



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 08:57 AM EDT

PDB ID : 4FE1 / pdb_00004fe1
Title : Improving the Accuracy of Macromolecular Structure Refinement at 7 Å Resolution
Authors : Fromme, R.; Adams, P.D.; Fromme, P.; Levitt, M.; Schroeder, G.F.; Brunger, A.T.
Deposited on : 2012-05-29
Resolution : 4.92 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

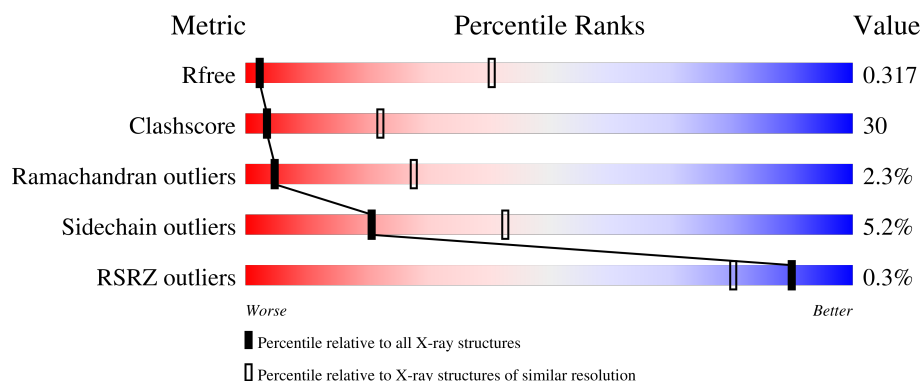
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.92 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	1008 (5.88-3.96)
Clashscore	190562	1020 (5.82-3.98)
Ramachandran outliers	187476	1125 (5.94-3.90)
Sidechain outliers	187428	1105 (5.94-3.90)
RSRZ outliers	180081	1003 (5.88-3.96)

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	
2	B	740	
3	C	80	
4	D	138	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	803	-	-	X	-
13	CLA	B	830	-	-	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 23997 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	740	Total	C	N	O	S	0	0	0
			5784	3794	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	N	O	S	0	0	0
			5879	3867	986	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	N	O	S	0	0	0
			598	367	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	N	O	S	0	0	0
			1075	682	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	N	O	0	0	0
			539	342	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	N	O	S	0	0	0
			1065	680	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	N	O	S	0	0	0
			301	208	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	N	O	S	0	0	0
			338	231	51	54	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	46	Total	C	N	O	S	0	0	0
			222	130	46	46				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	151	Total	C	N	O	S	0	0	0
			1119	735	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	N	O	S	0	0	0
			241	161	36	43	1			

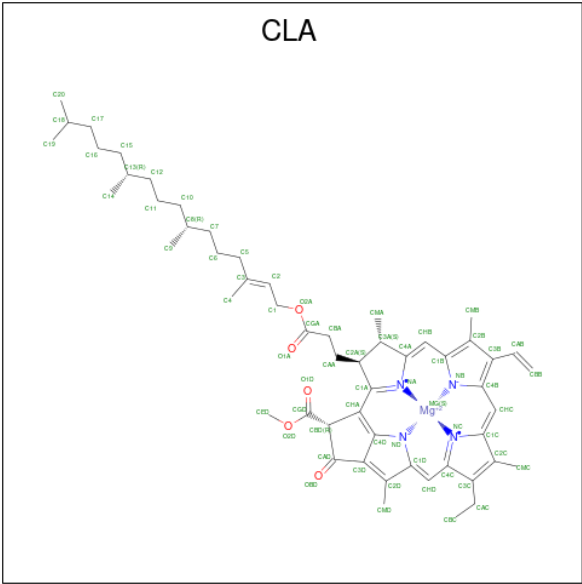
- Molecule 12 is a protein called Photosystem I 4.8K protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	X	29	Total	C	N	O	S	0	0	0
			233	164	34	35				

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	32	ALA	-	expression tag	UNP Q8DKP6
X	33	ALA	-	expression tag	UNP Q8DKP6
X	34	ALA	-	expression tag	UNP Q8DKP6
X	35	ALA	-	expression tag	UNP Q8DKP6

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
13	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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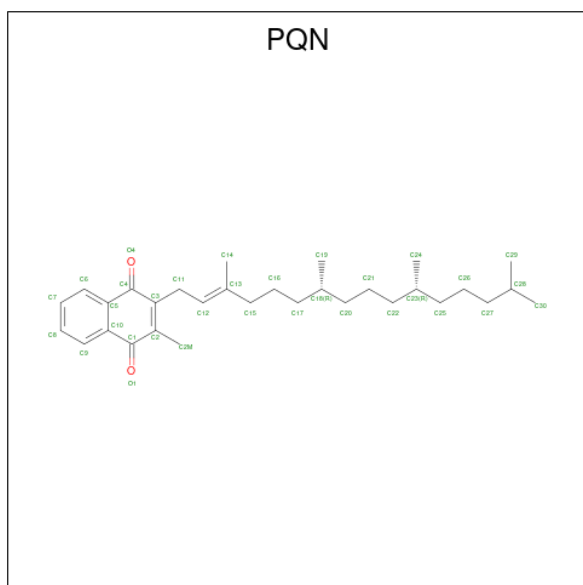
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 58	C 48	Mg 1	N 4	O 5	0	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	F	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	I	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	J	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	J	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
13	J	1	Total 37	C 31	Mg 1	N 4	O 1	0	0
13	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
13	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
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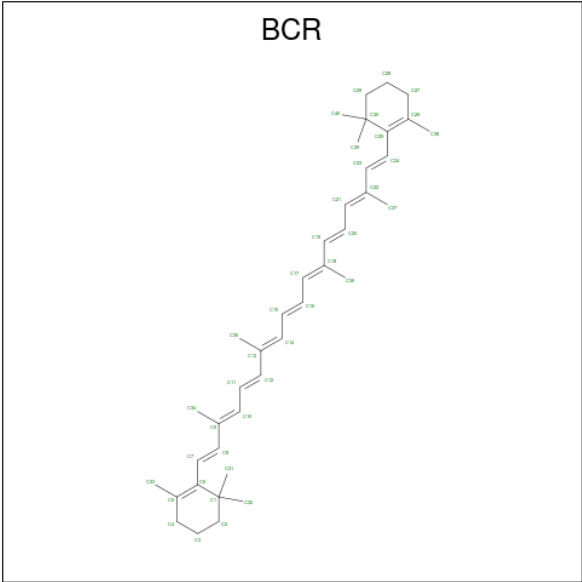
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	M	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	X	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

- Molecule 14 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



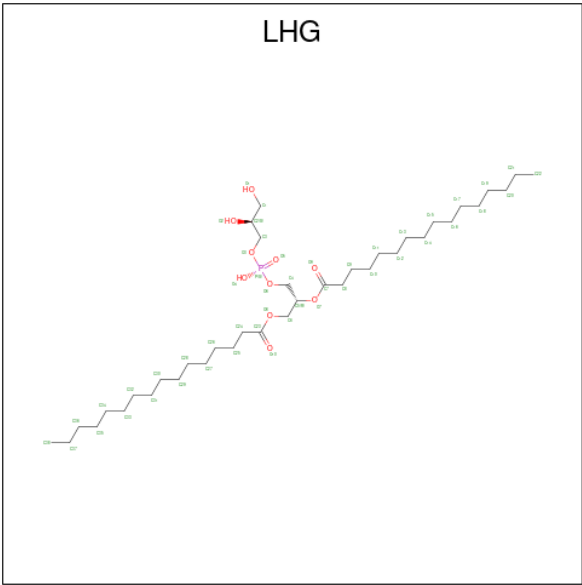
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	A	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 25 25	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0
15	B	1	Total C 40 40	0	0

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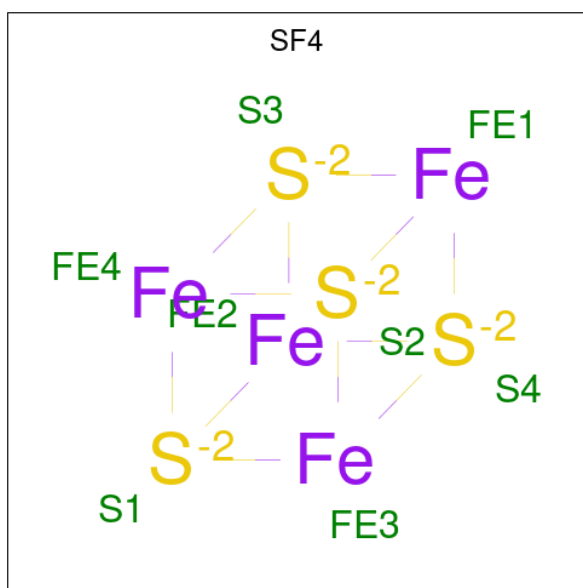
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total C 40 40	0	0
15	F	1	Total C 40 40	0	0
15	I	1	Total C 40 40	0	0
15	J	1	Total C 40 40	0	0
15	J	1	Total C 40 40	0	0
15	L	1	Total C 40 40	0	0
15	L	1	Total C 40 40	0	0
15	M	1	Total C 40 40	0	0

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



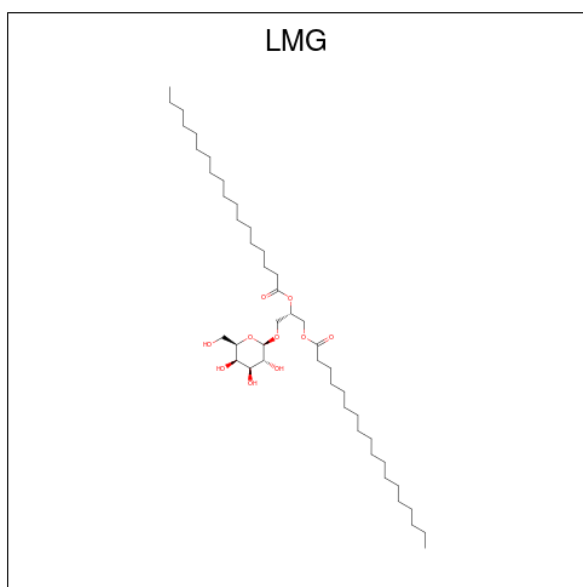
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total C O P 49 38 10 1	0	0
16	A	1	Total C O P 27 16 10 1	0	0
16	X	1	Total C O P 23 12 10 1	0	0

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $\text{C}_{45}\text{H}_{86}\text{O}_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	B	1	Total	C	O	0	0
			55	45	10		

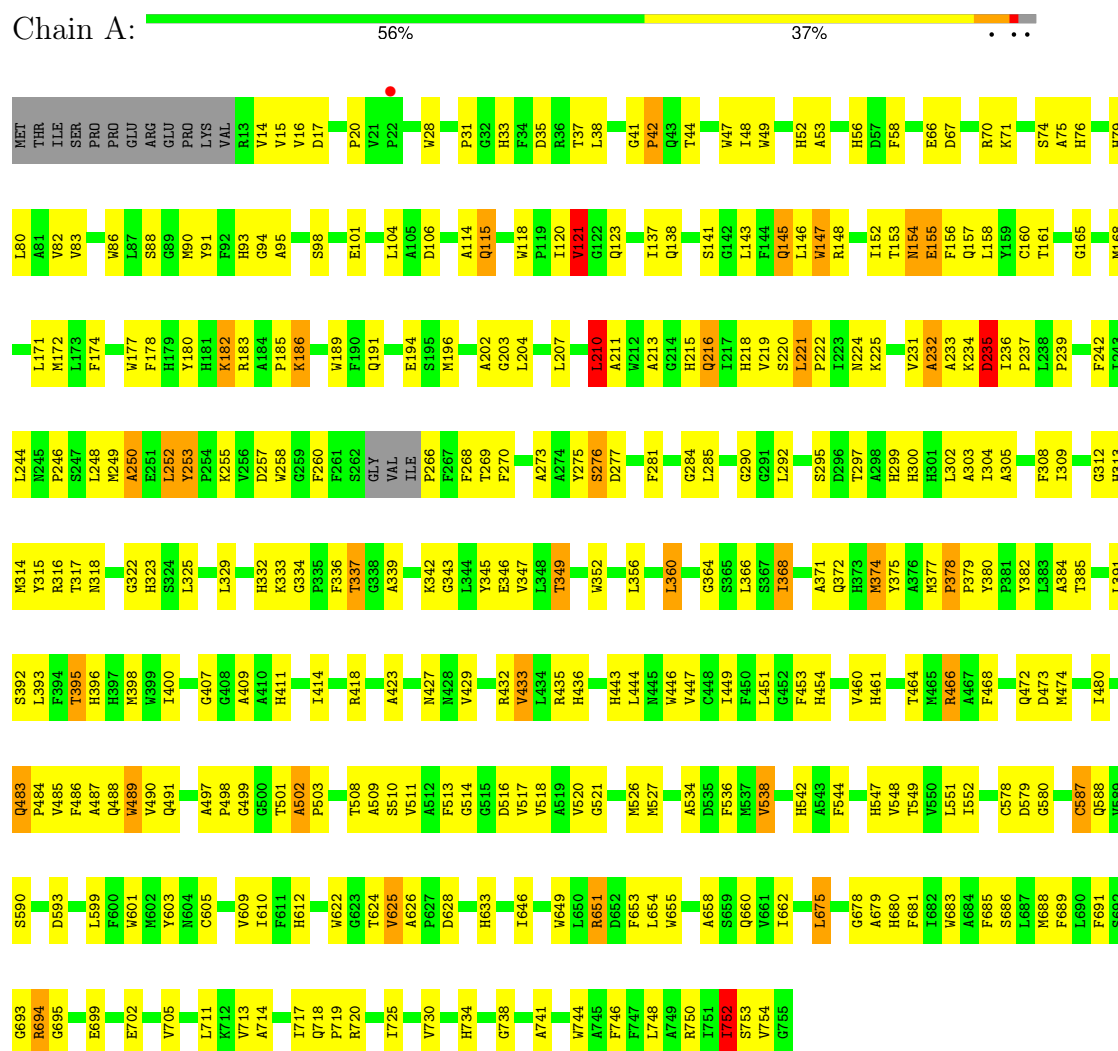
- Molecule 19 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	L	1	Total	Ca	0	0
			1	1		

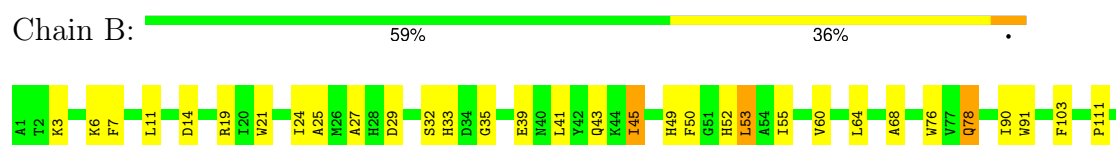
3 Residue-property plots

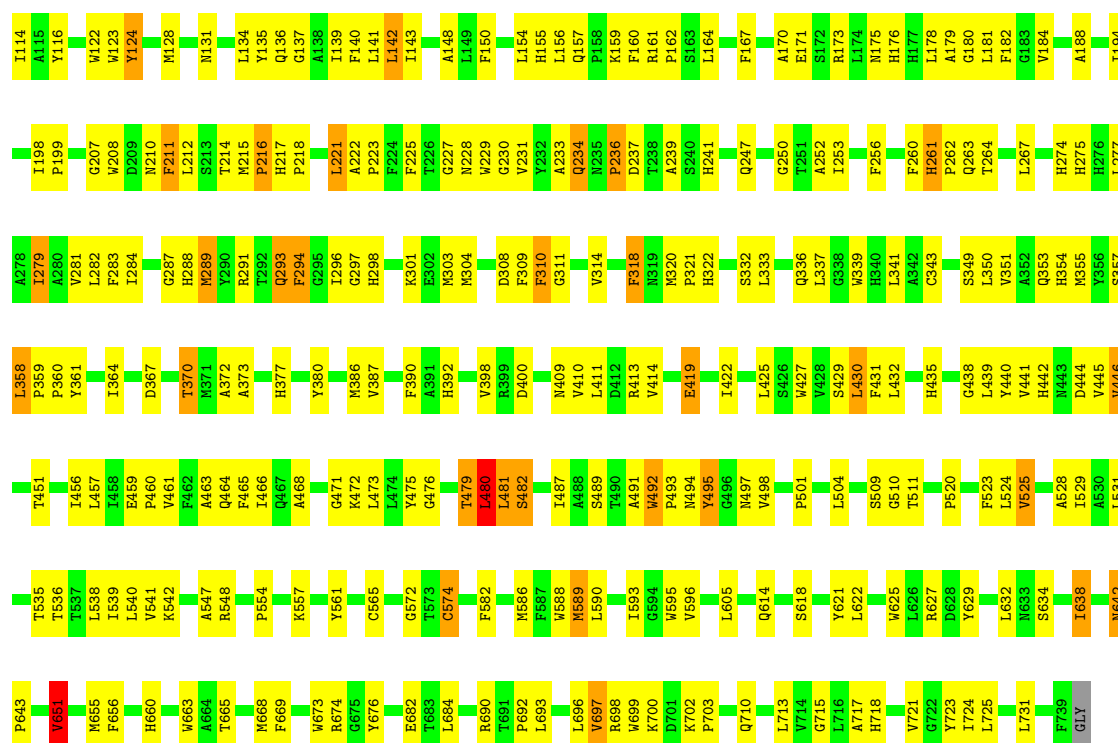
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





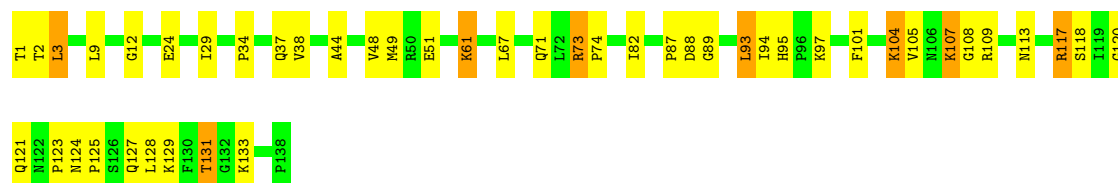
• Molecule 3: Photosystem I iron-sulfur center

Chain C: 71% 24% 5%



• Molecule 4: Photosystem I reaction center subunit II

Chain D: 67% 28% 6%



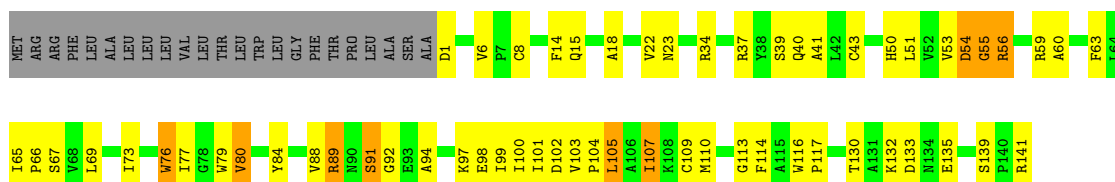
• Molecule 5: Photosystem I reaction center subunit IV

Chain E: 55% 33% 8%



• Molecule 6: Photosystem I reaction center subunit III

Chain F: 49% 31% 5% 14%



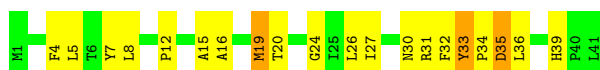
• Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 50% 42% 8%



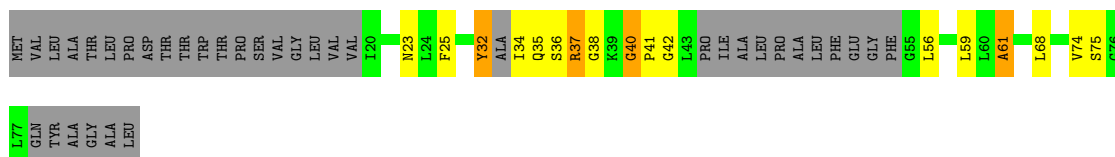
• Molecule 8: Photosystem I reaction center subunit IX

Chain J: 51% 41% 7%



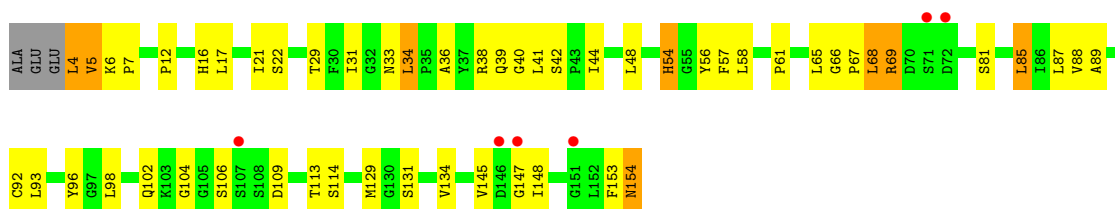
• Molecule 9: Photosystem I reaction center subunit PsaK

Chain K: 35% 16% 5% 45%



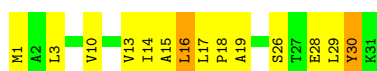
• Molecule 10: Photosystem I reaction center subunit XI

Chain L: 4% 63% 30% 5%



• Molecule 11: Photosystem I reaction center subunit XII

Chain M: 55% 39% 6%



• Molecule 12: Photosystem I 4.8K protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	281.00Å 281.00Å 165.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.97 – 4.92 97.97 – 4.92	Depositor EDS
% Data completeness (in resolution range)	96.4 (97.97-4.92) 96.3 (97.97-4.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.35 (at 4.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1058)	Depositor
R, R_{free}	0.274 , 0.315 0.276 , 0.317	Depositor DCC
R_{free} test set	1534 reflections (4.37%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 259.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.13$	Xtriage
Estimated twinning fraction	0.175 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	23997	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: CLA, LHG, CA, LMG, SF4, PQN, BCR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/5983	1.11	34/8158 (0.4%)
2	B	0.52	0/6096	1.08	31/8332 (0.4%)
3	C	0.50	0/608	1.25	7/824 (0.8%)
4	D	0.47	0/1101	1.06	3/1492 (0.2%)
5	E	0.52	0/551	1.16	2/750 (0.3%)
6	F	0.59	0/1087	1.15	6/1476 (0.4%)
7	I	0.51	0/312	1.10	2/425 (0.5%)
8	J	0.52	0/350	1.26	6/477 (1.3%)
9	K	0.61	0/220	1.71	10/300 (3.3%)
10	L	0.50	0/1148	1.16	12/1558 (0.8%)
11	M	0.73	0/244	1.37	2/332 (0.6%)
12	X	0.50	0/242	1.02	1/332 (0.3%)
All	All	0.52	0/17942	1.12	116/24456 (0.5%)

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	1
2	B	0	1
4	D	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	PRO	CA-C-N	11.32	131.07	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	PRO	C-N-CA	11.32	131.07	119.64
2	B	217	HIS	CA-C-N	11.03	133.62	119.84
2	B	217	HIS	C-N-CA	11.03	133.62	119.84
1	A	580	GLY	CA-C-N	10.30	129.91	119.82

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	337	THR	Mainchain
2	B	35	GLY	Mainchain
4	D	88	ASP	Mainchain

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	0	5639	340	0
2	B	5879	0	5632	344	0
3	C	598	0	580	16	0
4	D	1075	0	1077	31	0
5	E	539	0	528	14	0
6	F	1065	0	1077	53	0
7	I	301	0	306	24	0
8	J	338	0	347	24	0
9	K	222	0	111	9	0
10	L	1119	0	1125	49	1
11	M	241	0	264	23	0
12	X	233	0	231	11	0
13	A	2667	0	2635	435	0
13	B	2230	0	2182	406	0
13	F	45	0	33	4	0
13	I	65	0	72	15	0
13	J	147	0	129	15	0
13	L	195	0	216	26	0
13	M	99	0	81	16	0
13	X	45	0	33	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A	33	0	46	7	0
14	B	33	0	46	6	0
15	A	240	0	336	38	0
15	B	345	0	481	82	0
15	F	40	0	56	12	0
15	I	40	0	56	9	0
15	J	80	0	112	9	0
15	L	80	0	112	16	0
15	M	40	0	56	11	0
16	A	76	0	98	11	0
16	X	23	0	16	1	0
17	A	8	0	0	0	0
17	C	16	0	0	0	0
18	B	55	0	86	18	0
19	L	1	0	0	0	0
All	All	23997	0	23799	1418	1

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 30.

The worst 5 of 1418 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)
13:B:806:CLA:H12	7:I:18:VAL:HG21	1.35	1.08
13:A:803:CLA:H151	13:A:842:CLA:HAB	1.36	1.08
13:B:831:CLA:HED1	8:J:36:LEU:H	1.06	1.07
13:B:817:CLA:HBD	13:B:821:CLA:HED2	1.37	1.06
13:A:828:CLA:H51	15:A:852:BCR:H312	1.33	1.05

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:40:GLY:O	10:L:114:SER:OG[3_665]	2.17	0.03

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%)	685 (93%)	39 (5%)	12 (2%)	7	37
2	B	737/740 (100%)	691 (94%)	37 (5%)	9 (1%)	10	42
3	C	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	9	41
4	D	136/138 (99%)	123 (90%)	8 (6%)	5 (4%)	2	19
5	E	67/75 (89%)	53 (79%)	6 (9%)	8 (12%)	0	5
6	F	139/164 (85%)	127 (91%)	8 (6%)	4 (3%)	3	23
7	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	K	42/83 (51%)	30 (71%)	5 (12%)	7 (17%)	0	3
10	L	149/154 (97%)	138 (93%)	9 (6%)	2 (1%)	9	41
11	M	29/31 (94%)	26 (90%)	2 (7%)	1 (3%)	3	20
12	X	27/35 (77%)	21 (78%)	5 (18%)	1 (4%)	2	19
All	All	2215/2334 (95%)	2039 (92%)	126 (6%)	50 (2%)	5	28

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	VAL
1	A	235	ASP
2	B	211	PHE
2	B	234	GLN
2	B	480	LEU

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%)	561 (95%)	28 (5%)	23	45
2	B	595/597 (100%)	565 (95%)	30 (5%)	22	43
3	C	67/67 (100%)	64 (96%)	3 (4%)	24	46
4	D	115/115 (100%)	107 (93%)	8 (7%)	14	36
5	E	59/64 (92%)	57 (97%)	2 (3%)	32	54
6	F	109/128 (85%)	105 (96%)	4 (4%)	30	51
7	I	32/32 (100%)	30 (94%)	2 (6%)	16	38
8	J	36/36 (100%)	35 (97%)	1 (3%)	38	59
10	L	117/119 (98%)	108 (92%)	9 (8%)	12	32
11	M	26/26 (100%)	23 (88%)	3 (12%)	5	19
12	X	20/24 (83%)	19 (95%)	1 (5%)	22	43
All	All	1765/1811 (98%)	1674 (95%)	91 (5%)	21	43

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	698	ARG
6	F	1	ASP
3	C	65	ARG
4	D	104	LYS
7	I	10	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	228	ASN
2	B	261	HIS
10	L	119	GLN
4	D	127	GLN
5	E	18	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 128 ligands modelled in this entry, 1 is monoatomic - leaving 127 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$
17	SF4	A	856	2,1	0,12,12	-	-	-		
13	CLA	A	836	1	49,53,73	1.79	13 (26%)	58,89,113	1.94	6 (10%)
13	CLA	A	818	1	58,62,73	1.75	16 (27%)	68,99,113	2.06	10 (14%)
13	CLA	A	824	1	63,67,73	1.70	18 (28%)	74,105,113	1.99	13 (17%)
14	PQN	B	840	-	34,34,34	0.92	1 (2%)	43,45,45	1.40	5 (11%)
13	CLA	B	822	-	58,62,73	1.80	18 (31%)	68,99,113	2.03	10 (14%)
13	CLA	A	807	1	55,59,73	1.80	15 (27%)	64,96,113	2.12	11 (17%)
13	CLA	A	837	-	55,59,73	1.84	15 (27%)	64,96,113	2.08	14 (21%)
15	BCR	J	1104	-	41,41,41	2.14	20 (48%)	56,56,56	2.27	23 (41%)
15	BCR	B	841	-	41,41,41	2.12	20 (48%)	56,56,56	2.13	22 (39%)
16	LHG	X	101	-	22,22,48	1.35	2 (9%)	25,28,54	1.03	1 (4%)
13	CLA	B	808	2	69,73,73	1.63	15 (21%)	82,113,113	1.88	10 (12%)
13	CLA	B	815	2	63,67,73	1.70	17 (26%)	74,105,113	1.75	10 (13%)
15	BCR	B	849	-	41,41,41	2.04	18 (43%)	56,56,56	2.36	20 (35%)
13	CLA	B	802	-	69,73,73	1.65	18 (26%)	82,113,113	2.08	13 (15%)
13	CLA	A	833	1	69,73,73	1.62	17 (24%)	82,113,113	1.71	8 (9%)
13	CLA	A	855	-	49,53,73	1.79	13 (26%)	58,89,113	2.03	9 (15%)
15	BCR	A	847	-	41,41,41	2.14	21 (51%)	56,56,56	2.07	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BCR	B	844	-	25,25,41	2.19	13 (52%)	33,33,56	2.12	12 (36%)
13	CLA	B	805	-	69,73,73	1.59	16 (23%)	82,113,113	1.77	10 (12%)
13	CLA	A	813	1	64,68,73	1.66	15 (23%)	76,107,113	1.91	11 (14%)
15	BCR	A	851	-	41,41,41	2.12	20 (48%)	56,56,56	2.18	19 (33%)
13	CLA	B	833	-	49,53,73	1.78	13 (26%)	58,89,113	2.10	5 (8%)
13	CLA	A	835	1	58,62,73	1.76	18 (31%)	68,99,113	1.81	7 (10%)
13	CLA	A	822	1	53,57,73	1.78	13 (24%)	61,93,113	2.21	9 (14%)
13	CLA	A	830	1	69,73,73	1.57	16 (23%)	82,113,113	1.90	12 (14%)
15	BCR	B	845	-	41,41,41	2.10	18 (43%)	56,56,56	2.39	22 (39%)
13	CLA	B	803	-	69,73,73	1.63	18 (26%)	82,113,113	1.78	10 (12%)
13	CLA	M	1202	-	49,53,73	1.77	13 (26%)	58,89,113	2.12	9 (15%)
15	BCR	L	1005	-	41,41,41	2.10	20 (48%)	56,56,56	2.28	24 (42%)
13	CLA	A	803	-	69,73,73	1.62	16 (23%)	82,113,113	1.74	12 (14%)
13	CLA	A	816	-	53,57,73	1.74	13 (24%)	61,93,113	1.89	8 (13%)
13	CLA	A	829	1	69,73,73	1.60	18 (26%)	82,113,113	1.93	12 (14%)
18	LMG	B	848	-	55,55,55	1.06	8 (14%)	63,63,63	1.22	3 (4%)
15	BCR	B	843	-	41,41,41	2.09	21 (51%)	56,56,56	2.42	26 (46%)
13	CLA	A	809	1	69,73,73	1.64	17 (24%)	82,113,113	2.01	16 (19%)
15	BCR	M	1203	-	41,41,41	2.09	18 (43%)	56,56,56	2.30	21 (37%)
15	BCR	L	1006	-	41,41,41	2.13	21 (51%)	56,56,56	2.04	22 (39%)
13	CLA	X	102	12	49,53,73	1.81	15 (30%)	58,89,113	2.21	8 (13%)
15	BCR	A	850	-	41,41,41	2.18	21 (51%)	56,56,56	2.20	20 (35%)
13	CLA	A	806	-	69,73,73	1.60	15 (21%)	82,113,113	1.76	12 (14%)
13	CLA	B	809	2	49,53,73	1.78	14 (28%)	58,89,113	2.05	9 (15%)
13	CLA	A	804	13,1	63,67,73	1.71	16 (25%)	74,105,113	1.82	10 (13%)
13	CLA	A	812	1	58,62,73	1.74	16 (27%)	68,99,113	2.09	12 (17%)
13	CLA	A	805	-	69,73,73	1.61	17 (24%)	82,113,113	1.77	9 (10%)
14	PQN	A	846	-	34,34,34	0.99	1 (2%)	43,45,45	1.21	4 (9%)
17	SF4	C	102	3	0,12,12	-	-	-	-	-
13	CLA	J	1103	8	41,45,73	1.96	13 (31%)	50,78,113	1.68	4 (8%)
13	CLA	A	842	1	69,73,73	1.66	18 (26%)	82,113,113	1.63	9 (10%)
13	CLA	B	806	2	69,73,73	1.63	17 (24%)	82,113,113	1.88	12 (14%)
15	BCR	B	850	-	41,41,41	2.13	21 (51%)	56,56,56	2.38	23 (41%)
13	CLA	B	807	2	69,73,73	1.64	18 (26%)	82,113,113	1.92	11 (13%)
13	CLA	B	818	2	51,55,73	1.80	15 (29%)	60,91,113	1.84	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	810	2	49,53,73	1.80	15 (30%)	58,89,113	1.87	7 (12%)
13	CLA	A	845	16	56,60,73	1.74	16 (28%)	65,97,113	2.12	14 (21%)
13	CLA	A	810	1	49,53,73	1.76	13 (26%)	58,89,113	2.12	8 (13%)
13	CLA	B	821	2	49,53,73	1.81	13 (26%)	58,89,113	1.85	9 (15%)
13	CLA	B	804	-	69,73,73	1.61	16 (23%)	82,113,113	1.80	11 (13%)
13	CLA	A	819	1	69,73,73	1.59	17 (24%)	82,113,113	2.03	13 (15%)
13	CLA	A	821	-	69,73,73	1.61	17 (24%)	82,113,113	1.93	11 (13%)
13	CLA	A	801	1	69,73,73	1.65	18 (26%)	82,113,113	1.83	13 (15%)
13	CLA	A	826	-	69,73,73	1.65	15 (21%)	82,113,113	1.83	13 (15%)
15	BCR	B	847	-	41,41,41	2.12	20 (48%)	56,56,56	2.29	21 (37%)
13	CLA	L	1003	10	69,73,73	1.62	17 (24%)	82,113,113	1.95	14 (17%)
13	CLA	A	841	-	55,59,73	1.79	13 (23%)	64,96,113	1.86	8 (12%)
13	CLA	B	834	-	49,53,73	1.78	13 (26%)	58,89,113	2.04	8 (13%)
13	CLA	A	840	1	69,73,73	1.61	17 (24%)	82,113,113	1.89	12 (14%)
13	CLA	A	839	1	51,55,73	1.73	11 (21%)	60,91,113	2.10	8 (13%)
13	CLA	M	1201	2	58,62,73	1.76	17 (29%)	68,99,113	2.09	13 (19%)
15	BCR	I	102	-	41,41,41	2.02	17 (41%)	56,56,56	2.35	24 (42%)
13	CLA	B	813	2	49,53,73	1.81	14 (28%)	58,89,113	2.05	9 (15%)
15	BCR	F	1302	-	41,41,41	2.10	21 (51%)	56,56,56	2.22	21 (37%)
13	CLA	A	834	1	69,73,73	1.66	19 (27%)	82,113,113	1.75	9 (10%)
13	CLA	B	835	-	64,68,73	1.72	15 (23%)	76,107,113	1.89	15 (19%)
13	CLA	B	816	2	64,68,73	1.69	17 (26%)	76,107,113	1.84	13 (17%)
13	CLA	A	844	-	45,49,73	1.82	13 (28%)	54,83,113	1.67	8 (14%)
13	CLA	J	1102	8	49,53,73	1.77	12 (24%)	58,89,113	2.04	7 (12%)
13	CLA	B	824	2	69,73,73	1.62	15 (21%)	82,113,113	1.84	11 (13%)
13	CLA	B	826	2	69,73,73	1.62	17 (24%)	82,113,113	1.66	7 (8%)
13	CLA	B	823	-	50,54,73	1.81	13 (26%)	59,90,113	1.99	11 (18%)
13	CLA	A	802	-	69,73,73	1.65	18 (26%)	82,113,113	1.71	7 (8%)
13	CLA	J	1101	-	69,73,73	1.61	14 (20%)	82,113,113	1.88	14 (17%)
16	LHG	A	853	-	48,48,48	0.94	2 (4%)	51,54,54	1.07	2 (3%)
13	CLA	B	838	-	69,73,73	1.63	15 (21%)	82,113,113	1.92	13 (15%)
13	CLA	A	831	1	54,58,73	1.80	16 (29%)	64,95,113	1.92	9 (14%)
13	CLA	A	828	1	69,73,73	1.60	15 (21%)	82,113,113	1.84	11 (13%)
13	CLA	B	828	2	49,53,73	1.80	16 (32%)	58,89,113	1.96	7 (12%)
13	CLA	A	843	-	69,73,73	1.60	16 (23%)	82,113,113	1.87	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	820	-	59,63,73	1.74	16 (27%)	70,101,113	1.83	10 (14%)
13	CLA	I	101	-	69,73,73	1.65	18 (26%)	82,113,113	1.91	14 (17%)
15	BCR	B	846	-	41,41,41	2.13	20 (48%)	56,56,56	2.09	19 (33%)
13	CLA	A	811	13,1	69,73,73	1.62	16 (23%)	82,113,113	1.90	11 (13%)
13	CLA	B	832	2	49,53,73	1.79	14 (28%)	58,89,113	2.01	9 (15%)
13	CLA	A	832	1	69,73,73	1.62	17 (24%)	82,113,113	1.93	11 (13%)
13	CLA	A	820	1	65,69,73	1.70	18 (27%)	77,108,113	1.82	13 (16%)
13	CLA	B	819	2	49,53,73	1.79	15 (30%)	58,89,113	2.03	8 (13%)
13	CLA	B	830	2	69,73,73	1.61	16 (23%)	82,113,113	1.87	9 (10%)
16	LHG	A	854	13	26,26,48	1.27	2 (7%)	29,32,54	1.17	2 (6%)
13	CLA	A	808	1	69,73,73	1.66	15 (21%)	82,113,113	2.06	12 (14%)
15	BCR	A	849	-	41,41,41	2.03	18 (43%)	56,56,56	2.25	23 (41%)
13	CLA	B	839	2	69,73,73	1.61	17 (24%)	82,113,113	1.78	11 (13%)
17	SF4	C	101	3	0,12,12	-	-	-	-	-
13	CLA	L	1004	-	69,73,73	1.61	16 (23%)	82,113,113	1.86	10 (12%)
13	CLA	A	827	-	69,73,73	1.61	16 (23%)	82,113,113	1.84	11 (13%)
15	BCR	A	848	-	41,41,41	2.14	20 (48%)	56,56,56	2.15	21 (37%)
13	CLA	B	837	2	51,55,73	1.75	15 (29%)	60,91,113	1.98	8 (13%)
15	BCR	A	852	-	41,41,41	2.15	21 (51%)	56,56,56	2.29	19 (33%)
13	CLA	A	825	-	69,73,73	1.62	16 (23%)	82,113,113	1.86	11 (13%)
13	CLA	A	817	1	58,62,73	1.75	15 (25%)	68,99,113	1.83	11 (16%)
13	CLA	L	1002	10	69,73,73	1.62	18 (26%)	82,113,113	1.86	11 (13%)
13	CLA	B	817	-	69,73,73	1.62	17 (24%)	82,113,113	1.88	9 (10%)
13	CLA	B	825	2	69,73,73	1.64	15 (21%)	82,113,113	1.73	8 (9%)
13	CLA	B	814	2	59,63,73	1.70	15 (25%)	70,101,113	2.02	12 (17%)
13	CLA	B	812	2	69,73,73	1.63	18 (26%)	82,113,113	1.90	10 (12%)
13	CLA	A	823	1	55,59,73	1.79	16 (29%)	64,96,113	1.84	9 (14%)
13	CLA	F	1301	-	49,53,73	1.84	13 (26%)	58,89,113	2.11	11 (18%)
13	CLA	B	801	2	69,73,73	1.63	18 (26%)	82,113,113	1.80	11 (13%)
13	CLA	B	831	2	62,66,73	1.71	16 (25%)	73,104,113	2.10	12 (16%)
13	CLA	A	838	1	69,73,73	1.64	19 (27%)	82,113,113	1.89	12 (14%)
13	CLA	A	814	1	49,53,73	1.80	15 (30%)	58,89,113	1.92	9 (15%)
13	CLA	B	829	2	53,57,73	1.73	14 (26%)	61,93,113	1.84	11 (18%)
15	BCR	J	1105	-	41,41,41	2.14	20 (48%)	56,56,56	2.16	22 (39%)
15	BCR	B	842	-	41,41,41	2.16	21 (51%)	56,56,56	2.29	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	827	2	69,73,73	1.60	16 (23%)	82,113,113	1.95	13 (15%)
13	CLA	A	815	1	49,53,73	1.77	14 (28%)	58,89,113	2.06	11 (18%)
13	CLA	B	836	2	69,73,73	1.63	18 (26%)	82,113,113	1.81	11 (13%)
13	CLA	B	811	-	69,73,73	1.65	16 (23%)	82,113,113	1.85	9 (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
17	SF4	A	856	2,1	-	-	0/6/5/5
13	CLA	A	836	1	-	6/15/91/115	-
13	CLA	A	818	1	-	7/26/102/115	-
13	CLA	A	824	1	-	9/32/108/115	-
14	PQN	B	840	-	-	5/23/43/43	0/2/2/2
13	CLA	B	822	-	-	9/26/102/115	-
13	CLA	A	807	1	-	6/23/99/115	-
13	CLA	A	837	-	-	4/23/99/115	-
15	BCR	J	1104	-	-	11/29/63/63	0/2/2/2
15	BCR	B	841	-	-	8/29/63/63	0/2/2/2
16	LHG	X	101	-	-	8/26/26/53	-
13	CLA	B	808	2	-	9/39/115/115	-
13	CLA	B	815	2	-	9/32/108/115	-
15	BCR	B	849	-	-	14/29/63/63	0/2/2/2
13	CLA	B	802	-	-	12/39/115/115	-
13	CLA	A	833	1	-	8/39/115/115	-
13	CLA	A	855	-	-	2/15/91/115	-
15	BCR	A	847	-	-	8/29/63/63	0/2/2/2
15	BCR	B	844	-	-	6/18/35/63	0/1/1/2
13	CLA	B	805	-	-	7/39/115/115	-
13	CLA	A	813	1	-	9/33/109/115	-
15	BCR	A	851	-	-	8/29/63/63	0/2/2/2
13	CLA	B	833	-	-	6/15/91/115	-
13	CLA	A	835	1	-	7/26/102/115	-
13	CLA	A	822	1	-	7/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	830	1	-	10/39/115/115	-
15	BCR	B	845	-	-	10/29/63/63	0/2/2/2
13	CLA	B	803	-	-	13/39/115/115	-
13	CLA	M	1202	-	-	4/15/91/115	-
15	BCR	L	1005	-	-	9/29/63/63	0/2/2/2
13	CLA	A	803	-	-	8/39/115/115	-
13	CLA	A	816	-	-	5/20/96/115	-
13	CLA	A	829	1	-	10/39/115/115	-
18	LMG	B	848	-	-	11/50/70/70	0/1/1/1
15	BCR	B	843	-	-	9/29/63/63	0/2/2/2
13	CLA	A	809	1	-	10/39/115/115	-
15	BCR	M	1203	-	-	15/29/63/63	0/2/2/2
15	BCR	L	1006	-	-	8/29/63/63	0/2/2/2
13	CLA	X	102	12	-	7/15/91/115	-
15	BCR	A	850	-	-	6/29/63/63	0/2/2/2
13	CLA	A	806	-	-	8/39/115/115	-
13	CLA	B	809	2	-	4/15/91/115	-
13	CLA	A	804	13,1	-	8/32/108/115	-
13	CLA	A	812	1	-	9/26/102/115	-
13	CLA	A	805	-	-	9/39/115/115	-
14	PQN	A	846	-	-	6/23/43/43	0/2/2/2
17	SF4	C	102	3	-	-	0/6/5/5
13	CLA	J	1103	8	-	2/4/76/115	-
13	CLA	A	842	1	-	16/39/115/115	-
13	CLA	B	806	2	-	12/39/115/115	-
15	BCR	B	850	-	-	7/29/63/63	0/2/2/2
13	CLA	B	807	2	-	16/39/115/115	-
13	CLA	B	818	2	-	4/18/94/115	-
13	CLA	B	810	2	-	5/15/91/115	-
13	CLA	A	845	16	-	5/24/100/115	-
13	CLA	A	810	1	-	7/15/91/115	-
13	CLA	B	821	2	-	3/15/91/115	-
13	CLA	B	804	-	-	6/39/115/115	-
13	CLA	A	819	1	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	821	-	-	15/39/115/115	-
13	CLA	A	801	1	-	8/39/115/115	-
13	CLA	A	826	-	-	8/39/115/115	-
15	BCR	B	847	-	-	12/29/63/63	0/2/2/2
13	CLA	L	1003	10	-	15/39/115/115	-
13	CLA	A	841	-	-	5/23/99/115	-
13	CLA	B	834	-	-	3/15/91/115	-
13	CLA	A	840	1	-	12/39/115/115	-
13	CLA	A	839	1	-	5/18/94/115	-
13	CLA	M	1201	2	-	7/26/102/115	-
15	BCR	I	102	-	-	15/29/63/63	0/2/2/2
13	CLA	B	813	2	-	5/15/91/115	-
15	BCR	F	1302	-	-	10/29/63/63	0/2/2/2
13	CLA	A	834	1	-	12/39/115/115	-
13	CLA	B	835	-	-	9/33/109/115	-
13	CLA	B	816	2	-	6/33/109/115	-
13	CLA	A	844	-	-	4/9/81/115	-
13	CLA	J	1102	8	-	5/15/91/115	-
13	CLA	B	824	2	-	9/39/115/115	-
13	CLA	B	826	2	-	13/39/115/115	-
13	CLA	B	823	-	-	3/17/93/115	-
13	CLA	A	802	-	-	5/39/115/115	-
13	CLA	J	1101	-	-	7/39/115/115	-
16	LHG	A	853	-	-	20/53/53/53	-
13	CLA	B	838	-	-	14/39/115/115	-
13	CLA	A	831	1	-	3/21/97/115	-
13	CLA	A	828	1	-	16/39/115/115	-
13	CLA	B	828	2	-	5/15/91/115	-
13	CLA	A	843	-	-	8/39/115/115	-
13	CLA	B	820	-	-	8/27/103/115	-
13	CLA	I	101	-	-	11/39/115/115	-
15	BCR	B	846	-	-	8/29/63/63	0/2/2/2
13	CLA	A	811	13,1	-	15/39/115/115	-
13	CLA	B	832	2	-	3/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	832	1	-	17/39/115/115	-
13	CLA	A	820	1	-	10/35/111/115	-
13	CLA	B	819	2	-	2/15/91/115	-
13	CLA	B	830	2	-	11/39/115/115	-
16	LHG	A	854	13	-	8/31/31/53	-
13	CLA	A	808	1	-	12/39/115/115	-
15	BCR	A	849	-	-	5/29/63/63	0/2/2/2
13	CLA	B	839	2	-	8/39/115/115	-
17	SF4	C	101	3	-	-	0/6/5/5
13	CLA	L	1004	-	-	11/39/115/115	-
13	CLA	A	827	-	-	10/39/115/115	-
15	BCR	A	848	-	-	11/29/63/63	0/2/2/2
13	CLA	B	837	2	-	5/18/94/115	-
15	BCR	A	852	-	-	12/29/63/63	0/2/2/2
13	CLA	A	825	-	-	6/39/115/115	-
13	CLA	A	817	1	-	4/26/102/115	-
13	CLA	L	1002	10	-	10/39/115/115	-
13	CLA	B	817	-	-	10/39/115/115	-
13	CLA	B	825	2	-	11/39/115/115	-
13	CLA	B	814	2	-	6/27/103/115	-
13	CLA	B	812	2	-	12/39/115/115	-
13	CLA	A	823	1	-	4/23/99/115	-
13	CLA	F	1301	-	-	5/15/91/115	-
13	CLA	B	801	2	-	11/39/115/115	-
13	CLA	B	831	2	-	8/31/107/115	-
13	CLA	A	838	1	-	16/39/115/115	-
13	CLA	A	814	1	-	4/15/91/115	-
13	CLA	B	829	2	-	3/20/96/115	-
15	BCR	J	1105	-	-	14/29/63/63	0/2/2/2
15	BCR	B	842	-	-	12/29/63/63	0/2/2/2
13	CLA	B	827	2	-	8/39/115/115	-
13	CLA	A	815	1	-	2/15/91/115	-
13	CLA	B	836	2	-	11/39/115/115	-
13	CLA	B	811	-	-	12/39/115/115	-

The worst 5 of 1952 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J	1103	CLA	C3A-C2A	-4.48	1.50	1.54
13	A	808	CLA	MG-ND	-4.34	1.97	2.05
13	B	802	CLA	MG-ND	-4.27	1.97	2.05
13	A	824	CLA	CHB-C1B	-4.25	1.29	1.39
13	B	822	CLA	MG-ND	-4.23	1.97	2.05

The worst 5 of 1470 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	809	CLA	C4A-NA-C1A	11.40	111.88	106.68
13	A	808	CLA	C4A-NA-C1A	11.29	111.83	106.68
13	A	830	CLA	C4A-NA-C1A	11.20	111.79	106.68
13	M	1202	CLA	C4A-NA-C1A	11.11	111.75	106.68
13	B	827	CLA	C4A-NA-C1A	11.09	111.74	106.68

There are no chirality outliers.

5 of 1055 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	801	CLA	C2B-C3B-CAB-CBB
13	A	801	CLA	C4B-C3B-CAB-CBB
13	A	802	CLA	C4B-C3B-CAB-CBB
13	A	804	CLA	C2B-C3B-CAB-CBB
13	A	804	CLA	C4B-C3B-CAB-CBB

There are no ring outliers.

123 monomers are involved in 1016 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	836	CLA	9	0
13	A	818	CLA	11	0
13	A	824	CLA	6	0
14	B	840	PQN	6	0
13	B	822	CLA	20	0
13	A	807	CLA	11	0
13	A	837	CLA	12	0
15	J	1104	BCR	3	0
15	B	841	BCR	6	0
16	X	101	LHG	1	0
13	B	808	CLA	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	815	CLA	16	0
15	B	849	BCR	16	0
13	B	802	CLA	17	0
13	A	833	CLA	15	0
13	A	855	CLA	2	0
15	A	847	BCR	5	0
15	B	844	BCR	6	0
13	B	805	CLA	8	0
13	A	813	CLA	14	0
15	A	851	BCR	2	0
13	B	833	CLA	3	0
13	A	835	CLA	7	0
13	A	822	CLA	7	0
13	A	830	CLA	13	0
15	B	845	BCR	7	0
13	B	803	CLA	16	0
13	M	1202	CLA	1	0
15	L	1005	BCR	12	0
13	A	803	CLA	26	0
13	A	816	CLA	4	0
13	A	829	CLA	9	0
18	B	848	LMG	18	0
15	B	843	BCR	17	0
13	A	809	CLA	12	0
15	M	1203	BCR	11	0
15	L	1006	BCR	4	0
13	X	102	CLA	4	0
15	A	850	BCR	4	0
13	A	806	CLA	10	0
13	B	809	CLA	6	0
13	A	804	CLA	10	0
13	A	812	CLA	3	0
13	A	805	CLA	10	0
14	A	846	PQN	7	0
13	A	842	CLA	20	0
13	B	806	CLA	14	0
15	B	850	BCR	6	0
13	B	807	CLA	13	0
13	B	818	CLA	4	0
13	B	810	CLA	6	0
13	A	845	CLA	11	0
13	A	810	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	821	CLA	11	0
13	B	804	CLA	16	0
13	A	819	CLA	16	0
13	A	821	CLA	12	0
13	A	801	CLA	12	0
13	A	826	CLA	16	0
15	B	847	BCR	13	0
13	L	1003	CLA	16	0
13	A	841	CLA	5	0
13	B	834	CLA	4	0
13	A	840	CLA	16	0
13	A	839	CLA	13	0
13	M	1201	CLA	15	0
15	I	102	BCR	9	0
13	B	813	CLA	9	0
15	F	1302	BCR	12	0
13	A	834	CLA	18	0
13	B	835	CLA	15	0
13	B	816	CLA	15	0
13	A	844	CLA	2	0
13	J	1102	CLA	3	0
13	B	824	CLA	18	0
13	B	826	CLA	17	0
13	B	823	CLA	8	0
13	A	802	CLA	13	0
13	J	1101	CLA	12	0
16	A	853	LHG	9	0
13	B	838	CLA	15	0
13	A	831	CLA	9	0
13	A	828	CLA	15	0
13	B	828	CLA	5	0
13	A	843	CLA	10	0
13	B	820	CLA	11	0
13	I	101	CLA	15	0
15	B	846	BCR	7	0
13	A	811	CLA	13	0
13	B	832	CLA	9	0
13	A	832	CLA	19	0
13	A	820	CLA	7	0
13	B	819	CLA	2	0
13	B	830	CLA	23	0
16	A	854	LHG	2	0

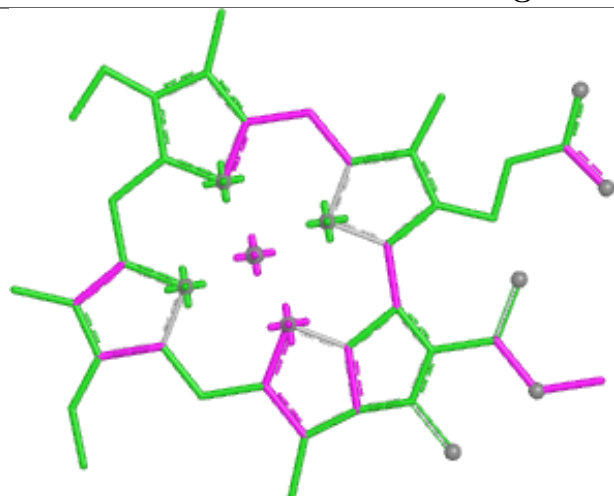
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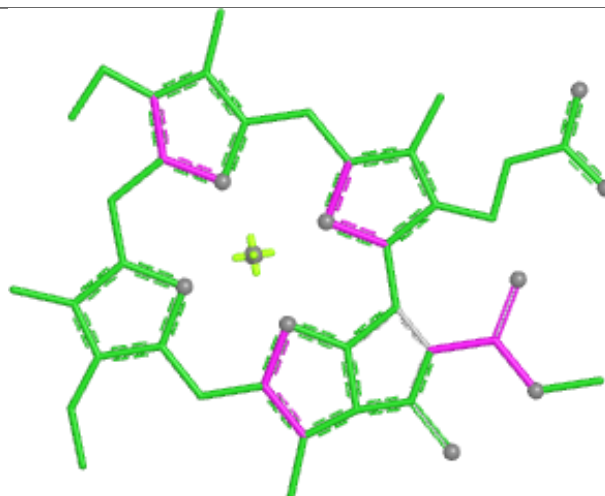
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	808	CLA	19	0
15	A	849	BCR	4	0
13	B	839	CLA	7	0
13	L	1004	CLA	5	0
13	A	827	CLA	13	0
15	A	848	BCR	5	0
13	B	837	CLA	6	0
15	A	852	BCR	19	0
13	A	825	CLA	20	0
13	A	817	CLA	8	0
13	L	1002	CLA	5	0
13	B	817	CLA	14	0
13	B	825	CLA	18	0
13	B	814	CLA	8	0
13	B	812	CLA	14	0
13	A	823	CLA	13	0
13	F	1301	CLA	4	0
13	B	801	CLA	12	0
13	B	831	CLA	12	0
13	A	838	CLA	8	0
13	A	814	CLA	9	0
13	B	829	CLA	6	0
15	J	1105	BCR	6	0
15	B	842	BCR	4	0
13	B	827	CLA	13	0
13	A	815	CLA	6	0
13	B	836	CLA	10	0
13	B	811	CLA	15	0

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

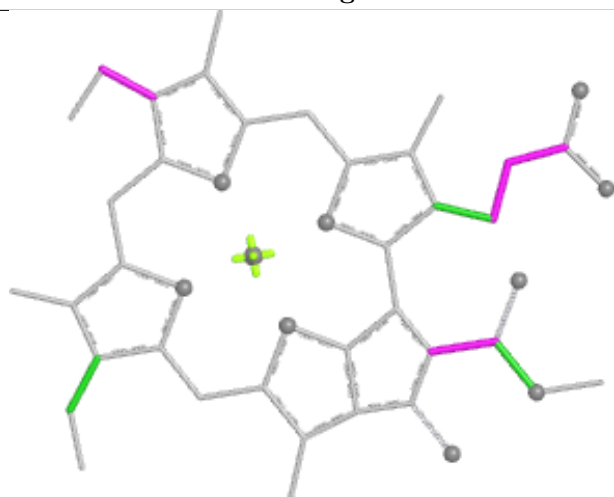
Ligand CLA A 836



Bond lengths



Bond angles

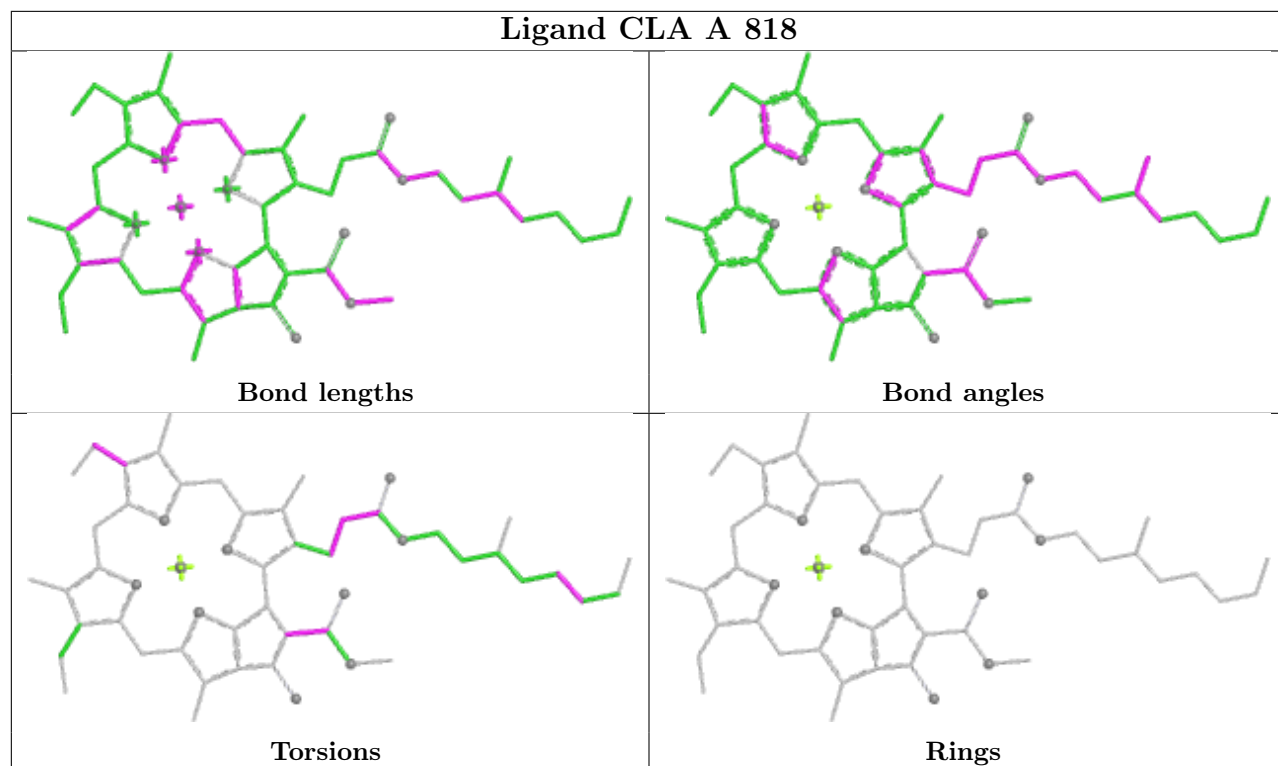


Torsions

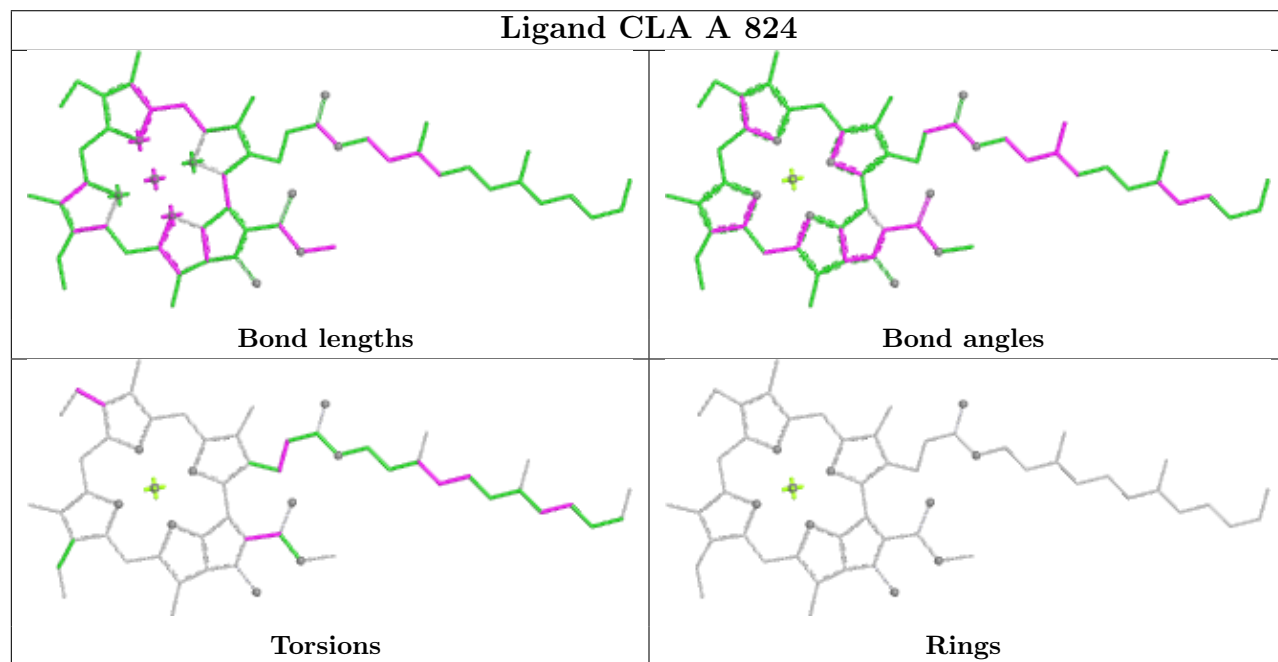


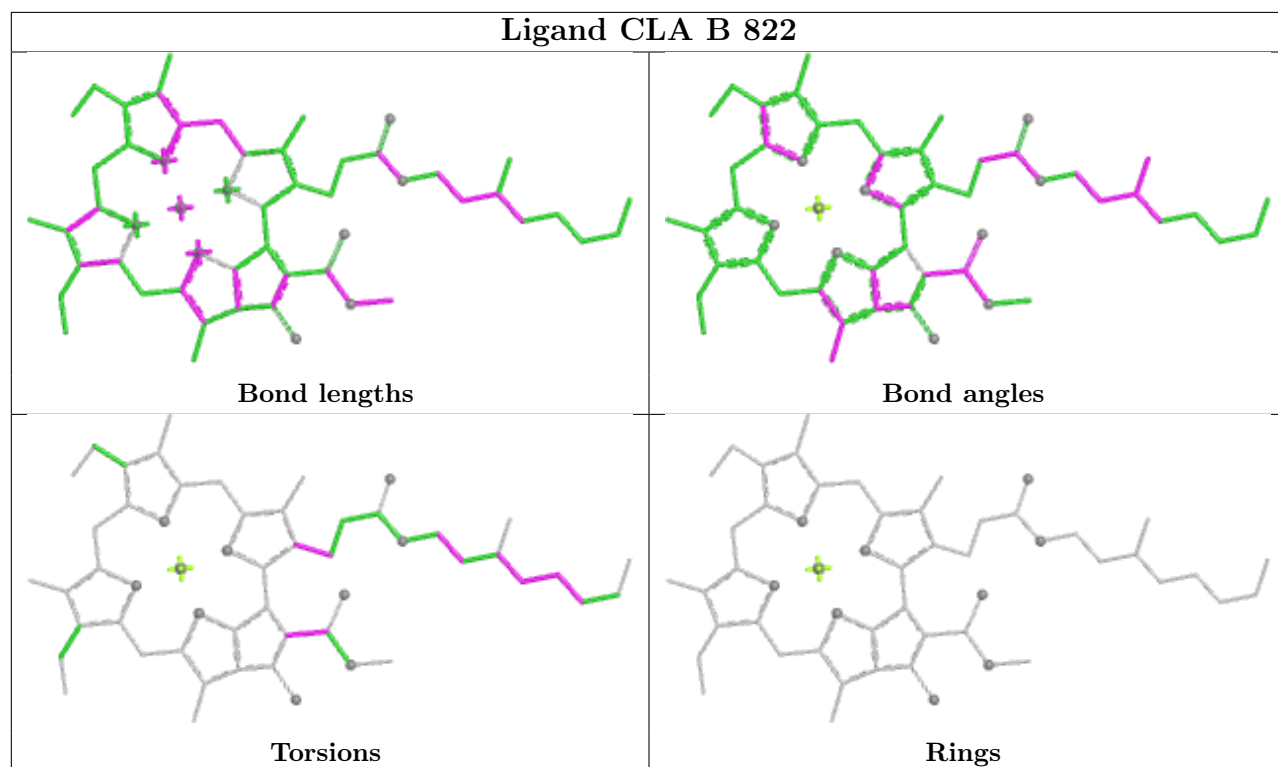
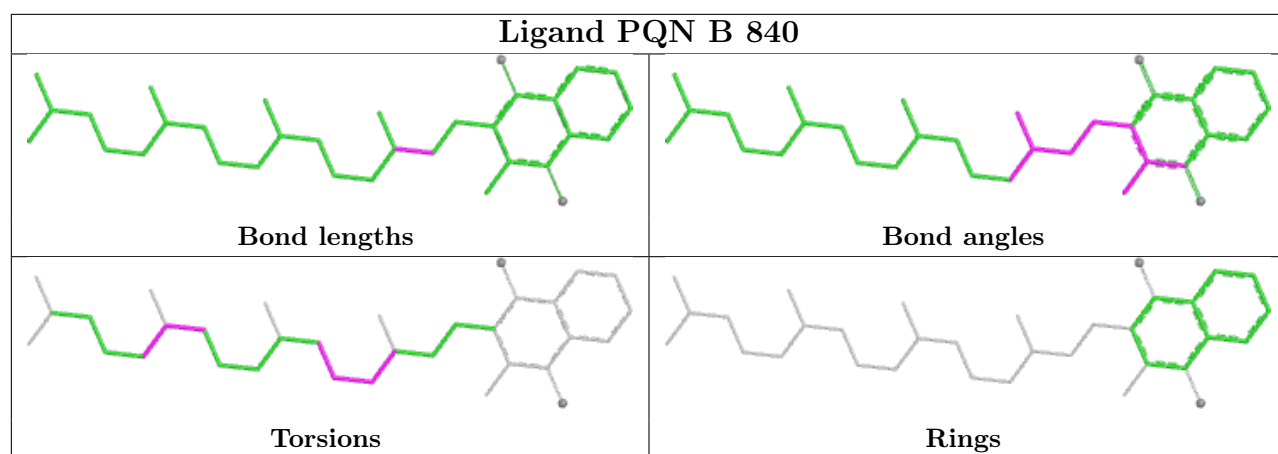
Rings

Ligand CLA A 818

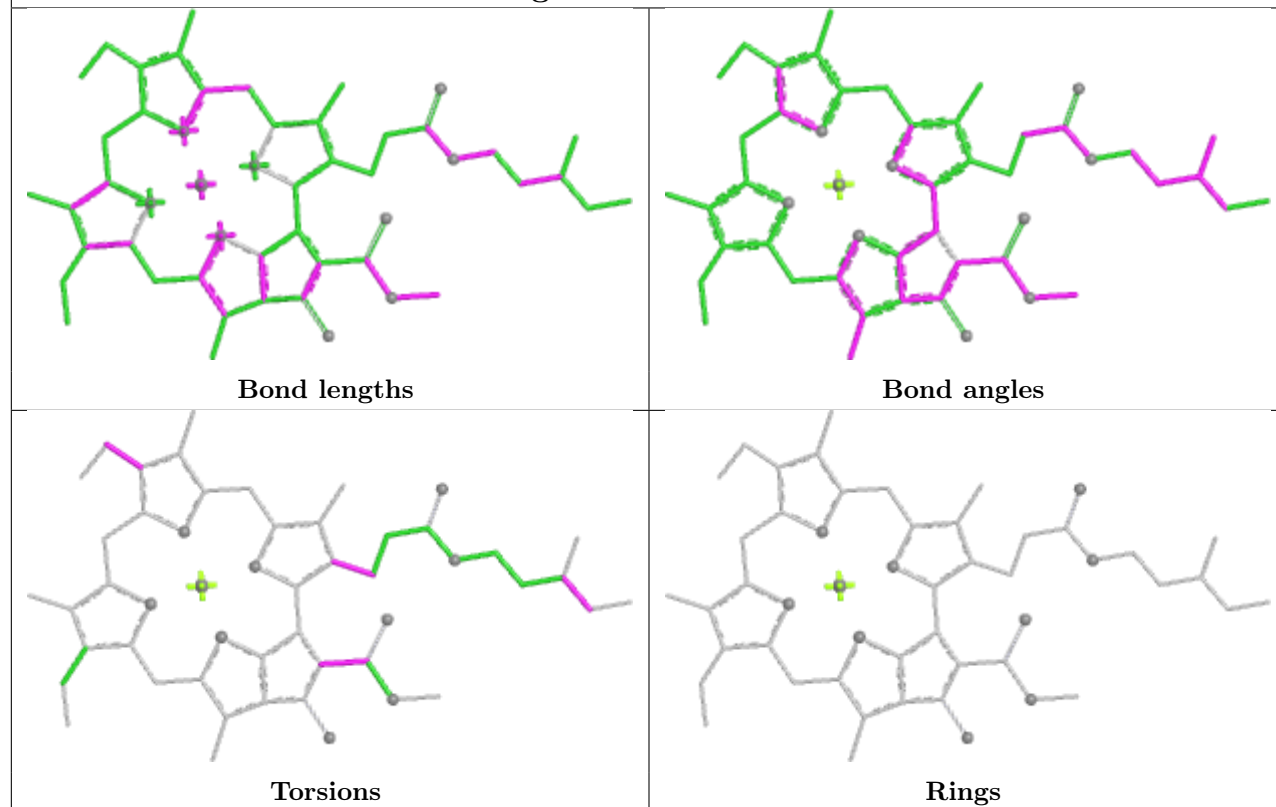


Ligand CLA A 824

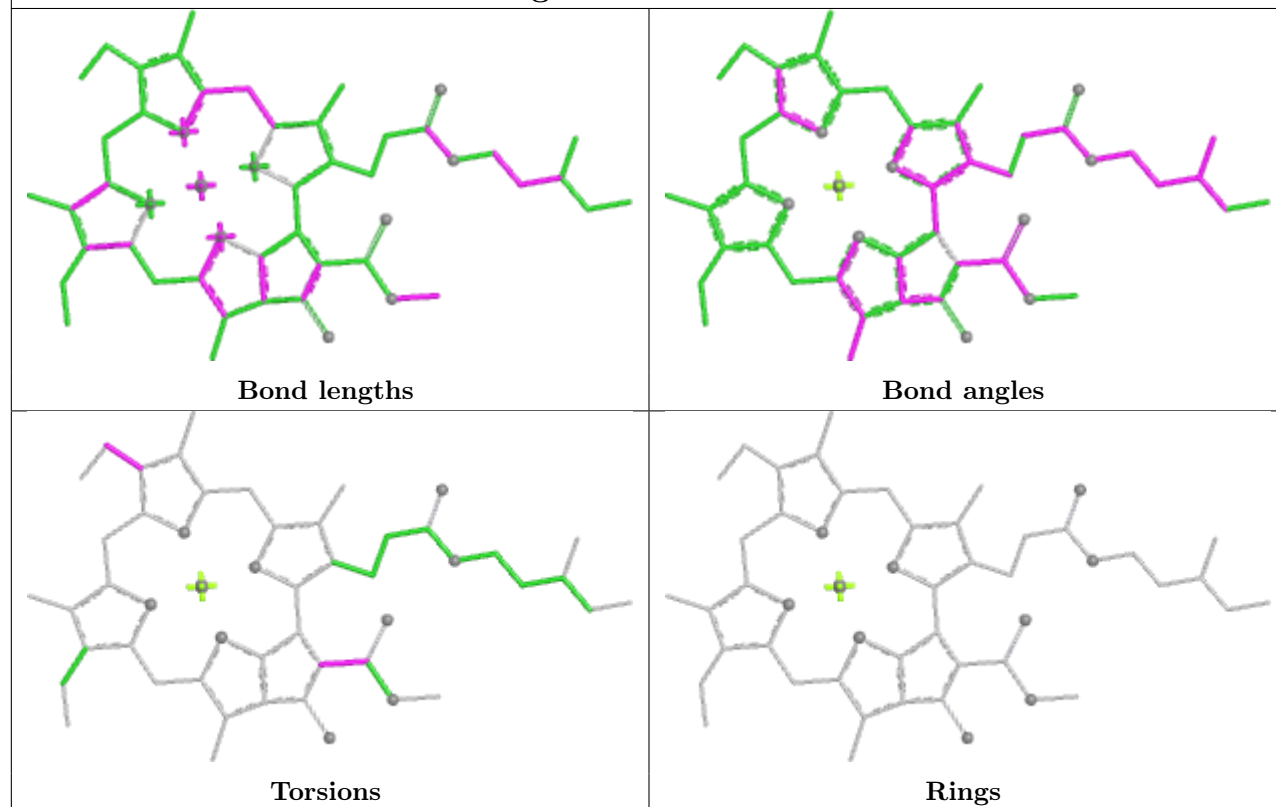


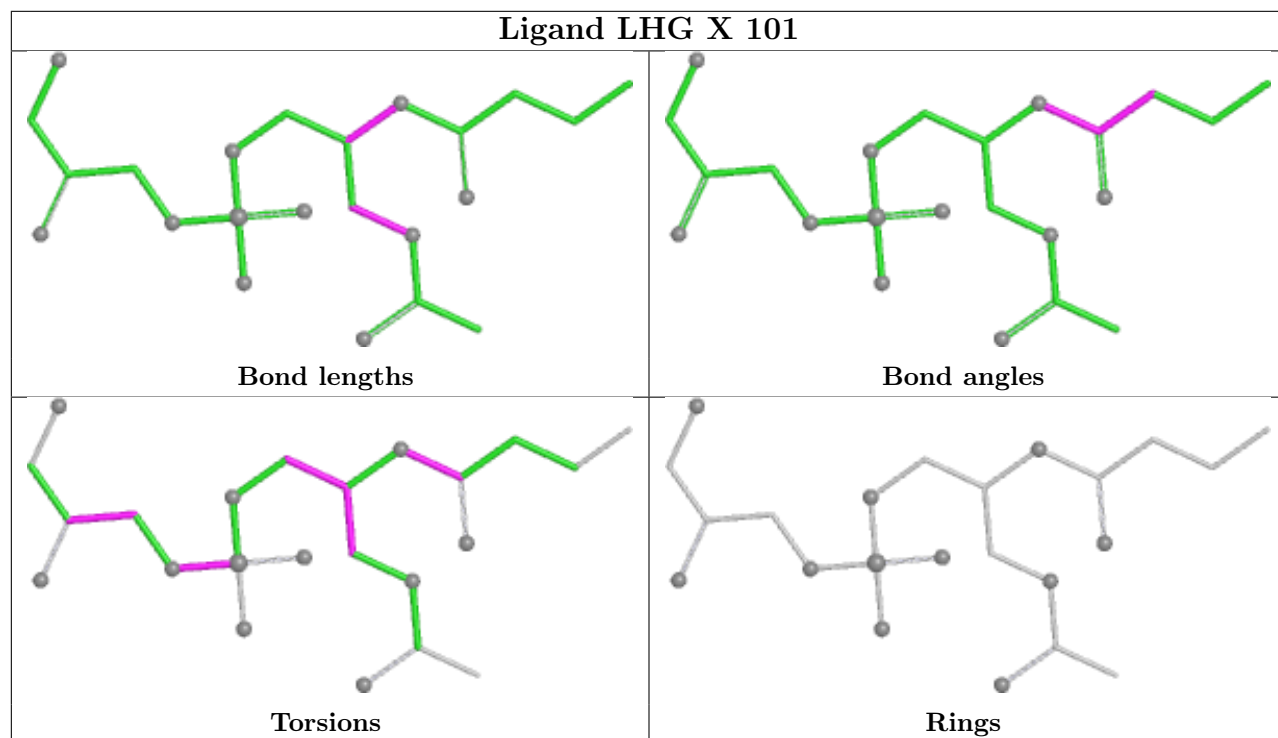
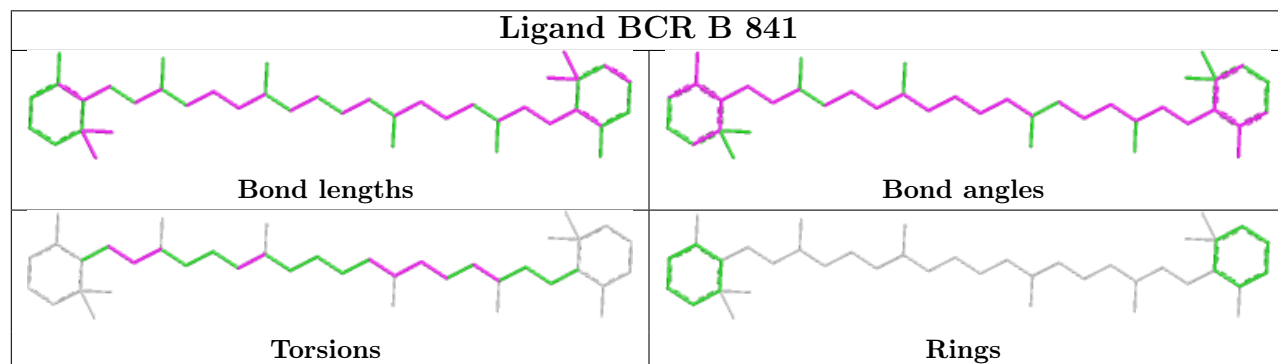
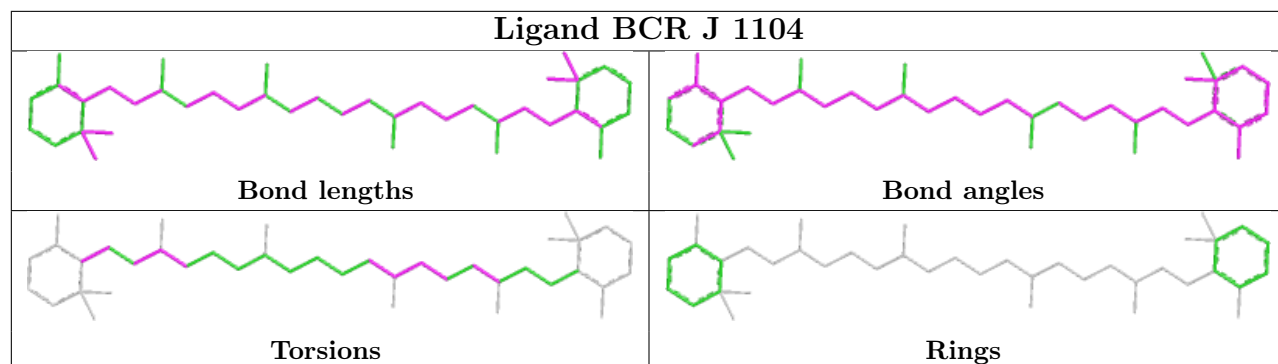


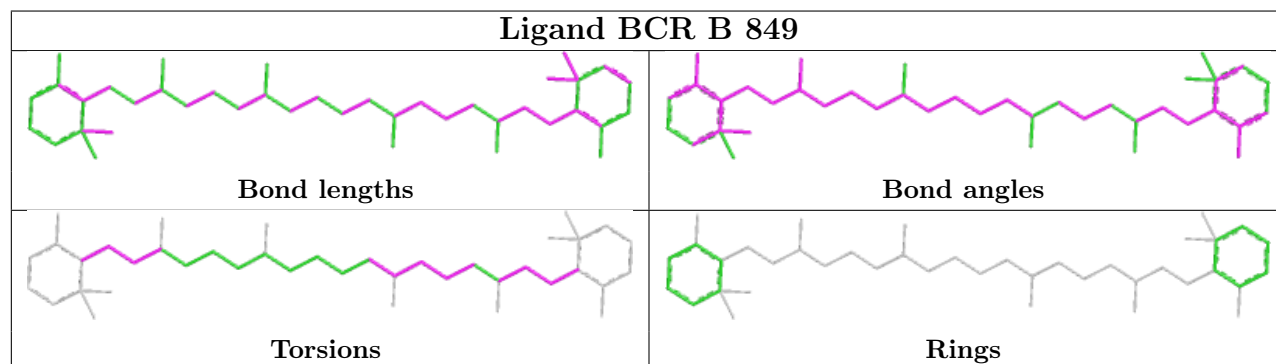
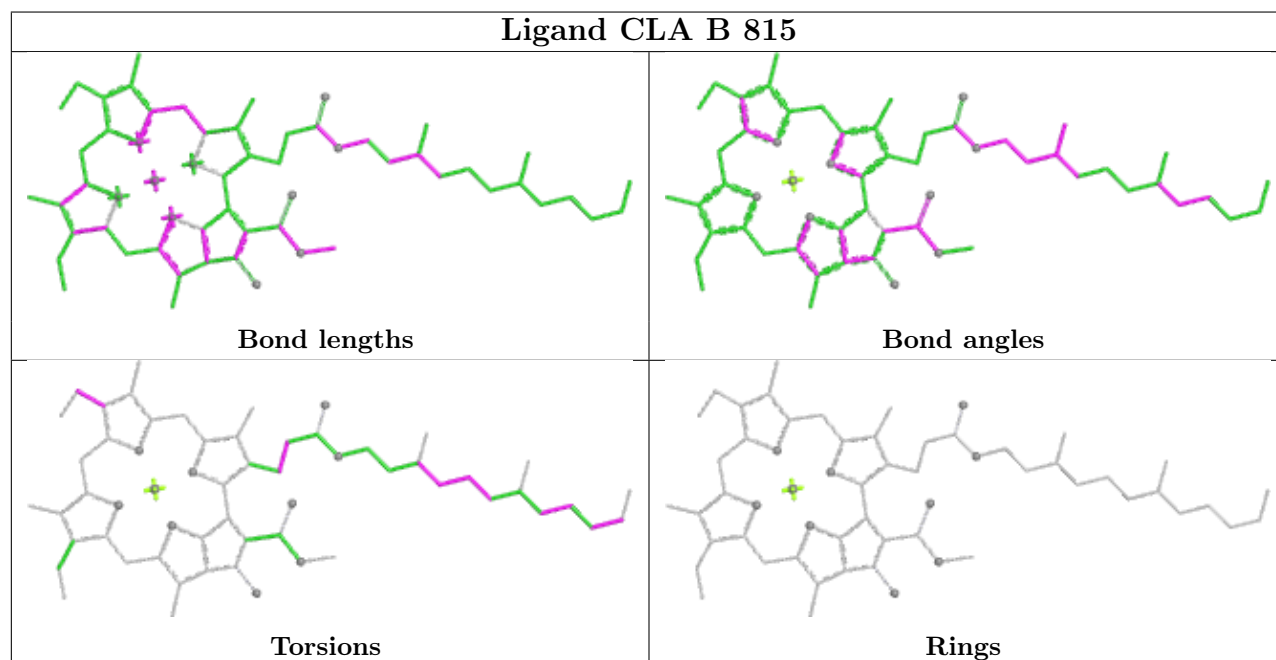
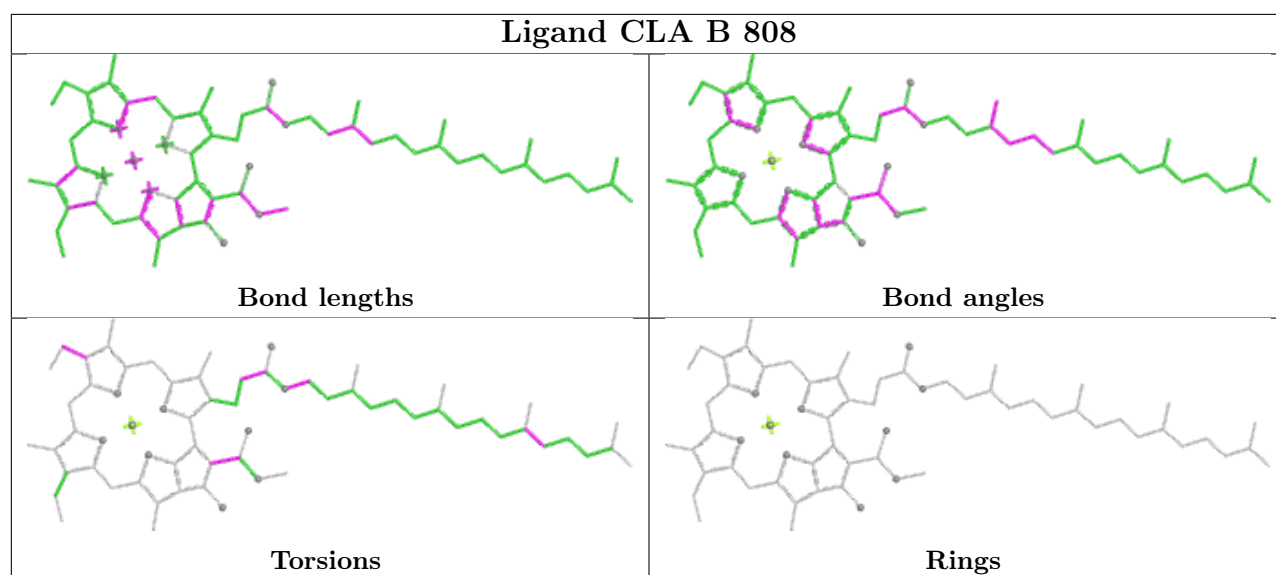
Ligand CLA A 807

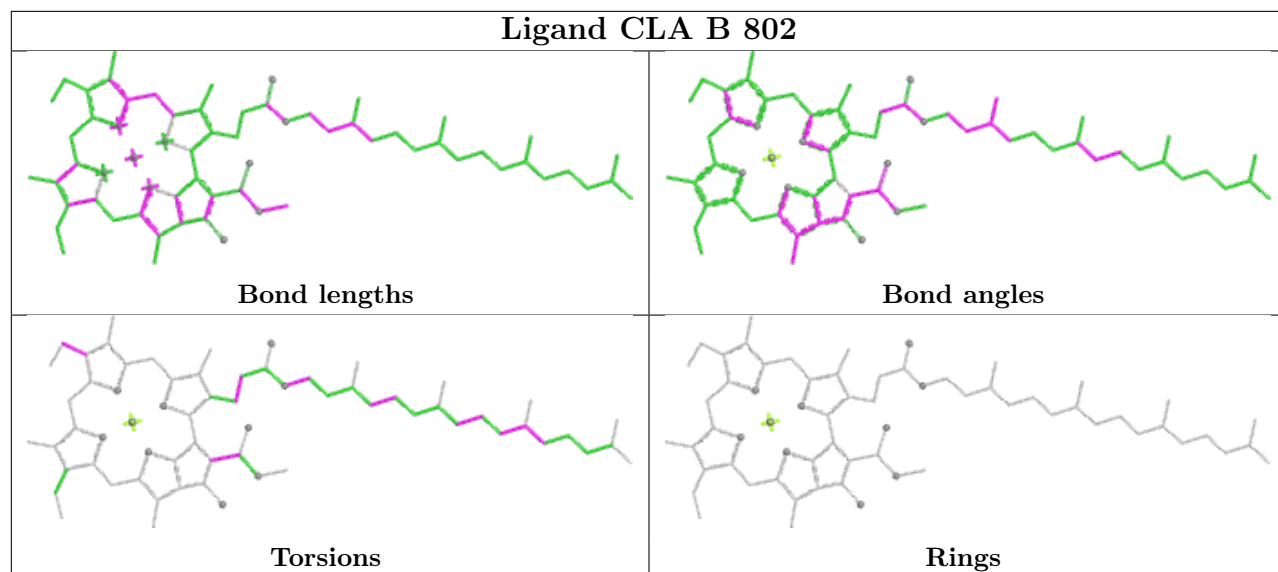
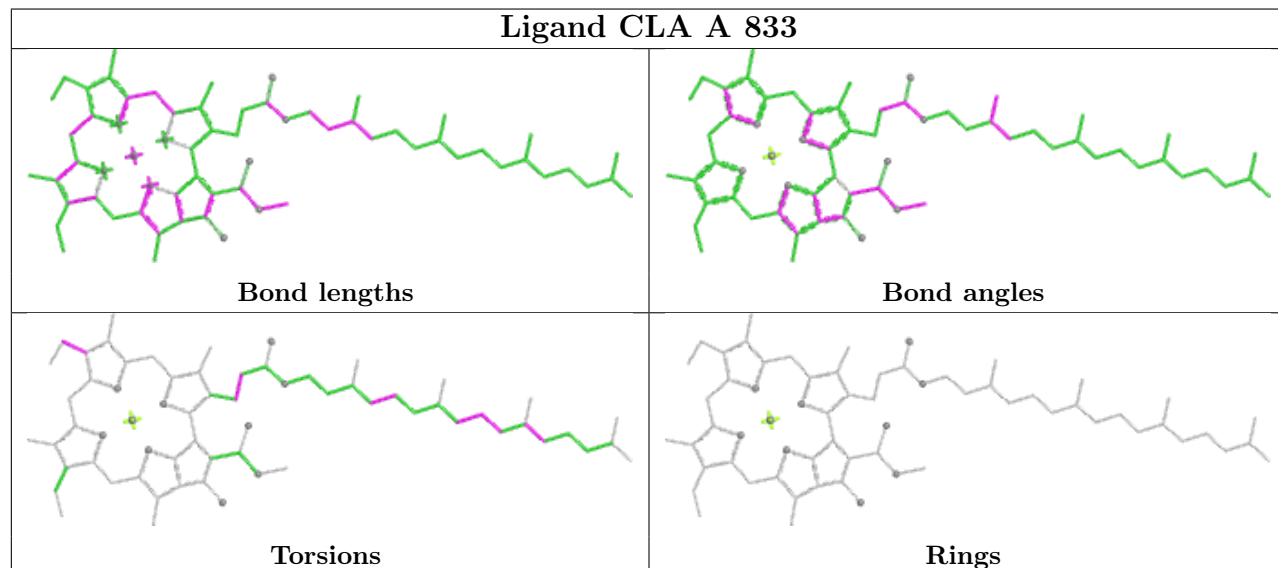


Ligand CLA A 837

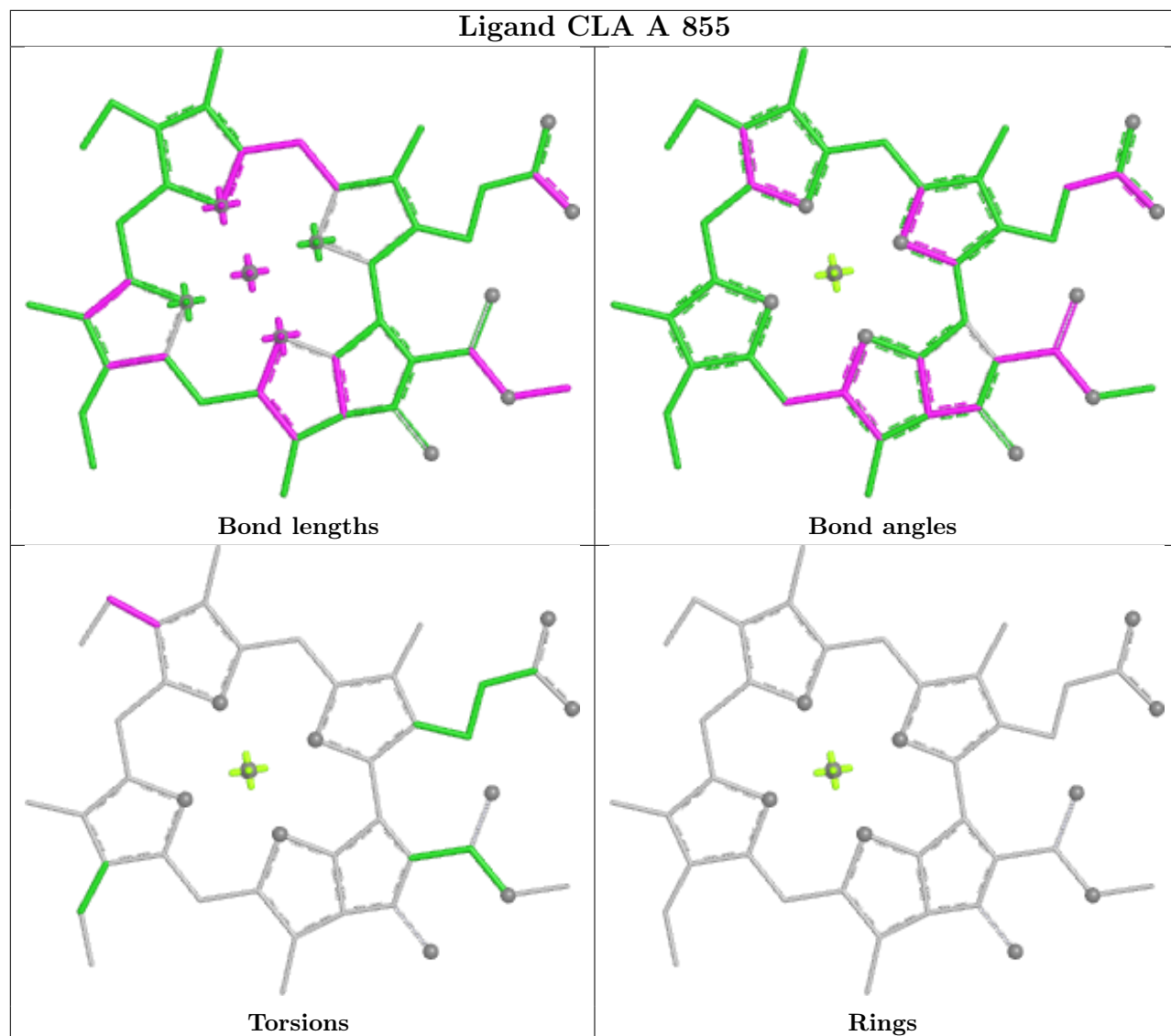




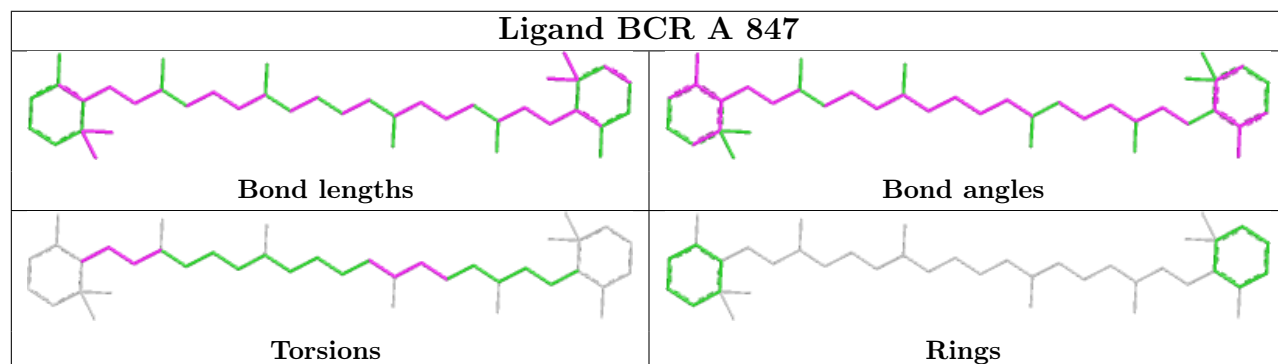


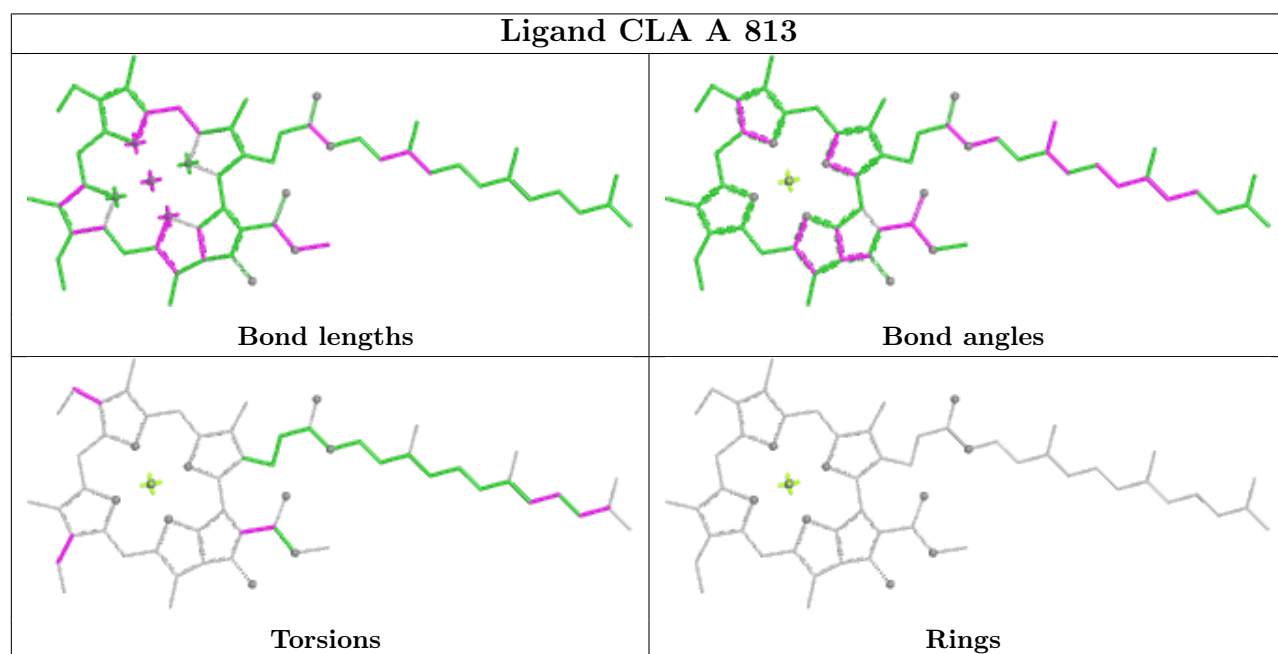
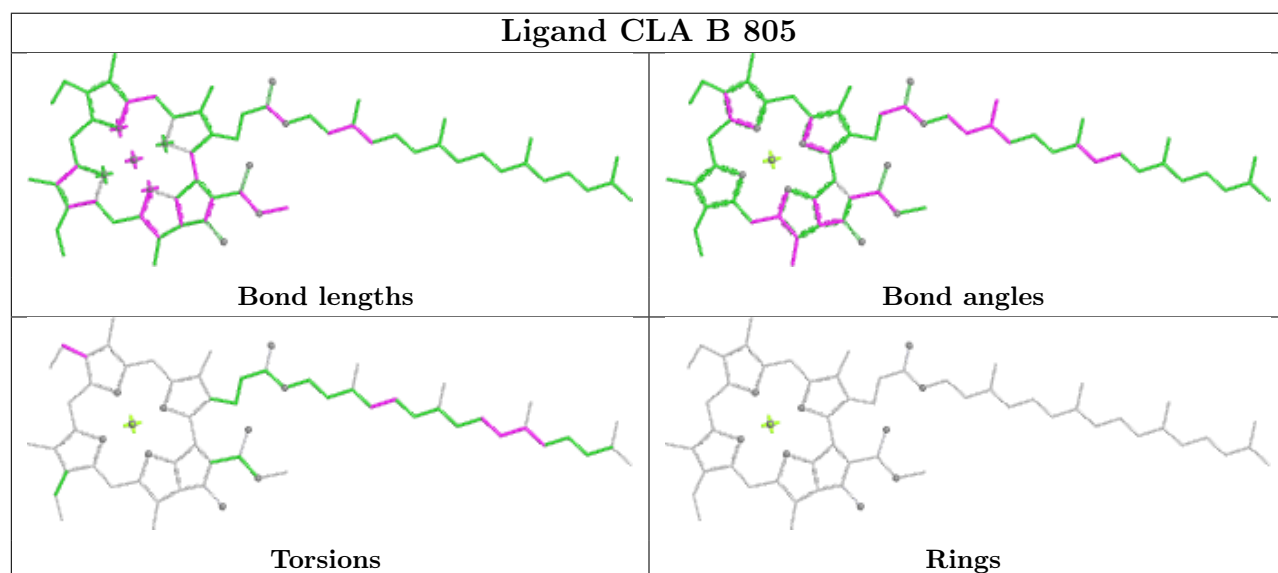
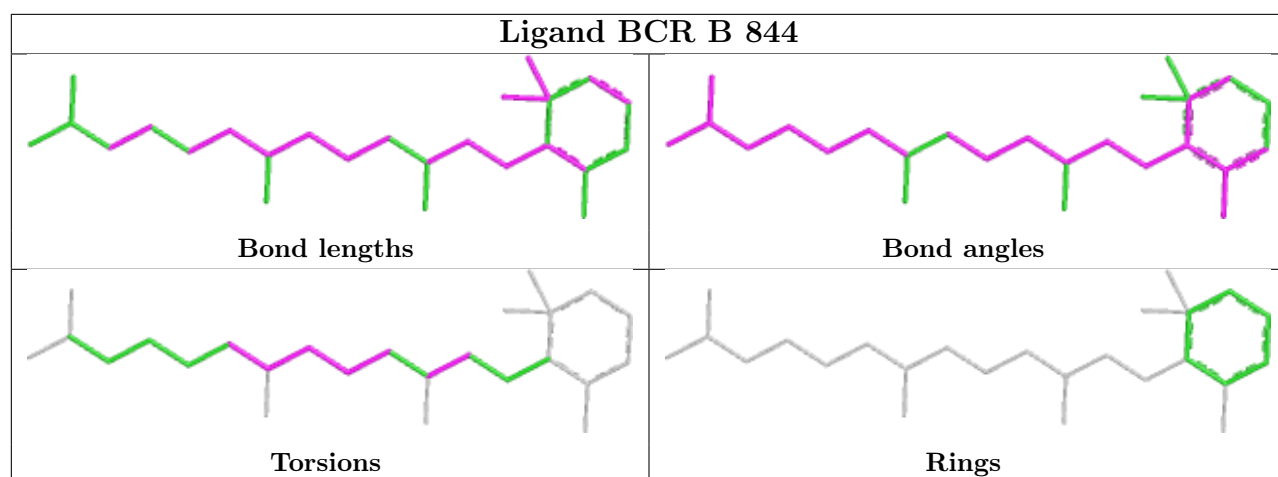
Ligand CLA B 802**Ligand CLA A 833**

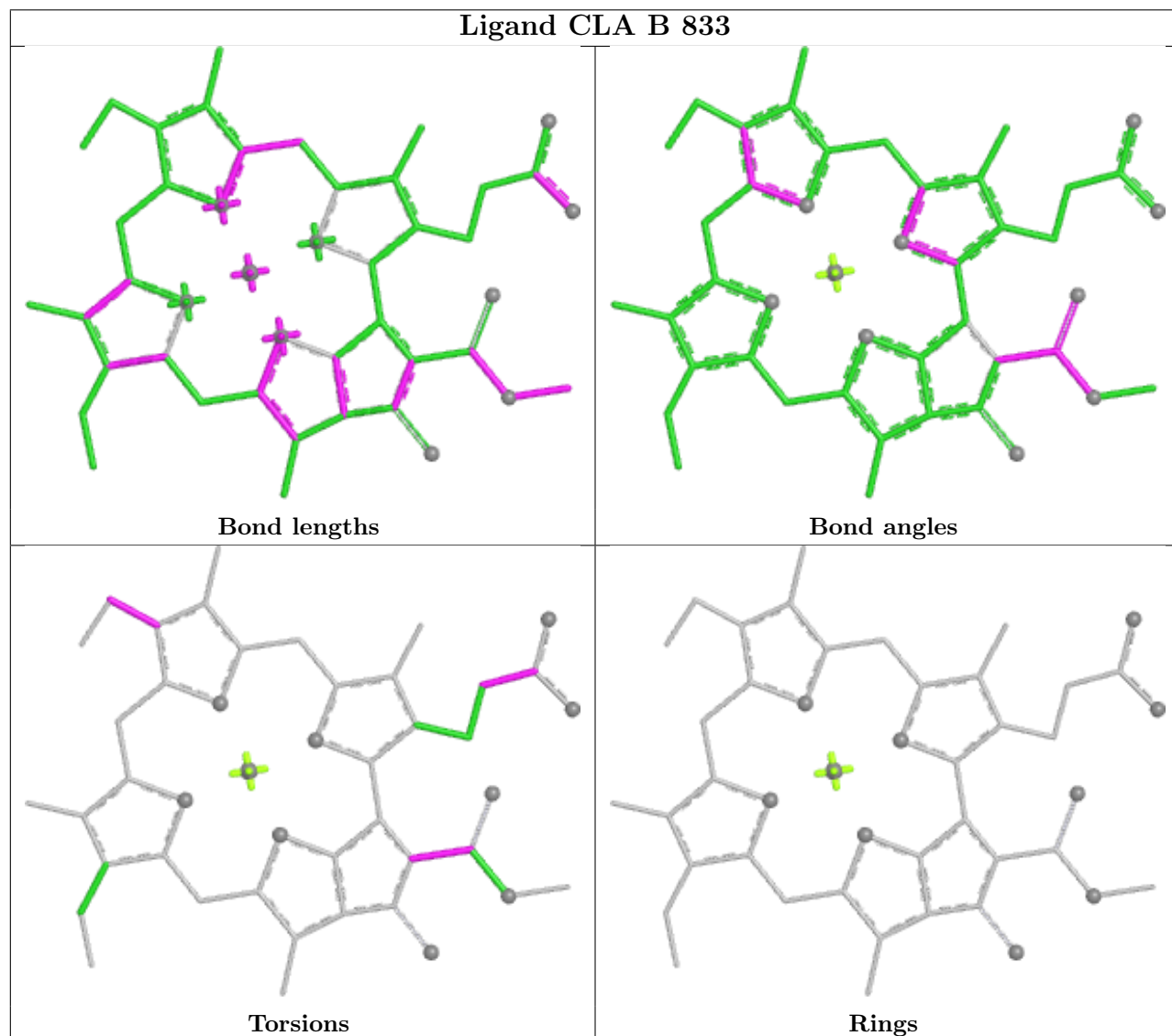
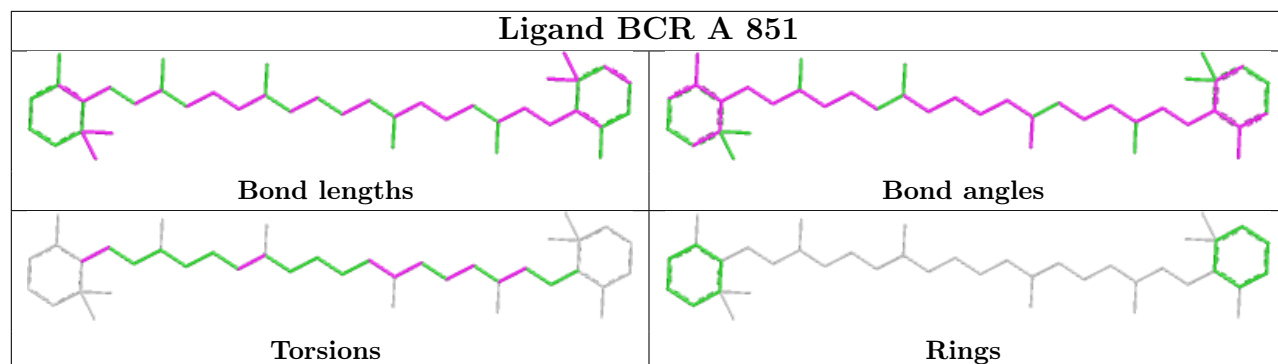
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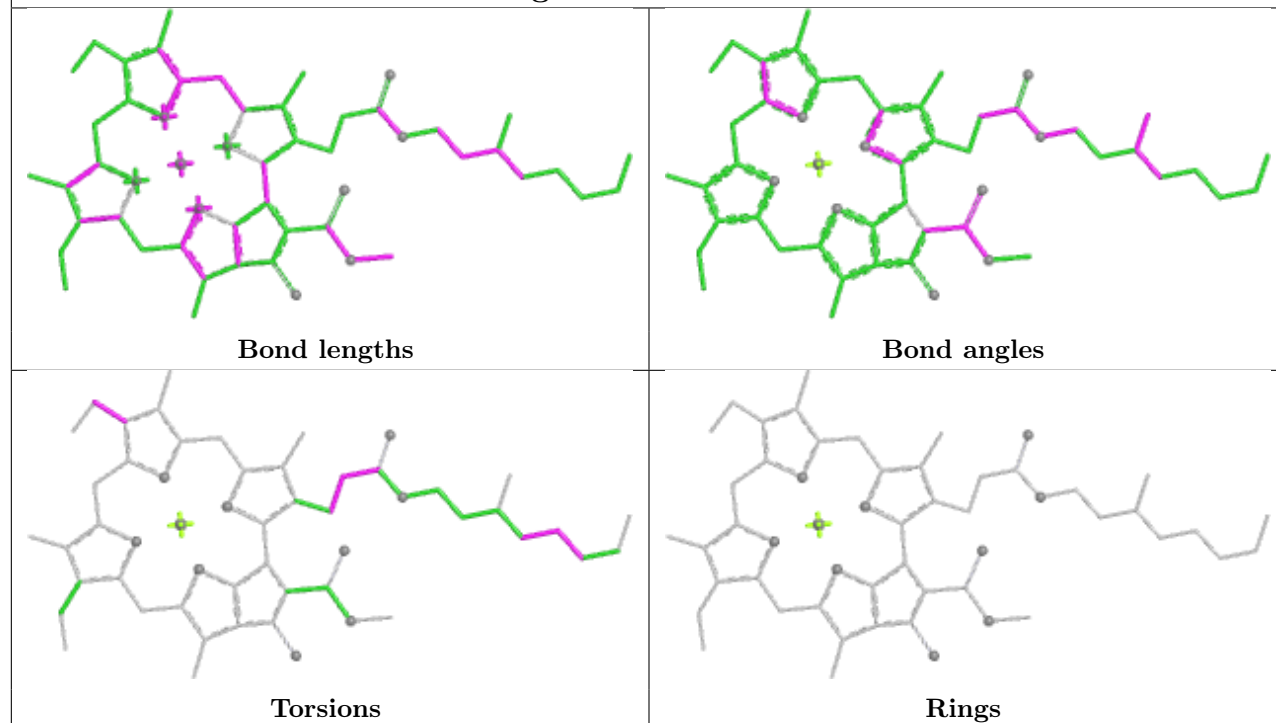
Ligand BCR A 847



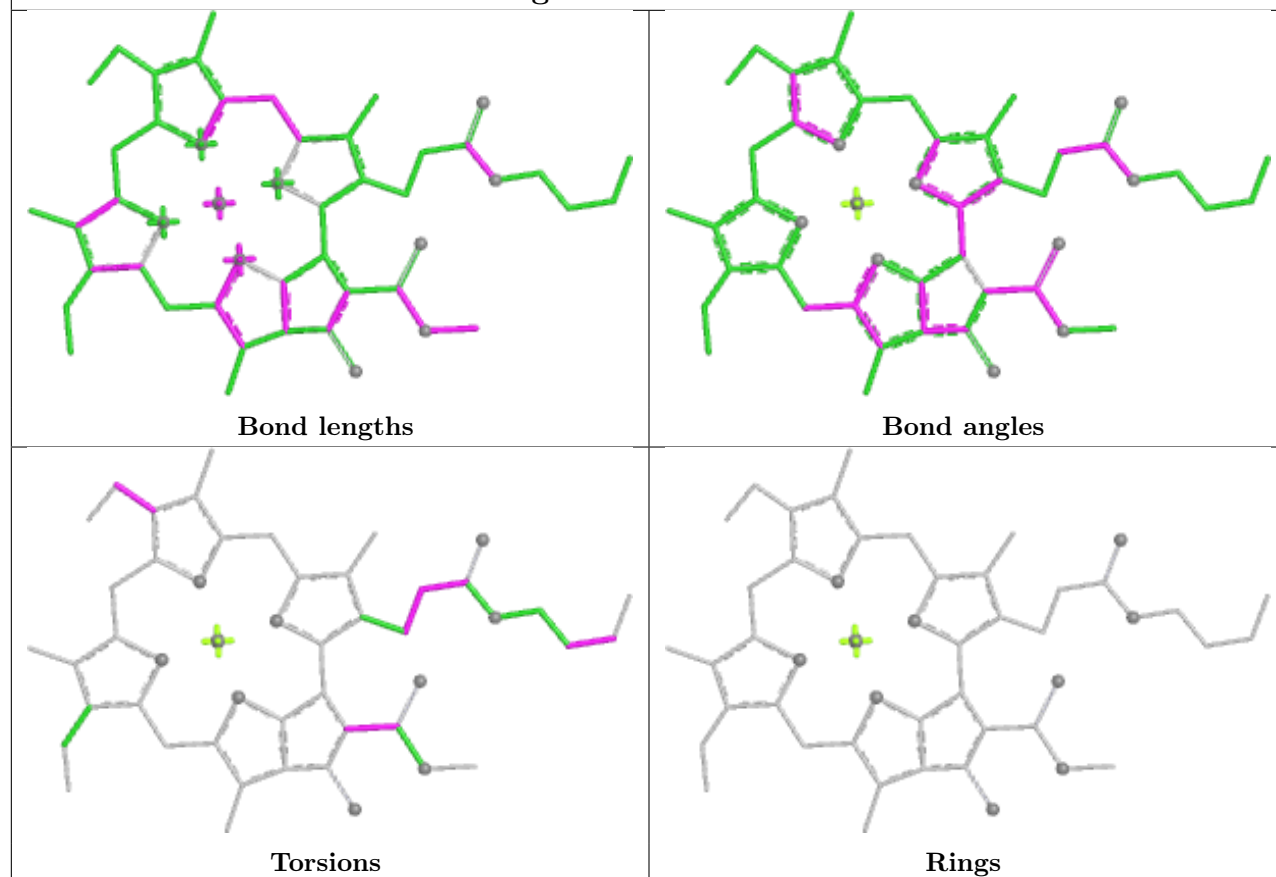


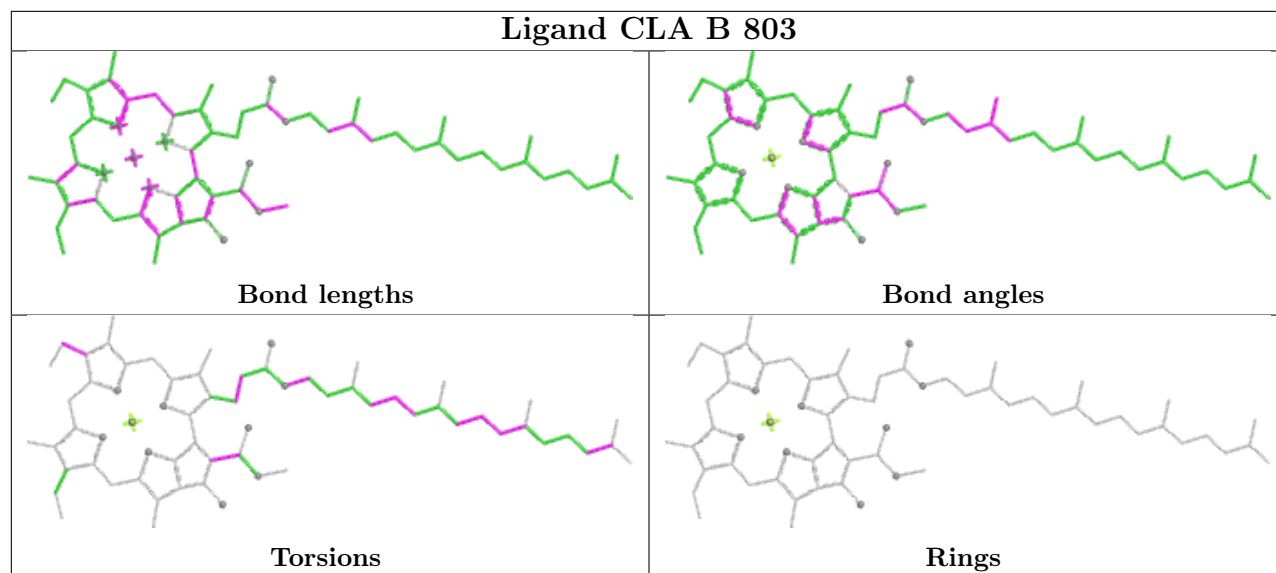
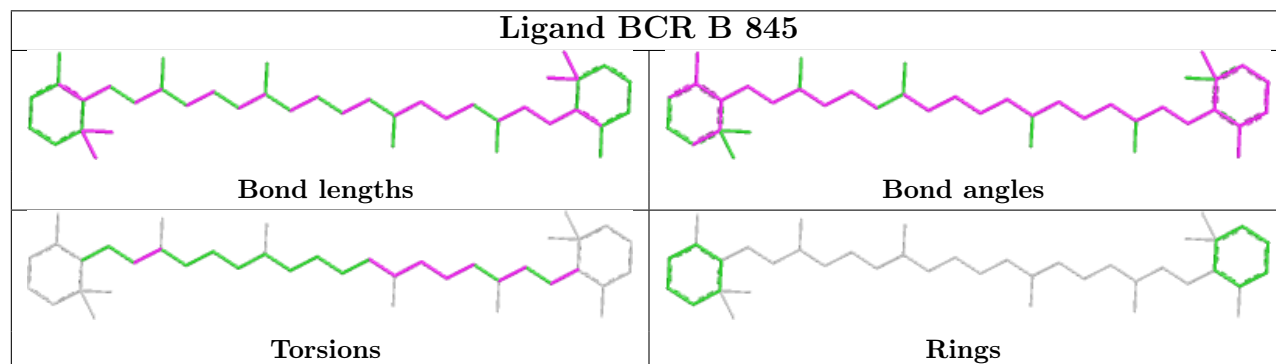
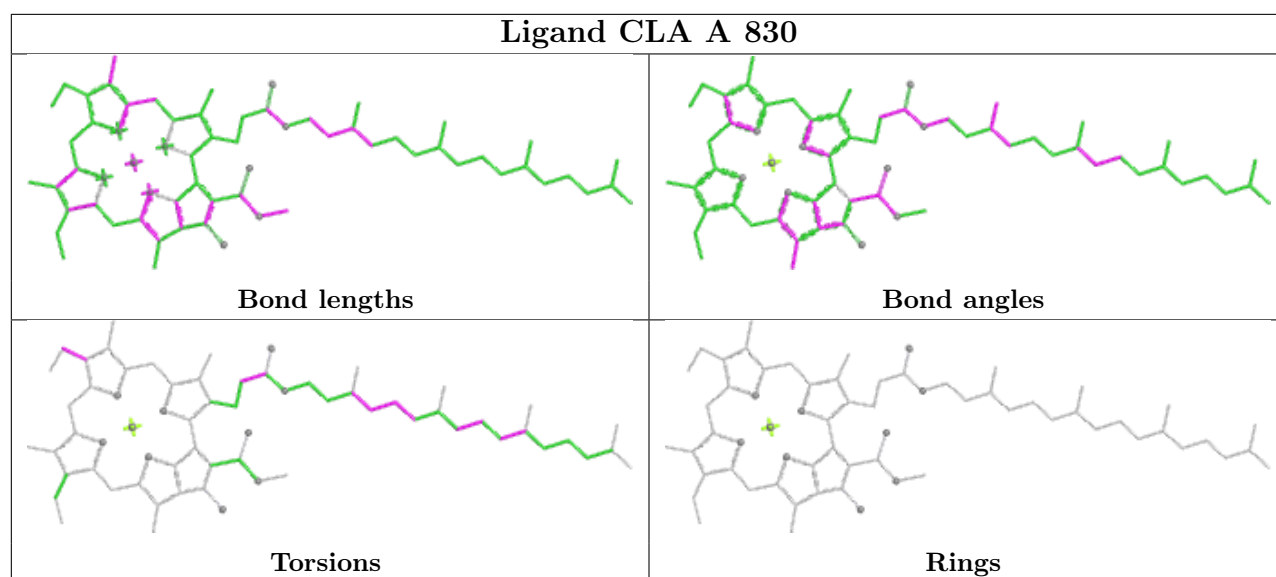


Ligand CLA A 835

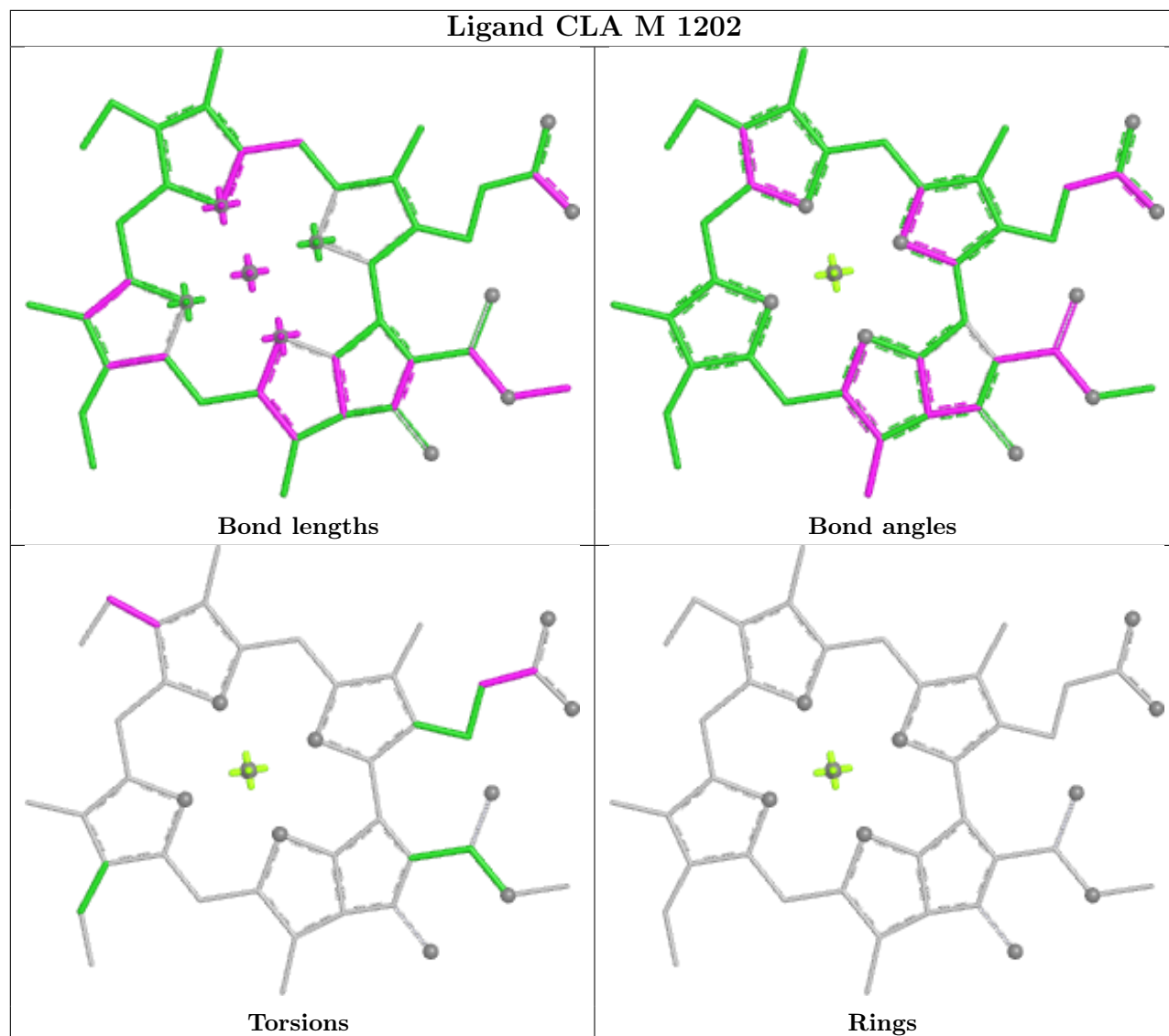


Ligand CLA A 822

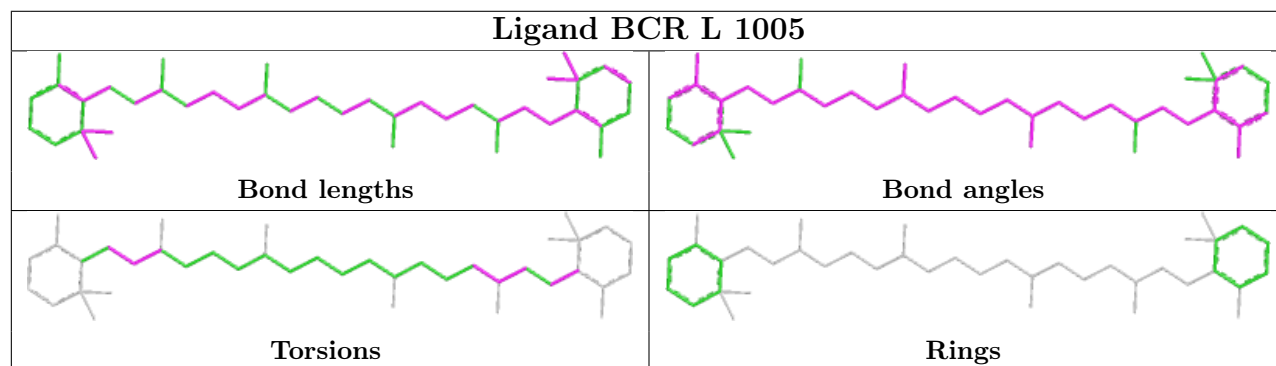




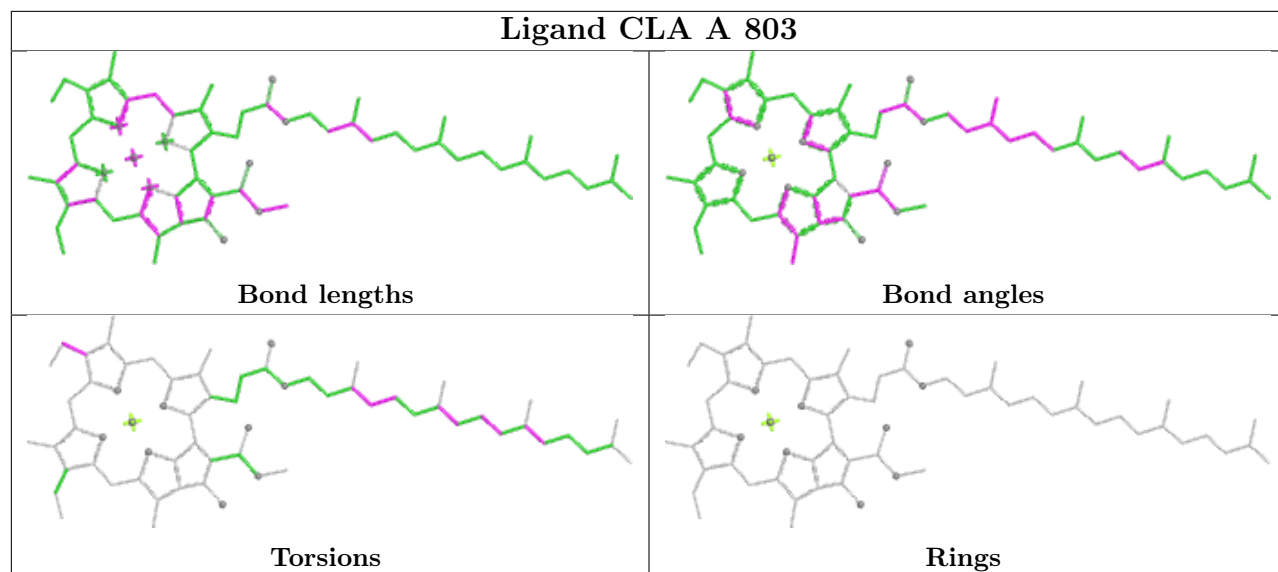
Ligand CLA M 1202



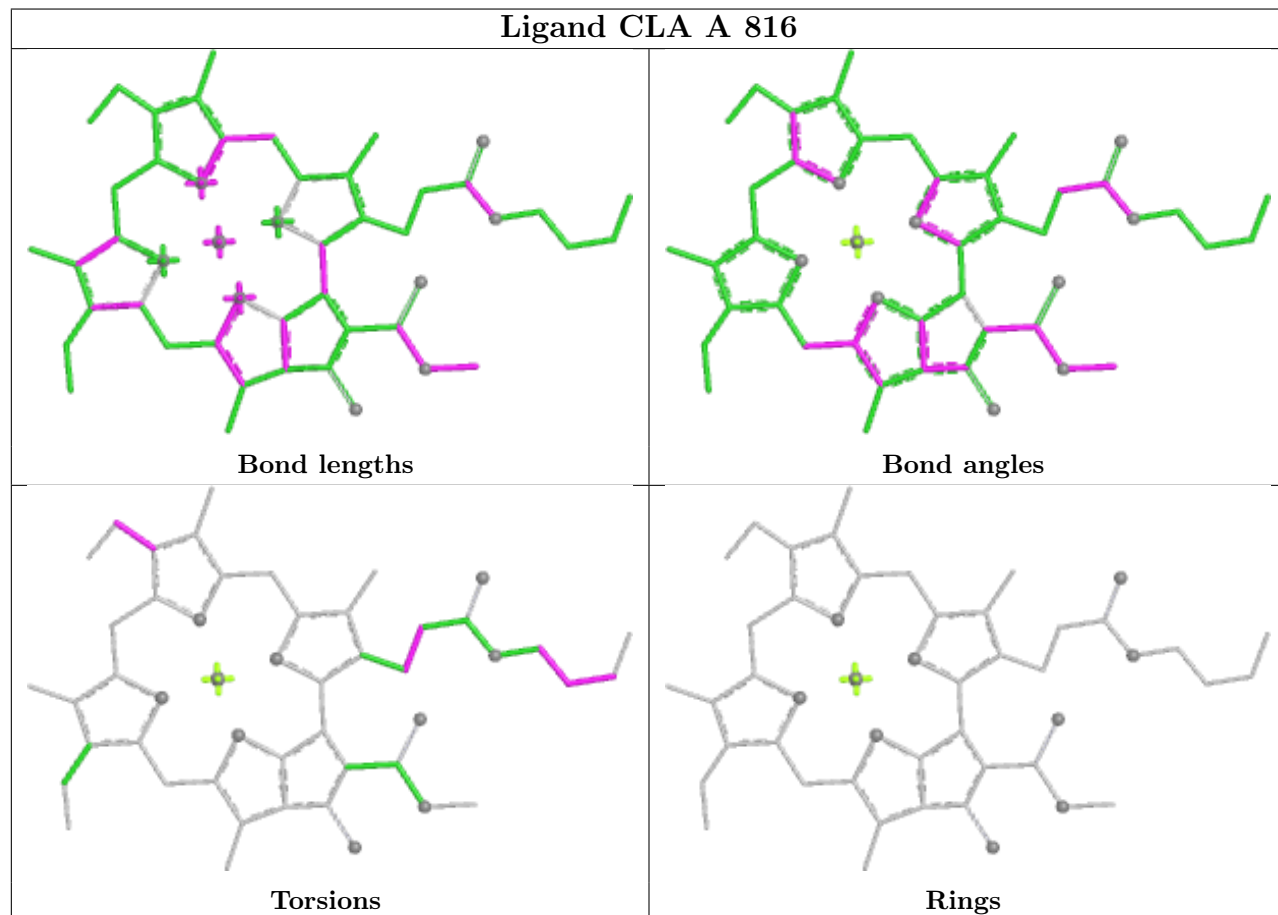
Ligand BCR L 1005

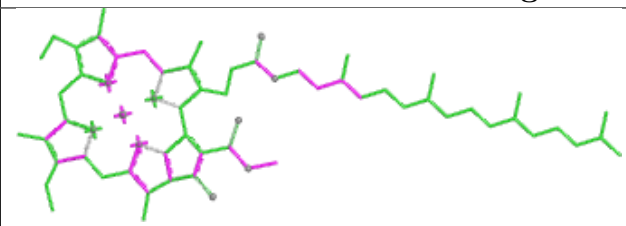
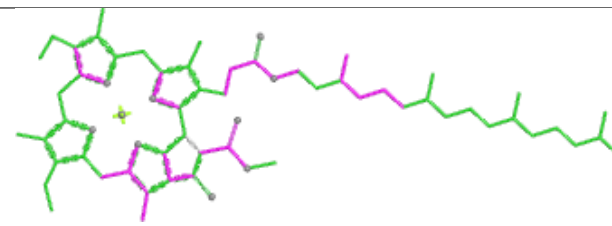
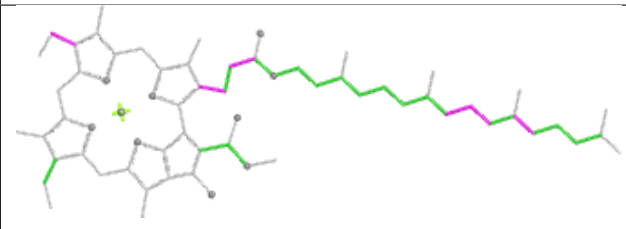
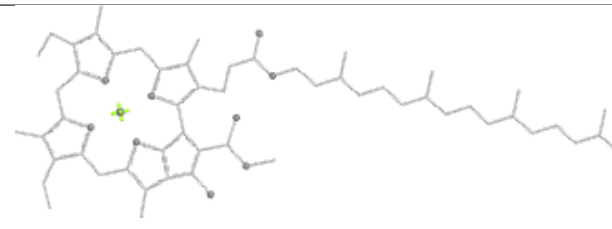


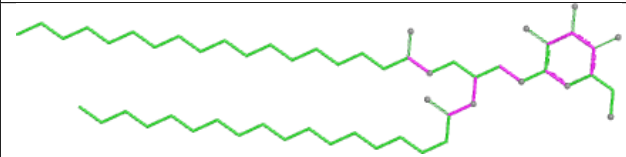
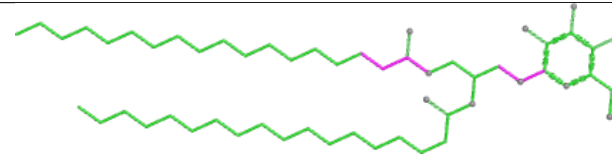
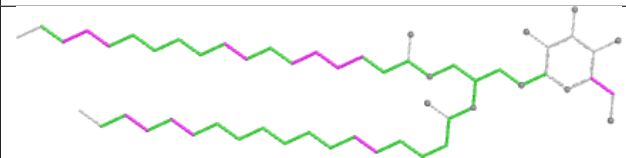
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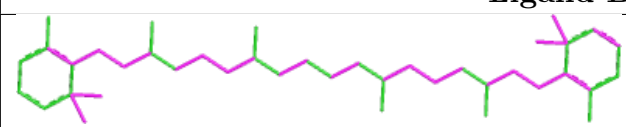
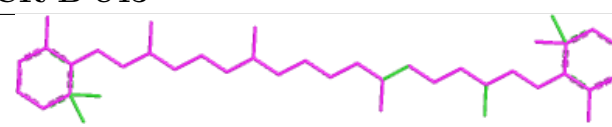
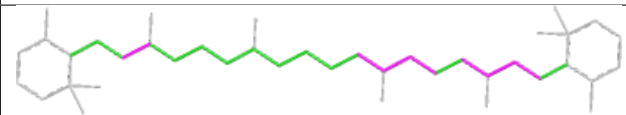
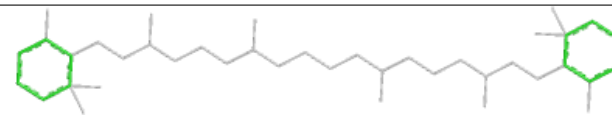


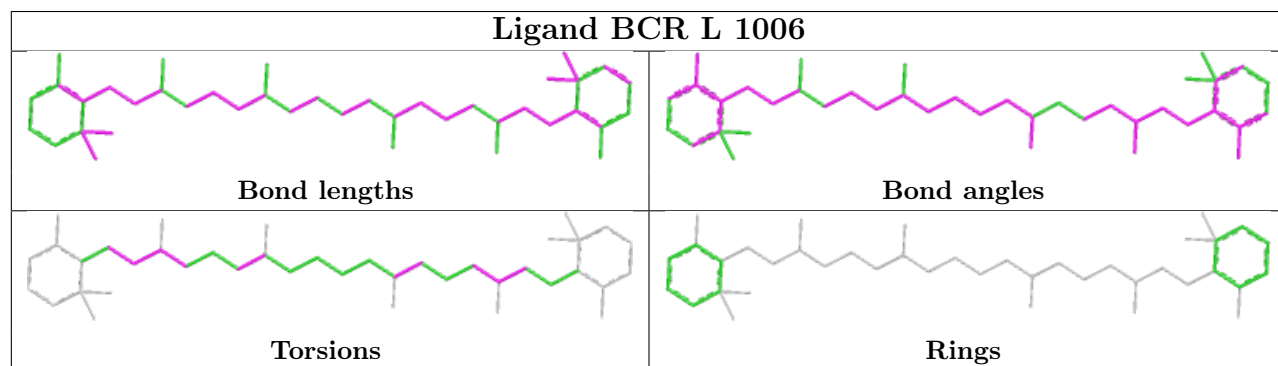
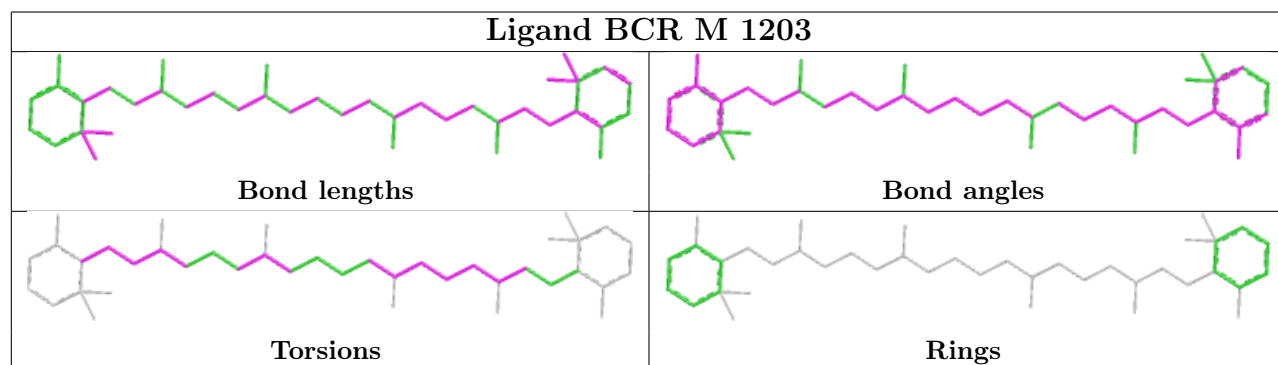
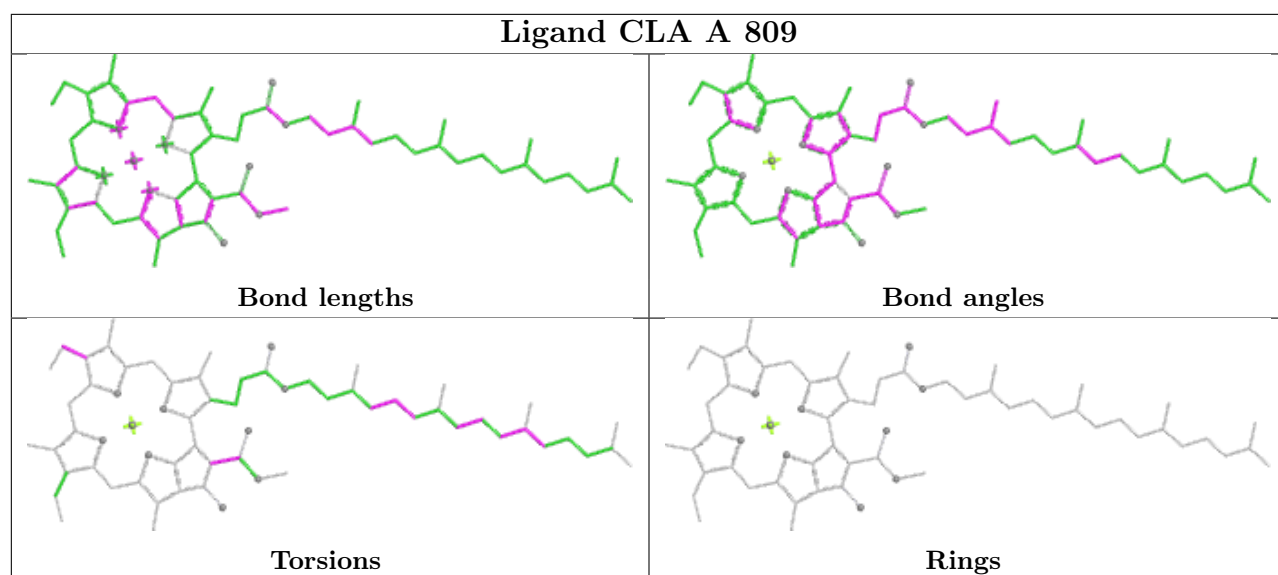
Ligand CLA A 816



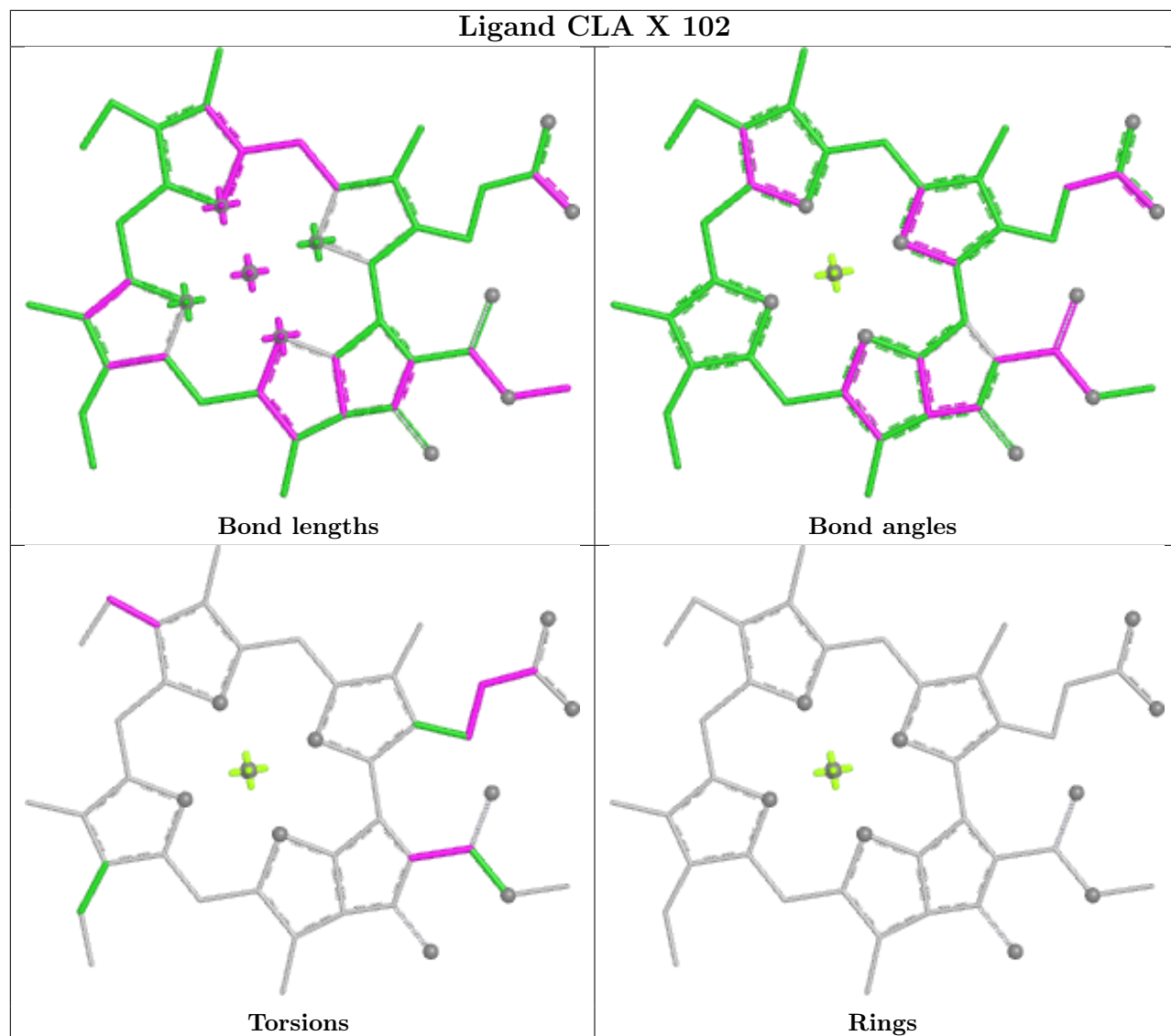
Ligand CLA A 829	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG B 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

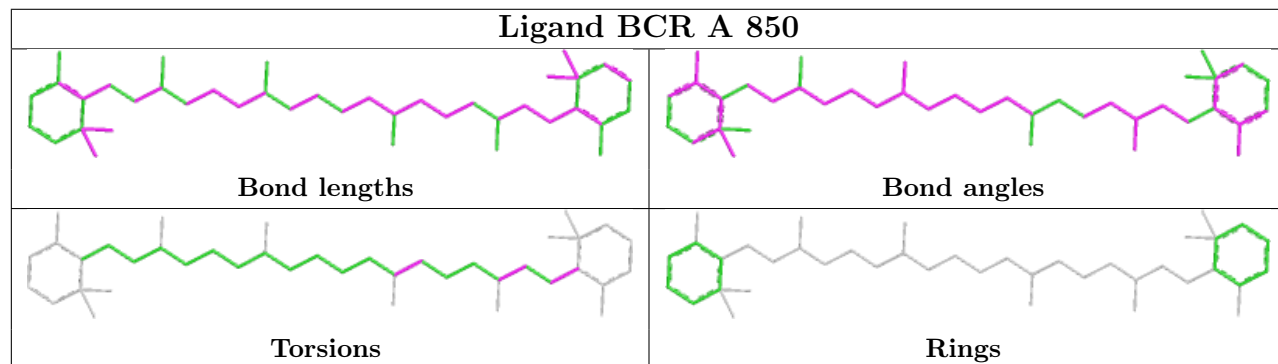
Ligand BCR B 843	
	
Bond lengths	Bond angles
	
Torsions	Rings



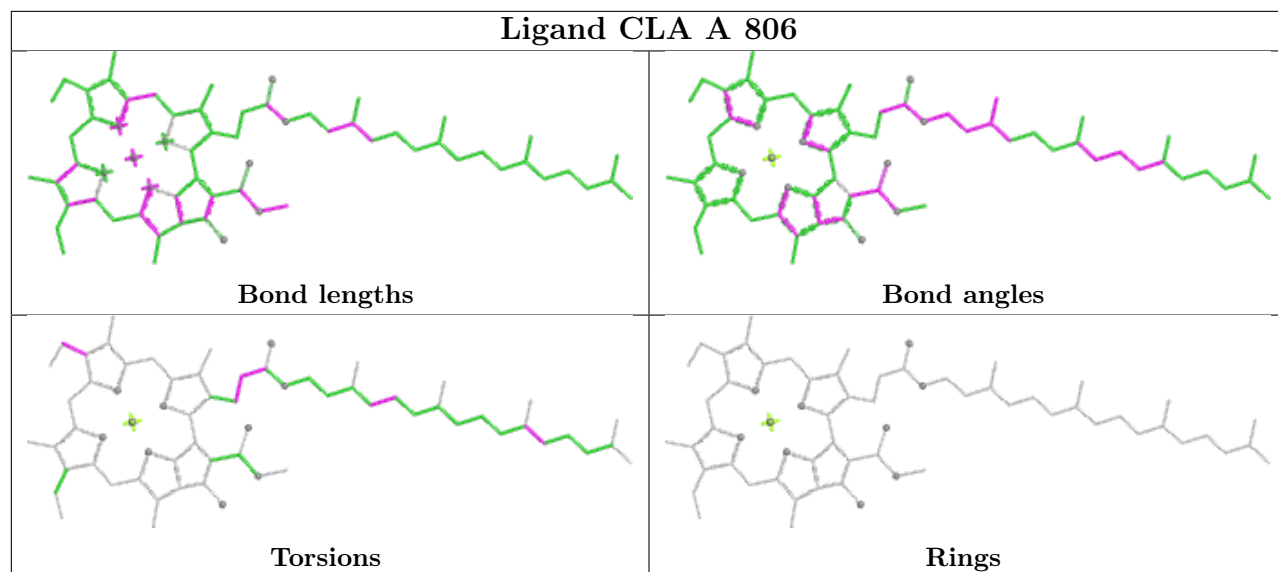
Ligand CLA X 102



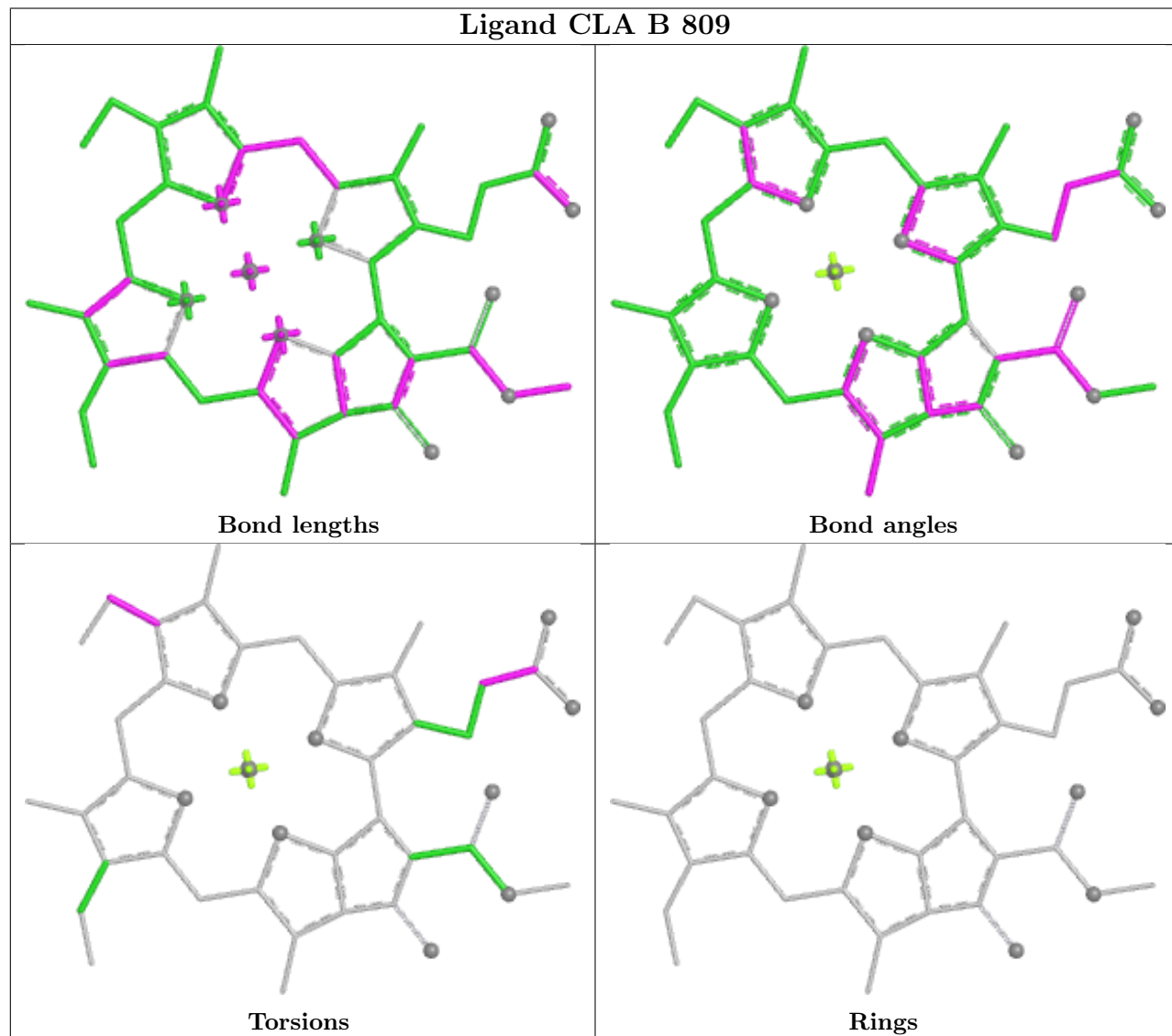
Ligand BCR A 850



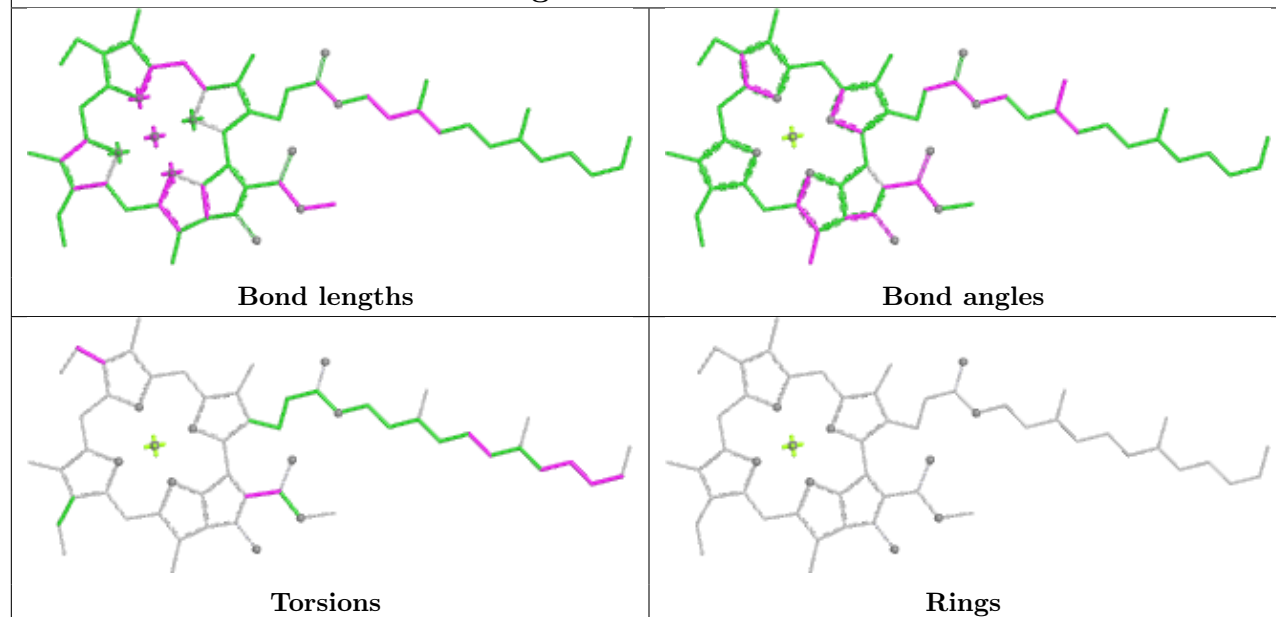
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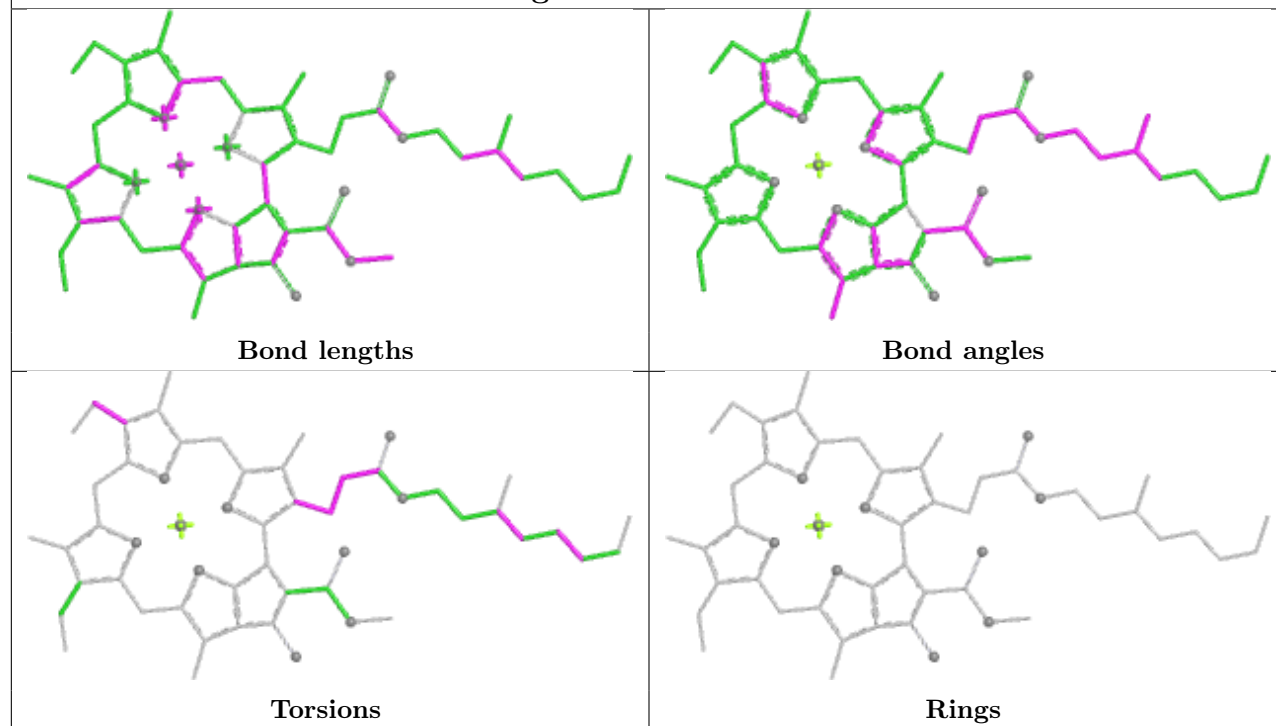
Ligand CLA B 809

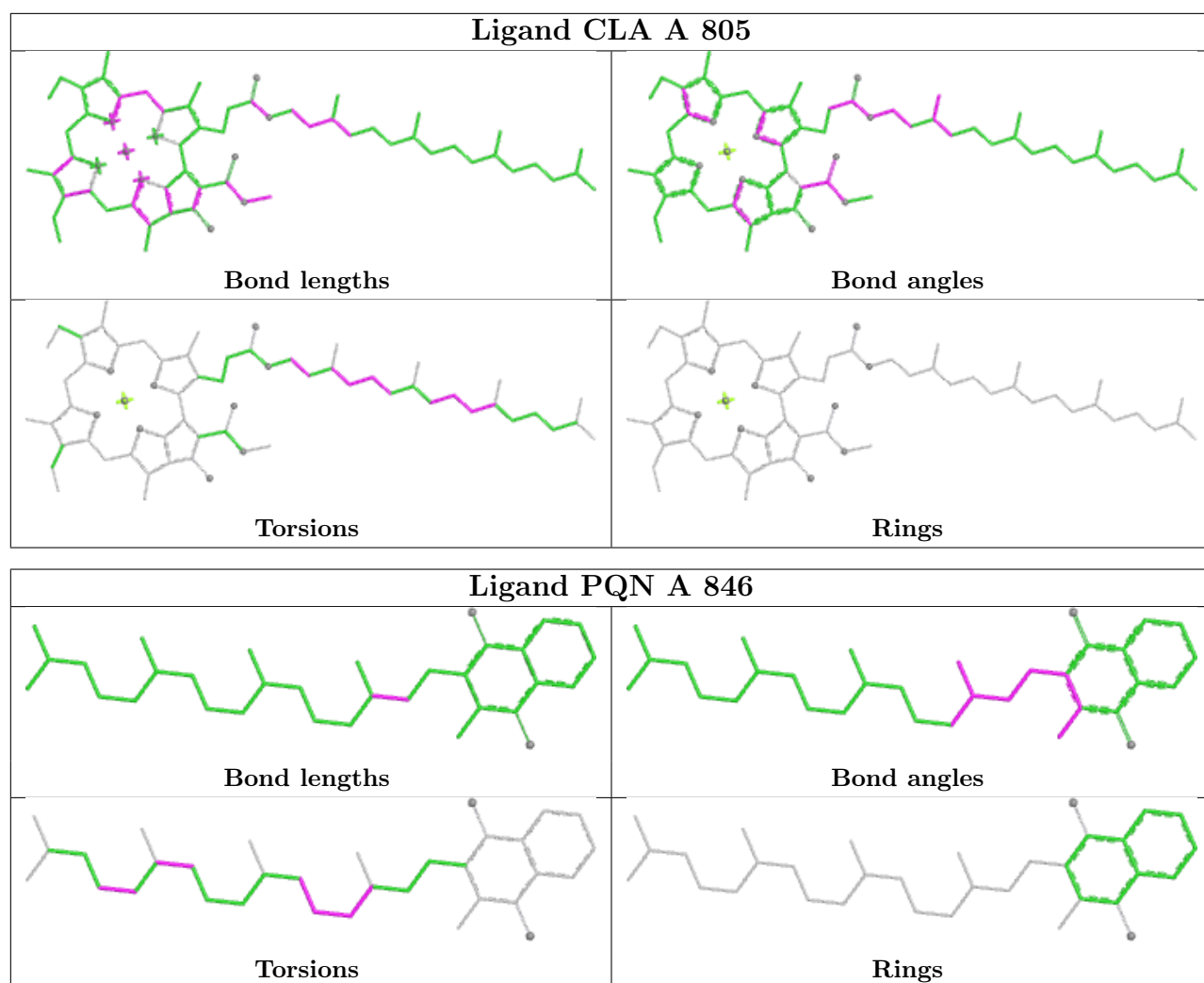


Ligand CLA A 804

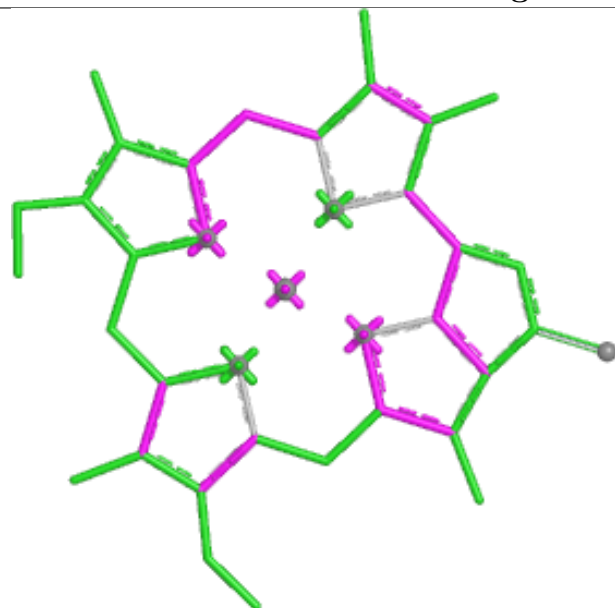


Ligand CLA A 812





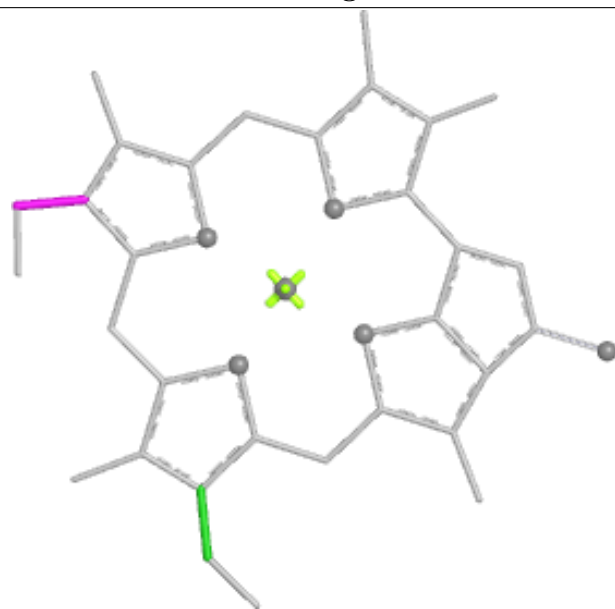
Ligand CLA J 1103



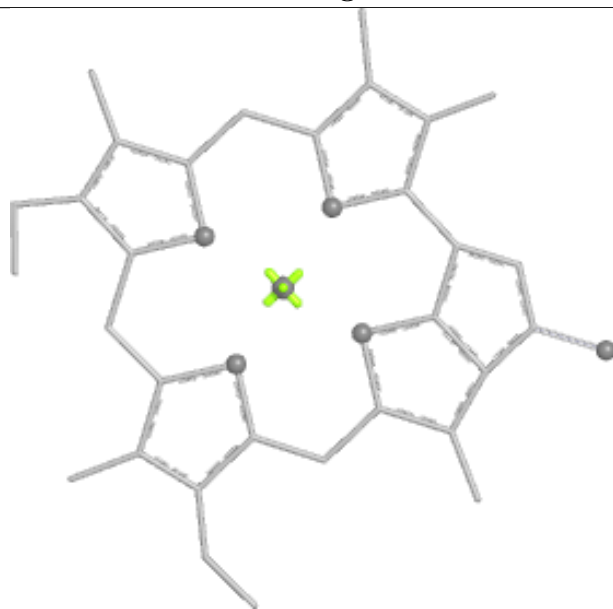
Bond lengths



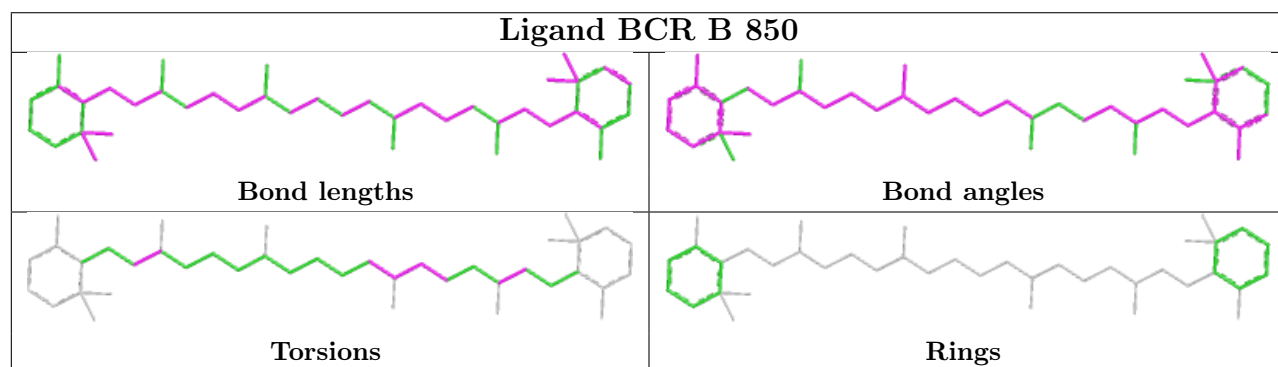
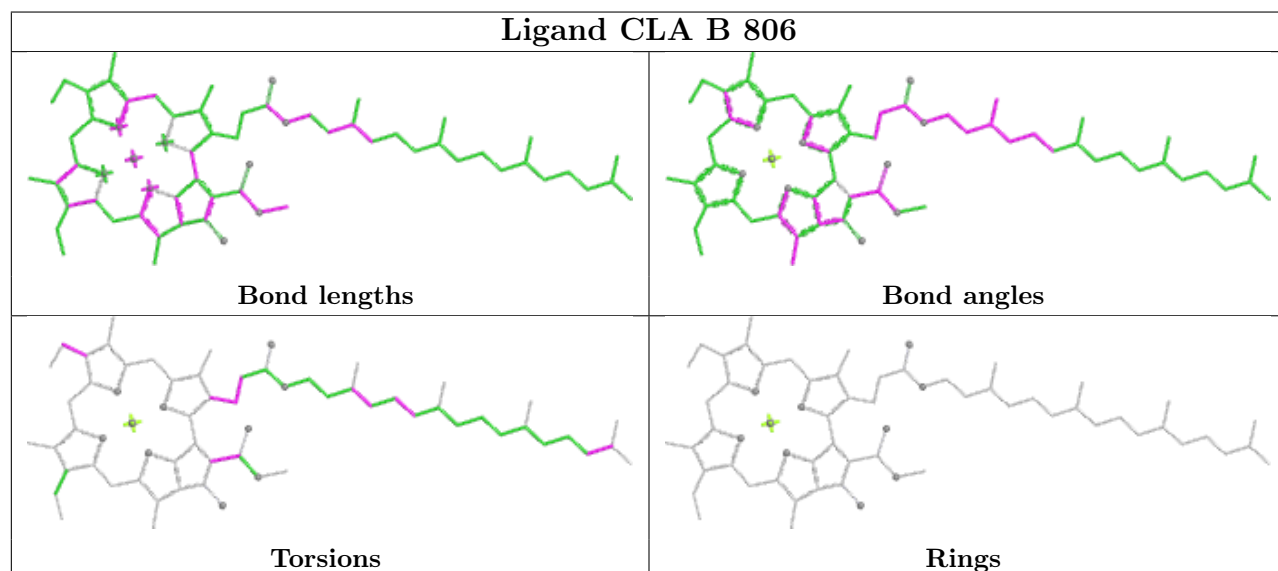
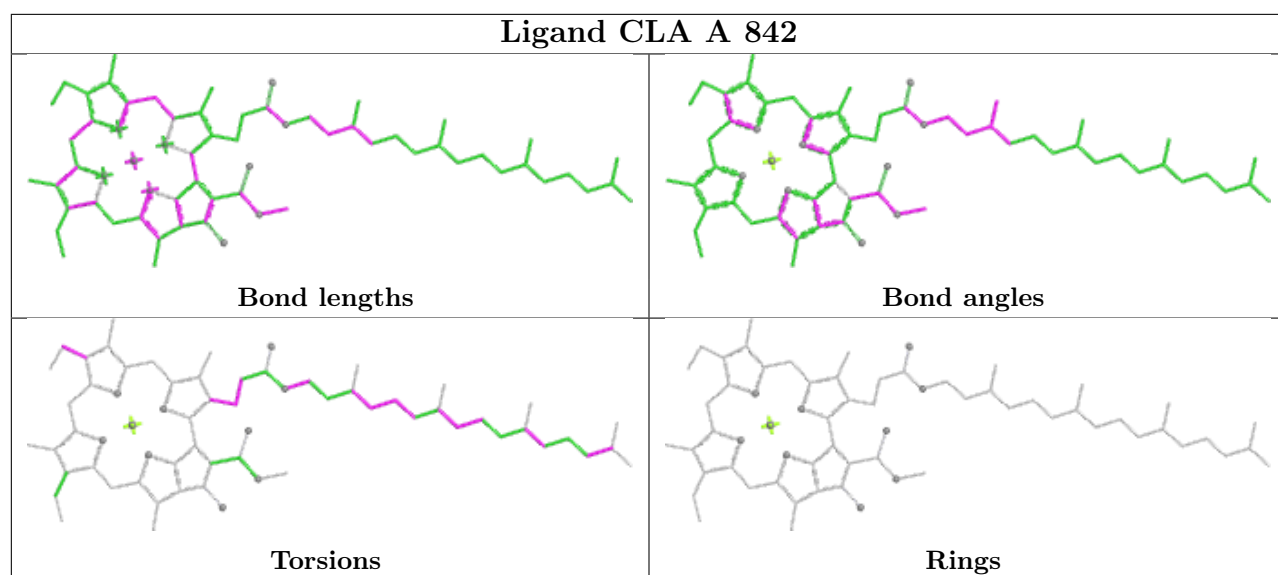
Bond angles



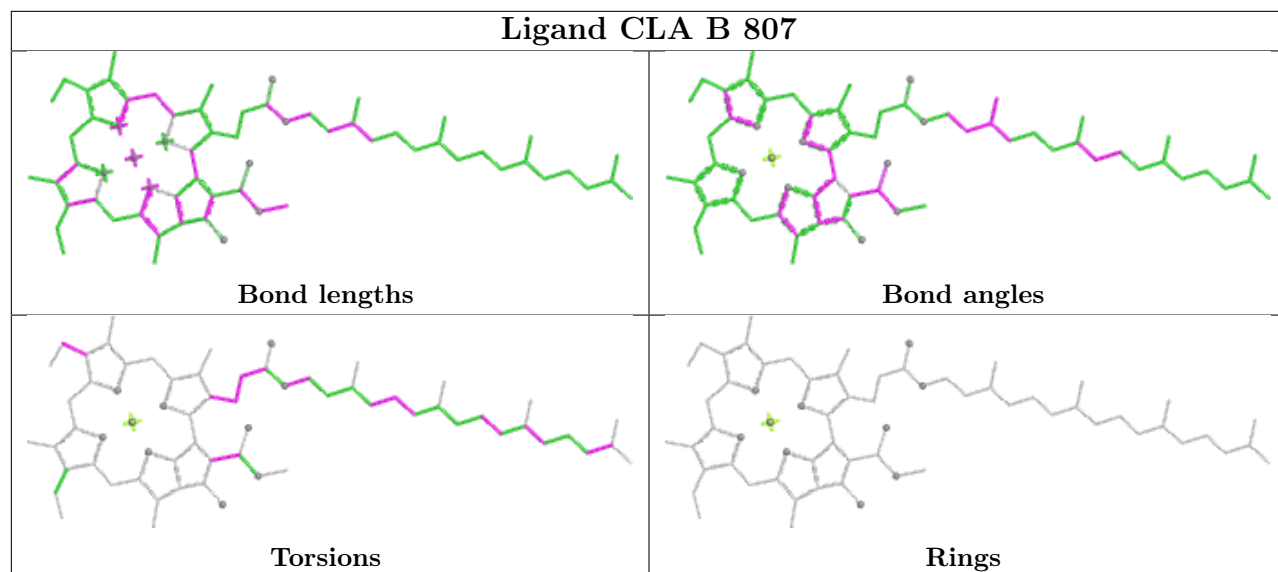
Torsions



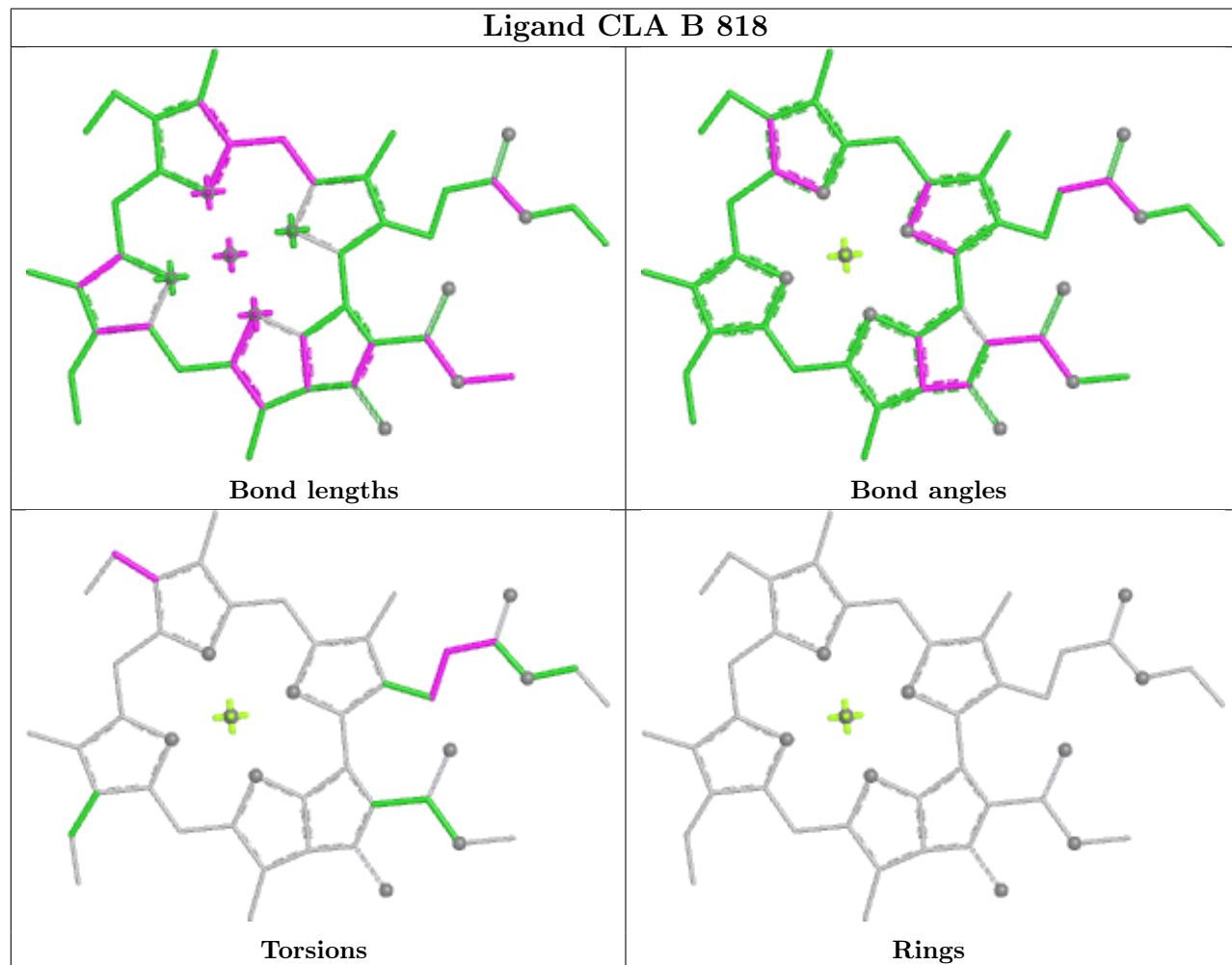
Rings



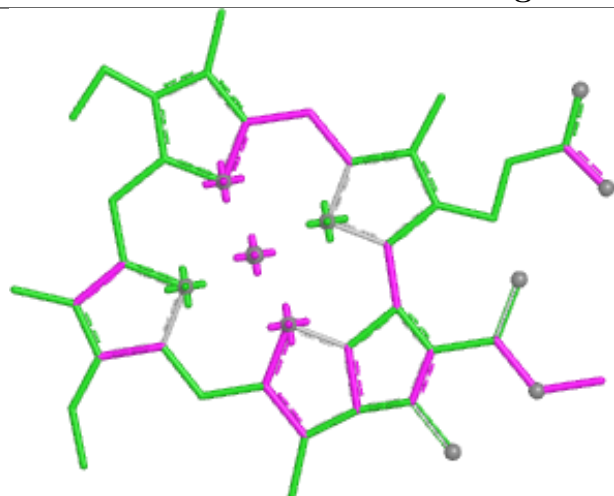
Ligand CLA B 807



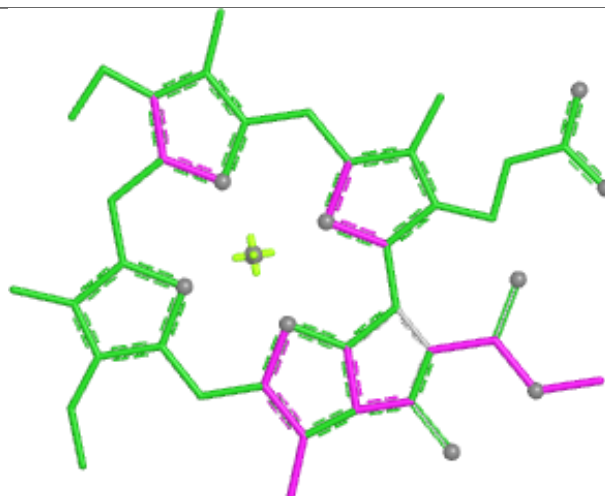
Ligand CLA B 818



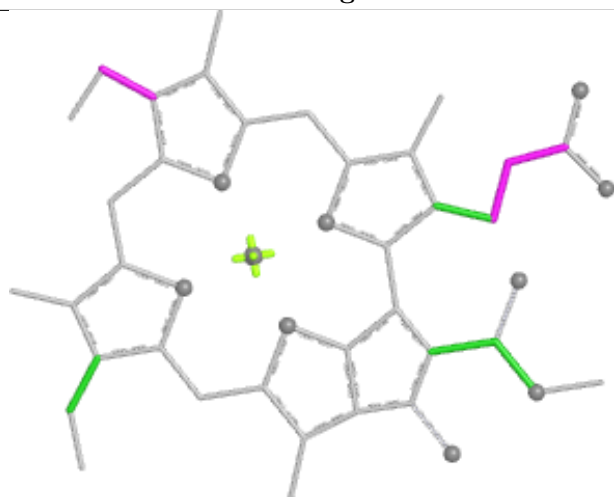
Ligand CLA B 810



Bond lengths



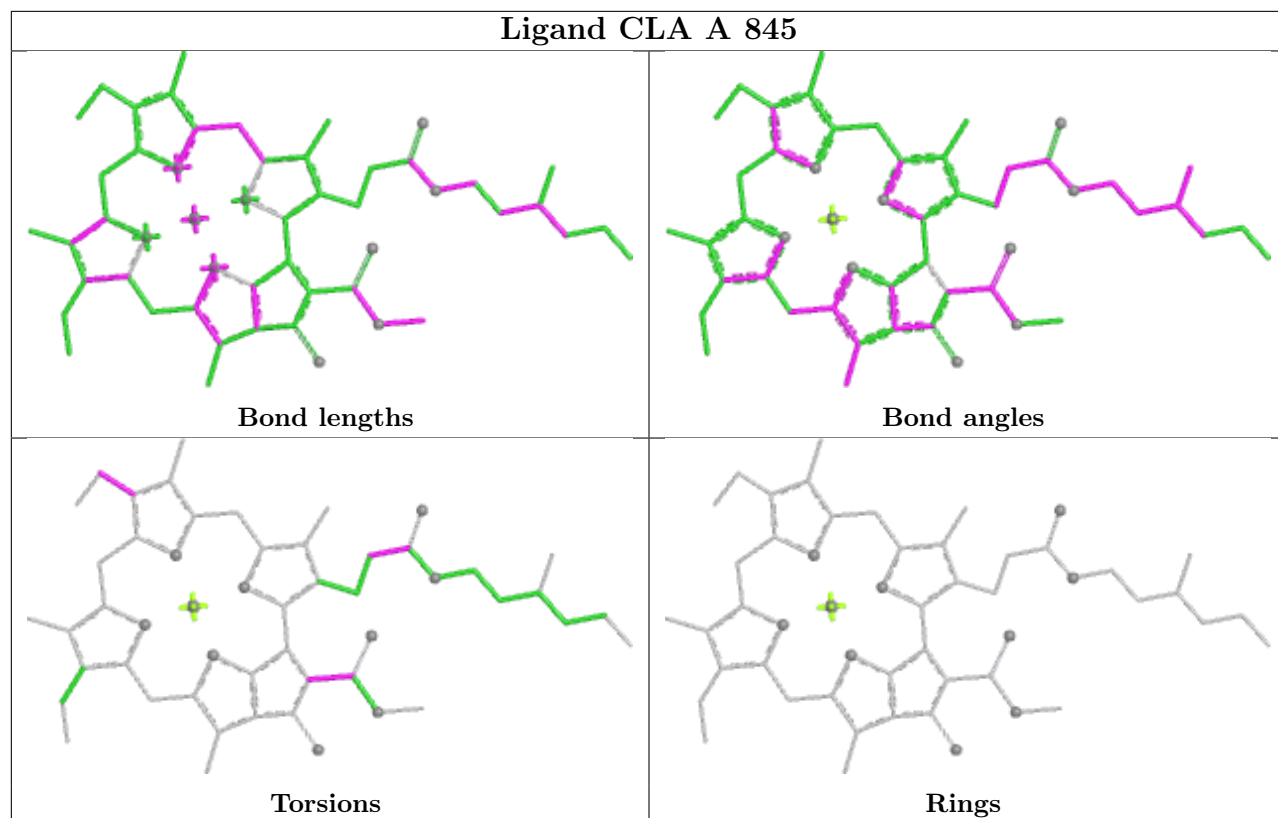
Bond angles



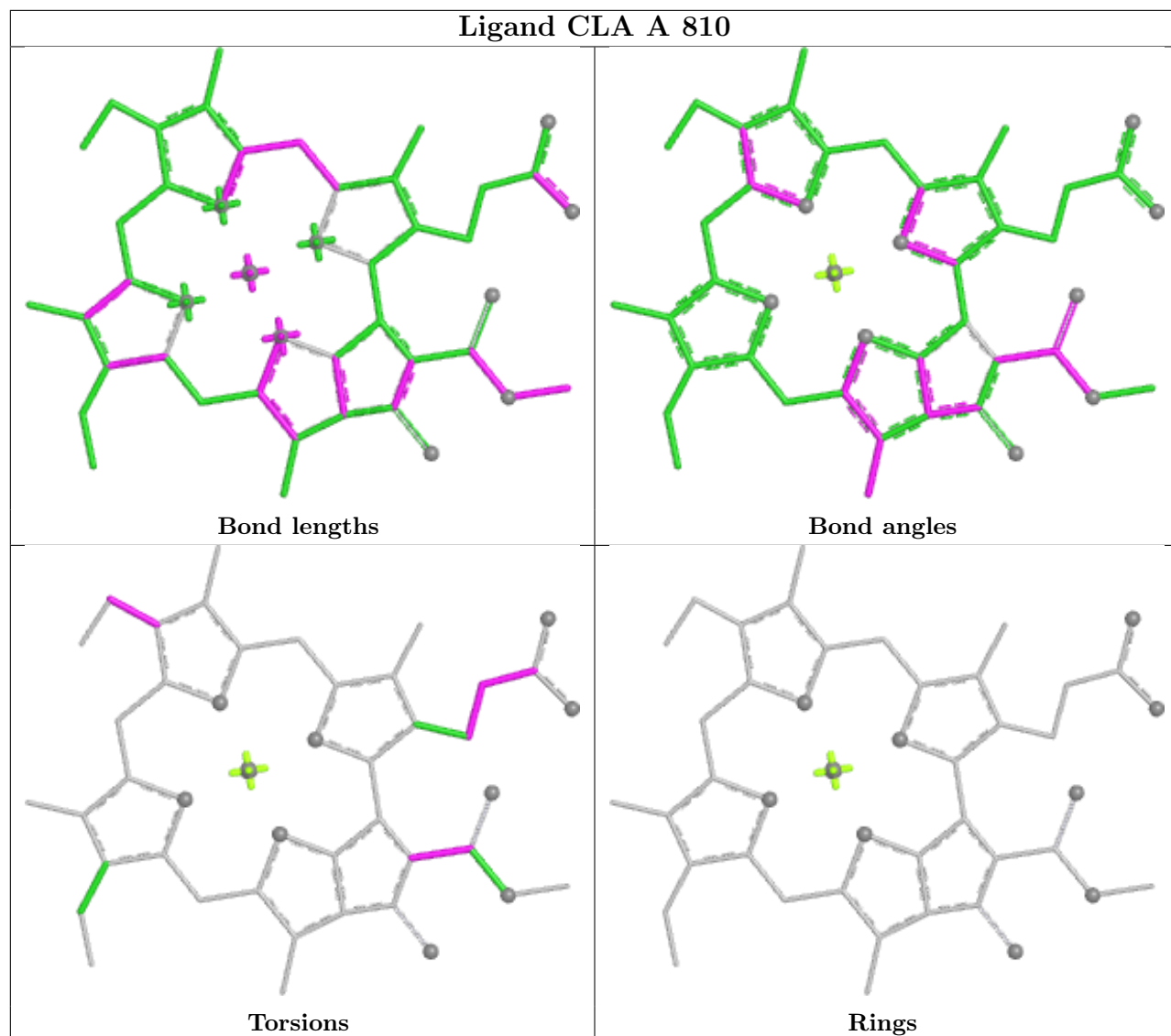
Torsions



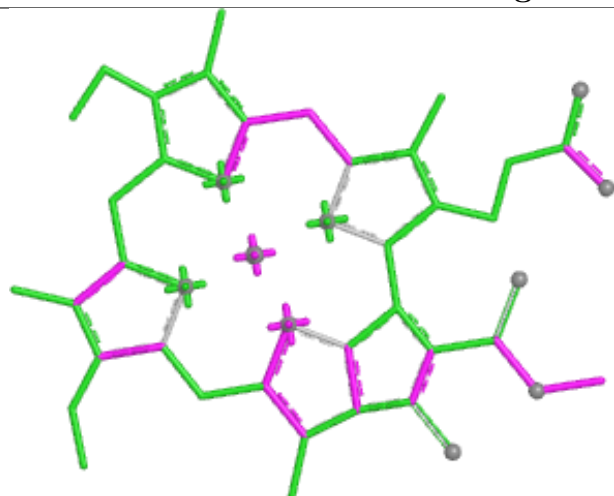
Rings



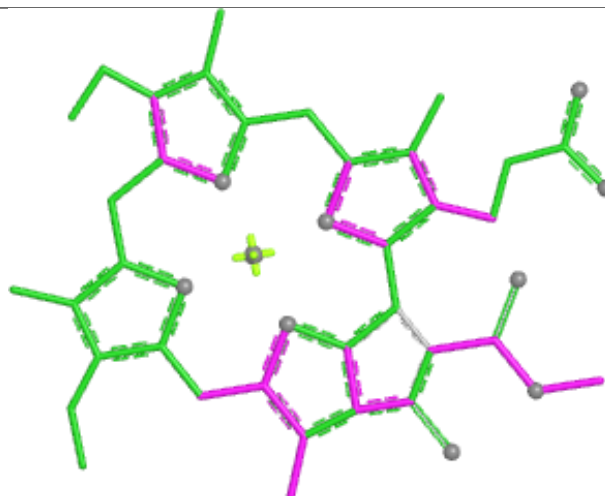
Ligand CLA A 810



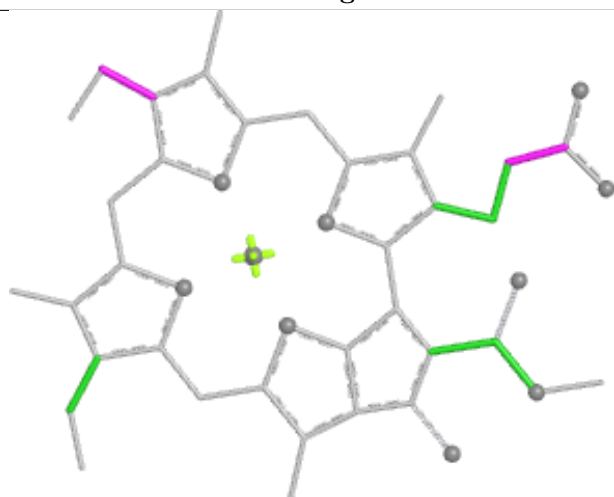
Ligand CLA B 821



Bond lengths



Bond angles

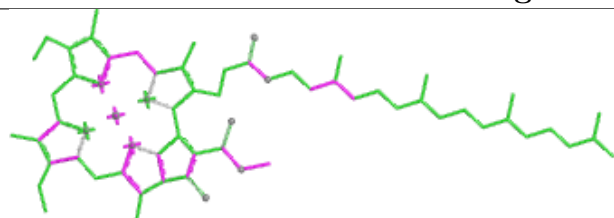


Torsions

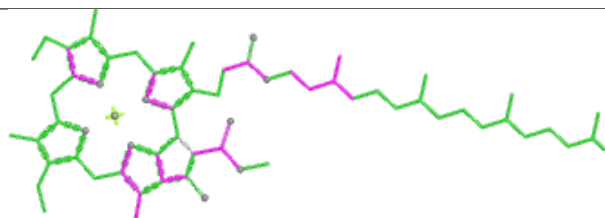


Rings

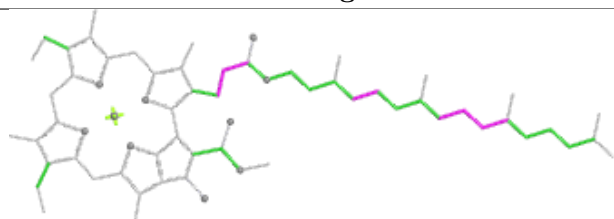
Ligand CLA B 804



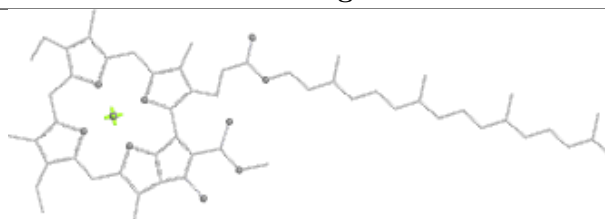
Bond lengths



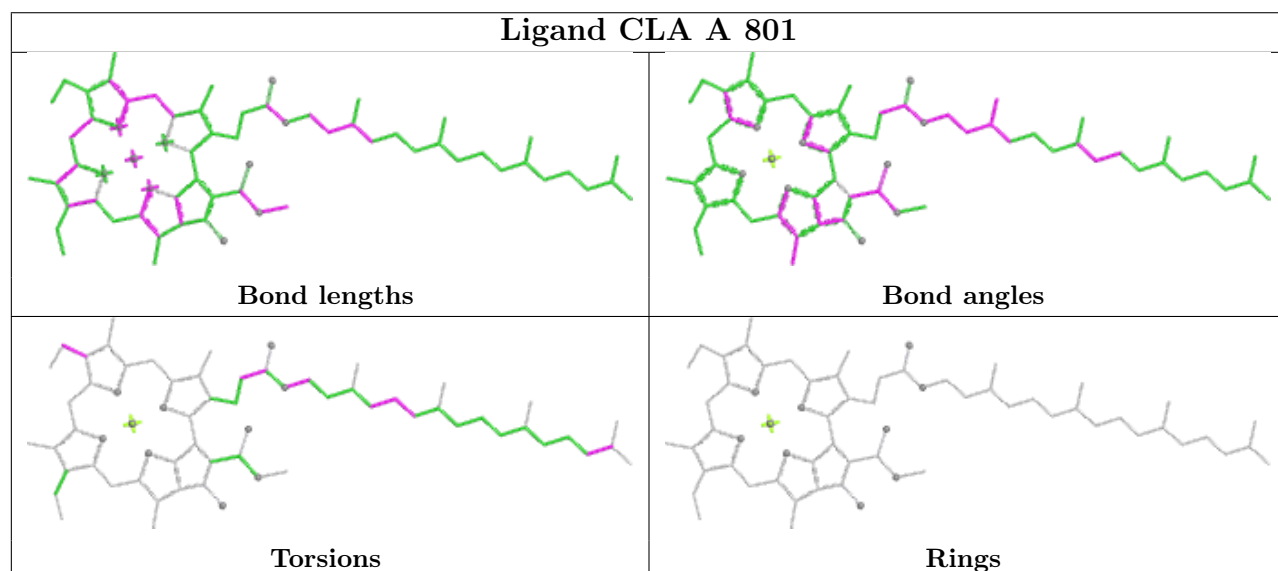
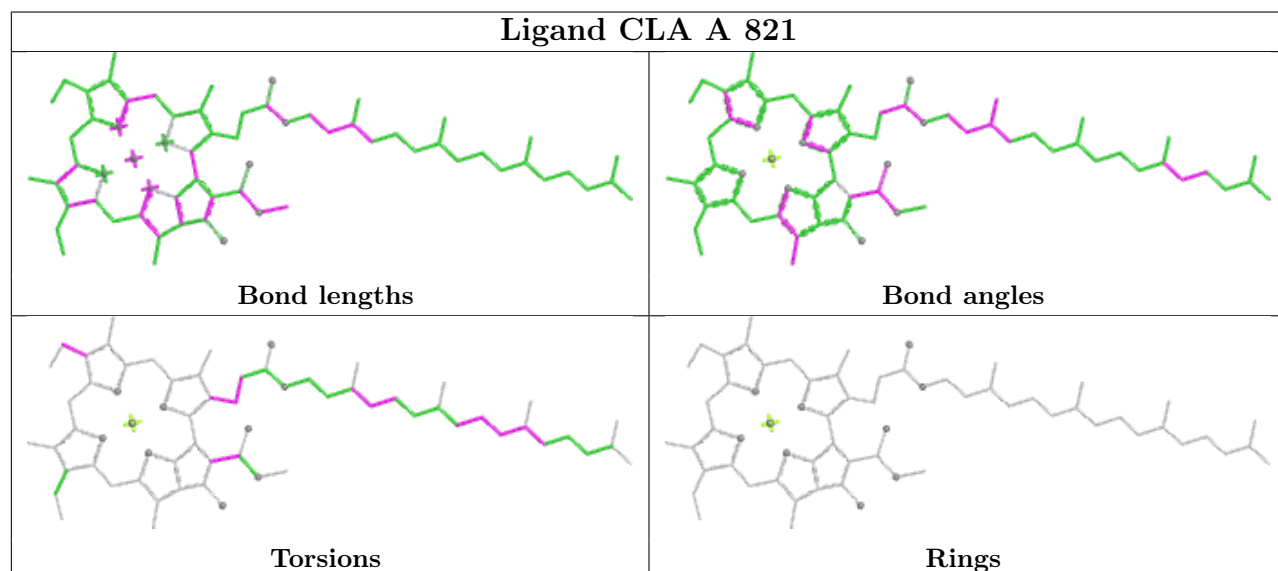
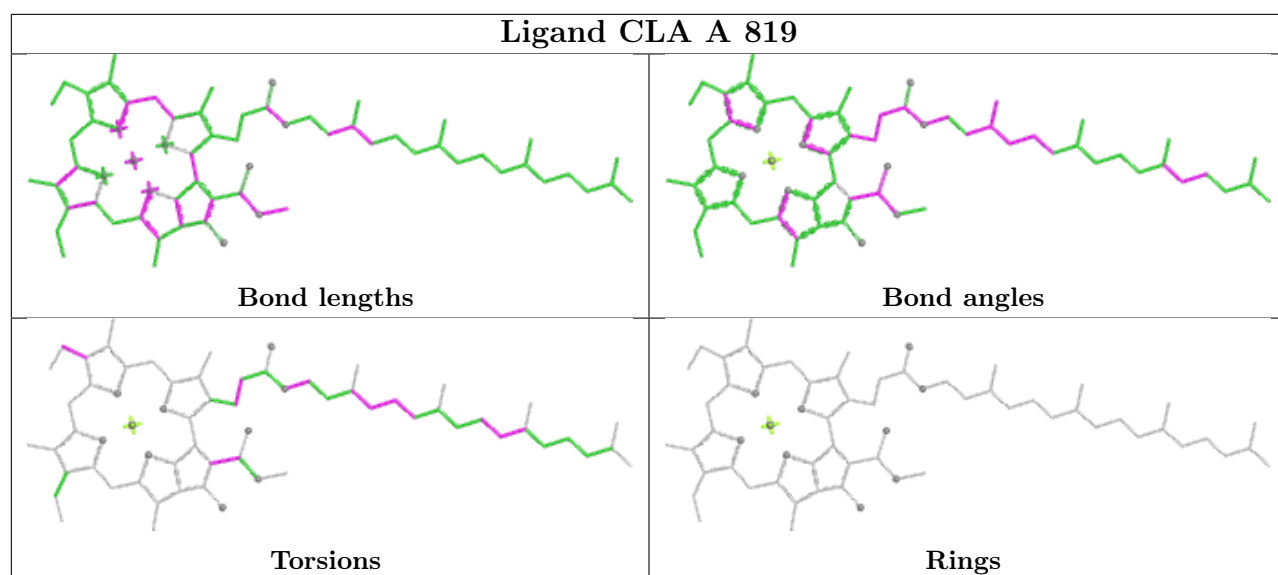
Bond angles

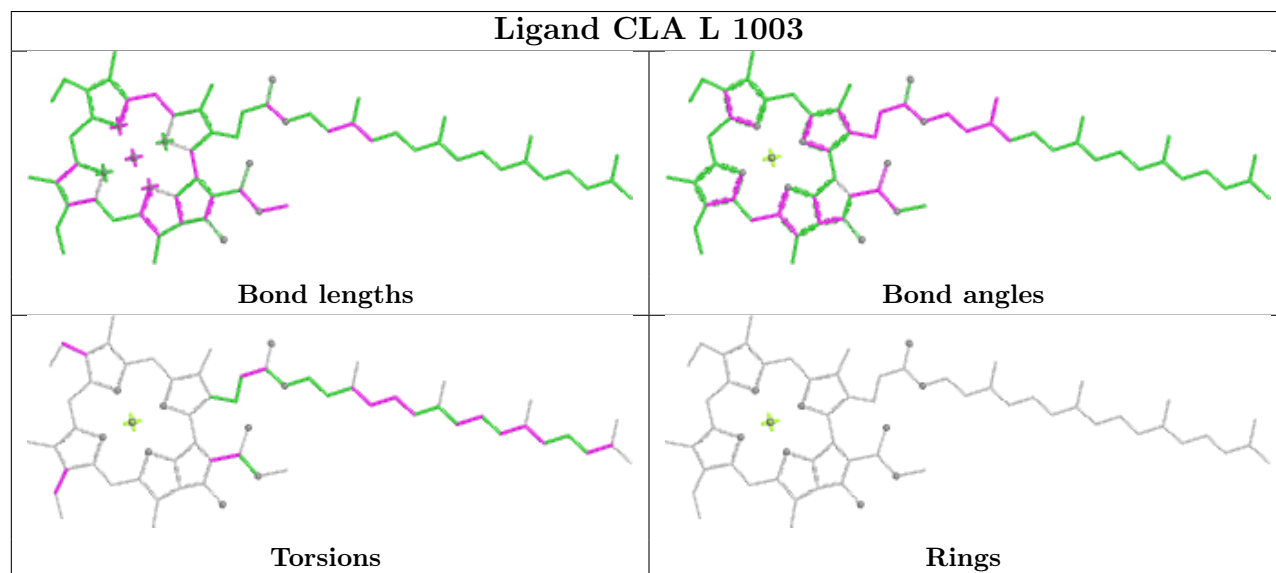
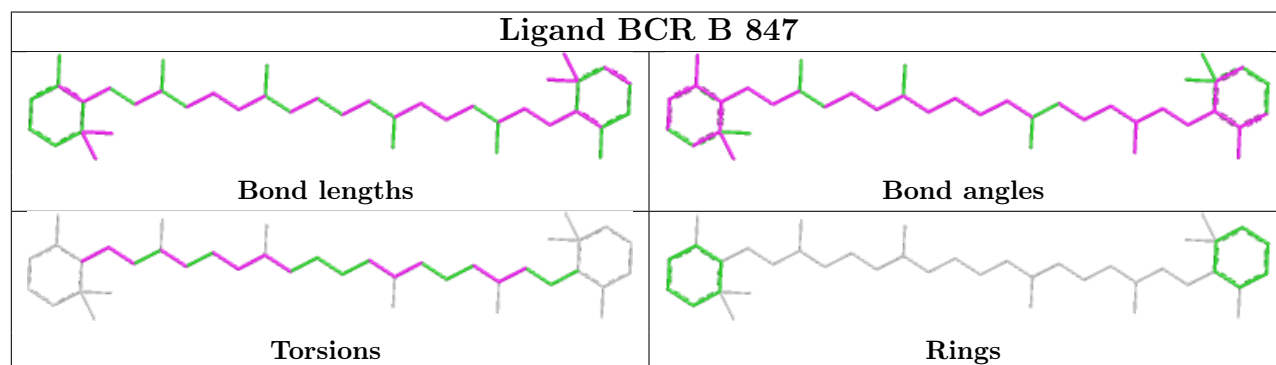
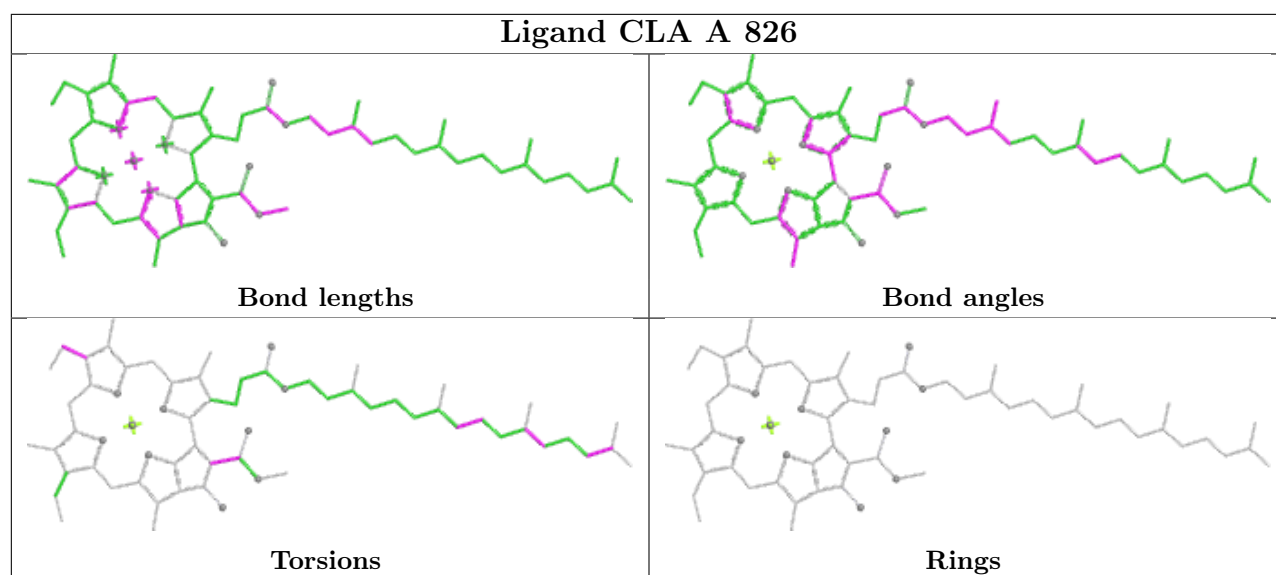


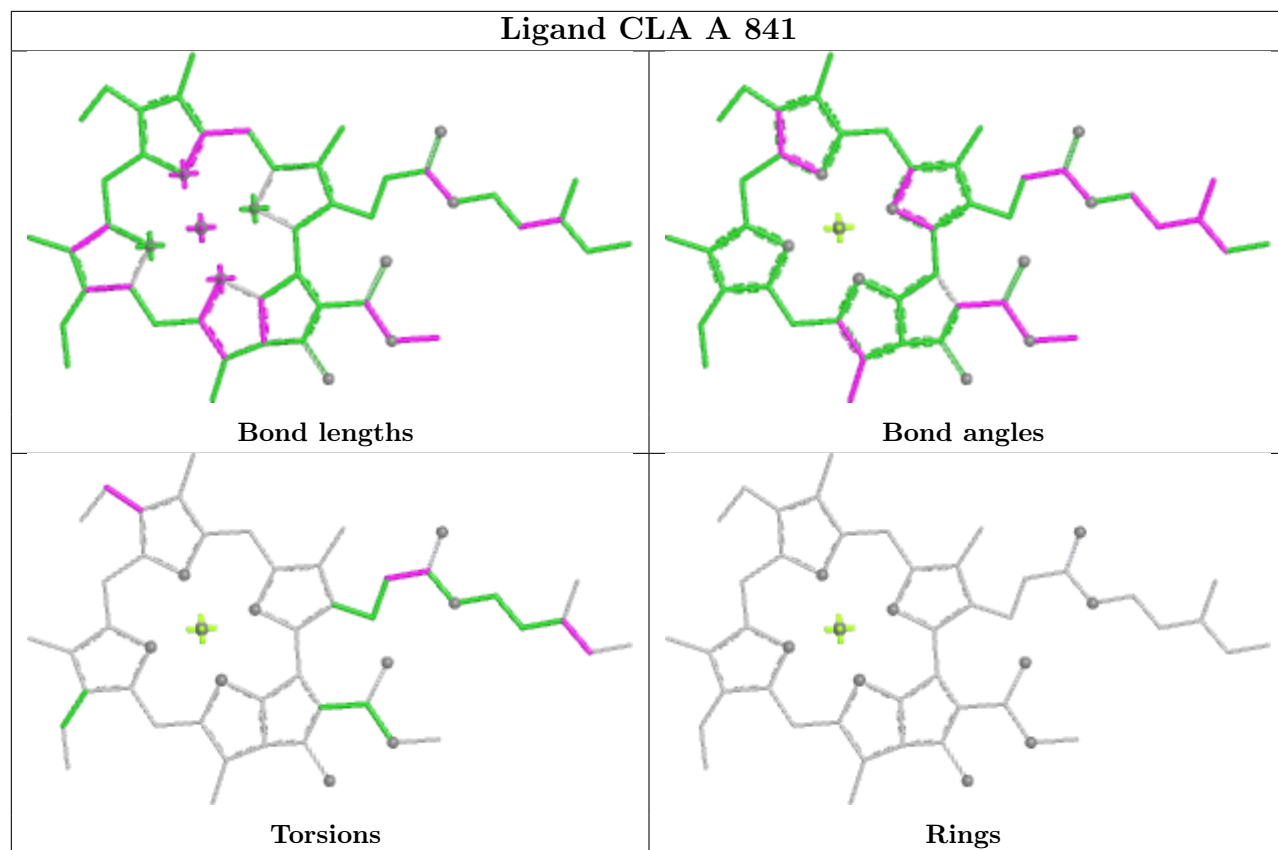
Torsions



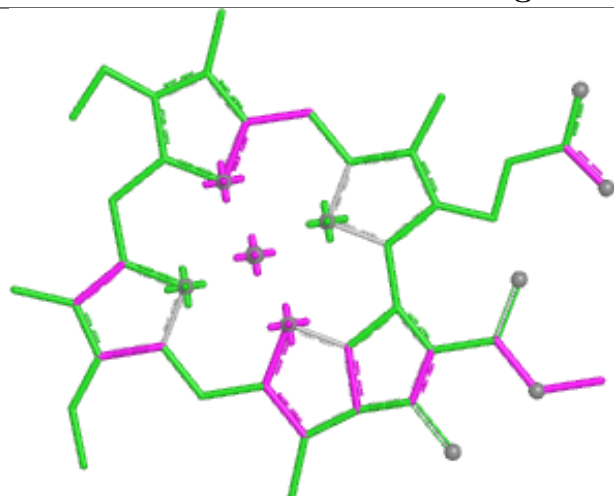
Rings



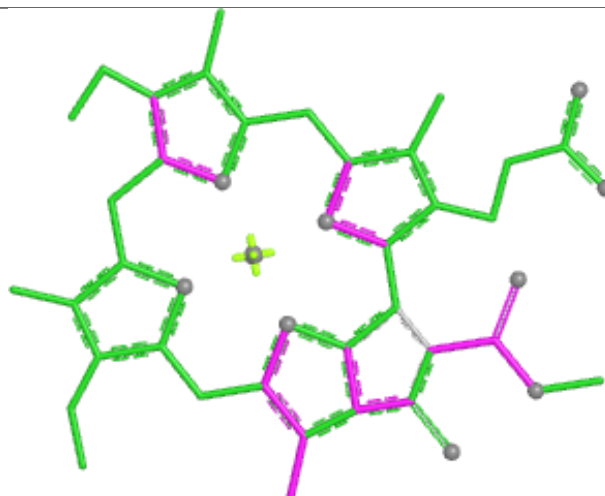




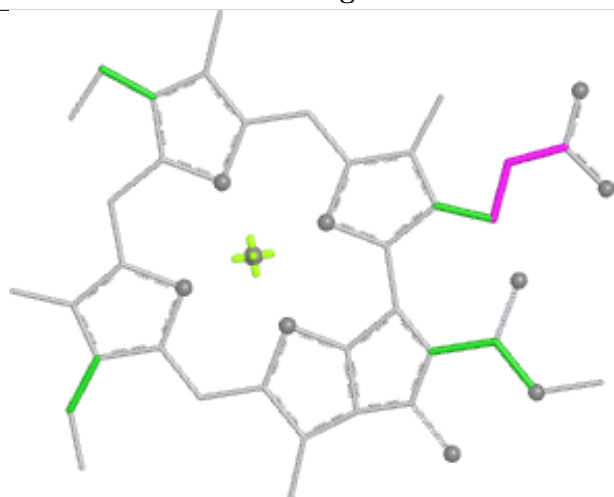
Ligand CLA B 834



Bond lengths



Bond angles

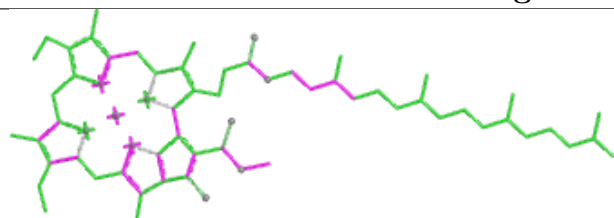


Torsions

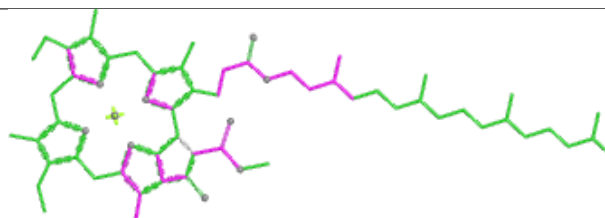


Rings

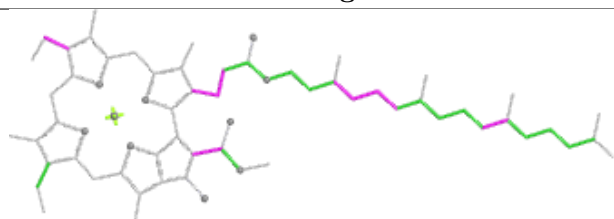
Ligand CLA A 840



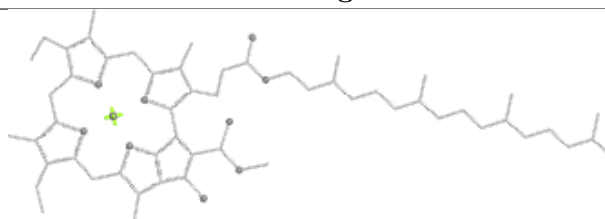
Bond lengths



Bond angles

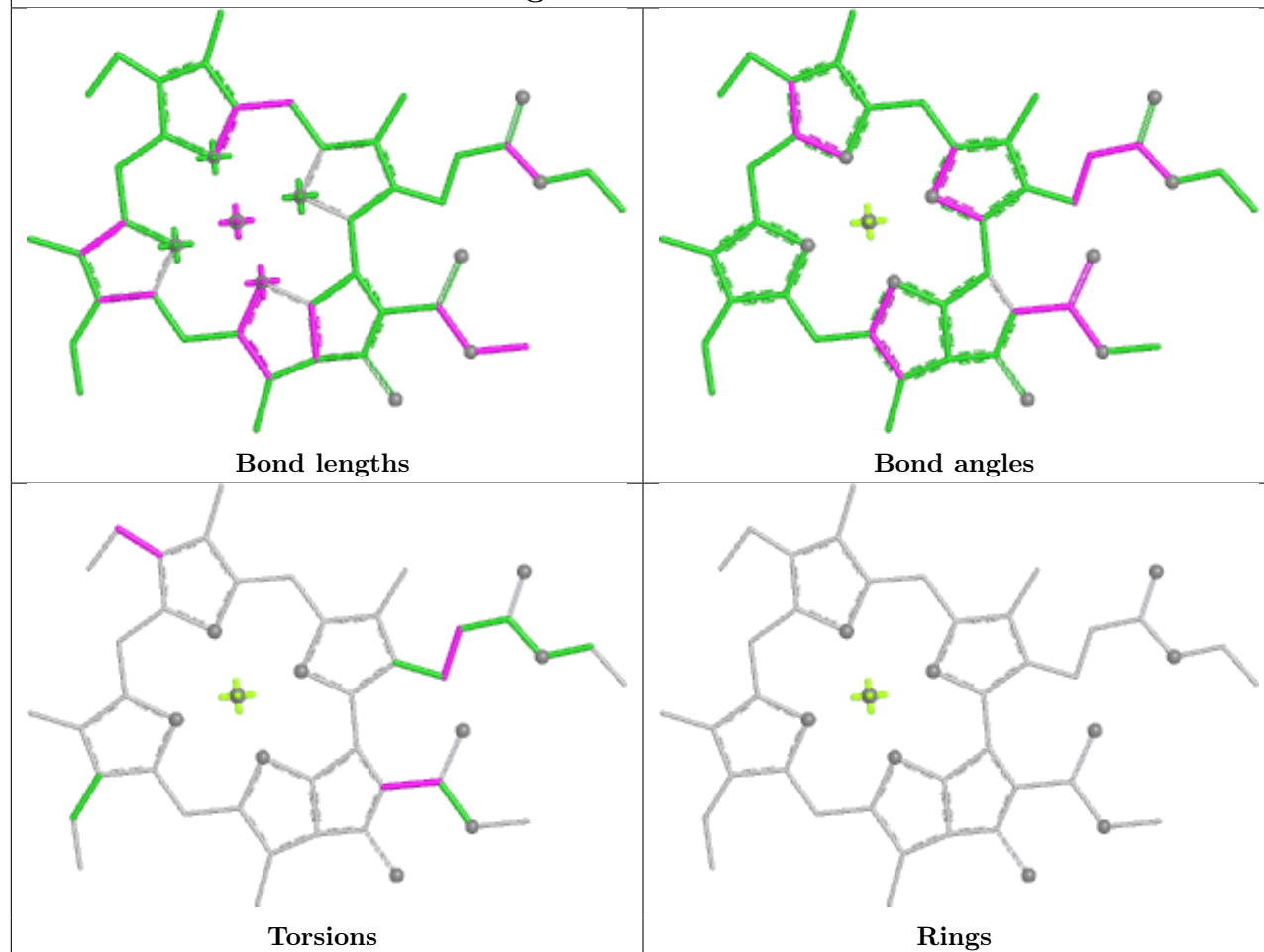


Torsions

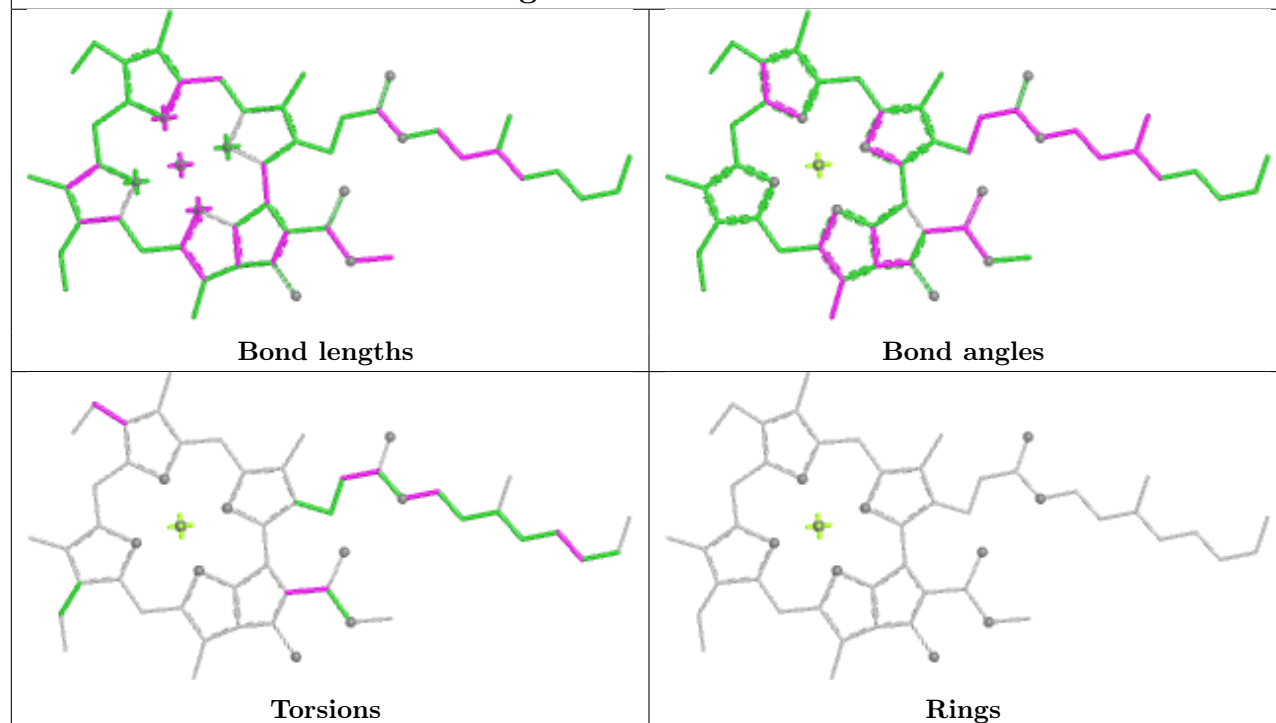


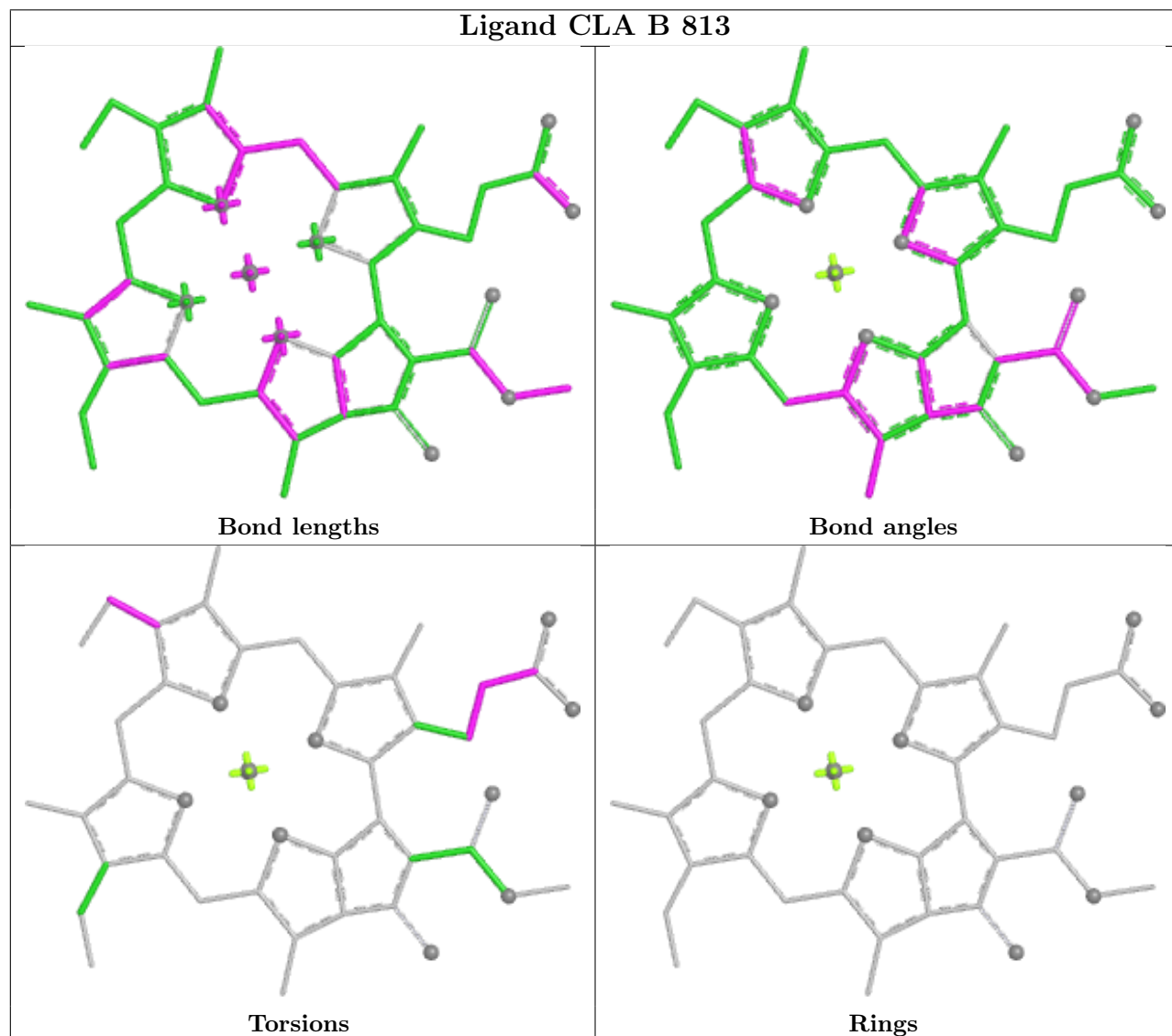
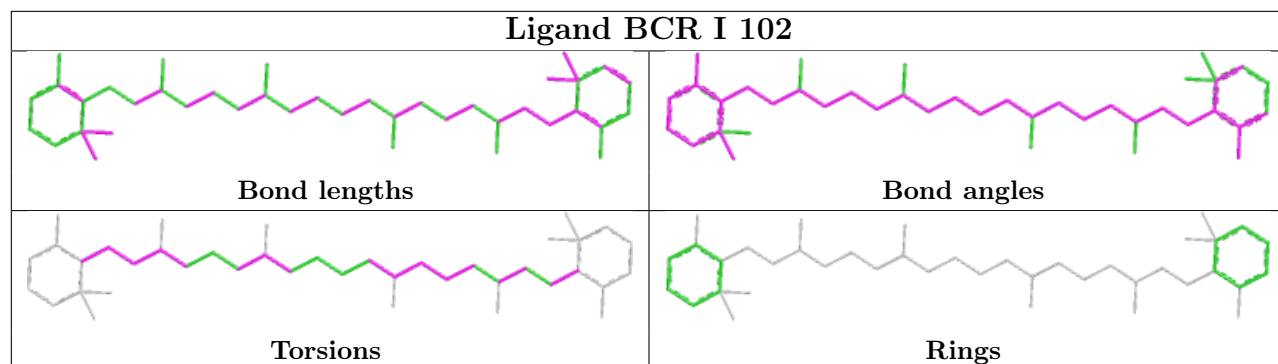
Rings

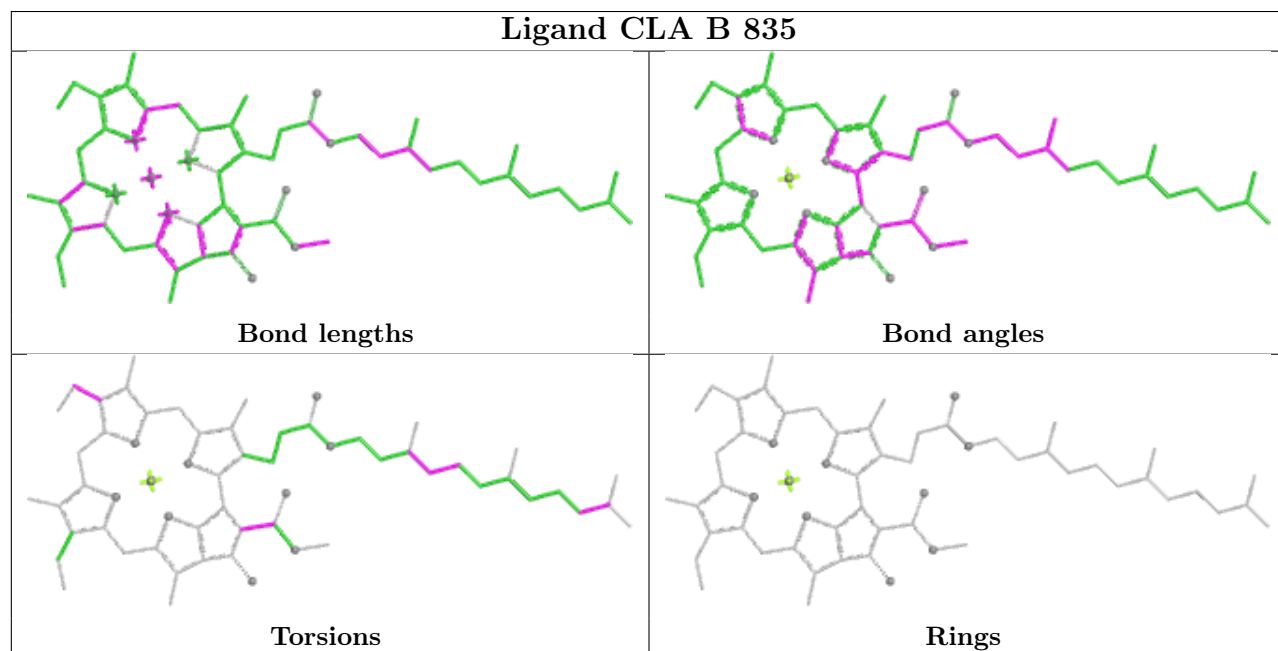
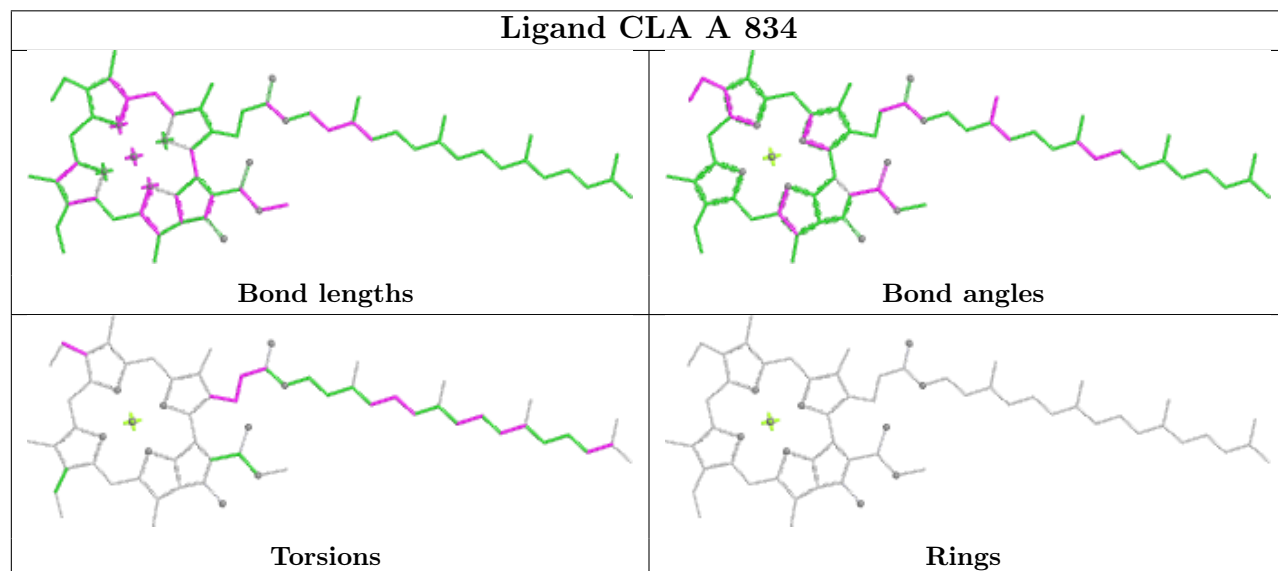
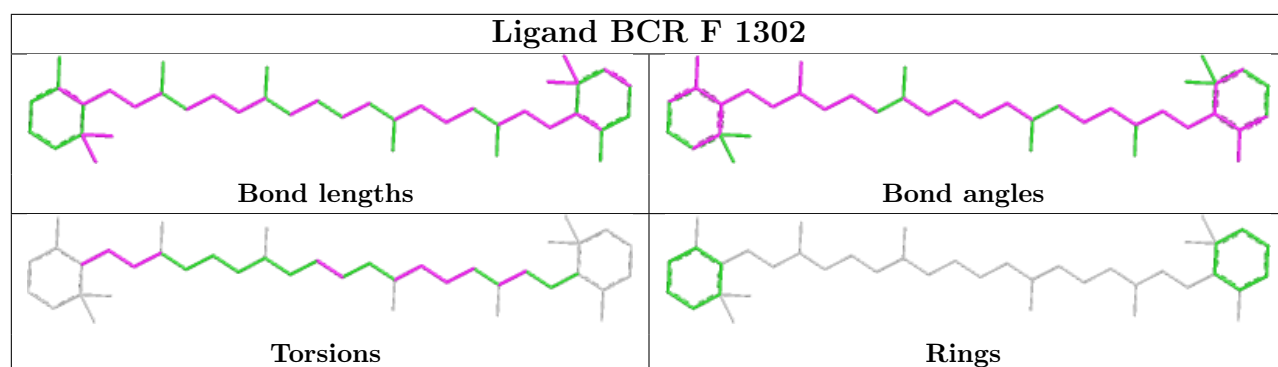
Ligand CLA A 839



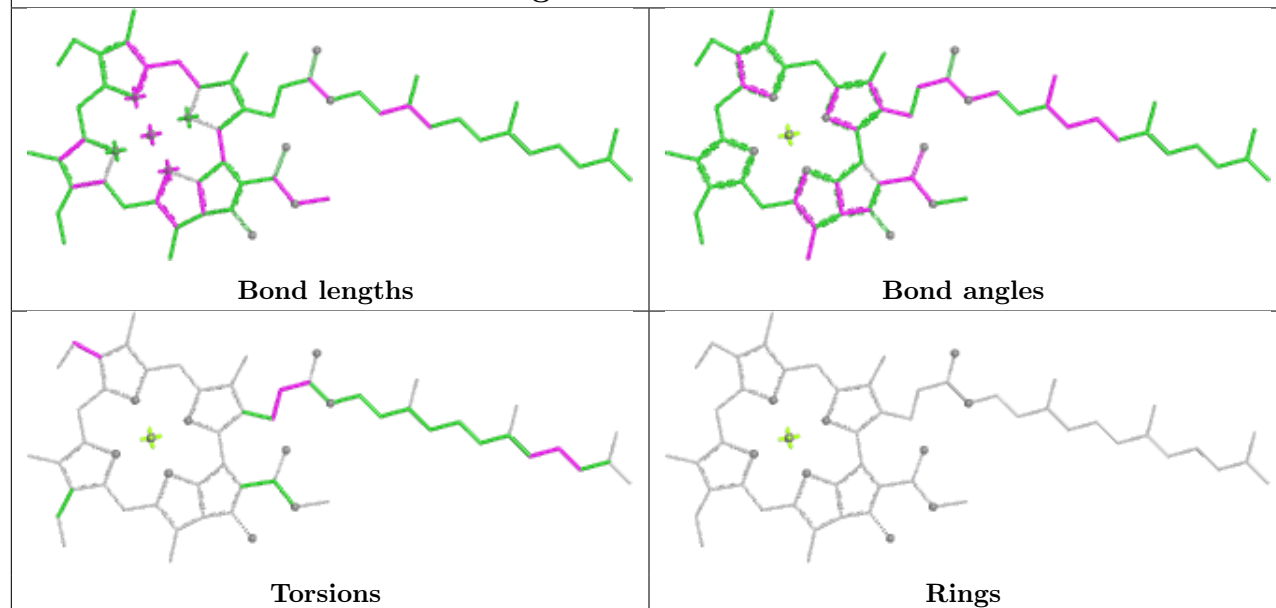
Ligand CLA M 1201



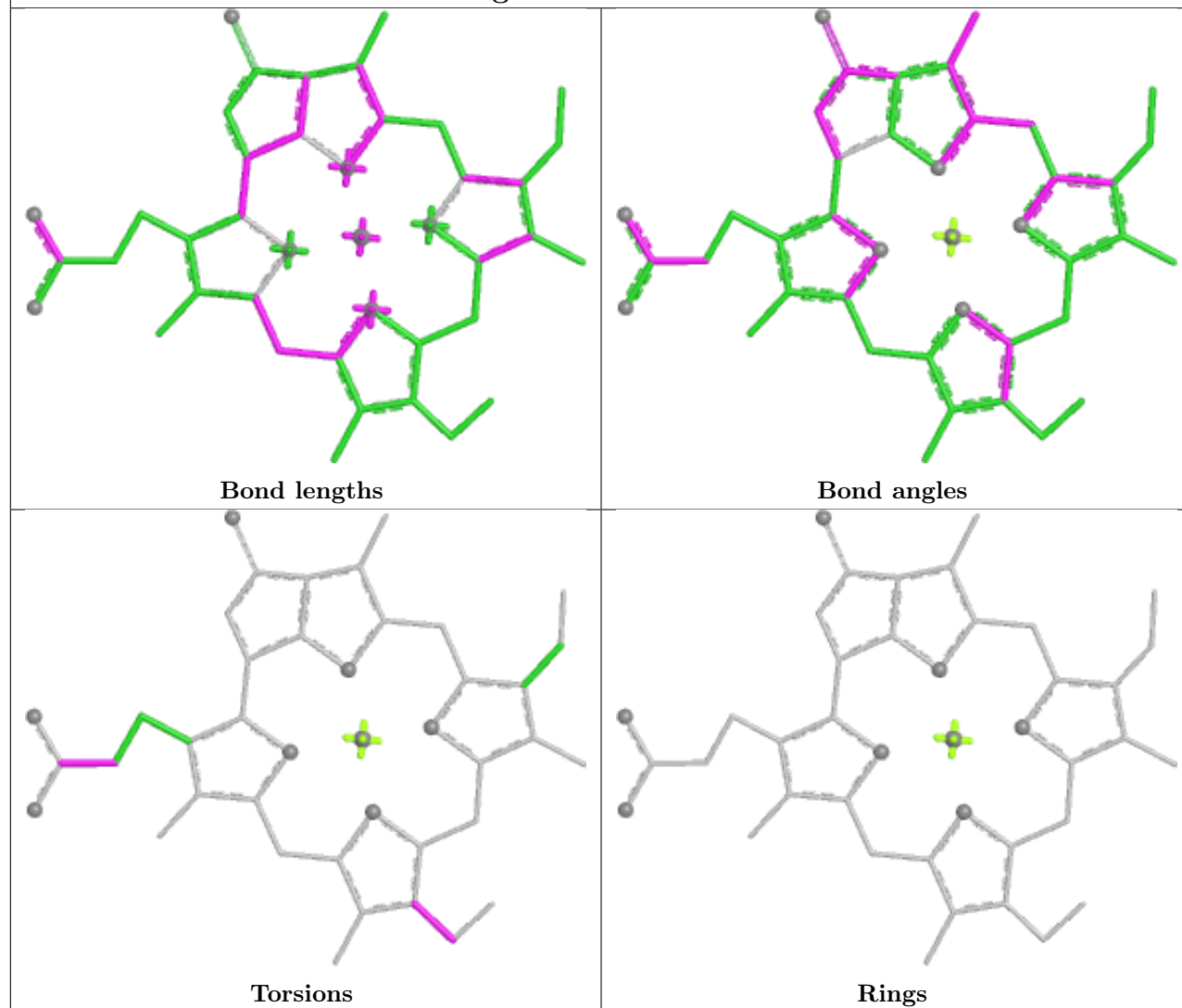


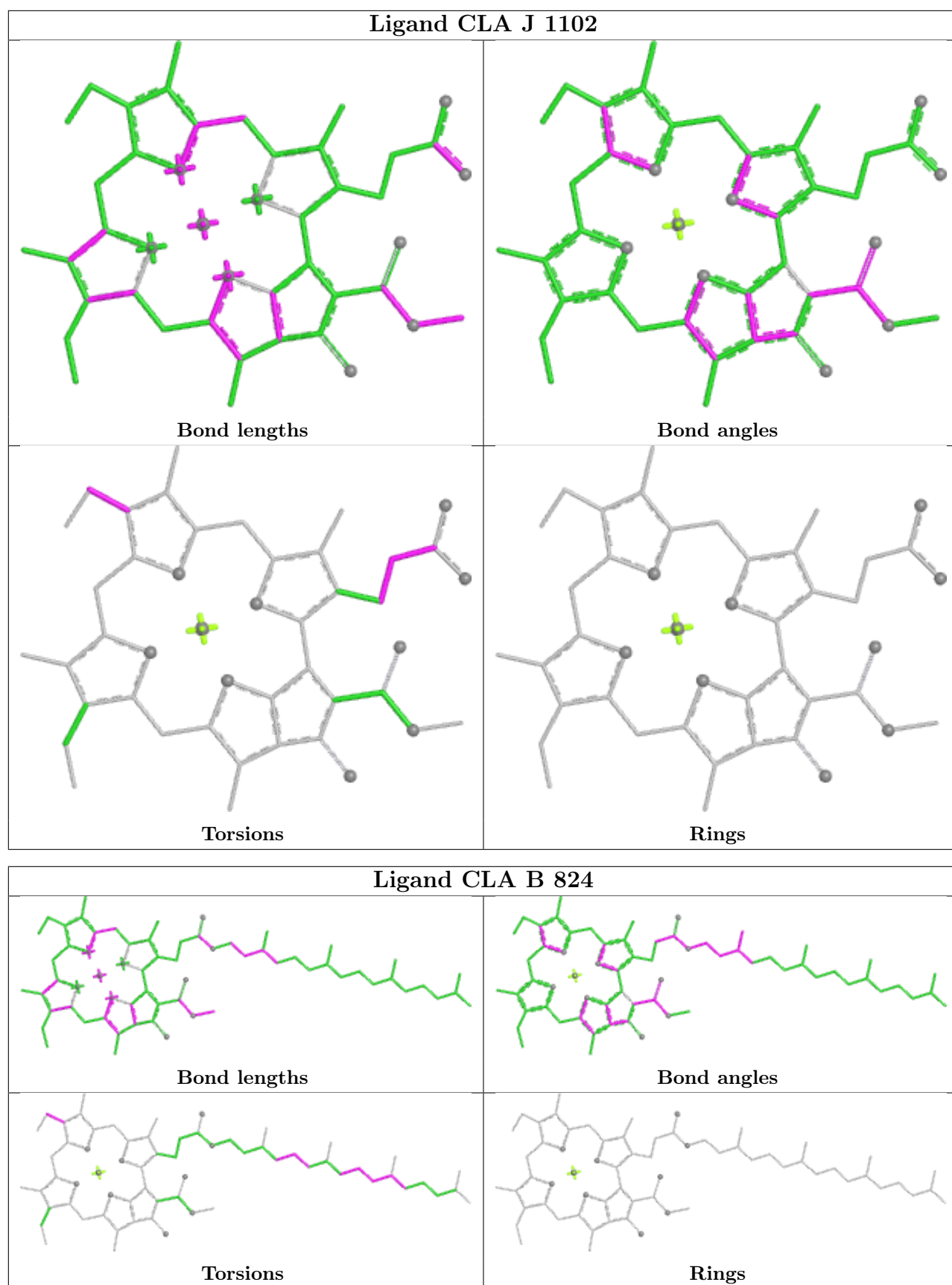


Ligand CLA B 816

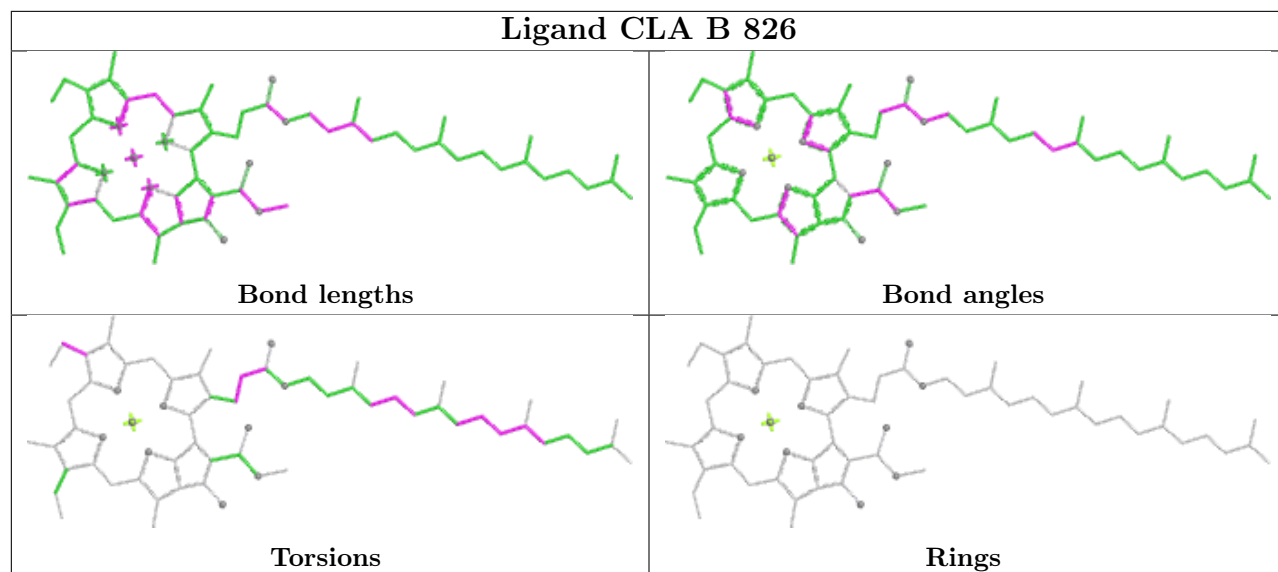


Ligand CLA A 844

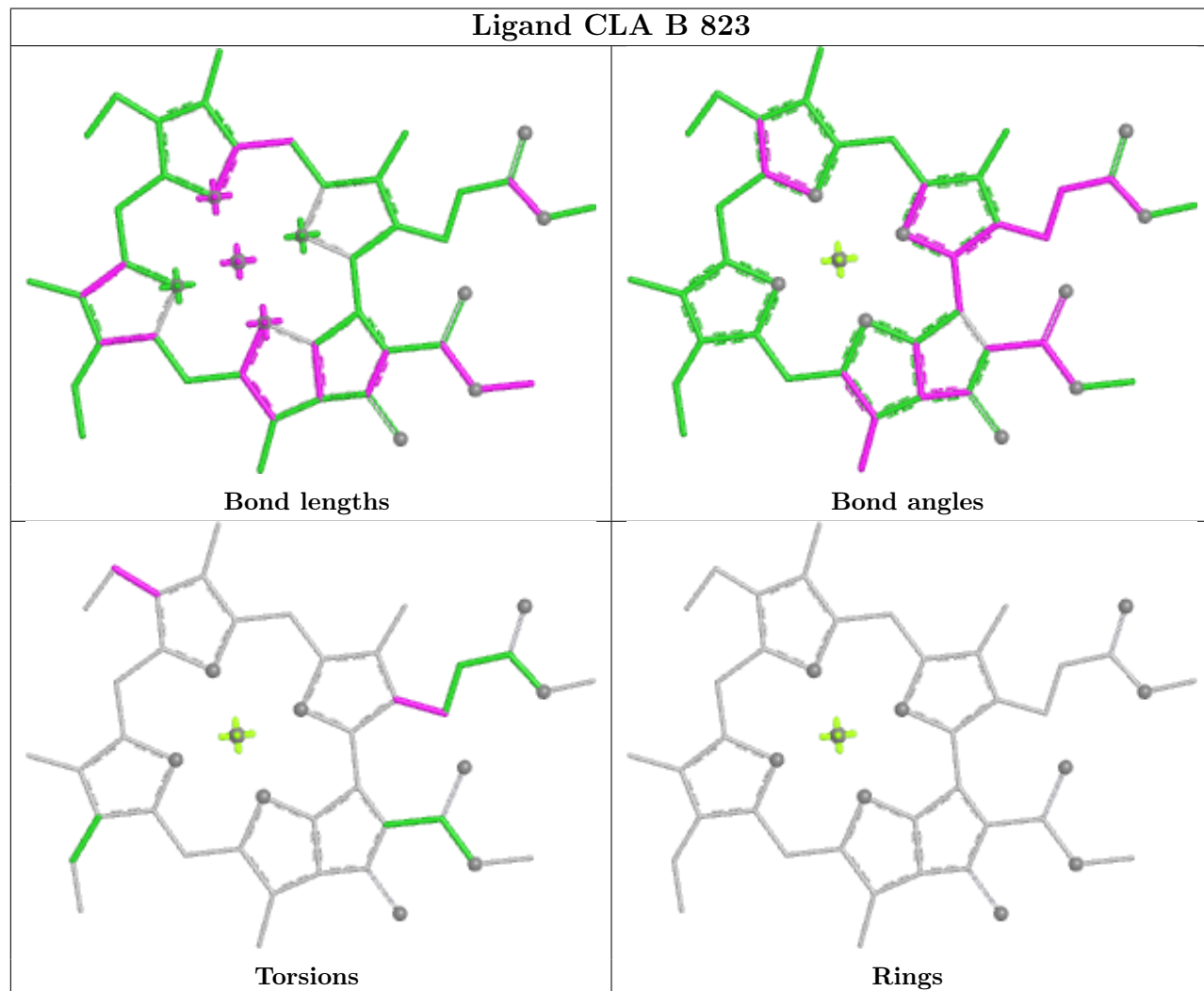


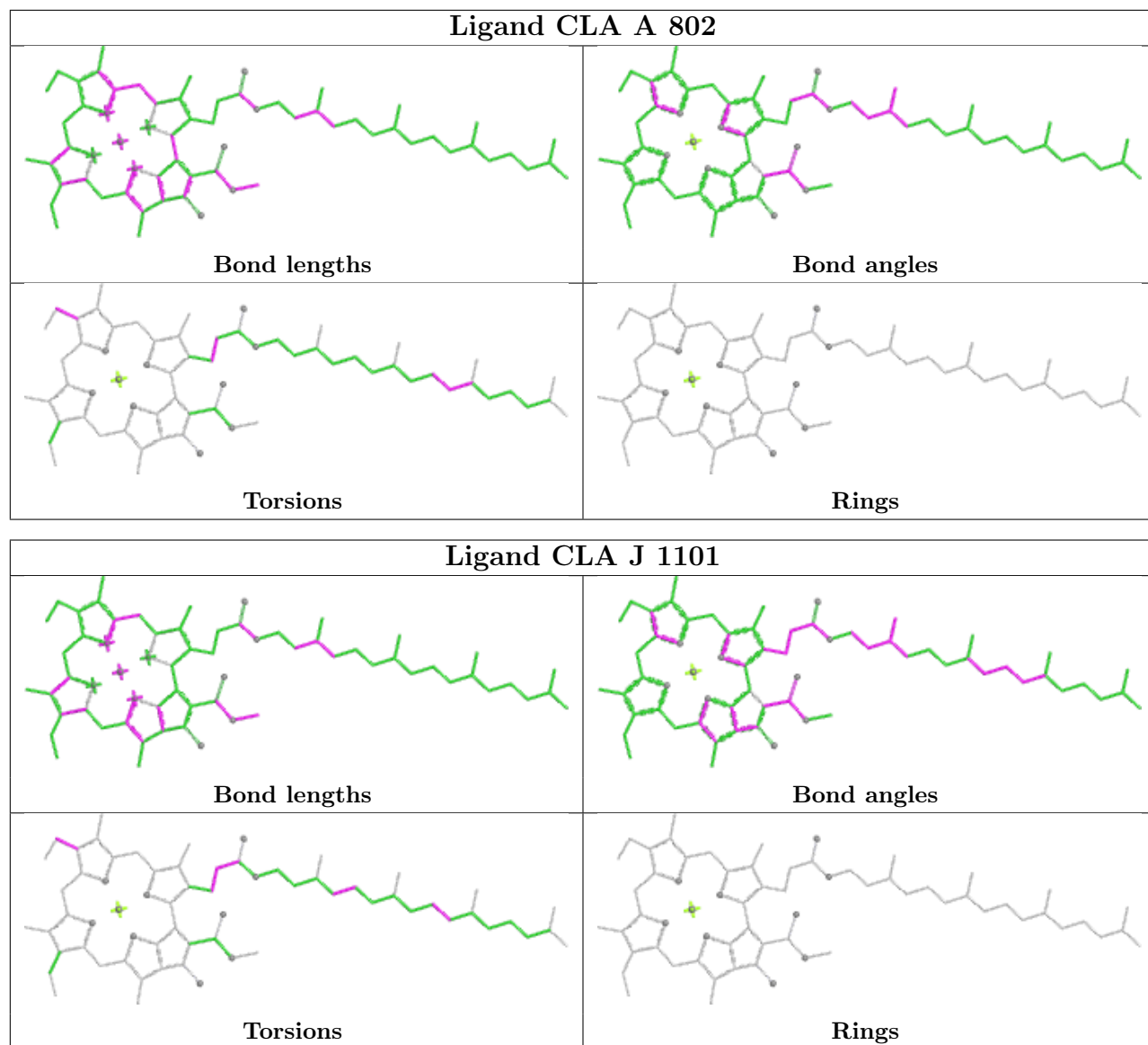


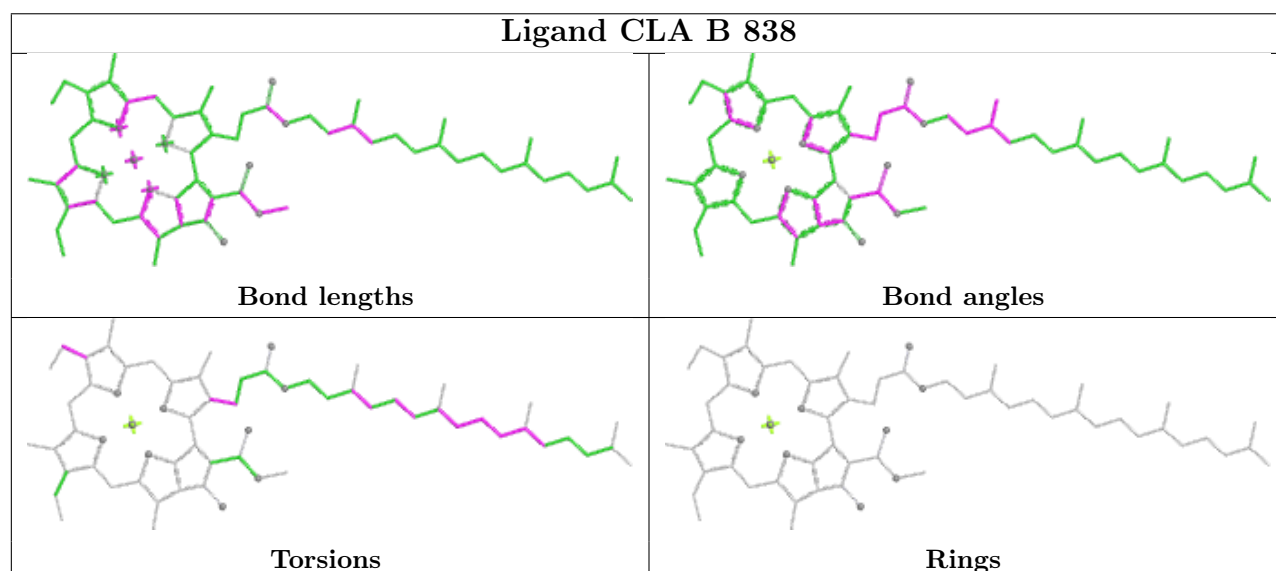
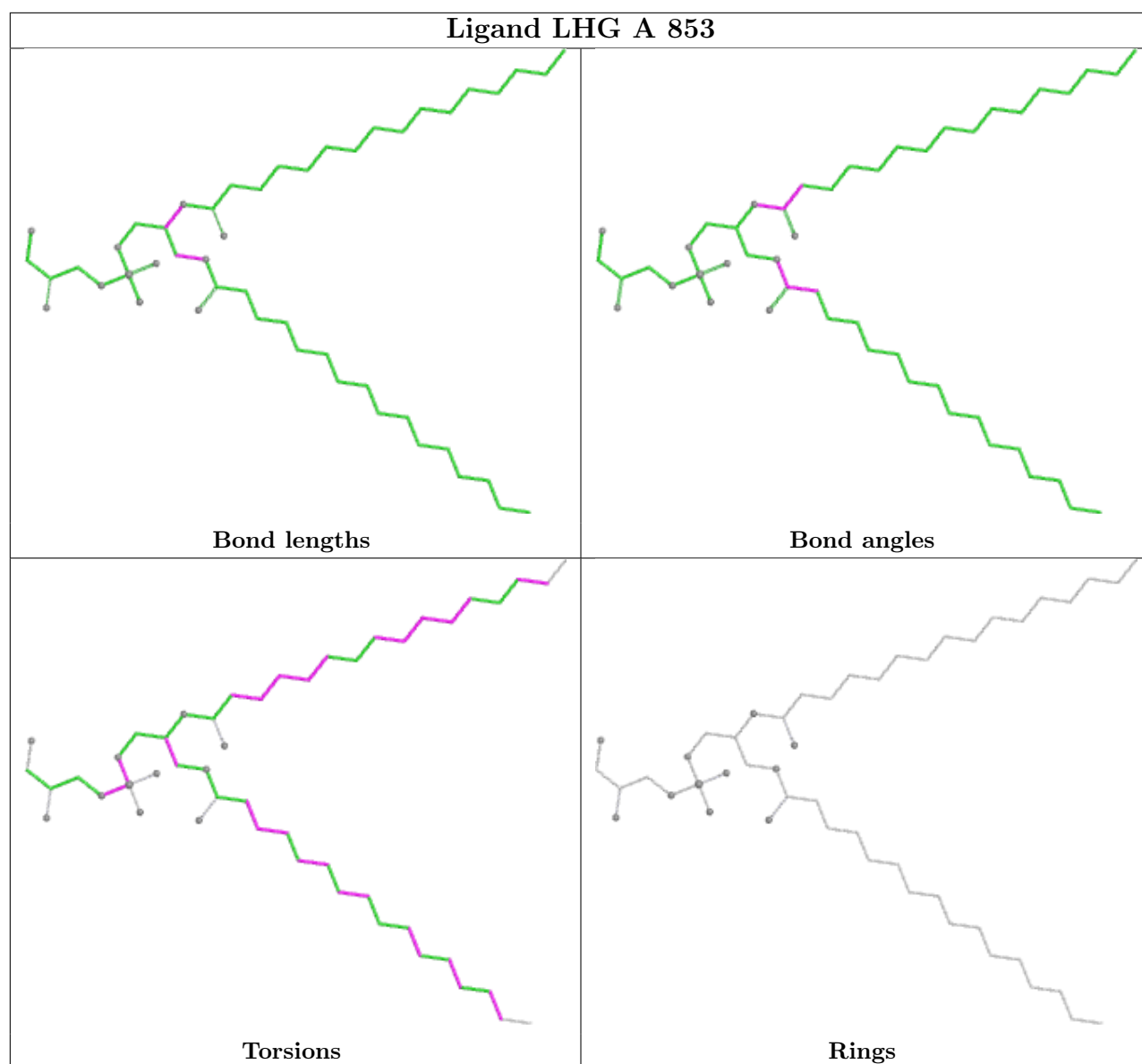
Ligand CLA B 826



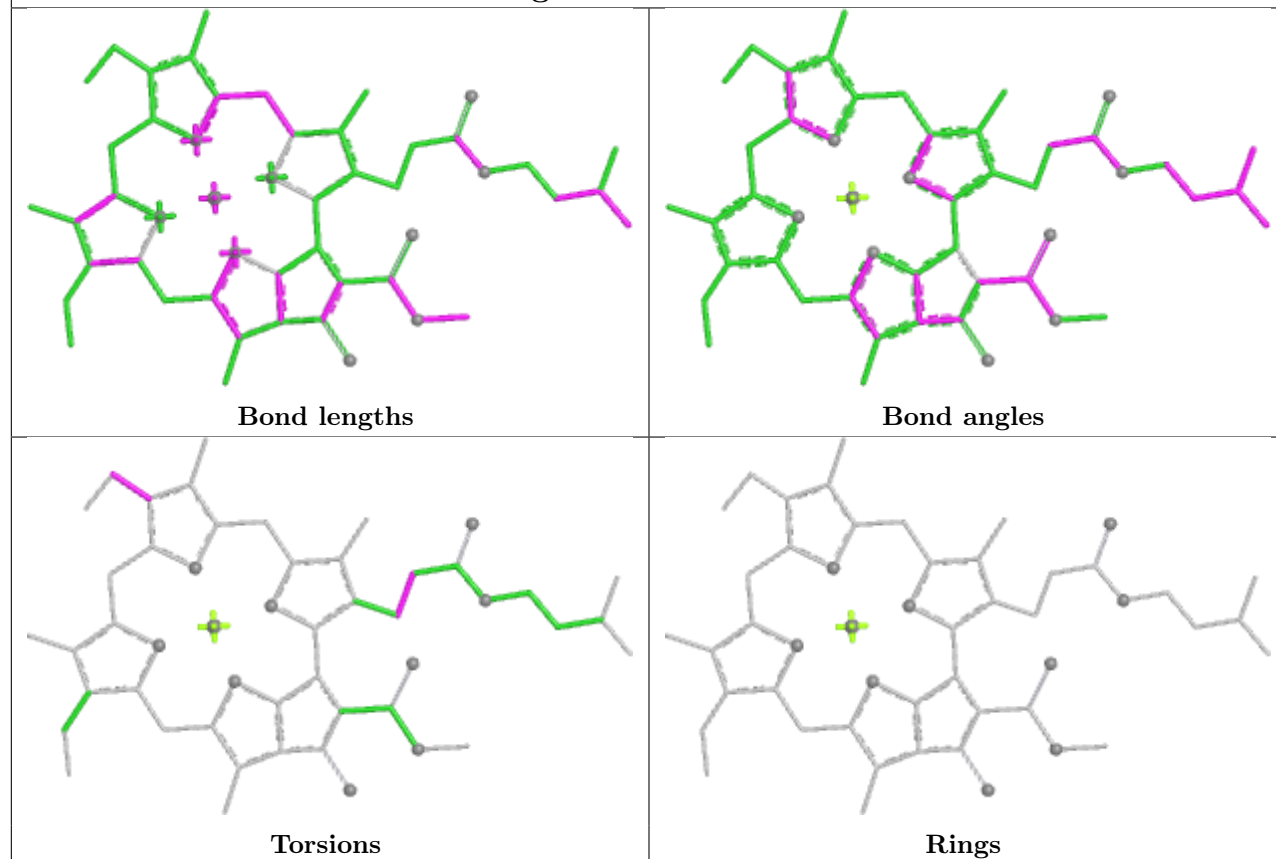
Ligand CLA B 823



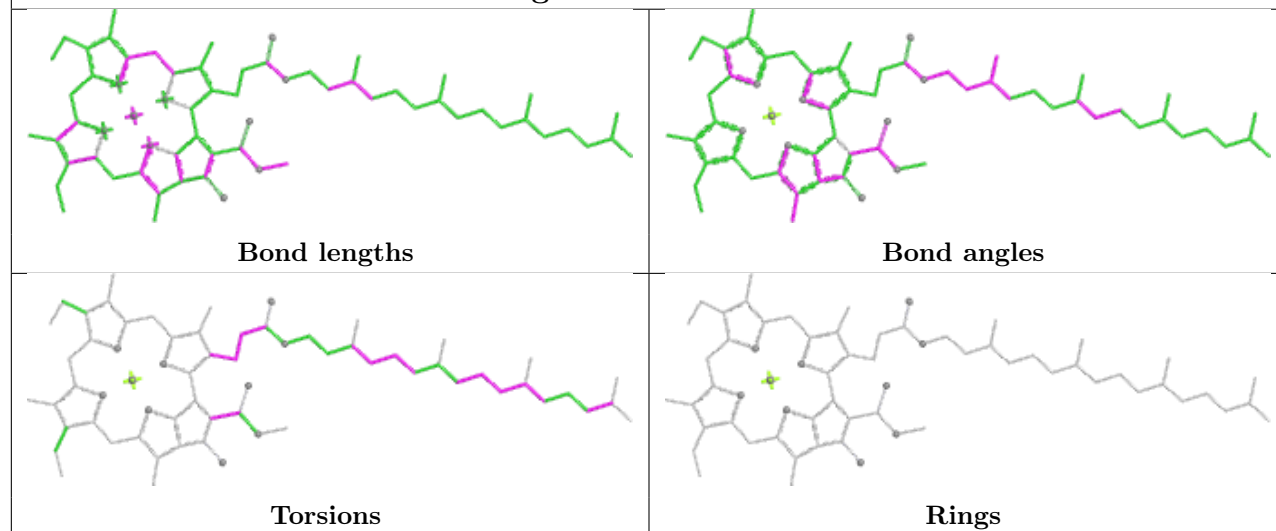




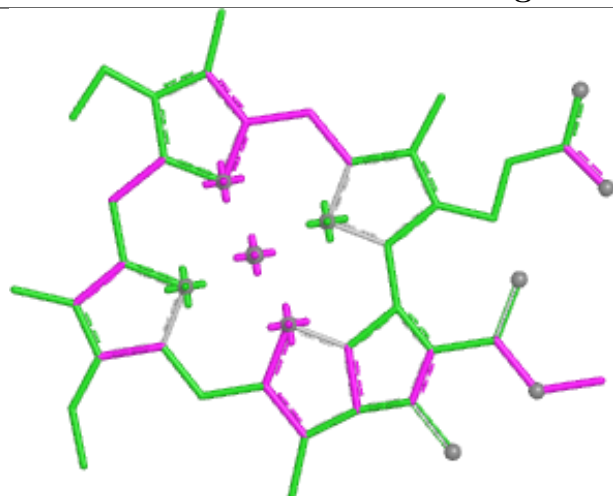
Ligand CLA A 831



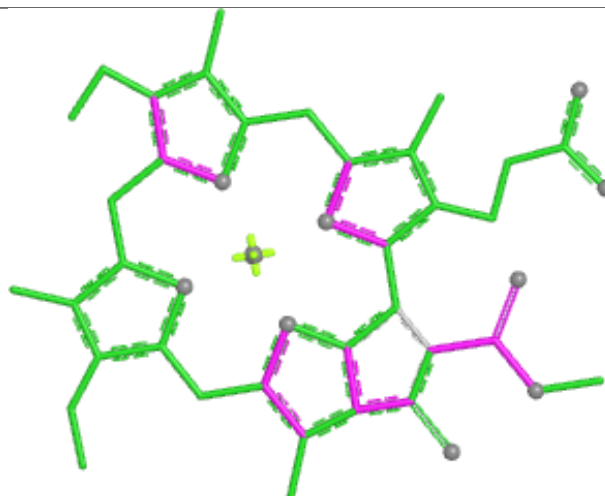
Ligand CLA A 828



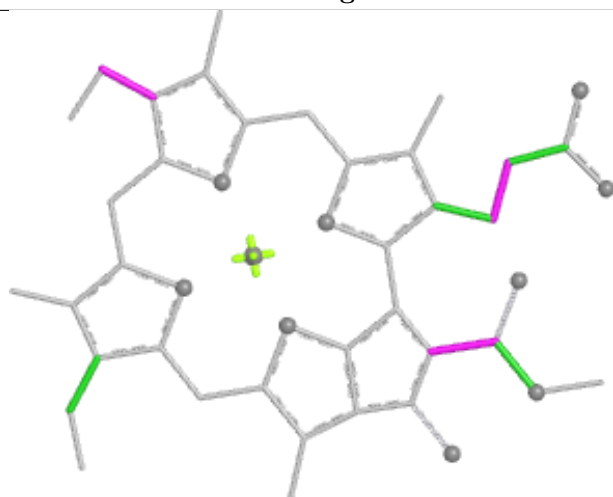
Ligand CLA B 828



Bond lengths



Bond angles

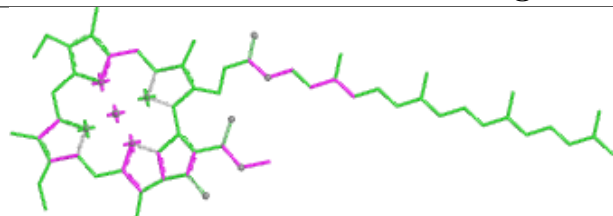


Torsions

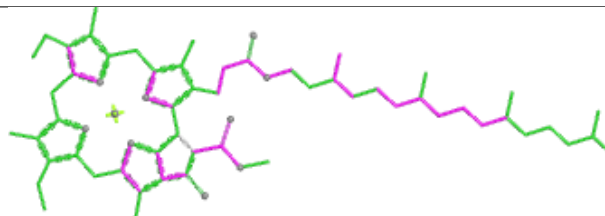


Rings

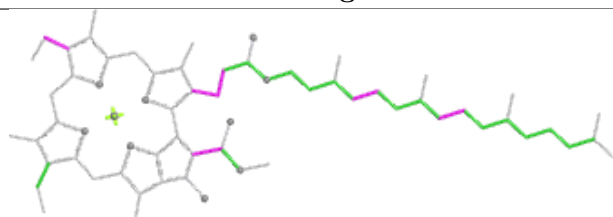
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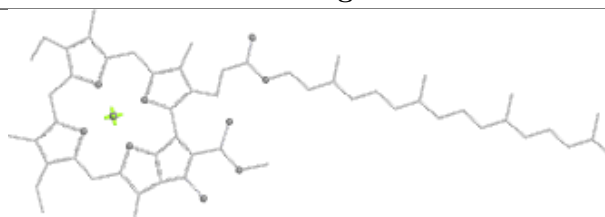
Bond lengths



Bond angles

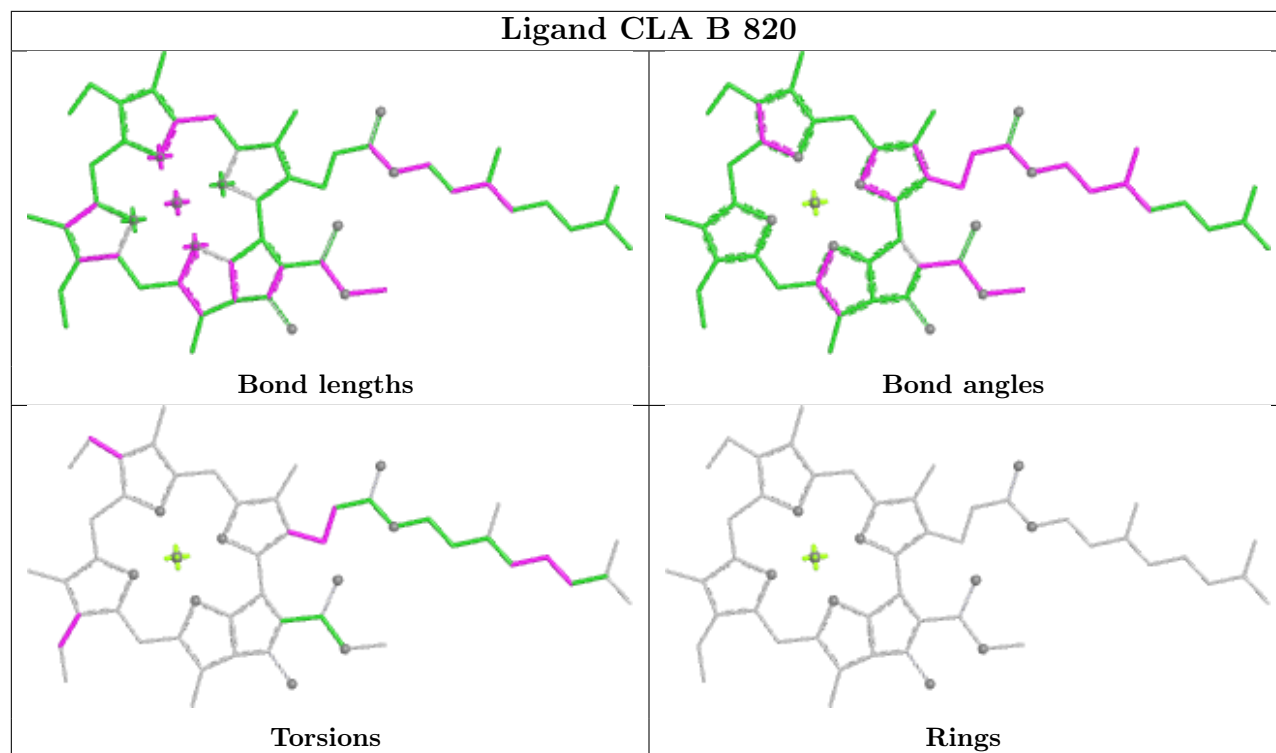


Torsions

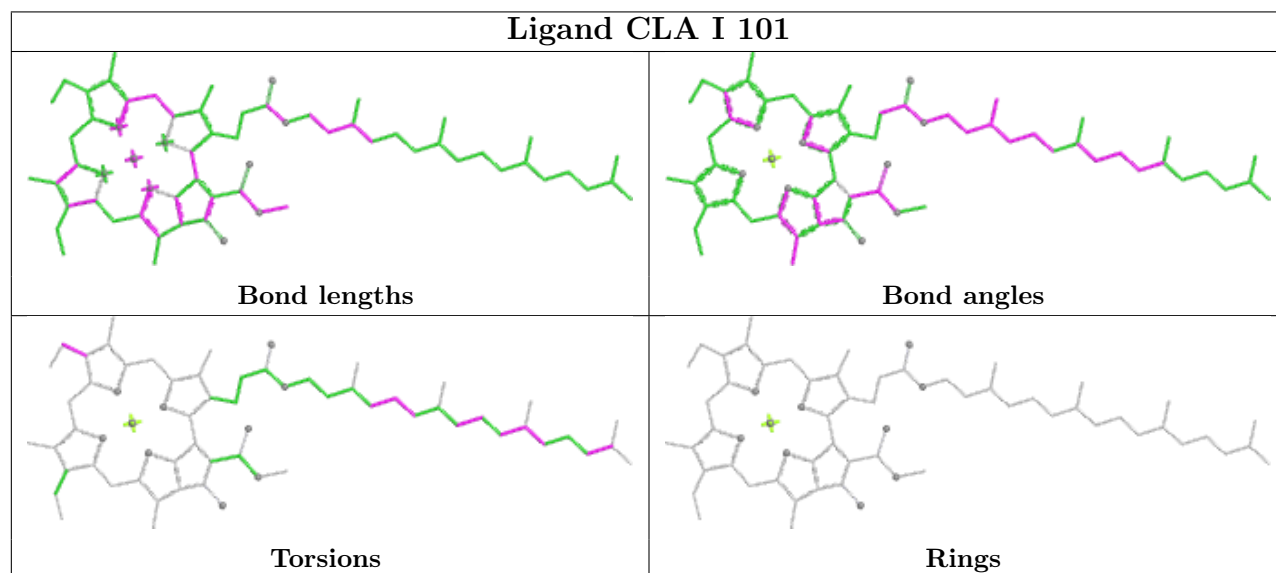


Rings

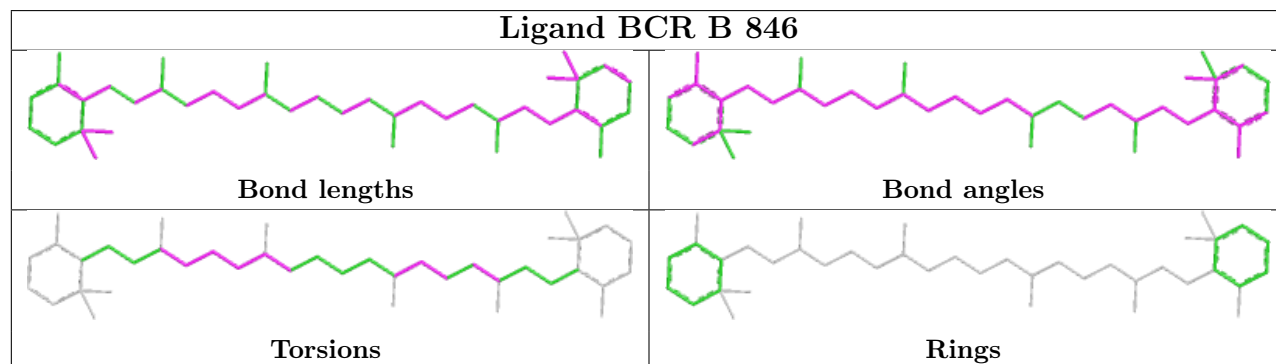
Ligand CLA B 820



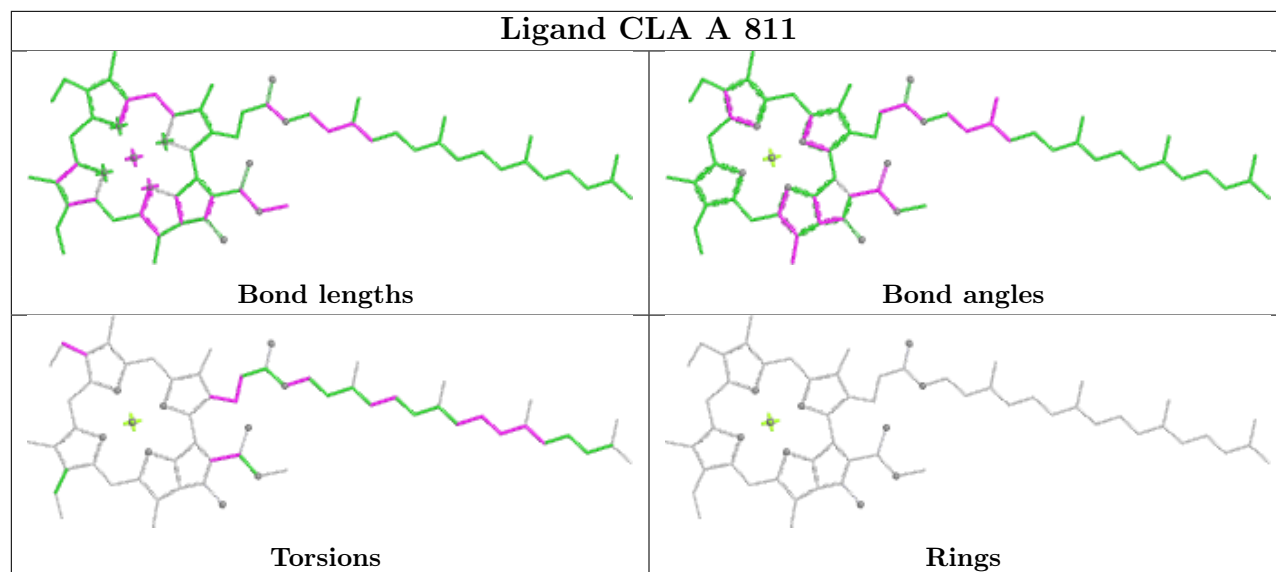
Ligand CLA I 101



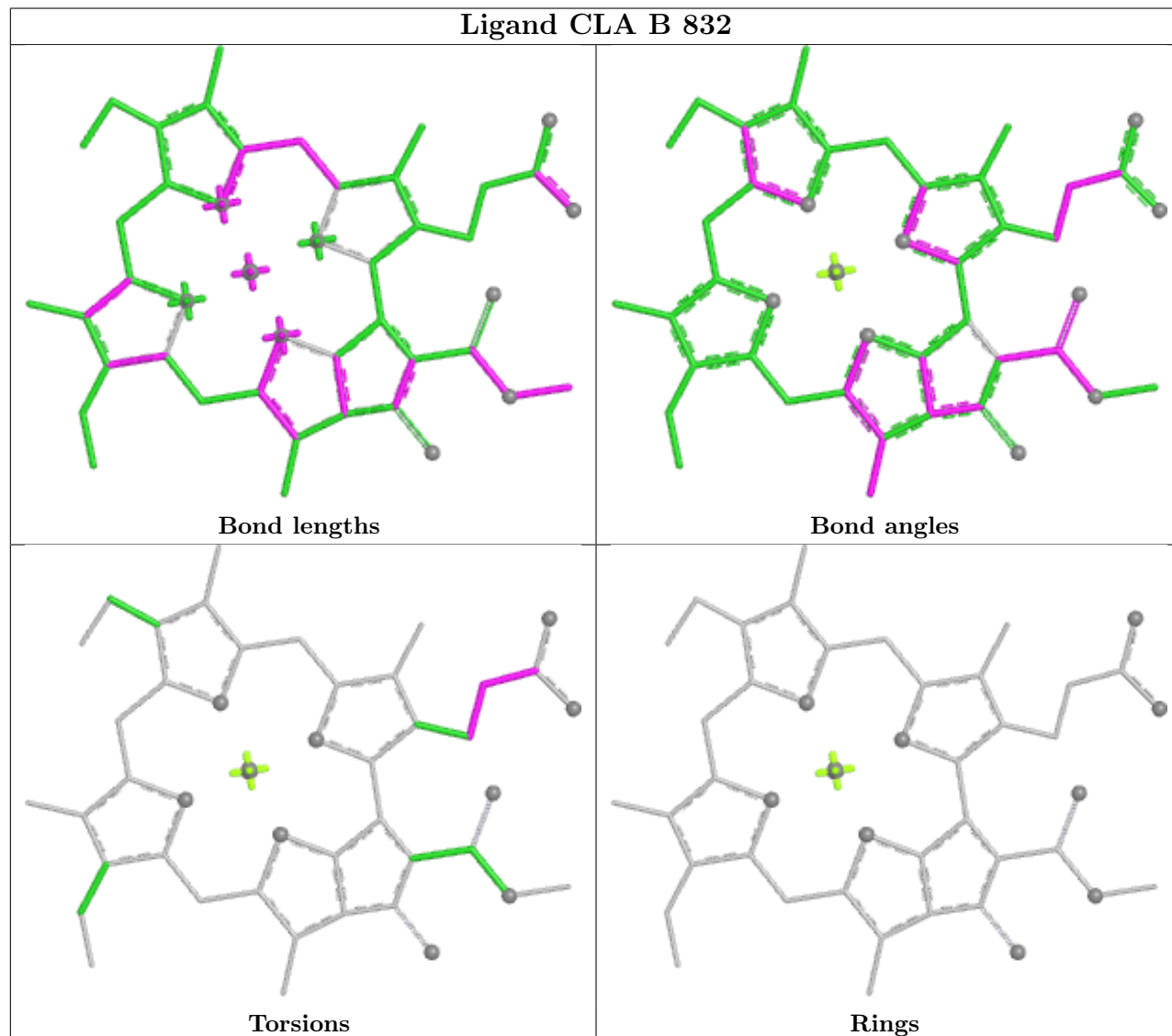
Ligand BCR B 846

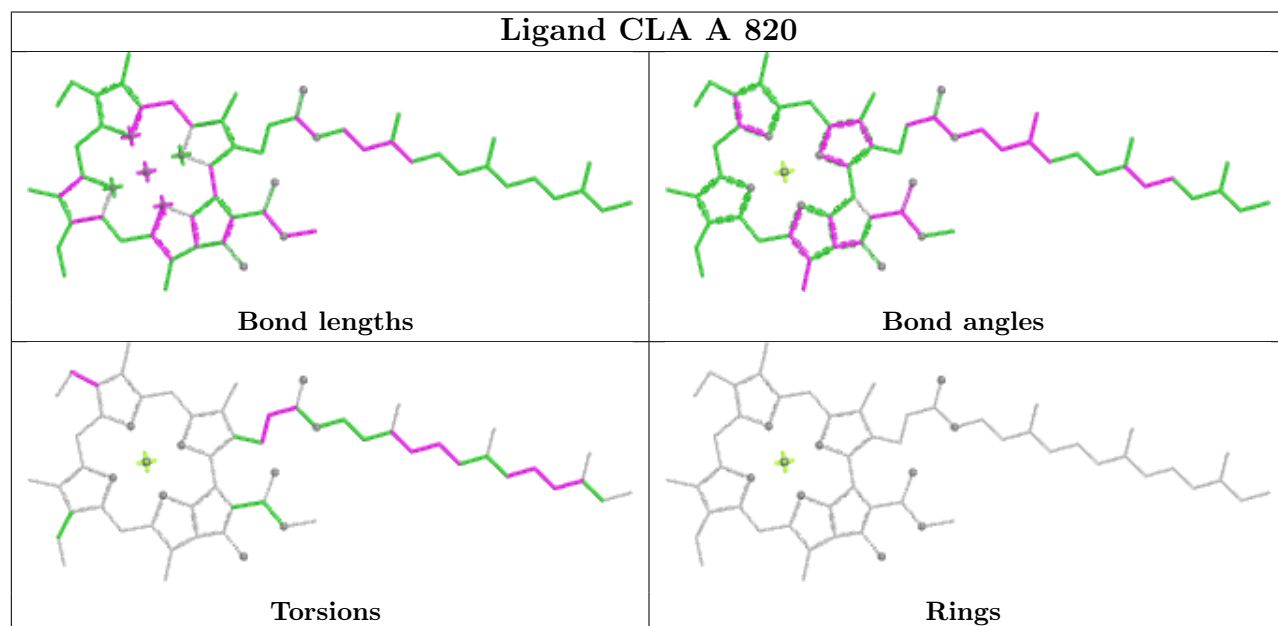
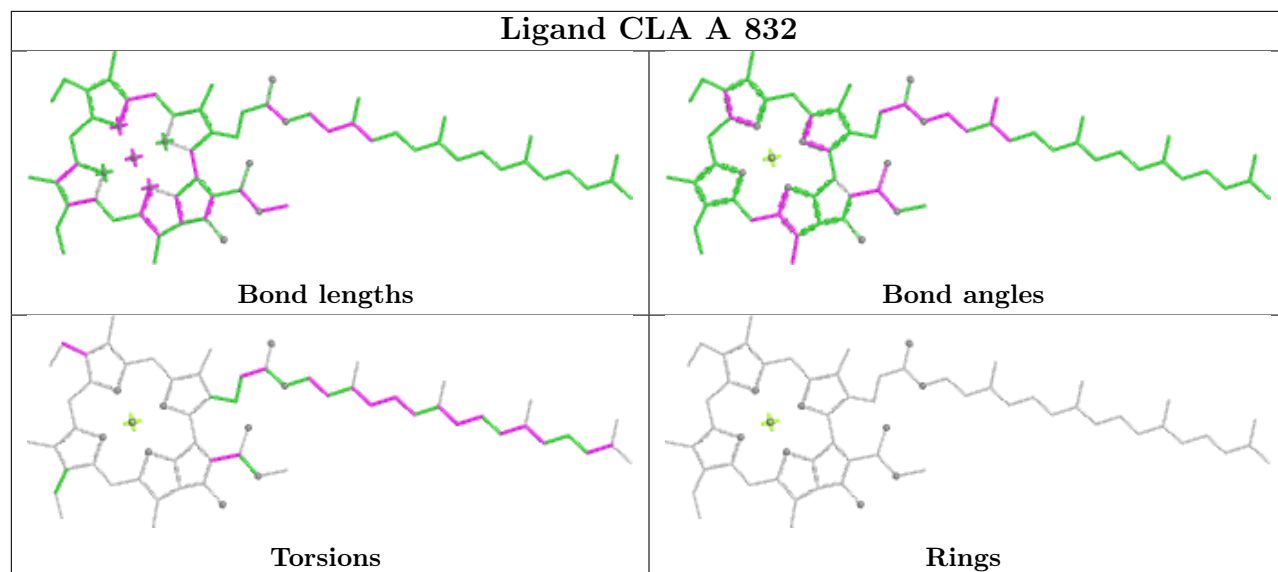


Ligand CLA A 811

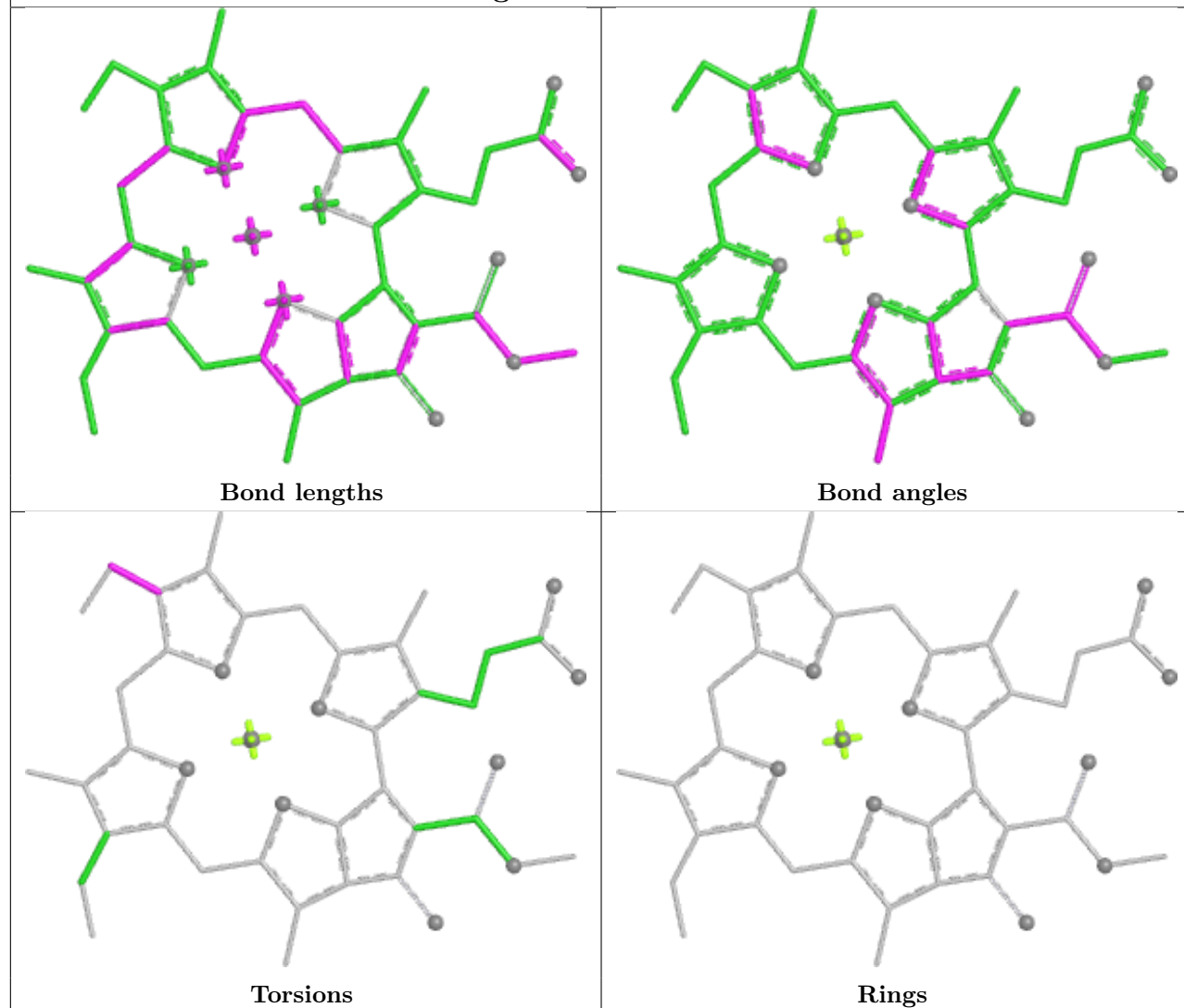


Ligand CLA B 832

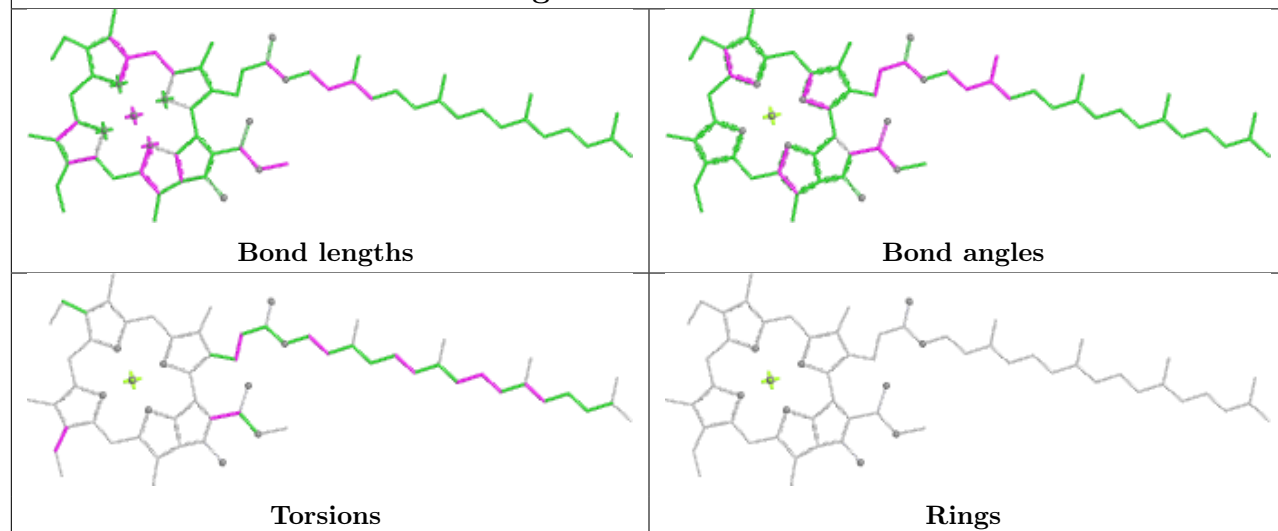


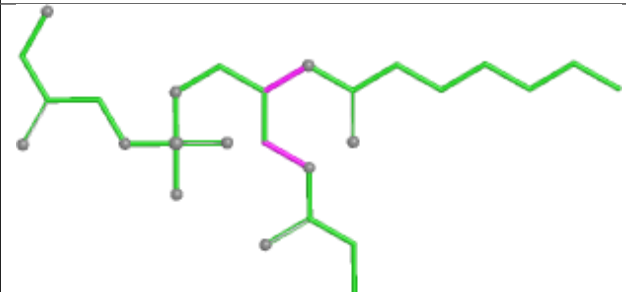
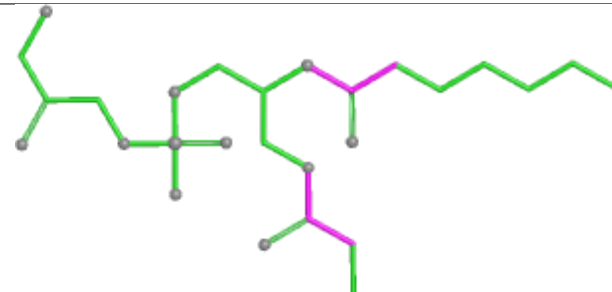
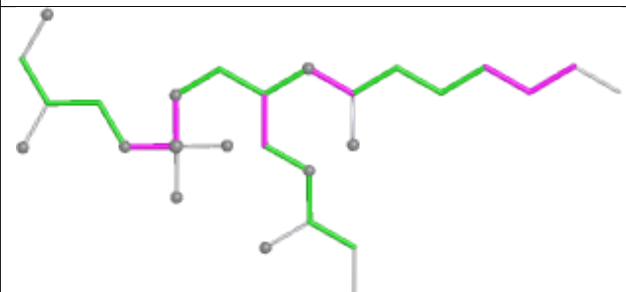
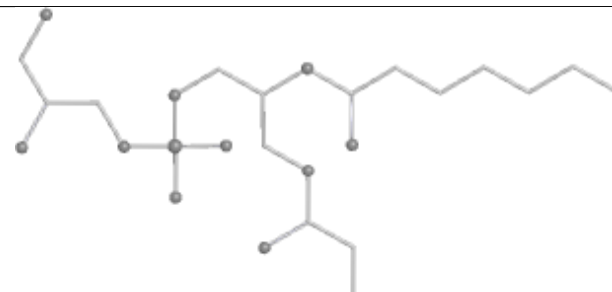


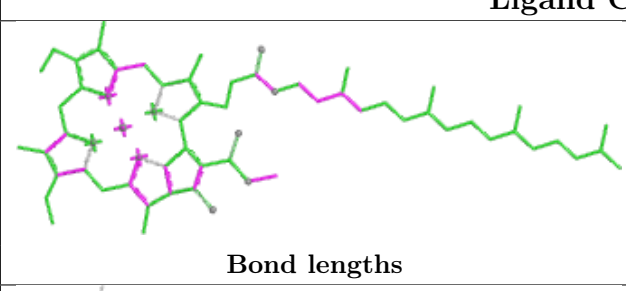
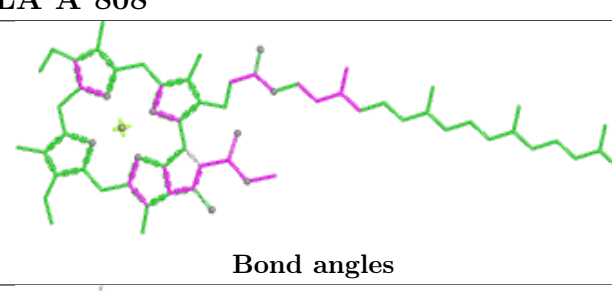
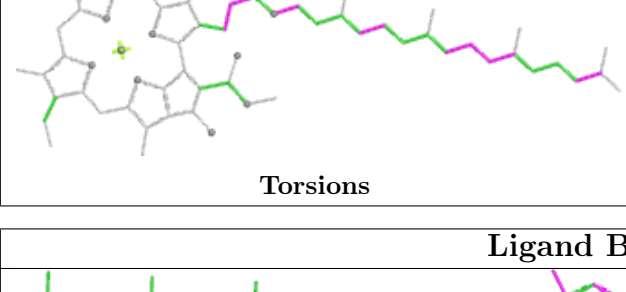
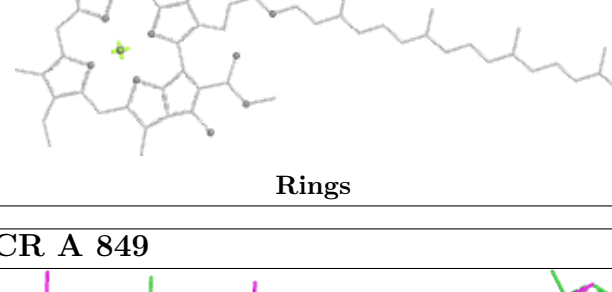
Ligand CLA B 819

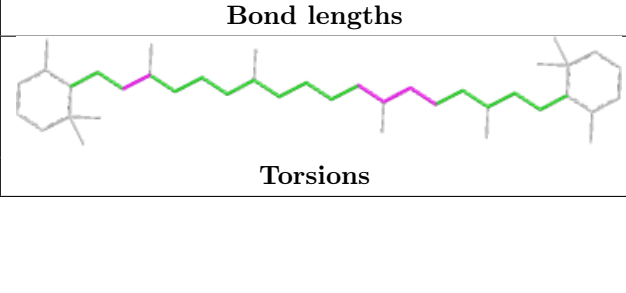
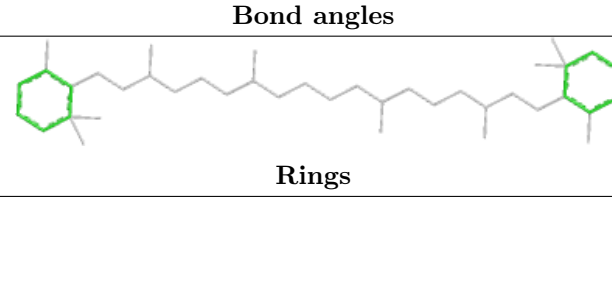


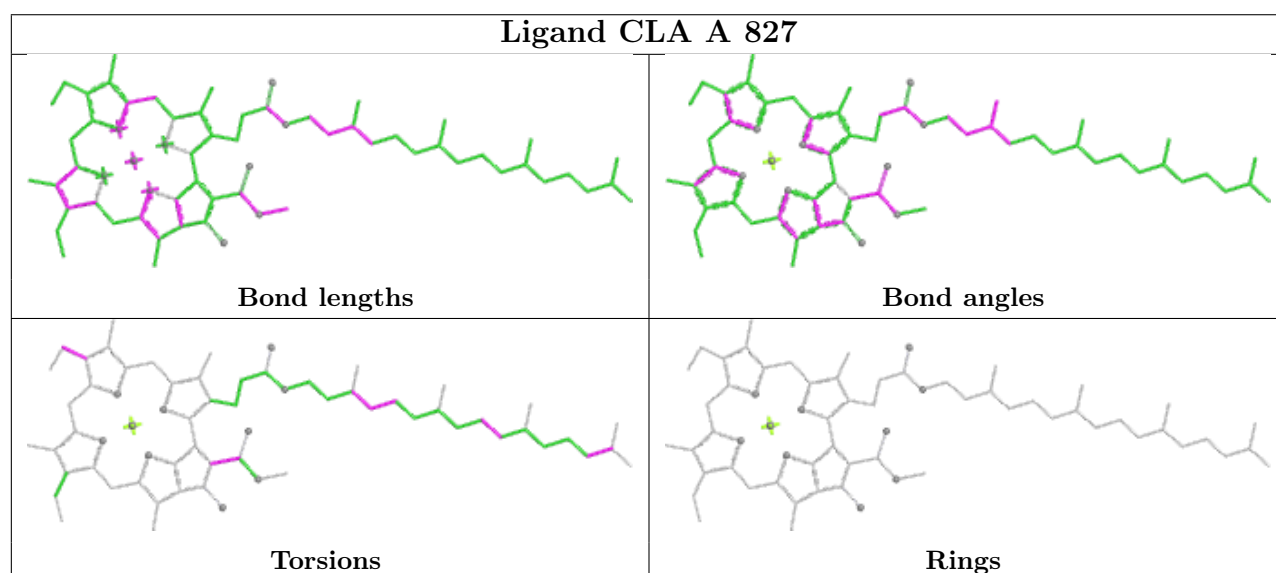
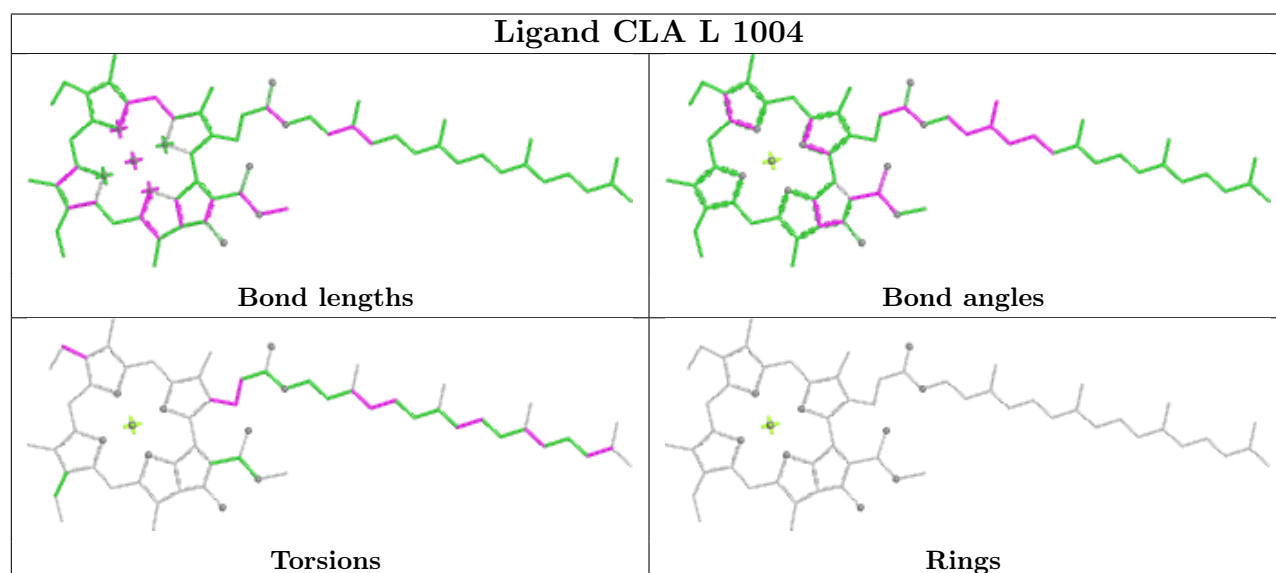
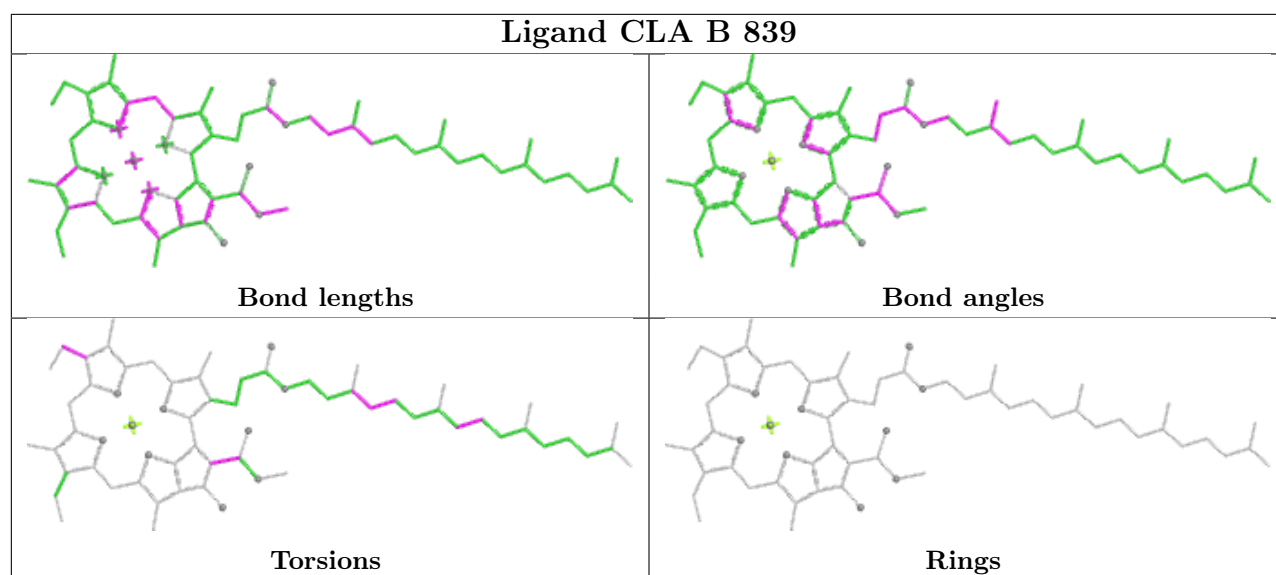
Ligand CLA B 830

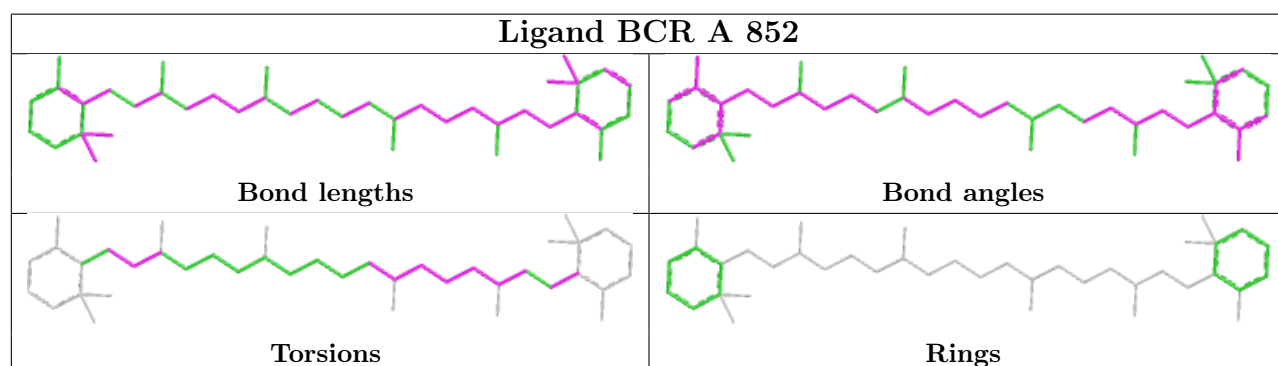
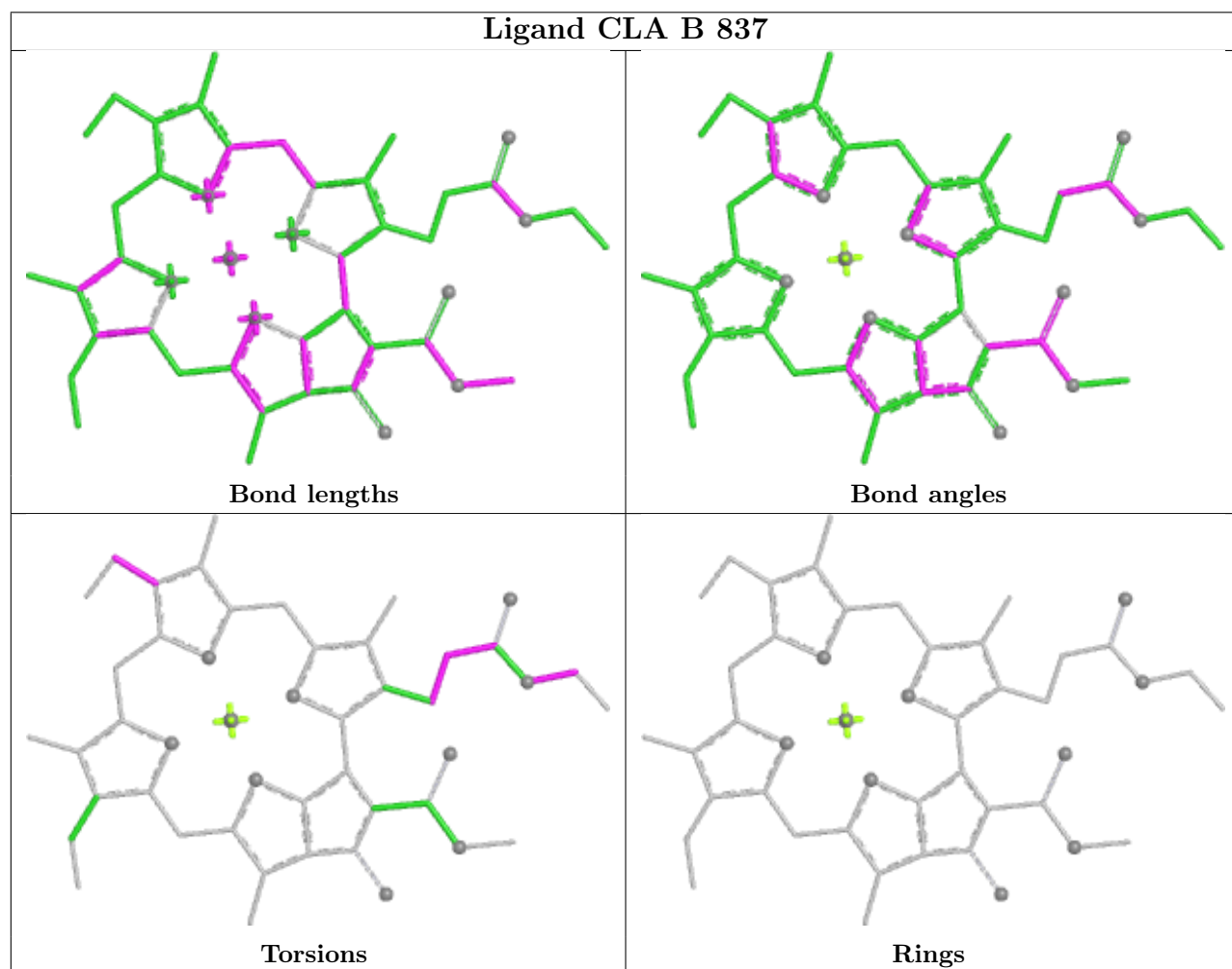
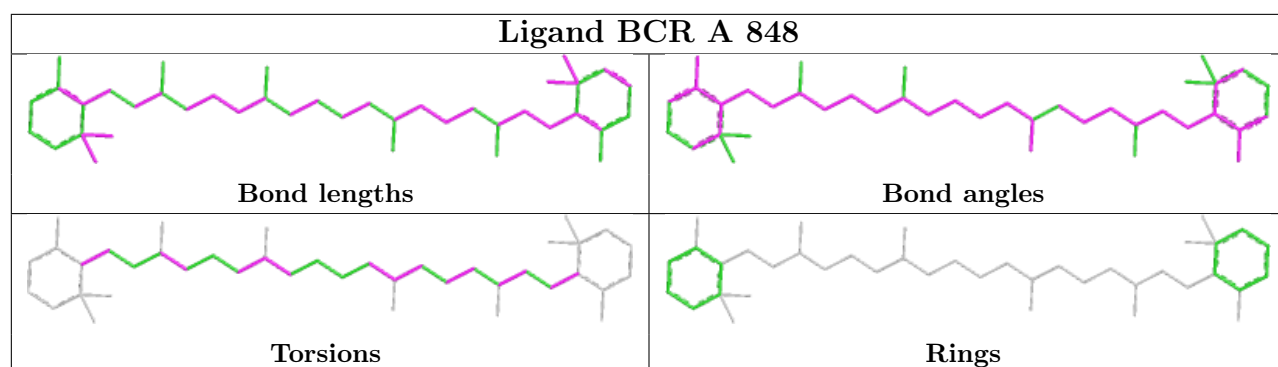


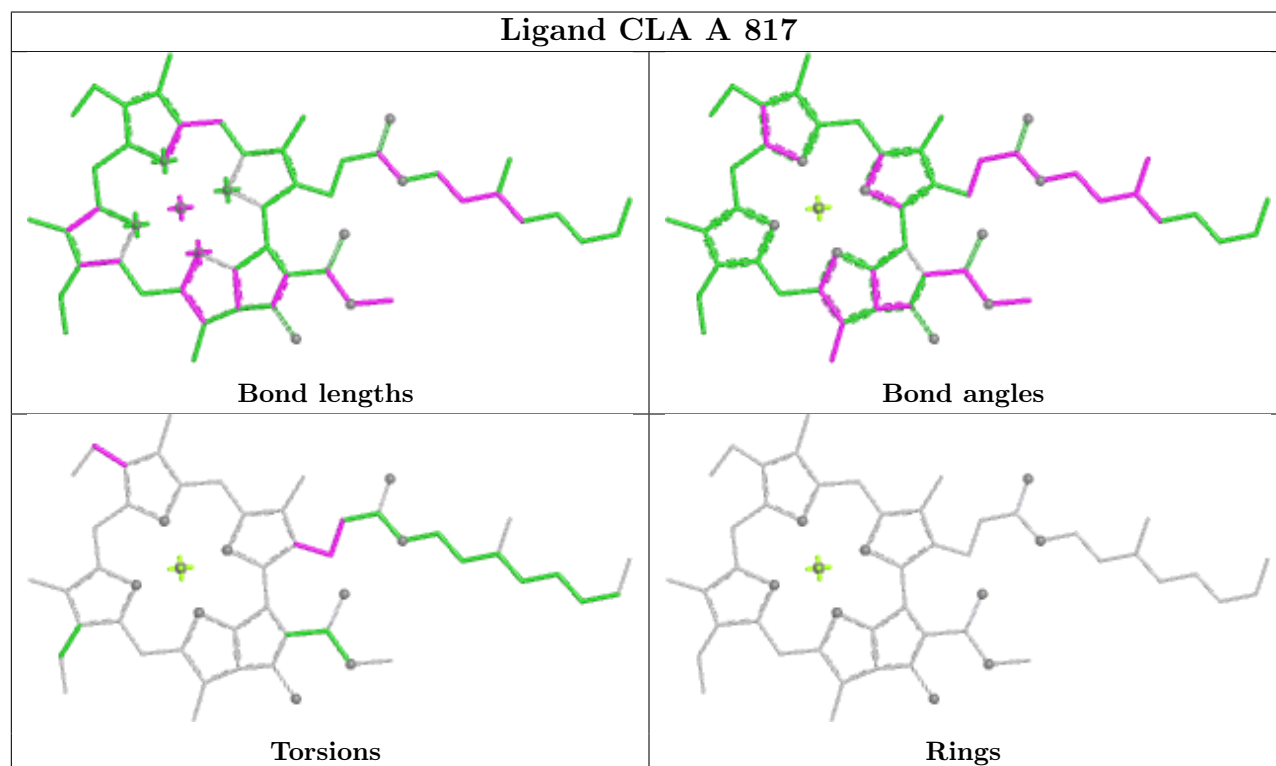
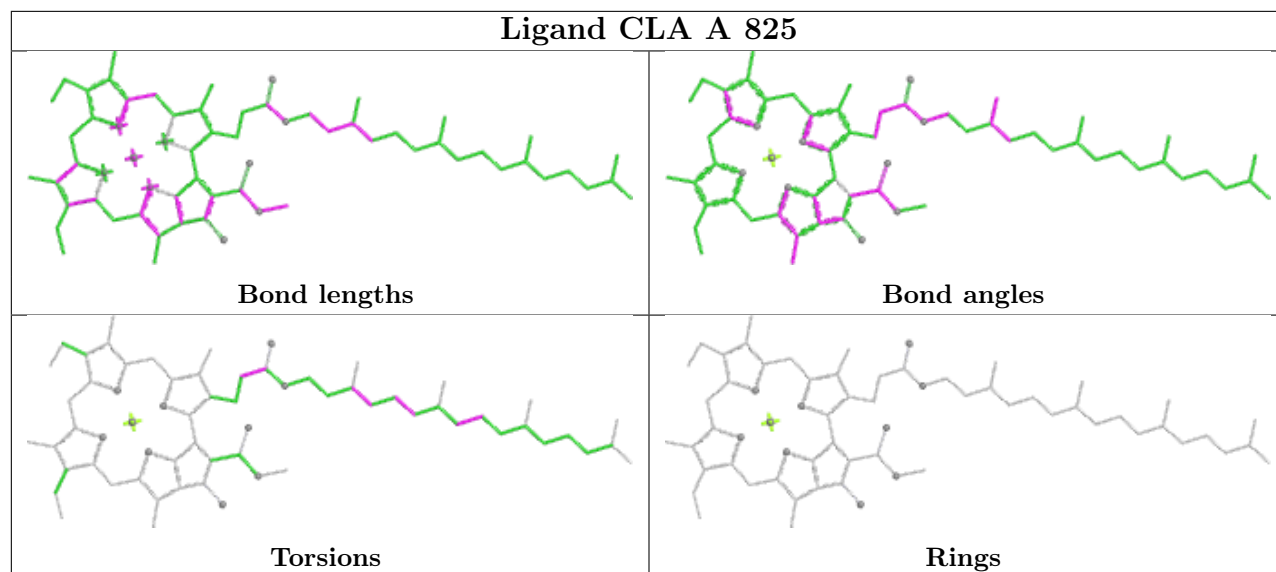
Ligand LHG A 854	
	
Bond lengths	Bond angles
	
Torsions	Rings

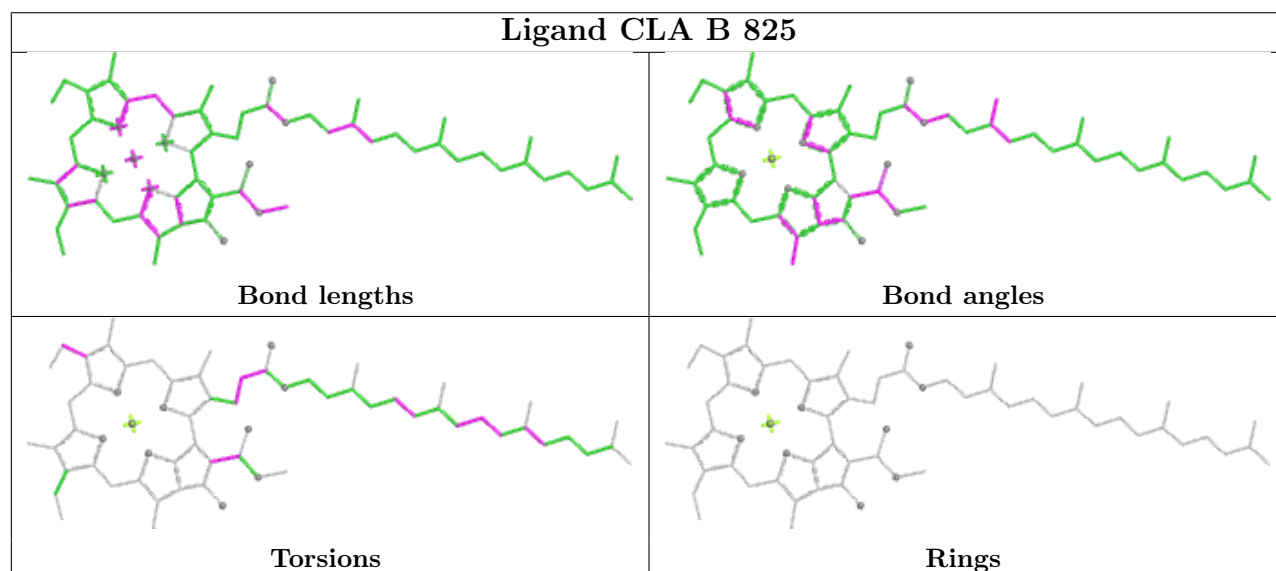
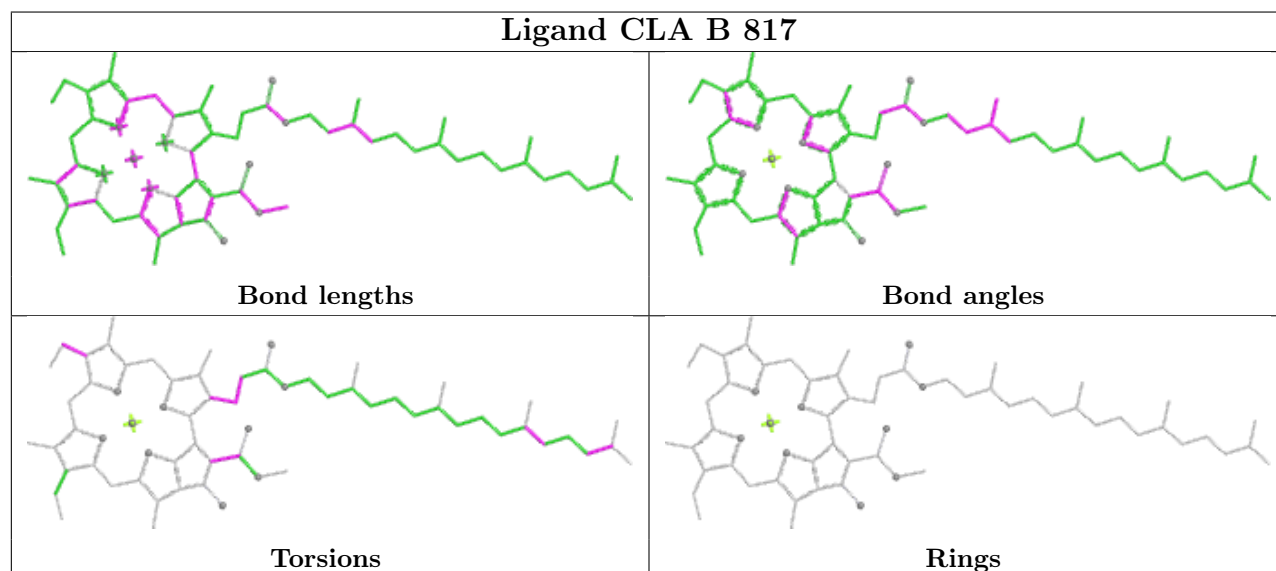
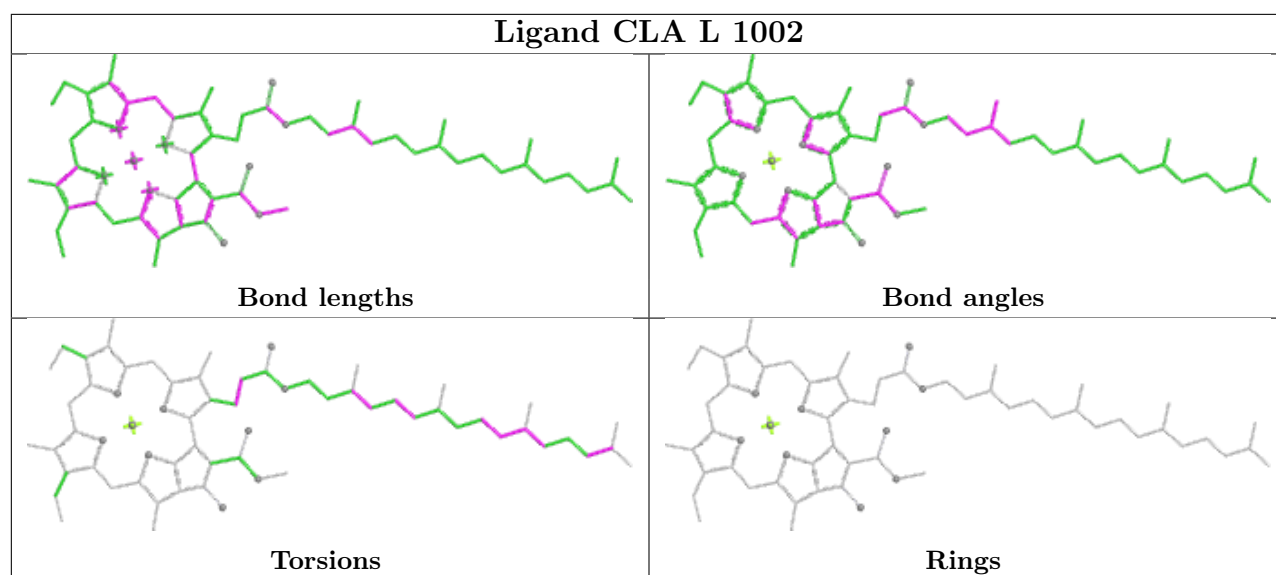
Ligand CLA A 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

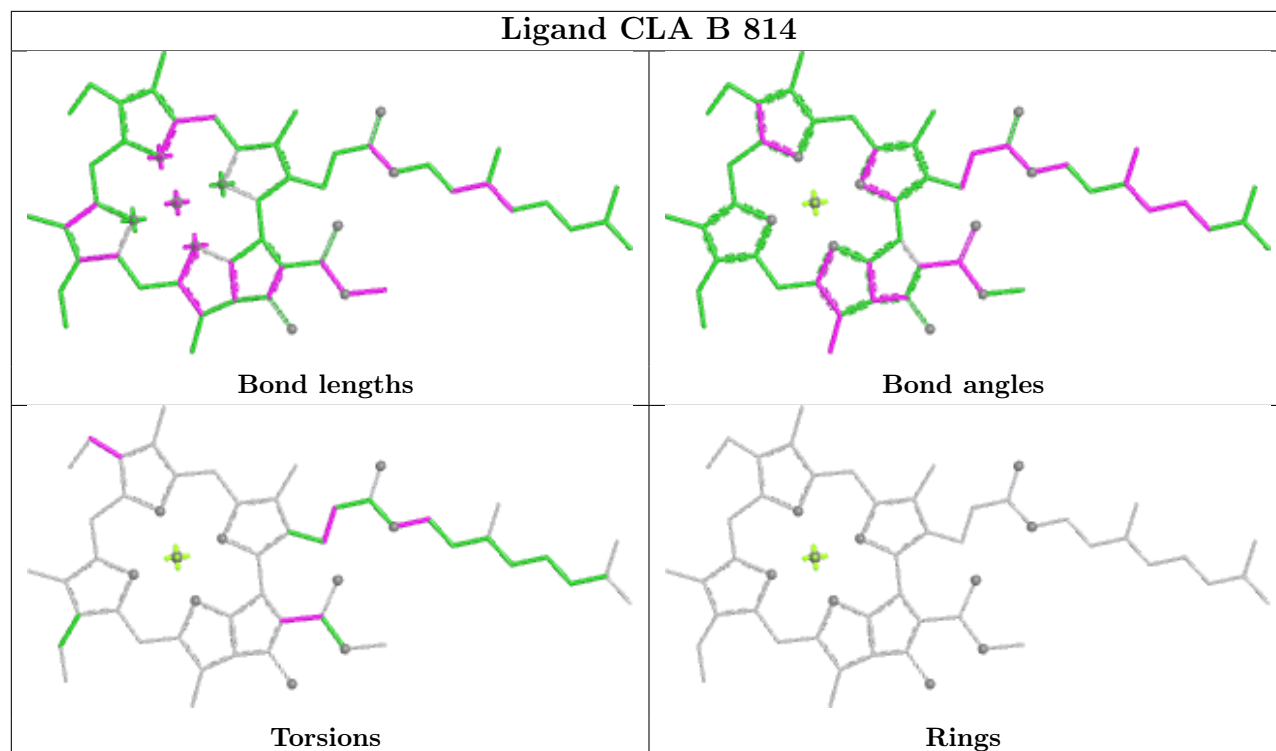




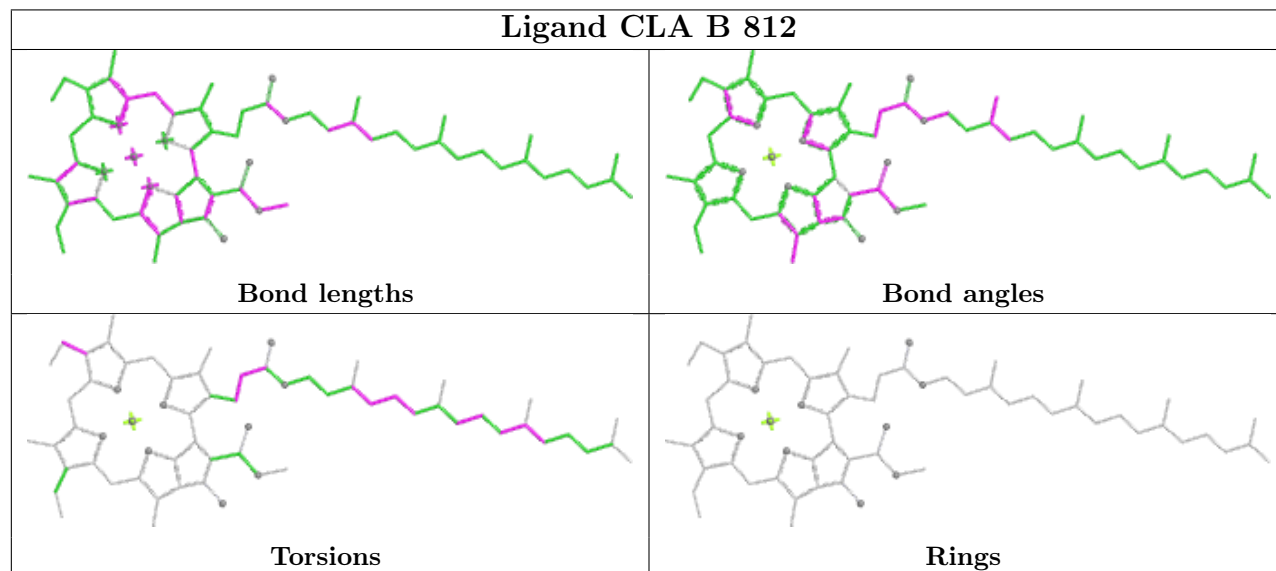


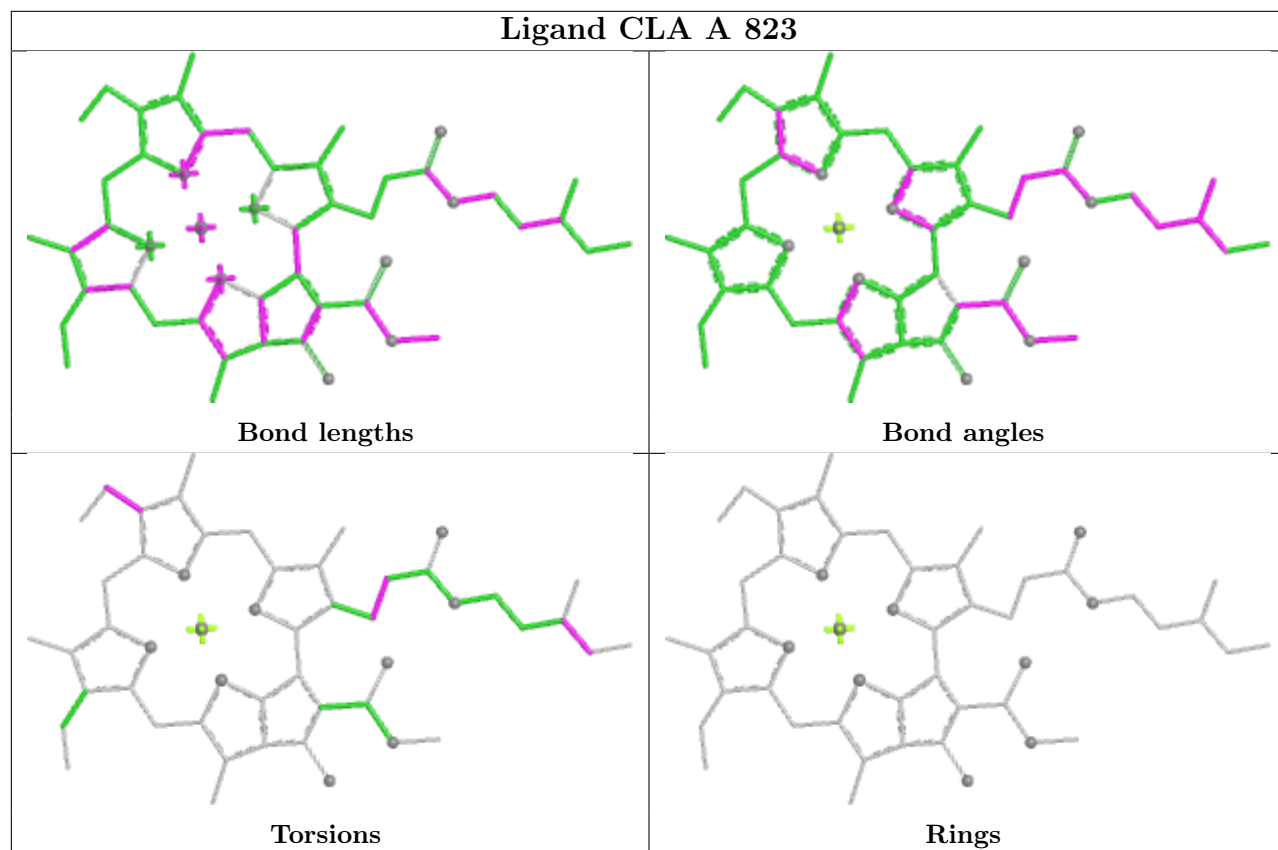


Ligand CLA B 814

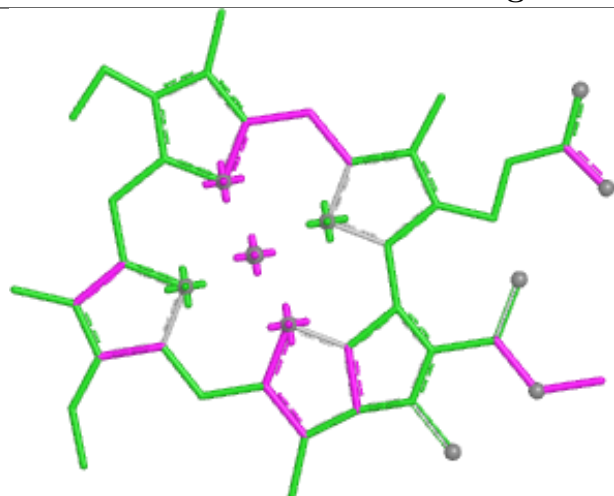


Ligand CLA B 812

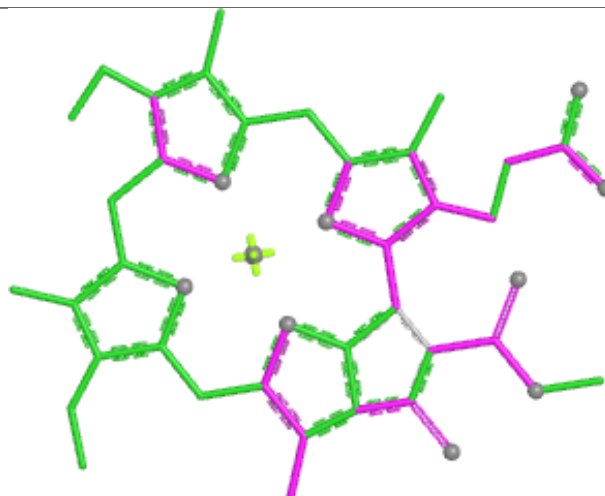




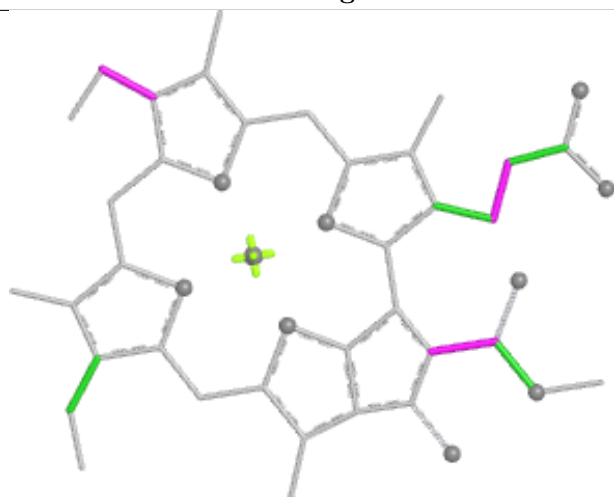
Ligand CLA F 1301



Bond lengths



Bond angles

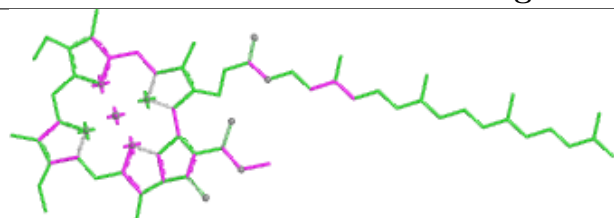


Torsions

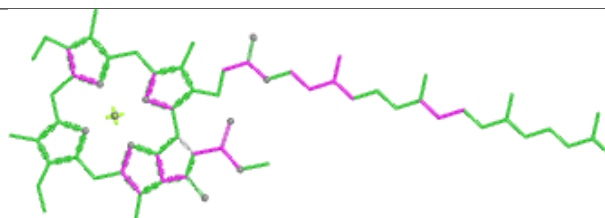


Rings

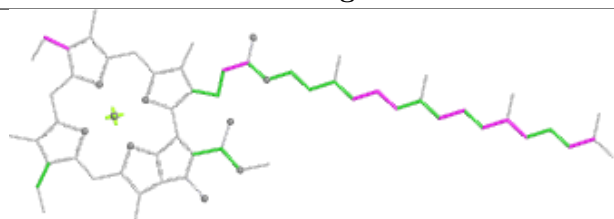
Ligand CLA B 801



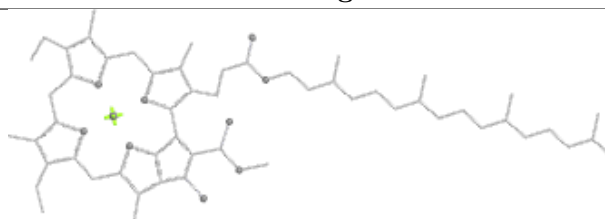
Bond lengths



Bond angles

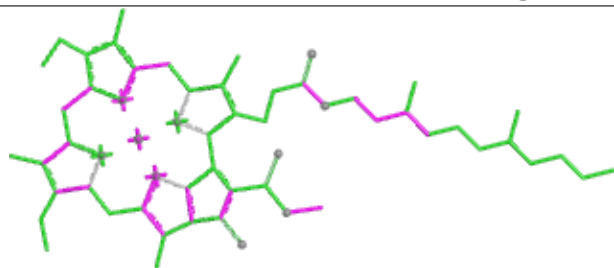


Torsions

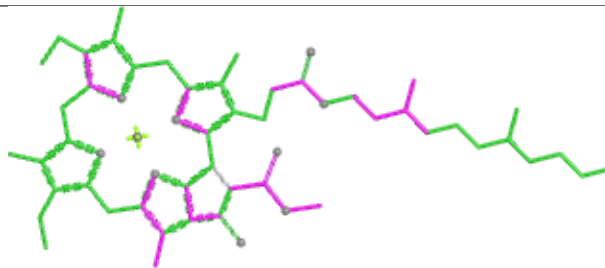


Rings

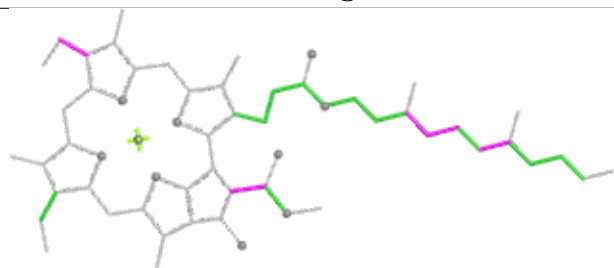
Ligand CLA B 831



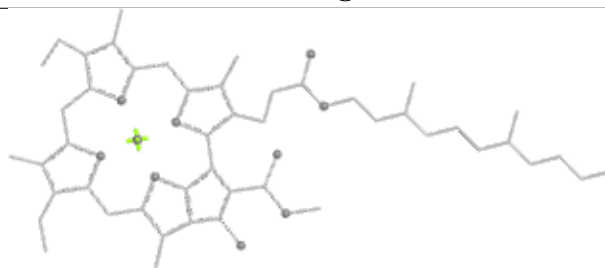
Bond lengths



Bond angles

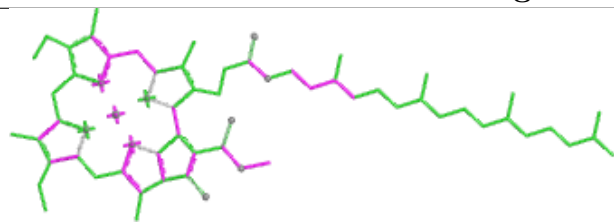


Torsions

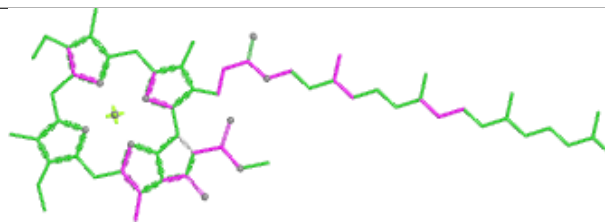


Rings

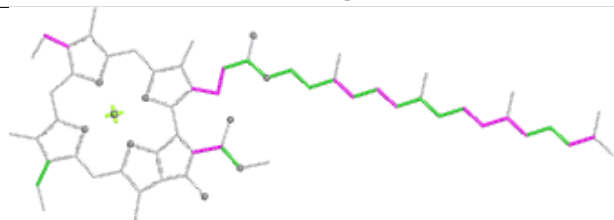
Ligand CLA A 838



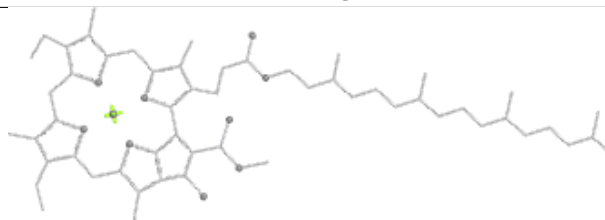
Bond lengths



Bond angles

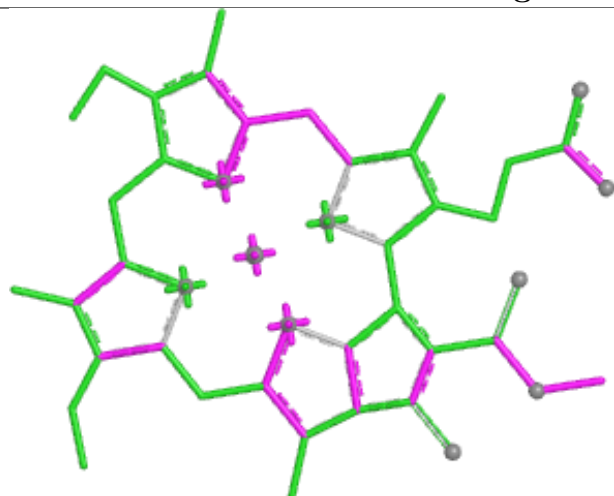


Torsions

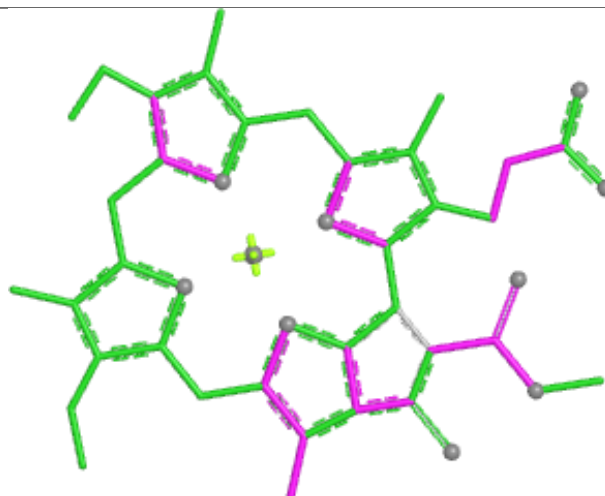


Rings

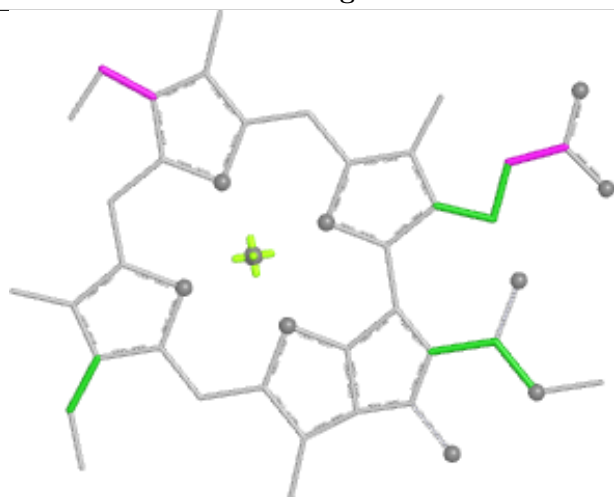
Ligand CLA A 814



Bond lengths



Bond angles

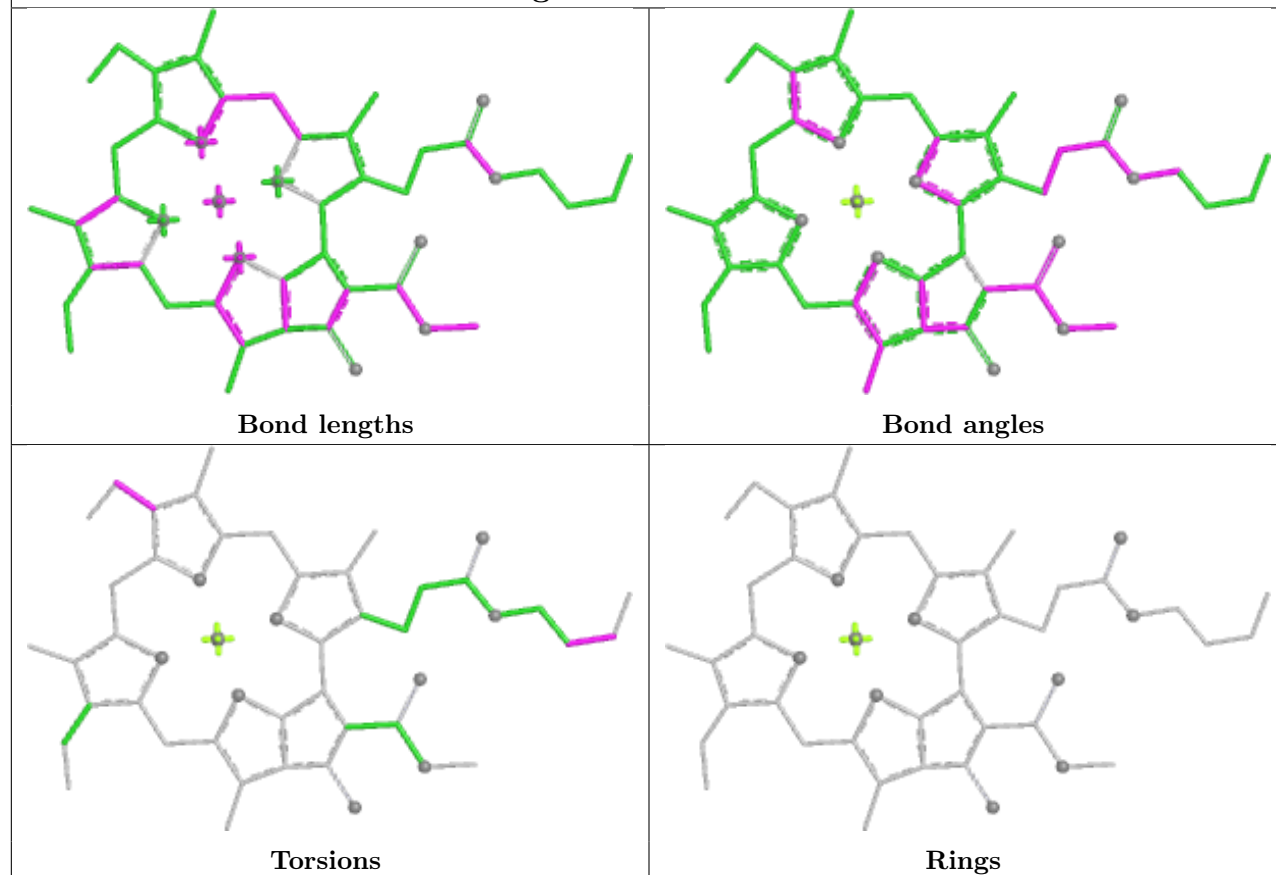


Torsions

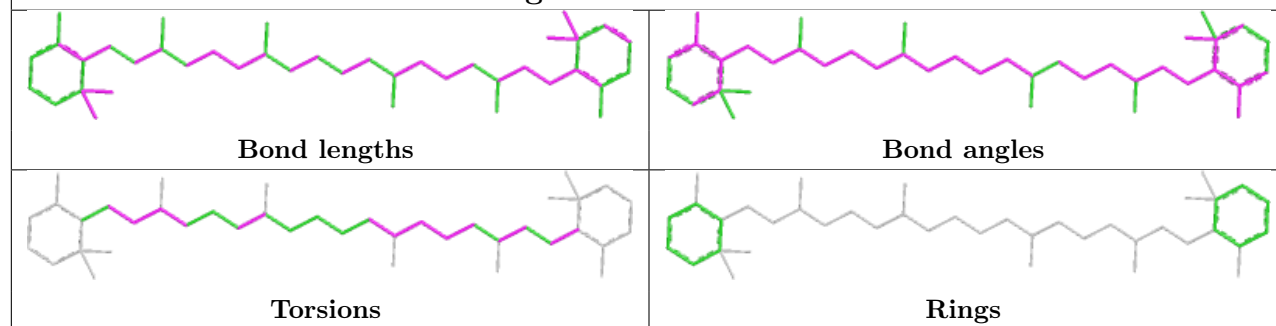


Rings

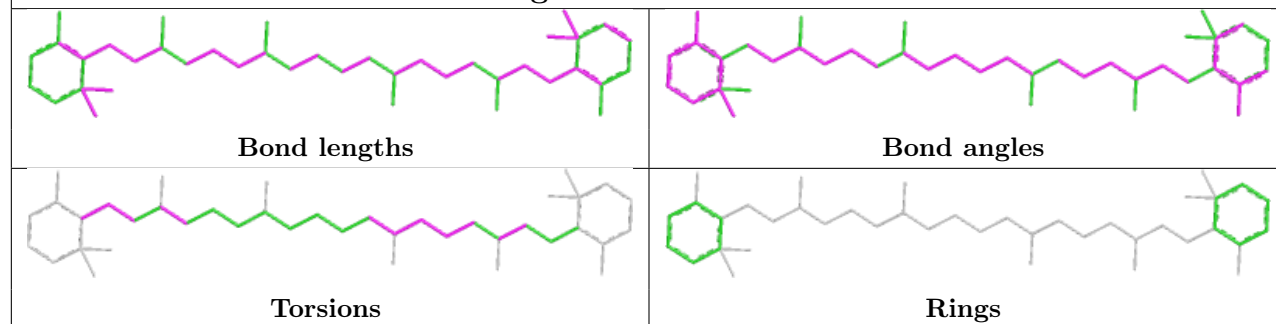
Ligand CLA B 829



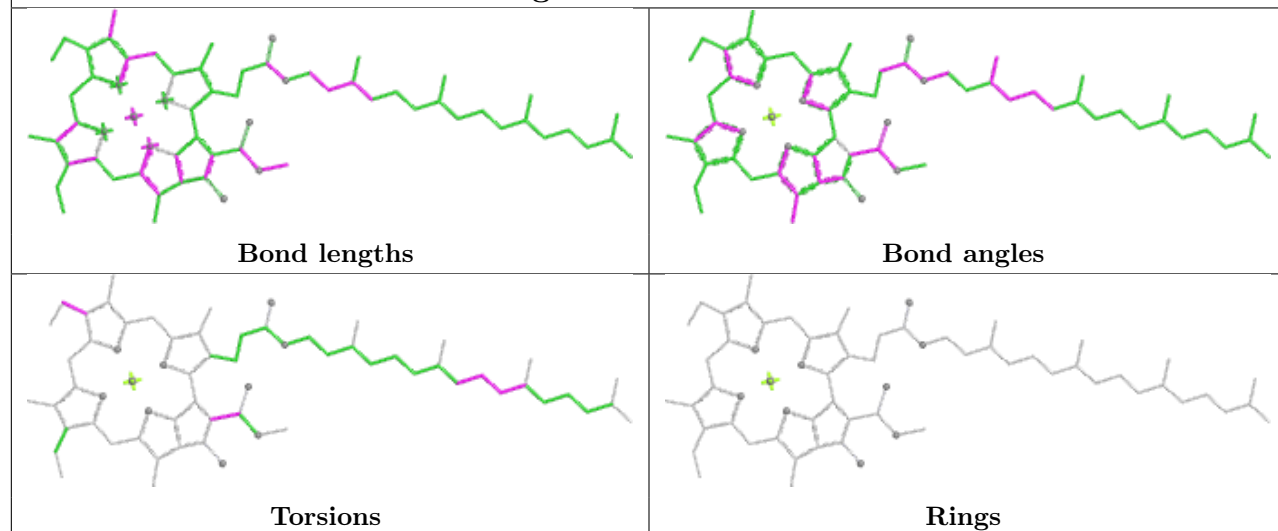
Ligand BCR J 1105



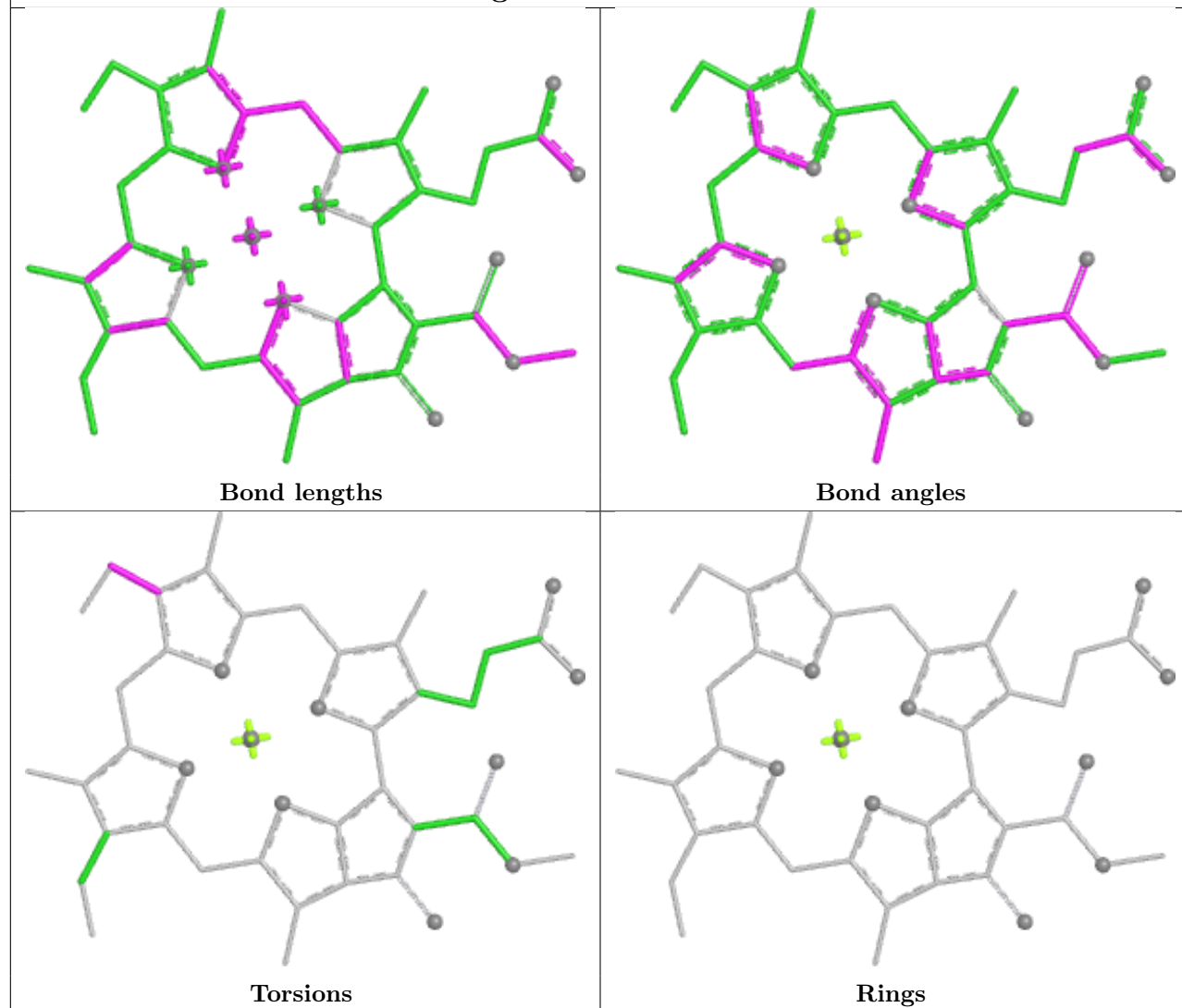
Ligand BCR B 842

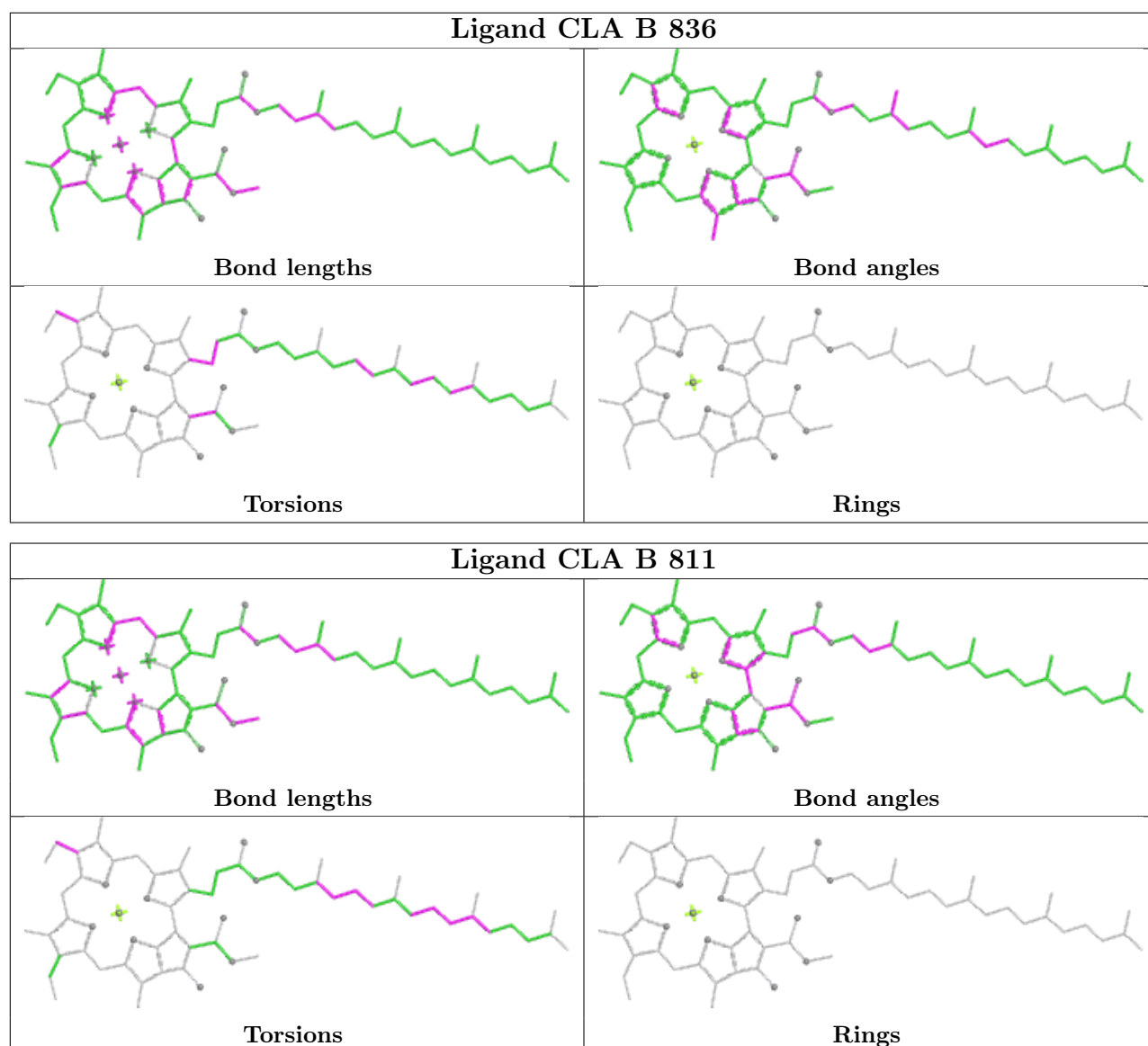


Ligand CLA B 827



Ligand CLA A 815





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	740/755 (98%)	-0.50	1 (0%) 92 87	42, 99, 157, 202	0
2	B	739/740 (99%)	-0.55	0 100 100	34, 76, 126, 215	0
3	C	80/80 (100%)	-0.70	0 100 100	46, 72, 126, 138	0
4	D	138/138 (100%)	-0.62	0 100 100	45, 72, 117, 137	0
5	E	69/75 (92%)	-0.58	0 100 100	77, 100, 148, 194	0
6	F	141/164 (85%)	-0.62	0 100 100	54, 83, 136, 158	0
7	I	38/38 (100%)	-0.65	0 100 100	10, 36, 74, 78	0
8	J	41/41 (100%)	-0.77	0 100 100	65, 89, 136, 165	0
9	K	46/83 (55%)	-0.67	0 100 100	55, 87, 141, 169	0
10	L	151/154 (98%)	-0.22	6 (3%) 42 37	14, 49, 104, 140	0
11	M	31/31 (100%)	-0.70	0 100 100	31, 51, 80, 92	0
12	X	29/35 (82%)	-0.56	0 100 100	59, 80, 120, 155	0
All	All	2243/2334 (96%)	-0.54	7 (0%) 90 80	10, 81, 141, 215	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	L	107	SER	3.8
10	L	146	ASP	3.8
1	A	22	PRO	3.3
10	L	147	GLY	3.1
10	L	72	ASP	2.6

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
13	CLA	A	812	54/65	0.97	0.11	136,181,240,396	0
13	CLA	B	829	49/65	0.97	0.11	80,85,125,141	0
13	CLA	B	832	45/65	0.97	0.12	71,121,142,247	0
13	CLA	B	834	45/65	0.97	0.10	91,118,151,158	0
15	BCR	A	847	40/40	0.97	0.12	98,140,151,162	0
15	BCR	A	849	40/40	0.97	0.12	95,136,179,183	0
18	LMG	B	848	55/55	0.97	0.12	42,51,67,114	0
13	CLA	A	813	60/65	0.98	0.08	115,146,178,366	0
13	CLA	A	815	45/65	0.98	0.09	111,150,177,185	0
13	CLA	A	816	49/65	0.98	0.12	119,163,187,193	0
13	CLA	A	817	54/65	0.98	0.08	83,104,164,172	0
13	CLA	A	820	61/65	0.98	0.09	119,135,166,198	0
13	CLA	A	822	49/65	0.98	0.10	102,126,157,235	0
13	CLA	A	823	51/65	0.98	0.09	74,129,153,156	0
13	CLA	A	827	65/65	0.98	0.10	68,103,137,248	0
13	CLA	A	829	65/65	0.98	0.10	83,108,179,197	0
13	CLA	A	835	54/65	0.98	0.11	54,79,117,204	0
13	CLA	A	839	47/65	0.98	0.08	48,51,119,202	0
13	CLA	A	840	65/65	0.98	0.10	77,87,117,198	0
13	CLA	A	841	51/65	0.98	0.09	80,105,182,204	0
13	CLA	A	842	65/65	0.98	0.09	62,82,149,162	0
13	CLA	A	843	65/65	0.98	0.10	56,83,169,197	0
13	CLA	A	844	41/65	0.98	0.08	116,136,148,281	0
13	CLA	A	845	52/65	0.98	0.09	56,78,188,214	0
13	CLA	A	855	45/65	0.98	0.08	95,118,140,153	0
13	CLA	B	802	65/65	0.98	0.09	61,82,112,165	0
13	CLA	B	803	65/65	0.98	0.11	40,68,95,180	0
13	CLA	B	808	65/65	0.98	0.10	36,41,97,103	0
13	CLA	B	810	45/65	0.98	0.09	47,84,145,182	0
13	CLA	B	812	65/65	0.98	0.10	37,42,111,117	0
13	CLA	B	813	45/65	0.98	0.09	51,86,132,141	0
13	CLA	B	814	55/65	0.98	0.10	77,122,182,325	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	CLA	B	815	59/65	0.98	0.10	55,58,76,293	0
13	CLA	B	820	55/65	0.98	0.09	77,105,141,146	0
13	CLA	B	821	45/65	0.98	0.09	63,69,105,191	0
13	CLA	B	823	46/65	0.98	0.09	59,68,120,137	0
13	CLA	B	824	65/65	0.98	0.10	58,65,88,96	0
13	CLA	B	828	45/65	0.98	0.09	70,80,132,193	0
13	CLA	A	804	59/65	0.98	0.09	83,99,117,144	0
13	CLA	B	831	58/65	0.98	0.10	80,101,148,333	0
13	CLA	A	807	51/65	0.98	0.09	87,100,151,177	0
13	CLA	B	833	45/65	0.98	0.09	77,104,141,148	0
13	CLA	A	809	65/65	0.98	0.11	78,117,148,152	0
13	CLA	B	835	60/65	0.98	0.08	65,106,240,292	0
13	CLA	B	838	65/65	0.98	0.11	35,45,102,125	0
13	CLA	B	839	65/65	0.98	0.09	35,49,151,215	0
13	CLA	F	1301	45/65	0.98	0.09	94,137,167,175	0
13	CLA	J	1102	45/65	0.98	0.08	75,111,128,280	0
14	PQN	A	846	33/33	0.98	0.09	55,64,82,82	0
14	PQN	B	840	33/33	0.98	0.10	56,84,105,121	0
13	CLA	A	810	45/65	0.98	0.10	109,136,151,223	0
15	BCR	A	848	40/40	0.98	0.11	112,132,147,157	0
13	CLA	A	811	65/65	0.98	0.11	95,134,173,321	0
15	BCR	B	841	40/40	0.98	0.13	65,105,151,155	0
15	BCR	B	843	40/40	0.98	0.10	45,59,82,86	0
15	BCR	B	845	40/40	0.98	0.09	60,66,78,82	0
15	BCR	B	846	40/40	0.98	0.10	75,91,131,137	0
15	BCR	B	847	40/40	0.98	0.11	40,51,116,126	0
15	BCR	B	849	40/40	0.98	0.09	12,43,147,152	0
15	BCR	B	850	40/40	0.98	0.09	83,107,144,146	0
15	BCR	J	1104	40/40	0.98	0.10	64,78,113,120	0
15	BCR	L	1005	40/40	0.98	0.10	11,16,81,93	0
15	BCR	L	1006	40/40	0.98	0.10	16,24,64,78	0
15	BCR	M	1203	40/40	0.98	0.09	43,48,87,92	0
16	LHG	X	101	23/49	0.98	0.08	78,81,207,208	0
13	CLA	A	801	65/65	0.98	0.09	44,53,82,89	0
19	CA	L	1001	1/1	0.98	0.10	22,22,22,22	0
13	CLA	B	822	54/65	0.99	0.08	61,86,118,158	0
13	CLA	A	836	45/65	0.99	0.08	63,96,163,234	0
13	CLA	A	837	51/65	0.99	0.07	52,56,96,147	0
13	CLA	B	825	65/65	0.99	0.08	40,60,136,157	0
13	CLA	B	826	65/65	0.99	0.08	42,47,127,149	0
13	CLA	B	827	65/65	0.99	0.08	44,66,95,108	0
13	CLA	A	838	65/65	0.99	0.08	45,81,109,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	CLA	A	818	54/65	0.99	0.07	92,136,168,207	0
13	CLA	B	830	65/65	0.99	0.08	82,91,129,139	0
13	CLA	A	819	65/65	0.99	0.08	97,140,181,328	0
13	CLA	A	803	65/65	0.99	0.09	76,100,142,222	0
13	CLA	A	821	65/65	0.99	0.08	72,100,164,266	0
13	CLA	A	808	65/65	0.99	0.08	72,89,172,177	0
13	CLA	A	814	45/65	0.99	0.07	108,150,172,174	0
13	CLA	B	836	65/65	0.99	0.09	69,98,146,234	0
13	CLA	B	837	47/65	0.99	0.08	65,71,119,193	0
13	CLA	A	824	59/65	0.99	0.08	59,101,164,321	0
13	CLA	A	825	65/65	0.99	0.07	74,102,152,193	0
13	CLA	B	801	65/65	0.99	0.08	57,68,123,322	0
13	CLA	I	101	65/65	0.99	0.08	33,57,85,338	0
13	CLA	J	1101	65/65	0.99	0.09	77,129,178,357	0
13	CLA	A	826	65/65	0.99	0.08	53,80,112,127	0
13	CLA	J	1103	37/65	0.99	0.07	85,117,155,158	0
13	CLA	L	1002	65/65	0.99	0.09	29,65,103,148	0
13	CLA	L	1003	65/65	0.99	0.08	16,52,179,216	0
13	CLA	L	1004	65/65	0.99	0.08	21,31,64,72	0
13	CLA	M	1201	54/65	0.99	0.07	34,42,121,127	0
13	CLA	M	1202	45/65	0.99	0.09	51,149,183,198	0
13	CLA	X	102	45/65	0.99	0.08	67,104,127,283	0
13	CLA	A	802	65/65	0.99	0.08	40,77,110,230	0
13	CLA	B	804	65/65	0.99	0.08	45,51,117,199	0
13	CLA	B	805	65/65	0.99	0.07	41,48,97,150	0
13	CLA	B	806	65/65	0.99	0.09	33,63,107,170	0
13	CLA	B	807	65/65	0.99	0.08	38,65,106,122	0
15	BCR	A	850	40/40	0.99	0.09	56,96,126,139	0
15	BCR	A	851	40/40	0.99	0.07	50,58,118,132	0
15	BCR	A	852	40/40	0.99	0.10	78,107,149,162	0
13	CLA	A	828	65/65	0.99	0.08	59,74,127,289	0
15	BCR	B	842	40/40	0.99	0.07	48,76,129,134	0
13	CLA	B	809	45/65	0.99	0.08	39,95,125,308	0
15	BCR	B	844	25/40	0.99	0.08	65,68,113,118	0
13	CLA	A	805	65/65	0.99	0.08	85,98,117,126	0
13	CLA	B	811	65/65	0.99	0.08	48,71,108,145	0
13	CLA	A	830	65/65	0.99	0.06	59,71,105,119	0
13	CLA	A	831	50/65	0.99	0.08	45,76,105,144	0
13	CLA	A	832	65/65	0.99	0.07	42,45,81,134	0
15	BCR	F	1302	40/40	0.99	0.11	70,94,125,128	0
15	BCR	I	102	40/40	0.99	0.08	19,20,48,52	0
13	CLA	A	833	65/65	0.99	0.09	39,45,110,121	0

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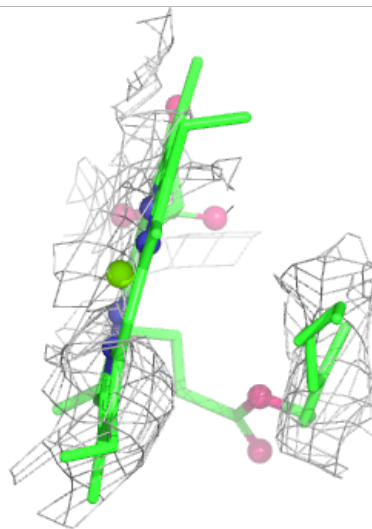
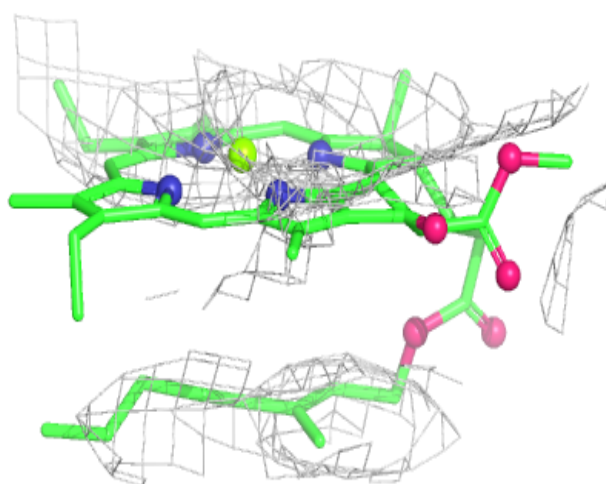
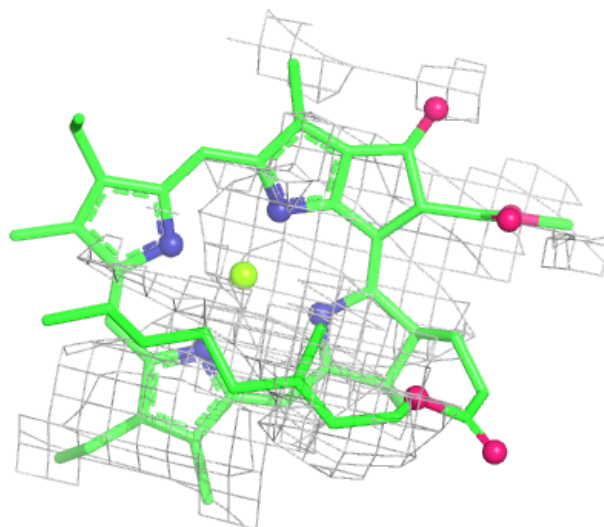
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	BCR	J	1105	40/40	0.99	0.07	63,67,71,71	0
13	CLA	B	816	60/65	0.99	0.09	46,53,111,221	0
13	CLA	B	817	65/65	0.99	0.09	57,65,113,125	0
13	CLA	B	818	47/65	0.99	0.09	56,99,146,292	0
16	LHG	A	853	49/49	0.99	0.09	57,74,107,127	0
16	LHG	A	854	27/49	0.99	0.06	49,58,88,122	0
13	CLA	B	819	45/65	0.99	0.10	98,131,171,173	0
13	CLA	A	834	65/65	0.99	0.08	39,40,92,96	0
13	CLA	A	806	65/65	0.99	0.09	63,80,155,164	0
17	SF4	C	102	8/8	1.00	0.03	47,48,122,359	0
17	SF4	A	856	8/8	1.00	0.04	49,50,150,174	0
17	SF4	C	101	8/8	1.00	0.03	48,48,49,62	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.

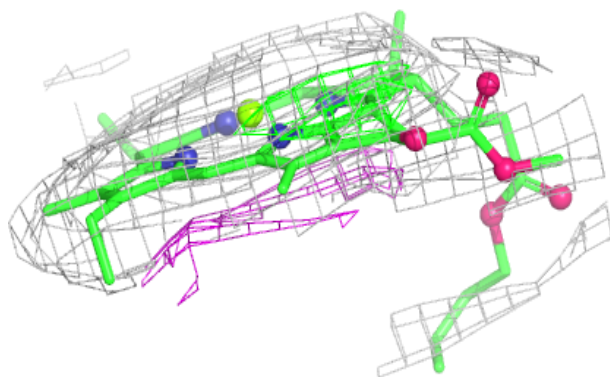
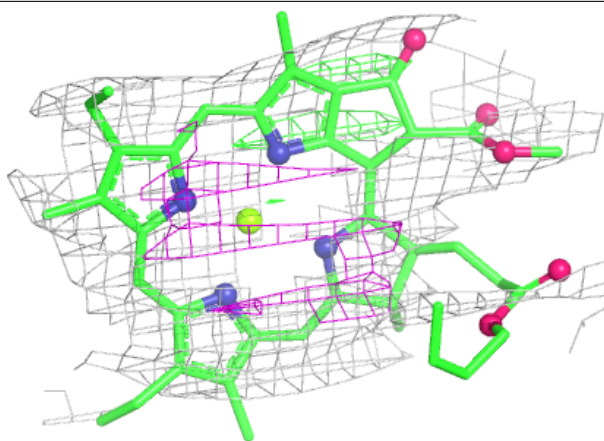
Electron density around CLA A 812:

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



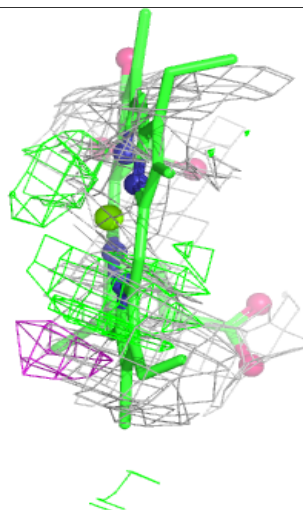
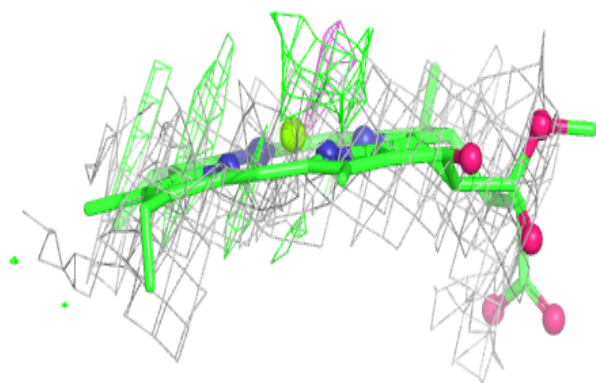
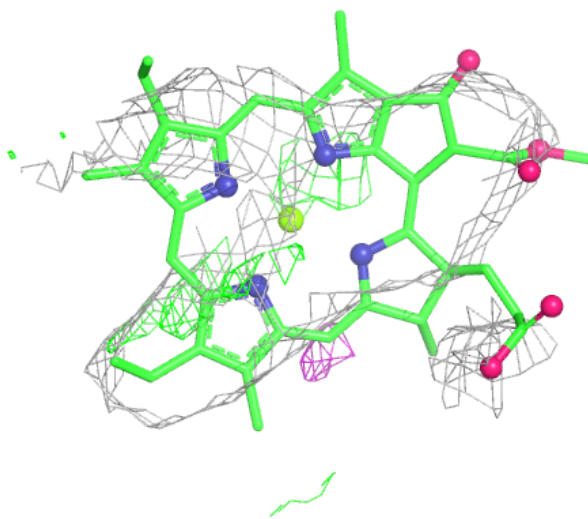
Electron density around CLA B 829:

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



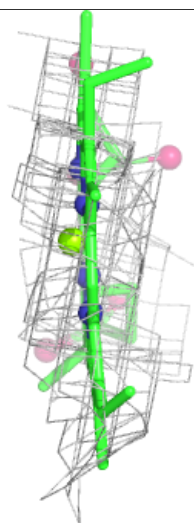
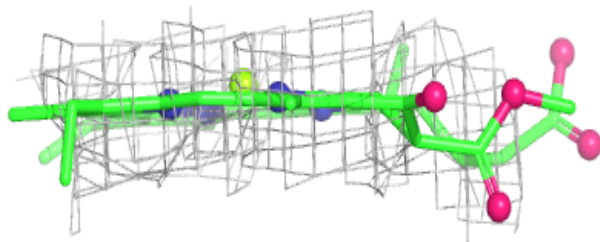
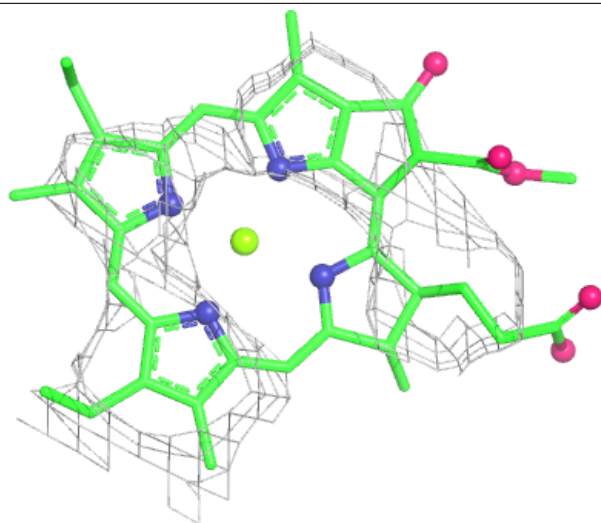
Electron density around CLA B 832:

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



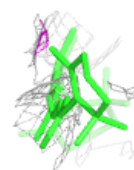
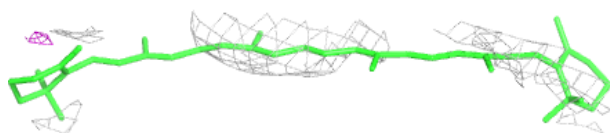
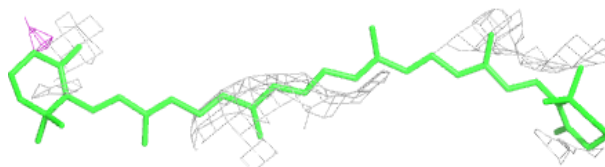
Electron density around CLA B 834:

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

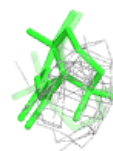
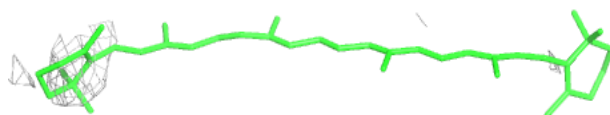


Electron density around BCR A 847:

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

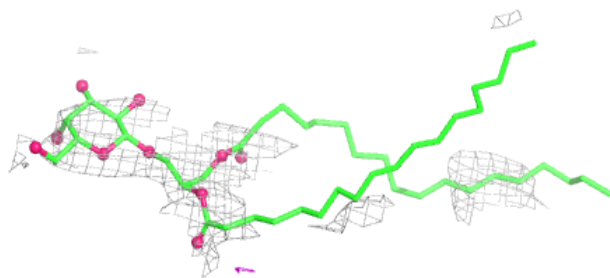
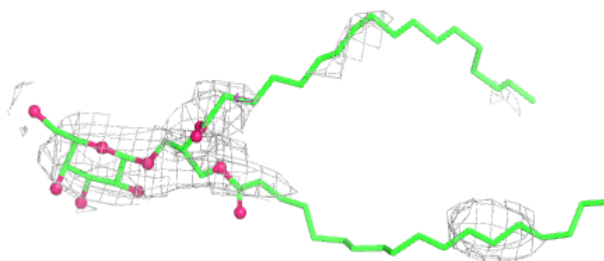
**Electron density around BCR A 849:**

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



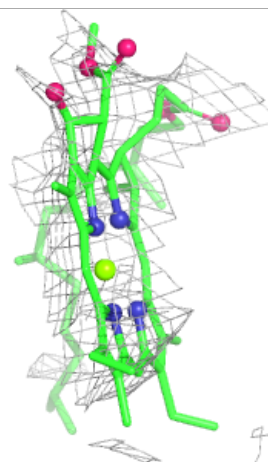
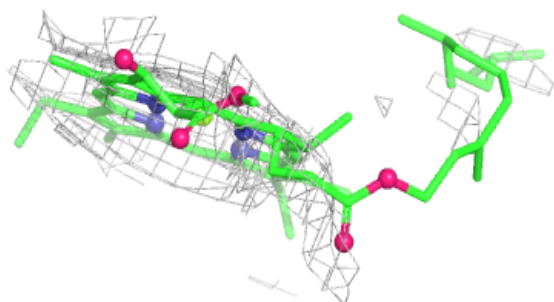
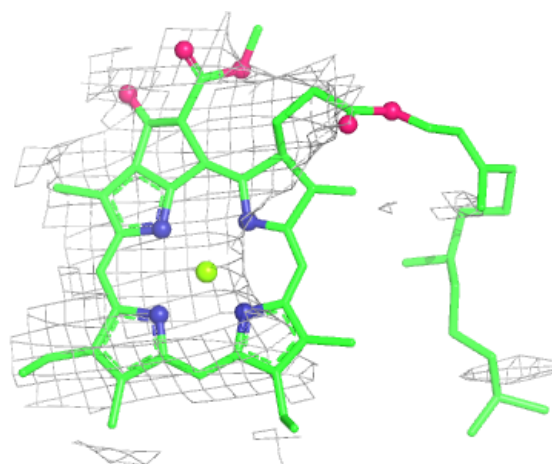
Electron density around LMG B 848:

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



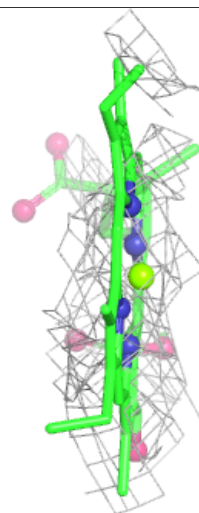
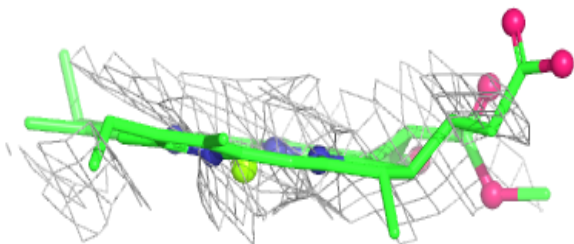
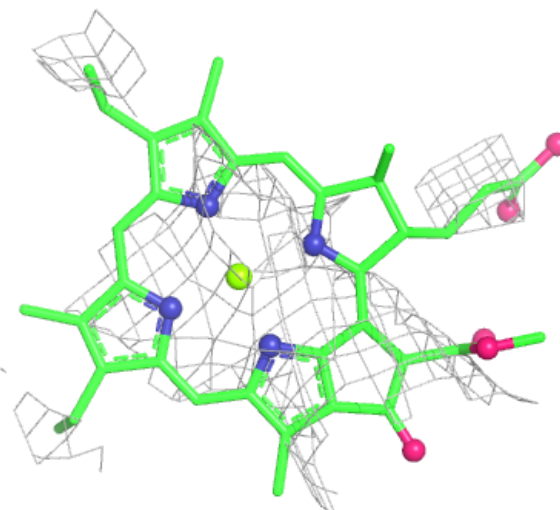
Electron density around CLA A 813:

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



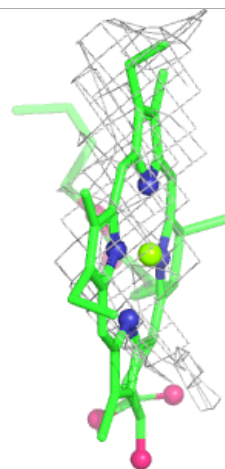
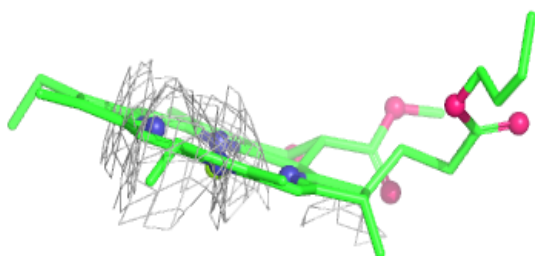
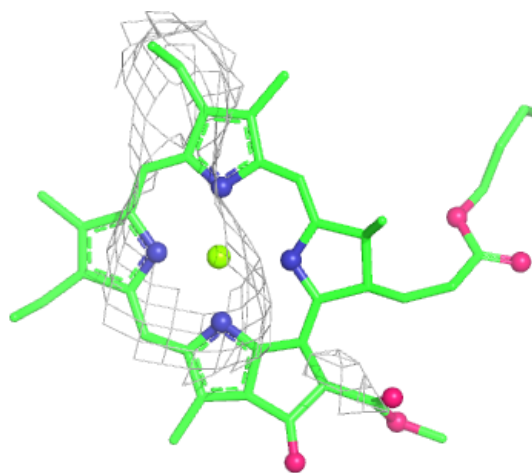
Electron density around CLA A 815:

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



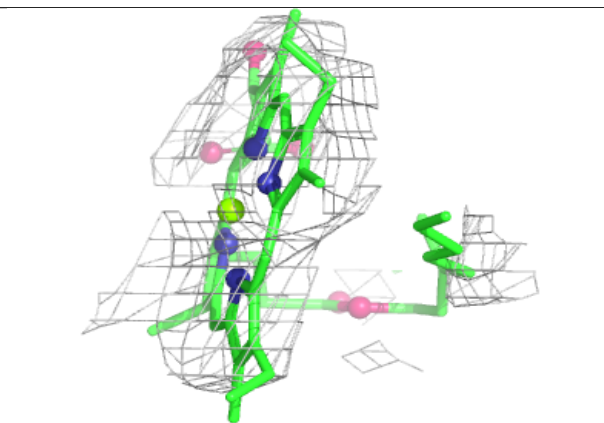
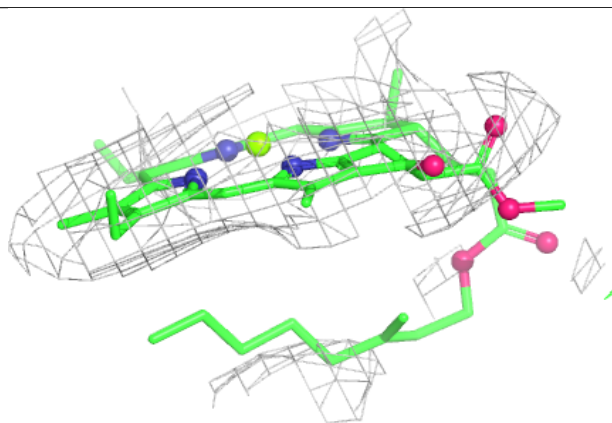
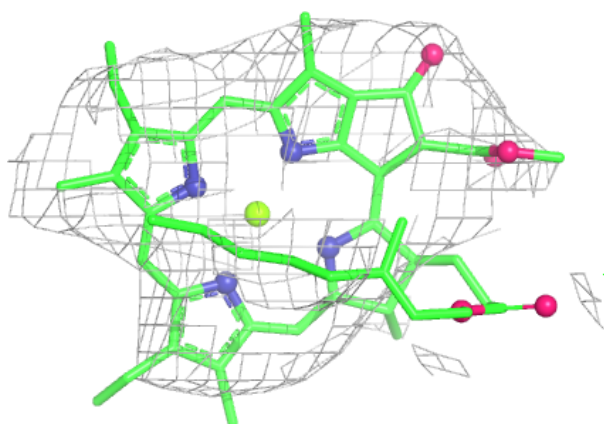
Electron density around CLA A 816:

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and green (positive)

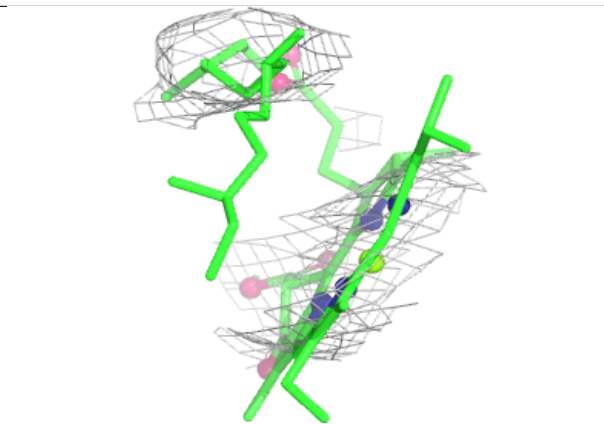
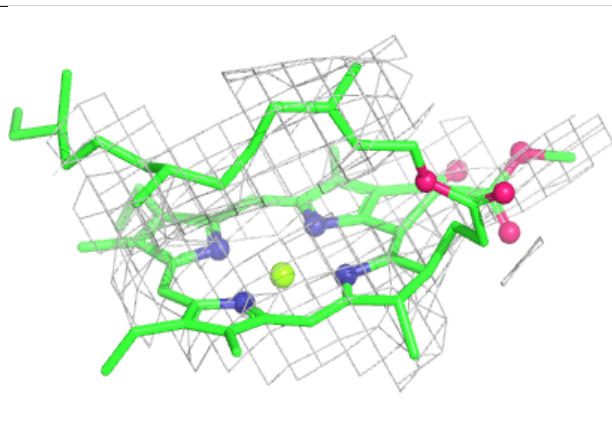
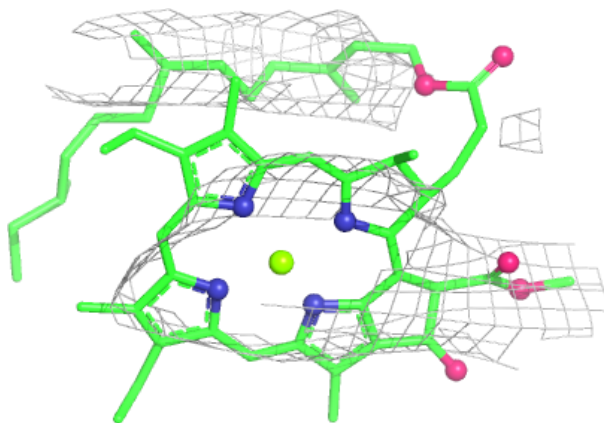


Electron density around CLA A 817:

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and green (positive)

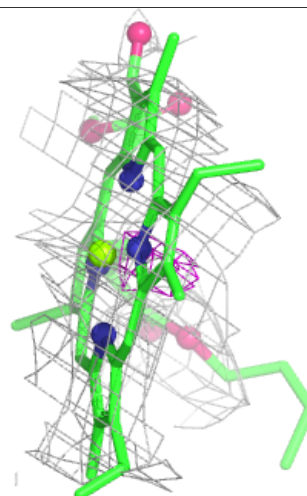
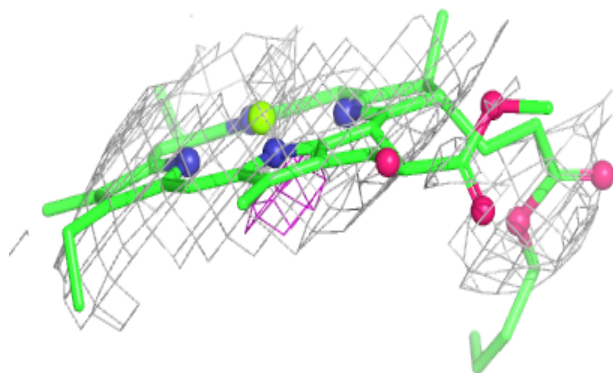
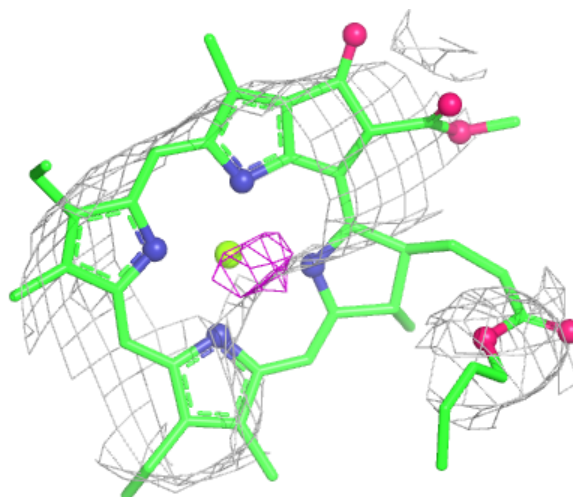
**Electron density around CLA A 820:**

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



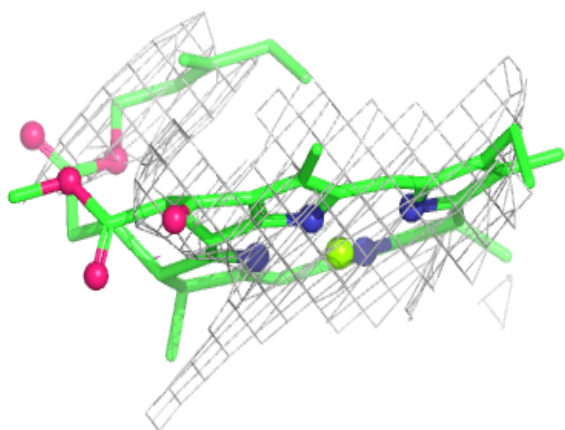
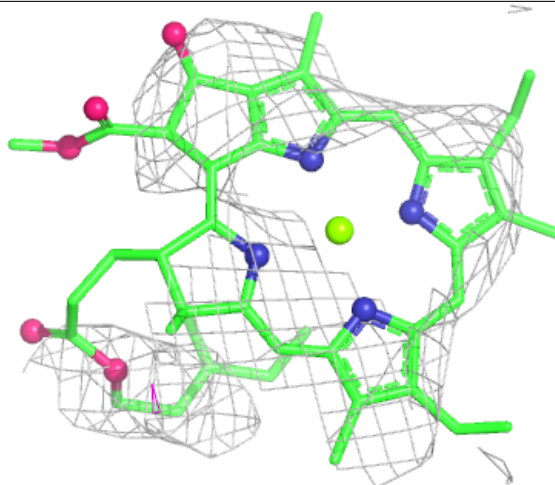
Electron density around CLA A 822:

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



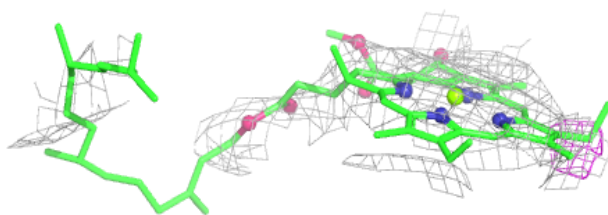
Electron density around CLA A 823:

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

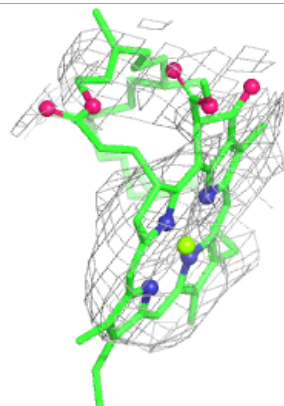
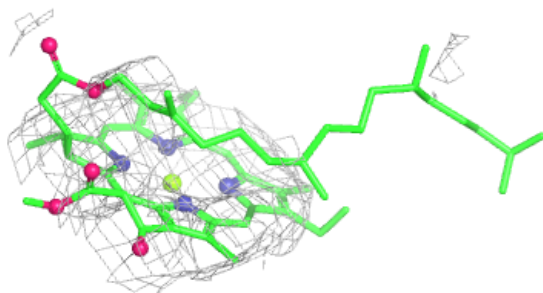
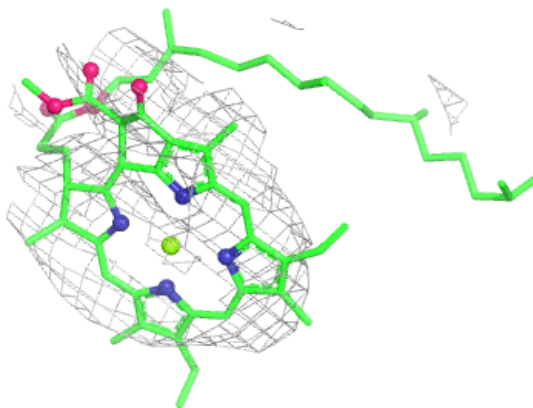


Electron density around CLA A 827:

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and green (positive)

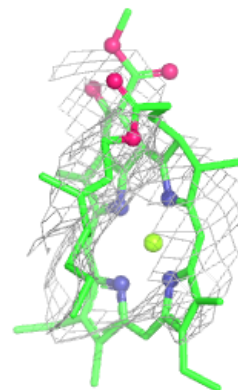
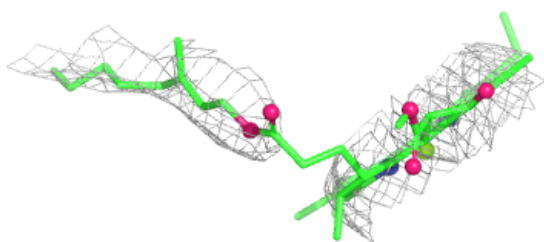
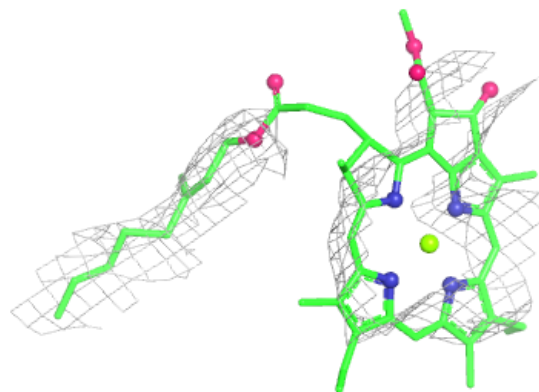
**Electron density around CLA A 829:**

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



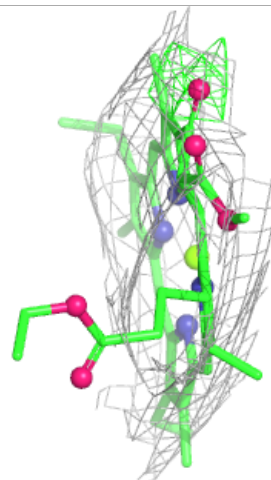
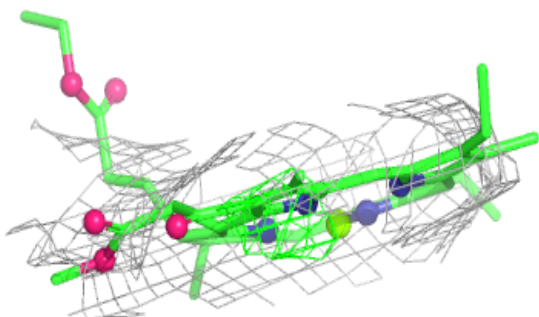
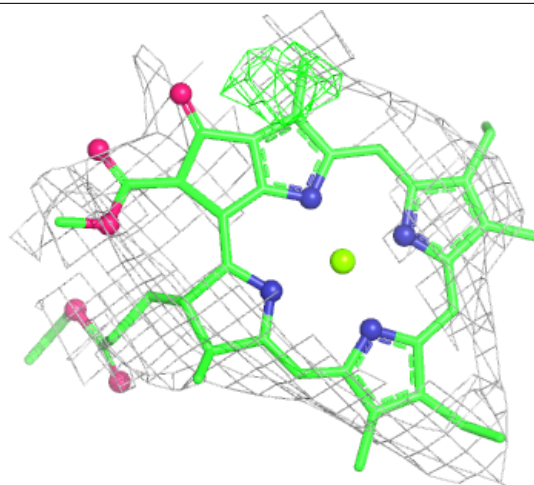
Electron density around CLA A 835:

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



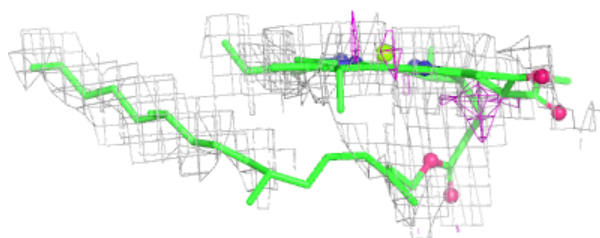
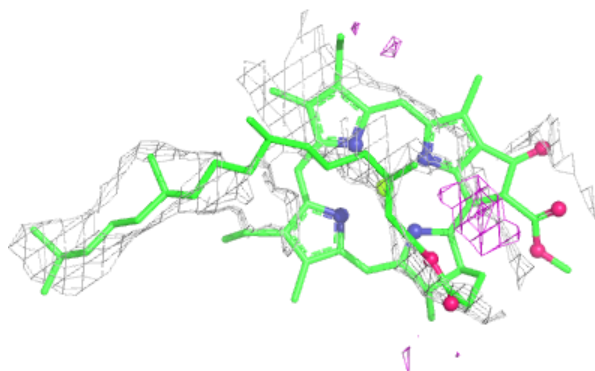
Electron density around CLA A 839:

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

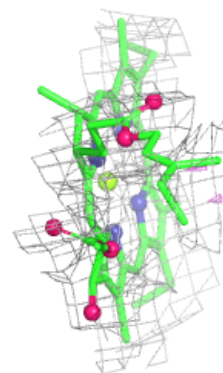
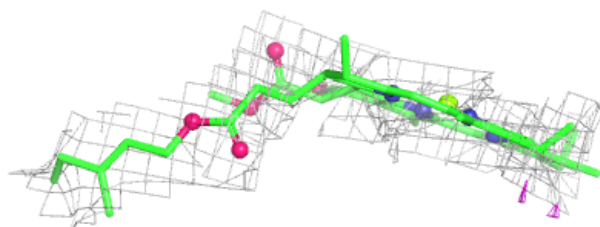
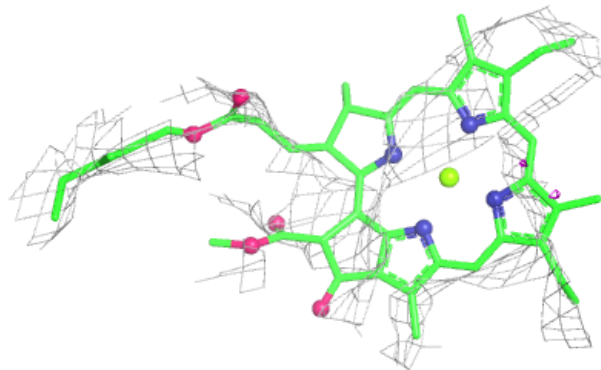


Electron density around CLA A 840:

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

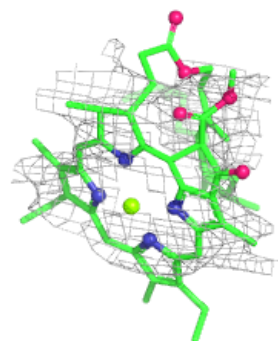
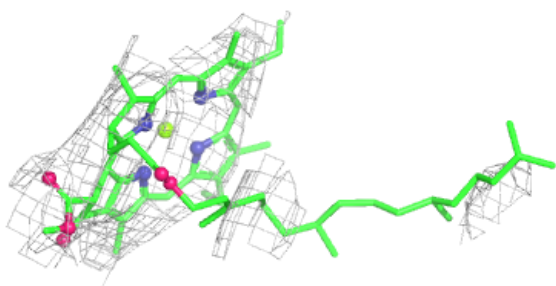
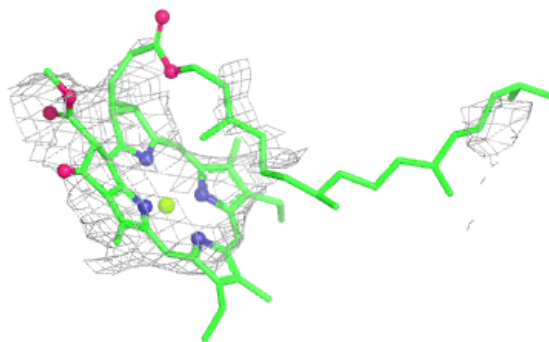
**Electron density around CLA A 841:**

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



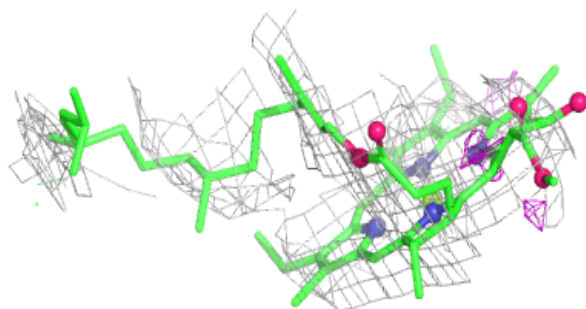
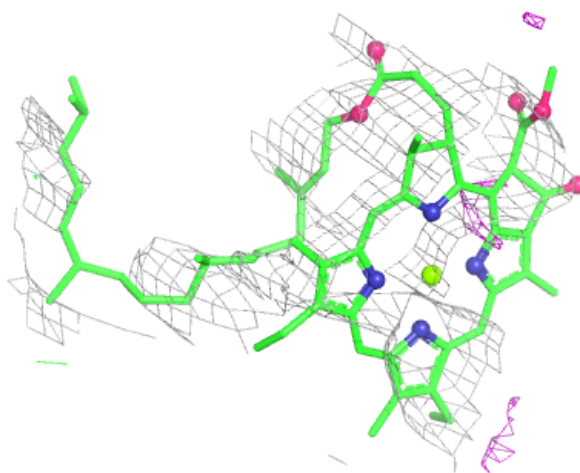
Electron density around CLA A 842:

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



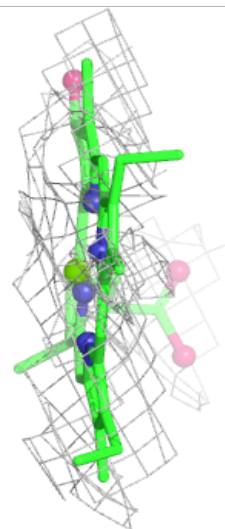
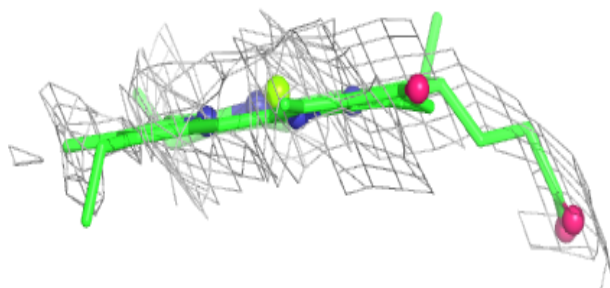
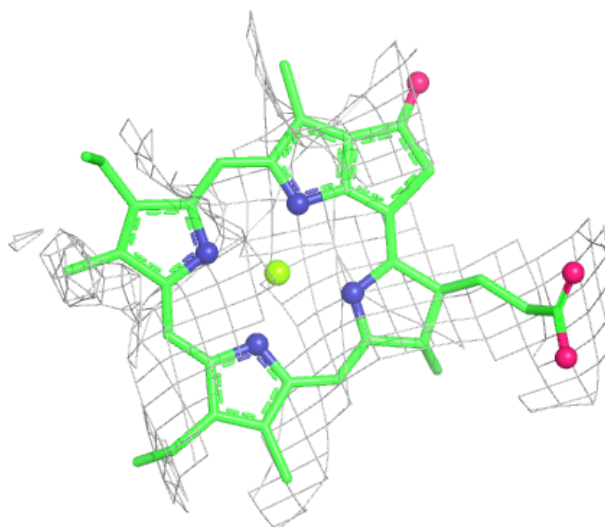
Electron density around CLA A 843:

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



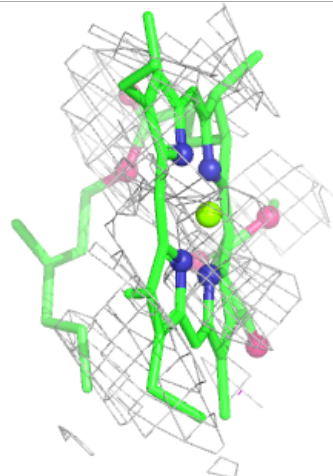
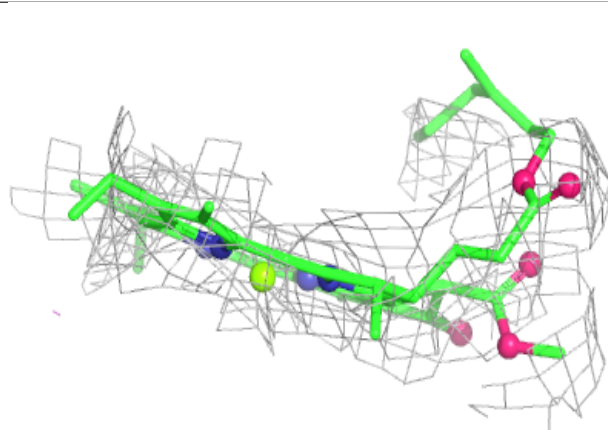
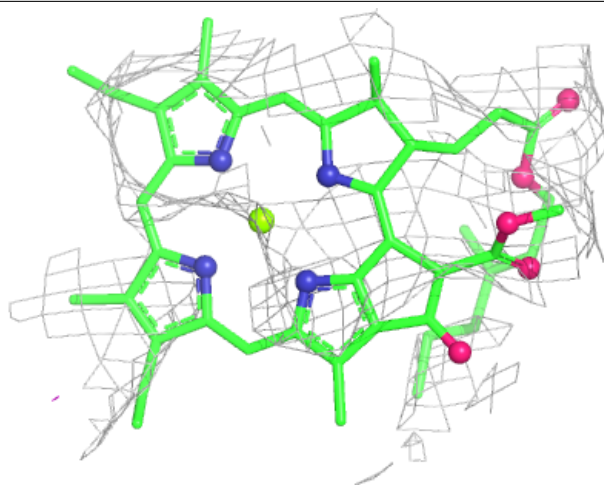
Electron density around CLA A 844:

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



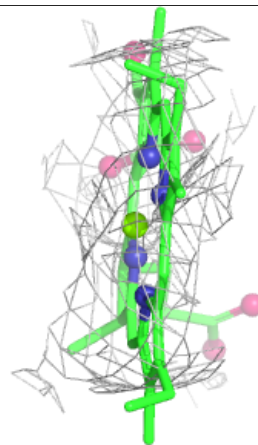
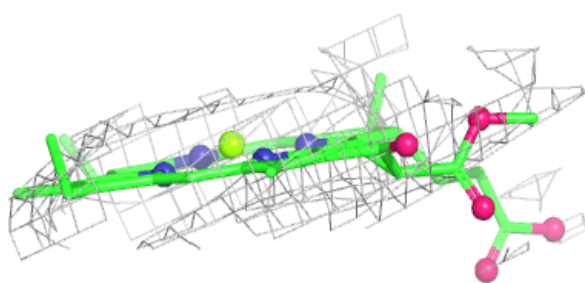
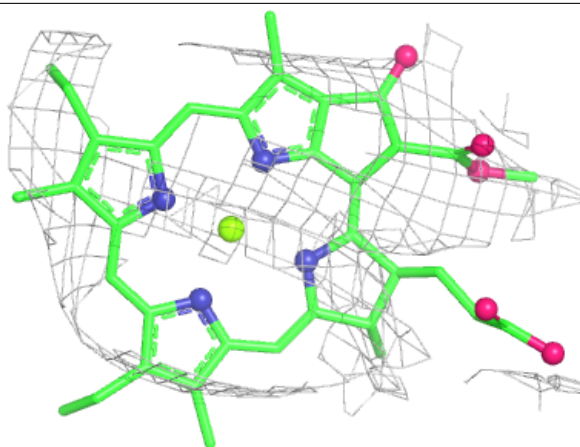
Electron density around CLA A 845:

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



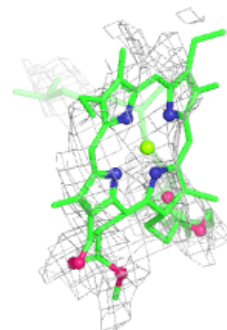
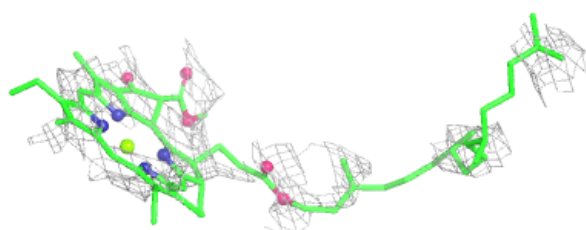
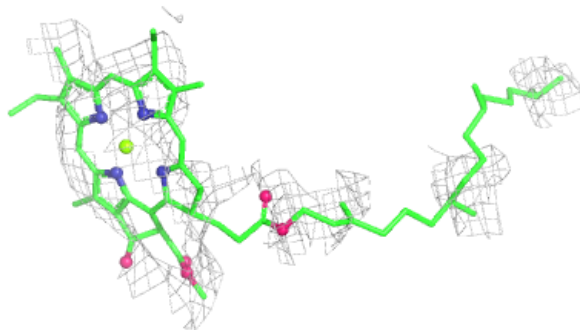
Electron density around CLA A 855:

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

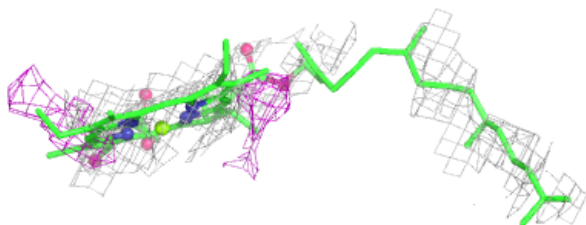
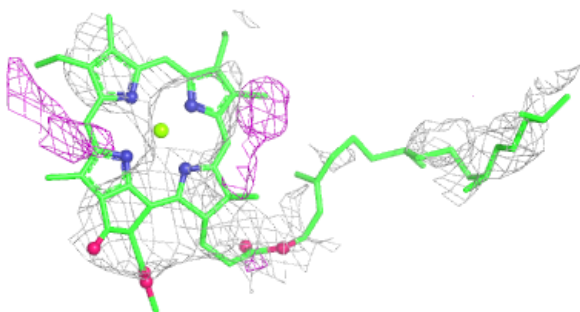


Electron density around CLA B 802:

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

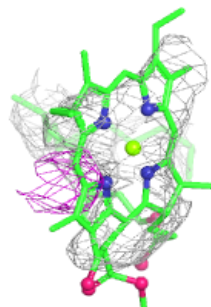
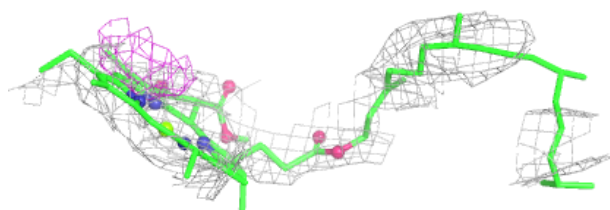
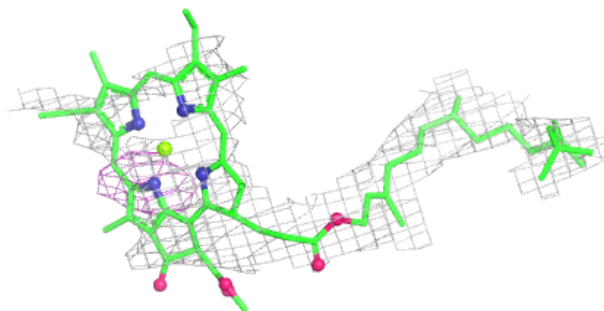
**Electron density around CLA B 803:**

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



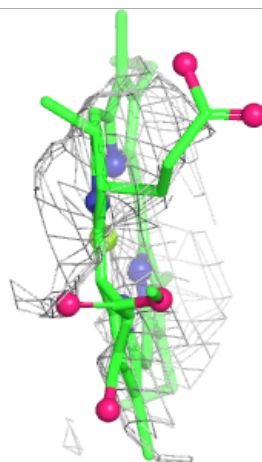
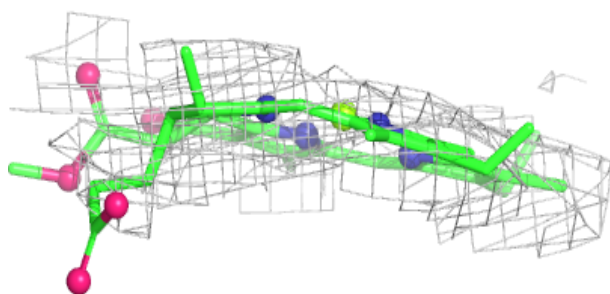
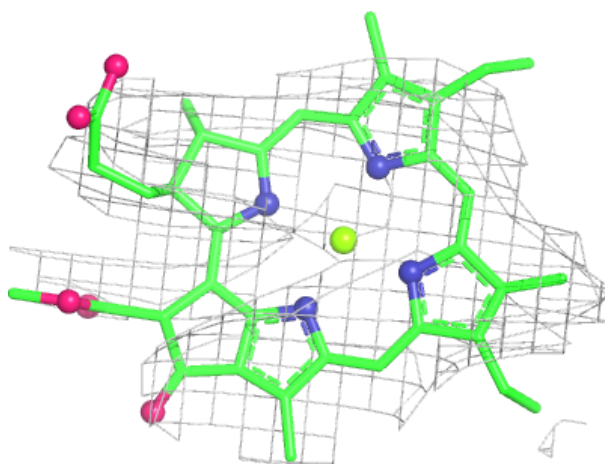
Electron density around CLA B 808:

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



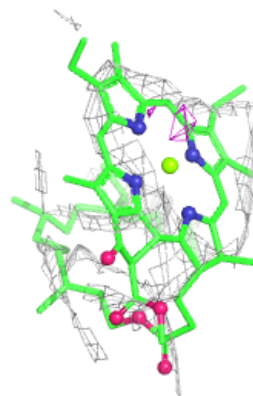
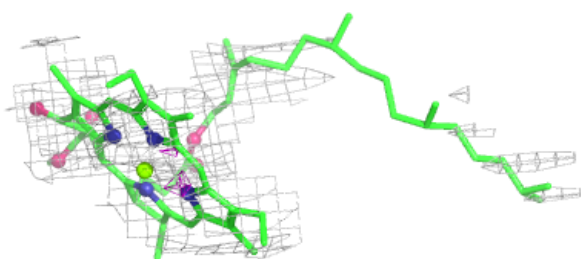
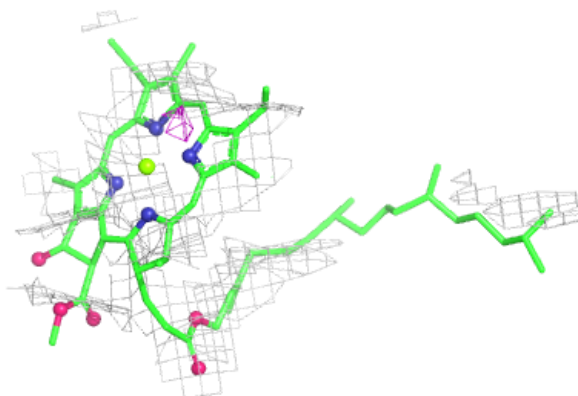
Electron density around CLA B 810:

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



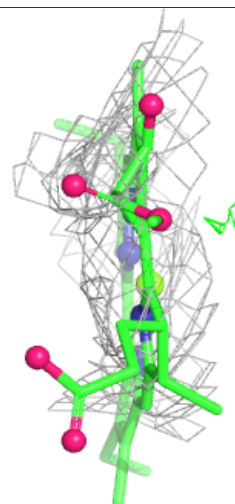
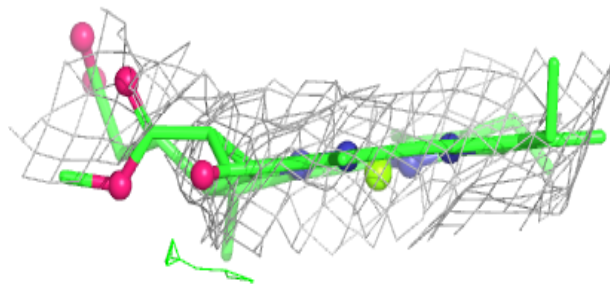
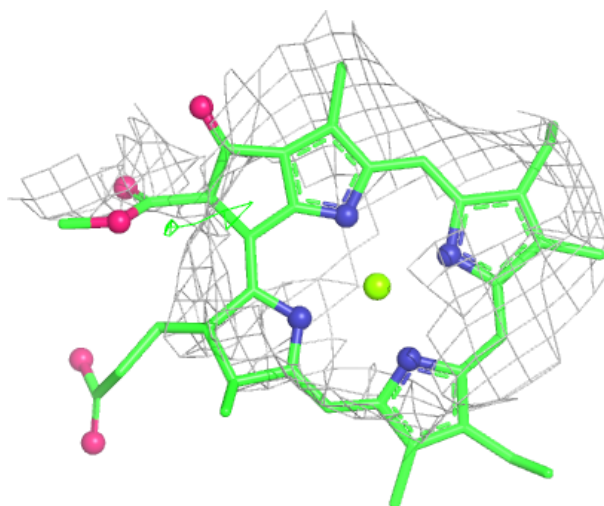
Electron density around CLA B 812:

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



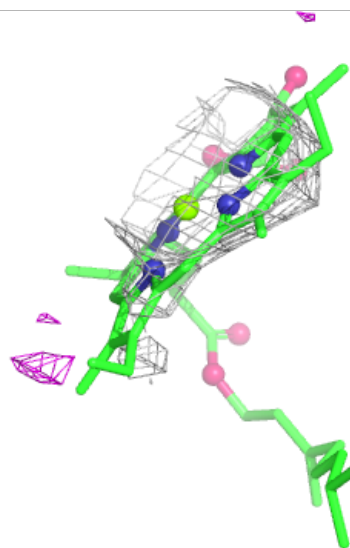
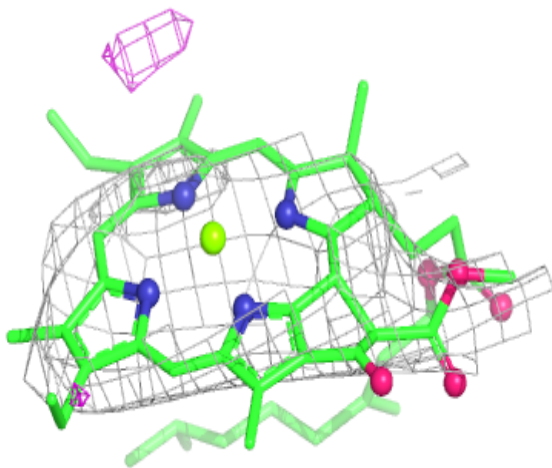
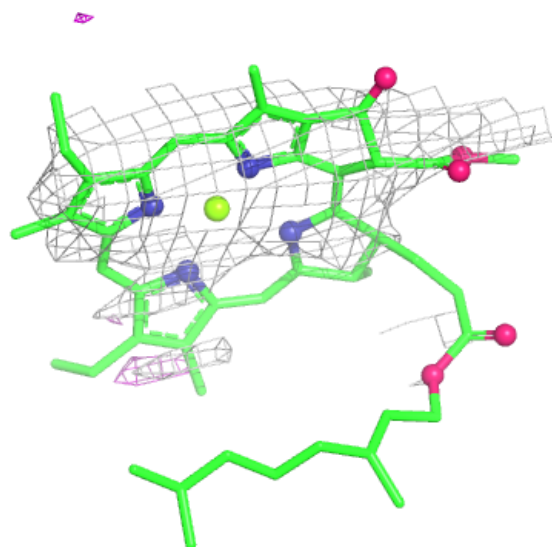
Electron density around CLA B 813:

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



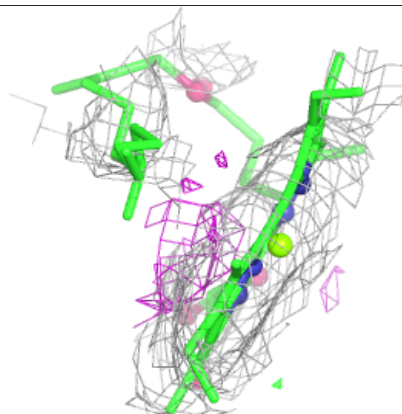
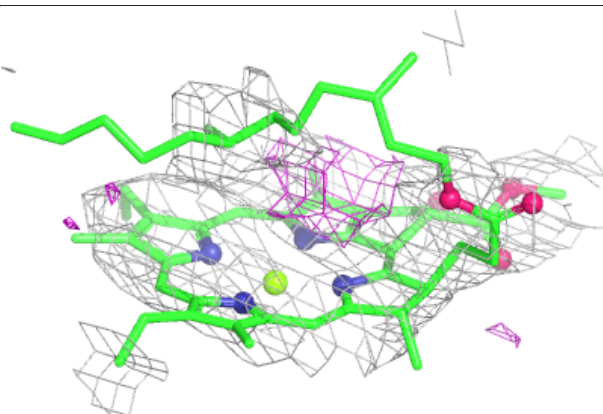
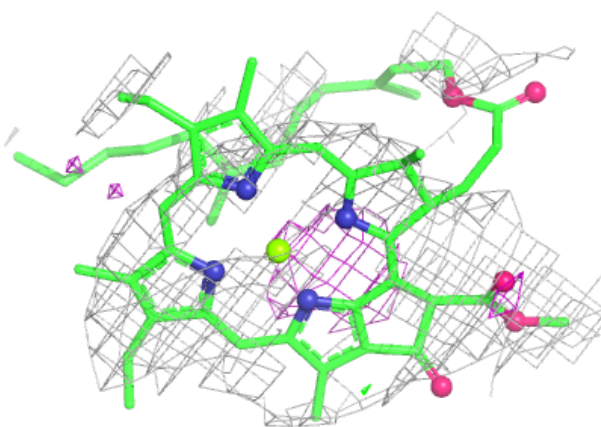
Electron density around CLA B 814:

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



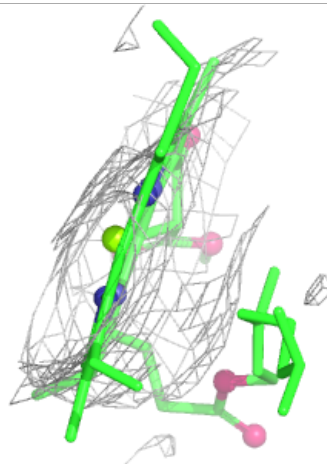
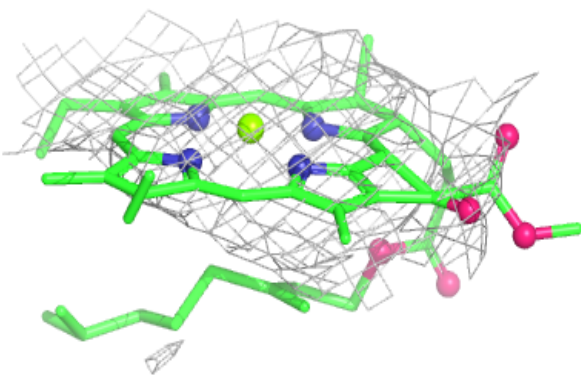
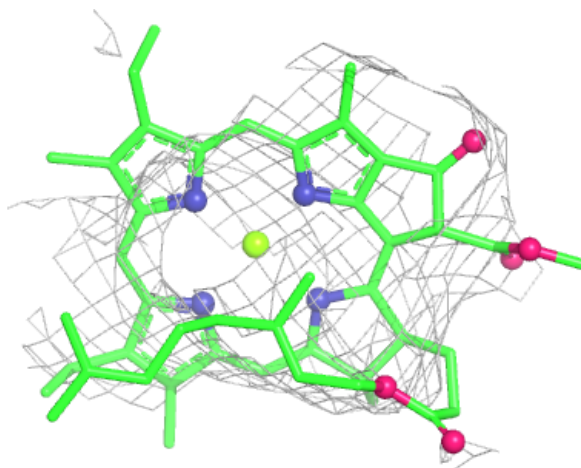
Electron density around CLA B 815:

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



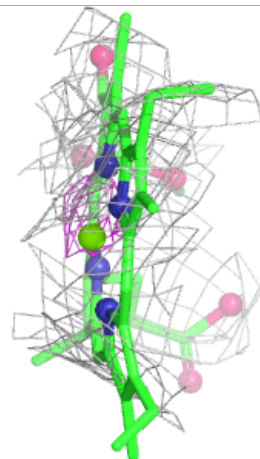
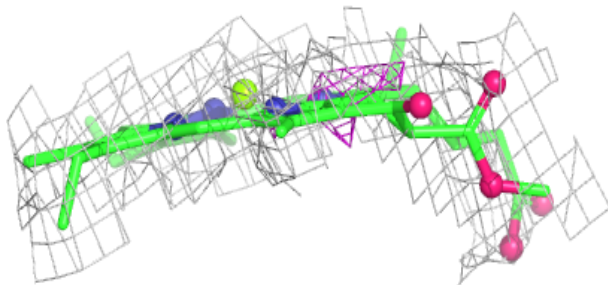
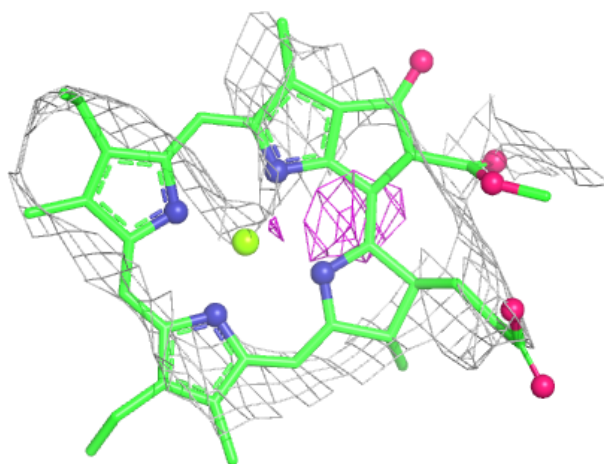
Electron density around CLA B 820:

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



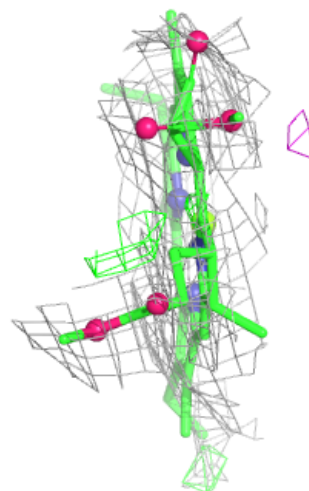
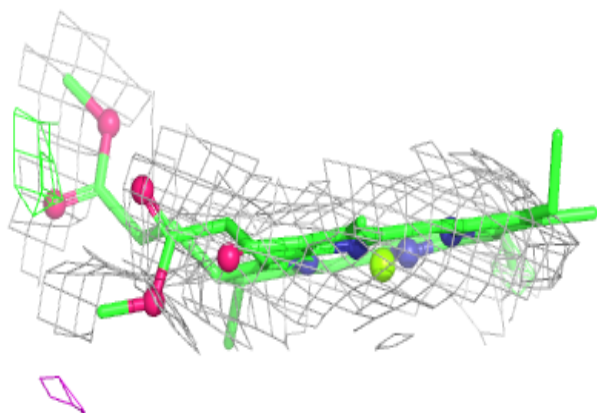
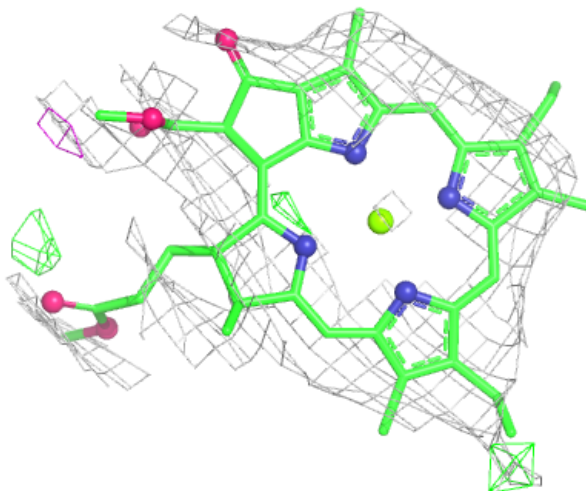
Electron density around CLA B 821:

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



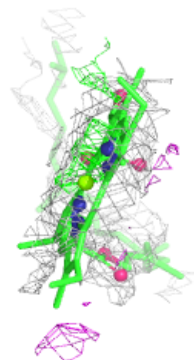
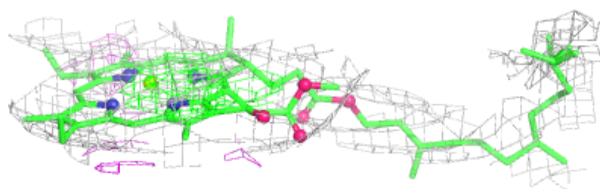
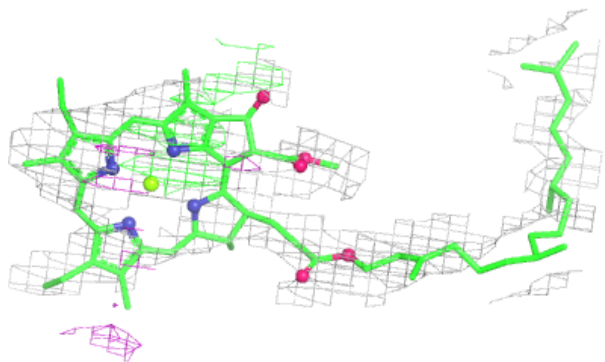
Electron density around CLA B 823:

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



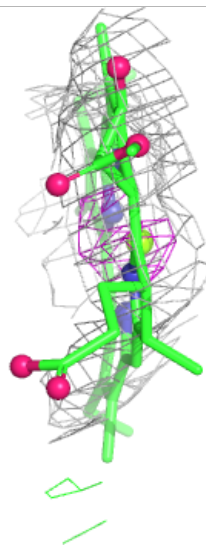
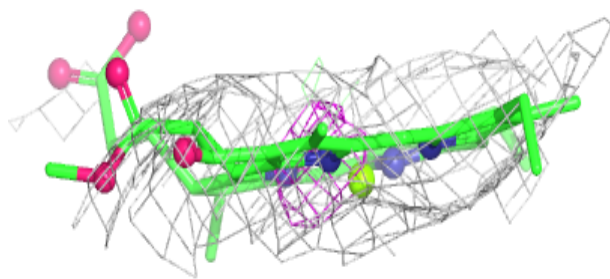
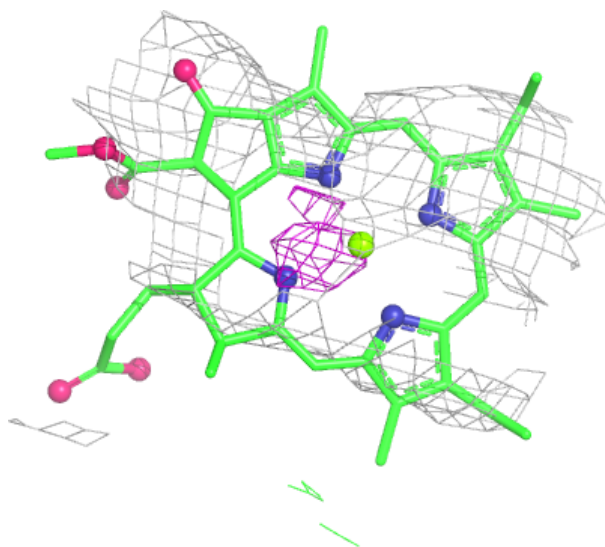
Electron density around CLA B 824:

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



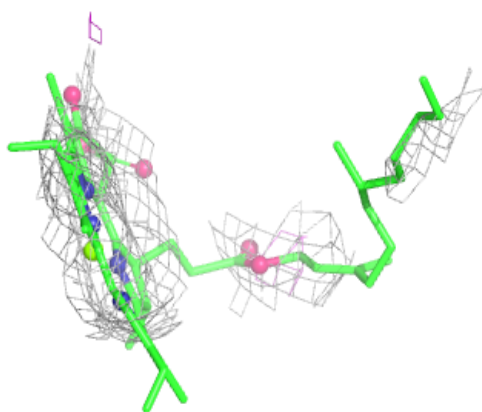
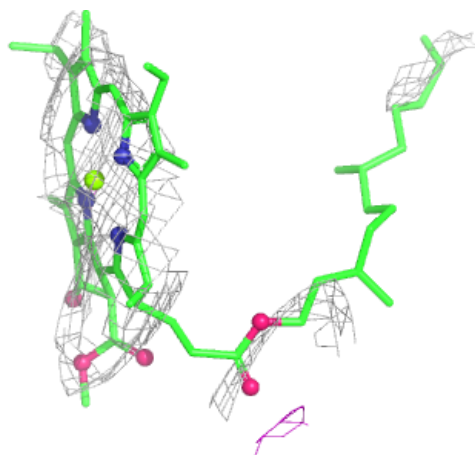
Electron density around CLA B 828:

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



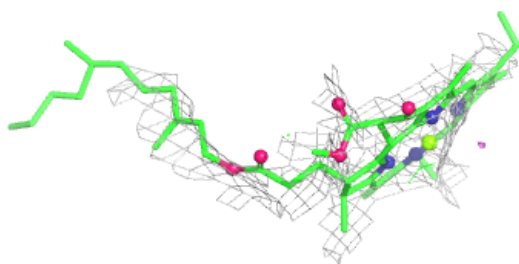
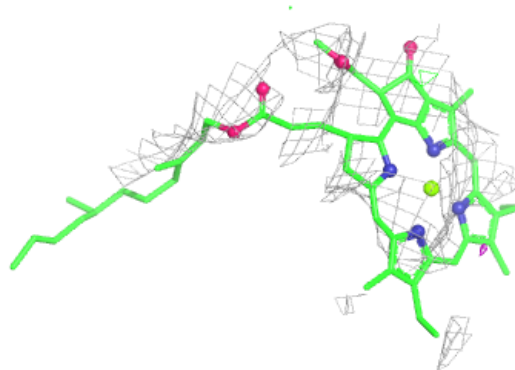
Electron density around CLA A 804:

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



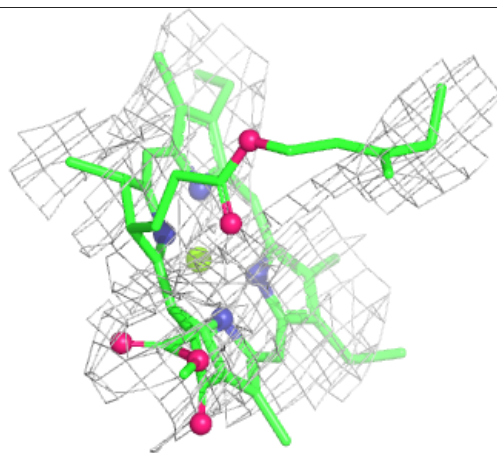
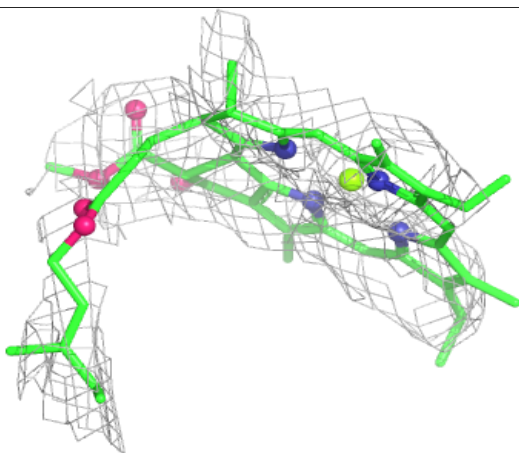
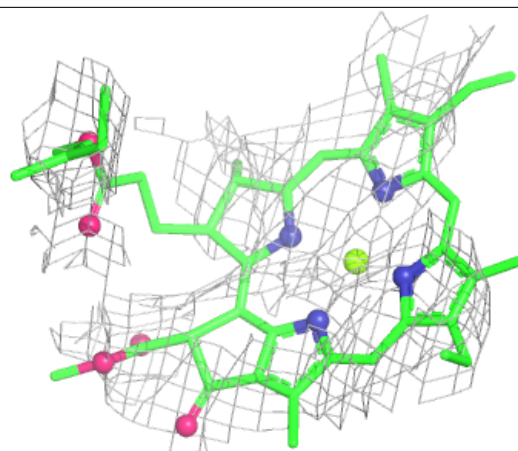
Electron density around CLA B 831:

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



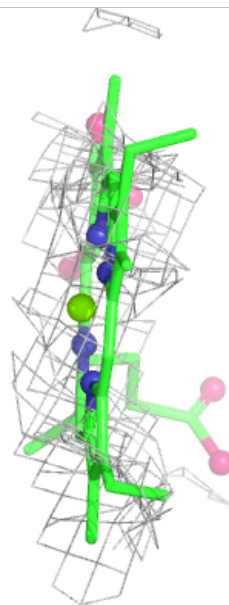
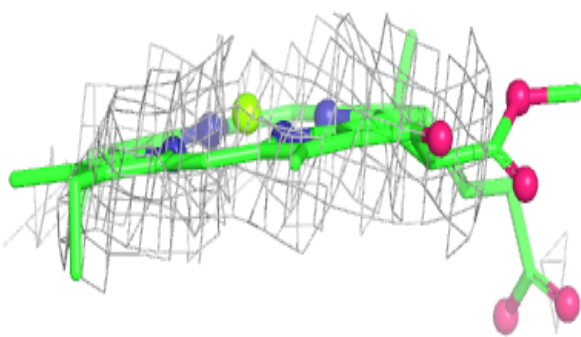
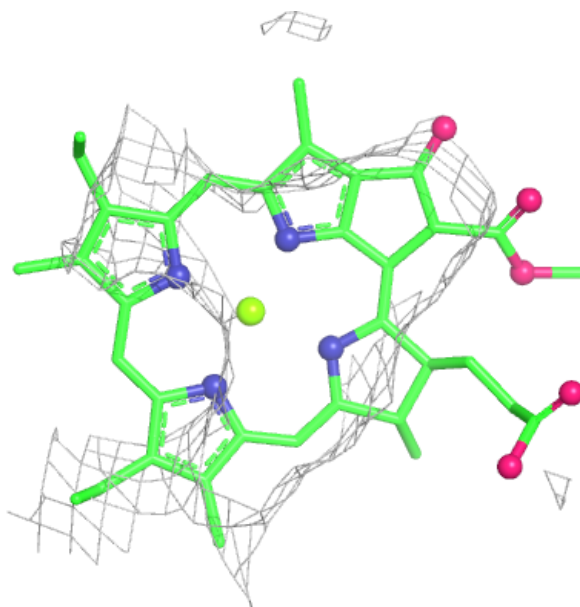
Electron density around CLA A 807:

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



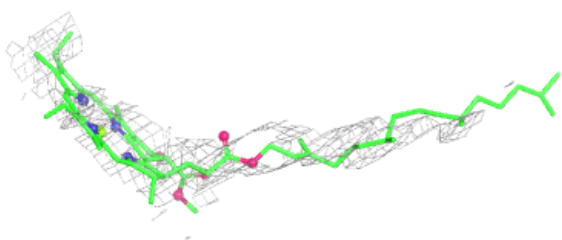
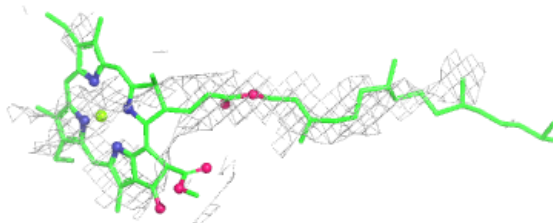
Electron density around CLA B 833:

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

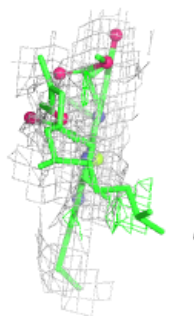
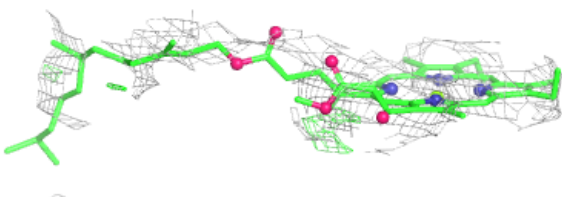


Electron density around CLA A 809:

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

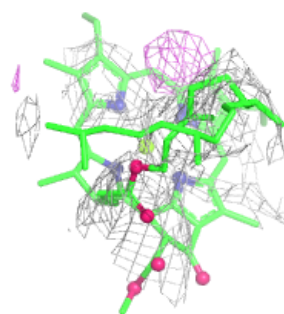
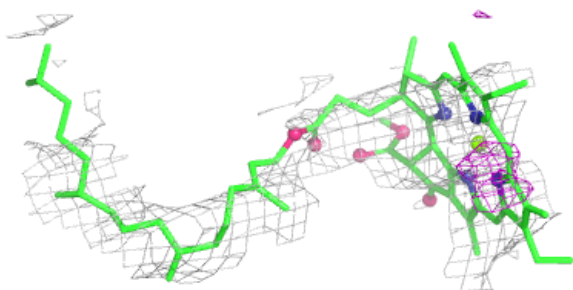
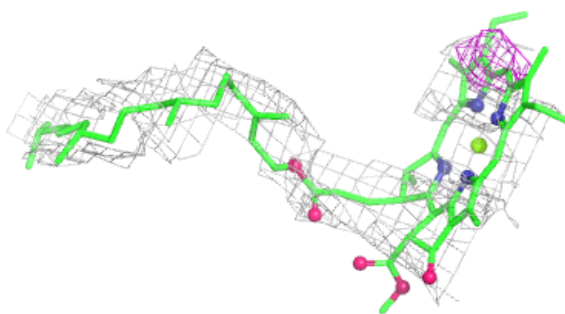
**Electron density around CLA B 835:**

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

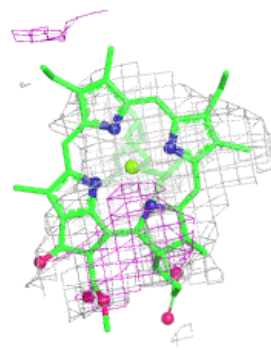
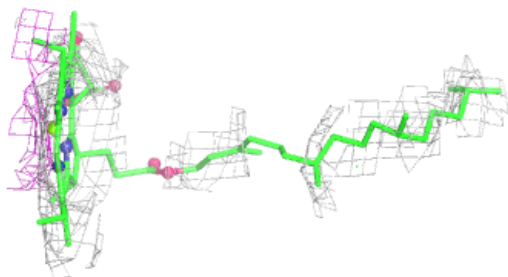
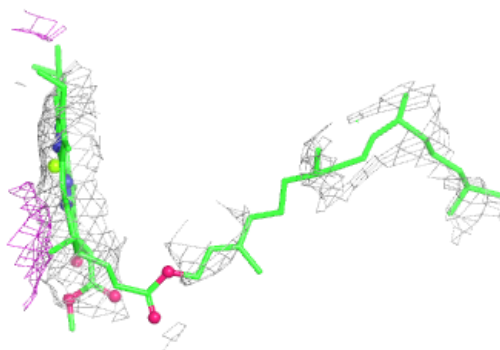


Electron density around CLA B 838:

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

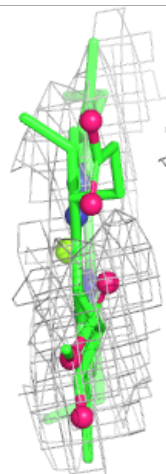
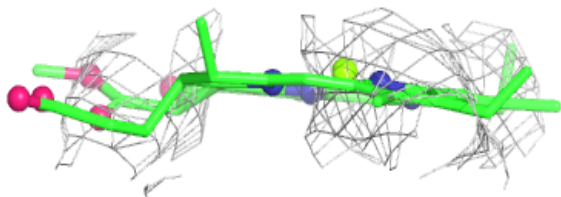
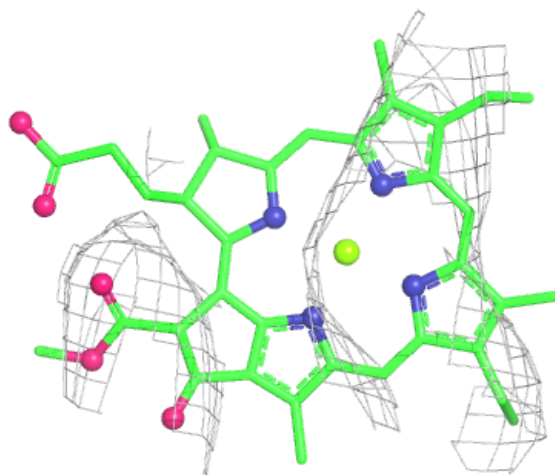
**Electron density around CLA B 839:**

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



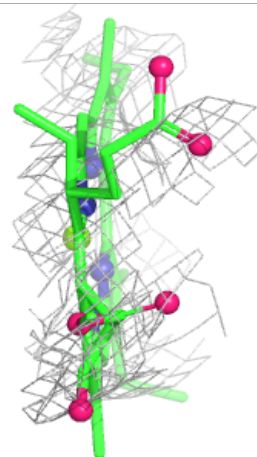
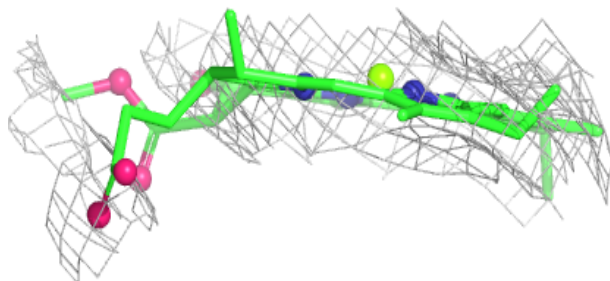
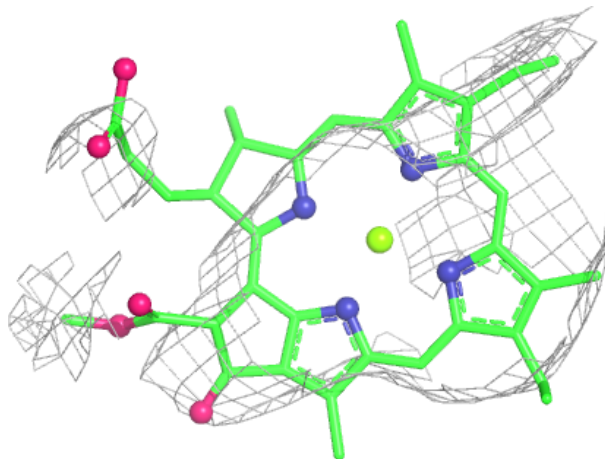
Electron density around CLA F 1301:

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



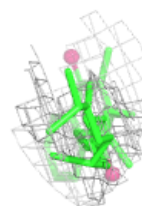
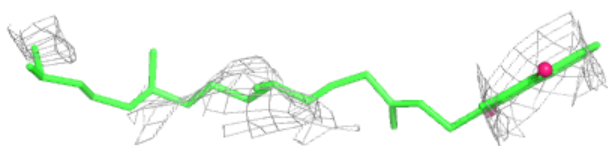
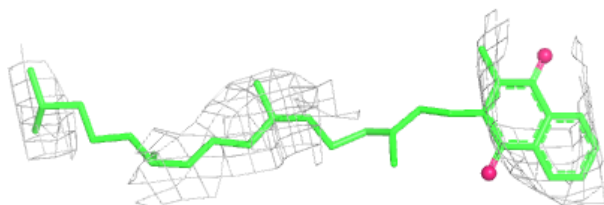
Electron density around CLA J 1102:

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

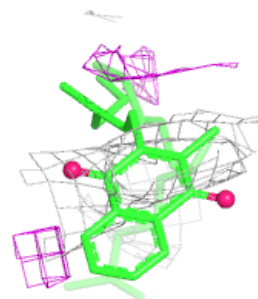
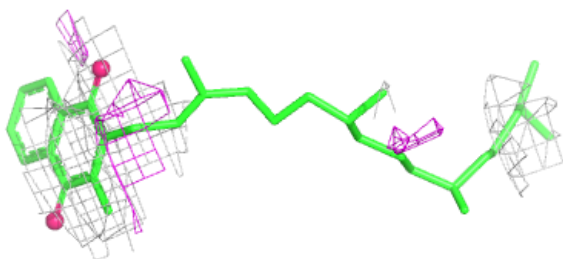
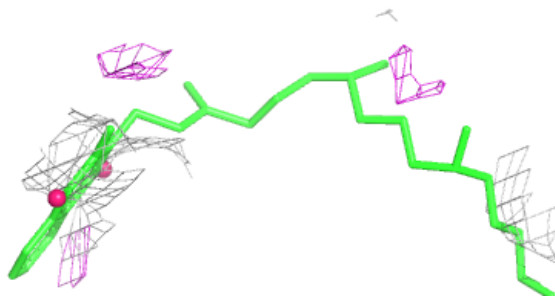


Electron density around PQN A 846:

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

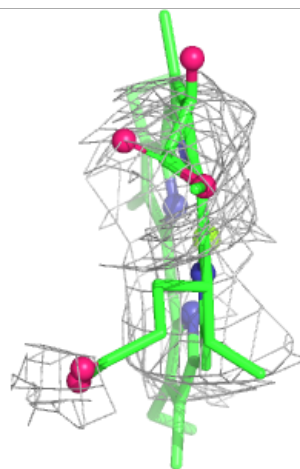
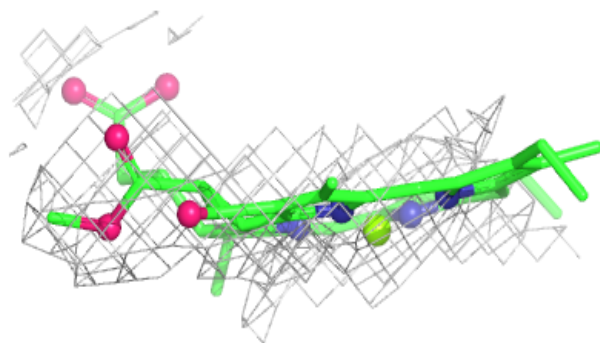
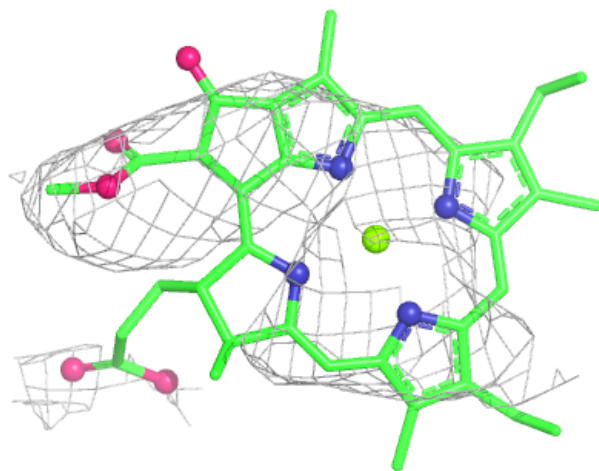
**Electron density around PQN B 840:**

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



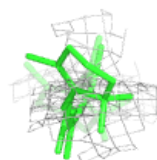
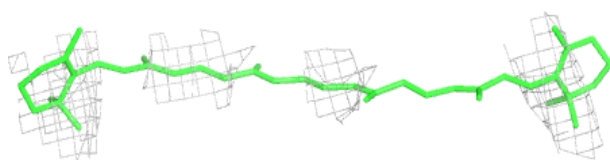
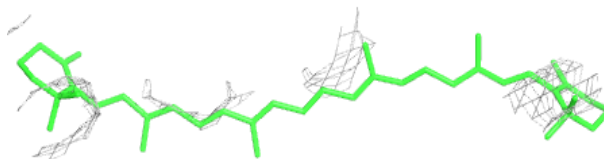
Electron density around CLA A 810:

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

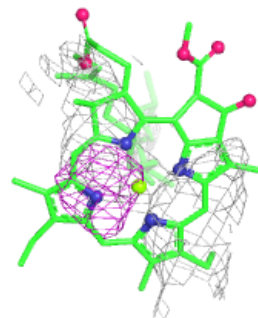
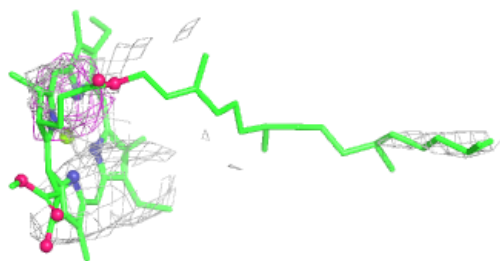
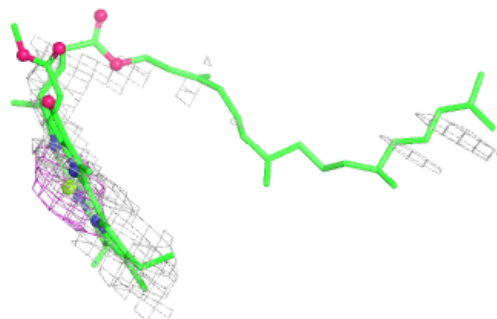


Electron density around BCR A 848:

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

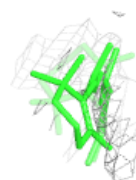
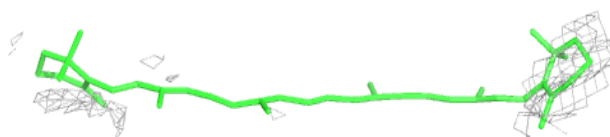
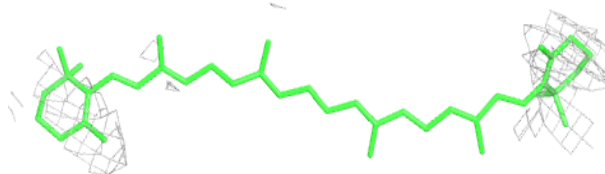
**Electron density around CLA A 811:**

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

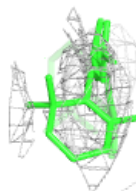
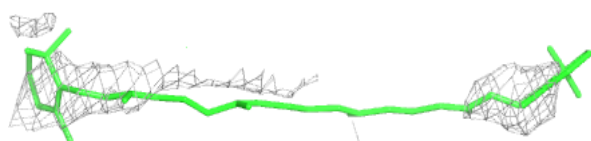


Electron density around BCR B 841:

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

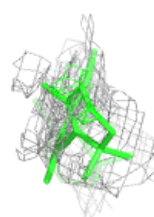
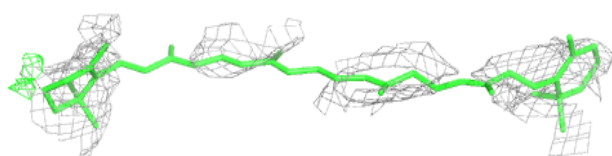
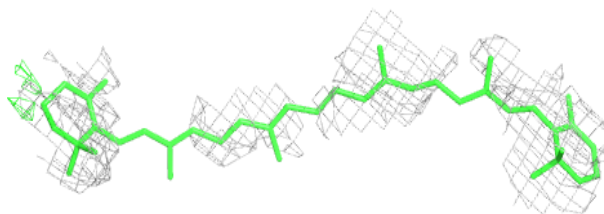
**Electron density around BCR B 843:**

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

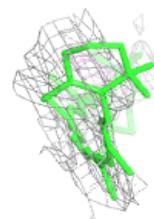
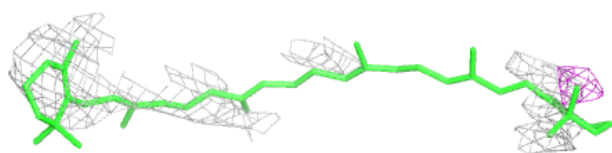
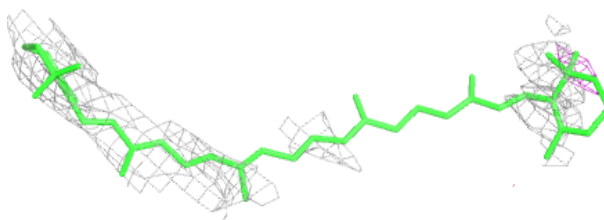


Electron density around BCR B 845:

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

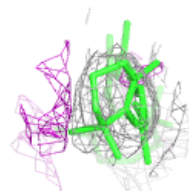
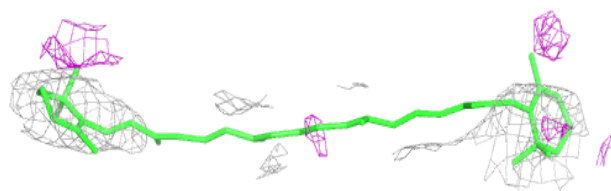
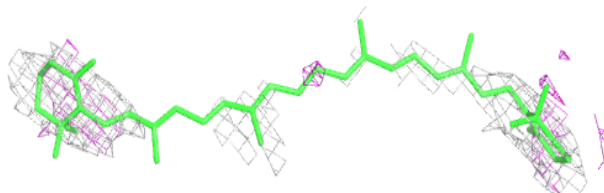
**Electron density around BCR B 846:**

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

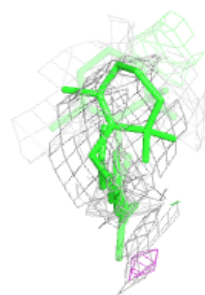
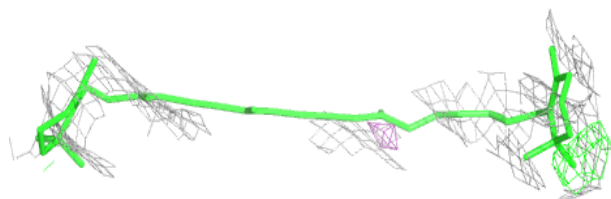
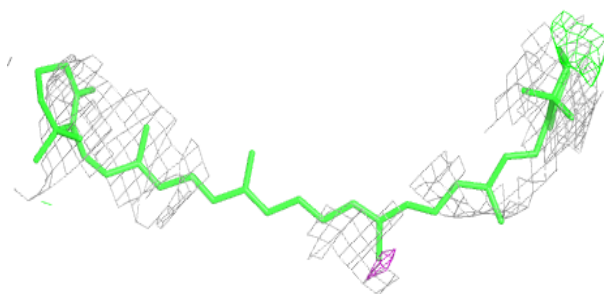


Electron density around BCR B 847:

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

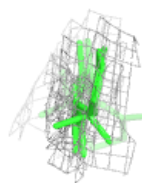
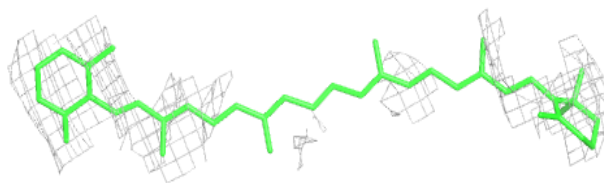
**Electron density around BCR B 849:**

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

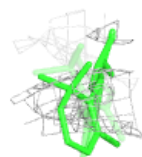
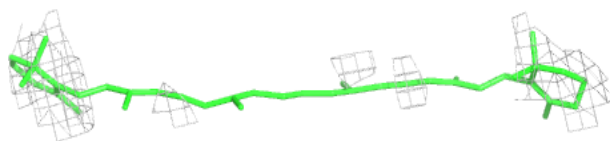
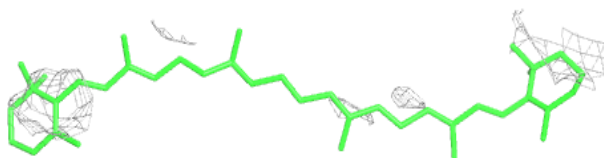


Electron density around BCR B 850:

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

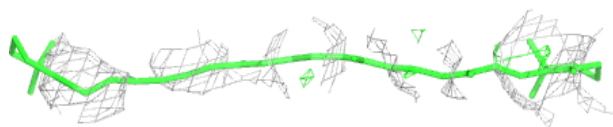
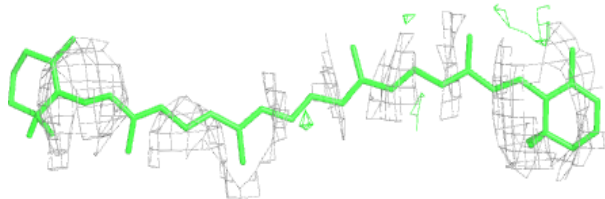
**Electron density around BCR J 1104:**

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

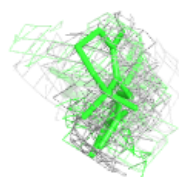
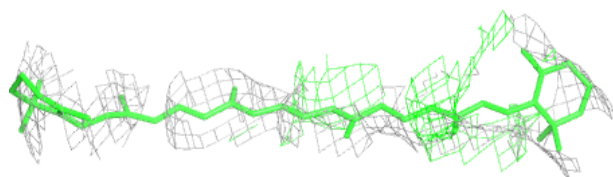
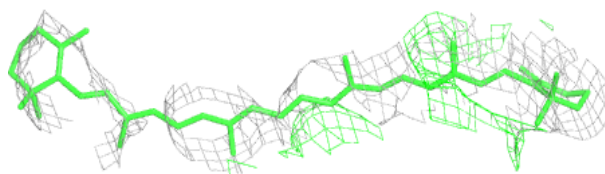


Electron density around BCR L 1005:

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

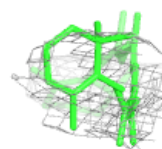
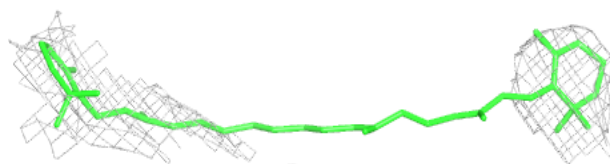
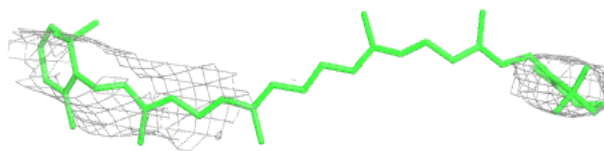
**Electron density around BCR L 1006:**

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



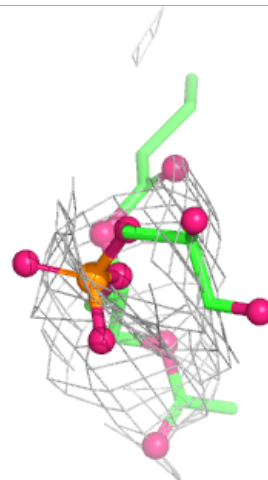
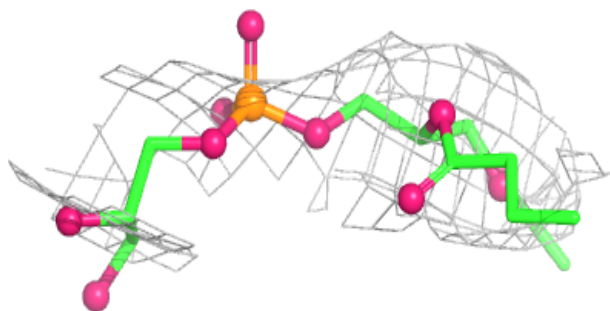
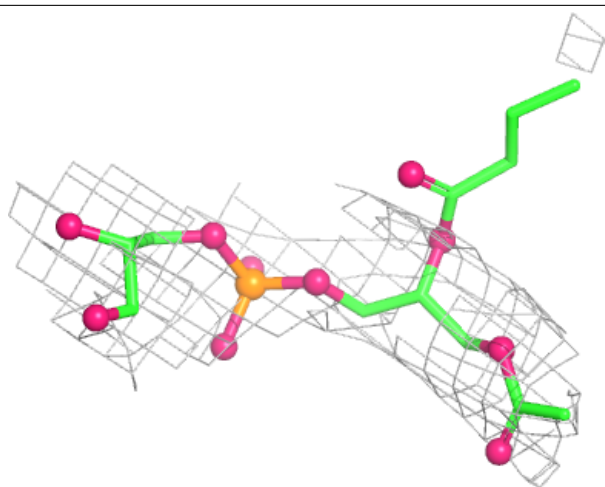
Electron density around BCR M 1203:

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



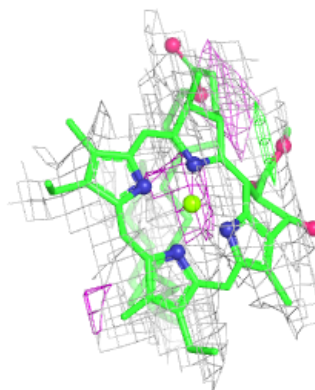
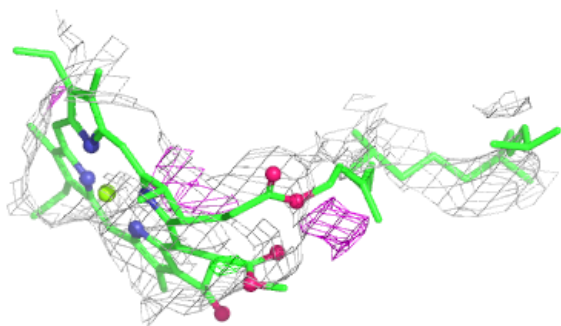
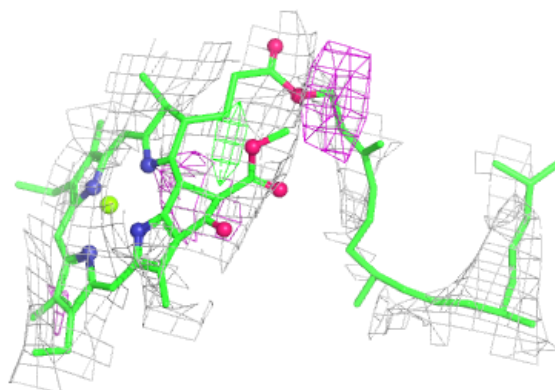
Electron density around LHG X 101:

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



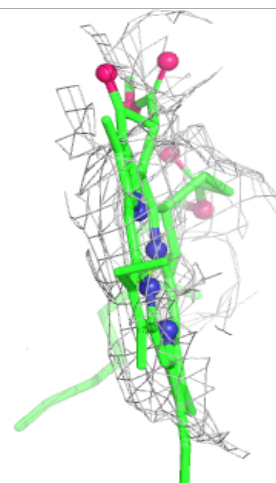
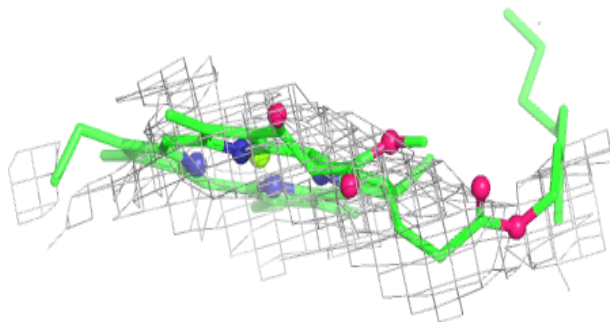
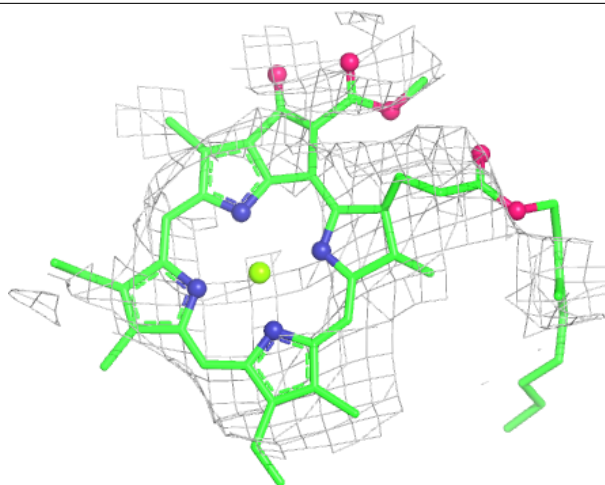
Electron density around CLA A 801:

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



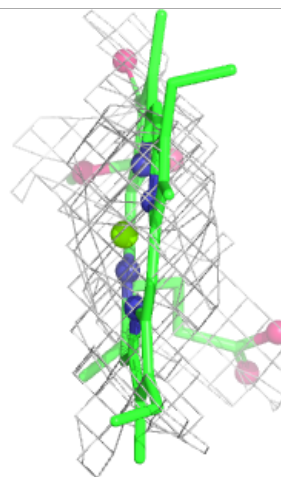
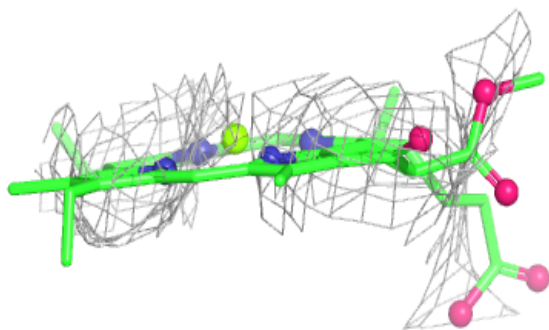
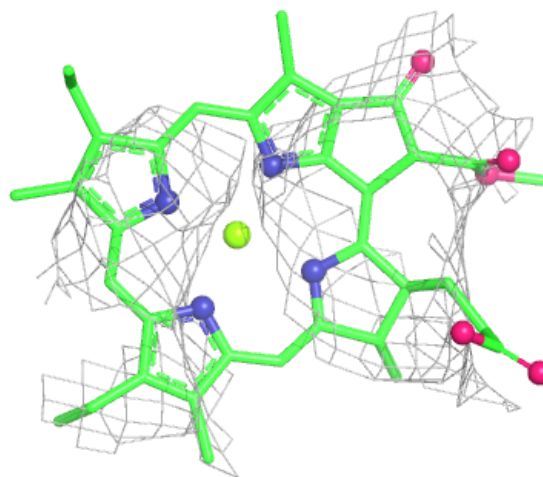
Electron density around CLA B 822:

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



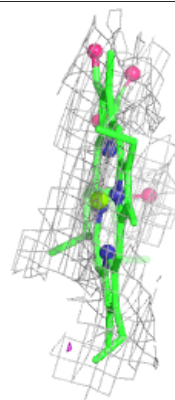
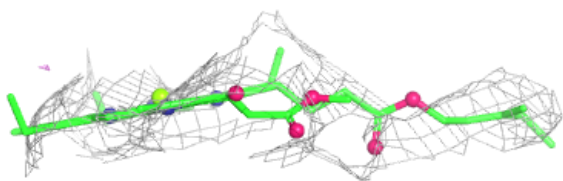
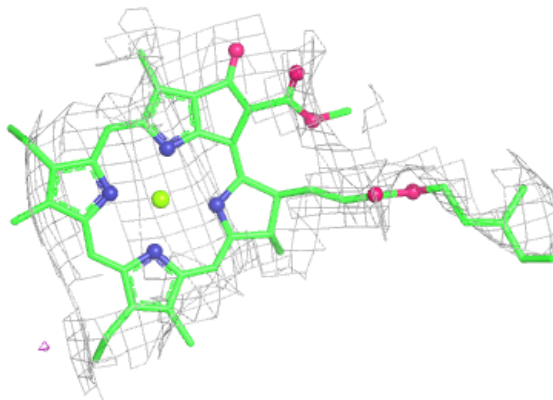
Electron density around CLA A 836:

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



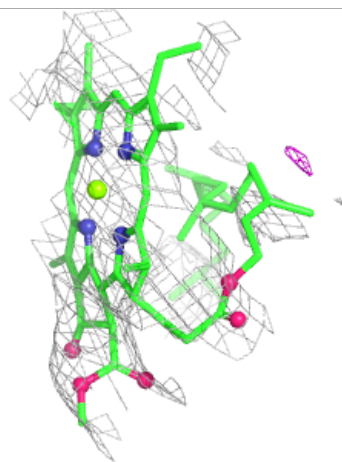
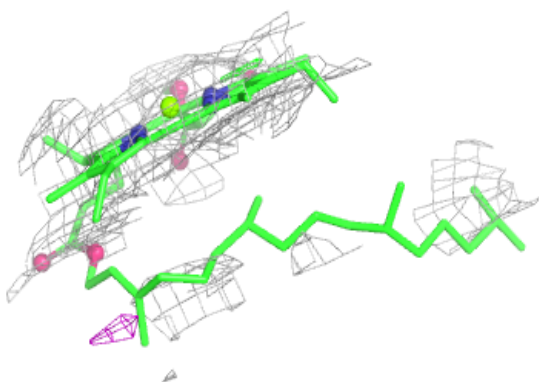
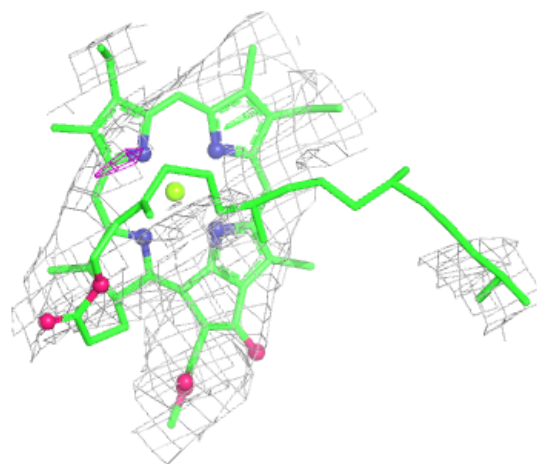
Electron density around CLA A 837:

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



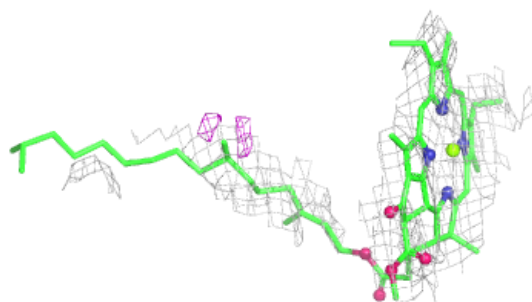
Electron density around CLA B 825:

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

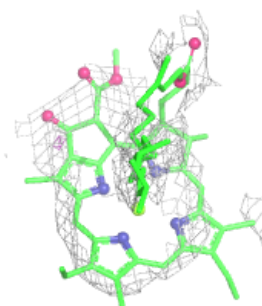
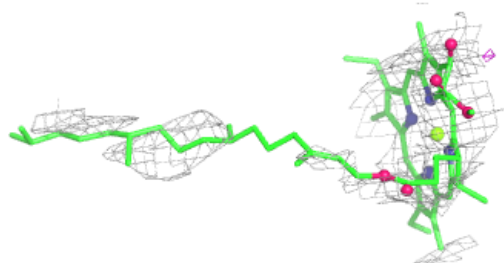
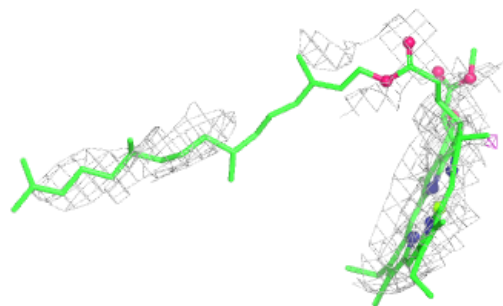


Electron density around CLA B 826:

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

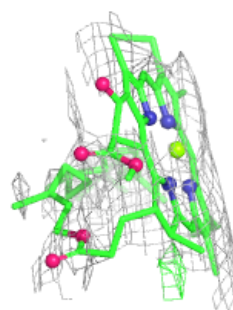
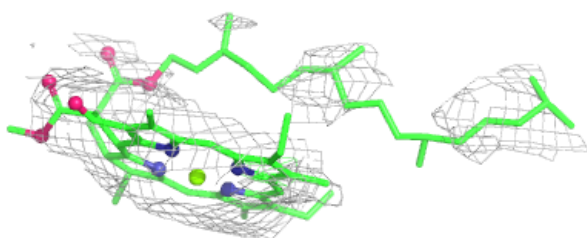
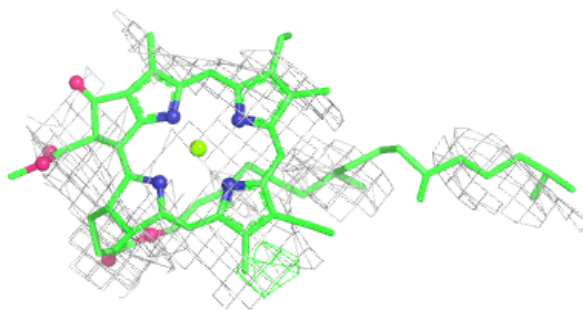
**Electron density around CLA B 827:**

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



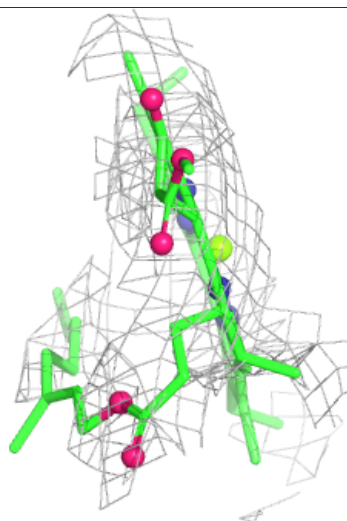
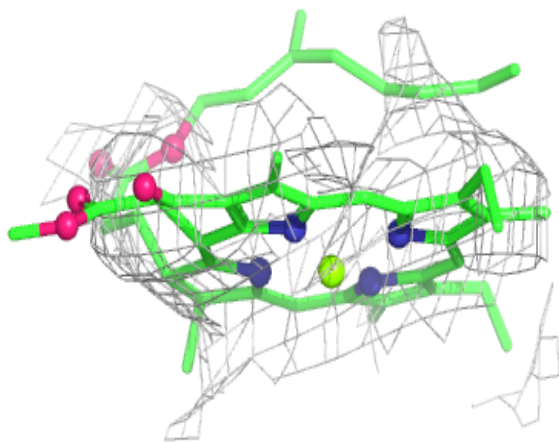
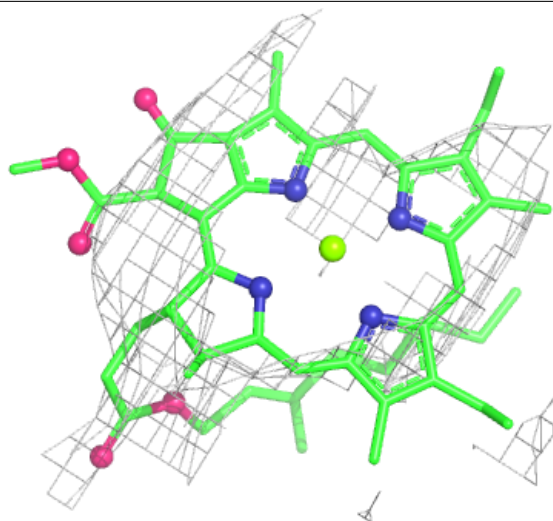
Electron density around CLA A 838:

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



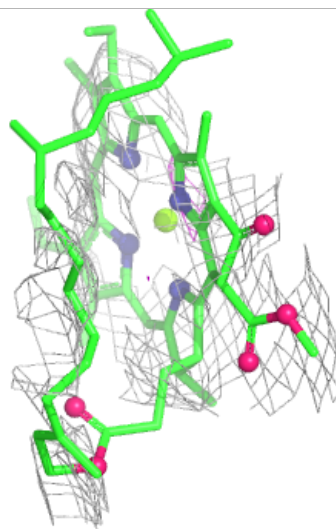
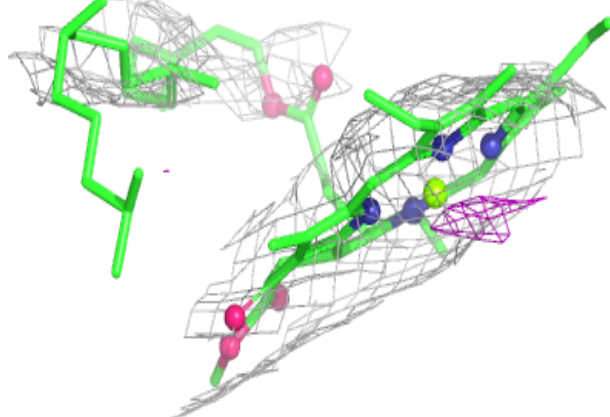
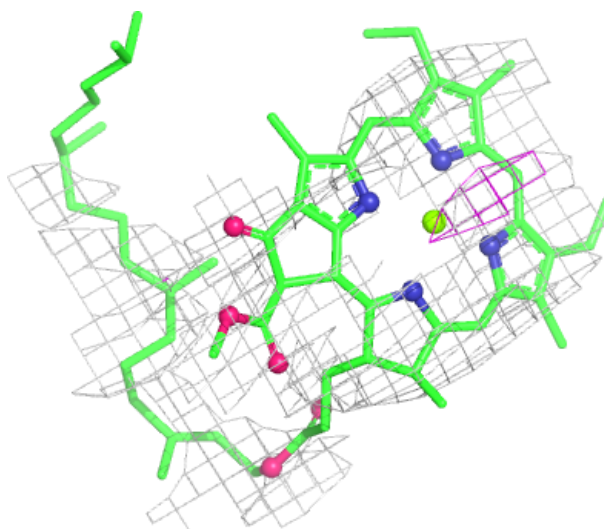
Electron density around CLA A 818:

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



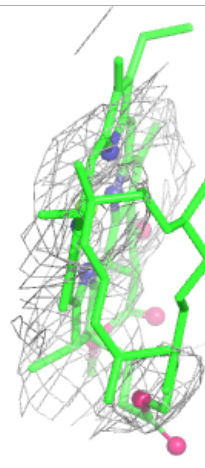
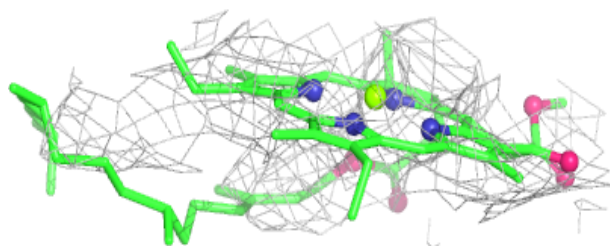
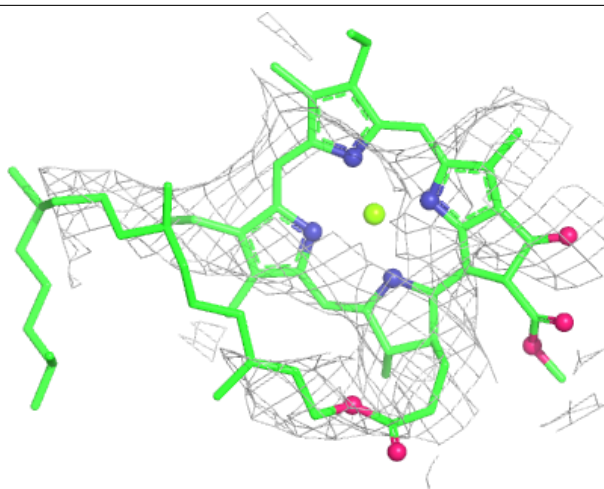
Electron density around CLA B 830:

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



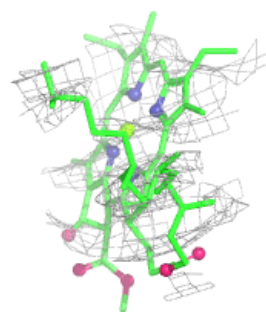
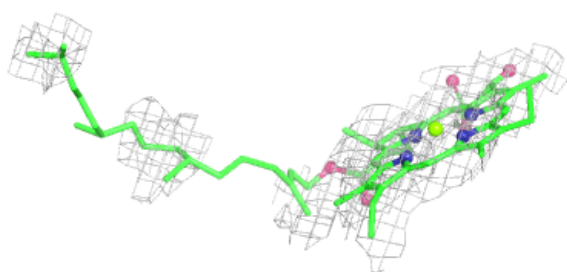
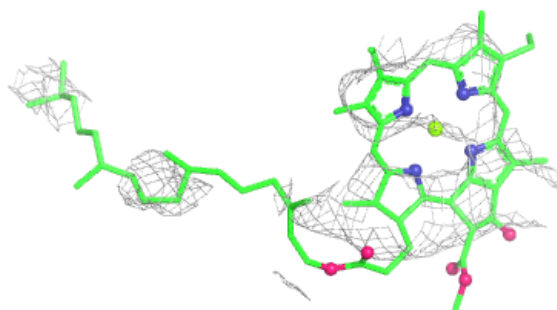
Electron density around CLA A 819:

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

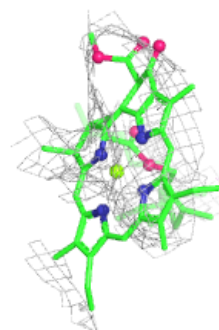
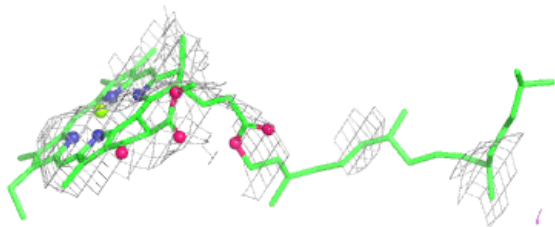
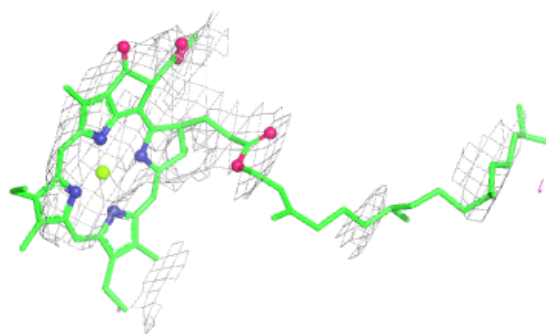


Electron density around CLA A 803:

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

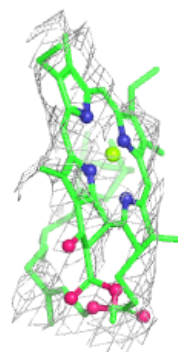
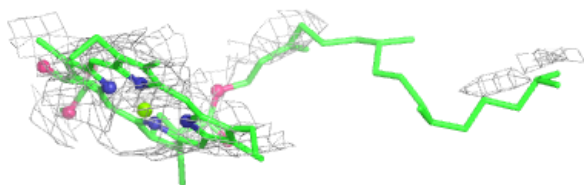
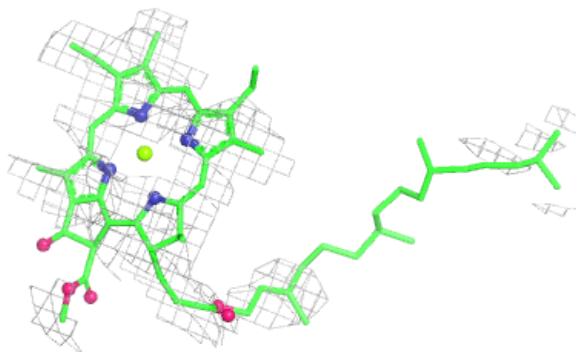
**Electron density around CLA A 821:**

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

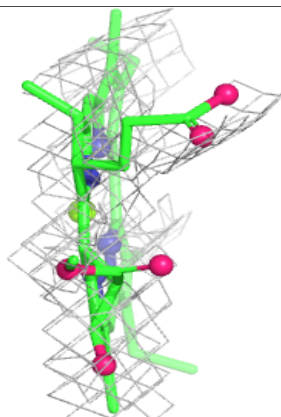
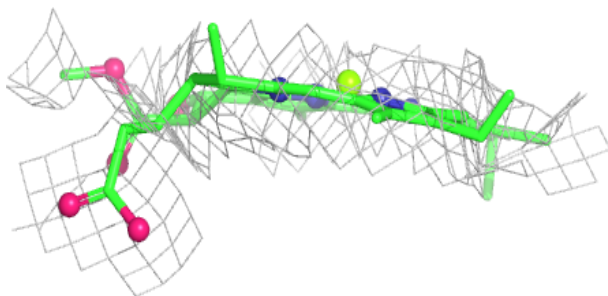
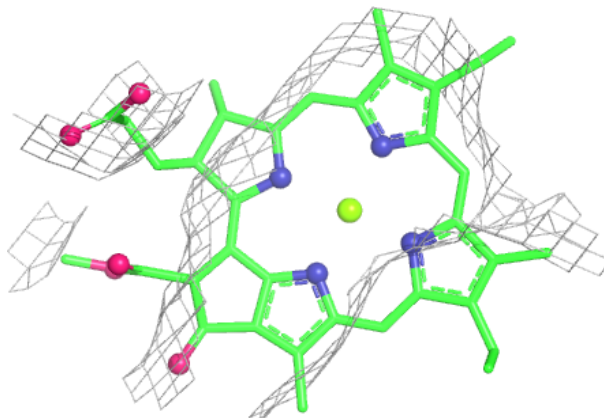


Electron density around CLA A 808:

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

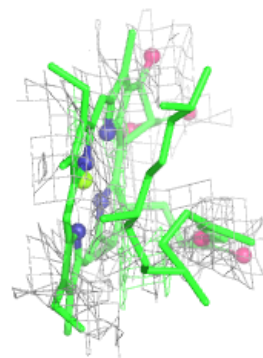
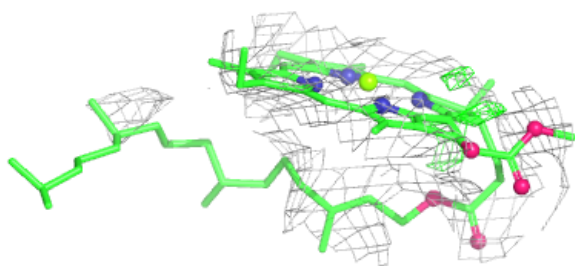
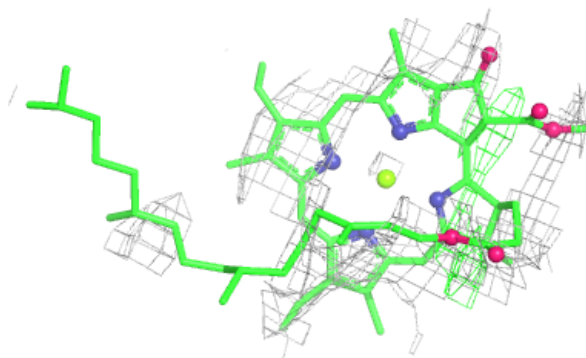
**Electron density around CLA A 814:**

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



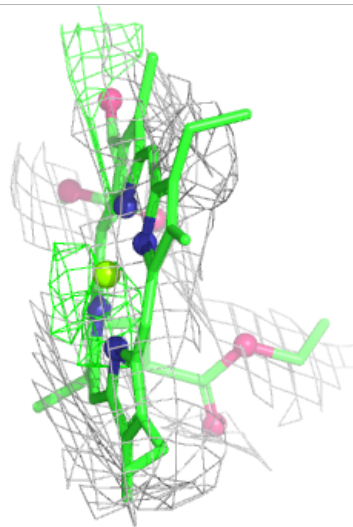
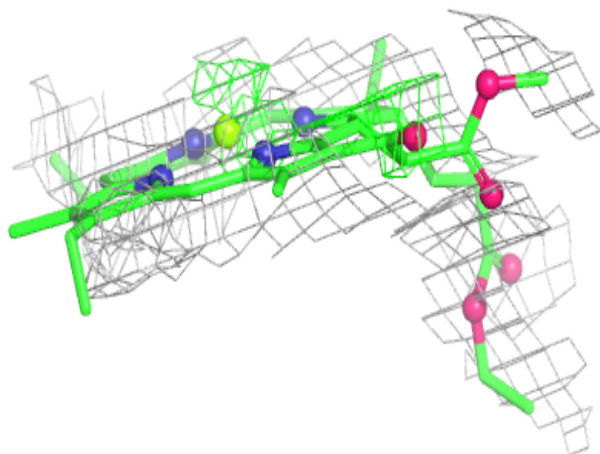
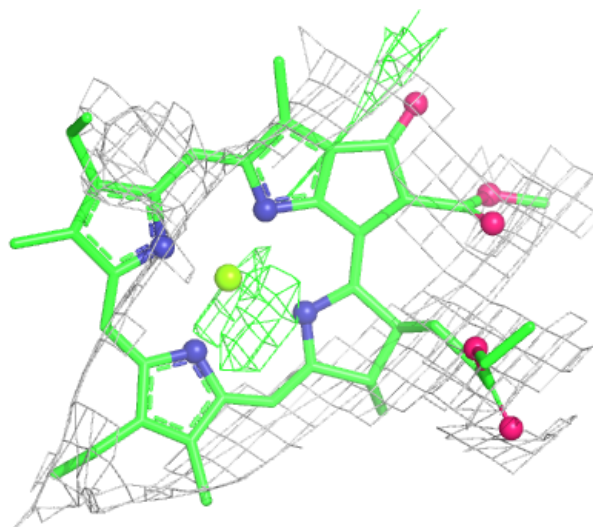
Electron density around CLA B 836:

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



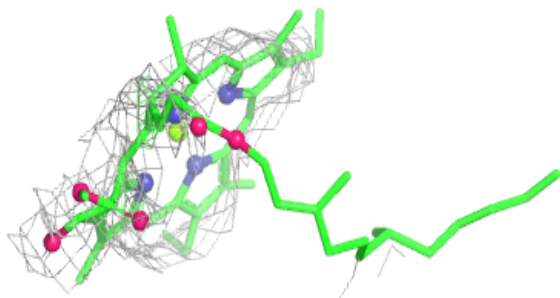
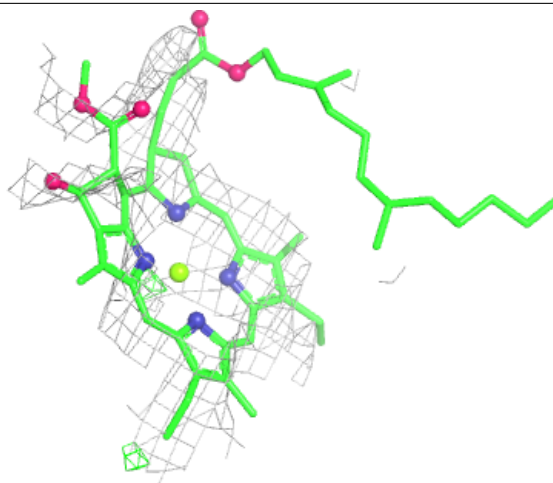
Electron density around CLA B 837:

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



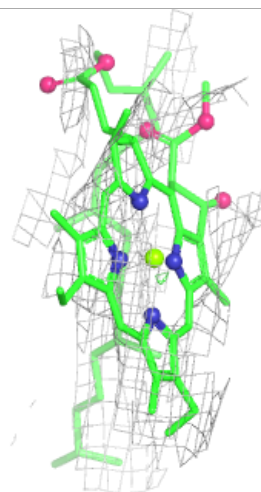
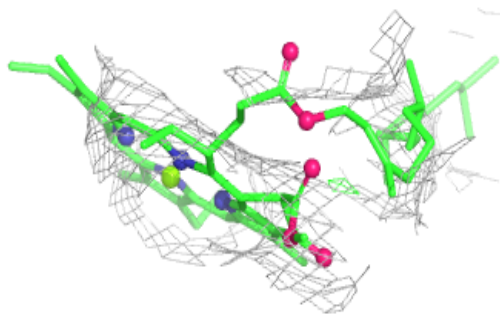
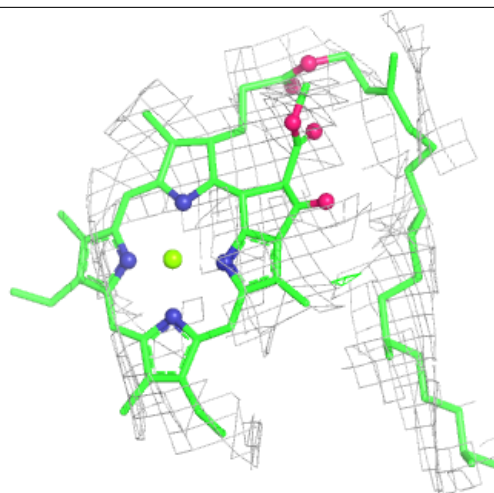
Electron density around CLA A 824:

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



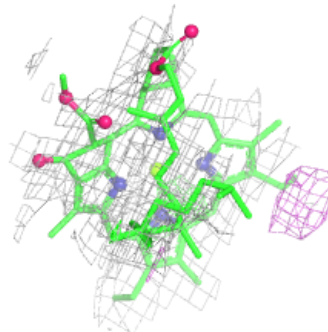
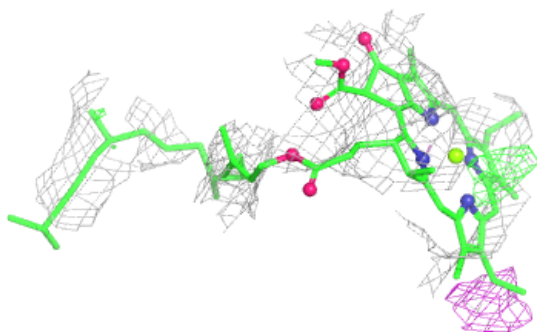
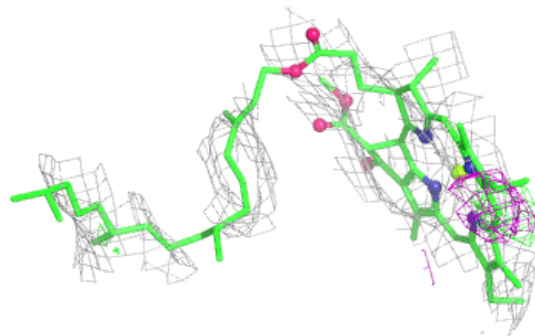
Electron density around CLA A 825:

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

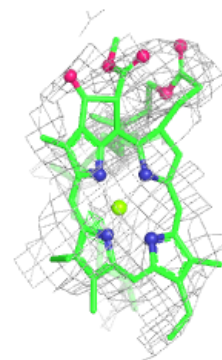
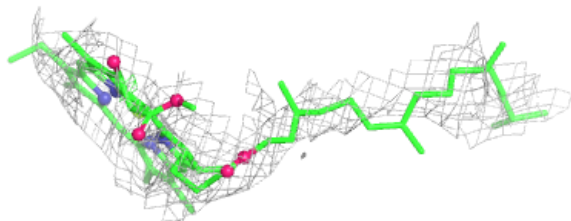
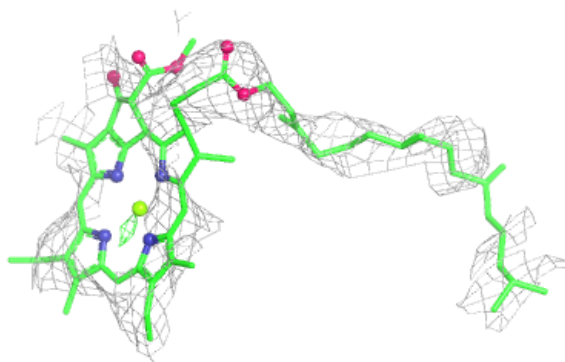


Electron density around CLA B 801:

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

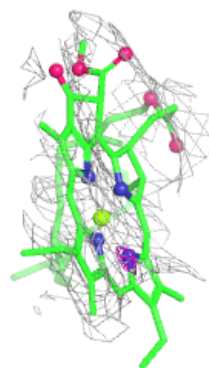
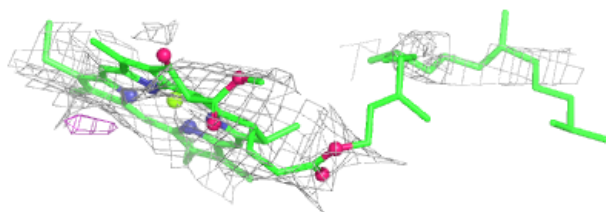
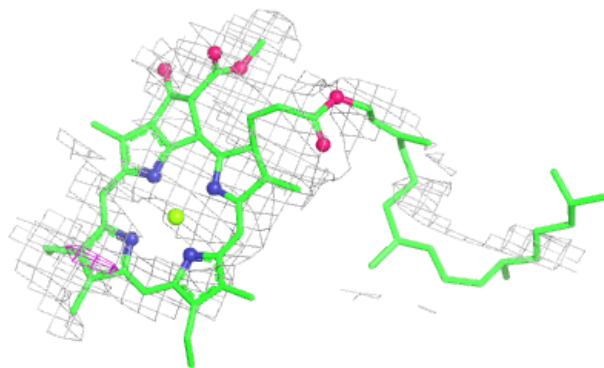
**Electron density around CLA I 101:**

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

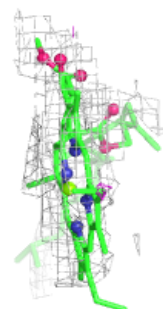
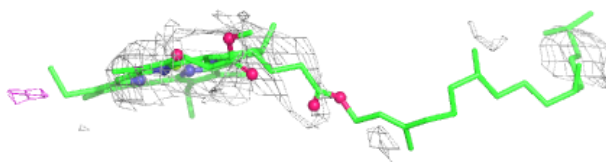
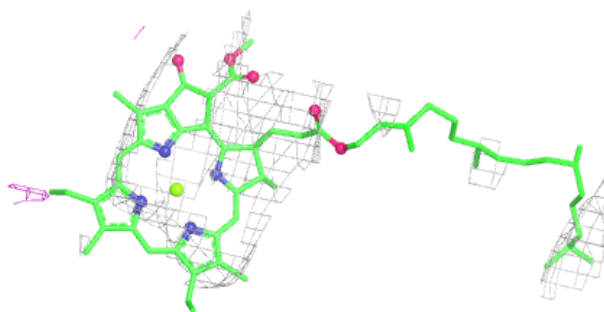


Electron density around CLA J 1101:

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

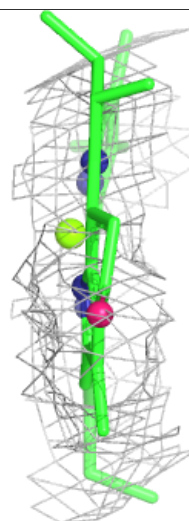
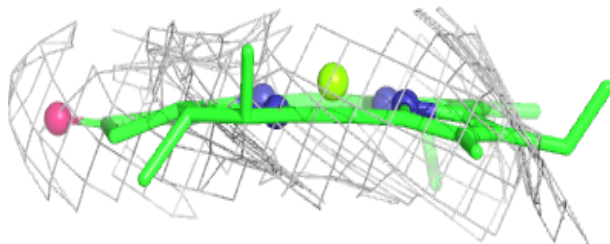
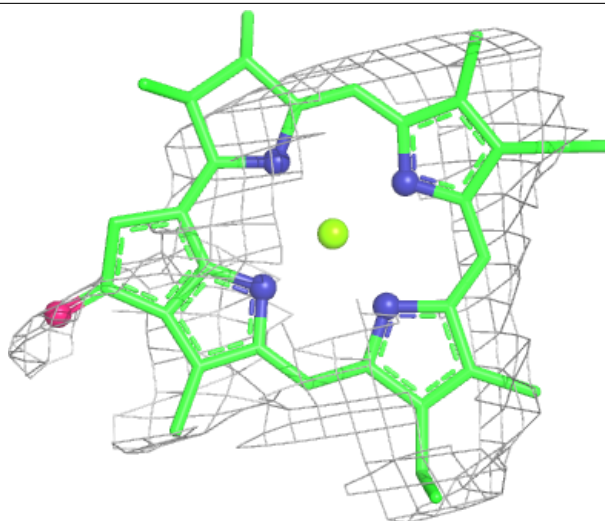
**Electron density around CLA A 826:**

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



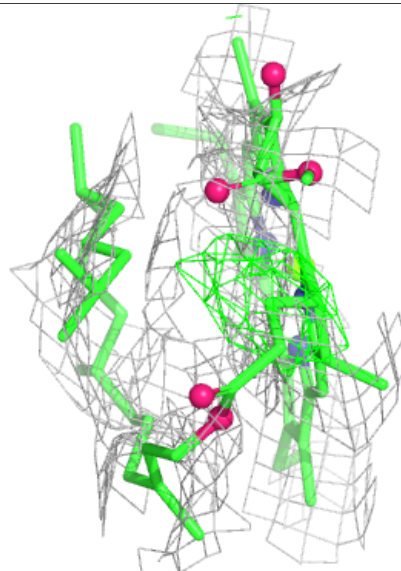
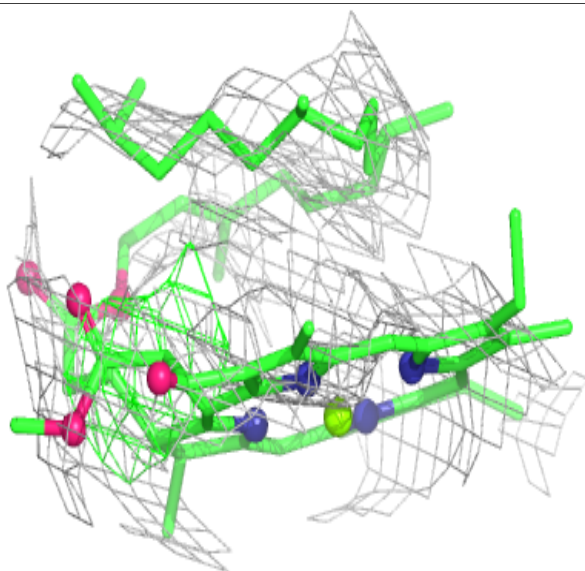
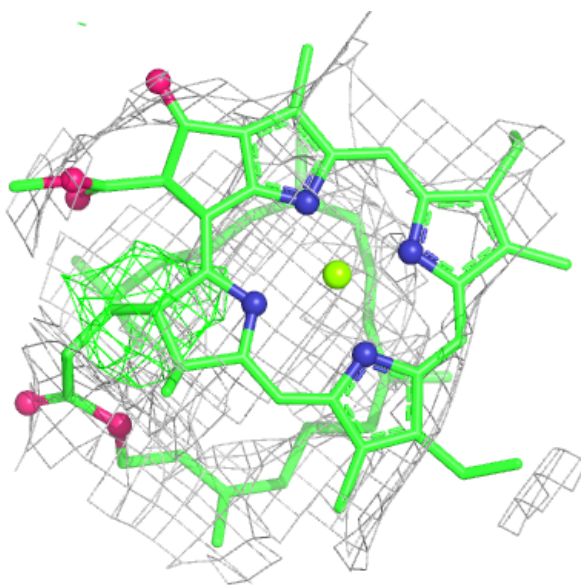
Electron density around CLA J 1103:

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



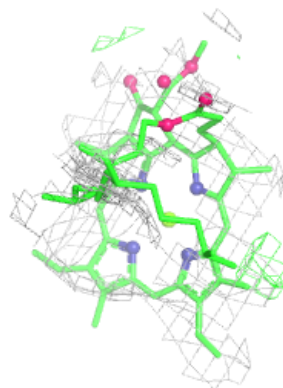
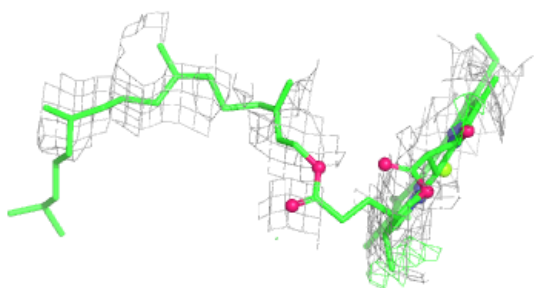
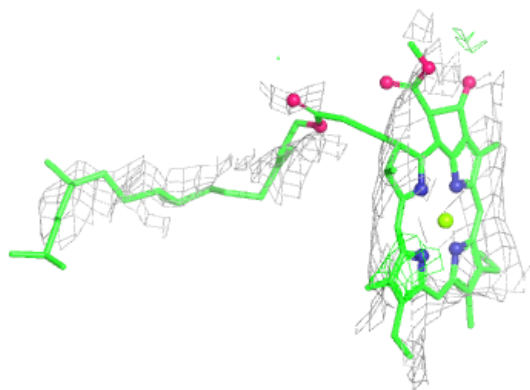
Electron density around CLA L 1002:

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

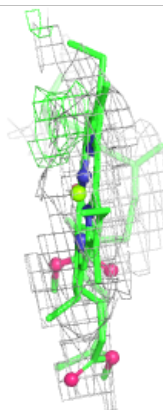
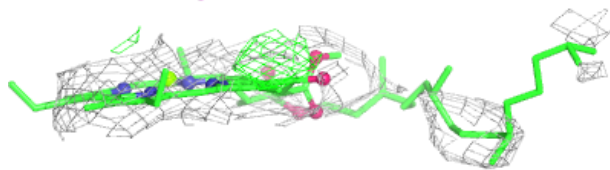
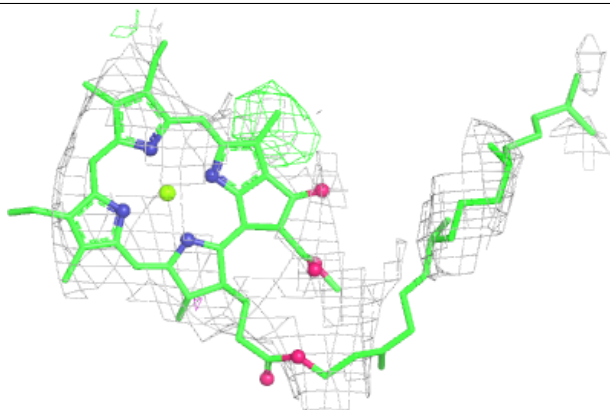


Electron density around CLA L 1003:

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

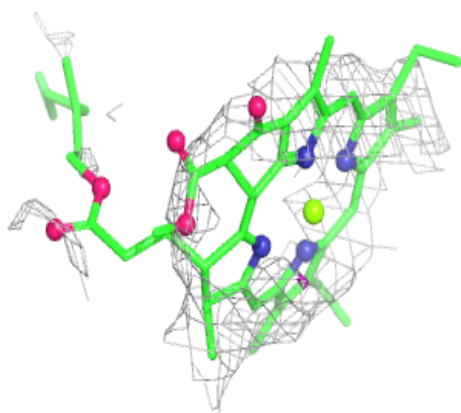
**Electron density around CLA L 1004:**

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



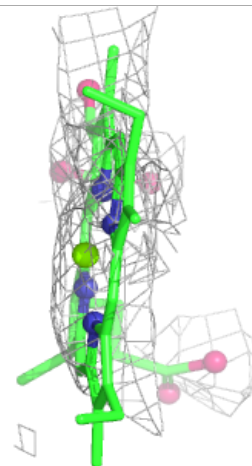
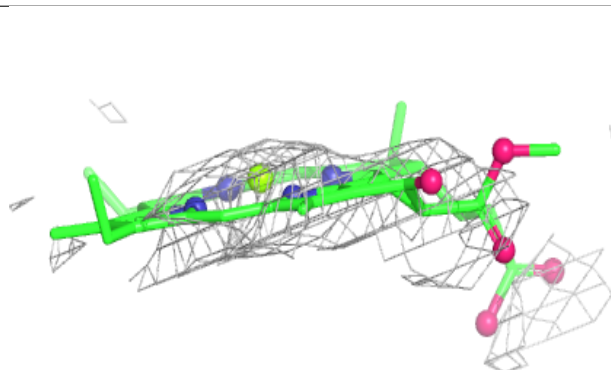
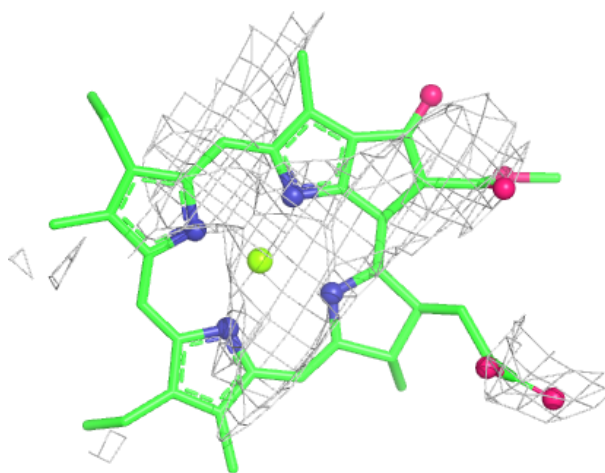
Electron density around CLA M 1201:

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



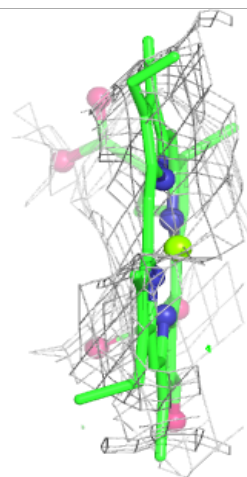
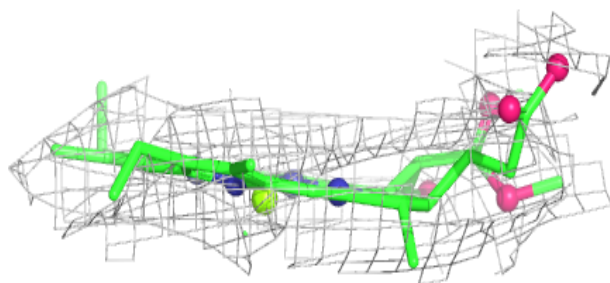
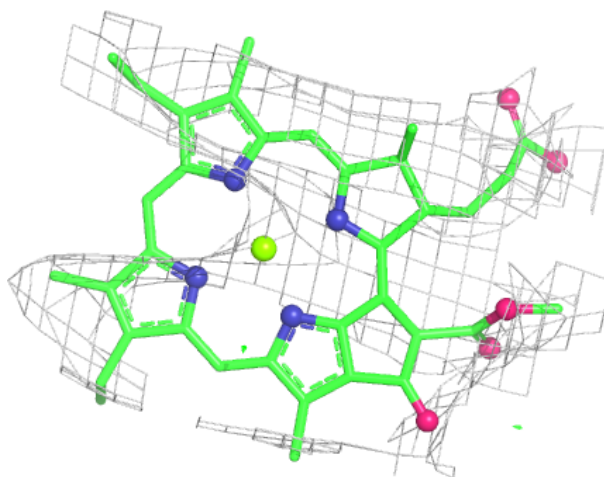
Electron density around CLA M 1202:

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



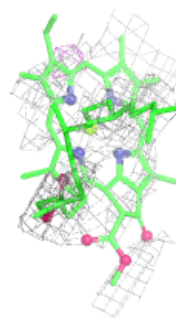
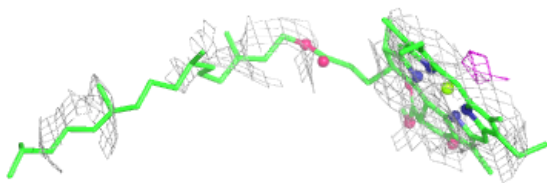
Electron density around CLA X 102:

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



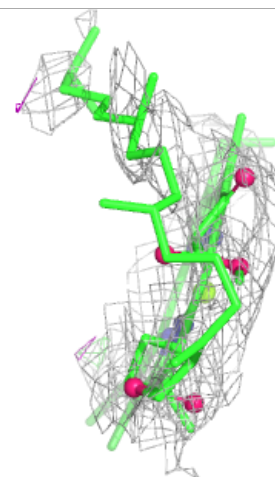
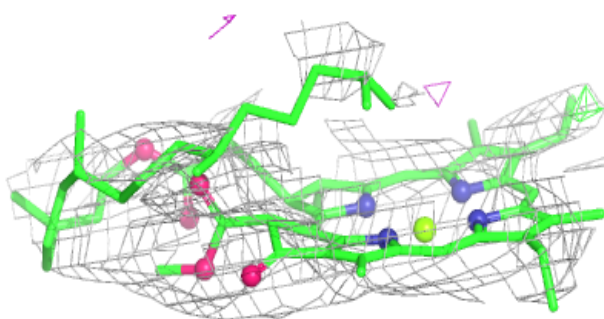
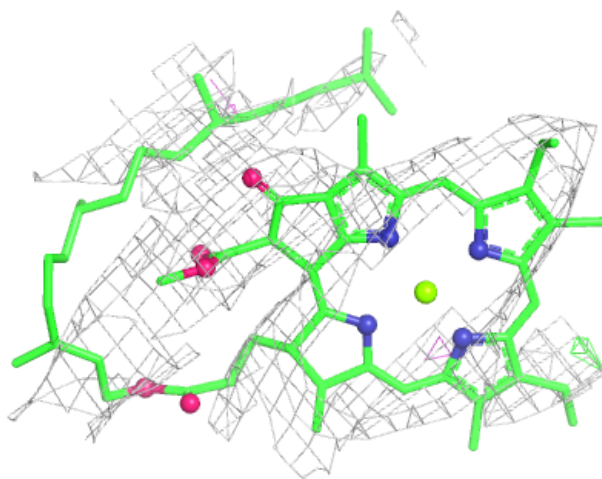
Electron density around CLA A 802:

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



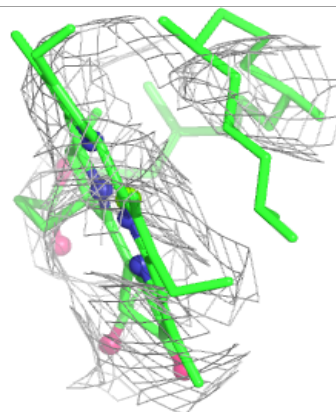
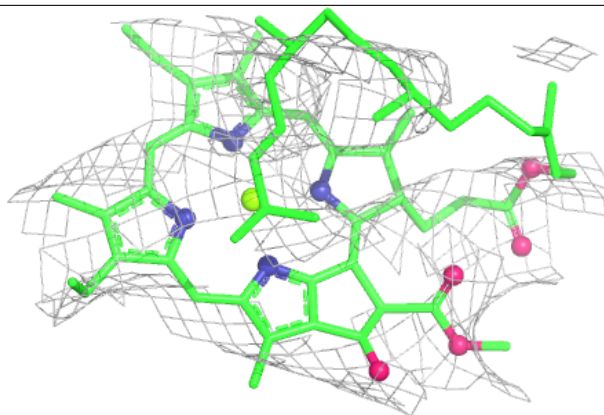
Electron density around CLA B 804:

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

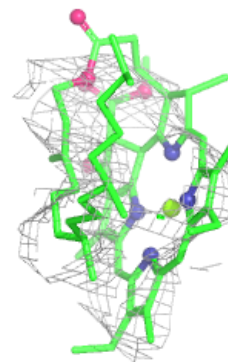
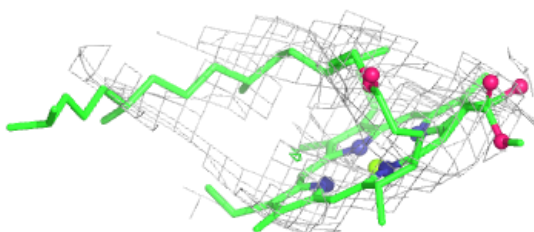
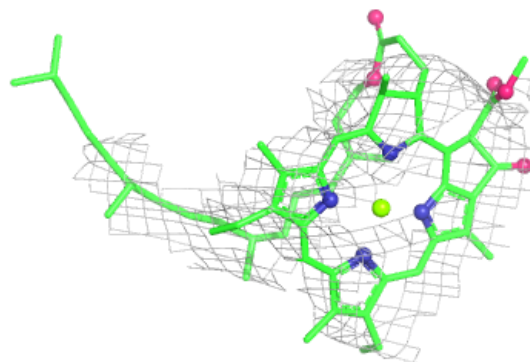


Electron density around CLA B 805:

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

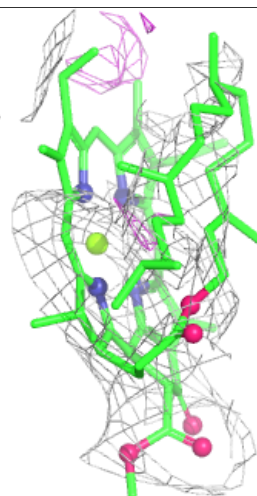
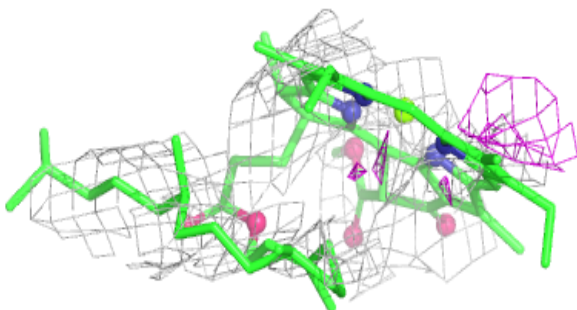
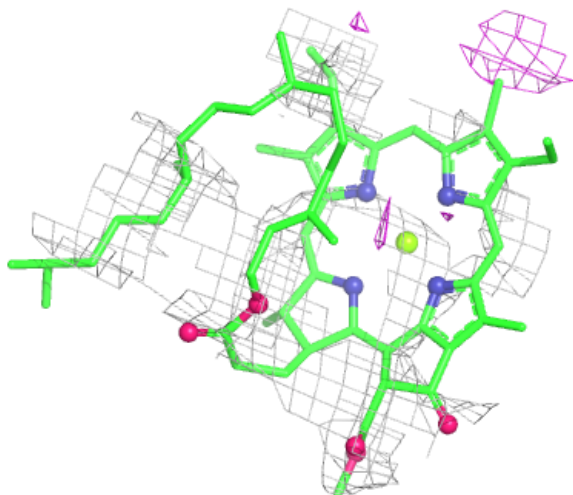
**Electron density around CLA B 806:**

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



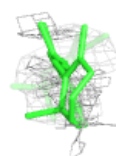
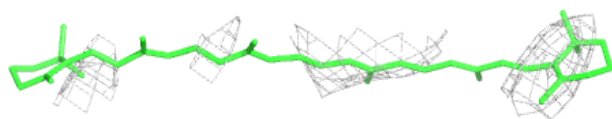
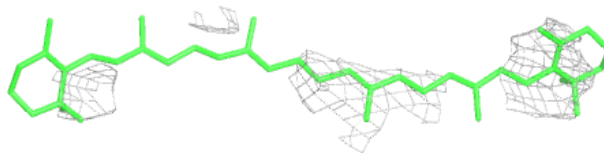
Electron density around CLA B 807:

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

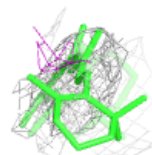
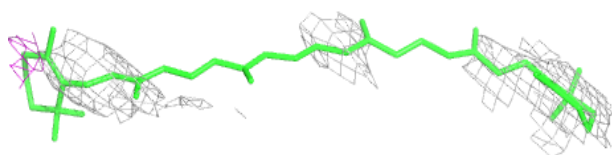
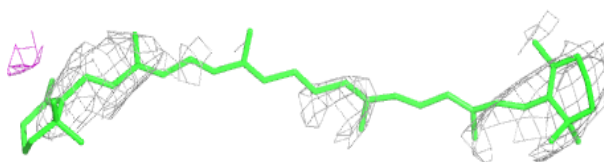


Electron density around BCR A 850:

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

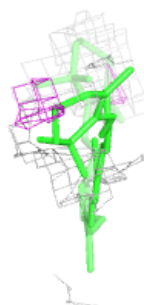
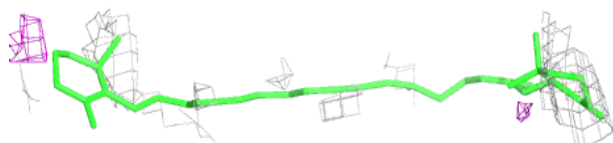
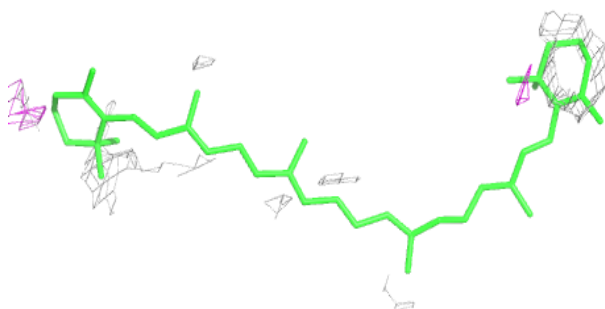
**Electron density around BCR A 851:**

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

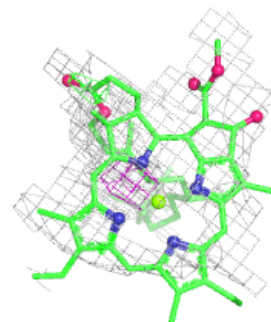
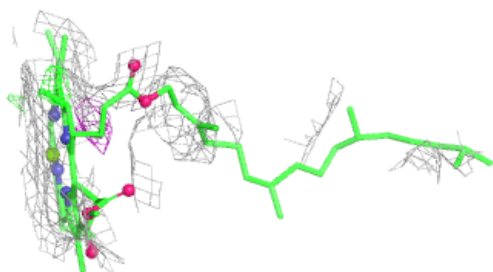
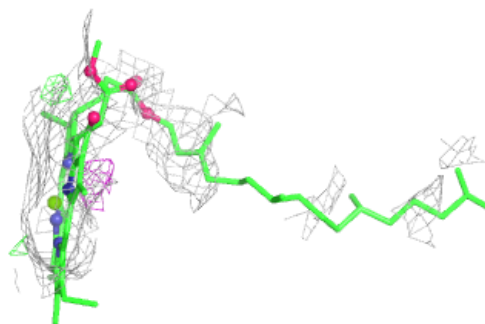


Electron density around BCR A 852:

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

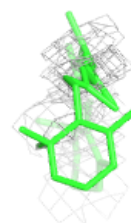
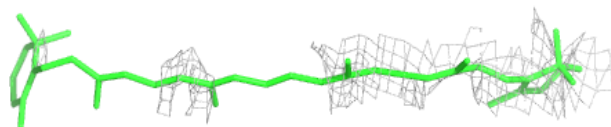
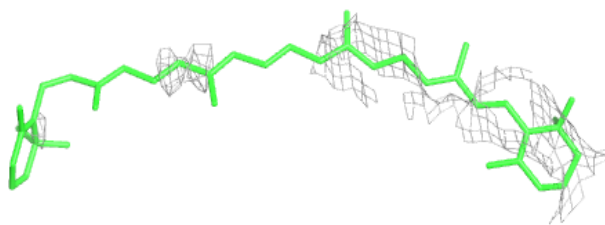
**Electron density around CLA A 828:**

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



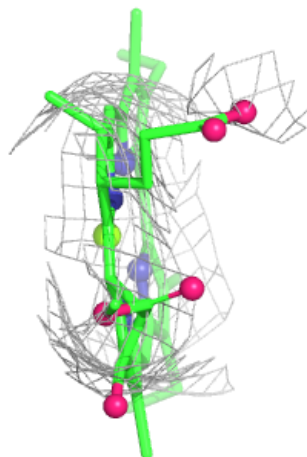
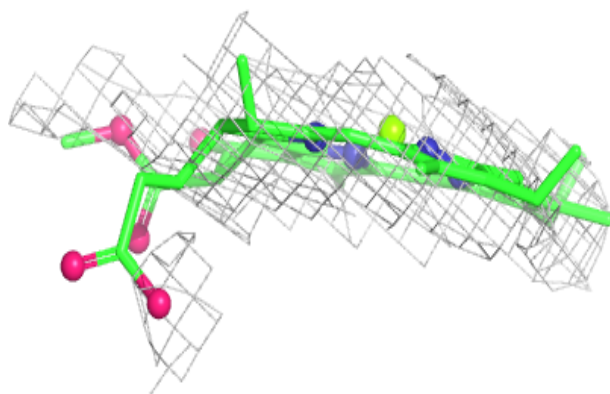
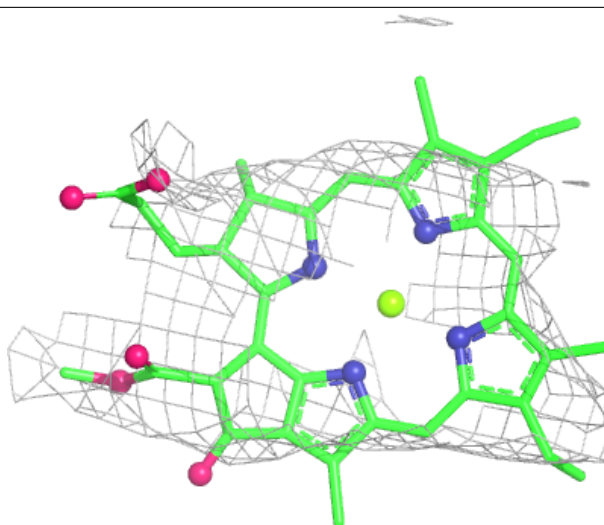
Electron density around BCR B 842:

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



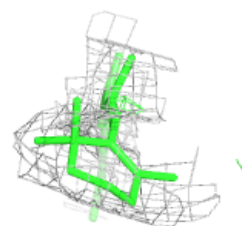
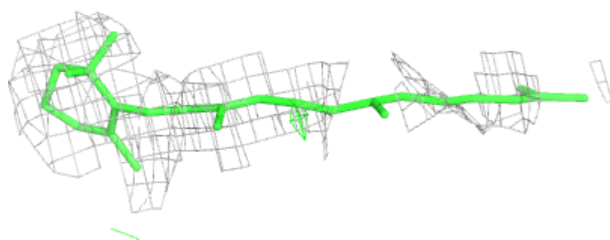
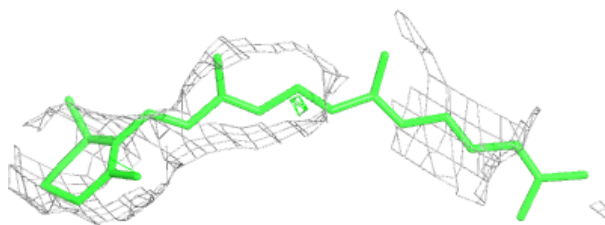
Electron density around CLA B 809:

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

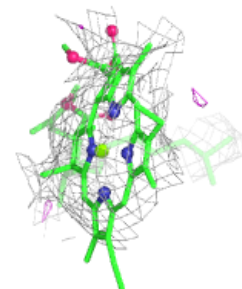
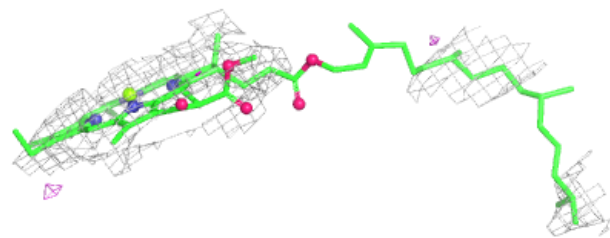
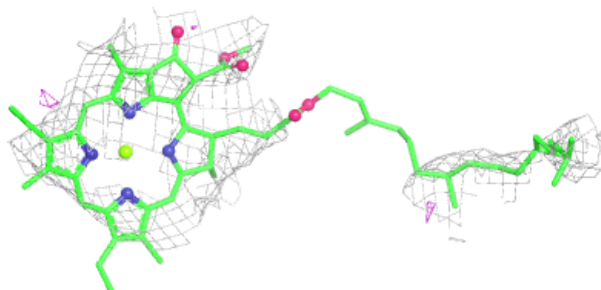


Electron density around BCR B 844:

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

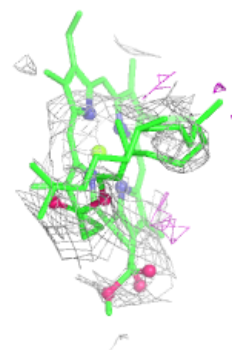
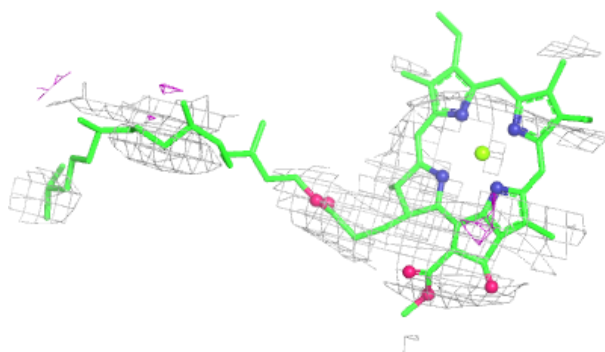
**Electron density around CLA A 805:**

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

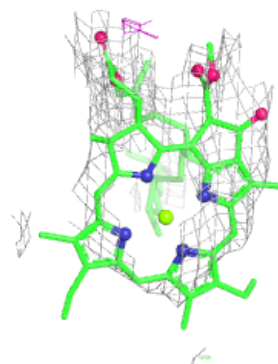
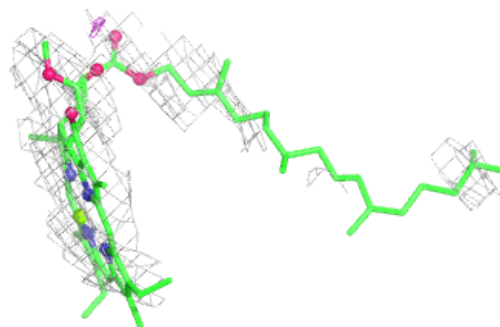


Electron density around CLA B 811:

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

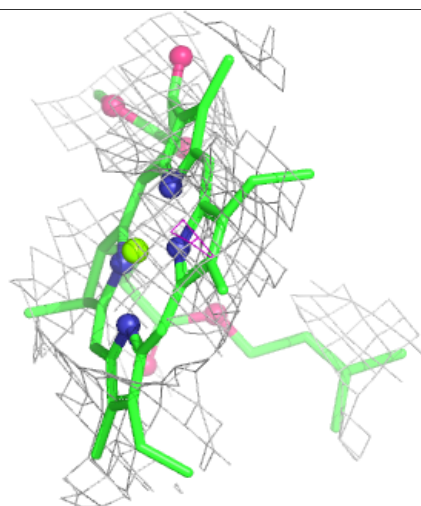
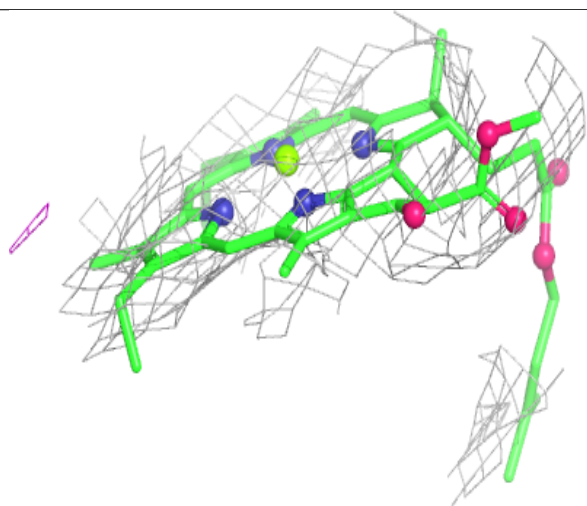
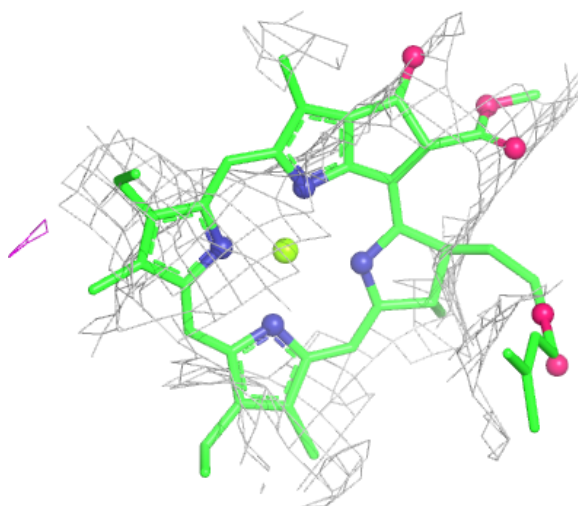
**Electron density around CLA A 830:**

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



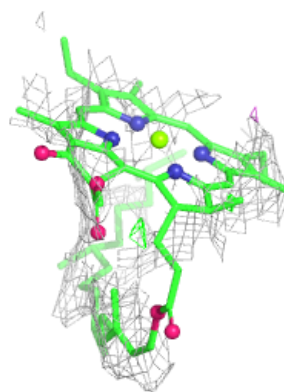
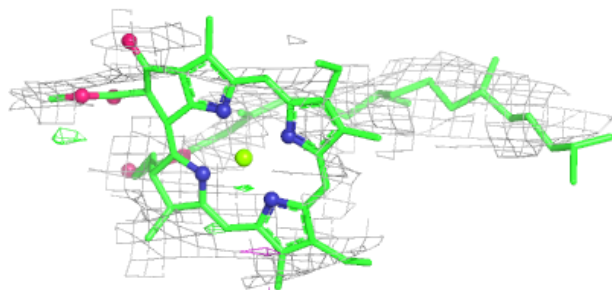
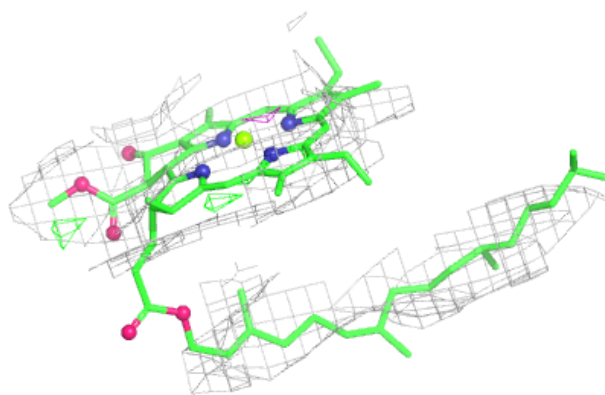
Electron density around CLA A 831:

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

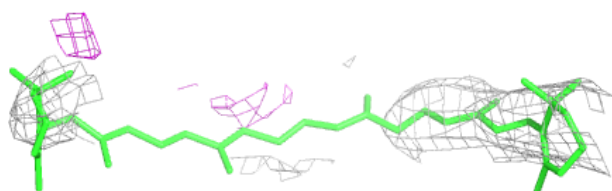
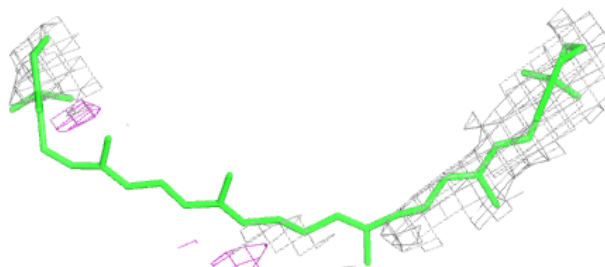


Electron density around CLA A 832:

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

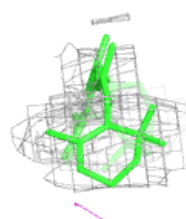
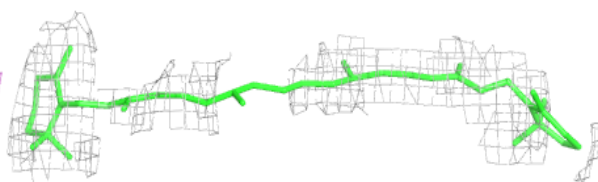
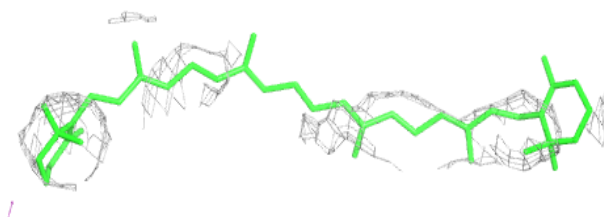
**Electron density around BCR F 1302:**

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

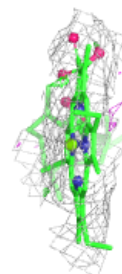
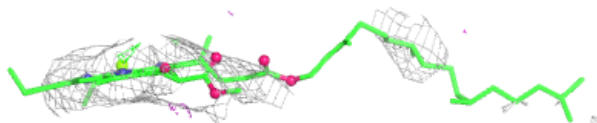


Electron density around BCR I 102:

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

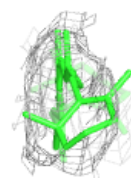
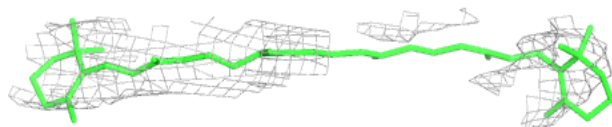
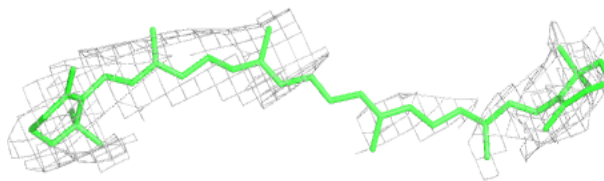
**Electron density around CLA A 833:**

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

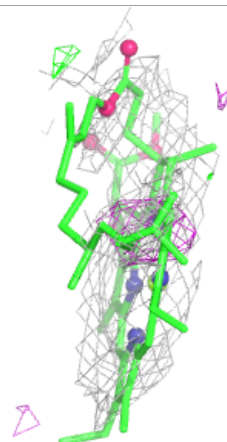
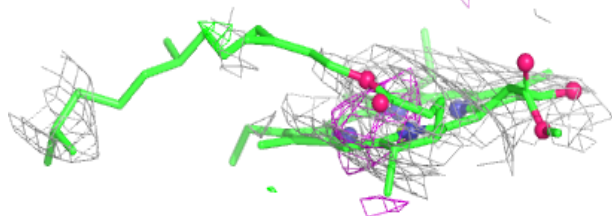
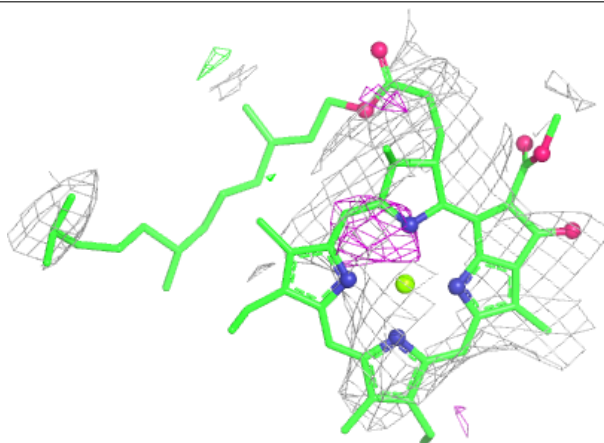


Electron density around BCR J 1105:

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

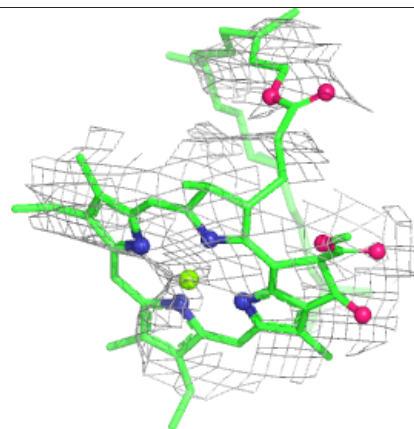
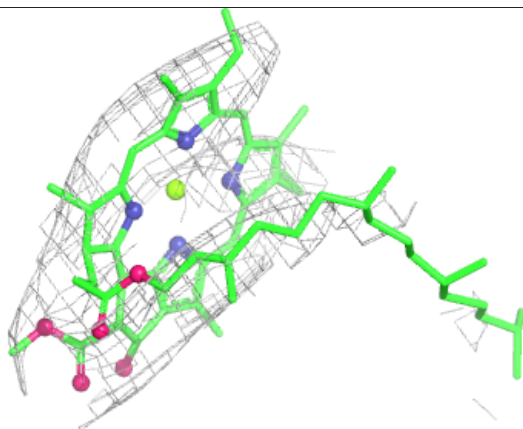
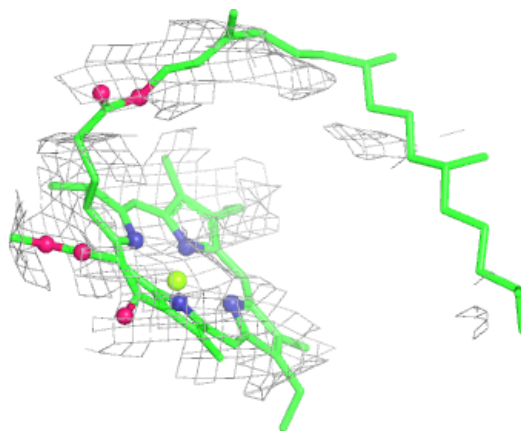
**Electron density around CLA B 816:**

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



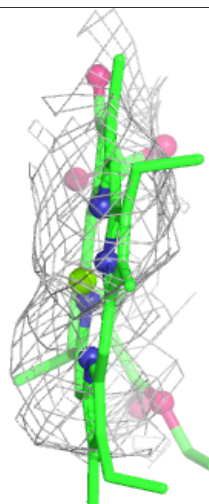
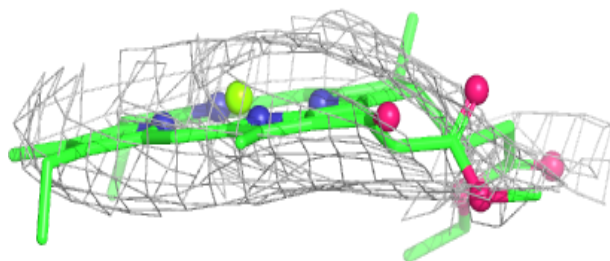
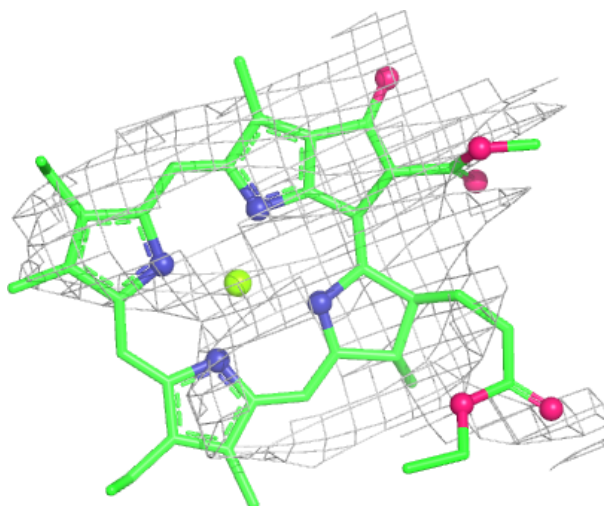
Electron density around CLA B 817:

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



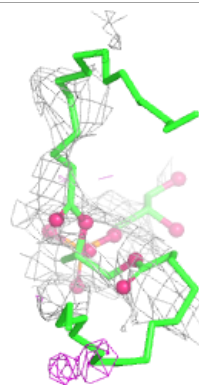
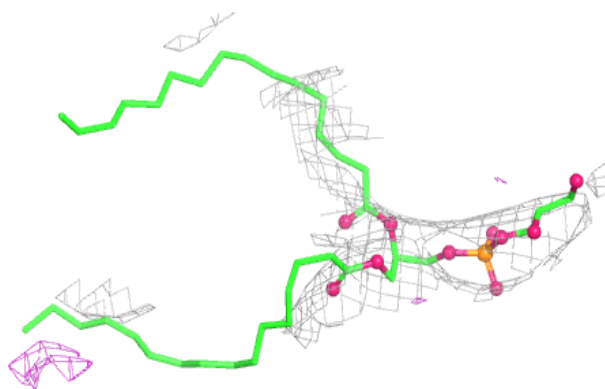
Electron density around CLA B 818:

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

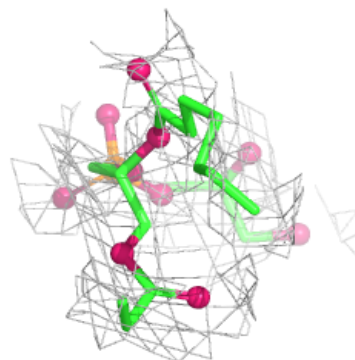
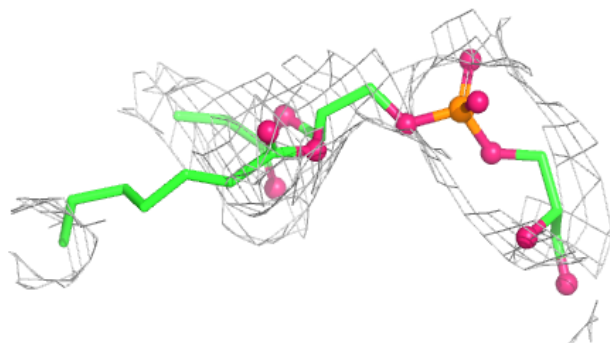
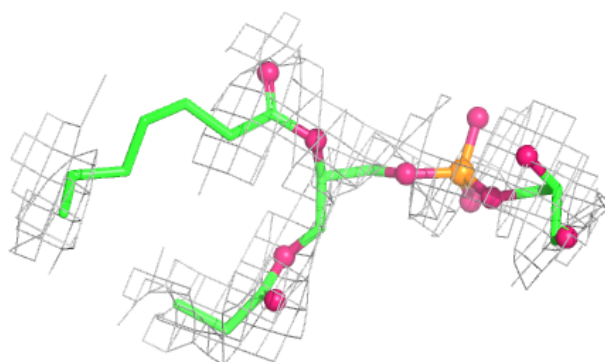


Electron density around LHG A 853:

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

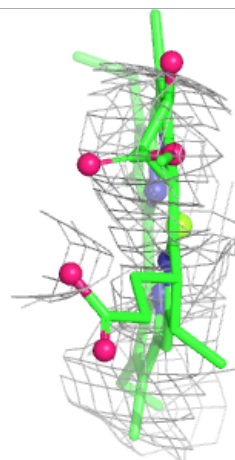
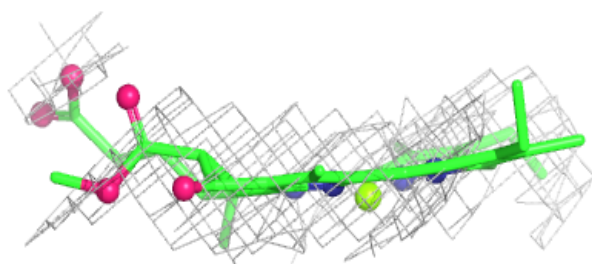
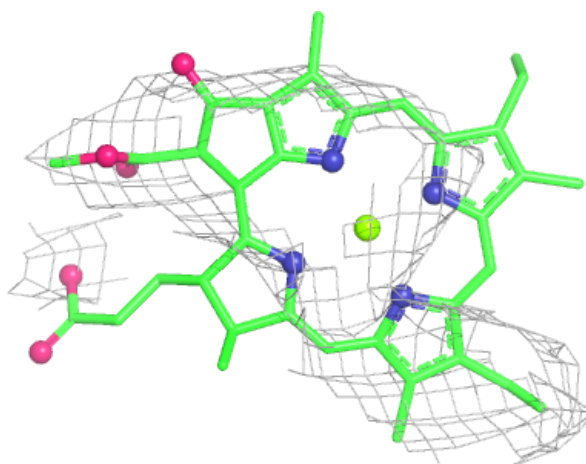
**Electron density around LHG A 854:**

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



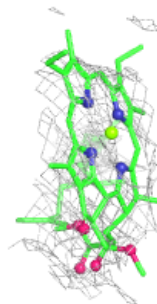
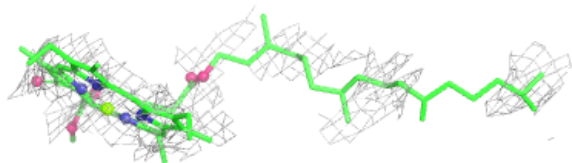
Electron density around CLA B 819:

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

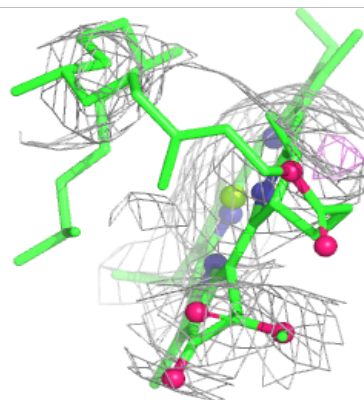
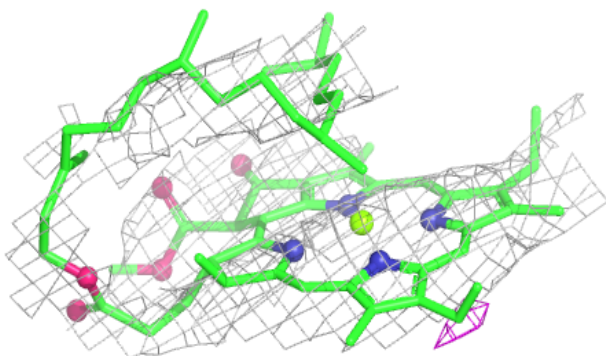
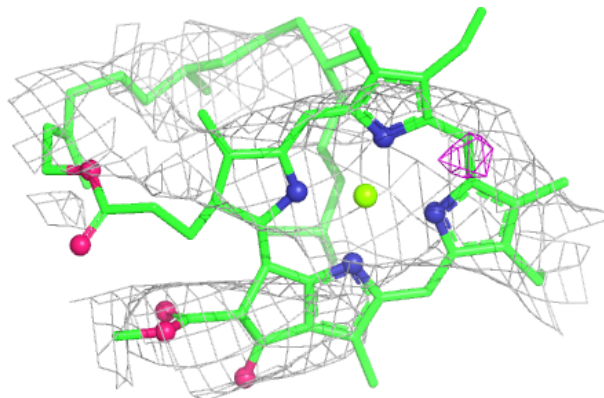


Electron density around CLA A 834:

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

**Electron density around CLA A 806:**

$2mF_o-DF_c$ (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.