



wwPDB X-ray Structure Validation Summary Report ⓘ

May 7, 2026 – 09:05 AM EDT

PDB ID : 7M75 / pdb_00007m75
Title : Room Temperature XFEL Crystallography reveals asymmetry in the vicinity of the two phylloquinones in Photosystem I
Authors : Keable, S.M.; Simon, P.S.; Kolsch, A.; Kern, J.; Yachandra, V.K.; Zouni, A.; Yano, J.
Deposited on : 2021-03-26
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

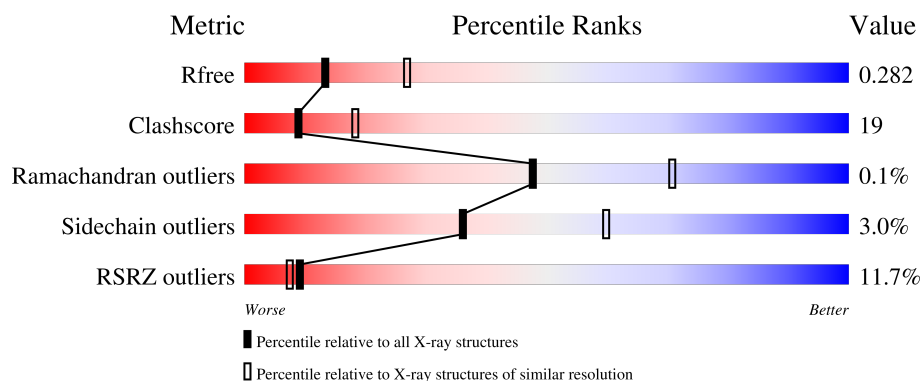
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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

Mol	Chain	Length	Quality of chain
1	A	755	16% 62% 35% ..
2	B	740	9% 69% 29% .
3	C	80	2% 56% 42% .
4	D	138	5% 74% 24% .

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Mol	Chain	Length	Quality of chain
5	E	75	
6	F	164	
7	I	38	
8	J	41	
9	K	83	
10	L	154	
11	M	31	
12	X	35	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CL0	A	801	X	-	-	-
14	CLA	A	802	X	-	-	-
14	CLA	A	803	X	-	-	-
14	CLA	A	804	X	-	-	-
14	CLA	A	805	X	-	-	-
14	CLA	A	806	X	-	-	-
14	CLA	A	807	X	-	-	-
14	CLA	A	808	X	-	-	-
14	CLA	A	809	X	-	-	-
14	CLA	A	810	X	-	-	-
14	CLA	A	811	X	-	-	-
14	CLA	A	812	X	-	-	-
14	CLA	A	813	X	-	-	-
14	CLA	A	814	X	-	-	-
14	CLA	A	815	X	-	-	-
14	CLA	A	816	X	-	-	-
14	CLA	A	817	X	-	-	-
14	CLA	A	818	X	-	-	-
14	CLA	A	819	X	-	-	-
14	CLA	A	820	X	-	-	-
14	CLA	A	821	X	-	-	-
14	CLA	A	822	X	-	-	-
14	CLA	A	823	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	824	X	-	-	-
14	CLA	A	825	X	-	-	-
14	CLA	A	826	X	-	-	-
14	CLA	A	827	X	-	-	-
14	CLA	A	828	X	-	-	-
14	CLA	A	829	X	-	-	-
14	CLA	A	830	X	-	-	-
14	CLA	A	831	X	-	-	-
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	839	X	-	-	-
14	CLA	A	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	842	X	-	-	-
14	CLA	A	843	X	-	-	-
14	CLA	A	844	X	-	-	-
14	CLA	A	845	X	-	-	-
14	CLA	A	856	X	-	-	-
14	CLA	B	3003	X	-	-	-
14	CLA	B	3004	X	-	-	-
14	CLA	B	3005	X	-	-	-
14	CLA	B	3006	X	-	-	-
14	CLA	B	3007	X	-	-	-
14	CLA	B	3008	X	-	-	-
14	CLA	B	3009	X	-	-	-
14	CLA	B	3010	X	-	-	-
14	CLA	B	3011	X	-	-	-
14	CLA	B	3012	X	-	-	-
14	CLA	B	3013	X	-	-	-
14	CLA	B	3014	X	-	-	-
14	CLA	B	3015	X	-	-	-
14	CLA	B	3016	X	-	-	-
14	CLA	B	3017	X	-	-	-
14	CLA	B	3018	X	-	-	-
14	CLA	B	3019	X	-	-	-
14	CLA	B	3020	X	-	-	-
14	CLA	B	3021	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	3022	X	-	-	-
14	CLA	B	3023	X	-	-	-
14	CLA	B	3024	X	-	-	-
14	CLA	B	3026	X	-	-	-
14	CLA	B	3027	X	-	-	-
14	CLA	B	3028	X	-	-	-
14	CLA	B	3029	X	-	-	-
14	CLA	B	3030	X	-	-	-
14	CLA	B	3031	X	-	-	-
14	CLA	B	3032	X	-	-	-
14	CLA	B	3033	X	-	-	-
14	CLA	B	3034	X	-	-	-
14	CLA	B	3035	X	-	-	-
14	CLA	B	3036	X	-	-	-
14	CLA	B	3037	X	-	-	-
14	CLA	B	3038	X	-	-	-
14	CLA	B	3039	X	-	-	-
14	CLA	B	3041	X	-	-	-
14	CLA	F	202	X	-	-	-
14	CLA	I	101	X	-	-	-
14	CLA	J	101	X	-	-	-
14	CLA	J	102	X	-	-	-
14	CLA	K	101	X	-	-	-
14	CLA	K	103	X	-	-	-
14	CLA	L	203	X	-	-	-
14	CLA	L	204	X	-	-	-
14	CLA	L	205	X	-	-	-
14	CLA	M	102	X	-	-	-
14	CLA	X	1701	X	-	-	-

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 48896 atoms, of which 24384 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	740	Total	C	H	N	O	S	0	0	0
			11422	3794	5638	988	976	26			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	739	Total	C	H	N	O	S	0	0	0
			11507	3876	5618	987	1005	21			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	80	Total	C	H	N	O	S	0	0	0
			1174	367	576	103	117	11			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	138	Total	C	H	N	O	S	0	0	0
			2152	682	1077	186	204	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	69	Total	C	H	N	O	0	0	0
			1067	342	528	93	104			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	F	141	Total	C	H	N	O	S	0	0	0
			2141	680	1076	184	197	4			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	I	38	Total	C	H	N	O	S	0	0	0
			607	208	306	40	48	5			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	J	41	Total	C	H	N	O	S	0	0	0
			685	231	347	51	54	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
9	K	47	Total	C	H	N	O	S	0	0	0
			687	217	354	58	57	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
10	L	151	Total	C	H	N	O	S	0	0	0
			2244	735	1125	179	201	4			

There is a discrepancy between the modelled and reference sequences:

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

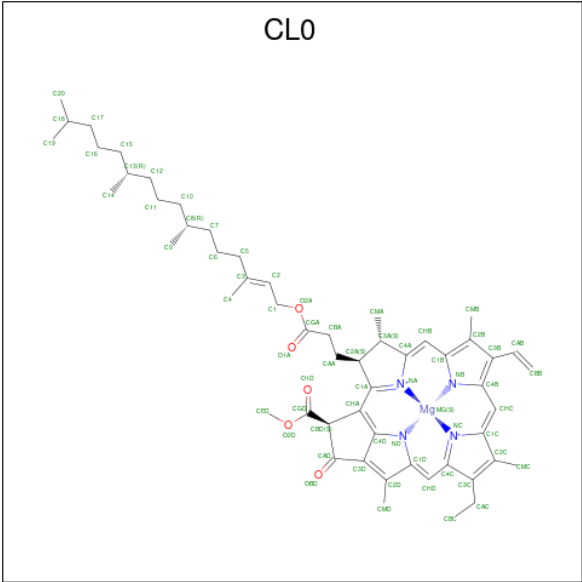
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
11	M	31	Total	C	H	N	O	S	0	0	0
			505	161	264	36	43	1			

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

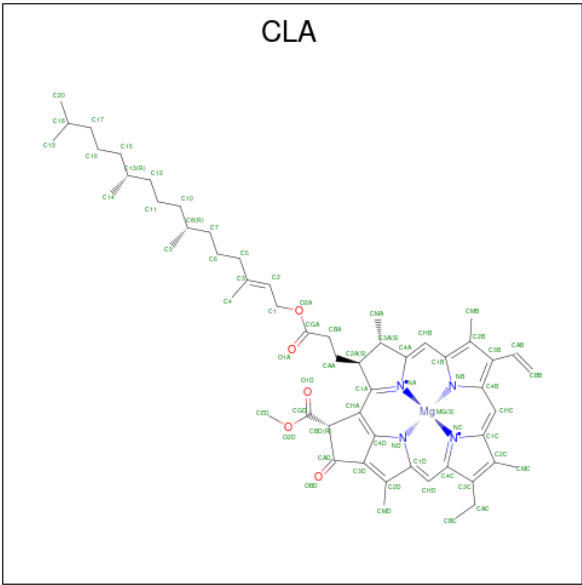
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
12	X	29	Total	C	H	N	O		0	0	0
			459	172	217	35	35				

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	Mg	N	O		
13	A	1	137	55	72	1	4	5	0	0

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	Mg	N	O		
14	A	1	137	55	72	1	4	5	0	0
14	A	1	137	55	72	1	4	5	0	0
14	A	1	137	55	72	1	4	5	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	A	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			92	41	41	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			88	39	39	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			72	35	29	1	4	3		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			88	39	39	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			92	41	41	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			89	40	39	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			92	41	41	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			82	37	35	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			92	41	41	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			95	42	43	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			104	45	49	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			82	37	35	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			104	45	49	1	4	5		

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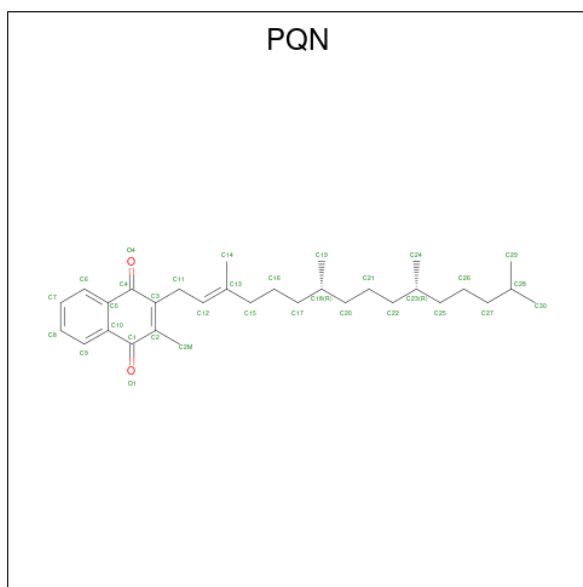
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
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			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			79	36	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			88	39	39	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			113	48	55	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			82	37	35	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	F	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	I	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	J	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		

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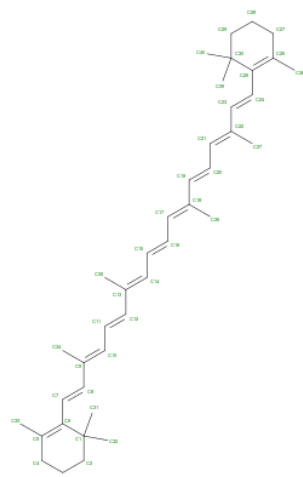
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	J	1	Total	C	H	Mg	N	O	0	0
			62	31	25	1	4	1		
14	K	1	Total	C	H	Mg	N	O	0	0
			70	33	29	1	4	3		
14	K	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	L	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	L	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	L	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	M	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	X	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	A	1	Total	C	H	O	0	0
			79	31	46	2		
15	B	1	Total	C	H	O	0	0
			79	31	46	2		

- Molecule 16 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).

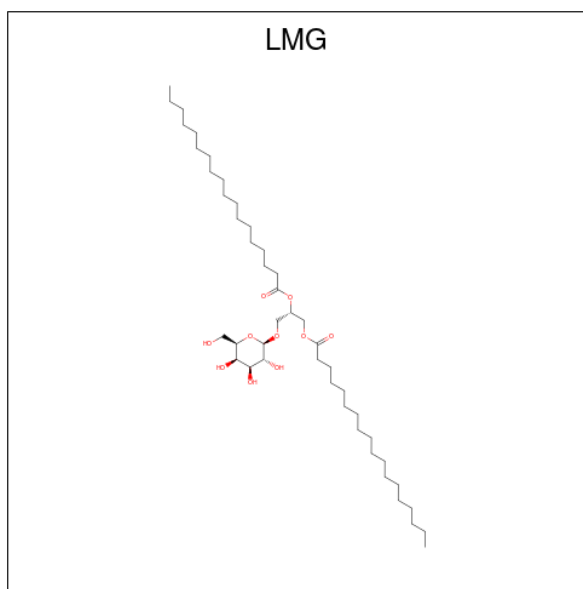


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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	I	1	Total	C	H	0	0
			96	40	56		
16	I	1	Total	C	H	0	0
			96	40	56		
16	J	1	Total	C	H	0	0
			96	40	56		
16	J	1	Total	C	H	0	0
			96	40	56		
16	J	1	Total	C	H	0	0
			96	40	56		
16	K	1	Total	C	H	0	0
			96	40	56		
16	L	1	Total	C	H	0	0
			96	40	56		
16	M	1	Total	C	H	0	0
			96	40	56		

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



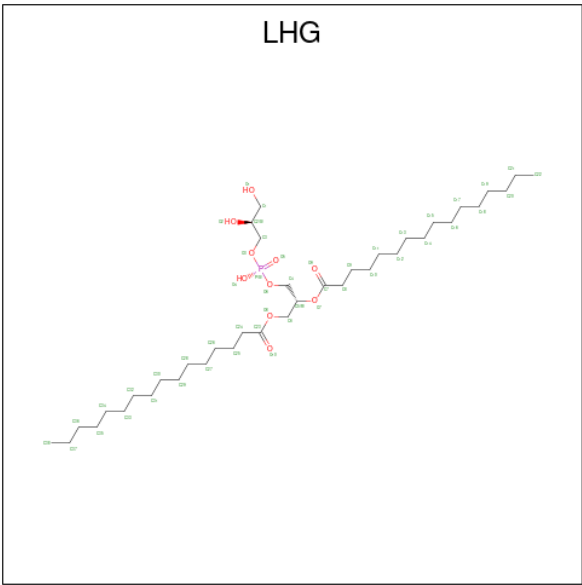
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	H	O	0	0
			118	38	70	10		
17	A	1	Total	C	H	O	0	0
			67	22	37	8		
17	B	1	Total	C	H	O	0	0
			141	45	86	10		

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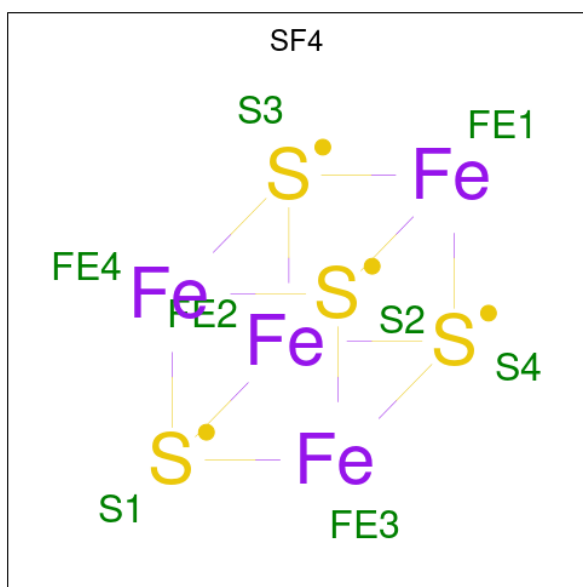
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	I	1	Total	C	H	O	0	0
			91	30	51	10		

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
18	A	1	Total	C	H	O	P	0	0
			53	16	26	10	1		
18	B	1	Total	C	H	O	P	0	0
			43	12	20	10	1		
18	M	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 19 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

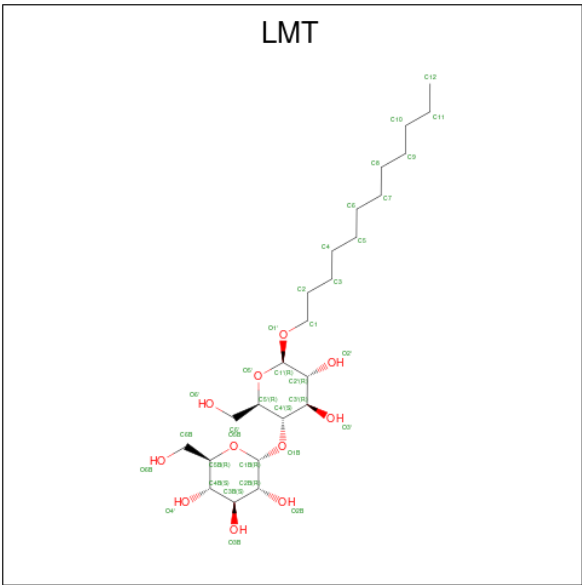


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	B	1	Total	Fe	S	0	0
			8	4	4		
19	C	1	Total	Fe	S	0	0
			8	4	4		
19	C	1	Total	Fe	S	0	0
			8	4	4		

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

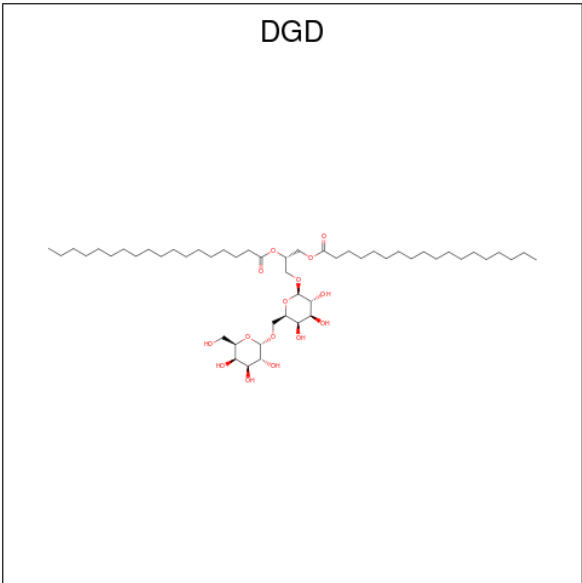
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	B	1	Total	Ca	0	0
			1	1		
20	L	1	Total	Ca	0	0
			1	1		

- Molecule 21 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	L	1	Total	C	H	O	0	0
			81	24	46	11		

- Molecule 22 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	L	1	Total	C	H	O	0	0
			162	51	96	15		

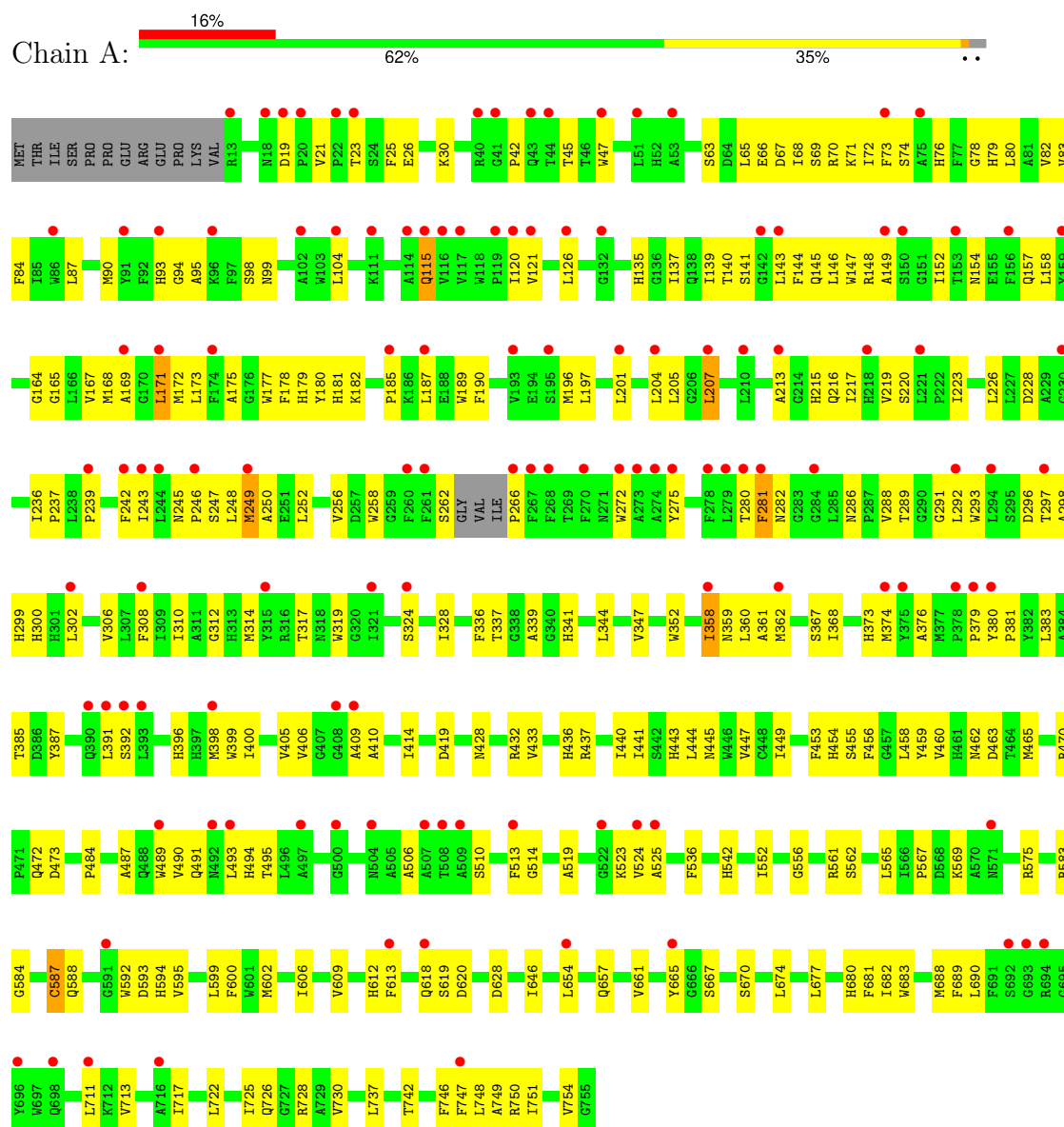
- Molecule 23 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	30	Total 30	O 30	0	0
23	B	41	Total 41	O 41	0	0
23	C	11	Total 11	O 11	0	0
23	D	14	Total 14	O 14	0	0
23	E	1	Total 1	O 1	0	0
23	F	2	Total 2	O 2	0	0
23	I	3	Total 3	O 3	0	0
23	J	1	Total 1	O 1	0	0
23	L	15	Total 15	O 15	0	0
23	M	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

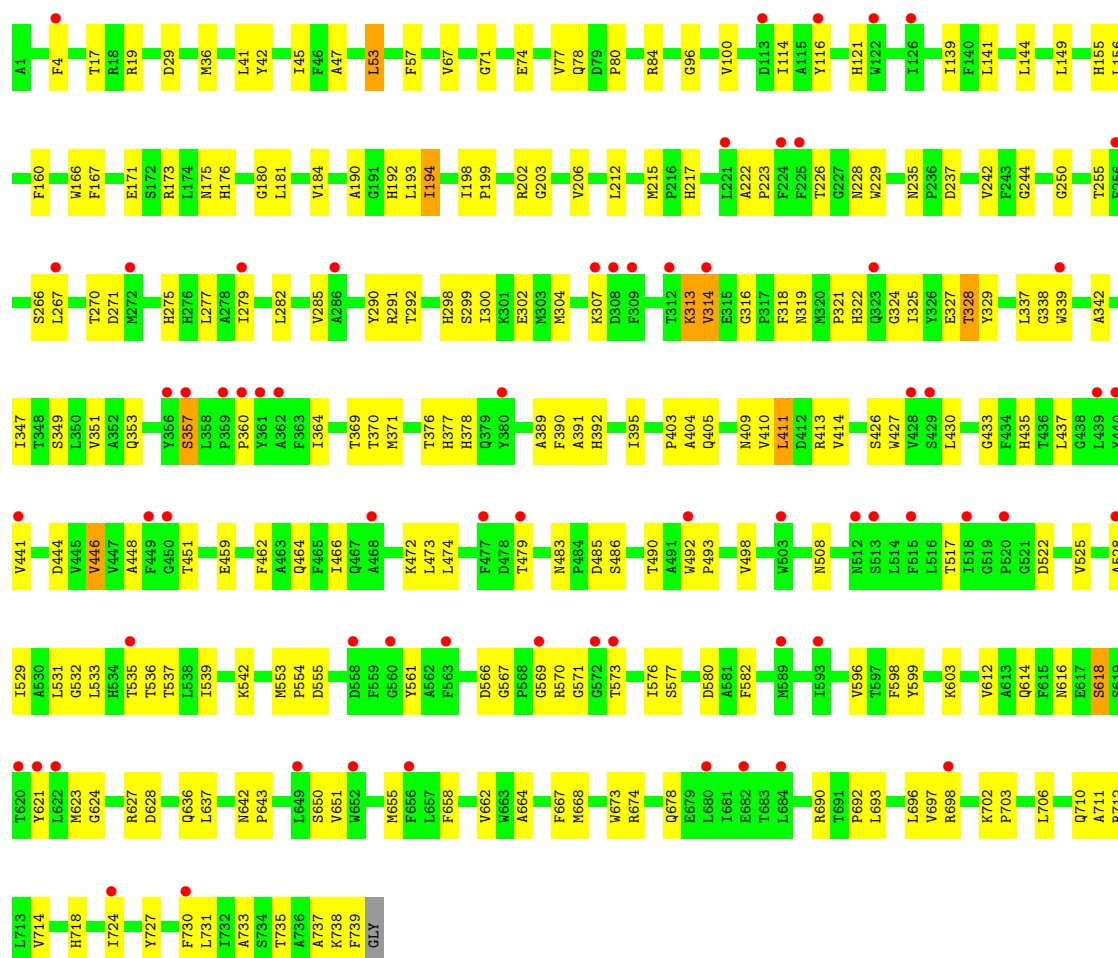
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

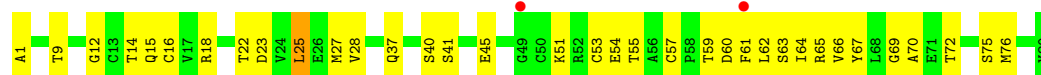


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





• Molecule 3: Photosystem I iron-sulfur center

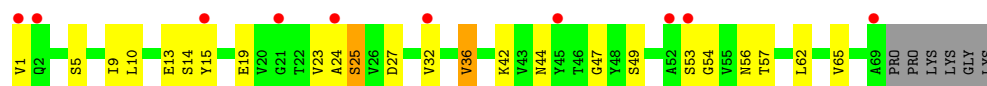


• Molecule 4: Photosystem I reaction center subunit II

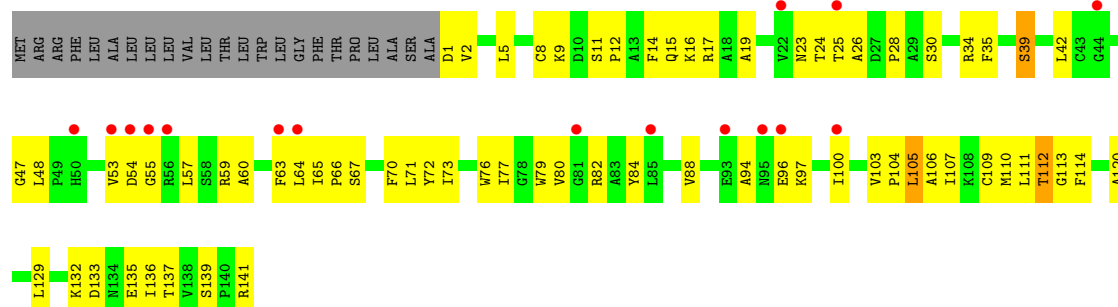


• Molecule 5: Photosystem I reaction center subunit IV

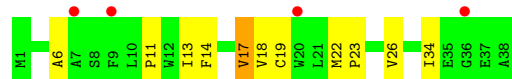




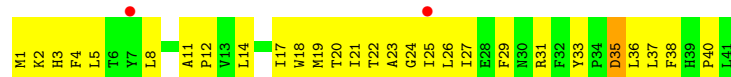
• Molecule 6: Photosystem I reaction center subunit III



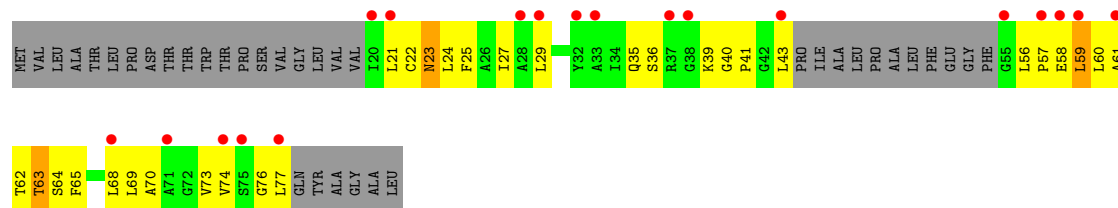
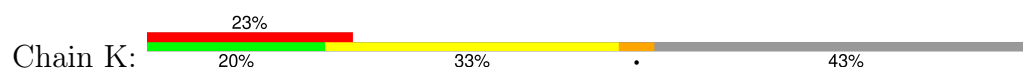
• Molecule 7: Photosystem I reaction center subunit VIII



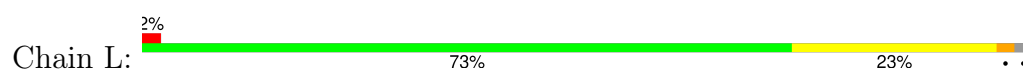
• Molecule 8: Photosystem I reaction center subunit IX



• Molecule 9: Photosystem I reaction center subunit Psak



• Molecule 10: Photosystem I reaction center subunit XI





● Molecule 11: Photosystem I reaction center subunit XII



● Molecule 12: Photosystem I 4.8K protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	285.43Å 285.43Å 166.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	56.71 – 2.75 56.71 – 2.75	Depositor EDS
% Data completeness (in resolution range)	95.0 (56.71-2.75) 91.4 (56.71-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.16 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.264 , 0.279 0.268 , 0.282	Depositor DCC
R_{free} test set	2009 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 84.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	48896	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.28	0/5983	0.52	1/8158 (0.0%)
2	B	0.27	0/6107	0.50	0/8345
3	C	0.26	0/608	0.52	0/824
4	D	0.22	0/1101	0.48	0/1492
5	E	0.22	0/551	0.48	0/750
6	F	0.28	0/1087	0.49	0/1476
7	I	0.27	0/312	0.68	0/425
8	J	0.33	0/350	0.58	0/477
9	K	0.28	0/337	0.66	0/454
10	L	0.27	0/1148	0.53	0/1558
11	M	0.32	0/244	0.58	0/332
12	X	0.30	0/251	0.49	0/342
All	All	0.27	0/18079	0.51	1/24633 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	MET	CA-CB-CG	5.33	124.75	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5784	5638	5639	306	0
2	B	5889	5618	5649	216	0
3	C	598	576	580	37	0
4	D	1075	1077	1077	30	0
5	E	539	528	528	18	0
6	F	1065	1076	1077	79	0
7	I	301	306	306	15	0
8	J	338	347	347	53	0
9	K	333	354	354	47	0
10	L	1119	1125	1125	30	0
11	M	241	264	264	12	0
12	X	242	217	249	14	0
13	A	65	72	72	2	0
14	A	2628	2615	2615	99	0
14	B	2219	2160	2160	75	0
14	F	45	33	33	8	0
14	I	65	72	72	8	0
14	J	82	58	58	0	0
14	K	86	62	62	3	0
14	L	195	216	216	4	0
14	M	45	33	33	3	0
14	X	45	33	33	2	0
15	A	33	46	46	7	0
15	B	33	46	46	3	0
16	A	200	280	280	16	0
16	B	240	336	336	13	0
16	F	80	112	112	8	0
16	I	120	168	168	8	0
16	J	120	168	168	13	0
16	K	40	56	56	4	0
16	L	40	56	56	2	0
16	M	40	56	56	2	0
17	A	78	107	105	0	0
17	B	55	86	86	1	0
17	I	40	51	50	0	0
18	A	76	100	98	4	0
18	B	23	20	16	2	0
18	M	49	74	74	1	0
19	B	8	0	0	0	0
19	C	16	0	0	0	0
20	B	1	0	0	0	0
20	L	1	0	0	0	0
21	L	35	46	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	L	66	96	96	2	0
23	A	30	0	0	5	0
23	B	41	0	0	5	0
23	C	11	0	0	2	0
23	D	14	0	0	1	0
23	E	1	0	0	0	0
23	F	2	0	0	0	0
23	I	3	0	0	2	0
23	J	1	0	0	0	0
23	L	15	0	0	0	0
23	M	1	0	0	0	0
All	All	24512	24384	24444	905	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 19.

The worst 5 of 905 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)
4:D:32:THR:OG1	4:D:79:ASP:OD2	1.81	0.98
4:D:3:LEU:HD21	4:D:91:THR:HG21	1.47	0.95
2:B:307:LYS:O	2:B:314:VAL:HG23	1.68	0.93
9:K:60:LEU:O	9:K:63:THR:OG1	1.87	0.93
1:A:661:VAL:HG21	1:A:746:PHE:HA	1.51	0.91

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	736/755 (98%)	678 (92%)	58 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	737/740 (100%)	684 (93%)	52 (7%)	1 (0%)	48	71
3	C	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
4	D	136/138 (99%)	123 (90%)	13 (10%)	0	100	100
5	E	67/75 (89%)	55 (82%)	11 (16%)	1 (2%)	8	15
6	F	139/164 (85%)	124 (89%)	15 (11%)	0	100	100
7	I	36/38 (95%)	29 (81%)	7 (19%)	0	100	100
8	J	39/41 (95%)	35 (90%)	4 (10%)	0	100	100
9	K	43/83 (52%)	35 (81%)	8 (19%)	0	100	100
10	L	149/154 (97%)	140 (94%)	9 (6%)	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100
12	X	27/35 (77%)	26 (96%)	1 (4%)	0	100	100
All	All	2216/2334 (95%)	2031 (92%)	183 (8%)	2 (0%)	48	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	25	SER
2	B	194	ILE

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	589/603 (98%)	578 (98%)	11 (2%)	50	70
2	B	597/597 (100%)	582 (98%)	15 (2%)	42	64
3	C	67/67 (100%)	64 (96%)	3 (4%)	24	46
4	D	115/115 (100%)	110 (96%)	5 (4%)	26	47
5	E	59/64 (92%)	56 (95%)	3 (5%)	21	40
6	F	109/128 (85%)	103 (94%)	6 (6%)	19	37
7	I	32/32 (100%)	30 (94%)	2 (6%)	16	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	J	36/36 (100%)	35 (97%)	1 (3%)	38 61
9	K	33/61 (54%)	30 (91%)	3 (9%)	9 17
10	L	117/119 (98%)	112 (96%)	5 (4%)	26 47
11	M	26/26 (100%)	26 (100%)	0	100 100
12	X	23/27 (85%)	23 (100%)	0	100 100
All	All	1803/1875 (96%)	1749 (97%)	54 (3%)	36 60

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	45	GLU
5	E	36	VAL
10	L	83	ILE
4	D	3	LEU
4	D	118	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	228	ASN
10	L	102	GLN
2	B	467	GLN
10	L	141	ASN
6	F	134	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 135 ligands modelled in this entry, 2 are monoatomic - leaving 133 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
14	CLA	J	102	-	41,45,73	1.51	6 (14%)	50,78,113	1.33	6 (12%)
14	CLA	L	204	-	69,73,73	1.16	8 (11%)	82,113,113	1.33	5 (6%)
14	CLA	A	811	-	49,53,73	1.41	8 (16%)	58,89,113	1.39	6 (10%)
14	CLA	B	3024	-	49,53,73	1.39	9 (18%)	58,89,113	1.42	6 (10%)
14	CLA	A	822	23	69,73,73	1.19	6 (8%)	82,113,113	1.19	6 (7%)
14	CLA	B	3036	23	49,53,73	1.43	6 (12%)	58,89,113	1.41	4 (6%)
14	CLA	B	3034	-	62,66,73	1.24	6 (9%)	73,104,113	1.34	7 (9%)
14	CLA	A	839	-	69,73,73	1.16	7 (10%)	82,113,113	1.37	7 (8%)
14	CLA	B	3032	-	53,57,73	1.34	8 (15%)	61,93,113	1.41	10 (16%)
14	CLA	B	3005	-	58,62,73	1.31	5 (8%)	68,99,113	1.41	4 (5%)
16	BCR	A	849	-	41,41,41	1.13	3 (7%)	56,56,56	1.22	5 (8%)
14	CLA	A	809	1	69,73,73	1.17	6 (8%)	82,113,113	1.23	6 (7%)
14	CLA	B	3010	2	69,73,73	1.22	7 (10%)	82,113,113	1.38	9 (10%)
16	BCR	J	105	-	41,41,41	1.14	3 (7%)	56,56,56	1.31	8 (14%)
14	CLA	L	203	10	69,73,73	1.18	5 (7%)	82,113,113	1.47	7 (8%)
14	CLA	J	101	8	49,53,73	1.44	5 (10%)	58,89,113	1.33	4 (6%)
14	CLA	A	856	23	69,73,73	1.18	8 (11%)	82,113,113	1.28	6 (7%)
14	CLA	A	834	-	69,73,73	1.21	7 (10%)	82,113,113	1.21	4 (4%)
14	CLA	K	101	-	45,49,73	1.42	6 (13%)	54,83,113	1.35	4 (7%)
16	BCR	A	847	-	41,41,41	1.21	3 (7%)	56,56,56	1.23	6 (10%)
16	BCR	B	3047	-	41,41,41	1.14	3 (7%)	56,56,56	1.29	8 (14%)
15	PQN	B	3042	-	34,34,34	1.98	7 (20%)	43,45,45	1.23	5 (11%)
14	CLA	A	824	-	55,59,73	1.33	5 (9%)	64,96,113	1.31	6 (9%)
14	CLA	B	3031	-	49,53,73	1.41	6 (12%)	58,89,113	1.53	6 (10%)
14	CLA	B	3012	-	49,53,73	1.42	7 (14%)	58,89,113	1.48	7 (12%)
14	CLA	K	103	-	49,53,73	1.40	6 (12%)	58,89,113	1.37	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	M	102	23	49,53,73	1.49	10 (20%)	58,89,113	1.39	9 (15%)
14	CLA	A	803	-	69,73,73	1.20	7 (10%)	82,113,113	1.24	6 (7%)
14	CLA	B	3030	-	69,73,73	1.19	6 (8%)	82,113,113	1.27	7 (8%)
19	SF4	C	101	3	0,12,12	-	-	-	-	-
18	LHG	A	853	-	48,48,48	0.62	1 (2%)	51,54,54	1.24	4 (7%)
16	BCR	I	103	-	41,41,41	1.20	3 (7%)	56,56,56	1.40	7 (12%)
14	CLA	B	3029	-	69,73,73	1.18	7 (10%)	82,113,113	1.28	5 (6%)
16	BCR	B	3050	-	41,41,41	1.23	3 (7%)	56,56,56	1.26	7 (12%)
18	LHG	A	854	14	26,26,48	1.00	1 (3%)	29,32,54	1.31	3 (10%)
14	CLA	B	3017	-	59,63,73	1.29	7 (11%)	70,101,113	1.28	5 (7%)
14	CLA	A	812	14	69,73,73	1.20	8 (11%)	82,113,113	1.23	5 (6%)
14	CLA	B	3041	-	69,73,73	1.22	7 (10%)	82,113,113	1.34	5 (6%)
19	SF4	C	102	3	0,12,12	-	-	-	-	-
14	CLA	A	829	-	69,73,73	1.18	5 (7%)	82,113,113	1.17	4 (4%)
14	CLA	B	3025	2	58,62,73	1.32	6 (10%)	68,99,113	1.38	7 (10%)
14	CLA	A	825	-	63,67,73	1.27	5 (7%)	74,105,113	1.23	5 (6%)
16	BCR	I	105	-	41,41,41	1.18	3 (7%)	56,56,56	1.44	9 (16%)
14	CLA	B	3022	-	49,53,73	1.41	6 (12%)	58,89,113	1.37	5 (8%)
14	CLA	F	202	23	49,53,73	1.46	7 (14%)	58,89,113	1.29	5 (8%)
14	CLA	A	836	-	58,62,73	1.30	7 (12%)	68,99,113	1.32	5 (7%)
14	CLA	A	838	-	55,59,73	1.36	7 (12%)	64,96,113	1.30	5 (7%)
13	CL0	A	801	-	58,73,73	2.24	10 (17%)	60,113,113	1.59	14 (23%)
14	CLA	B	3013	-	49,53,73	1.42	5 (10%)	58,89,113	1.40	5 (8%)
14	CLA	A	806	-	69,73,73	1.18	6 (8%)	82,113,113	1.29	6 (7%)
16	BCR	M	103	-	41,41,41	1.19	3 (7%)	56,56,56	1.13	3 (5%)
14	CLA	A	843	-	69,73,73	1.20	7 (10%)	82,113,113	1.24	5 (6%)
14	CLA	B	3015	-	69,73,73	1.18	6 (8%)	82,113,113	1.22	4 (4%)
14	CLA	B	3037	23	49,53,73	1.43	5 (10%)	58,89,113	1.34	4 (6%)
14	CLA	A	835	-	69,73,73	1.15	6 (8%)	82,113,113	1.23	7 (8%)
16	BCR	A	850	-	41,41,41	1.13	3 (7%)	56,56,56	1.24	6 (10%)
14	CLA	A	813	-	58,62,73	1.29	6 (10%)	68,99,113	1.31	5 (7%)
14	CLA	A	805	14	63,67,73	1.27	7 (11%)	74,105,113	1.24	5 (6%)
14	CLA	B	3021	-	51,55,73	1.36	6 (11%)	60,91,113	1.39	4 (6%)
14	CLA	B	3023	23	59,63,73	1.29	7 (11%)	70,101,113	1.29	4 (5%)
14	CLA	B	3007	-	69,73,73	1.20	6 (8%)	82,113,113	1.27	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	833	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	3 (3%)
14	CLA	A	804	-	69,73,73	1.20	7 (10%)	82,113,113	1.15	4 (4%)
14	CLA	B	3039	-	69,73,73	1.19	6 (8%)	82,113,113	1.25	6 (7%)
14	CLA	A	818	-	58,62,73	1.31	6 (10%)	68,99,113	1.32	4 (5%)
14	CLA	B	3028	-	69,73,73	1.19	7 (10%)	82,113,113	1.19	5 (6%)
14	CLA	A	826	23	69,73,73	1.18	7 (10%)	82,113,113	1.24	6 (7%)
16	BCR	B	3043	-	41,41,41	1.15	3 (7%)	56,56,56	1.22	6 (10%)
14	CLA	A	816	-	49,53,73	1.40	5 (10%)	58,89,113	1.51	4 (6%)
14	CLA	X	1701	12	49,53,73	1.41	7 (14%)	58,89,113	1.46	5 (8%)
14	CLA	A	807	-	69,73,73	1.22	6 (8%)	82,113,113	1.18	4 (4%)
14	CLA	B	3018	-	63,67,73	1.23	6 (9%)	74,105,113	1.30	6 (8%)
14	CLA	B	3027	-	69,73,73	1.20	5 (7%)	82,113,113	1.20	5 (6%)
16	BCR	I	102	-	41,41,41	1.09	3 (7%)	56,56,56	1.36	8 (14%)
16	BCR	A	848	-	41,41,41	1.18	3 (7%)	56,56,56	1.29	6 (10%)
14	CLA	A	815	-	49,53,73	1.40	7 (14%)	58,89,113	1.36	5 (8%)
14	CLA	B	3016	-	49,53,73	1.40	7 (14%)	58,89,113	1.44	5 (8%)
16	BCR	A	851	-	41,41,41	1.16	3 (7%)	56,56,56	1.39	5 (8%)
14	CLA	B	3004	-	69,73,73	1.24	9 (13%)	82,113,113	1.29	8 (9%)
16	BCR	B	3044	-	41,41,41	1.17	3 (7%)	56,56,56	1.21	6 (10%)
14	CLA	A	845	18	56,60,73	1.32	5 (8%)	65,97,113	1.47	6 (9%)
14	CLA	A	841	-	69,73,73	1.18	5 (7%)	82,113,113	1.31	5 (6%)
14	CLA	L	205	23	69,73,73	1.17	8 (11%)	82,113,113	1.36	8 (9%)
14	CLA	A	837	1	49,53,73	1.42	5 (10%)	58,89,113	1.35	4 (6%)
14	CLA	B	3006	-	69,73,73	1.20	6 (8%)	82,113,113	1.28	5 (6%)
14	CLA	A	820	-	69,73,73	1.17	6 (8%)	82,113,113	1.40	8 (9%)
18	LHG	B	3049	-	22,22,48	1.17	2 (9%)	25,28,54	1.24	1 (4%)
14	CLA	A	814	-	64,68,73	1.24	7 (10%)	76,107,113	1.27	5 (6%)
14	CLA	A	810	1	69,73,73	1.21	8 (11%)	82,113,113	1.28	6 (7%)
14	CLA	B	3040	-	51,55,73	1.38	6 (11%)	60,91,113	1.37	4 (6%)
14	CLA	A	819	-	58,62,73	1.31	9 (15%)	68,99,113	1.37	9 (13%)
14	CLA	A	831	-	69,73,73	1.19	8 (11%)	82,113,113	1.23	5 (6%)
16	BCR	B	3046	-	41,41,41	1.15	3 (7%)	56,56,56	1.30	7 (12%)
14	CLA	A	840	-	51,55,73	1.42	6 (11%)	60,91,113	1.39	6 (10%)
14	CLA	B	3020	23	69,73,73	1.17	9 (13%)	82,113,113	1.28	6 (7%)
14	CLA	I	101	-	69,73,73	1.21	4 (5%)	82,113,113	1.38	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	J	103	-	41,41,41	1.17	3 (7%)	56,56,56	1.21	6 (10%)
16	BCR	L	207	-	41,41,41	1.17	3 (7%)	56,56,56	1.27	6 (10%)
16	BCR	J	104	-	41,41,41	1.19	3 (7%)	56,56,56	1.26	6 (10%)
14	CLA	A	817	23	53,57,73	1.35	6 (11%)	61,93,113	1.30	4 (6%)
14	CLA	B	3033	-	69,73,73	1.20	6 (8%)	82,113,113	1.26	5 (6%)
14	CLA	B	3009	-	69,73,73	1.18	5 (7%)	82,113,113	1.31	5 (6%)
16	BCR	K	102	-	41,41,41	1.11	3 (7%)	56,56,56	1.41	9 (16%)
17	LMG	A	855	-	30,30,55	1.16	2 (6%)	37,37,63	1.26	4 (10%)
14	CLA	A	823	-	53,57,73	1.35	5 (9%)	61,93,113	1.43	6 (9%)
15	PQN	A	846	-	34,34,34	2.09	7 (20%)	43,45,45	1.30	6 (13%)
14	CLA	B	3014	-	69,73,73	1.22	6 (8%)	82,113,113	1.26	5 (6%)
14	CLA	B	3035	-	49,53,73	1.42	7 (14%)	58,89,113	1.43	4 (6%)
14	CLA	B	3011	2	69,73,73	1.20	9 (13%)	82,113,113	1.27	7 (8%)
17	LMG	A	852	-	48,48,55	0.84	1 (2%)	56,56,63	1.26	5 (8%)
14	CLA	A	821	-	46,50,73	1.42	7 (15%)	54,84,113	1.45	9 (16%)
17	LMG	I	104	-	40,40,55	1.14	4 (10%)	48,48,63	1.16	3 (6%)
14	CLA	A	844	23	69,73,73	1.18	8 (11%)	82,113,113	1.32	7 (8%)
21	LMT	L	201	-	36,36,36	1.08	4 (11%)	47,47,47	1.18	4 (8%)
16	BCR	B	3045	-	41,41,41	1.14	3 (7%)	56,56,56	1.23	8 (14%)
14	CLA	B	3003	-	69,73,73	1.20	8 (11%)	82,113,113	1.34	4 (4%)
16	BCR	F	201	-	41,41,41	1.21	3 (7%)	56,56,56	1.22	5 (8%)
22	DGD	L	206	-	67,67,67	0.99	4 (5%)	81,81,81	1.29	8 (9%)
14	CLA	A	802	23	69,73,73	1.18	6 (8%)	82,113,113	1.24	6 (7%)
14	CLA	B	3026	23	50,54,73	1.39	6 (12%)	59,90,113	1.47	6 (10%)
18	LHG	M	101	-	48,48,48	0.63	1 (2%)	51,54,54	1.19	3 (5%)
17	LMG	B	3048	-	55,55,55	0.72	0	63,63,63	1.33	6 (9%)
14	CLA	A	808	-	55,59,73	1.36	6 (10%)	64,96,113	1.35	6 (9%)
14	CLA	A	842	23	55,59,73	1.32	7 (12%)	64,96,113	1.42	5 (7%)
14	CLA	A	828	-	69,73,73	1.23	5 (7%)	82,113,113	1.23	6 (7%)
14	CLA	B	3019	-	64,68,73	1.24	5 (7%)	76,107,113	1.25	6 (7%)
16	BCR	F	203	-	41,41,41	1.16	3 (7%)	56,56,56	1.23	5 (8%)
19	SF4	B	3001	1,2	0,12,12	-	-	-	-	-
14	CLA	B	3038	-	64,68,73	1.26	6 (9%)	76,107,113	1.23	5 (6%)
14	CLA	A	830	-	69,73,73	1.20	5 (7%)	82,113,113	1.19	5 (6%)
14	CLA	A	827	23	69,73,73	1.17	7 (10%)	82,113,113	1.22	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	3008	-	69,73,73	1.18	6 (8%)	82,113,113	1.32	4 (4%)
14	CLA	A	832	-	54,58,73	1.34	8 (14%)	64,95,113	1.43	8 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	J	102	-	1/1/12/20	0/4/76/115	-
14	CLA	L	204	-	1/1/20/20	5/39/115/115	-
14	CLA	A	811	-	1/1/15/20	8/15/91/115	-
14	CLA	B	3024	-	1/1/15/20	4/15/91/115	-
14	CLA	A	822	23	1/1/20/20	14/39/115/115	-
14	CLA	B	3036	23	1/1/15/20	6/15/91/115	-
14	CLA	B	3034	-	1/1/18/20	9/31/107/115	-
14	CLA	A	839	-	1/1/20/20	8/39/115/115	-
14	CLA	B	3032	-	1/1/16/20	7/20/96/115	-
14	CLA	B	3005	-	1/1/17/20	5/26/102/115	-
16	BCR	A	849	-	-	7/29/63/63	0/2/2/2
14	CLA	A	809	1	1/1/20/20	15/39/115/115	-
14	CLA	B	3010	2	1/1/20/20	16/39/115/115	-
16	BCR	J	105	-	-	11/29/63/63	0/2/2/2
14	CLA	L	203	10	1/1/20/20	13/39/115/115	-
14	CLA	J	101	8	1/1/15/20	6/15/91/115	-
14	CLA	A	856	23	1/1/20/20	15/39/115/115	-
14	CLA	A	834	-	1/1/20/20	9/39/115/115	-
14	CLA	K	101	-	1/1/13/20	1/9/81/115	-
16	BCR	A	847	-	-	13/29/63/63	0/2/2/2
16	BCR	B	3047	-	-	2/29/63/63	0/2/2/2
15	PQN	B	3042	-	-	8/23/43/43	0/2/2/2
14	CLA	A	824	-	1/1/17/20	2/23/99/115	-
14	CLA	B	3031	-	1/1/15/20	8/15/91/115	-
14	CLA	B	3012	-	1/1/15/20	2/15/91/115	-
14	CLA	K	103	-	1/1/15/20	8/15/91/115	-
14	CLA	M	102	23	1/1/15/20	9/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	803	-	1/1/20/20	5/39/115/115	-
14	CLA	B	3030	-	1/1/20/20	13/39/115/115	-
19	SF4	C	101	3	-	-	0/6/5/5
18	LHG	A	853	-	-	23/53/53/53	-
16	BCR	I	103	-	-	5/29/63/63	0/2/2/2
14	CLA	B	3029	-	1/1/20/20	16/39/115/115	-
16	BCR	B	3050	-	-	10/29/63/63	0/2/2/2
18	LHG	A	854	14	-	10/31/31/53	-
14	CLA	B	3017	-	1/1/18/20	5/27/103/115	-
14	CLA	A	812	14	1/1/20/20	9/39/115/115	-
14	CLA	B	3041	-	1/1/20/20	7/39/115/115	-
19	SF4	C	102	3	-	-	0/6/5/5
14	CLA	A	829	-	1/1/20/20	9/39/115/115	-
14	CLA	B	3025	2	-	9/26/102/115	-
14	CLA	A	825	-	1/1/18/20	11/32/108/115	-
16	BCR	I	105	-	-	17/29/63/63	0/2/2/2
14	CLA	B	3022	-	1/1/15/20	6/15/91/115	-
14	CLA	F	202	23	1/1/15/20	6/15/91/115	-
14	CLA	A	836	-	1/1/17/20	7/26/102/115	-
14	CLA	A	838	-	1/1/17/20	6/23/99/115	-
13	CL0	A	801	-	3/3/25/25	12/37/135/135	-
14	CLA	B	3013	-	1/1/15/20	5/15/91/115	-
14	CLA	A	806	-	1/1/20/20	17/39/115/115	-
16	BCR	M	103	-	-	8/29/63/63	0/2/2/2
14	CLA	A	843	-	1/1/20/20	6/39/115/115	-
14	CLA	B	3015	-	1/1/20/20	13/39/115/115	-
14	CLA	B	3037	23	1/1/15/20	4/15/91/115	-
14	CLA	A	835	-	1/1/20/20	9/39/115/115	-
16	BCR	A	850	-	-	9/29/63/63	0/2/2/2
14	CLA	A	813	-	1/1/17/20	5/26/102/115	-
14	CLA	A	805	14	1/1/18/20	9/32/108/115	-
14	CLA	B	3021	-	1/1/15/20	11/18/94/115	-
14	CLA	B	3023	23	1/1/18/20	6/27/103/115	-
14	CLA	B	3007	-	1/1/20/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	833	-	1/1/20/20	6/39/115/115	-
14	CLA	A	804	-	1/1/20/20	9/39/115/115	-
14	CLA	B	3039	-	1/1/20/20	10/39/115/115	-
14	CLA	A	818	-	1/1/17/20	3/26/102/115	-
14	CLA	B	3028	-	1/1/20/20	12/39/115/115	-
14	CLA	A	826	23	1/1/20/20	12/39/115/115	-
16	BCR	B	3043	-	-	7/29/63/63	0/2/2/2
14	CLA	A	816	-	1/1/15/20	4/15/91/115	-
14	CLA	X	1701	12	1/1/15/20	4/15/91/115	-
14	CLA	A	807	-	1/1/20/20	13/39/115/115	-
14	CLA	B	3018	-	1/1/18/20	11/32/108/115	-
14	CLA	B	3027	-	1/1/20/20	8/39/115/115	-
16	BCR	I	102	-	-	5/29/63/63	0/2/2/2
16	BCR	A	848	-	-	7/29/63/63	0/2/2/2
14	CLA	A	815	-	1/1/15/20	2/15/91/115	-
14	CLA	B	3016	-	1/1/15/20	3/15/91/115	-
16	BCR	A	851	-	-	17/29/63/63	0/2/2/2
14	CLA	B	3004	-	1/1/20/20	8/39/115/115	-
16	BCR	B	3044	-	-	11/29/63/63	0/2/2/2
14	CLA	A	845	18	1/1/17/20	7/24/100/115	-
14	CLA	A	841	-	1/1/20/20	7/39/115/115	-
14	CLA	L	205	23	1/1/20/20	8/39/115/115	-
14	CLA	A	837	1	1/1/15/20	6/15/91/115	-
14	CLA	B	3006	-	1/1/20/20	14/39/115/115	-
14	CLA	A	820	-	1/1/20/20	18/39/115/115	-
18	LHG	B	3049	-	-	11/26/26/53	-
14	CLA	A	814	-	1/1/19/20	4/33/109/115	-
14	CLA	A	810	1	1/1/20/20	8/39/115/115	-
14	CLA	B	3040	-	-	5/18/94/115	-
14	CLA	A	819	-	1/1/17/20	10/26/102/115	-
14	CLA	A	831	-	1/1/20/20	8/39/115/115	-
16	BCR	B	3046	-	-	14/29/63/63	0/2/2/2
14	CLA	A	840	-	1/1/15/20	4/18/94/115	-
14	CLA	B	3020	23	1/1/20/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	I	101	-	1/1/20/20	9/39/115/115	-
16	BCR	J	103	-	-	12/29/63/63	0/2/2/2
16	BCR	L	207	-	-	9/29/63/63	0/2/2/2
16	BCR	J	104	-	-	15/29/63/63	0/2/2/2
14	CLA	A	817	23	1/1/16/20	7/20/96/115	-
14	CLA	B	3033	-	1/1/20/20	17/39/115/115	-
14	CLA	B	3009	-	1/1/20/20	7/39/115/115	-
16	BCR	K	102	-	-	9/29/63/63	0/2/2/2
17	LMG	A	855	-	-	12/23/43/70	0/1/1/1
14	CLA	A	823	-	1/1/16/20	11/20/96/115	-
15	PQN	A	846	-	-	10/23/43/43	0/2/2/2
14	CLA	B	3014	-	1/1/20/20	12/39/115/115	-
14	CLA	B	3035	-	1/1/15/20	6/15/91/115	-
14	CLA	B	3011	2	1/1/20/20	13/39/115/115	-
17	LMG	A	852	-	-	24/43/63/70	0/1/1/1
14	CLA	A	821	-	1/1/14/20	4/10/86/115	-
17	LMG	I	104	-	-	17/35/55/70	0/1/1/1
14	CLA	A	844	23	1/1/20/20	10/39/115/115	-
21	LMT	L	201	-	-	11/21/61/61	0/2/2/2
16	BCR	B	3045	-	-	10/29/63/63	0/2/2/2
14	CLA	B	3003	-	1/1/20/20	14/39/115/115	-
16	BCR	F	201	-	-	9/29/63/63	0/2/2/2
22	DGD	L	206	-	-	19/55/95/95	0/2/2/2
14	CLA	A	802	23	1/1/20/20	10/39/115/115	-
14	CLA	B	3026	23	1/1/15/20	2/17/93/115	-
18	LHG	M	101	-	-	26/53/53/53	-
17	LMG	B	3048	-	-	24/50/70/70	0/1/1/1
14	CLA	A	808	-	1/1/17/20	12/23/99/115	-
14	CLA	A	842	23	1/1/17/20	4/23/99/115	-
14	CLA	A	828	-	1/1/20/20	6/39/115/115	-
14	CLA	B	3019	-	1/1/19/20	10/33/109/115	-
16	BCR	F	203	-	-	12/29/63/63	0/2/2/2
19	SF4	B	3001	1,2	-	-	0/6/5/5
14	CLA	B	3038	-	1/1/19/20	9/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	830	-	1/1/20/20	14/39/115/115	-
14	CLA	A	827	23	1/1/20/20	10/39/115/115	-
14	CLA	B	3008	-	1/1/20/20	9/39/115/115	-
14	CLA	A	832	-	1/1/17/20	6/21/97/115	-

The worst 5 of 728 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	801	CL0	C1B-C2B	8.94	1.49	1.39
13	A	801	CL0	C3B-C4B	7.85	1.49	1.41
13	A	801	CL0	C1D-C2D	7.40	1.48	1.39
15	B	3042	PQN	O1-C1	5.97	1.35	1.23
15	A	846	PQN	O4-C4	5.93	1.35	1.23

The worst 5 of 737 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3033	CLA	C4A-NA-C1A	7.67	110.18	106.68
14	A	842	CLA	C4A-NA-C1A	7.65	110.17	106.68
14	I	101	CLA	C4A-NA-C1A	7.56	110.13	106.68
14	A	816	CLA	C4A-NA-C1A	7.50	110.10	106.68
14	B	3005	CLA	C4A-NA-C1A	7.45	110.08	106.68

5 of 96 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	801	CL0	ND
13	A	801	CL0	NA
13	A	801	CL0	NC
14	A	802	CLA	ND
14	A	803	CLA	ND

5 of 1221 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	801	CL0	C3A-C2A-CAA-CBA
14	A	805	CLA	CHA-CBD-CGD-O2D
14	A	806	CLA	C1A-C2A-CAA-CBA
14	A	806	CLA	CAD-CBD-CGD-O1D
14	A	806	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

107 monomers are involved in 267 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	L	204	CLA	1	0
14	A	811	CLA	8	0
14	B	3024	CLA	2	0
14	A	822	CLA	2	0
14	B	3034	CLA	5	0
14	B	3032	CLA	2	0
14	B	3005	CLA	1	0
16	A	849	BCR	2	0
14	A	809	CLA	3	0
14	B	3010	CLA	6	0
16	J	105	BCR	6	0
14	L	203	CLA	2	0
14	A	856	CLA	3	0
14	A	834	CLA	1	0
14	K	101	CLA	3	0
16	A	847	BCR	4	0
15	B	3042	PQN	3	0
14	B	3031	CLA	2	0
14	B	3012	CLA	1	0
14	M	102	CLA	3	0
14	A	803	CLA	4	0
14	B	3030	CLA	4	0
18	A	853	LHG	2	0
16	I	103	BCR	1	0
14	B	3029	CLA	1	0
16	B	3050	BCR	2	0
18	A	854	LHG	2	0
14	B	3017	CLA	3	0
14	B	3041	CLA	1	0
14	A	829	CLA	8	0
14	B	3025	CLA	5	0
14	A	825	CLA	1	0
16	I	105	BCR	3	0
14	B	3022	CLA	1	0
14	F	202	CLA	8	0
14	A	836	CLA	1	0
14	A	838	CLA	1	0
13	A	801	CL0	2	0
14	B	3013	CLA	2	0
14	A	806	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	M	103	BCR	2	0
14	A	843	CLA	3	0
14	B	3015	CLA	1	0
14	B	3037	CLA	2	0
14	A	835	CLA	1	0
16	A	850	BCR	5	0
14	A	813	CLA	2	0
14	B	3021	CLA	2	0
14	B	3007	CLA	1	0
14	A	833	CLA	1	0
14	A	804	CLA	4	0
14	B	3039	CLA	1	0
14	A	818	CLA	2	0
14	B	3028	CLA	2	0
14	A	826	CLA	4	0
14	X	1701	CLA	2	0
14	B	3018	CLA	4	0
14	B	3027	CLA	1	0
16	I	102	BCR	4	0
14	A	815	CLA	1	0
14	B	3016	CLA	1	0
16	A	851	BCR	6	0
14	B	3004	CLA	5	0
16	B	3044	BCR	3	0
14	A	845	CLA	2	0
14	A	841	CLA	3	0
14	L	205	CLA	1	0
14	B	3006	CLA	1	0
14	A	820	CLA	4	0
18	B	3049	LHG	2	0
14	A	814	CLA	8	0
14	A	810	CLA	3	0
14	A	819	CLA	3	0
14	A	831	CLA	2	0
16	B	3046	BCR	5	0
14	A	840	CLA	1	0
14	I	101	CLA	8	0
16	J	103	BCR	4	0
16	L	207	BCR	2	0
16	J	104	BCR	3	0
14	A	817	CLA	3	0
14	B	3033	CLA	2	0

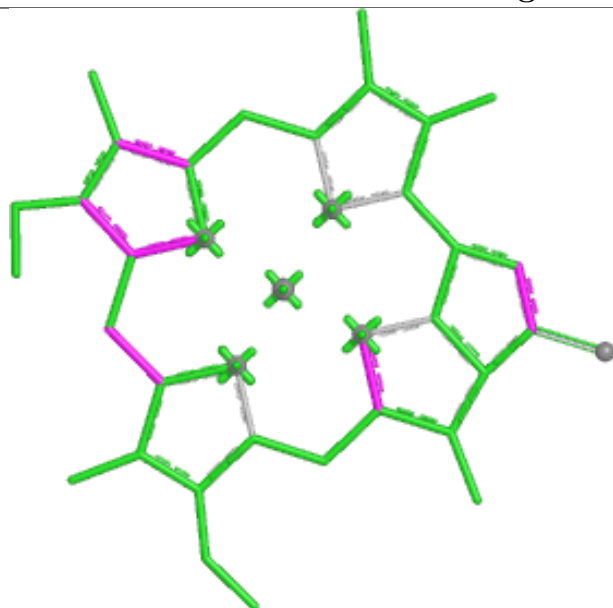
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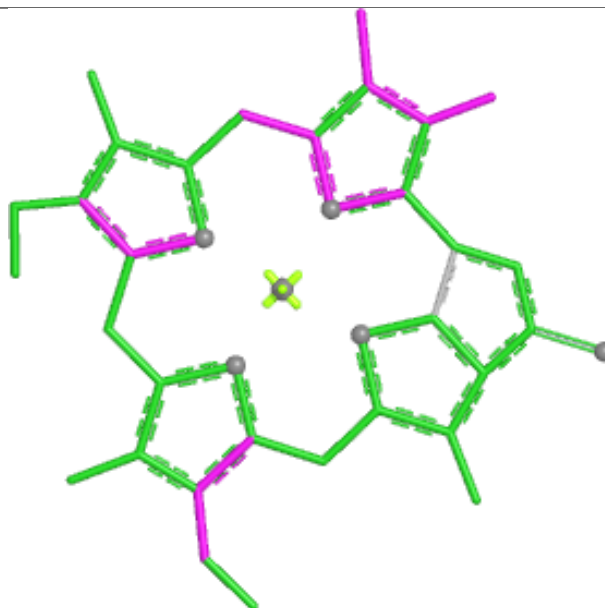
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	3009	CLA	1	0
16	K	102	BCR	4	0
14	A	823	CLA	1	0
15	A	846	PQN	7	0
14	B	3014	CLA	5	0
14	B	3011	CLA	4	0
14	A	821	CLA	5	0
14	A	844	CLA	3	0
16	B	3045	BCR	3	0
14	B	3003	CLA	4	0
16	F	201	BCR	5	0
22	L	206	DGD	2	0
14	A	802	CLA	2	0
14	B	3026	CLA	2	0
18	M	101	LHG	1	0
17	B	3048	LMG	1	0
14	A	808	CLA	1	0
14	A	828	CLA	3	0
14	B	3019	CLA	2	0
16	F	203	BCR	3	0
14	B	3038	CLA	3	0
14	A	830	CLA	2	0
14	A	827	CLA	2	0
14	B	3008	CLA	2	0
14	A	832	CLA	3	0

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

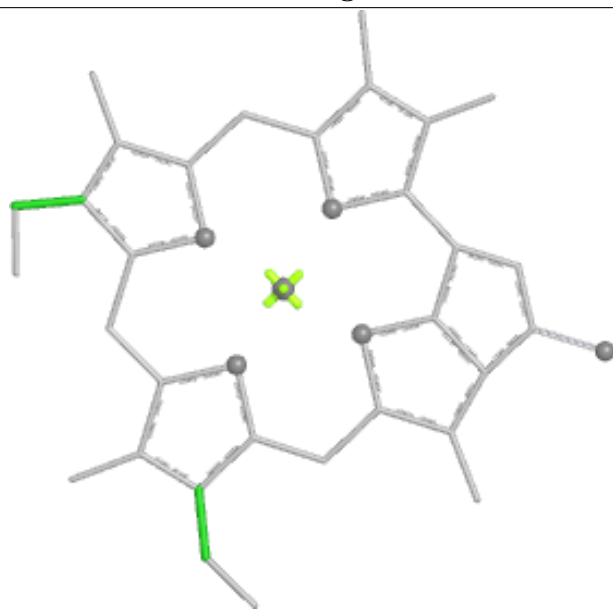
Ligand CLA J 102



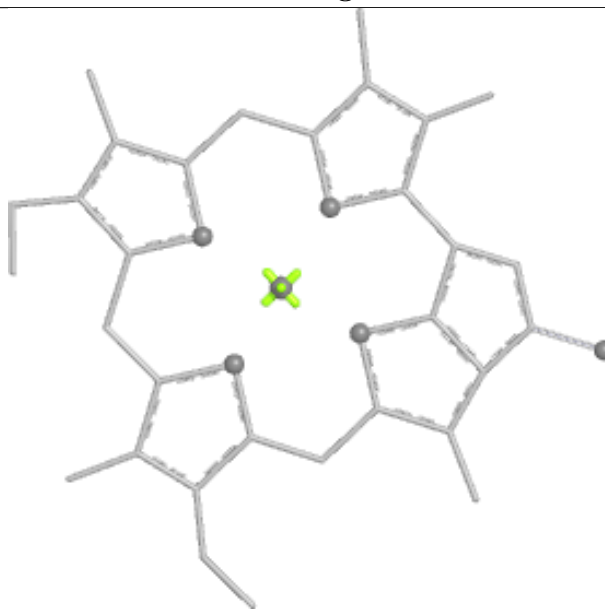
Bond lengths



Bond angles

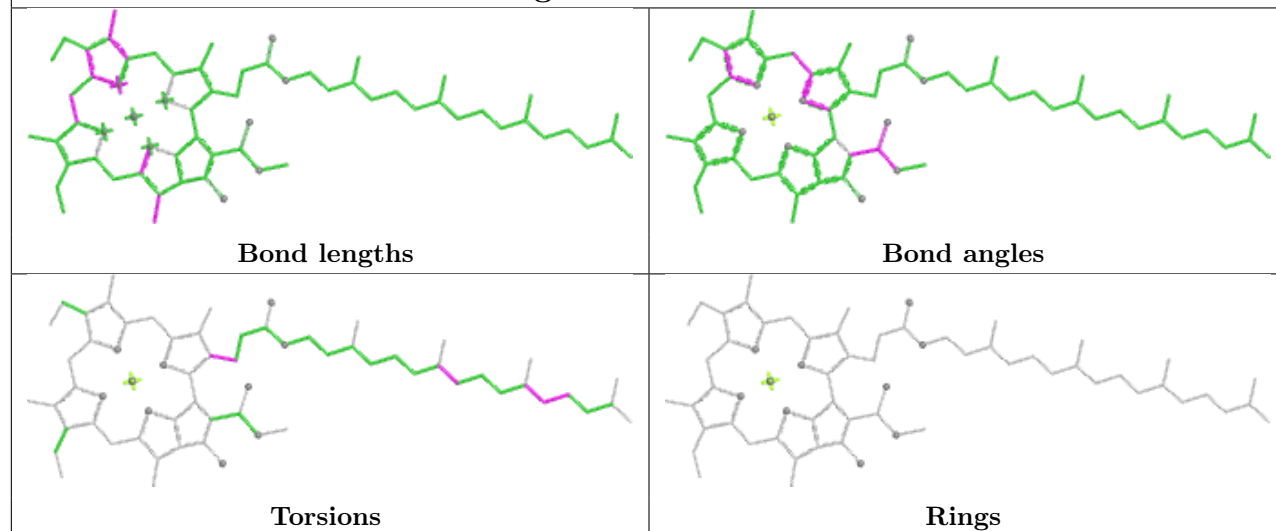


Torsions

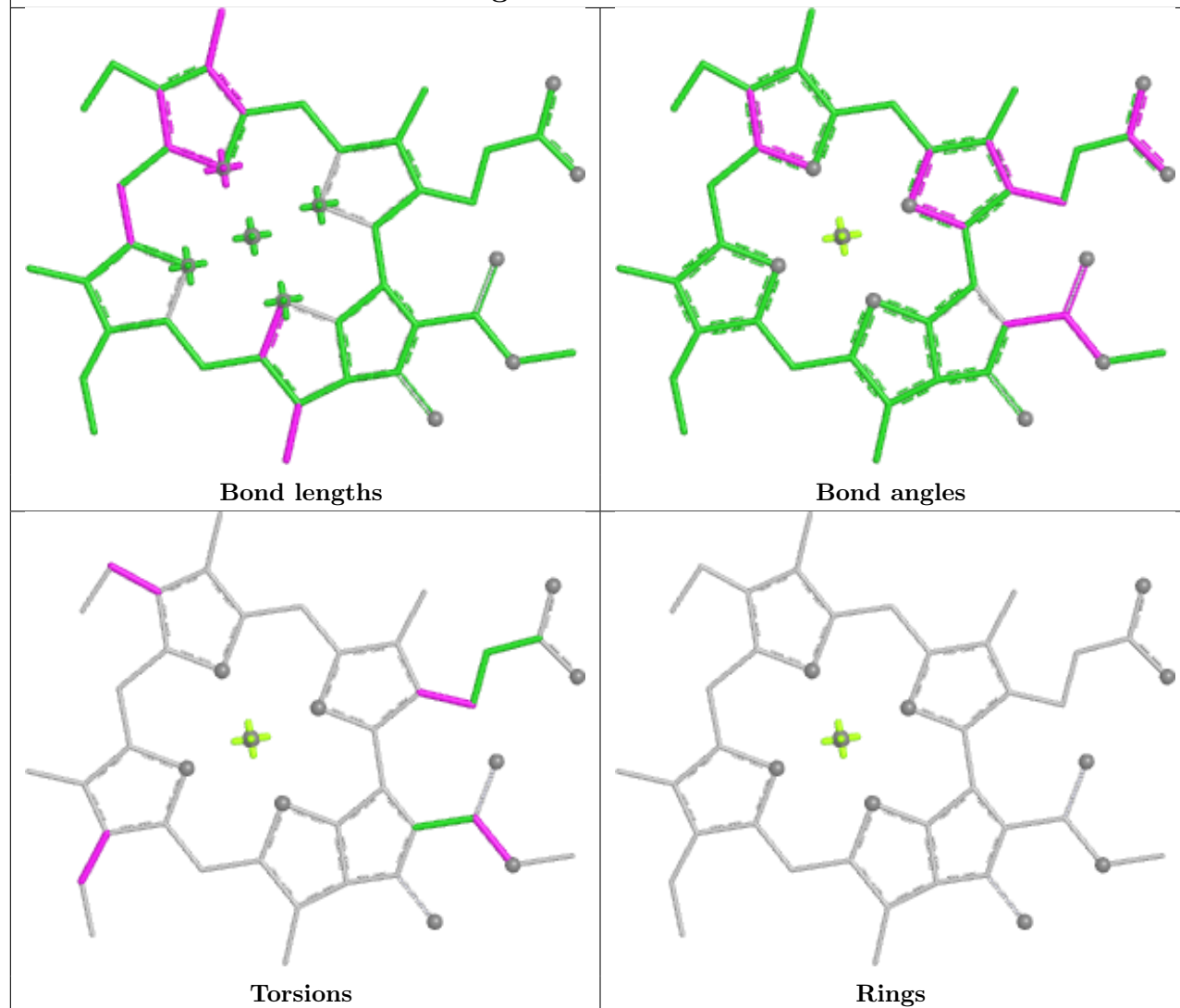


Rings

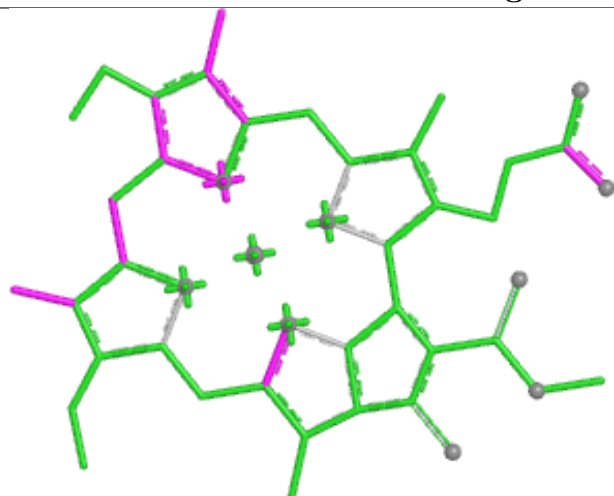
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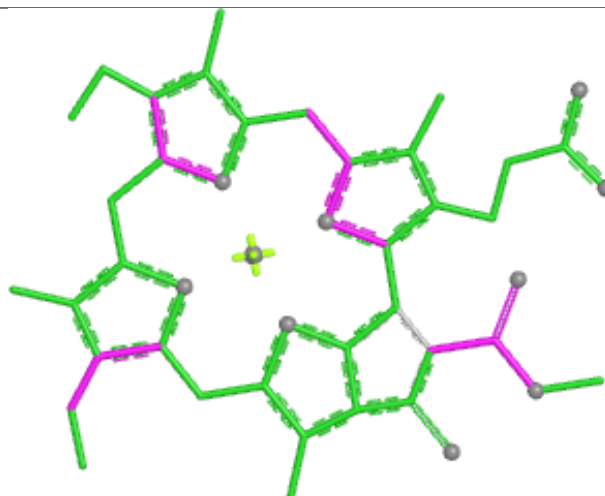
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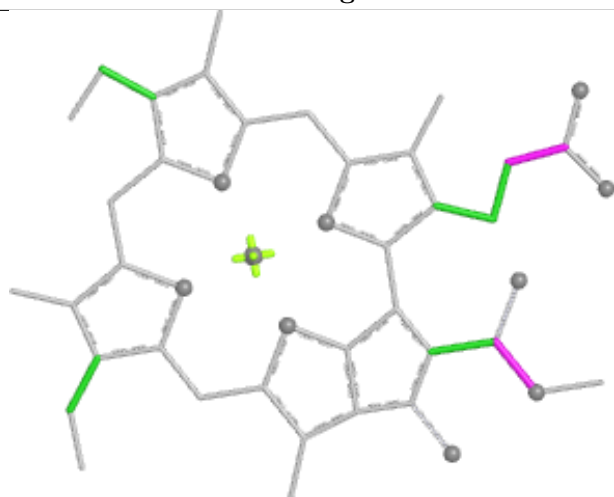
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Bond lengths



Bond angles

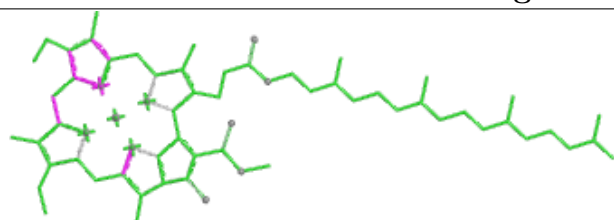


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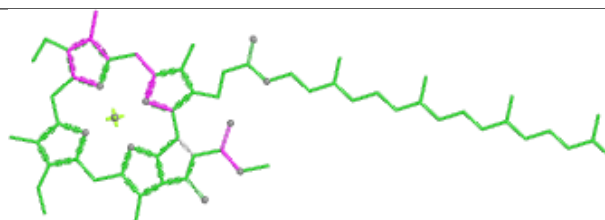


Rings

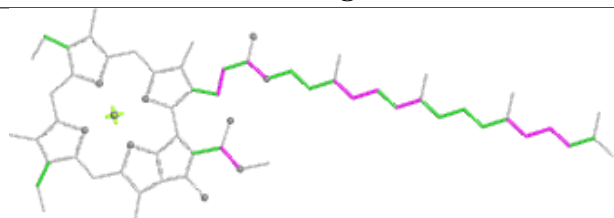
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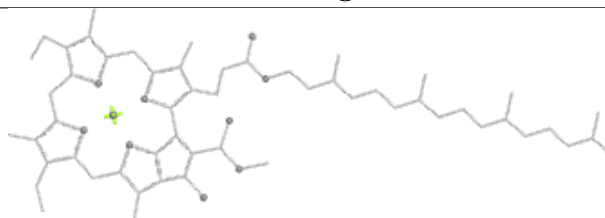
Bond lengths



Bond angles

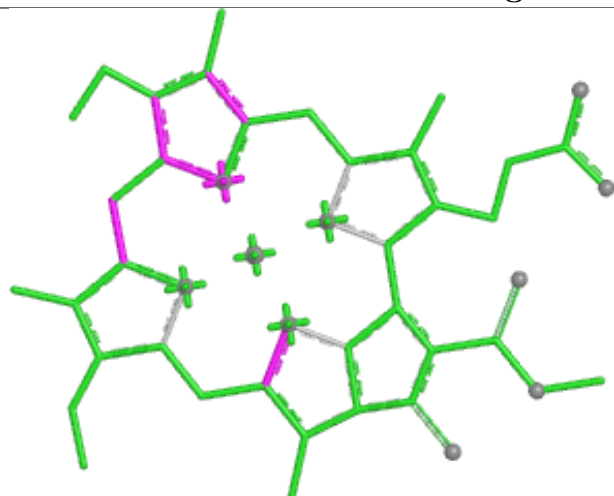


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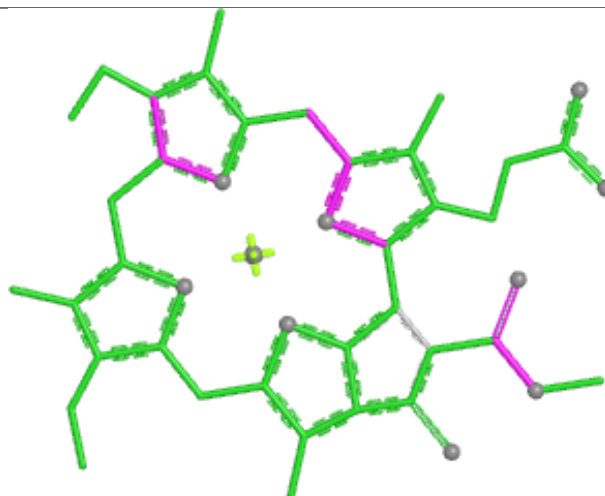


Rings

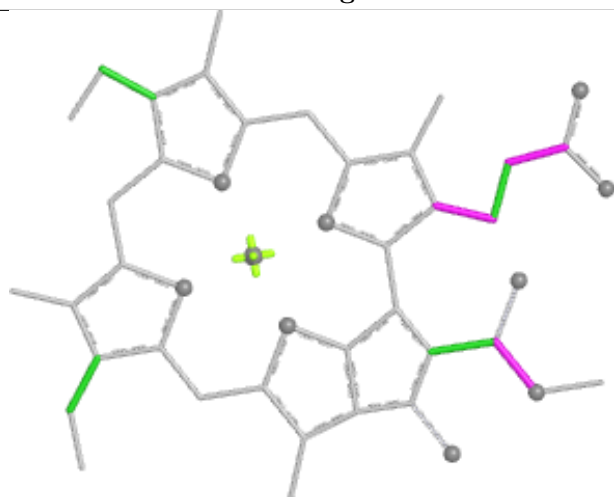
Ligand CLA B 3036



Bond lengths



Bond angles

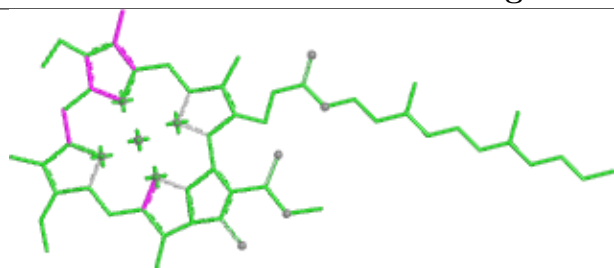


Torsions

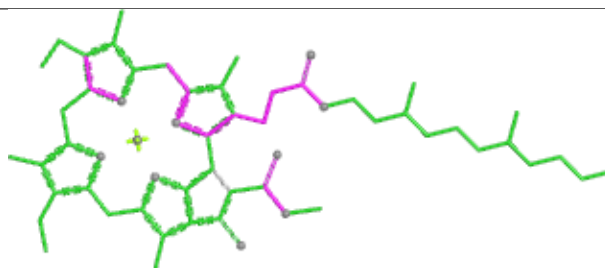


Rings

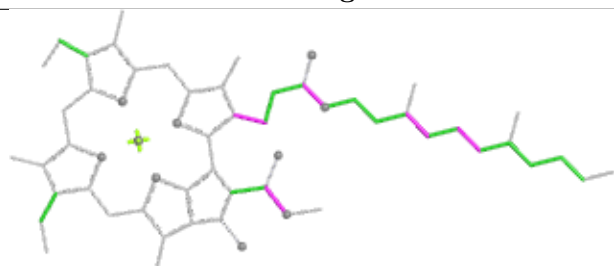
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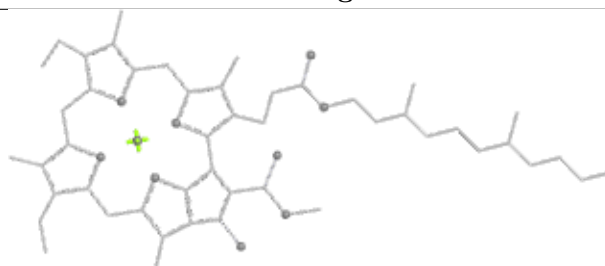
Bond lengths



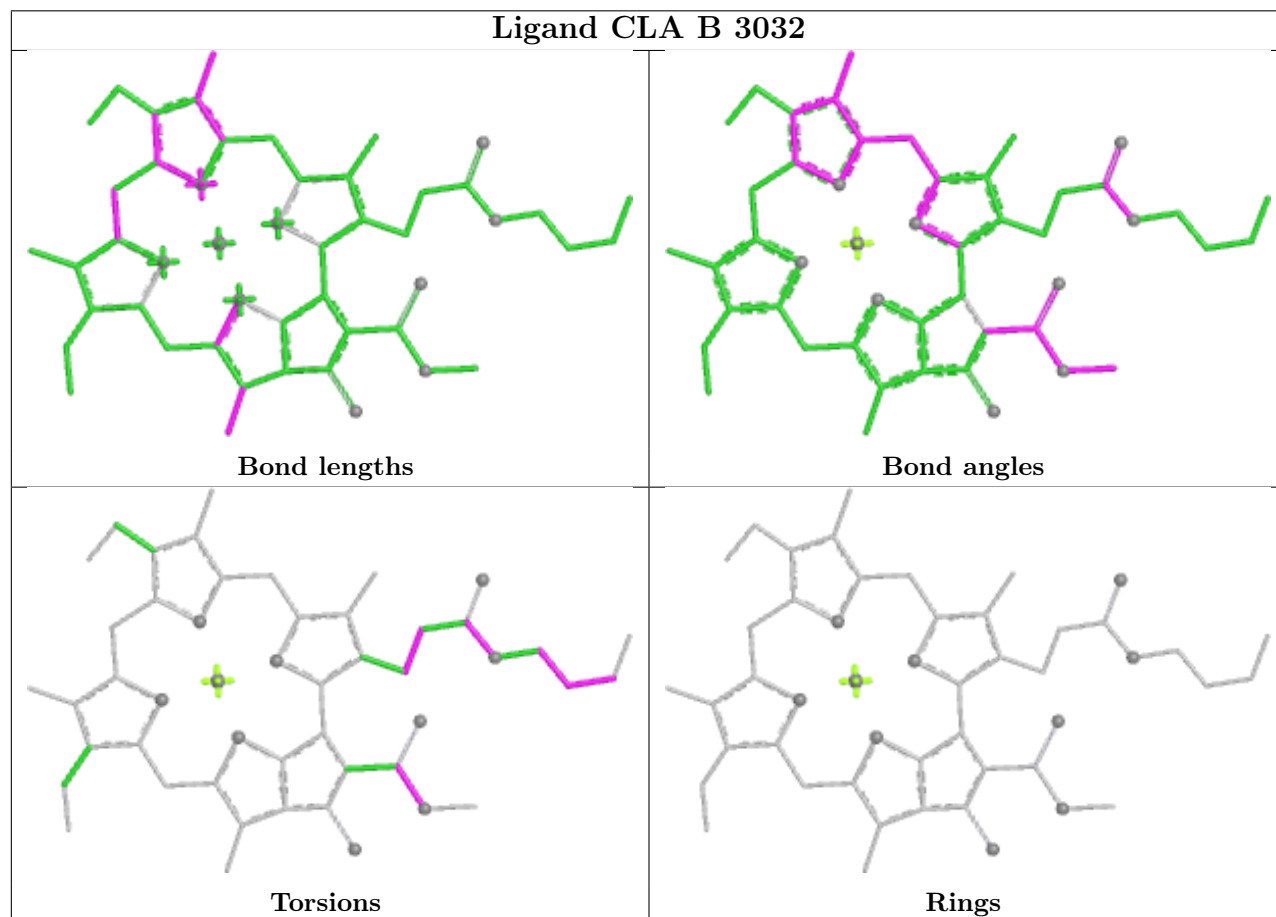
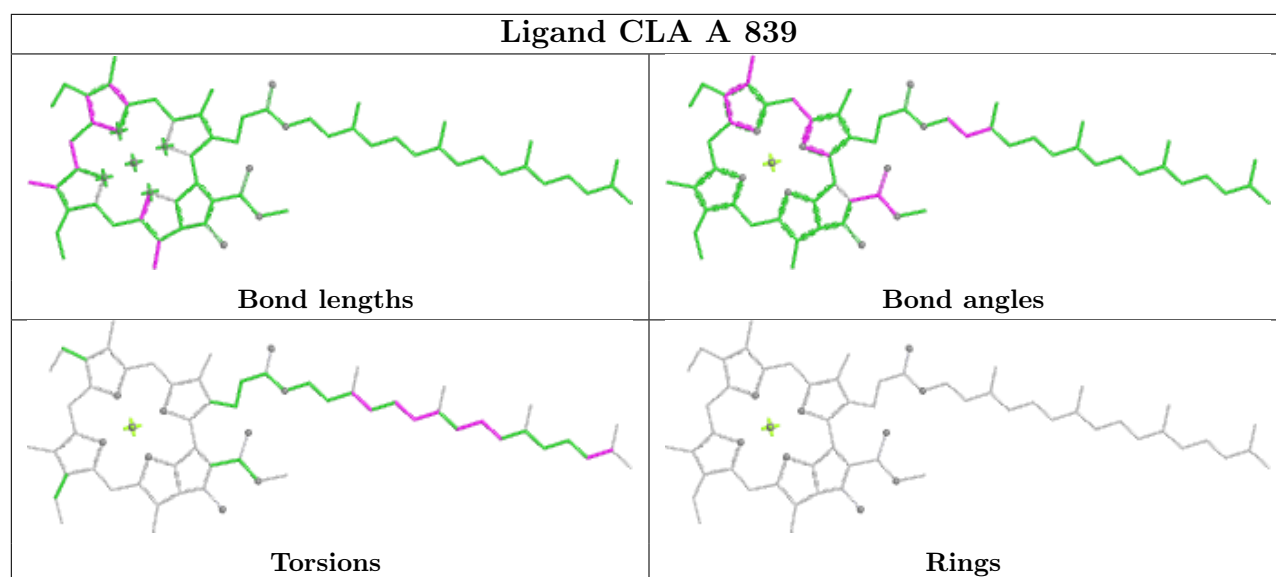
Bond angles

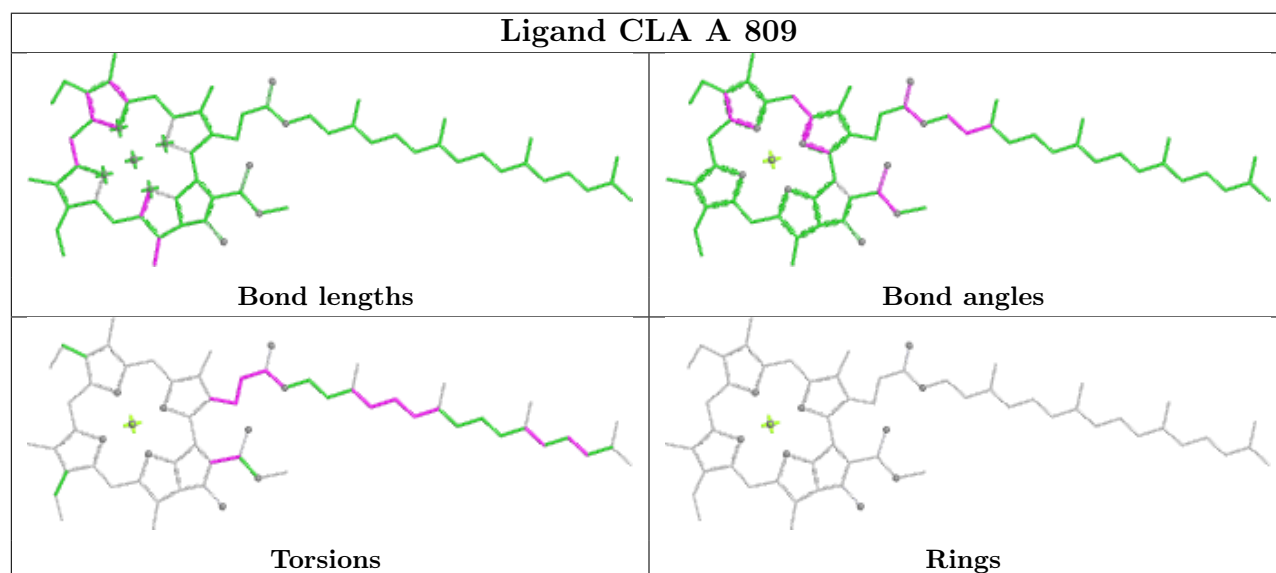
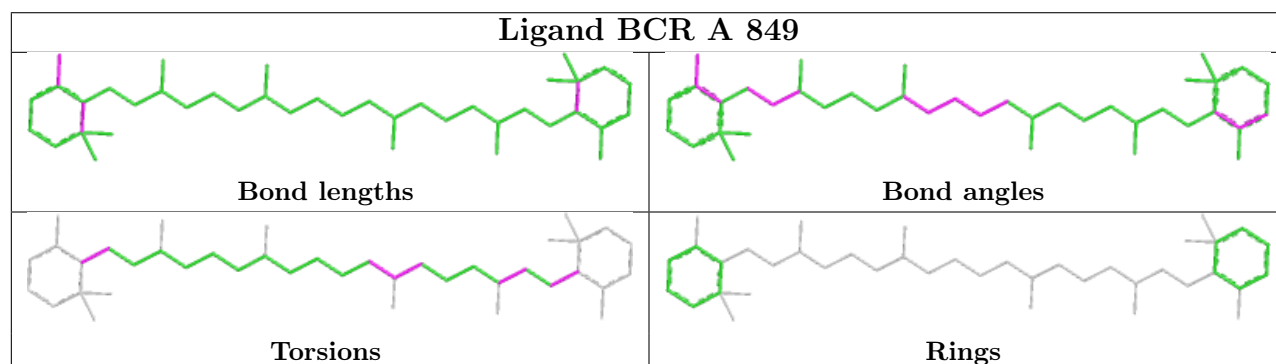
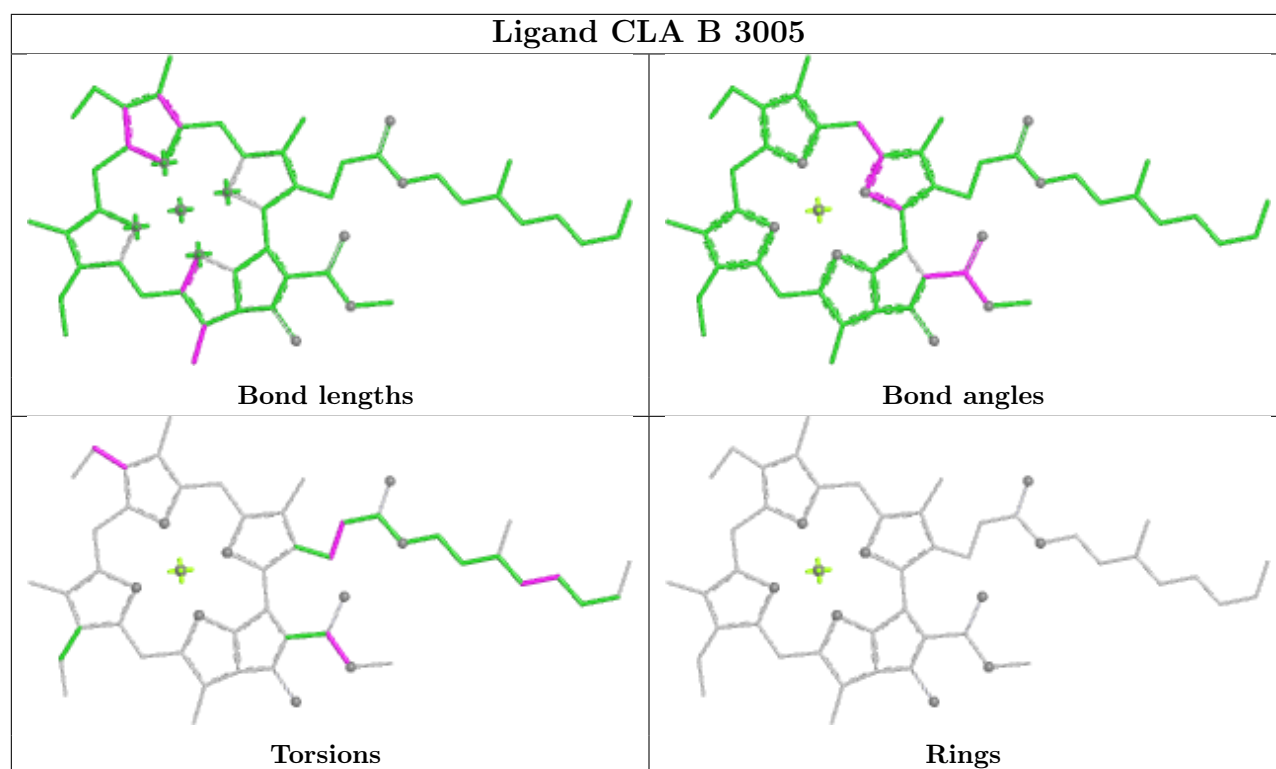


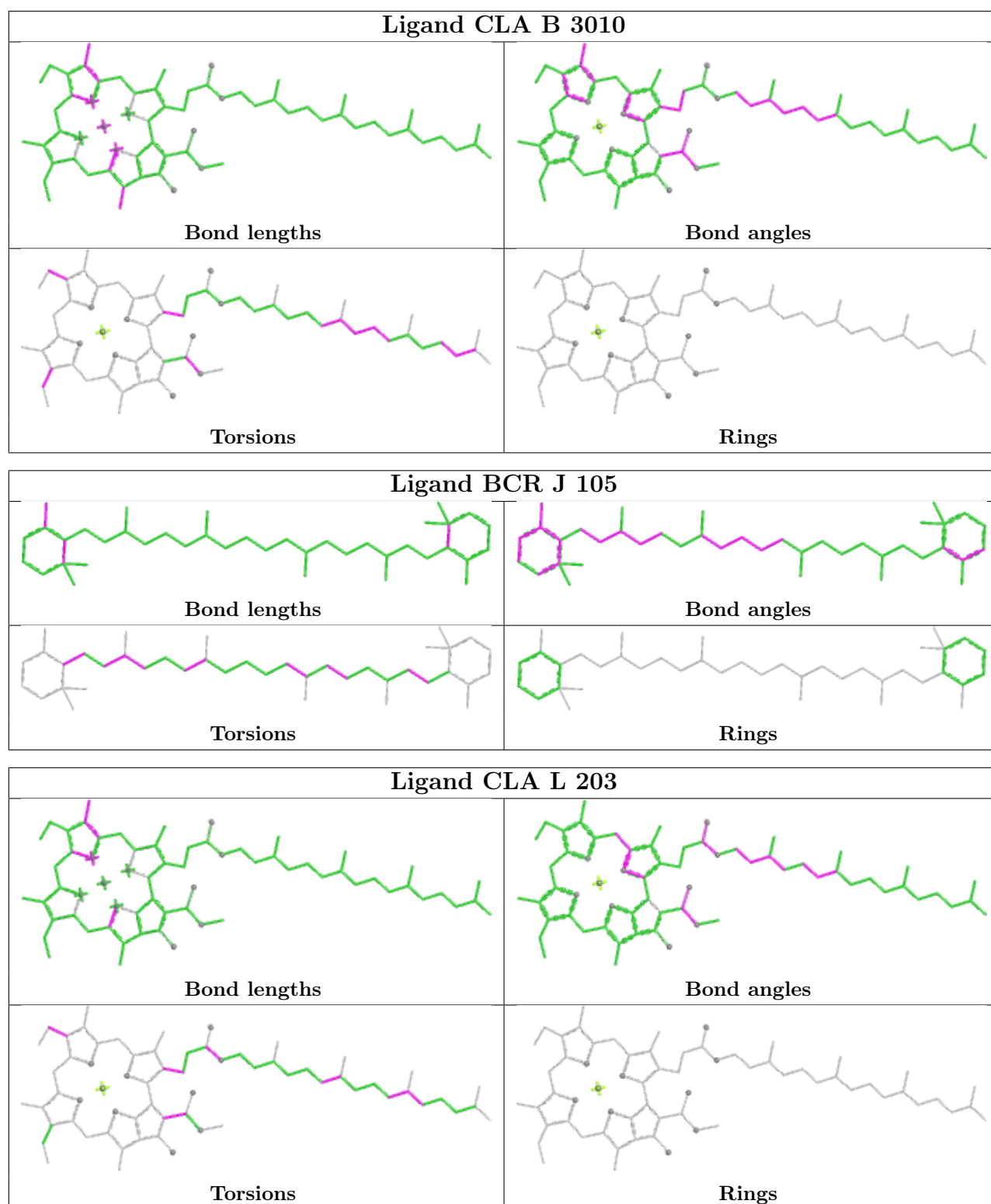
Torsions



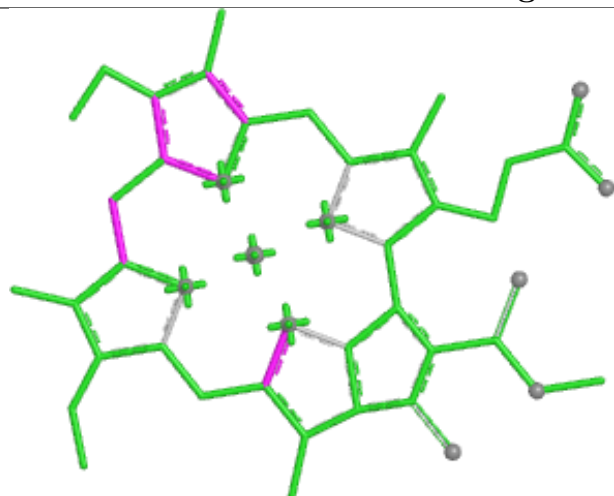
Rings



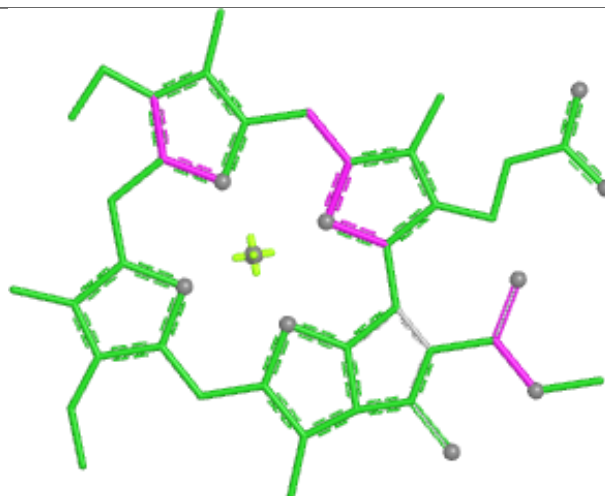




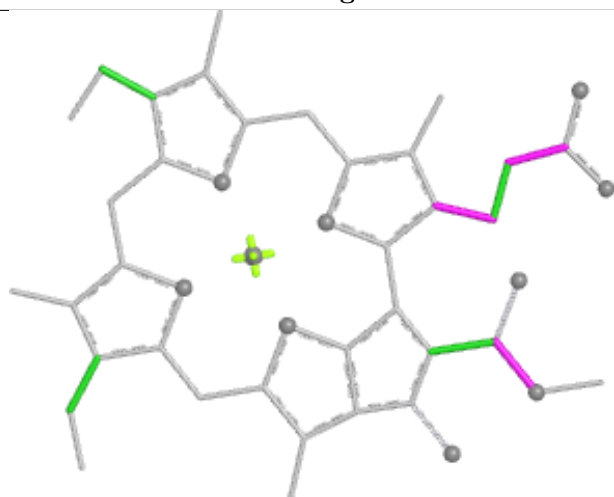
Ligand CLA J 101



Bond lengths



Bond angles

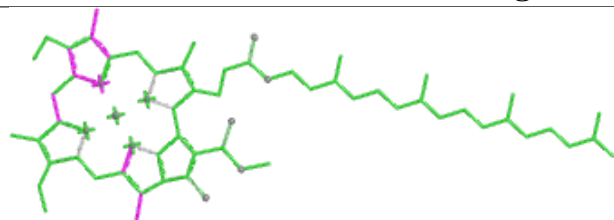


Torsions

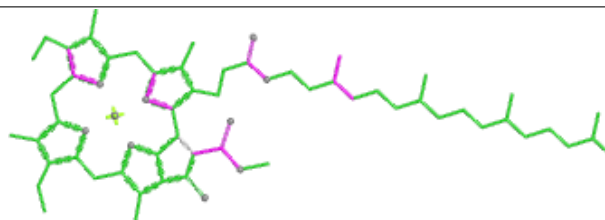


Rings

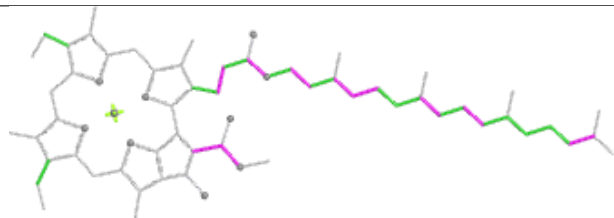
Ligand CLA A 856



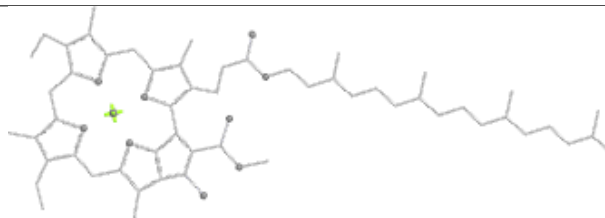
Bond lengths



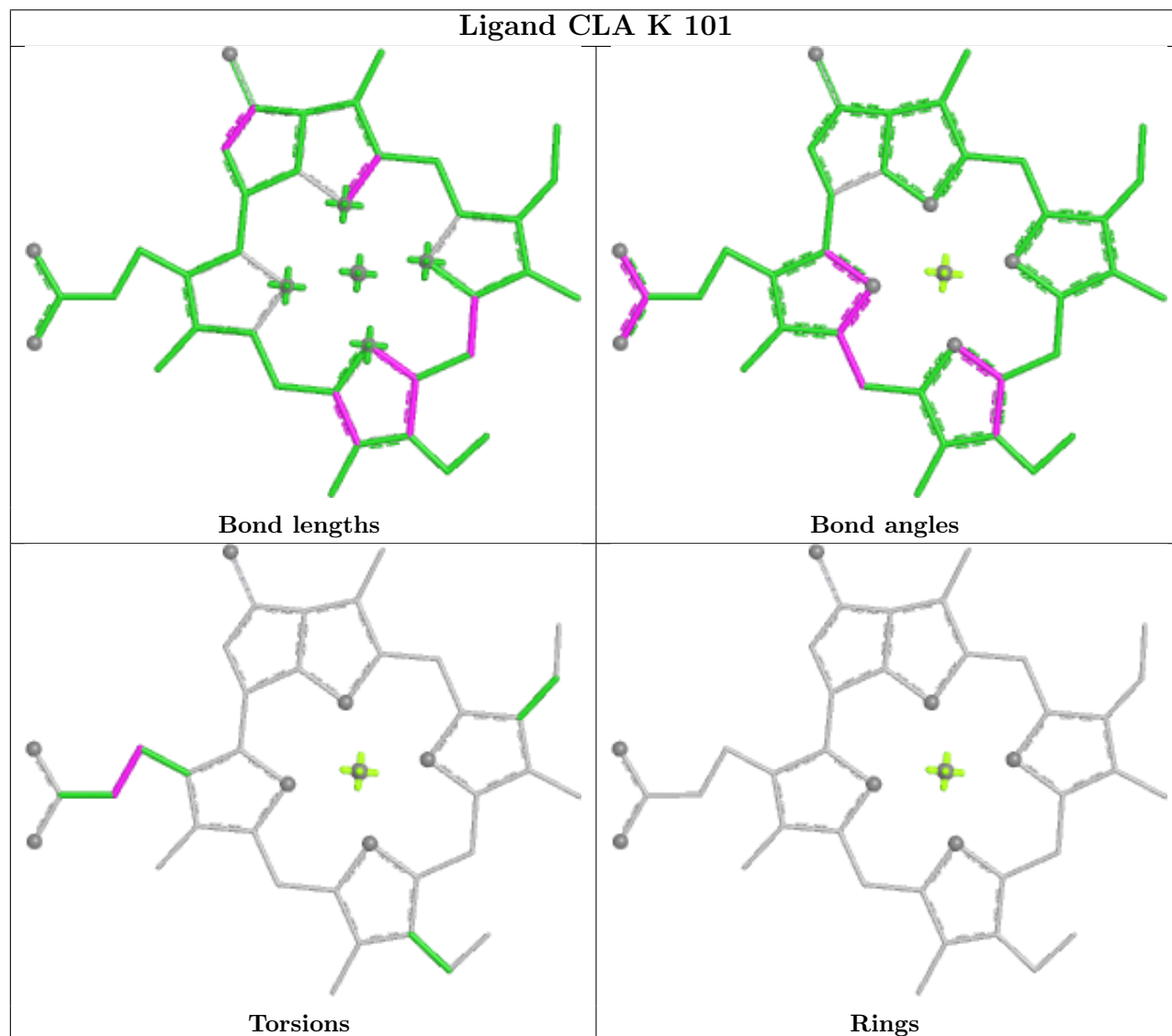
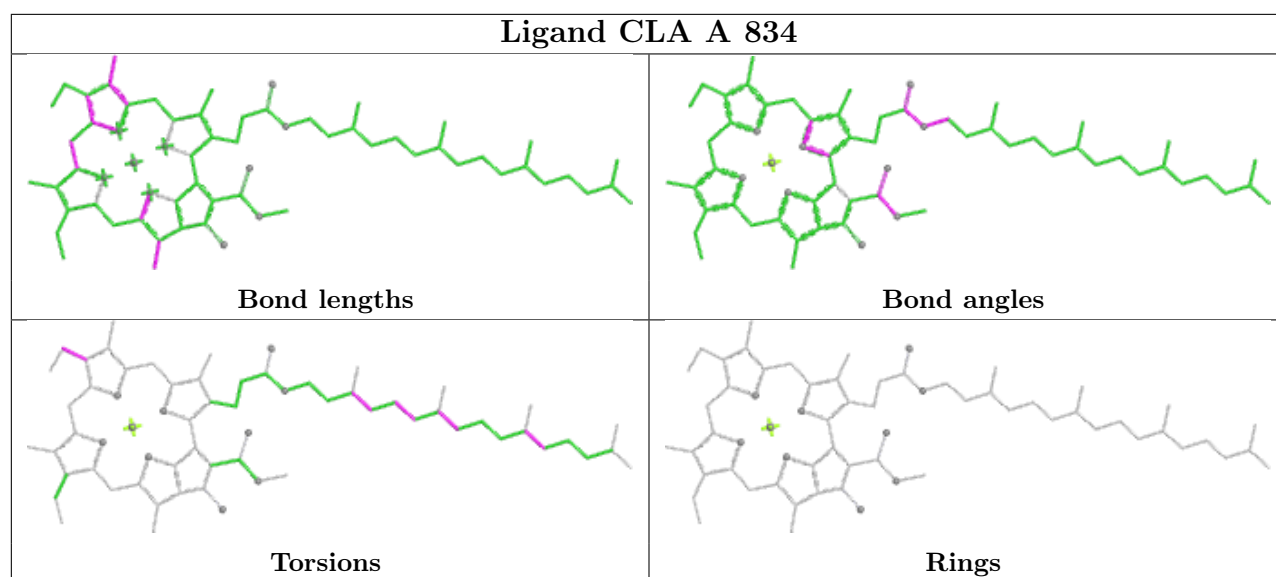
Bond angles

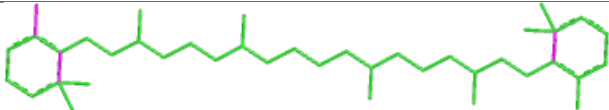
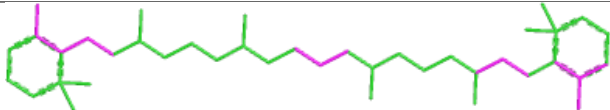
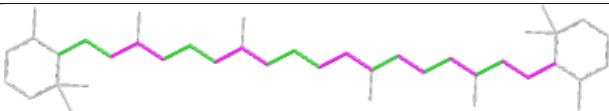
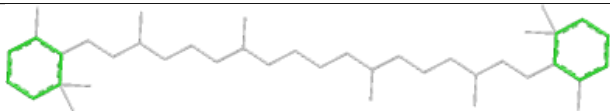


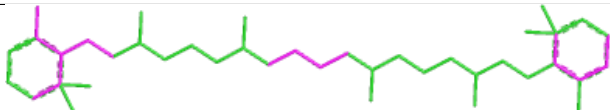
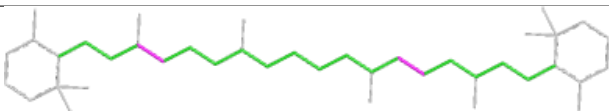
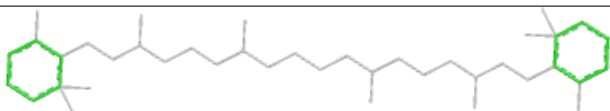
Torsions

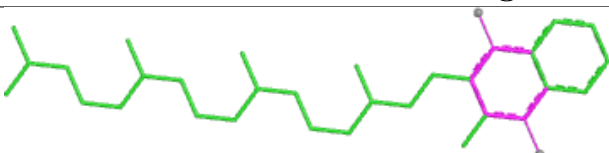
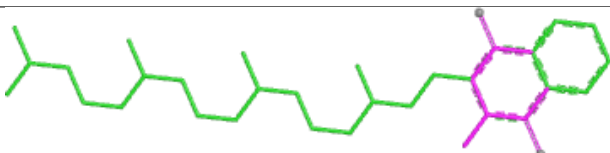
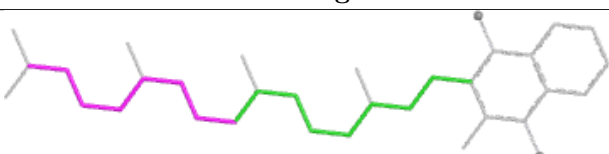
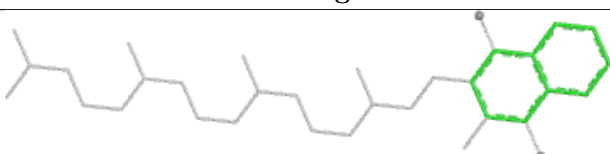


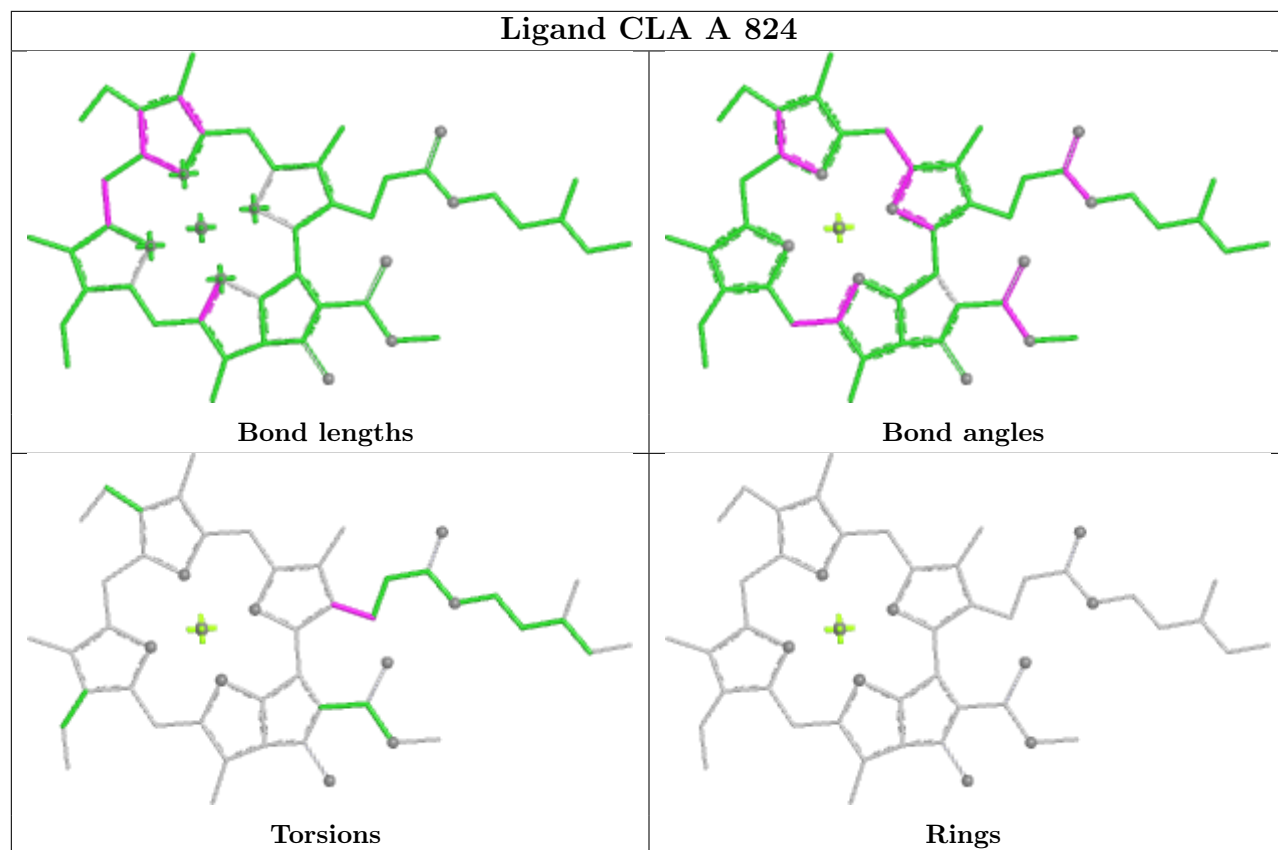
Rings



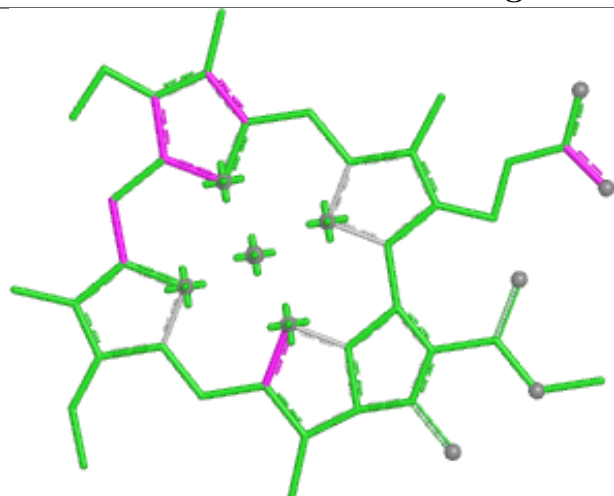
Ligand BCR A 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 3047	
	
Bond lengths	Bond angles
	
Torsions	Rings

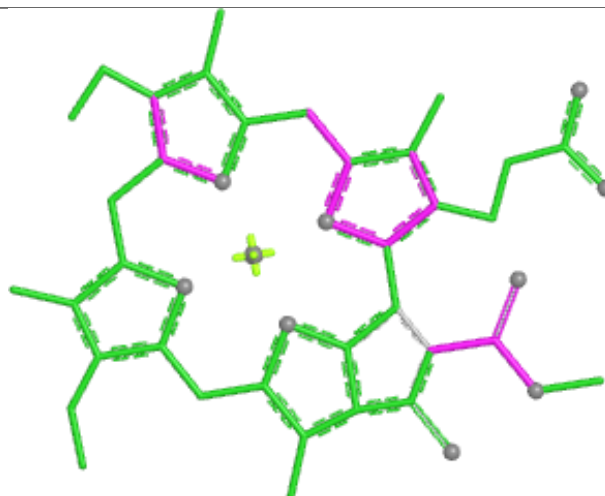
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Bond lengths	Bond angles
	
Torsions	Rings



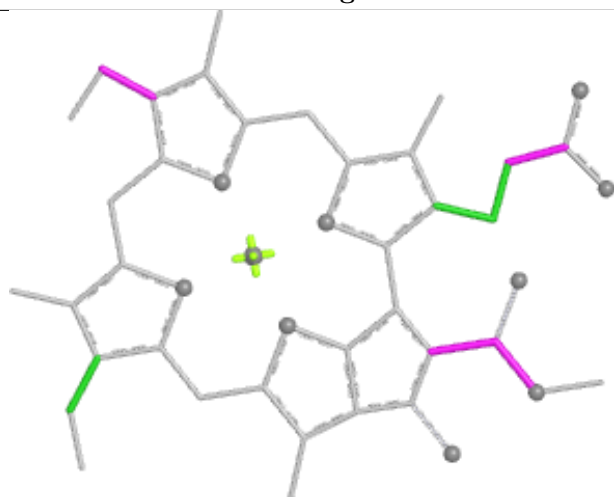
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Bond lengths



Bond angles

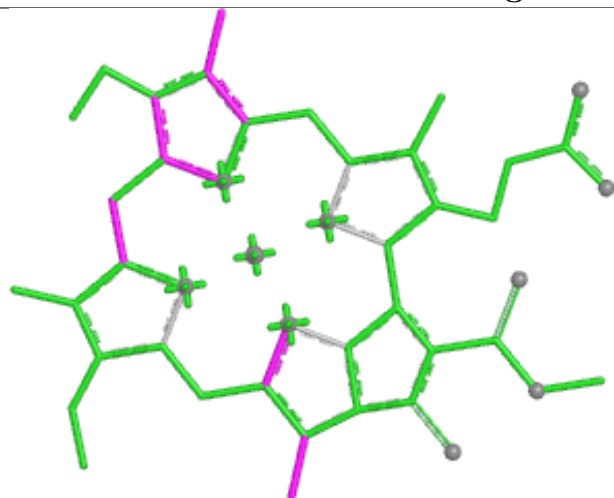


Torsions

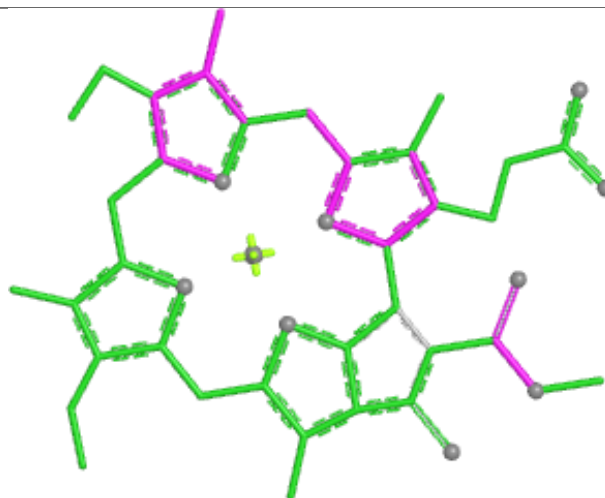


Rings

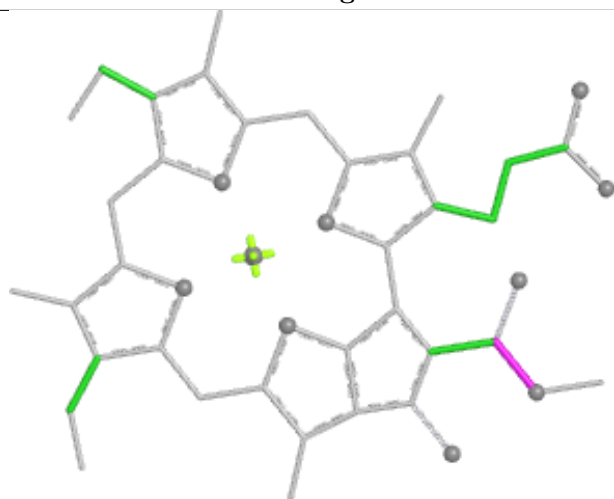
Ligand CLA B 3012



Bond lengths



Bond angles

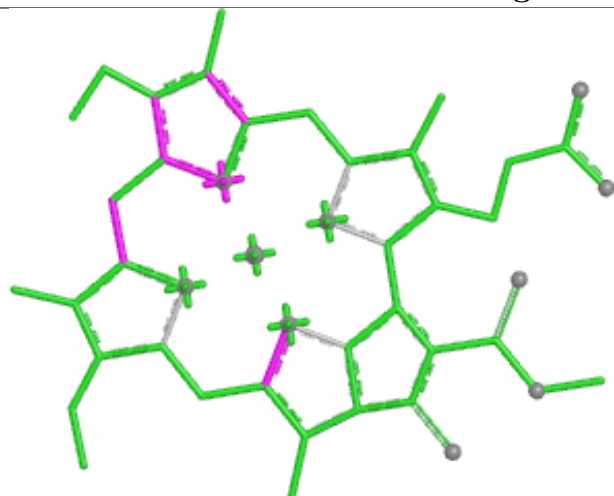


Torsions

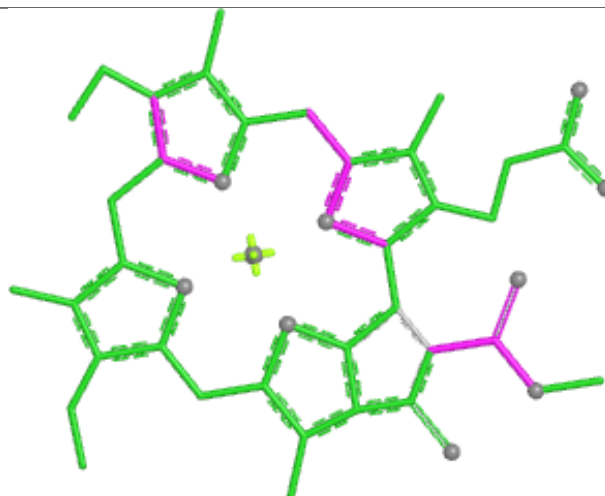


Rings

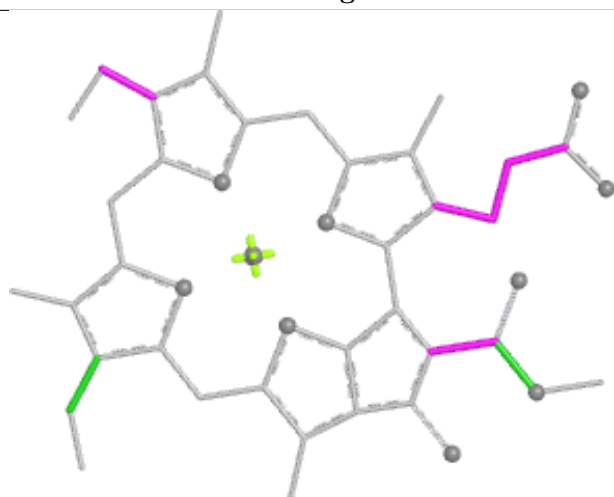
Ligand CLA K 103



Bond lengths



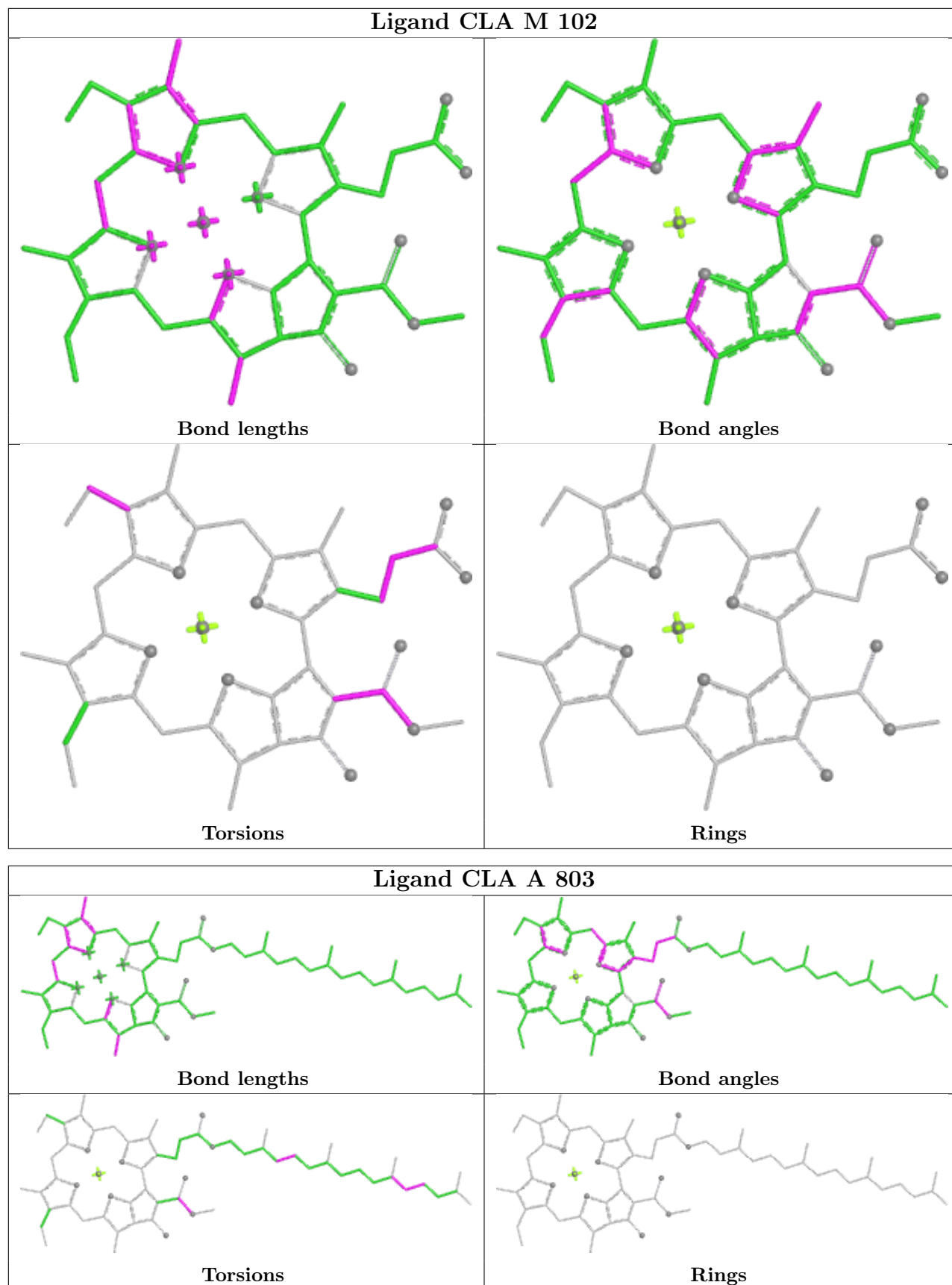
Bond angles

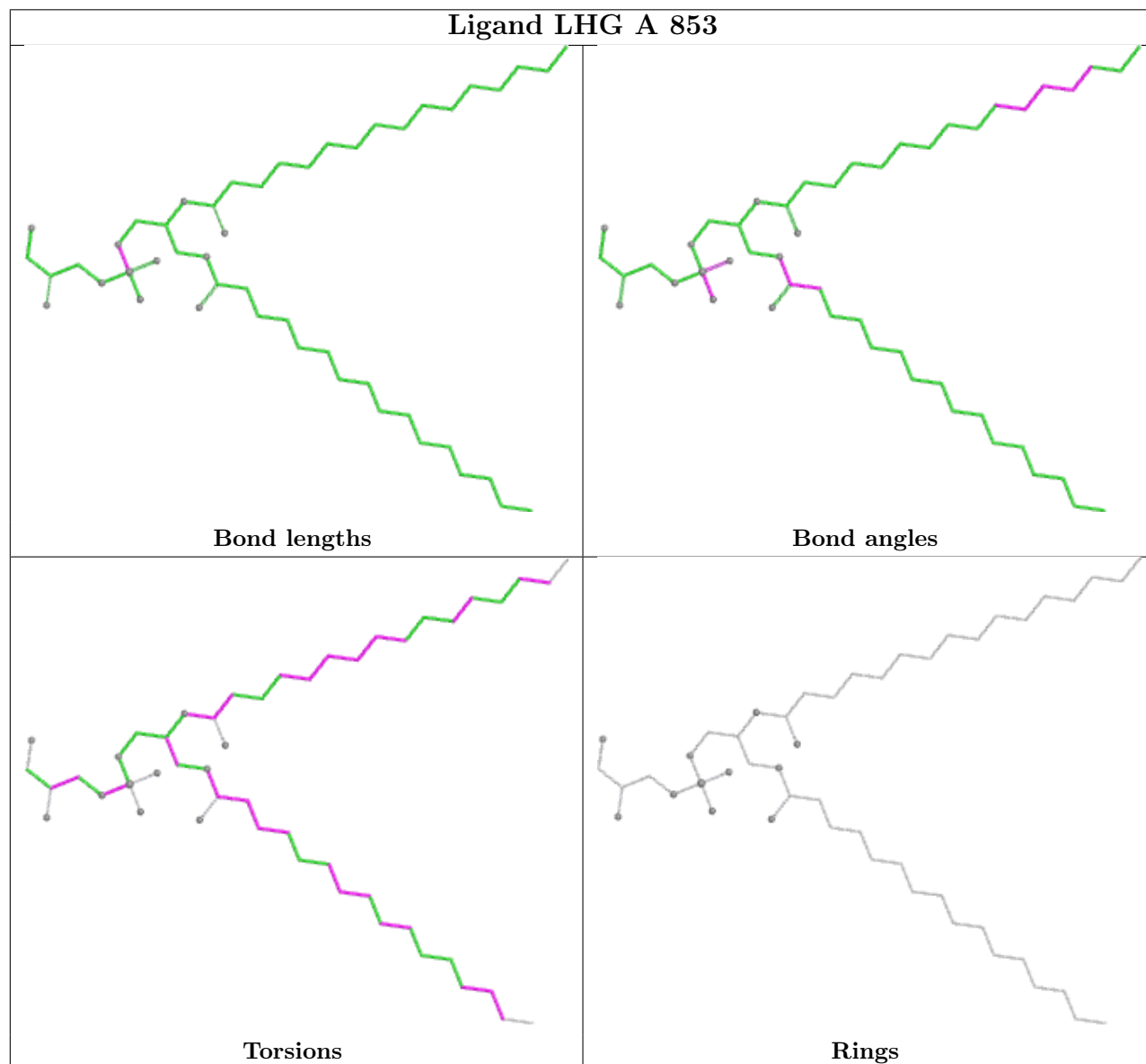
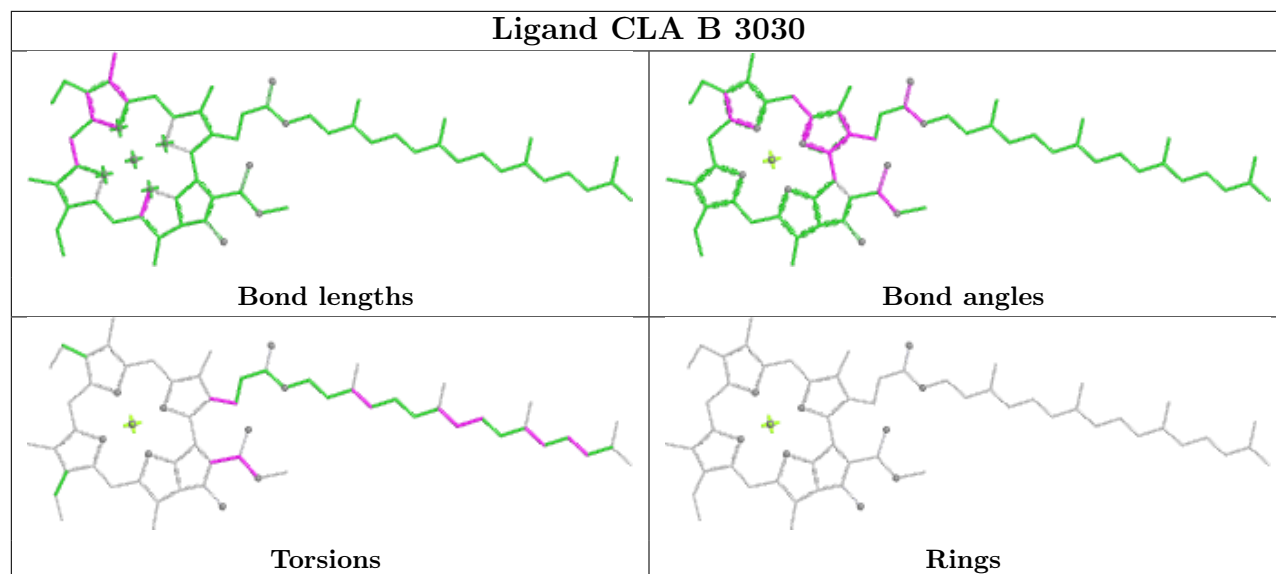


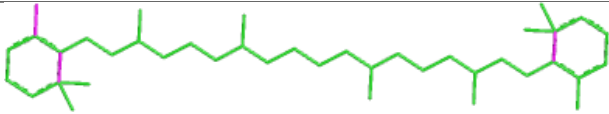
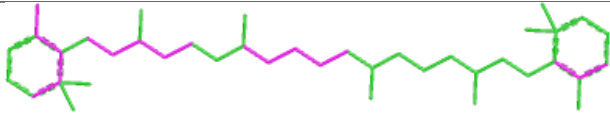
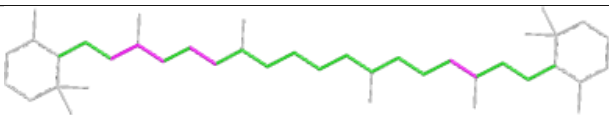
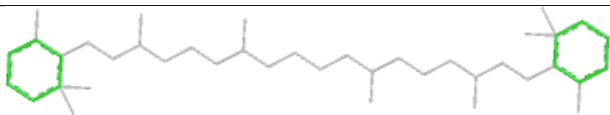
Torsions

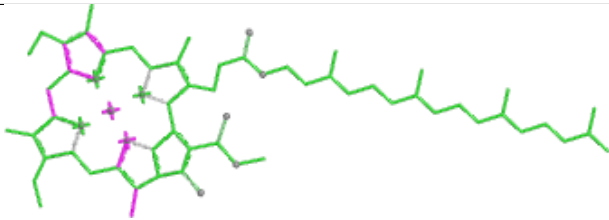
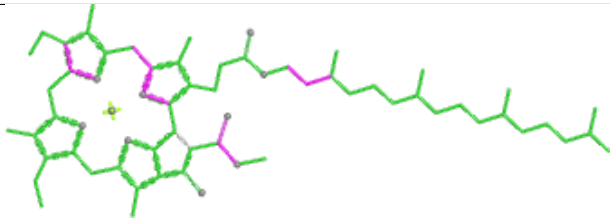
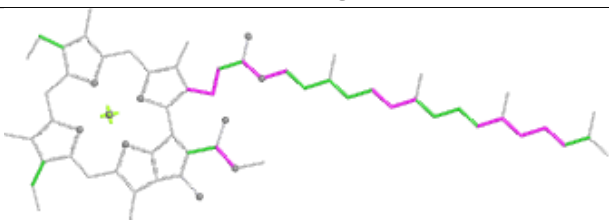
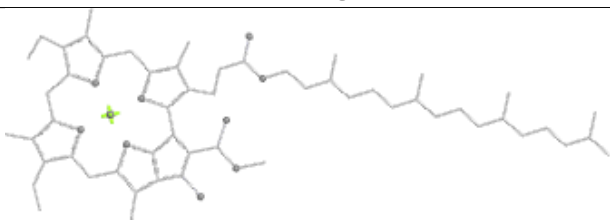


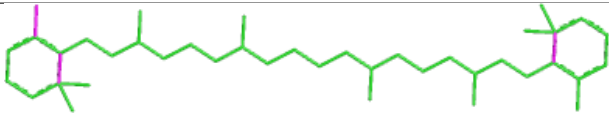
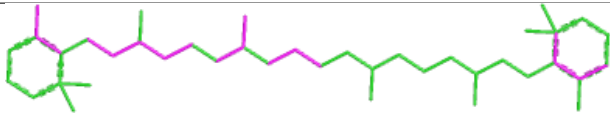
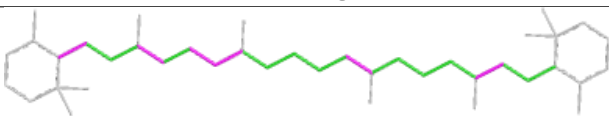
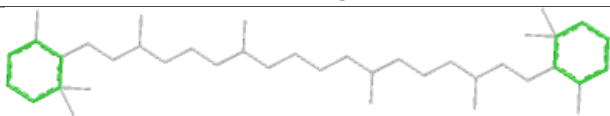
Rings

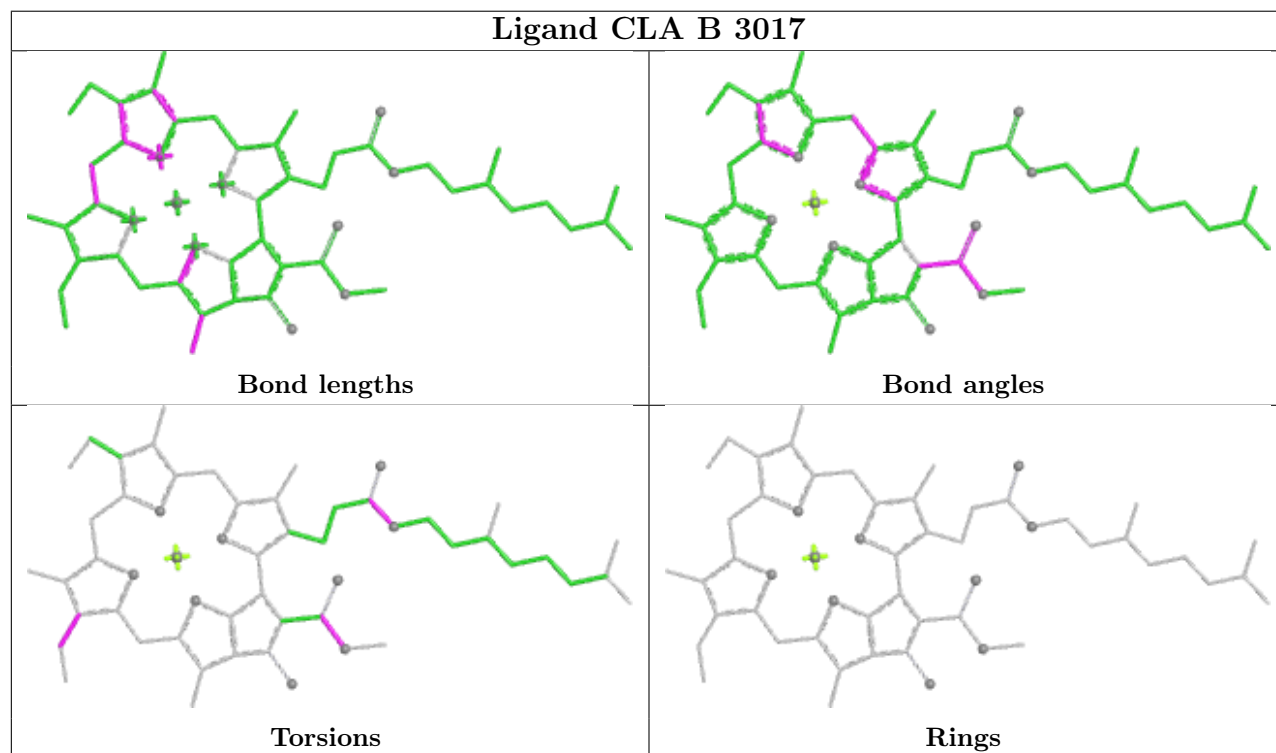
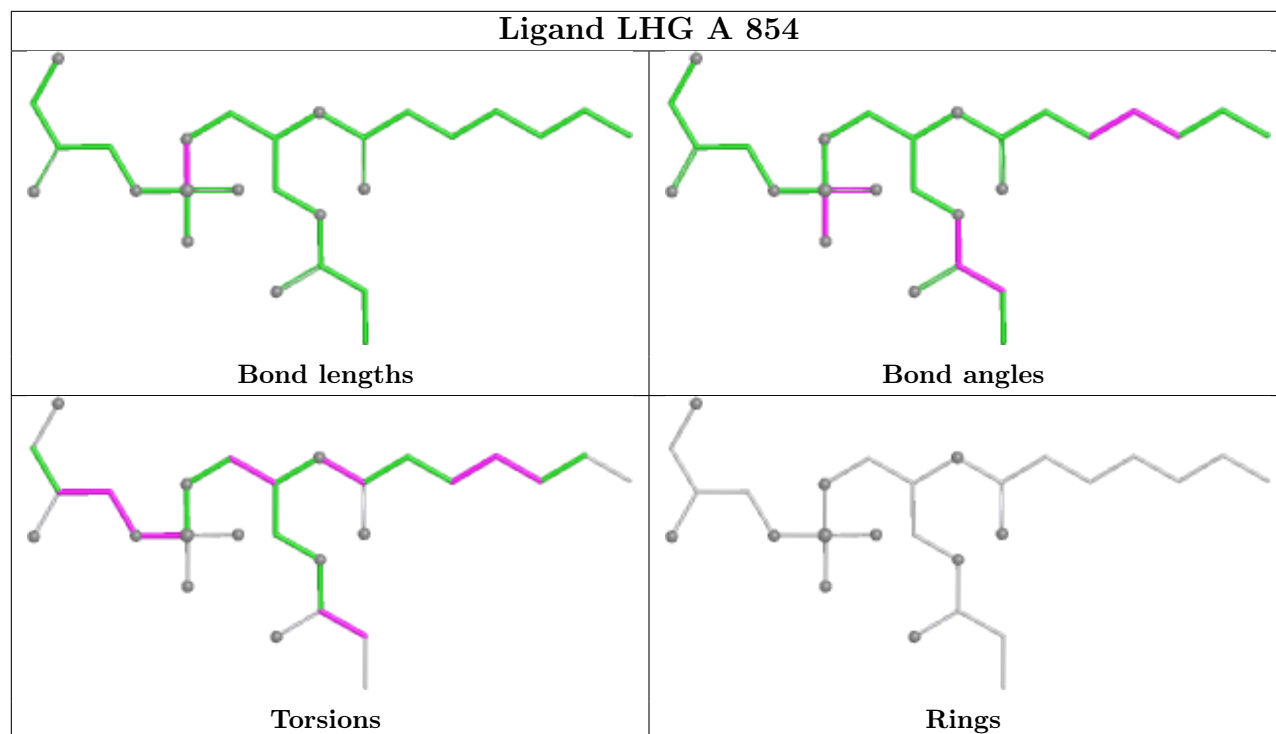


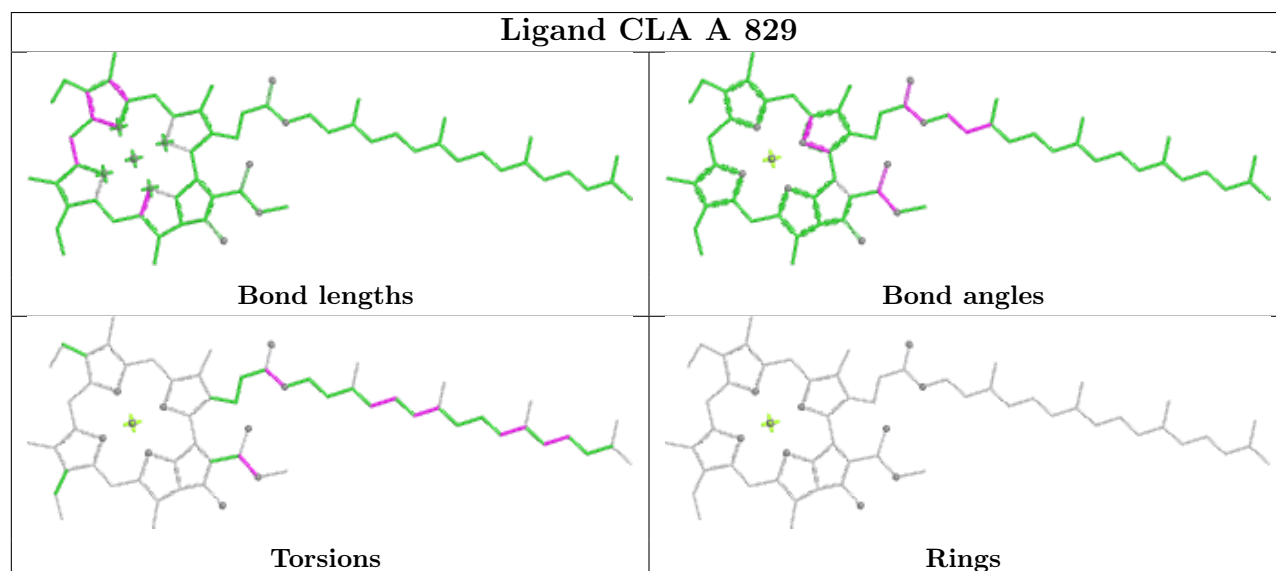
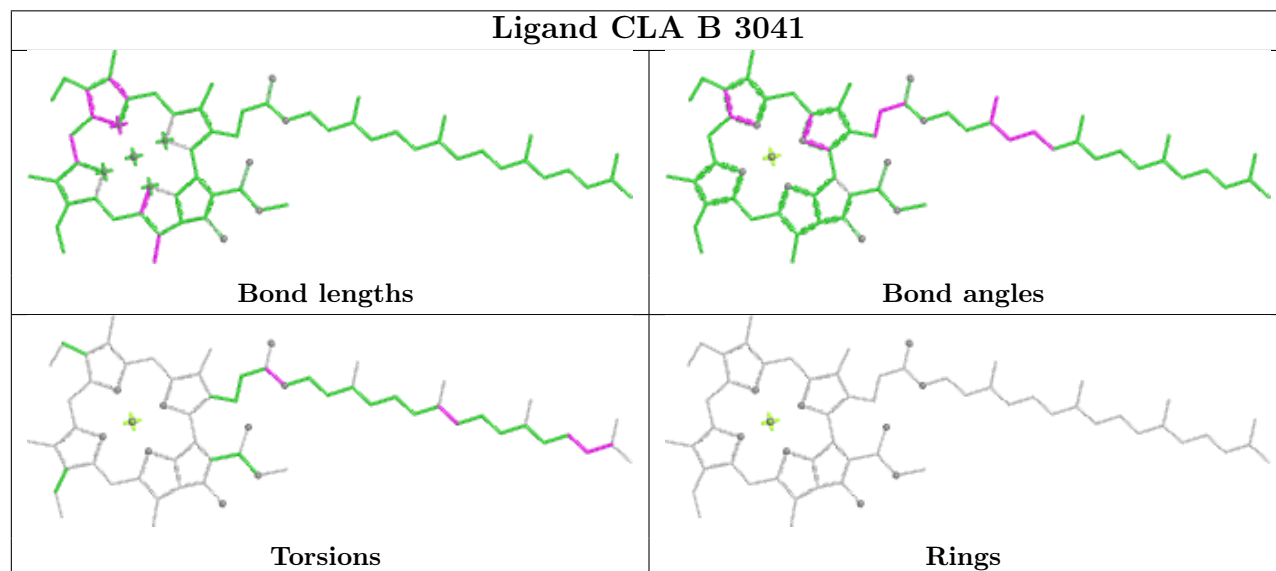
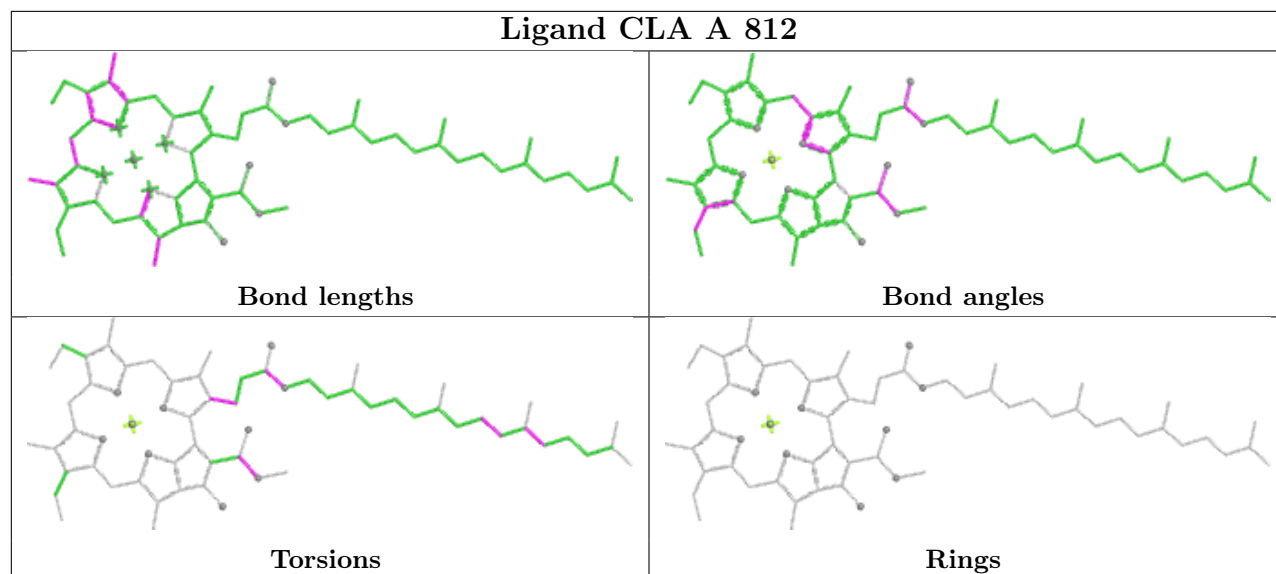


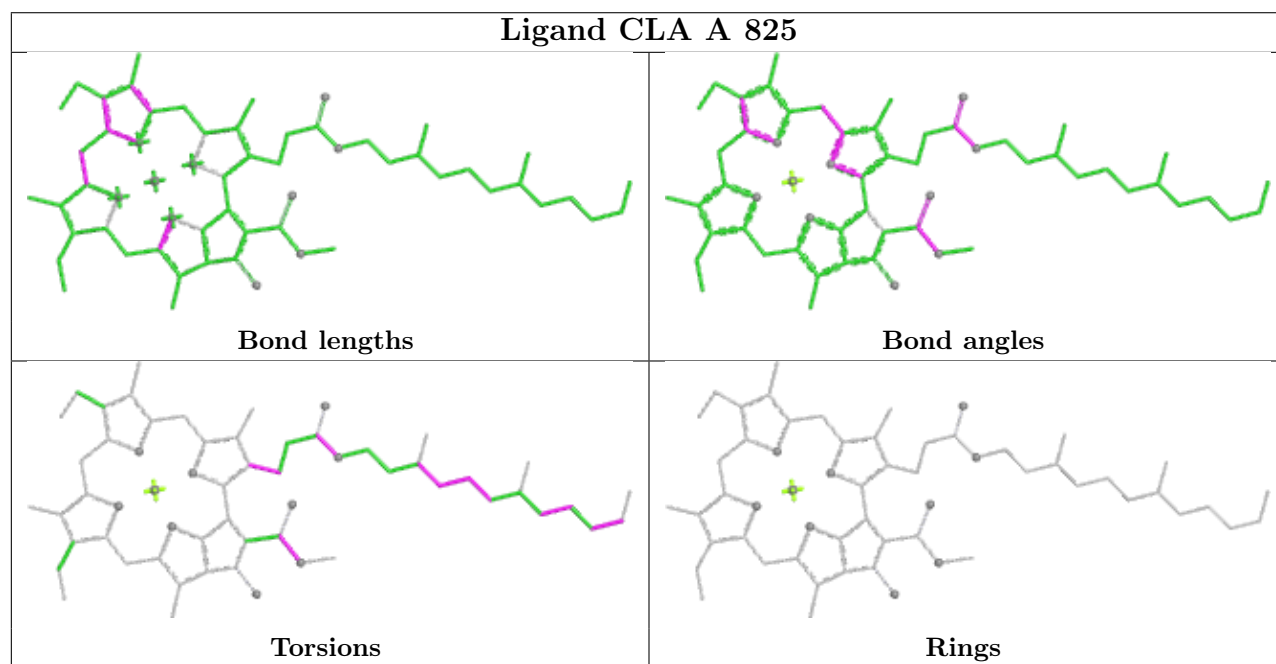
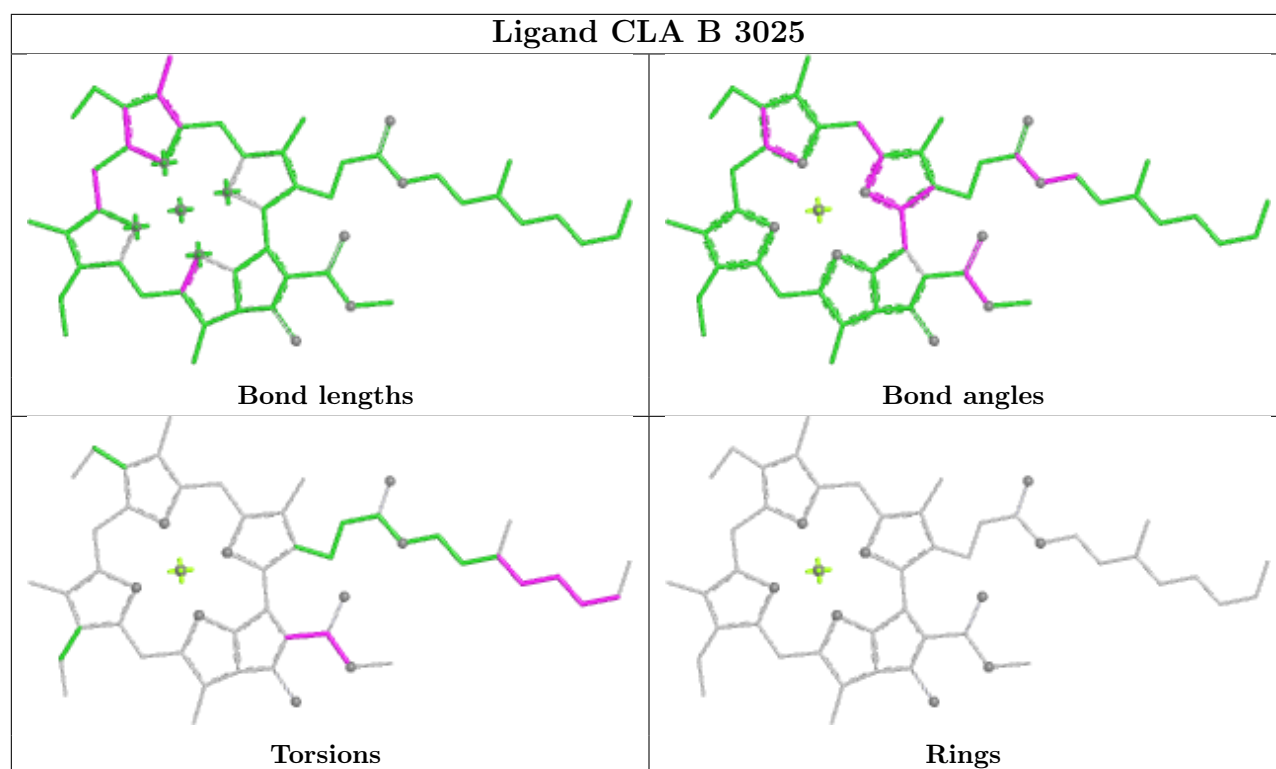
Ligand BCR I 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

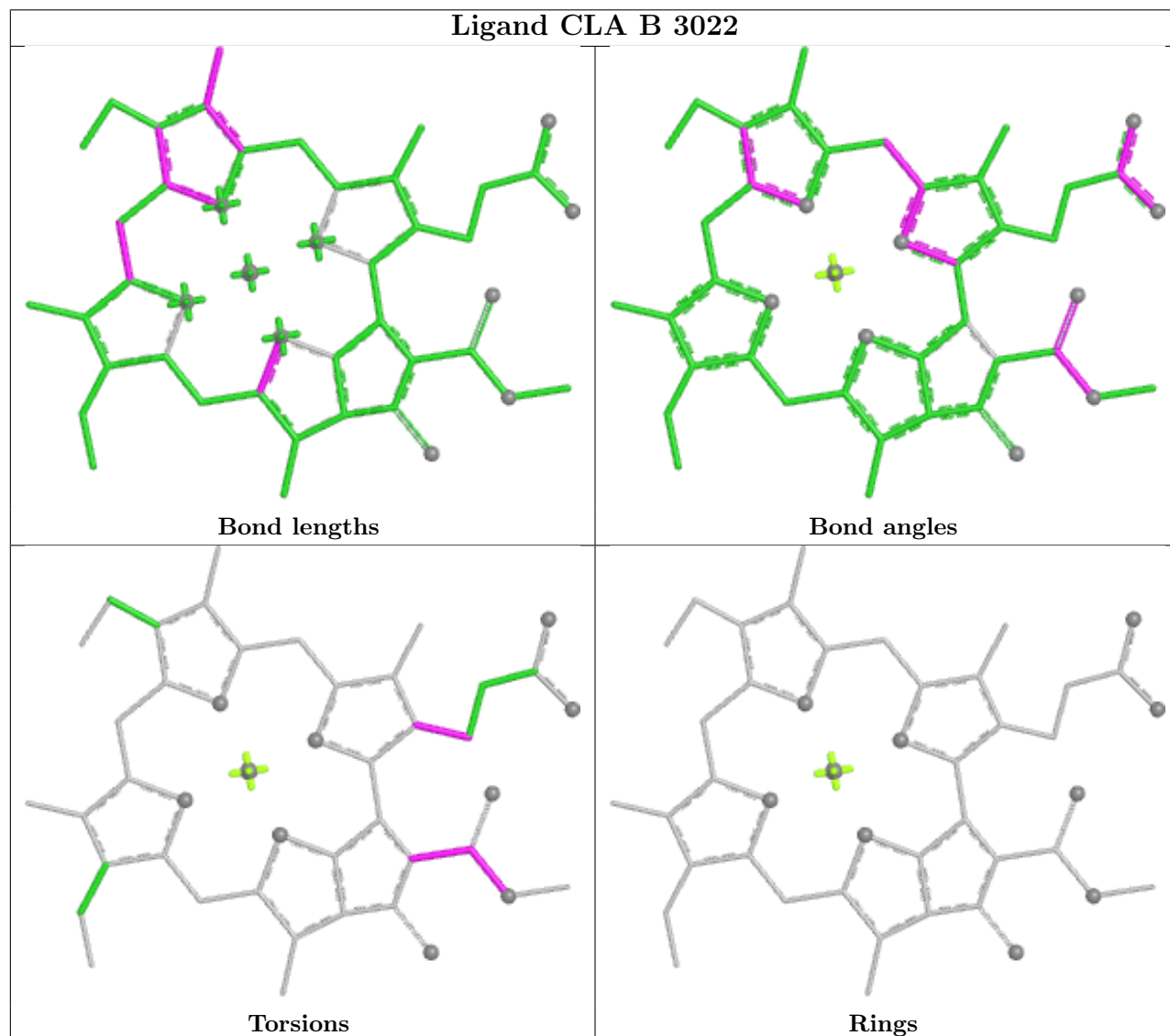
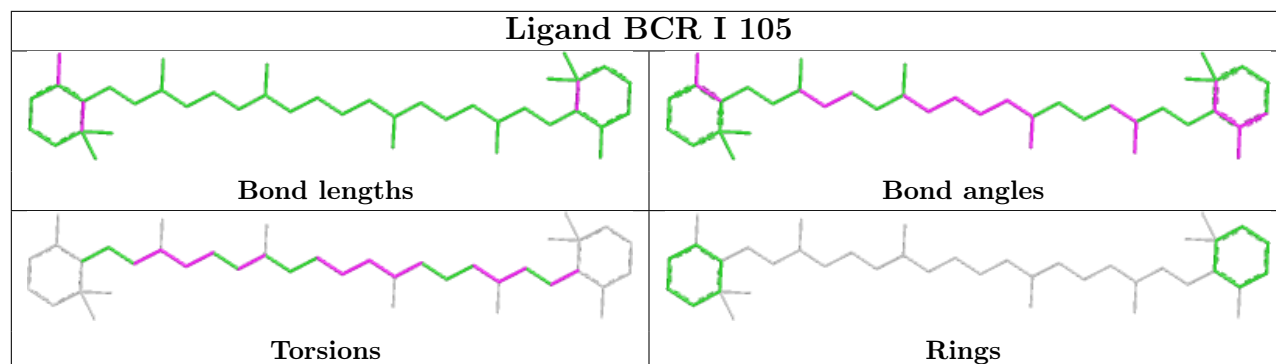
Ligand CLA B 3029	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 3050	
	
Bond lengths	Bond angles
	
Torsions	Rings

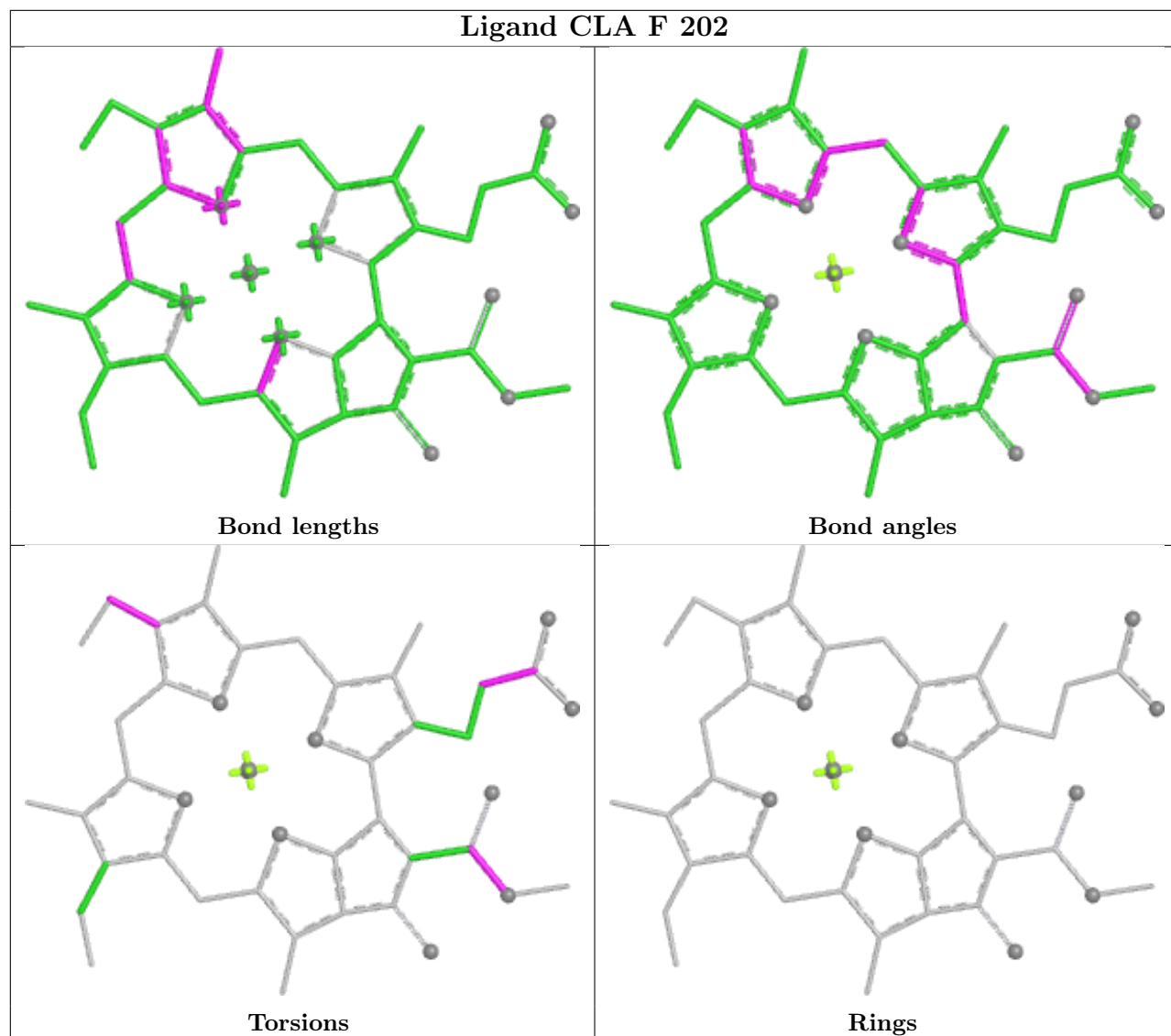




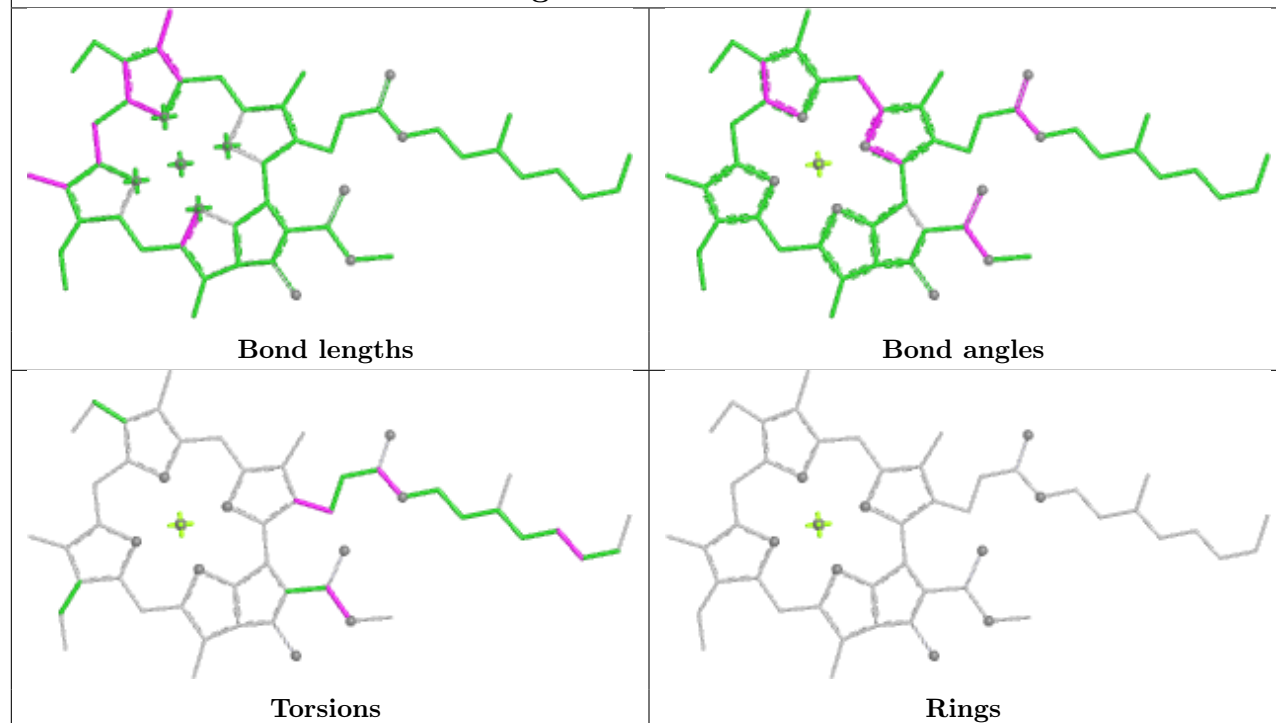




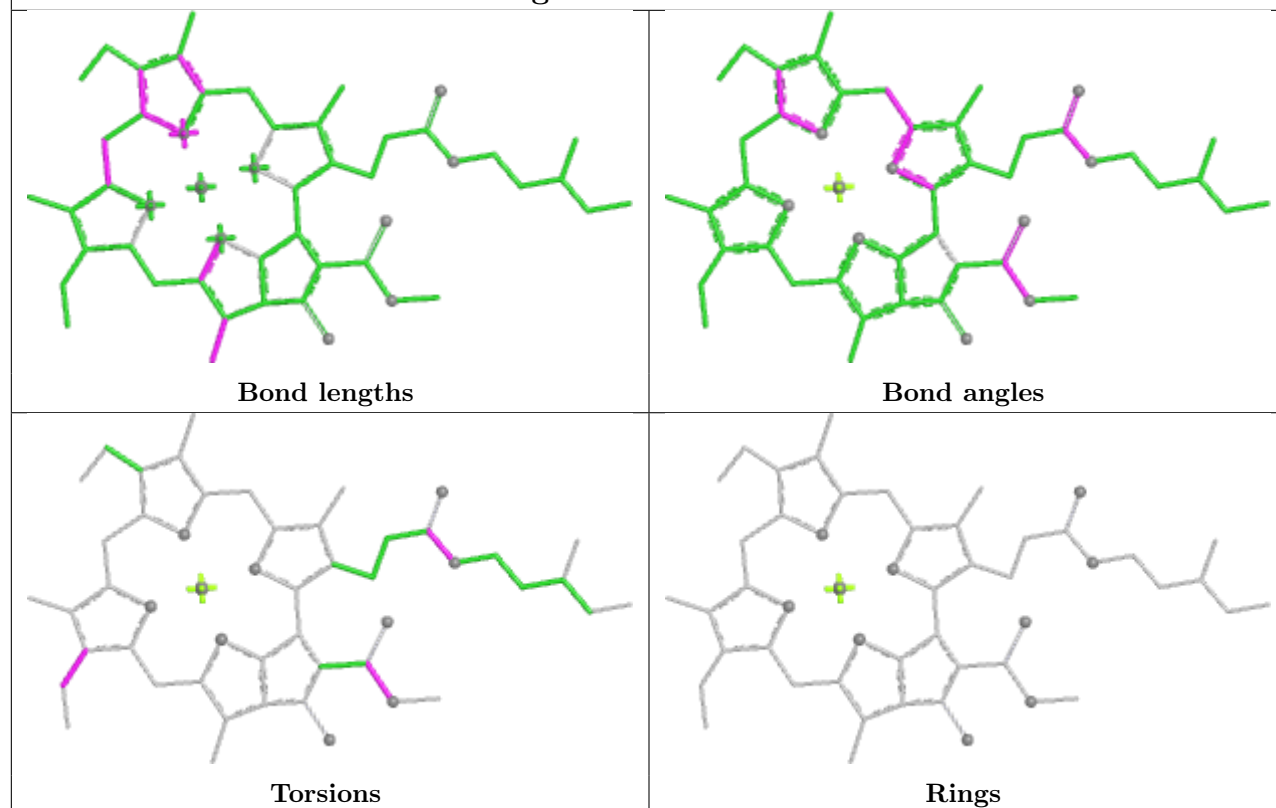
Ligand CLA F 202



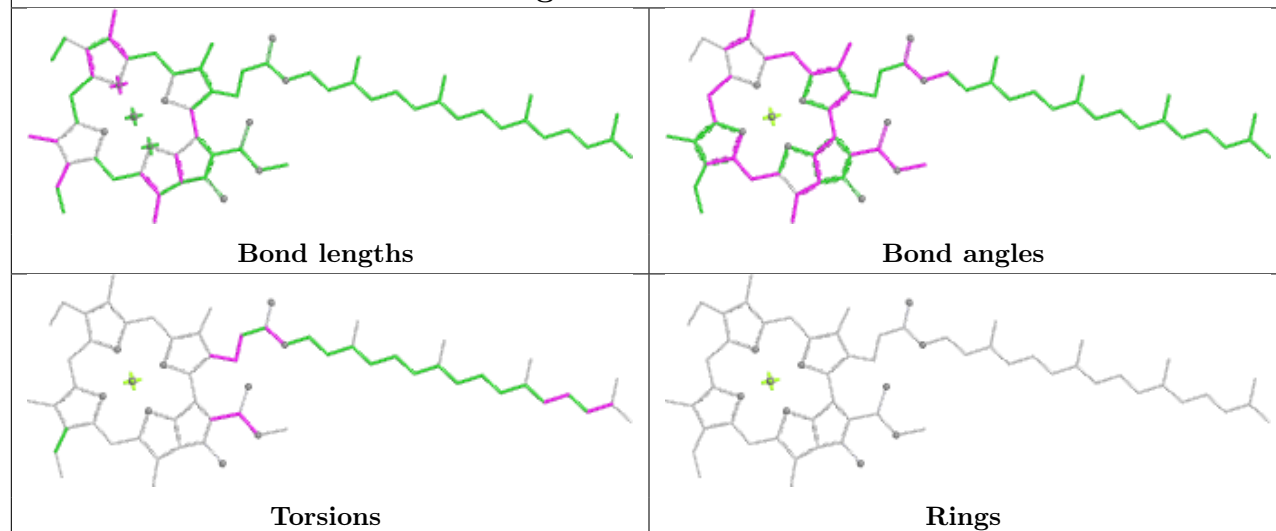
Ligand CLA A 836



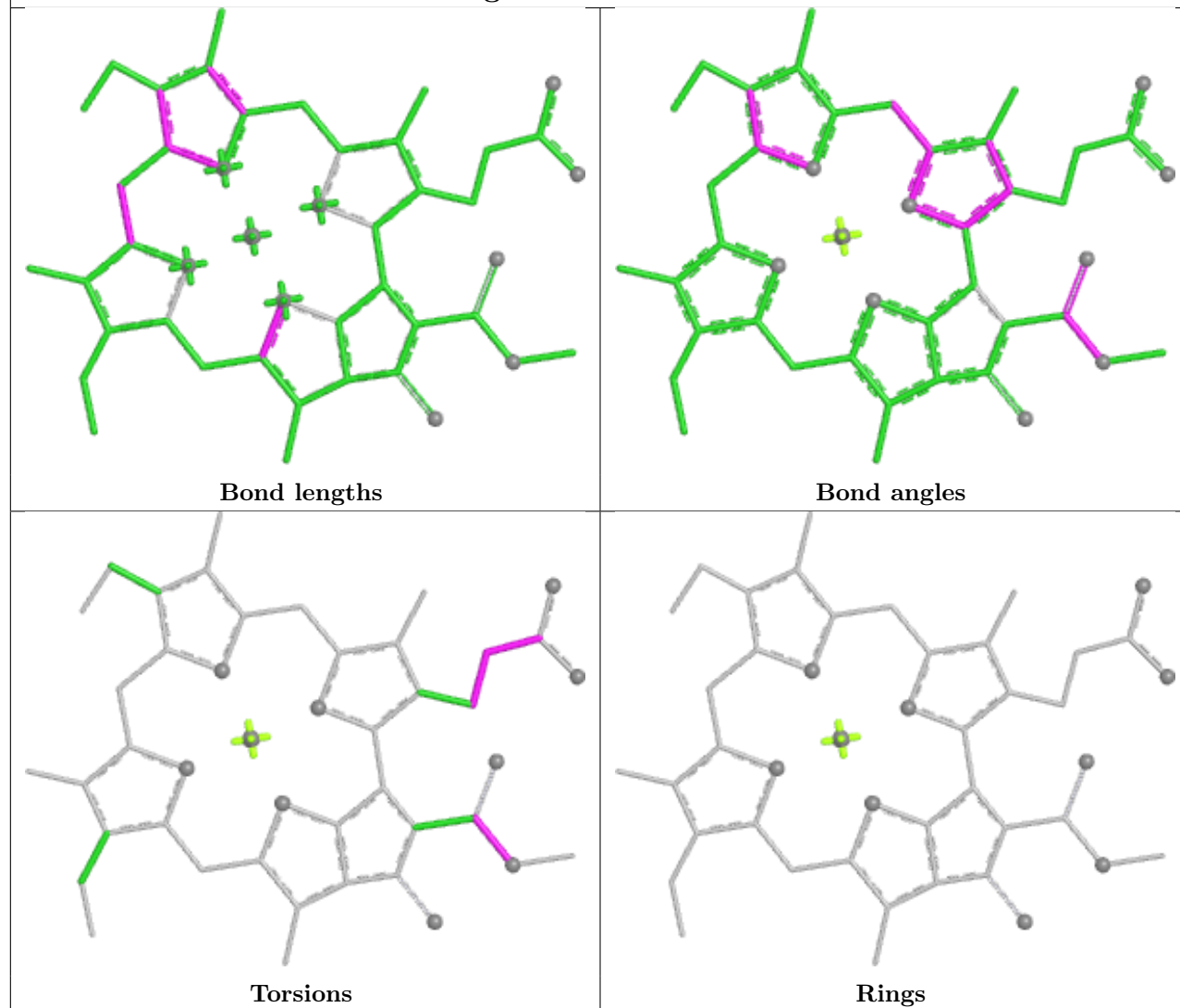
Ligand CLA A 838

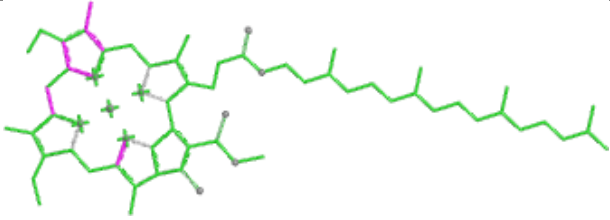
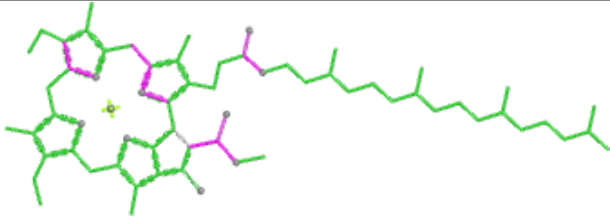
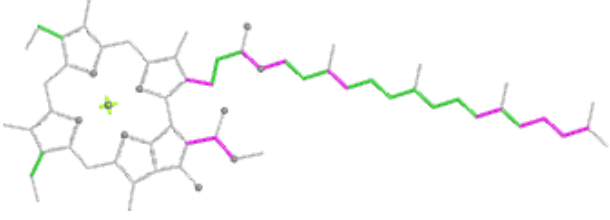
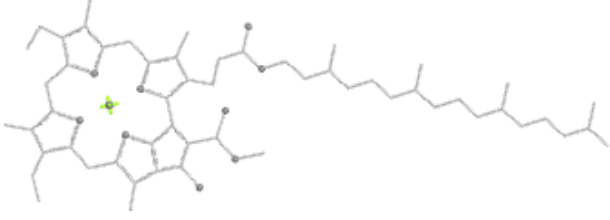
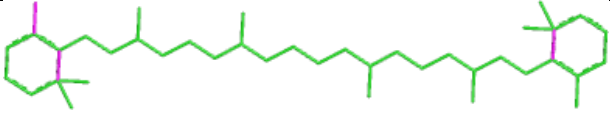
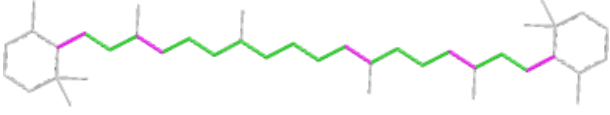
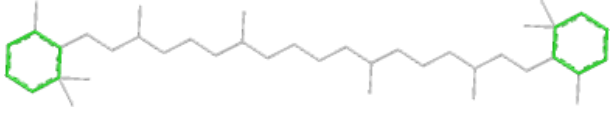
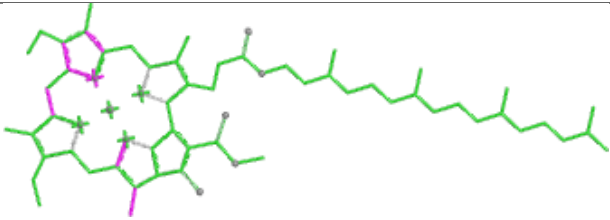
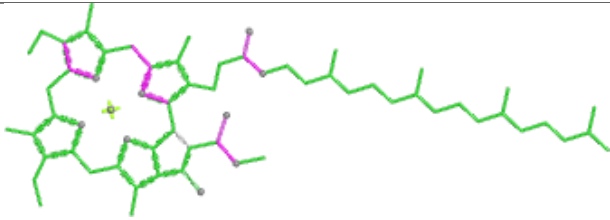
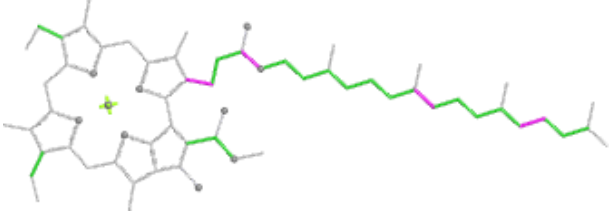
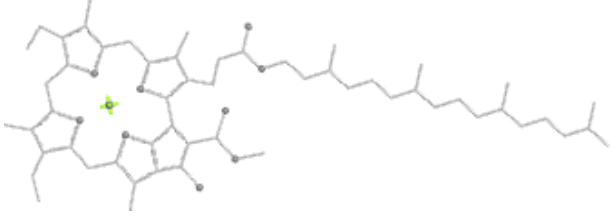


Ligand CL0 A 801

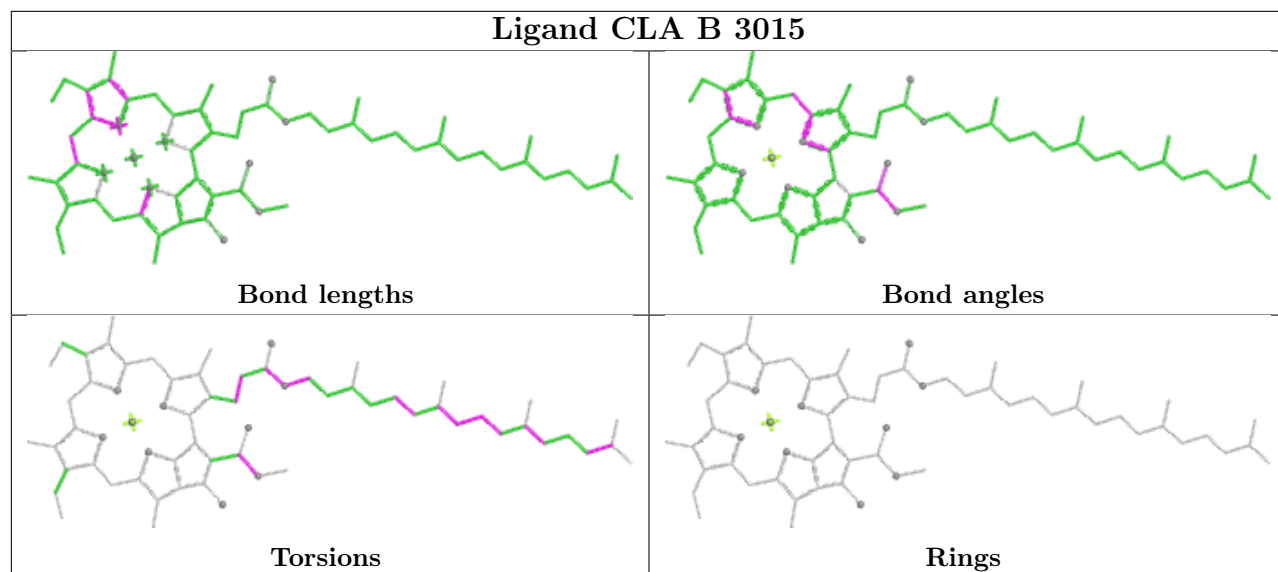


Ligand CLA B 3013

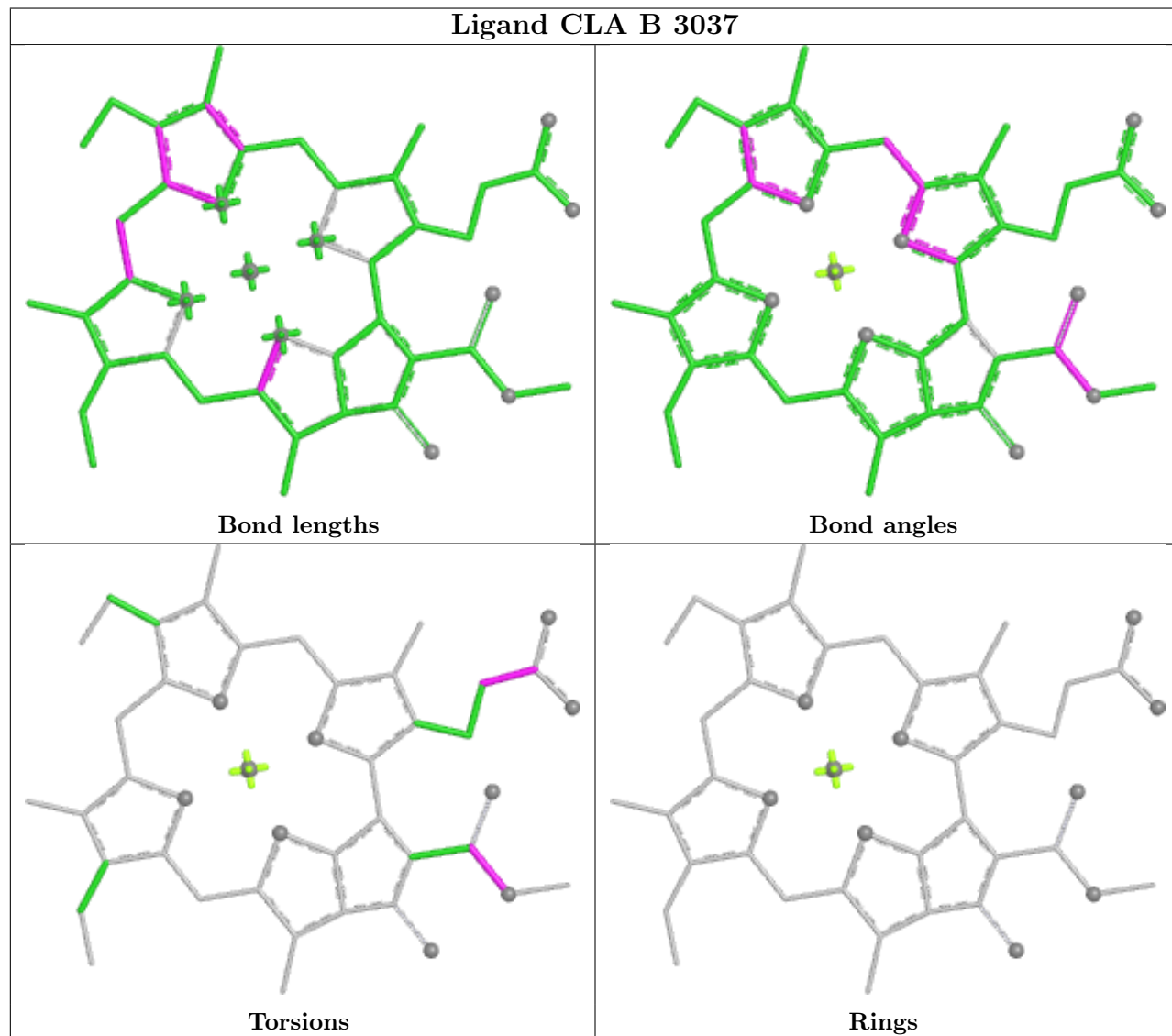


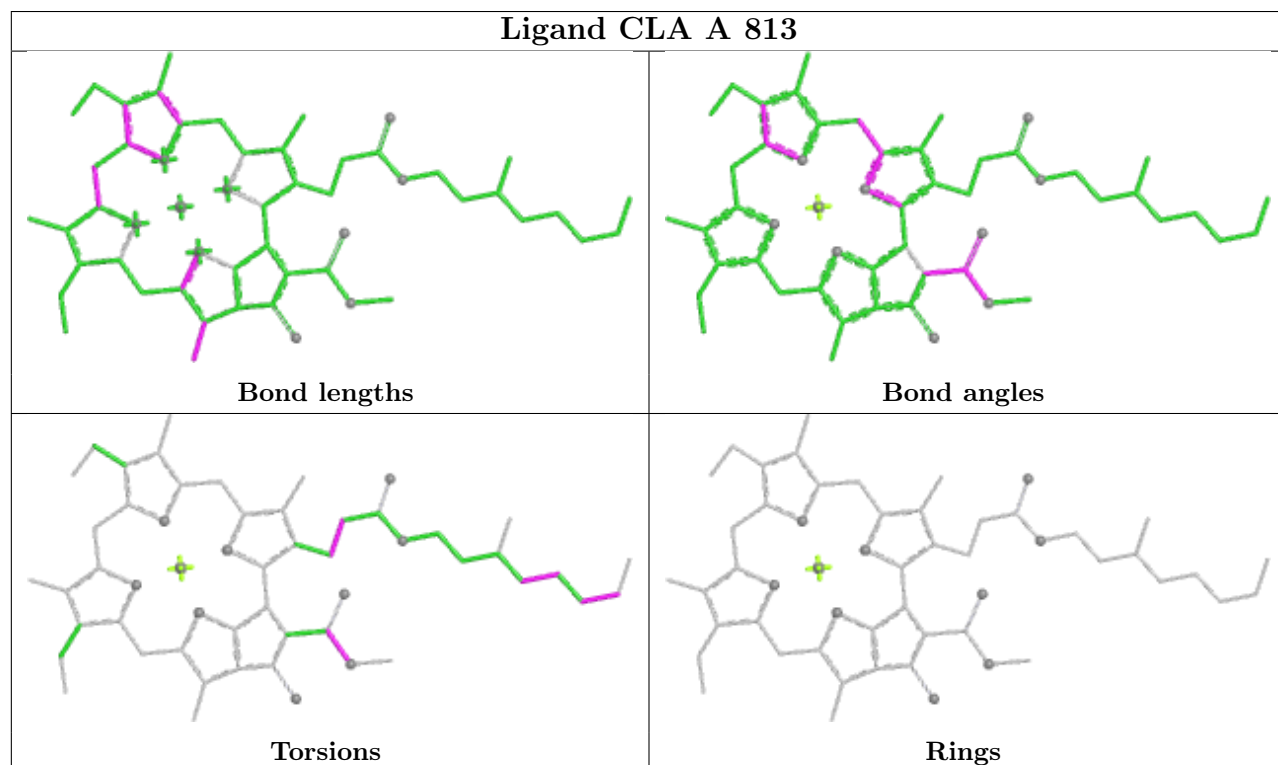
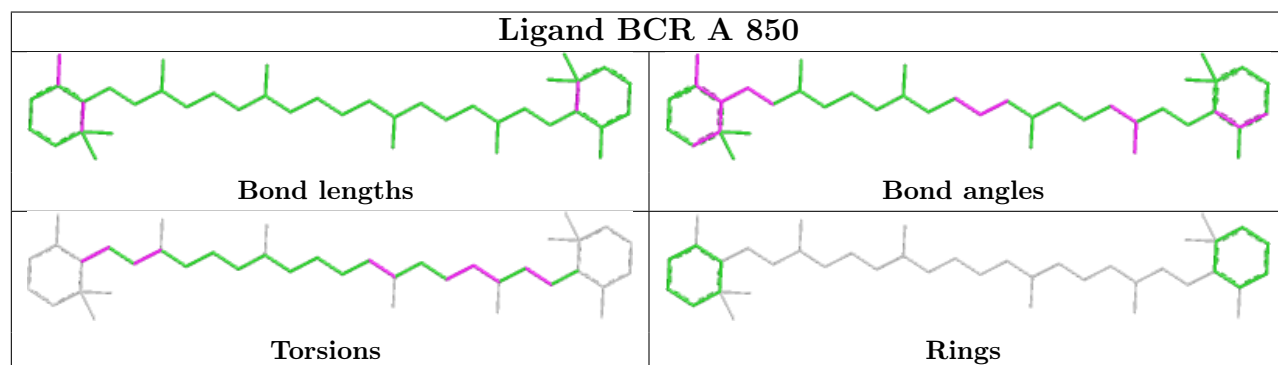
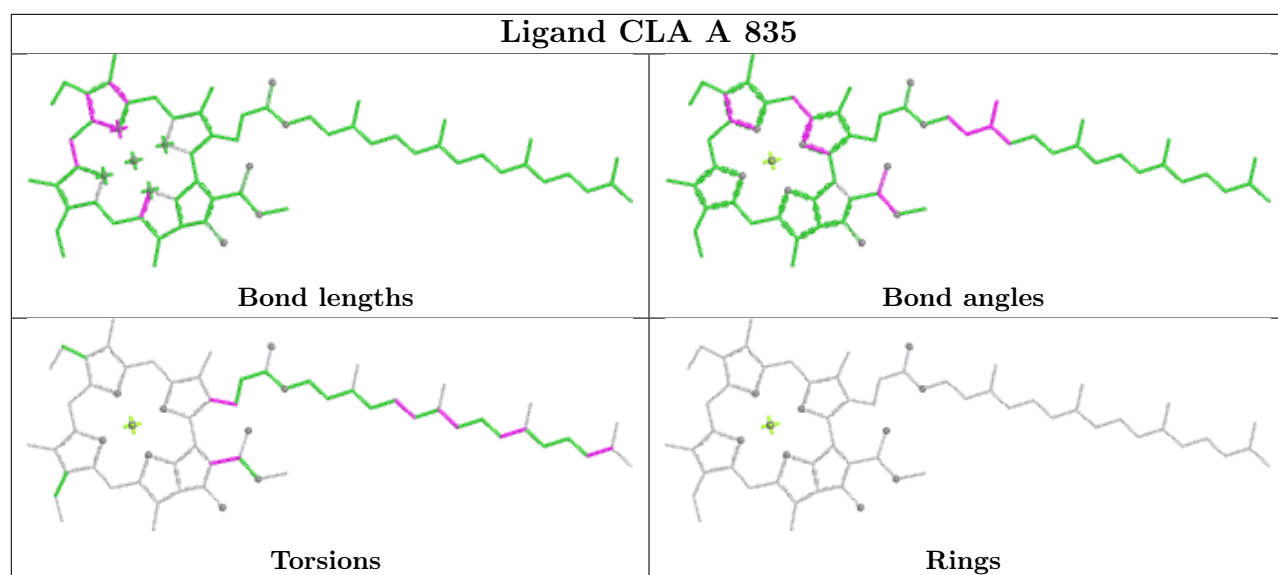
Ligand CLA A 806	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR M 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA A 843	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 3015

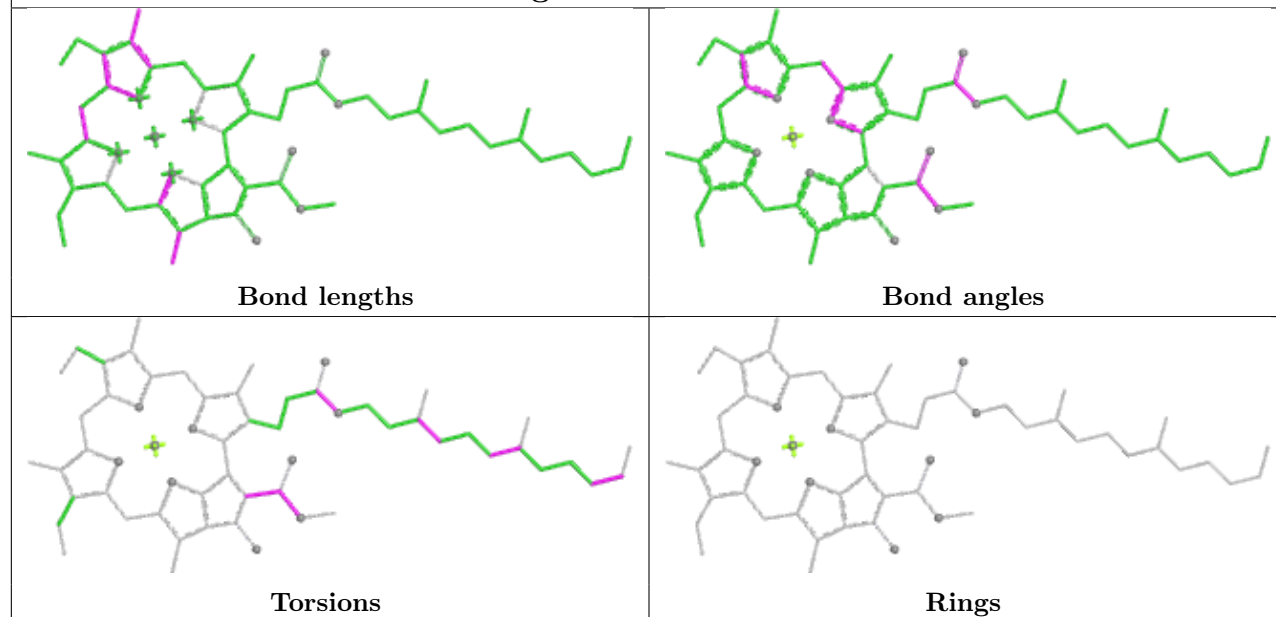


Ligand CLA B 3037

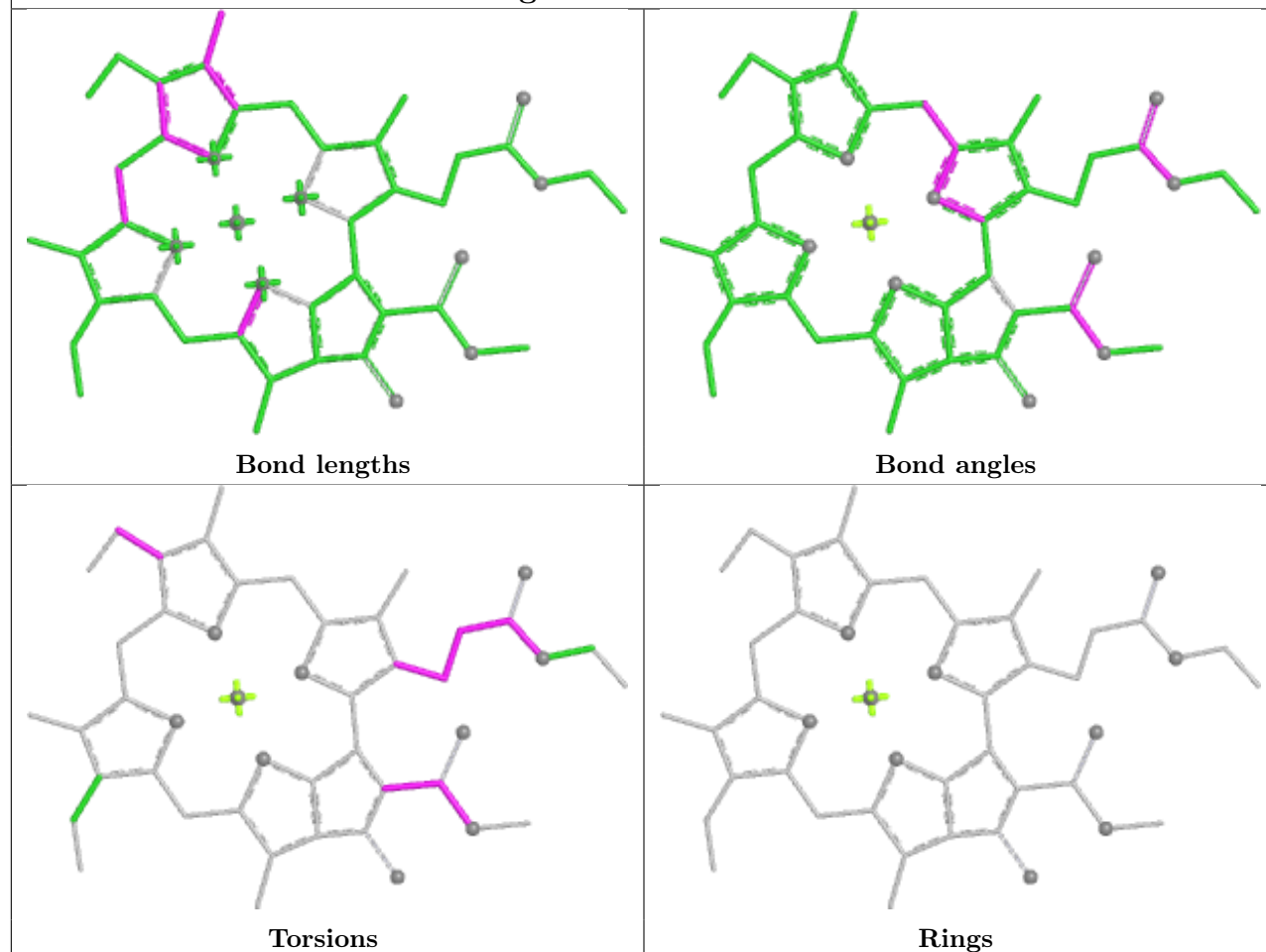




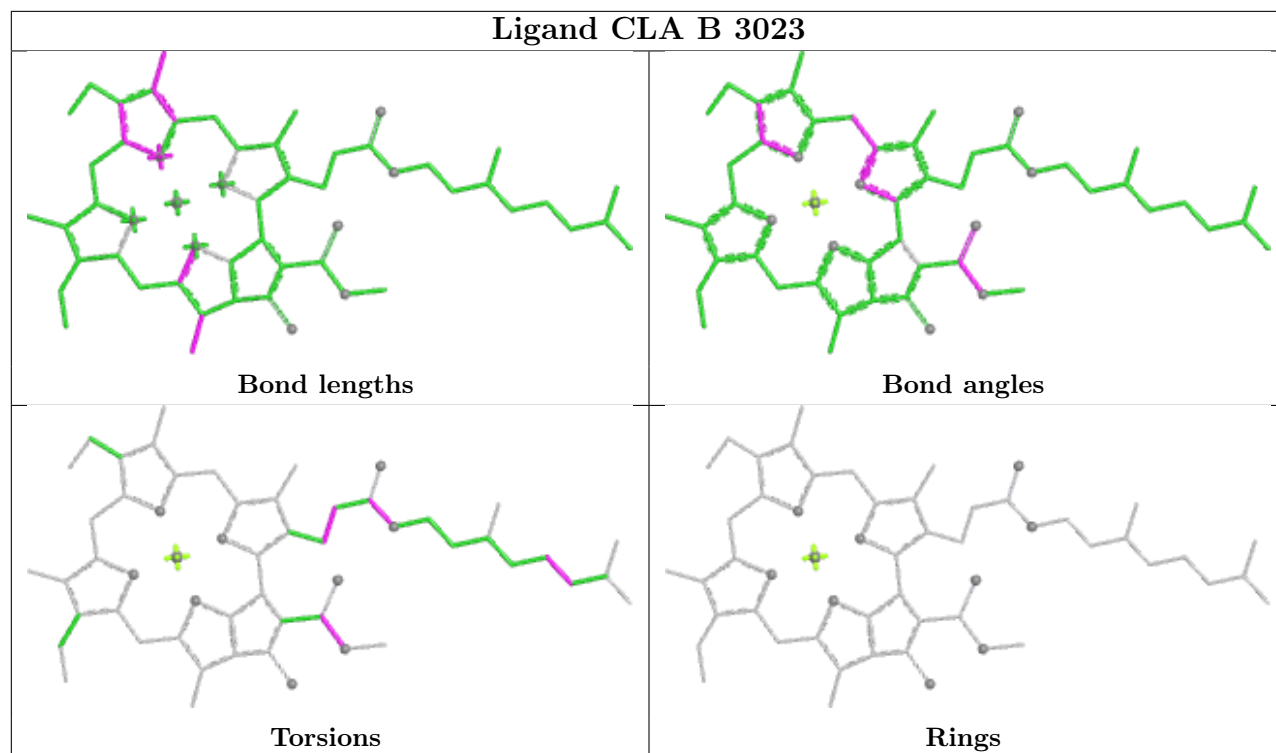
Ligand CLA A 805



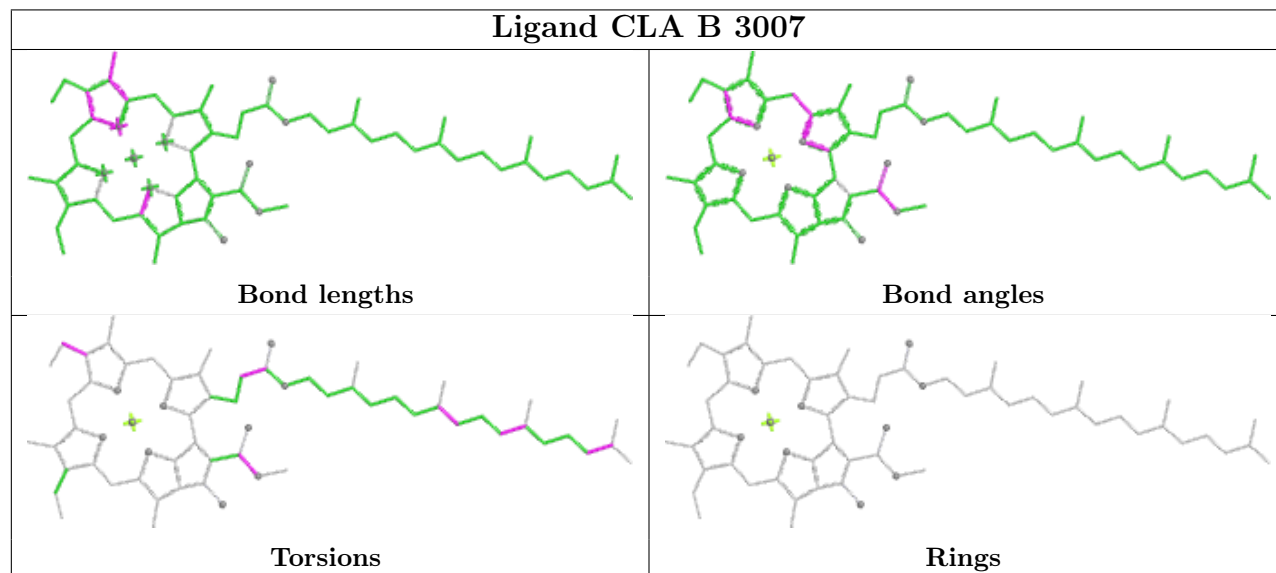
Ligand CLA B 3021

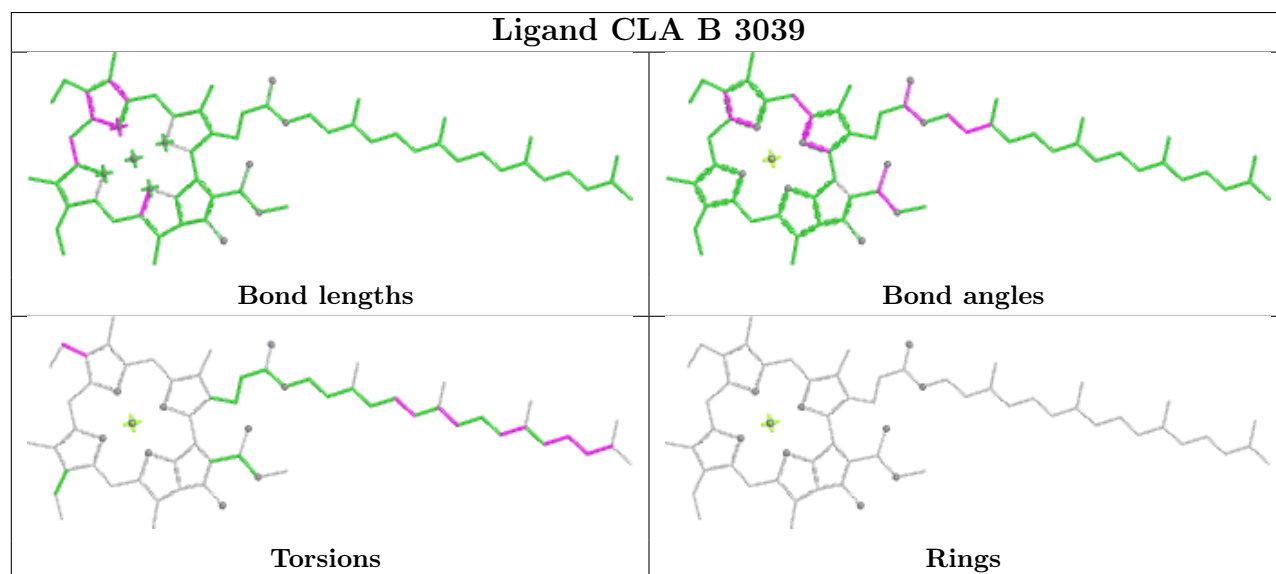
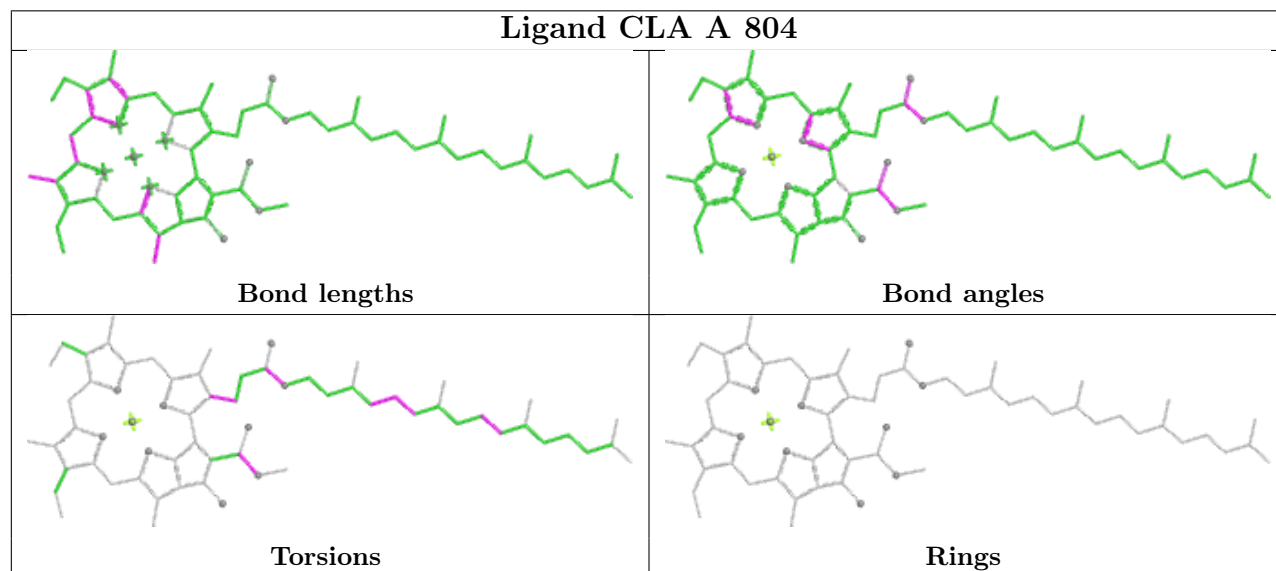
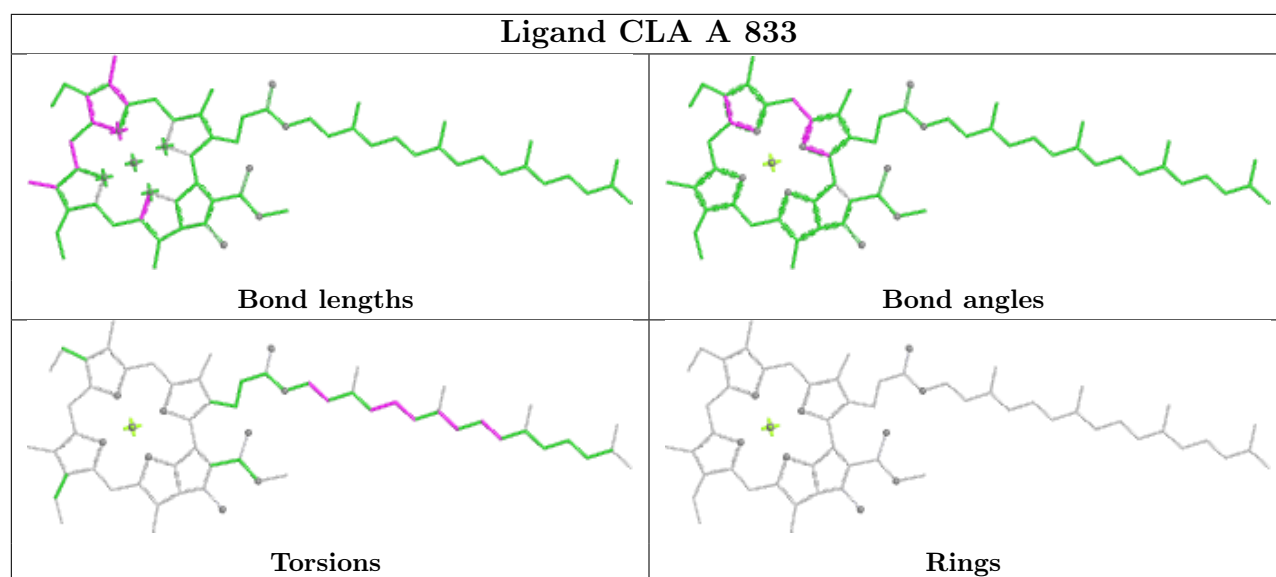


Ligand CLA B 3023

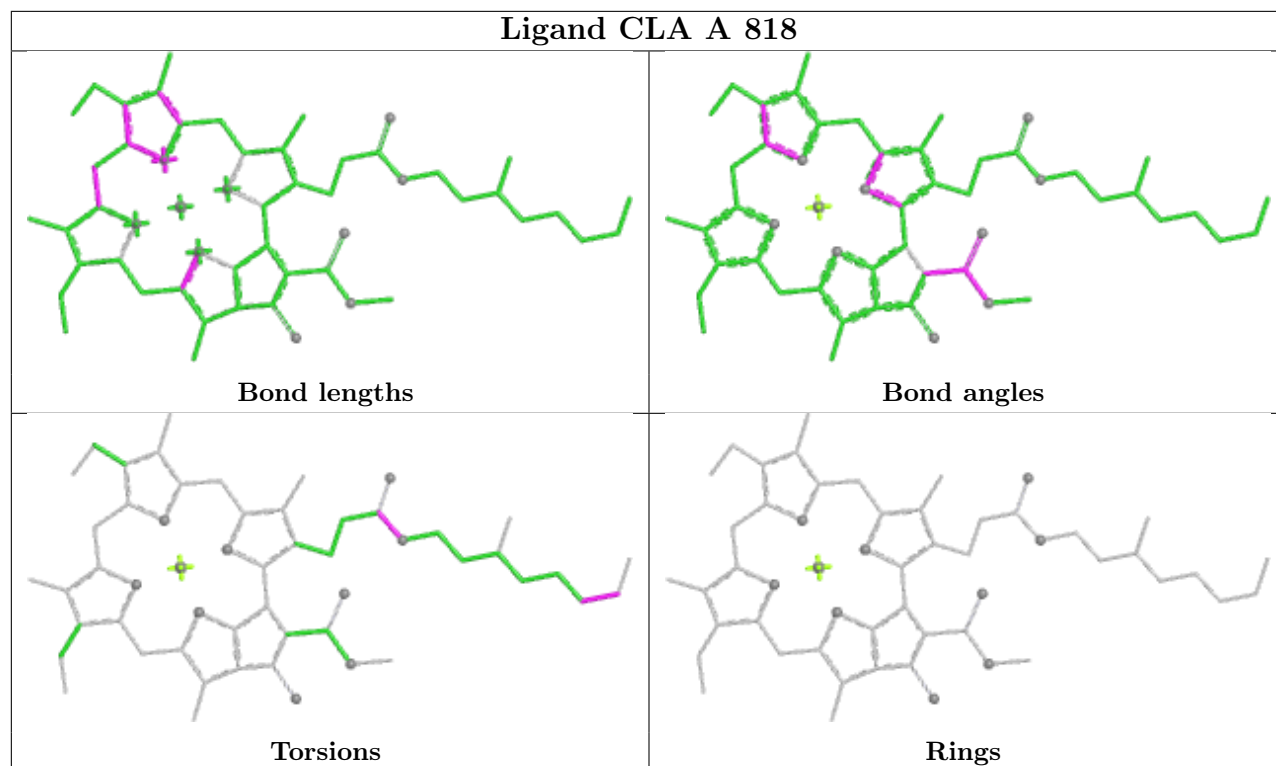


Ligand CLA B 3007

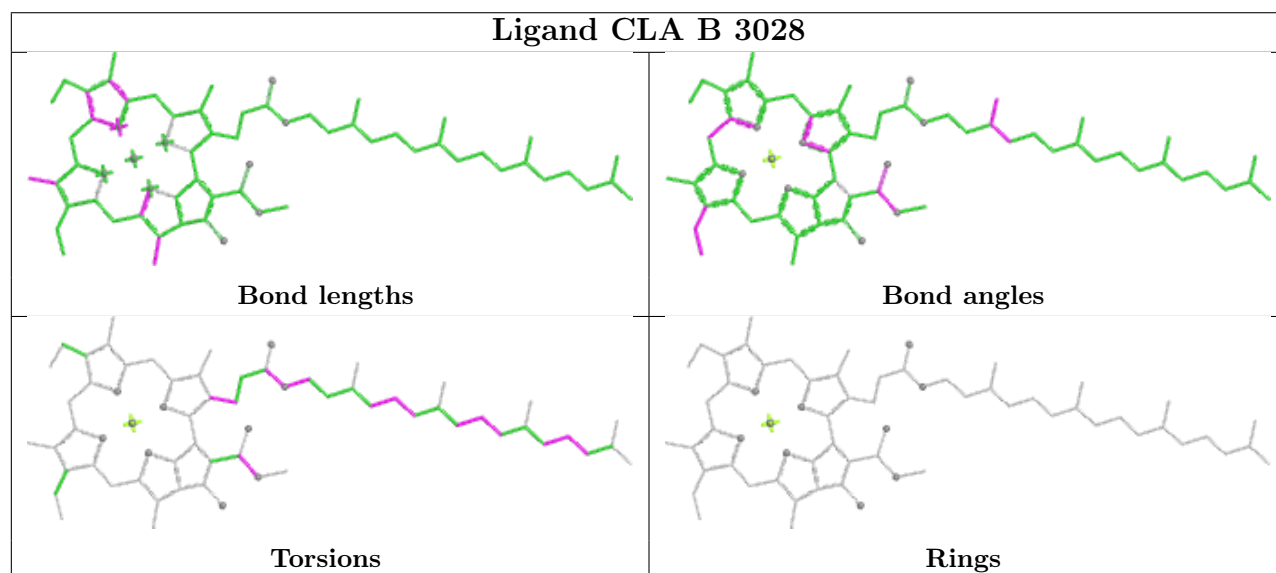


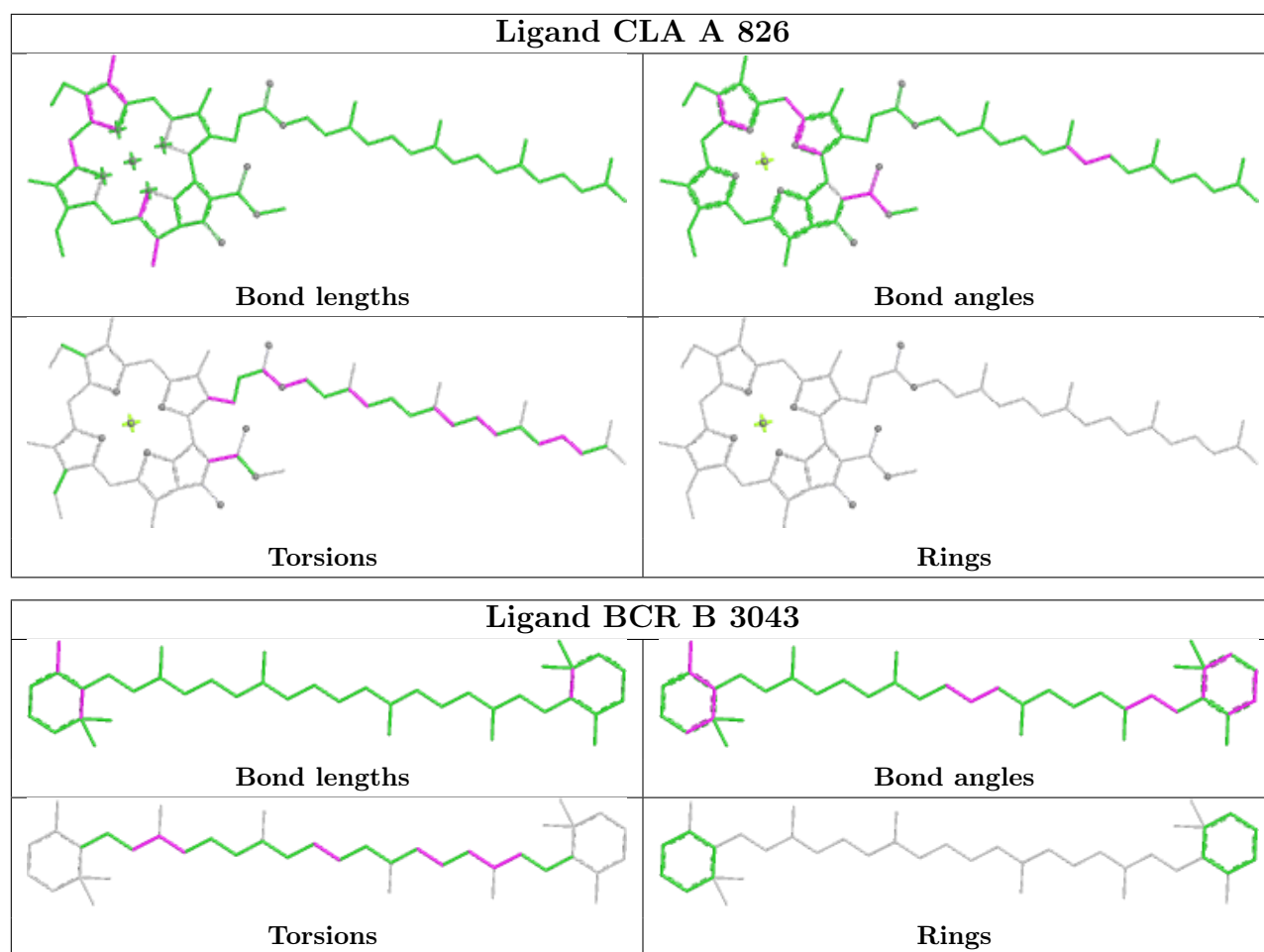


Ligand CLA A 818

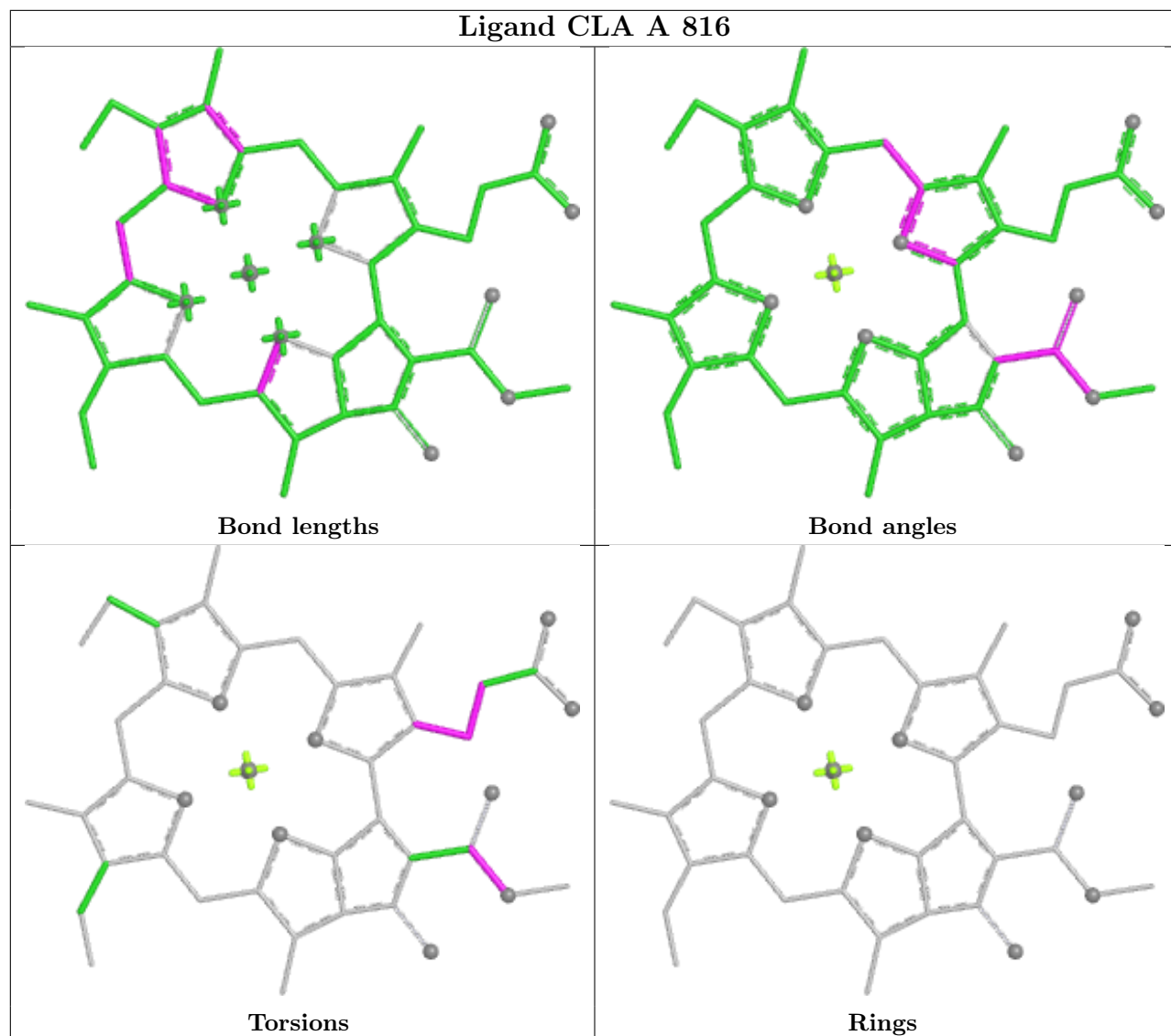


Ligand CLA B 3028

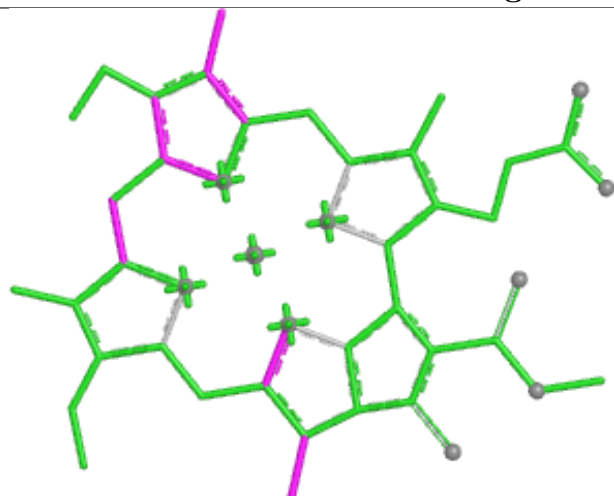




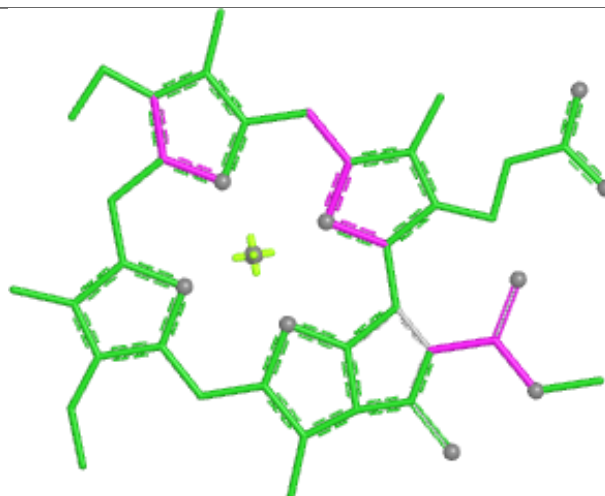
Ligand CLA A 816



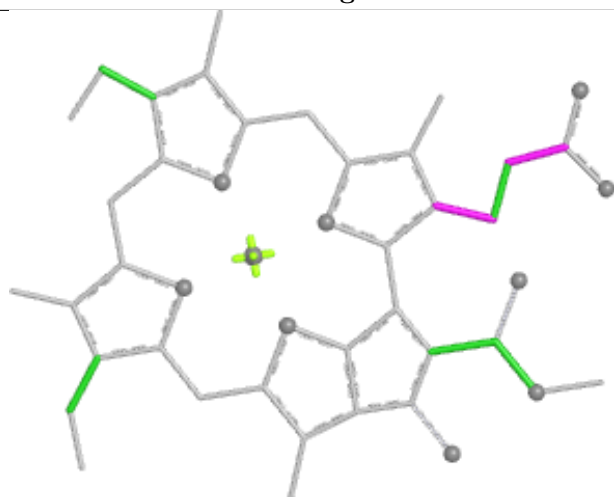
Ligand CLA X 1701



Bond lengths



Bond angles

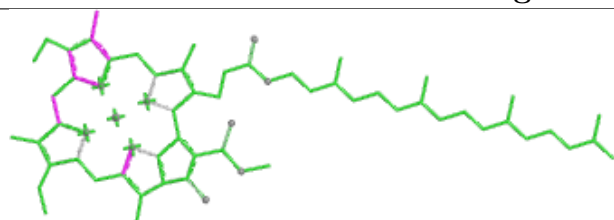


Torsions

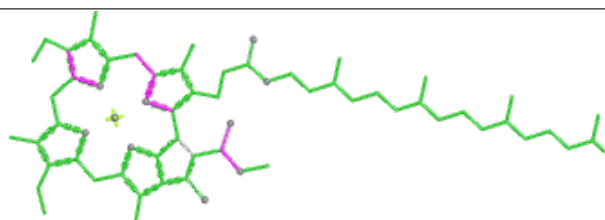


Rings

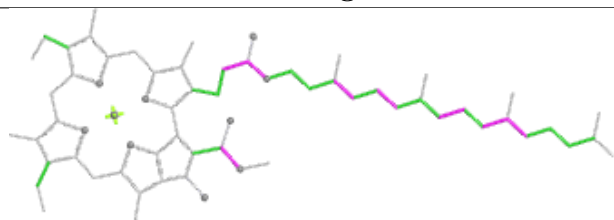
Ligand CLA A 807



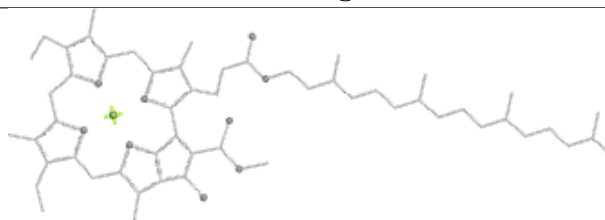
Bond lengths



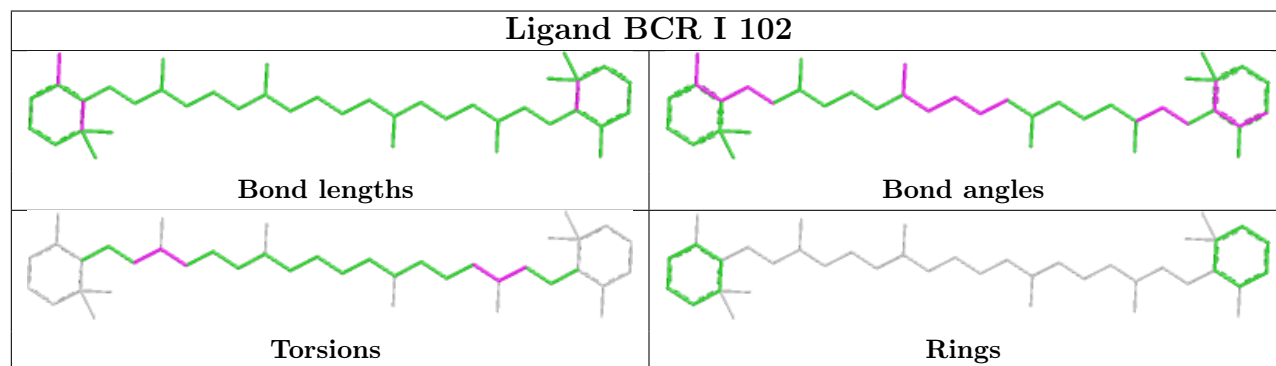
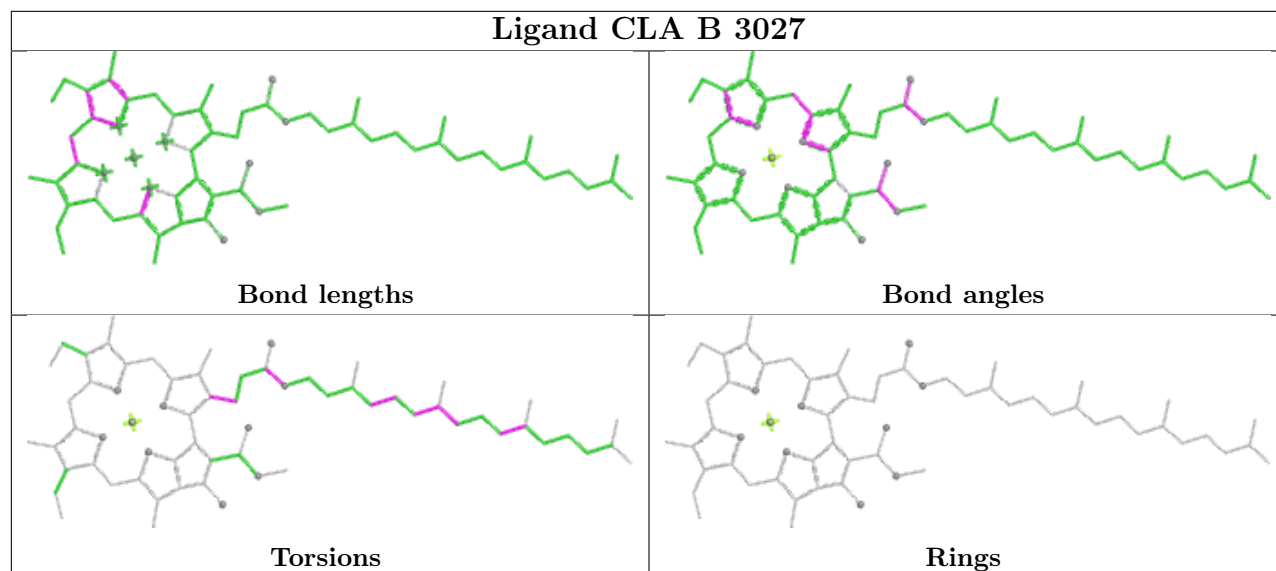
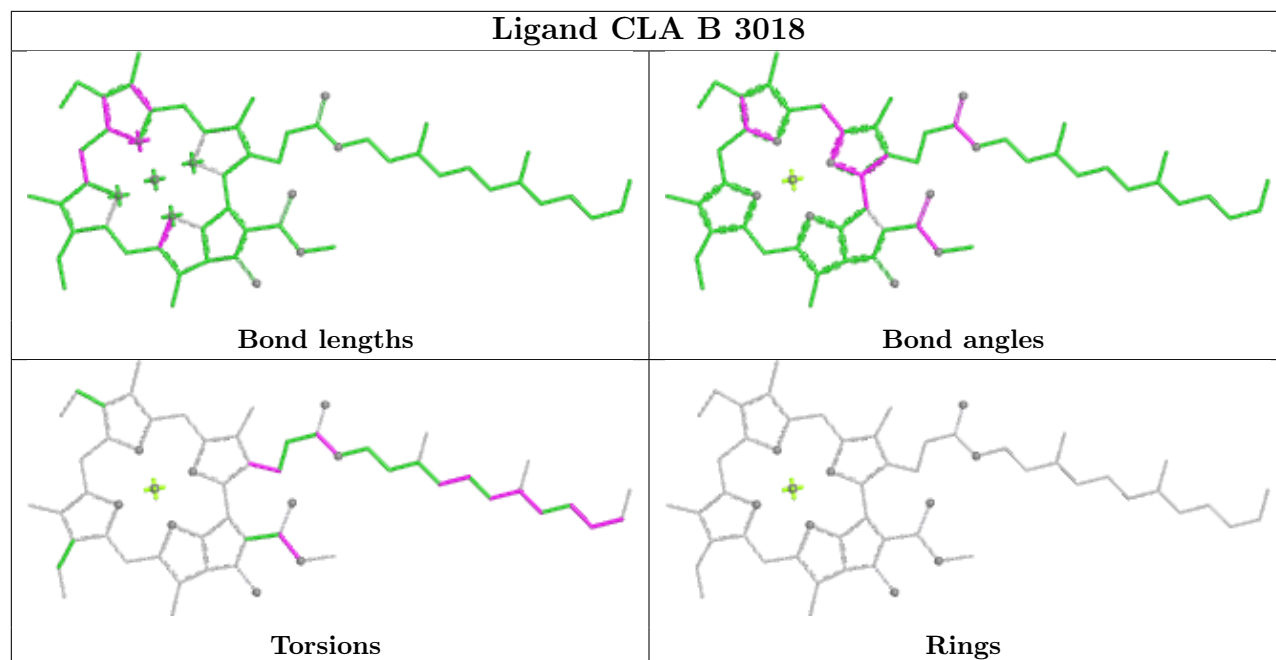
Bond angles

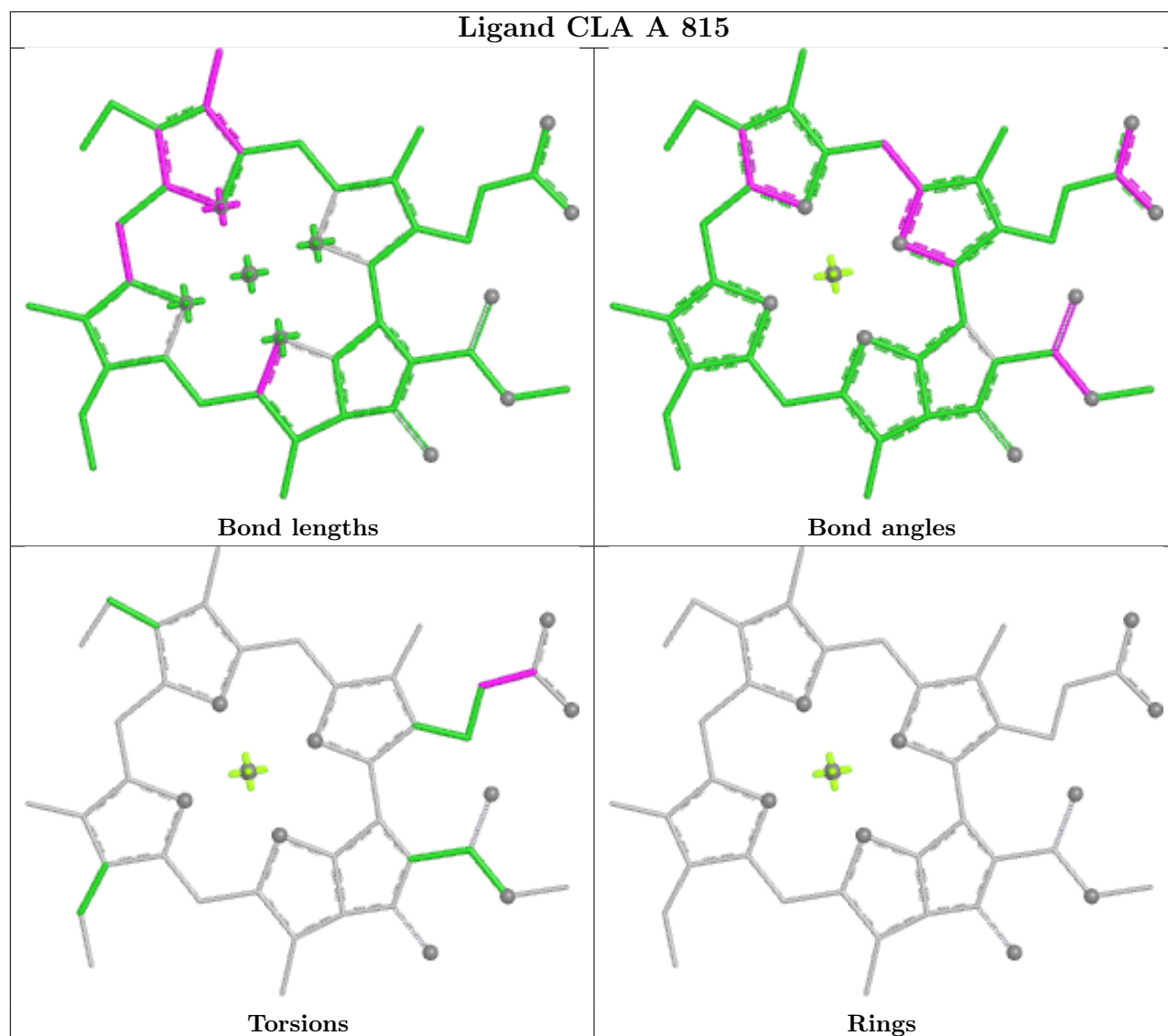
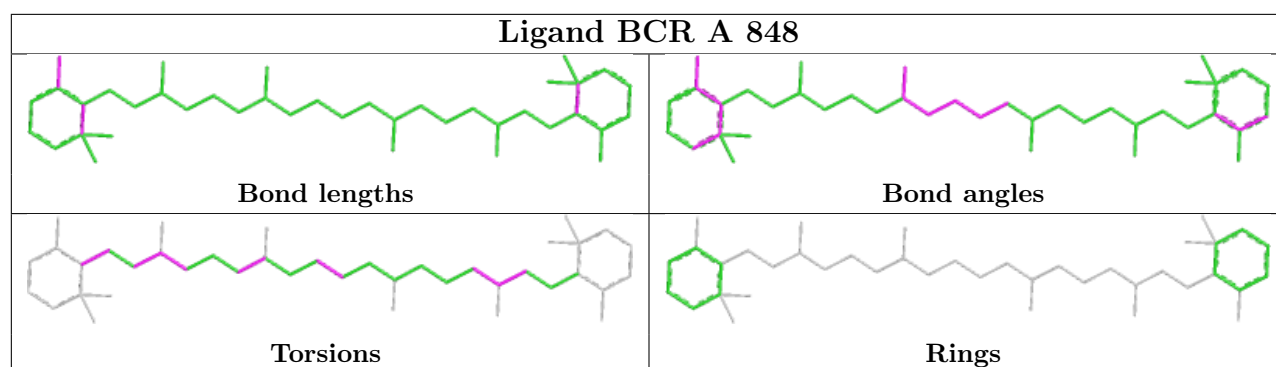


Torsions

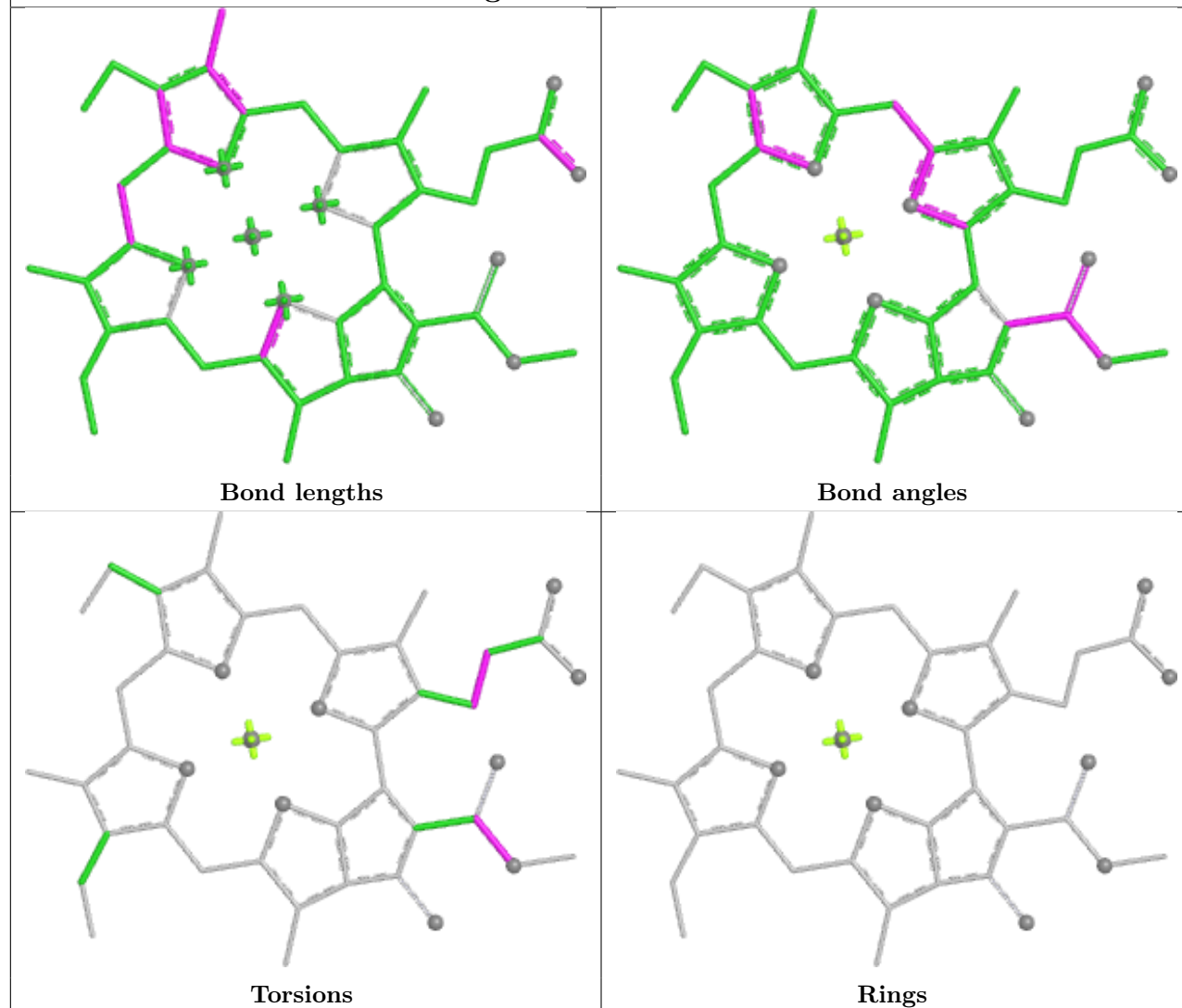


Rings

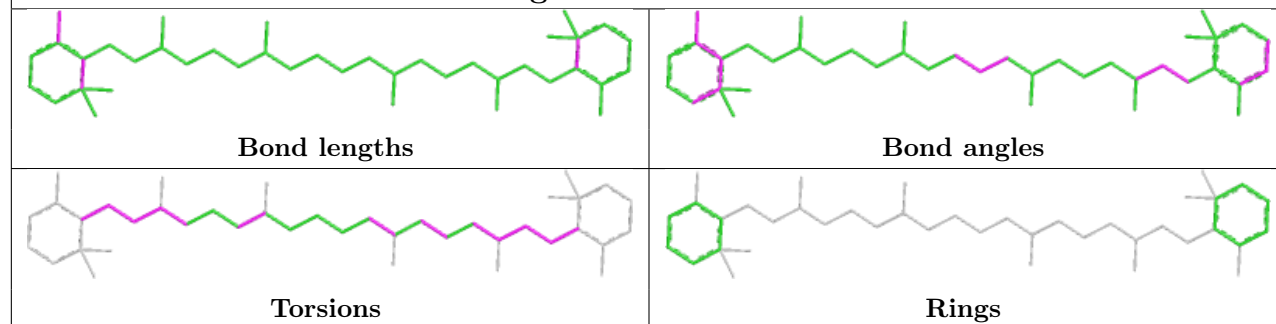


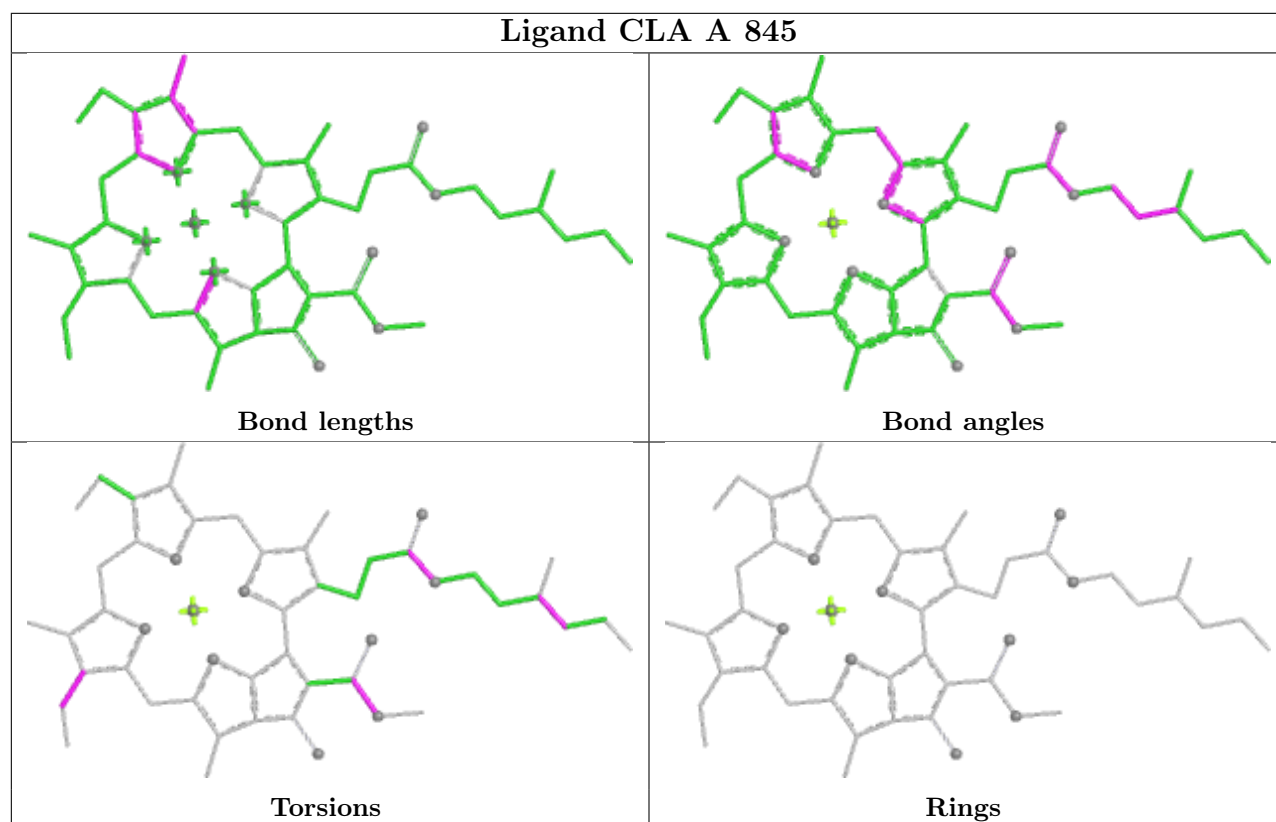
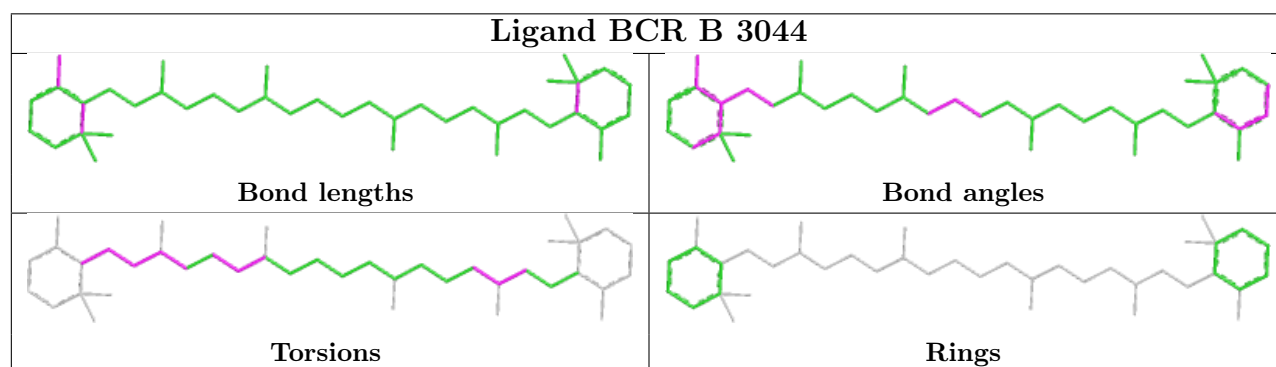
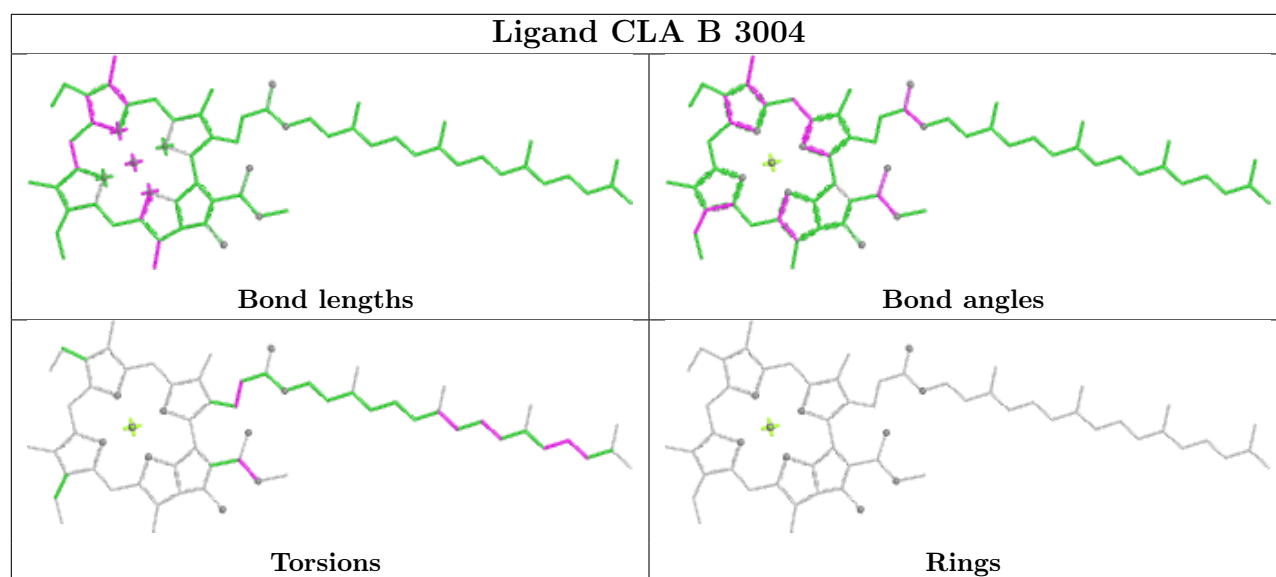


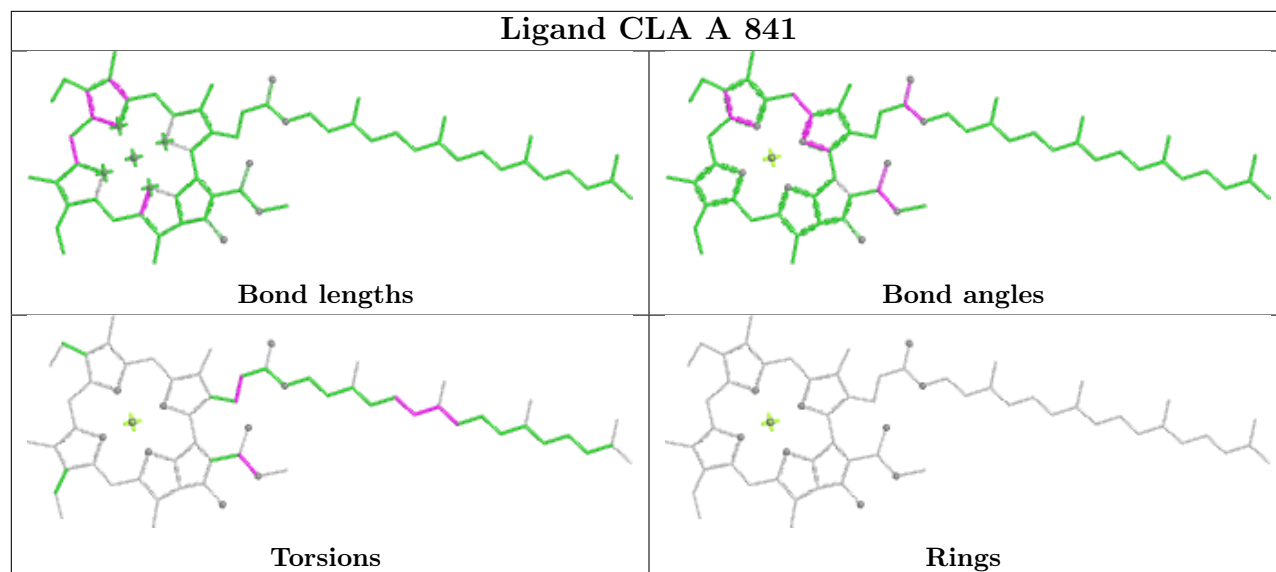
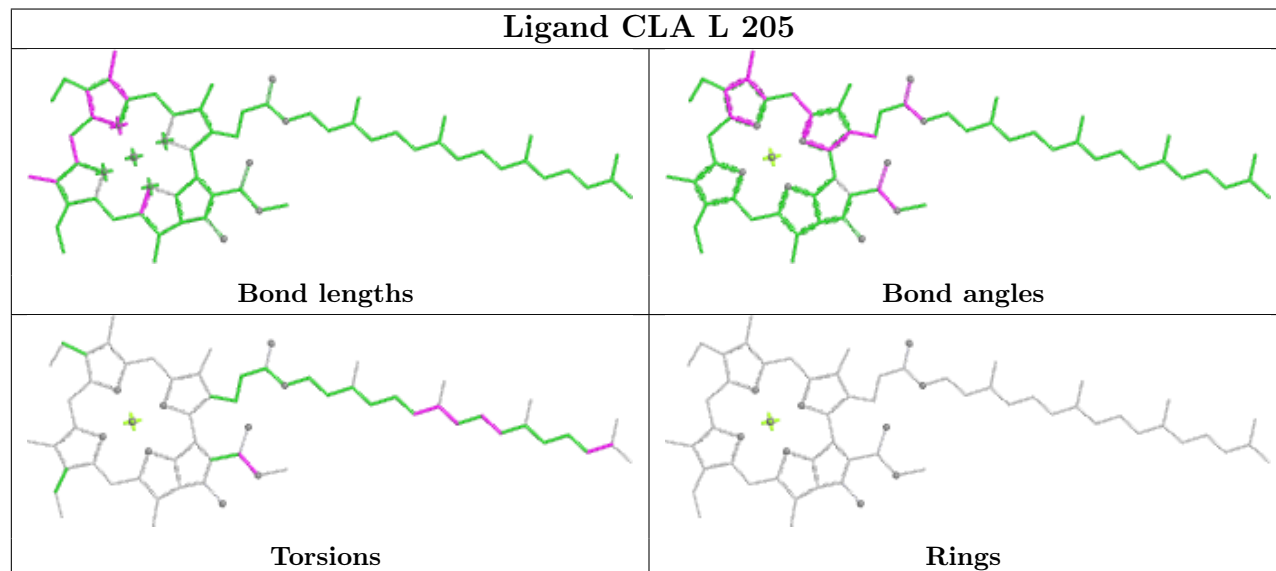
Ligand CLA B 3016



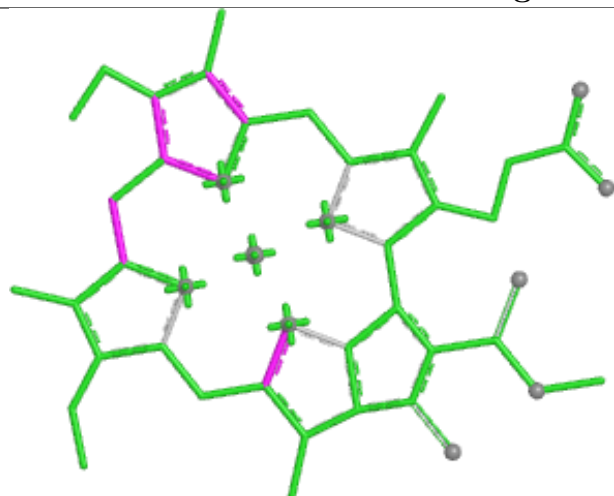
Ligand BCR A 851



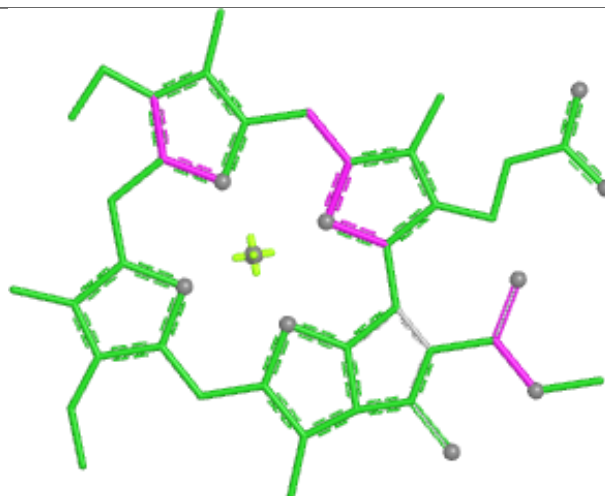


Ligand CLA A 841**Ligand CLA L 205**

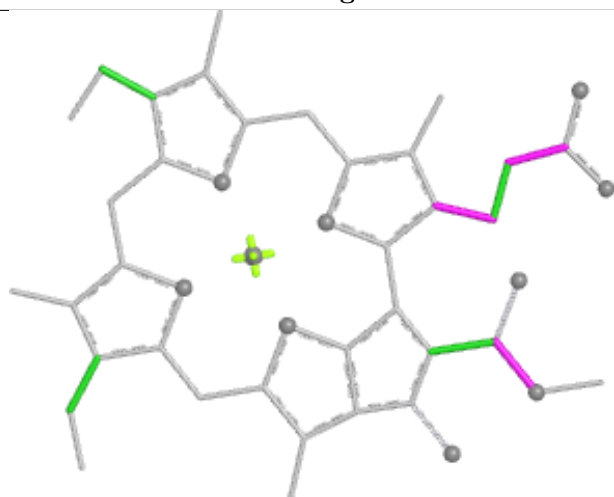
Ligand CLA A 837



Bond lengths



Bond angles

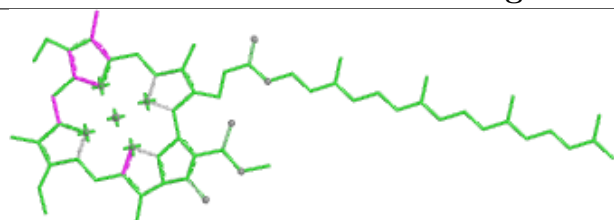


Torsions

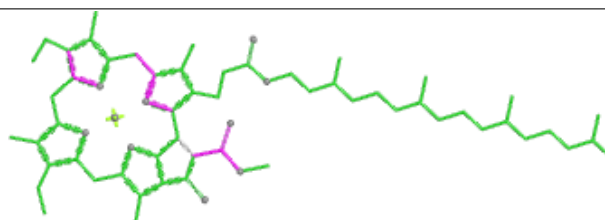


Rings

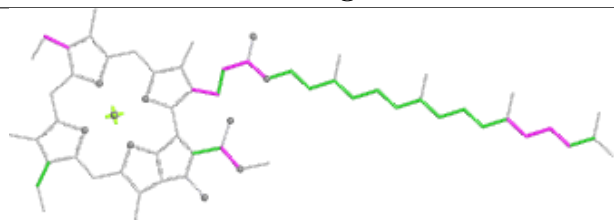
Ligand CLA B 3006



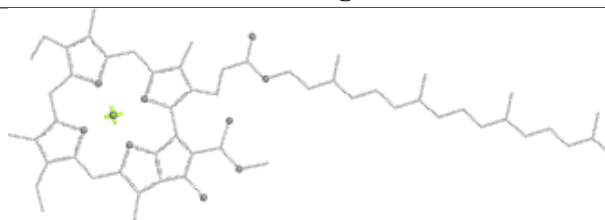
Bond lengths



Bond angles

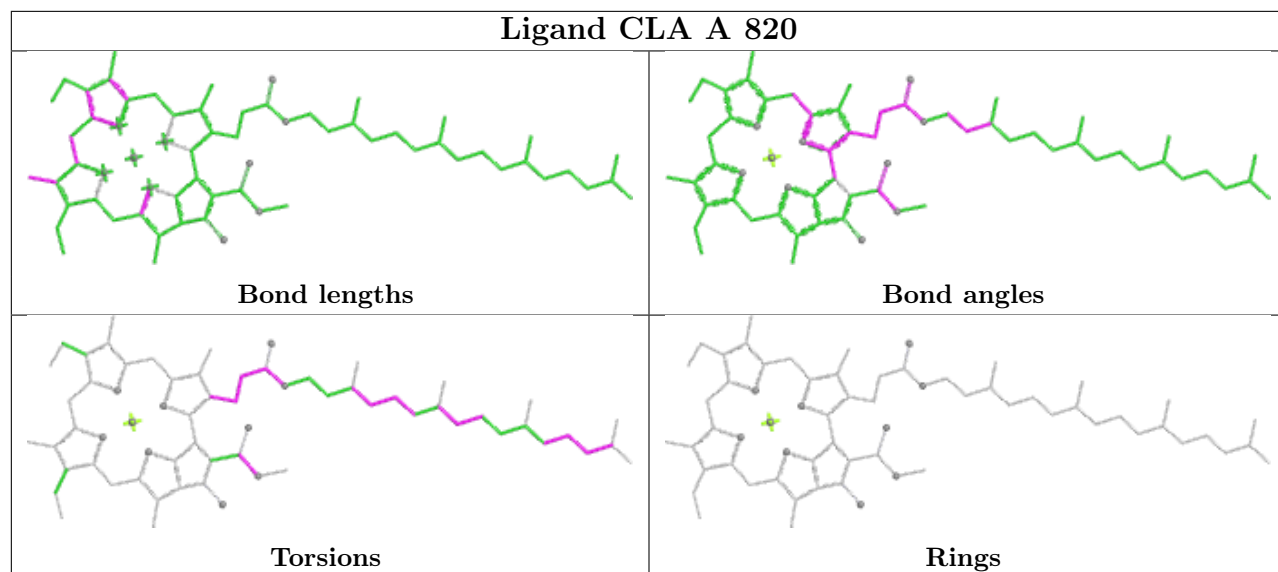


Torsions

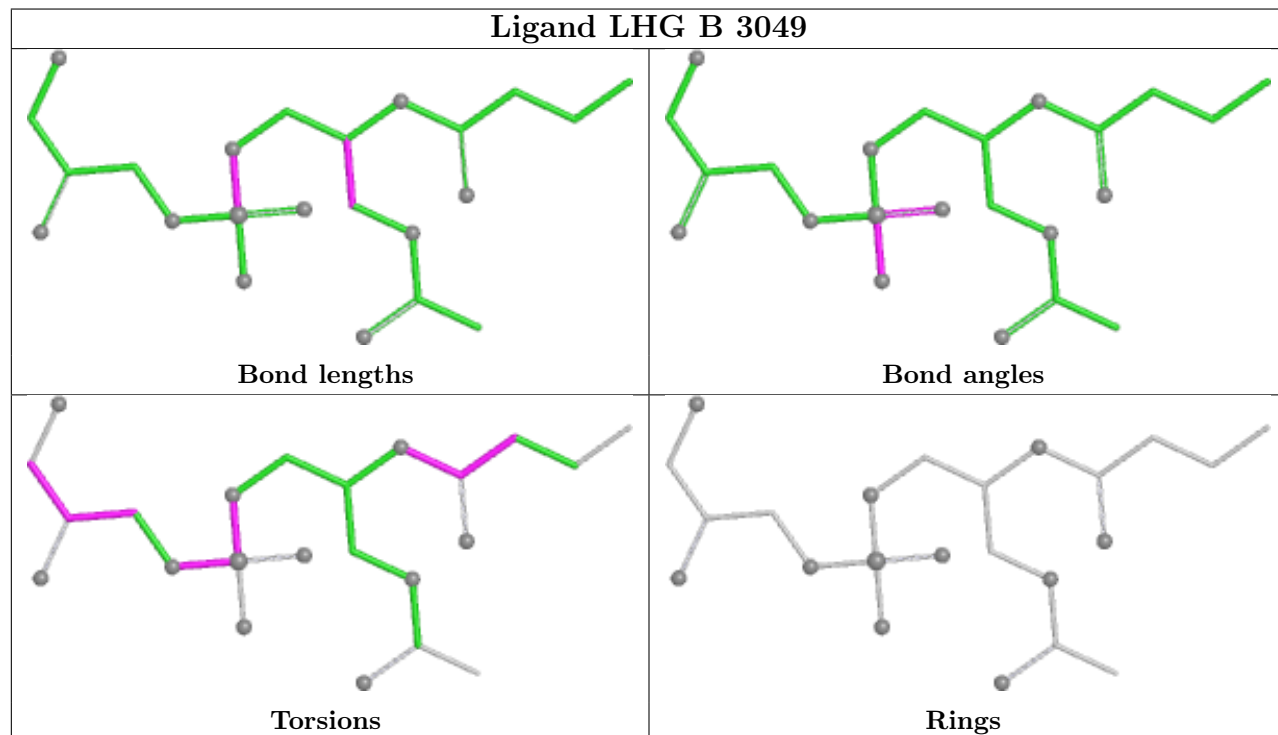


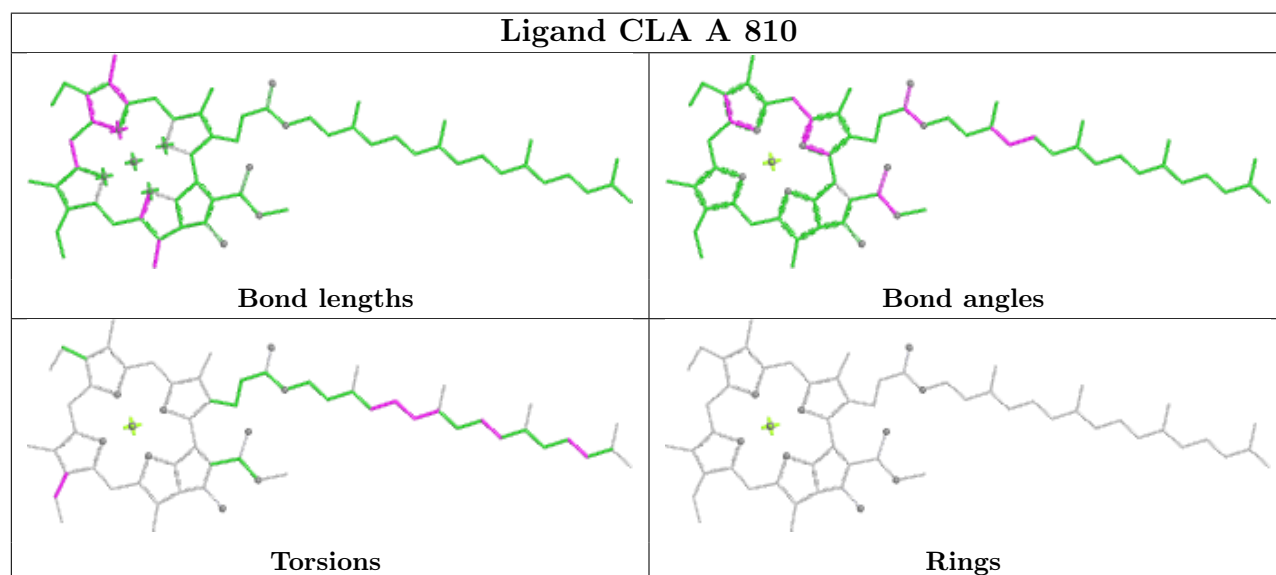
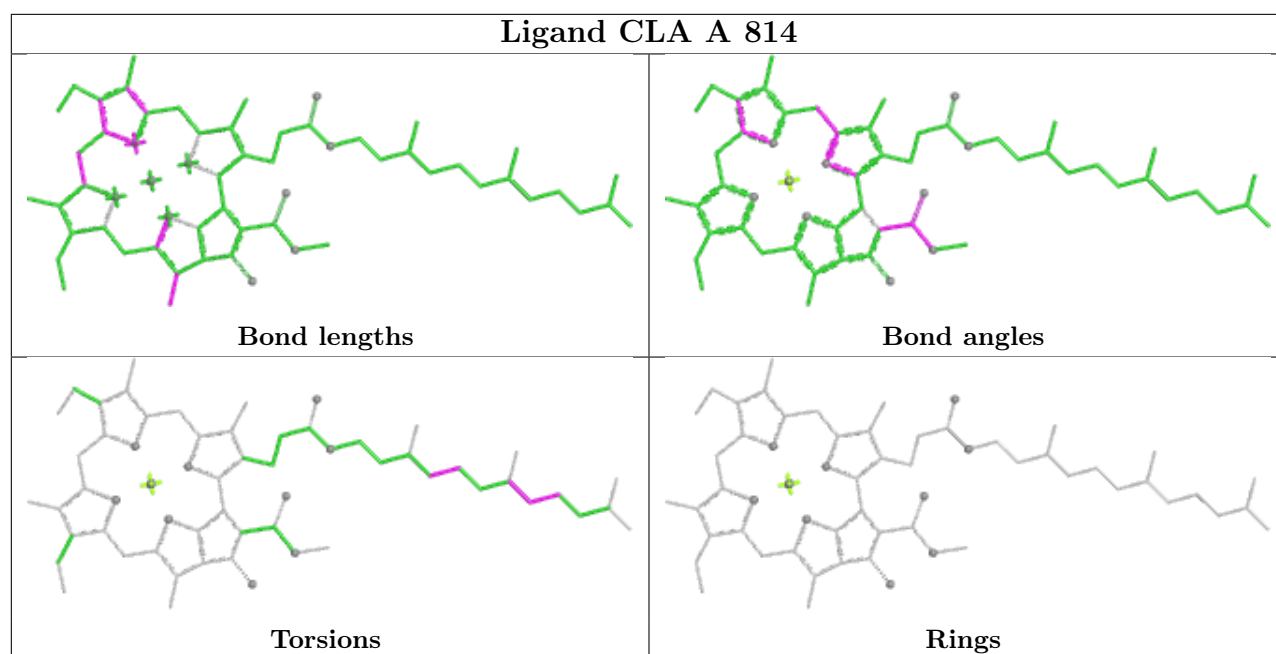
Rings

Ligand CLA A 820

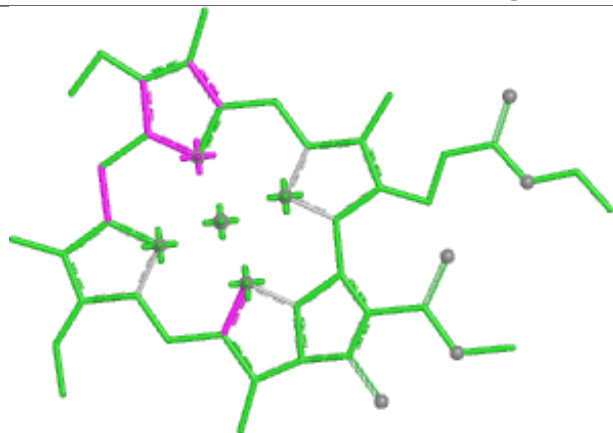


Ligand LHG B 3049

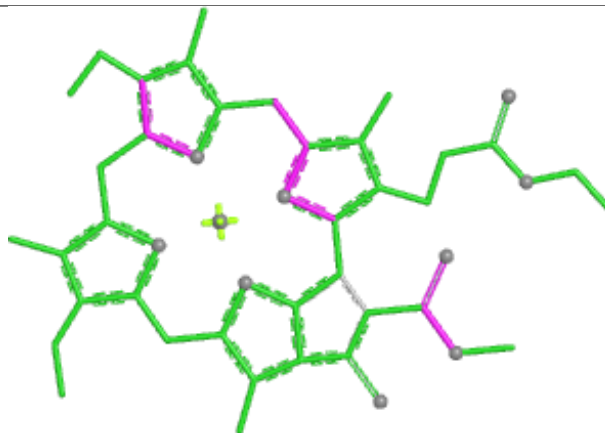




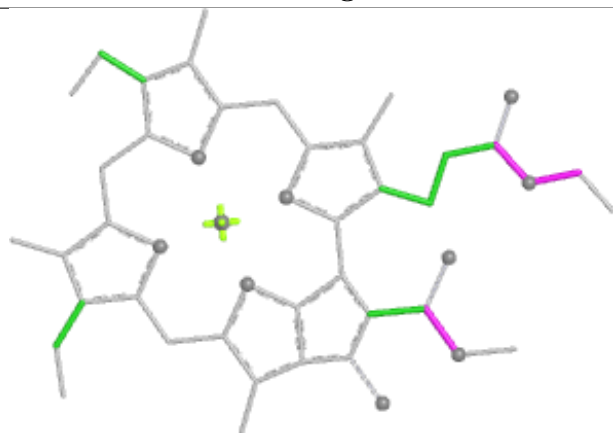
Ligand CLA B 3040



Bond lengths



Bond angles

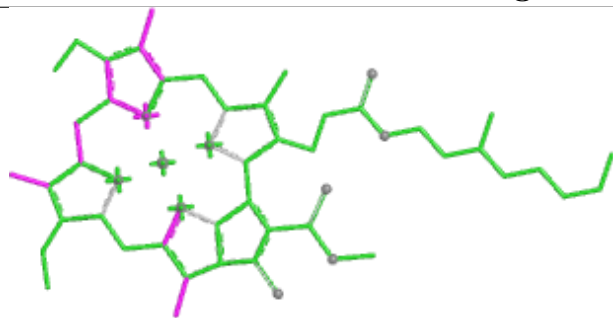


Torsions

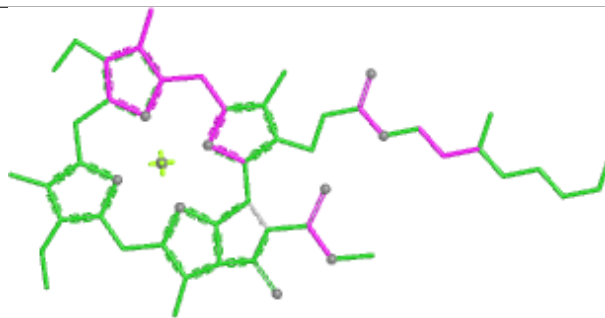


Rings

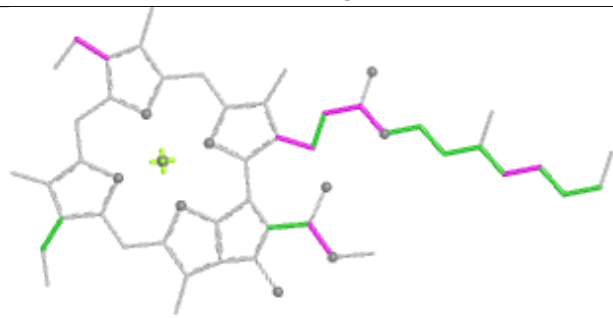
Ligand CLA A 819



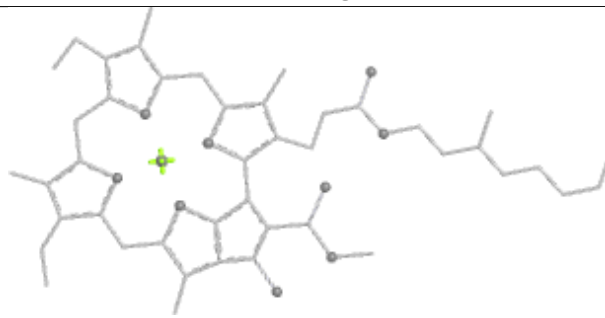
Bond lengths



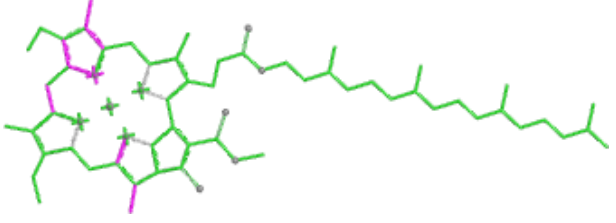
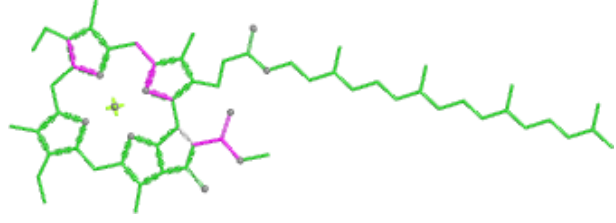
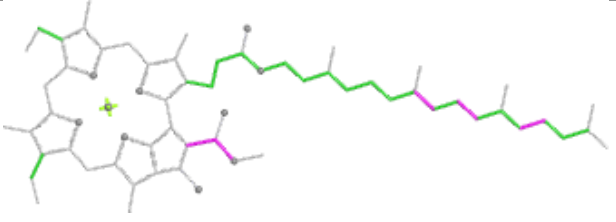
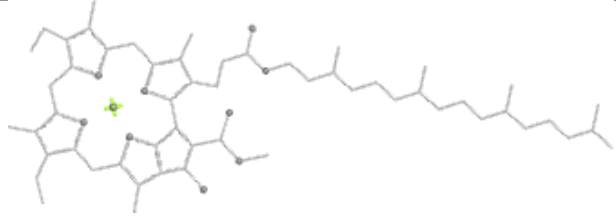
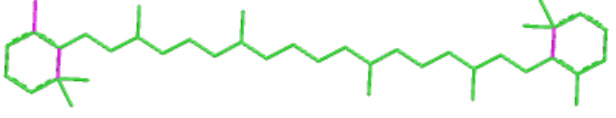
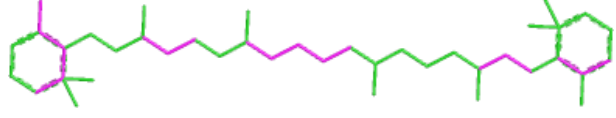
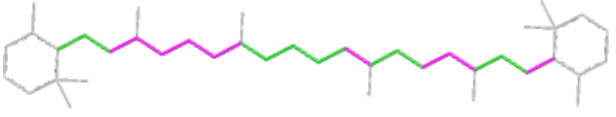
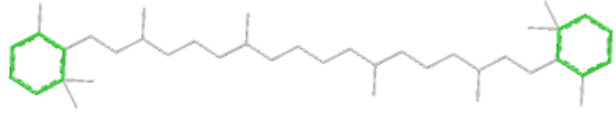
Bond angles



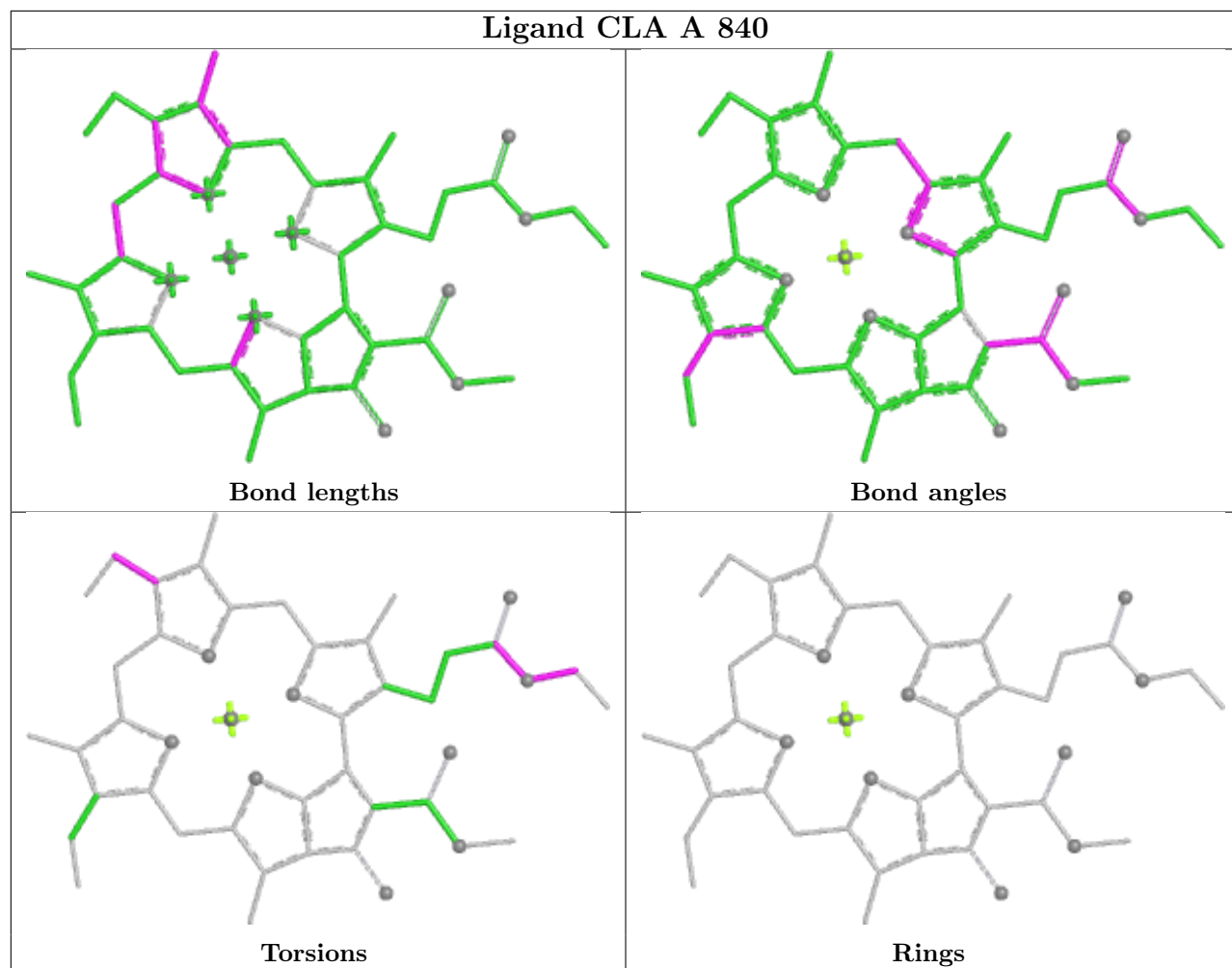
Torsions



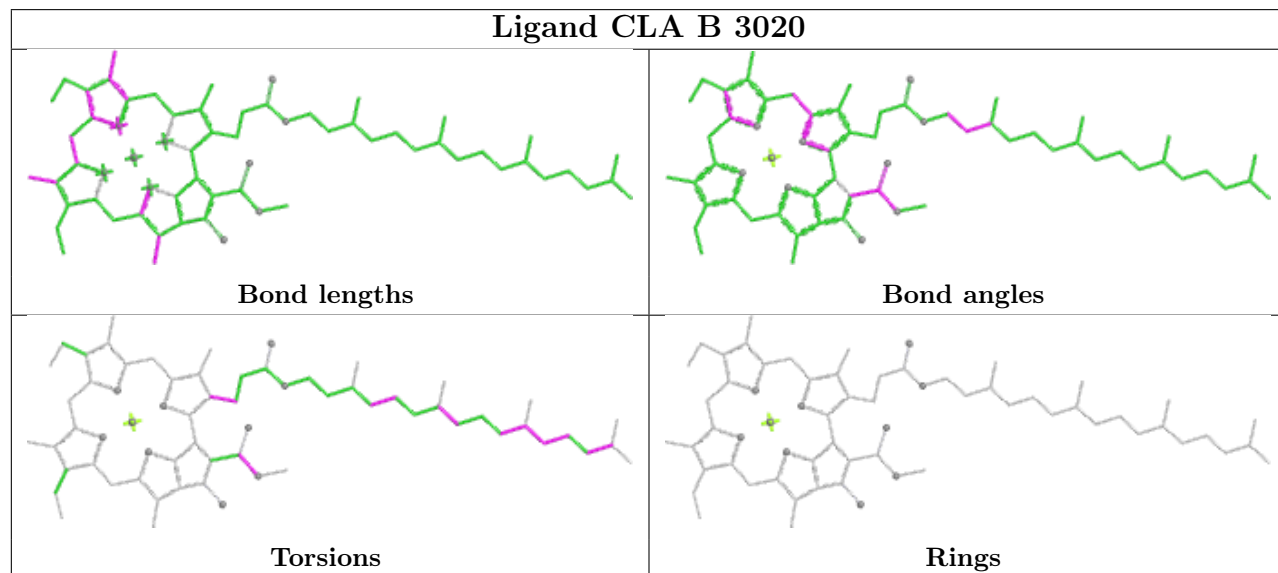
Rings

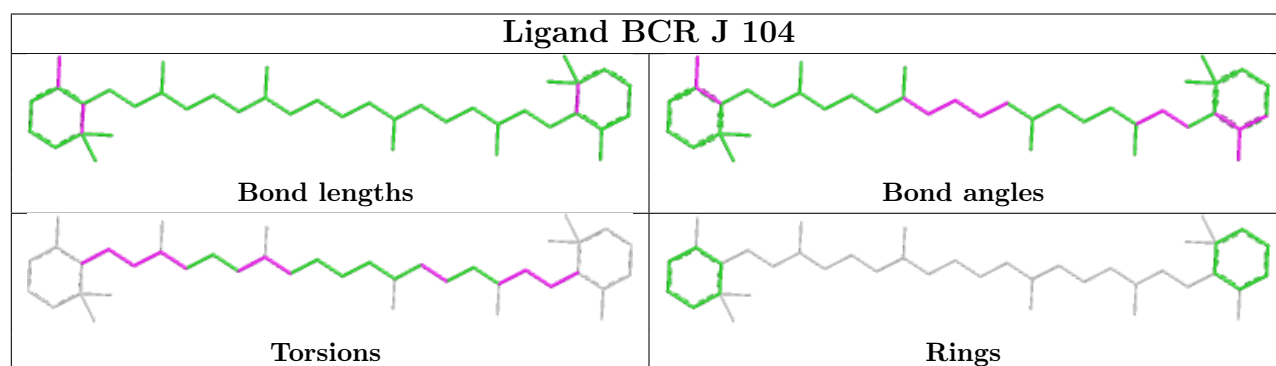
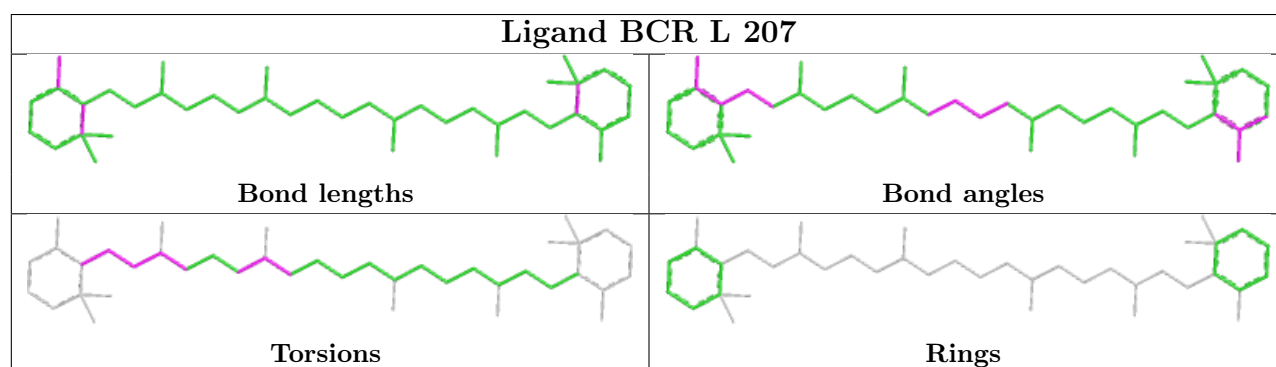
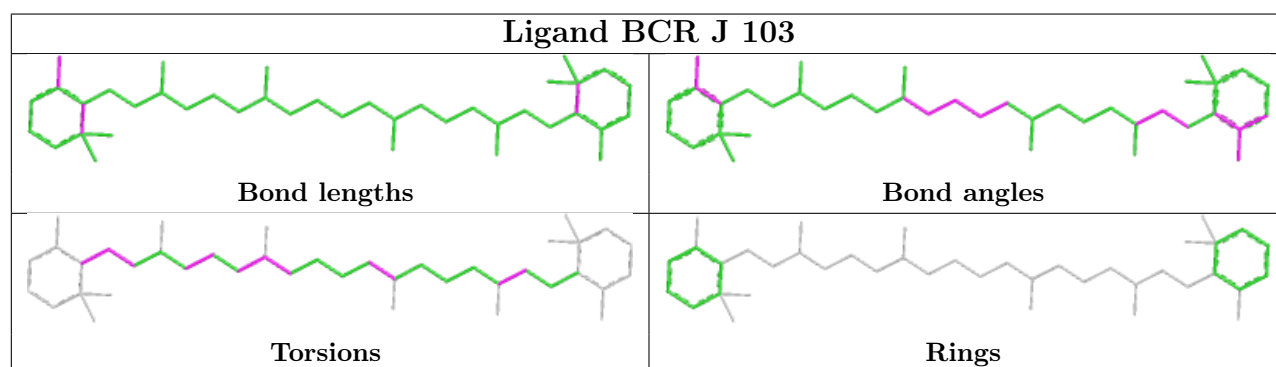
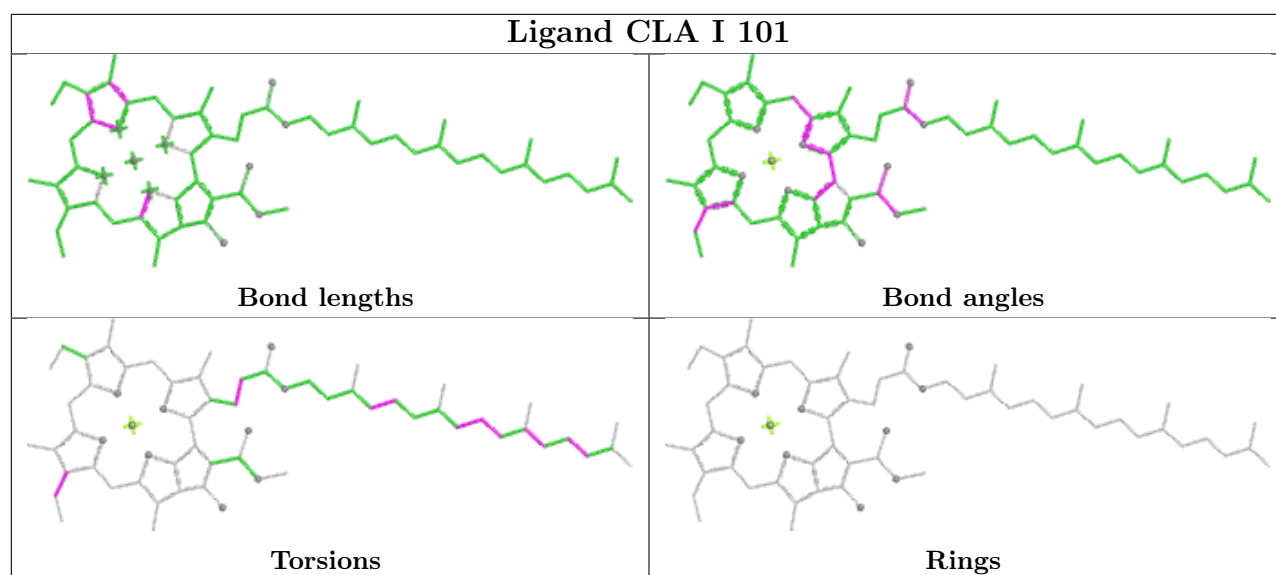
Ligand CLA A 831	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 3046	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 840

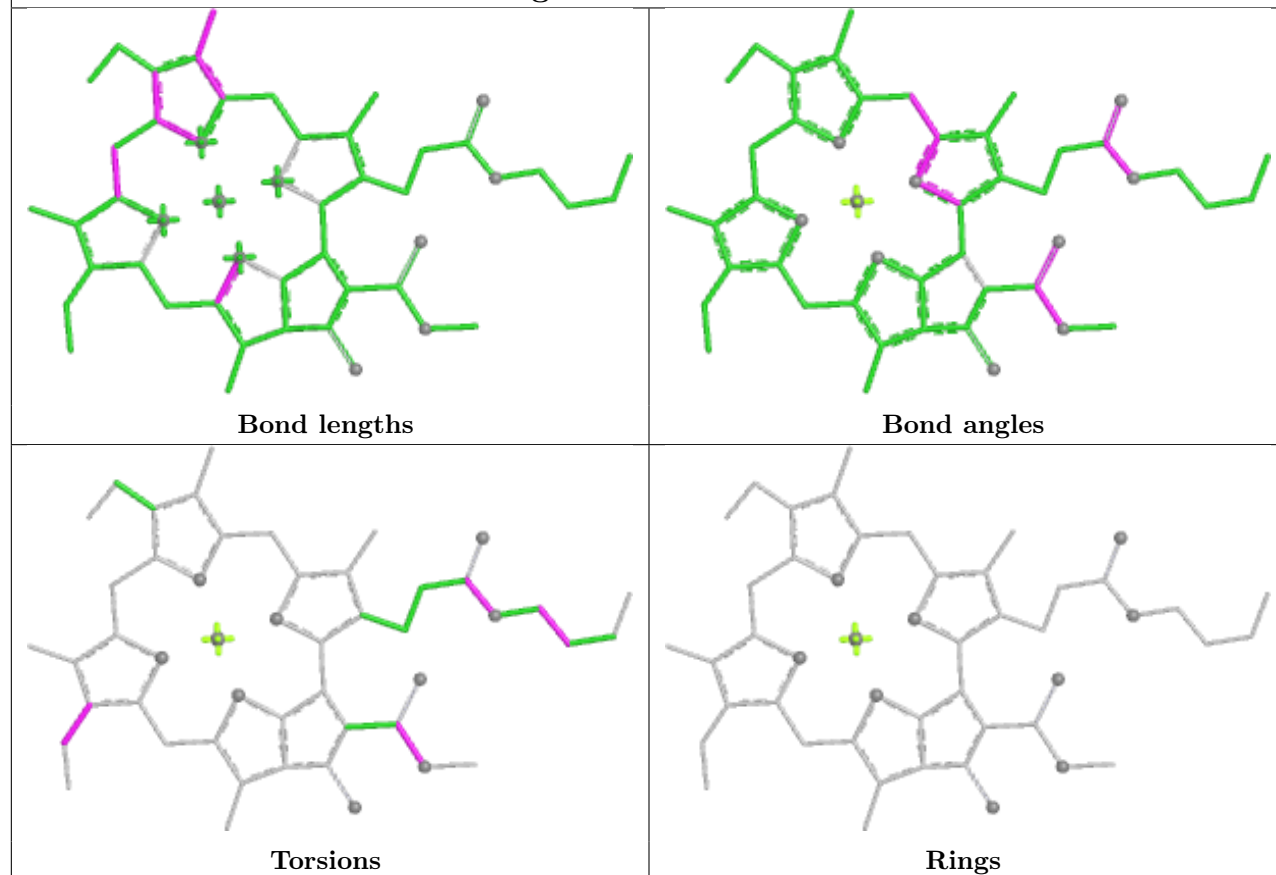


Ligand CLA B 3020

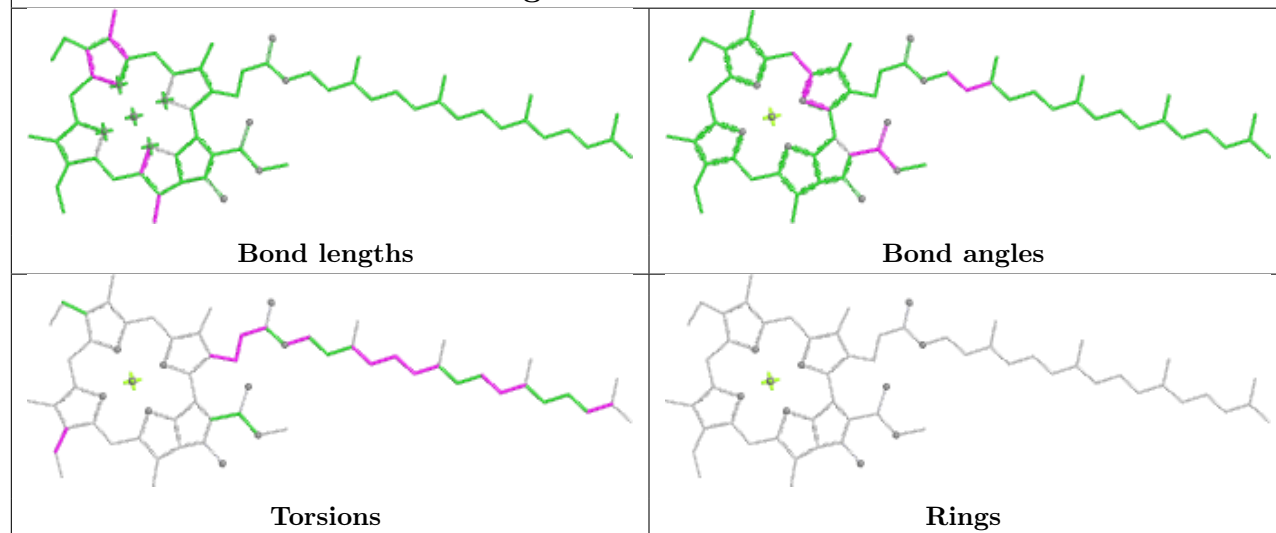


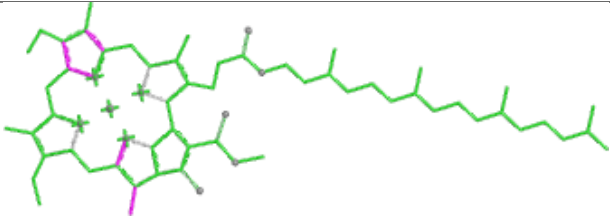
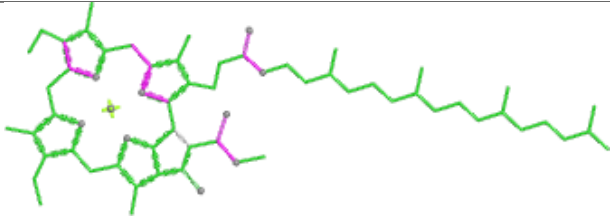
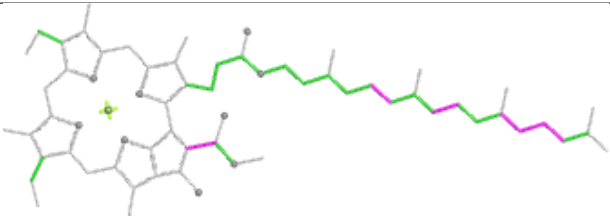
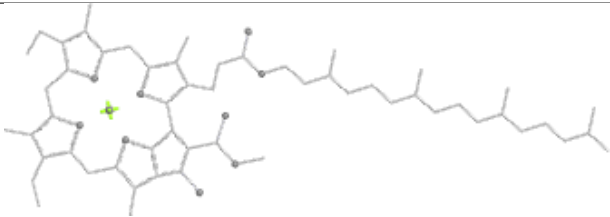
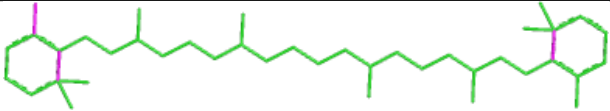
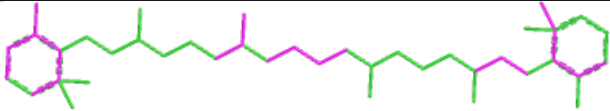
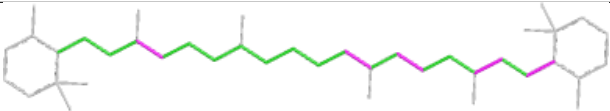
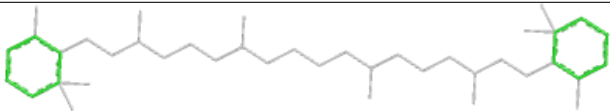
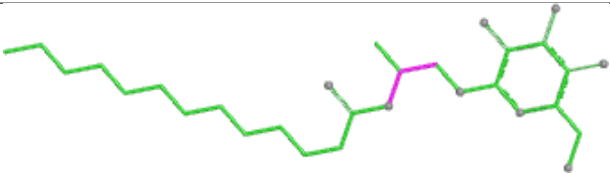
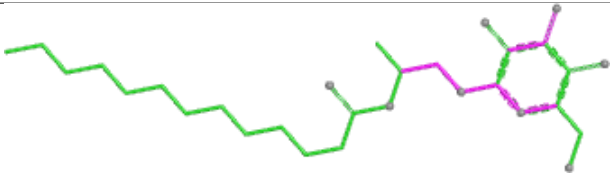
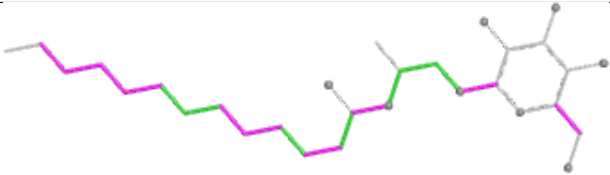
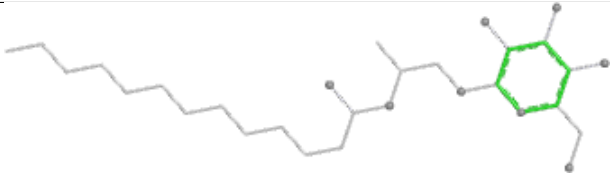


Ligand CLA A 817

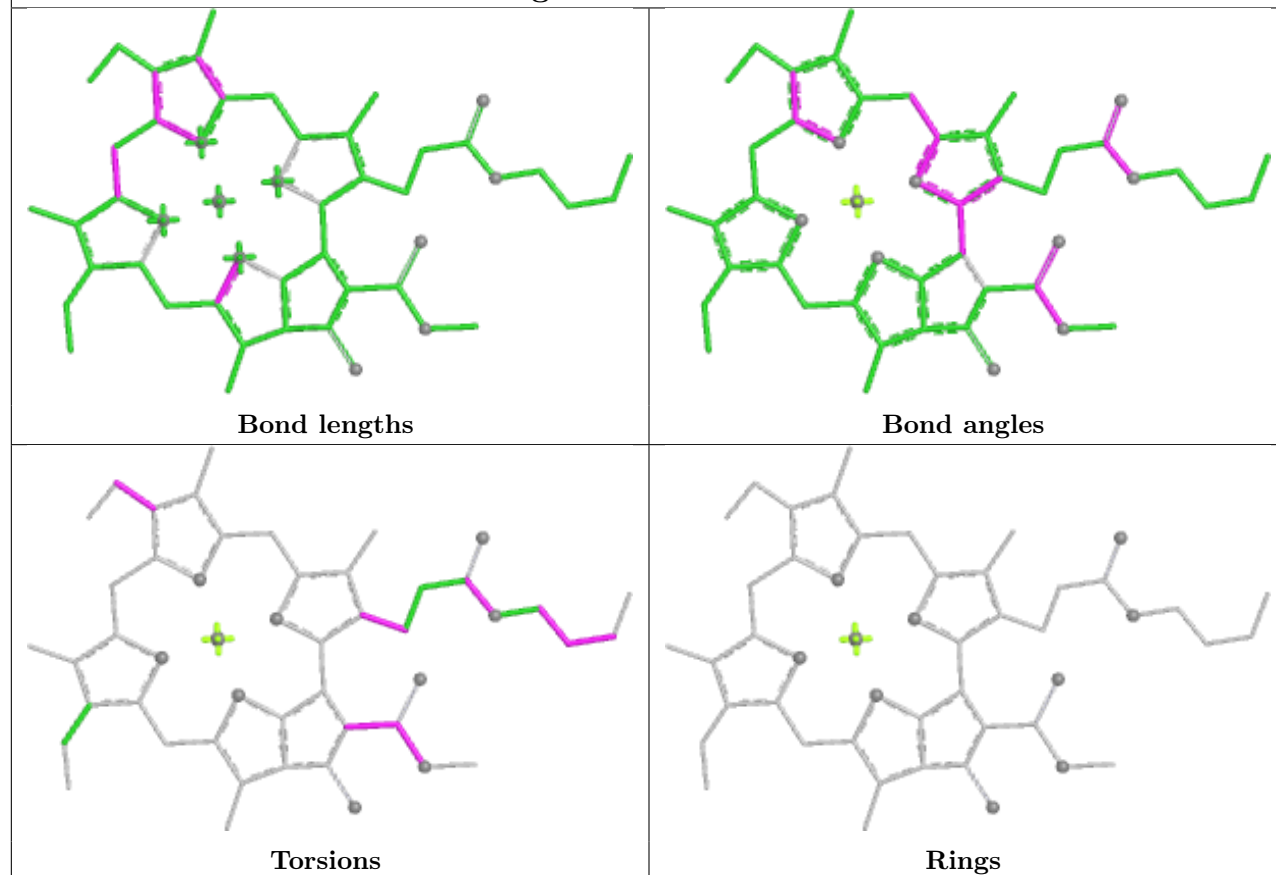


Ligand CLA B 3033

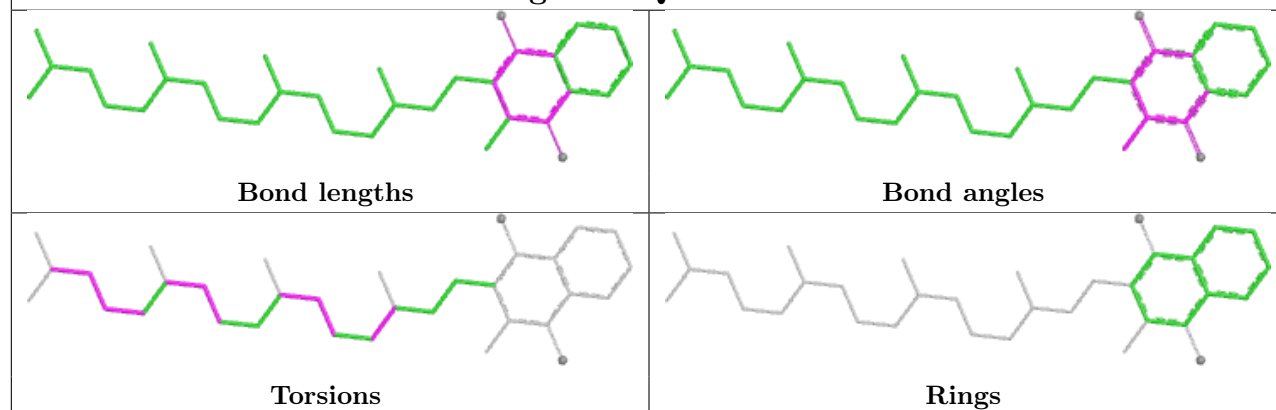


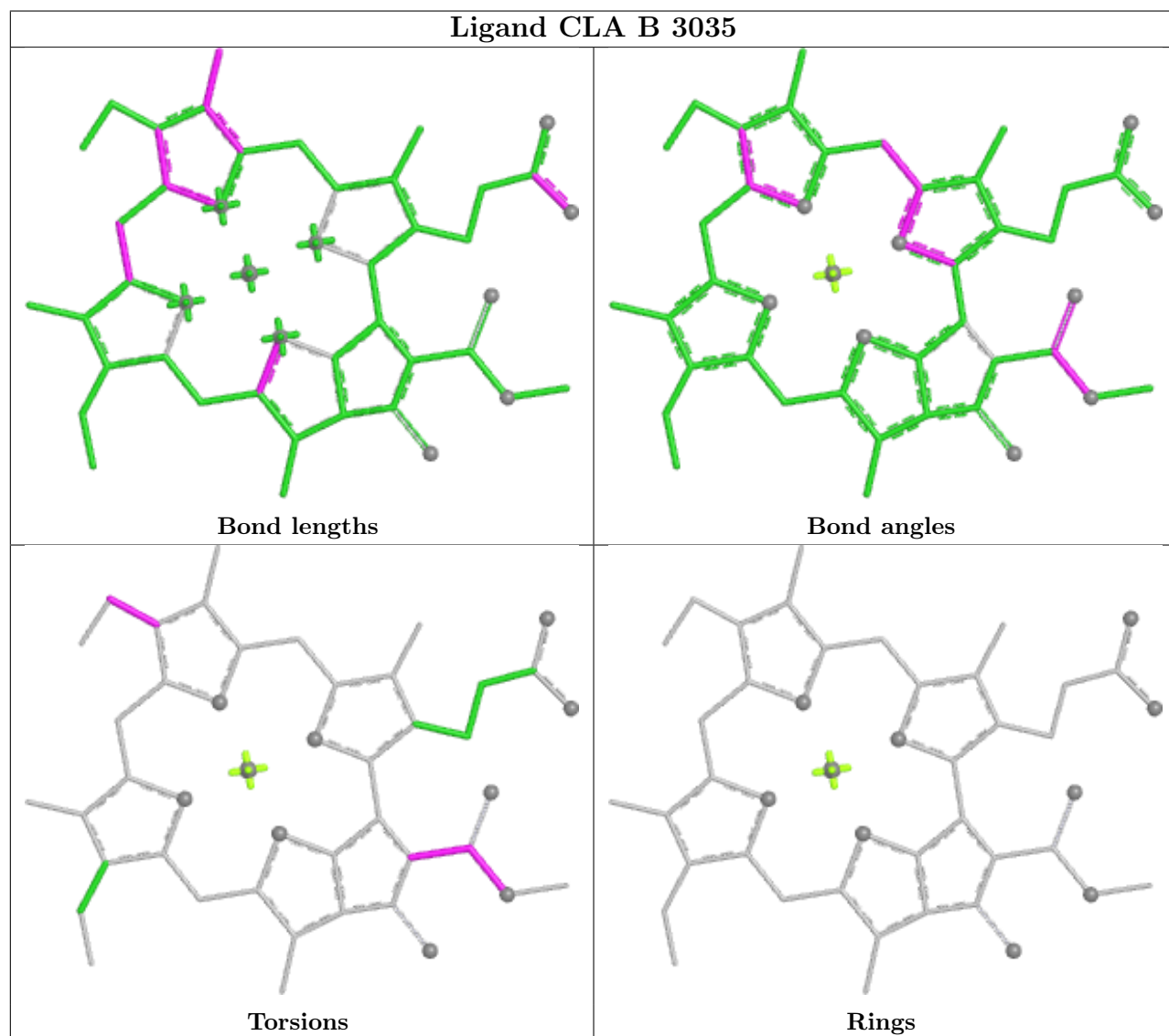
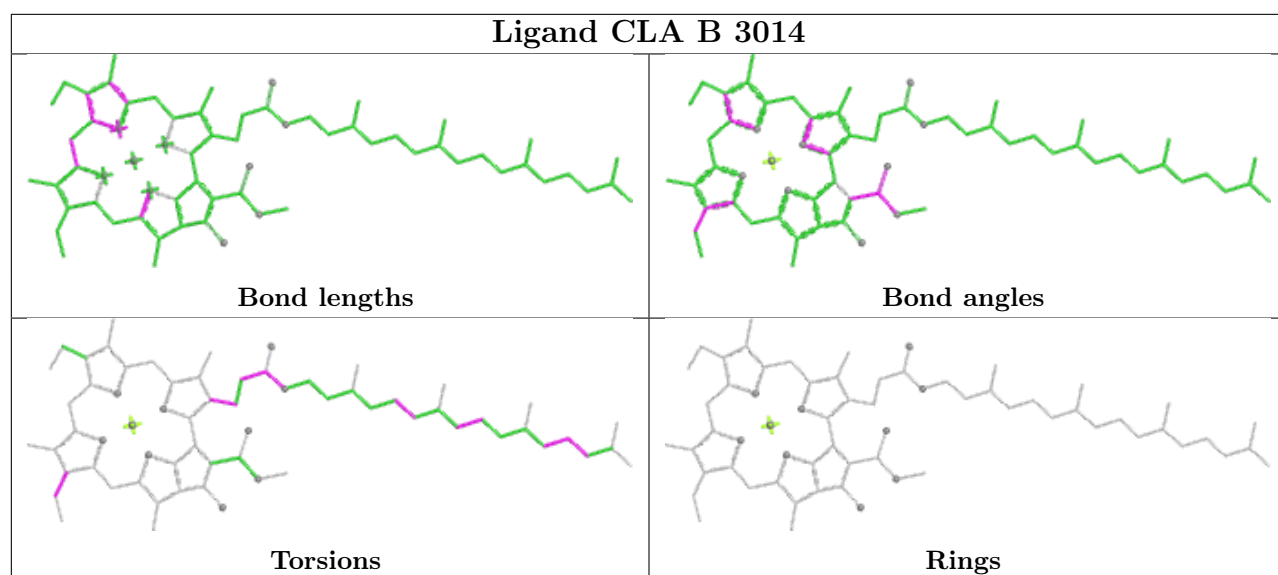
Ligand CLA B 3009	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR K 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG A 855	
 Bond lengths	 Bond angles
 Torsions	 Rings

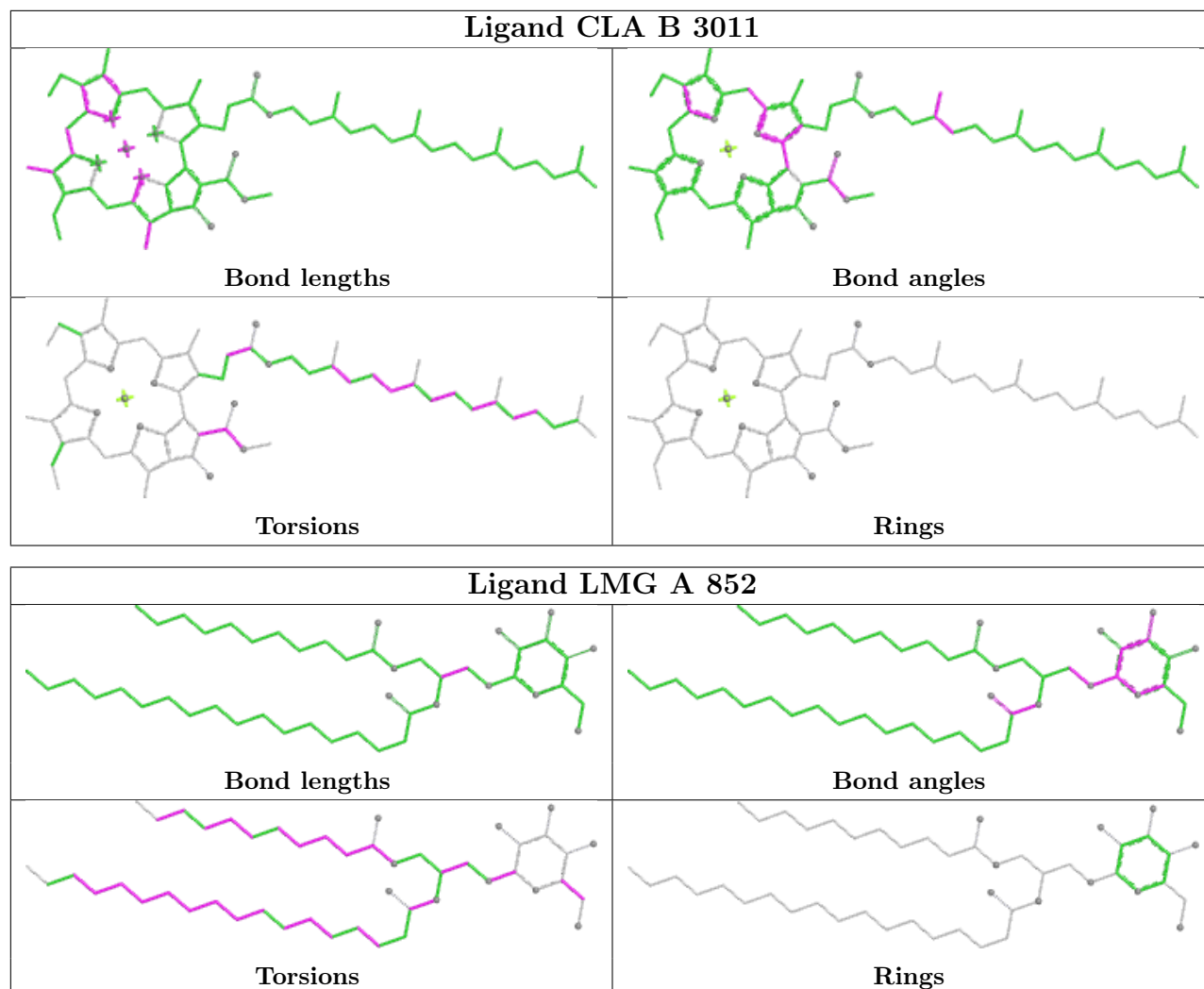
Ligand CLA A 823



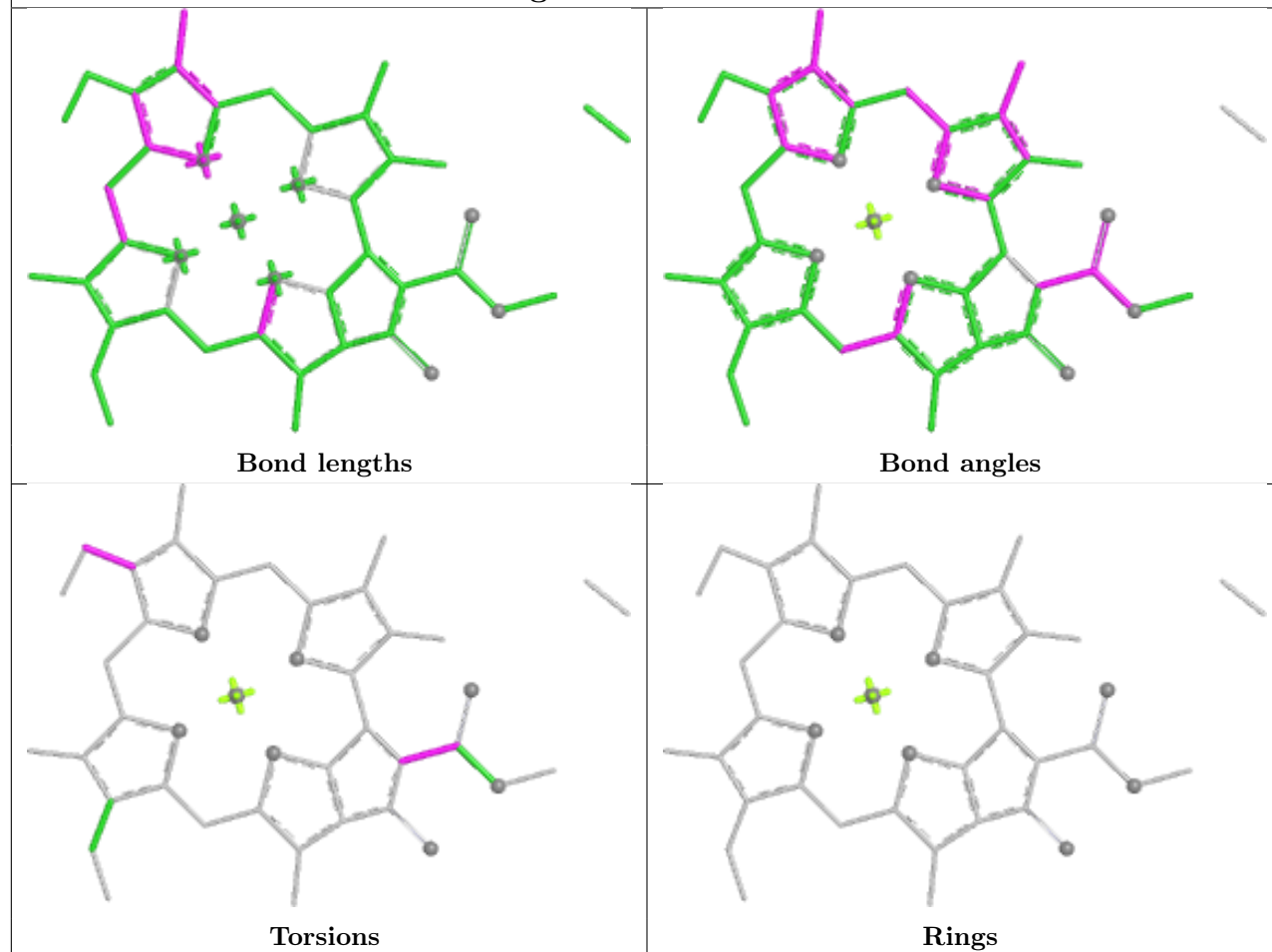
Ligand PQN A 846



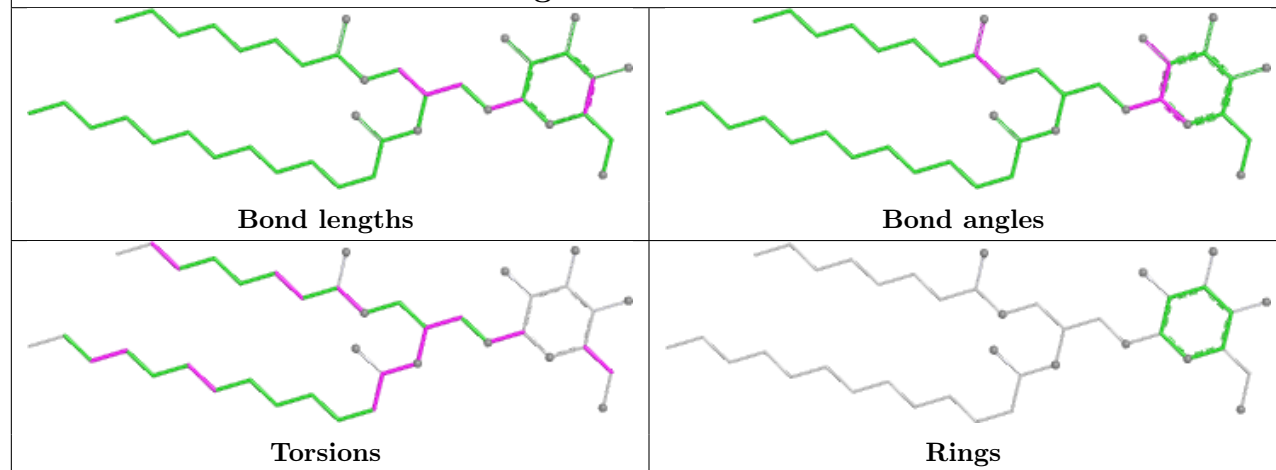


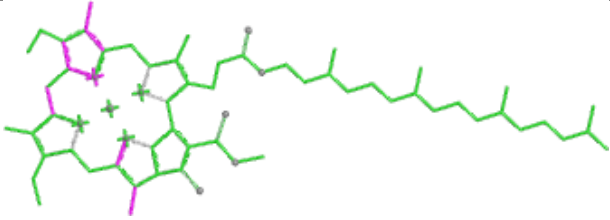
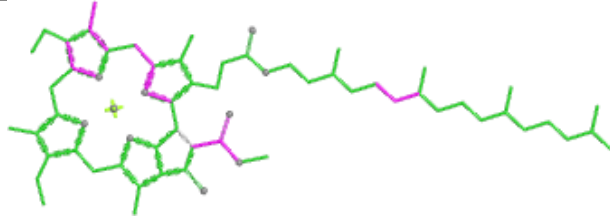
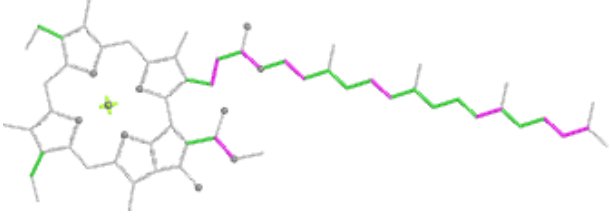
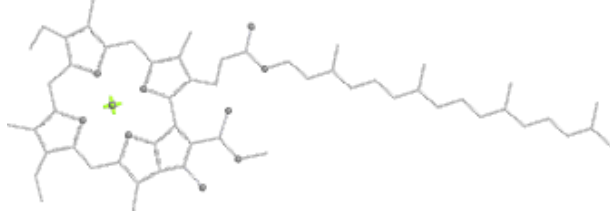
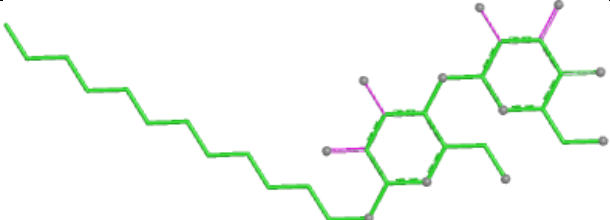
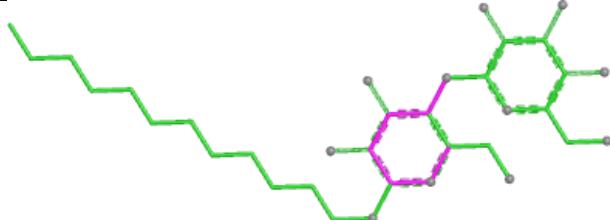
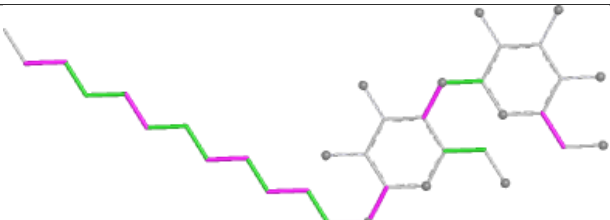
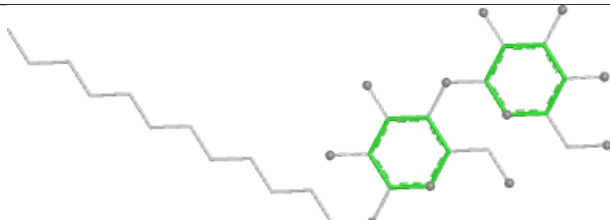
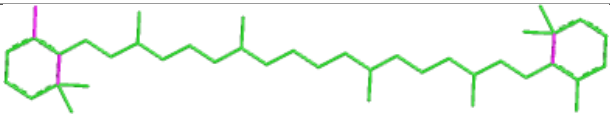
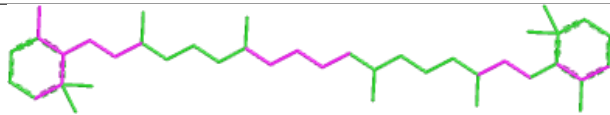
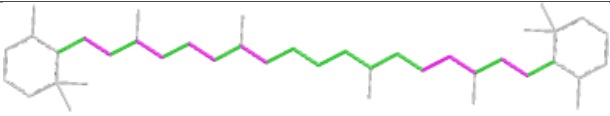
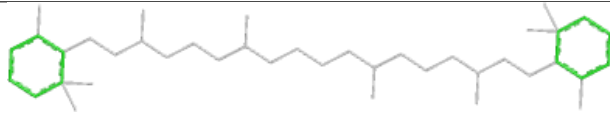


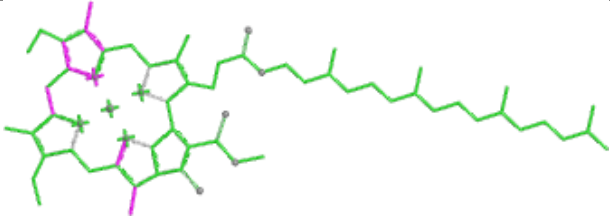
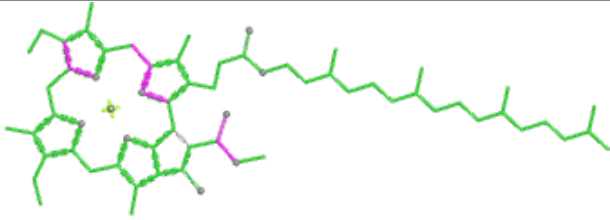
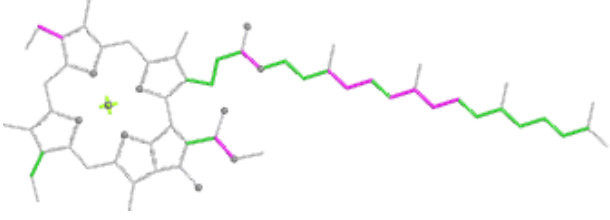
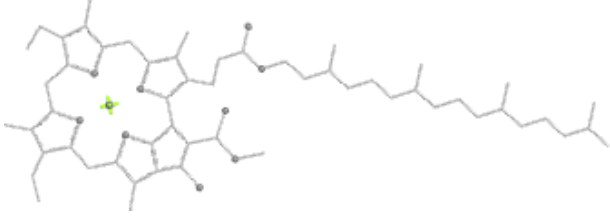
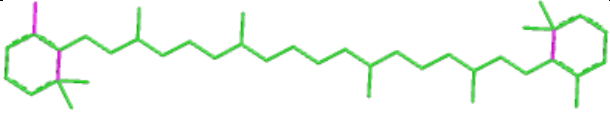
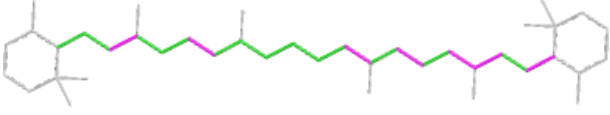
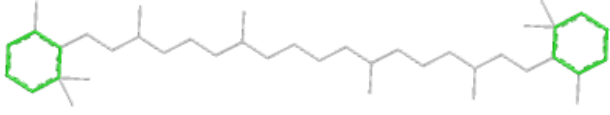
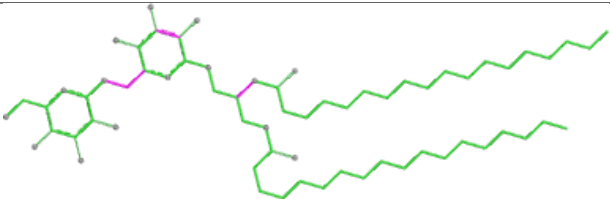
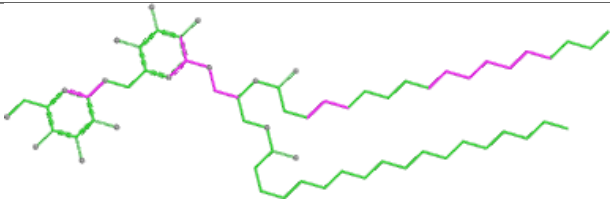
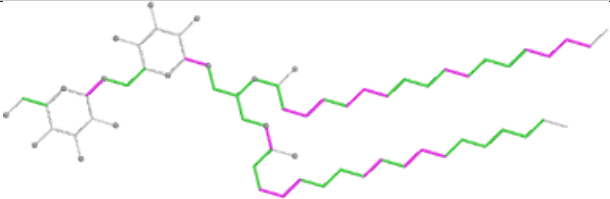
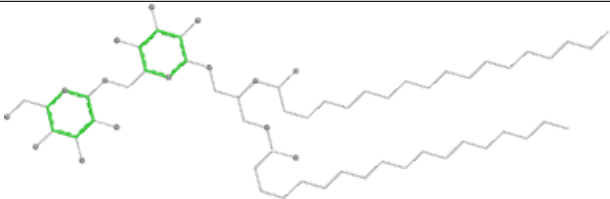
Ligand CLA A 821



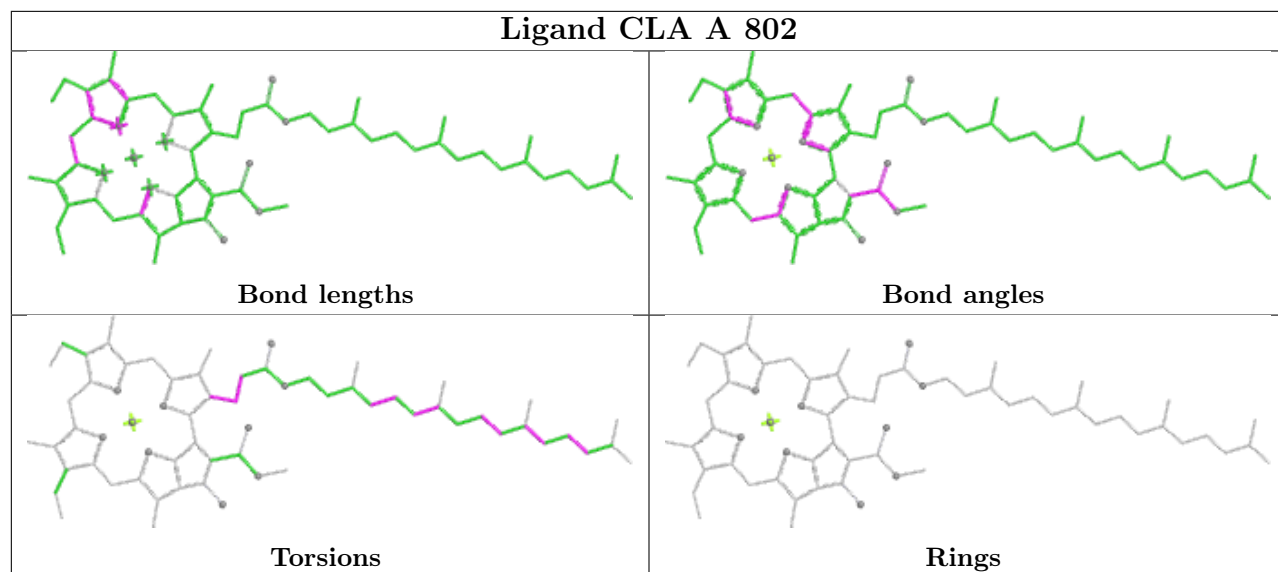
Ligand LMG I 104



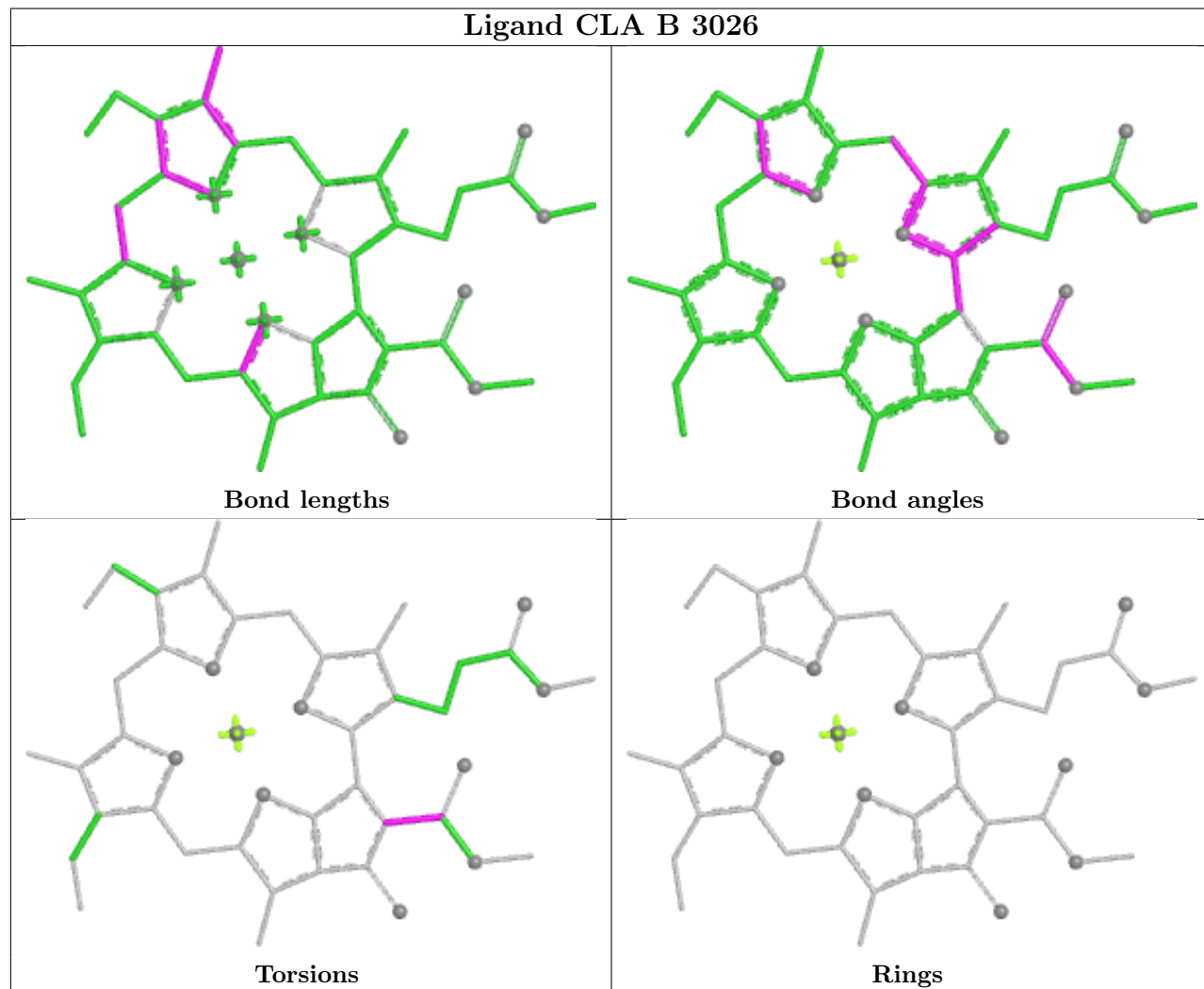
Ligand CLA A 844	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT L 201	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 3045	
 Bond lengths	 Bond angles
 Torsions	 Rings

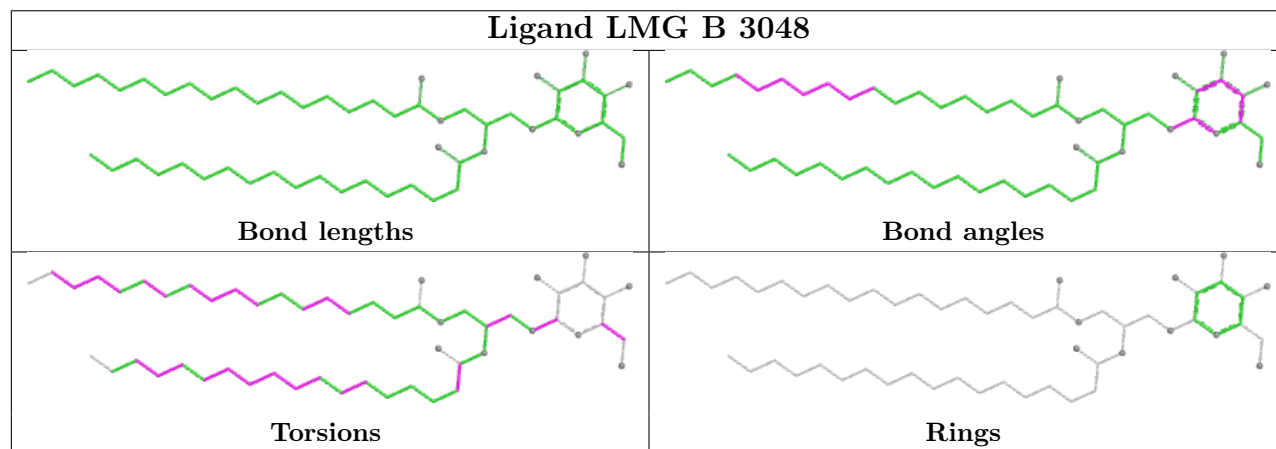
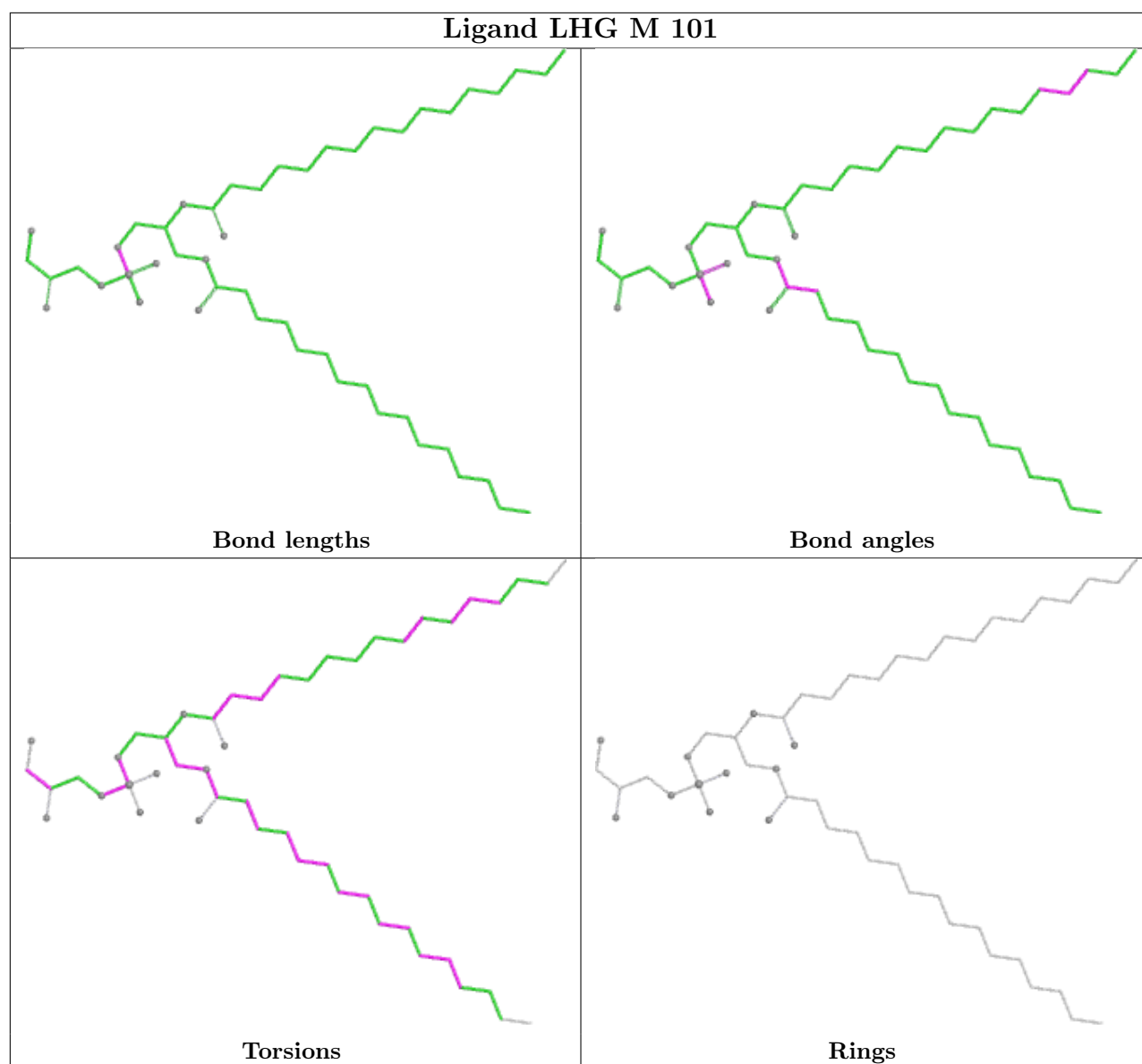
Ligand CLA B 3003	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR F 201	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD L 206	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 802

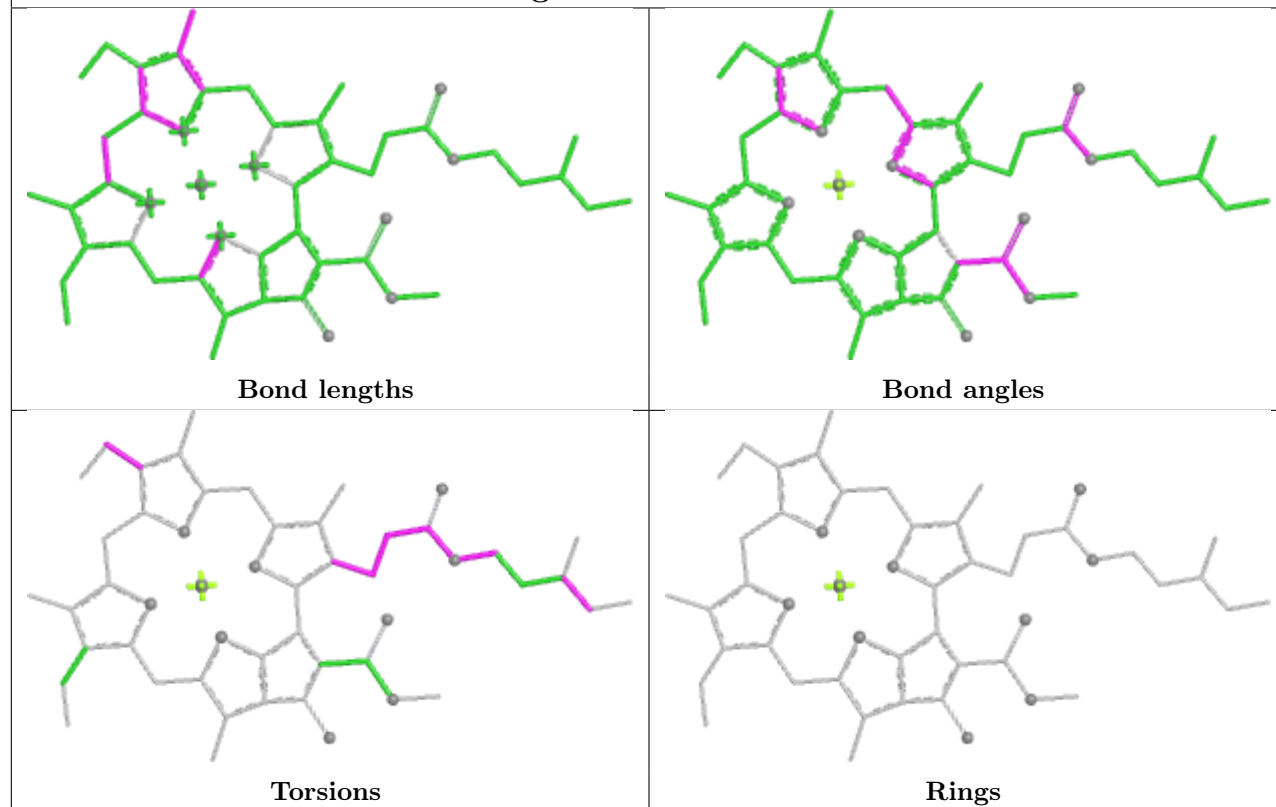


Ligand CLA B 3026

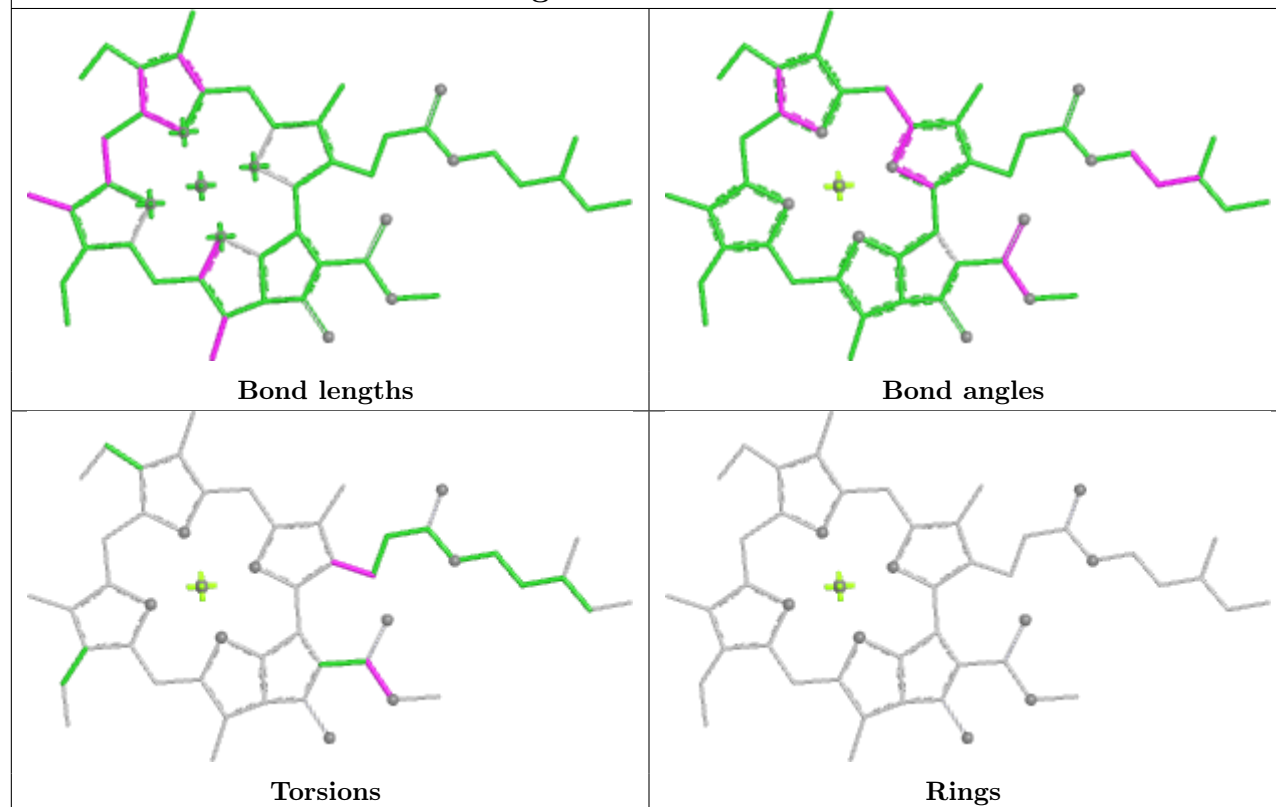


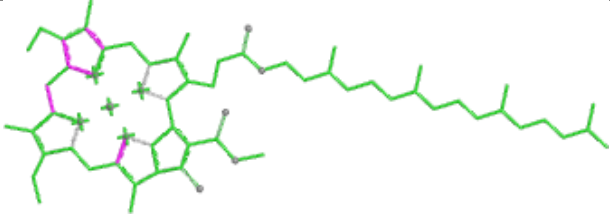
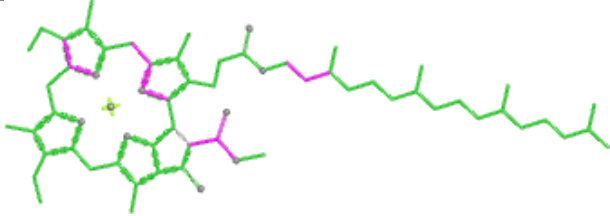
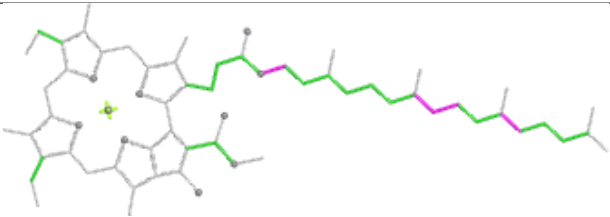
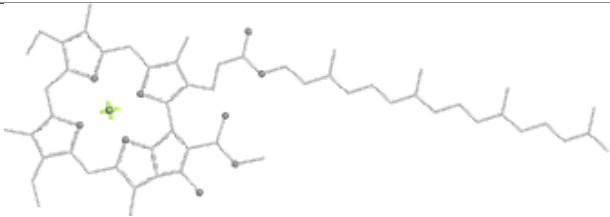
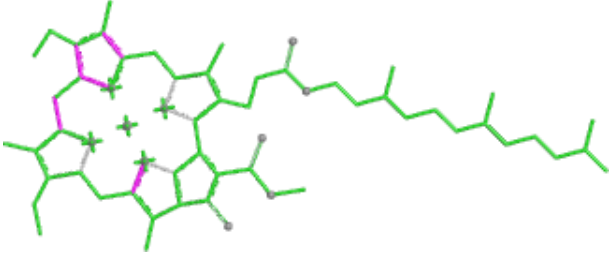
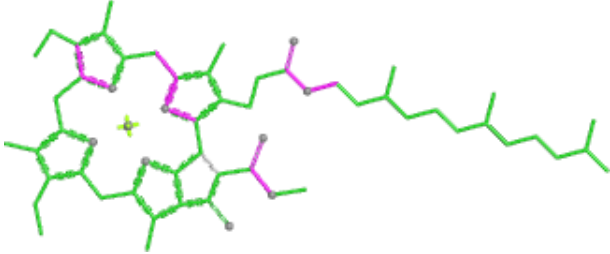
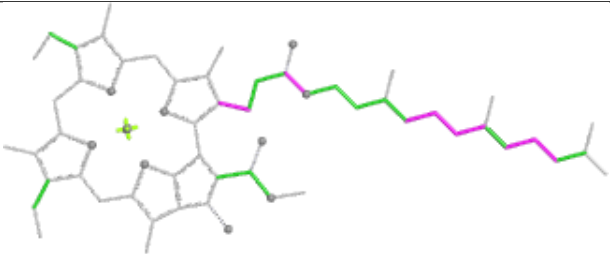
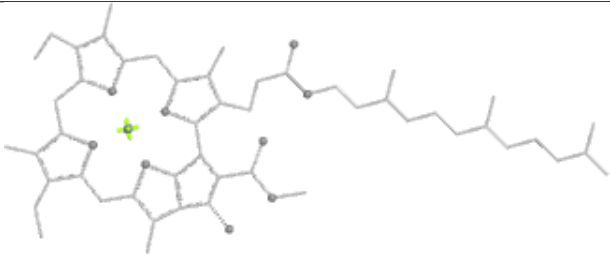
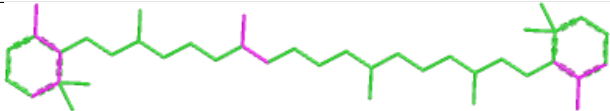
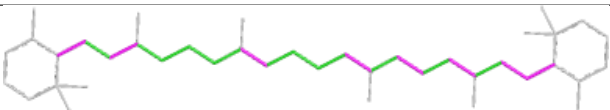
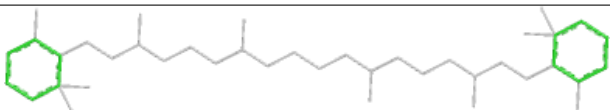


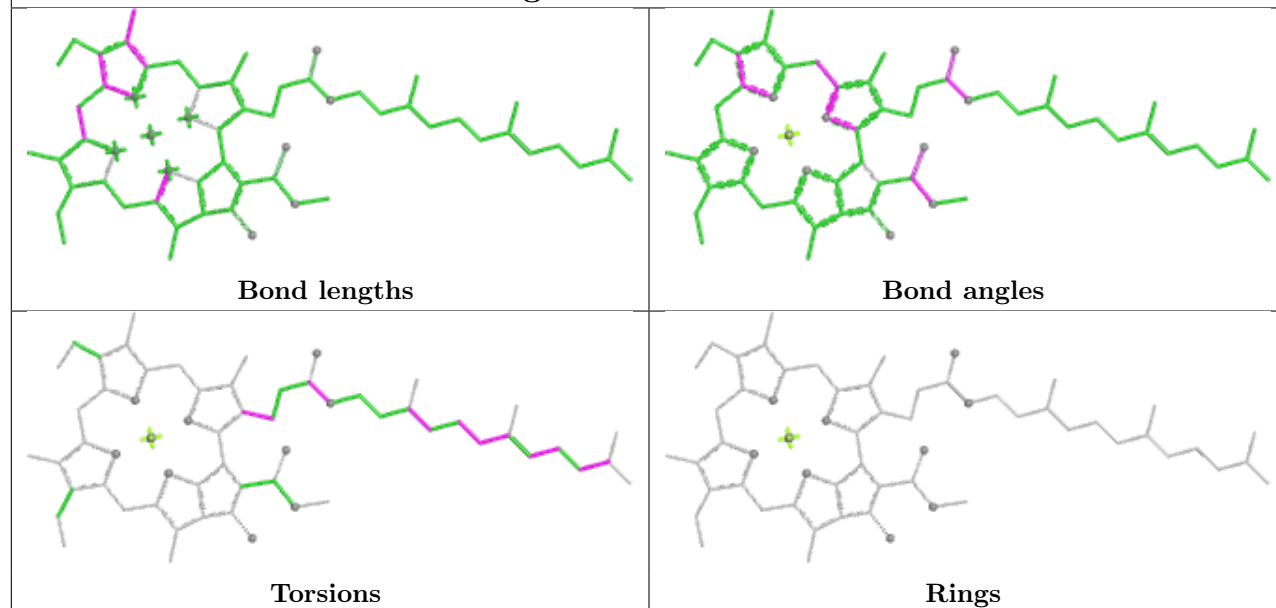
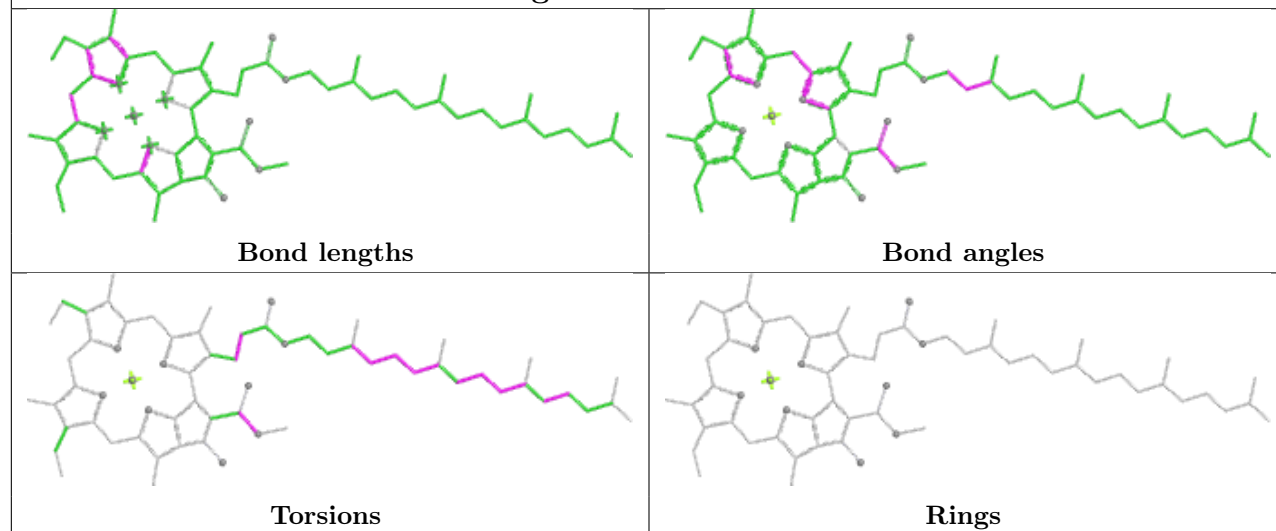
Ligand CLA A 808

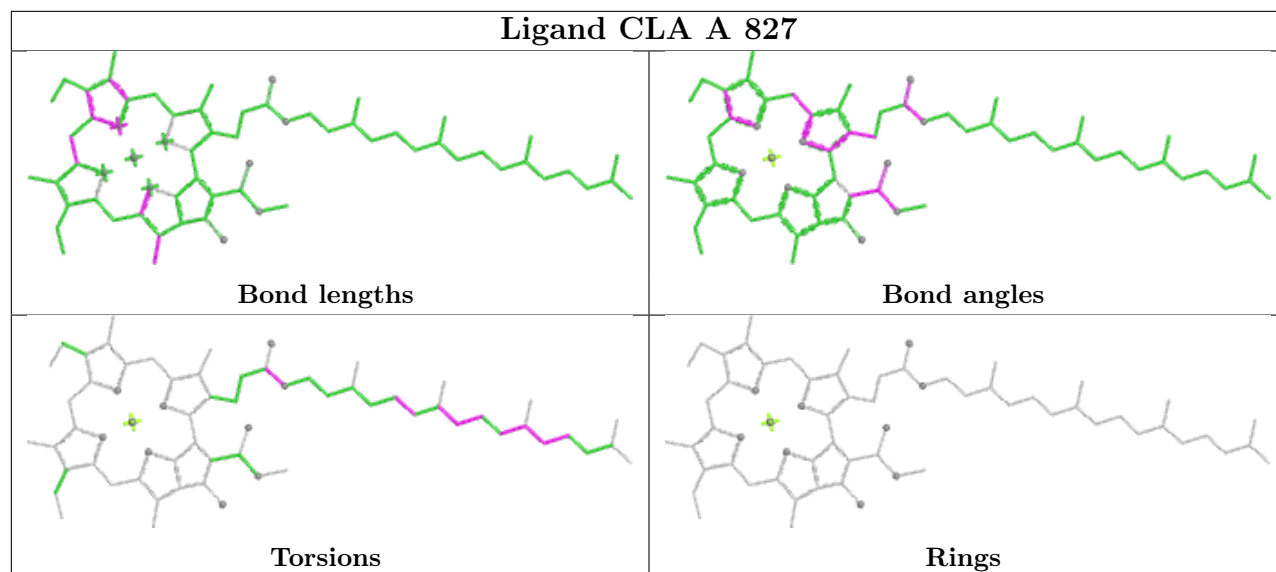
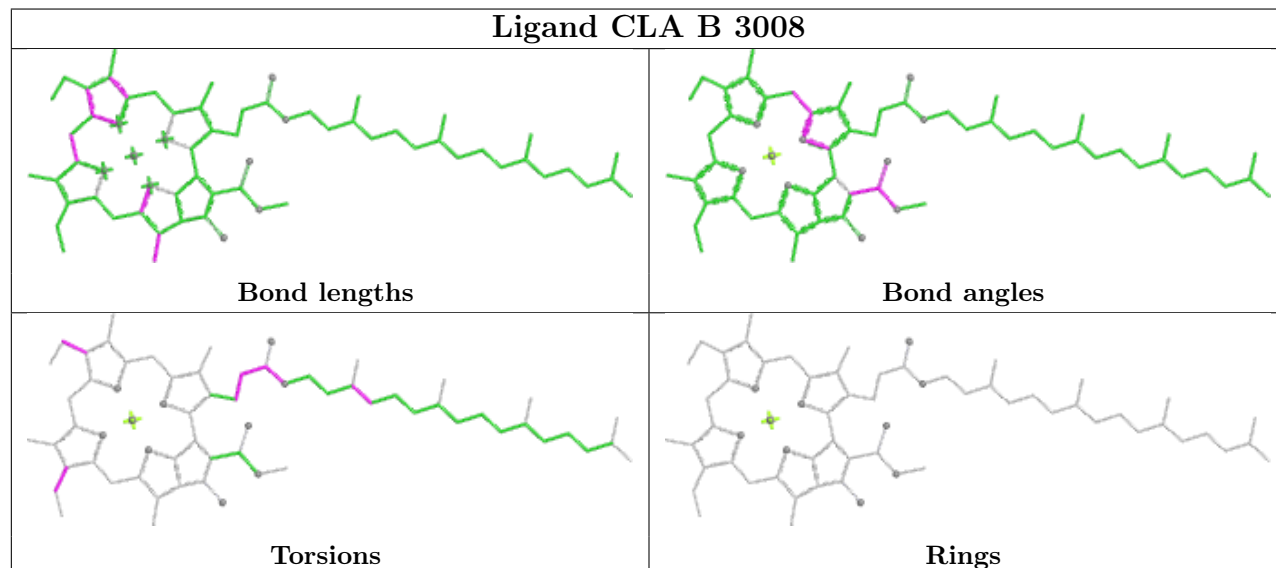


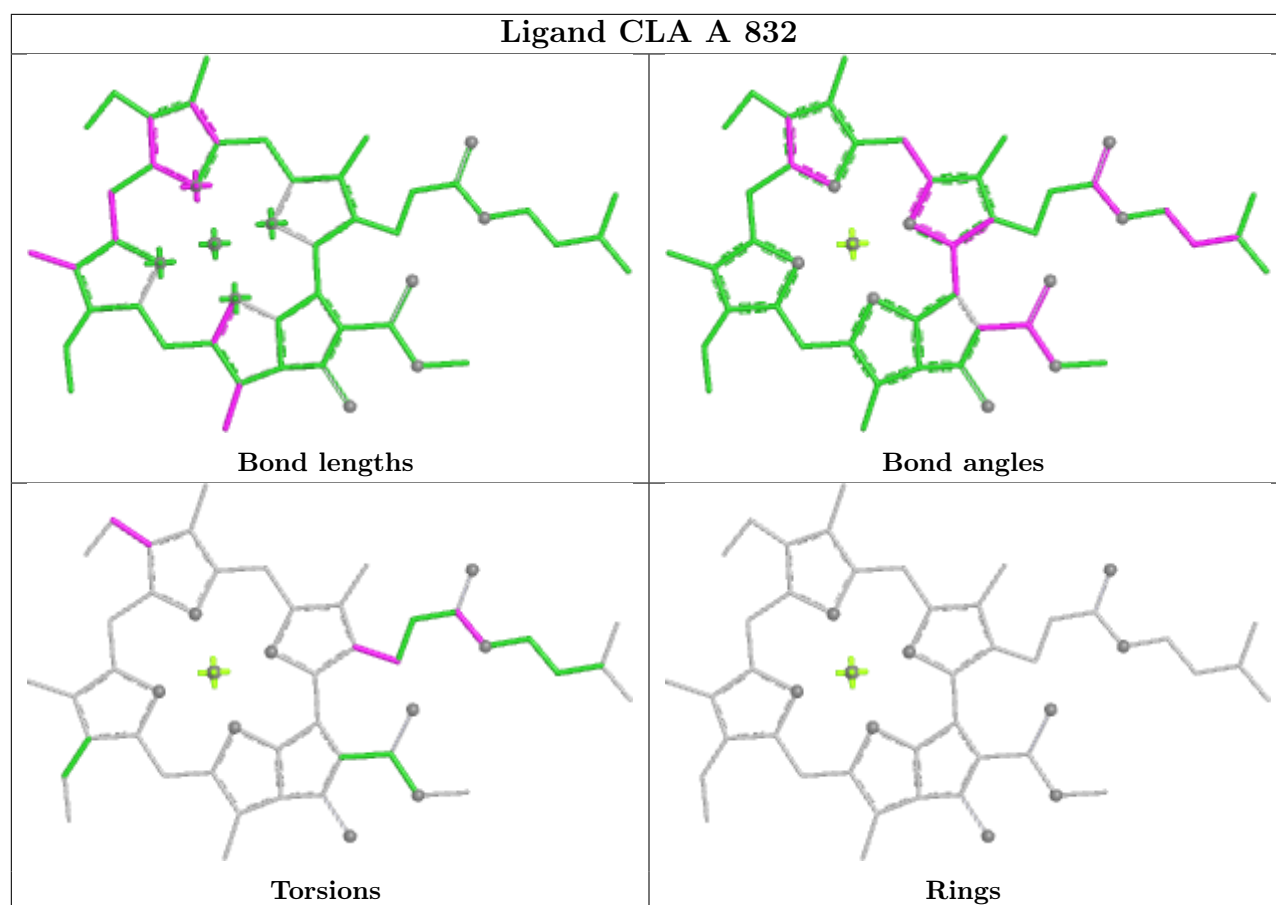
Ligand CLA A 842



Ligand CLA A 828	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 3019	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR F 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 3038**Ligand CLA A 830**

Ligand CLA A 827**Ligand CLA B 3008**



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	740/755 (98%)	1.05	123 (16%) 4 4	32, 97, 149, 195	0
2	B	739/740 (99%)	0.68	66 (8%) 15 15	23, 70, 117, 151	0
3	C	80/80 (100%)	0.36	2 (2%) 58 56	22, 63, 91, 101	0
4	D	138/138 (100%)	0.35	7 (5%) 33 33	40, 75, 102, 157	0
5	E	69/75 (92%)	1.05	10 (14%) 6 5	64, 92, 114, 130	0
6	F	141/164 (85%)	0.83	16 (11%) 10 8	64, 116, 135, 143	0
7	I	38/38 (100%)	0.67	4 (10%) 11 11	27, 44, 72, 106	0
8	J	41/41 (100%)	0.85	2 (4%) 35 34	107, 126, 140, 160	0
9	K	47/83 (56%)	2.06	19 (40%) 0 0	142, 176, 193, 210	0
10	L	151/154 (98%)	0.29	3 (1%) 65 63	24, 43, 82, 131	0
11	M	31/31 (100%)	0.57	4 (12%) 7 6	40, 63, 88, 113	0
12	X	29/35 (82%)	1.23	7 (24%) 2 1	73, 97, 127, 140	0
All	All	2244/2334 (96%)	0.80	263 (11%) 9 7	22, 81, 142, 210	0

The worst 5 of 263 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	ALA	14.7
1	A	379	PRO	6.4
1	A	281	PHE	6.3
1	A	43	GLN	5.7
1	A	278	PHE	5.5

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	DGD	L	206	66/66	0.62	0.21	55,109,166,179	0
14	CLA	M	102	45/65	0.65	0.26	93,141,177,190	0
21	LMT	L	201	35/35	0.66	0.19	84,152,189,202	0
17	LMG	I	104	40/55	0.70	0.29	59,95,131,154	0
17	LMG	A	852	48/55	0.71	0.20	66,123,163,170	0
14	CLA	J	101	45/65	0.72	0.16	128,147,182,186	0
18	LHG	B	3049	23/49	0.72	0.22	83,121,149,155	0
14	CLA	A	816	45/65	0.78	0.21	116,153,179,189	0
14	CLA	K	103	45/65	0.78	0.19	111,142,174,176	0
16	BCR	K	102	40/40	0.79	0.29	117,157,176,186	0
18	LHG	M	101	49/49	0.79	0.23	57,99,174,191	0
14	CLA	J	102	37/65	0.79	0.17	112,135,160,173	0
16	BCR	B	3043	40/40	0.79	0.24	85,120,154,171	0
14	CLA	A	817	49/65	0.81	0.16	73,138,169,170	0
17	LMG	A	855	30/55	0.82	0.17	42,93,155,172	0
14	CLA	A	845	52/65	0.82	0.16	54,94,121,130	0
14	CLA	A	818	54/65	0.82	0.19	106,134,161,172	0
14	CLA	F	202	45/65	0.83	0.15	96,125,156,161	0
14	CLA	K	101	41/65	0.83	0.17	122,159,195,204	0
16	BCR	A	847	40/40	0.83	0.29	106,141,172,186	0
14	CLA	A	828	65/65	0.85	0.21	69,103,138,145	0
16	BCR	J	104	40/40	0.85	0.22	88,126,155,160	0
16	BCR	B	3046	40/40	0.86	0.26	64,90,110,116	0
14	CLA	A	811	45/65	0.86	0.16	102,135,162,170	0
16	BCR	A	848	40/40	0.87	0.30	88,129,181,187	0
14	CLA	A	813	54/65	0.87	0.14	84,111,138,146	0
14	CLA	A	823	49/65	0.88	0.13	88,126,156,168	0
14	CLA	B	3021	47/65	0.88	0.14	79,108,139,145	0
16	BCR	B	3050	40/40	0.88	0.20	56,94,138,144	0
16	BCR	A	849	40/40	0.88	0.22	71,101,165,167	0
16	BCR	J	105	40/40	0.88	0.22	77,124,164,171	0
16	BCR	A	850	40/40	0.88	0.19	51,84,118,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	BCR	M	103	40/40	0.88	0.14	31,58,86,92	0
14	CLA	A	837	45/65	0.89	0.14	90,114,137,148	0
14	CLA	A	808	51/65	0.89	0.15	91,113,140,144	0
14	CLA	B	3018	59/65	0.89	0.19	57,91,119,127	0
14	CLA	A	824	51/65	0.89	0.14	77,111,142,148	0
16	BCR	F	203	40/40	0.89	0.22	53,104,137,157	0
14	CLA	B	3032	49/65	0.89	0.15	44,79,107,132	0
14	CLA	A	821	43/65	0.89	0.16	82,140,180,186	0
14	CLA	A	836	54/65	0.89	0.20	57,97,138,146	0
14	CLA	A	820	65/65	0.90	0.17	76,110,135,144	0
14	CLA	A	815	45/65	0.90	0.15	96,124,160,166	0
16	BCR	F	201	40/40	0.90	0.23	55,101,134,142	0
14	CLA	A	814	60/65	0.90	0.19	83,125,150,151	0
14	CLA	B	3034	58/65	0.90	0.16	73,108,147,151	0
14	CLA	A	819	54/65	0.90	0.15	71,104,126,142	0
16	BCR	B	3044	40/40	0.90	0.19	58,84,124,133	0
16	BCR	L	207	40/40	0.90	0.14	7,48,96,108	0
14	CLA	B	3027	65/65	0.91	0.17	48,75,102,107	0
14	CLA	B	3015	65/65	0.91	0.15	56,87,122,127	0
16	BCR	B	3045	40/40	0.91	0.15	53,86,141,153	0
14	CLA	B	3017	55/65	0.91	0.14	71,107,143,176	0
14	CLA	X	1701	45/65	0.91	0.14	85,114,144,150	0
14	CLA	B	3038	60/65	0.91	0.17	51,91,123,132	0
14	CLA	A	838	51/65	0.91	0.14	46,69,90,112	0
16	BCR	J	103	40/40	0.91	0.21	71,112,135,139	0
20	CA	B	3002	1/1	0.91	0.12	80,80,80,80	0
14	CLA	B	3013	45/65	0.91	0.11	67,99,126,129	0
14	CLA	B	3023	55/65	0.91	0.15	79,105,132,133	0
14	CLA	B	3022	45/65	0.92	0.11	77,103,130,130	0
14	CLA	B	3012	45/65	0.92	0.10	55,77,98,121	0
16	BCR	A	851	40/40	0.92	0.19	30,73,100,103	0
14	CLA	B	3025	54/65	0.92	0.15	58,75,97,98	0
14	CLA	A	822	65/65	0.92	0.18	61,97,131,137	0
14	CLA	B	3031	45/65	0.92	0.13	56,83,106,123	0
14	CLA	L	205	65/65	0.92	0.15	31,56,85,95	0
14	CLA	B	3019	60/65	0.92	0.16	60,81,110,117	0
14	CLA	B	3020	65/65	0.92	0.20	58,101,131,143	0
14	CLA	A	812	65/65	0.92	0.17	91,124,154,157	0
16	BCR	I	103	40/40	0.92	0.13	12,44,69,71	0
16	BCR	I	105	40/40	0.92	0.13	13,38,58,75	0
14	CLA	B	3039	65/65	0.92	0.17	52,98,138,154	0
14	CLA	I	101	65/65	0.93	0.12	2,28,62,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	A	839	65/65	0.93	0.12	31,69,107,130	0
14	CLA	A	842	51/65	0.93	0.15	46,85,134,153	0
14	CLA	A	803	65/65	0.93	0.17	52,77,98,118	0
14	CLA	B	3003	65/65	0.93	0.15	26,59,80,87	0
14	CLA	B	3026	46/65	0.93	0.15	46,74,99,100	0
14	CLA	A	826	65/65	0.93	0.17	81,111,141,144	0
14	CLA	B	3029	65/65	0.93	0.15	37,71,89,107	0
15	PQN	A	846	33/33	0.93	0.19	61,89,118,121	0
14	CLA	A	810	65/65	0.93	0.15	54,109,158,171	0
14	CLA	A	833	65/65	0.93	0.15	34,73,145,150	0
14	CLA	B	3033	65/65	0.93	0.15	66,96,122,131	0
14	CLA	A	834	65/65	0.93	0.12	20,47,75,81	0
14	CLA	B	3036	45/65	0.93	0.14	54,90,117,121	0
18	LHG	A	853	49/49	0.93	0.20	48,94,118,128	0
14	CLA	A	804	65/65	0.93	0.17	69,108,135,142	0
14	CLA	A	805	59/65	0.93	0.16	85,108,135,151	0
14	CLA	B	3040	47/65	0.93	0.14	59,84,103,115	0
14	CLA	A	807	65/65	0.93	0.17	66,94,120,127	0
16	BCR	B	3047	40/40	0.93	0.13	25,44,71,71	0
14	CLA	A	829	65/65	0.94	0.17	69,96,120,127	0
14	CLA	A	843	65/65	0.94	0.15	47,83,127,146	0
14	CLA	A	830	65/65	0.94	0.14	65,98,128,131	0
14	CLA	A	856	65/65	0.94	0.17	48,75,101,112	0
16	BCR	I	102	40/40	0.94	0.11	8,39,60,78	0
14	CLA	A	832	50/65	0.94	0.12	43,71,101,127	0
14	CLA	L	203	65/65	0.94	0.12	21,51,82,104	0
14	CLA	L	204	65/65	0.94	0.12	18,55,127,140	0
14	CLA	B	3004	65/65	0.94	0.12	20,43,63,75	0
14	CLA	B	3008	65/65	0.94	0.12	20,45,77,99	0
14	CLA	B	3030	65/65	0.94	0.14	30,57,90,108	0
14	CLA	A	802	65/65	0.94	0.12	30,49,65,85	0
15	PQN	B	3042	33/33	0.94	0.13	27,47,66,70	0
13	CL0	A	801	65/65	0.94	0.14	11,56,81,84	0
14	CLA	B	3014	65/65	0.94	0.13	52,82,109,112	0
17	LMG	B	3048	55/55	0.94	0.14	30,68,94,97	0
14	CLA	A	825	59/65	0.94	0.18	60,93,133,145	0
14	CLA	B	3035	45/65	0.94	0.11	65,83,105,108	0
18	LHG	A	854	27/49	0.94	0.13	56,89,126,128	0
14	CLA	B	3016	45/65	0.94	0.10	71,92,125,128	0
14	CLA	A	809	65/65	0.94	0.16	48,94,134,139	0
14	CLA	A	827	65/65	0.94	0.17	40,78,156,177	0
14	CLA	A	806	65/65	0.94	0.18	77,111,146,152	0

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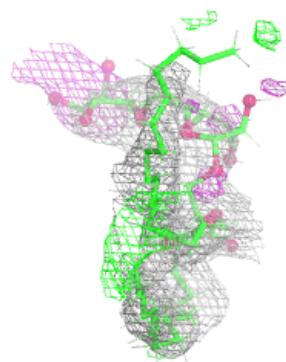
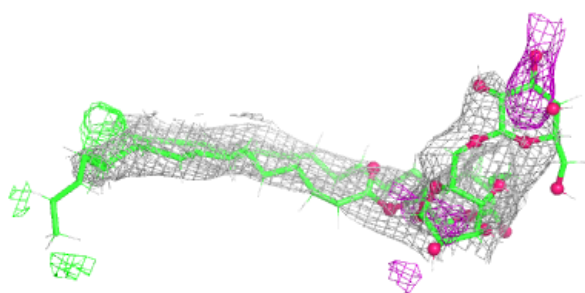
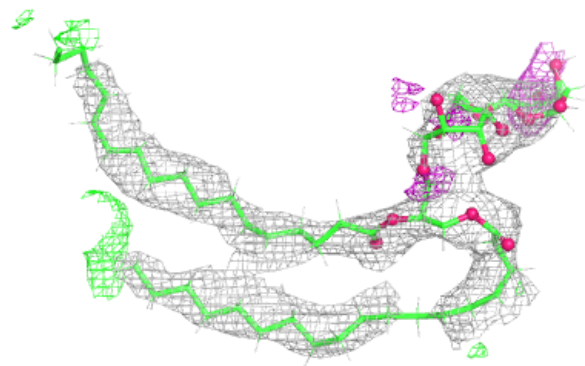
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	A	840	47/65	0.94	0.12	32,65,86,103	0
14	CLA	B	3010	65/65	0.95	0.10	16,48,76,100	0
14	CLA	A	844	65/65	0.95	0.10	2,28,60,69	0
14	CLA	A	831	65/65	0.95	0.18	66,97,120,129	0
14	CLA	B	3041	65/65	0.95	0.12	14,39,62,65	0
14	CLA	B	3005	54/65	0.95	0.12	33,58,77,85	0
14	CLA	B	3006	65/65	0.95	0.12	37,66,100,111	0
14	CLA	B	3007	65/65	0.95	0.12	32,61,87,100	0
14	CLA	A	841	65/65	0.95	0.13	42,79,133,142	0
20	CA	L	202	1/1	0.95	0.06	37,37,37,37	0
14	CLA	B	3009	65/65	0.95	0.10	20,49,82,86	0
14	CLA	B	3037	45/65	0.95	0.10	74,99,130,131	0
19	SF4	B	3001	8/8	0.96	0.09	40,56,98,128	0
19	SF4	C	101	8/8	0.96	0.08	33,61,68,81	0
14	CLA	A	835	65/65	0.96	0.10	11,42,72,100	0
14	CLA	B	3011	65/65	0.96	0.09	4,34,70,79	0
14	CLA	B	3024	45/65	0.96	0.09	40,71,104,116	0
14	CLA	B	3028	65/65	0.96	0.14	25,58,110,112	0
19	SF4	C	102	8/8	0.99	0.03	48,55,72,74	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.

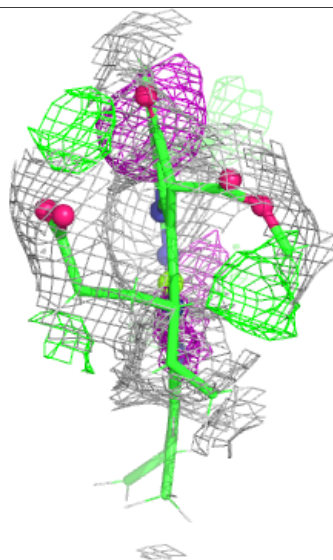
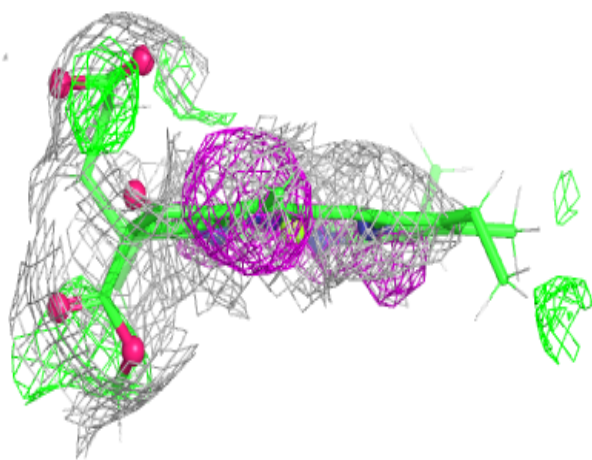
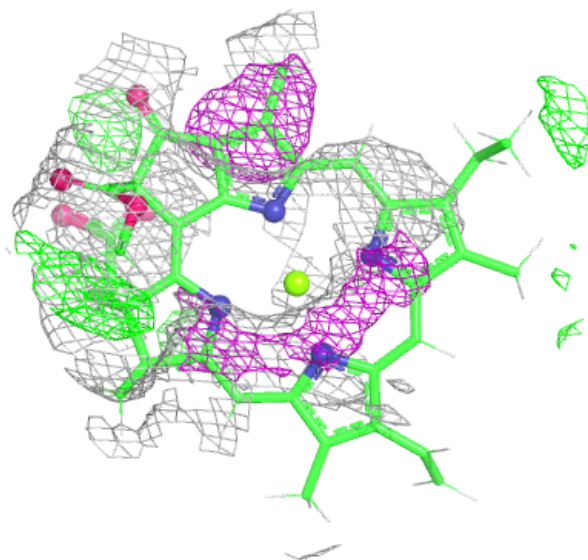
Electron density around DGD L 206:

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



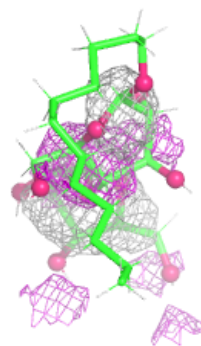
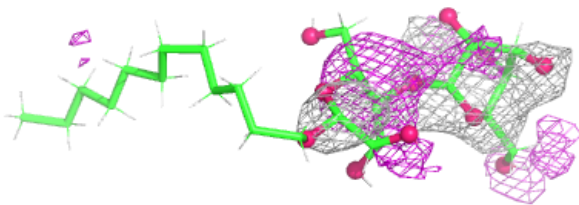
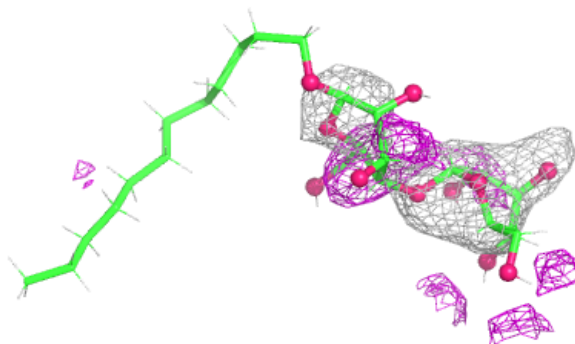
Electron density around CLA M 102:

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

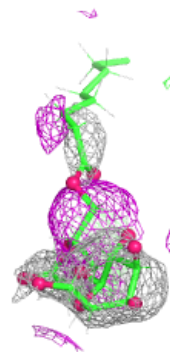
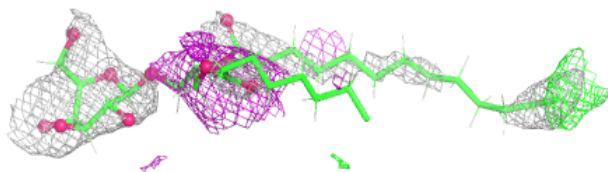
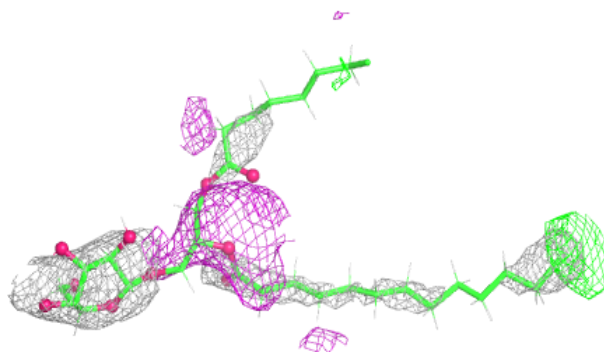


Electron density around LMT L 201:

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

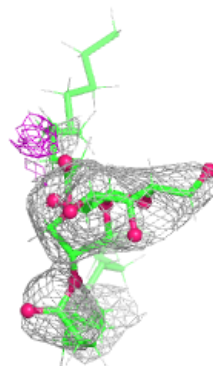
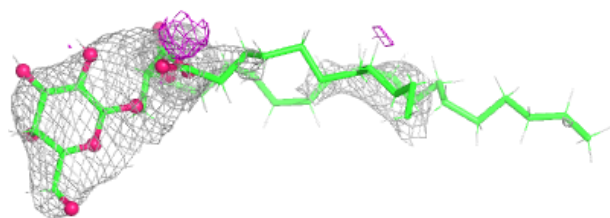
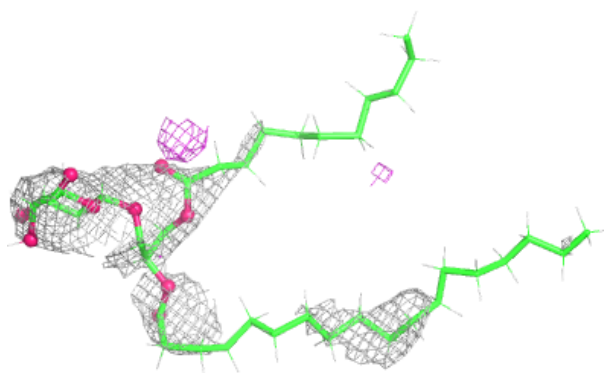
**Electron density around LMG I 104:**

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



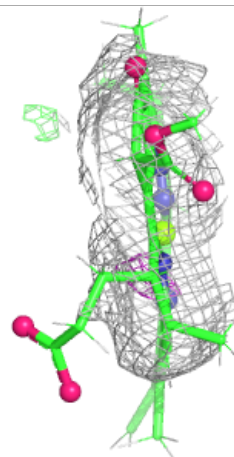
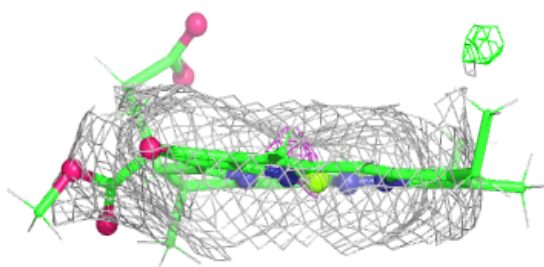
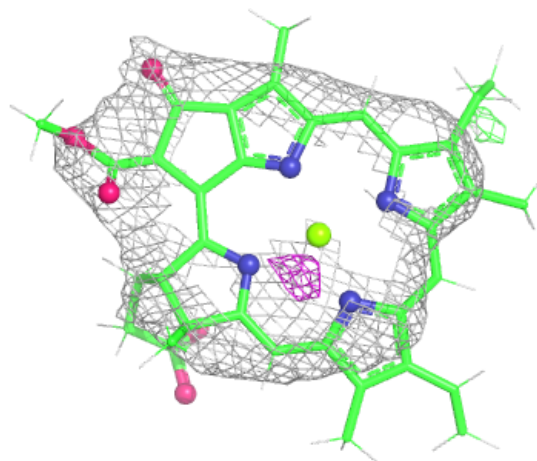
Electron density around LMG A 852:

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



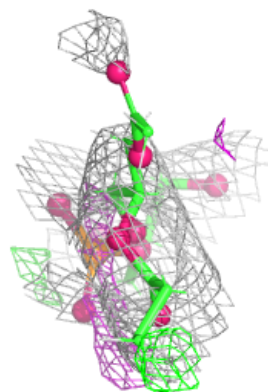
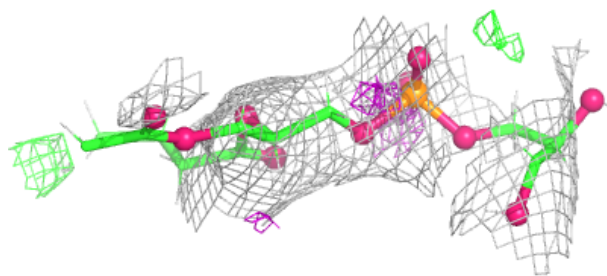
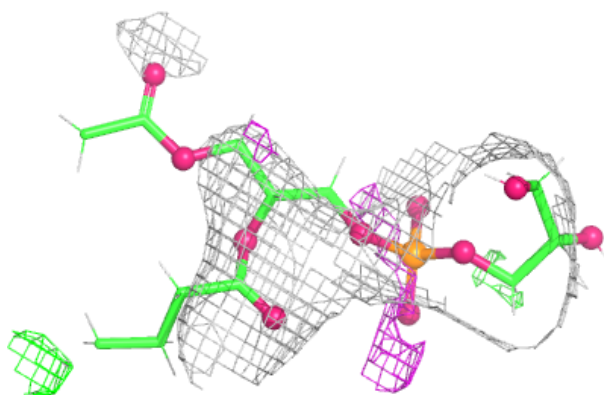
Electron density around CLA J 101:

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



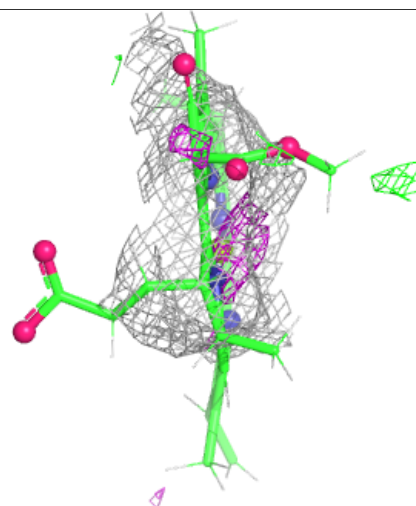
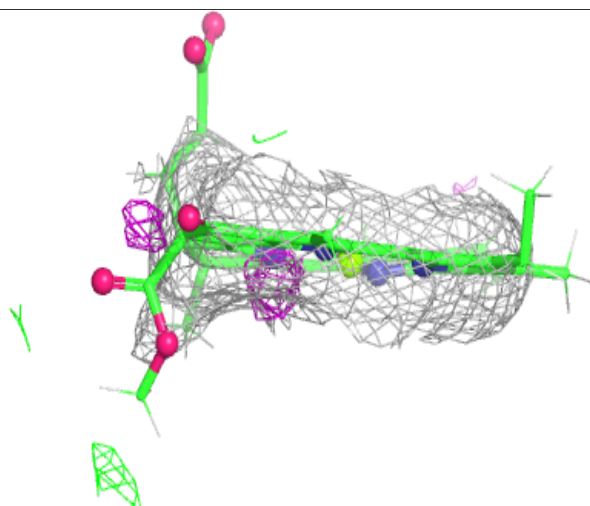
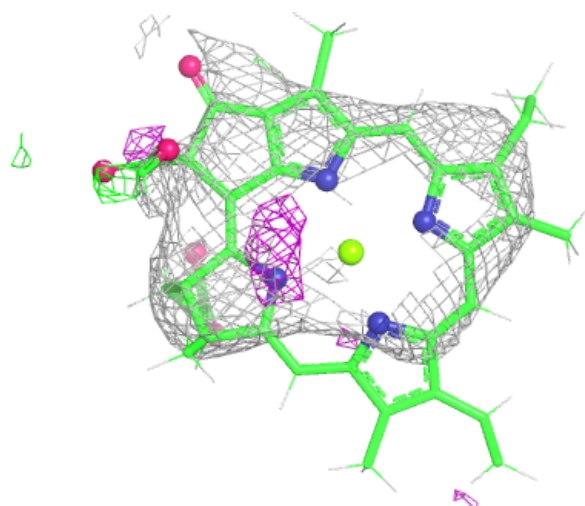
Electron density around LHG B 3049:

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



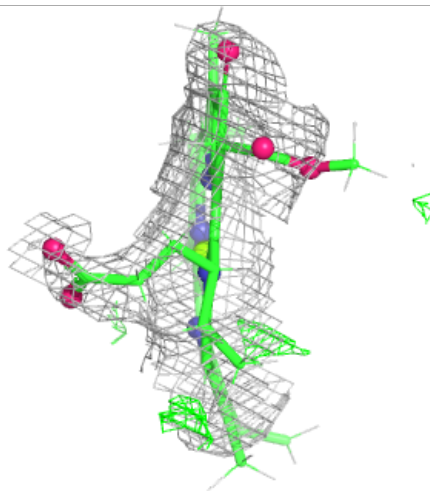
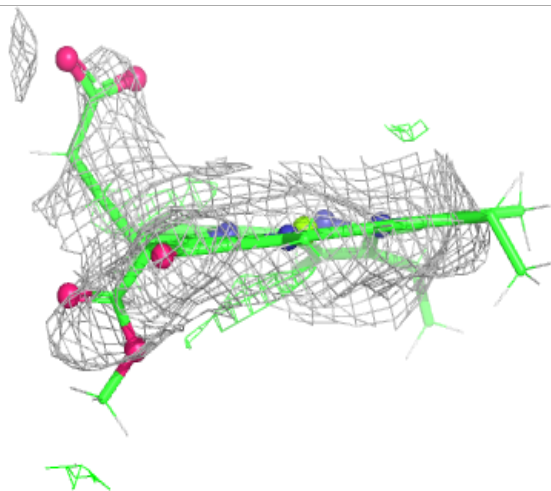
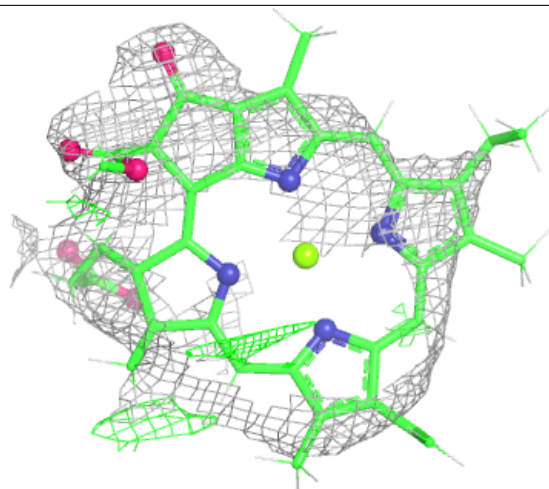
Electron density around CLA A 816:

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and green (positive)



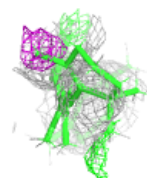
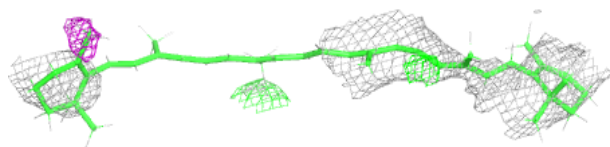
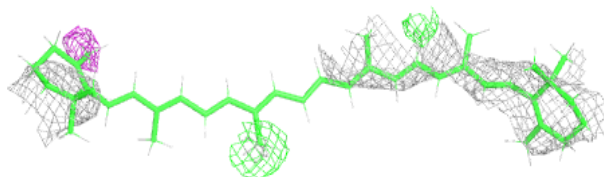
Electron density around CLA K 103:

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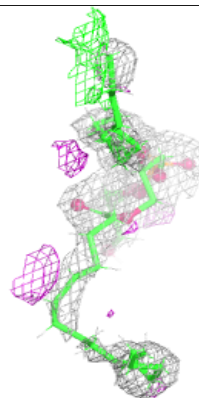
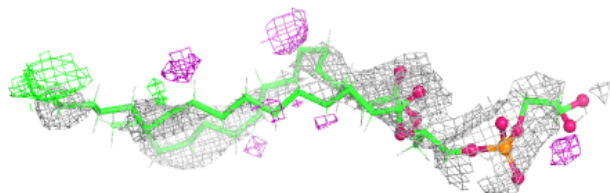
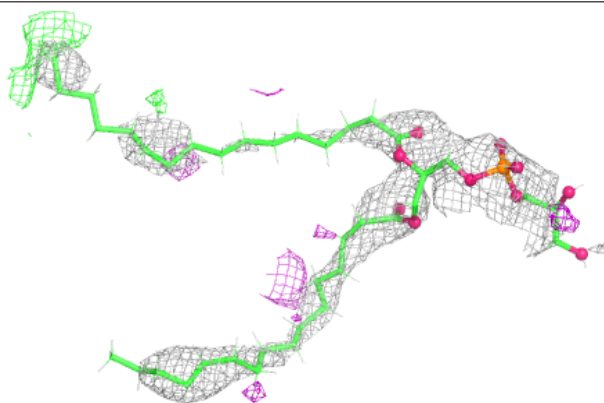


Electron density around BCR K 102:

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and green (positive)

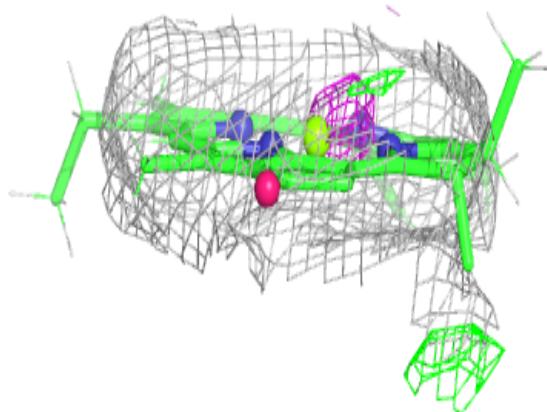
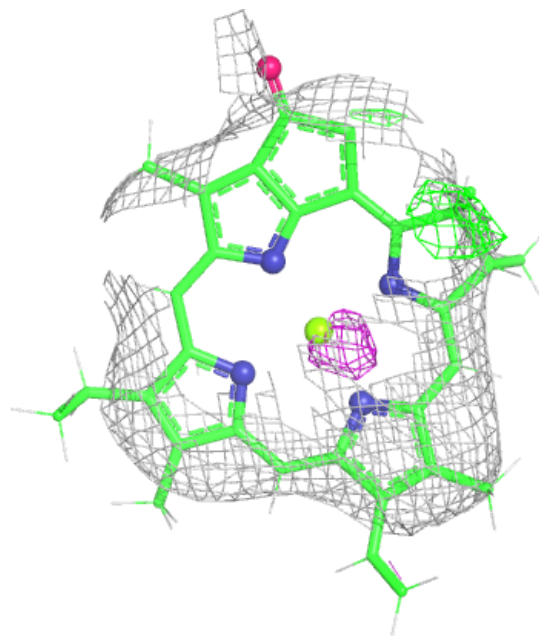
**Electron density around LHG M 101:**

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



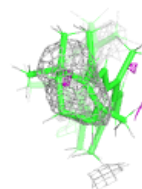
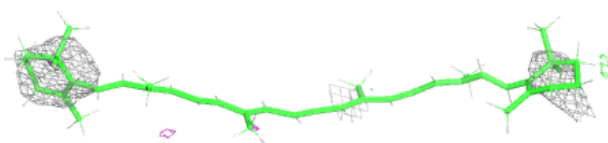
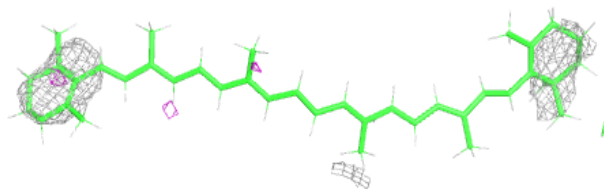
Electron density around CLA J 102:

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



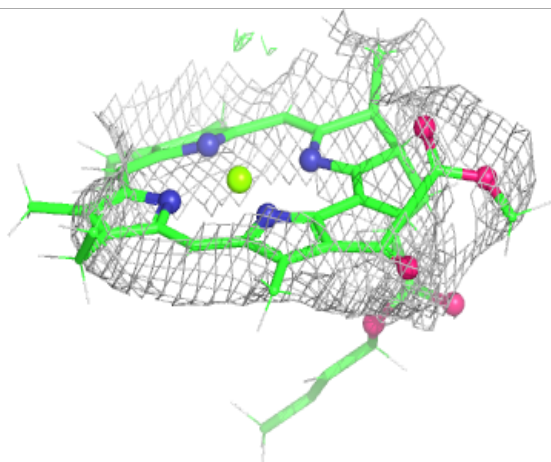
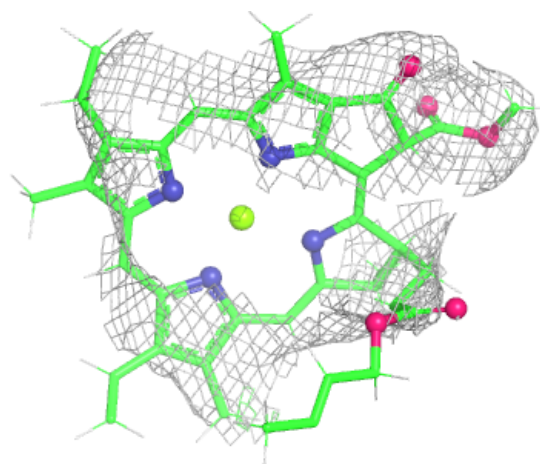
Electron density around BCR B 3043:

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



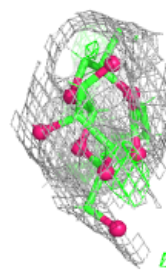
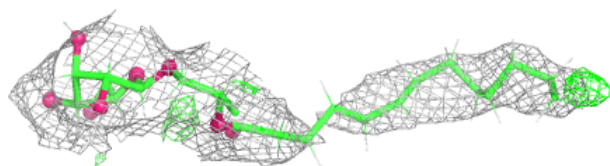
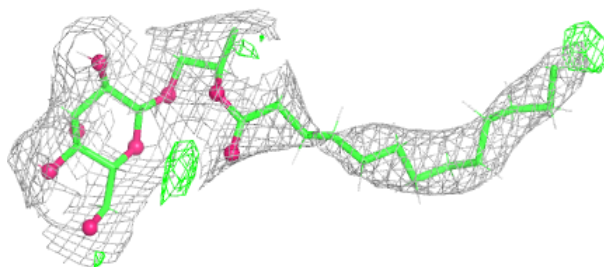
Electron density around CLA A 817:

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



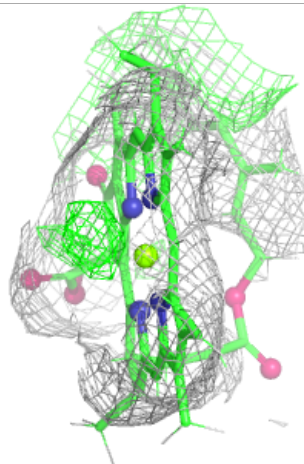
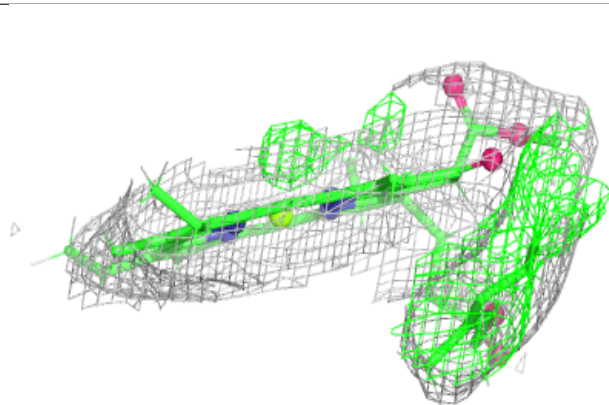
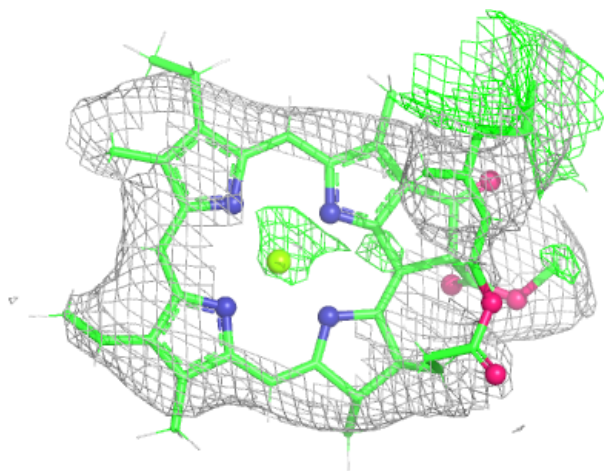
Electron density around LMG A 855:

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



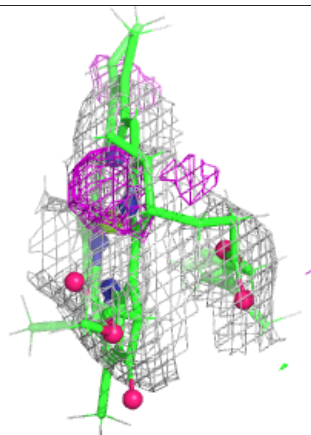
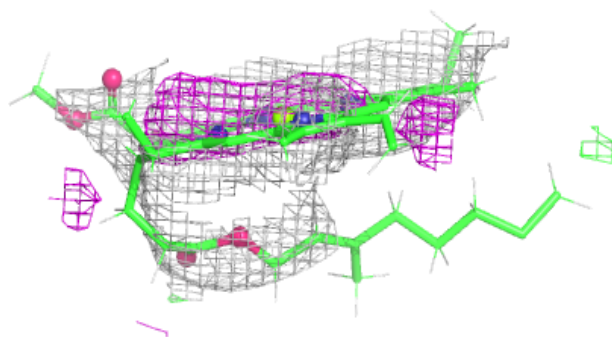
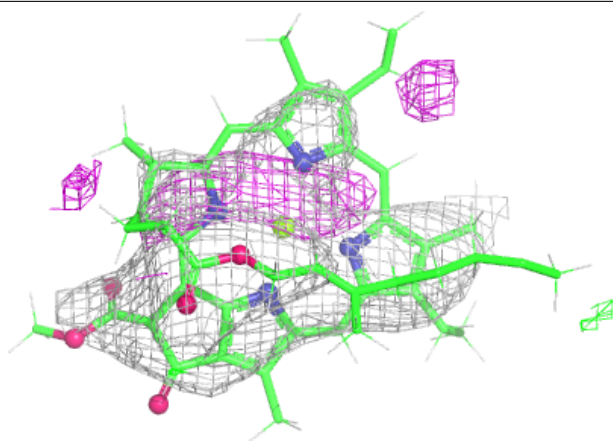
Electron density around CLA A 845:

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



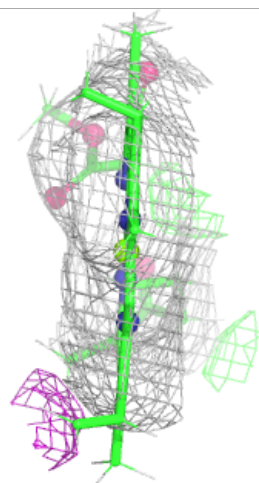
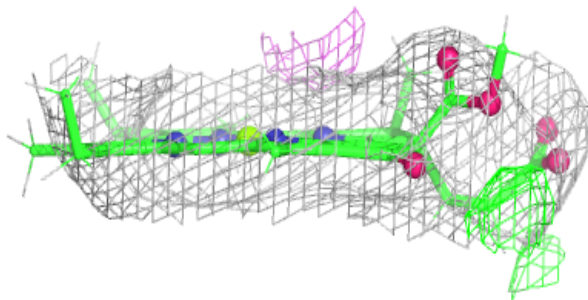
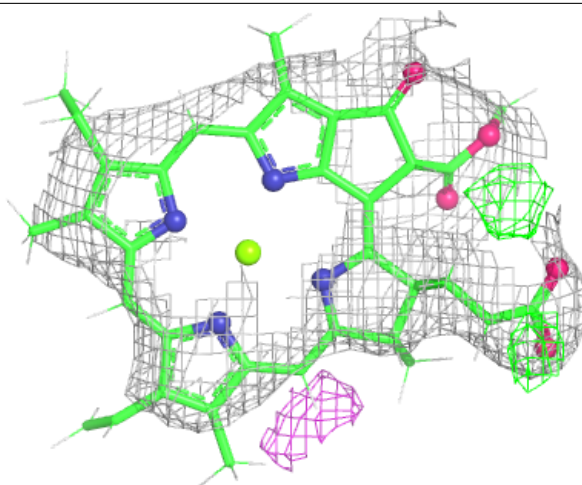
Electron density around CLA A 818:

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



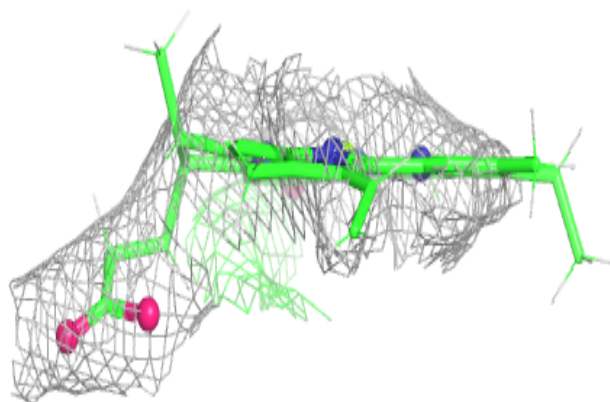
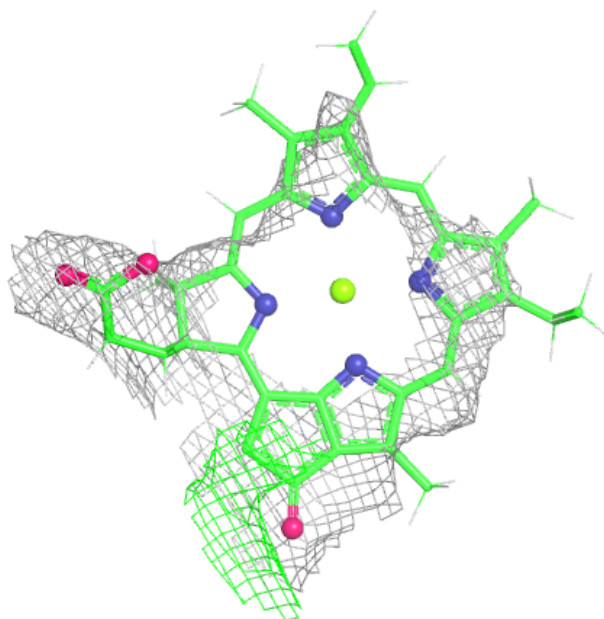
Electron density around CLA F 202:

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



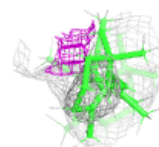
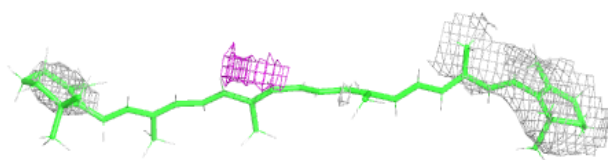
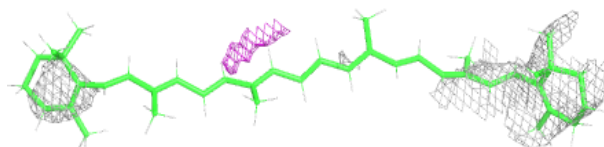
Electron density around CLA K 101:

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

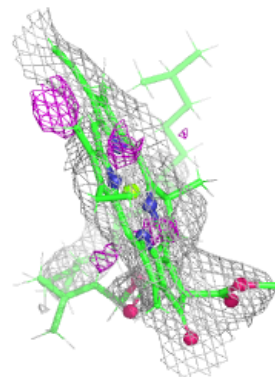
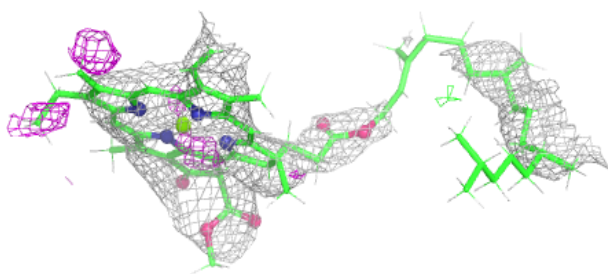
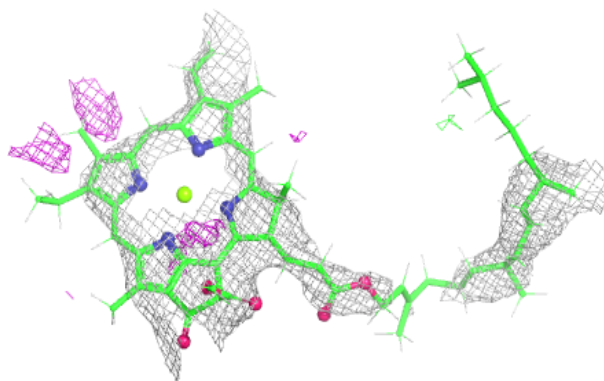


Electron density around BCR A 847:

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

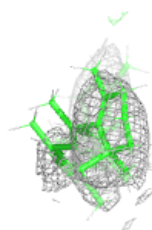
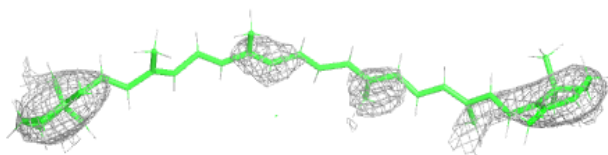
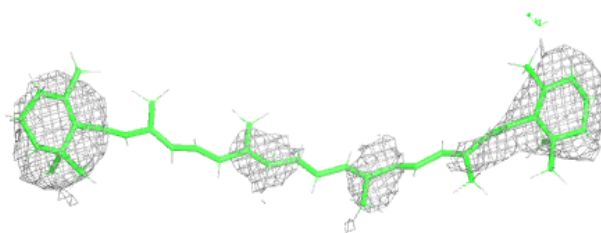
**Electron density around CLA A 828:**

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

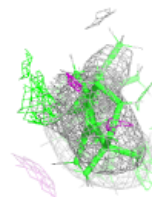
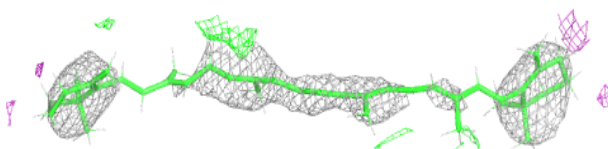
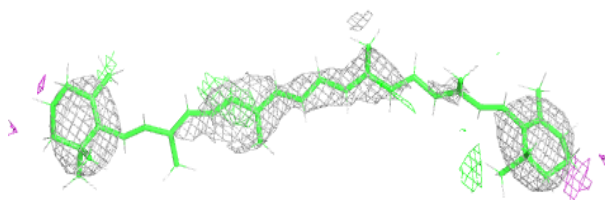


Electron density around BCR J 104:

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

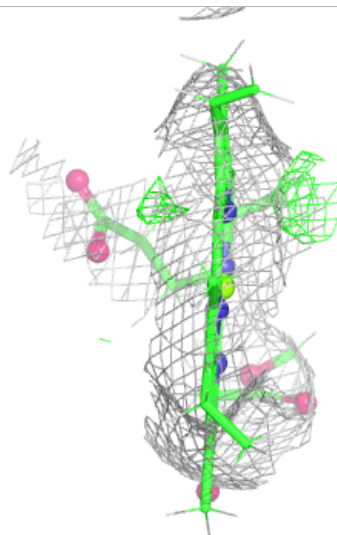
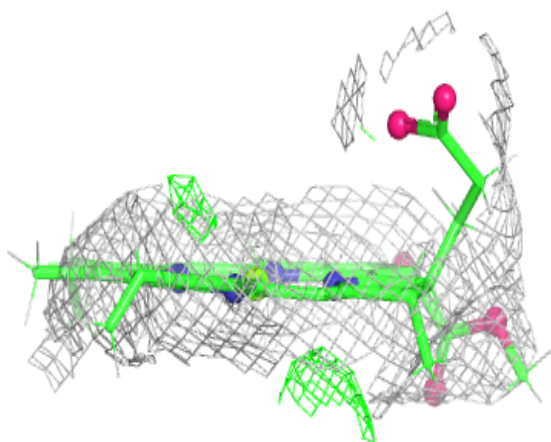
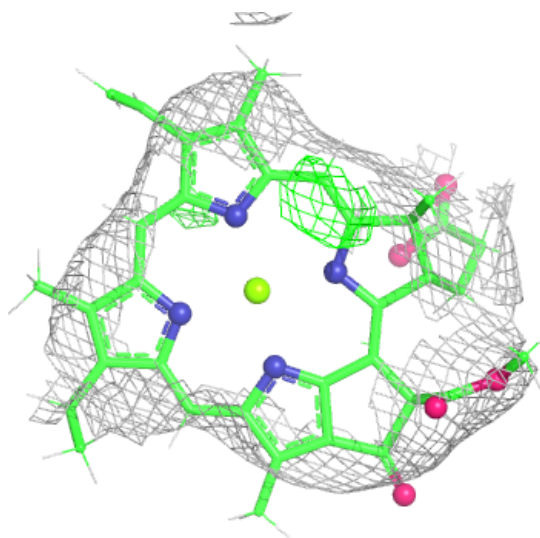
**Electron density around BCR B 3046:**

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



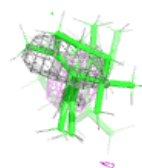
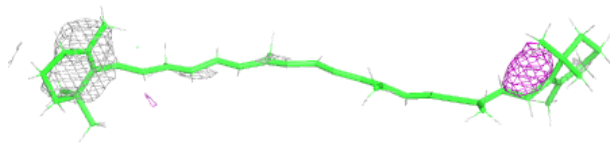
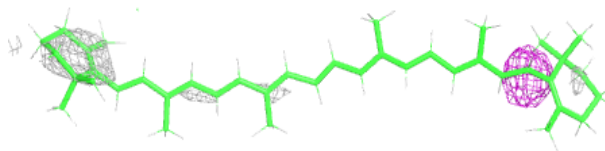
Electron density around CLA A 811:

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



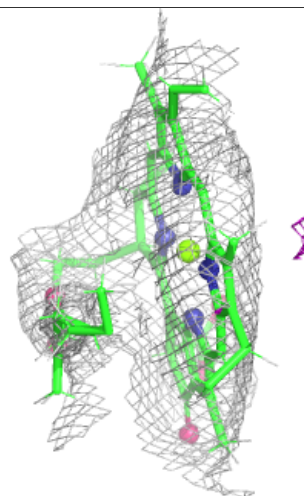
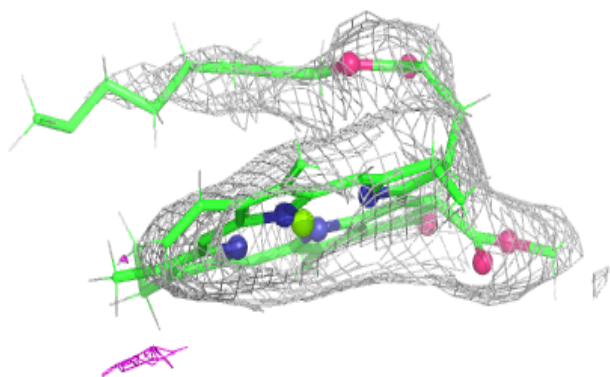
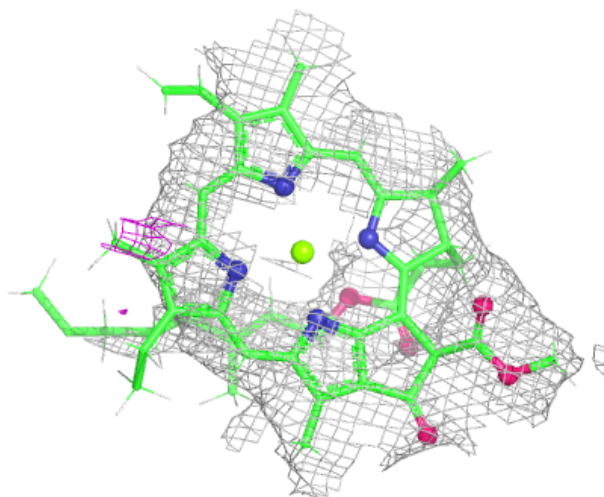
Electron density around BCR A 848:

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



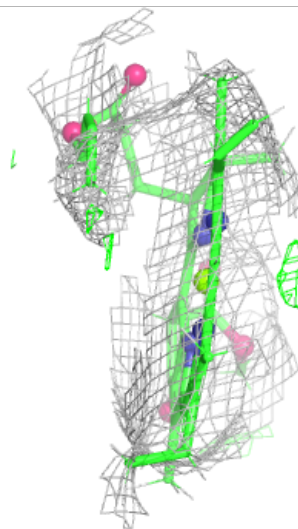
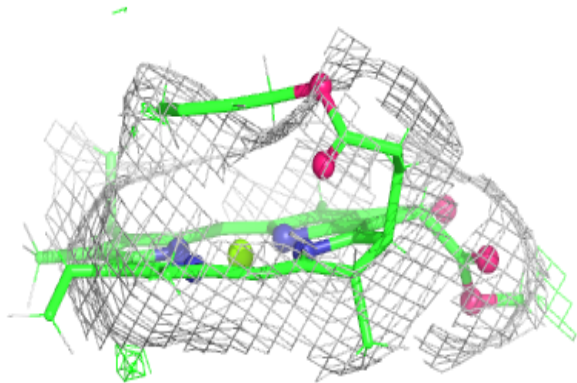
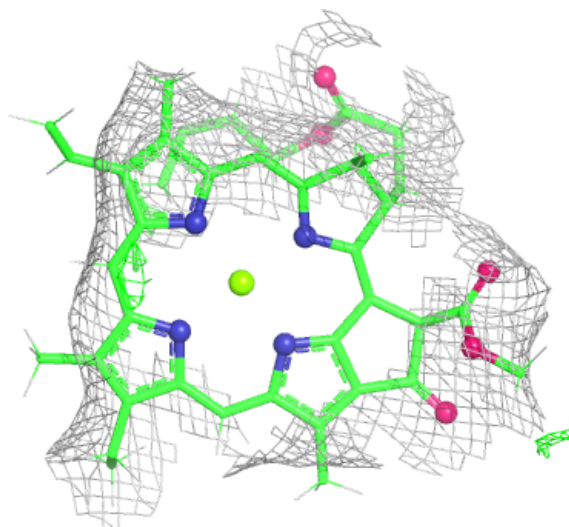
Electron density around CLA A 813:

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



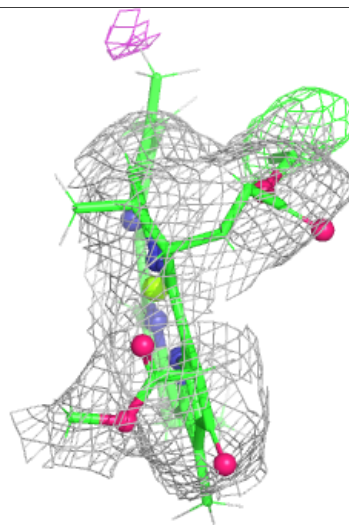
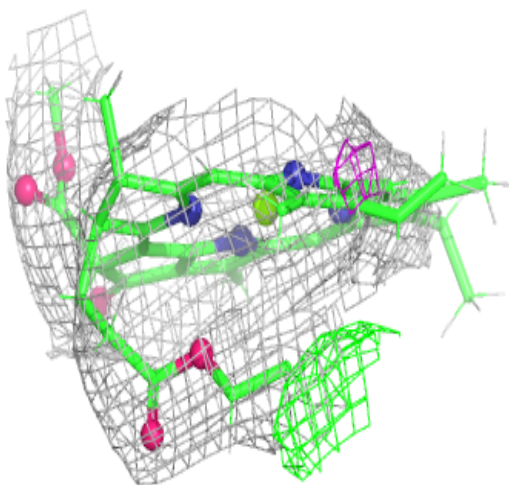
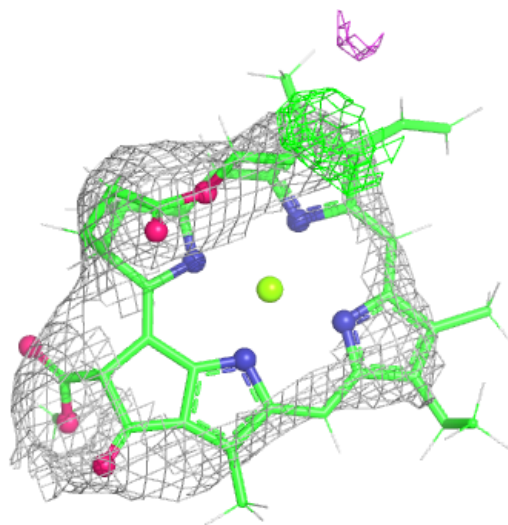
Electron density around CLA A 823:

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



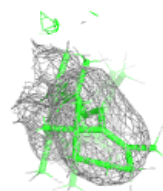
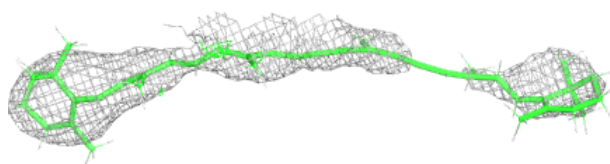
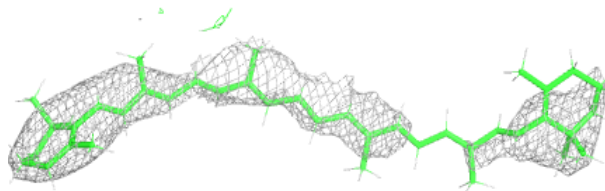
Electron density around CLA B 3021:

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

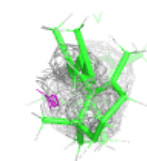
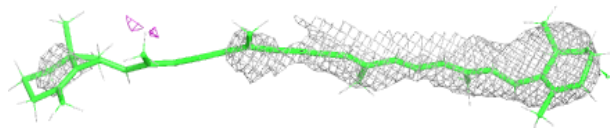
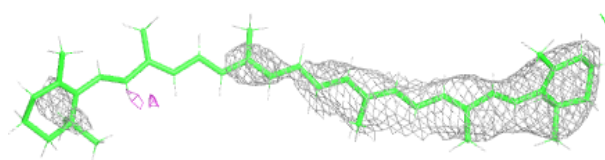


Electron density around BCR B 3050:

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

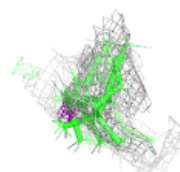
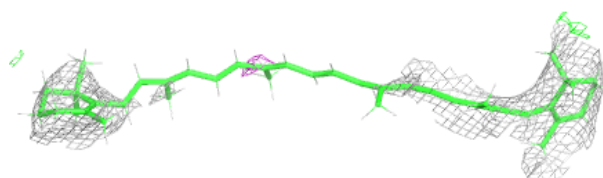
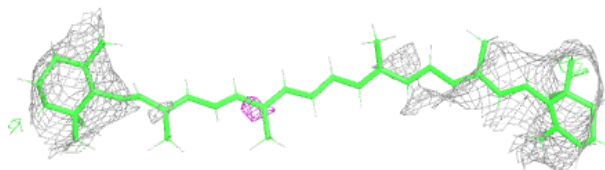
**Electron density around BCR A 849:**

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

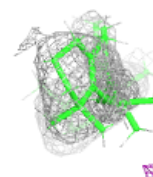
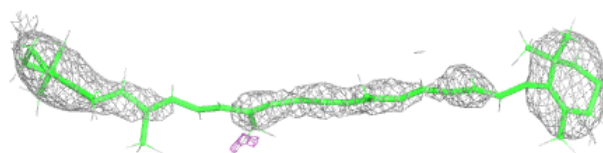
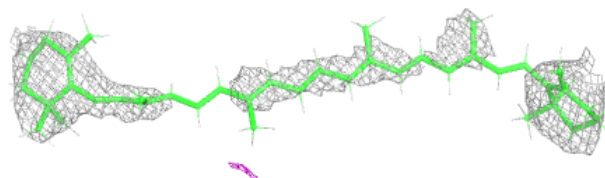


Electron density around BCR J 105:

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

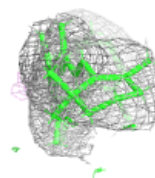
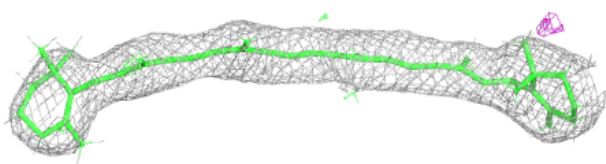
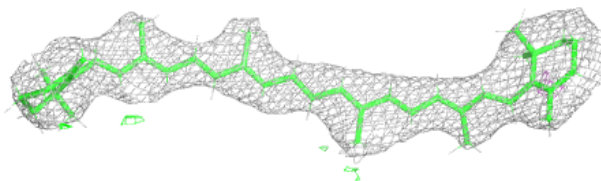
**Electron density around BCR A 850:**

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



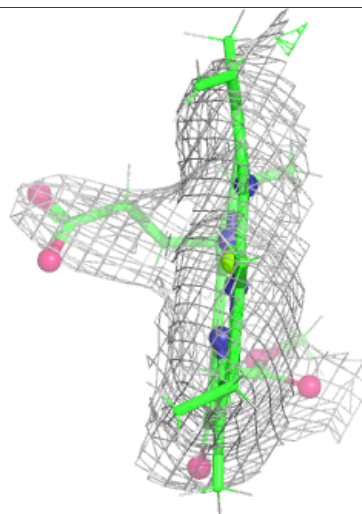
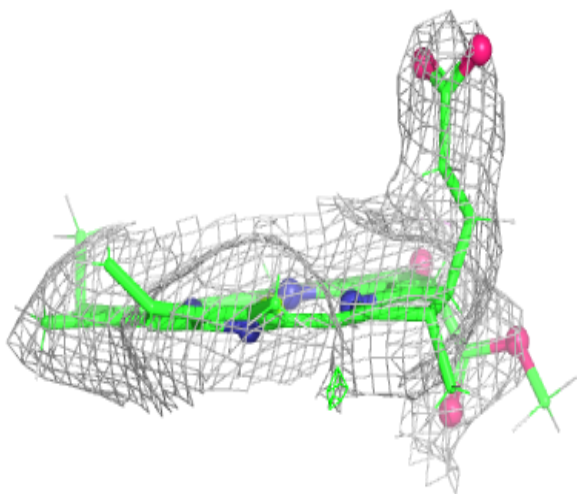
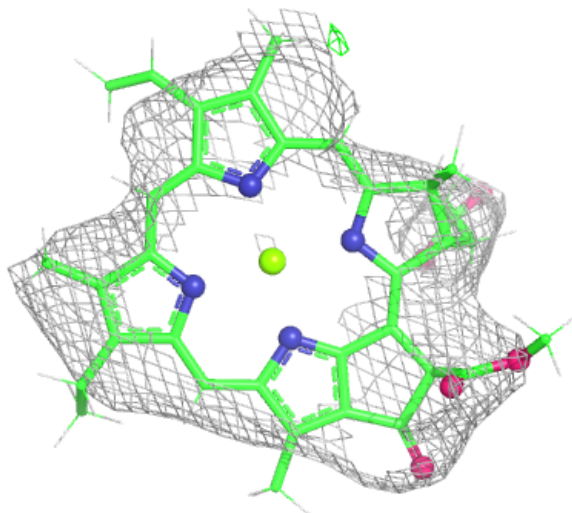
Electron density around BCR M 103:

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



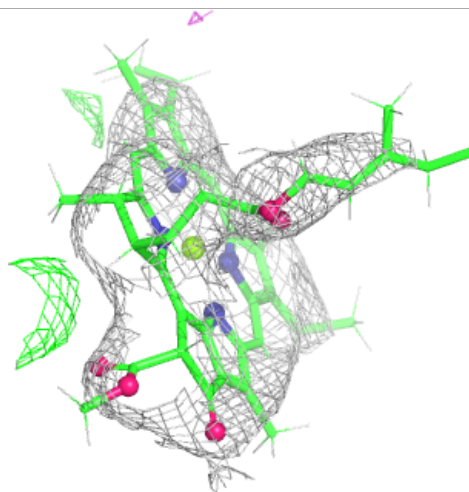
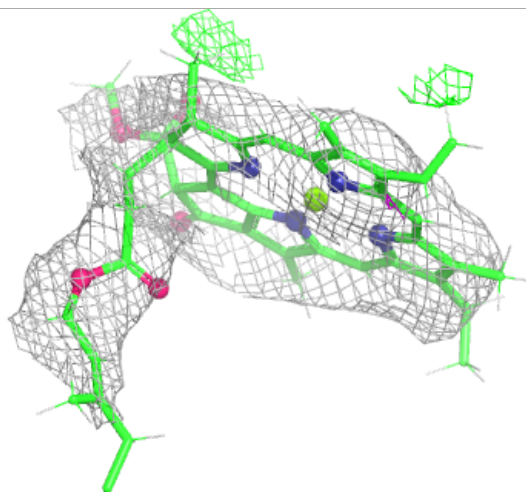
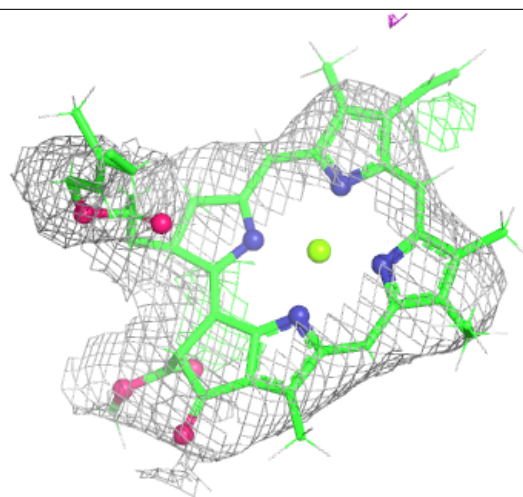
Electron density around CLA A 837:

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



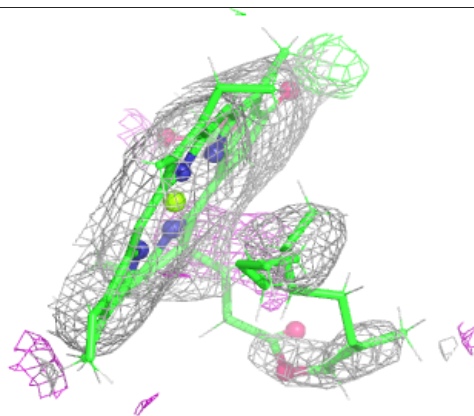
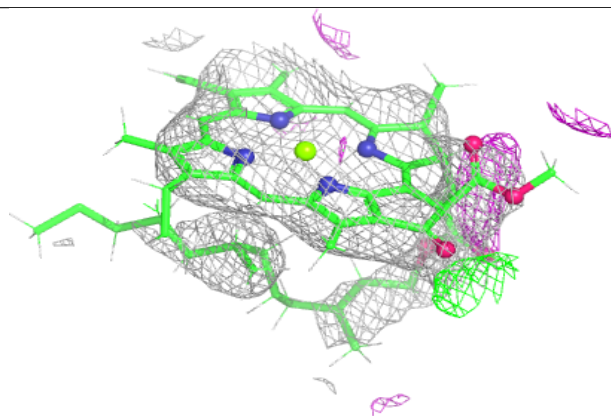
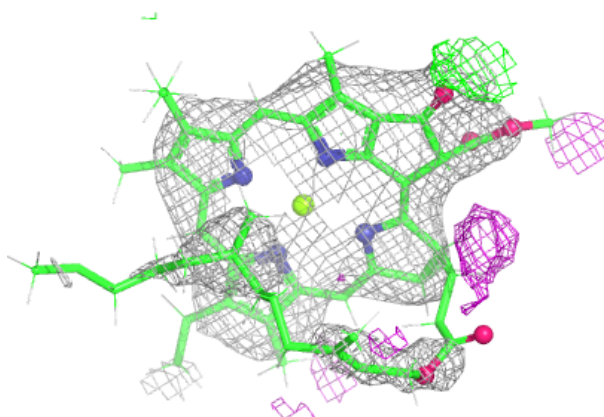
Electron density around CLA A 808:

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



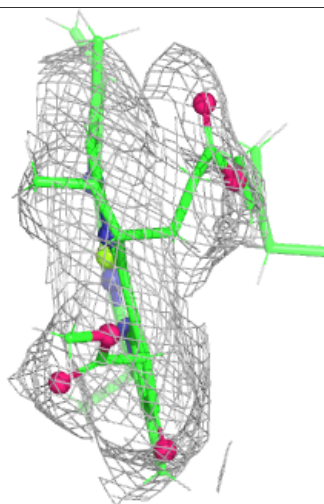
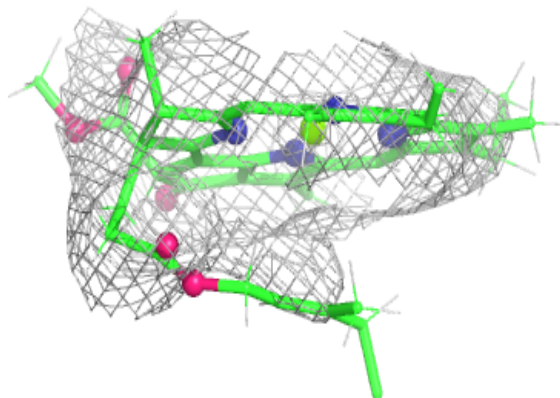
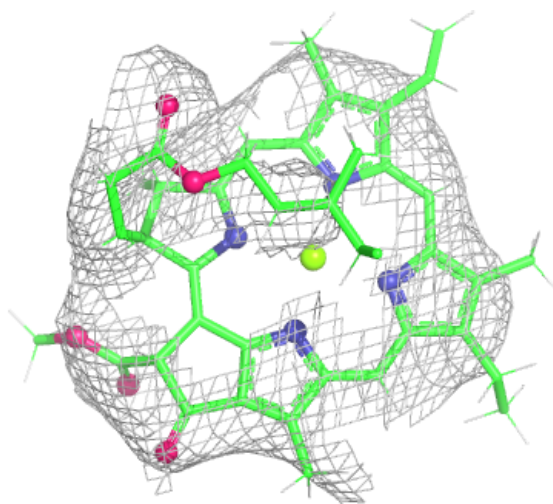
Electron density around CLA B 3018:

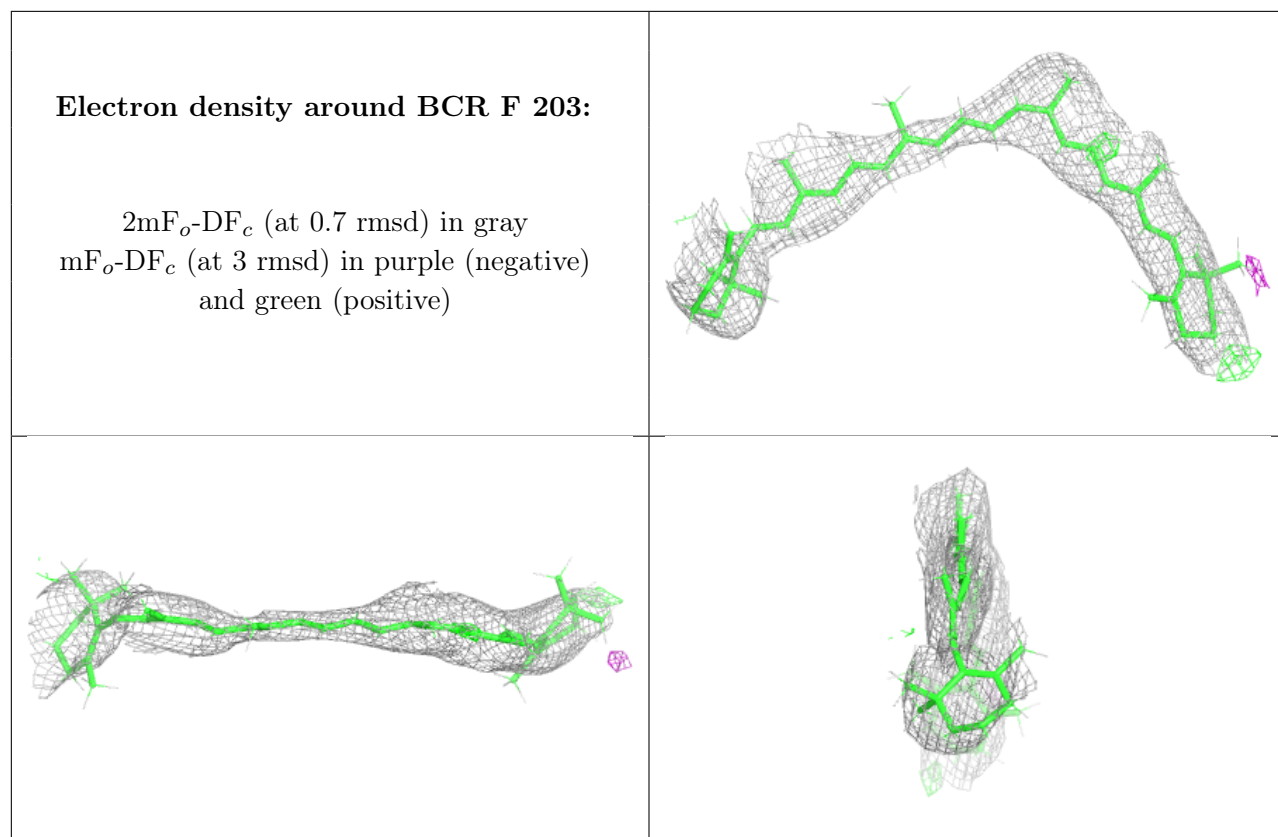
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA A 824:

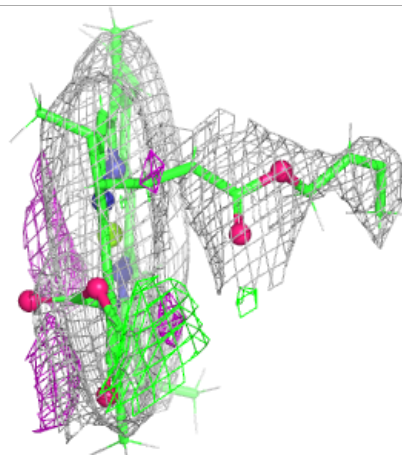
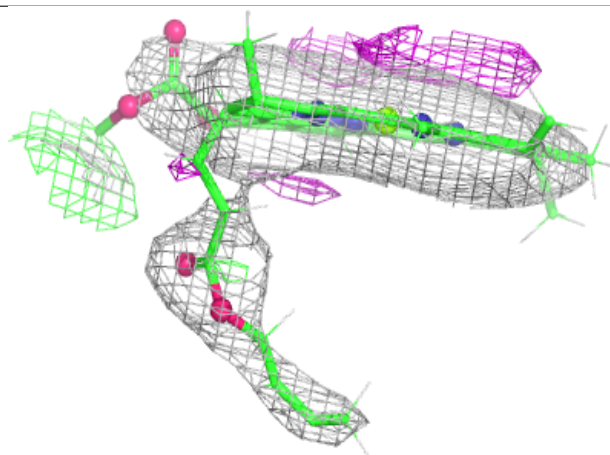
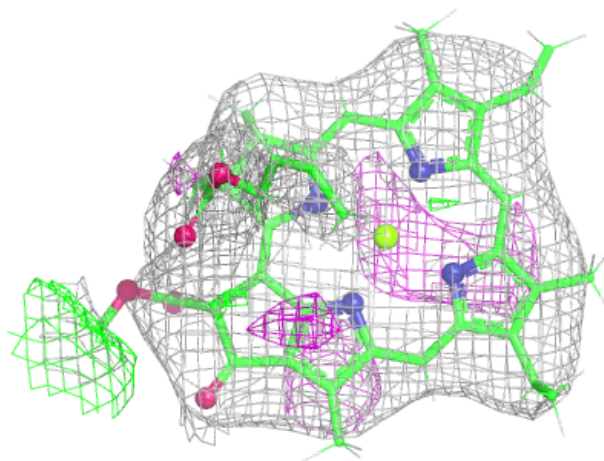
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





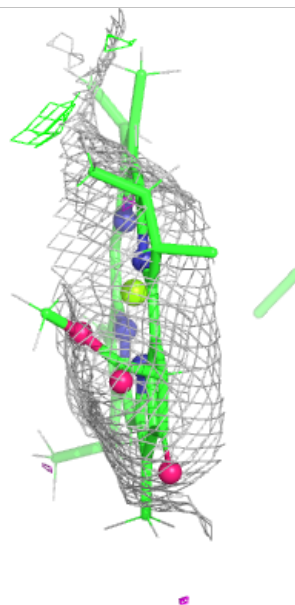
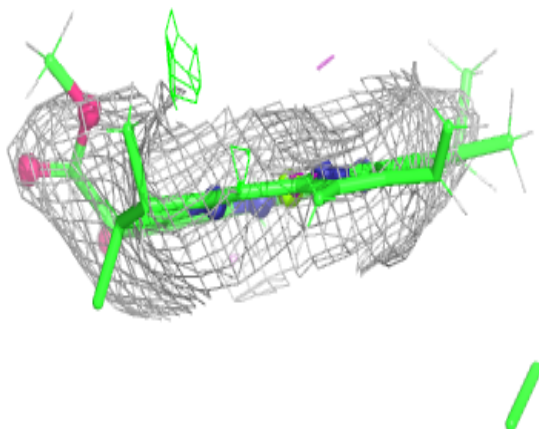
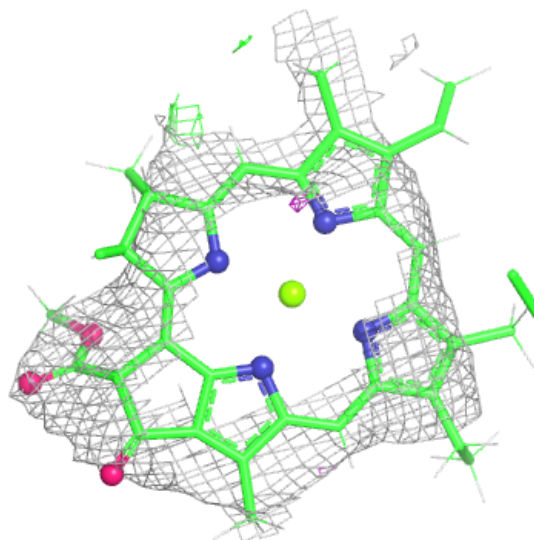
Electron density around CLA B 3032:

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



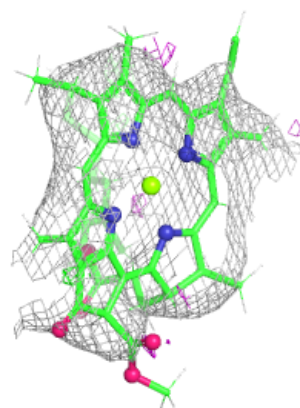
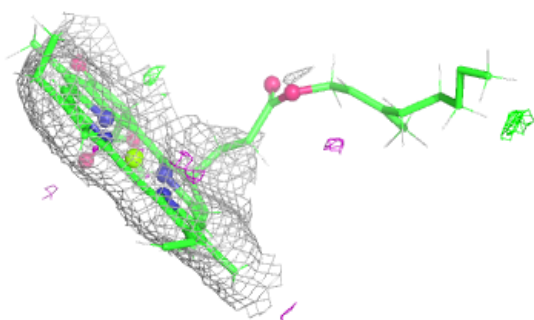
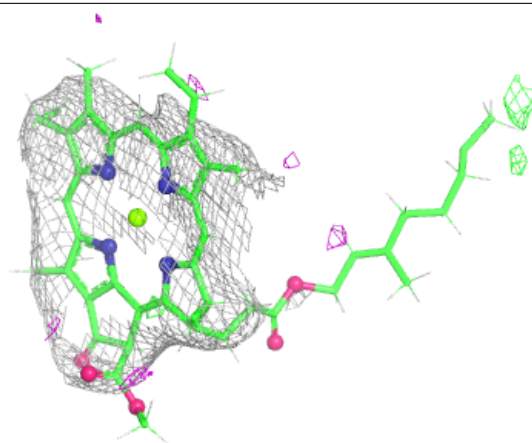
Electron density around CLA A 821:

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

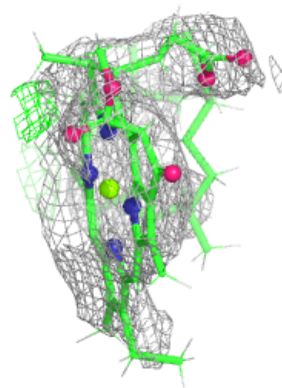
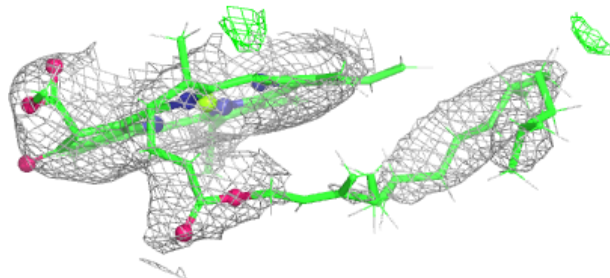
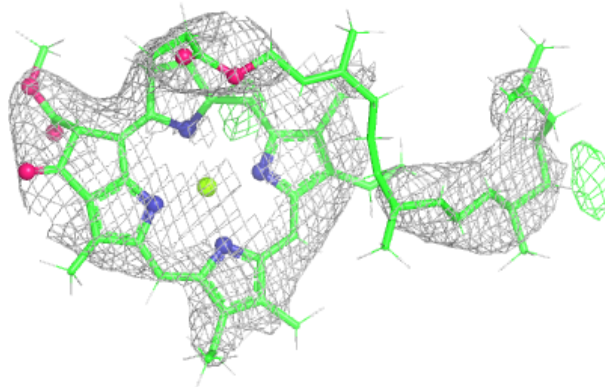


Electron density around CLA A 836:

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

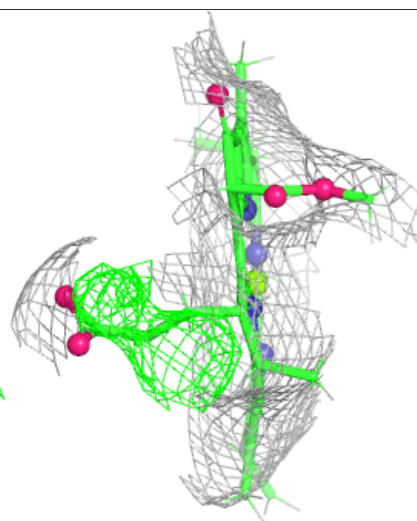
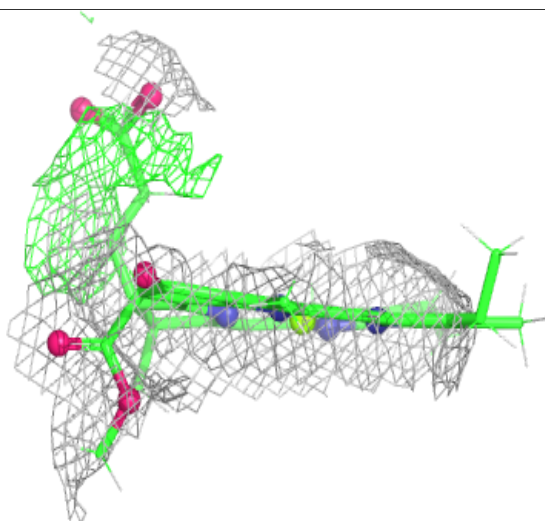
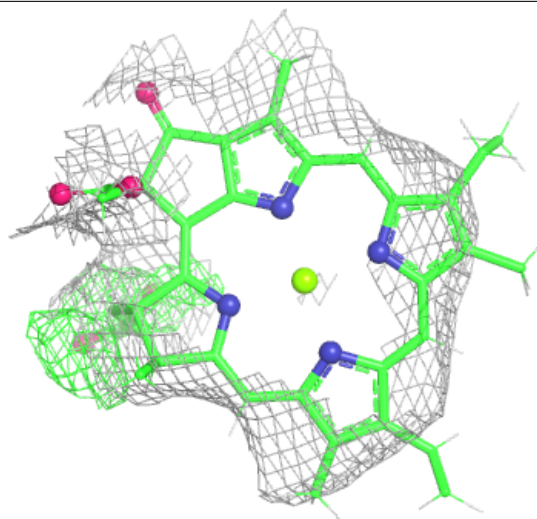
**Electron density around CLA A 820:**

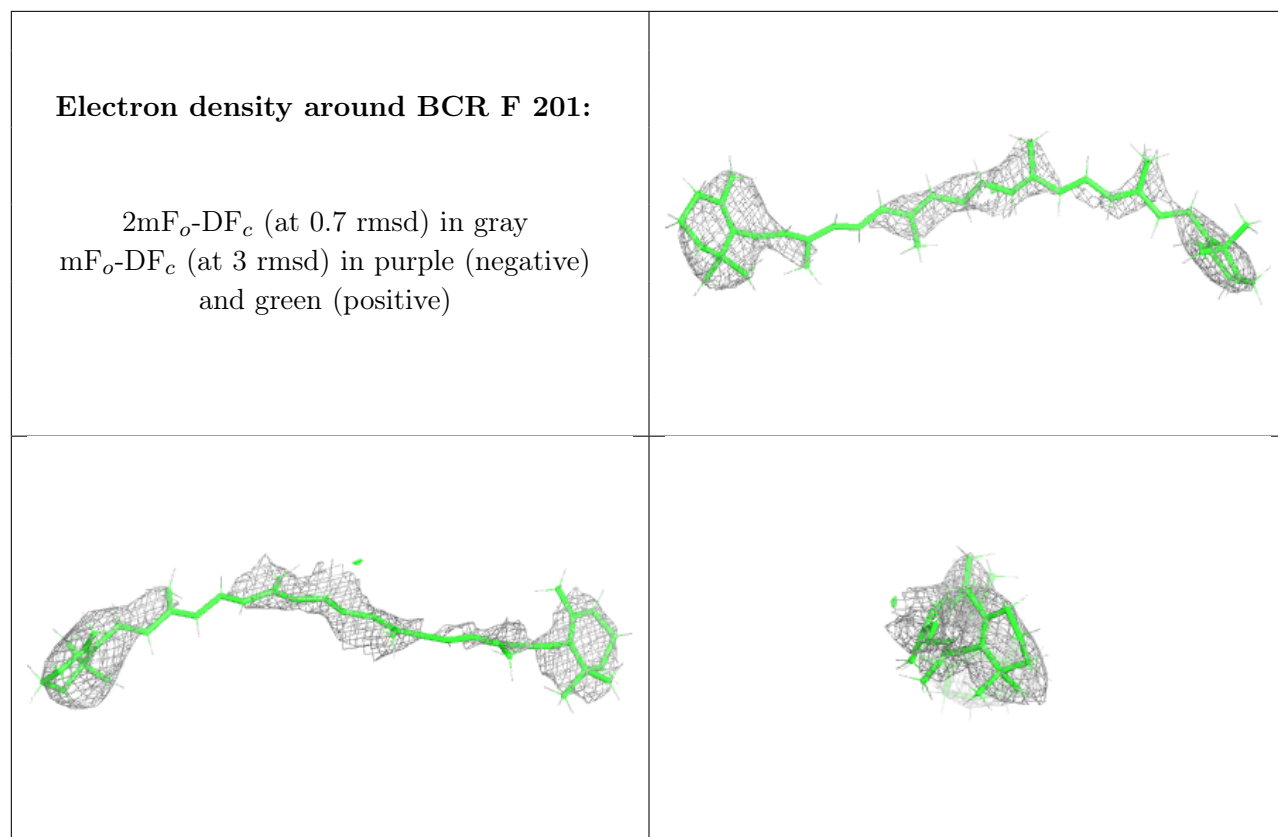
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA A 815:

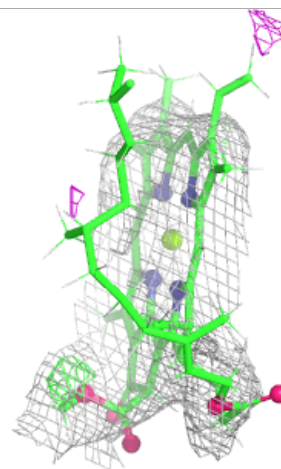
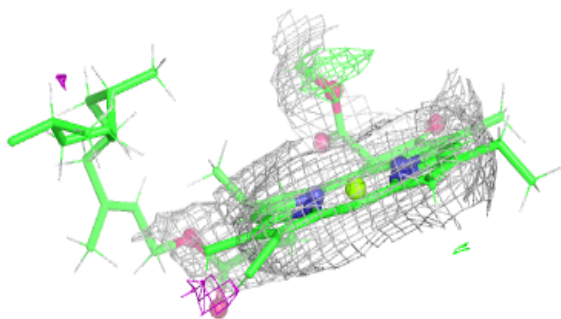
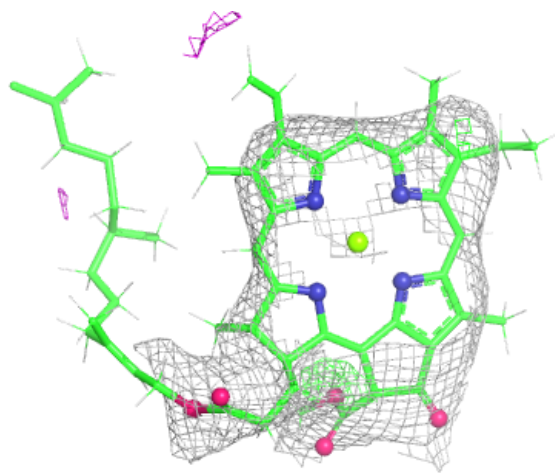
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





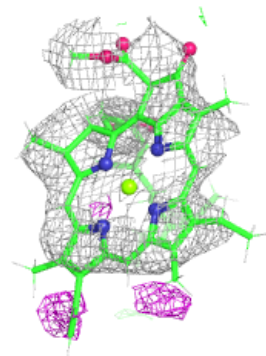
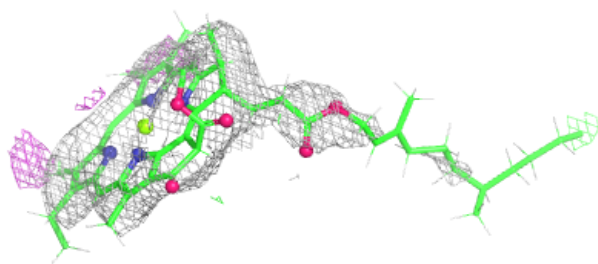
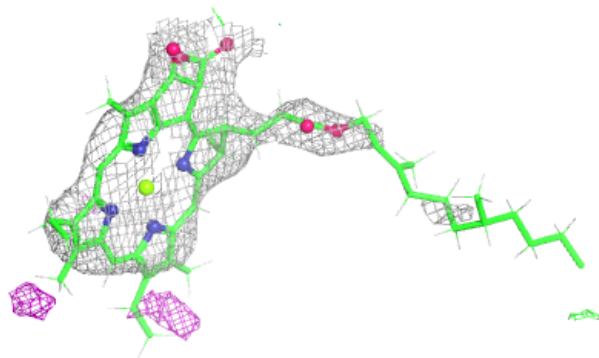
Electron density around CLA A 814:

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



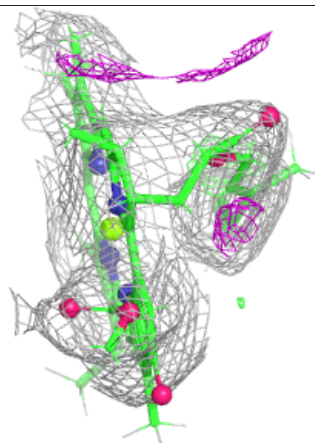
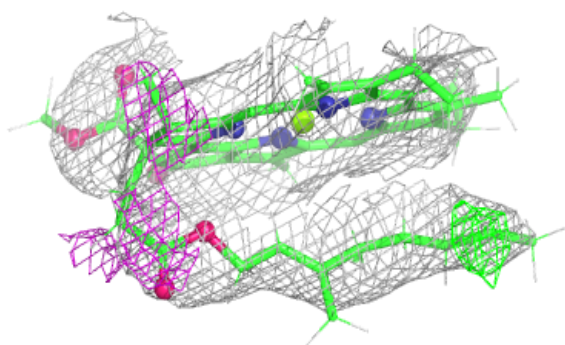
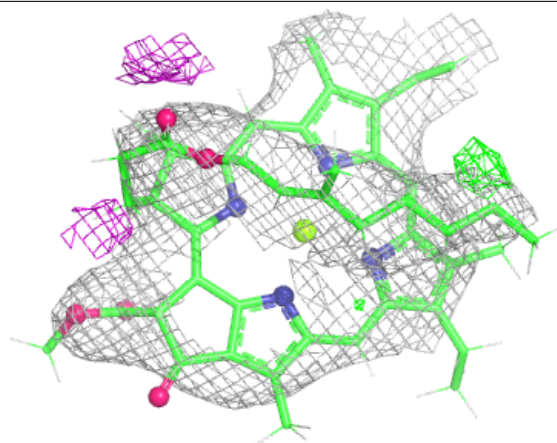
Electron density around CLA B 3034:

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

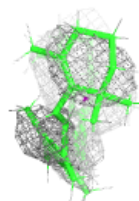
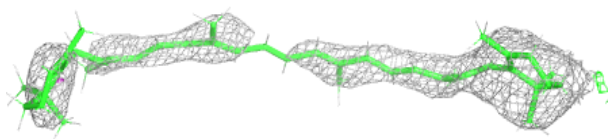
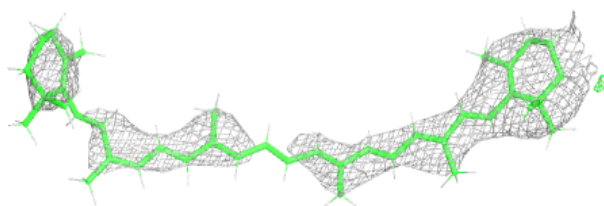


Electron density around CLA A 819:

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

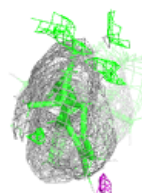
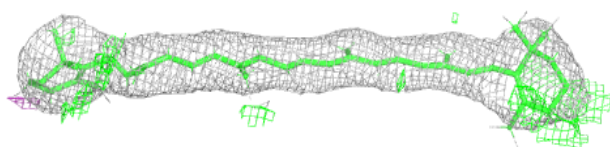
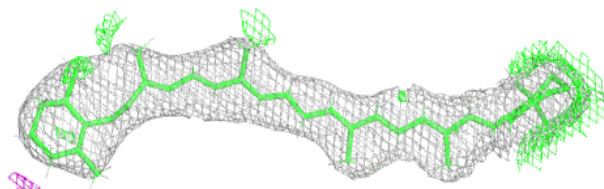
**Electron density around BCR B 3044:**

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

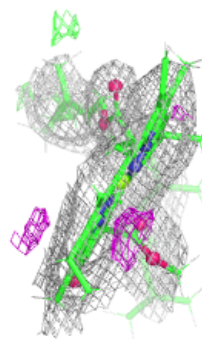
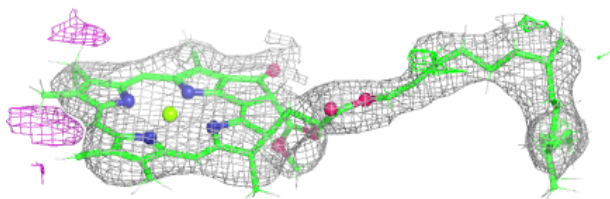
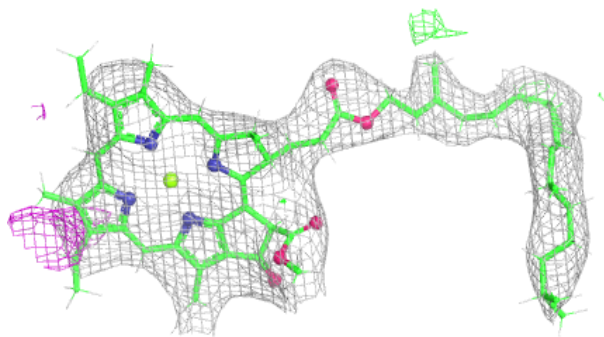


Electron density around BCR L 207:

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

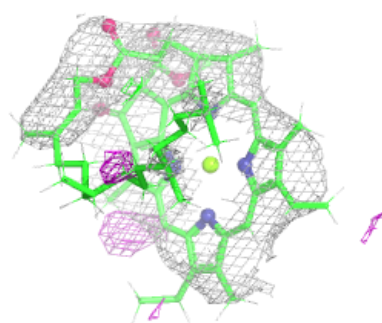
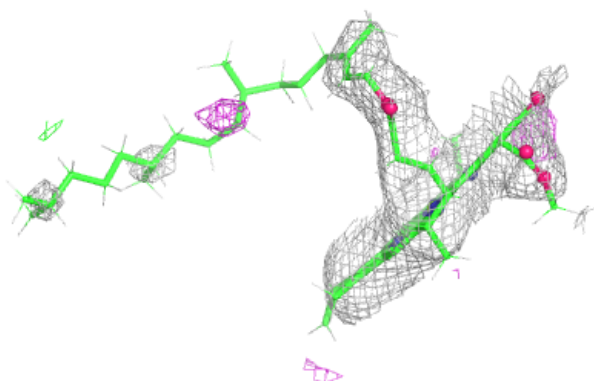
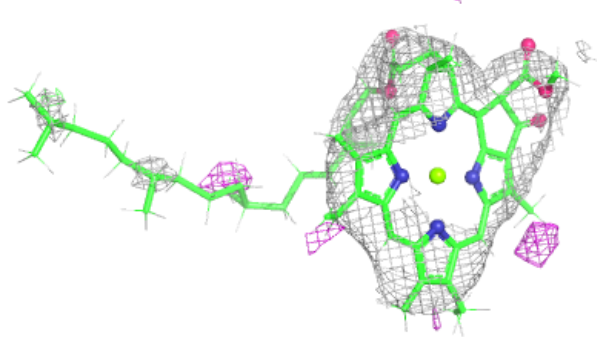
**Electron density around CLA B 3027:**

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

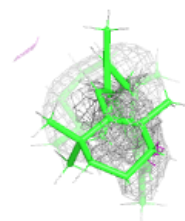
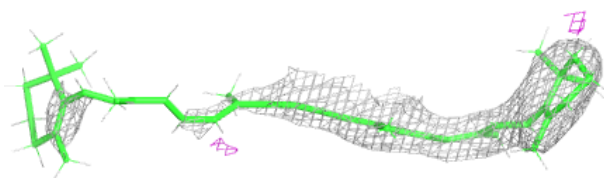
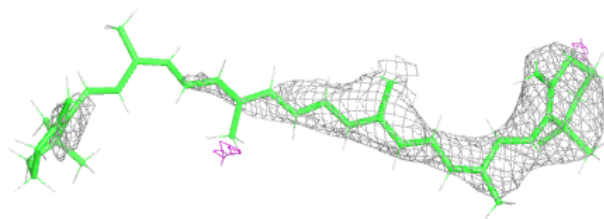


Electron density around CLA B 3015:

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

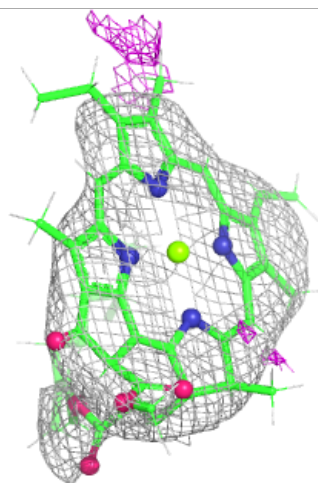
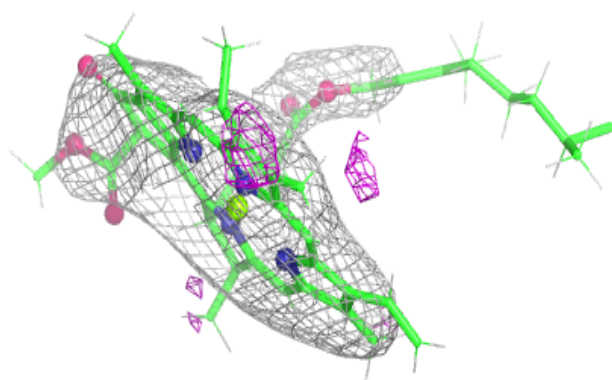
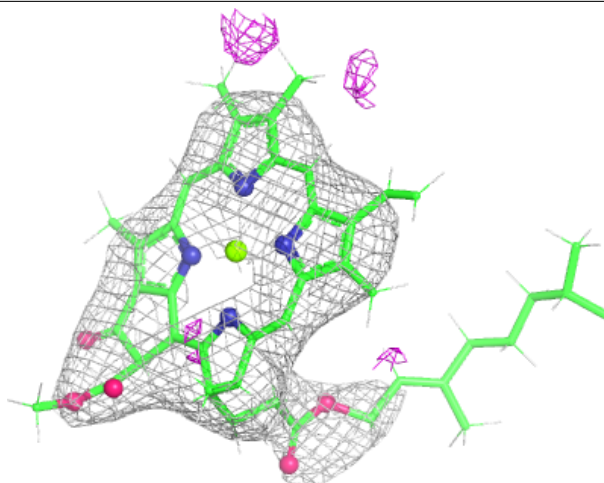
**Electron density around BCR B 3045:**

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



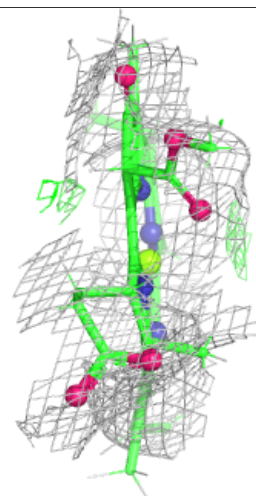
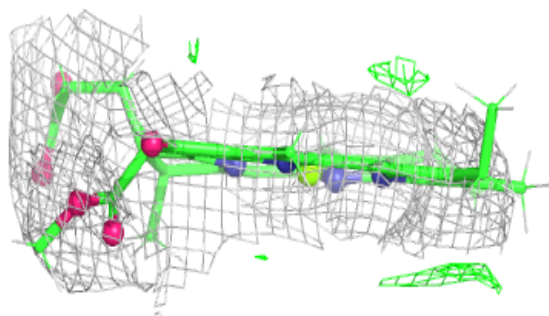
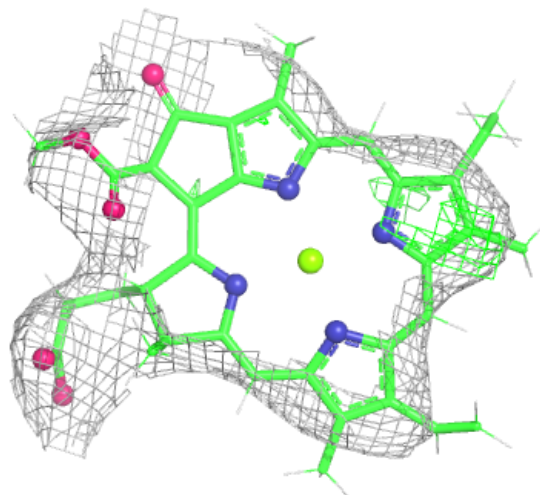
Electron density around CLA B 3017:

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



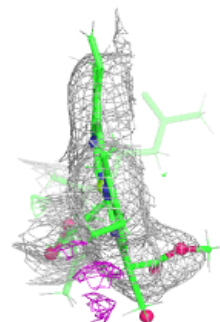
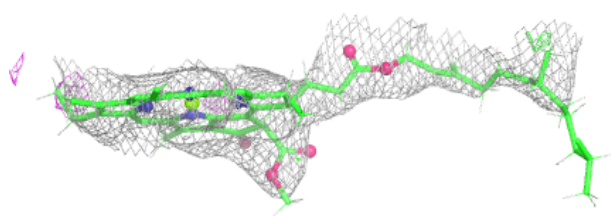
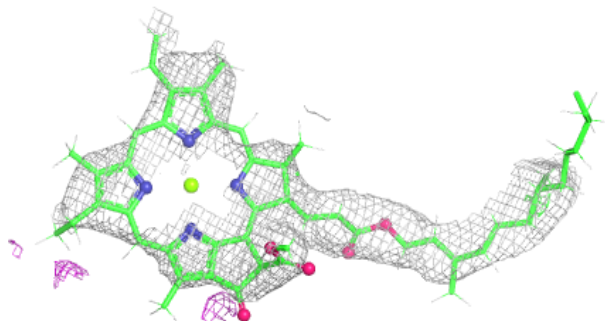
Electron density around CLA X 1701:

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

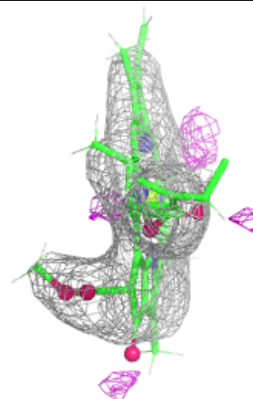
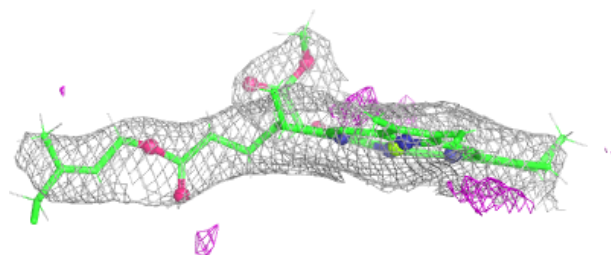
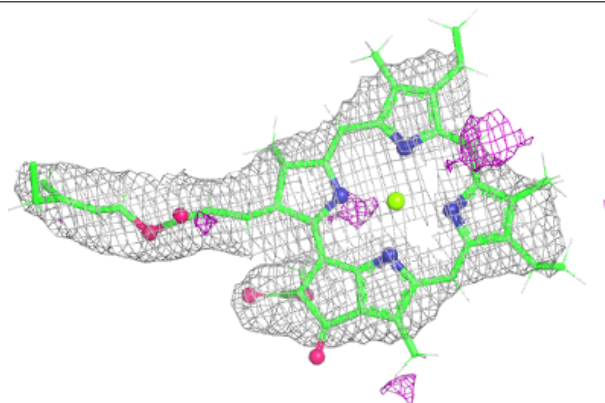


Electron density around CLA B 3038:

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

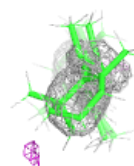
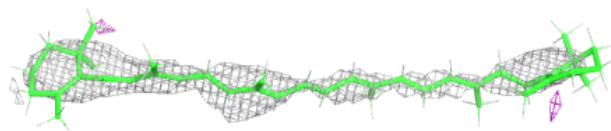
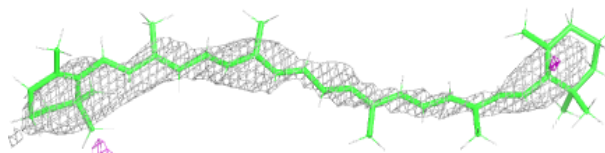
**Electron density around CLA A 838:**

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



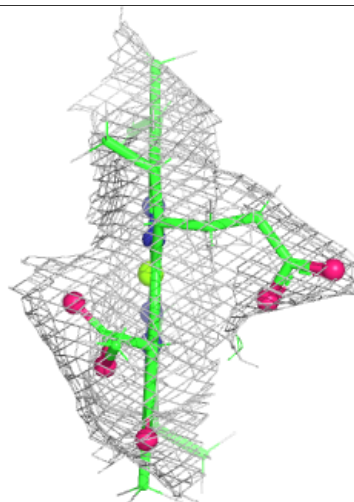
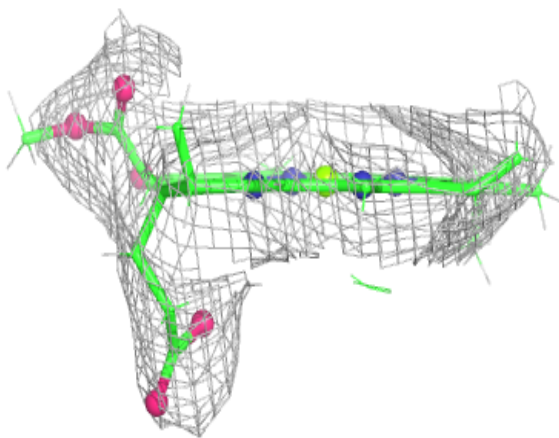
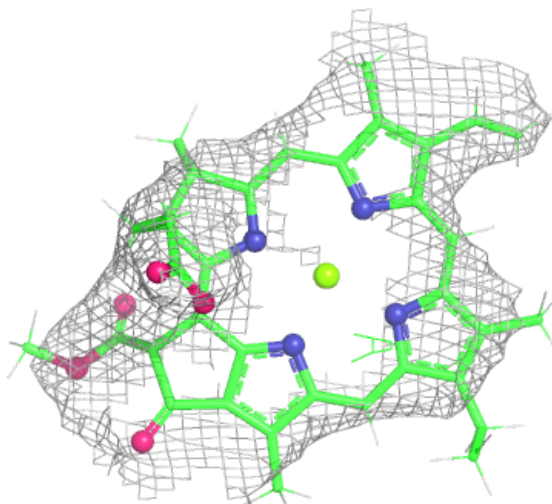
Electron density around BCR J 103:

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



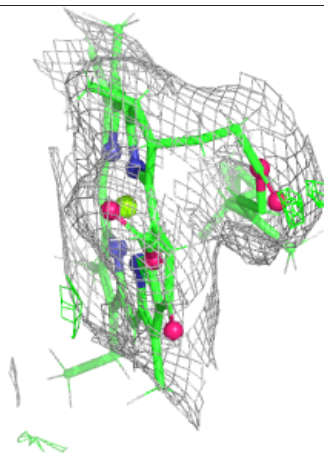
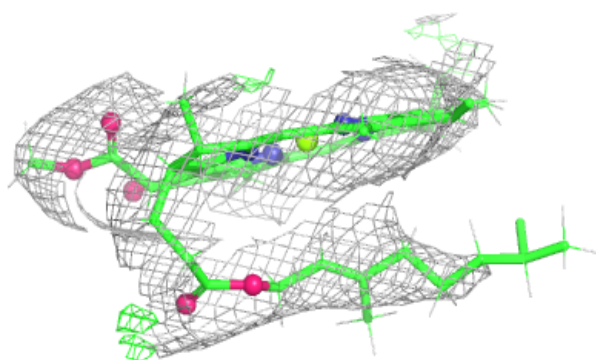
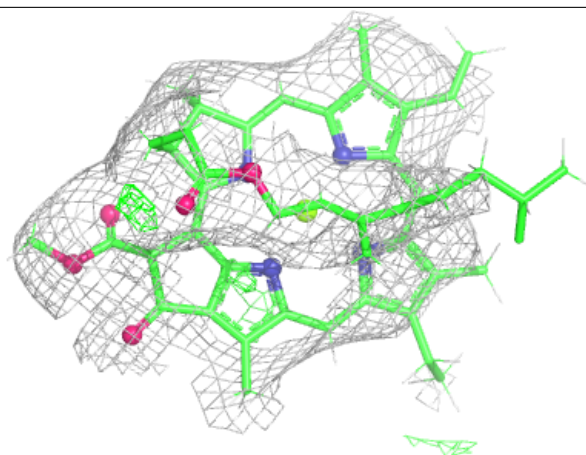
Electron density around CLA B 3013:

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



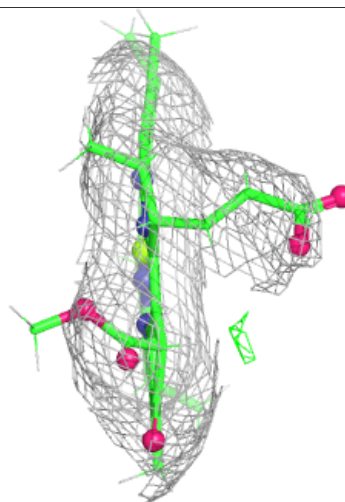
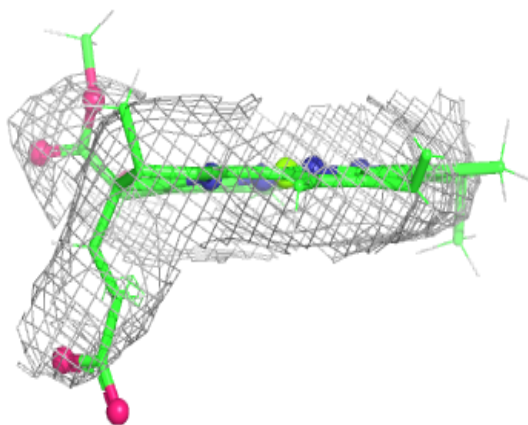
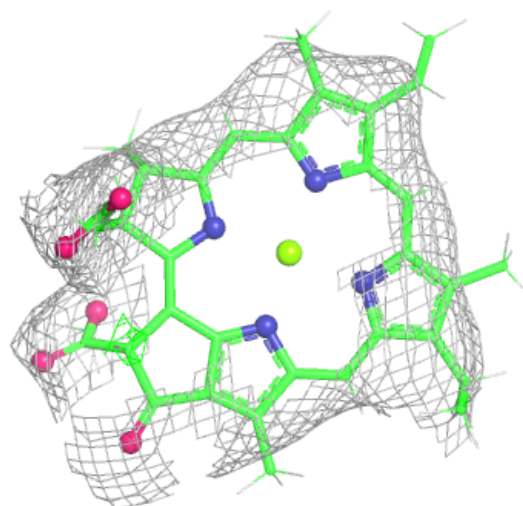
Electron density around CLA B 3023:

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



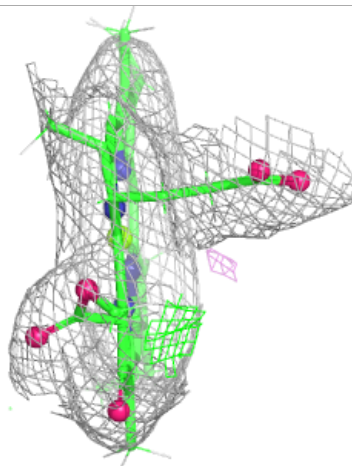
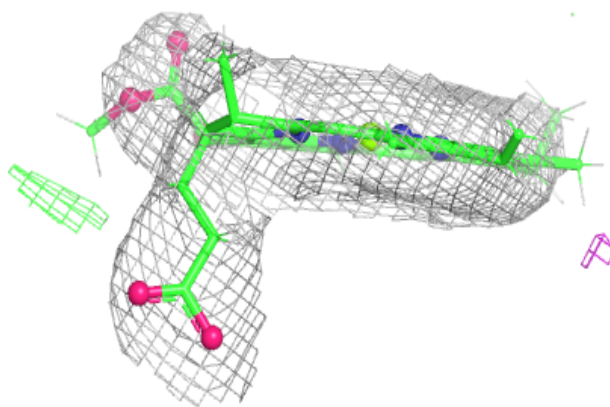
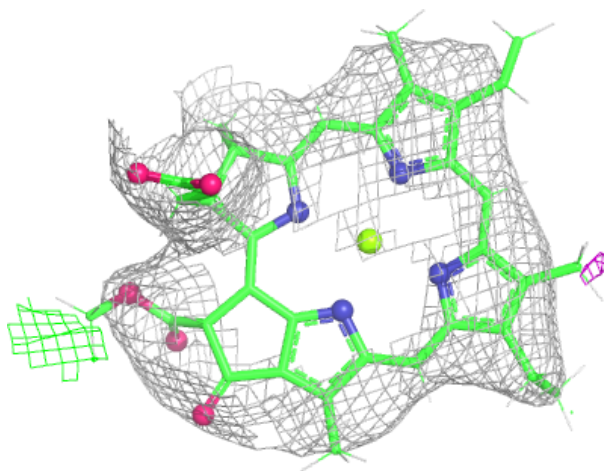
Electron density around CLA B 3022:

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



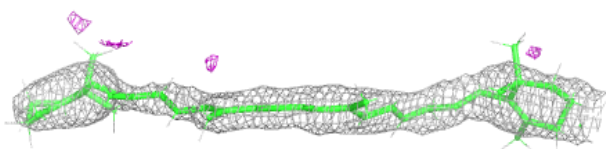
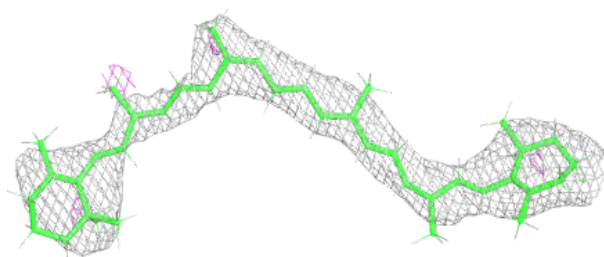
Electron density around CLA B 3012:

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



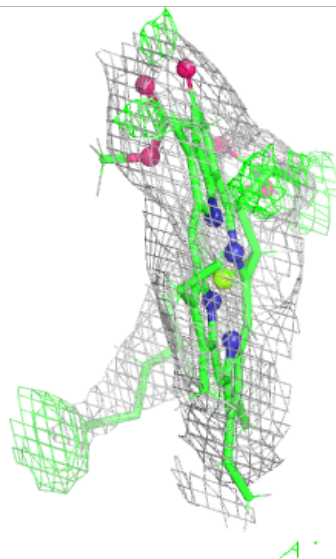
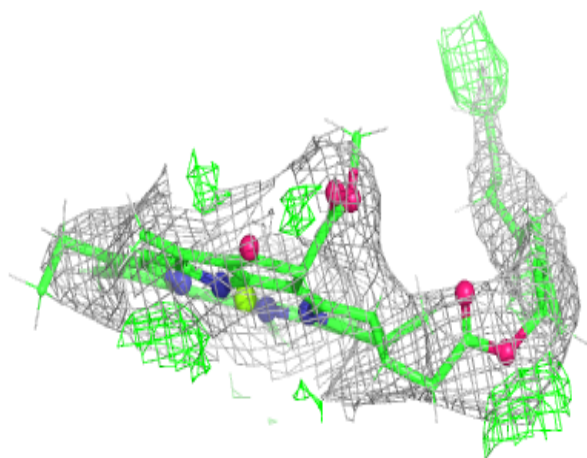
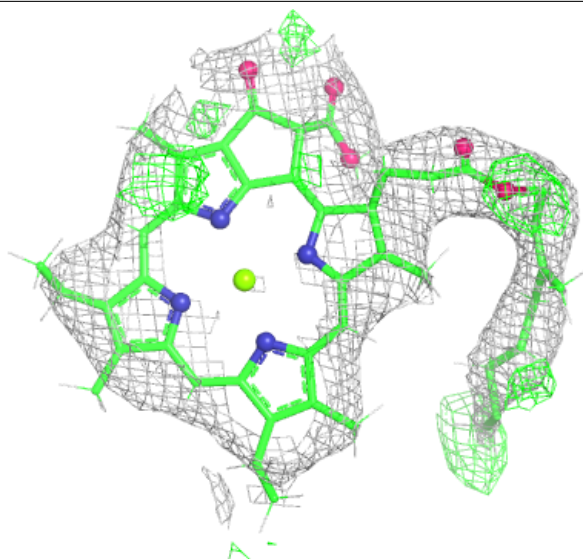
Electron density around BCR A 851:

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



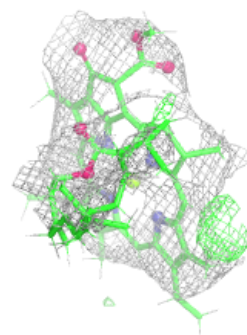
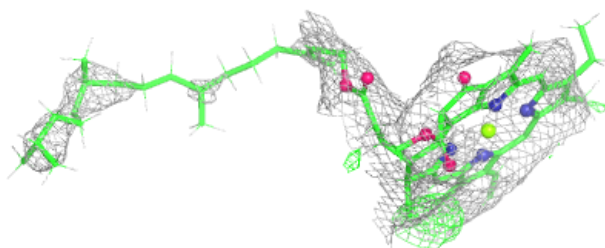
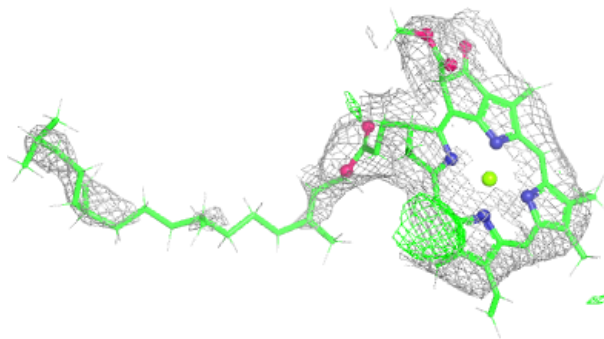
Electron density around CLA B 3025:

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



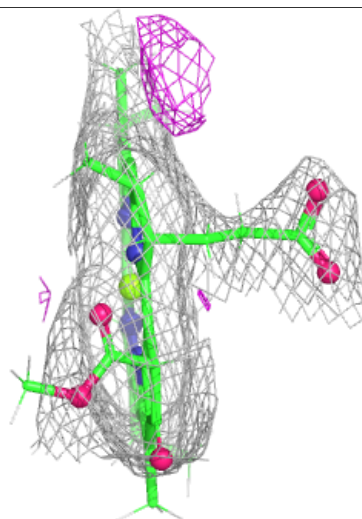
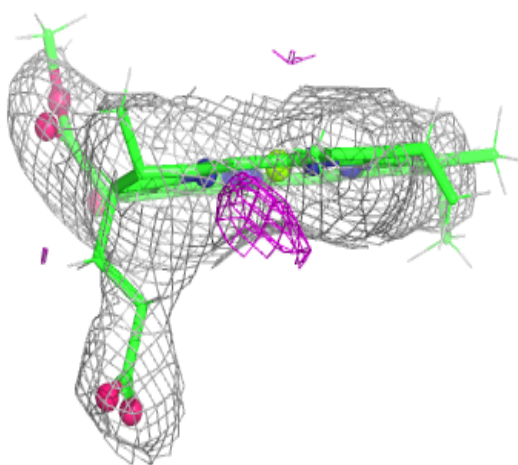
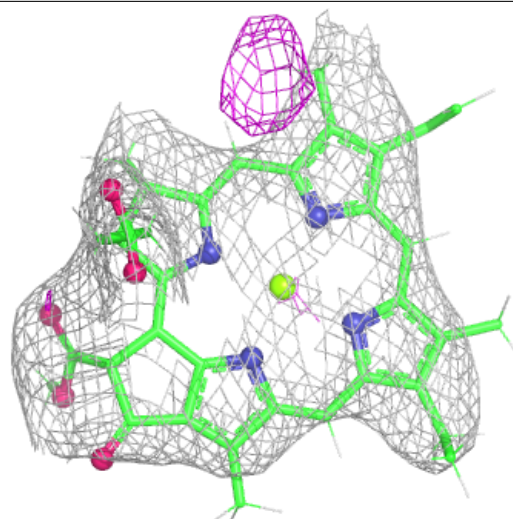
Electron density around CLA A 822:

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



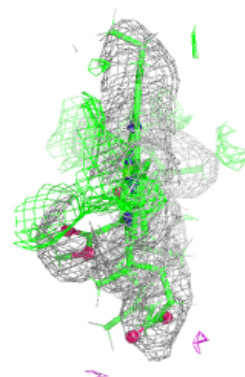
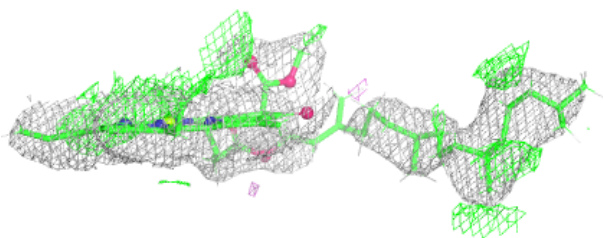
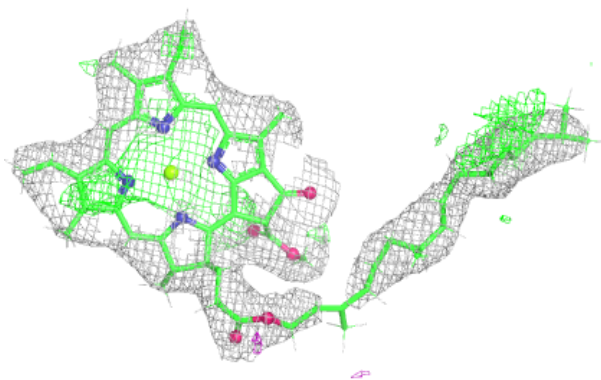
Electron density around CLA B 3031:

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

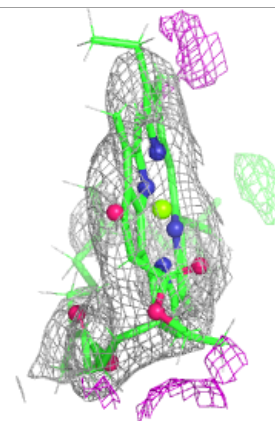
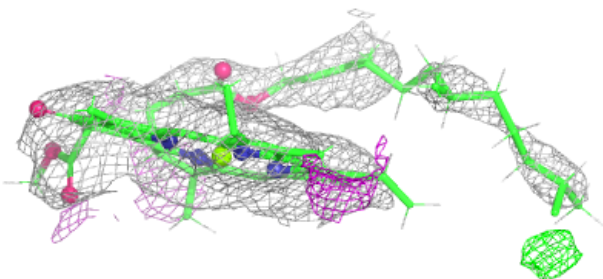
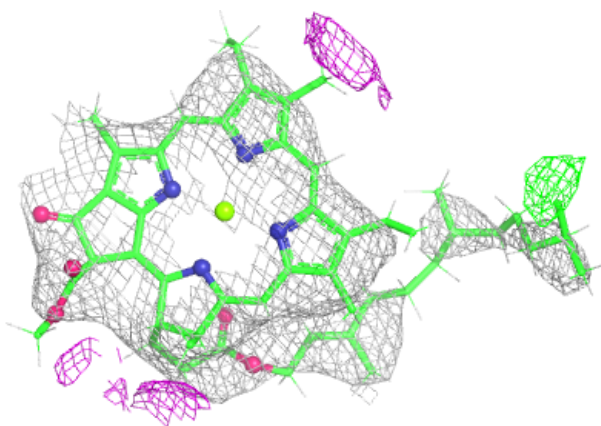


Electron density around CLA L 205:

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

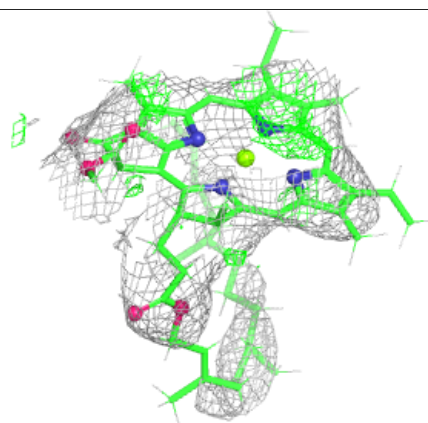
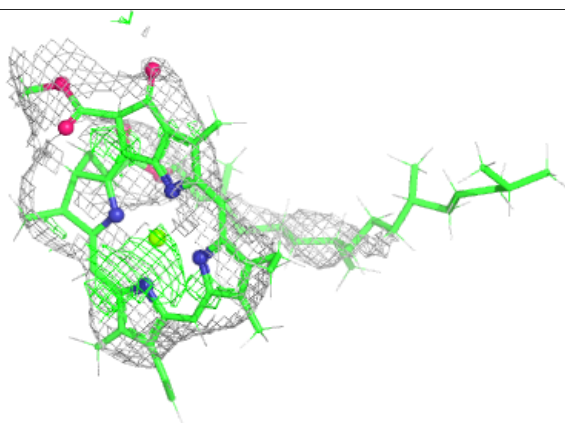
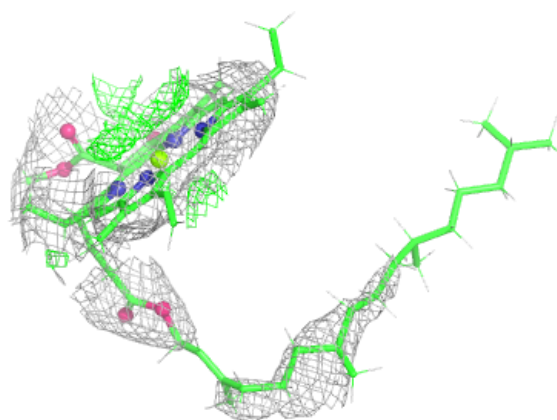
**Electron density around CLA B 3019:**

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

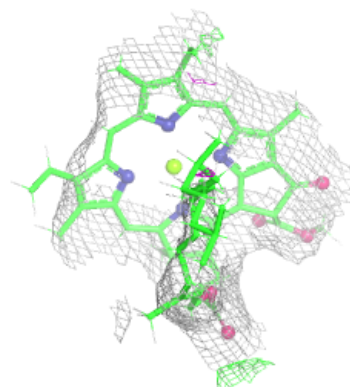
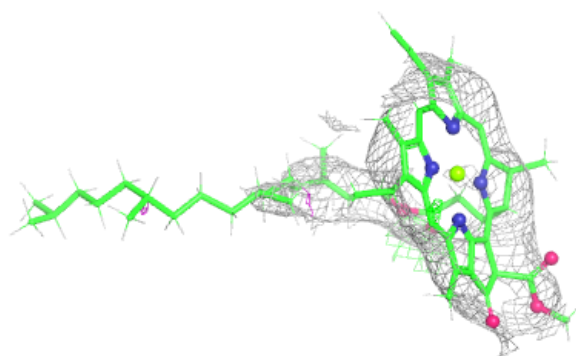
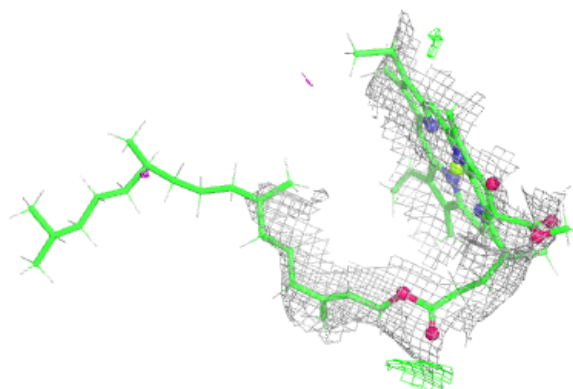


Electron density around CLA B 3020:

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

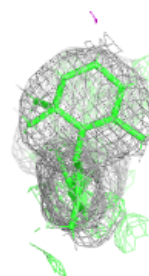
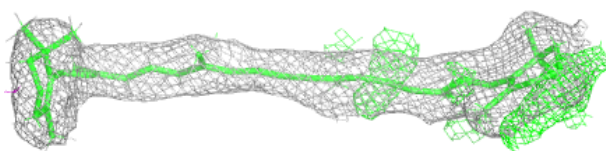
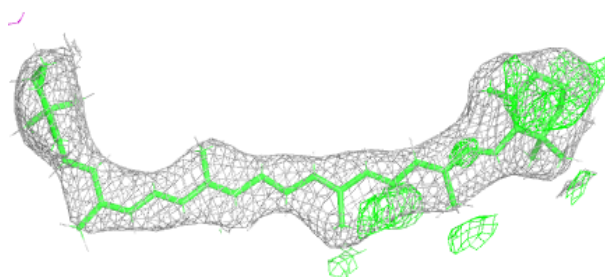
**Electron density around CLA A 812:**

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

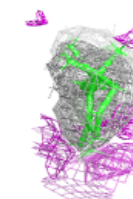
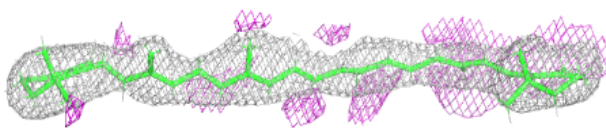
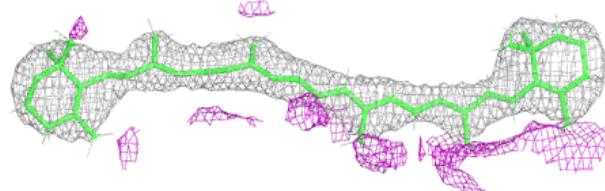


Electron density around BCR I 103:

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

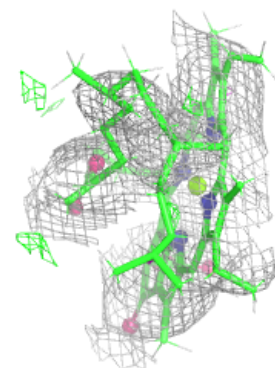
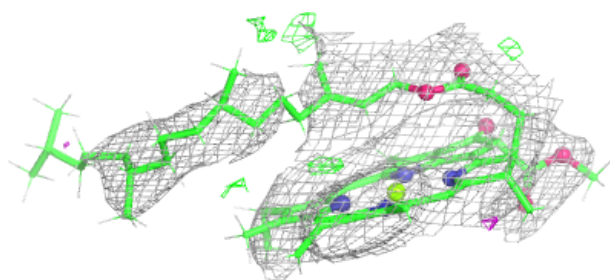
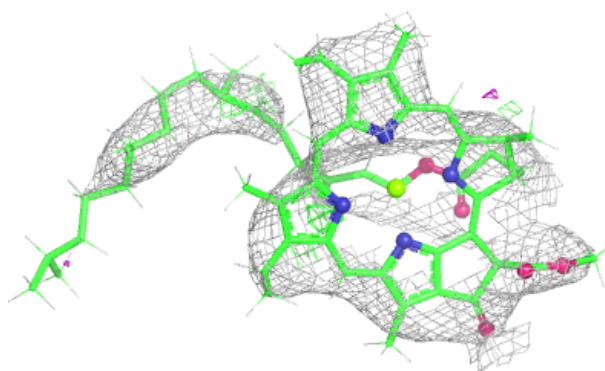
**Electron density around BCR I 105:**

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

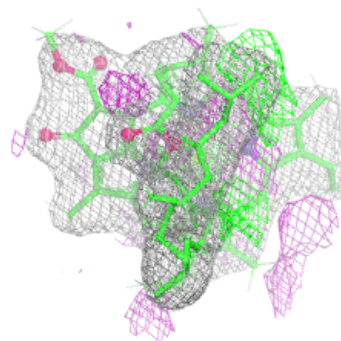
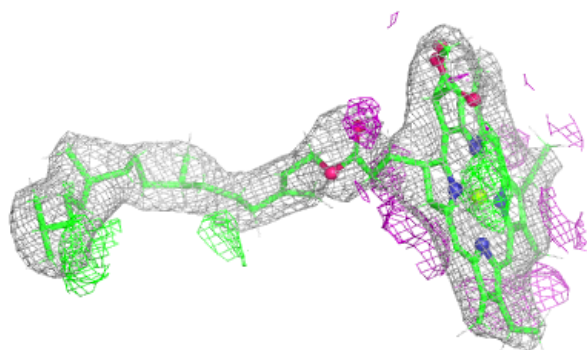
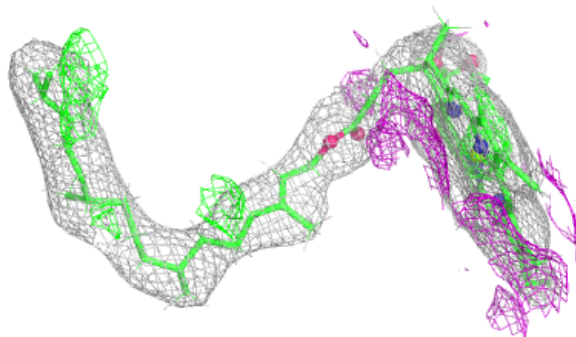


Electron density around CLA B 3039:

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

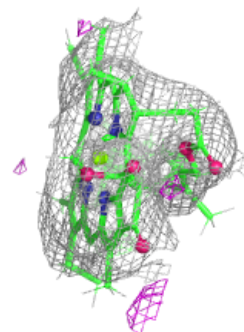
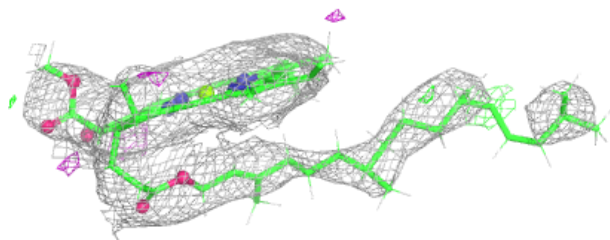
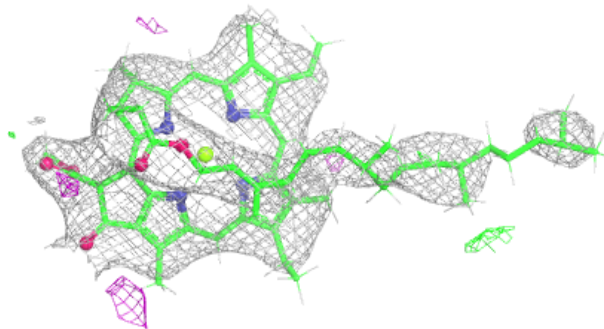
**Electron density around CLA I 101:**

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

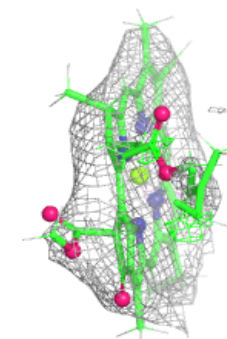
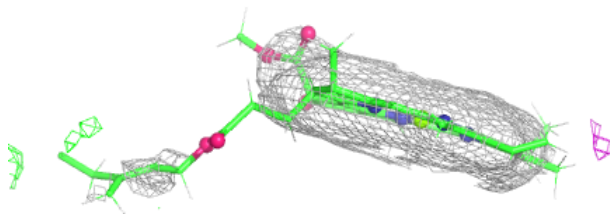
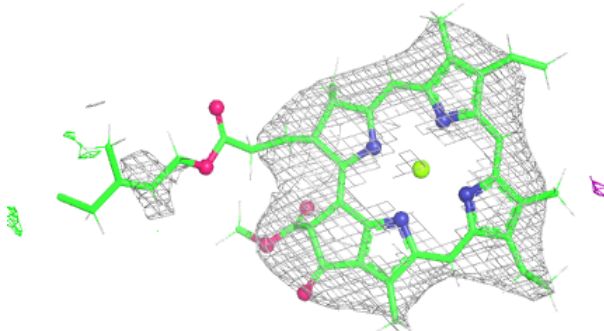


Electron density around CLA A 839:

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

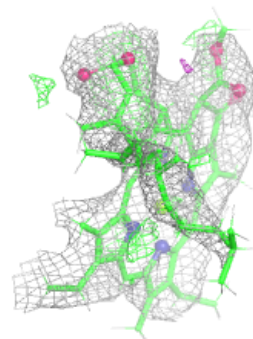
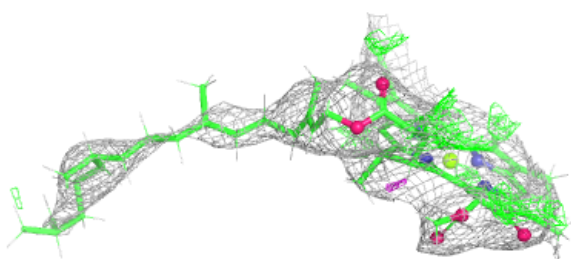
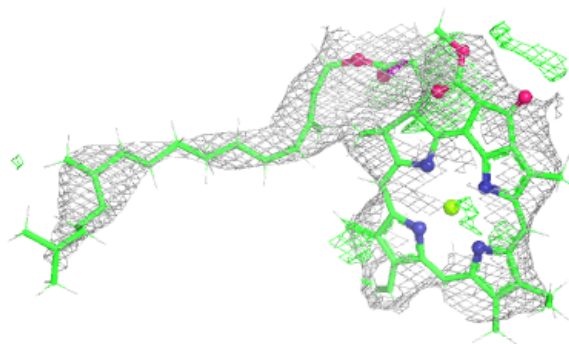
**Electron density around CLA A 842:**

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

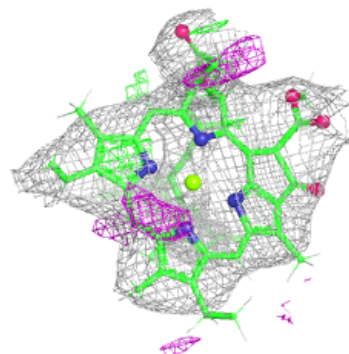
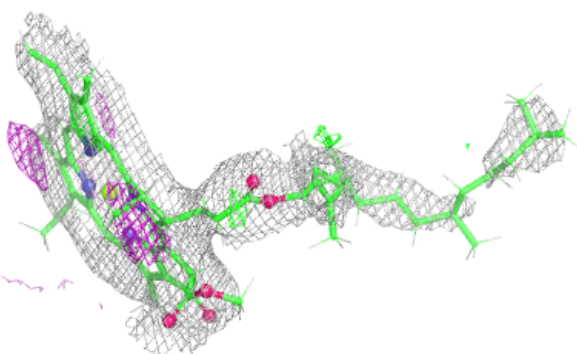
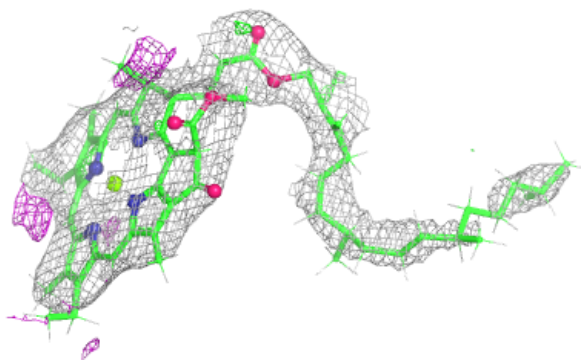


Electron density around CLA A 803:

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

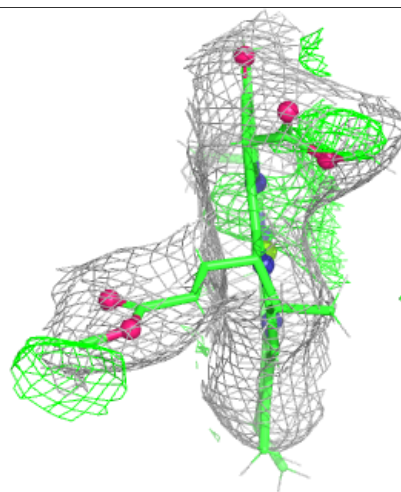
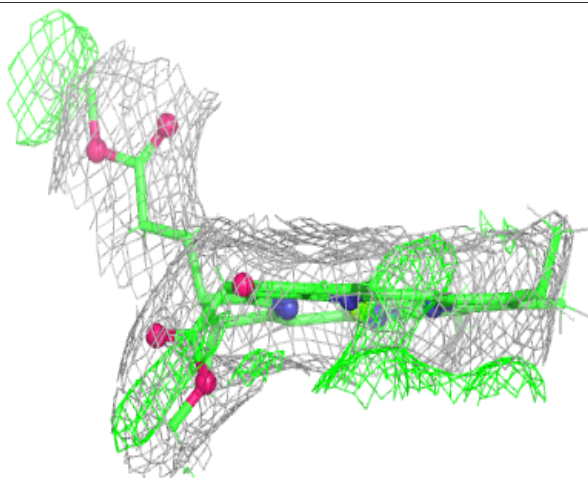
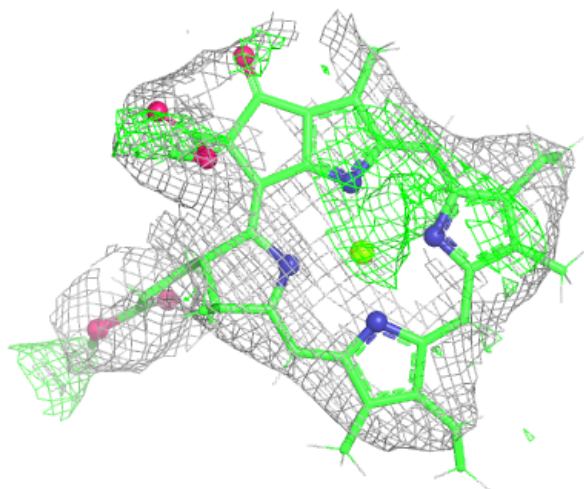
**Electron density around CLA B 3003:**

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



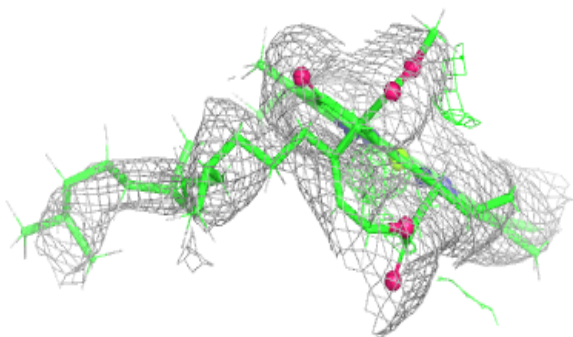
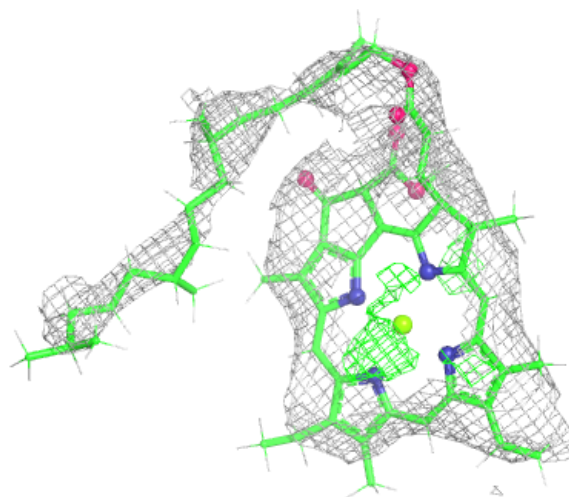
Electron density around CLA B 3026:

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



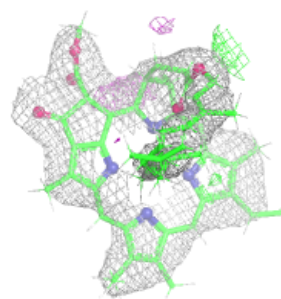
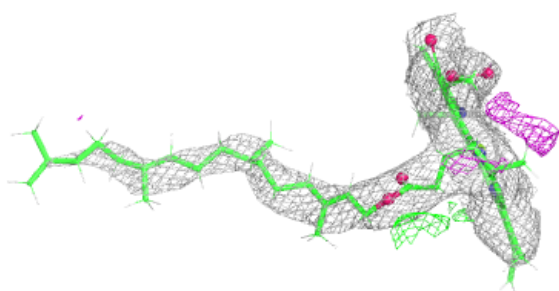
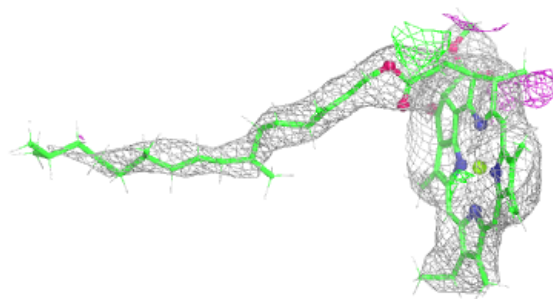
Electron density around CLA A 826:

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

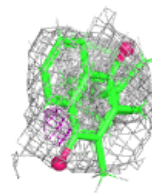
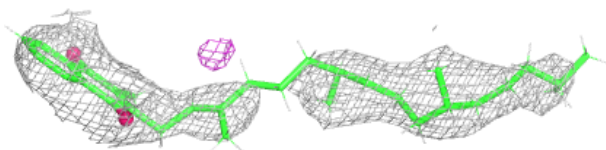
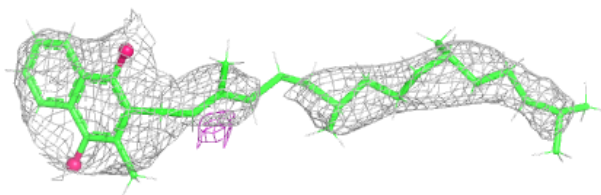


Electron density around CLA B 3029:

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

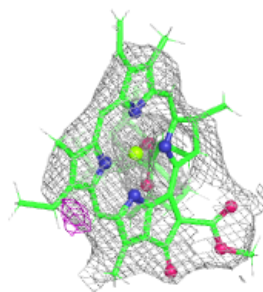
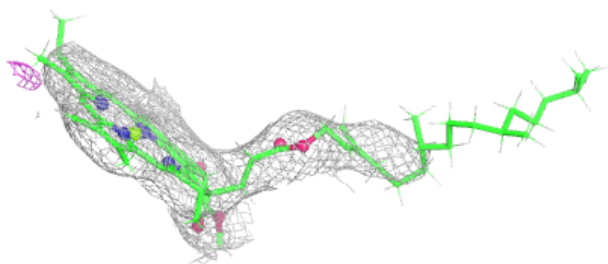
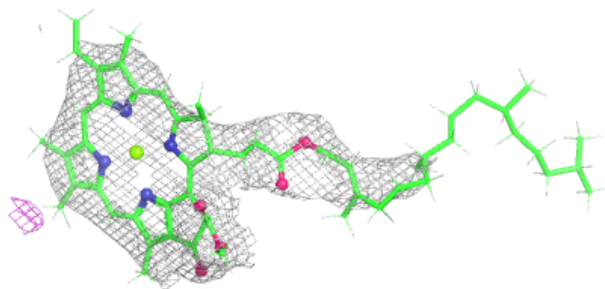
**Electron density around PQN A 846:**

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

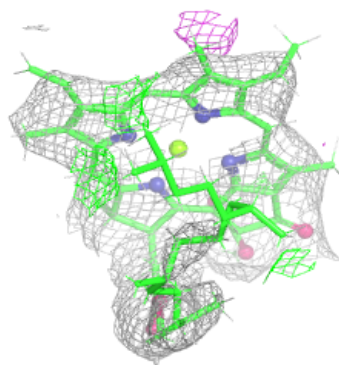
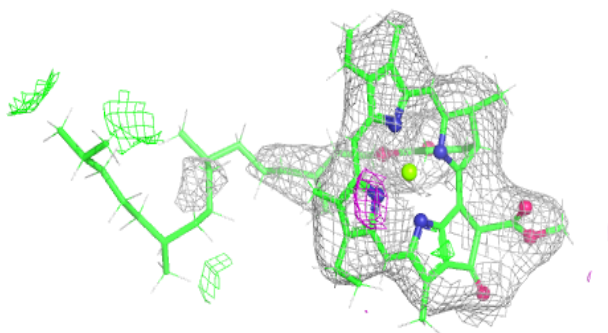
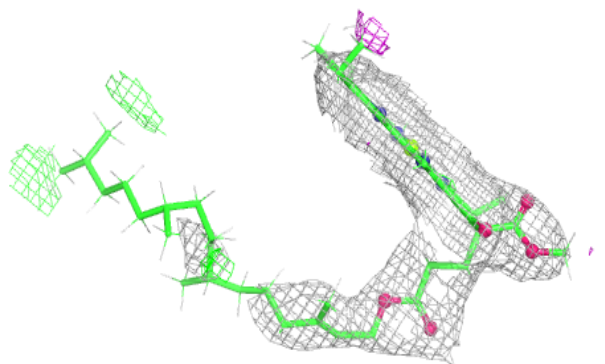


Electron density around CLA A 810:

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

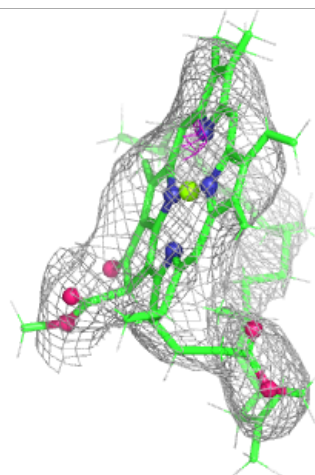
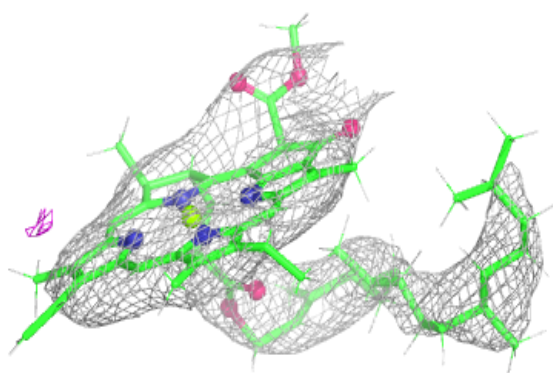
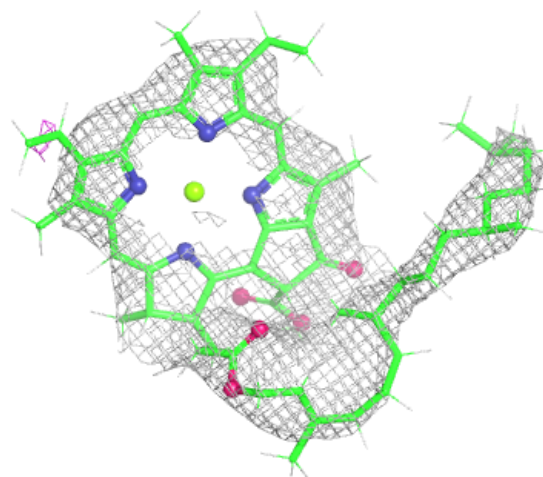
**Electron density around CLA A 833:**

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



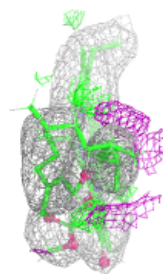
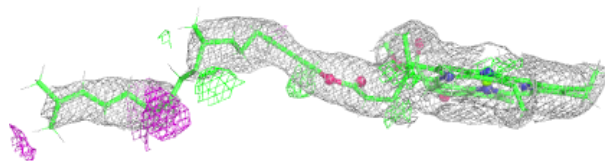
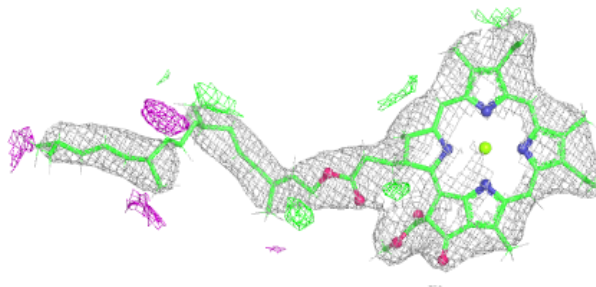
Electron density around CLA B 3033:

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



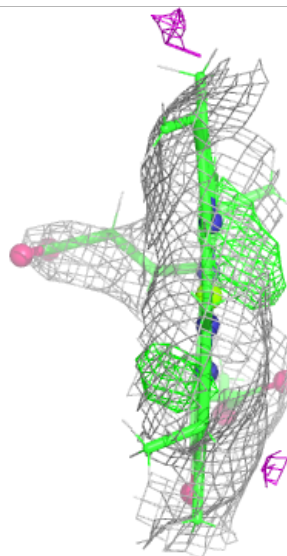
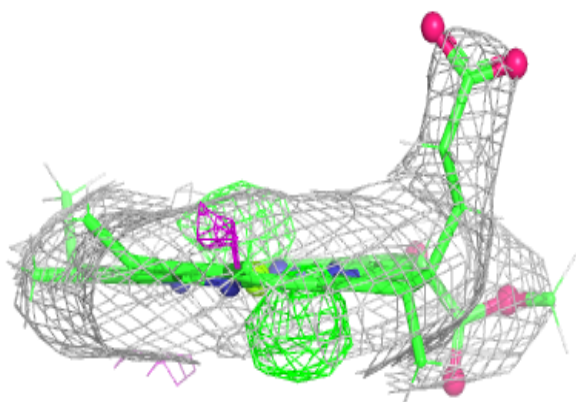
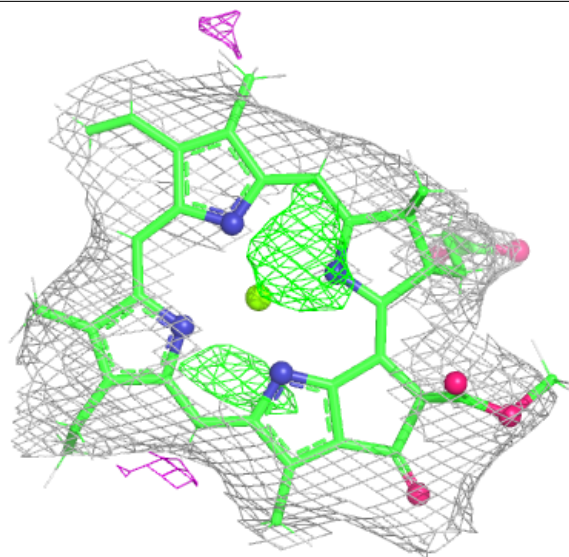
Electron density around CLA A 834:

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



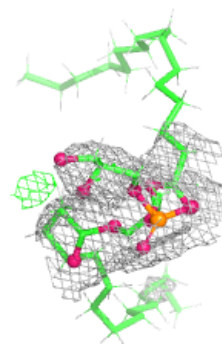
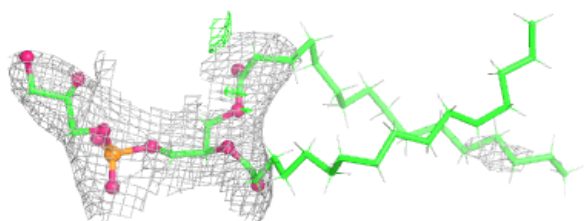
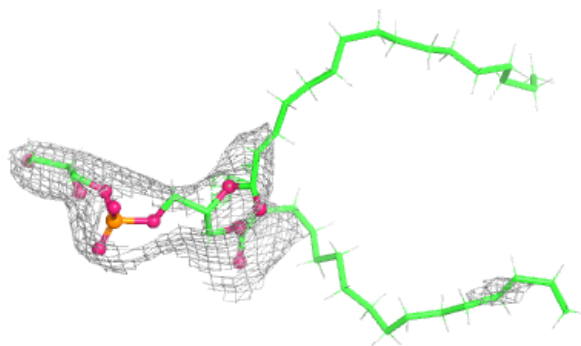
Electron density around CLA B 3036:

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

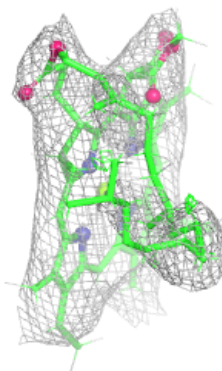
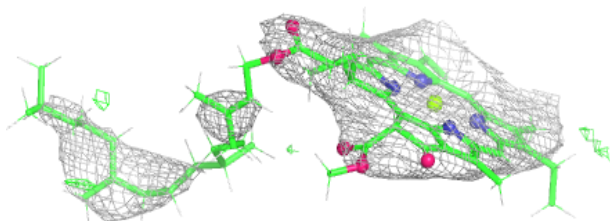
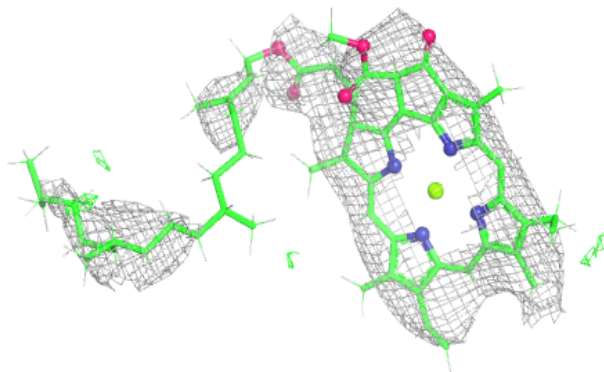


Electron density around LHG A 853:

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

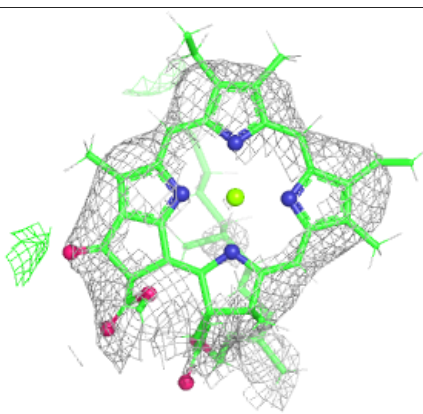
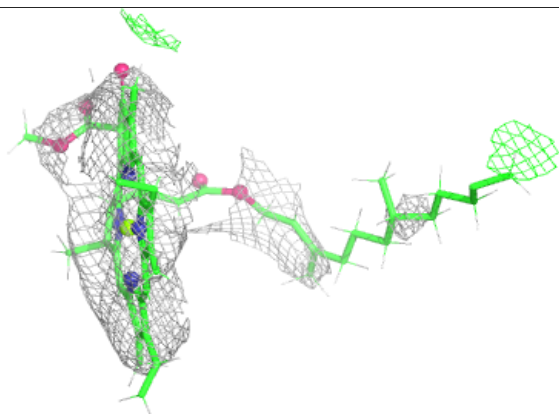
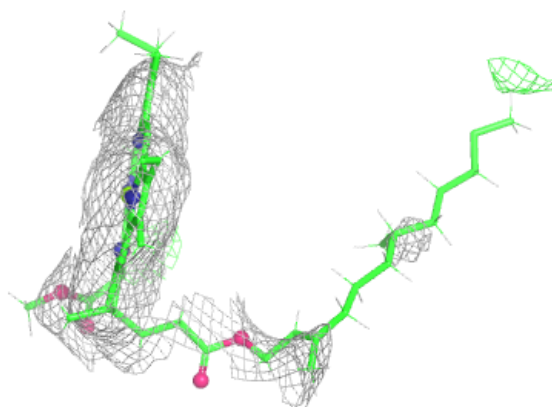
**Electron density around CLA A 804:**

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



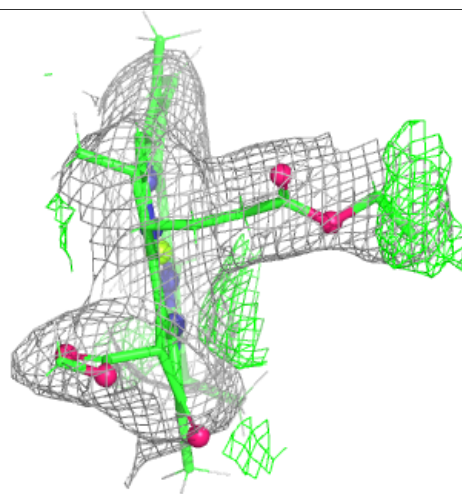
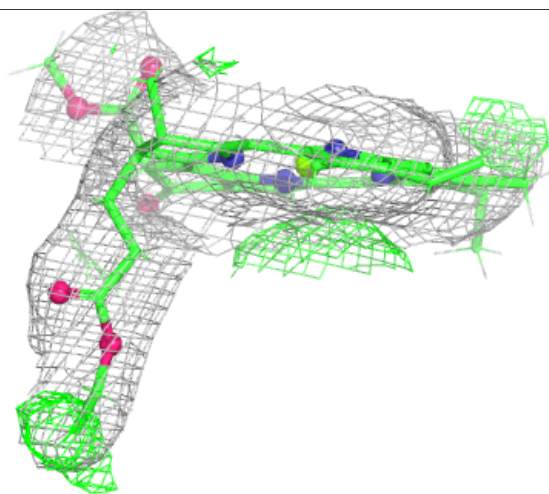
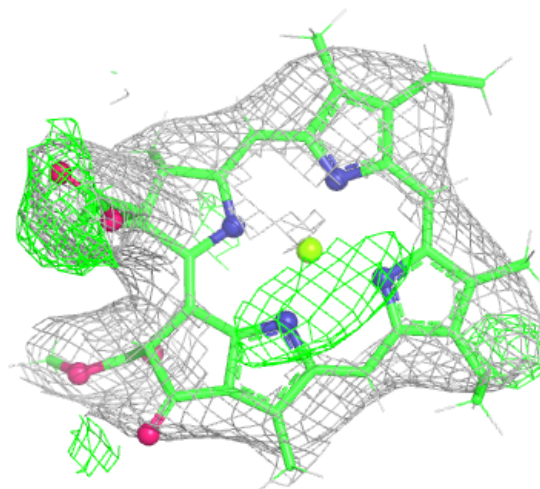
Electron density around CLA A 805:

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



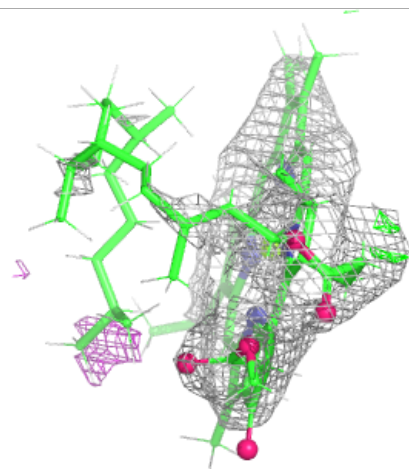
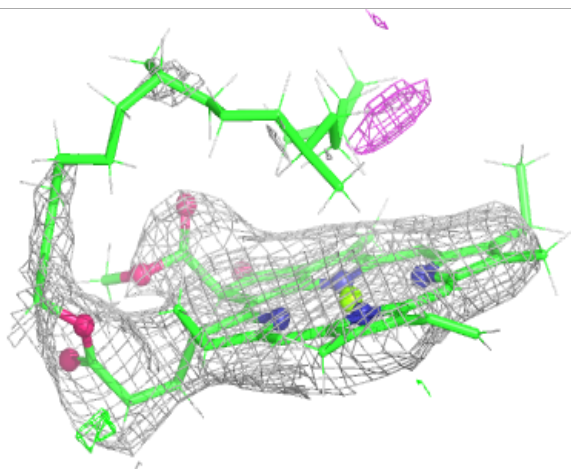
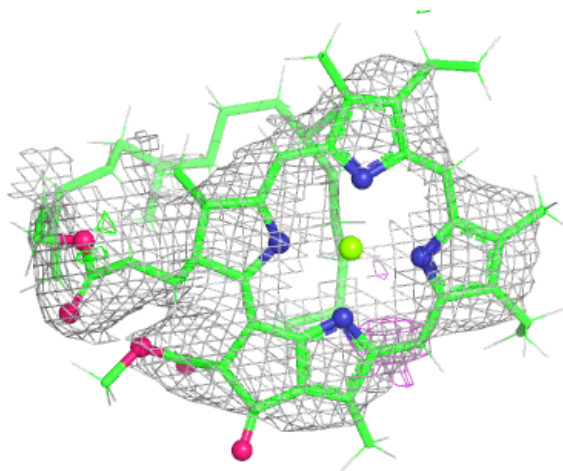
Electron density around CLA B 3040:

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



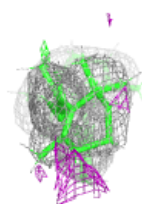
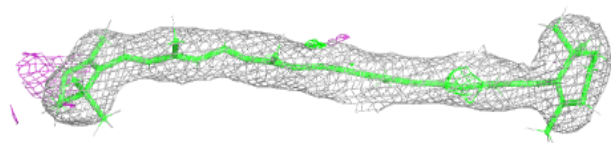
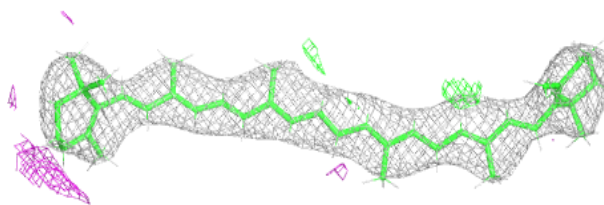
Electron density around CLA A 807:

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

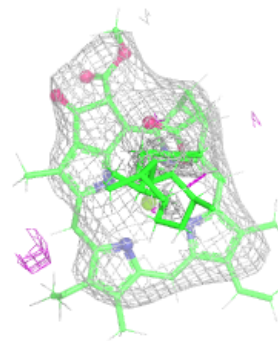
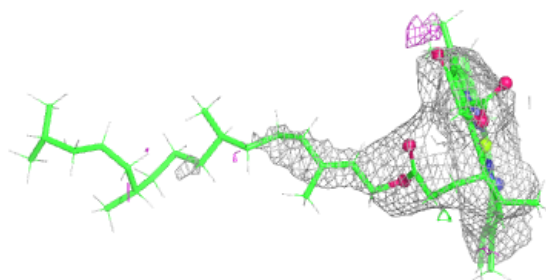
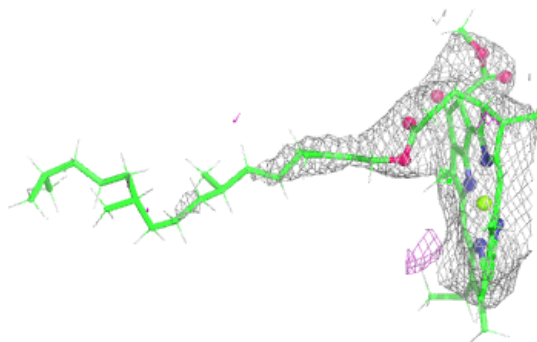


Electron density around BCR B 3047:

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

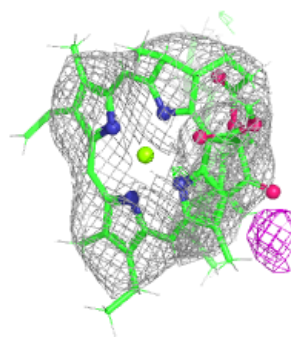
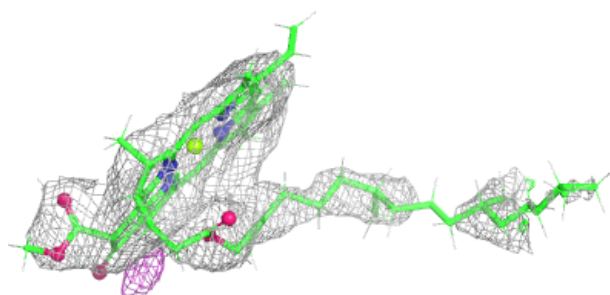
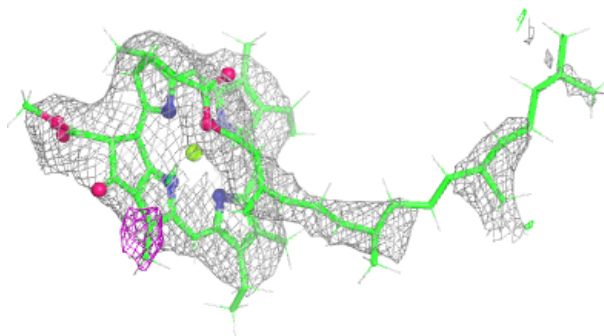
**Electron density around CLA A 829:**

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



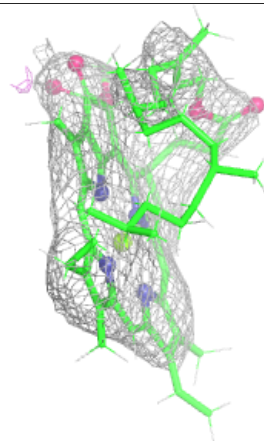
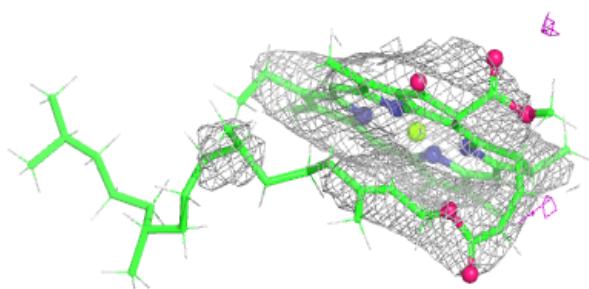
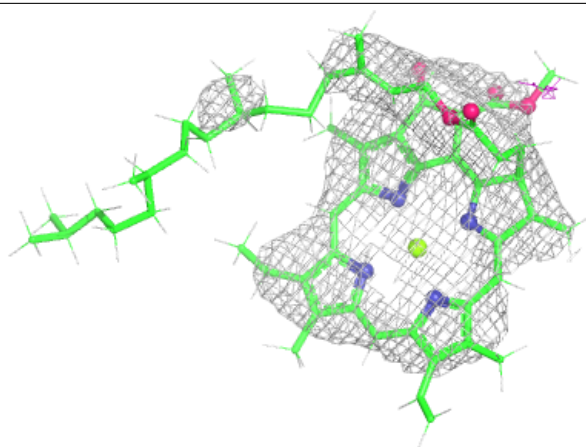
Electron density around CLA A 843:

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



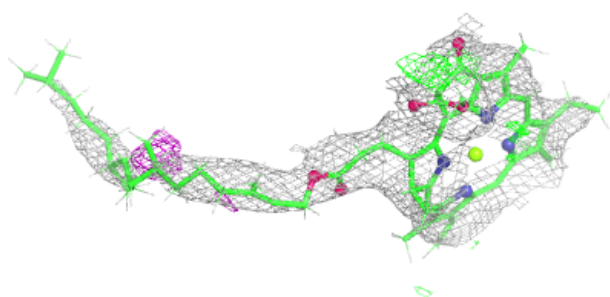
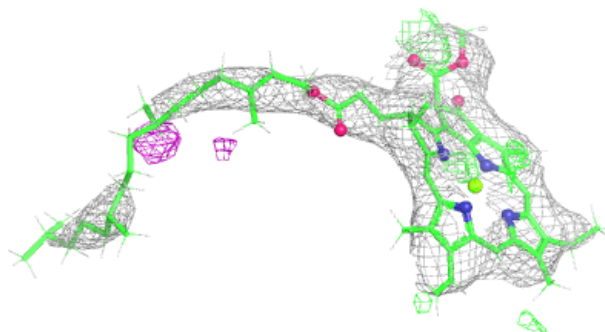
Electron density around CLA A 830:

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

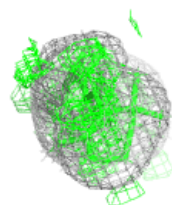
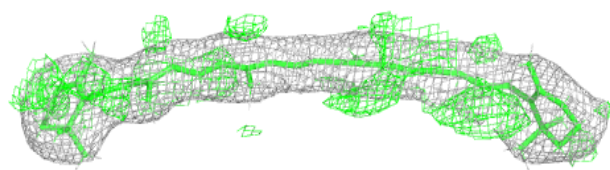
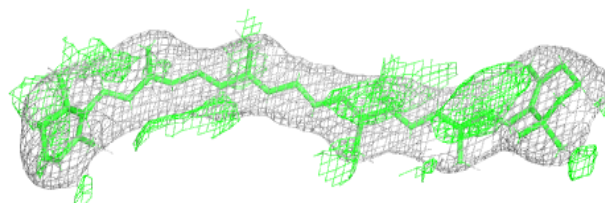


Electron density around CLA A 856:

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

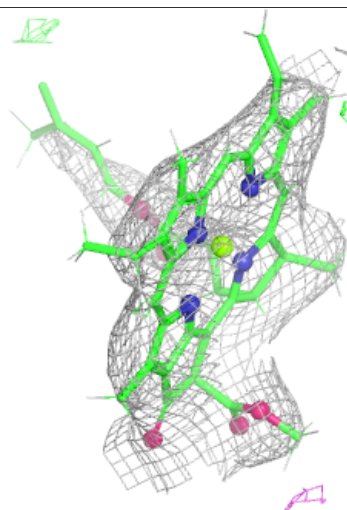
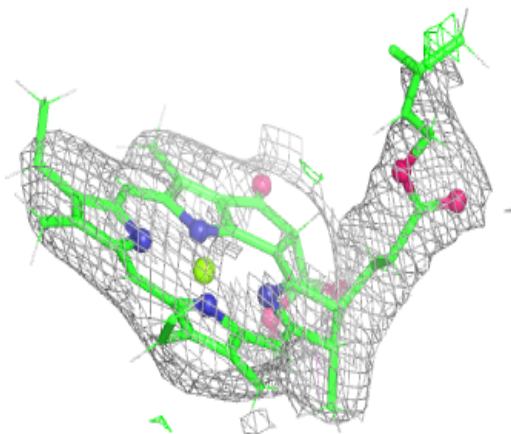
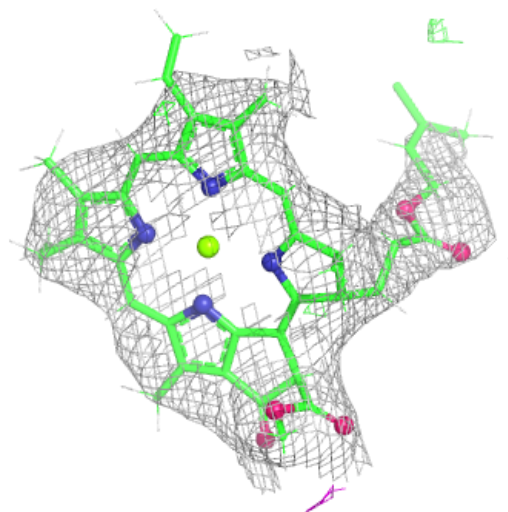
**Electron density around BCR I 102:**

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



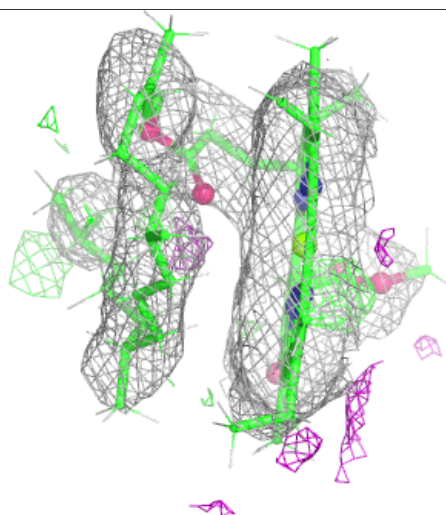
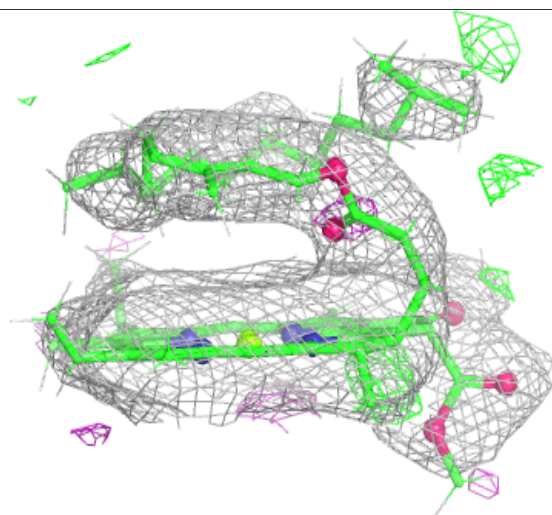
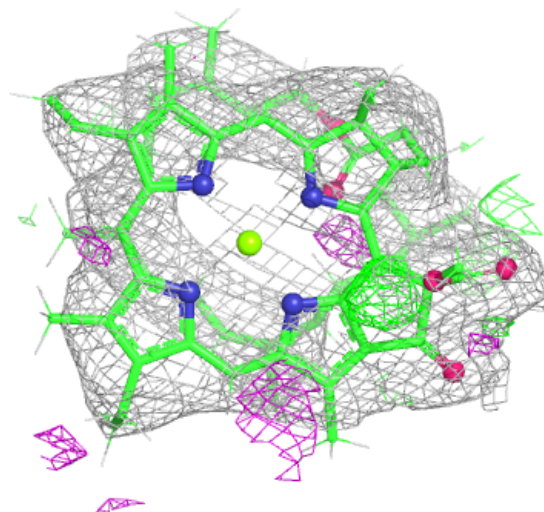
Electron density around CLA A 832:

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



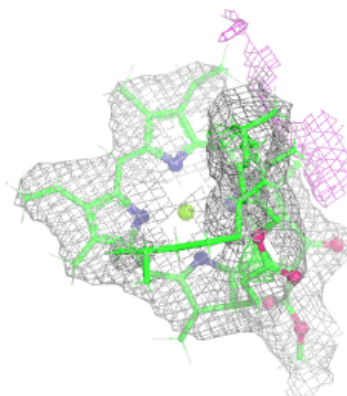
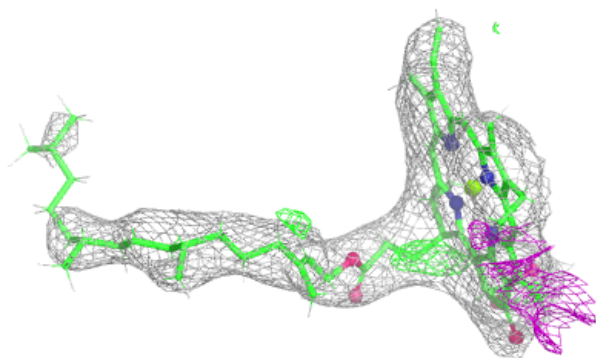
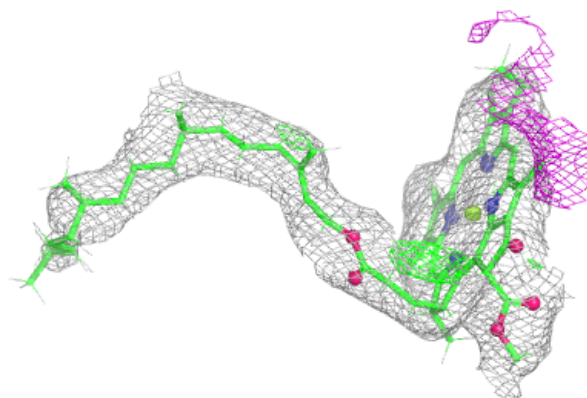
Electron density around CLA L 203:

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

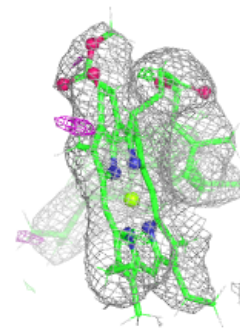
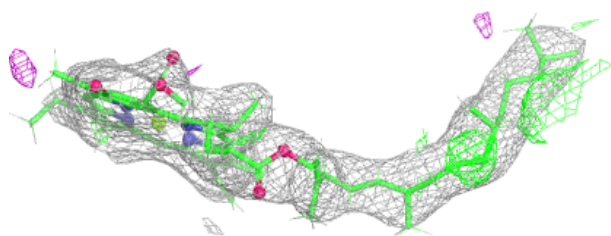
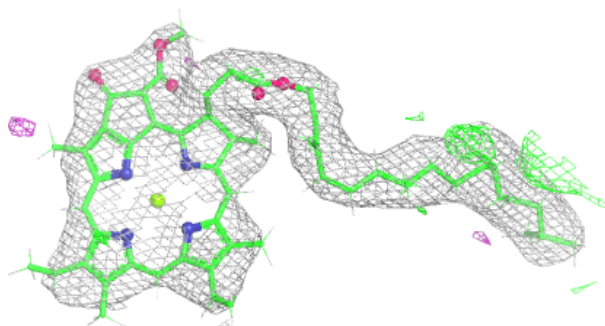


Electron density around CLA L 204:

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

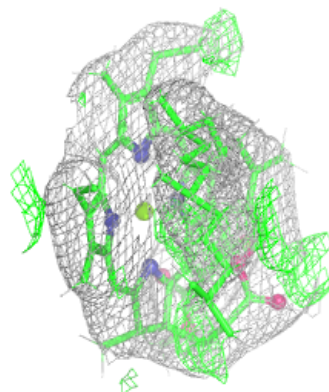
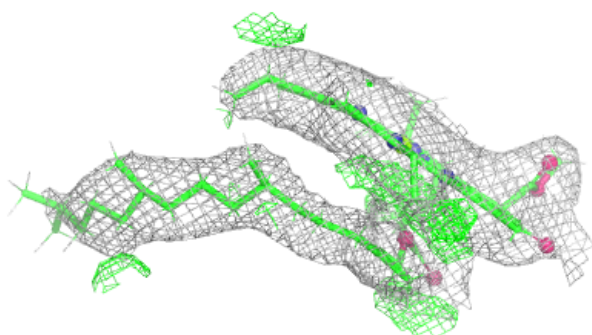
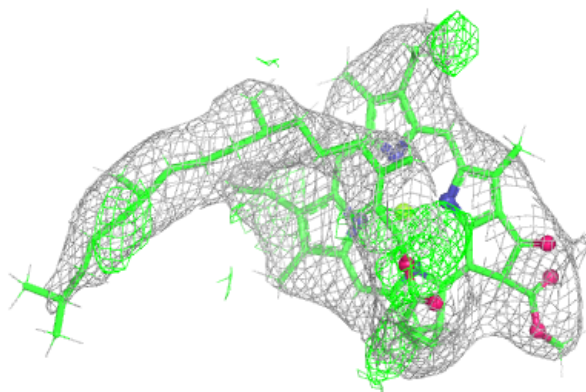
**Electron density around CLA B 3004:**

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

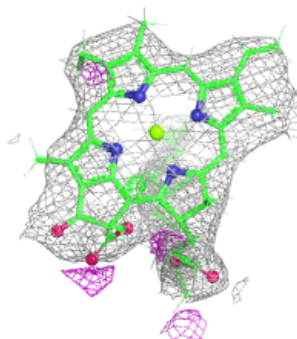
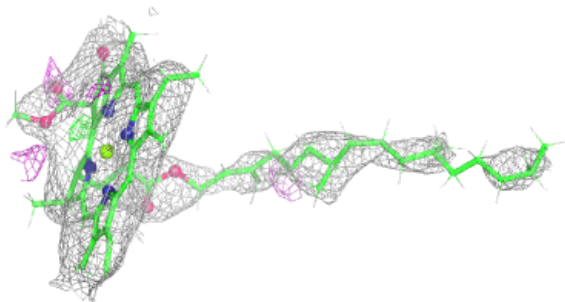
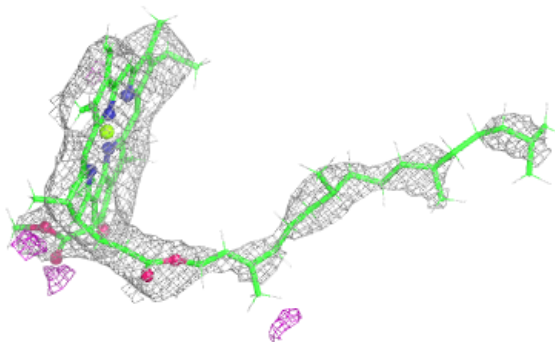


Electron density around CLA B 3008:

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

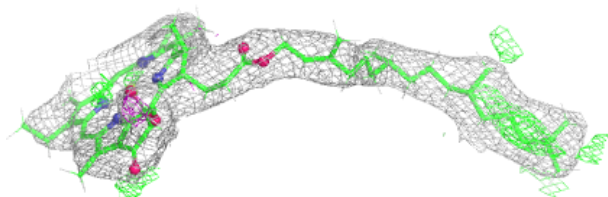
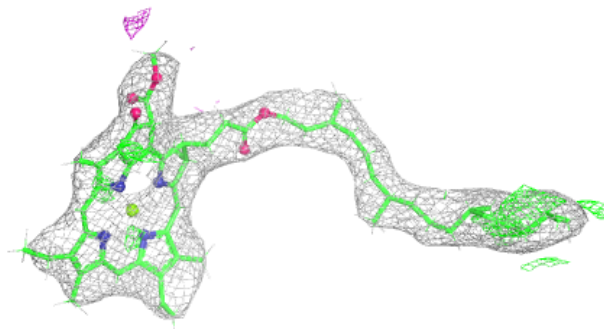
**Electron density around CLA B 3030:**

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

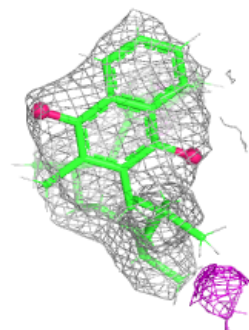
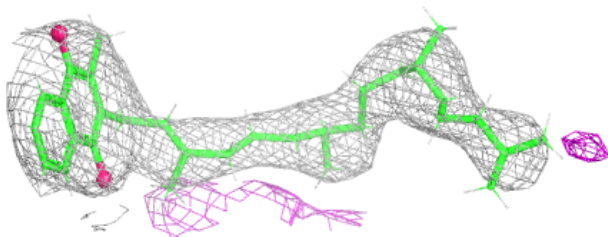
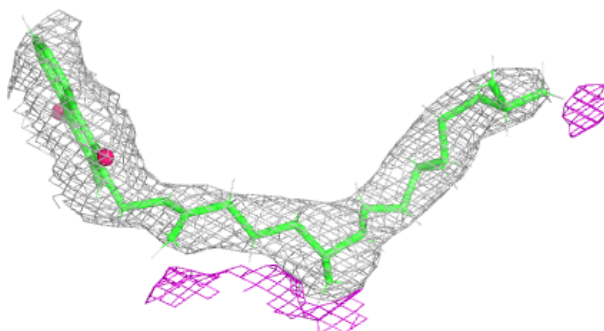


Electron density around CLA A 802:

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

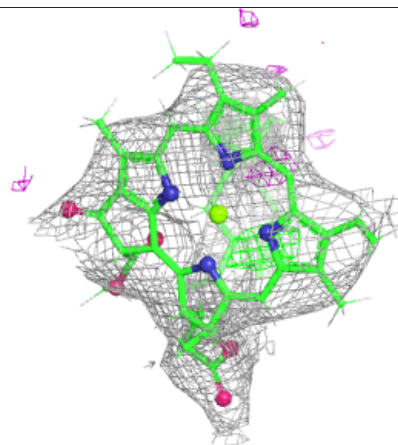
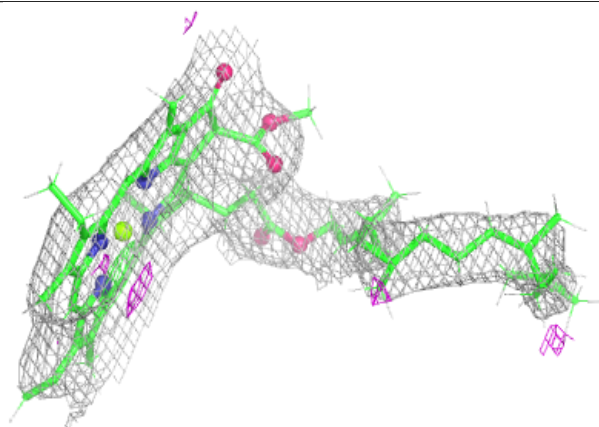
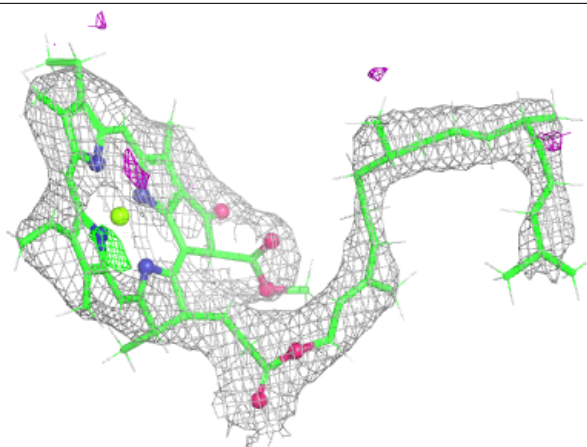
**Electron density around PQN B 3042:**

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

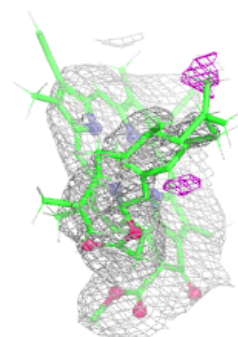
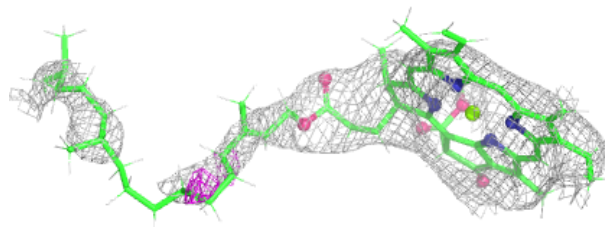
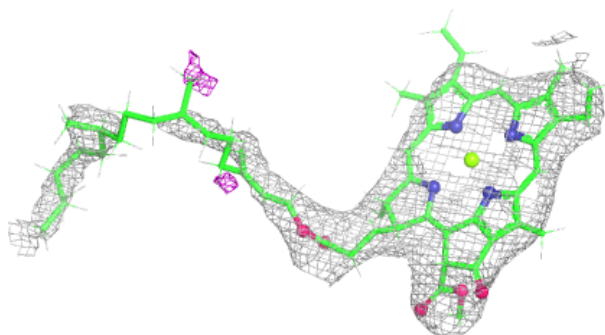


Electron density around CL0 A 801:

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

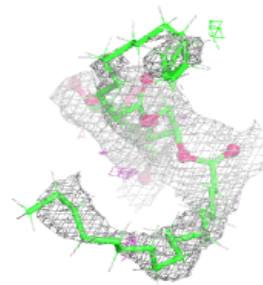
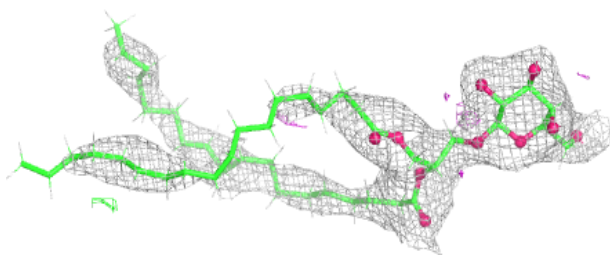
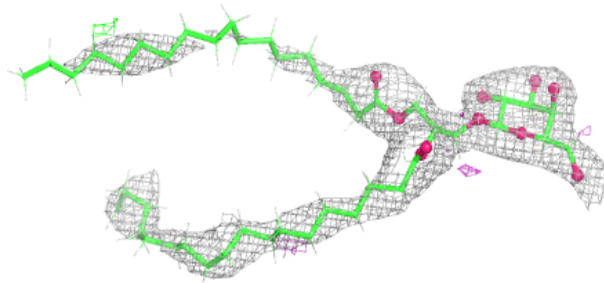
**Electron density around CLA B 3014:**

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

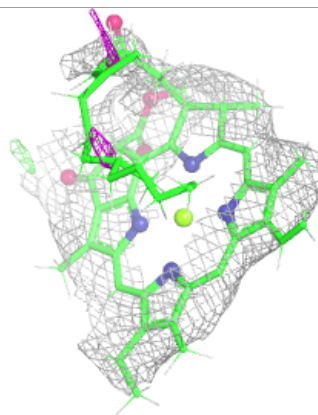
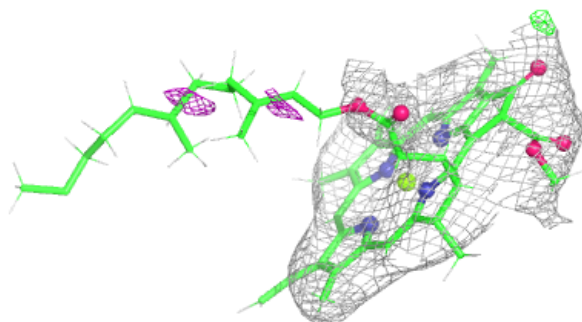
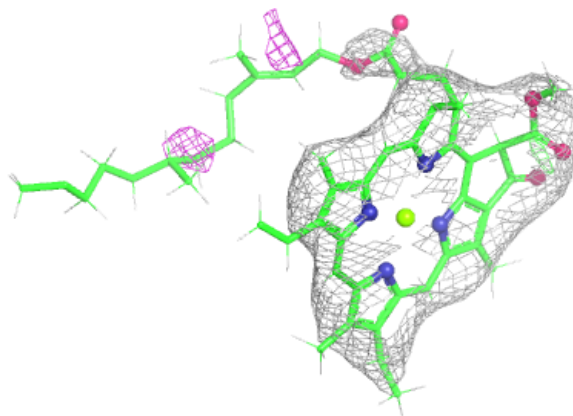


Electron density around LMG B 3048:

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

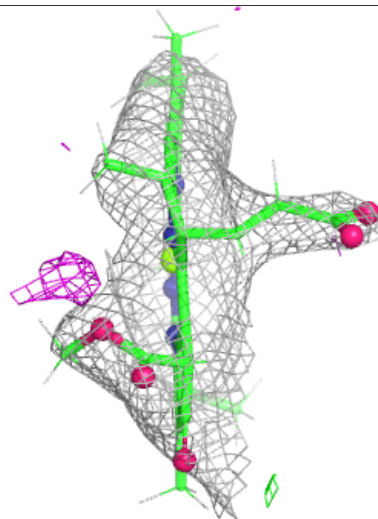
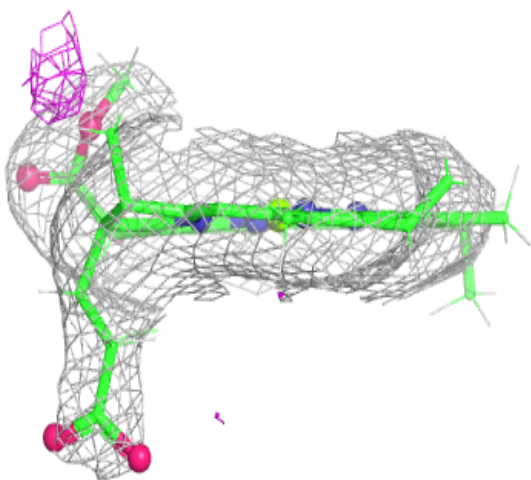
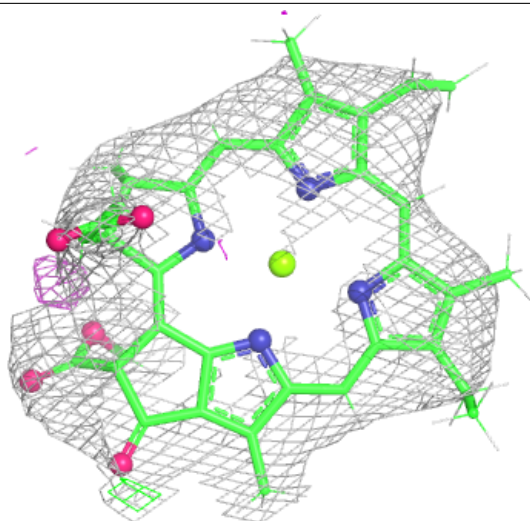
**Electron density around CLA A 825:**

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



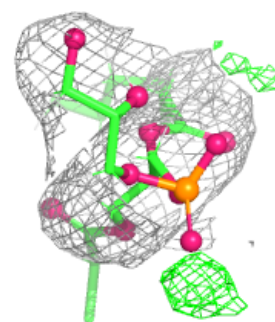
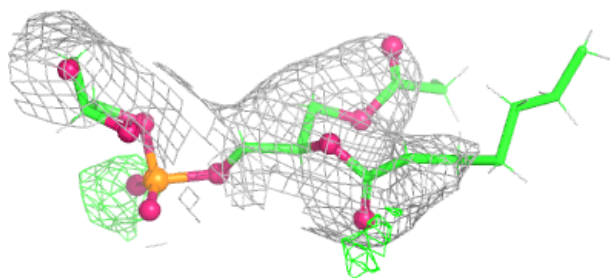
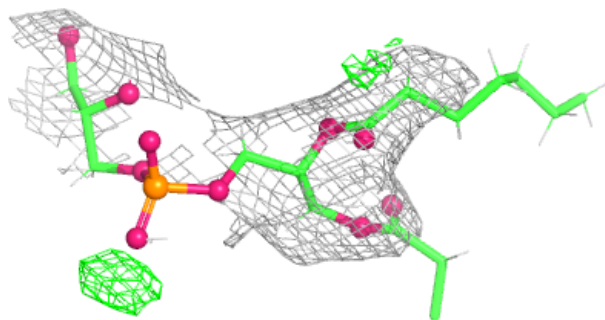
Electron density around CLA B 3035:

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



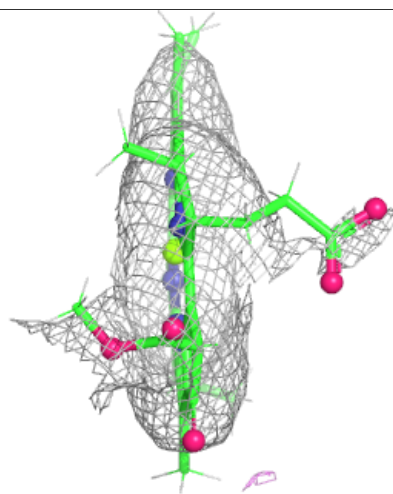
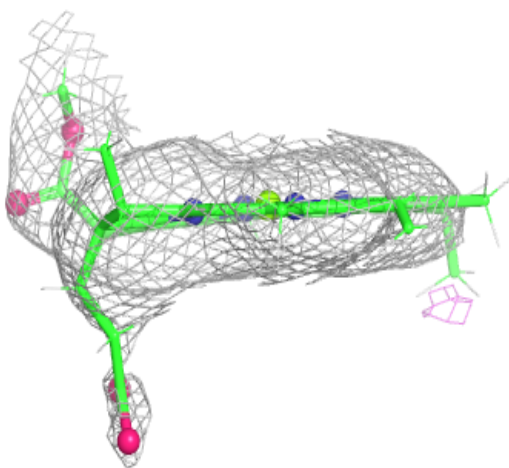
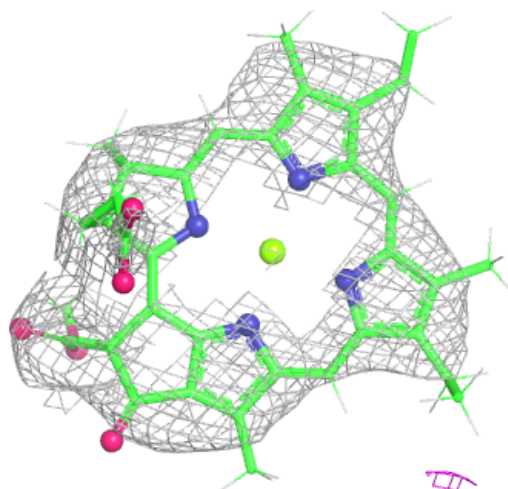
Electron density around LHG A 854:

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



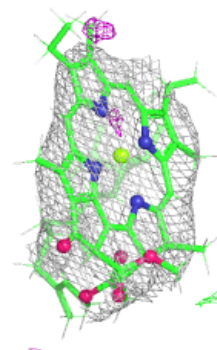
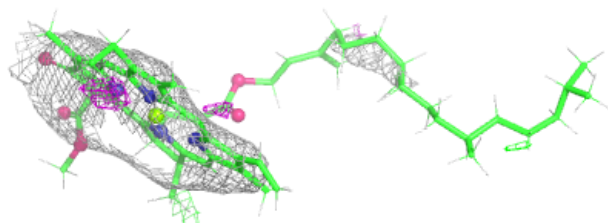
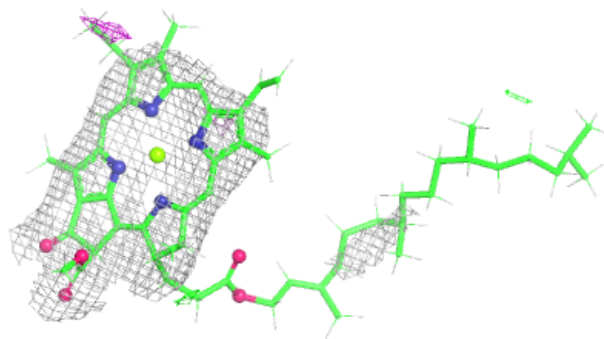
Electron density around CLA B 3016:

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

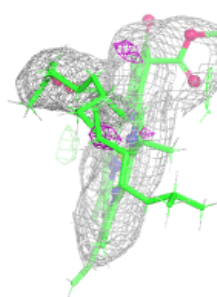
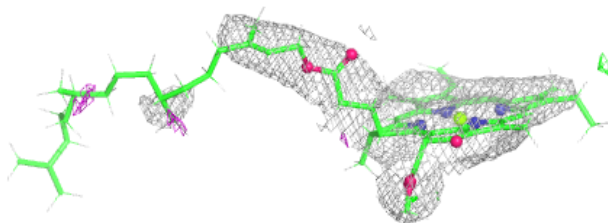
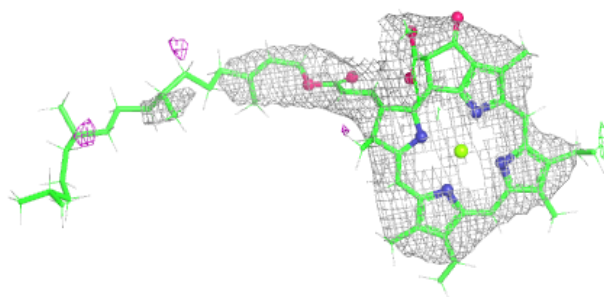


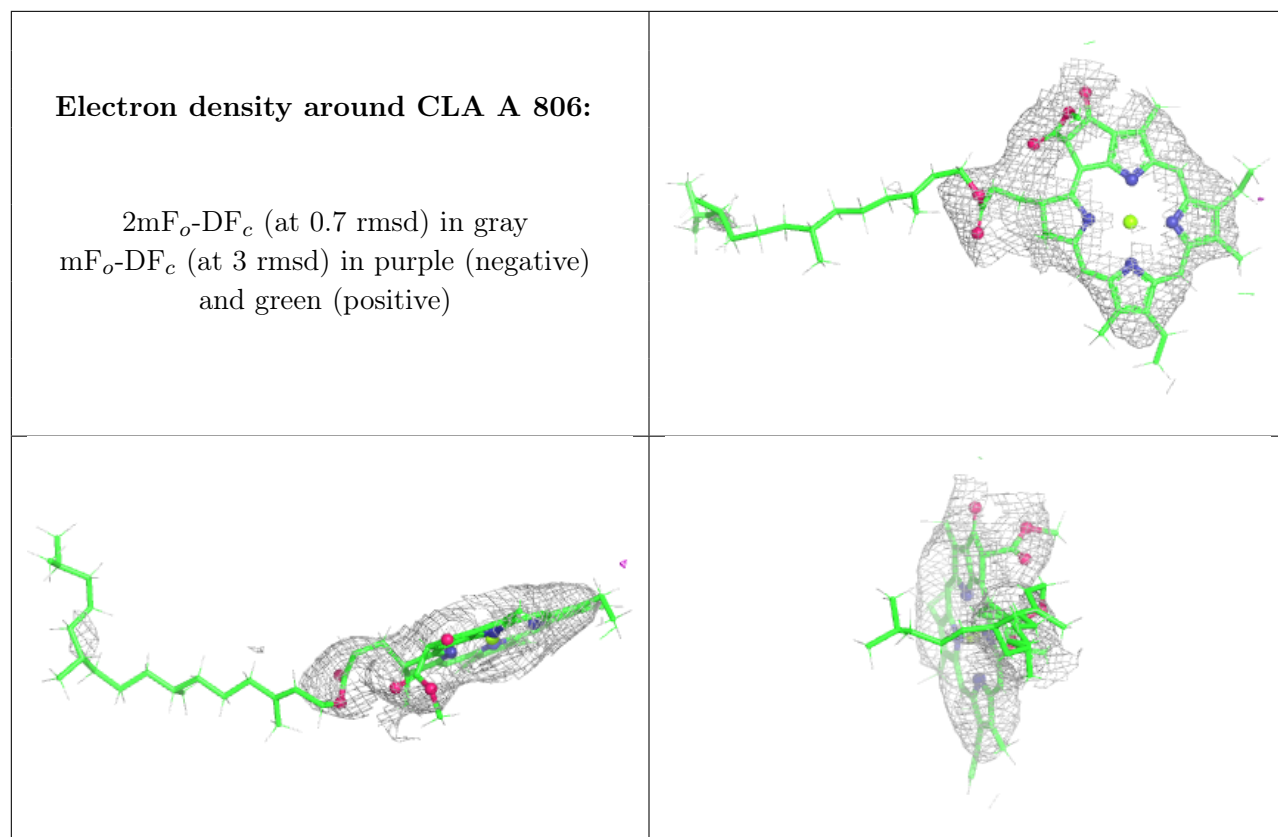
Electron density around CLA A 809:

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

**Electron density around CLA A 827:**

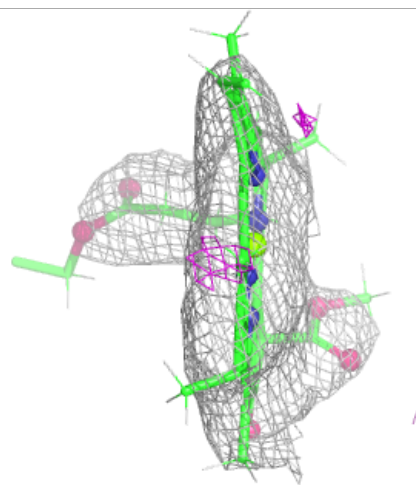
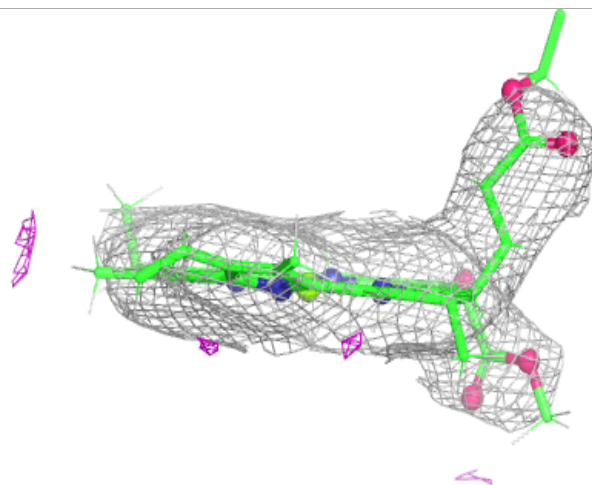
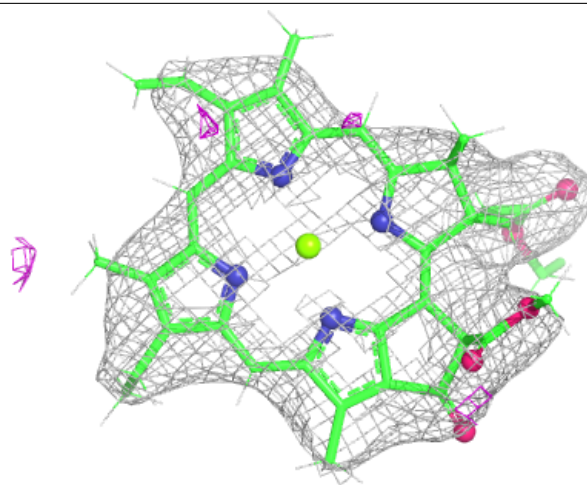
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





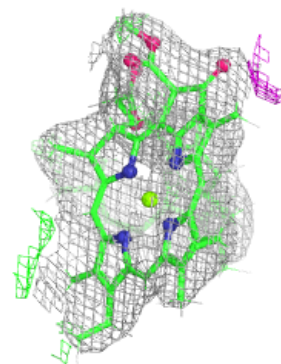
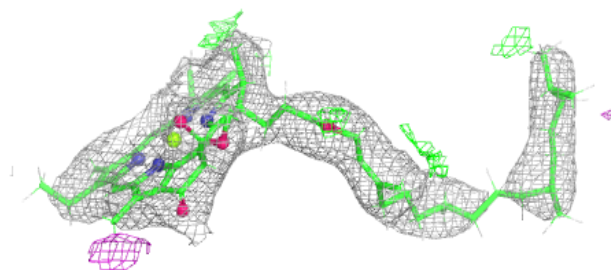
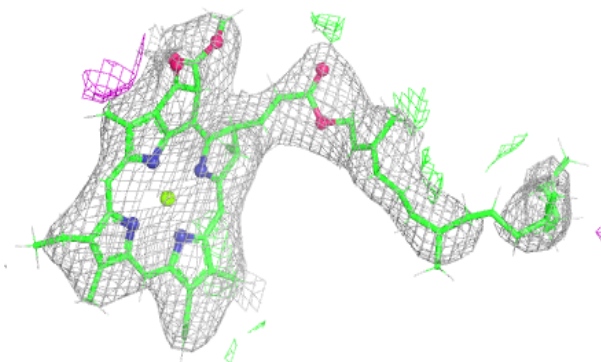
Electron density around CLA A 840:

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

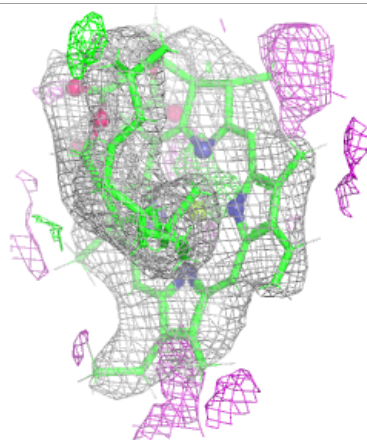
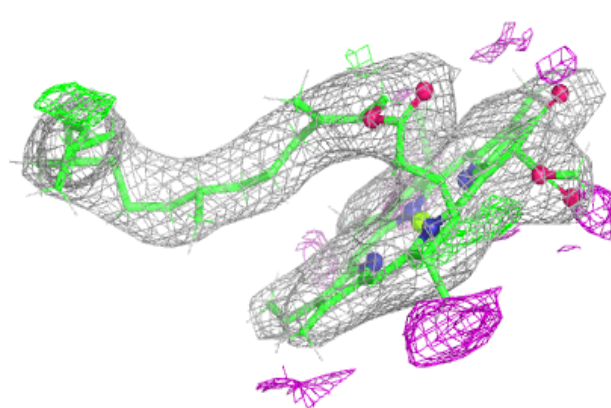
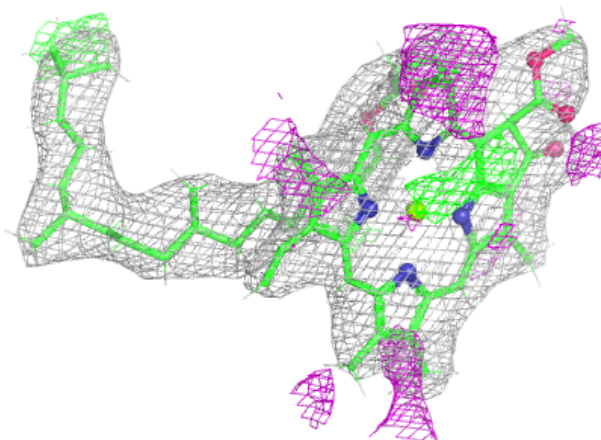


Electron density around CLA B 3010:

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

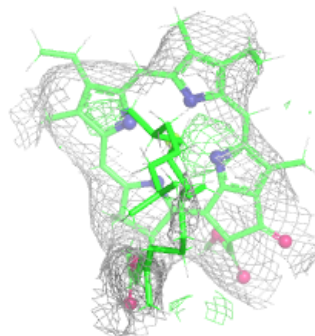
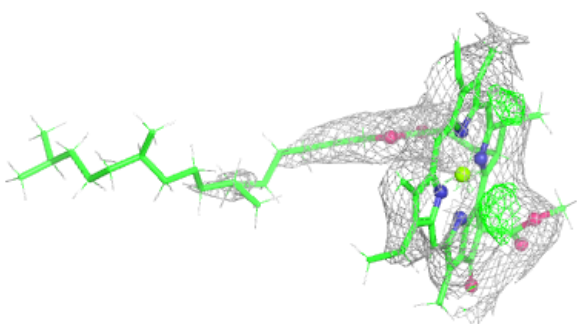
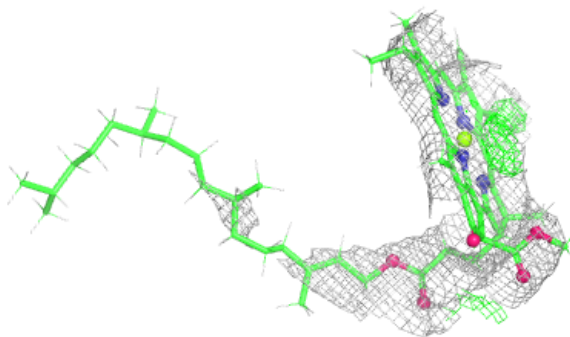
**Electron density around CLA A 844:**

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

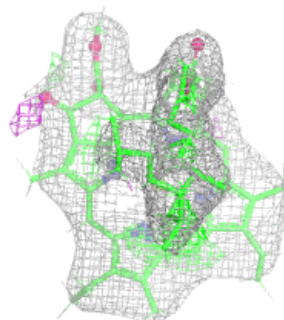
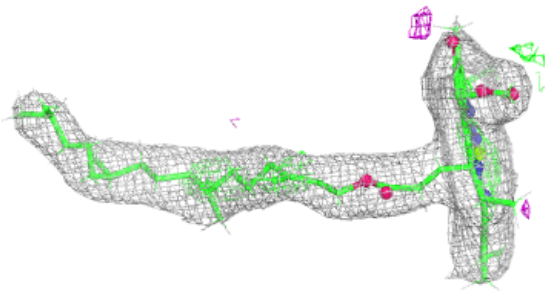
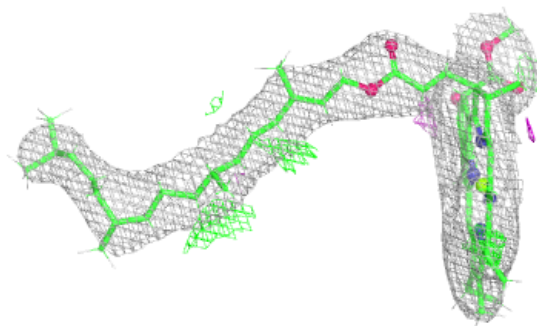


Electron density around CLA A 831:

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

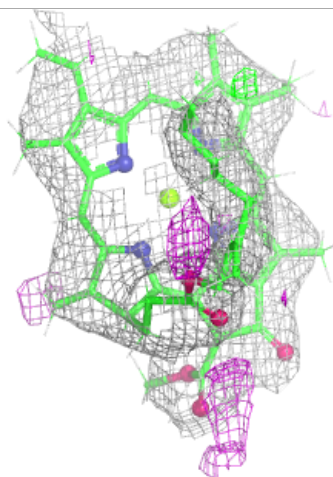
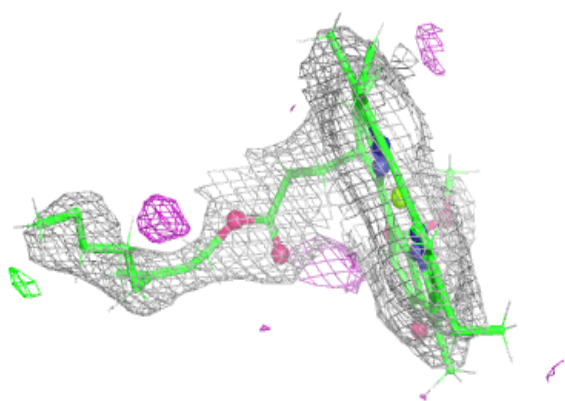
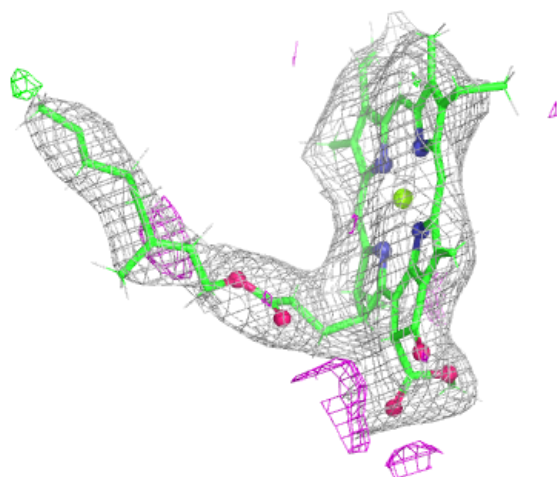
**Electron density around CLA B 3041:**

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



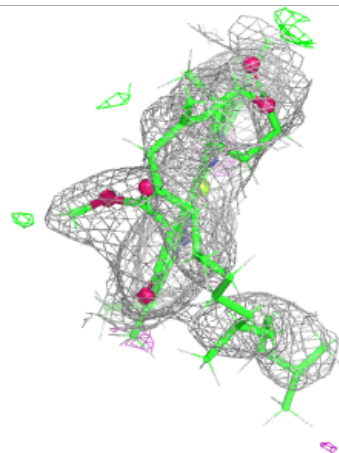
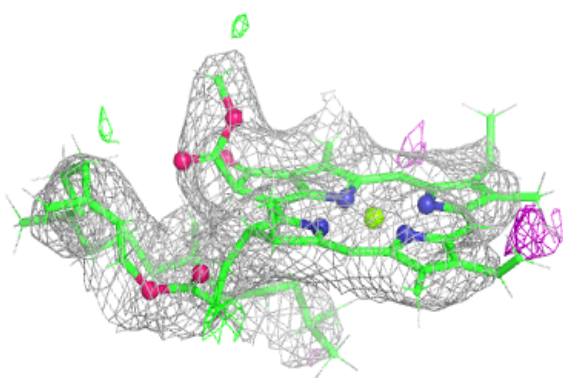
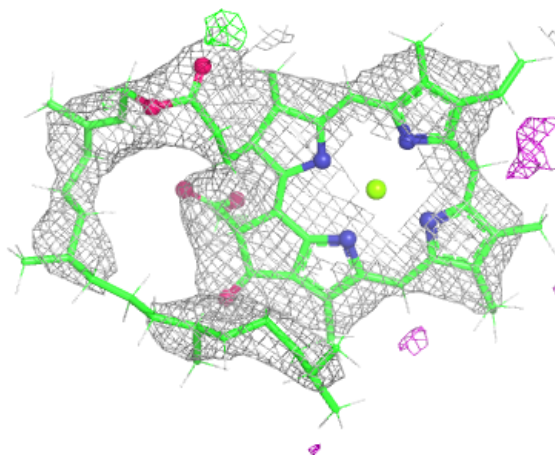
Electron density around CLA B 3005:

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



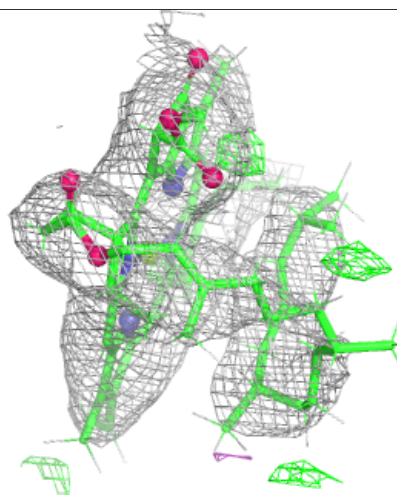
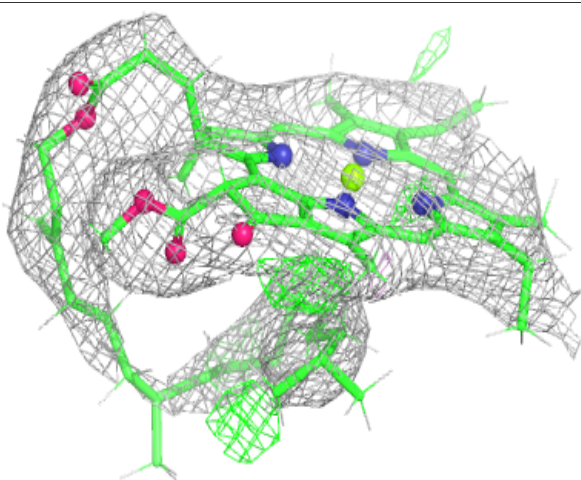
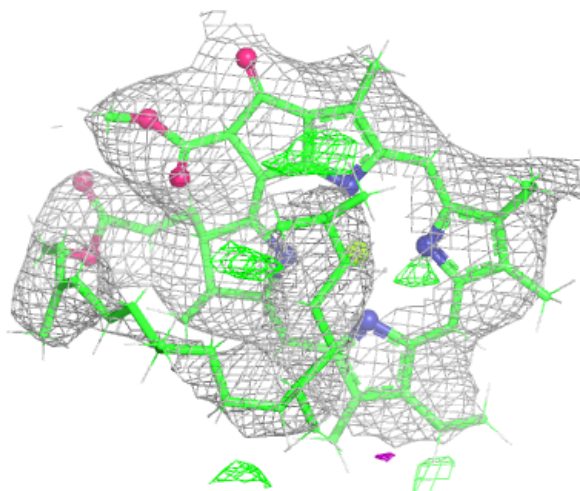
Electron density around CLA B 3006:

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



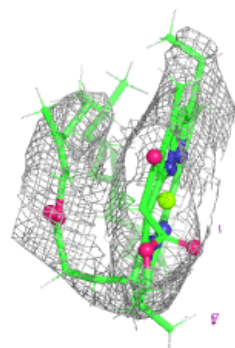
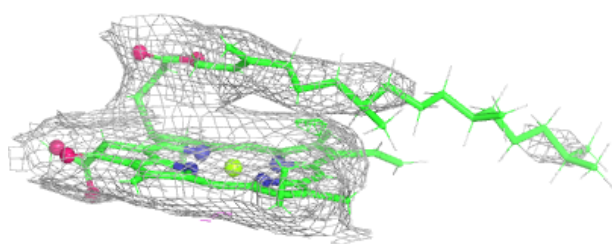
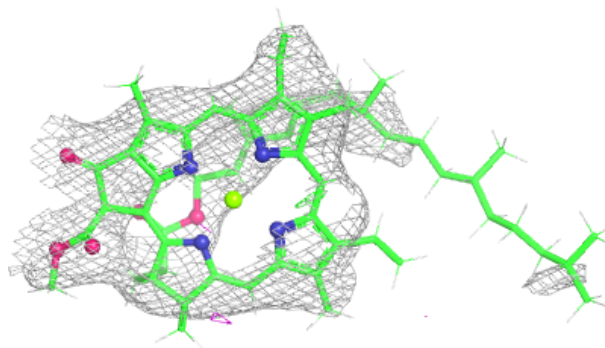
Electron density around CLA B 3007:

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



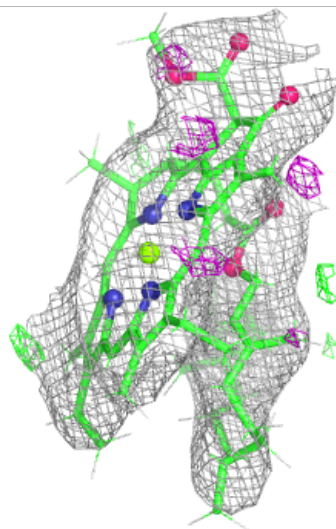
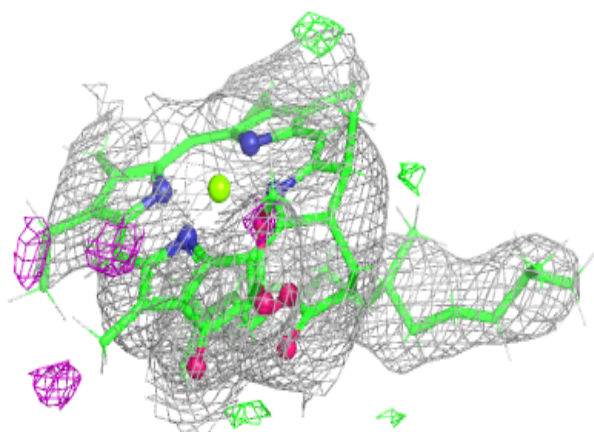
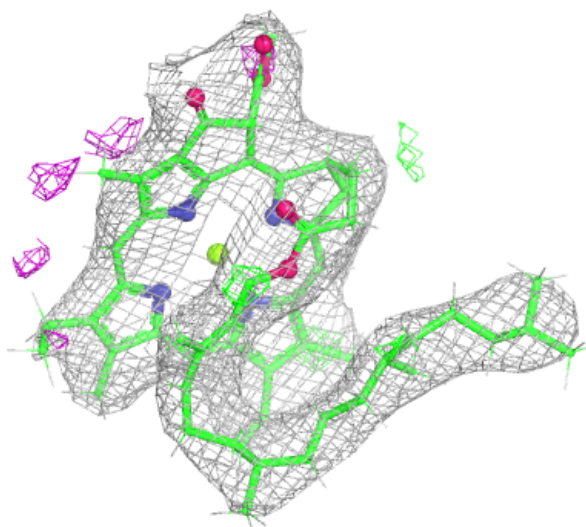
Electron density around CLA A 841:

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



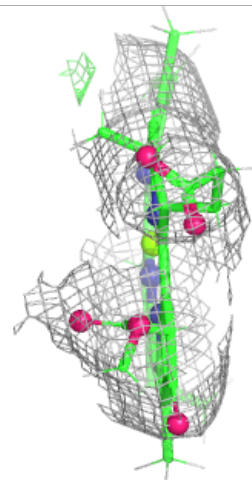
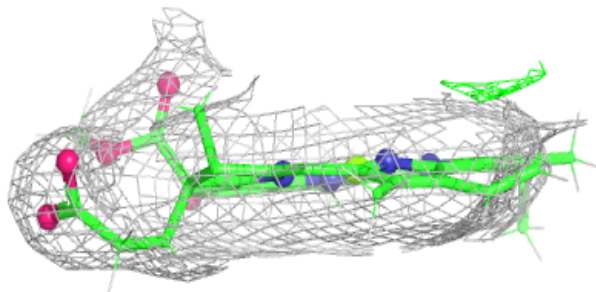
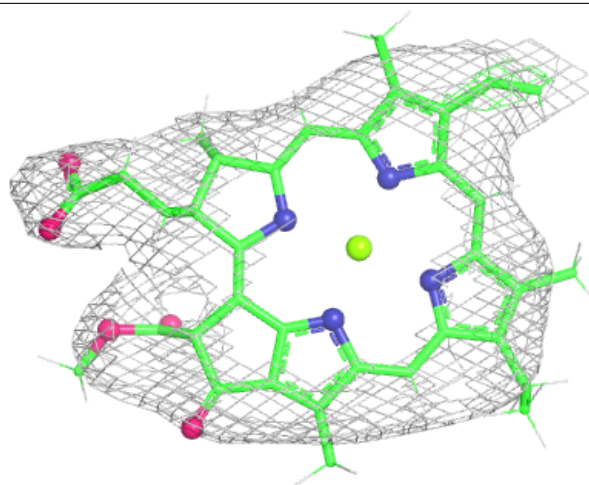
Electron density around CLA B 3009:

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



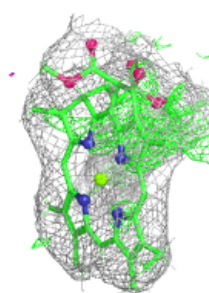
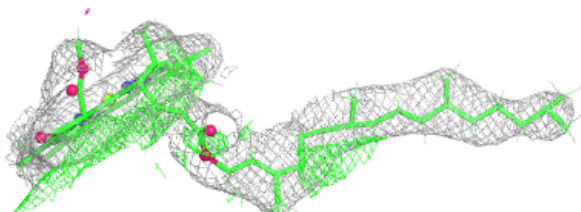
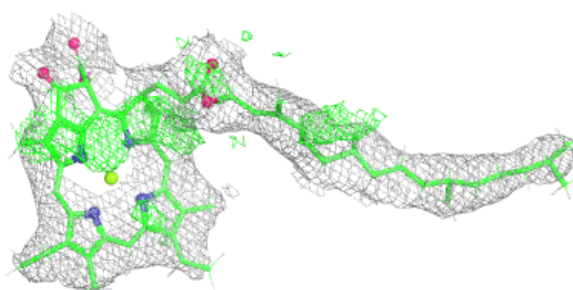
Electron density around CLA B 3037:

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

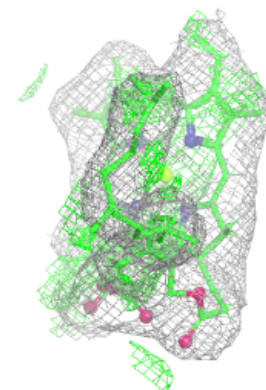
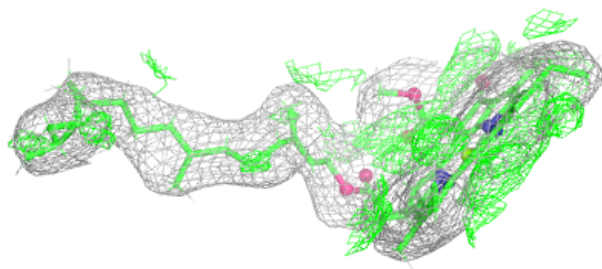
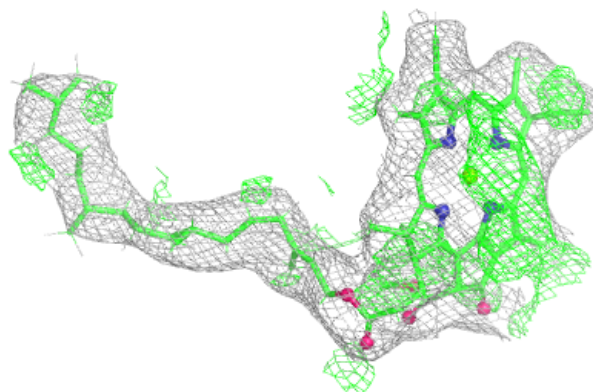


Electron density around CLA A 835:

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

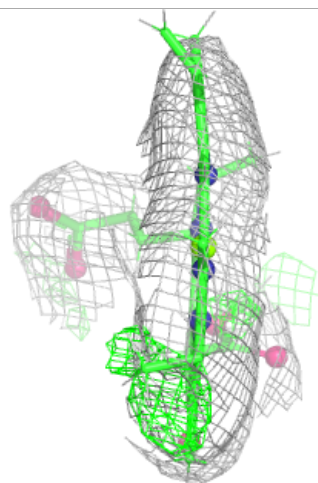
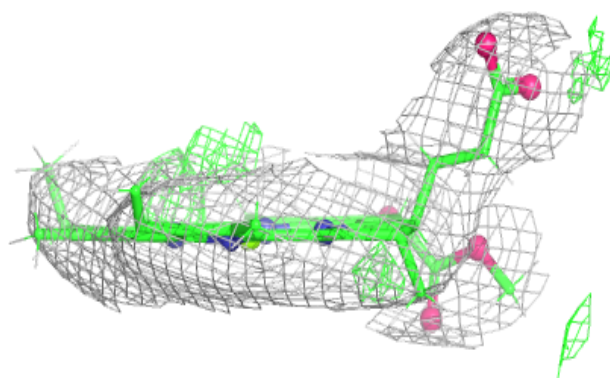
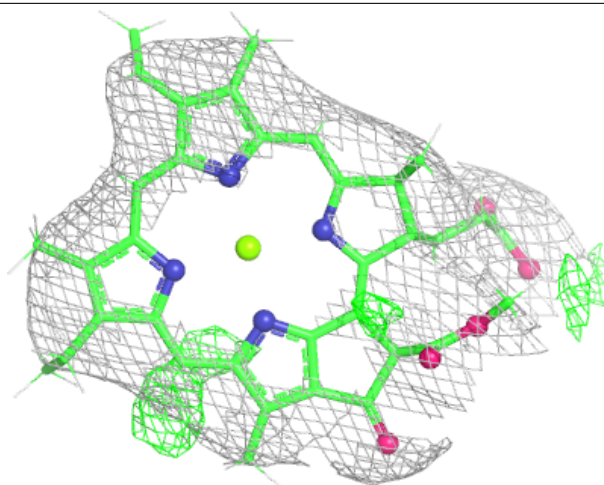
**Electron density around CLA B 3011:**

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



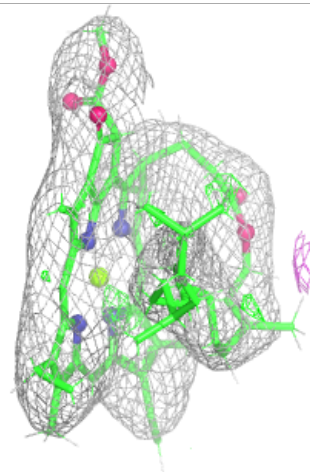
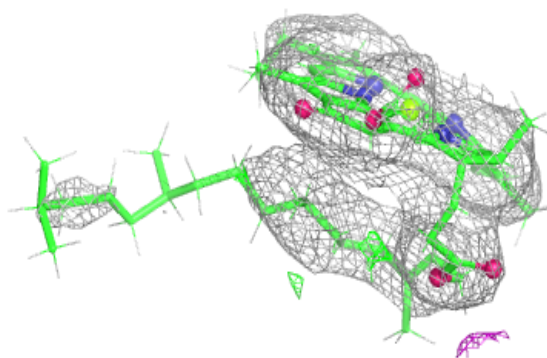
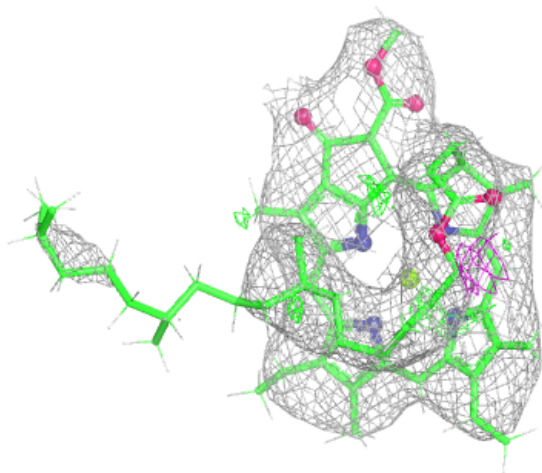
Electron density around CLA B 3024:

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



Electron density around CLA B 3028:

$2mF_o-DF_c$ (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.