



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 15, 2021 – 12:45 PM EST

PDB ID : 7M76
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 : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

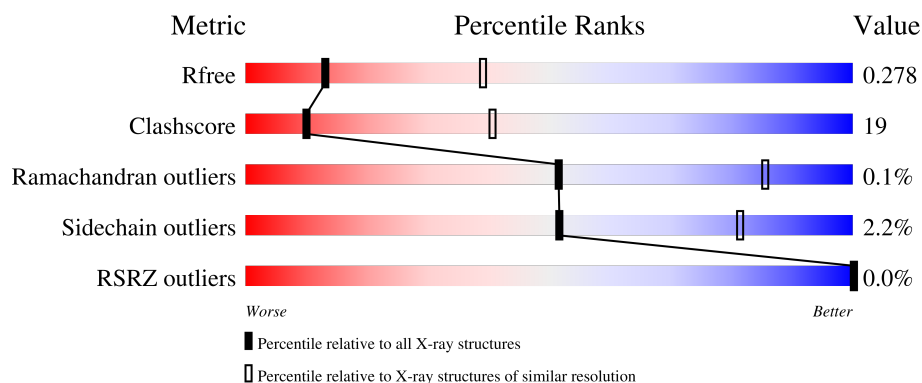
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



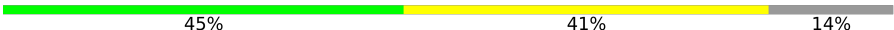


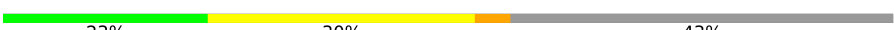



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	755	 59% 38% ..
2	B	740	 66% 34% .
3	C	80	 62% 36% .
4	D	138	 68% 32%
5	E	75	 67% 23% .. 8%

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Mol	Chain	Length	Quality of chain
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	-	-	-
14	CLA	A	824	X	-	-	-
14	CLA	A	825	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	826	X	-	-	-
14	CLA	A	827	X	-	-	-
14	CLA	A	828	X	-	-	-
14	CLA	A	829	X	-	-	-
14	CLA	A	830	X	-	-	-
14	CLA	A	831	X	-	-	-
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	839	X	-	-	-
14	CLA	A	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	842	X	-	-	-
14	CLA	A	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	-	-	-
14	CLA	B	3022	X	-	-	-
14	CLA	B	3023	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	3039	X	-	-	-
14	CLA	B	3041	X	-	-	-
14	CLA	B	3042	X	-	-	-
14	CLA	F	202	X	-	-	-
14	CLA	J	101	X	-	-	-
14	CLA	J	102	X	-	-	-
14	CLA	K	101	X	-	-	-
14	CLA	K	103	X	-	-	-
14	CLA	L	204	X	-	-	-
14	CLA	L	205	X	-	-	-
14	CLA	L	206	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 48797 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

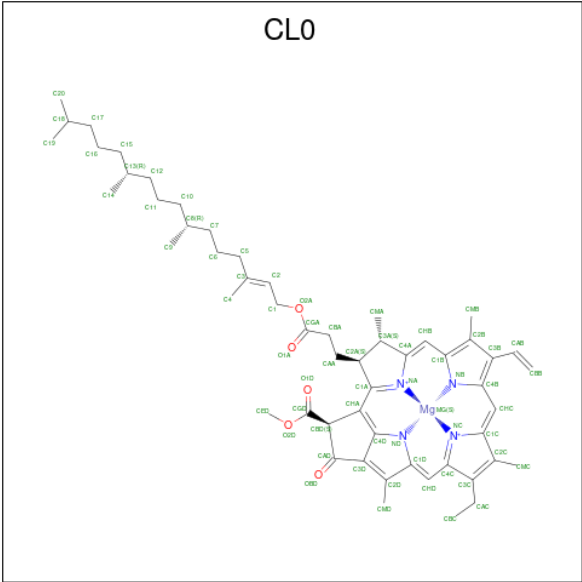
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

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.

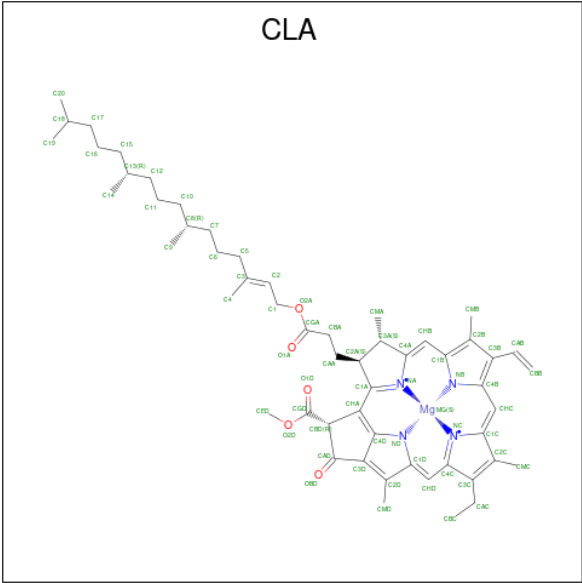
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	X	29	Total	C	H	N	O	0	0	0
			459	172	217	35	35			

- Molecule 13 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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		

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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
			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		

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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
			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		

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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	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		

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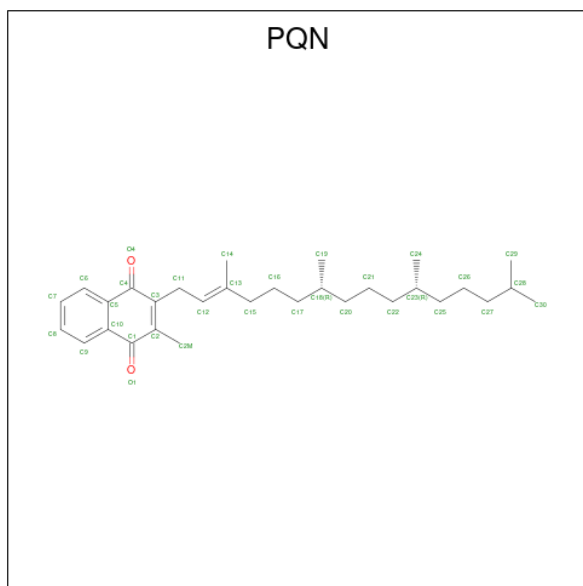
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	B	1	Total	C	H	Mg	N	O	0	0
			104	45	49	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			79	36	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	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	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		

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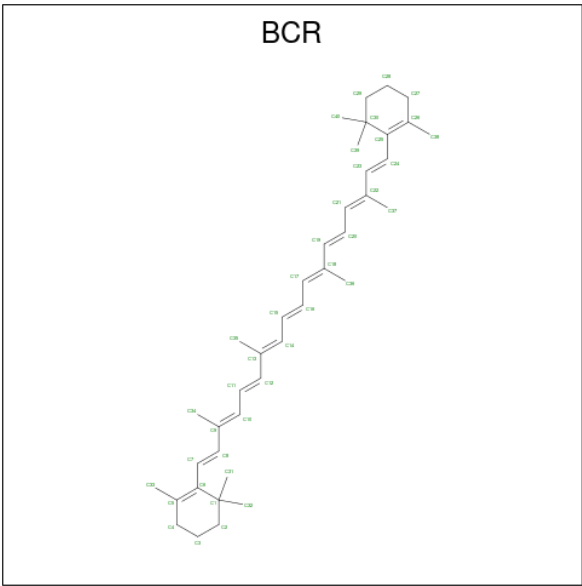
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	J	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	J	1	Total	C	H	Mg	N	O	0	0
			62	31	25	1	4	1		
14	K	1	Total	C	H	Mg	N	O	0	0
			70	33	29	1	4	3		
14	K	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	L	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	L	1	Total	C	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 (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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 (three-letter code: BCR) (formula: C₄₀H₅₆).



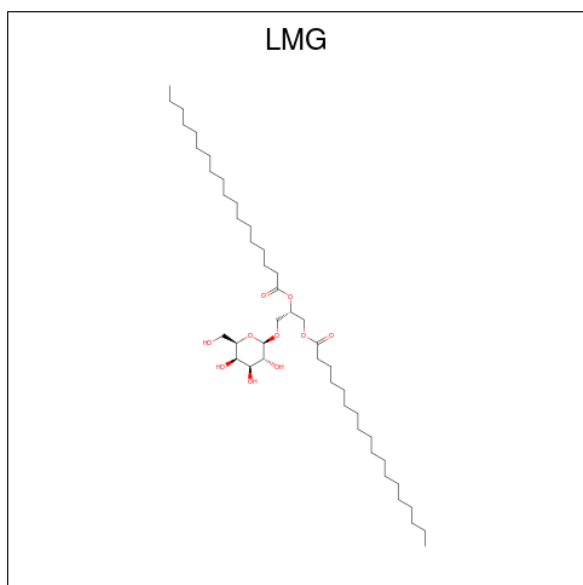
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	A	1	Total	C	H	0	0
			96	40	56		
16	A	1	Total	C	H	0	0
			96	40	56		
16	A	1	Total	C	H	0	0
			96	40	56		
16	A	1	Total	C	H	0	0
			96	40	56		
16	A	1	Total	C	H	0	0
			96	40	56		
16	B	1	Total	C	H	0	0
			96	40	56		
16	B	1	Total	C	H	0	0
			96	40	56		
16	B	1	Total	C	H	0	0
			96	40	56		
16	B	1	Total	C	H	0	0
			96	40	56		
16	B	1	Total	C	H	0	0
			96	40	56		
16	F	1	Total	C	H	0	0
			96	40	56		
16	F	1	Total	C	H	0	0
			96	40	56		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	L	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 (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



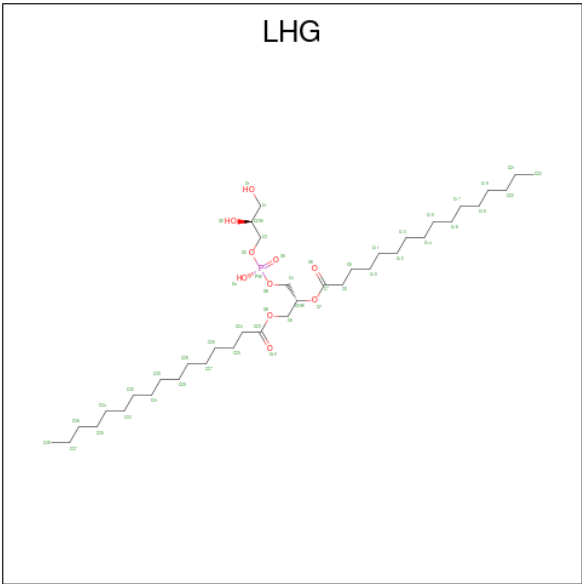
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	H	O	0	0
			118	38	70	10		
17	A	1	Total	C	H	O	0	0
			67	22	37	8		

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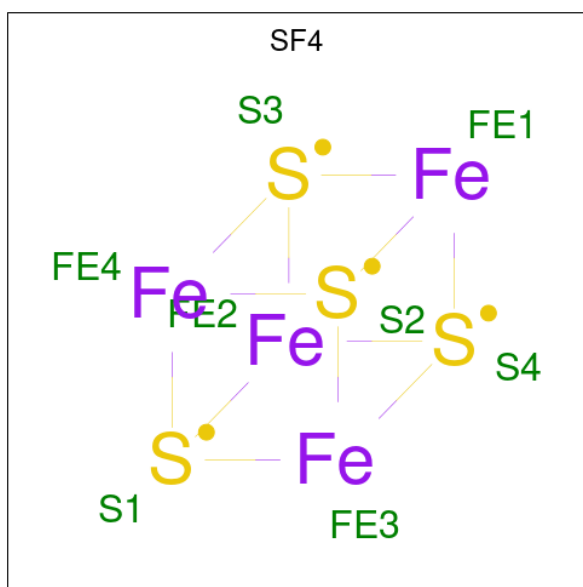
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	B	1	Total	C	H	O	0	0
			141	45	86	10		
17	I	1	Total	C	H	O	0	0
			91	30	51	10		

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: 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 (three-letter code: SF4) (formula: Fe₄S₄).

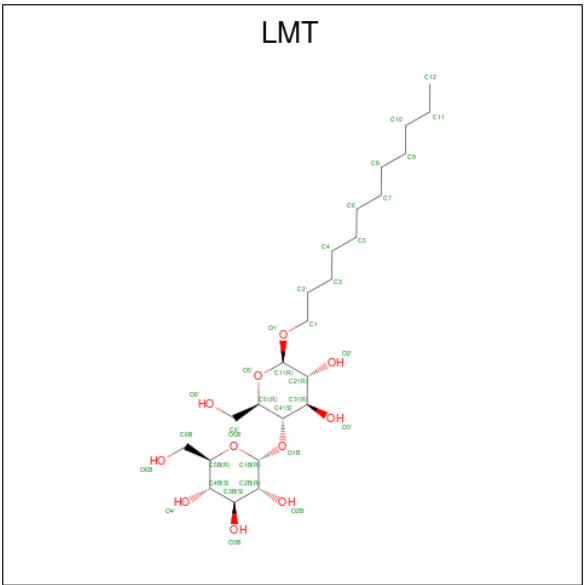


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	B	1	Total	Fe	S	0	0
			8	4	4		
19	C	1	Total	Fe	S	0	0
			8	4	4		
19	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 20 is CALCIUM ION (three-letter code: CA) (formula: Ca).

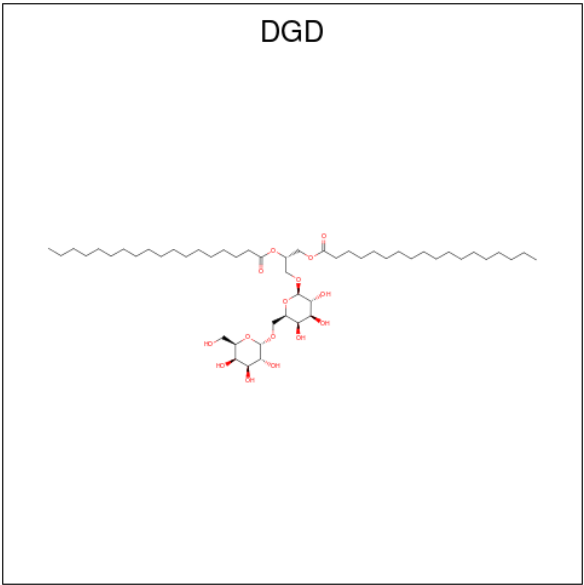
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	B	1	Total	Ca	0	0
			1	1		
20	L	1	Total	Ca	0	0
			1	1		

- Molecule 21 is DODECYL-BETA-D-MALTOSIDE (three-letter code: 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) (three-letter code: 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		

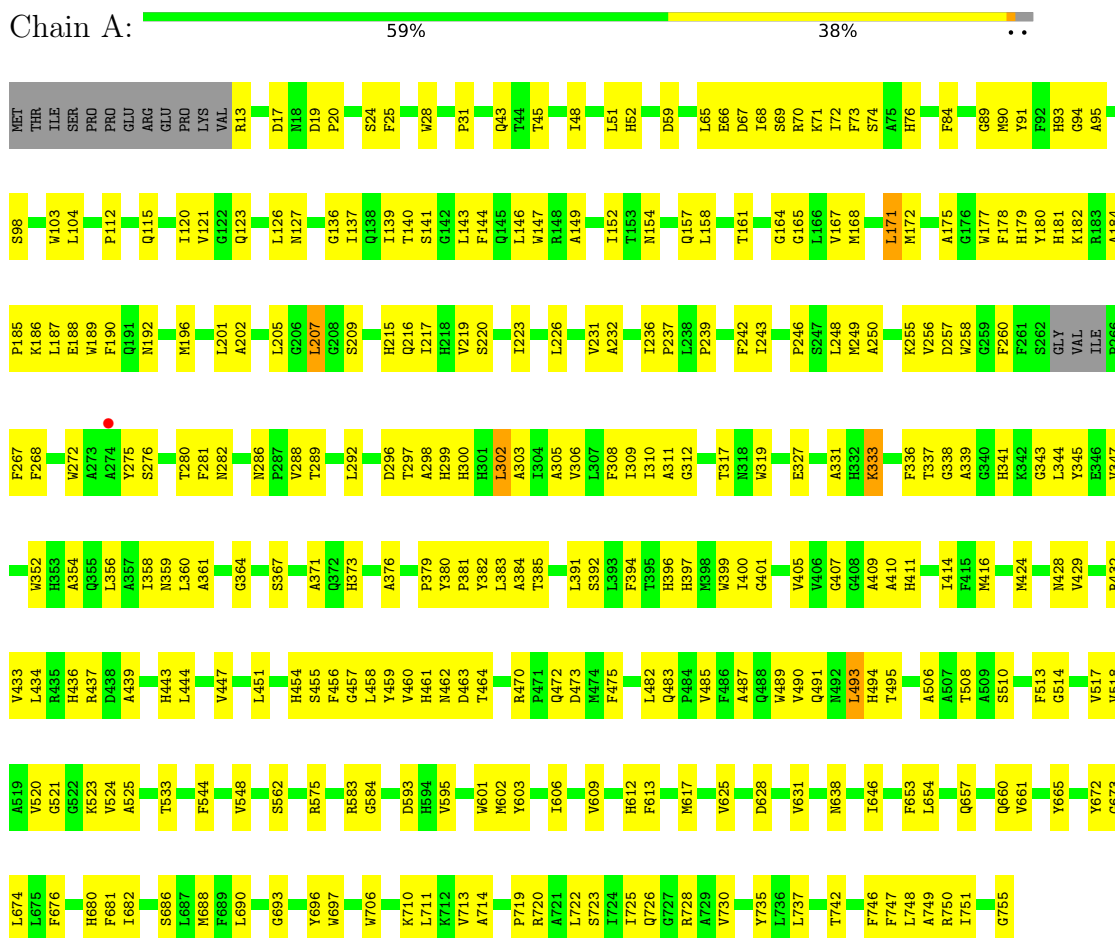
- Molecule 23 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	8	Total 8	O 8	0	0
23	B	8	Total 8	O 8	0	0
23	J	1	Total 1	O 1	0	0
23	L	2	Total 2	O 2	0	0
23	M	1	Total 1	O 1	0	0

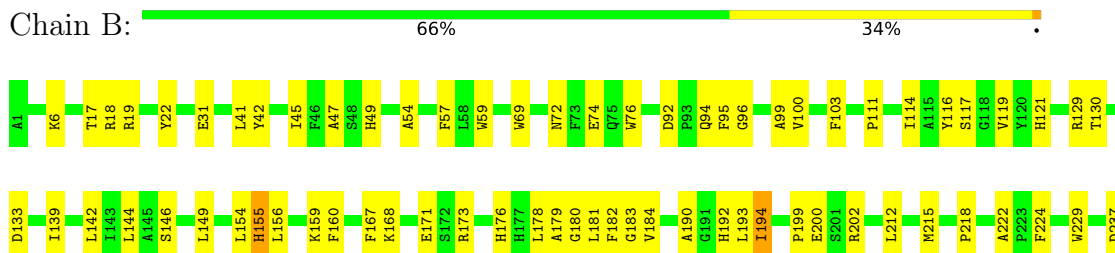
3 Residue-property plots

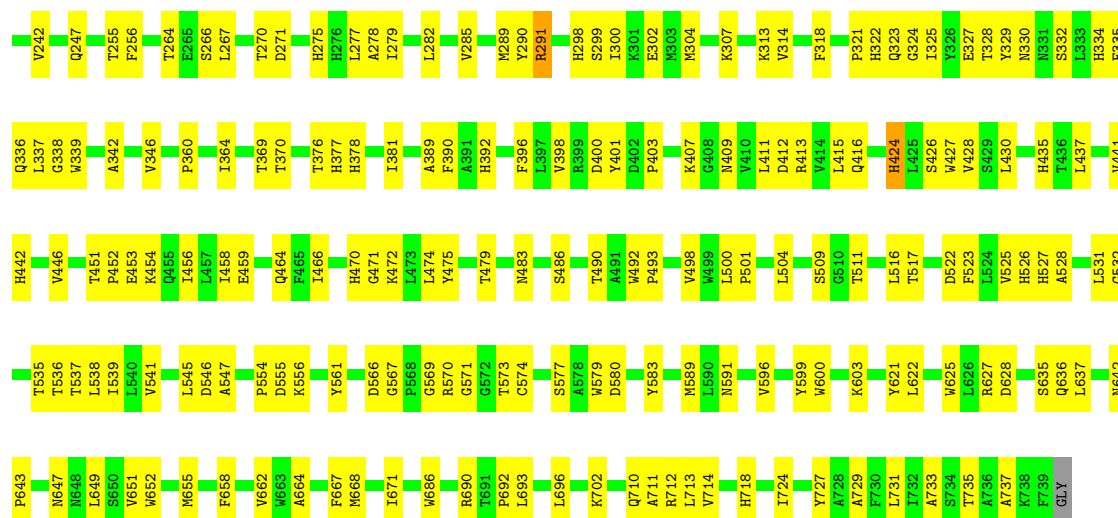
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

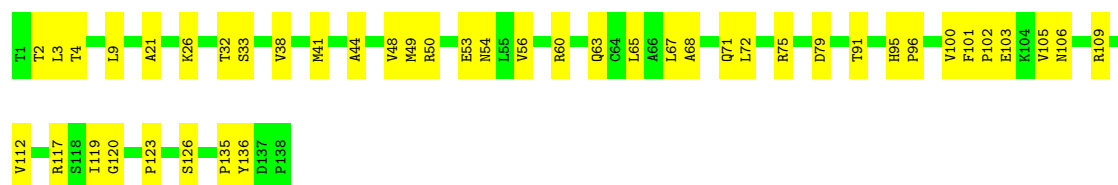




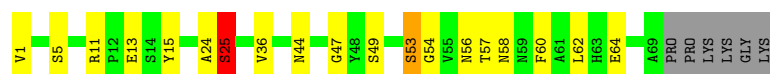
• Molecule 3: Photosystem I iron-sulfur center



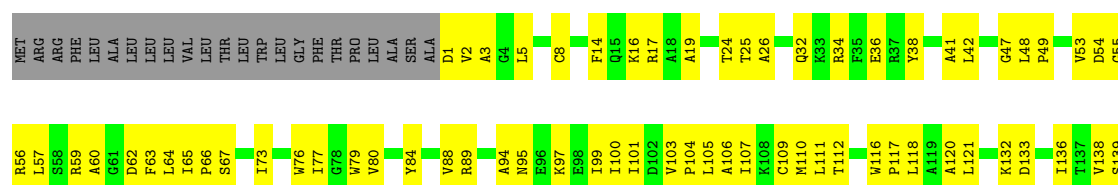
• Molecule 4: Photosystem I reaction center subunit II



• Molecule 5: Photosystem I reaction center subunit IV



• Molecule 6: Photosystem I reaction center subunit III





- Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 58% 42%



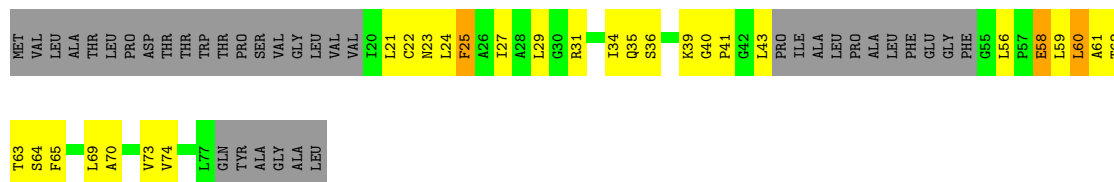
- Molecule 8: Photosystem I reaction center subunit IX

Chain J: 46% 54%



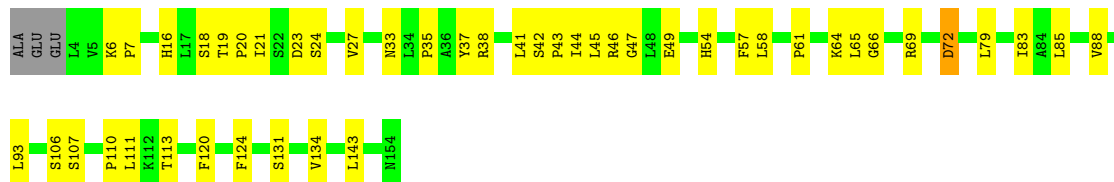
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain K: 23% 30% 43%



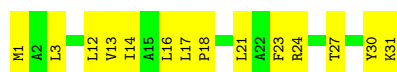
- Molecule 10: Photosystem I reaction center subunit XI

Chain L: 68% 29% ..



- Molecule 11: Photosystem I reaction center subunit XII

Chain M: 55% 45%



- Molecule 12: Photosystem I 4.8K protein

Chain X: 40% 37% 6% 17%

ALA	THR	LYS	SER	ALA	LYS	P7	T8	Y9		R12	T13	F14	W15	A16	V17	L18	L19	L20		N23	F24	L25		Y29	Y30	F31		L34	K35
-----	-----	-----	-----	-----	-----	----	----	----	--	-----	-----	-----	-----	-----	-----	-----	-----	-----	--	-----	-----	-----	--	-----	-----	-----	--	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	284.27Å 284.27Å 165.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.23 – 3.00 25.23 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (25.23-3.00) 83.1 (25.23-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.23 (at 2.99Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.268 , 0.278 0.268 , 0.278	Depositor DCC
R_{free} test set	1997 reflections (1.32%)	wwPDB-VP
Wilson B-factor (Å ²)	60.8	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , -11.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.045 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	48797	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.33	0/5983	0.60	3/8158 (0.0%)
2	B	0.33	0/6107	0.56	0/8345
3	C	0.37	0/608	0.60	0/824
4	D	0.33	0/1101	0.60	0/1492
5	E	0.33	0/551	0.59	0/750
6	F	0.35	0/1087	0.64	0/1476
7	I	0.32	0/312	0.61	0/425
8	J	0.34	0/350	0.59	0/477
9	K	0.32	0/337	0.75	0/454
10	L	0.34	0/1148	0.59	0/1558
11	M	0.39	0/244	0.59	0/332
12	X	0.37	0/251	0.59	0/342
All	All	0.33	0/18079	0.59	3/24633 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
3	C	0	1
9	K	0	1
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	LEU	CA-CB-CG	5.48	127.90	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	493	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	171	LEU	CA-CB-CG	5.13	127.10	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	521	GLY	Peptide
1	A	617	MET	Peptide
3	C	60	ASP	Peptide
9	K	58	GLU	Peptide

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	290	0
2	B	5889	5618	5649	222	0
3	C	598	576	580	27	0
4	D	1075	1077	1077	33	0
5	E	539	528	528	14	0
6	F	1065	1076	1077	70	0
7	I	301	306	306	18	0
8	J	338	347	347	27	0
9	K	333	354	354	38	0
10	L	1119	1125	1125	32	0
11	M	241	264	264	15	0
12	X	242	217	249	16	0
13	A	65	72	72	3	0
14	A	2628	2615	2615	157	0
14	B	2284	2232	2232	108	0
14	F	45	33	33	8	0
14	J	82	58	58	4	0
14	K	86	62	62	5	0
14	L	195	216	216	5	0
14	M	45	33	33	4	0
14	X	45	33	33	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	A	33	46	46	9	0
15	B	33	46	46	2	0
16	A	200	280	280	20	0
16	B	240	336	336	18	0
16	F	80	112	112	8	0
16	I	40	56	56	4	0
16	J	120	168	168	20	0
16	K	40	56	56	5	0
16	L	120	168	168	7	0
16	M	40	56	56	2	0
17	A	78	107	105	1	0
17	B	55	86	86	0	0
17	I	40	51	50	3	0
18	A	76	100	98	7	0
18	B	23	20	16	2	0
18	M	49	74	74	3	0
19	B	8	0	0	0	0
19	C	16	0	0	1	0
20	B	1	0	0	0	0
20	L	1	0	0	0	0
21	L	35	46	45	0	0
22	L	66	96	96	2	0
23	A	8	0	0	4	0
23	B	8	0	0	0	0
23	J	1	0	0	0	0
23	L	2	0	0	0	0
23	M	1	0	0	0	0
All	All	24413	24384	24443	928	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 928 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)
9:K:60:LEU:O	9:K:63:THR:N	1.88	1.04
1:A:454:HIS:O	1:A:458:LEU:HD13	1.61	0.98
1:A:661:VAL:HG22	1:A:749:ALA:HB3	1.47	0.97
1:A:661:VAL:HG21	1:A:746:PHE:HA	1.46	0.97
4:D:3:LEU:HD21	4:D:91:THR:HG21	1.52	0.91

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	736/755 (98%)	671 (91%)	65 (9%)	0	100	100
2	B	737/740 (100%)	680 (92%)	56 (8%)	1 (0%)	51	85
3	C	78/80 (98%)	71 (91%)	7 (9%)	0	100	100
4	D	136/138 (99%)	122 (90%)	14 (10%)	0	100	100
5	E	67/75 (89%)	56 (84%)	10 (15%)	1 (2%)	10	42
6	F	139/164 (85%)	121 (87%)	18 (13%)	0	100	100
7	I	36/38 (95%)	30 (83%)	6 (17%)	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%)	136 (91%)	13 (9%)	0	100	100
11	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
12	X	27/35 (77%)	24 (89%)	3 (11%)	0	100	100
All	All	2216/2334 (95%)	2009 (91%)	205 (9%)	2 (0%)	51	85

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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%)	577 (98%)	12 (2%)	55	83
2	B	597/597 (100%)	583 (98%)	14 (2%)	50	80
3	C	67/67 (100%)	64 (96%)	3 (4%)	27	64
4	D	115/115 (100%)	114 (99%)	1 (1%)	78	92
5	E	59/64 (92%)	57 (97%)	2 (3%)	37	72
6	F	109/128 (85%)	108 (99%)	1 (1%)	78	92
7	I	32/32 (100%)	32 (100%)	0	100	100
8	J	36/36 (100%)	36 (100%)	0	100	100
9	K	33/61 (54%)	30 (91%)	3 (9%)	9	34
10	L	117/119 (98%)	116 (99%)	1 (1%)	78	92
11	M	26/26 (100%)	26 (100%)	0	100	100
12	X	23/27 (85%)	20 (87%)	3 (13%)	4	19
All	All	1803/1875 (96%)	1763 (98%)	40 (2%)	52	81

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	18	ARG
9	K	60	LEU
4	D	33	SER
6	F	95	ASN
12	X	12	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	591	ASN
5	E	59	ASN
4	D	78	ASN
6	F	90	ASN
1	A	718	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	825	-	50,67,73	1.67	4 (8%)	47,105,113	1.57	8 (17%)
14	CLA	A	816	-	33,53,73	2.00	5 (15%)	27,89,113	2.27	11 (40%)
14	CLA	B	3036	23	33,53,73	2.14	5 (15%)	27,89,113	1.98	9 (33%)
14	CLA	K	101	-	29,49,73	2.10	4 (13%)	20,83,113	2.25	6 (30%)
16	BCR	B	3047	-	41,41,41	1.15	3 (7%)	56,56,56	1.34	8 (14%)
14	CLA	K	103	-	33,53,73	2.06	5 (15%)	27,89,113	1.99	9 (33%)
14	CLA	A	839	-	56,73,73	1.56	5 (8%)	55,113,113	1.70	11 (20%)
14	CLA	B	3035	-	33,53,73	2.12	5 (15%)	27,89,113	1.91	7 (25%)
14	CLA	L	206	23	56,73,73	1.59	5 (8%)	55,113,113	1.68	9 (16%)
19	SF4	C	102	3	0,12,12	-	-	-	-	-
14	CLA	A	820	-	56,73,73	1.55	5 (8%)	55,113,113	1.73	12 (21%)
16	BCR	L	208	-	41,41,41	1.12	3 (7%)	56,56,56	1.44	12 (21%)
14	CLA	A	808	-	42,59,73	1.93	4 (9%)	38,96,113	1.63	7 (18%)
15	PQN	A	846	-	34,34,34	2.03	7 (20%)	42,45,45	1.29	6 (14%)
14	CLA	A	856	23	56,73,73	1.59	5 (8%)	55,113,113	1.60	9 (16%)
14	CLA	B	3033	-	56,73,73	1.59	5 (8%)	55,113,113	1.64	10 (18%)
14	CLA	B	3007	-	56,73,73	1.59	6 (10%)	55,113,113	1.53	9 (16%)
17	LMG	A	852	-	48,48,55	0.86	2 (4%)	56,56,63	1.27	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	818	-	45,62,73	1.85	6 (13%)	41,99,113	1.70	8 (19%)
16	BCR	F	203	-	41,41,41	1.12	3 (7%)	56,56,56	1.31	7 (12%)
14	CLA	B	3030	-	56,73,73	1.62	7 (12%)	55,113,113	1.71	13 (23%)
16	BCR	L	201	-	41,41,41	1.13	3 (7%)	56,56,56	1.21	5 (8%)
14	CLA	B	3013	-	33,53,73	2.07	6 (18%)	27,89,113	2.06	8 (29%)
16	BCR	L	209	-	41,41,41	1.17	3 (7%)	56,56,56	1.31	7 (12%)
14	CLA	A	813	-	45,62,73	1.78	6 (13%)	41,99,113	1.83	10 (24%)
16	BCR	B	3045	-	41,41,41	1.14	3 (7%)	56,56,56	1.26	6 (10%)
14	CLA	B	3017	-	46,63,73	1.78	4 (8%)	43,101,113	1.71	8 (18%)
14	CLA	B	3023	23	46,63,73	1.74	6 (13%)	43,101,113	1.67	7 (16%)
14	CLA	B	3028	-	56,73,73	1.57	7 (12%)	55,113,113	1.65	7 (12%)
14	CLA	B	3020	23	56,73,73	1.58	6 (10%)	55,113,113	1.68	11 (20%)
17	LMG	I	102	-	40,40,55	1.37	6 (15%)	48,48,63	1.23	4 (8%)
14	CLA	A	810	1	56,73,73	1.62	5 (8%)	55,113,113	1.48	8 (14%)
18	LHG	A	853	-	48,48,48	0.69	2 (4%)	51,54,54	1.23	6 (11%)
14	CLA	B	3041	23	56,73,73	1.78	7 (12%)	55,113,113	1.42	5 (9%)
14	CLA	B	3022	-	33,53,73	2.05	5 (15%)	27,89,113	2.08	9 (33%)
16	BCR	A	850	-	41,41,41	1.07	3 (7%)	56,56,56	1.20	4 (7%)
14	CLA	A	806	-	56,73,73	1.55	6 (10%)	55,113,113	1.69	9 (16%)
16	BCR	M	103	-	41,41,41	1.16	3 (7%)	56,56,56	1.14	2 (3%)
14	CLA	A	827	23	56,73,73	1.63	6 (10%)	55,113,113	1.55	9 (16%)
14	CLA	A	830	-	56,73,73	1.59	5 (8%)	55,113,113	1.59	9 (16%)
14	CLA	B	3027	-	56,73,73	1.63	6 (10%)	55,113,113	1.51	8 (14%)
16	BCR	B	3044	-	41,41,41	1.10	3 (7%)	56,56,56	1.21	6 (10%)
16	BCR	B	3051	-	41,41,41	1.16	3 (7%)	56,56,56	1.18	3 (5%)
14	CLA	A	812	14	56,73,73	1.62	8 (14%)	55,113,113	1.56	9 (16%)
14	CLA	A	824	-	42,59,73	1.81	5 (11%)	38,96,113	1.88	9 (23%)
14	CLA	B	3034	-	49,66,73	1.67	4 (8%)	46,104,113	1.69	12 (26%)
14	CLA	B	3038	-	51,68,73	1.65	6 (11%)	49,107,113	1.66	9 (18%)
14	CLA	B	3008	-	56,73,73	1.65	7 (12%)	55,113,113	1.62	9 (16%)
16	BCR	J	105	-	41,41,41	1.12	3 (7%)	56,56,56	1.35	9 (16%)
14	CLA	J	102	-	28,45,73	2.23	5 (17%)	19,78,113	2.03	6 (31%)
14	CLA	A	811	-	33,53,73	2.00	5 (15%)	27,89,113	2.04	9 (33%)
14	CLA	A	822	23	56,73,73	1.54	4 (7%)	55,113,113	1.55	11 (20%)
14	CLA	B	3004	-	56,73,73	1.58	7 (12%)	55,113,113	1.62	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	3015	-	56,73,73	1.64	5 (8%)	55,113,113	1.37	9 (16%)
14	CLA	A	817	23	40,57,73	1.92	5 (12%)	34,93,113	1.87	7 (20%)
14	CLA	B	3032	-	40,57,73	1.84	5 (12%)	34,93,113	1.97	10 (29%)
14	CLA	A	814	-	51,68,73	1.74	5 (9%)	49,107,113	1.50	9 (18%)
15	PQN	B	3043	-	34,34,34	2.15	7 (20%)	42,45,45	1.22	5 (11%)
14	CLA	A	844	23	56,73,73	1.63	5 (8%)	55,113,113	1.70	9 (16%)
14	CLA	A	835	-	56,73,73	1.60	5 (8%)	55,113,113	1.66	10 (18%)
14	CLA	B	3031	-	33,53,73	2.14	5 (15%)	27,89,113	2.06	6 (22%)
22	DGD	L	207	-	67,67,67	1.04	3 (4%)	81,81,81	1.18	8 (9%)
17	LMG	A	855	-	30,30,55	1.40	4 (13%)	37,37,63	1.32	4 (10%)
18	LHG	B	3050	-	22,22,48	1.57	5 (22%)	25,28,54	1.24	3 (12%)
14	CLA	B	3010	2	56,73,73	1.64	8 (14%)	55,113,113	1.79	12 (21%)
14	CLA	B	3042	-	56,73,73	1.62	6 (10%)	55,113,113	1.71	7 (12%)
18	LHG	A	854	14	26,26,48	0.97	1 (3%)	29,32,54	1.32	3 (10%)
16	BCR	J	104	-	41,41,41	1.18	3 (7%)	56,56,56	1.30	6 (10%)
14	CLA	B	3006	-	56,73,73	1.61	6 (10%)	55,113,113	1.56	9 (16%)
16	BCR	F	201	-	41,41,41	1.14	3 (7%)	56,56,56	1.26	6 (10%)
16	BCR	A	847	-	41,41,41	1.17	3 (7%)	56,56,56	1.25	6 (10%)
14	CLA	A	837	1	33,53,73	2.04	6 (18%)	27,89,113	2.11	8 (29%)
16	BCR	J	103	-	41,41,41	1.10	3 (7%)	56,56,56	1.20	2 (3%)
14	CLA	B	3019	-	51,68,73	1.66	4 (7%)	49,107,113	1.72	12 (24%)
14	CLA	A	843	-	56,73,73	1.66	5 (8%)	55,113,113	1.65	9 (16%)
14	CLA	B	3018	-	50,67,73	1.66	5 (10%)	47,105,113	1.81	9 (19%)
14	CLA	A	841	-	56,73,73	1.58	5 (8%)	55,113,113	1.63	12 (21%)
16	BCR	K	102	-	41,41,41	1.10	3 (7%)	56,56,56	1.36	8 (14%)
14	CLA	A	828	-	56,73,73	1.68	7 (12%)	55,113,113	1.50	7 (12%)
18	LHG	M	101	-	48,48,48	0.71	1 (2%)	51,54,54	1.20	3 (5%)
14	CLA	B	3037	23	33,53,73	2.13	6 (18%)	27,89,113	2.00	7 (25%)
14	CLA	A	815	-	33,53,73	2.09	5 (15%)	27,89,113	1.90	6 (22%)
14	CLA	B	3029	-	56,73,73	1.62	4 (7%)	55,113,113	1.57	10 (18%)
14	CLA	B	3014	-	56,73,73	1.64	5 (8%)	55,113,113	1.54	9 (16%)
14	CLA	A	807	-	56,73,73	1.64	4 (7%)	55,113,113	1.43	10 (18%)
16	BCR	A	848	-	41,41,41	1.14	3 (7%)	56,56,56	1.22	6 (10%)
14	CLA	B	3003	-	56,73,73	1.63	7 (12%)	55,113,113	1.61	7 (12%)
14	CLA	A	802	23	56,73,73	1.62	6 (10%)	55,113,113	1.61	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CL0	A	801	-	59,73,73	1.48	5 (8%)	67,113,113	1.40	10 (14%)
14	CLA	A	803	-	56,73,73	1.62	6 (10%)	55,113,113	1.69	10 (18%)
14	CLA	A	831	-	56,73,73	1.58	6 (10%)	55,113,113	1.59	11 (20%)
14	CLA	X	1701	12	33,53,73	2.08	6 (18%)	27,89,113	2.02	8 (29%)
14	CLA	B	3021	-	38,55,73	1.96	6 (15%)	33,91,113	1.88	8 (24%)
14	CLA	A	805	14	50,67,73	1.74	5 (10%)	47,105,113	1.54	5 (10%)
14	CLA	A	829	-	56,73,73	1.57	6 (10%)	55,113,113	1.55	9 (16%)
19	SF4	C	101	3	0,12,12	-	-	-	-	-
14	CLA	B	3012	-	33,53,73	2.04	5 (15%)	27,89,113	2.26	9 (33%)
14	CLA	B	3040	-	38,55,73	1.95	4 (10%)	33,91,113	2.02	10 (30%)
14	CLA	L	204	10	56,73,73	1.56	7 (12%)	55,113,113	1.82	13 (23%)
14	CLA	A	838	-	42,59,73	1.86	6 (14%)	38,96,113	1.89	10 (26%)
14	CLA	A	821	-	33,50,73	2.01	4 (12%)	26,84,113	2.28	10 (38%)
14	CLA	B	3016	-	33,53,73	2.03	5 (15%)	27,89,113	1.92	6 (22%)
21	LMT	L	202	-	36,36,36	1.15	5 (13%)	47,47,47	1.36	7 (14%)
14	CLA	A	836	-	45,62,73	1.80	6 (13%)	41,99,113	1.78	9 (21%)
14	CLA	A	845	18	43,60,73	1.77	5 (11%)	39,97,113	1.87	12 (30%)
16	BCR	B	3046	-	41,41,41	1.13	3 (7%)	56,56,56	1.26	7 (12%)
14	CLA	B	3005	-	45,62,73	1.77	6 (13%)	41,99,113	1.87	9 (21%)
14	CLA	J	101	8	33,53,73	2.07	4 (12%)	27,89,113	1.96	9 (33%)
16	BCR	A	849	-	41,41,41	1.14	3 (7%)	56,56,56	1.32	7 (12%)
14	CLA	B	3009	-	56,73,73	1.60	6 (10%)	55,113,113	1.59	10 (18%)
16	BCR	B	3048	-	41,41,41	1.10	3 (7%)	56,56,56	1.18	4 (7%)
14	CLA	B	3024	-	33,53,73	2.11	4 (12%)	27,89,113	1.88	7 (25%)
14	CLA	F	202	23	33,53,73	2.10	4 (12%)	27,89,113	2.06	9 (33%)
14	CLA	L	205	-	56,73,73	1.56	5 (8%)	55,113,113	1.60	10 (18%)
17	LMG	B	3049	-	55,55,55	0.81	1 (1%)	63,63,63	1.36	4 (6%)
16	BCR	A	851	-	41,41,41	1.16	3 (7%)	56,56,56	1.40	8 (14%)
14	CLA	A	833	-	56,73,73	1.55	7 (12%)	55,113,113	1.59	10 (18%)
14	CLA	B	3025	2	45,62,73	1.77	4 (8%)	41,99,113	1.91	13 (31%)
16	BCR	I	101	-	41,41,41	1.03	2 (4%)	56,56,56	1.26	7 (12%)
14	CLA	M	102	23	33,53,73	2.15	6 (18%)	27,89,113	1.98	12 (44%)
14	CLA	A	823	-	40,57,73	1.88	5 (12%)	34,93,113	1.97	10 (29%)
14	CLA	A	809	1	56,73,73	1.62	6 (10%)	55,113,113	1.55	7 (12%)
14	CLA	A	832	-	41,58,73	1.82	6 (14%)	37,95,113	1.87	10 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	804	-	56,73,73	1.62	6 (10%)	55,113,113	1.44	6 (10%)
14	CLA	A	826	-	56,73,73	1.59	5 (8%)	55,113,113	1.55	11 (20%)
14	CLA	B	3011	2	56,73,73	1.58	4 (7%)	55,113,113	1.53	11 (20%)
14	CLA	B	3026	23	37,54,73	1.97	7 (18%)	32,90,113	1.96	8 (25%)
14	CLA	A	842	23	42,59,73	1.76	7 (16%)	38,96,113	2.00	10 (26%)
14	CLA	B	3039	-	56,73,73	1.65	6 (10%)	55,113,113	1.56	9 (16%)
14	CLA	A	834	-	56,73,73	1.66	7 (12%)	55,113,113	1.56	8 (14%)
14	CLA	A	819	-	45,62,73	1.75	7 (15%)	41,99,113	1.90	10 (24%)
14	CLA	A	840	-	38,55,73	2.04	6 (15%)	33,91,113	1.99	10 (30%)
19	SF4	B	3001	1,2	0,12,12	-	-	-	-	-

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	A	825	-	1/1/18/20	13/30/108/115	-
14	CLA	A	816	-	1/1/15/20	4/11/91/115	-
14	CLA	B	3036	23	1/1/15/20	4/11/91/115	-
14	CLA	K	101	-	1/1/13/20	2/5/81/115	-
16	BCR	B	3047	-	-	15/29/63/63	0/2/2/2
14	CLA	K	103	-	1/1/15/20	5/11/91/115	-
14	CLA	A	839	-	1/1/20/20	9/37/115/115	-
14	CLA	B	3035	-	1/1/15/20	4/11/91/115	-
14	CLA	L	206	23	1/1/20/20	7/37/115/115	-
19	SF4	C	102	3	-	-	0/6/5/5
14	CLA	A	820	-	1/1/20/20	20/37/115/115	-
16	BCR	L	208	-	-	15/29/63/63	0/2/2/2
14	CLA	A	808	-	1/1/17/20	10/21/99/115	-
15	PQN	A	846	-	-	10/23/43/43	0/2/2/2
14	CLA	A	856	23	1/1/20/20	16/37/115/115	-
14	CLA	B	3033	-	1/1/20/20	18/37/115/115	-
14	CLA	B	3007	-	1/1/20/20	10/37/115/115	-
17	LMG	A	852	-	-	27/43/63/70	0/1/1/1
14	CLA	A	818	-	1/1/17/20	5/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	F	203	-	-	11/29/63/63	0/2/2/2
14	CLA	B	3030	-	1/1/20/20	15/37/115/115	-
16	BCR	L	201	-	-	8/29/63/63	0/2/2/2
14	CLA	B	3013	-	1/1/15/20	3/11/91/115	-
16	BCR	L	209	-	-	10/29/63/63	0/2/2/2
14	CLA	A	813	-	1/1/17/20	7/24/102/115	-
16	BCR	B	3045	-	-	11/29/63/63	0/2/2/2
14	CLA	B	3017	-	1/1/18/20	4/25/103/115	-
14	CLA	B	3023	23	1/1/18/20	9/25/103/115	-
14	CLA	B	3028	-	1/1/20/20	13/37/115/115	-
14	CLA	B	3020	23	1/1/20/20	14/37/115/115	-
17	LMG	I	102	-	-	11/35/55/70	0/1/1/1
14	CLA	A	810	1	1/1/20/20	10/37/115/115	-
18	LHG	A	853	-	-	27/53/53/53	-
14	CLA	B	3041	23	1/1/20/20	11/37/115/115	-
14	CLA	B	3022	-	1/1/15/20	8/11/91/115	-
16	BCR	A	850	-	-	11/29/63/63	0/2/2/2
14	CLA	A	806	-	1/1/20/20	21/37/115/115	-
16	BCR	M	103	-	-	7/29/63/63	0/2/2/2
14	CLA	A	827	23	1/1/20/20	10/37/115/115	-
14	CLA	A	830	-	1/1/20/20	15/37/115/115	-
14	CLA	B	3027	-	1/1/20/20	16/37/115/115	-
16	BCR	B	3044	-	-	8/29/63/63	0/2/2/2
16	BCR	B	3051	-	-	12/29/63/63	0/2/2/2
14	CLA	A	812	14	1/1/20/20	11/37/115/115	-
14	CLA	A	824	-	1/1/17/20	6/21/99/115	-
14	CLA	B	3034	-	1/1/18/20	11/29/107/115	-
14	CLA	B	3038	-	-	6/31/109/115	-
14	CLA	B	3008	-	1/1/20/20	5/37/115/115	-
16	BCR	J	105	-	-	12/29/63/63	0/2/2/2
14	CLA	J	102	-	1/1/12/20	0/2/76/115	-
14	CLA	A	811	-	1/1/15/20	9/11/91/115	-
14	CLA	A	822	23	1/1/20/20	15/37/115/115	-
14	CLA	B	3004	-	1/1/20/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	3015	-	1/1/20/20	13/37/115/115	-
14	CLA	A	817	23	1/1/16/20	8/18/96/115	-
14	CLA	B	3032	-	1/1/16/20	9/18/96/115	-
14	CLA	A	814	-	1/1/19/20	6/31/109/115	-
15	PQN	B	3043	-	-	8/23/43/43	0/2/2/2
14	CLA	A	844	23	1/1/20/20	13/37/115/115	-
14	CLA	A	835	-	1/1/20/20	14/37/115/115	-
14	CLA	B	3031	-	1/1/15/20	4/11/91/115	-
22	DGD	L	207	-	-	22/55/95/95	0/2/2/2
17	LMG	A	855	-	-	15/23/43/70	0/1/1/1
18	LHG	B	3050	-	-	11/26/26/53	-
14	CLA	B	3010	2	1/1/20/20	11/37/115/115	-
14	CLA	B	3042	-	1/1/20/20	7/37/115/115	-
18	LHG	A	854	14	-	14/31/31/53	-
16	BCR	J	104	-	-	15/29/63/63	0/2/2/2
14	CLA	B	3006	-	1/1/20/20	16/37/115/115	-
16	BCR	F	201	-	-	7/29/63/63	0/2/2/2
16	BCR	A	847	-	-	16/29/63/63	0/2/2/2
14	CLA	A	837	1	1/1/15/20	7/11/91/115	-
16	BCR	J	103	-	-	14/29/63/63	0/2/2/2
14	CLA	B	3019	-	1/1/19/20	11/31/109/115	-
14	CLA	A	843	-	1/1/20/20	7/37/115/115	-
14	CLA	B	3018	-	1/1/18/20	11/30/108/115	-
14	CLA	A	841	-	1/1/20/20	6/37/115/115	-
16	BCR	K	102	-	-	12/29/63/63	0/2/2/2
14	CLA	A	828	-	1/1/20/20	8/37/115/115	-
18	LHG	M	101	-	-	26/53/53/53	-
14	CLA	B	3037	23	1/1/15/20	2/11/91/115	-
14	CLA	A	815	-	1/1/15/20	0/11/91/115	-
14	CLA	B	3029	-	1/1/20/20	21/37/115/115	-
14	CLA	B	3014	-	1/1/20/20	12/37/115/115	-
14	CLA	A	807	-	1/1/20/20	15/37/115/115	-
16	BCR	A	848	-	-	7/29/63/63	0/2/2/2
14	CLA	B	3003	-	1/1/20/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	802	23	1/1/20/20	10/37/115/115	-
13	CL0	A	801	-	3/3/25/25	11/37/135/135	-
14	CLA	A	803	-	1/1/20/20	8/37/115/115	-
14	CLA	A	831	-	1/1/20/20	10/37/115/115	-
14	CLA	X	1701	12	1/1/15/20	1/11/91/115	-
14	CLA	B	3021	-	1/1/15/20	13/16/94/115	-
14	CLA	A	805	14	1/1/18/20	5/30/108/115	-
14	CLA	A	829	-	1/1/20/20	13/37/115/115	-
19	SF4	C	101	3	-	-	0/6/5/5
14	CLA	B	3012	-	1/1/15/20	5/11/91/115	-
14	CLA	B	3040	-	-	5/16/94/115	-
14	CLA	L	204	10	1/1/20/20	11/37/115/115	-
14	CLA	A	838	-	1/1/17/20	5/21/99/115	-
14	CLA	A	821	-	1/1/14/20	4/8/86/115	-
14	CLA	B	3016	-	1/1/15/20	7/11/91/115	-
21	LMT	L	202	-	-	12/21/61/61	0/2/2/2
14	CLA	A	836	-	1/1/17/20	11/24/102/115	-
14	CLA	A	845	18	1/1/17/20	9/22/100/115	-
16	BCR	B	3046	-	-	11/29/63/63	0/2/2/2
14	CLA	B	3005	-	1/1/17/20	8/24/102/115	-
14	CLA	J	101	8	1/1/15/20	4/11/91/115	-
16	BCR	A	849	-	-	12/29/63/63	0/2/2/2
14	CLA	B	3009	-	1/1/20/20	11/37/115/115	-
16	BCR	B	3048	-	-	4/29/63/63	0/2/2/2
14	CLA	B	3024	-	1/1/15/20	4/11/91/115	-
14	CLA	F	202	23	1/1/15/20	2/11/91/115	-
14	CLA	L	205	-	1/1/20/20	3/37/115/115	-
17	LMG	B	3049	-	-	23/50/70/70	0/1/1/1
16	BCR	A	851	-	-	17/29/63/63	0/2/2/2
14	CLA	A	833	-	1/1/20/20	9/37/115/115	-
14	CLA	B	3025	2	-	7/24/102/115	-
16	BCR	I	101	-	-	4/29/63/63	0/2/2/2
14	CLA	M	102	23	1/1/15/20	5/11/91/115	-
14	CLA	A	823	-	1/1/16/20	12/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	809	1	1/1/20/20	19/37/115/115	-
14	CLA	A	832	-	1/1/17/20	6/19/97/115	-
14	CLA	A	804	-	1/1/20/20	8/37/115/115	-
14	CLA	A	826	-	1/1/20/20	15/37/115/115	-
14	CLA	B	3011	2	1/1/20/20	17/37/115/115	-
14	CLA	B	3026	23	1/1/15/20	2/15/93/115	-
14	CLA	A	842	23	1/1/17/20	7/21/99/115	-
14	CLA	B	3039	-	1/1/20/20	9/37/115/115	-
14	CLA	A	834	-	1/1/20/20	8/37/115/115	-
14	CLA	A	819	-	1/1/17/20	6/24/102/115	-
14	CLA	A	840	-	1/1/15/20	5/16/94/115	-
19	SF4	B	3001	1,2	-	-	0/6/5/5

The worst 5 of 635 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	3041	CLA	C4B-NB	8.54	1.42	1.35
14	B	3037	CLA	C4B-NB	8.31	1.42	1.35
14	A	828	CLA	C4B-NB	8.31	1.42	1.35
14	A	843	CLA	C4B-NB	8.28	1.42	1.35
14	A	817	CLA	C4B-NB	8.25	1.42	1.35

The worst 5 of 1062 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	842	CLA	C4A-NA-C1A	8.06	110.33	106.71
14	A	806	CLA	C4A-NA-C1A	7.97	110.29	106.71
14	B	3042	CLA	C4A-NA-C1A	7.78	110.20	106.71
14	B	3033	CLA	C4A-NA-C1A	7.66	110.15	106.71
14	A	803	CLA	C4A-NA-C1A	7.63	110.14	106.71

5 of 95 chirality outliers are listed below:

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

5 of 1307 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	801	CL0	C1A-C2A-CAA-CBA
13	A	801	CL0	C3A-C2A-CAA-CBA
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.

124 monomers are involved in 376 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	825	CLA	3	0
14	B	3036	CLA	1	0
14	K	101	CLA	4	0
16	B	3047	BCR	3	0
14	K	103	CLA	1	0
14	A	839	CLA	3	0
14	B	3035	CLA	3	0
14	L	206	CLA	1	0
14	A	820	CLA	6	0
16	L	208	BCR	2	0
14	A	808	CLA	4	0
15	A	846	PQN	9	0
14	A	856	CLA	7	0
14	B	3033	CLA	4	0
14	B	3007	CLA	3	0
14	A	818	CLA	5	0
16	F	203	BCR	4	0
14	B	3030	CLA	3	0
16	L	201	BCR	3	0
14	B	3013	CLA	4	0
16	L	209	BCR	2	0
14	A	813	CLA	9	0
16	B	3045	BCR	8	0
14	B	3017	CLA	4	0
14	B	3023	CLA	2	0
14	B	3028	CLA	4	0
14	B	3020	CLA	2	0
17	I	102	LMG	3	0
14	A	810	CLA	3	0
18	A	853	LHG	3	0
14	B	3041	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	3022	CLA	2	0
16	A	850	BCR	4	0
14	A	806	CLA	3	0
16	M	103	BCR	2	0
14	A	827	CLA	2	0
14	A	830	CLA	5	0
14	B	3027	CLA	1	0
16	B	3044	BCR	1	0
16	B	3051	BCR	4	0
14	A	812	CLA	5	0
14	A	824	CLA	1	0
14	B	3034	CLA	5	0
14	B	3038	CLA	4	0
14	B	3008	CLA	3	0
16	J	105	BCR	11	0
14	J	102	CLA	1	0
14	A	811	CLA	7	0
14	A	822	CLA	4	0
14	B	3004	CLA	4	0
14	B	3015	CLA	1	0
14	A	817	CLA	3	0
14	B	3032	CLA	2	0
14	A	814	CLA	2	0
15	B	3043	PQN	2	0
14	A	844	CLA	4	0
14	A	835	CLA	4	0
14	B	3031	CLA	3	0
22	L	207	DGD	2	0
17	A	855	LMG	1	0
18	B	3050	LHG	2	0
14	B	3010	CLA	8	0
14	B	3042	CLA	1	0
18	A	854	LHG	4	0
16	J	104	BCR	6	0
14	B	3006	CLA	2	0
16	F	201	BCR	4	0
16	A	847	BCR	7	0
16	J	103	BCR	3	0
14	B	3019	CLA	3	0
14	A	843	CLA	5	0
14	B	3018	CLA	7	0
14	A	841	CLA	6	0

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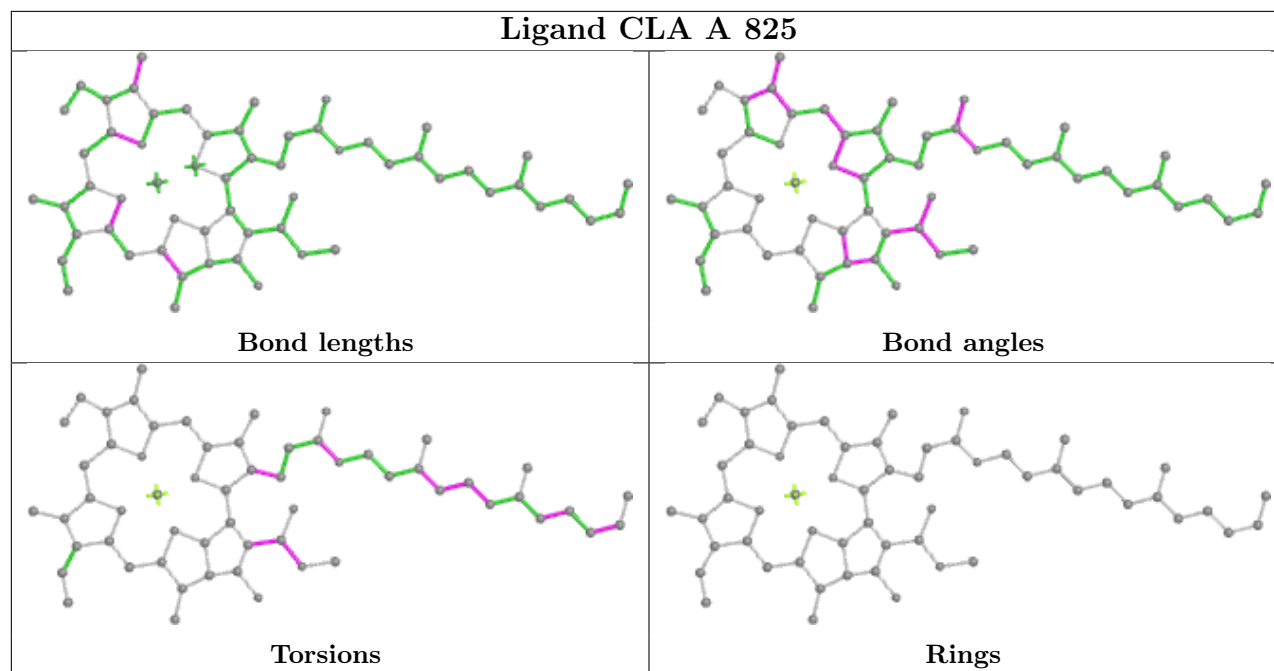
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	K	102	BCR	5	0
14	A	828	CLA	5	0
18	M	101	LHG	3	0
14	B	3037	CLA	2	0
14	A	815	CLA	4	0
14	B	3029	CLA	1	0
14	B	3014	CLA	7	0
14	A	807	CLA	1	0
14	B	3003	CLA	4	0
14	A	802	CLA	3	0
13	A	801	CL0	3	0
14	A	803	CLA	3	0
14	A	831	CLA	6	0
14	X	1701	CLA	3	0
14	B	3021	CLA	2	0
14	A	805	CLA	2	0
14	A	829	CLA	9	0
19	C	101	SF4	1	0
14	B	3012	CLA	2	0
14	B	3040	CLA	3	0
14	L	204	CLA	2	0
14	A	838	CLA	2	0
14	A	821	CLA	3	0
14	B	3016	CLA	1	0
14	A	836	CLA	3	0
14	A	845	CLA	6	0
16	B	3046	BCR	3	0
14	B	3005	CLA	2	0
14	J	101	CLA	3	0
16	A	849	BCR	2	0
14	B	3009	CLA	1	0
14	B	3024	CLA	5	0
14	F	202	CLA	8	0
14	L	205	CLA	3	0
16	A	851	BCR	8	0
14	A	833	CLA	4	0
14	B	3025	CLA	4	0
16	I	101	BCR	4	0
14	M	102	CLA	4	0
14	A	823	CLA	2	0
14	A	809	CLA	6	0
14	A	832	CLA	8	0

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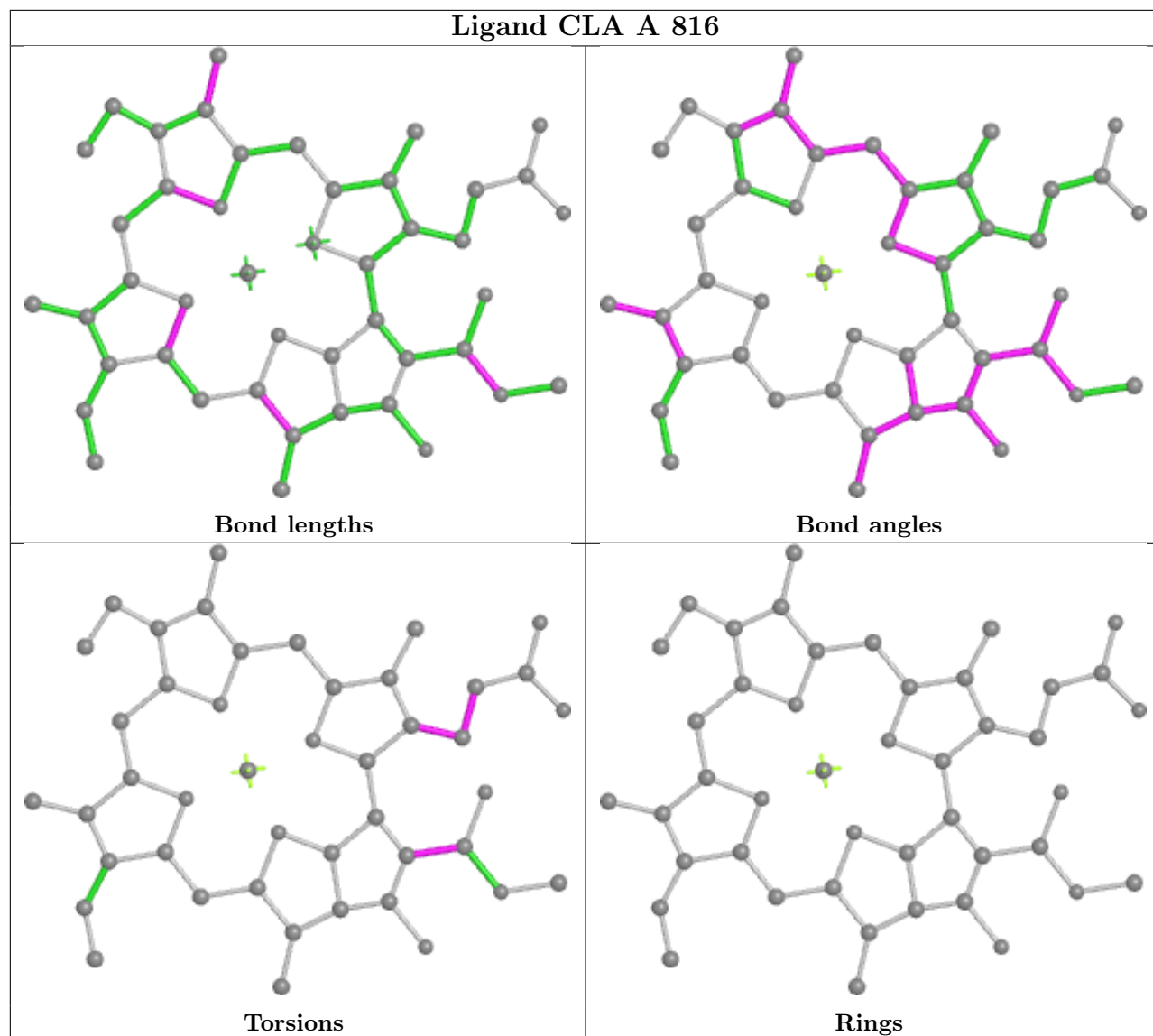
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	804	CLA	10	0
14	A	826	CLA	8	0
14	B	3011	CLA	2	0
14	B	3026	CLA	5	0
14	A	842	CLA	4	0
14	B	3039	CLA	3	0
14	A	834	CLA	2	0
14	A	819	CLA	7	0
14	A	840	CLA	2	0

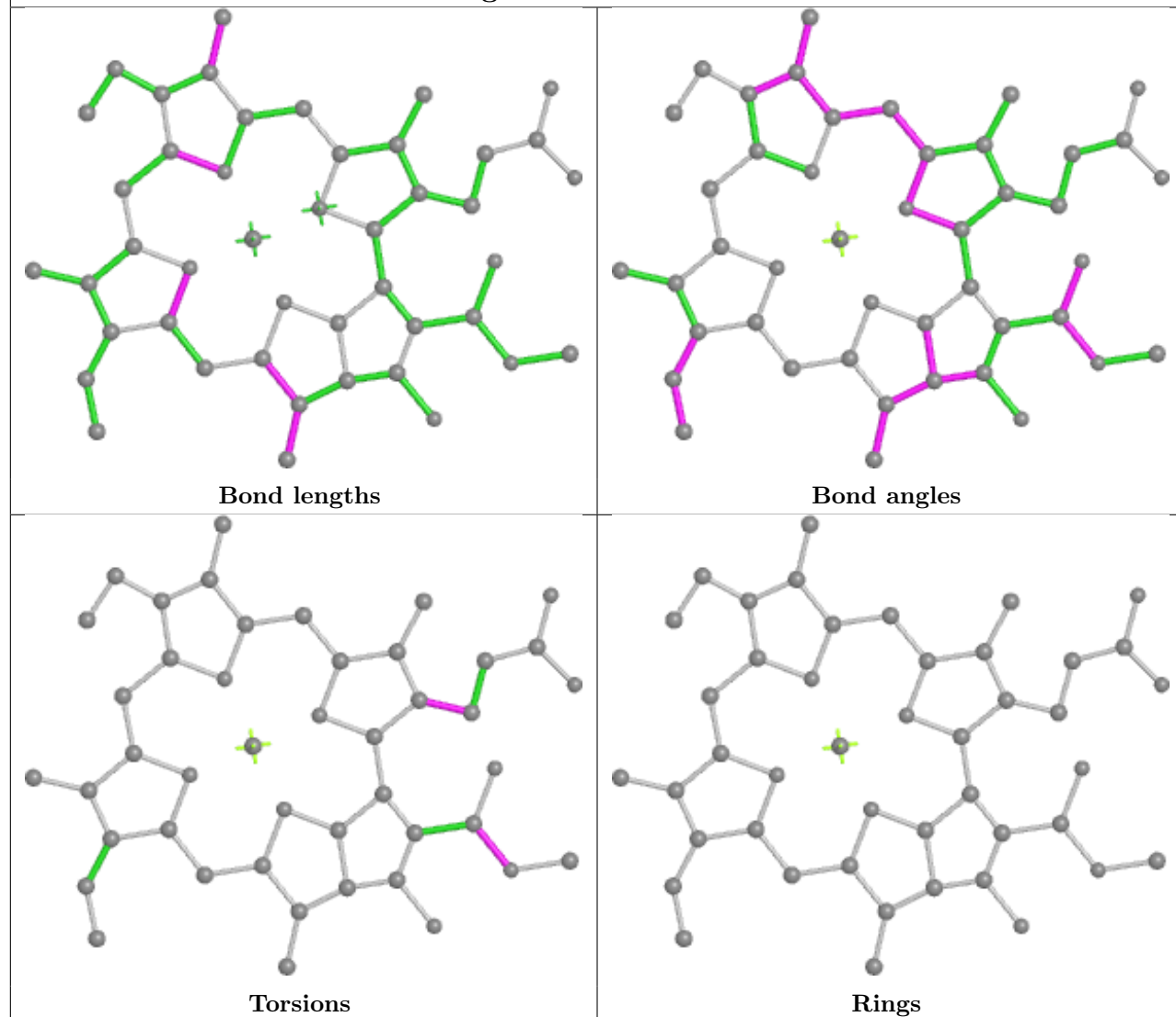
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



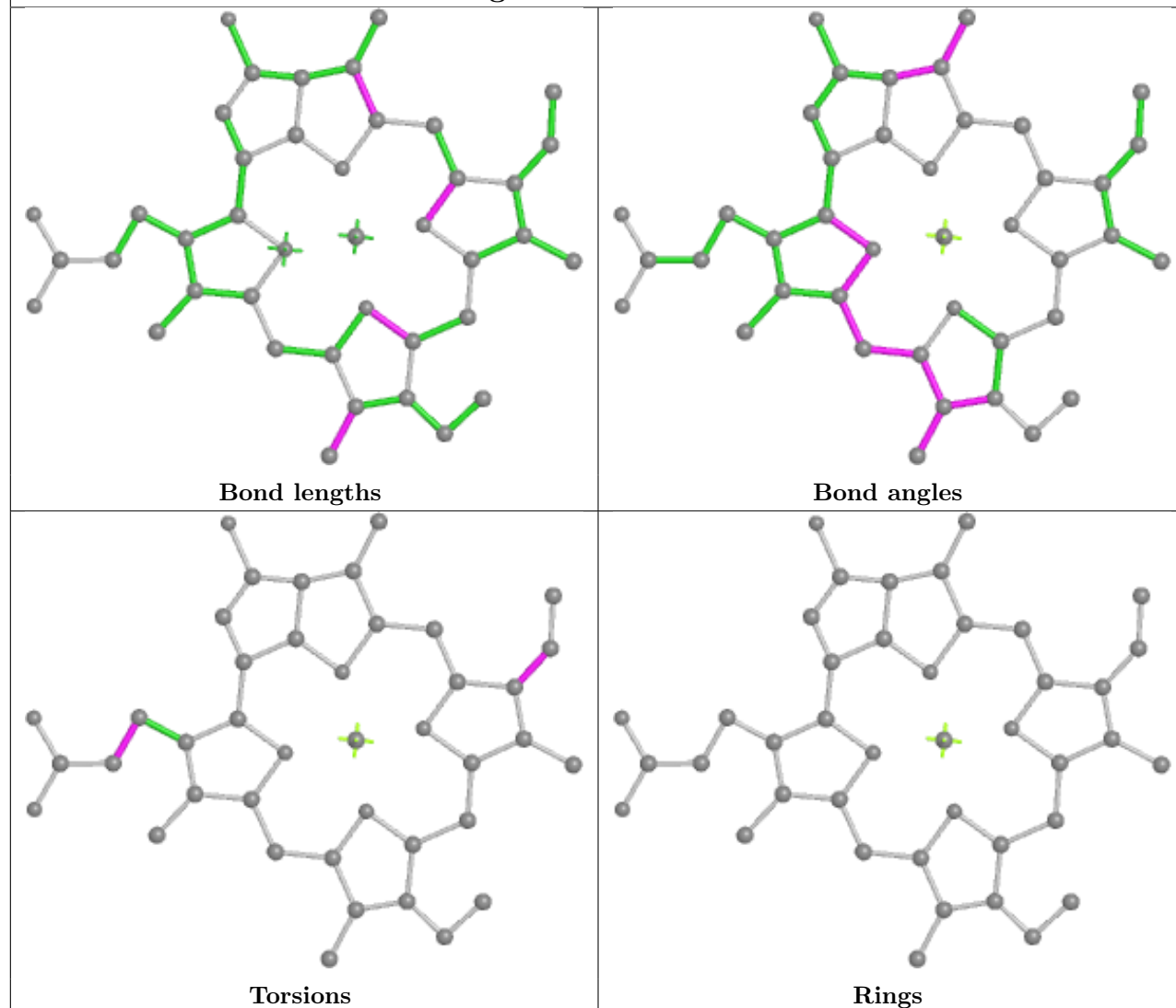
Ligand CLA A 816



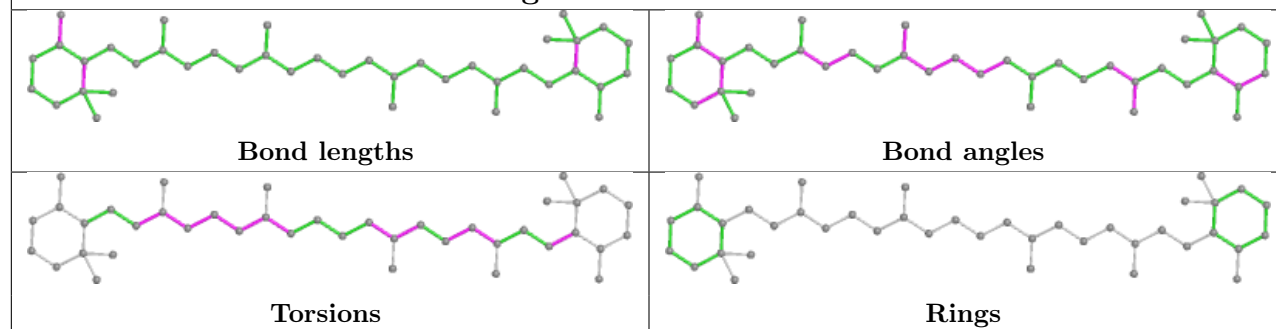
Ligand CLA B 3036



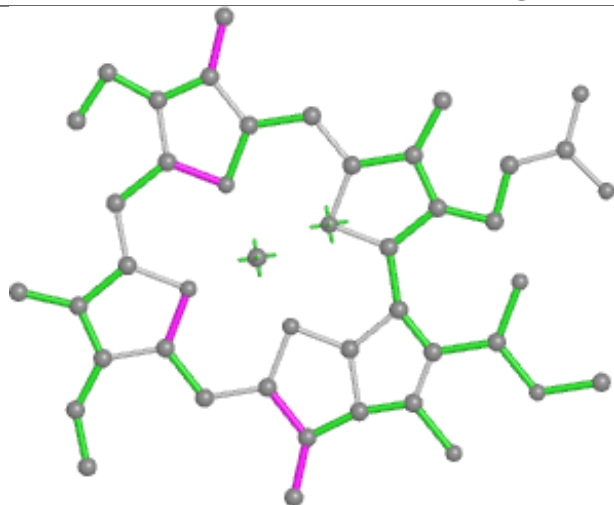
Ligand CLA K 101



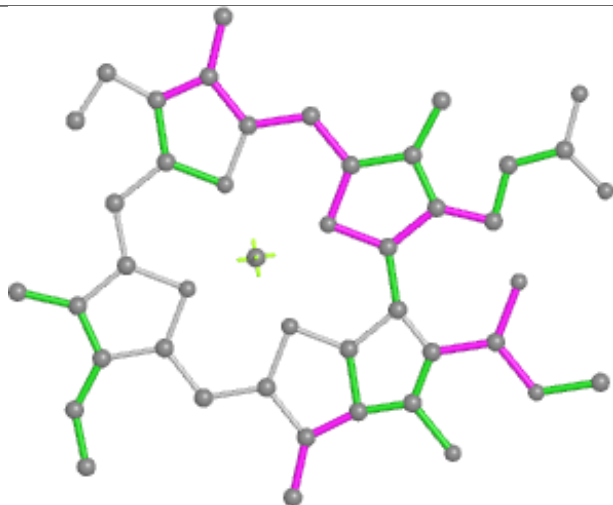
Ligand BCR B 3047



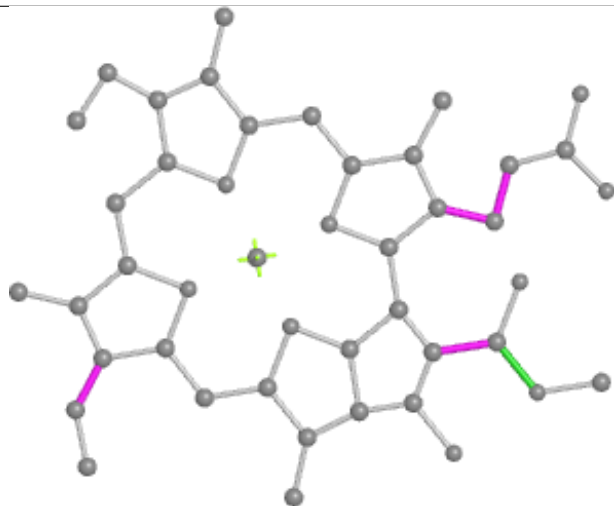
Ligand CLA K 103



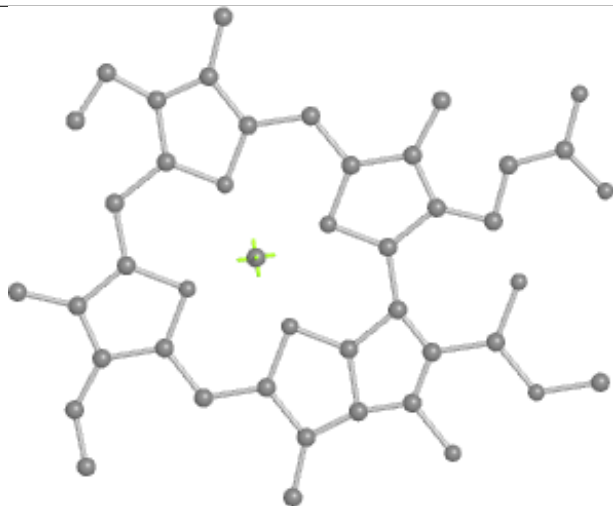
Bond lengths



Bond angles

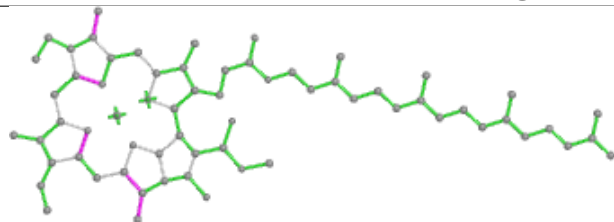


Torsions

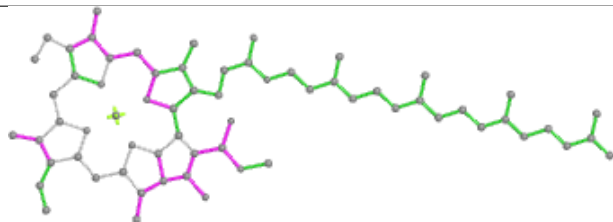


Rings

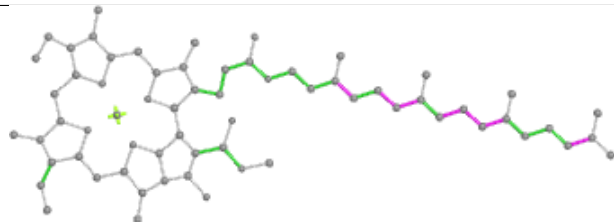
Ligand CLA A 839



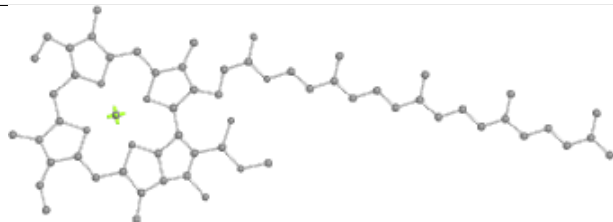
Bond lengths



Bond angles

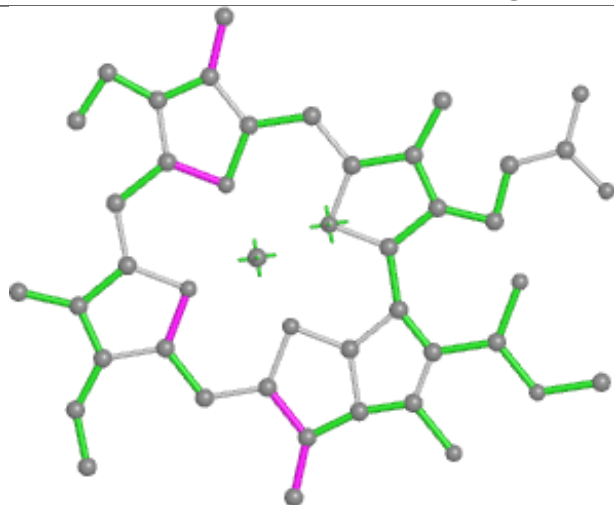


Torsions

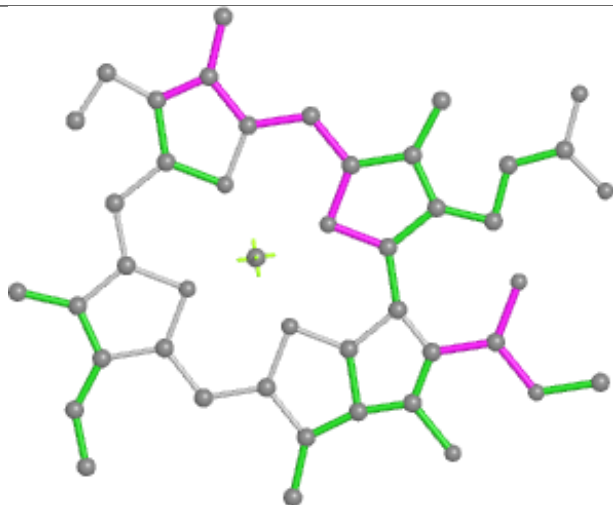


Rings

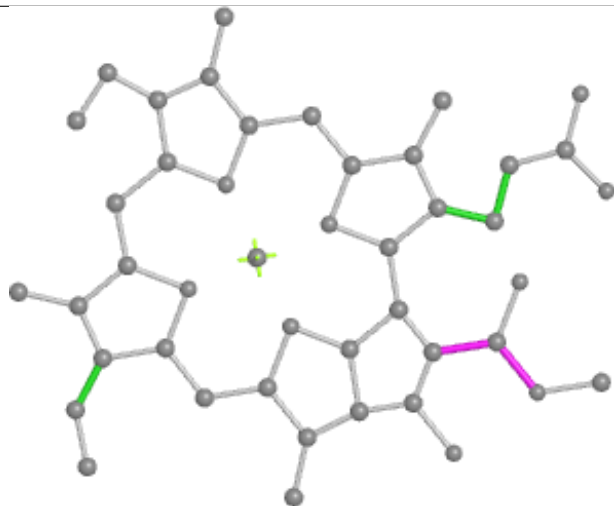
Ligand CLA B 3035



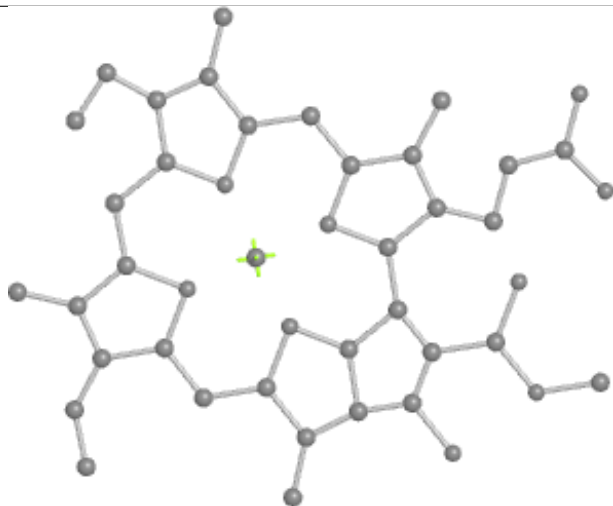
Bond lengths



Bond angles

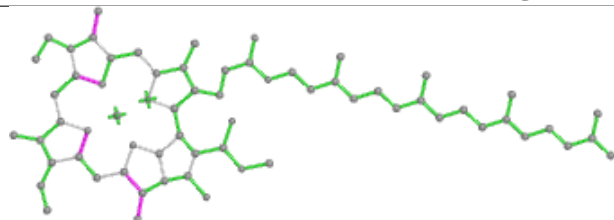


Torsions

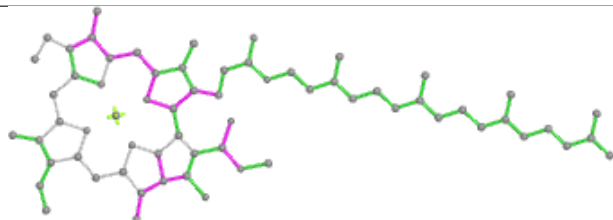


Rings

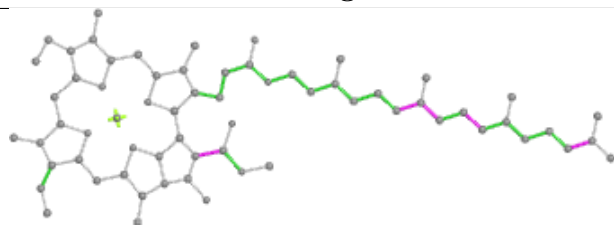
Ligand CLA L 206



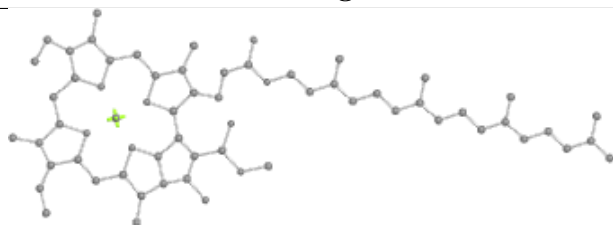
Bond lengths



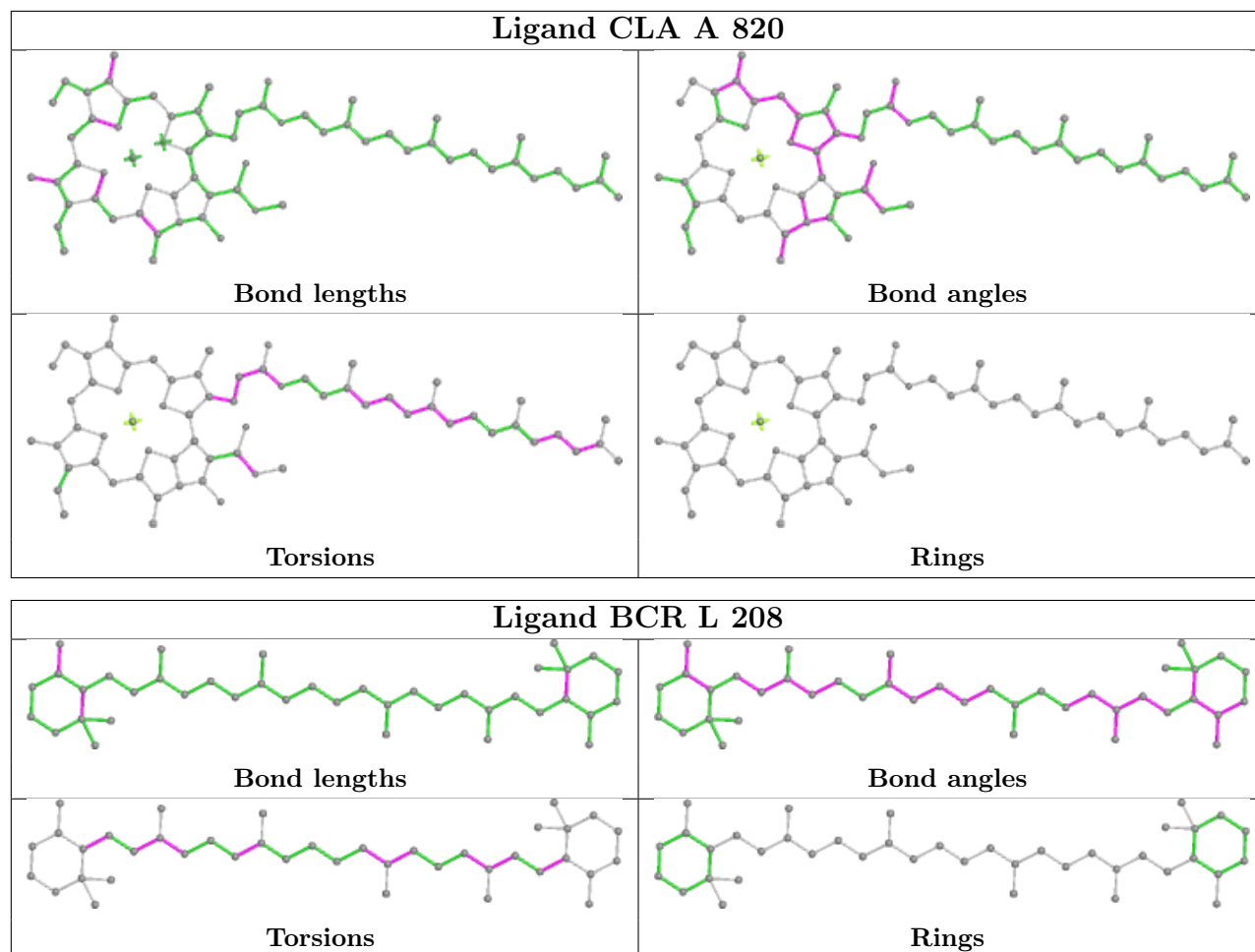
Bond angles



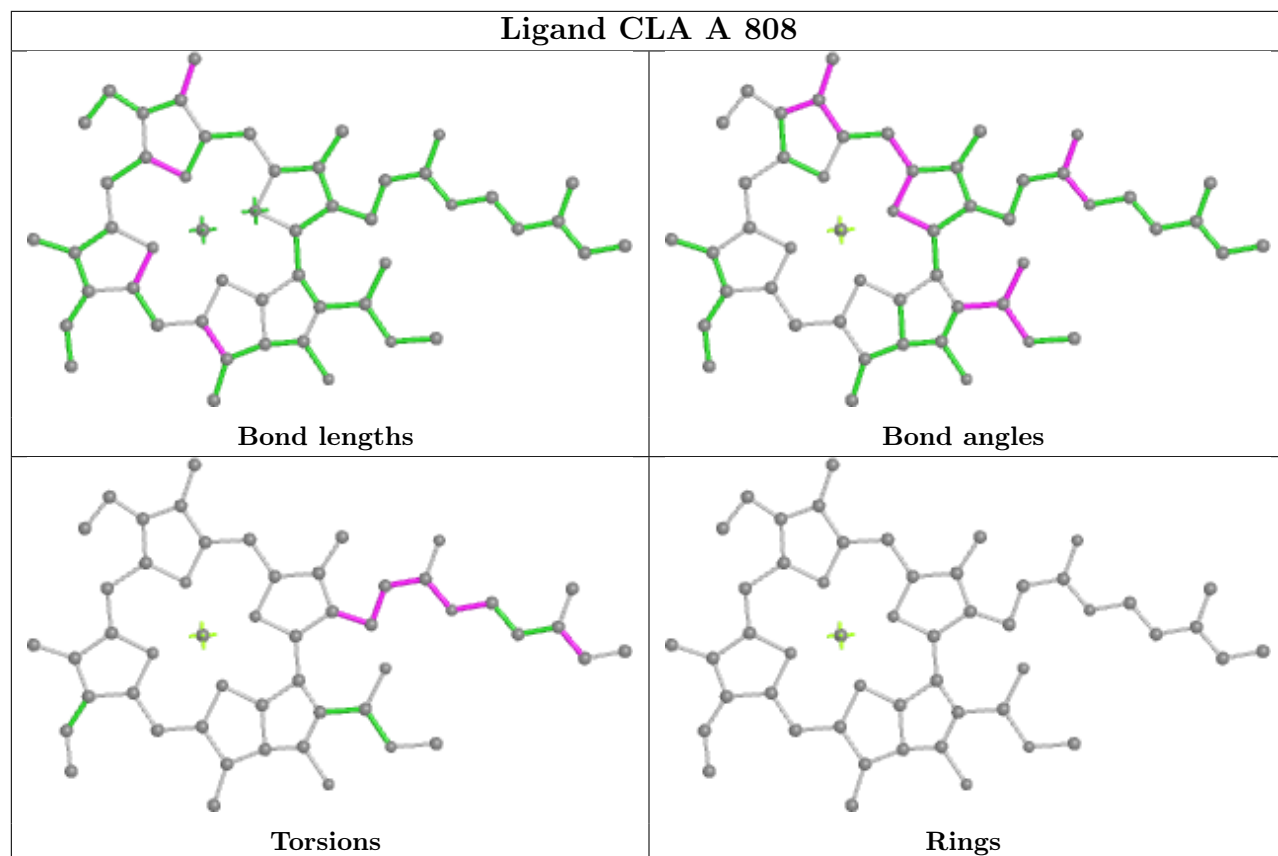
Torsions



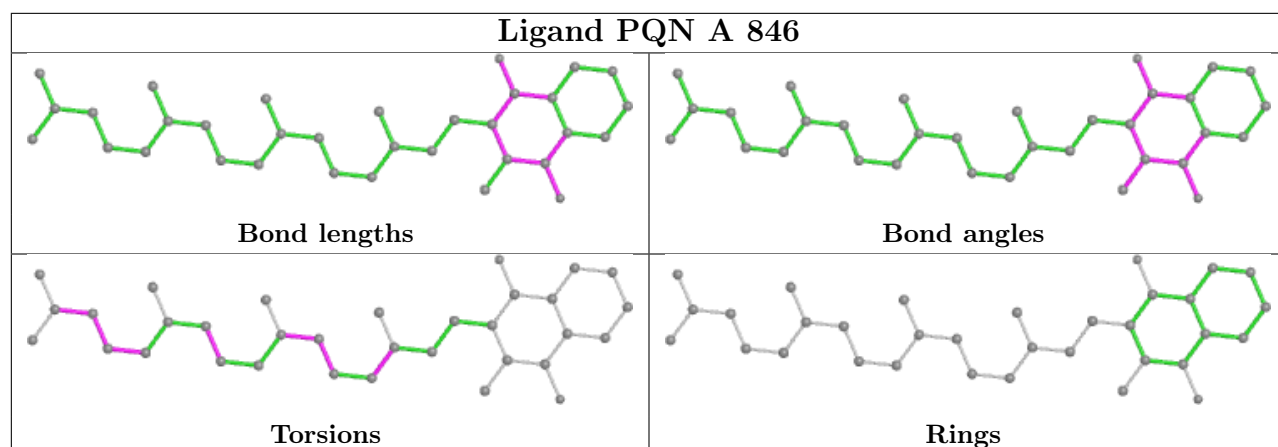
Rings



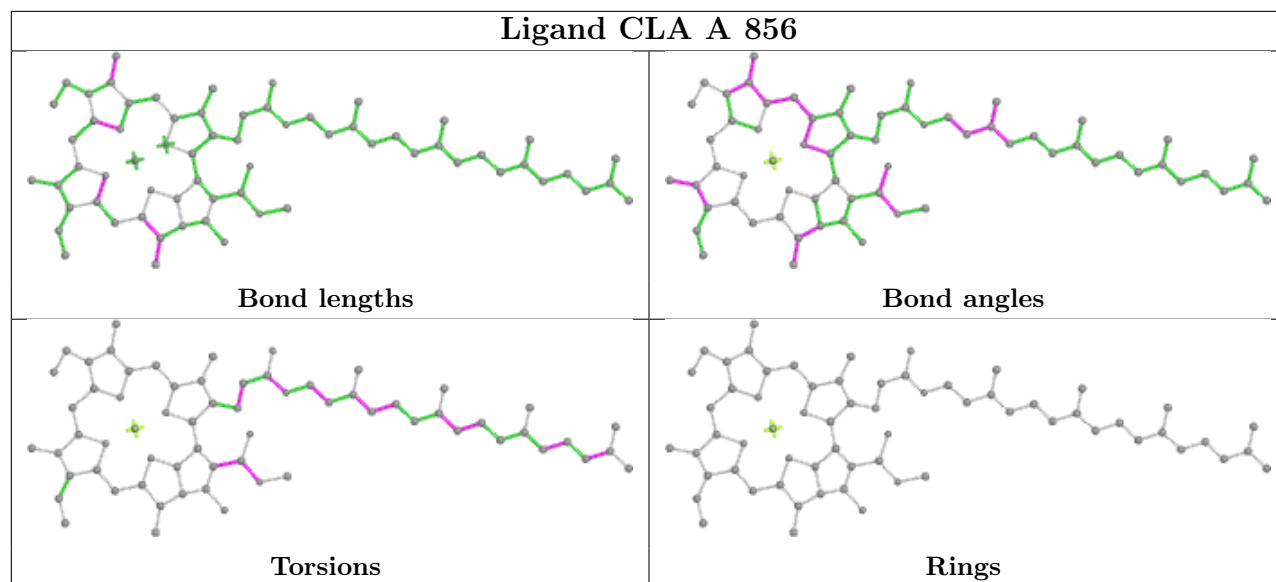
Ligand CLA A 808



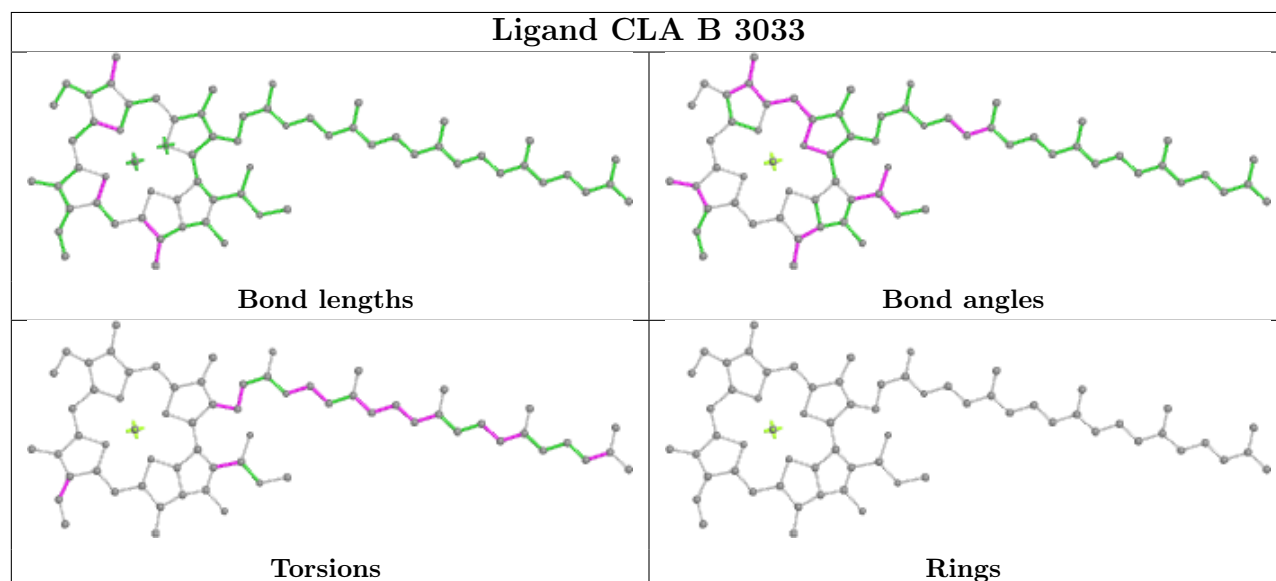
Ligand PQN A 846



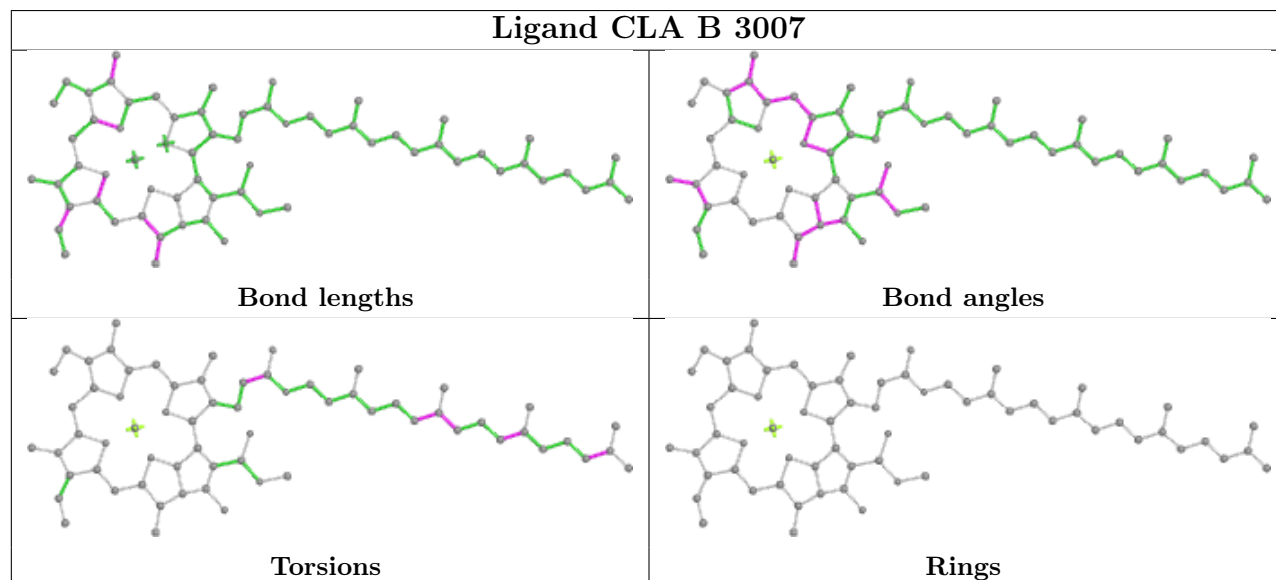
Ligand CLA A 856

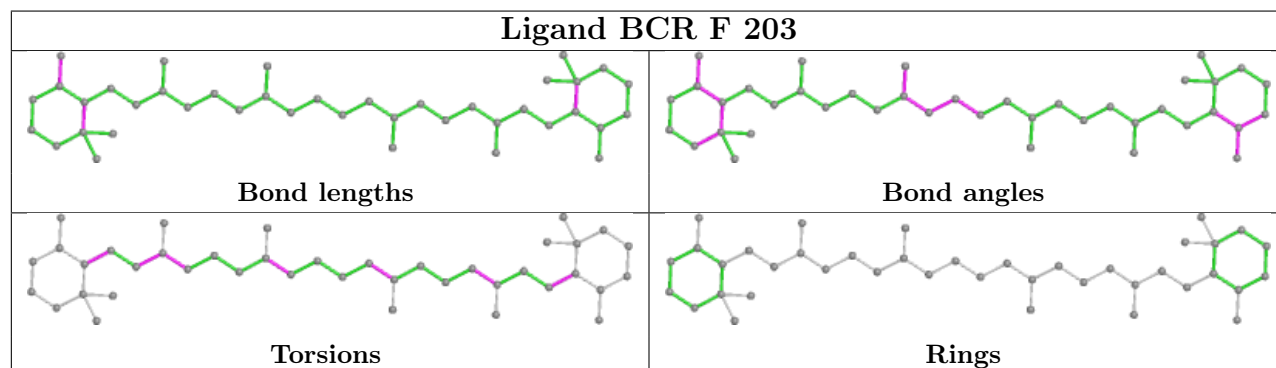
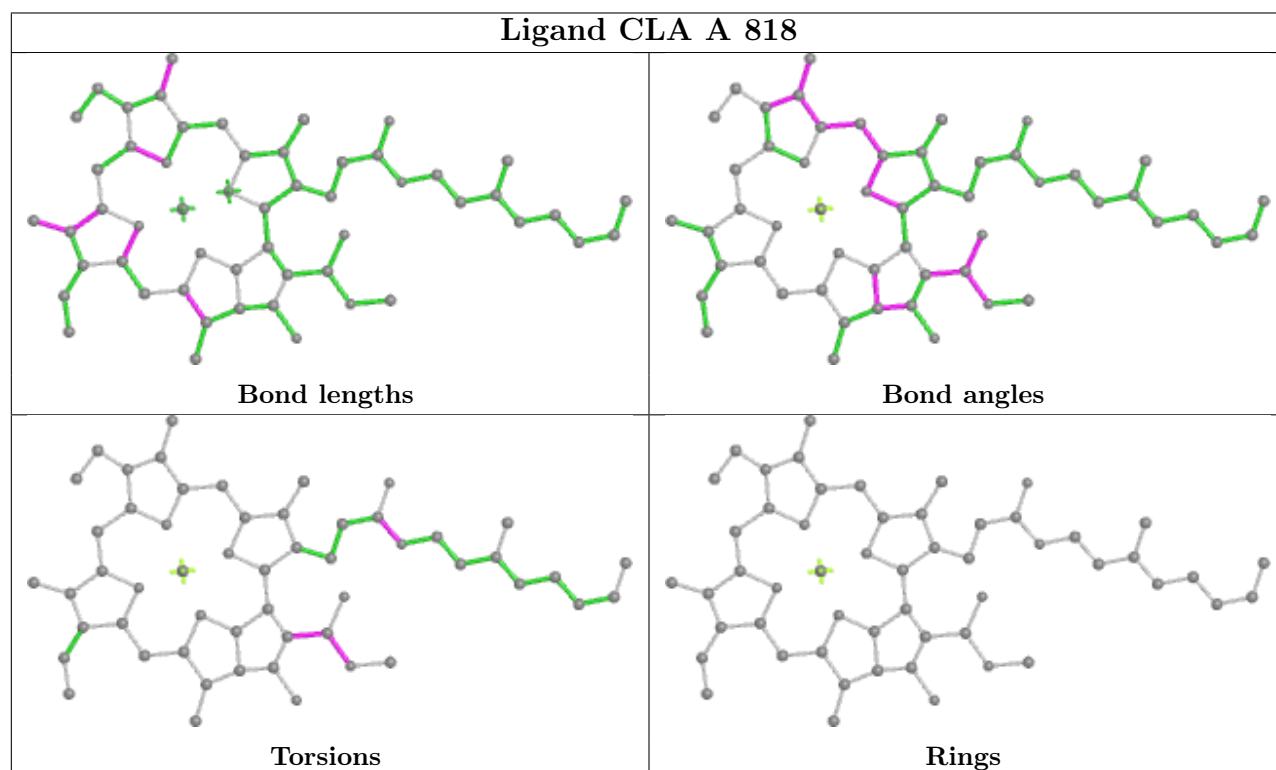
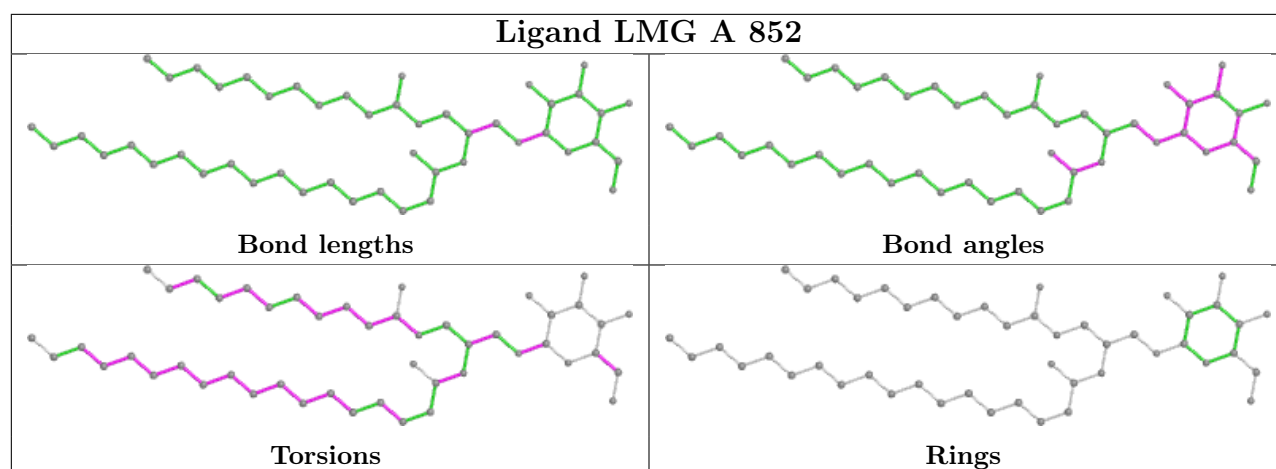


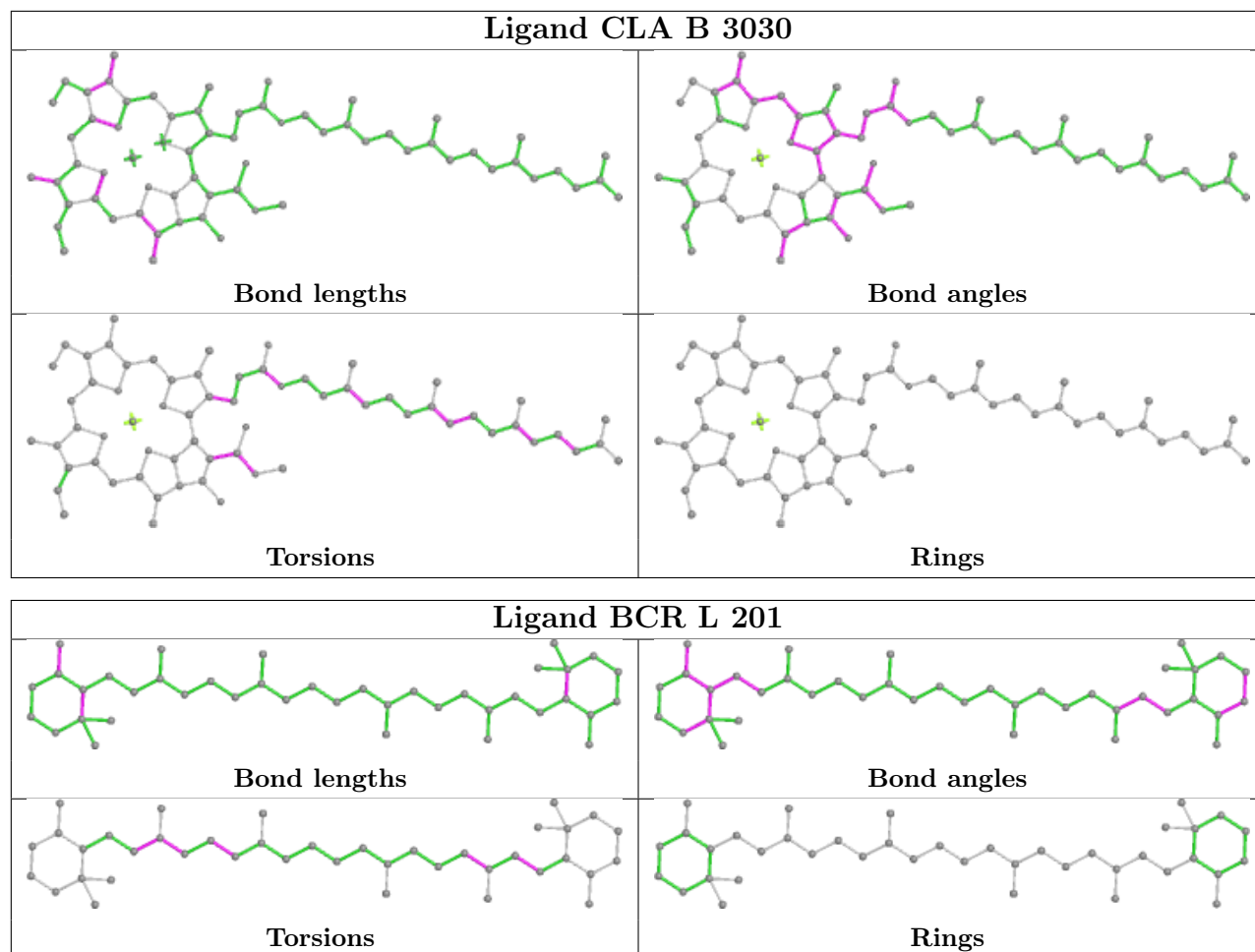
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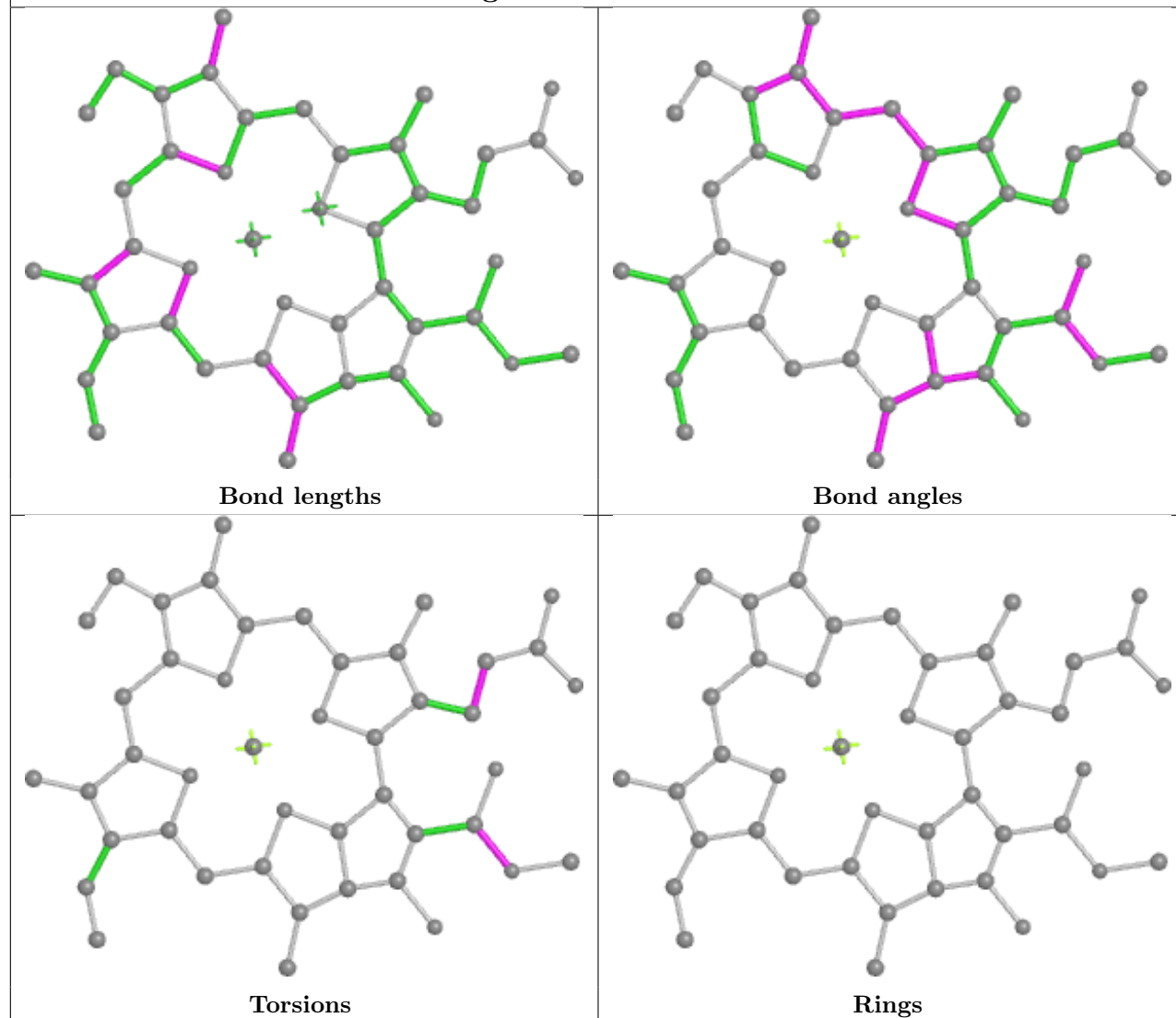
Ligand CLA B 3007



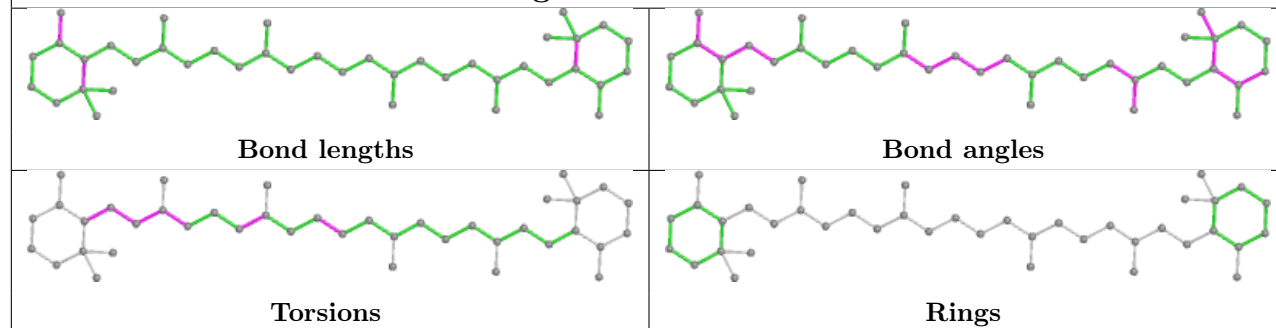


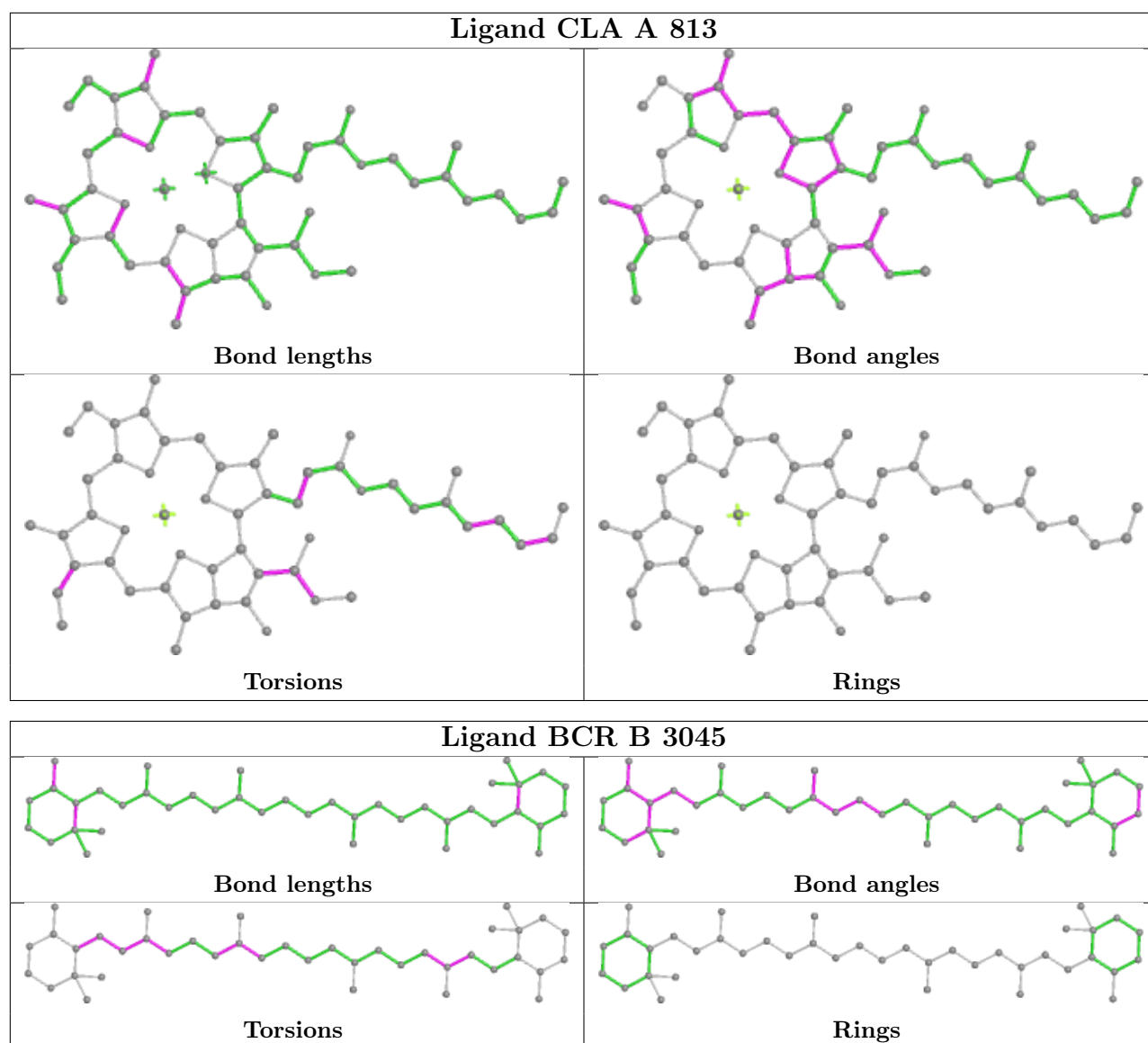


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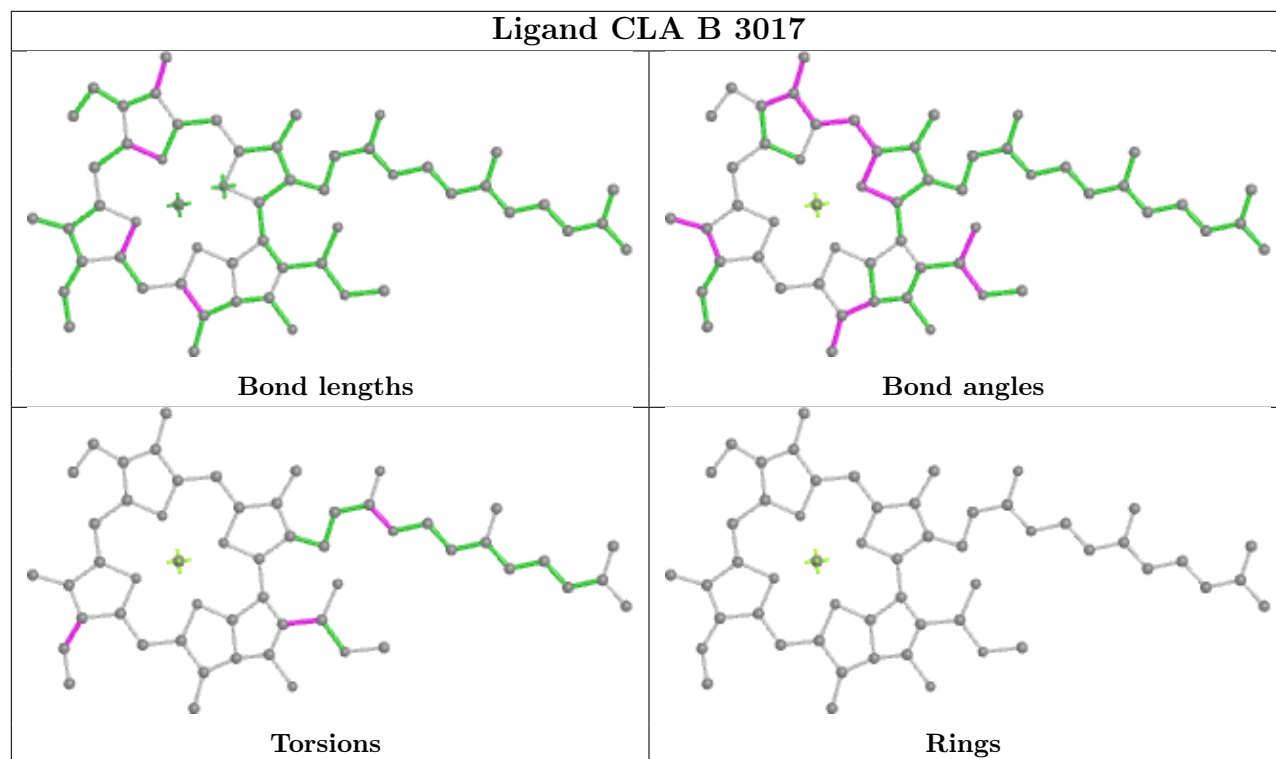


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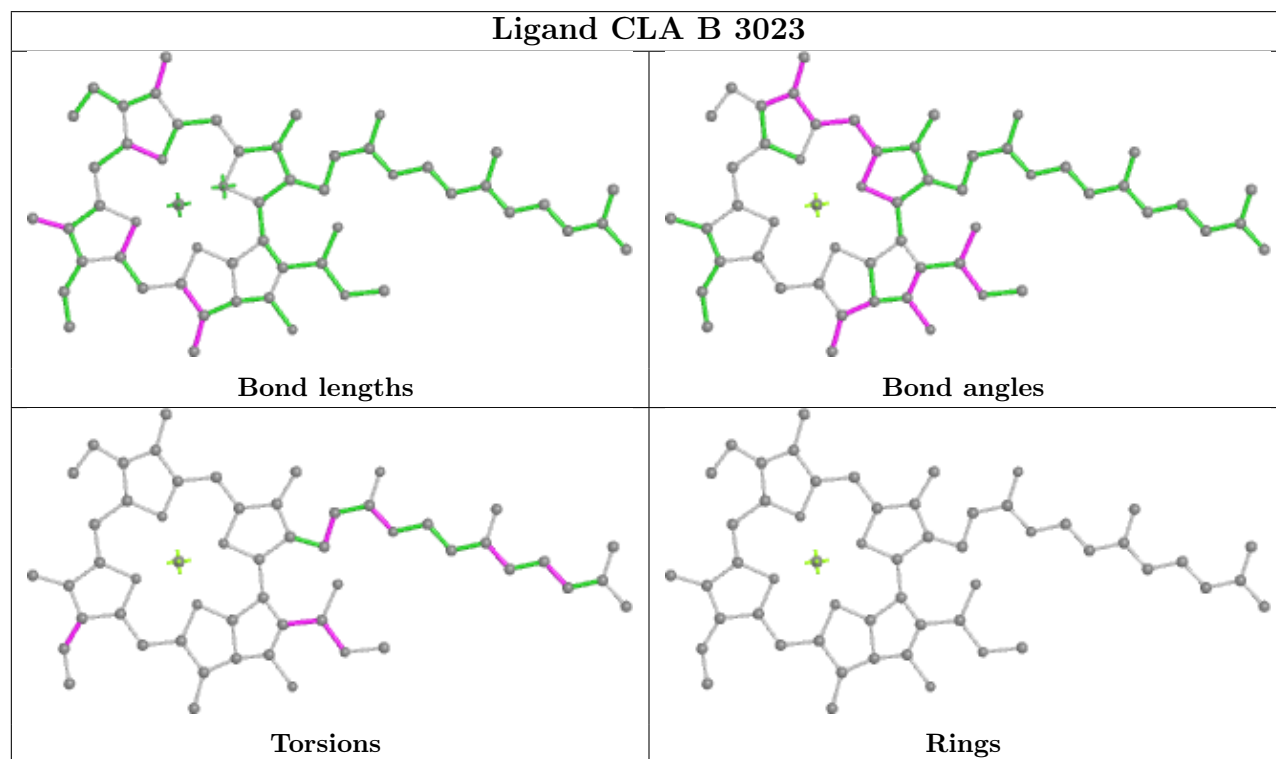


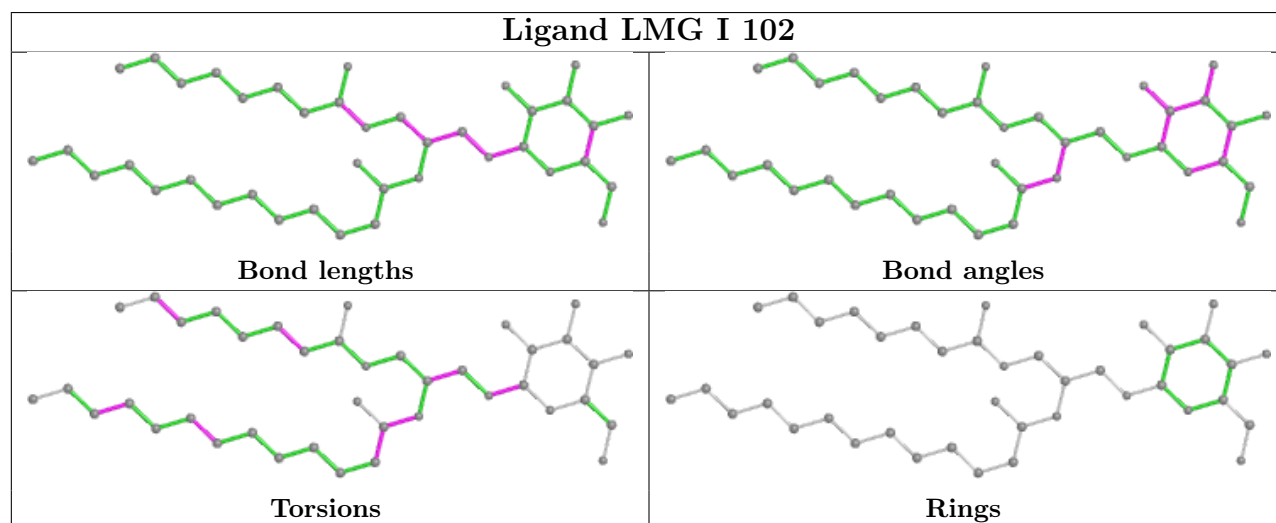
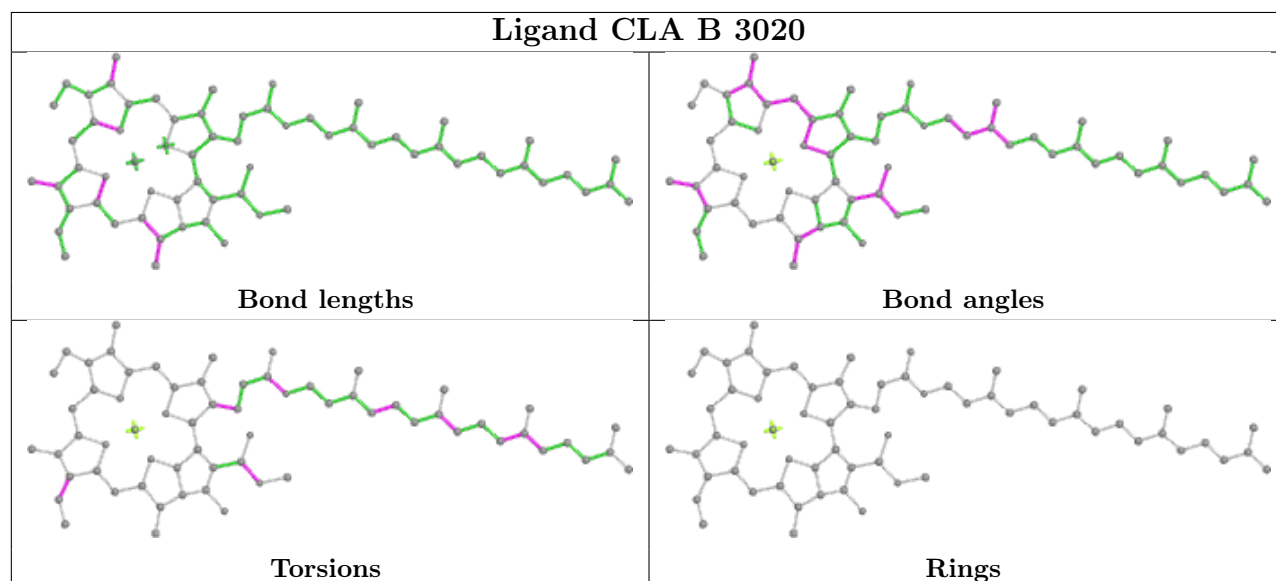
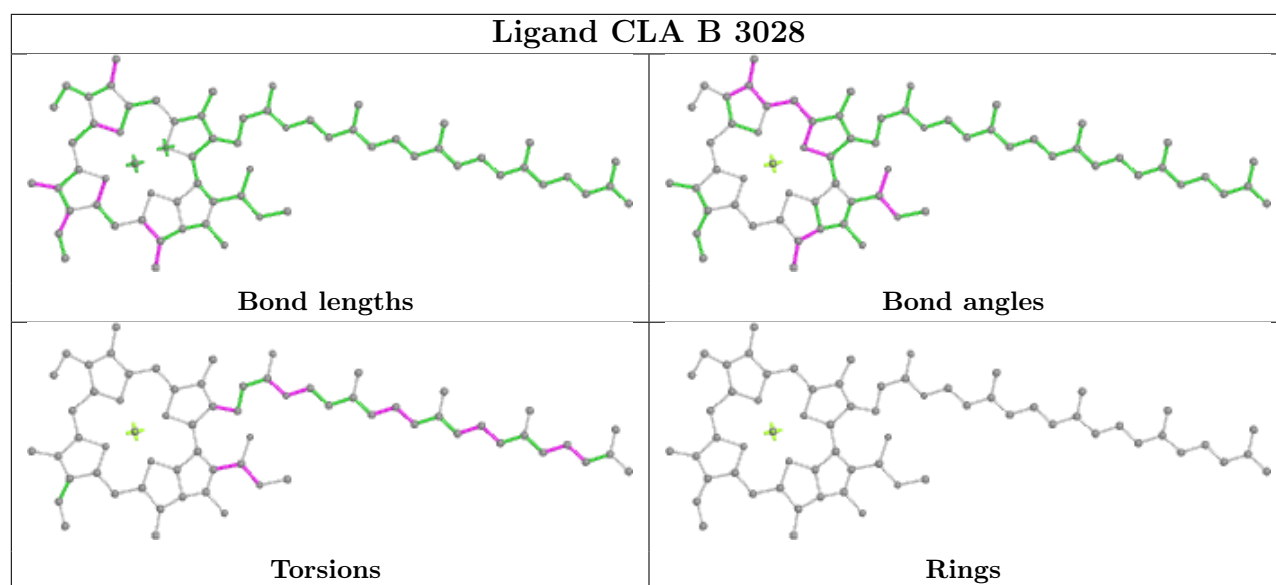


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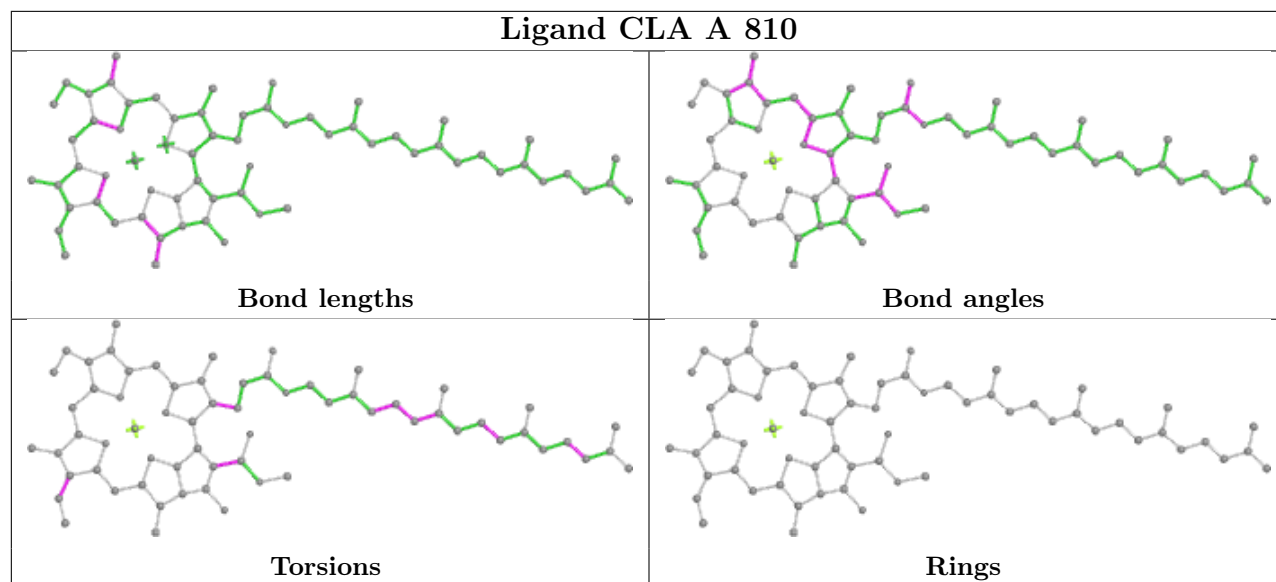


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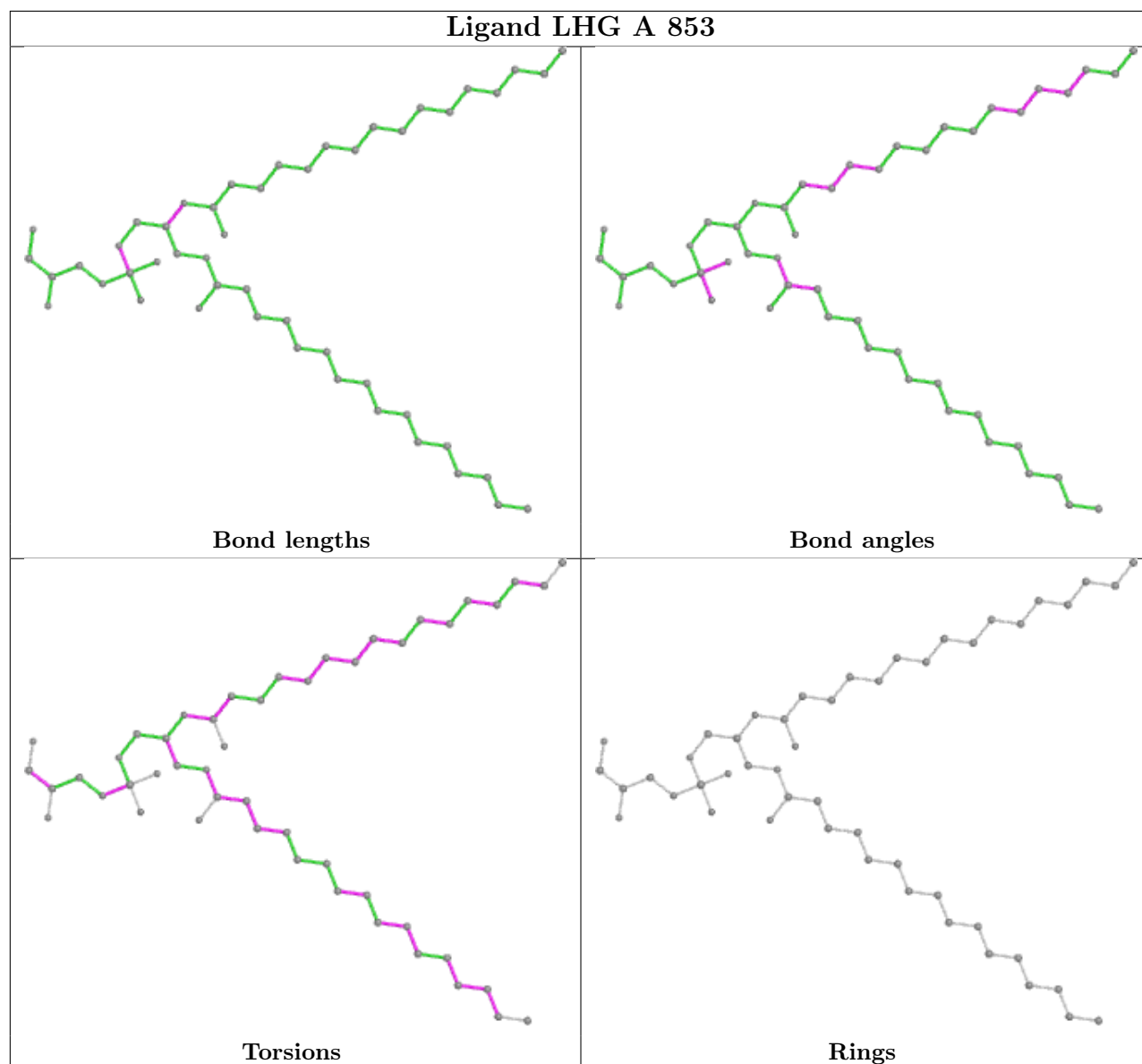




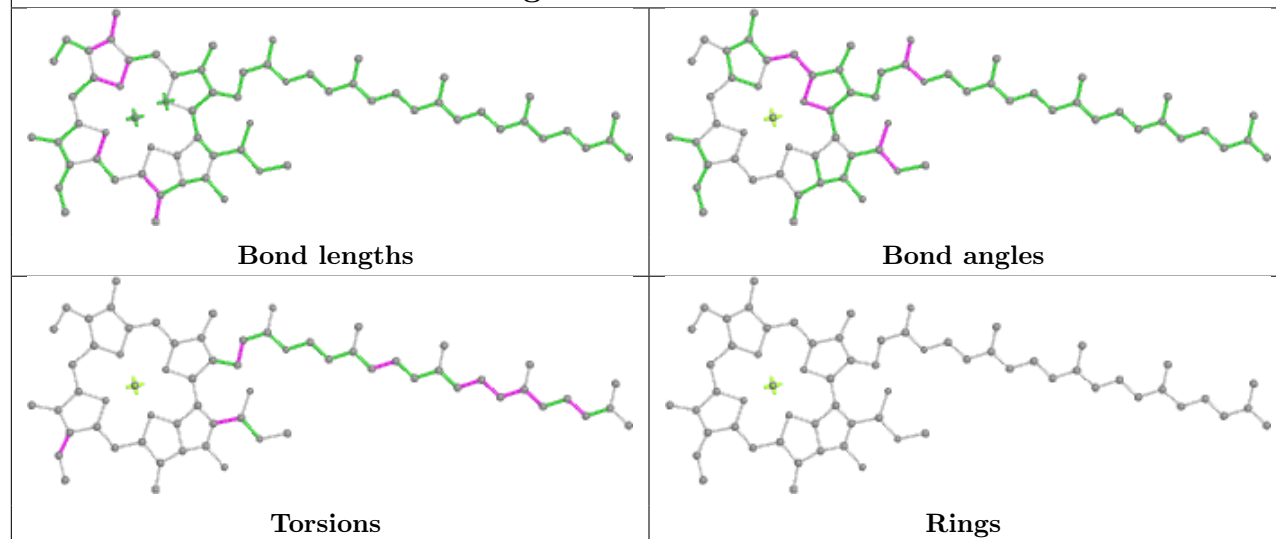
Ligand CLA A 810



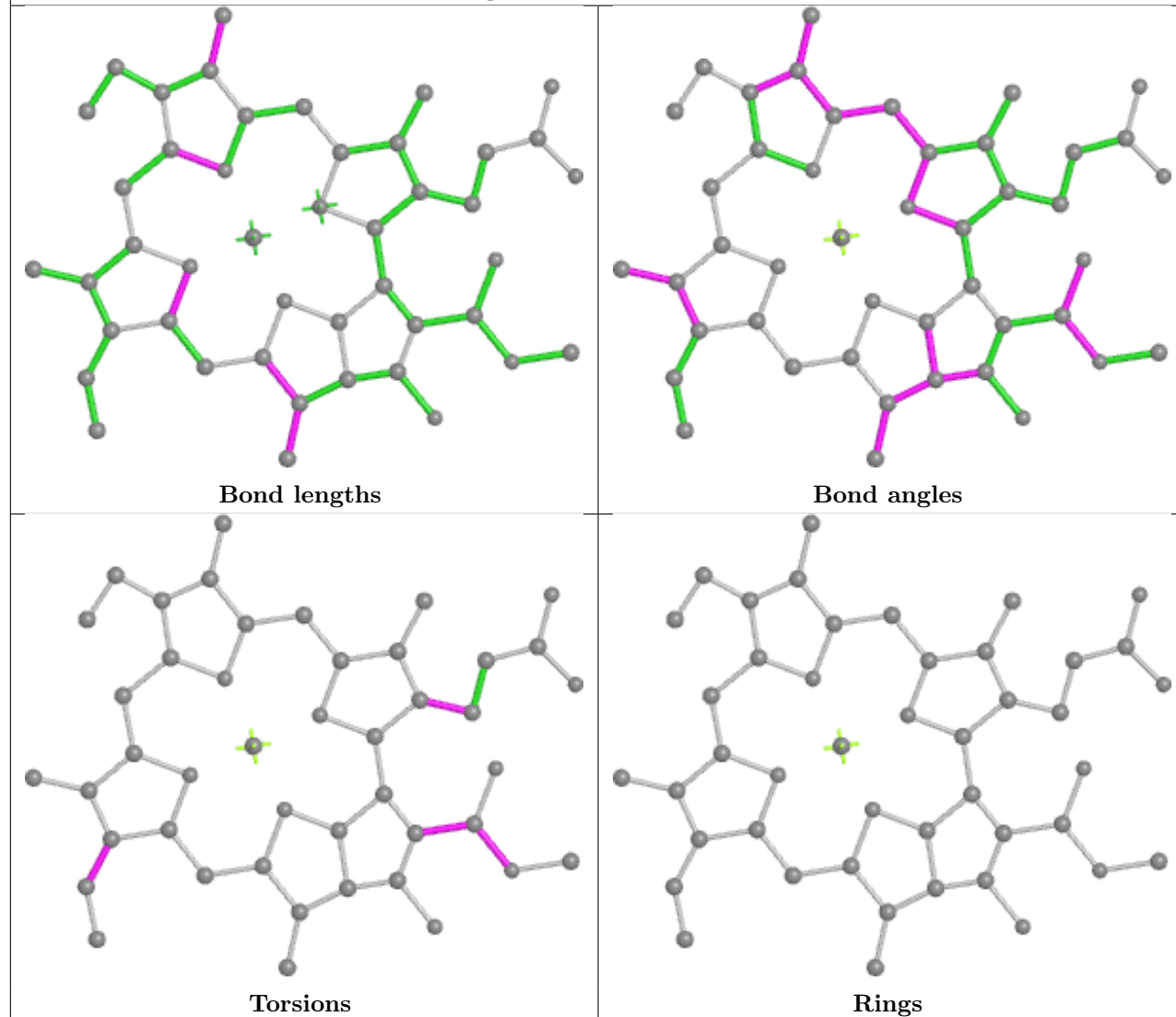
Ligand LHG A 853

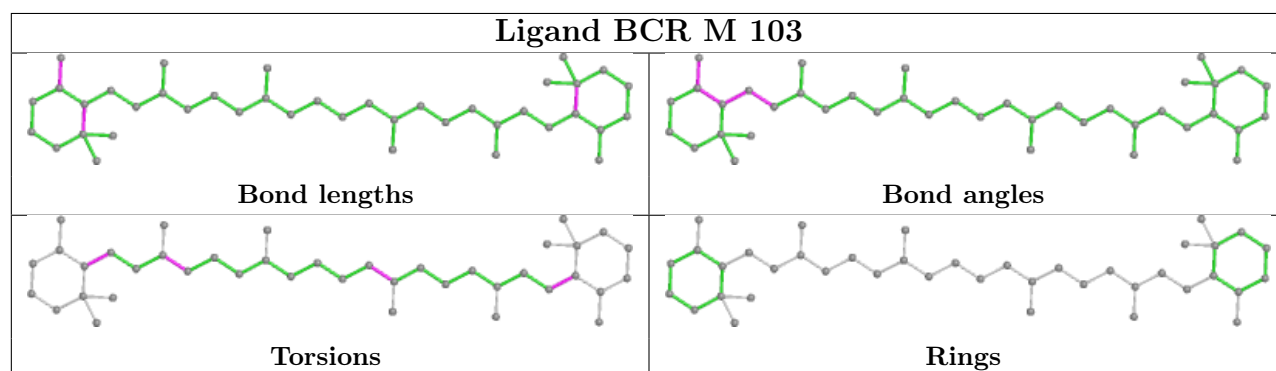
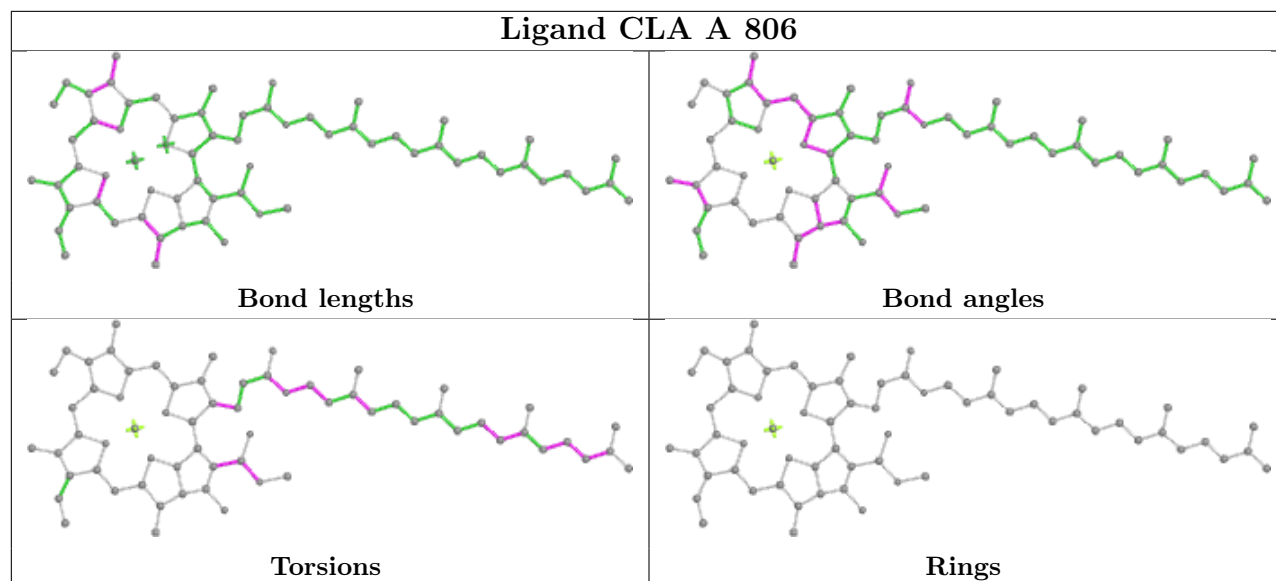
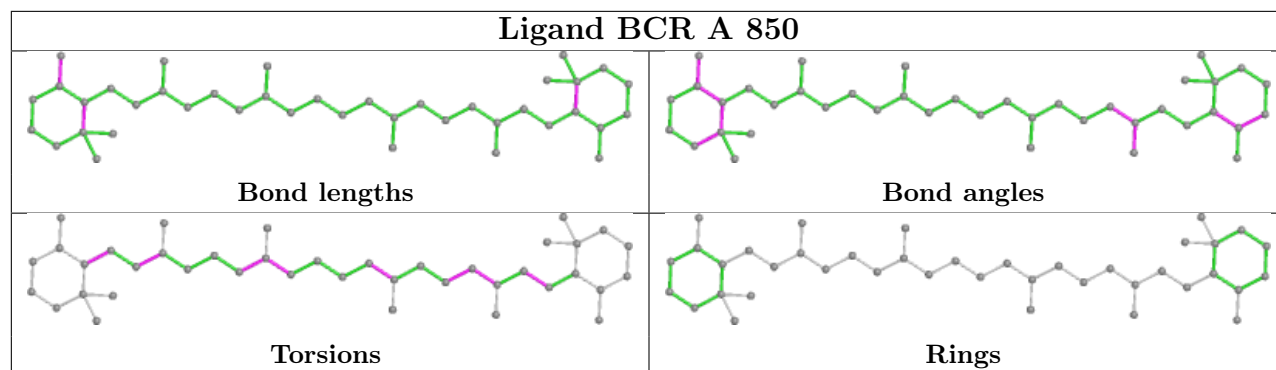


Ligand CLA B 3041

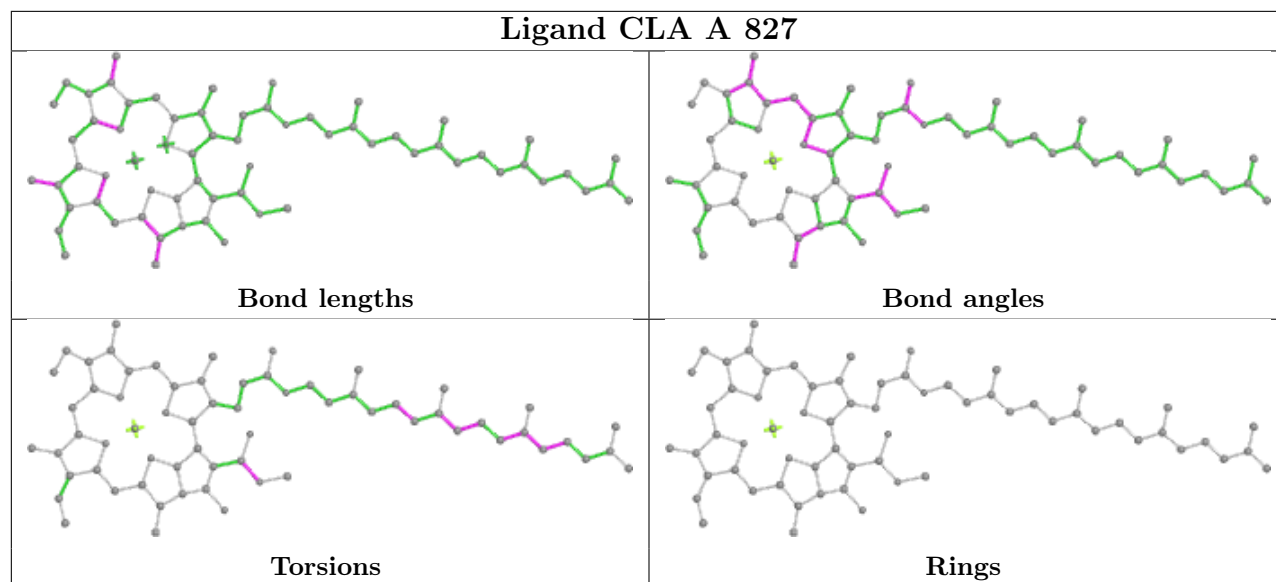


Ligand CLA B 3022

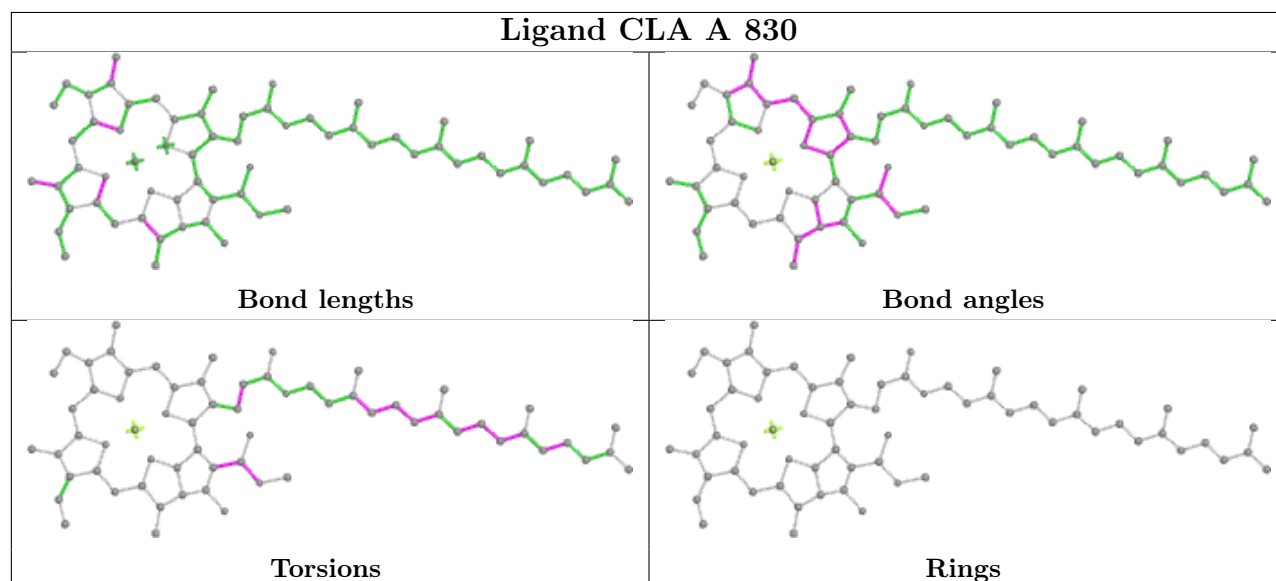




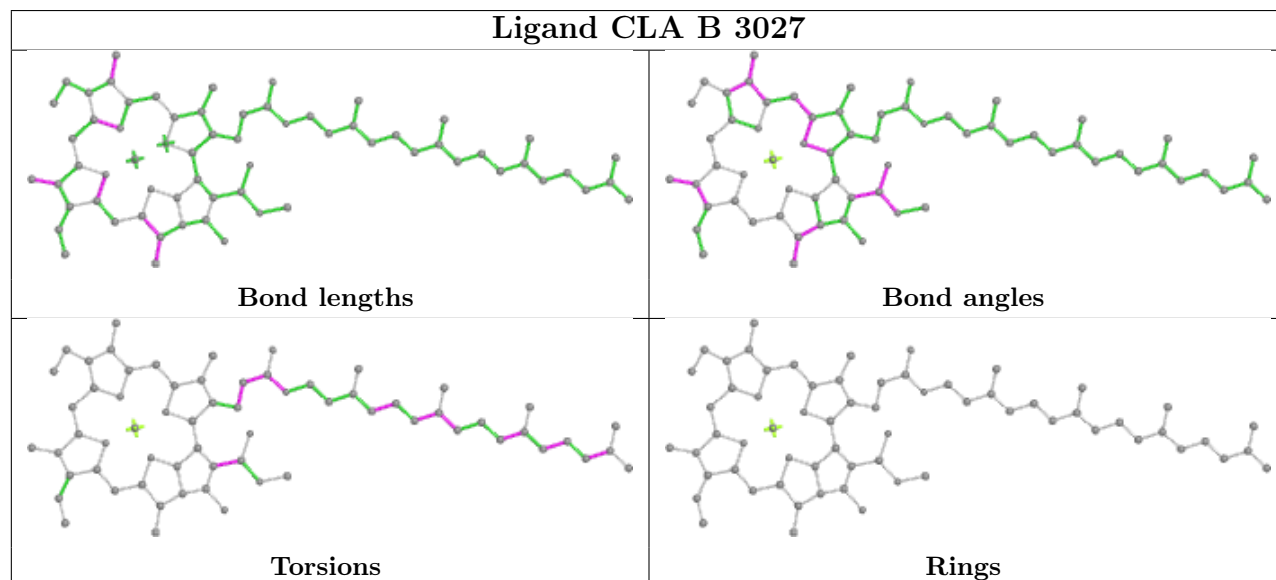
Ligand CLA A 827

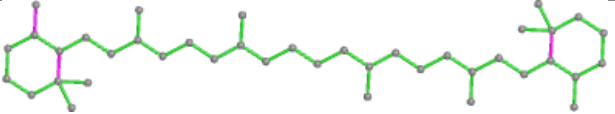
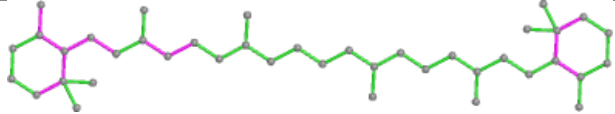
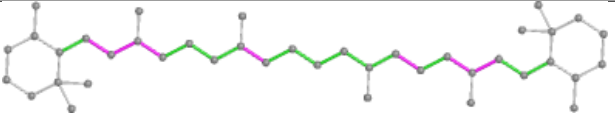
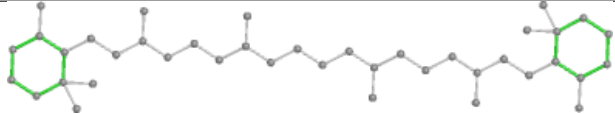
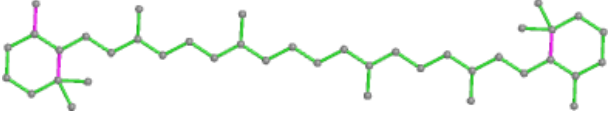
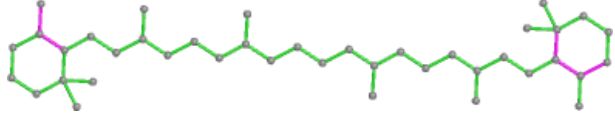
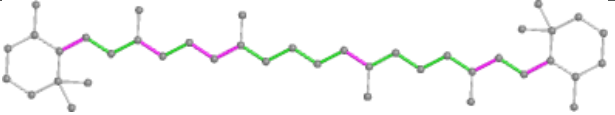
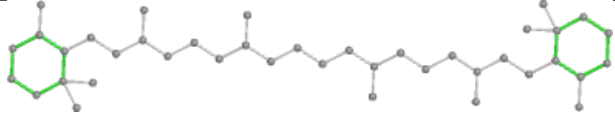
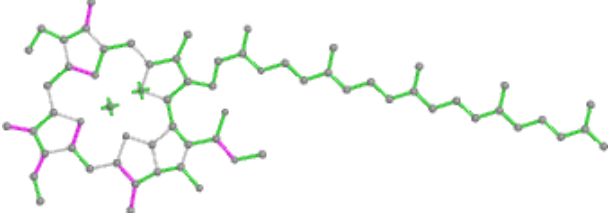
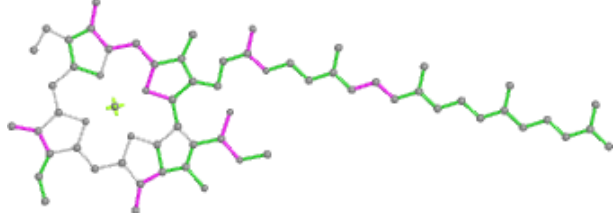
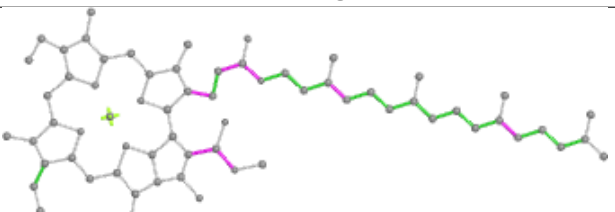
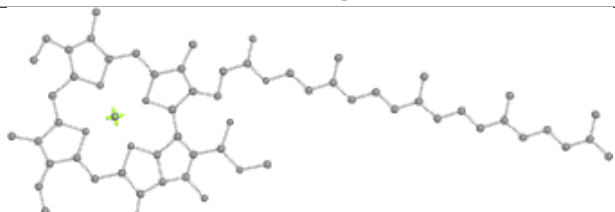


Ligand CLA A 830

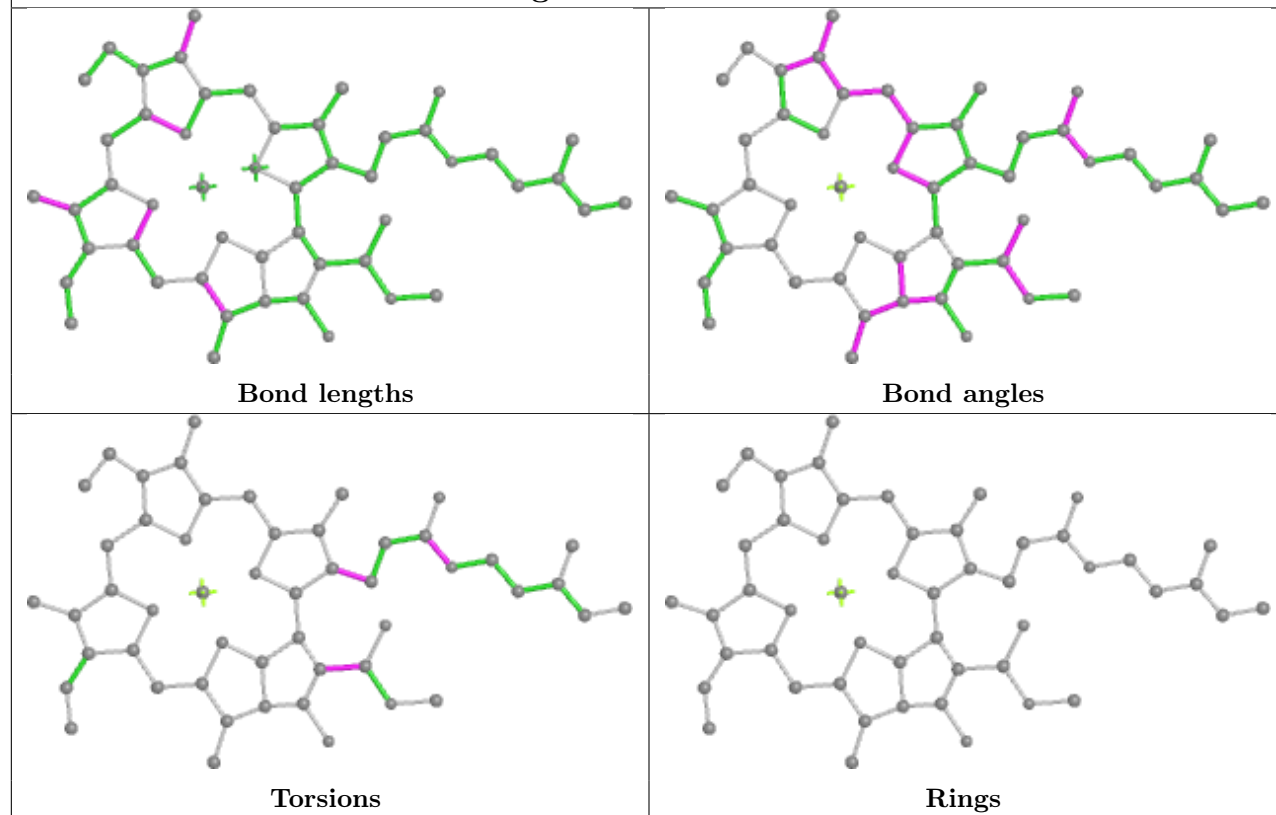


Ligand CLA B 3027

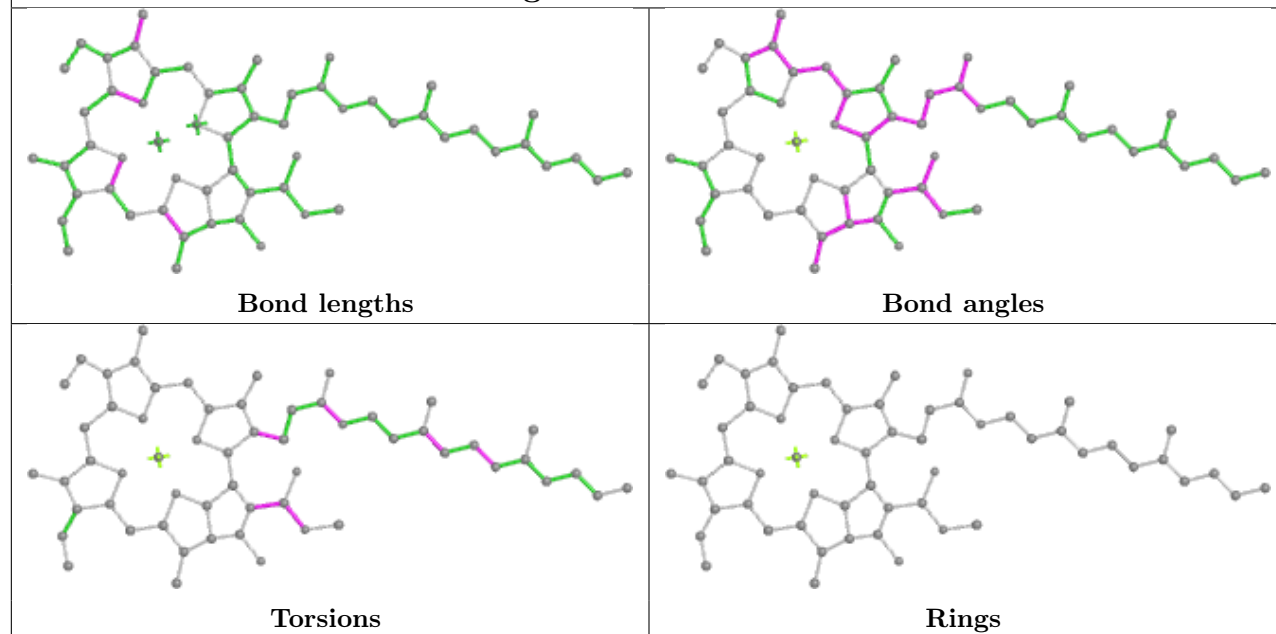


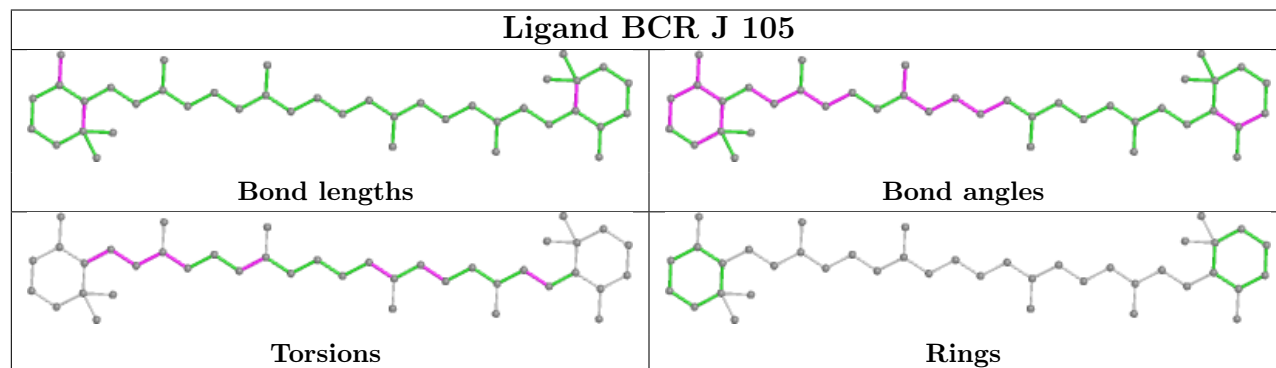
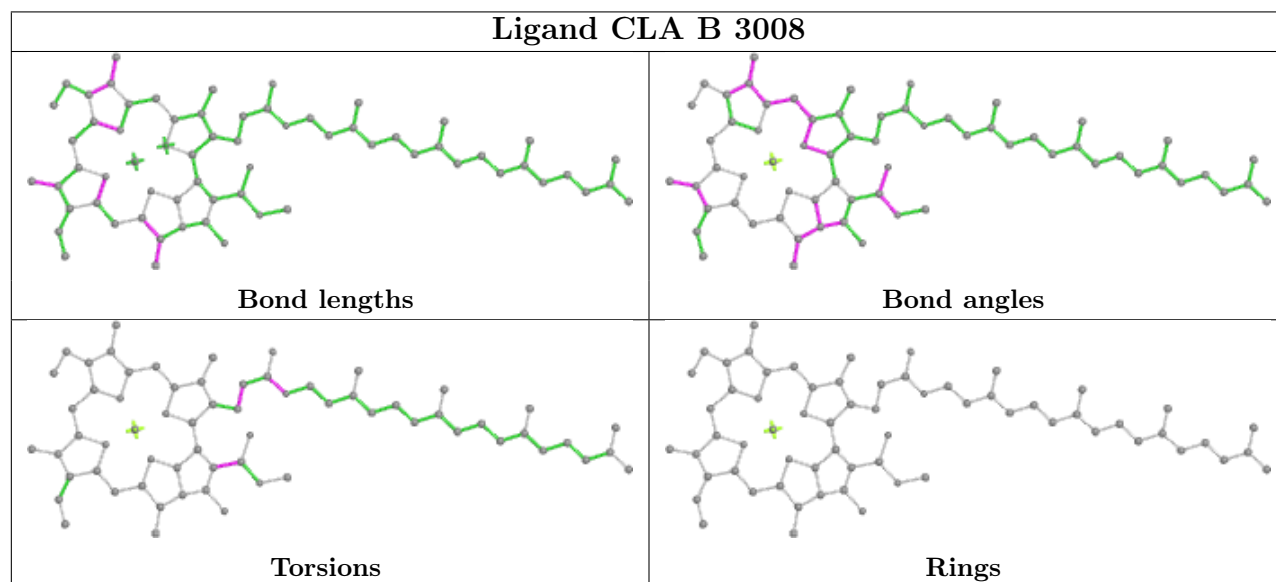
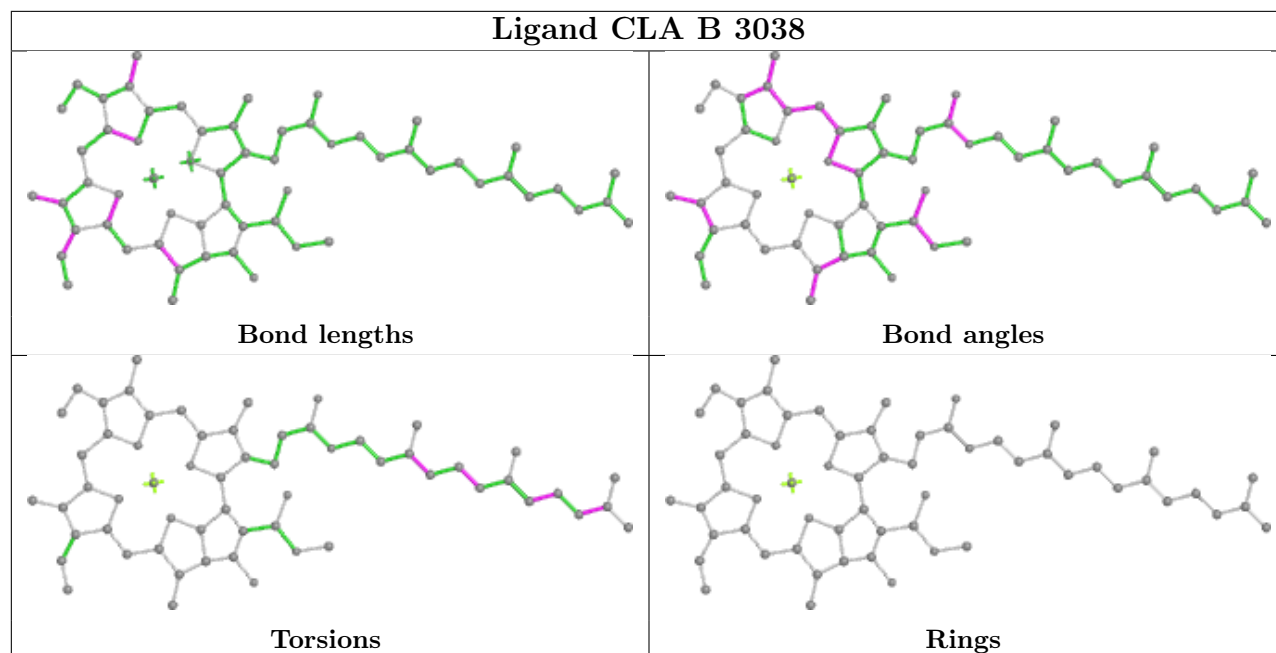
Ligand BCR B 3044	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR B 3051	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA A 812	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

Ligand CLA A 824

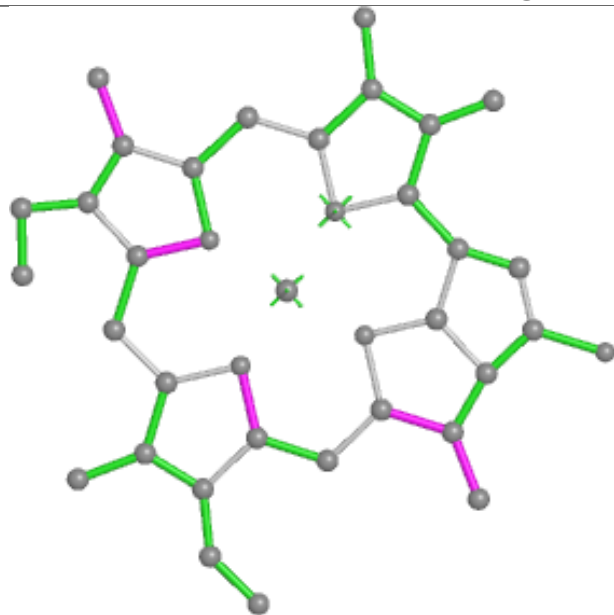


Ligand CLA B 3034

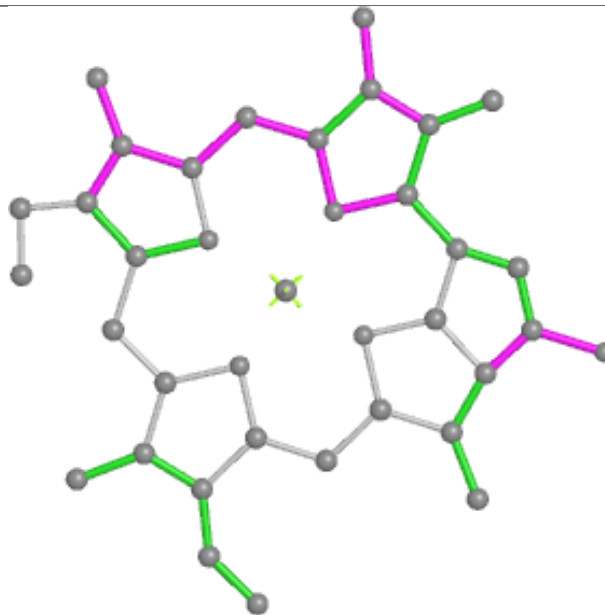




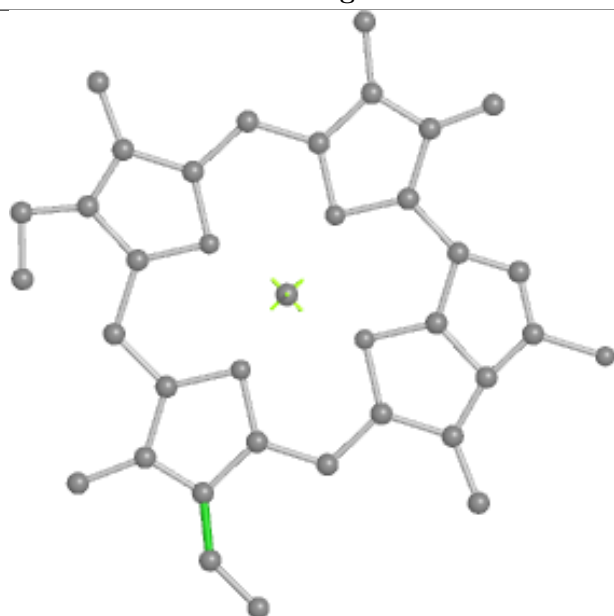
Ligand CLA J 102



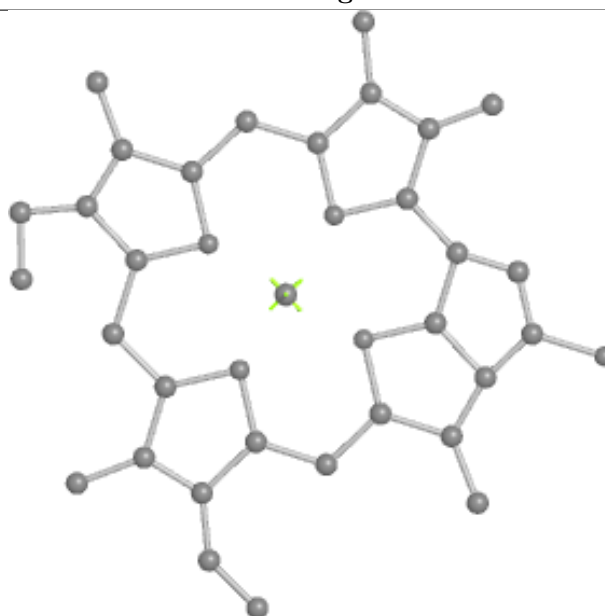
Bond lengths



Bond angles

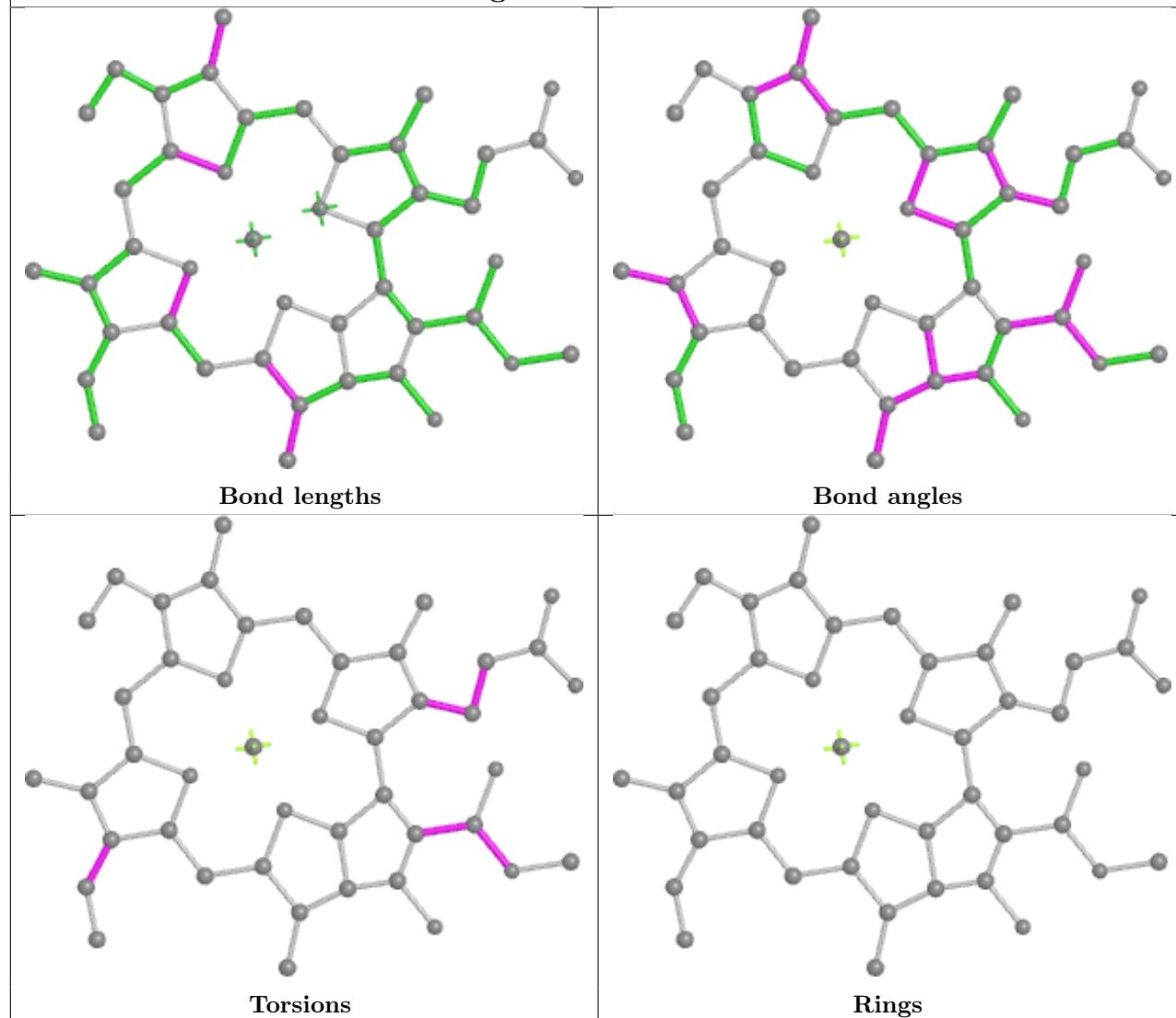


Torsions

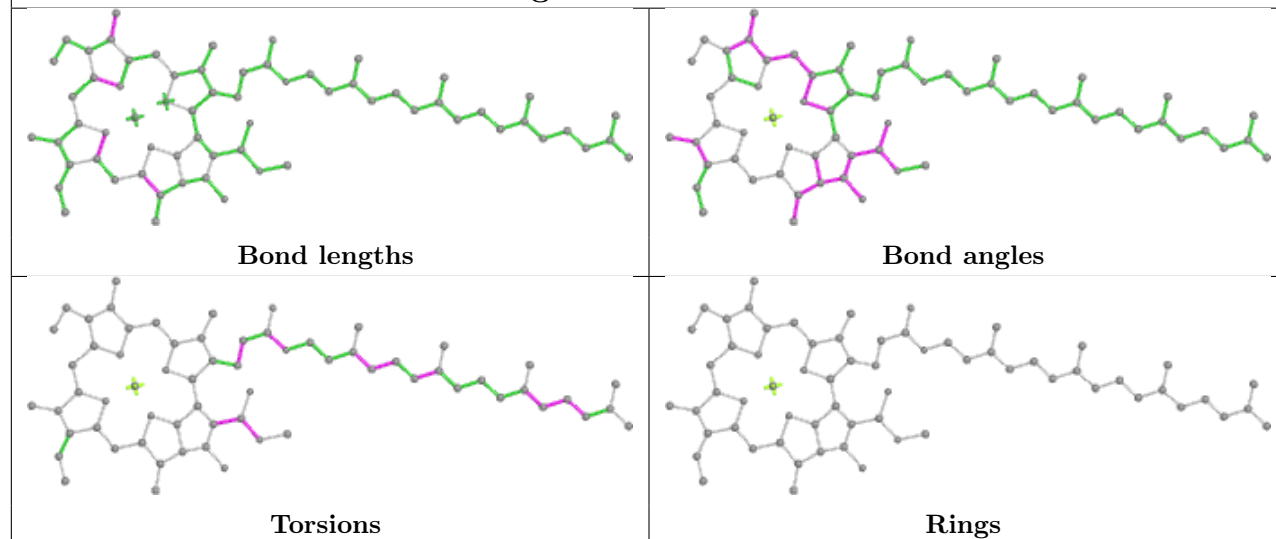


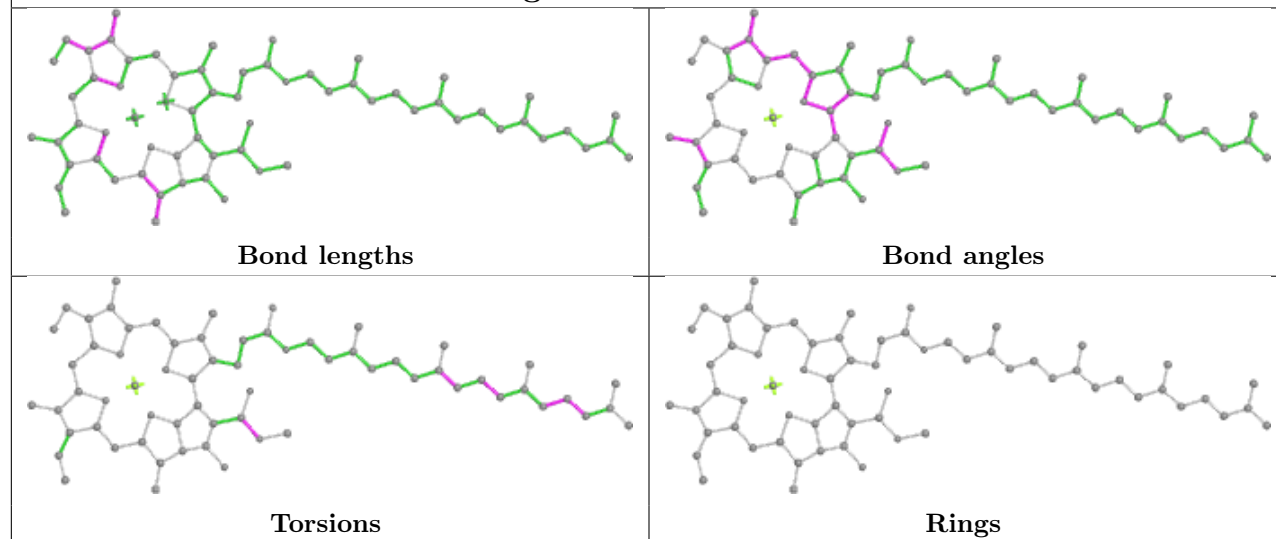
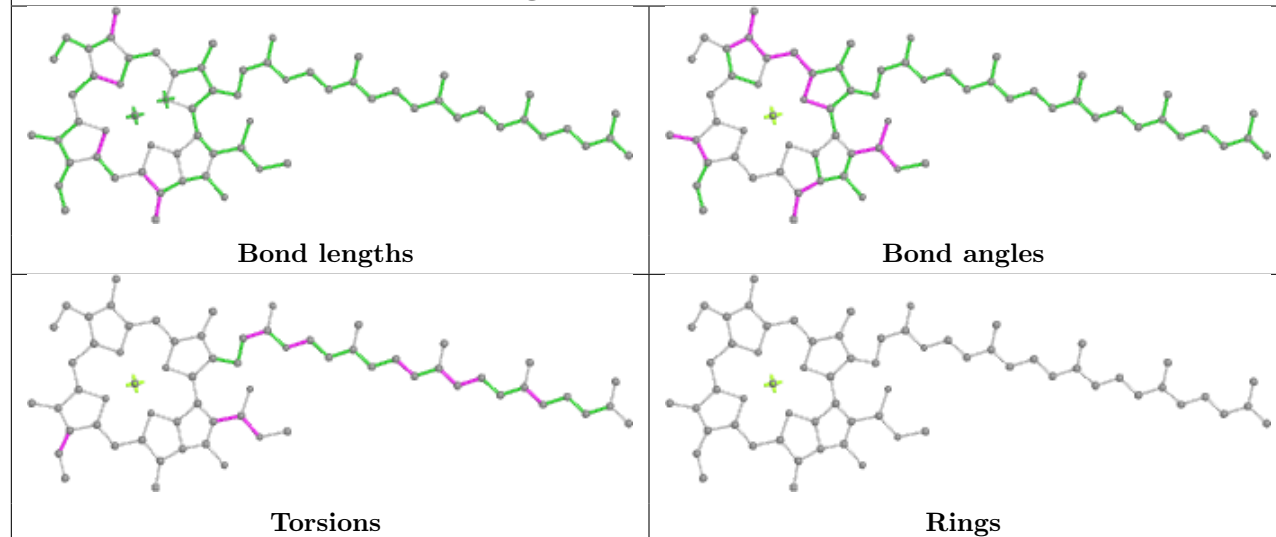
Rings

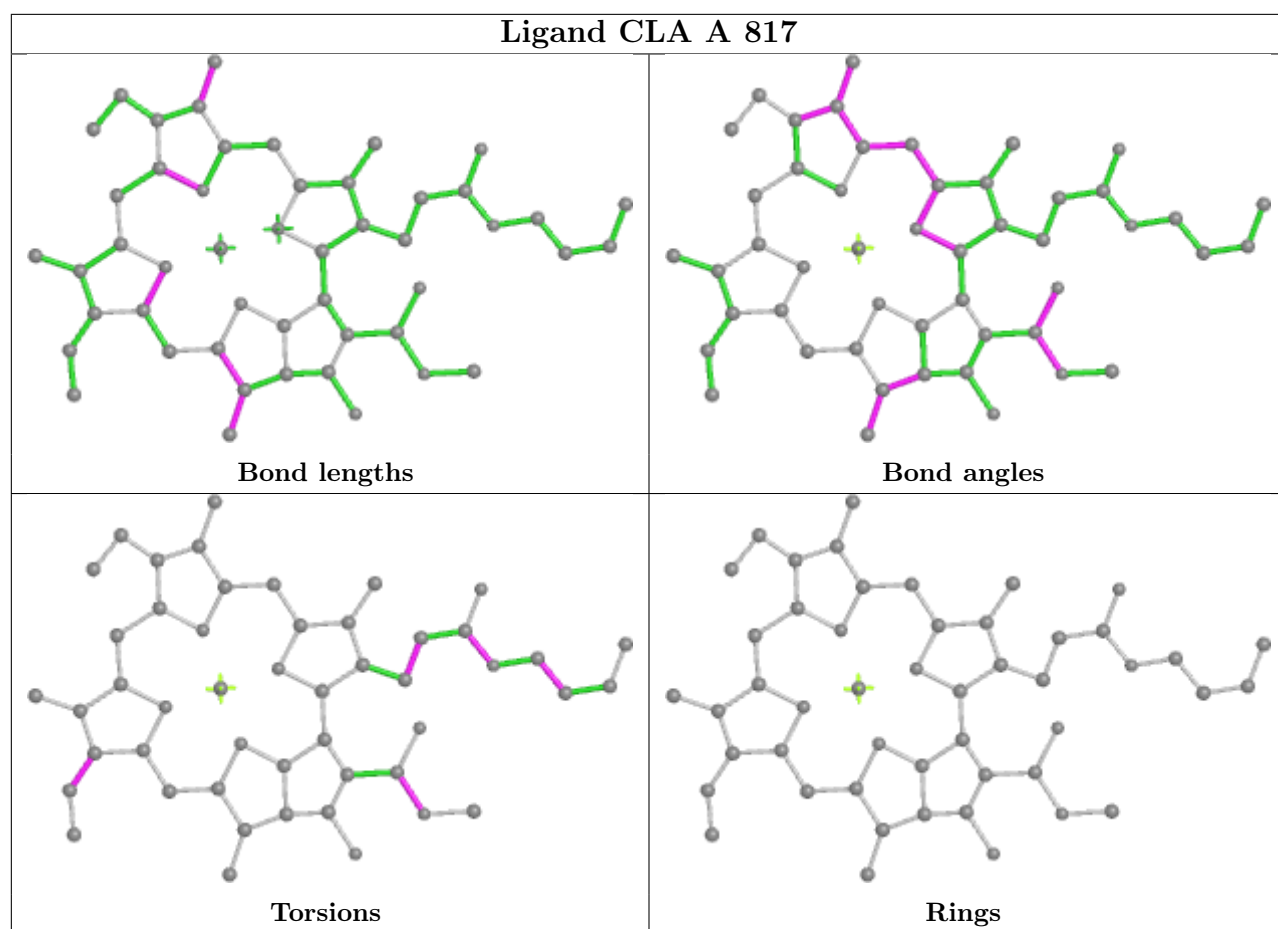
Ligand CLA A 811



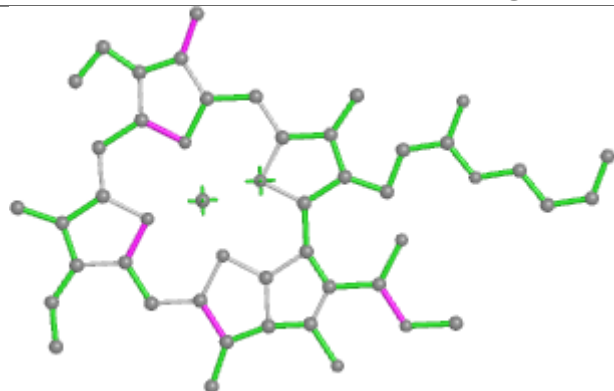
Ligand CLA A 822



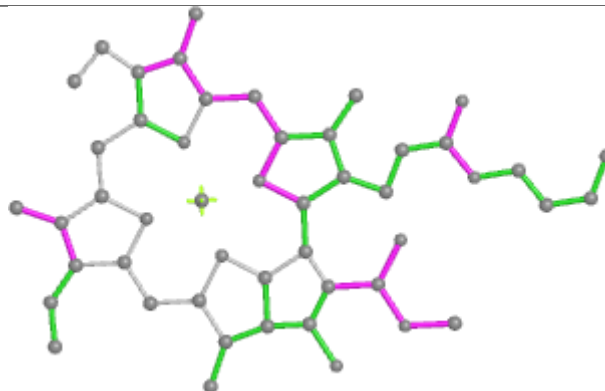
Ligand CLA B 3004**Ligand CLA B 3015**



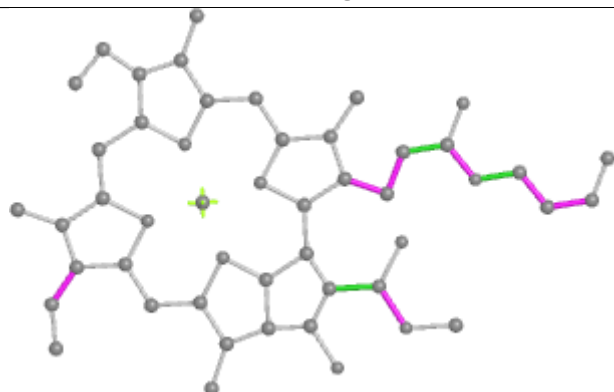
Ligand CLA B 3032



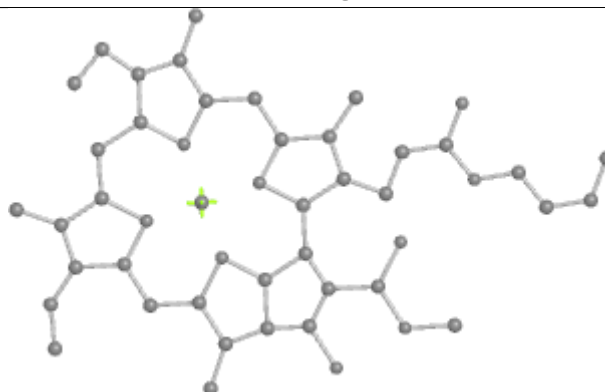
Bond lengths



Bond angles

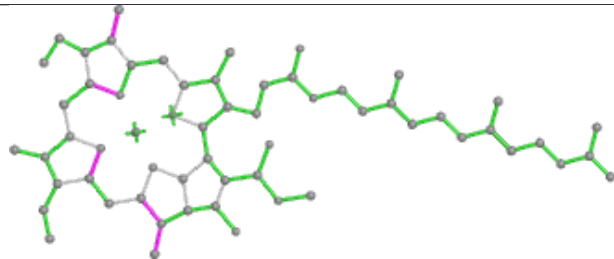


Torsions

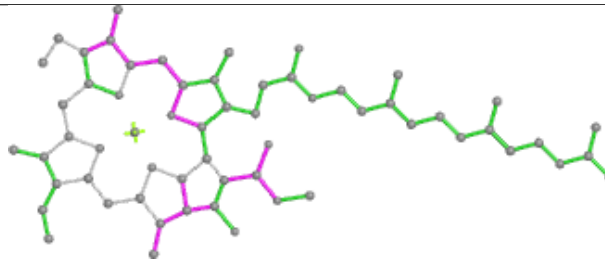


Rings

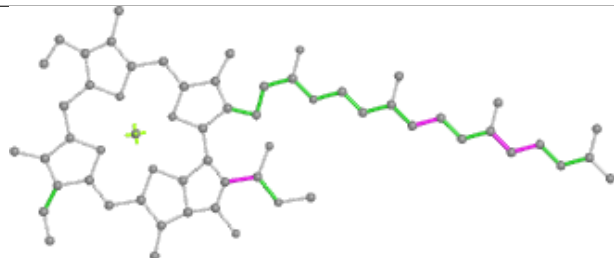
Ligand CLA A 814



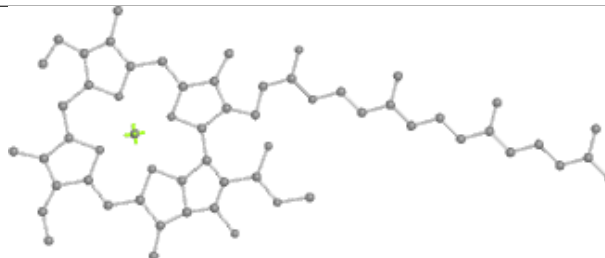
Bond lengths



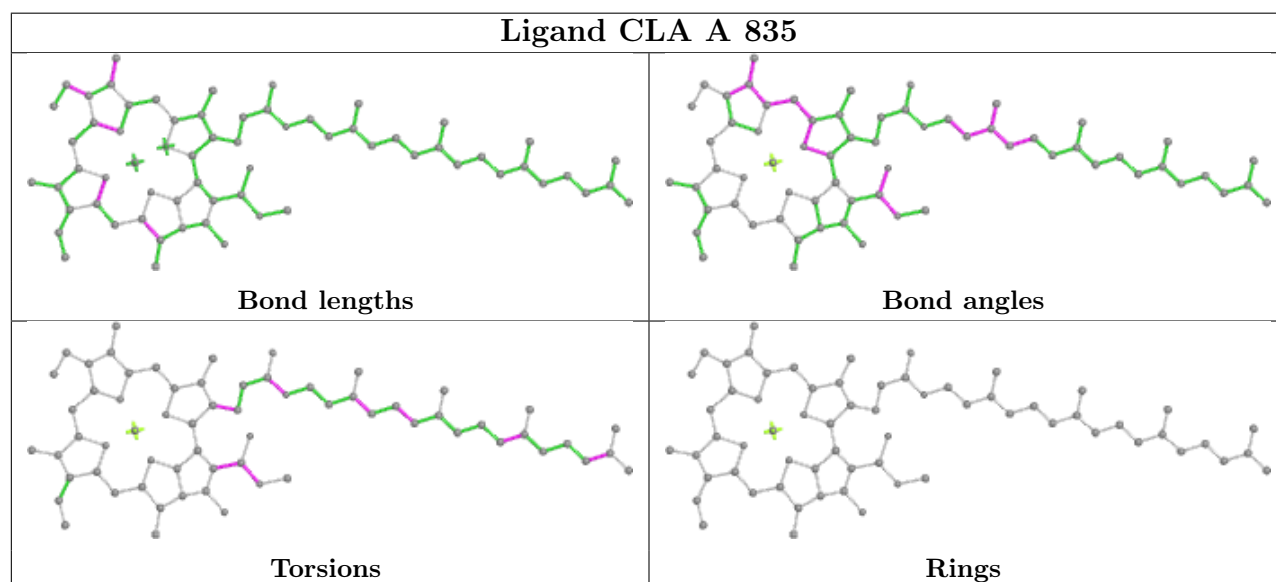
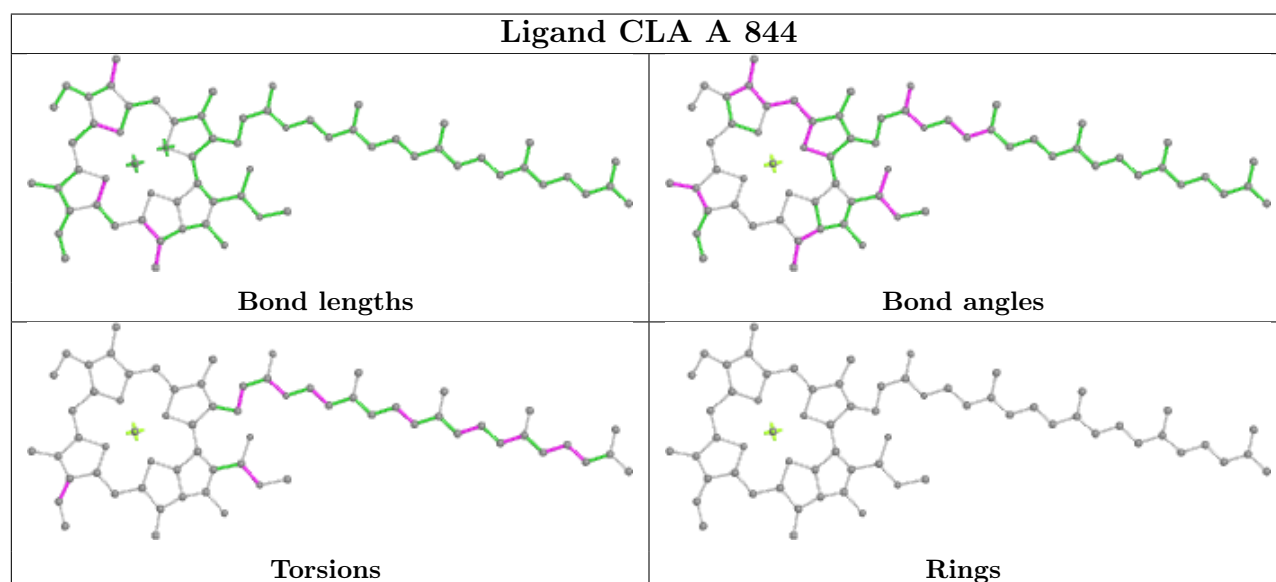
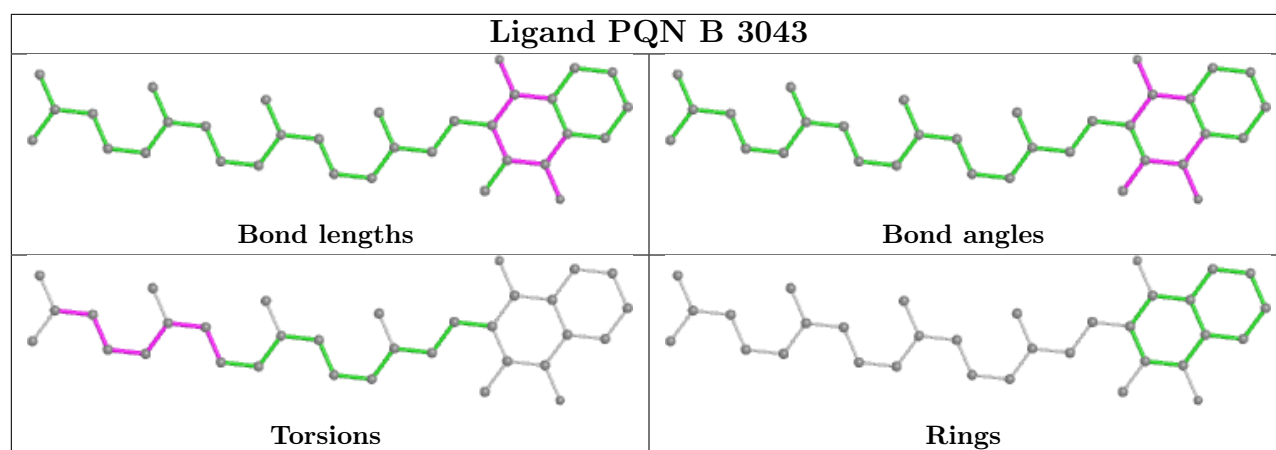
Bond angles



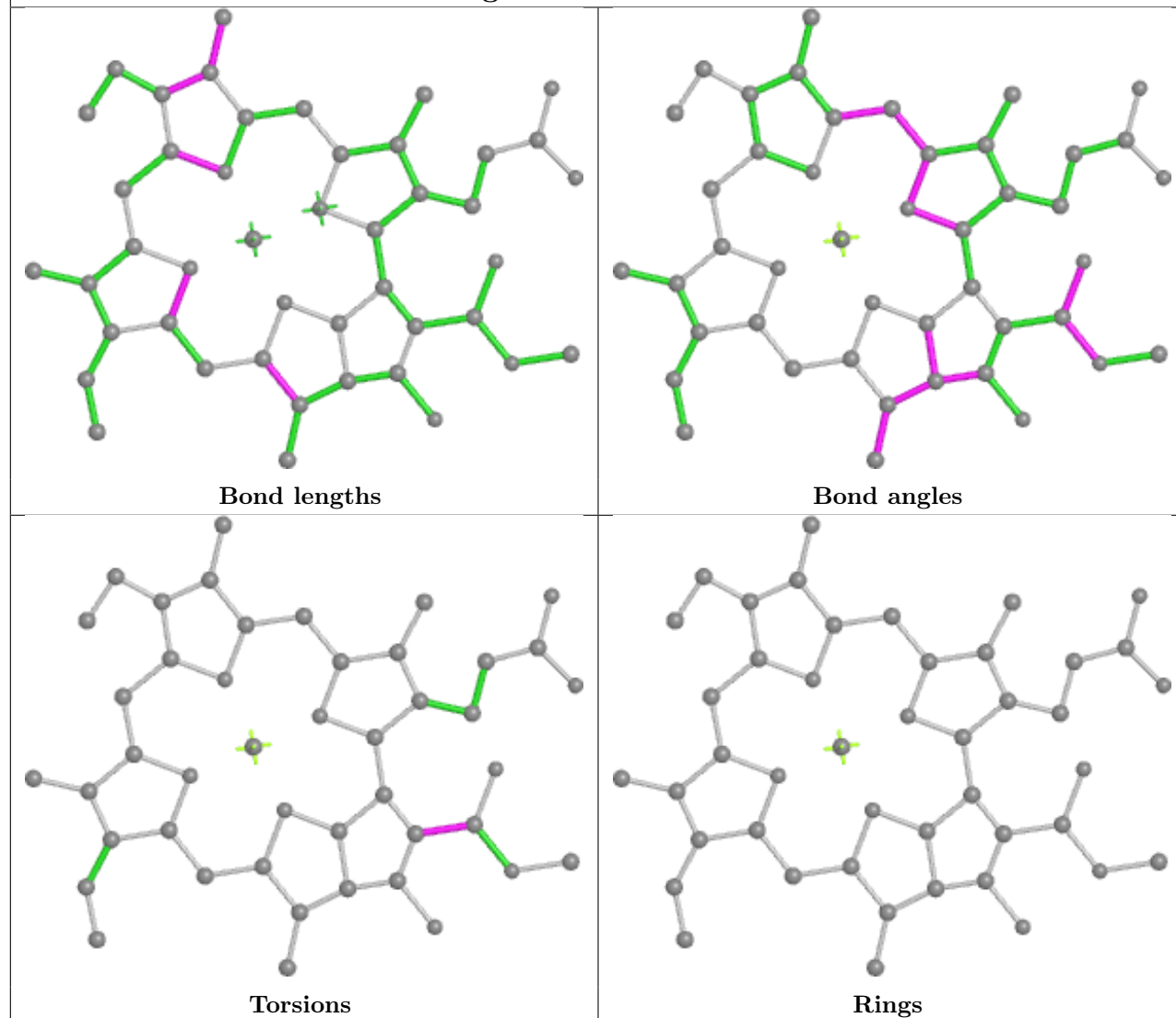
Torsions



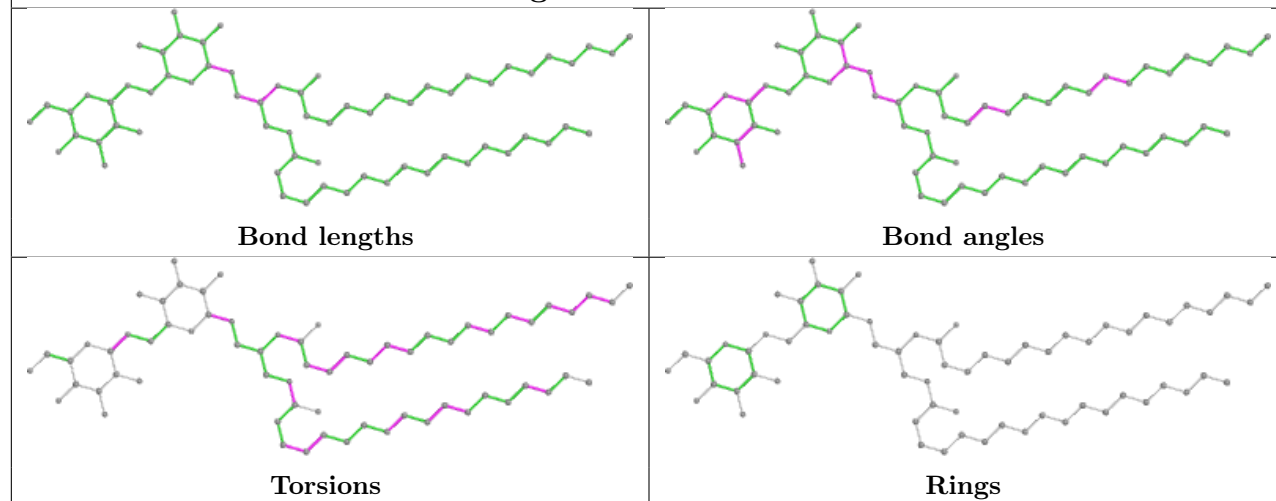
Rings

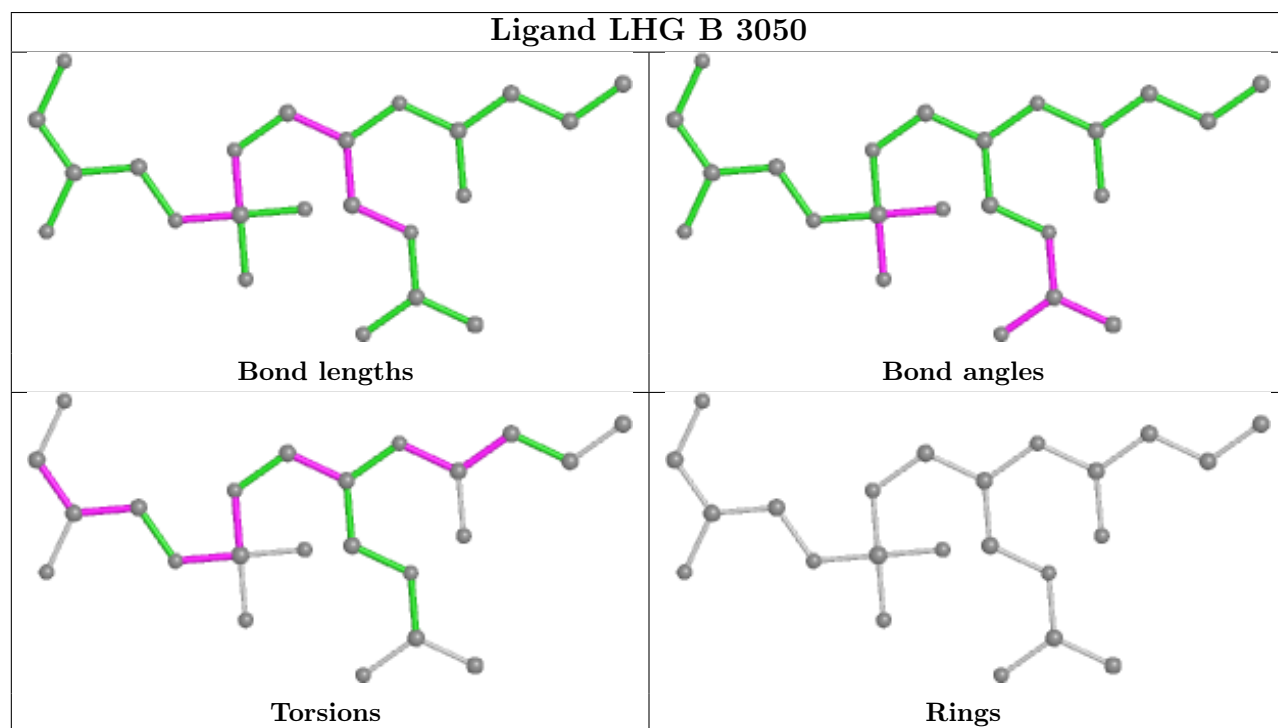
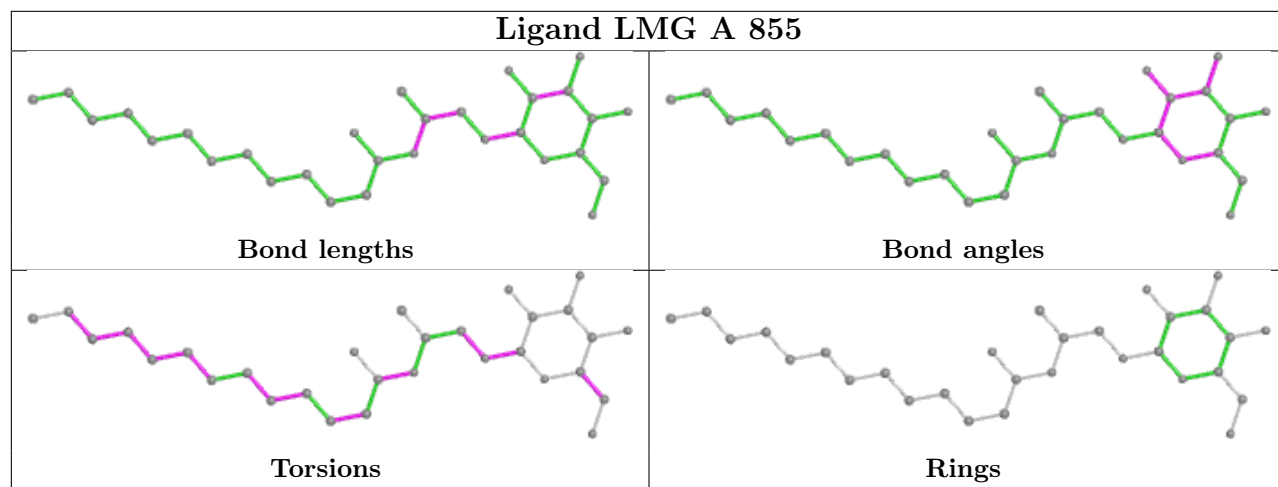


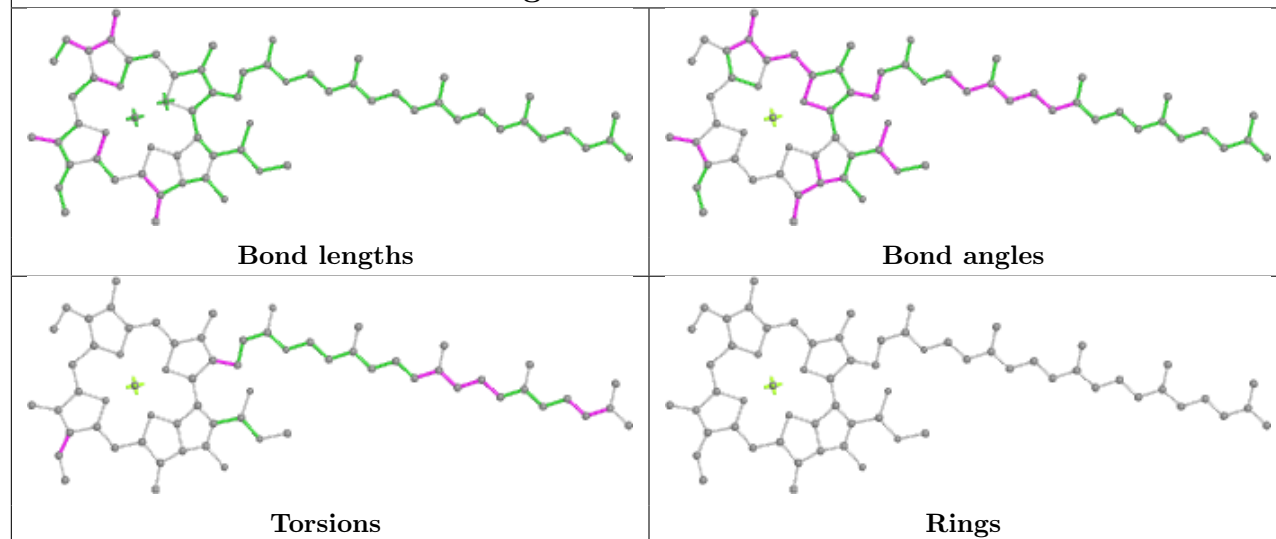
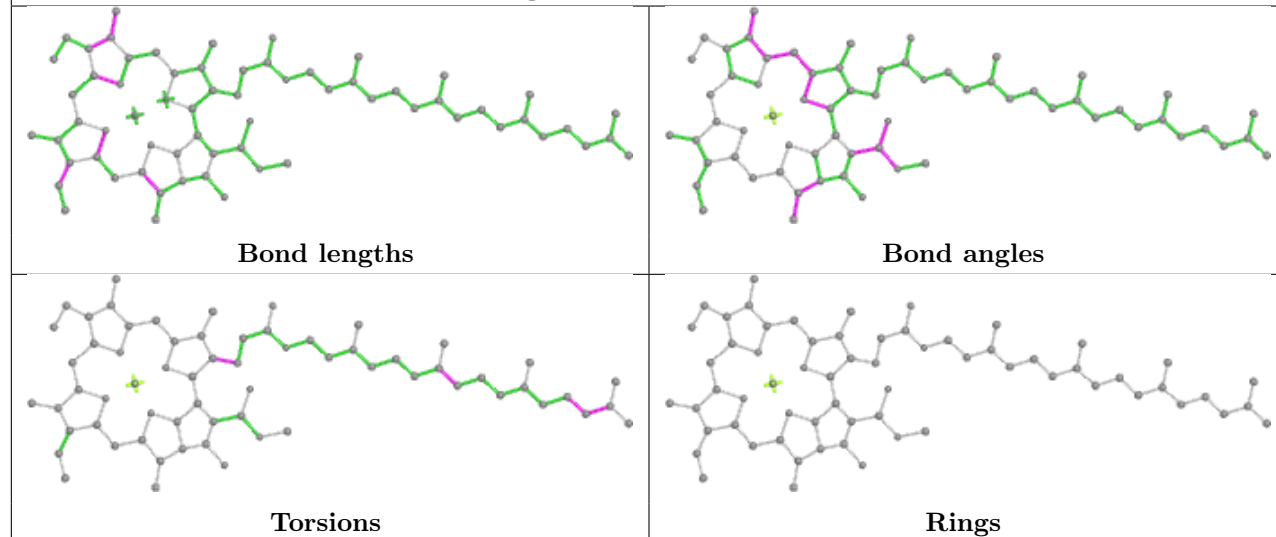
Ligand CLA B 3031

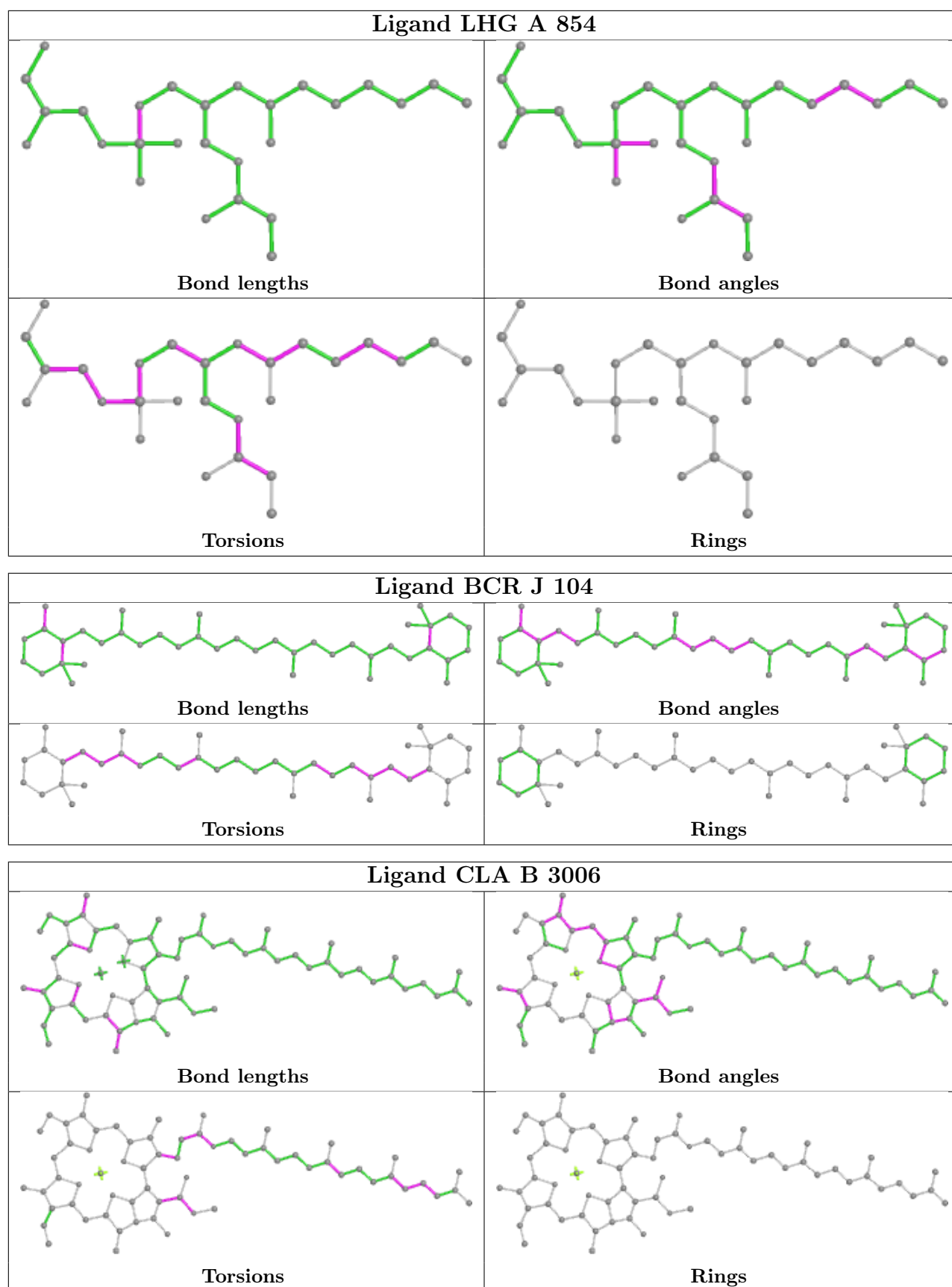


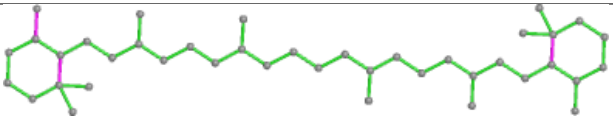
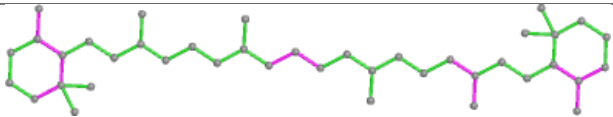
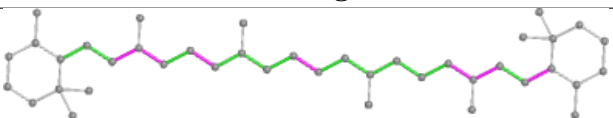
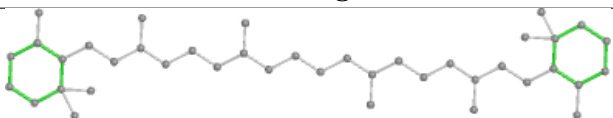
Ligand DGD L 207

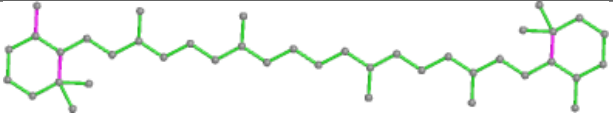
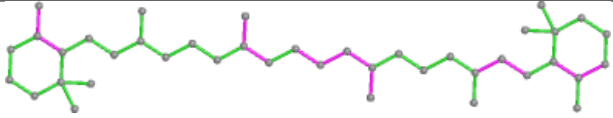
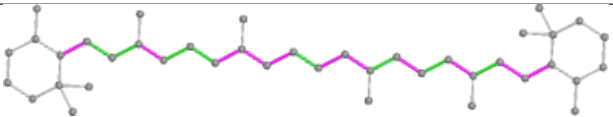
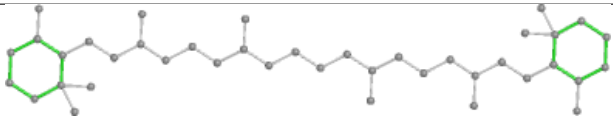




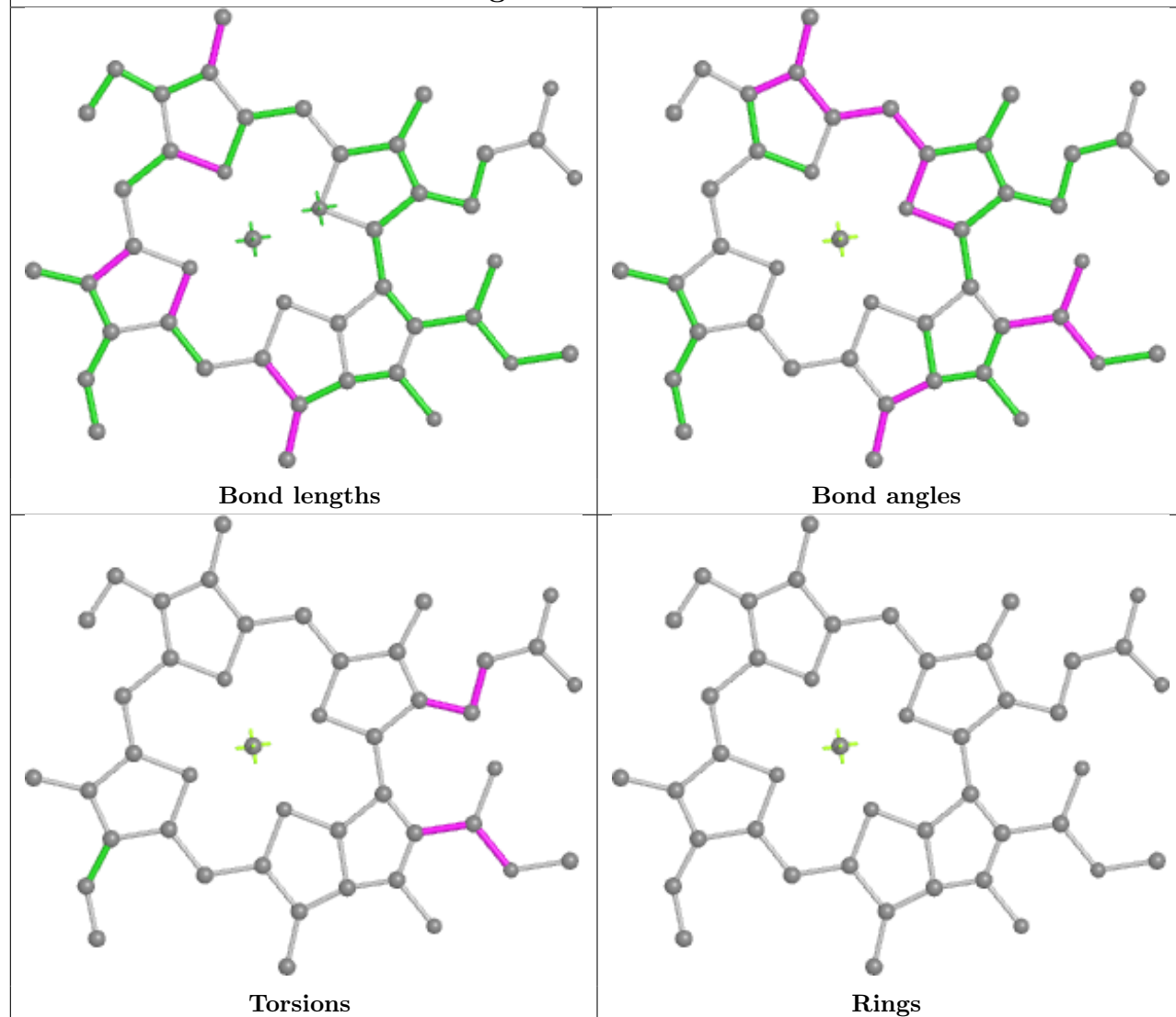
Ligand CLA B 3010**Ligand CLA B 3042**



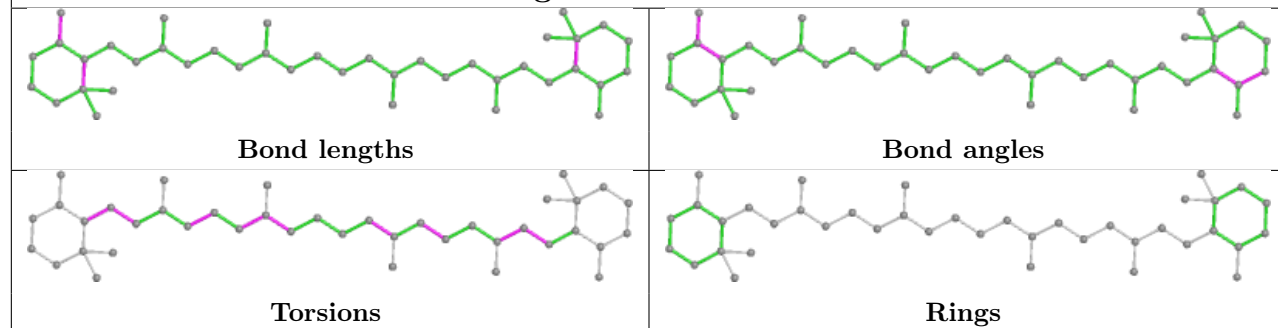
Ligand BCR F 201	
	Bond lengths
	Bond angles
	Torsions
	Rings

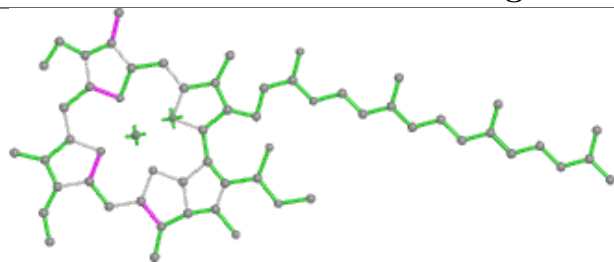
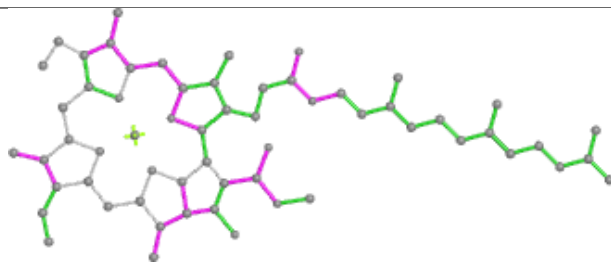
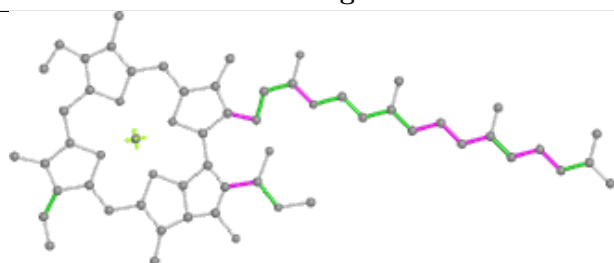
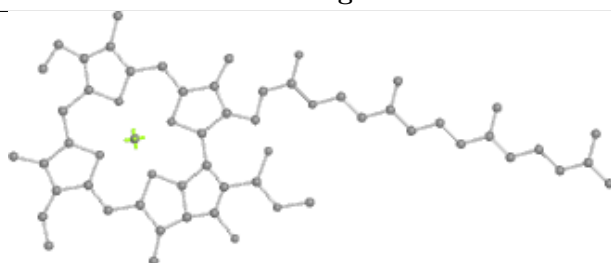
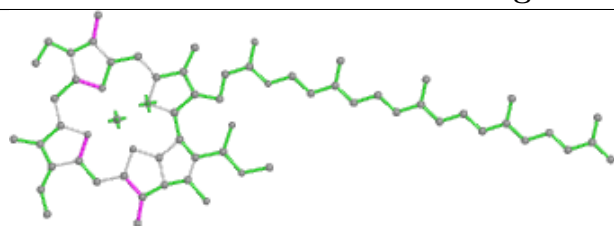
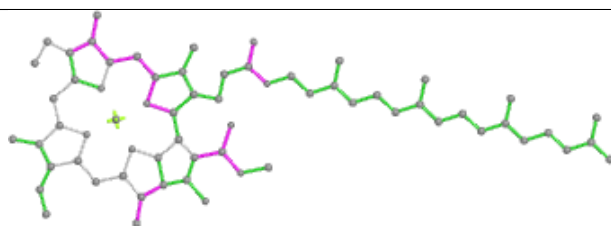
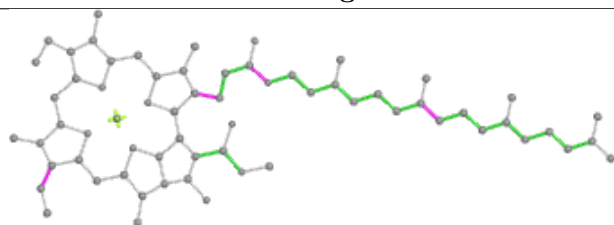
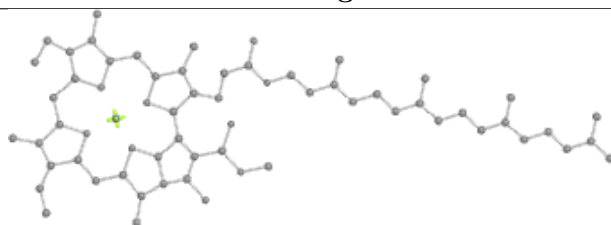
Ligand BCR A 847	
	Bond lengths
	Bond angles
	Torsions
	Rings

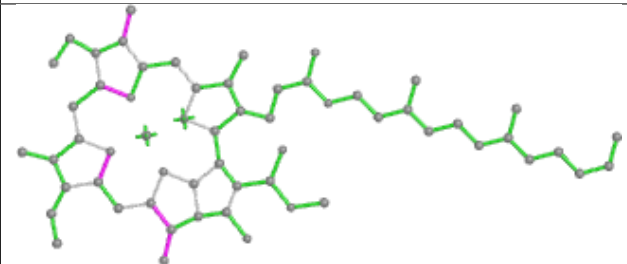
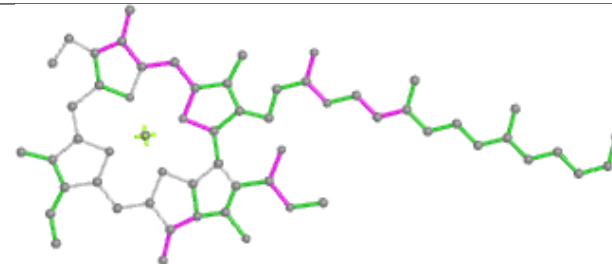
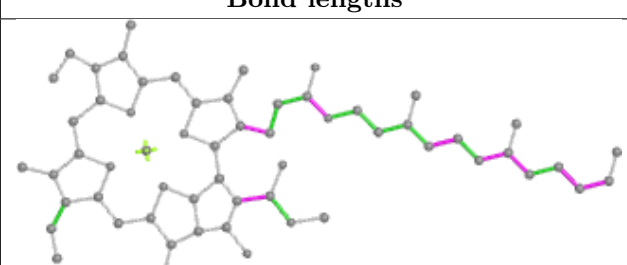
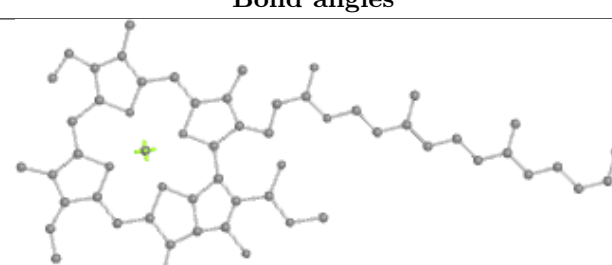
Ligand CLA A 837

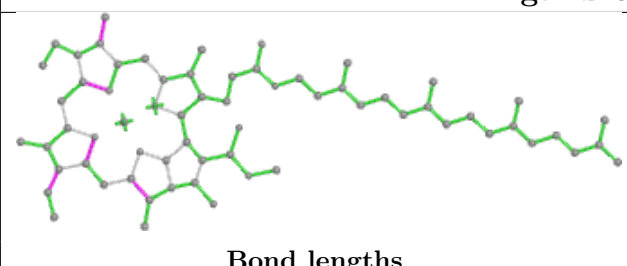
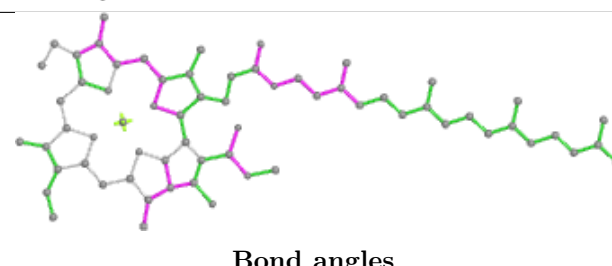
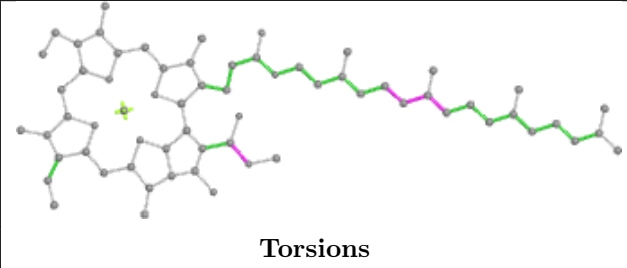
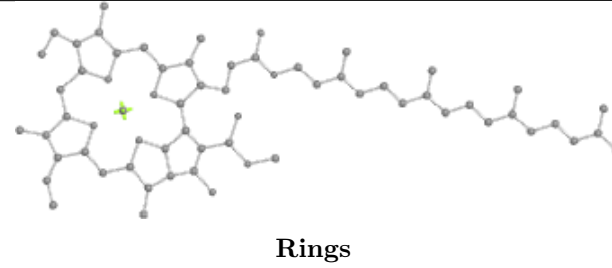


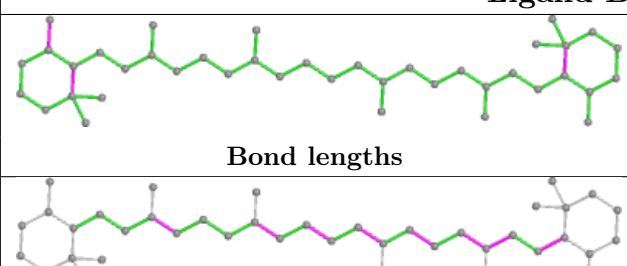
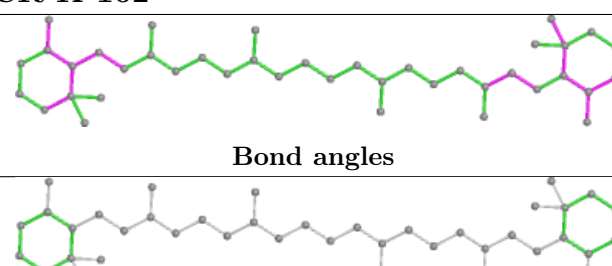


Ligand BCR J 103



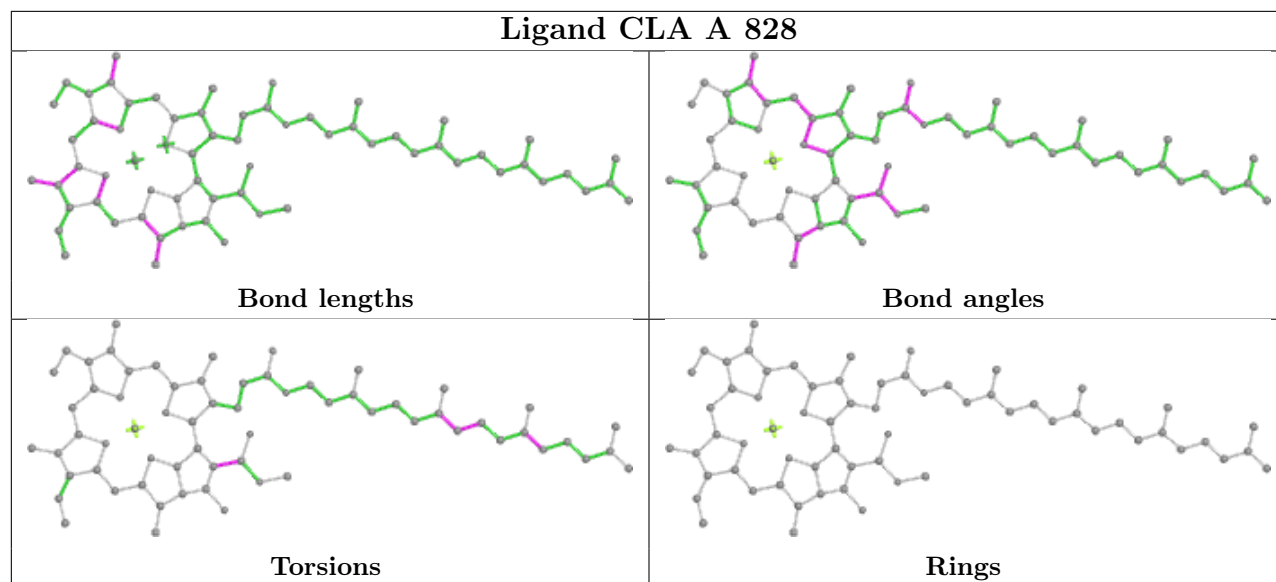
Ligand CLA B 3019**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 843****Bond lengths****Bond angles****Torsions****Rings**

Ligand CLA B 3018	
	
Bond lengths	Bond angles
	
Torsions	Rings

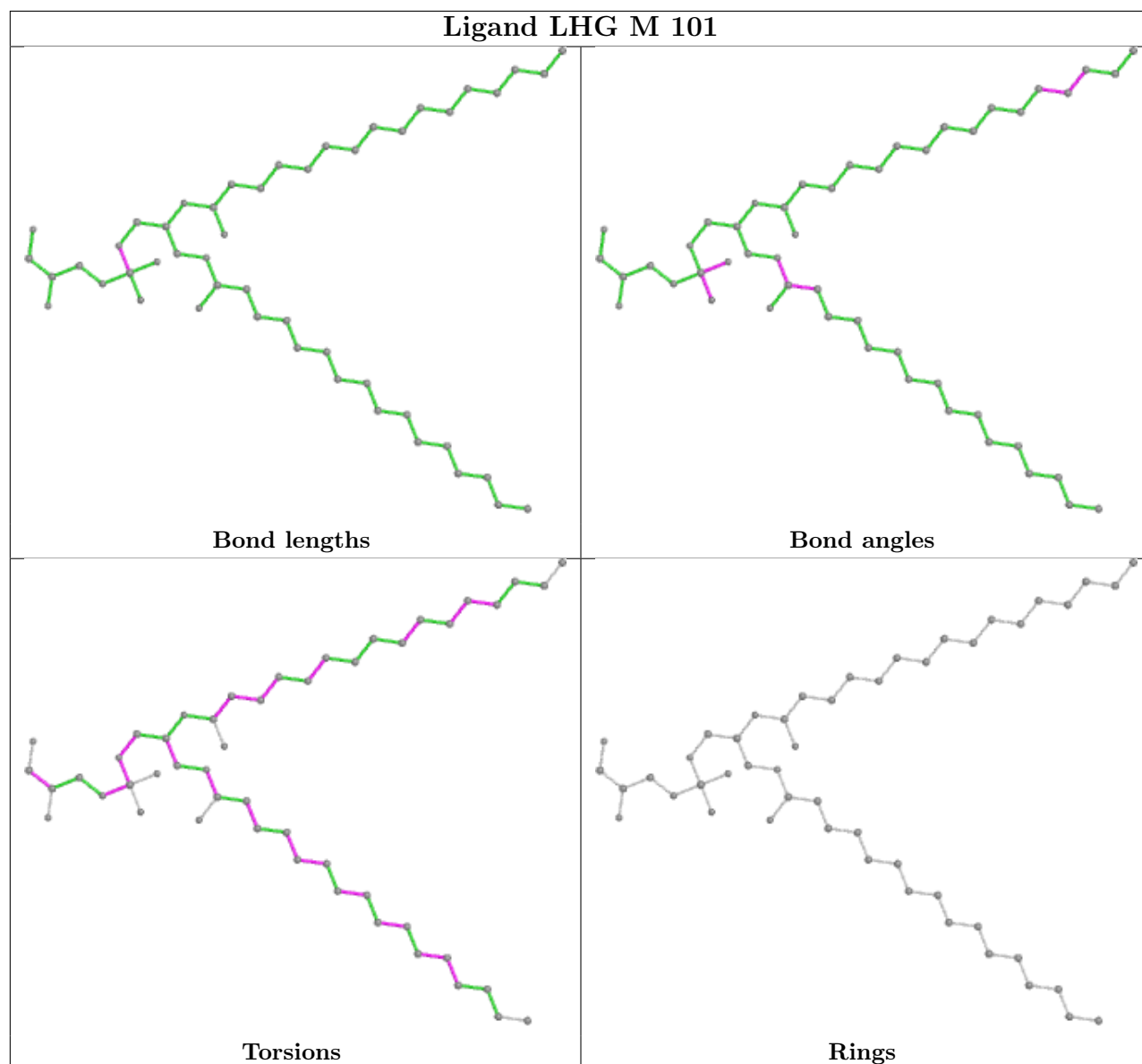
Ligand CLA A 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

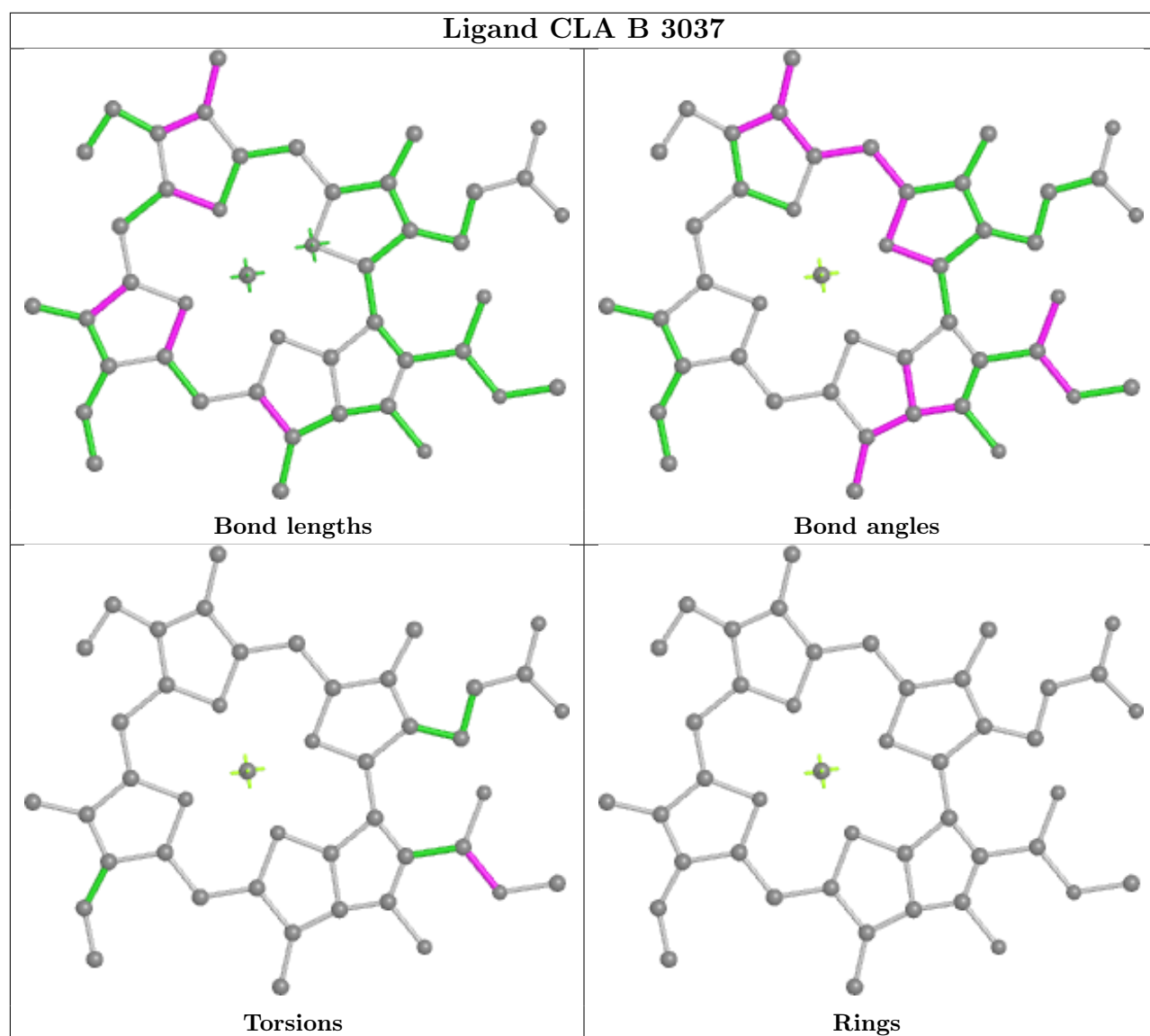
Ligand BCR K 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 828

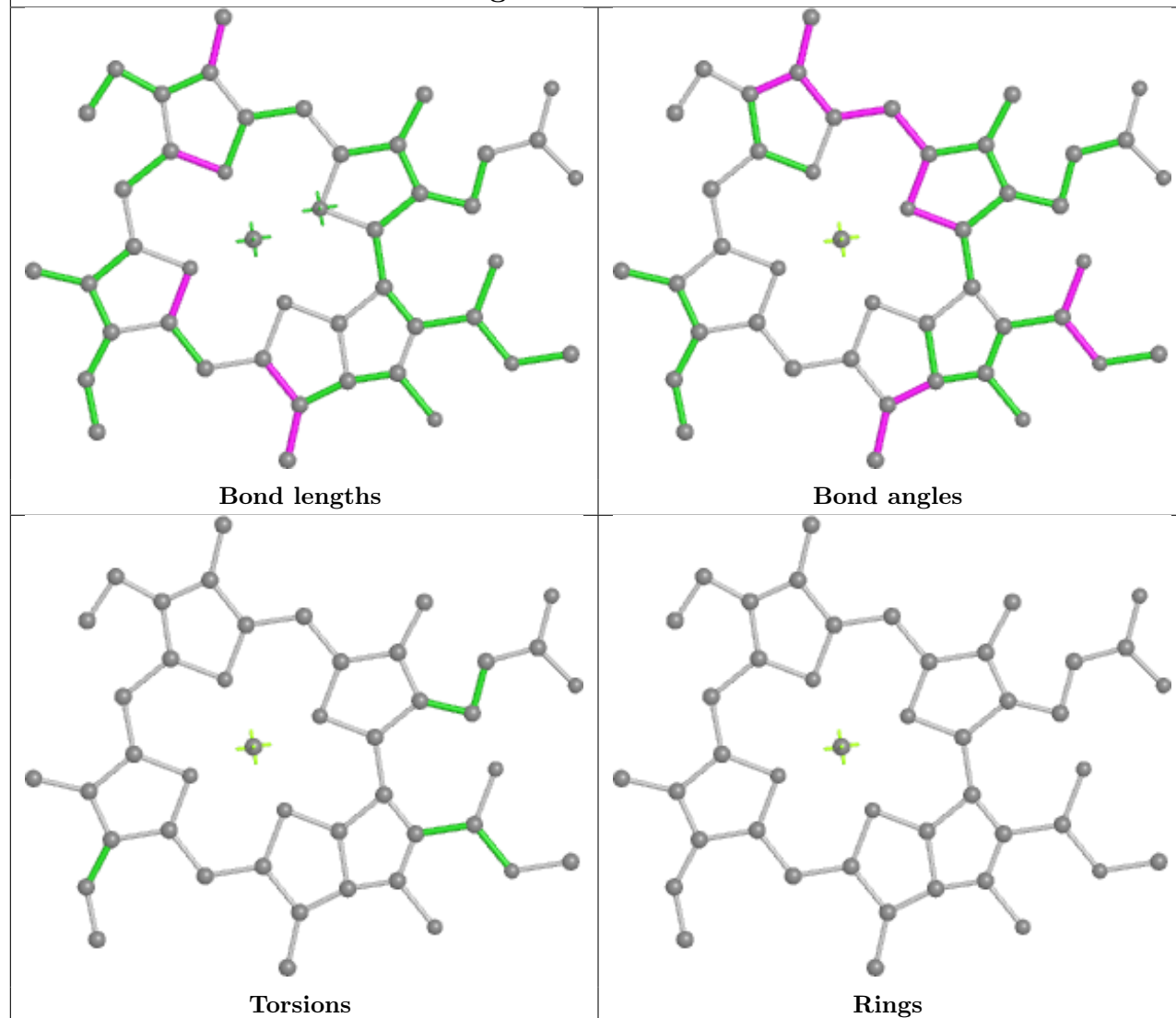


Ligand LHG M 101

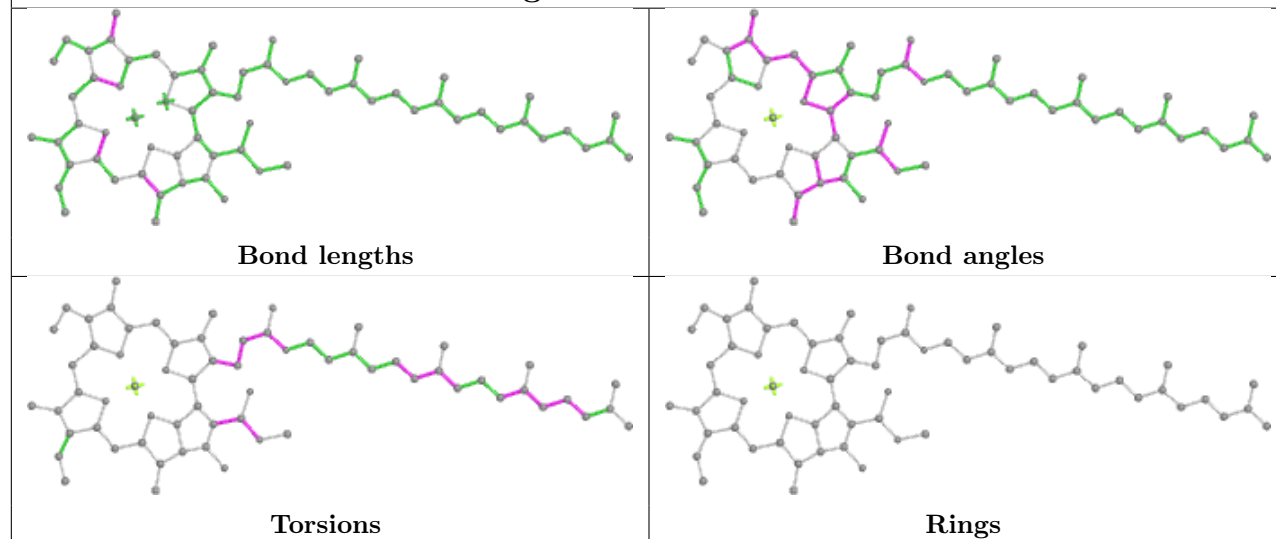




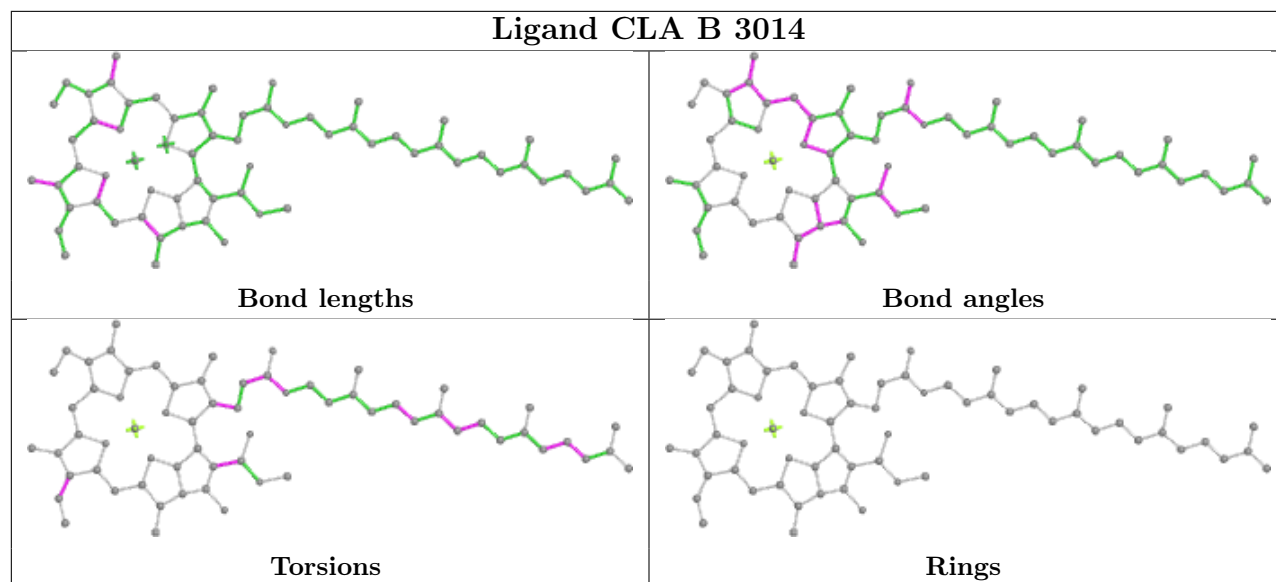
Ligand CLA A 815



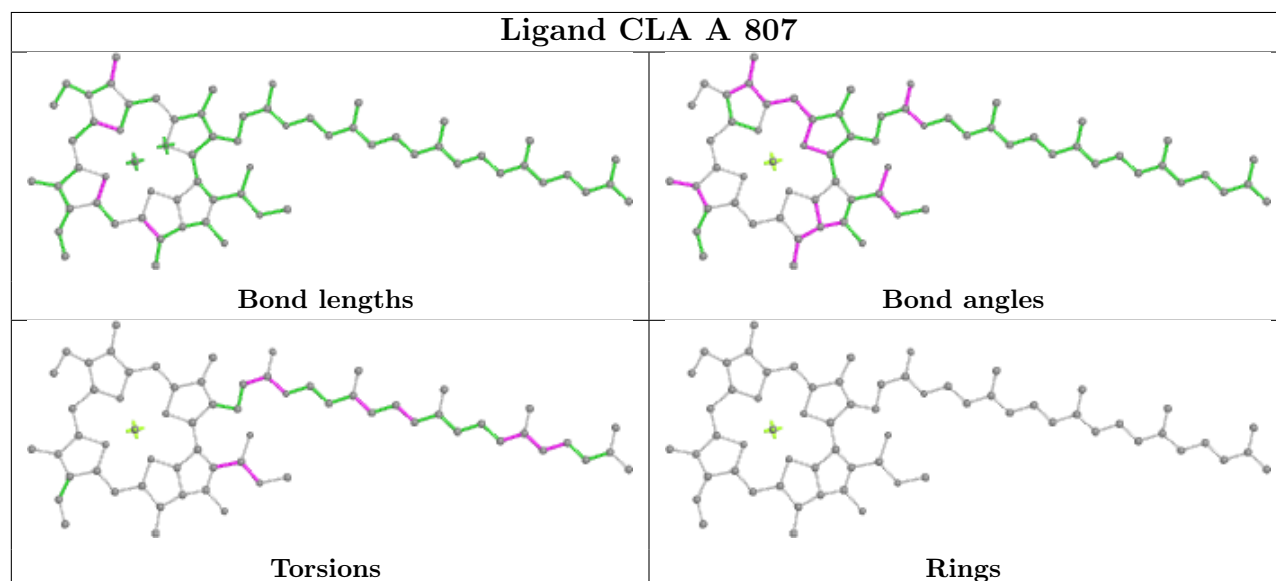
Ligand CLA B 3029



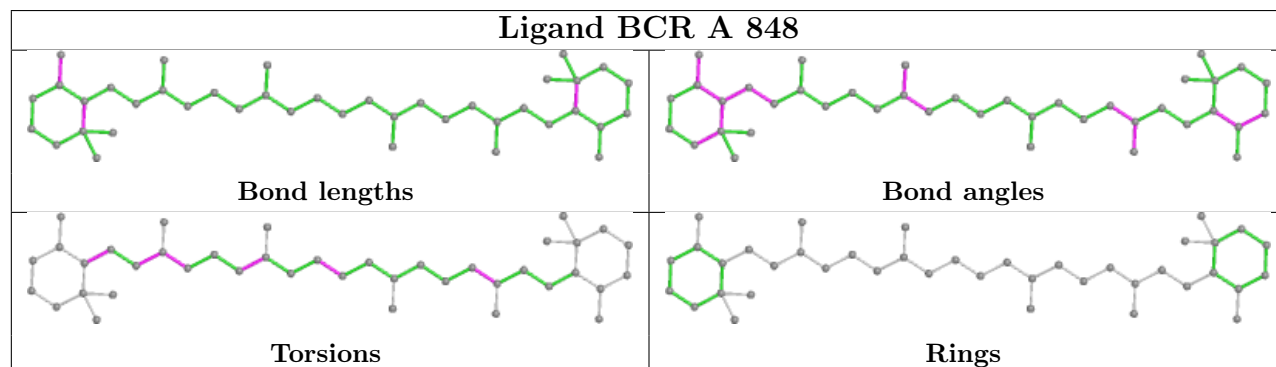
Ligand CLA B 3014

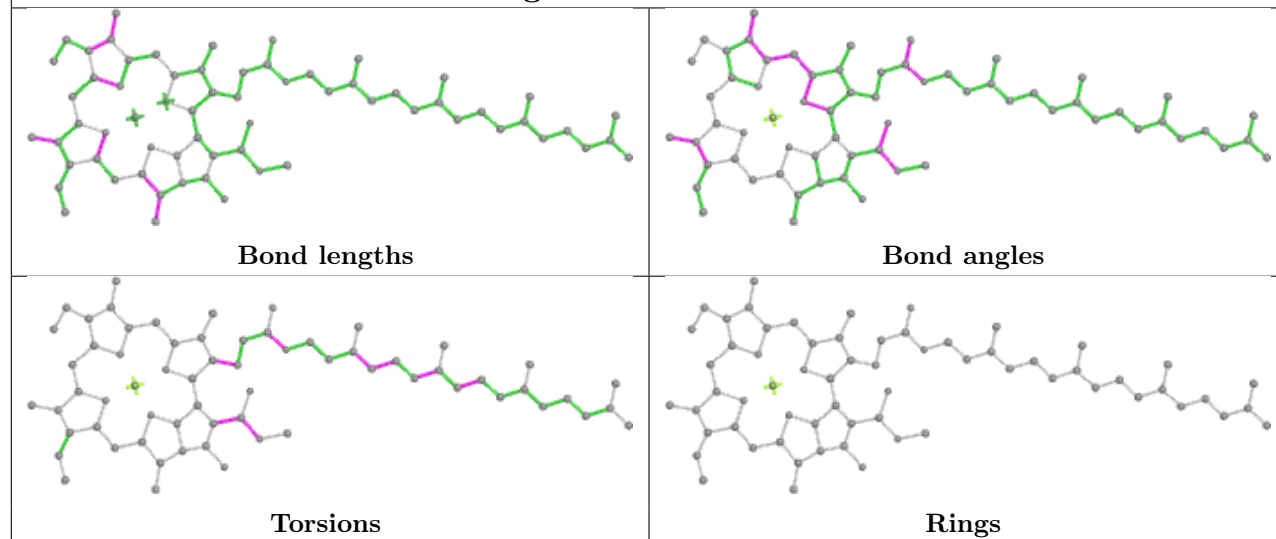
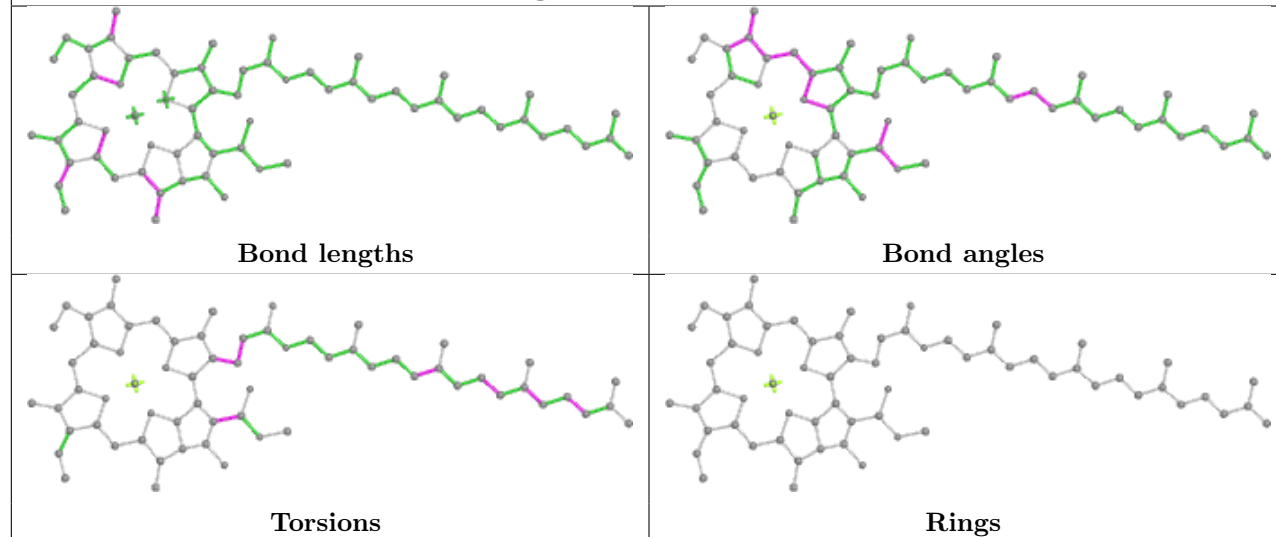
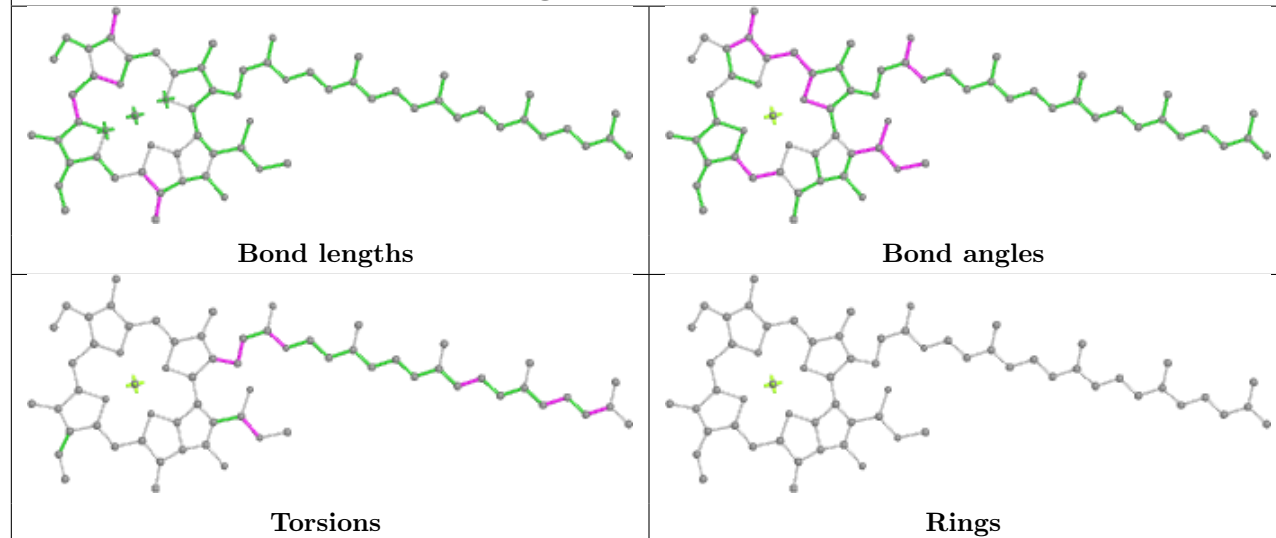


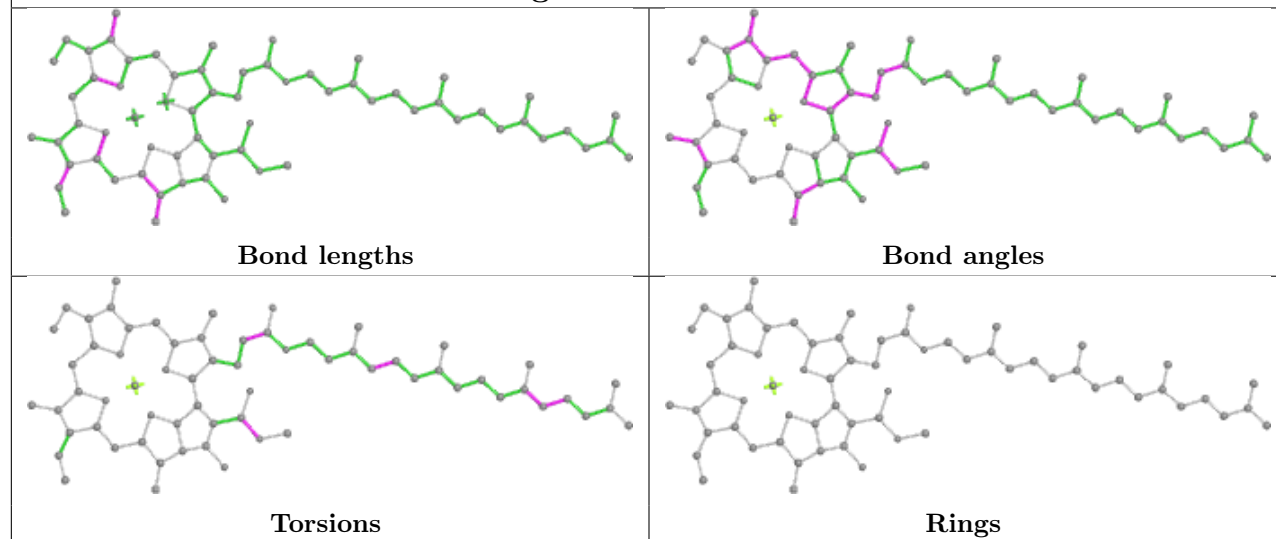
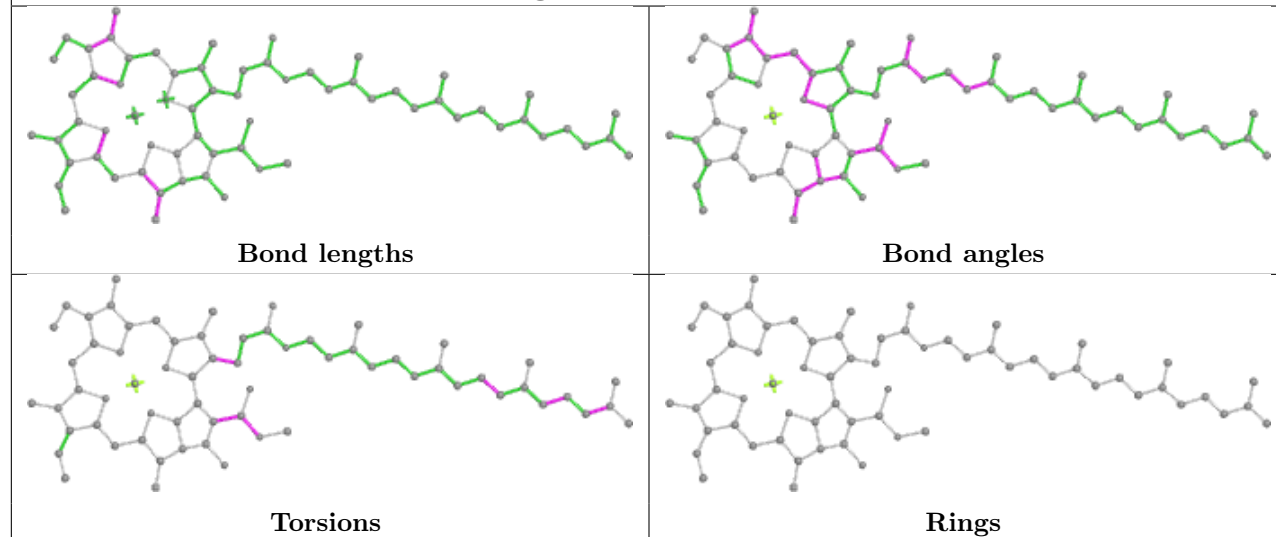
Ligand CLA A 807



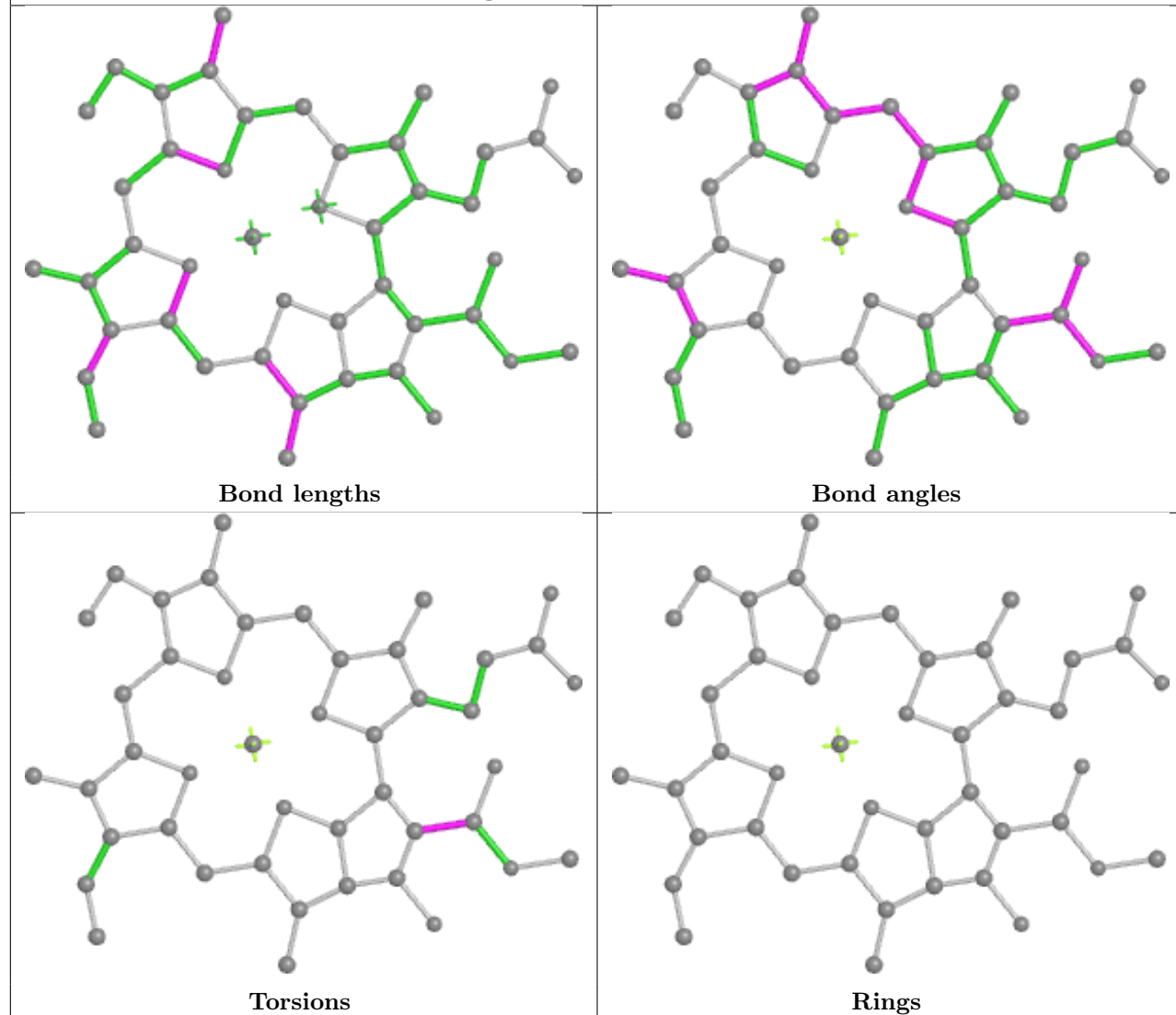
Ligand BCR A 848



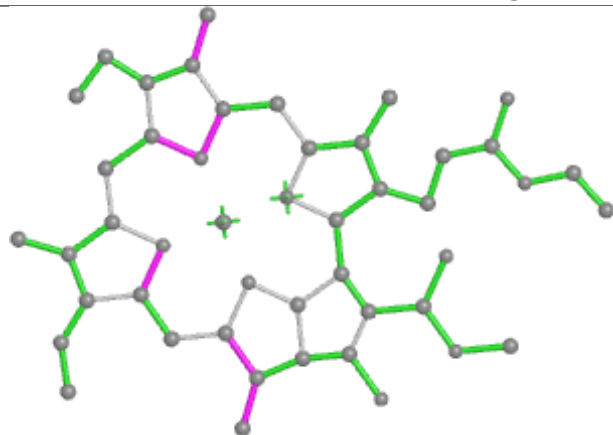
Ligand CLA B 3003**Ligand CLA A 802****Ligand CL0 A 801**

Ligand CLA A 803**Ligand CLA A 831**

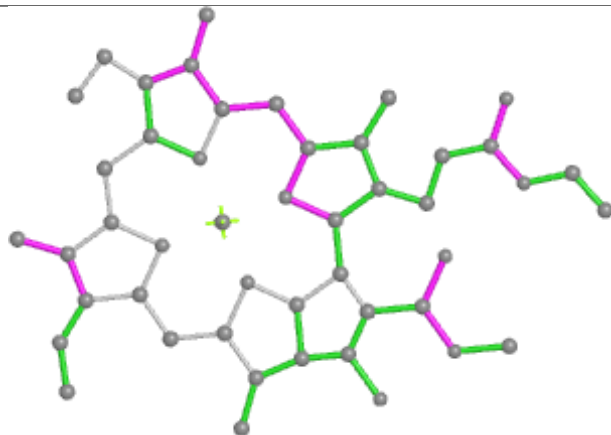
Ligand CLA X 1701



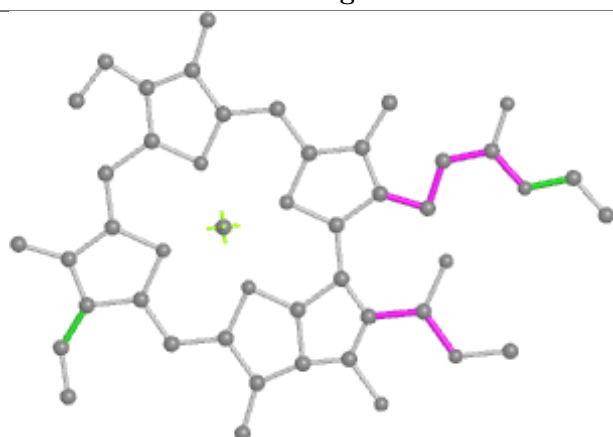
Ligand CLA B 3021



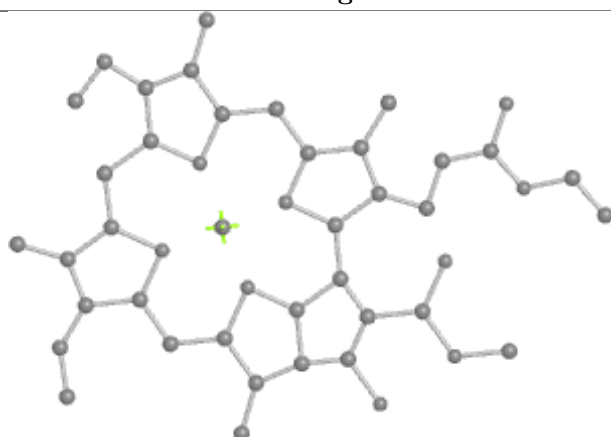
Bond lengths



Bond angles

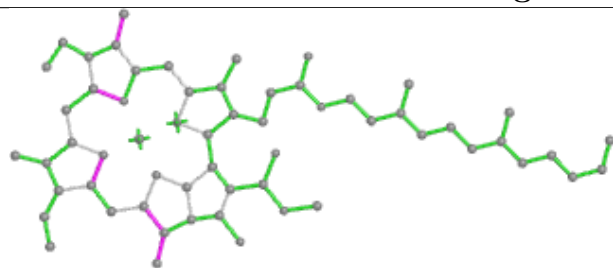


Torsions

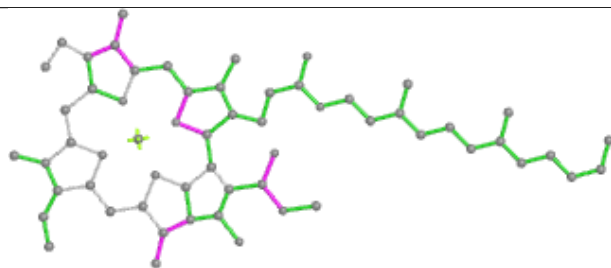


Rings

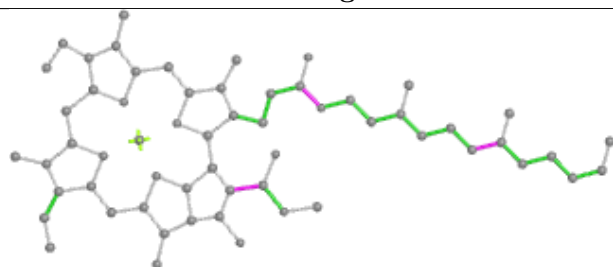
Ligand CLA A 805



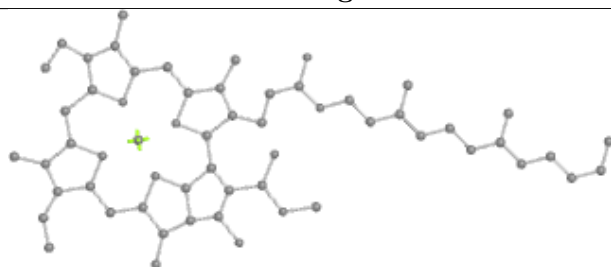
Bond lengths



Bond angles

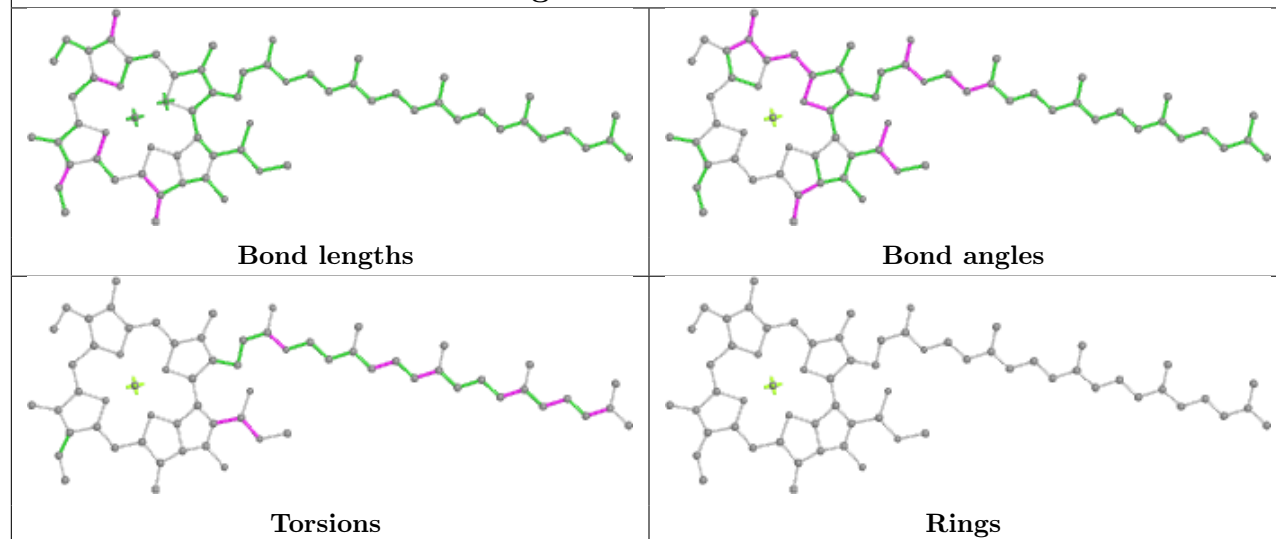


Torsions

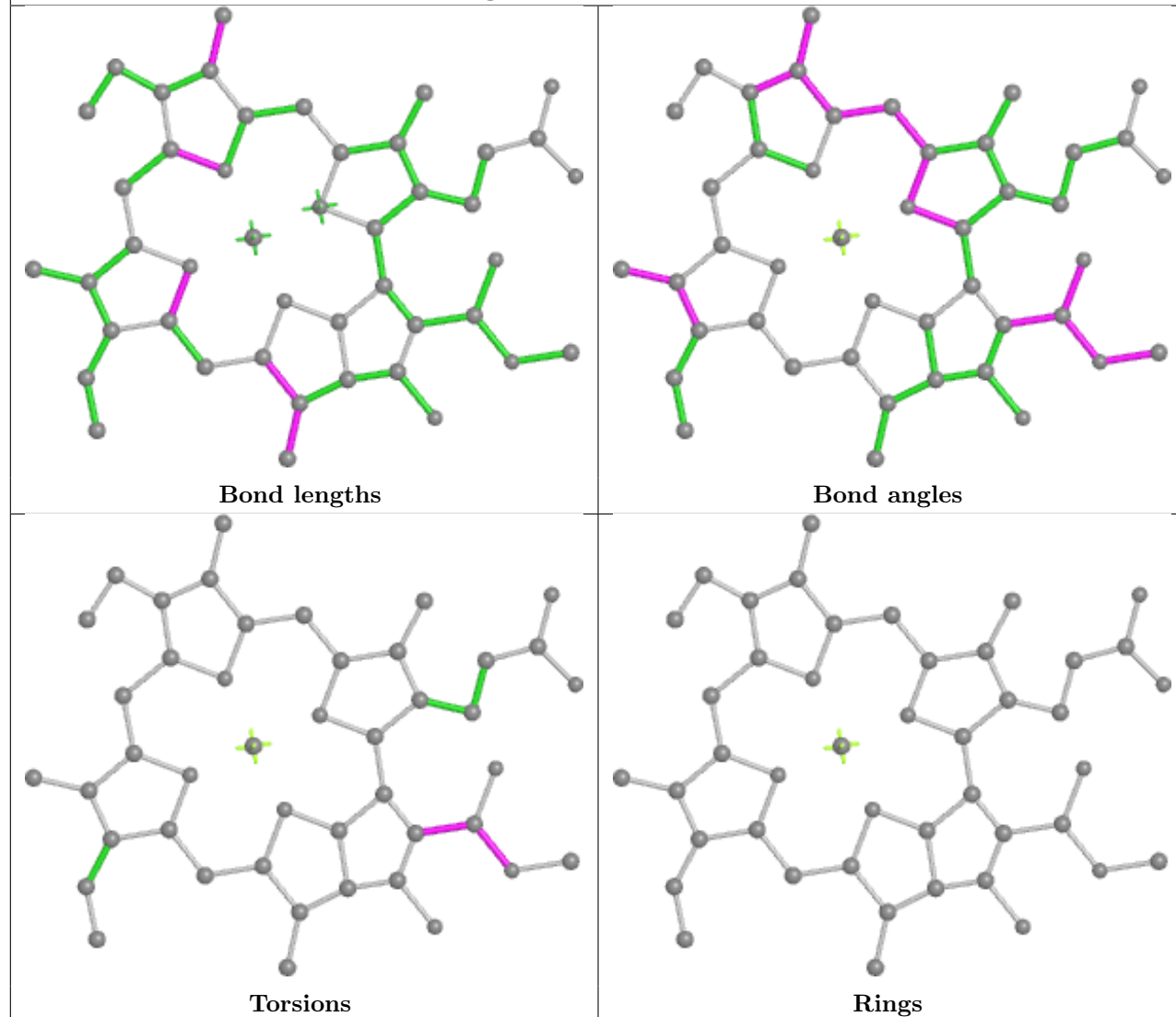


Rings

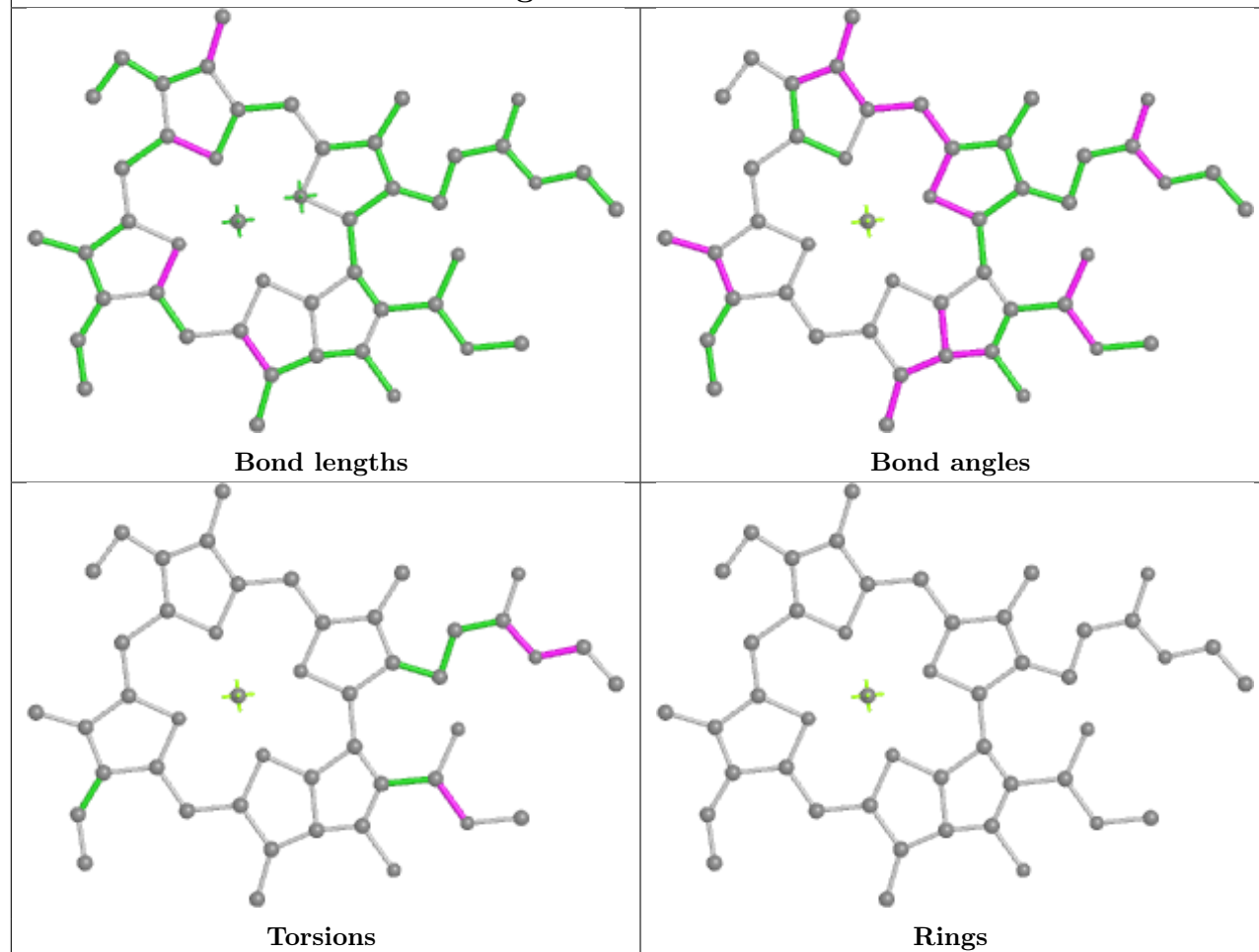
Ligand CLA A 829



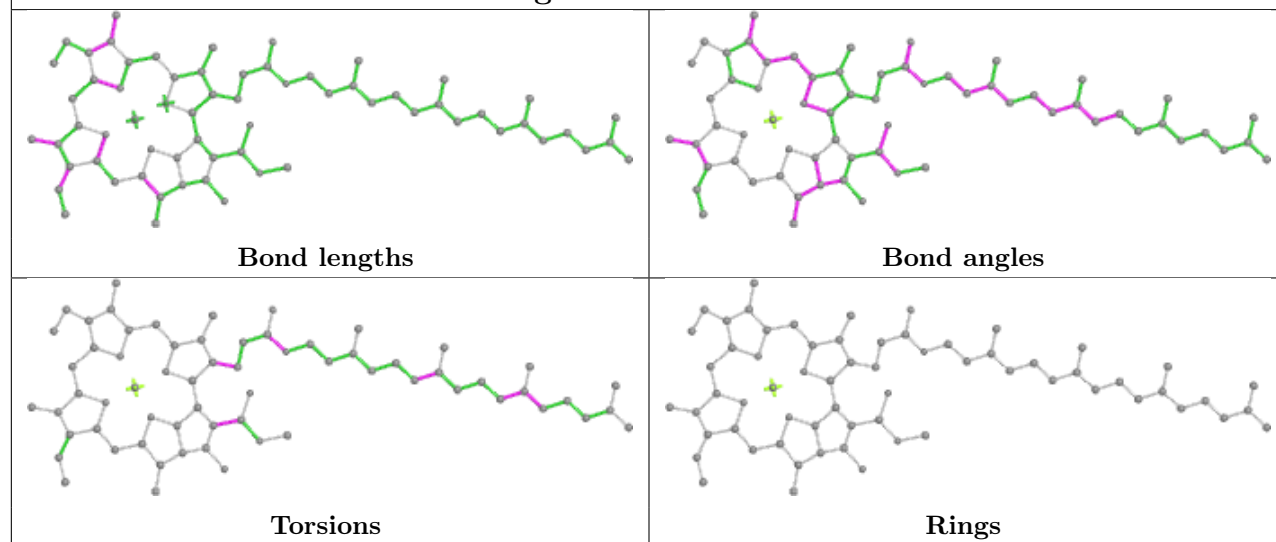
Ligand CLA B 3012



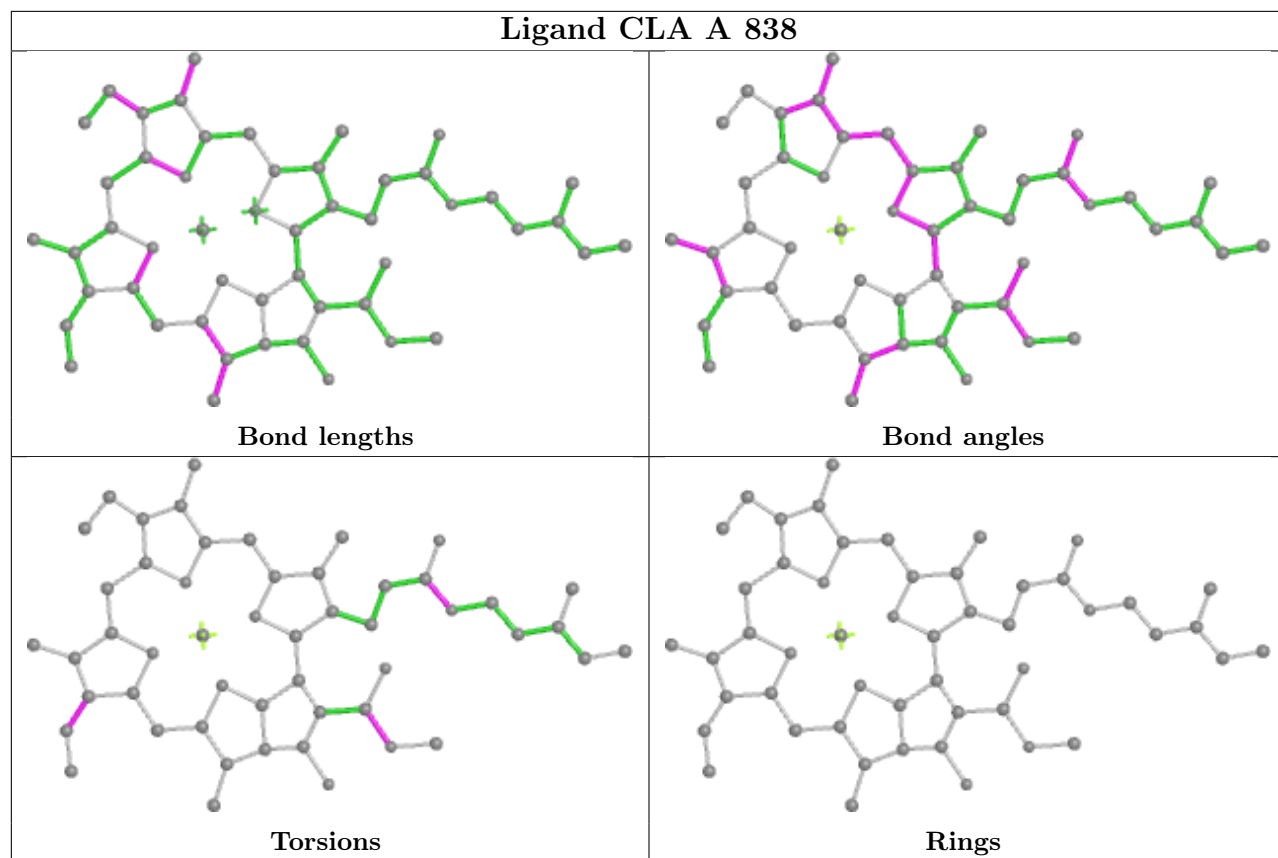
Ligand CLA B 3040

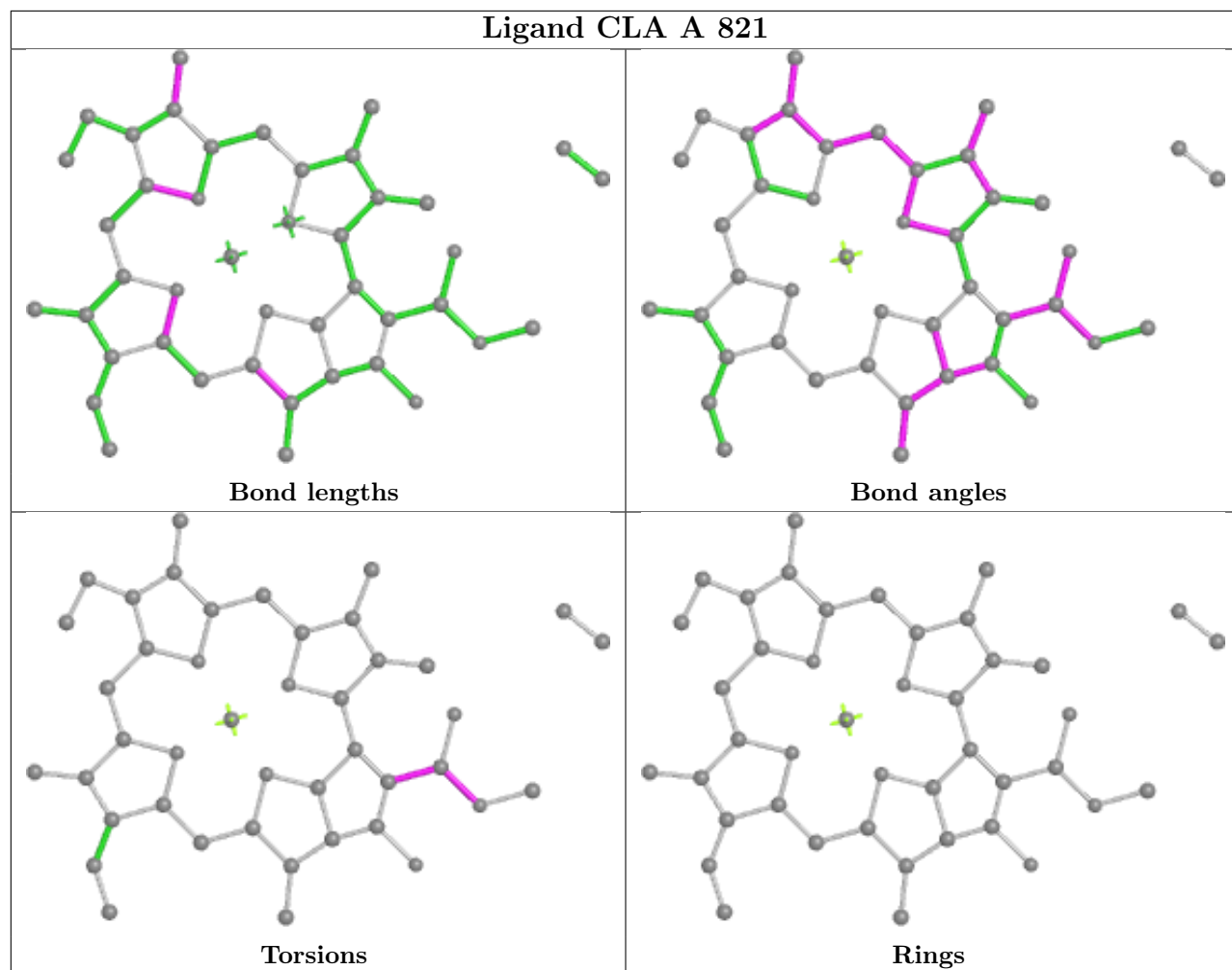


Ligand CLA L 204

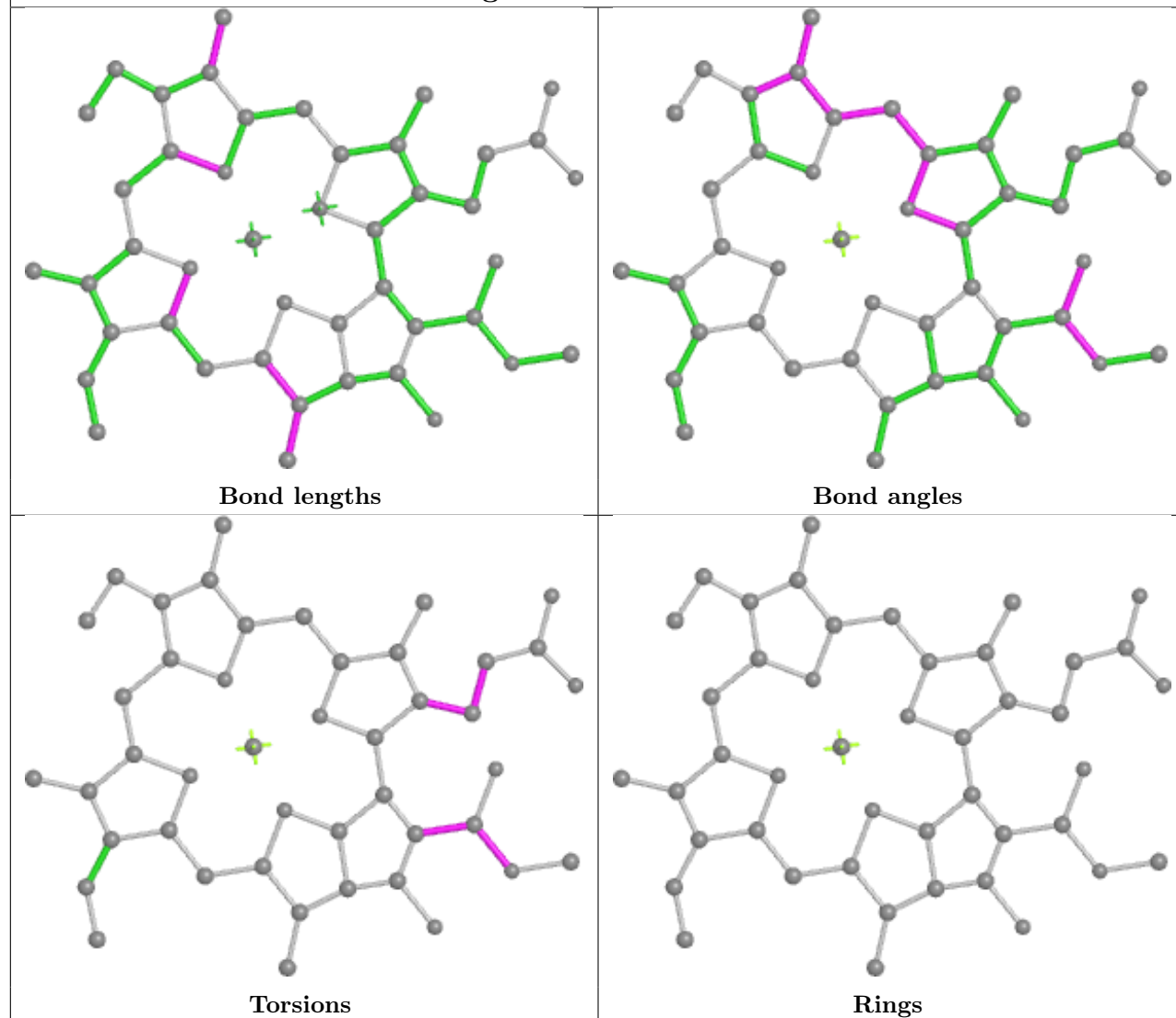


Ligand CLA A 838

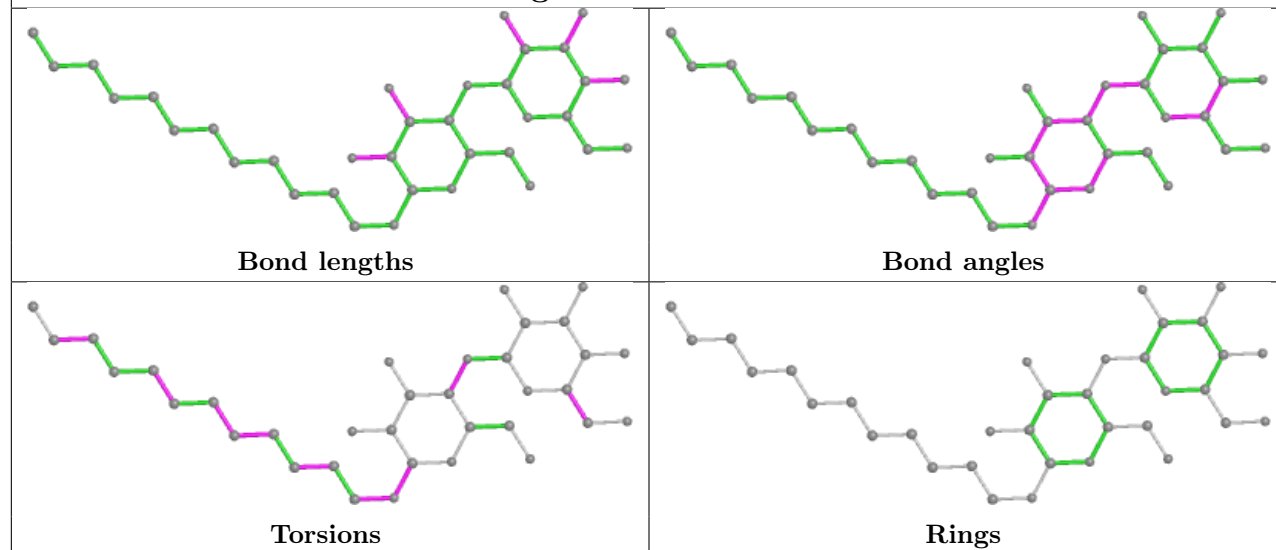




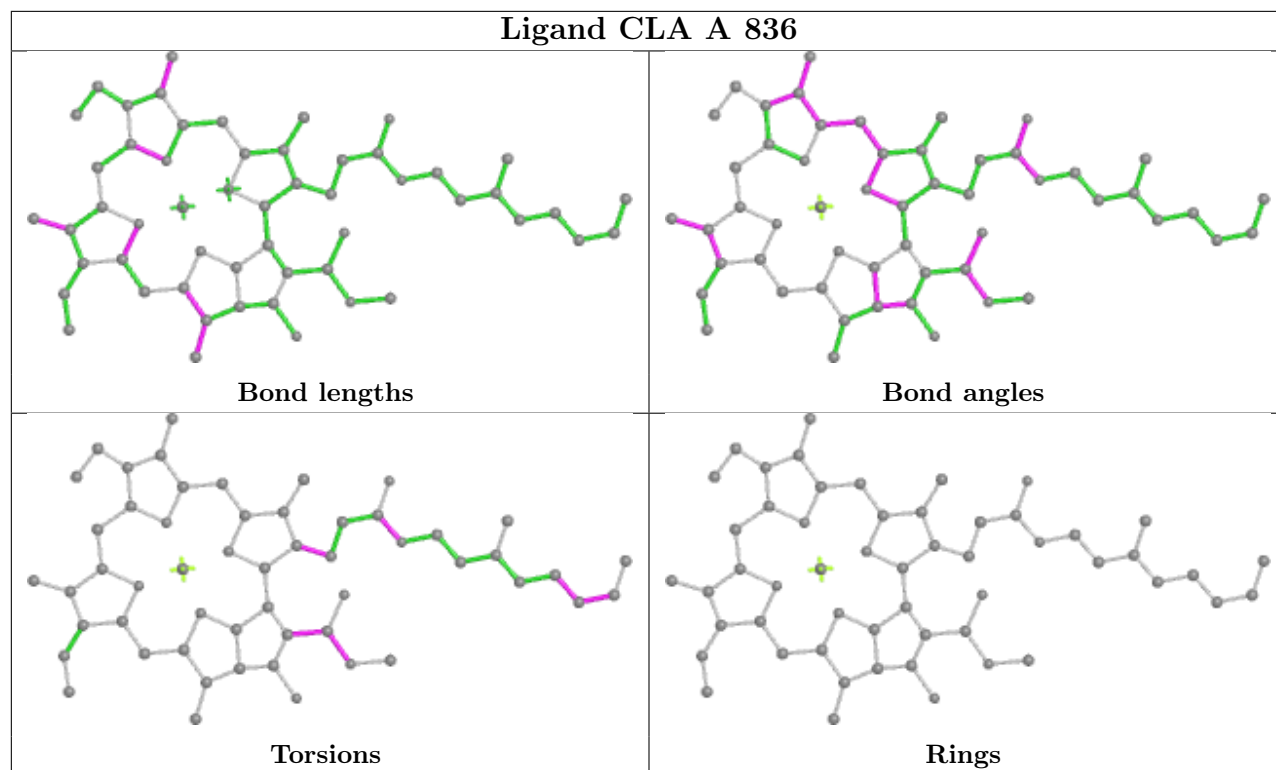
Ligand CLA B 3016



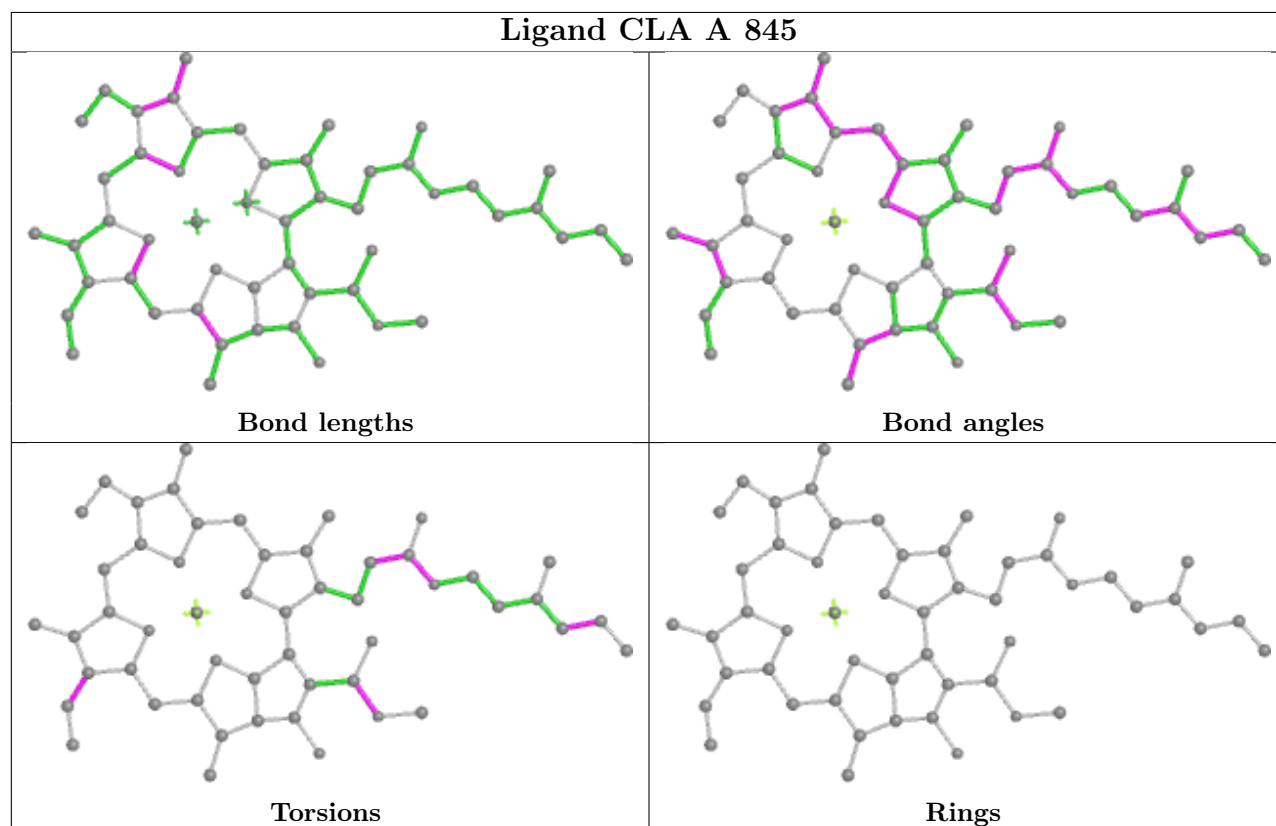
Ligand LMT L 202

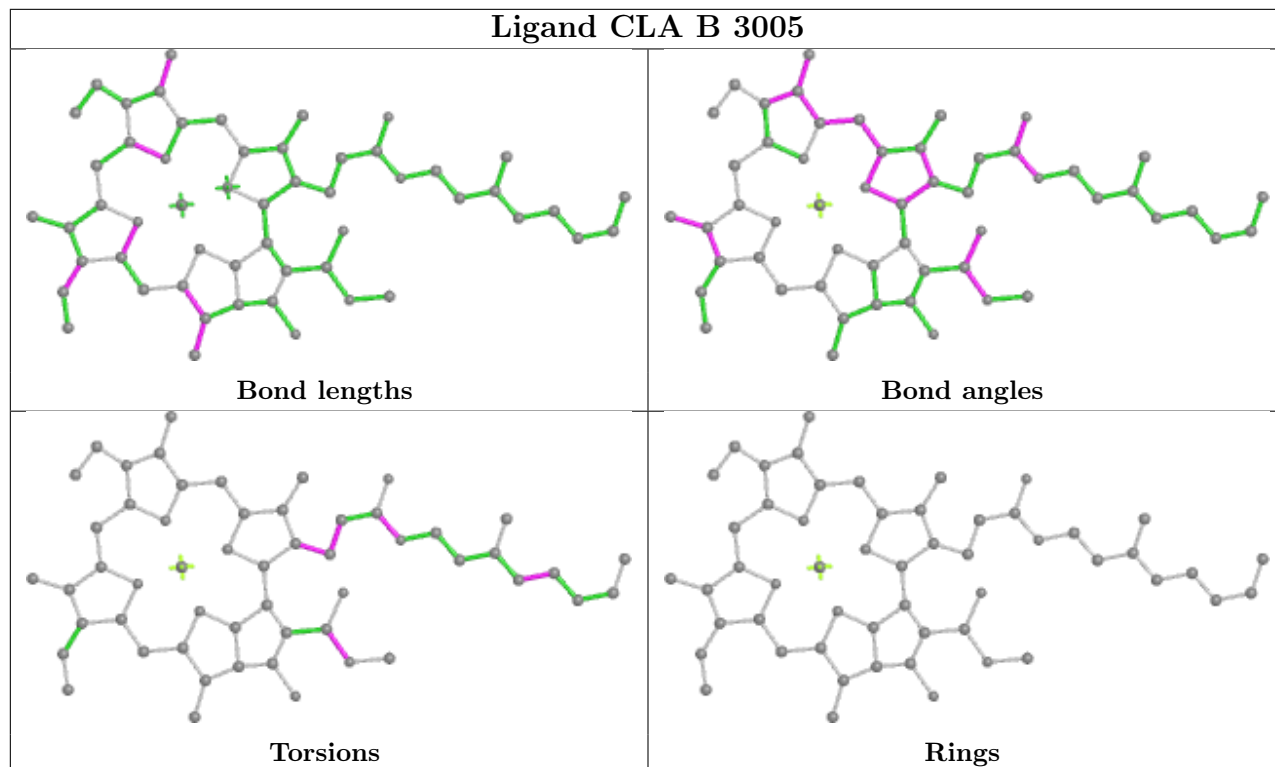
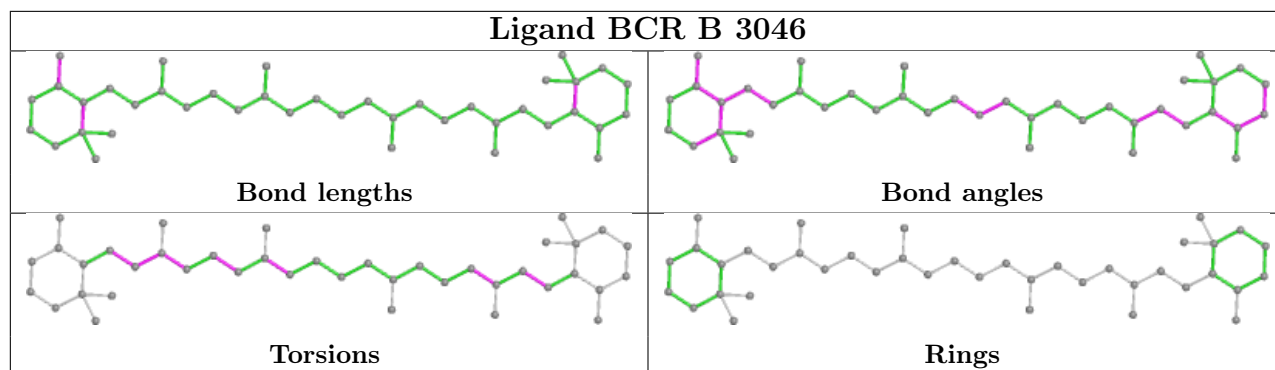


Ligand CLA A 836

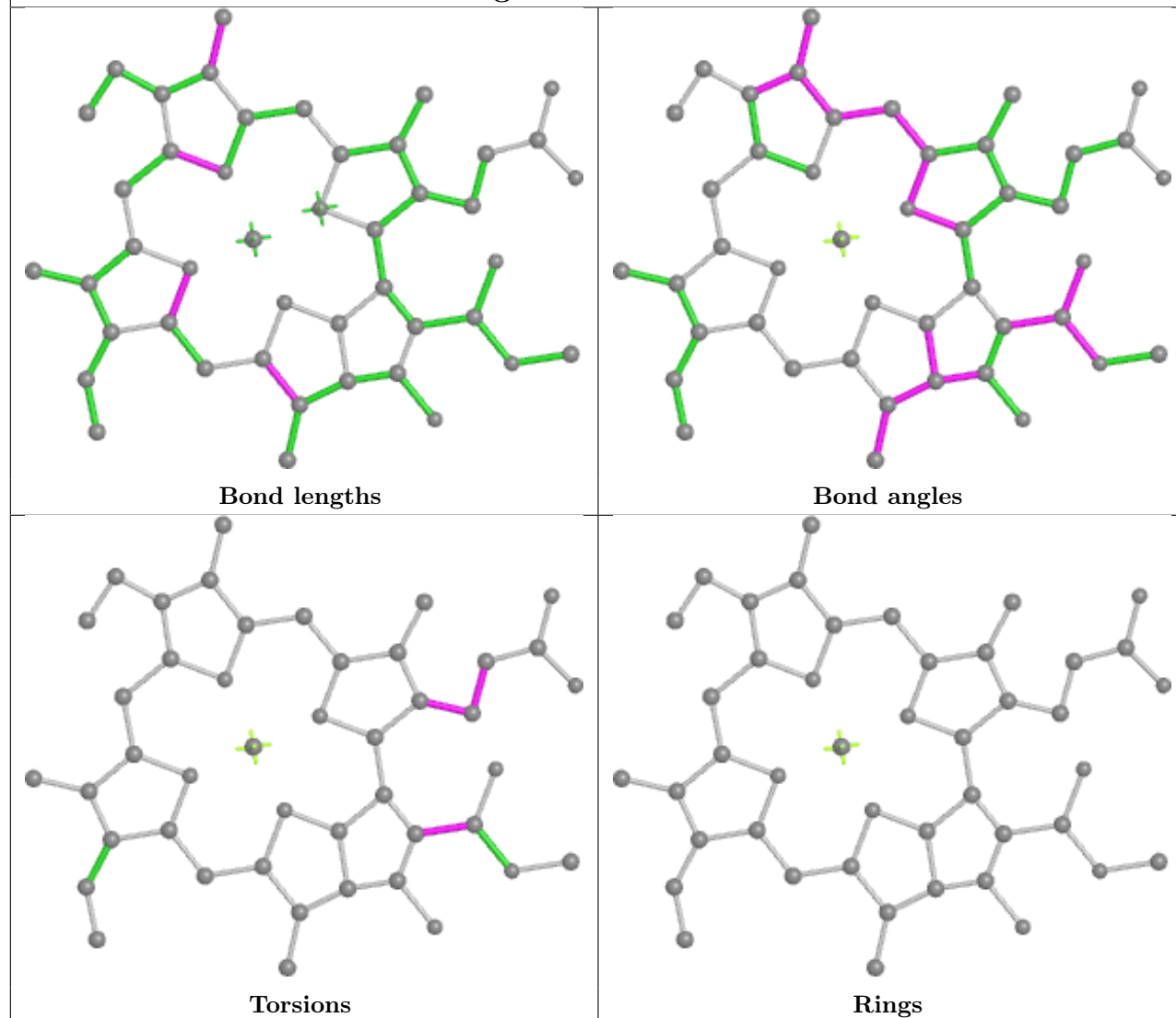


Ligand CLA A 845

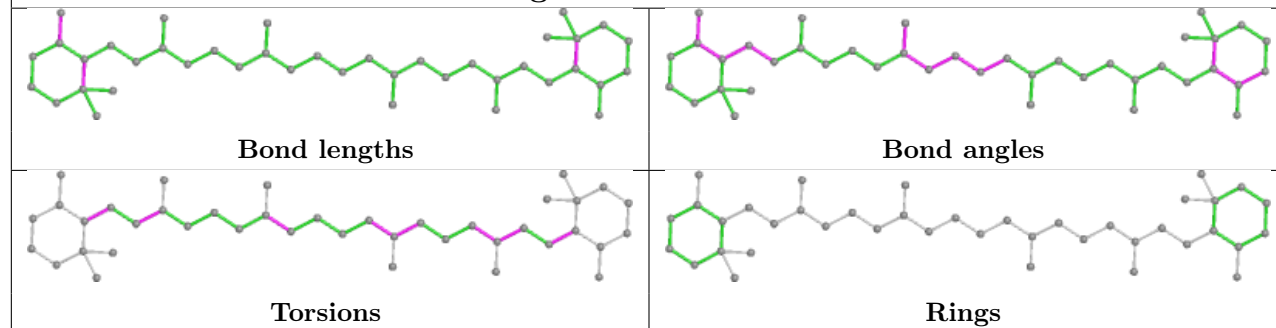


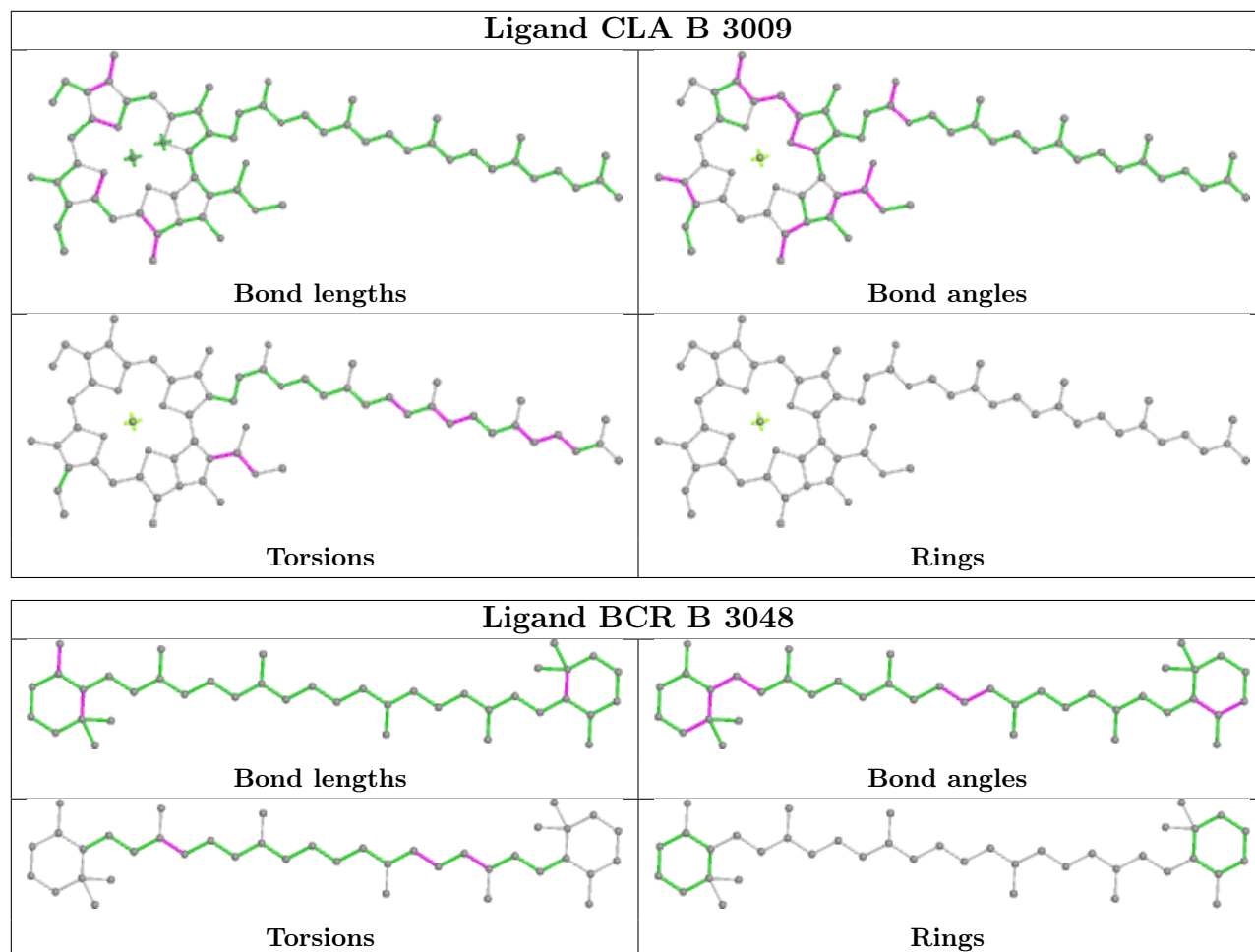


Ligand CLA J 101

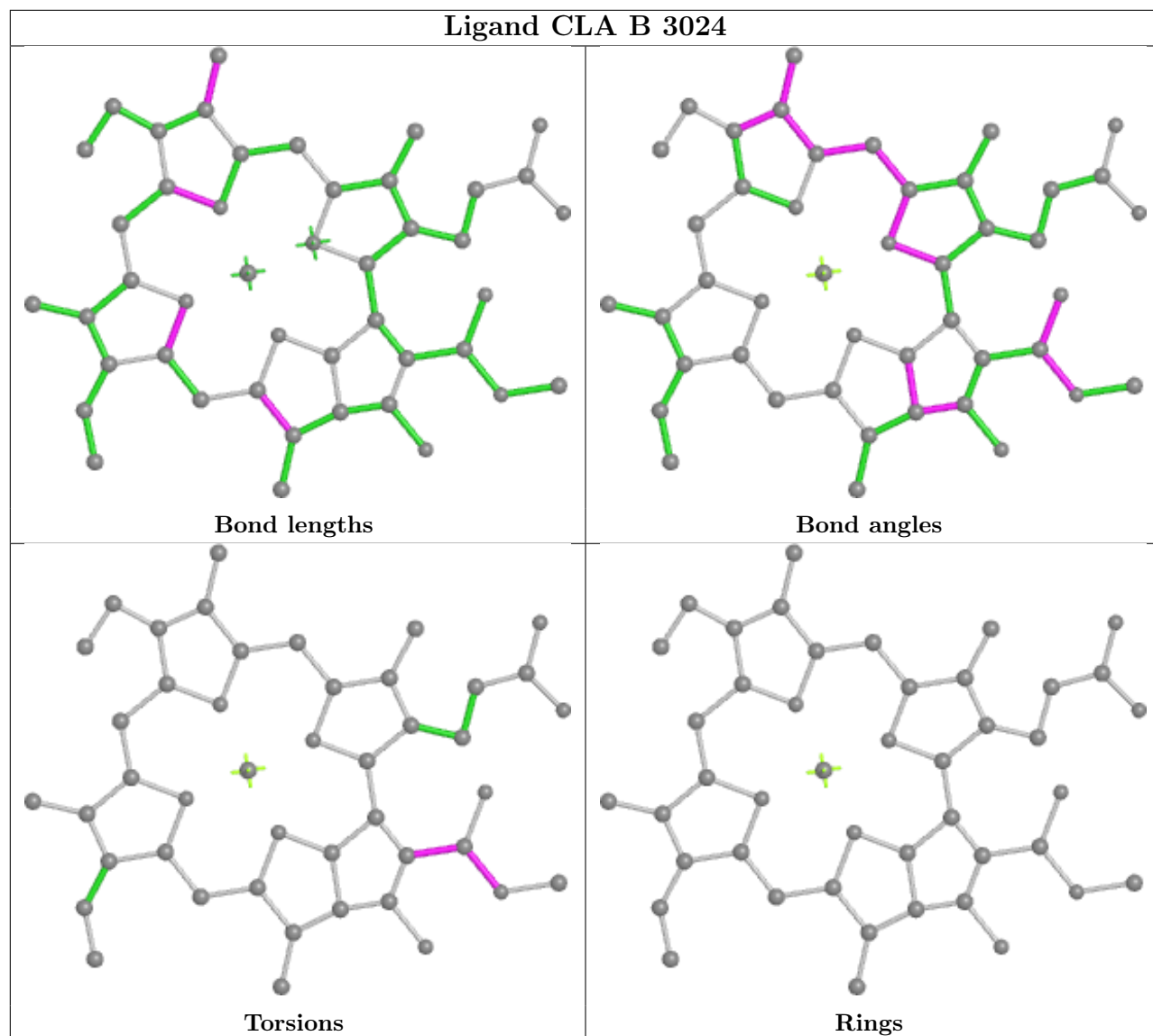


Ligand BCR A 849

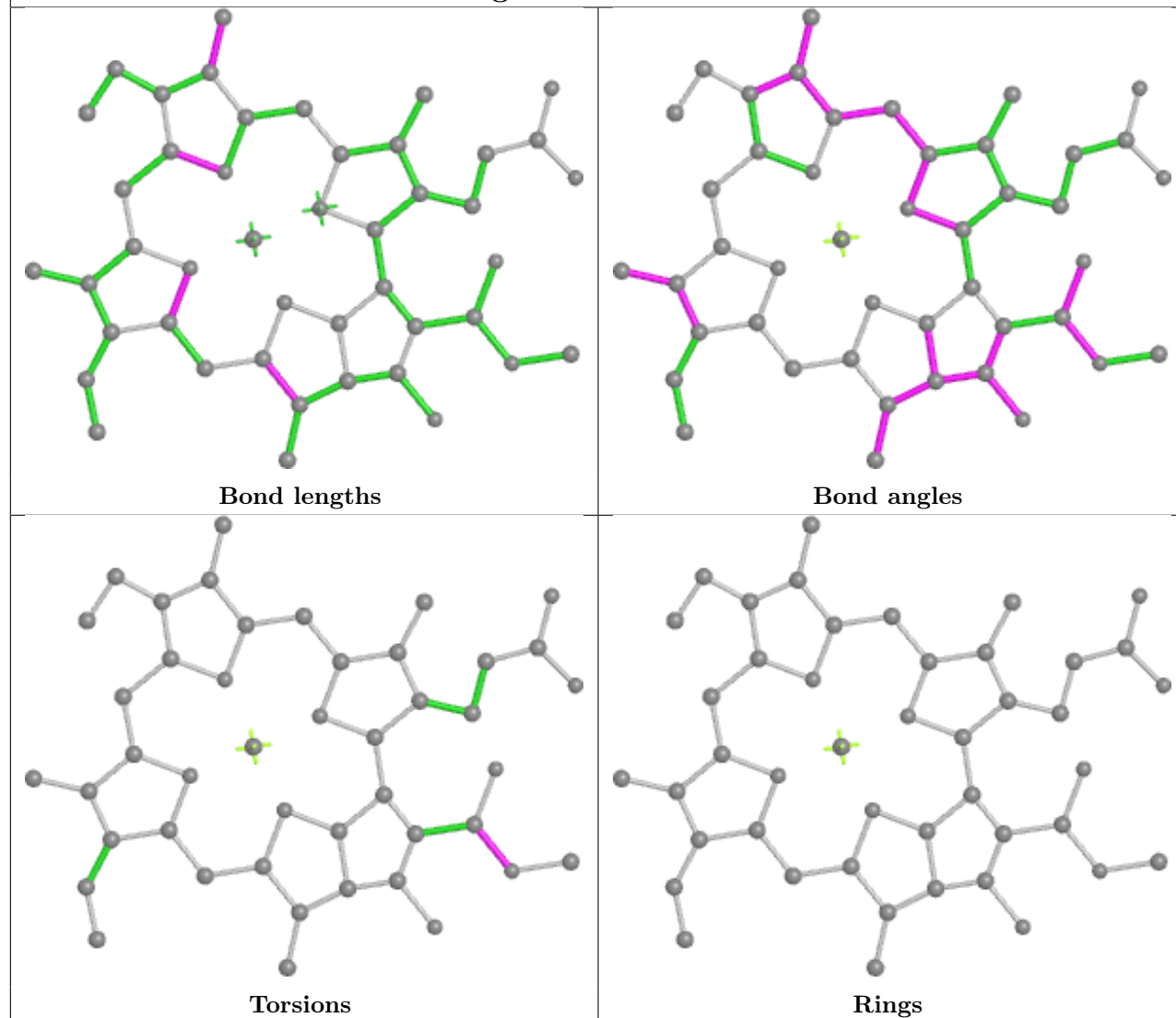




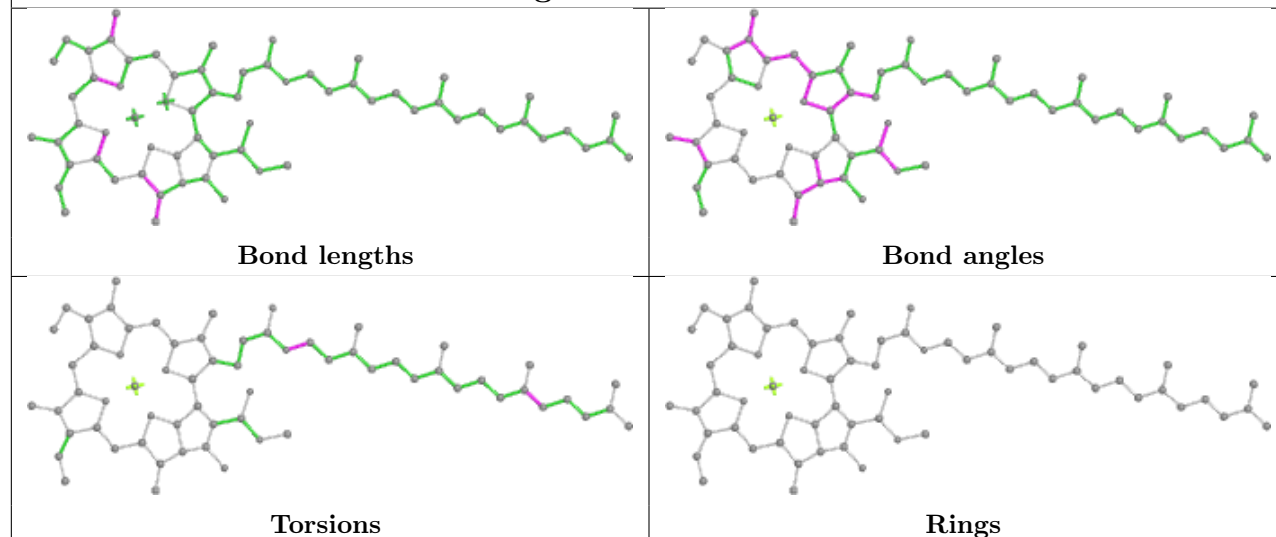
Ligand CLA B 3024

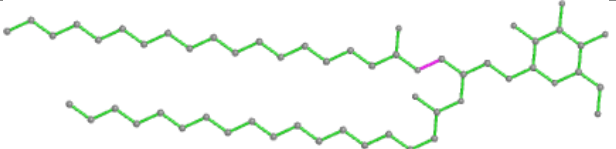
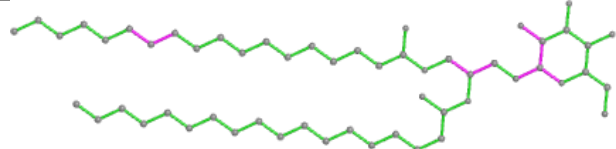
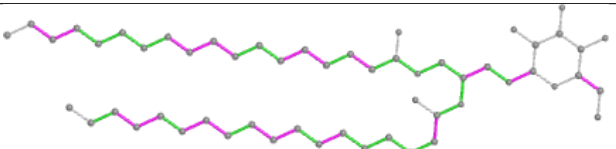
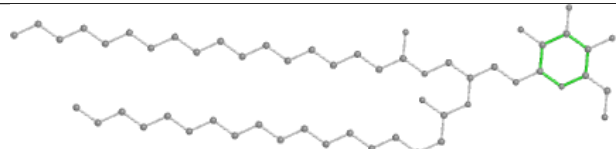


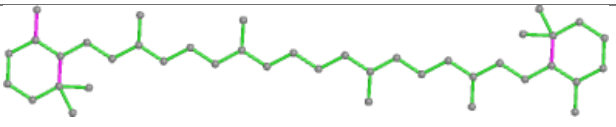
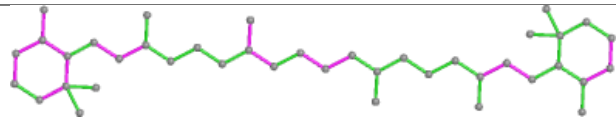
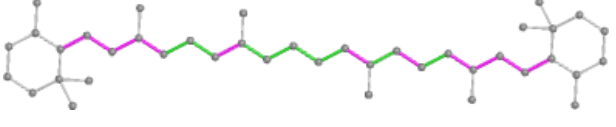
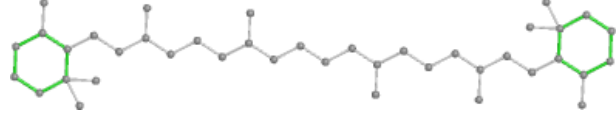
Ligand CLA F 202

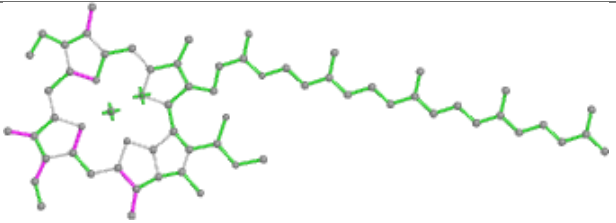
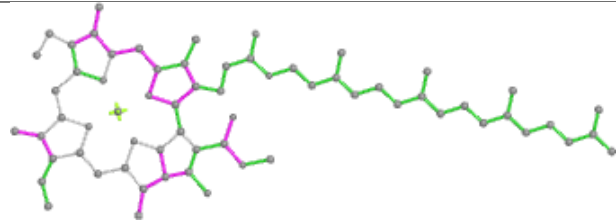
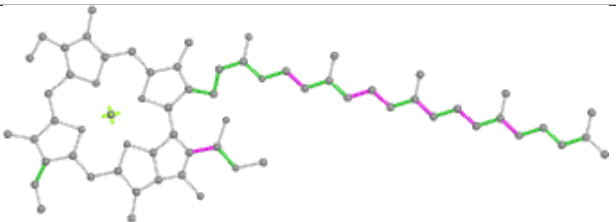
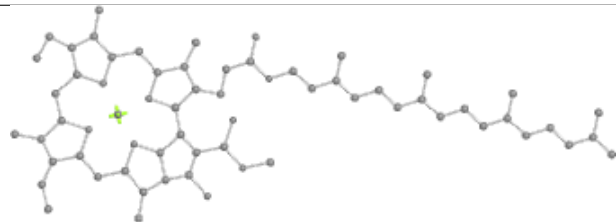


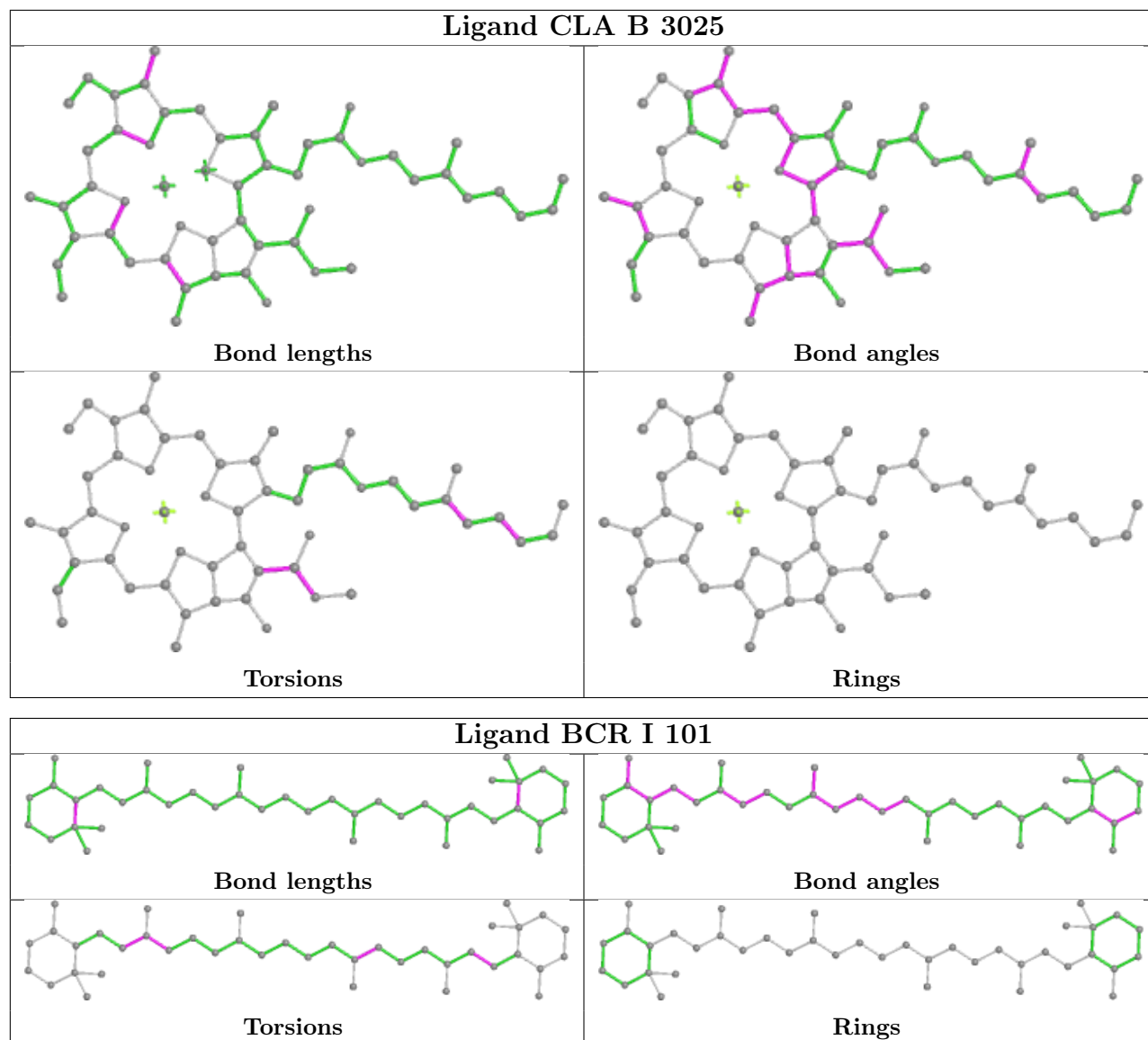
Ligand CLA L 205

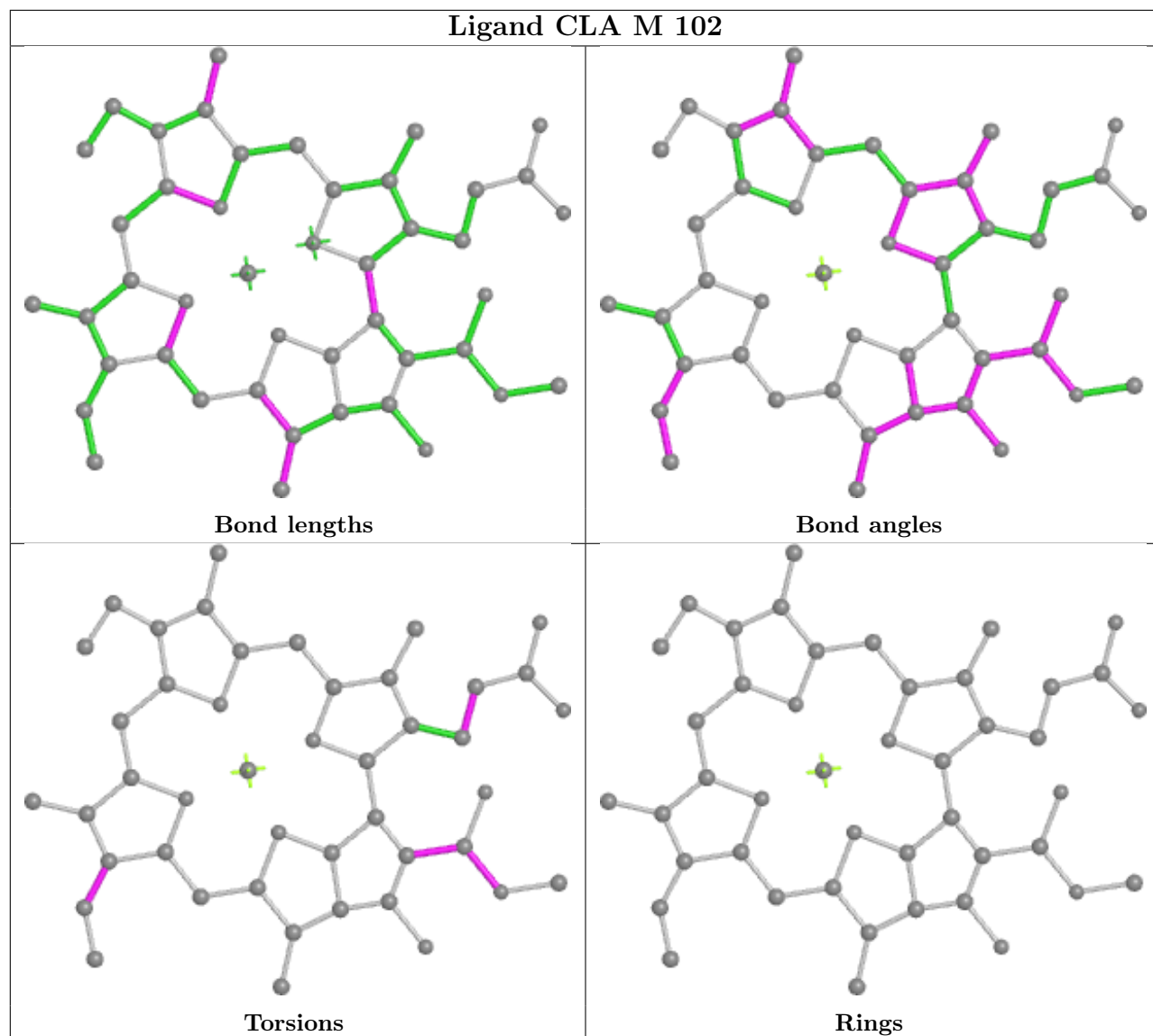


Ligand LMG B 3049	
	
Bond lengths	Bond angles
	
Torsions	Rings

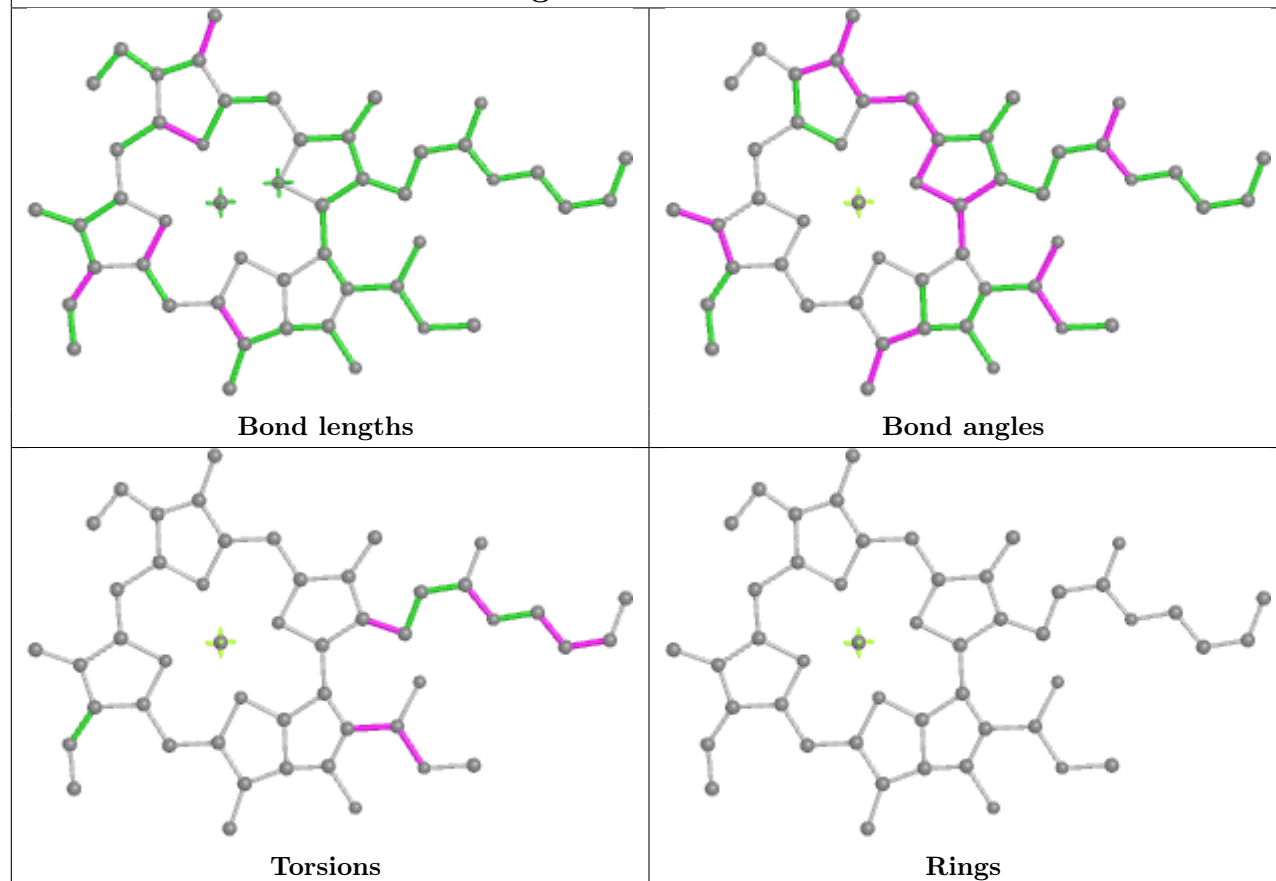
Ligand BCR A 851	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 833	
	
Bond lengths	Bond angles
	
Torsions	Rings

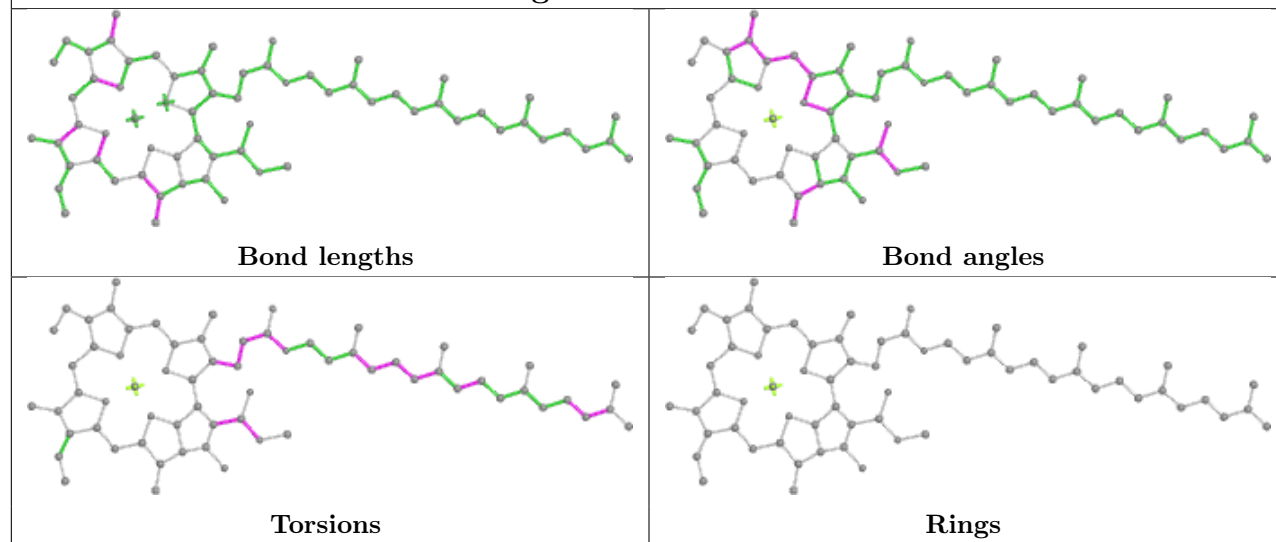




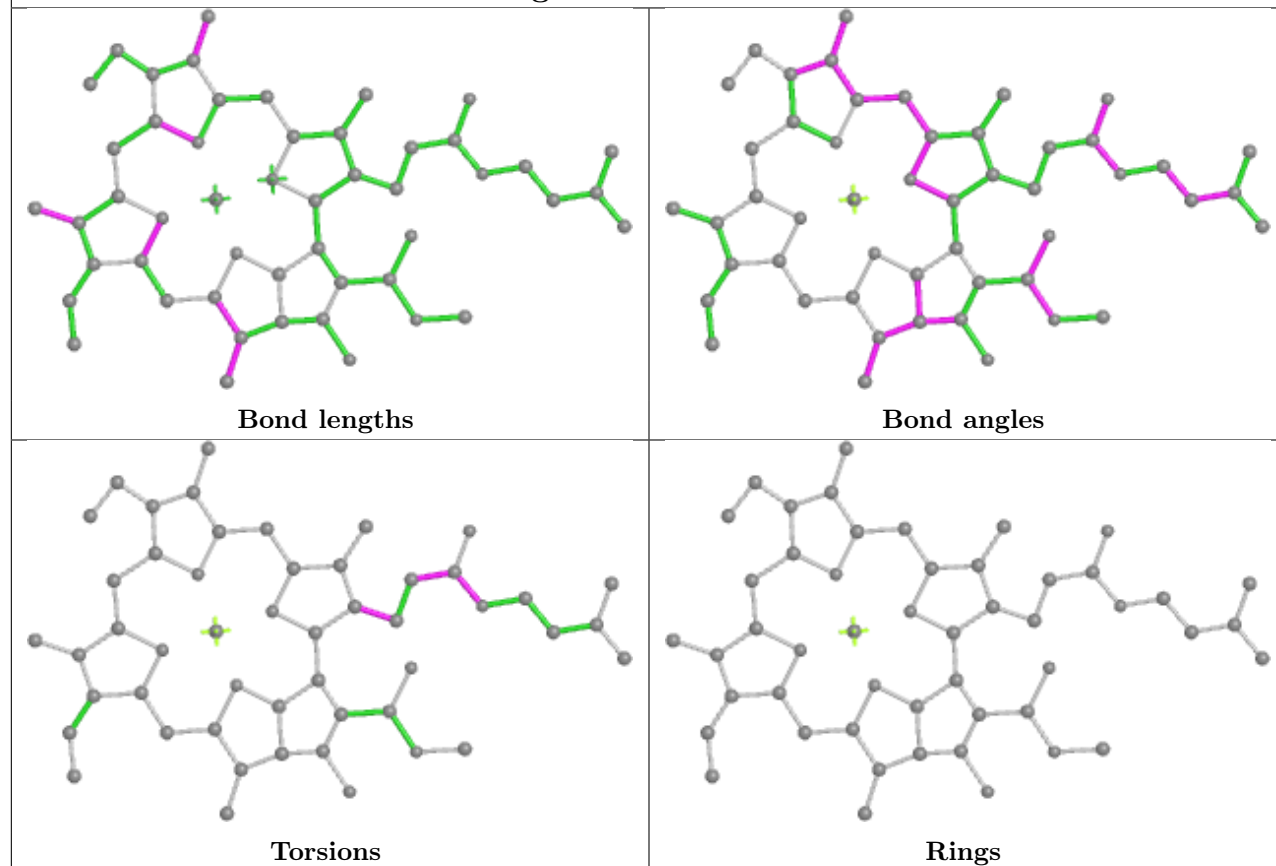
Ligand CLA A 823



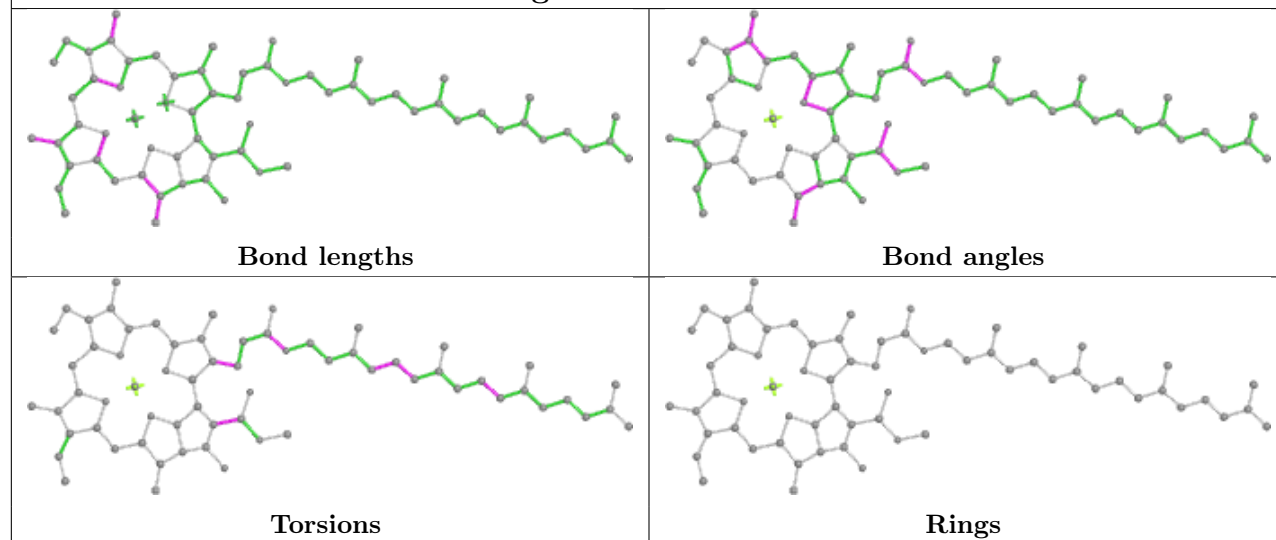
Ligand CLA A 809

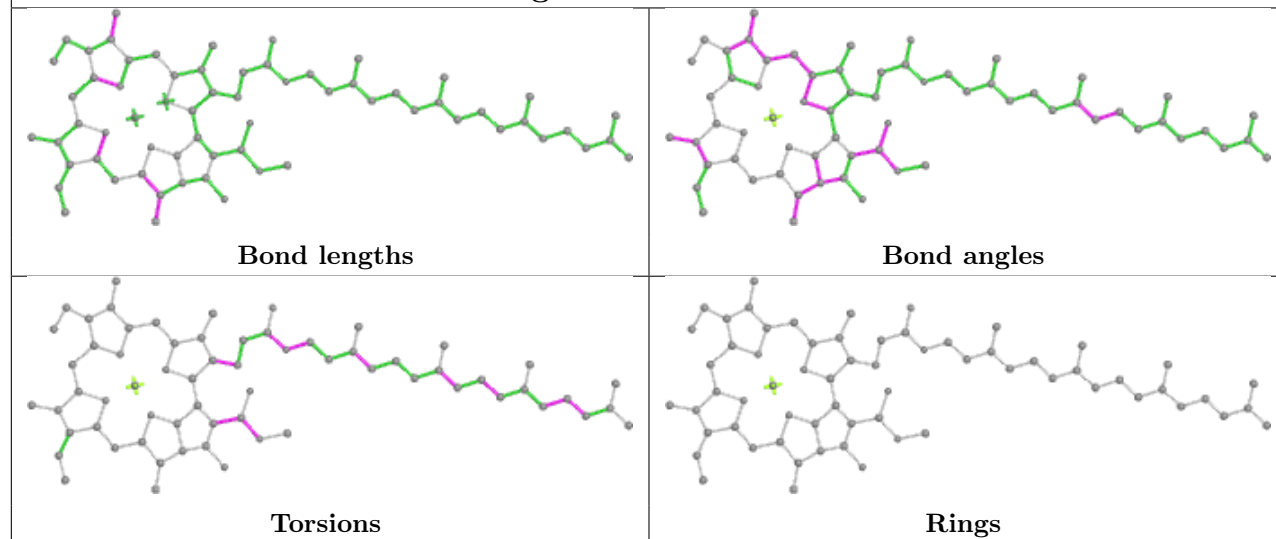
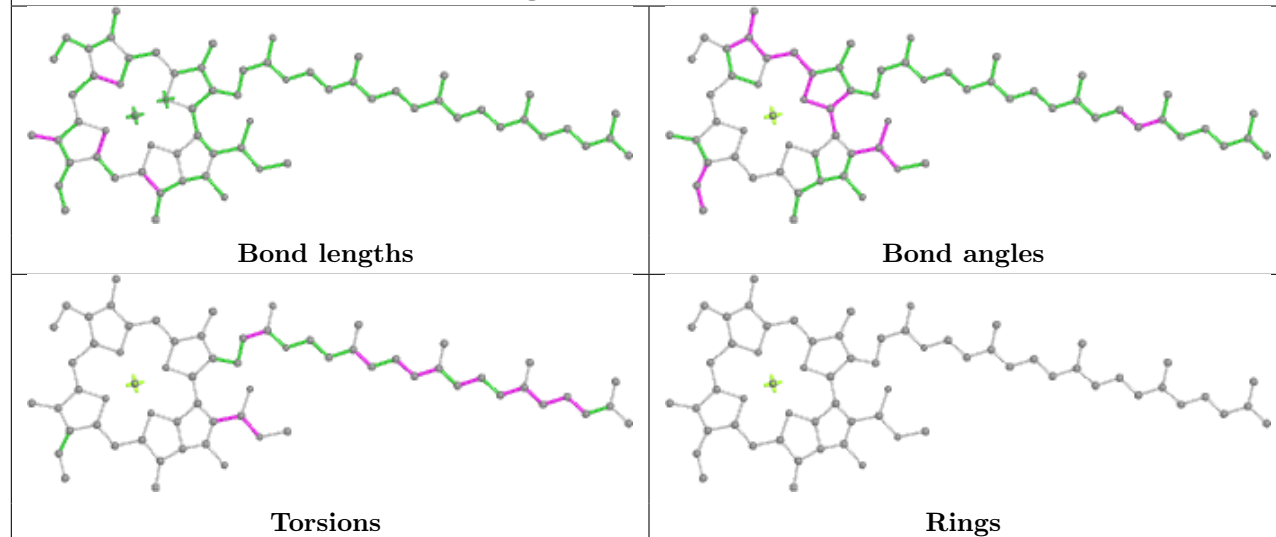


Ligand CLA A 832

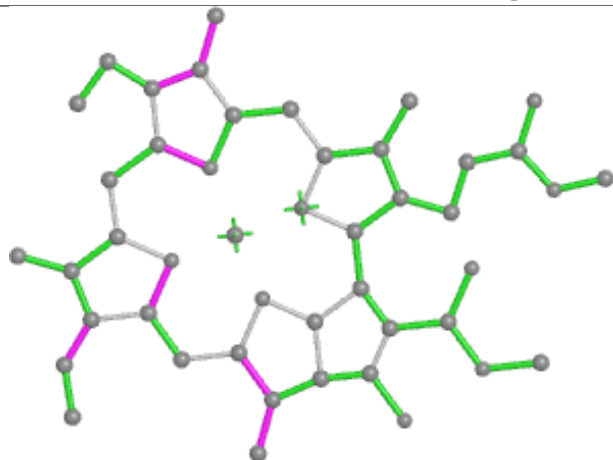


Ligand CLA A 804

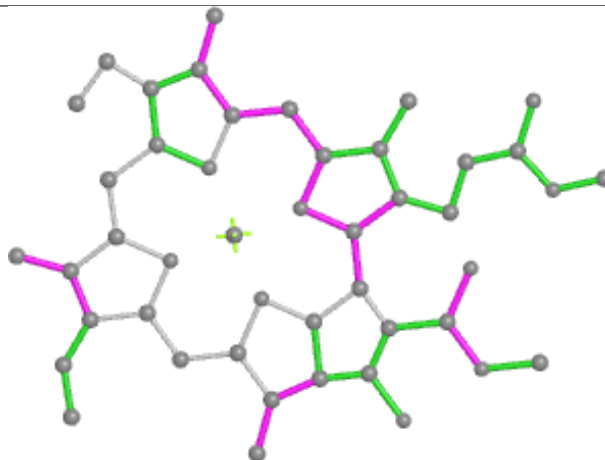


Ligand CLA A 826**Ligand CLA B 3011**

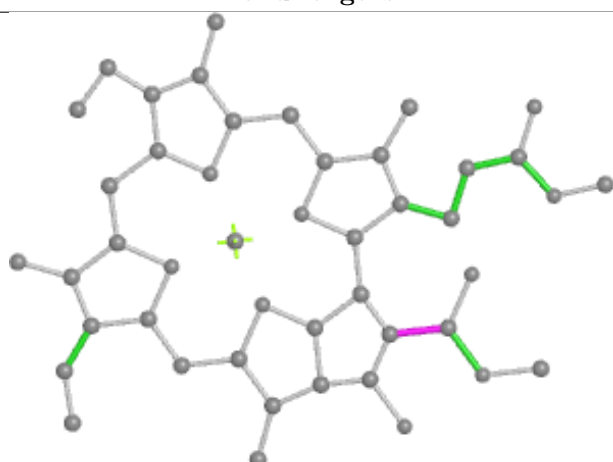
Ligand CLA B 3026



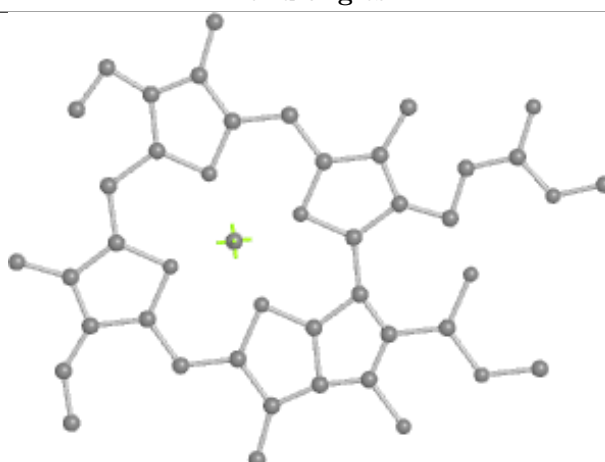
Bond lengths



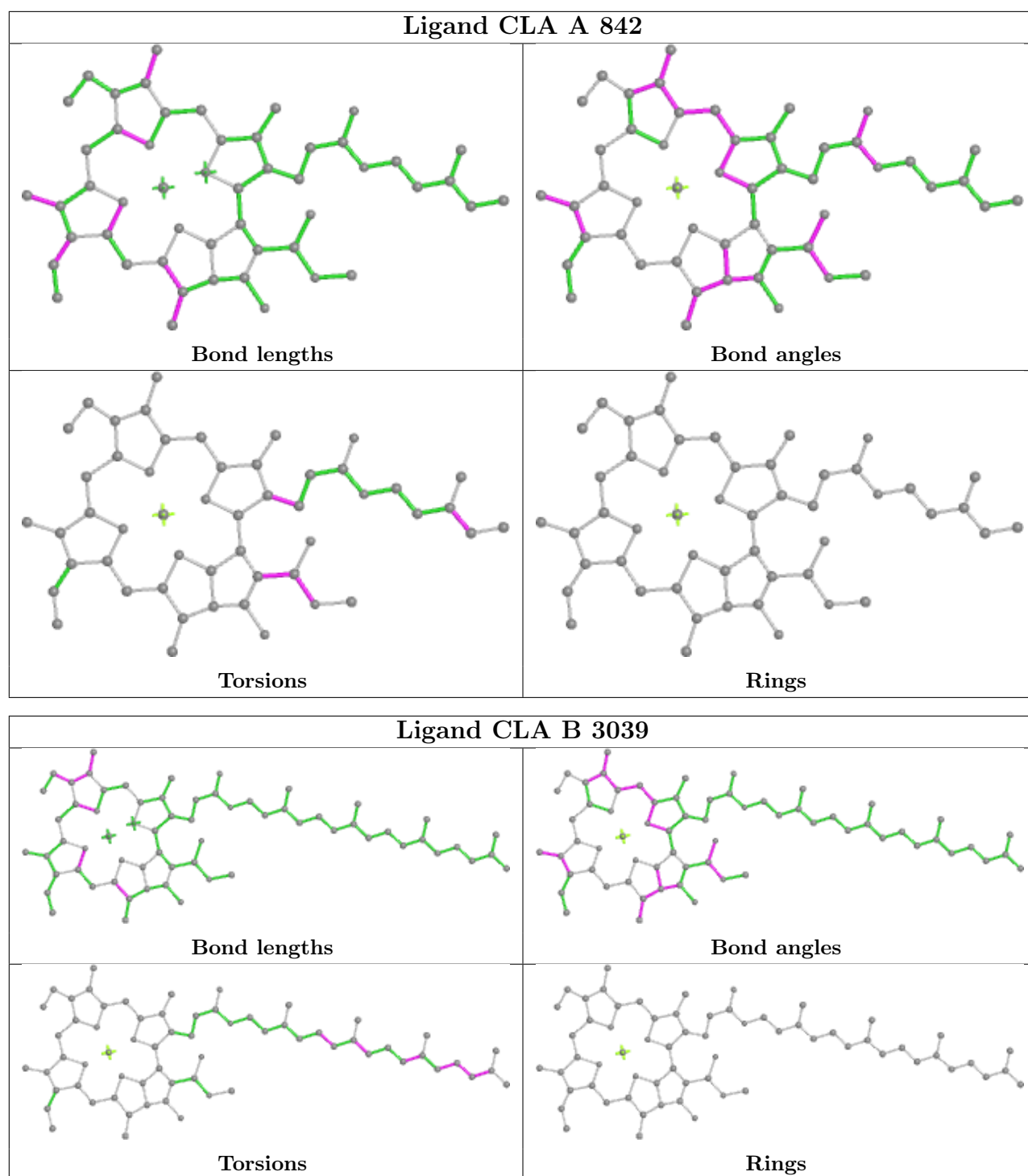
Bond angles



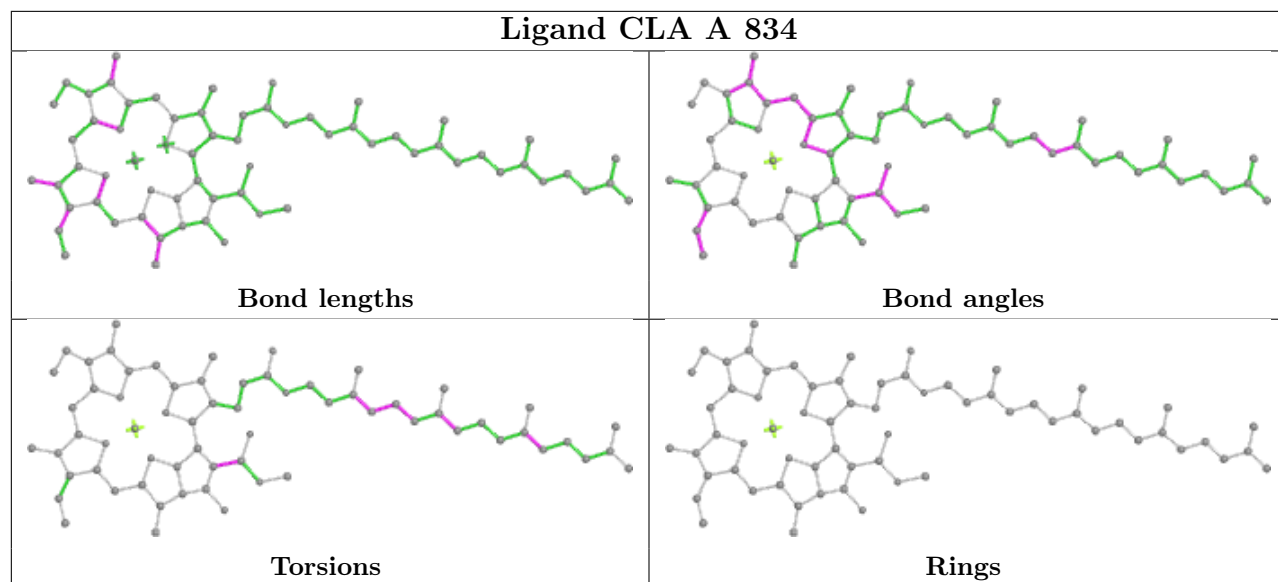
Torsions



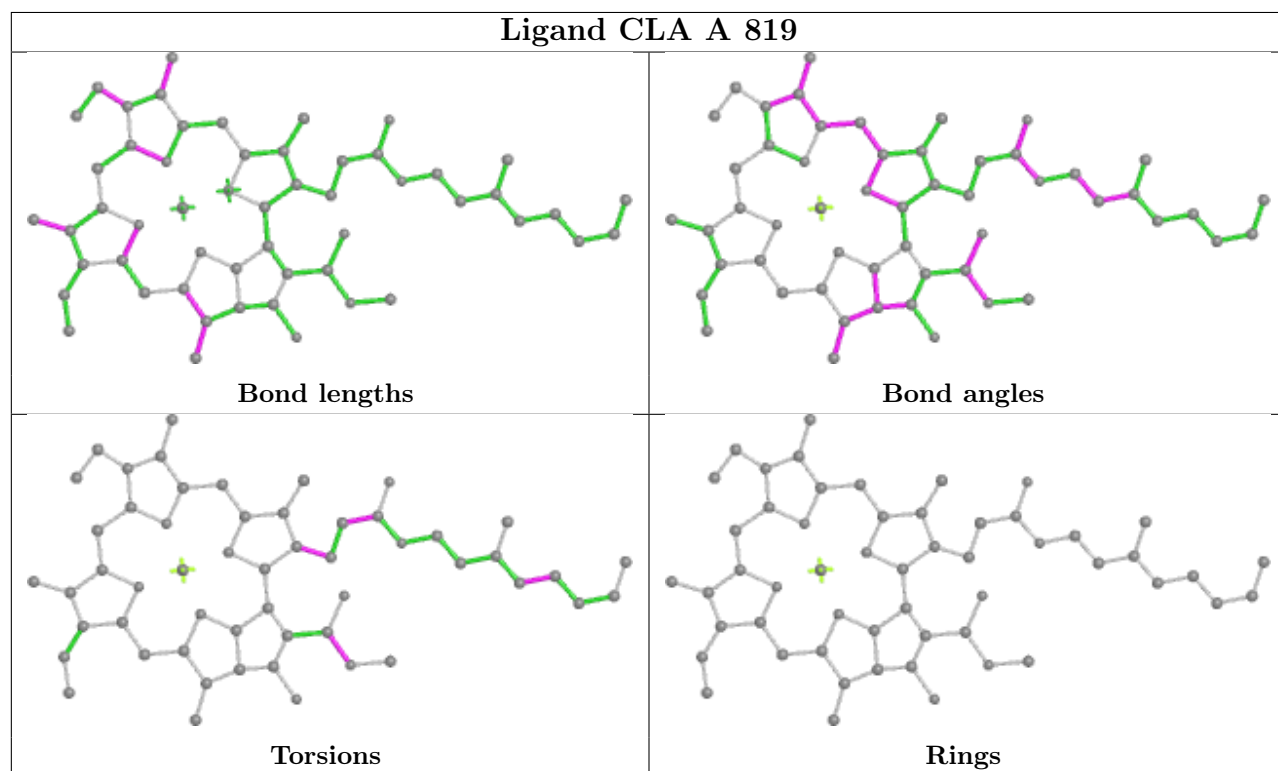
Rings

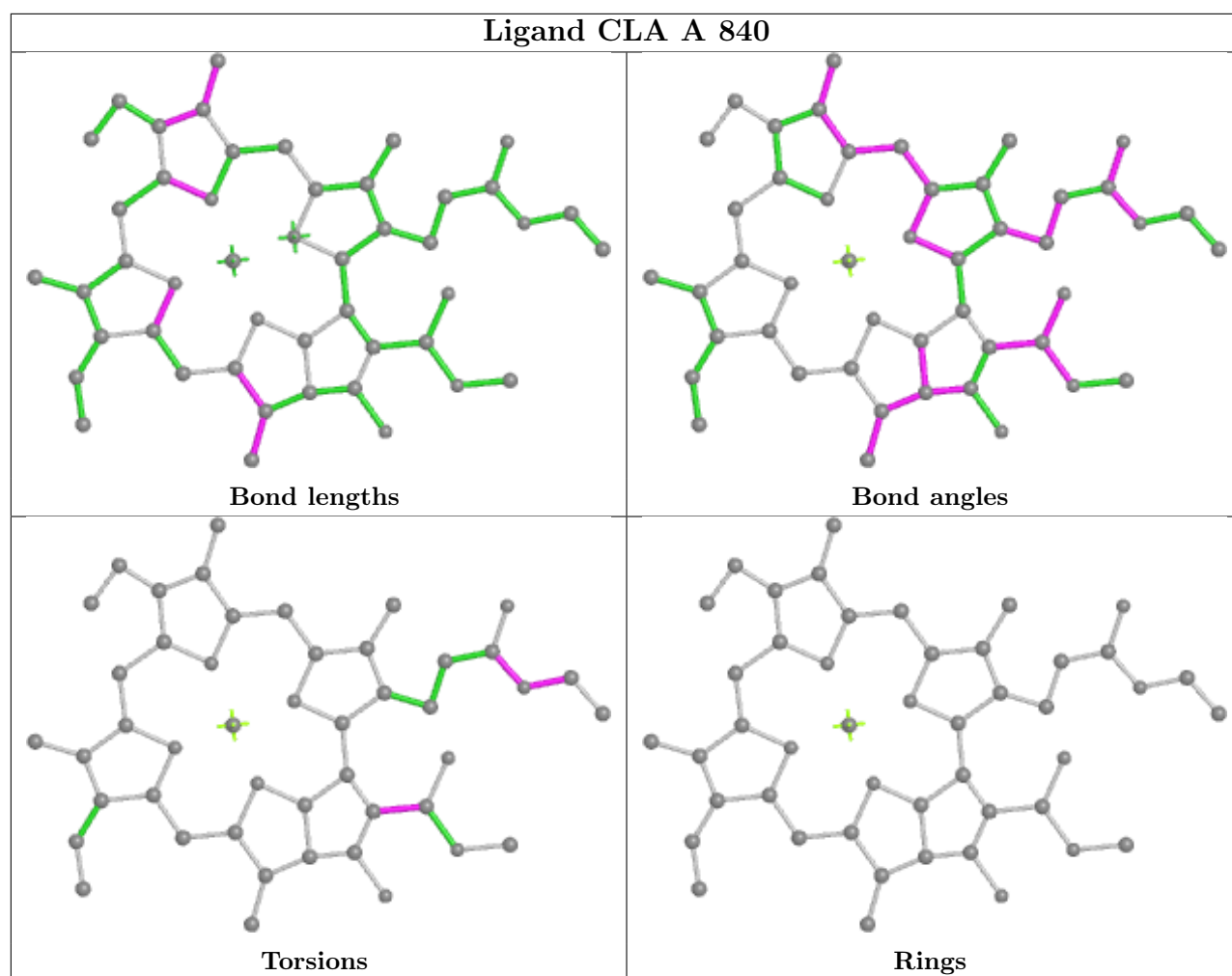


Ligand CLA A 834



Ligand CLA A 819





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	740/755 (98%)	-0.68	1 (0%) 95 89	17, 77, 124, 161	0
2	B	739/740 (99%)	-0.62	0 100 100	11, 52, 94, 129	0
3	C	80/80 (100%)	-0.69	0 100 100	13, 46, 70, 76	0
4	D	138/138 (100%)	-0.74	0 100 100	24, 57, 81, 127	0
5	E	69/75 (92%)	-0.91	0 100 100	48, 71, 92, 105	0
6	F	141/164 (85%)	-0.75	0 100 100	46, 94, 111, 118	0
7	I	38/38 (100%)	-0.46	0 100 100	14, 27, 55, 79	0
8	J	41/41 (100%)	-0.76	0 100 100	88, 105, 117, 132	0
9	K	47/83 (56%)	-0.54	0 100 100	113, 149, 164, 180	0
10	L	151/154 (98%)	-0.44	0 100 100	8, 26, 60, 110	0
11	M	31/31 (100%)	-0.54	0 100 100	26, 42, 64, 92	0
12	X	29/35 (82%)	-0.64	0 100 100	57, 78, 104, 118	0
All	All	2244/2334 (96%)	-0.65	1 (0%) 100 100	8, 61, 118, 180	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	ALA	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	LMG	I	102	40/55	0.83	0.33	49,85,120,144	0
14	CLA	M	102	45/65	0.84	0.30	83,131,166,180	0
18	LHG	M	101	49/49	0.85	0.36	47,89,164,181	0
16	BCR	K	102	40/40	0.87	0.44	107,147,166,175	0
17	LMG	A	855	30/55	0.87	0.27	32,83,145,162	0
16	BCR	A	848	40/40	0.88	0.57	77,119,171,177	0
16	BCR	J	105	40/40	0.88	0.40	67,114,154,161	0
16	BCR	A	847	40/40	0.89	0.44	96,131,161,175	0
16	BCR	J	104	40/40	0.89	0.31	78,116,145,150	0
17	LMG	A	852	48/55	0.89	0.36	56,113,152,160	0
21	LMT	L	202	35/35	0.89	0.28	74,142,179,192	0
22	DGD	L	207	66/66	0.90	0.25	45,99,155,168	0
16	BCR	B	3044	40/40	0.91	0.47	75,110,143,161	0
14	CLA	J	101	45/65	0.91	0.25	118,137,171,176	0
14	CLA	A	816	45/65	0.92	0.21	105,143,169,179	0
18	LHG	B	3050	23/49	0.92	0.18	73,111,139,145	0
14	CLA	K	101	41/65	0.92	0.17	112,149,185,194	0
14	CLA	K	103	45/65	0.92	0.23	101,132,164,166	0
17	LMG	B	3049	55/55	0.92	0.24	20,58,84,87	0
14	CLA	F	202	45/65	0.93	0.19	86,115,145,151	0
16	BCR	A	849	40/40	0.93	0.41	61,91,155,157	0
14	CLA	A	811	45/65	0.94	0.18	92,125,152,159	0
14	CLA	A	817	49/65	0.94	0.20	63,127,159,160	0
14	CLA	J	102	37/65	0.94	0.26	102,125,149,163	0
14	CLA	A	821	43/65	0.94	0.27	72,130,170,176	0
16	BCR	B	3046	40/40	0.94	0.36	43,76,131,143	0
16	BCR	B	3051	40/40	0.94	0.38	46,84,127,134	0
16	BCR	F	203	40/40	0.94	0.30	43,94,126,147	0
14	CLA	A	823	49/65	0.94	0.20	78,116,146,158	0
14	CLA	A	845	52/65	0.94	0.19	44,84,111,120	0
14	CLA	B	3022	45/65	0.95	0.21	67,93,119,120	0
16	BCR	B	3045	40/40	0.95	0.28	48,74,114,123	0
14	CLA	A	818	54/65	0.95	0.26	95,124,151,161	0
14	CLA	A	837	45/65	0.95	0.17	80,104,127,137	0
16	BCR	F	201	40/40	0.95	0.39	45,91,124,132	0
18	LHG	A	853	49/49	0.95	0.30	38,84,108,118	0
14	CLA	A	812	65/65	0.95	0.24	81,114,144,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	BCR	J	103	40/40	0.95	0.41	60,102,125,129	0
20	CA	B	3002	1/1	0.95	0.15	69,69,69,69	0
14	CLA	B	3020	65/65	0.95	0.31	48,91,121,132	0
16	BCR	A	850	40/40	0.95	0.36	41,74,108,125	0
14	CLA	A	808	51/65	0.96	0.20	81,103,130,133	0
14	CLA	B	3031	45/65	0.96	0.20	46,73,95,113	0
14	CLA	B	3032	49/65	0.96	0.22	34,69,97,122	0
16	BCR	B	3047	40/40	0.96	0.44	54,79,99,106	0
14	CLA	B	3034	58/65	0.96	0.28	63,98,137,141	0
14	CLA	B	3036	45/65	0.96	0.19	44,79,107,111	0
14	CLA	B	3037	45/65	0.96	0.19	64,88,120,121	0
14	CLA	B	3038	60/65	0.96	0.21	41,81,112,122	0
14	CLA	B	3039	65/65	0.96	0.28	42,88,128,143	0
14	CLA	A	826	65/65	0.96	0.25	71,100,131,134	0
14	CLA	A	828	65/65	0.96	0.24	59,93,128,135	0
16	BCR	M	103	40/40	0.96	0.23	21,48,76,82	0
14	CLA	A	819	54/65	0.96	0.20	61,94,116,132	0
14	CLA	A	813	54/65	0.96	0.20	74,100,128,136	0
14	CLA	B	3012	45/65	0.96	0.19	45,67,88,111	0
14	CLA	B	3013	45/65	0.96	0.17	57,89,115,119	0
14	CLA	X	1701	45/65	0.96	0.17	75,104,134,140	0
15	PQN	A	846	33/33	0.96	0.27	61,89,118,121	0
14	CLA	B	3015	65/65	0.96	0.28	45,77,112,117	0
14	CLA	B	3017	55/65	0.96	0.28	61,96,133,166	0
14	CLA	A	822	65/65	0.96	0.28	51,87,121,127	0
14	CLA	B	3021	47/65	0.96	0.21	69,98,129,135	0
14	CLA	L	206	65/65	0.97	0.23	21,46,75,85	0
14	CLA	A	807	65/65	0.97	0.25	56,84,110,116	0
14	CLA	A	856	65/65	0.97	0.24	38,65,91,102	0
13	CL0	A	801	65/65	0.97	0.22	2,46,71,74	0
14	CLA	A	810	65/65	0.97	0.24	44,99,148,161	0
14	CLA	A	820	65/65	0.97	0.25	65,100,125,134	0
14	CLA	B	3016	45/65	0.97	0.21	61,82,115,118	0
14	CLA	A	803	65/65	0.97	0.24	42,67,87,108	0
16	BCR	A	851	40/40	0.97	0.28	20,63,90,93	0
14	CLA	B	3018	59/65	0.97	0.24	47,81,109,117	0
14	CLA	A	804	65/65	0.97	0.27	59,98,125,132	0
14	CLA	A	805	59/65	0.97	0.21	75,98,125,141	0
14	CLA	A	824	51/65	0.97	0.22	67,101,132,138	0
14	CLA	B	3023	55/65	0.97	0.21	69,94,122,122	0
14	CLA	B	3027	65/65	0.97	0.25	38,65,91,97	0
14	CLA	B	3028	65/65	0.97	0.25	15,48,100,102	0

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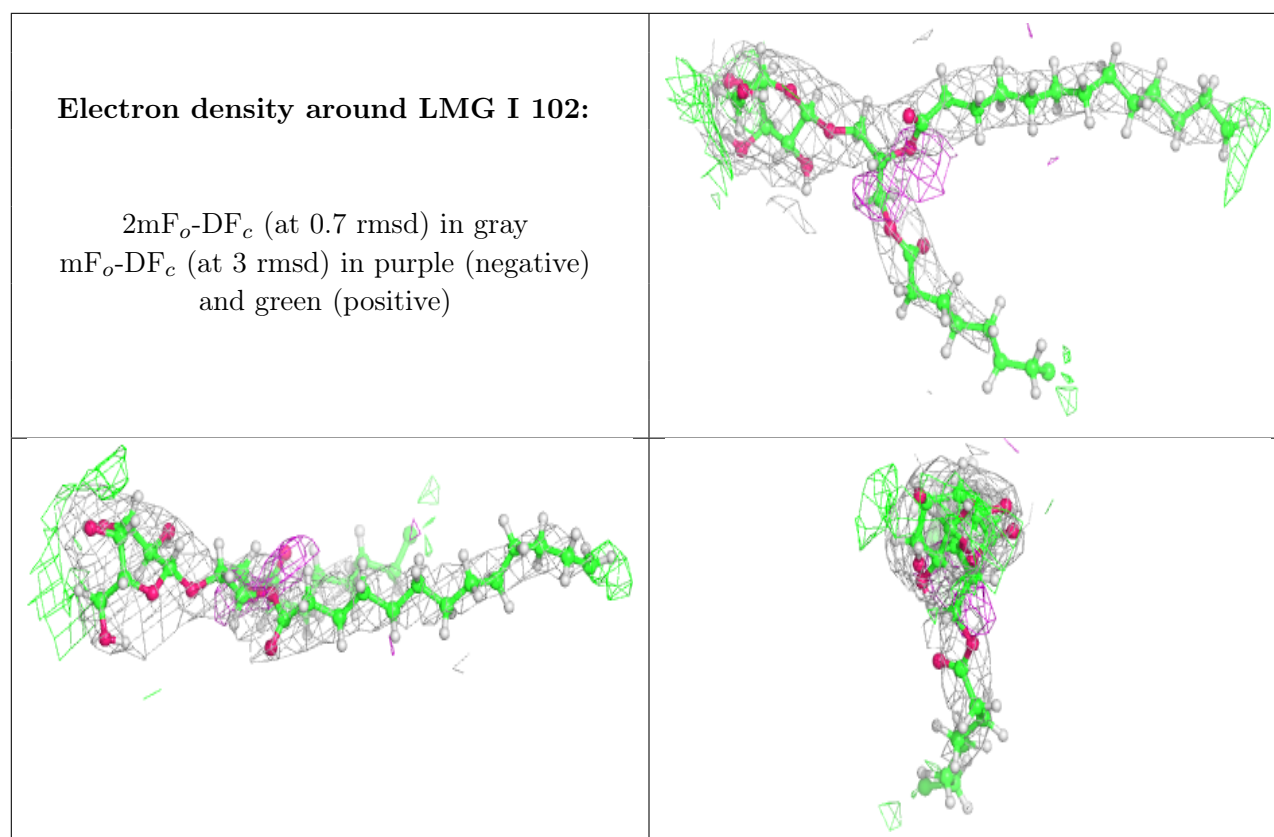
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	CLA	B	3029	65/65	0.97	0.23	27,61,79,97	0
14	CLA	A	825	59/65	0.97	0.30	49,83,123,135	0
14	CLA	A	814	60/65	0.97	0.28	73,115,140,141	0
14	CLA	A	827	65/65	0.97	0.30	29,68,145,167	0
14	CLA	B	3035	45/65	0.97	0.20	55,73,95,97	0
14	CLA	A	815	45/65	0.97	0.17	85,114,150,156	0
14	CLA	A	829	65/65	0.97	0.27	59,85,110,117	0
14	CLA	A	830	65/65	0.97	0.22	55,88,118,121	0
14	CLA	A	833	65/65	0.97	0.27	24,63,135,140	0
14	CLA	B	3040	47/65	0.97	0.21	49,74,93,105	0
18	LHG	A	854	27/49	0.97	0.21	46,79,116,117	0
14	CLA	A	836	54/65	0.97	0.26	47,87,128,136	0
14	CLA	A	806	65/65	0.97	0.24	67,101,136,142	0
14	CLA	A	839	65/65	0.97	0.26	21,59,97,120	0
14	CLA	A	840	47/65	0.97	0.22	22,55,75,93	0
14	CLA	A	844	65/65	0.97	0.24	2,17,50,59	0
14	CLA	B	3024	45/65	0.98	0.20	30,61,94,106	0
15	PQN	B	3043	33/33	0.98	0.24	27,47,66,70	0
14	CLA	B	3025	54/65	0.98	0.19	48,64,87,87	0
14	CLA	B	3026	46/65	0.98	0.21	36,64,89,90	0
14	CLA	B	3004	65/65	0.98	0.21	9,33,53,64	0
14	CLA	B	3005	54/65	0.98	0.20	23,48,67,74	0
14	CLA	B	3006	65/65	0.98	0.25	26,56,90,101	0
14	CLA	B	3030	65/65	0.98	0.23	20,47,80,98	0
14	CLA	B	3007	65/65	0.98	0.25	22,50,77,90	0
14	CLA	B	3008	65/65	0.98	0.24	10,35,66,89	0
14	CLA	B	3033	65/65	0.98	0.26	56,86,112,121	0
16	BCR	B	3048	40/40	0.98	0.24	14,34,61,61	0
14	CLA	B	3009	65/65	0.98	0.24	10,39,72,76	0
14	CLA	B	3010	65/65	0.98	0.22	5,38,66,90	0
14	CLA	B	3011	65/65	0.98	0.24	2,24,59,69	0
16	BCR	I	101	40/40	0.98	0.24	2,28,50,68	0
14	CLA	A	838	51/65	0.98	0.20	36,59,79,102	0
14	CLA	A	832	50/65	0.98	0.21	33,61,91,117	0
14	CLA	B	3014	65/65	0.98	0.21	42,72,99,102	0
14	CLA	A	809	65/65	0.98	0.28	38,84,123,129	0
16	BCR	L	201	40/40	0.98	0.24	2,34,59,61	0
16	BCR	L	208	40/40	0.98	0.27	3,28,48,65	0
16	BCR	L	209	40/40	0.98	0.24	2,38,86,98	0
14	CLA	B	3041	65/65	0.98	0.22	2,18,52,58	0
14	CLA	B	3042	65/65	0.98	0.25	4,29,52,55	0
14	CLA	A	841	65/65	0.98	0.24	32,69,123,132	0

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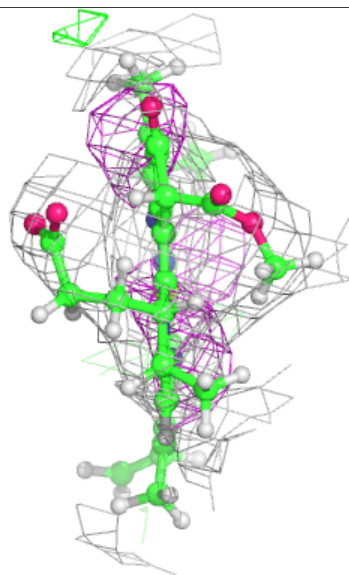
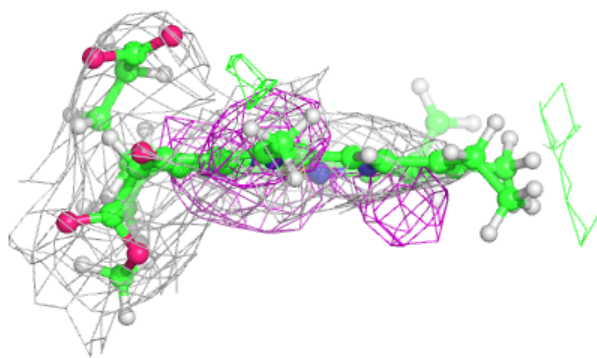
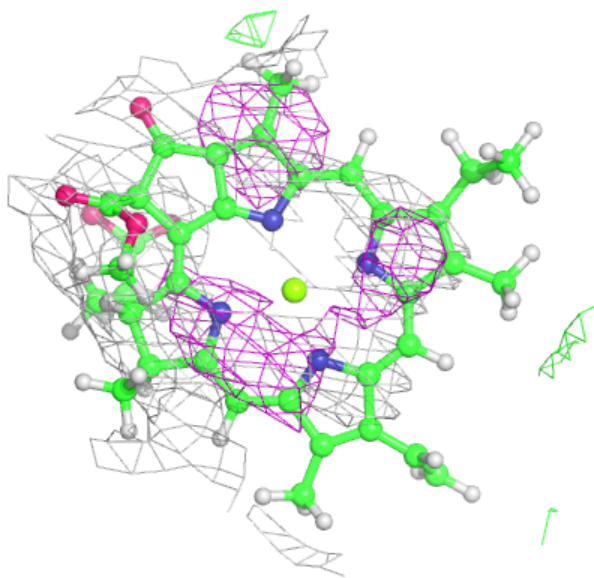
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	CLA	A	842	51/65	0.98	0.26	36,75,124,143	0
14	CLA	A	843	65/65	0.98	0.27	37,73,117,135	0
14	CLA	B	3019	60/65	0.98	0.25	49,70,100,107	0
14	CLA	A	834	65/65	0.98	0.24	10,37,65,71	0
14	CLA	L	204	65/65	0.98	0.23	11,41,72,93	0
14	CLA	L	205	65/65	0.98	0.25	8,45,117,130	0
14	CLA	A	802	65/65	0.98	0.21	20,38,54,75	0
14	CLA	A	831	65/65	0.98	0.25	55,87,110,118	0
14	CLA	B	3003	65/65	0.98	0.23	16,49,70,76	0
20	CA	L	203	1/1	0.99	0.19	27,27,27,27	0
19	SF4	B	3001	8/8	0.99	0.30	29,46,88,118	0
14	CLA	A	835	65/65	0.99	0.23	2,32,62,90	0
19	SF4	C	101	8/8	1.00	0.29	23,51,58,71	0
19	SF4	C	102	8/8	1.00	0.28	38,45,62,64	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



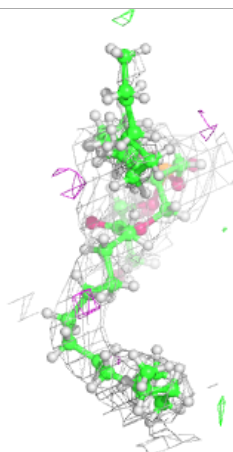
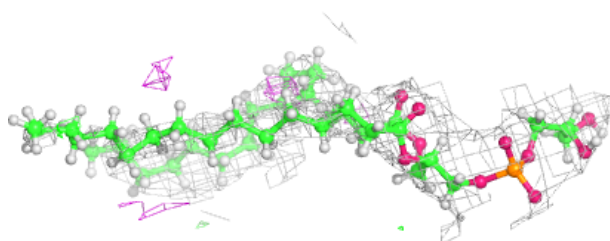
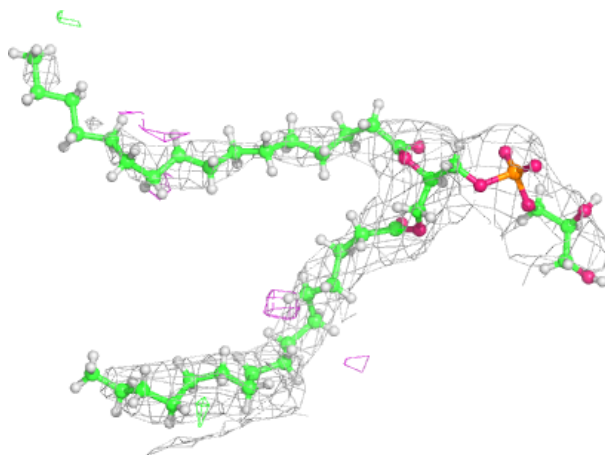
Electron density around CLA M 102:

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



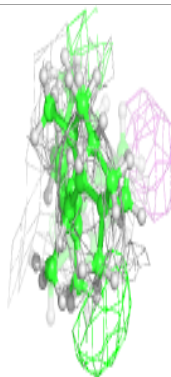
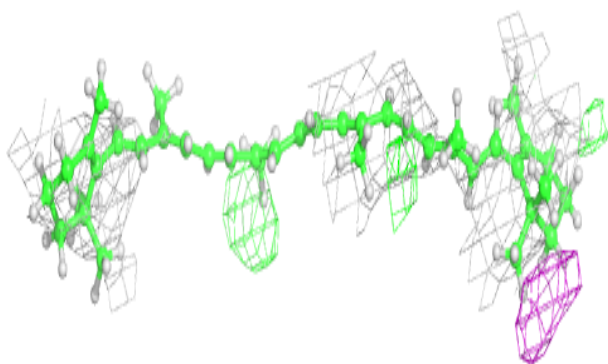
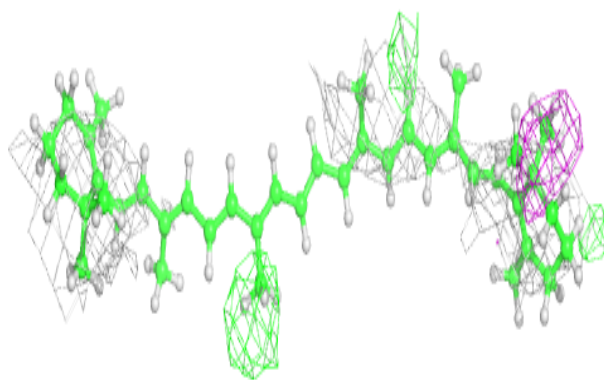
Electron density around LHG M 101:

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

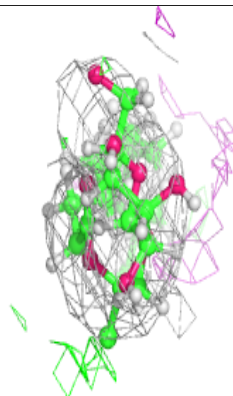
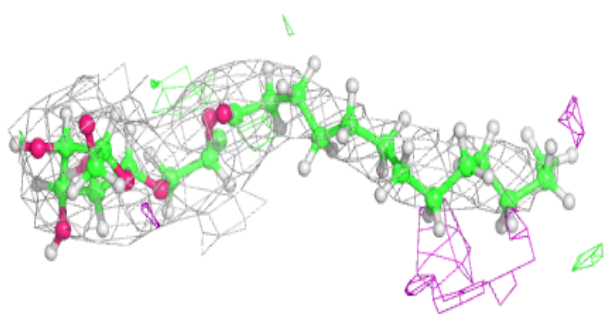
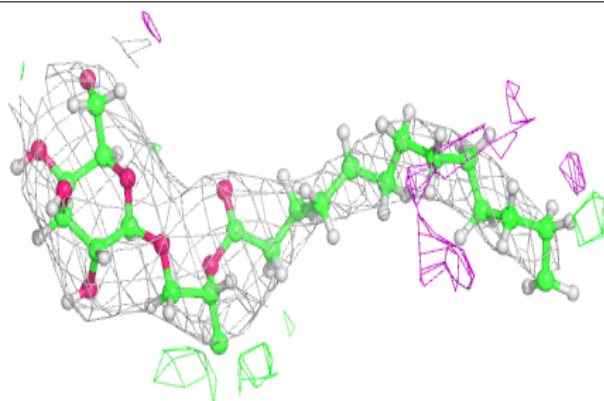


Electron density around BCR K 102:

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

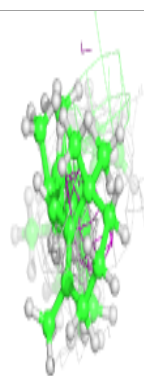
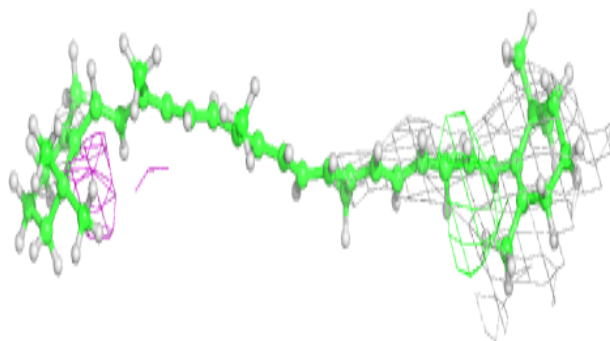
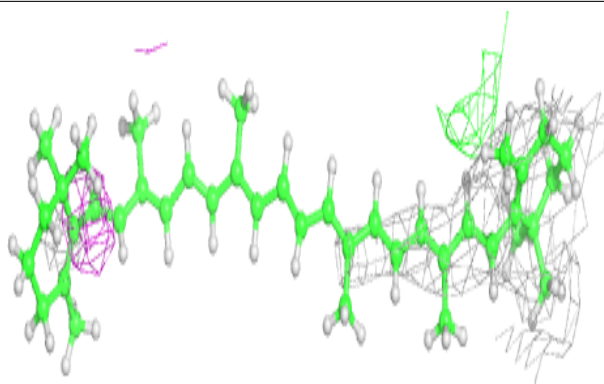
**Electron density around LMG A 855:**

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

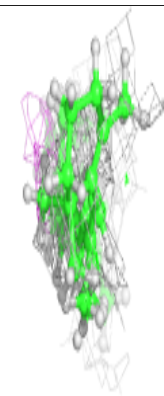
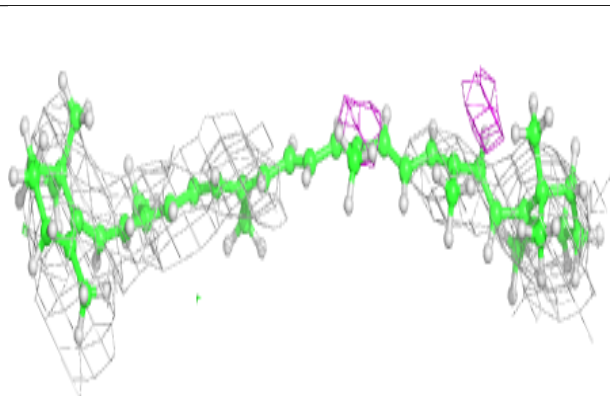
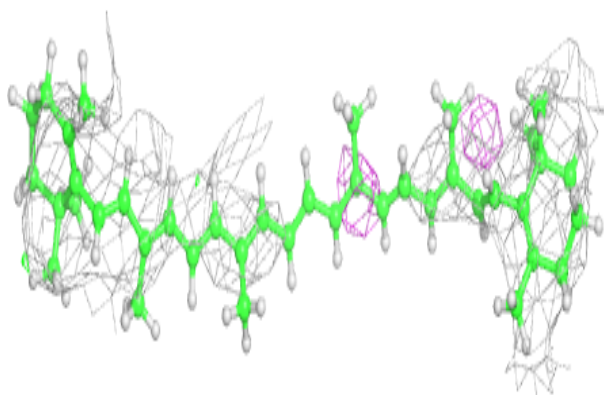


Electron density around BCR A 848:

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

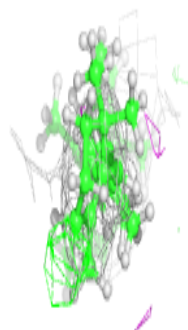
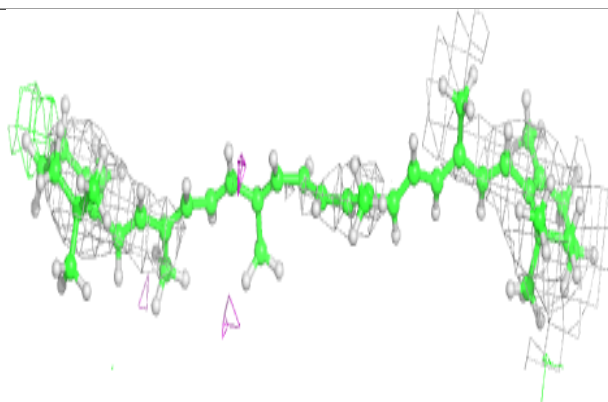
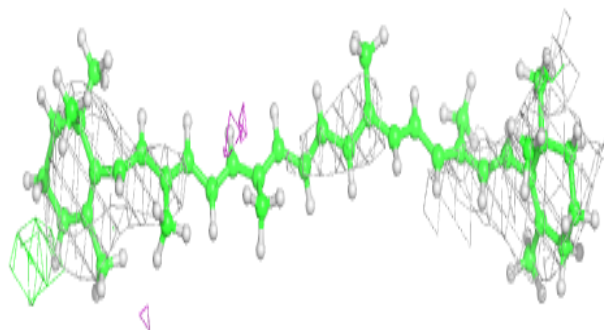
**Electron density around BCR J 105:**

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

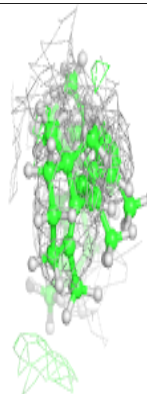
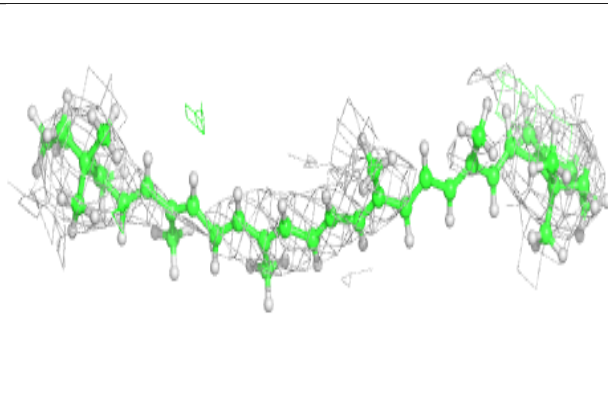
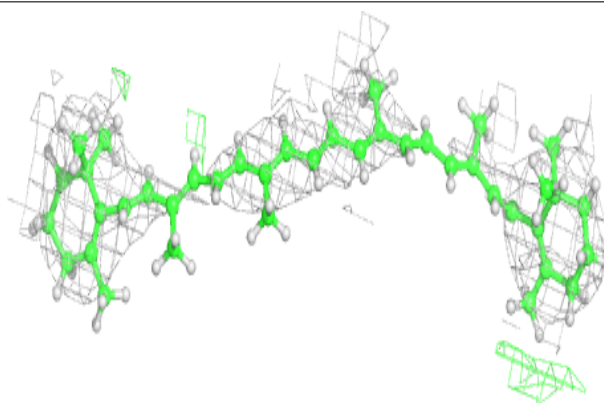


Electron density around BCR A 847:

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

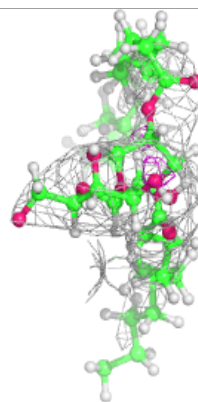
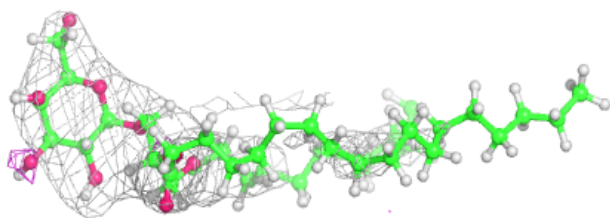
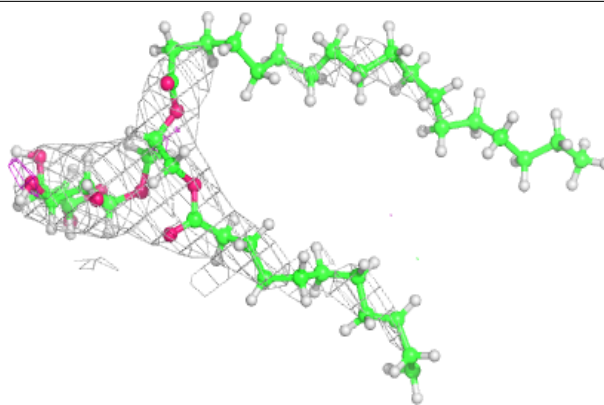
**Electron density around BCR J 104:**

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

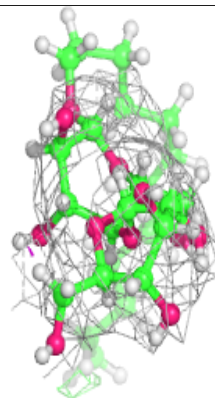
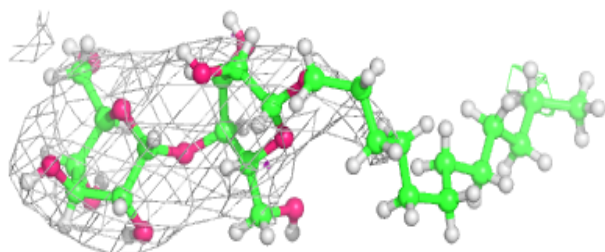
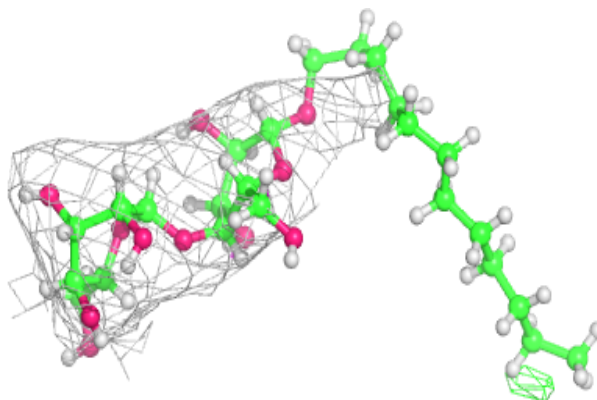


Electron density around LMG A 852:

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

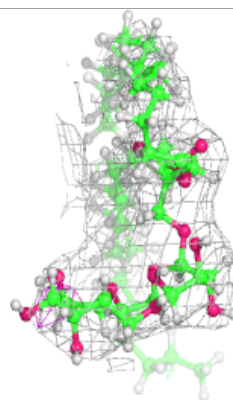
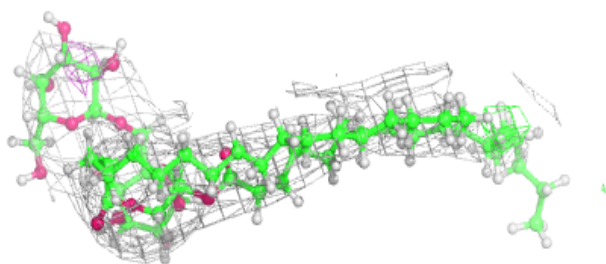
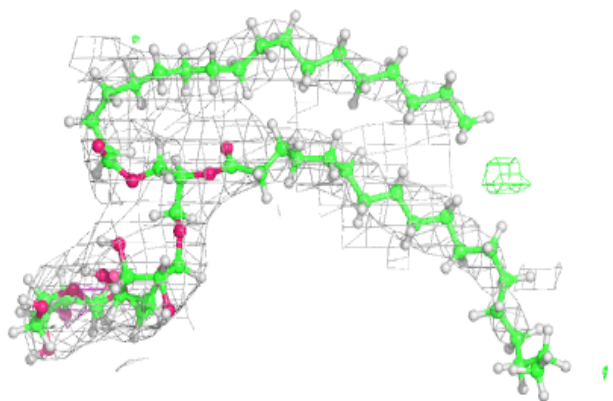
**Electron density around LMT L 202:**

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

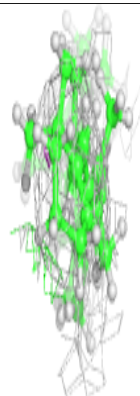
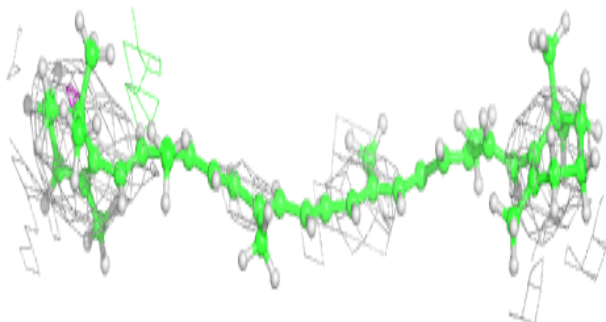
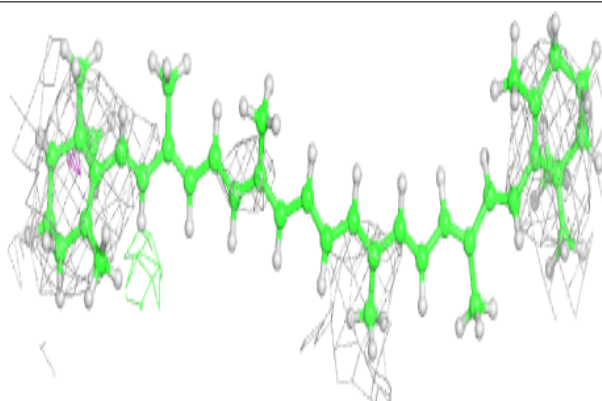


Electron density around DGD L 207:

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

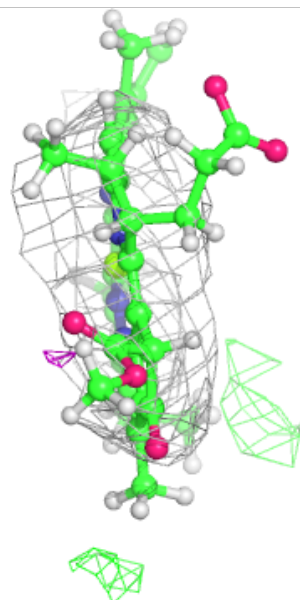
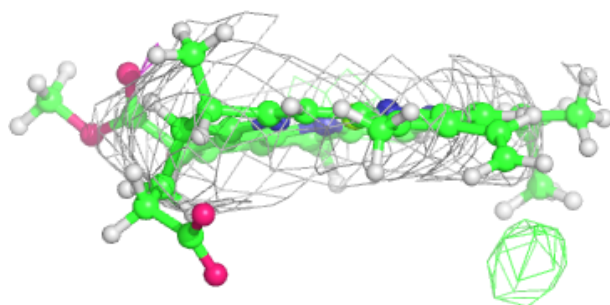
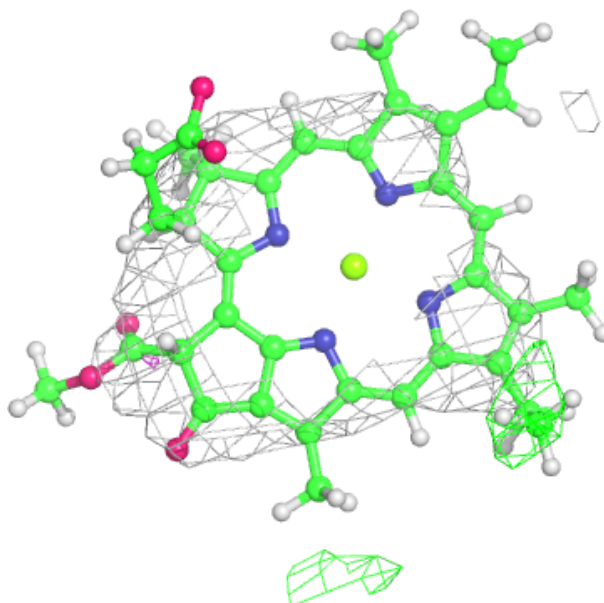
**Electron density around BCR B 3044:**

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



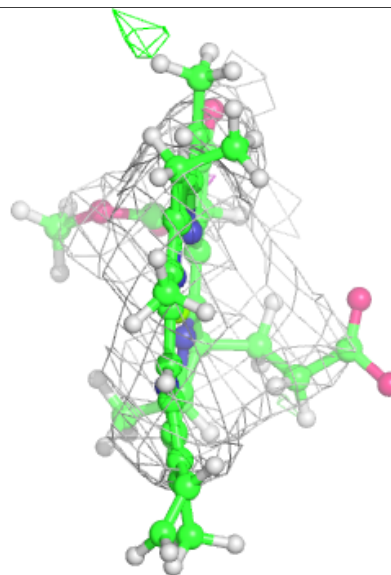
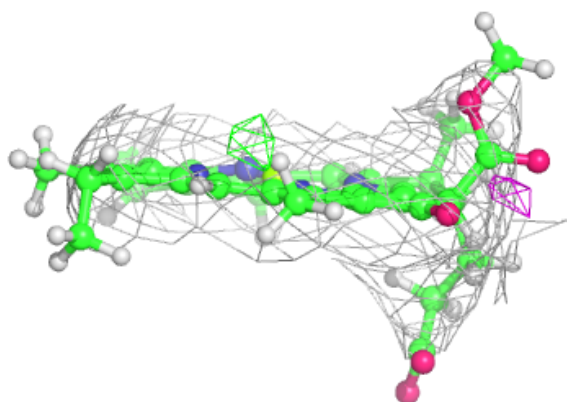
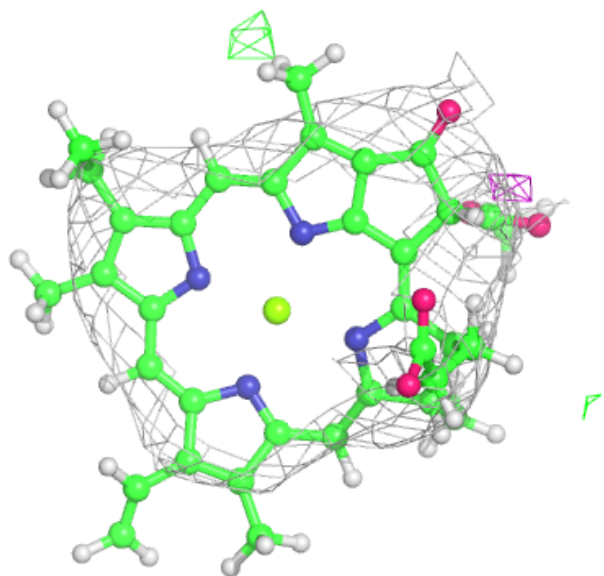
Electron density around CLA J 101:

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



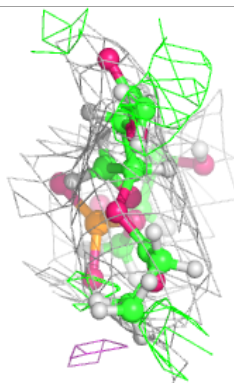
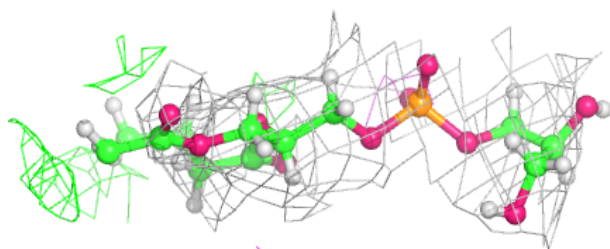
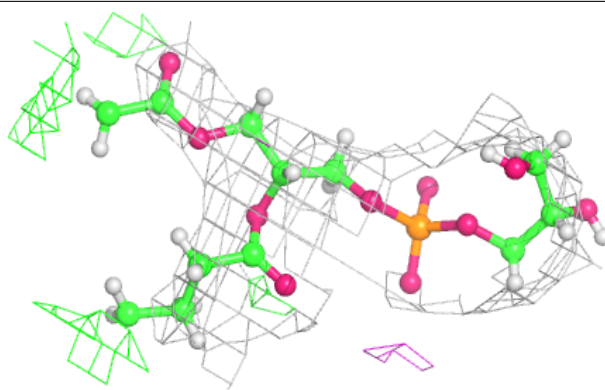
Electron density around CLA A 816:

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



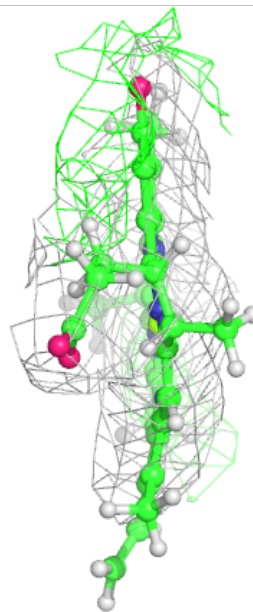
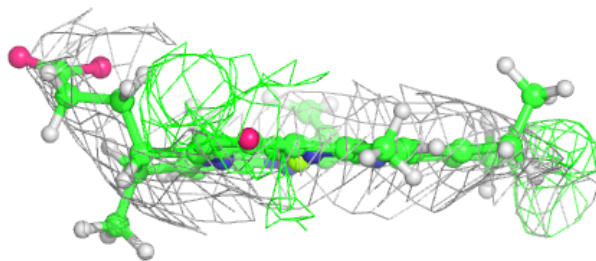
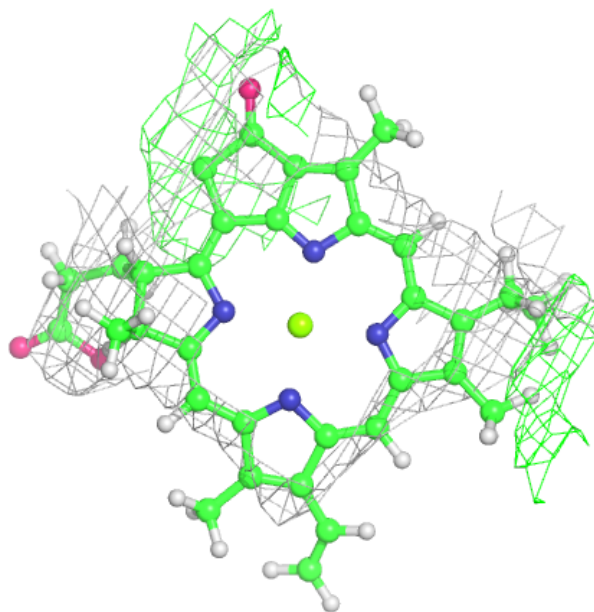
Electron density around LHG B 3050:

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



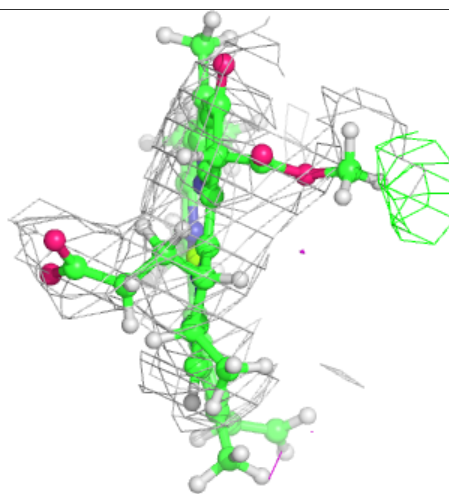
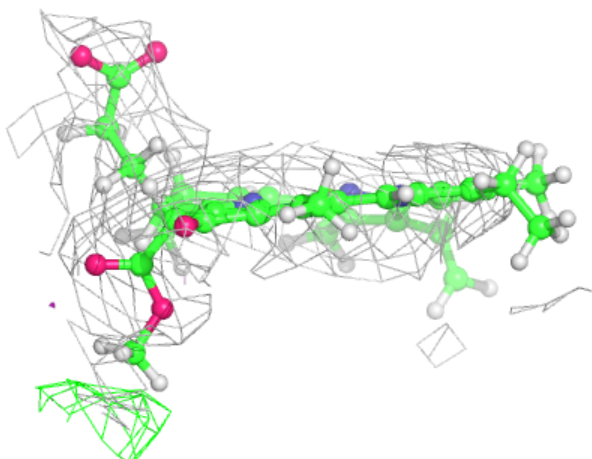
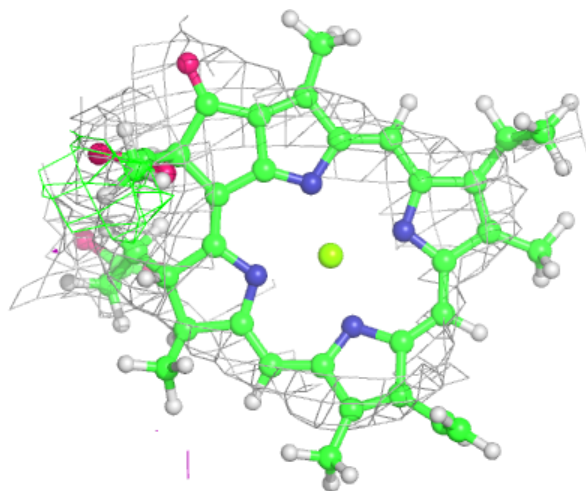
Electron density around CLA K 101:

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



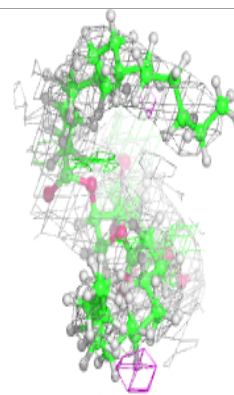
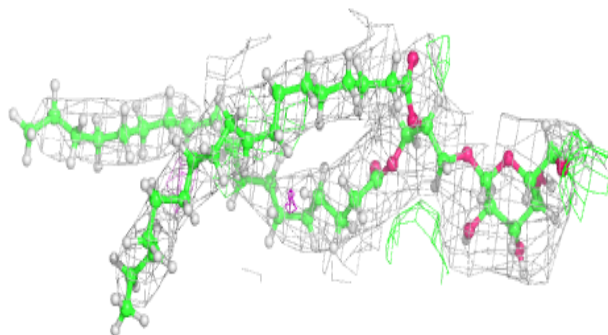
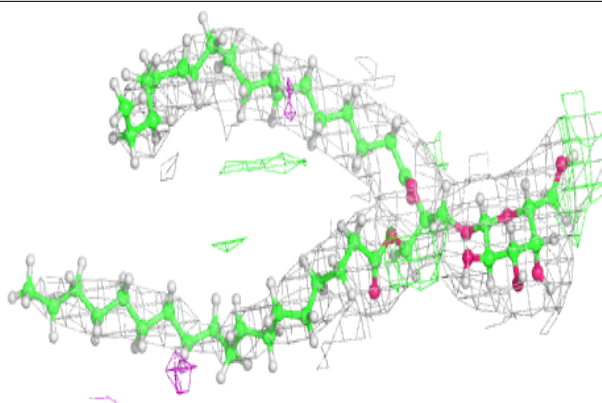
Electron density around CLA K 103:

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



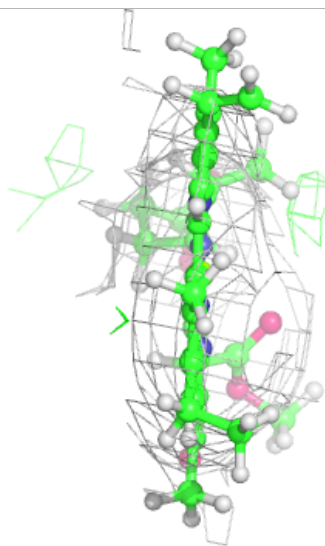
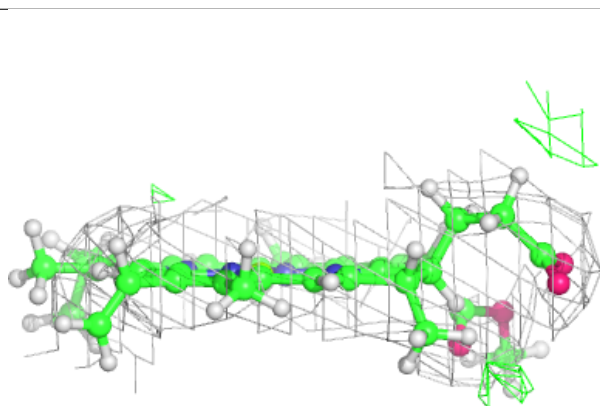
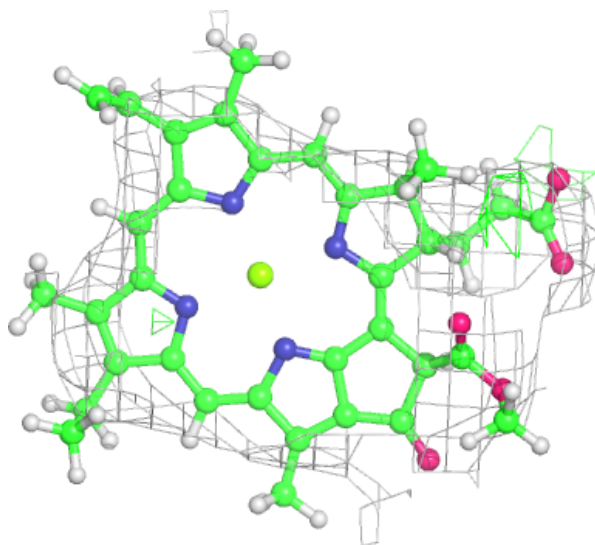
Electron density around LMG B 3049:

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



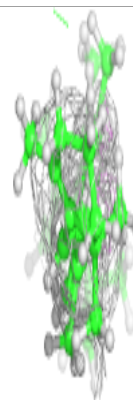
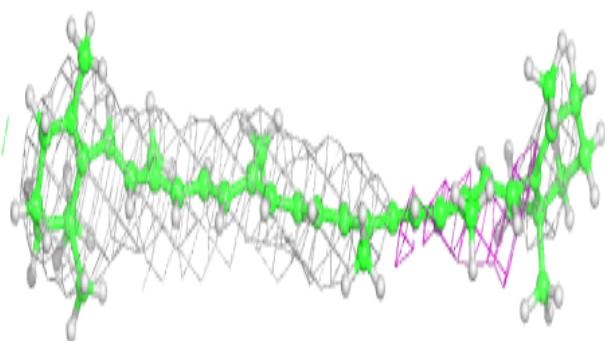
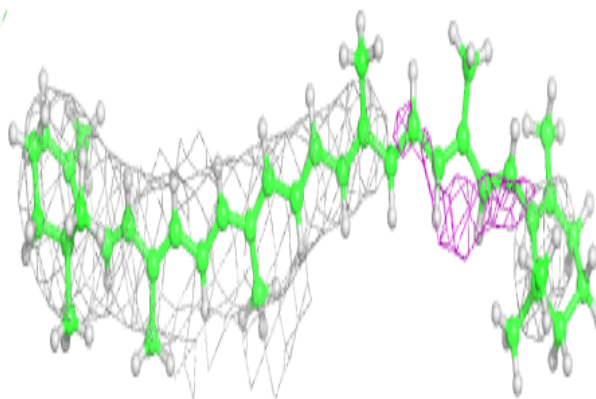
Electron density around CLA F 202:

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



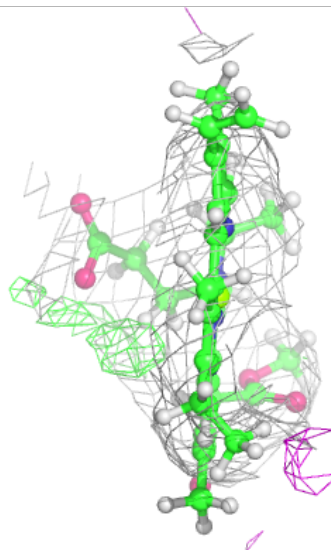
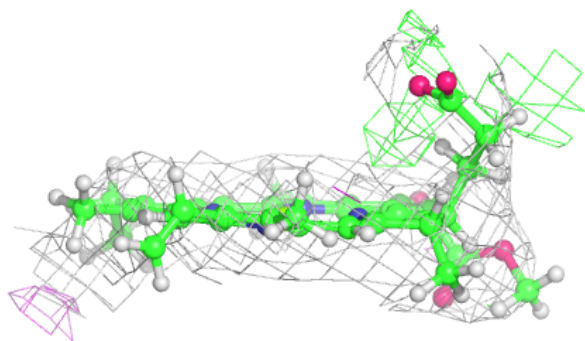
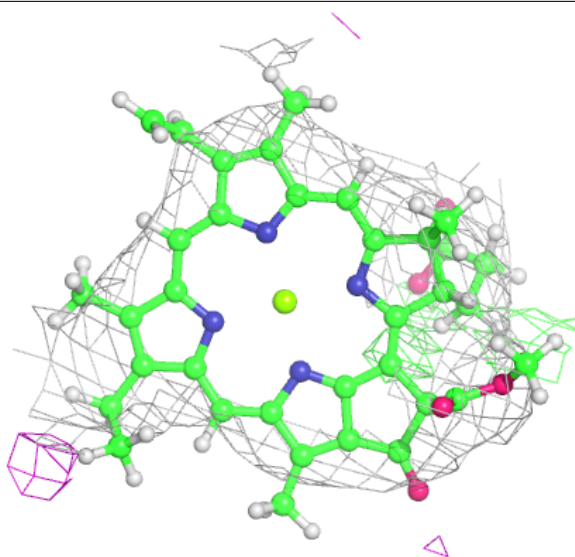
Electron density around BCR A 849:

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



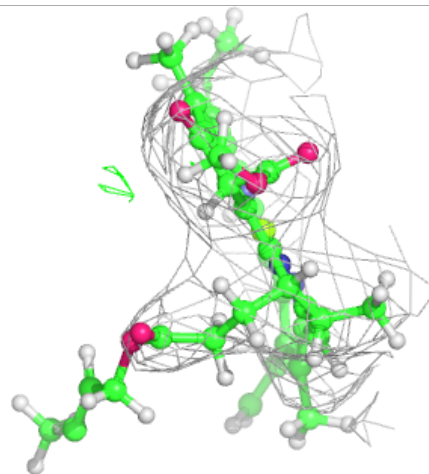
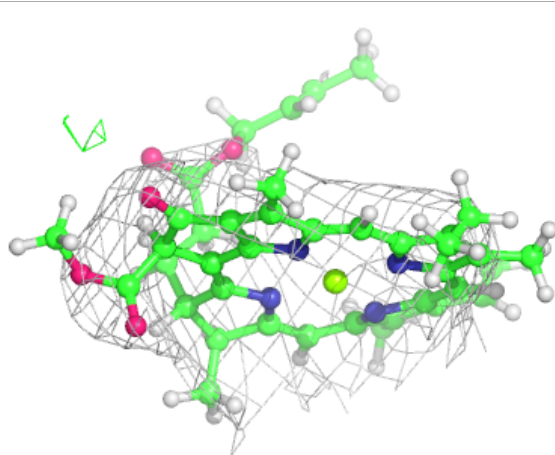
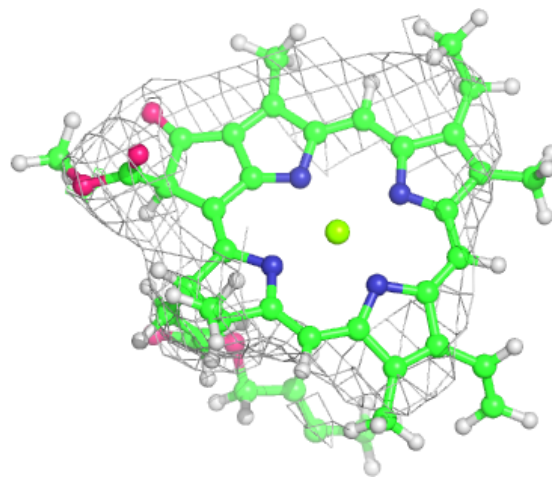
Electron density around CLA A 811:

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



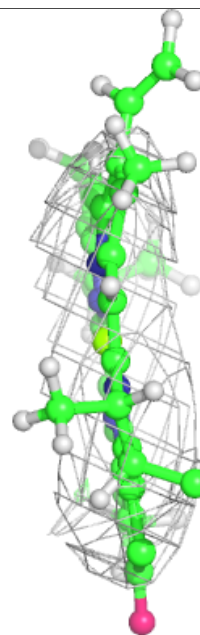
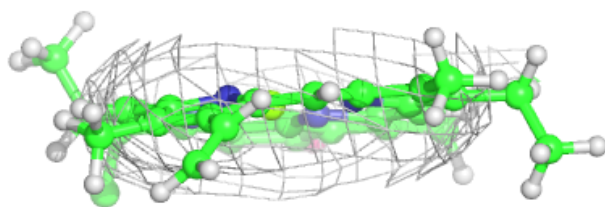
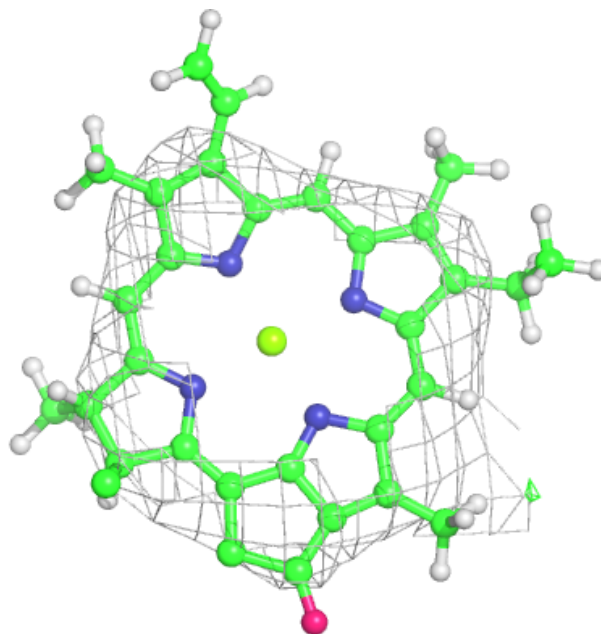
Electron density around CLA A 817:

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



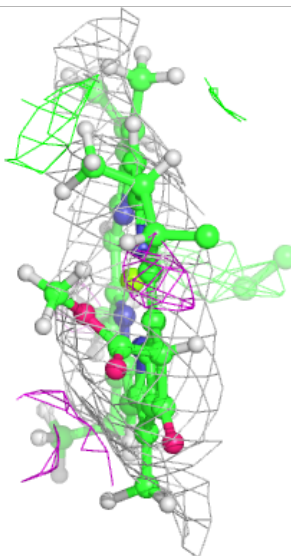
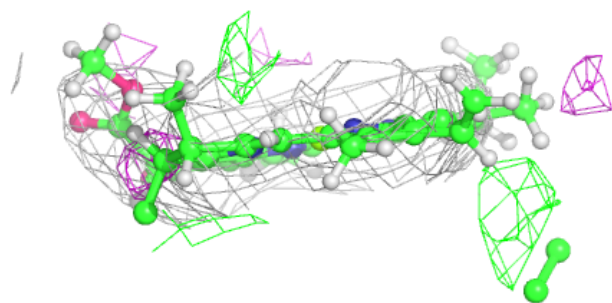
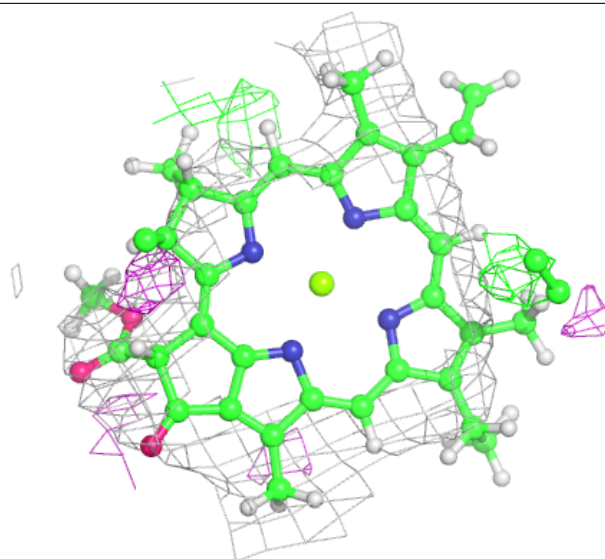
Electron density around CLA J 102:

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



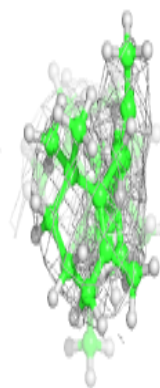
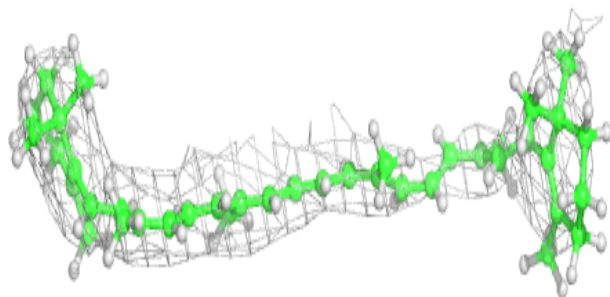
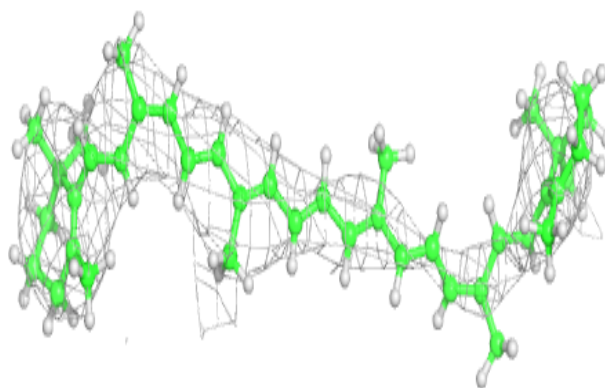
Electron density around CLA A 821:

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

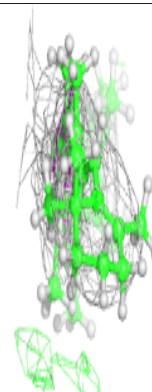
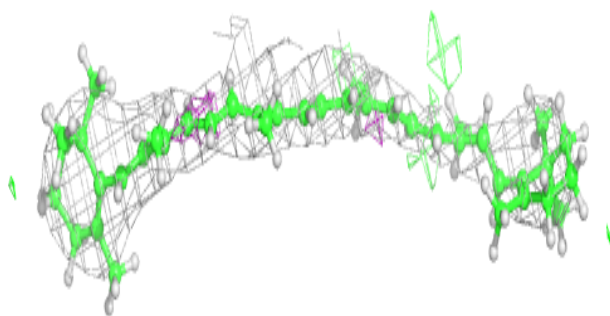
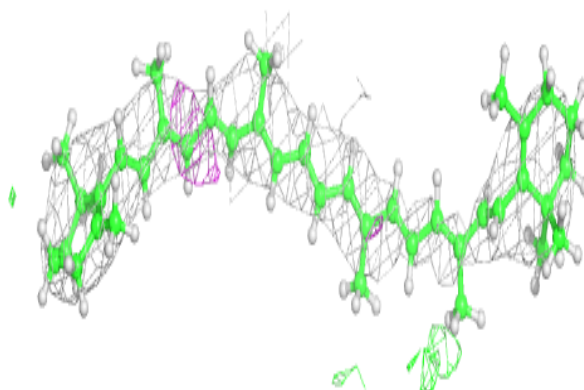


Electron density around BCR B 3046:

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

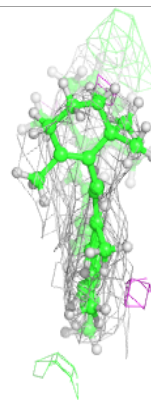
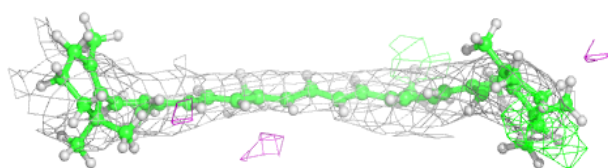
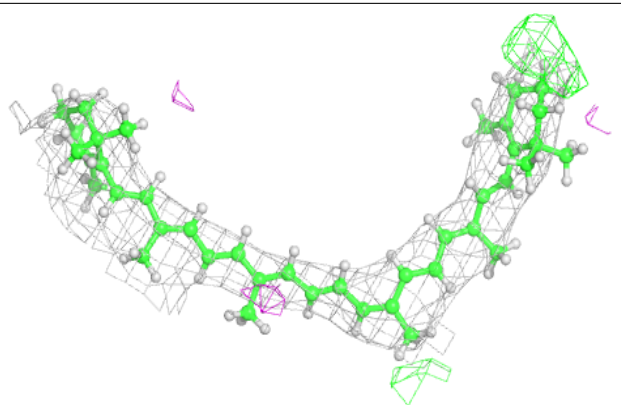
**Electron density around BCR B 3051:**

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



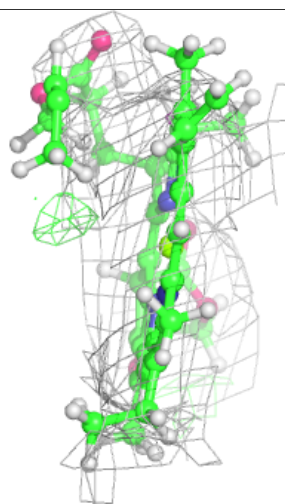
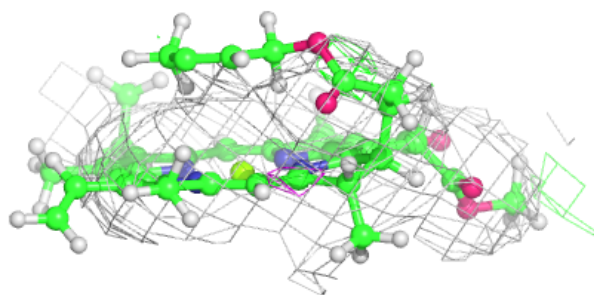
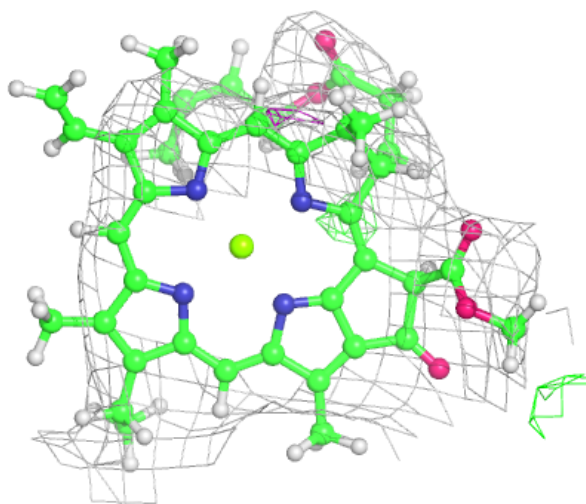
Electron density around BCR F 203:

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



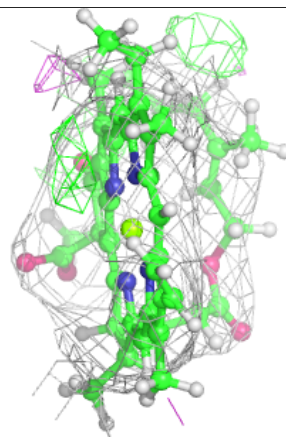
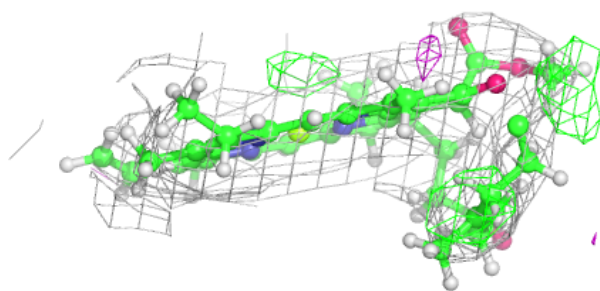
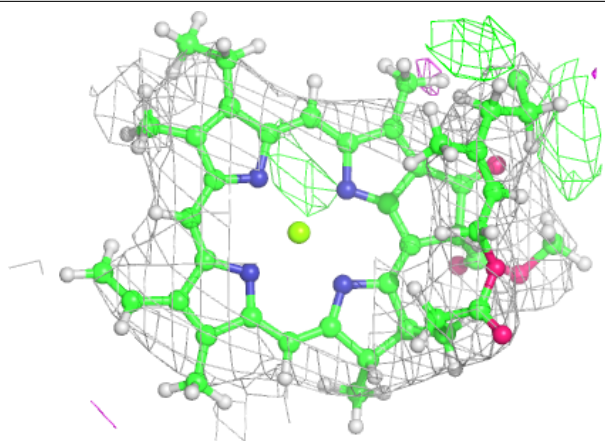
Electron density around CLA A 823:

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



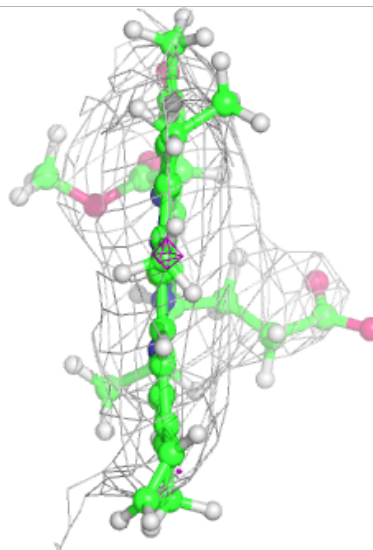
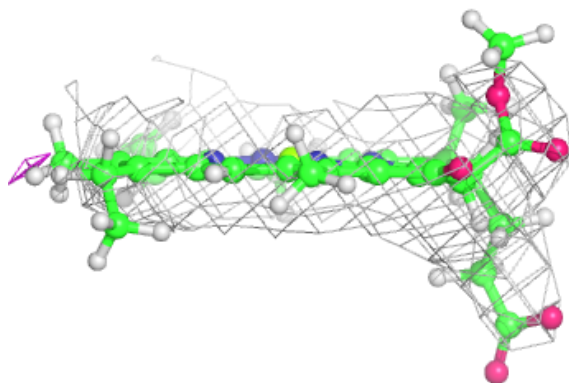
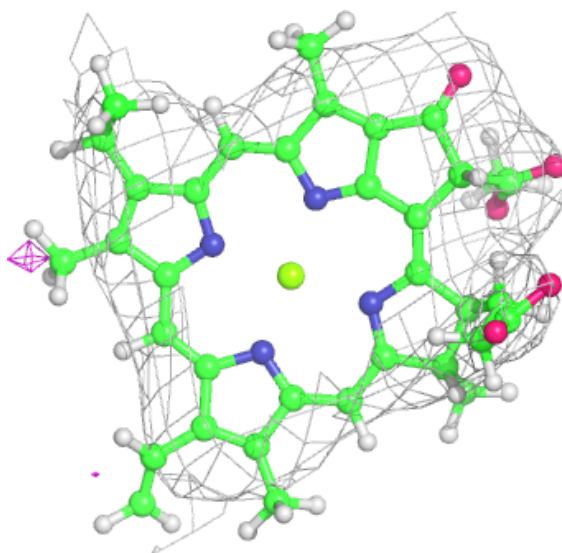
Electron density around CLA A 845:

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



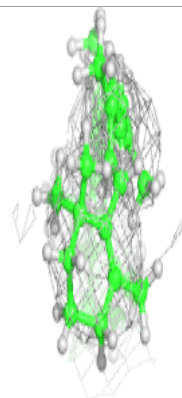
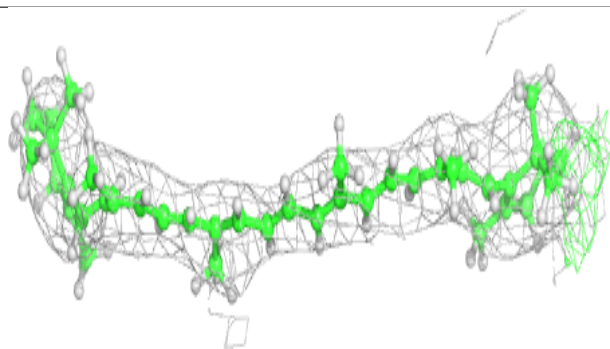
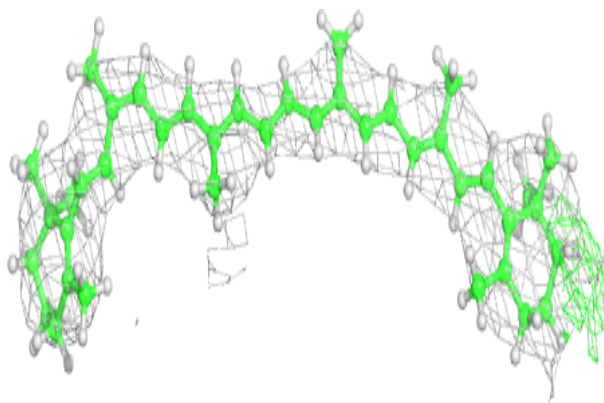
Electron density around CLA B 3022:

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



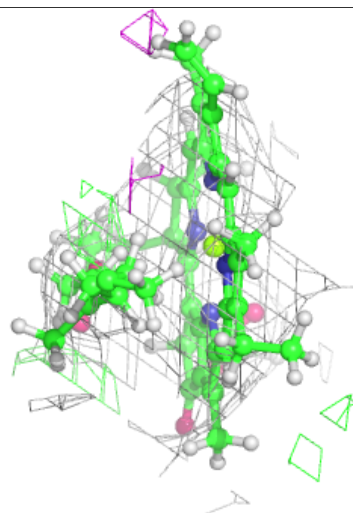
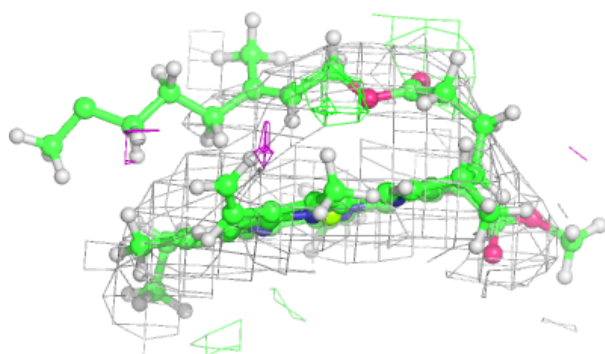
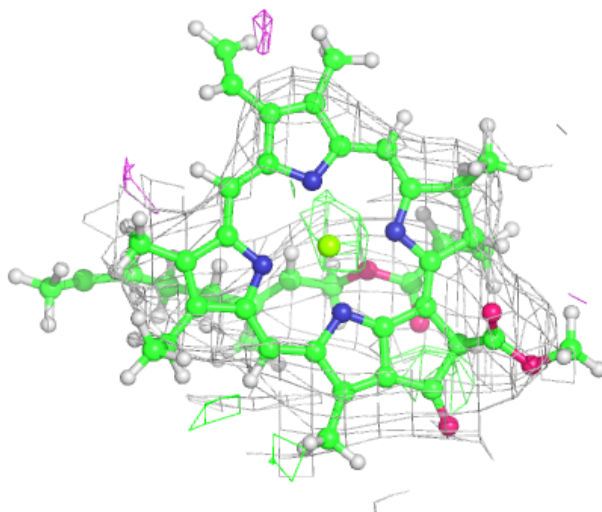
Electron density around BCR B 3045:

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



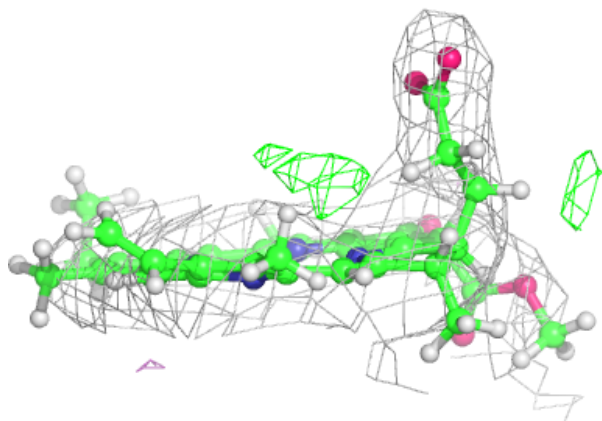
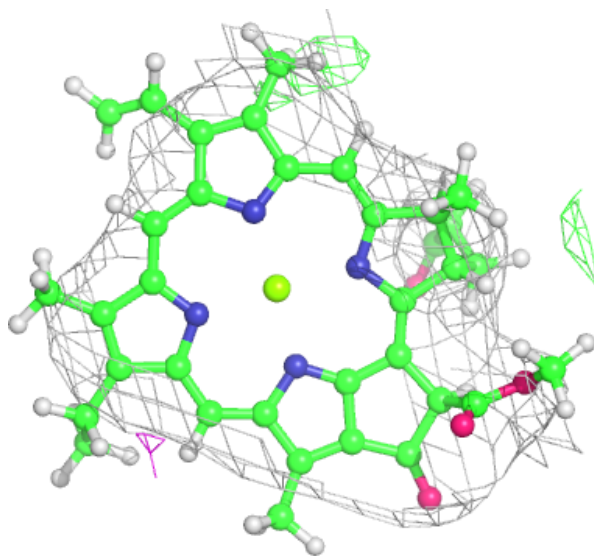
Electron density around CLA A 818:

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



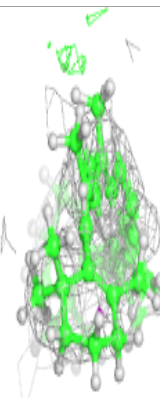
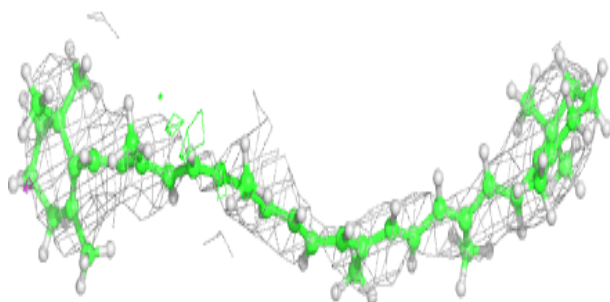
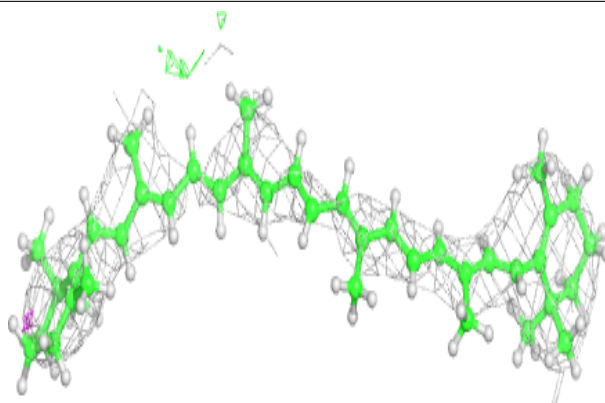
Electron density around CLA A 837:

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

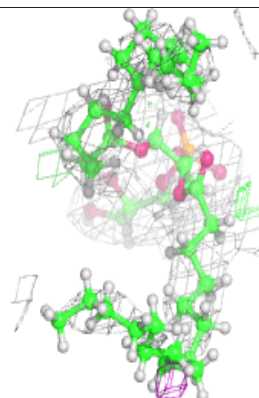
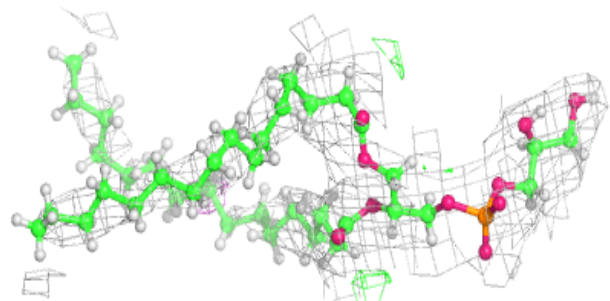
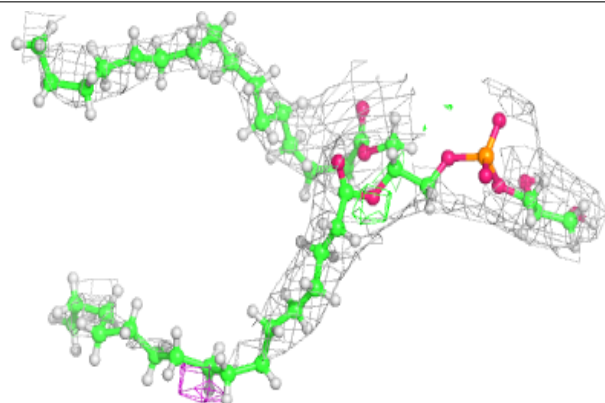


Electron density around BCR F 201:

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

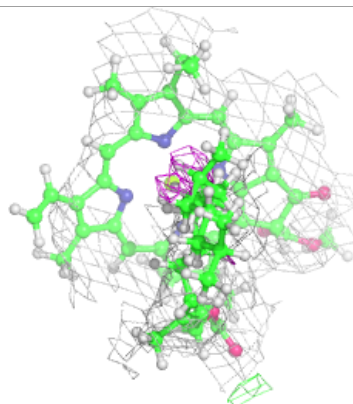
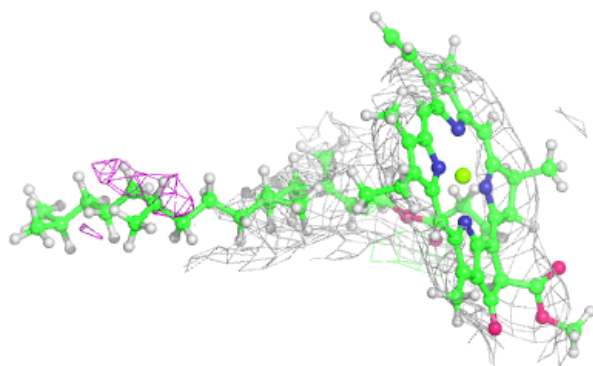
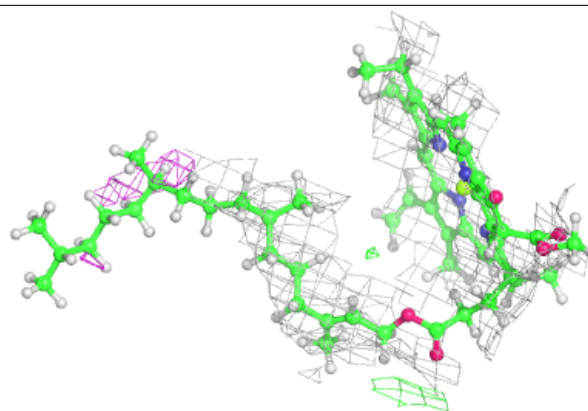
**Electron density around LHG A 853:**

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

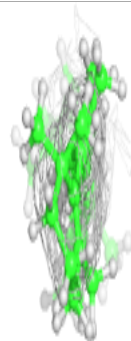
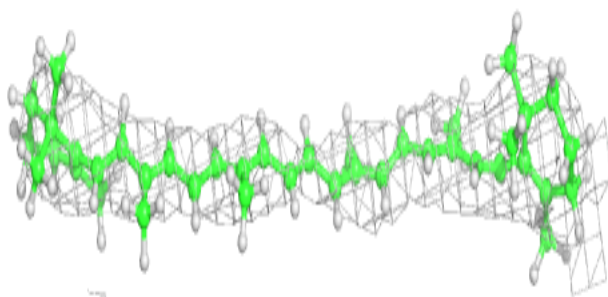
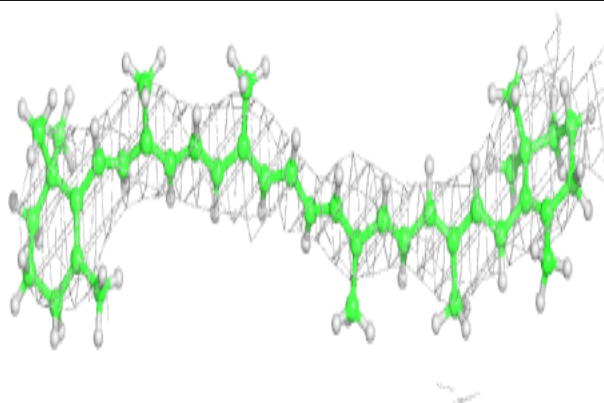


Electron density around CLA A 812:

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

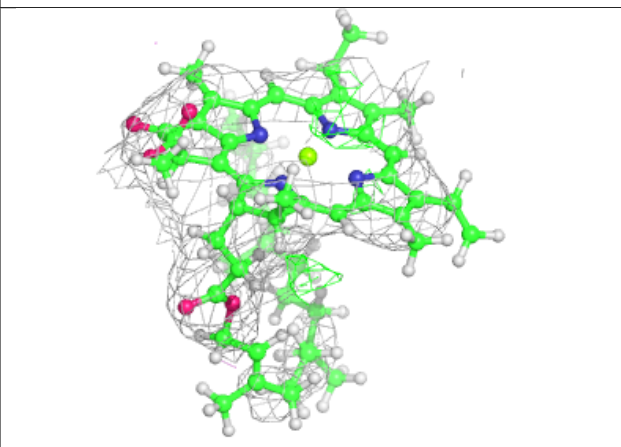
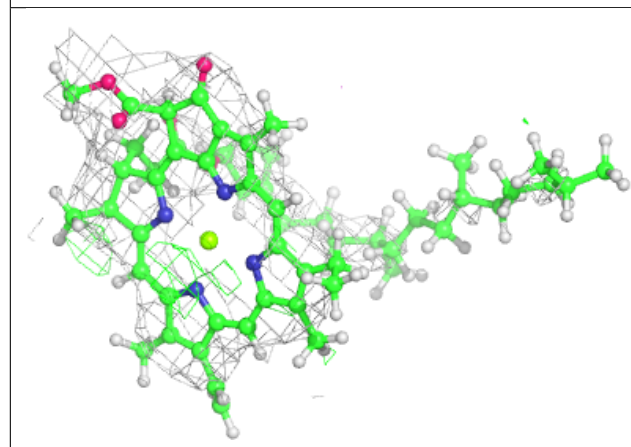
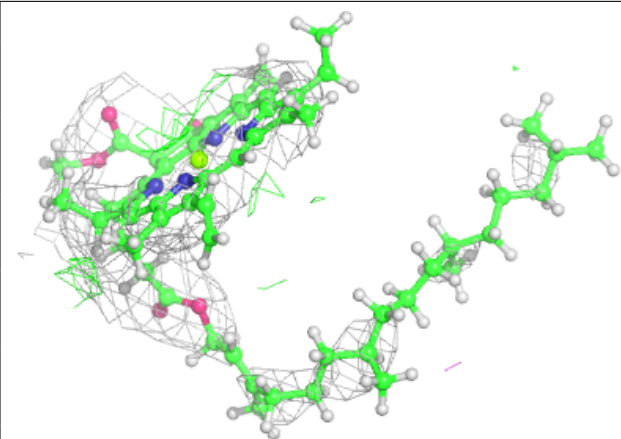
**Electron density around BCR J 103:**

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

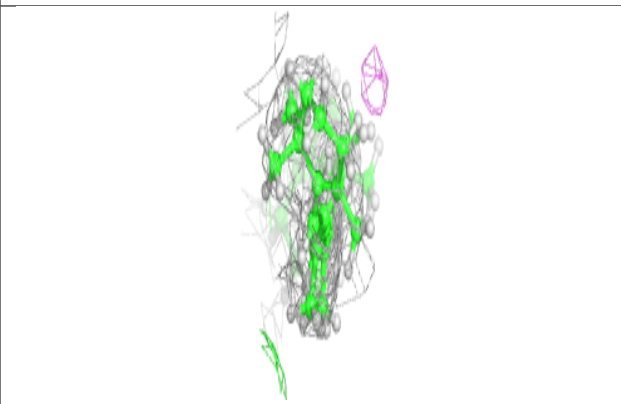
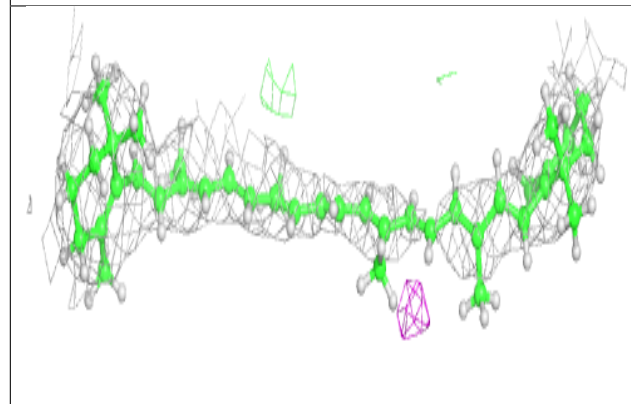
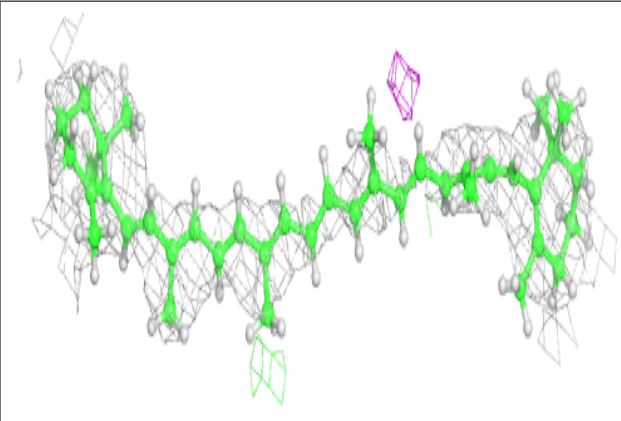


Electron density around CLA B 3020:

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

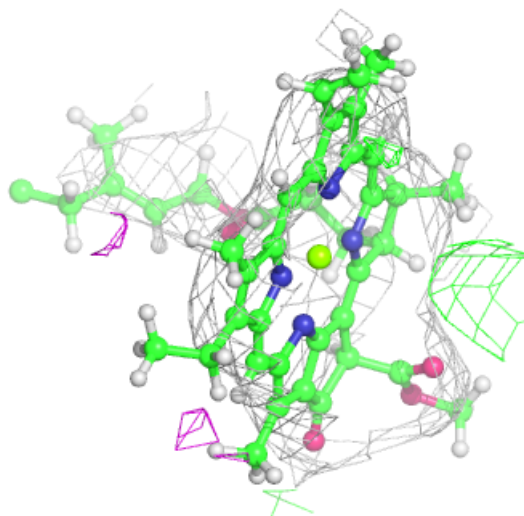
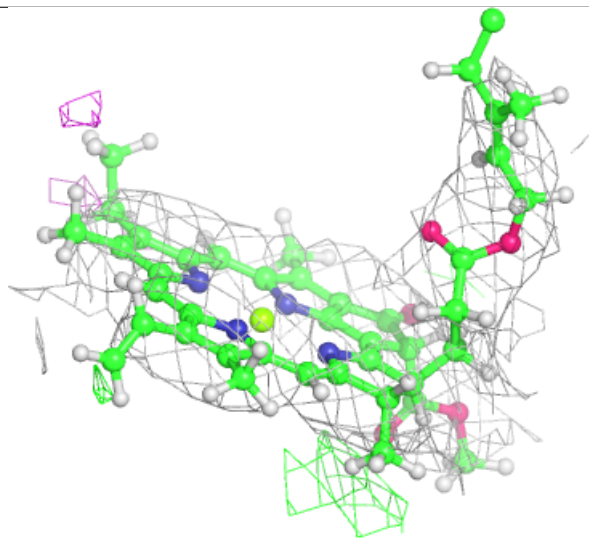
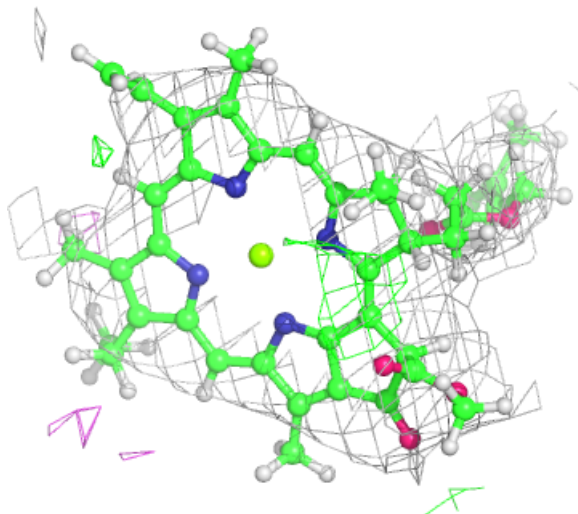
**Electron density around BCR A 850:**

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



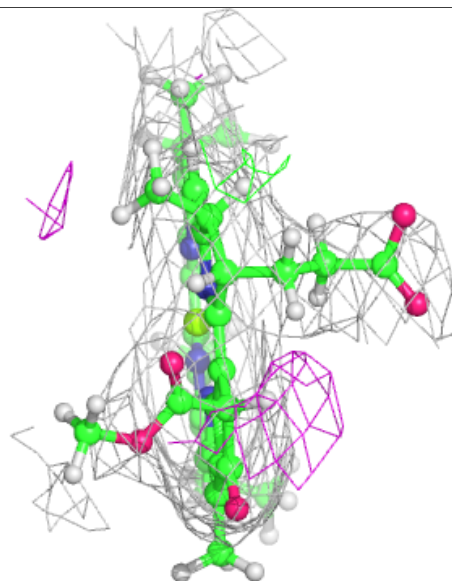
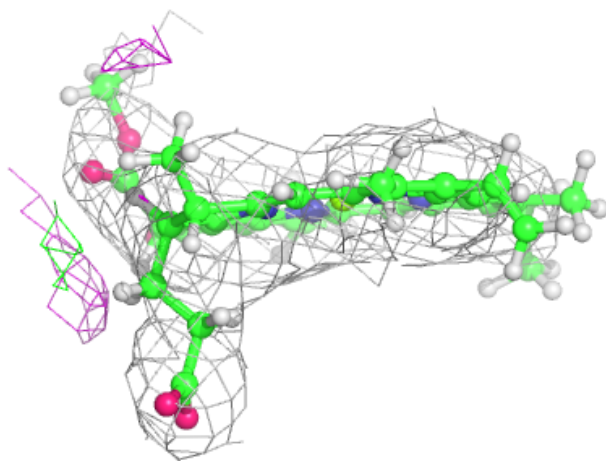
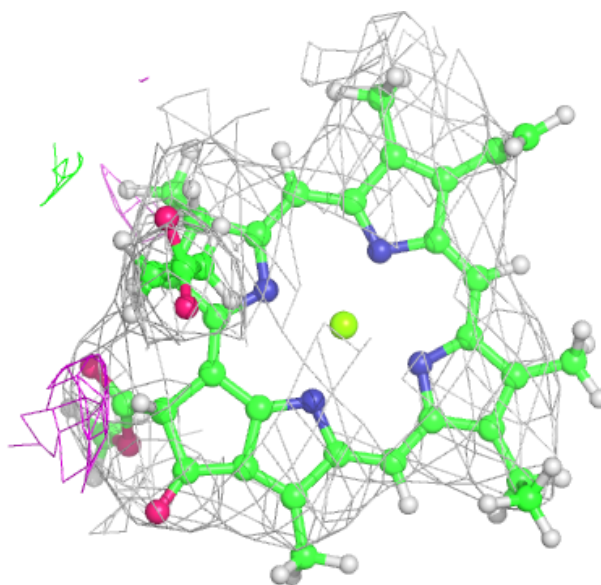
Electron density around CLA A 808:

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



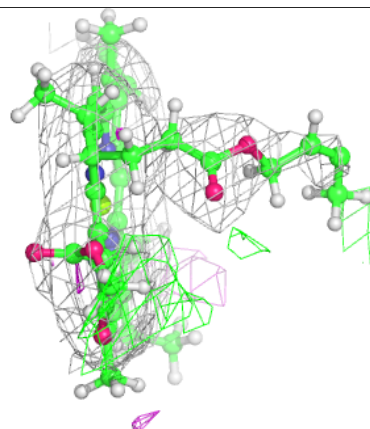
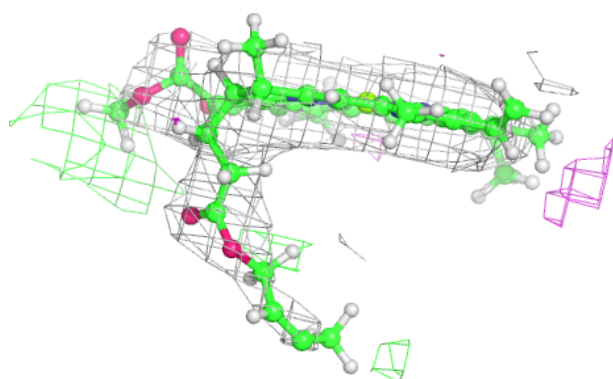
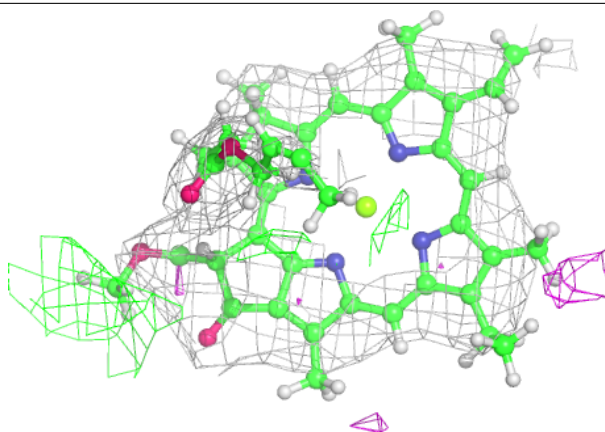
Electron density around CLA B 3031:

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

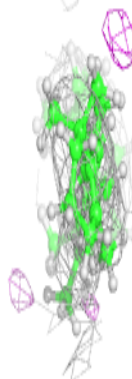
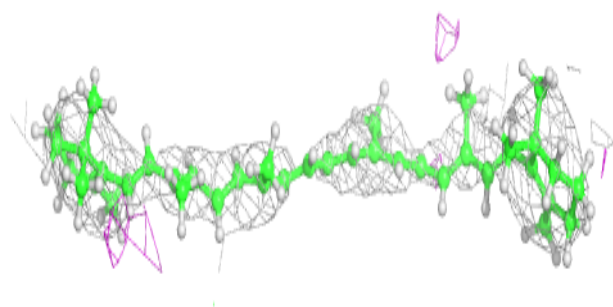
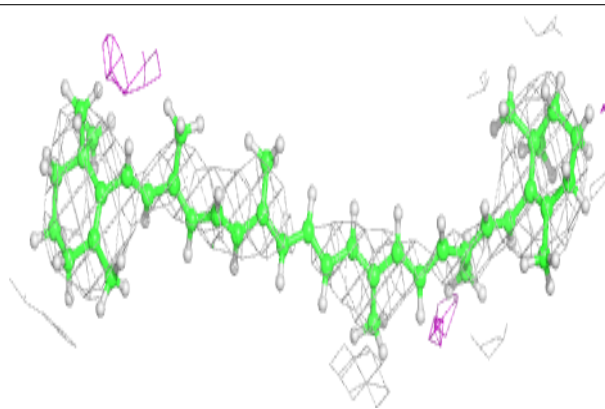


Electron density around CLA B 3032:

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

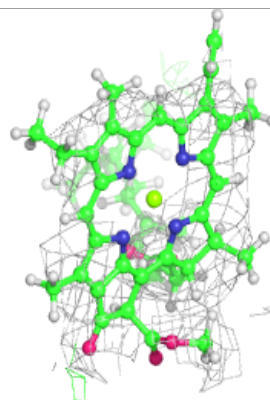
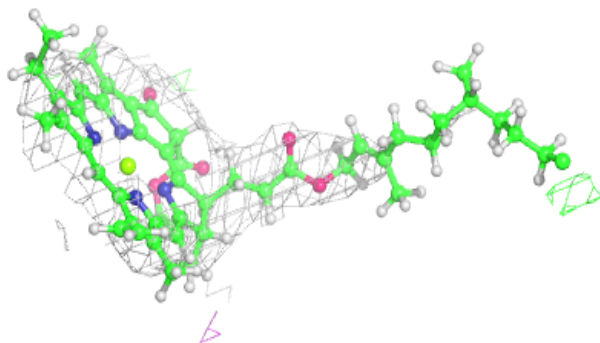
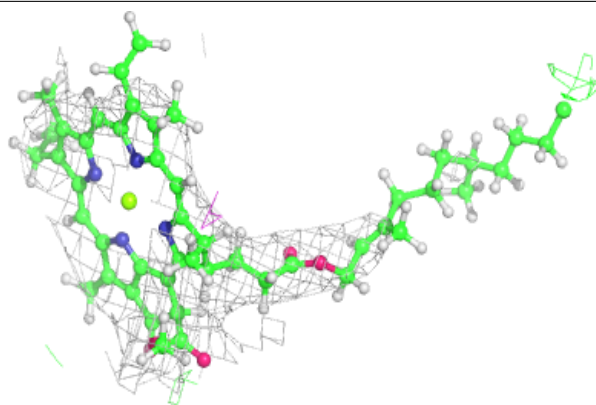
**Electron density around BCR B 3047:**

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



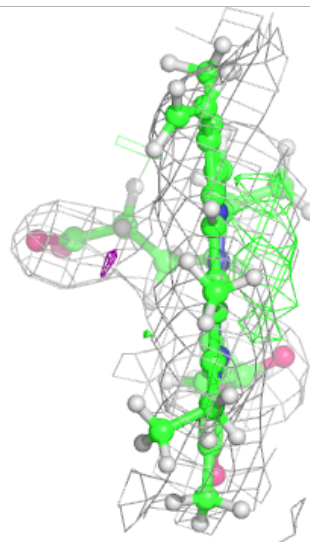
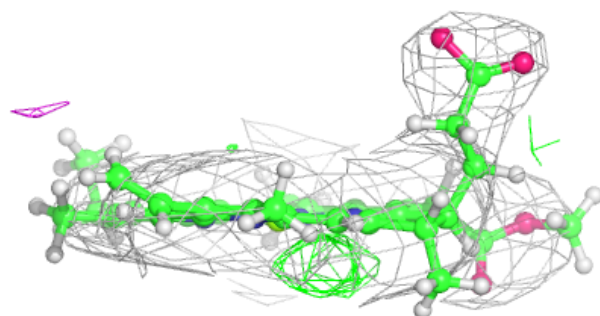
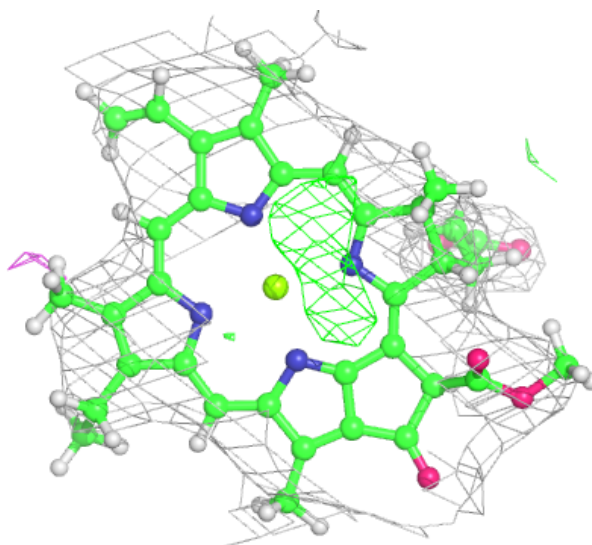
Electron density around CLA B 3034:

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



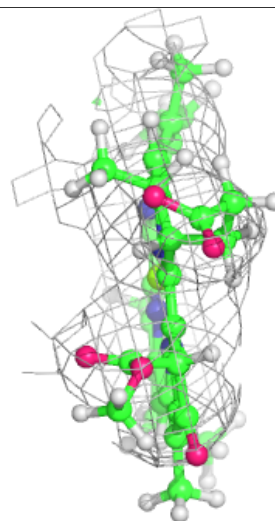
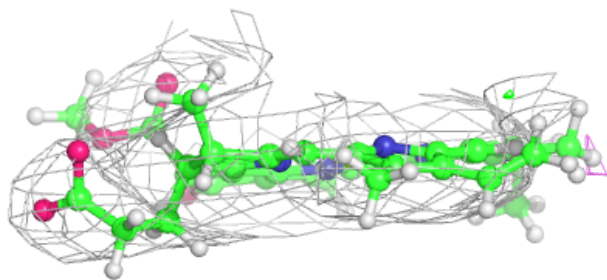
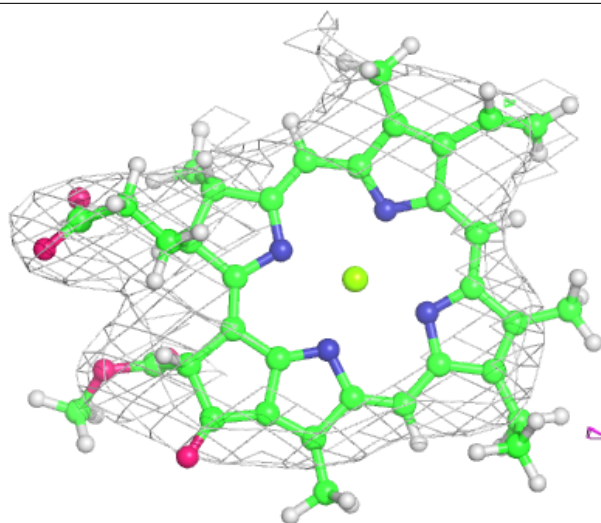
Electron density around CLA B 3036:

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



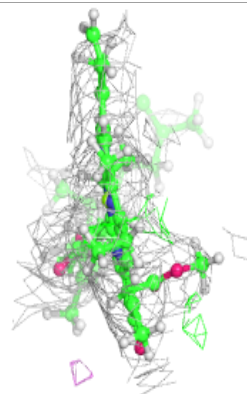
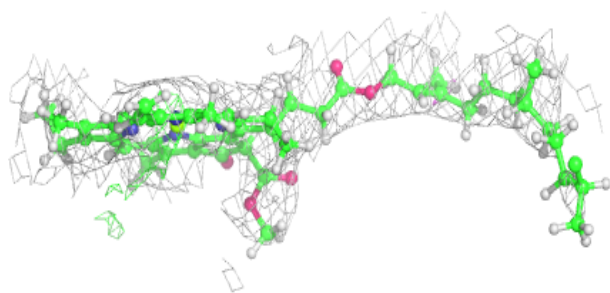
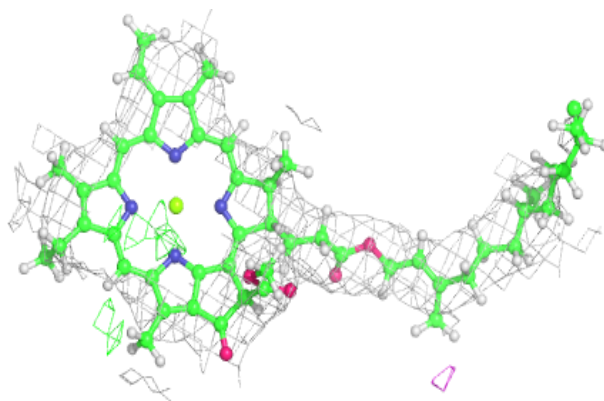
Electron density around CLA B 3037:

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

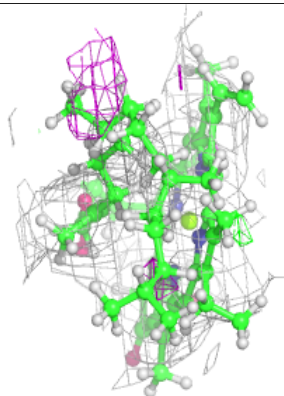
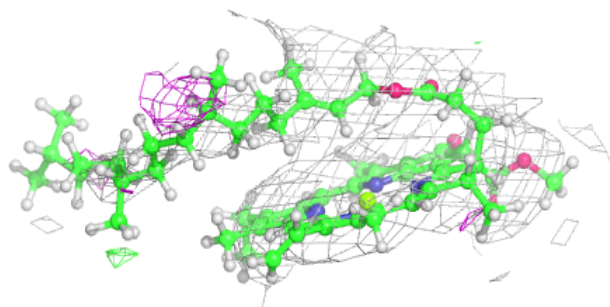
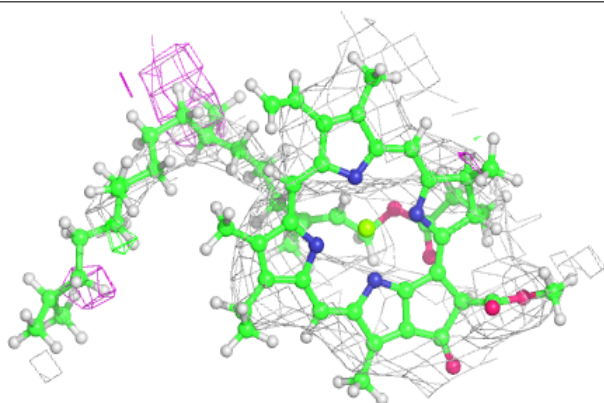


Electron density around CLA B 3038:

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

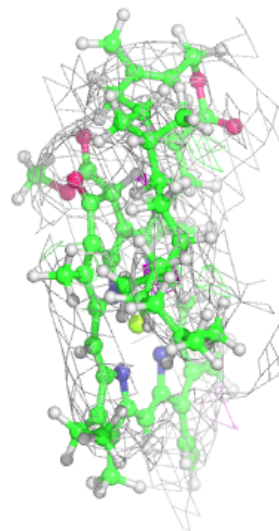
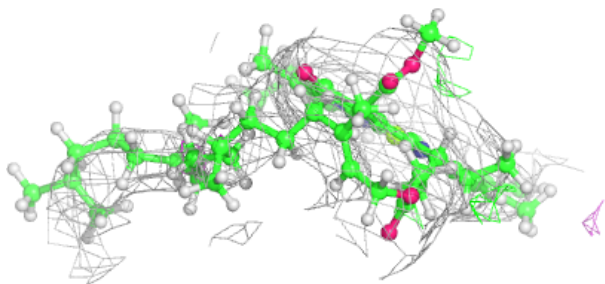
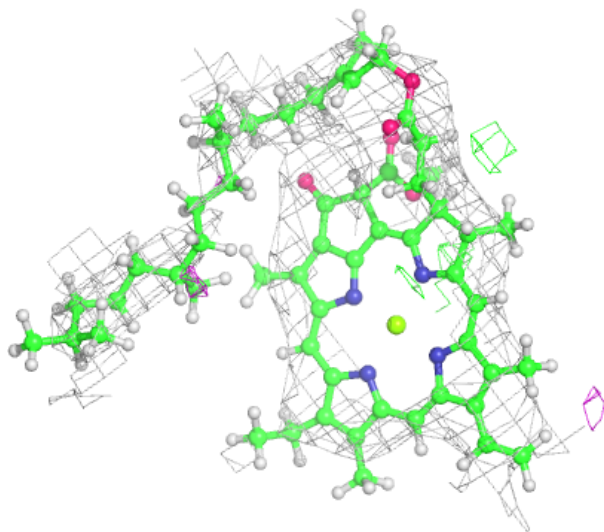
**Electron density around CLA B 3039:**

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



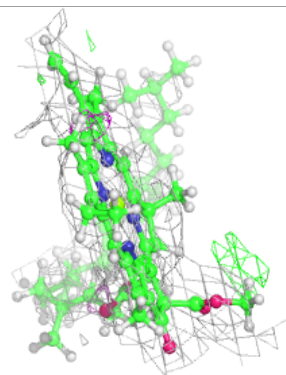
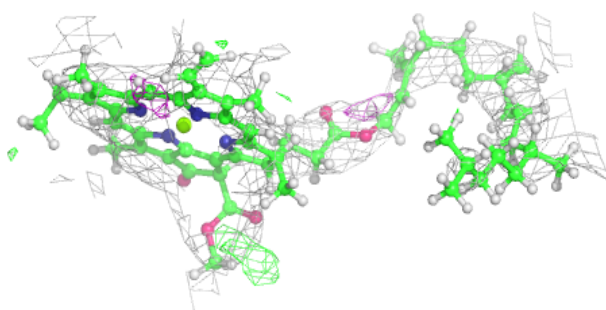
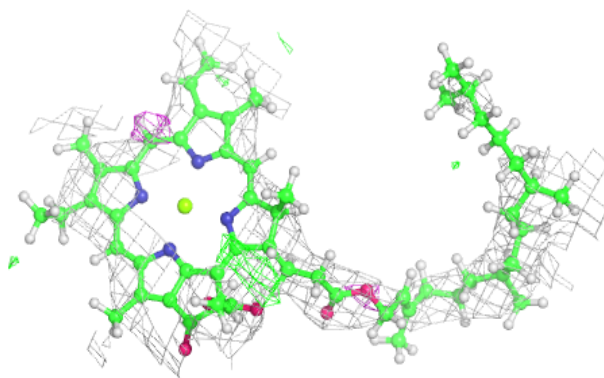
Electron density around CLA A 826:

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

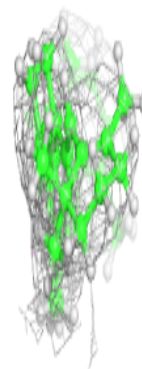
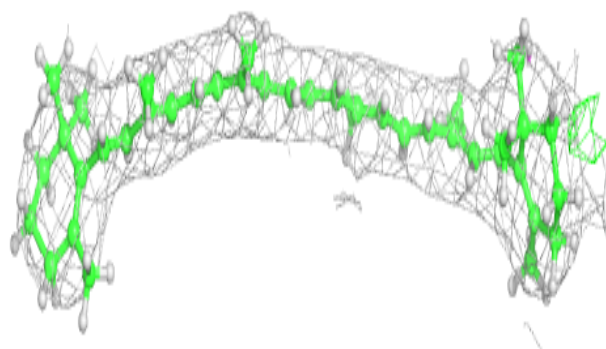
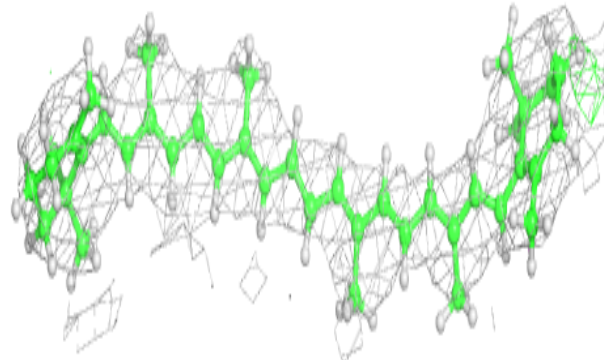


Electron density around CLA A 828:

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

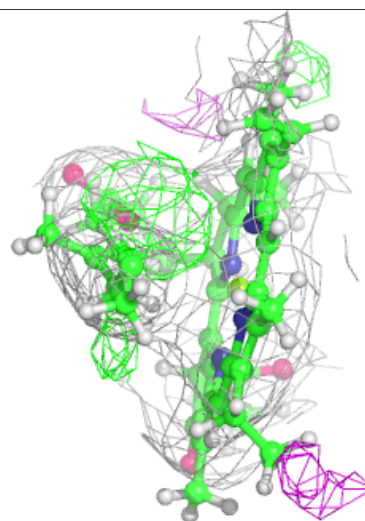
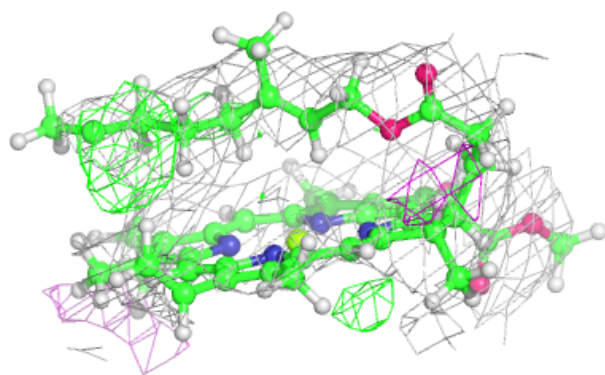
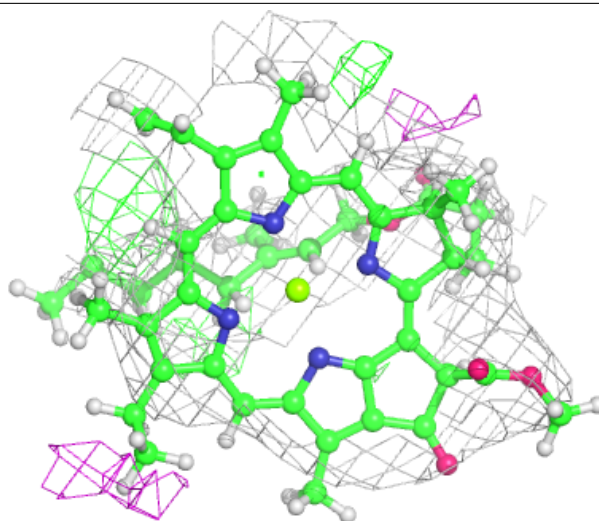
**Electron density around BCR M 103:**

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



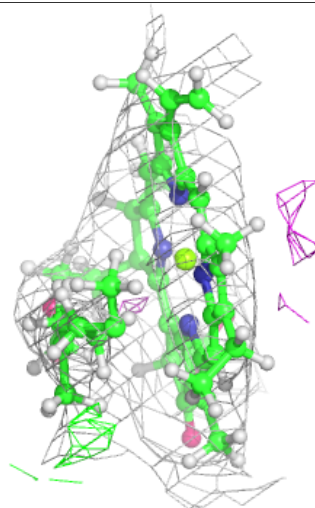
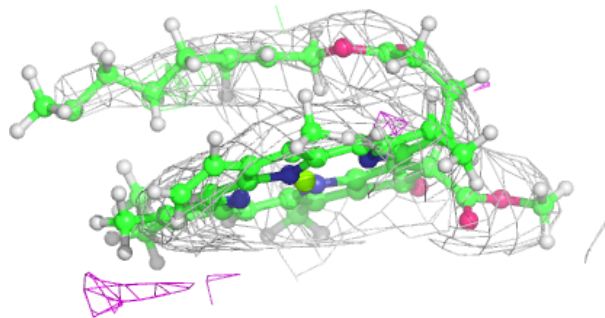
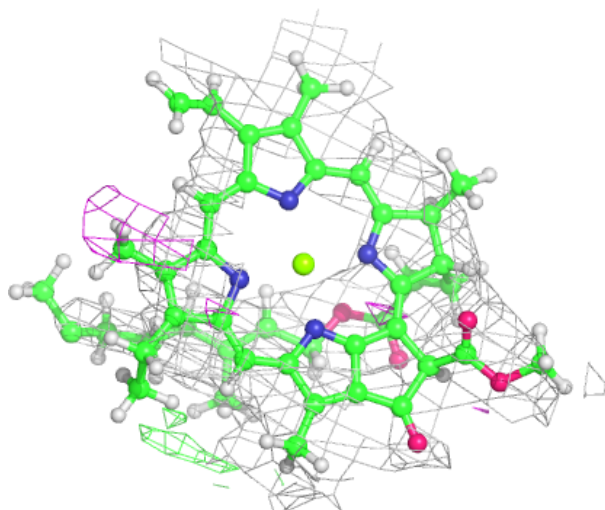
Electron density around CLA A 819:

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



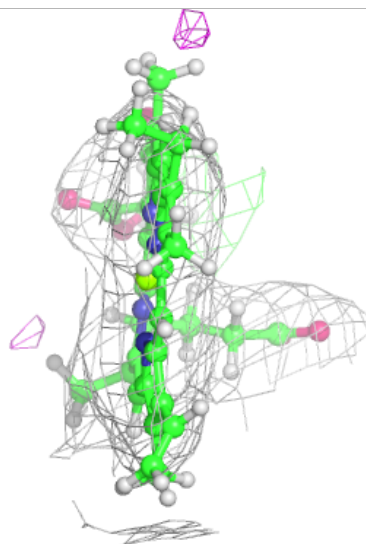
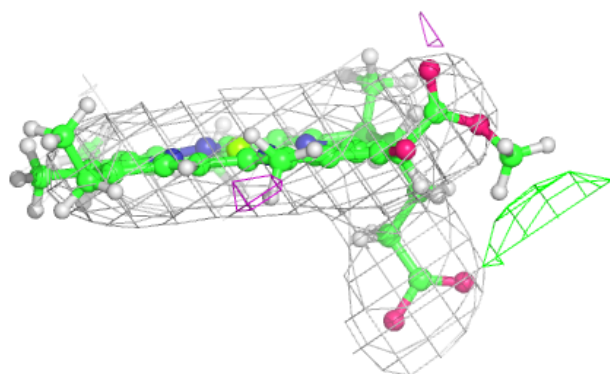
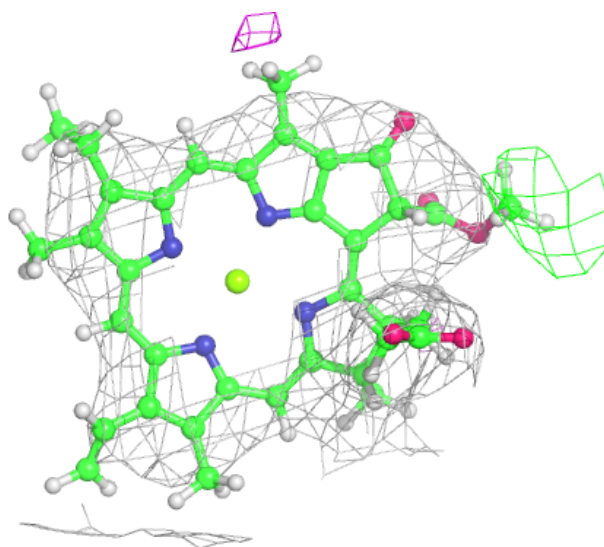
Electron density around CLA A 813:

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



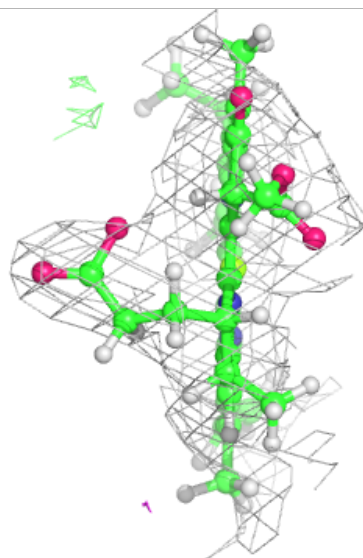
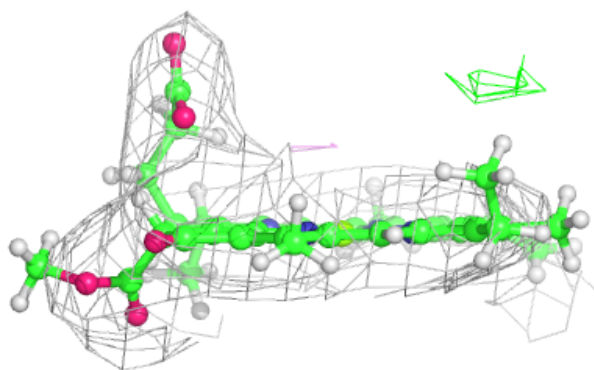
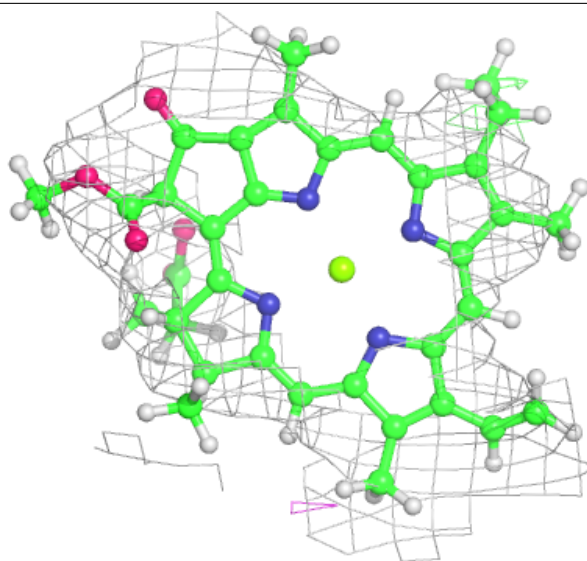
Electron density around CLA B 3012:

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



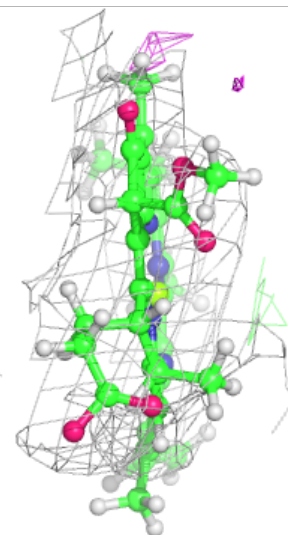
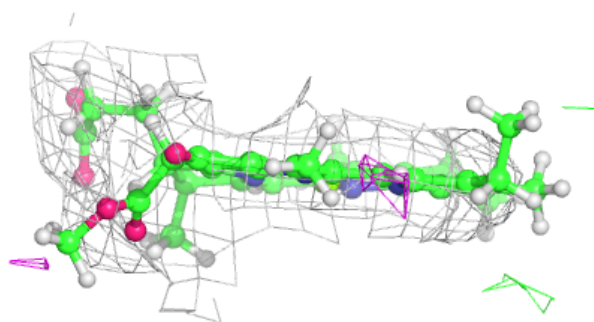
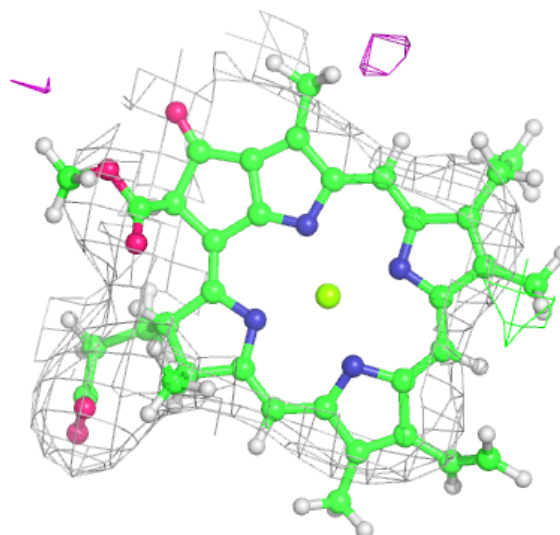
Electron density around CLA B 3013:

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



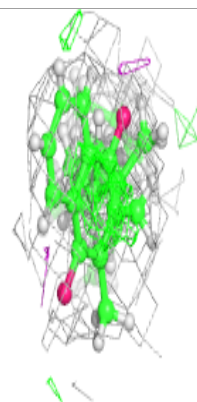
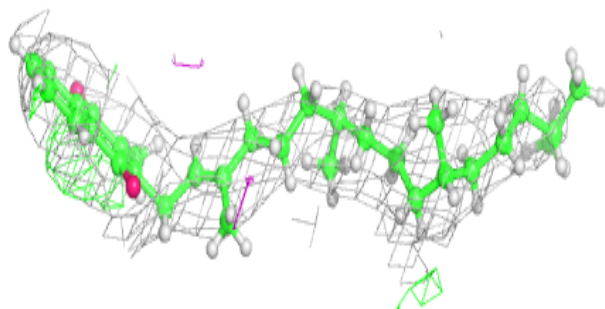
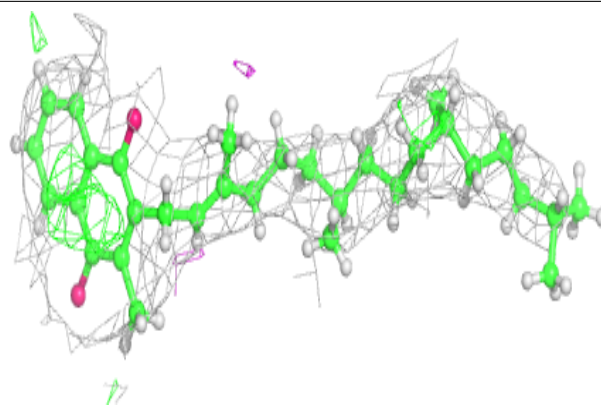
Electron density around CLA X 1701:

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

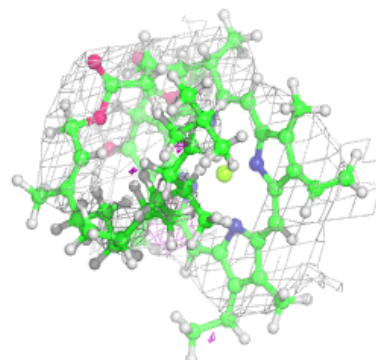
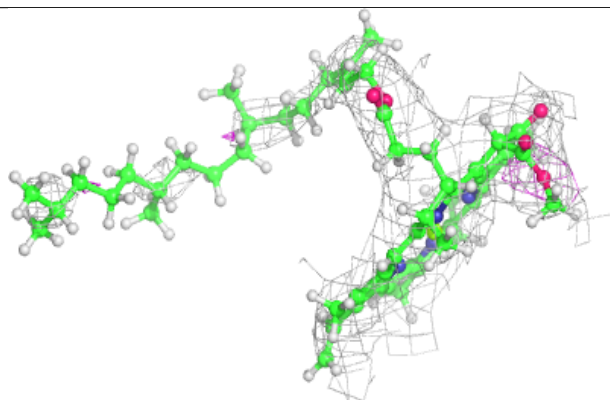
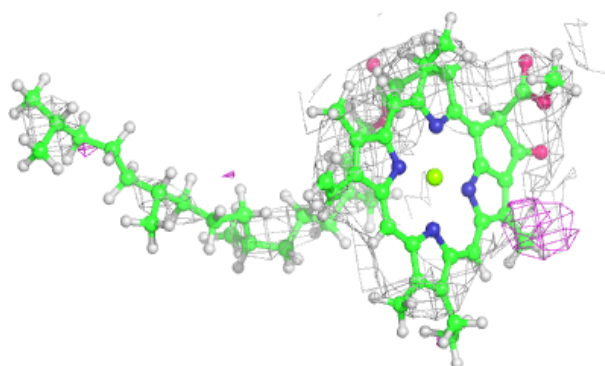


Electron density around PQN A 846:

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

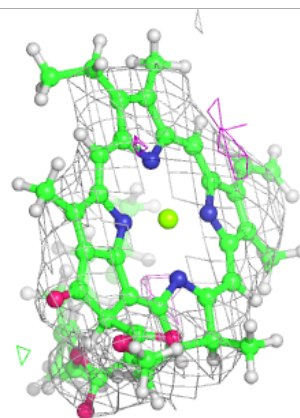
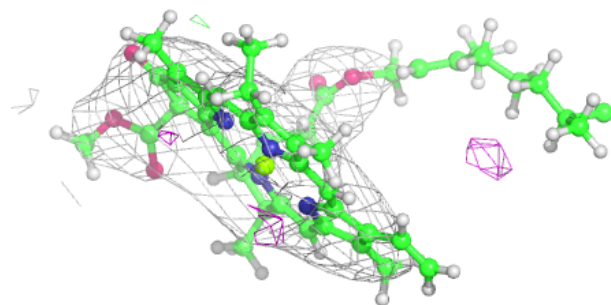
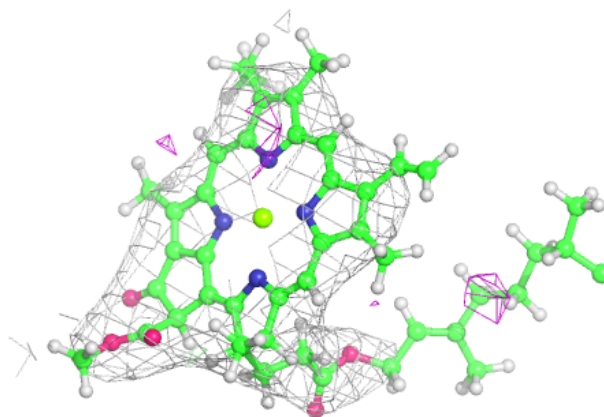
**Electron density around CLA B 3015:**

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



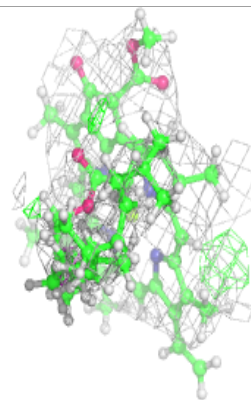
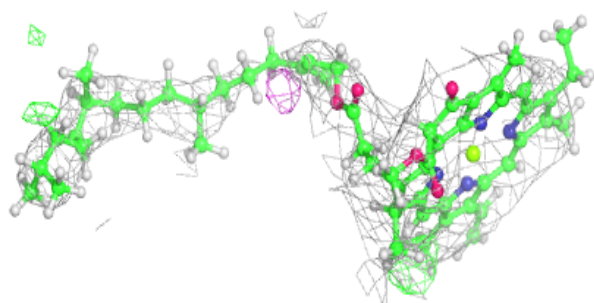
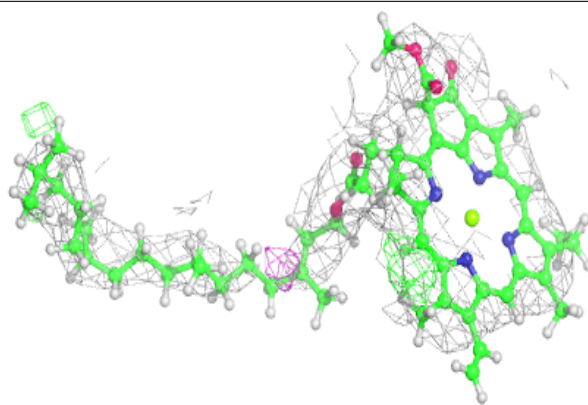
Electron density around CLA B 3017:

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



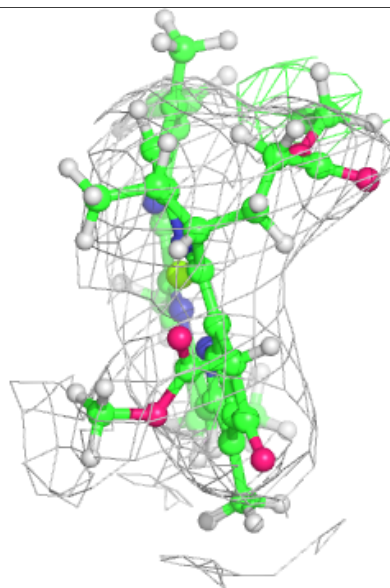
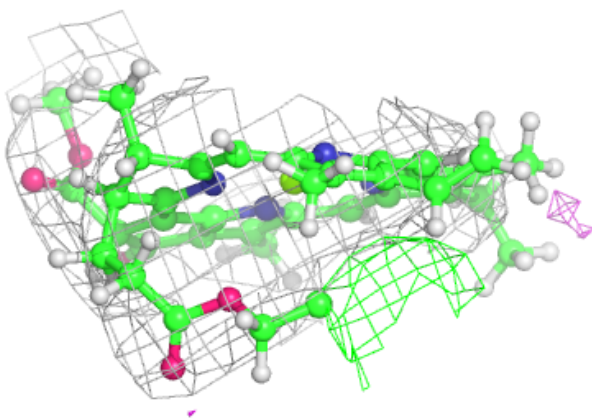
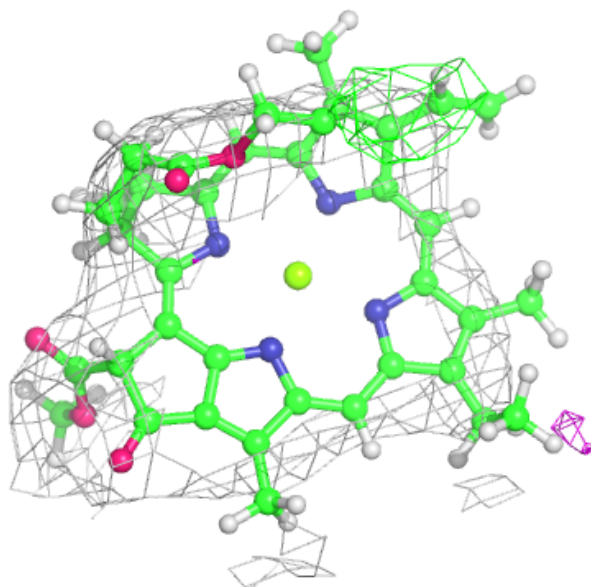
Electron density around CLA A 822:

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



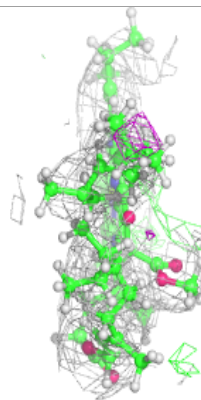
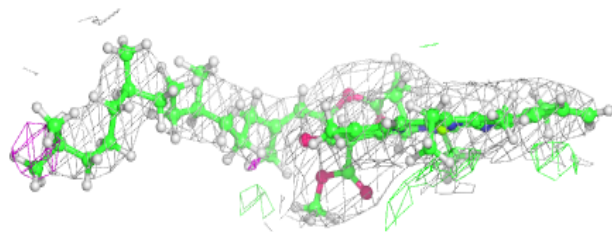
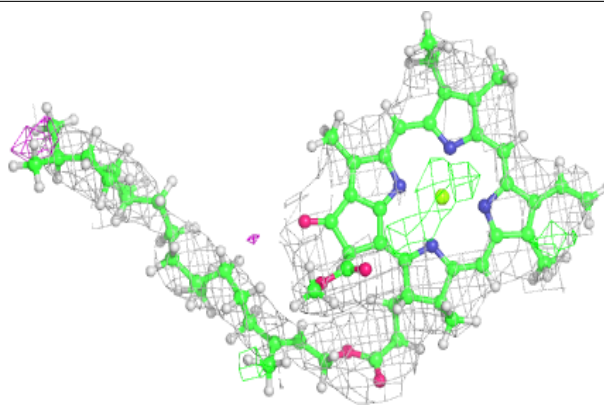
Electron density around CLA B 3021:

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

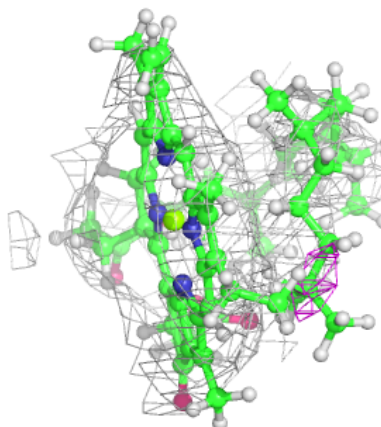
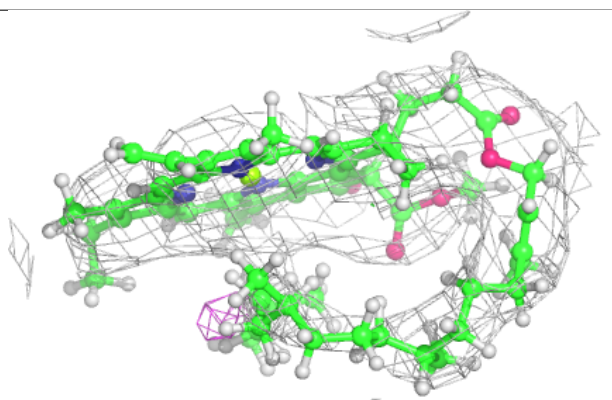
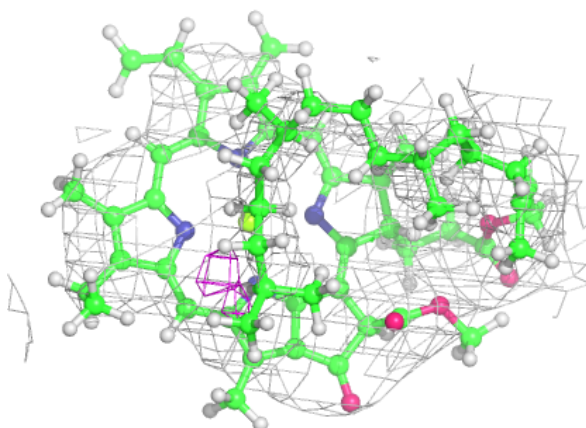


Electron density around CLA L 206:

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

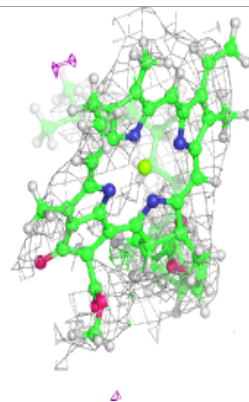
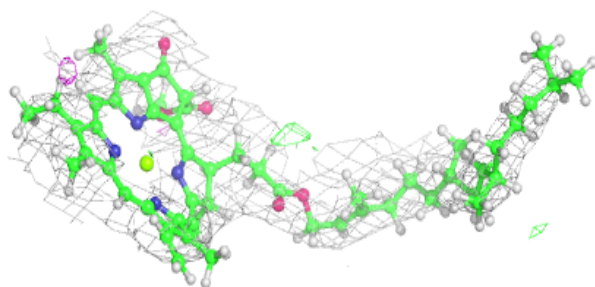
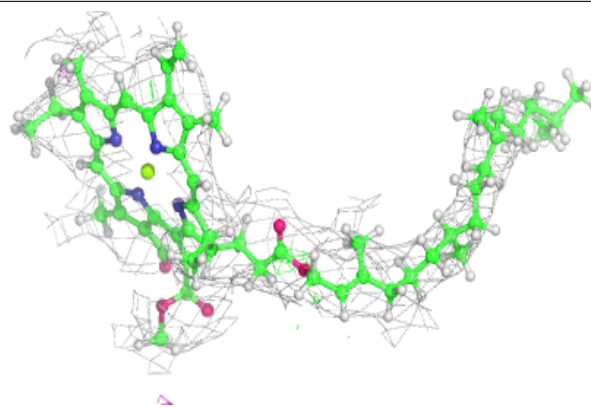
**Electron density around CLA A 807:**

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

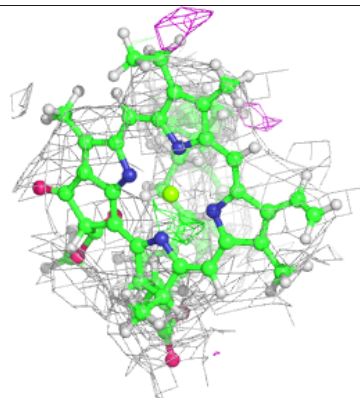
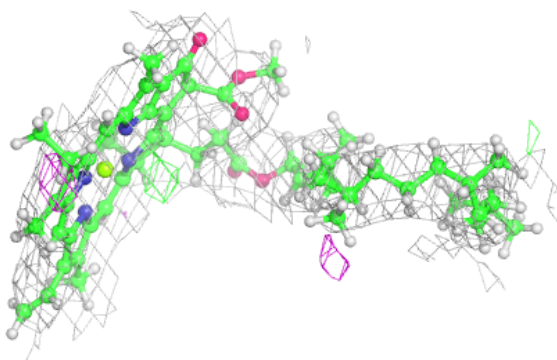
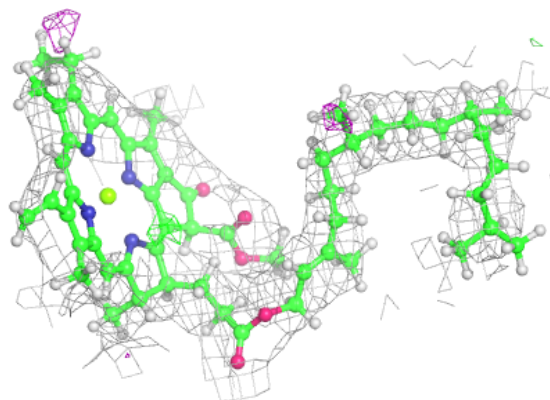


Electron density around CLA A 856:

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

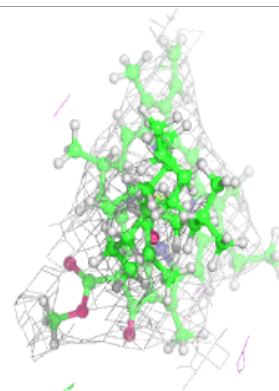
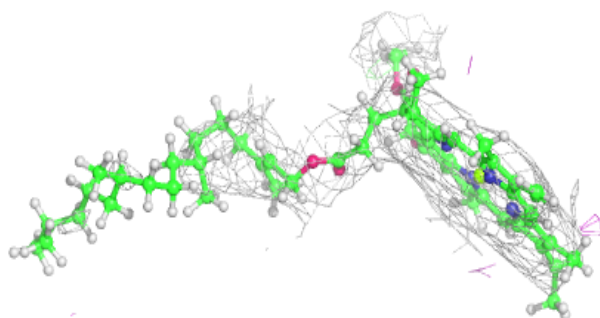
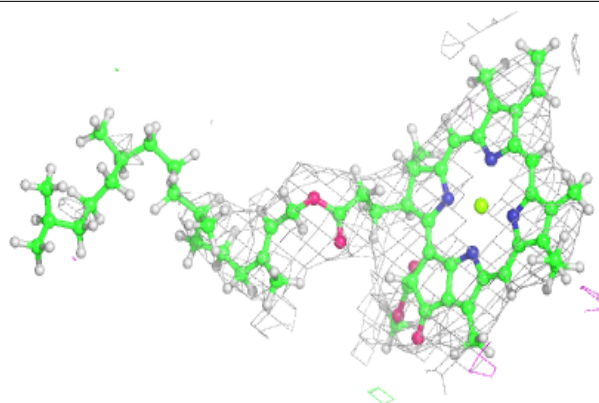
**Electron density around CL0 A 801:**

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

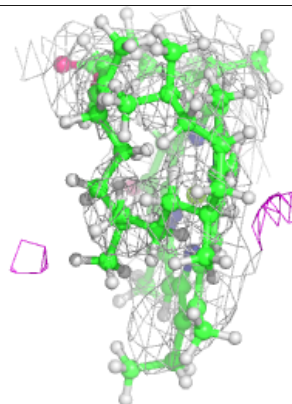
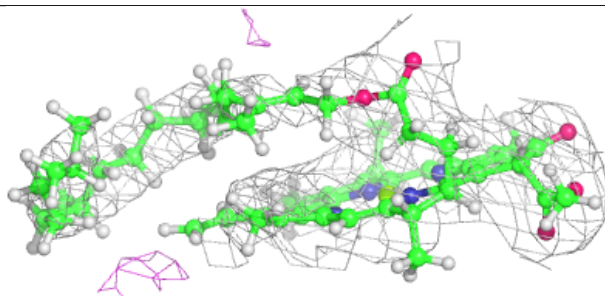
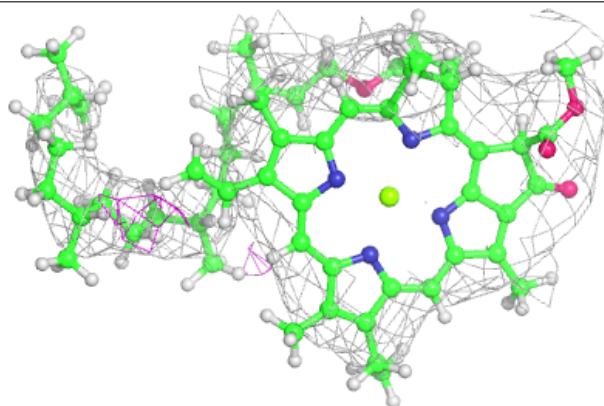


Electron density around CLA A 810:

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

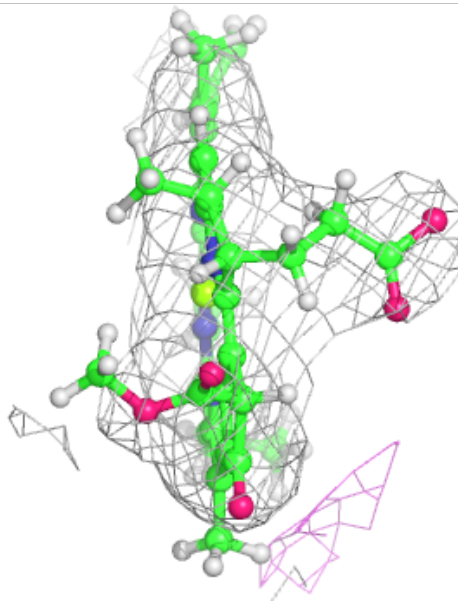
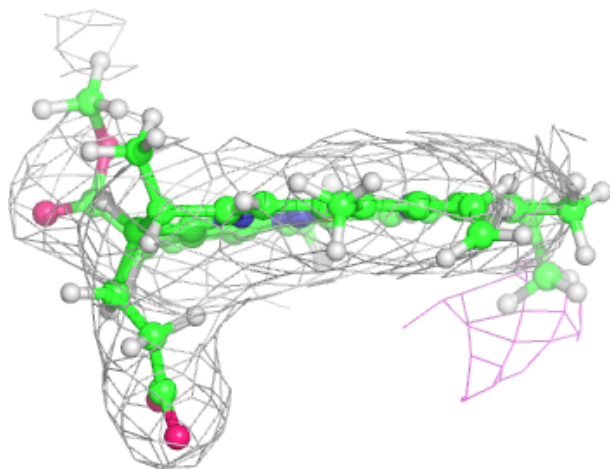
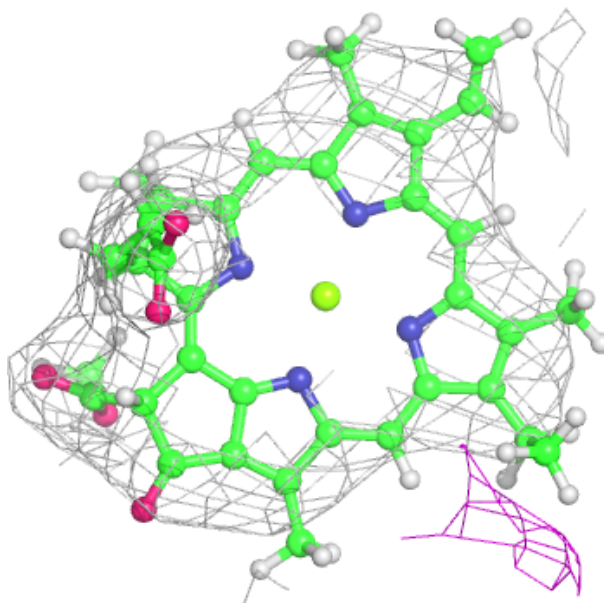
**Electron density around CLA A 820:**

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



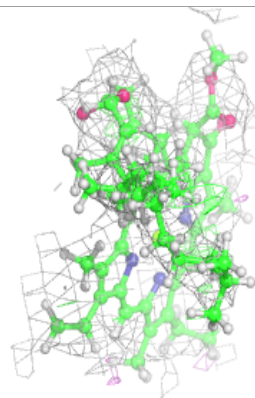
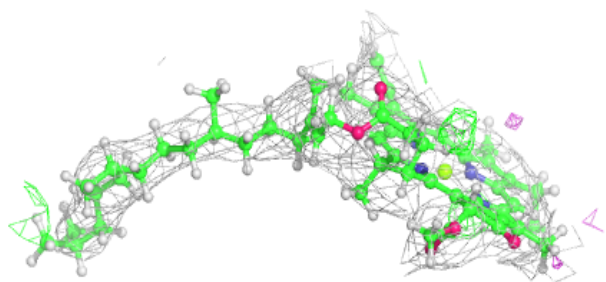
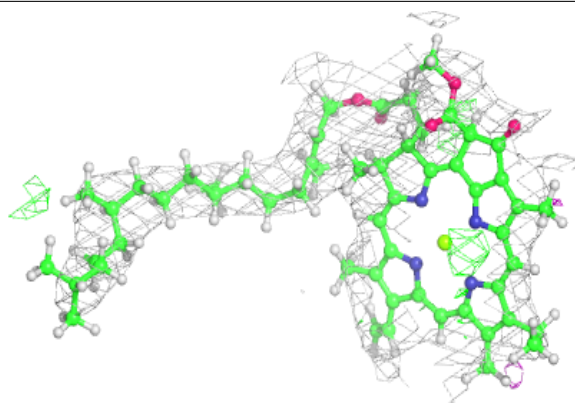
Electron density around CLA B 3016:

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

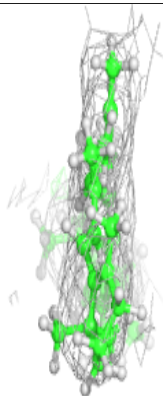
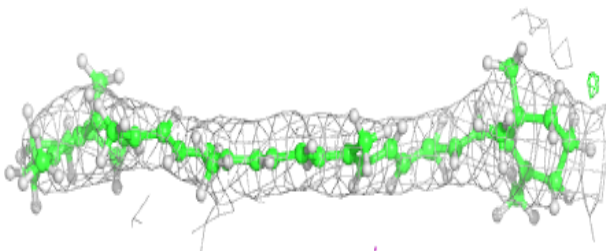
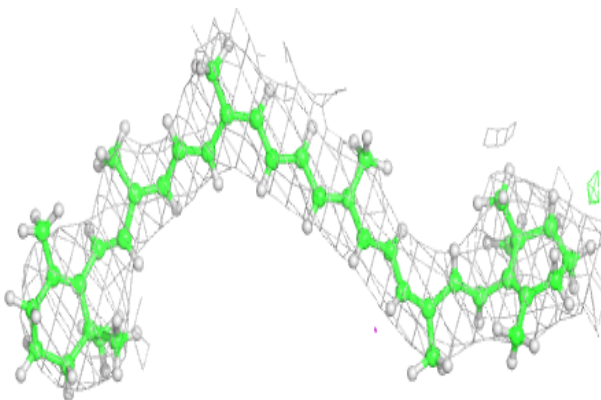


Electron density around CLA A 803:

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

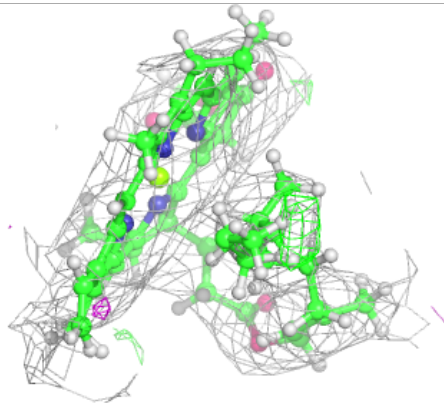
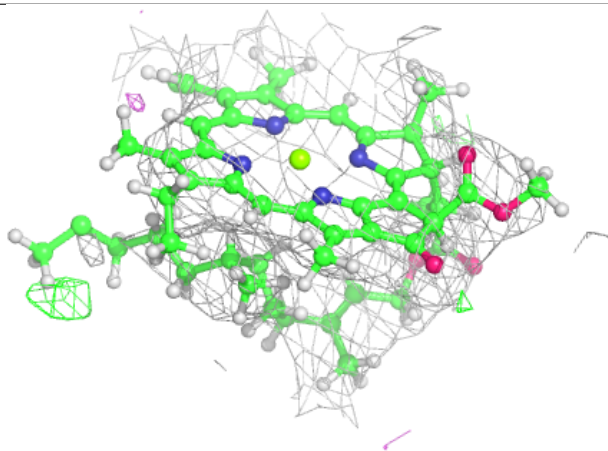
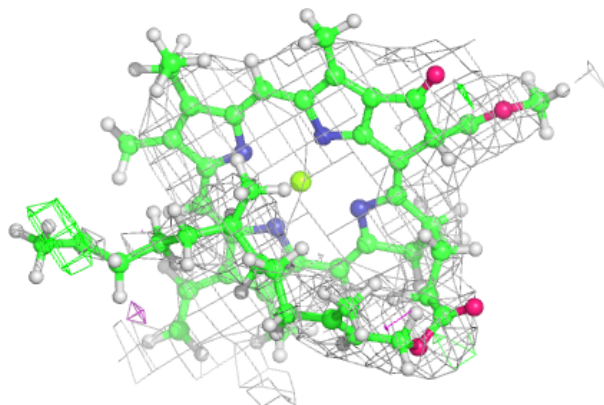
**Electron density around BCR A 851:**

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



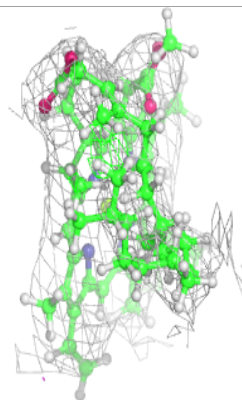
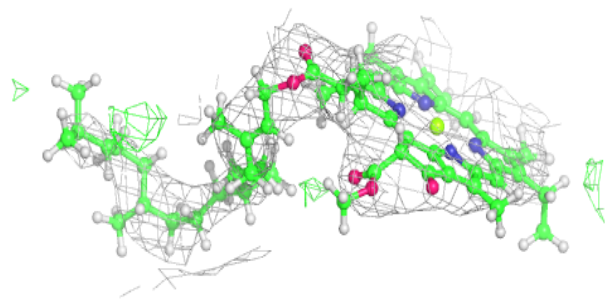
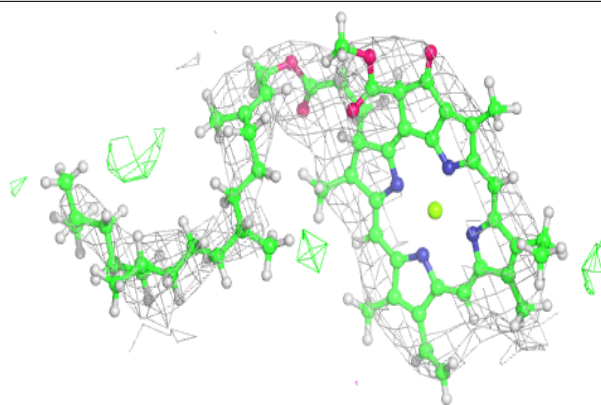
Electron density around CLA B 3018:

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



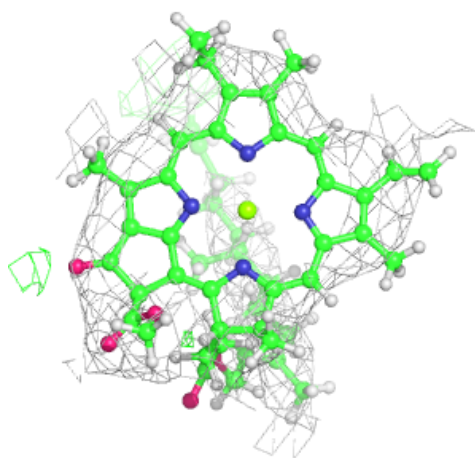
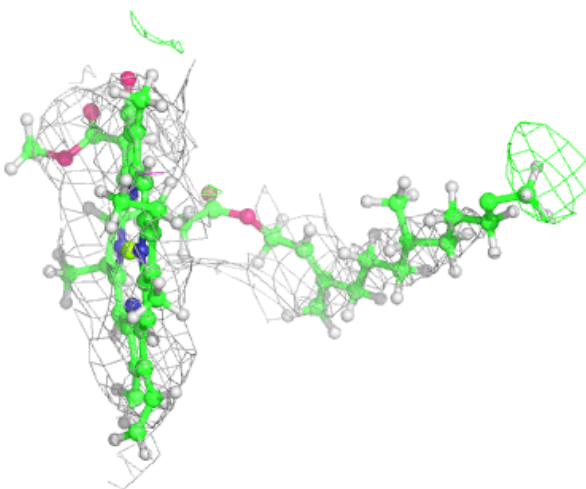
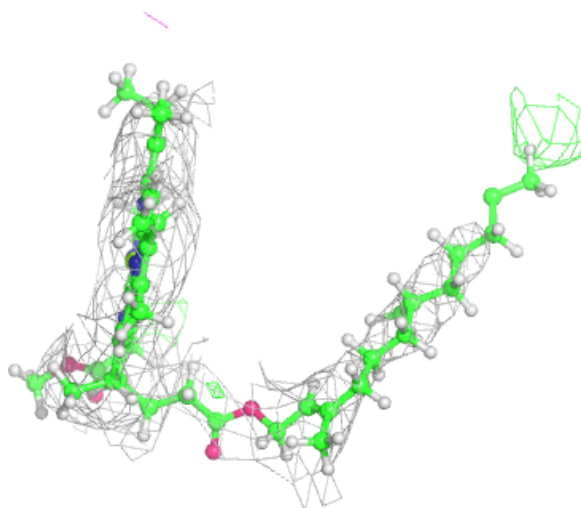
Electron density around CLA A 804:

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



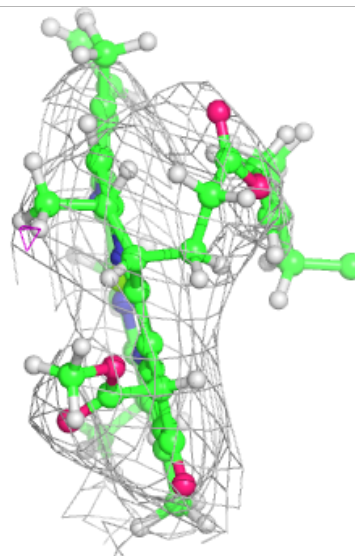
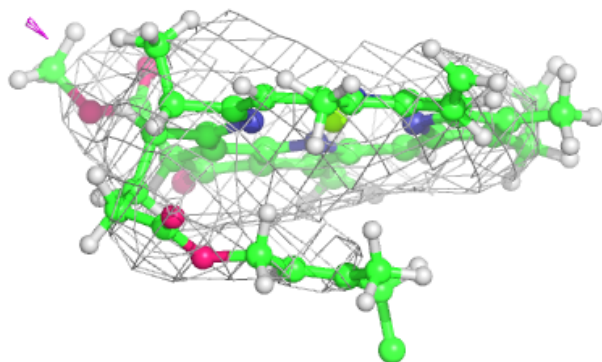
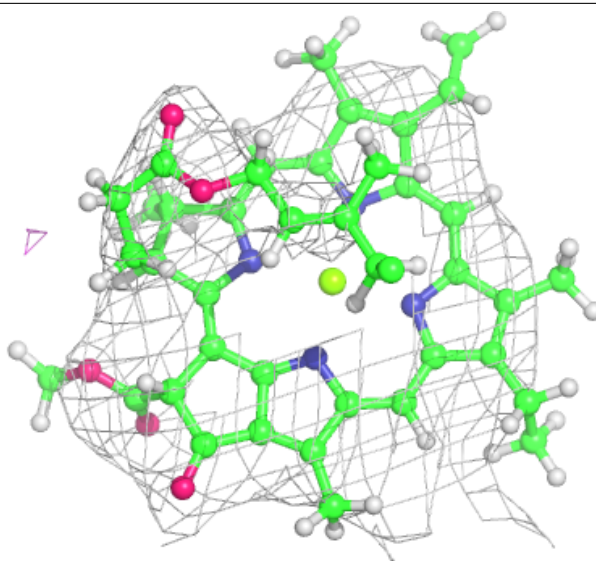
Electron density around CLA A 805:

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



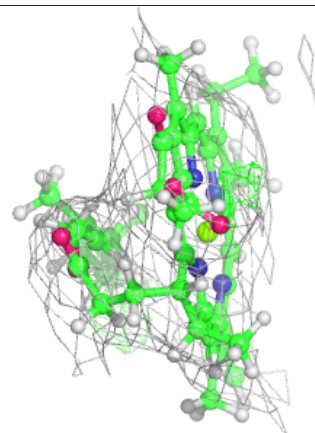
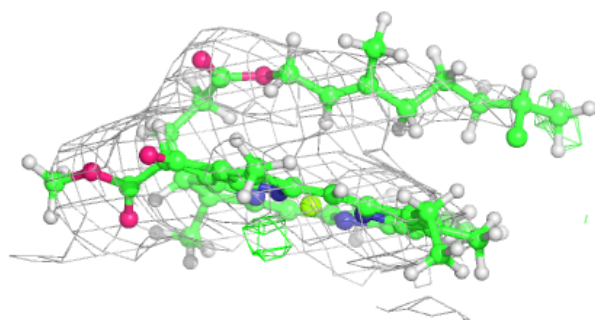
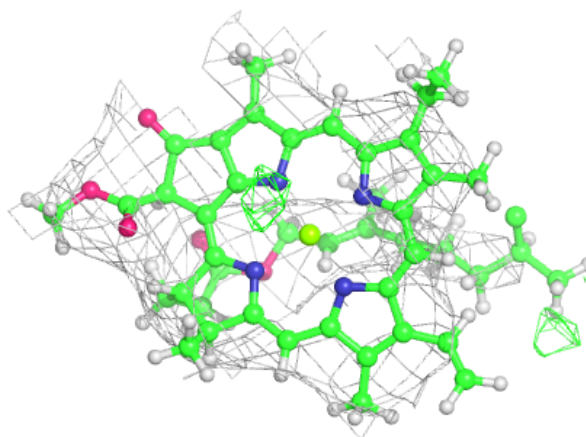
Electron density around CLA A 824:

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

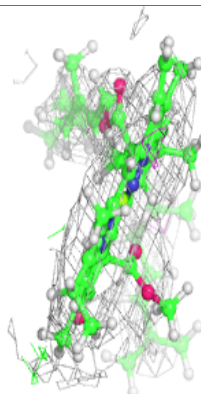
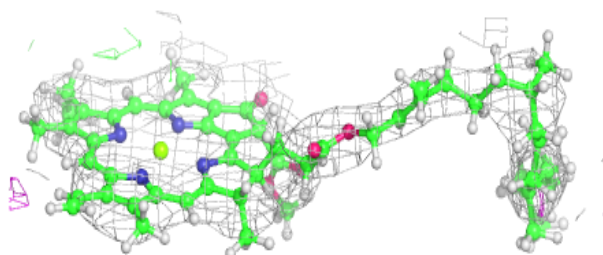
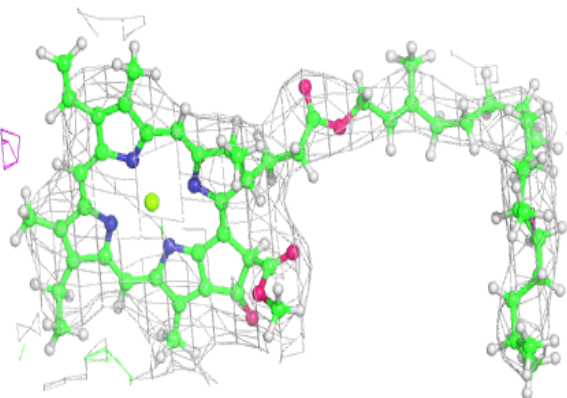


Electron density around CLA B 3023:

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

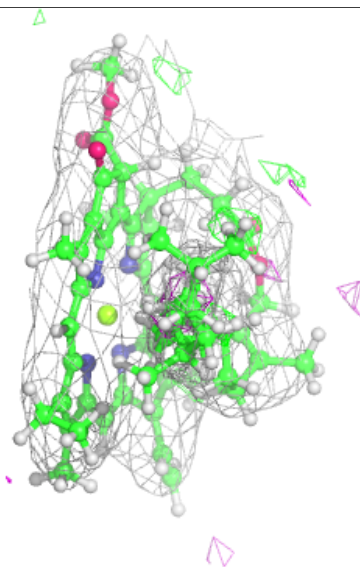
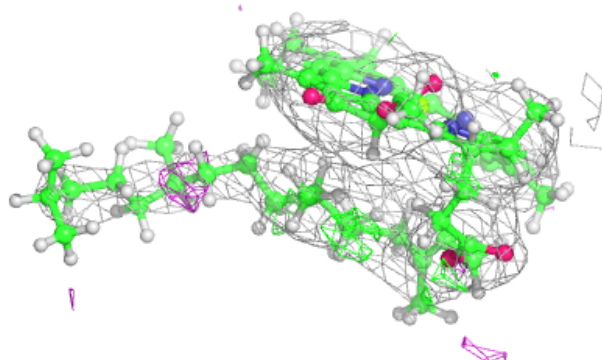
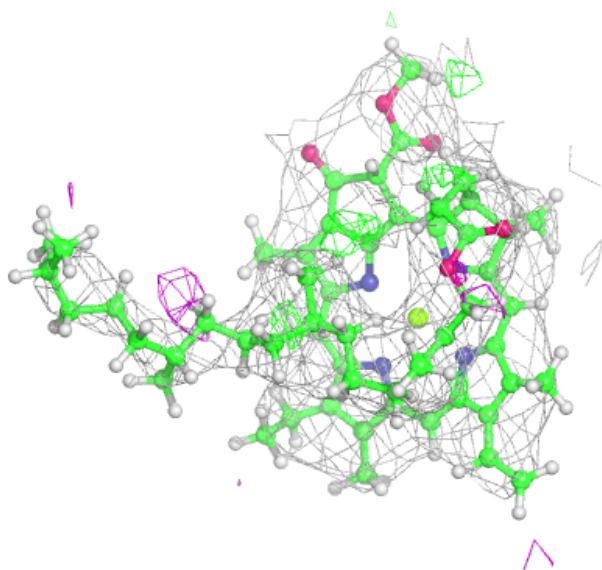
**Electron density around CLA B 3027:**

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



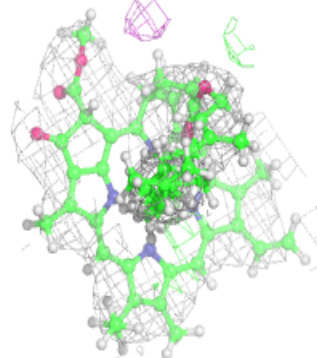
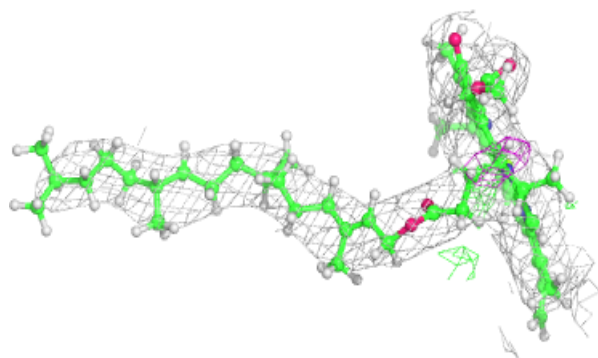
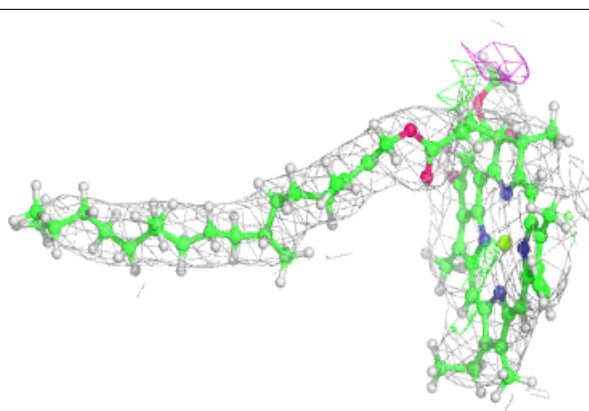
Electron density around CLA B 3028:

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



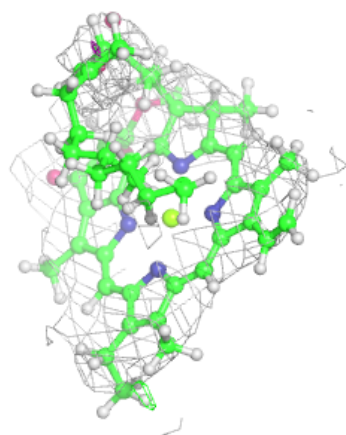
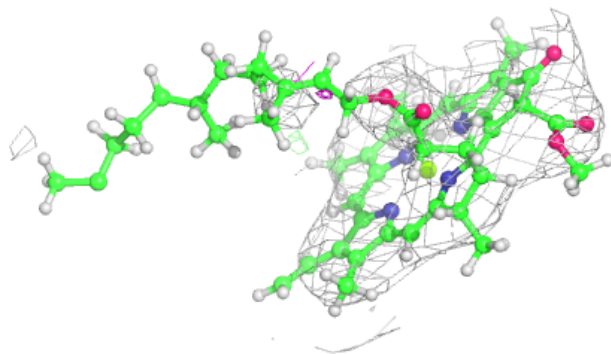
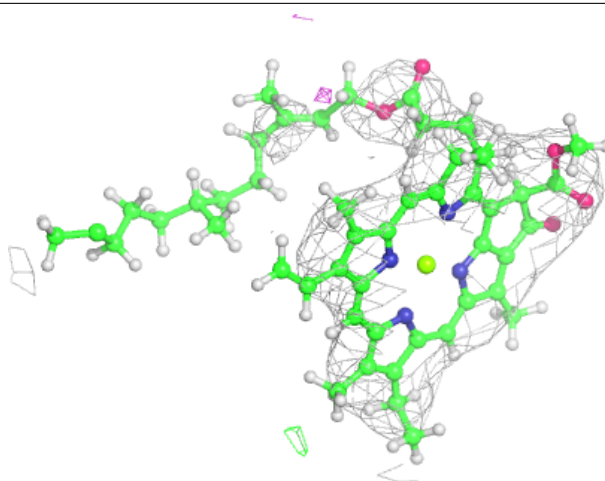
Electron density around CLA B 3029:

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



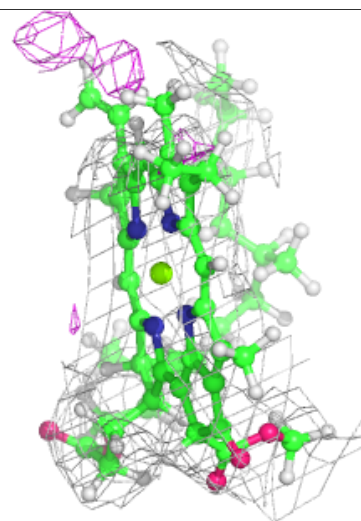
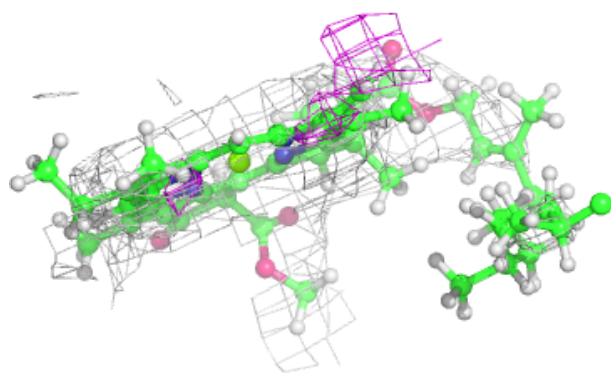
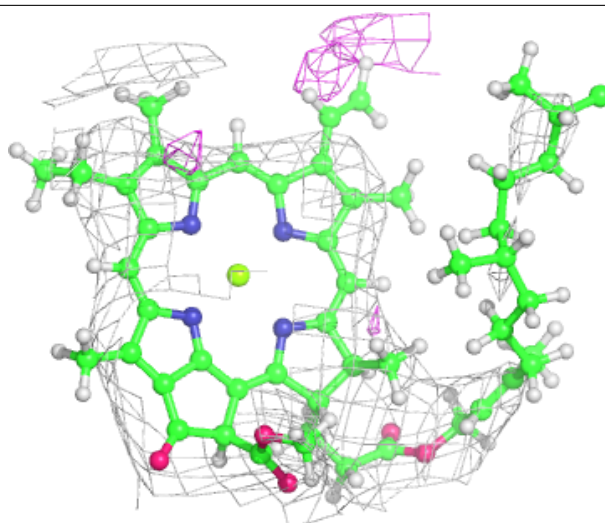
Electron density around CLA A 825:

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



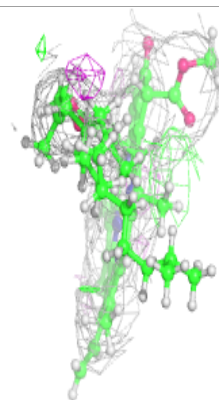
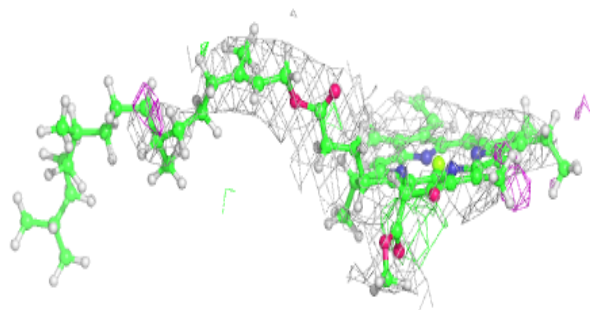
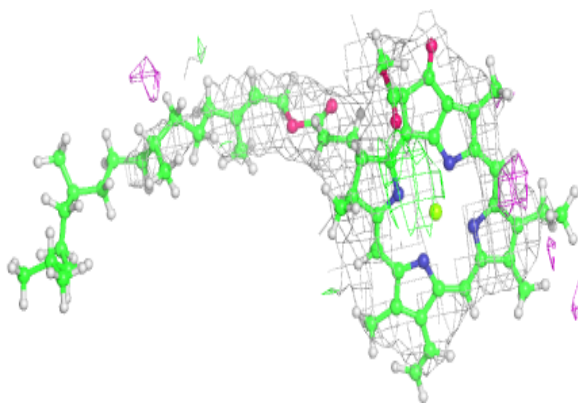
Electron density around CLA A 814:

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



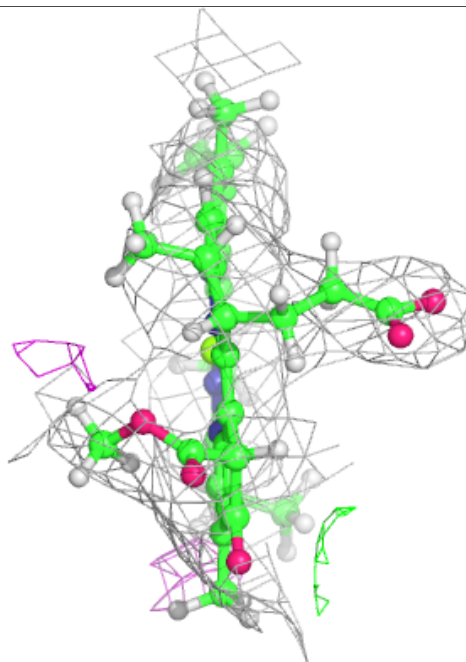
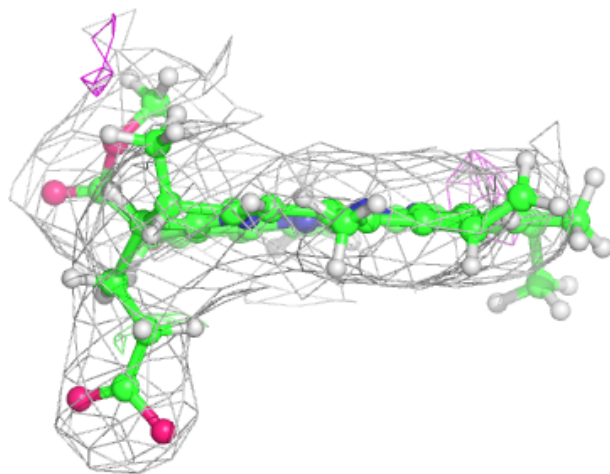
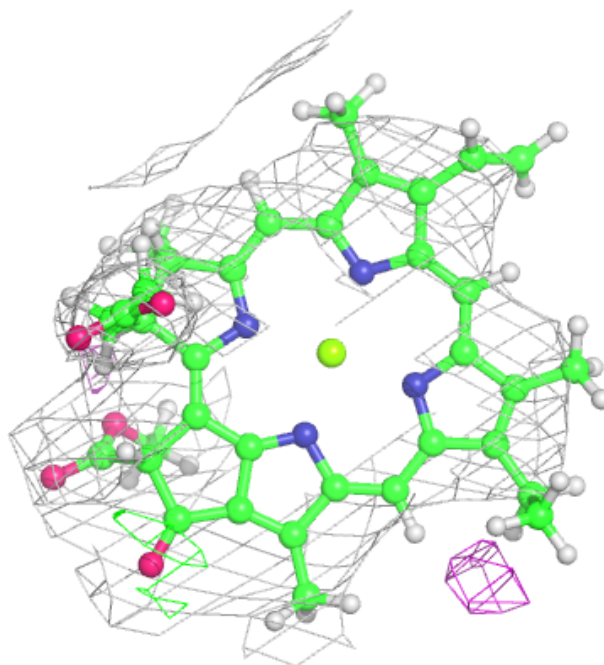
Electron density around CLA A 827:

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



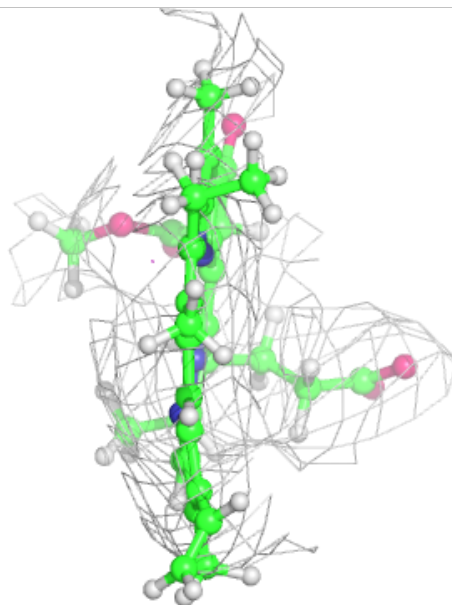
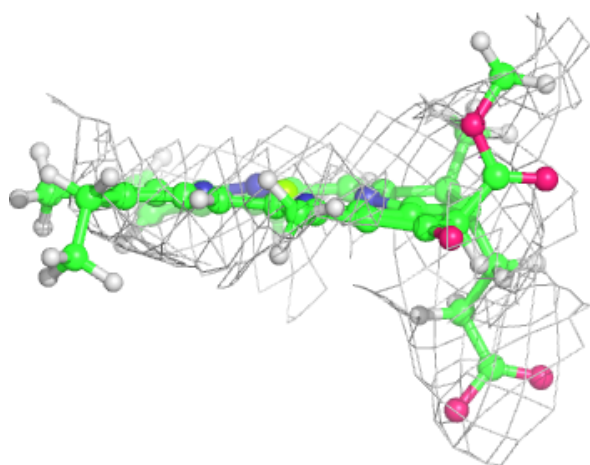
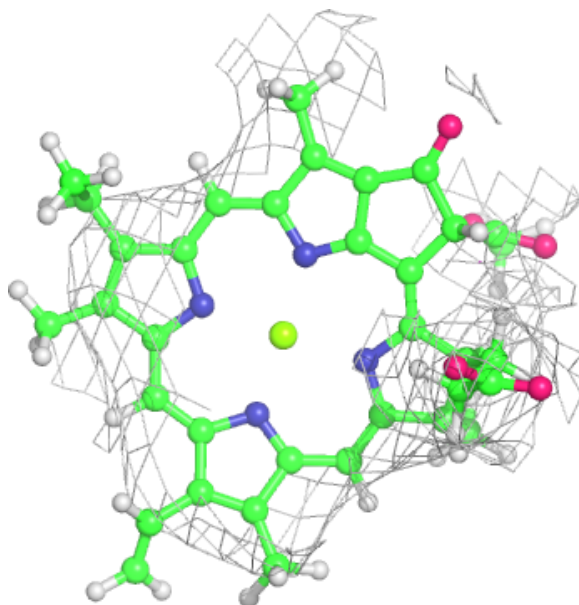
Electron density around CLA B 3035:

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



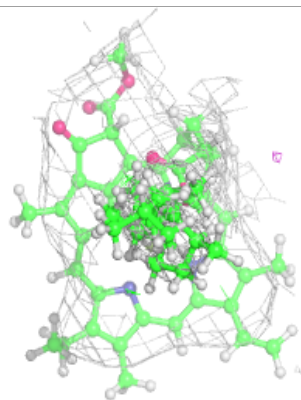
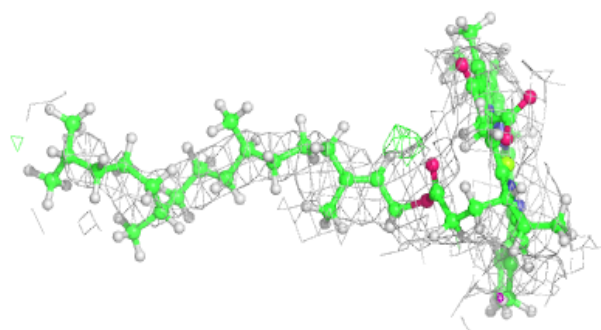
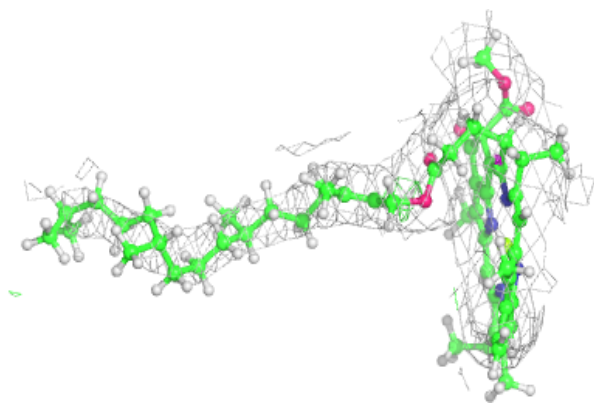
Electron density around CLA A 815:

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



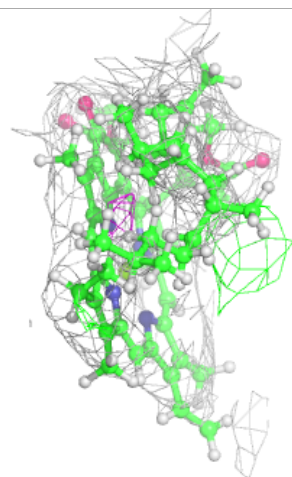
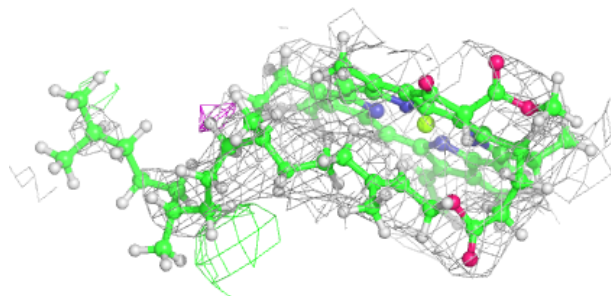
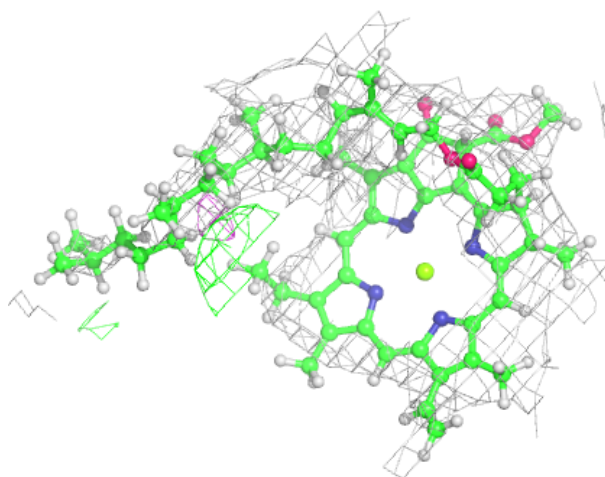
Electron density around CLA A 829:

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



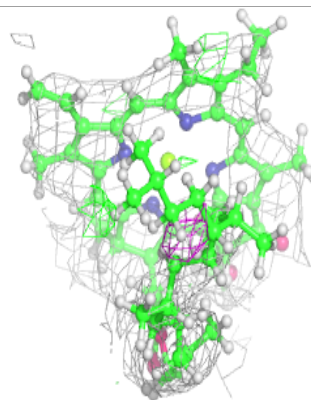
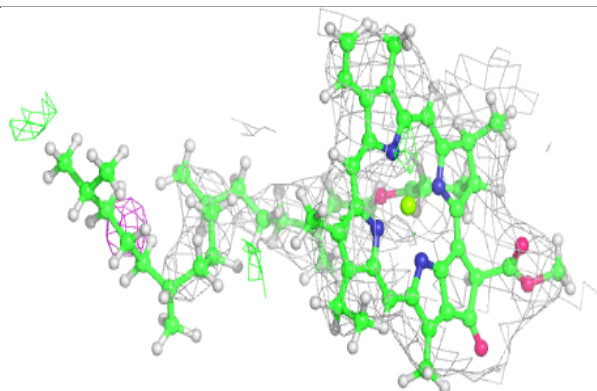
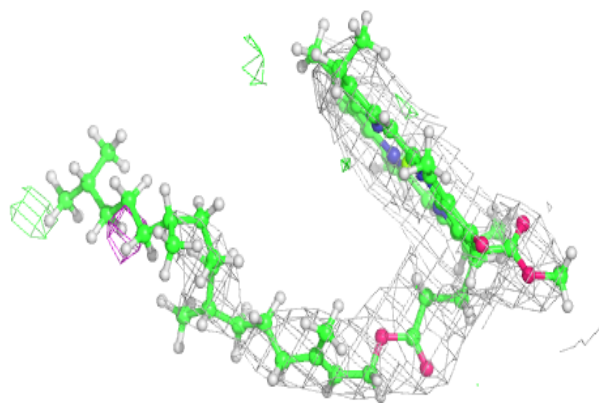
Electron density around CLA A 830:

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



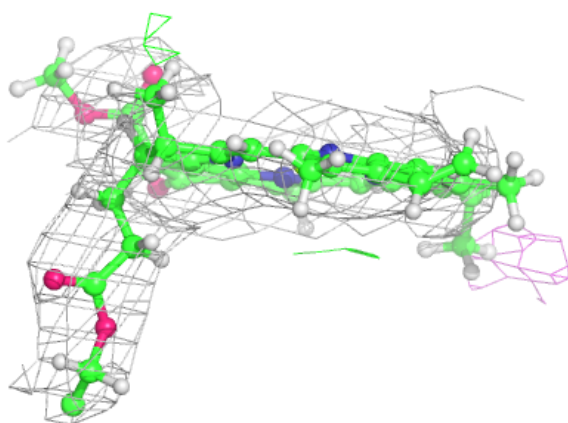
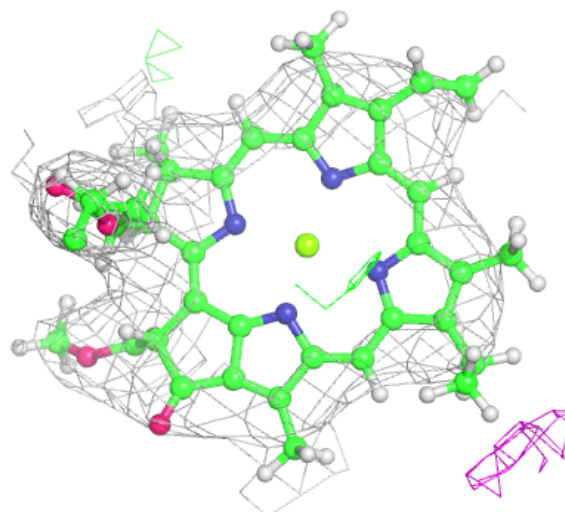
Electron density around CLA A 833:

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



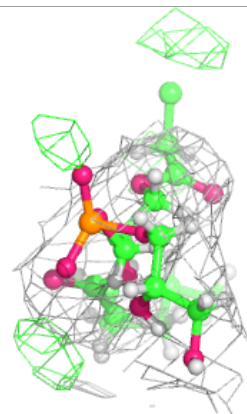
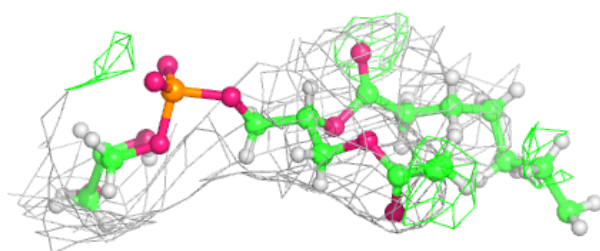
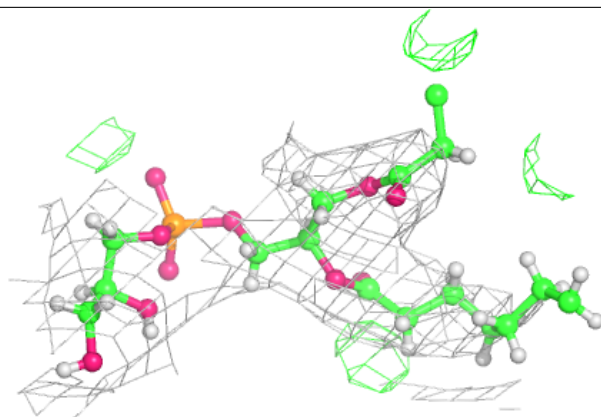
Electron density around CLA B 3040:

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



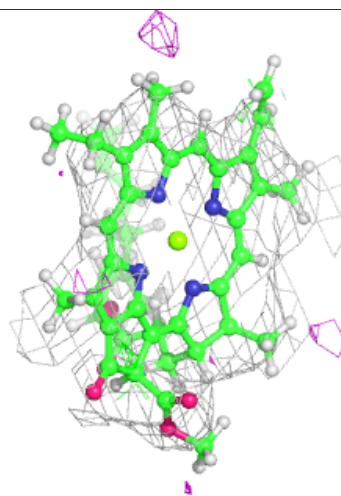
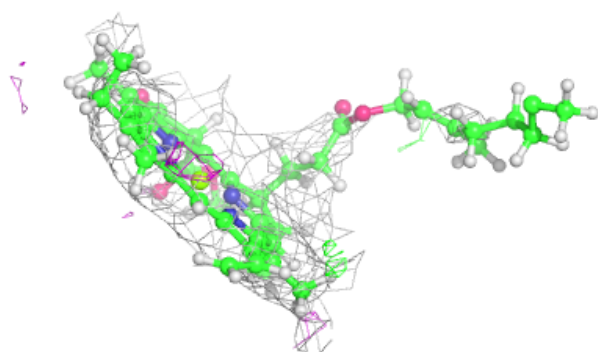
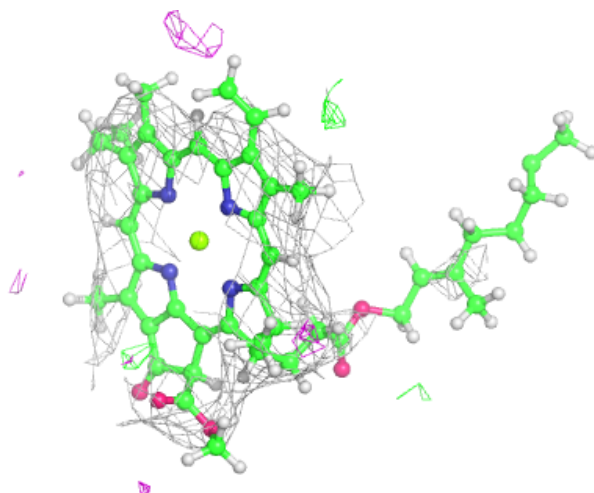
Electron density around LHG A 854:

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



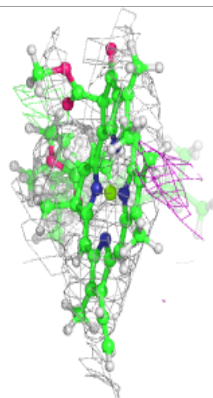
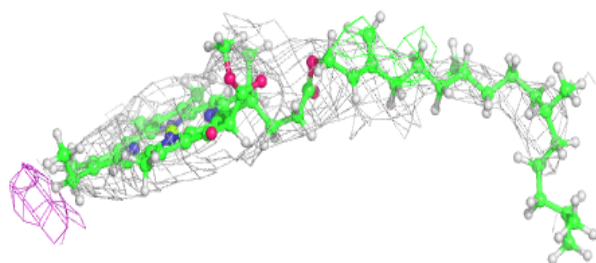
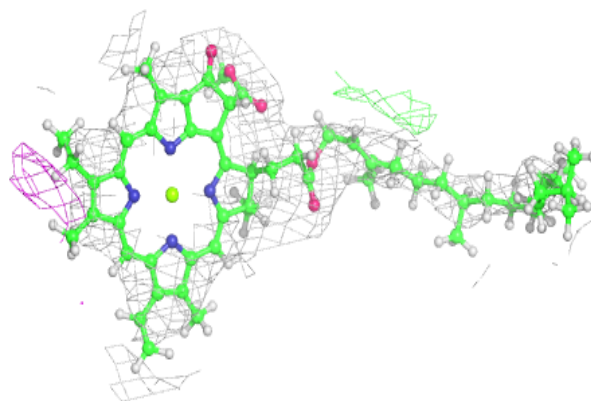
Electron density around CLA A 836:

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

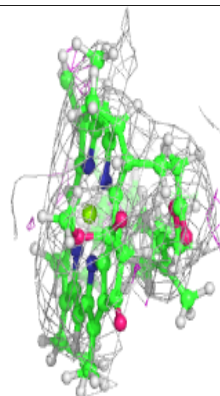
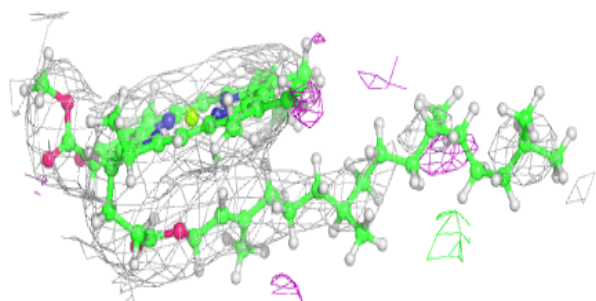
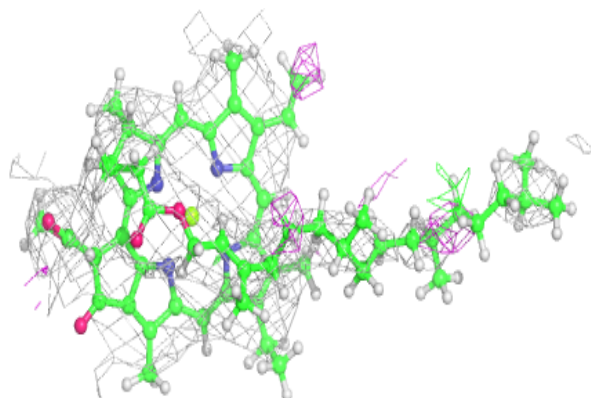


Electron density around CLA A 806:

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

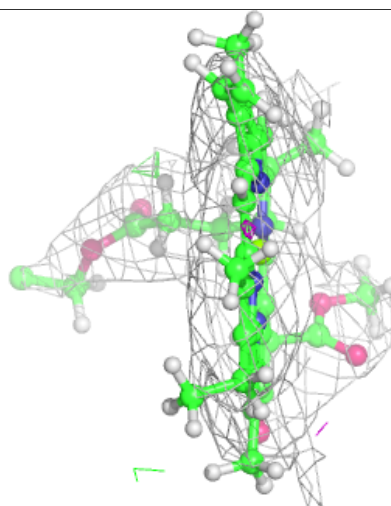
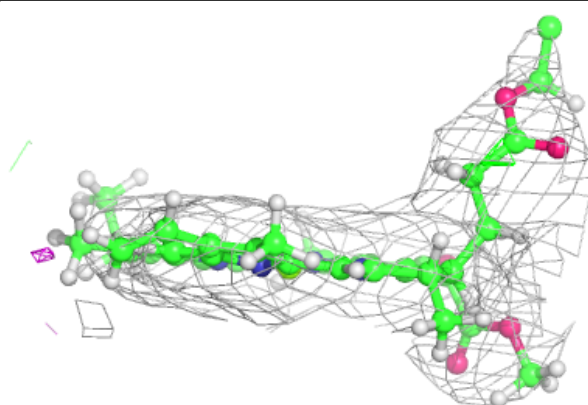
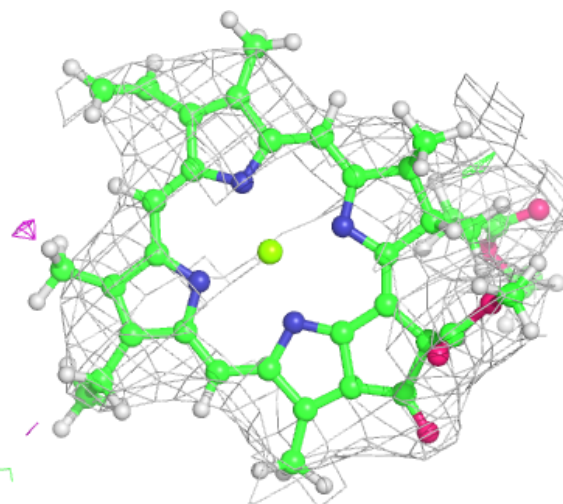
**Electron density around CLA A 839:**

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



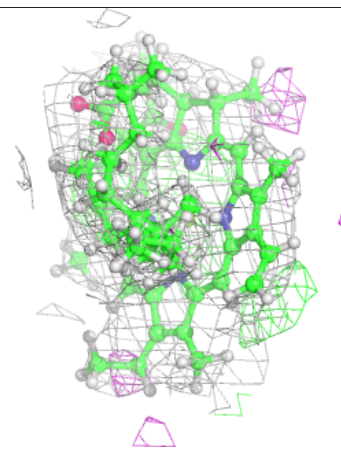
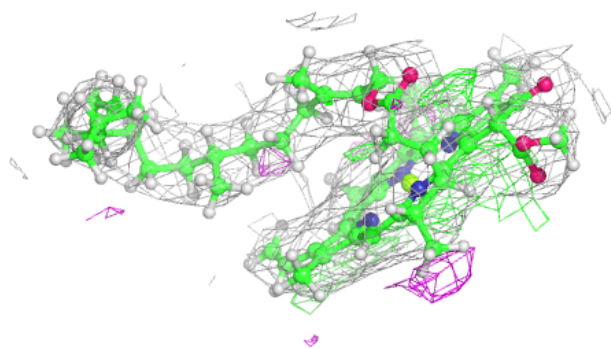
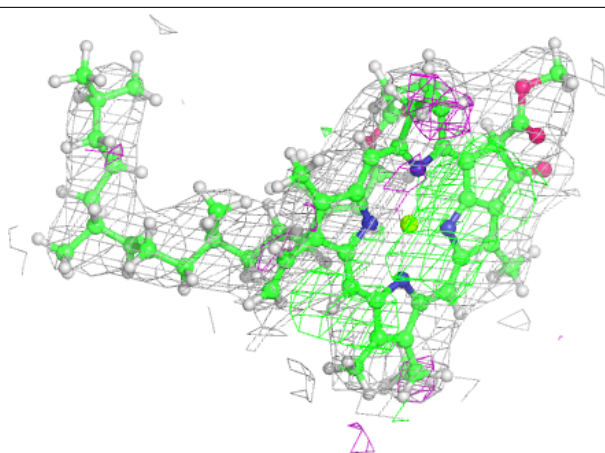
Electron density around CLA A 840:

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



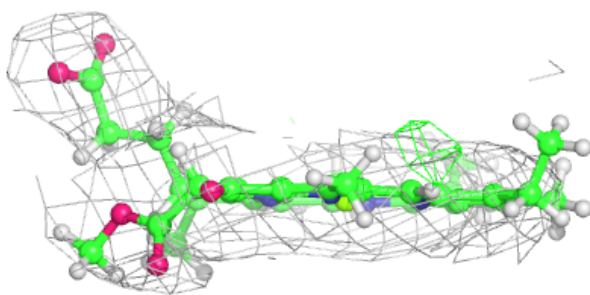
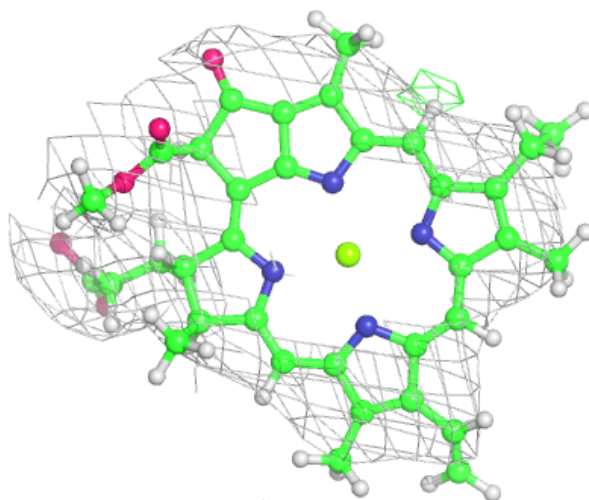
Electron density around CLA A 844:

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



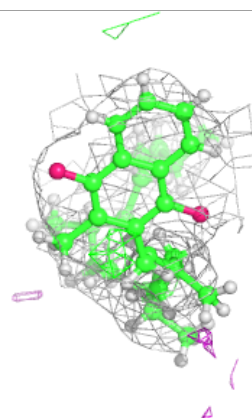
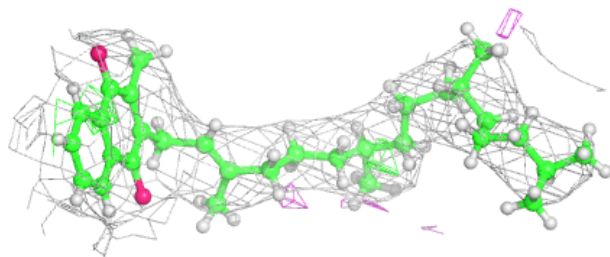
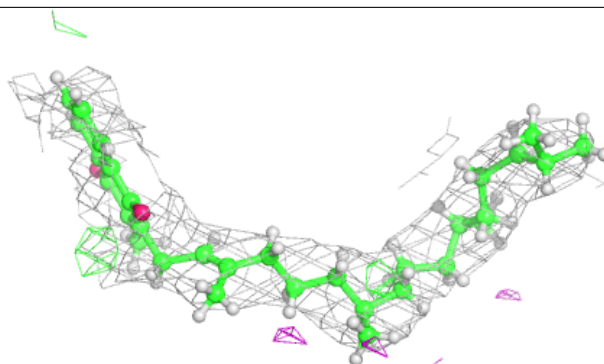
Electron density around CLA B 3024:

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



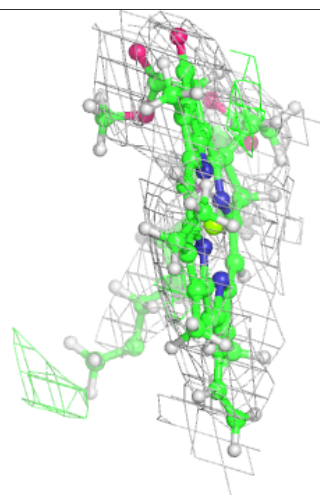
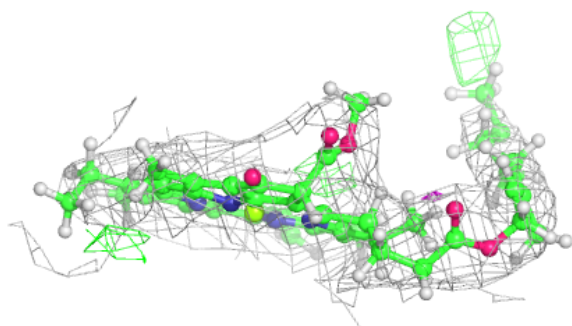
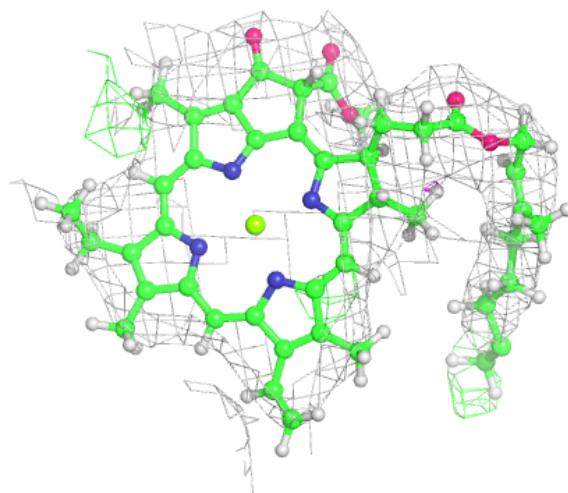
Electron density around PQN B 3043:

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



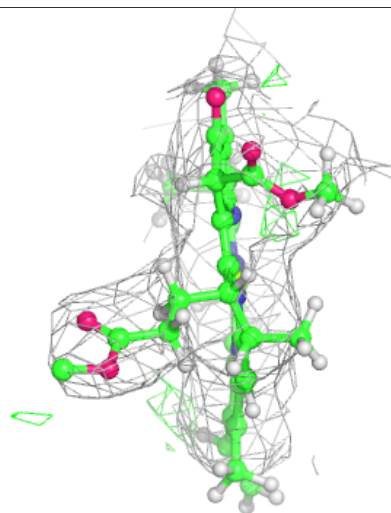
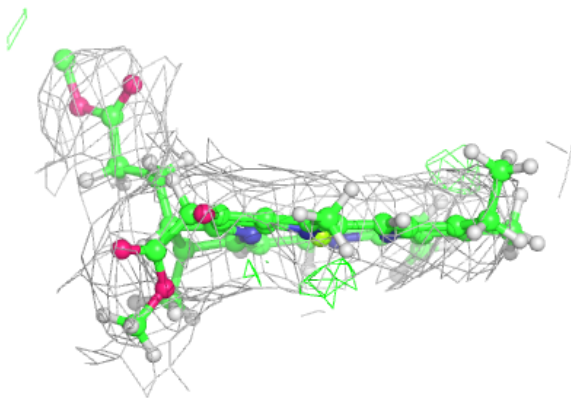
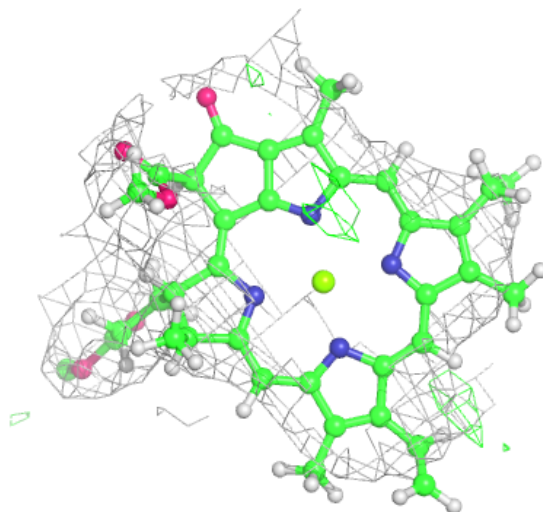
Electron density around CLA B 3025:

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



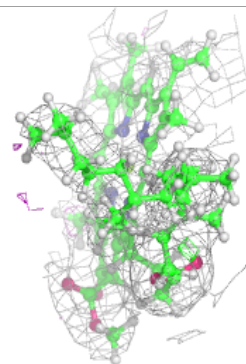
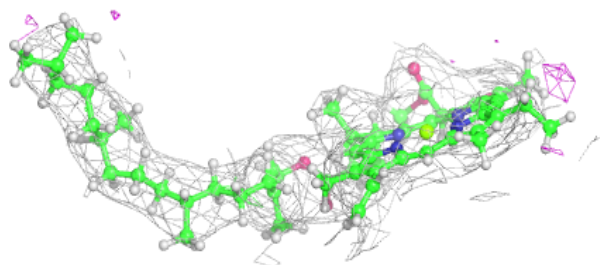
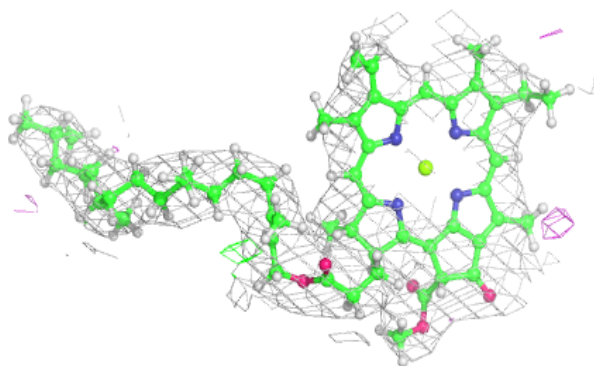
Electron density around CLA B 3026:

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



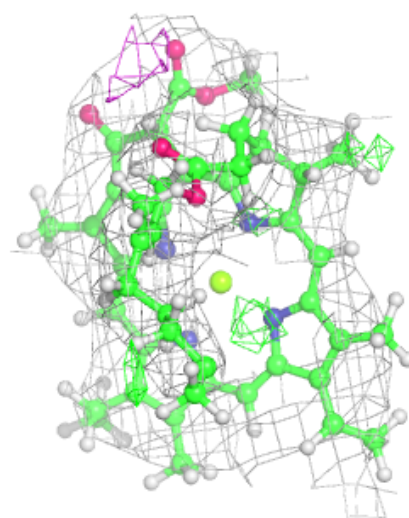
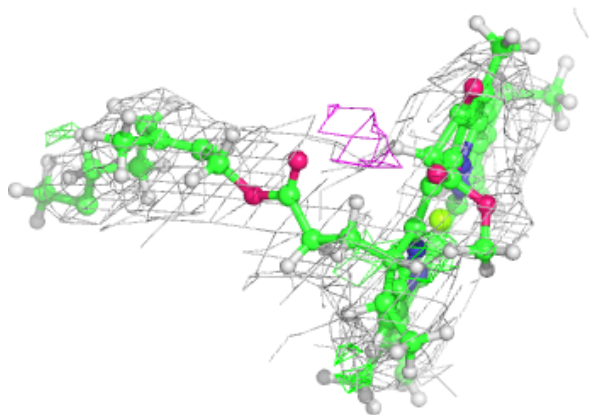
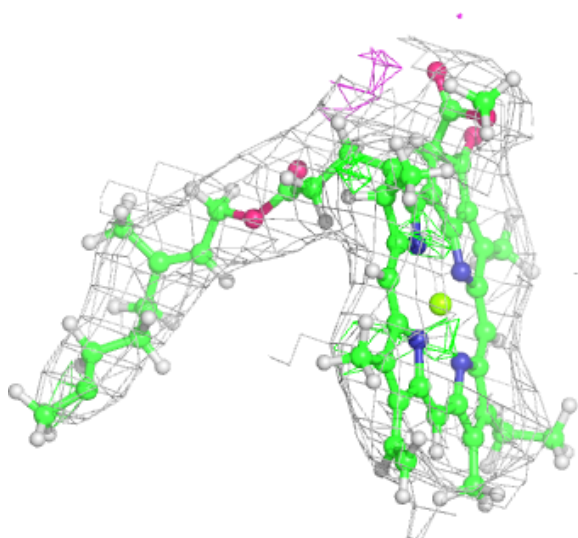
Electron density around CLA B 3004:

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



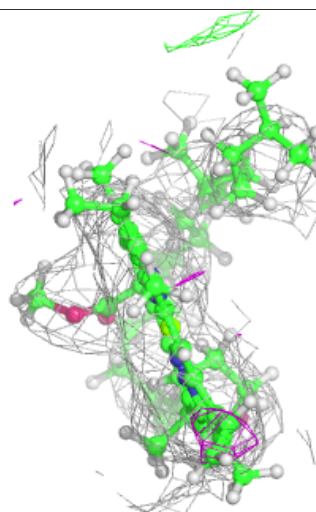
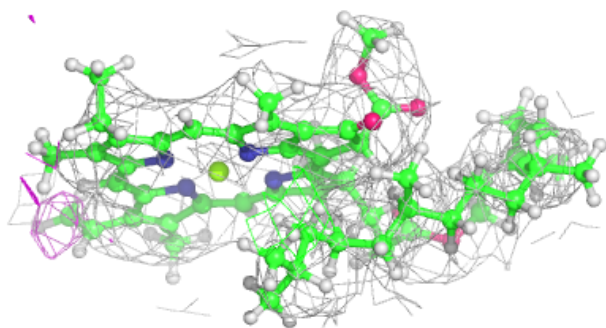
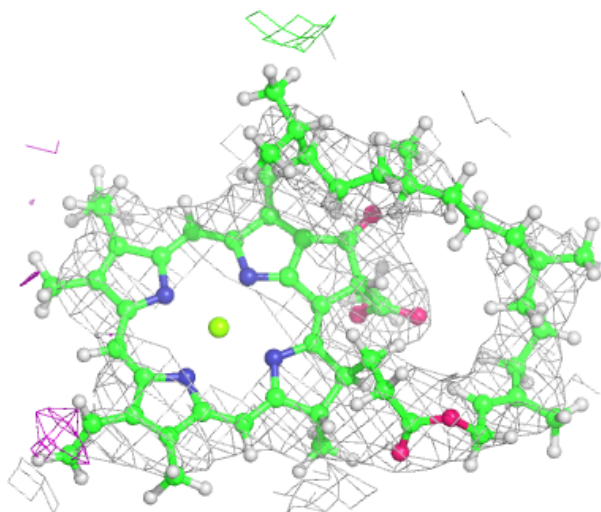
Electron density around CLA B 3005:

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



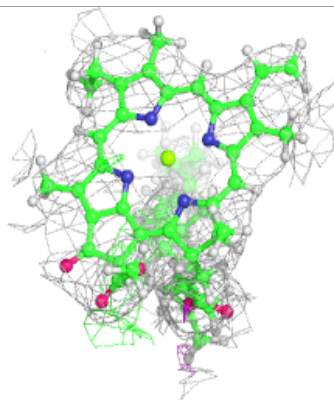
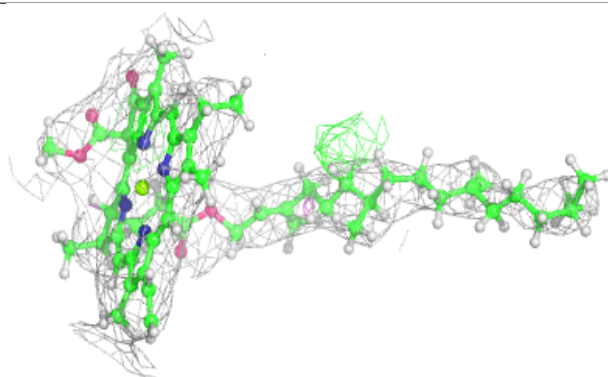
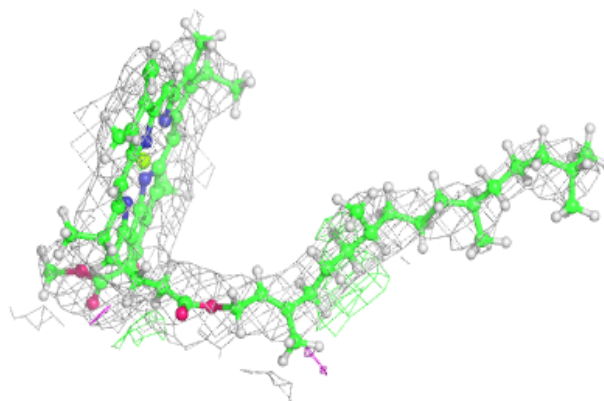
Electron density around CLA B 3006:

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



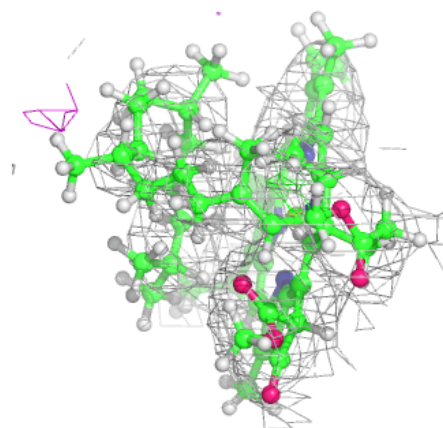
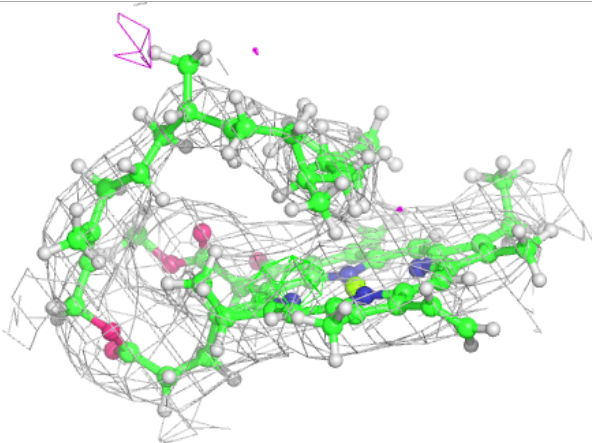
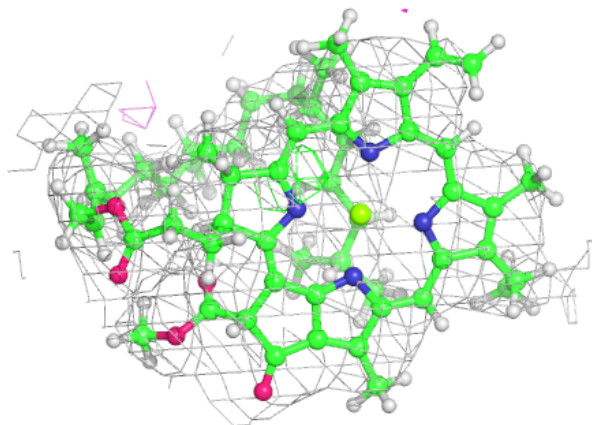
Electron density around CLA B 3030:

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



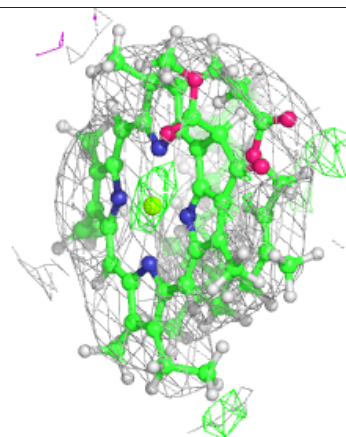
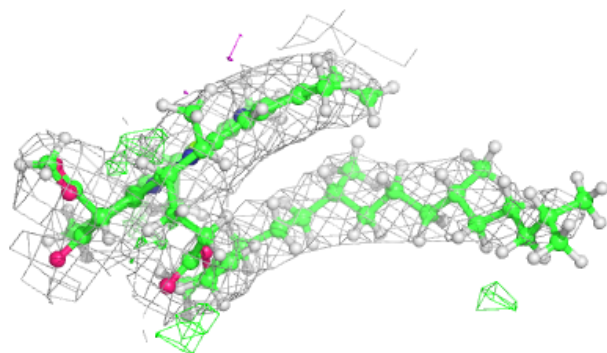
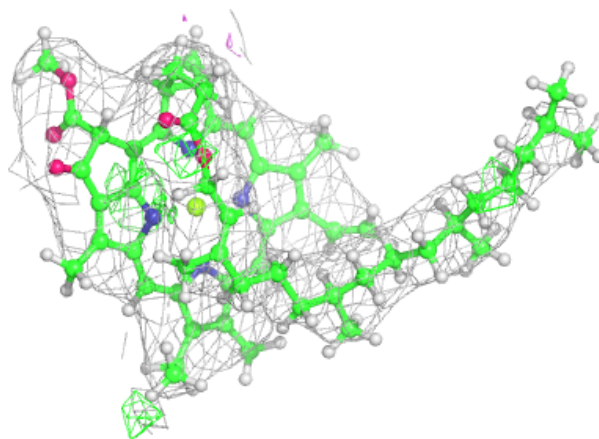
Electron density around CLA B 3007:

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



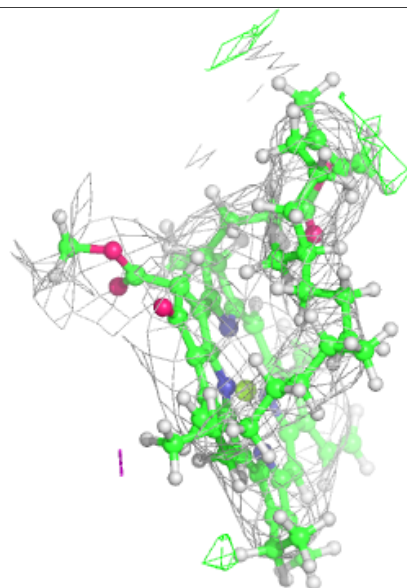
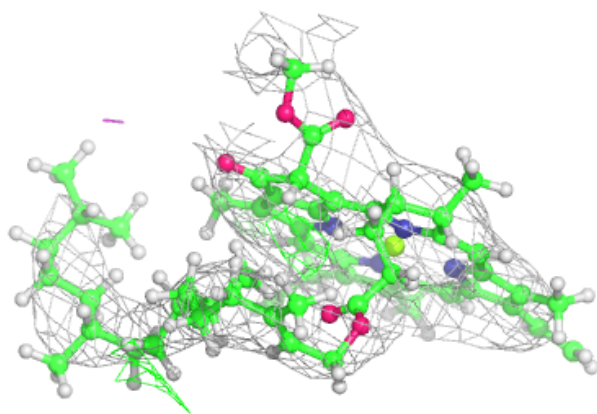
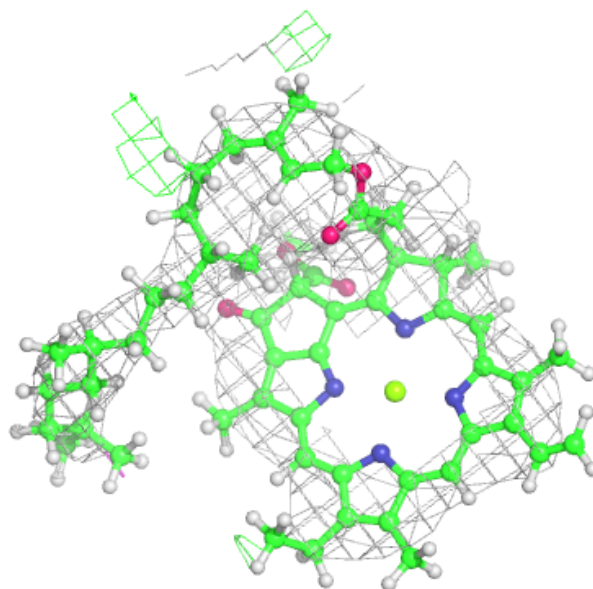
Electron density around CLA B 3008:

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



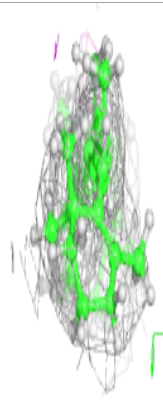
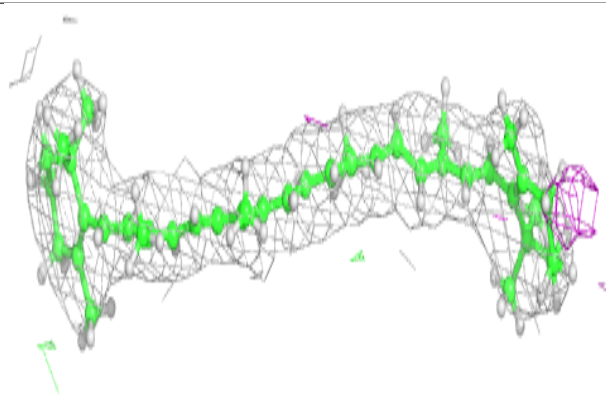
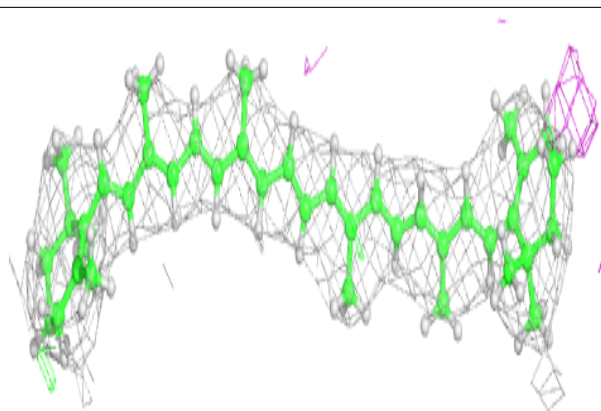
Electron density around CLA B 3033:

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



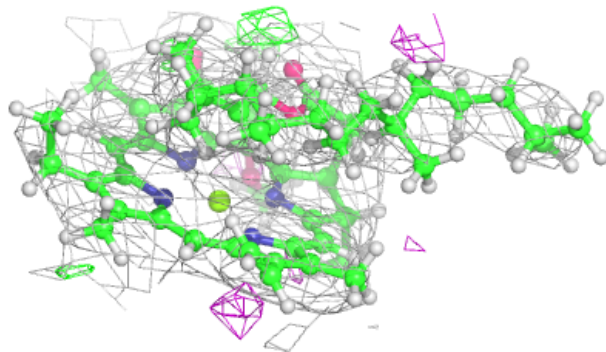
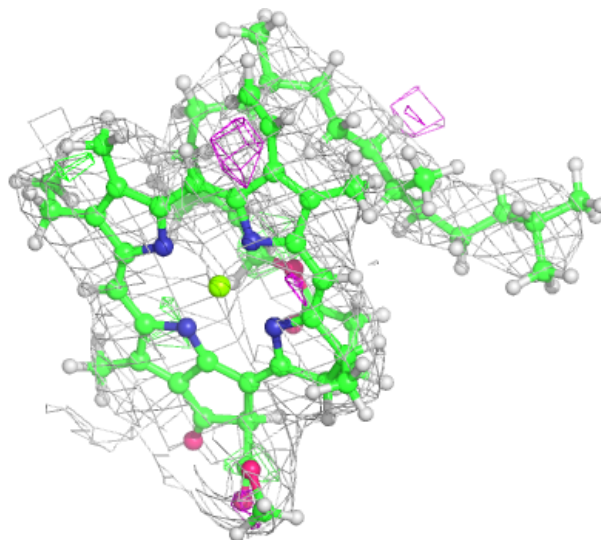
Electron density around BCR B 3048:

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



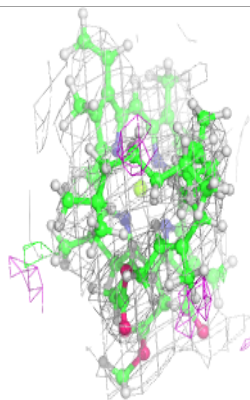
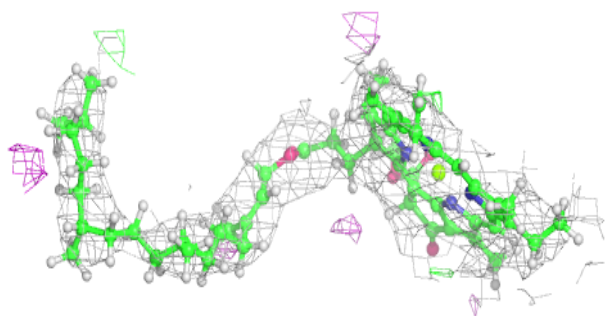
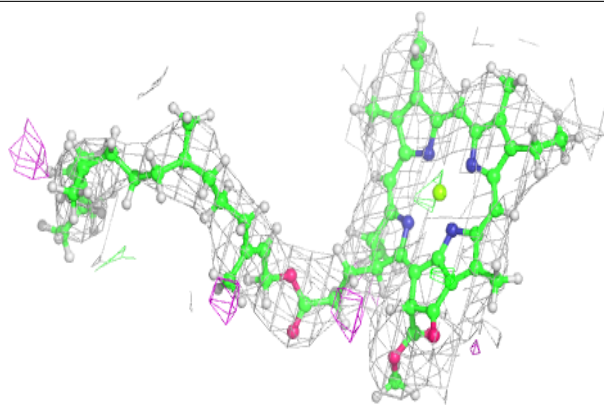
Electron density around CLA B 3009:

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

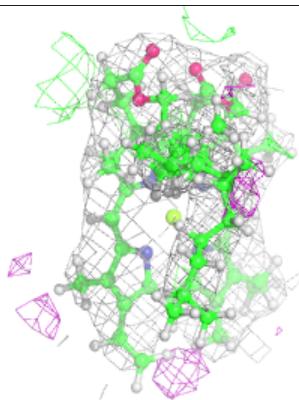
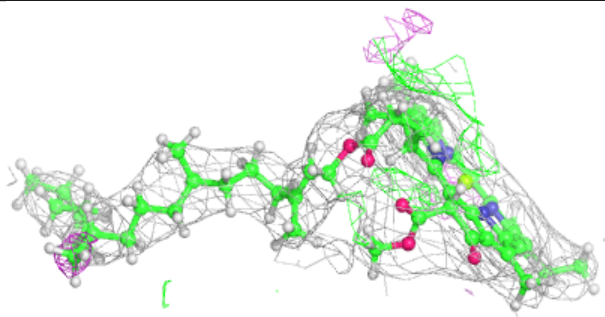
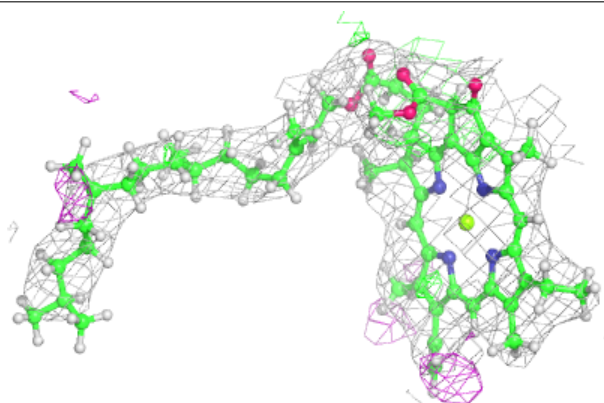


Electron density around CLA B 3010:

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

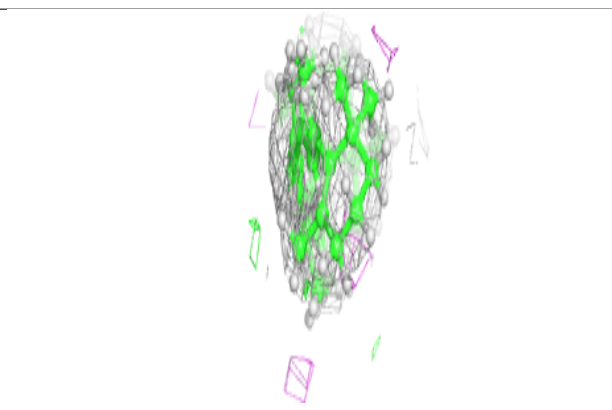
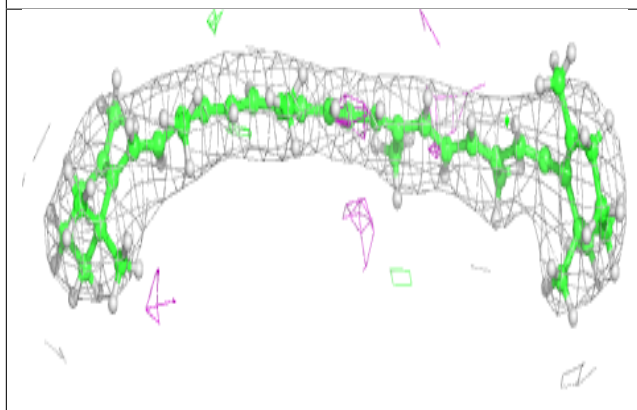
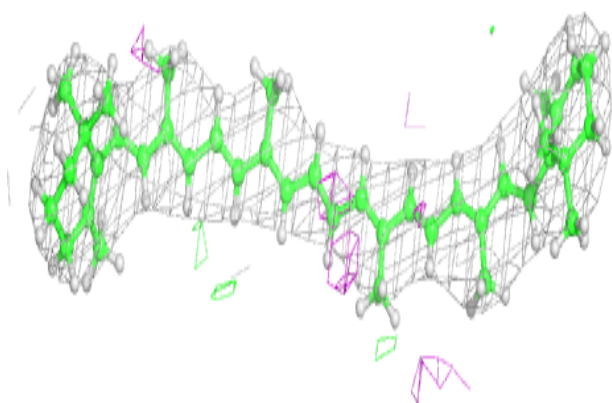
**Electron density around CLA B 3011:**

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

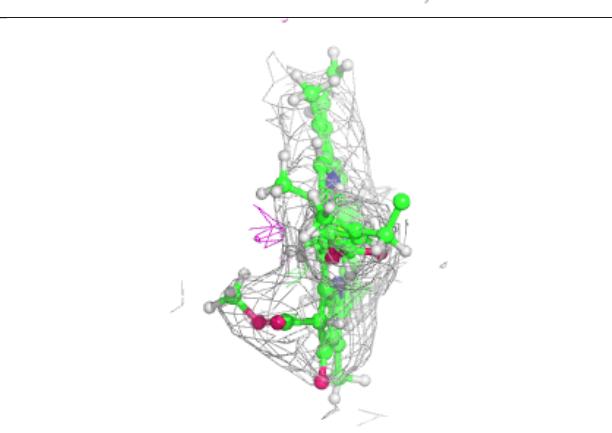
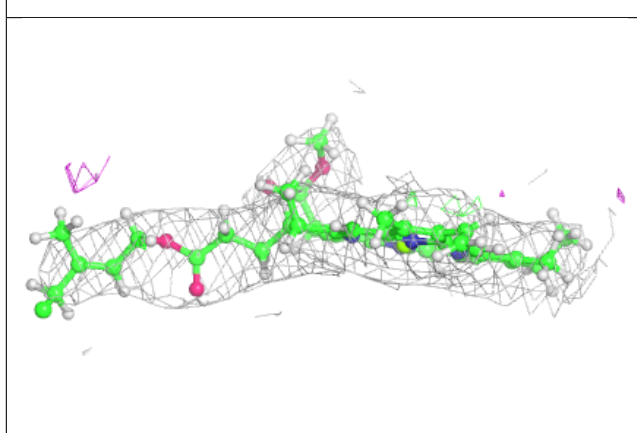
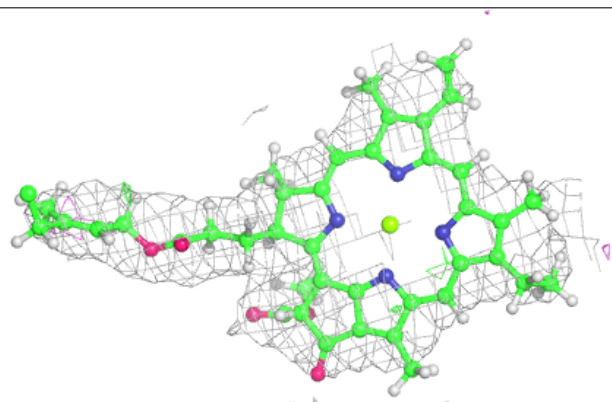


Electron density around BCR I 101:

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

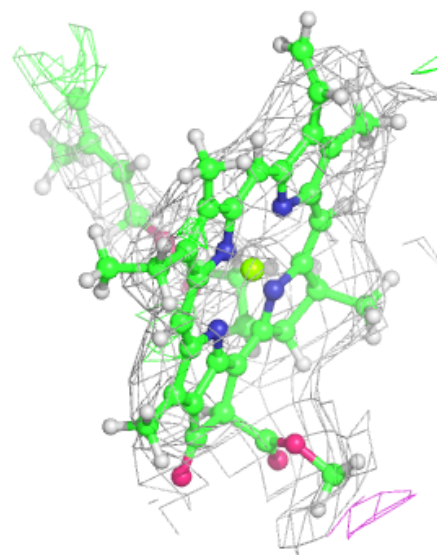
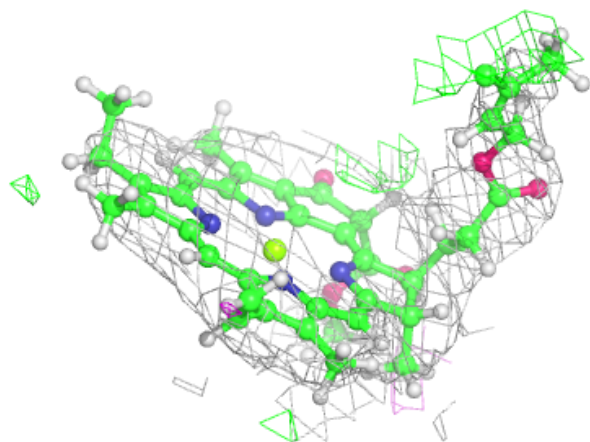
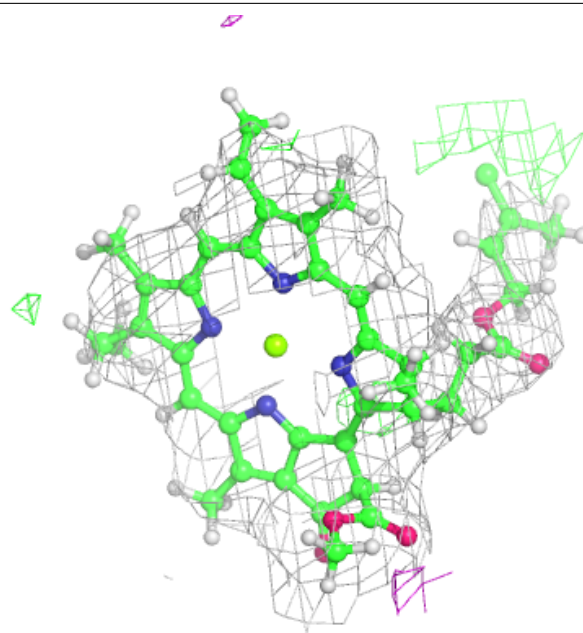
**Electron density around CLA A 838:**

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



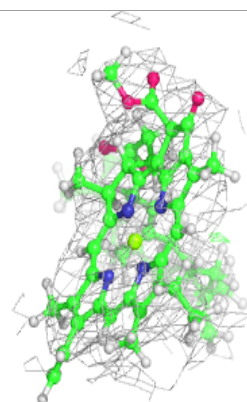
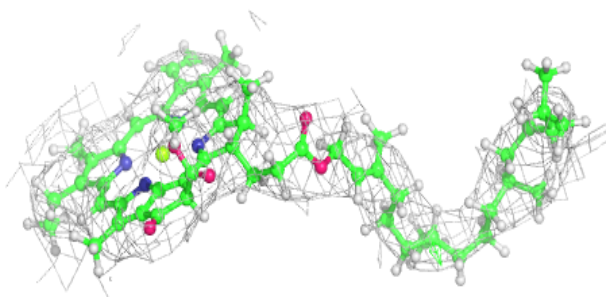
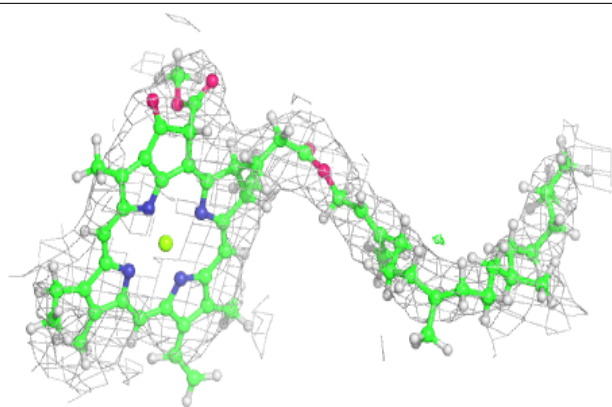
Electron density around CLA A 832:

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

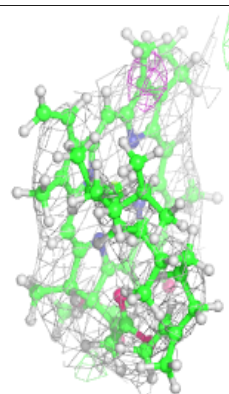
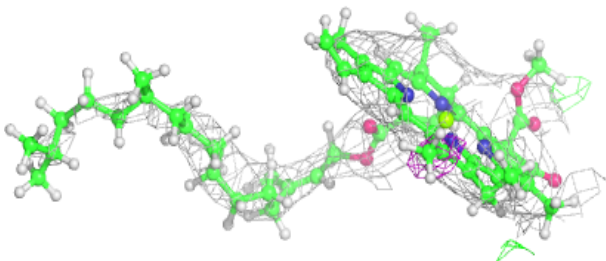
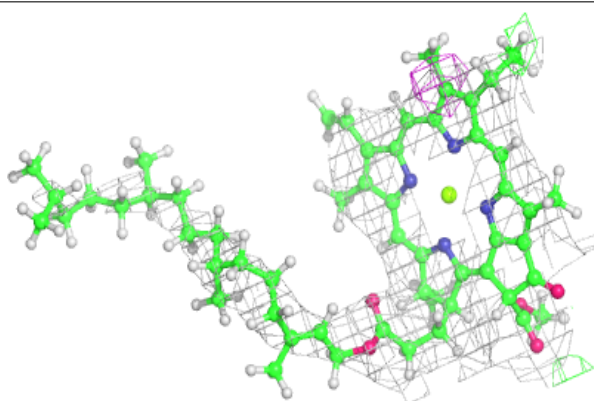


Electron density around CLA B 3014:

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

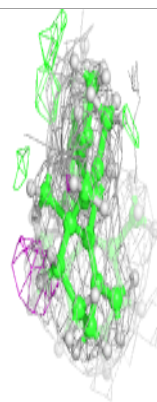
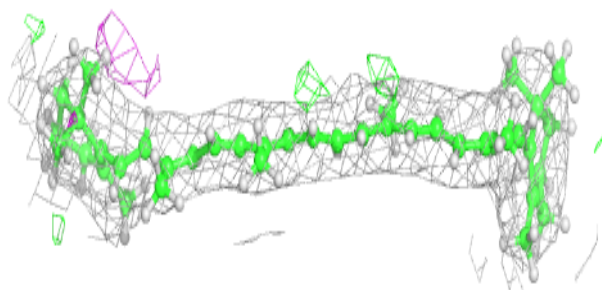
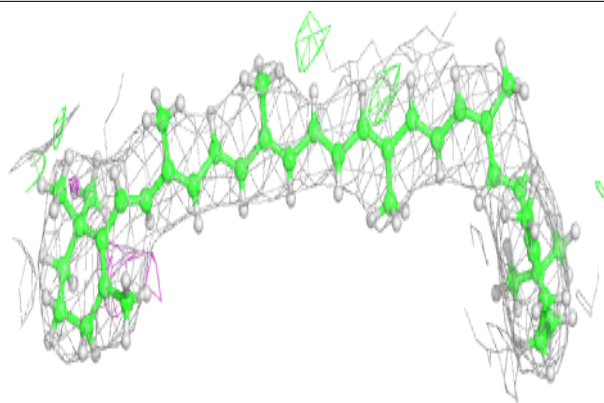
**Electron density around CLA A 809:**

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

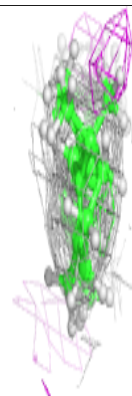
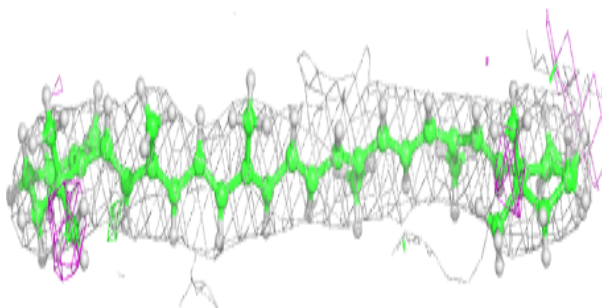
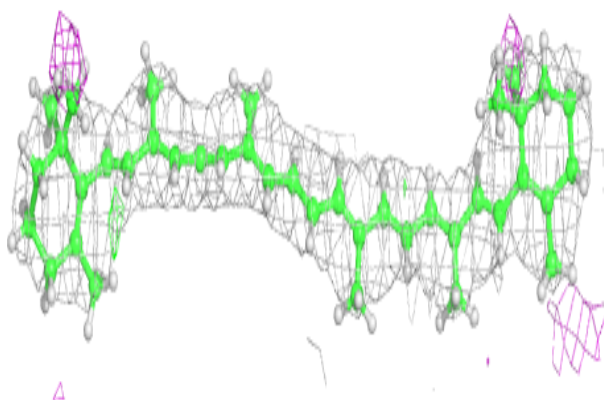


Electron density around BCR L 201:

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

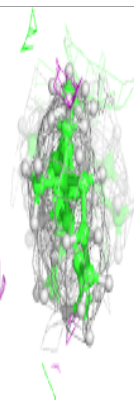
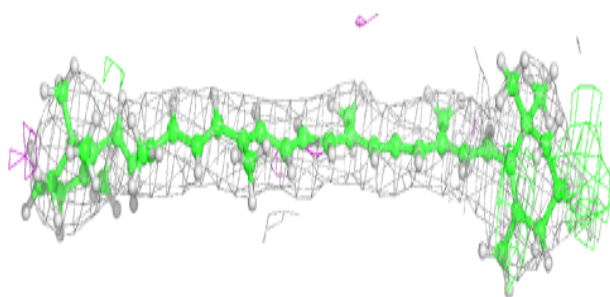
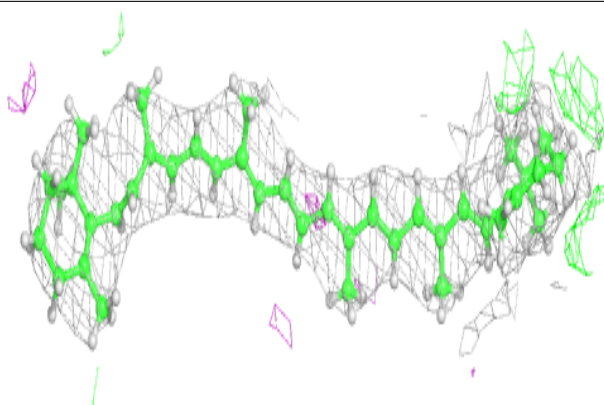
**Electron density around BCR L 208:**

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

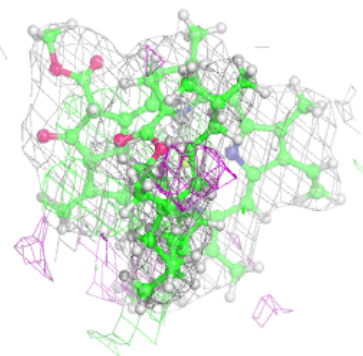
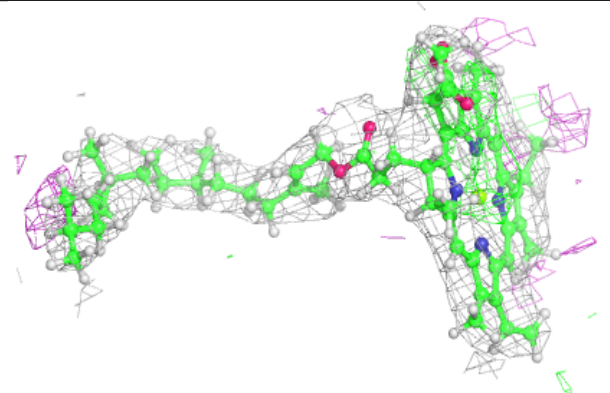
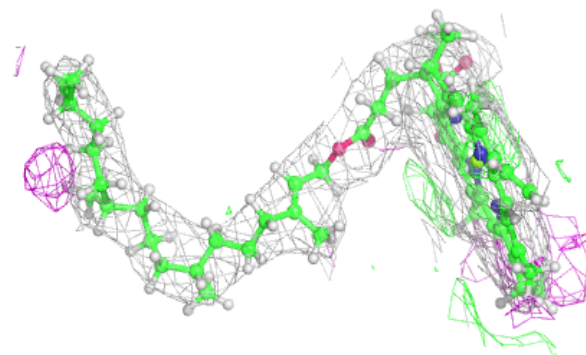


Electron density around BCR L 209:

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

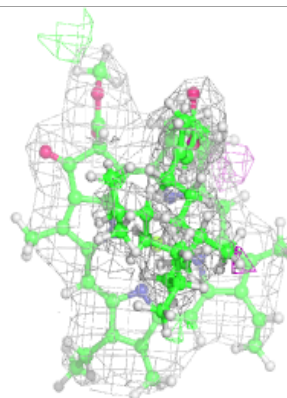
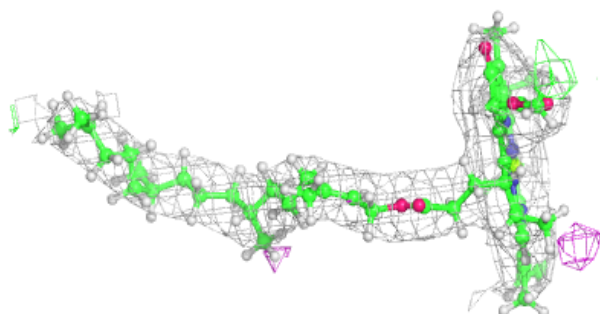
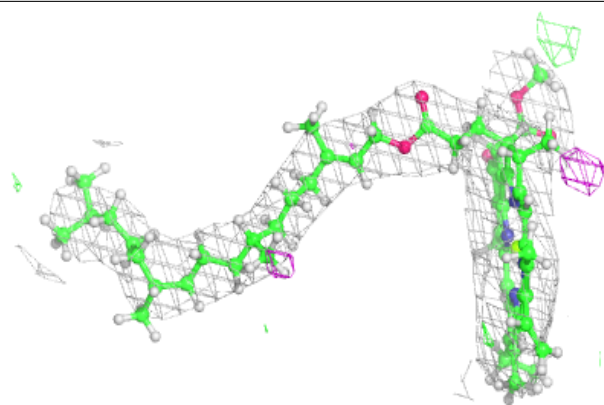
**Electron density around CLA B 3041:**

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

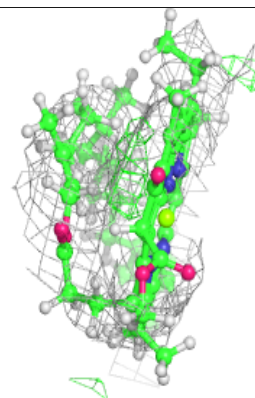
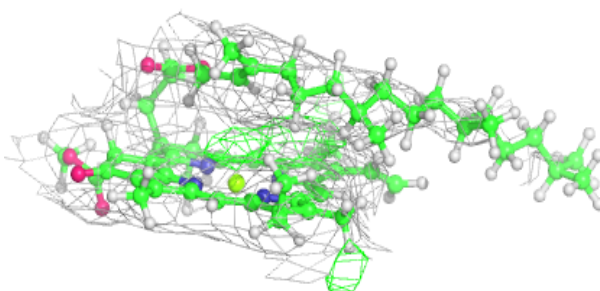
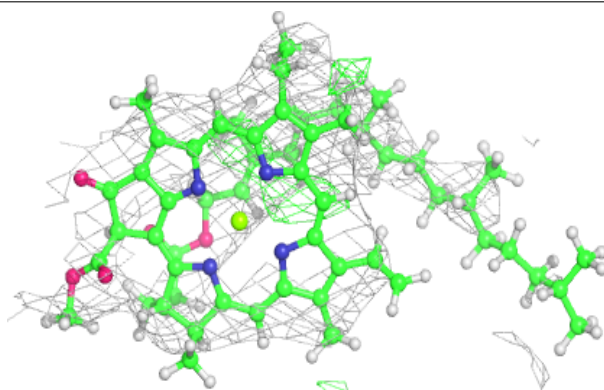


Electron density around CLA B 3042:

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

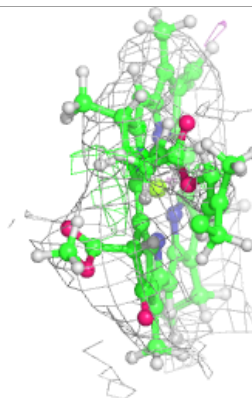
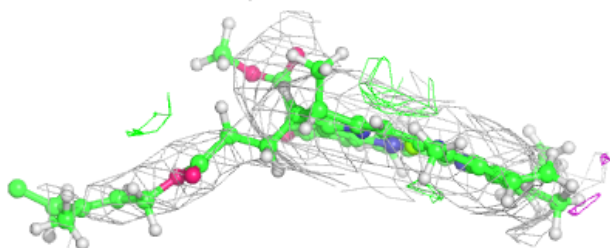
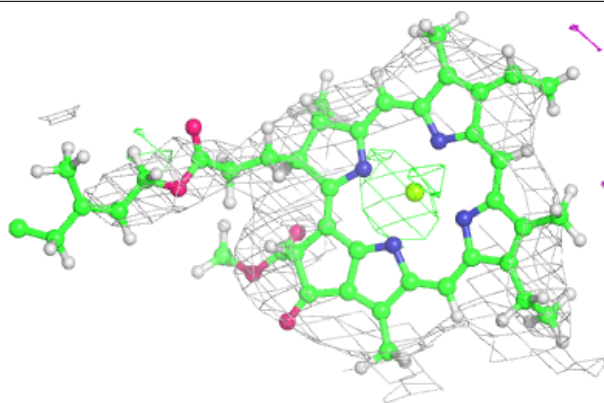
**Electron density around CLA A 841:**

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

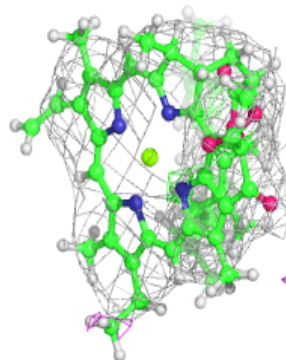
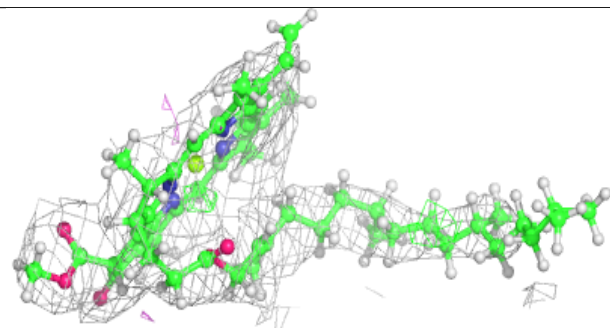
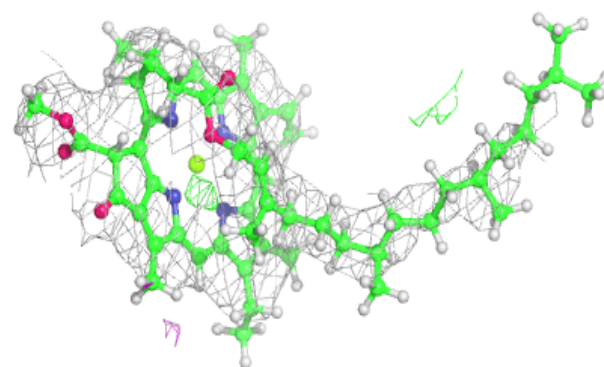


Electron density around CLA A 842:

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

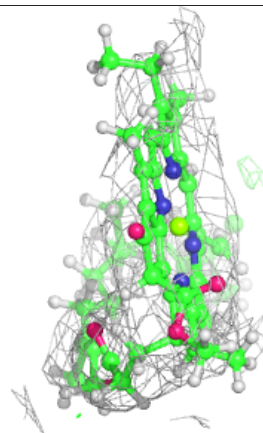
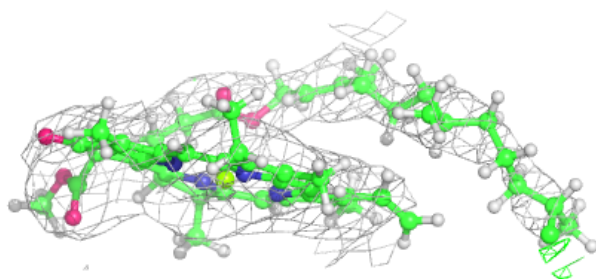
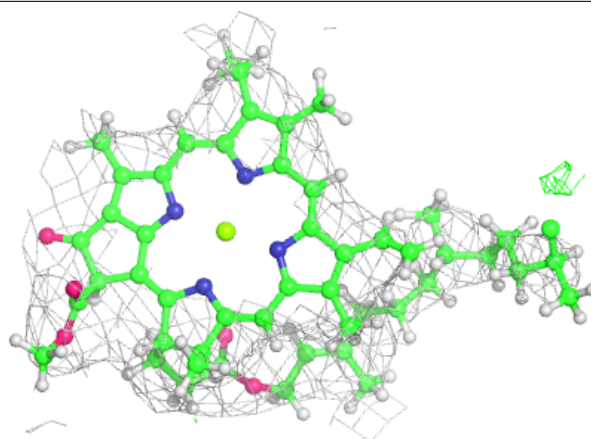
**Electron density around CLA A 843:**

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

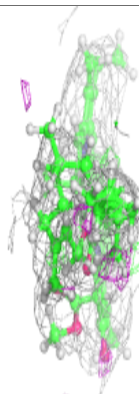
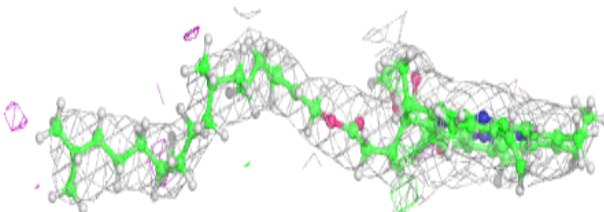
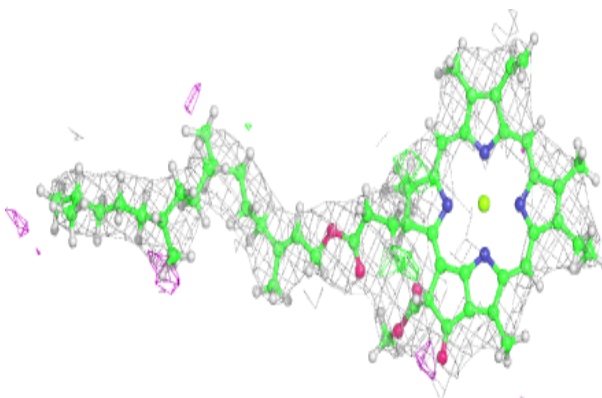


Electron density around CLA B 3019:

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

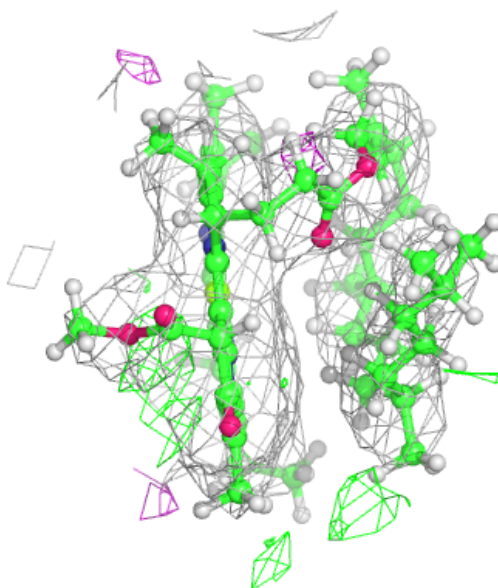
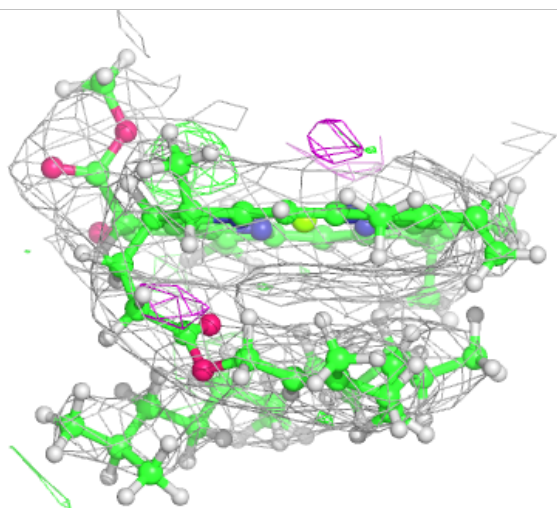
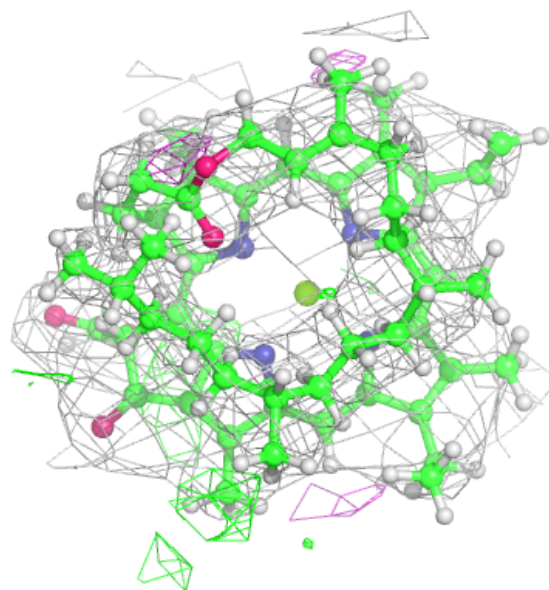
**Electron density around CLA A 834:**

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



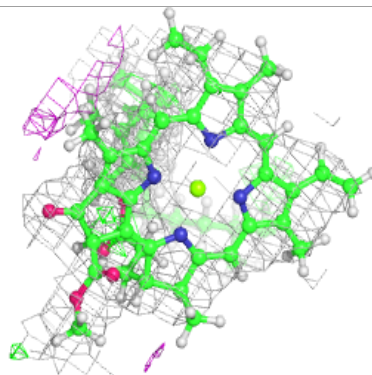
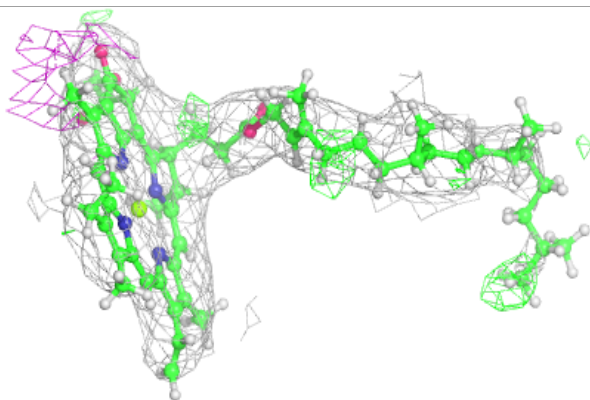
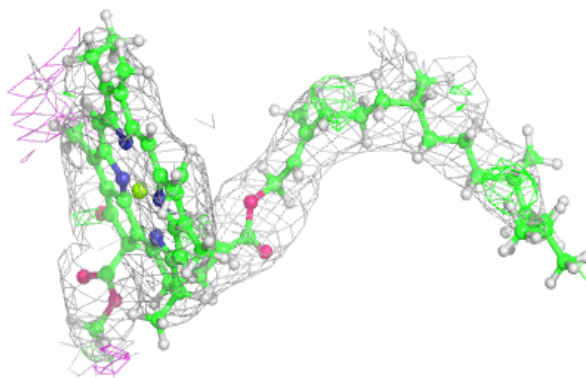
Electron density around CLA L 204:

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

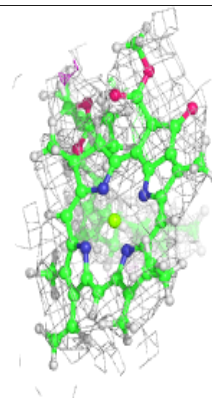
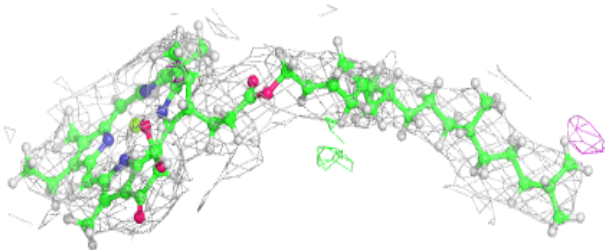
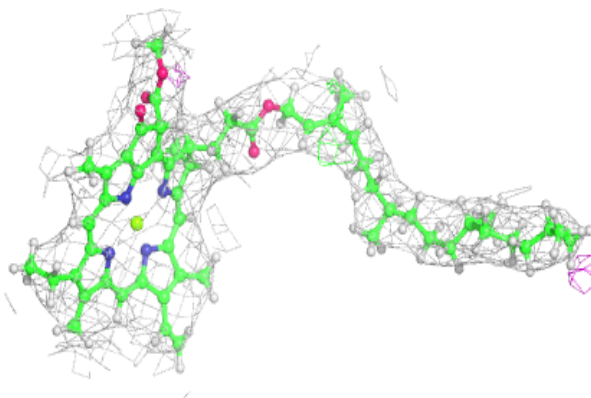


Electron density around CLA L 205:

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

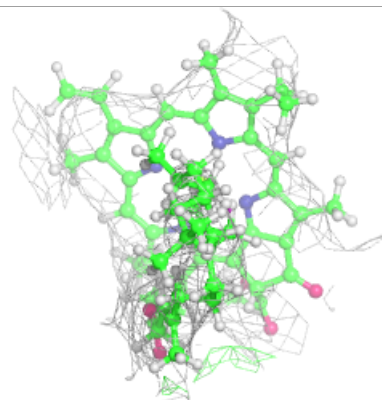
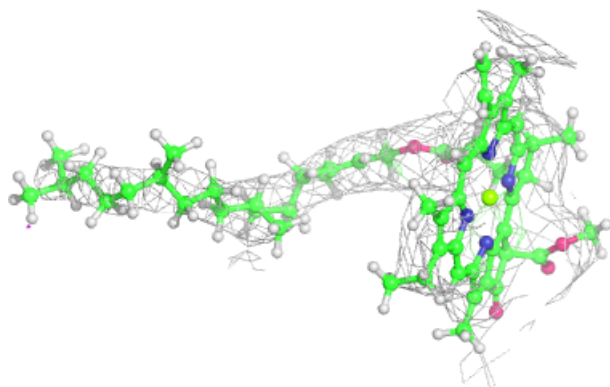
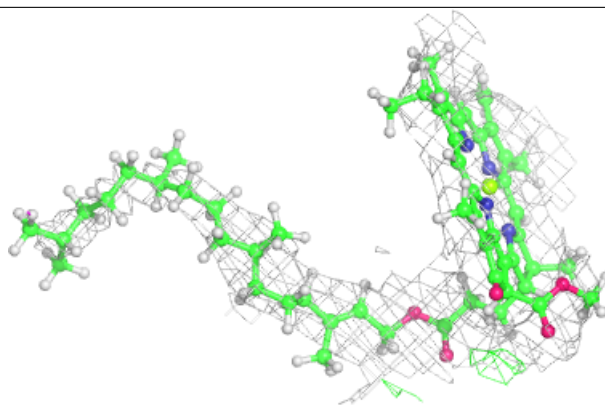
**Electron density around CLA A 802:**

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

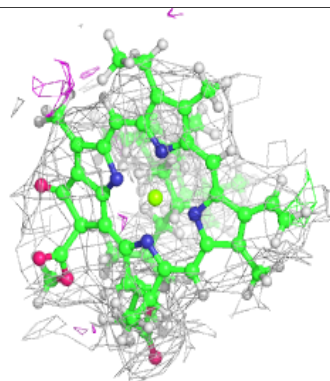
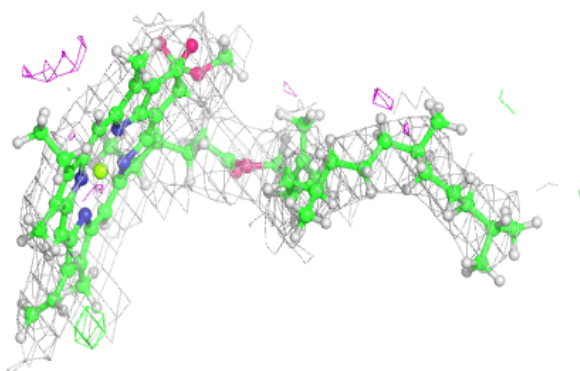
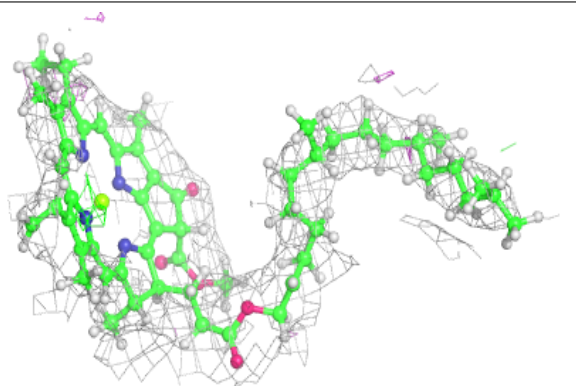


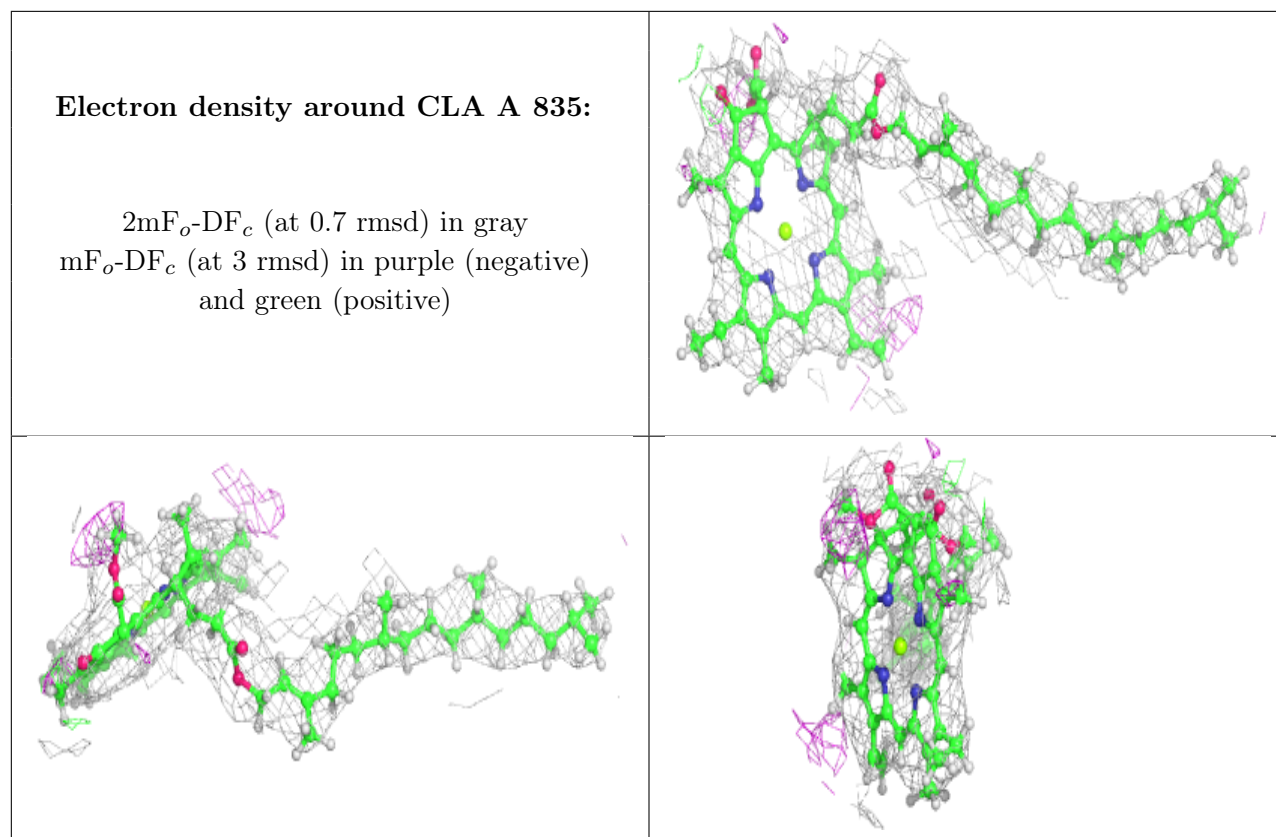
Electron density around CLA A 831:

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

**Electron density around CLA B 3003:**

$2mF_o-DF_c$ (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.