



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 12:10 AM EDT

PDB ID : 7M76 / pdb_00007m76
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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

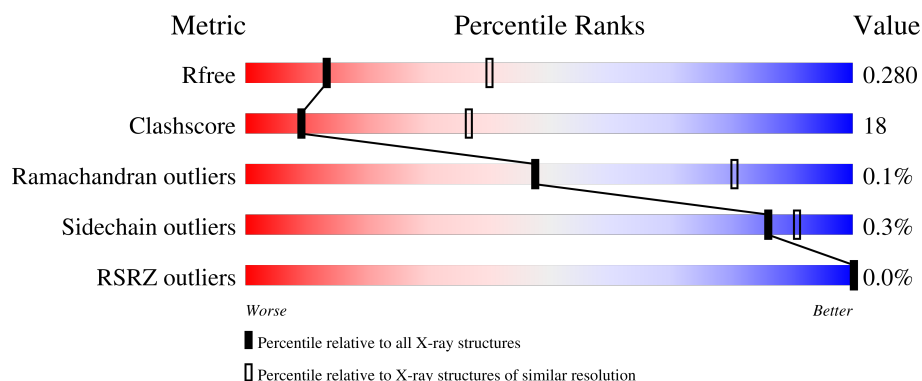
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	755	59% 39% .
2	B	740	66% 34%
3	C	80	68% 31% .
4	D	138	68% 32%

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

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

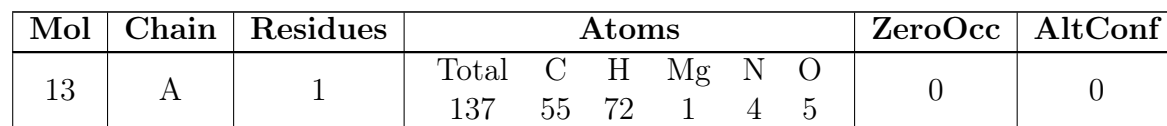
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

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 (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



- # CLA

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



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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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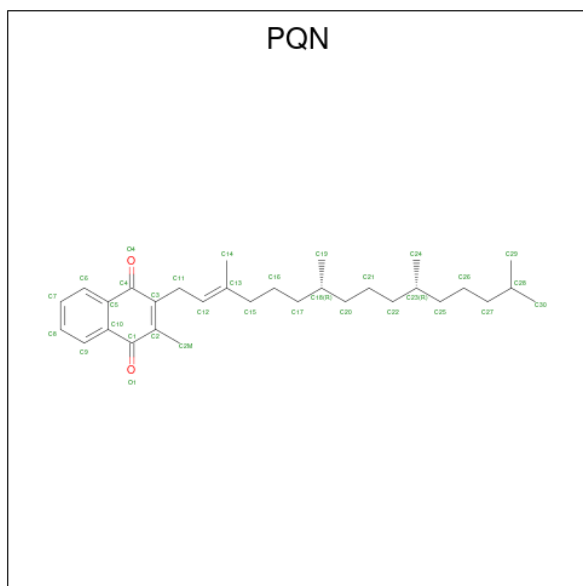
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	B	1	Total	C	H	Mg	N	O	0	0
			104	45	49	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			79	36	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	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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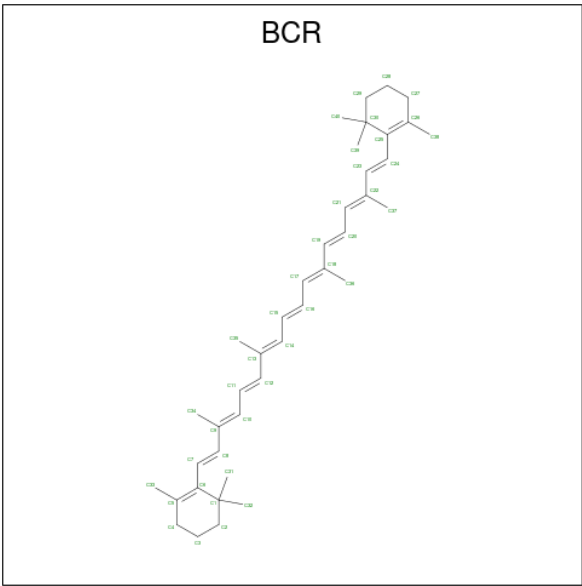
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	J	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	J	1	Total	C	H	Mg	N	O	0	0
			62	31	25	1	4	1		
14	K	1	Total	C	H	Mg	N	O	0	0
			70	33	29	1	4	3		
14	K	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	L	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	L	1	Total	C	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 (CCD ID: 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 (CCD ID: BCR) (formula: C₄₀H₅₆).



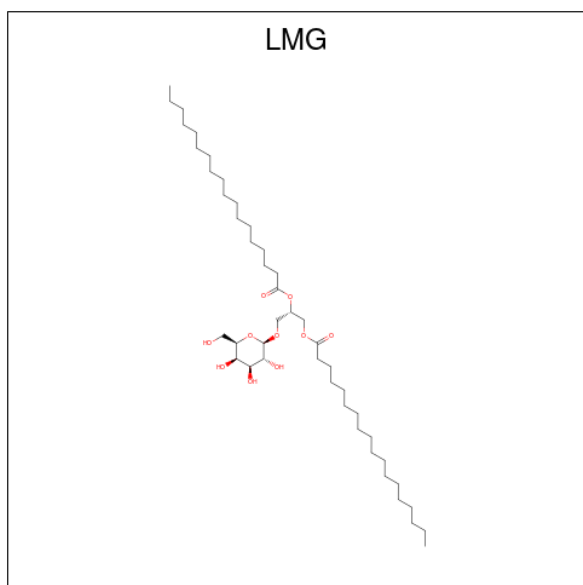
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	A	1	Total	C	H	0	0
			96	40	56		
16	A	1	Total	C	H	0	0
			96	40	56		
16	A	1	Total	C	H	0	0
			96	40	56		
16	A	1	Total	C	H	0	0
			96	40	56		
16	A	1	Total	C	H	0	0
			96	40	56		
16	B	1	Total	C	H	0	0
			96	40	56		
16	B	1	Total	C	H	0	0
			96	40	56		
16	B	1	Total	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 (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



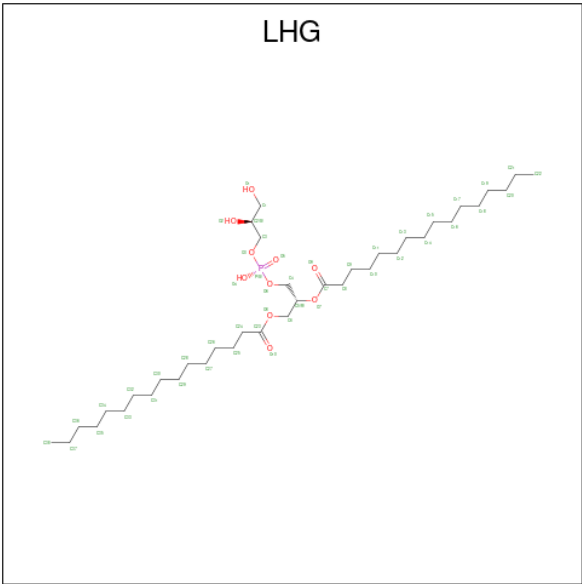
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	H	O	0	0
			118	38	70	10		
17	A	1	Total	C	H	O	0	0
			67	22	37	8		

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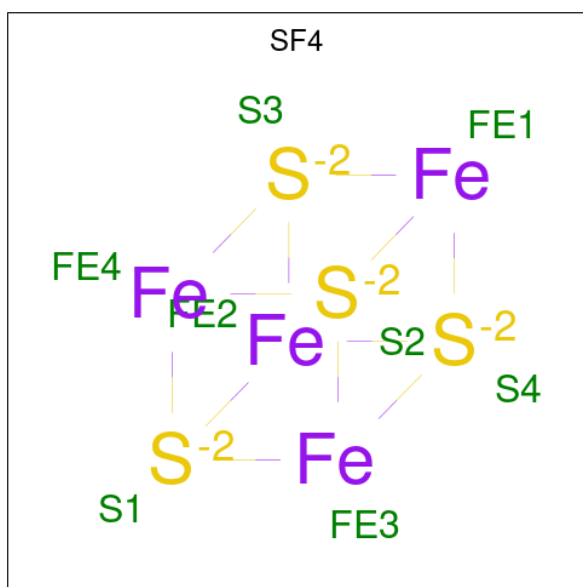
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	B	1	Total	C	H	O	0	0
			141	45	86	10		
17	I	1	Total	C	H	O	0	0
			91	30	51	10		

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



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

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

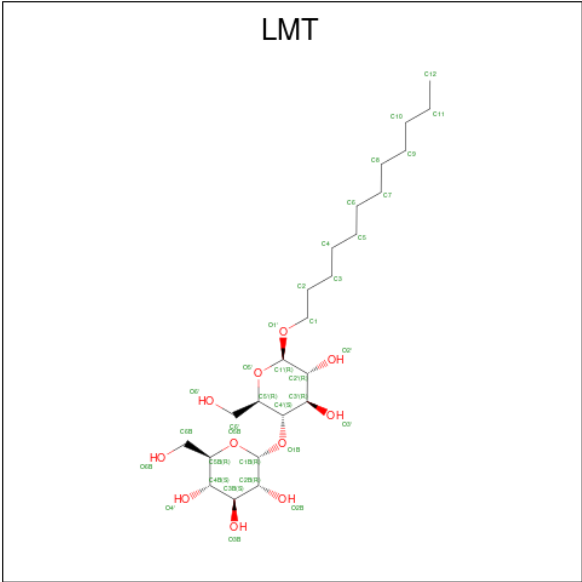


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	B	1	Total	Fe	S	0	0
			8	4	4		
19	C	1	Total	Fe	S	0	0
			8	4	4		
19	C	1	Total	Fe	S	0	0
			8	4	4		

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

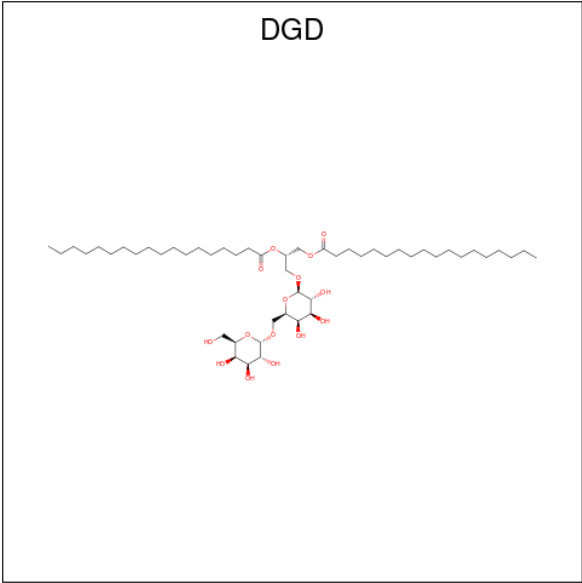
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	B	1	Total	Ca	0	0
			1	1		
20	L	1	Total	Ca	0	0
			1	1		

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



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

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



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

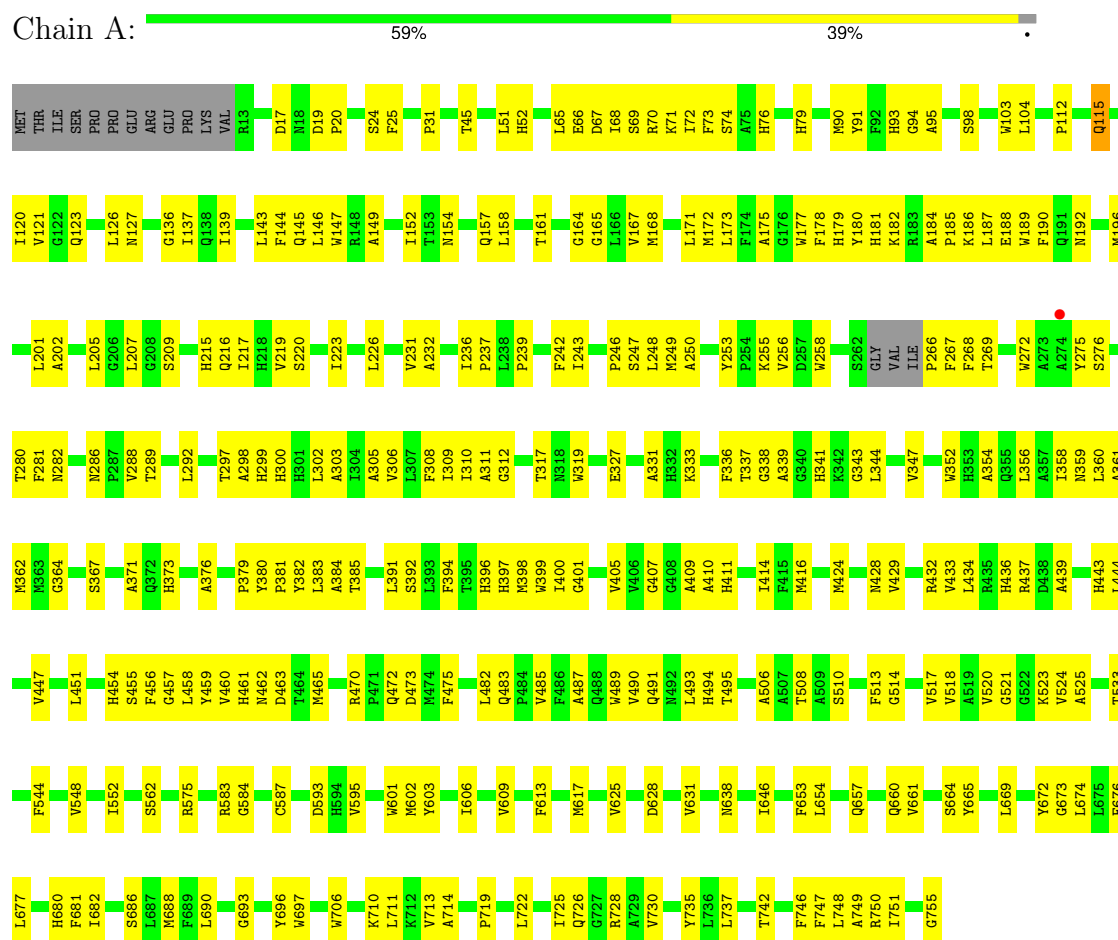
- Molecule 23 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	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

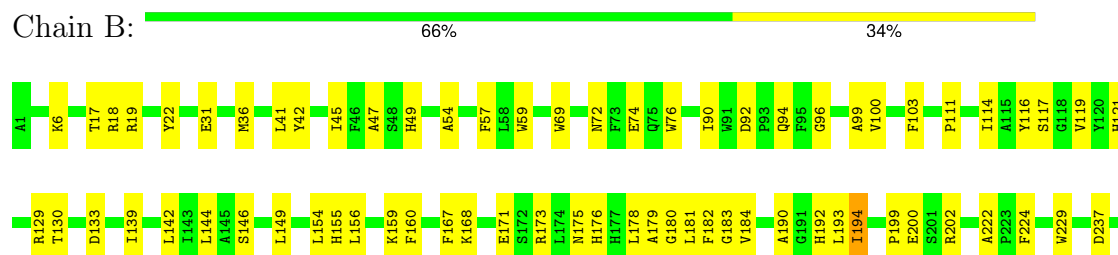
3 Residue-property plots

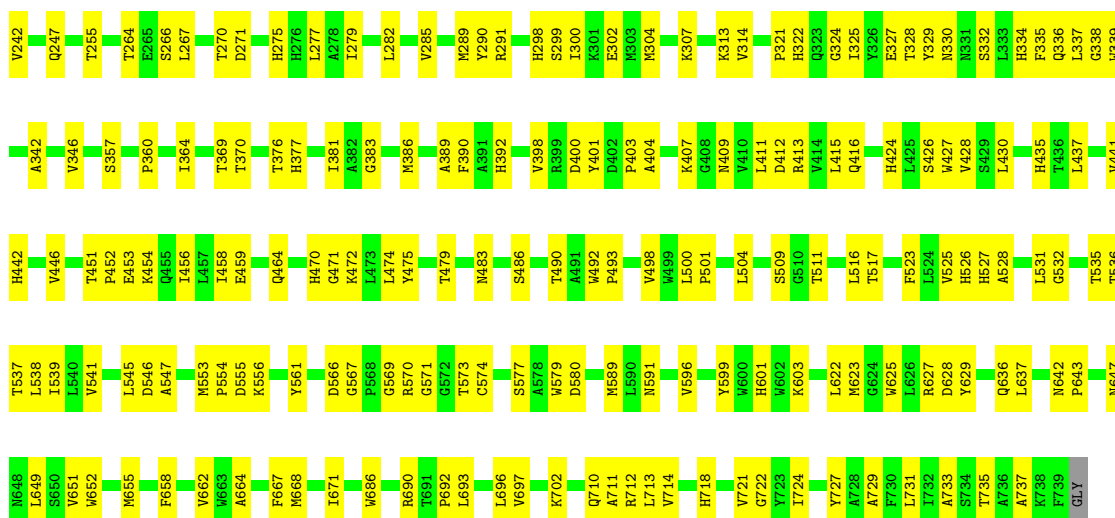
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

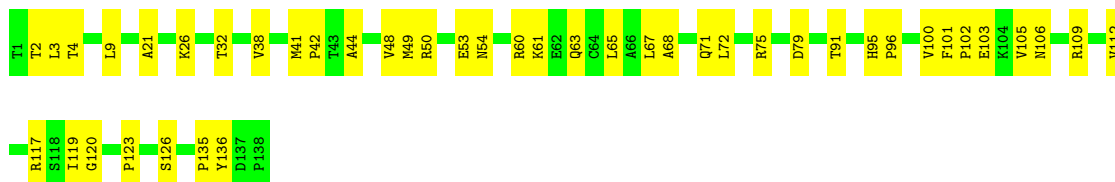




• Molecule 3: Photosystem I iron-sulfur center



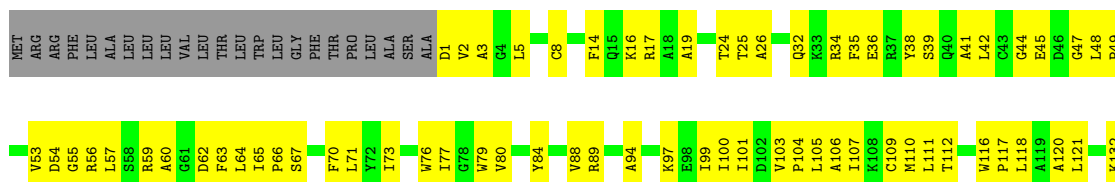
• Molecule 4: Photosystem I reaction center subunit II



• Molecule 5: Photosystem I reaction center subunit IV



• Molecule 6: Photosystem I reaction center subunit III





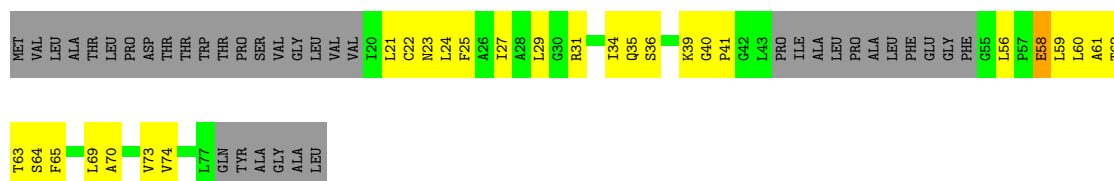
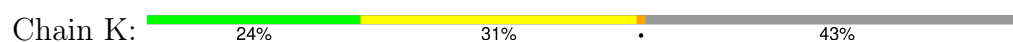
• Molecule 7: Photosystem I reaction center subunit VIII



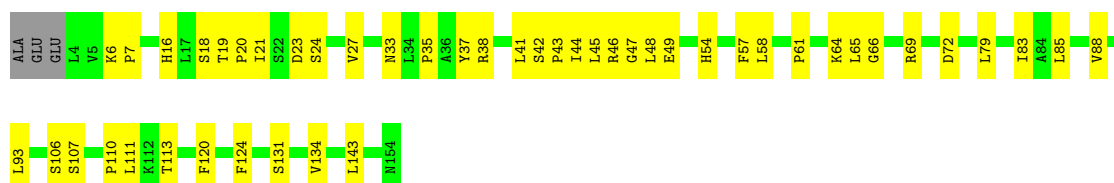
• Molecule 8: Photosystem I reaction center subunit IX



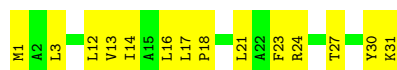
• Molecule 9: Photosystem I reaction center subunit PsaK



• Molecule 10: Photosystem I reaction center subunit XI



• Molecule 11: Photosystem I reaction center subunit XII



• Molecule 12: Photosystem I 4.8K protein



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 0.270 , 0.280	Depositor DCC
R_{free} test set	1997 reflections (1.31%)	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)	0.24 , 60.3	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	0.91	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: PQN, CA, LMG, BCR, LHG, CLA, DGD, SF4, CL0, LMT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/5983	0.54	1/8158 (0.0%)
2	B	0.26	0/6107	0.51	0/8345
3	C	0.29	0/608	0.54	0/824
4	D	0.21	0/1101	0.50	0/1492
5	E	0.26	0/551	0.54	0/750
6	F	0.28	0/1087	0.54	0/1476
7	I	0.27	0/312	0.65	0/425
8	J	0.30	0/350	0.60	0/477
9	K	0.28	0/337	0.67	0/454
10	L	0.26	0/1148	0.55	0/1558
11	M	0.33	0/244	0.60	0/332
12	X	0.30	0/251	0.49	0/342
All	All	0.27	0/18079	0.54	1/24633 (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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	TYR	O-C-N	5.61	124.11	121.53

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

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	295	0
2	B	5889	5618	5649	227	0
3	C	598	576	580	28	0
4	D	1075	1077	1077	34	0
5	E	539	528	528	14	0
6	F	1065	1076	1077	75	0
7	I	301	306	306	18	0
8	J	338	347	347	28	0
9	K	333	354	354	44	0
10	L	1119	1125	1125	36	0
11	M	241	264	264	16	0
12	X	242	217	249	16	0
13	A	65	72	72	1	0
14	A	2628	2615	2615	112	0
14	B	2284	2232	2232	82	0
14	F	45	33	33	9	0
14	J	82	58	58	3	0
14	K	86	62	62	6	0
14	L	195	216	216	5	0
14	M	45	33	33	4	0
14	X	45	33	33	3	0
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	20	0
16	F	80	112	112	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	I	40	56	56	4	0
16	J	120	168	168	19	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	4	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	891	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 18.

The worst 5 of 891 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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	736/755 (98%)	671 (91%)	65 (9%)	0	100	100
2	B	737/740 (100%)	680 (92%)	56 (8%)	1 (0%)	48	80
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%)	8	35
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%)	48	80

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	589/603 (98%)	587 (100%)	2 (0%)	86	91
2	B	597/597 (100%)	595 (100%)	2 (0%)	86	91
3	C	67/67 (100%)	66 (98%)	1 (2%)	57	80
4	D	115/115 (100%)	115 (100%)	0	100	100
5	E	59/64 (92%)	59 (100%)	0	100	100
6	F	109/128 (85%)	109 (100%)	0	100	100
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%)	33 (100%)	0	100	100
10	L	117/119 (98%)	117 (100%)	0	100	100
11	M	26/26 (100%)	26 (100%)	0	100	100
12	X	23/27 (85%)	23 (100%)	0	100	100
All	All	1803/1875 (96%)	1798 (100%)	5 (0%)	86	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	587	CYS
2	B	424	HIS
2	B	526	HIS
3	C	16	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	336	GLN
2	B	591	ASN
6	F	134	ASN
2	B	467	GLN
2	B	688	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 135 ligands modelled in this entry, 2 are monoatomic - leaving 133 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
19	SF4	B	3001	1,2	0,12,12	-	-	-		
14	CLA	B	3017	2	59,63,73	1.32	6 (10%)	70,101,113	1.28	5 (7%)
16	BCR	L	201	-	41,41,41	1.16	3 (7%)	56,56,56	1.23	5 (8%)
14	CLA	L	205	10	69,73,73	1.17	7 (10%)	82,113,113	1.30	7 (8%)
14	CLA	A	833	1	69,73,73	1.17	9 (13%)	82,113,113	1.28	5 (6%)
14	CLA	B	3038	2	64,68,73	1.24	7 (10%)	76,107,113	1.28	6 (7%)
16	BCR	I	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.25	7 (12%)
14	CLA	A	856	23	69,73,73	1.19	9 (13%)	82,113,113	1.24	6 (7%)
14	CLA	B	3039	2	69,73,73	1.21	7 (10%)	82,113,113	1.24	4 (4%)
16	BCR	A	851	-	41,41,41	1.18	3 (7%)	56,56,56	1.41	8 (14%)
16	BCR	J	103	-	41,41,41	1.12	3 (7%)	56,56,56	1.22	2 (3%)
14	CLA	B	3040	2	51,55,73	1.39	7 (13%)	60,91,113	1.39	5 (8%)
17	LMG	A	855	-	30,30,55	1.40	4 (13%)	37,37,63	1.33	4 (10%)
17	LMG	I	102	-	40,40,55	1.36	6 (15%)	48,48,63	1.24	5 (10%)
14	CLA	B	3008	2	69,73,73	1.20	7 (10%)	82,113,113	1.29	4 (4%)
19	SF4	C	101	3	0,12,12	-	-	-		
16	BCR	A	847	-	41,41,41	1.20	4 (9%)	56,56,56	1.26	5 (8%)
14	CLA	A	805	14,1	63,67,73	1.28	8 (12%)	74,105,113	1.21	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	3024	2	49,53,73	1.45	5 (10%)	58,89,113	1.36	6 (10%)
14	CLA	B	3035	2	49,53,73	1.44	6 (12%)	58,89,113	1.47	6 (10%)
14	CLA	A	821	1	46,50,73	1.41	6 (13%)	54,84,113	1.50	9 (16%)
14	CLA	B	3006	2	69,73,73	1.20	5 (7%)	82,113,113	1.25	5 (6%)
14	CLA	A	842	23	55,59,73	1.33	7 (12%)	64,96,113	1.48	5 (7%)
16	BCR	B	3051	-	41,41,41	1.20	3 (7%)	56,56,56	1.20	3 (5%)
14	CLA	A	838	1	55,59,73	1.37	8 (14%)	64,96,113	1.47	7 (10%)
14	CLA	B	3029	2	69,73,73	1.19	5 (7%)	82,113,113	1.26	6 (7%)
14	CLA	B	3016	2	49,53,73	1.41	5 (10%)	58,89,113	1.44	6 (10%)
22	DGD	L	207	-	67,67,67	1.05	3 (4%)	81,81,81	1.18	7 (8%)
14	CLA	B	3023	23	59,63,73	1.28	8 (13%)	70,101,113	1.27	4 (5%)
13	CL0	A	801	1	69,73,73	1.21	8 (11%)	82,113,113	1.25	7 (8%)
14	CLA	A	841	1	69,73,73	1.18	5 (7%)	82,113,113	1.36	7 (8%)
14	CLA	B	3022	2	49,53,73	1.42	7 (14%)	58,89,113	1.37	5 (8%)
14	CLA	A	840	1	51,55,73	1.40	7 (13%)	60,91,113	1.48	7 (11%)
14	CLA	A	809	1	69,73,73	1.19	6 (8%)	82,113,113	1.24	5 (6%)
16	BCR	A	848	-	41,41,41	1.19	3 (7%)	56,56,56	1.23	4 (7%)
14	CLA	X	1701	12	49,53,73	1.42	6 (12%)	58,89,113	1.45	5 (8%)
14	CLA	A	812	14,1	69,73,73	1.21	7 (10%)	82,113,113	1.32	6 (7%)
18	LHG	A	854	14	26,26,48	0.98	1 (3%)	29,32,54	1.31	3 (10%)
14	CLA	B	3034	2	62,66,73	1.25	6 (9%)	73,104,113	1.34	9 (12%)
14	CLA	A	815	1	49,53,73	1.42	8 (16%)	58,89,113	1.33	3 (5%)
14	CLA	B	3028	2	69,73,73	1.18	7 (10%)	82,113,113	1.29	3 (3%)
14	CLA	B	3031	2	49,53,73	1.43	7 (14%)	58,89,113	1.47	5 (8%)
14	CLA	K	101	9	45,49,73	1.40	7 (15%)	54,83,113	1.34	5 (9%)
14	CLA	A	808	1	55,59,73	1.40	6 (10%)	64,96,113	1.41	7 (10%)
14	CLA	B	3030	2	69,73,73	1.18	7 (10%)	82,113,113	1.37	9 (10%)
16	BCR	B	3046	-	41,41,41	1.16	3 (7%)	56,56,56	1.28	7 (12%)
14	CLA	A	806	1	69,73,73	1.18	6 (8%)	82,113,113	1.38	5 (6%)
21	LMT	L	202	-	36,36,36	1.12	5 (13%)	47,47,47	1.38	7 (14%)
14	CLA	B	3033	2	69,73,73	1.19	6 (8%)	82,113,113	1.29	6 (7%)
14	CLA	A	826	-	69,73,73	1.20	6 (8%)	82,113,113	1.28	5 (6%)
14	CLA	A	803	-	69,73,73	1.18	7 (10%)	82,113,113	1.39	6 (7%)
14	CLA	J	102	8	41,45,73	1.51	7 (17%)	50,78,113	1.31	5 (10%)
14	CLA	A	810	1	69,73,73	1.23	5 (7%)	82,113,113	1.23	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	3013	2	49,53,73	1.41	6 (12%)	58,89,113	1.38	4 (6%)
17	LMG	A	852	-	48,48,55	0.85	2 (4%)	56,56,63	1.26	5 (8%)
18	LHG	M	101	-	48,48,48	0.72	1 (2%)	51,54,54	1.22	3 (5%)
19	SF4	C	102	3	0,12,12	-	-	-	-	-
14	CLA	A	824	1	55,59,73	1.32	5 (9%)	64,96,113	1.38	5 (7%)
16	BCR	B	3048	-	41,41,41	1.13	3 (7%)	56,56,56	1.20	7 (12%)
14	CLA	B	3037	23	49,53,73	1.43	7 (14%)	58,89,113	1.32	3 (5%)
17	LMG	B	3049	-	55,55,55	0.81	1 (1%)	63,63,63	1.36	4 (6%)
14	CLA	B	3004	-	69,73,73	1.19	8 (11%)	82,113,113	1.36	5 (6%)
14	CLA	A	811	1	49,53,73	1.40	8 (16%)	58,89,113	1.39	6 (10%)
14	CLA	A	819	1	58,62,73	1.29	8 (13%)	68,99,113	1.46	10 (14%)
14	CLA	A	814	1	64,68,73	1.26	5 (7%)	76,107,113	1.24	5 (6%)
14	CLA	B	3025	2	58,62,73	1.33	7 (12%)	68,99,113	1.41	8 (11%)
14	CLA	A	823	1	53,57,73	1.36	6 (11%)	61,93,113	1.46	5 (8%)
14	CLA	B	3027	2	69,73,73	1.23	7 (10%)	82,113,113	1.21	5 (6%)
14	CLA	A	822	23	69,73,73	1.18	6 (8%)	82,113,113	1.21	6 (7%)
14	CLA	B	3005	2	58,62,73	1.30	6 (10%)	68,99,113	1.45	5 (7%)
14	CLA	B	3042	2	69,73,73	1.20	7 (10%)	82,113,113	1.38	6 (7%)
14	CLA	M	102	23	49,53,73	1.52	12 (24%)	58,89,113	1.57	12 (20%)
14	CLA	A	835	1	69,73,73	1.20	7 (10%)	82,113,113	1.44	10 (12%)
16	BCR	A	849	-	41,41,41	1.16	3 (7%)	56,56,56	1.34	7 (12%)
16	BCR	B	3047	-	41,41,41	1.18	3 (7%)	56,56,56	1.35	8 (14%)
14	CLA	K	103	-	49,53,73	1.41	6 (12%)	58,89,113	1.44	6 (10%)
14	CLA	A	827	23	69,73,73	1.17	7 (10%)	82,113,113	1.27	7 (8%)
14	CLA	A	843	1	69,73,73	1.20	7 (10%)	82,113,113	1.37	6 (7%)
15	PQN	B	3043	-	34,34,34	2.15	7 (20%)	43,45,45	1.21	4 (9%)
14	CLA	A	825	1	63,67,73	1.26	7 (11%)	74,105,113	1.28	6 (8%)
14	CLA	B	3014	2	69,73,73	1.21	7 (10%)	82,113,113	1.23	6 (7%)
16	BCR	F	203	-	41,41,41	1.16	3 (7%)	56,56,56	1.30	8 (14%)
14	CLA	A	807	1	69,73,73	1.22	5 (7%)	82,113,113	1.18	5 (6%)
14	CLA	A	836	1	58,62,73	1.30	8 (13%)	68,99,113	1.34	6 (8%)
14	CLA	A	804	1	69,73,73	1.20	6 (8%)	82,113,113	1.17	4 (4%)
14	CLA	A	820	1	69,73,73	1.16	6 (8%)	82,113,113	1.38	8 (9%)
16	BCR	J	105	-	41,41,41	1.17	3 (7%)	56,56,56	1.36	8 (14%)
14	CLA	B	3036	23	49,53,73	1.44	5 (10%)	58,89,113	1.40	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	3018	2	63,67,73	1.23	6 (9%)	74,105,113	1.37	6 (8%)
16	BCR	L	208	-	41,41,41	1.15	3 (7%)	56,56,56	1.43	10 (17%)
14	CLA	A	834	1	69,73,73	1.21	7 (10%)	82,113,113	1.29	6 (7%)
14	CLA	A	802	23	69,73,73	1.20	6 (8%)	82,113,113	1.25	6 (7%)
14	CLA	L	206	23	69,73,73	1.19	7 (10%)	82,113,113	1.35	9 (10%)
14	CLA	A	832	1	54,58,73	1.33	7 (12%)	64,95,113	1.41	6 (9%)
14	CLA	A	818	1	58,62,73	1.31	6 (10%)	68,99,113	1.39	6 (8%)
14	CLA	A	837	1	49,53,73	1.40	7 (14%)	58,89,113	1.39	5 (8%)
14	CLA	B	3011	2	69,73,73	1.20	6 (8%)	82,113,113	1.32	11 (13%)
14	CLA	B	3015	2	69,73,73	1.22	5 (7%)	82,113,113	1.14	5 (6%)
14	CLA	J	101	8	49,53,73	1.44	5 (10%)	58,89,113	1.32	5 (8%)
18	LHG	B	3050	-	22,22,48	1.58	5 (22%)	25,28,54	1.27	3 (12%)
14	CLA	L	204	10	69,73,73	1.19	5 (7%)	82,113,113	1.48	8 (9%)
14	CLA	A	845	18	56,60,73	1.32	6 (10%)	65,97,113	1.43	7 (10%)
15	PQN	A	846	-	34,34,34	2.03	7 (20%)	43,45,45	1.28	6 (13%)
14	CLA	B	3026	23	50,54,73	1.40	5 (10%)	59,90,113	1.48	4 (6%)
14	CLA	B	3041	23	69,73,73	1.25	7 (10%)	82,113,113	1.37	8 (9%)
16	BCR	B	3044	-	41,41,41	1.14	3 (7%)	56,56,56	1.24	6 (10%)
14	CLA	B	3007	2	69,73,73	1.18	7 (10%)	82,113,113	1.25	4 (4%)
16	BCR	J	104	-	41,41,41	1.21	3 (7%)	56,56,56	1.31	7 (12%)
14	CLA	A	813	1	58,62,73	1.30	9 (15%)	68,99,113	1.36	5 (7%)
14	CLA	A	828	1	69,73,73	1.24	6 (8%)	82,113,113	1.23	6 (7%)
14	CLA	A	829	1	69,73,73	1.17	6 (8%)	82,113,113	1.23	6 (7%)
14	CLA	B	3012	2	49,53,73	1.42	6 (12%)	58,89,113	1.57	6 (10%)
14	CLA	B	3009	2	69,73,73	1.19	7 (10%)	82,113,113	1.32	8 (9%)
14	CLA	B	3020	23	69,73,73	1.18	9 (13%)	82,113,113	1.33	7 (8%)
16	BCR	M	103	-	41,41,41	1.20	3 (7%)	56,56,56	1.17	3 (5%)
14	CLA	A	844	23	69,73,73	1.20	7 (10%)	82,113,113	1.39	6 (7%)
14	CLA	A	831	1	69,73,73	1.18	6 (8%)	82,113,113	1.25	7 (8%)
18	LHG	A	853	-	48,48,48	0.70	3 (6%)	51,54,54	1.25	5 (9%)
14	CLA	B	3032	2	53,57,73	1.38	6 (11%)	61,93,113	1.50	8 (13%)
14	CLA	A	830	1	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
14	CLA	A	817	23	53,57,73	1.35	7 (13%)	61,93,113	1.32	2 (3%)
14	CLA	A	839	1	69,73,73	1.16	6 (8%)	82,113,113	1.33	5 (6%)
14	CLA	F	202	23	49,53,73	1.43	7 (14%)	58,89,113	1.36	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	K	102	-	41,41,41	1.14	3 (7%)	56,56,56	1.39	7 (12%)
14	CLA	B	3019	2	64,68,73	1.22	6 (9%)	76,107,113	1.30	8 (10%)
14	CLA	B	3010	2	69,73,73	1.21	9 (13%)	82,113,113	1.47	10 (12%)
14	CLA	A	816	1	49,53,73	1.40	7 (14%)	58,89,113	1.50	5 (8%)
14	CLA	B	3021	2	51,55,73	1.36	7 (13%)	60,91,113	1.36	4 (6%)
16	BCR	A	850	-	41,41,41	1.11	3 (7%)	56,56,56	1.20	4 (7%)
16	BCR	B	3045	-	41,41,41	1.17	3 (7%)	56,56,56	1.27	6 (10%)
14	CLA	B	3003	2	69,73,73	1.20	7 (10%)	82,113,113	1.31	5 (6%)
16	BCR	F	201	-	41,41,41	1.18	4 (9%)	56,56,56	1.29	4 (7%)
16	BCR	L	209	-	41,41,41	1.21	3 (7%)	56,56,56	1.33	6 (10%)

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
19	SF4	B	3001	1,2	-	-	0/6/5/5
14	CLA	B	3017	2	-	5/27/103/115	-
16	BCR	L	201	-	-	8/29/63/63	0/2/2/2
14	CLA	L	205	10	-	4/39/115/115	-
14	CLA	A	833	1	-	5/39/115/115	-
14	CLA	B	3038	2	-	6/33/109/115	-
16	BCR	I	101	-	-	4/29/63/63	0/2/2/2
14	CLA	A	856	23	-	15/39/115/115	-
14	CLA	B	3039	2	-	9/39/115/115	-
16	BCR	A	851	-	-	16/29/63/63	0/2/2/2
16	BCR	J	103	-	-	14/29/63/63	0/2/2/2
14	CLA	B	3040	2	-	5/18/94/115	-
17	LMG	A	855	-	-	15/23/43/70	0/1/1/1
17	LMG	I	102	-	-	11/35/55/70	0/1/1/1
14	CLA	B	3008	2	-	6/39/115/115	-
19	SF4	C	101	3	-	-	0/6/5/5
16	BCR	A	847	-	-	16/29/63/63	0/2/2/2
14	CLA	A	805	14,1	-	5/32/108/115	-
14	CLA	B	3024	2	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	3035	2	-	5/15/91/115	-
14	CLA	A	821	1	-	6/10/86/115	-
14	CLA	B	3006	2	-	14/39/115/115	-
14	CLA	A	842	23	-	6/23/99/115	-
16	BCR	B	3051	-	-	12/29/63/63	0/2/2/2
14	CLA	A	838	1	-	6/23/99/115	-
14	CLA	B	3029	2	-	17/39/115/115	-
14	CLA	B	3016	2	-	4/15/91/115	-
22	DGD	L	207	-	-	23/55/95/95	0/2/2/2
14	CLA	B	3023	23	-	8/27/103/115	-
13	CL0	A	801	1	-	11/39/115/115	-
14	CLA	A	841	1	-	6/39/115/115	-
14	CLA	B	3022	2	-	8/15/91/115	-
14	CLA	A	840	1	-	4/18/94/115	-
14	CLA	A	809	1	-	18/39/115/115	-
16	BCR	A	848	-	-	7/29/63/63	0/2/2/2
14	CLA	X	1701	12	-	3/15/91/115	-
14	CLA	A	812	14,1	-	9/39/115/115	-
18	LHG	A	854	14	-	10/31/31/53	-
14	CLA	B	3034	2	-	9/31/107/115	-
14	CLA	A	815	1	-	2/15/91/115	-
14	CLA	B	3028	2	-	12/39/115/115	-
14	CLA	B	3031	2	-	6/15/91/115	-
14	CLA	K	101	9	-	1/9/81/115	-
14	CLA	A	808	1	-	12/23/99/115	-
14	CLA	B	3030	2	-	15/39/115/115	-
16	BCR	B	3046	-	-	11/29/63/63	0/2/2/2
14	CLA	A	806	1	-	18/39/115/115	-
21	LMT	L	202	-	-	12/21/61/61	0/2/2/2
14	CLA	B	3033	2	-	16/39/115/115	-
14	CLA	A	826	-	-	16/39/115/115	-
14	CLA	A	803	-	-	8/39/115/115	-
14	CLA	J	102	8	-	0/4/76/115	-
14	CLA	A	810	1	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	3013	2	-	6/15/91/115	-
17	LMG	A	852	-	-	27/43/63/70	0/1/1/1
18	LHG	M	101	-	-	26/53/53/53	-
19	SF4	C	102	3	-	-	0/6/5/5
14	CLA	A	824	1	-	4/23/99/115	-
16	BCR	B	3048	-	-	4/29/63/63	0/2/2/2
14	CLA	B	3037	23	-	4/15/91/115	-
17	LMG	B	3049	-	-	23/50/70/70	0/1/1/1
14	CLA	B	3004	-	-	7/39/115/115	-
14	CLA	A	811	1	-	9/15/91/115	-
14	CLA	A	819	1	-	8/26/102/115	-
14	CLA	A	814	1	-	4/33/109/115	-
14	CLA	B	3025	2	-	8/26/102/115	-
14	CLA	A	823	1	-	10/20/96/115	-
14	CLA	B	3027	2	-	13/39/115/115	-
14	CLA	A	822	23	-	15/39/115/115	-
14	CLA	B	3005	2	-	8/26/102/115	-
14	CLA	B	3042	2	-	8/39/115/115	-
14	CLA	M	102	23	-	11/15/91/115	-
14	CLA	A	835	1	-	16/39/115/115	-
16	BCR	A	849	-	-	12/29/63/63	0/2/2/2
16	BCR	B	3047	-	-	15/29/63/63	0/2/2/2
14	CLA	K	103	-	-	10/15/91/115	-
14	CLA	A	827	23	-	10/39/115/115	-
14	CLA	A	843	1	-	8/39/115/115	-
15	PQN	B	3043	-	-	8/23/43/43	0/2/2/2
14	CLA	A	825	1	-	10/32/108/115	-
14	CLA	B	3014	2	-	13/39/115/115	-
16	BCR	F	203	-	-	11/29/63/63	0/2/2/2
14	CLA	A	807	1	-	12/39/115/115	-
14	CLA	A	836	1	-	8/26/102/115	-
14	CLA	A	804	1	-	7/39/115/115	-
14	CLA	A	820	1	-	18/39/115/115	-
16	BCR	J	105	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	3036	23	-	6/15/91/115	-
14	CLA	B	3018	2	-	11/32/108/115	-
16	BCR	L	208	-	-	12/29/63/63	0/2/2/2
14	CLA	A	834	1	-	9/39/115/115	-
14	CLA	A	802	23	-	9/39/115/115	-
14	CLA	L	206	23	-	6/39/115/115	-
14	CLA	A	832	1	-	6/21/97/115	-
14	CLA	A	818	1	-	4/26/102/115	-
14	CLA	A	837	1	-	6/15/91/115	-
14	CLA	B	3011	2	-	14/39/115/115	-
14	CLA	B	3015	2	-	11/39/115/115	-
14	CLA	J	101	8	-	5/15/91/115	-
18	LHG	B	3050	-	-	10/26/26/53	-
14	CLA	L	204	10	-	12/39/115/115	-
14	CLA	A	845	18	-	9/24/100/115	-
15	PQN	A	846	-	-	9/23/43/43	0/2/2/2
14	CLA	B	3026	23	-	2/17/93/115	-
14	CLA	B	3041	23	-	10/39/115/115	-
16	BCR	B	3044	-	-	8/29/63/63	0/2/2/2
14	CLA	B	3007	2	-	9/39/115/115	-
16	BCR	J	104	-	-	15/29/63/63	0/2/2/2
14	CLA	A	813	1	-	6/26/102/115	-
14	CLA	A	828	1	-	5/39/115/115	-
14	CLA	A	829	1	-	11/39/115/115	-
14	CLA	B	3012	2	-	2/15/91/115	-
14	CLA	B	3009	2	-	10/39/115/115	-
14	CLA	B	3020	23	-	13/39/115/115	-
16	BCR	M	103	-	-	7/29/63/63	0/2/2/2
14	CLA	A	844	23	-	12/39/115/115	-
14	CLA	A	831	1	-	9/39/115/115	-
18	LHG	A	853	-	-	23/53/53/53	-
14	CLA	B	3032	2	-	7/20/96/115	-
14	CLA	A	830	1	-	13/39/115/115	-
14	CLA	A	817	23	-	8/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	839	1	-	9/39/115/115	-
14	CLA	F	202	23	-	6/15/91/115	-
16	BCR	K	102	-	-	12/29/63/63	0/2/2/2
14	CLA	B	3019	2	-	10/33/109/115	-
14	CLA	B	3010	2	-	14/39/115/115	-
14	CLA	A	816	1	-	2/15/91/115	-
14	CLA	B	3021	2	-	12/18/94/115	-
16	BCR	A	850	-	-	11/29/63/63	0/2/2/2
16	BCR	B	3045	-	-	11/29/63/63	0/2/2/2
14	CLA	B	3003	2	-	13/39/115/115	-
16	BCR	F	201	-	-	6/29/63/63	0/2/2/2
16	BCR	L	209	-	-	10/29/63/63	0/2/2/2

The worst 5 of 752 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	3043	PQN	O1-C1	6.03	1.35	1.23
15	A	846	PQN	O1-C1	5.97	1.35	1.23
15	A	846	PQN	O4-C4	5.94	1.35	1.23
15	B	3043	PQN	O4-C4	5.93	1.35	1.23
15	B	3043	PQN	C10-C1	-5.52	1.37	1.48

The worst 5 of 766 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	842	CLA	C4A-NA-C1A	8.00	110.33	106.68
14	A	806	CLA	C4A-NA-C1A	7.90	110.28	106.68
14	B	3042	CLA	C4A-NA-C1A	7.73	110.20	106.68
14	B	3033	CLA	C4A-NA-C1A	7.62	110.16	106.68
14	A	803	CLA	C4A-NA-C1A	7.58	110.14	106.68

There are no chirality outliers.

5 of 1263 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	805	CLA	CHA-CBD-CGD-O1D
14	A	805	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	A	806	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

115 monomers are involved in 304 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	3017	CLA	2	0
16	L	201	BCR	3	0
14	L	205	CLA	4	0
14	A	833	CLA	1	0
14	B	3038	CLA	1	0
16	I	101	BCR	4	0
14	A	856	CLA	5	0
14	B	3039	CLA	1	0
16	A	851	BCR	8	0
16	J	103	BCR	3	0
14	B	3040	CLA	1	0
17	A	855	LMG	1	0
17	I	102	LMG	3	0
14	B	3008	CLA	3	0
19	C	101	SF4	1	0
16	A	847	BCR	7	0
14	B	3024	CLA	3	0
14	B	3035	CLA	1	0
14	A	821	CLA	3	0
14	B	3006	CLA	2	0
14	A	842	CLA	3	0
16	B	3051	BCR	4	0
14	A	838	CLA	1	0
14	B	3016	CLA	2	0
22	L	207	DGD	2	0
13	A	801	CL0	1	0
14	A	841	CLA	5	0
14	B	3022	CLA	1	0
14	A	809	CLA	1	0
14	X	1701	CLA	3	0
14	A	812	CLA	4	0
18	A	854	LHG	1	0
14	B	3034	CLA	3	0
14	A	815	CLA	3	0
14	B	3028	CLA	3	0
14	B	3031	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	K	101	CLA	5	0
14	A	808	CLA	3	0
14	B	3030	CLA	1	0
16	B	3046	BCR	4	0
14	A	806	CLA	4	0
14	B	3033	CLA	3	0
14	A	826	CLA	3	0
14	A	803	CLA	3	0
14	J	102	CLA	1	0
14	A	810	CLA	1	0
14	B	3013	CLA	2	0
18	M	101	LHG	3	0
14	B	3037	CLA	2	0
14	B	3004	CLA	5	0
14	A	811	CLA	6	0
14	A	819	CLA	5	0
14	A	814	CLA	1	0
14	B	3025	CLA	4	0
14	A	823	CLA	2	0
14	B	3027	CLA	2	0
14	B	3005	CLA	2	0
14	B	3042	CLA	1	0
14	M	102	CLA	4	0
14	A	835	CLA	4	0
16	A	849	BCR	2	0
16	B	3047	BCR	4	0
14	K	103	CLA	1	0
14	A	827	CLA	2	0
14	A	843	CLA	4	0
15	B	3043	PQN	2	0
14	A	825	CLA	2	0
14	B	3014	CLA	4	0
16	F	203	BCR	4	0
14	A	807	CLA	1	0
14	A	836	CLA	2	0
14	A	804	CLA	7	0
14	A	820	CLA	5	0
16	J	105	BCR	10	0
14	B	3018	CLA	6	0
16	L	208	BCR	2	0
14	A	834	CLA	2	0
14	A	802	CLA	2	0

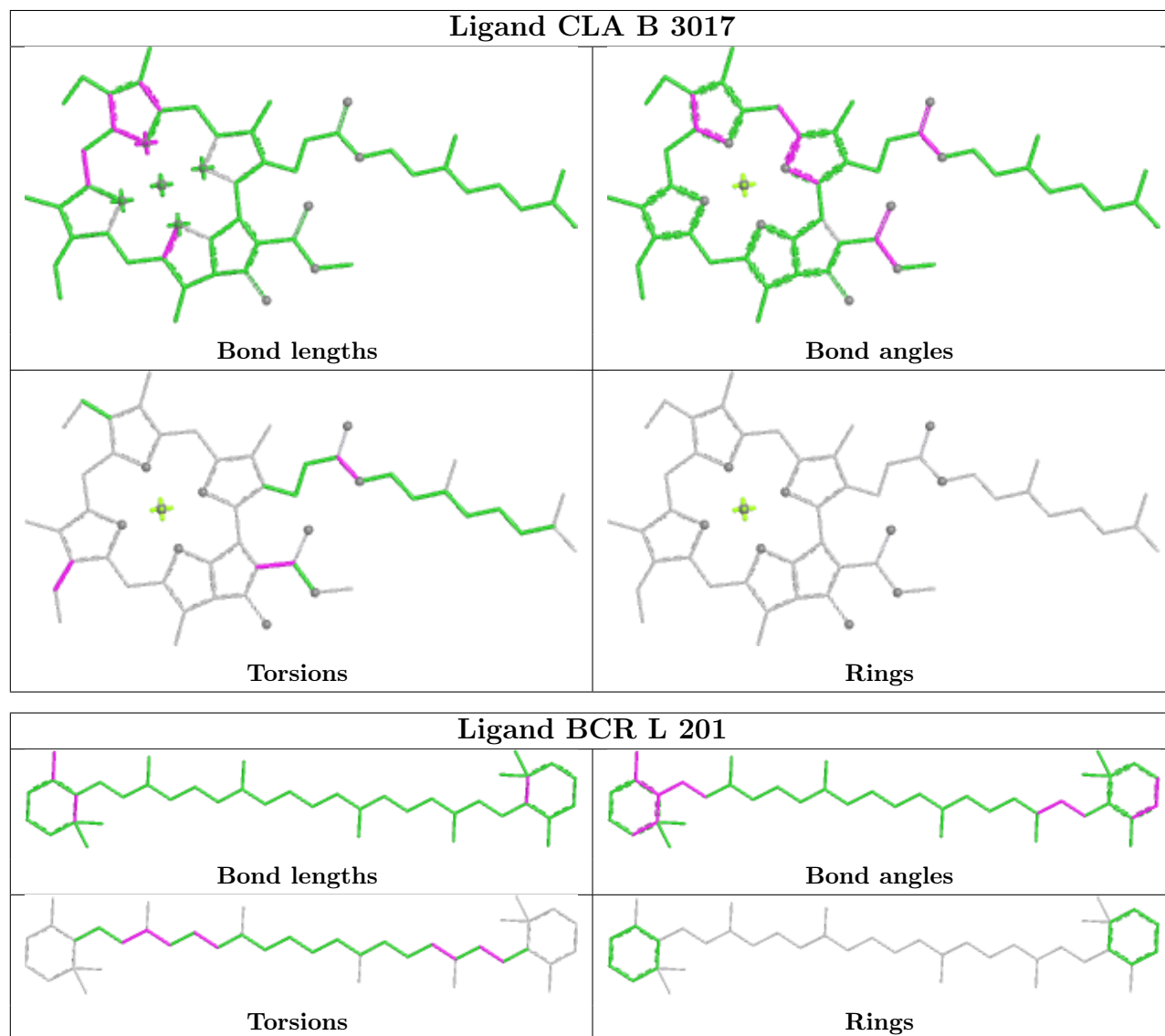
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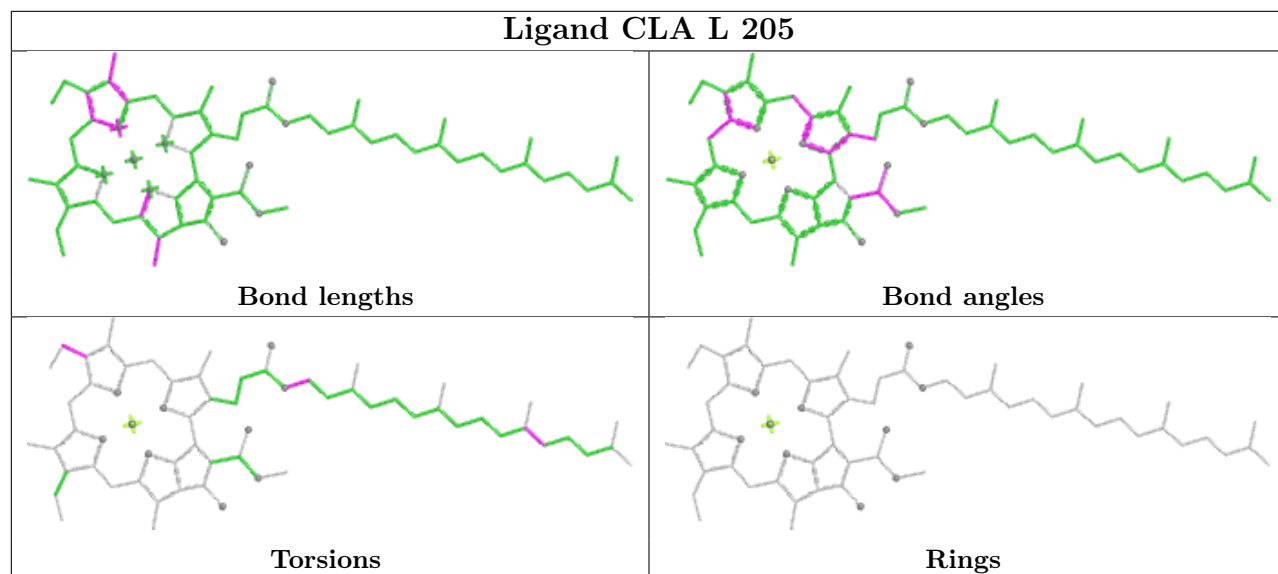
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	832	CLA	5	0
14	A	818	CLA	3	0
14	B	3011	CLA	1	0
14	B	3015	CLA	1	0
14	J	101	CLA	2	0
18	B	3050	LHG	2	0
14	L	204	CLA	2	0
14	A	845	CLA	2	0
15	A	846	PQN	9	0
14	B	3026	CLA	2	0
14	B	3041	CLA	3	0
16	B	3044	BCR	1	0
14	B	3007	CLA	3	0
16	J	104	BCR	6	0
14	A	813	CLA	5	0
14	A	828	CLA	3	0
14	A	829	CLA	8	0
14	B	3012	CLA	1	0
14	B	3020	CLA	2	0
16	M	103	BCR	2	0
14	A	844	CLA	4	0
14	A	831	CLA	5	0
18	A	853	LHG	3	0
14	B	3032	CLA	2	0
14	A	830	CLA	3	0
14	A	817	CLA	2	0
14	A	839	CLA	1	0
14	F	202	CLA	9	0
16	K	102	BCR	5	0
14	B	3019	CLA	3	0
14	B	3010	CLA	7	0
14	B	3021	CLA	2	0
16	A	850	BCR	4	0
16	B	3045	BCR	8	0
14	B	3003	CLA	4	0
16	F	201	BCR	4	0
16	L	209	BCR	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.

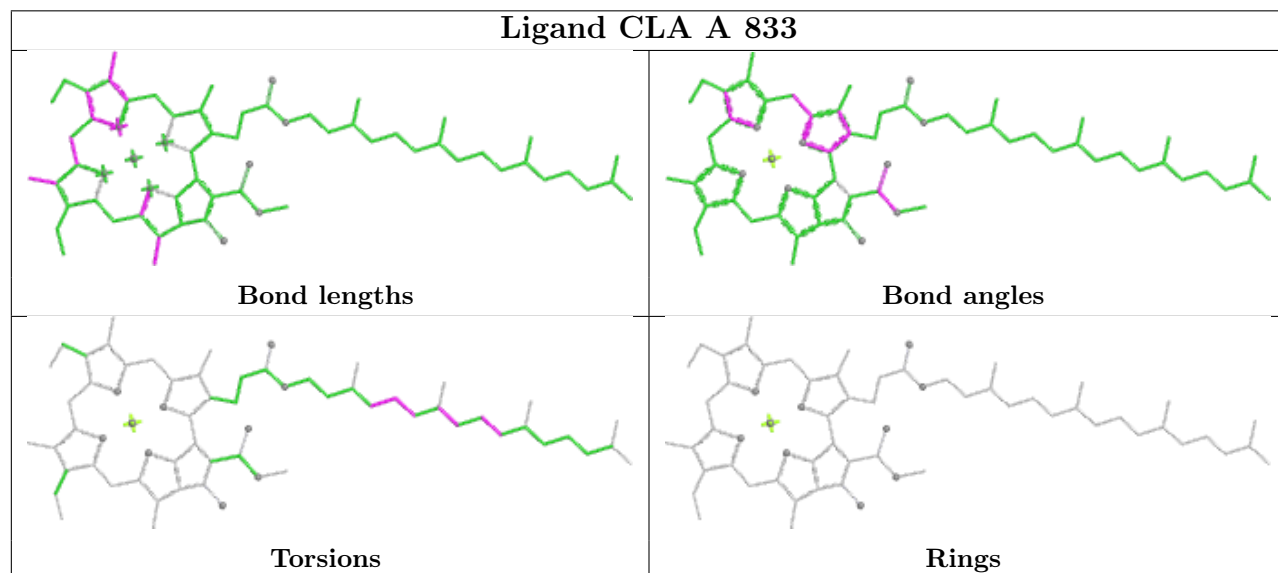
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

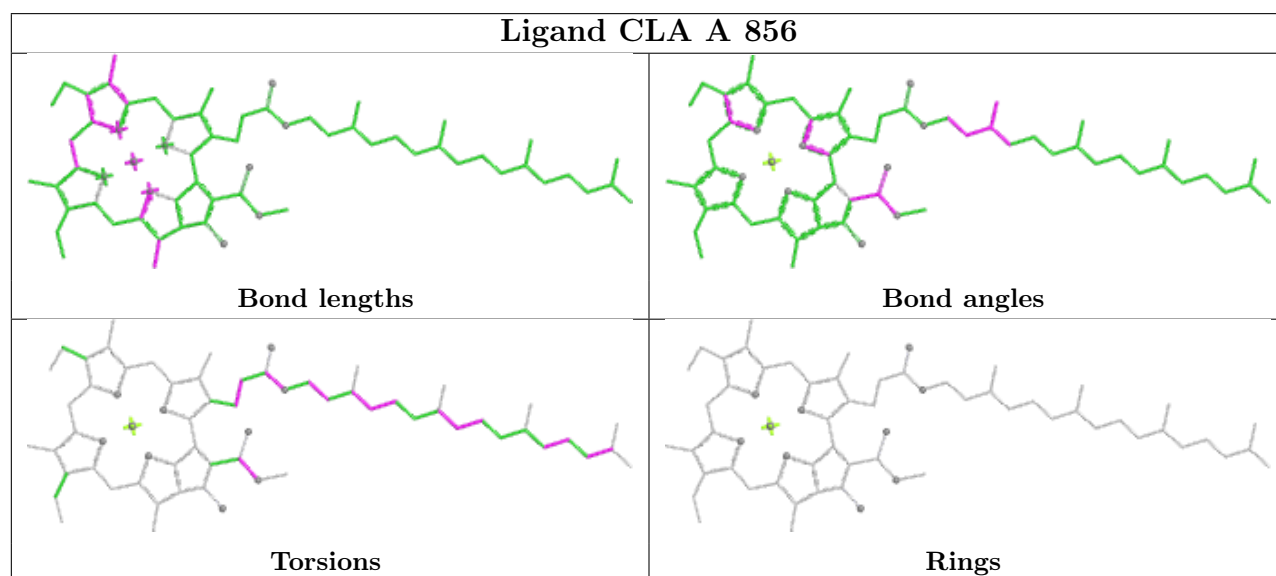
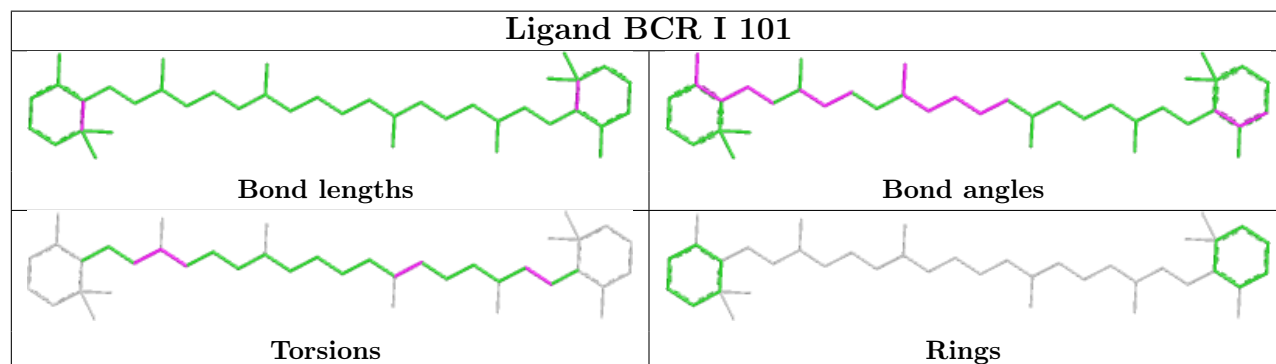
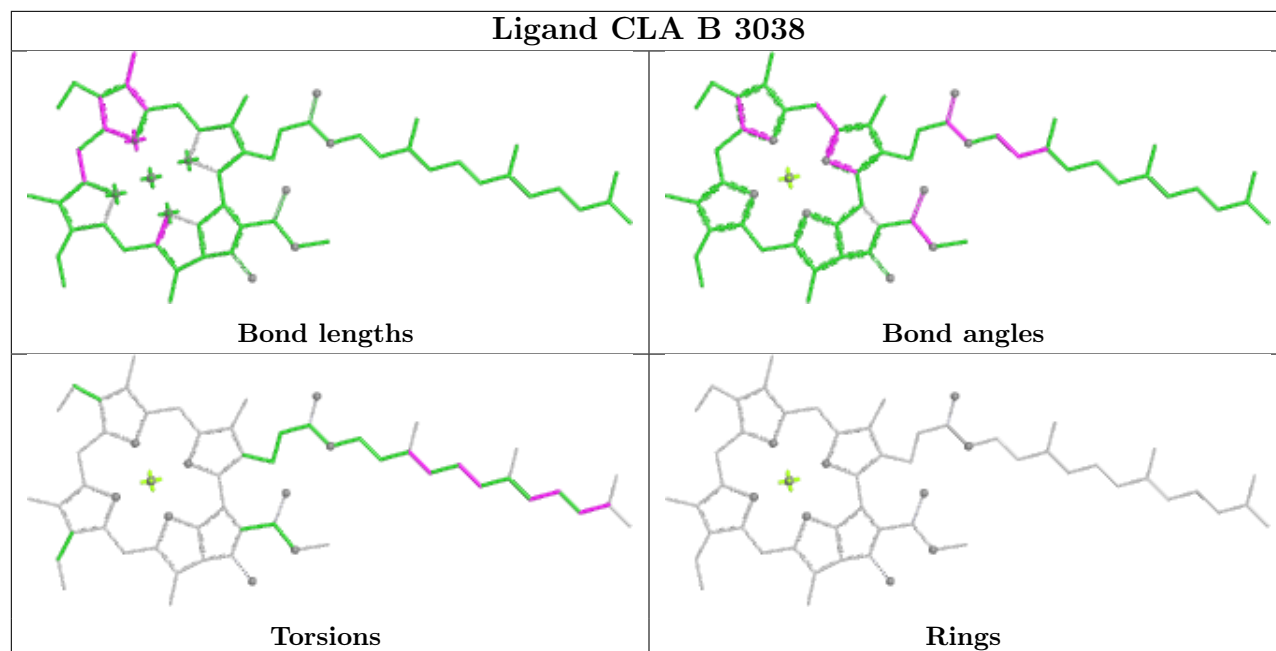


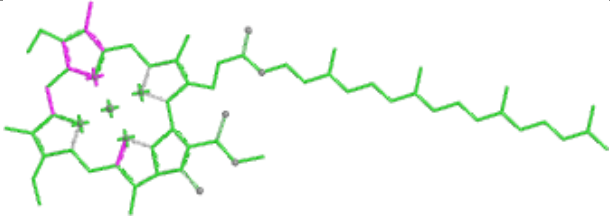
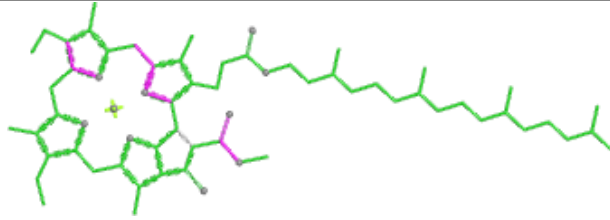
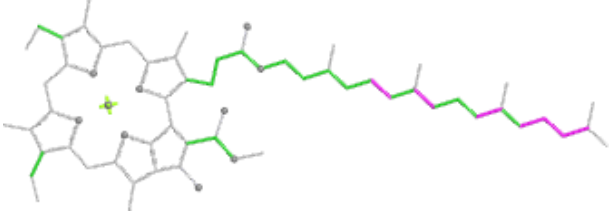
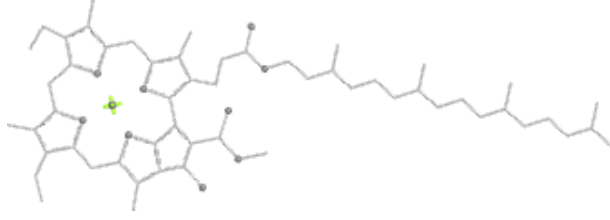
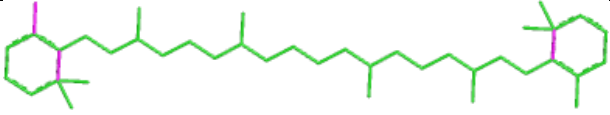
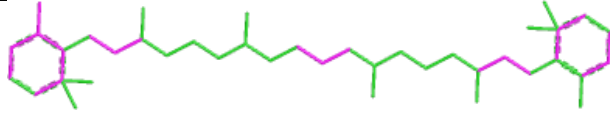
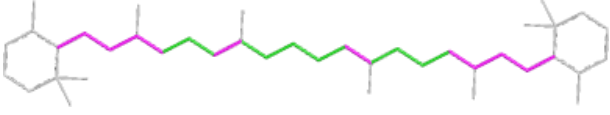
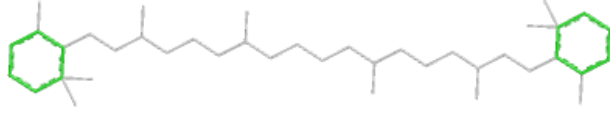
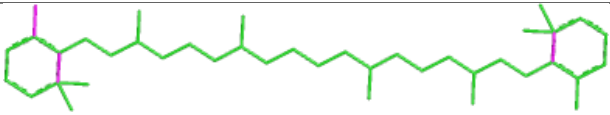
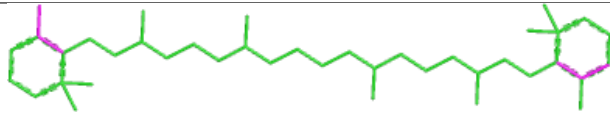
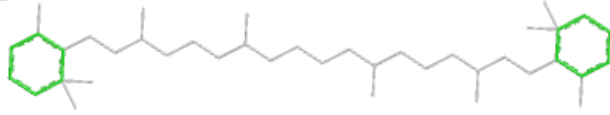
Ligand CLA L 205

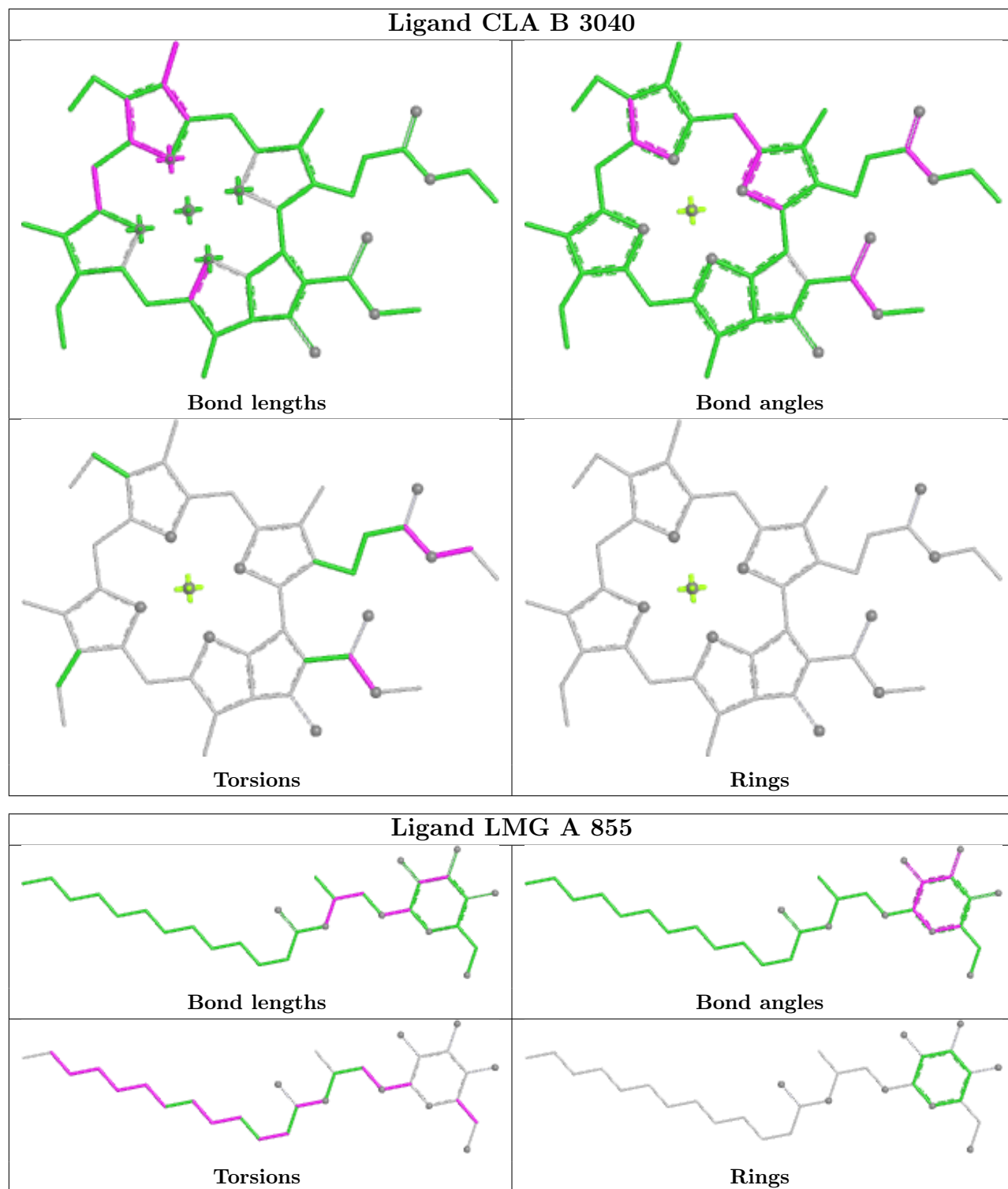


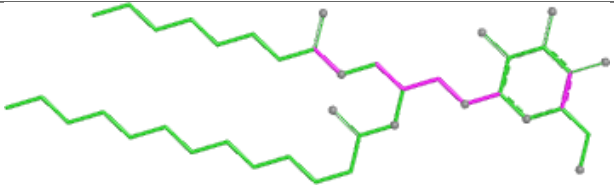
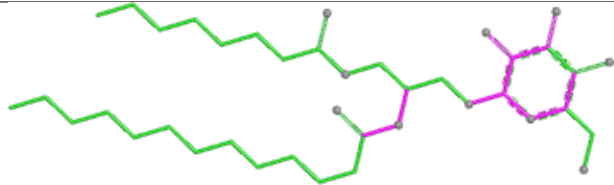
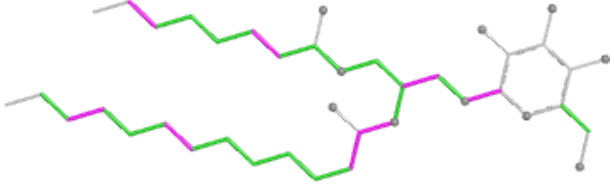
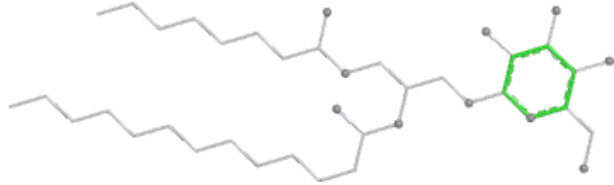
Ligand CLA A 833

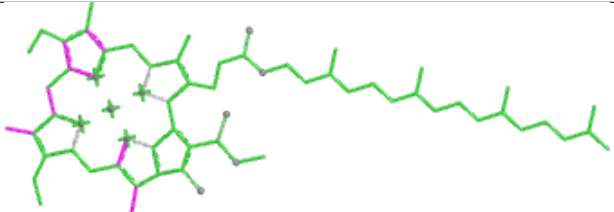
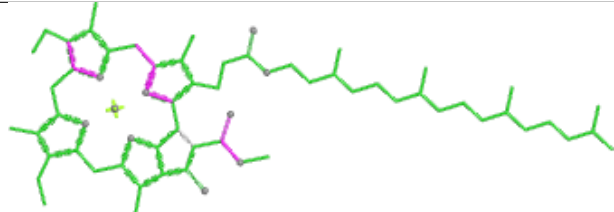
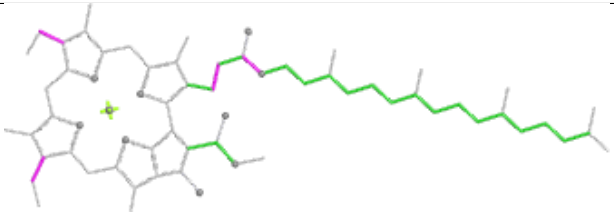
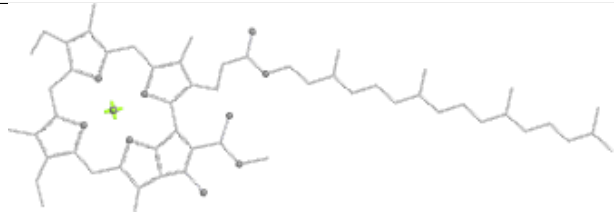


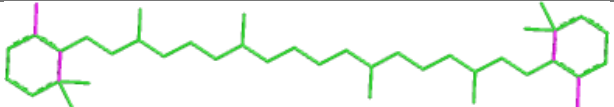
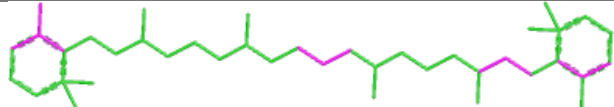
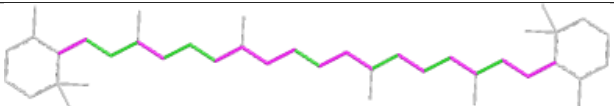
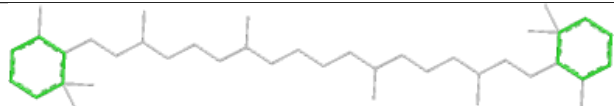


Ligand CLA B 3039	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 851	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR J 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

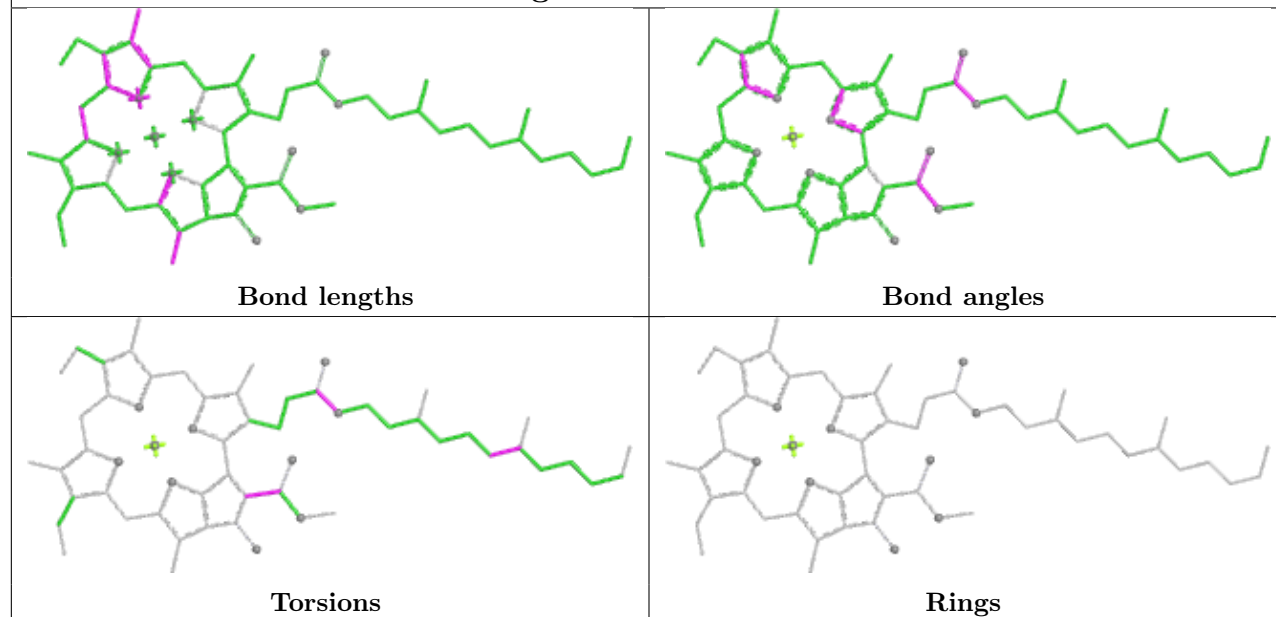


Ligand LMG I 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

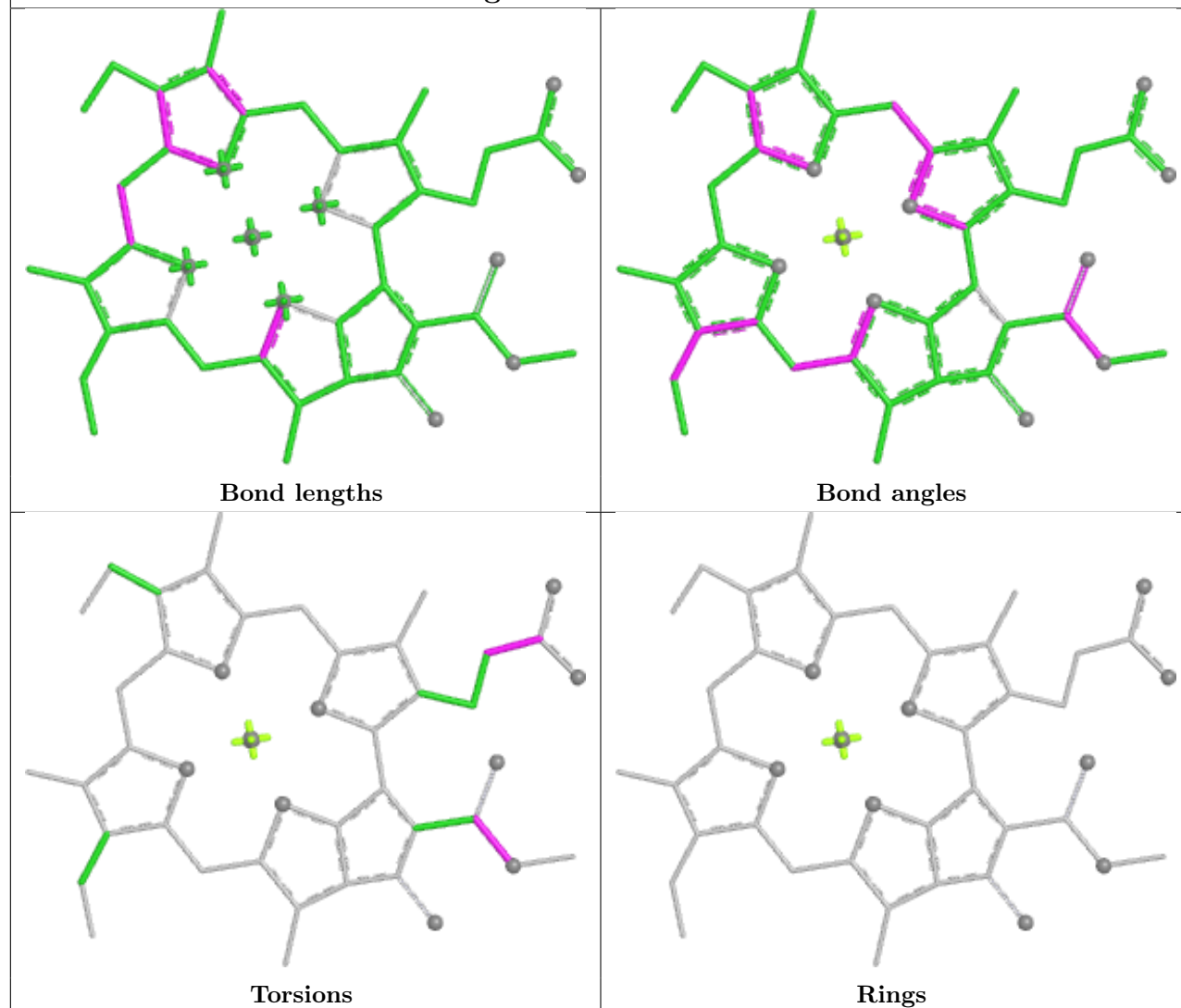
Ligand CLA B 3008	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

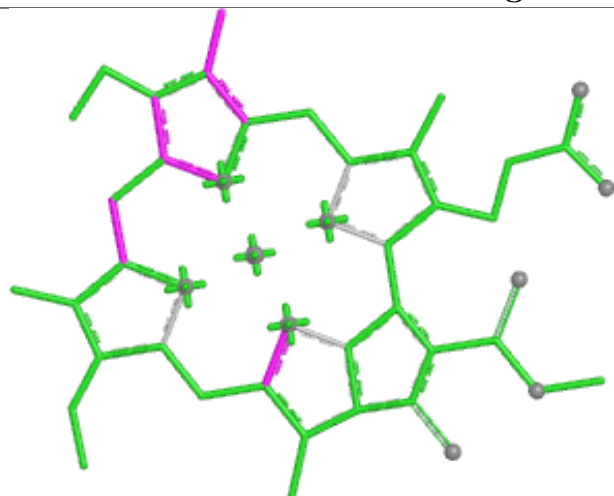
Ligand CLA A 805



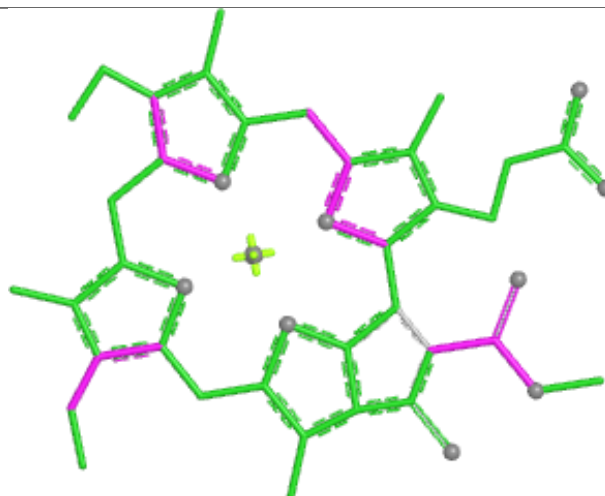
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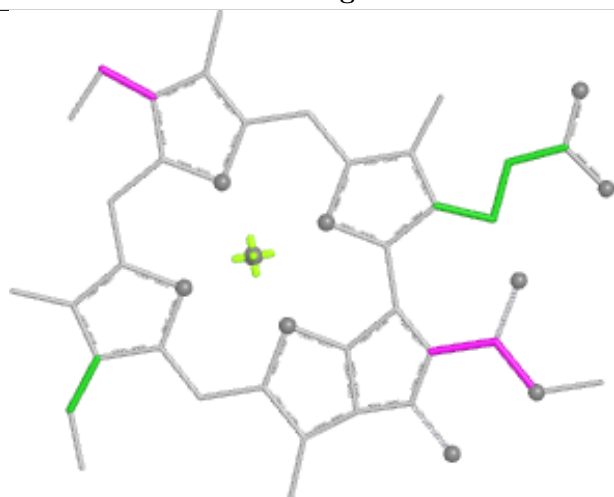
Ligand CLA B 3035



Bond lengths



Bond angles

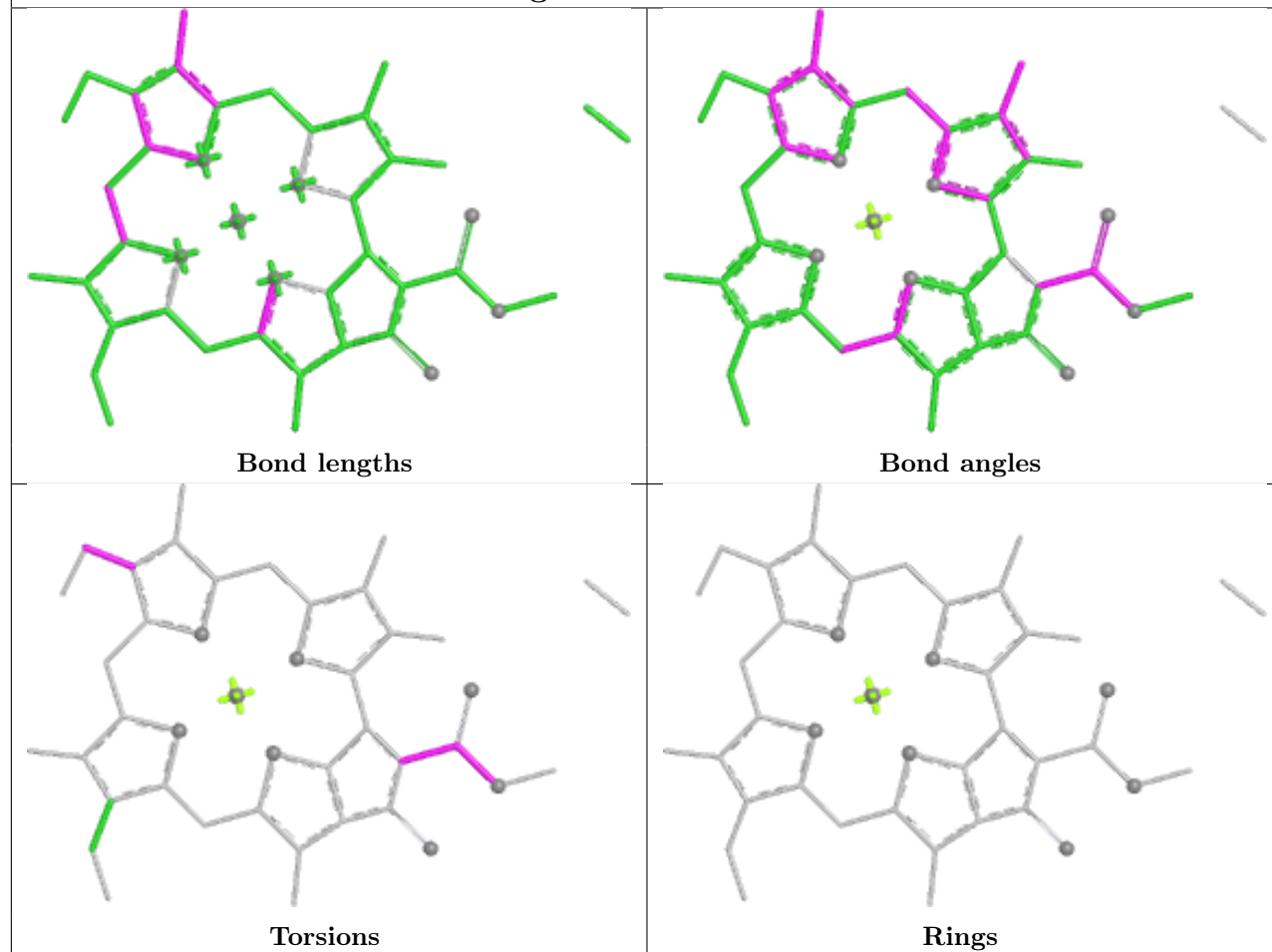


Torsions

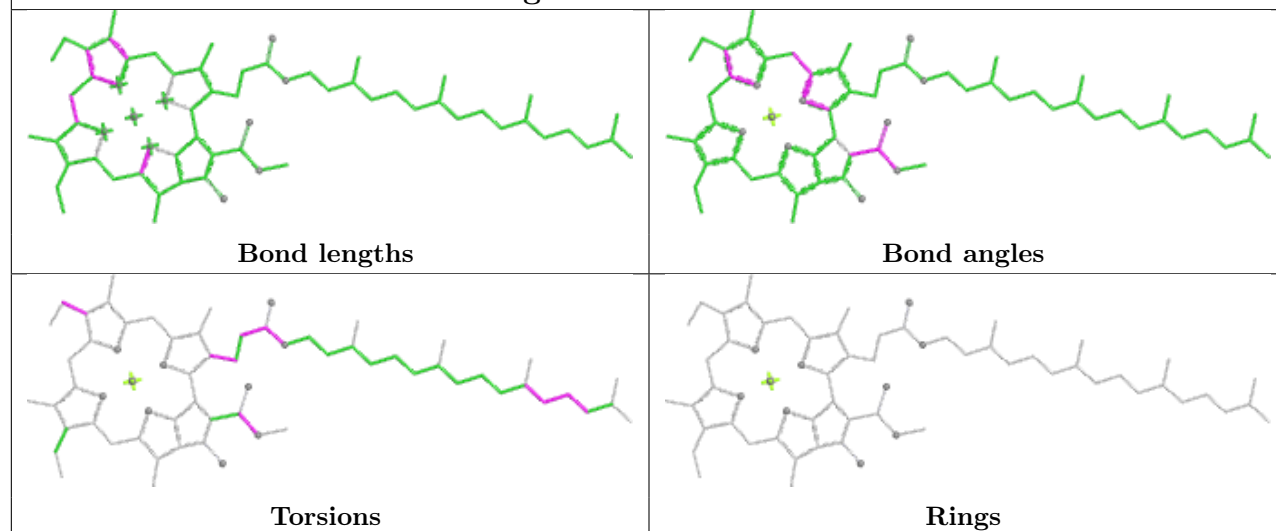


Rings

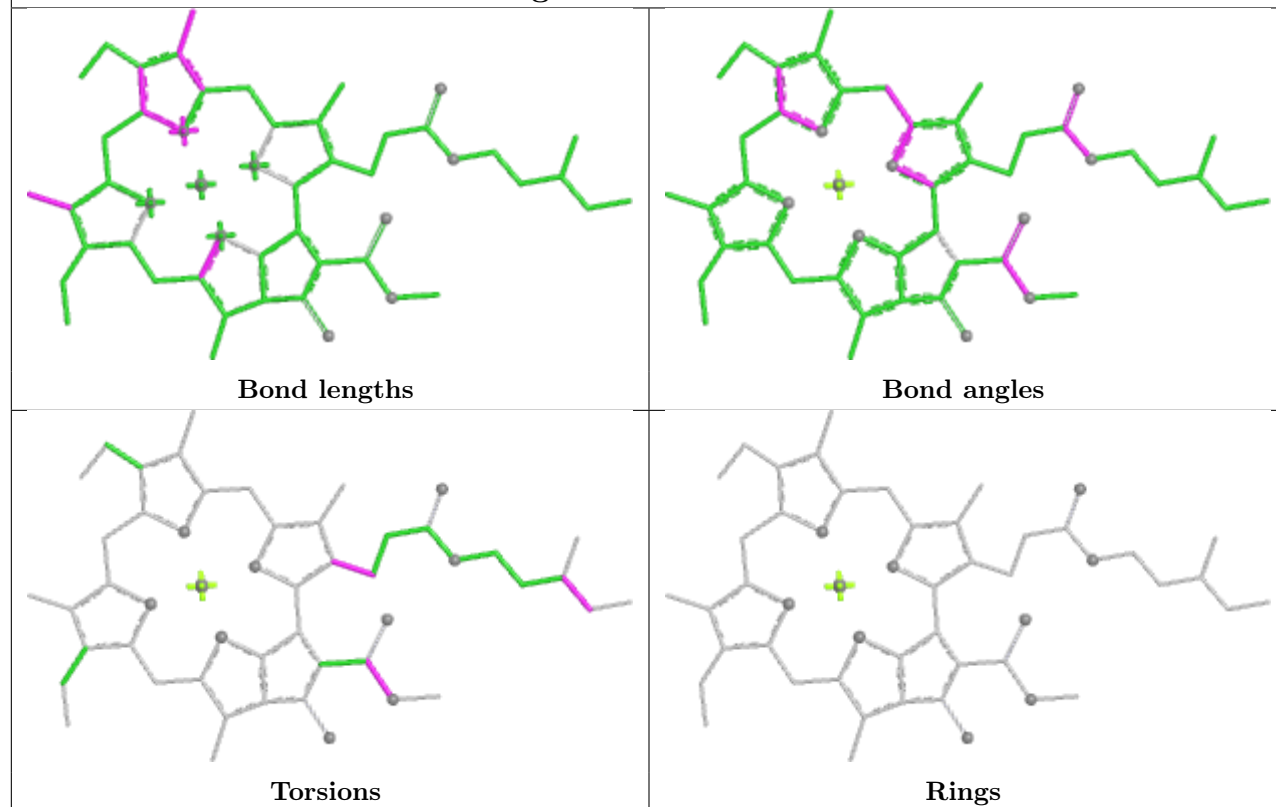
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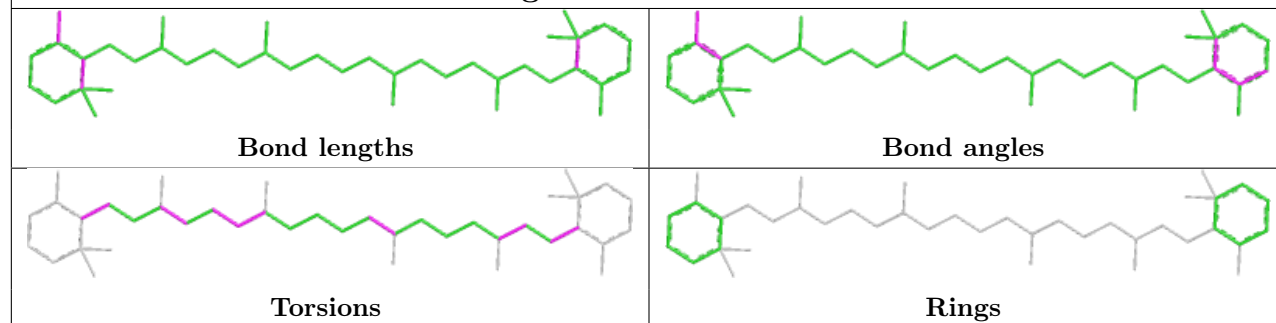
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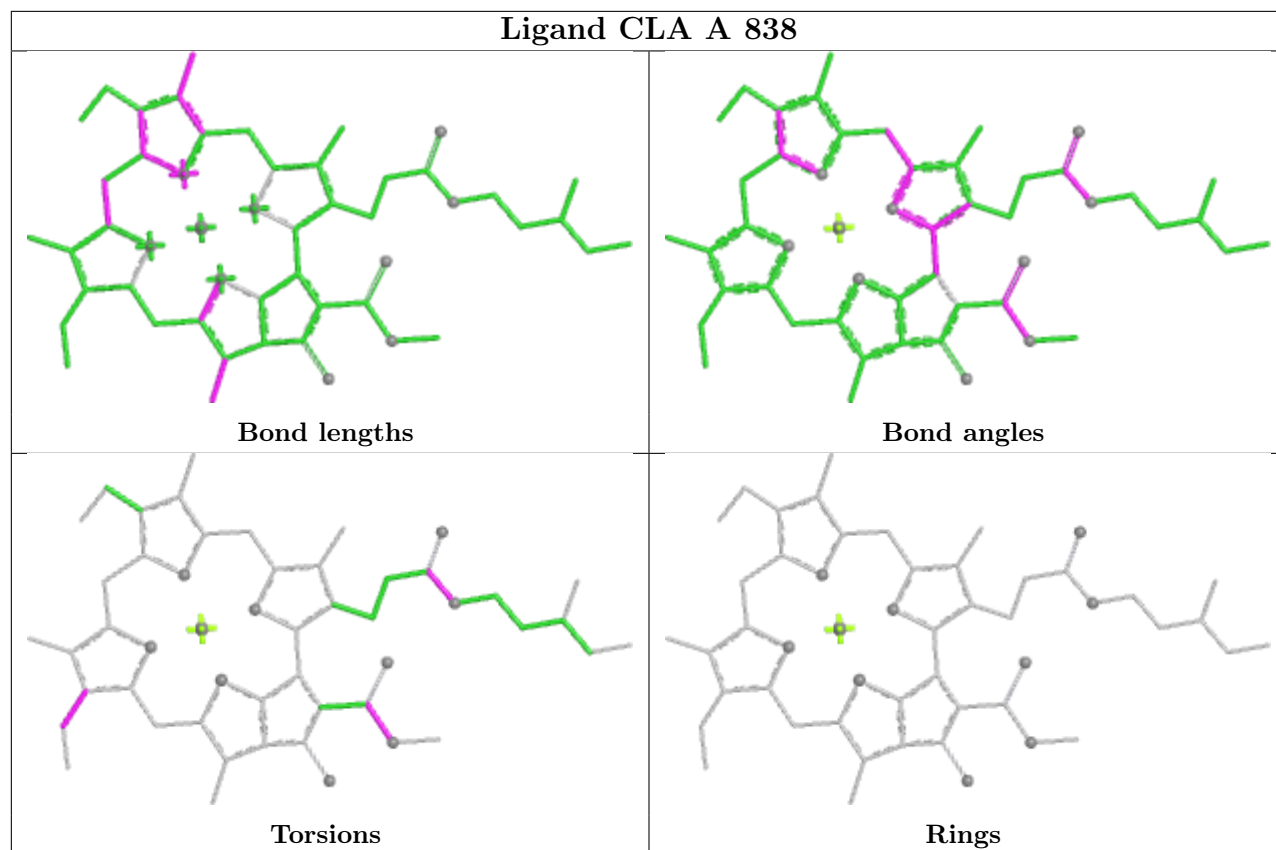
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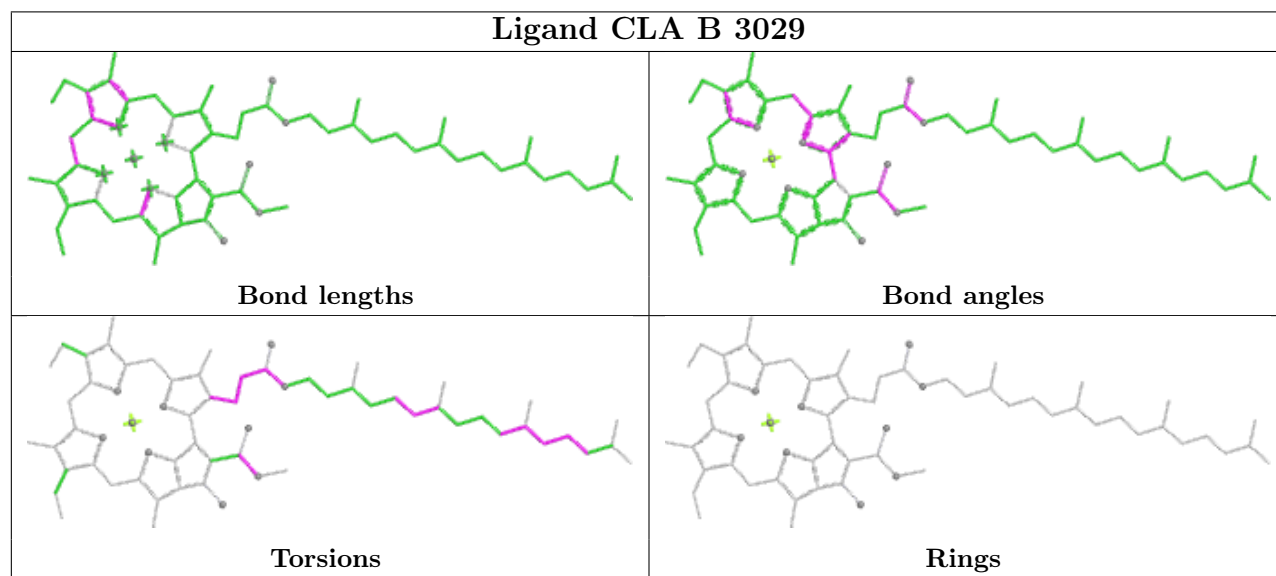
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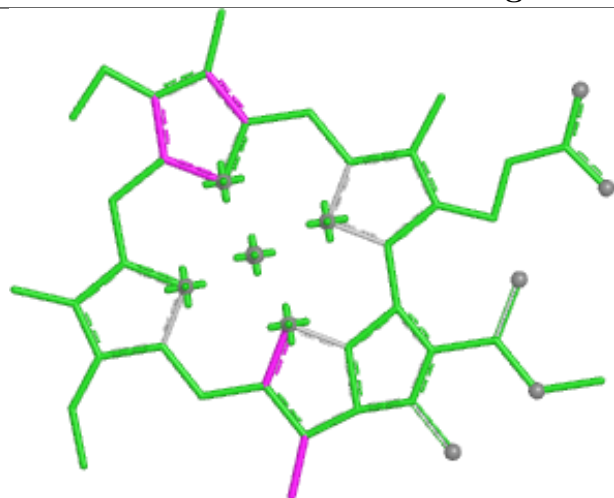
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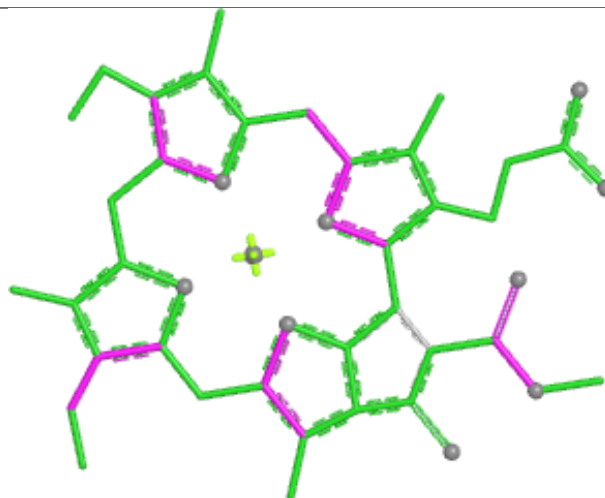
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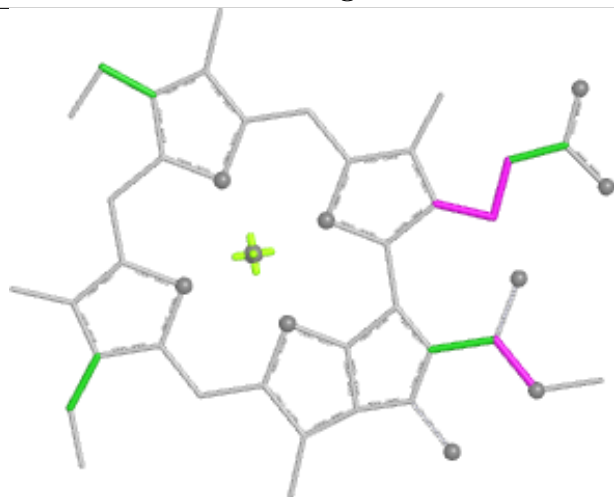
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Bond lengths



Bond angles

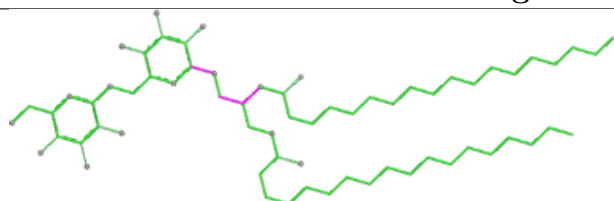


Torsions

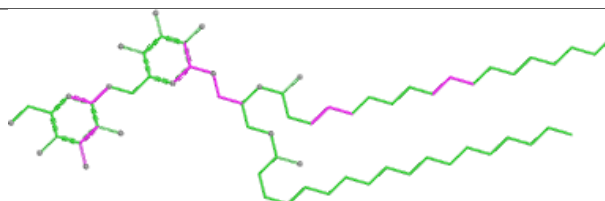


Rings

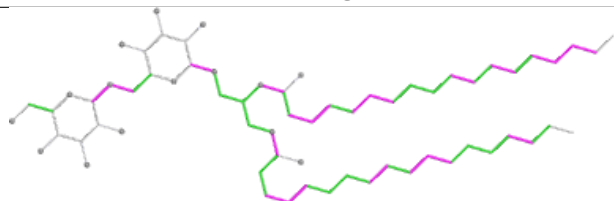
Ligand DGD L 207



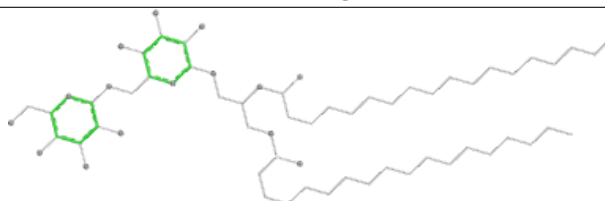
Bond lengths



Bond angles

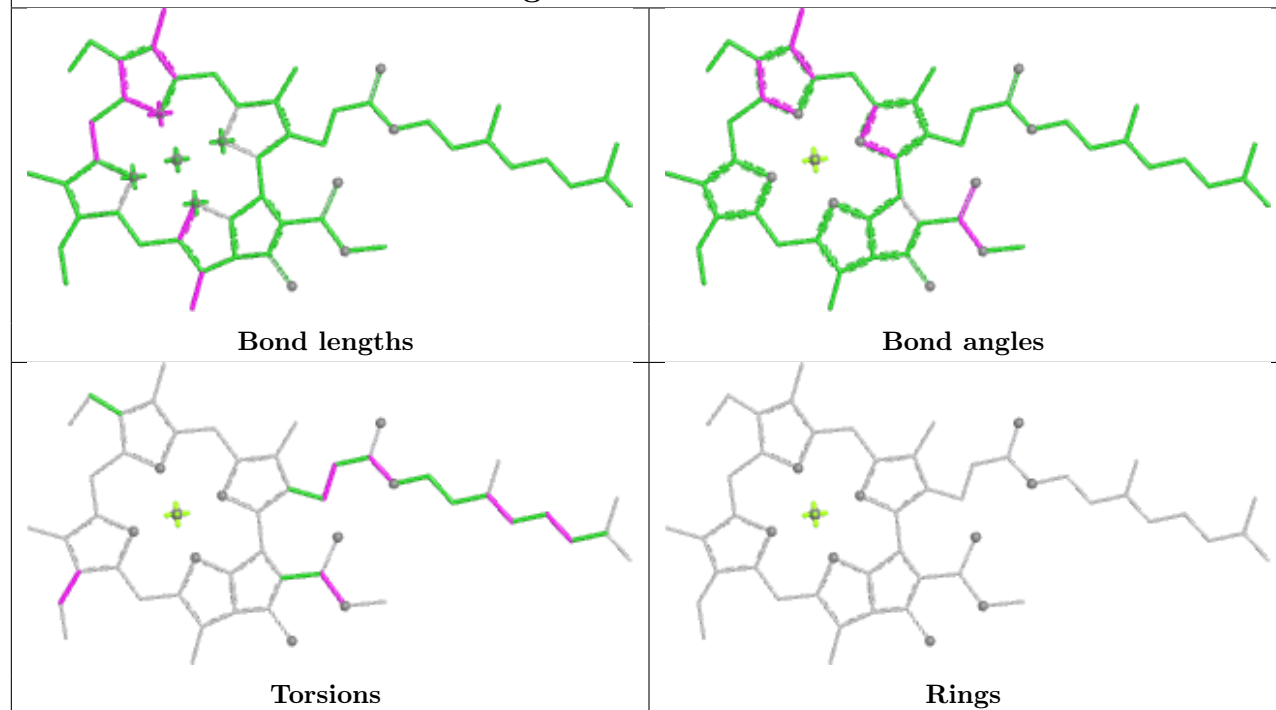


Torsions

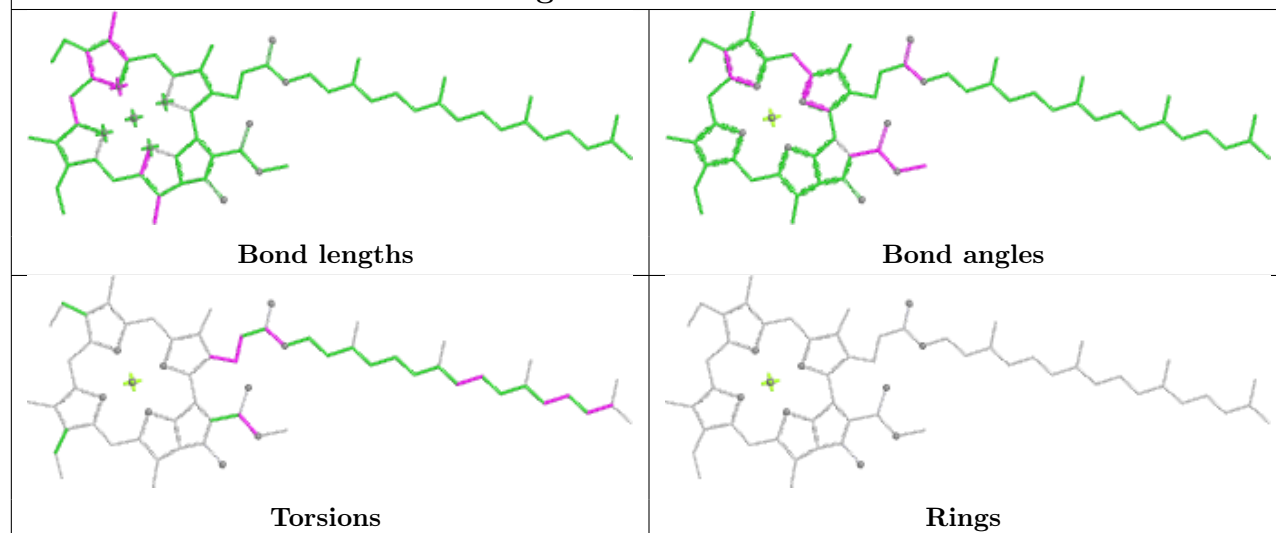


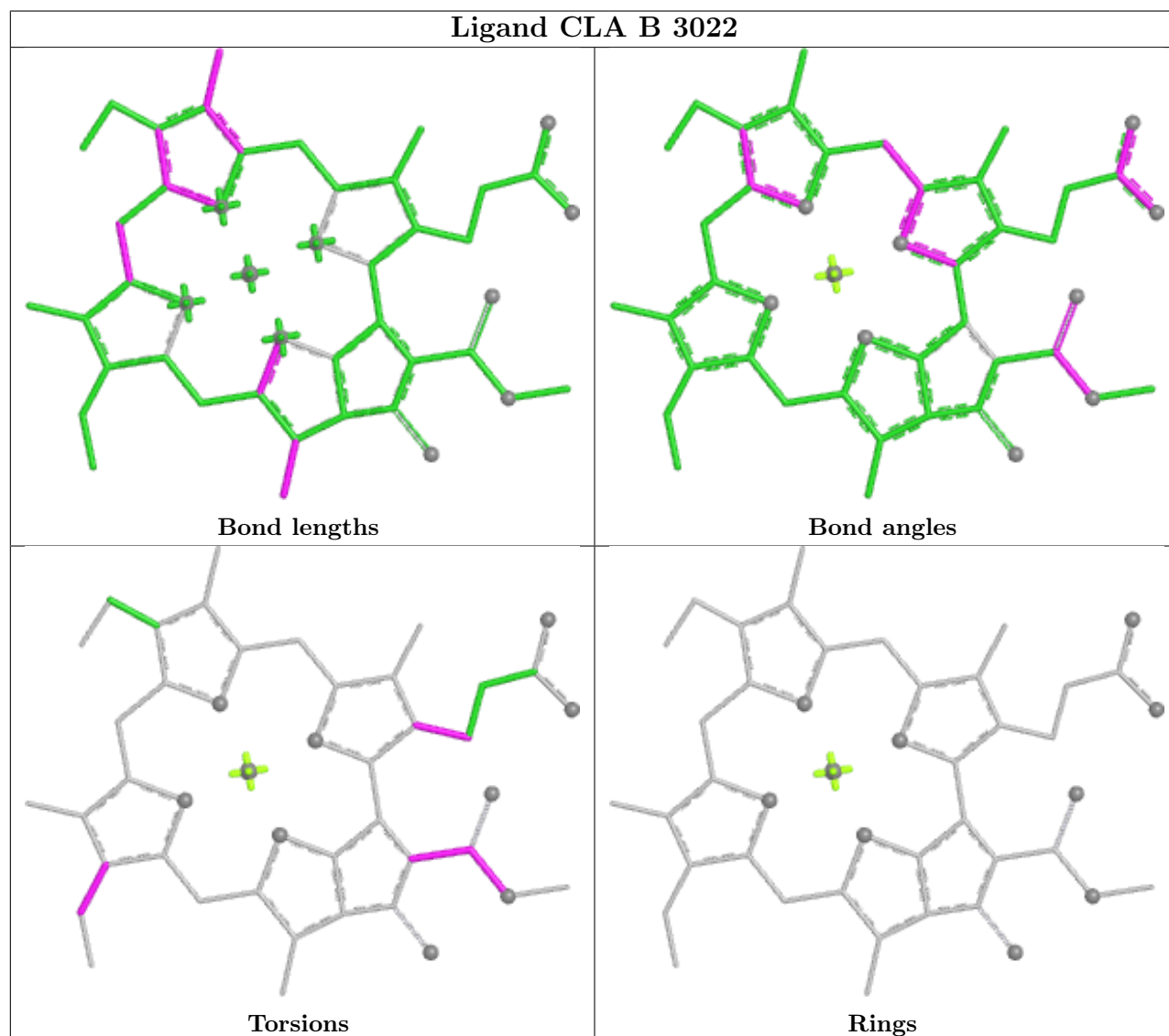
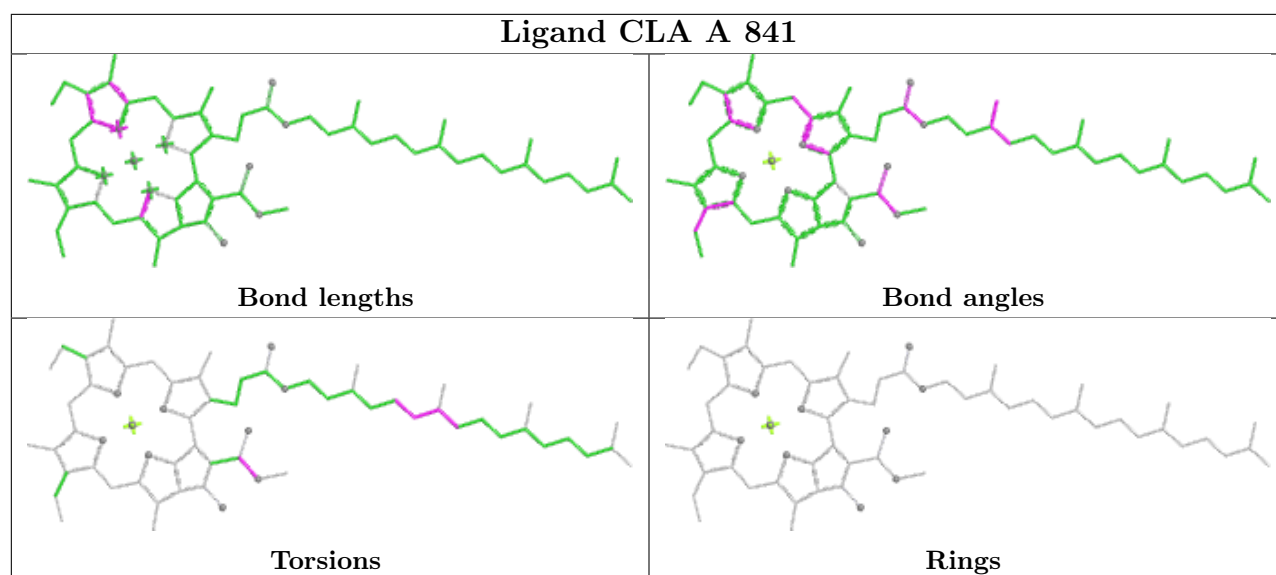
Rings

Ligand CLA B 3023

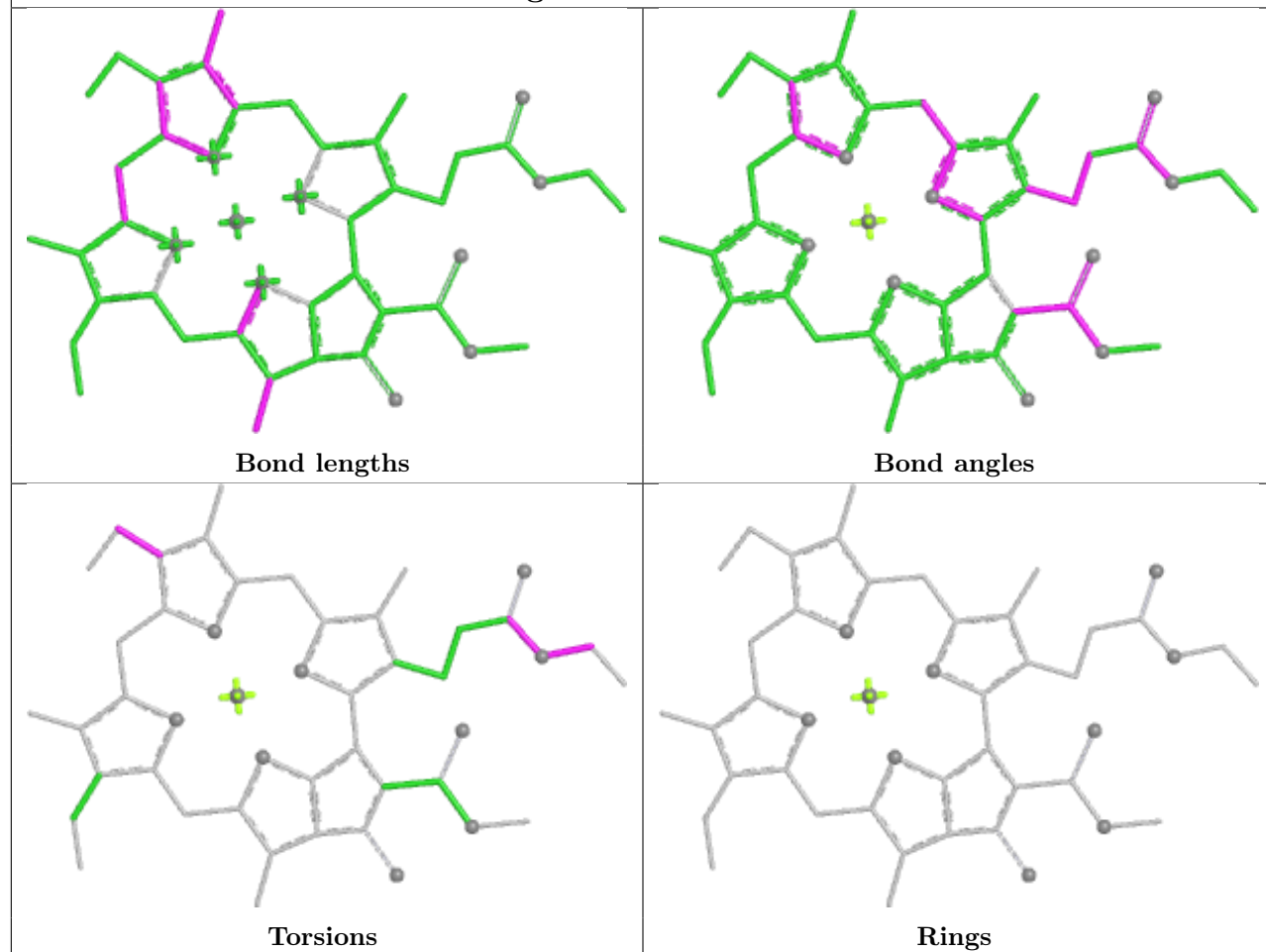


Ligand CL0 A 801

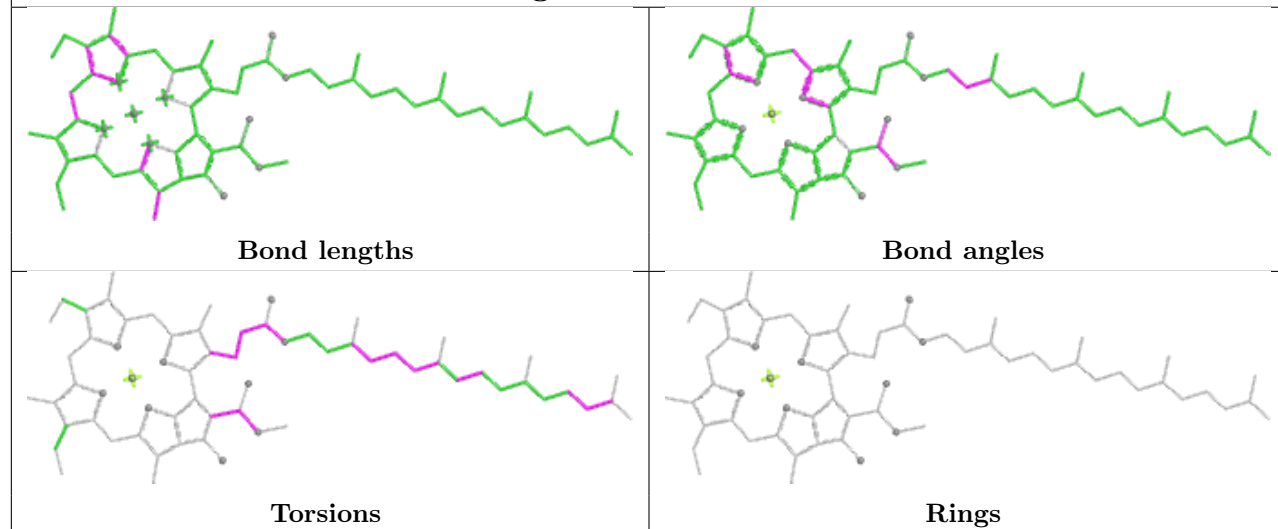


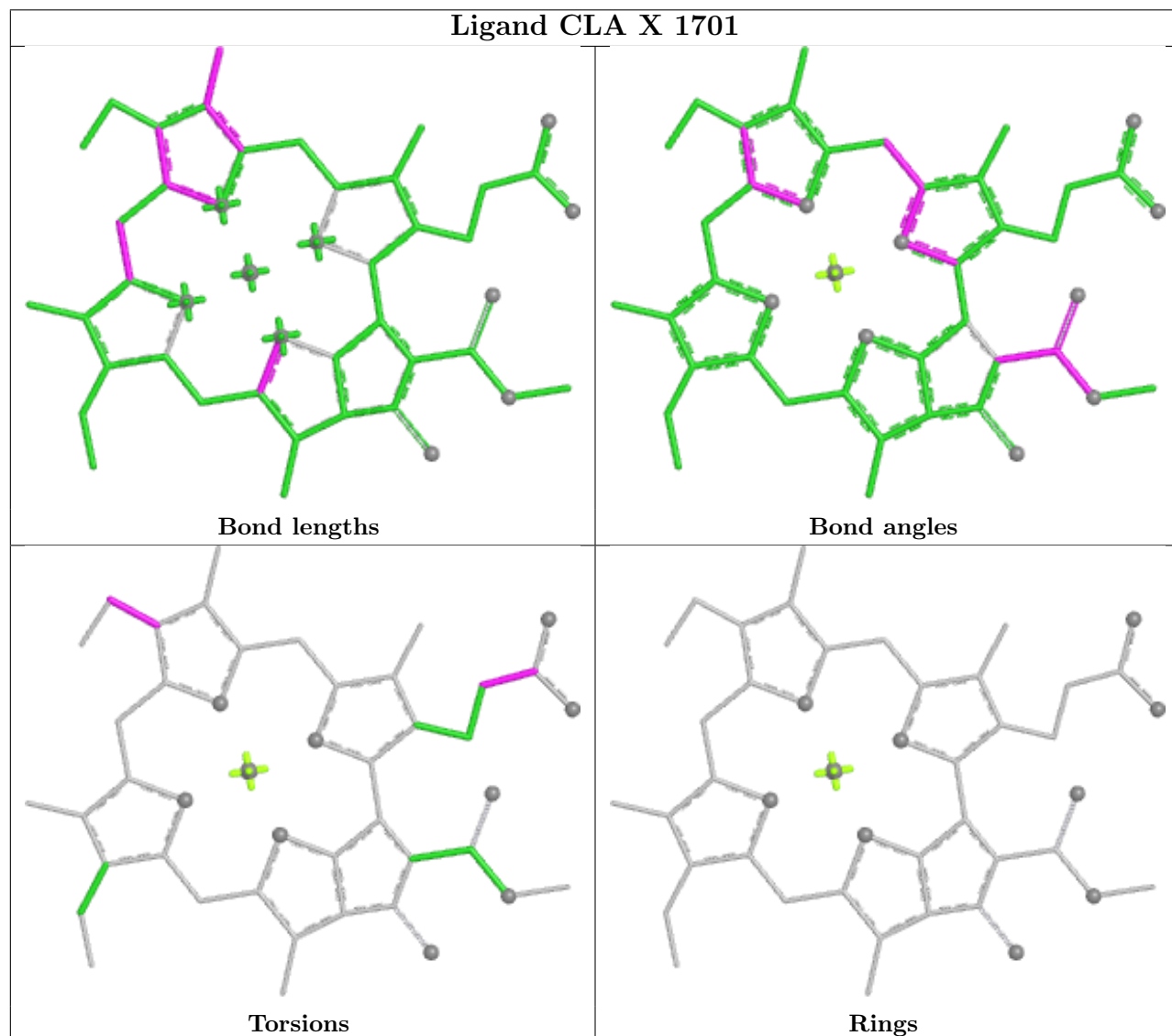
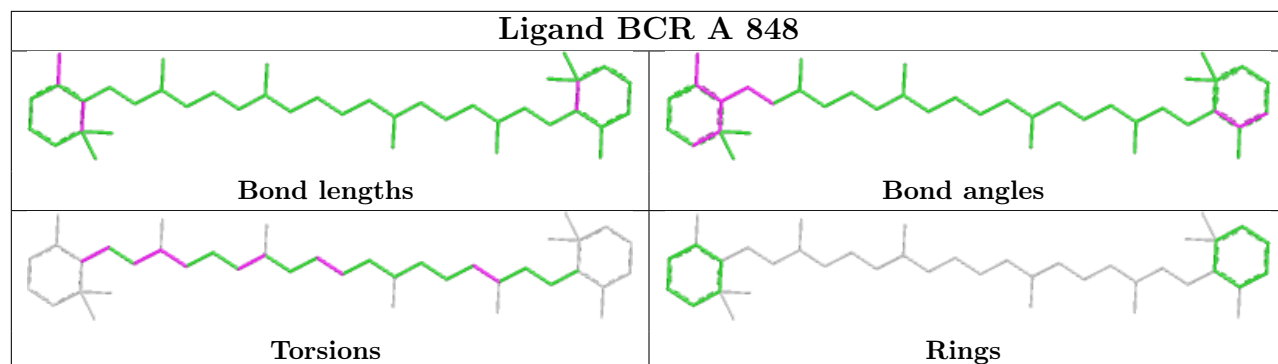


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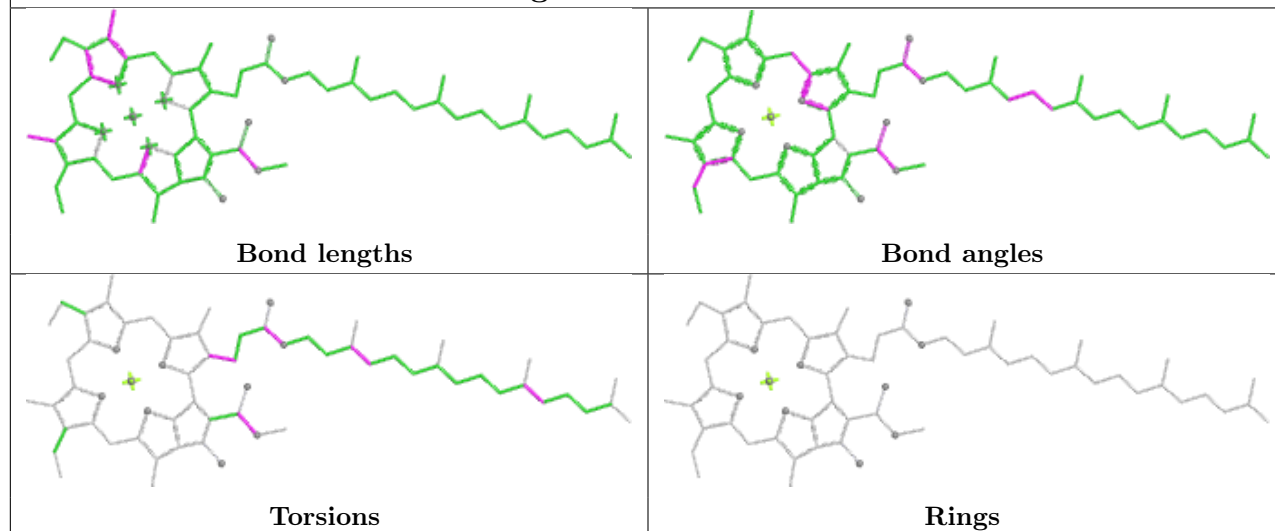


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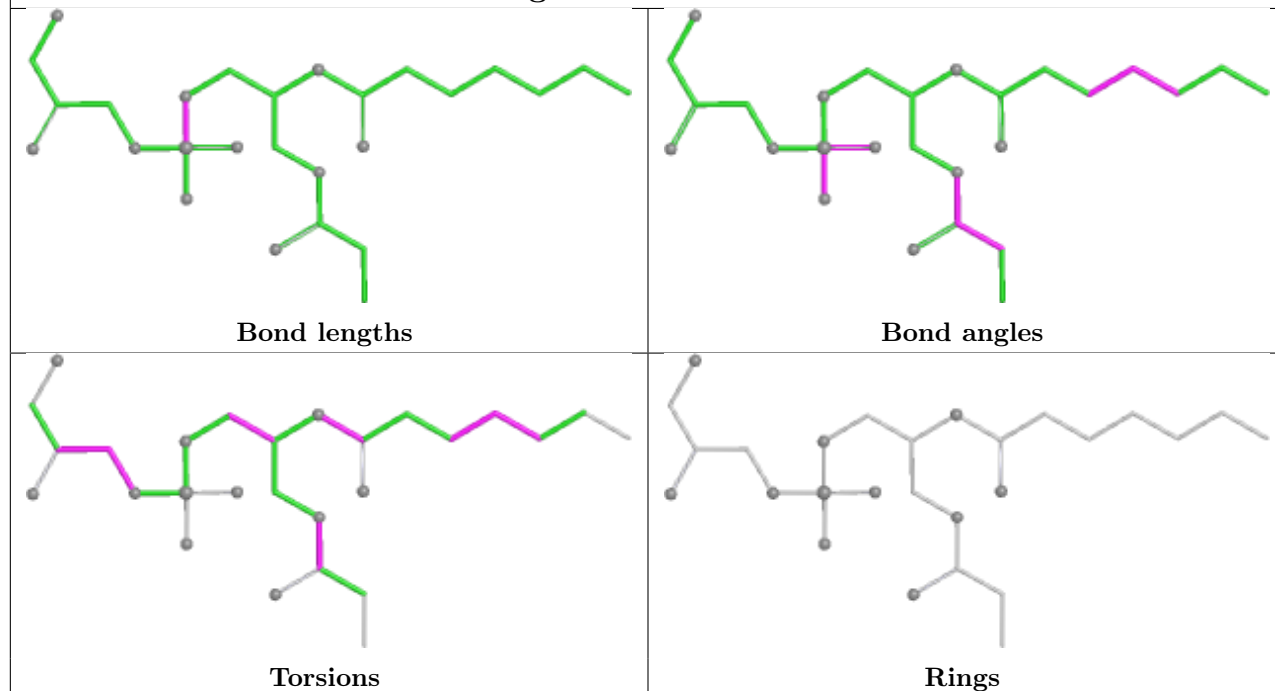




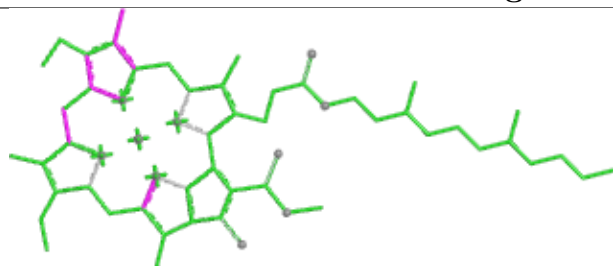
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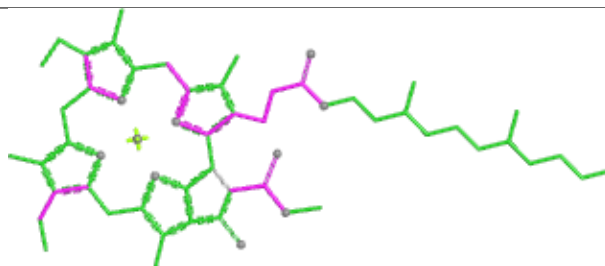
Ligand LHG A 854



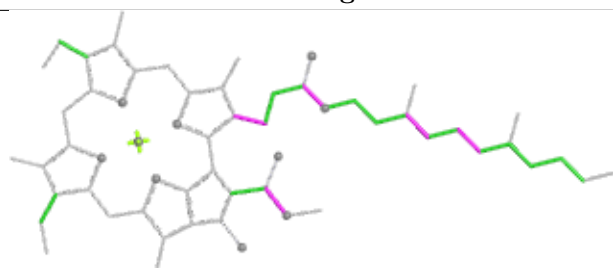
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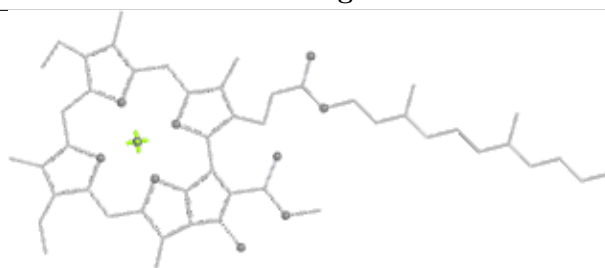
Bond lengths



Bond angles

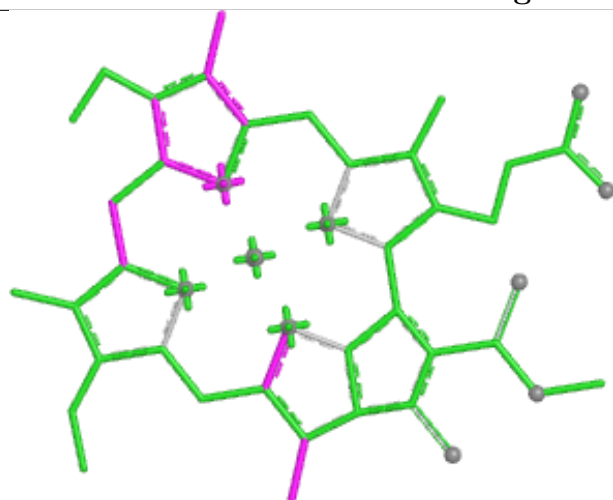


Torsions

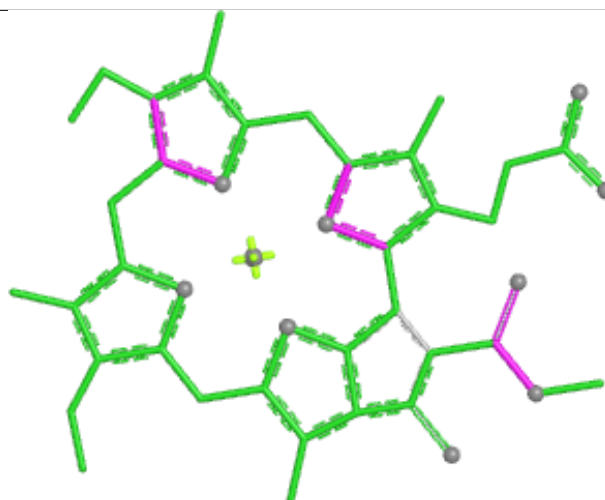


Rings

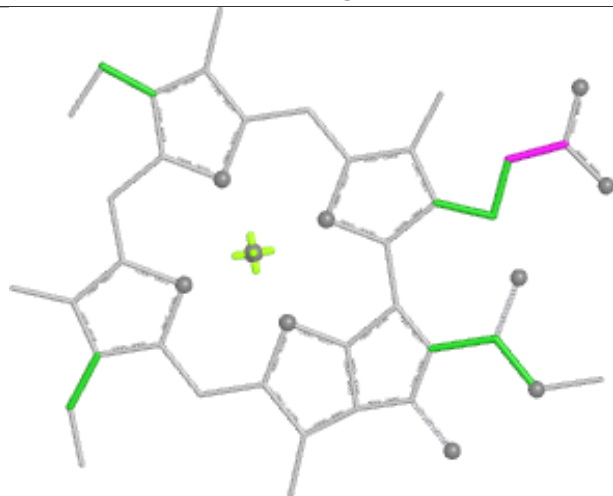
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Bond lengths



Bond angles

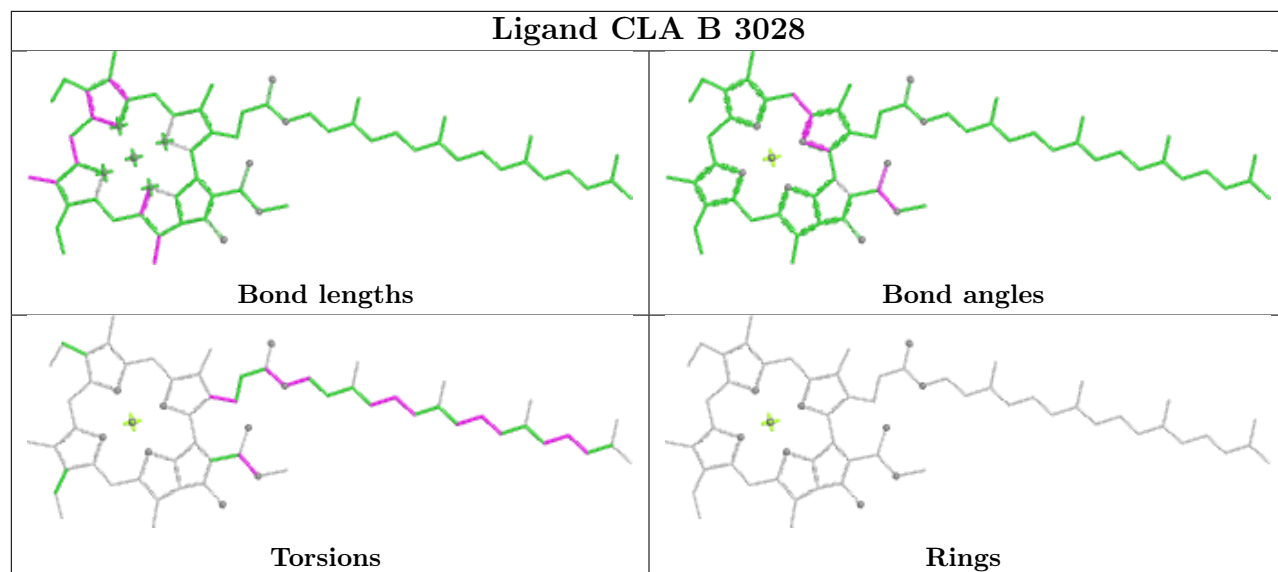


Torsions

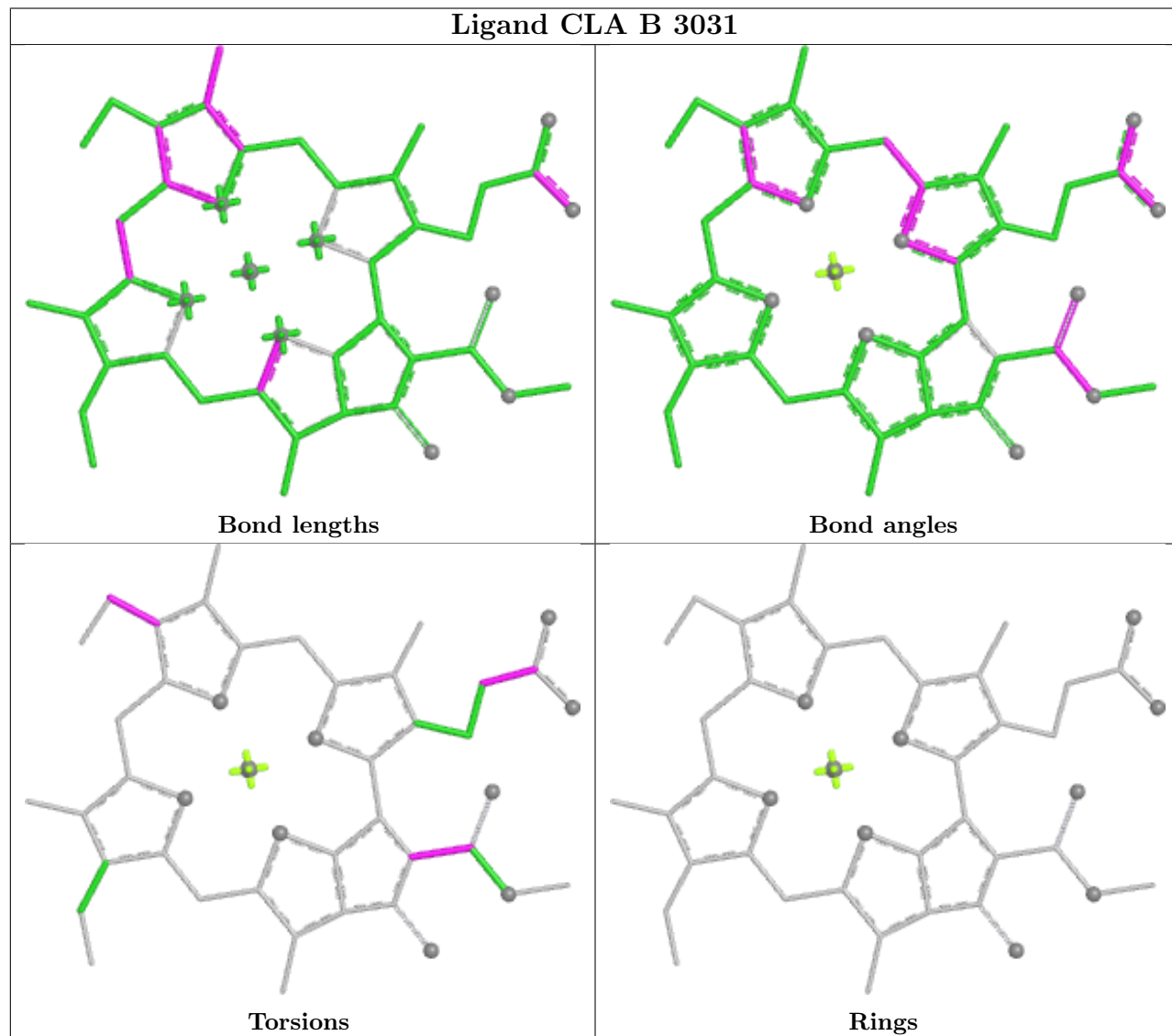


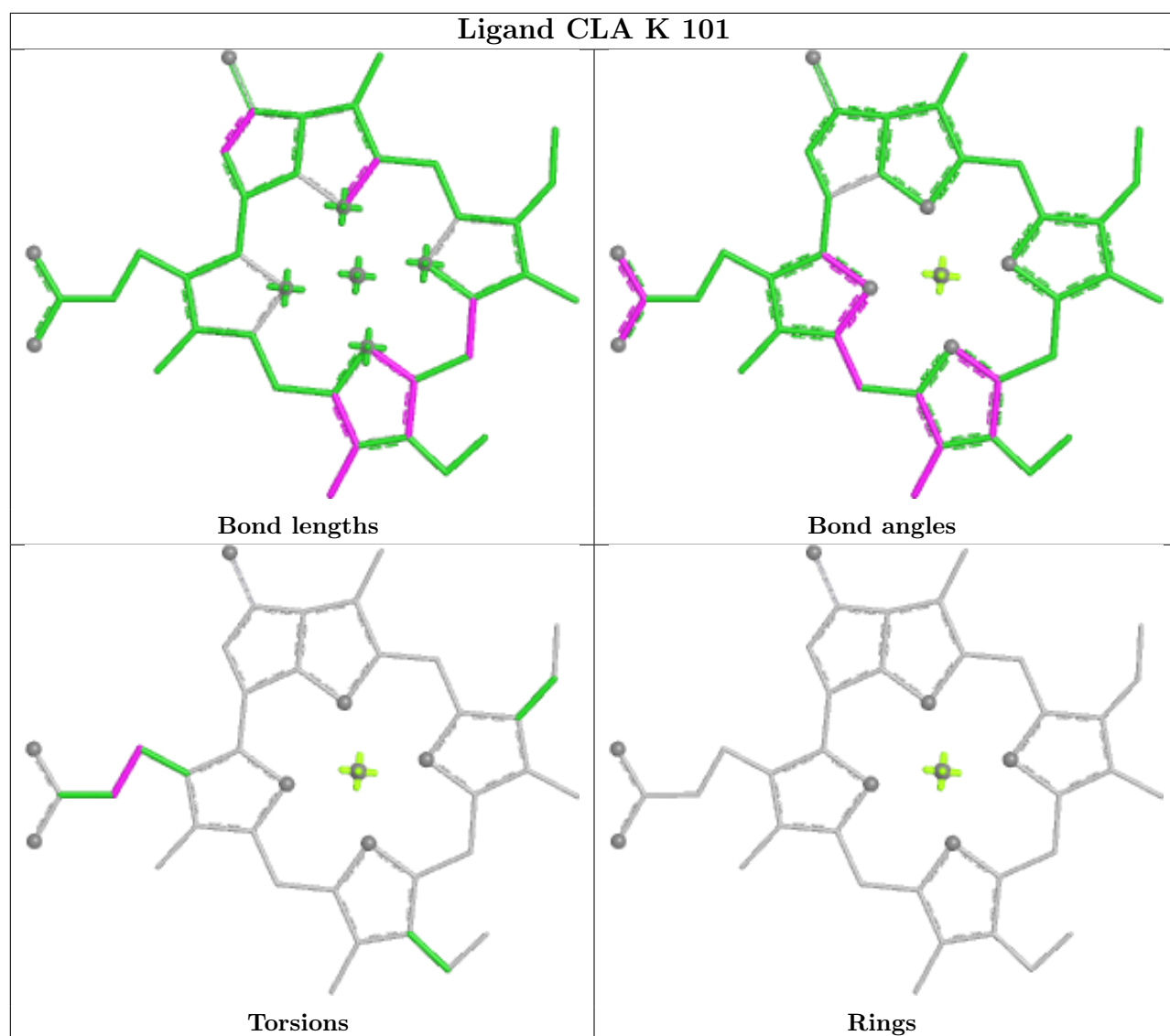
Rings

Ligand CLA B 3028

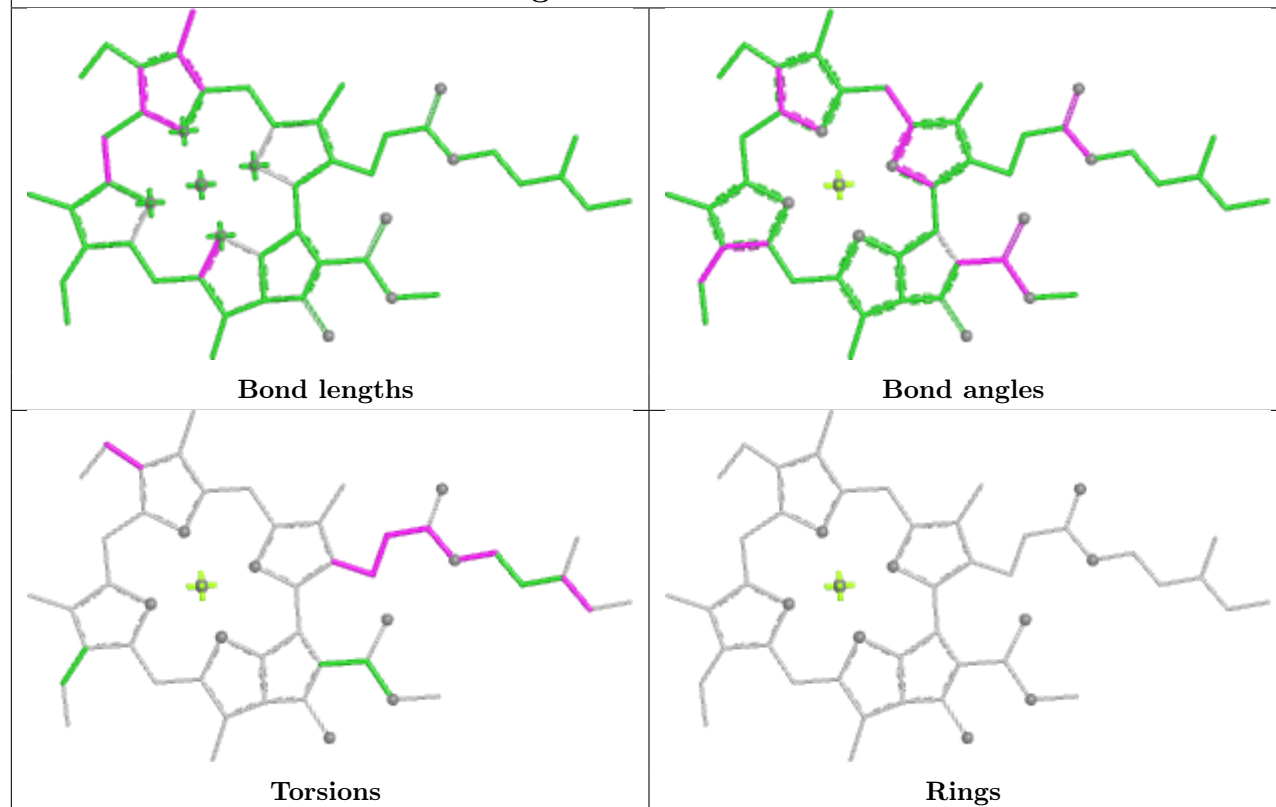


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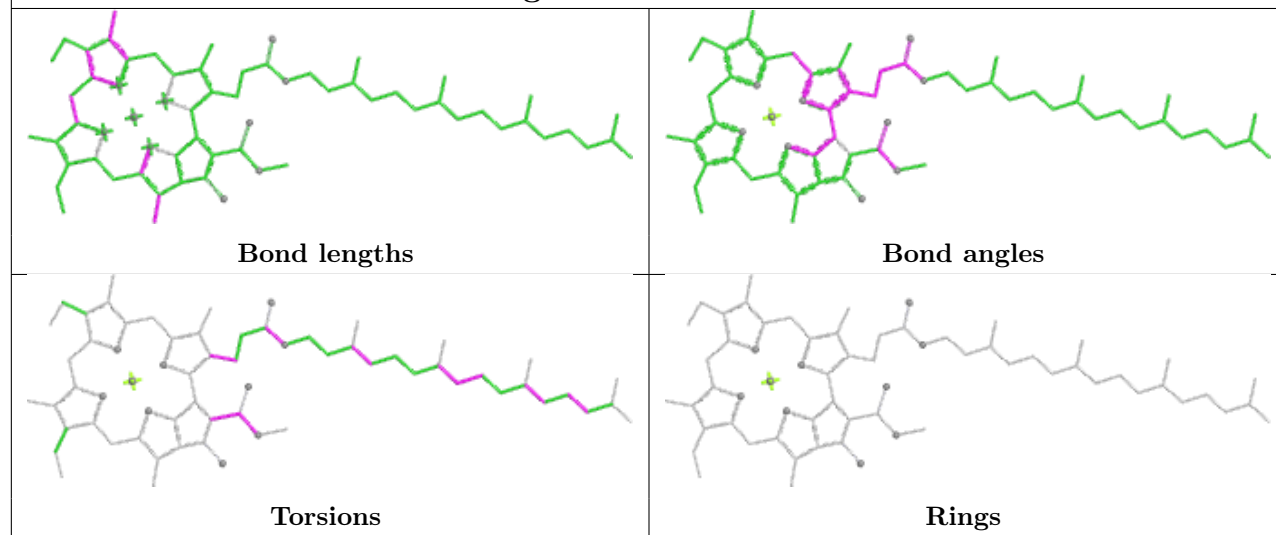


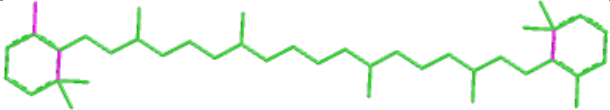
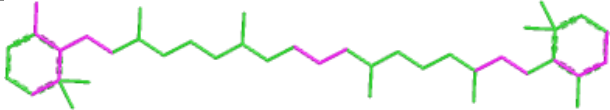
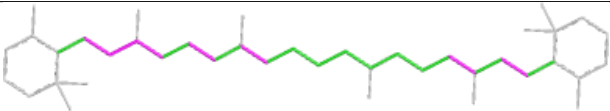
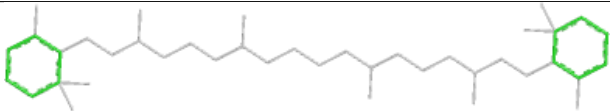
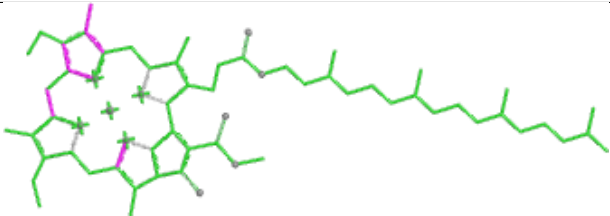
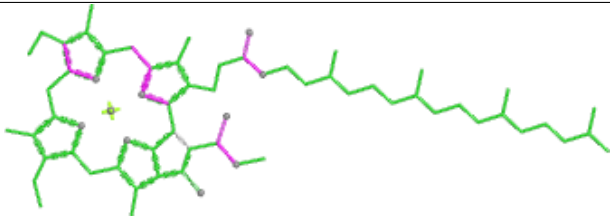
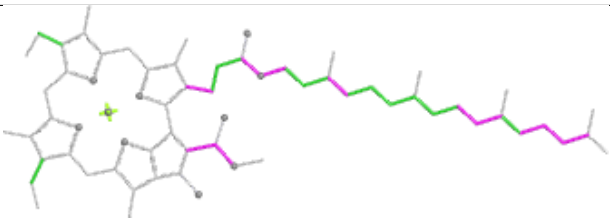
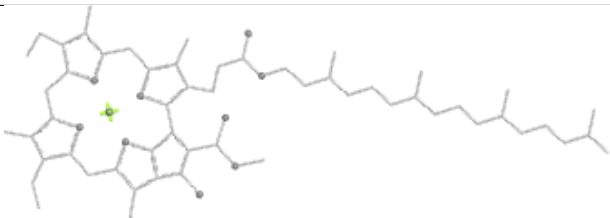
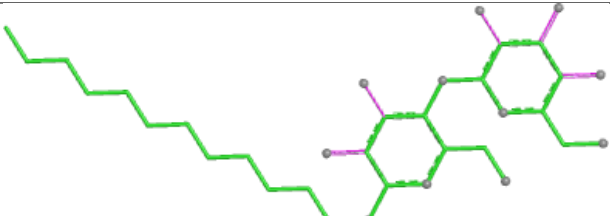
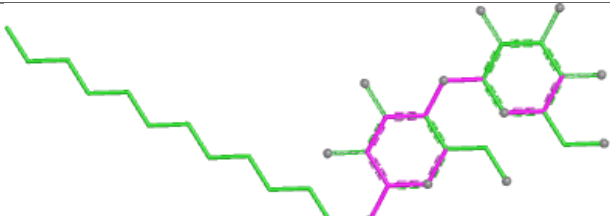
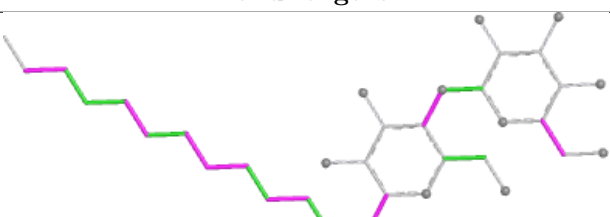
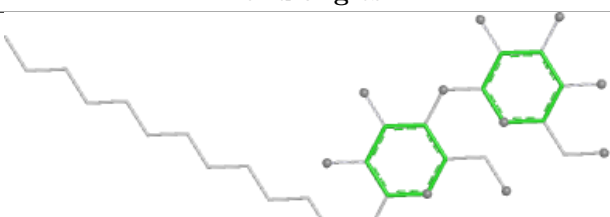


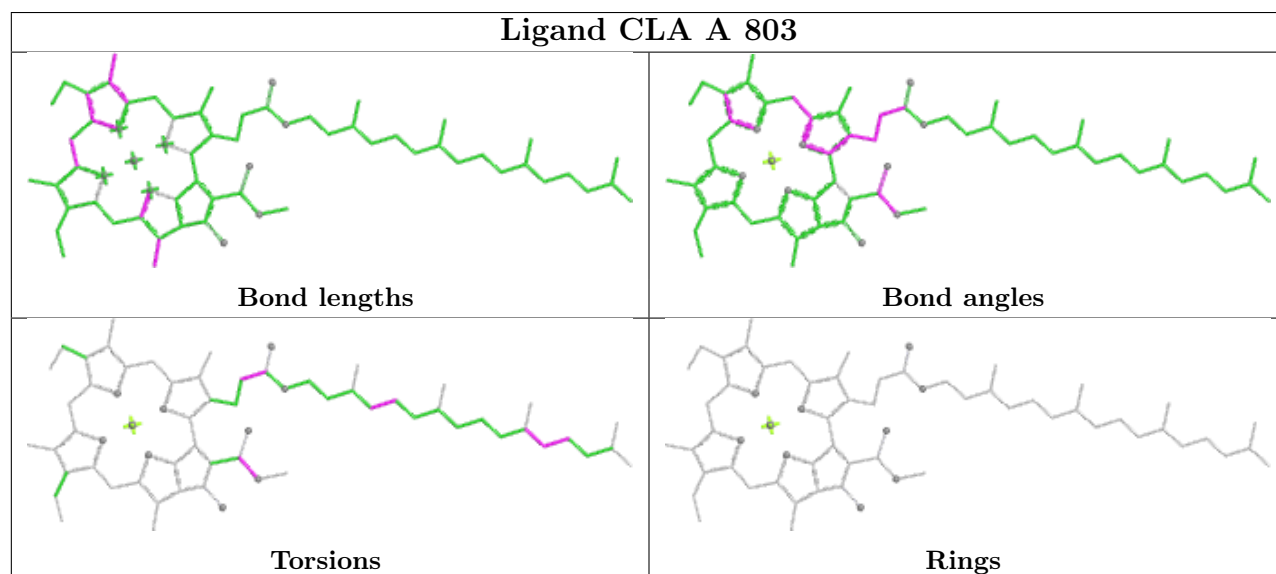
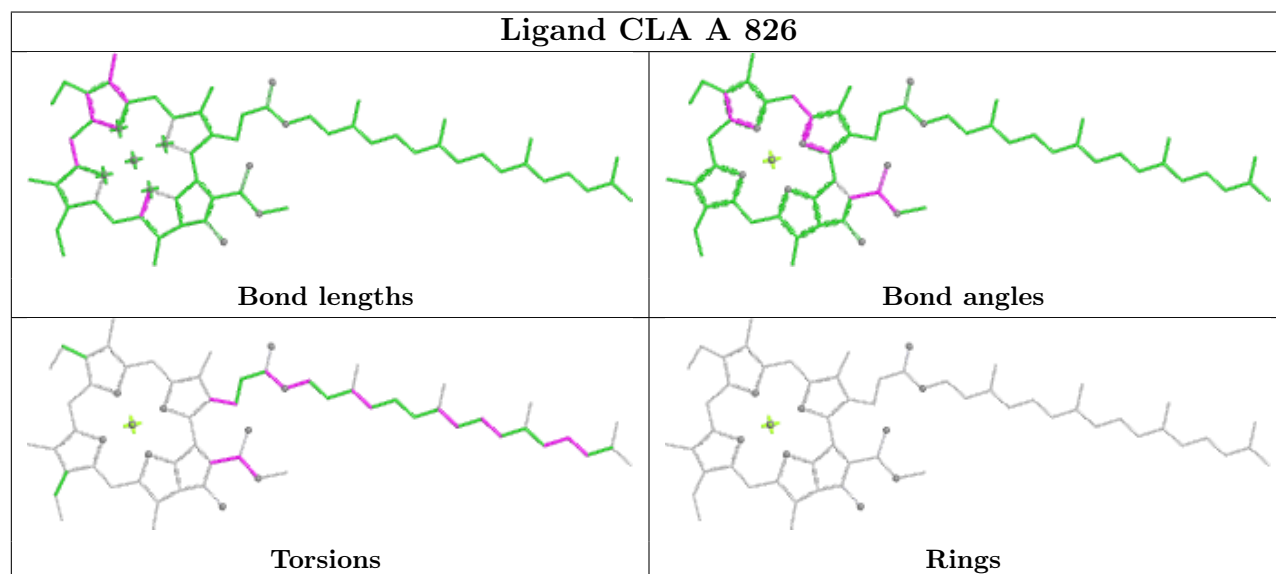
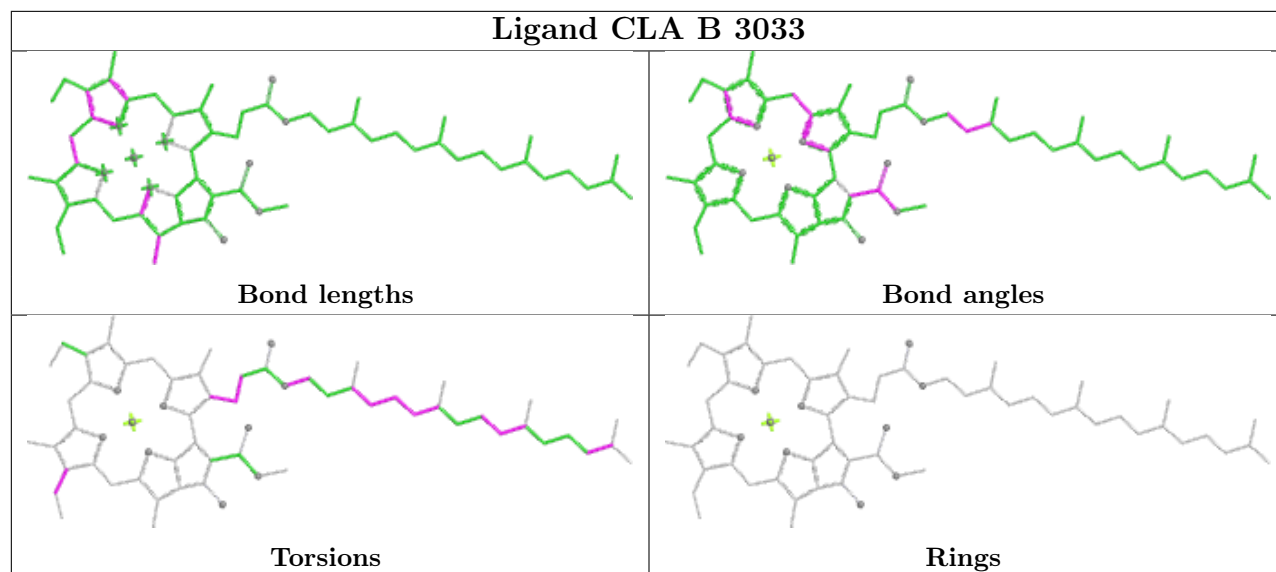
Ligand CLA A 808



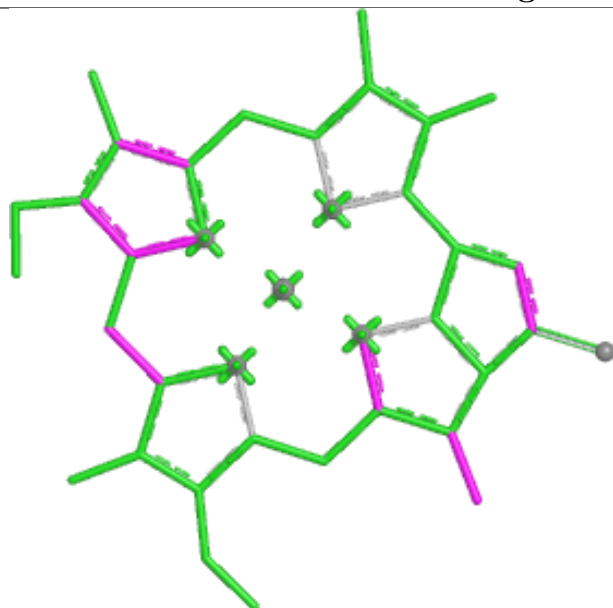
Ligand CLA B 3030



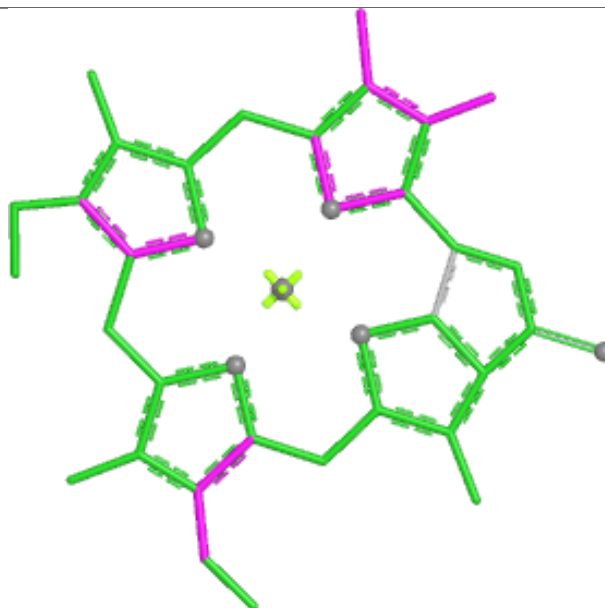
Ligand BCR B 3046	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA A 806	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT L 202	
 Bond lengths	 Bond angles
 Torsions	 Rings



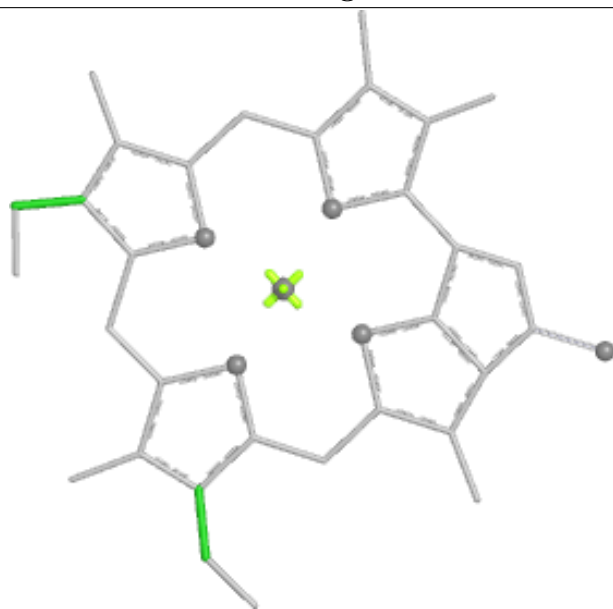
Ligand CLA J 102



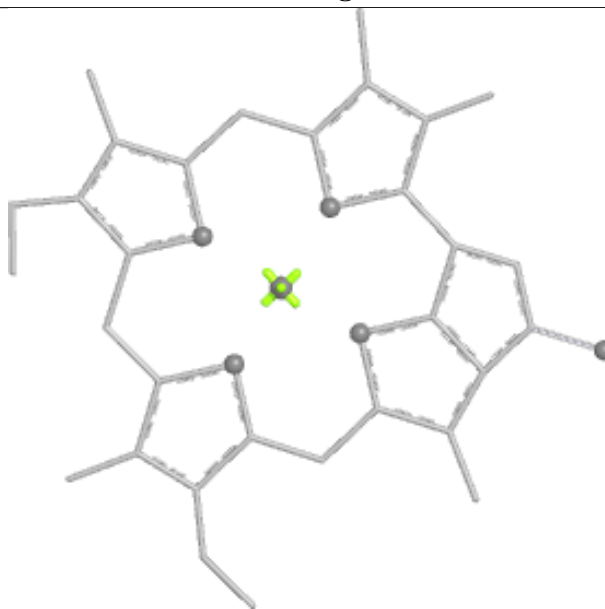
Bond lengths



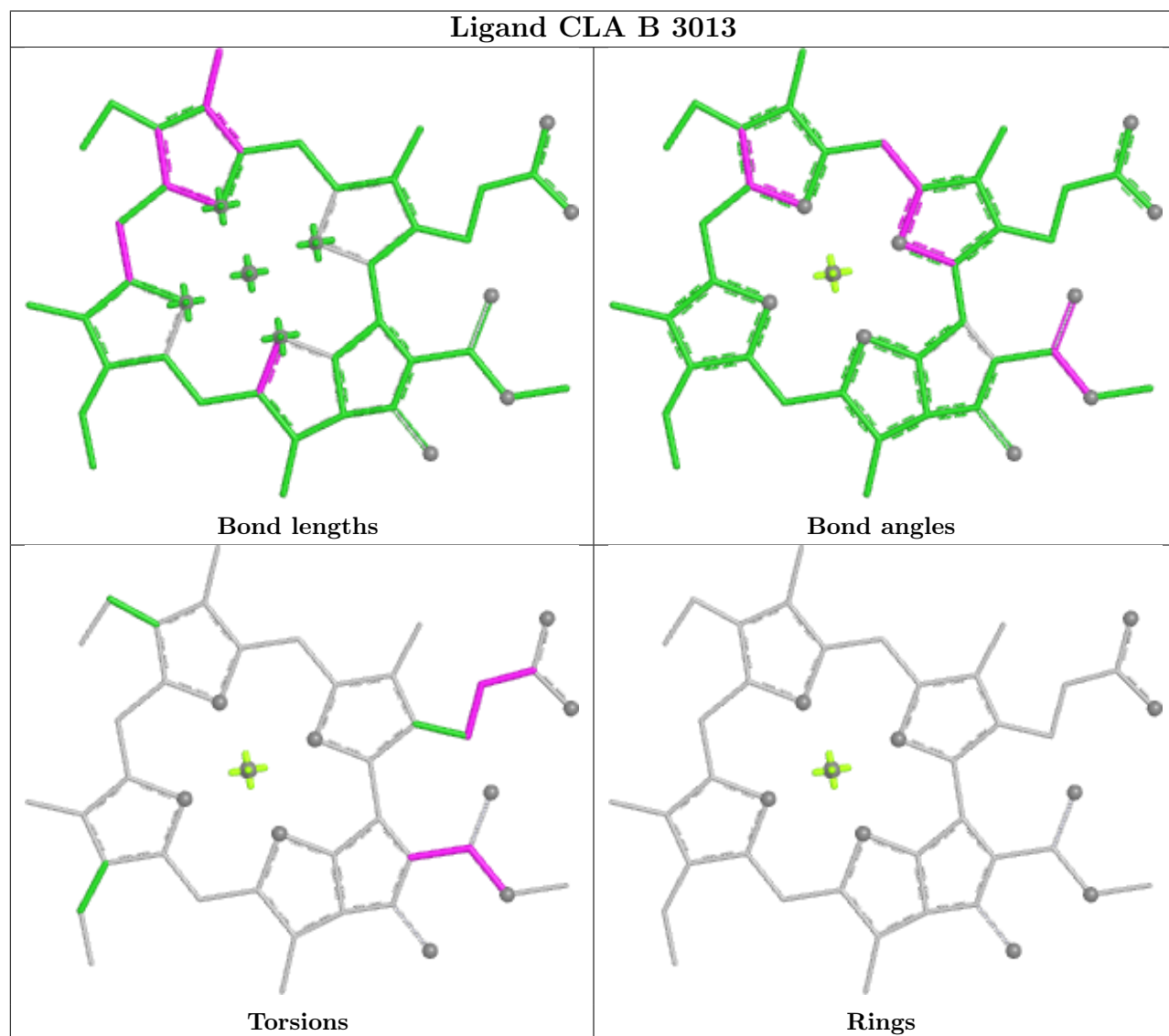
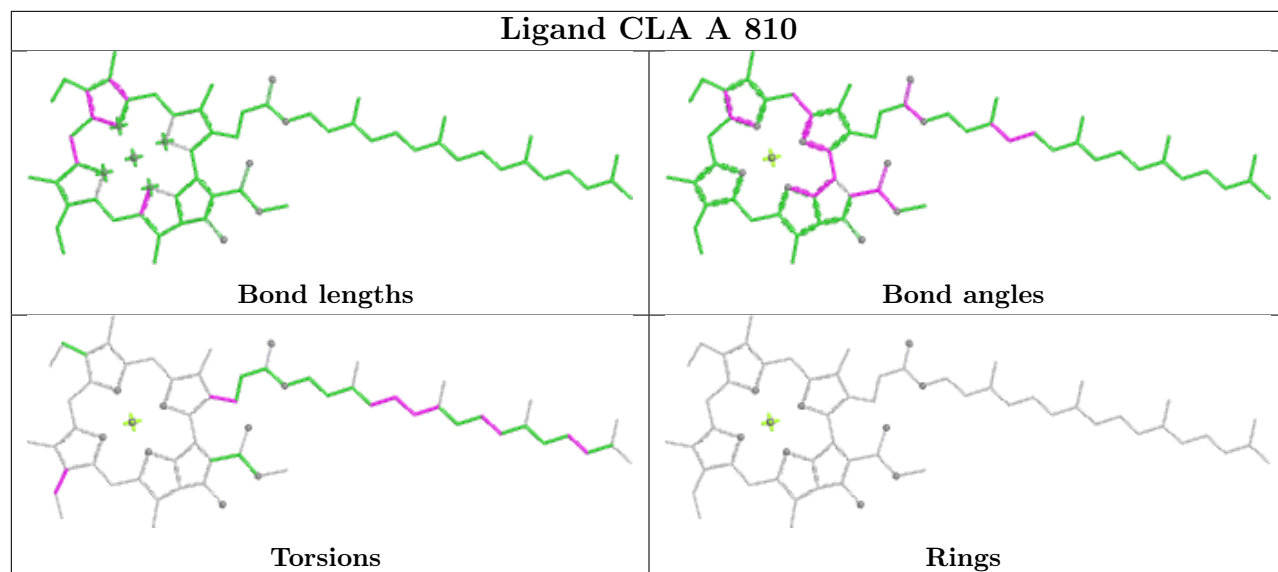
Bond angles

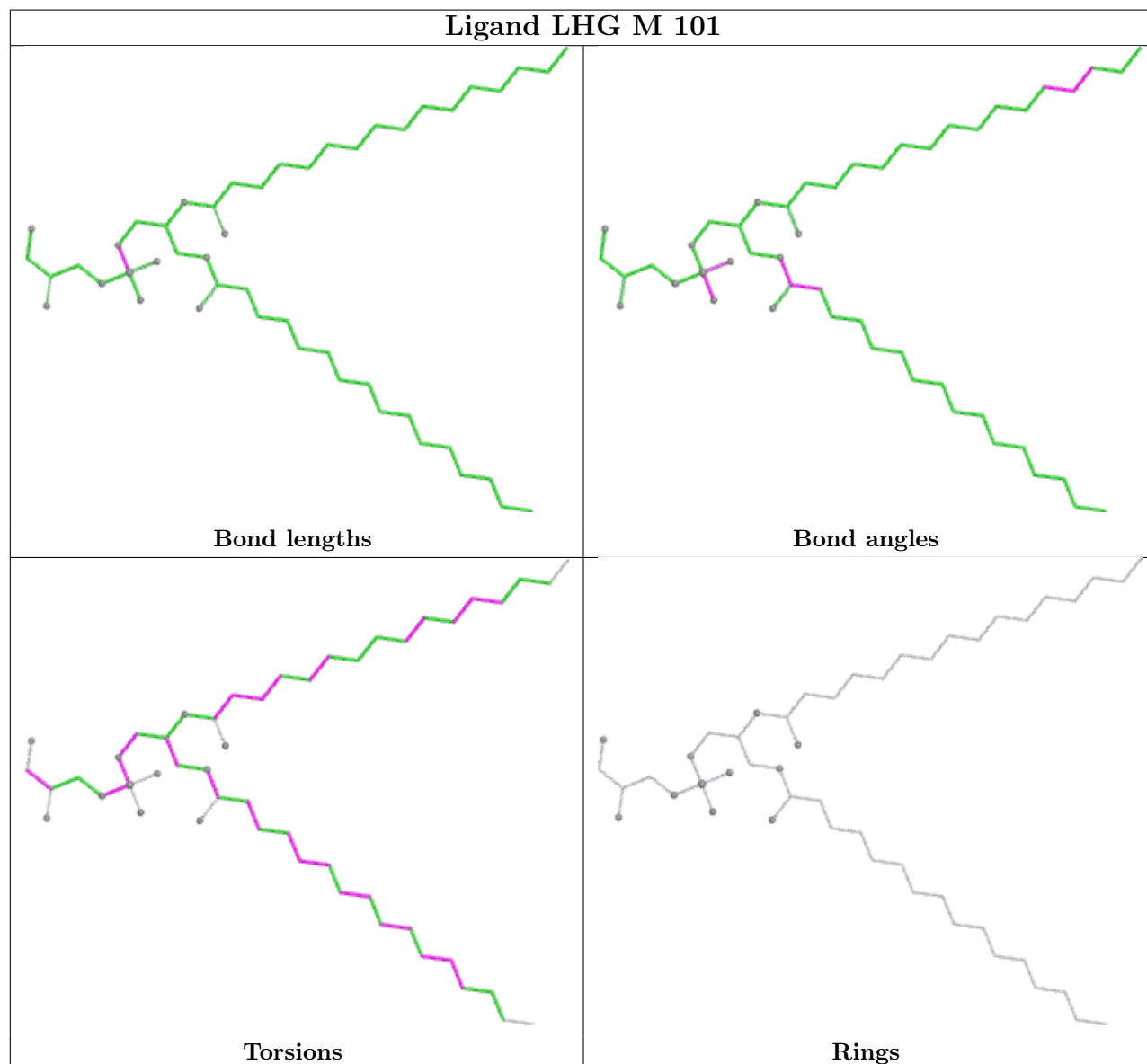
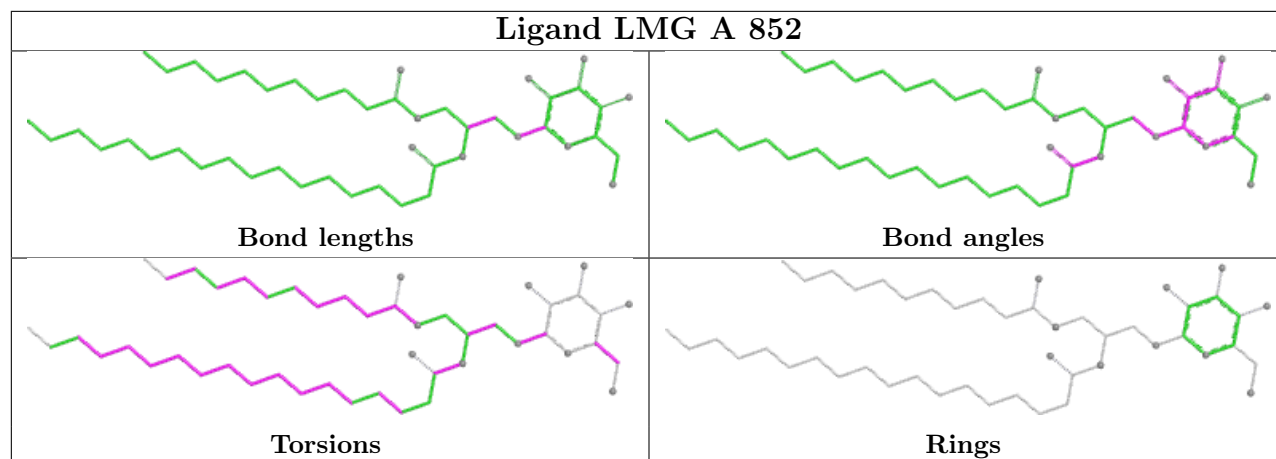


Torsions

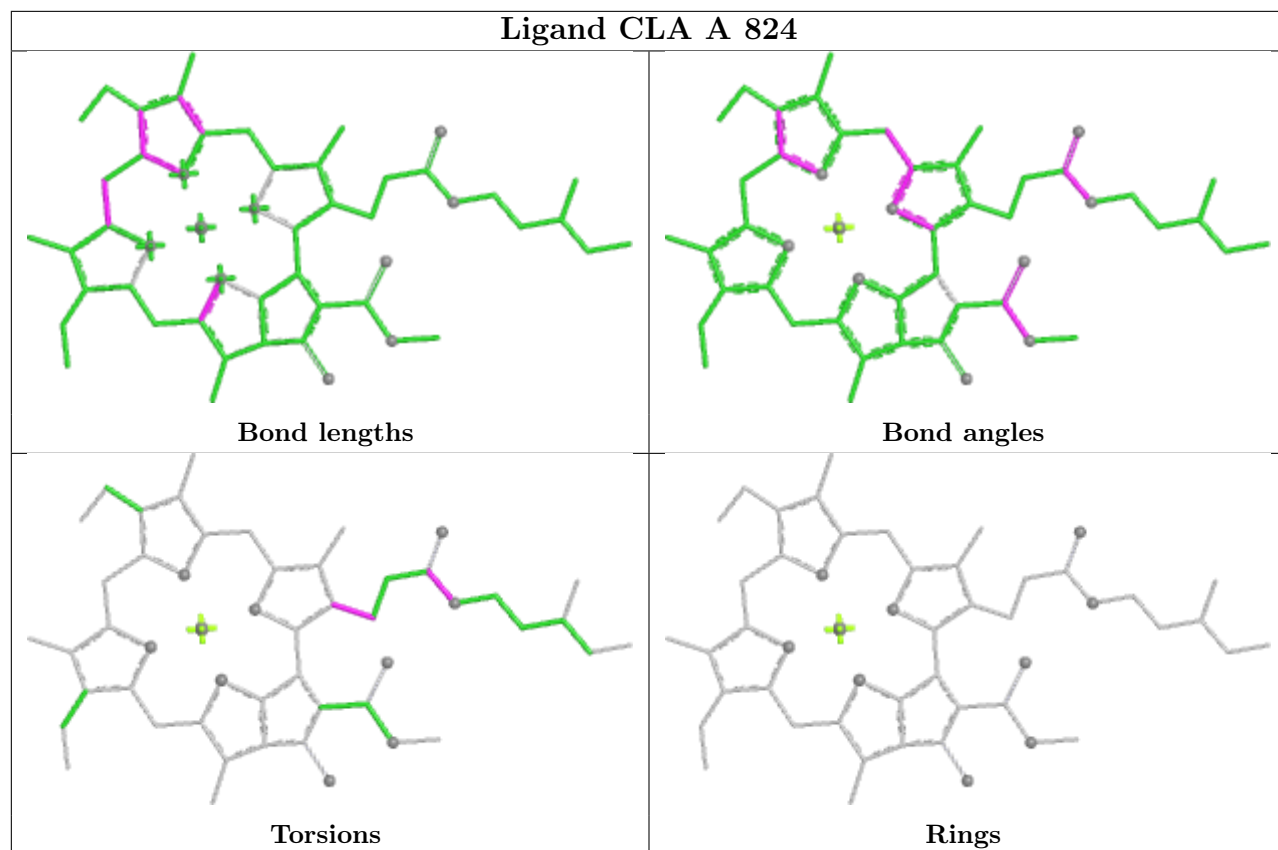


Rings

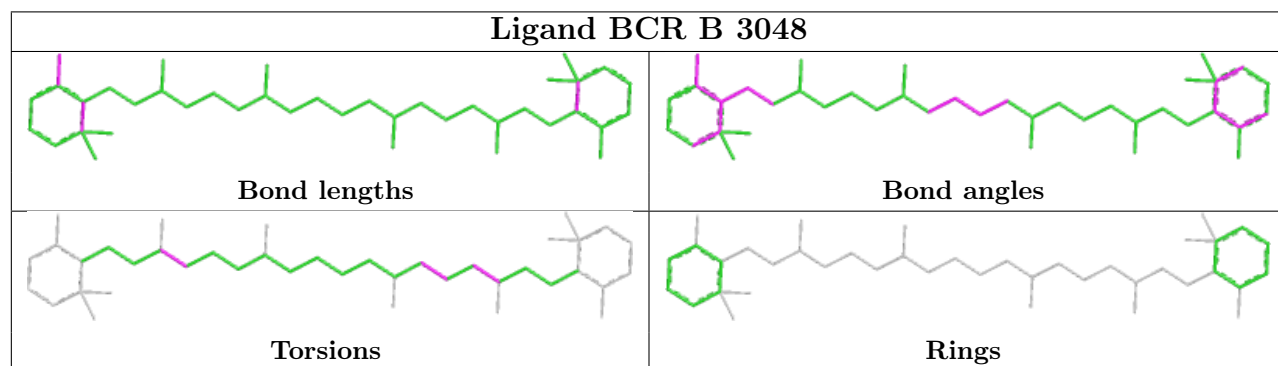




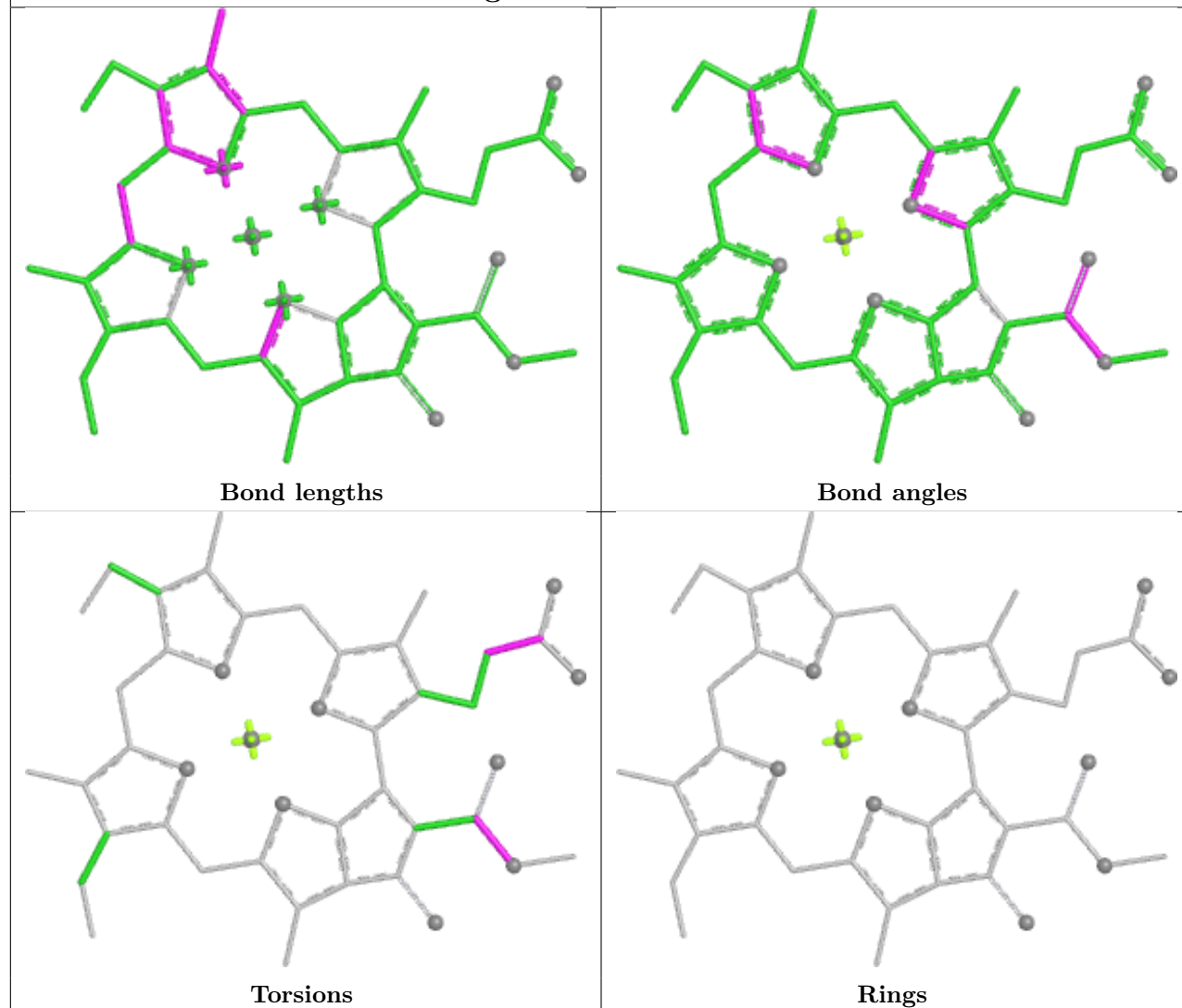
Ligand CLA A 824



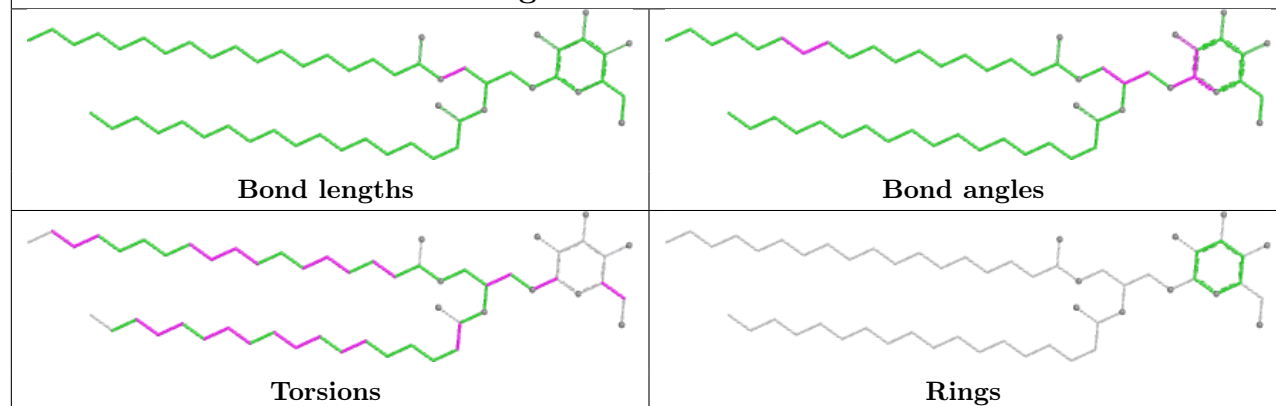
Ligand BCR B 3048



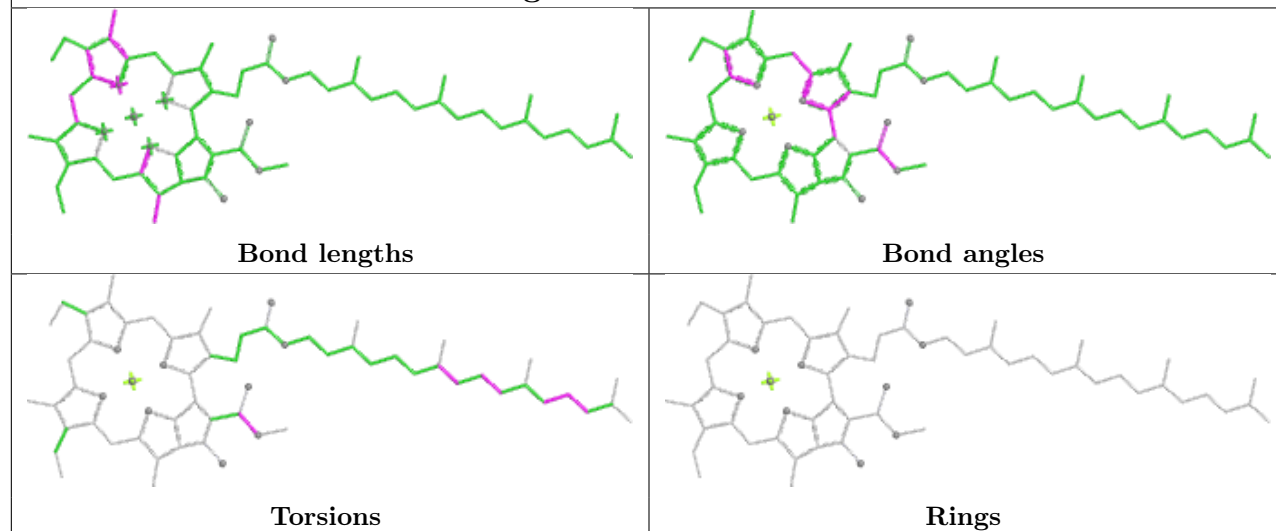
Ligand CLA B 3037



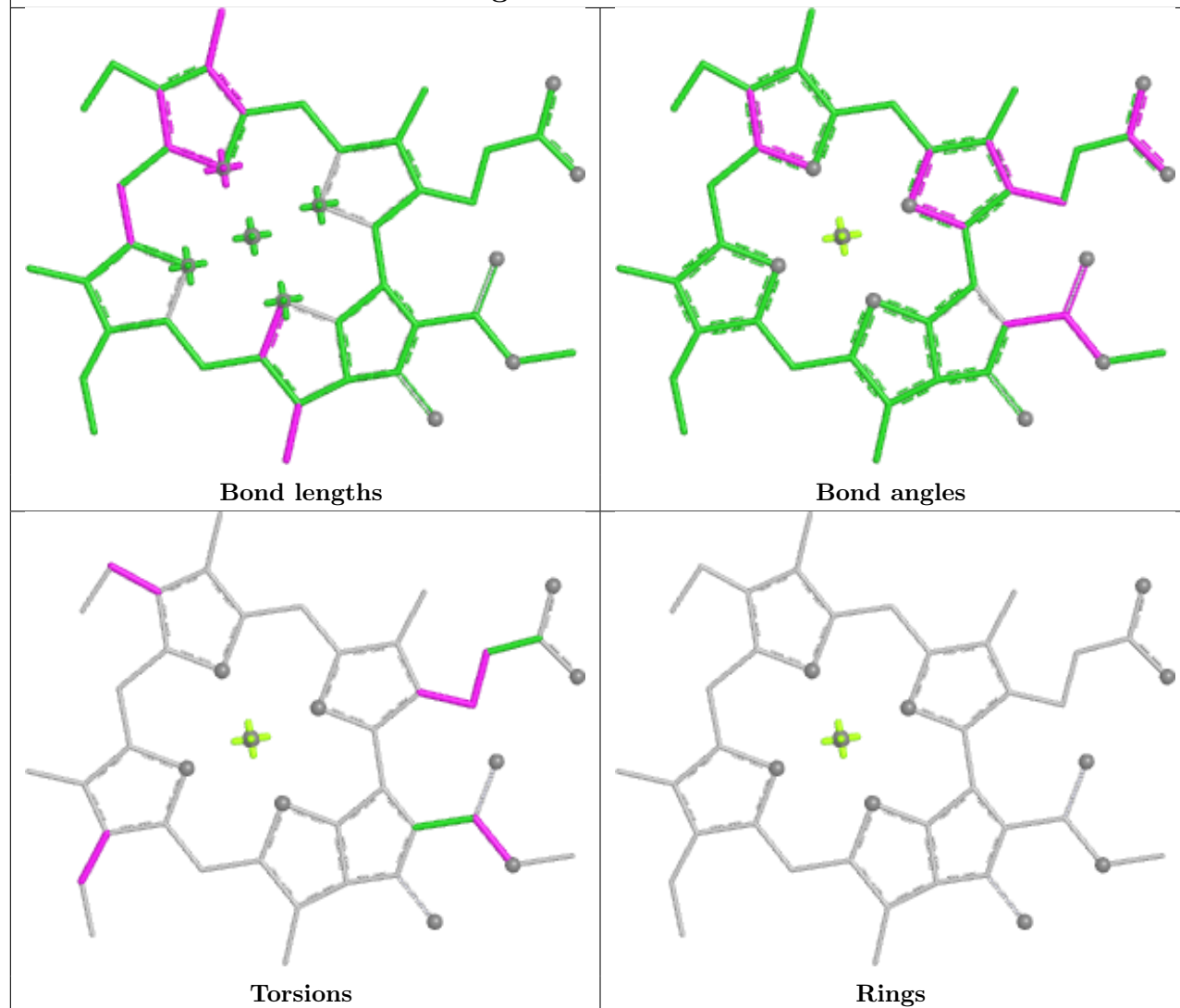
Ligand LMG B 3049



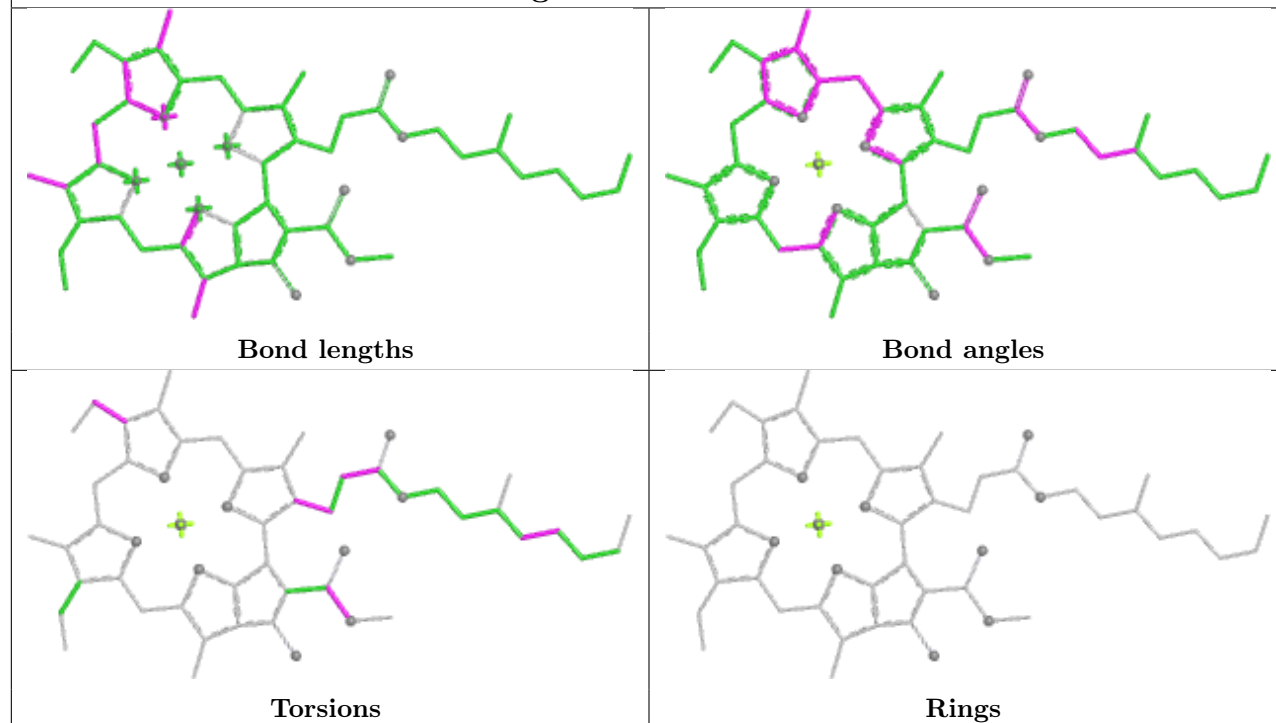
Ligand CLA B 3004



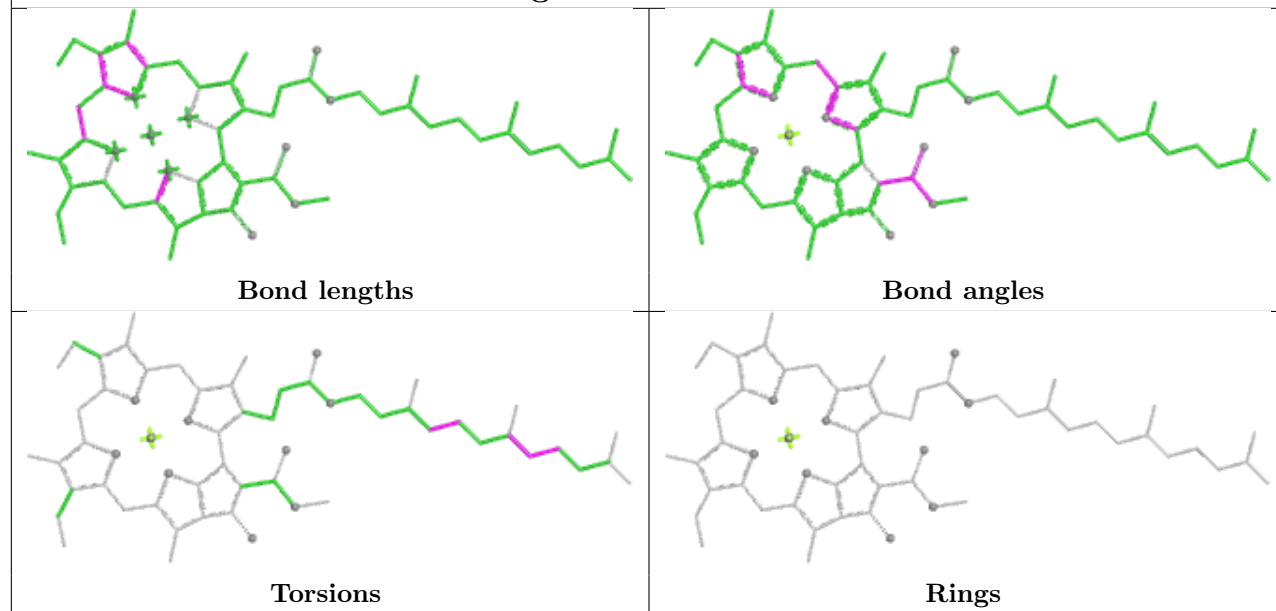
Ligand CLA A 811



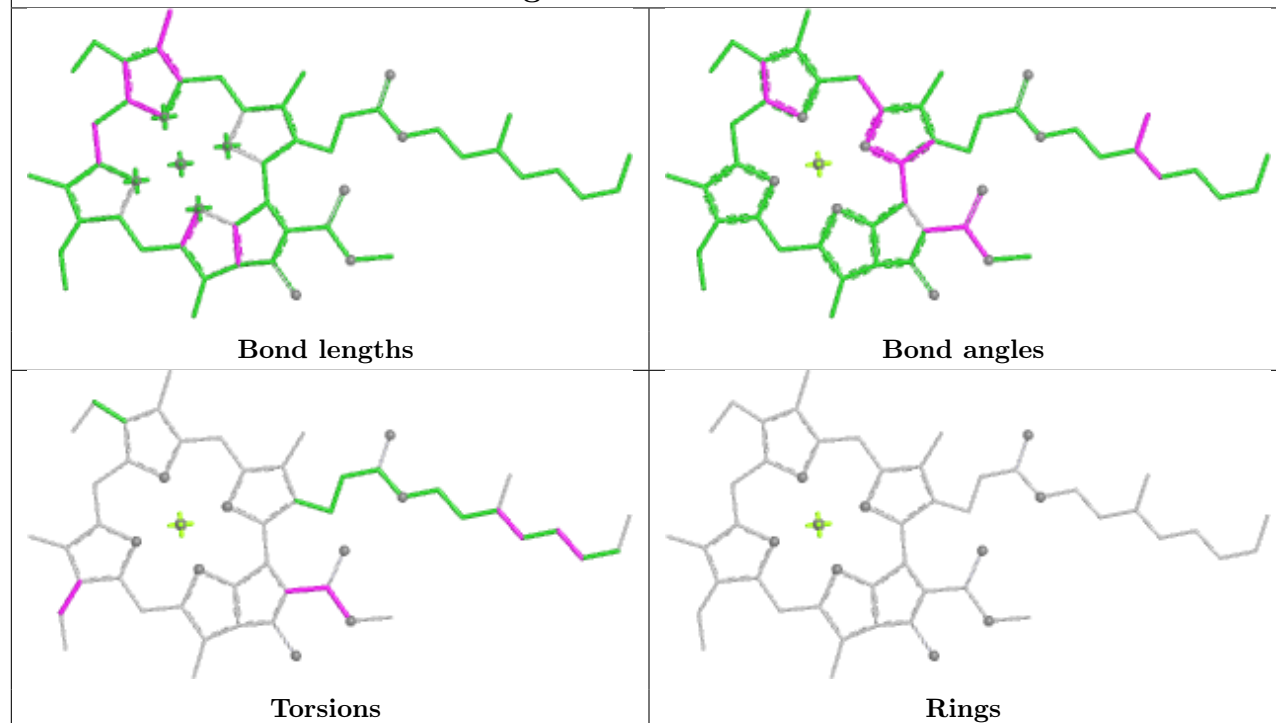
Ligand CLA A 819



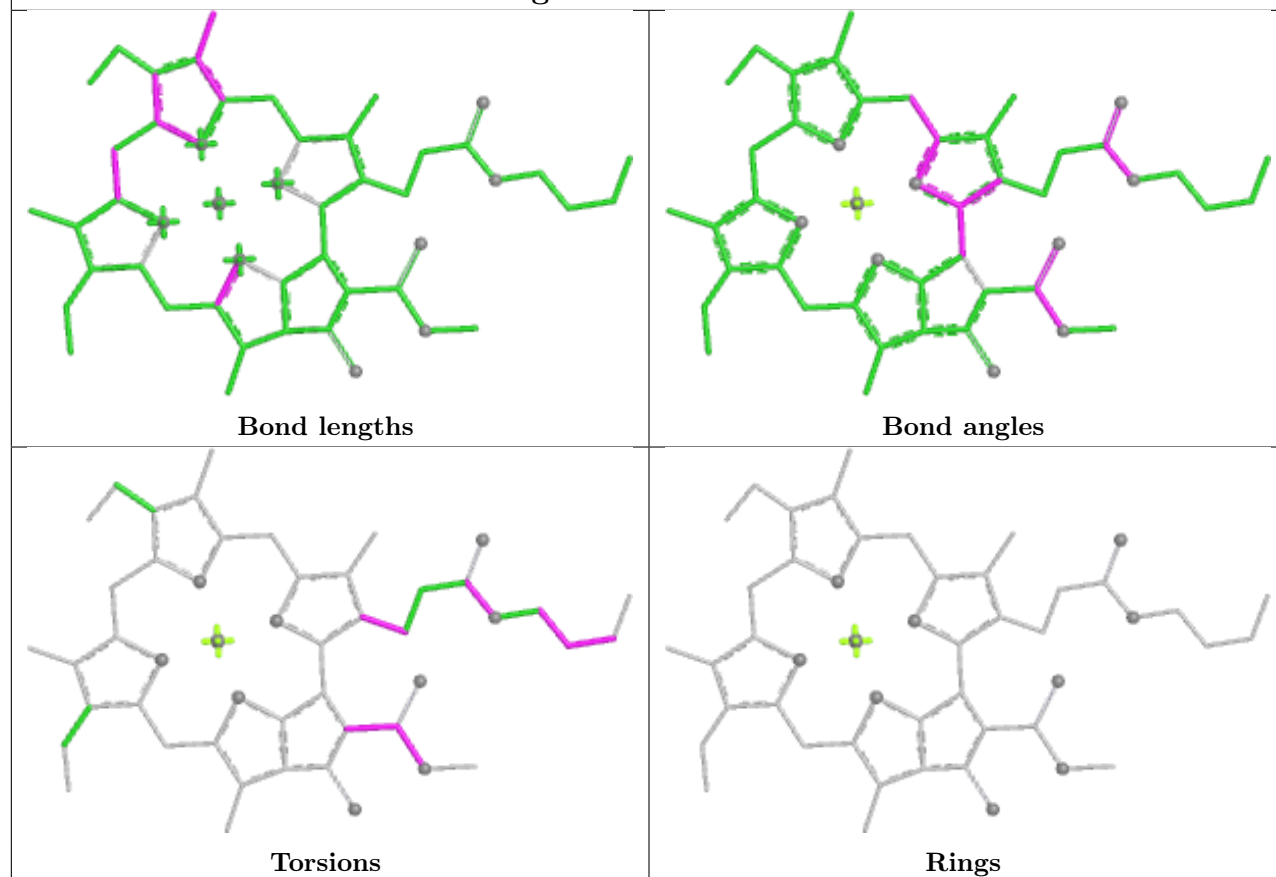
Ligand CLA A 814

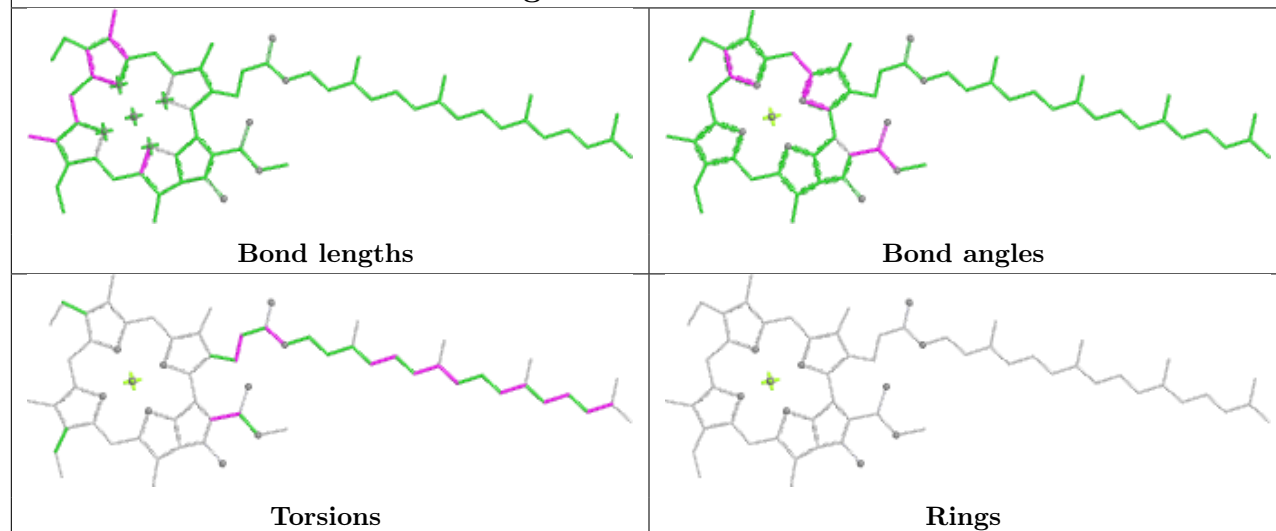
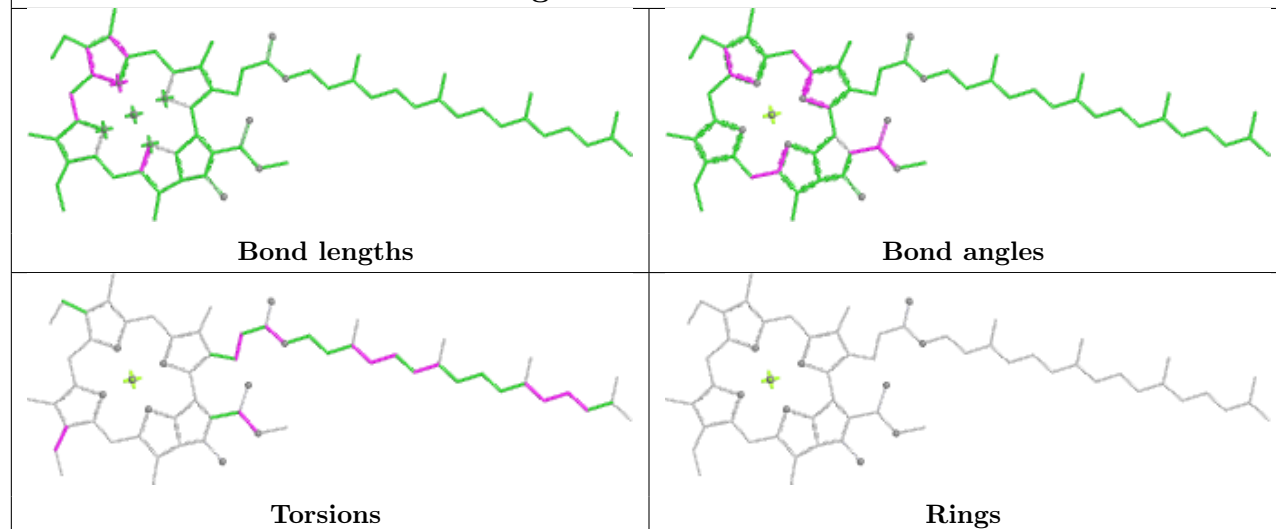


Ligand CLA B 3025

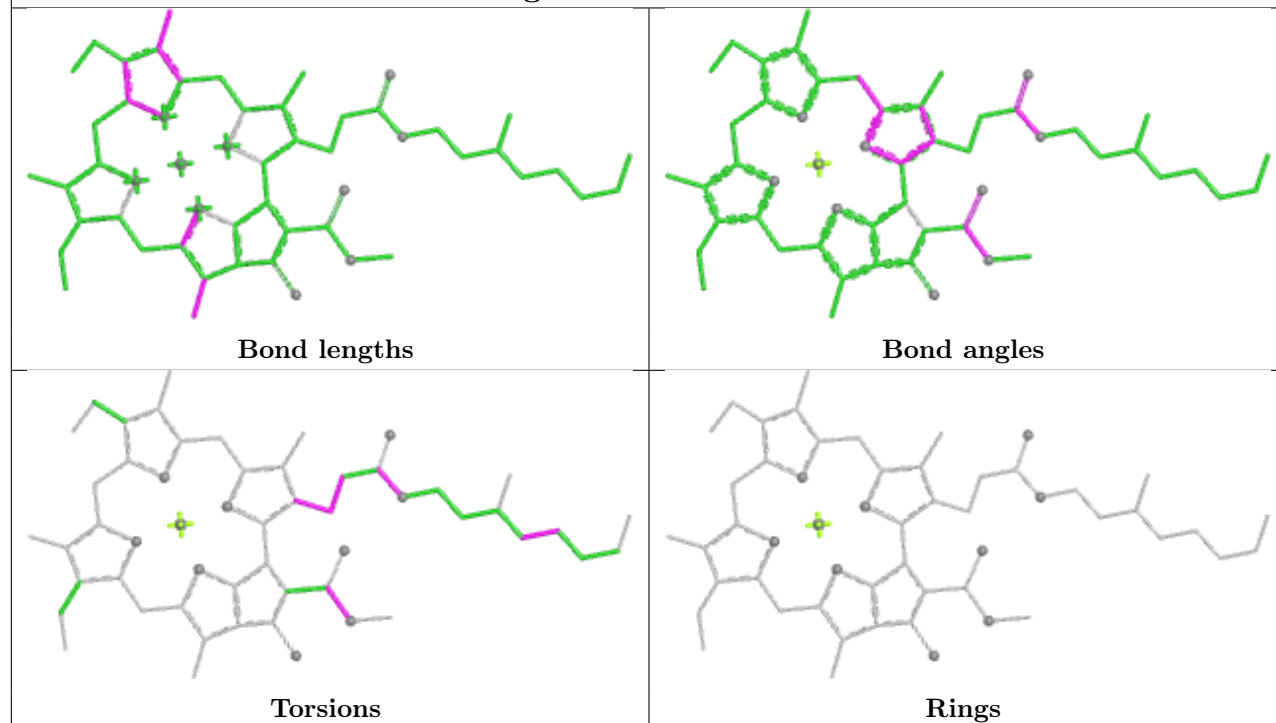


Ligand CLA A 823

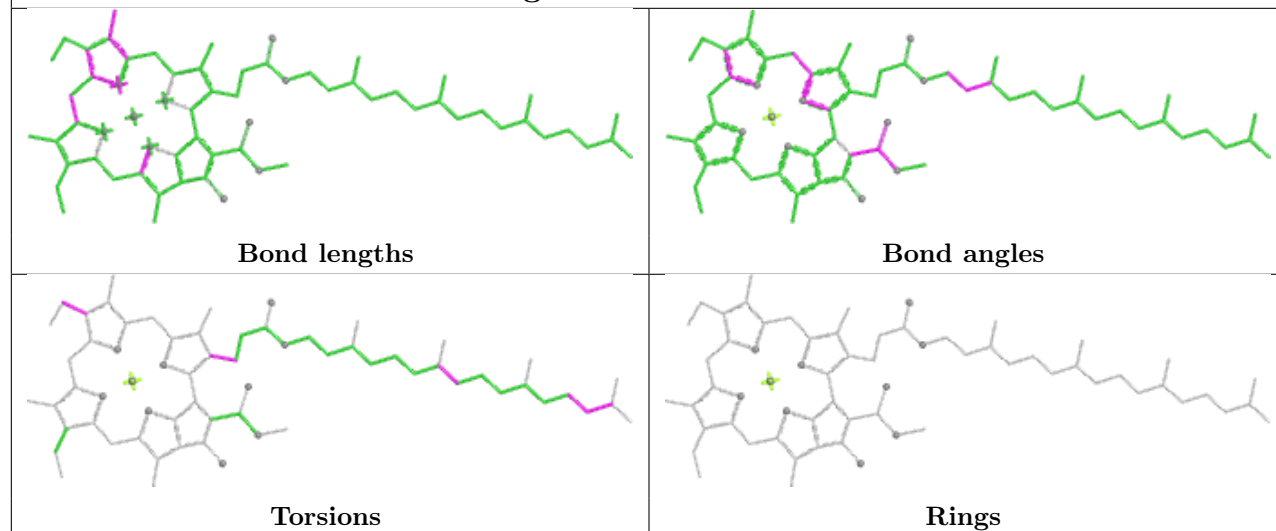


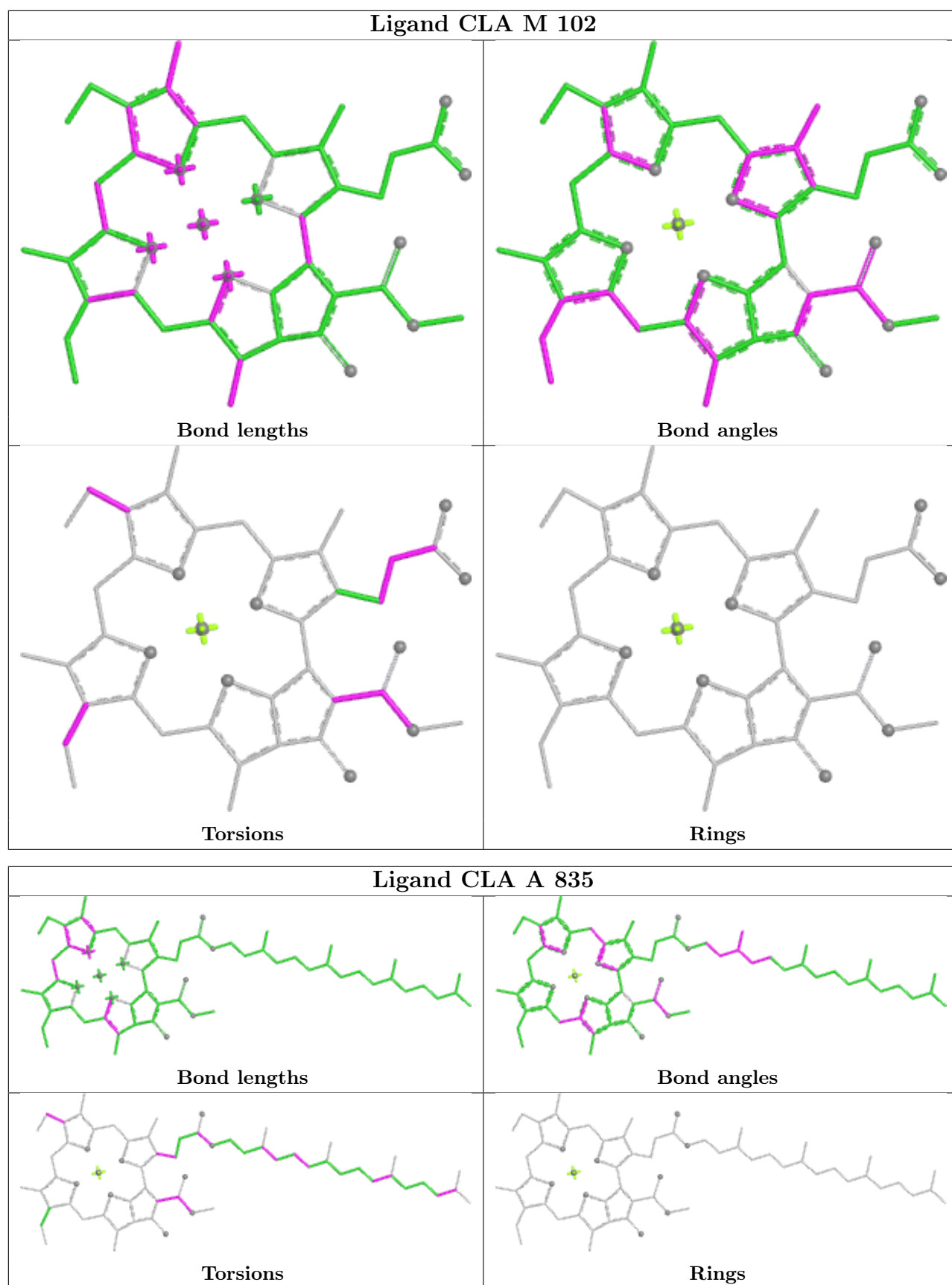
Ligand CLA B 3027**Ligand CLA A 822**

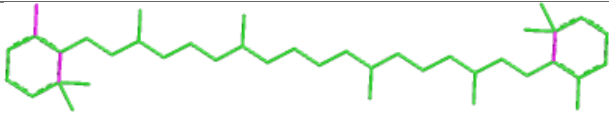
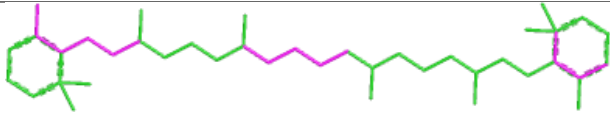
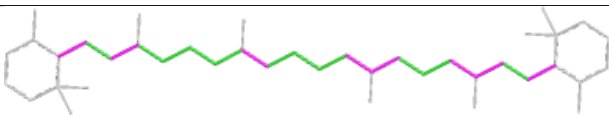
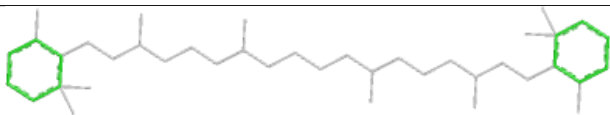
Ligand CLA B 3005

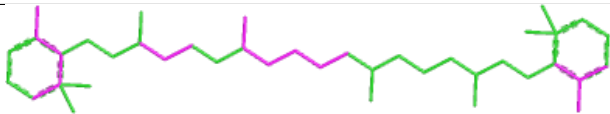
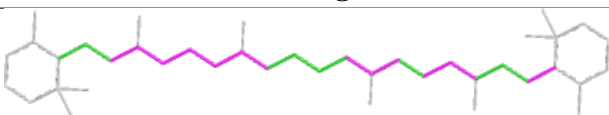
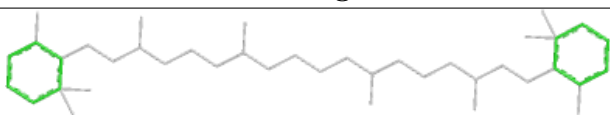


Ligand CLA B 3042

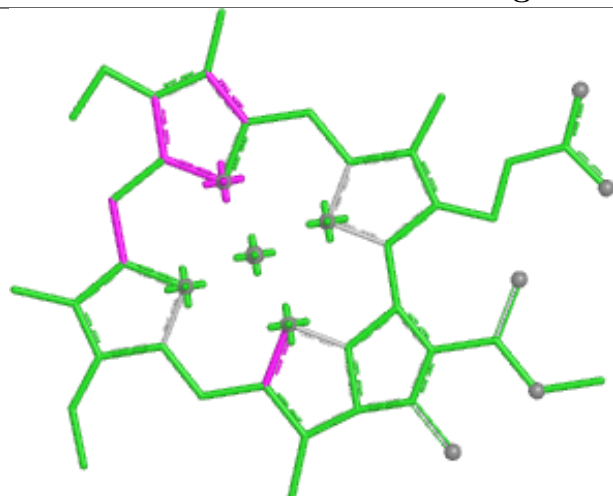




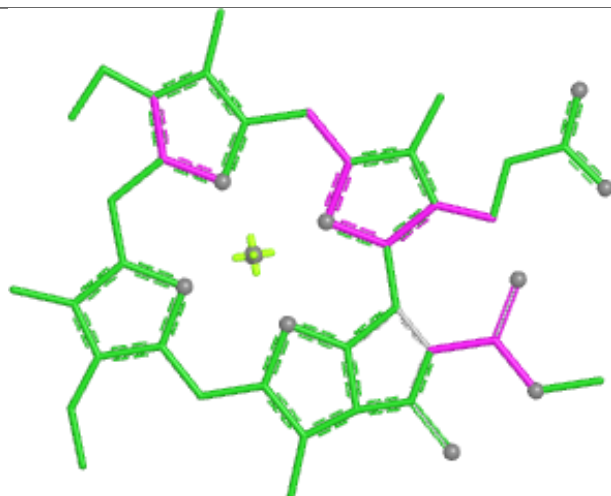
Ligand BCR A 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 3047	
	
Bond lengths	Bond angles
	
Torsions	Rings

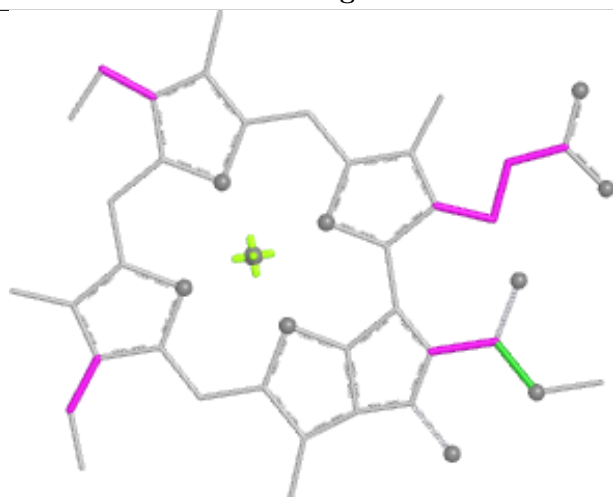
Ligand CLA K 103



Bond lengths



Bond angles

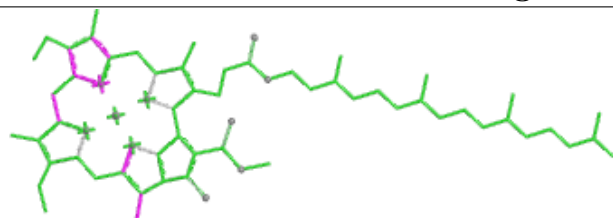


Torsions

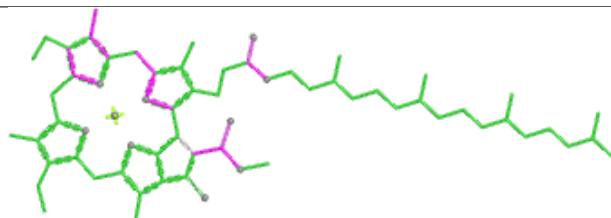


Rings

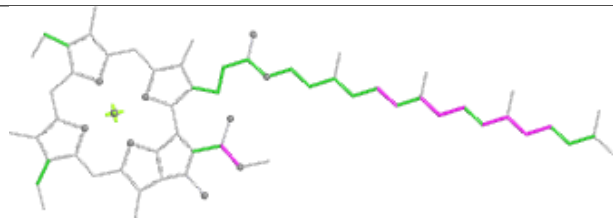
Ligand CLA A 827



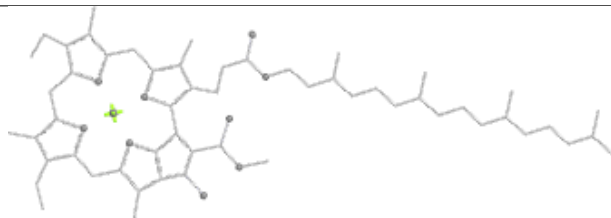
Bond lengths



Bond angles

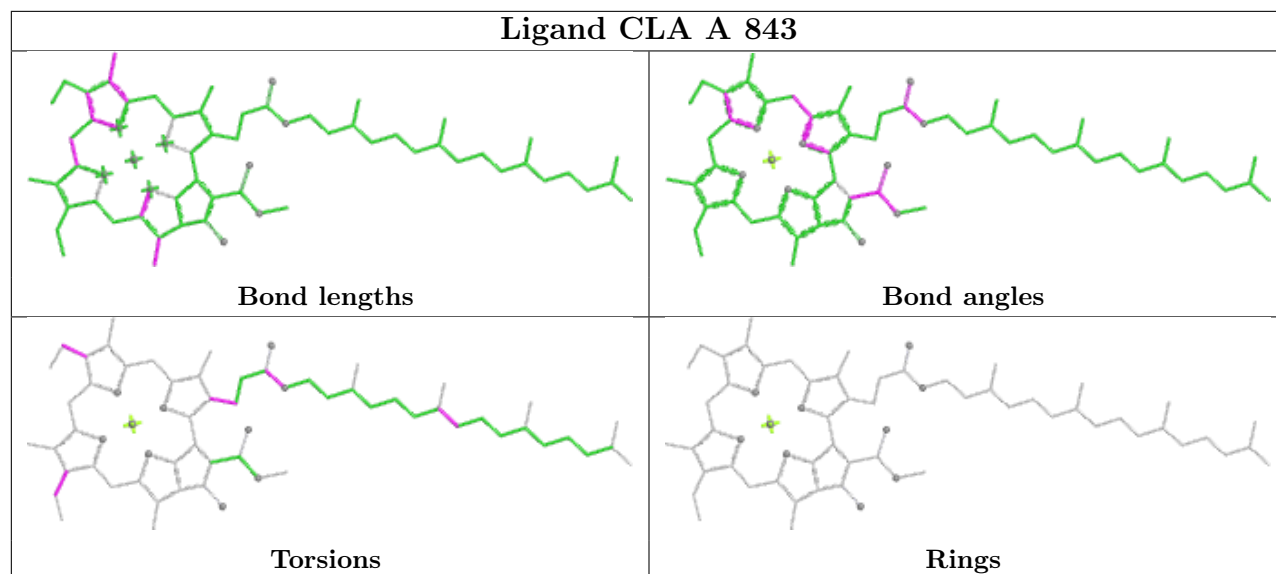


Torsions

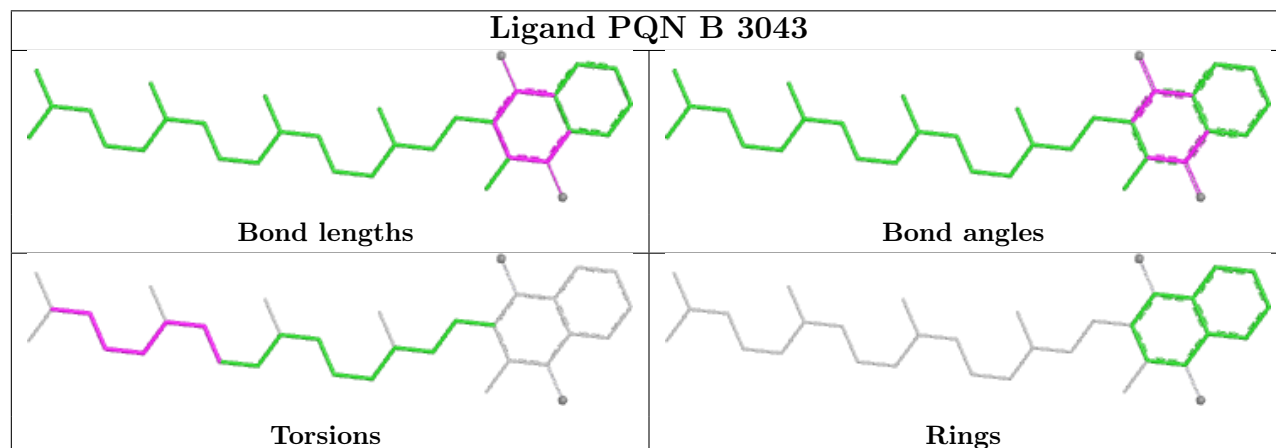


Rings

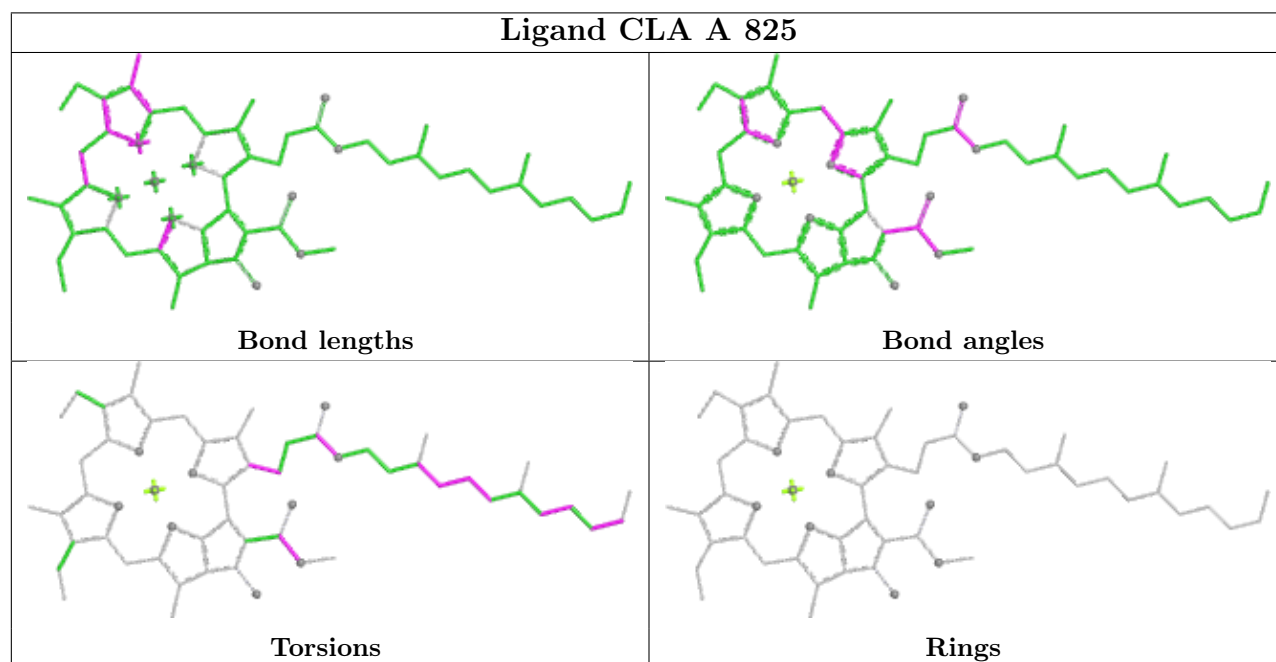
Ligand CLA A 843

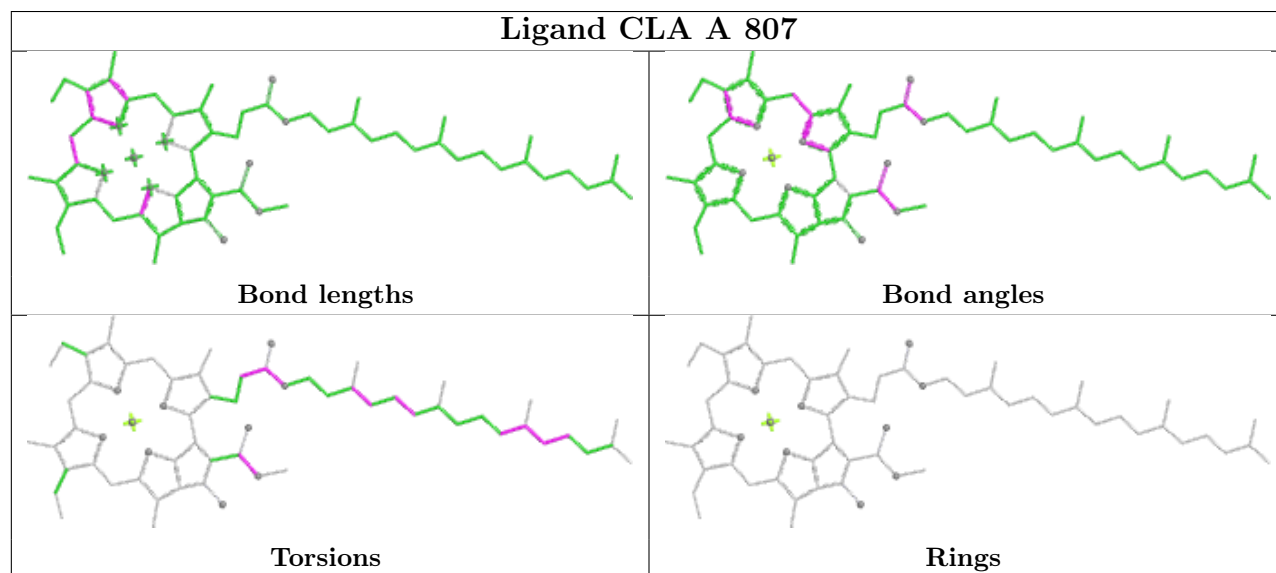
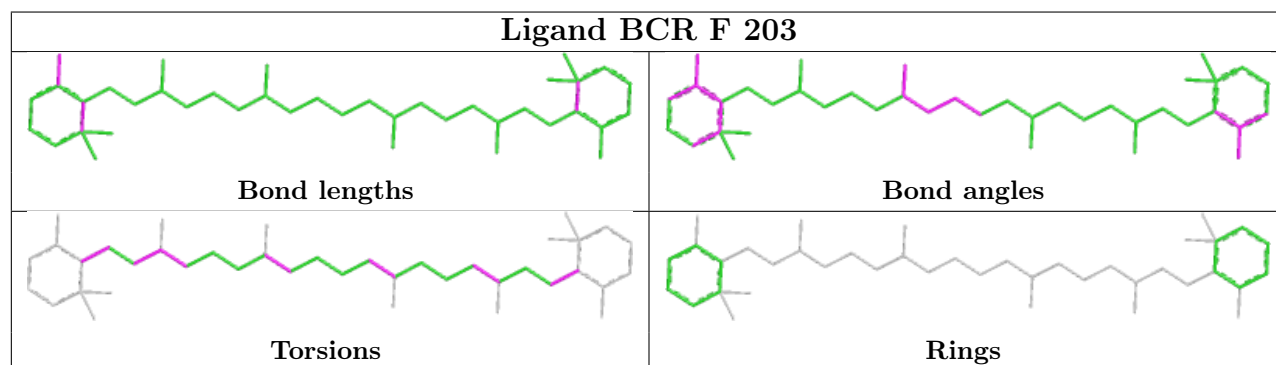
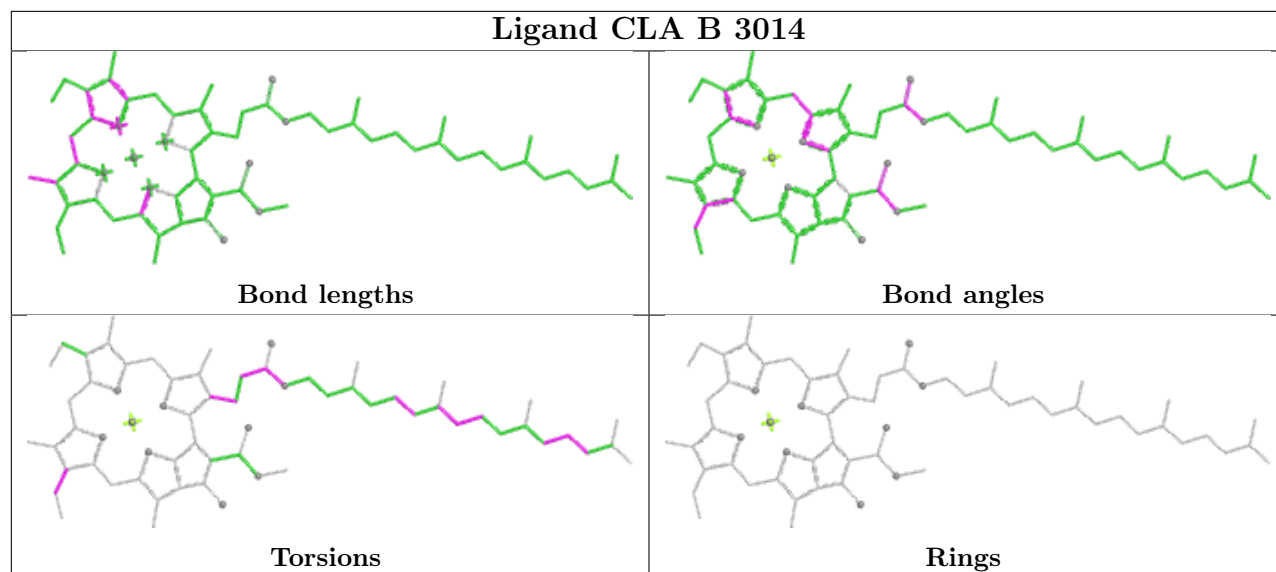


Ligand PQN B 3043

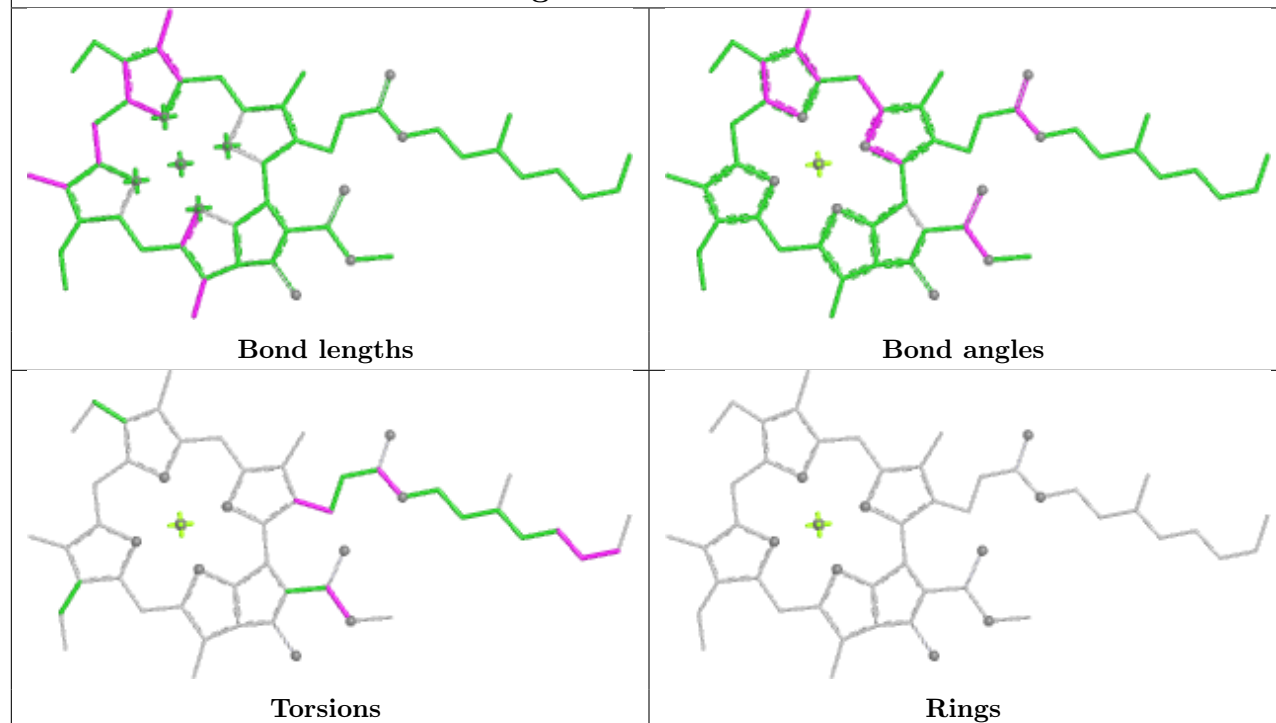


Ligand CLA A 825

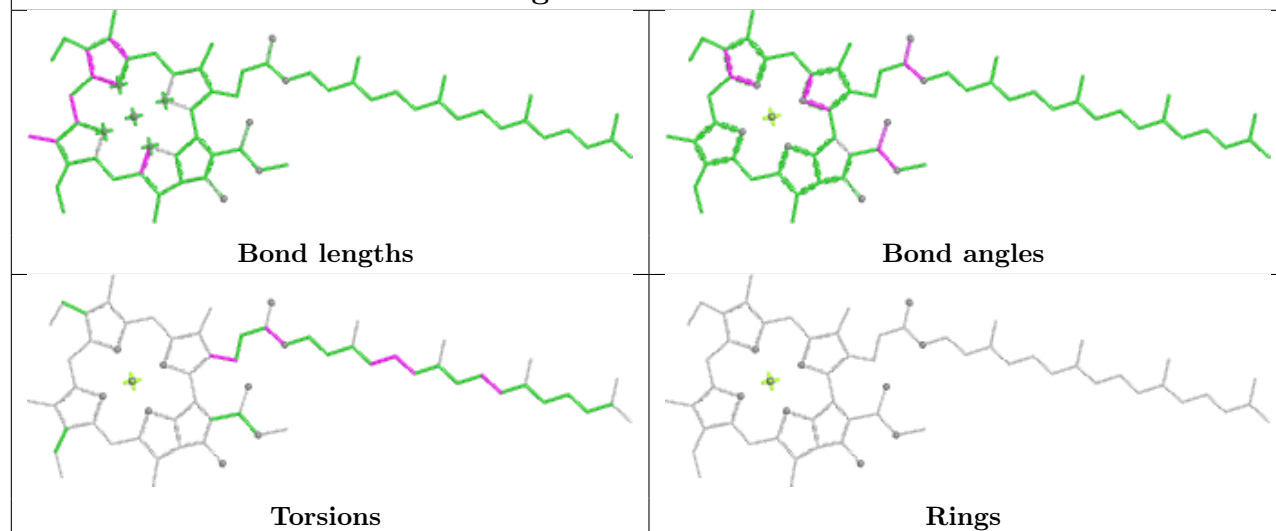


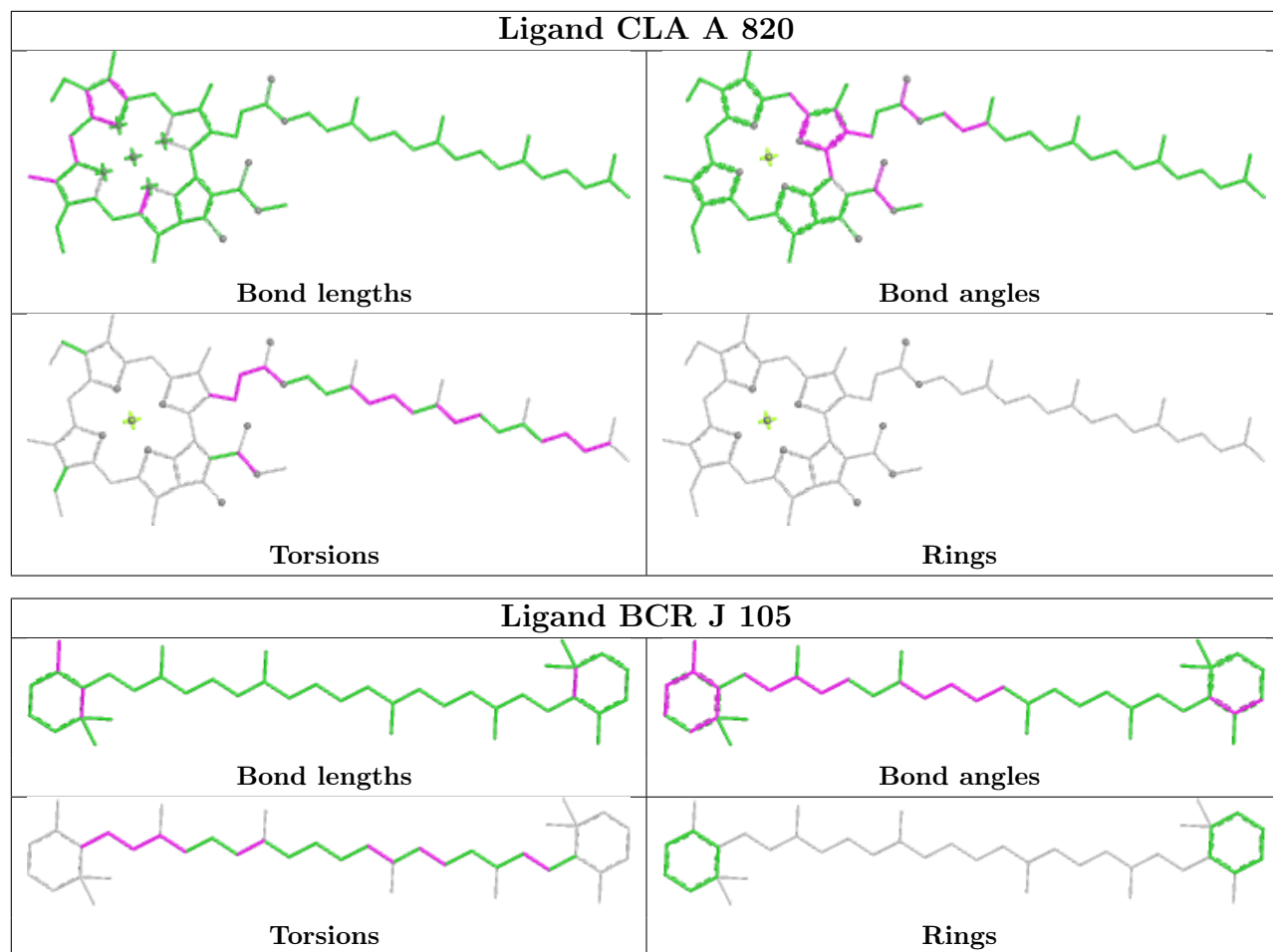


Ligand CLA A 836

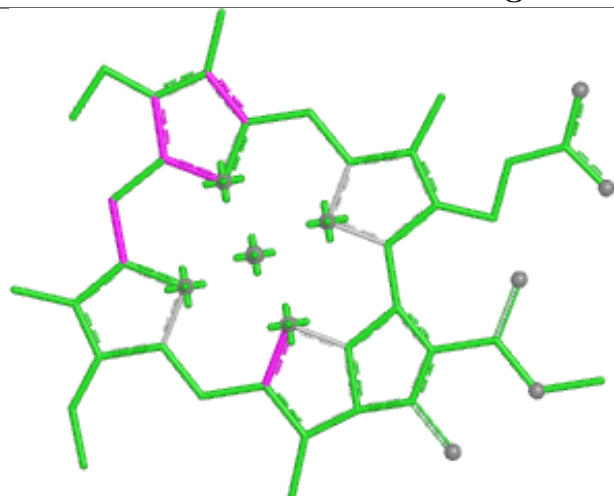


Ligand CLA A 804

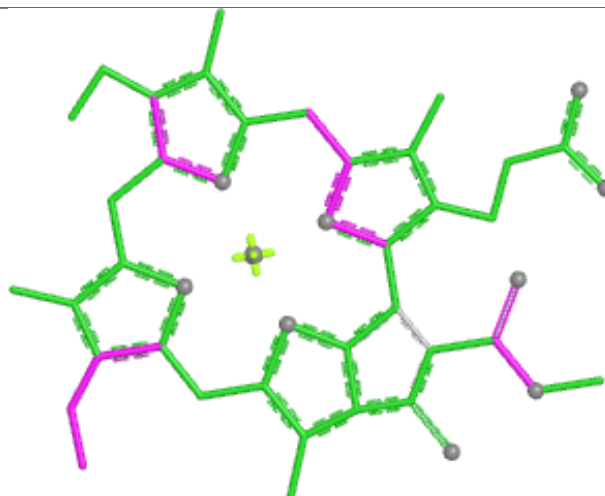




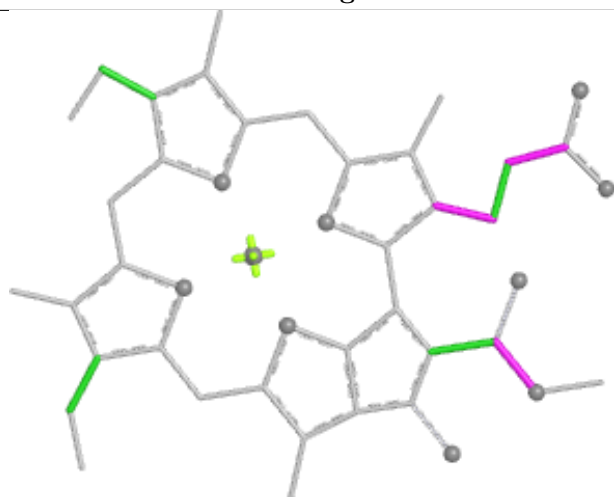
Ligand CLA B 3036



Bond lengths



Bond angles

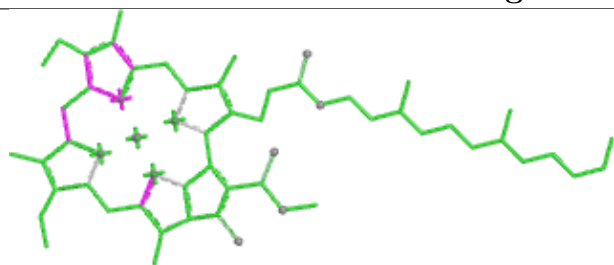


Torsions

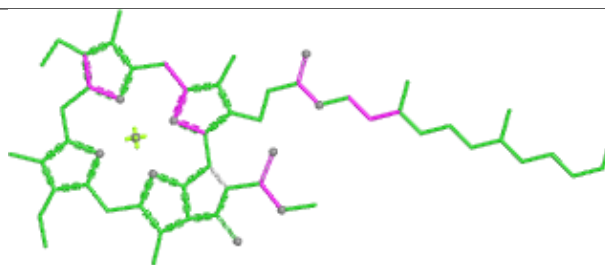


Rings

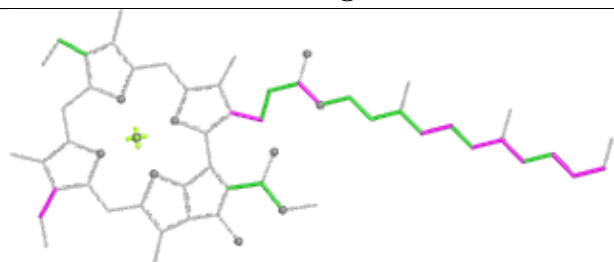
Ligand CLA B 3018



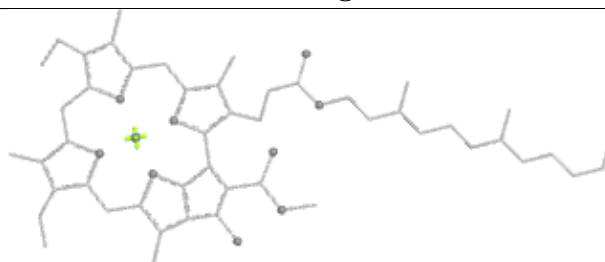
Bond lengths



Bond angles

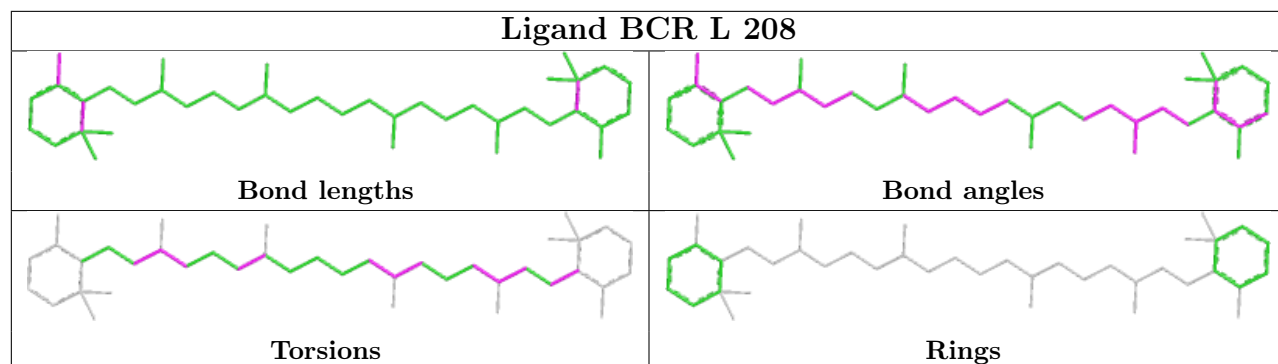


Torsions

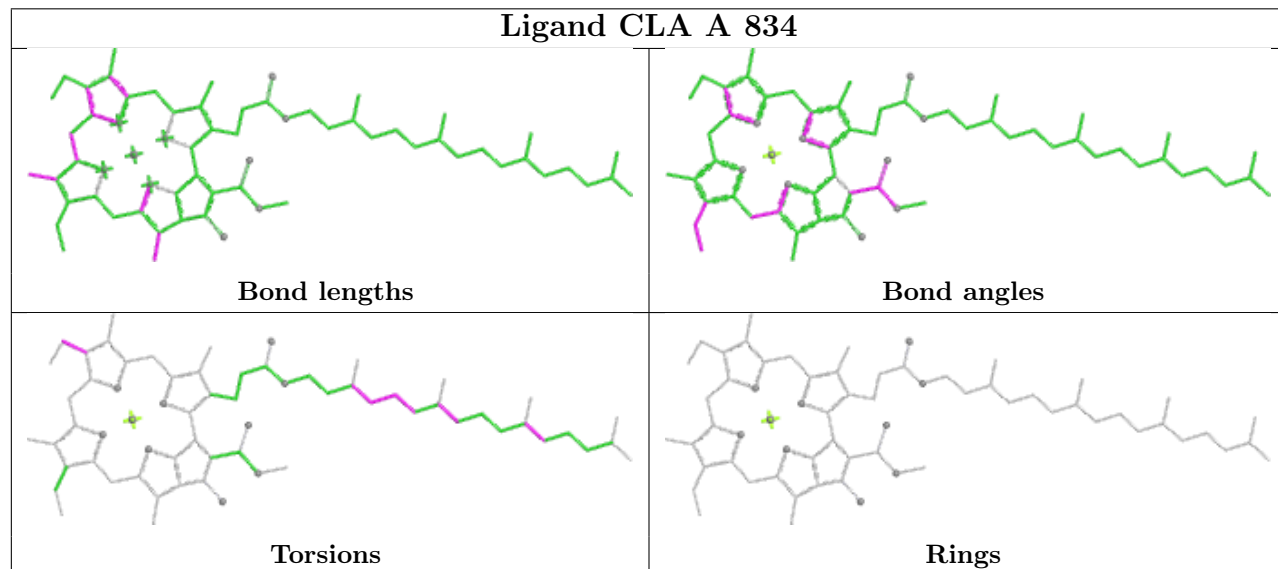


Rings

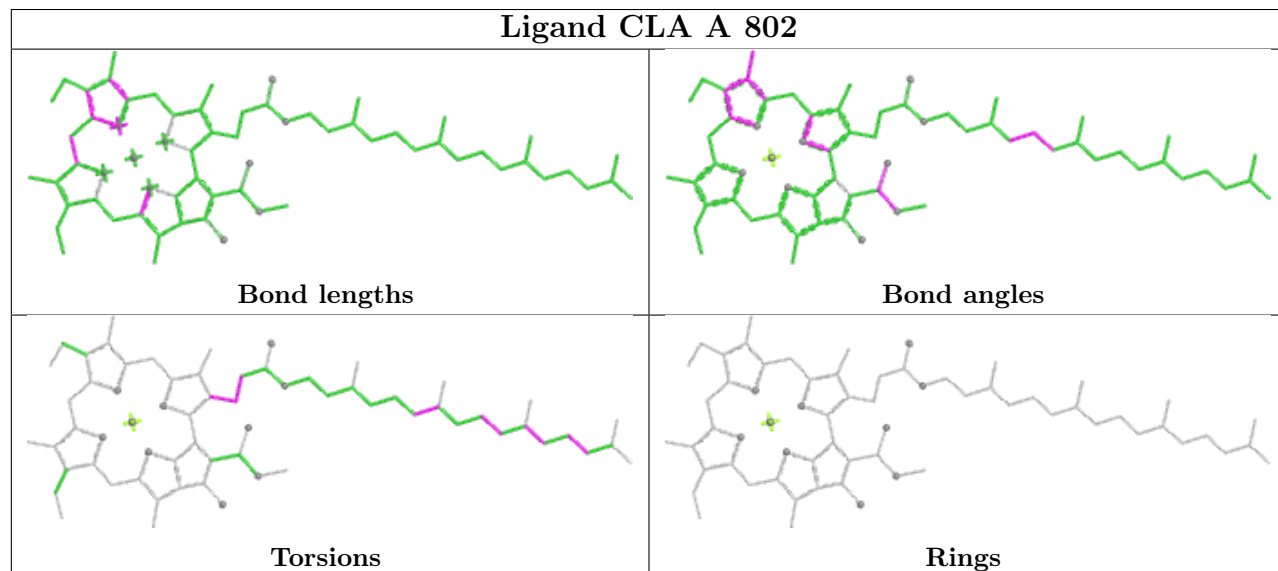
Ligand BCR L 208



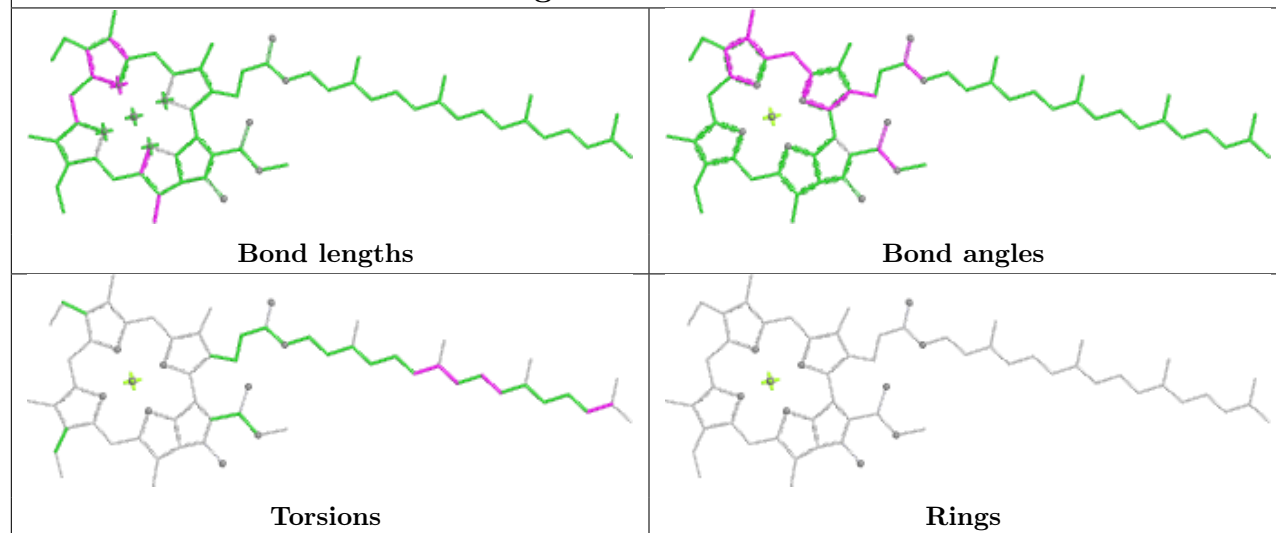
Ligand CLA A 834



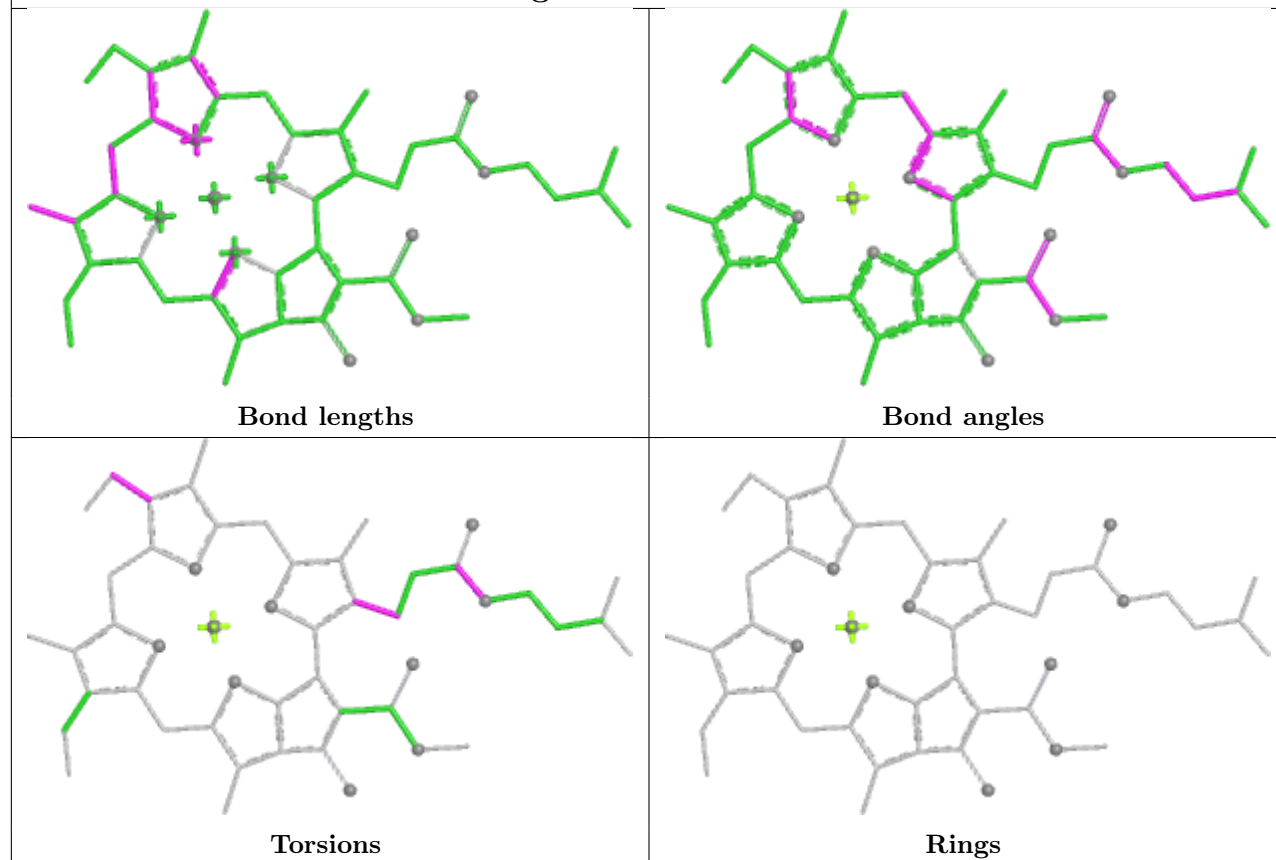
Ligand CLA A 802

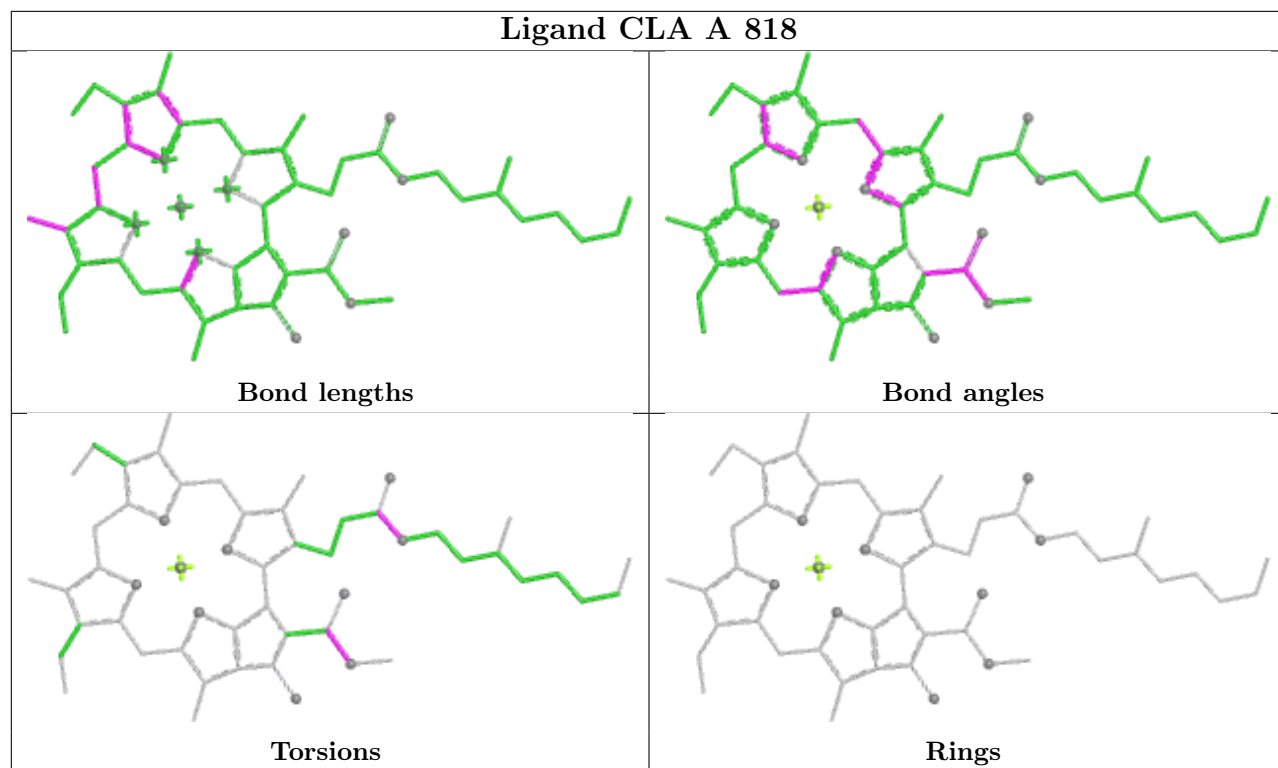


Ligand CLA L 206

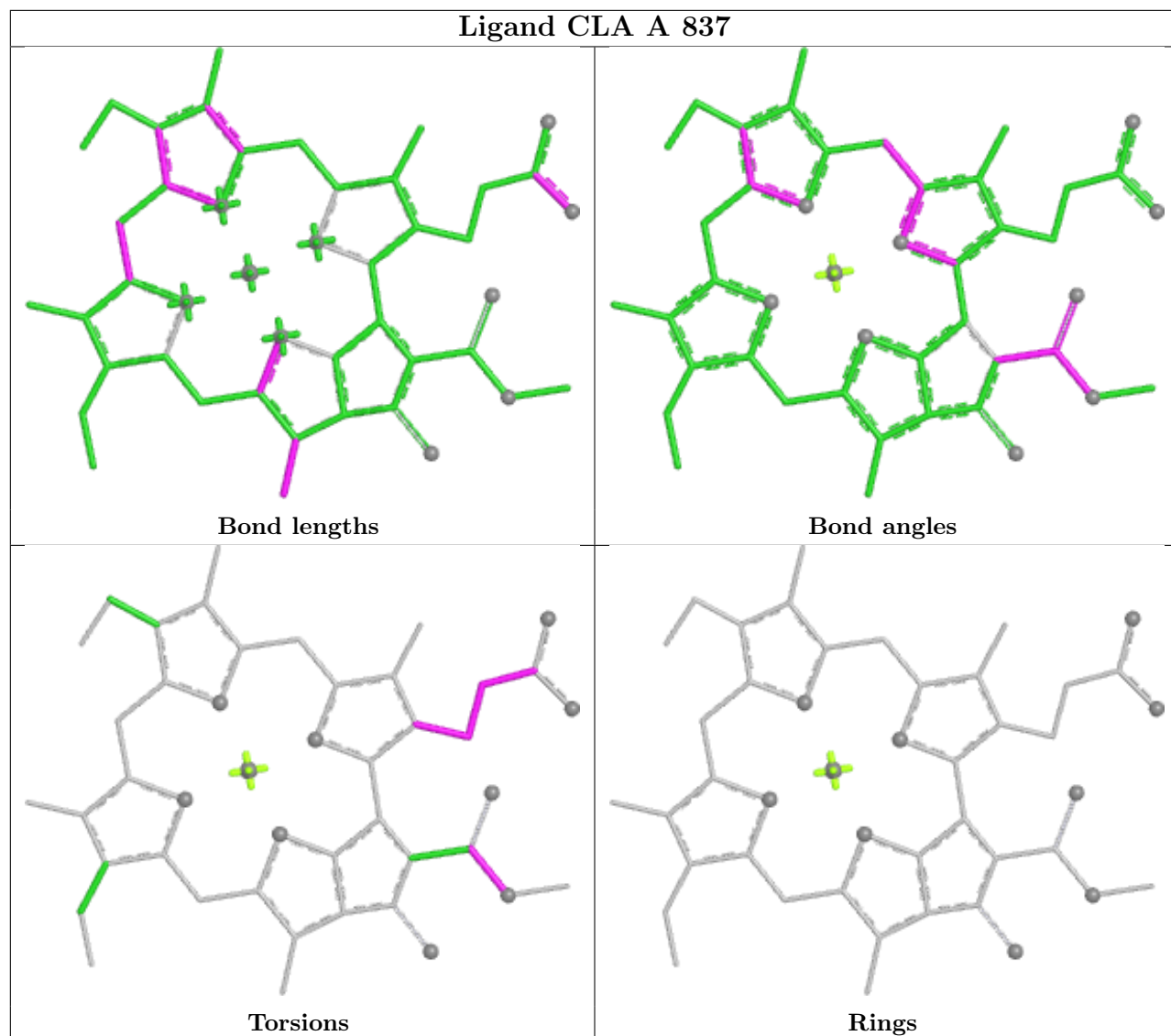


Ligand CLA A 832

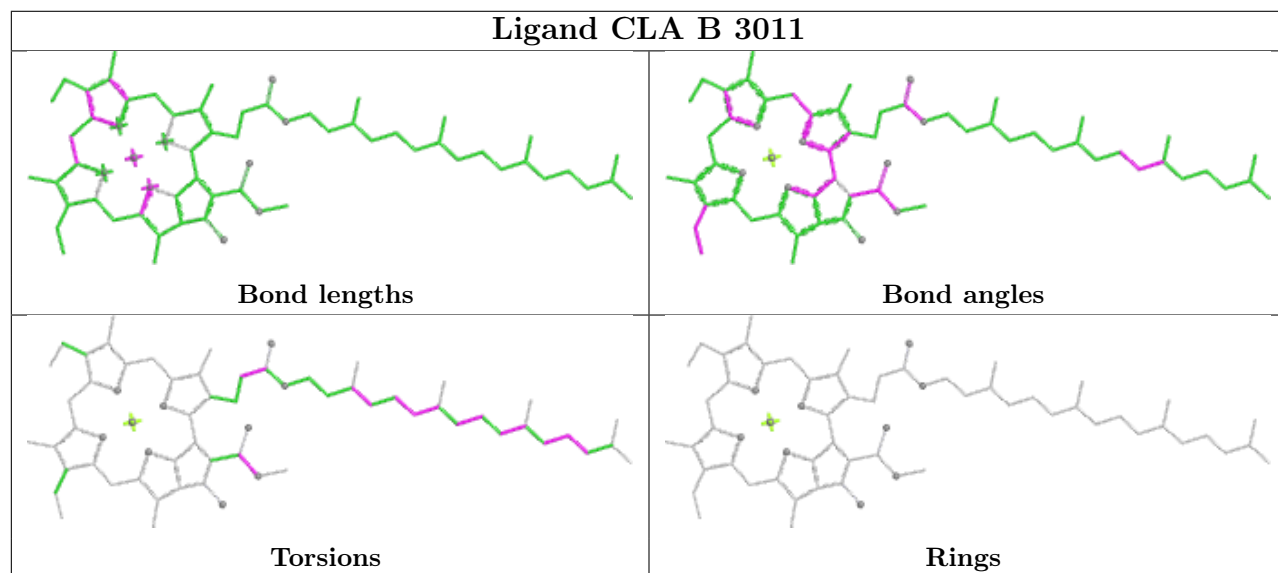




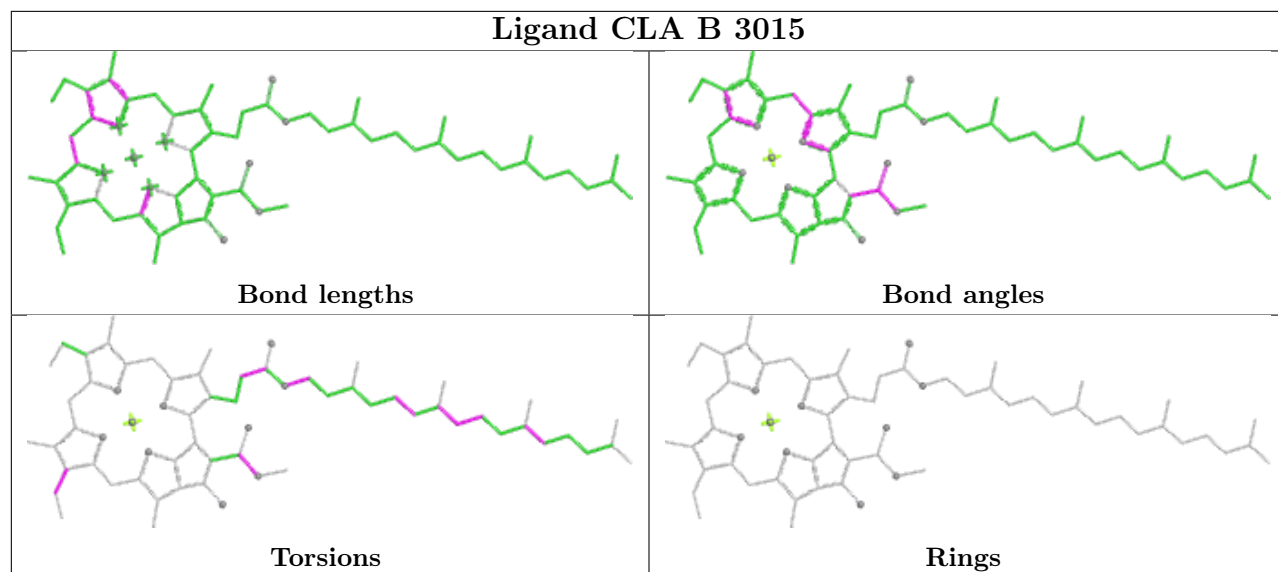
Ligand CLA A 837



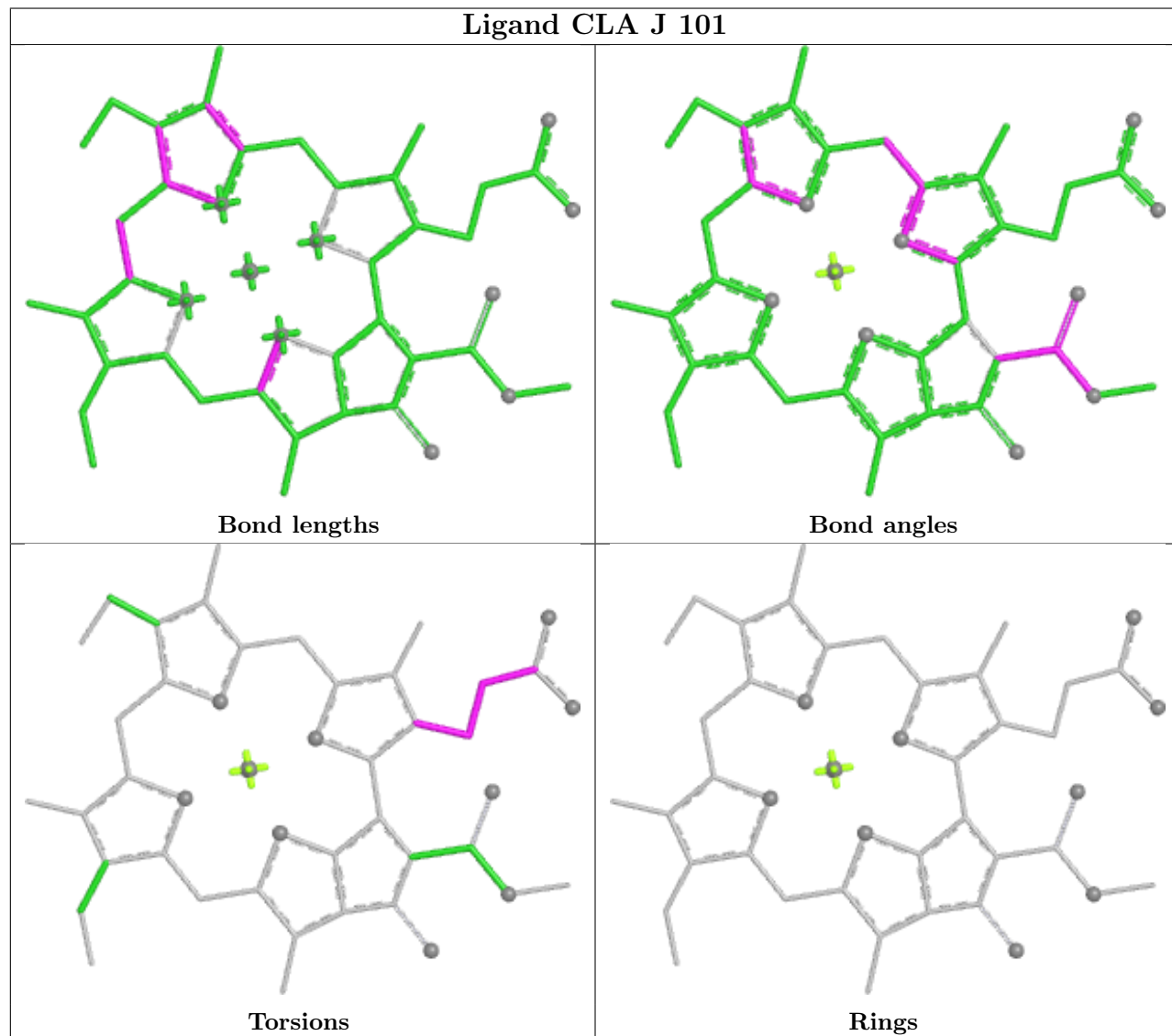
Ligand CLA B 3011

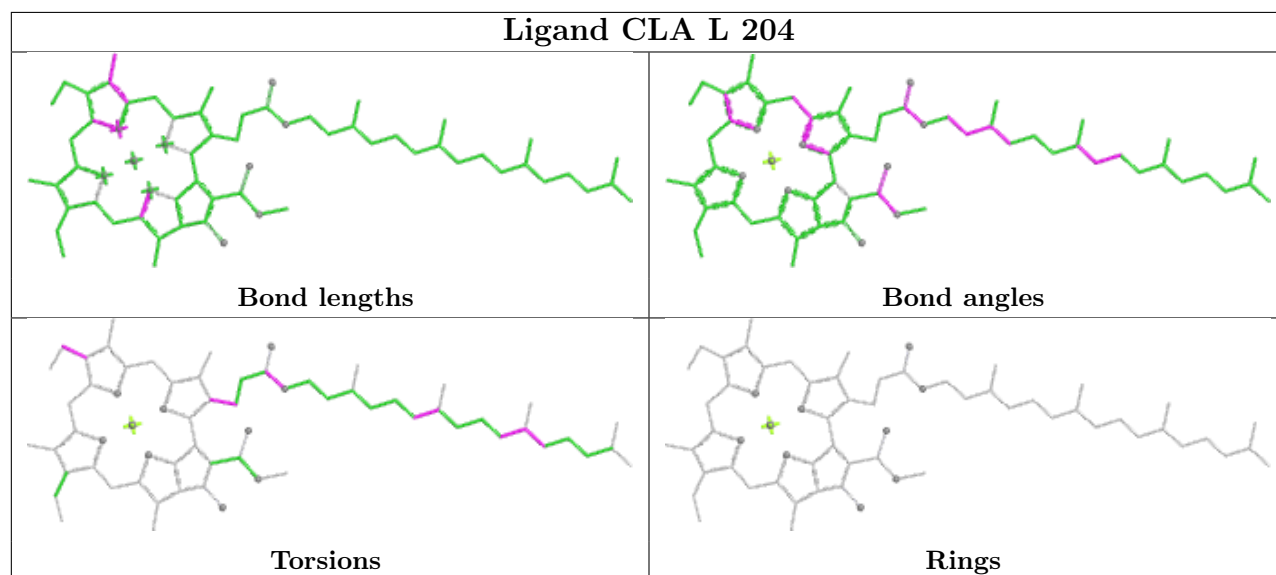
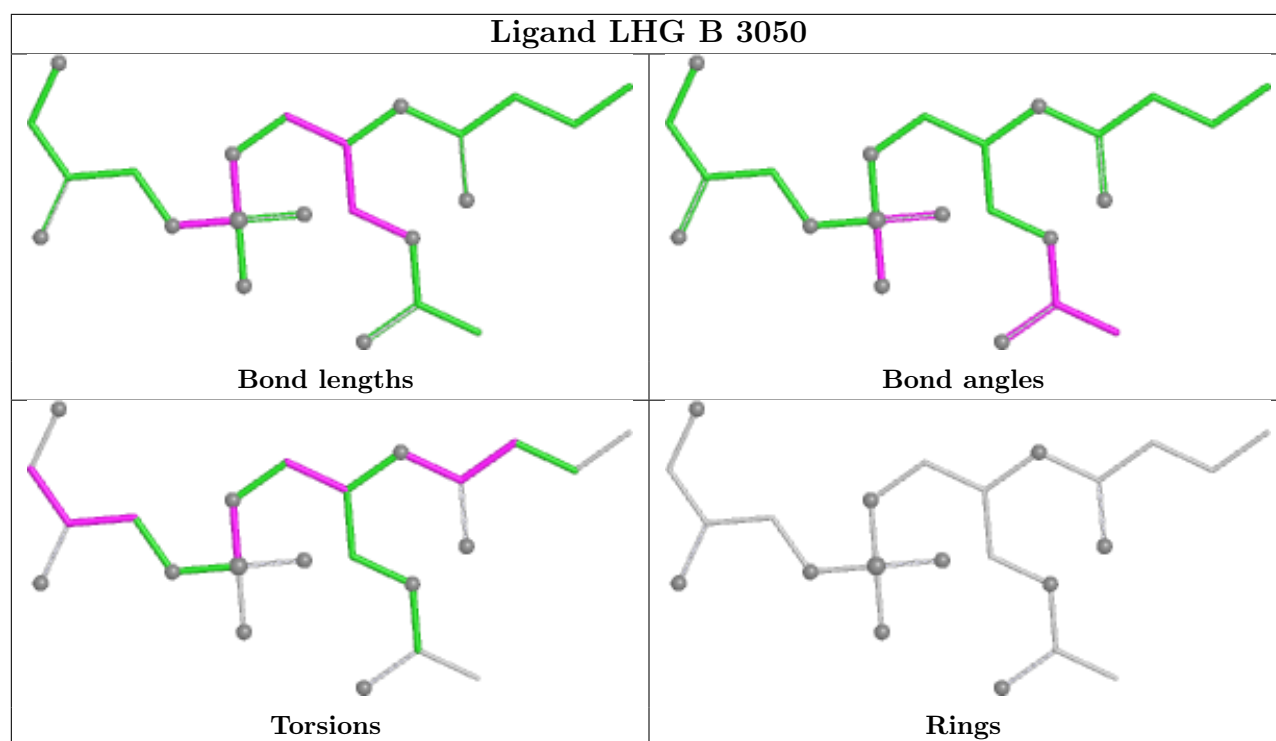


Ligand CLA B 3015

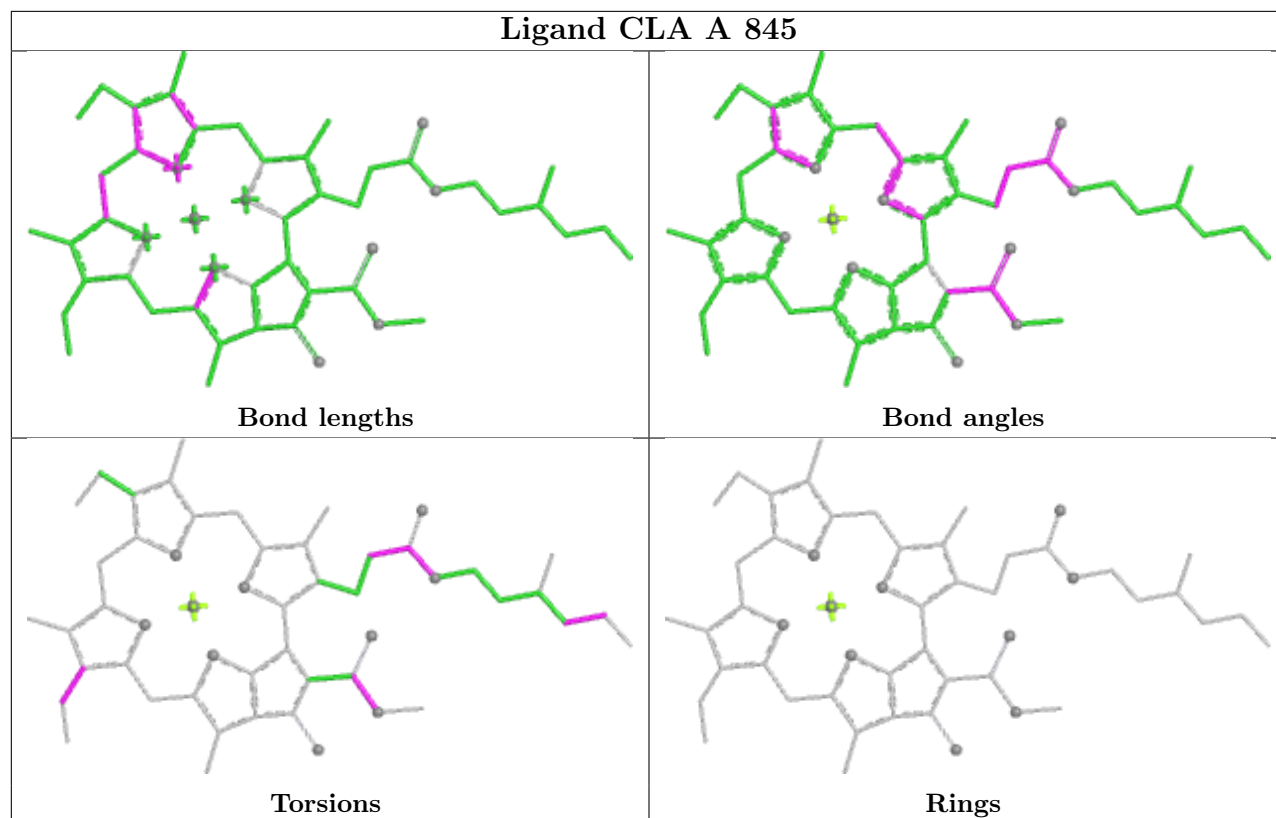


Ligand CLA J 101

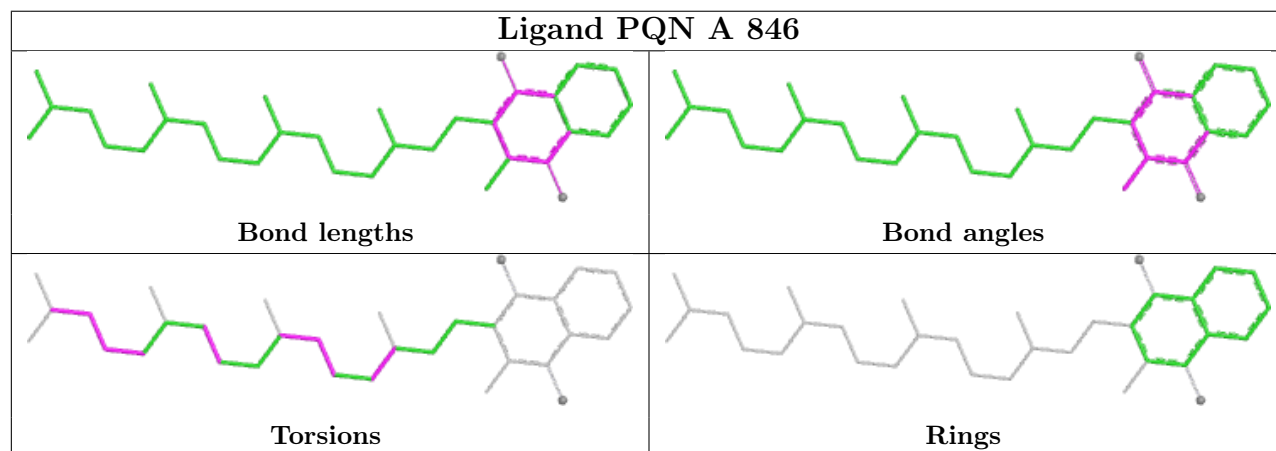




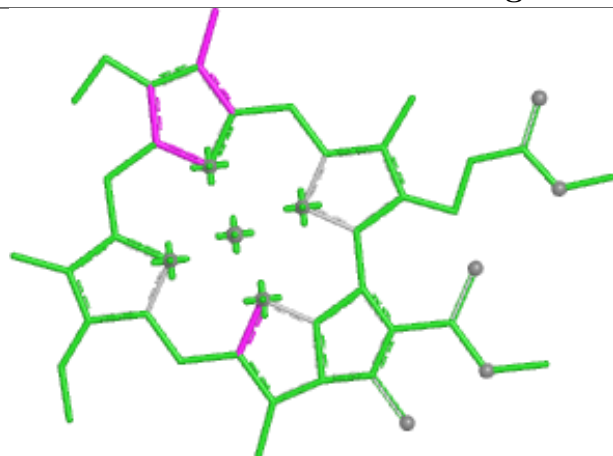
Ligand CLA A 845



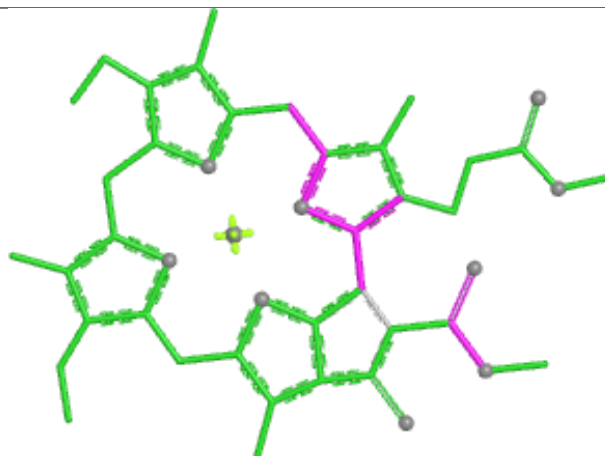
Ligand PQN A 846



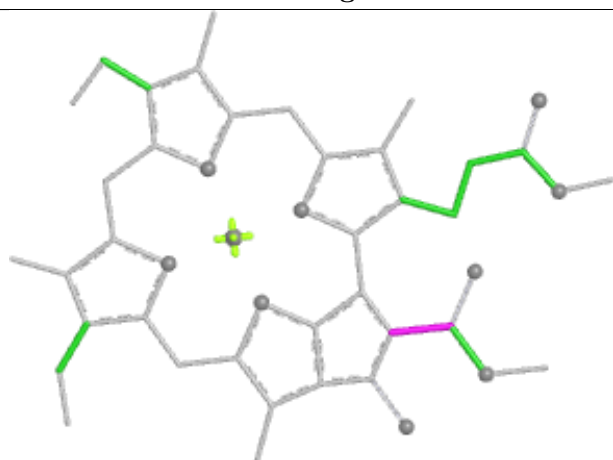
Ligand CLA B 3026



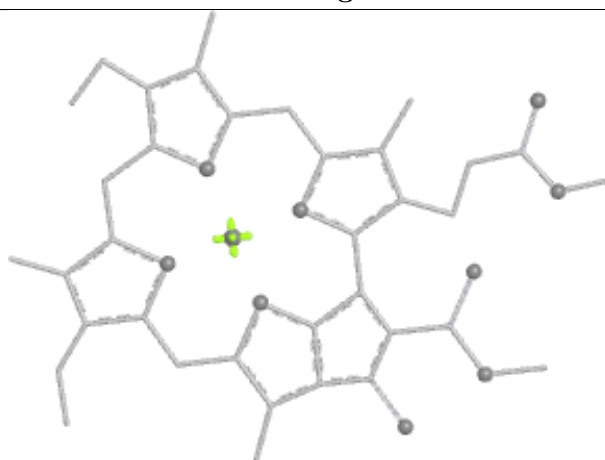
Bond lengths



Bond angles

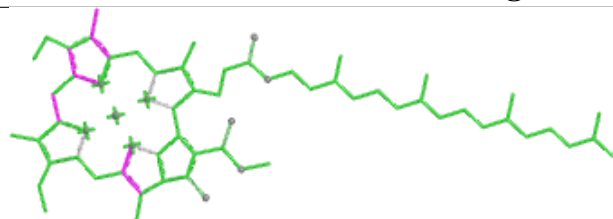


Torsions

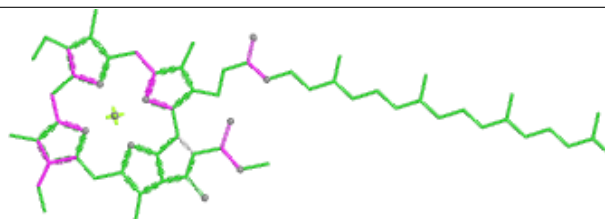


Rings

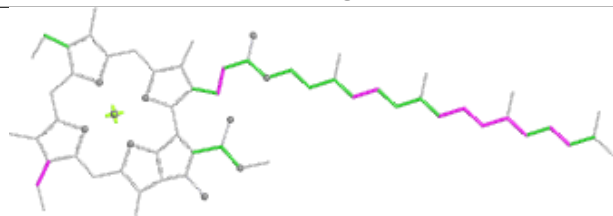
Ligand CLA B 3041



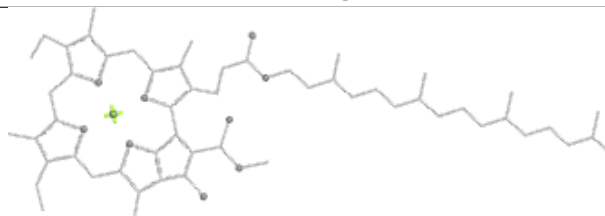
Bond lengths



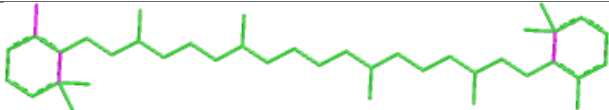
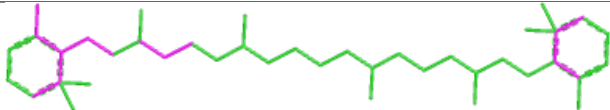
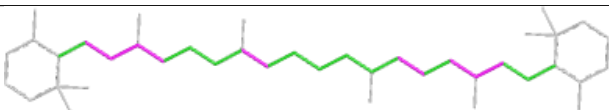
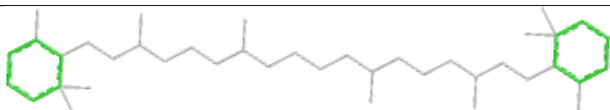
Bond angles

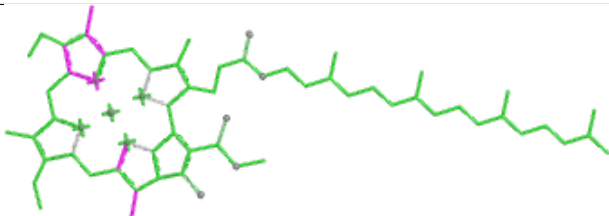
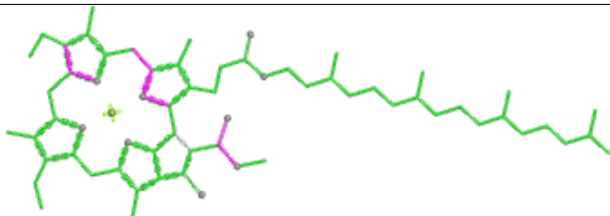
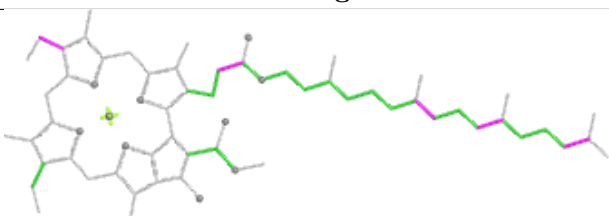
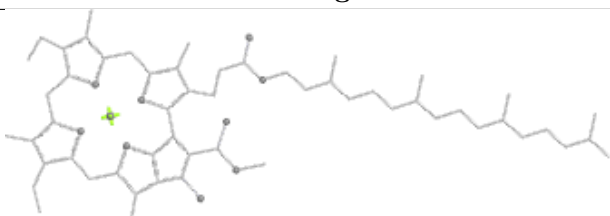


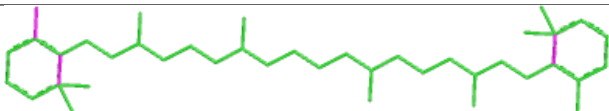
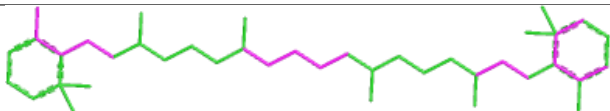
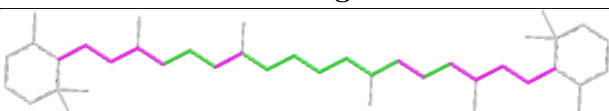
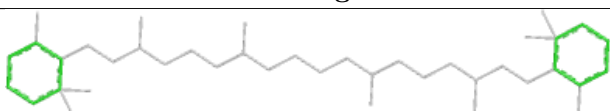
Torsions



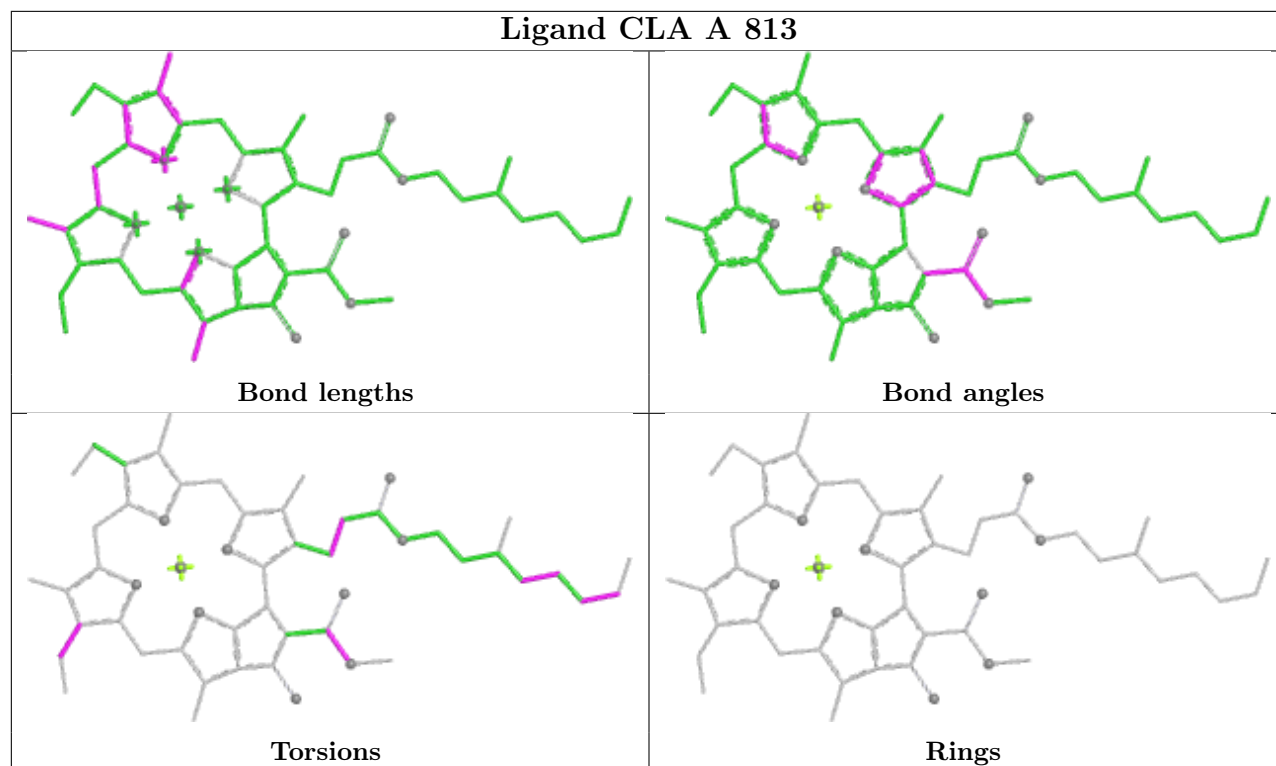
Rings

Ligand BCR B 3044	
	
Bond lengths	Bond angles
	
Torsions	Rings

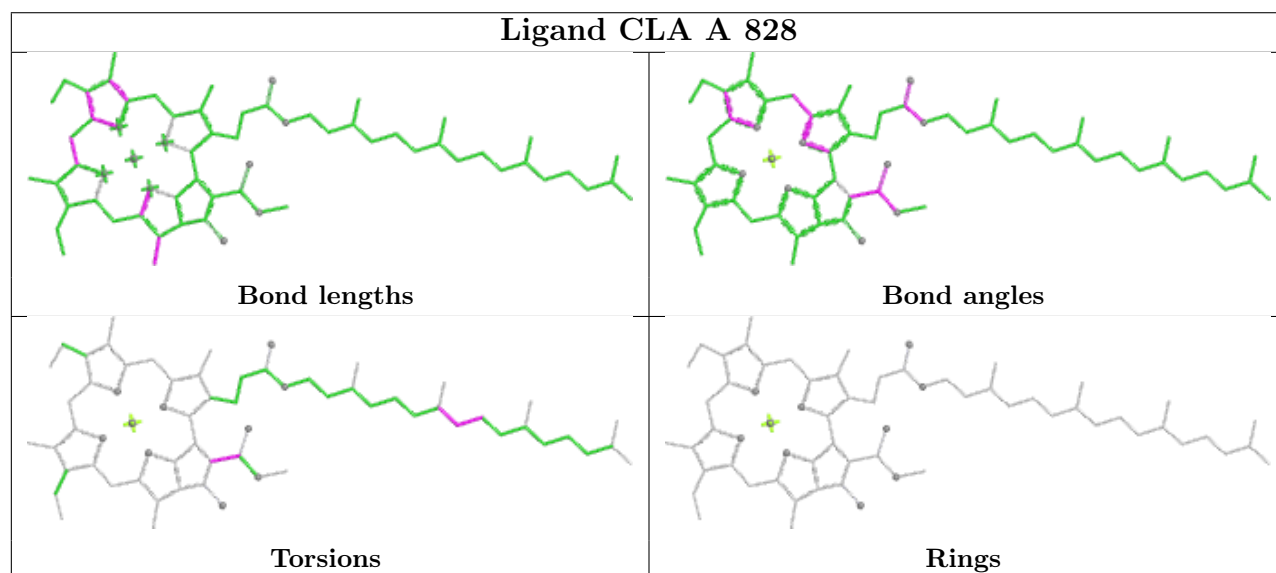
Ligand CLA B 3007	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR J 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

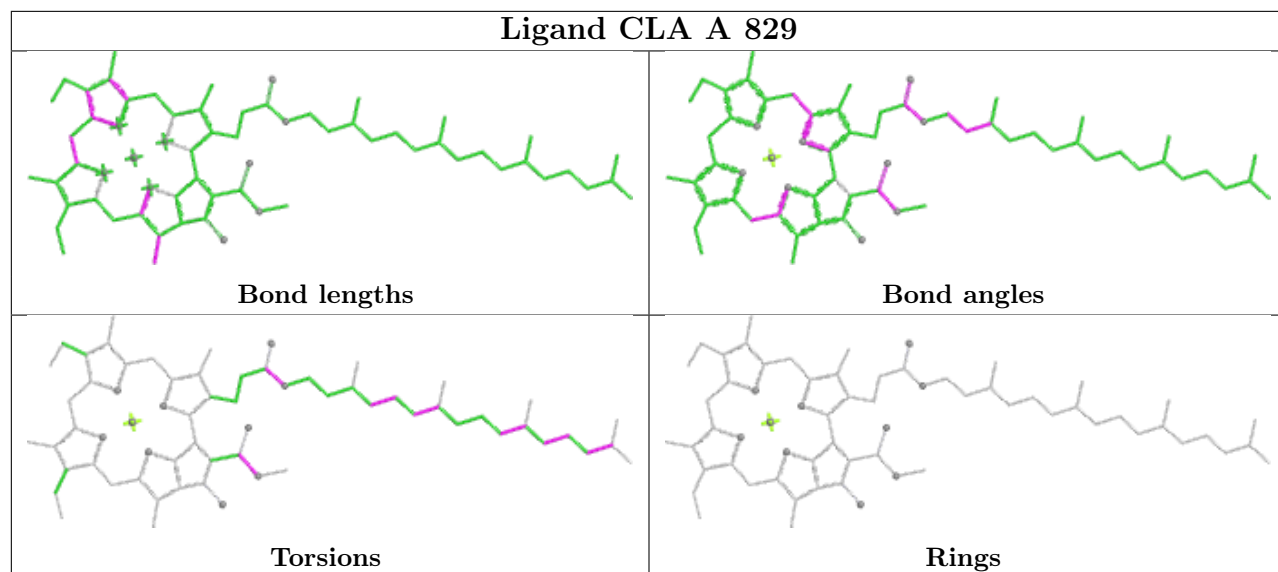
Ligand CLA A 813



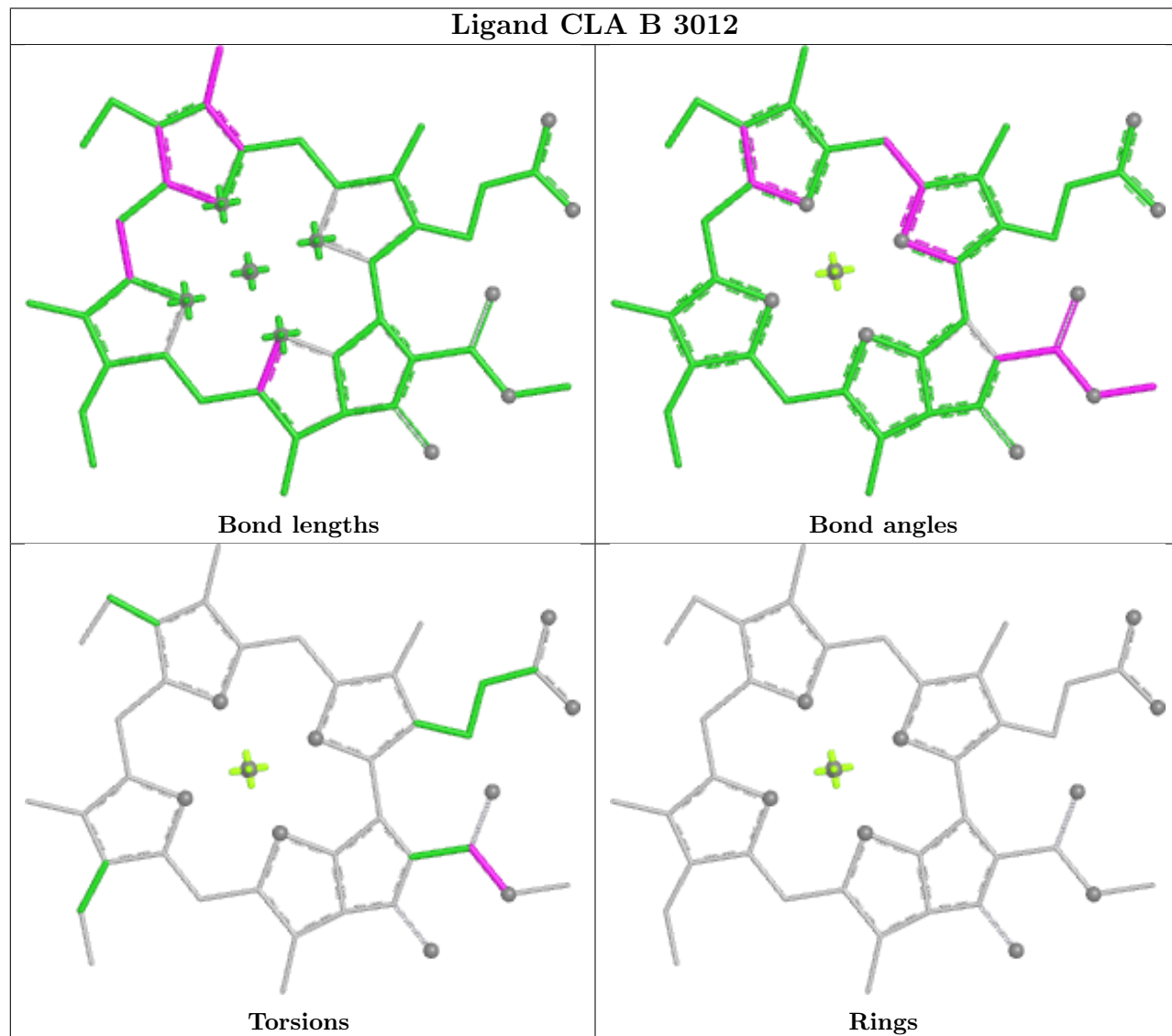
Ligand CLA A 828

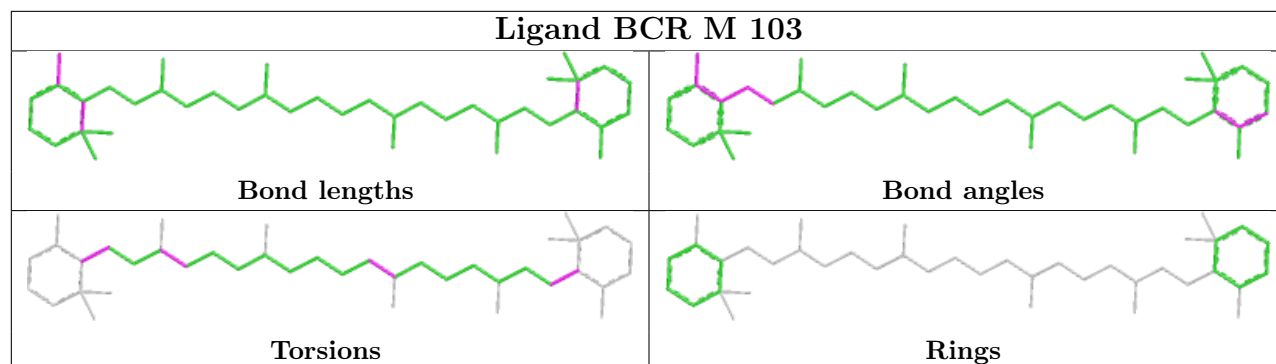
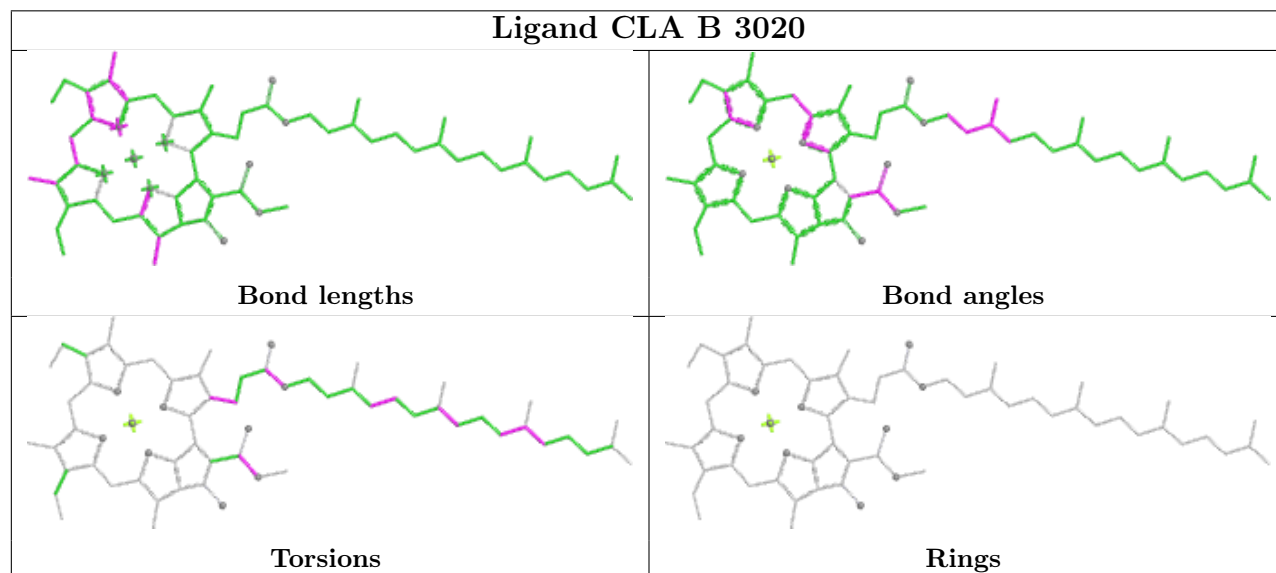
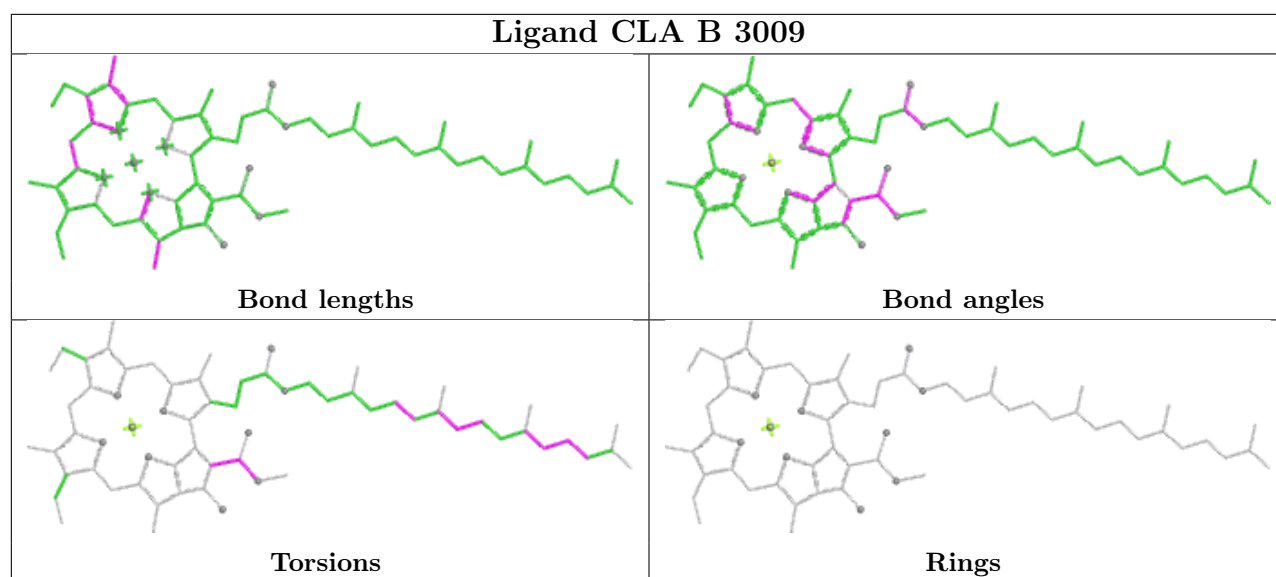


Ligand CLA A 829

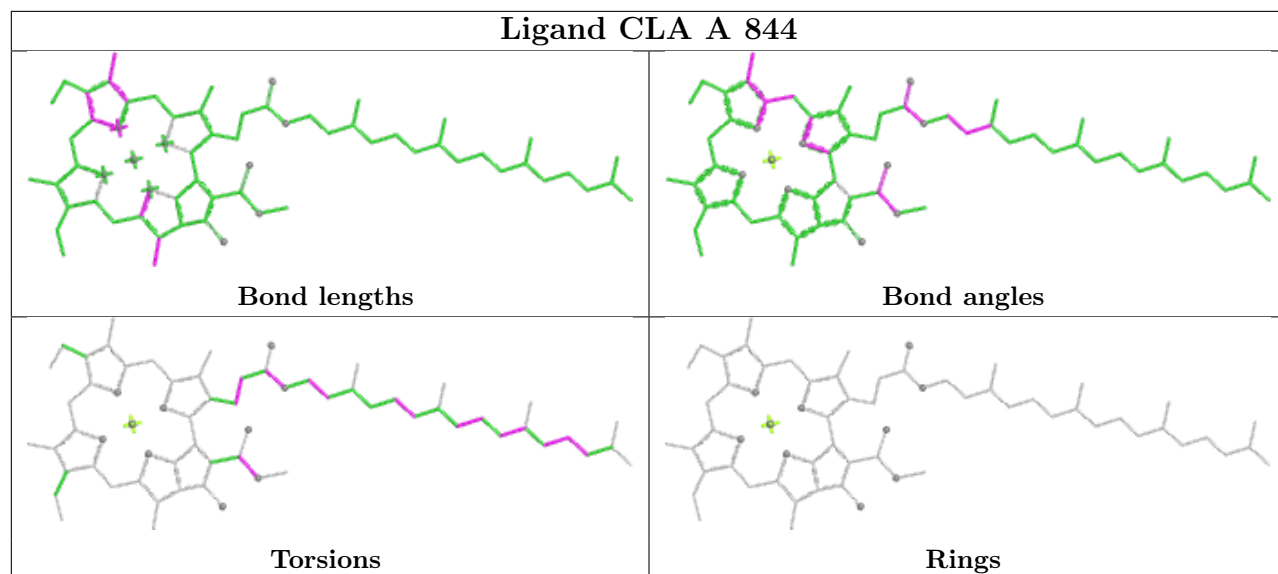


Ligand CLA B 3012

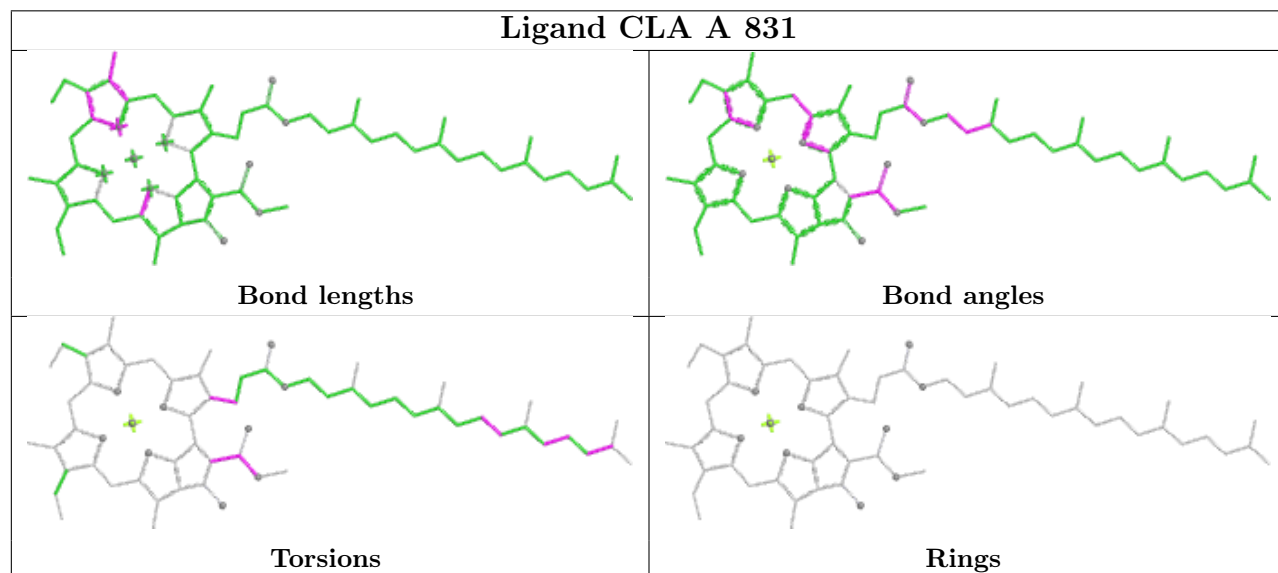


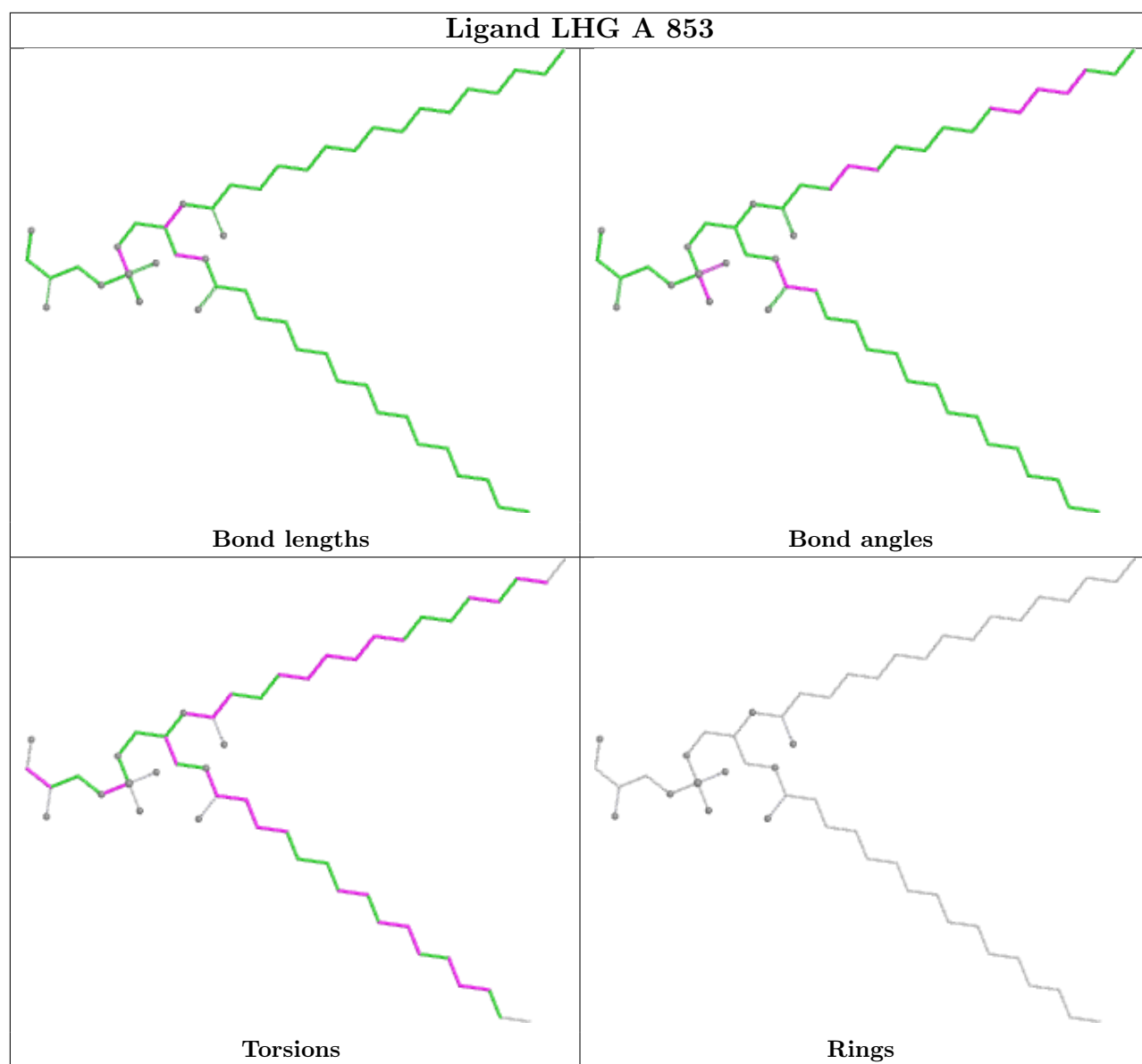


Ligand CLA A 844

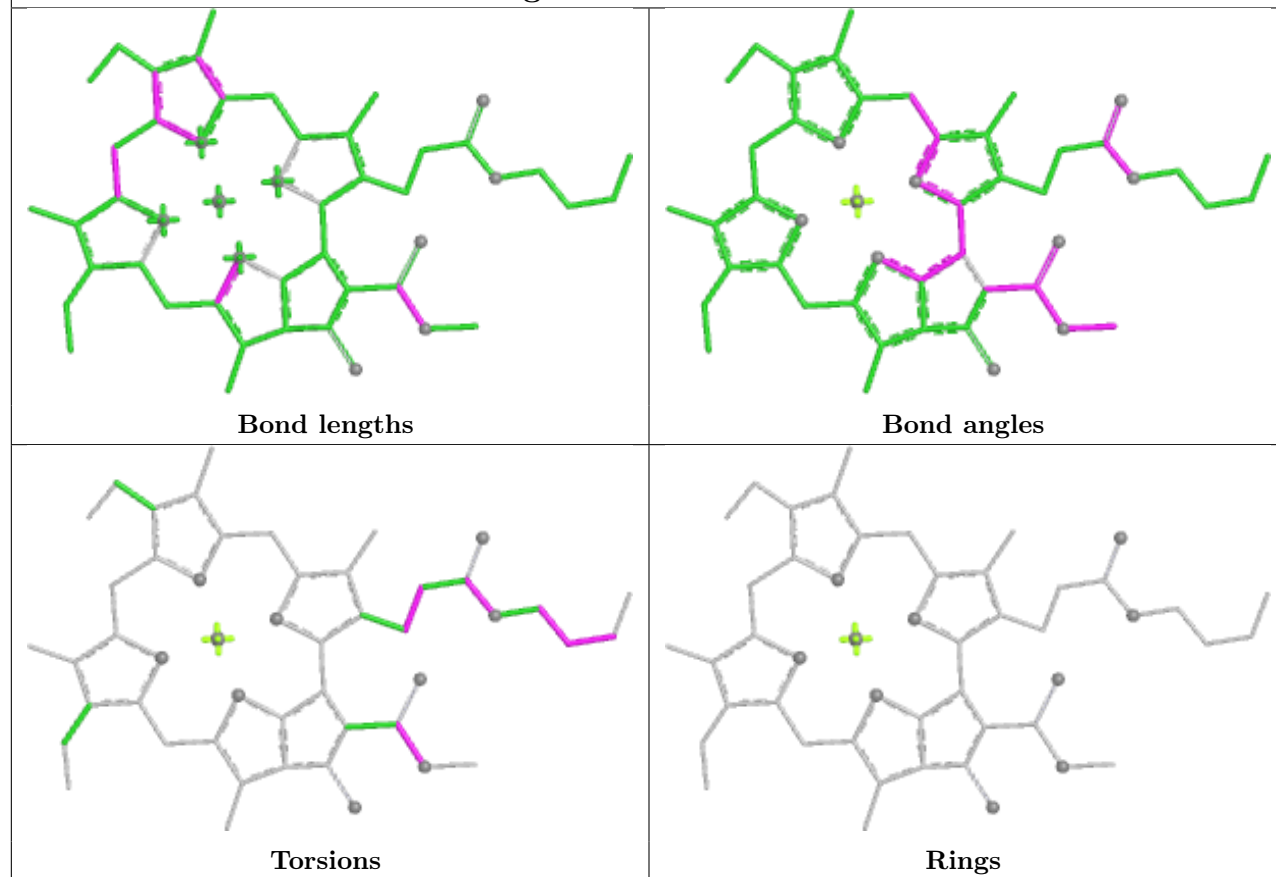


Ligand CLA A 831

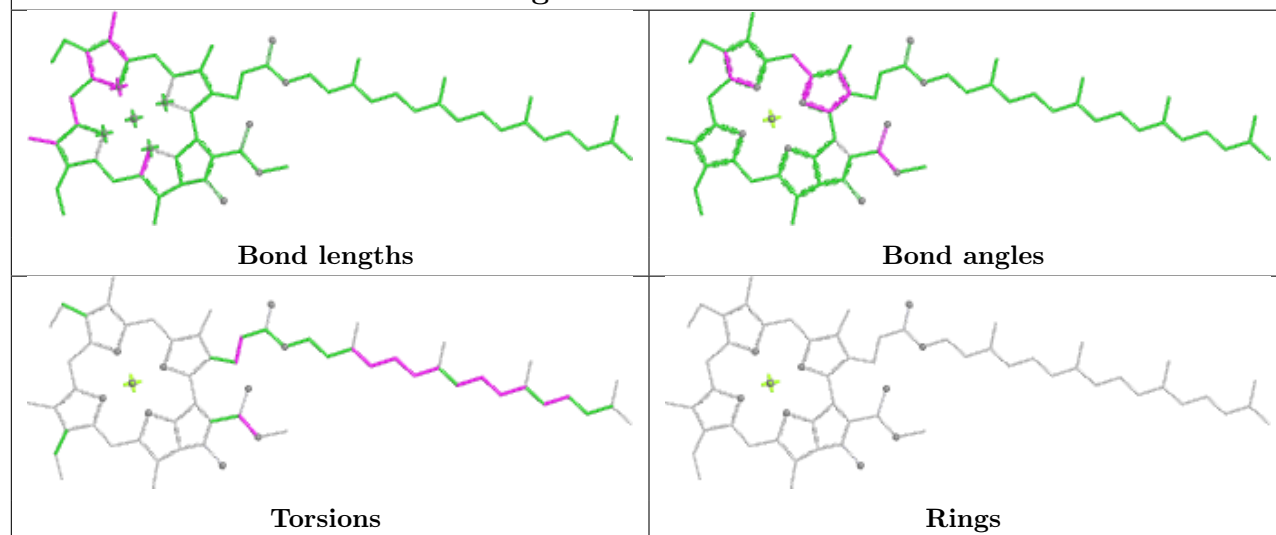




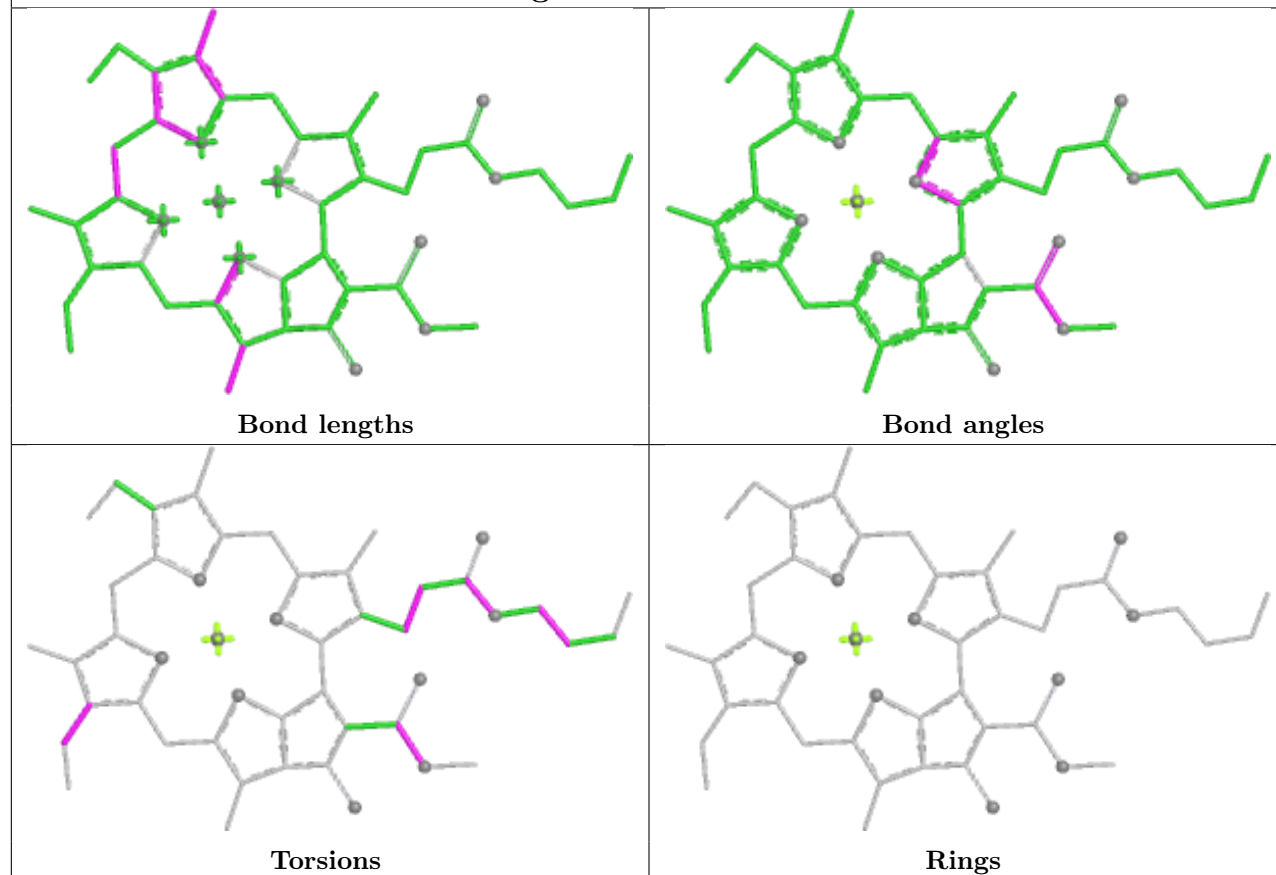
Ligand CLA B 3032



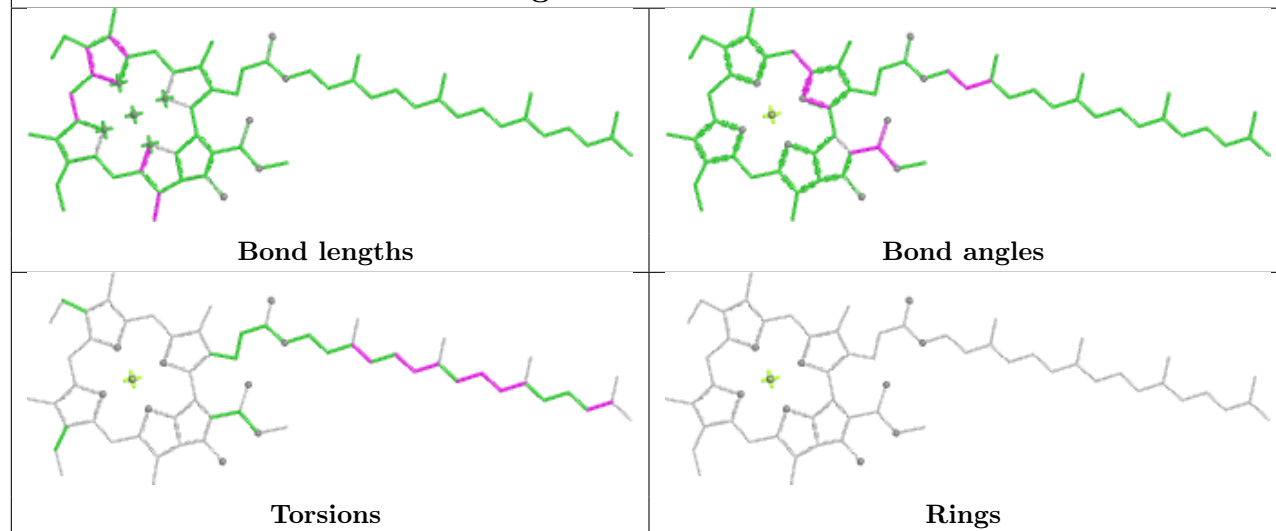
Ligand CLA A 830



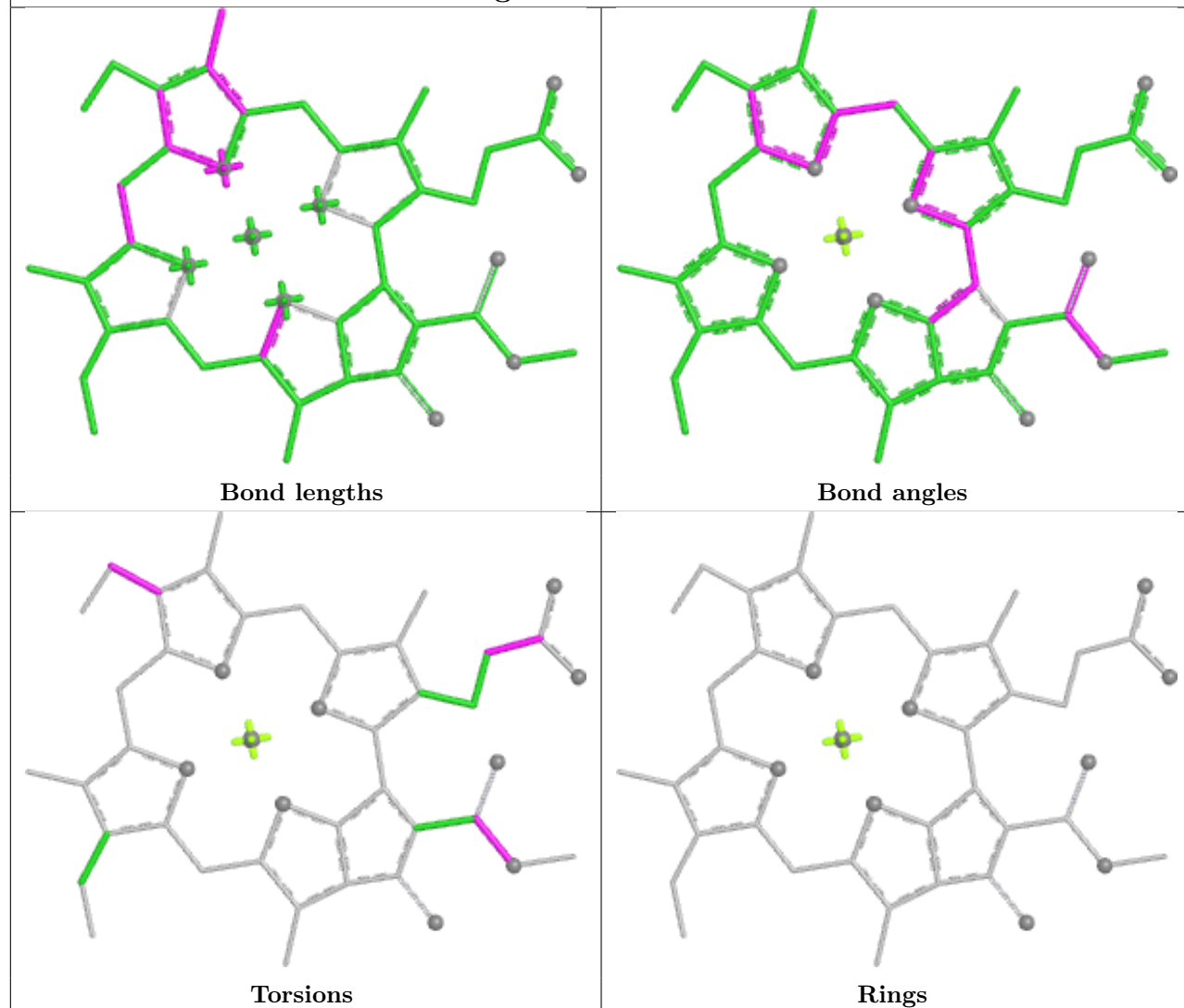
Ligand CLA A 817



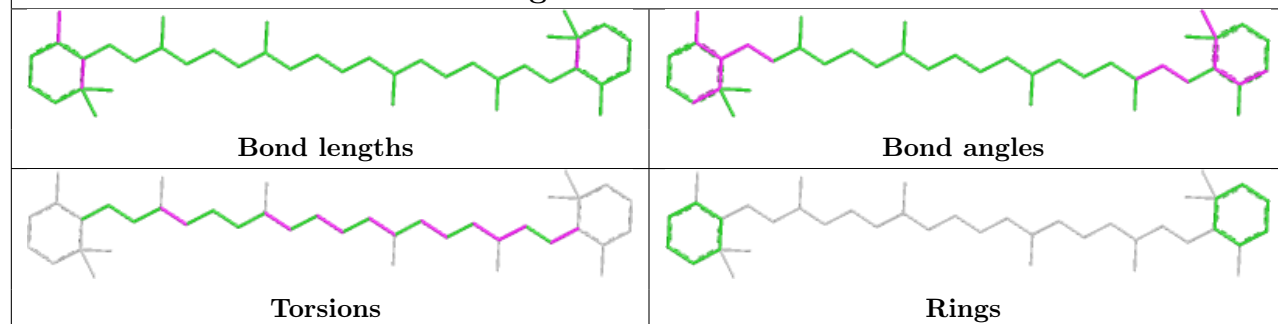
Ligand CLA A 839

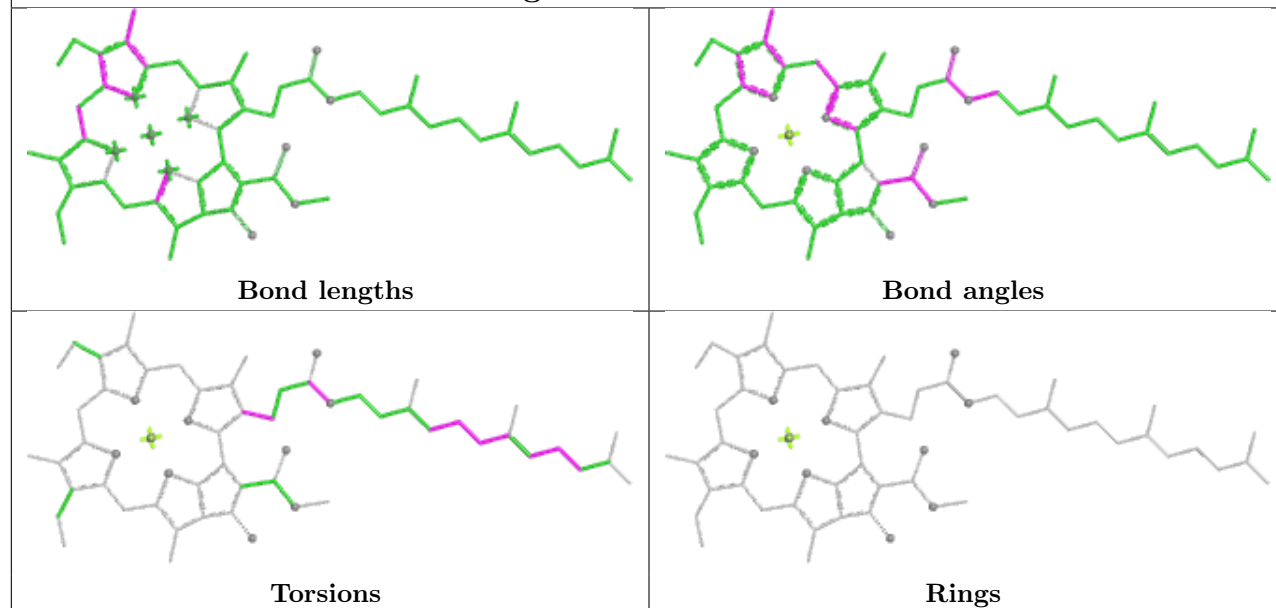
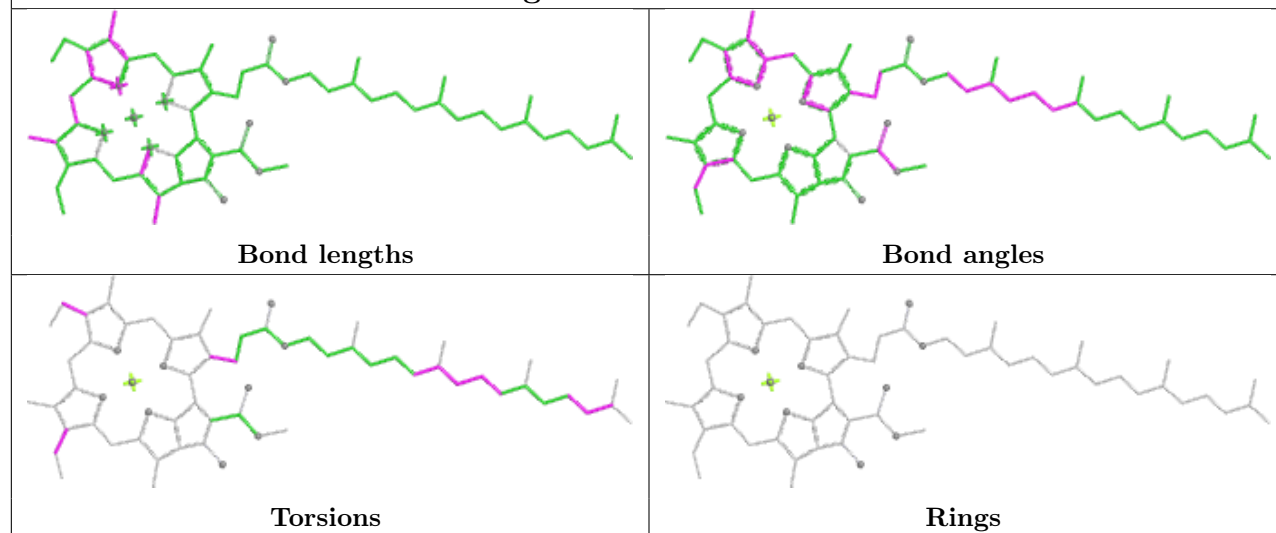


Ligand CLA F 202

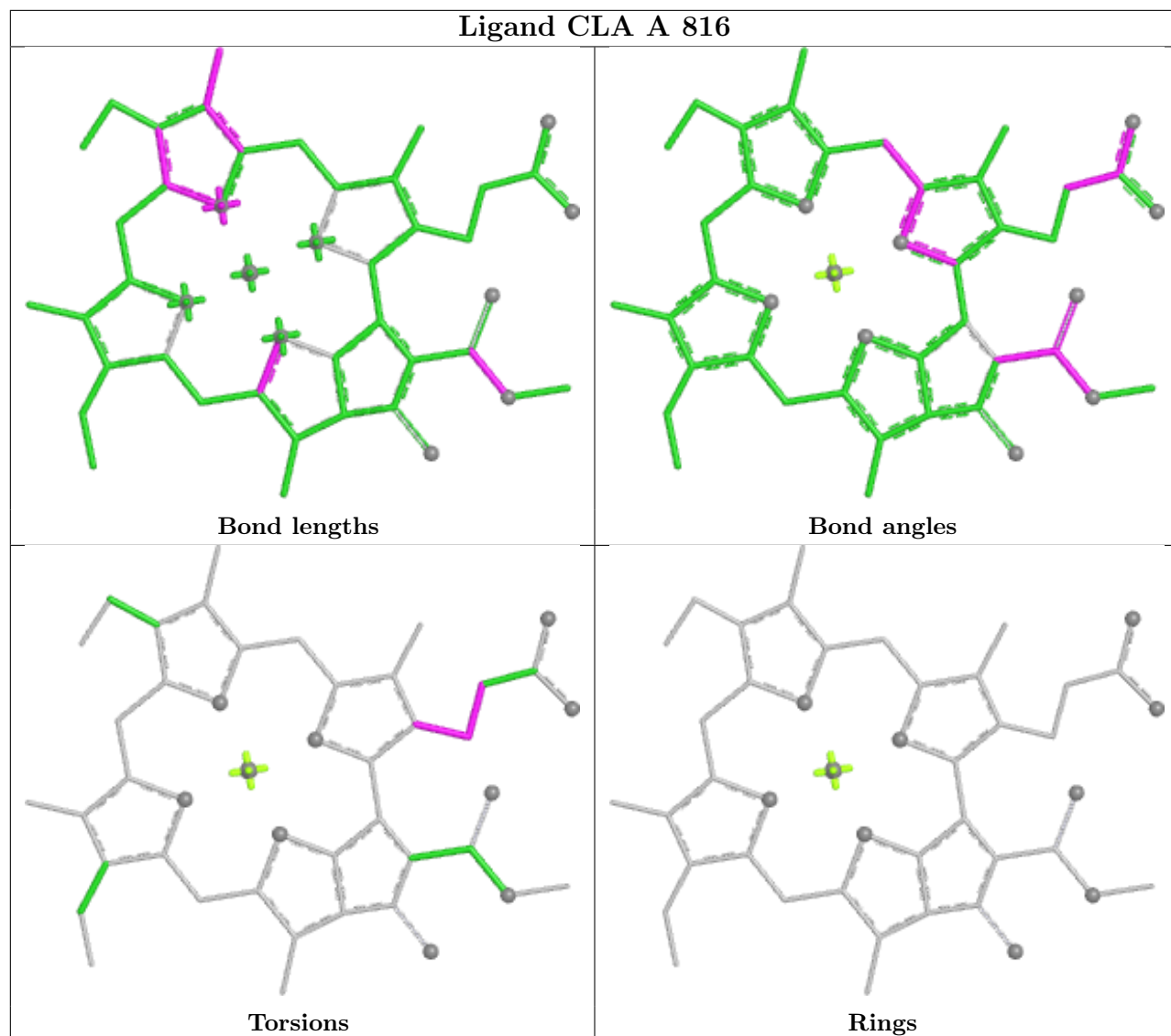


Ligand BCR K 102

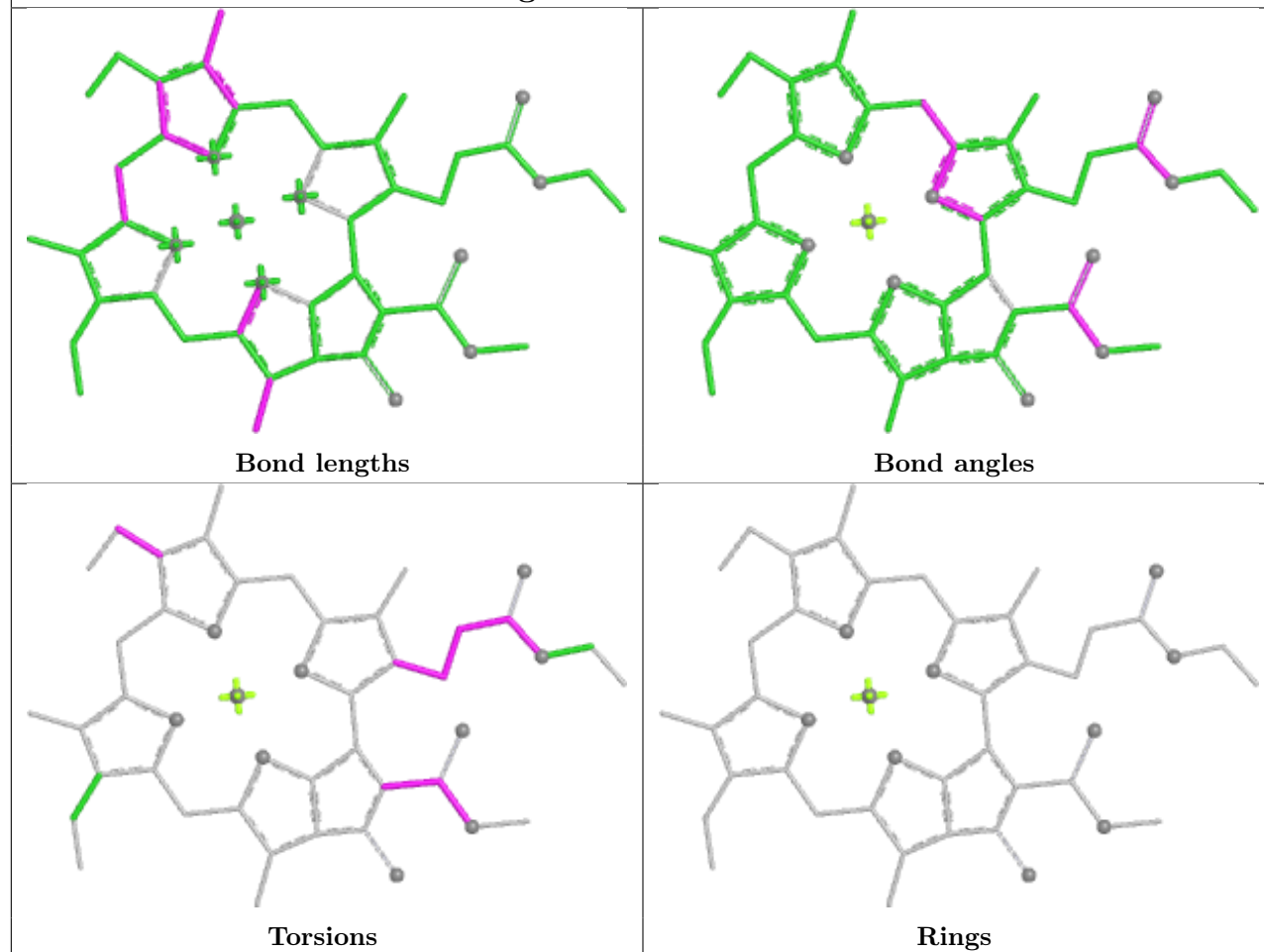


Ligand CLA B 3019**Ligand CLA B 3010**

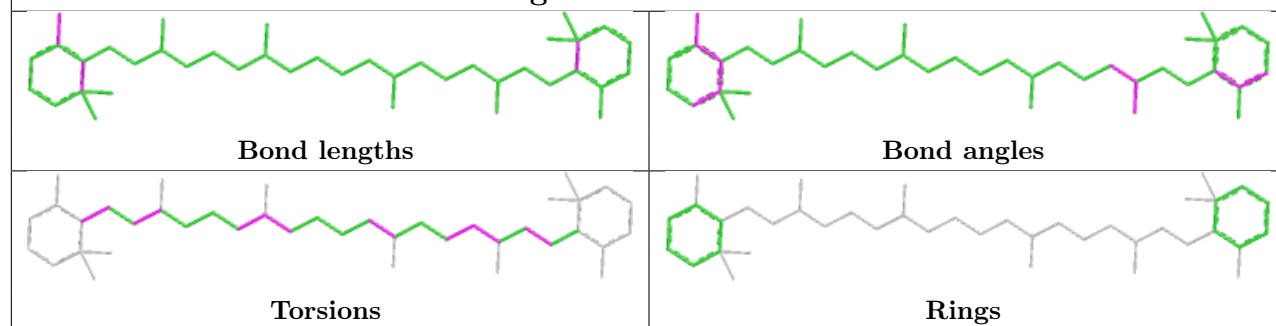
Ligand CLA A 816



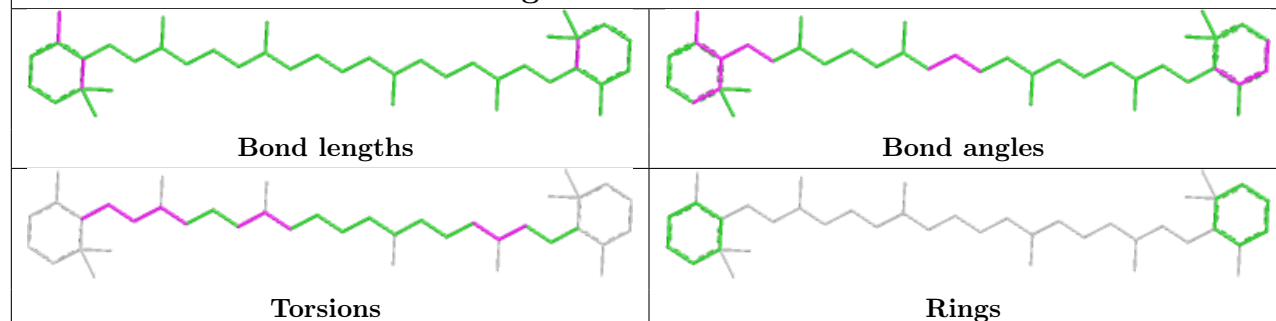
Ligand CLA B 3021

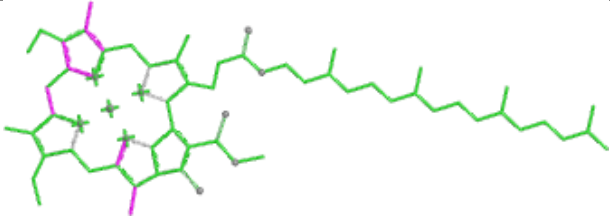
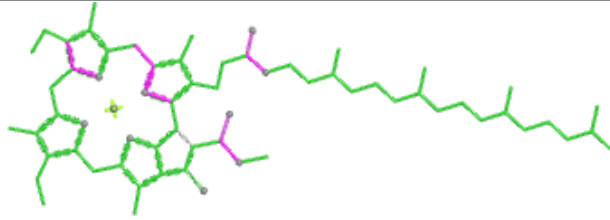
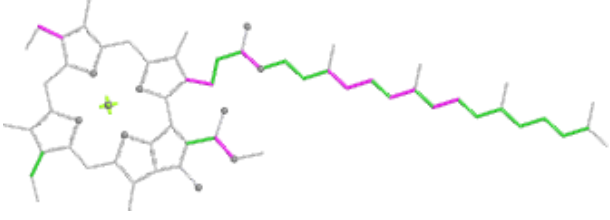
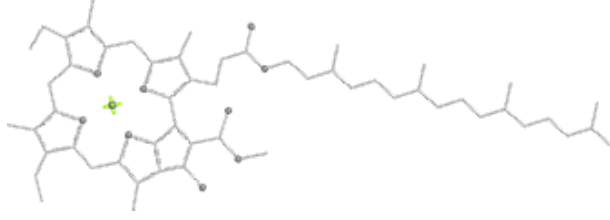


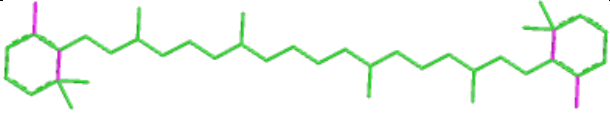
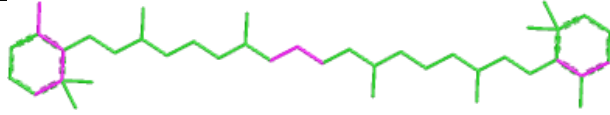
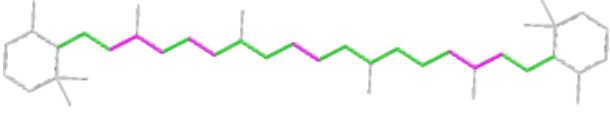
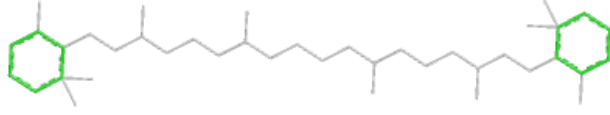
Ligand BCR A 850

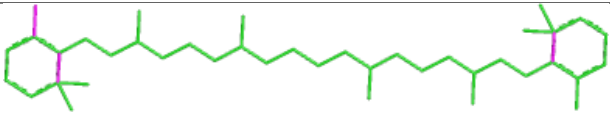
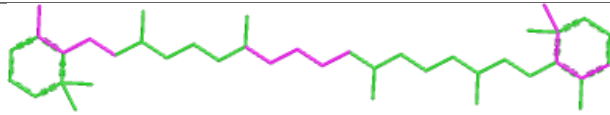
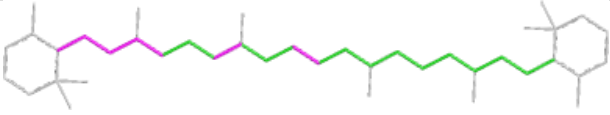
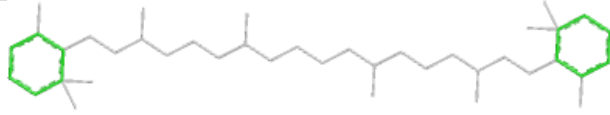


Ligand BCR B 3045



Ligand CLA B 3003			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand BCR F 201			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand BCR L 209			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	740/755 (98%)	-1.51	1 (0%) 92 86	21, 87, 139, 184	0
2	B	739/740 (99%)	-1.78	0 100 100	13, 60, 106, 141	0
3	C	80/80 (100%)	-1.79	0 100 100	12, 53, 81, 91	0
4	D	138/138 (100%)	-1.84	0 100 100	30, 65, 92, 147	0
5	E	69/75 (92%)	-1.72	0 100 100	54, 82, 104, 120	0
6	F	141/164 (85%)	-1.53	0 100 100	54, 106, 125, 133	0
7	I	38/38 (100%)	-1.90	0 100 100	17, 34, 62, 96	0
8	J	41/41 (100%)	-1.28	0 100 100	97, 116, 130, 149	0
9	K	47/83 (56%)	-0.69	0 100 100	132, 166, 183, 200	0
10	L	151/154 (98%)	-1.90	0 100 100	13, 33, 72, 120	0
11	M	31/31 (100%)	-1.79	0 100 100	30, 53, 78, 102	0
12	X	29/35 (82%)	-1.64	0 100 100	67, 87, 116, 130	0
All	All	2244/2334 (96%)	-1.65	1 (0%) 100 100	12, 70, 132, 200	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	ALA	2.5

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 oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	K	101	41/65	0.96	0.10	112,149,185,194	0
14	CLA	A	816	45/65	0.97	0.11	105,143,169,179	0
14	CLA	A	817	49/65	0.97	0.07	63,127,159,160	0
14	CLA	A	821	43/65	0.97	0.10	72,130,170,176	0
14	CLA	A	813	54/65	0.97	0.07	74,100,128,136	0
14	CLA	A	818	54/65	0.98	0.09	95,124,151,161	0
14	CLA	A	812	65/65	0.98	0.09	81,114,144,146	0
14	CLA	A	823	49/65	0.98	0.07	78,116,146,158	0
14	CLA	J	101	45/65	0.98	0.06	118,137,171,176	0
14	CLA	J	102	37/65	0.98	0.05	102,125,149,163	0
14	CLA	A	815	45/65	0.98	0.09	85,114,150,156	0
14	CLA	K	103	45/65	0.98	0.05	101,132,164,166	0
14	CLA	X	1701	45/65	0.98	0.06	75,104,134,140	0
16	BCR	A	847	40/40	0.98	0.06	96,131,161,175	0
16	BCR	J	104	40/40	0.98	0.05	78,116,145,150	0
16	BCR	K	102	40/40	0.98	0.09	107,147,166,175	0
17	LMG	A	852	48/55	0.98	0.06	56,113,152,160	0
18	LHG	B	3050	23/49	0.98	0.05	73,111,139,145	0
21	LMT	L	202	35/35	0.98	0.06	74,142,179,192	0
22	DGD	L	207	66/66	0.98	0.05	45,99,155,168	0
14	CLA	A	829	65/65	0.99	0.05	59,85,110,117	0
14	CLA	A	831	65/65	0.99	0.04	55,87,110,118	0
14	CLA	A	836	54/65	0.99	0.04	47,87,128,136	0
14	CLA	A	837	45/65	0.99	0.05	80,104,127,137	0
14	CLA	B	3012	45/65	0.99	0.03	45,67,88,111	0
14	CLA	B	3013	45/65	0.99	0.04	57,89,115,119	0
14	CLA	B	3017	55/65	0.99	0.04	61,96,133,166	0
14	CLA	B	3020	65/65	0.99	0.04	48,91,121,132	0
14	CLA	B	3021	47/65	0.99	0.04	69,98,129,135	0
14	CLA	B	3022	45/65	0.99	0.04	67,93,119,120	0
14	CLA	B	3023	55/65	0.99	0.04	69,94,122,122	0
14	CLA	B	3036	45/65	0.99	0.03	44,79,107,111	0
14	CLA	B	3037	45/65	0.99	0.04	64,88,120,121	0
14	CLA	F	202	45/65	0.99	0.06	86,115,145,151	0
14	CLA	A	808	51/65	0.99	0.04	81,103,130,133	0
14	CLA	A	810	65/65	0.99	0.04	44,99,148,161	0
14	CLA	A	811	45/65	0.99	0.06	92,125,152,159	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	A	805	59/65	0.99	0.04	75,98,125,141	0
14	CLA	M	102	45/65	0.99	0.09	83,131,166,180	0
14	CLA	A	819	54/65	0.99	0.05	61,94,116,132	0
14	CLA	A	820	65/65	0.99	0.04	65,100,125,134	0
16	BCR	A	848	40/40	0.99	0.06	77,119,171,177	0
16	BCR	A	849	40/40	0.99	0.04	61,91,155,157	0
16	BCR	A	850	40/40	0.99	0.04	41,74,108,125	0
16	BCR	B	3044	40/40	0.99	0.06	75,110,143,161	0
16	BCR	B	3046	40/40	0.99	0.05	43,76,131,143	0
16	BCR	B	3047	40/40	0.99	0.04	54,79,99,106	0
16	BCR	B	3051	40/40	0.99	0.04	46,84,127,134	0
16	BCR	F	201	40/40	0.99	0.07	45,91,124,132	0
16	BCR	F	203	40/40	0.99	0.04	43,94,126,147	0
14	CLA	A	806	65/65	0.99	0.04	67,101,136,142	0
16	BCR	J	105	40/40	0.99	0.06	67,114,154,161	0
14	CLA	A	822	65/65	0.99	0.04	51,87,121,127	0
16	BCR	M	103	40/40	0.99	0.03	21,48,76,82	0
14	CLA	A	814	60/65	0.99	0.08	73,115,140,141	0
17	LMG	A	855	30/55	0.99	0.06	32,83,145,162	0
17	LMG	I	102	40/55	0.99	0.07	49,85,120,144	0
14	CLA	A	824	51/65	0.99	0.05	67,101,132,138	0
18	LHG	M	101	49/49	0.99	0.05	47,89,164,181	0
14	CLA	A	826	65/65	0.99	0.05	71,100,131,134	0
14	CLA	A	828	65/65	0.99	0.05	59,93,128,135	0
14	CLA	B	3018	59/65	1.00	0.04	47,81,109,117	0
14	CLA	B	3019	60/65	1.00	0.03	49,70,100,107	0
14	CLA	A	803	65/65	1.00	0.02	42,67,87,108	0
14	CLA	A	809	65/65	1.00	0.03	38,84,123,129	0
14	CLA	A	830	65/65	1.00	0.04	55,88,118,121	0
14	CLA	A	804	65/65	1.00	0.03	59,98,125,132	0
14	CLA	B	3024	45/65	1.00	0.02	30,61,94,106	0
14	CLA	B	3025	54/65	1.00	0.02	48,64,87,87	0
14	CLA	B	3026	46/65	1.00	0.02	36,64,89,90	0
14	CLA	B	3027	65/65	1.00	0.03	38,65,91,97	0
14	CLA	B	3028	65/65	1.00	0.03	15,48,100,102	0
14	CLA	B	3029	65/65	1.00	0.02	27,61,79,97	0
14	CLA	B	3030	65/65	1.00	0.02	20,47,80,98	0
14	CLA	B	3031	45/65	1.00	0.03	46,73,95,113	0
14	CLA	B	3032	49/65	1.00	0.03	34,69,97,122	0
14	CLA	B	3033	65/65	1.00	0.03	56,86,112,121	0
14	CLA	B	3034	58/65	1.00	0.05	63,98,137,141	0
14	CLA	B	3035	45/65	1.00	0.03	55,73,95,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	A	832	50/65	1.00	0.03	33,61,91,117	0
14	CLA	A	833	65/65	1.00	0.03	24,63,135,140	0
14	CLA	B	3038	60/65	1.00	0.03	41,81,112,122	0
14	CLA	B	3039	65/65	1.00	0.03	42,88,128,143	0
14	CLA	B	3040	47/65	1.00	0.02	49,74,93,105	0
14	CLA	B	3041	65/65	1.00	0.01	2,18,52,58	0
14	CLA	B	3042	65/65	1.00	0.02	4,29,52,55	0
14	CLA	A	834	65/65	1.00	0.02	10,37,65,71	0
14	CLA	A	835	65/65	1.00	0.02	2,32,62,90	0
13	CL0	A	801	65/65	1.00	0.03	2,46,71,74	0
14	CLA	A	802	65/65	1.00	0.02	20,38,54,75	0
14	CLA	A	838	51/65	1.00	0.02	36,59,79,102	0
14	CLA	L	204	65/65	1.00	0.02	11,41,72,93	0
14	CLA	L	205	65/65	1.00	0.02	8,45,117,130	0
14	CLA	L	206	65/65	1.00	0.02	21,46,75,85	0
14	CLA	A	839	65/65	1.00	0.03	21,59,97,120	0
14	CLA	A	840	47/65	1.00	0.03	22,55,75,93	0
15	PQN	A	846	33/33	1.00	0.04	61,89,118,121	0
15	PQN	B	3043	33/33	1.00	0.03	27,47,66,70	0
14	CLA	A	841	65/65	1.00	0.02	32,69,123,132	0
14	CLA	A	842	51/65	1.00	0.04	36,75,124,143	0
14	CLA	A	843	65/65	1.00	0.02	37,73,117,135	0
14	CLA	A	844	65/65	1.00	0.02	2,17,50,59	0
16	BCR	A	851	40/40	1.00	0.03	20,63,90,93	0
14	CLA	A	845	52/65	1.00	0.03	44,84,111,120	0
16	BCR	B	3045	40/40	1.00	0.02	48,74,114,123	0
14	CLA	A	856	65/65	1.00	0.03	38,65,91,102	0
14	CLA	B	3003	65/65	1.00	0.03	16,49,70,76	0
16	BCR	B	3048	40/40	1.00	0.02	14,34,61,61	0
14	CLA	B	3004	65/65	1.00	0.02	9,33,53,64	0
14	CLA	B	3005	54/65	1.00	0.02	23,48,67,74	0
14	CLA	B	3006	65/65	1.00	0.02	26,56,90,101	0
16	BCR	I	101	40/40	1.00	0.02	2,28,50,68	0
16	BCR	J	103	40/40	1.00	0.04	60,102,125,129	0
14	CLA	B	3007	65/65	1.00	0.02	22,50,77,90	0
14	CLA	B	3008	65/65	1.00	0.02	10,35,66,89	0
14	CLA	B	3009	65/65	1.00	0.02	10,39,72,76	0
16	BCR	L	201	40/40	1.00	0.02	2,34,59,61	0
16	BCR	L	208	40/40	1.00	0.02	3,28,48,65	0
16	BCR	L	209	40/40	1.00	0.02	2,38,86,98	0
14	CLA	B	3010	65/65	1.00	0.02	5,38,66,90	0
14	CLA	B	3011	65/65	1.00	0.02	2,24,59,69	0

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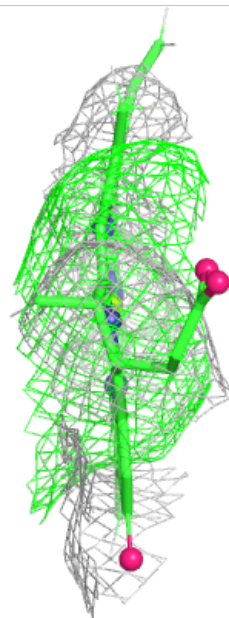
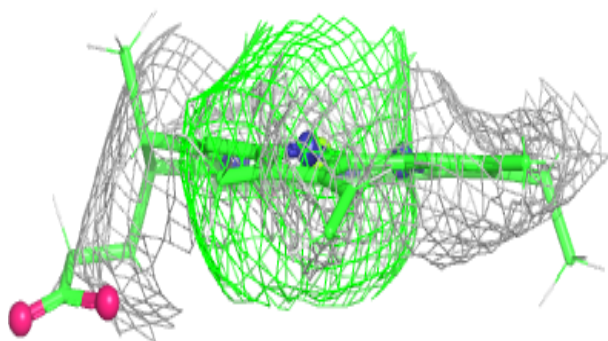
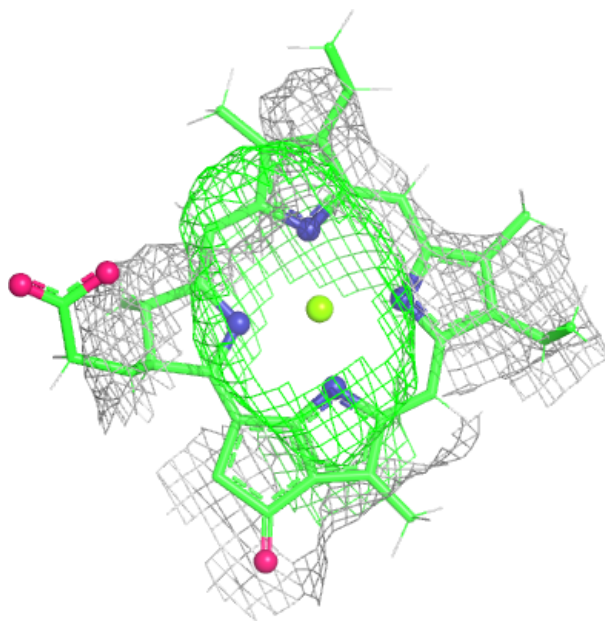
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CLA	A	825	59/65	1.00	0.03	49,83,123,135	0
17	LMG	B	3049	55/55	1.00	0.03	20,58,84,87	0
14	CLA	A	807	65/65	1.00	0.03	56,84,110,116	0
18	LHG	A	853	49/49	1.00	0.04	38,84,108,118	0
18	LHG	A	854	27/49	1.00	0.03	46,79,116,117	0
14	CLA	B	3014	65/65	1.00	0.03	42,72,99,102	0
14	CLA	B	3015	65/65	1.00	0.03	45,77,112,117	0
19	SF4	B	3001	8/8	1.00	0.01	29,46,88,118	0
19	SF4	C	101	8/8	1.00	0.01	23,51,58,71	0
19	SF4	C	102	8/8	1.00	0.01	38,45,62,64	0
20	CA	B	3002	1/1	1.00	0.02	69,69,69,69	0
20	CA	L	203	1/1	1.00	0.00	27,27,27,27	0
14	CLA	B	3016	45/65	1.00	0.03	61,82,115,118	0
14	CLA	A	827	65/65	1.00	0.03	29,68,145,167	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.

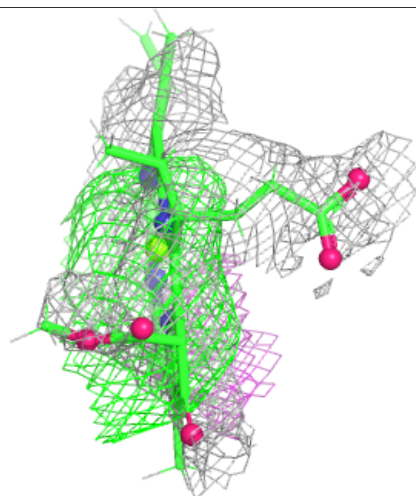
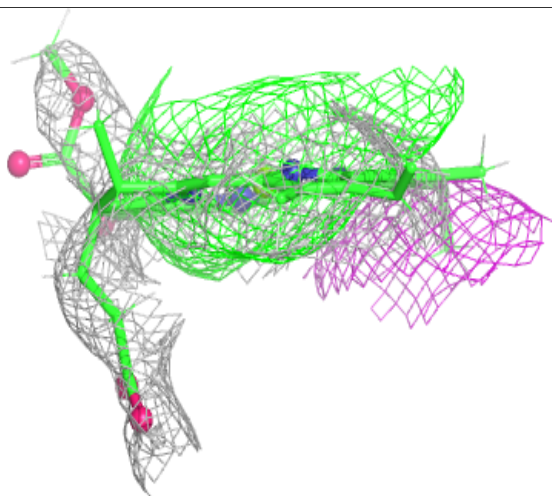
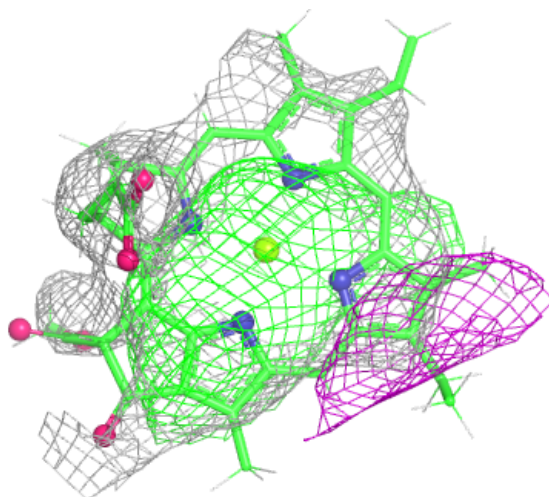
Electron density around CLA K 101:

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



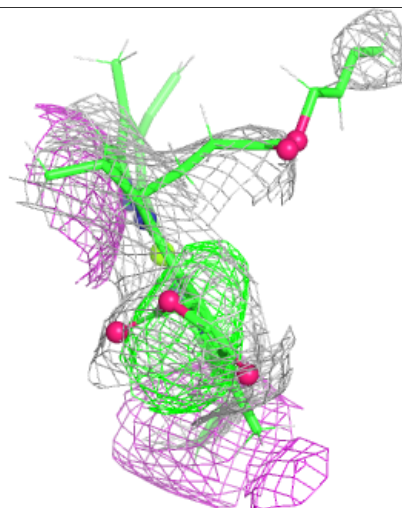
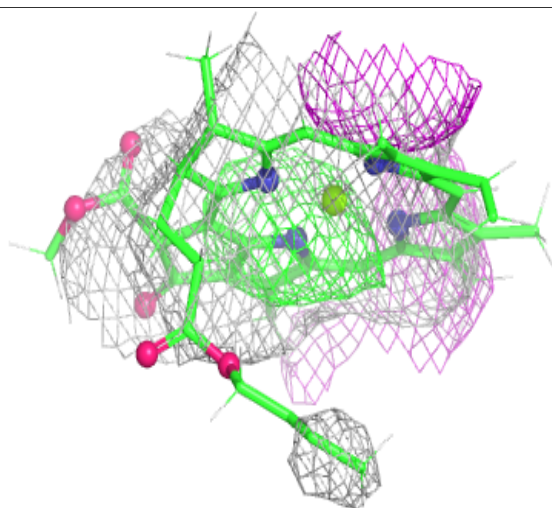
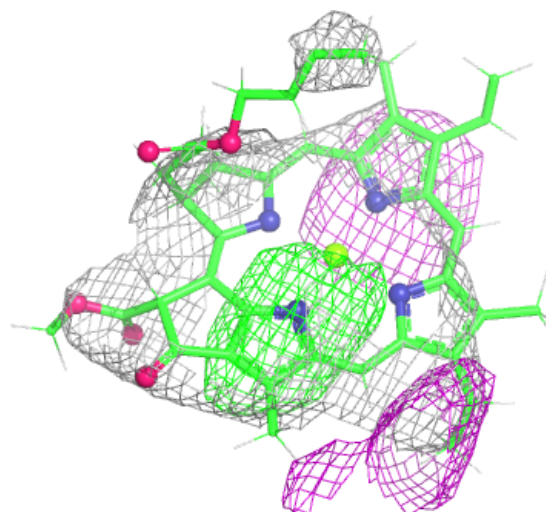
Electron density around CLA A 816:

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



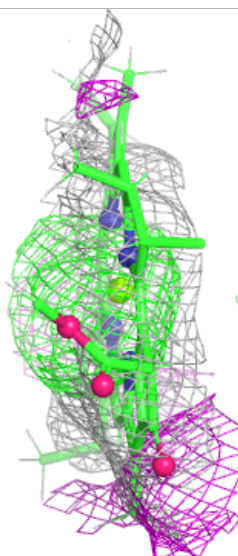
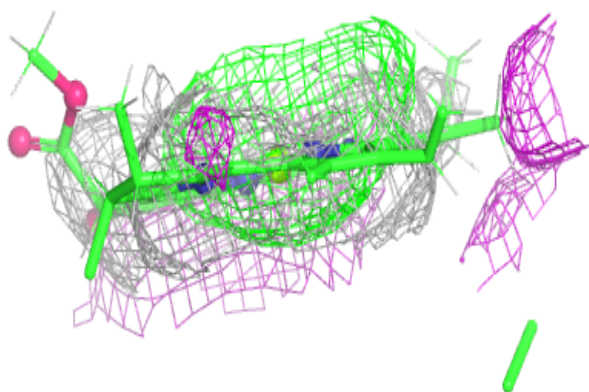
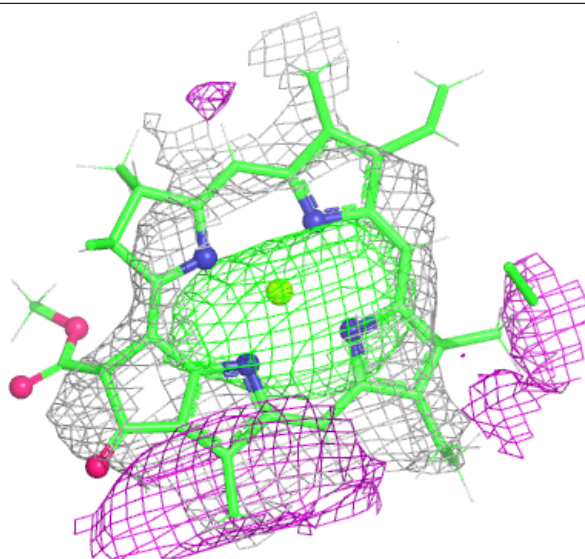
Electron density around CLA A 817:

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



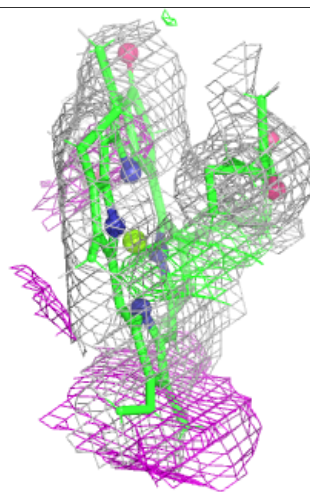
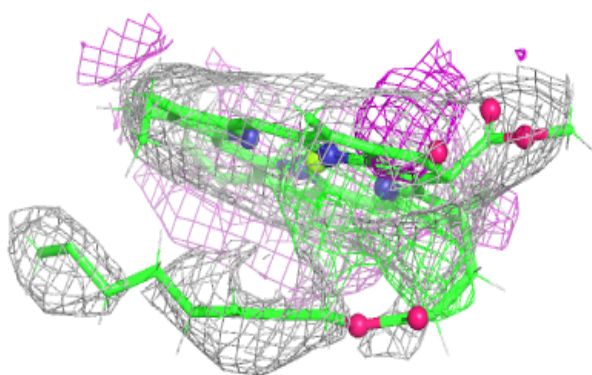
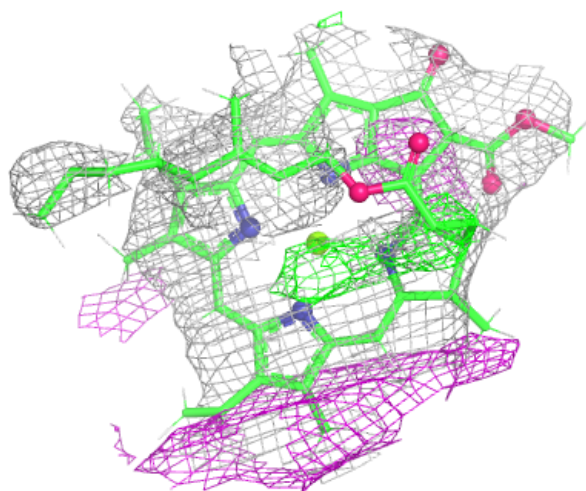
Electron density around CLA A 821:

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and green (positive)



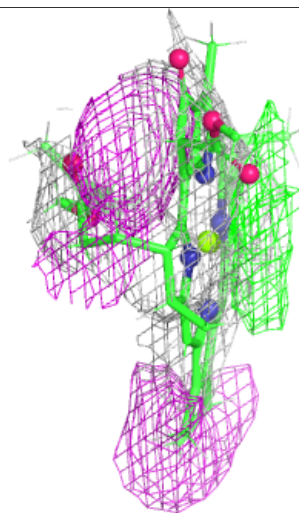
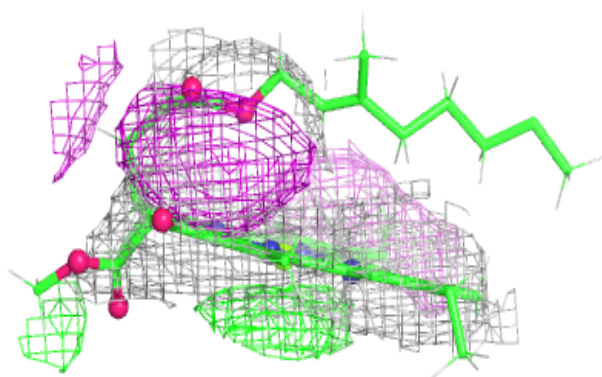
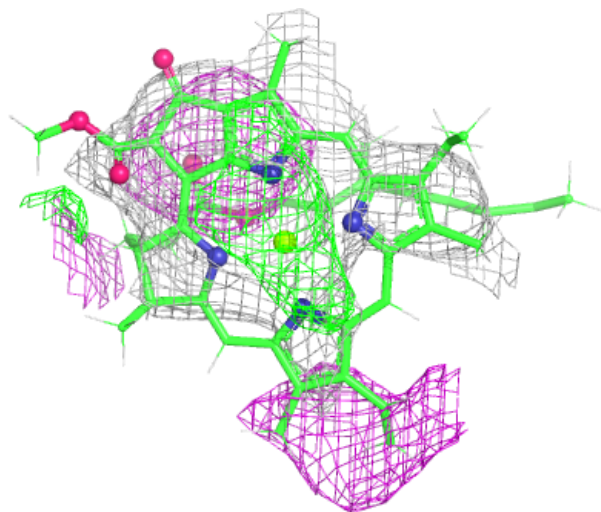
Electron density around CLA A 813:

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



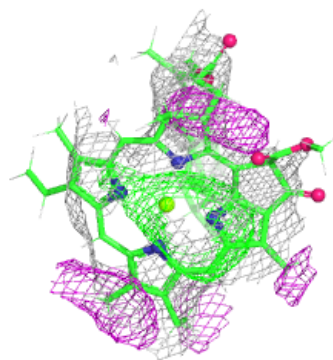
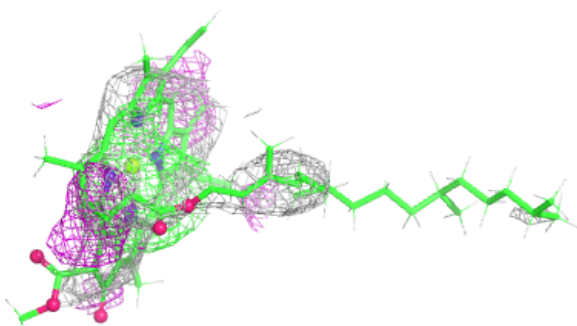
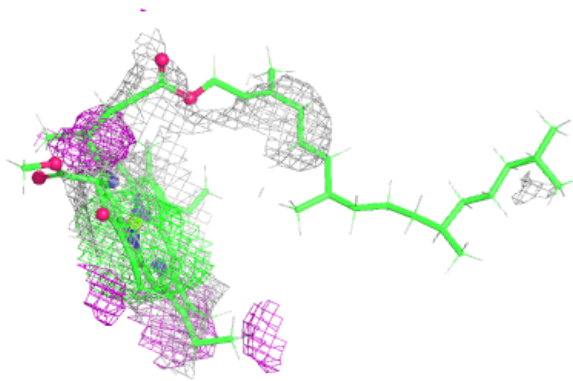
Electron density around CLA A 818:

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



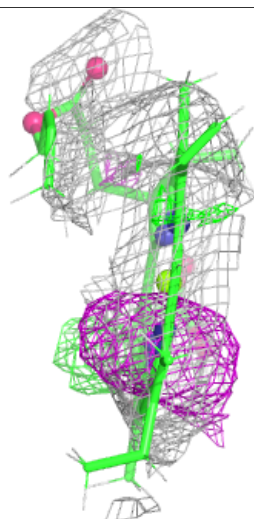
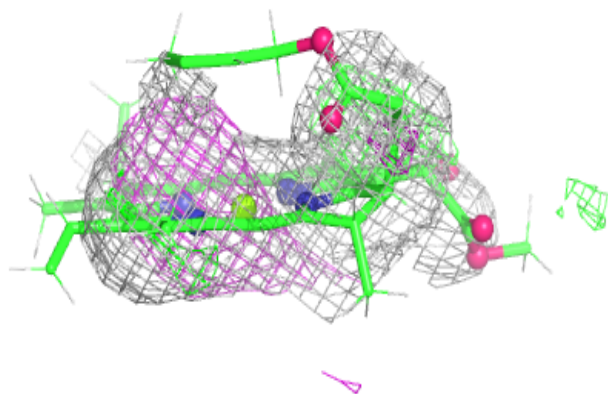
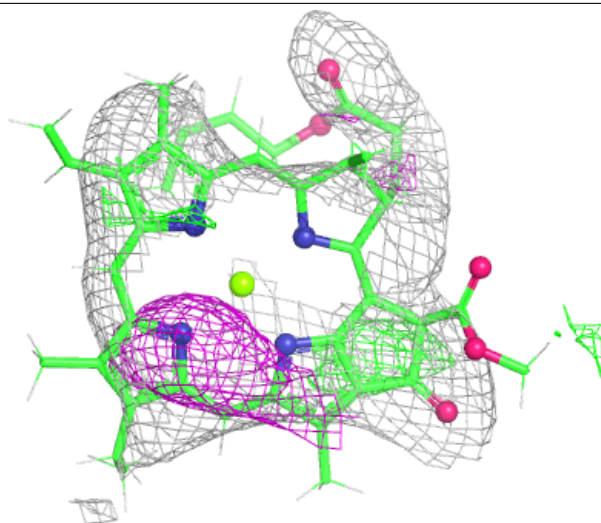
Electron density around CLA A 812:

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



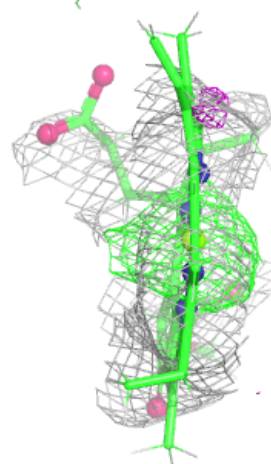
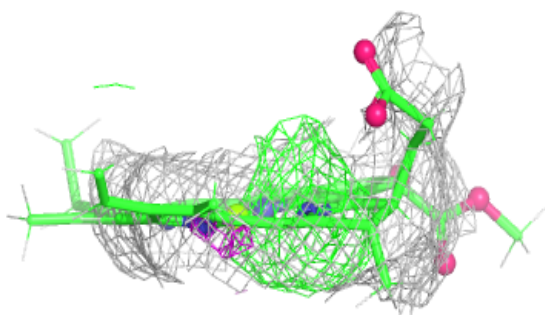
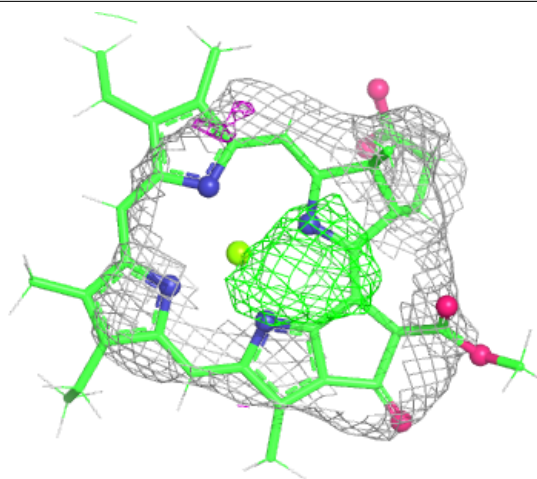
Electron density around CLA A 823:

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and green (positive)



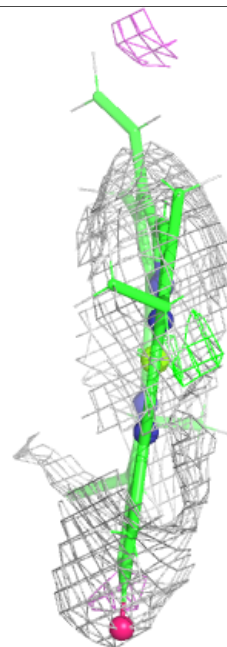
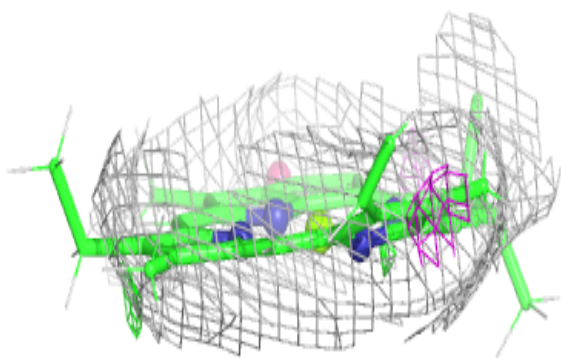
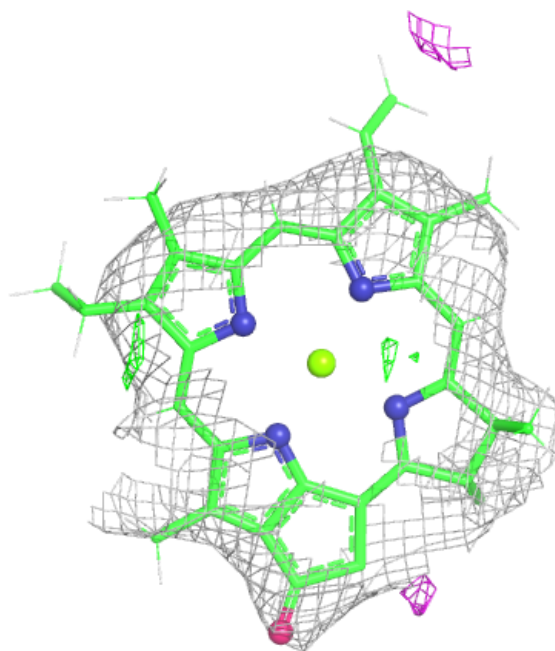
Electron density around CLA J 101:

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



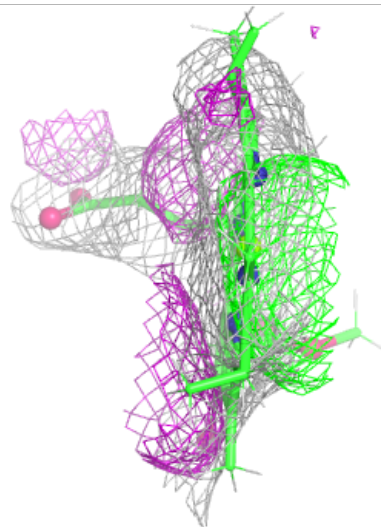
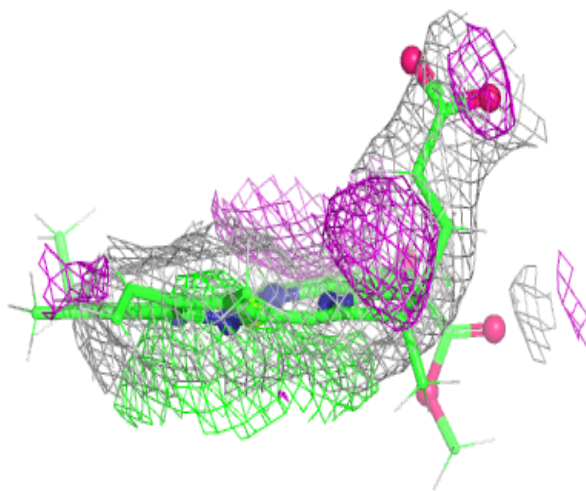
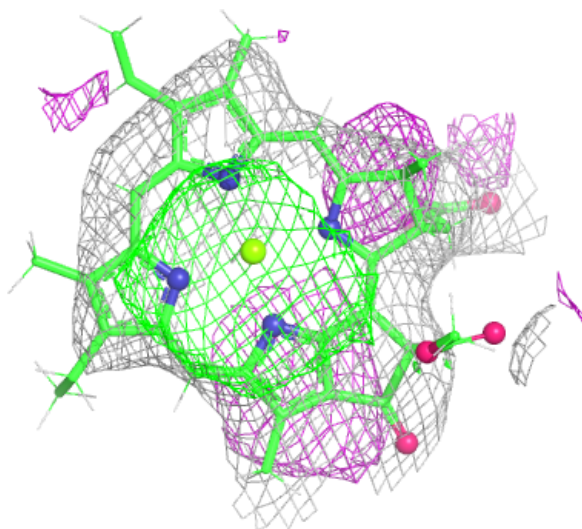
Electron density around CLA J 102:

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and green (positive)



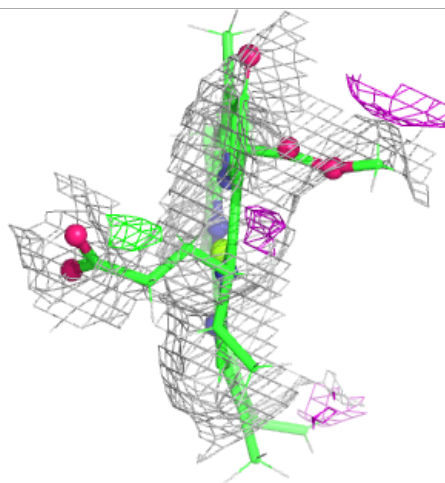
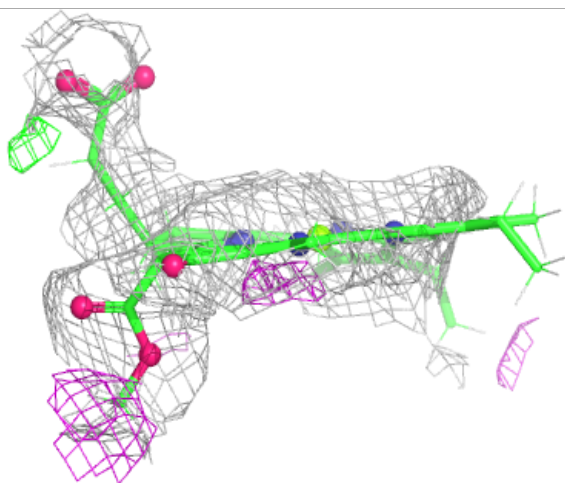
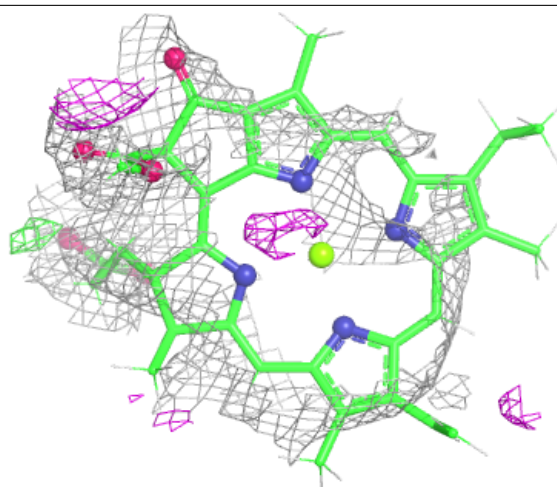
Electron density around CLA A 815:

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and green (positive)



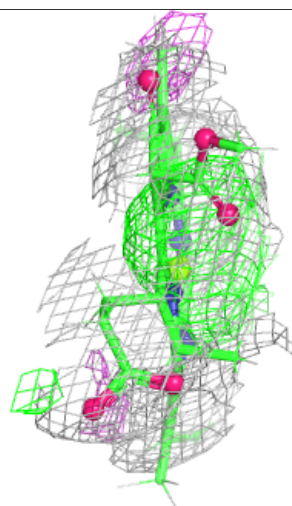
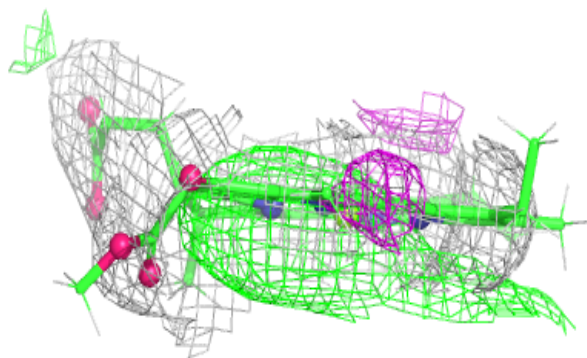
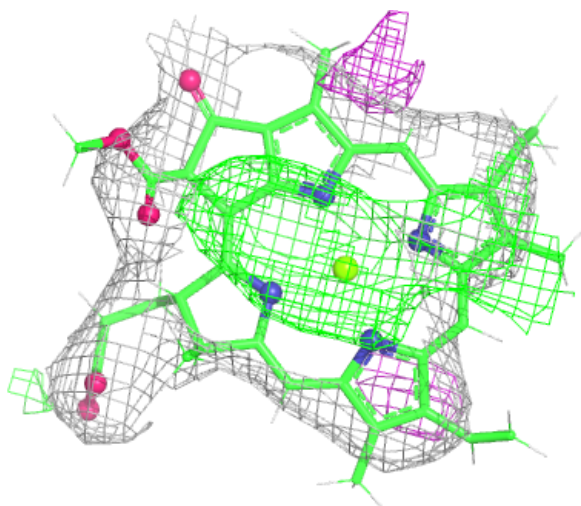
Electron density around CLA K 103:

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and green (positive)



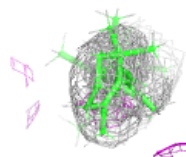
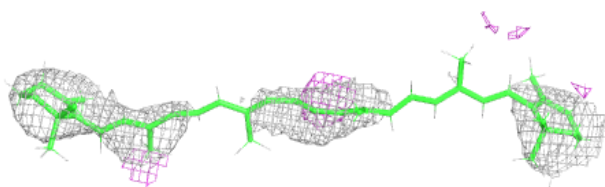
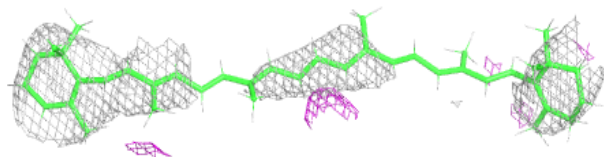
Electron density around CLA X 1701:

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and green (positive)

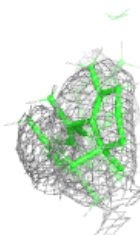
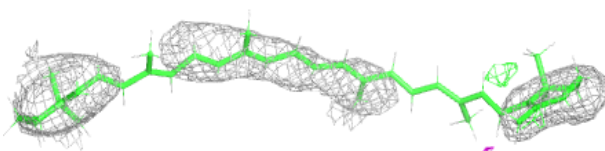
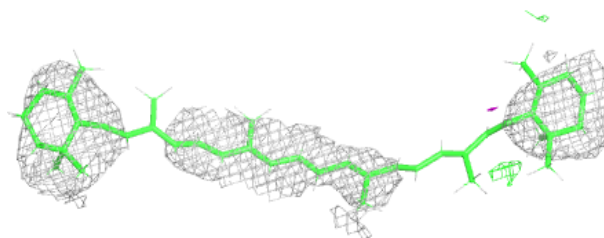


Electron density around BCR A 847:

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and green (positive)

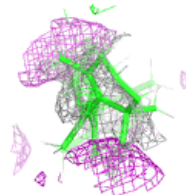
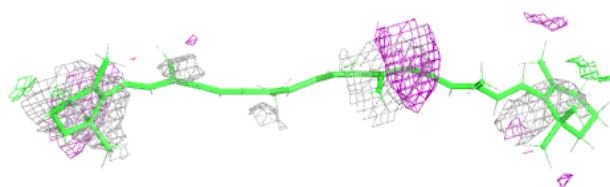
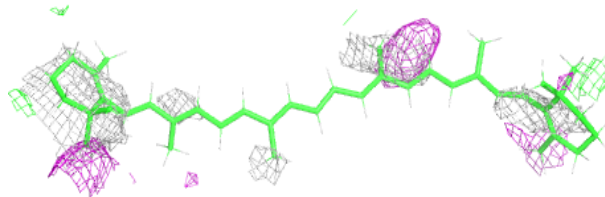
**Electron density around BCR J 104:**

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and green (positive)

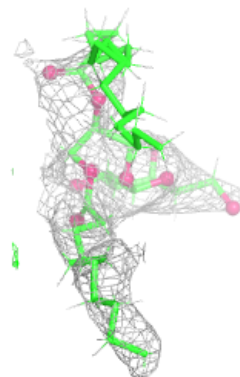
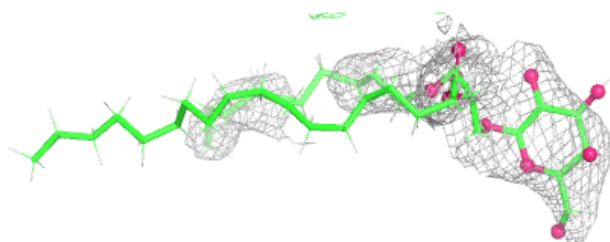
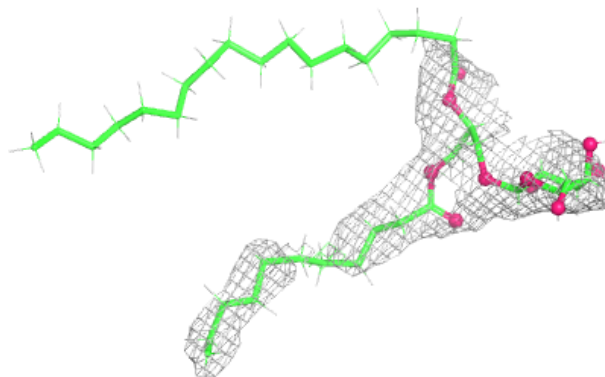


Electron density around BCR K 102:

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and green (positive)

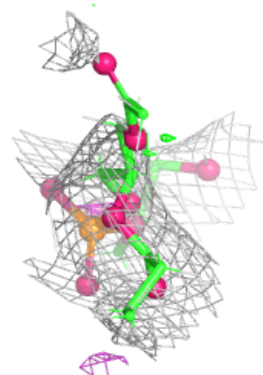
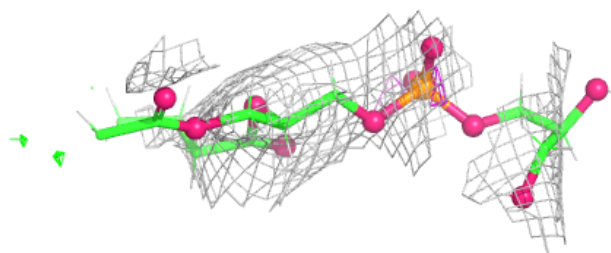
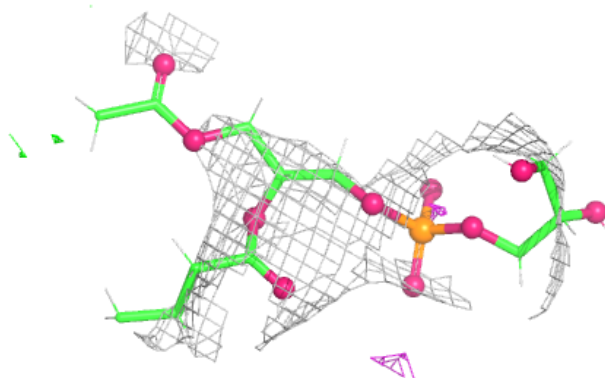
**Electron density around LMG A 852:**

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and green (positive)

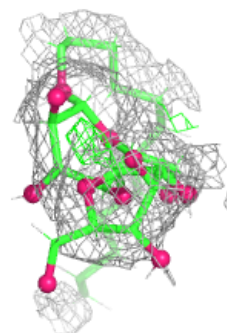
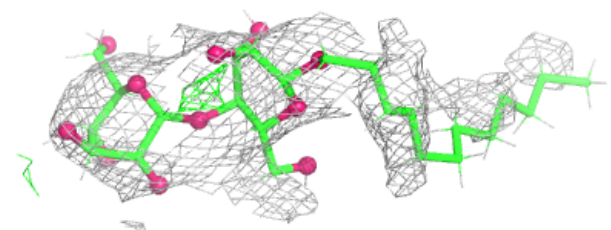
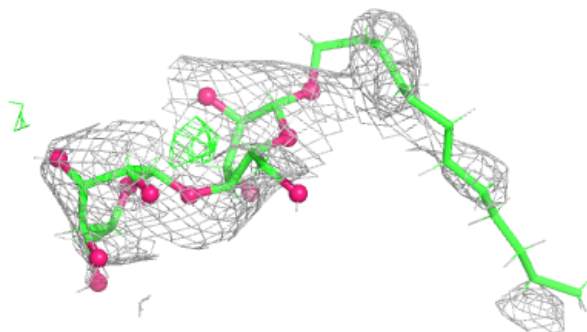


Electron density around LHG B 3050:

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and green (positive)

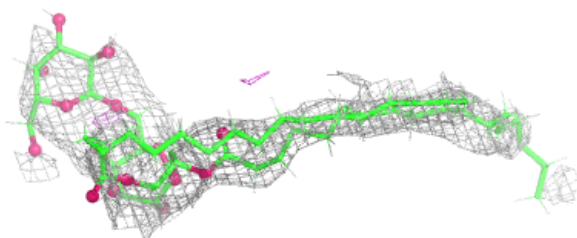
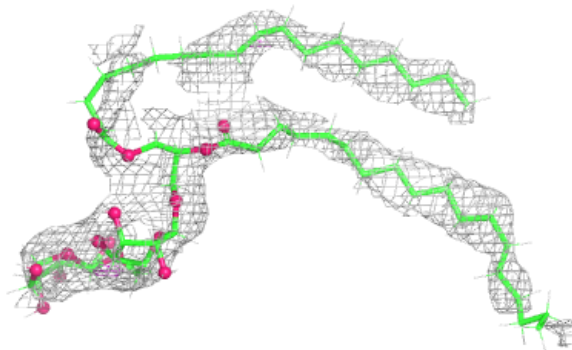
**Electron density around LMT L 202:**

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

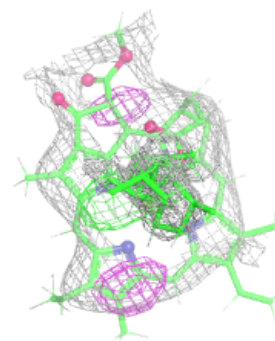
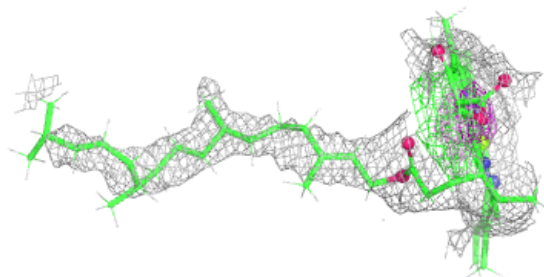
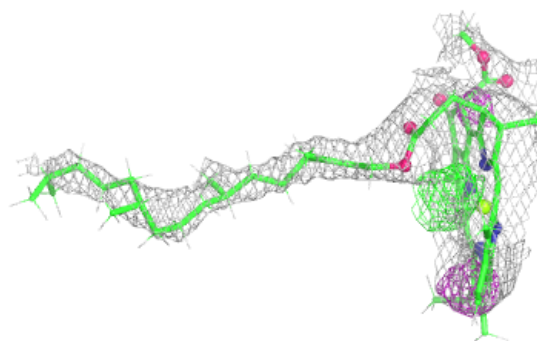


Electron density around DGD L 207:

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and green (positive)

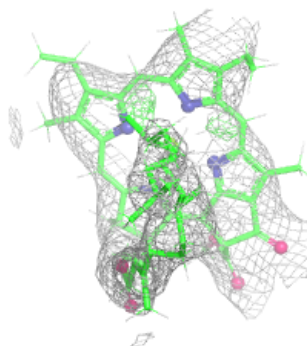
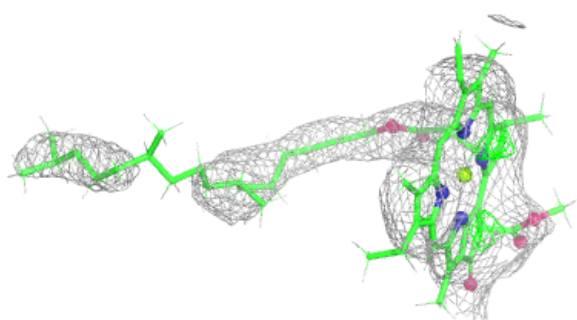
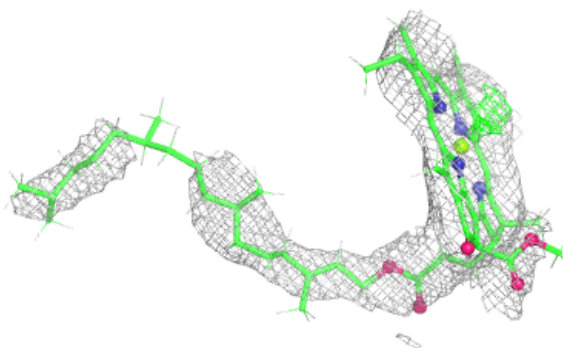
**Electron density around CLA A 829:**

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

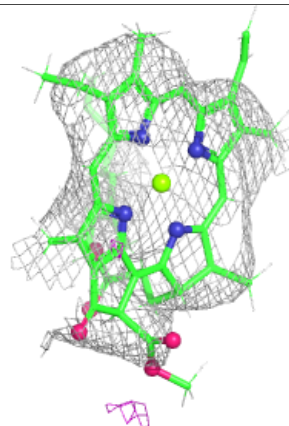
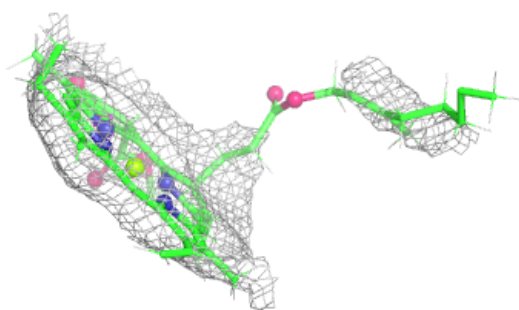
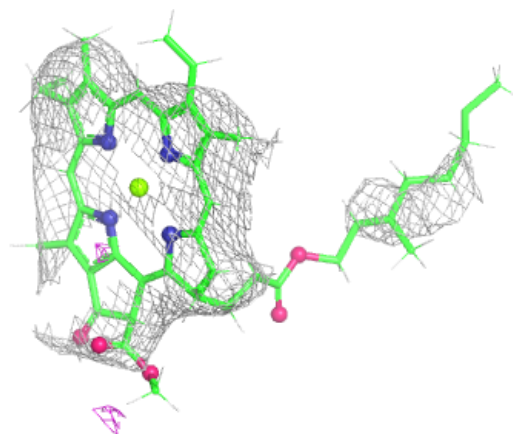


Electron density around CLA A 831:

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and green (positive)

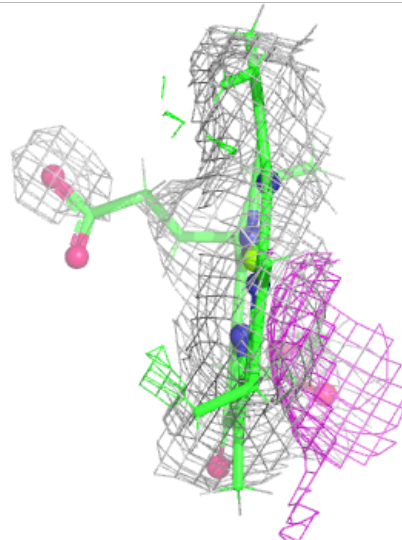
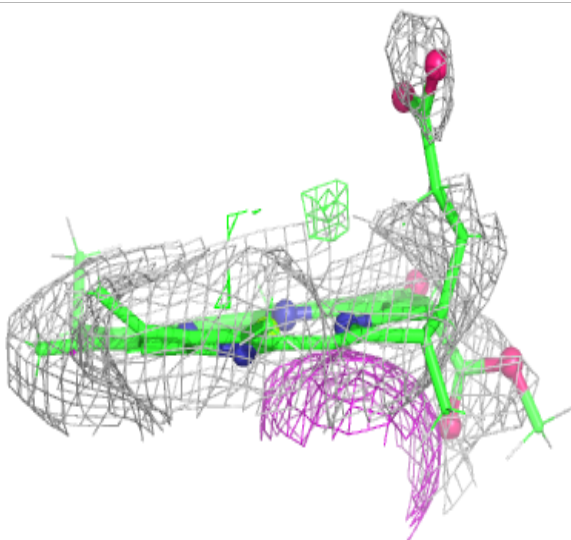
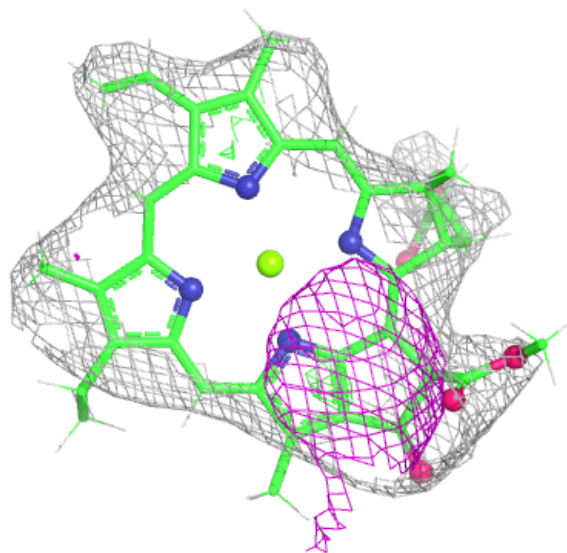
**Electron density around CLA A 836:**

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and green (positive)



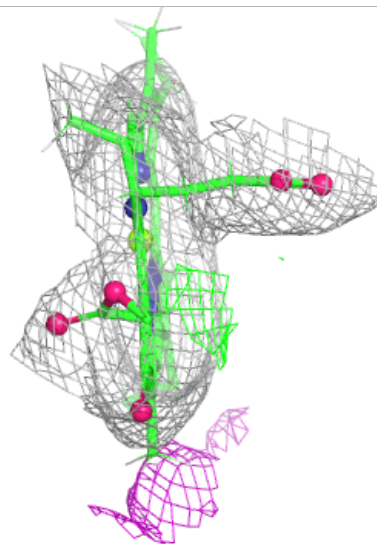
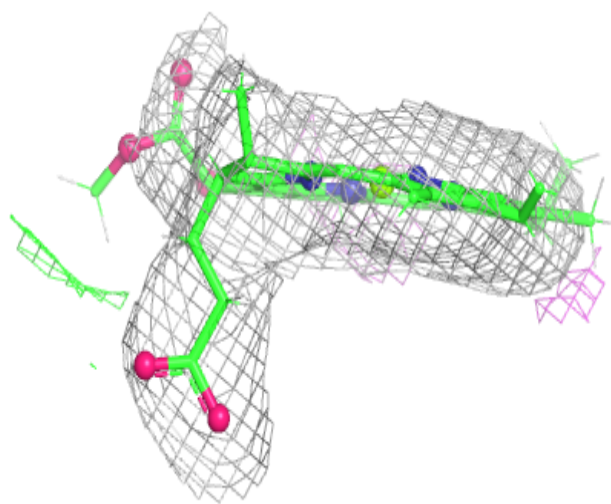
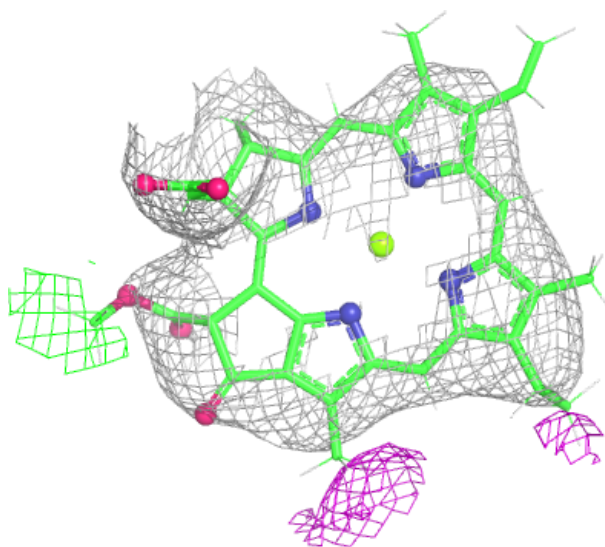
Electron density around CLA A 837:

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



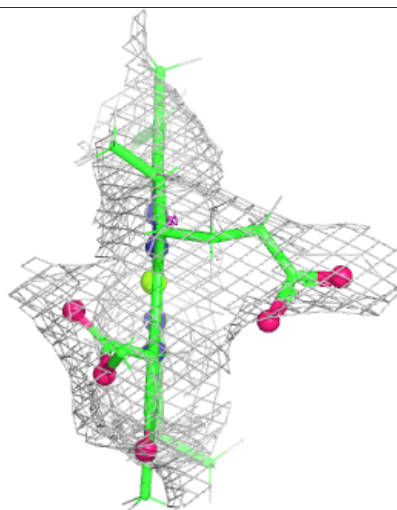
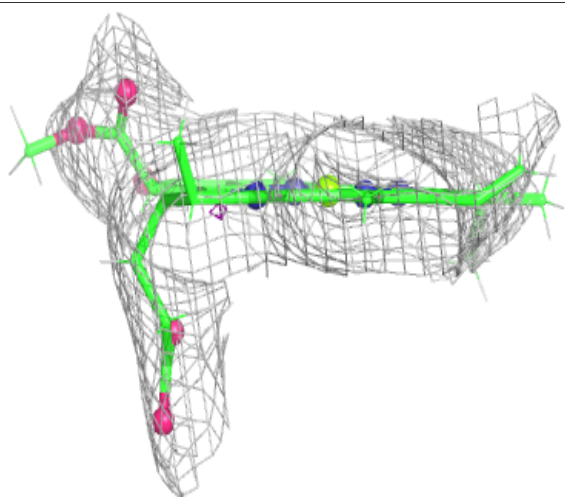
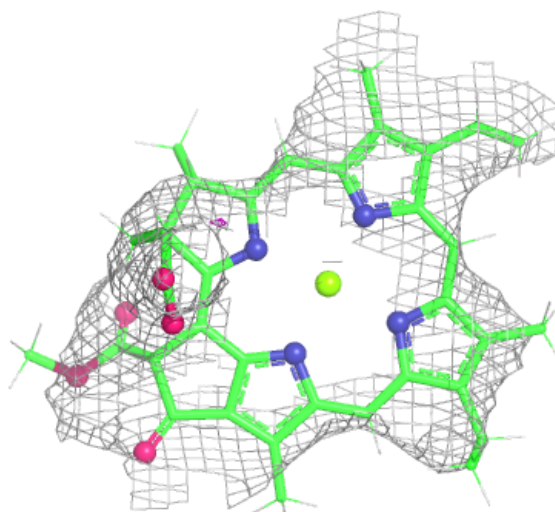
Electron density around CLA B 3012:

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



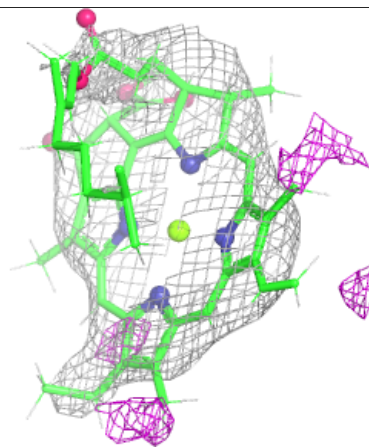
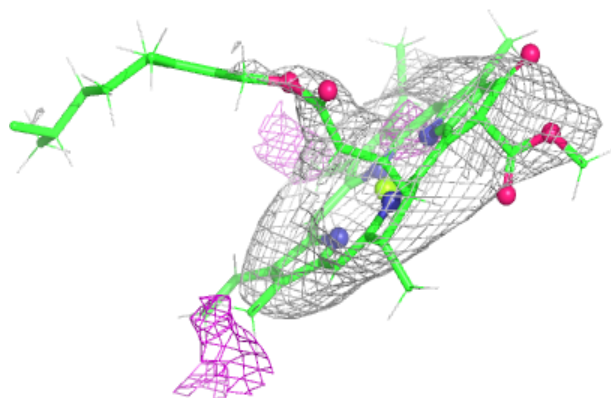
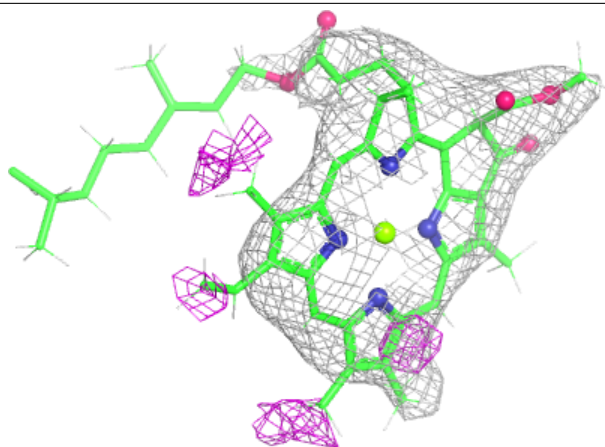
Electron density around CLA B 3013:

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



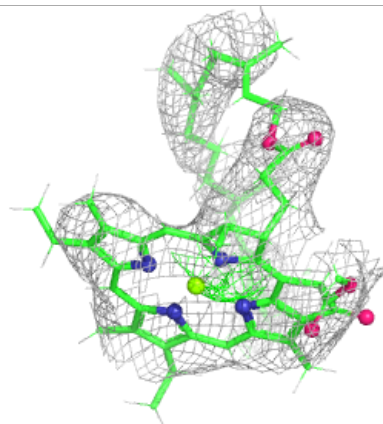
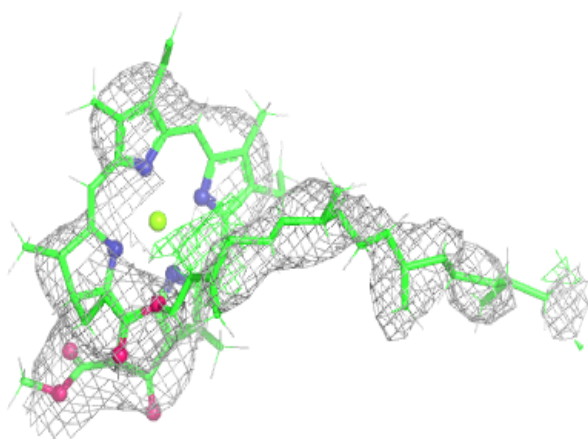
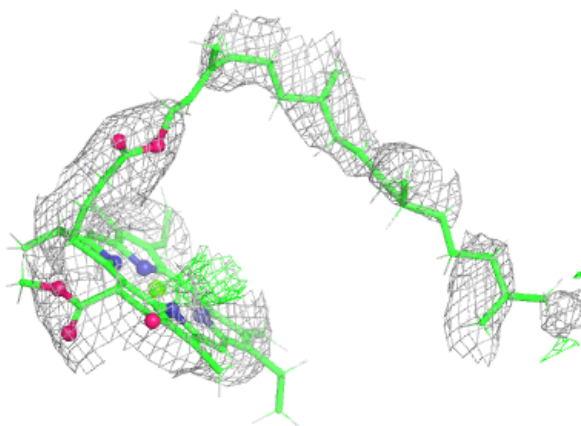
Electron density around CLA B 3017:

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



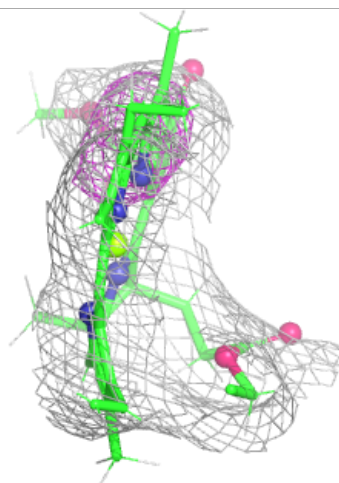
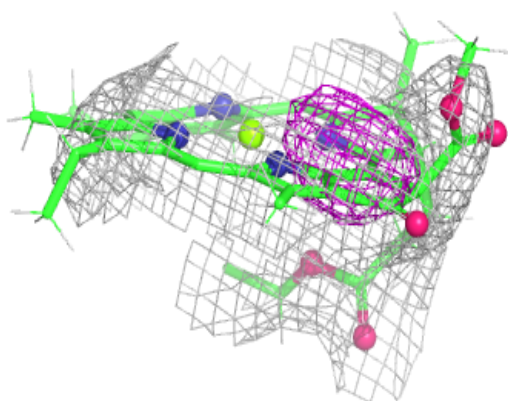
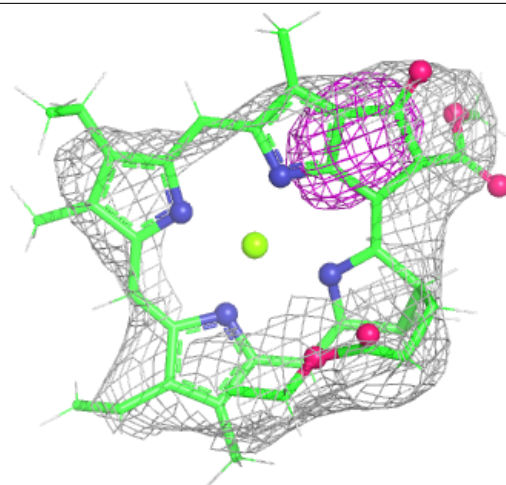
Electron density around CLA B 3020:

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



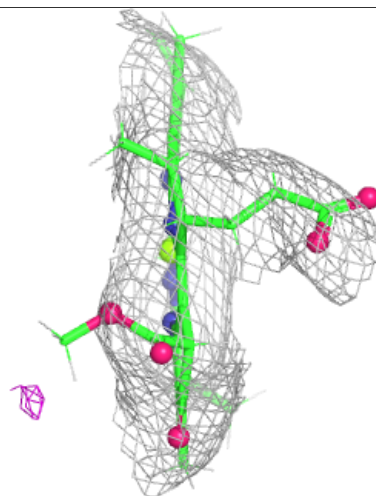
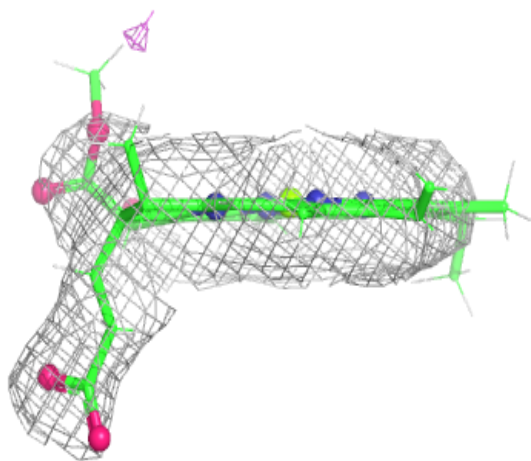
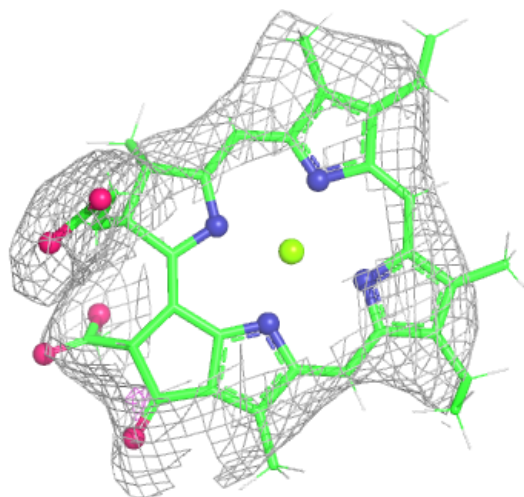
Electron density around CLA B 3021:

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



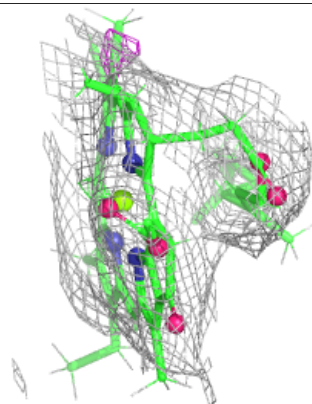
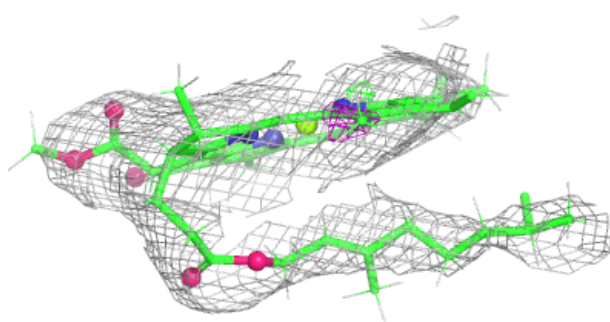
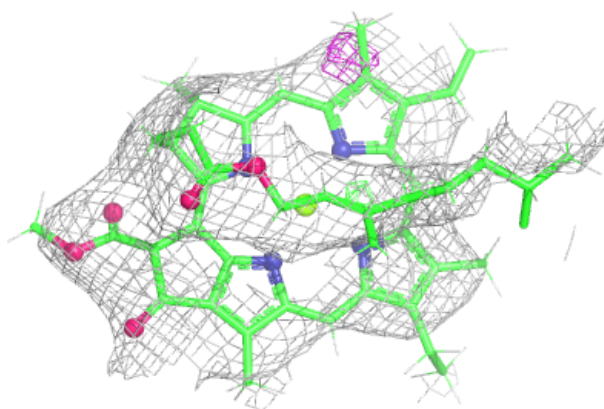
Electron density around CLA B 3022:

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



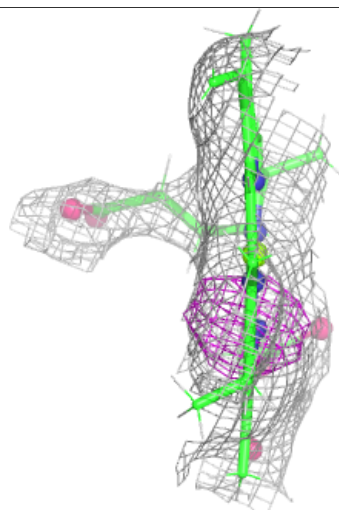
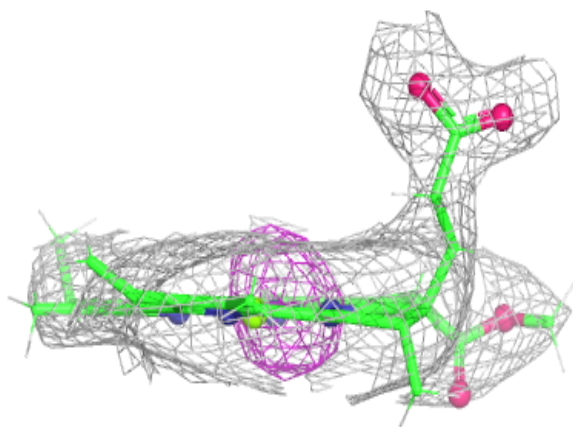
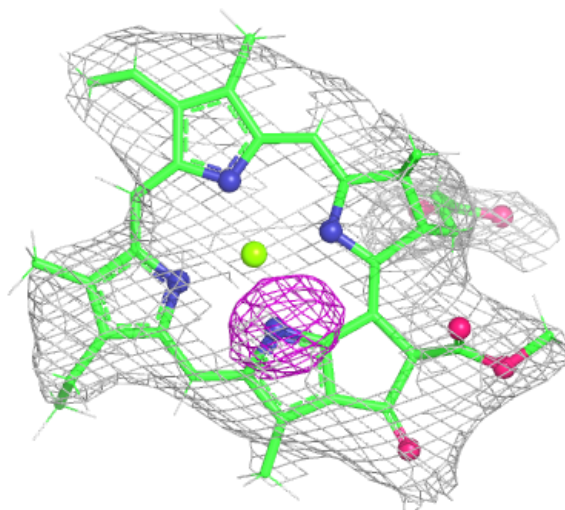
Electron density around CLA B 3023:

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



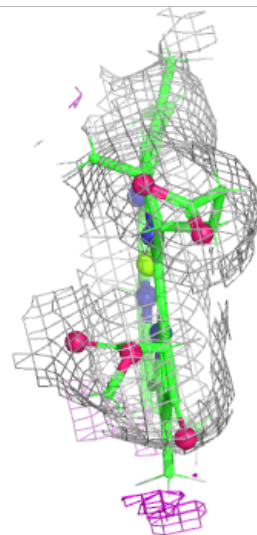
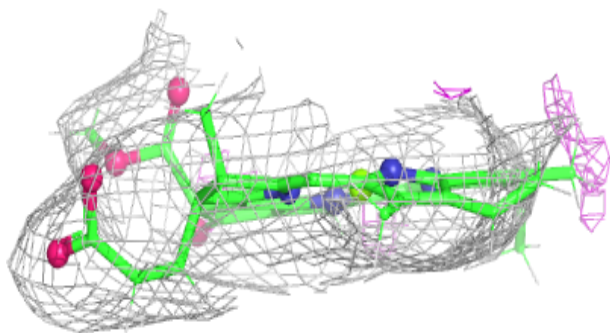
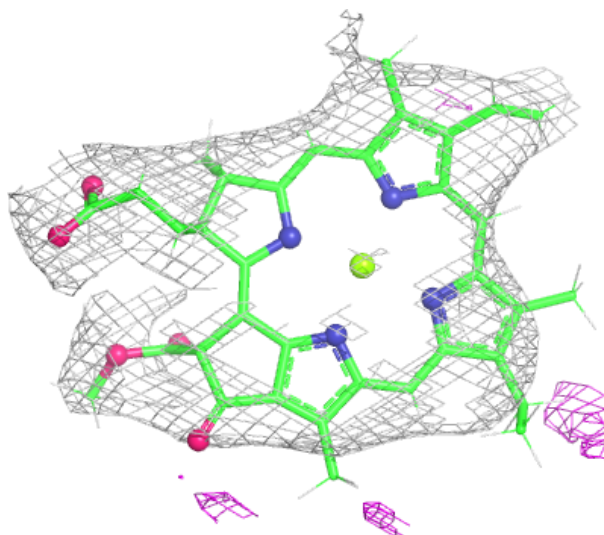
Electron density around CLA B 3036:

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



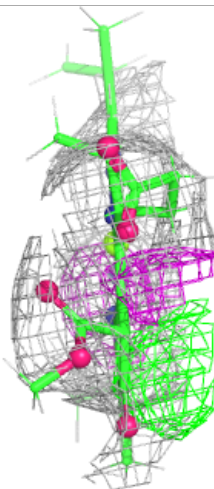
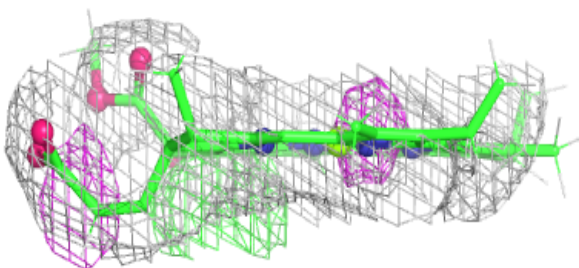
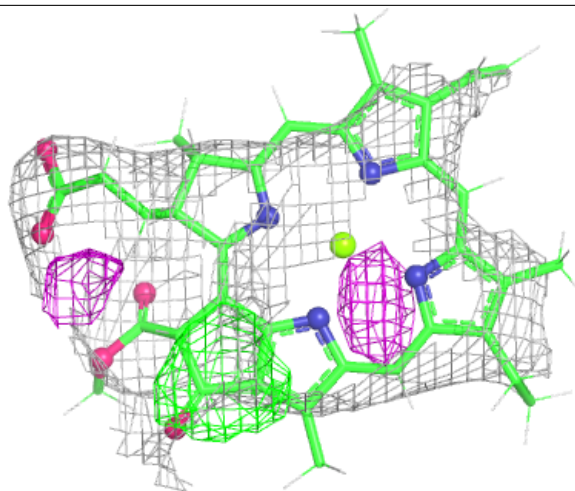
Electron density around CLA B 3037:

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



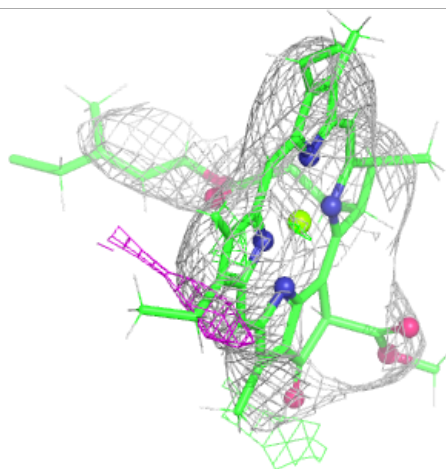
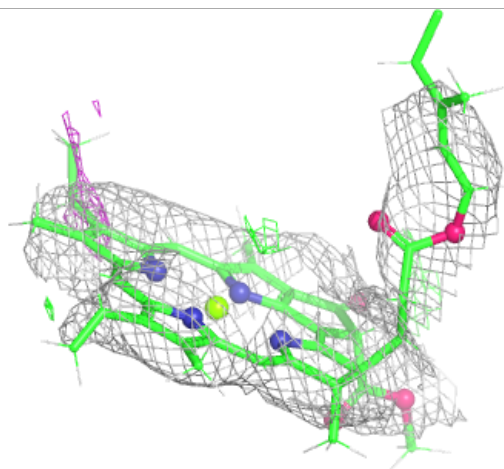
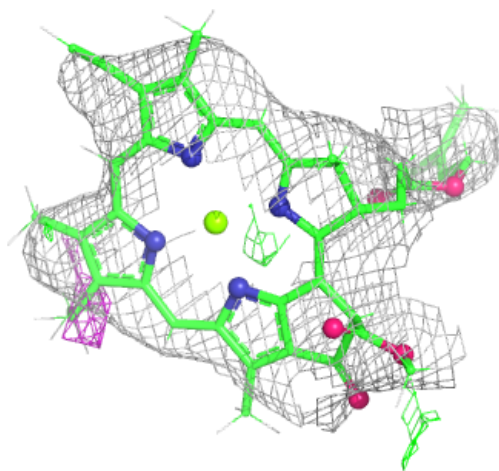
Electron density around CLA F 202:

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



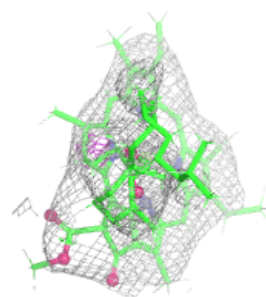
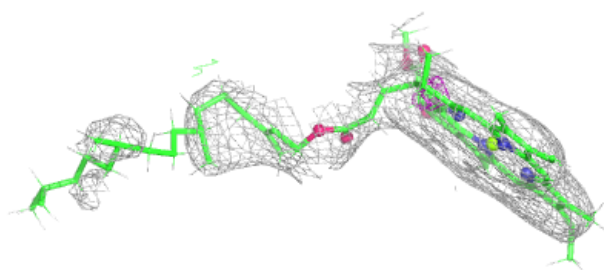
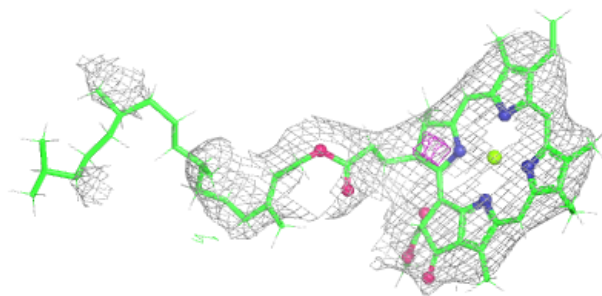
Electron density around CLA A 808:

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



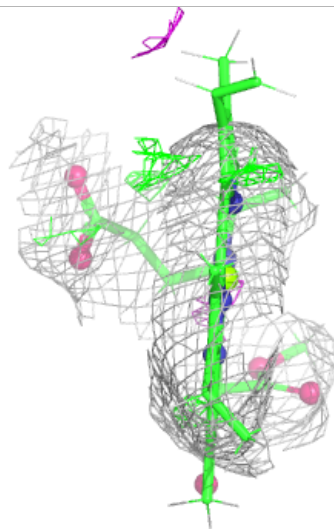
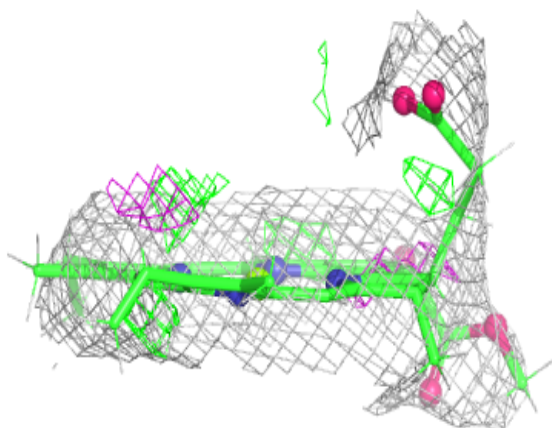
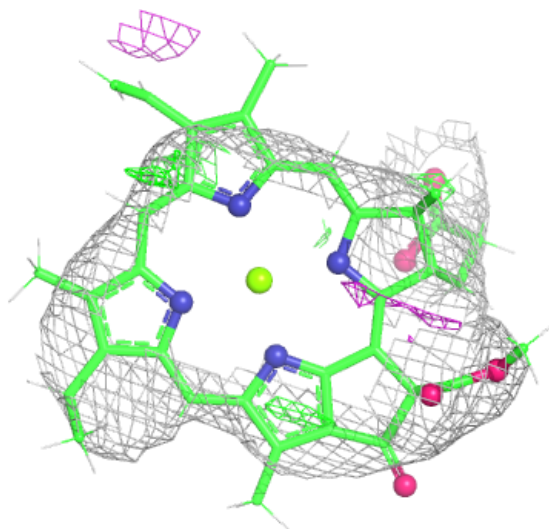
Electron density around CLA A 810:

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



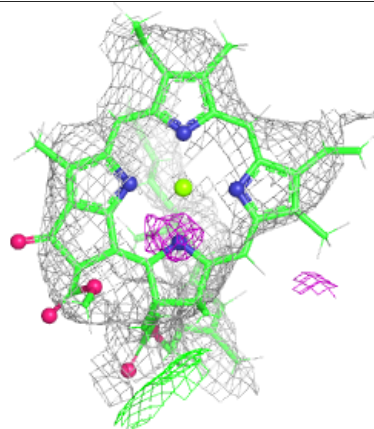
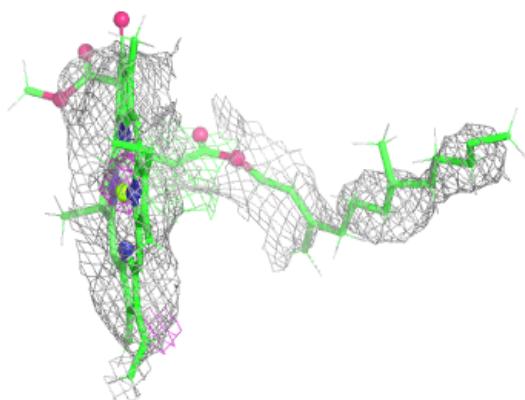
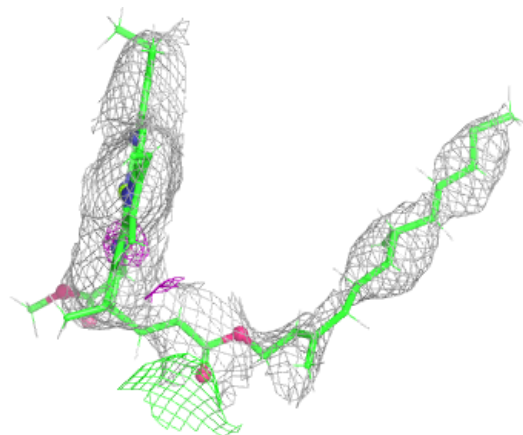
Electron density around CLA A 811:

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



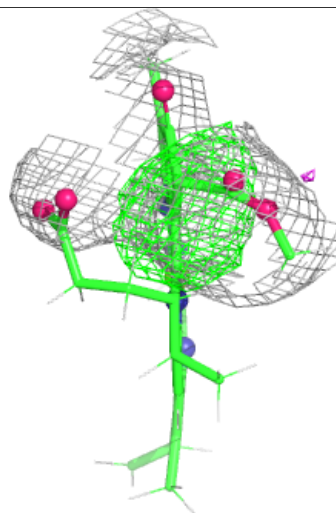
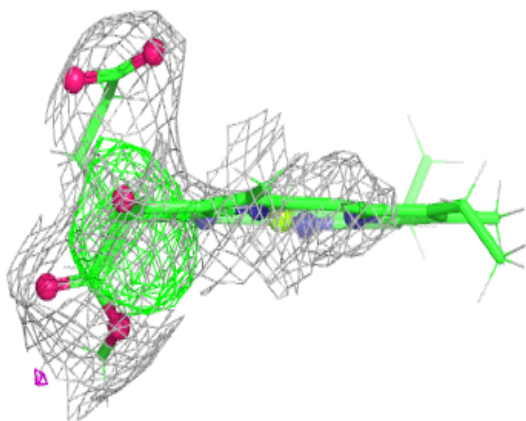
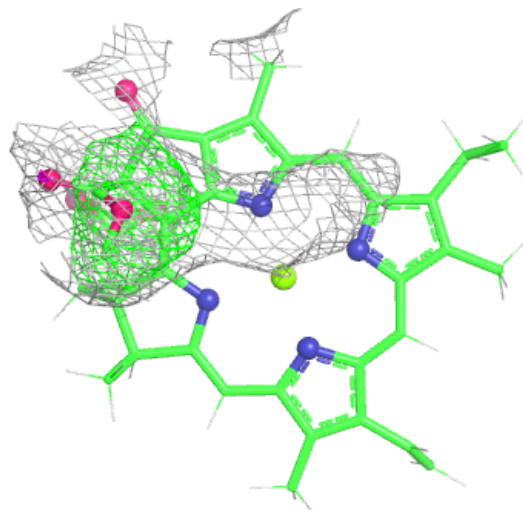
Electron density around CLA A 805:

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



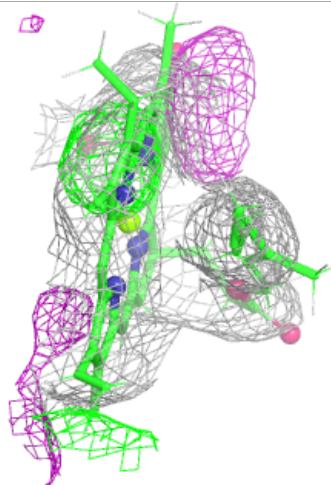
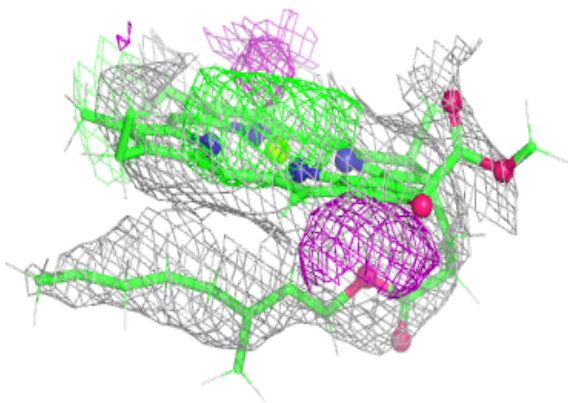
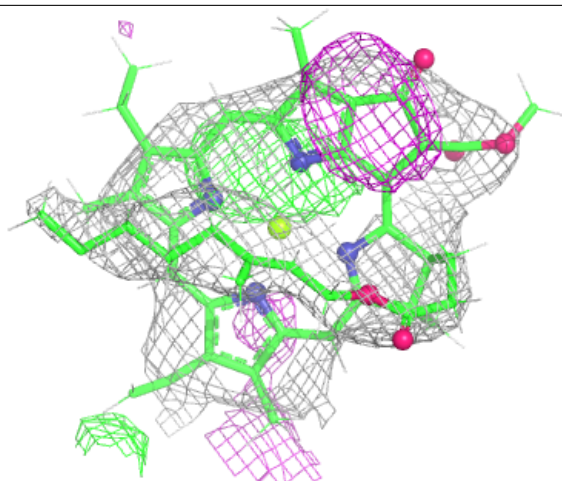
Electron density around CLA M 102:

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



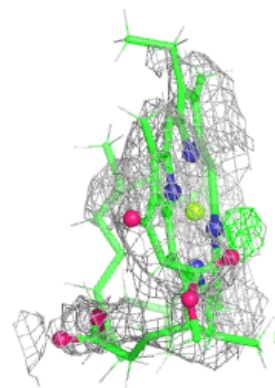
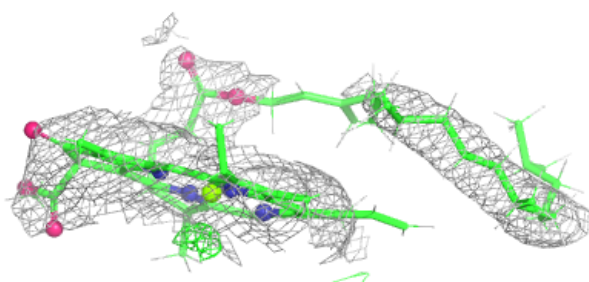
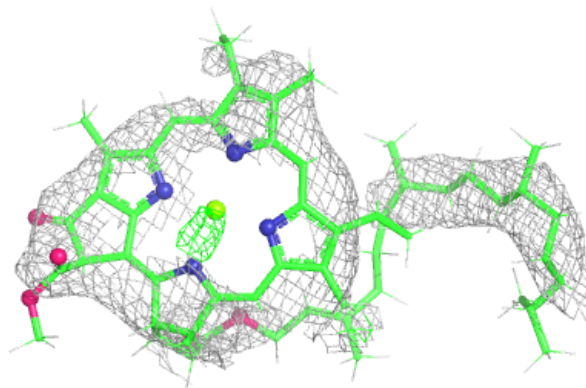
Electron density around CLA A 819:

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

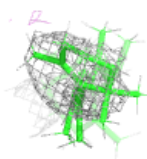
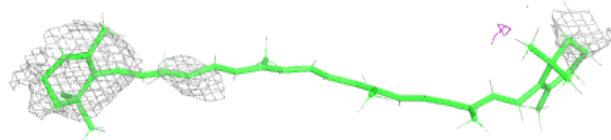
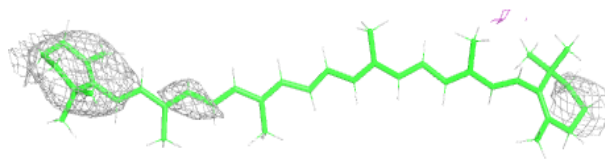


Electron density around CLA A 820:

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

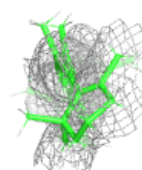
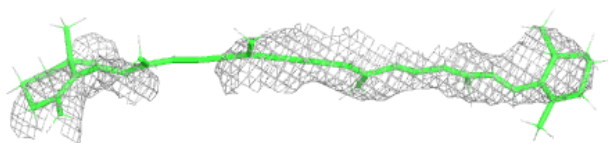
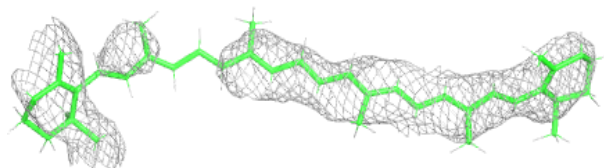
**Electron density around BCR A 848:**

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

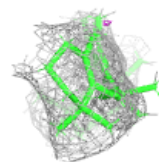
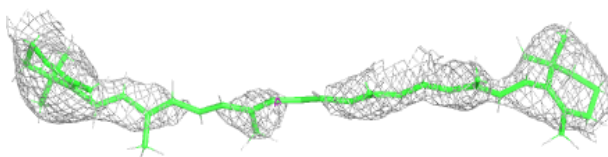
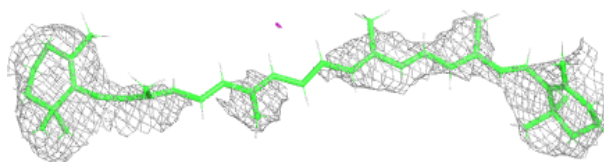


Electron density around BCR A 849:

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

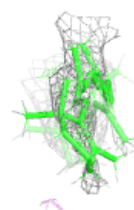
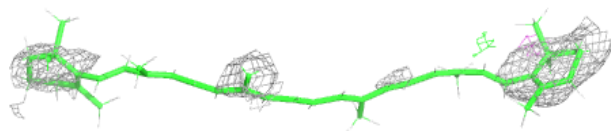
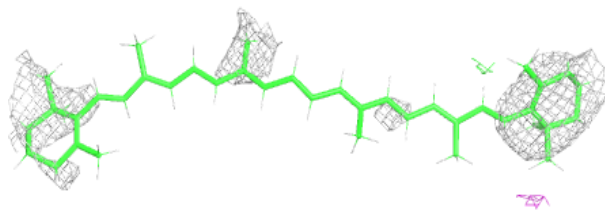
**Electron density around BCR A 850:**

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

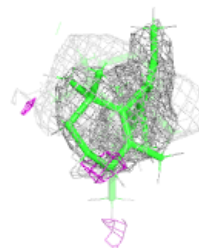
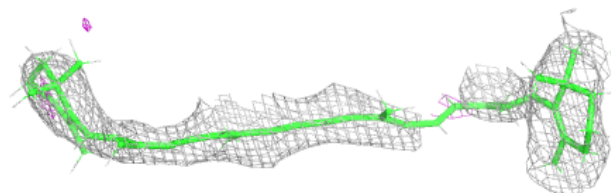
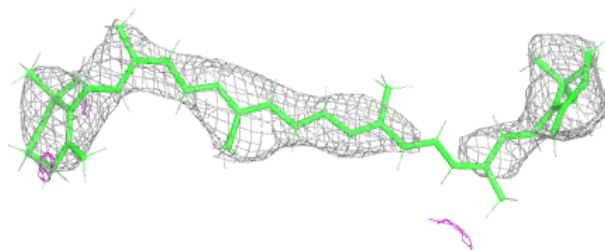


Electron density around BCR B 3044:

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

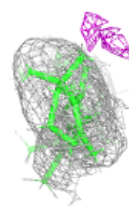
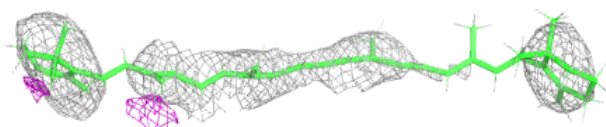
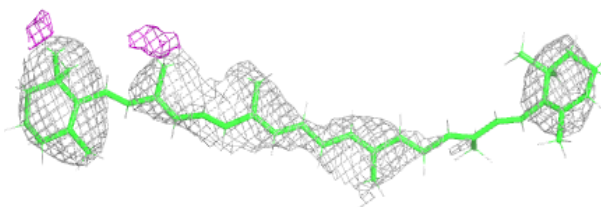
**Electron density around BCR B 3046:**

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

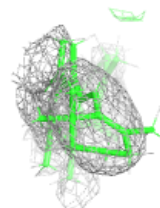
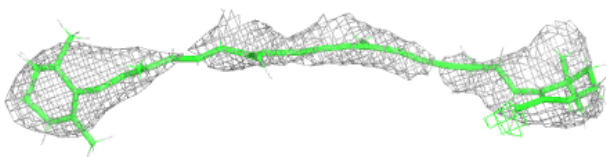
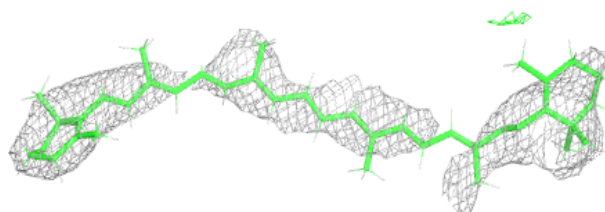


Electron density around BCR B 3047:

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

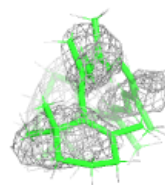
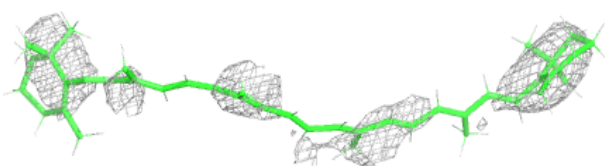
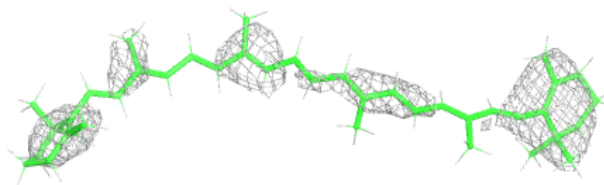
**Electron density around BCR B 3051:**

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

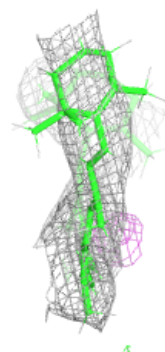
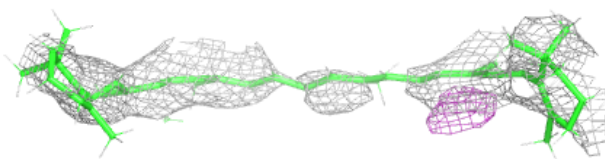
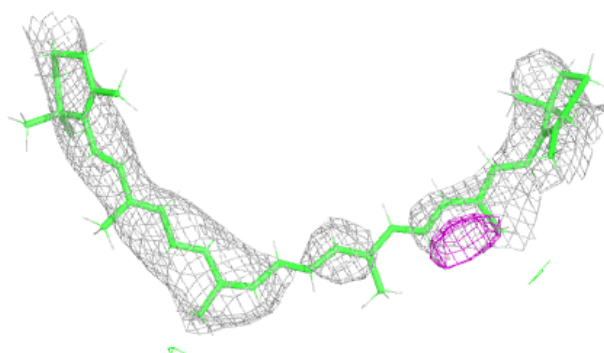


Electron density around BCR F 201:

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

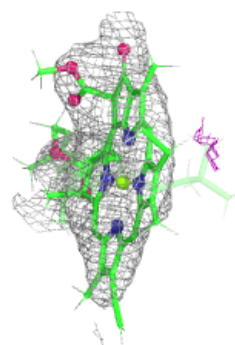
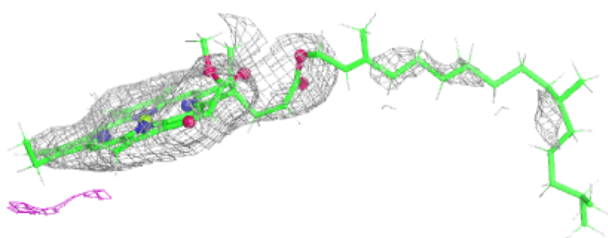
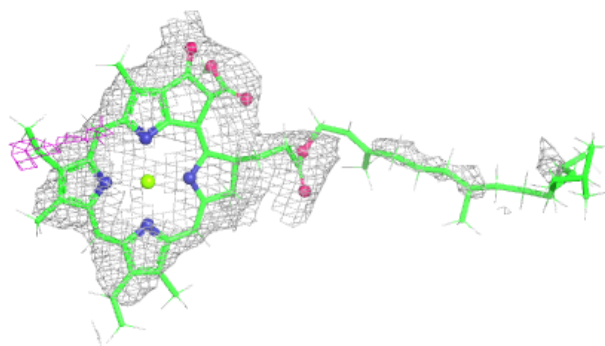
**Electron density around BCR F 203:**

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

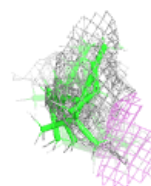
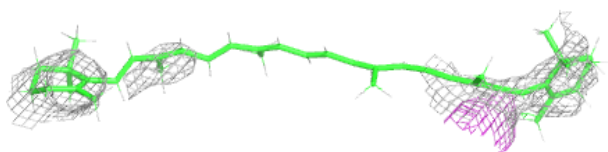
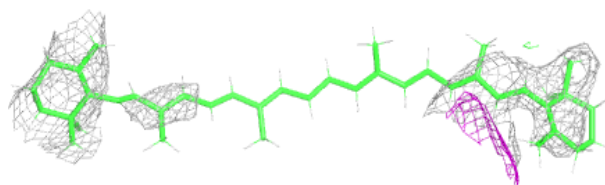


Electron density around CLA A 806:

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

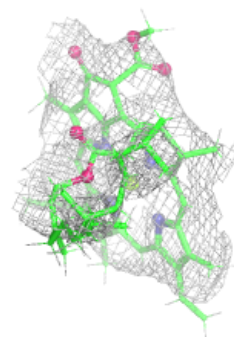
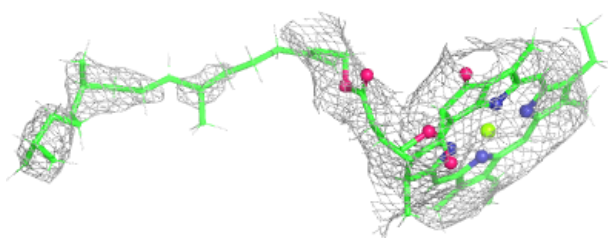
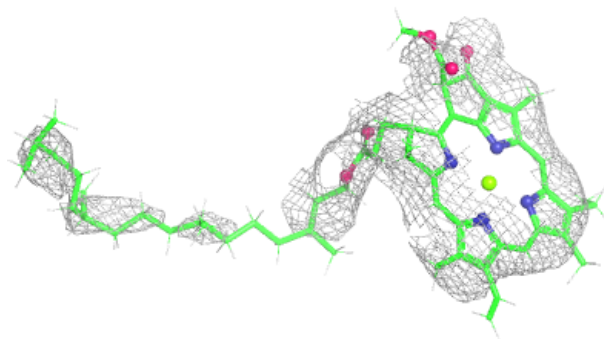
**Electron density around BCR J 105:**

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

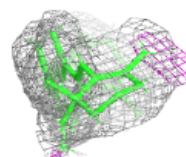
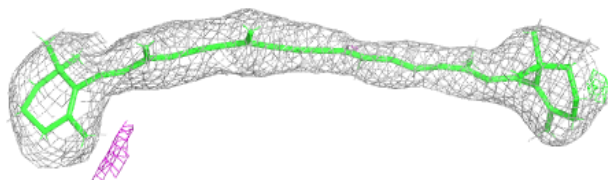
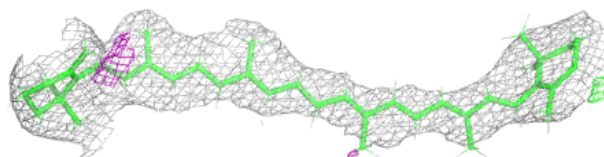


Electron density around CLA A 822:

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

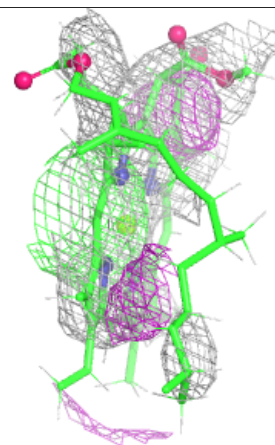
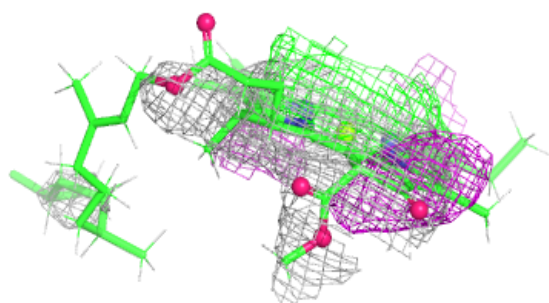
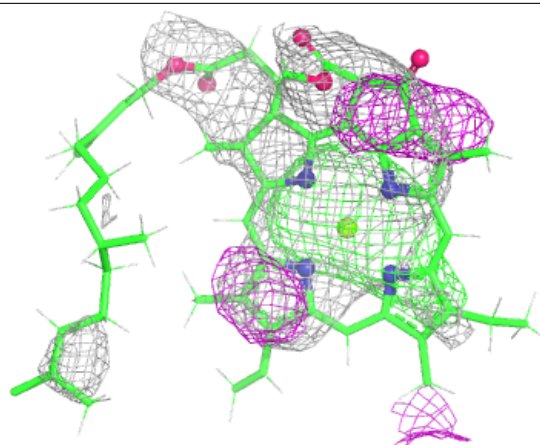
**Electron density around BCR M 103:**

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

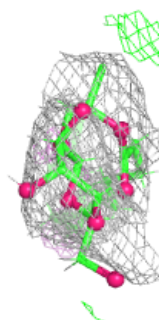
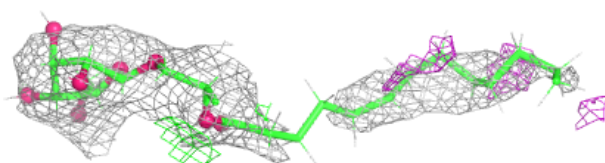
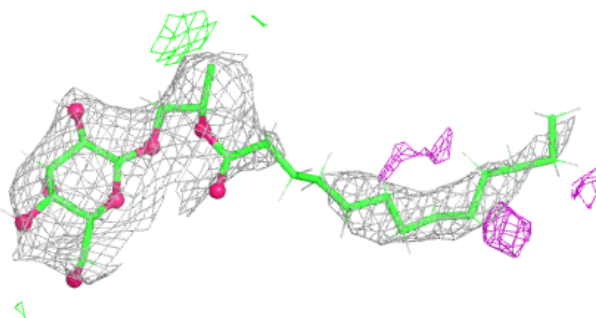


Electron density around CLA A 814:

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

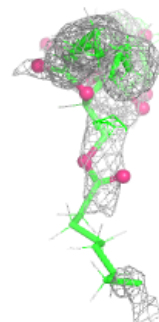
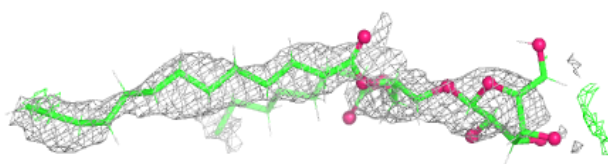
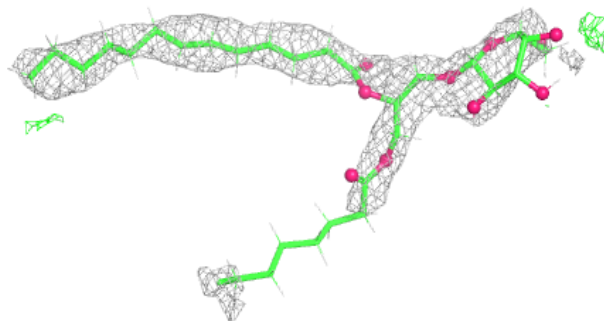
**Electron density around LMG A 855:**

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



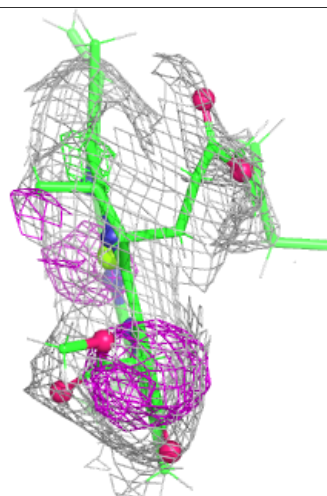
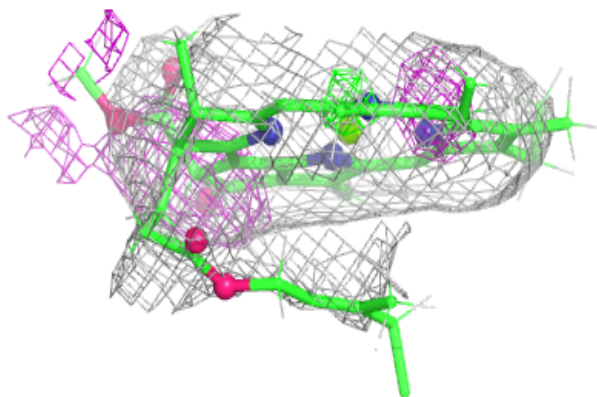
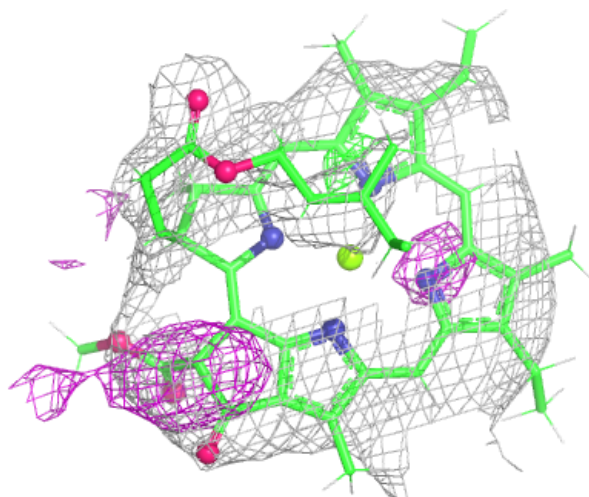
Electron density around LMG I 102:

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



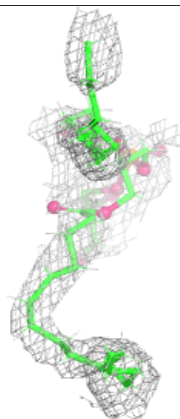
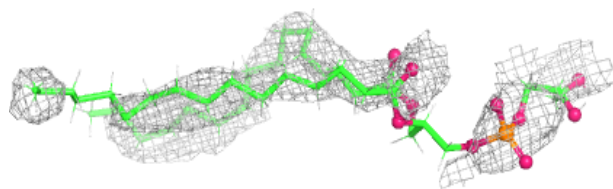
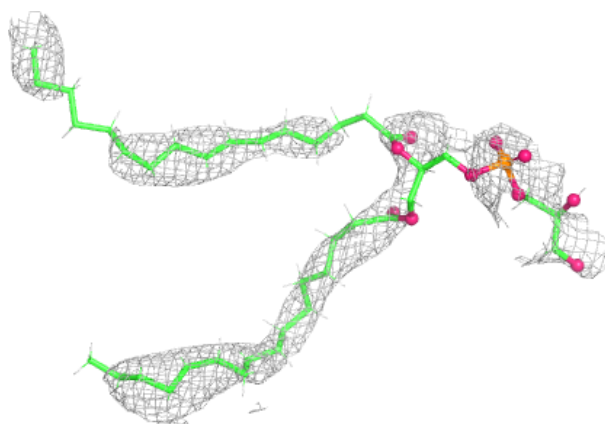
Electron density around CLA A 824:

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



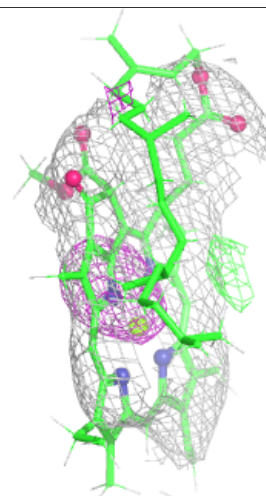
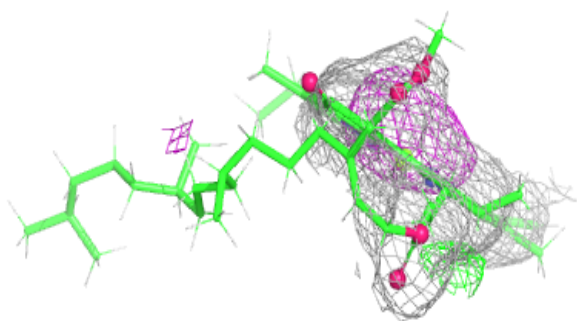
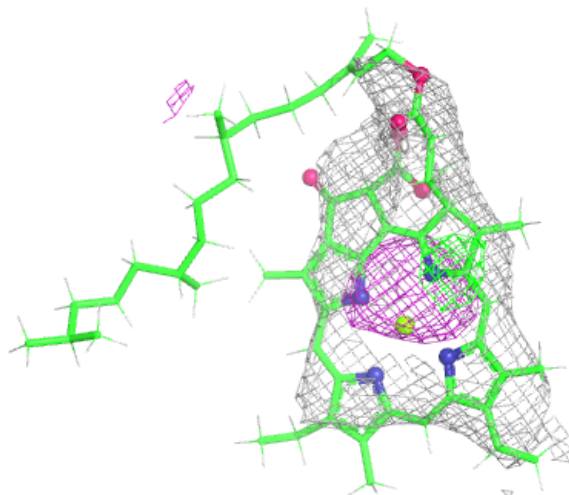
Electron density around LHG M 101:

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



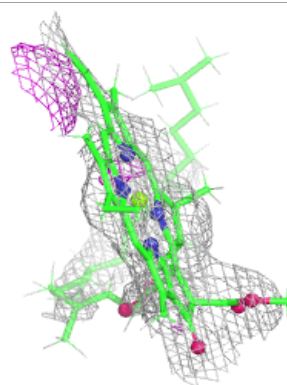
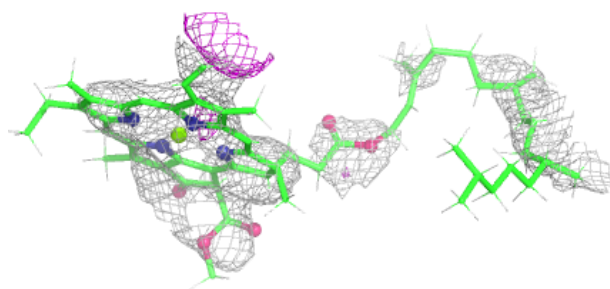
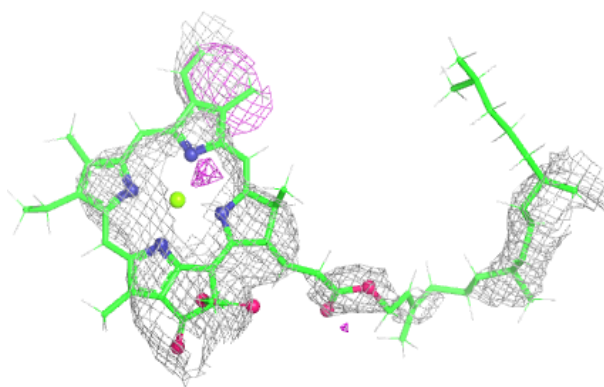
Electron density around CLA A 826:

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

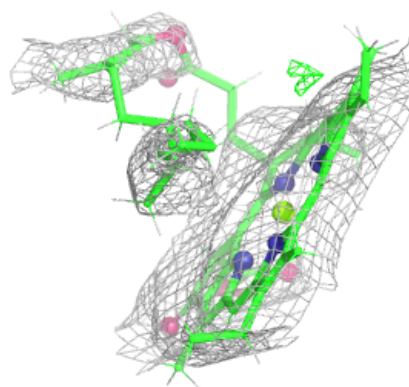
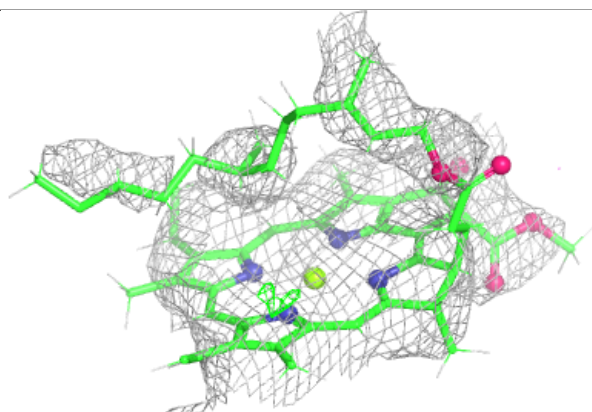
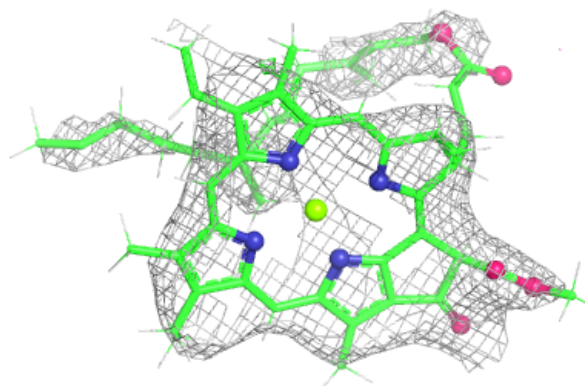


Electron density around CLA A 828:

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

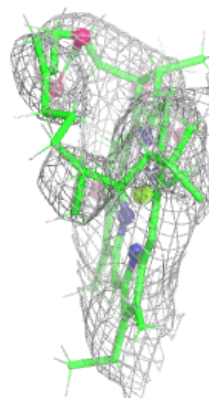
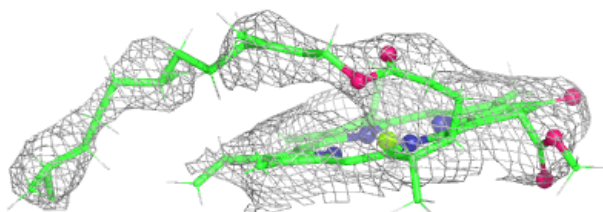
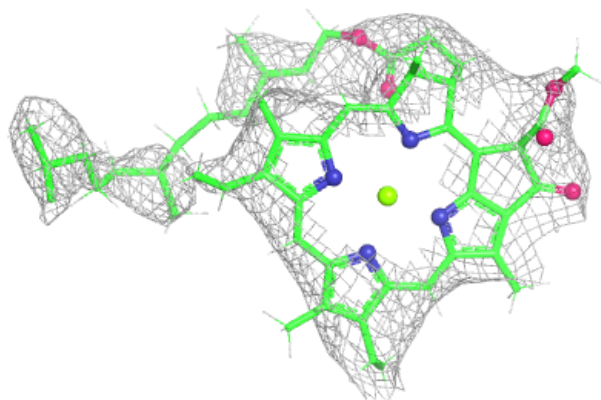
**Electron density around CLA B 3018:**

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

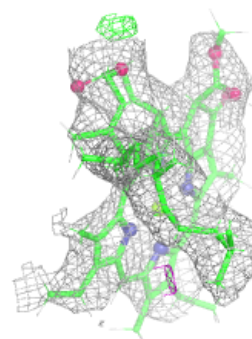
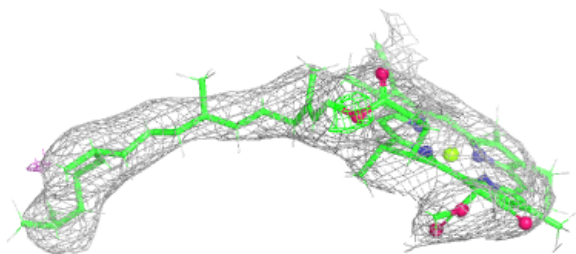
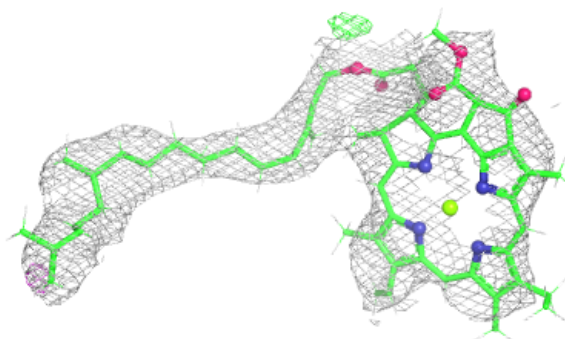


Electron density around CLA B 3019:

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

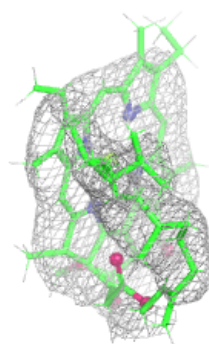
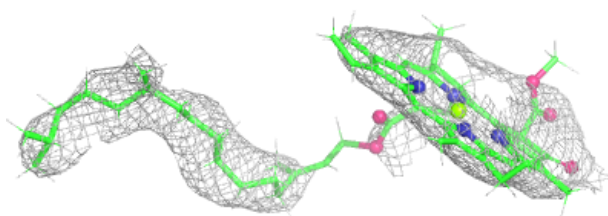
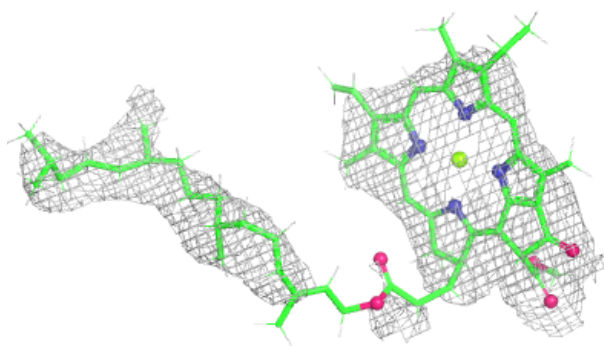
**Electron density around CLA A 803:**

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

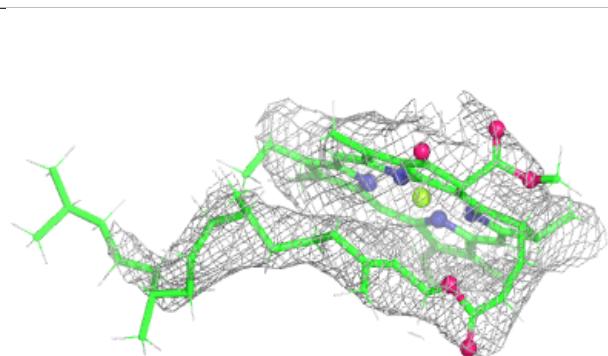
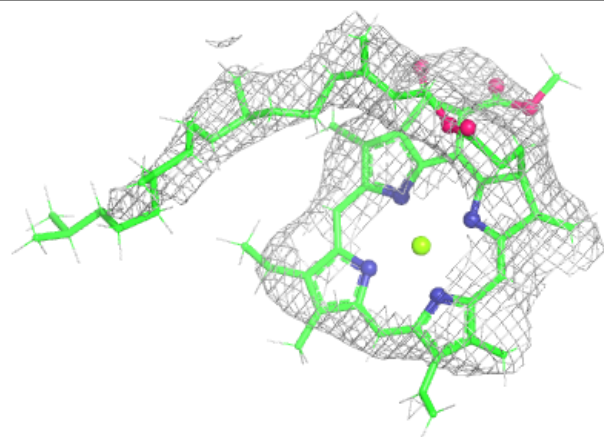


Electron density around CLA A 809:

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

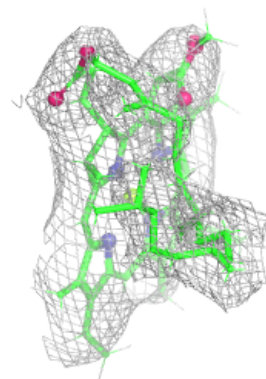
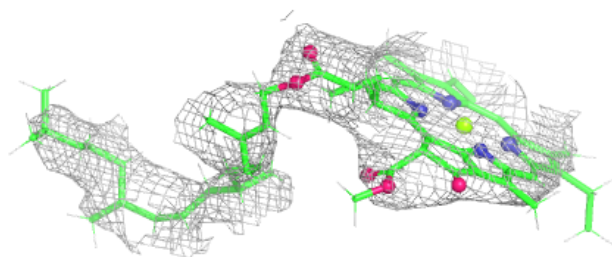
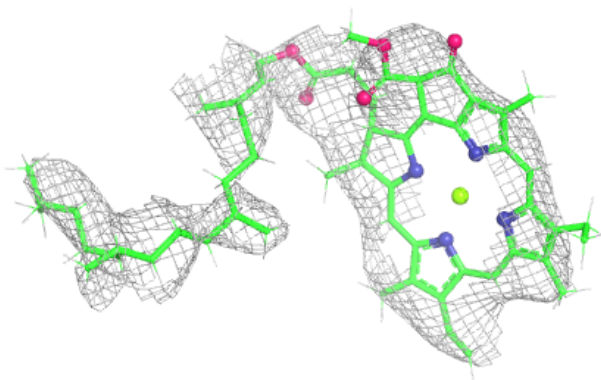
**Electron density around CLA A 830:**

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



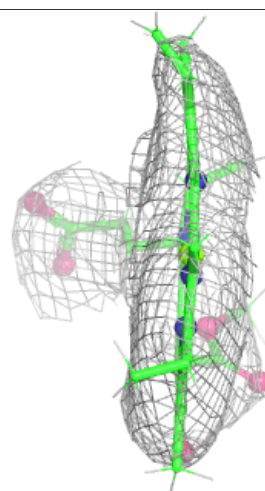
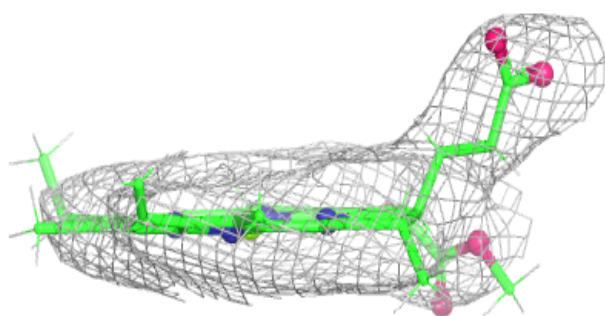
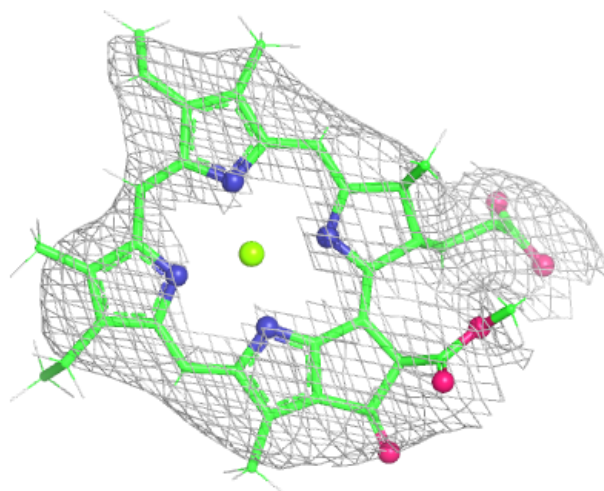
Electron density around CLA A 804:

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



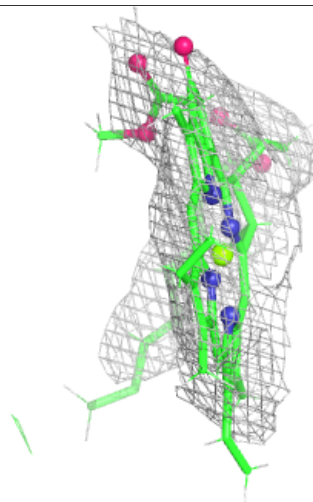
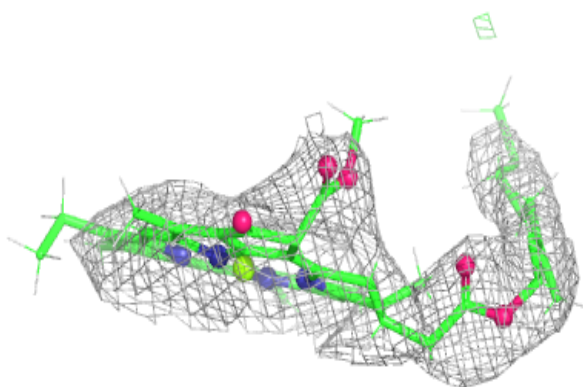
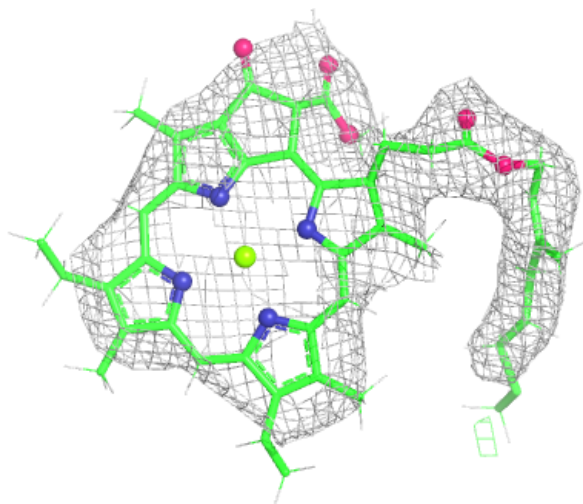
Electron density around CLA B 3024:

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



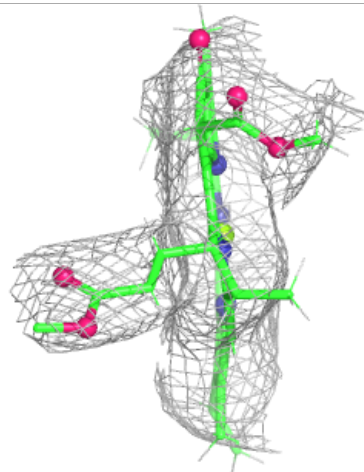
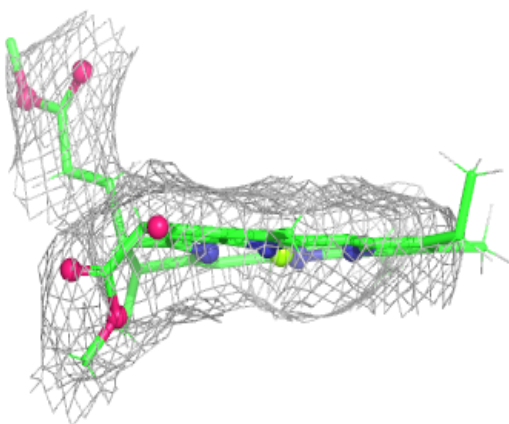
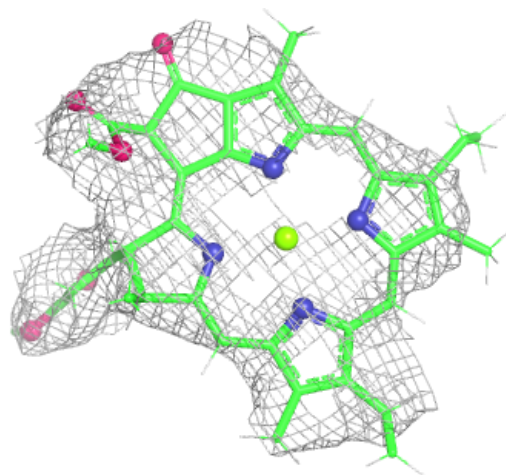
Electron density around CLA B 3025:

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



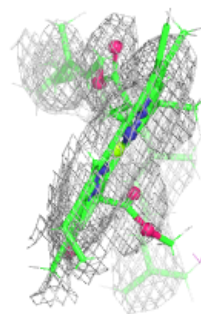
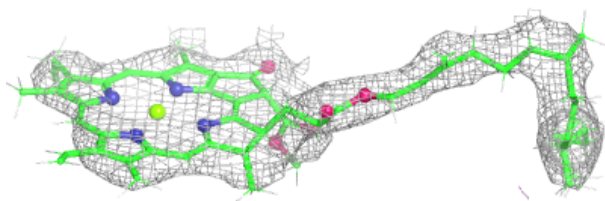
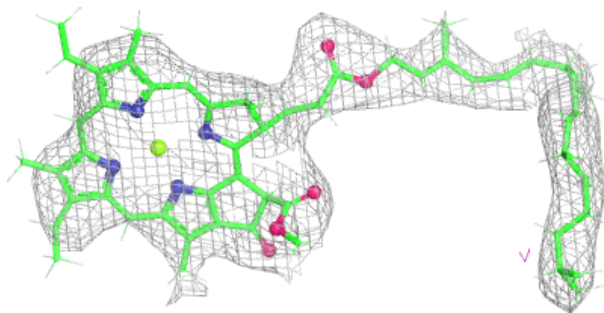
Electron density around CLA B 3026:

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



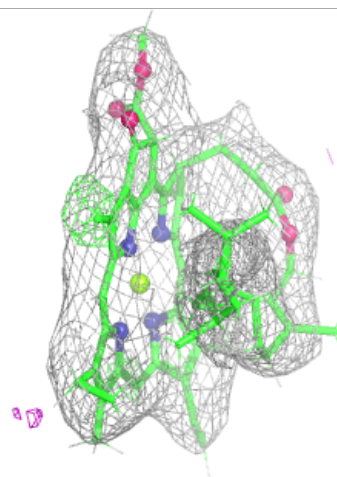
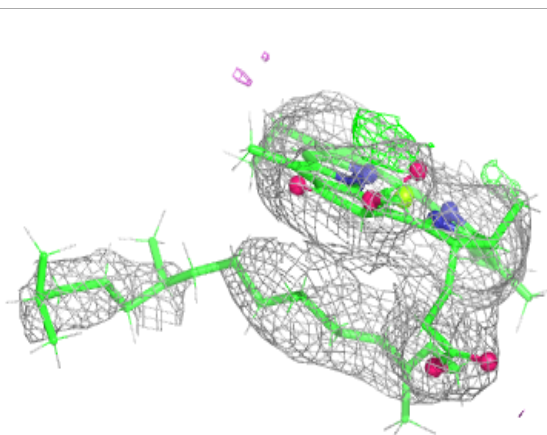
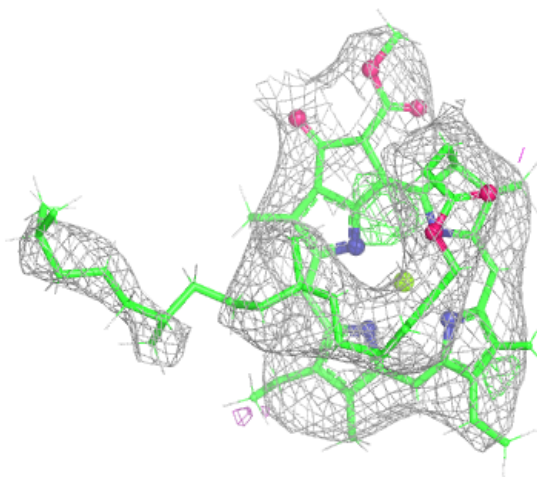
Electron density around CLA B 3027:

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



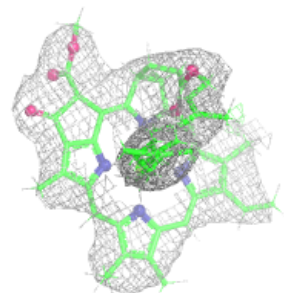
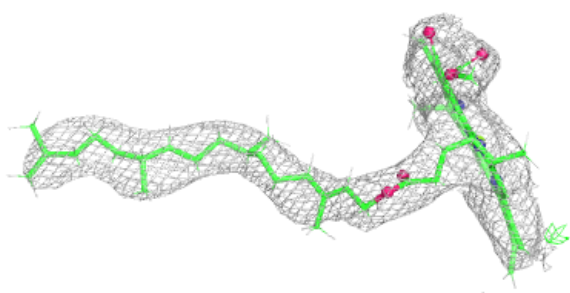
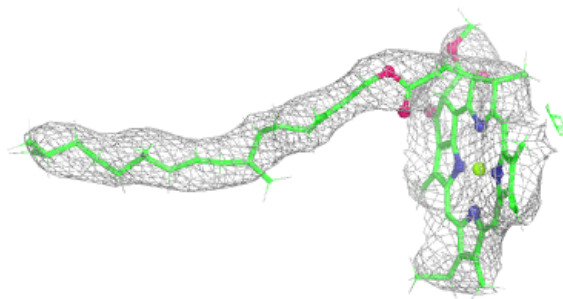
Electron density around CLA B 3028:

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

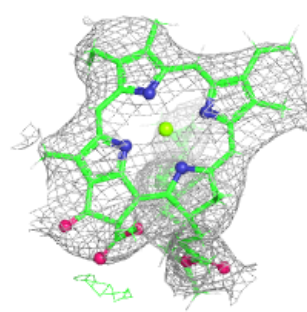
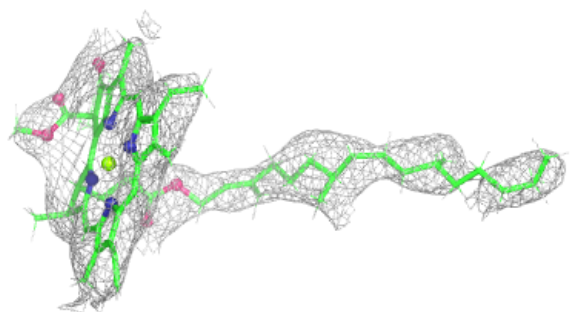
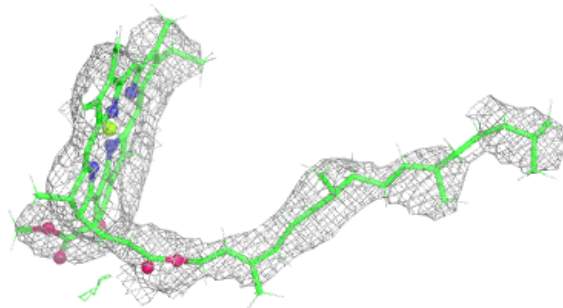


Electron density around CLA B 3029:

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

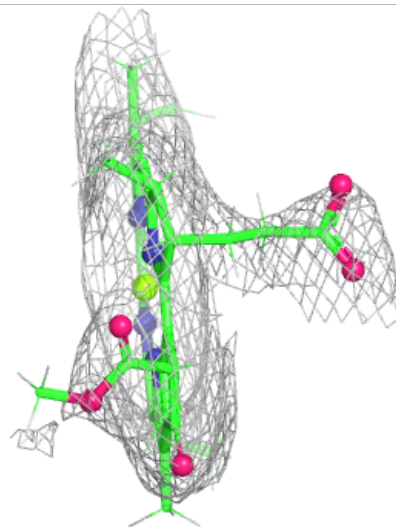
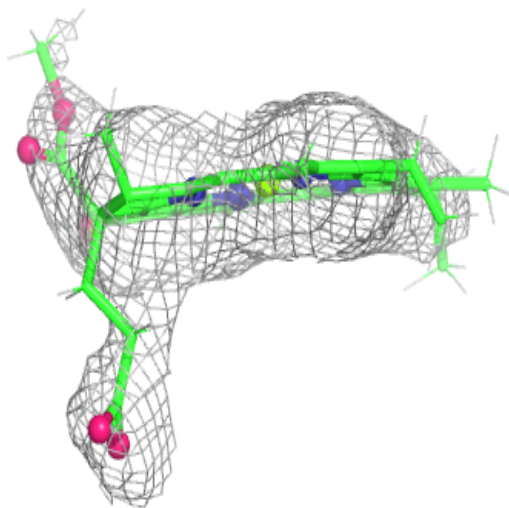
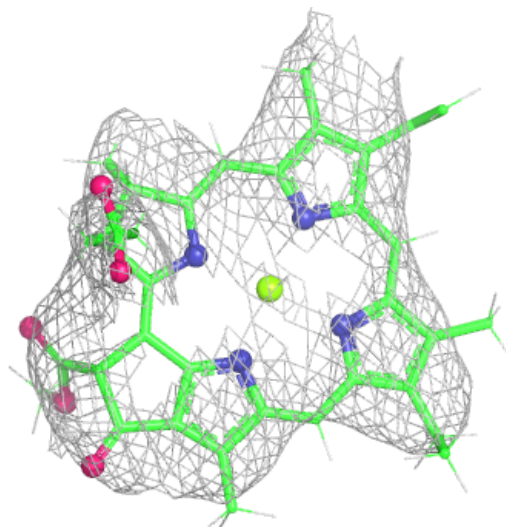
**Electron density around CLA B 3030:**

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



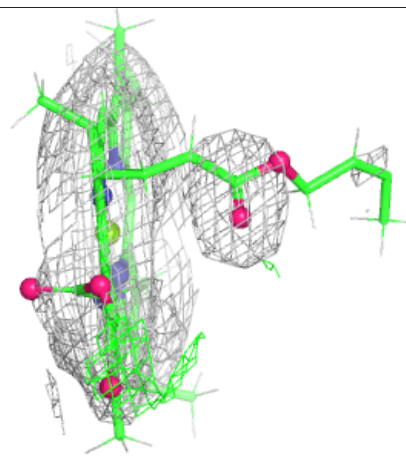
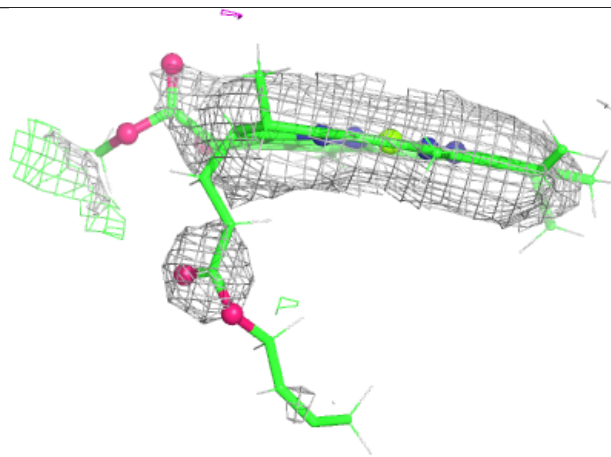
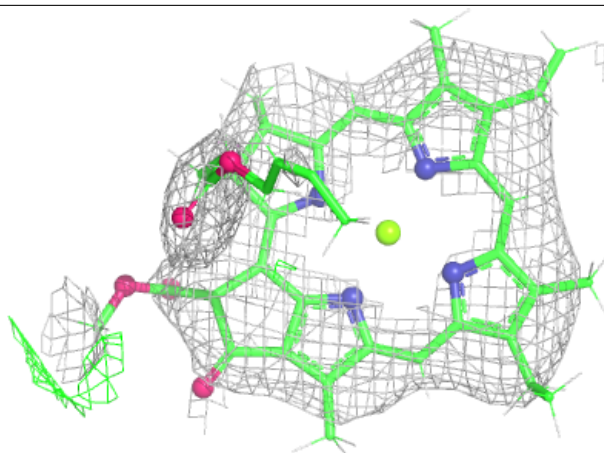
Electron density around CLA B 3031:

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



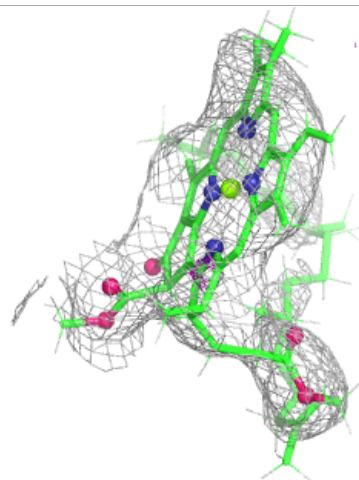
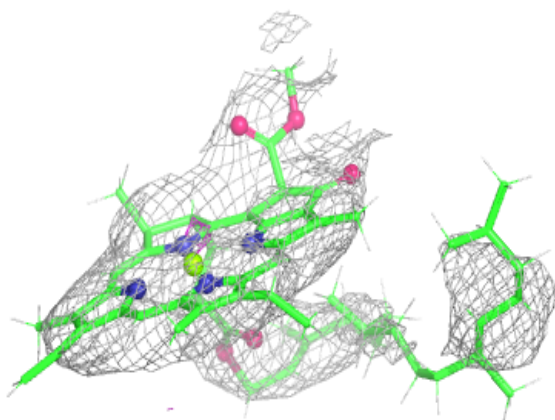
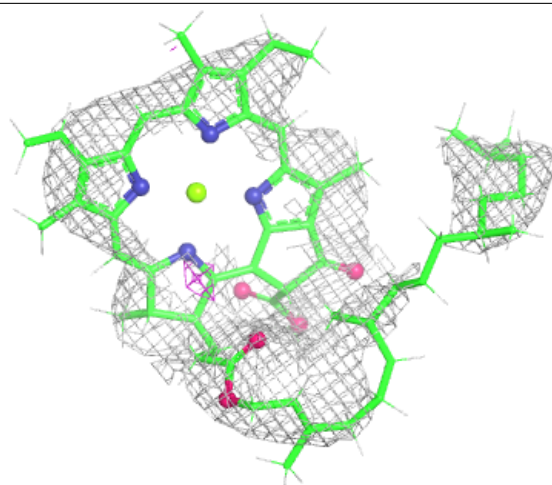
Electron density around CLA B 3032:

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



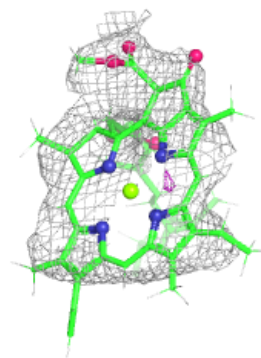
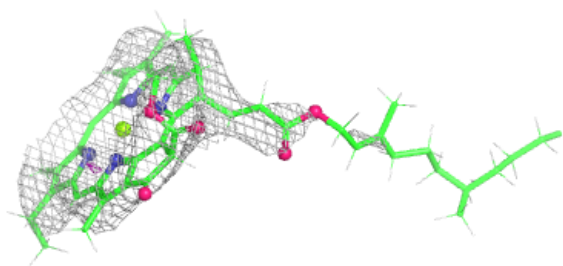
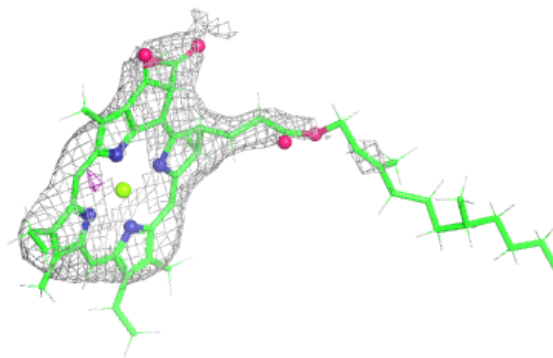
Electron density around CLA B 3033:

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



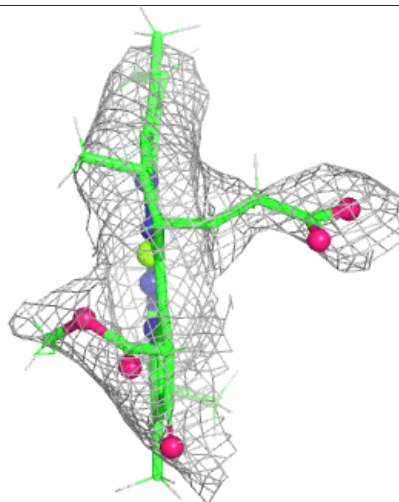
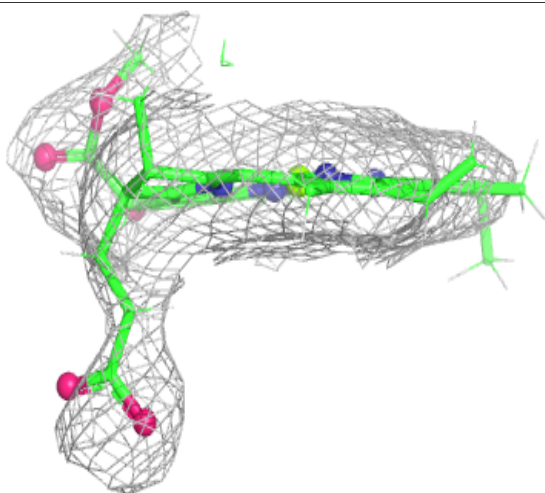
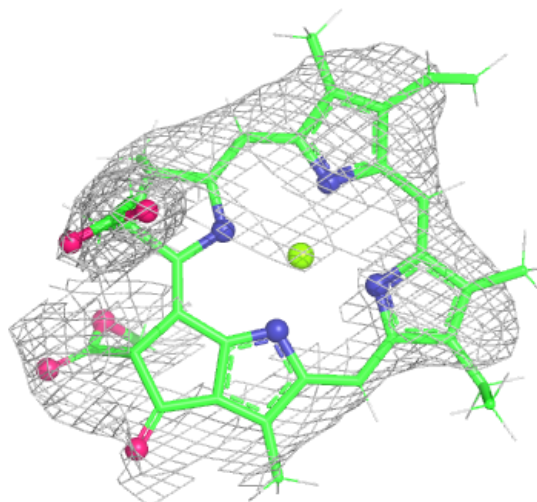
Electron density around CLA B 3034:

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



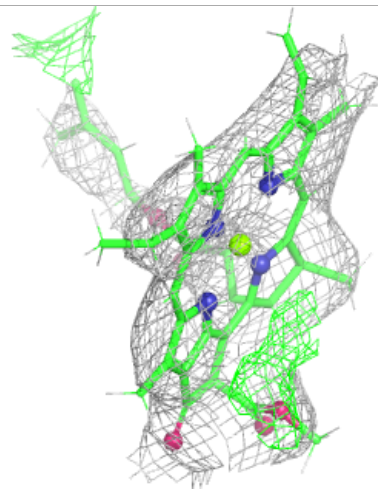
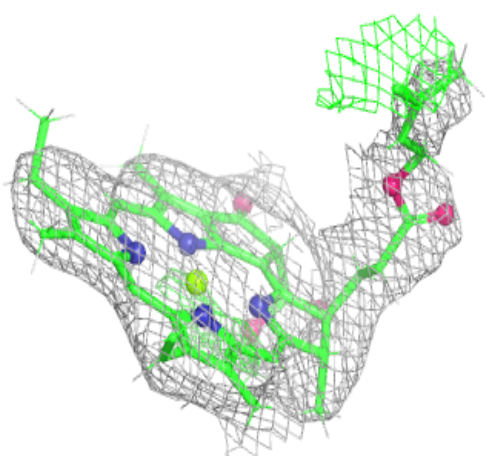
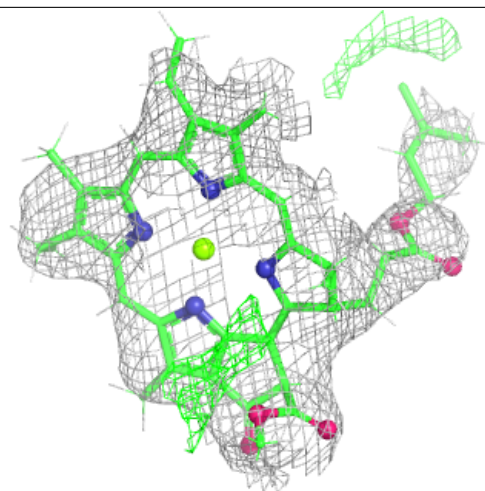
Electron density around CLA B 3035:

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



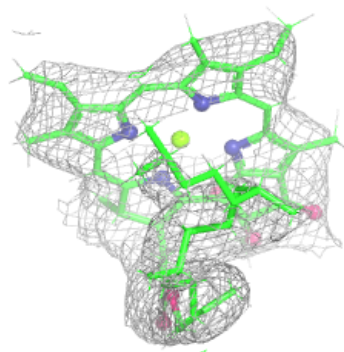
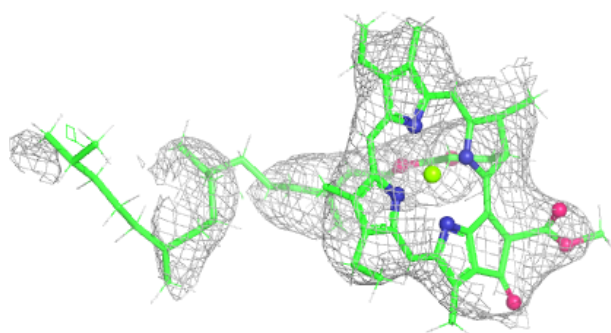
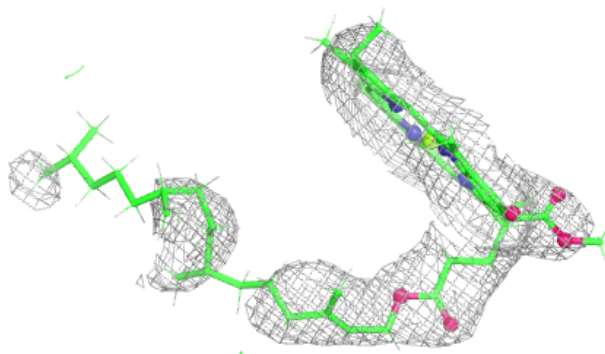
Electron density around CLA A 832:

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

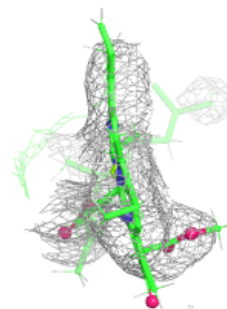
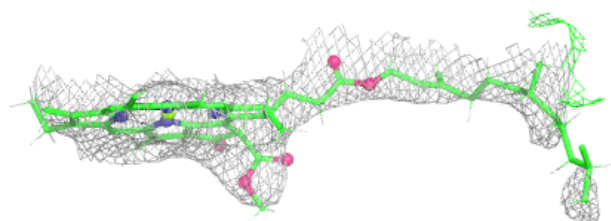
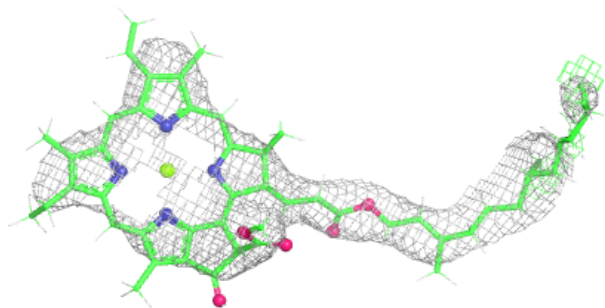


Electron density around CLA A 833:

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

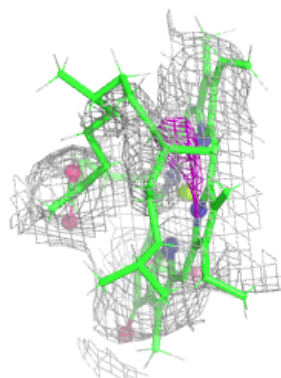
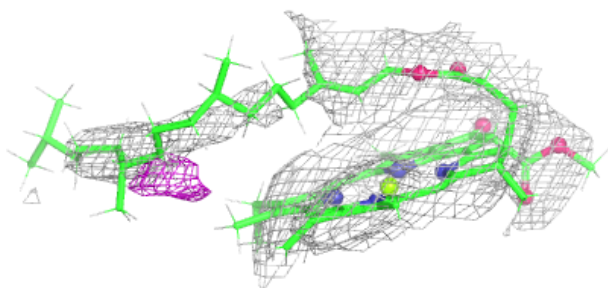
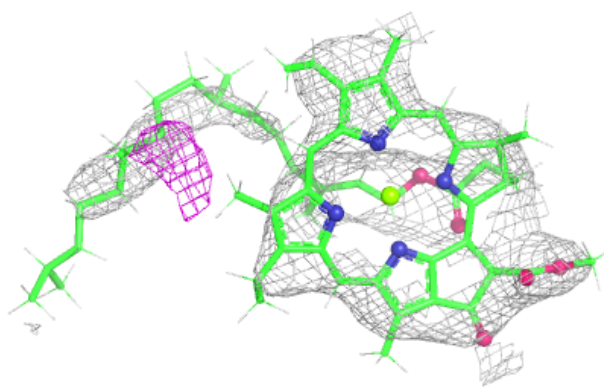
**Electron density around CLA B 3038:**

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



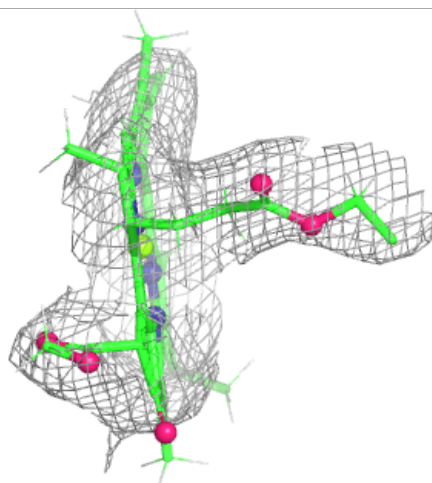
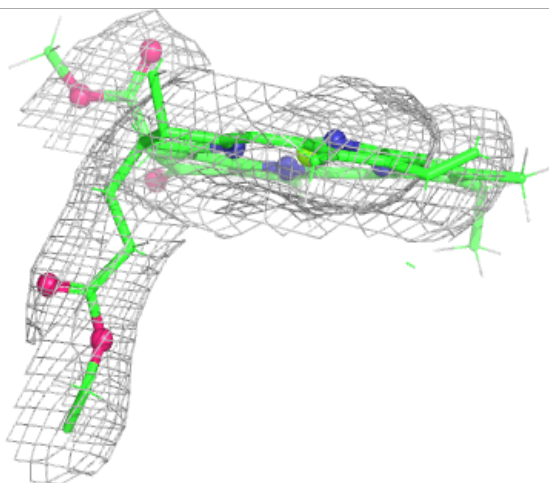
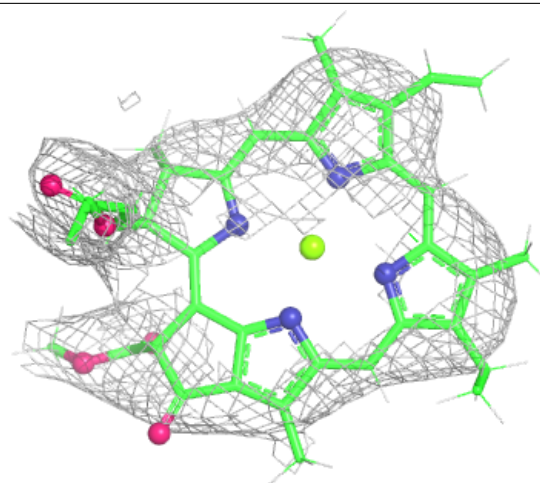
Electron density around CLA B 3039:

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



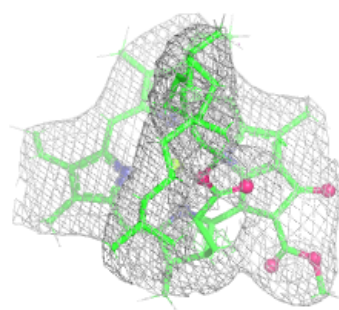
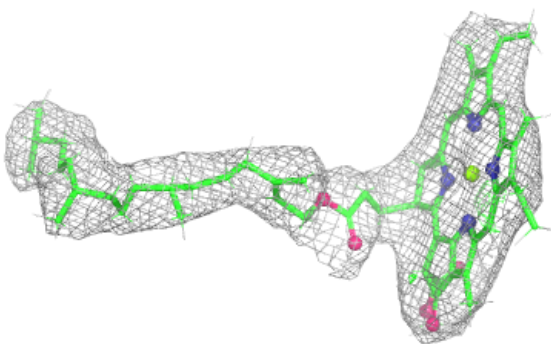
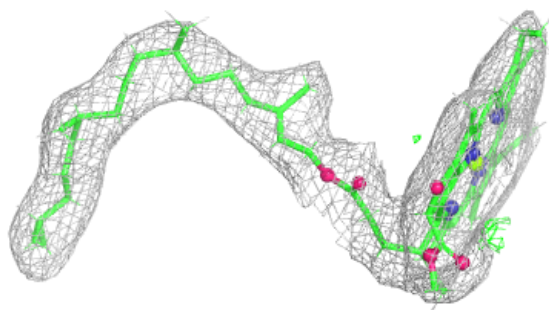
Electron density around CLA B 3040:

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

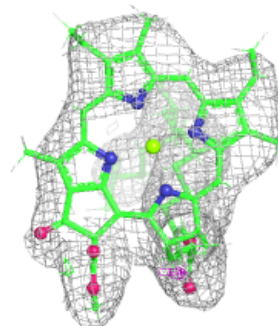
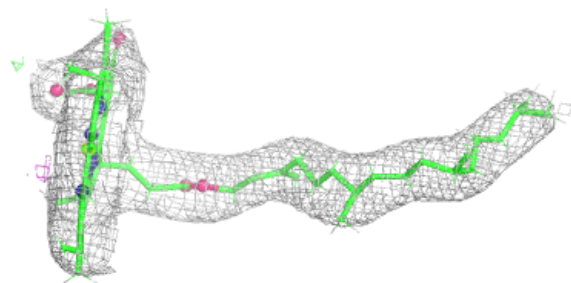
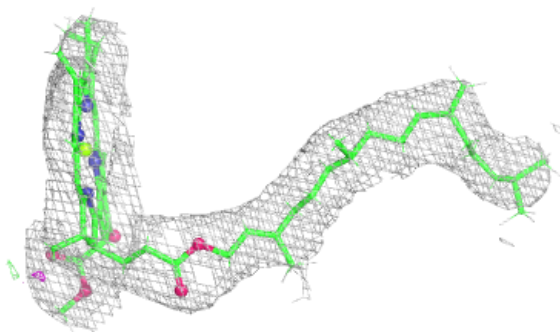


Electron density around CLA B 3041:

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

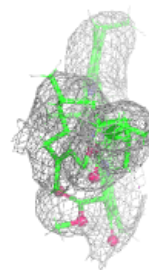
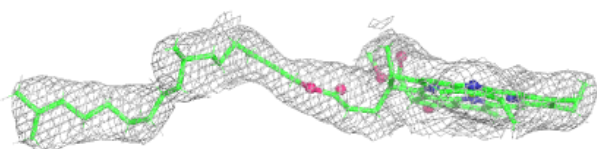
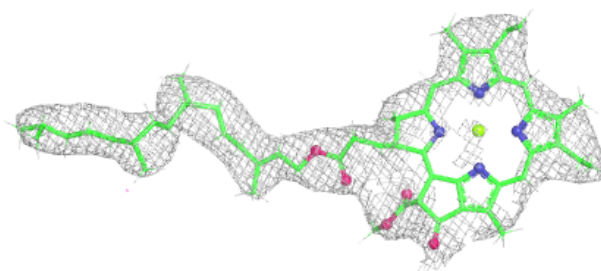
**Electron density around CLA B 3042:**

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

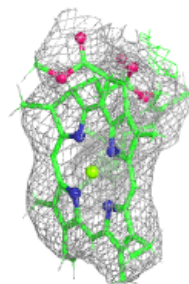
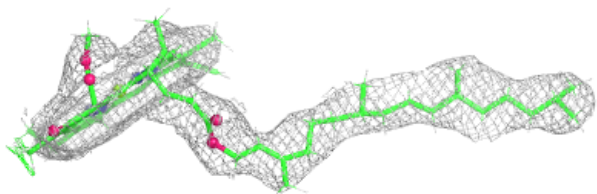
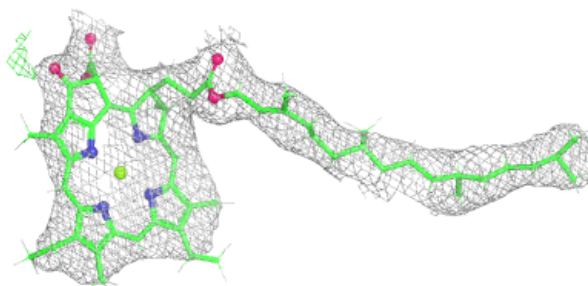


Electron density around CLA A 834:

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

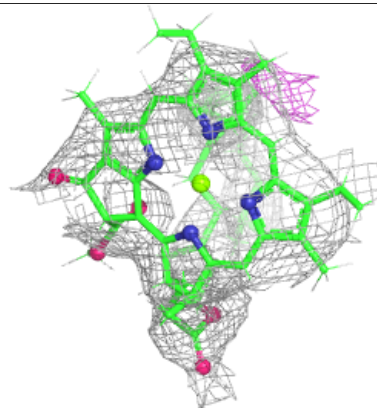
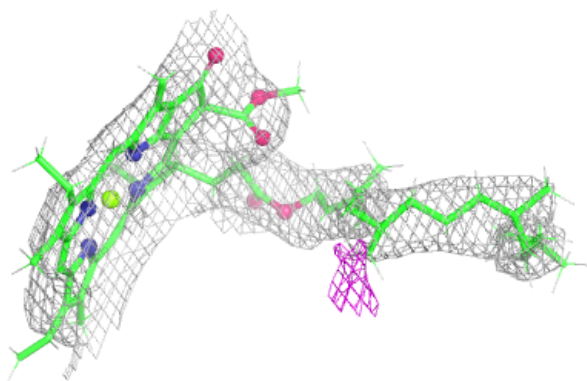
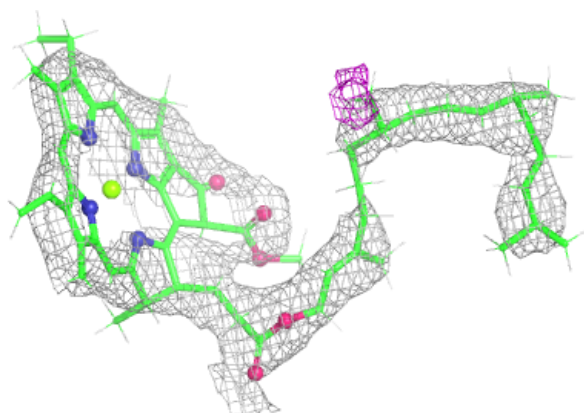
**Electron density around CLA A 835:**

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

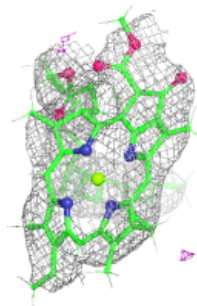
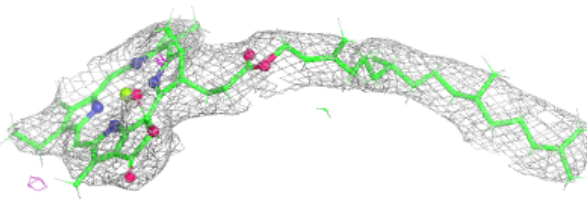
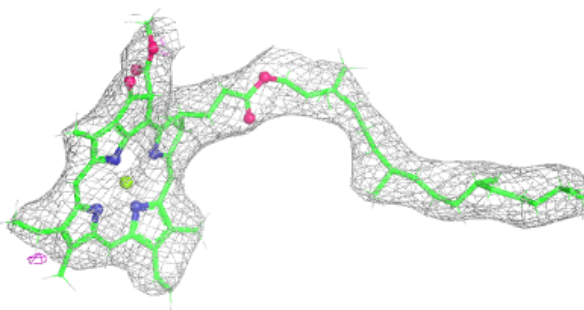


Electron density around CL0 A 801:

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

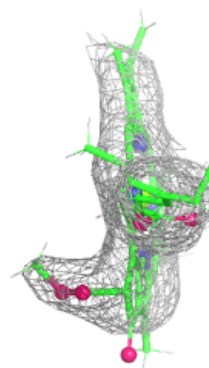
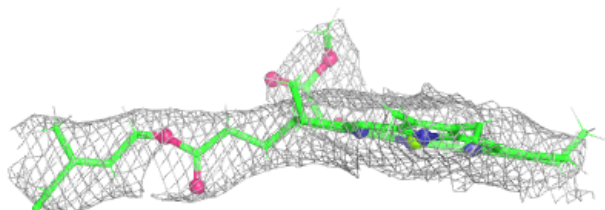
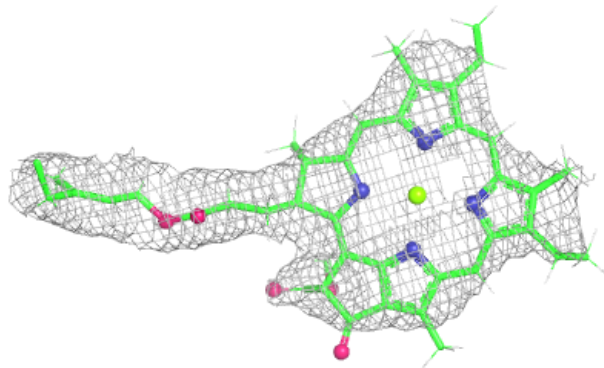
**Electron density around CLA A 802:**

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



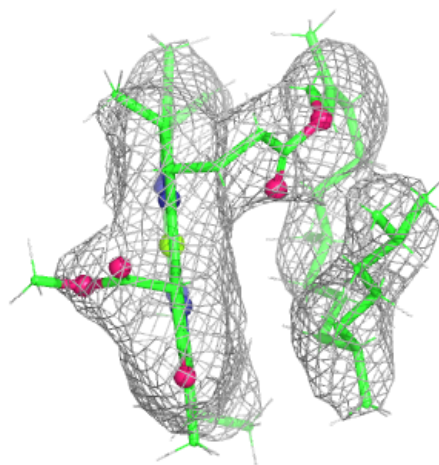
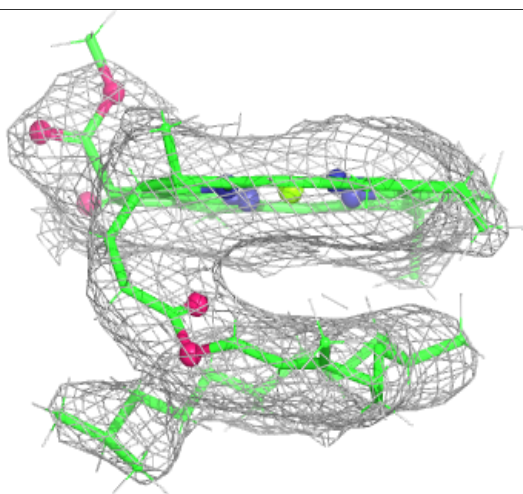
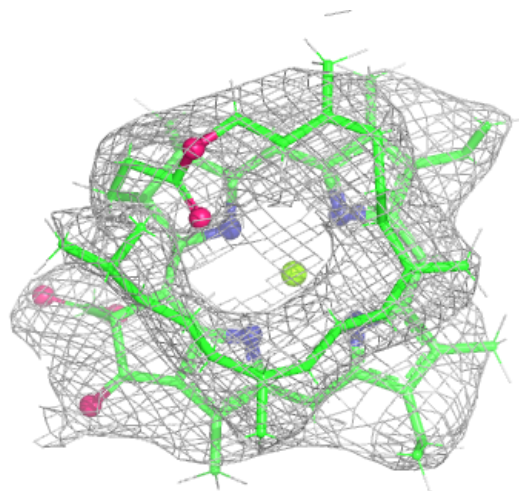
Electron density around CLA A 838:

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



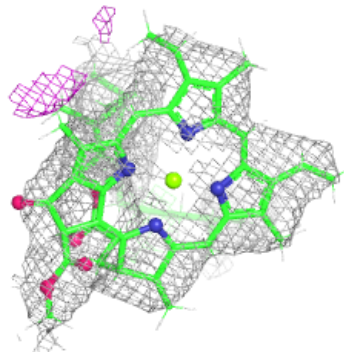
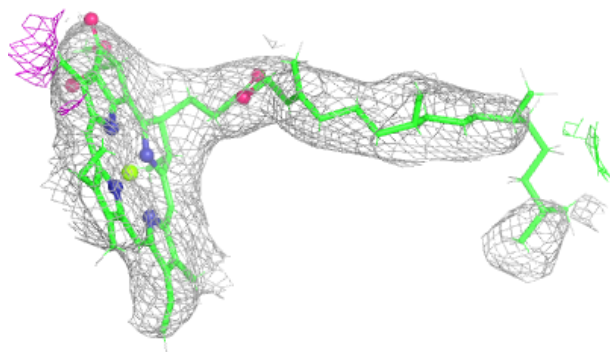
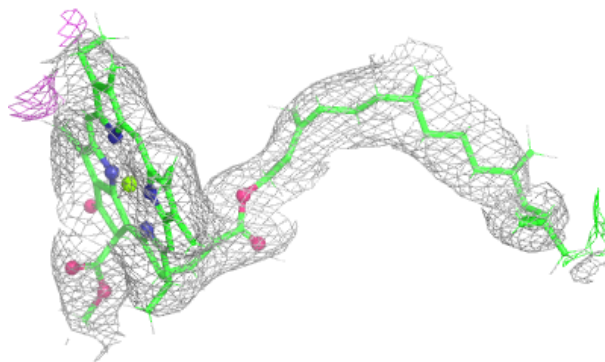
Electron density around CLA L 204:

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

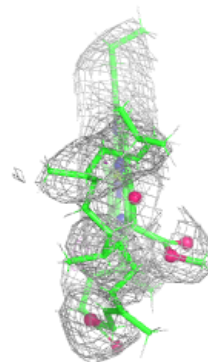
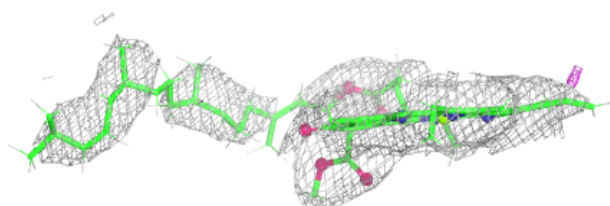
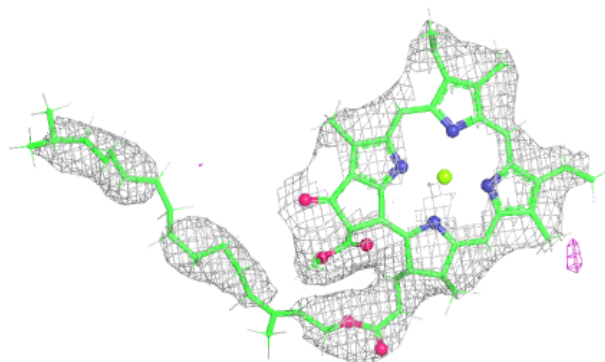


Electron density around CLA L 205:

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

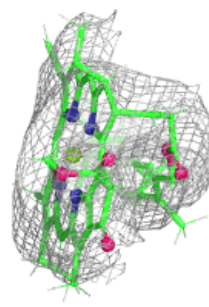
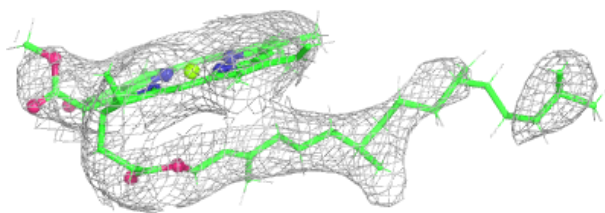
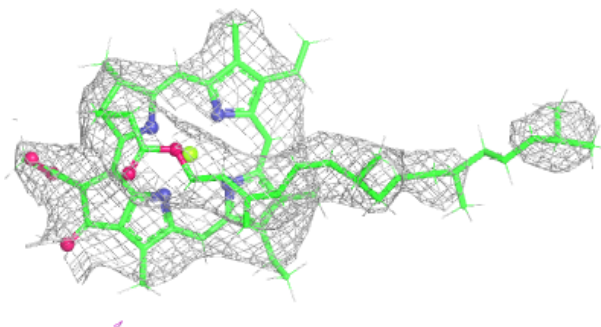
**Electron density around CLA L 206:**

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



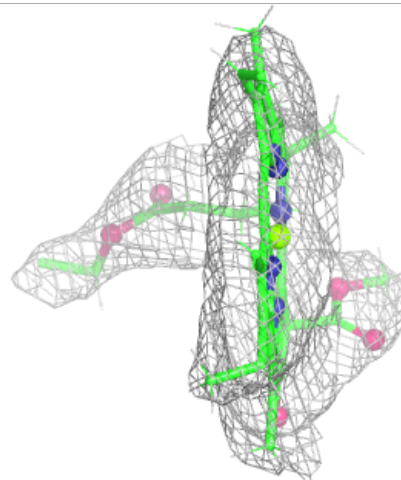
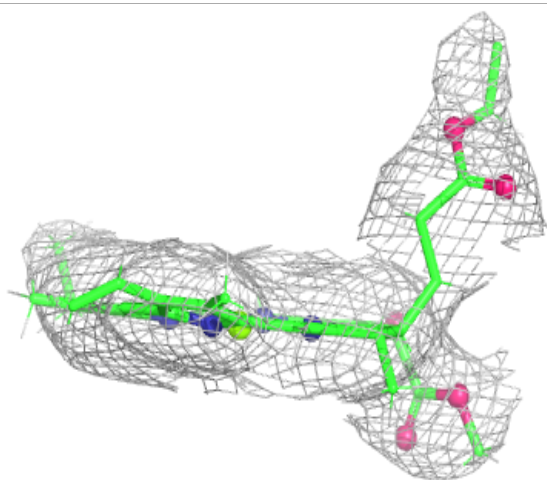
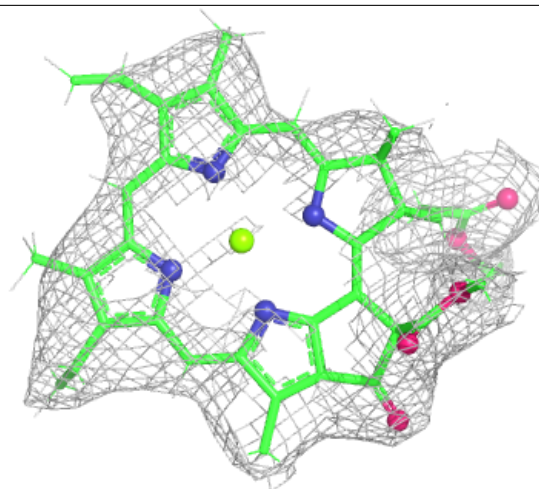
Electron density around CLA A 839:

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



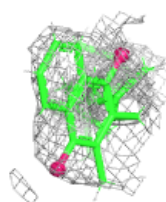
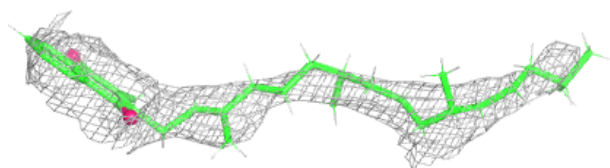
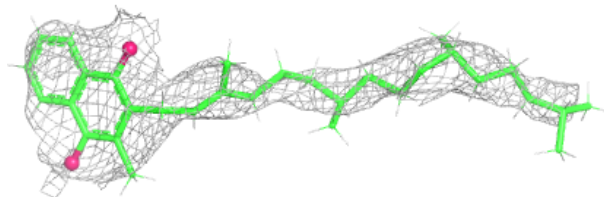
Electron density around CLA A 840:

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

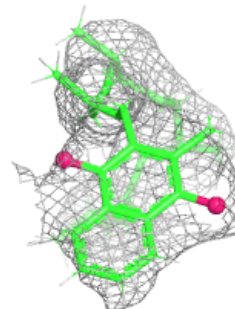
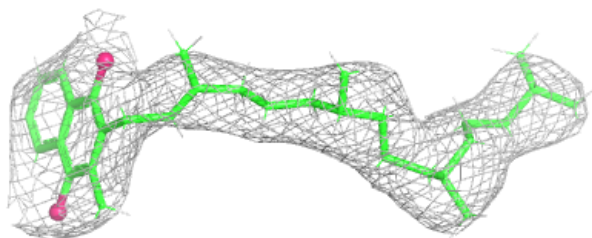
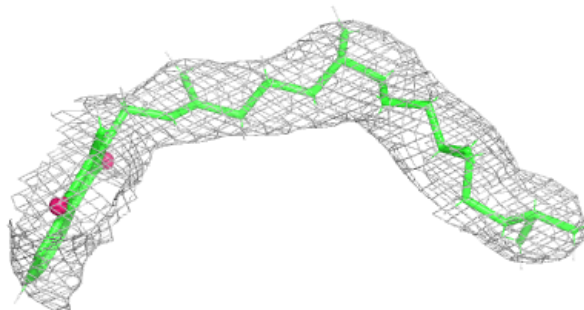


Electron density around PQN A 846:

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

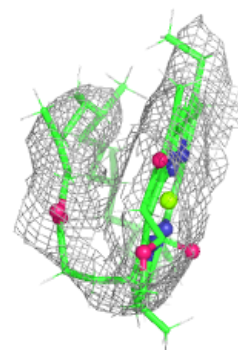
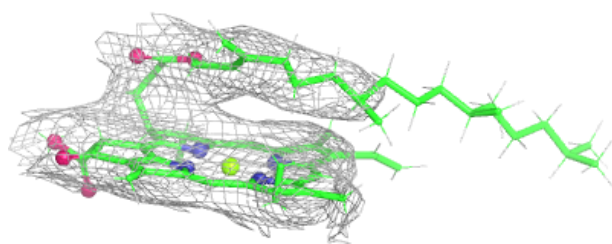
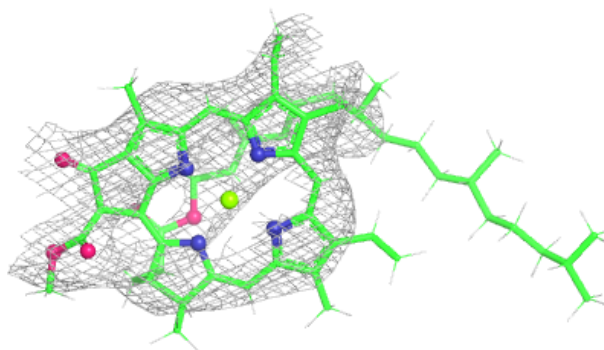
**Electron density around PQN B 3043:**

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

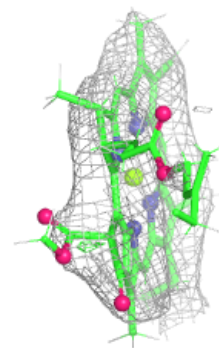
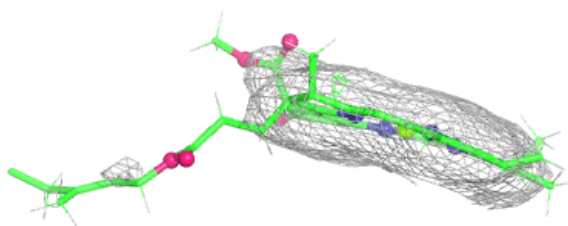
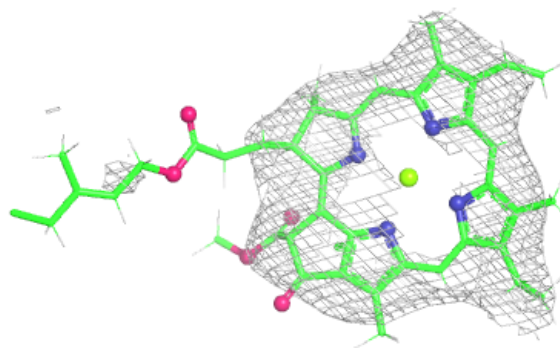


Electron density around CLA A 841:

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

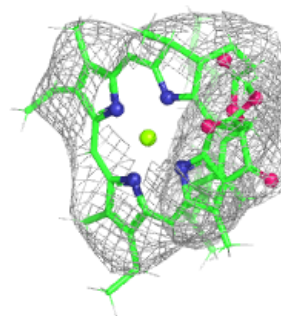
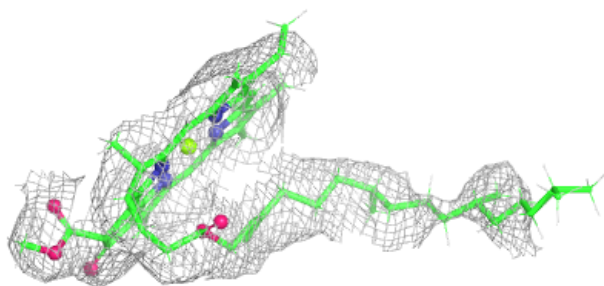
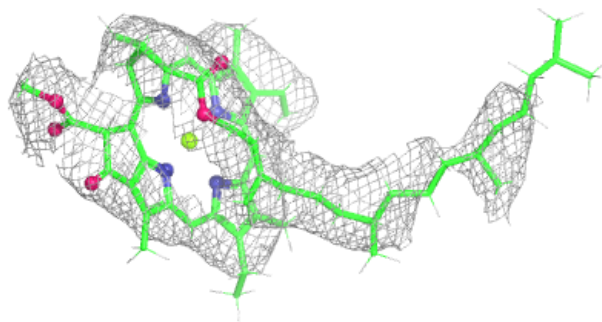
**Electron density around CLA A 842:**

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

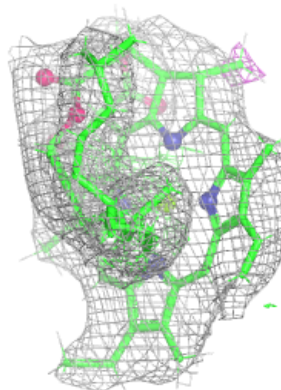
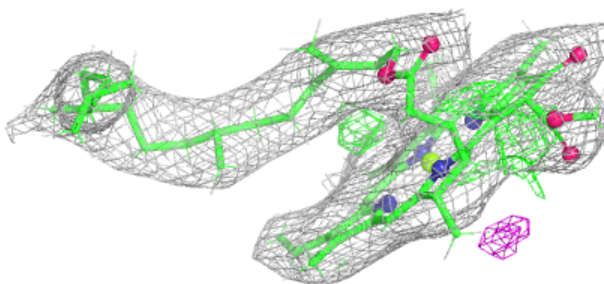
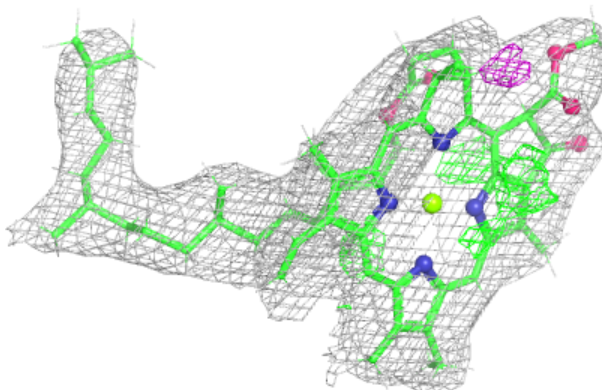


Electron density around CLA A 843:

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

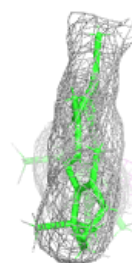
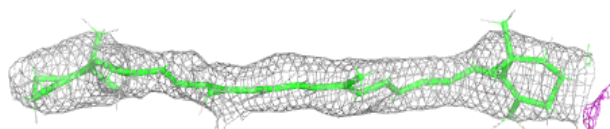
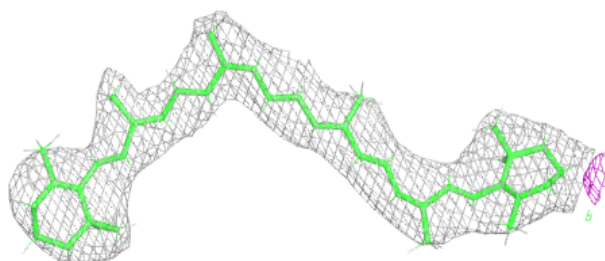
**Electron density around CLA A 844:**

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

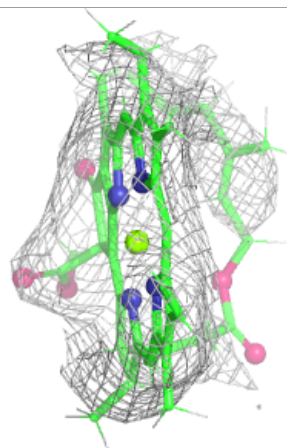
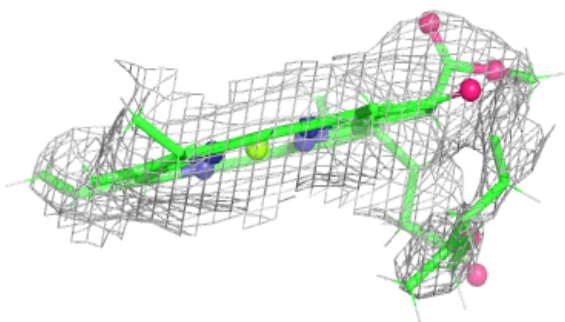
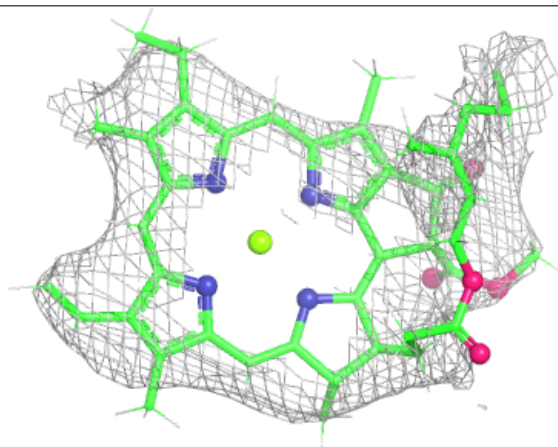


Electron density around BCR A 851:

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

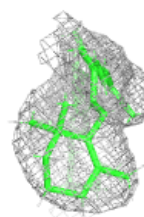
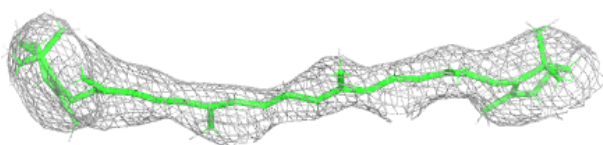
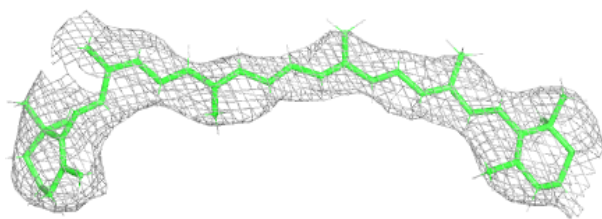
**Electron density around CLA A 845:**

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

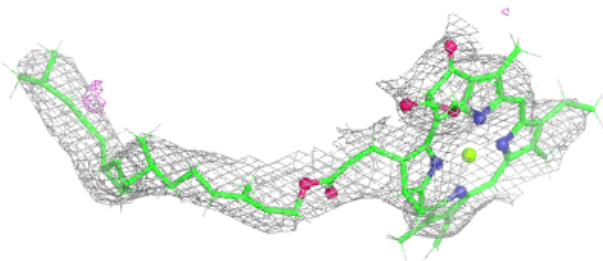
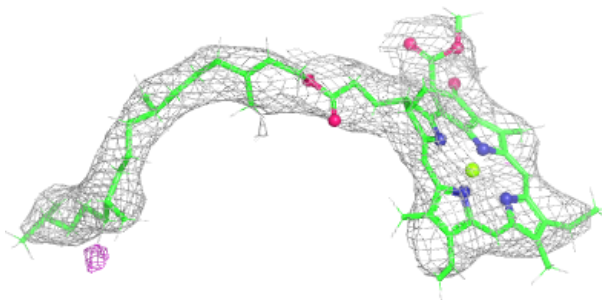


Electron density around BCR B 3045:

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

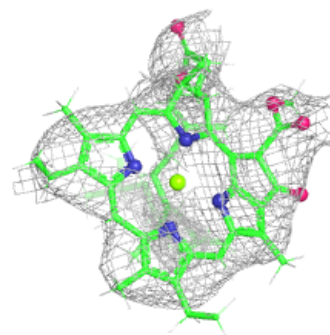
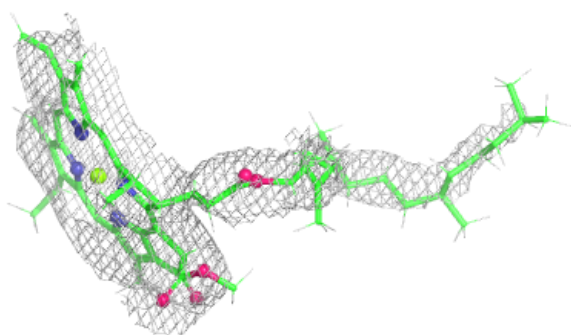
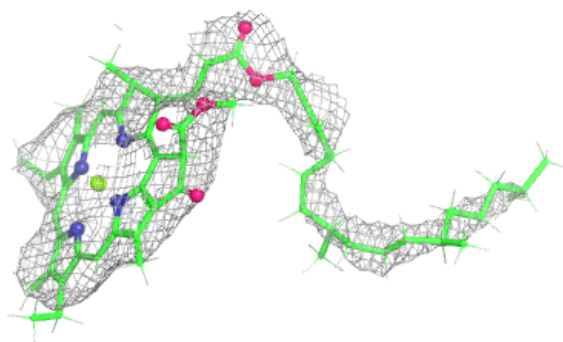
**Electron density around CLA A 856:**

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

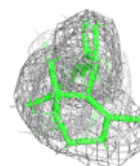
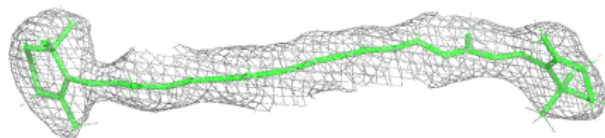
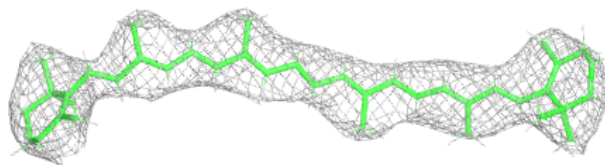


Electron density around CLA B 3003:

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

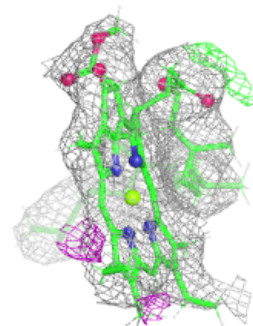
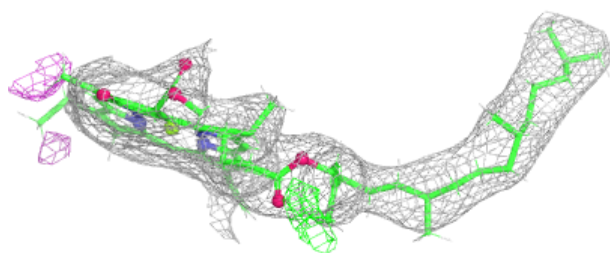
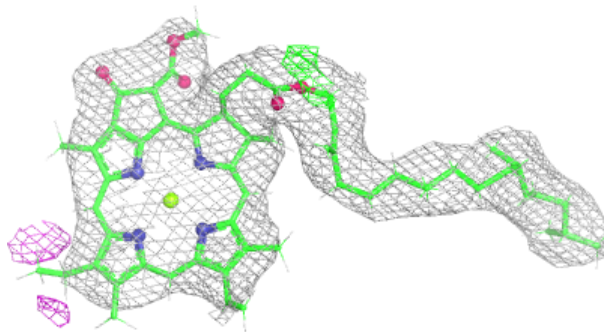
**Electron density around BCR B 3048:**

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

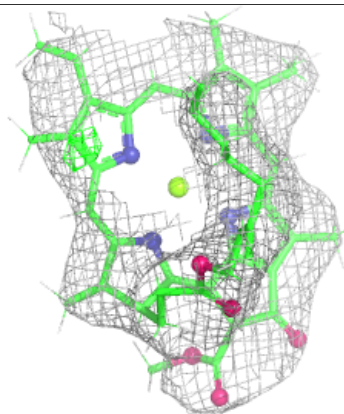
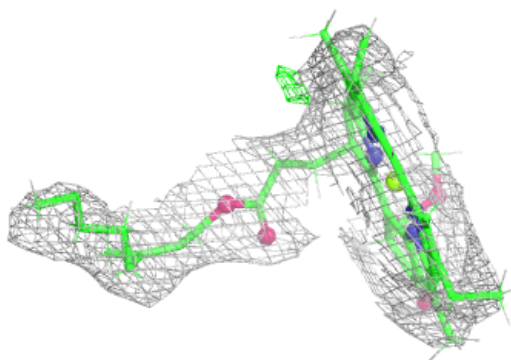
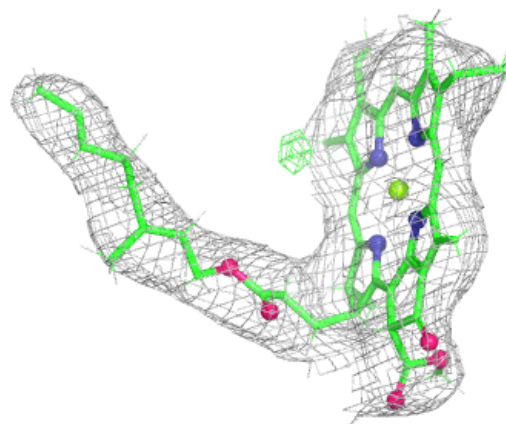


Electron density around CLA B 3004:

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

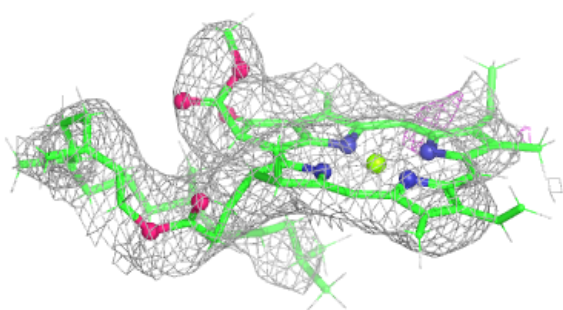
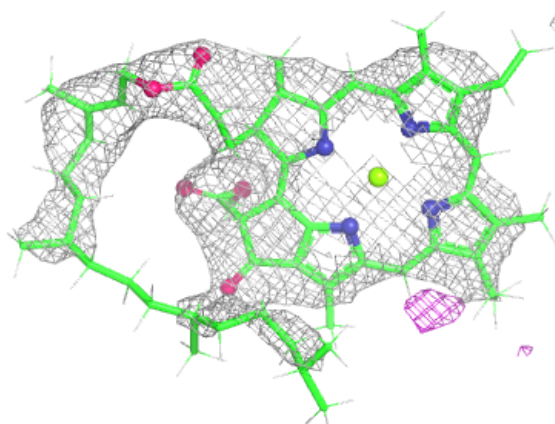
**Electron density around CLA B 3005:**

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

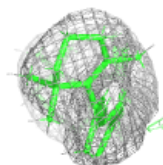
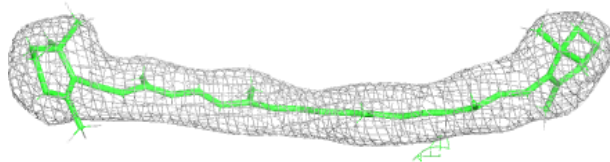
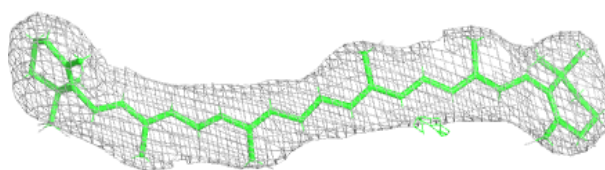


Electron density around CLA B 3006:

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

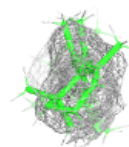
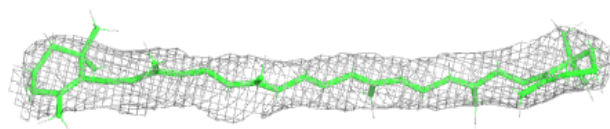
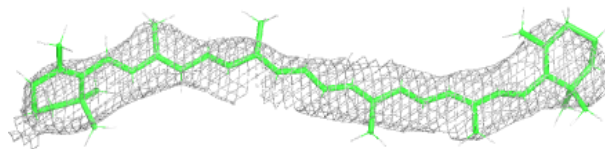
**Electron density around BCR I 101:**

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



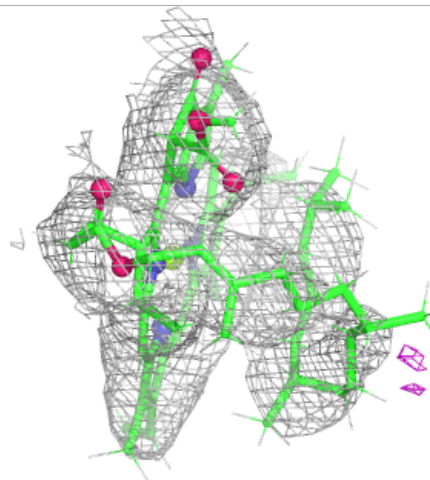
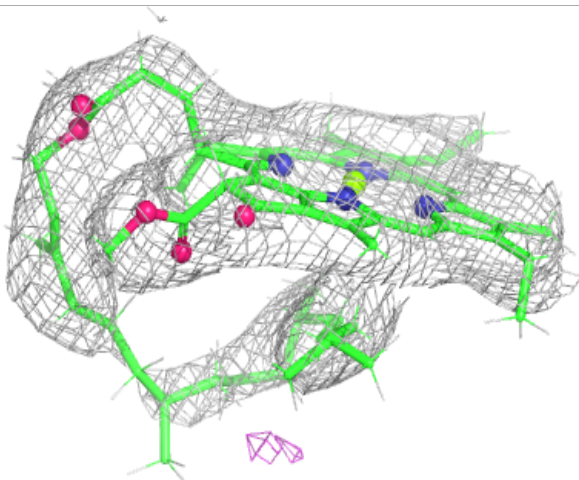
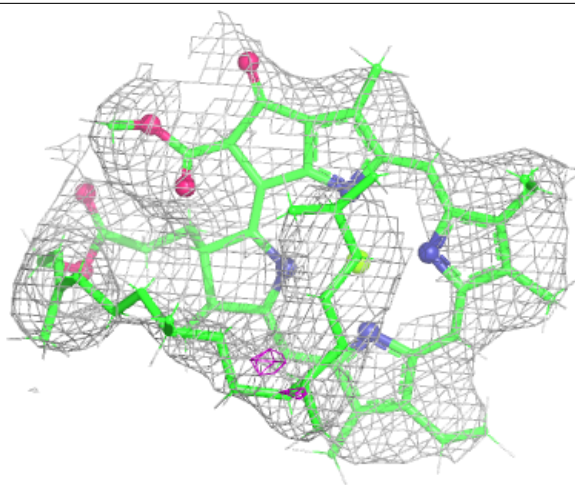
Electron density around BCR J 103:

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



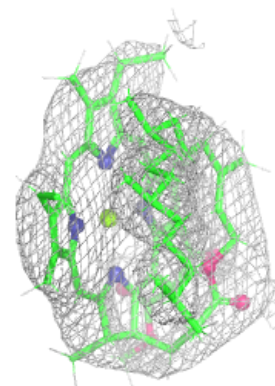
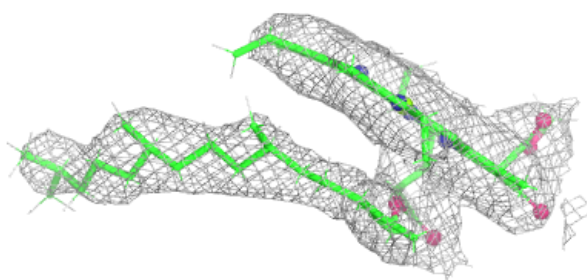
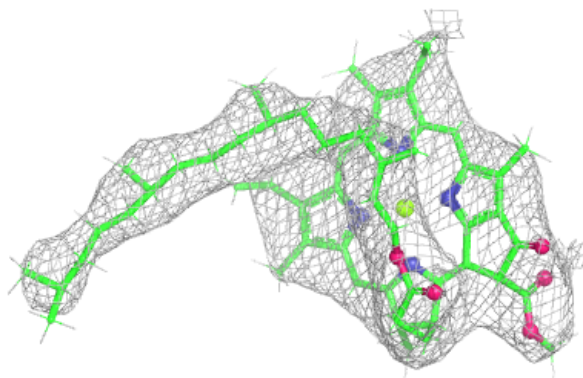
Electron density around CLA B 3007:

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



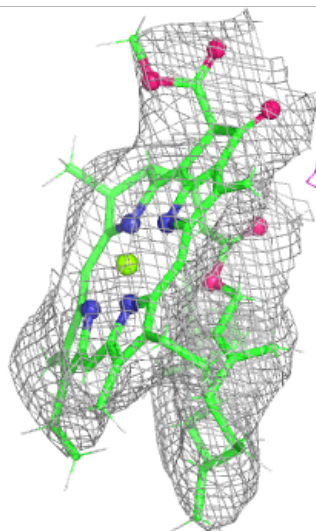
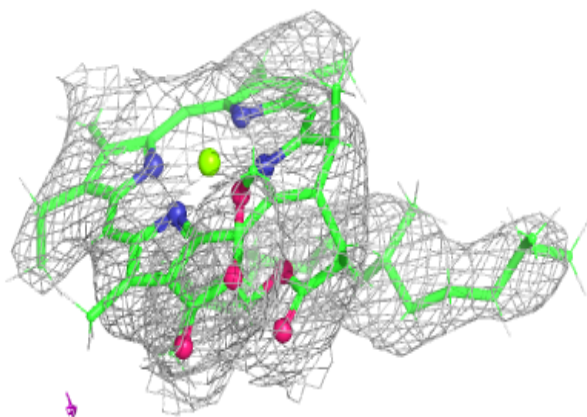
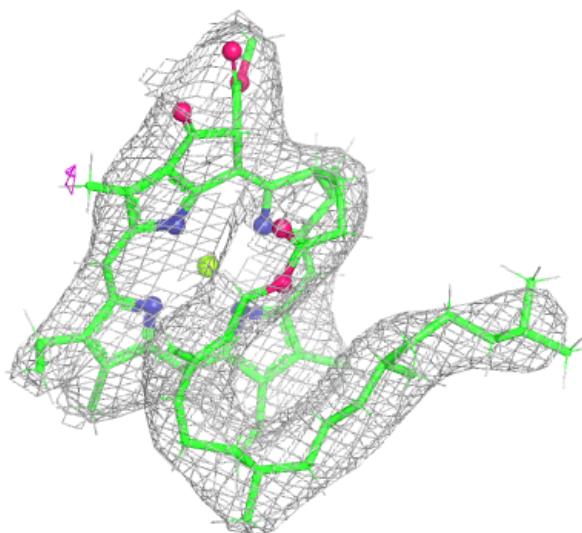
Electron density around CLA B 3008:

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



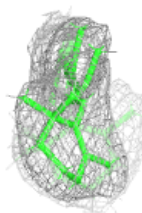
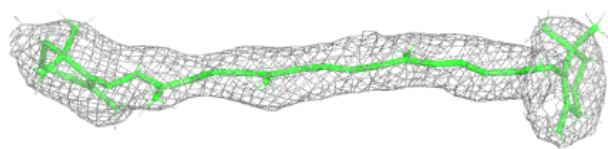
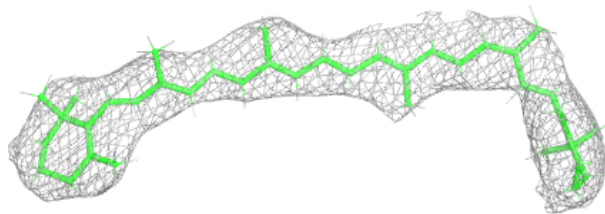
Electron density around CLA B 3009:

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

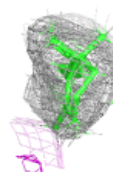
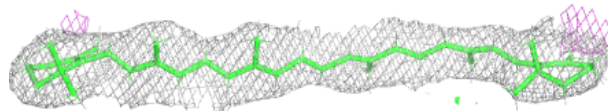
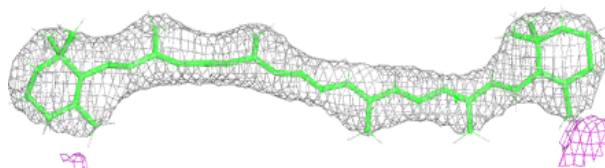


Electron density around BCR L 201:

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

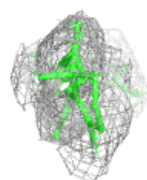
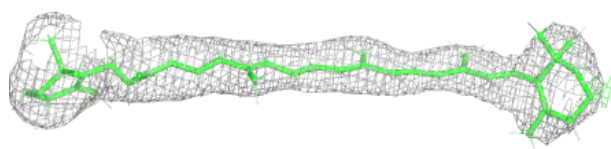
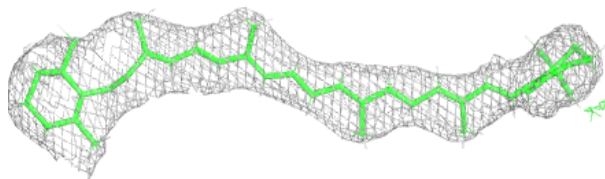
**Electron density around BCR L 208:**

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

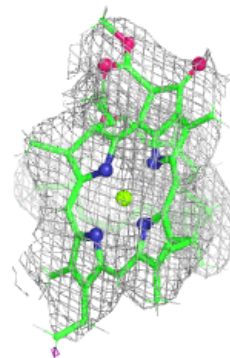
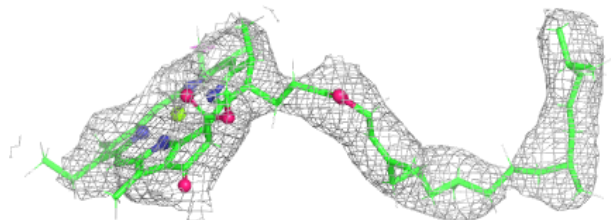
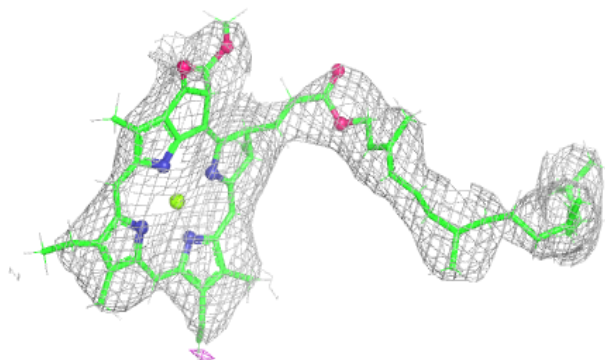


Electron density around BCR L 209:

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

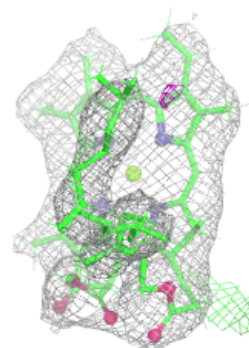
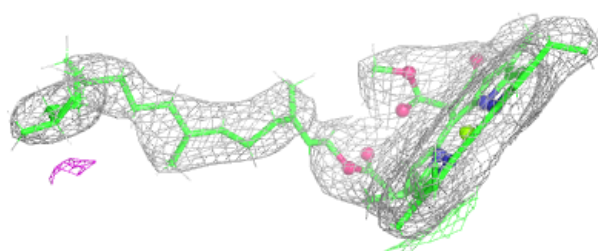
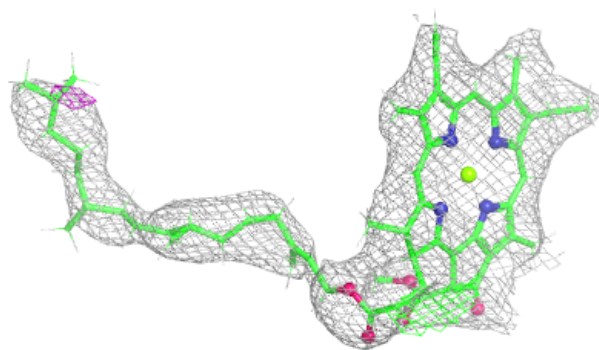
**Electron density around CLA B 3010:**

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



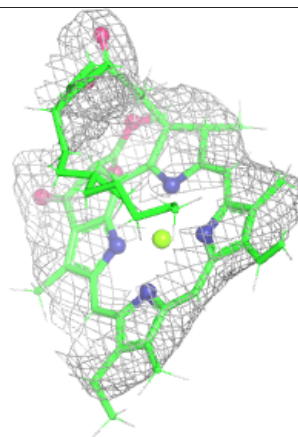
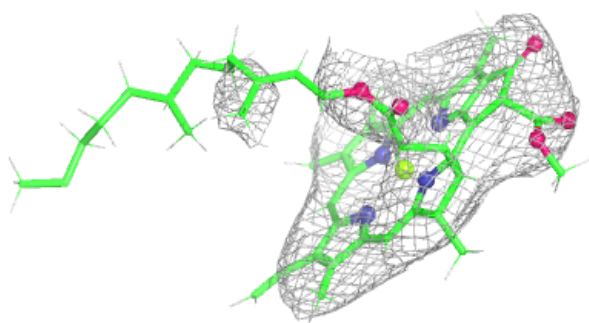
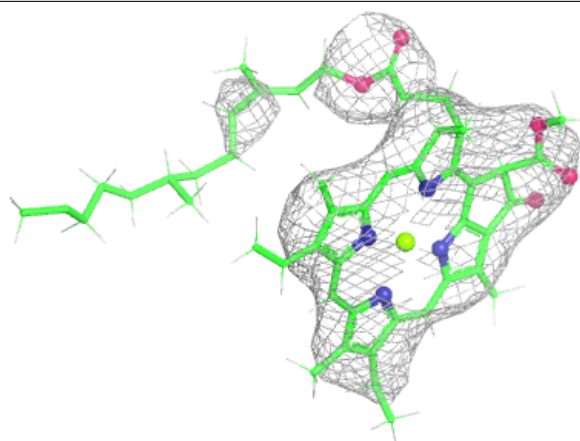
Electron density around CLA B 3011:

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

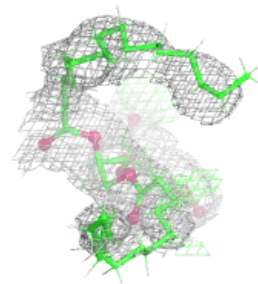
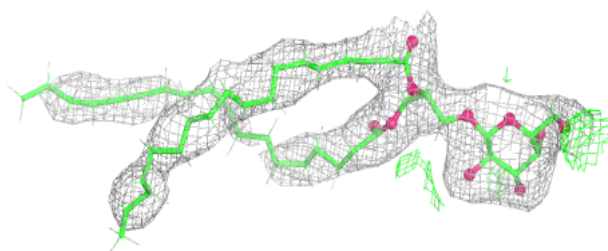
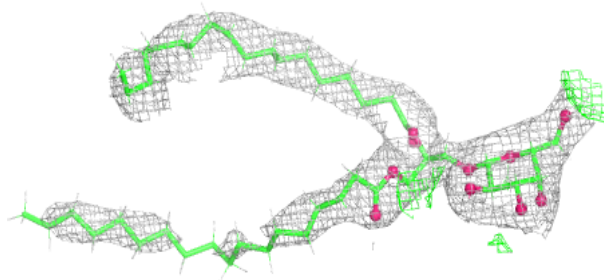


Electron density around CLA A 825:

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

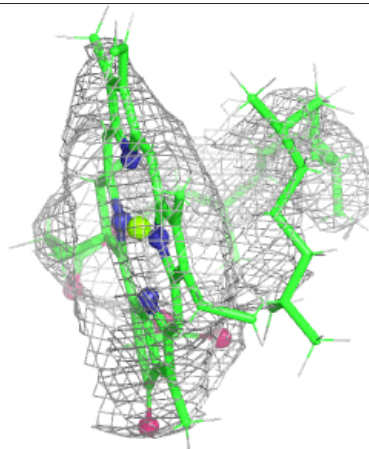
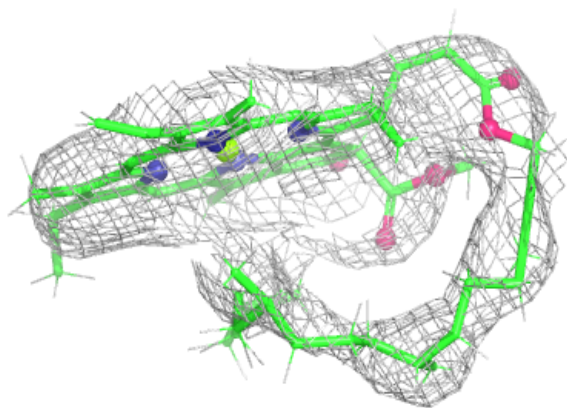
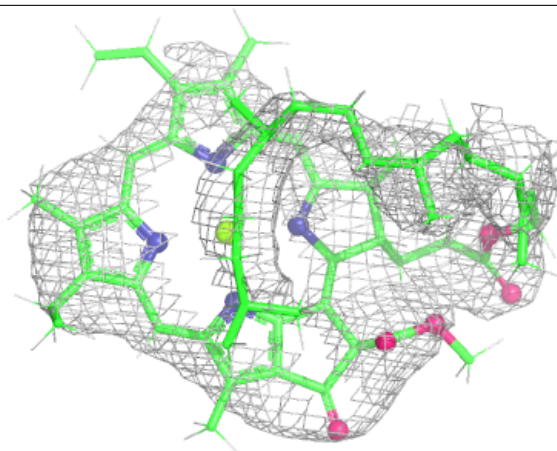
**Electron density around LMG B 3049:**

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



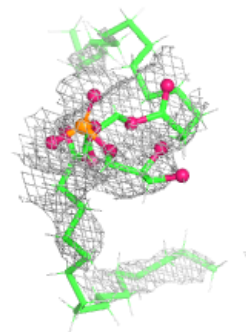
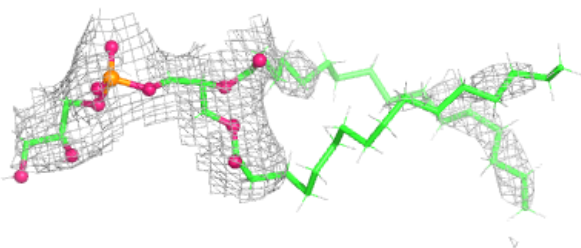
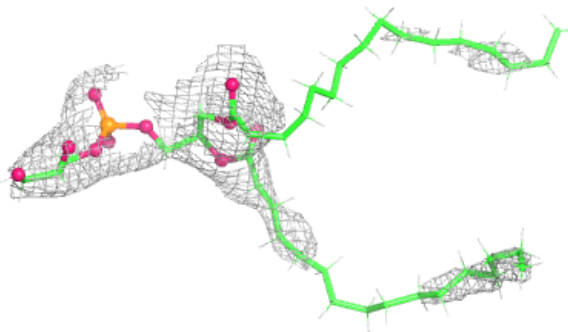
Electron density around CLA A 807:

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

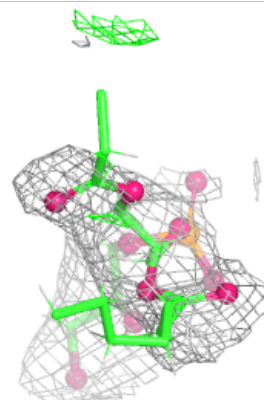
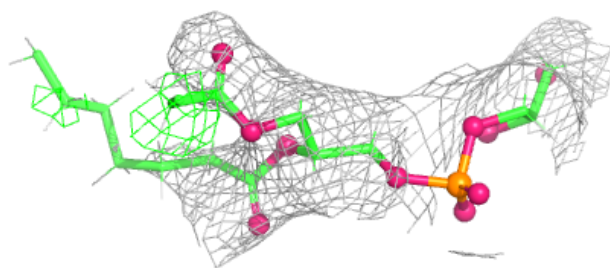
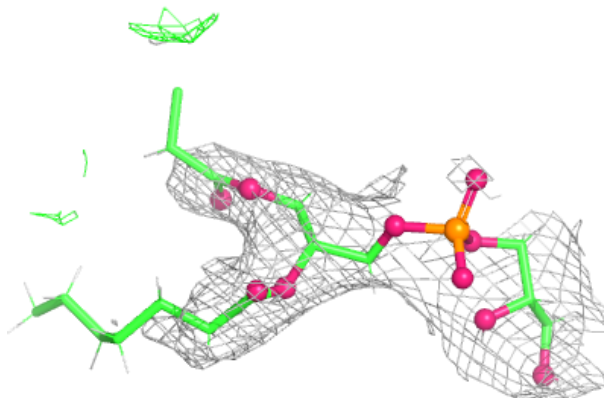


Electron density around LHG A 853:

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

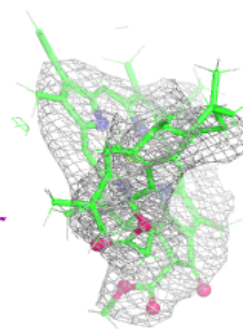
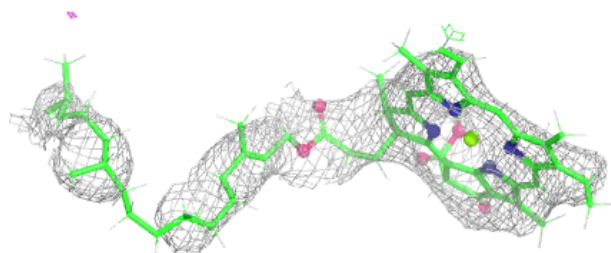
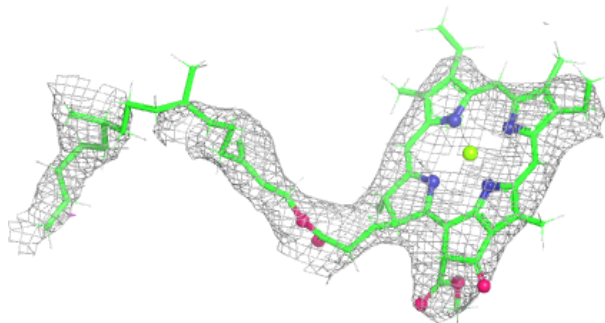
**Electron density around LHG A 854:**

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

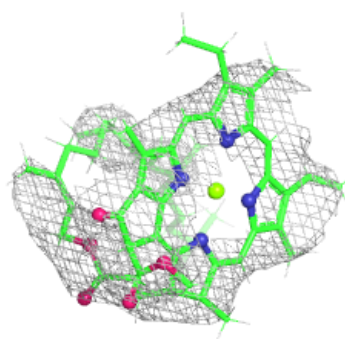
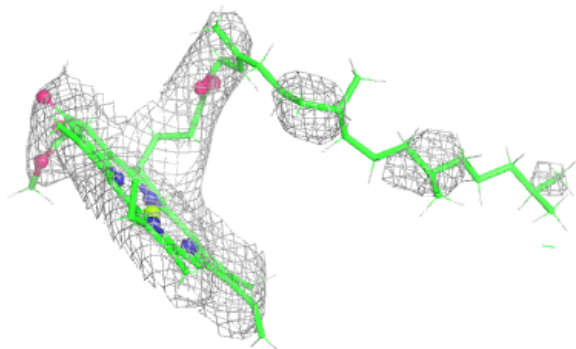
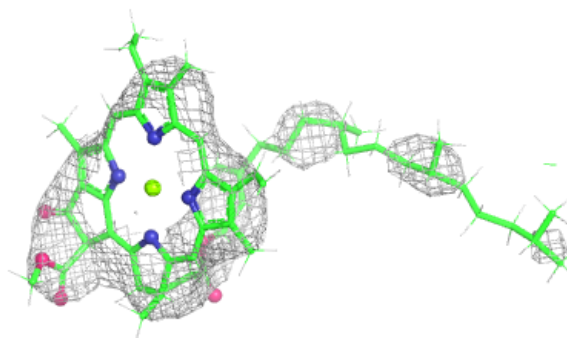


Electron density around CLA B 3014:

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

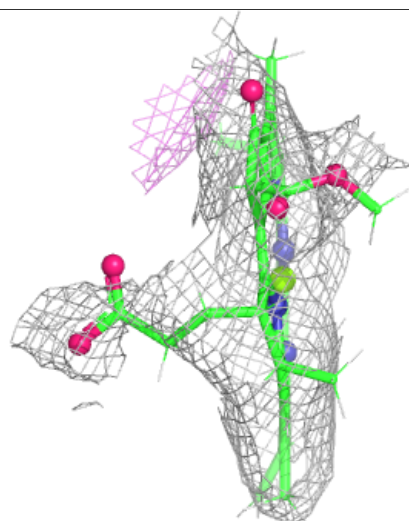
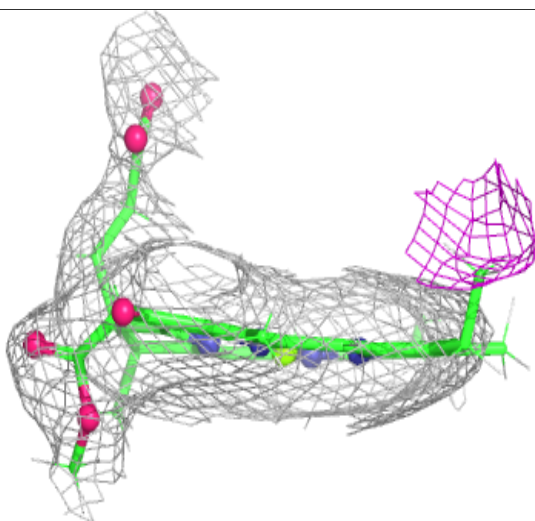
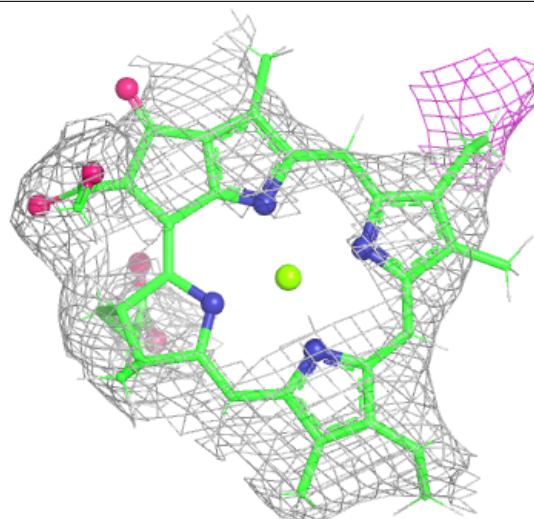
**Electron density around CLA B 3015:**

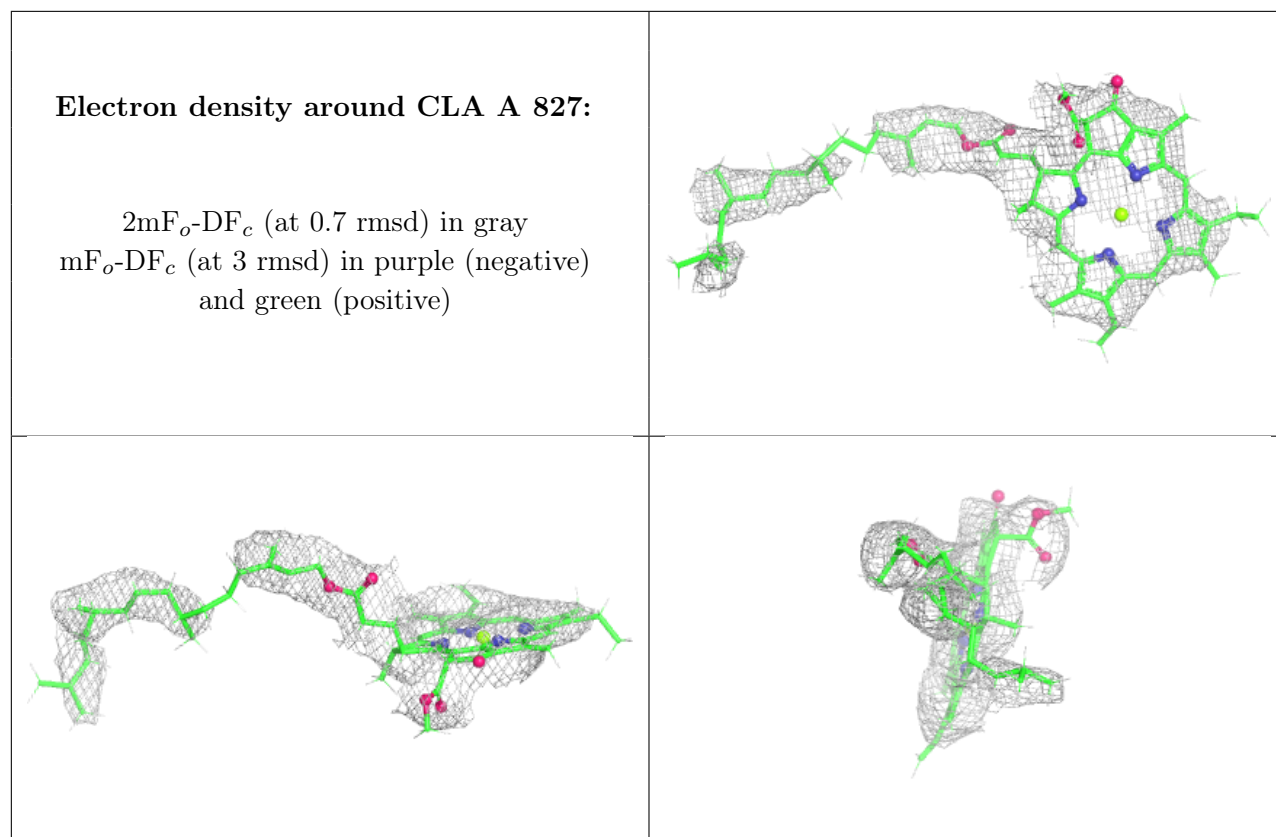
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 3016:

$2mF_o-DF_c$ (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.