



wwPDB EM Validation Summary Report ⓘ

Oct 5, 2026 – 08:34 PM EDT

PDB ID : 9YL7 / pdb_00009yl7
EMDB ID : EMD-73077
Title : Structure of photosystem I with plastoquinone-9 bound
Authors : Brininger, C.M.; Gisriel, C.J.
Deposited on : 2025-10-08
Resolution : 1.68 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>

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:

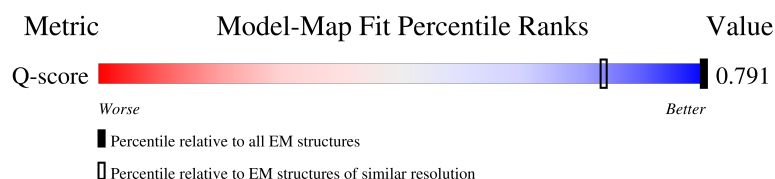
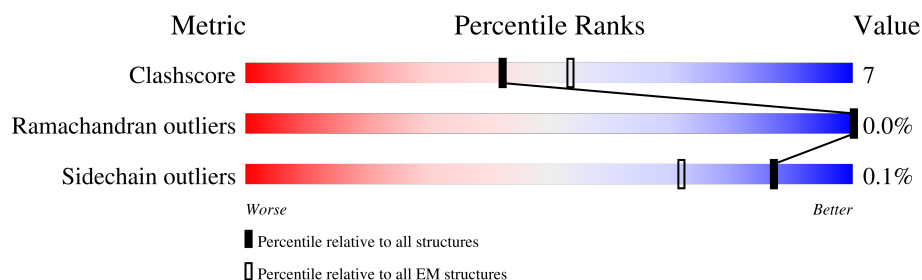
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.2
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 1.68 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	466 (1.19 - 2.18)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	751	 91% 8% .
2	B	731	 87% 12%
3	C	81	 85% 14% .
4	D	141	 84% 12% ..

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Mol	Chain	Length	Quality of chain
5	E	74	 81% 11% 7%
6	F	165	 73% 12% 15%
7	I	40	 85% 10% 5%
8	J	40	 72% 22% 6%
9	K	86	 74% 15% 9%
10	L	157	 86% 11% 3%
11	M	31	 84% 13% 3%

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 25616 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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					AltConf	Trace
1	A	742	Total	C	N	O	S	0	0
			5783	3791	981	984	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	729	Total	C	N	O	S	0	0
			5759	3792	967	986	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	369	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	139	Total	C	N	O	S	0	0
			1075	680	186	206	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	69	Total	C	N	O	0	0
			537	337	95	105		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1084	700	180	199	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	38	Total	C	N	O	S	0	0
			297	202	42	50	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	39	Total	C	N	O	S	0	0
			311	210	46	53	2		

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	78	Total	C	N	O	S	0	0
			545	358	89	94	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	37	PHE	LEU	conflict	UNP P72712
K	43	SER	ASN	conflict	UNP P72712

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	154	Total	C	N	O	S	0	0
			1152	751	188	211	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			238	159	36	42	1		

- Molecule 12 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
12	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
12	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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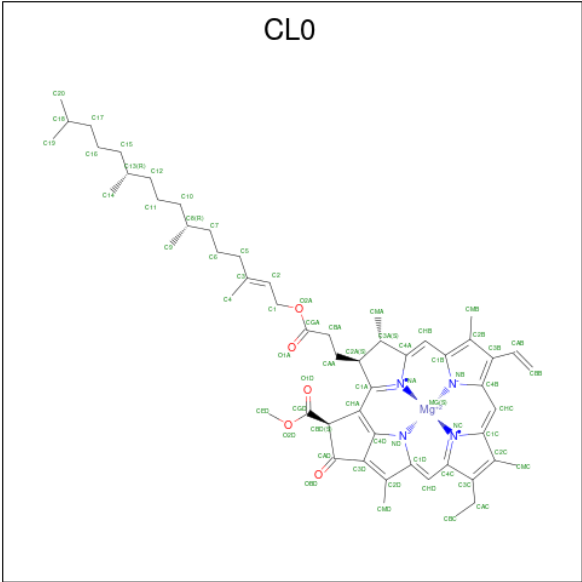
Mol	Chain	Residues	Atoms					AltConf
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12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 55	C 45	Mg 1	N 4	O 5	0

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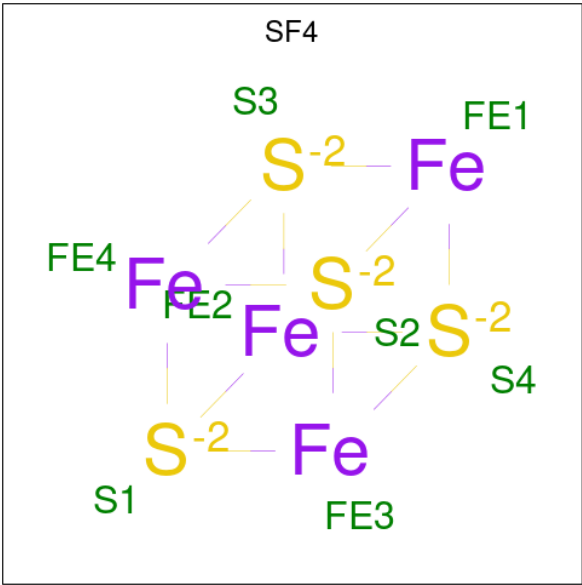
Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	J	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	K	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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



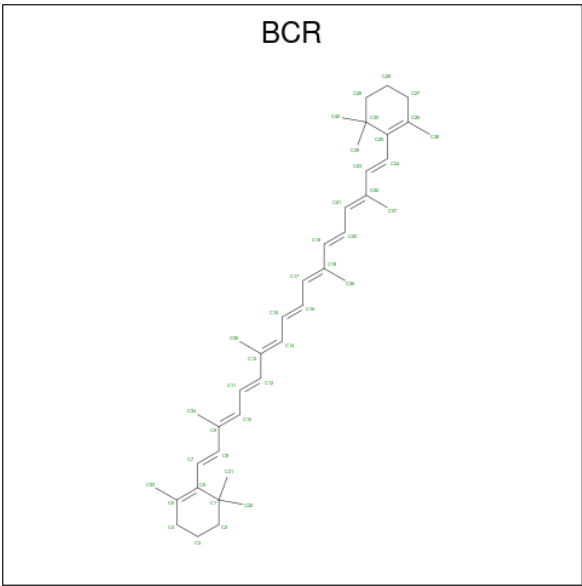
Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



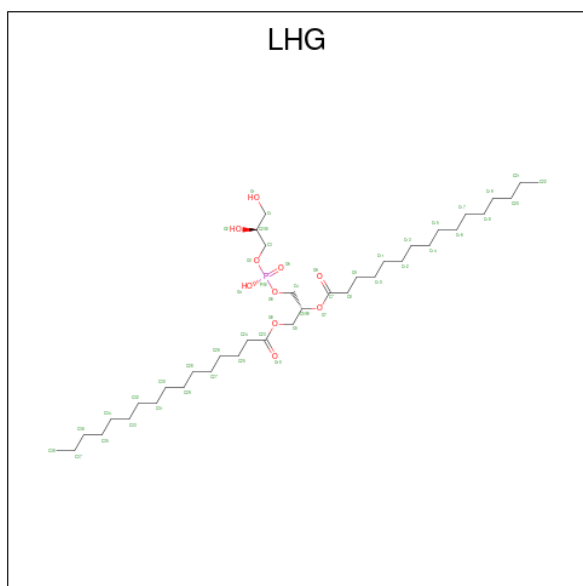
Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	C	0
			40	40	
15	A	1	Total	C	0
			40	40	
15	A	1	Total	C	0
			40	40	
15	A	1	Total	C	0
			40	40	
15	B	1	Total	C	0
			40	40	
15	B	1	Total	C	0
			40	40	
15	B	1	Total	C	0
			40	40	
15	B	1	Total	C	0
			25	25	
15	B	1	Total	C	0
			40	40	
15	F	1	Total	C	0
			40	40	
15	F	1	Total	C	0
			40	40	
15	I	1	Total	C	0
			40	40	
15	J	1	Total	C	0
			14	14	

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Mol	Chain	Residues	Atoms	AltConf
15	J	1	Total C 40 40	0
15	J	1	Total C 40 40	0
15	K	1	Total C 40 40	0
15	K	1	Total C 40 40	0
15	L	1	Total C 40 40	0
15	L	1	Total C 40 40	0

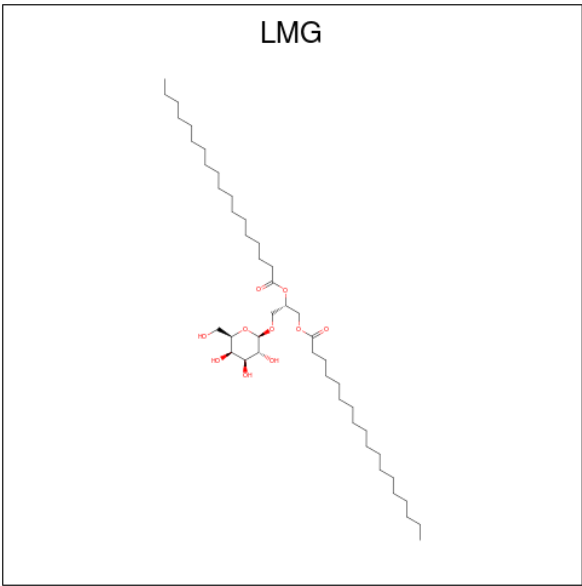
- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
16	A	1	Total C O P 49 38 10 1	0
16	A	1	Total C O P 37 26 10 1	0
16	B	1	Total C O P 49 38 10 1	0
16	M	1	Total C O P 44 33 10 1	0

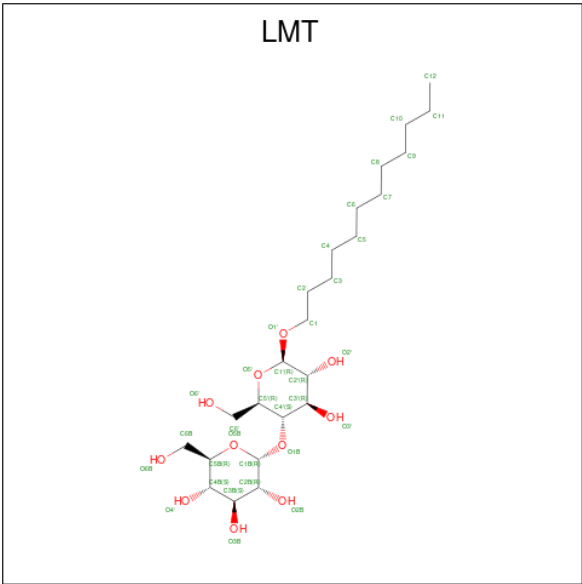
- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID:

LMG) (formula: C₄₅H₈₆O₁₀).



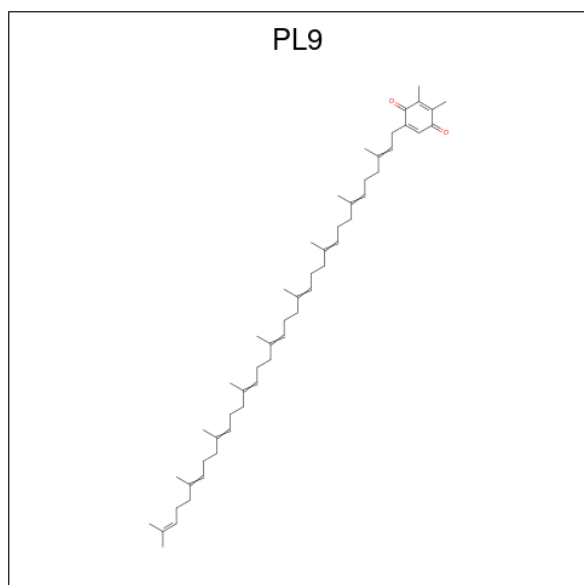
Mol	Chain	Residues	Atoms			AltConf
17	A	1	Total	C	O	0
			50	40	10	
17	A	1	Total	C	O	0
			46	36	10	
17	B	1	Total	C	O	0
			51	41	10	

- Molecule 18 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



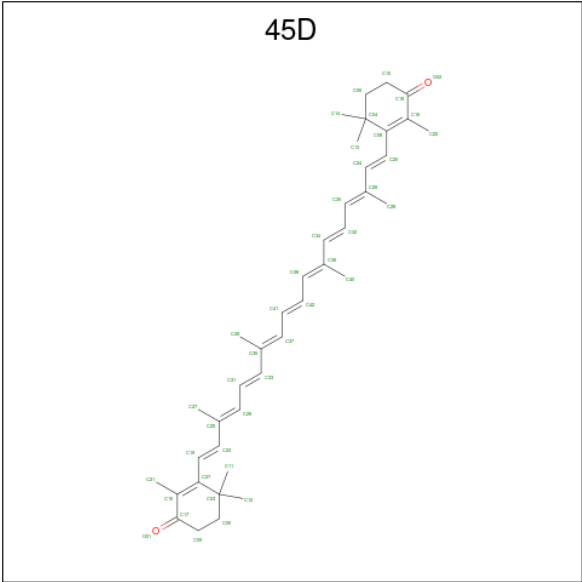
Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	C	O	0
			35	24	11	
18	A	1	Total	C	O	0
			35	24	11	
18	A	1	Total	C	O	0
			35	24	11	
18	B	1	Total	C	O	0
			29	18	11	
18	B	1	Total	C	O	0
			35	24	11	
18	F	1	Total	C	O	0
			31	20	11	
18	J	1	Total	C	O	0
			31	20	11	
18	L	1	Total	C	O	0
			35	24	11	

- Molecule 19 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	C	O	0
			30	28	2	

- Molecule 20 is beta,beta-carotene-4,4'-dione (CCD ID: 45D) (formula: C₄₀H₅₂O₂).

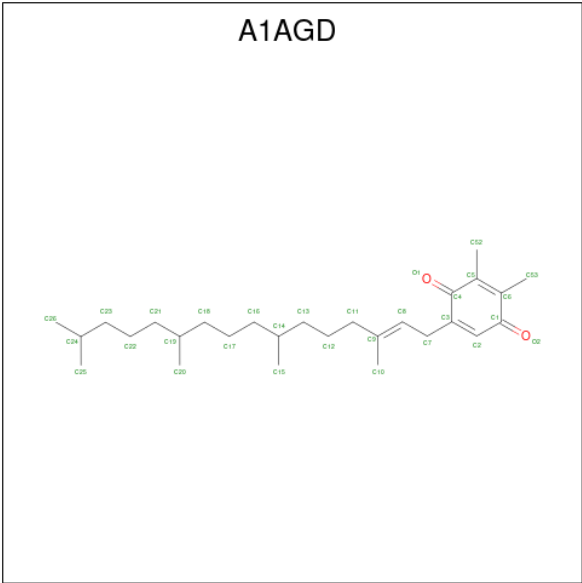


Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			42	40	2	

- Molecule 21 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

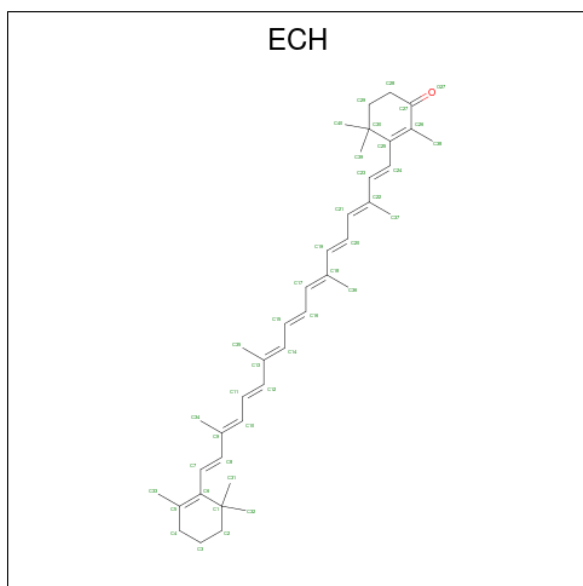
Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	Cl	0
			1	1	

- Molecule 22 is 2,3-dimethyl-5-[(2E,7R,11R)-3,7,11,15-tetramethylhexadec-2-en-1-yl]cyclohexa-2,5-diene-1,4-dione (CCD ID: A1AGD) (formula: C₂₈H₄₆O₂).



Mol	Chain	Residues	Atoms			AltConf
22	B	1	Total	C	O	0
			30	28	2	

- Molecule 23 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: $C_{40}H_{54}O$).

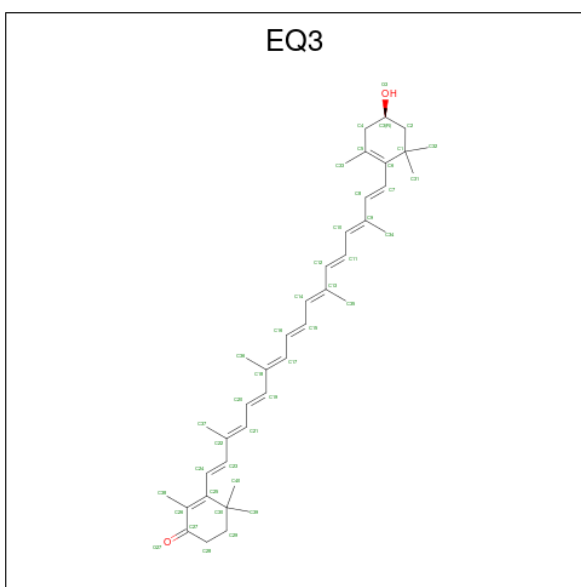


Mol	Chain	Residues	Atoms			AltConf
23	B	1	Total	C	O	0
			41	40	1	
23	M	1	Total	C	O	0
			41	40	1	

- Molecule 24 is CALCIUM ION (CCD ID: CA) (formula: Ca).

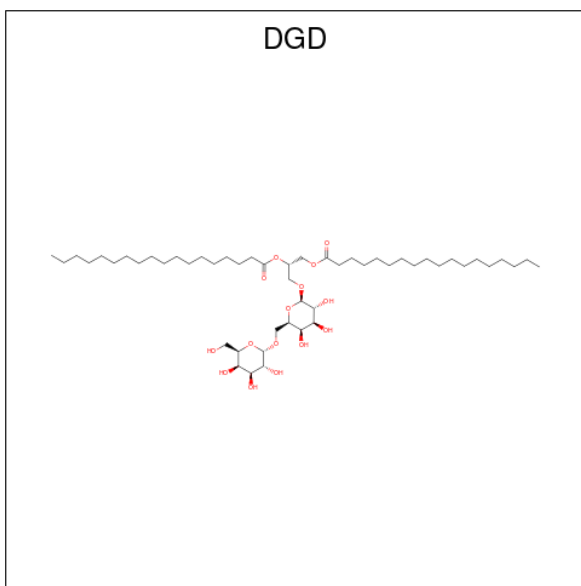
Mol	Chain	Residues	Atoms		AltConf
24	B	1	Total	Ca	0
			1	1	
24	L	1	Total	Ca	0
			1	1	

- Molecule 25 is (3'R)-3'-hydroxy-beta,beta-caroten-4-one (CCD ID: EQ3) (formula: $C_{40}H_{54}O_2$).



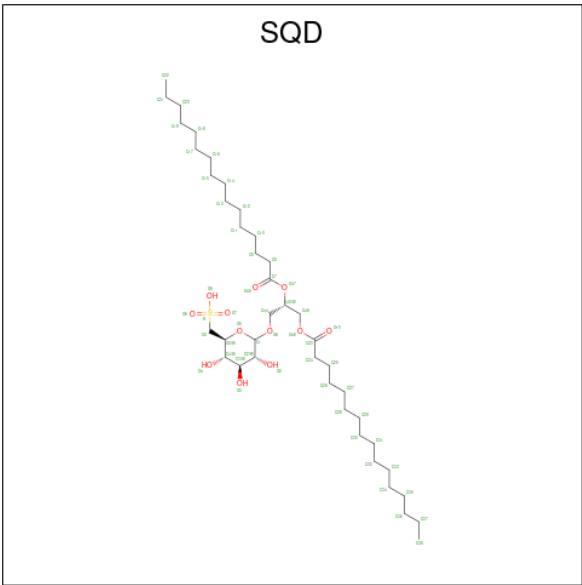
Mol	Chain	Residues	Atoms			AltConf
25	L	1	Total	C	O	0
			42	40	2	

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



Mol	Chain	Residues	Atoms			AltConf
26	L	1	Total	C	O	0
			49	39	10	

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
27	M	1	54	41	12	1	0

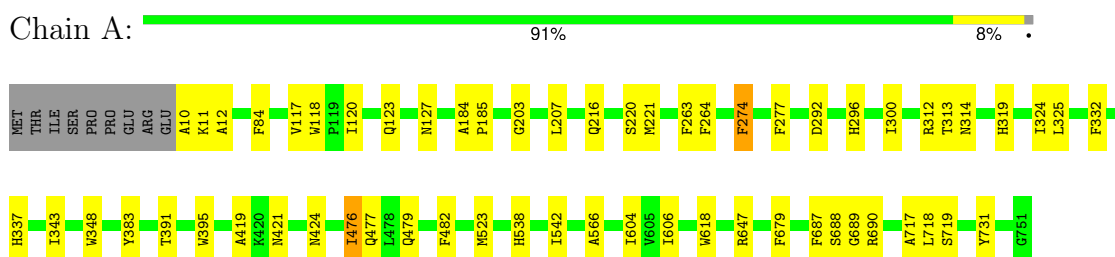
- Molecule 28 is water.

Mol	Chain	Residues	Atoms		AltConf
28	A	267	Total	O	0
			267	267	
28	B	291	Total	O	0
			291	291	
28	C	68	Total	O	0
			68	68	
28	D	68	Total	O	0
			68	68	
28	E	26	Total	O	0
			26	26	
28	F	11	Total	O	0
			11	11	
28	I	6	Total	O	0
			6	6	
28	J	3	Total	O	0
			3	3	
28	K	7	Total	O	0
			7	7	
28	L	39	Total	O	0
			39	39	
28	M	7	Total	O	0
			7	7	

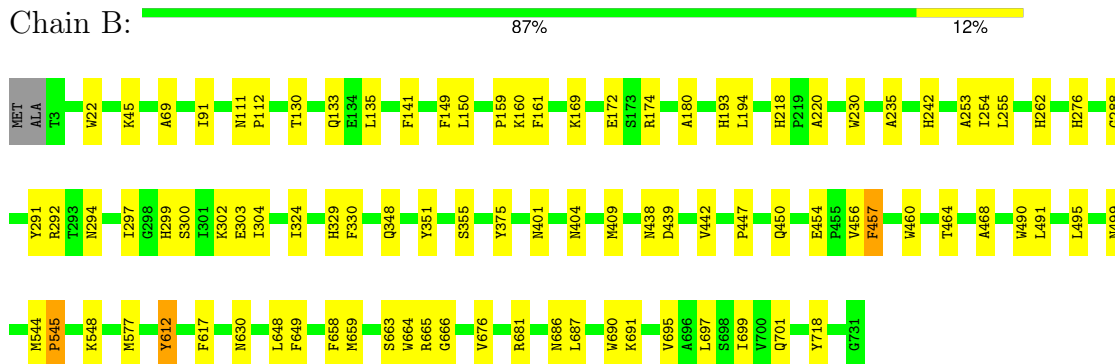
3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

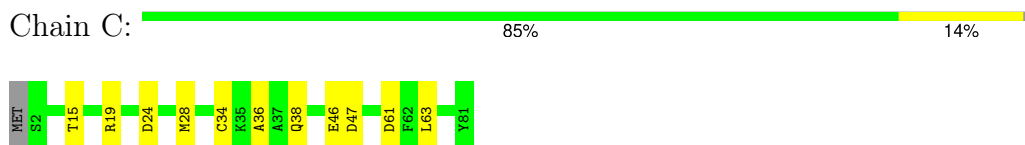
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



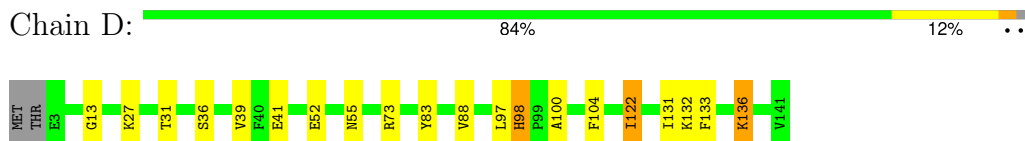
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center

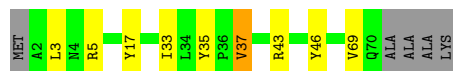


- Molecule 4: Photosystem I reaction center subunit II



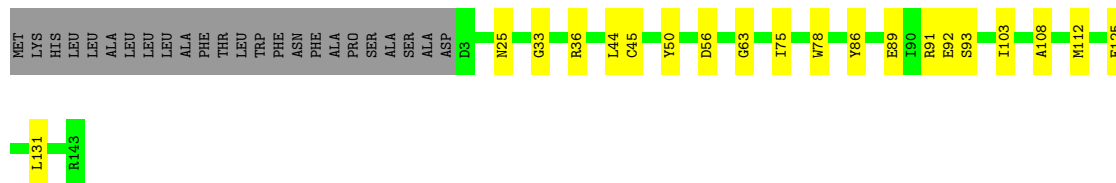
- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  81% 11% • 7%



- Molecule 6: Photosystem I reaction center subunit III

Chain F:  73% 12% 15%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:  85% 10% 5%



- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  72% 22% • •



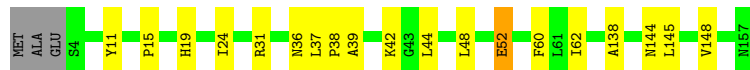
- Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain K:  74% 15% • 9%



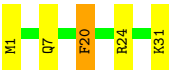
- Molecule 10: Photosystem I reaction center subunit XI

Chain L:  86% 11% • •



- Molecule 11: Photosystem I reaction center subunit XII

Chain M:  84% 13% •



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1243569	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.571	Depositor
Minimum map value	-1.161	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.0353	Depositor
Map size (Å)	350.28, 350.28, 350.28	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, A1AGD, BCR, DGD, LHG, CA, EQ3, ECH, CL0, CL, CLA, SF4, SQD, LMG, 45D, PL9

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	0.68	20/5981 (0.3%)	0.69	8/8156 (0.1%)
2	B	0.93	46/5970 (0.8%)	0.97	17/8165 (0.2%)
3	C	0.65	2/610 (0.3%)	1.01	1/826 (0.1%)
4	D	0.64	4/1099 (0.4%)	0.94	7/1484 (0.5%)
5	E	0.86	2/546 (0.4%)	1.23	5/740 (0.7%)
6	F	0.72	1/1114 (0.1%)	1.07	3/1518 (0.2%)
7	I	0.38	0/308	0.78	0/421
8	J	0.65	0/320	1.08	3/433 (0.7%)
9	K	0.82	3/557 (0.5%)	1.01	1/754 (0.1%)
10	L	0.56	3/1182 (0.3%)	0.81	1/1606 (0.1%)
11	M	0.67	2/241 (0.8%)	0.62	0/326
All	All	0.77	83/17928 (0.5%)	0.89	46/24429 (0.2%)

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
2	B	0	2
3	C	0	1
4	D	0	2
5	E	0	3
6	F	0	1
7	I	0	1
10	L	0	1
All	All	0	11

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	THR	CA-C	16.23	1.60	1.52
1	A	731	TYR	C-O	-13.06	1.08	1.24
2	B	695	VAL	C-O	-13.02	1.09	1.23
2	B	649	PHE	C-O	-11.44	1.10	1.24
2	B	297	ILE	C-O	-11.44	1.10	1.24

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	92	GLU	N-CA-C	-8.45	104.02	112.97
2	B	665	ARG	N-CA-C	8.26	120.28	111.28
4	D	136	LYS	CA-CB-CG	8.18	130.46	114.10
9	K	14	LEU	N-CA-C	8.04	122.74	109.95
3	C	63	LEU	CA-C-O	-6.90	113.60	121.19

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	292	ARG	Sidechain
2	B	294	ASN	Mainchain
3	C	19	ARG	Sidechain
4	D	122	ILE	Mainchain
4	D	52	GLU	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5783	0	5630	30	0
2	B	5759	0	5532	41	0
3	C	600	0	581	5	0
4	D	1075	0	1056	8	0
5	E	537	0	511	2	0
6	F	1084	0	1059	9	0
7	I	297	0	295	2	0
8	J	311	0	316	10	0
9	K	545	0	567	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	L	1152	0	1123	12	0
11	M	238	0	260	8	0
12	A	2530	0	2581	83	0
12	B	2530	0	2667	85	0
12	F	90	0	66	3	0
12	J	150	0	124	4	0
12	K	150	0	123	10	0
12	L	260	0	288	6	0
13	A	65	0	72	1	0
14	A	8	0	0	0	0
14	C	16	0	0	0	0
15	A	160	0	224	6	0
15	B	185	0	257	10	0
15	F	80	0	112	6	0
15	I	40	0	56	4	0
15	J	94	0	132	7	0
15	K	80	0	112	5	0
15	L	80	0	112	4	0
16	A	86	0	118	9	0
16	B	49	0	74	5	0
16	M	44	0	61	1	0
17	A	96	0	135	4	0
17	B	51	0	75	1	0
18	A	105	0	138	5	0
18	B	64	0	77	4	0
18	F	31	0	35	1	0
18	J	31	0	35	1	0
18	L	35	0	46	3	0
19	A	30	0	37	10	0
20	A	42	0	52	3	0
21	A	1	0	0	0	0
22	B	30	0	0	0	0
23	B	41	0	54	1	0
23	M	41	0	54	0	0
24	B	1	0	0	0	0
24	L	1	0	0	0	0
25	L	42	0	0	0	0
26	L	49	0	70	2	0
27	M	54	0	78	5	0
28	A	267	0	0	0	0
28	B	291	0	0	0	0
28	C	68	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	D	68	0	0	0	0
28	E	26	0	0	1	0
28	F	11	0	0	0	0
28	I	6	0	0	0	0
28	J	3	0	0	0	0
28	K	7	0	0	0	0
28	L	39	0	0	0	0
28	M	7	0	0	0	0
All	All	25616	0	24995	334	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 334 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)
8:J:31:ARG:HD3	15:J:105:BCR:H313	1.48	0.95
12:B:847:CLA:HHC	12:B:847:CLA:HBB1	1.49	0.94
1:A:12:ALA:H	1:A:314:ASN:HD21	1.03	0.93
12:A:843:CLA:H92	12:A:846:CLA:C6	2.05	0.86
8:J:31:ARG:HD3	15:J:105:BCR:C31	2.08	0.83

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	740/751 (98%)	722 (98%)	17 (2%)	1 (0%)	48	31
2	B	727/731 (100%)	695 (96%)	32 (4%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	137/141 (97%)	134 (98%)	3 (2%)	0	100	100
5	E	67/74 (90%)	64 (96%)	3 (4%)	0	100	100
6	F	139/165 (84%)	133 (96%)	6 (4%)	0	100	100
7	I	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
8	J	37/40 (92%)	37 (100%)	0	0	100	100
9	K	76/86 (88%)	73 (96%)	3 (4%)	0	100	100
10	L	152/157 (97%)	145 (95%)	7 (5%)	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100
All	All	2218/2297 (97%)	2142 (97%)	75 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	LYS

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 PDB entries followed by that with respect to all EM entries.

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%)	589 (100%)	0	100	100
2	B	579/583 (99%)	579 (100%)	0	100	100
3	C	68/69 (99%)	68 (100%)	0	100	100
4	D	111/116 (96%)	111 (100%)	0	100	100
5	E	56/60 (93%)	56 (100%)	0	100	100
6	F	114/137 (83%)	112 (98%)	2 (2%)	51	27
7	I	31/32 (97%)	31 (100%)	0	100	100
8	J	34/35 (97%)	34 (100%)	0	100	100
9	K	55/62 (89%)	55 (100%)	0	100	100
10	L	115/118 (98%)	115 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	M	25/25 (100%)	25 (100%)	0	100	100
All	All	1777/1840 (97%)	1775 (100%)	2 (0%)	87	83

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	44	LEU
6	F	89	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	331	GLN
2	B	624	ASN
10	L	108	GLN
2	B	401	ASN
2	B	499	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 144 ligands modelled in this entry, 3 are monoatomic - leaving 141 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
12	CLA	A	828	1	69,73,73	2.18	23 (33%)	82,113,113	2.42	24 (29%)
12	CLA	A	817	1	54,58,73	2.52	22 (40%)	64,95,113	2.69	23 (35%)
12	CLA	F	203	28	49,53,73	2.54	20 (40%)	58,89,113	2.61	23 (39%)
12	CLA	B	823	2	59,63,73	2.45	24 (40%)	70,101,113	2.52	24 (34%)
12	CLA	A	843	1	64,68,73	2.28	22 (34%)	76,107,113	2.58	28 (36%)
12	CLA	B	852	2	54,58,73	2.60	23 (42%)	64,95,113	2.75	25 (39%)
16	LHG	M	103	-	43,43,48	1.04	2 (4%)	46,49,54	1.26	5 (10%)
17	LMG	A	840	-	50,50,55	1.49	8 (16%)	58,58,63	1.52	8 (13%)
12	CLA	A	808	1	54,58,73	2.52	21 (38%)	64,95,113	2.75	27 (42%)
12	CLA	B	807	2	69,73,73	2.22	23 (33%)	82,113,113	2.44	25 (30%)
12	CLA	F	204	6	49,53,73	2.58	22 (44%)	58,89,113	2.81	25 (43%)
15	BCR	B	835	-	41,41,41	4.66	24 (58%)	56,56,56	2.24	23 (41%)
14	SF4	A	834	1,2	0,12,12	-	-	-	-	-
12	CLA	A	823	1	69,73,73	2.22	22 (31%)	82,113,113	2.43	25 (30%)
12	CLA	B	846	2	59,63,73	2.28	21 (35%)	70,101,113	2.96	29 (41%)
15	BCR	B	832	-	41,41,41	4.80	24 (58%)	56,56,56	2.06	18 (32%)
16	LHG	A	839	-	48,48,48	0.92	2 (4%)	51,54,54	0.97	3 (5%)
15	BCR	F	201	-	41,41,41	4.80	24 (58%)	56,56,56	2.17	23 (41%)
12	CLA	A	804	1	69,73,73	2.19	23 (33%)	82,113,113	2.45	25 (30%)
12	CLA	B	828	28	69,73,73	2.21	22 (31%)	82,113,113	2.36	23 (28%)
15	BCR	A	835	-	41,41,41	4.74	24 (58%)	56,56,56	2.25	23 (41%)
27	SQD	M	102	-	52,54,54	1.52	7 (13%)	62,65,65	1.53	10 (16%)
12	CLA	B	809	2	69,73,73	2.23	20 (28%)	82,113,113	2.32	23 (28%)
12	CLA	A	818	28	69,73,73	2.24	22 (31%)	82,113,113	2.51	25 (30%)
12	CLA	A	846	1	59,63,73	2.45	20 (33%)	70,101,113	2.79	25 (35%)
12	CLA	B	830	16	49,53,73	2.55	22 (44%)	58,89,113	2.81	24 (41%)
12	CLA	A	849	1	69,73,73	2.21	22 (31%)	82,113,113	2.37	25 (30%)
12	CLA	A	811	1	49,53,73	2.51	21 (42%)	58,89,113	2.71	22 (37%)
12	CLA	B	814	2	69,73,73	2.26	24 (34%)	82,113,113	2.41	24 (29%)
18	LMT	A	842	-	36,36,36	0.55	0	47,47,47	0.87	1 (2%)
12	CLA	B	812	2	69,73,73	2.20	22 (31%)	82,113,113	2.45	27 (32%)
12	CLA	B	826	28	69,73,73	2.24	23 (33%)	82,113,113	2.47	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BCR	L	207	-	41,41,41	4.72	24 (58%)	56,56,56	2.37	25 (44%)
16	LHG	A	850	12	36,36,48	1.20	4 (11%)	39,42,54	1.65	6 (15%)
25	EQ3	L	202	-	43,43,43	1.31	8 (18%)	55,60,60	1.57	8 (14%)
15	BCR	B	836	-	25,25,41	4.34	12 (48%)	33,33,56	2.81	16 (48%)
12	CLA	B	802	28	69,73,73	2.22	22 (31%)	82,113,113	2.45	26 (31%)
12	CLA	A	809	1,12	69,73,73	2.16	21 (30%)	82,113,113	2.69	31 (37%)
12	CLA	A	845	1	69,73,73	2.21	22 (31%)	82,113,113	2.41	26 (31%)
18	LMT	B	839	-	30,30,36	0.59	0	41,41,47	0.82	1 (2%)
12	CLA	A	810	1	54,58,73	2.50	20 (37%)	64,95,113	2.70	23 (35%)
12	CLA	B	805	28	49,53,73	2.54	22 (44%)	58,89,113	4.41	21 (36%)
18	LMT	A	853	-	36,36,36	0.55	0	47,47,47	0.85	3 (6%)
23	ECH	M	101	-	42,42,42	0.44	0	55,58,58	0.90	3 (5%)
12	CLA	B	819	2	69,73,73	2.19	21 (30%)	82,113,113	2.40	23 (28%)
12	CLA	A	830	1	69,73,73	2.24	23 (33%)	82,113,113	2.36	27 (32%)
12	CLA	A	814	1	69,73,73	2.21	22 (31%)	82,113,113	2.30	25 (30%)
18	LMT	J	106	-	32,32,36	0.56	0	43,43,47	1.09	3 (6%)
12	CLA	B	804	2	69,73,73	2.25	22 (31%)	82,113,113	2.45	26 (31%)
12	CLA	A	848	1	69,73,73	2.20	22 (31%)	82,113,113	2.45	25 (30%)
12	CLA	B	825	2	59,63,73	2.42	23 (38%)	70,101,113	2.62	27 (38%)
13	CL0	A	802	1	69,73,73	2.20	23 (33%)	82,113,113	2.40	23 (28%)
12	CLA	B	843	28	69,73,73	2.22	22 (31%)	82,113,113	2.41	25 (30%)
12	CLA	B	808	2	69,73,73	2.24	23 (33%)	82,113,113	2.34	21 (25%)
12	CLA	A	819	28	64,68,73	2.32	23 (35%)	76,107,113	2.54	25 (32%)
12	CLA	B	811	2	69,73,73	2.17	21 (30%)	82,113,113	2.57	28 (34%)
12	CLA	B	849	2	64,68,73	2.29	21 (32%)	76,107,113	2.71	26 (34%)
14	SF4	C	101	3	0,12,12	-	-	-	-	-
17	LMG	B	837	-	51,51,55	1.44	7 (13%)	59,59,63	1.07	5 (8%)
12	CLA	A	822	1	69,73,73	2.24	21 (30%)	82,113,113	2.30	20 (24%)
12	CLA	B	853	2	69,73,73	2.21	22 (31%)	82,113,113	2.80	26 (31%)
12	CLA	K	4003	9	49,53,73	1.44	8 (16%)	58,89,113	1.09	5 (8%)
12	CLA	L	204	-	69,73,73	2.24	23 (33%)	82,113,113	2.44	24 (29%)
12	CLA	A	855	28	69,73,73	2.21	23 (33%)	82,113,113	2.56	28 (34%)
12	CLA	B	815	2	49,53,73	2.55	22 (44%)	58,89,113	2.64	21 (36%)
15	BCR	A	837	-	41,41,41	4.69	24 (58%)	56,56,56	2.46	22 (39%)
12	CLA	A	816	28	69,73,73	2.25	23 (33%)	82,113,113	2.34	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	SF4	C	102	3	0,12,12	-	-	-		
12	CLA	B	829	2	69,73,73	2.19	23 (33%)	82,113,113	2.46	23 (28%)
12	CLA	A	826	1	69,73,73	2.20	22 (31%)	82,113,113	2.41	24 (29%)
12	CLA	A	833	16	54,58,73	2.53	23 (42%)	64,95,113	2.74	25 (39%)
18	LMT	B	840	-	36,36,36	0.48	0	47,47,47	1.47	6 (12%)
12	CLA	K	4002	9	49,53,73	2.54	21 (42%)	58,89,113	2.80	28 (48%)
12	CLA	J	102	-	49,53,73	2.54	22 (44%)	58,89,113	2.70	22 (37%)
12	CLA	A	831	28	69,73,73	2.22	22 (31%)	82,113,113	2.59	26 (31%)
12	CLA	L	201	1	69,73,73	2.22	22 (31%)	82,113,113	2.49	22 (26%)
12	CLA	A	852	28	59,63,73	2.58	24 (40%)	70,101,113	2.79	28 (40%)
12	CLA	A	844	1	69,73,73	2.12	19 (27%)	82,113,113	2.78	28 (34%)
12	CLA	B	827	2	49,53,73	2.51	20 (40%)	58,89,113	2.82	19 (32%)
15	BCR	K	4001	-	41,41,41	4.79	24 (58%)	56,56,56	2.30	21 (37%)
12	CLA	B	847	2	69,73,73	2.04	19 (27%)	82,113,113	2.49	24 (29%)
12	CLA	A	825	1	64,68,73	2.28	23 (35%)	76,107,113	2.59	27 (35%)
12	CLA	B	803	28	69,73,73	2.22	20 (28%)	82,113,113	2.85	28 (34%)
18	LMT	A	841	-	36,36,36	0.56	0	47,47,47	0.71	0
12	CLA	A	858	-	69,73,73	2.17	21 (30%)	82,113,113	2.53	27 (32%)
12	CLA	B	824	2	69,73,73	2.10	18 (26%)	82,113,113	2.66	27 (32%)
15	BCR	J	105	-	41,41,41	4.77	25 (60%)	56,56,56	3.14	28 (50%)
12	CLA	A	832	1	54,58,73	2.53	22 (40%)	64,95,113	2.71	24 (37%)
12	CLA	B	820	2	69,73,73	2.21	21 (30%)	82,113,113	2.41	24 (29%)
16	LHG	B	851	12	48,48,48	0.98	2 (4%)	51,54,54	1.34	7 (13%)
12	CLA	B	817	2	69,73,73	2.19	21 (30%)	82,113,113	2.48	29 (35%)
12	CLA	K	4004	28	64,68,73	2.25	22 (34%)	76,107,113	3.03	32 (42%)
12	CLA	B	813	2	69,73,73	2.22	23 (33%)	82,113,113	2.53	26 (31%)
18	LMT	F	205	-	32,32,36	0.58	0	43,43,47	0.88	2 (4%)
12	CLA	B	850	2	69,73,73	2.26	23 (33%)	82,113,113	2.37	29 (35%)
12	CLA	A	847	1	69,73,73	2.19	22 (31%)	82,113,113	2.39	25 (30%)
12	CLA	A	821	1	69,73,73	2.23	22 (31%)	82,113,113	2.46	24 (29%)
12	CLA	B	816	2	69,73,73	2.22	23 (33%)	82,113,113	2.40	25 (30%)
12	CLA	J	101	1	64,68,73	2.41	23 (35%)	76,107,113	2.65	28 (36%)
12	CLA	B	818	28	69,73,73	2.21	22 (31%)	82,113,113	2.49	29 (35%)
12	CLA	A	824	1	59,63,73	2.39	23 (38%)	70,101,113	2.61	27 (38%)
12	CLA	A	829	1	69,73,73	2.24	24 (34%)	82,113,113	2.55	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BCR	B	841	-	41,41,41	4.73	24 (58%)	56,56,56	2.34	20 (35%)
12	CLA	A	820	1	69,73,73	2.20	21 (30%)	82,113,113	2.44	26 (31%)
12	CLA	A	803	1	69,73,73	2.24	22 (31%)	82,113,113	2.47	27 (32%)
12	CLA	A	813	1	64,68,73	2.32	23 (35%)	76,107,113	2.48	27 (35%)
15	BCR	F	202	-	41,41,41	4.79	24 (58%)	56,56,56	2.27	21 (37%)
12	CLA	A	812	28	49,53,73	2.55	23 (46%)	58,89,113	2.72	23 (39%)
15	BCR	K	4005	-	41,41,41	4.77	24 (58%)	56,56,56	2.12	28 (50%)
12	CLA	A	801	1,12	64,68,73	2.29	23 (35%)	76,107,113	2.62	28 (36%)
12	CLA	B	810	2	69,73,73	2.22	22 (31%)	82,113,113	2.33	23 (28%)
15	BCR	B	834	-	41,41,41	4.74	24 (58%)	56,56,56	2.25	25 (44%)
15	BCR	J	107	-	41,41,41	4.72	24 (58%)	56,56,56	2.60	24 (42%)
22	A1AGD	B	831	-	30,30,30	0.84	1 (3%)	38,39,39	1.45	5 (13%)
15	BCR	A	836	-	41,41,41	4.75	24 (58%)	56,56,56	2.29	23 (41%)
17	LMG	A	851	-	46,46,55	1.42	6 (13%)	54,54,63	1.75	11 (20%)
12	CLA	B	842	2	69,73,73	2.22	23 (33%)	82,113,113	2.41	24 (29%)
12	CLA	B	845	2	69,73,73	2.23	22 (31%)	82,113,113	2.44	26 (31%)
26	DGD	L	209	-	49,49,67	1.42	6 (12%)	57,57,81	1.16	3 (5%)
12	CLA	B	821	2	69,73,73	2.23	22 (31%)	82,113,113	2.35	25 (30%)
12	CLA	A	827	1	69,73,73	2.21	23 (33%)	82,113,113	2.42	27 (32%)
19	PL9	A	854	-	30,30,55	0.93	2 (6%)	38,39,69	2.03	15 (39%)
15	BCR	J	104	-	14,14,41	5.39	8 (57%)	20,20,56	2.81	9 (45%)
12	CLA	B	844	2	64,68,73	2.24	23 (35%)	76,107,113	3.15	27 (35%)
12	CLA	B	801	-	69,73,73	2.20	22 (31%)	82,113,113	2.51	27 (32%)
12	CLA	A	807	1	59,63,73	2.39	23 (38%)	70,101,113	2.70	25 (35%)
12	CLA	A	805	1	69,73,73	2.24	22 (31%)	82,113,113	2.57	30 (36%)
12	CLA	B	848	2	69,73,73	2.27	23 (33%)	82,113,113	2.48	25 (30%)
12	CLA	B	822	2	69,73,73	2.21	22 (31%)	82,113,113	2.45	27 (32%)
15	BCR	A	838	-	41,41,41	4.75	24 (58%)	56,56,56	2.25	20 (35%)
12	CLA	B	806	2	69,73,73	2.24	22 (31%)	82,113,113	2.42	25 (30%)
12	CLA	L	206	28	69,73,73	2.24	23 (33%)	82,113,113	2.46	24 (29%)
18	LMT	L	210	-	36,36,36	0.50	0	47,47,47	1.07	4 (8%)
15	BCR	I	101	-	41,41,41	4.81	24 (58%)	56,56,56	2.18	19 (33%)
12	CLA	A	815	1	69,73,73	2.23	22 (31%)	82,113,113	2.44	24 (29%)
12	CLA	J	103	8	49,53,73	2.59	24 (48%)	58,89,113	3.04	26 (44%)
20	45D	A	856	-	43,43,43	1.50	8 (18%)	54,60,60	1.80	17 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	L	205	10	69,73,73	2.20	21 (30%)	82,113,113	2.52	25 (30%)
15	BCR	L	208	-	41,41,41	4.80	24 (58%)	56,56,56	2.27	20 (35%)
12	CLA	A	806	1	49,53,73	2.52	21 (42%)	58,89,113	2.77	22 (37%)
23	ECH	B	833	-	42,42,42	0.40	0	55,58,58	0.75	1 (1%)

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
12	CLA	A	828	1	-	16/39/115/115	-
12	CLA	A	817	1	-	6/21/97/115	-
12	CLA	F	203	28	-	1/15/91/115	-
12	CLA	B	823	2	-	9/27/103/115	-
12	CLA	A	843	1	-	13/33/109/115	-
12	CLA	B	852	2	-	3/21/97/115	-
16	LHG	M	103	-	-	25/48/48/53	-
17	LMG	A	840	-	-	18/45/65/70	0/1/1/1
12	CLA	A	808	1	-	8/21/97/115	-
12	CLA	B	807	2	-	9/39/115/115	-
12	CLA	F	204	6	-	9/15/91/115	-
15	BCR	B	835	-	-	2/29/63/63	0/2/2/2
14	SF4	A	834	1,2	-	-	0/6/5/5
12	CLA	A	823	1	-	15/39/115/115	-
12	CLA	B	846	2	-	12/27/103/115	-
15	BCR	B	832	-	-	4/29/63/63	0/2/2/2
16	LHG	A	839	-	-	24/53/53/53	-
15	BCR	F	201	-	-	5/29/63/63	0/2/2/2
12	CLA	A	804	1	-	19/39/115/115	-
12	CLA	B	828	28	-	6/39/115/115	-
15	BCR	A	835	-	-	8/29/63/63	0/2/2/2
27	SQD	M	102	-	-	28/49/69/69	0/1/1/1
12	CLA	B	809	2	-	10/39/115/115	-
12	CLA	A	818	28	-	7/39/115/115	-
12	CLA	A	846	1	-	11/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	830	16	-	4/15/91/115	-
12	CLA	A	849	1	-	14/39/115/115	-
12	CLA	A	811	1	-	3/15/91/115	-
12	CLA	B	814	2	-	17/39/115/115	-
18	LMT	A	842	-	-	12/21/61/61	0/2/2/2
12	CLA	B	812	2	-	6/39/115/115	-
12	CLA	B	826	28	-	11/39/115/115	-
15	BCR	L	207	-	-	6/29/63/63	0/2/2/2
16	LHG	A	850	12	-	14/41/41/53	-
25	EQ3	L	202	-	-	5/29/68/68	0/2/2/2
15	BCR	B	836	-	-	8/18/35/63	0/1/1/2
12	CLA	B	802	28	-	10/39/115/115	-
12	CLA	A	809	1,12	-	17/39/115/115	-
12	CLA	A	845	1	-	11/39/115/115	-
18	LMT	B	839	-	-	5/15/55/61	0/2/2/2
12	CLA	A	810	1	-	5/21/97/115	-
12	CLA	B	805	28	-	3/15/91/115	-
18	LMT	A	853	-	-	4/21/61/61	0/2/2/2
23	ECH	M	101	-	-	6/29/66/66	0/2/2/2
12	CLA	B	819	2	-	4/39/115/115	-
12	CLA	A	830	1	-	6/39/115/115	-
12	CLA	A	814	1	-	6/39/115/115	-
18	LMT	J	106	-	-	10/17/57/61	0/2/2/2
12	CLA	B	804	2	-	13/39/115/115	-
12	CLA	A	848	1	-	21/39/115/115	-
12	CLA	B	825	2	-	11/27/103/115	-
13	CL0	A	802	1	-	5/39/115/115	-
12	CLA	B	843	28	-	19/39/115/115	-
12	CLA	B	808	2	-	11/39/115/115	-
12	CLA	A	819	28	-	8/33/109/115	-
12	CLA	B	811	2	-	7/39/115/115	-
12	CLA	B	849	2	-	11/33/109/115	-
17	LMG	B	837	-	-	12/46/66/70	0/1/1/1
14	SF4	C	101	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	822	1	-	5/39/115/115	-
12	CLA	B	853	2	-	5/39/115/115	-
12	CLA	K	4003	9	-	2/15/91/115	-
12	CLA	L	204	-	-	16/39/115/115	-
12	CLA	A	855	28	-	7/39/115/115	-
12	CLA	B	815	2	-	3/15/91/115	-
15	BCR	A	837	-	-	4/29/63/63	0/2/2/2
12	CLA	A	816	28	-	5/39/115/115	-
14	SF4	C	102	3	-	-	0/6/5/5
12	CLA	B	829	2	-	15/39/115/115	-
12	CLA	A	826	1	-	13/39/115/115	-
12	CLA	A	833	16	-	6/21/97/115	-
18	LMT	B	840	-	-	12/21/61/61	0/2/2/2
12	CLA	K	4002	9	-	9/15/91/115	-
12	CLA	J	102	-	-	7/15/91/115	-
12	CLA	A	831	28	-	15/39/115/115	-
12	CLA	L	201	1	-	7/39/115/115	-
12	CLA	A	852	28	-	4/27/103/115	-
12	CLA	A	844	1	-	12/39/115/115	-
12	CLA	B	827	2	-	3/15/91/115	-
15	BCR	K	4001	-	-	4/29/63/63	0/2/2/2
12	CLA	B	847	2	-	4/39/115/115	-
12	CLA	A	825	1	-	12/33/109/115	-
12	CLA	B	803	28	-	3/39/115/115	-
18	LMT	A	841	-	-	9/21/61/61	0/2/2/2
12	CLA	A	858	-	-	10/39/115/115	-
12	CLA	B	824	2	-	9/39/115/115	-
15	BCR	J	105	-	-	7/29/63/63	0/2/2/2
12	CLA	A	832	1	-	7/21/97/115	-
12	CLA	B	820	2	-	19/39/115/115	-
16	LHG	B	851	12	-	26/53/53/53	-
12	CLA	B	817	2	-	14/39/115/115	-
12	CLA	K	4004	28	-	9/33/109/115	-
12	CLA	B	813	2	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LMT	F	205	-	-	4/17/57/61	0/2/2/2
12	CLA	B	850	2	-	9/39/115/115	-
12	CLA	A	847	1	-	18/39/115/115	-
12	CLA	A	821	1	-	10/39/115/115	-
12	CLA	B	816	2	-	19/39/115/115	-
12	CLA	J	101	1	-	16/33/109/115	-
12	CLA	B	818	28	-	14/39/115/115	-
12	CLA	A	824	1	-	14/27/103/115	-
12	CLA	A	829	1	-	12/39/115/115	-
15	BCR	B	841	-	-	9/29/63/63	0/2/2/2
12	CLA	A	820	1	-	6/39/115/115	-
12	CLA	A	803	1	-	12/39/115/115	-
12	CLA	A	813	1	-	11/33/109/115	-
15	BCR	F	202	-	-	2/29/63/63	0/2/2/2
12	CLA	A	812	28	-	6/15/91/115	-
15	BCR	K	4005	-	-	8/29/63/63	0/2/2/2
12	CLA	A	801	1,12	-	12/33/109/115	-
12	CLA	B	810	2	-	10/39/115/115	-
15	BCR	B	834	-	-	2/29/63/63	0/2/2/2
15	BCR	J	107	-	-	10/29/63/63	0/2/2/2
22	A1AGD	B	831	-	-	10/23/43/43	0/1/1/1
15	BCR	A	836	-	-	1/29/63/63	0/2/2/2
17	LMG	A	851	-	-	21/41/61/70	0/1/1/1
12	CLA	B	842	2	-	17/39/115/115	-
12	CLA	B	845	2	-	13/39/115/115	-
26	DGD	L	209	-	-	23/44/64/95	0/1/1/2
12	CLA	B	821	2	-	6/39/115/115	-
12	CLA	A	827	1	-	16/39/115/115	-
19	PL9	A	854	-	-	5/23/43/73	0/1/1/1
15	BCR	J	104	-	-	3/5/22/63	0/1/1/2
12	CLA	B	844	2	-	11/33/109/115	-
12	CLA	B	801	-	-	6/39/115/115	-
12	CLA	A	807	1	-	8/27/103/115	-
12	CLA	A	805	1	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	848	2	-	23/39/115/115	-
12	CLA	B	822	2	-	14/39/115/115	-
15	BCR	A	838	-	-	7/29/63/63	0/2/2/2
12	CLA	B	806	2	-	21/39/115/115	-
12	CLA	L	206	28	-	19/39/115/115	-
18	LMT	L	210	-	-	14/21/61/61	0/2/2/2
15	BCR	I	101	-	-	4/29/63/63	0/2/2/2
12	CLA	A	815	1	-	12/39/115/115	-
12	CLA	J	103	8	-	7/15/91/115	-
20	45D	A	856	-	-	5/29/69/69	0/2/2/2
12	CLA	L	205	10	-	10/39/115/115	-
15	BCR	L	208	-	-	2/29/63/63	0/2/2/2
12	CLA	A	806	1	-	6/15/91/115	-
23	ECH	B	833	-	-	5/29/66/66	0/2/2/2

The worst 5 of 2593 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	K	4001	BCR	C26-C25	16.71	1.62	1.34
15	F	201	BCR	C26-C25	16.11	1.61	1.34
15	I	101	BCR	C26-C25	16.09	1.61	1.34
15	A	836	BCR	C26-C25	16.02	1.61	1.34
15	B	834	BCR	C26-C25	15.90	1.61	1.34

The worst 5 of 2951 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	805	CLA	O2A-CGA-O1A	-20.40	70.86	123.33
12	B	844	CLA	C4A-NA-C1A	13.79	112.97	106.68
12	B	805	CLA	O2A-CGA-CBA	12.91	154.79	114.00
12	B	805	CLA	O1A-CGA-CBA	-12.34	83.95	123.09
12	B	803	CLA	C4A-NA-C1A	11.82	112.07	106.68

There are no chirality outliers.

5 of 1368 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	803	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	A	803	CLA	CBA-CGA-O2A-C1
12	A	803	CLA	O1A-CGA-O2A-C1
12	A	804	CLA	C1A-C2A-CAA-CBA
12	A	804	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

113 monomers are involved in 242 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	828	CLA	3	0
12	F	203	CLA	1	0
12	B	823	CLA	2	0
12	A	843	CLA	8	0
12	B	852	CLA	2	0
16	M	103	LHG	1	0
17	A	840	LMG	2	0
12	B	807	CLA	3	0
12	F	204	CLA	2	0
15	B	835	BCR	1	0
12	A	823	CLA	2	0
12	B	846	CLA	1	0
15	B	832	BCR	2	0
16	A	839	LHG	4	0
15	F	201	BCR	3	0
12	A	804	CLA	2	0
12	B	828	CLA	2	0
15	A	835	BCR	3	0
27	M	102	SQD	5	0
12	B	809	CLA	2	0
12	A	846	CLA	9	0
12	A	849	CLA	4	0
12	B	814	CLA	2	0
18	A	842	LMT	4	0
12	B	826	CLA	1	0
15	L	207	BCR	3	0
16	A	850	LHG	5	0
15	B	836	BCR	3	0
12	B	802	CLA	5	0
12	A	809	CLA	6	0
12	A	845	CLA	1	0
12	A	810	CLA	1	0
12	B	805	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	819	CLA	6	0
12	A	830	CLA	3	0
12	A	814	CLA	3	0
18	J	106	LMT	1	0
12	A	848	CLA	4	0
12	B	825	CLA	1	0
13	A	802	CL0	1	0
12	B	843	CLA	3	0
12	B	808	CLA	1	0
12	A	819	CLA	1	0
12	B	811	CLA	4	0
12	B	849	CLA	2	0
17	B	837	LMG	1	0
12	B	853	CLA	3	0
12	K	4003	CLA	6	0
12	L	204	CLA	3	0
12	A	855	CLA	1	0
15	A	837	BCR	3	0
12	A	816	CLA	2	0
12	A	826	CLA	2	0
12	A	833	CLA	1	0
18	B	840	LMT	4	0
12	J	102	CLA	2	0
12	A	831	CLA	3	0
12	L	201	CLA	1	0
12	A	844	CLA	8	0
12	B	827	CLA	4	0
12	B	847	CLA	5	0
12	A	825	CLA	3	0
12	B	803	CLA	4	0
18	A	841	LMT	1	0
12	A	858	CLA	2	0
12	B	824	CLA	6	0
15	J	105	BCR	4	0
12	A	832	CLA	2	0
12	B	820	CLA	3	0
16	B	851	LHG	5	0
12	B	817	CLA	1	0
12	K	4004	CLA	4	0
12	B	813	CLA	2	0
18	F	205	LMT	1	0
12	B	850	CLA	5	0

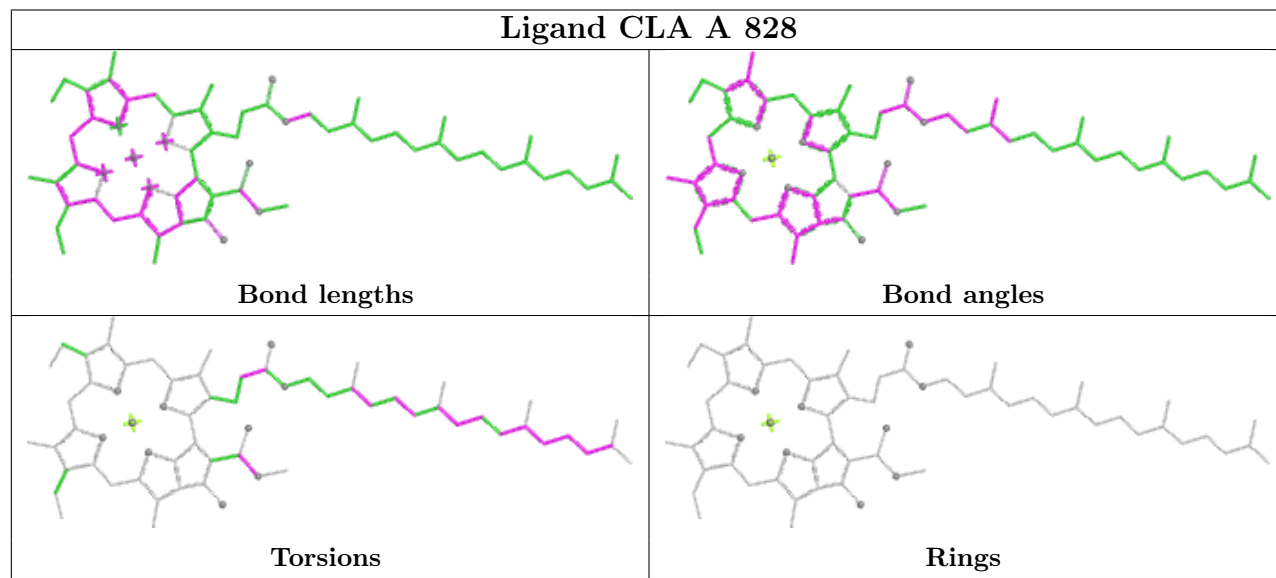
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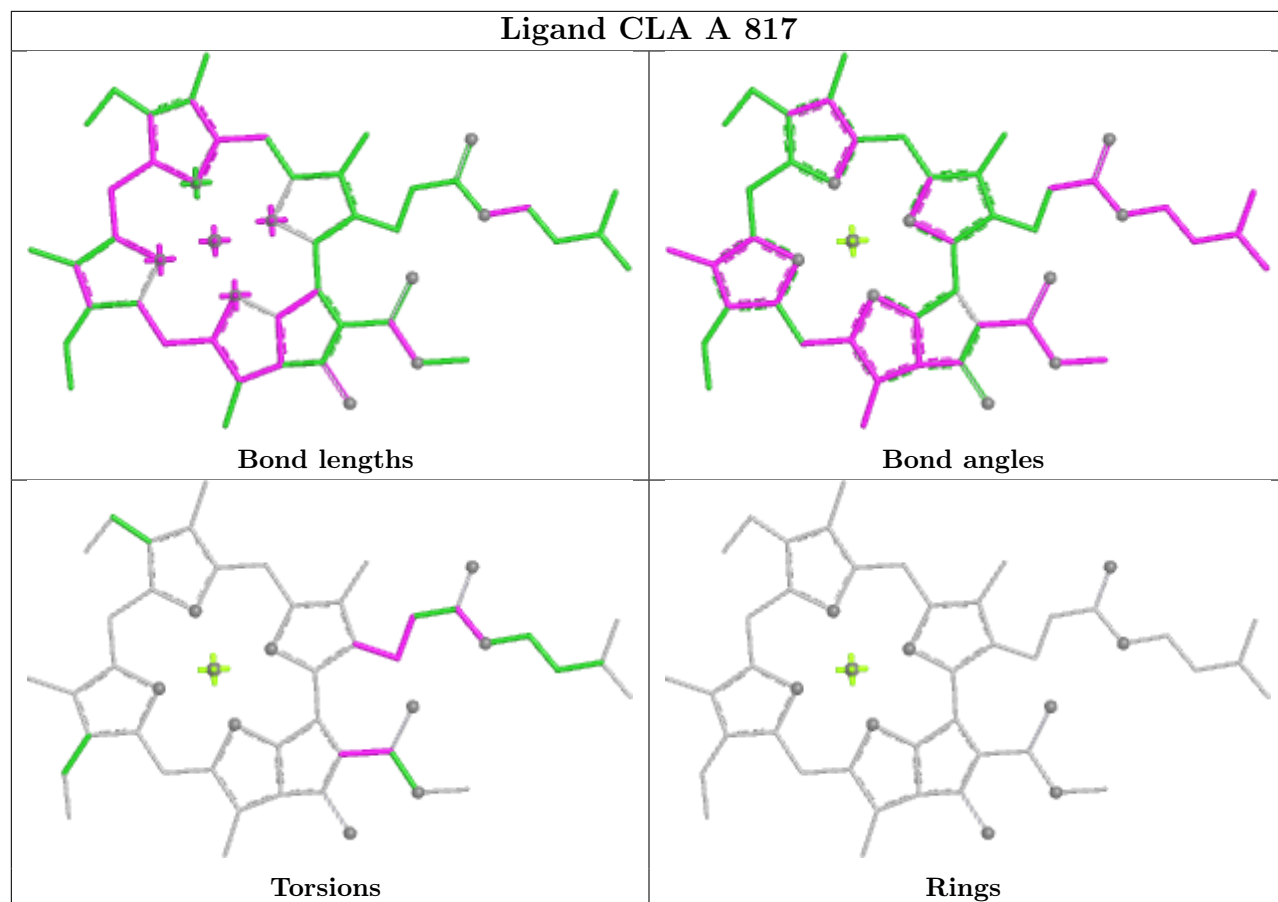
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	847	CLA	2	0
12	A	821	CLA	4	0
12	B	816	CLA	1	0
12	J	101	CLA	2	0
12	B	818	CLA	2	0
12	A	824	CLA	2	0
12	A	829	CLA	3	0
15	B	841	BCR	1	0
12	A	820	CLA	2	0
12	A	803	CLA	1	0
12	A	813	CLA	2	0
15	F	202	BCR	3	0
15	K	4005	BCR	5	0
12	A	801	CLA	1	0
12	B	810	CLA	3	0
15	B	834	BCR	3	0
15	J	107	BCR	3	0
15	A	836	BCR	2	0
17	A	851	LMG	2	0
12	B	842	CLA	3	0
12	B	845	CLA	3	0
26	L	209	DGD	2	0
12	B	821	CLA	1	0
12	A	827	CLA	5	0
19	A	854	PL9	10	0
12	B	844	CLA	4	0
12	B	801	CLA	2	0
12	A	807	CLA	1	0
12	B	848	CLA	5	0
12	B	822	CLA	1	0
12	B	806	CLA	5	0
12	L	206	CLA	2	0
18	L	210	LMT	3	0
15	I	101	BCR	4	0
12	A	815	CLA	3	0
20	A	856	45D	3	0
15	L	208	BCR	1	0
23	B	833	ECH	1	0

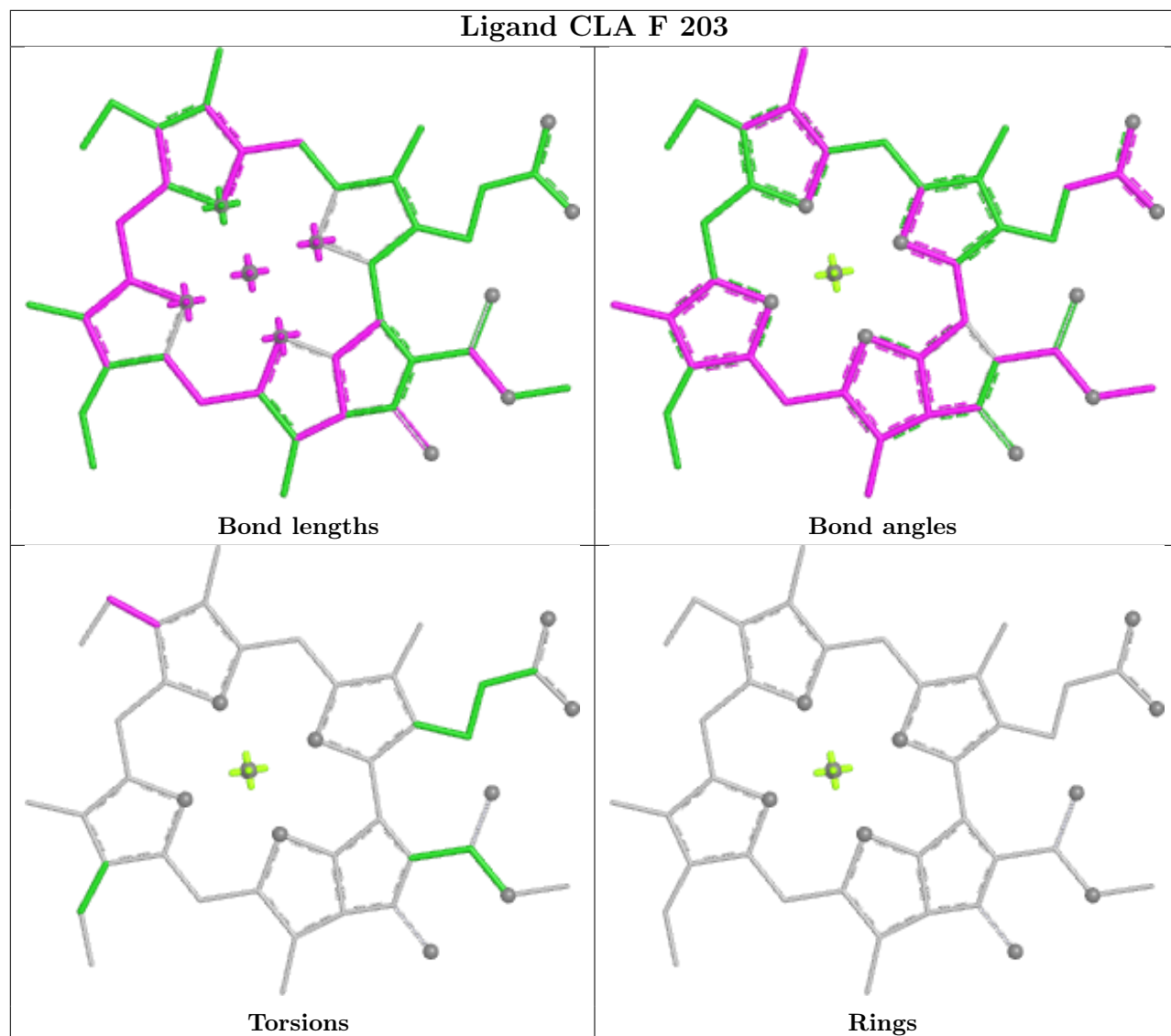
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

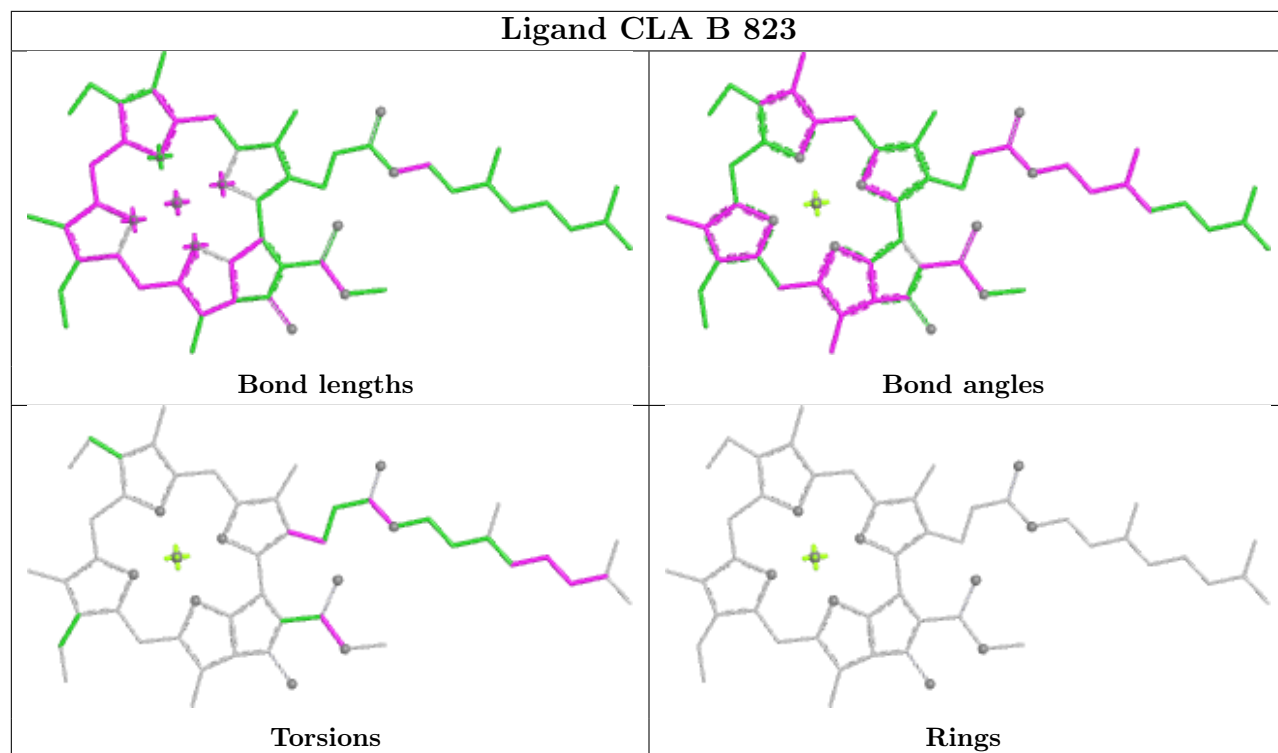




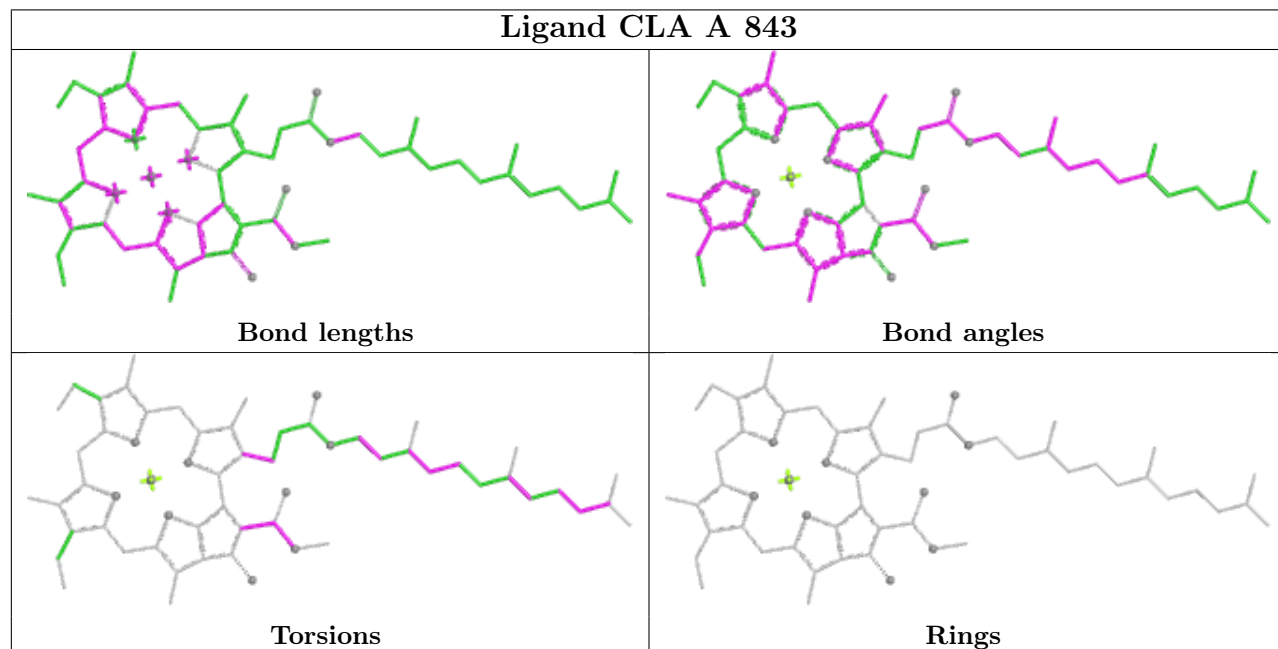
Ligand CLA F 203

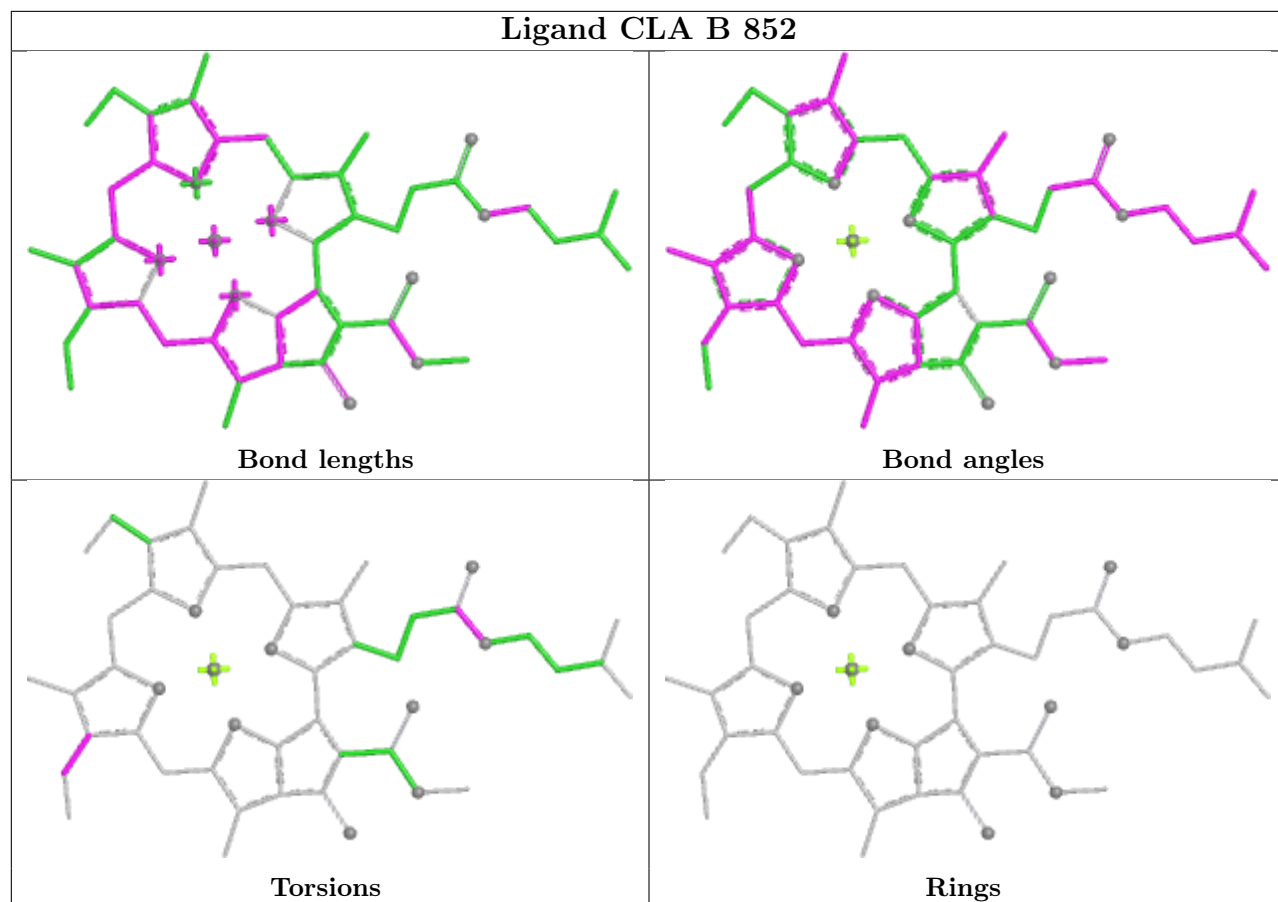


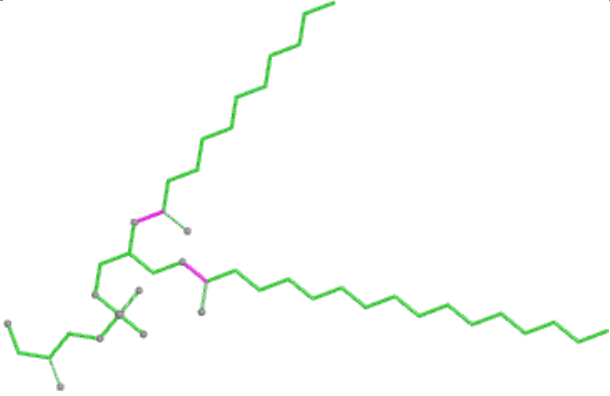
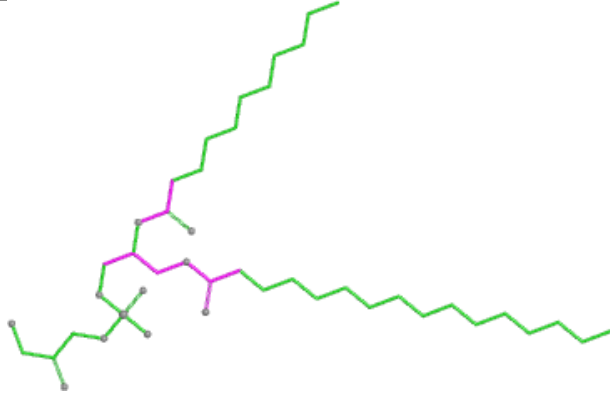
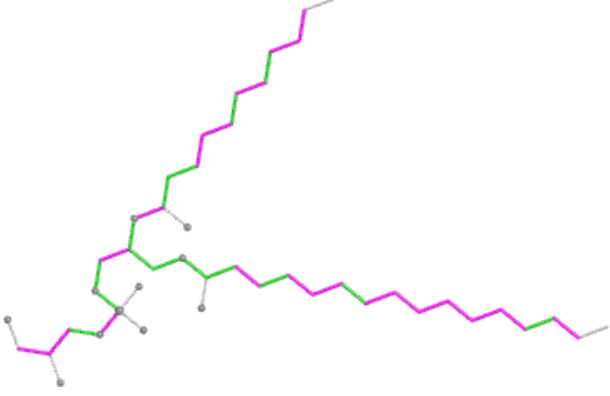
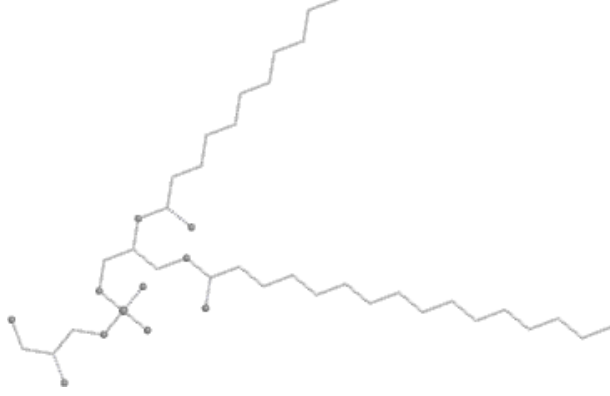
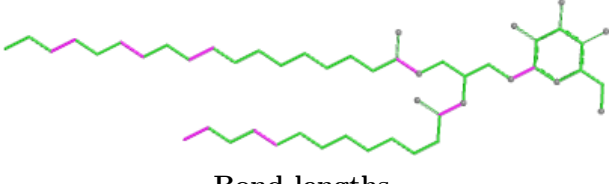
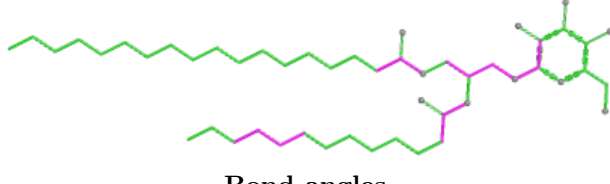
Ligand CLA B 823

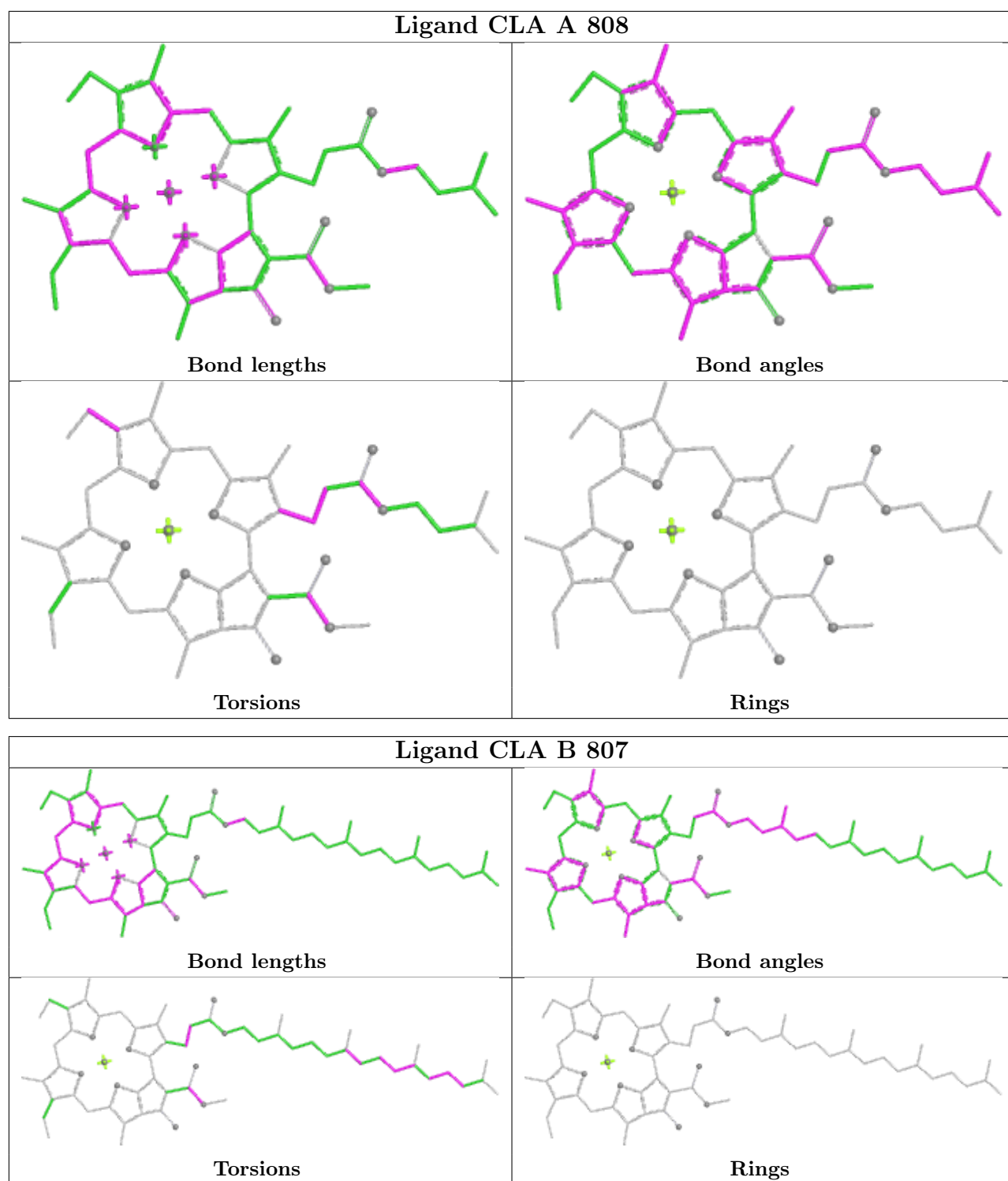


Ligand CLA A 843

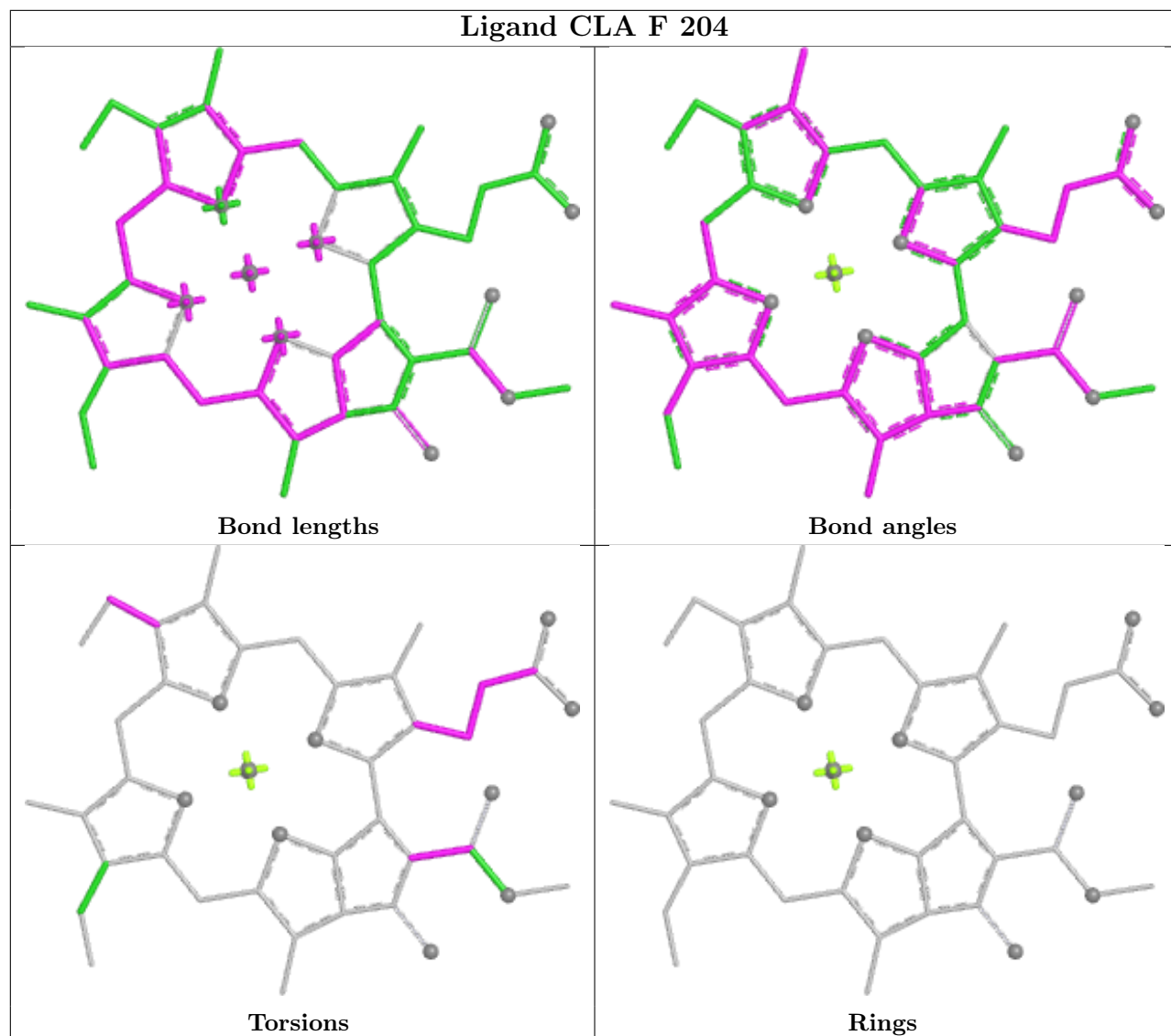




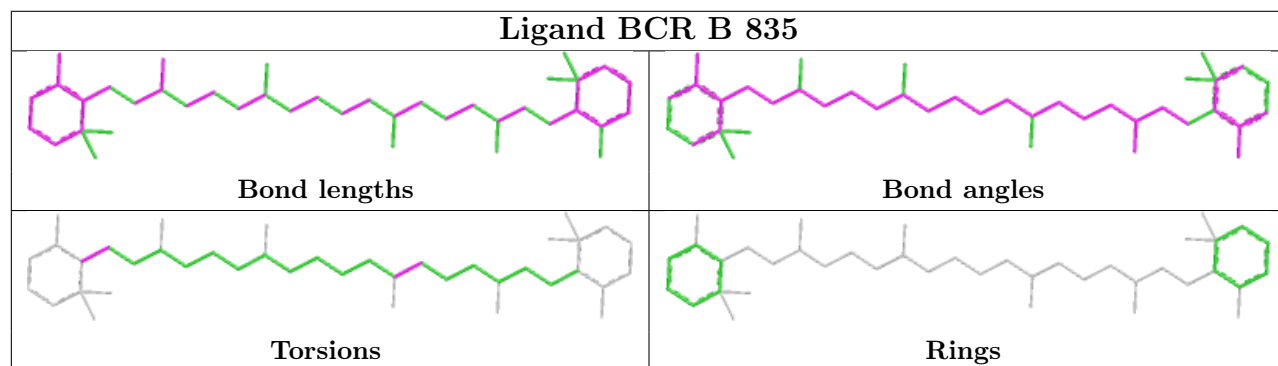
Ligand LHG M 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG A 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

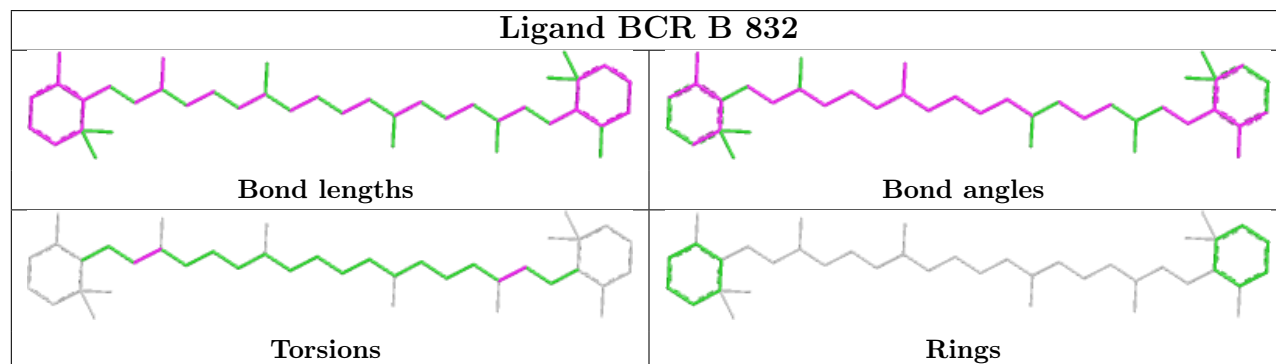
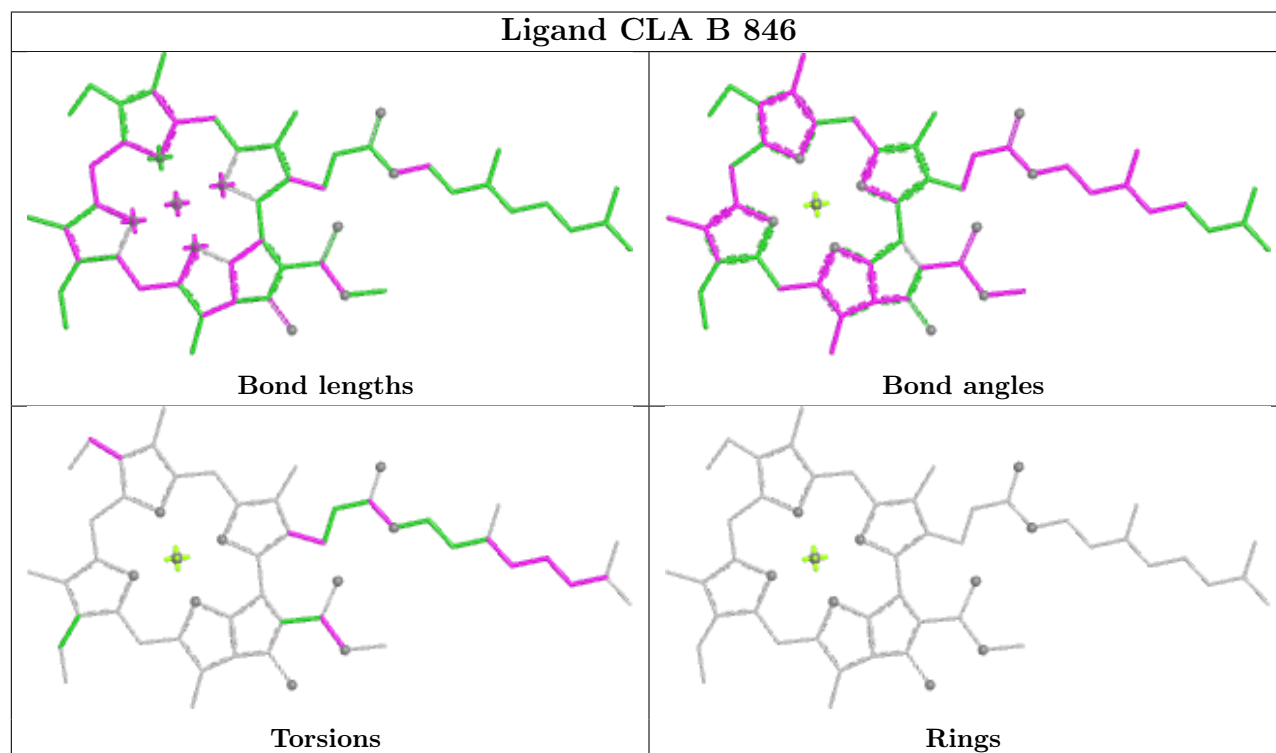
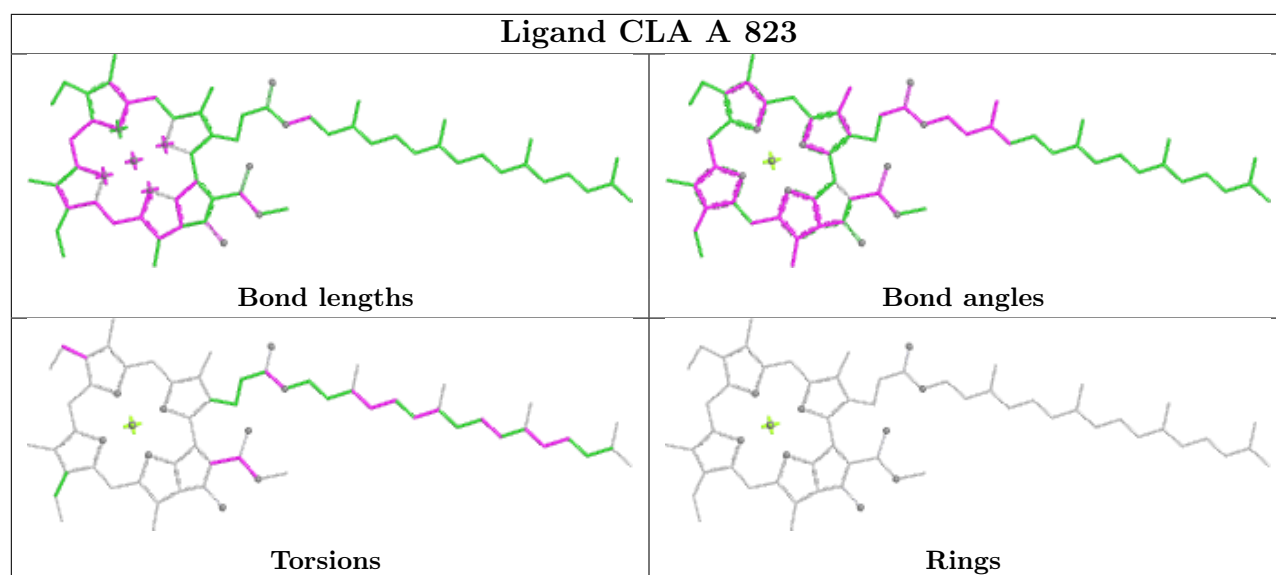


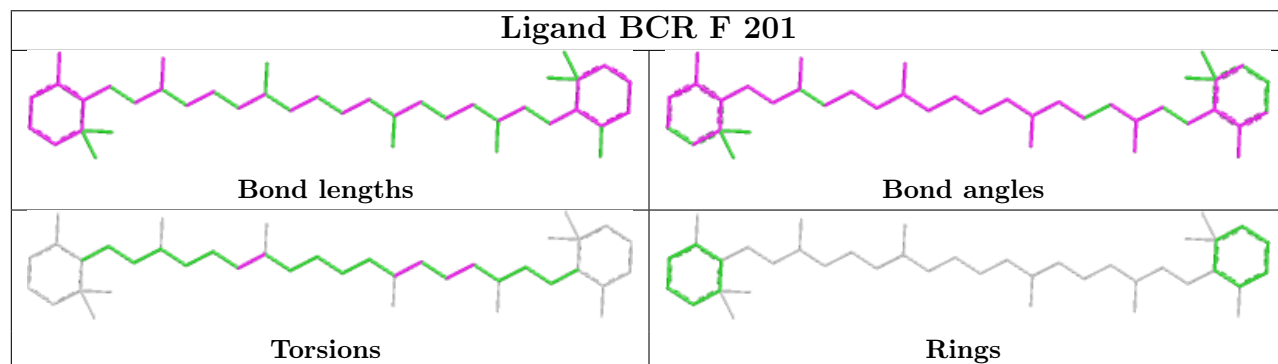
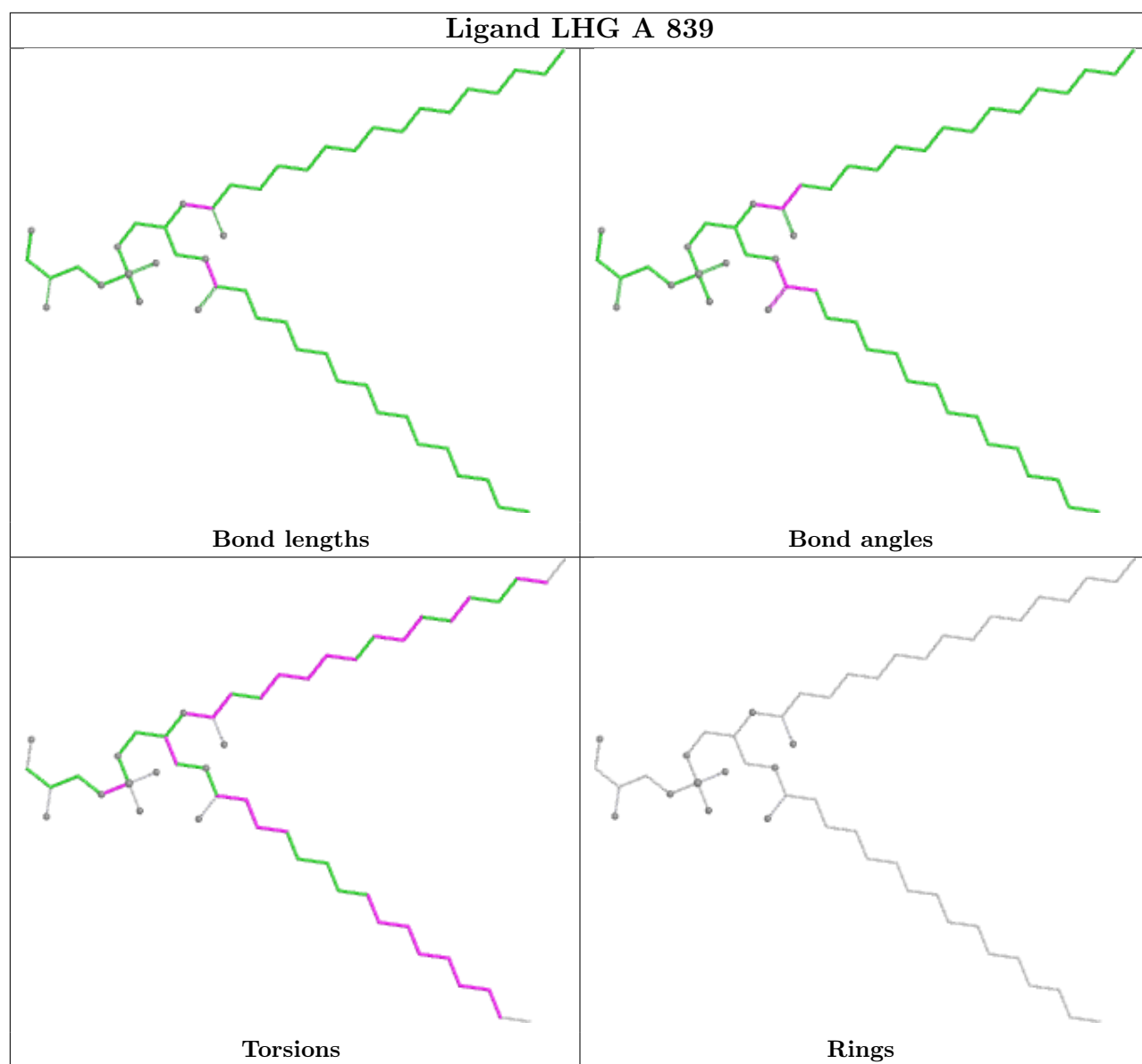
Ligand CLA F 204

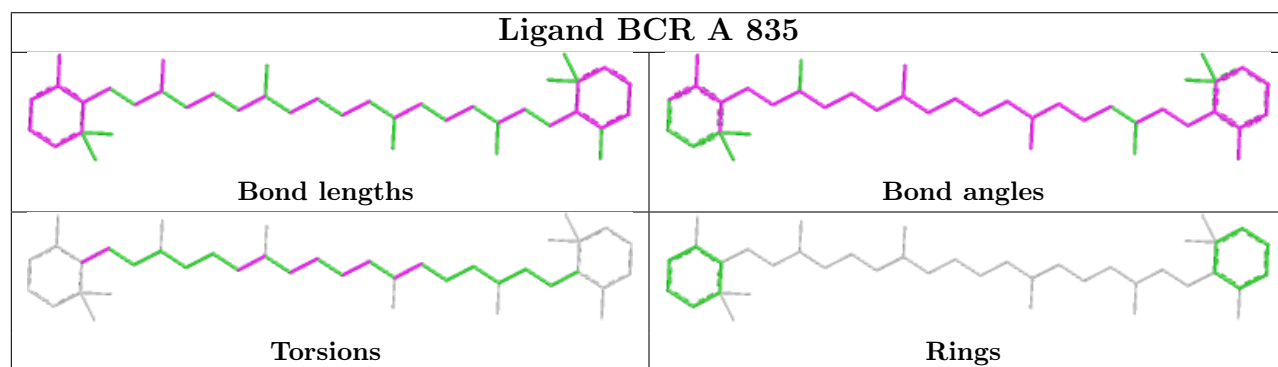
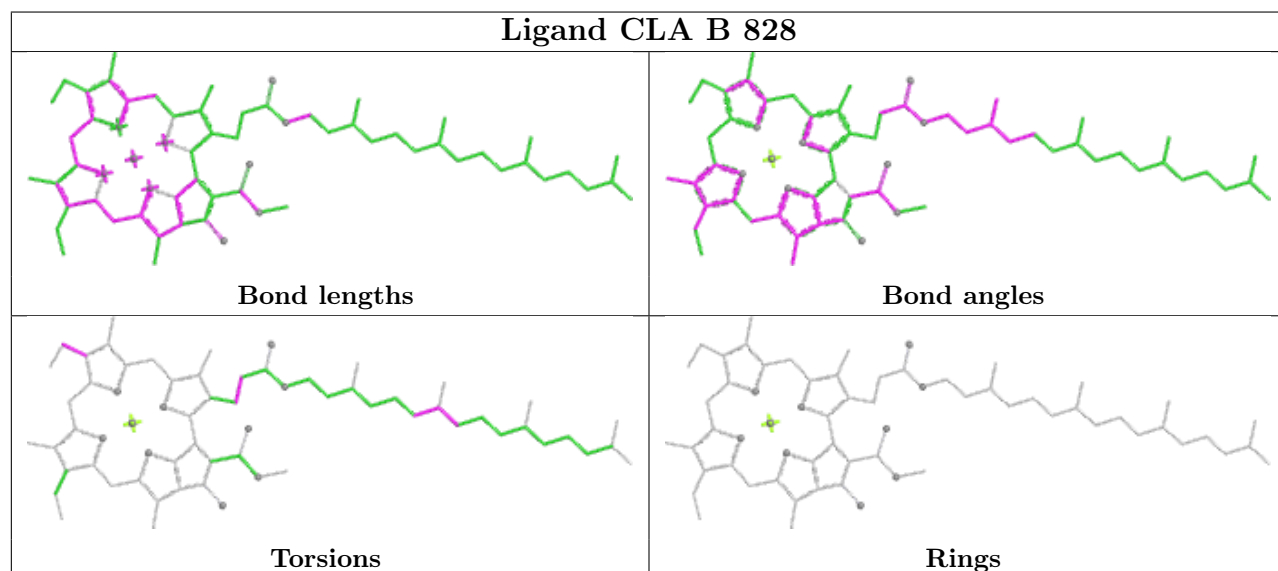
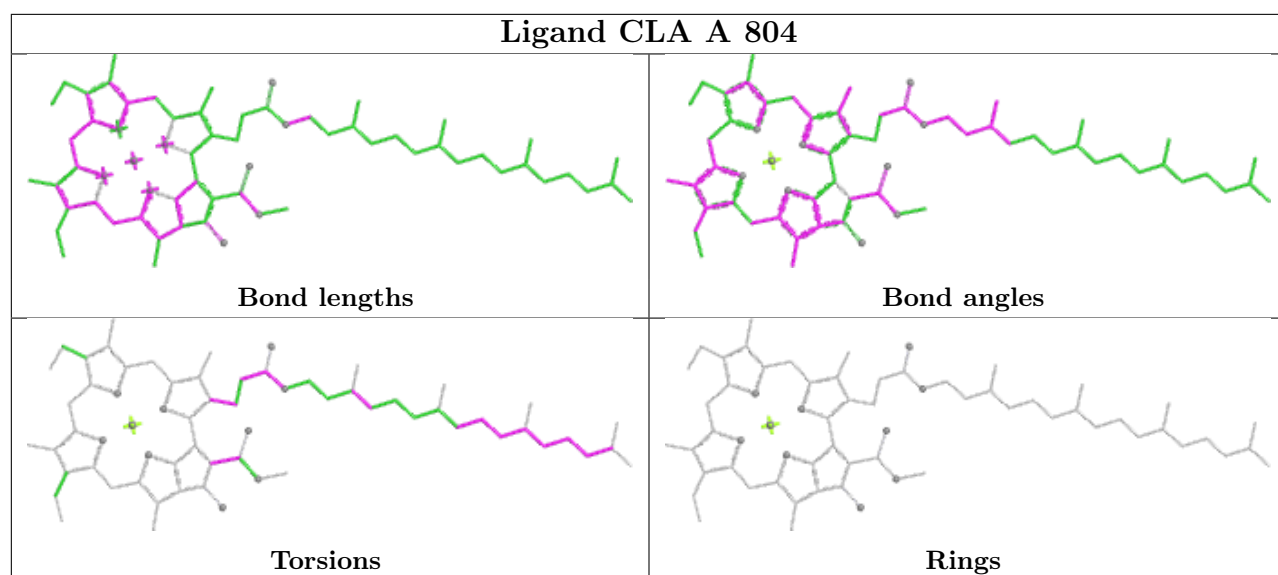


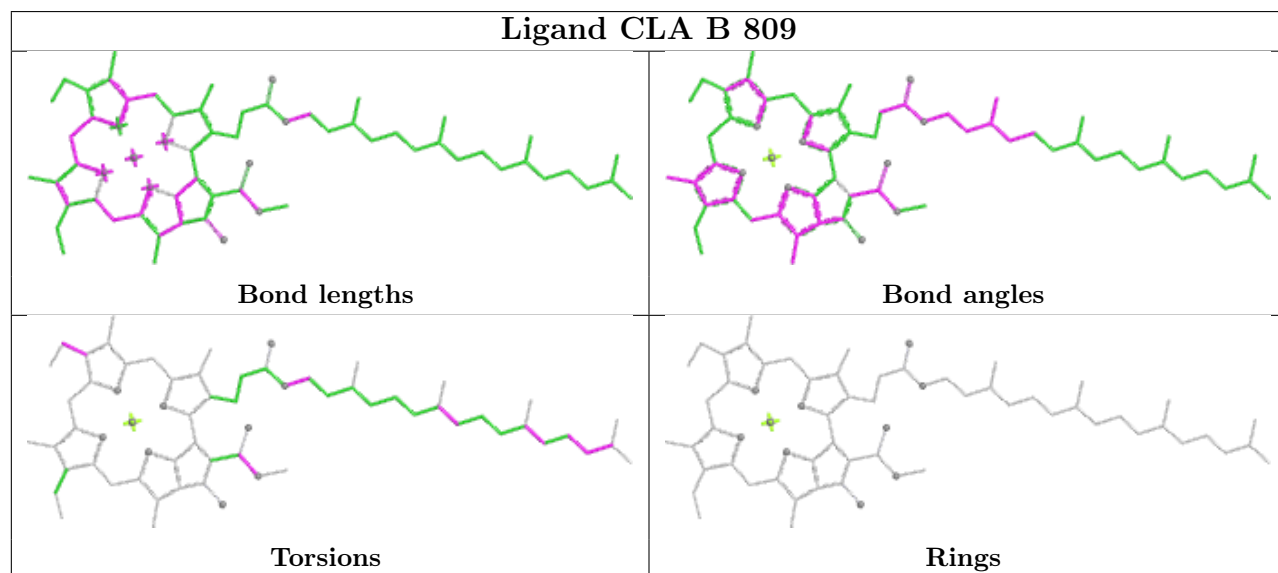
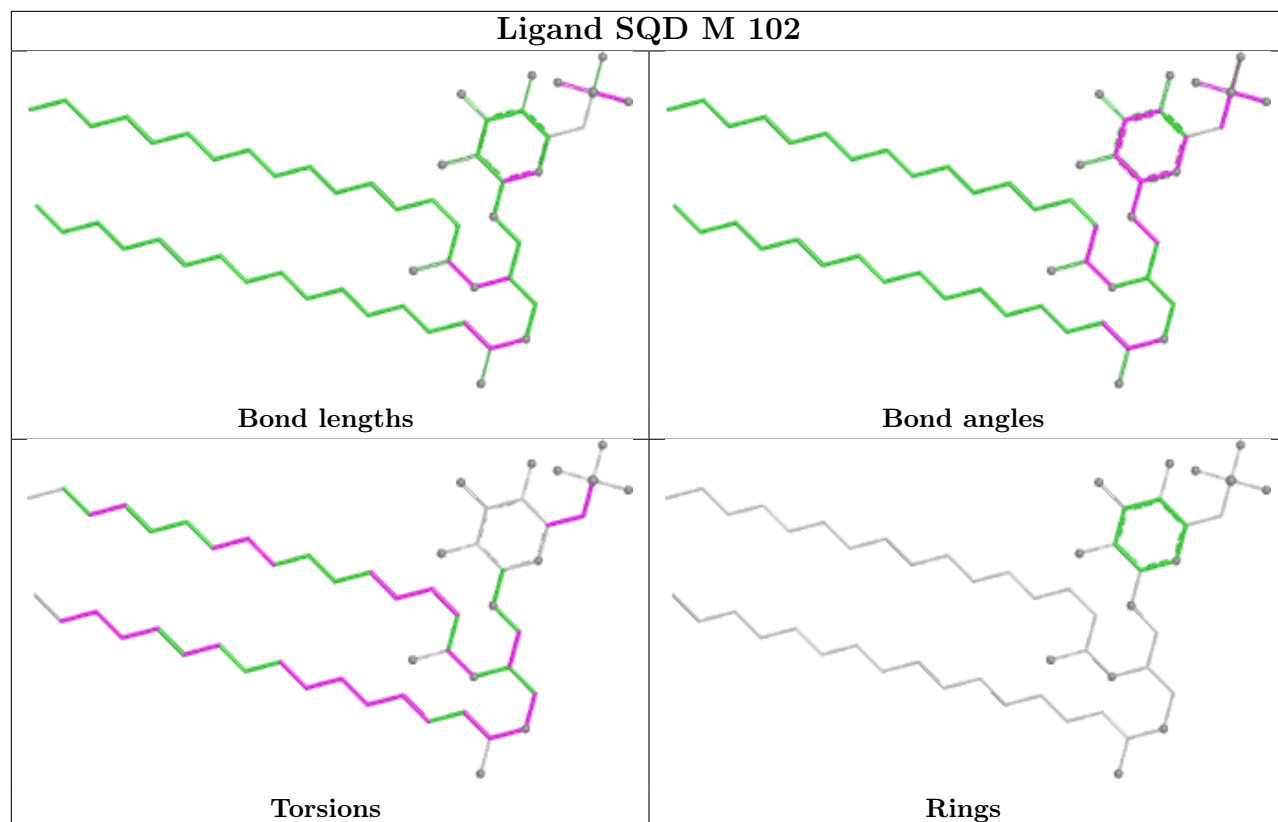
Ligand BCR B 835

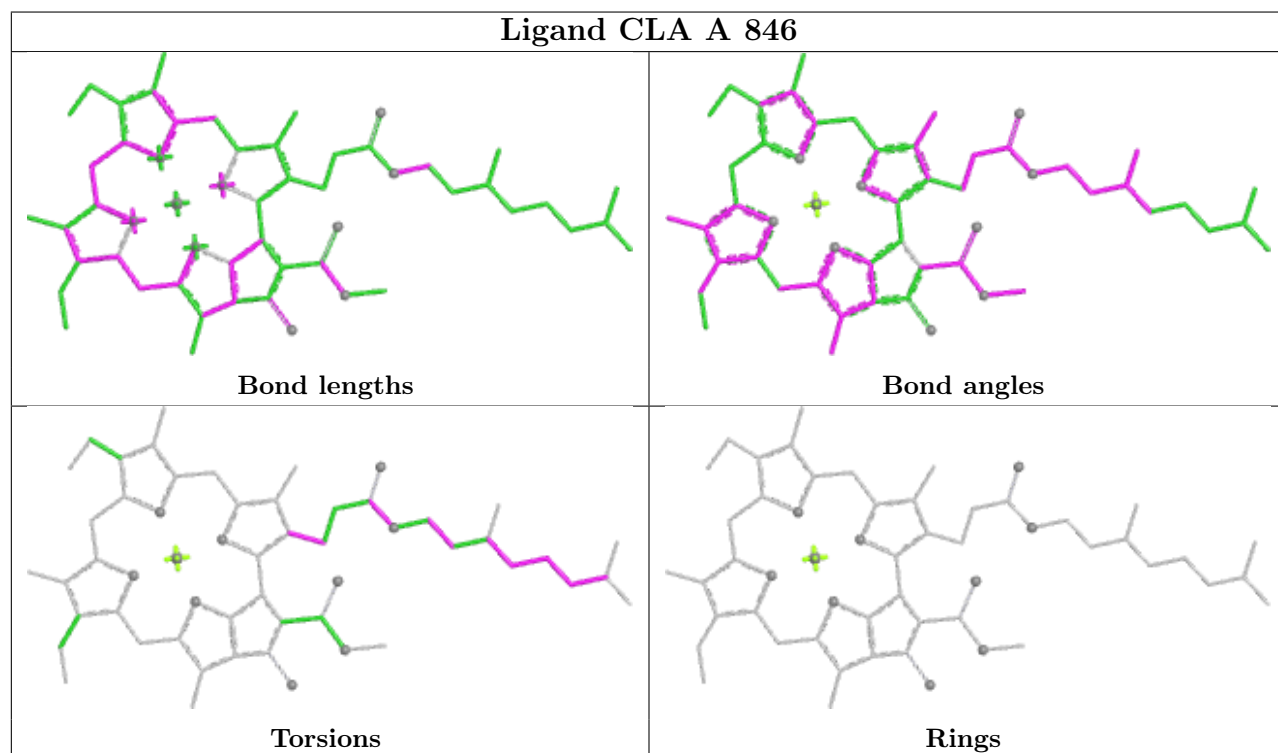
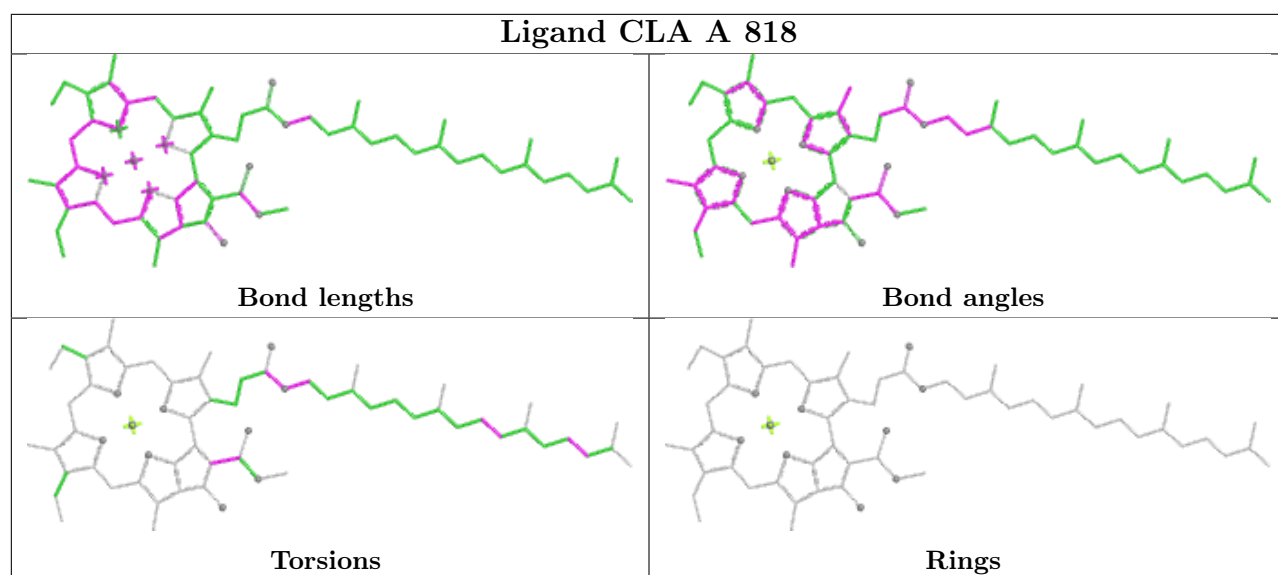




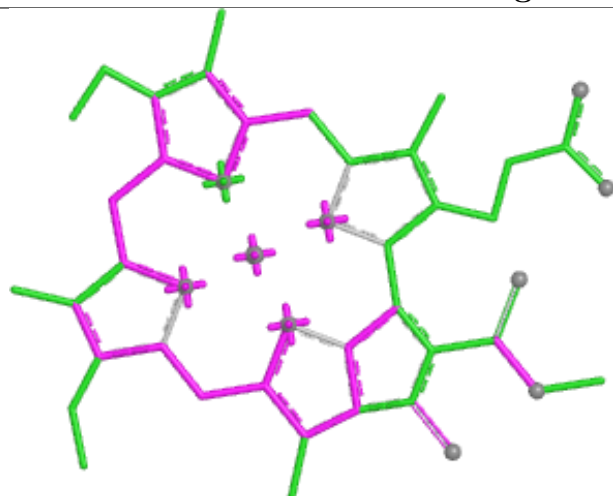




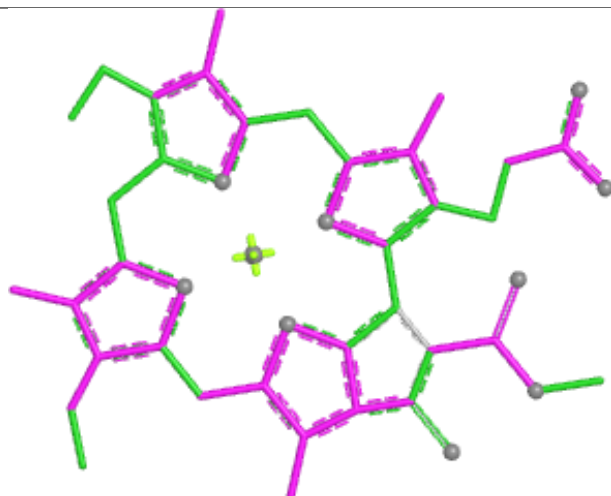




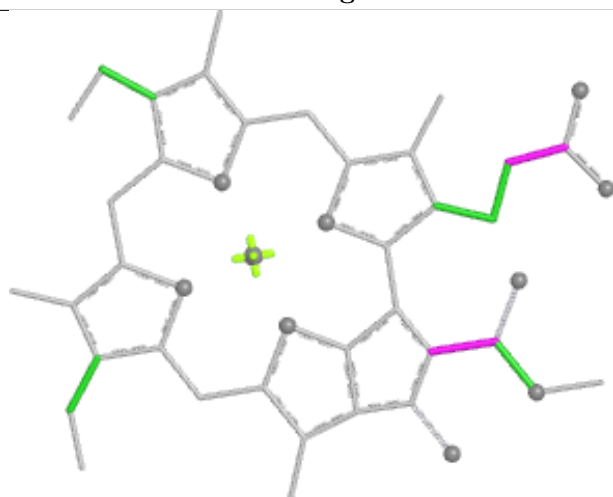
Ligand CLA B 830



Bond lengths



Bond angles

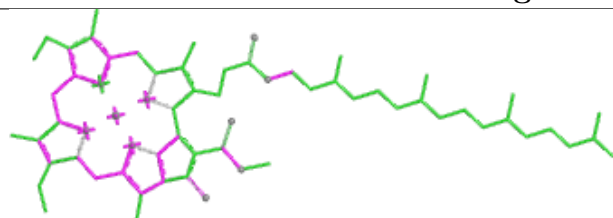


Torsions

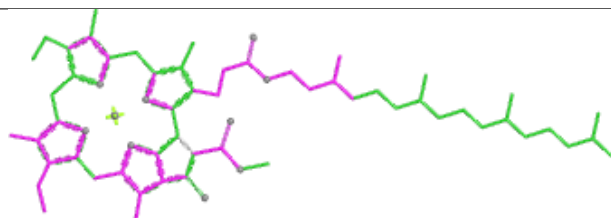


Rings

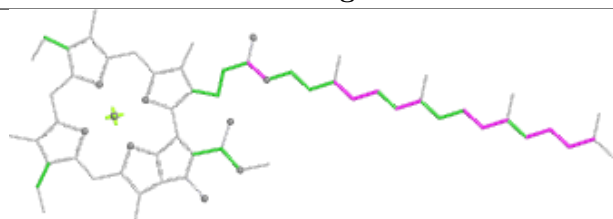
Ligand CLA A 849



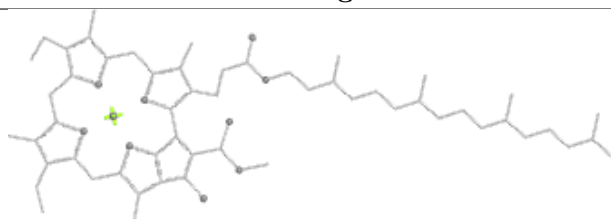
Bond lengths



Bond angles

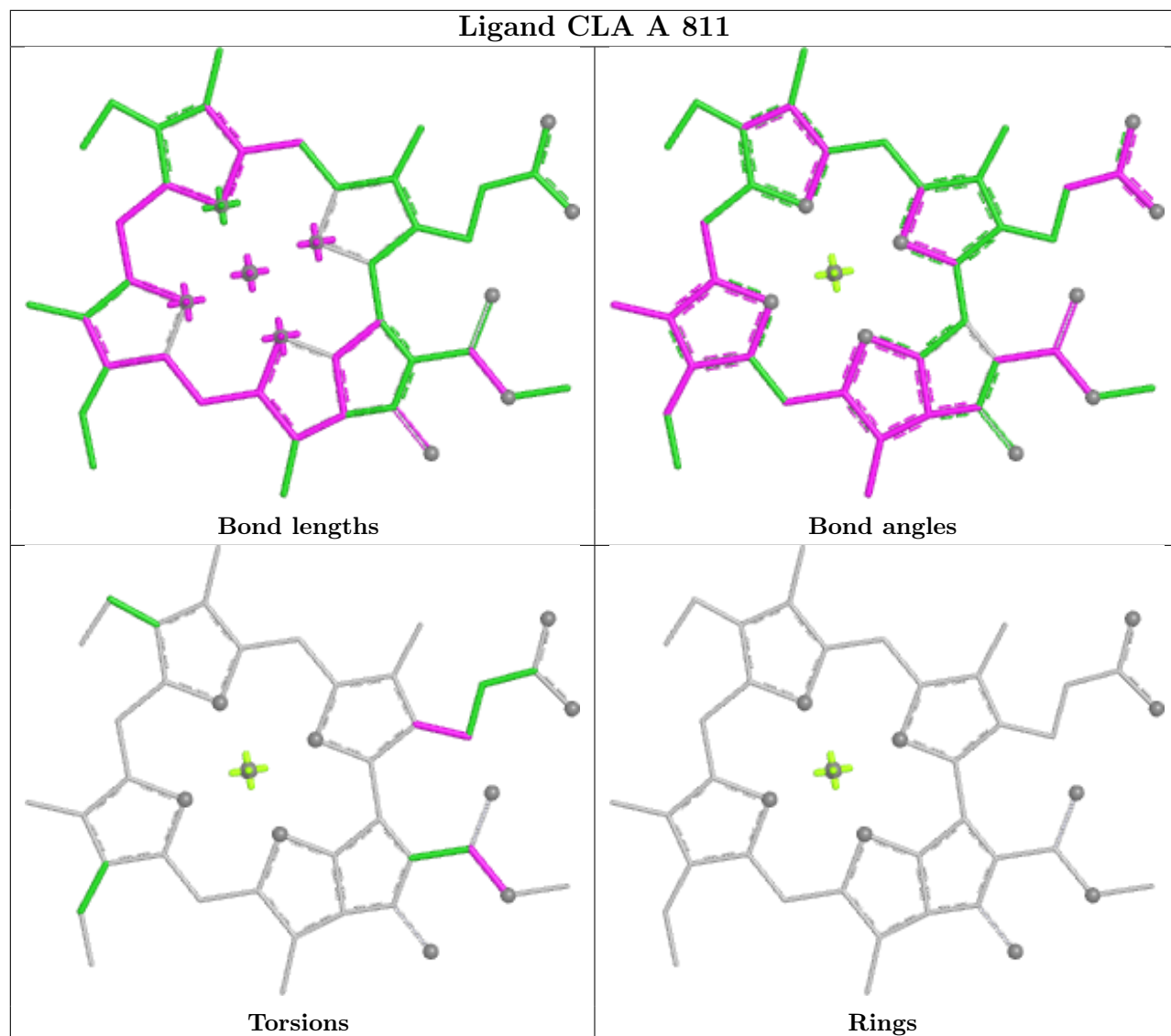


Torsions

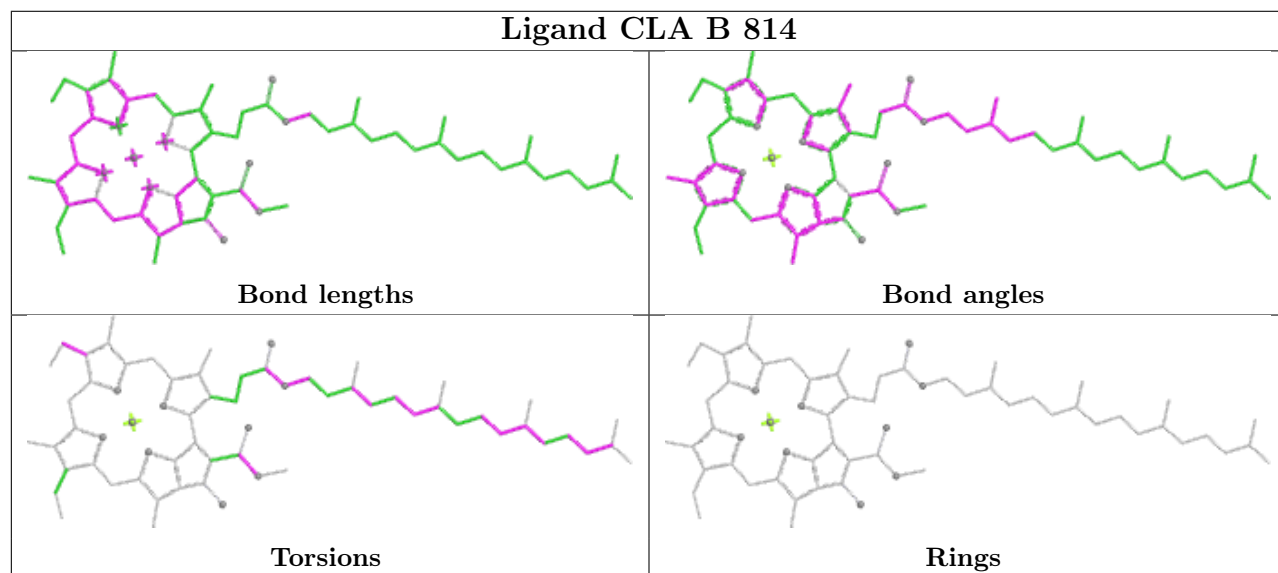


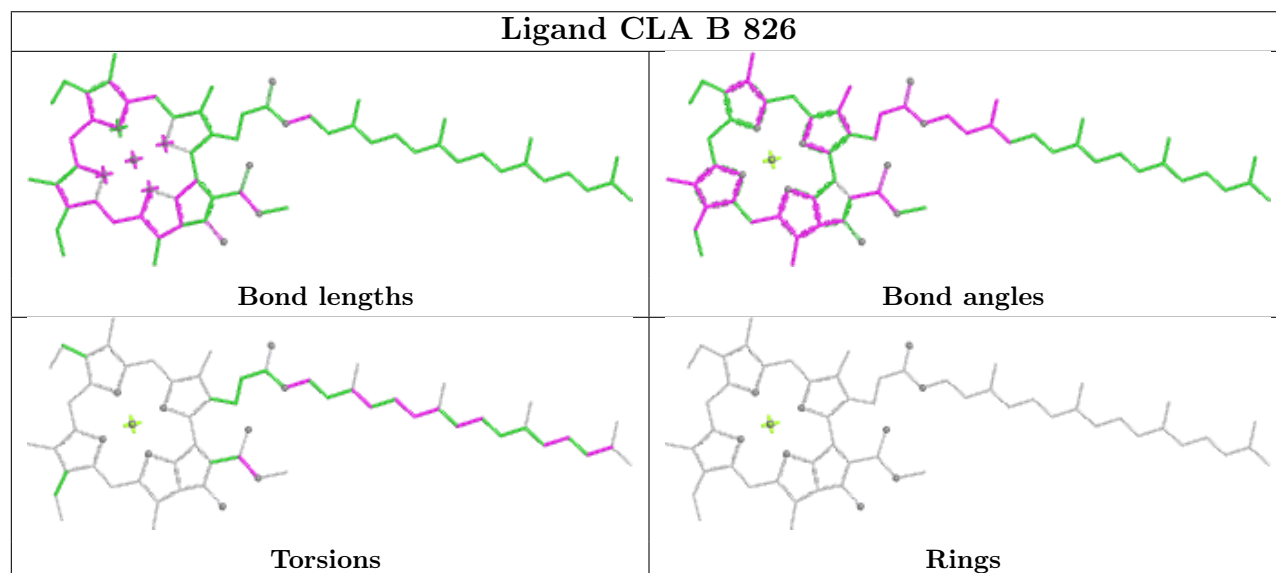
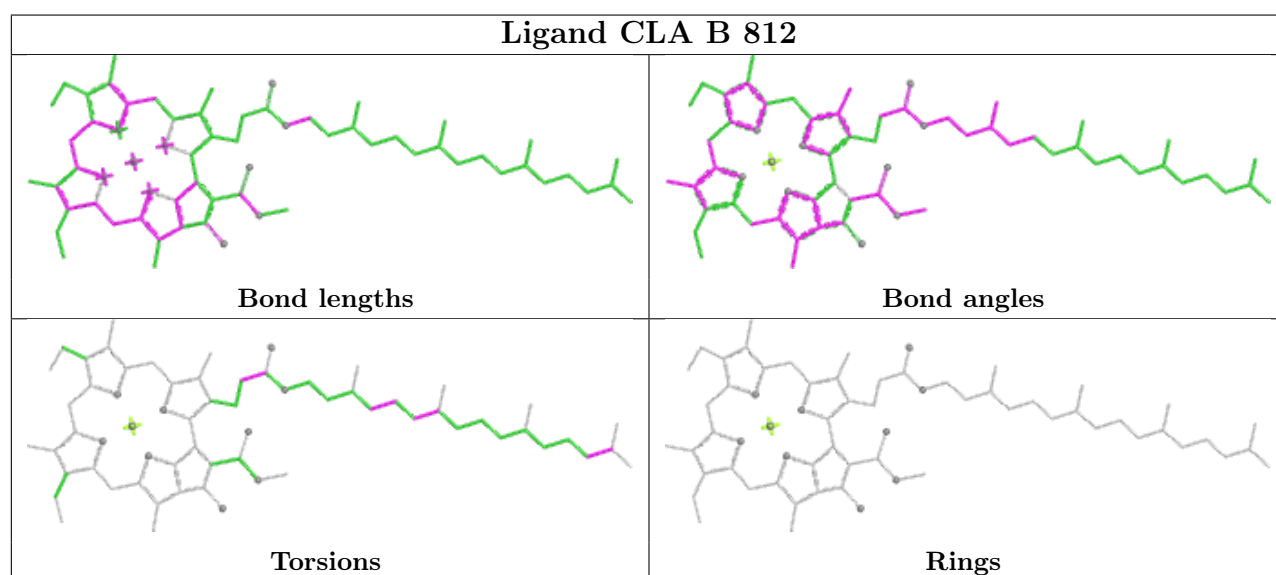
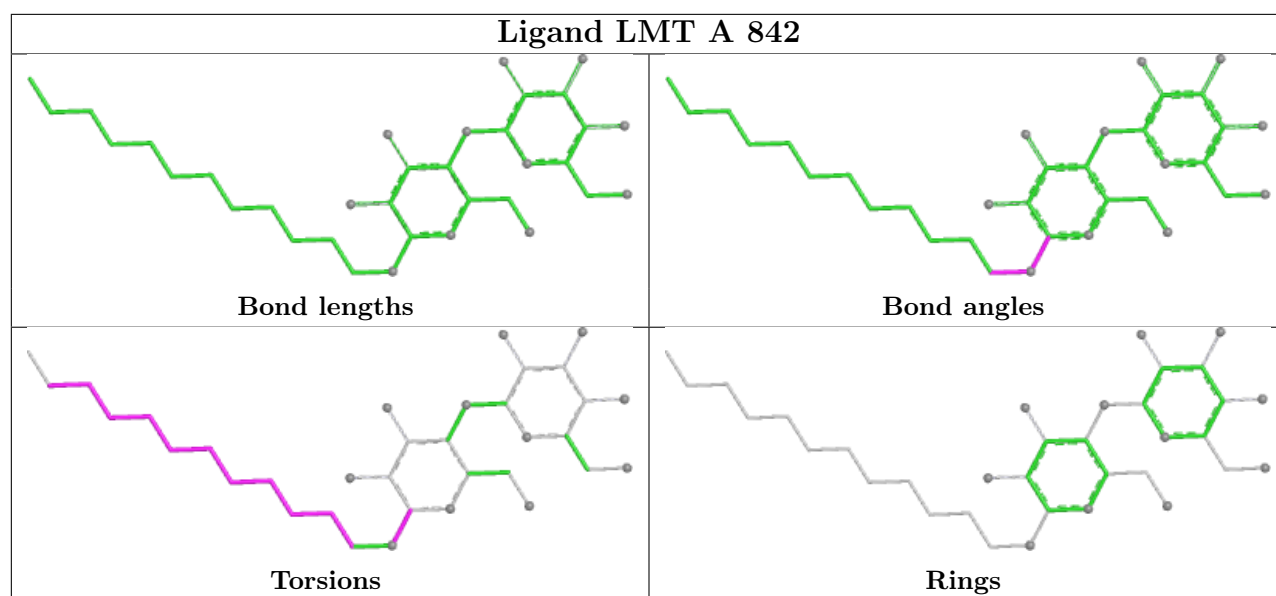
Rings

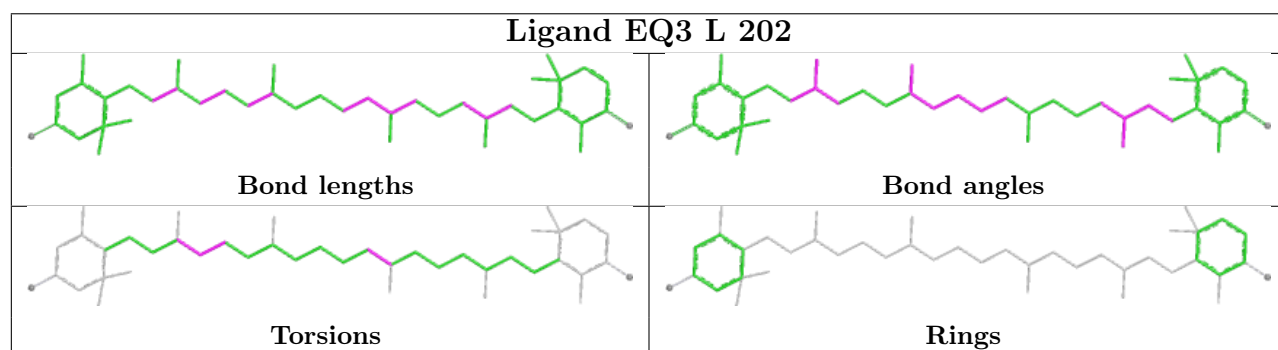
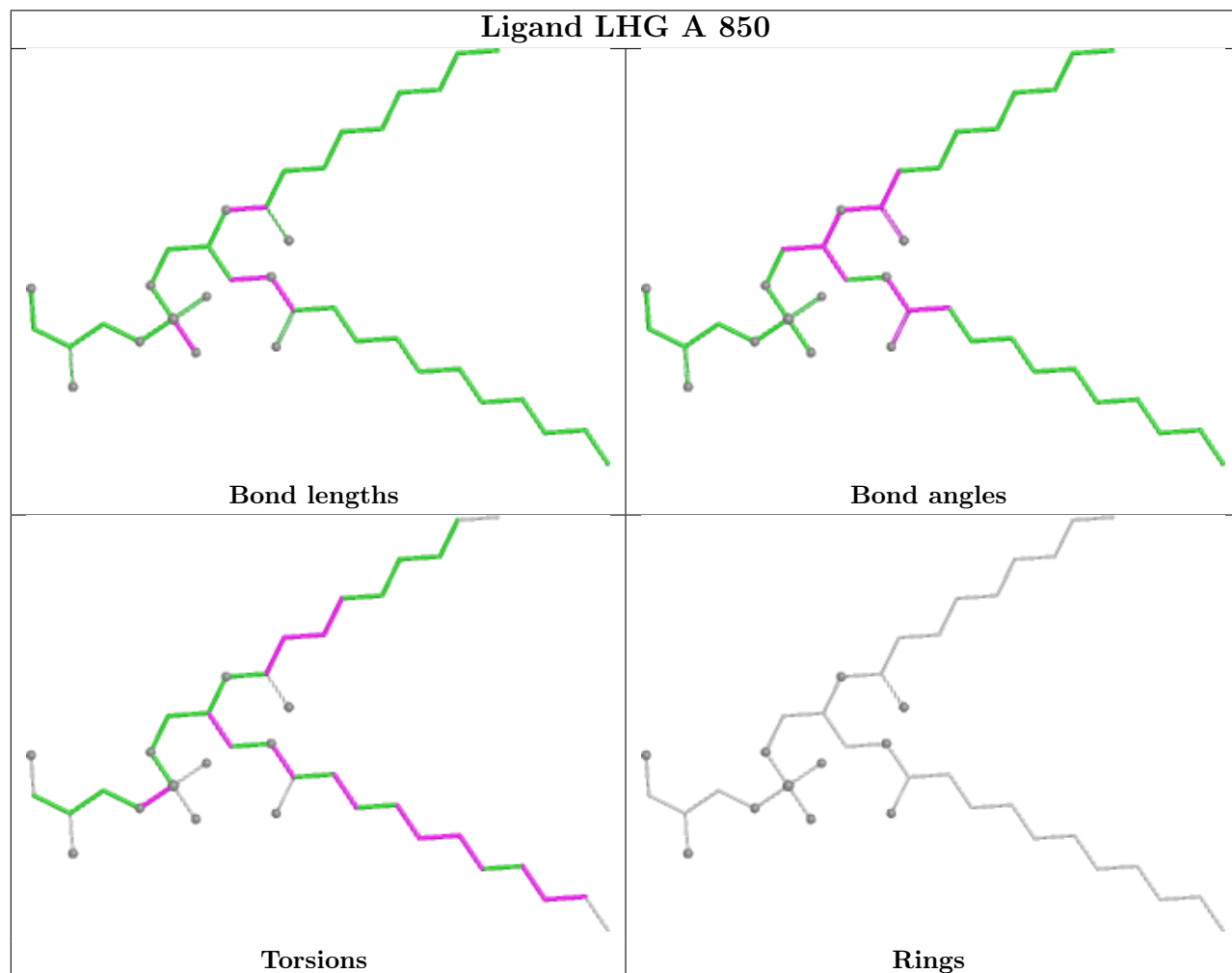
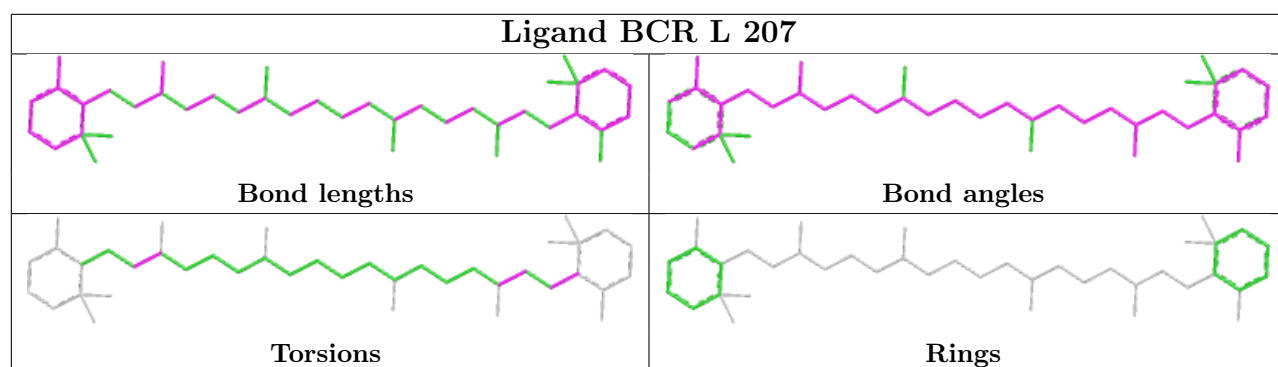
Ligand CLA A 811

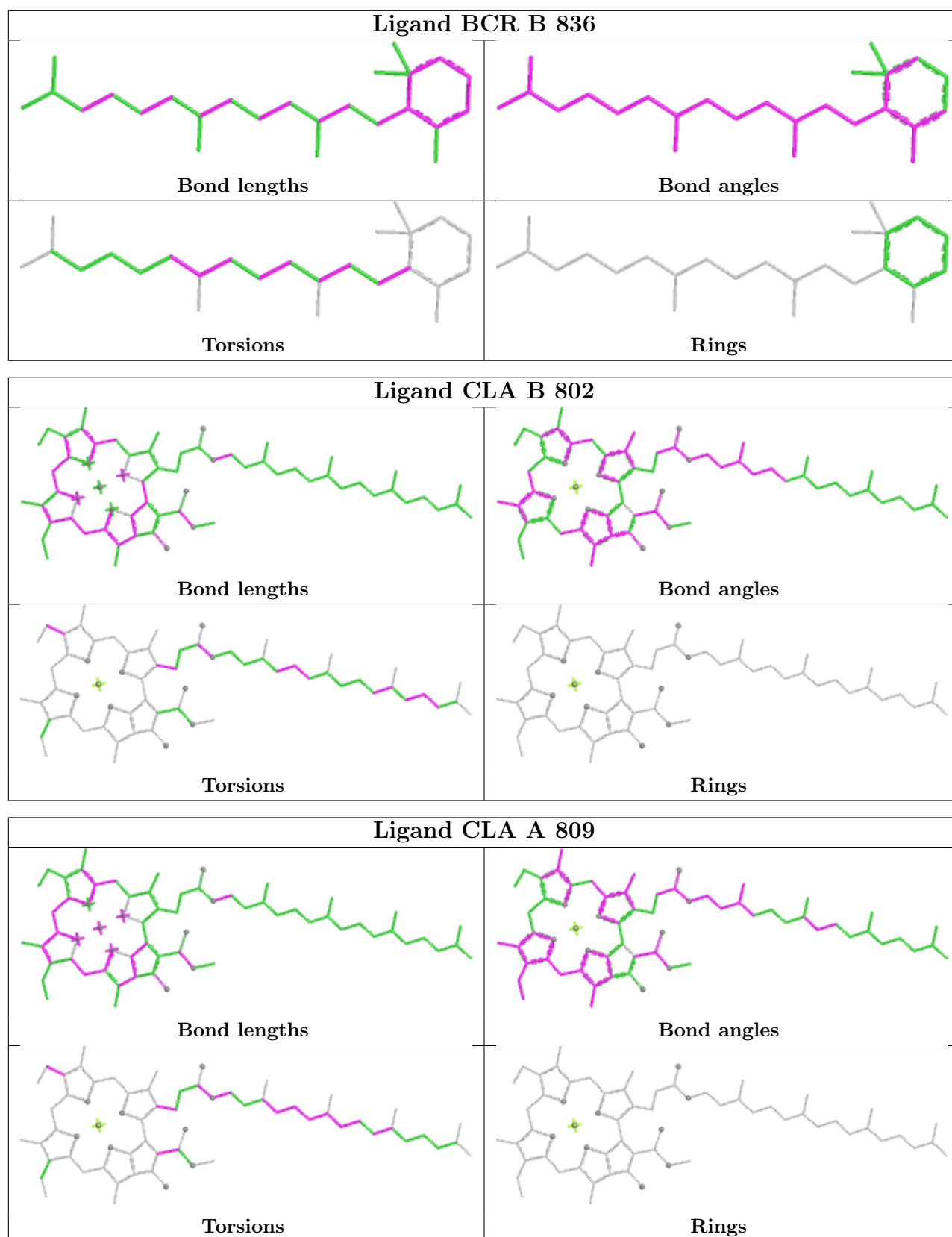


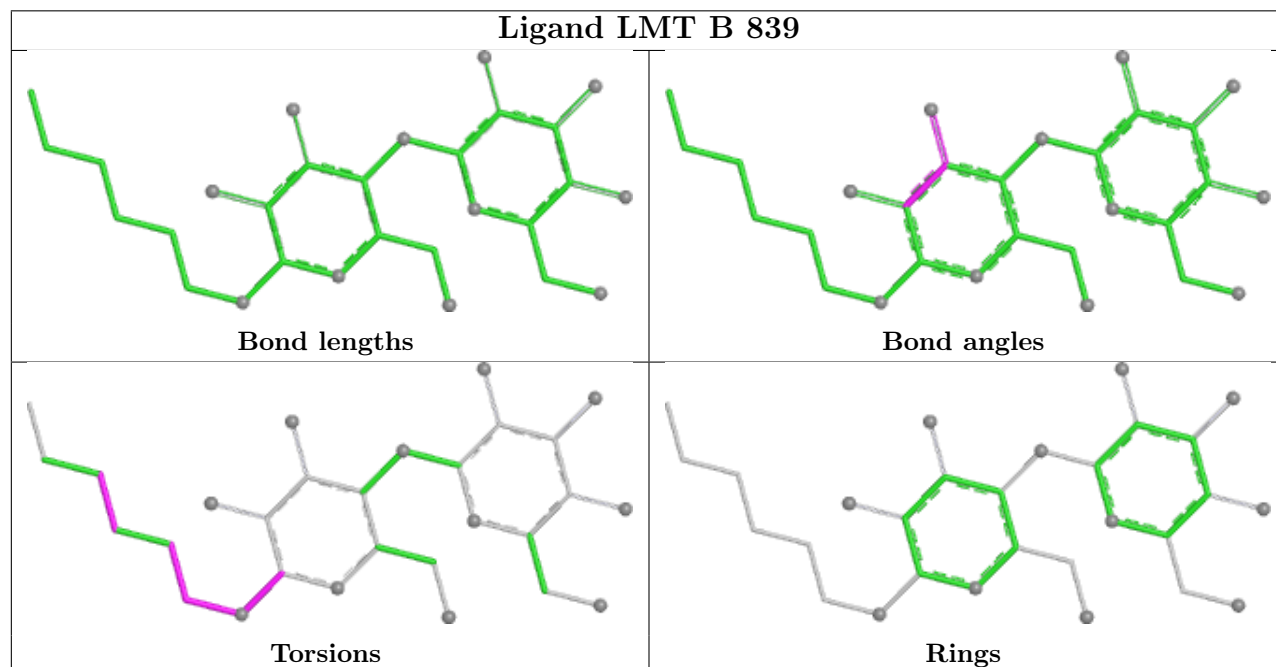
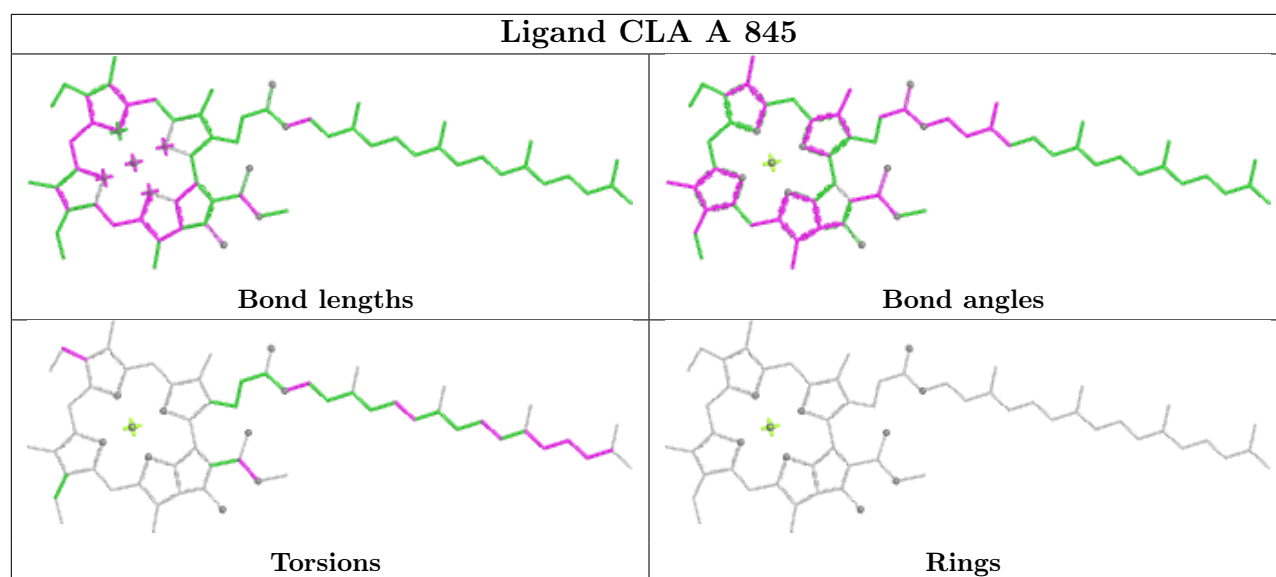
Ligand CLA B 814

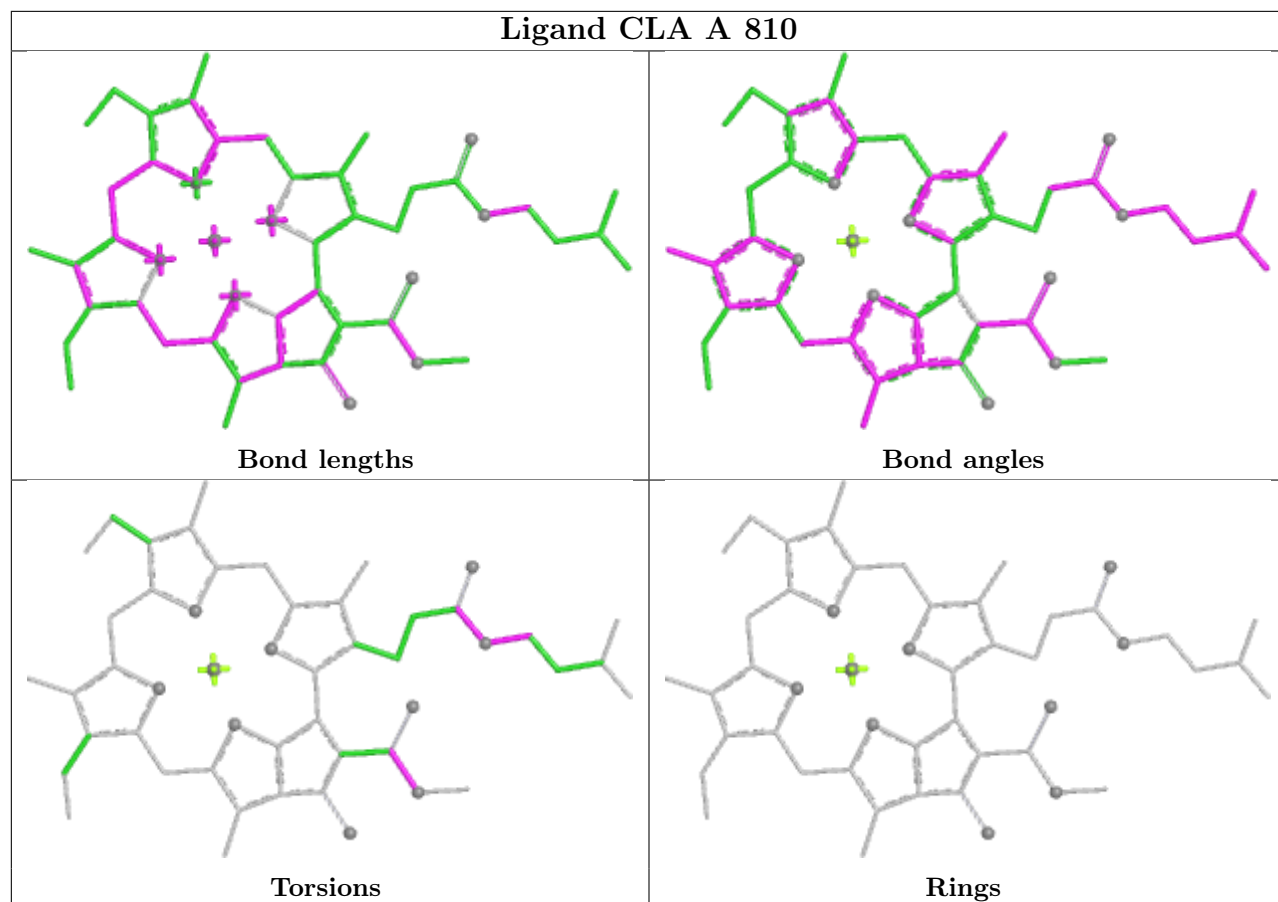




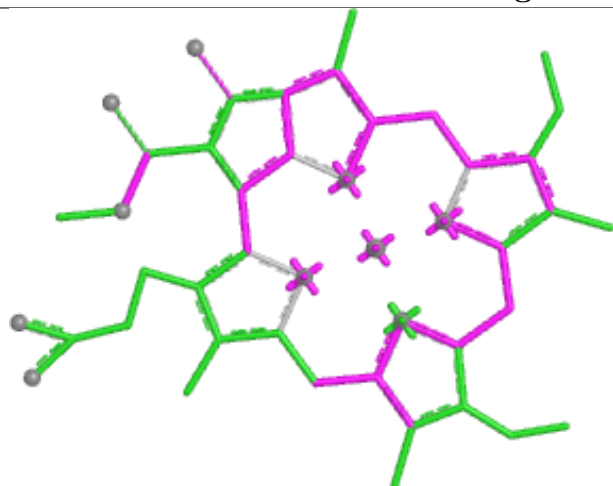




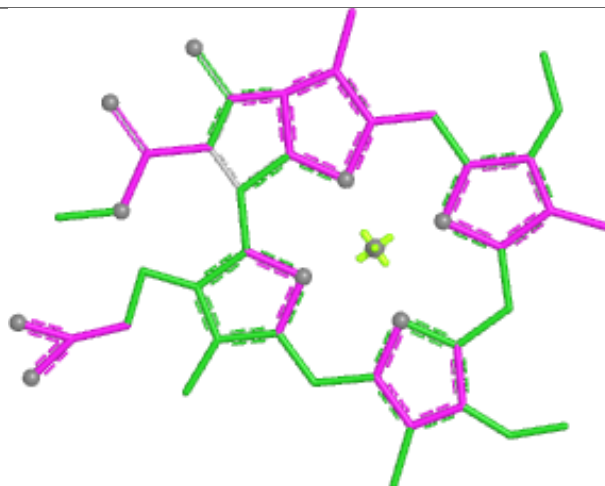




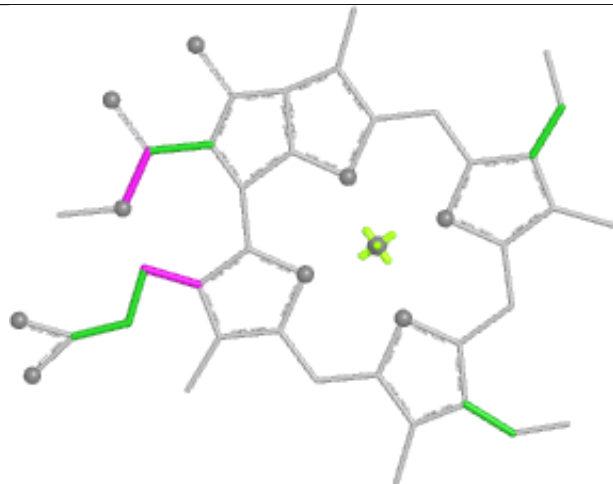
Ligand CLA B 805



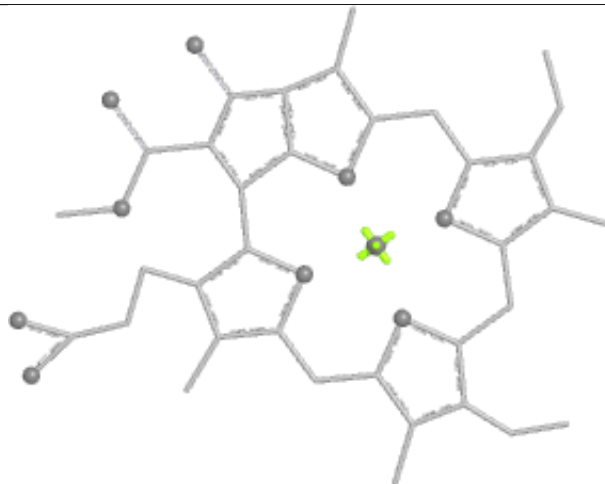
Bond lengths



Bond angles

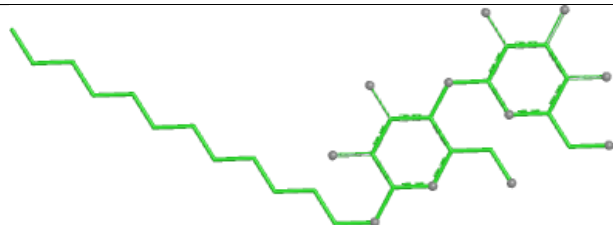


Torsions

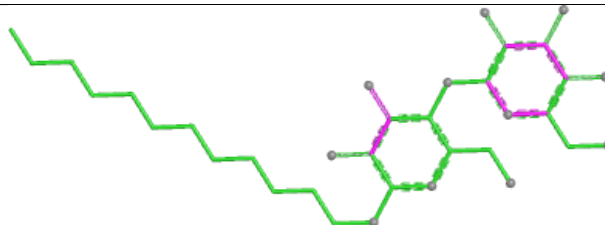


Rings

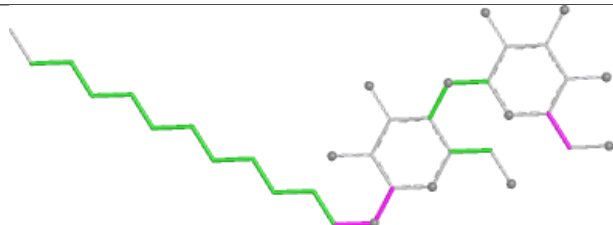
Ligand LMT A 853



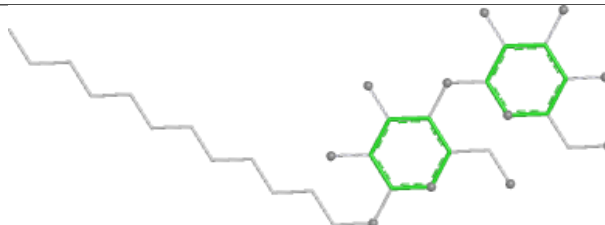
Bond lengths



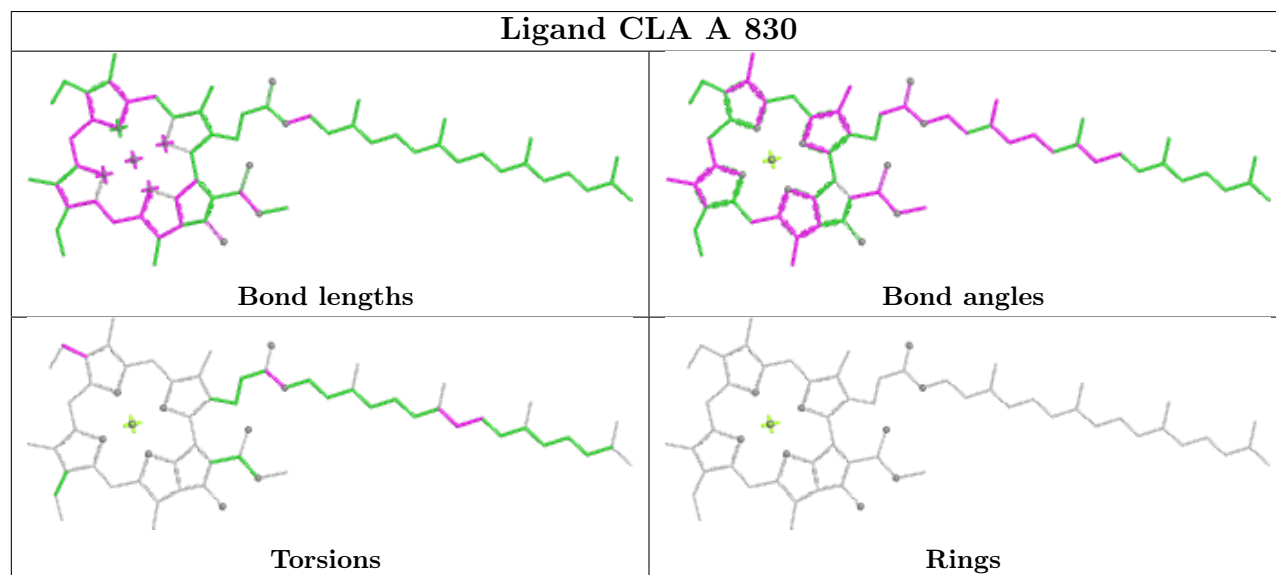
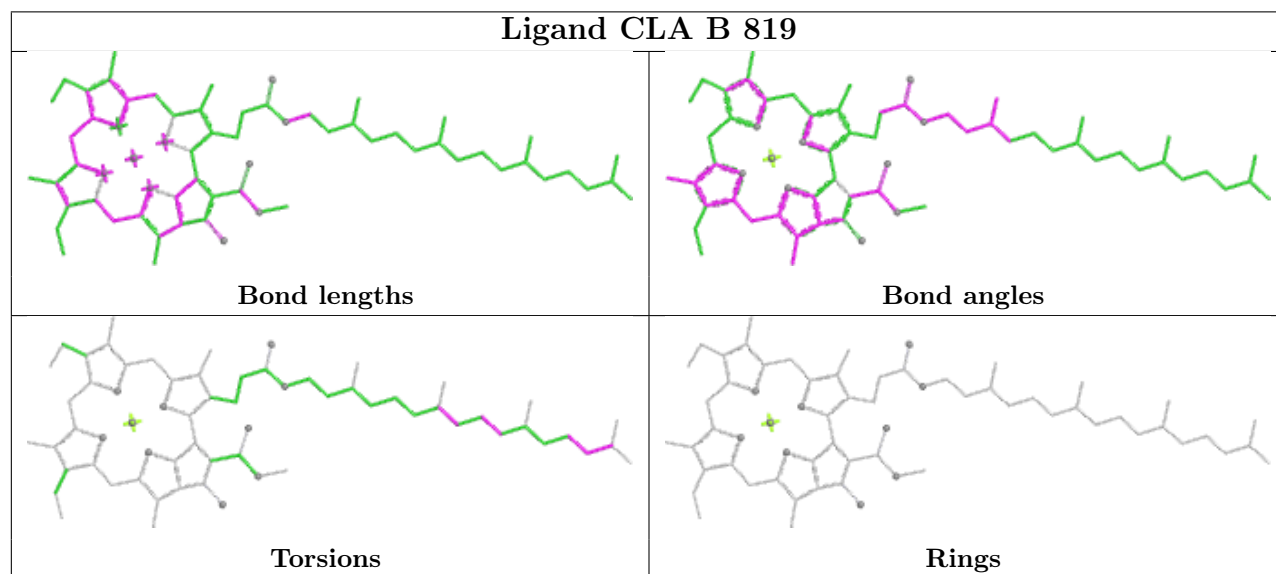
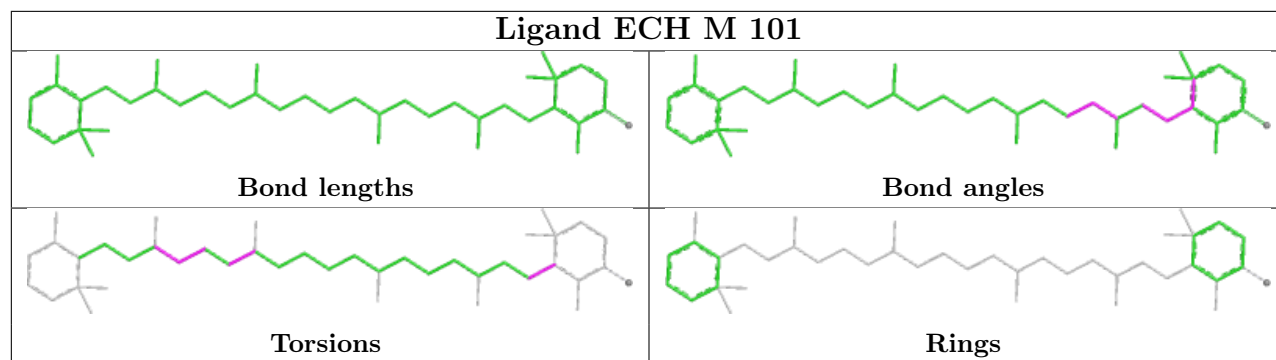
Bond angles

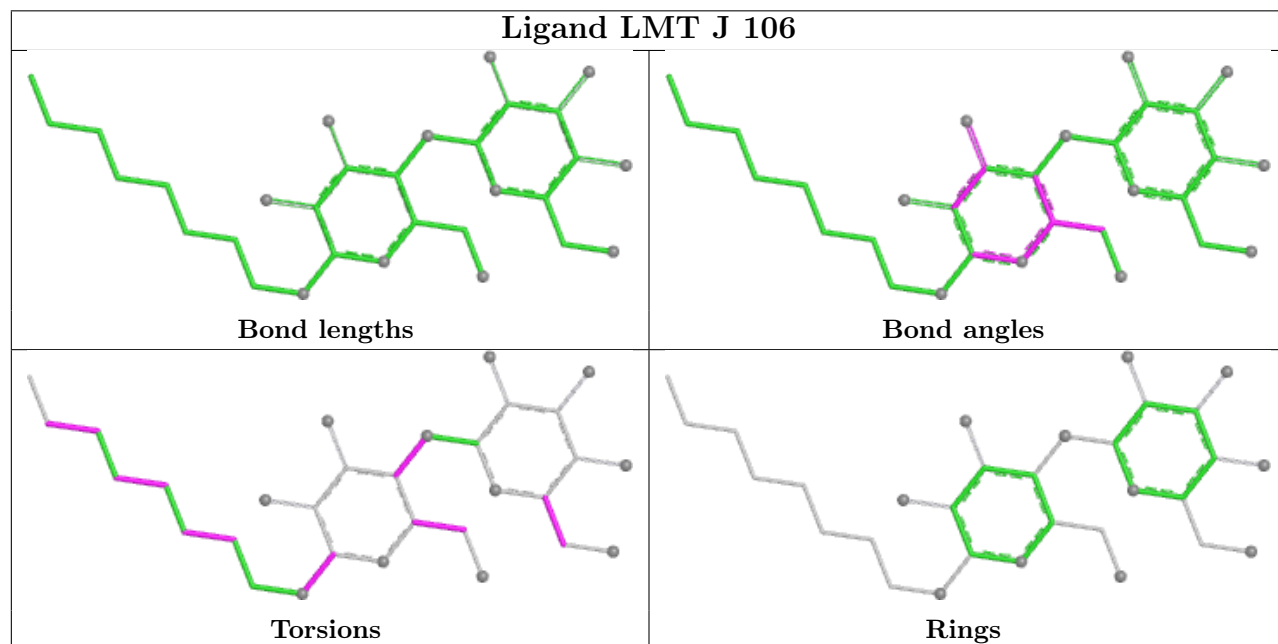
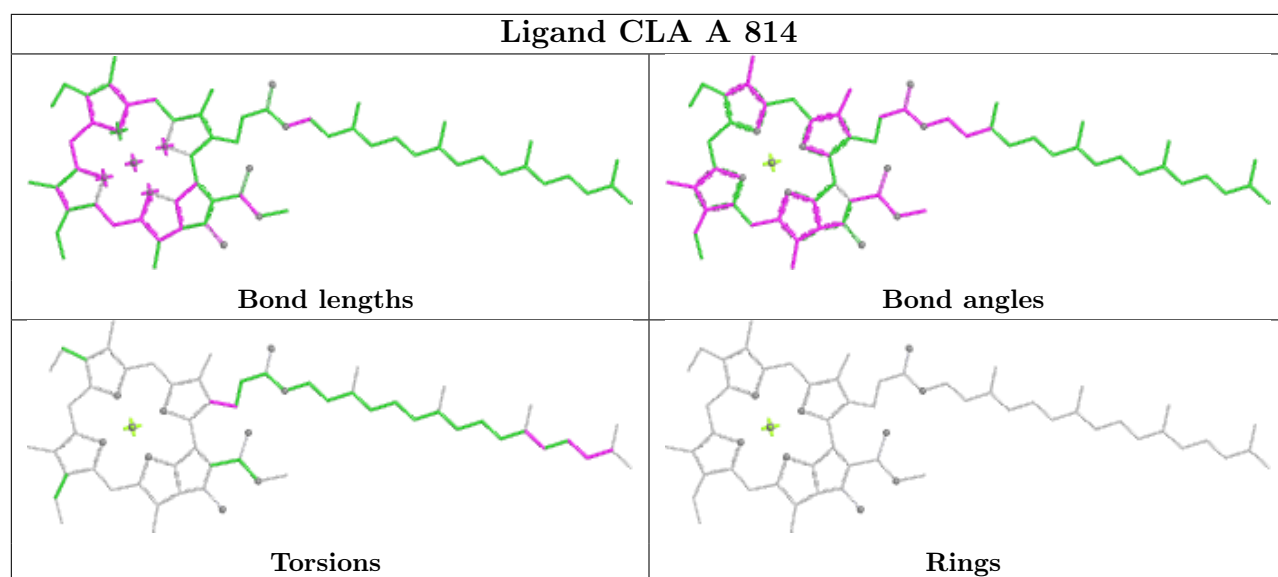


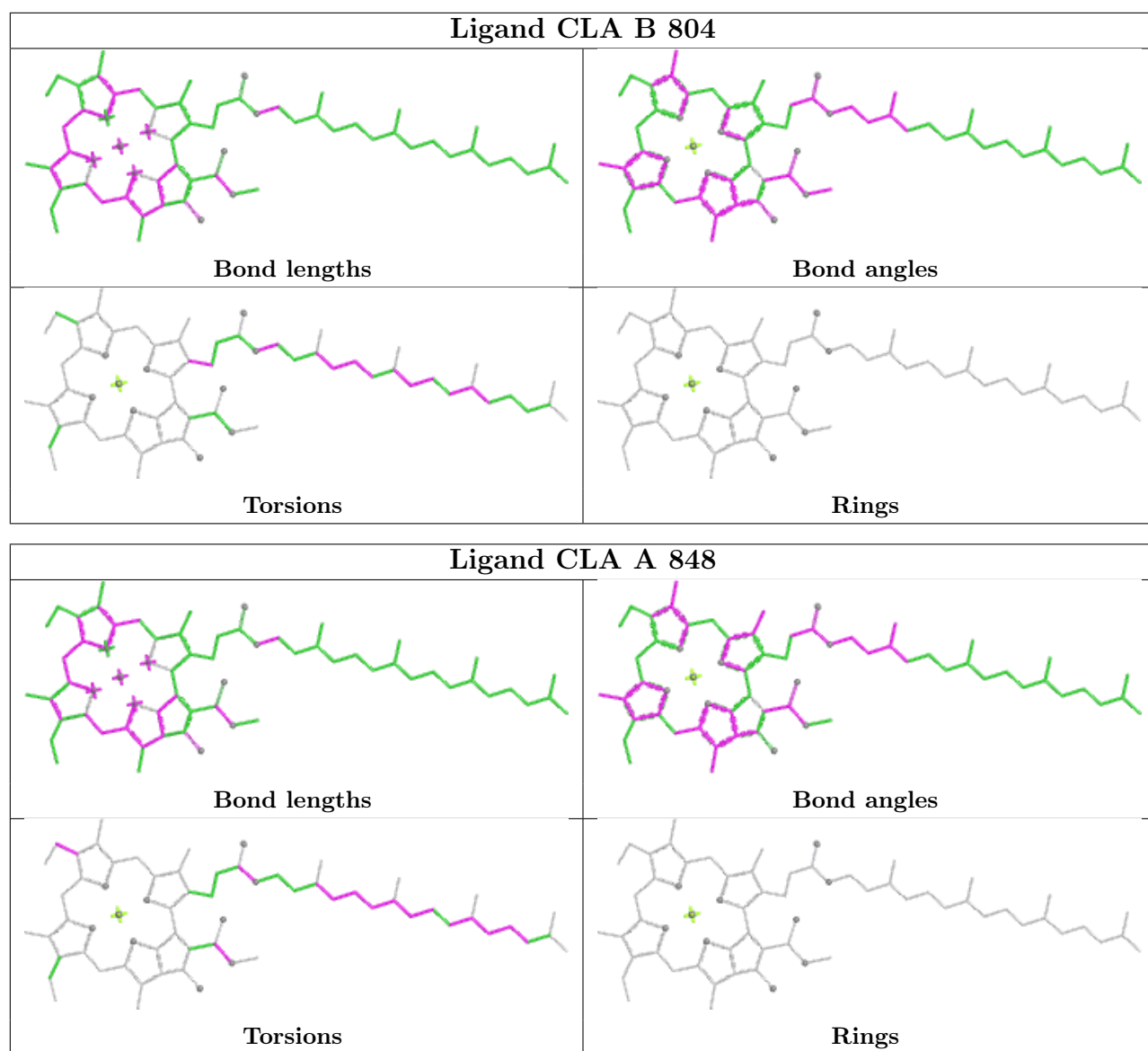
Torsions

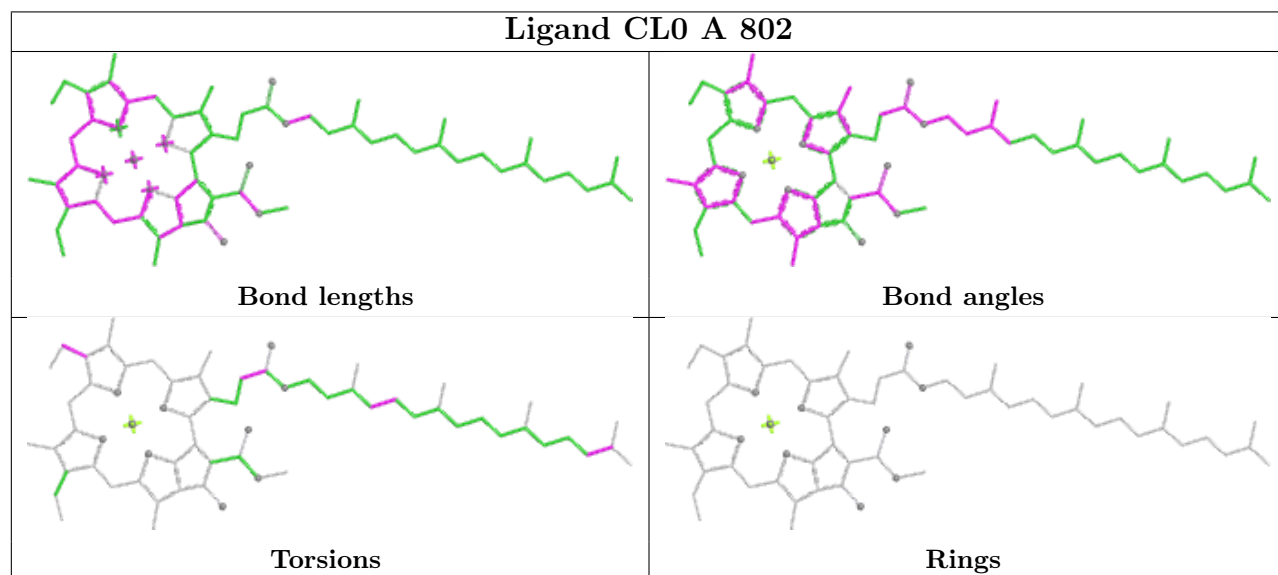
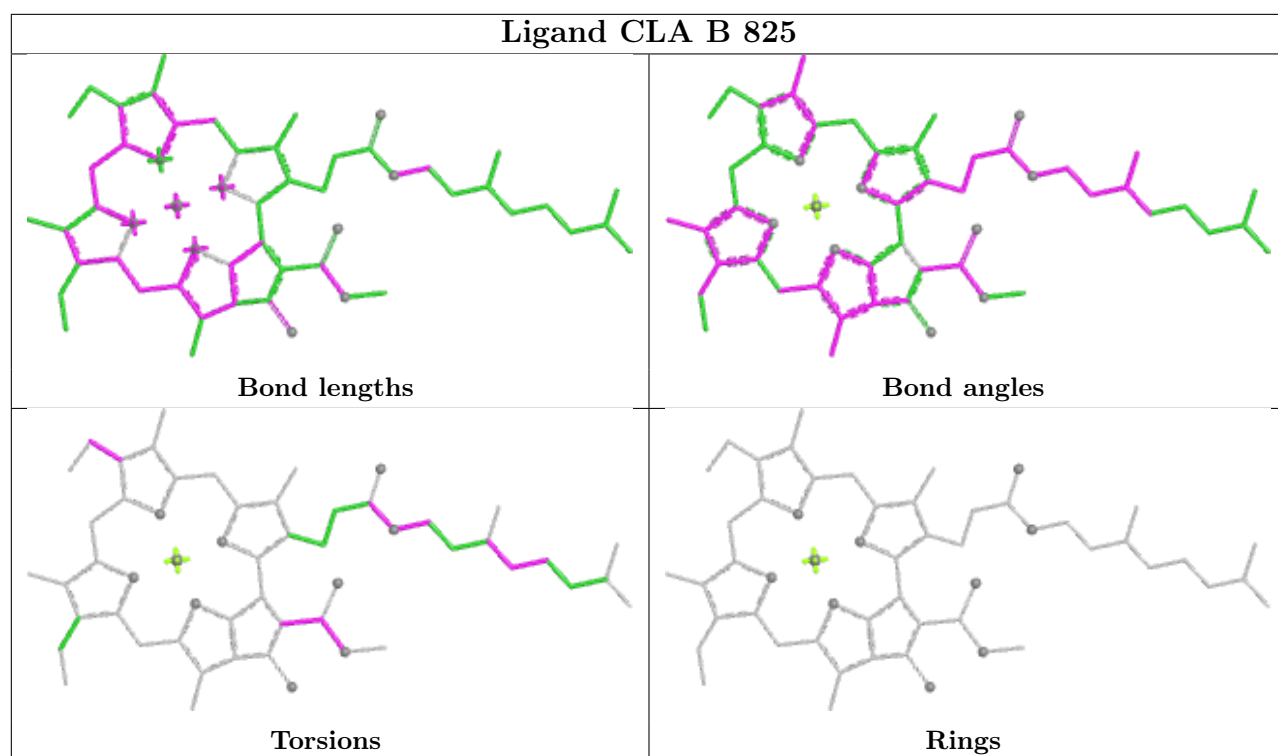


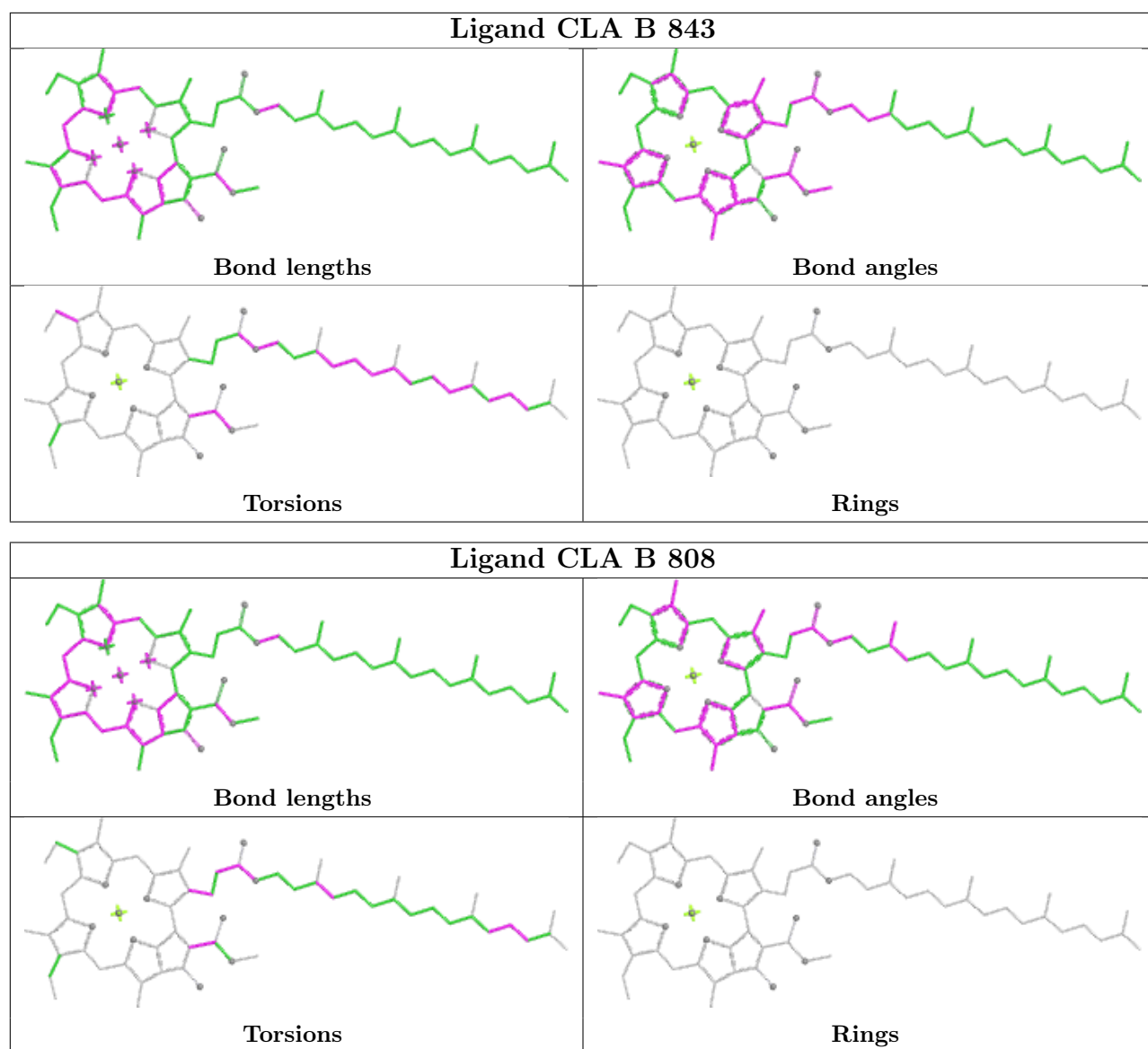
Rings

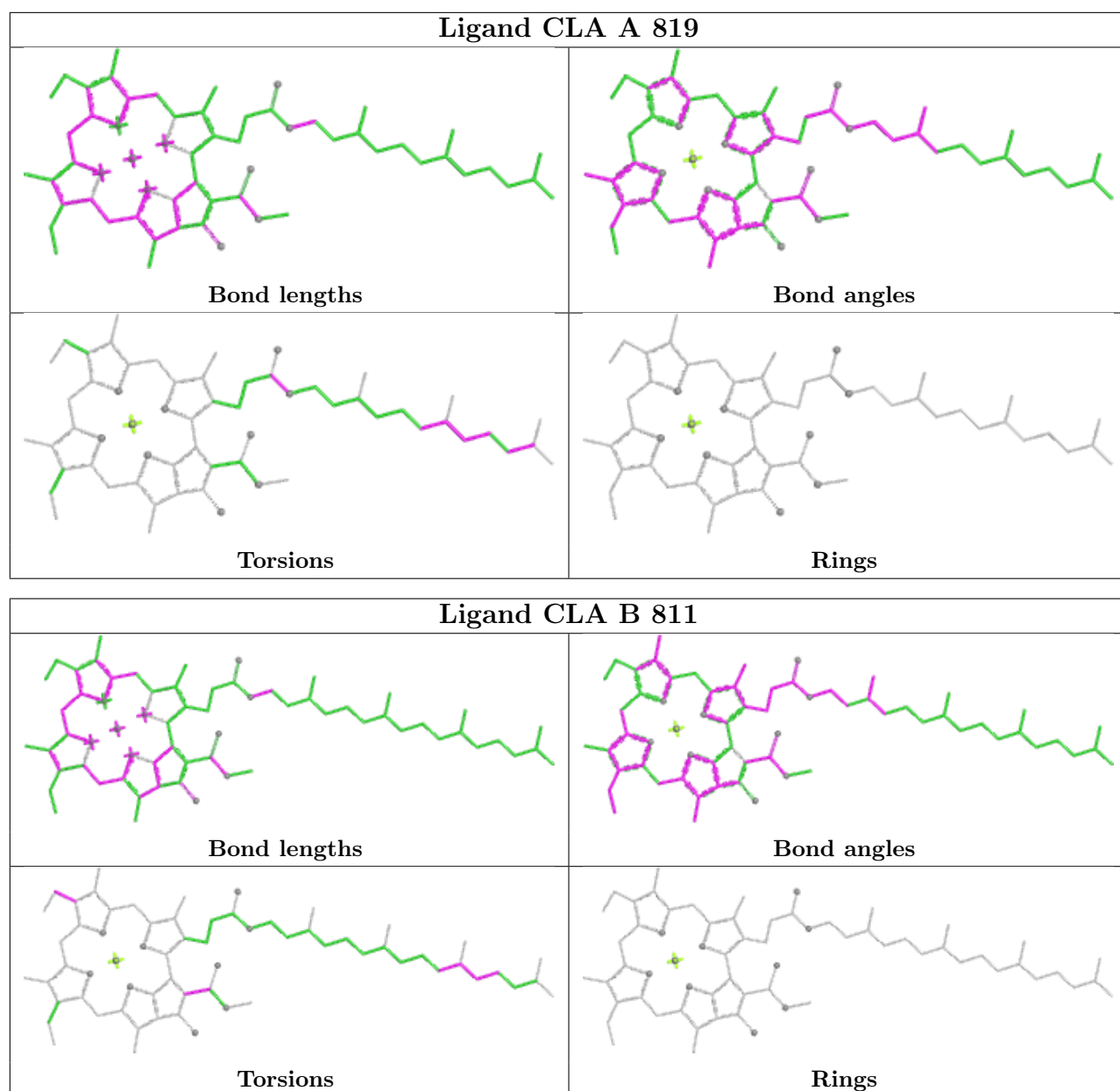


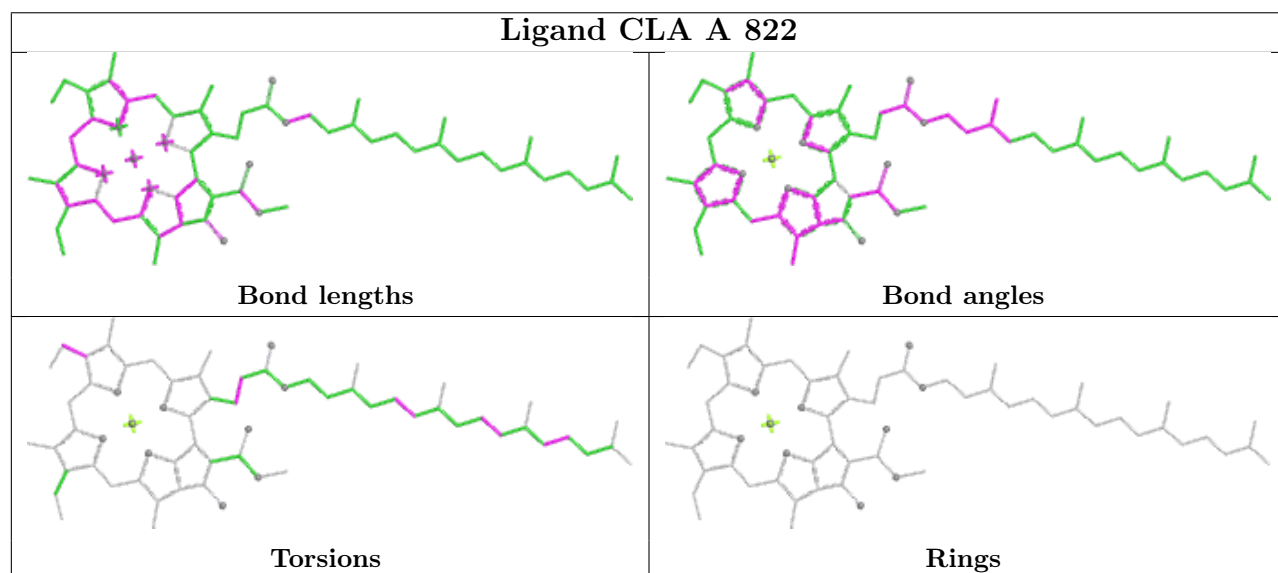
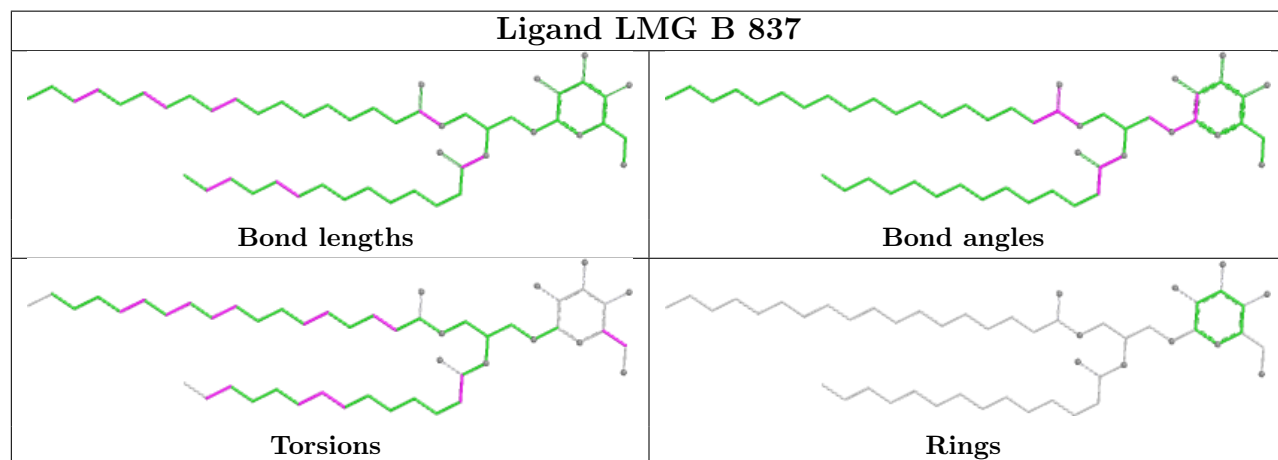
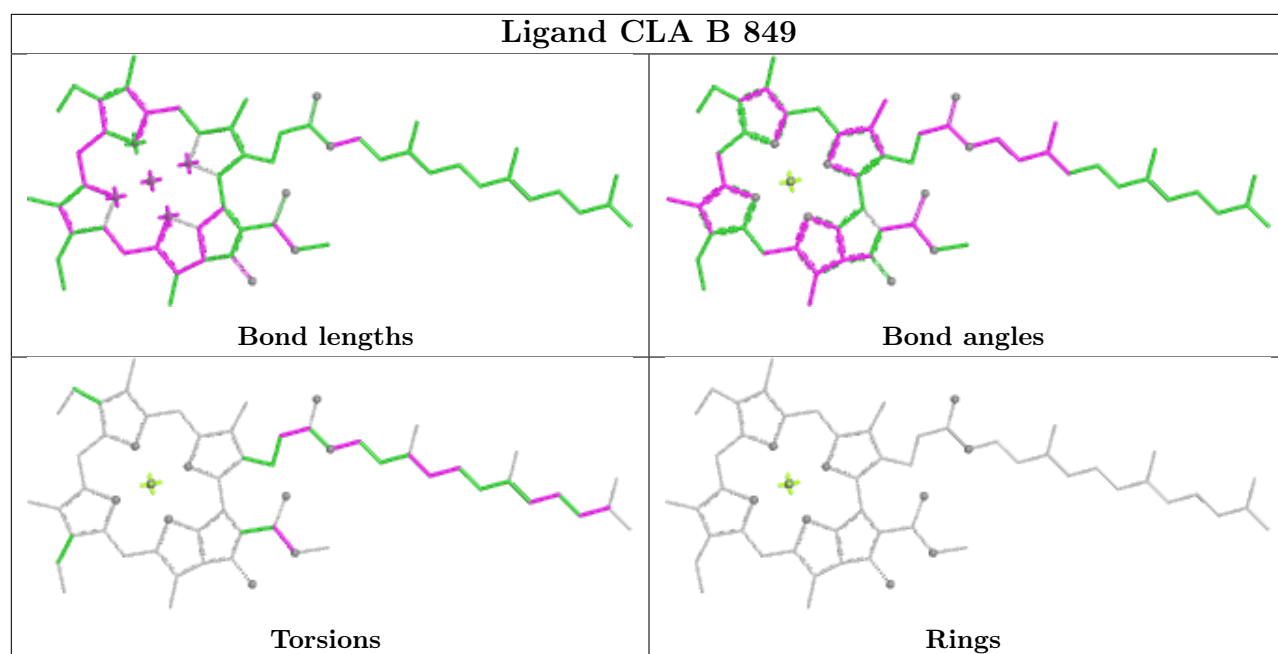


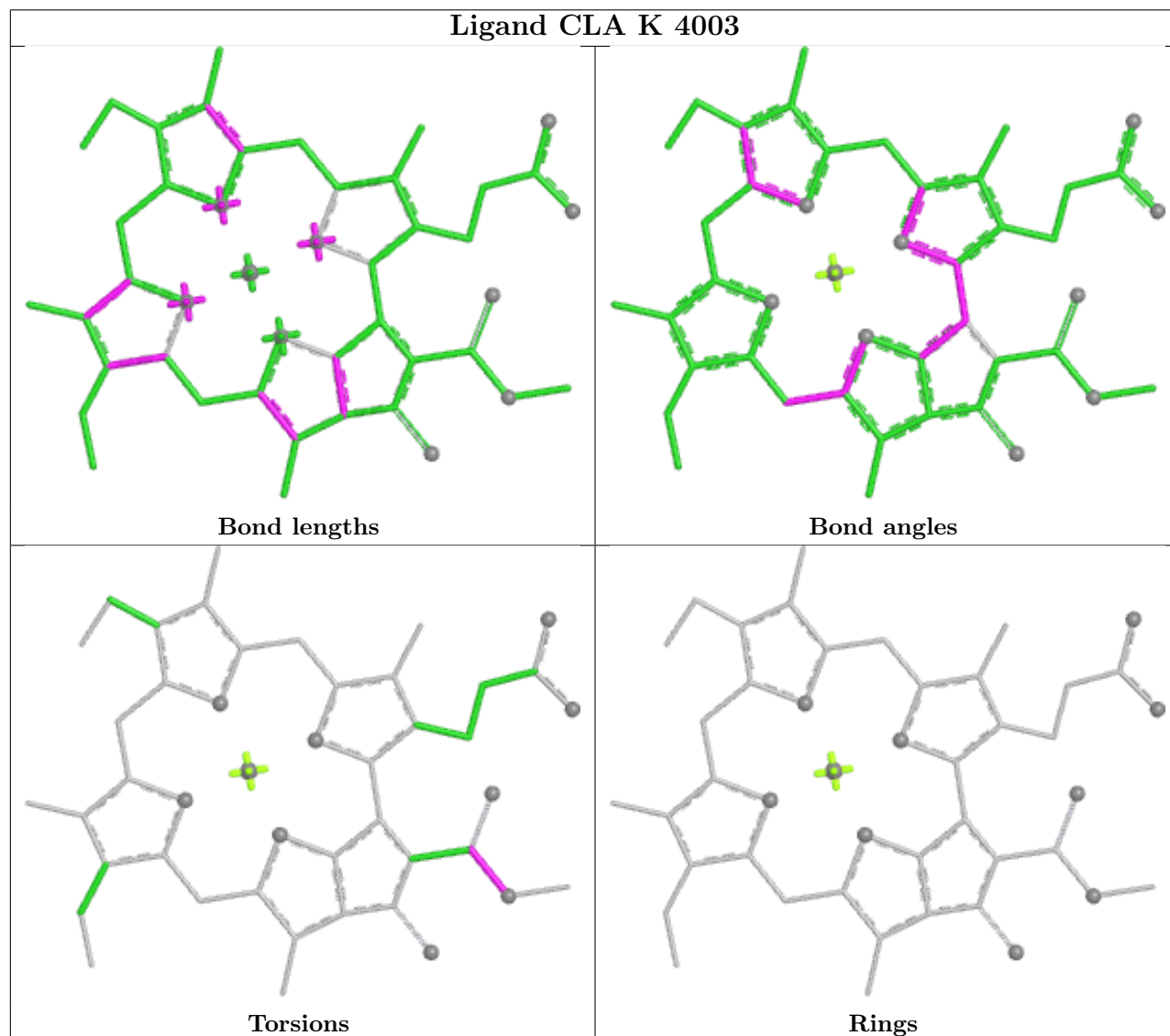
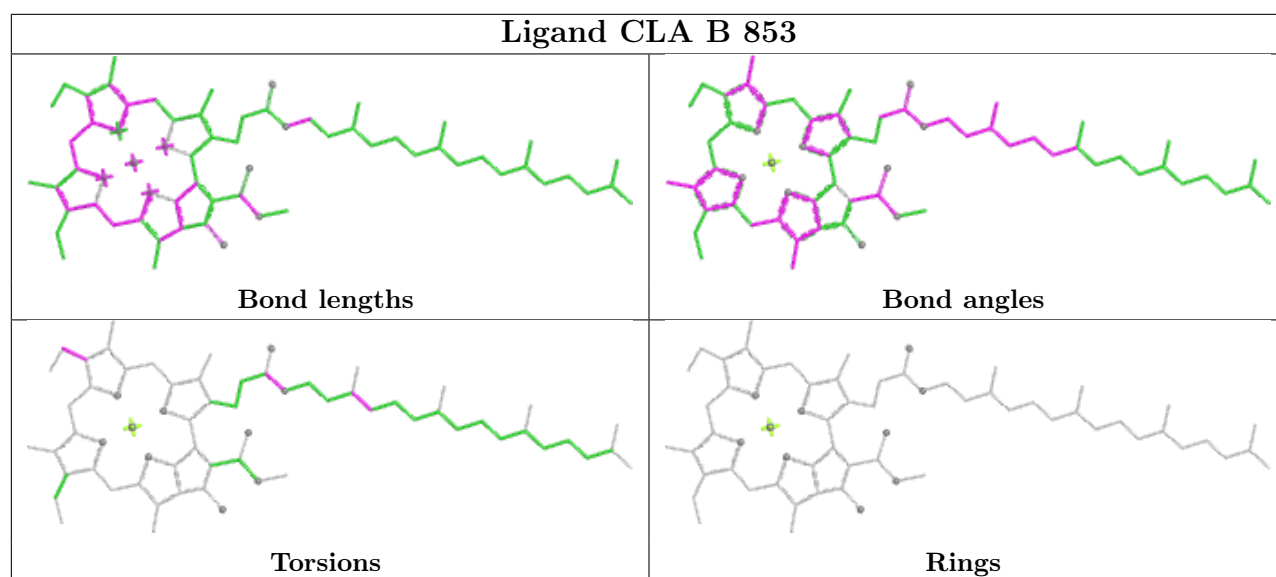


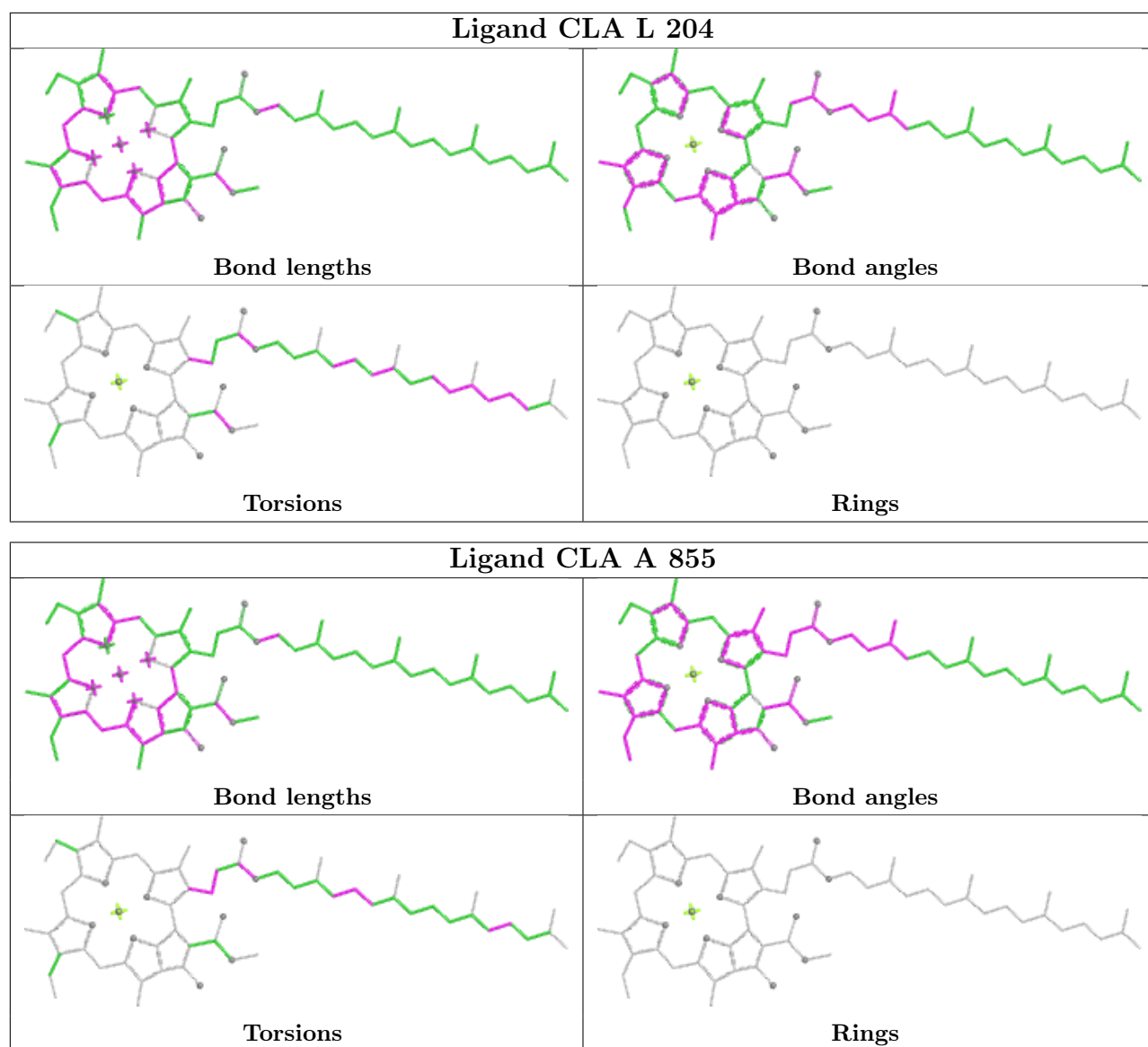




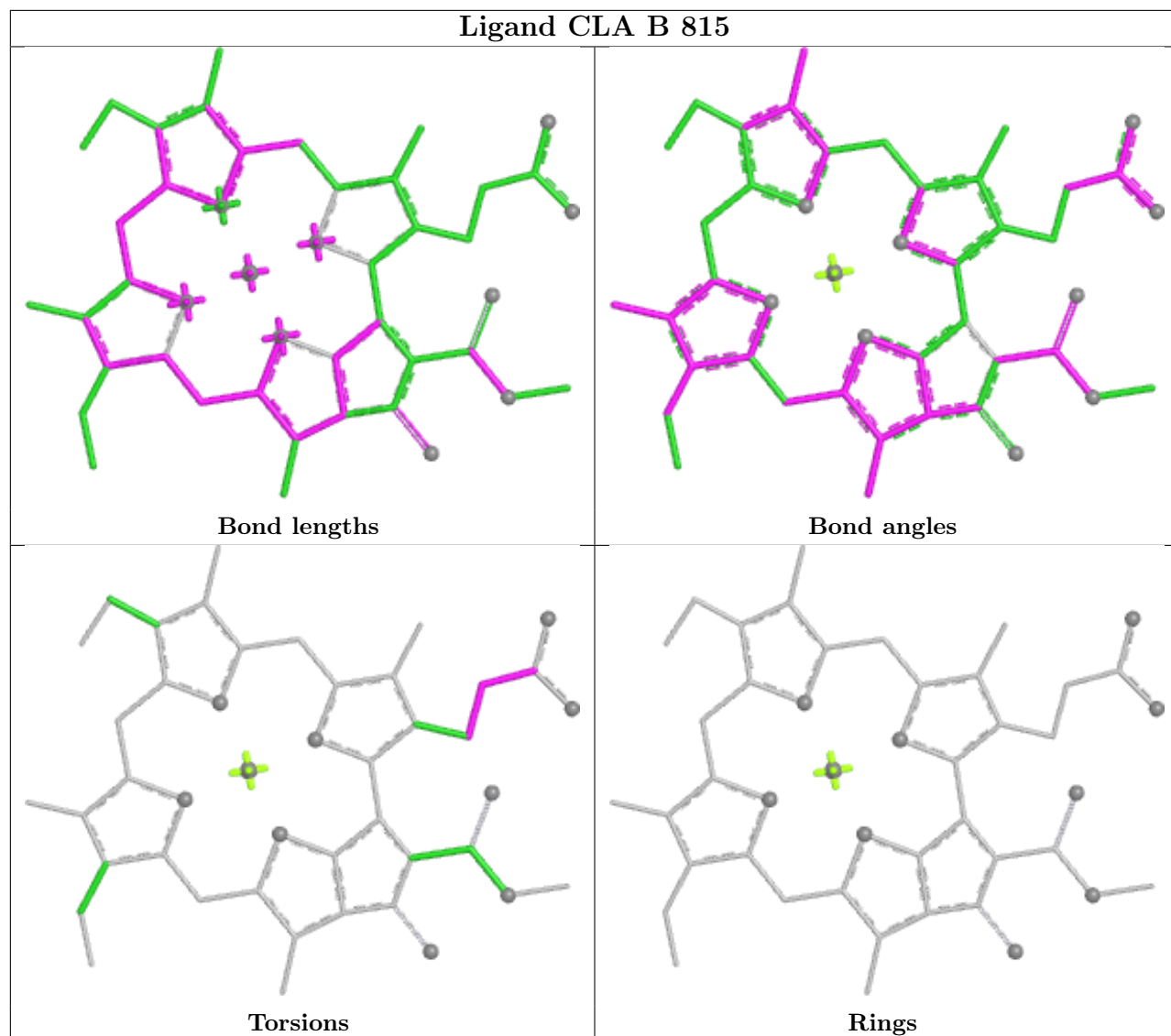




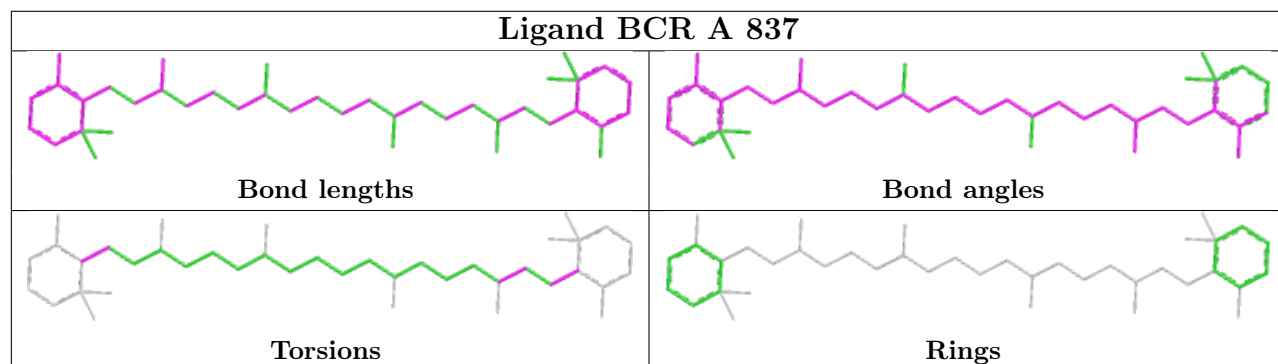


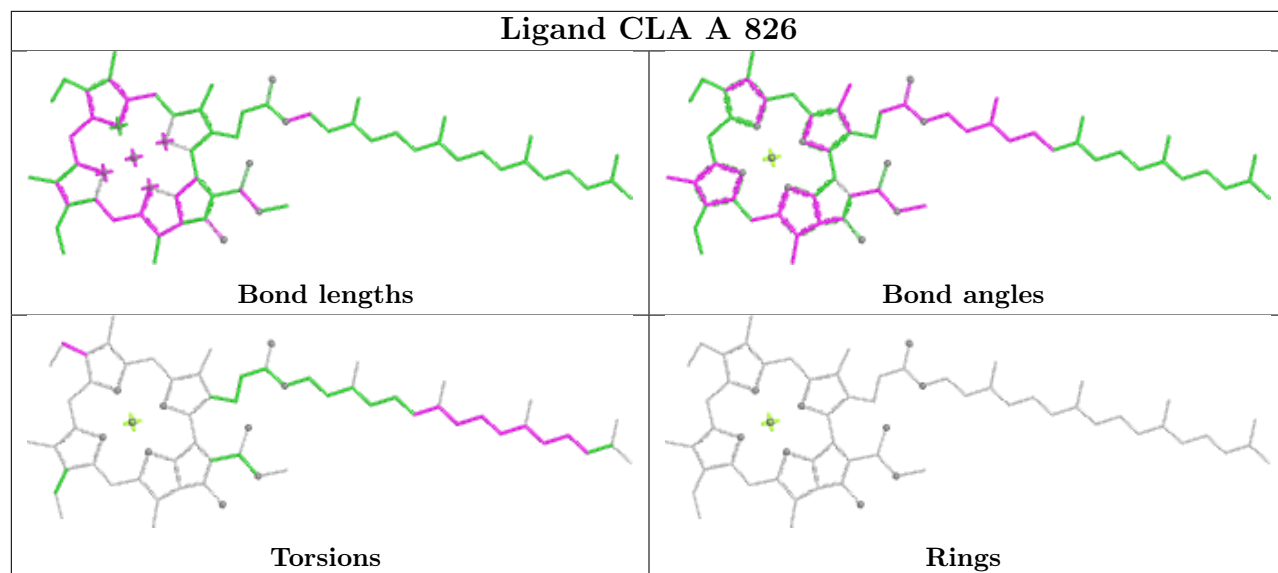
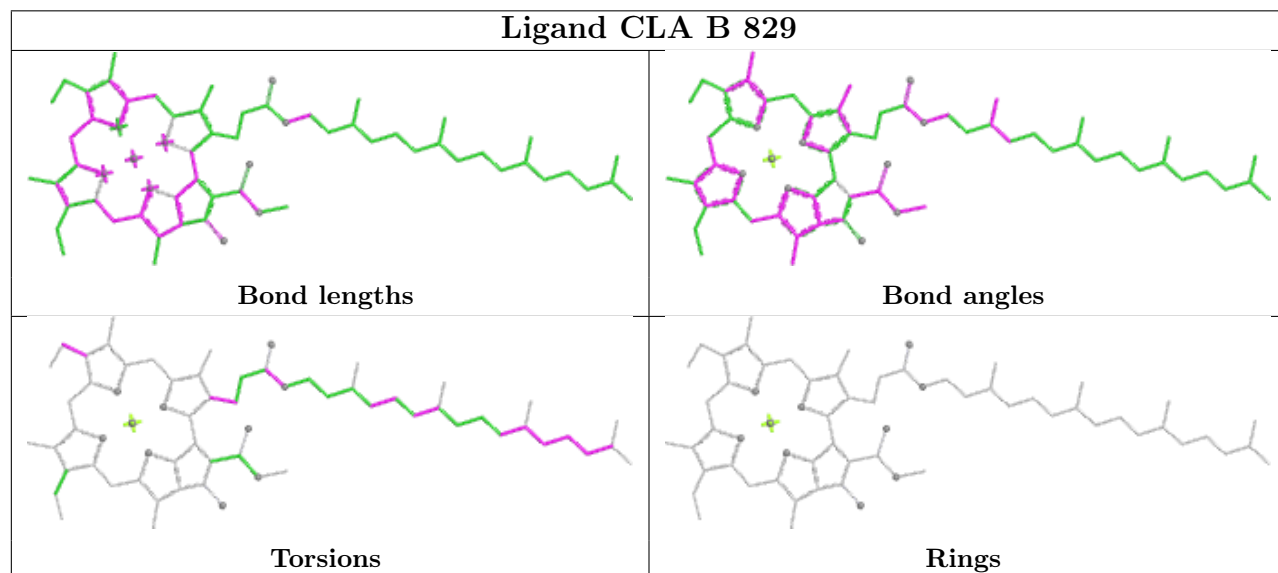
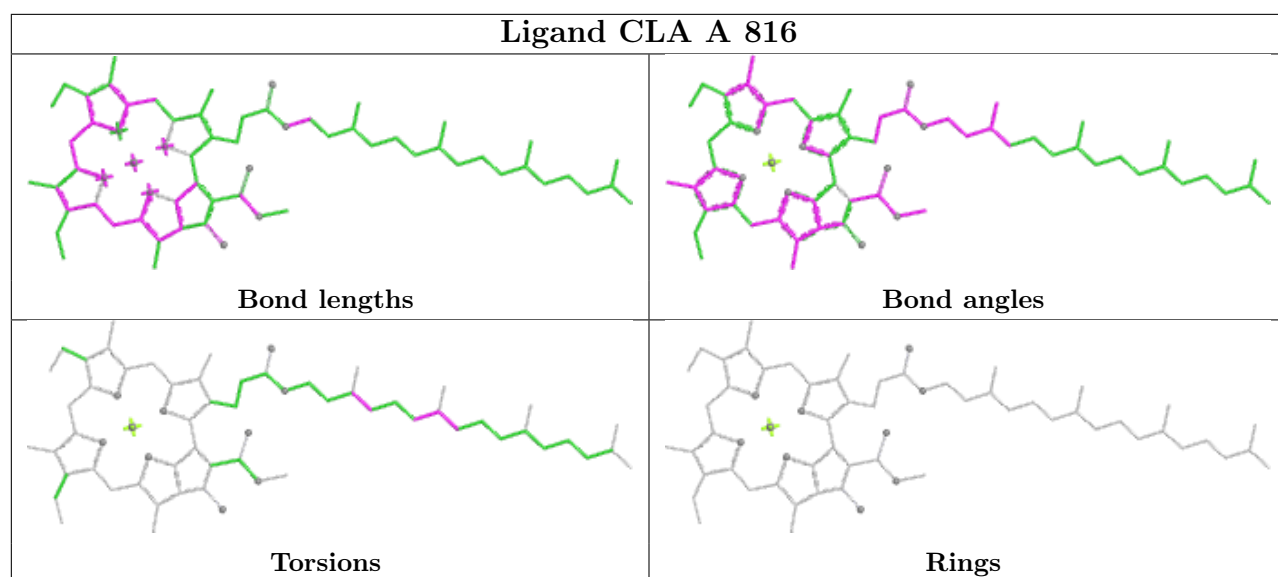


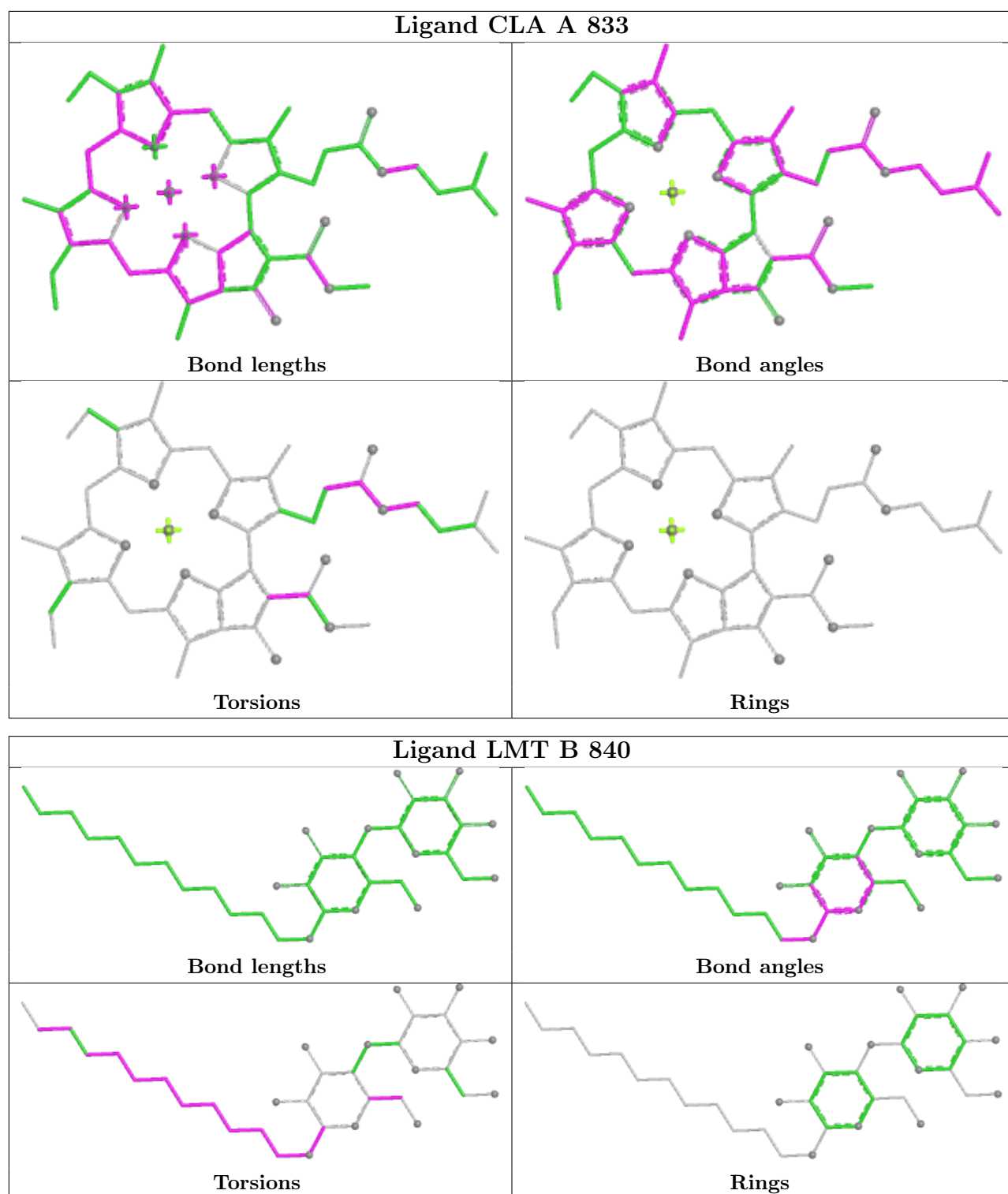
Ligand CLA B 815

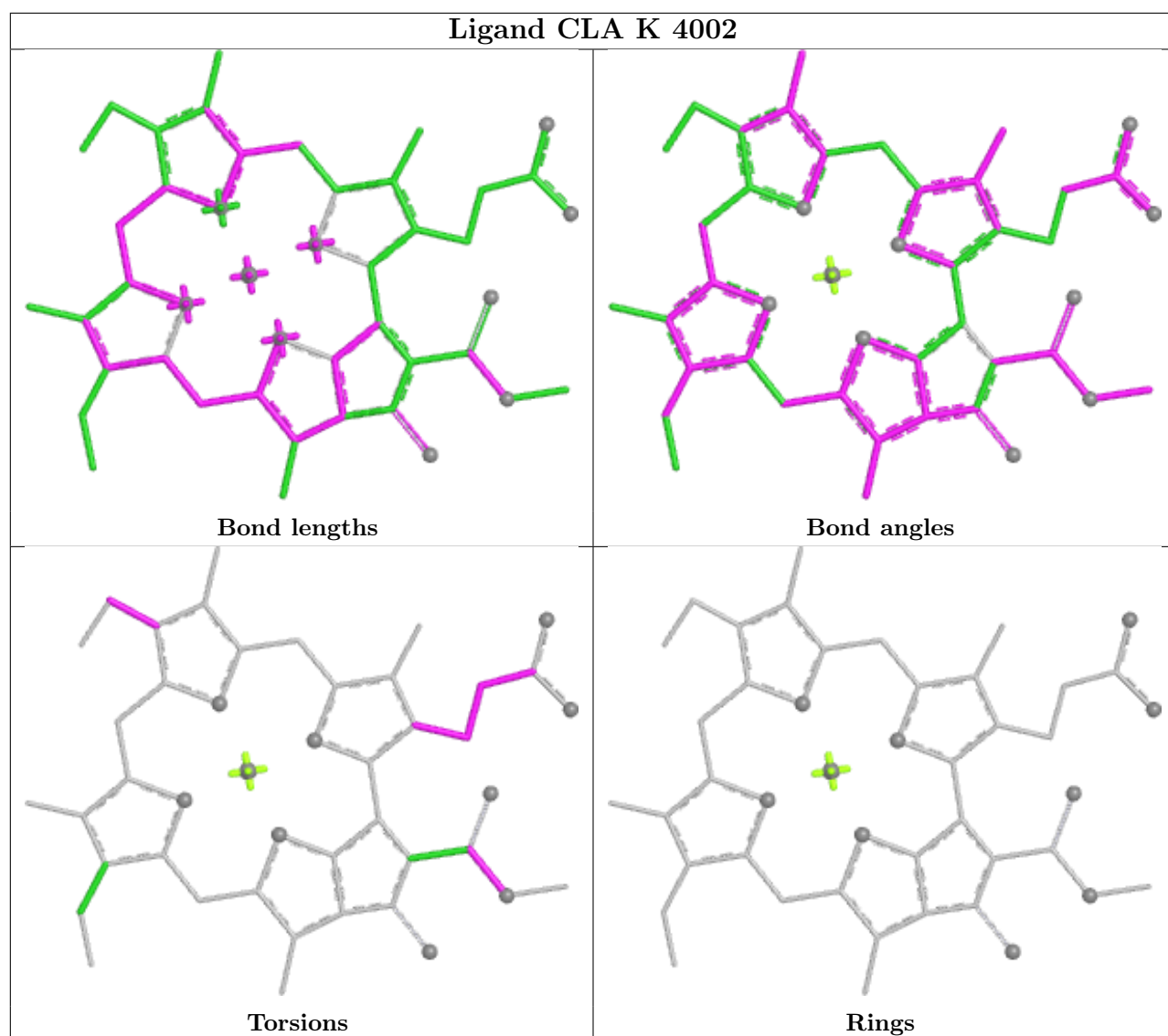


Ligand BCR A 837

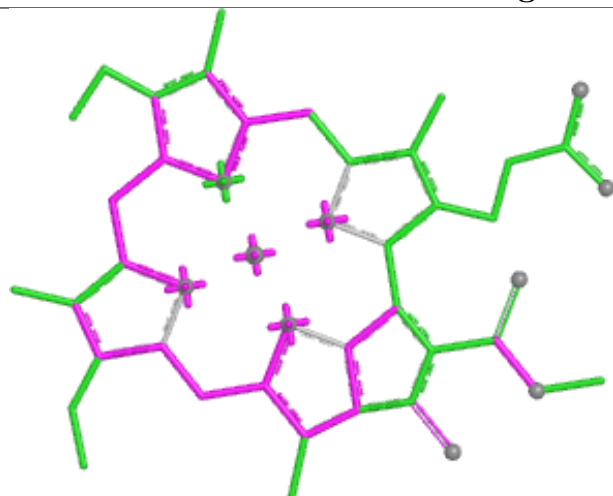




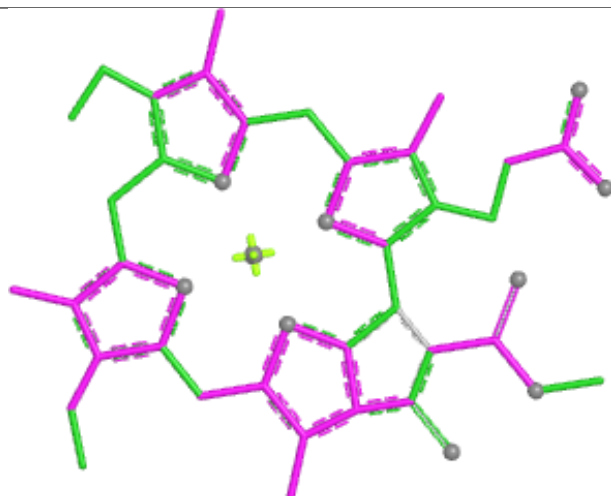




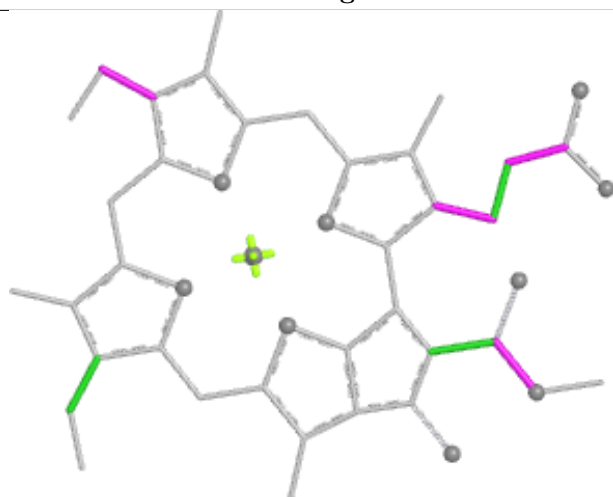
Ligand CLA J 102



Bond lengths



Bond angles

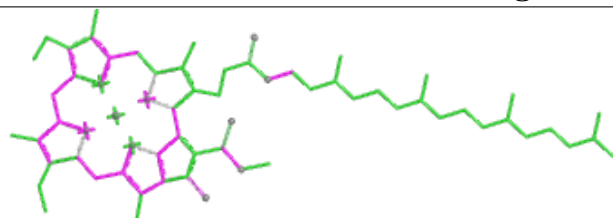


Torsions

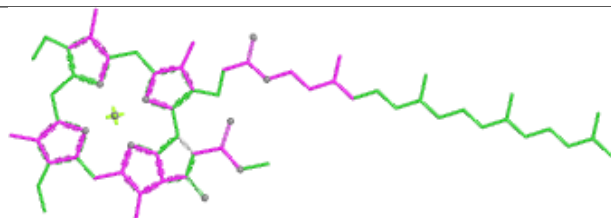


Rings

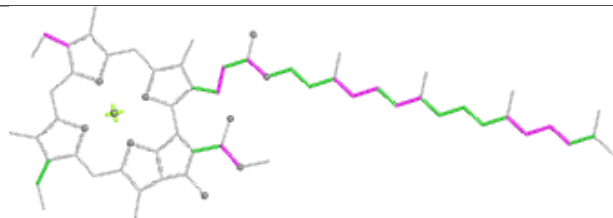
Ligand CLA A 831



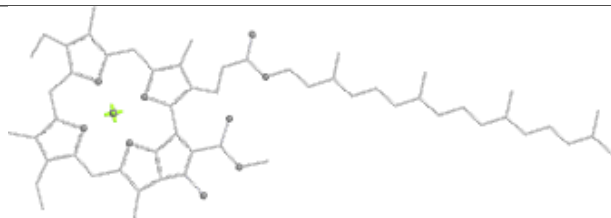
Bond lengths



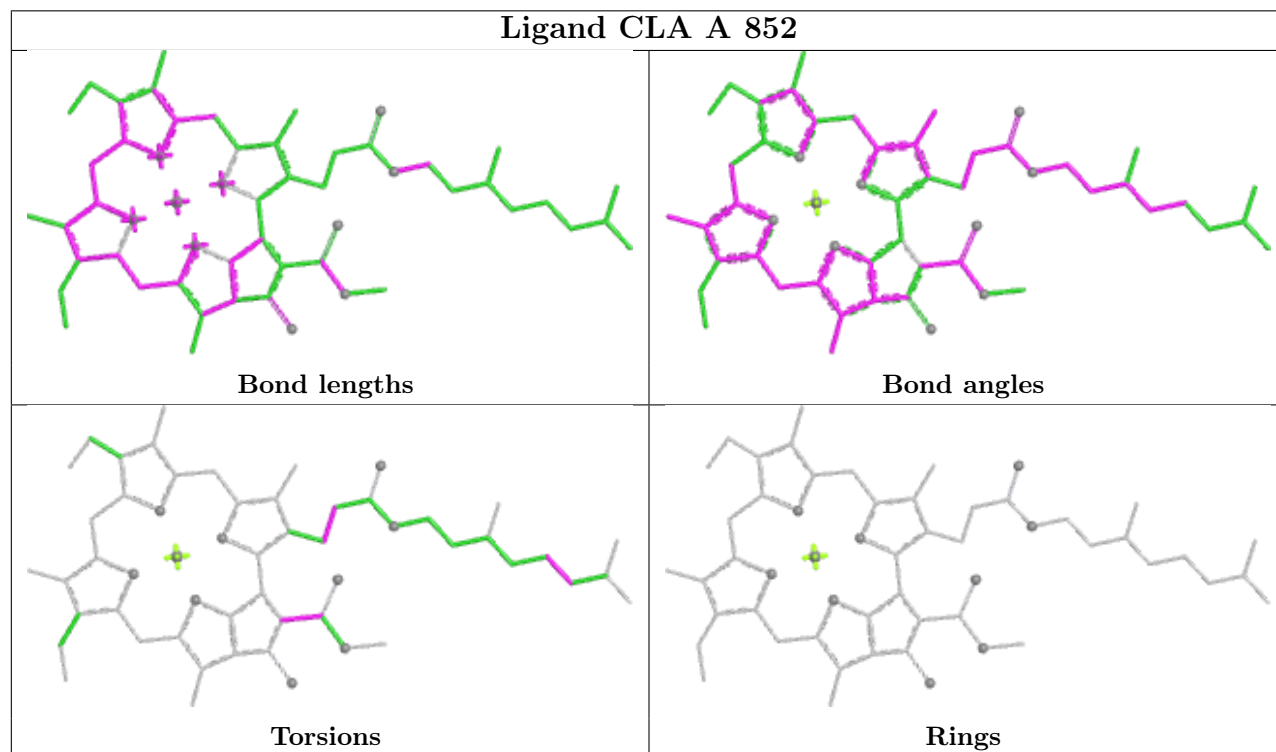
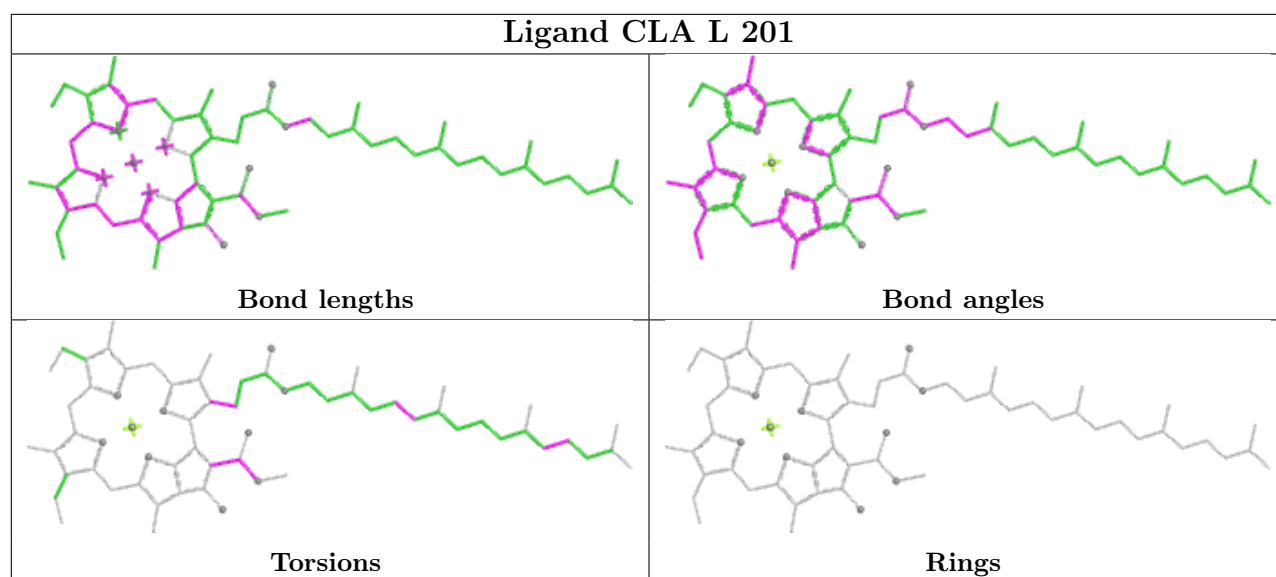
Bond angles

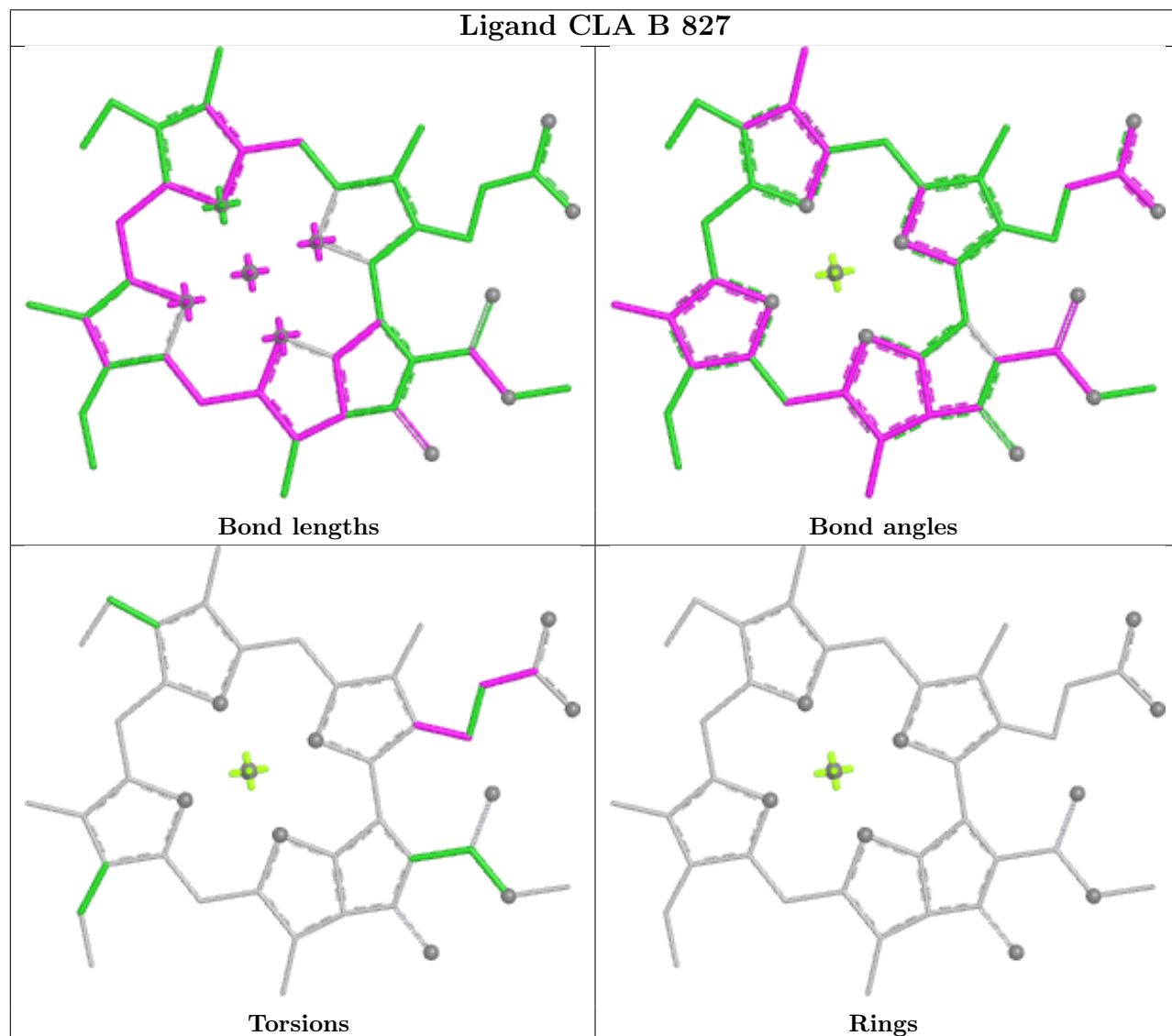
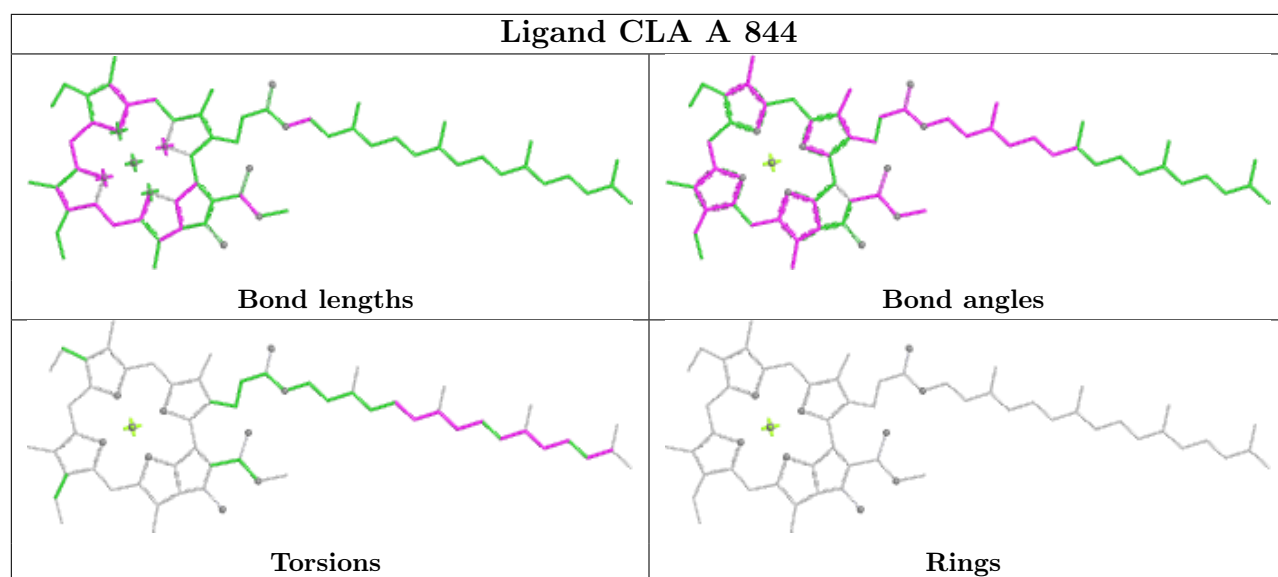


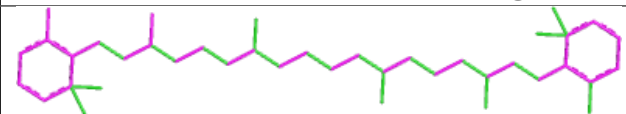
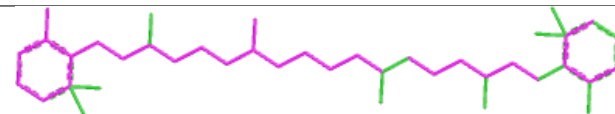
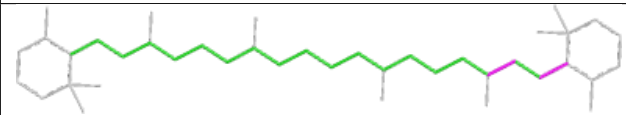
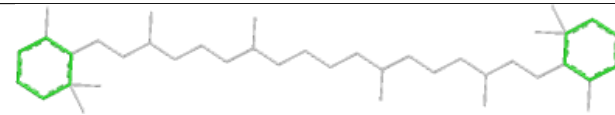
Torsions

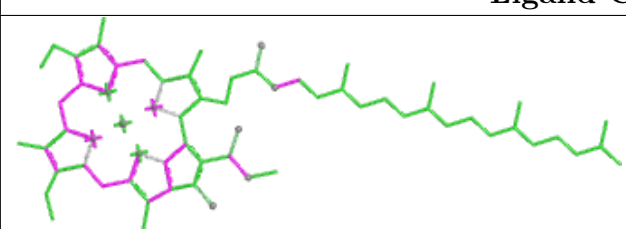
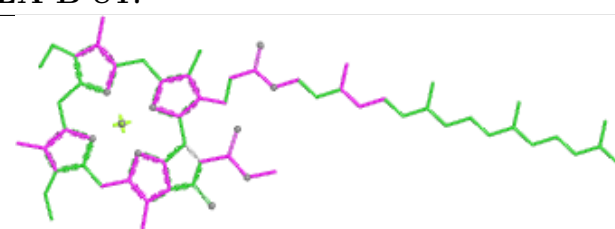
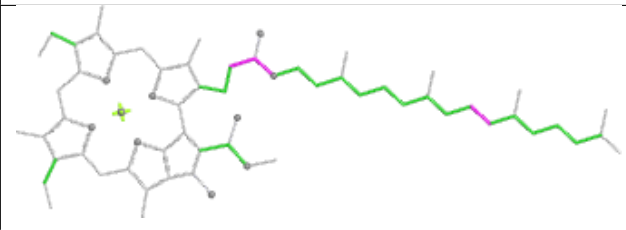
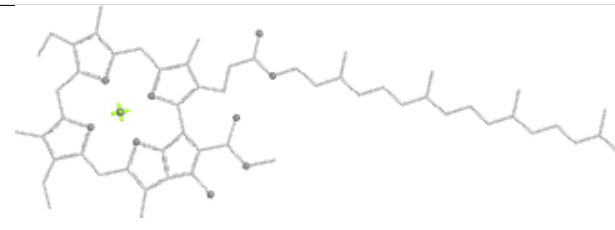


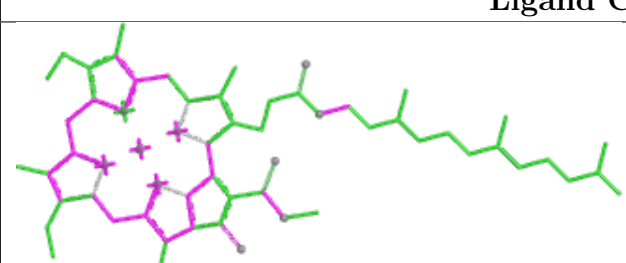
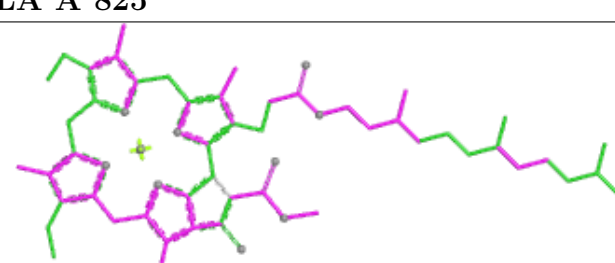
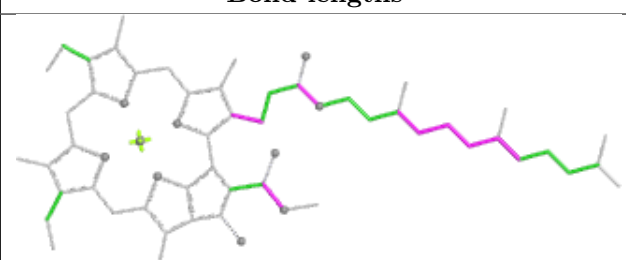
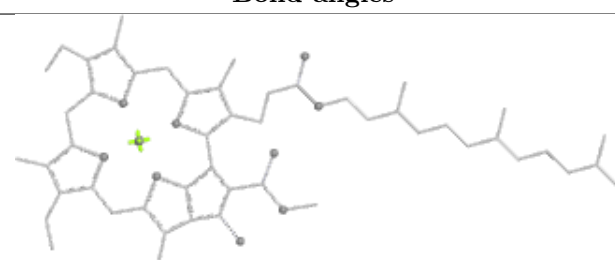
Rings

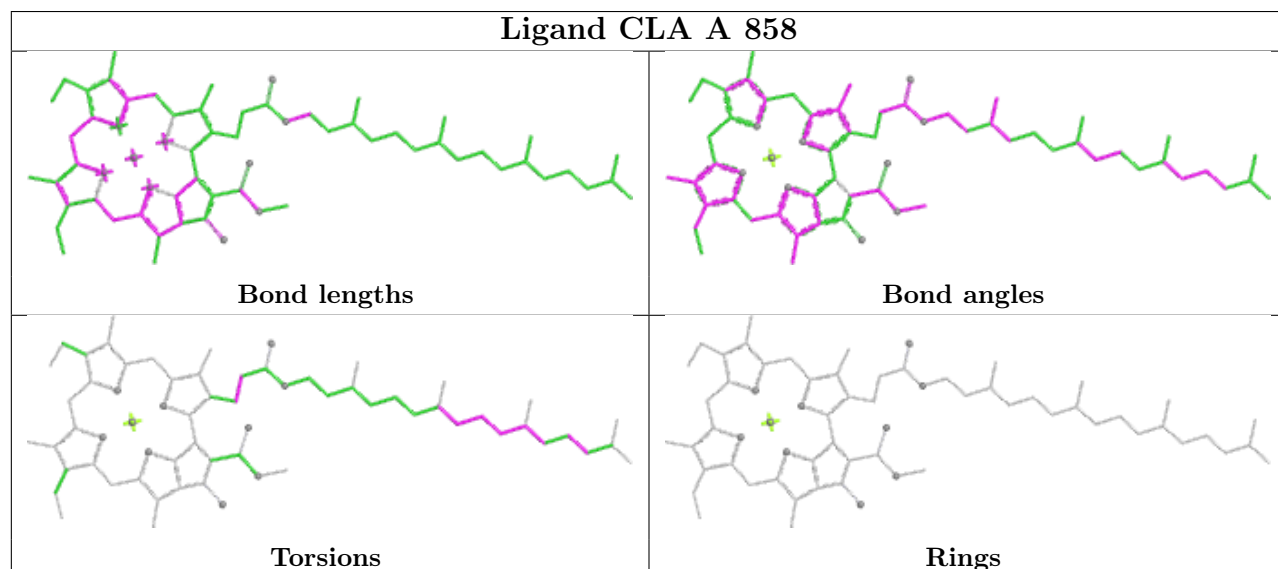
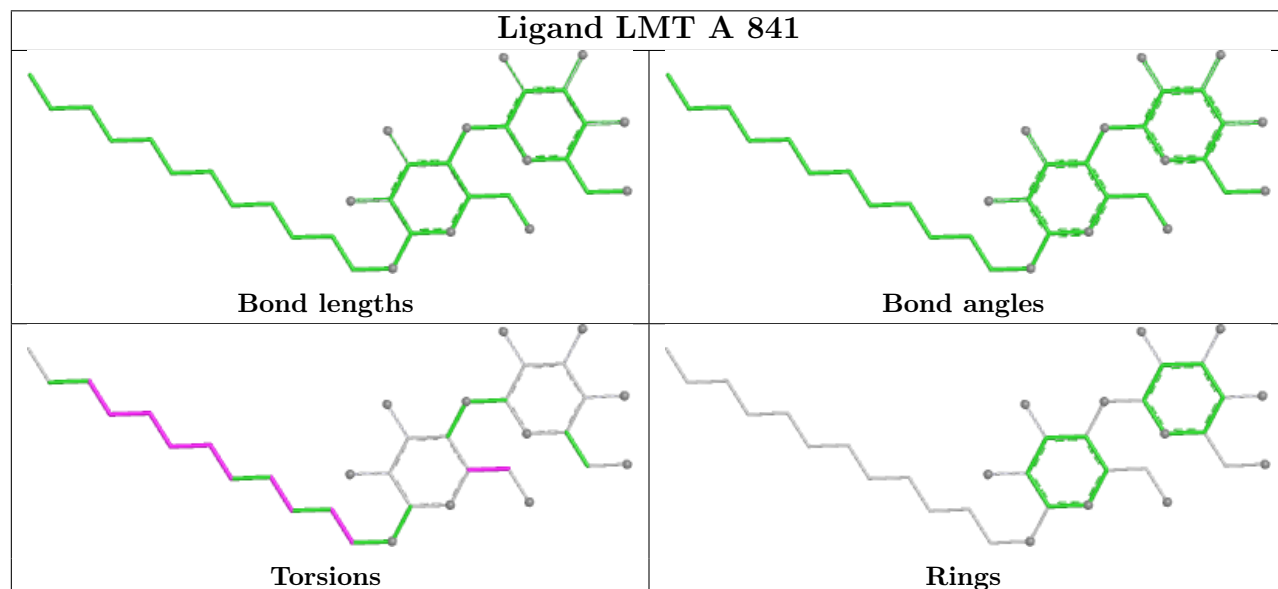
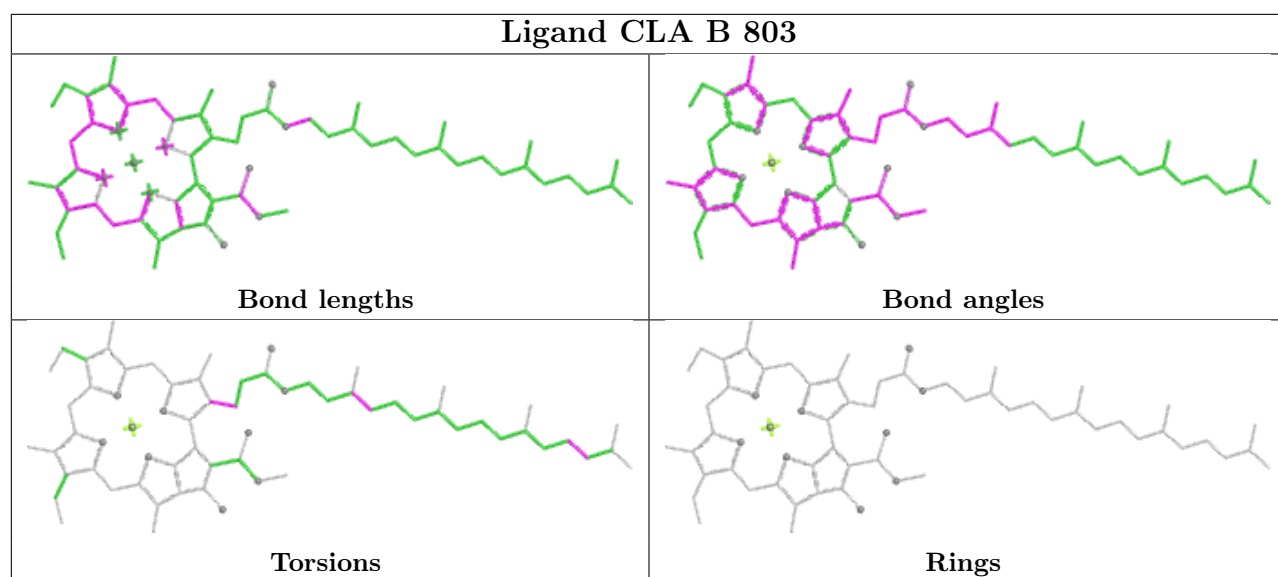


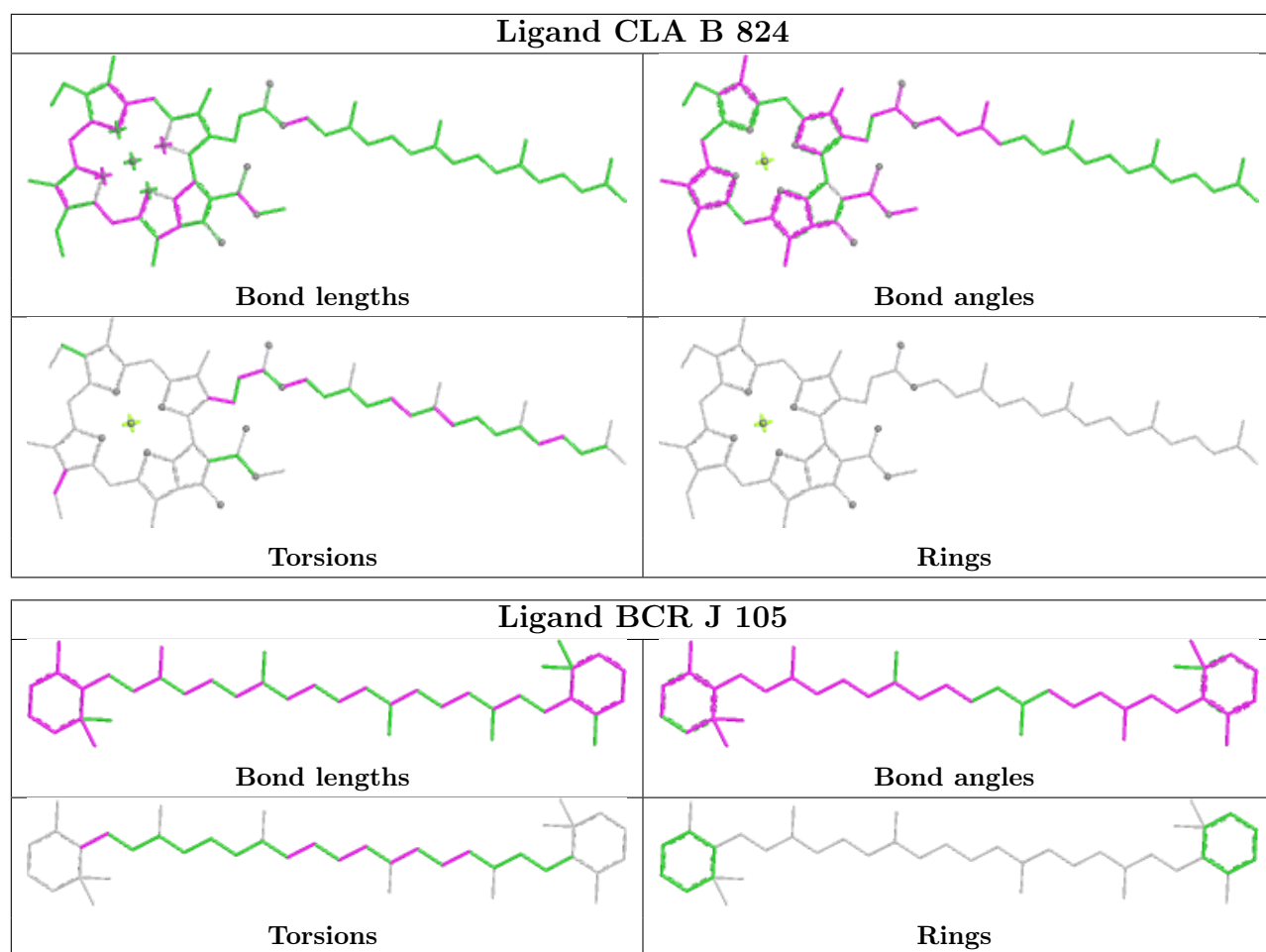


Ligand BCR K 4001	
	
Bond lengths	Bond angles
	
Torsions	Rings

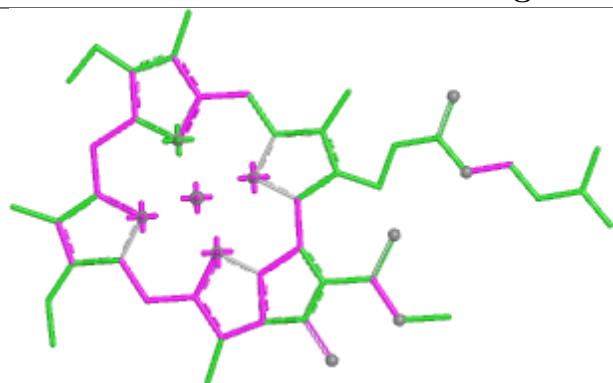
Ligand CLA B 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

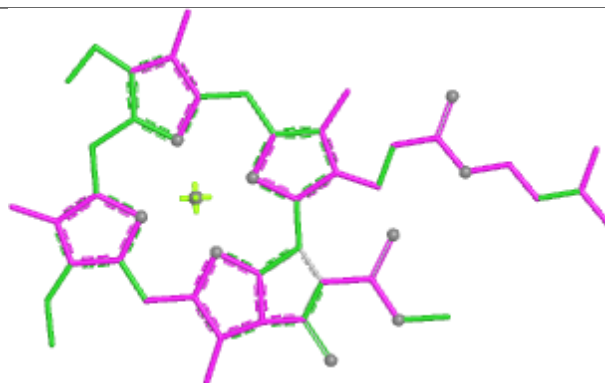




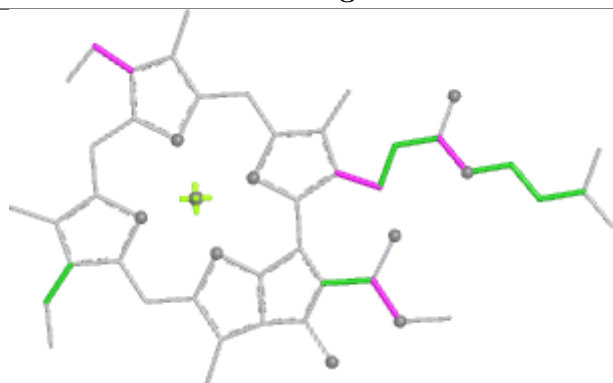
Ligand CLA A 832



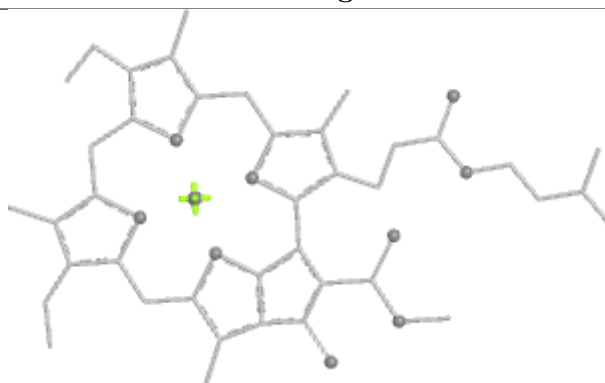
Bond lengths



Bond angles

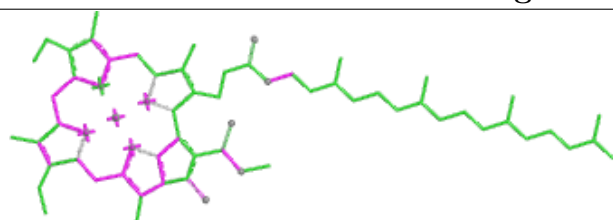


Torsions

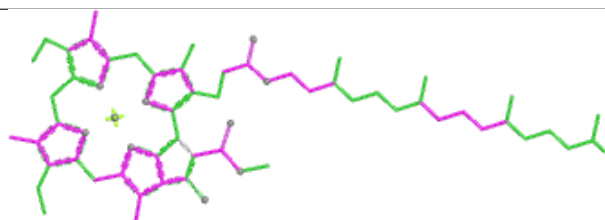


Rings

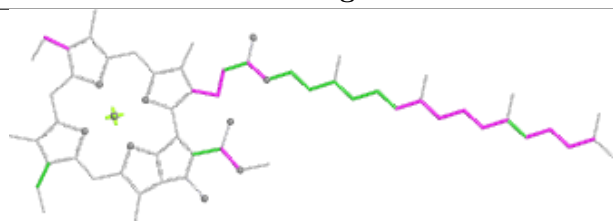
Ligand CLA B 820



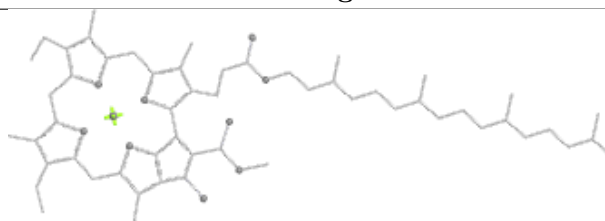
Bond lengths



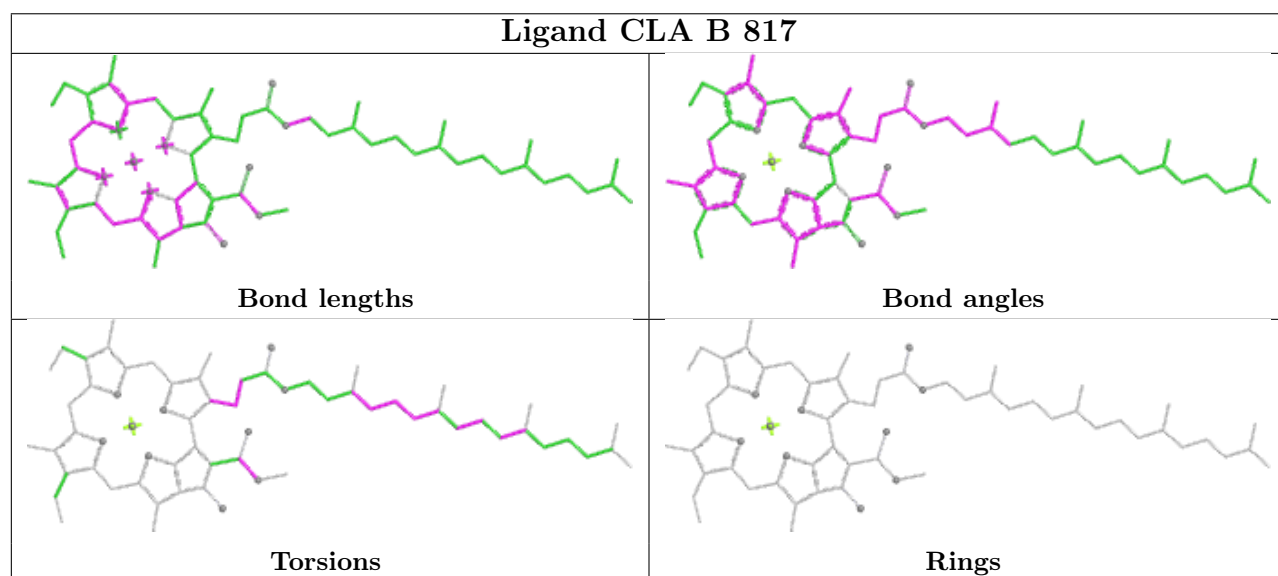
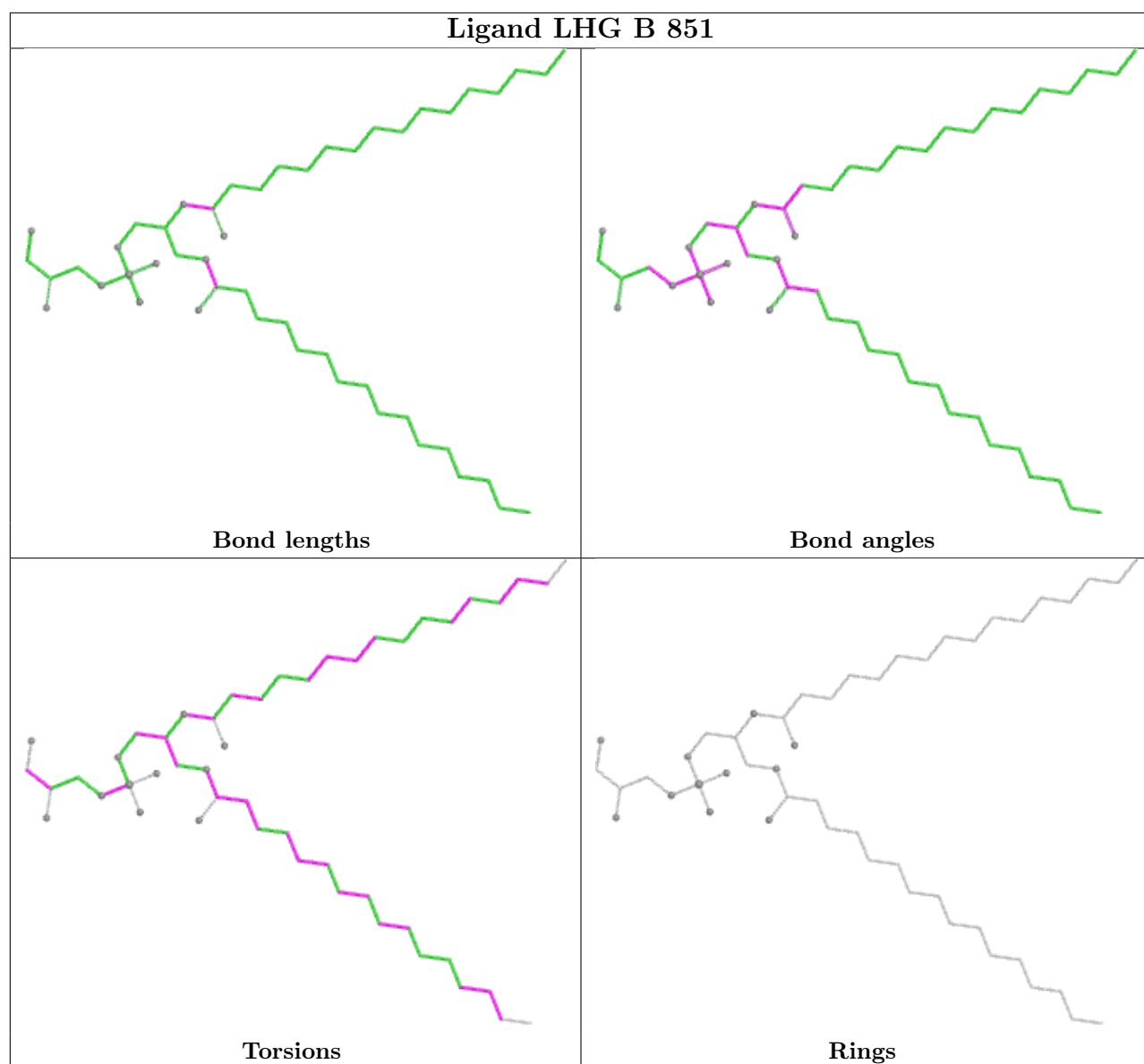
Bond angles

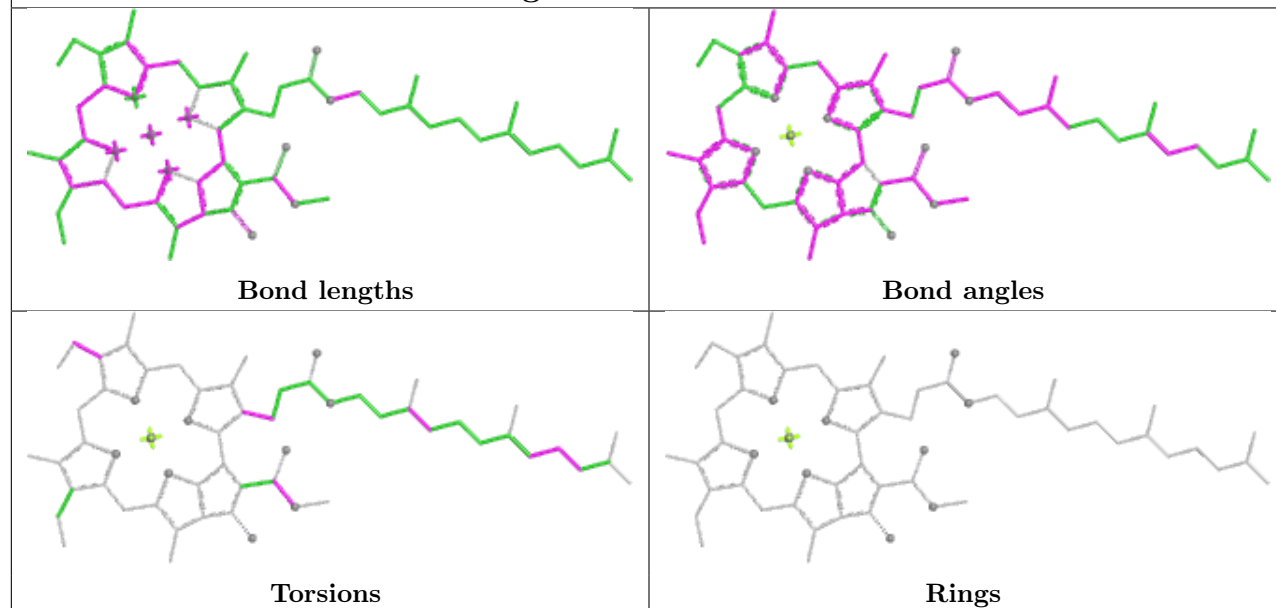
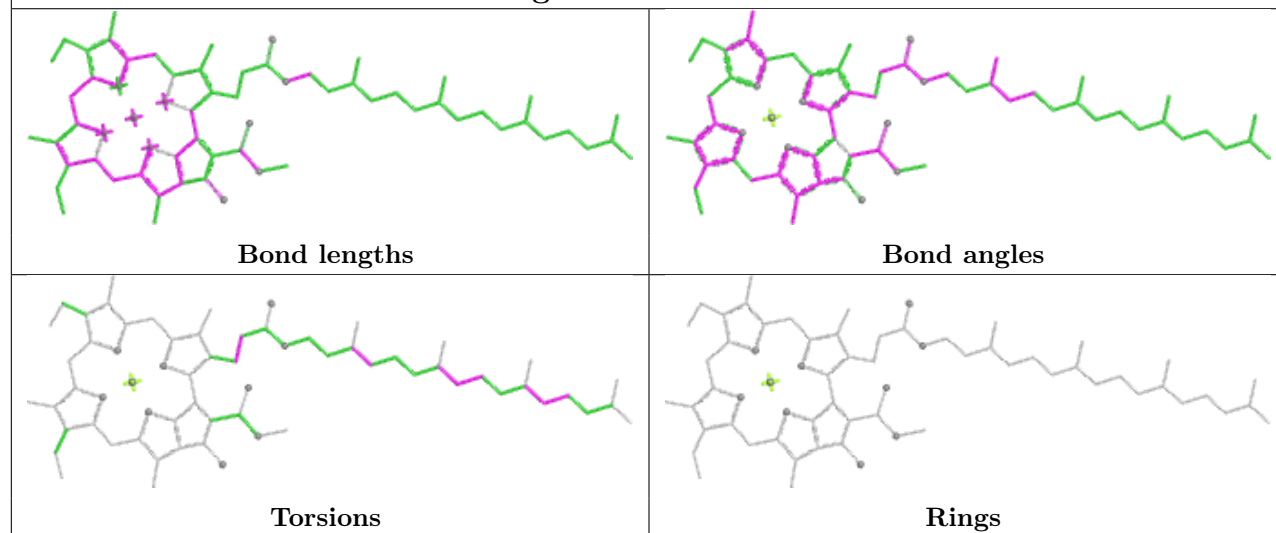


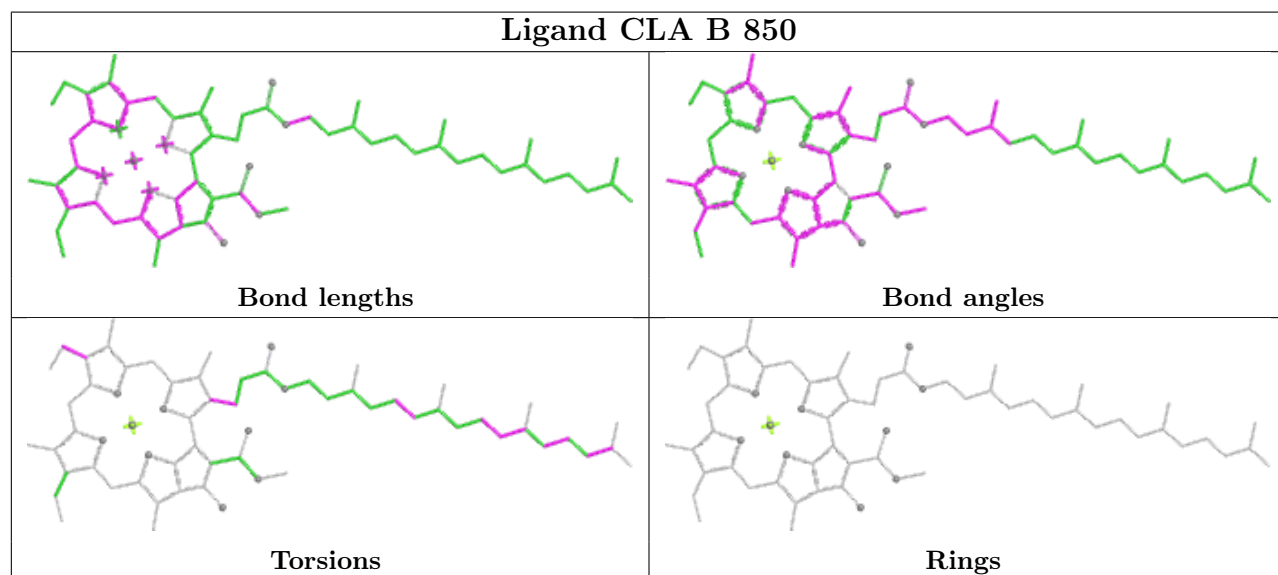
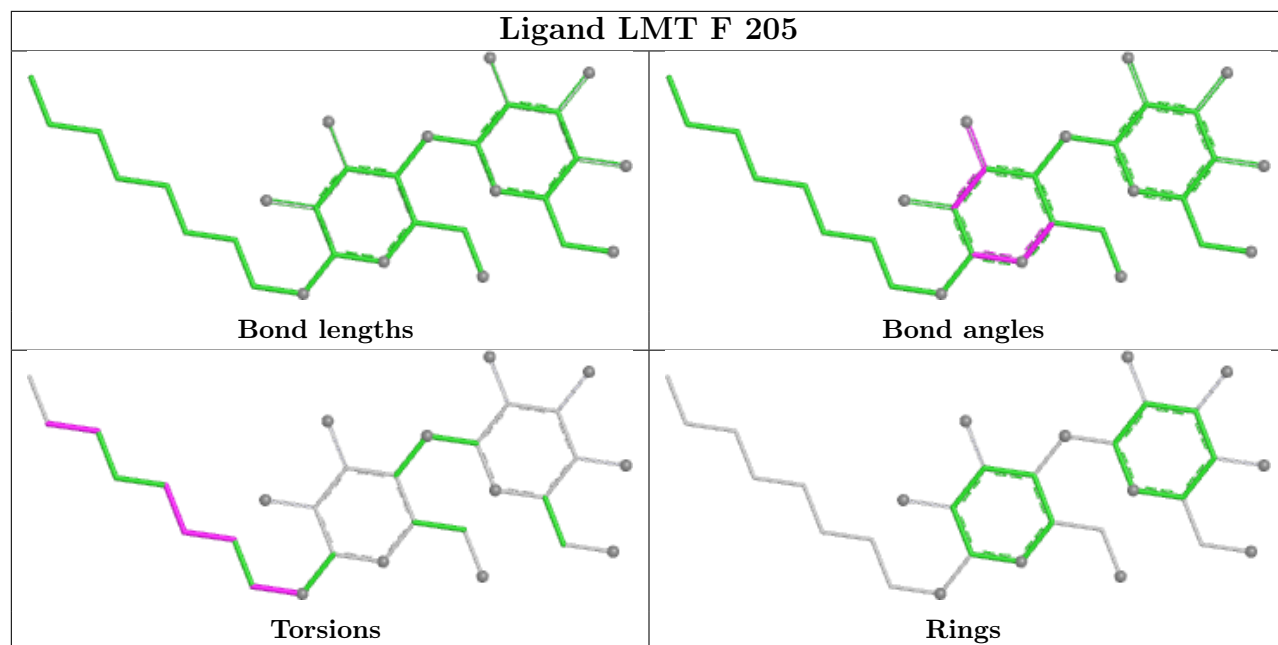
Torsions

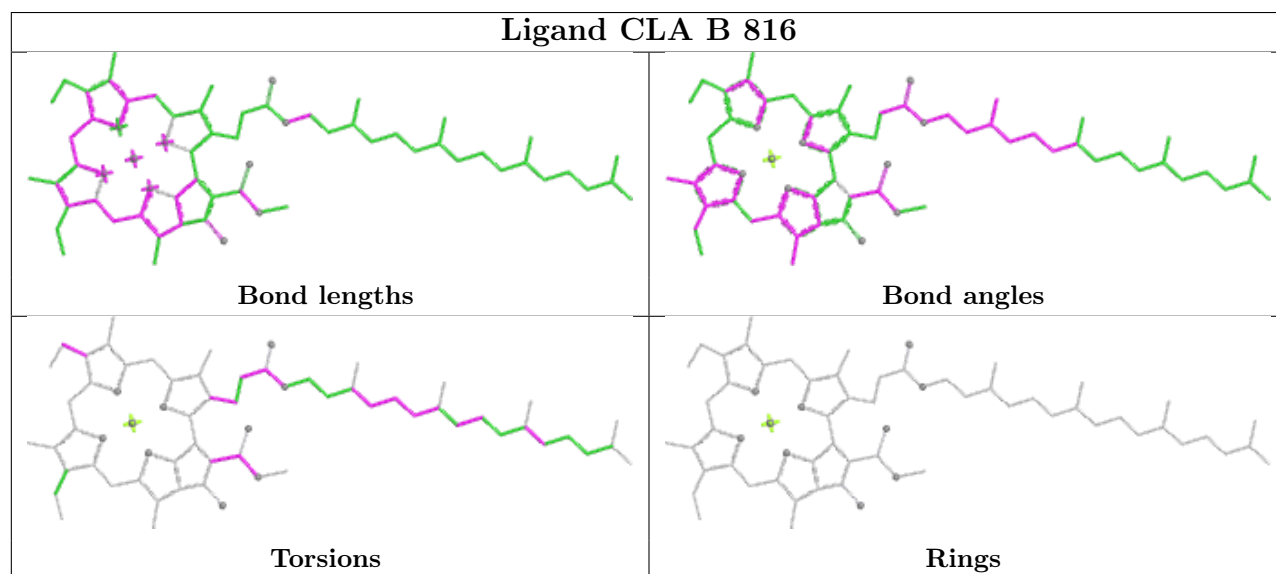
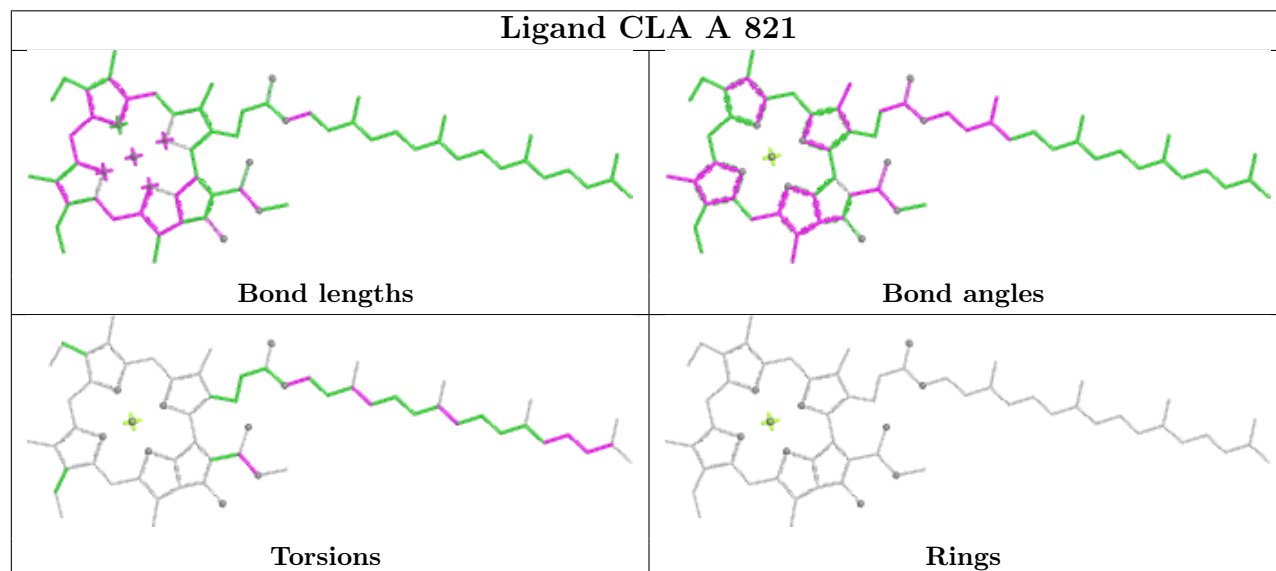
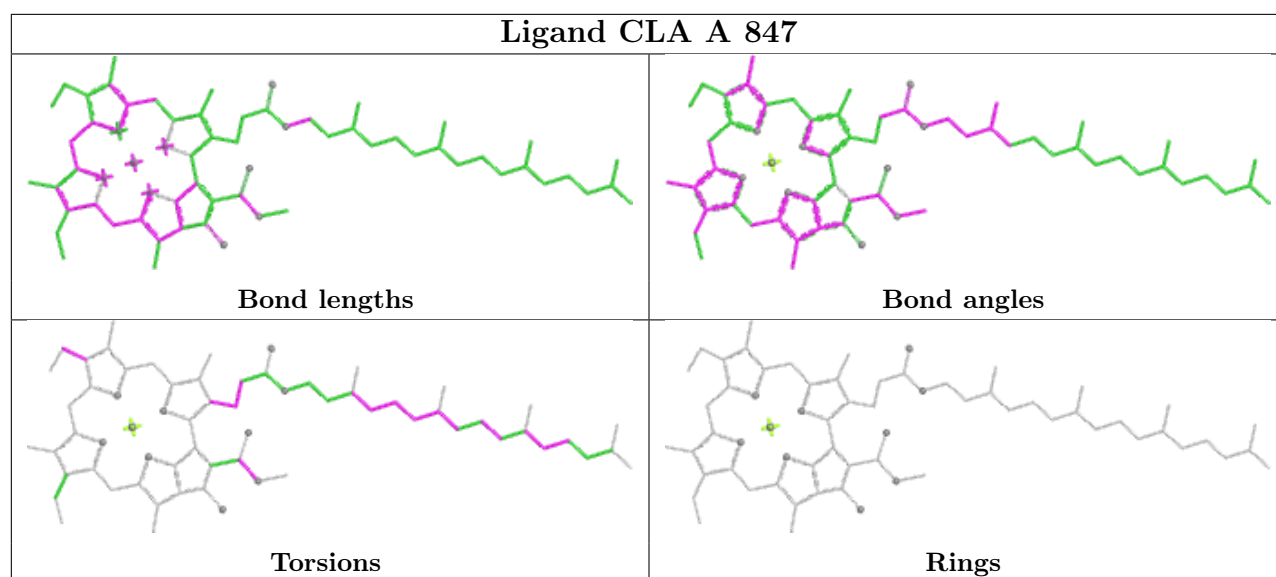


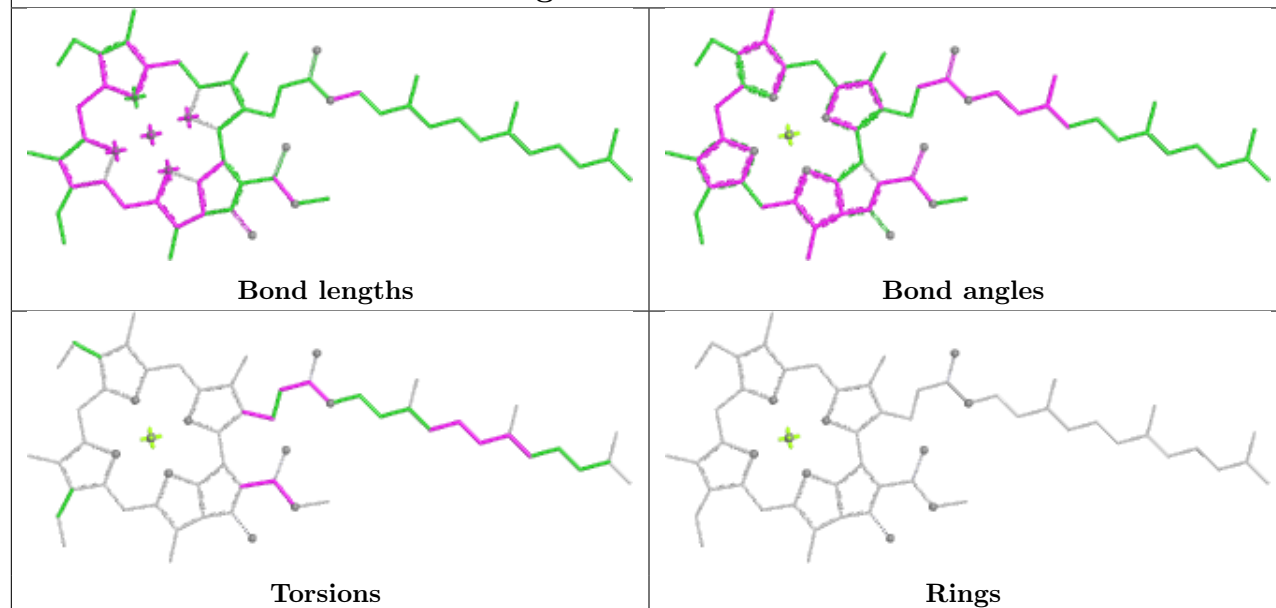
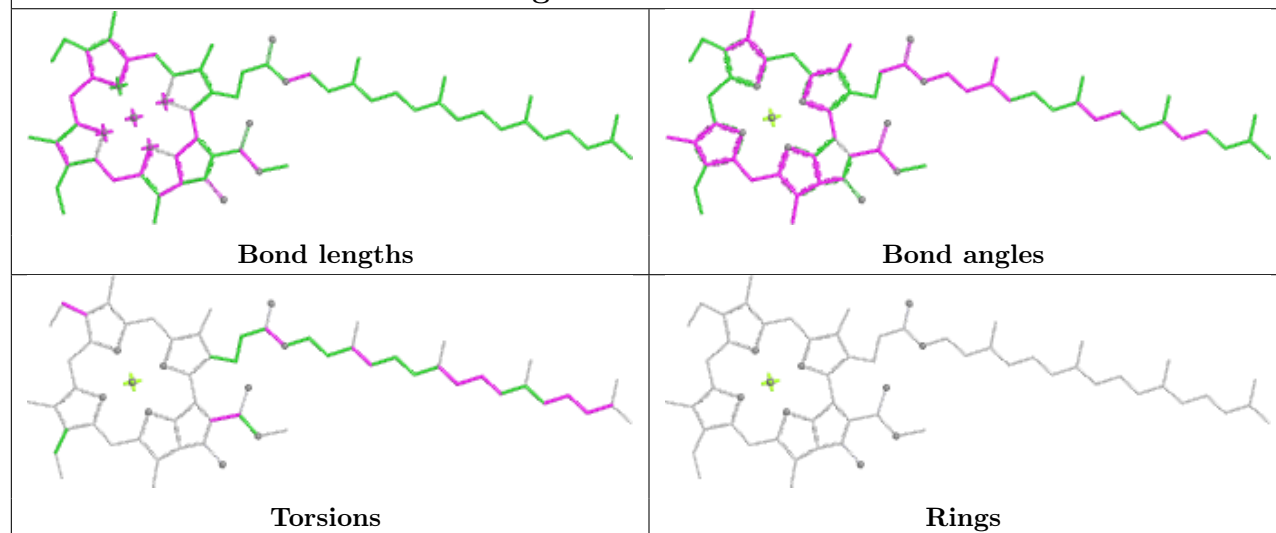
Rings

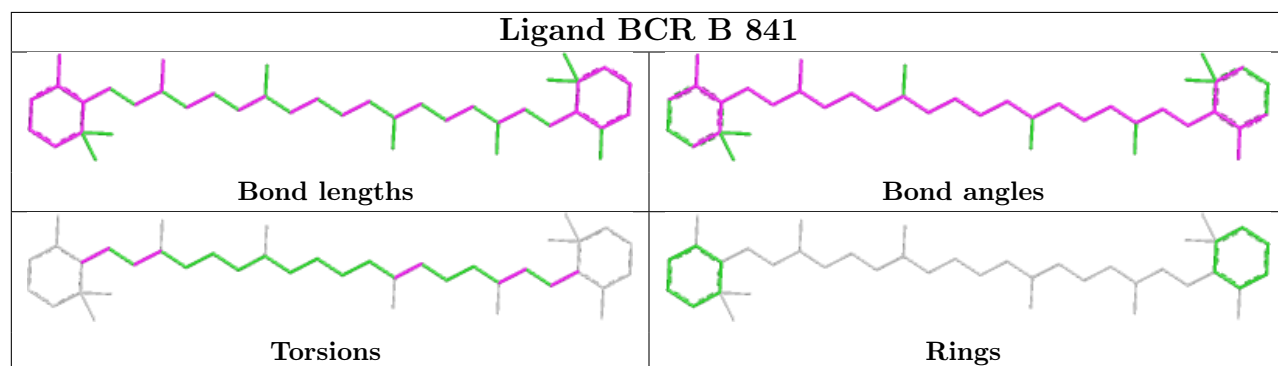
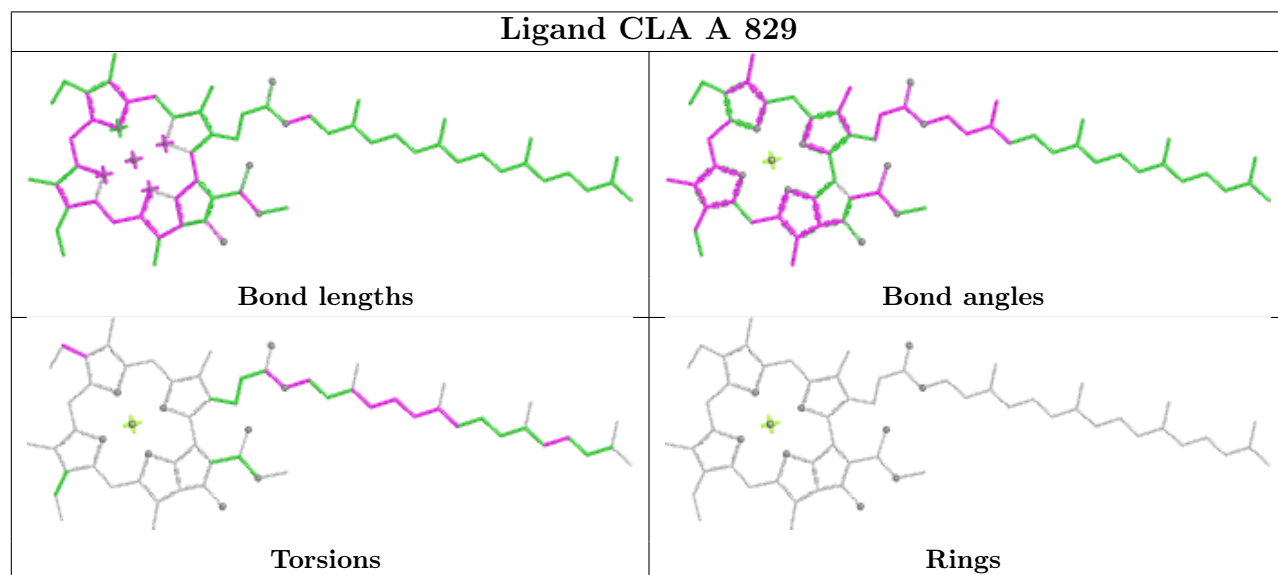
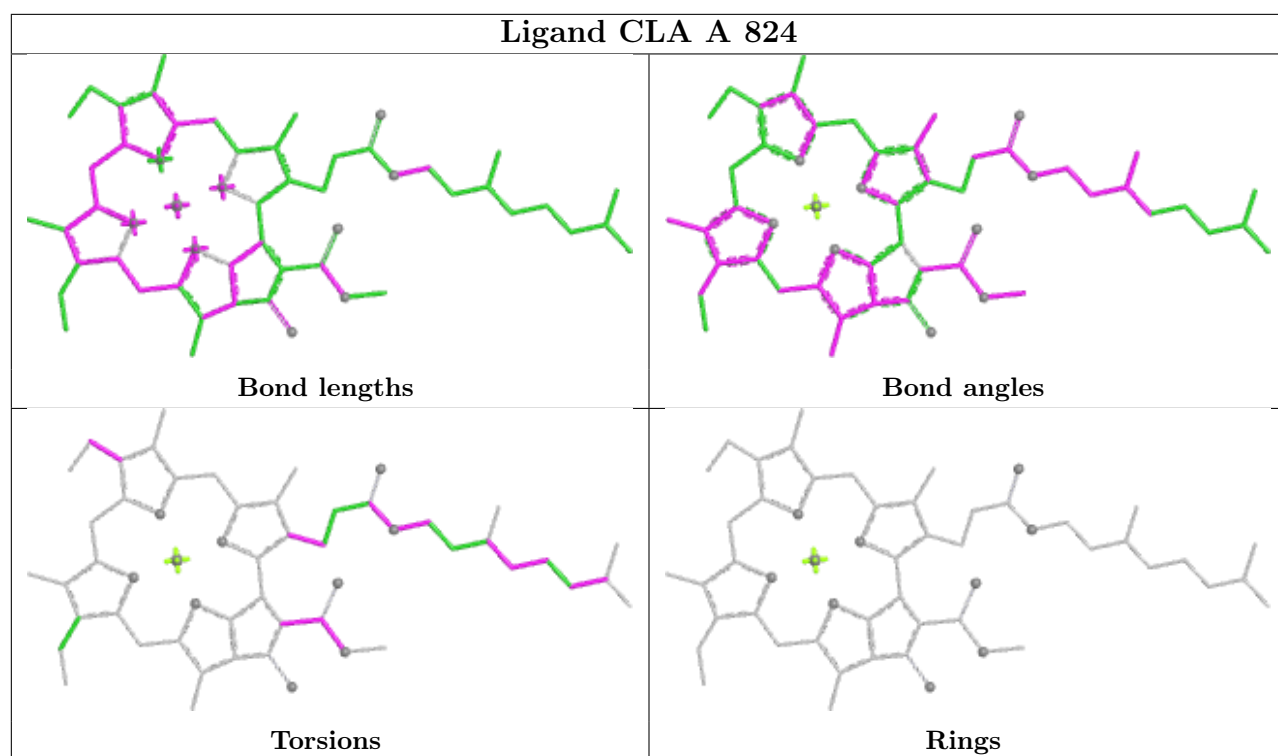


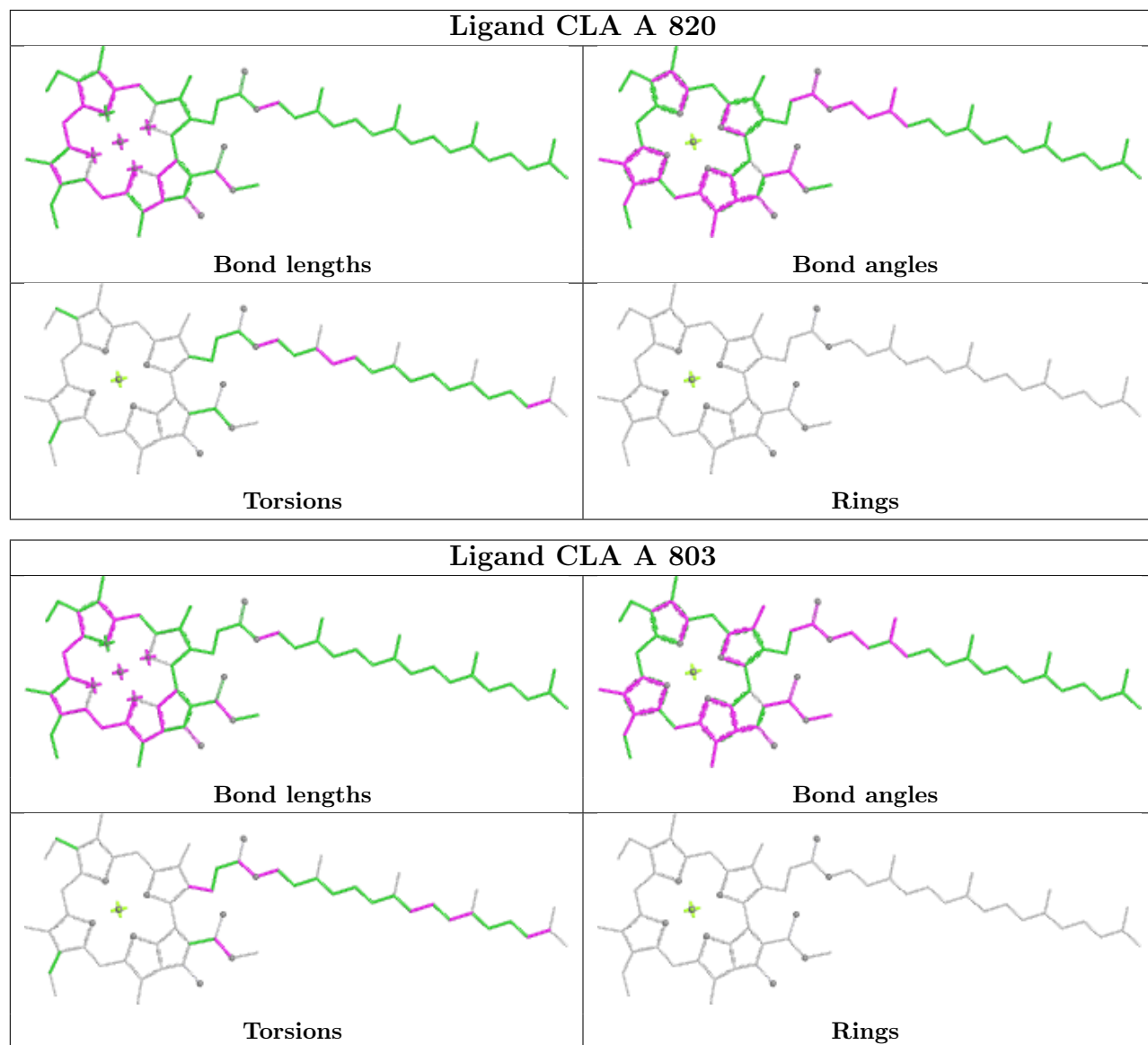
Ligand CLA K 4004**Ligand CLA B 813**

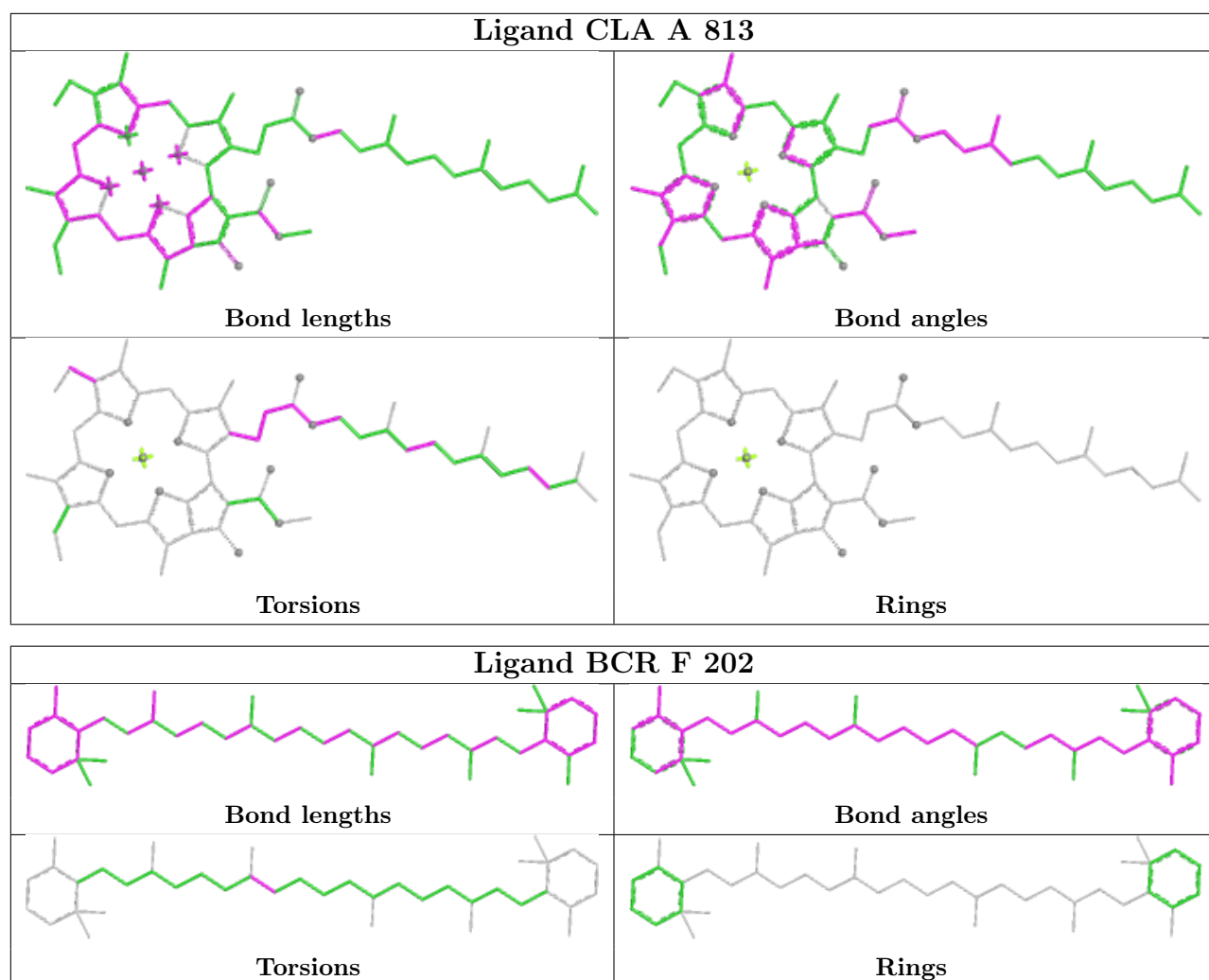


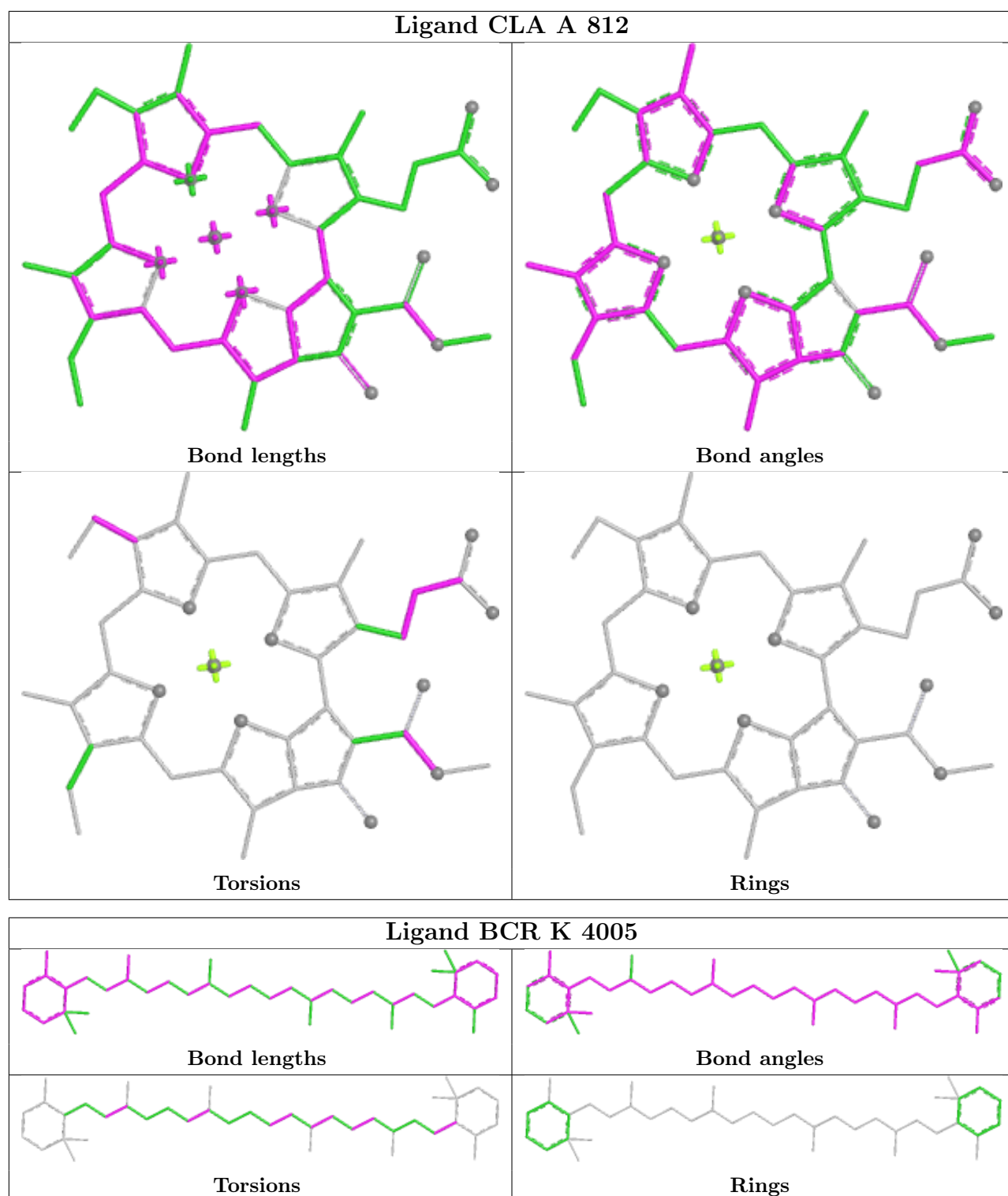


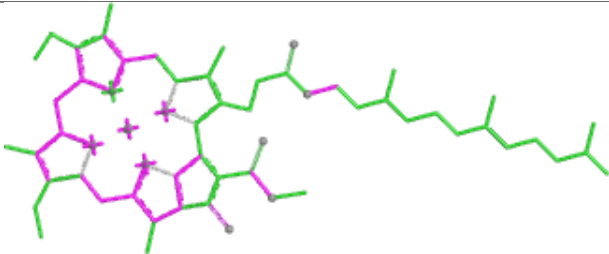
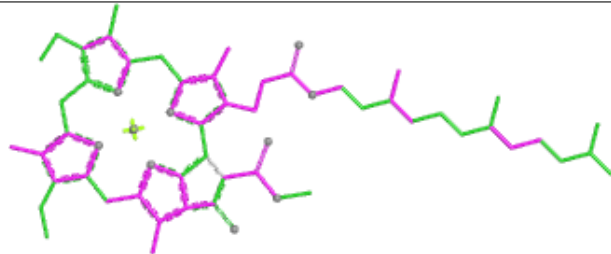
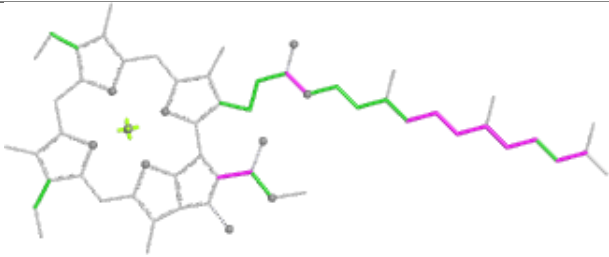
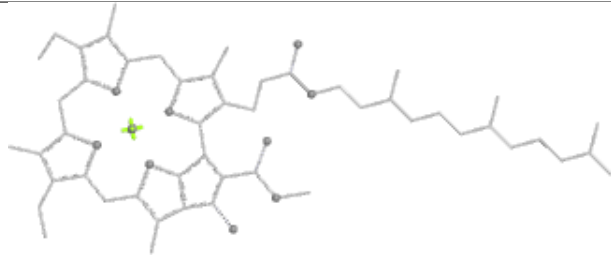
Ligand CLA J 101**Ligand CLA B 818**

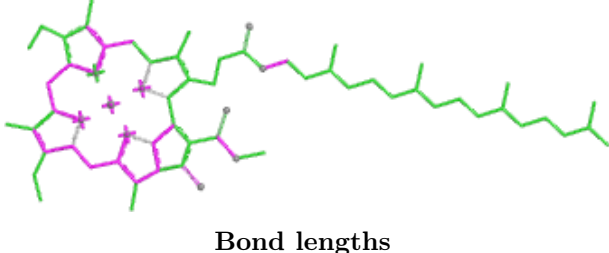
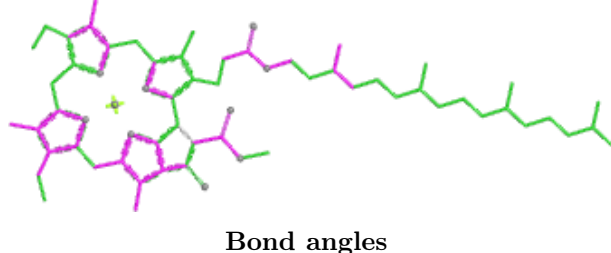
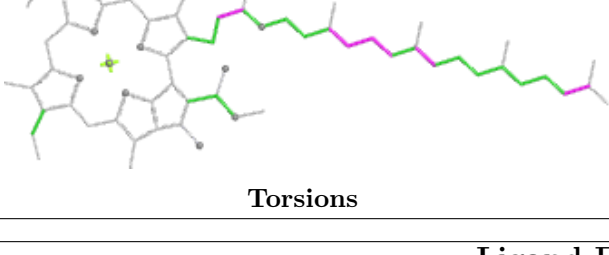
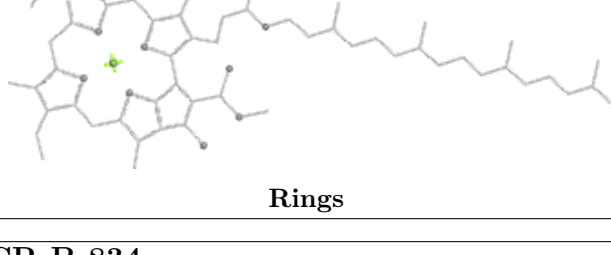


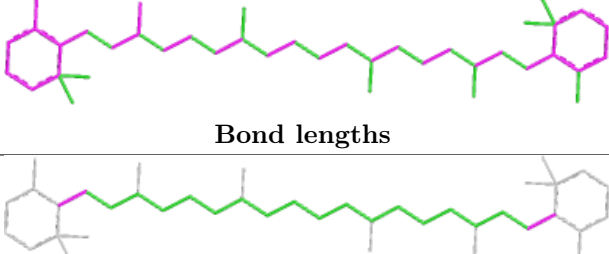
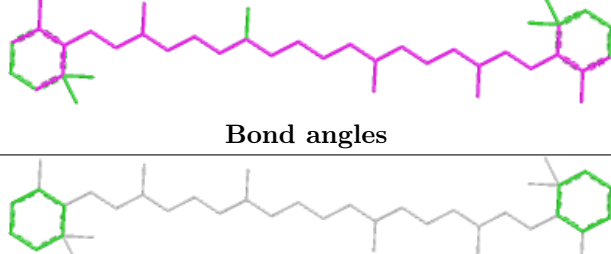


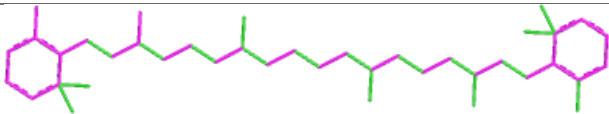
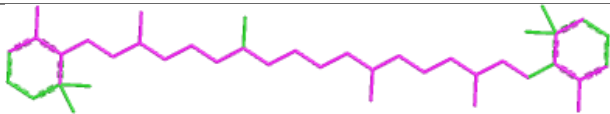
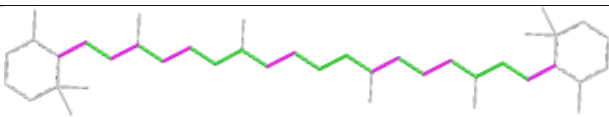
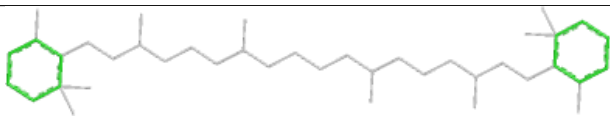


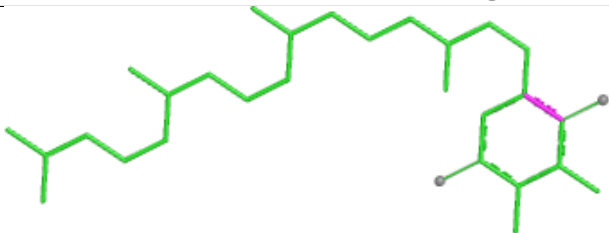
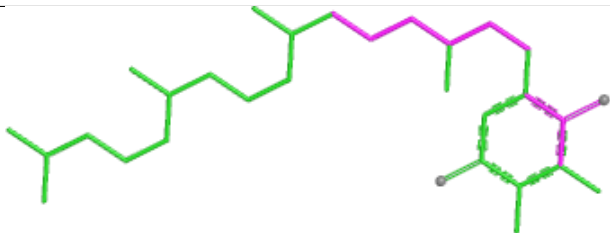
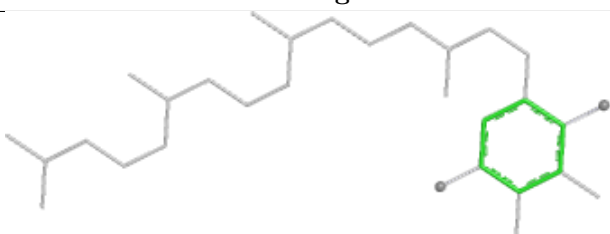


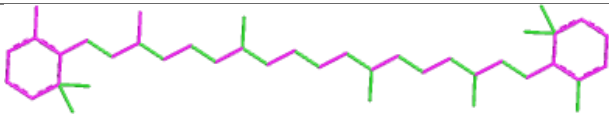
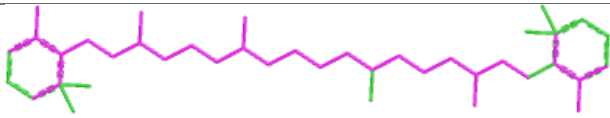
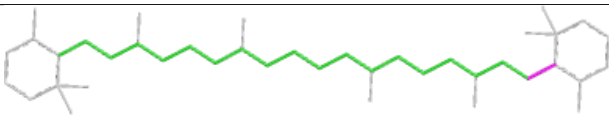
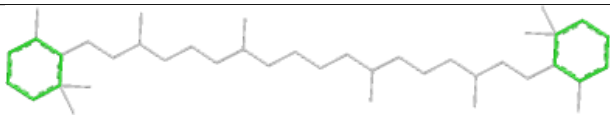
Ligand CLA A 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

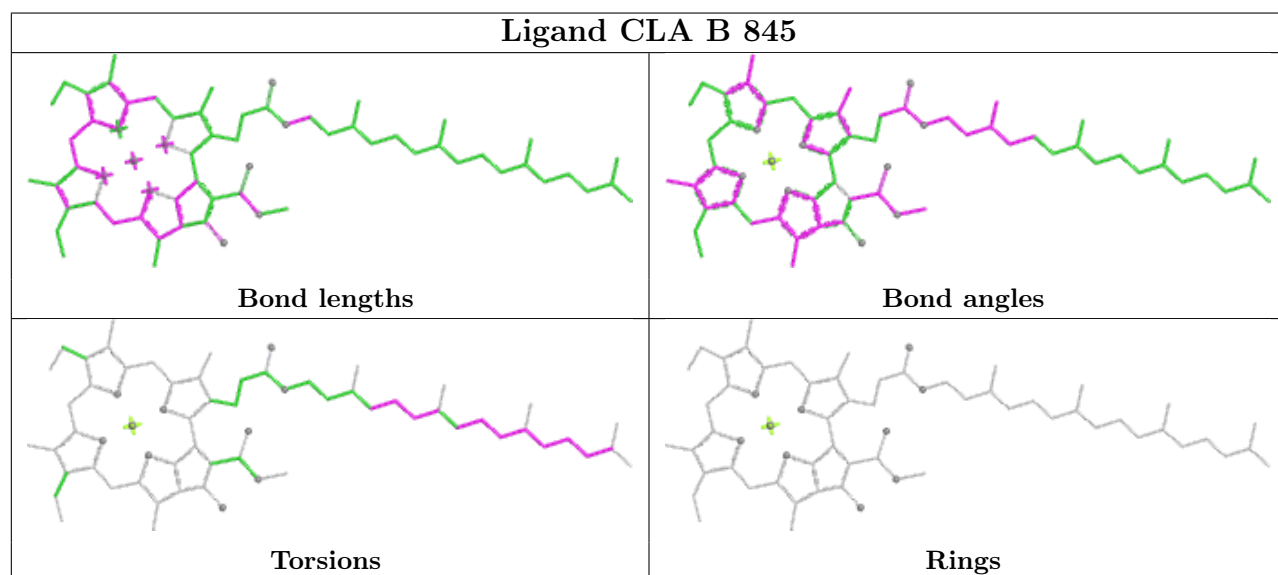
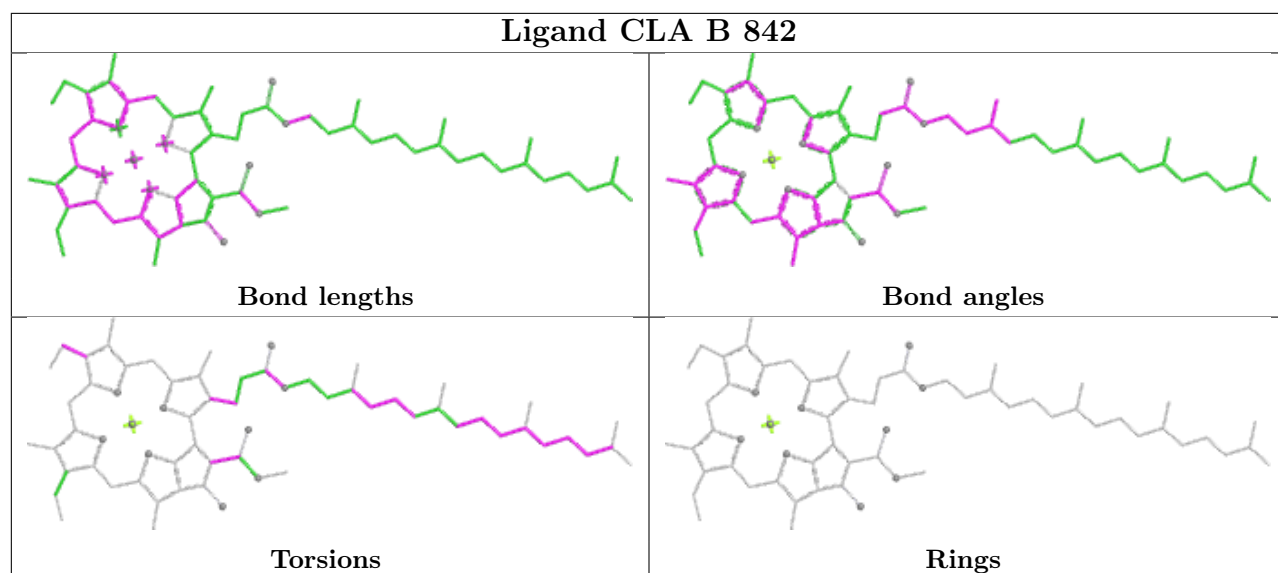
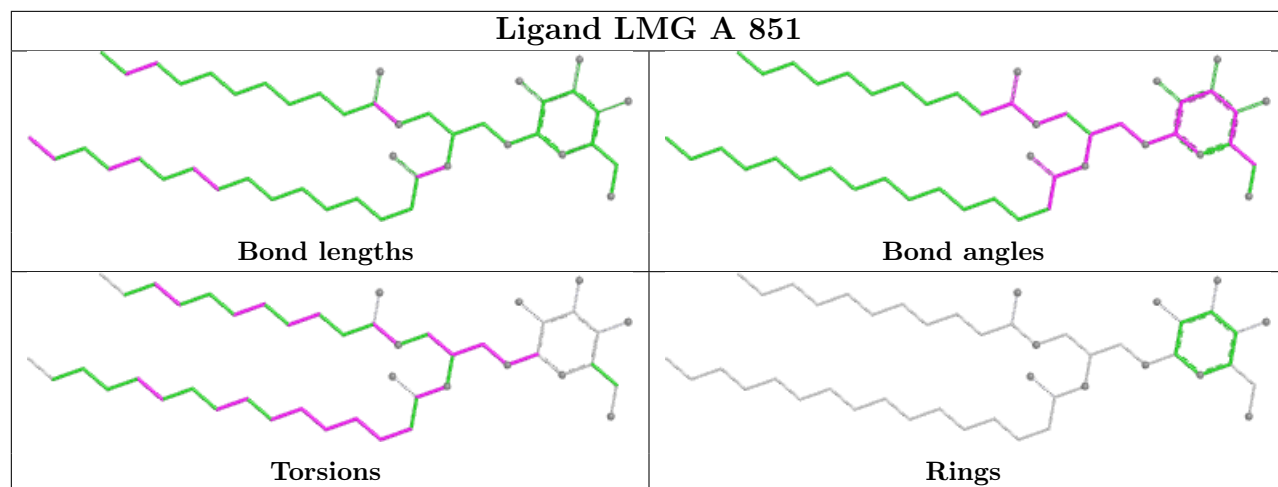
Ligand CLA B 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

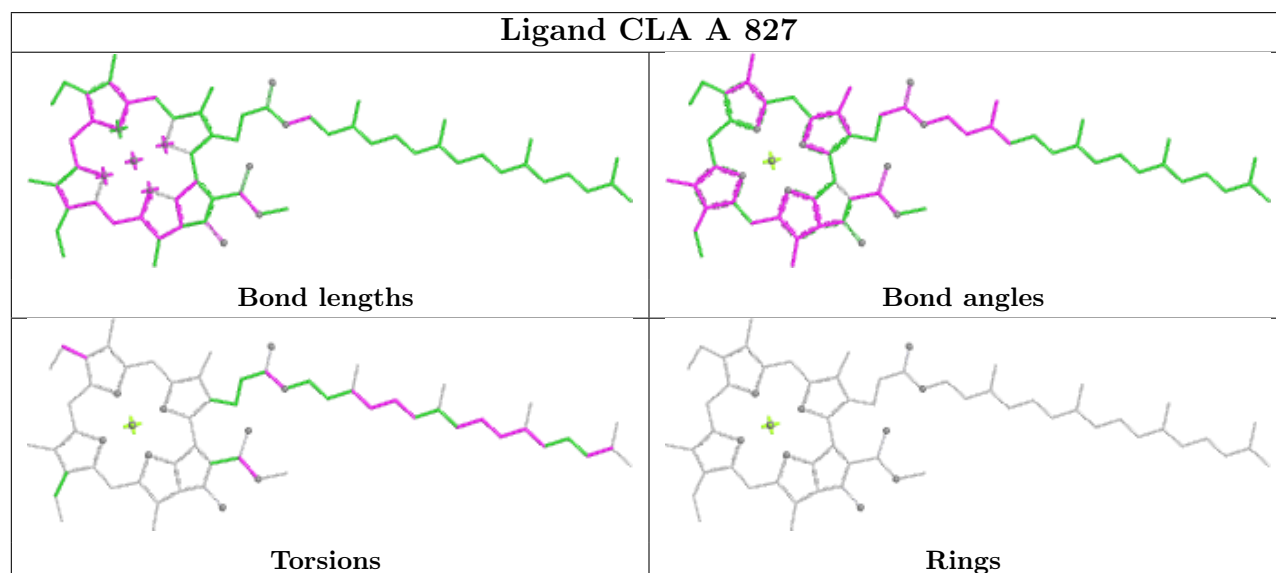
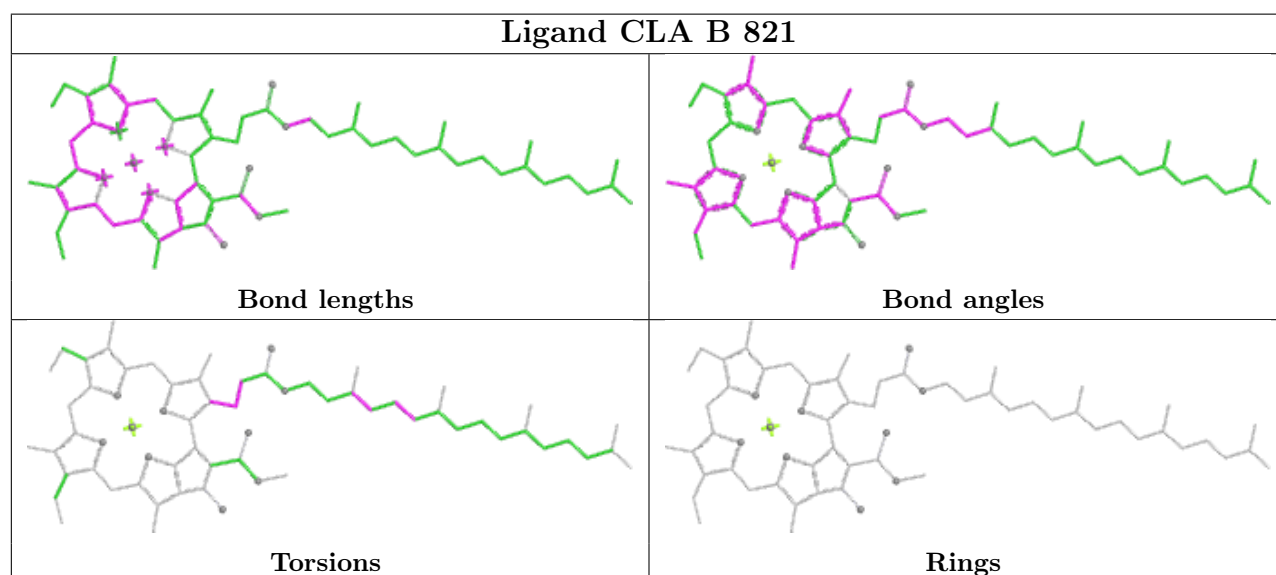
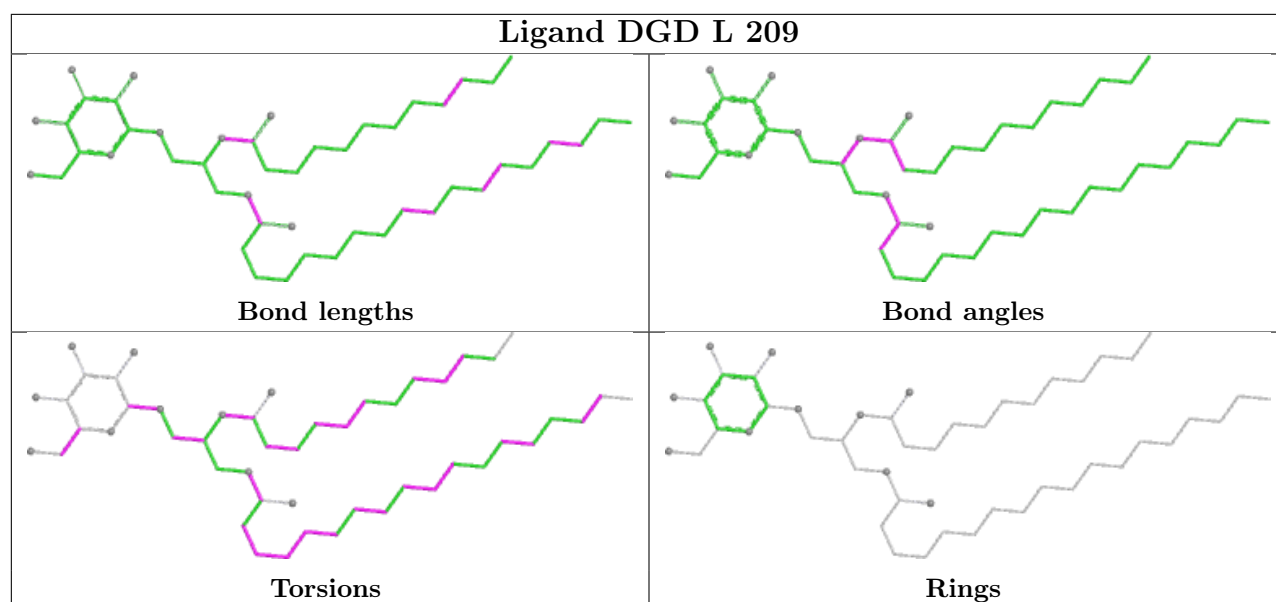
Ligand BCR B 834	
	
Bond lengths	Bond angles
Torsions	Rings

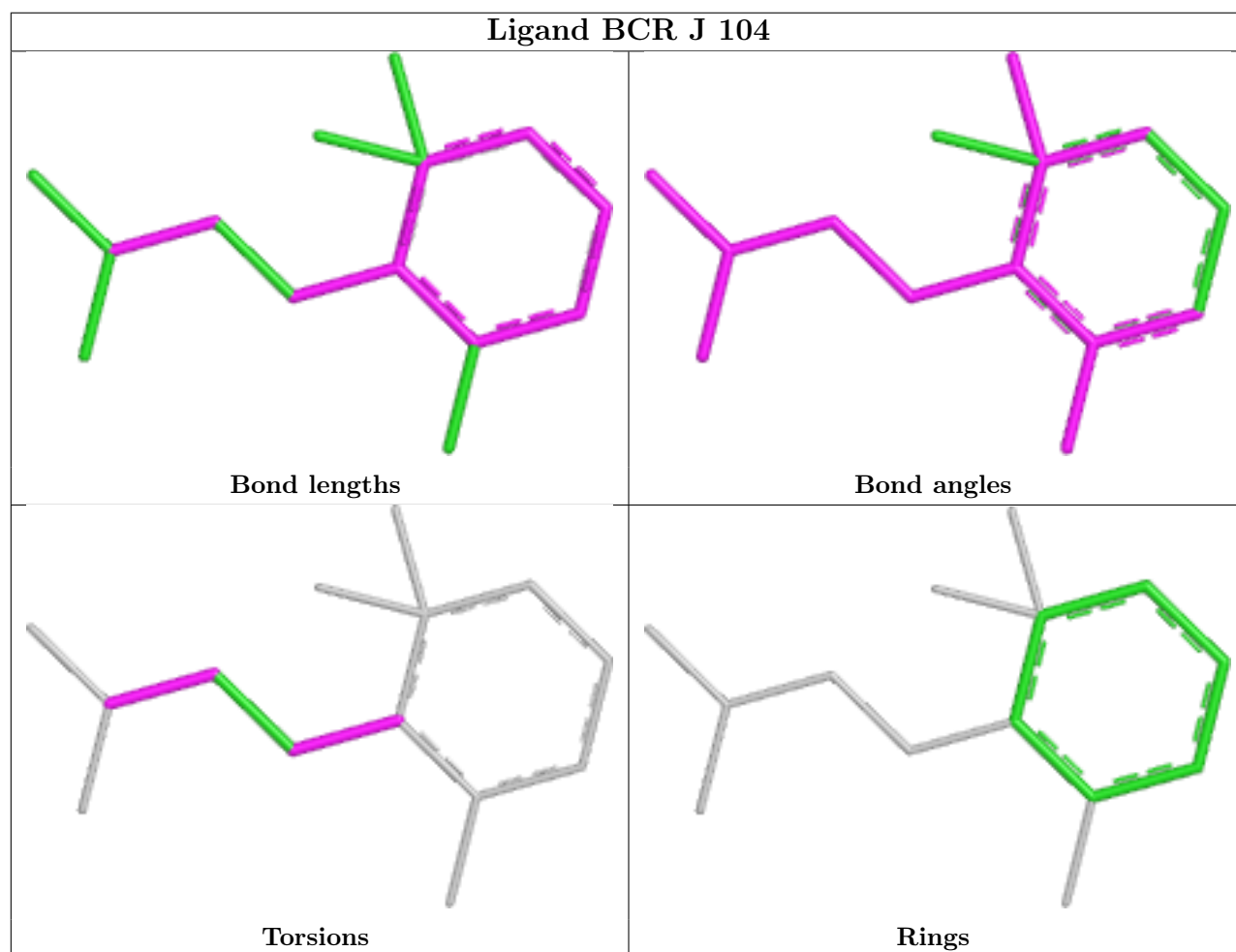
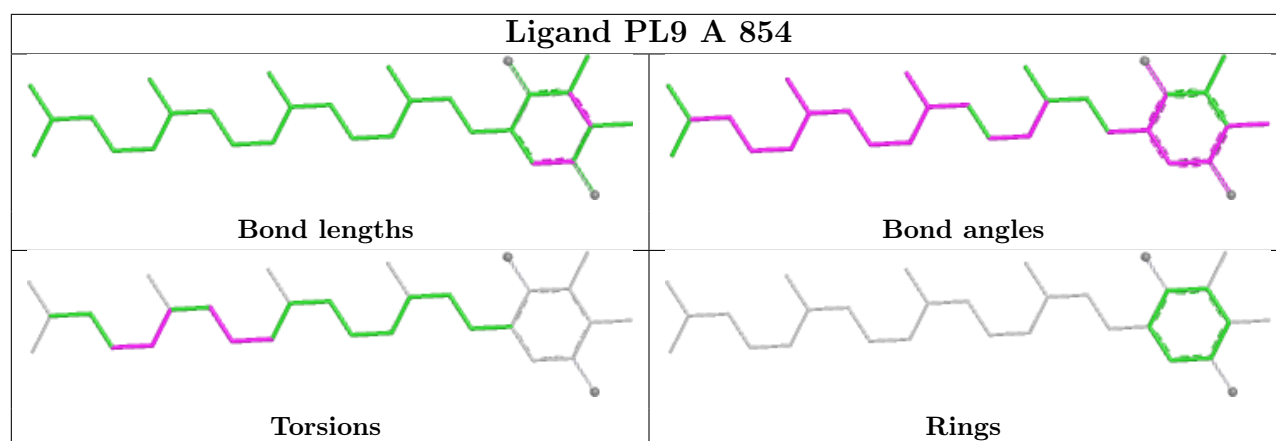
Ligand BCR J 107	
	
Bond lengths	Bond angles
	
Torsions	Rings

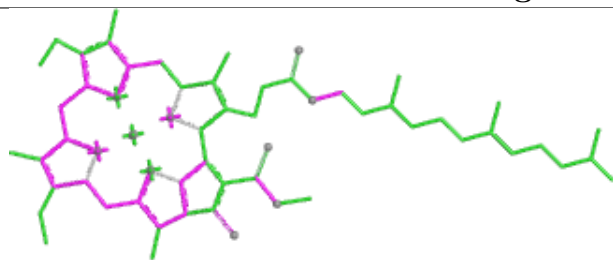
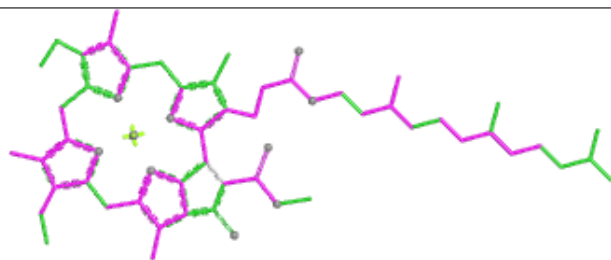
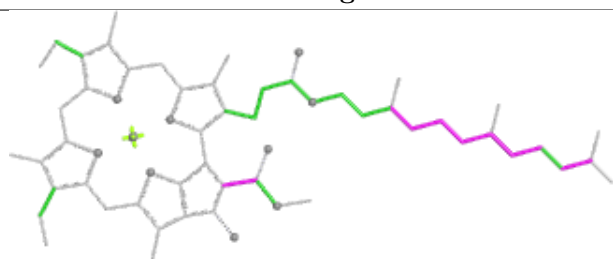
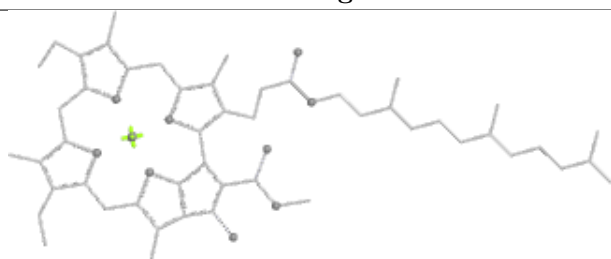
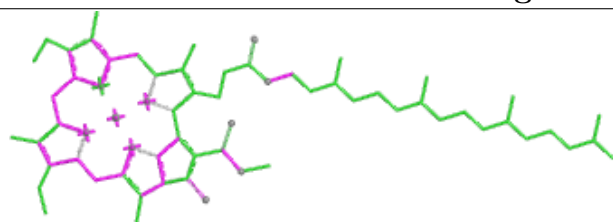
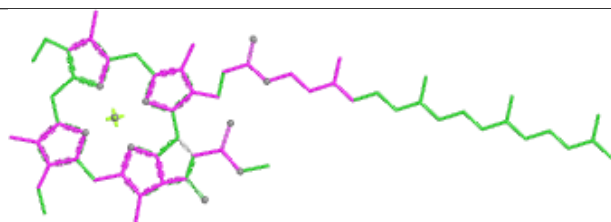
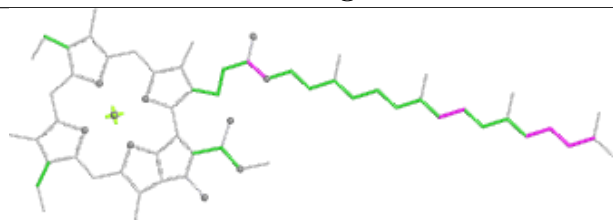
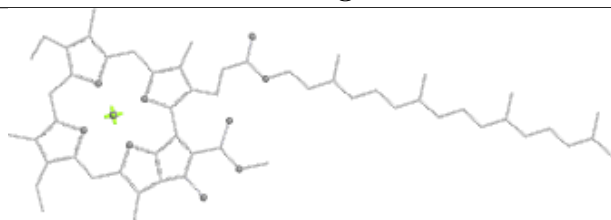
Ligand A1AGD B 831	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 836	
	
Bond lengths	Bond angles
	
Torsions	Rings

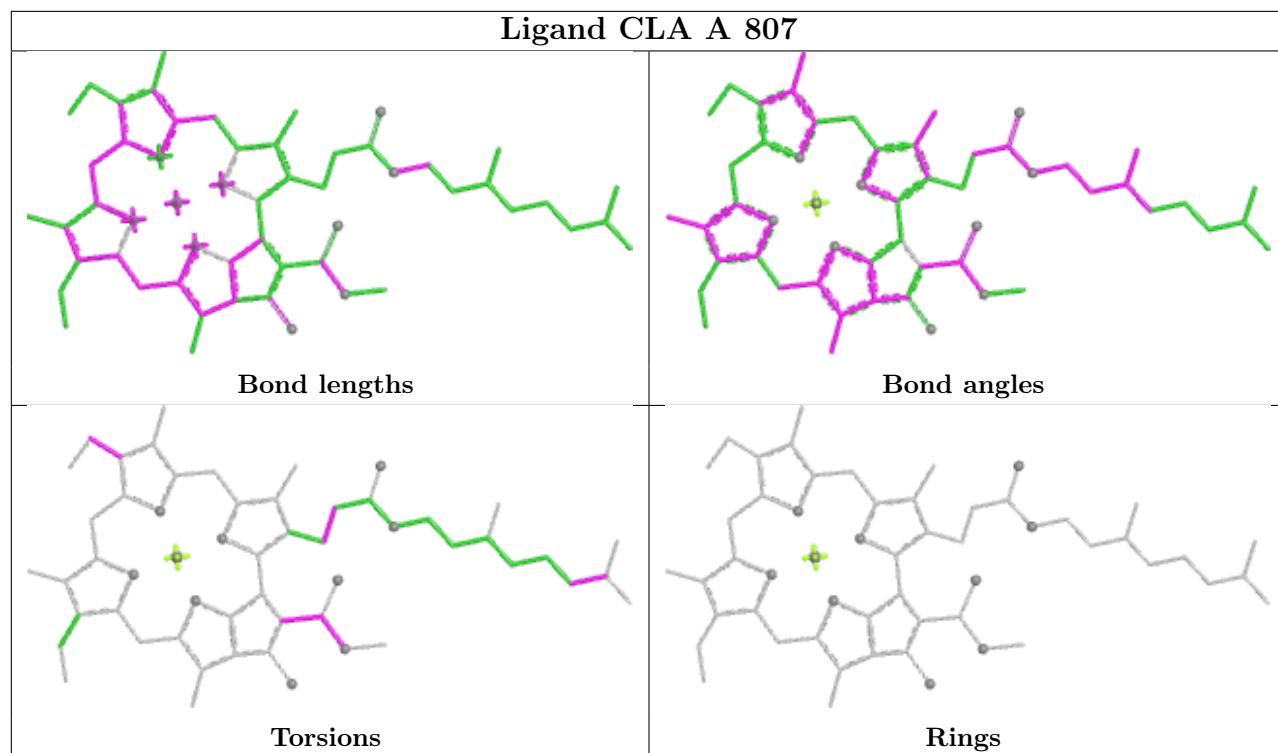




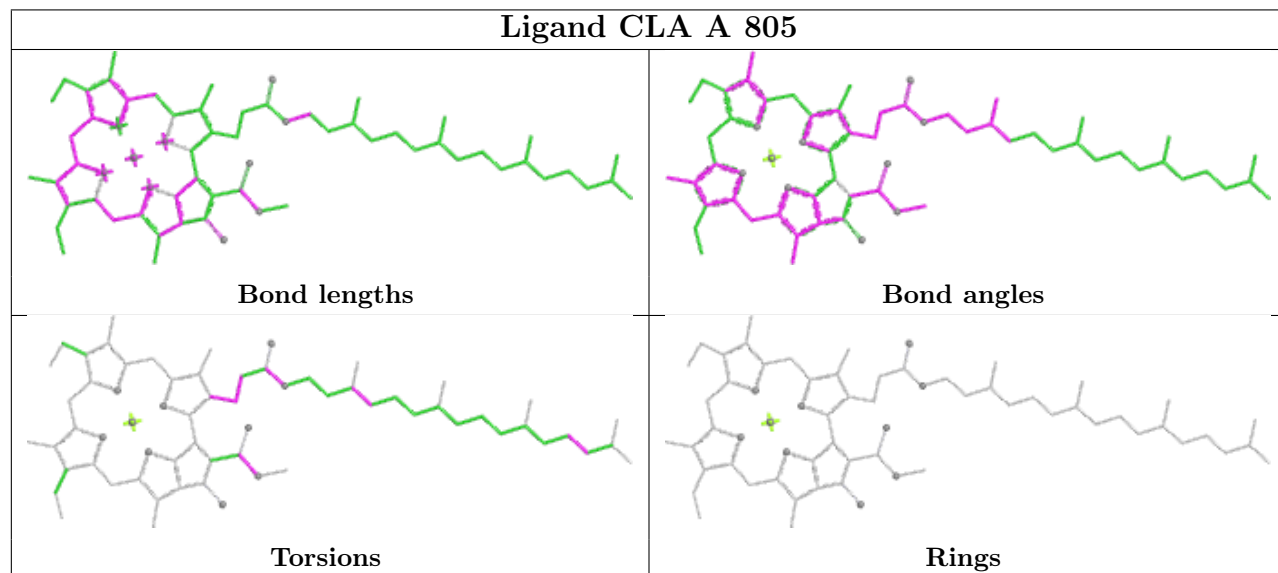


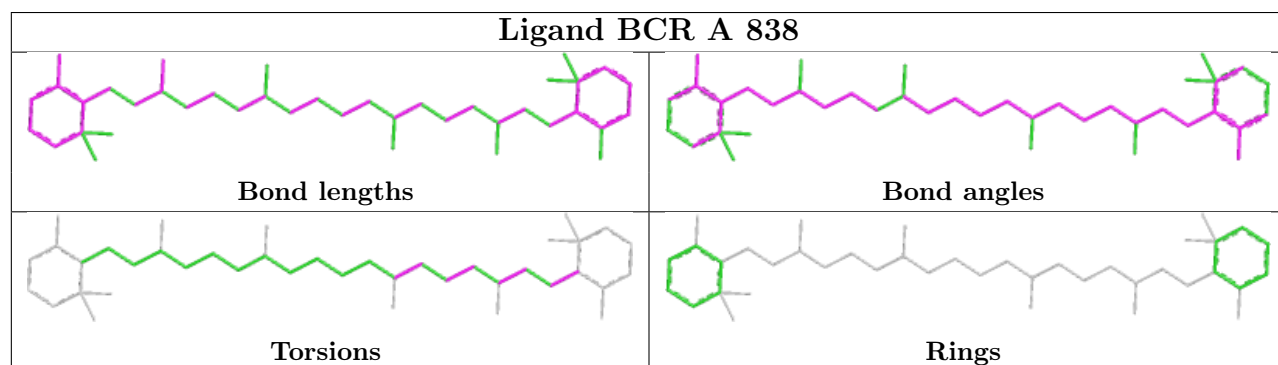
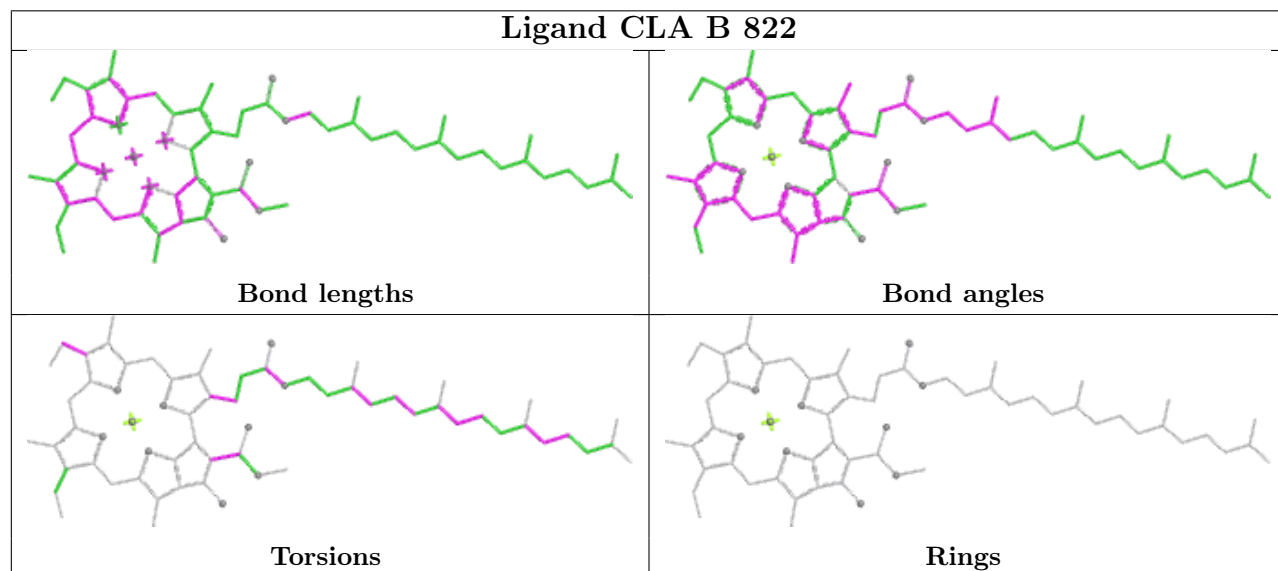
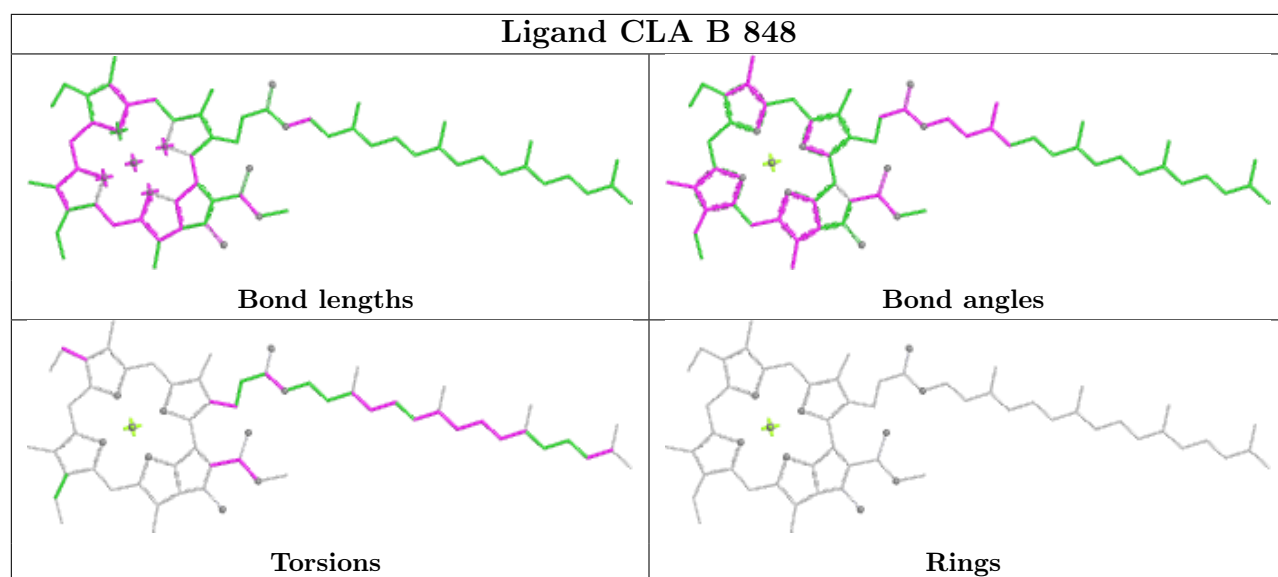
Ligand CLA B 844**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 801****Bond lengths****Bond angles****Torsions****Rings**

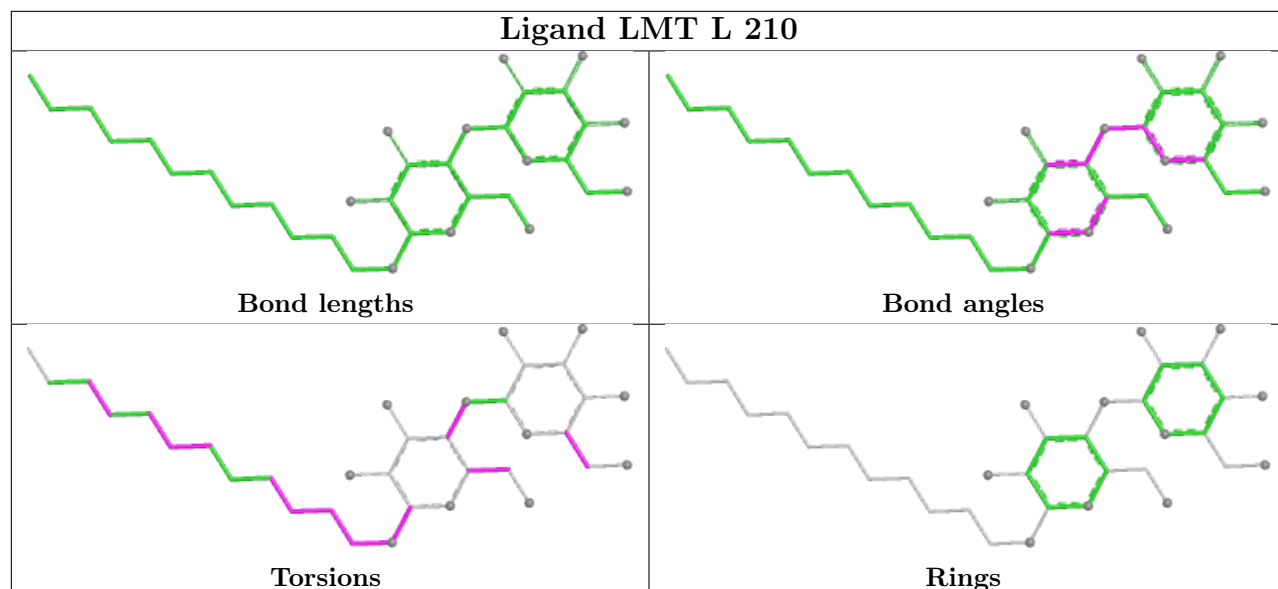
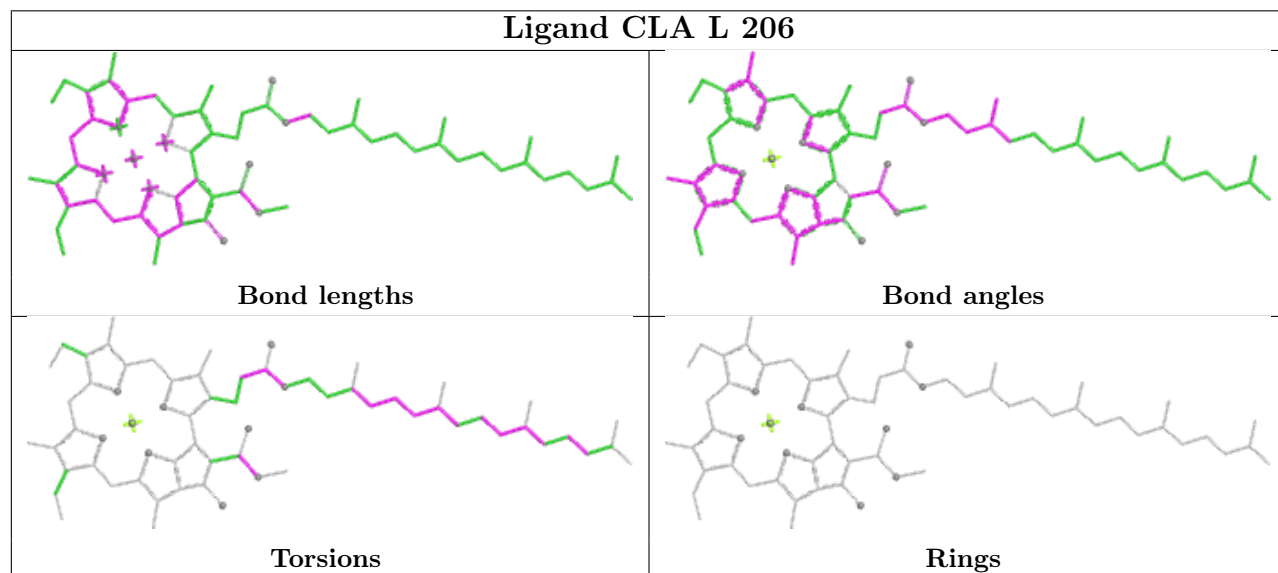
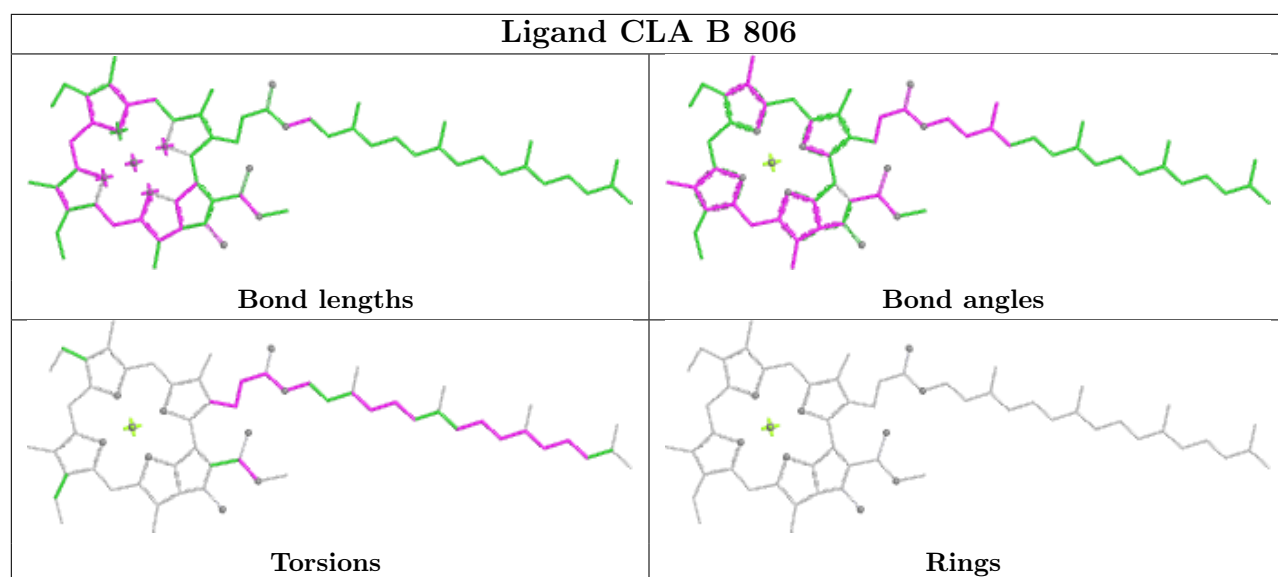
Ligand CLA A 807

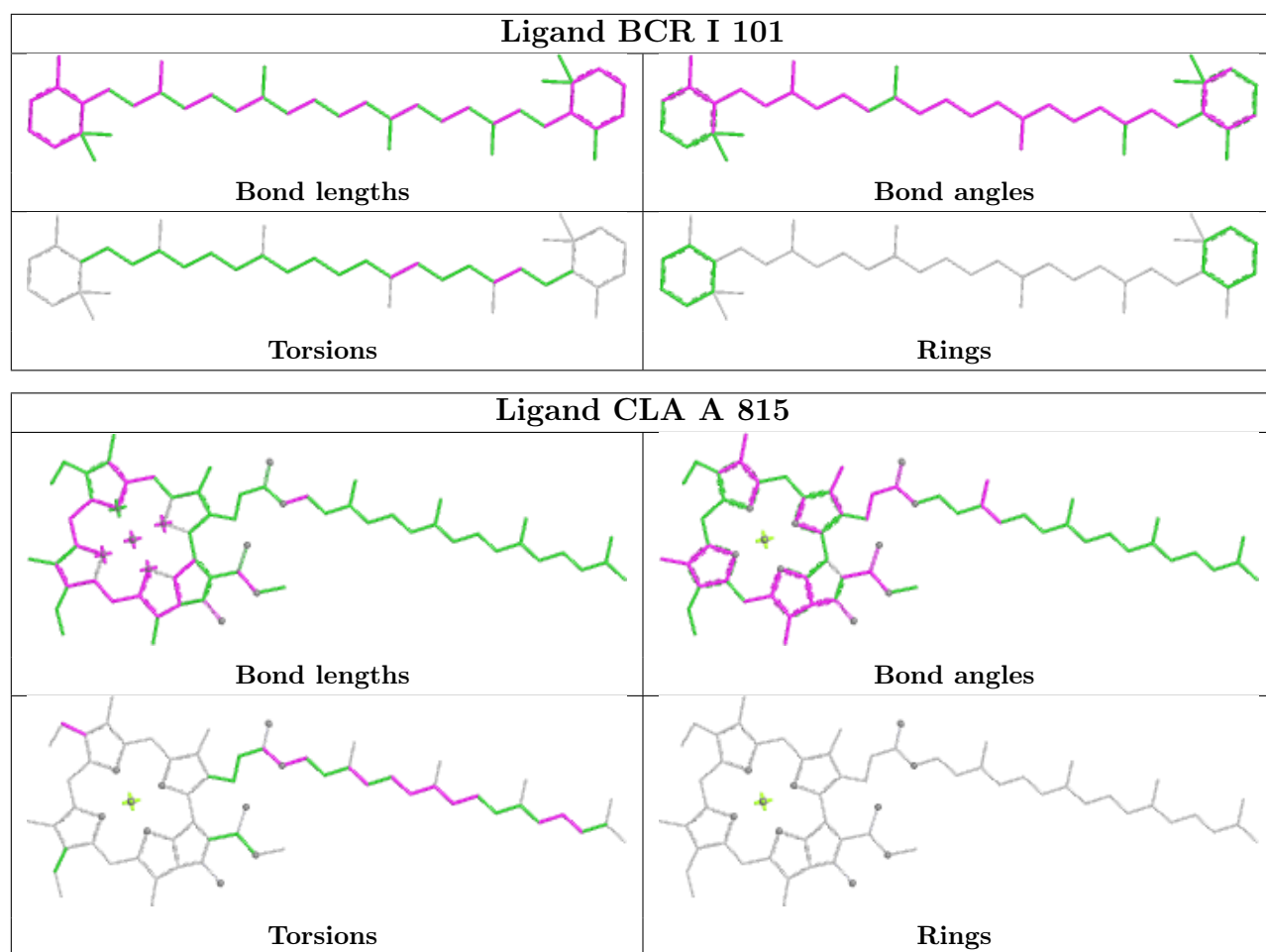


Ligand CLA A 805

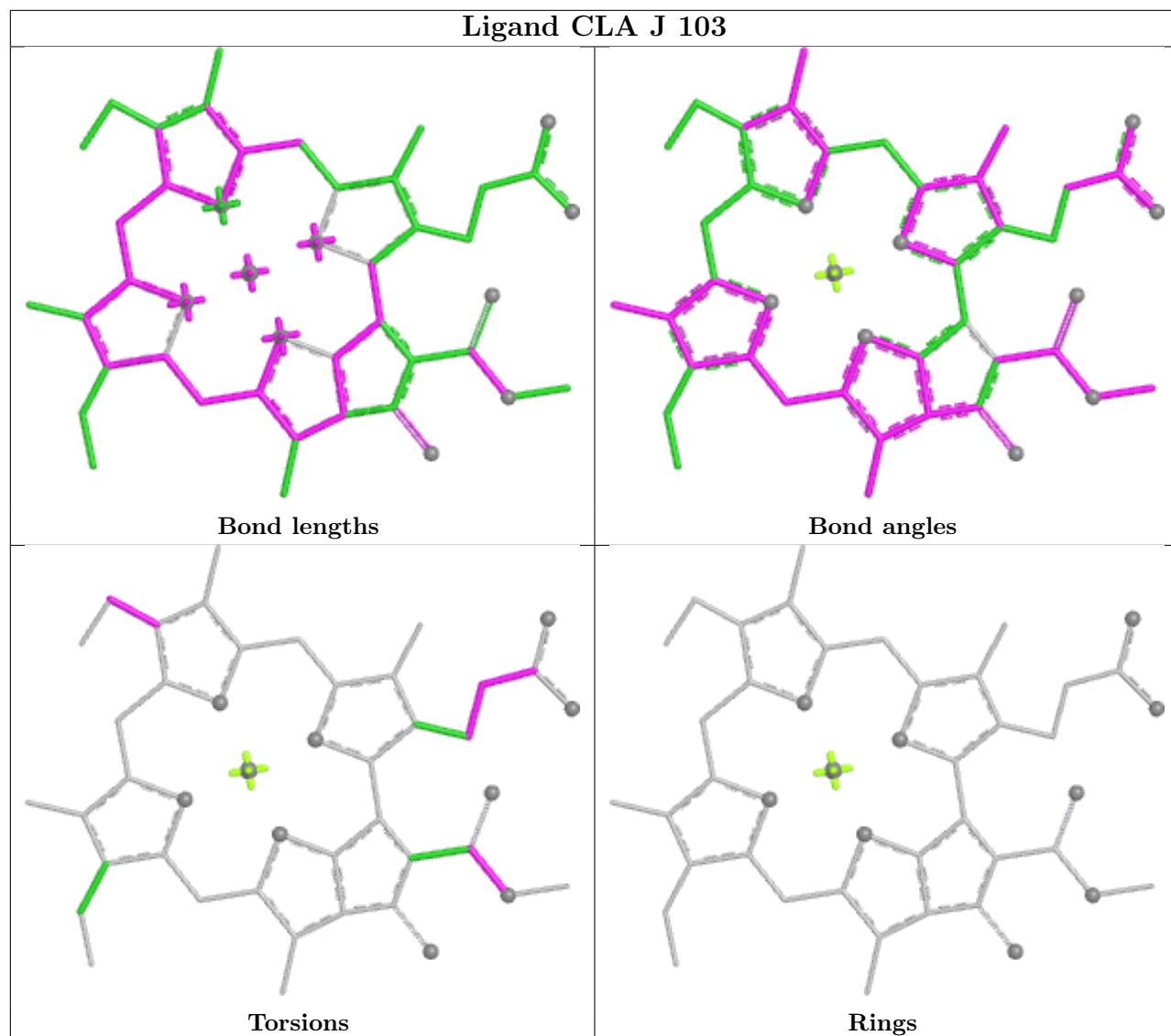




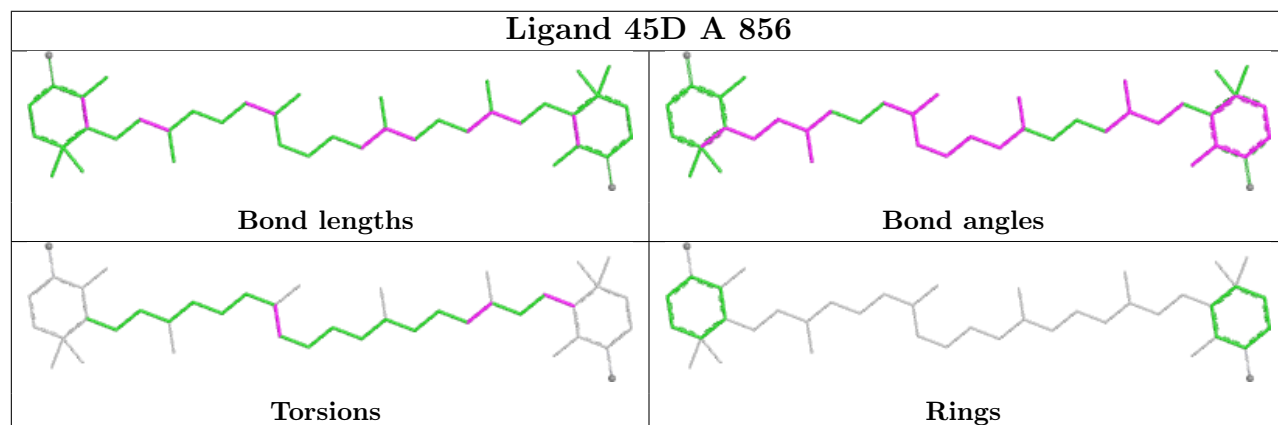


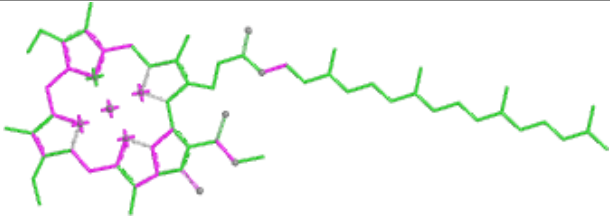
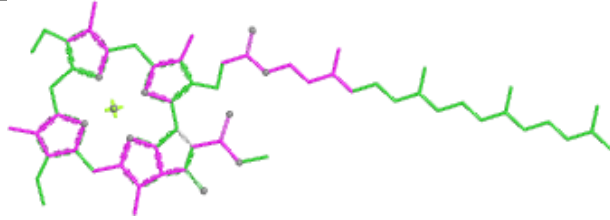
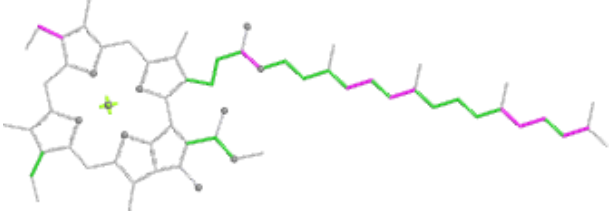
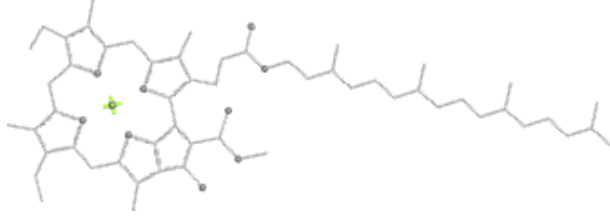


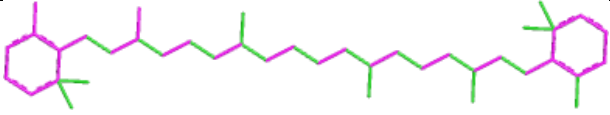
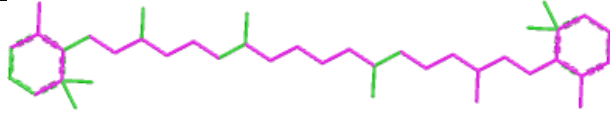
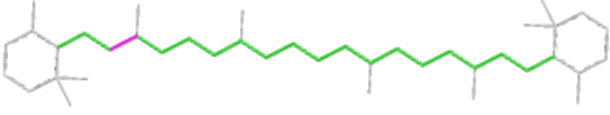
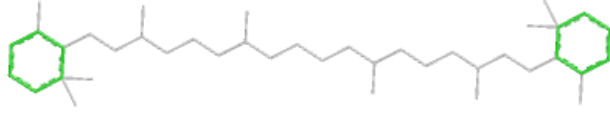
Ligand CLA J 103

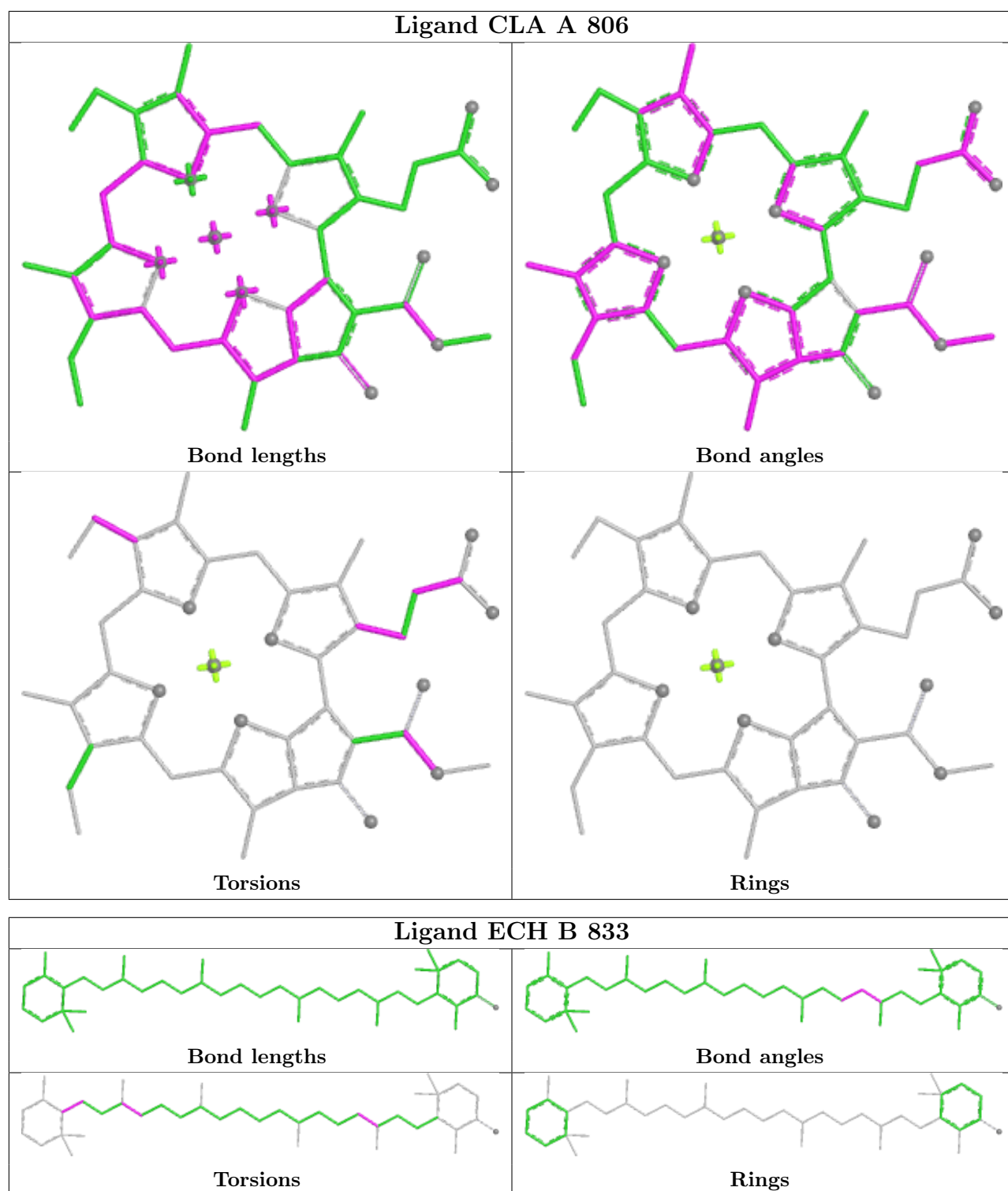


Ligand 45D A 856



Ligand CLA L 205			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand BCR L 208			
			
Bond lengths	Bond angles		
			
Torsions	Rings		



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

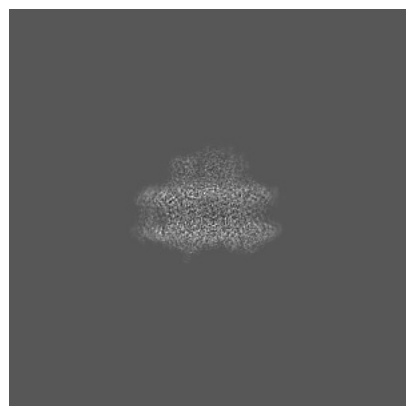
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73077. These allow visual inspection of the internal detail of the map and identification of artifacts.

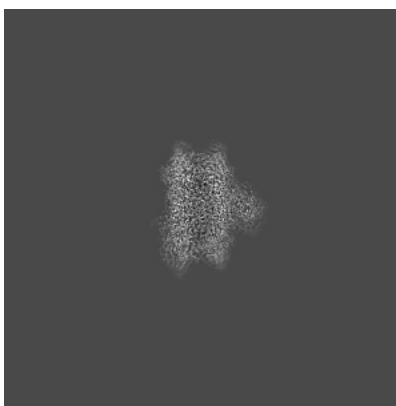
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

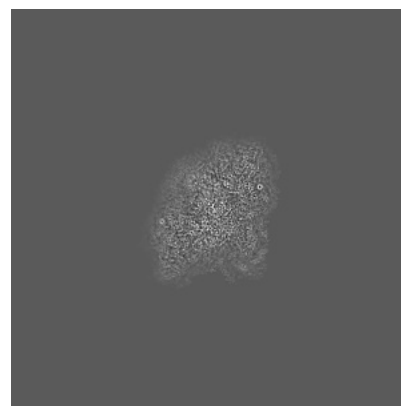
6.1.1 Primary map



X

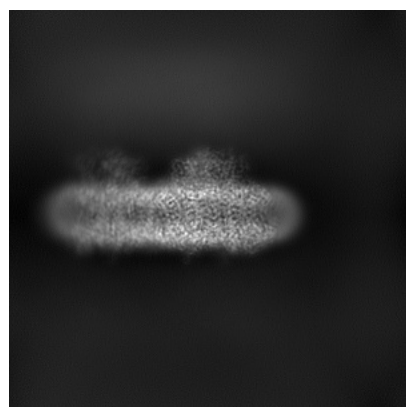


Y

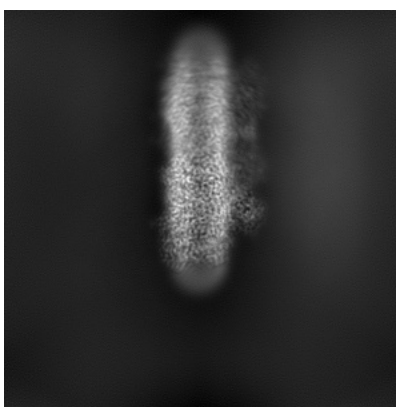


Z

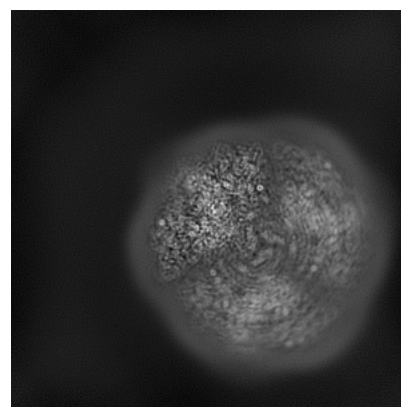
6.1.2 Raw map



X



Y

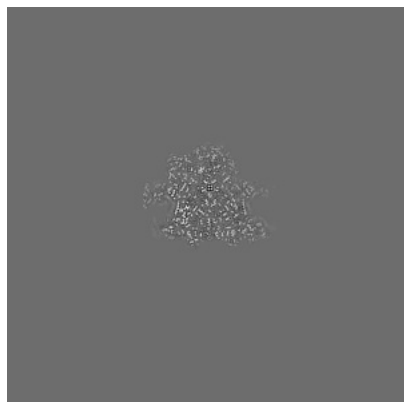


Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

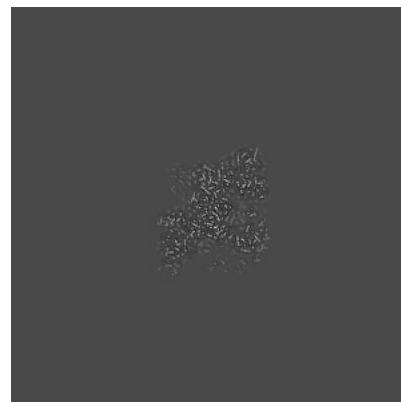
6.2.1 Primary map



X Index: 210

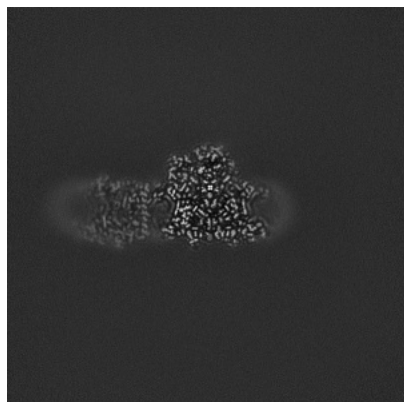


Y Index: 210

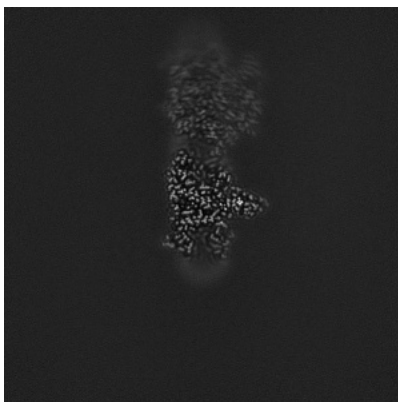


Z Index: 210

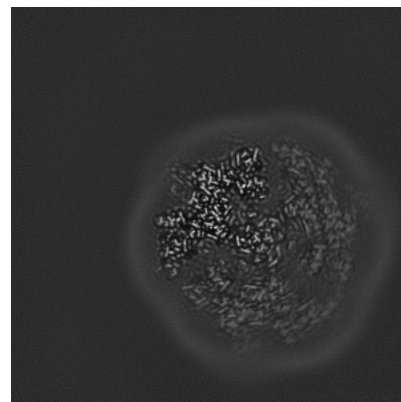
6.2.2 Raw map



X Index: 210



Y Index: 210

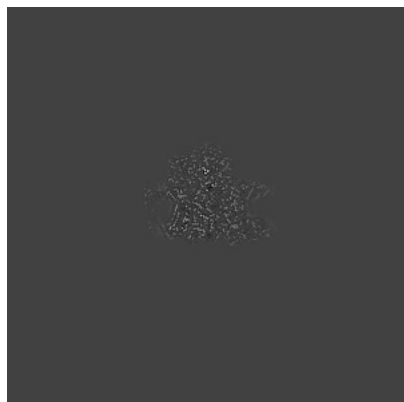


Z Index: 210

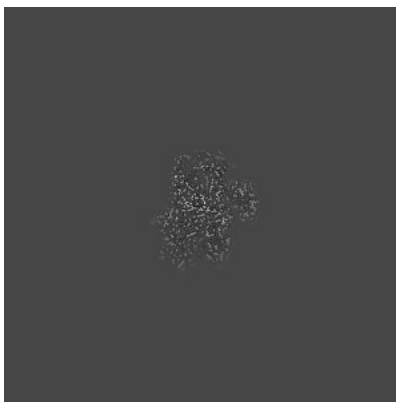
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 213

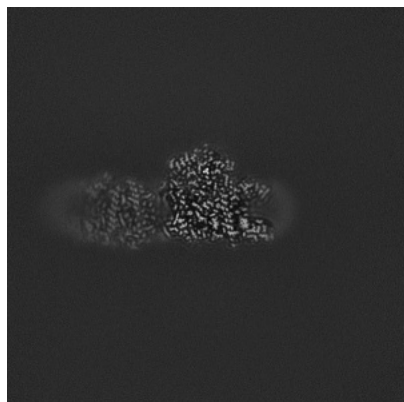


Y Index: 188

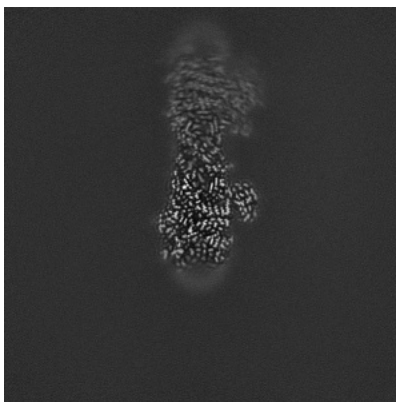


Z Index: 191

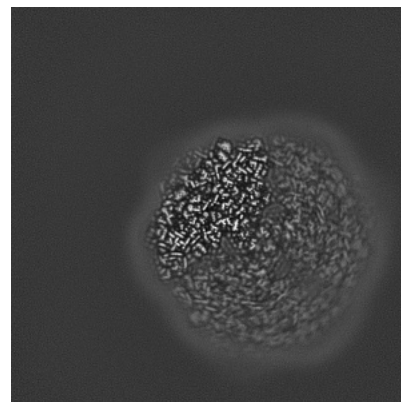
6.3.2 Raw map



X Index: 215



Y Index: 191

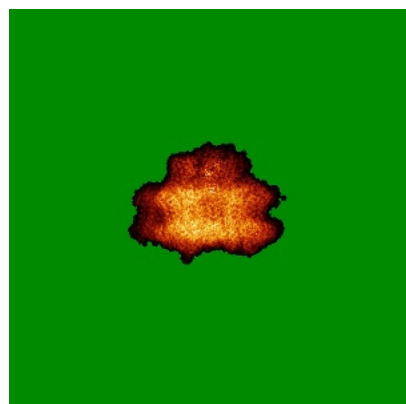


Z Index: 191

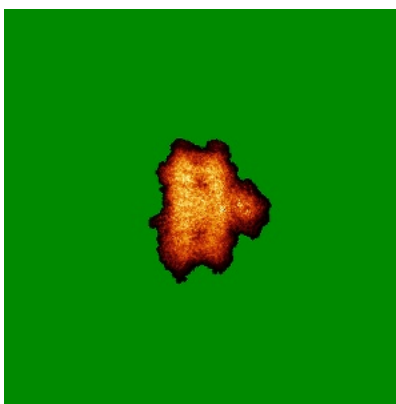
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

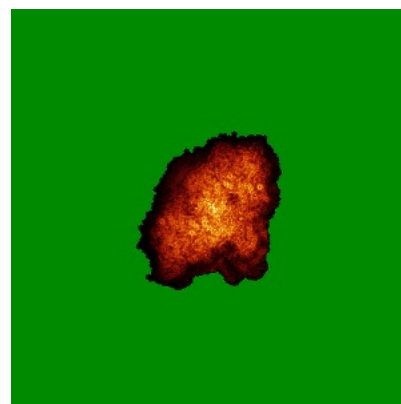
6.4.1 Primary map



X

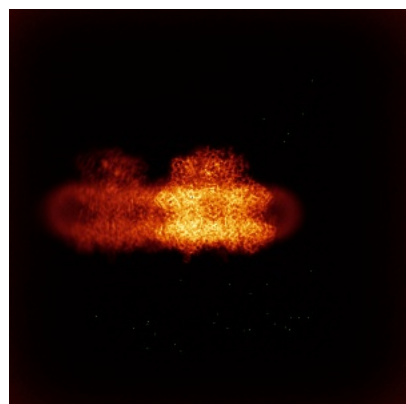


Y

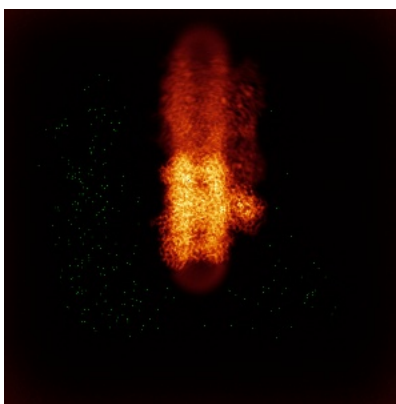


Z

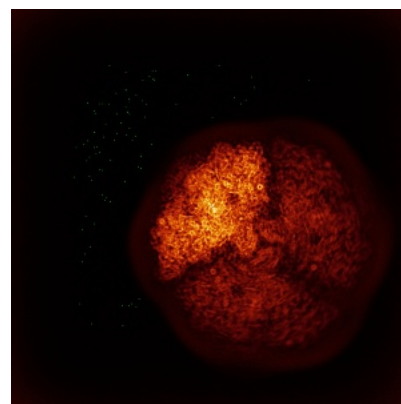
6.4.2 Raw map



X



Y

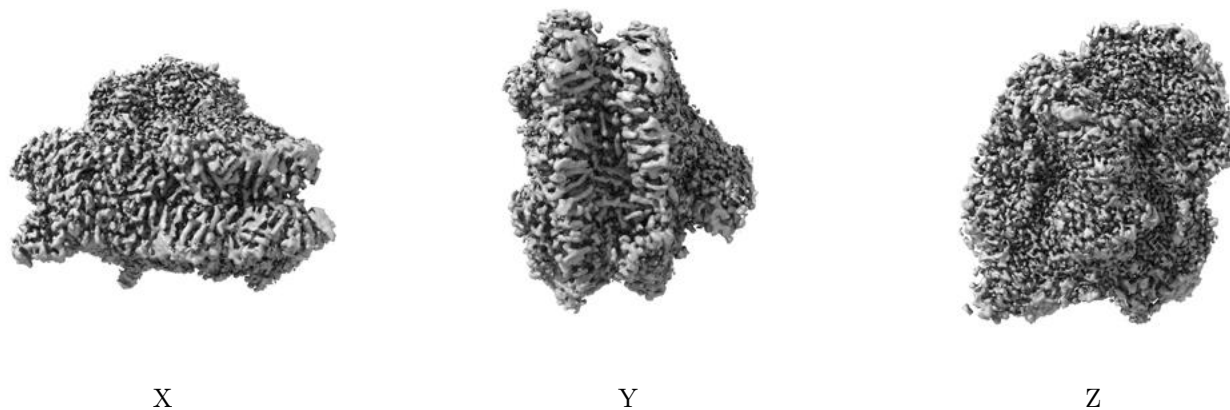


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

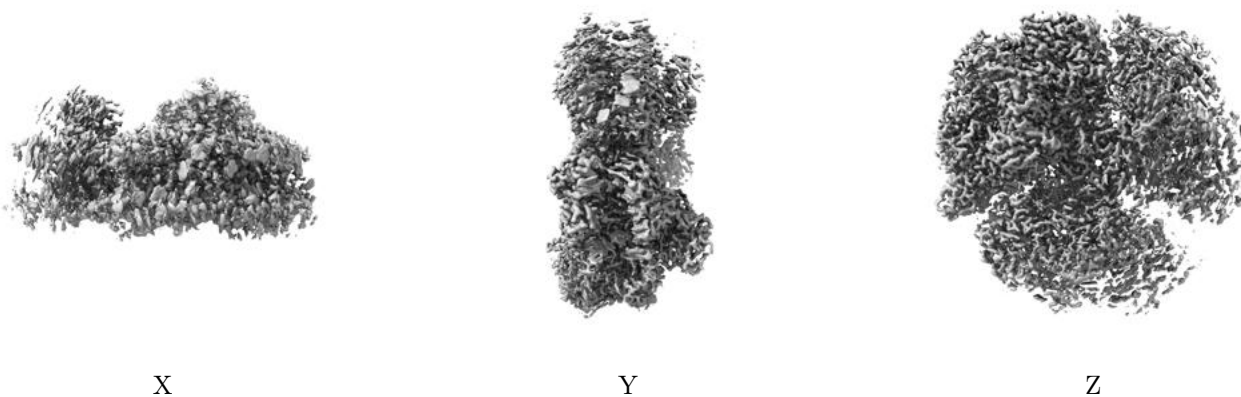
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0353. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

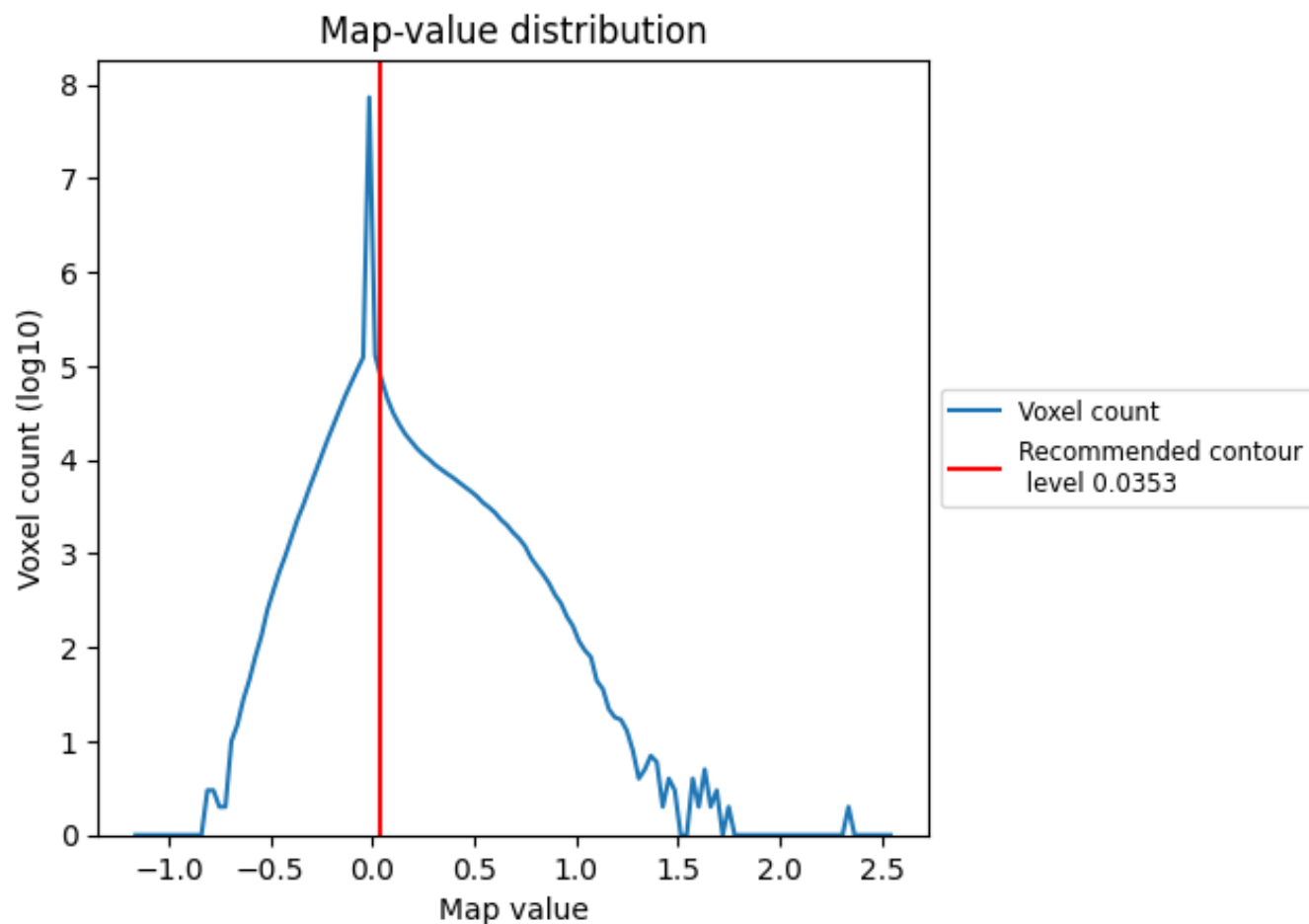
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

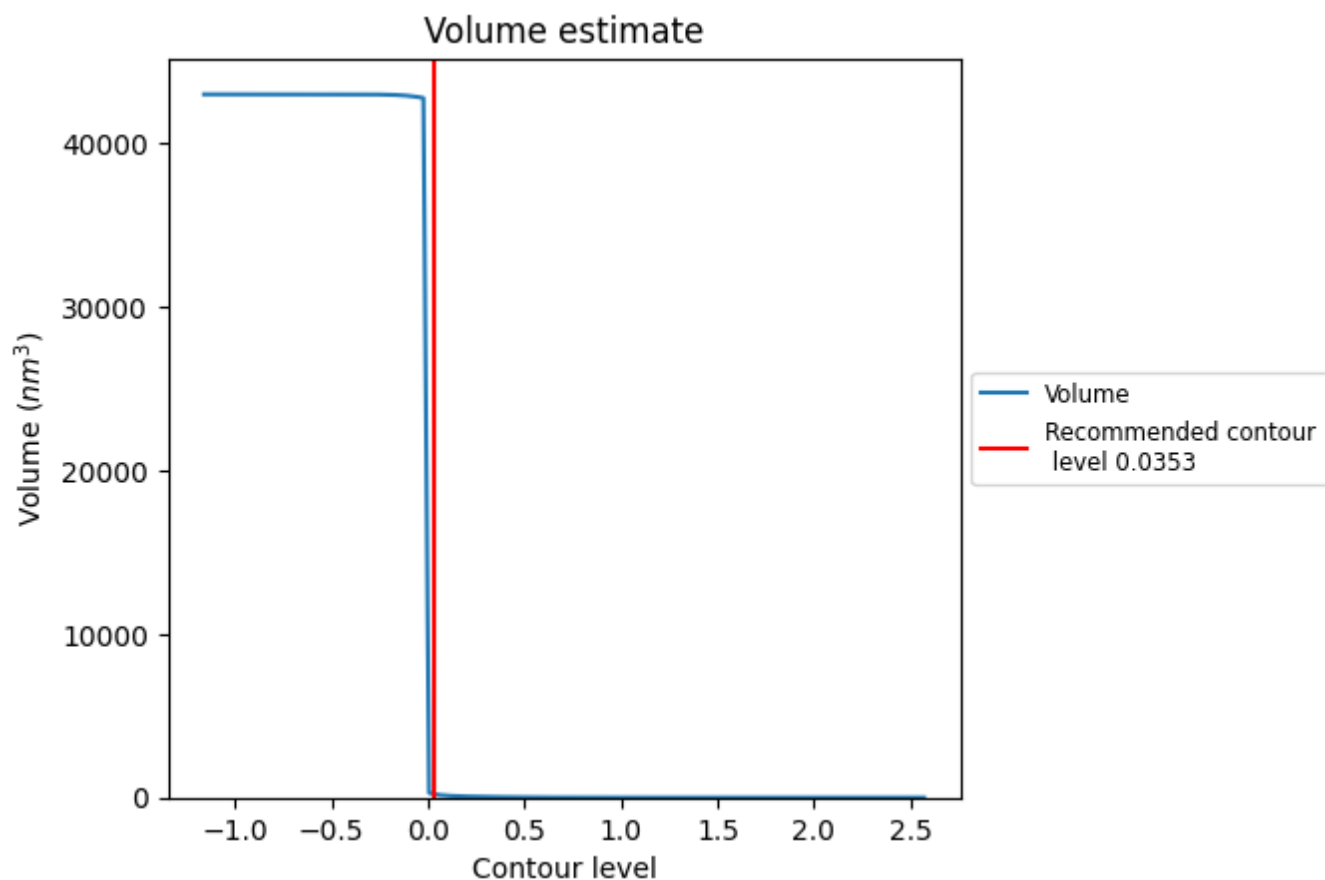
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

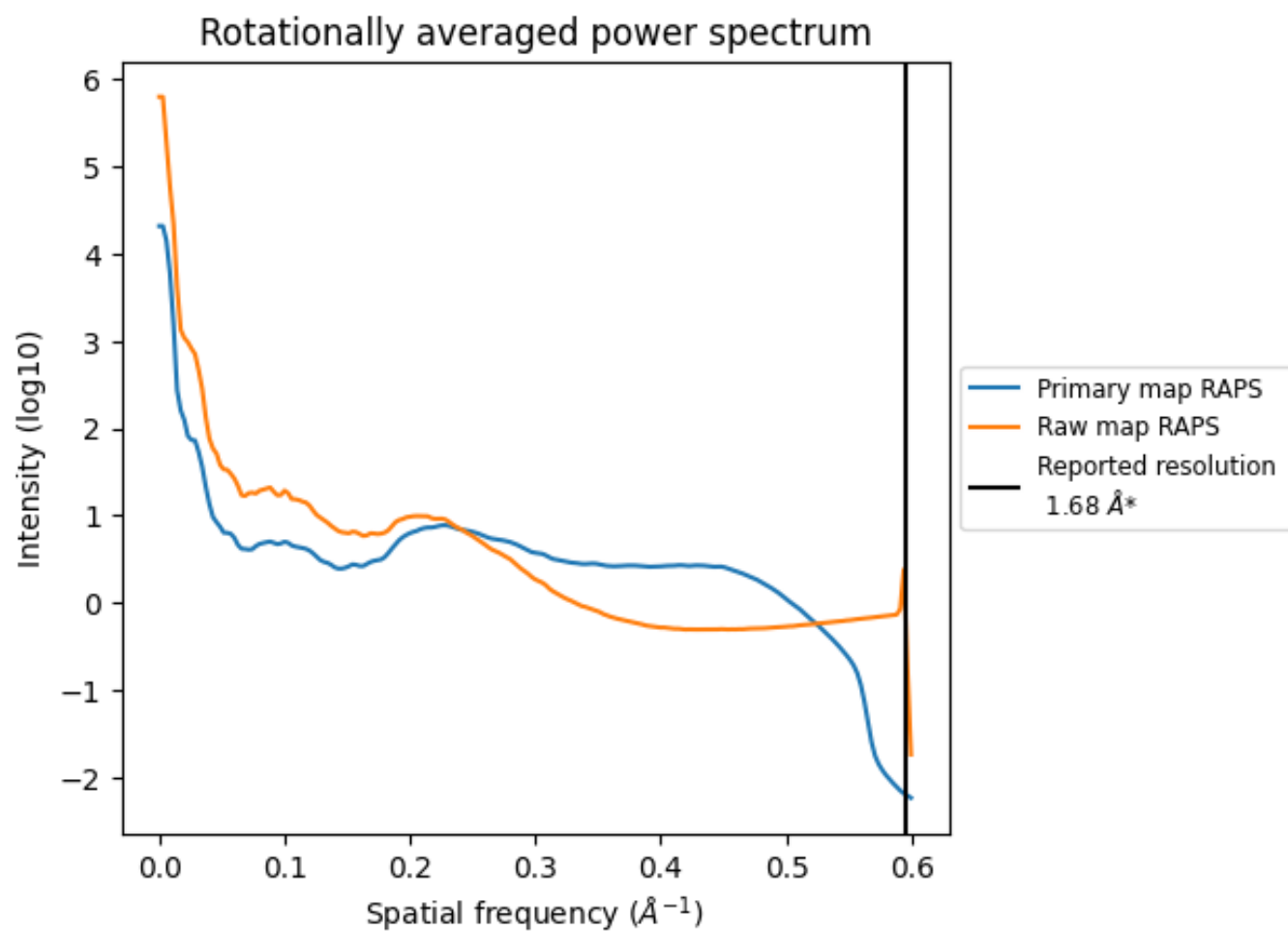
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 203 nm^3 ; this corresponds to an approximate mass of 183 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

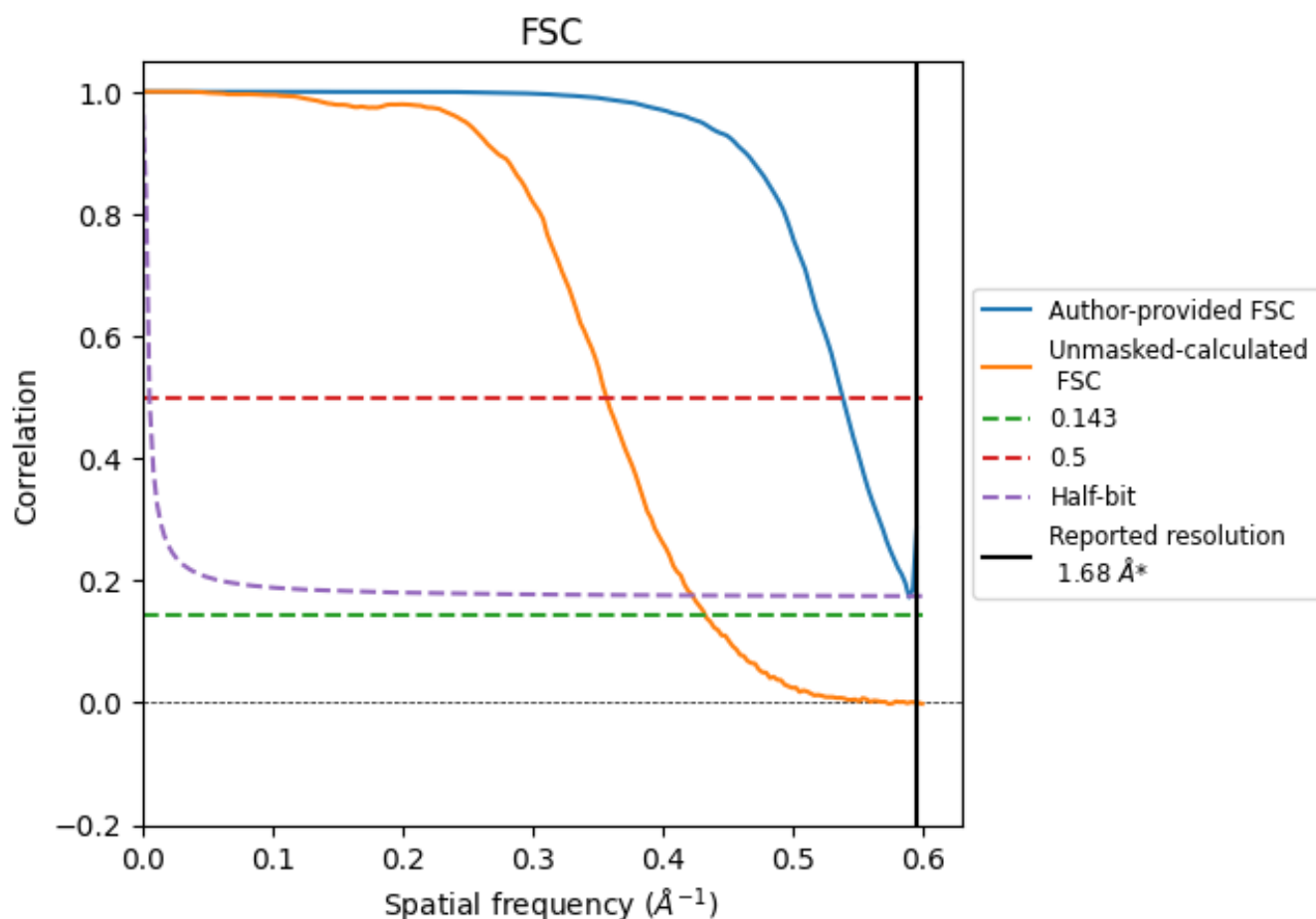


*Reported resolution corresponds to spatial frequency of 0.595 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.595 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

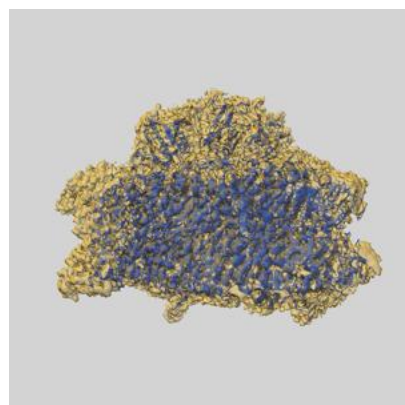
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.68	-	-
Author-provided FSC curve	-	1.86	1.70
Unmasked-calculated*	2.31	2.80	2.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.31 differs from the reported value 1.68 by more than 10 %

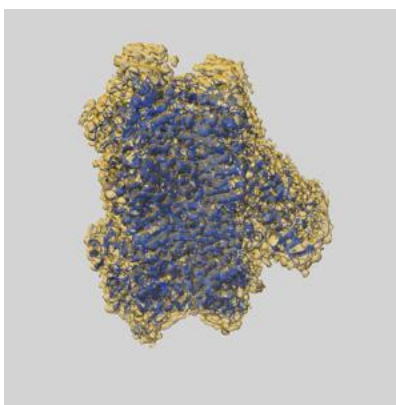
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73077 and PDB model 9YL7. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

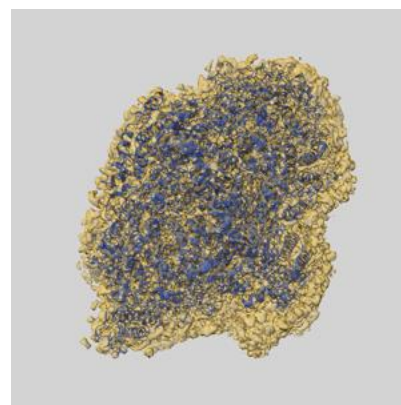
9.1 Map-model overlay [i](#)



X



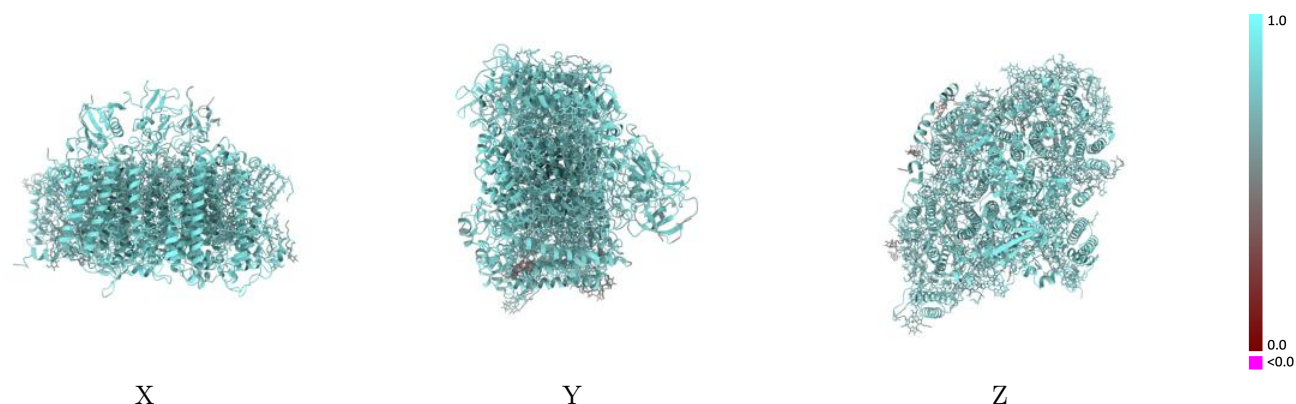
Y



Z

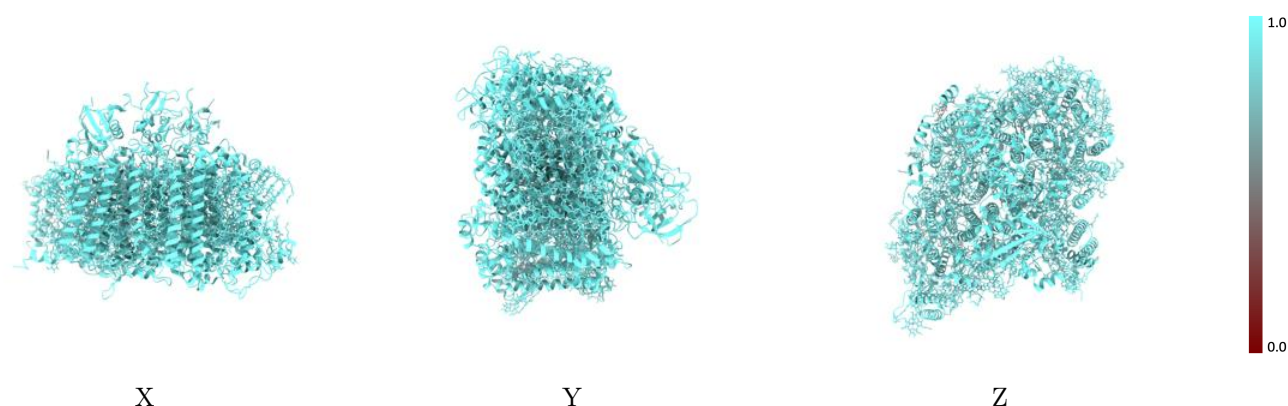
The images above show the 3D surface view of the map at the recommended contour level 0.0353 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



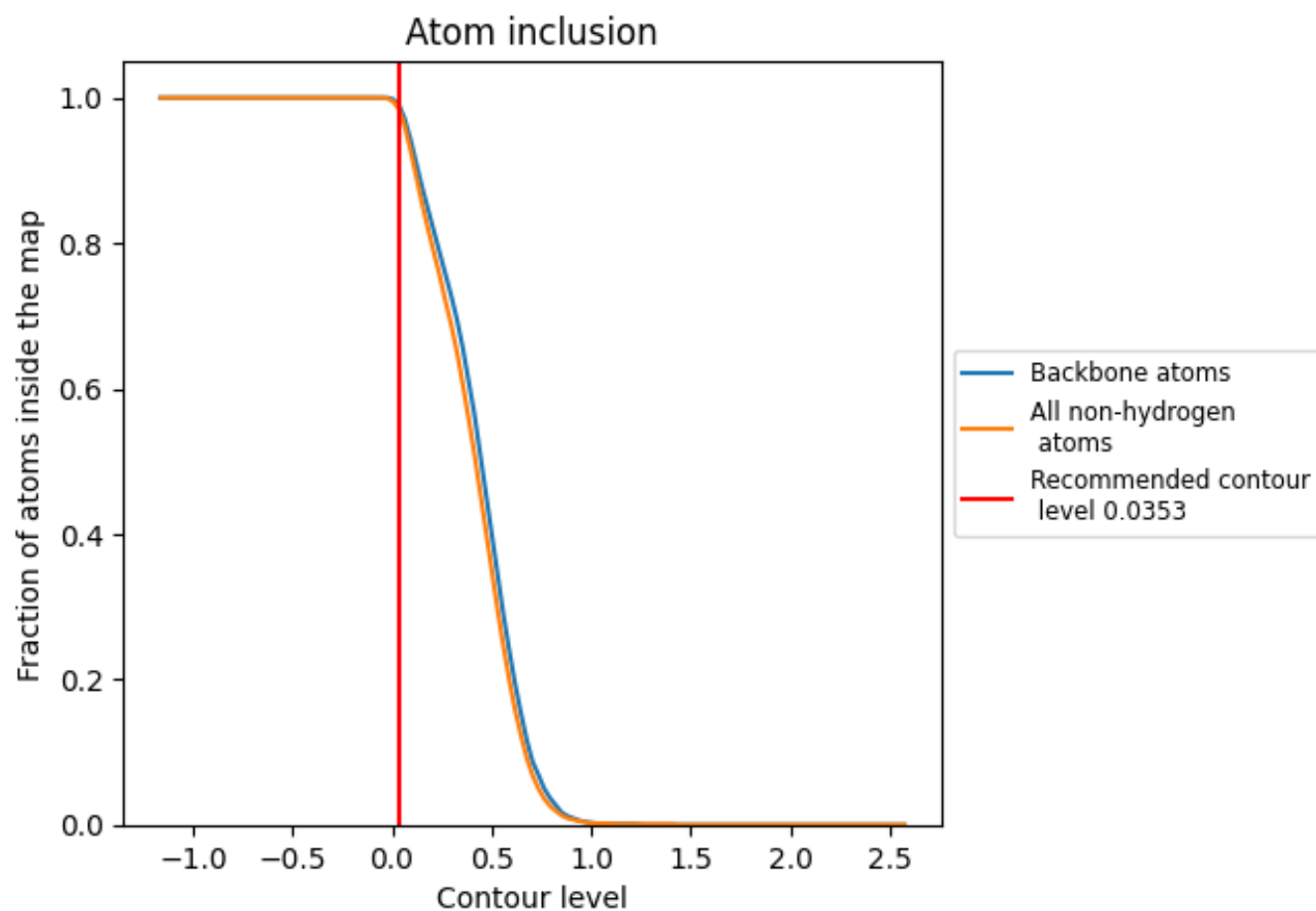
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0353).

9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0353) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9840	0.7910
A	0.9880	0.8000
B	0.9900	0.8060
C	0.9970	0.8320
D	0.9870	0.7960
E	0.9580	0.7350
F	0.9690	0.7330
I	0.9970	0.8220
J	0.9020	0.6570
K	0.9800	0.7450
L	0.9820	0.7830
M	0.9810	0.7560

1.0

0.0

<0.0