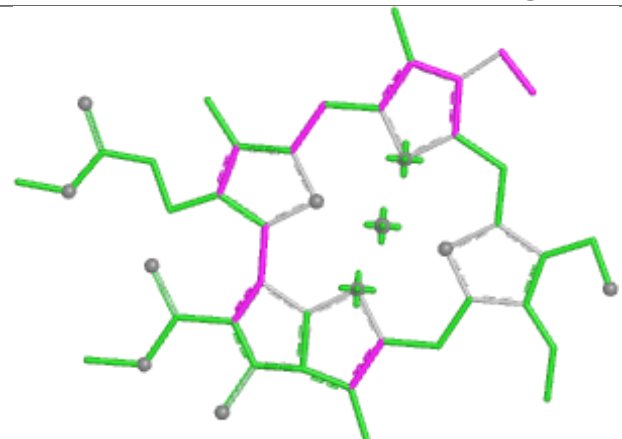


Torsions

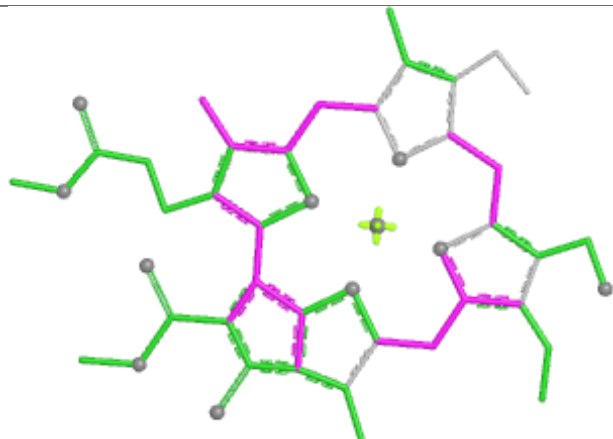


Rings

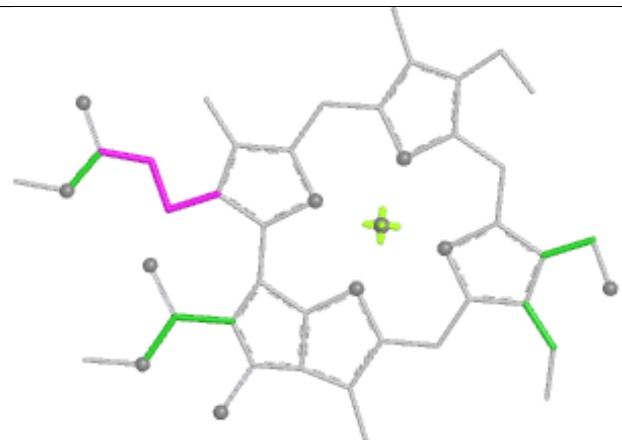
Ligand CHL 3 316



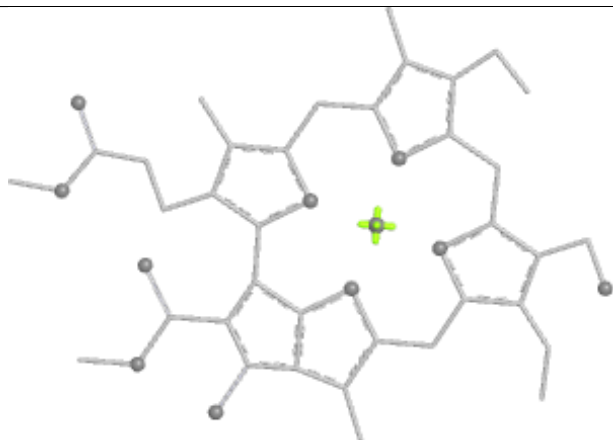
Bond lengths



Bond angles

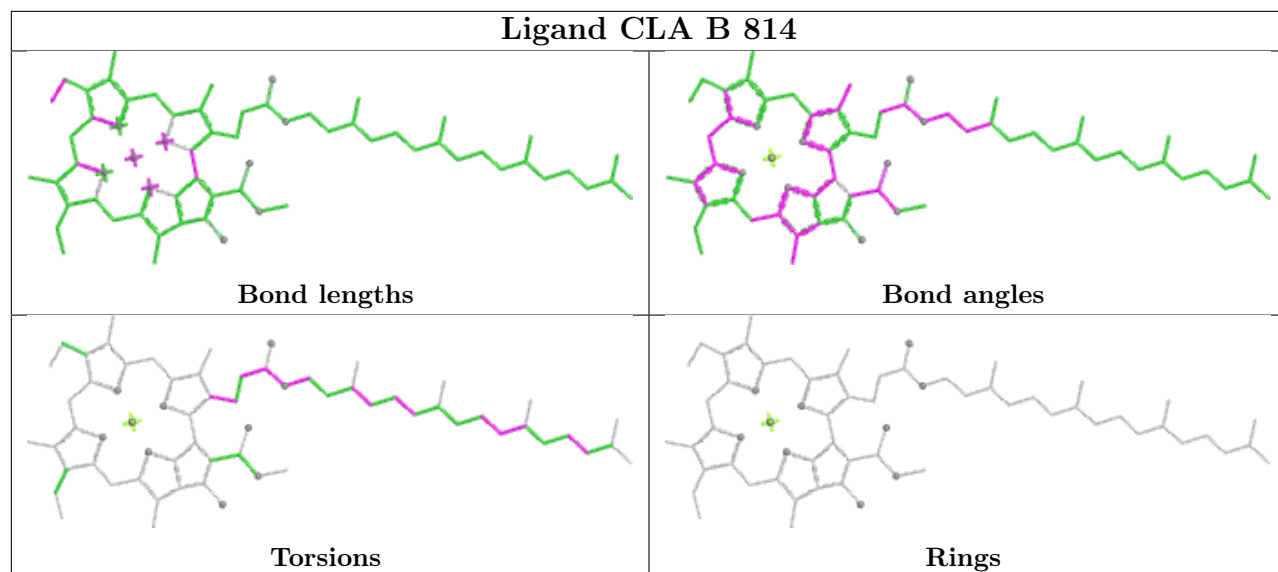


Torsions

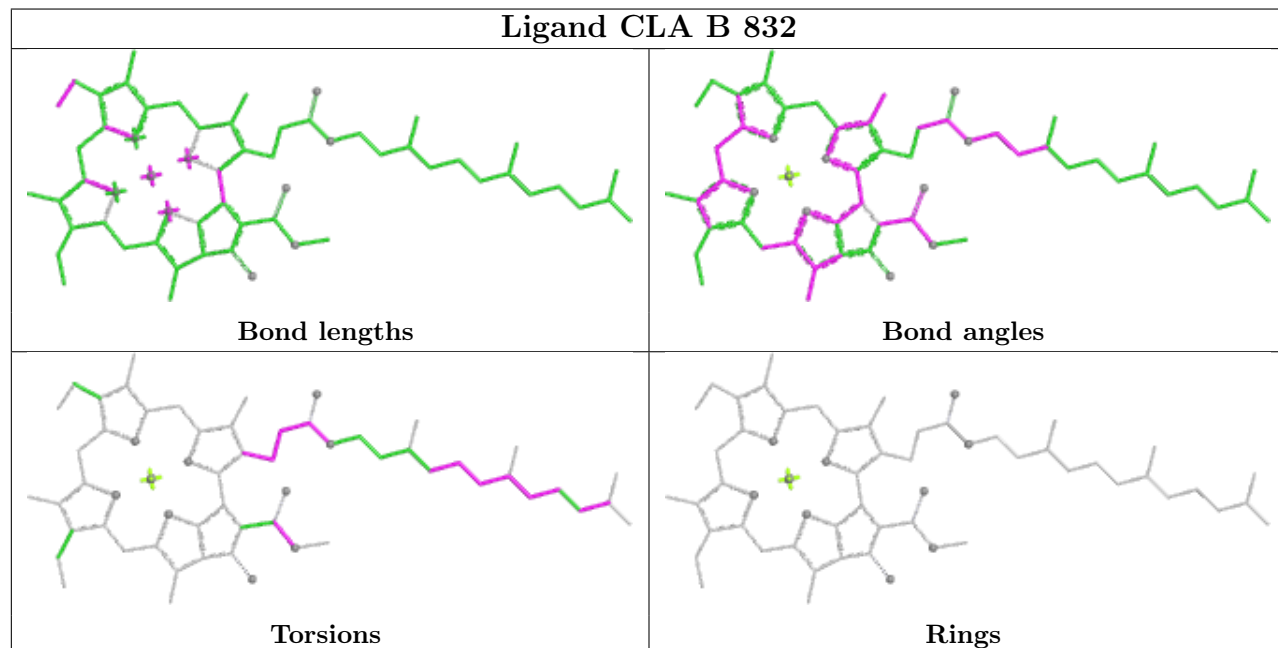


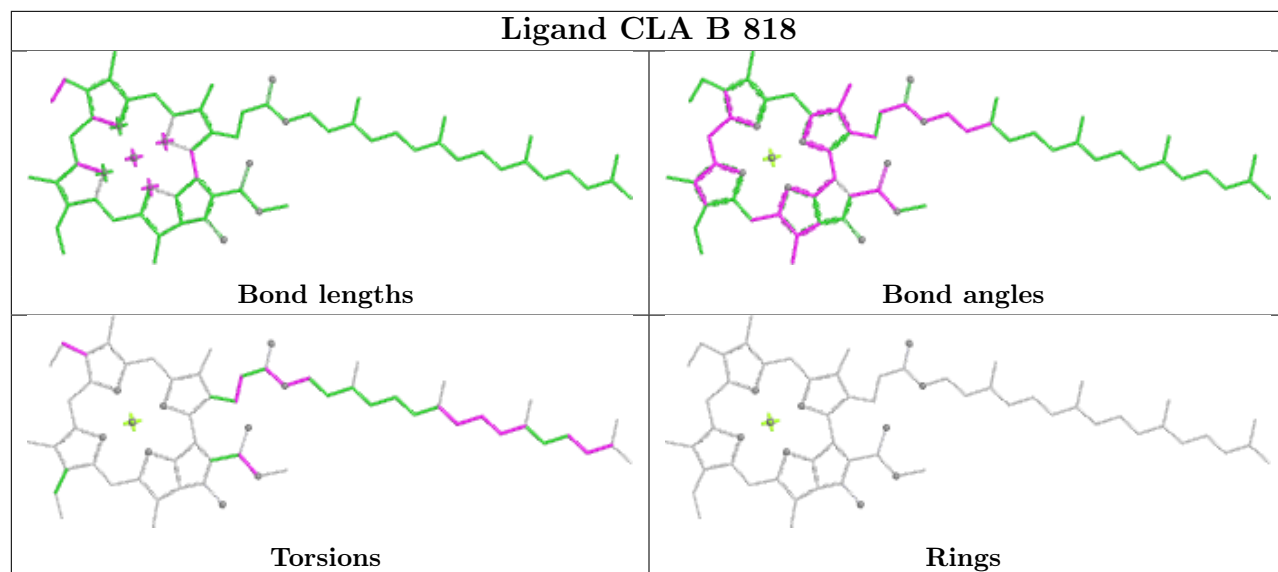
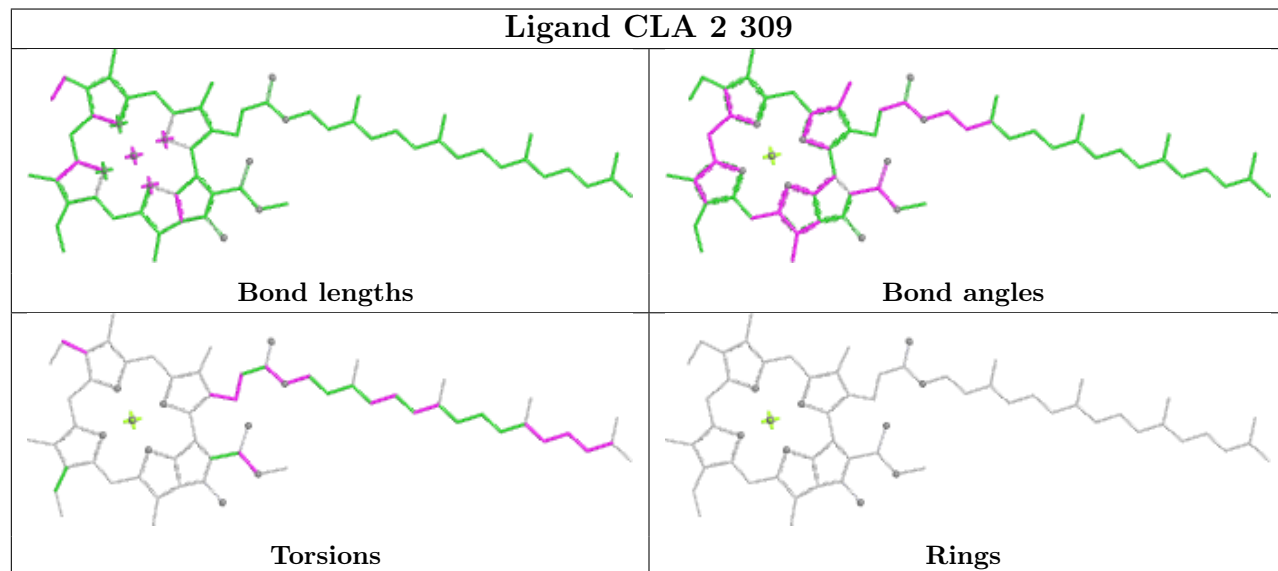
Rings

Ligand CLA B 814

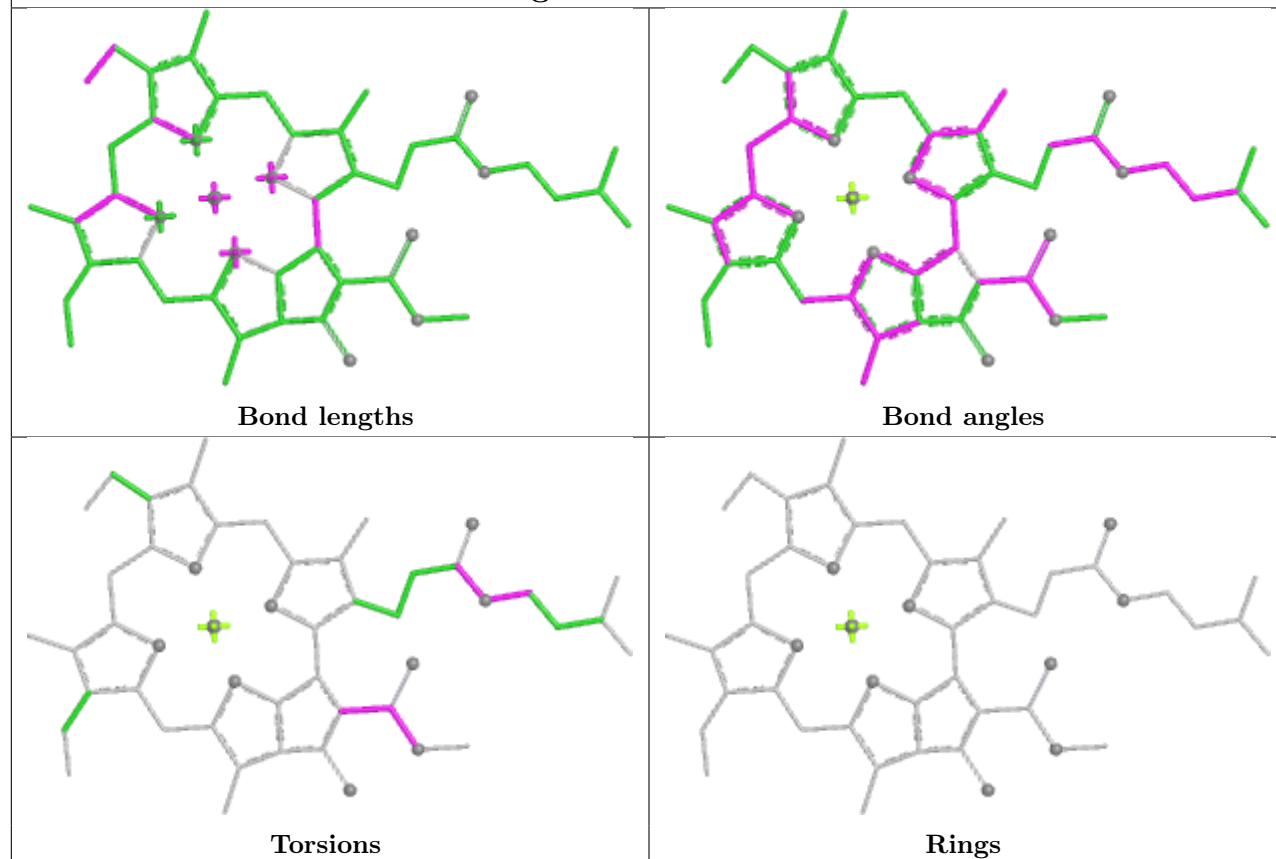


Ligand CLA B 832

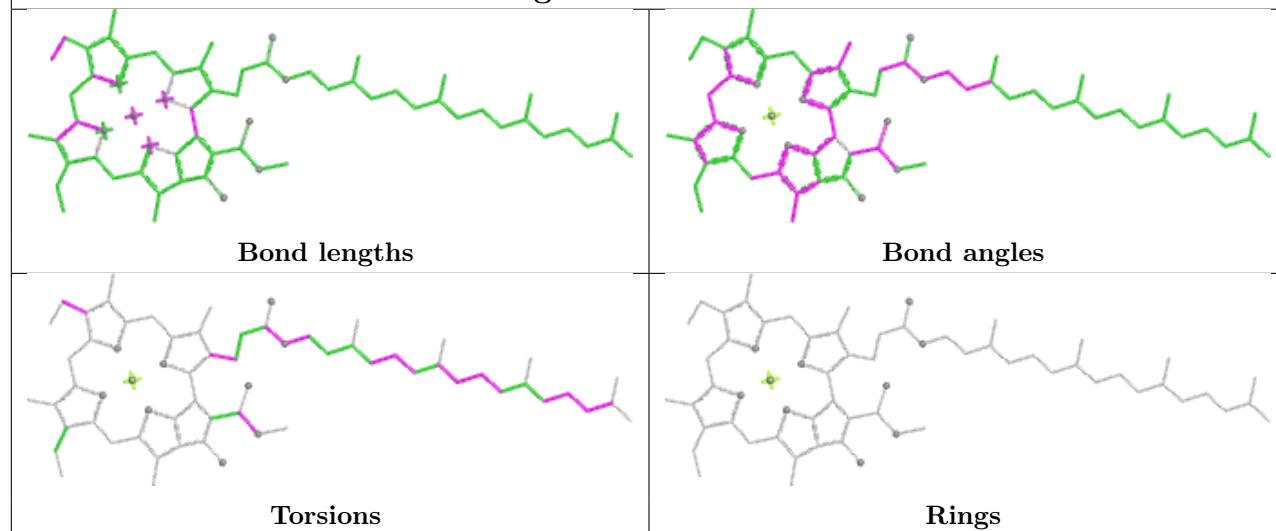


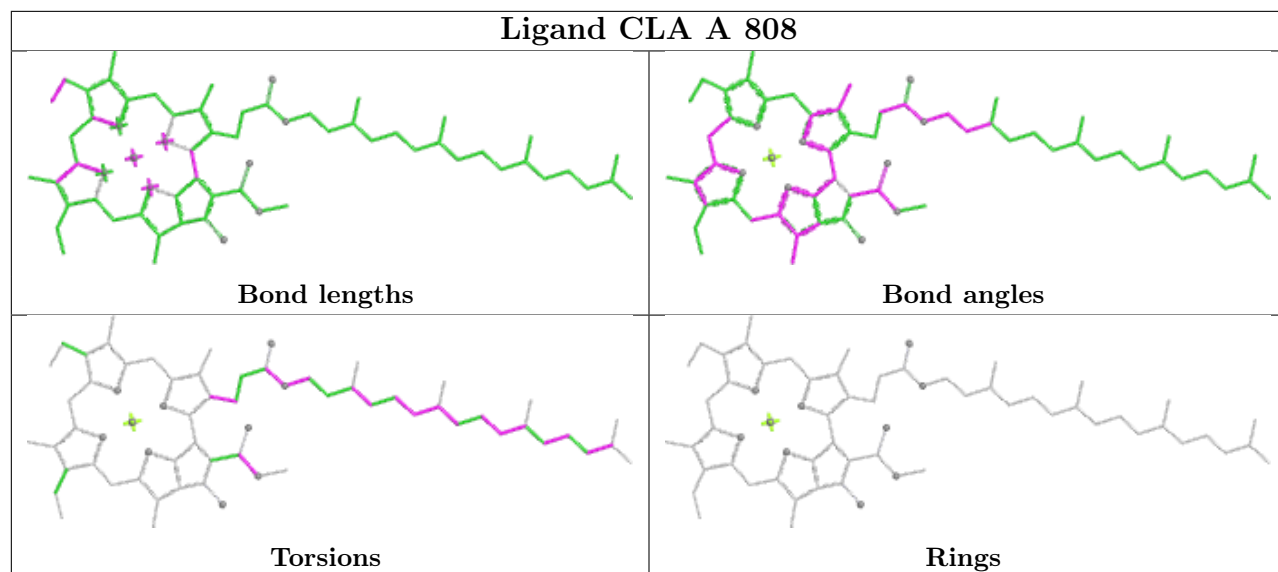
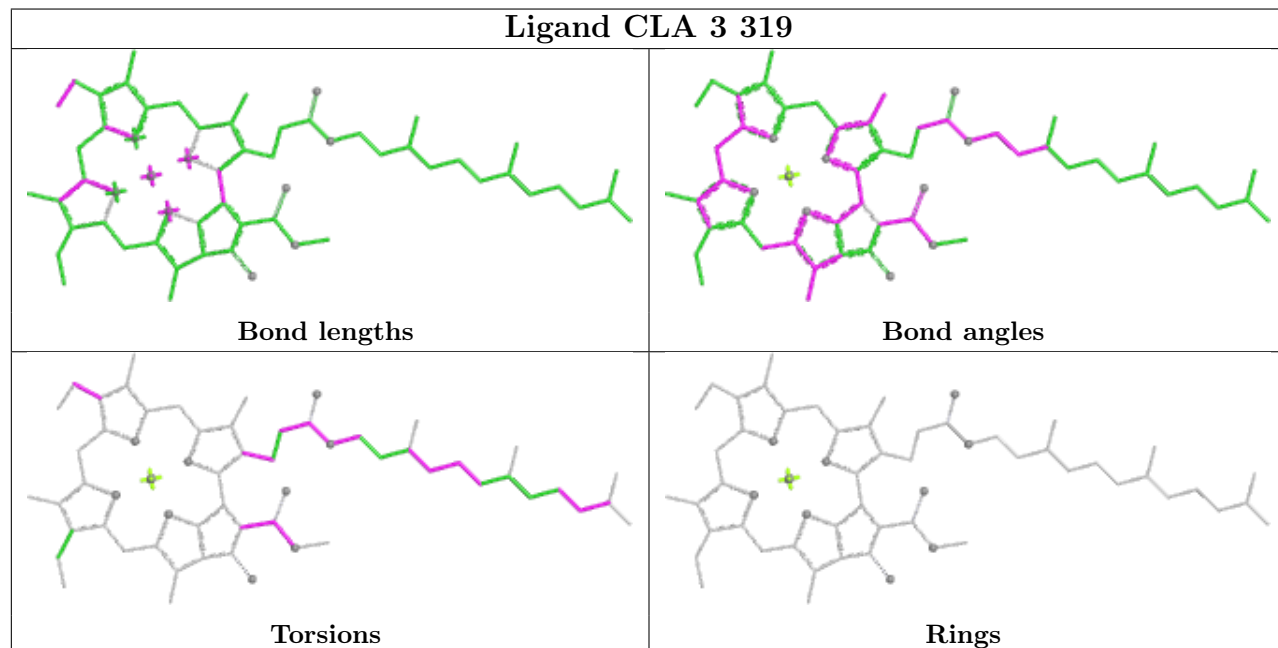
Ligand CLA B 818**Ligand CLA 2 309**

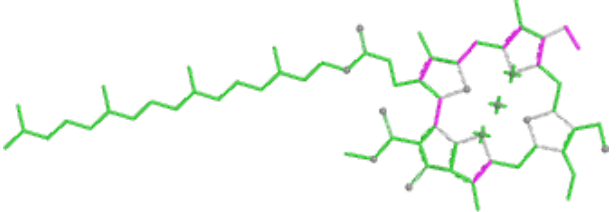
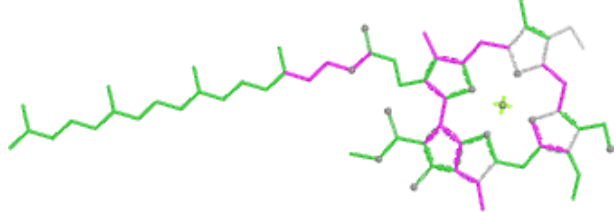
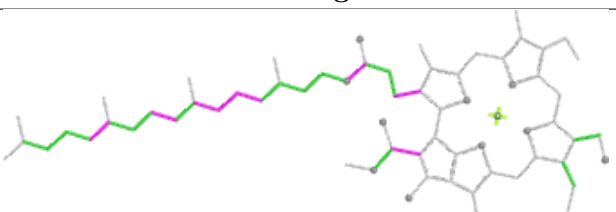
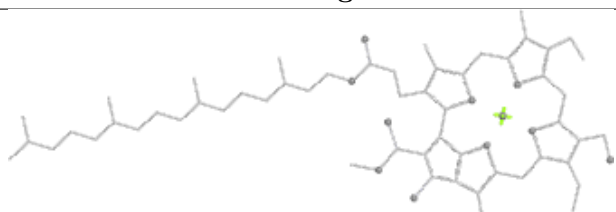
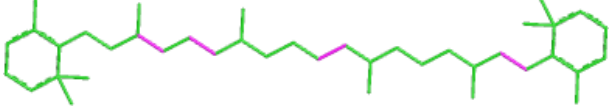
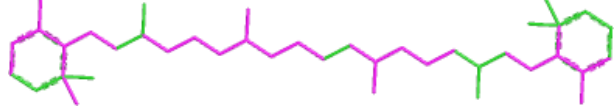
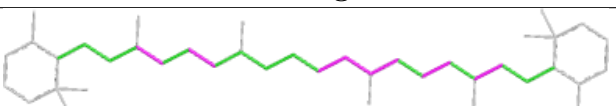
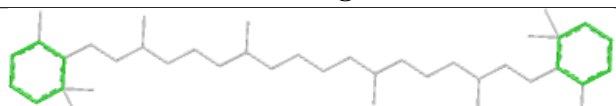
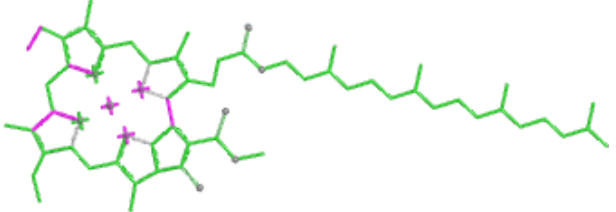
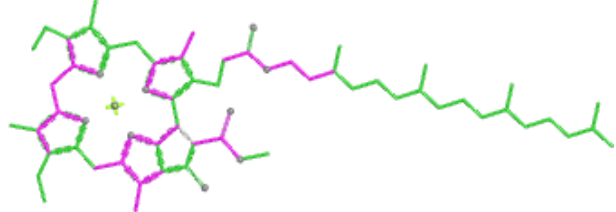
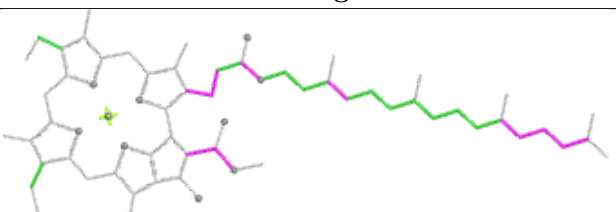
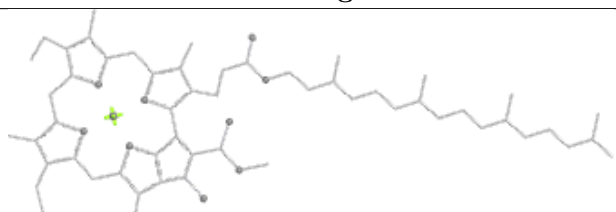
Ligand CLA A 818

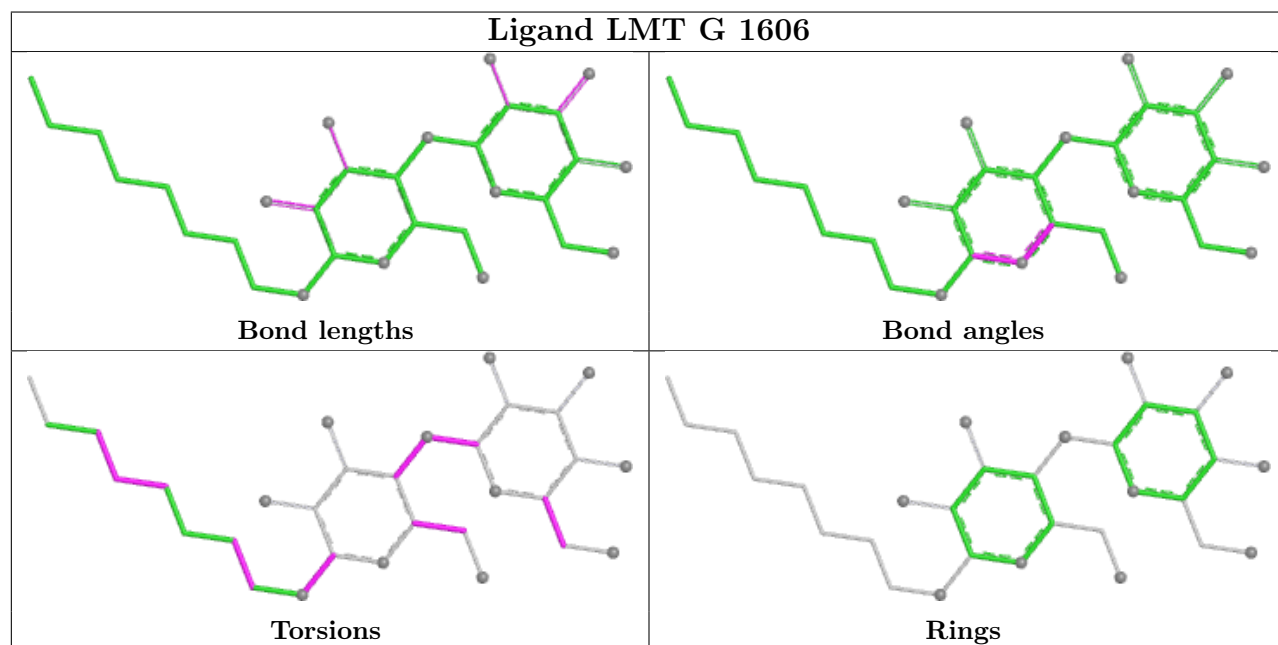
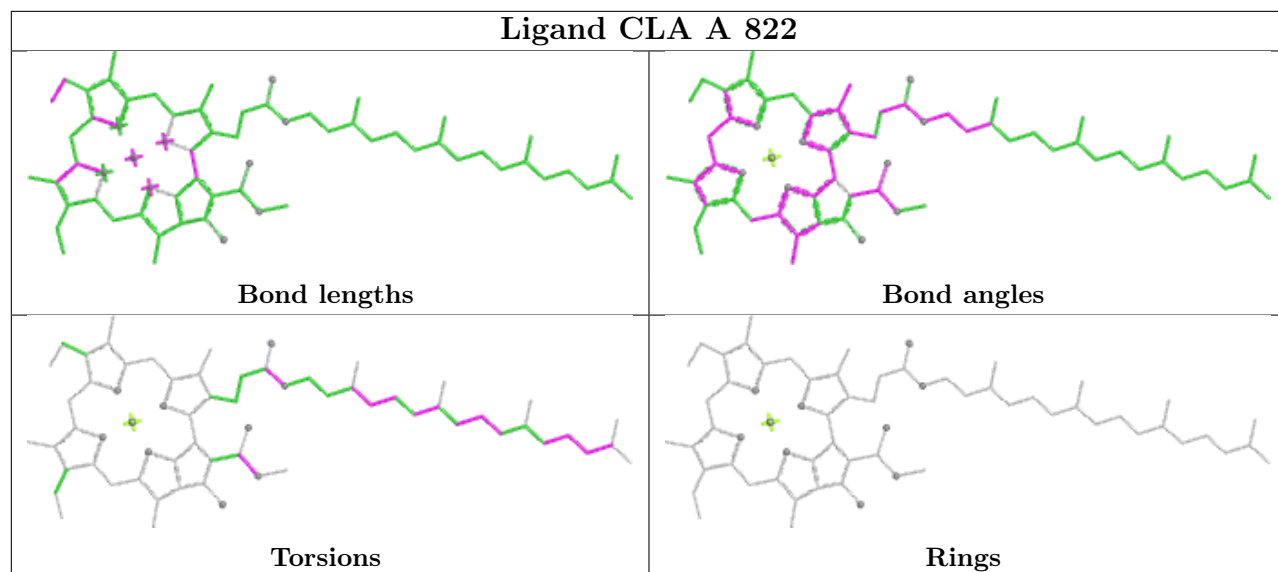


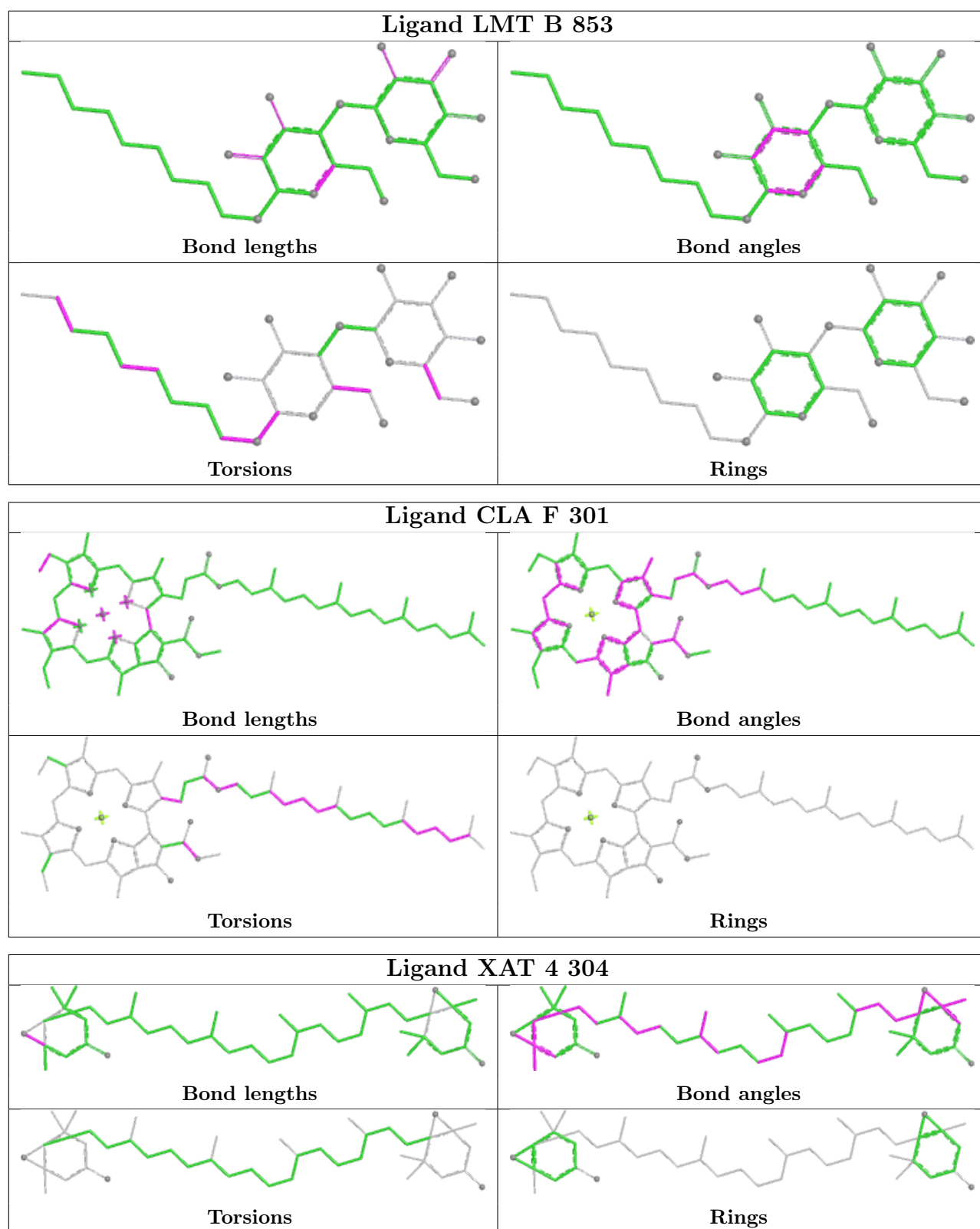
Ligand CLA F 303



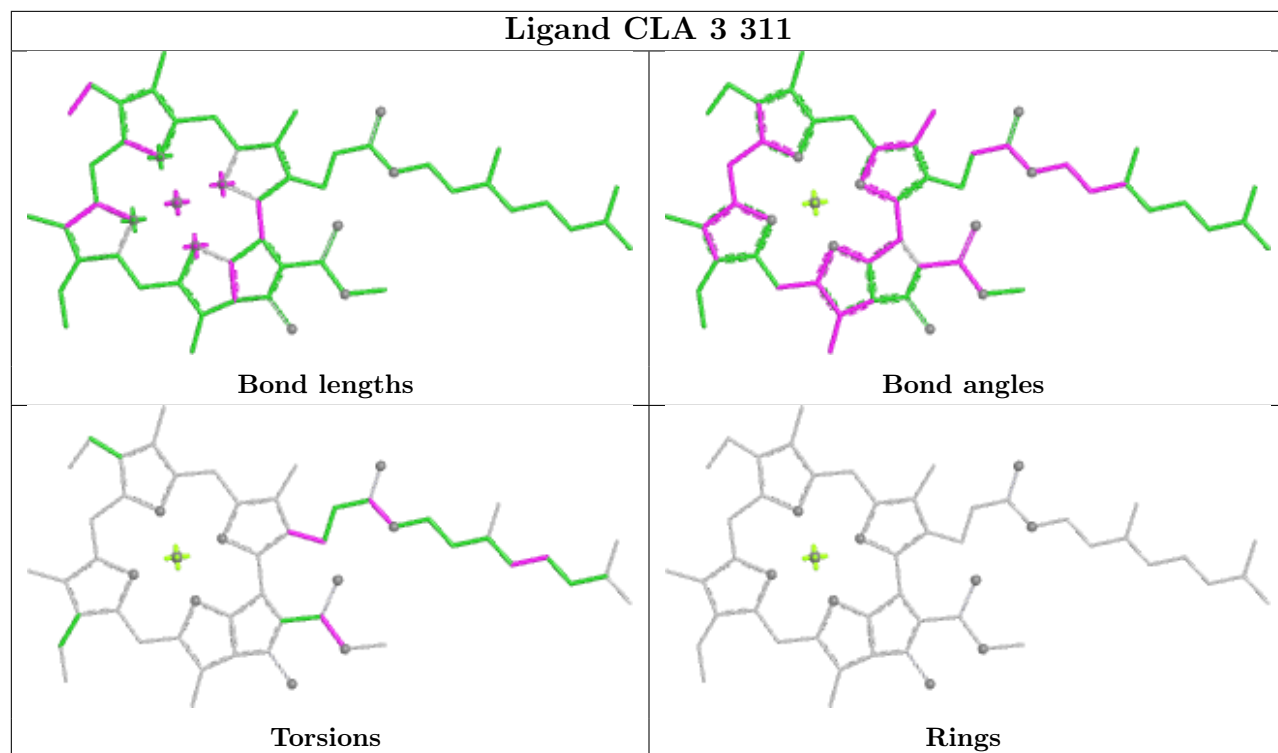
Ligand CLA A 808**Ligand CLA 3 319**

Ligand CHL 3 310	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 845	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

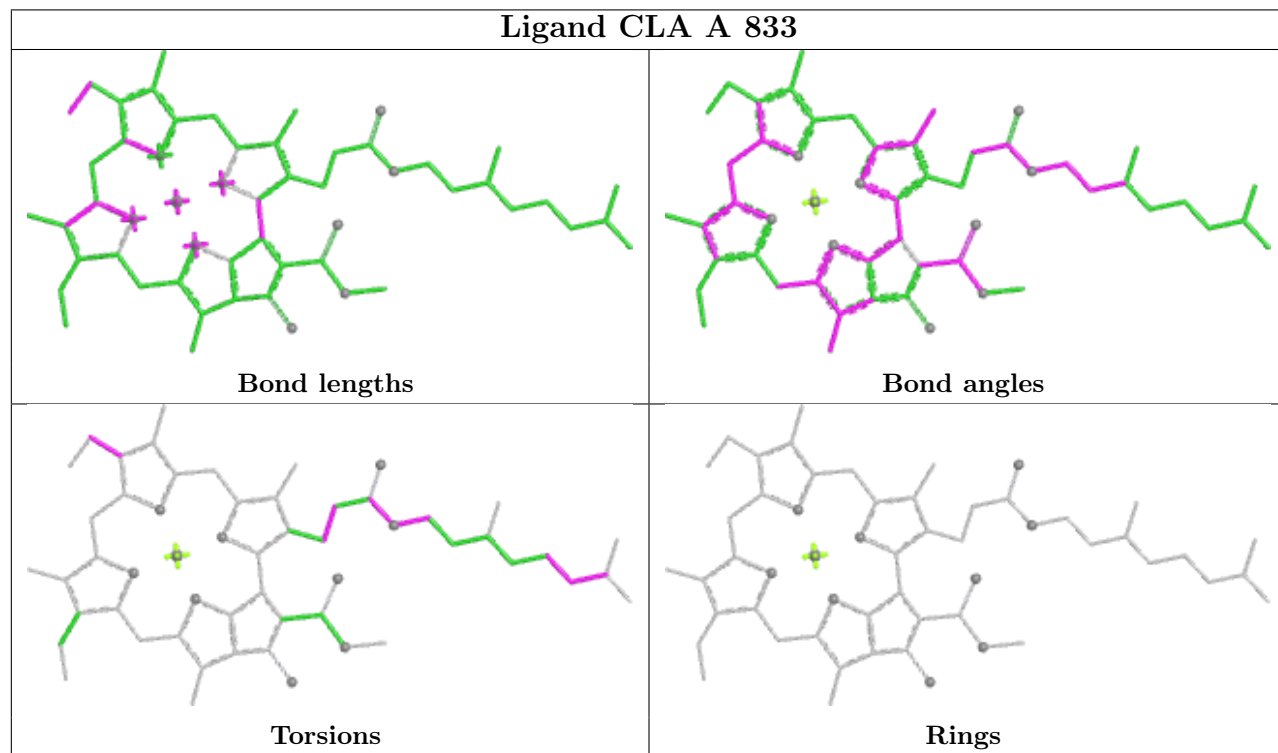


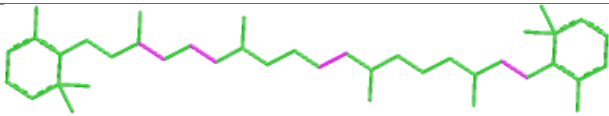
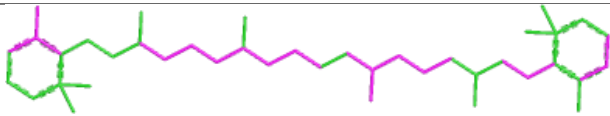
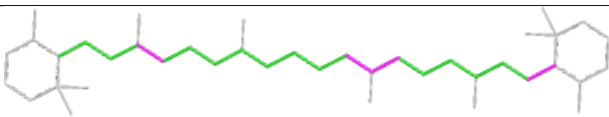
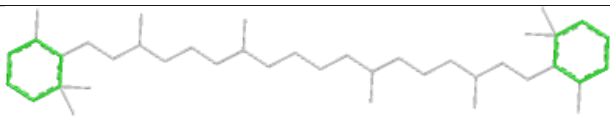


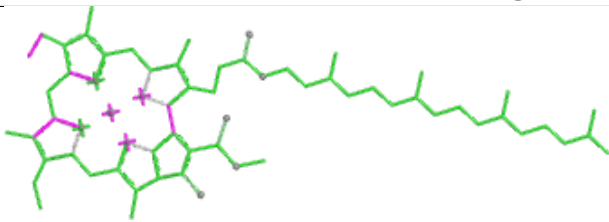
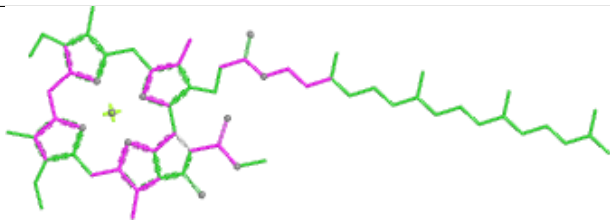
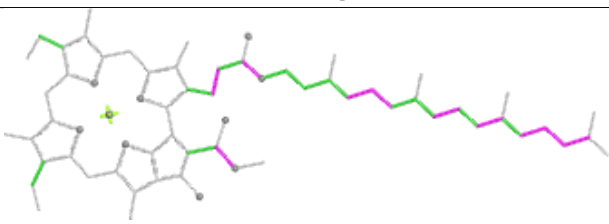
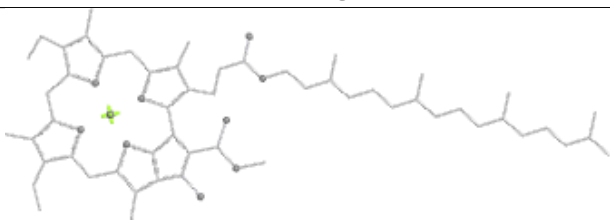
Ligand CLA 3 311

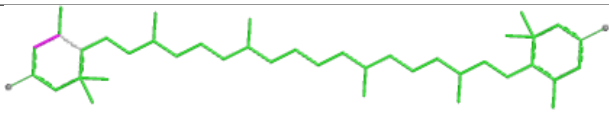
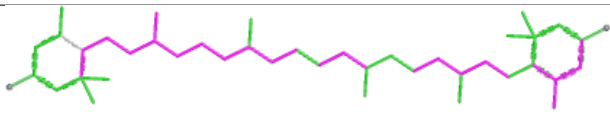
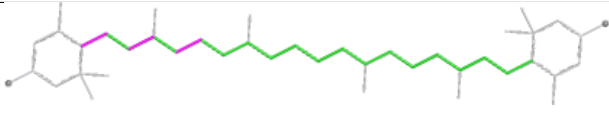
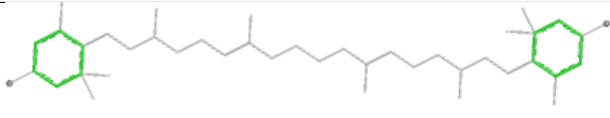


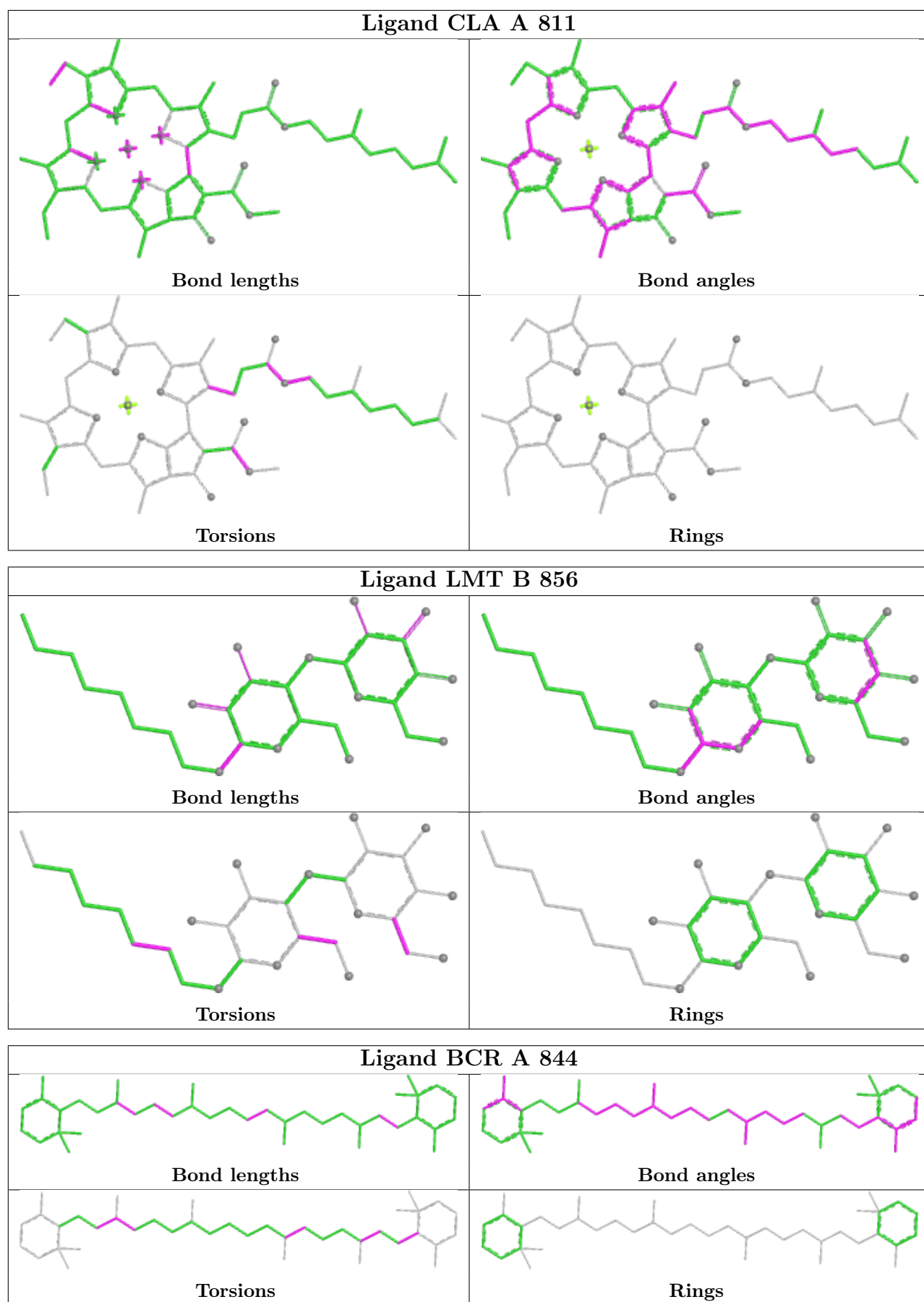
Ligand CLA A 833



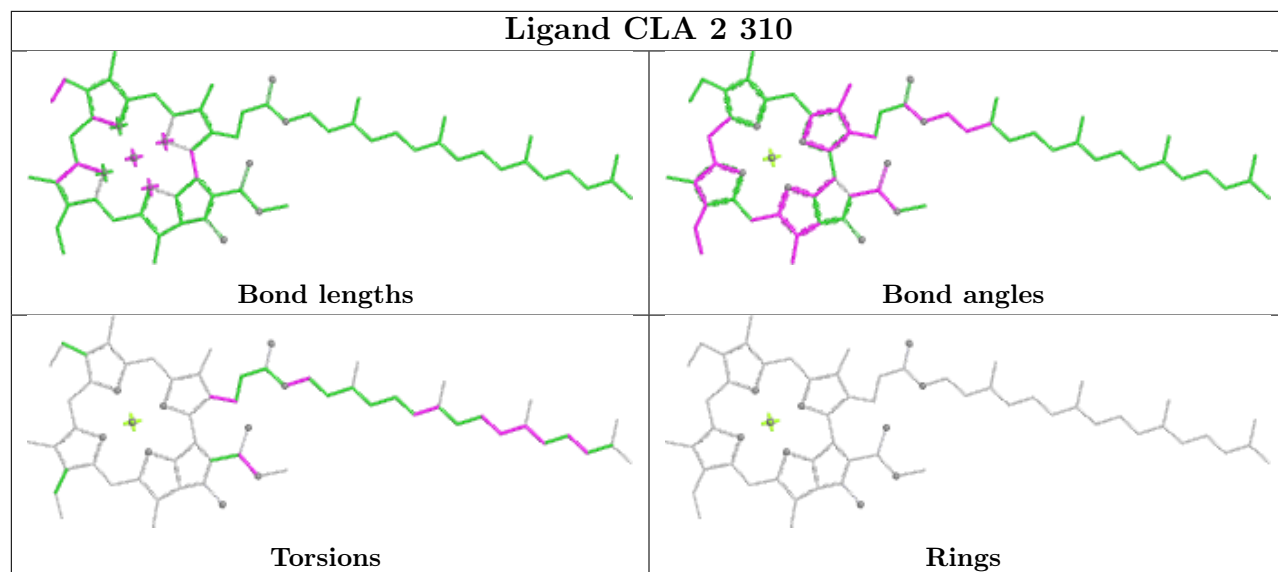
Ligand BCR G 1604	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

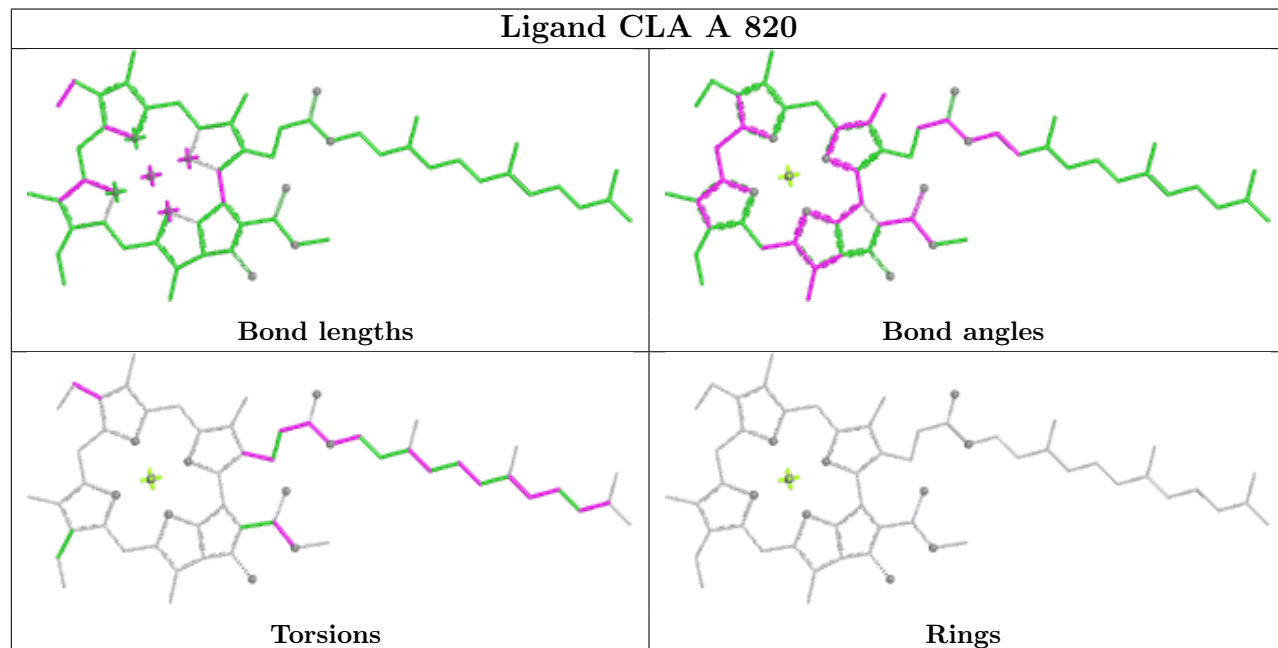
Ligand LUT 1 5004	
	
Bond lengths	Bond angles
	
Torsions	Rings



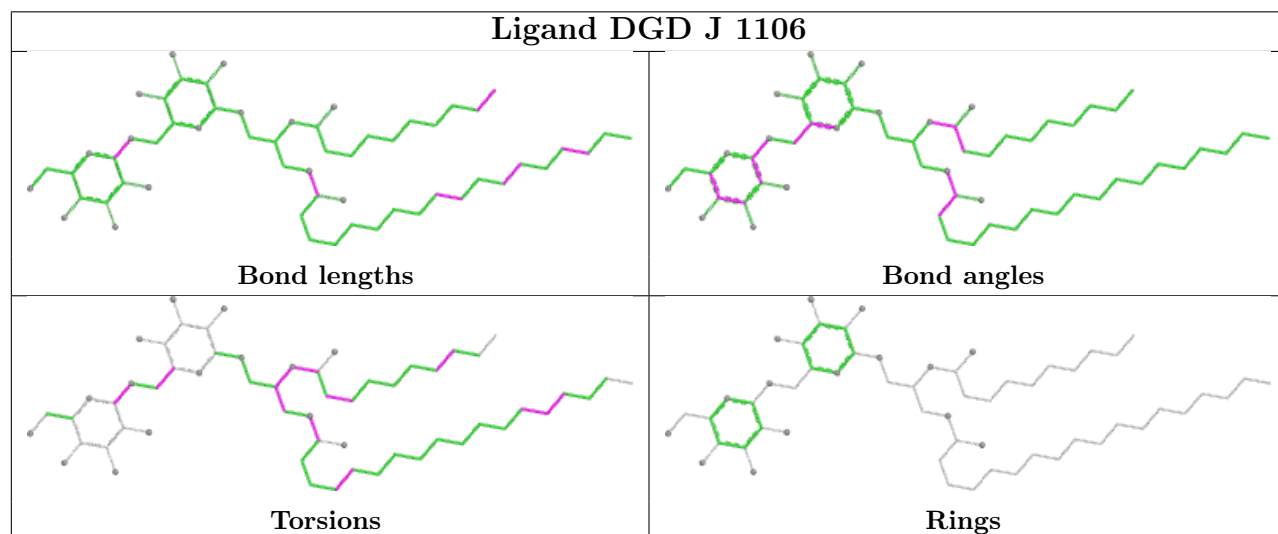
Ligand CLA 2 310

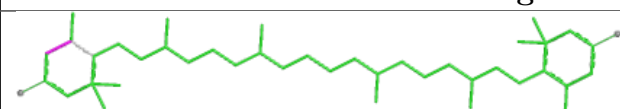
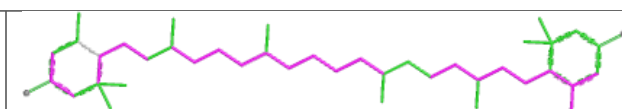
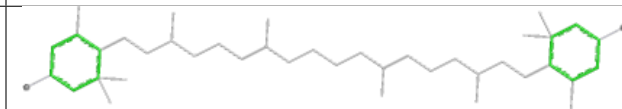


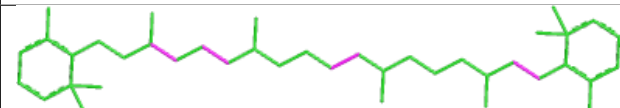
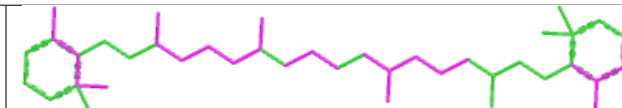
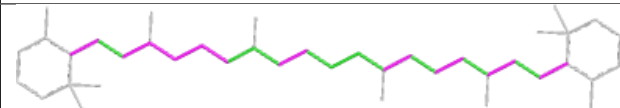
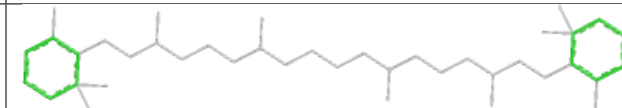
Ligand CLA A 820

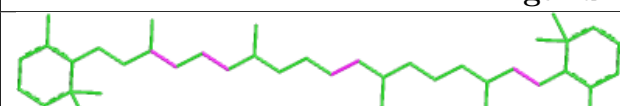
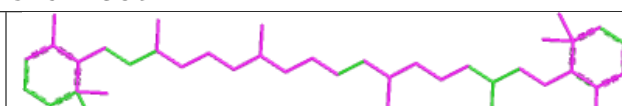
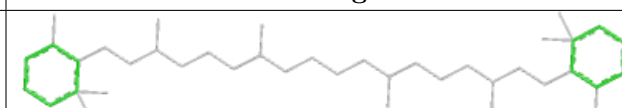


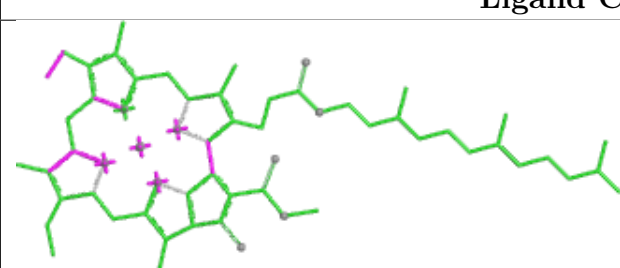
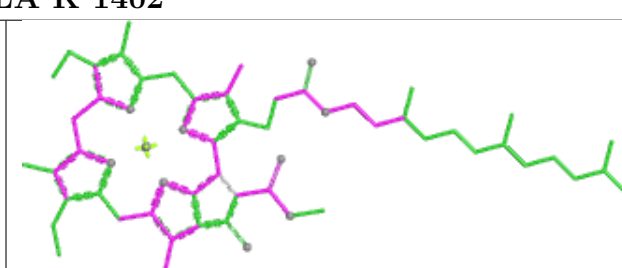
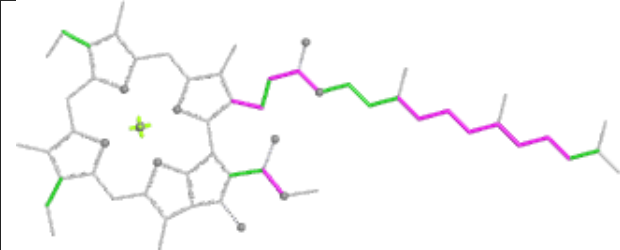
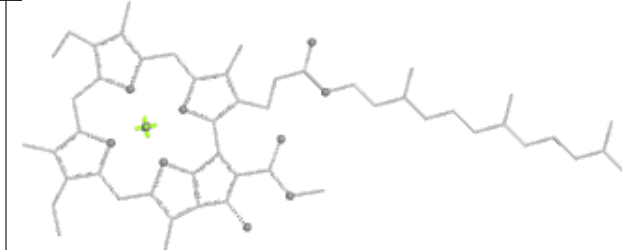
Ligand DGD J 1106

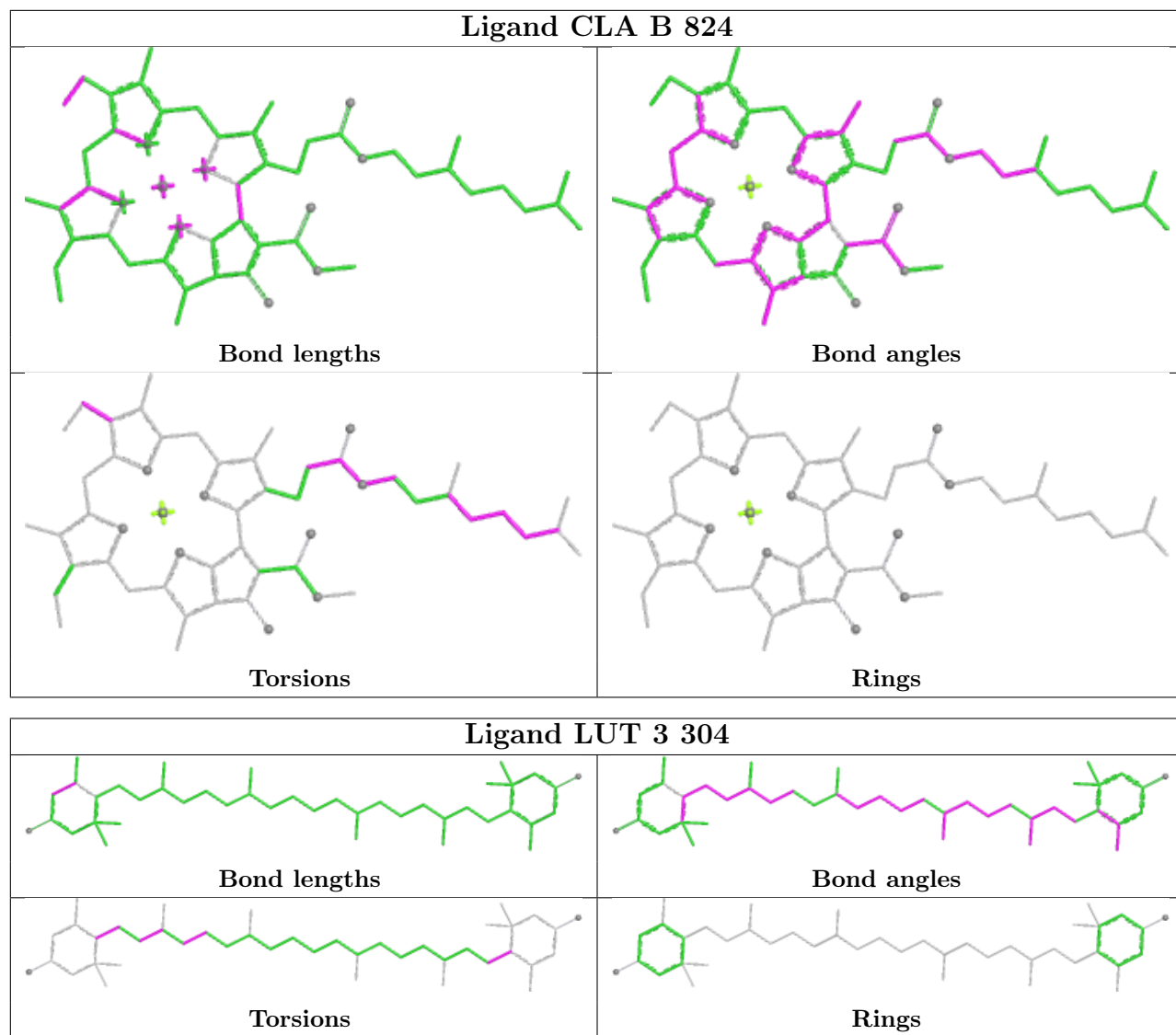


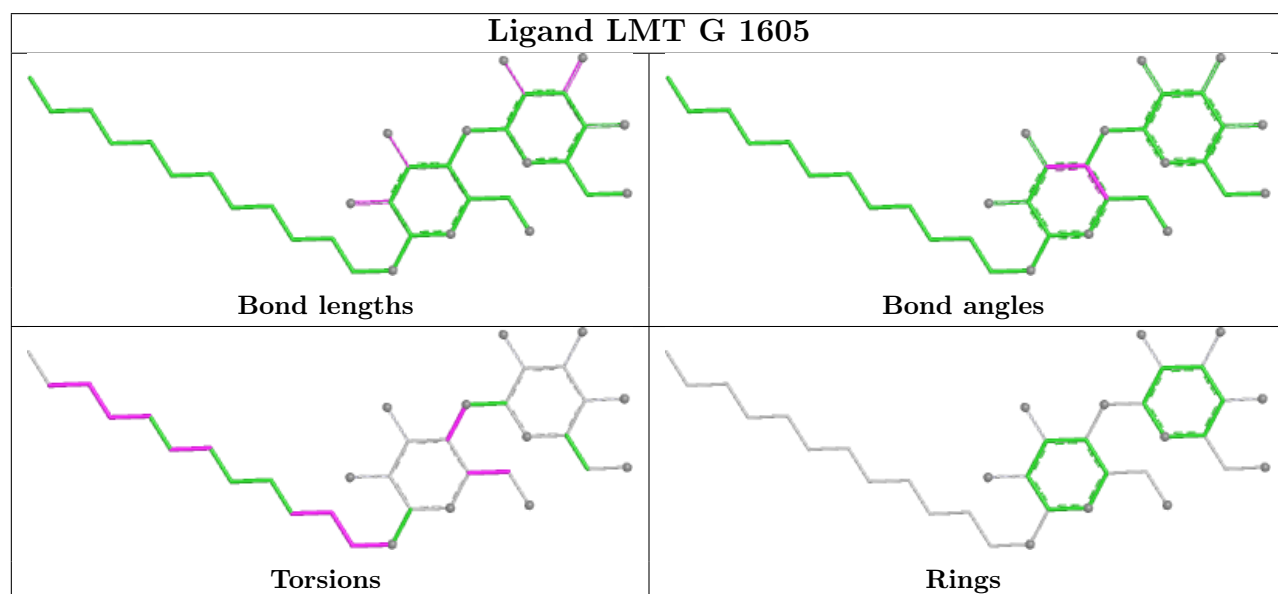
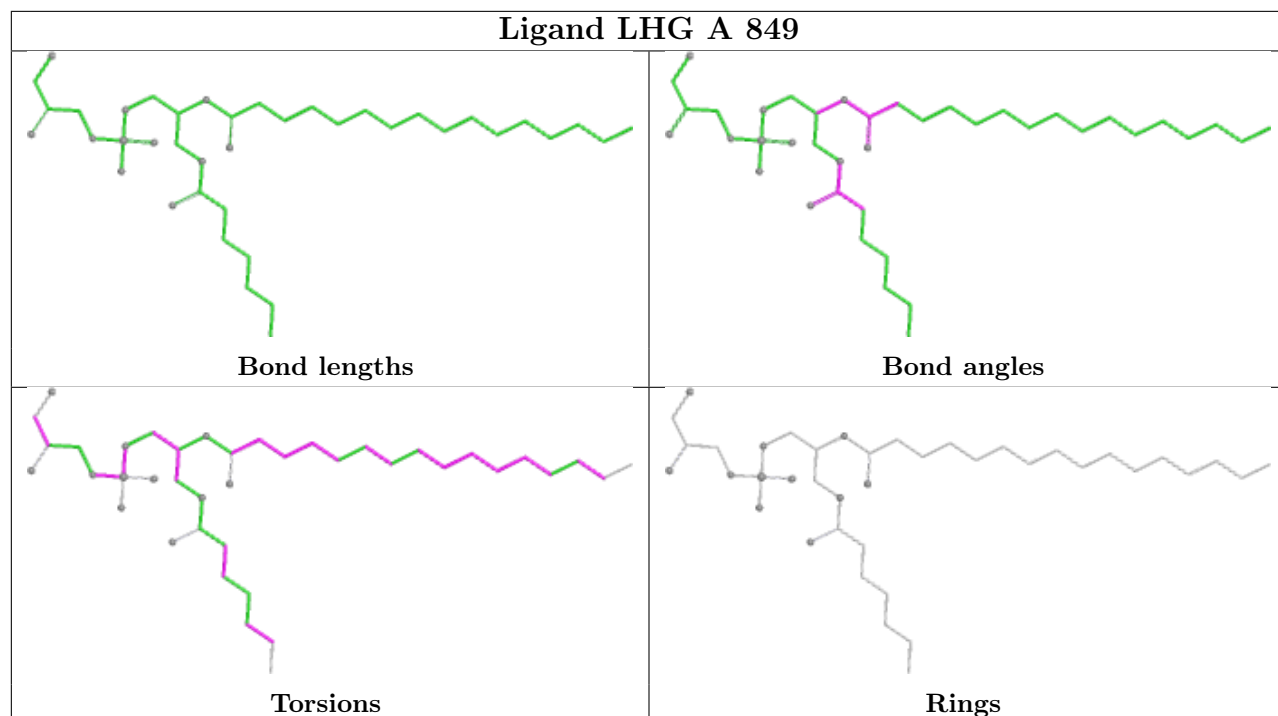
Ligand LUT 1 5003	
	
Bond lengths	Bond angles
	
Torsions	Rings

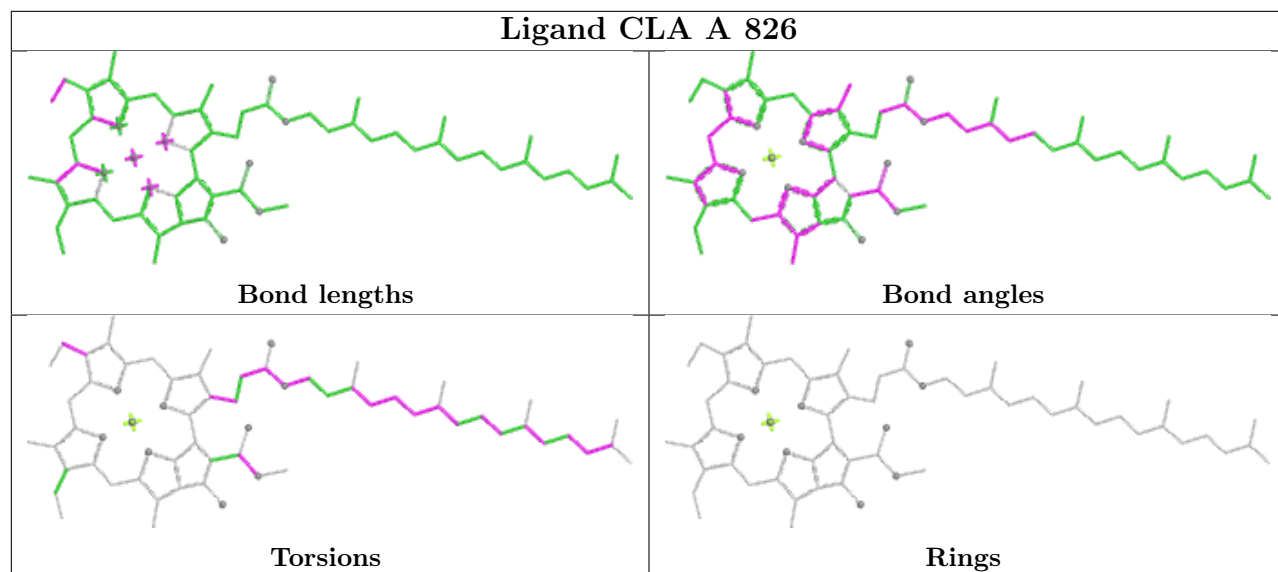
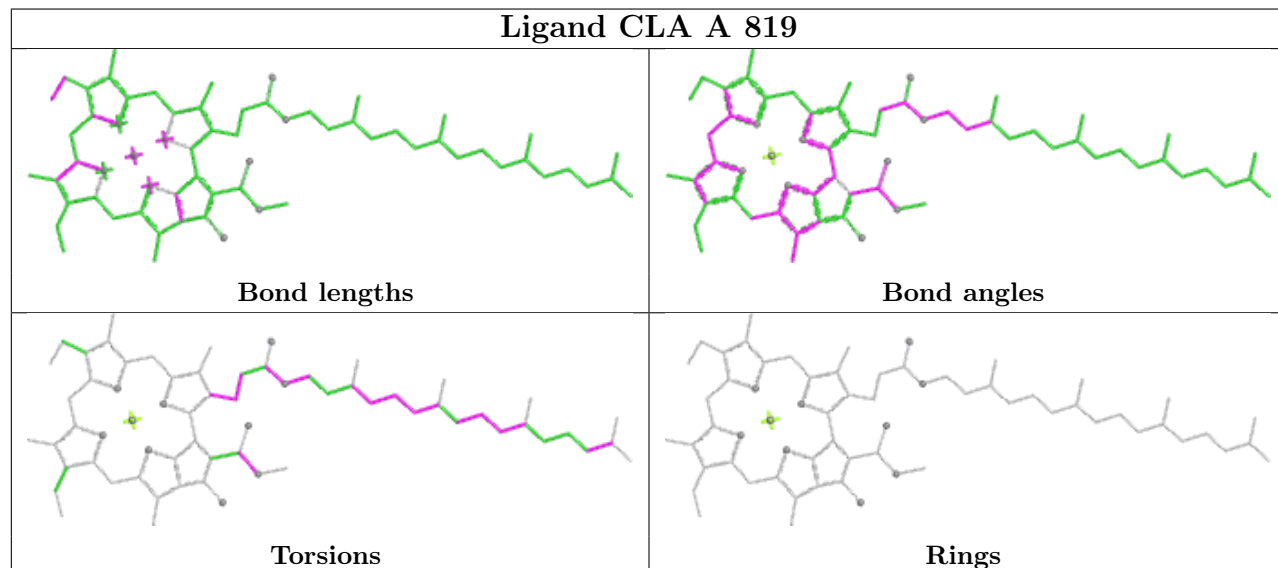
Ligand BCR I 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

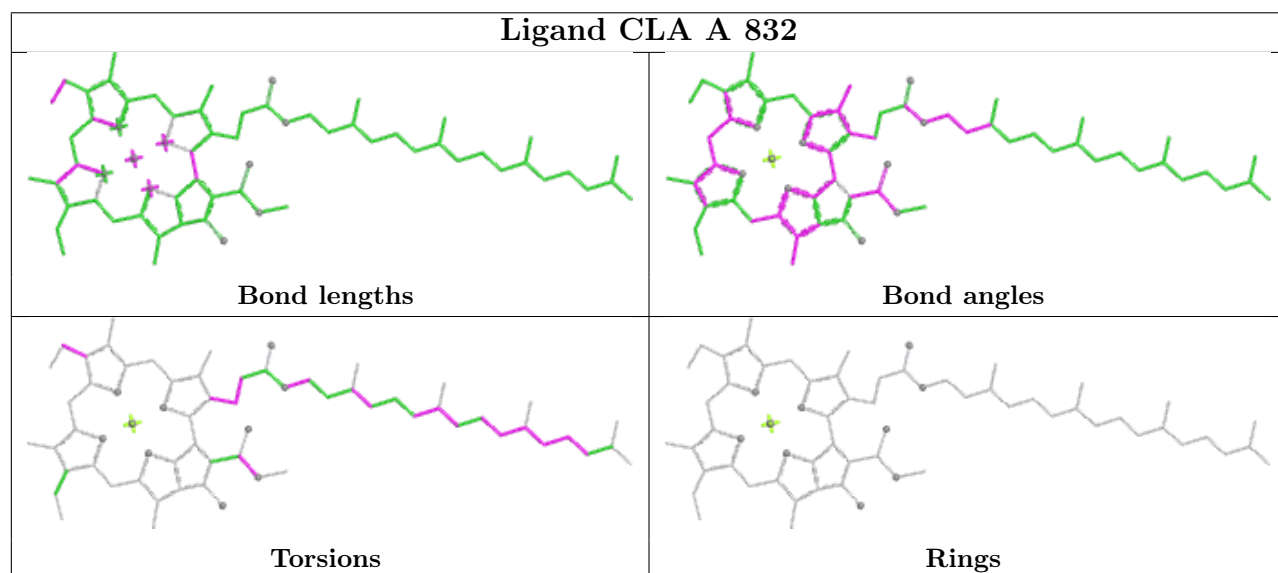
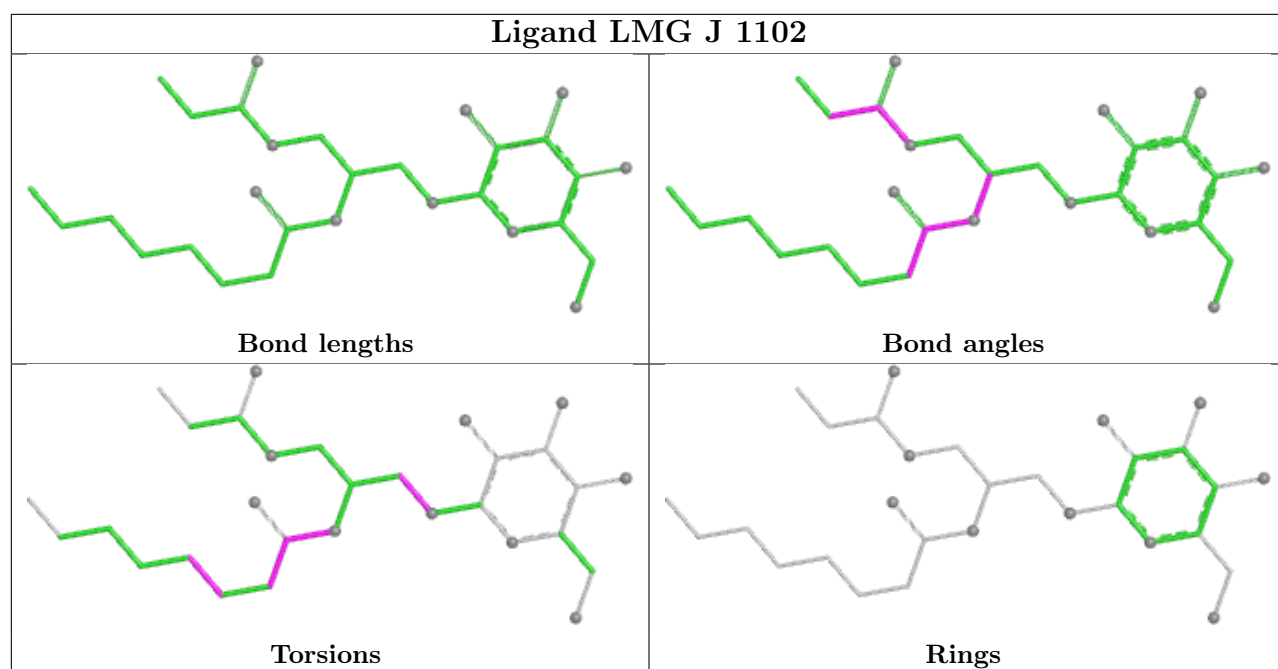
Ligand BCR 2 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

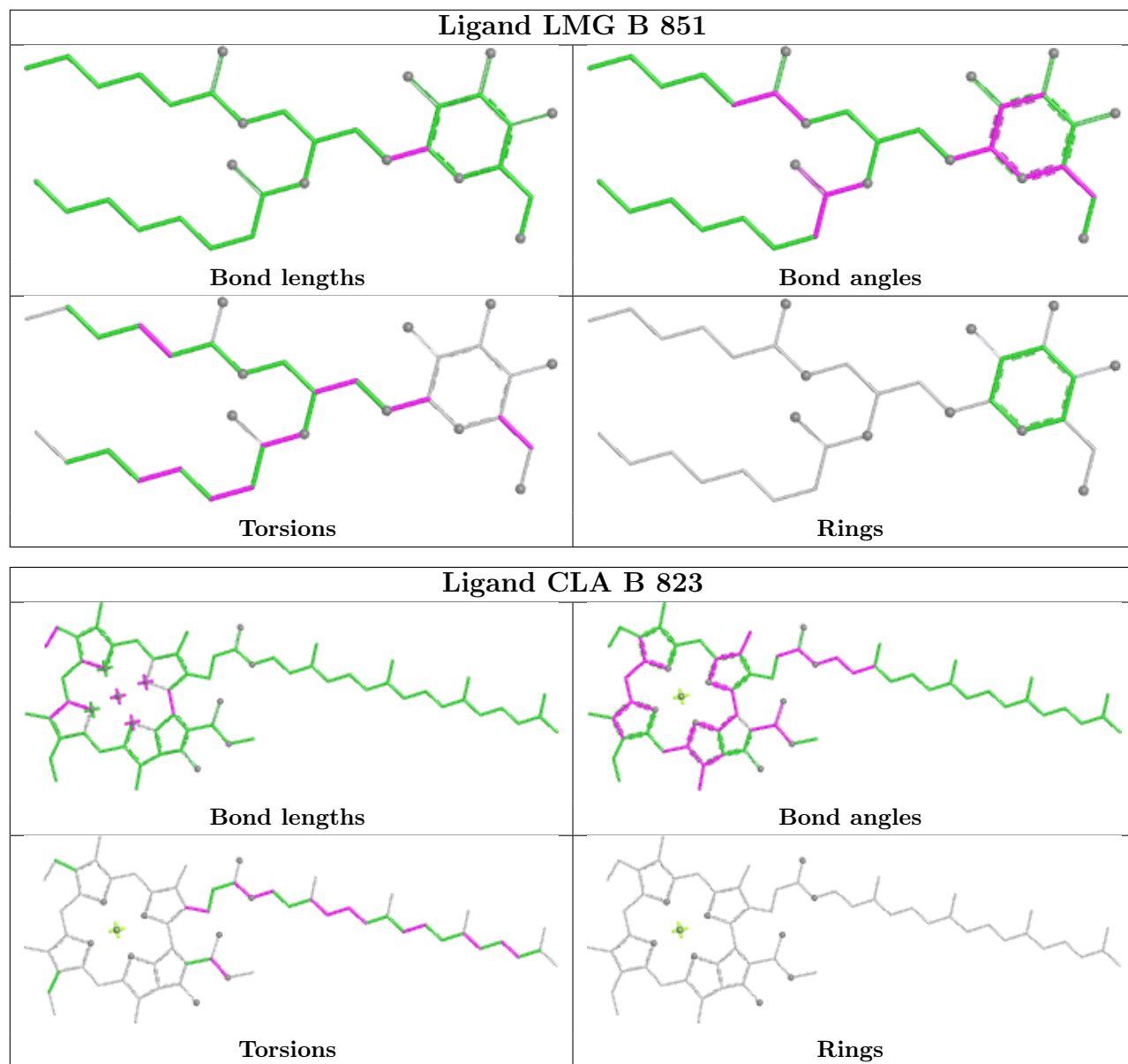
Ligand CLA K 1402	
	
Bond lengths	Bond angles
	
Torsions	Rings





Ligand CLA A 826**Ligand CLA A 819**





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	743/743 (100%)	0.26	41 (5%) 30 15	68, 103, 151, 196	0
2	B	733/733 (100%)	0.42	68 (9%) 14 7	67, 101, 138, 182	0
3	C	80/80 (100%)	0.53	7 (8%) 15 8	77, 95, 158, 180	0
4	D	143/143 (100%)	0.60	17 (11%) 9 5	77, 105, 128, 151	0
5	E	66/66 (100%)	0.35	7 (10%) 11 6	85, 113, 168, 180	0
6	F	154/154 (100%)	0.06	6 (3%) 43 24	82, 105, 141, 156	0
7	G	97/97 (100%)	0.53	12 (12%) 8 5	109, 139, 165, 199	0
8	H	88/88 (100%)	0.36	8 (9%) 15 8	100, 132, 160, 169	0
9	I	30/30 (100%)	0.30	3 (10%) 12 7	97, 115, 132, 154	0
10	J	42/42 (100%)	-0.16	2 (4%) 35 19	82, 96, 138, 171	0
11	K	80/80 (100%)	0.22	3 (3%) 44 24	142, 177, 208, 219	0
12	L	157/157 (100%)	0.76	26 (16%) 4 3	96, 125, 173, 204	0
13	1	193/193 (100%)	0.77	27 (13%) 6 4	124, 156, 201, 228	0
14	2	208/208 (100%)	0.39	17 (8%) 17 9	106, 134, 168, 200	0
15	3	221/221 (100%)	0.91	40 (18%) 3 2	124, 161, 218, 248	0
16	4	198/198 (100%)	0.44	19 (9%) 13 7	110, 136, 174, 204	0
All	All	3233/3233 (100%)	0.43	303 (9%) 14 7	67, 118, 178, 248	0

The worst 5 of 303 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	566	GLY	11.9
2	B	565	GLY	10.5
15	3	87	GLU	9.8
3	C	35	LYS	9.7
2	B	294	ASN	8.8

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	LMT	J	1107	25/35	0.21	0.17	151,182,201,206	0
23	LMT	2	325	35/35	0.24	0.17	157,224,241,245	0
18	CLA	K	1404	46/65	0.43	0.17	170,208,235,242	0
24	LMG	2	302	13/55	0.51	0.24	130,165,187,190	0
23	LMT	G	1606	31/35	0.53	0.15	144,198,232,237	0
24	LMG	2	301	13/55	0.56	0.14	148,168,192,202	0
23	LMT	A	850	35/35	0.57	0.18	79,146,165,174	0
26	DGD	1	5002	35/66	0.64	0.27	125,209,233,236	0
24	LMG	A	851	50/55	0.65	0.17	136,173,197,203	0
23	LMT	B	852	35/35	0.65	0.13	114,212,231,232	0
24	LMG	2	323	13/55	0.68	0.16	126,164,190,192	0
24	LMG	4	320	13/55	0.68	0.15	166,194,213,219	0
24	LMG	B	850	35/55	0.68	0.21	74,146,176,185	0
18	CLA	3	314	48/65	0.69	0.17	159,194,205,208	0
18	CLA	K	1403	48/65	0.70	0.14	166,197,226,242	0
21	BCR	2	305	40/40	0.71	0.26	131,154,181,186	0
18	CLA	H	1701	60/65	0.72	0.19	148,175,199,206	0
24	LMG	1	5001	49/55	0.73	0.26	91,156,219,221	0
24	LMG	2	321	25/55	0.74	0.15	114,144,164,168	0
18	CLA	K	1402	60/65	0.74	0.16	100,164,183,192	0
18	CLA	J	1103	50/65	0.75	0.17	92,155,195,209	0
24	LMG	2	324	13/55	0.76	0.11	159,183,205,212	0
24	LMG	F	307	36/55	0.76	0.21	125,159,194,197	0
25	GOL	4	321	6/6	0.76	0.19	135,146,153,158	0
22	LHG	B	849	49/49	0.76	0.21	101,139,196,220	0
18	CLA	1	5015	65/65	0.77	0.20	140,176,193,202	0
24	LMG	B	851	33/55	0.77	0.20	133,208,223,227	0

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Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	LMT	B	856	31/35	0.77	0.12	138,156,173,179	0
30	CHL	3	313	51/66	0.77	0.17	185,220,249,260	0
21	BCR	L	302	40/40	0.78	0.16	118,167,216,221	0
24	LMG	J	1102	30/55	0.78	0.14	103,123,146,159	0
18	CLA	K	1401	45/65	0.79	0.14	133,166,181,194	0
21	BCR	K	1405	40/40	0.79	0.17	138,166,194,201	0
24	LMG	2	322	36/55	0.79	0.14	111,177,212,217	0
21	BCR	3	306	40/40	0.80	0.17	134,160,182,188	0
30	CHL	3	312	51/66	0.80	0.12	141,157,177,183	0
24	LMG	G	1607	25/55	0.80	0.19	130,194,215,220	0
23	LMT	B	853	32/35	0.81	0.13	121,153,174,179	0
24	LMG	B	854	13/55	0.82	0.14	131,170,201,202	0
23	LMT	G	1605	35/35	0.82	0.12	116,177,214,218	0
18	CLA	G	1603	65/65	0.82	0.23	127,161,197,202	0
23	LMT	4	319	35/35	0.82	0.14	95,179,207,207	0
24	LMG	1	5020	46/55	0.83	0.18	88,157,201,209	0
18	CLA	1	5006	65/65	0.83	0.16	137,169,186,193	0
18	CLA	G	1602	46/65	0.83	0.11	132,158,180,206	0
26	DGD	F	309	57/66	0.83	0.21	105,158,186,192	0
22	LHG	1	5019	49/49	0.83	0.21	112,135,168,176	0
30	CHL	2	315	56/66	0.83	0.12	109,151,170,175	0
21	BCR	1	5005	40/40	0.83	0.15	135,175,224,229	0
18	CLA	A	840	60/65	0.83	0.13	101,147,196,206	0
18	CLA	3	308	52/65	0.84	0.12	165,202,217,224	0
24	LMG	F	308	34/55	0.84	0.13	102,163,181,202	0
26	DGD	2	327	51/66	0.84	0.16	99,129,165,174	0
30	CHL	4	317	43/66	0.84	0.12	125,162,177,190	0
30	CHL	2	319	56/66	0.85	0.15	117,147,181,192	0
29	LUT	4	303	42/42	0.85	0.19	106,128,148,160	0
29	LUT	2	303	42/42	0.85	0.19	114,132,145,159	0
30	CHL	4	313	47/66	0.85	0.13	104,133,160,176	0
30	CHL	2	318	46/66	0.85	0.12	117,142,157,175	0
21	BCR	A	846	40/40	0.86	0.20	72,100,129,147	0
18	CLA	2	311	50/65	0.86	0.10	116,139,154,158	0
18	CLA	3	319	60/65	0.86	0.17	118,140,186,194	0
21	BCR	L	307	40/40	0.86	0.15	102,130,153,164	0
29	LUT	1	5003	42/42	0.87	0.15	117,157,181,193	0
18	CLA	1	5011	50/65	0.87	0.12	146,167,182,191	0
29	LUT	3	303	42/42	0.87	0.13	145,166,176,181	0
21	BCR	G	1604	40/40	0.87	0.14	106,133,171,173	0
18	CLA	B	835	55/65	0.87	0.14	99,115,163,178	0
18	CLA	1	5018	60/65	0.87	0.18	88,137,192,196	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	CLA	L	304	50/65	0.87	0.14	123,151,170,179	0
18	CLA	L	306	50/65	0.87	0.14	101,134,155,170	0
18	CLA	B	808	65/65	0.87	0.16	87,100,144,165	0
18	CLA	1	5007	46/65	0.87	0.12	122,149,167,180	0
30	CHL	4	316	61/66	0.87	0.19	121,144,165,172	0
29	LUT	J	1105	42/42	0.87	0.16	89,122,148,163	0
31	XAT	2	304	44/44	0.87	0.16	106,124,144,150	0
18	CLA	1	5013	46/65	0.88	0.16	118,159,175,202	0
18	CLA	B	834	60/65	0.88	0.15	82,106,129,140	0
21	BCR	3	305	40/40	0.88	0.18	120,134,155,161	0
18	CLA	4	311	60/65	0.88	0.14	117,134,155,167	0
18	CLA	A	803	65/65	0.88	0.17	67,91,146,172	0
21	BCR	B	843	40/40	0.88	0.23	104,121,144,166	0
18	CLA	A	836	65/65	0.88	0.14	80,107,169,181	0
18	CLA	2	317	55/65	0.88	0.17	91,126,157,174	0
18	CLA	1	5012	46/65	0.88	0.12	117,149,168,183	0
18	CLA	3	309	55/65	0.88	0.13	132,175,204,219	0
22	LHG	A	849	40/49	0.89	0.14	88,125,152,155	0
30	CHL	2	316	48/66	0.89	0.17	107,124,145,160	0
18	CLA	A	833	55/65	0.89	0.14	113,137,165,171	0
18	CLA	4	312	46/65	0.89	0.14	115,145,160,175	0
25	GOL	A	854	6/6	0.89	0.13	124,136,142,142	0
29	LUT	1	5004	42/42	0.89	0.17	105,145,165,174	0
18	CLA	B	805	65/65	0.89	0.15	89,123,175,194	0
26	DGD	B	855	61/66	0.89	0.17	70,100,132,155	0
24	LMG	F	306	47/55	0.89	0.11	96,131,158,169	0
30	CHL	1	5016	61/66	0.89	0.12	114,154,166,171	0
18	CLA	3	307	55/65	0.90	0.12	148,169,183,191	0
21	BCR	B	845	40/40	0.90	0.17	92,121,179,183	0
21	BCR	B	846	40/40	0.90	0.20	73,106,123,130	0
21	BCR	B	847	40/40	0.90	0.20	73,99,115,120	0
18	CLA	G	1601	55/65	0.90	0.10	120,147,172,177	0
18	CLA	A	814	46/65	0.90	0.13	127,143,167,179	0
18	CLA	1	5017	45/65	0.90	0.11	159,182,206,210	0
21	BCR	L	303	40/40	0.90	0.18	90,108,127,135	0
30	CHL	3	310	66/66	0.90	0.16	107,148,166,194	0
18	CLA	B	816	55/65	0.90	0.13	107,133,154,171	0
18	CLA	4	310	50/65	0.90	0.14	125,146,176,189	0
28	ZEX	F	310	42/42	0.90	0.16	104,141,157,167	0
18	CLA	2	306	60/65	0.90	0.13	115,134,164,175	0
18	CLA	A	825	65/65	0.90	0.15	85,116,136,143	0
18	CLA	A	806	60/65	0.90	0.12	79,112,152,161	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	CLA	2	307	52/65	0.91	0.12	120,144,157,159	0
18	CLA	B	822	65/65	0.91	0.15	95,114,160,165	0
21	BCR	A	855	40/40	0.91	0.20	128,148,176,177	0
18	CLA	B	823	65/65	0.91	0.17	87,114,150,162	0
18	CLA	B	826	65/65	0.91	0.15	67,88,122,124	0
30	CHL	1	5014	47/66	0.91	0.13	139,168,192,198	0
18	CLA	A	815	65/65	0.91	0.15	135,149,171,179	0
18	CLA	A	829	65/65	0.91	0.14	78,118,173,180	0
18	CLA	B	839	65/65	0.91	0.16	82,101,124,130	0
21	BCR	I	102	40/40	0.91	0.20	83,115,133,139	0
21	BCR	J	1104	40/40	0.91	0.16	67,92,114,125	0
26	DGD	J	1106	58/66	0.91	0.13	67,115,186,193	0
18	CLA	3	318	46/65	0.91	0.10	140,158,170,172	0
18	CLA	F	302	65/65	0.91	0.17	73,107,198,210	0
27	CA	B	857	1/1	0.91	0.07	123,123,123,123	0
30	CHL	4	314	51/66	0.91	0.17	120,144,159,172	0
27	CA	3	302	1/1	0.91	0.09	129,129,129,129	0
18	CLA	B	810	65/65	0.91	0.15	87,116,141,161	0
18	CLA	A	832	65/65	0.91	0.14	92,120,139,165	0
18	CLA	B	818	65/65	0.92	0.18	82,102,119,128	0
18	CLA	4	305	60/65	0.92	0.11	119,141,161,167	0
18	CLA	A	810	65/65	0.92	0.11	70,97,115,128	0
18	CLA	2	310	65/65	0.92	0.14	107,128,155,166	0
18	CLA	1	5008	55/65	0.92	0.14	114,142,159,162	0
30	CHL	2	314	66/66	0.92	0.12	99,128,151,165	0
18	CLA	2	312	60/65	0.92	0.11	122,139,161,183	0
21	BCR	A	847	40/40	0.92	0.16	63,75,103,105	0
18	CLA	F	303	65/65	0.92	0.13	83,116,145,166	0
22	LHG	B	848	21/49	0.92	0.12	88,113,140,155	0
18	CLA	A	816	56/65	0.92	0.15	93,129,143,150	0
18	CLA	A	824	55/65	0.92	0.15	82,99,124,135	0
18	CLA	B	811	65/65	0.92	0.15	82,109,139,151	0
30	CHL	3	316	47/66	0.92	0.13	135,159,171,181	0
18	CLA	3	311	55/65	0.92	0.15	113,139,155,160	0
18	CLA	L	305	60/65	0.92	0.14	93,121,133,146	0
18	CLA	3	315	65/65	0.92	0.13	115,153,164,191	0
18	CLA	3	317	50/65	0.92	0.14	111,145,156,171	0
18	CLA	B	801	65/65	0.92	0.17	63,84,96,109	0
31	XAT	4	304	44/44	0.92	0.13	92,127,146,156	0
21	BCR	A	844	40/40	0.93	0.20	87,115,169,186	0
21	BCR	A	845	40/40	0.93	0.12	79,99,155,162	0
18	CLA	A	838	65/65	0.93	0.14	64,84,119,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	CLA	A	809	50/65	0.93	0.14	97,128,146,159	0
18	CLA	A	852	65/65	0.93	0.14	70,91,105,112	0
18	CLA	A	853	65/65	0.93	0.14	84,105,130,138	0
21	BCR	B	844	40/40	0.93	0.15	81,109,151,165	0
18	CLA	A	820	60/65	0.93	0.12	121,148,178,189	0
18	CLA	B	827	65/65	0.93	0.14	74,94,112,120	0
18	CLA	B	828	65/65	0.93	0.16	72,100,128,141	0
21	BCR	F	305	40/40	0.93	0.14	76,98,116,120	0
29	LUT	3	304	42/42	0.93	0.17	116,146,169,173	0
18	CLA	2	313	50/65	0.93	0.09	121,134,153,157	0
18	CLA	B	829	65/65	0.93	0.16	78,93,111,127	0
18	CLA	B	832	60/65	0.93	0.15	70,99,137,153	0
18	CLA	L	301	55/65	0.93	0.15	89,120,136,145	0
18	CLA	B	833	58/65	0.93	0.12	65,87,107,117	0
18	CLA	A	821	60/65	0.93	0.12	122,149,190,193	0
18	CLA	A	823	65/65	0.93	0.16	82,110,130,137	0
18	CLA	B	837	65/65	0.93	0.12	68,88,105,114	0
18	CLA	B	838	50/65	0.93	0.13	69,91,103,126	0
18	CLA	A	834	51/65	0.93	0.14	81,106,134,147	0
18	CLA	1	5009	65/65	0.93	0.11	91,137,151,157	0
21	BCR	4	301	40/40	0.93	0.20	120,140,157,165	0
30	CHL	4	302	56/66	0.93	0.12	109,129,143,148	0
18	CLA	B	840	65/65	0.93	0.14	74,97,120,127	0
18	CLA	4	306	50/65	0.93	0.11	118,145,159,169	0
18	CLA	B	841	65/65	0.93	0.12	72,107,126,133	0
18	CLA	A	811	55/65	0.93	0.13	102,127,140,151	0
18	CLA	B	812	60/65	0.93	0.11	94,128,153,169	0
18	CLA	4	315	65/65	0.93	0.16	107,134,164,176	0
18	CLA	A	822	65/65	0.94	0.13	78,93,121,129	0
18	CLA	A	826	65/65	0.94	0.12	66,88,109,121	0
18	CLA	B	815	65/65	0.94	0.10	96,116,136,155	0
22	LHG	2	320	35/49	0.94	0.14	101,131,149,160	0
18	CLA	2	308	65/65	0.94	0.12	113,132,152,167	0
21	BCR	F	304	40/40	0.94	0.14	67,85,100,105	0
18	CLA	A	835	65/65	0.94	0.13	89,114,148,162	0
18	CLA	4	308	60/65	0.94	0.10	92,118,142,153	0
21	BCR	I	101	40/40	0.94	0.14	85,108,125,129	0
18	CLA	B	830	65/65	0.94	0.13	77,98,128,139	0
18	CLA	B	831	65/65	0.94	0.14	69,88,115,121	0
18	CLA	B	817	60/65	0.94	0.15	110,133,148,156	0
18	CLA	A	813	65/65	0.94	0.13	104,133,165,180	0
21	BCR	A	843	40/40	0.94	0.18	86,116,155,162	0

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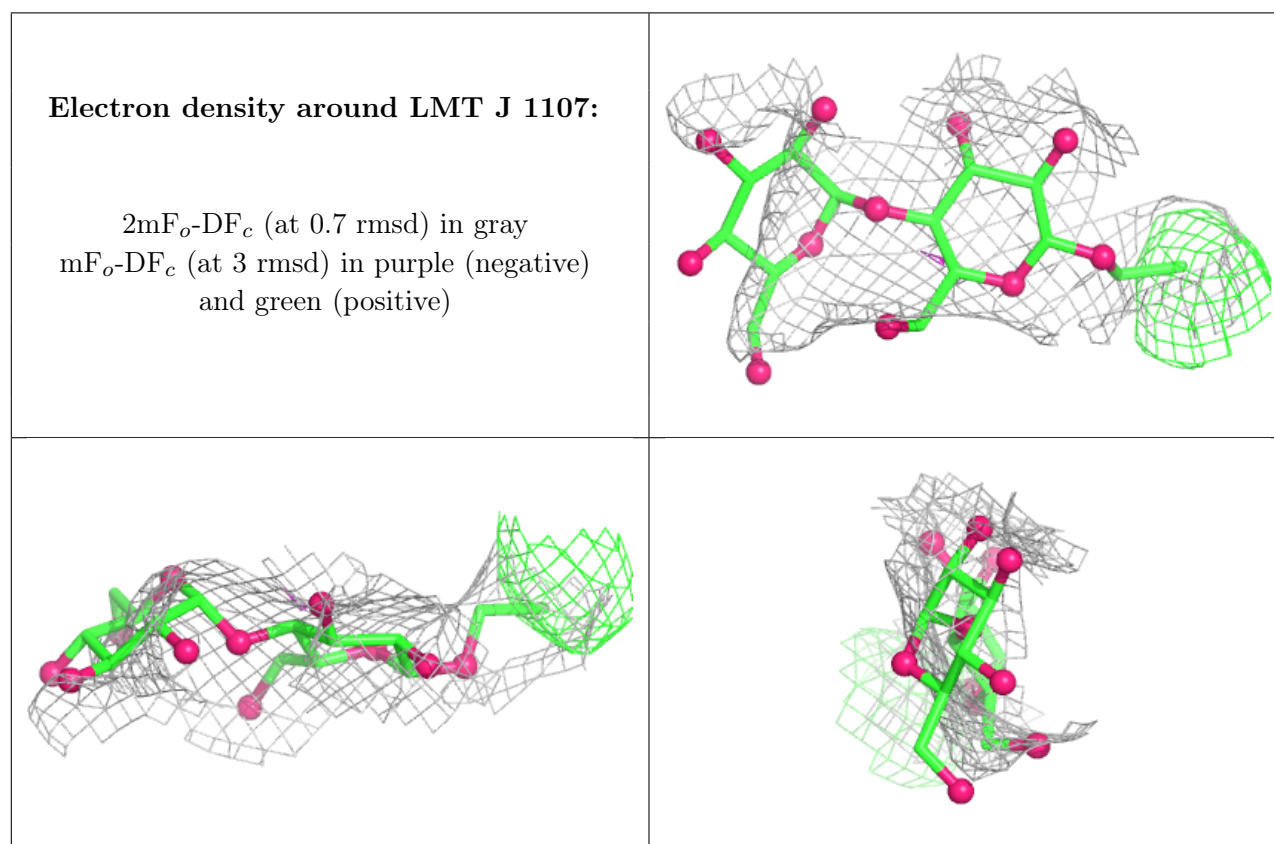
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	CLA	B	820	65/65	0.94	0.14	84,106,123,152	0
18	CLA	J	1101	65/65	0.94	0.10	65,87,114,129	0
18	CLA	B	821	46/65	0.94	0.12	110,126,143,155	0
18	CLA	B	836	55/65	0.94	0.12	74,92,108,115	0
18	CLA	A	831	65/65	0.94	0.14	81,104,128,146	0
21	BCR	B	802	40/40	0.94	0.16	72,100,119,128	0
22	LHG	A	848	49/49	0.94	0.15	63,90,107,112	0
18	CLA	A	807	65/65	0.94	0.13	66,84,106,119	0
18	CLA	B	825	65/65	0.95	0.12	77,94,120,134	0
18	CLA	A	828	65/65	0.95	0.13	64,79,99,118	0
18	CLA	B	813	46/65	0.95	0.09	107,126,142,166	0
18	CLA	A	817	65/65	0.95	0.18	84,115,134,143	0
18	CLA	B	803	65/65	0.95	0.14	64,81,98,107	0
18	CLA	F	301	65/65	0.95	0.10	65,87,105,109	0
18	CLA	A	830	65/65	0.95	0.13	77,95,108,122	0
18	CLA	B	806	65/65	0.95	0.12	76,92,112,121	0
18	CLA	A	802	65/65	0.95	0.11	62,77,96,111	0
18	CLA	B	809	65/65	0.95	0.13	79,108,122,129	0
18	CLA	A	812	65/65	0.95	0.13	92,113,130,139	0
18	CLA	4	307	65/65	0.95	0.12	109,135,157,165	0
17	CL0	A	801	65/65	0.95	0.14	65,86,99,118	0
18	CLA	4	309	60/65	0.95	0.12	83,123,138,143	0
18	CLA	B	824	55/65	0.95	0.12	82,105,123,133	0
18	CLA	1	5010	65/65	0.95	0.12	89,146,162,180	0
18	CLA	2	326	50/65	0.95	0.11	94,114,150,160	0
30	CHL	4	318	56/66	0.95	0.12	109,134,178,182	0
18	CLA	3	301	45/65	0.95	0.11	120,138,174,192	0
19	PQN	B	842	33/33	0.95	0.13	67,84,105,120	0
18	CLA	B	814	65/65	0.96	0.11	84,107,122,131	0
18	CLA	A	827	65/65	0.96	0.14	81,99,115,120	0
18	CLA	A	839	65/65	0.96	0.10	61,82,97,106	0
18	CLA	B	807	65/65	0.96	0.10	73,93,108,115	0
18	CLA	2	309	65/65	0.96	0.12	99,121,132,145	0
18	CLA	A	819	65/65	0.96	0.11	78,111,133,145	0
19	PQN	A	841	33/33	0.96	0.14	63,82,97,104	0
18	CLA	B	819	65/65	0.96	0.14	82,104,123,132	0
18	CLA	A	804	65/65	0.96	0.11	78,91,114,138	0
18	CLA	A	805	65/65	0.96	0.10	65,86,103,115	0
18	CLA	A	808	65/65	0.96	0.10	67,85,132,144	0
18	CLA	A	837	65/65	0.96	0.10	63,77,94,114	0
18	CLA	B	804	65/65	0.96	0.12	69,90,105,117	0
18	CLA	A	818	50/65	0.97	0.11	101,128,151,163	0

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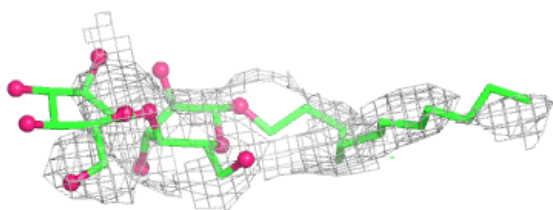
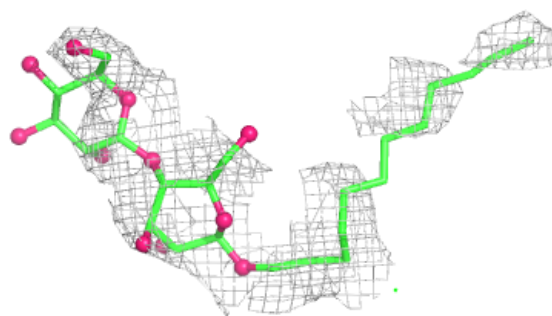
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	SF4	A	842	8/8	0.98	0.08	70,71,119,144	0
20	SF4	C	102	8/8	0.98	0.06	79,89,122,145	0
20	SF4	C	101	8/8	0.99	0.05	69,86,120,124	0

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.



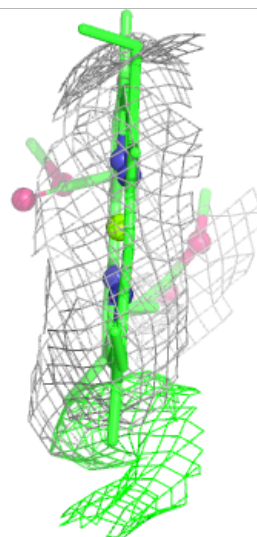
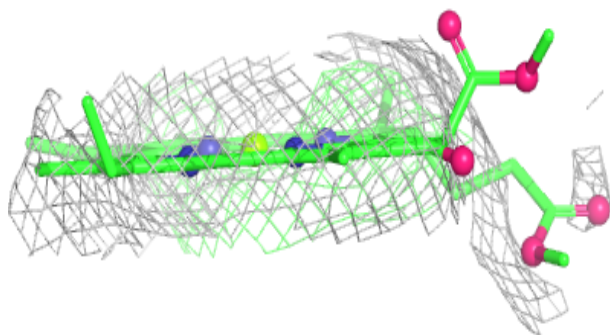
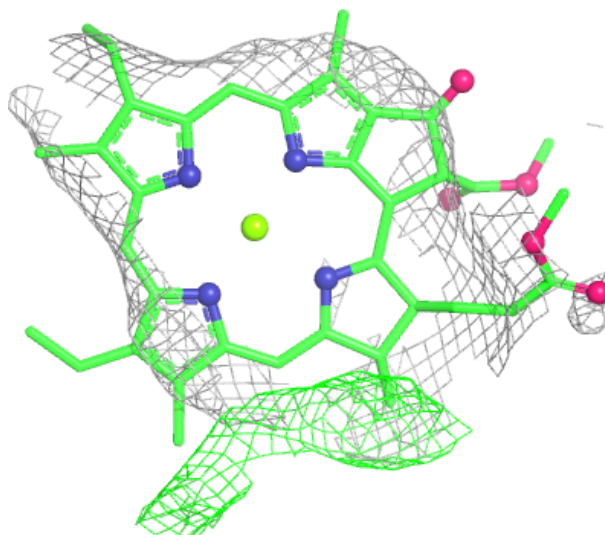
Electron density around LMT 2 325:

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



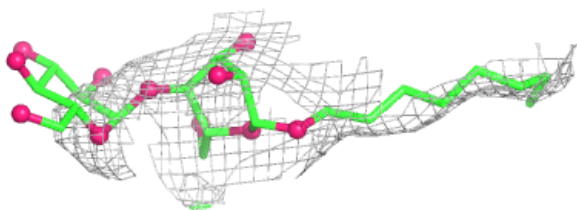
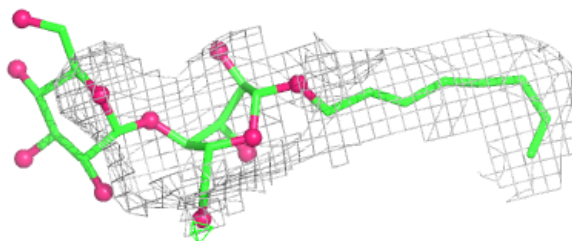
Electron density around CLA K 1404:

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

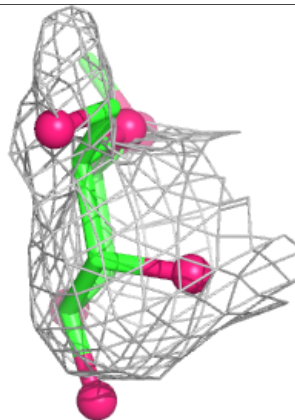
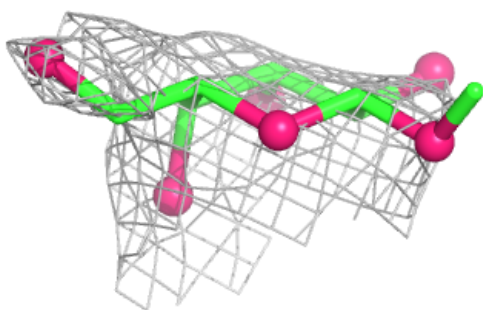
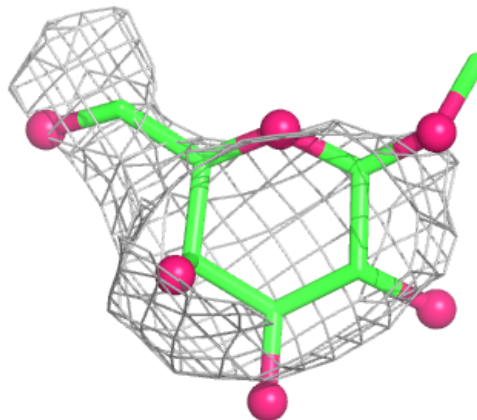


Electron density around LMT G 1606:

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

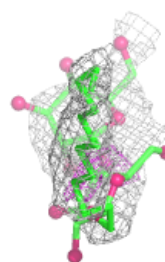
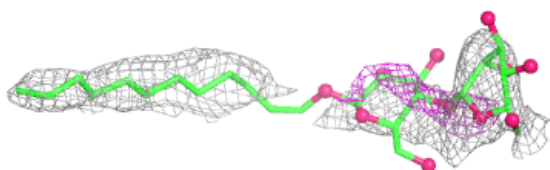
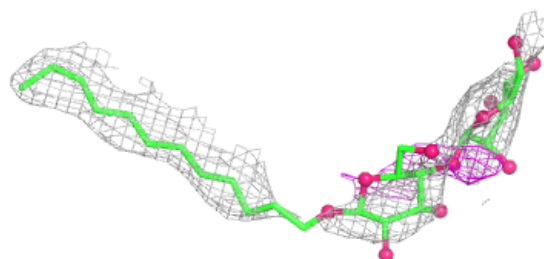
**Electron density around LMG 2 301:**

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

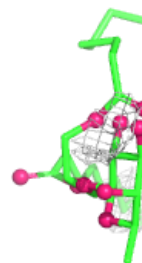
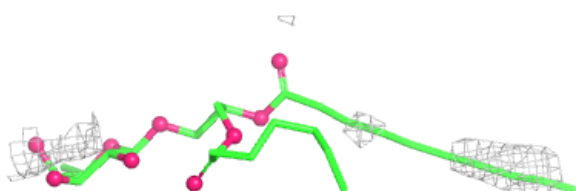
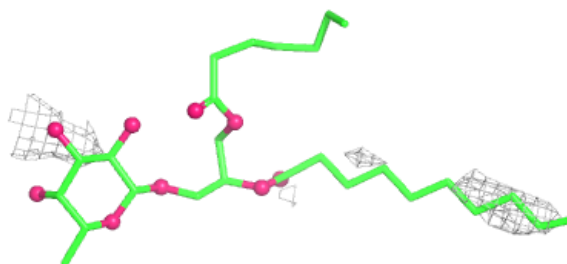


Electron density around LMT A 850:

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

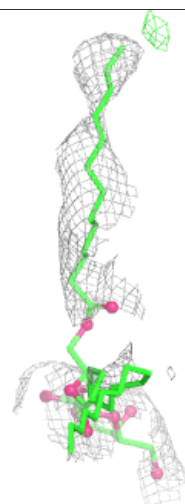
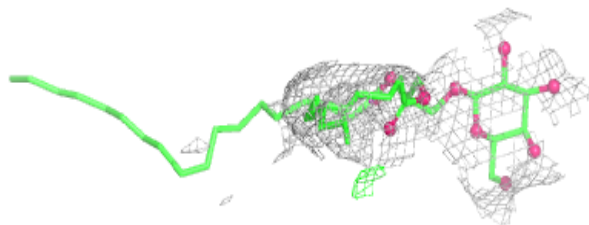
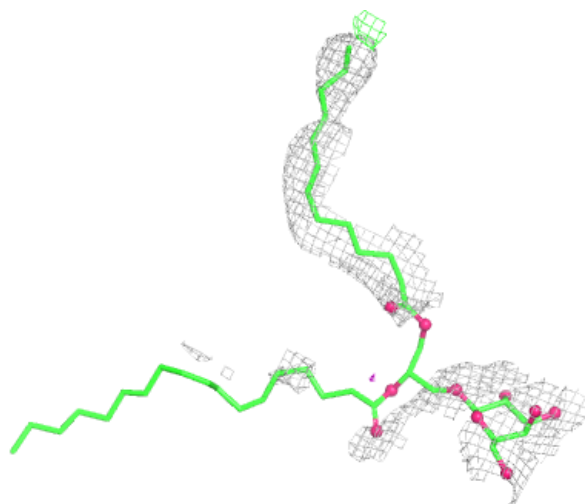
**Electron density around DGD 1 5002:**

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



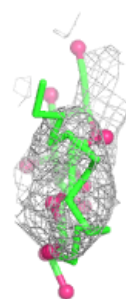
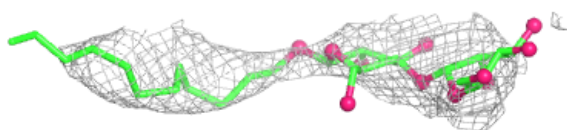
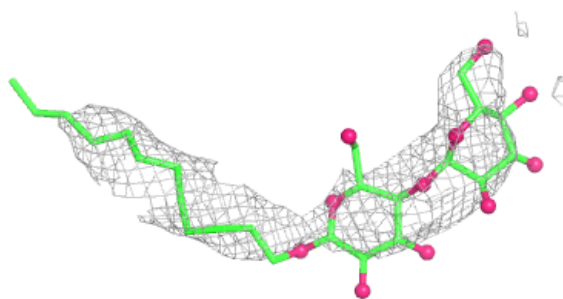
Electron density around LMG A 851:

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

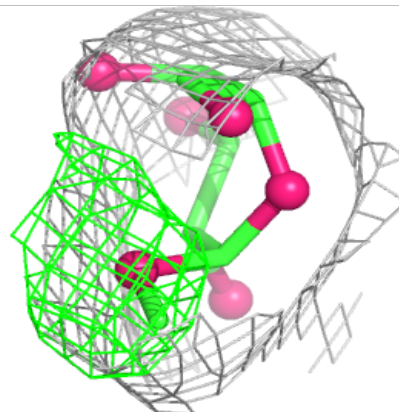
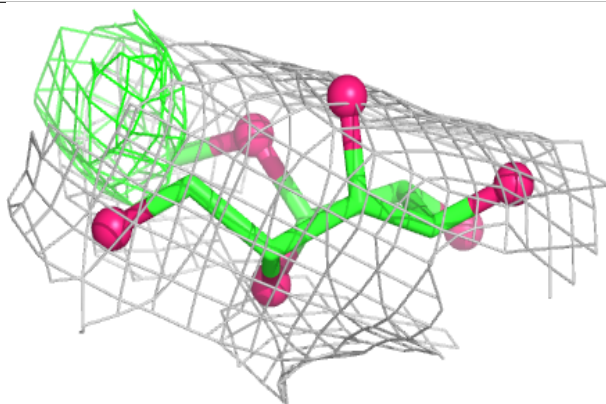
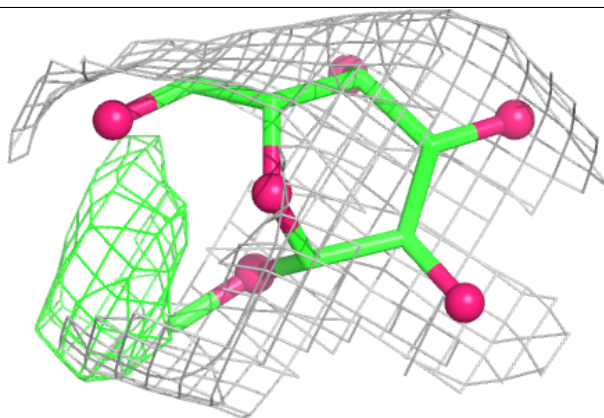


Electron density around LMT B 852:

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

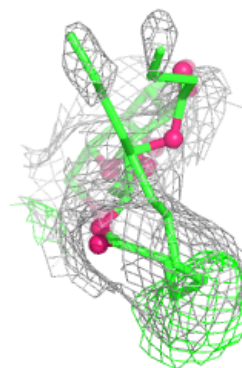
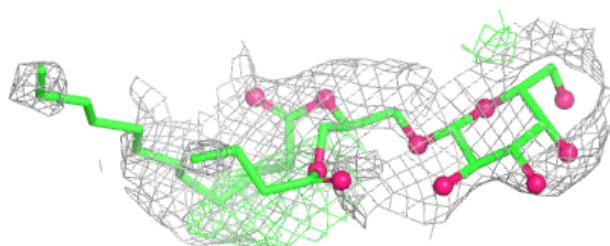
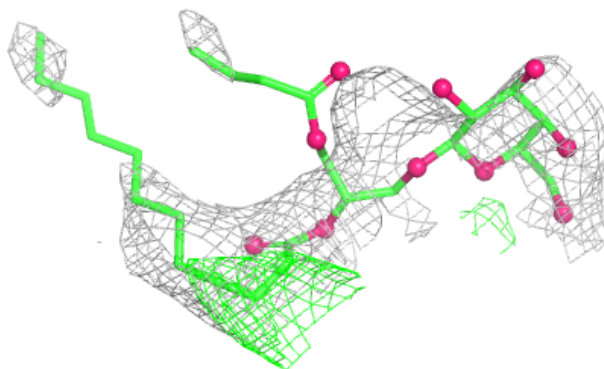
**Electron density around LMG 2 323:**

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

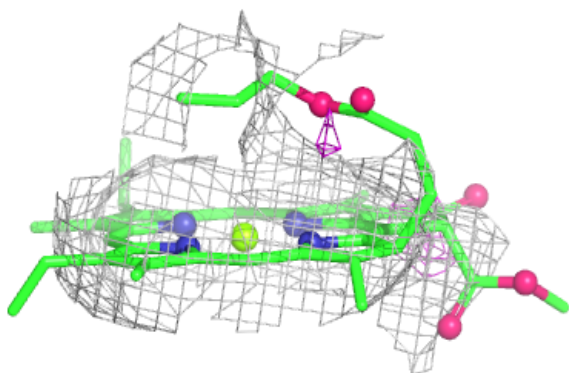
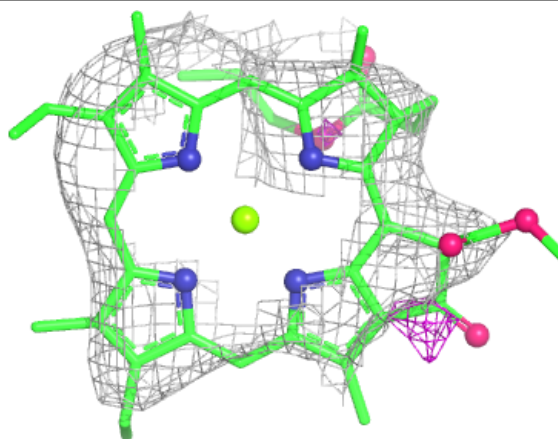


Electron density around LMG B 850:

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

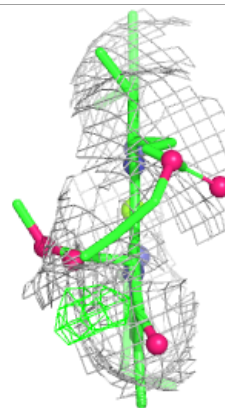
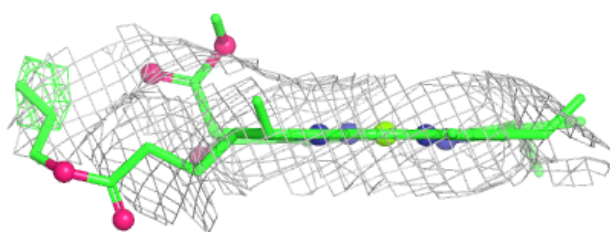
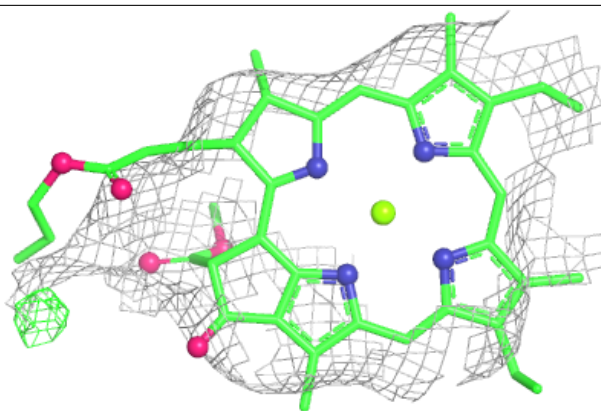
**Electron density around CLA 3 314:**

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

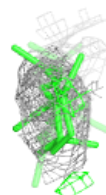
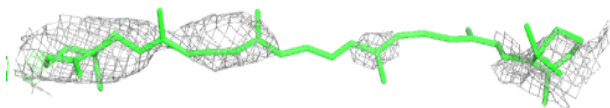
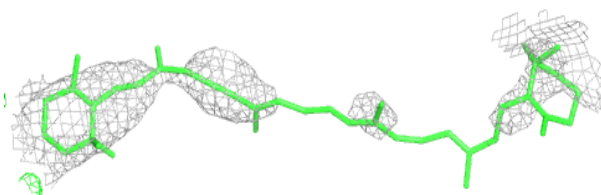


Electron density around CLA K 1403:

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

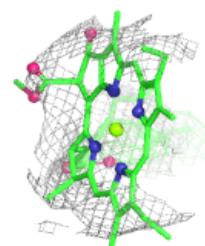
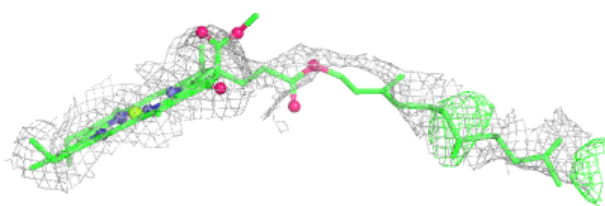
**Electron density around BCR 2 305:**

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



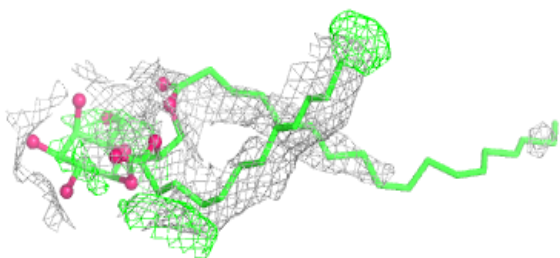
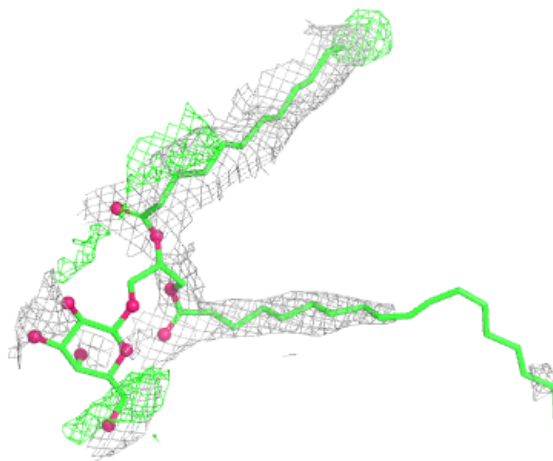
Electron density around CLA H 1701:

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



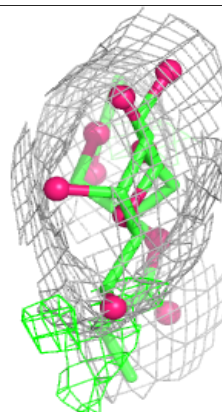
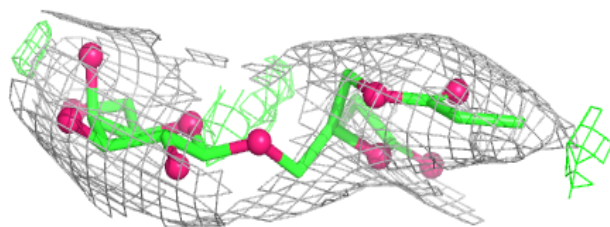
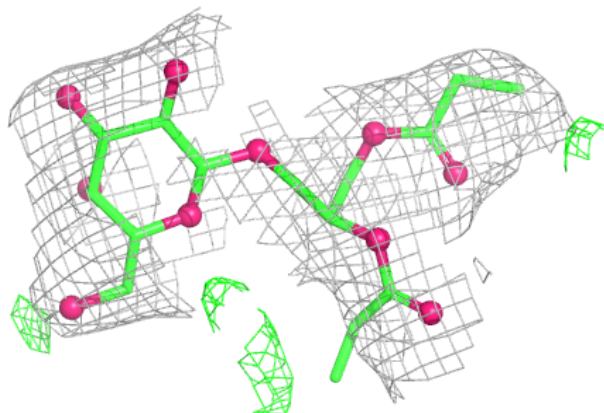
Electron density around LMG 1 5001:

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

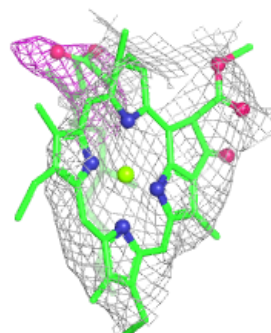
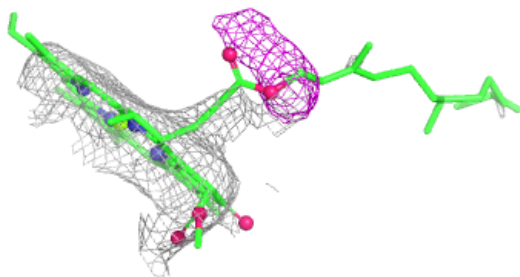
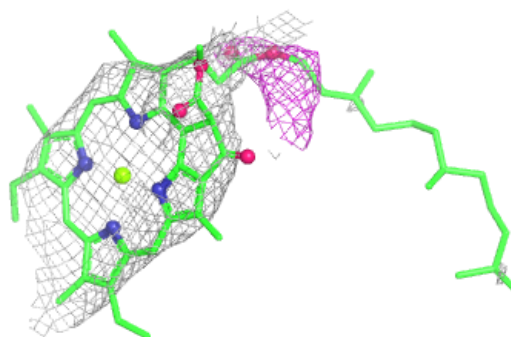


Electron density around LMG 2 321:

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

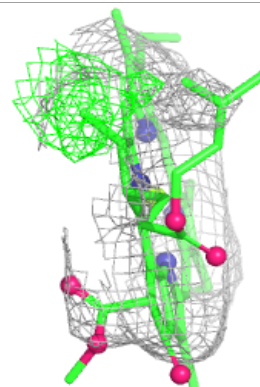
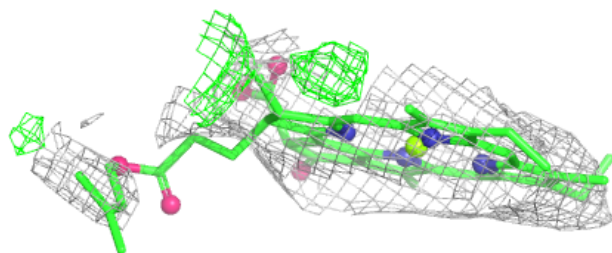
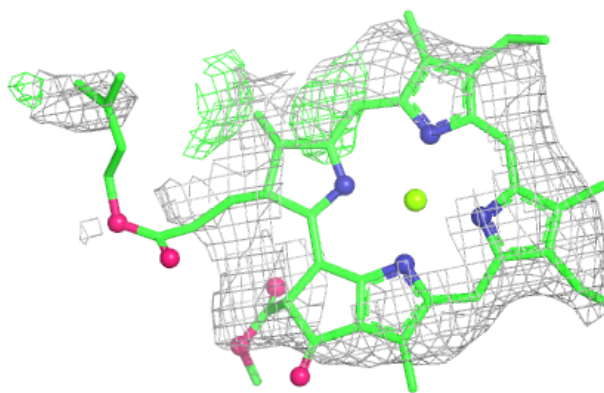
**Electron density around CLA K 1402:**

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



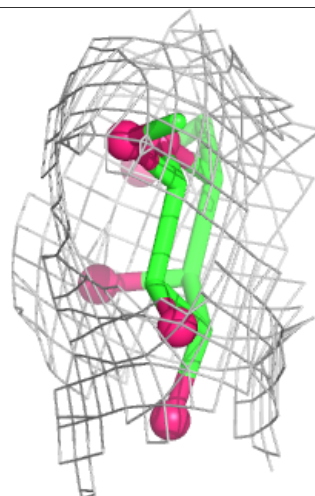
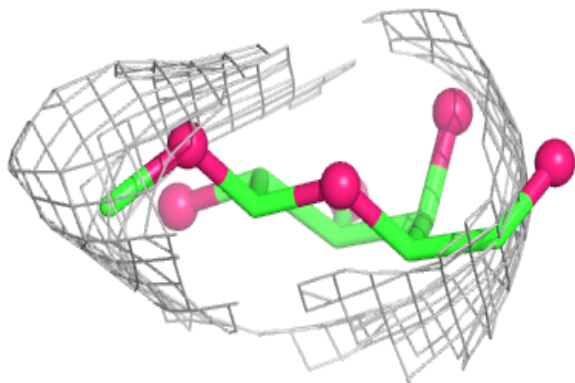
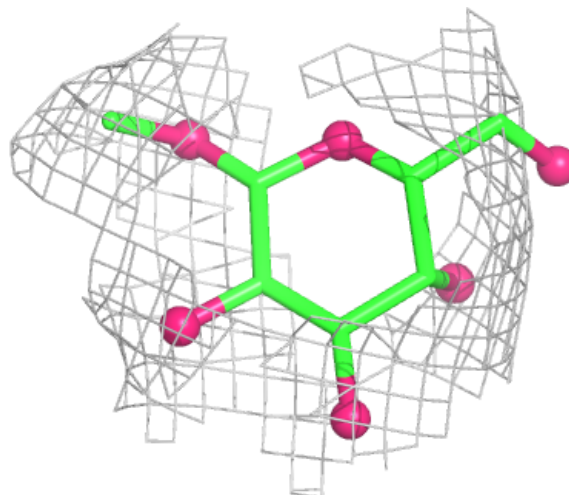
Electron density around CLA J 1103:

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



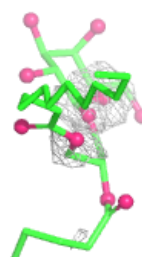
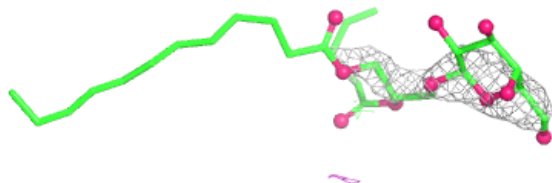
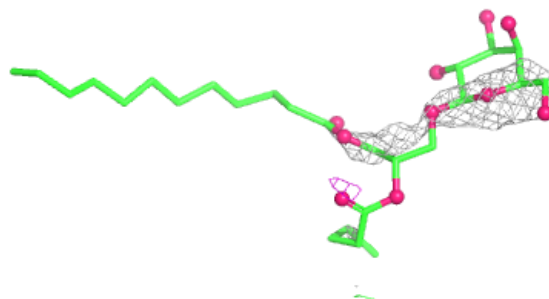
Electron density around LMG 2 324:

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

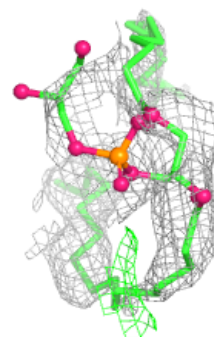
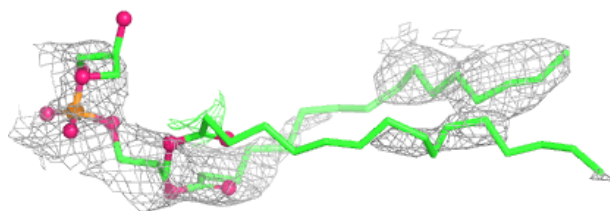
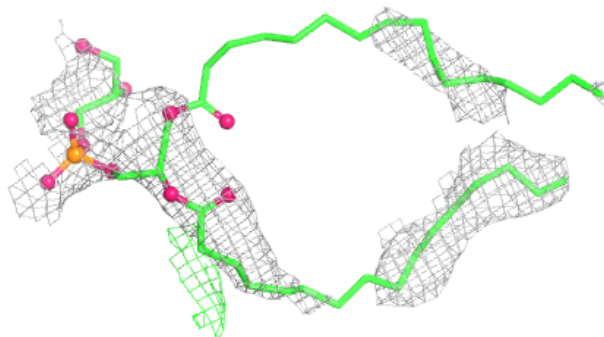


Electron density around LMG F 307:

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

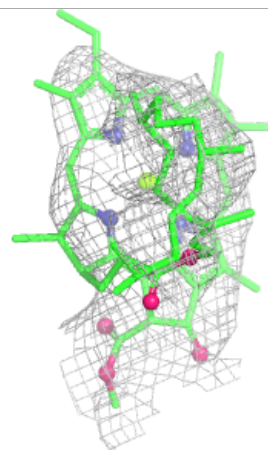
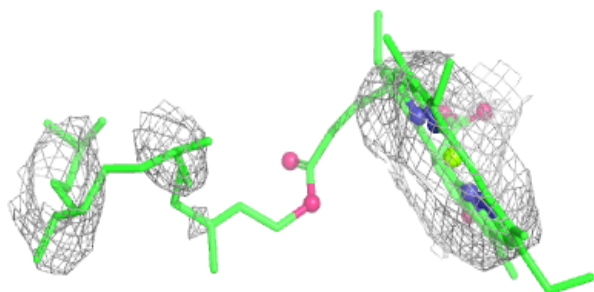
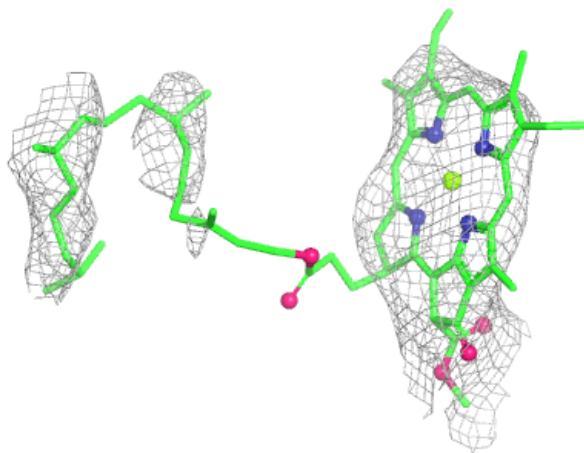
**Electron density around LHG B 849:**

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



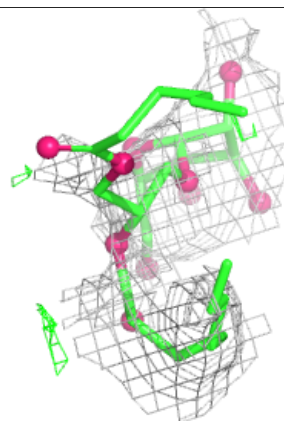
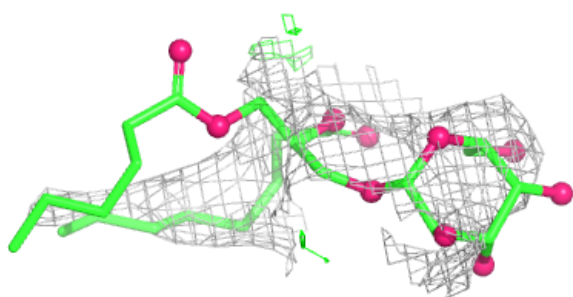
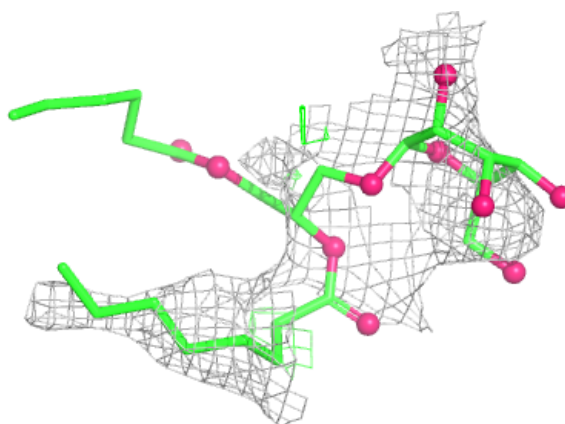
Electron density around CLA 1 5015:

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

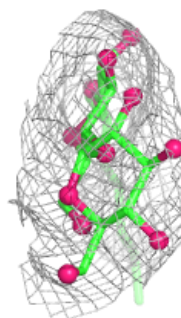
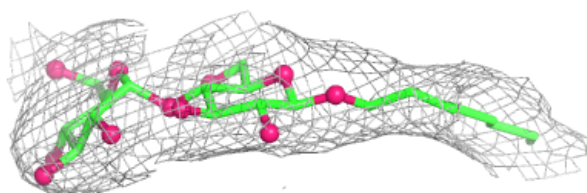
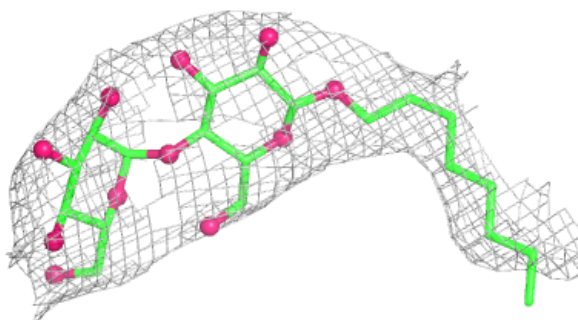


Electron density around LMG B 851:

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

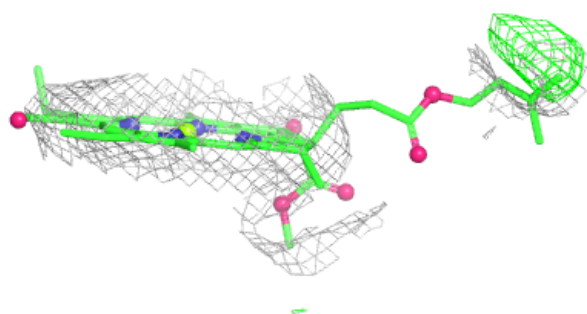
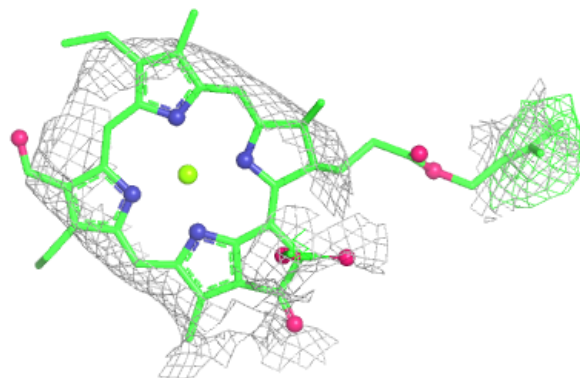
**Electron density around LMT B 856:**

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

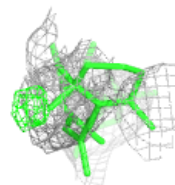
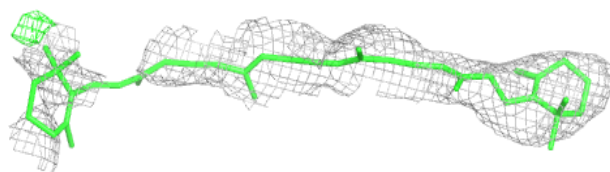
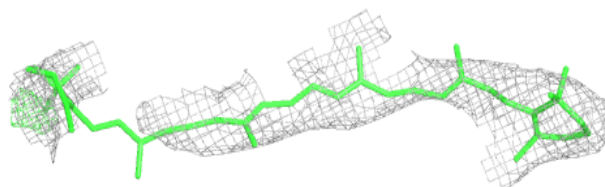


Electron density around CHL 3 313:

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

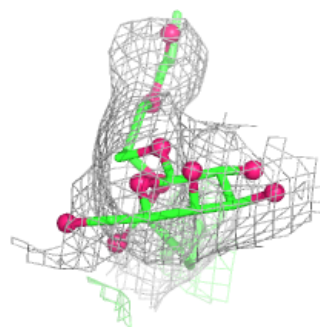
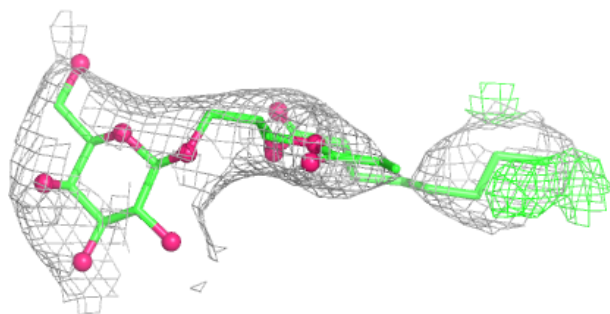
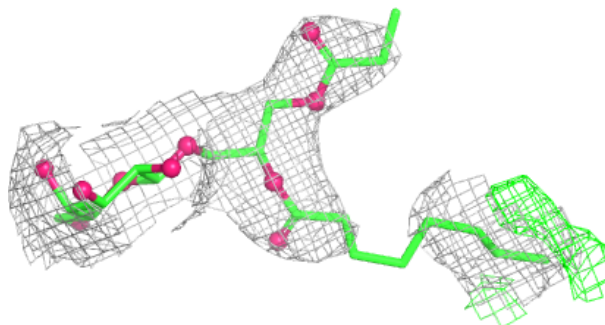
**Electron density around BCR L 302:**

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



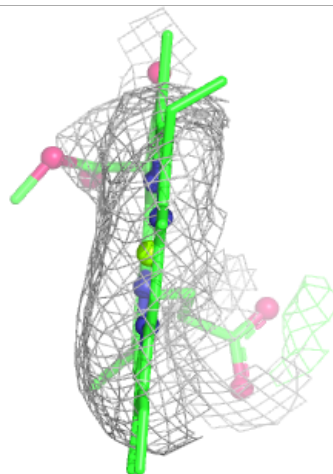
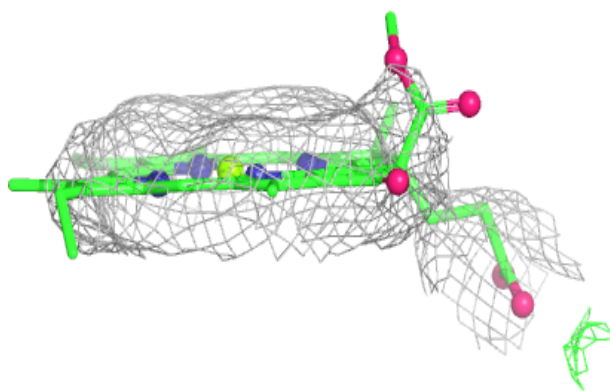
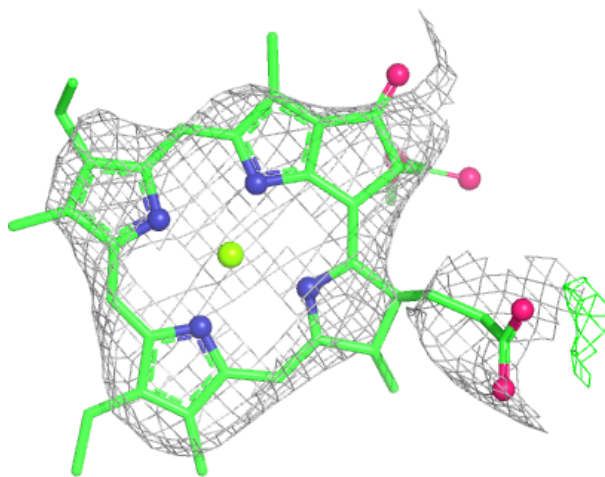
Electron density around LMG J 1102:

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



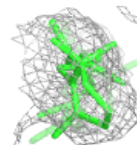
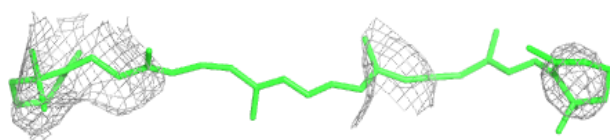
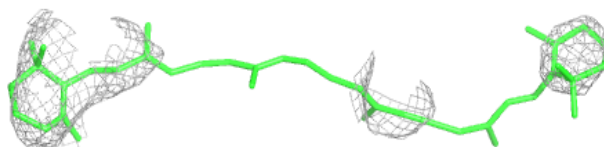
Electron density around CLA K 1401:

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

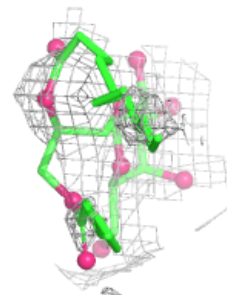
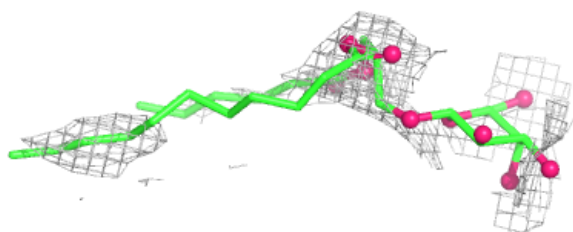


Electron density around BCR K 1405:

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

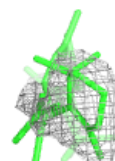
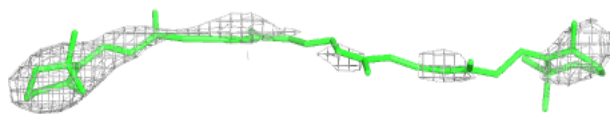
**Electron density around LMG 2 322:**

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



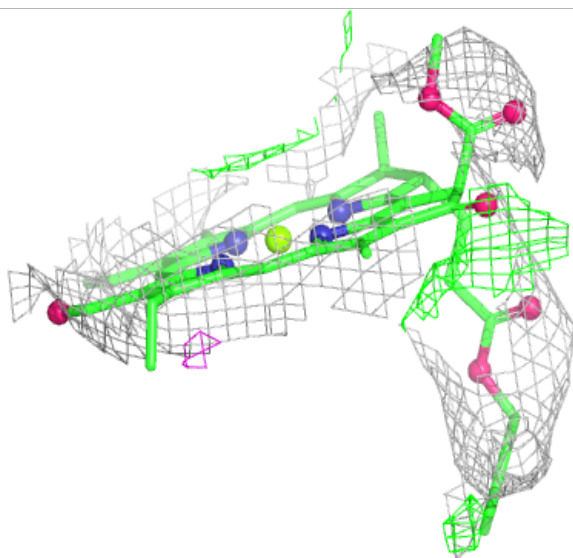
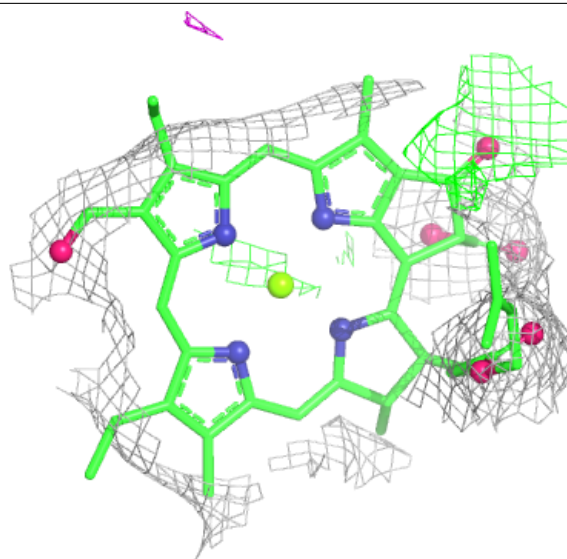
Electron density around BCR 3 306:

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



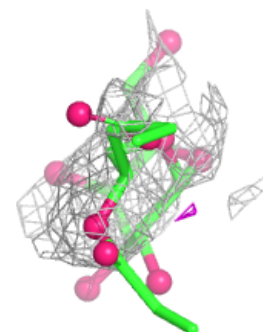
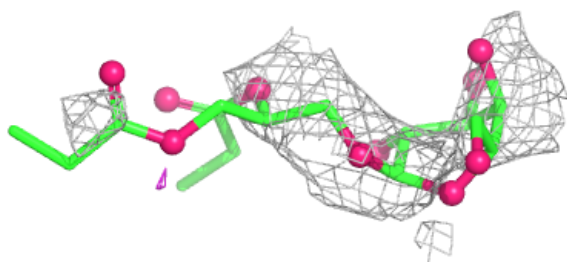
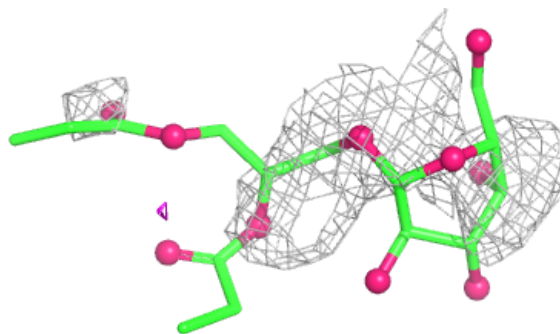
Electron density around CHL 3 312:

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

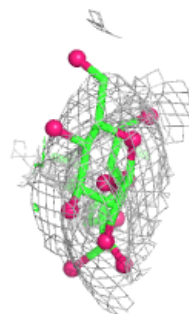
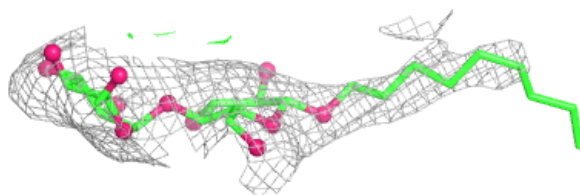
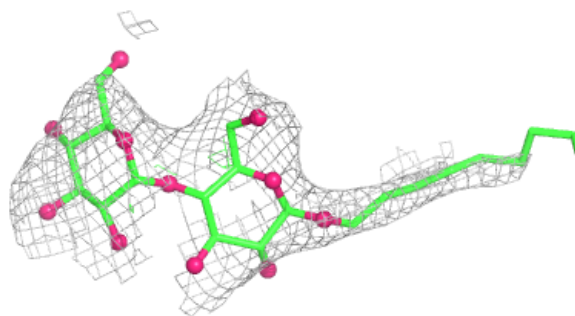


Electron density around LMG G 1607:

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

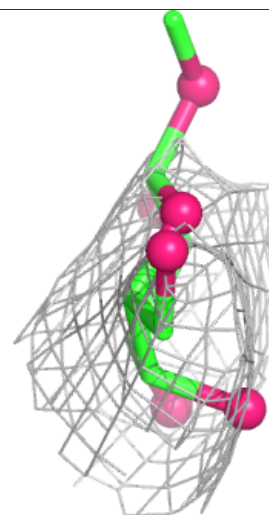
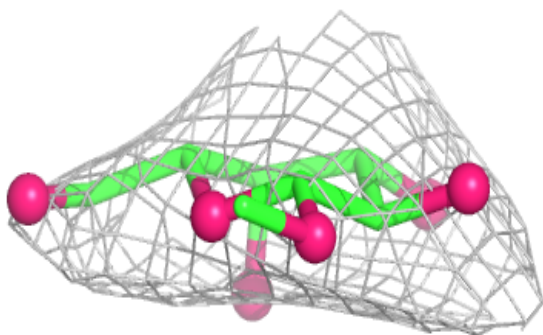
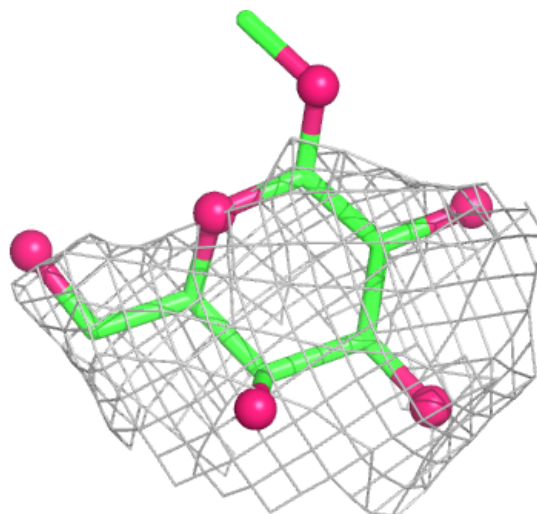
**Electron density around LMT B 853:**

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



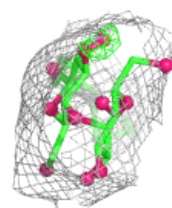
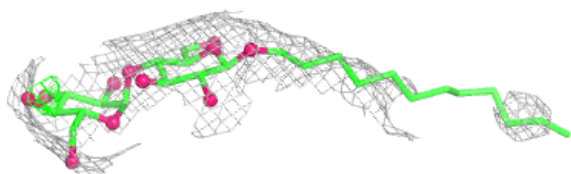
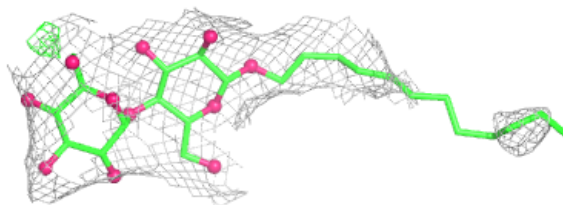
Electron density around LMG B 854:

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

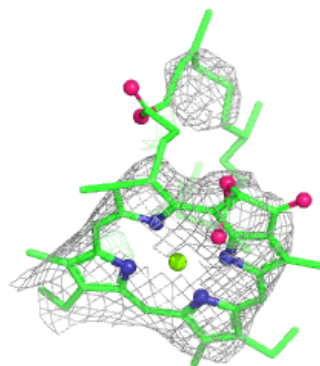
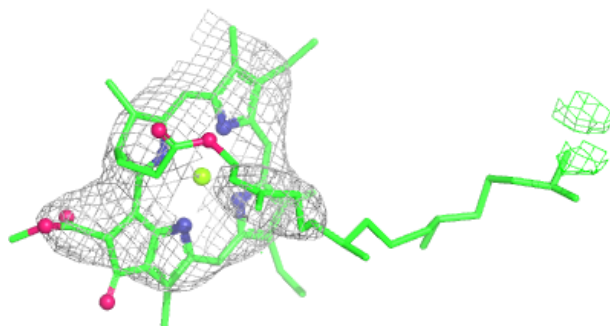
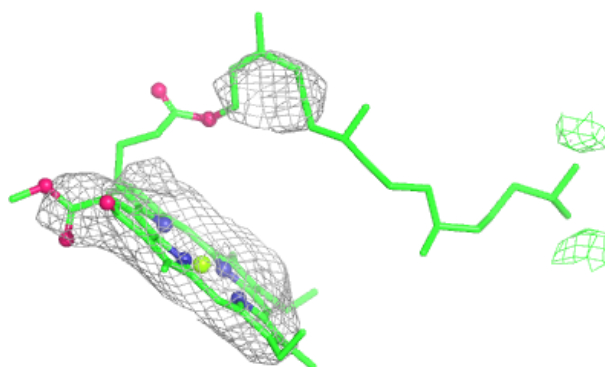


Electron density around LMT G 1605:

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

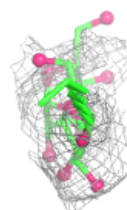
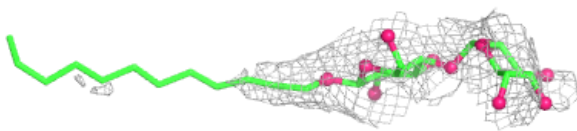
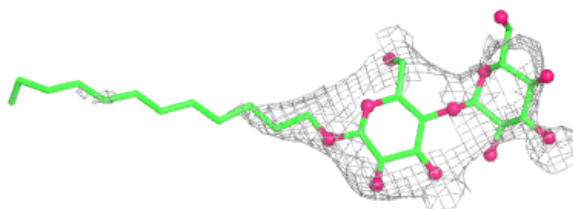
**Electron density around CLA G 1603:**

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

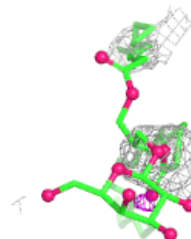
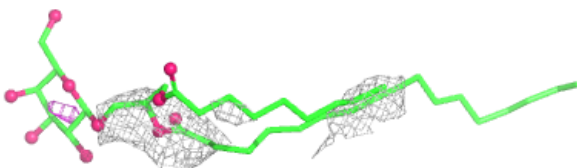
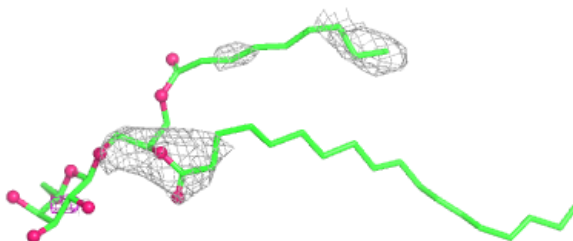


Electron density around LMT 4 319:

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

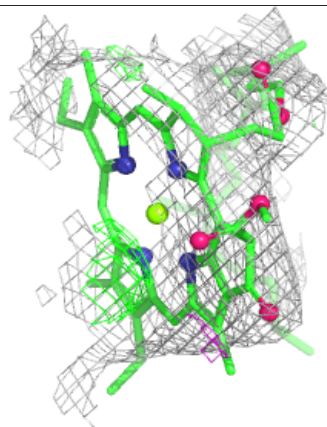
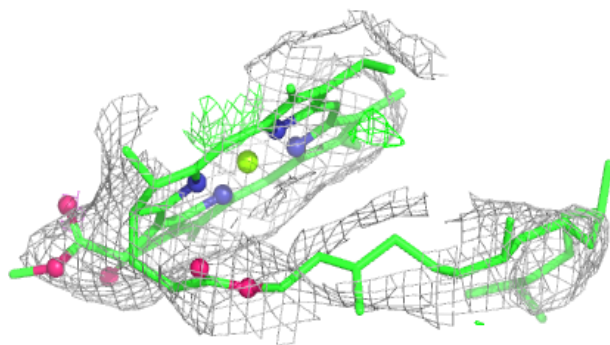
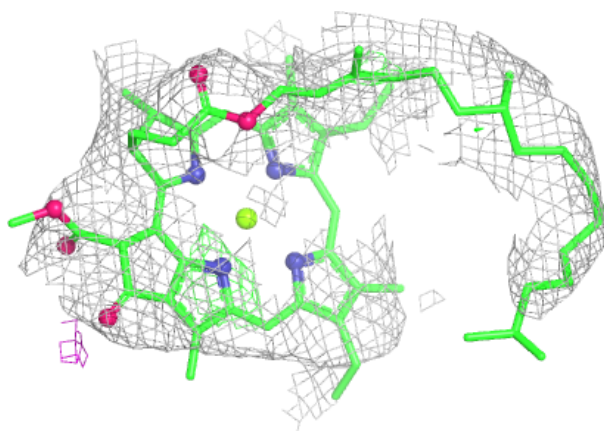
**Electron density around LMG 1 5020:**

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



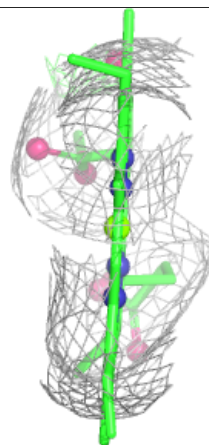
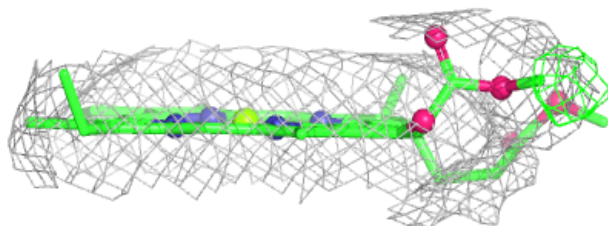
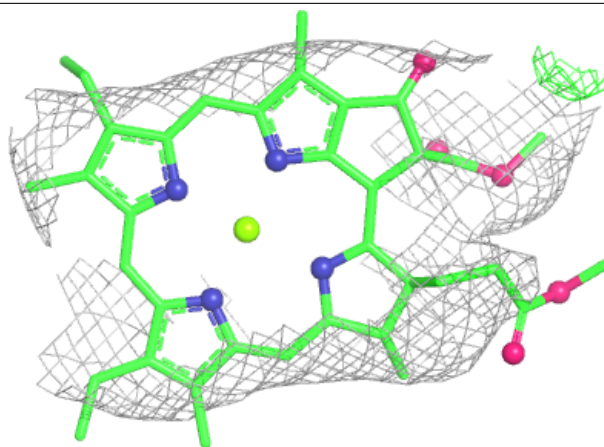
Electron density around CLA 1 5006:

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



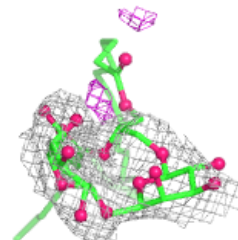
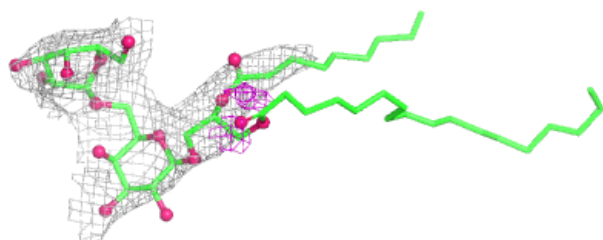
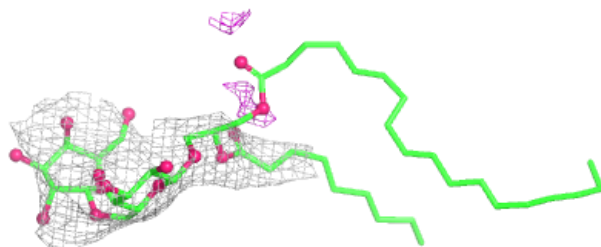
Electron density around CLA G 1602:

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

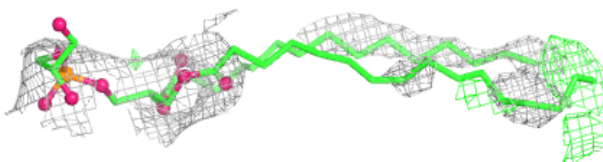


Electron density around DGD F 309:

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

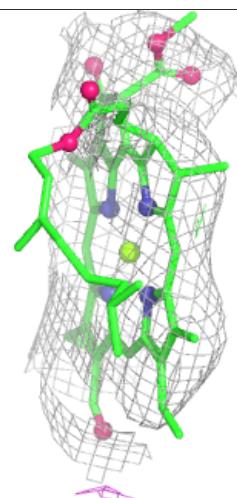
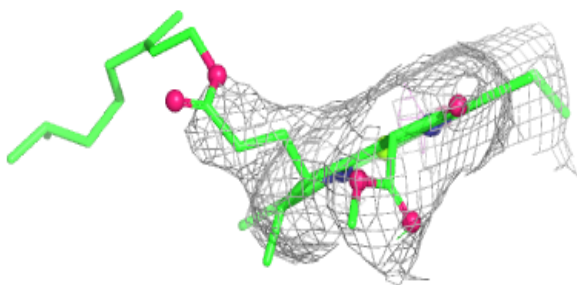
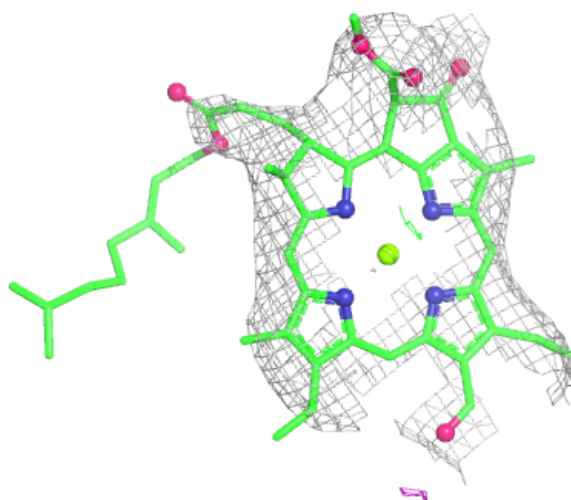
**Electron density around LHG 1 5019:**

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



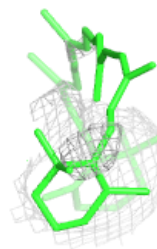
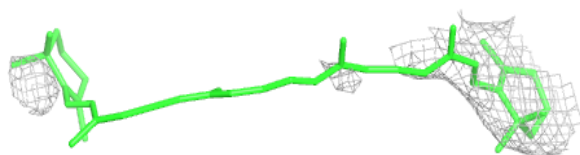
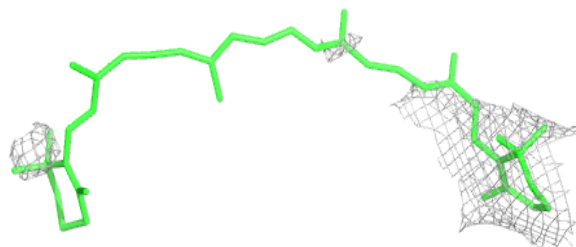
Electron density around CHL 2 315:

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



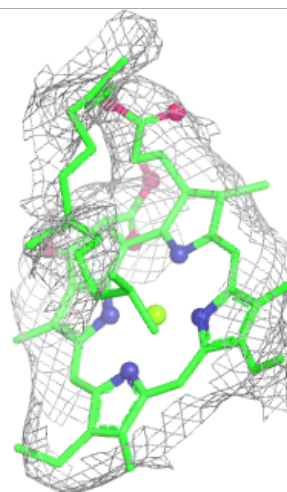
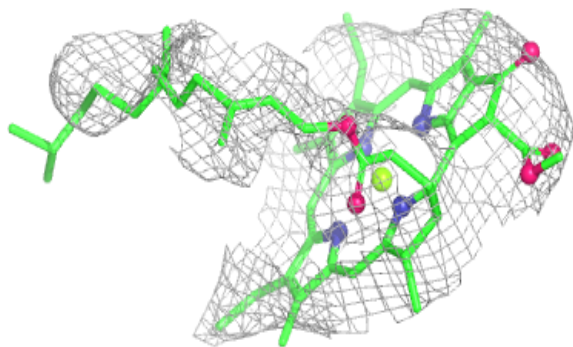
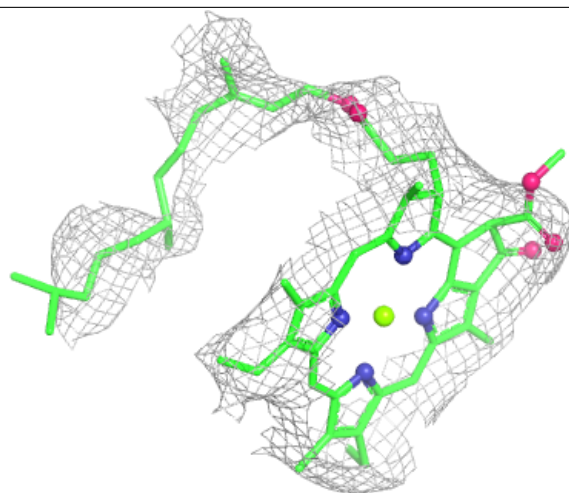
Electron density around BCR 1 5005:

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



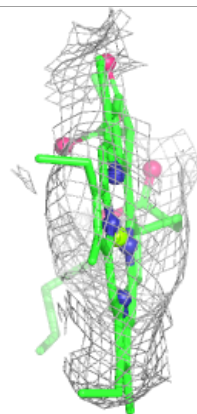
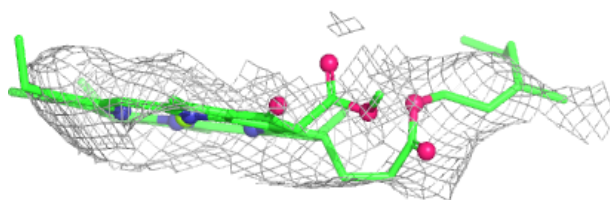
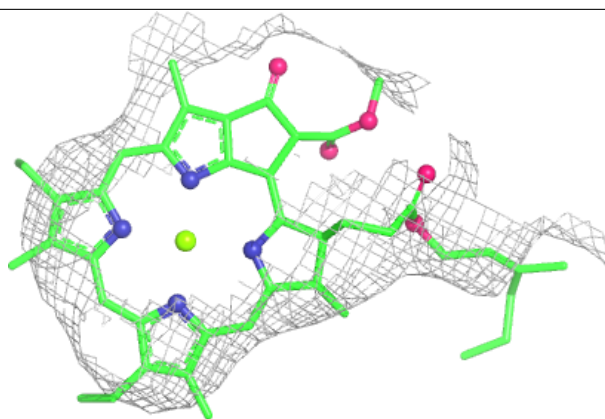
Electron density around CLA A 840:

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

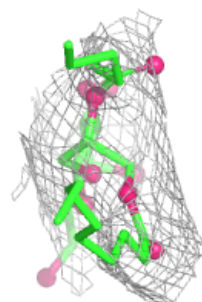
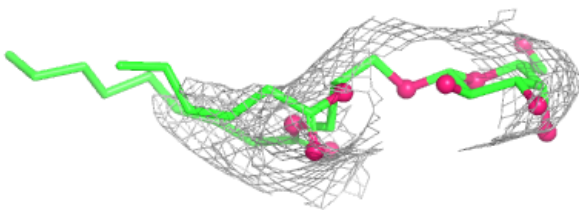
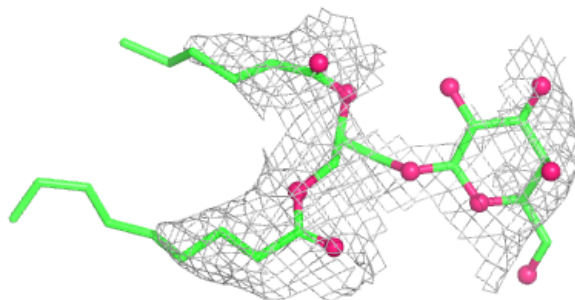


Electron density around CLA 3 308:

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

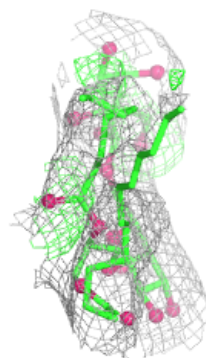
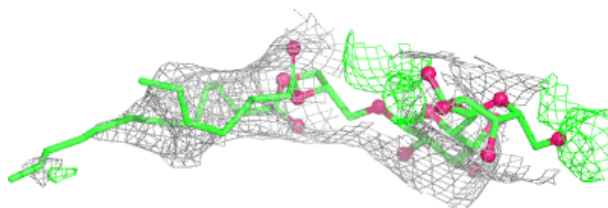
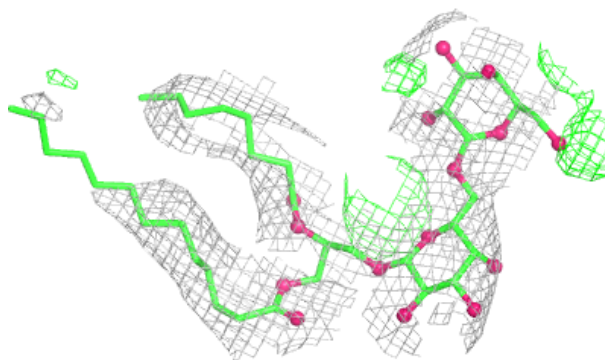
**Electron density around LMG F 308:**

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



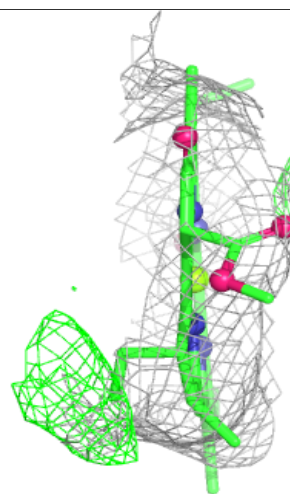
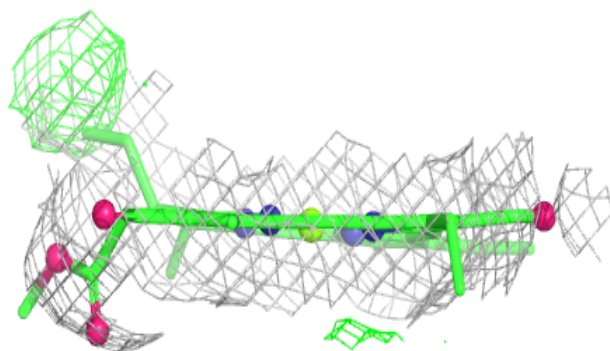
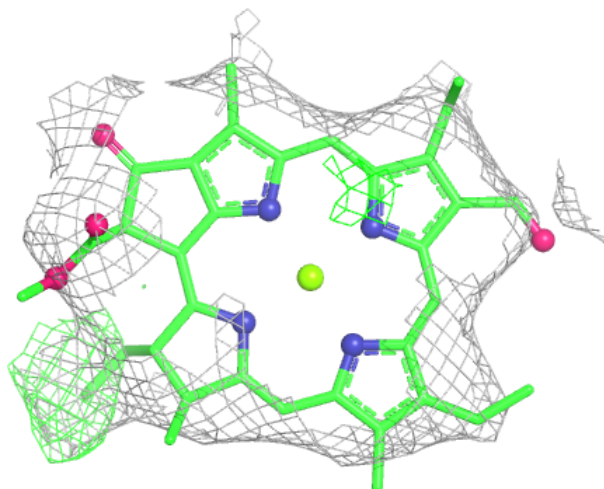
Electron density around DGD 2 327:

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



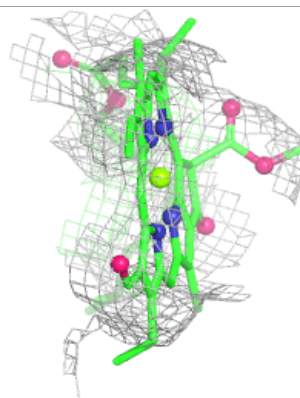
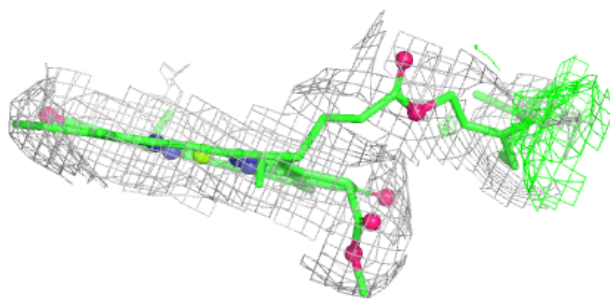
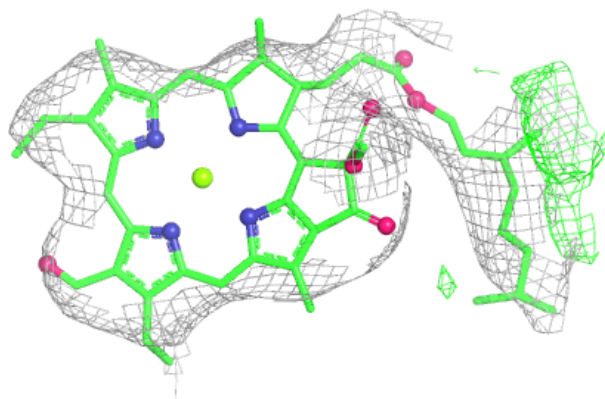
Electron density around CHL 4 317:

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

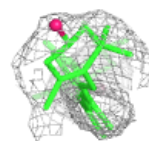
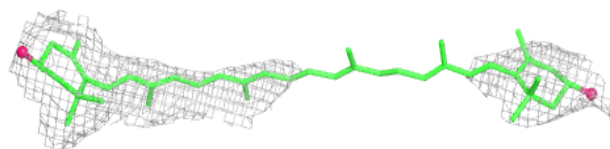
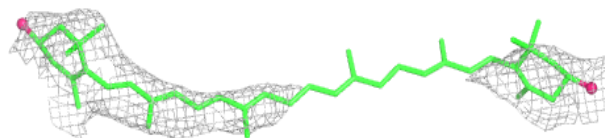


Electron density around CHL 2 319:

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

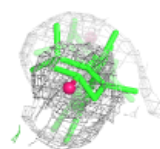
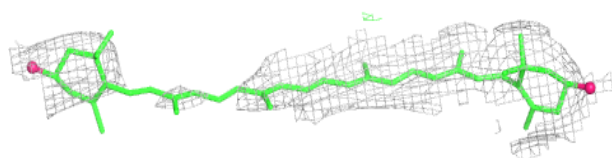
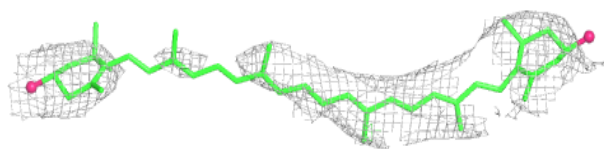
**Electron density around LUT 4 303:**

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

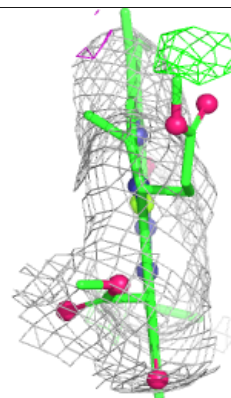
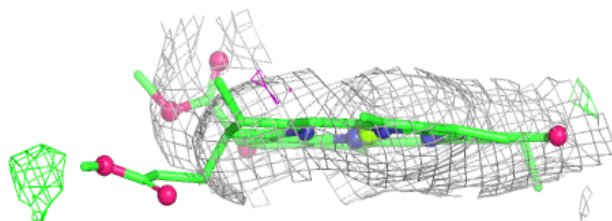
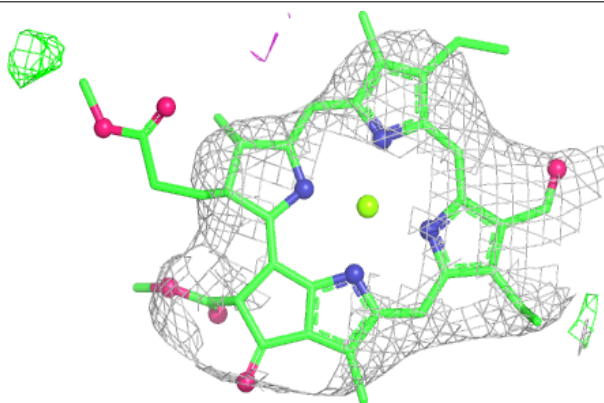


Electron density around LUT 2 303:

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

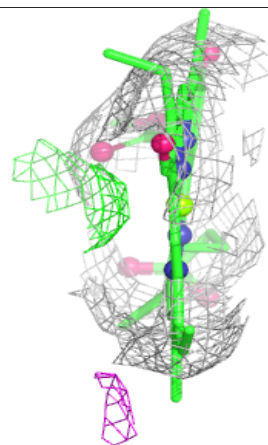
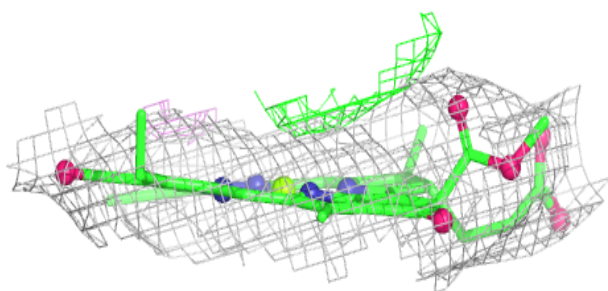
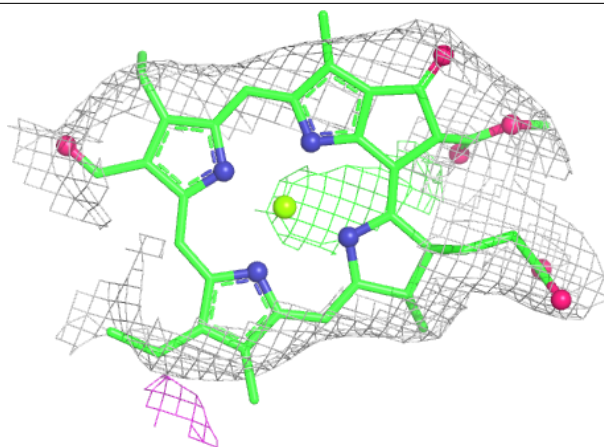
**Electron density around CHL 4 313:**

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

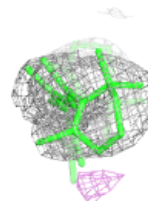
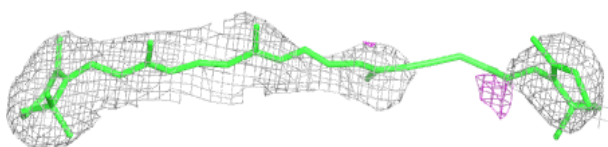
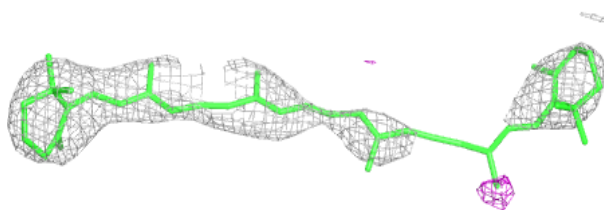


Electron density around CHL 2 318:

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

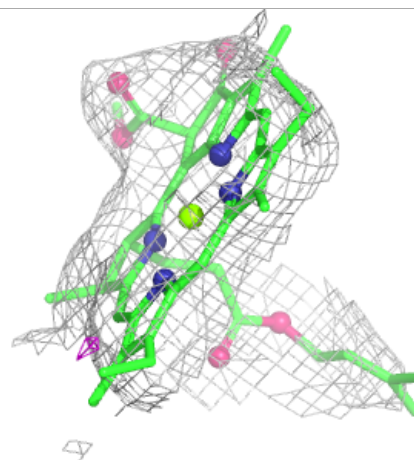
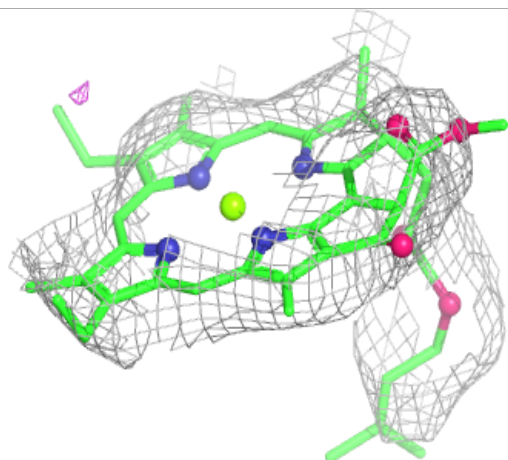
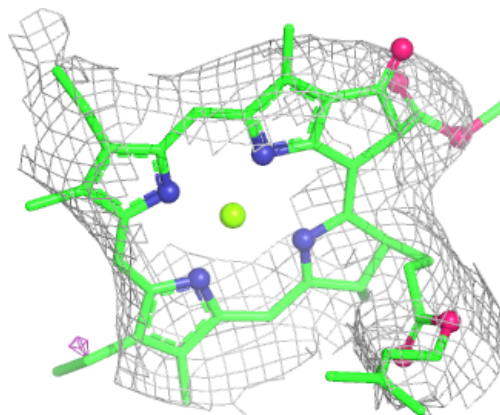
**Electron density around BCR A 846:**

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



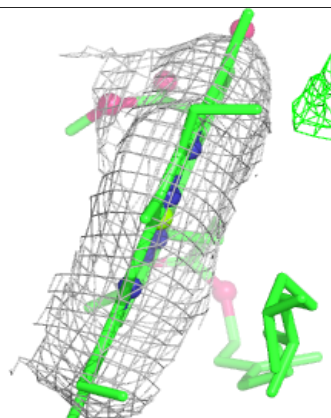
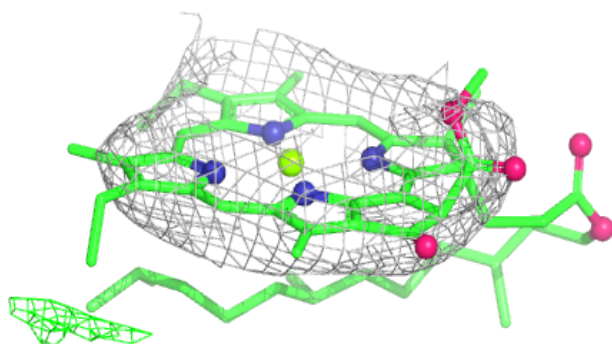
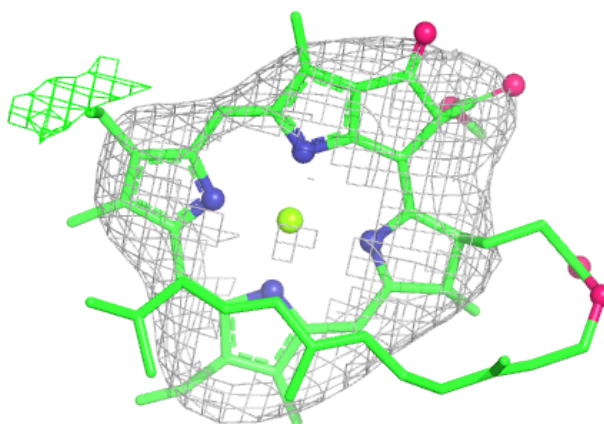
Electron density around CLA 2 311:

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

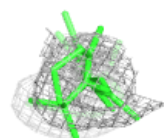
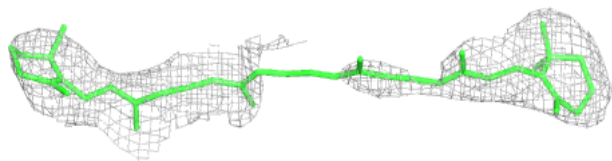
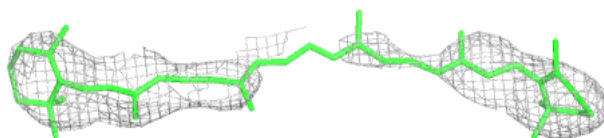


Electron density around CLA 3 319:

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

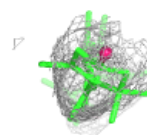
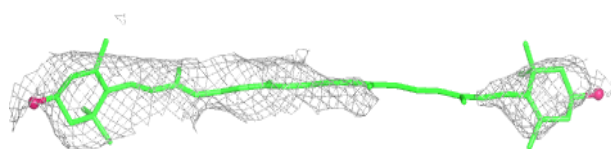
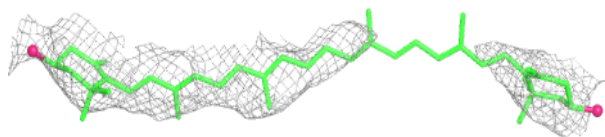
**Electron density around BCR L 307:**

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

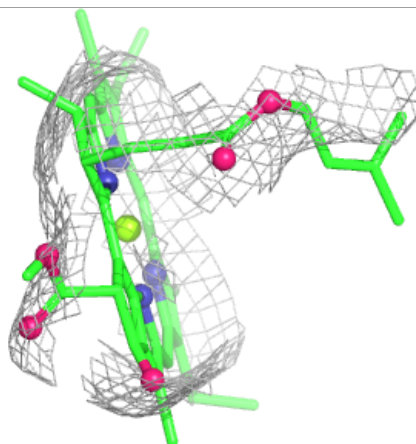
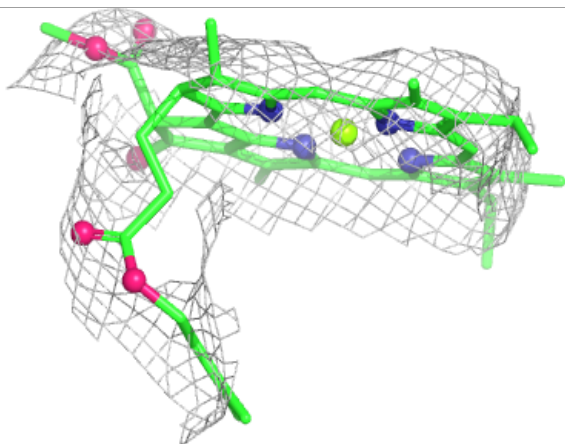
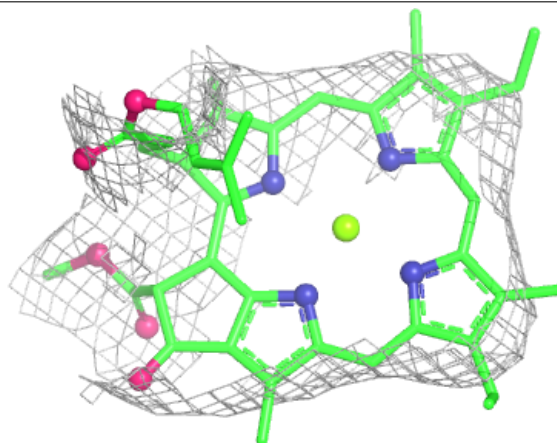


Electron density around LUT 1 5003:

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

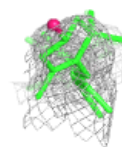
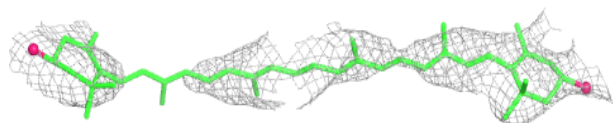
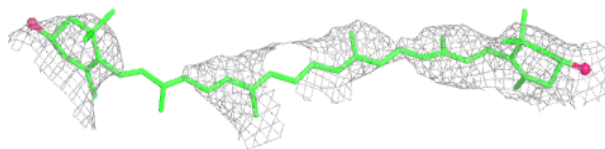
**Electron density around CLA 1 5011:**

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

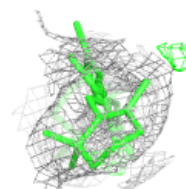
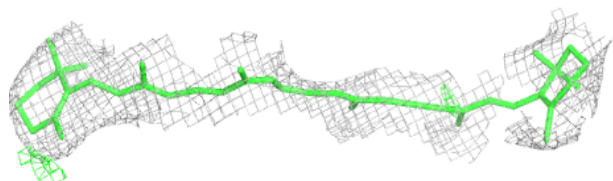
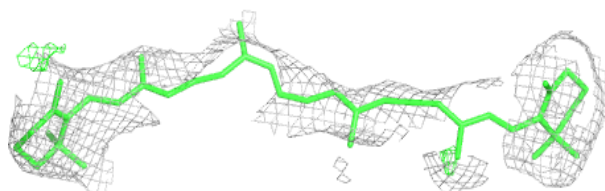


Electron density around LUT 3 303:

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

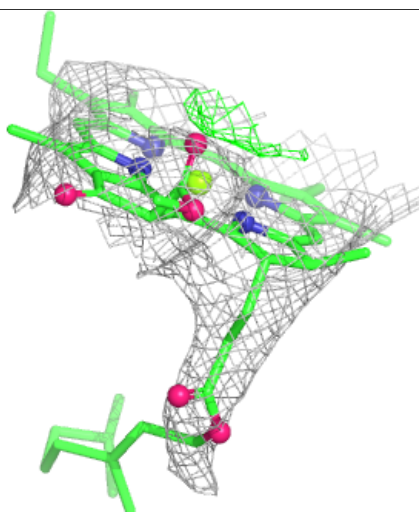
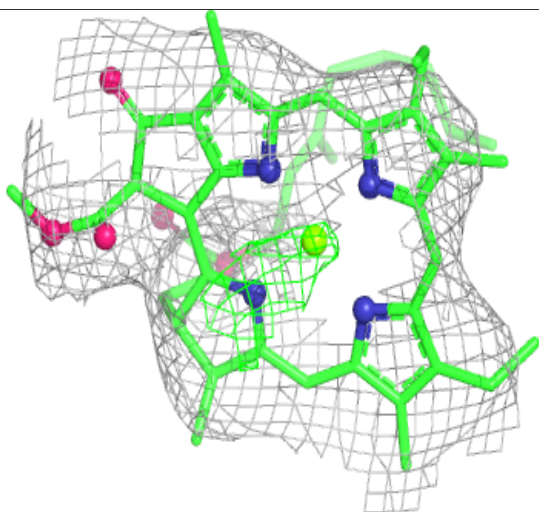
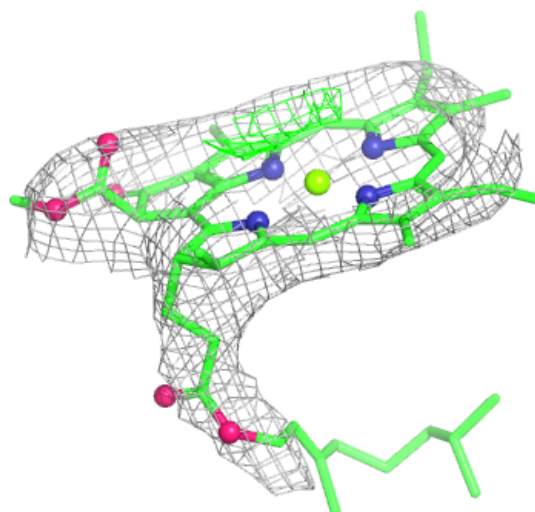
**Electron density around BCR G 1604:**

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



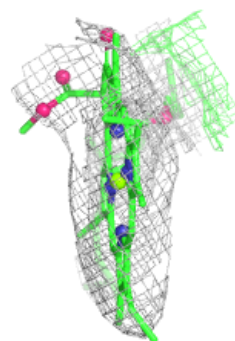
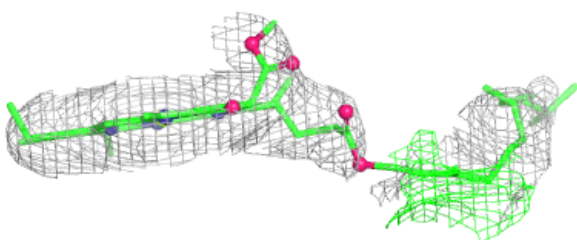
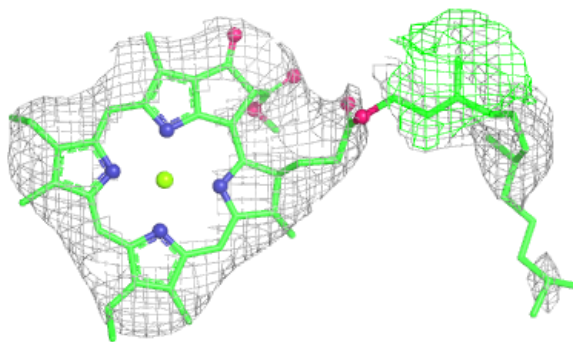
Electron density around CLA B 835:

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



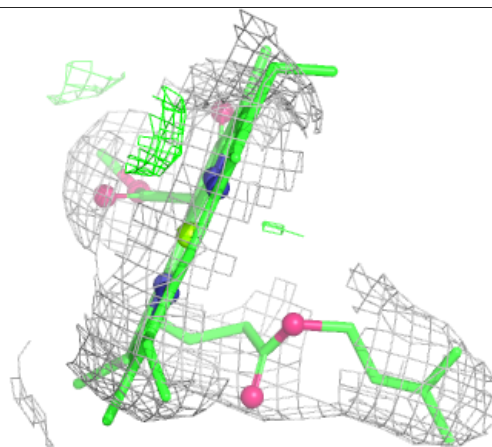
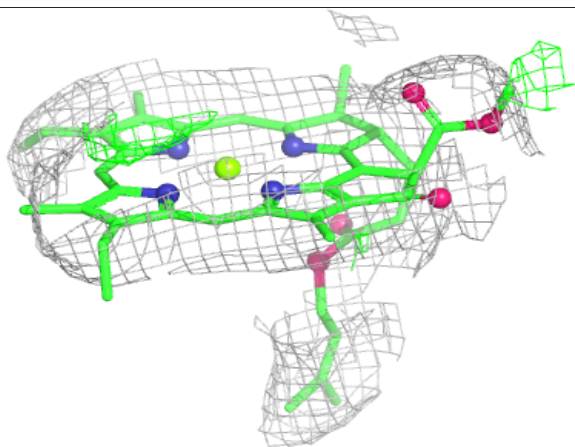
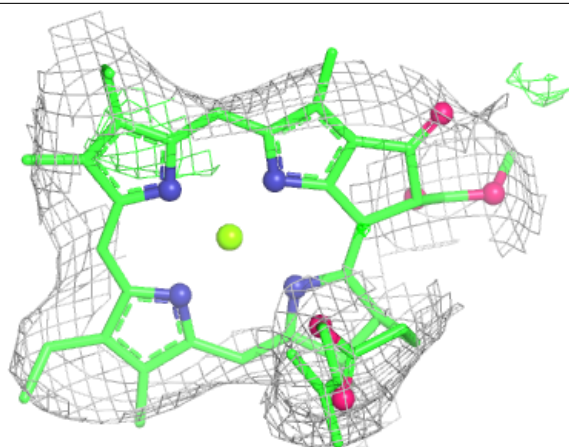
Electron density around CLA 1 5018:

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



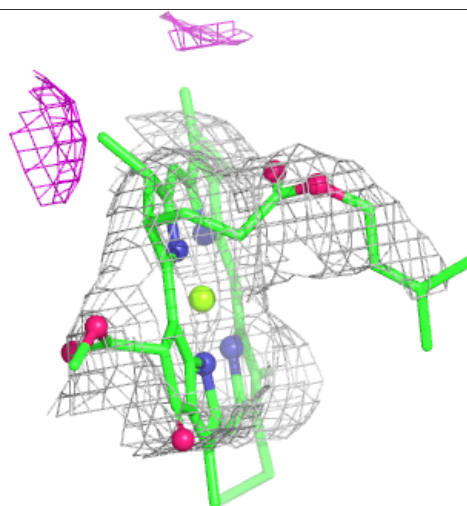
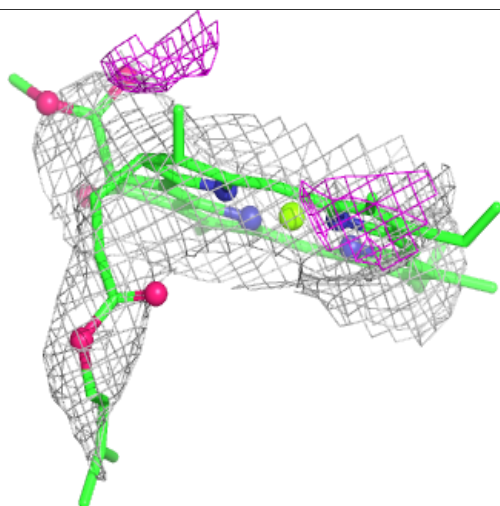
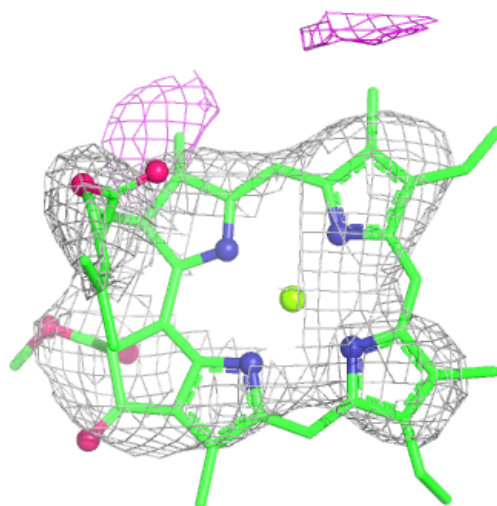
Electron density around CLA L 304:

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



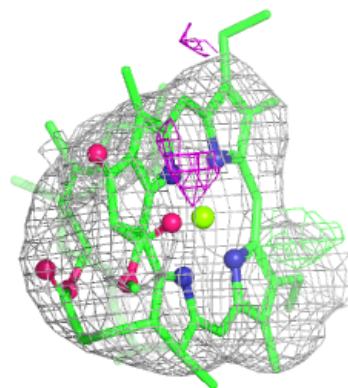
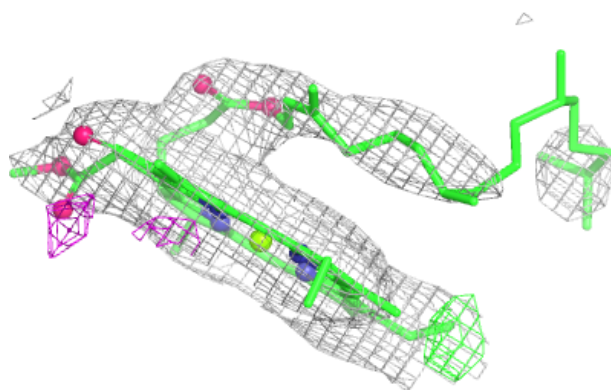
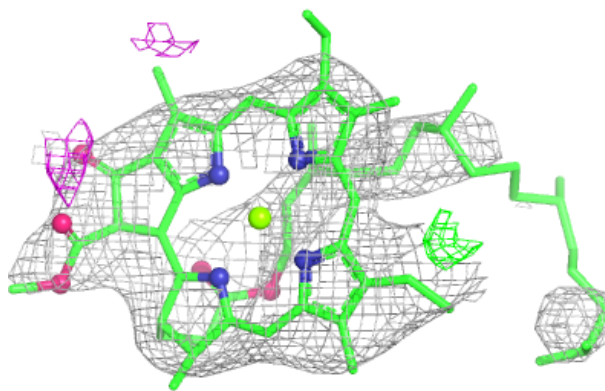
Electron density around CLA L 306:

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



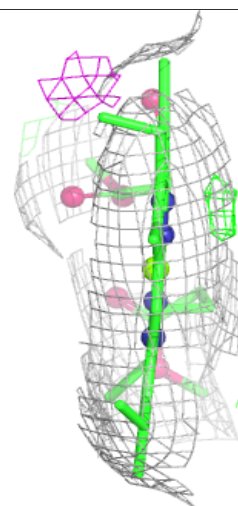
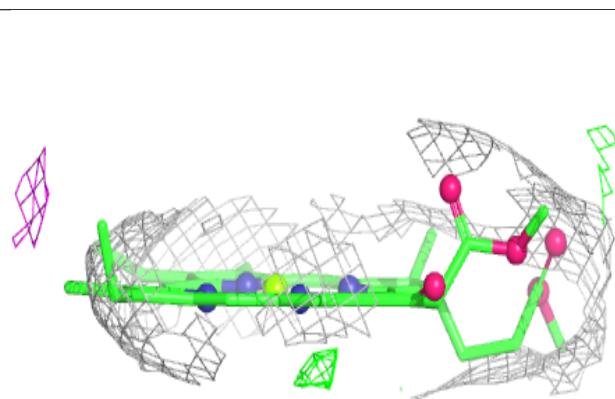
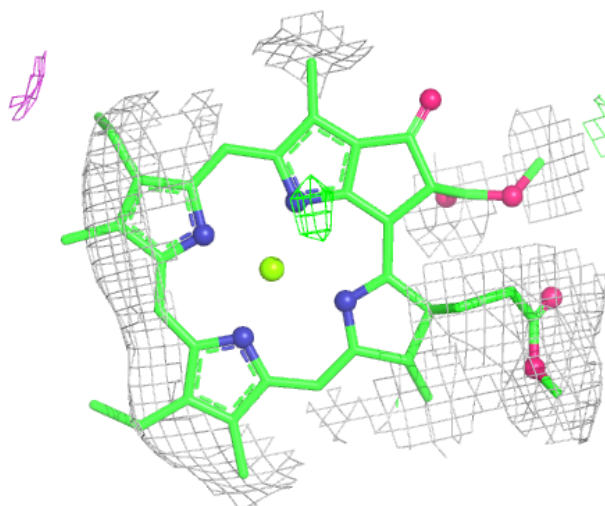
Electron density around CLA B 808:

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



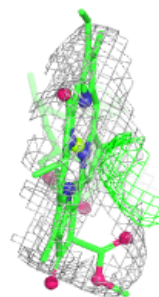
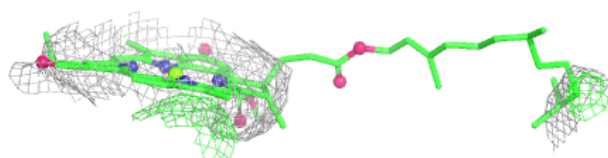
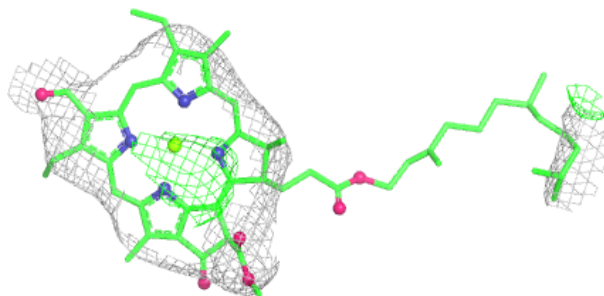
Electron density around CLA 1 5007:

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

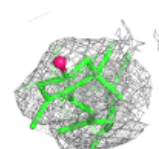
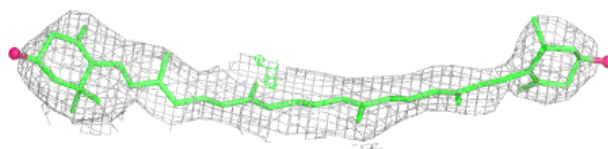


Electron density around CHL 4 316:

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

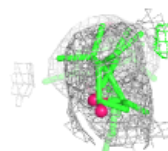
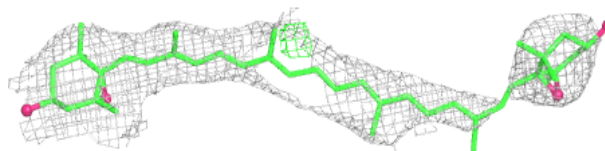
**Electron density around LUT J 1105:**

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



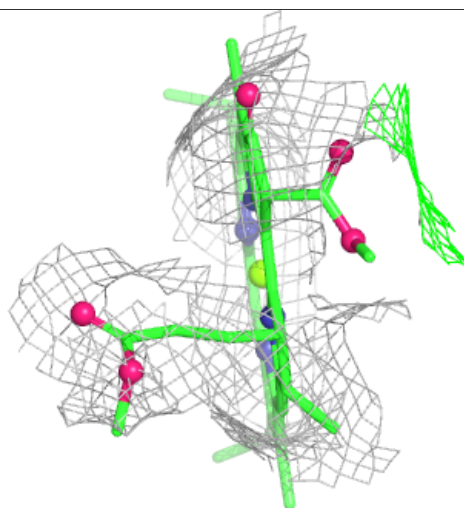
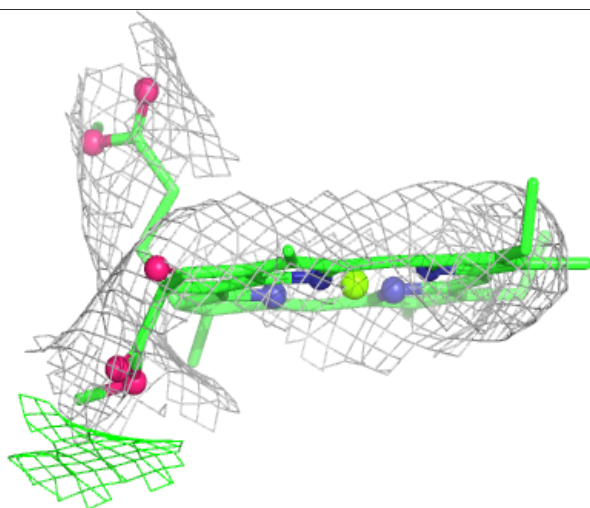
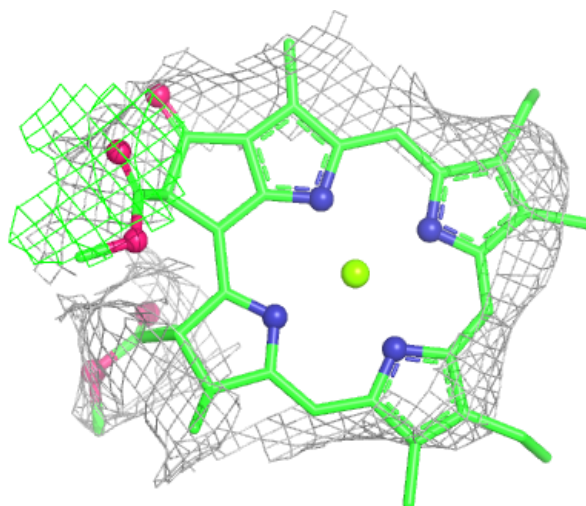
Electron density around XAT 2 304:

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



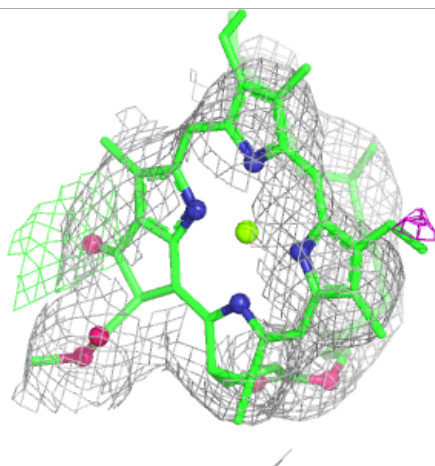
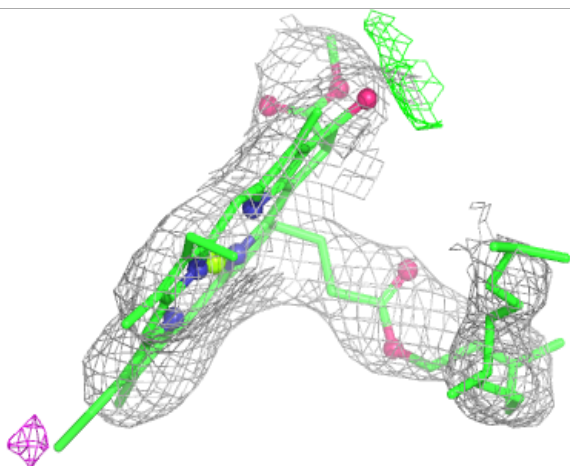
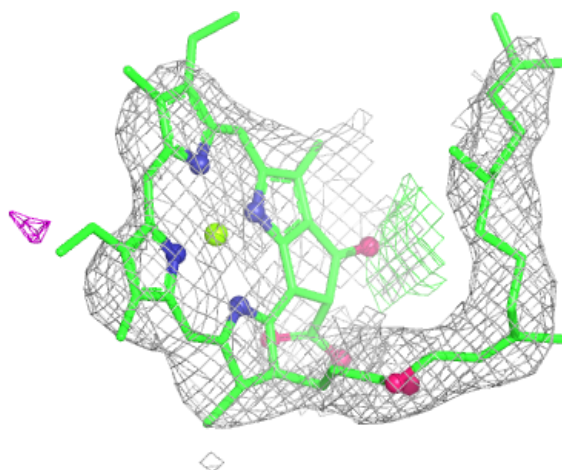
Electron density around CLA 1 5013:

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



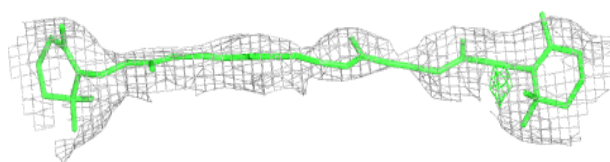
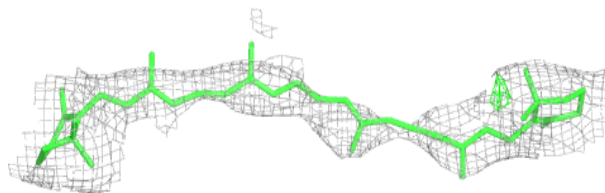
Electron density around CLA B 834:

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

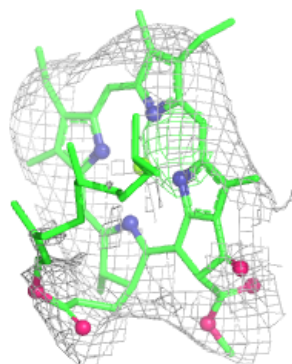
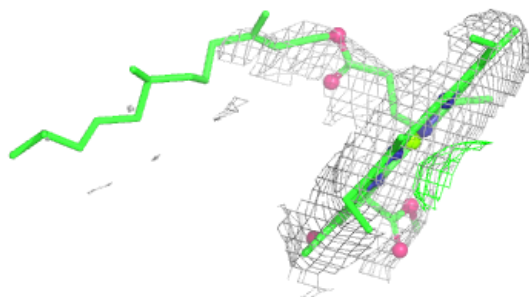
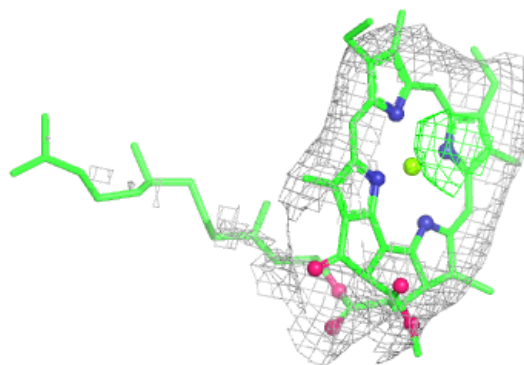


Electron density around BCR 3 305:

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

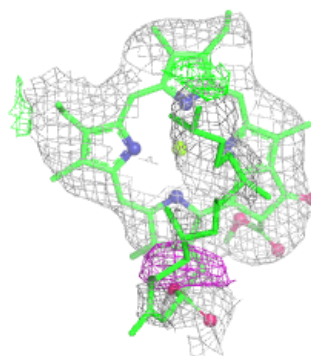
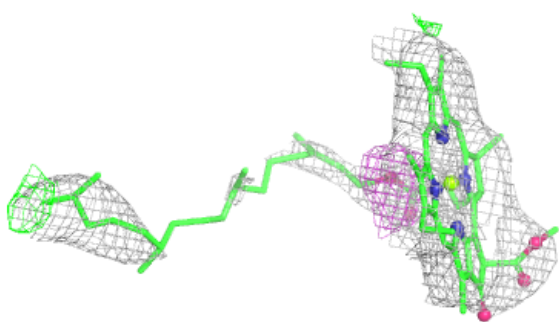
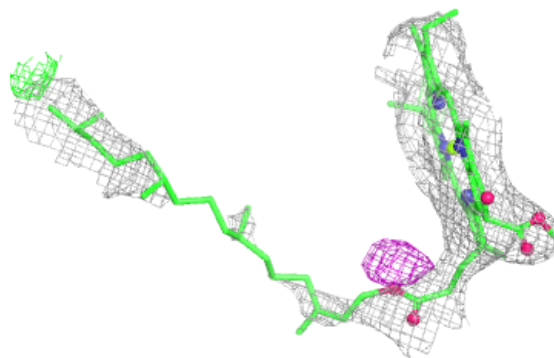
**Electron density around CLA 4 311:**

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

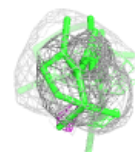
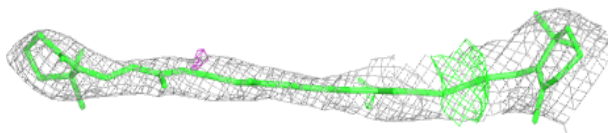
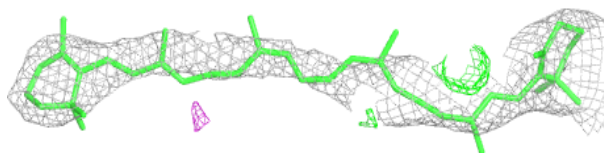


Electron density around CLA A 803:

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

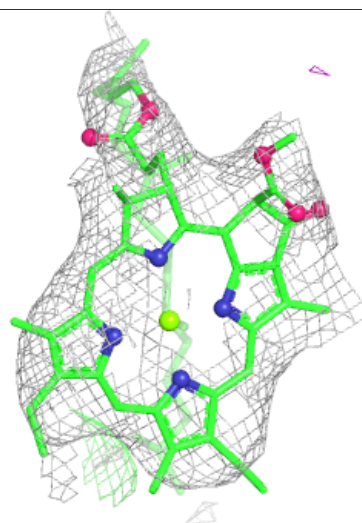
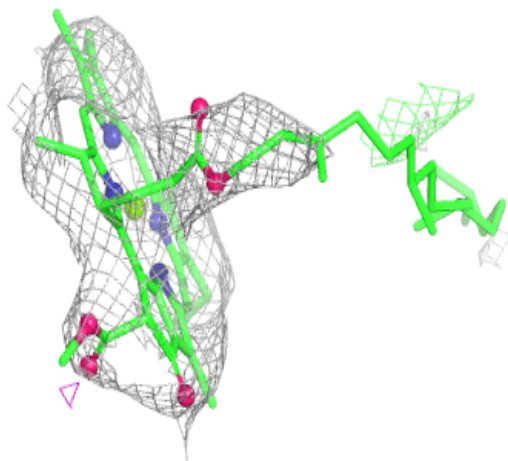
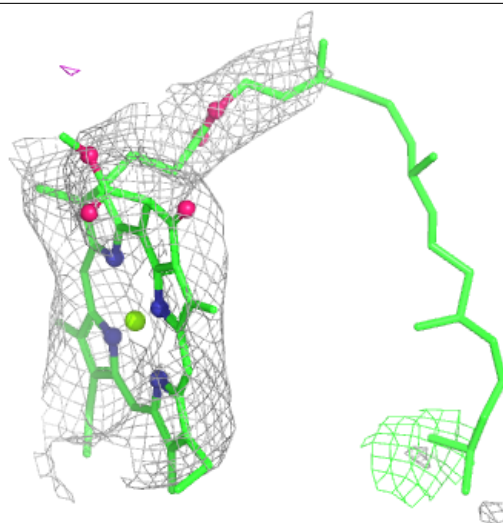
**Electron density around BCR B 843:**

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



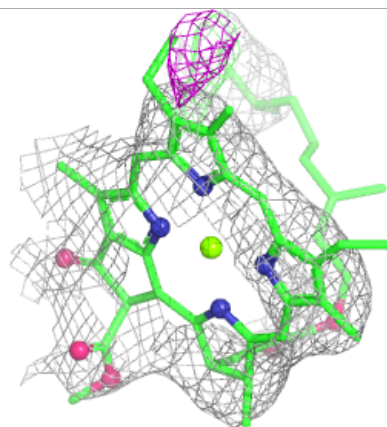
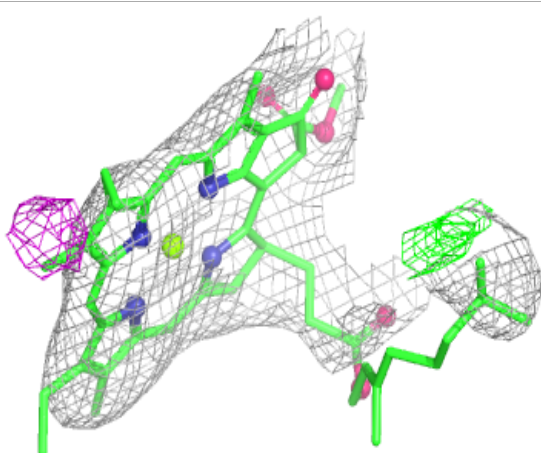
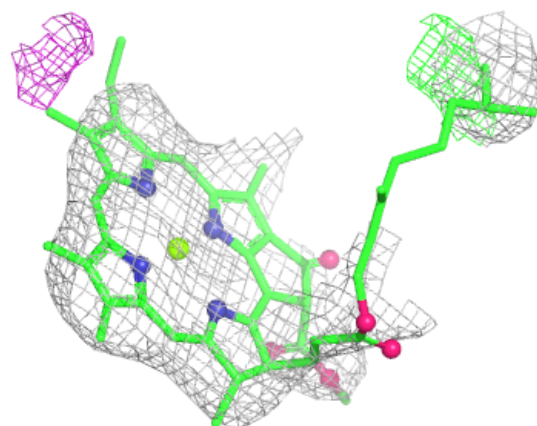
Electron density around CLA A 836:

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



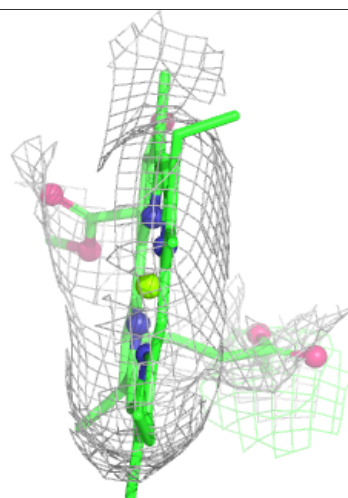
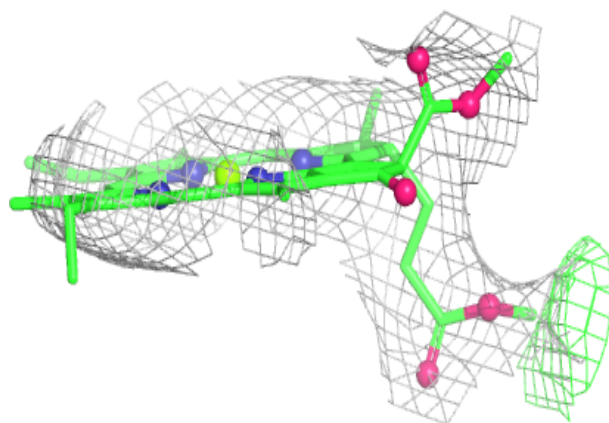
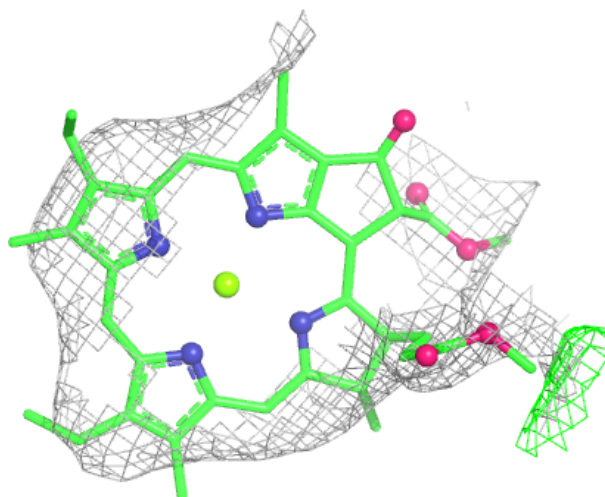
Electron density around CLA 2 317:

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



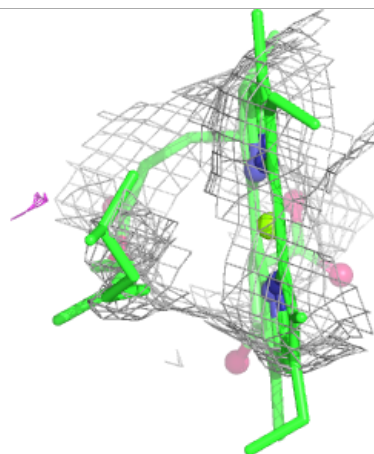
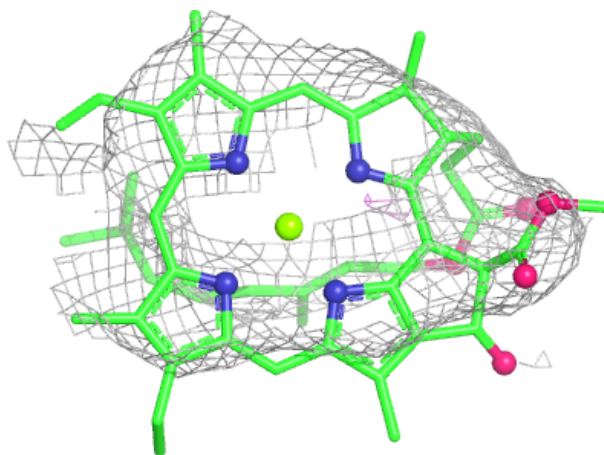
Electron density around CLA 1 5012:

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



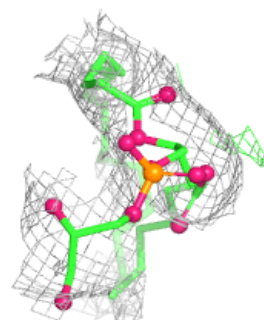
Electron density around CLA 3 309:

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

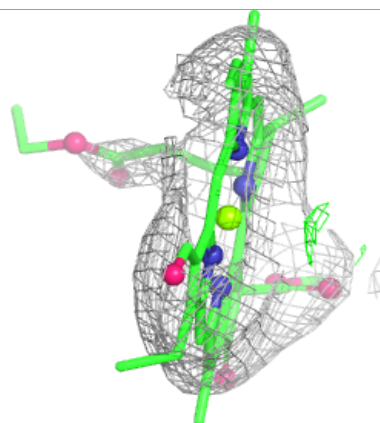
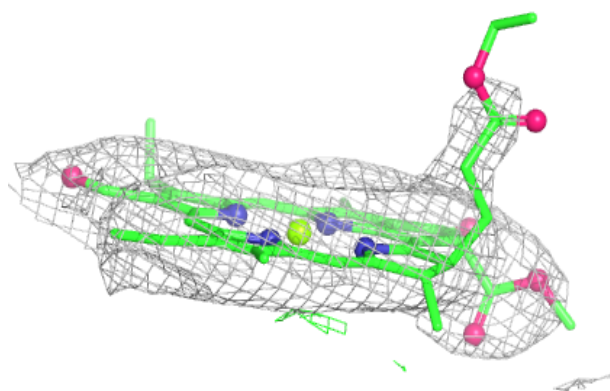
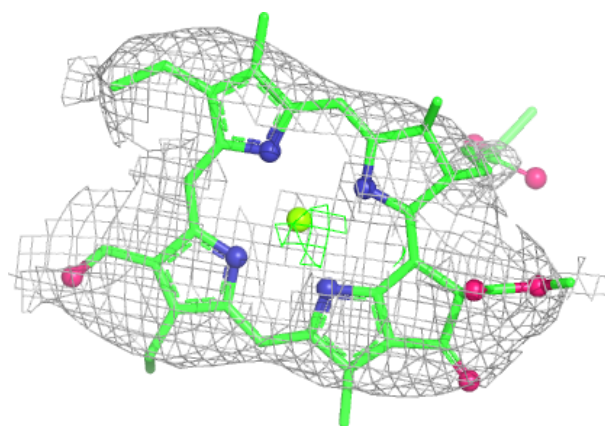


Electron density around LHG A 849:

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

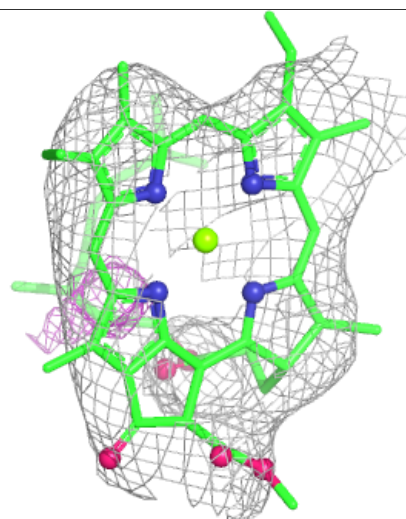
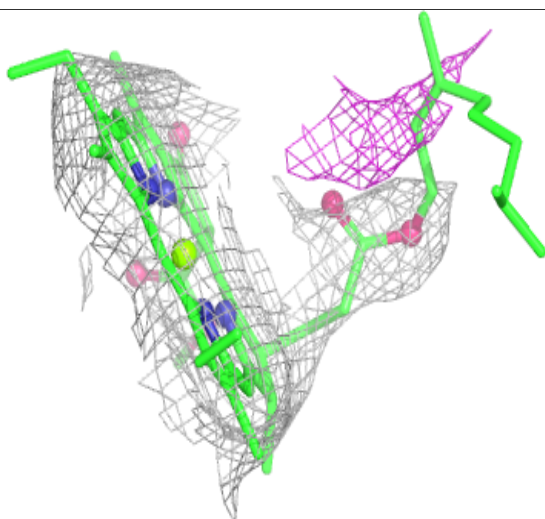
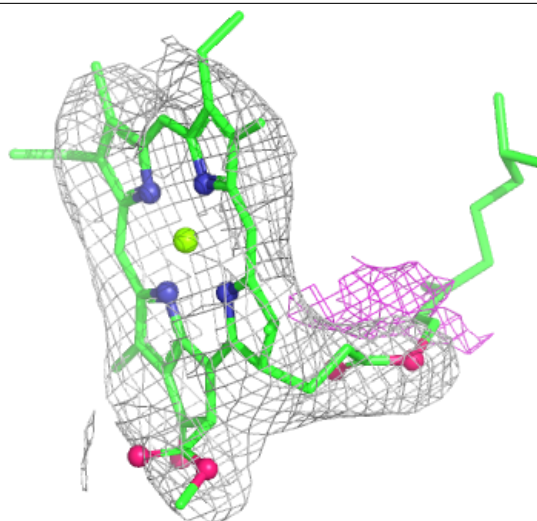
**Electron density around CHL 2 316:**

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



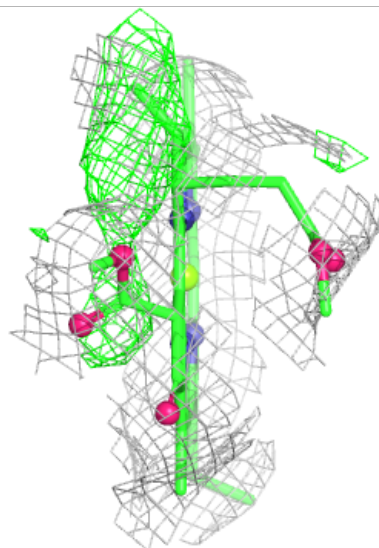
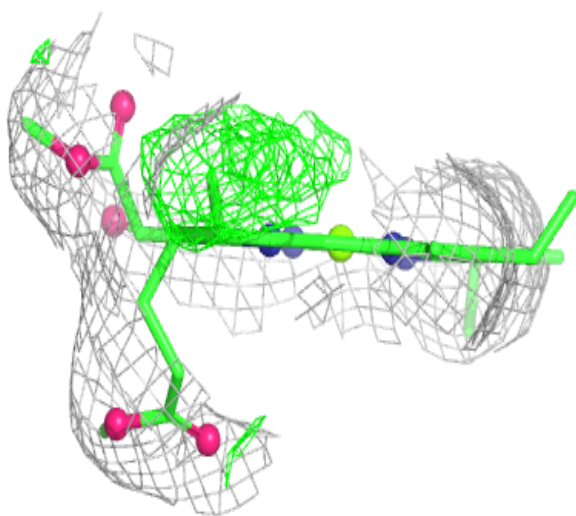
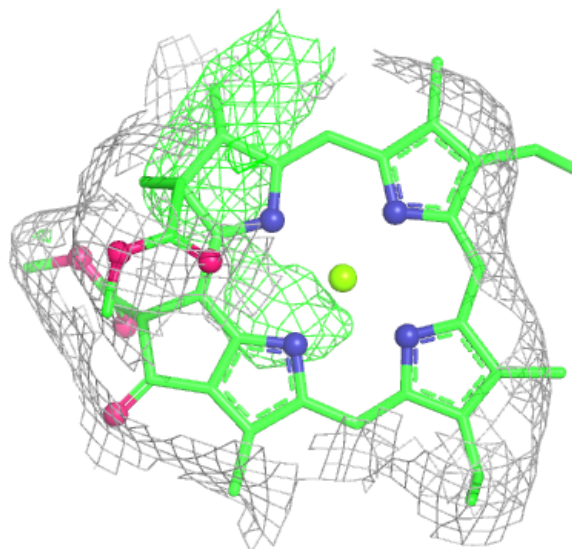
Electron density around CLA A 833:

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



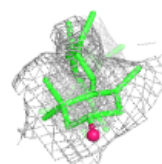
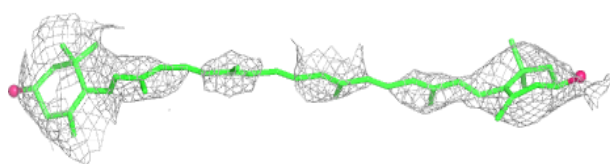
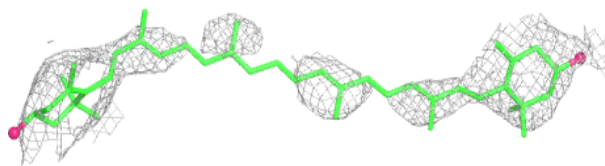
Electron density around CLA 4 312:

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

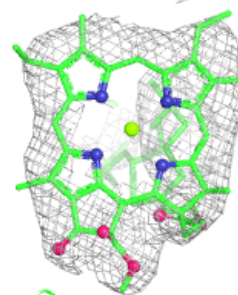
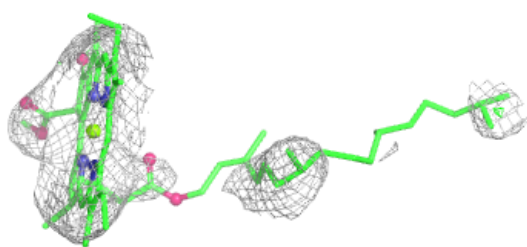
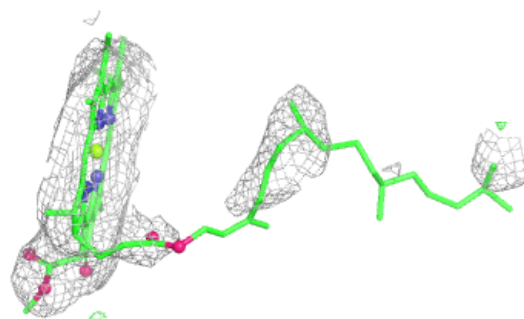


Electron density around LUT 1 5004:

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

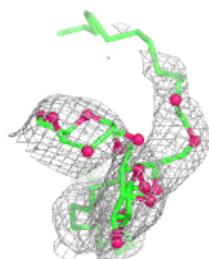
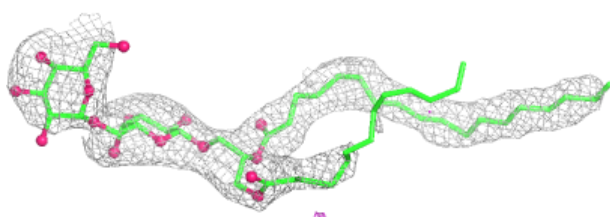
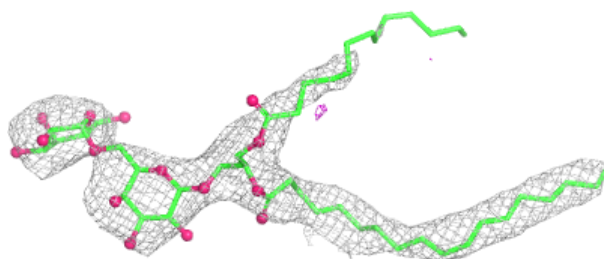
**Electron density around CLA B 805:**

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

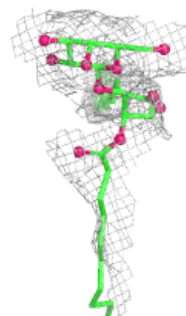
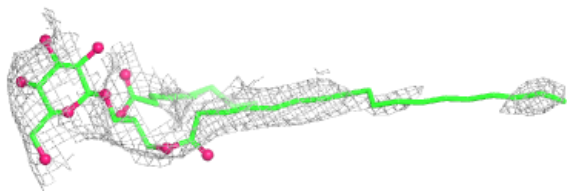


Electron density around DGD B 855:

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

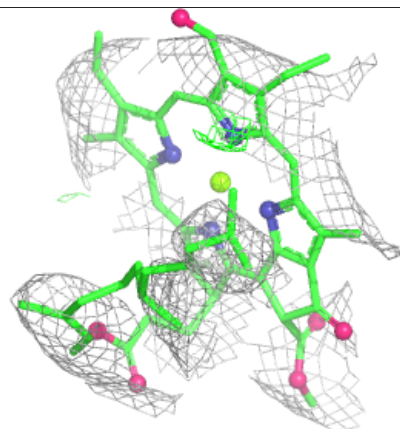
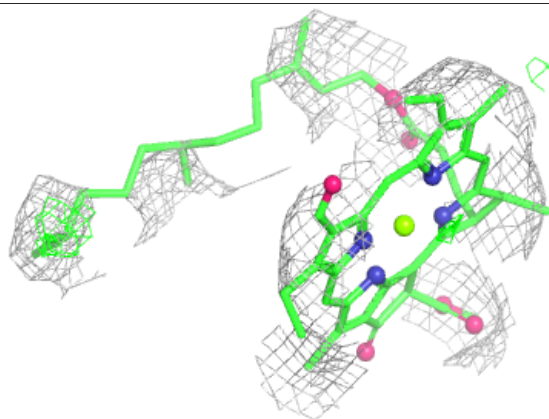
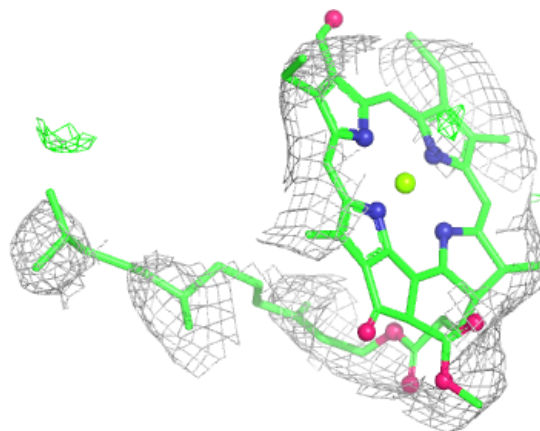
**Electron density around LMG F 306:**

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



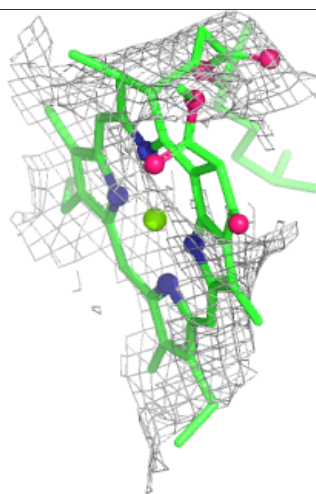
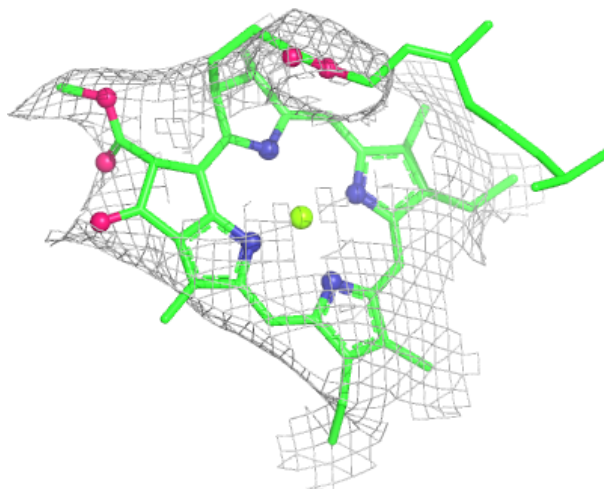
Electron density around CHL 1 5016:

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



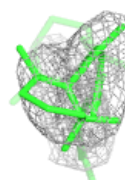
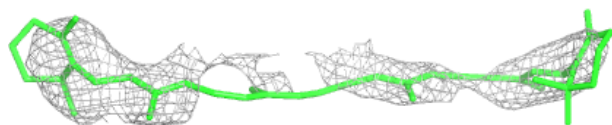
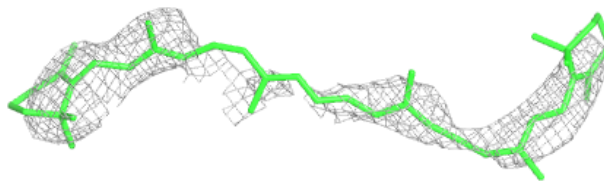
Electron density around CLA 3 307:

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

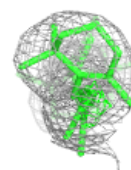
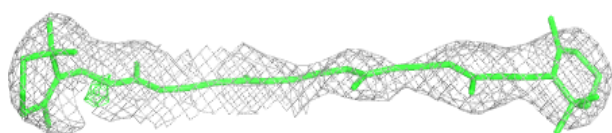
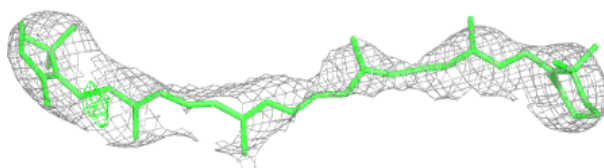


Electron density around BCR B 845:

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

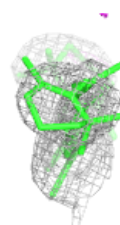
**Electron density around BCR B 846:**

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

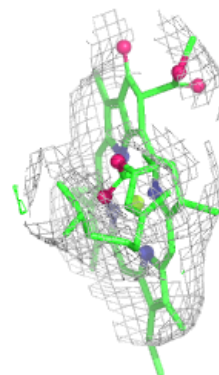
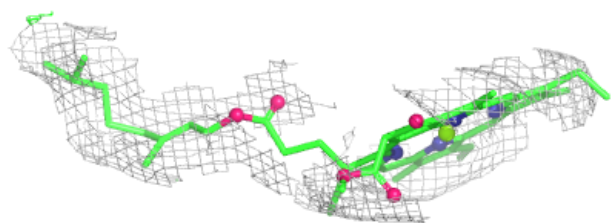
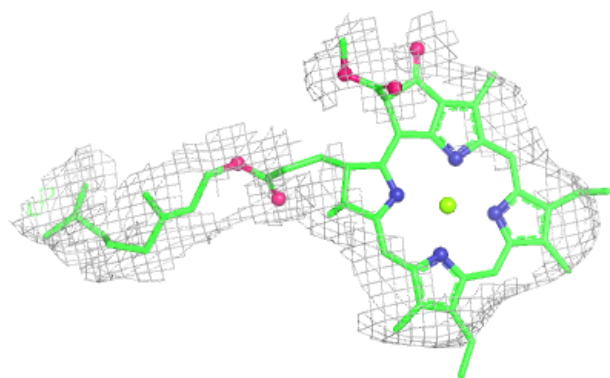


Electron density around BCR B 847:

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

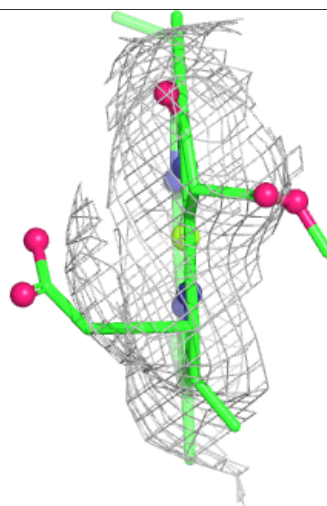
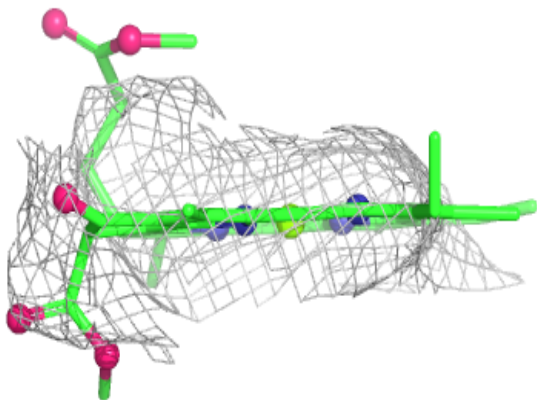
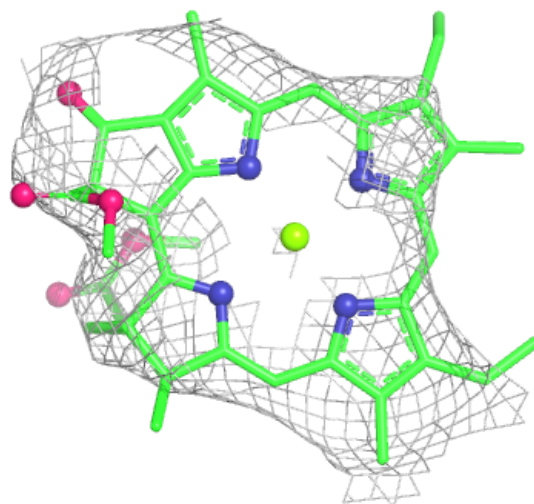
**Electron density around CLA G 1601:**

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



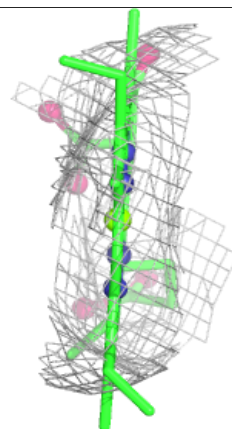
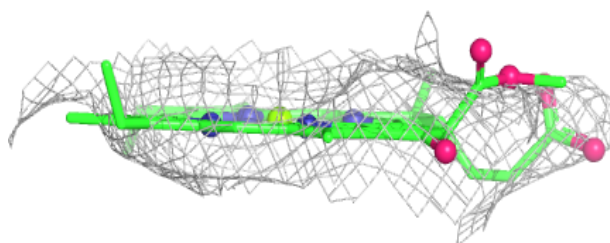
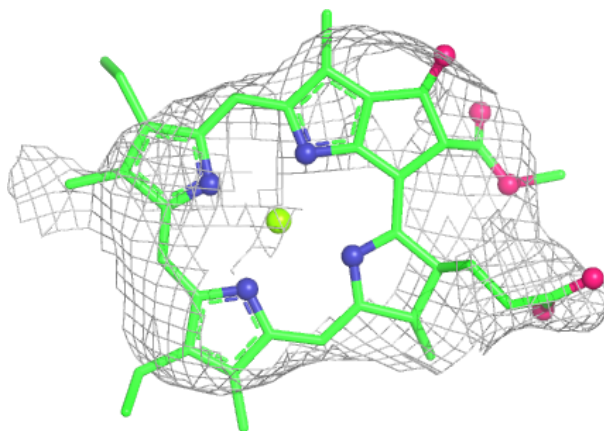
Electron density around CLA A 814:

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

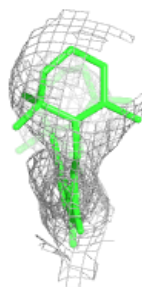
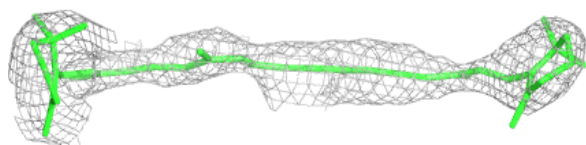
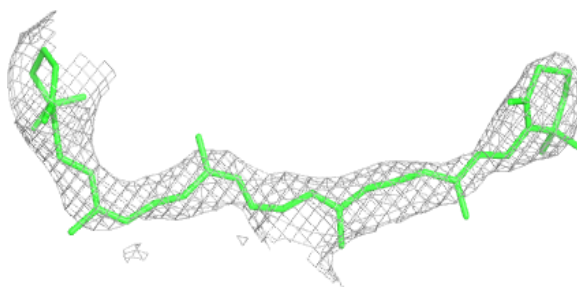


Electron density around CLA 1 5017:

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

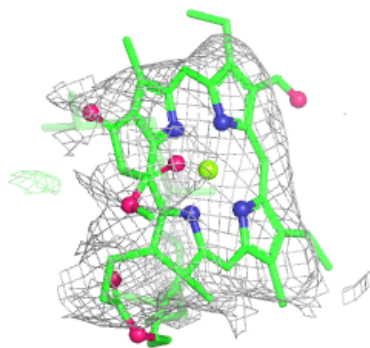
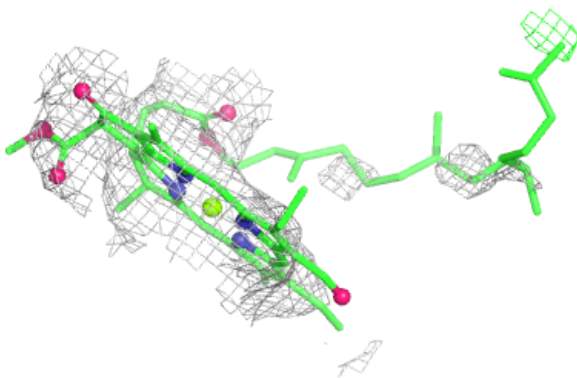
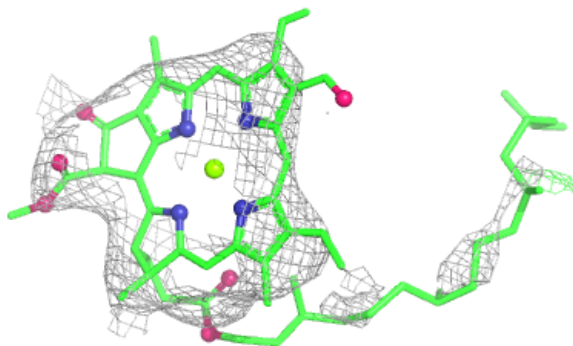
**Electron density around BCR L 303:**

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



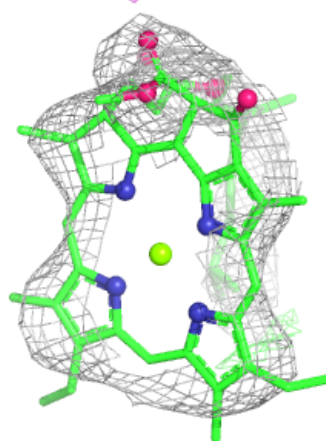
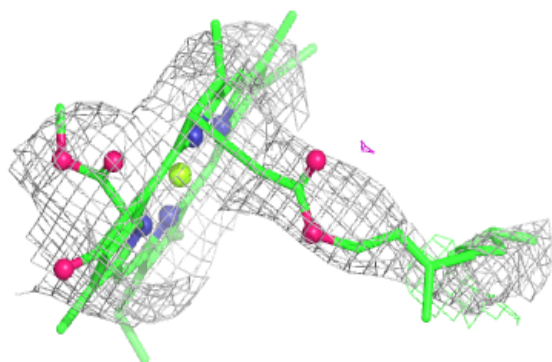
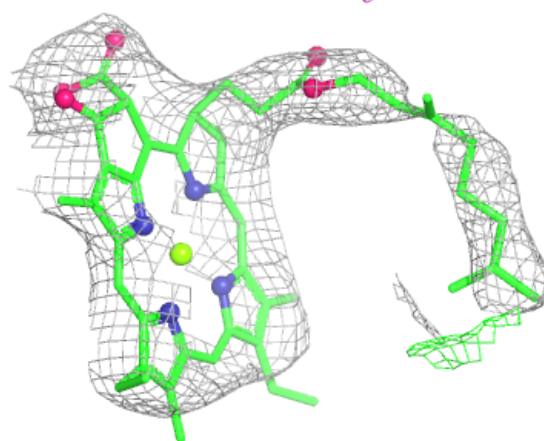
Electron density around CHL 3 310:

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



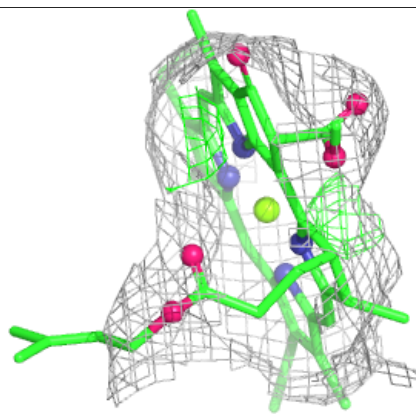
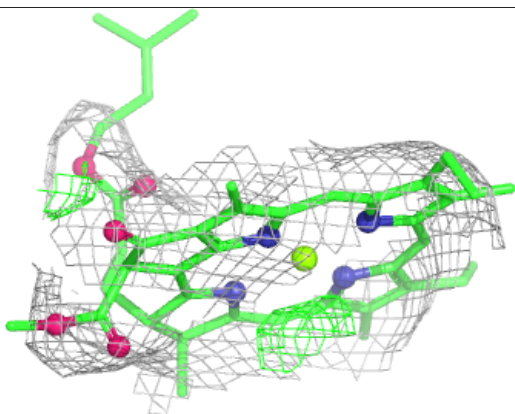
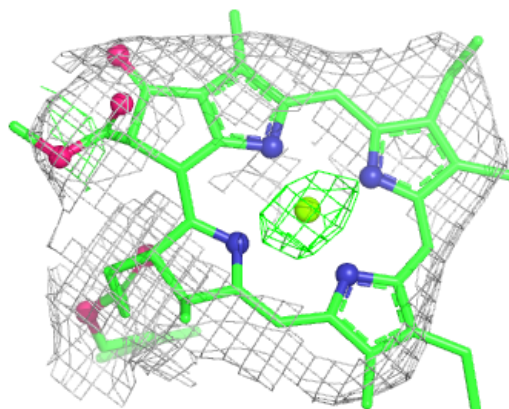
Electron density around CLA B 816:

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

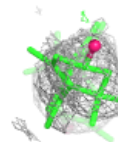
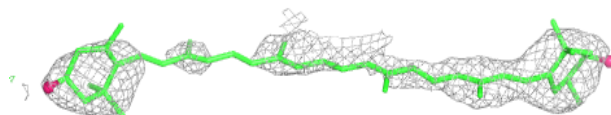
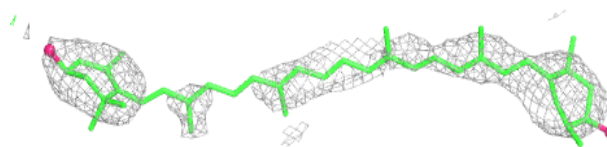


Electron density around CLA 4 310:

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

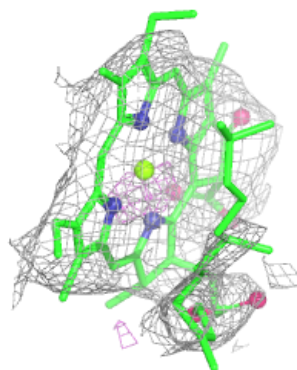
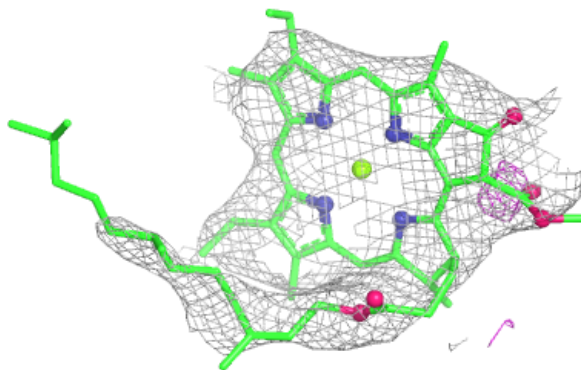
**Electron density around ZEX F 310:**

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

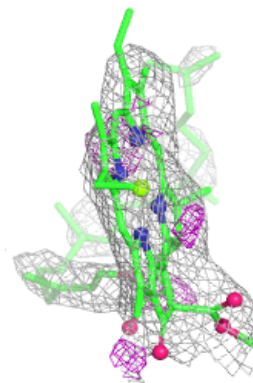
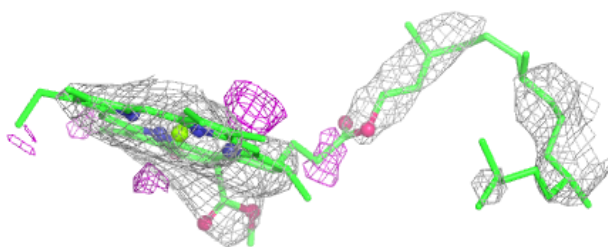
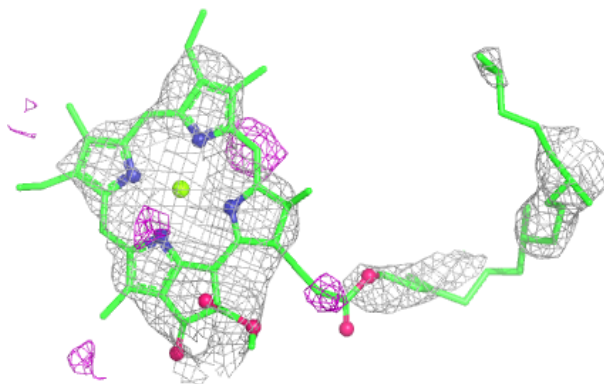


Electron density around CLA 2 306:

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

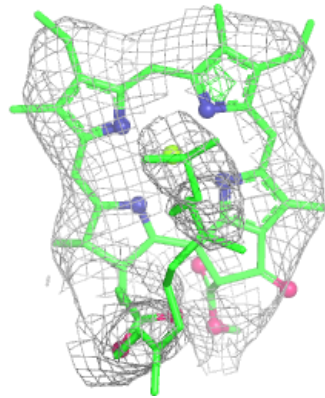
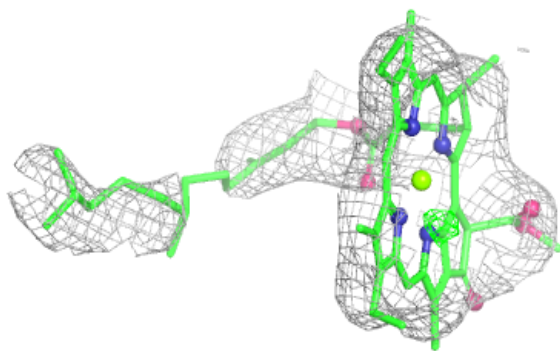
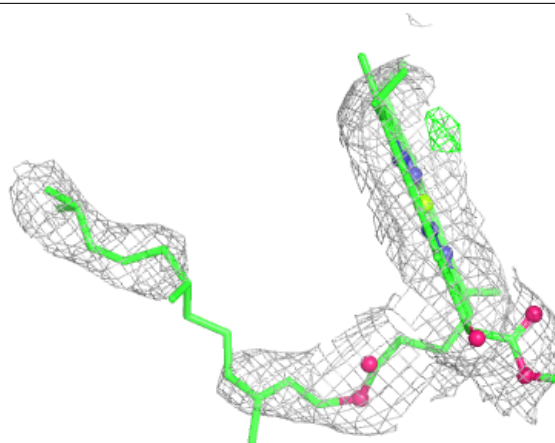
**Electron density around CLA A 825:**

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



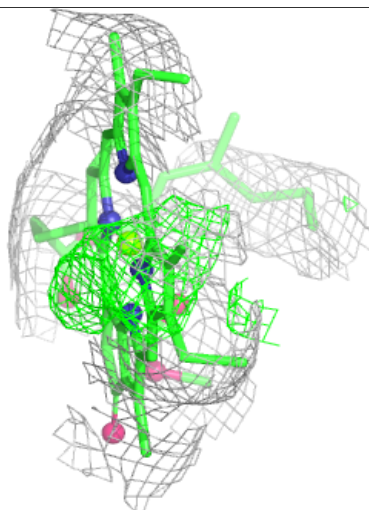
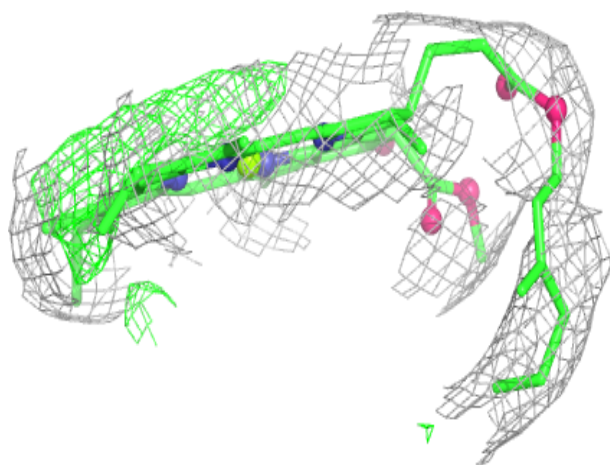
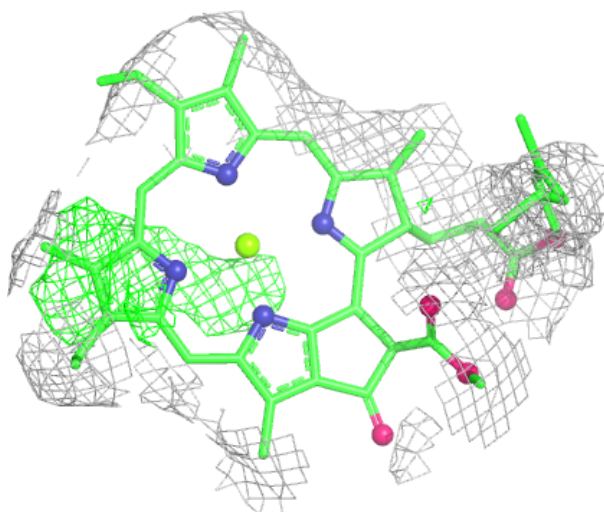
Electron density around CLA A 806:

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



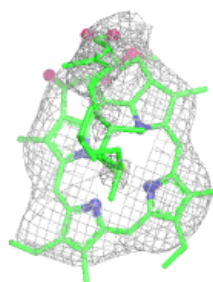
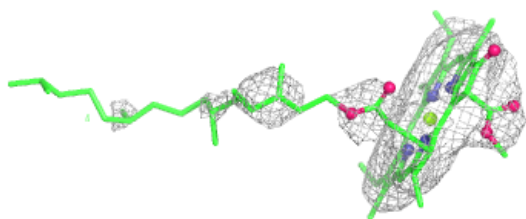
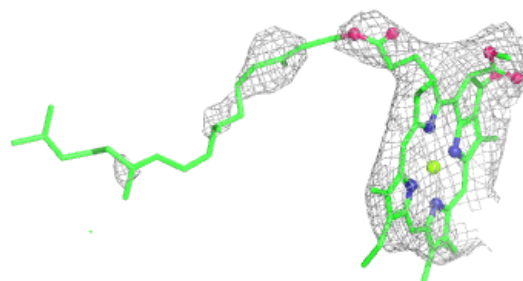
Electron density around CLA 2 307:

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

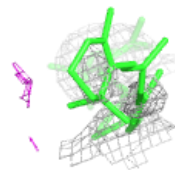
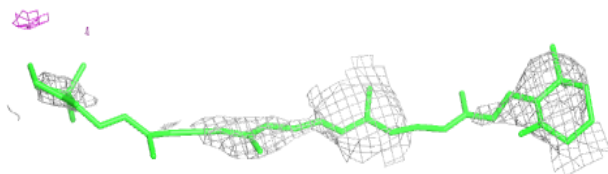
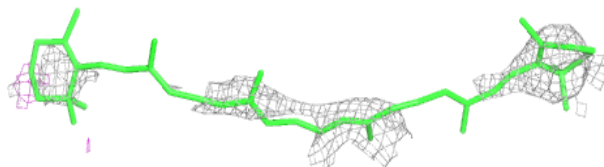


Electron density around CLA B 822:

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

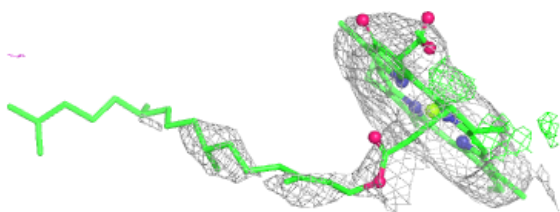
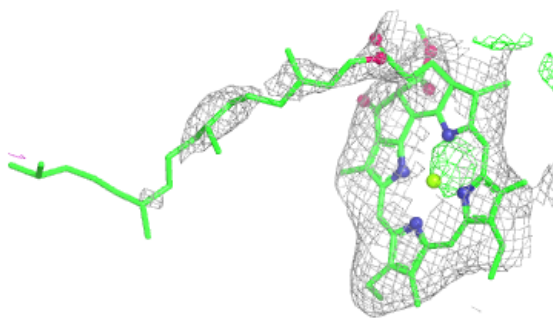
**Electron density around BCR A 855:**

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

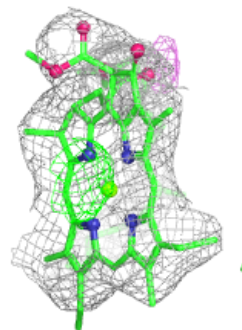
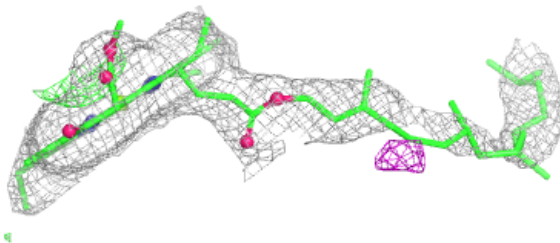
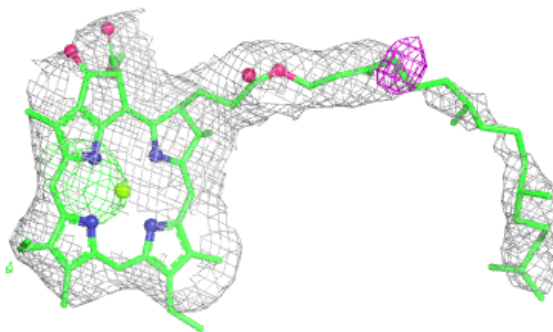


Electron density around CLA B 823:

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

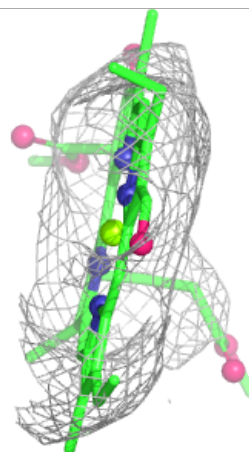
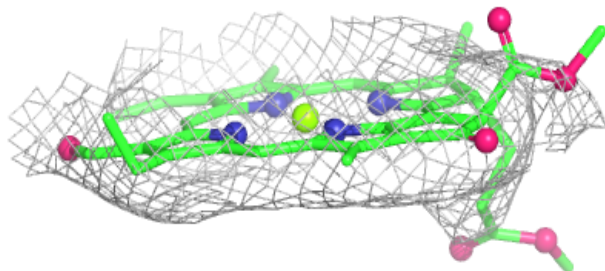
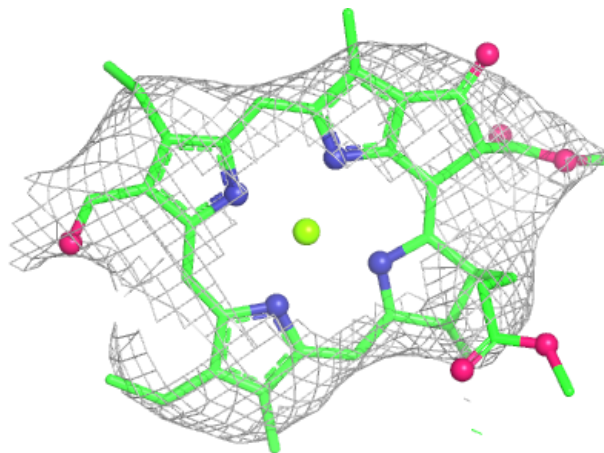
**Electron density around CLA B 826:**

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



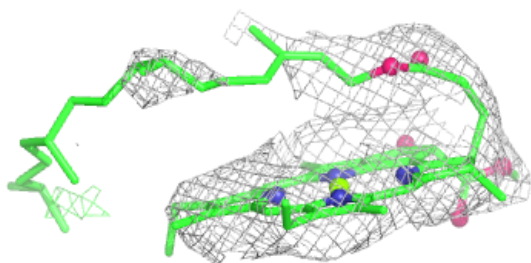
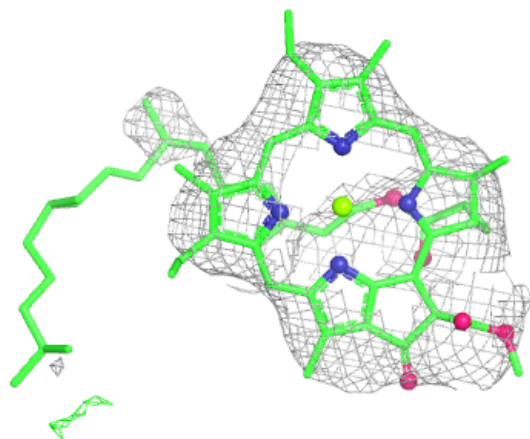
Electron density around CHL 1 5014:

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



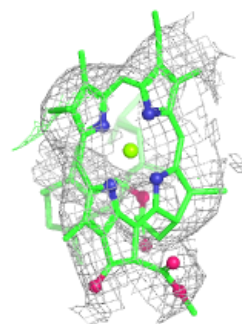
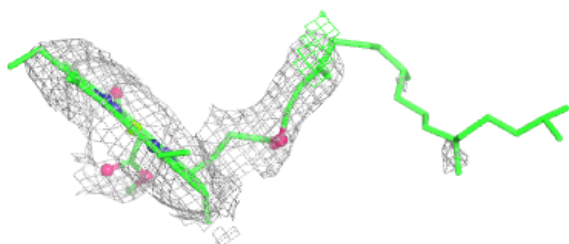
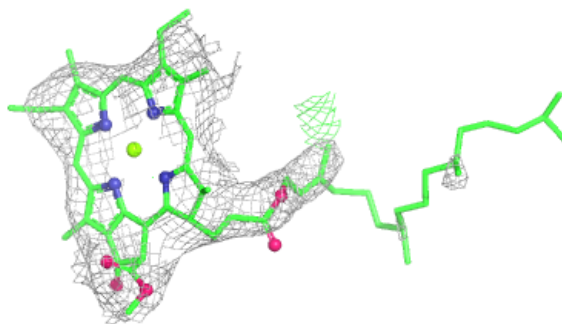
Electron density around CLA A 815:

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

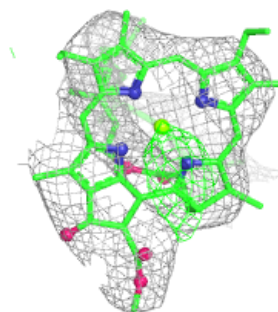
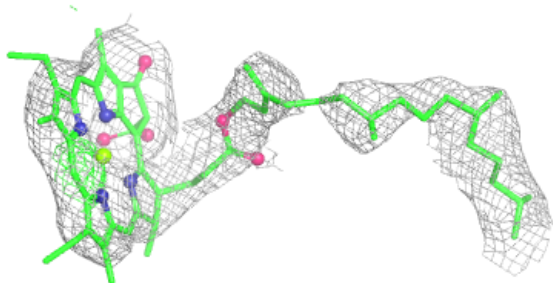
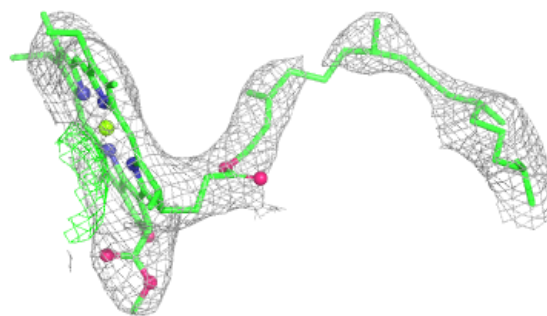


Electron density around CLA A 829:

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

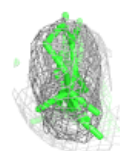
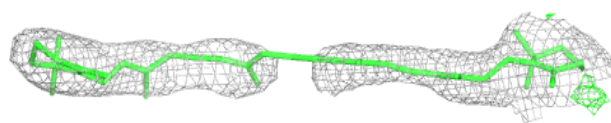
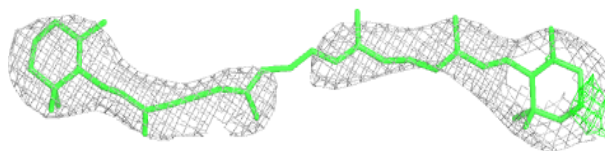
**Electron density around CLA B 839:**

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

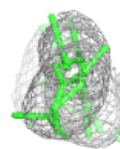
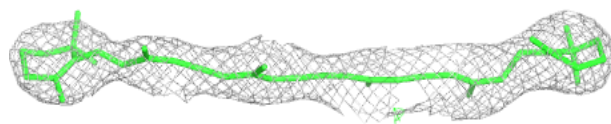
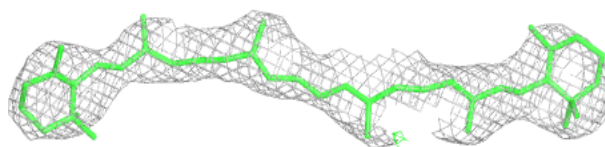


Electron density around BCR I 102:

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

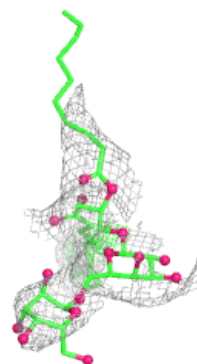
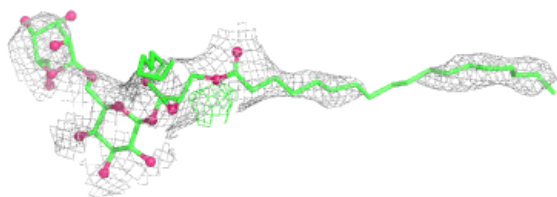
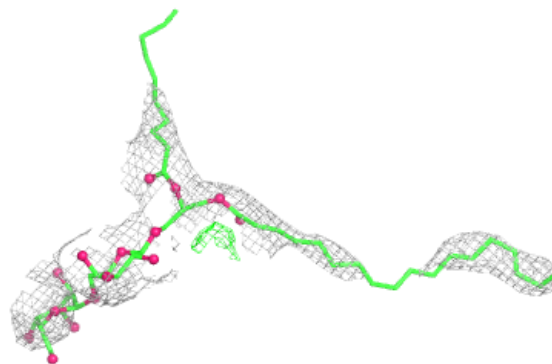
**Electron density around BCR J 1104:**

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

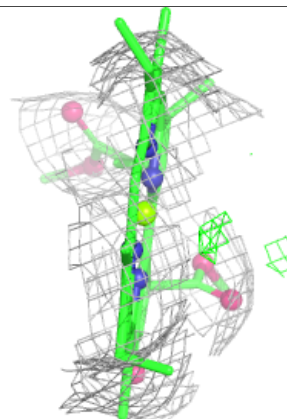
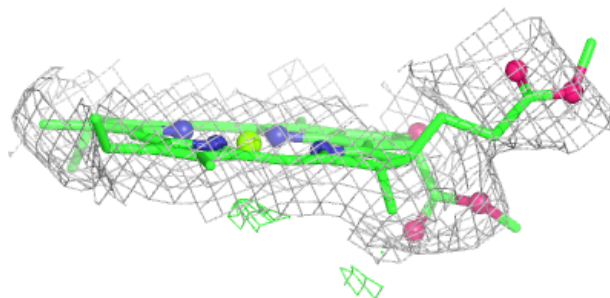
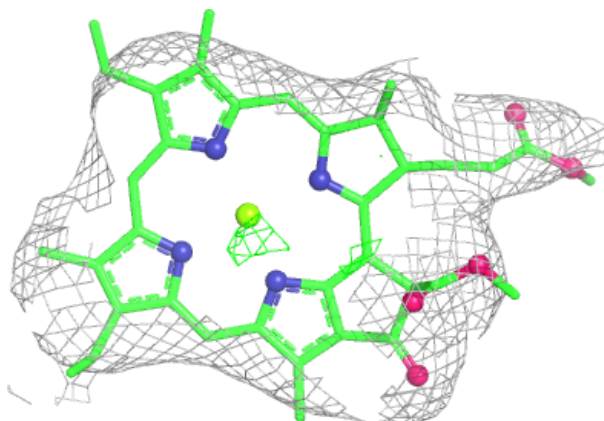


Electron density around DGD J 1106:

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

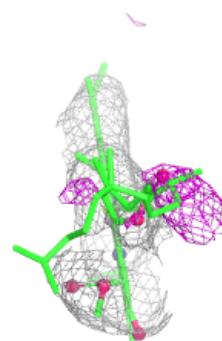
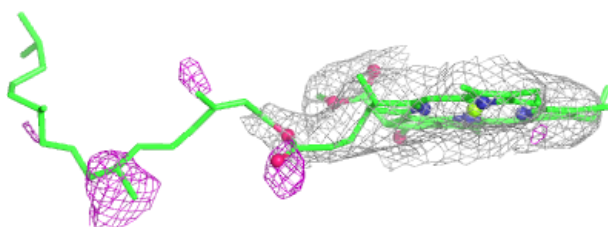
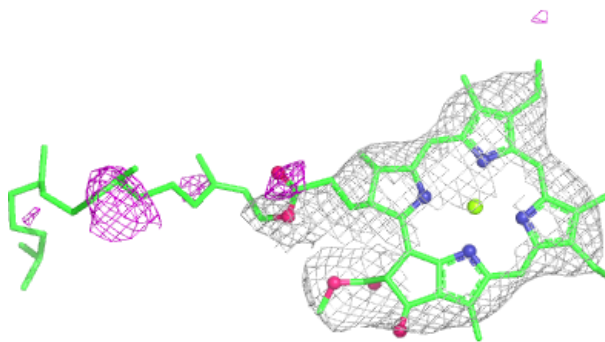
**Electron density around CLA 3 318:**

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

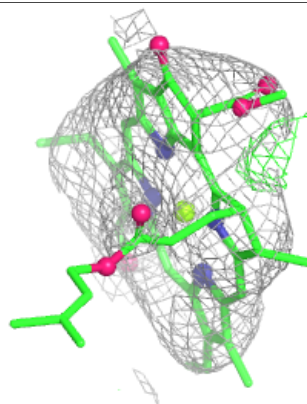
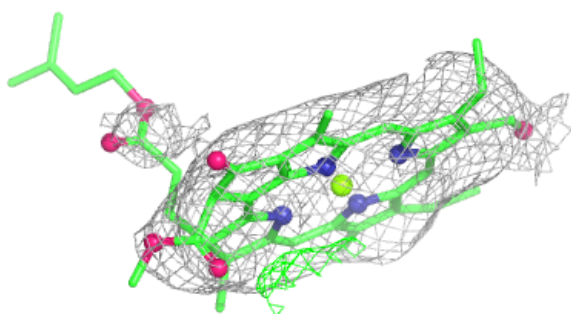
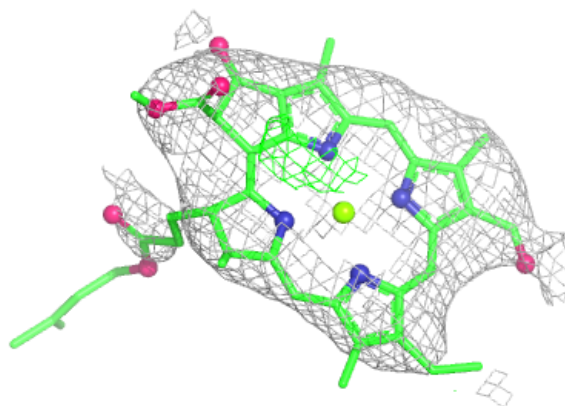


Electron density around CLA F 302:

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

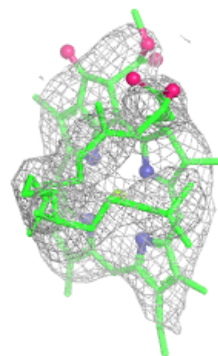
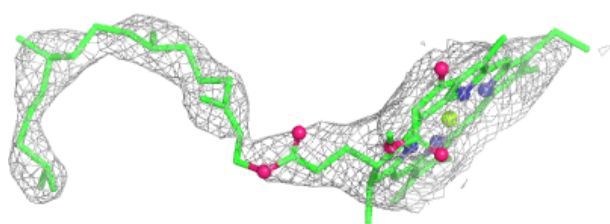
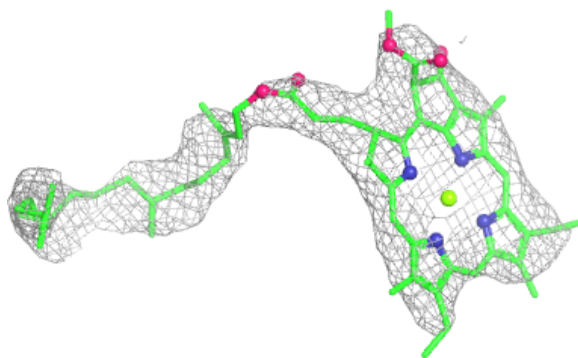
**Electron density around CHL 4 314:**

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

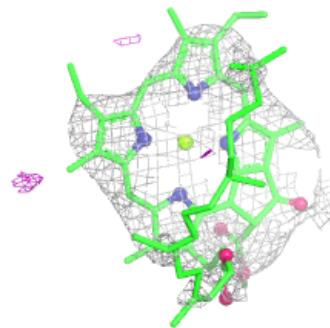
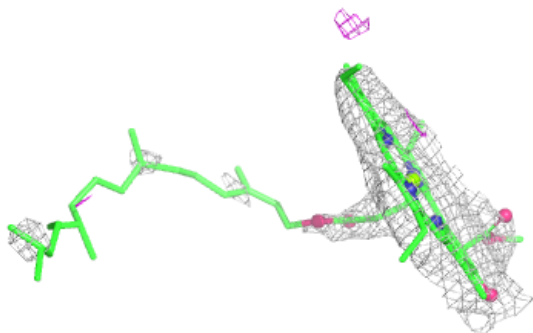
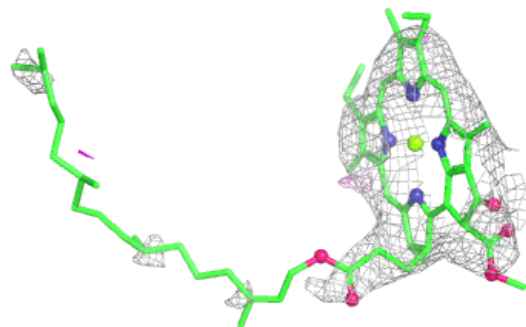


Electron density around CLA B 810:

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

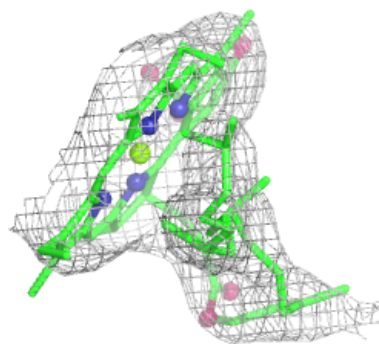
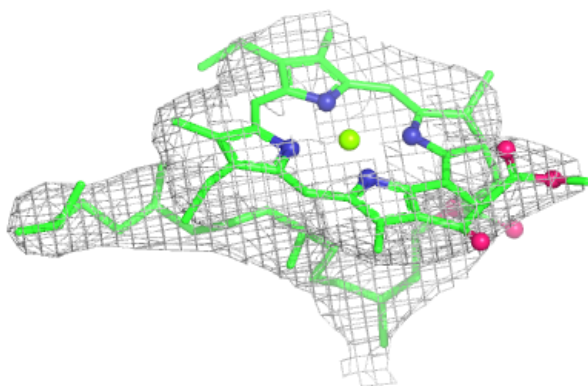
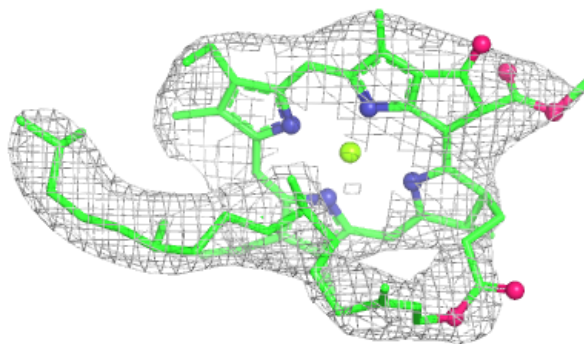
**Electron density around CLA A 832:**

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

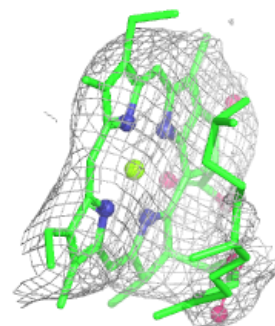
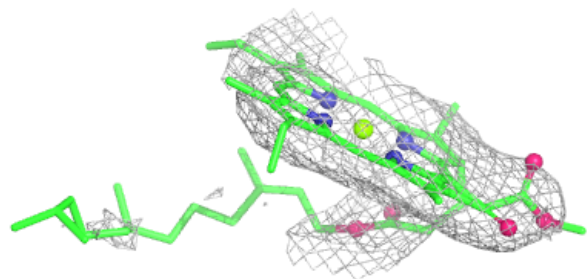
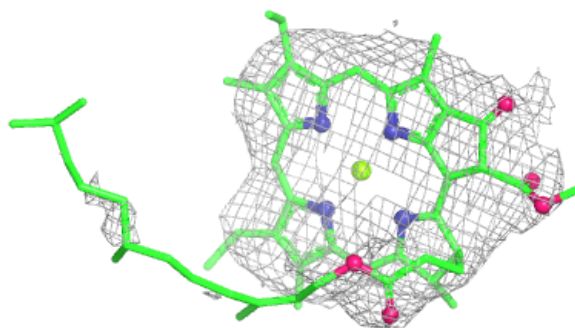


Electron density around CLA B 818:

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

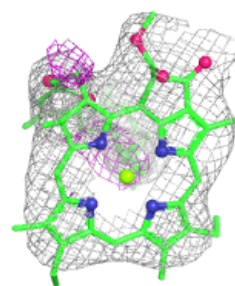
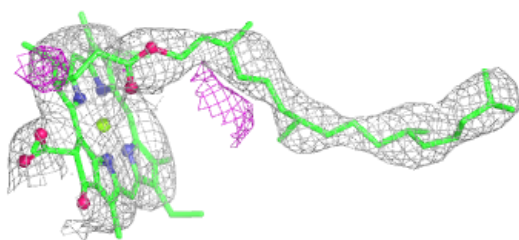
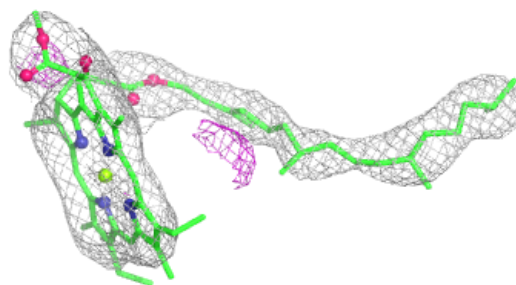
**Electron density around CLA 4 305:**

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



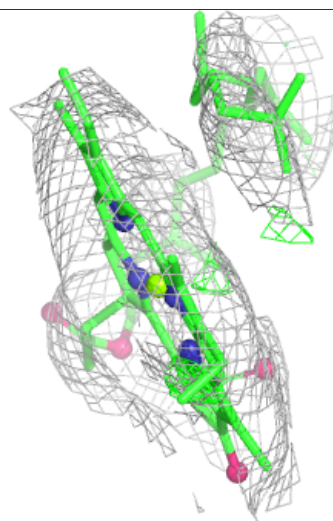
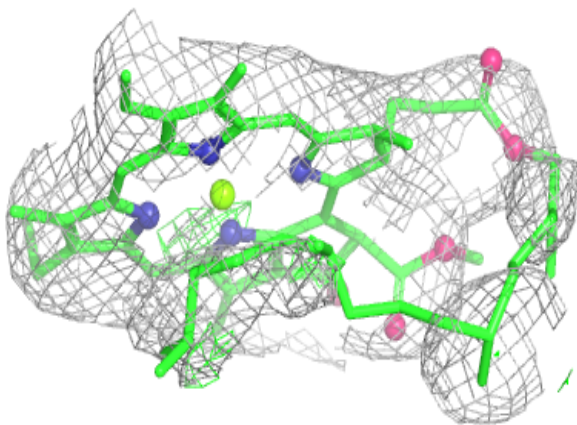
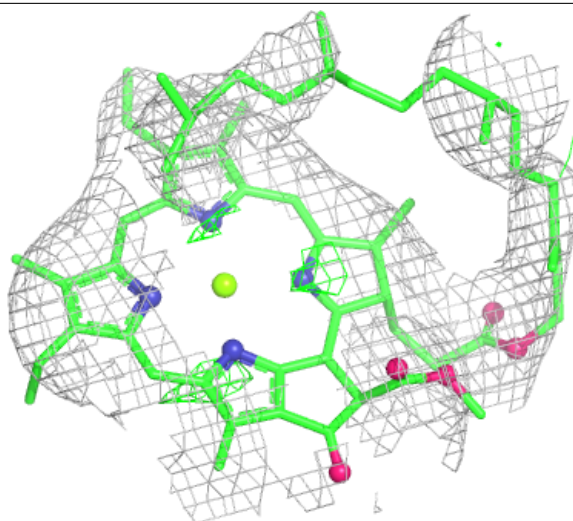
Electron density around CLA A 810:

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



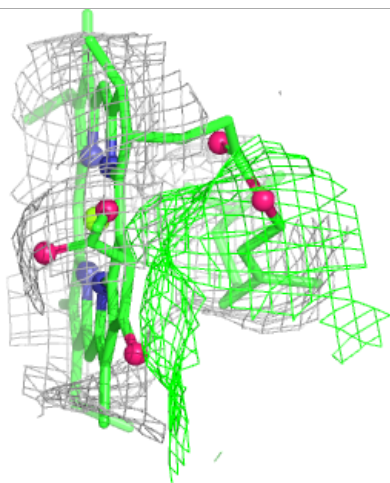
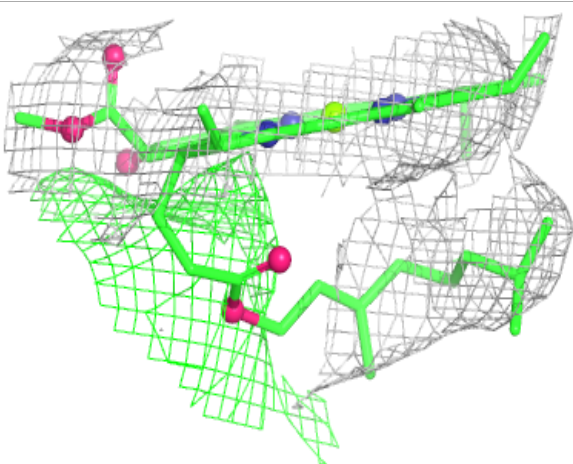
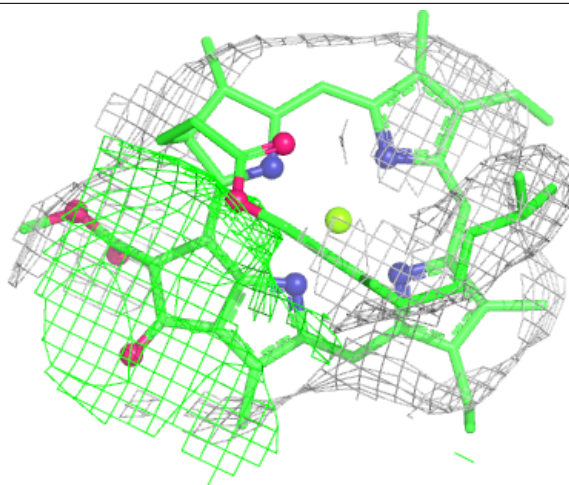
Electron density around CLA 2 310:

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



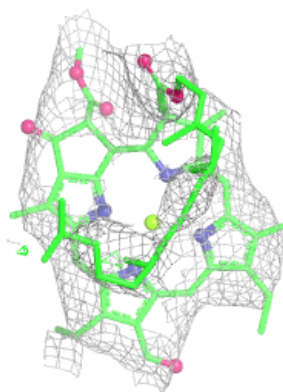
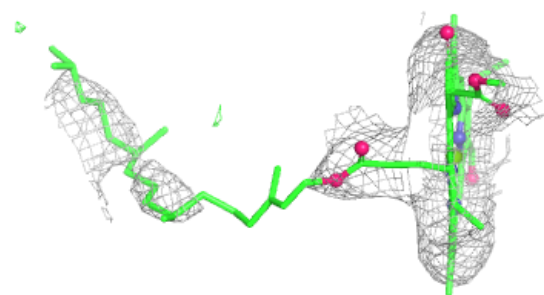
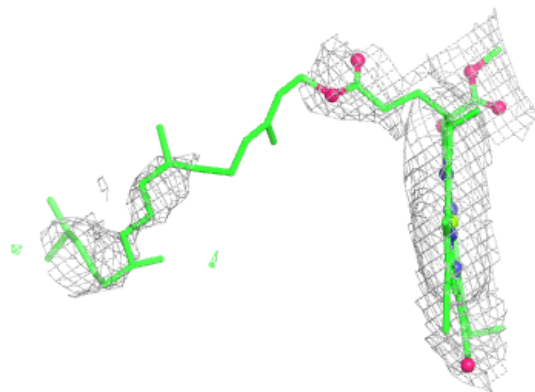
Electron density around CLA 1 5008:

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

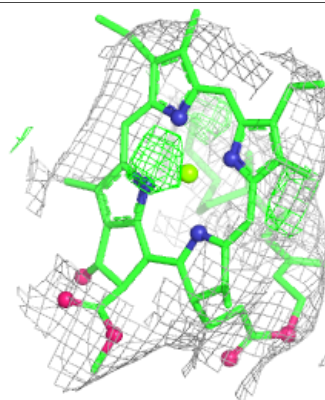
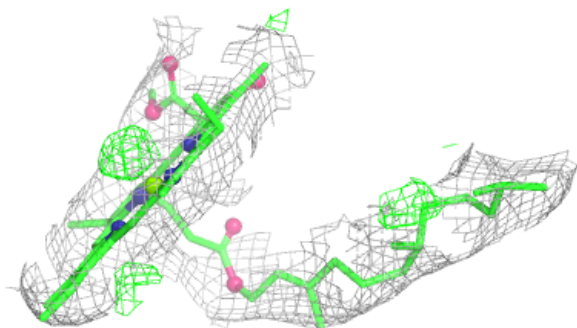
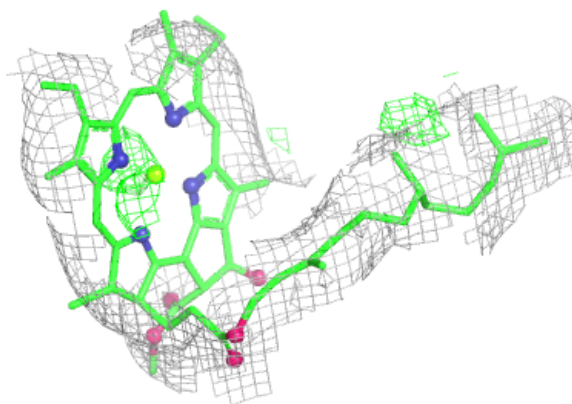


Electron density around CHL 2 314:

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

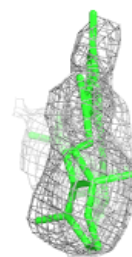
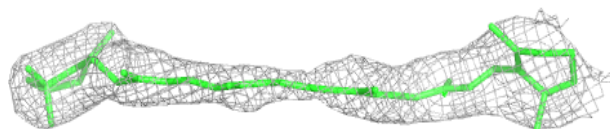
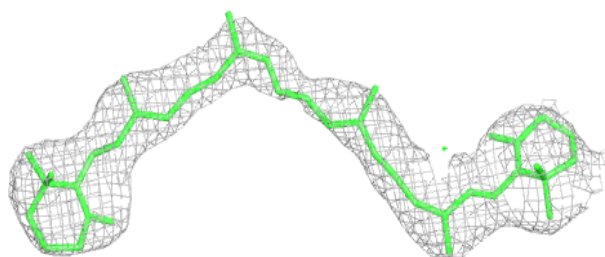
**Electron density around CLA 2 312:**

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

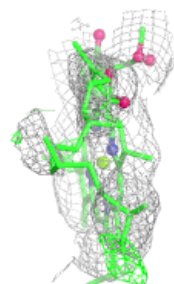
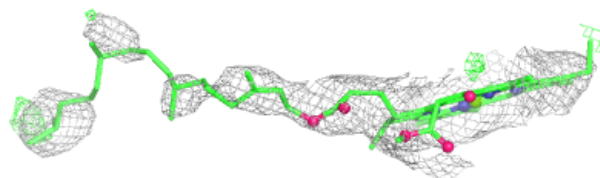
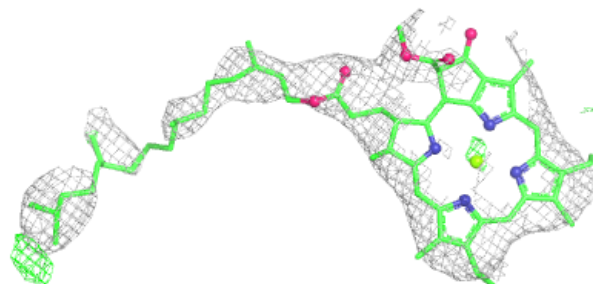


Electron density around BCR A 847:

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

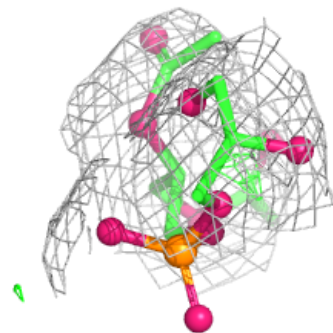
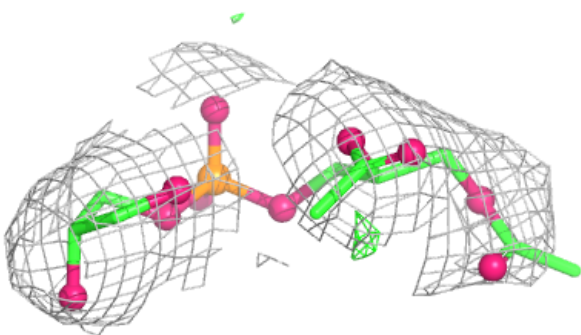
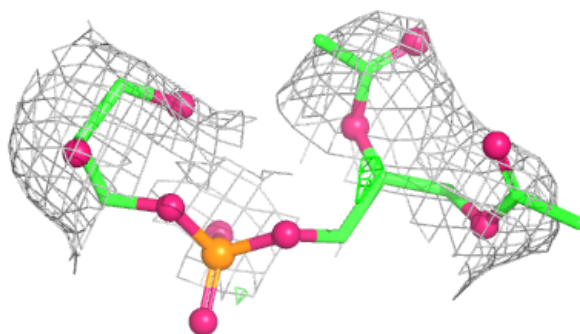
**Electron density around CLA F 303:**

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



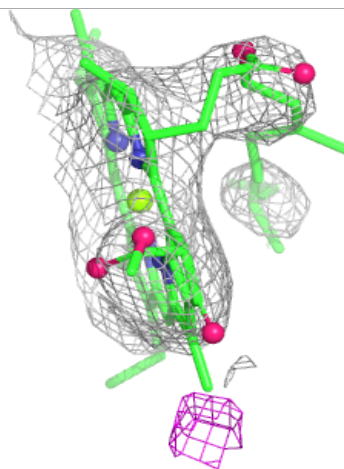
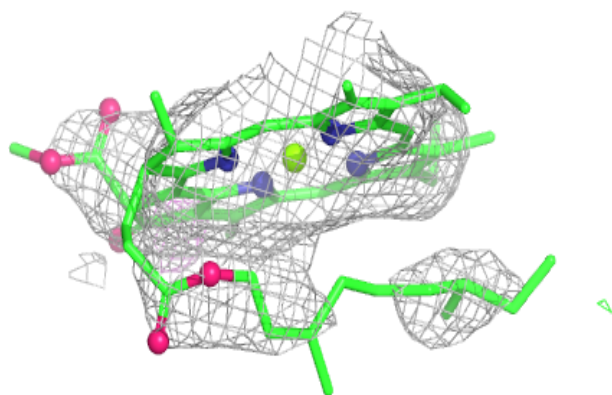
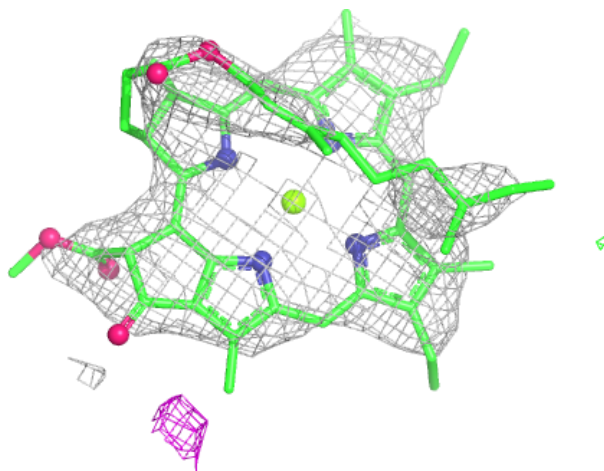
Electron density around LHG B 848:

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



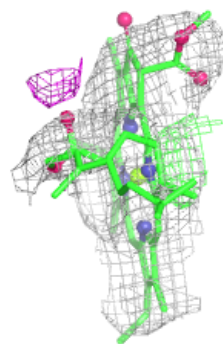
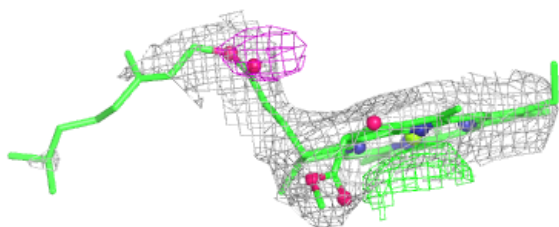
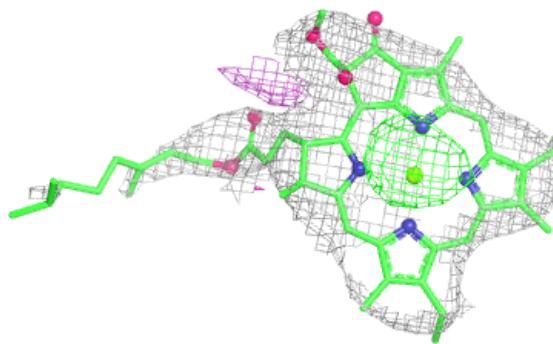
Electron density around CLA A 816:

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



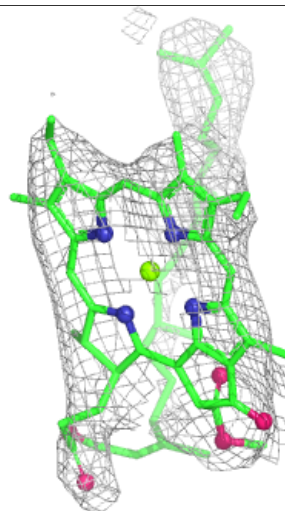
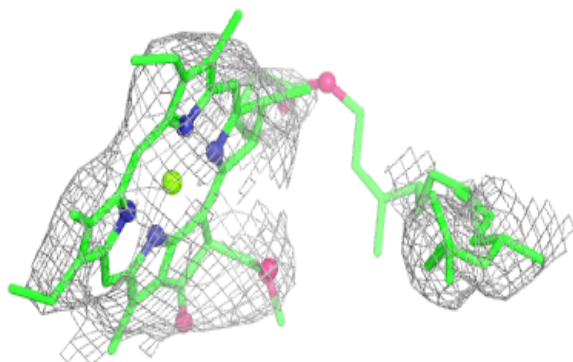
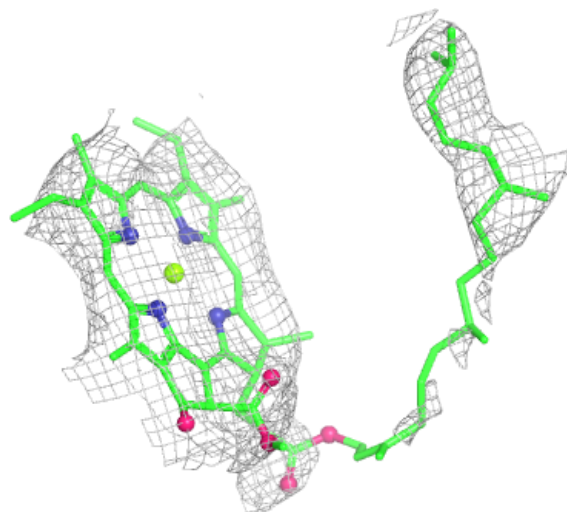
Electron density around CLA A 824:

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



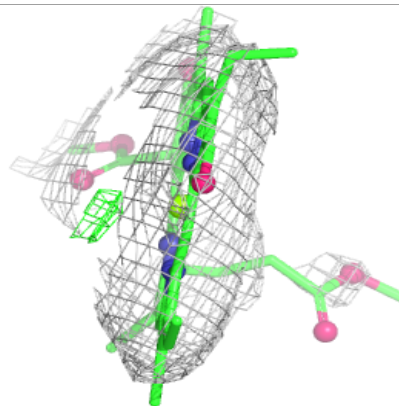
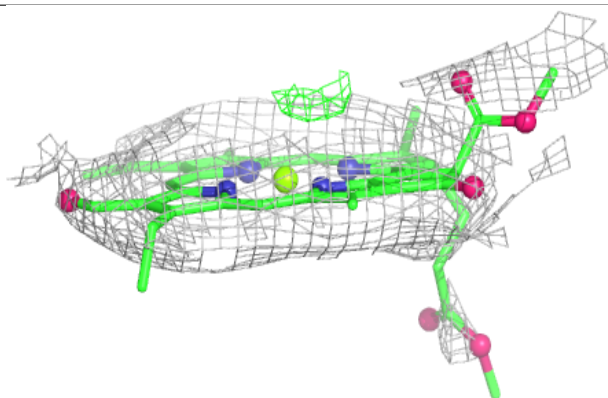
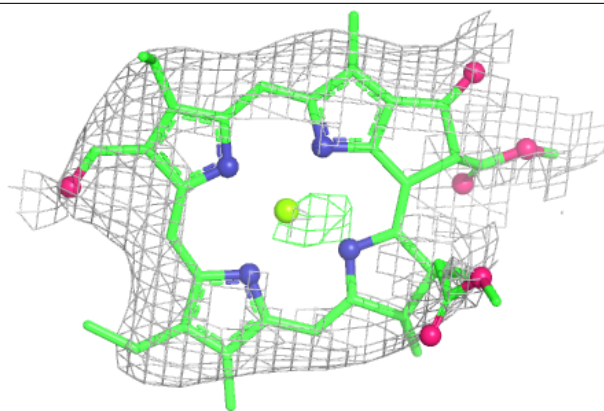
Electron density around CLA B 811:

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



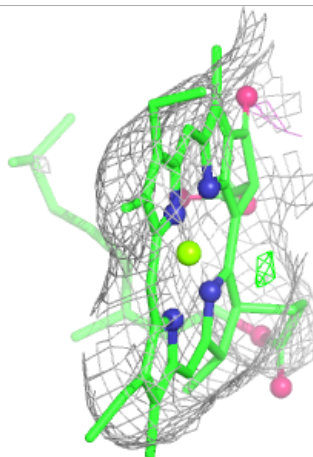
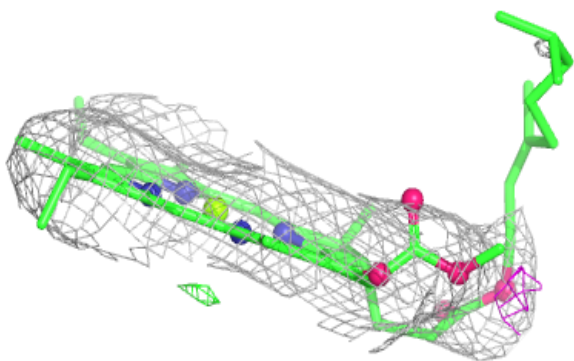
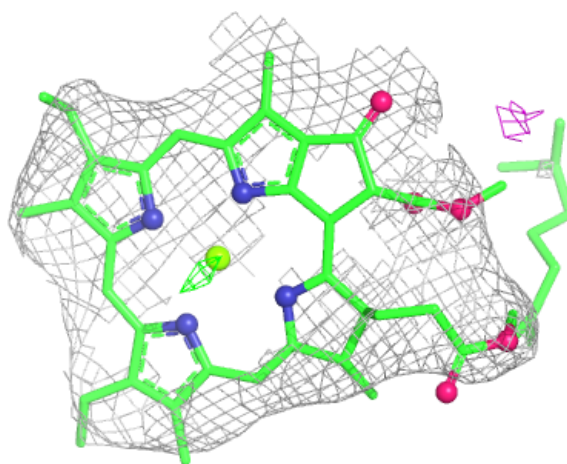
Electron density around CHL 3 316:

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



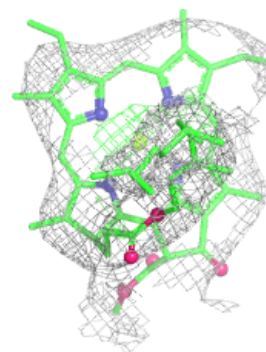
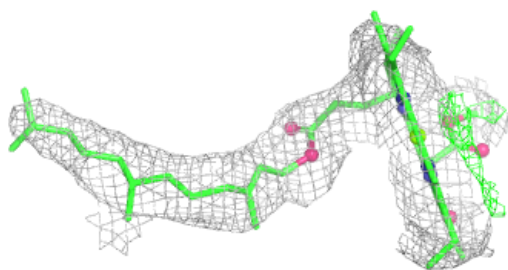
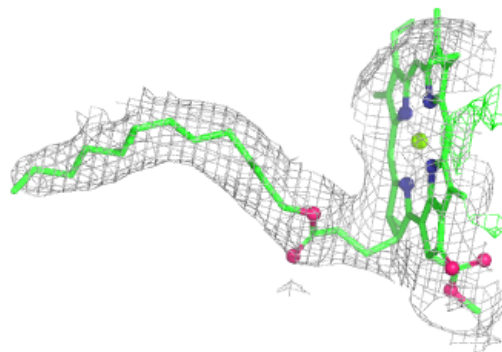
Electron density around CLA 3 311:

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



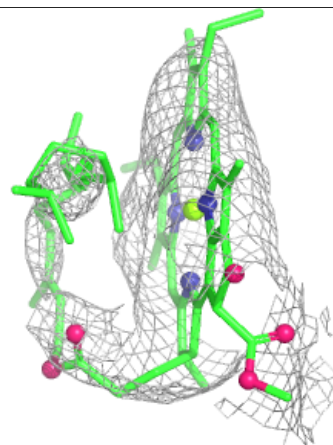
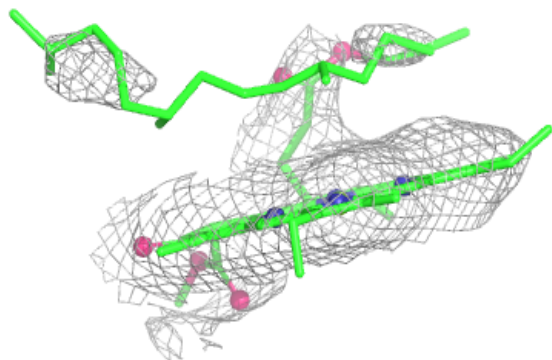
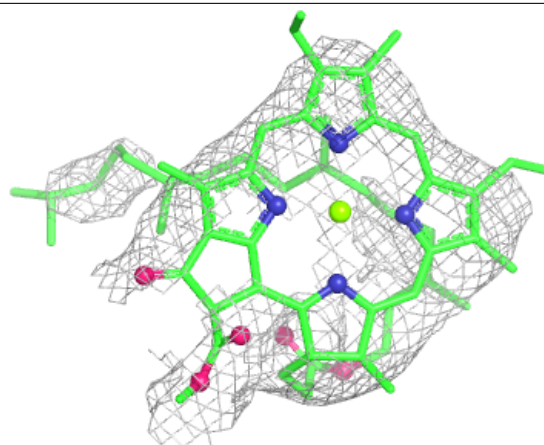
Electron density around CLA L 305:

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



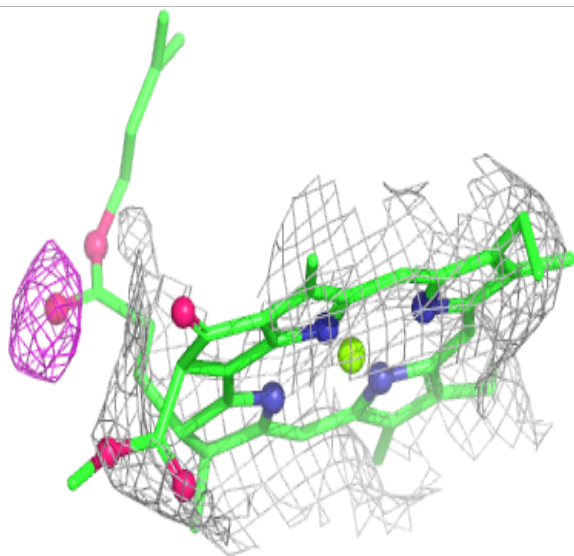
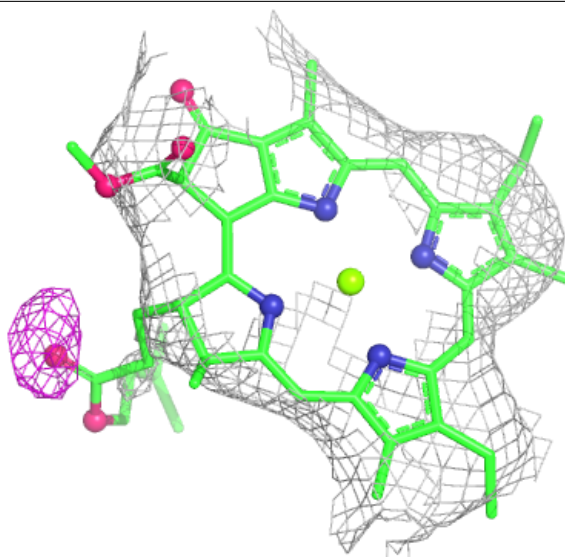
Electron density around CLA 3 315:

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



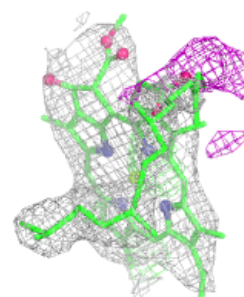
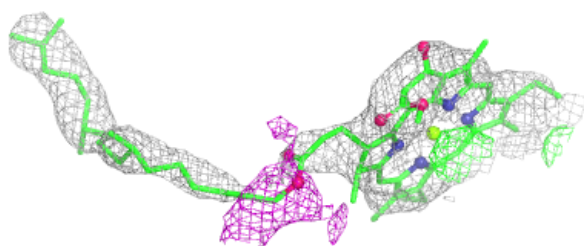
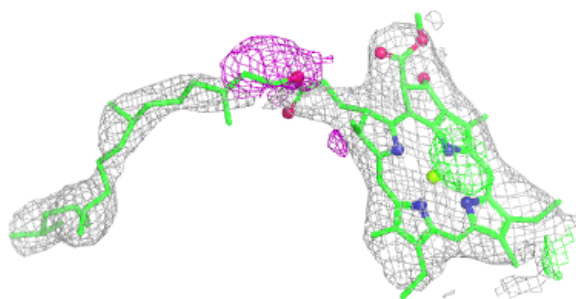
Electron density around CLA 3 317:

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

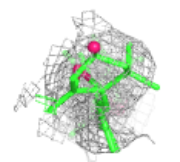
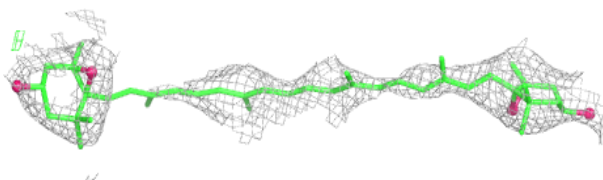
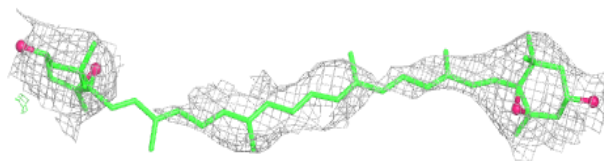


Electron density around CLA B 801:

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

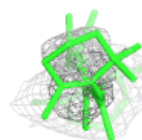
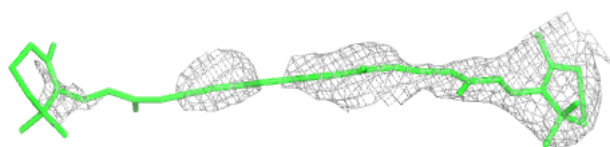
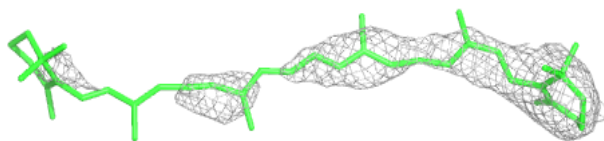
**Electron density around XAT 4 304:**

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

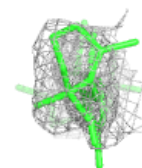
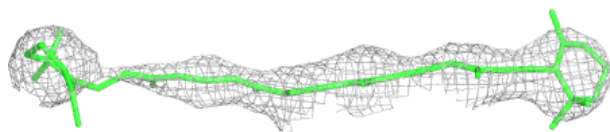


Electron density around BCR A 844:

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

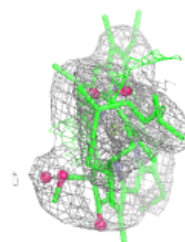
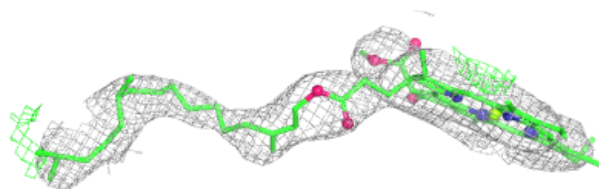
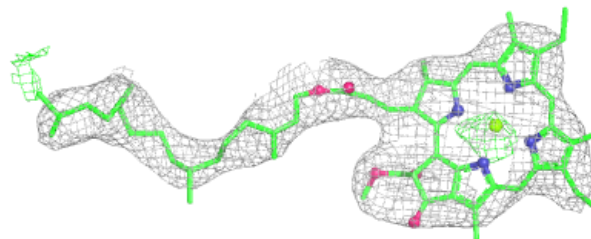
**Electron density around BCR A 845:**

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



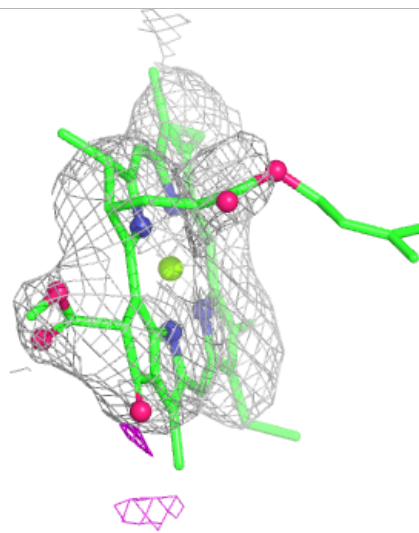
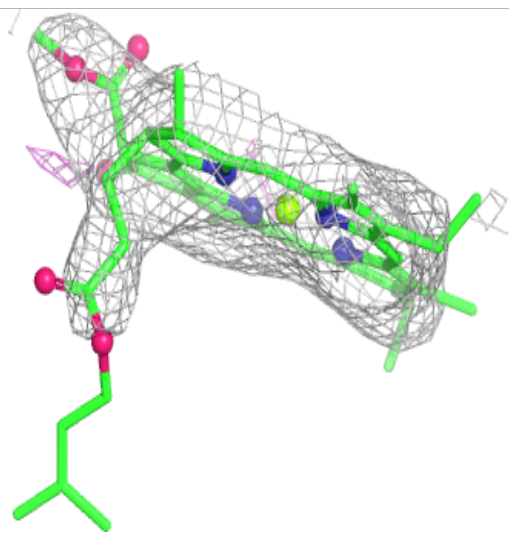
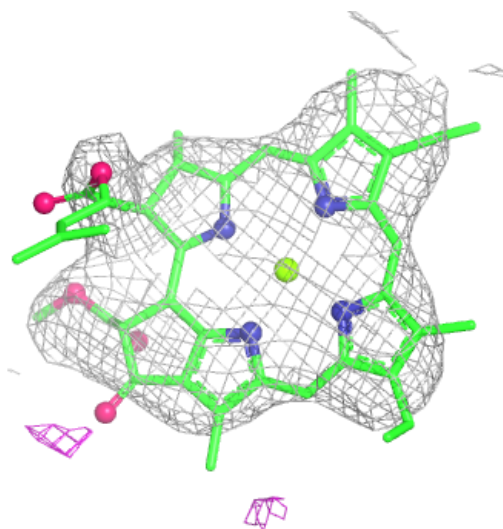
Electron density around CLA A 838:

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



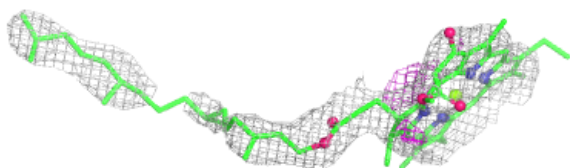
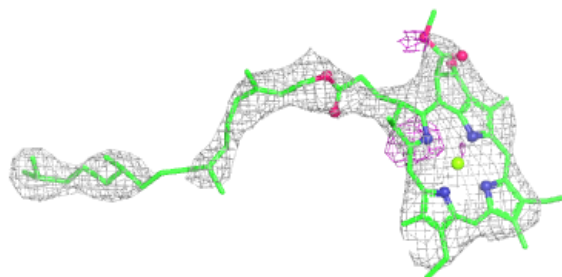
Electron density around CLA A 809:

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

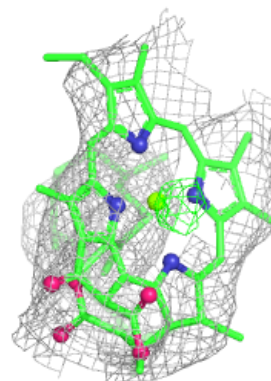
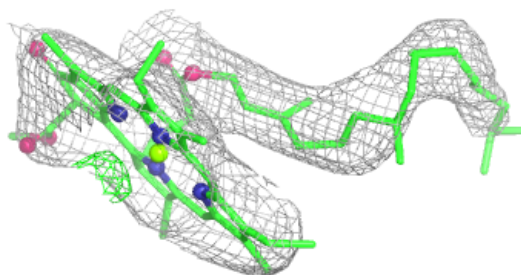
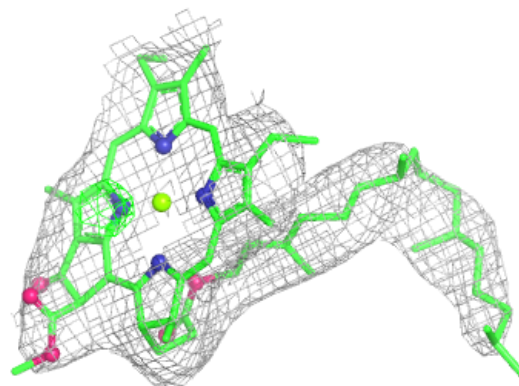


Electron density around CLA A 852:

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

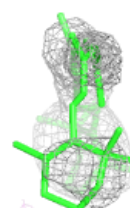
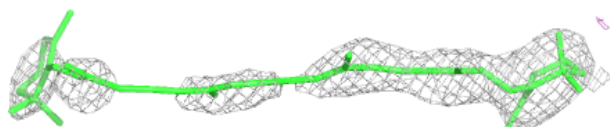
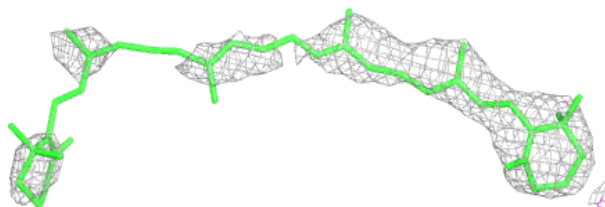
**Electron density around CLA A 853:**

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

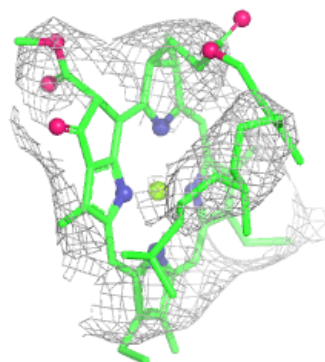
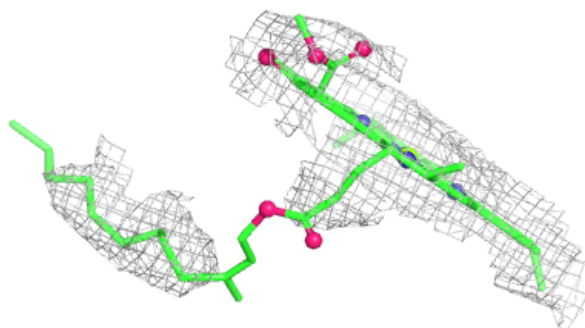
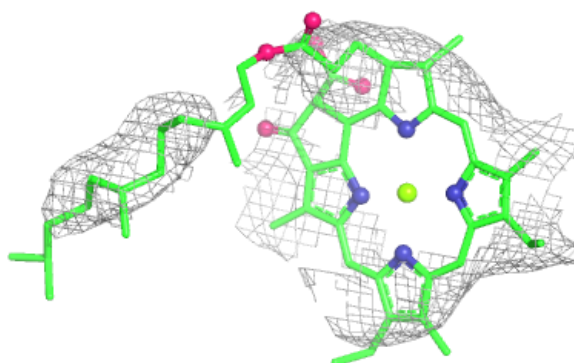


Electron density around BCR B 844:

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

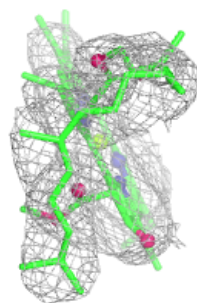
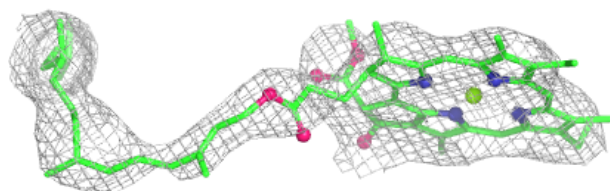
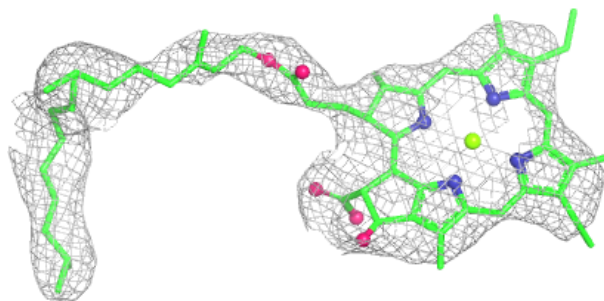
**Electron density around CLA A 820:**

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

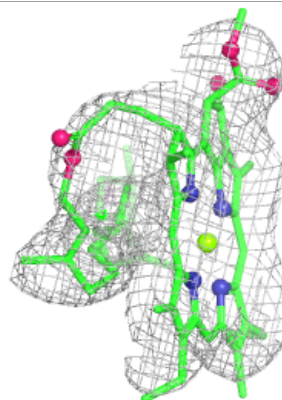
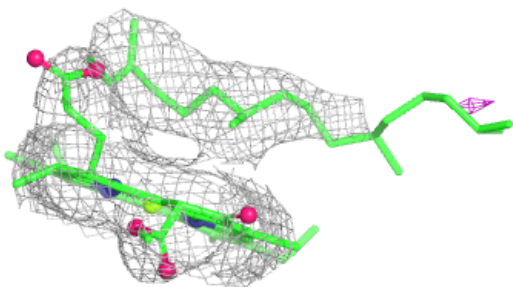
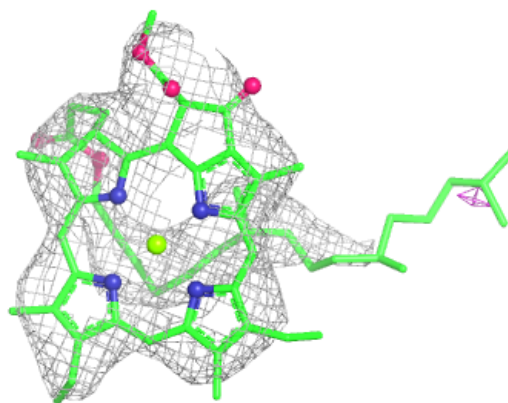


Electron density around CLA B 827:

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

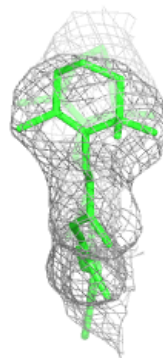
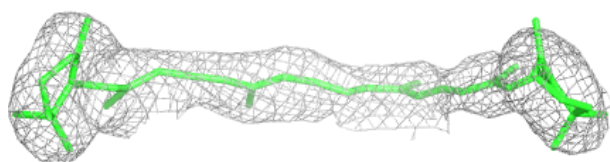
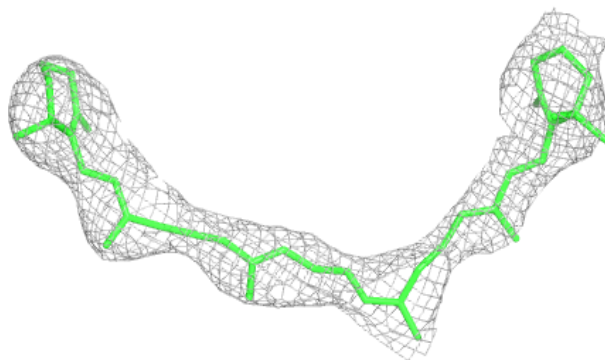
**Electron density around CLA B 828:**

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

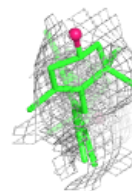
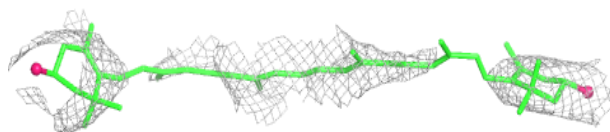
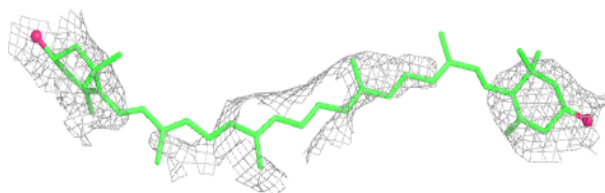


Electron density around BCR F 305:

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

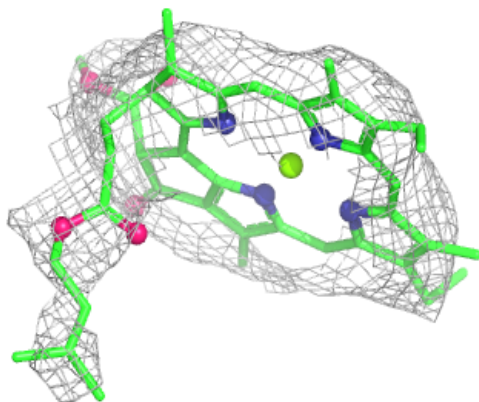
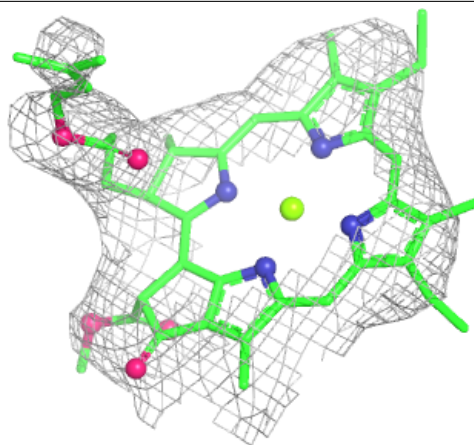
**Electron density around LUT 3 304:**

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



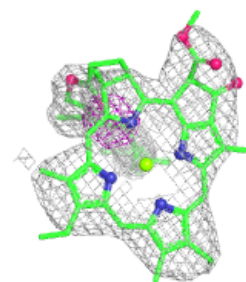
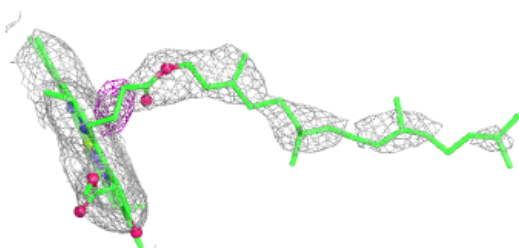
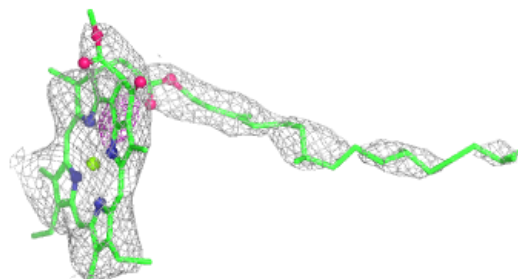
Electron density around CLA 2 313:

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

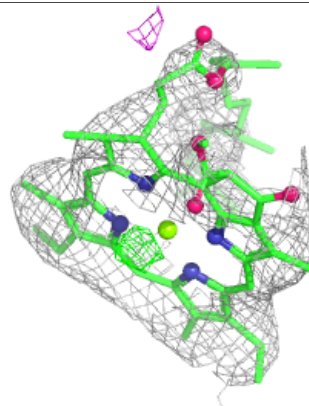
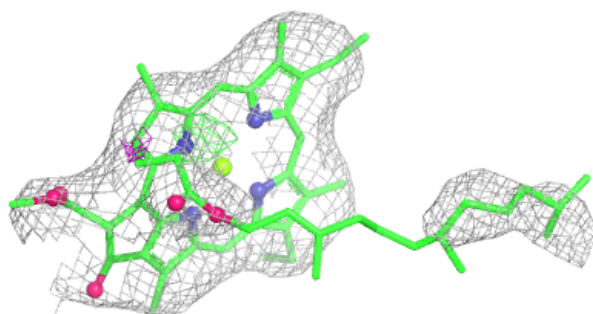
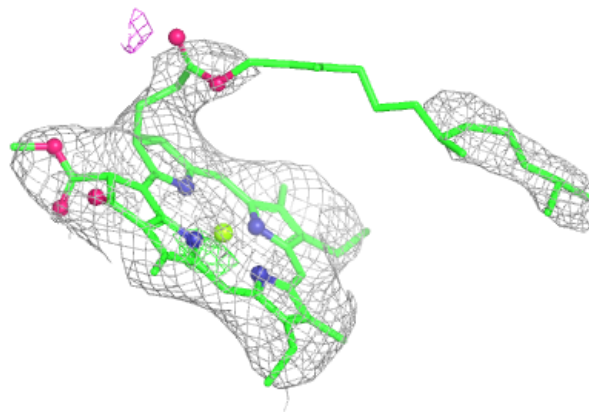


Electron density around CLA B 829:

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

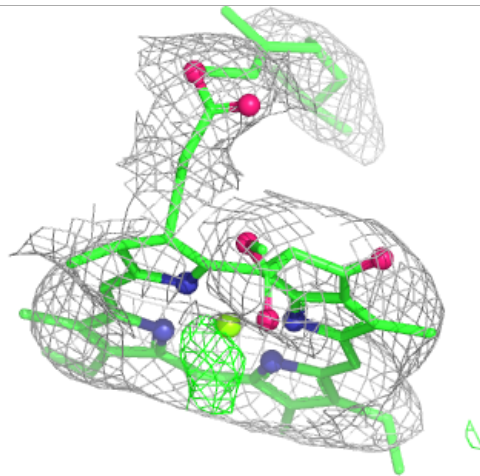
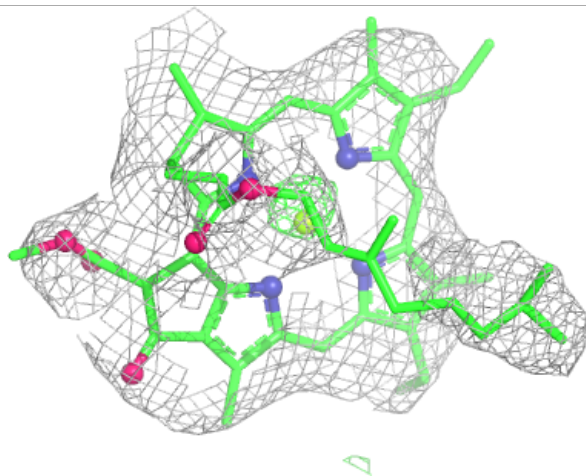
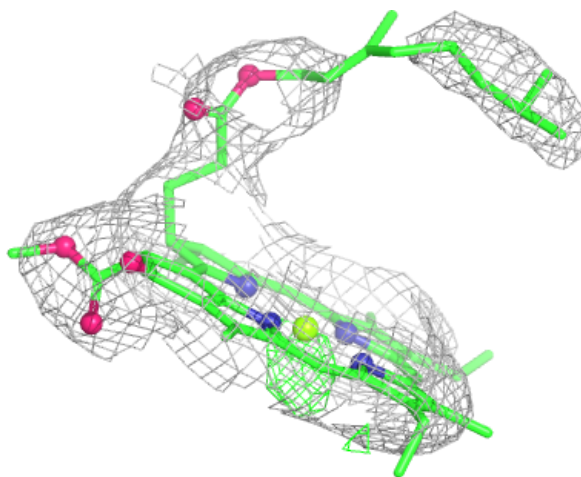
**Electron density around CLA B 832:**

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



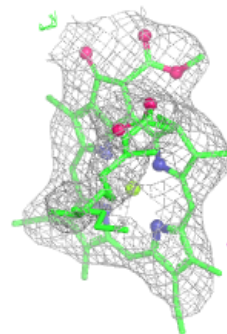
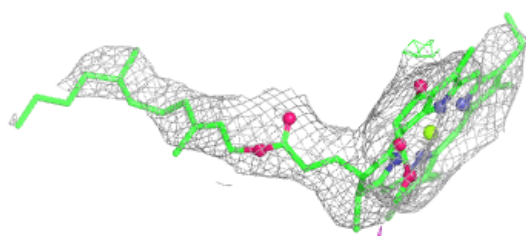
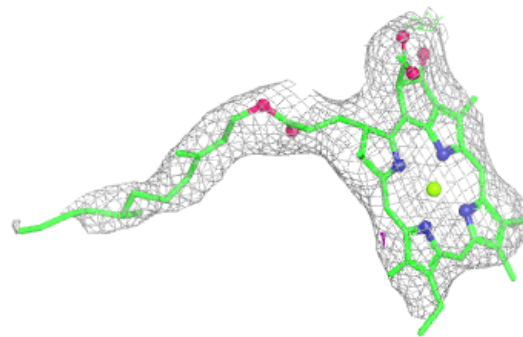
Electron density around CLA L 301:

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



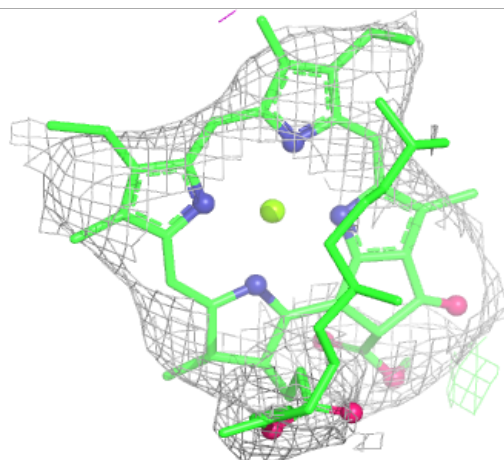
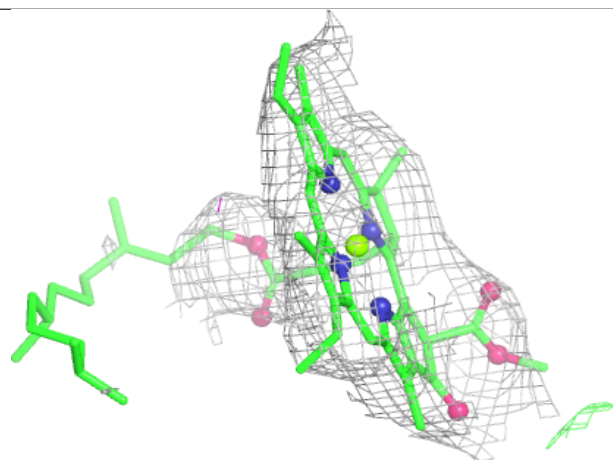
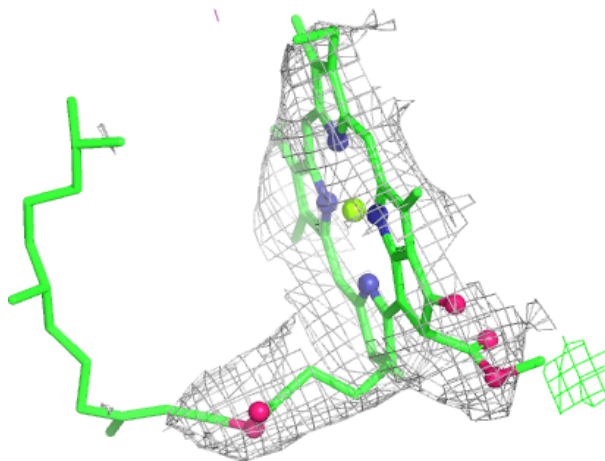
Electron density around CLA B 833:

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



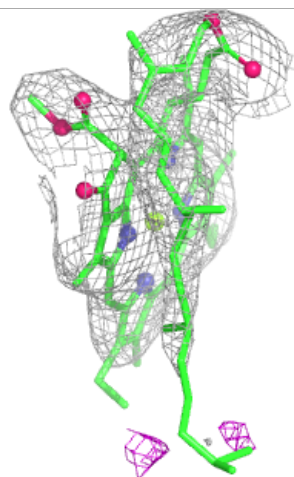
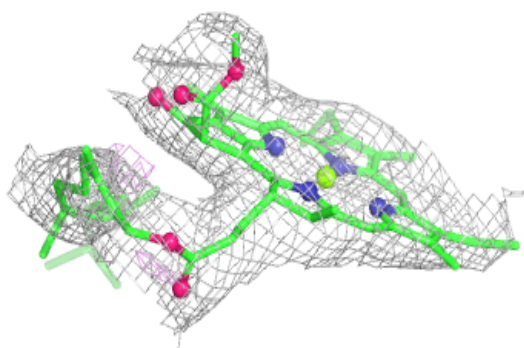
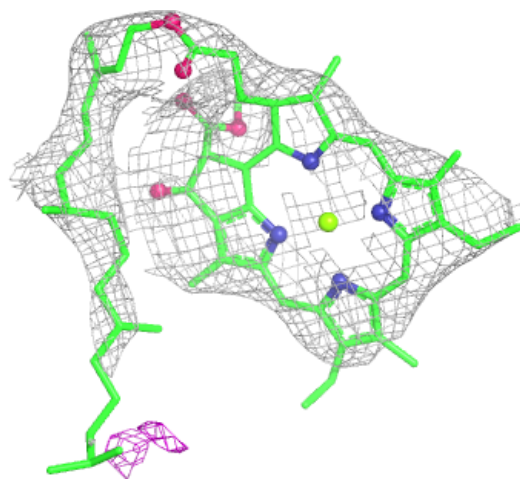
Electron density around CLA A 821:

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



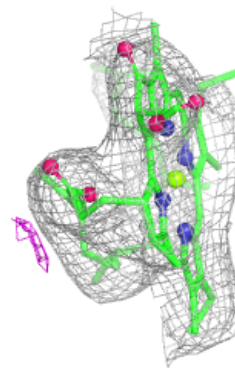
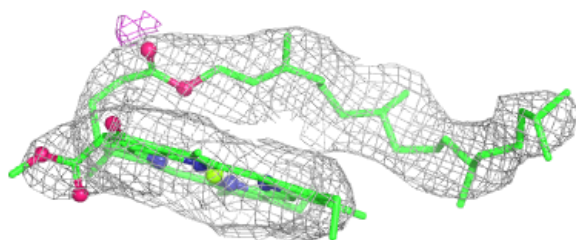
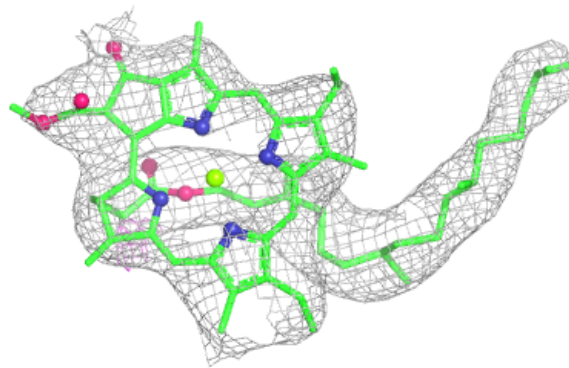
Electron density around CLA A 823:

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



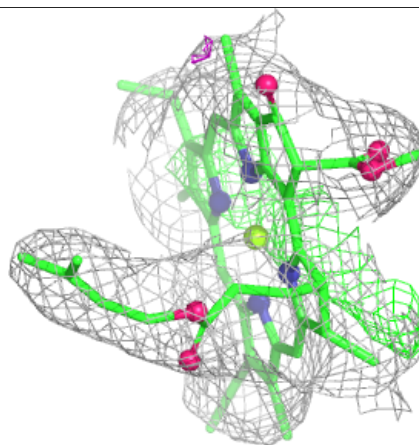
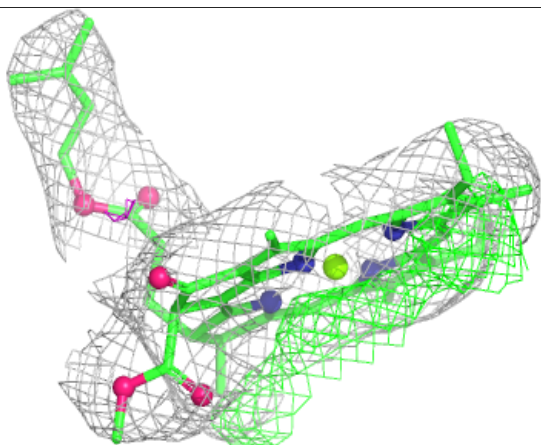
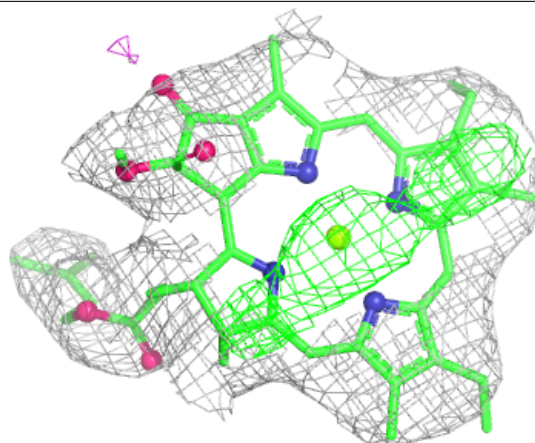
Electron density around CLA B 837:

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



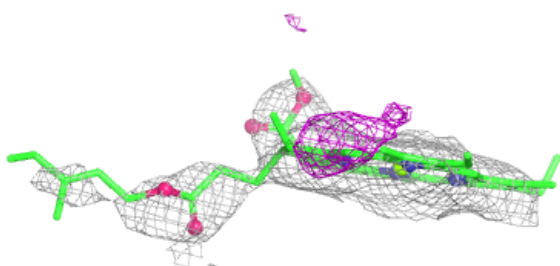
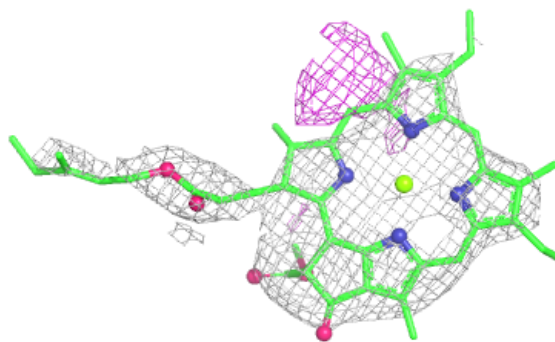
Electron density around CLA B 838:

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

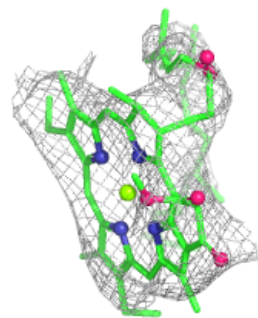
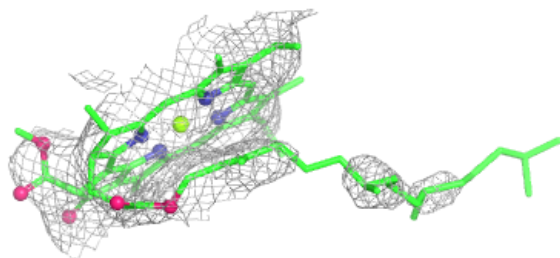
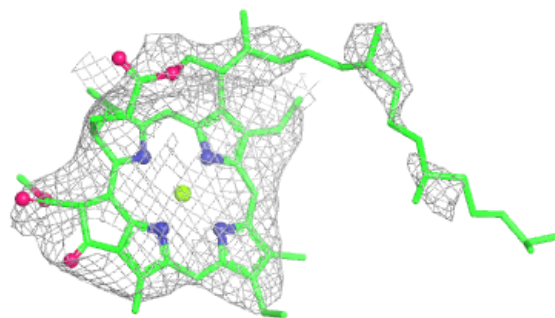


Electron density around CLA A 834:

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

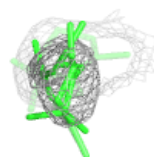
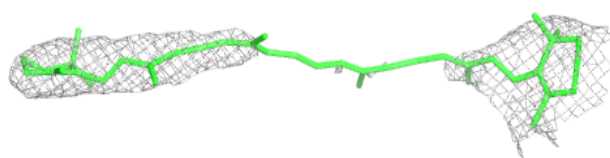
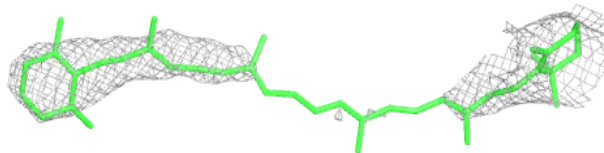
**Electron density around CLA 1 5009:**

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



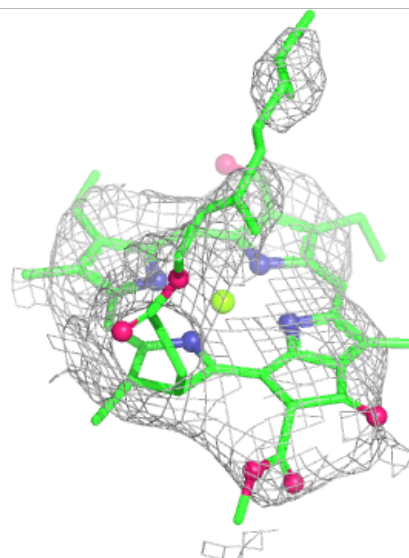
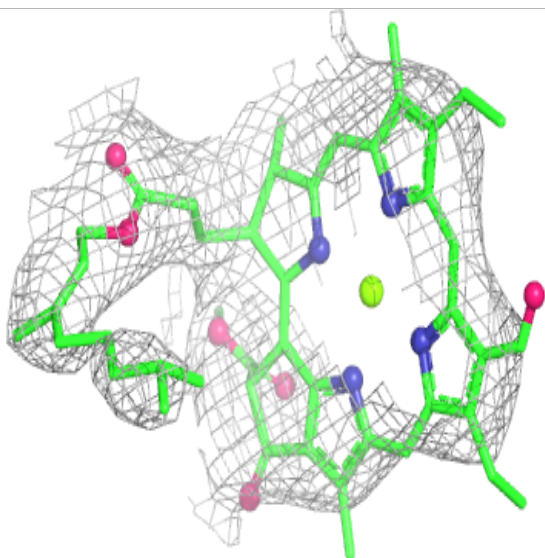
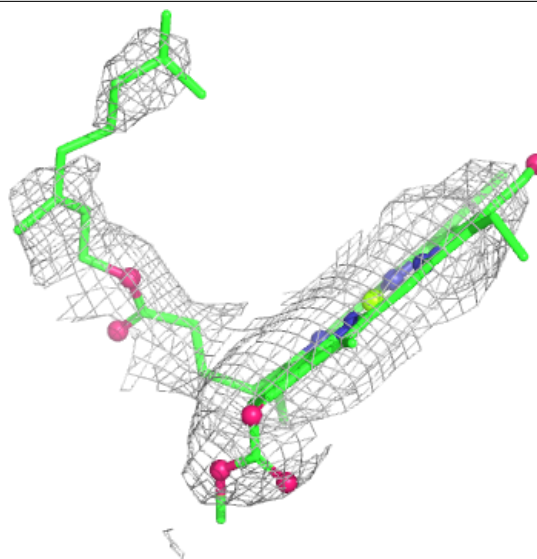
Electron density around BCR 4 301:

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



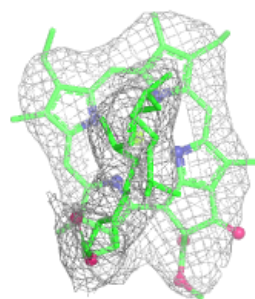
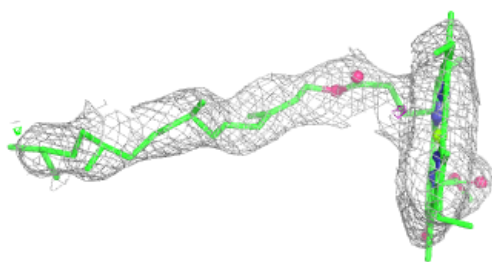
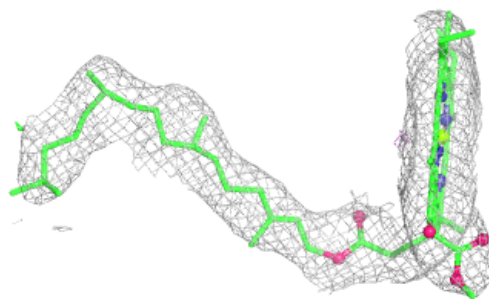
Electron density around CHL 4 302:

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



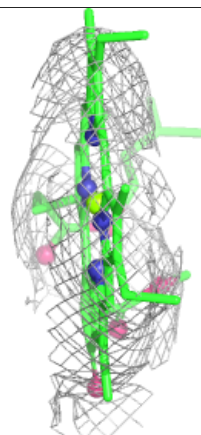
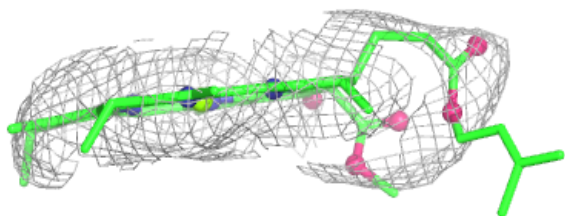
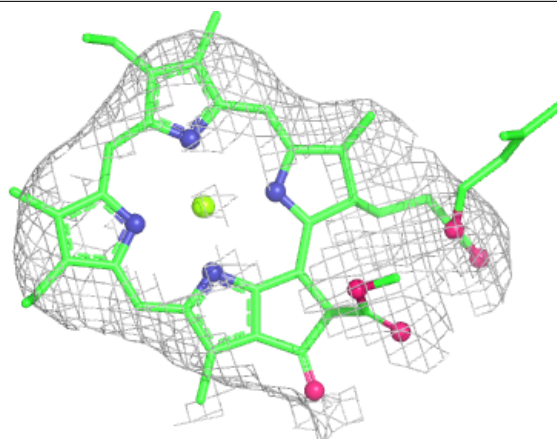
Electron density around CLA B 840:

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

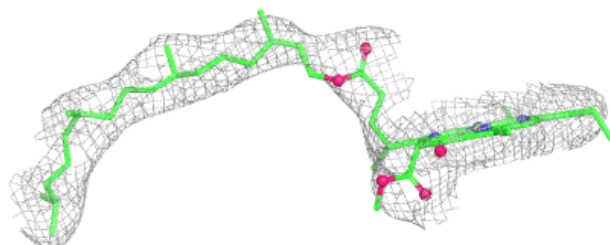
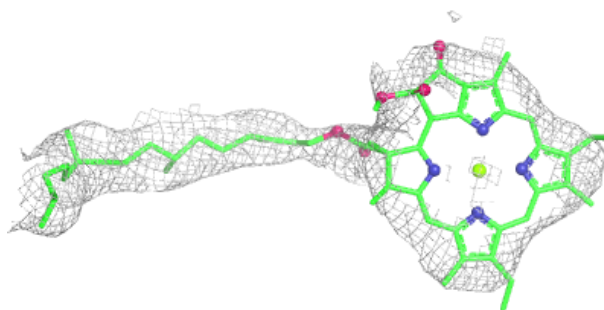


Electron density around CLA 4 306:

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

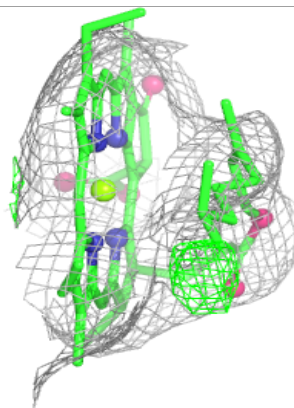
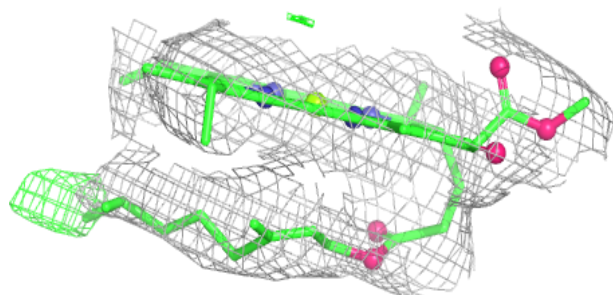
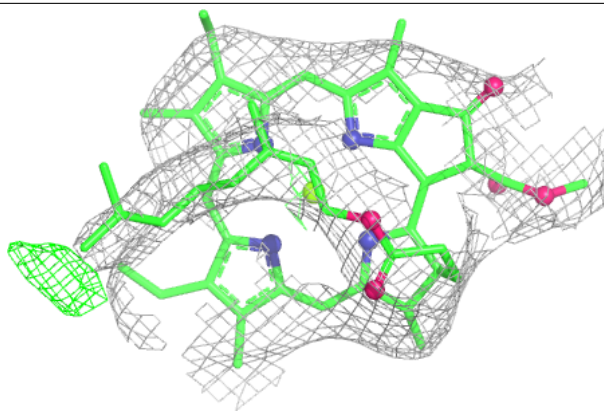
**Electron density around CLA B 841:**

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



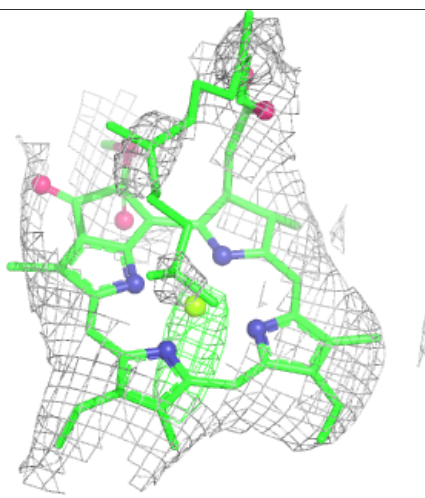
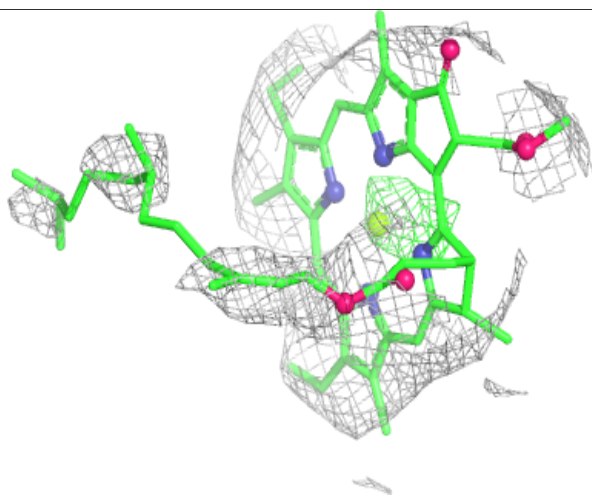
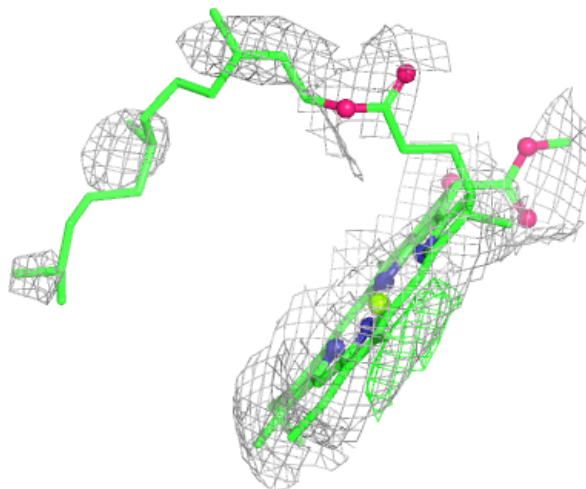
Electron density around CLA A 811:

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



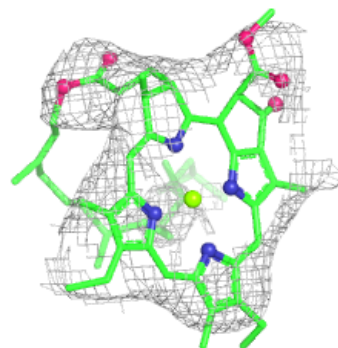
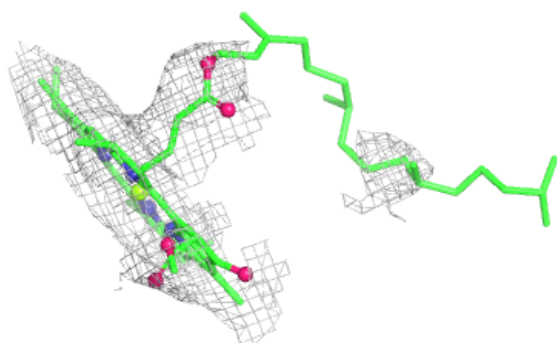
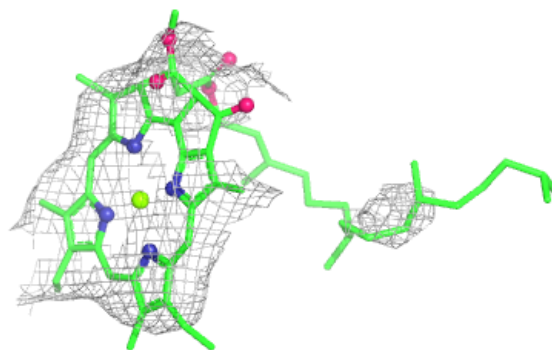
Electron density around CLA B 812:

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

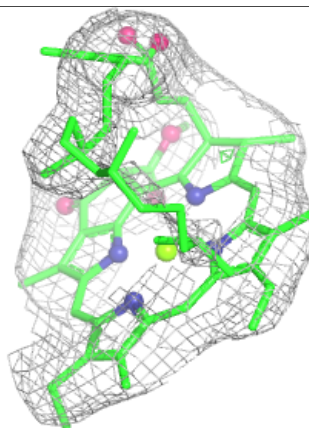
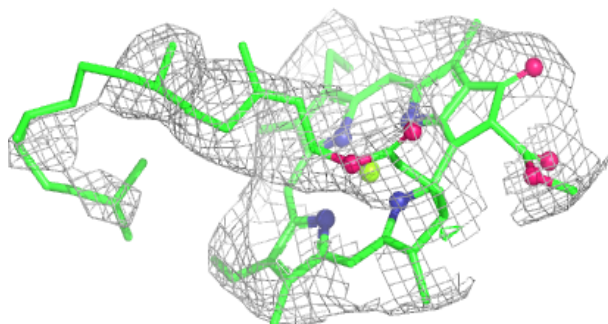
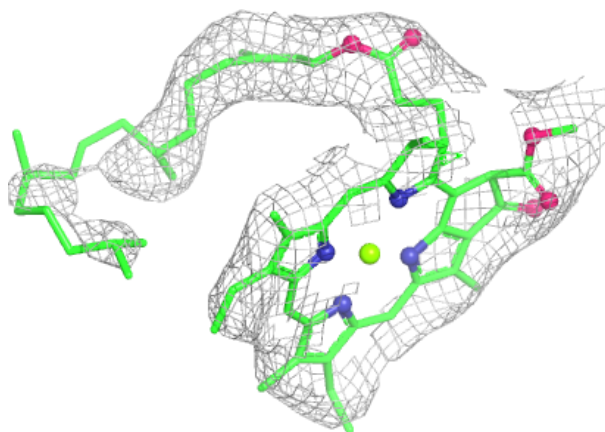


Electron density around CLA 4 315:

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

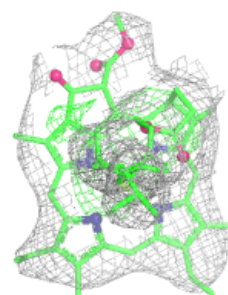
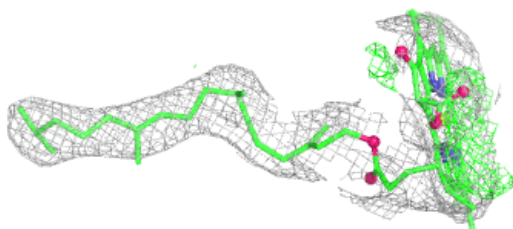
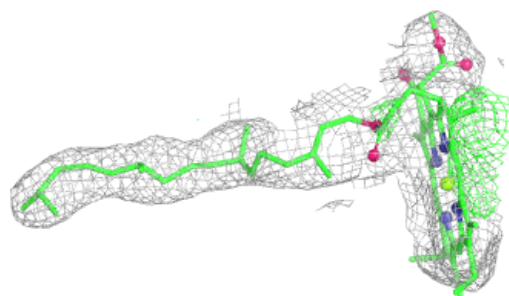
**Electron density around CLA A 822:**

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

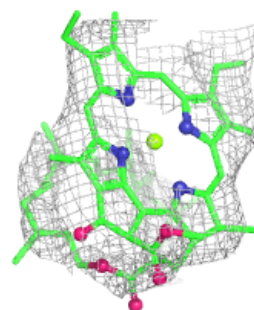
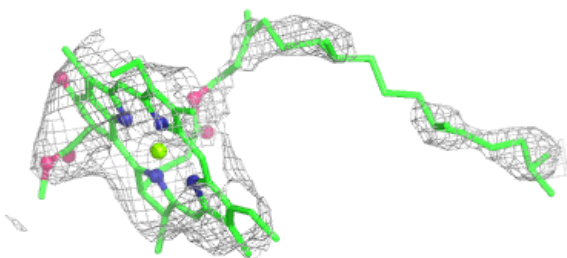
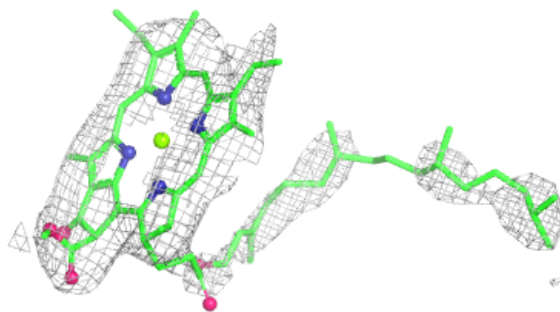


Electron density around CLA A 826:

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

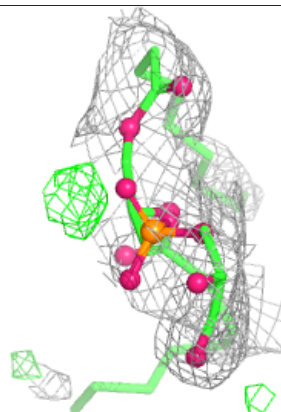
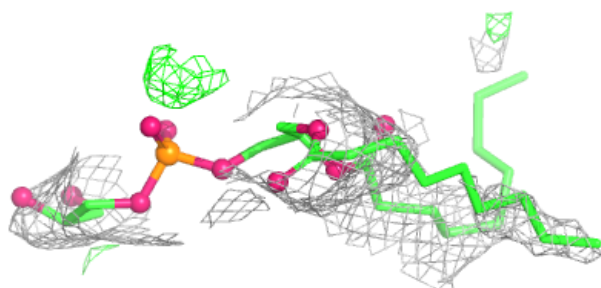
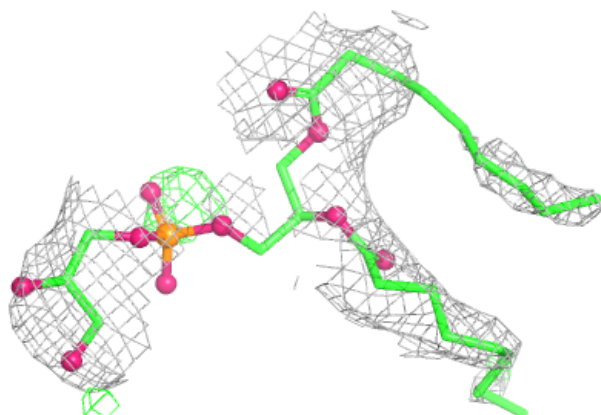
**Electron density around CLA B 815:**

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

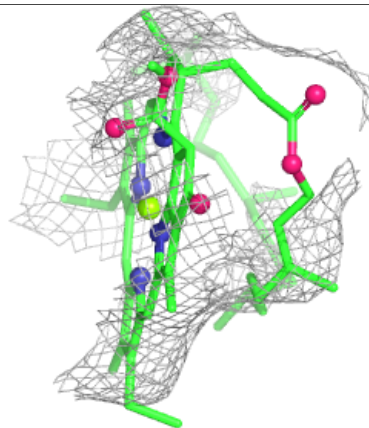
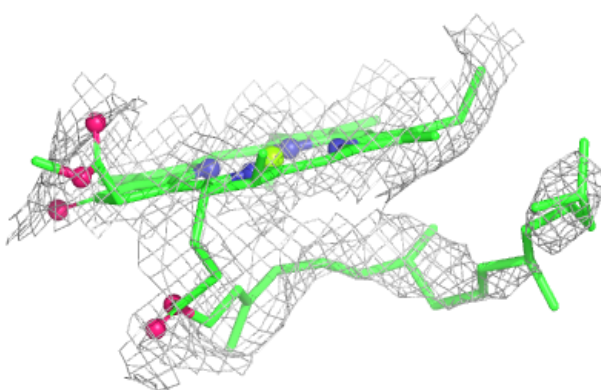
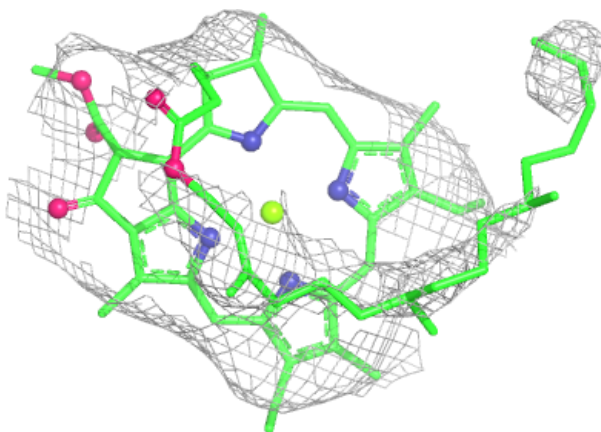


Electron density around LHG 2 320:

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

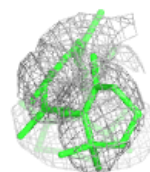
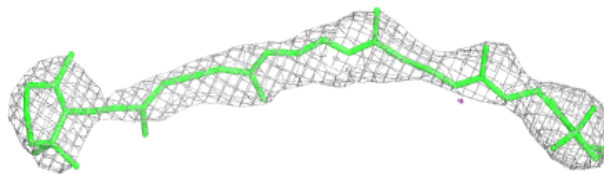
**Electron density around CLA 2 308:**

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

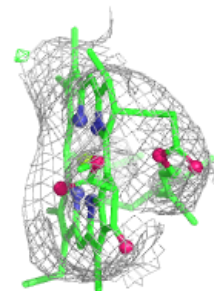
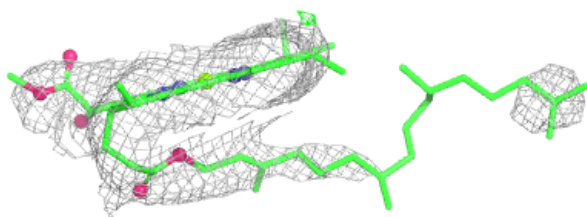
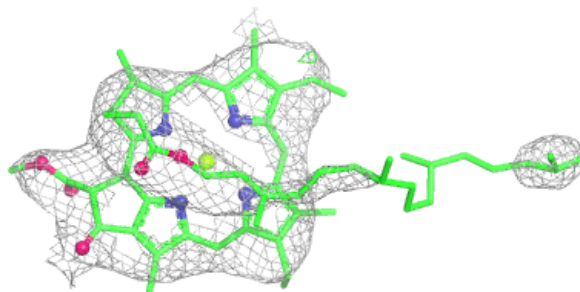


Electron density around BCR F 304:

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

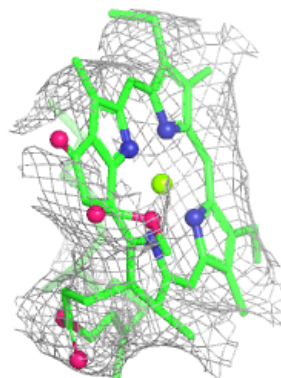
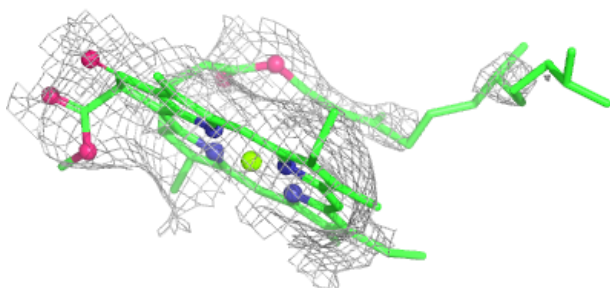
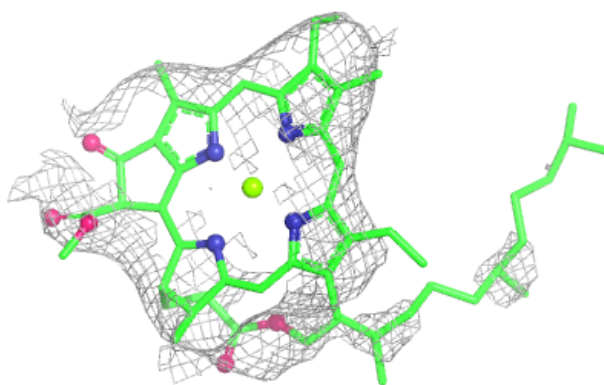
**Electron density around CLA A 835:**

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

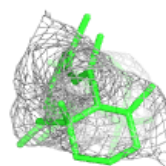
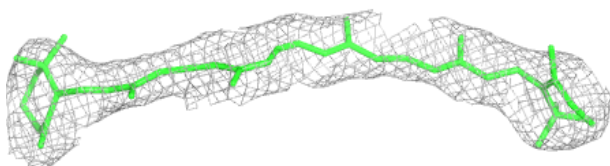
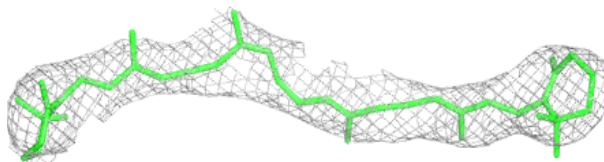


Electron density around CLA 4 308:

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

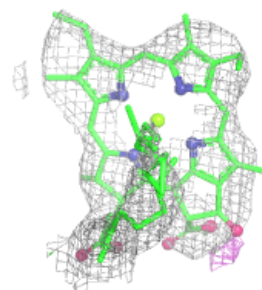
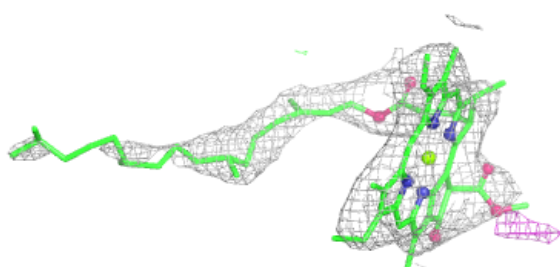
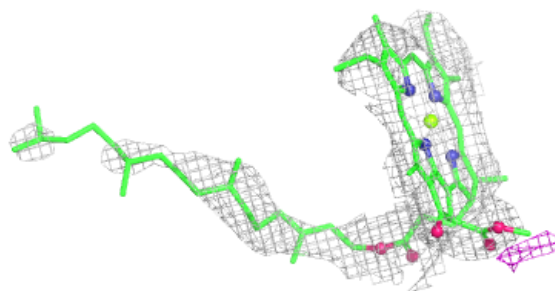
**Electron density around BCR I 101:**

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

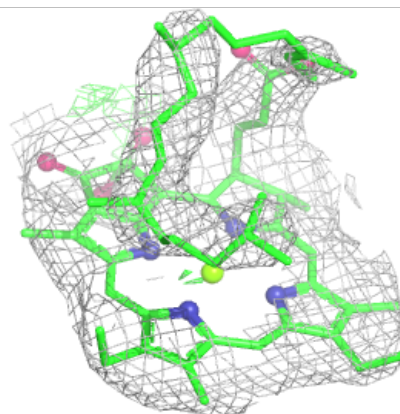
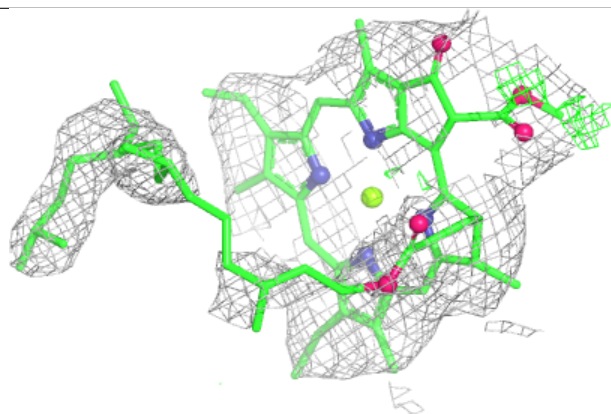
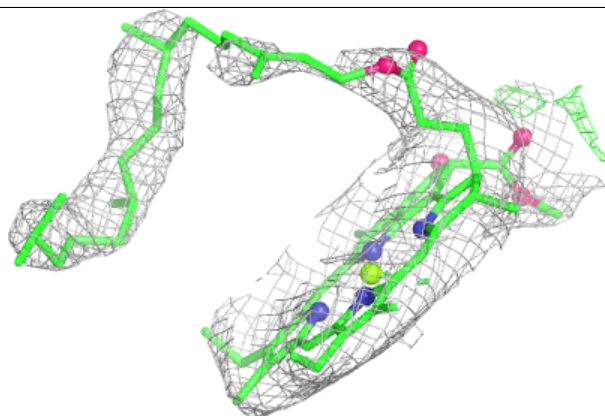


Electron density around CLA B 830:

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

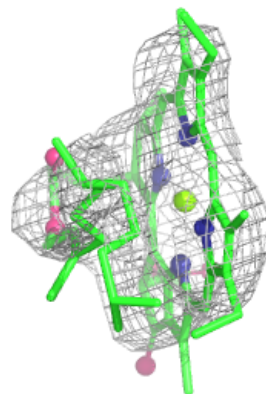
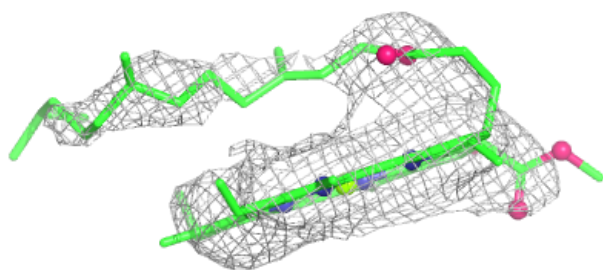
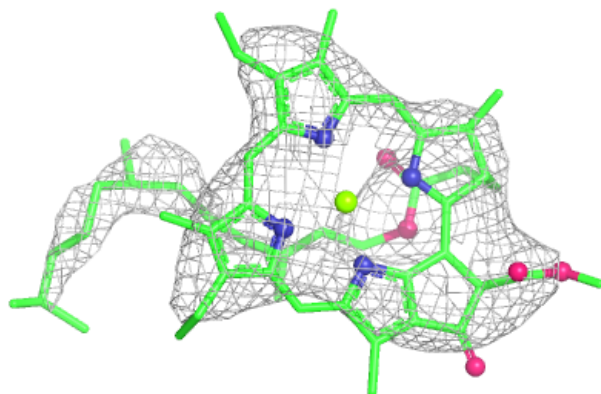
**Electron density around CLA B 831:**

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

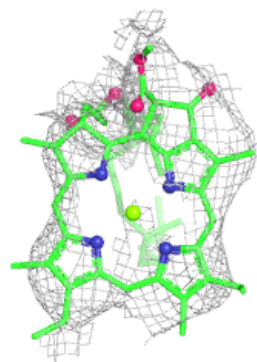
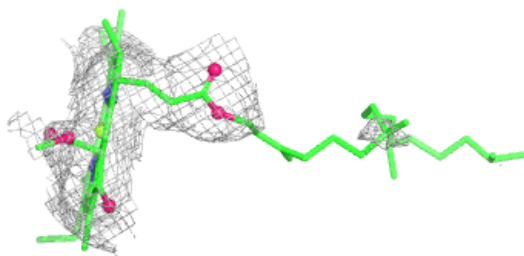
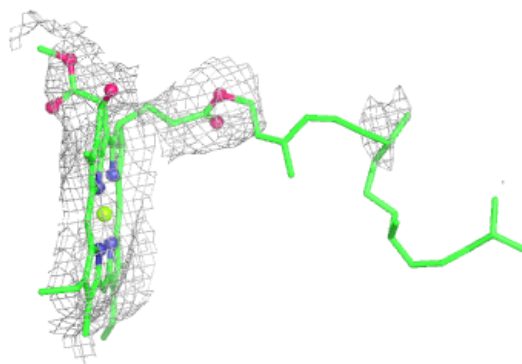


Electron density around CLA B 817:

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

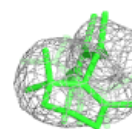
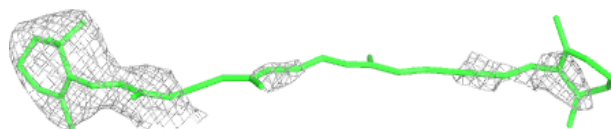
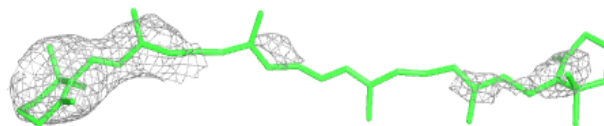
**Electron density around CLA A 813:**

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



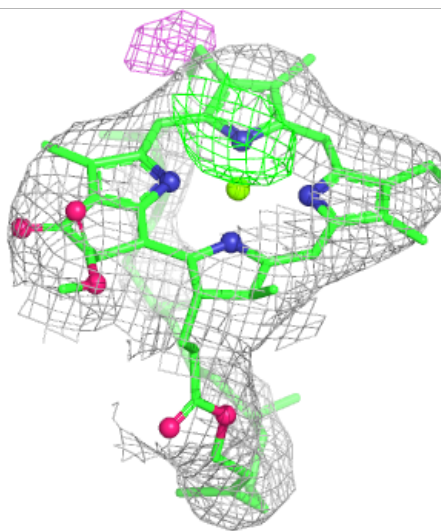
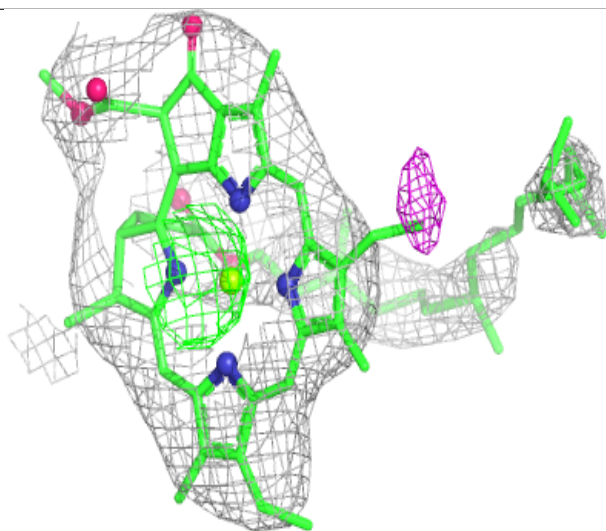
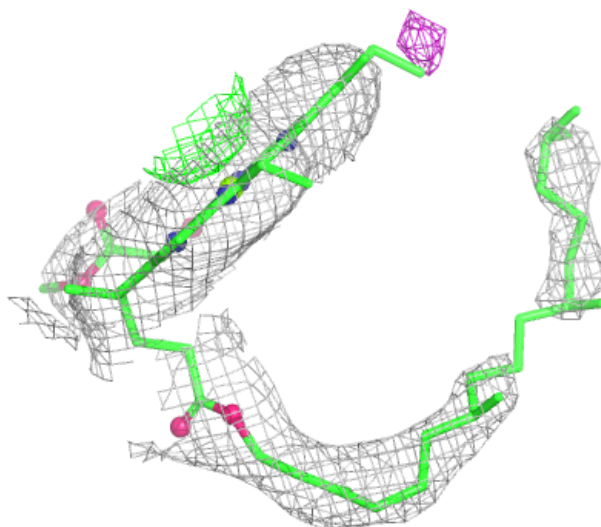
Electron density around BCR A 843:

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



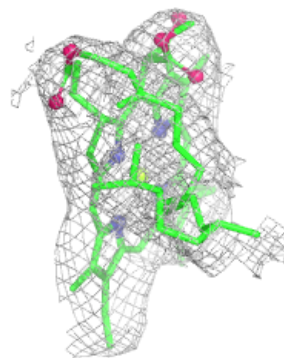
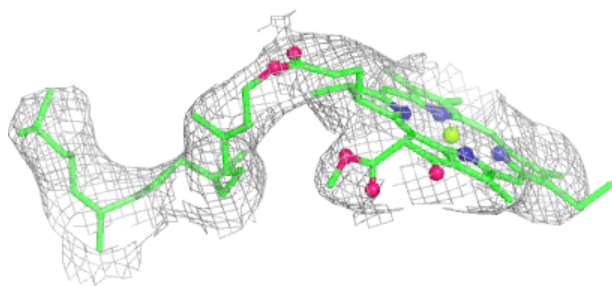
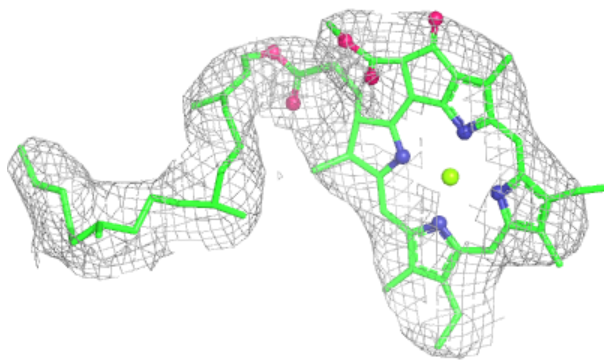
Electron density around CLA B 820:

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



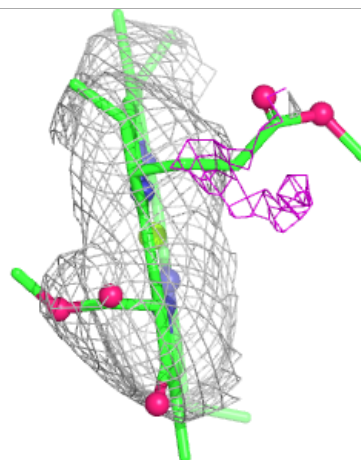
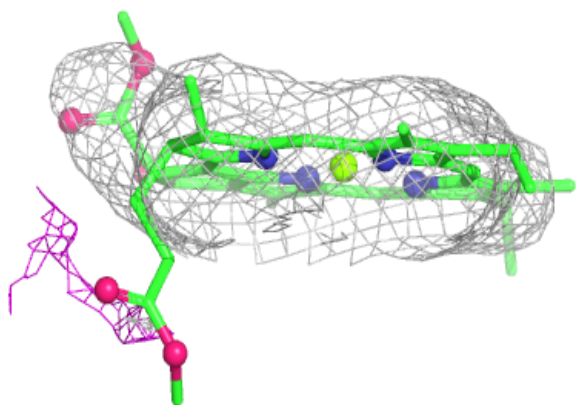
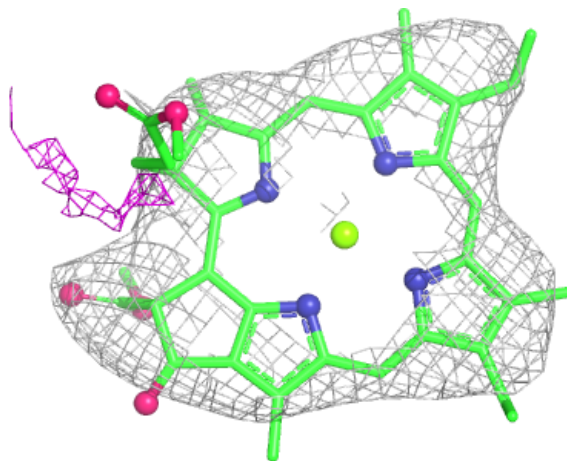
Electron density around CLA J 1101:

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



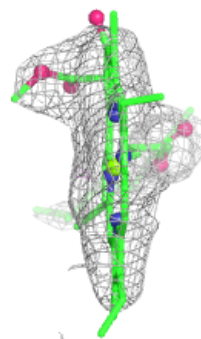
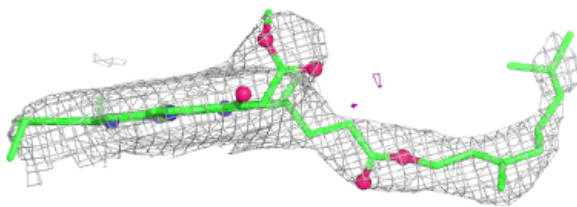
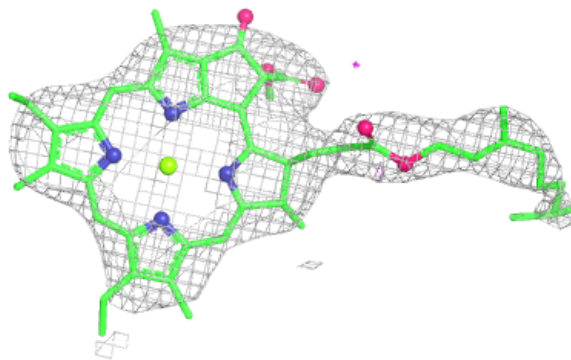
Electron density around CLA B 821:

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

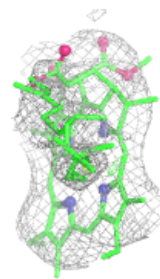
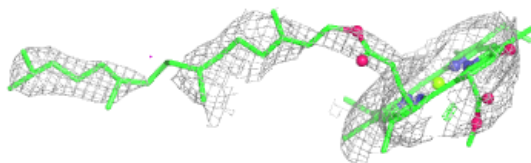
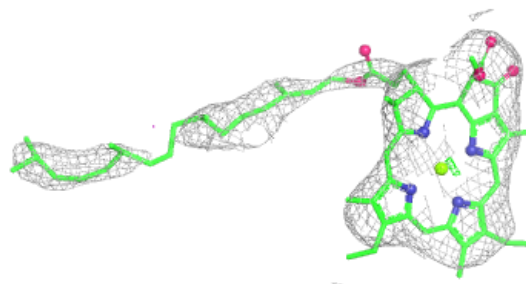


Electron density around CLA B 836:

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

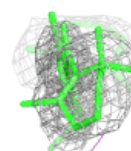
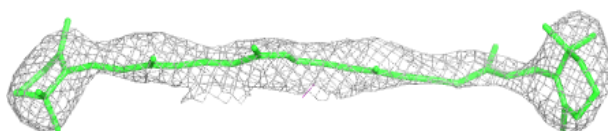
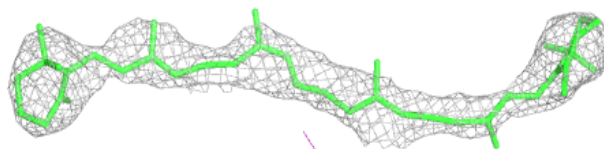
**Electron density around CLA A 831:**

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

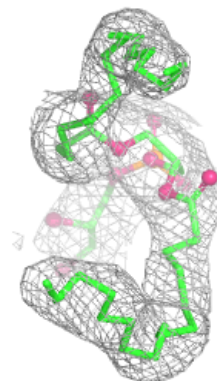
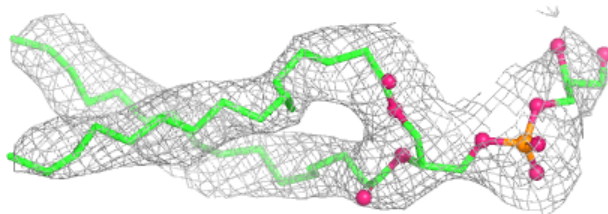
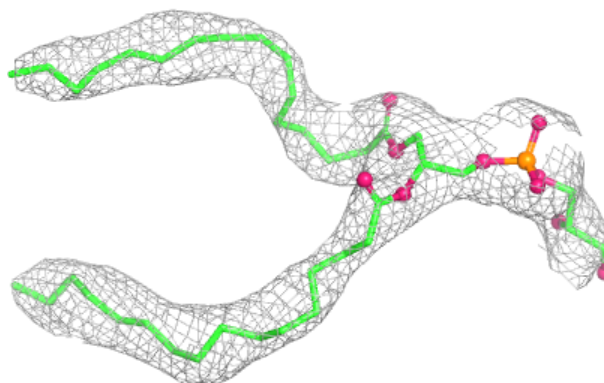


Electron density around BCR B 802:

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

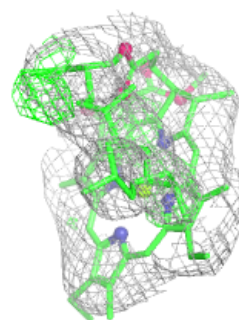
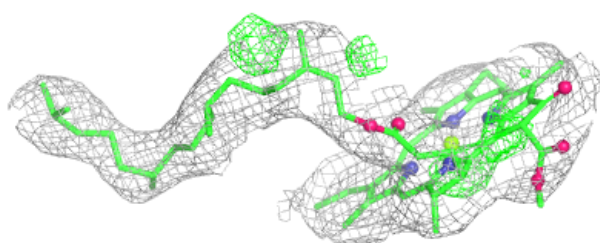
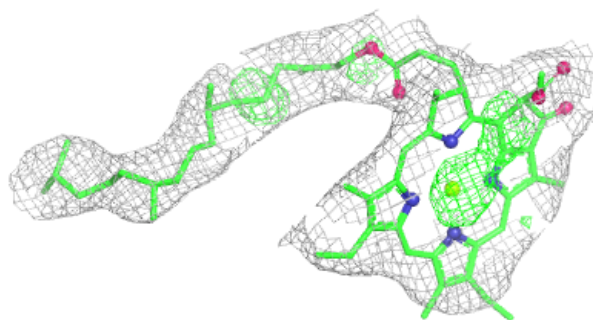
**Electron density around LHG A 848:**

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

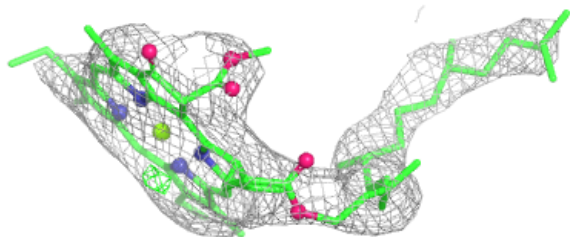
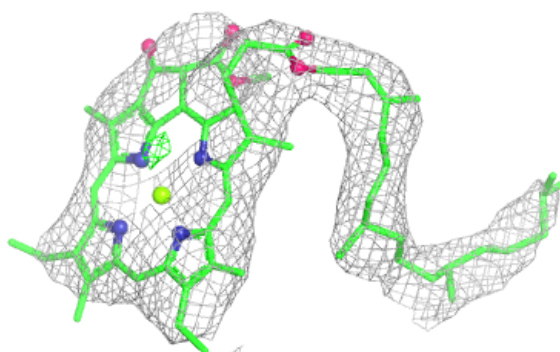


Electron density around CLA A 807:

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

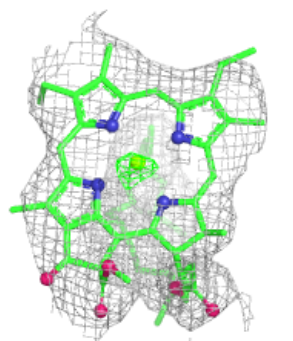
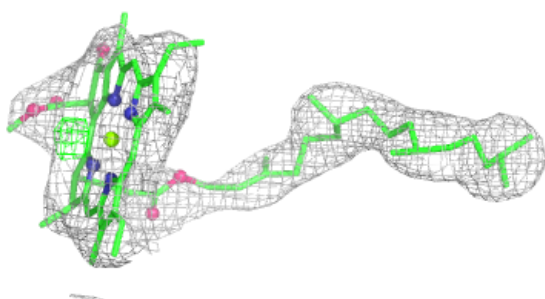
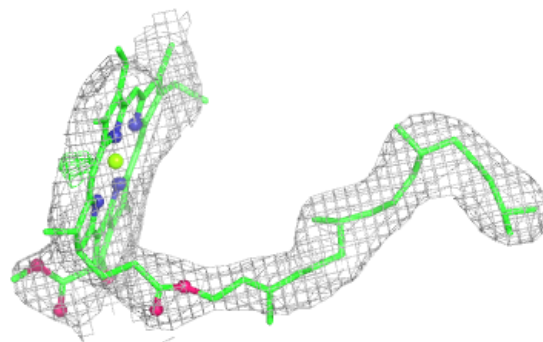
**Electron density around CLA B 825:**

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



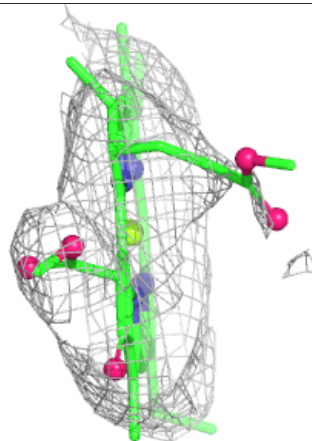
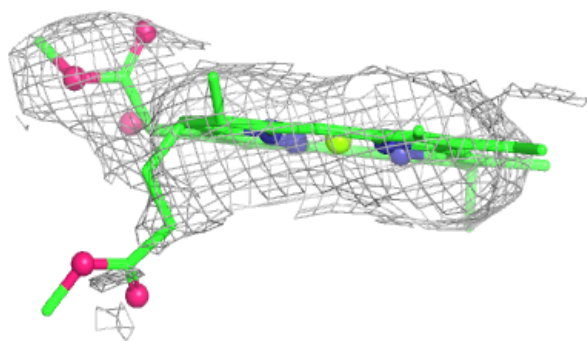
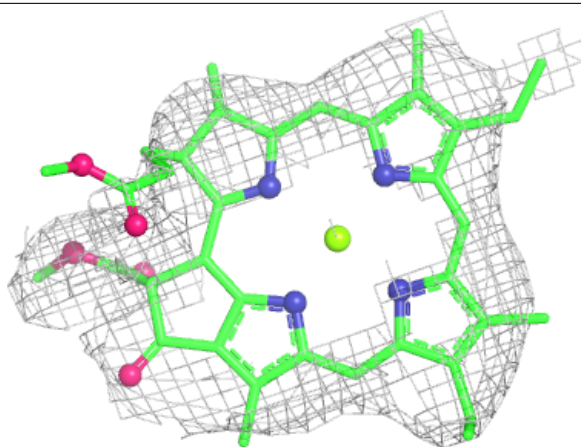
Electron density around CLA A 828:

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



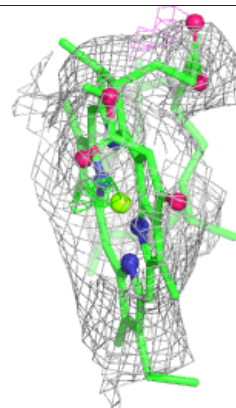
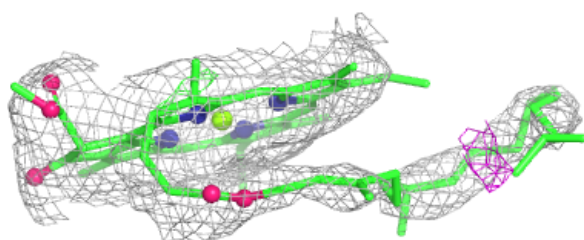
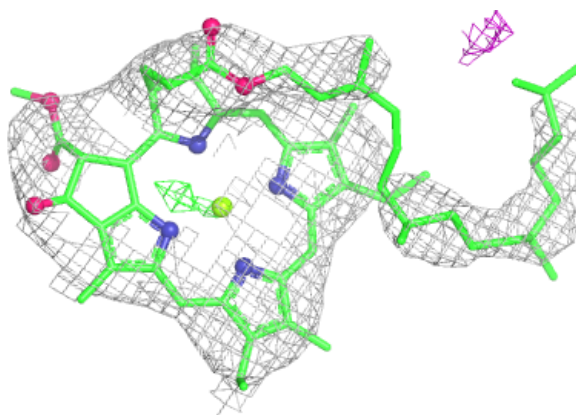
Electron density around CLA B 813:

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

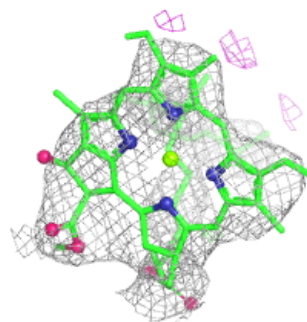
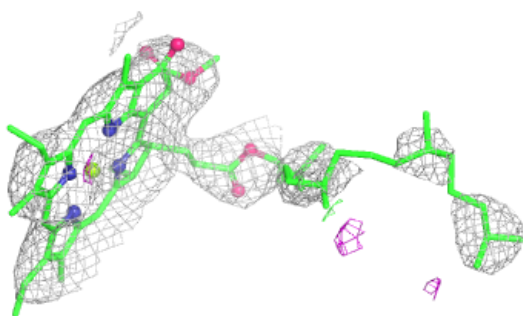
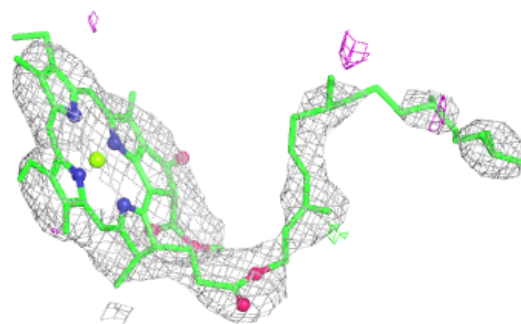


Electron density around CLA A 817:

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

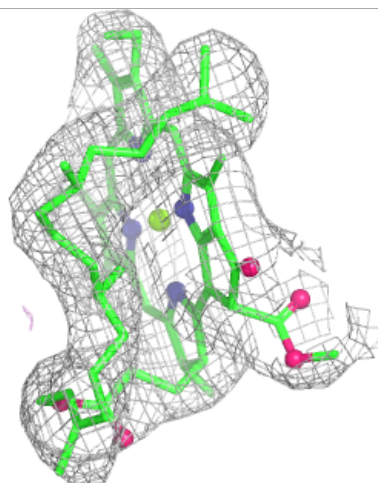
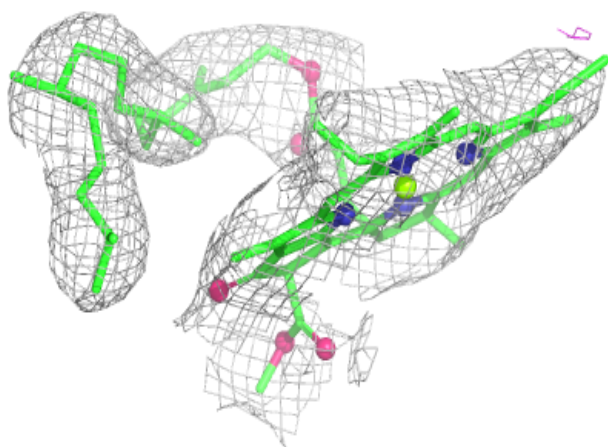
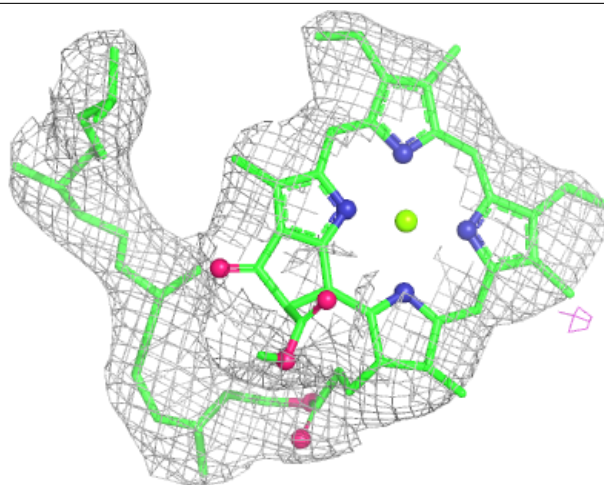
**Electron density around CLA B 803:**

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



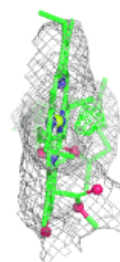
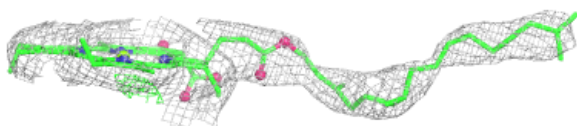
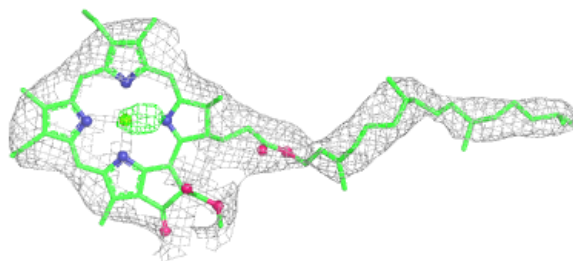
Electron density around CLA F 301:

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



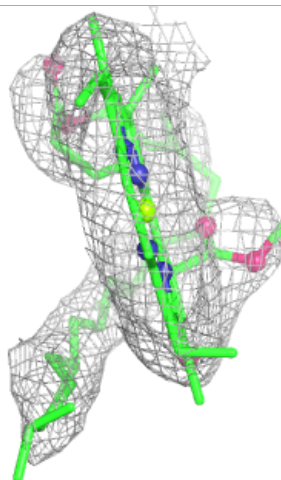
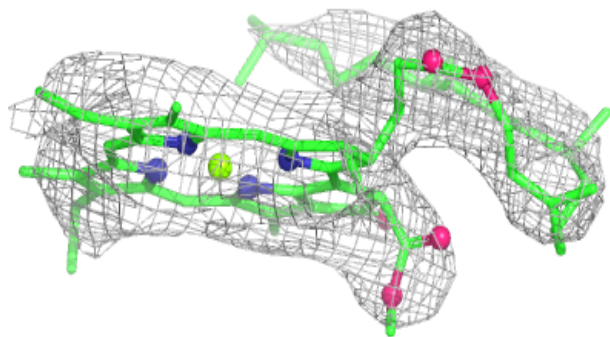
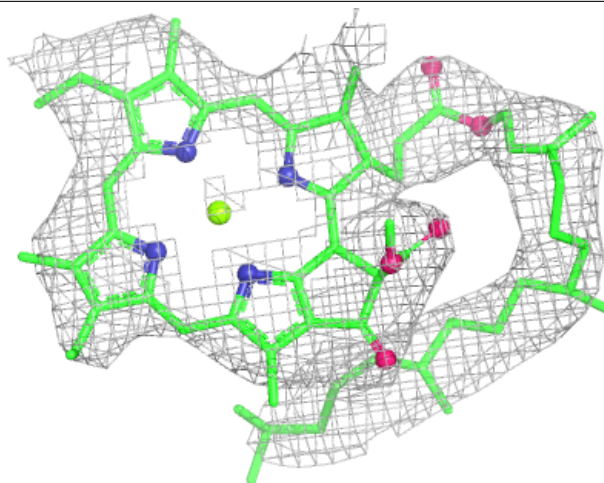
Electron density around CLA A 830:

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



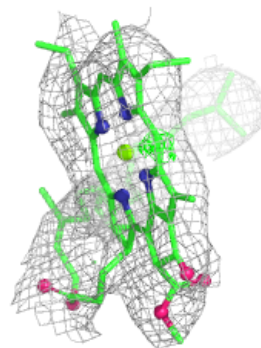
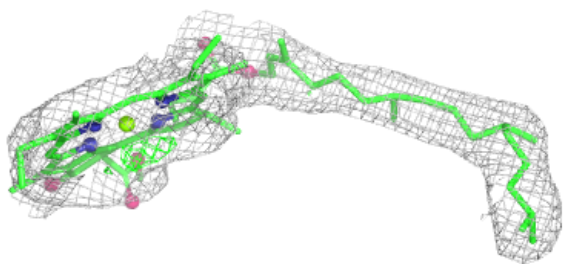
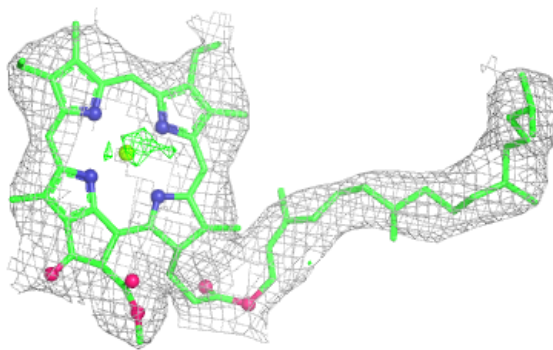
Electron density around CLA B 806:

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



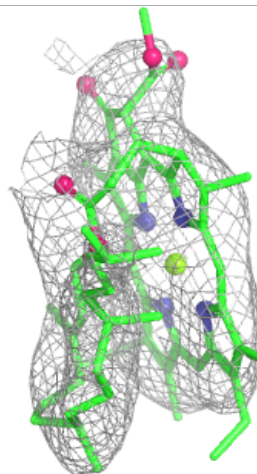
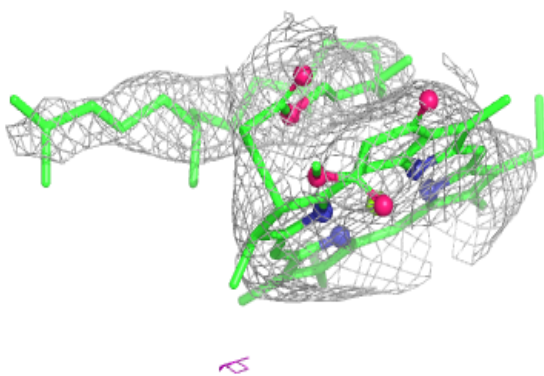
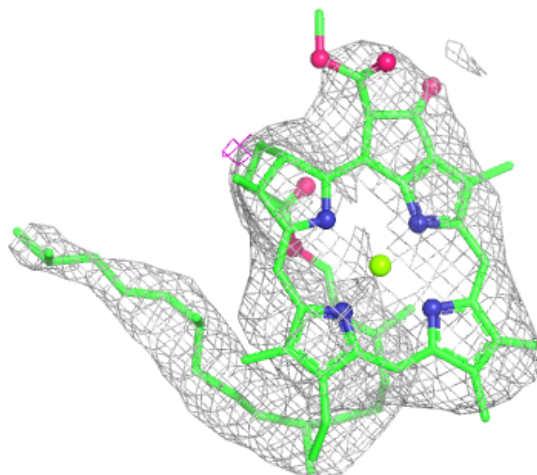
Electron density around CLA A 802:

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



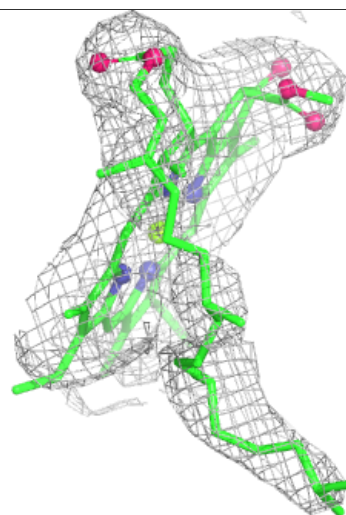
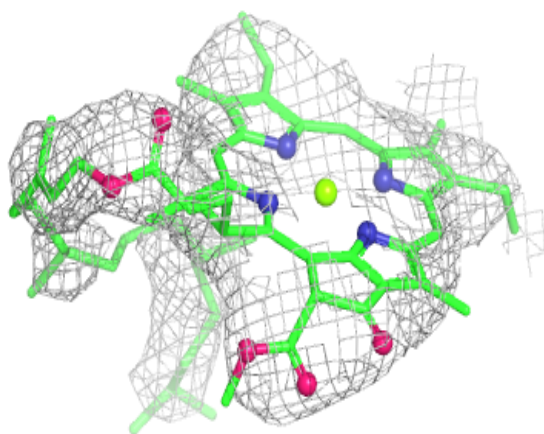
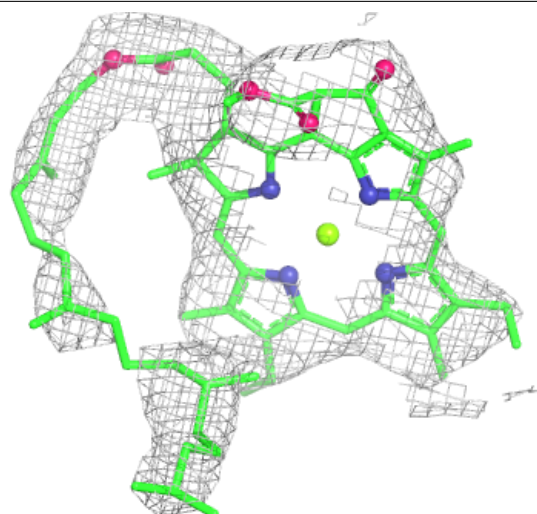
Electron density around CLA B 809:

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



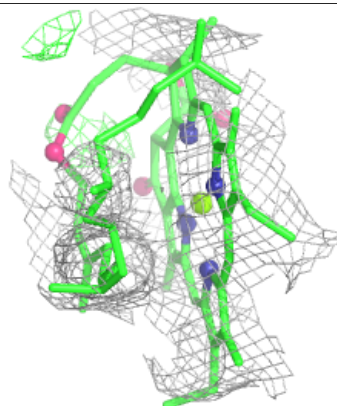
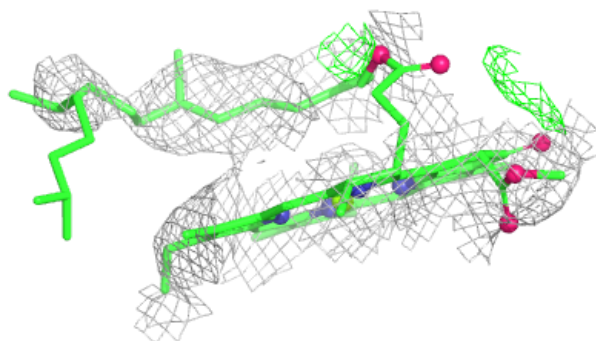
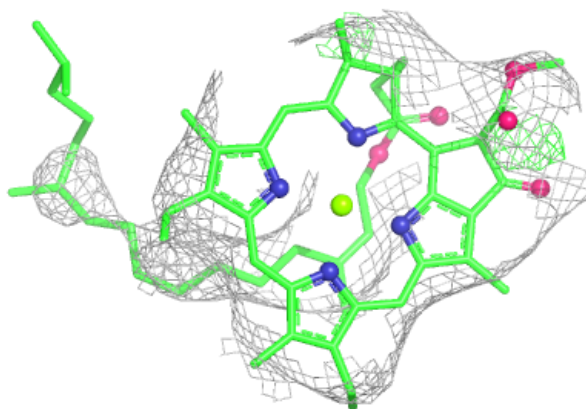
Electron density around CLA A 812:

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

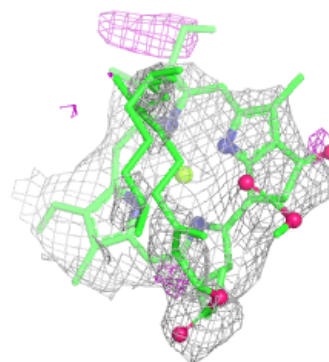
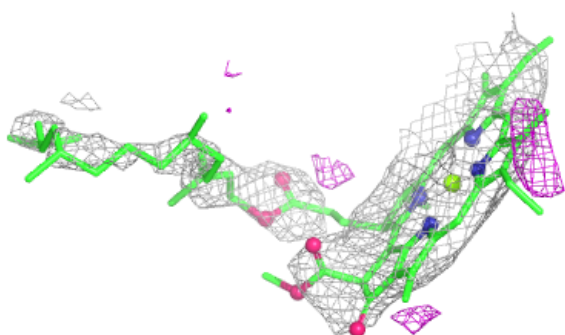
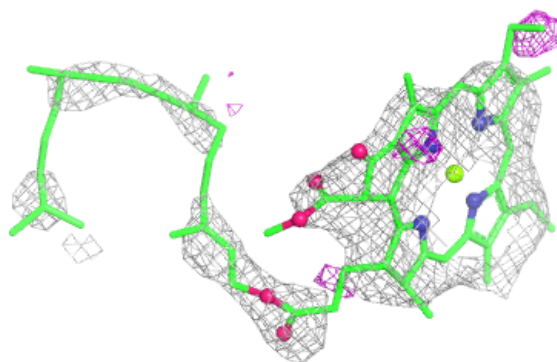


Electron density around CLA 4 307:

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

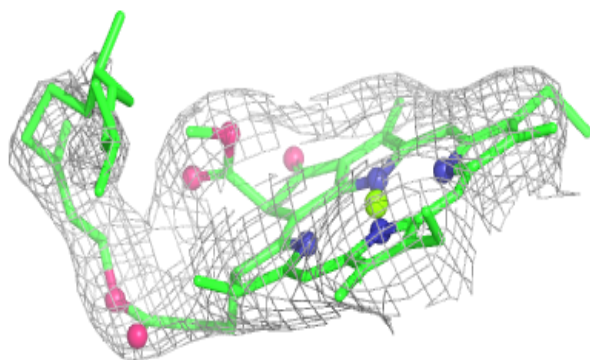
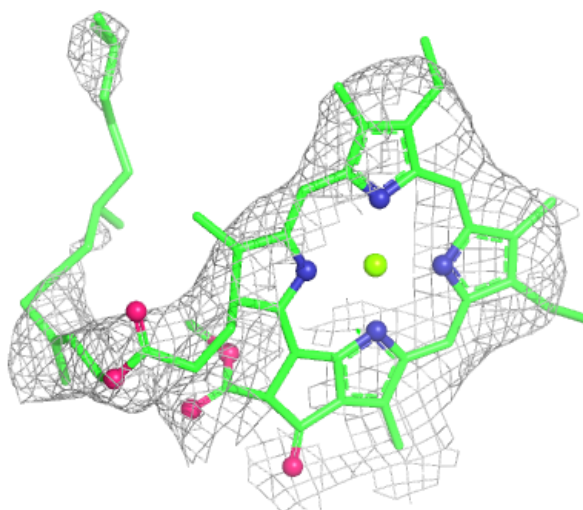
**Electron density around CL0 A 801:**

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



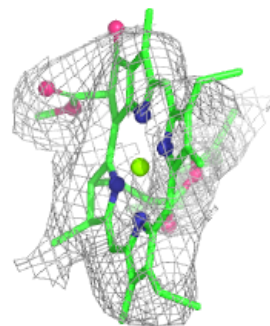
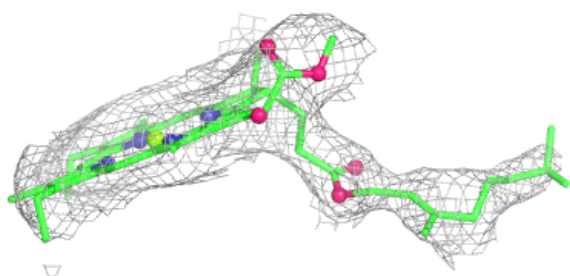
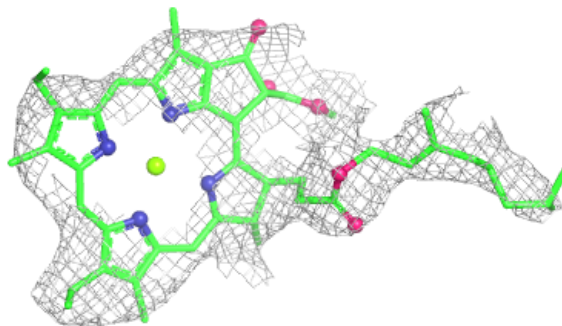
Electron density around CLA 4 309:

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



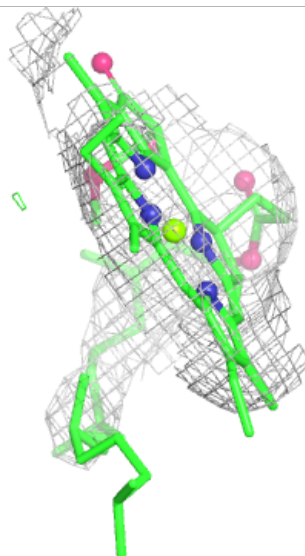
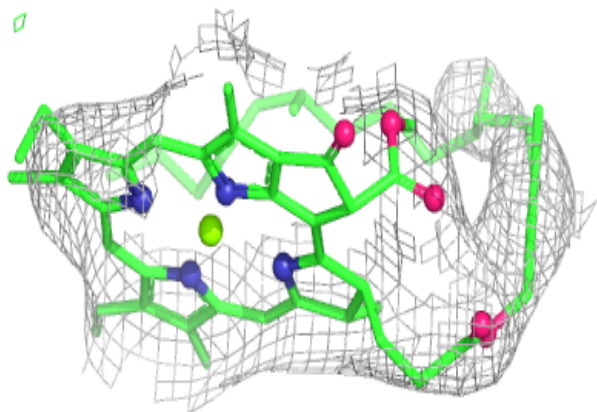
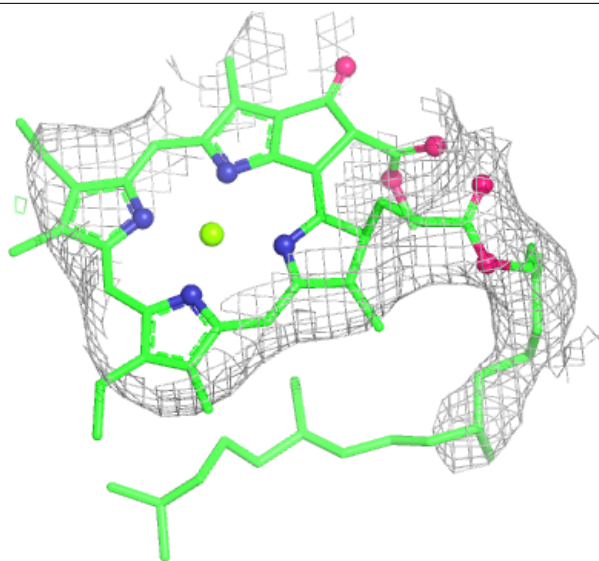
Electron density around CLA B 824:

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



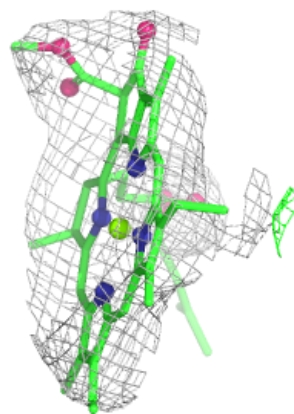
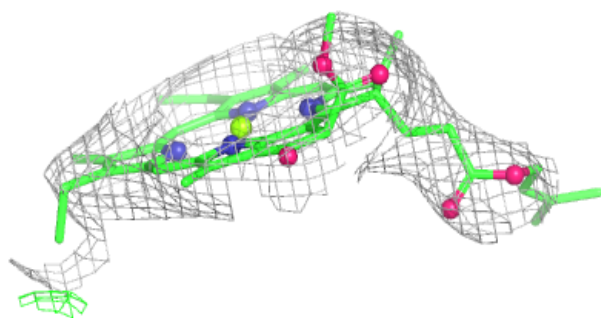
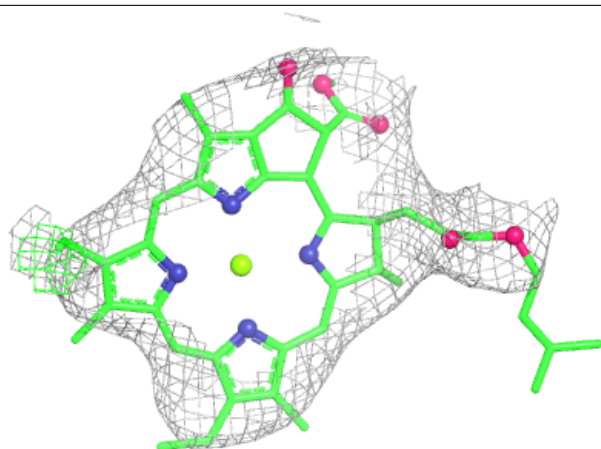
Electron density around CLA 1 5010:

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



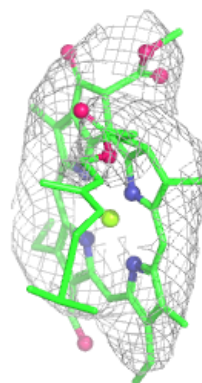
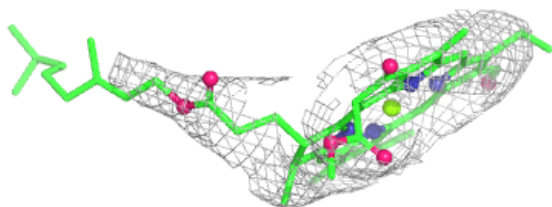
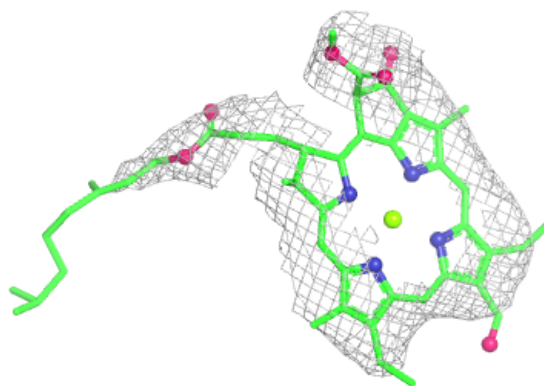
Electron density around CLA 2 326:

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



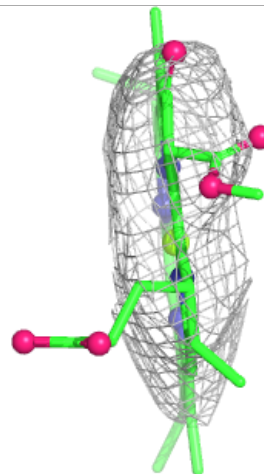
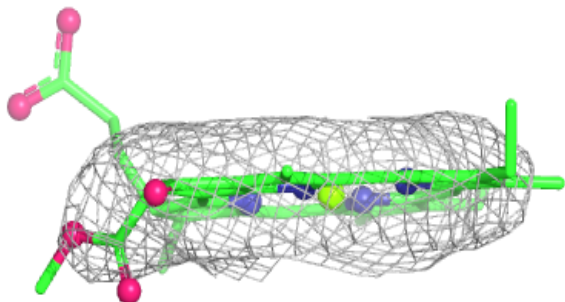
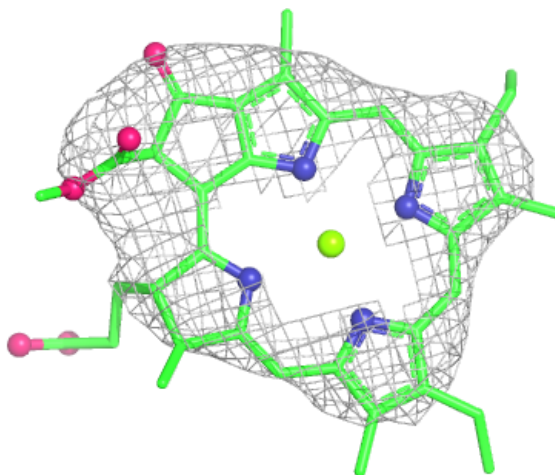
Electron density around CHL 4 318:

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



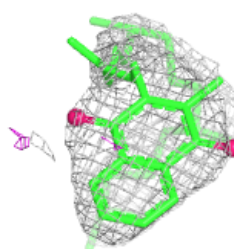
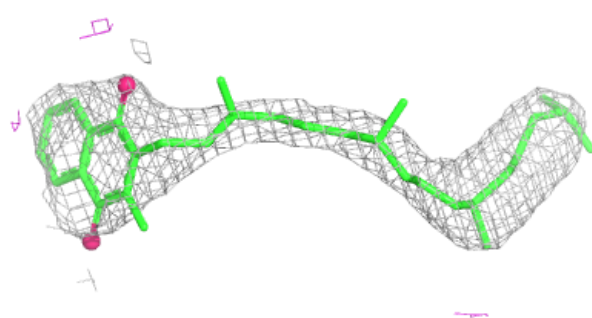
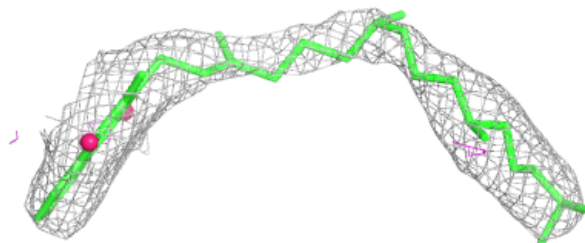
Electron density around CLA 3 301:

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

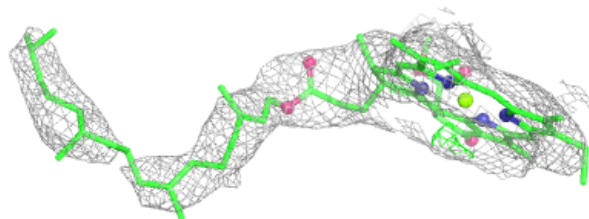
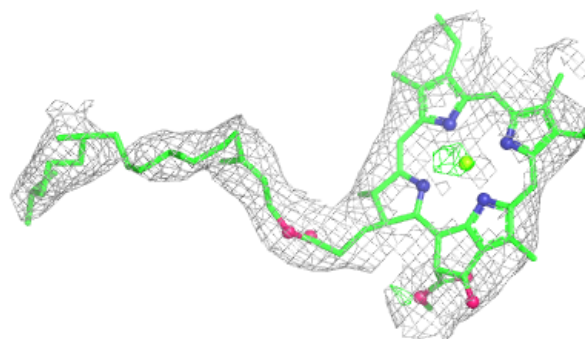


Electron density around PQN B 842:

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

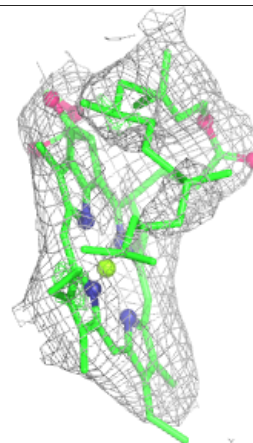
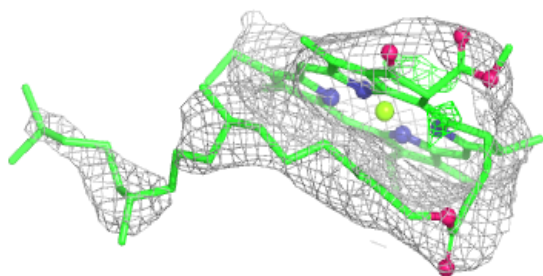
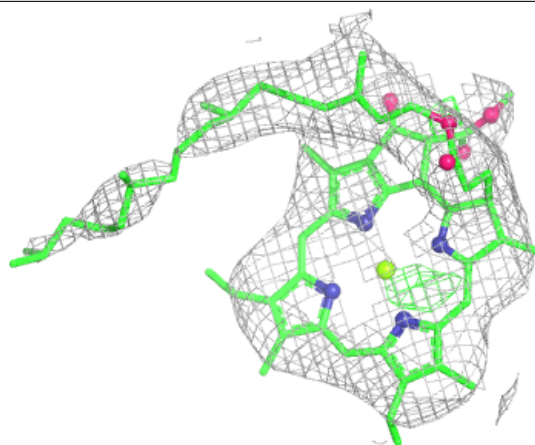
**Electron density around CLA B 814:**

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



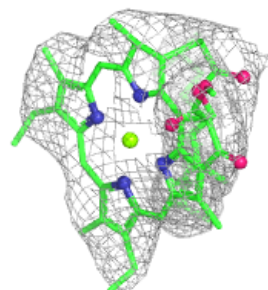
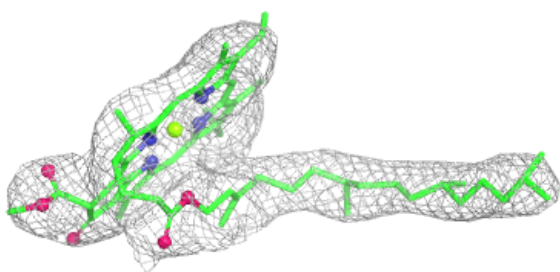
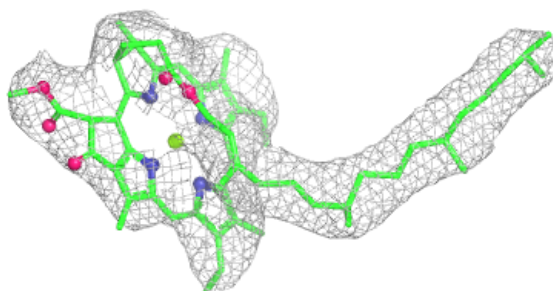
Electron density around CLA A 827:

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

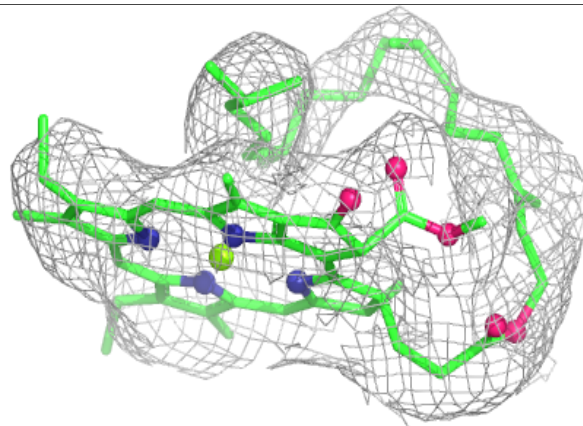
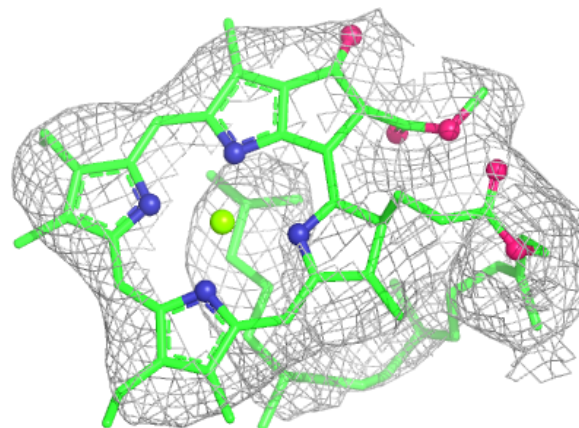


Electron density around CLA A 839:

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

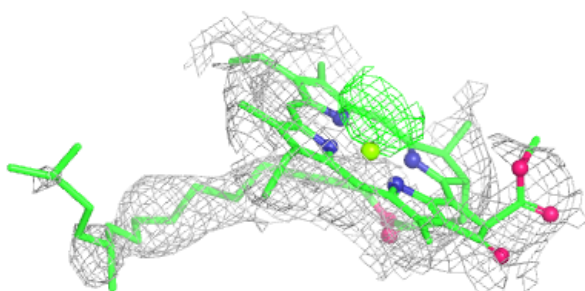
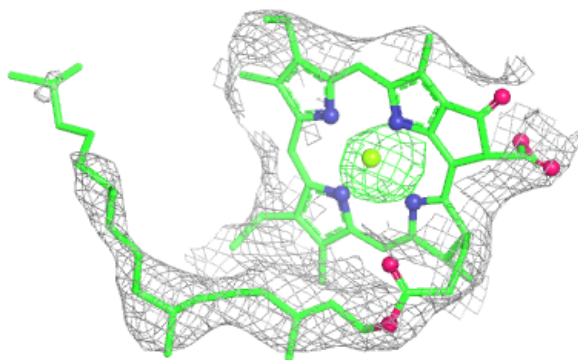
**Electron density around CLA B 807:**

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

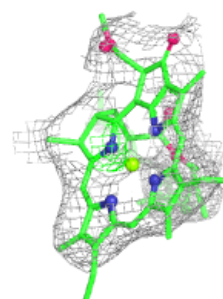
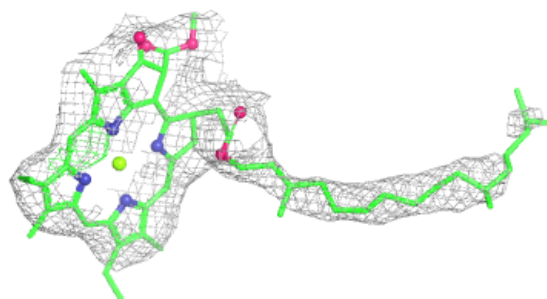


Electron density around CLA 2 309:

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

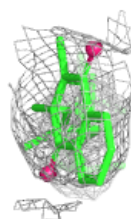
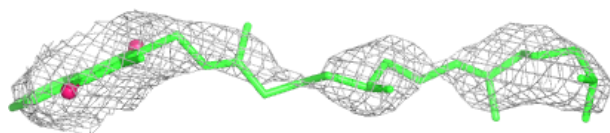
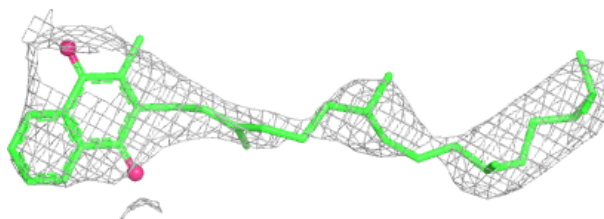
**Electron density around CLA A 819:**

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

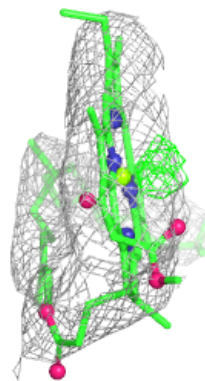
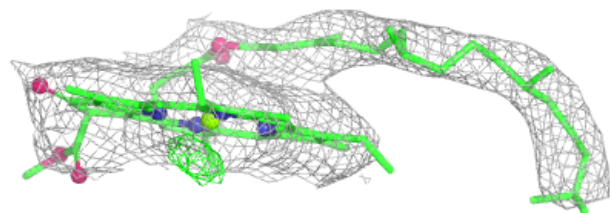
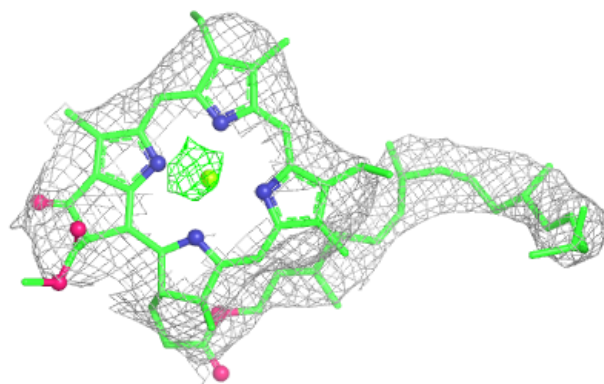


Electron density around PQN A 841:

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

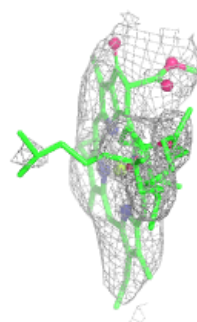
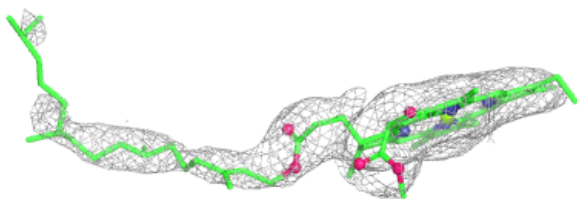
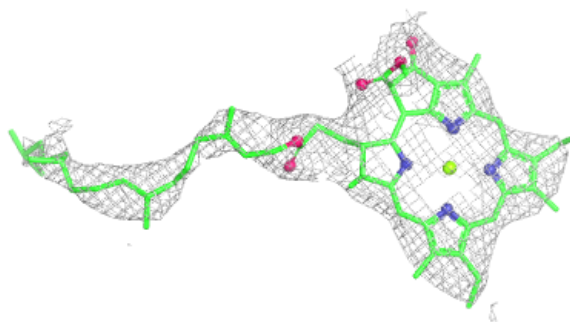
**Electron density around CLA B 819:**

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



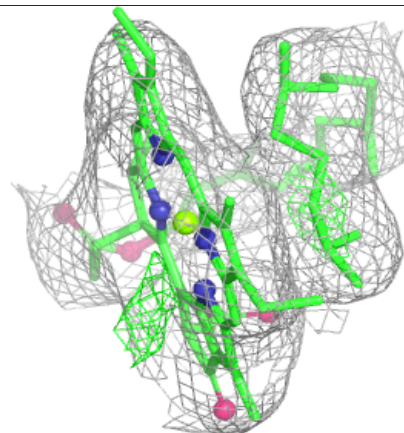
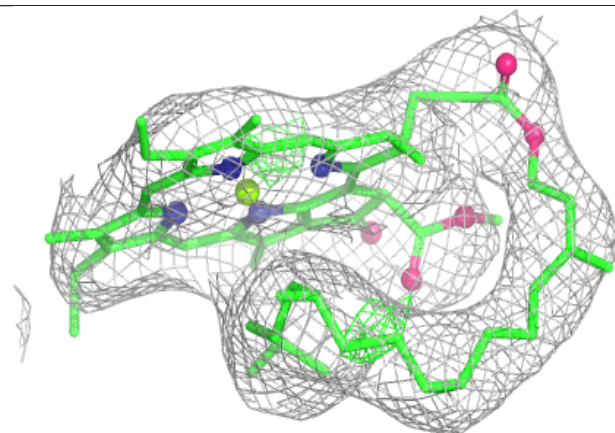
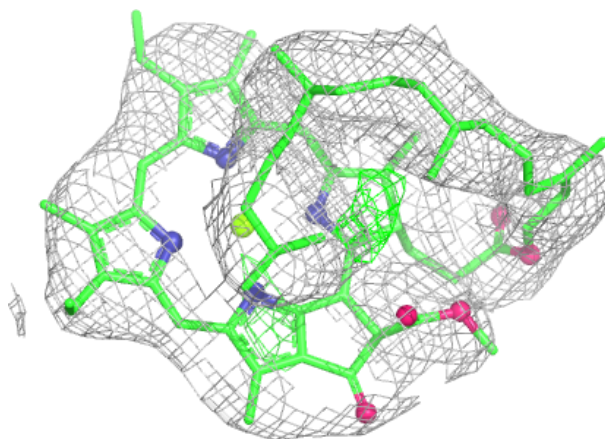
Electron density around CLA A 804:

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



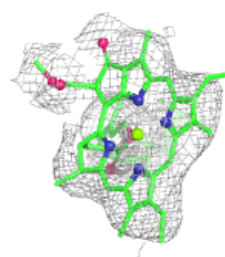
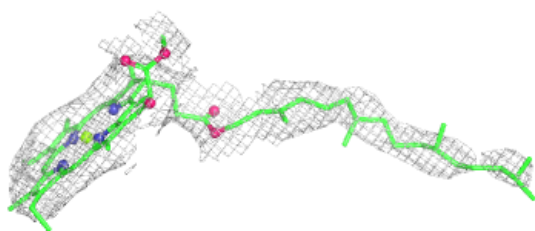
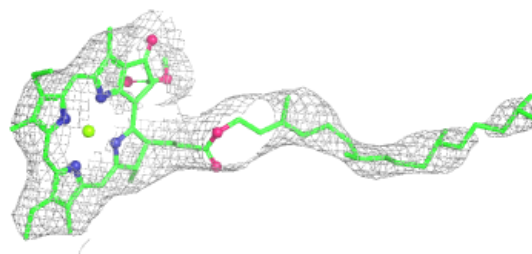
Electron density around CLA A 805:

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

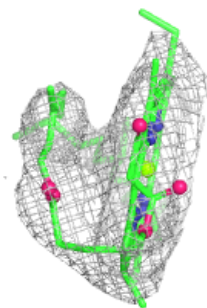
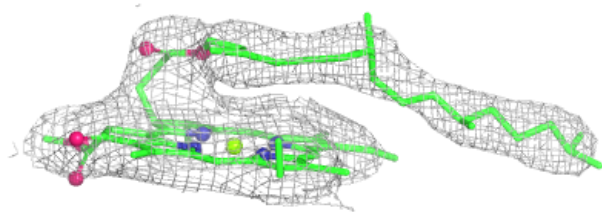
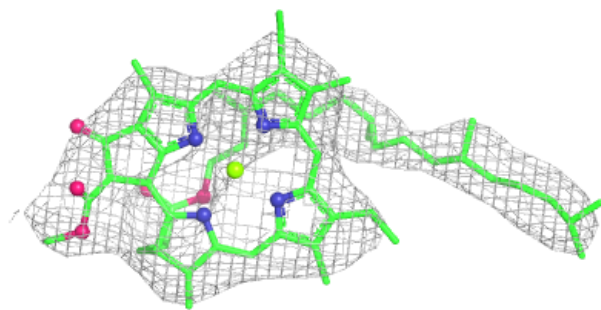


Electron density around CLA A 808:

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

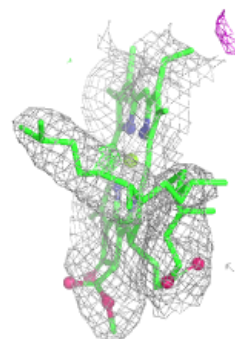
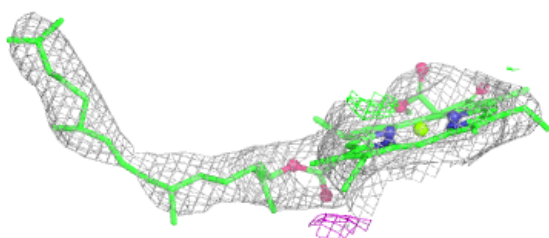
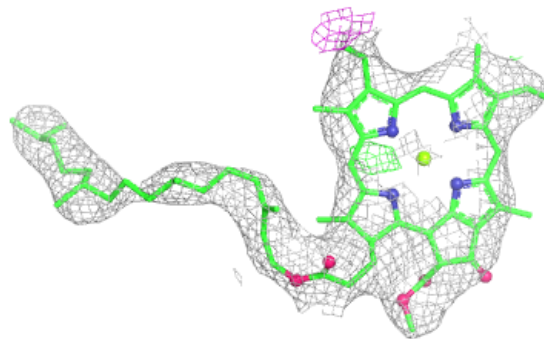
**Electron density around CLA A 837:**

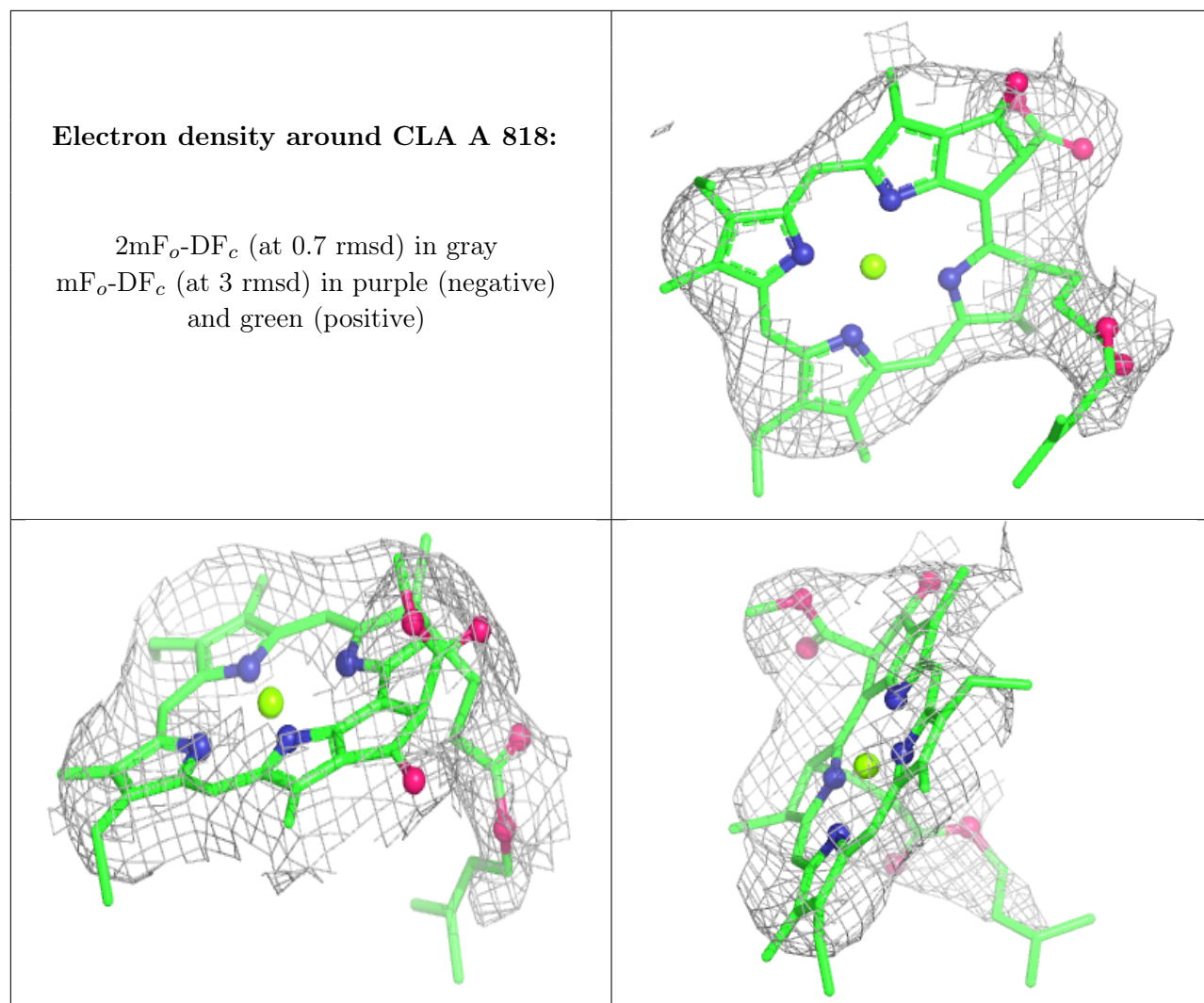
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 804:

$2mF_o-DF_c$ (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.