



wwPDB EM Validation Summary Report ⓘ

Sep 8, 2026 – 12:50 PM EDT

PDB ID : 10KF / pdb_000010kf
EMDB ID : EMD-75232
Title : Cryo-EM structure of a chemically treated Cyanobacterial Photosystem I core with bound platinum nanoparticles
Authors : Emerson, M.D.; Gisriel, C.J.
Deposited on : 2026-01-23
Resolution : 3.57 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:

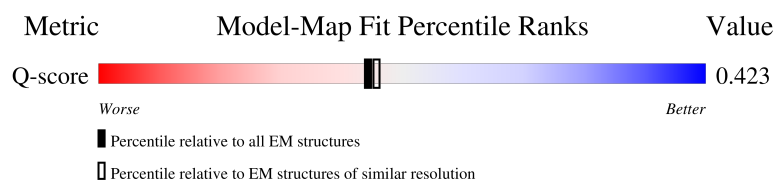
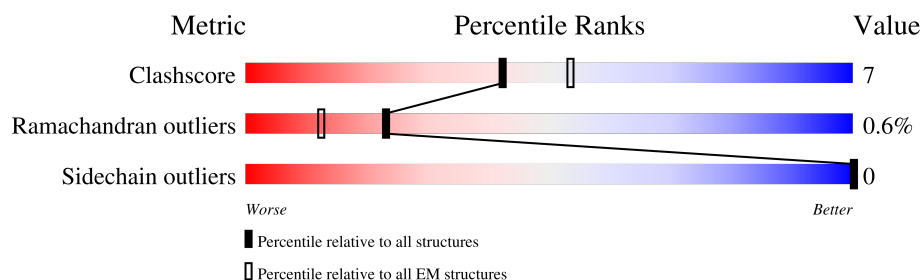
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 3.57 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	12682 (3.07 - 4.07)

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	763	 80% 16%
2	B	734	 84% 15%
3	F	159	 13% 44% 55%
4	I	38	 76% 8% 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	J	44	36% 89% 5% 7%
6	K	80	40% 90% 10%
7	M	29	86% 14%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 18035 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	737	Total	C	N	O	S	0	0
			5739	3763	982	977	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5789	3811	970	994	14		

- Molecule 3 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	72	Total	C	N	O	0	0
			353	209	72	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	32	Total	C	N	O	S	0	0
			235	163	32	39	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	J	41	Total	C	N	O	0	0
			204	121	41	42		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	MET	-	insertion	UNP Q5N5C7
J	2	LEU	-	insertion	UNP Q5N5C7
J	3	ALA	-	insertion	UNP Q5N5C7

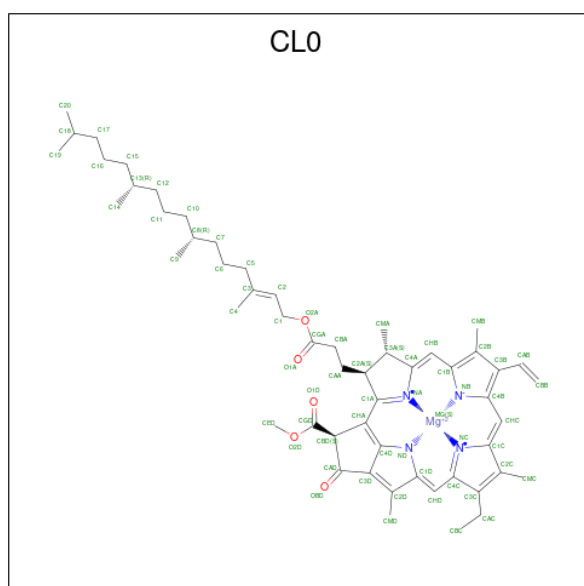
- Molecule 6 is a protein called Photosystem I reaction center subunit Psak.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	72	Total	C	N	O	0	0
			351	206	72	73		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	29	Total	C	N	O	S	0	0
			228	151	36	40	1		

- Molecule 8 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

- Molecule 9 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

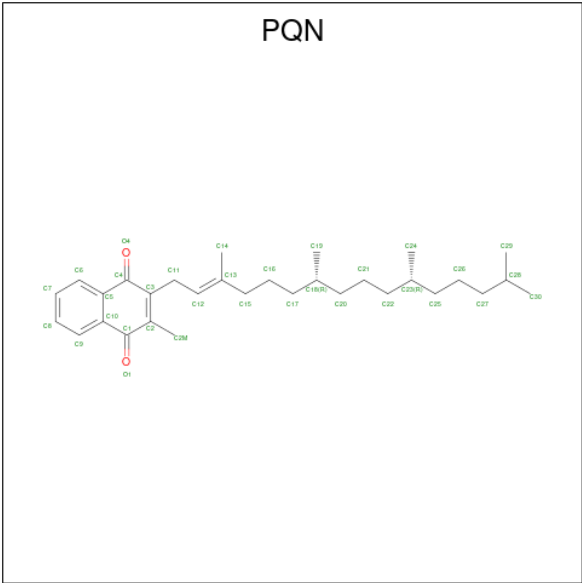
Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			45	35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

Continued on next page...

Continued from previous page...

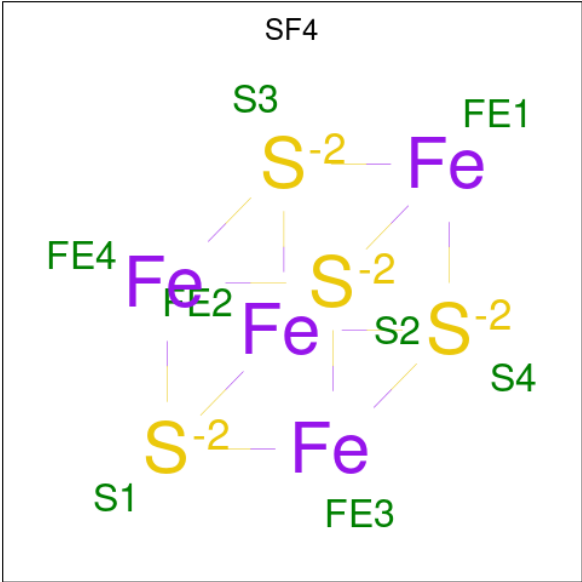
Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 10 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



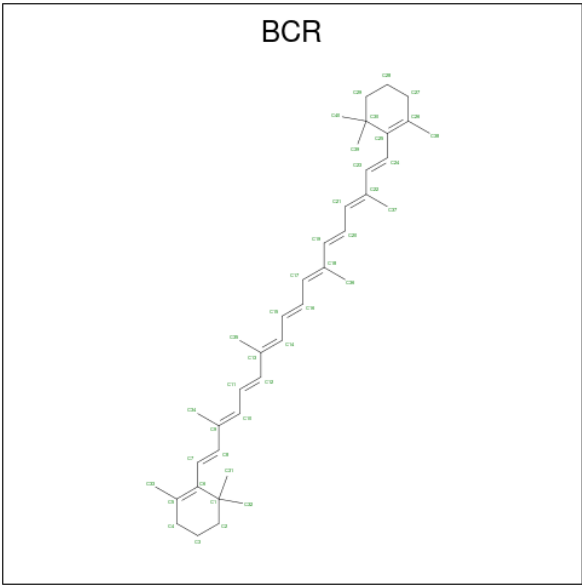
Mol	Chain	Residues	Atoms			AltConf
10	A	1	Total	C	O	0
			33	31	2	
10	B	1	Total	C	O	0
			33	31	2	

- Molecule 11 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 12 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



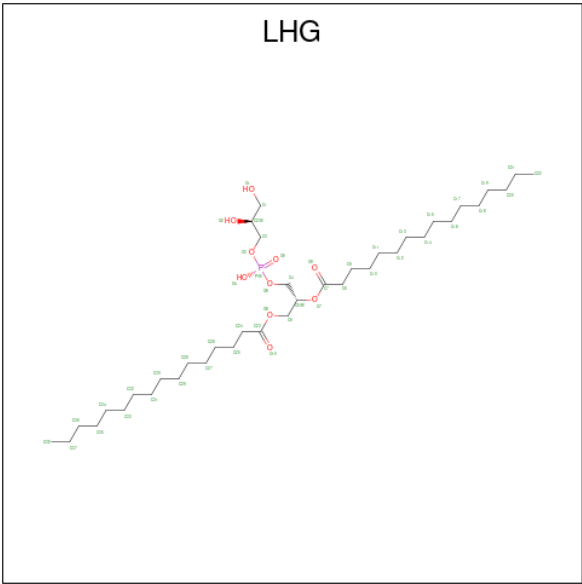
Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total	C	0
			40	40	
12	A	1	Total	C	0
			40	40	
12	A	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total	C	0
			40	40	
12	A	1	Total	C	0
			40	40	
12	B	1	Total	C	0
			40	40	
12	B	1	Total	C	0
			40	40	
12	B	1	Total	C	0
			40	40	
12	B	1	Total	C	0
			40	40	
12	B	1	Total	C	0
			40	40	
12	F	1	Total	C	0
			40	40	
12	M	1	Total	C	0
			40	40	

- Molecule 13 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



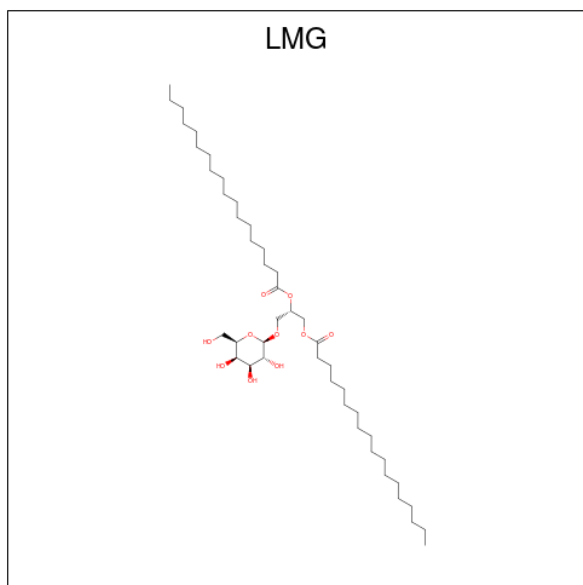
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			49	38	10	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
13	A	1	27	16	10	1	0

- Molecule 14 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).

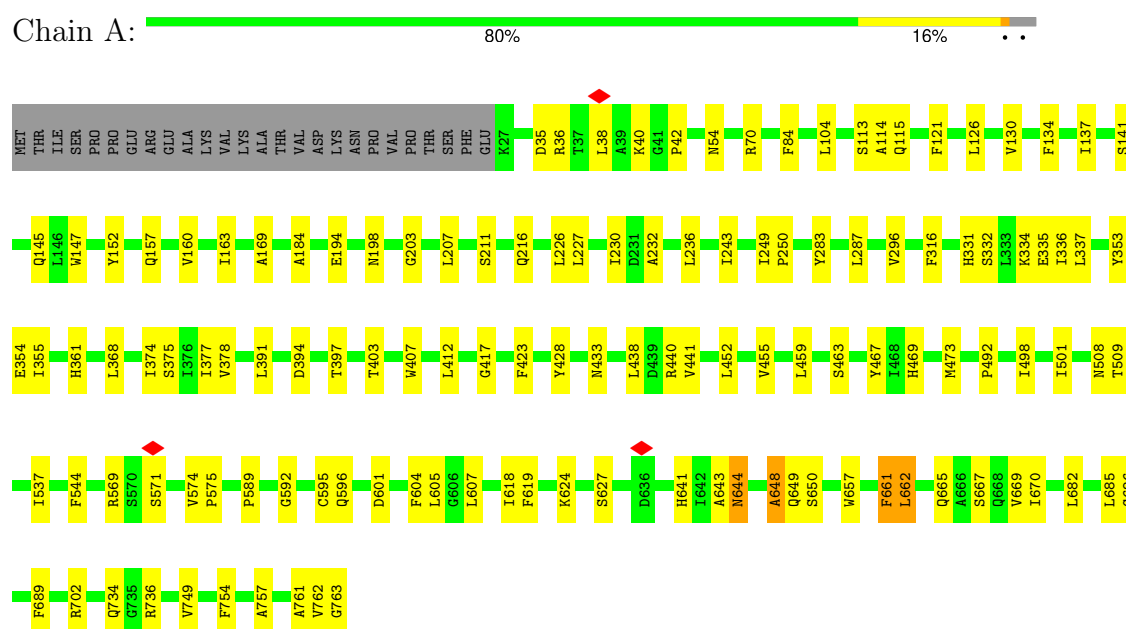


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O		
14	B	1	49	39	10		0

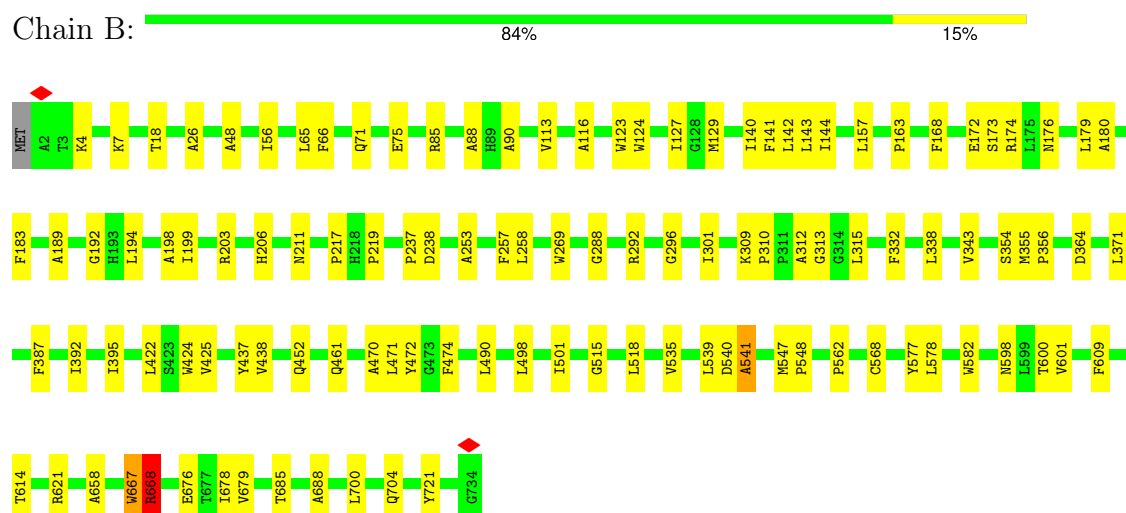
3 Residue-property plots

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

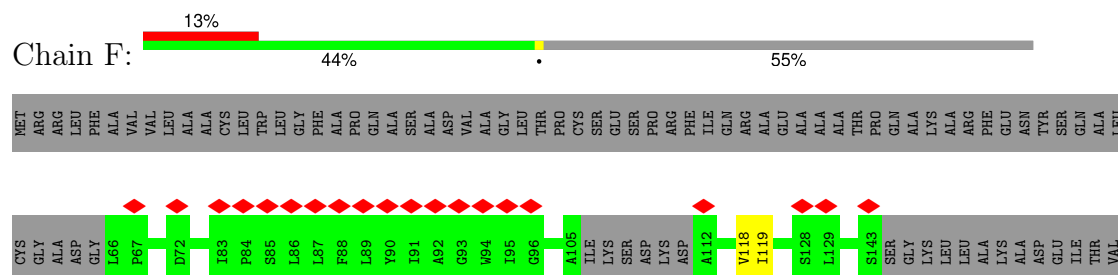
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



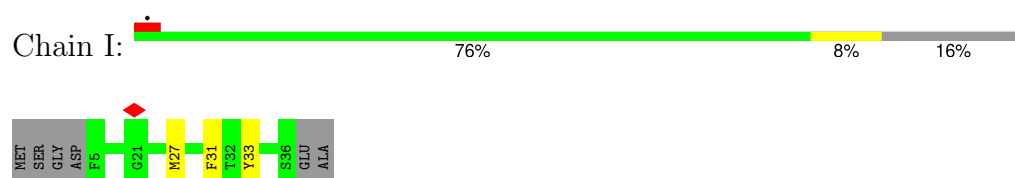
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



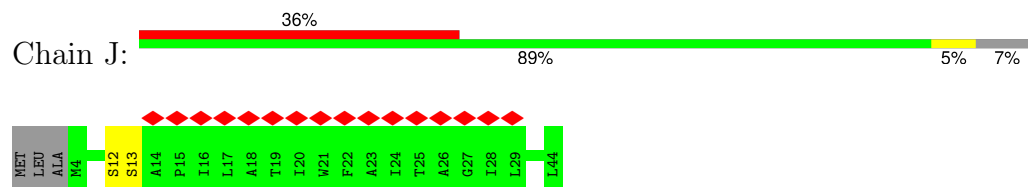
- Molecule 3: Photosystem I reaction center subunit III



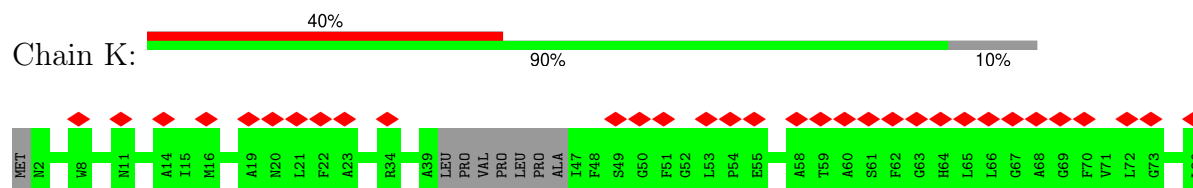
- Molecule 4: Photosystem I reaction center subunit VIII



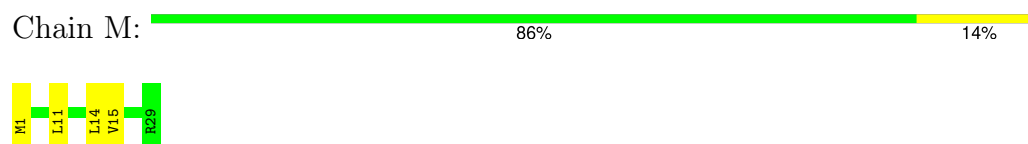
- Molecule 5: Photosystem I reaction center subunit IX



- Molecule 6: Photosystem I reaction center subunit PsaK



- Molecule 7: Photosystem I reaction center subunit XII



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53098	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.612	Depositor
Minimum map value	-0.201	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.164	Depositor
Map size ($\text{\AA}$)	272.384, 272.384, 272.384	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.064, 1.064, 1.064	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.32	0/5932	0.75	6/8094 (0.1%)
2	B	0.33	0/5999	0.78	10/8199 (0.1%)
3	F	0.14	0/351	0.43	0/484
4	I	0.42	0/241	1.03	0/331
5	J	0.16	0/203	0.52	0/280
6	K	0.19	0/349	0.59	0/478
7	M	0.63	1/231 (0.4%)	1.03	0/314
All	All	0.33	1/13306 (0.0%)	0.76	16/18180 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	4
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	15	VAL	C-N	7.14	1.42	1.33

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	PRO	CA-N-CD	-9.94	98.09	112.00
2	B	217	PRO	CA-C-N	5.84	132.34	122.65
2	B	217	PRO	C-N-CA	5.84	132.34	122.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	219	PRO	CA-N-CD	-5.83	103.84	112.00
2	B	309	LYS	CA-CB-CG	5.77	125.63	114.10

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	648	ALA	Peptide
1	A	661	PHE	Peptide
2	B	183	PHE	Peptide
2	B	312	ALA	Peptide
2	B	313	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5739	0	5601	79	0
2	B	5789	0	5575	80	0
3	F	353	0	172	2	0
4	I	235	0	249	2	0
5	J	204	0	92	2	0
6	K	351	0	188	0	0
7	M	228	0	246	3	0
8	A	60	0	59	5	0
9	A	2200	0	1880	32	0
9	B	2071	0	1799	52	0
9	I	45	0	32	1	0
9	K	41	0	28	0	0
10	A	33	0	46	3	0
10	B	33	0	46	4	0
11	A	8	0	0	0	0
12	A	200	0	245	14	0
12	B	240	0	293	15	0
12	F	40	0	48	2	0
12	M	40	0	49	4	0
13	A	76	0	98	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	B	49	0	71	6	0
All	All	18035	0	16817	235	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 235 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)
2:B:301:ILE:HG21	9:B:824:CLA:HAC1	1.69	0.75
2:B:56:ILE:HD11	12:M:101:BCR:HC7	1.71	0.72
2:B:189:ALA:HA	9:B:815:CLA:HBB2	1.74	0.68
10:B:841:PQN:H301	14:B:848:LMG:H192	1.73	0.68
2:B:387:PHE:HZ	9:B:825:CLA:HAB	1.61	0.65

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	735/763 (96%)	685 (93%)	45 (6%)	5 (1%)	18	51
2	B	731/734 (100%)	667 (91%)	59 (8%)	5 (1%)	18	51
3	F	68/159 (43%)	60 (88%)	8 (12%)	0	100	100
4	I	30/38 (79%)	29 (97%)	1 (3%)	0	100	100
5	J	39/44 (89%)	37 (95%)	2 (5%)	0	100	100
6	K	68/80 (85%)	60 (88%)	8 (12%)	0	100	100
7	M	27/29 (93%)	27 (100%)	0	0	100	100
All	All	1698/1847 (92%)	1565 (92%)	123 (7%)	10 (1%)	23	54

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	644	ASN
1	A	667	SER
1	A	762	VAL
2	B	471	LEU
2	B	668	ARG

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	583/611 (95%)	583 (100%)	0	100	100
2	B	583/584 (100%)	583 (100%)	0	100	100
4	I	25/30 (83%)	25 (100%)	0	100	100
7	M	24/24 (100%)	24 (100%)	0	100	100
All	All	1215/1249 (97%)	1215 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	414	HIS
2	B	496	ASN
7	M	5	GLN
2	B	528	HIS
1	A	367	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](#)

105 ligands are modelled in this entry.

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	$\# Z > 2$
9	CLA	A	844	13	49,53,73	2.58	22 (44%)	58,89,113	2.79	22 (37%)
9	CLA	A	835	-	49,53,73	2.56	22 (44%)	58,89,113	2.78	23 (39%)
9	CLA	A	807	1	49,53,73	2.54	22 (44%)	58,89,113	2.83	23 (39%)
9	CLA	B	836	-	59,63,73	2.44	23 (38%)	70,101,113	2.60	28 (40%)
9	CLA	B	806	-	64,68,73	2.34	24 (37%)	76,107,113	2.61	29 (38%)
12	BCR	A	849	-	41,41,41	2.61	6 (14%)	56,56,56	6.72	26 (46%)
9	CLA	B	810	-	49,53,73	2.56	21 (42%)	58,89,113	2.76	22 (37%)
12	BCR	A	847	-	41,41,41	2.60	6 (14%)	56,56,56	6.62	25 (44%)
8	CL0	A	801	-	64,68,73	2.35	23 (35%)	76,107,113	2.47	32 (42%)
13	LHG	A	853	9	26,26,48	1.26	2 (7%)	29,32,54	1.31	3 (10%)
12	BCR	B	846	-	41,41,41	2.65	6 (14%)	56,56,56	6.79	28 (50%)
9	CLA	A	813	1	64,68,73	2.29	23 (35%)	76,107,113	2.57	30 (39%)
9	CLA	B	803	-	69,73,73	2.20	20 (28%)	82,113,113	2.40	26 (31%)
9	CLA	B	818	2	64,68,73	2.33	24 (37%)	76,107,113	2.54	26 (34%)
9	CLA	B	827	2	59,63,73	2.40	21 (35%)	70,101,113	2.57	26 (37%)
9	CLA	B	809	2	69,73,73	2.25	22 (31%)	82,113,113	2.55	27 (32%)
9	CLA	A	825	-	69,73,73	2.25	23 (33%)	82,113,113	2.62	30 (36%)
9	CLA	B	823	2	49,53,73	2.58	25 (51%)	58,89,113	2.79	24 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CLA	B	831	-	49,53,73	2.56	22 (44%)	58,89,113	2.71	23 (39%)
12	BCR	B	845	-	41,41,41	2.66	6 (14%)	56,56,56	6.79	25 (44%)
9	CLA	B	807	-	69,73,73	2.25	23 (33%)	82,113,113	2.45	26 (31%)
12	BCR	M	101	-	41,41,41	2.58	6 (14%)	56,56,56	6.76	20 (35%)
9	CLA	A	838	-	49,53,73	2.54	22 (44%)	58,89,113	2.82	26 (44%)
9	CLA	A	836	-	49,53,73	2.58	22 (44%)	58,89,113	2.80	23 (39%)
9	CLA	A	803	1	49,53,73	2.55	22 (44%)	58,89,113	2.83	24 (41%)
9	CLA	B	813	-	69,73,73	2.24	23 (33%)	82,113,113	2.59	27 (32%)
12	BCR	B	842	-	41,41,41	2.64	6 (14%)	56,56,56	6.57	25 (44%)
9	CLA	A	822	-	49,53,73	2.56	23 (46%)	58,89,113	2.80	25 (43%)
9	CLA	B	811	-	49,53,73	2.55	22 (44%)	58,89,113	2.77	23 (39%)
9	CLA	B	825	-	49,53,73	2.57	22 (44%)	58,89,113	2.77	25 (43%)
9	CLA	B	805	-	49,53,73	2.55	23 (46%)	58,89,113	2.82	23 (39%)
9	CLA	B	837	-	64,68,73	2.33	23 (35%)	76,107,113	2.54	27 (35%)
9	CLA	A	815	1	49,53,73	2.56	22 (44%)	58,89,113	2.80	24 (41%)
9	CLA	A	828	1	69,73,73	2.25	23 (33%)	82,113,113	2.51	27 (32%)
9	CLA	A	837	-	49,53,73	2.55	22 (44%)	58,89,113	2.83	23 (39%)
9	CLA	B	838	-	49,53,73	2.56	21 (42%)	58,89,113	2.81	24 (41%)
12	BCR	B	847	-	41,41,41	2.60	6 (14%)	56,56,56	6.62	19 (33%)
12	BCR	F	201	-	41,41,41	2.56	6 (14%)	56,56,56	6.65	27 (48%)
9	CLA	B	816	-	49,53,73	2.56	22 (44%)	58,89,113	2.80	24 (41%)
9	CLA	B	835	-	49,53,73	2.56	23 (46%)	58,89,113	2.77	23 (39%)
9	CLA	A	819	1	69,73,73	2.25	23 (33%)	82,113,113	2.52	28 (34%)
9	CLA	A	843	-	49,53,73	2.55	23 (46%)	58,89,113	2.80	24 (41%)
9	CLA	B	814	-	59,63,73	2.41	21 (35%)	70,101,113	2.73	30 (42%)
9	CLA	A	802	-	69,73,73	2.26	22 (31%)	82,113,113	2.44	31 (37%)
11	SF4	A	846	2,1	0,12,12	-	-	-	-	-
12	BCR	A	851	-	41,41,41	2.63	6 (14%)	56,56,56	6.90	25 (44%)
9	CLA	A	817	-	54,58,73	2.54	22 (40%)	64,95,113	2.78	26 (40%)
9	CLA	A	809	-	54,58,73	2.53	23 (42%)	64,95,113	2.75	26 (40%)
9	CLA	B	830	-	49,53,73	2.58	23 (46%)	58,89,113	2.76	27 (46%)
9	CLA	A	826	-	64,68,73	2.33	24 (37%)	76,107,113	2.59	26 (34%)
9	CLA	A	821	-	69,73,73	2.27	22 (31%)	82,113,113	2.39	29 (35%)
9	CLA	A	841	-	49,53,73	2.54	23 (46%)	58,89,113	2.80	24 (41%)
9	CLA	B	808	2	49,53,73	2.54	21 (42%)	58,89,113	2.94	25 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CLA	A	806	1	69,73,73	2.25	21 (30%)	82,113,113	2.47	24 (29%)
9	CLA	B	817	-	59,63,73	2.44	22 (37%)	70,101,113	2.64	31 (44%)
9	CLA	B	833	2	49,53,73	2.56	23 (46%)	58,89,113	2.75	23 (39%)
9	CLA	A	812	-	49,53,73	2.57	23 (46%)	58,89,113	2.80	23 (39%)
9	CLA	B	819	-	59,63,73	2.44	24 (40%)	70,101,113	2.64	25 (35%)
9	CLA	B	821	-	49,53,73	2.56	22 (44%)	58,89,113	2.81	24 (41%)
12	BCR	A	850	-	41,41,41	2.68	6 (14%)	56,56,56	6.49	23 (41%)
9	CLA	B	802	-	69,73,73	2.25	22 (31%)	82,113,113	2.46	24 (29%)
9	CLA	A	829	-	69,73,73	2.25	22 (31%)	82,113,113	2.37	26 (31%)
9	CLA	A	834	1	49,53,73	2.56	22 (44%)	58,89,113	2.87	25 (43%)
9	CLA	B	839	-	49,53,73	2.53	22 (44%)	58,89,113	2.89	23 (39%)
12	BCR	A	848	-	41,41,41	2.62	6 (14%)	56,56,56	6.56	22 (39%)
13	LHG	A	852	-	48,48,48	0.94	2 (4%)	51,54,54	1.01	3 (5%)
14	LMG	B	848	-	49,49,55	1.40	6 (12%)	57,57,63	1.15	4 (7%)
9	CLA	B	824	-	49,53,73	2.51	22 (44%)	58,89,113	2.91	25 (43%)
12	BCR	B	843	-	41,41,41	2.65	6 (14%)	56,56,56	6.64	26 (46%)
9	CLA	B	834	-	49,53,73	2.55	23 (46%)	58,89,113	2.80	23 (39%)
9	CLA	A	808	1	49,53,73	2.53	21 (42%)	58,89,113	2.81	25 (43%)
9	CLA	B	815	2	49,53,73	2.53	22 (44%)	58,89,113	2.83	24 (41%)
12	BCR	B	844	-	41,41,41	2.58	6 (14%)	56,56,56	6.70	21 (37%)
10	PQN	B	841	-	34,34,34	1.62	2 (5%)	43,45,45	1.01	2 (4%)
10	PQN	A	845	-	34,34,34	1.62	2 (5%)	43,45,45	1.09	3 (6%)
9	CLA	A	831	-	49,53,73	2.56	23 (46%)	58,89,113	2.74	24 (41%)
9	CLA	A	842	1	54,58,73	2.55	23 (42%)	64,95,113	2.83	26 (40%)
9	CLA	B	804	-	69,73,73	2.22	22 (31%)	82,113,113	2.29	26 (31%)
9	CLA	A	804	9	49,53,73	2.56	23 (46%)	58,89,113	2.84	25 (43%)
9	CLA	B	822	-	49,53,73	2.55	23 (46%)	58,89,113	2.76	23 (39%)
9	CLA	B	840	-	49,53,73	2.52	22 (44%)	58,89,113	2.88	25 (43%)
9	CLA	A	816	-	49,53,73	2.54	22 (44%)	58,89,113	2.79	23 (39%)
9	CLA	A	814	1	49,53,73	2.56	23 (46%)	58,89,113	2.82	25 (43%)
9	CLA	I	101	-	49,53,73	2.54	22 (44%)	58,89,113	2.81	25 (43%)
9	CLA	A	830	1	69,73,73	2.23	24 (34%)	82,113,113	2.49	26 (31%)
9	CLA	B	812	-	49,53,73	2.56	22 (44%)	58,89,113	2.76	25 (43%)
9	CLA	A	827	-	69,73,73	2.24	22 (31%)	82,113,113	2.54	29 (35%)
9	CLA	B	828	-	69,73,73	2.26	22 (31%)	82,113,113	2.36	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CLA	A	840	-	54,58,73	2.54	24 (44%)	64,95,113	2.76	27 (42%)
9	CLA	B	801	-	64,68,73	2.30	22 (34%)	76,107,113	2.51	27 (35%)
9	CLA	B	829	-	49,53,73	2.55	22 (44%)	58,89,113	2.82	25 (43%)
9	CLA	A	823	-	49,53,73	2.56	23 (46%)	58,89,113	2.81	23 (39%)
9	CLA	A	811	9	49,53,73	2.56	23 (46%)	58,89,113	2.84	23 (39%)
9	CLA	B	826	-	69,73,73	2.26	23 (33%)	82,113,113	2.49	28 (34%)
9	CLA	A	818	1	54,58,73	2.55	23 (42%)	64,95,113	2.74	28 (43%)
9	CLA	A	810	-	49,53,73	2.55	22 (44%)	58,89,113	2.80	22 (37%)
9	CLA	B	832	2	49,53,73	2.56	22 (44%)	58,89,113	2.79	23 (39%)
9	CLA	A	824	-	49,53,73	2.56	23 (46%)	58,89,113	2.80	26 (44%)
9	CLA	B	820	2	49,53,73	2.55	22 (44%)	58,89,113	2.80	24 (41%)
9	CLA	A	805	-	69,73,73	2.21	21 (30%)	82,113,113	2.51	28 (34%)
9	CLA	A	832	-	49,53,73	2.56	23 (46%)	58,89,113	2.80	24 (41%)
9	CLA	A	820	-	59,63,73	2.40	21 (35%)	70,101,113	2.74	30 (42%)
9	CLA	A	839	-	49,53,73	2.55	22 (44%)	58,89,113	2.79	24 (41%)
9	CLA	K	101	-	45,49,73	2.50	21 (46%)	54,83,113	2.79	20 (37%)
9	CLA	A	833	1	49,53,73	2.56	22 (44%)	58,89,113	2.76	25 (43%)

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
9	CLA	A	844	13	-	11/15/91/115	-
9	CLA	A	835	-	-	9/15/91/115	-
9	CLA	A	807	1	-	8/15/91/115	-
9	CLA	B	836	-	-	11/27/103/115	-
9	CLA	B	806	-	-	12/33/109/115	-
12	BCR	A	849	-	-	9/29/63/63	0/2/2/2
9	CLA	B	810	-	-	8/15/91/115	-
12	BCR	A	847	-	-	6/29/63/63	0/2/2/2
8	CL0	A	801	-	-	15/33/109/115	-
13	LHG	A	853	9	-	16/31/31/53	-
12	BCR	B	846	-	-	11/29/63/63	0/2/2/2
9	CLA	A	813	1	-	17/33/109/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	B	803	-	-	17/39/115/115	-
9	CLA	B	818	2	-	15/33/109/115	-
9	CLA	B	827	2	-	13/27/103/115	-
9	CLA	B	809	2	-	15/39/115/115	-
9	CLA	A	825	-	-	16/39/115/115	-
9	CLA	B	823	2	-	2/15/91/115	-
9	CLA	B	831	-	-	5/15/91/115	-
12	BCR	B	845	-	-	6/29/63/63	0/2/2/2
9	CLA	B	807	-	-	15/39/115/115	-
12	BCR	M	101	-	-	9/29/63/63	0/2/2/2
9	CLA	A	838	-	-	3/15/91/115	-
9	CLA	A	836	-	-	7/15/91/115	-
9	CLA	A	803	1	-	10/15/91/115	-
9	CLA	B	813	-	-	23/39/115/115	-
12	BCR	B	842	-	-	11/29/63/63	0/2/2/2
9	CLA	A	822	-	-	7/15/91/115	-
9	CLA	B	811	-	-	5/15/91/115	-
9	CLA	B	825	-	-	4/15/91/115	-
9	CLA	B	805	-	-	5/15/91/115	-
9	CLA	B	837	-	-	13/33/109/115	-
9	CLA	A	815	1	-	7/15/91/115	-
9	CLA	A	828	1	-	17/39/115/115	-
9	CLA	A	837	-	-	8/15/91/115	-
9	CLA	B	838	-	-	5/15/91/115	-
12	BCR	B	847	-	-	7/29/63/63	0/2/2/2
12	BCR	F	201	-	-	5/29/63/63	0/2/2/2
9	CLA	B	816	-	-	7/15/91/115	-
9	CLA	B	835	-	-	5/15/91/115	-
9	CLA	A	819	1	-	15/39/115/115	-
9	CLA	A	843	-	-	8/15/91/115	-
9	CLA	B	814	-	-	12/27/103/115	-
9	CLA	A	802	-	-	17/39/115/115	-
11	SF4	A	846	2,1	-	-	0/6/5/5
12	BCR	A	851	-	-	9/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	A	817	-	-	7/21/97/115	-
9	CLA	A	809	-	-	6/21/97/115	-
9	CLA	B	830	-	-	11/15/91/115	-
9	CLA	A	826	-	-	9/33/109/115	-
9	CLA	A	821	-	-	14/39/115/115	-
9	CLA	A	841	-	-	7/15/91/115	-
9	CLA	B	808	2	-	7/15/91/115	-
9	CLA	A	806	1	-	12/39/115/115	-
9	CLA	B	817	-	-	8/27/103/115	-
9	CLA	B	833	2	-	6/15/91/115	-
9	CLA	A	812	-	-	6/15/91/115	-
9	CLA	B	819	-	-	5/27/103/115	-
9	CLA	B	821	-	-	7/15/91/115	-
12	BCR	A	850	-	-	9/29/63/63	0/2/2/2
9	CLA	B	802	-	-	16/39/115/115	-
9	CLA	A	829	-	-	15/39/115/115	-
9	CLA	A	834	1	-	7/15/91/115	-
9	CLA	B	839	-	-	7/15/91/115	-
12	BCR	A	848	-	-	10/29/63/63	0/2/2/2
13	LHG	A	852	-	-	34/53/53/53	-
14	LMG	B	848	-	-	23/44/64/70	0/1/1/1
9	CLA	B	824	-	-	9/15/91/115	-
12	BCR	B	843	-	-	9/29/63/63	0/2/2/2
9	CLA	B	834	-	-	6/15/91/115	-
9	CLA	A	808	1	-	9/15/91/115	-
9	CLA	B	815	2	-	9/15/91/115	-
12	BCR	B	844	-	-	9/29/63/63	0/2/2/2
10	PQN	B	841	-	-	9/23/43/43	0/2/2/2
10	PQN	A	845	-	-	4/23/43/43	0/2/2/2
9	CLA	A	831	-	-	7/15/91/115	-
9	CLA	A	842	1	-	8/21/97/115	-
9	CLA	B	804	-	-	12/39/115/115	-
9	CLA	A	804	9	-	8/15/91/115	-
9	CLA	B	822	-	-	8/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	B	840	-	-	7/15/91/115	-
9	CLA	A	816	-	-	7/15/91/115	-
9	CLA	A	814	1	-	4/15/91/115	-
9	CLA	I	101	-	-	8/15/91/115	-
9	CLA	A	830	1	-	14/39/115/115	-
9	CLA	B	812	-	-	5/15/91/115	-
9	CLA	A	827	-	-	12/39/115/115	-
9	CLA	B	828	-	-	14/39/115/115	-
9	CLA	A	840	-	-	6/21/97/115	-
9	CLA	B	801	-	-	10/33/109/115	-
9	CLA	B	829	-	-	5/15/91/115	-
9	CLA	A	823	-	-	8/15/91/115	-
9	CLA	A	811	9	-	7/15/91/115	-
9	CLA	B	826	-	-	17/39/115/115	-
9	CLA	A	818	1	-	10/21/97/115	-
9	CLA	A	810	-	-	5/15/91/115	-
9	CLA	B	832	2	-	3/15/91/115	-
9	CLA	A	824	-	-	8/15/91/115	-
9	CLA	B	820	2	-	8/15/91/115	-
9	CLA	A	805	-	-	22/39/115/115	-
9	CLA	A	832	-	-	5/15/91/115	-
9	CLA	A	820	-	-	10/27/103/115	-
9	CLA	A	839	-	-	7/15/91/115	-
9	CLA	K	101	-	-	4/9/81/115	-
9	CLA	A	833	1	-	6/15/91/115	-

The worst 5 of 2017 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	842	BCR	C8-C9	-8.41	1.28	1.46
12	A	848	BCR	C8-C9	-8.34	1.28	1.46
12	B	845	BCR	C11-C10	-8.33	1.17	1.43
12	B	846	BCR	C11-C10	-8.30	1.17	1.43
12	B	843	BCR	C8-C9	-8.27	1.28	1.46

The worst 5 of 2509 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	847	BCR	C15-C16-C17	22.88	170.33	123.52
12	A	851	BCR	C20-C21-C22	22.83	159.29	127.28
12	B	844	BCR	C20-C21-C22	22.51	158.84	127.28
12	B	845	BCR	C20-C21-C22	22.29	158.54	127.28
12	B	845	BCR	C16-C17-C18	21.77	157.80	127.28

There are no chirality outliers.

5 of 1001 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	801	CL0	C1A-C2A-CAA-CBA
8	A	801	CL0	C3A-C2A-CAA-CBA
8	A	801	CL0	C4-C3-C5-C6
9	A	802	CLA	C4B-C3B-CAB-CBB
9	A	803	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

71 monomers are involved in 126 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	835	CLA	2	0
9	A	807	CLA	2	0
9	B	836	CLA	2	0
9	B	806	CLA	1	0
12	A	849	BCR	2	0
9	B	810	CLA	2	0
12	A	847	BCR	3	0
8	A	801	CL0	5	0
12	B	846	BCR	1	0
9	A	813	CLA	1	0
9	B	803	CLA	4	0
9	B	818	CLA	2	0
9	B	827	CLA	1	0
9	B	809	CLA	3	0
9	A	825	CLA	2	0
9	B	831	CLA	1	0
12	B	845	BCR	2	0
9	B	807	CLA	3	0
12	M	101	BCR	4	0
9	A	838	CLA	2	0
9	B	813	CLA	3	0
12	B	842	BCR	2	0

Continued on next page...

Continued from previous page...

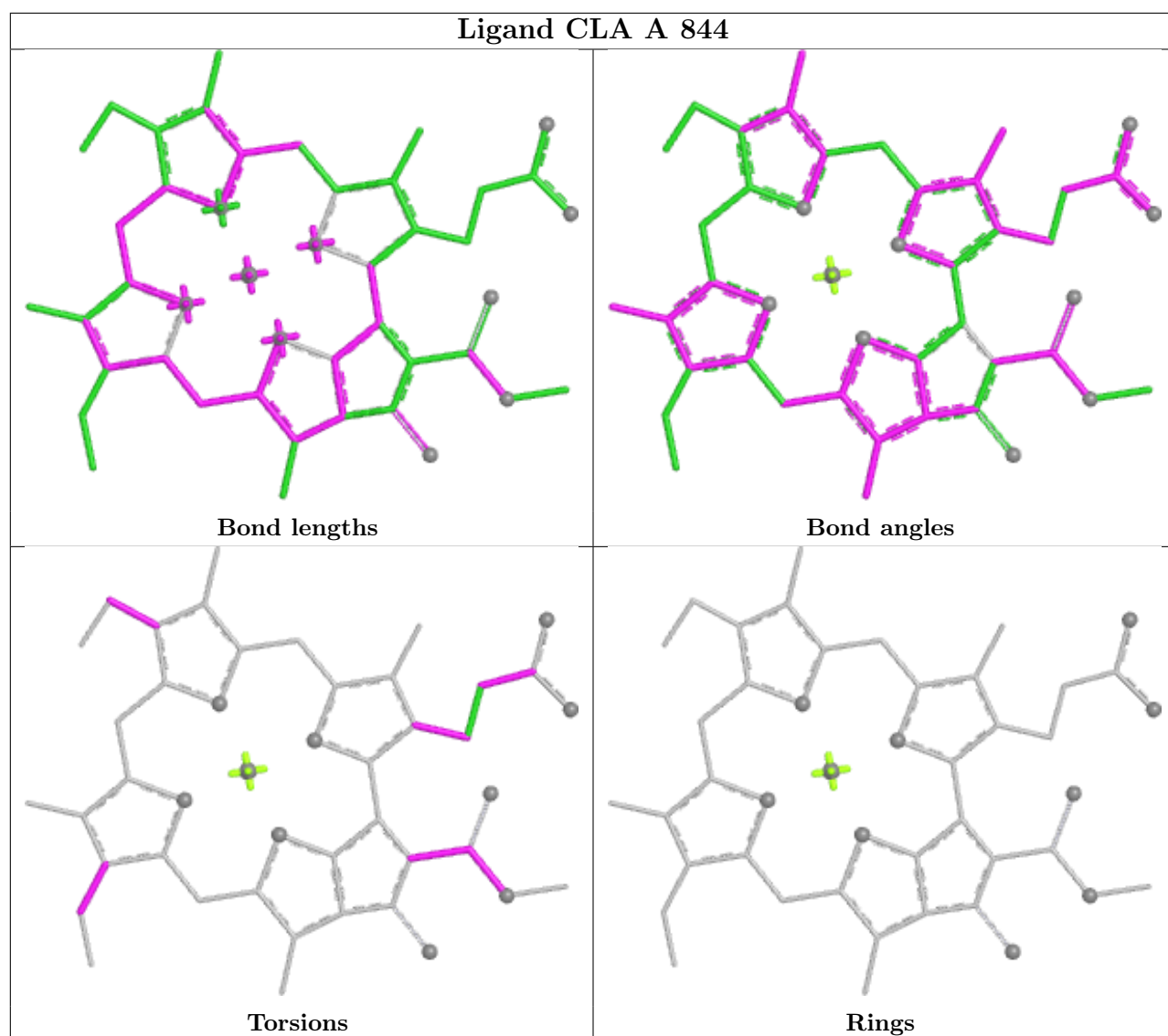
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	825	CLA	3	0
9	A	828	CLA	4	0
9	B	838	CLA	1	0
12	B	847	BCR	4	0
12	F	201	BCR	2	0
9	B	816	CLA	1	0
9	A	819	CLA	2	0
9	A	802	CLA	1	0
12	A	851	BCR	4	0
9	A	809	CLA	1	0
9	B	830	CLA	3	0
9	A	826	CLA	2	0
9	A	821	CLA	3	0
9	A	841	CLA	1	0
9	B	808	CLA	1	0
9	A	806	CLA	1	0
9	B	817	CLA	1	0
9	B	819	CLA	1	0
12	A	850	BCR	3	0
9	B	802	CLA	5	0
9	A	829	CLA	1	0
9	B	839	CLA	2	0
12	A	848	BCR	2	0
13	A	852	LHG	3	0
14	B	848	LMG	6	0
9	B	824	CLA	1	0
12	B	843	BCR	2	0
9	B	834	CLA	1	0
9	A	808	CLA	1	0
9	B	815	CLA	3	0
12	B	844	BCR	4	0
10	B	841	PQN	4	0
10	A	845	PQN	3	0
9	A	831	CLA	1	0
9	B	804	CLA	1	0
9	B	840	CLA	1	0
9	A	814	CLA	1	0
9	I	101	CLA	1	0
9	A	830	CLA	2	0
9	A	827	CLA	1	0
9	B	828	CLA	5	0
9	A	840	CLA	1	0

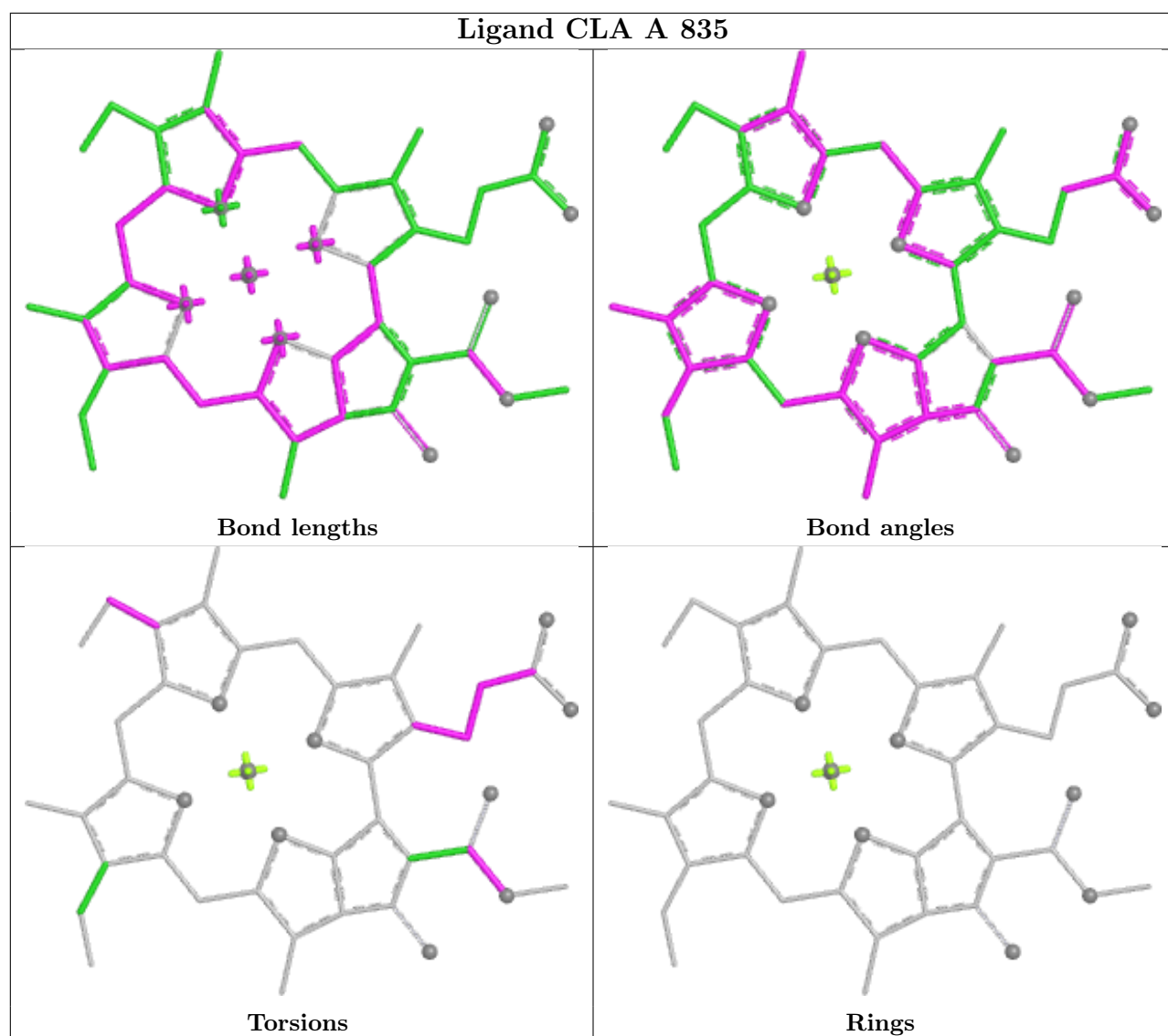
Continued on next page...

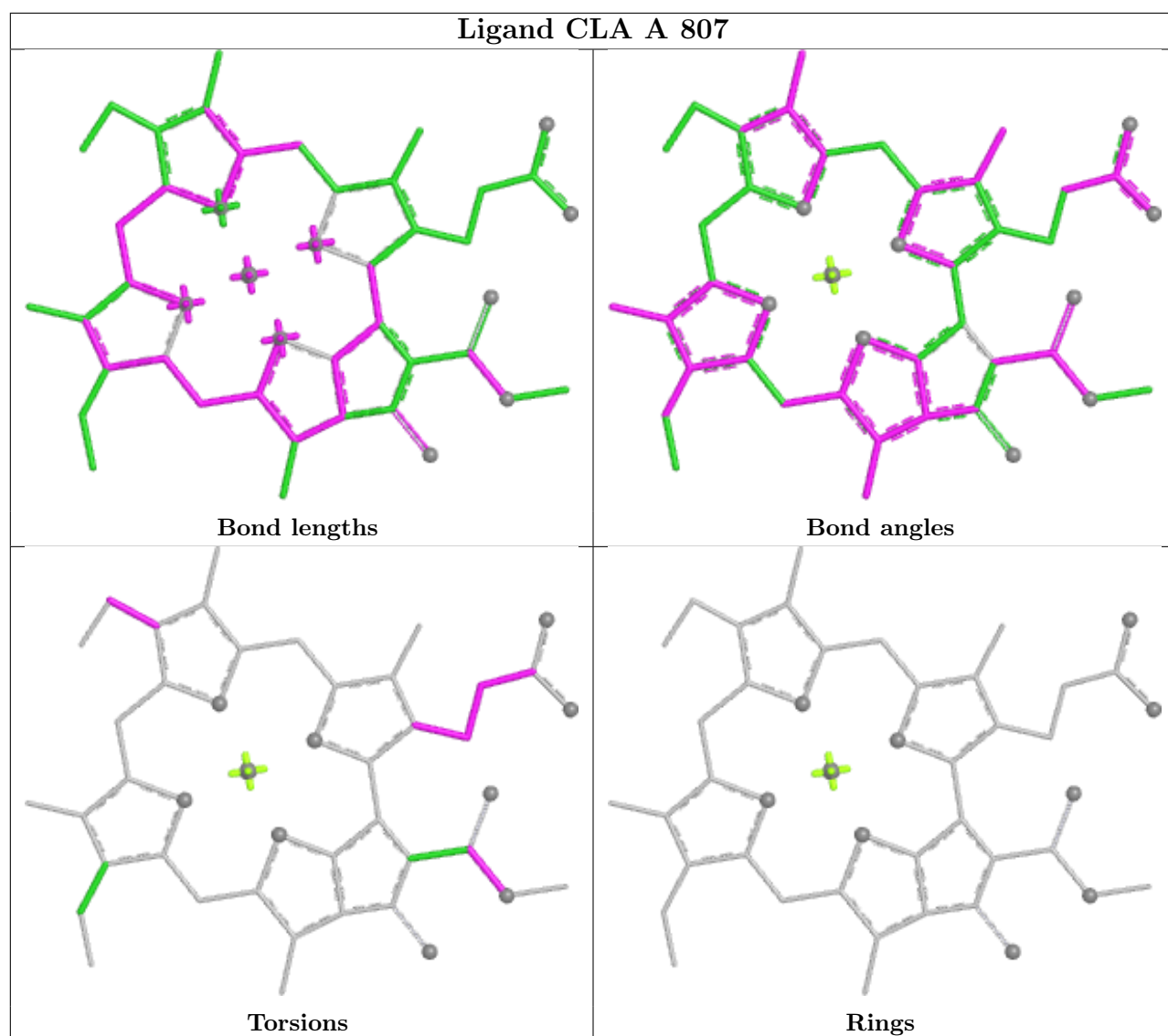
Continued from previous page...

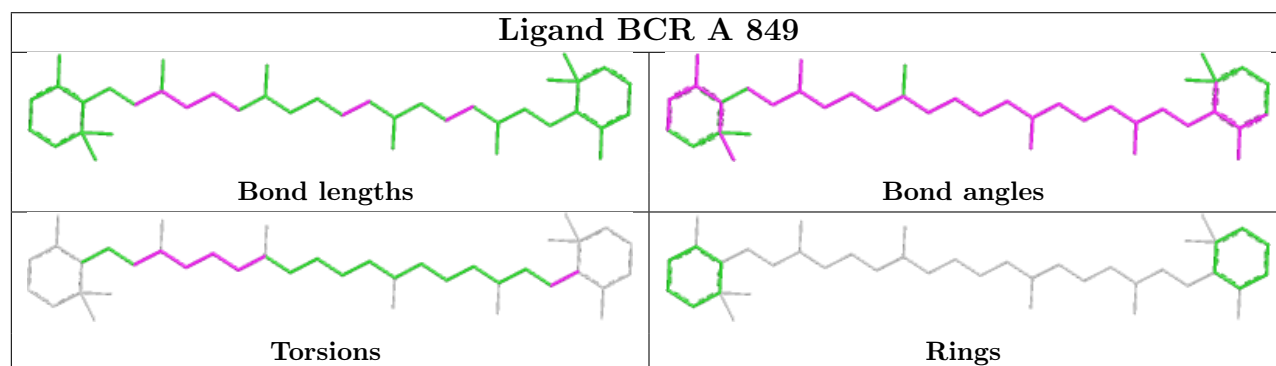
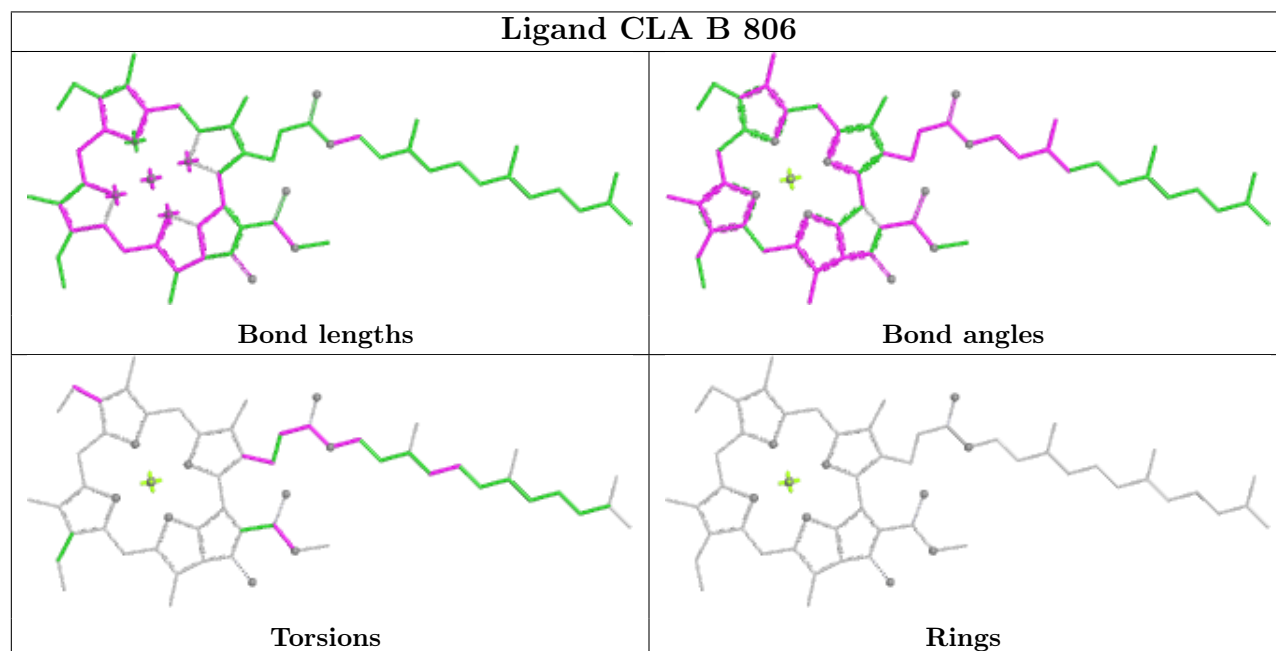
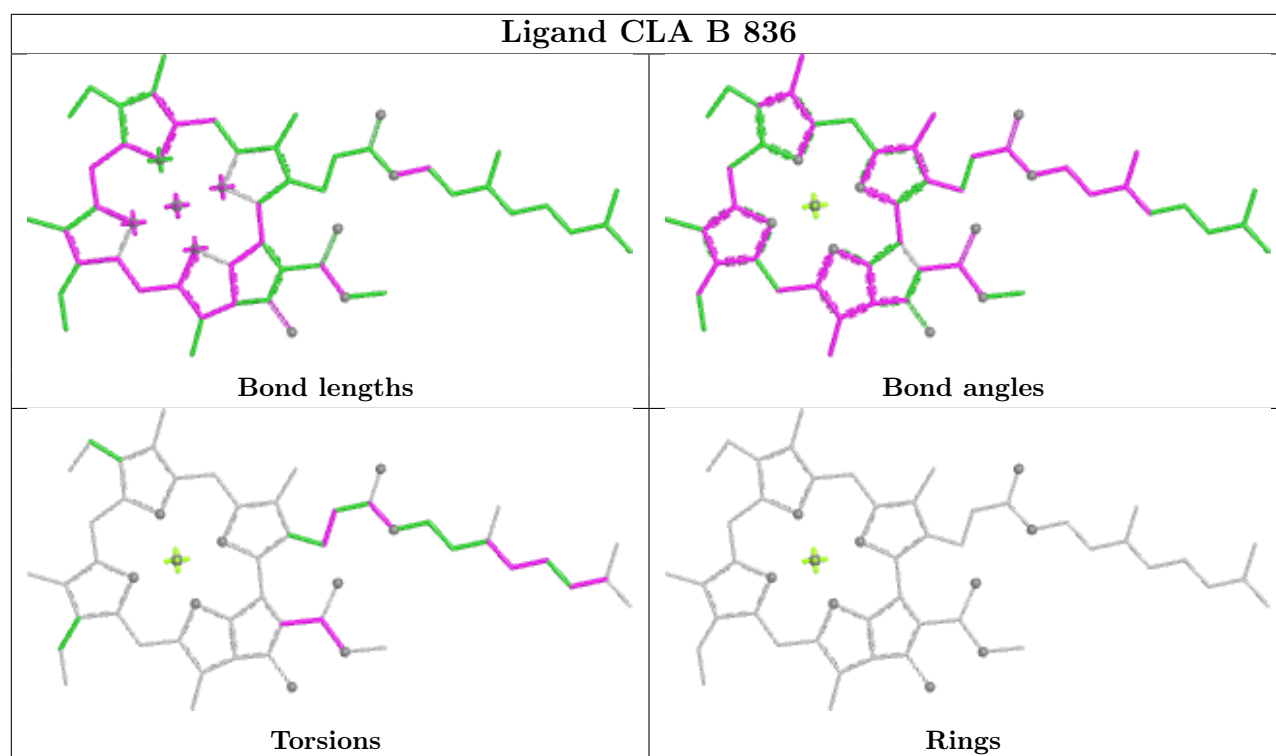
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	801	CLA	2	0
9	B	829	CLA	1	0
9	B	826	CLA	1	0
9	A	818	CLA	1	0
9	B	832	CLA	1	0
9	A	805	CLA	2	0
9	A	820	CLA	1	0

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.

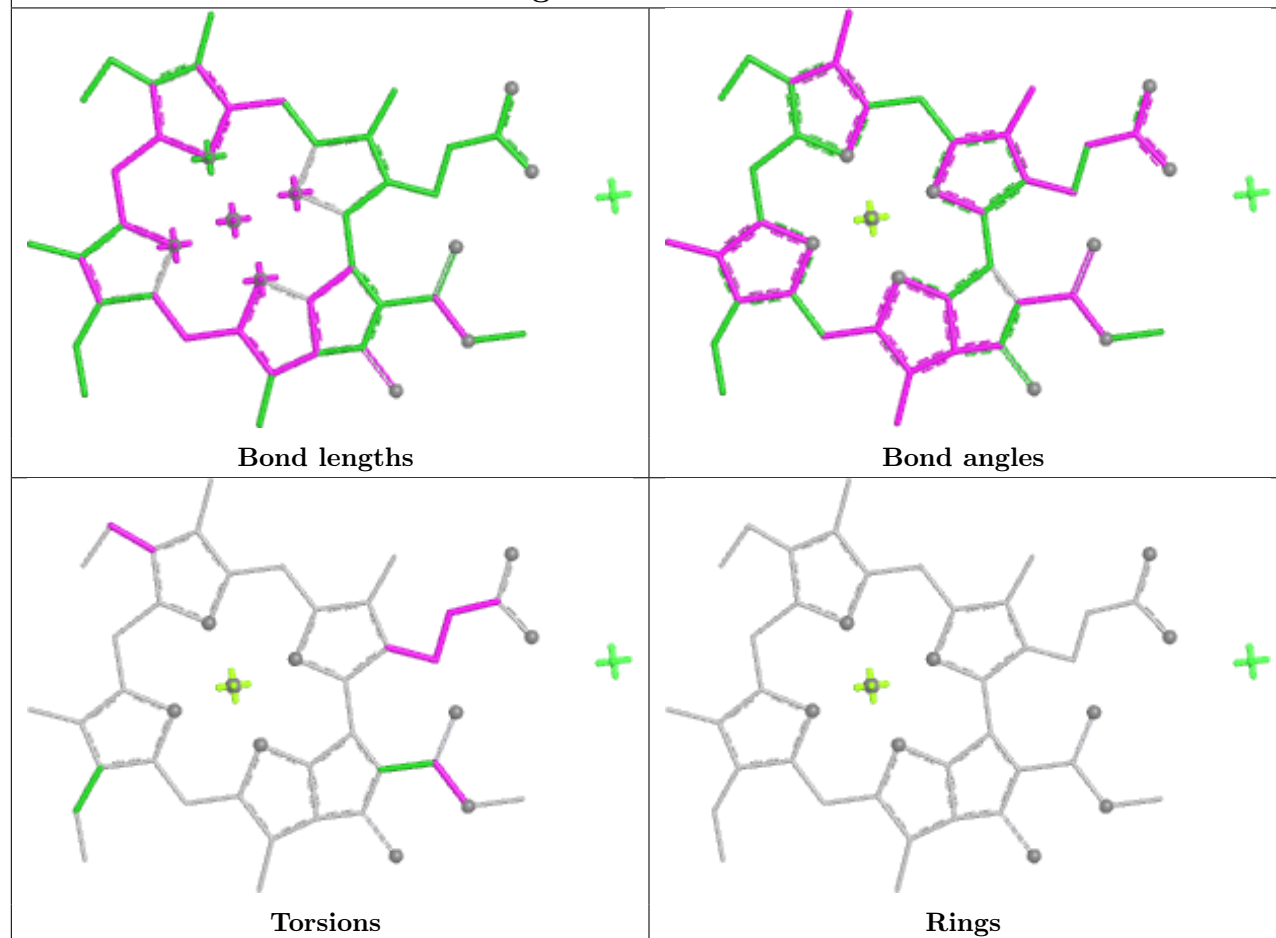




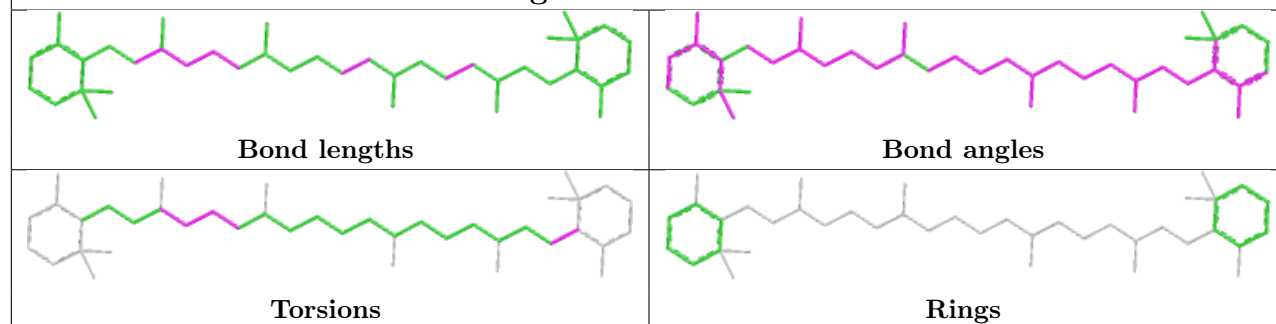


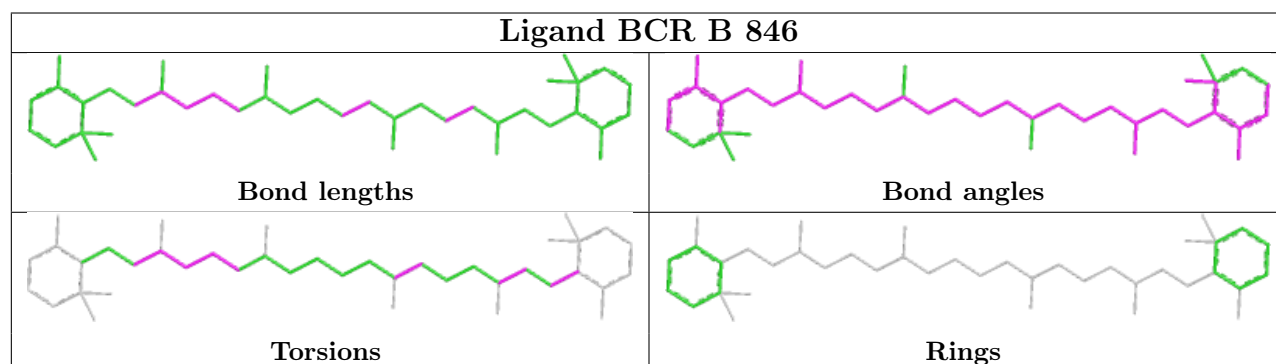
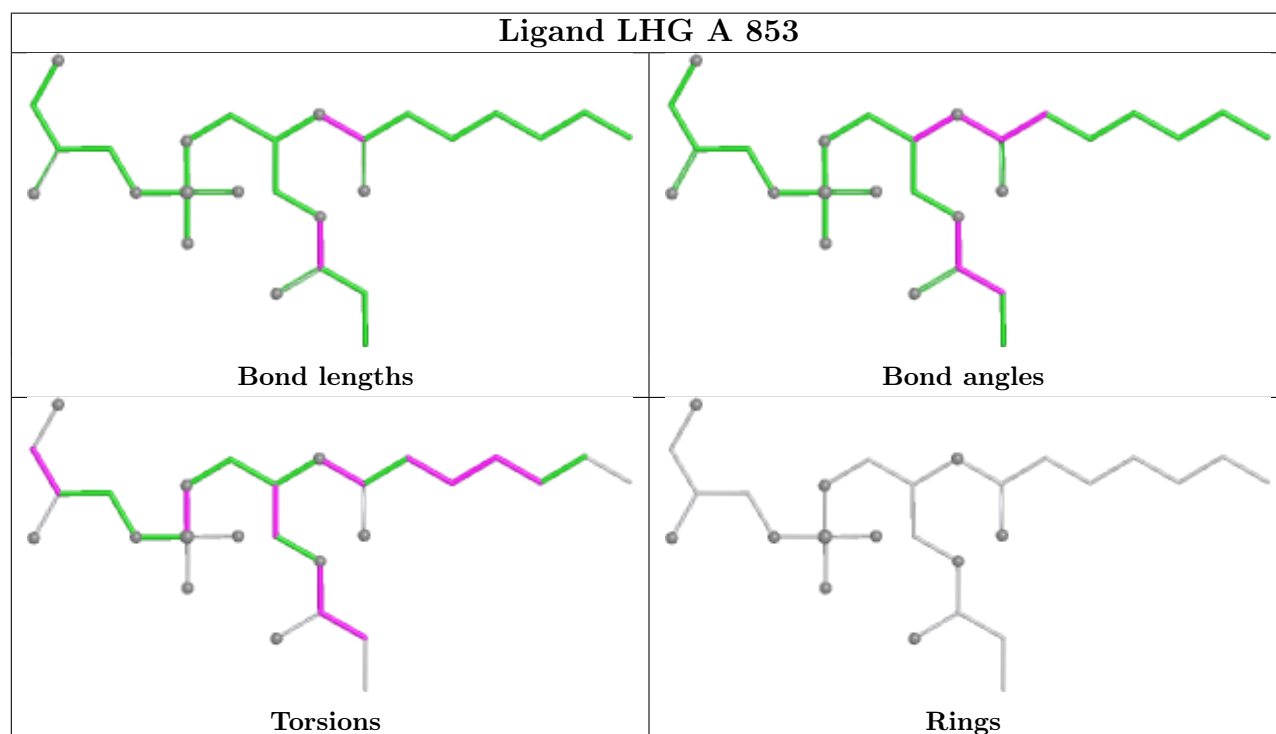
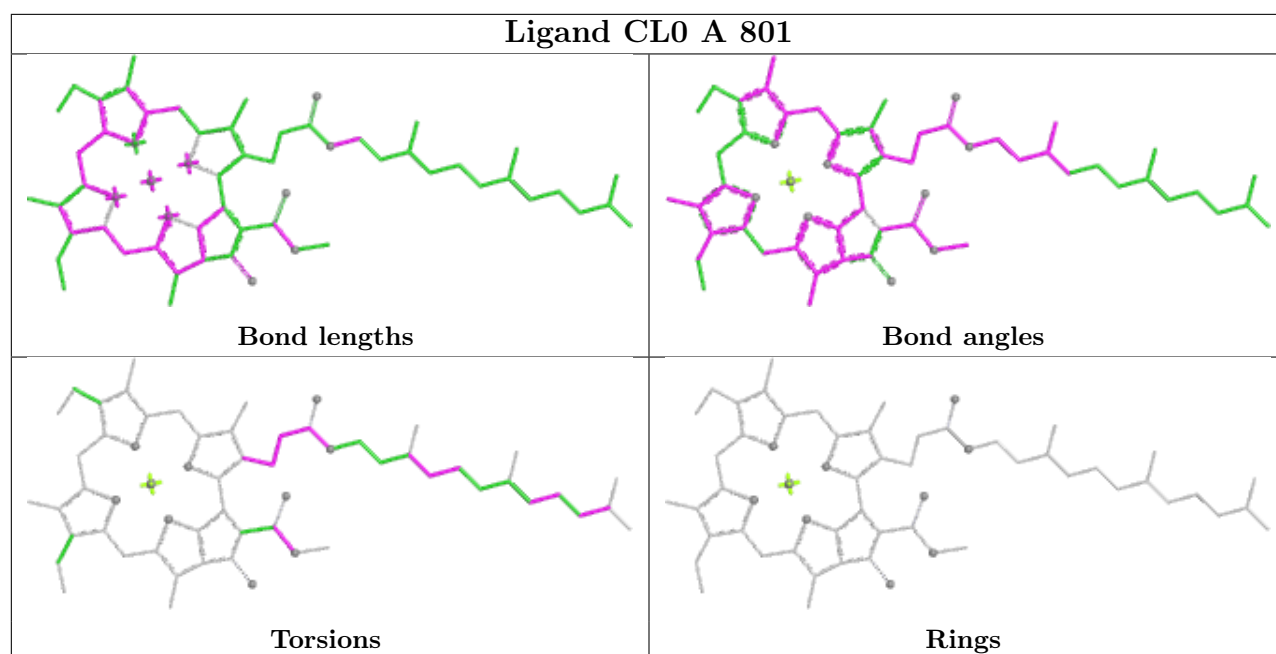


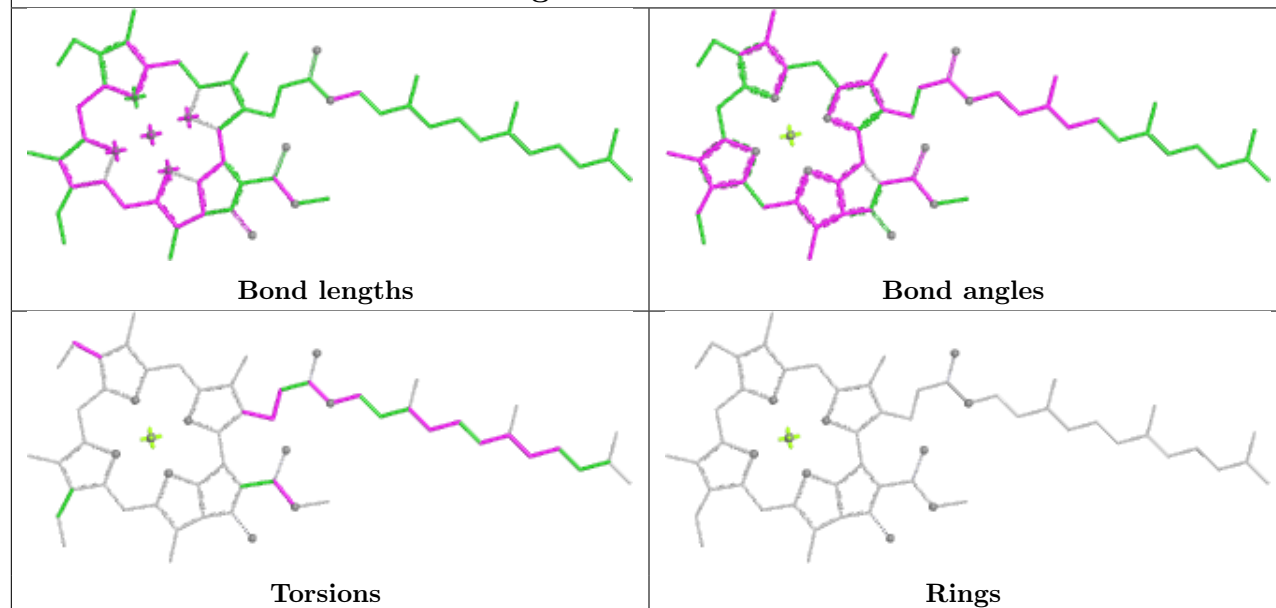
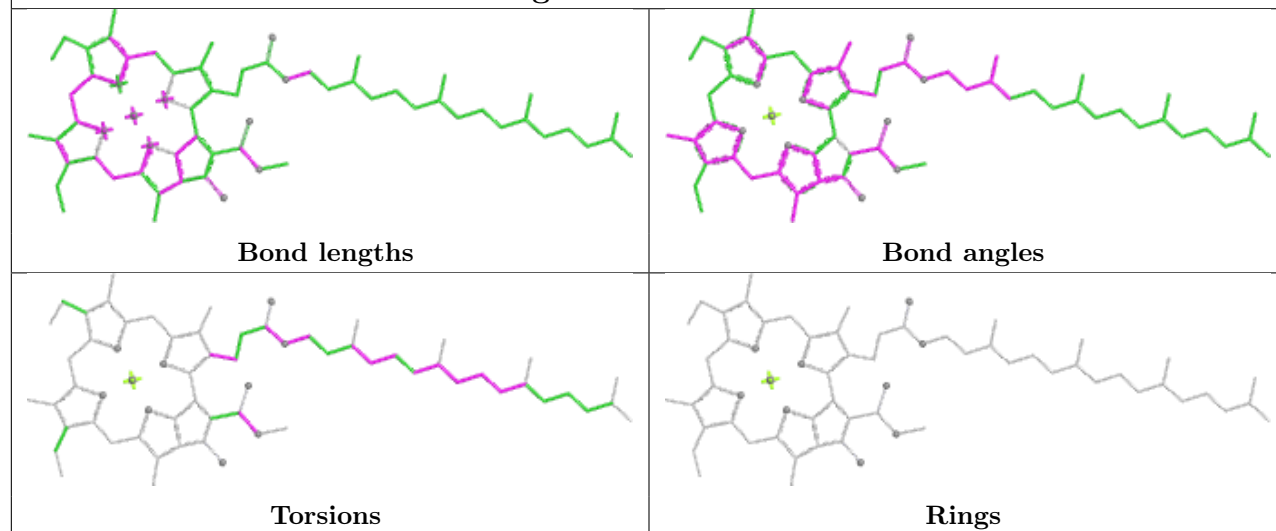
Ligand CLA B 810

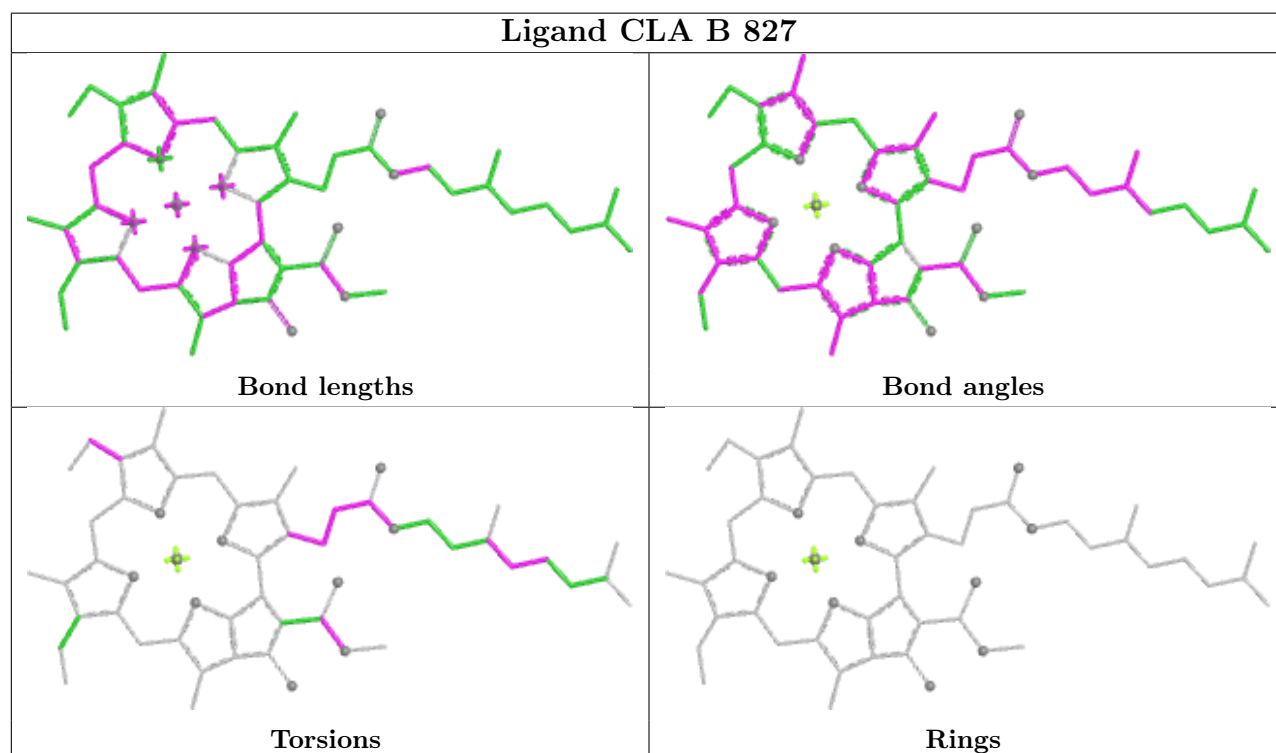
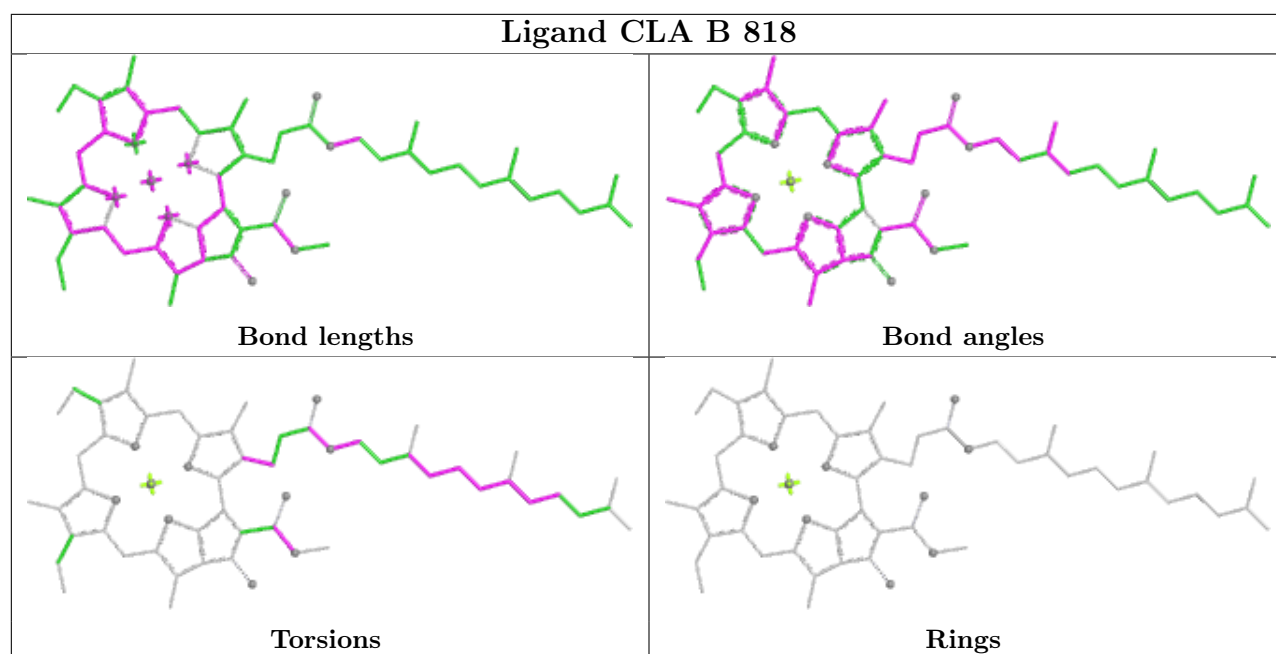


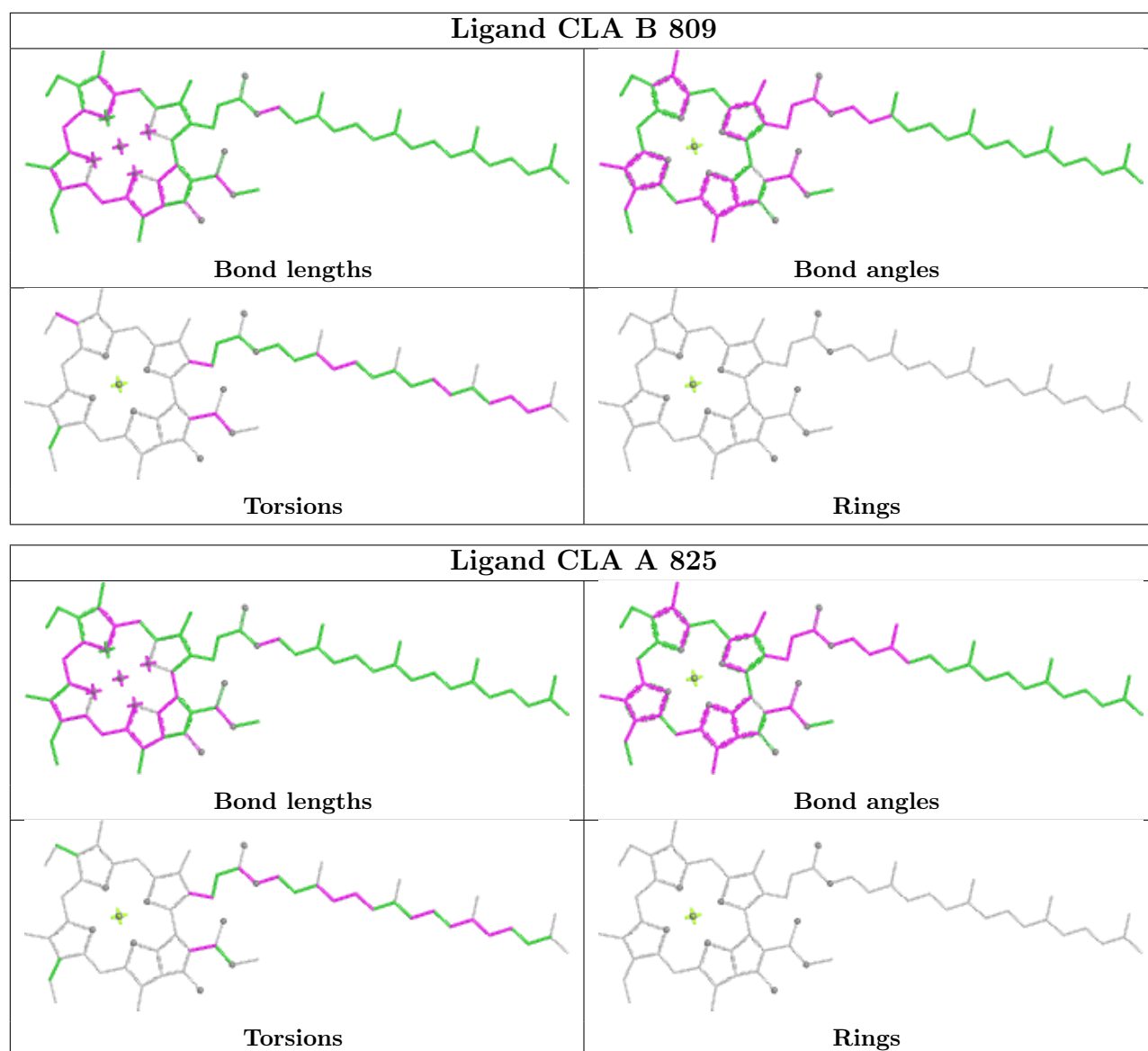
Ligand BCR A 847



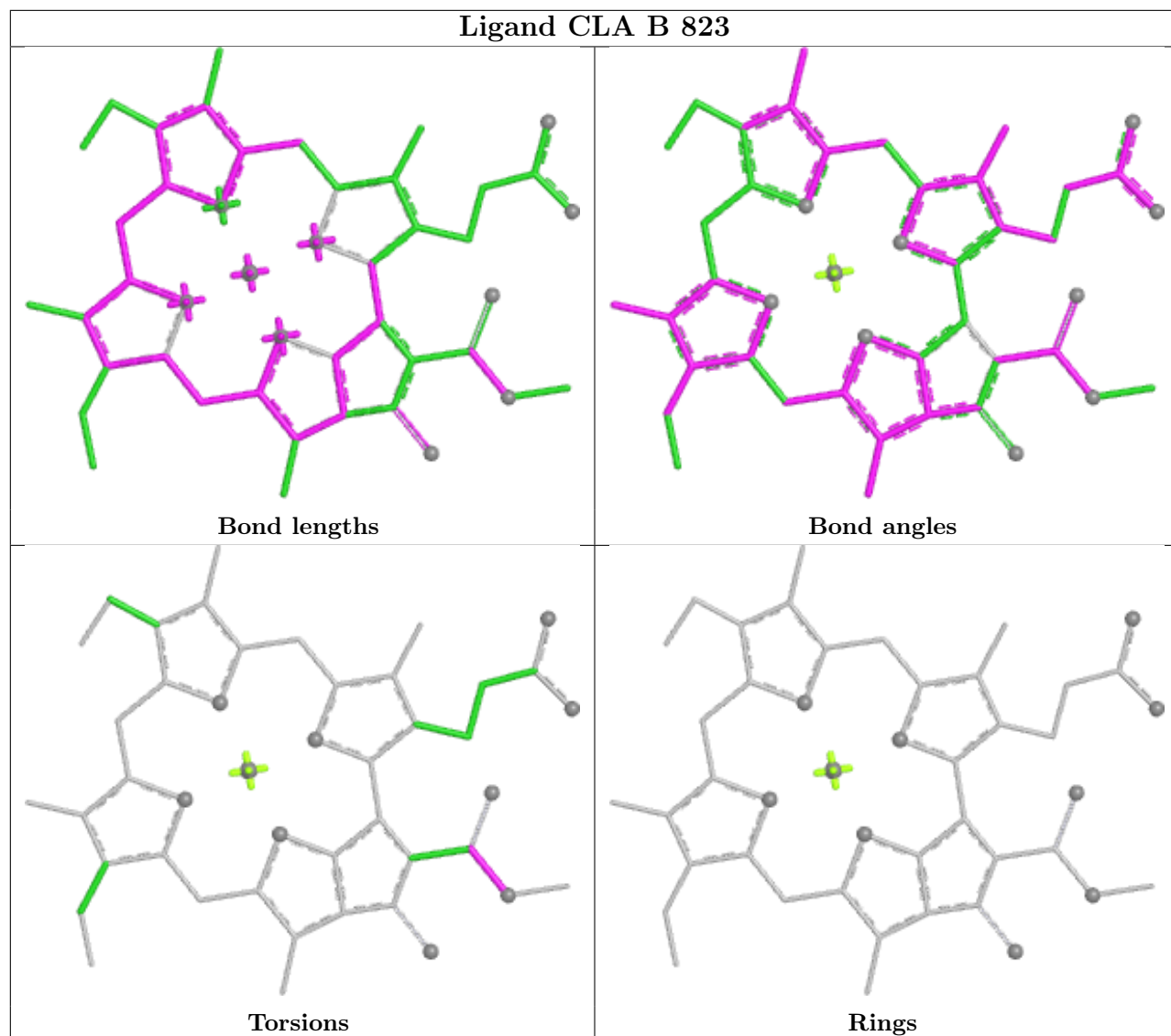


Ligand CLA A 813**Ligand CLA B 803**

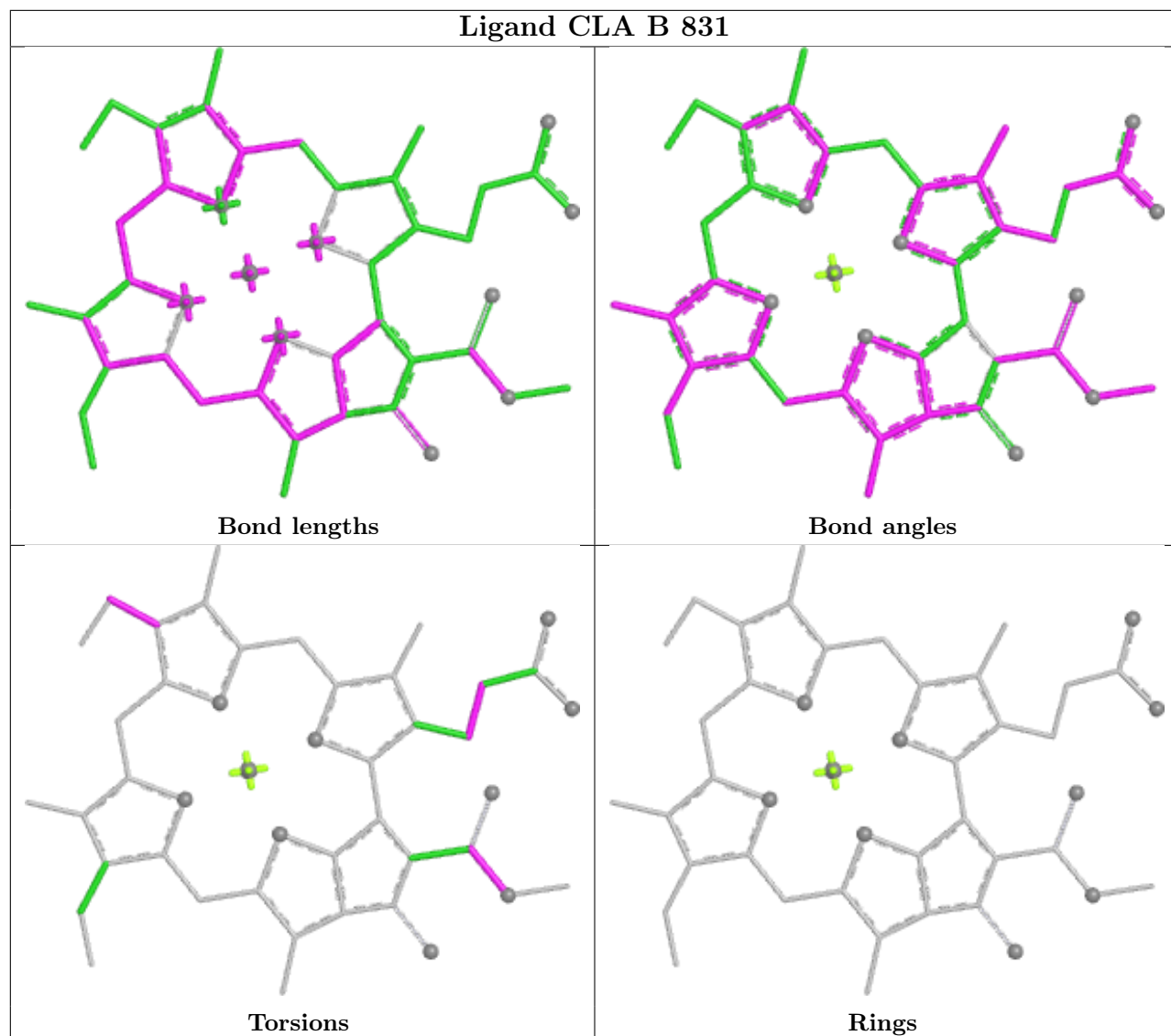




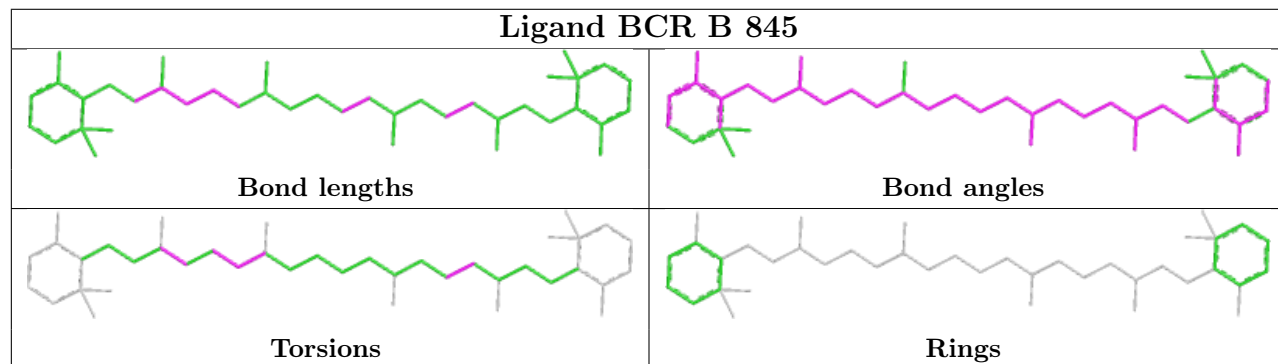
Ligand CLA B 823

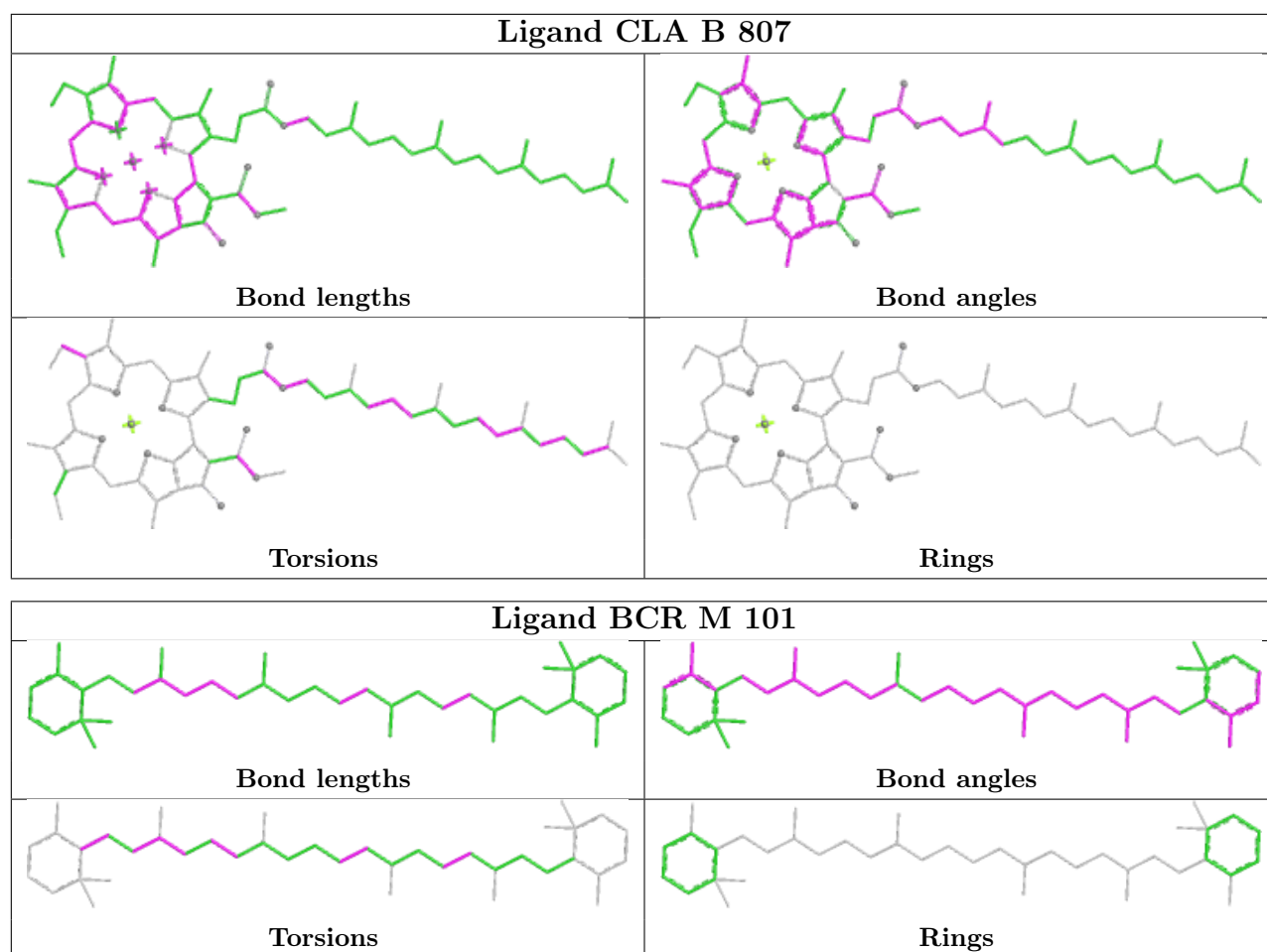


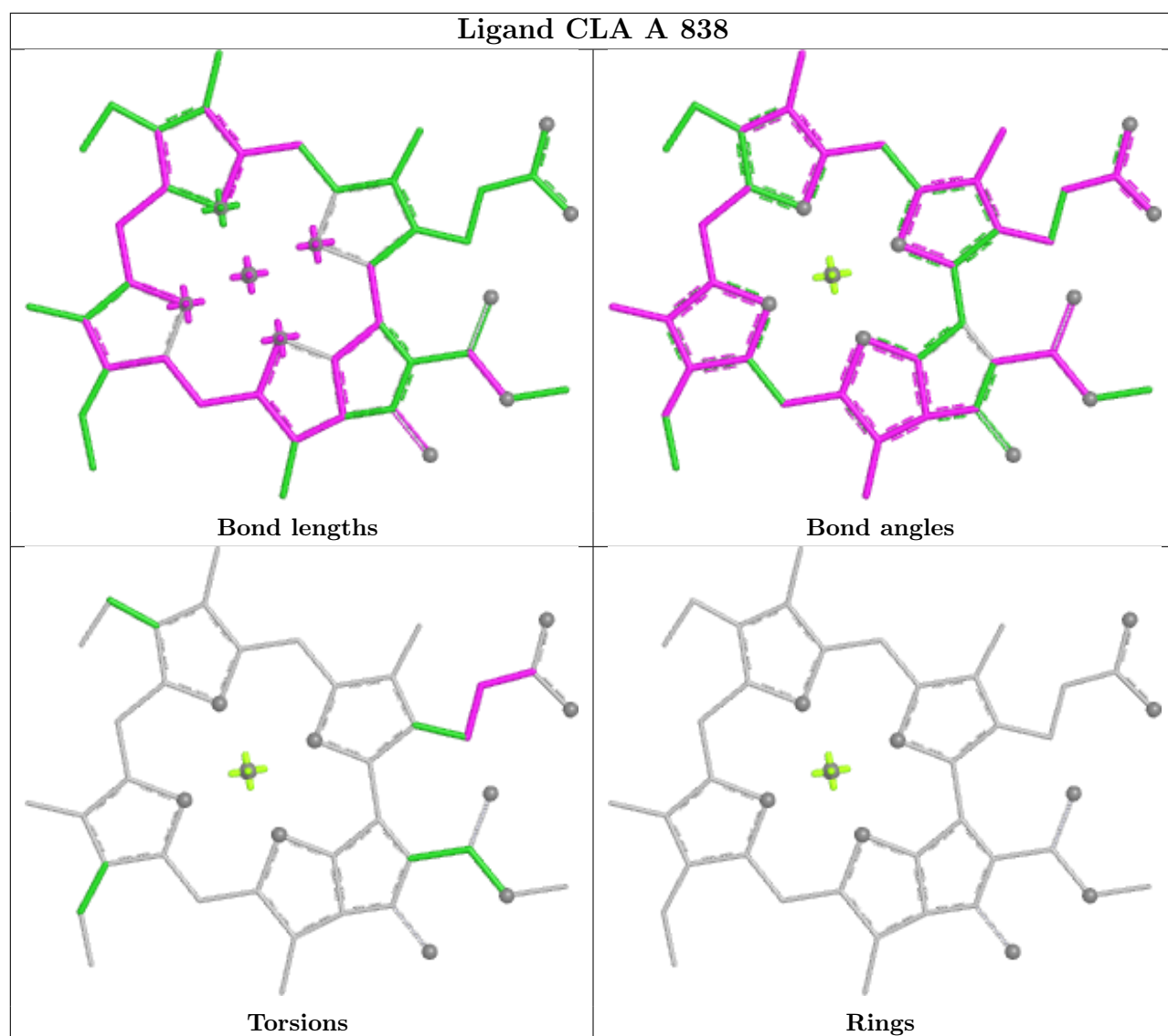
Ligand CLA B 831

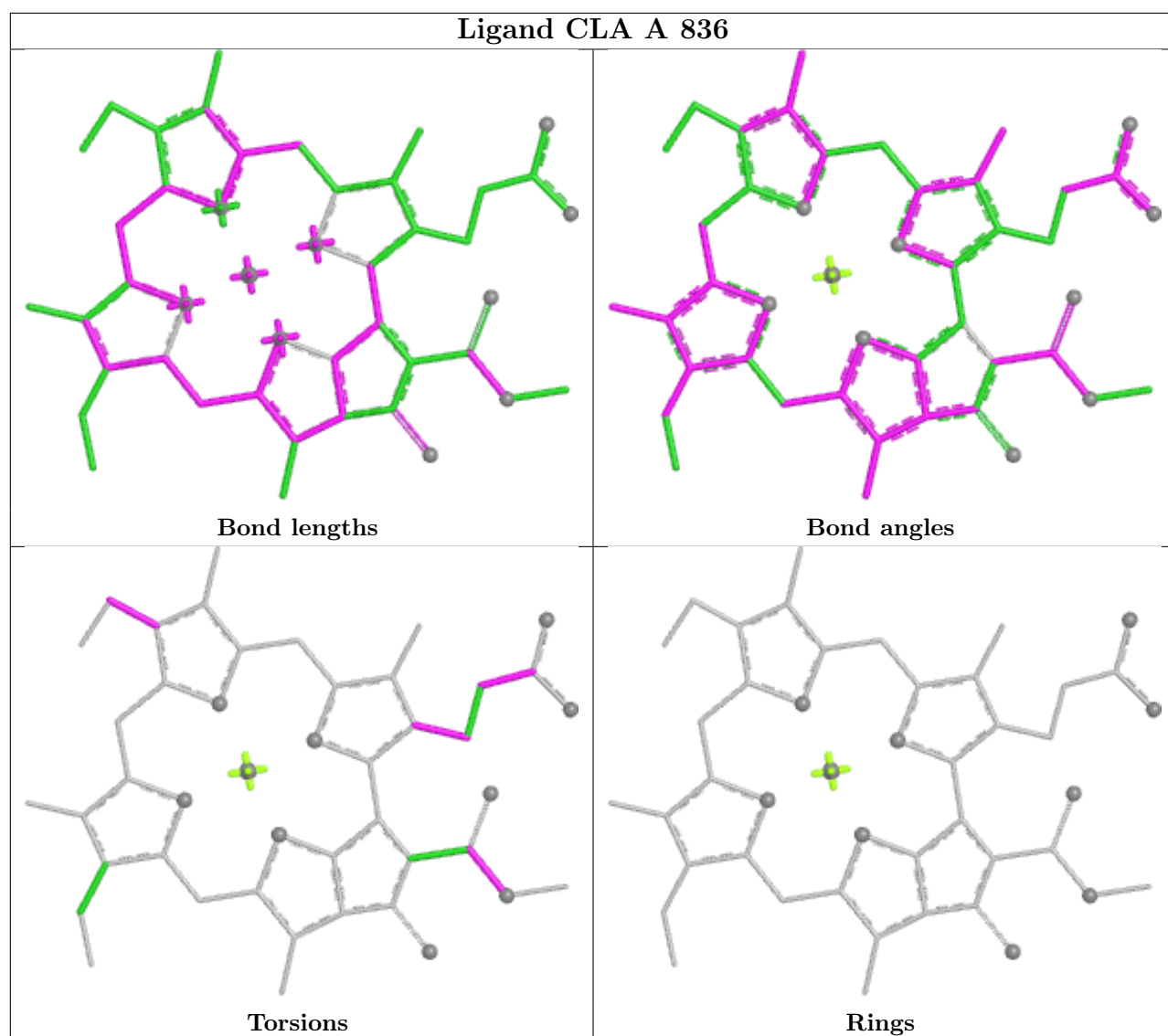


Ligand BCR B 845

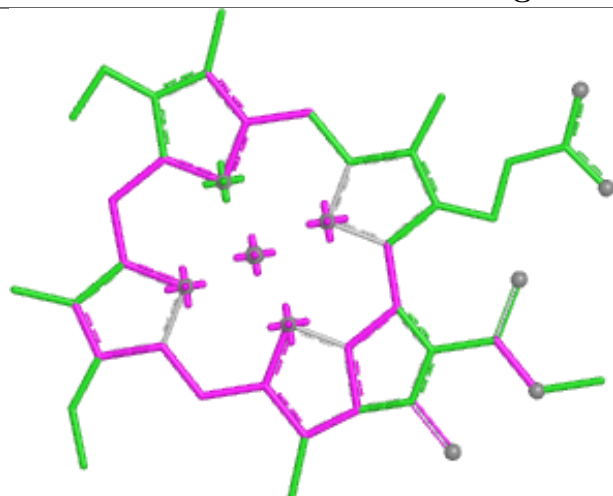




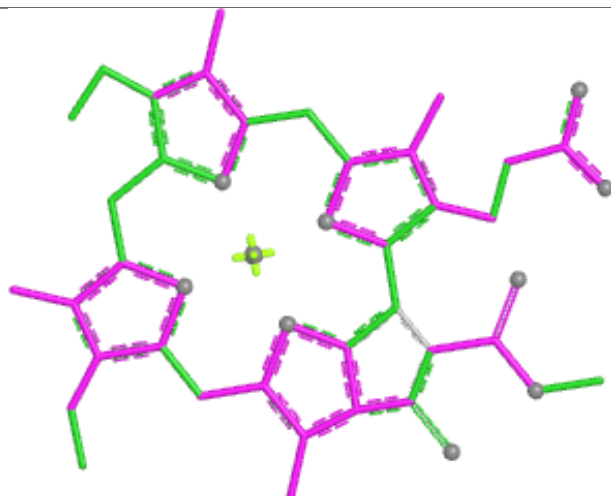




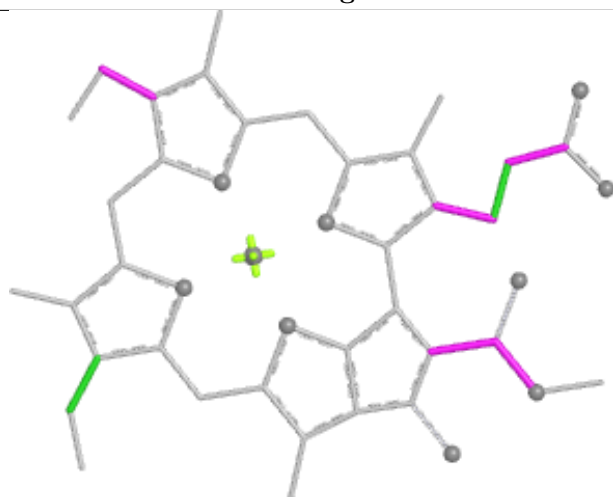
Ligand CLA A 803



Bond lengths



Bond angles

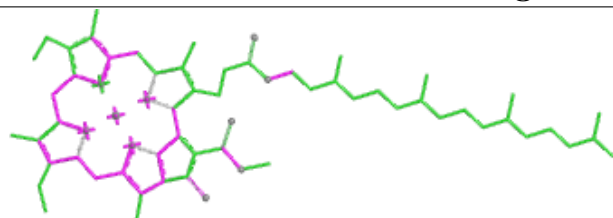


Torsions

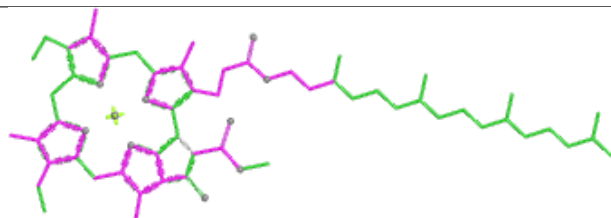


Rings

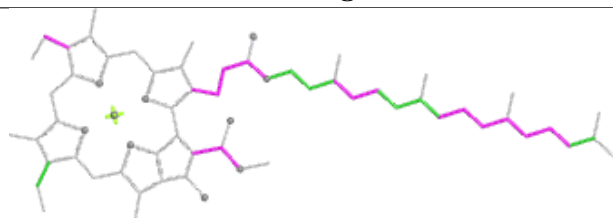
Ligand CLA B 813



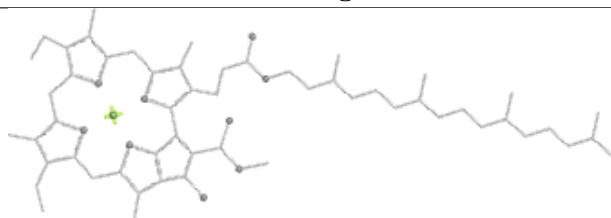
Bond lengths



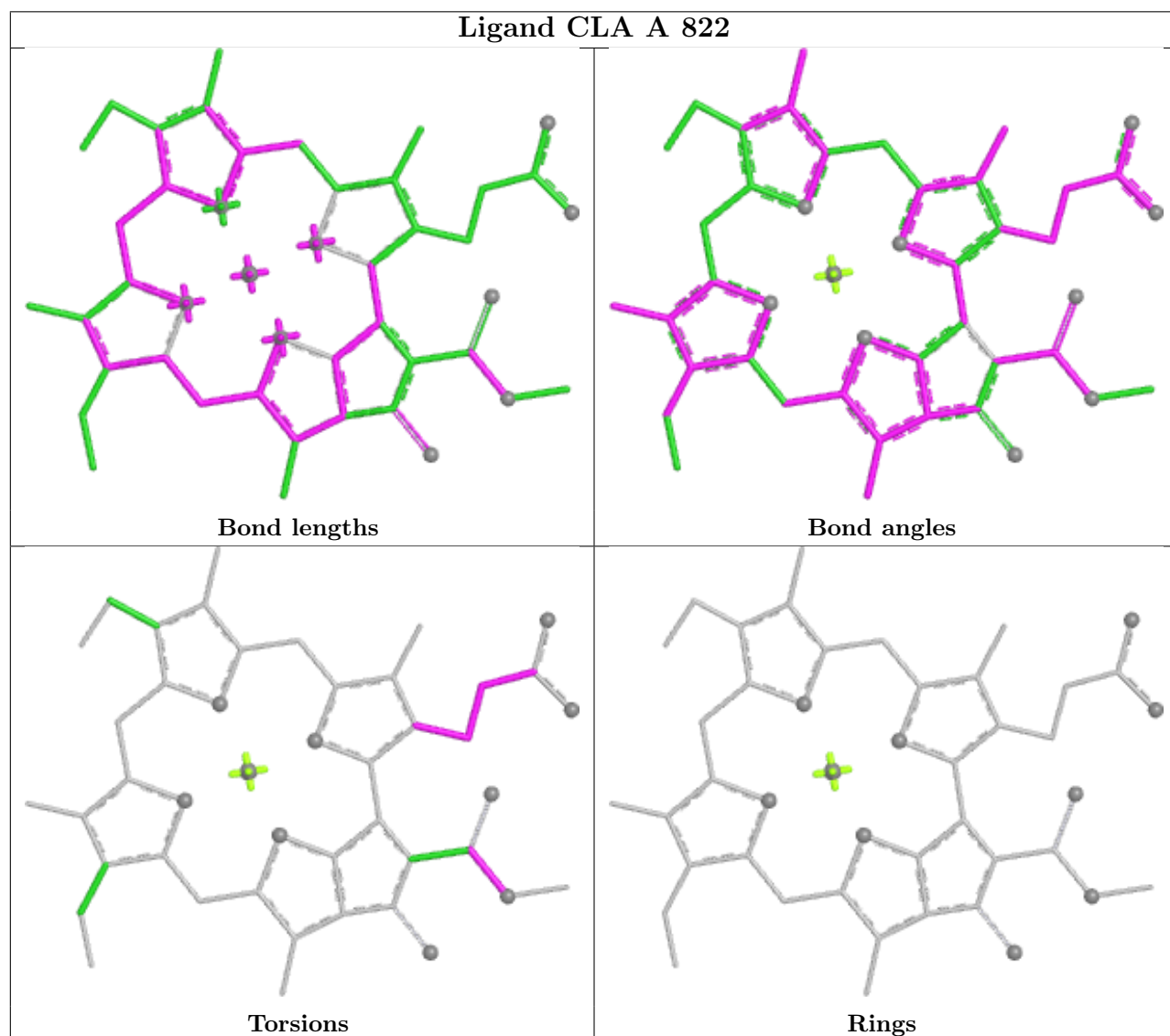
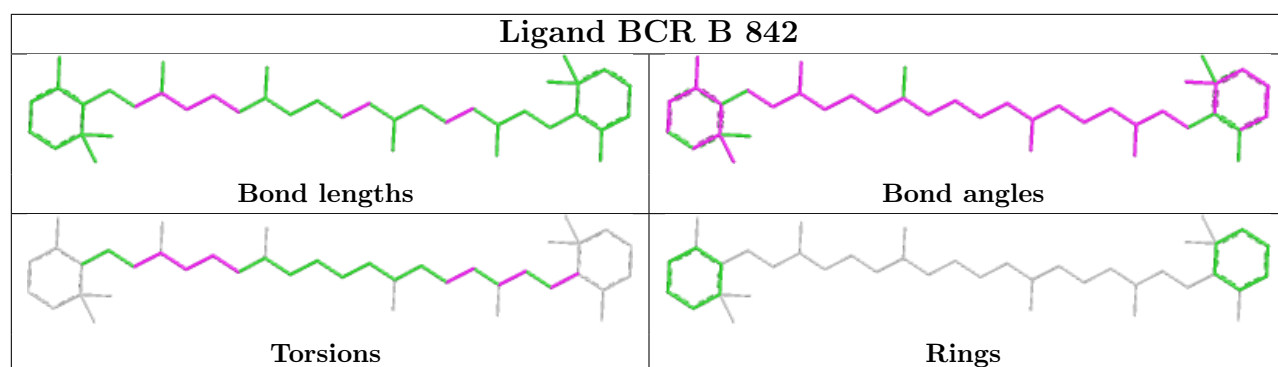
Bond angles



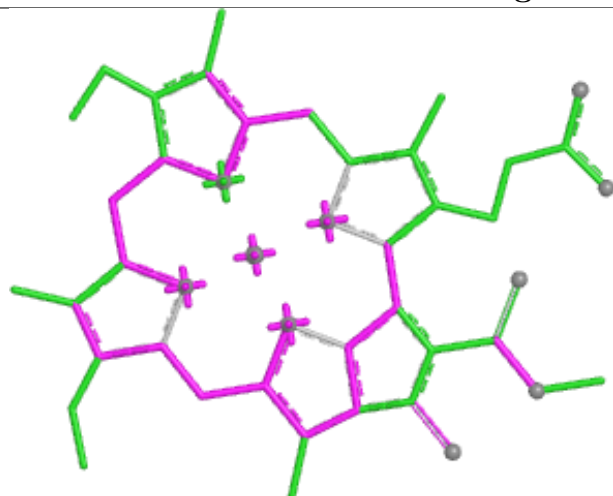
Torsions



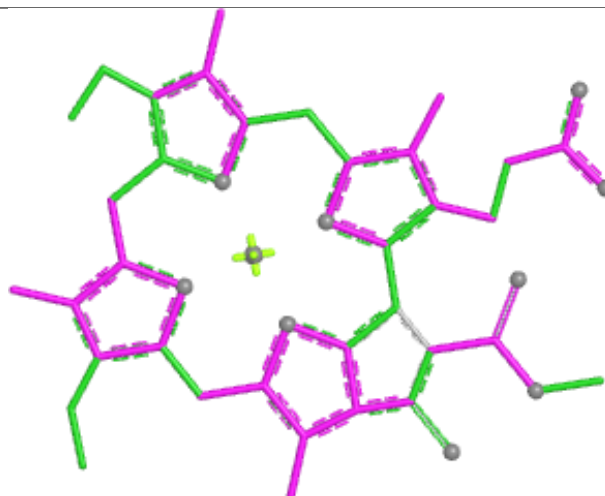
Rings



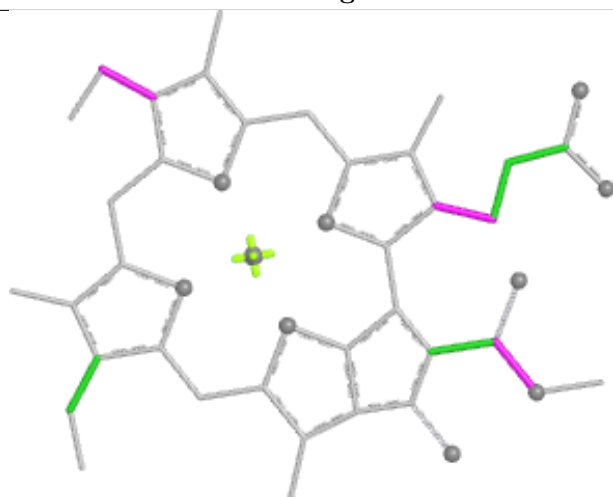
Ligand CLA B 811



Bond lengths



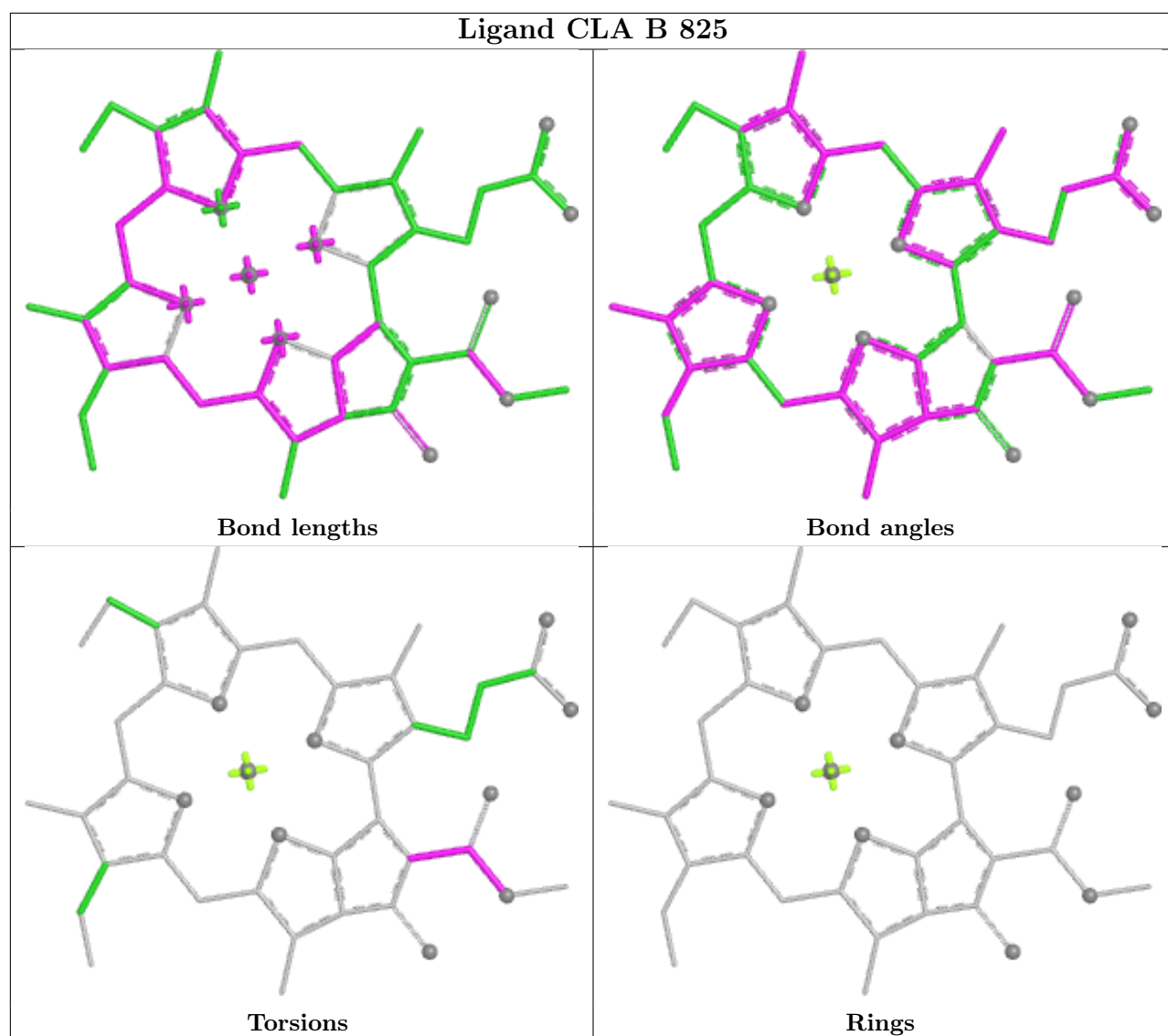
Bond angles



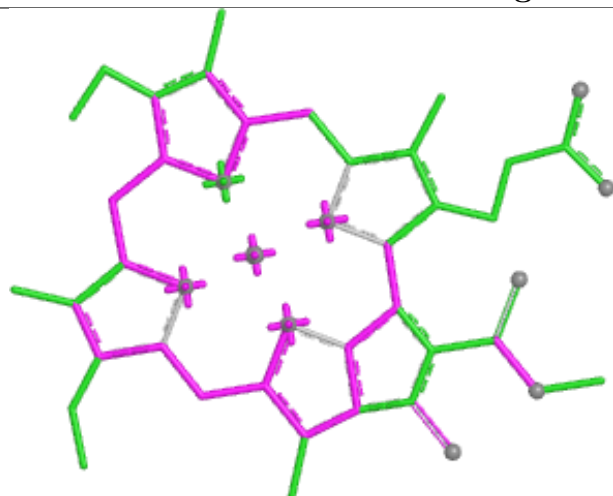
Torsions



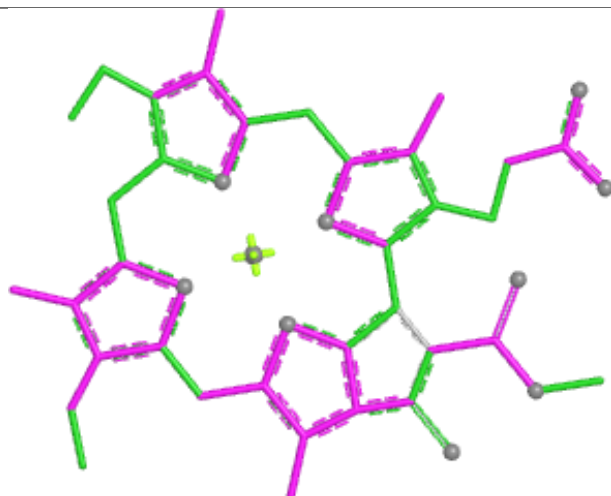
Rings



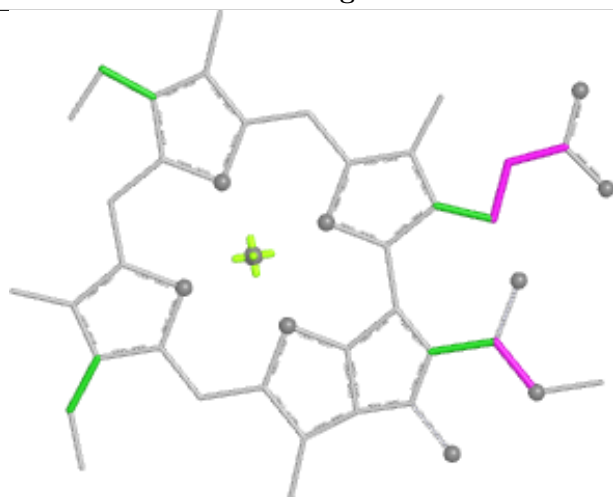
Ligand CLA B 805



Bond lengths



Bond angles

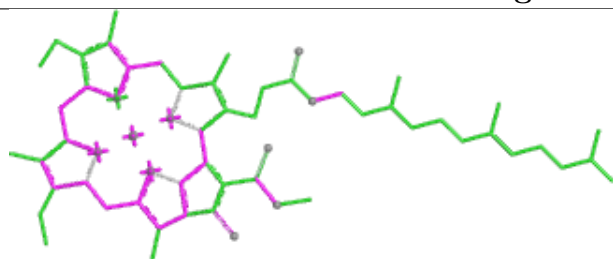


Torsions

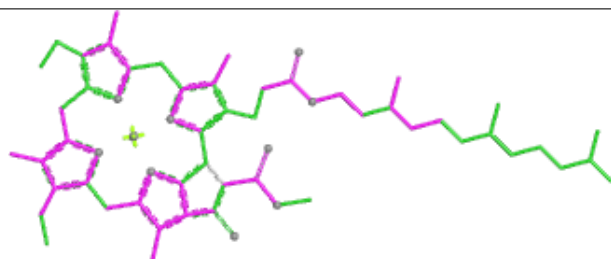


Rings

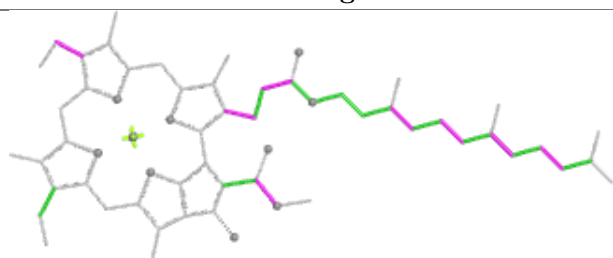
Ligand CLA B 837



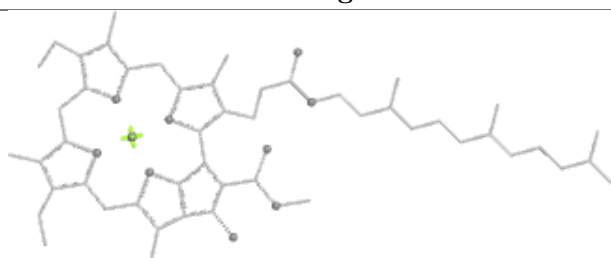
Bond lengths



Bond angles

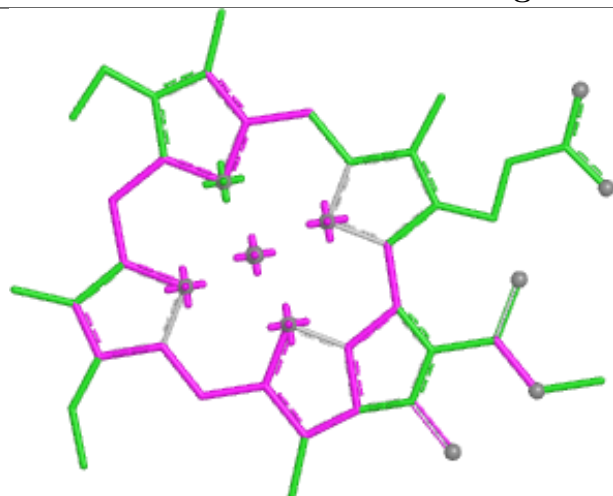


Torsions

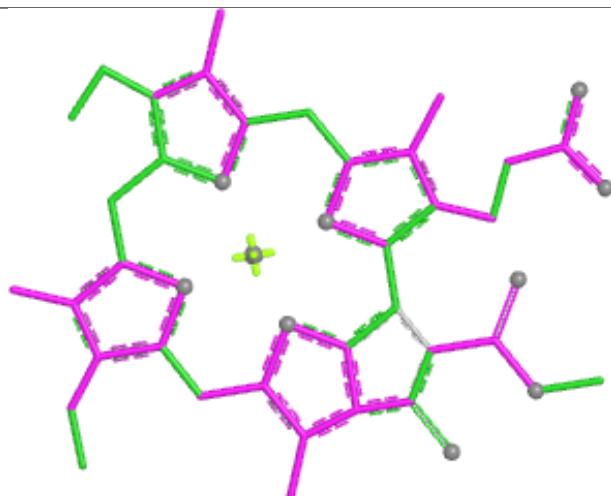


Rings

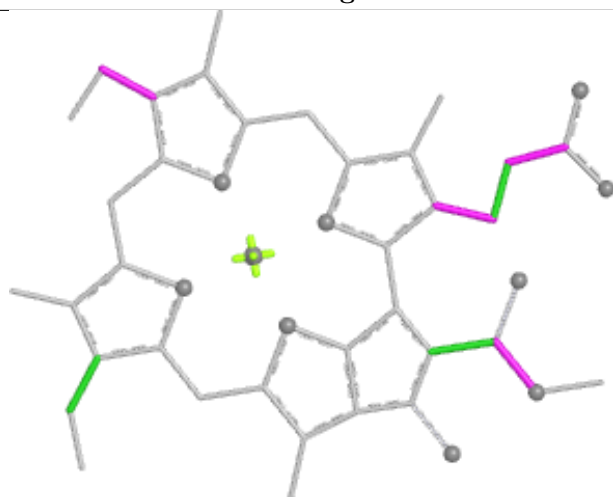
Ligand CLA A 815



Bond lengths



Bond angles

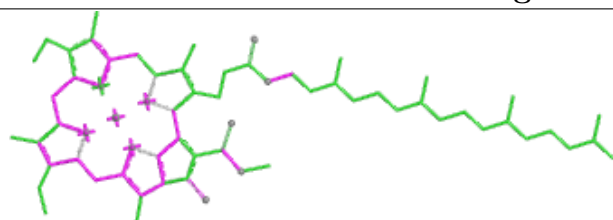


Torsions

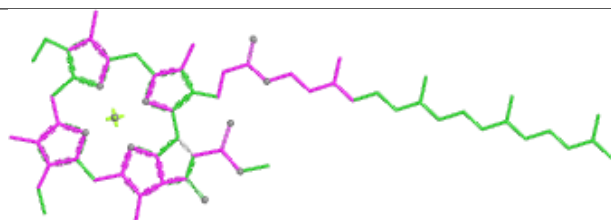


Rings

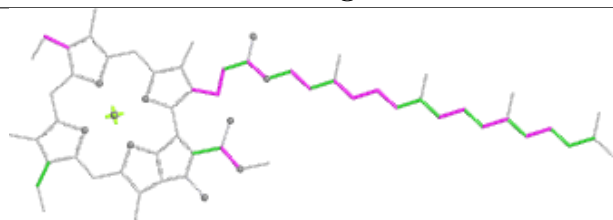
Ligand CLA A 828



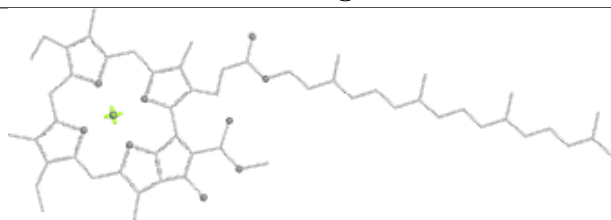
Bond lengths



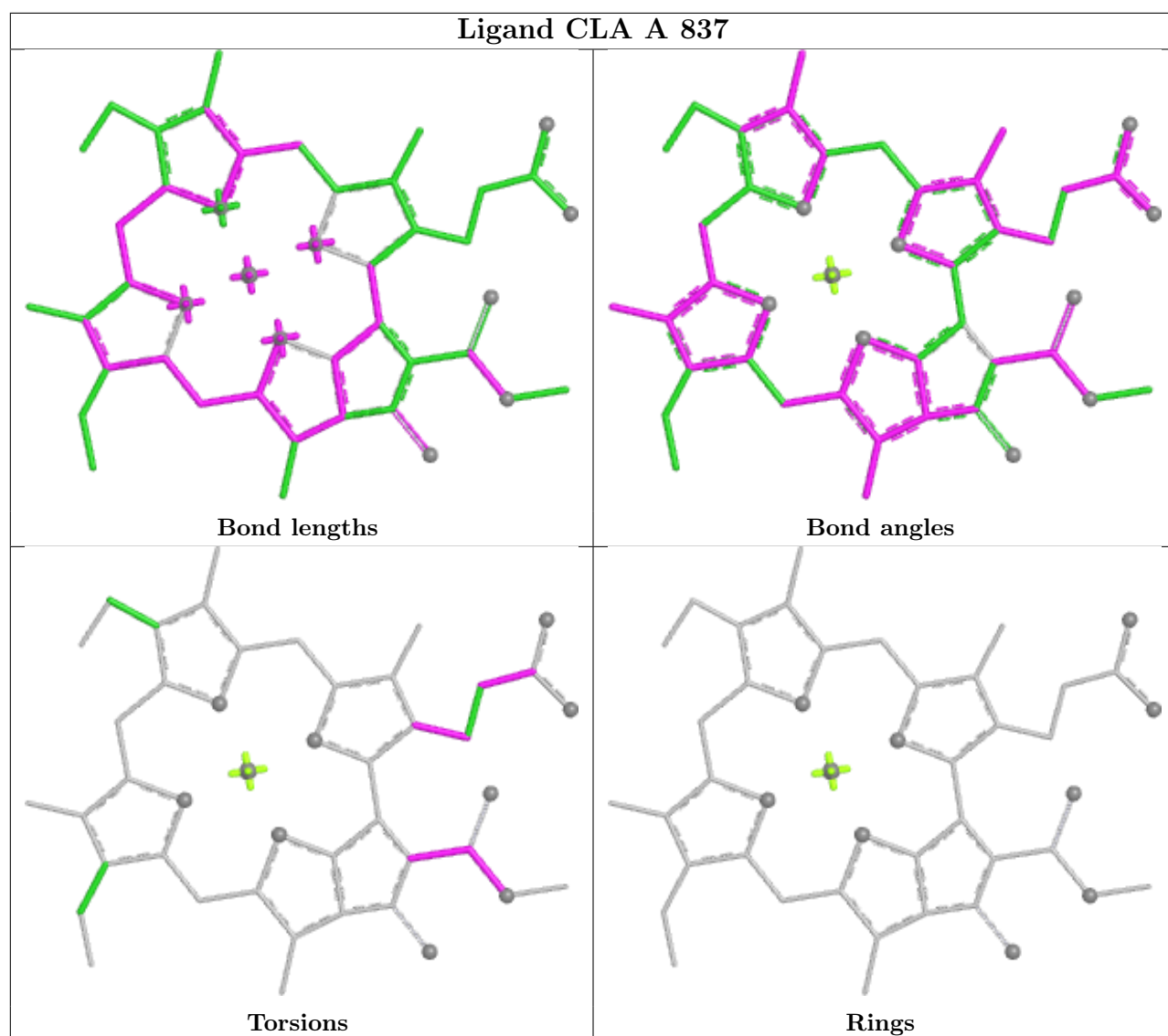
Bond angles



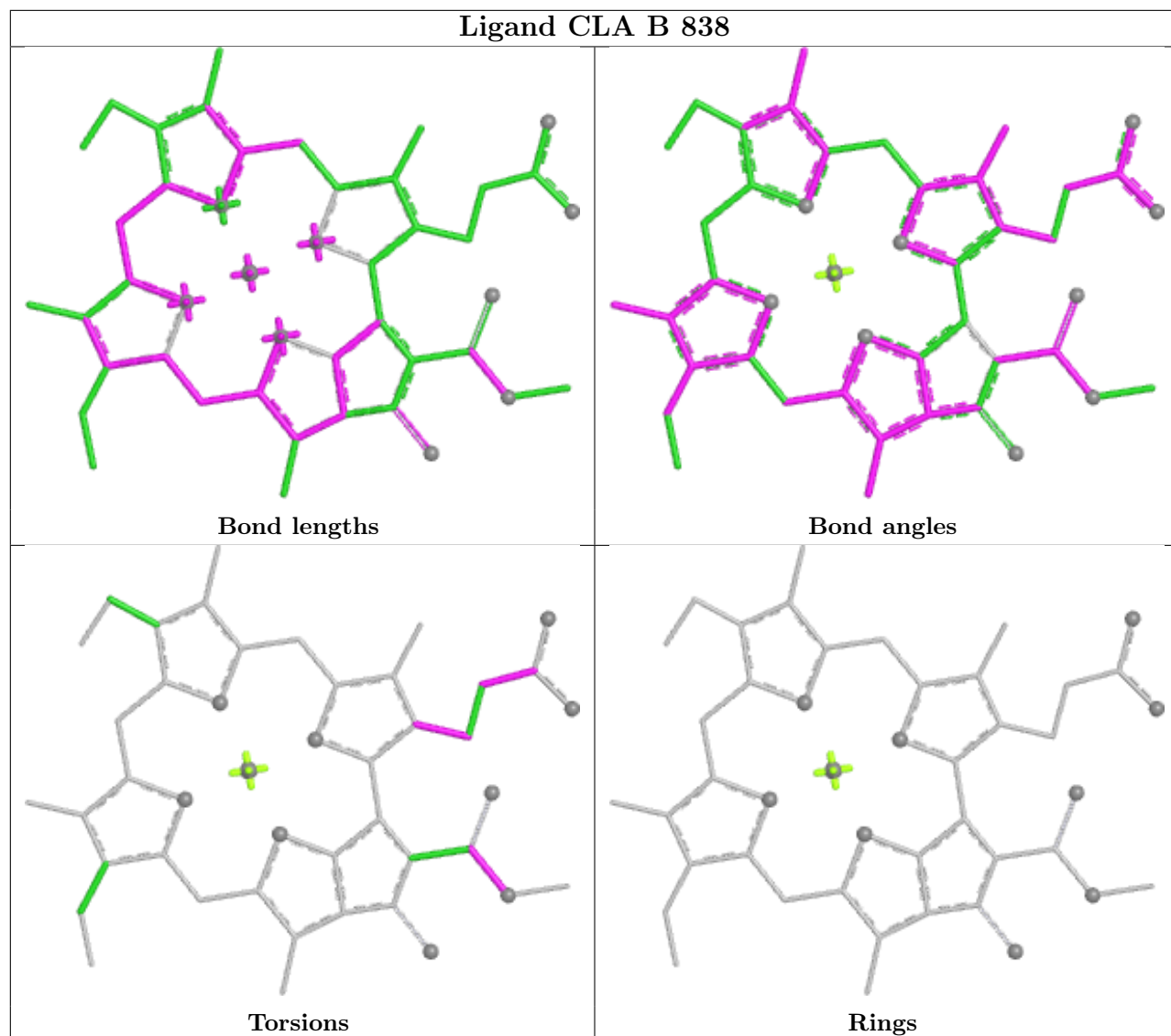
Torsions



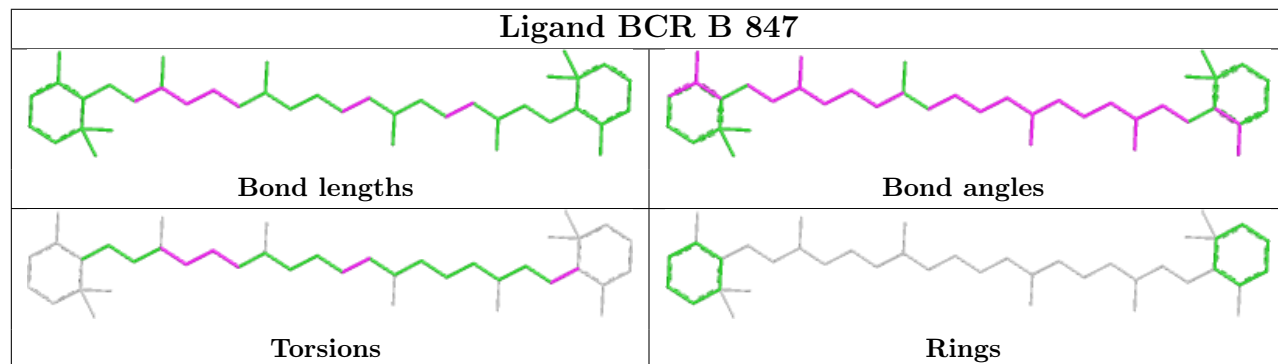
Rings

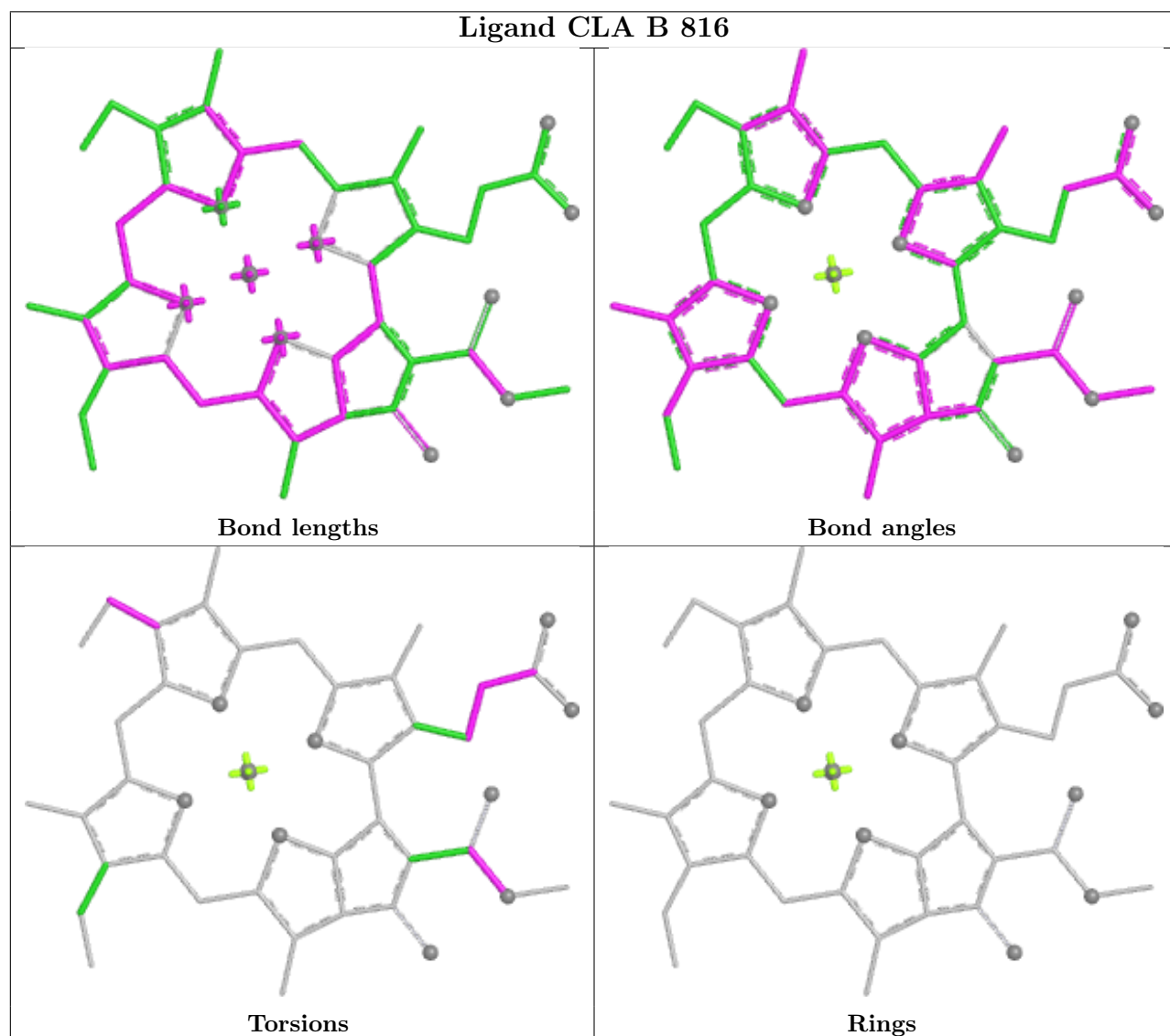
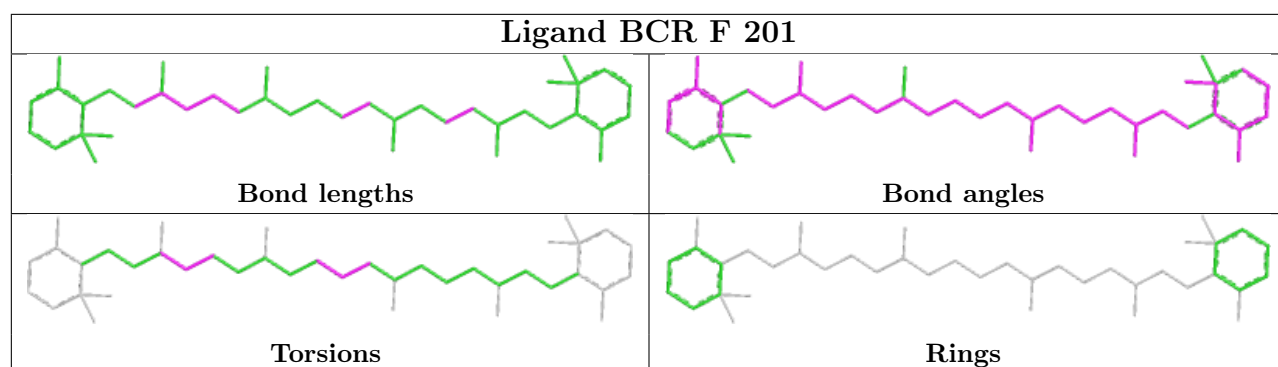


Ligand CLA B 838

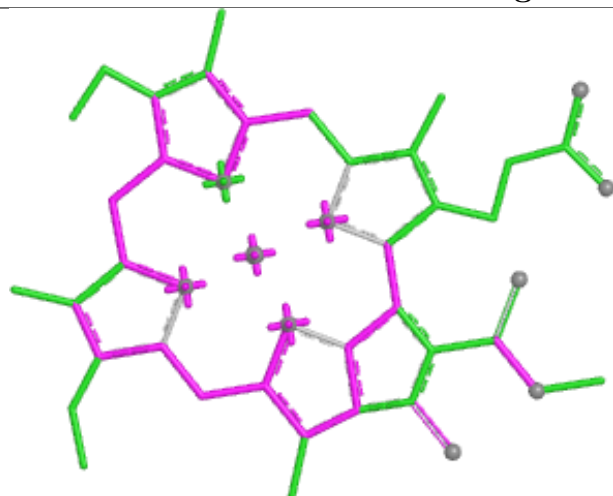


Ligand BCR B 847

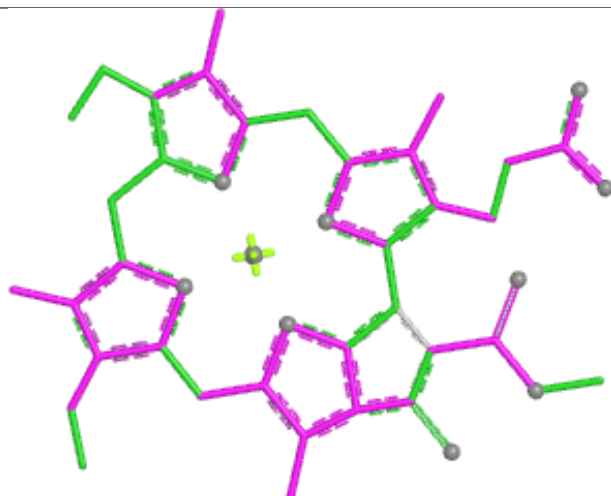




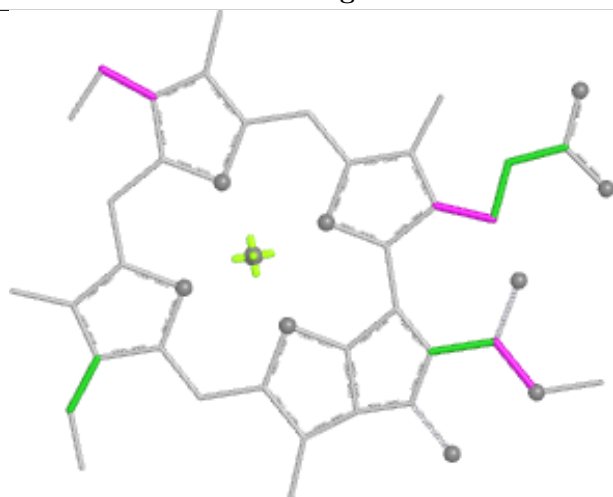
Ligand CLA B 835



Bond lengths



Bond angles

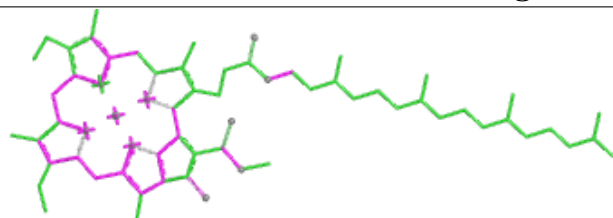


Torsions

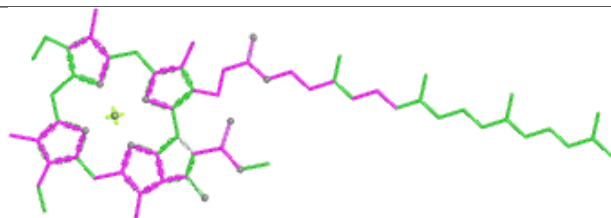


Rings

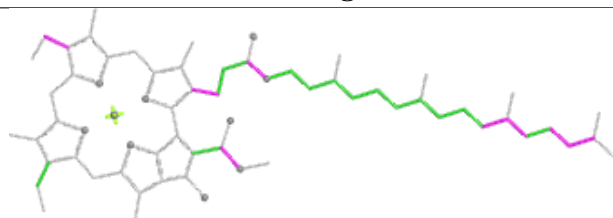
Ligand CLA A 819



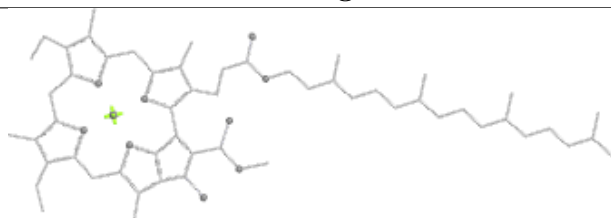
Bond lengths



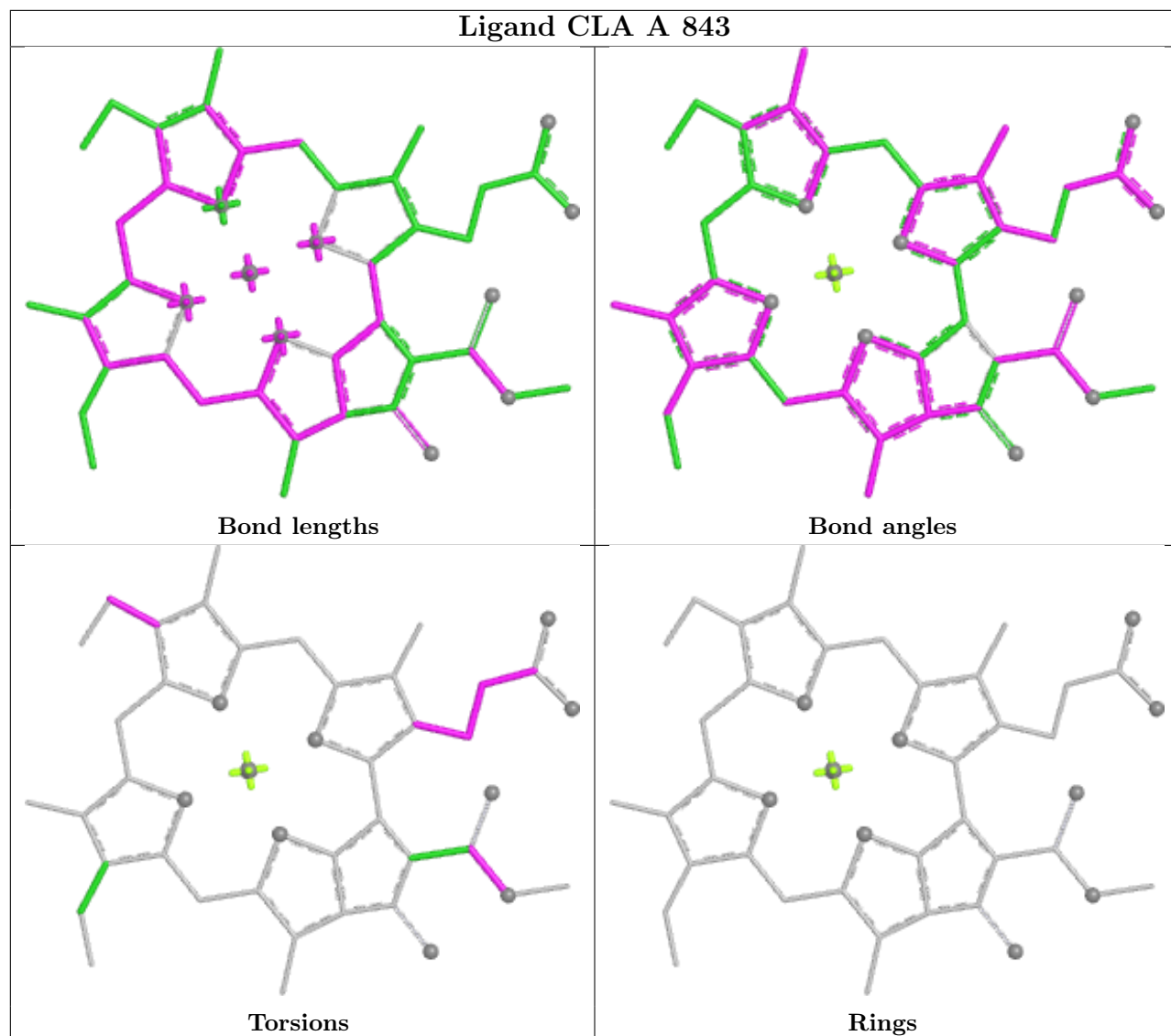
Bond angles

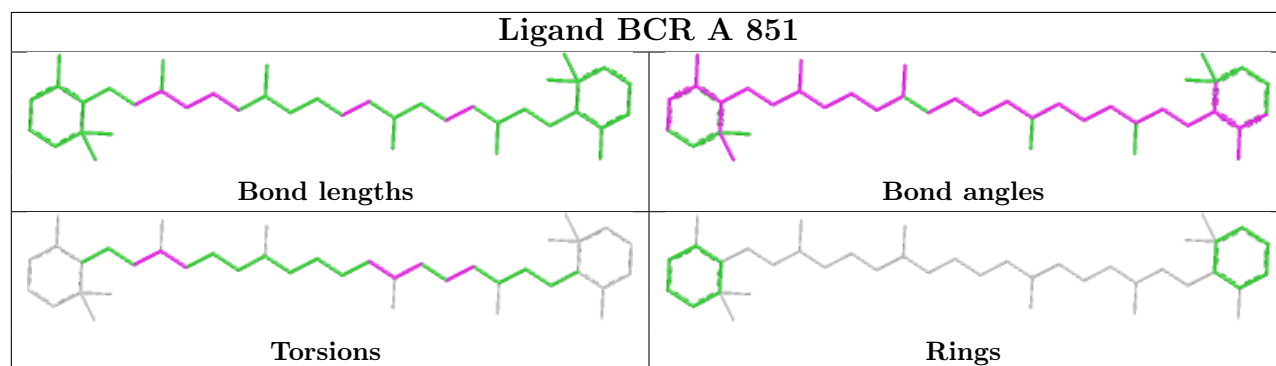
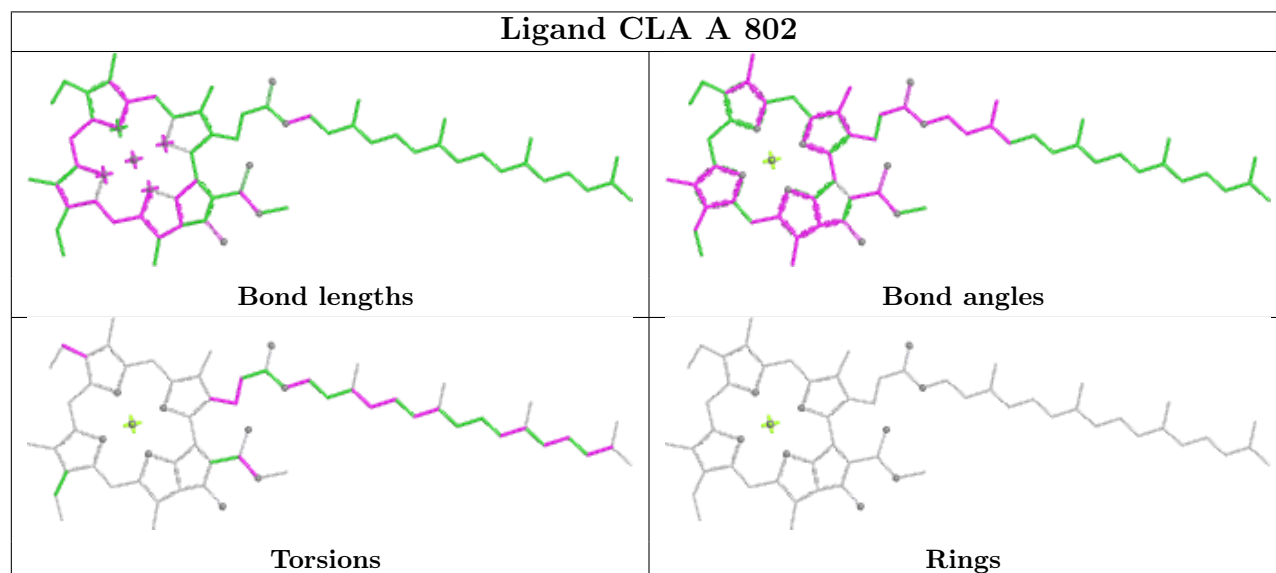
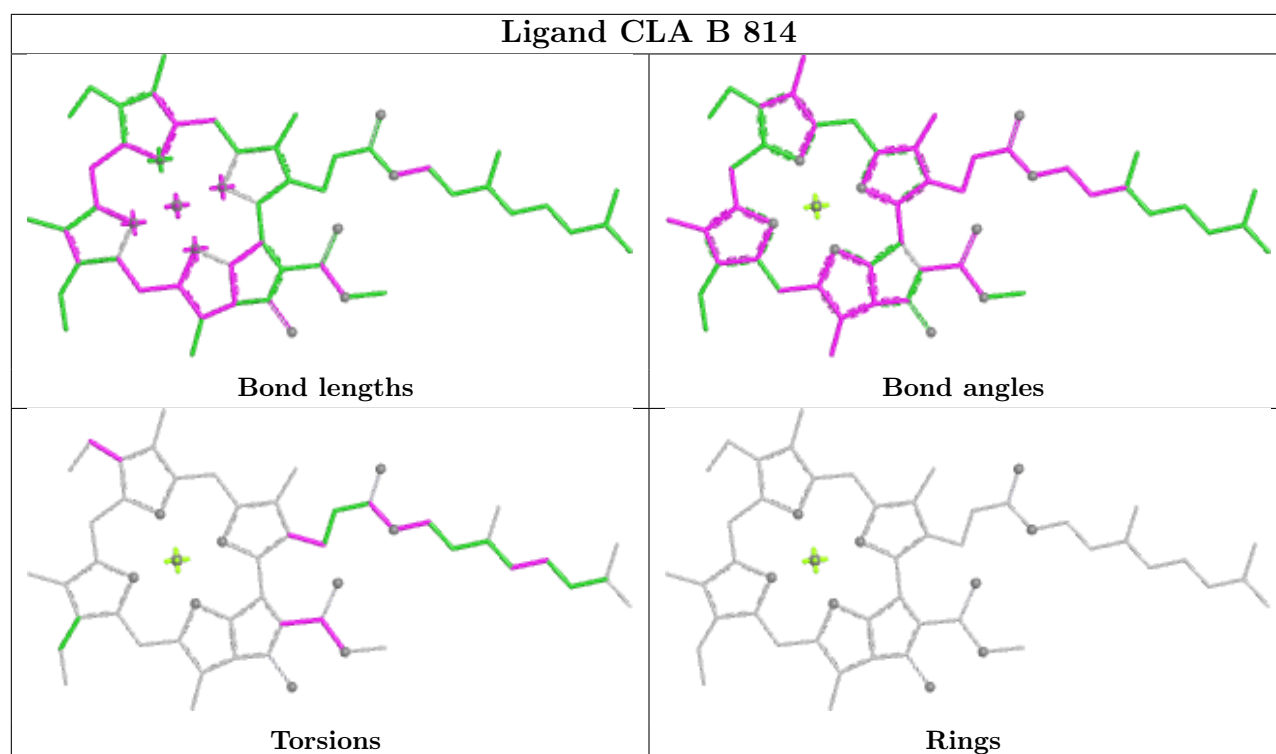


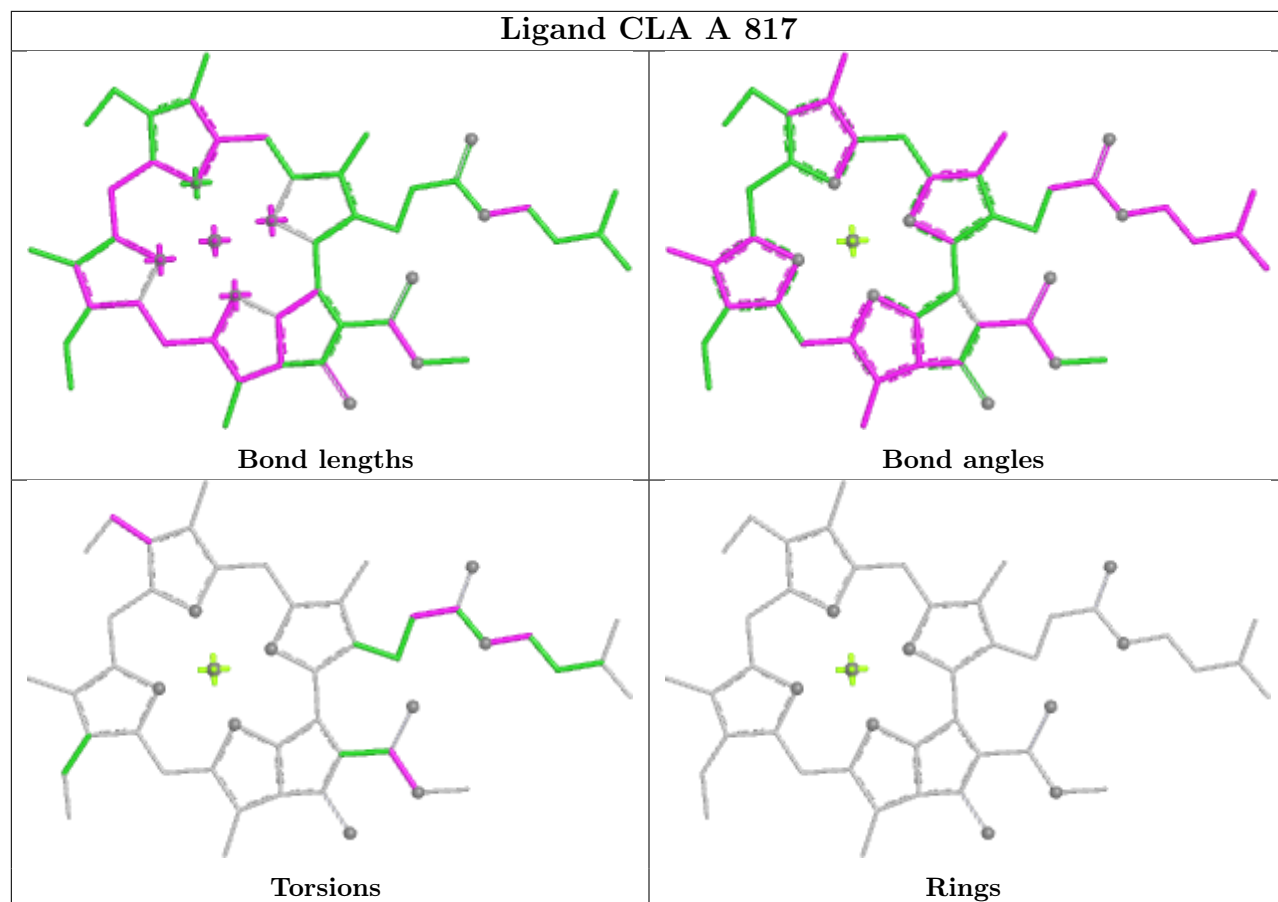
Torsions

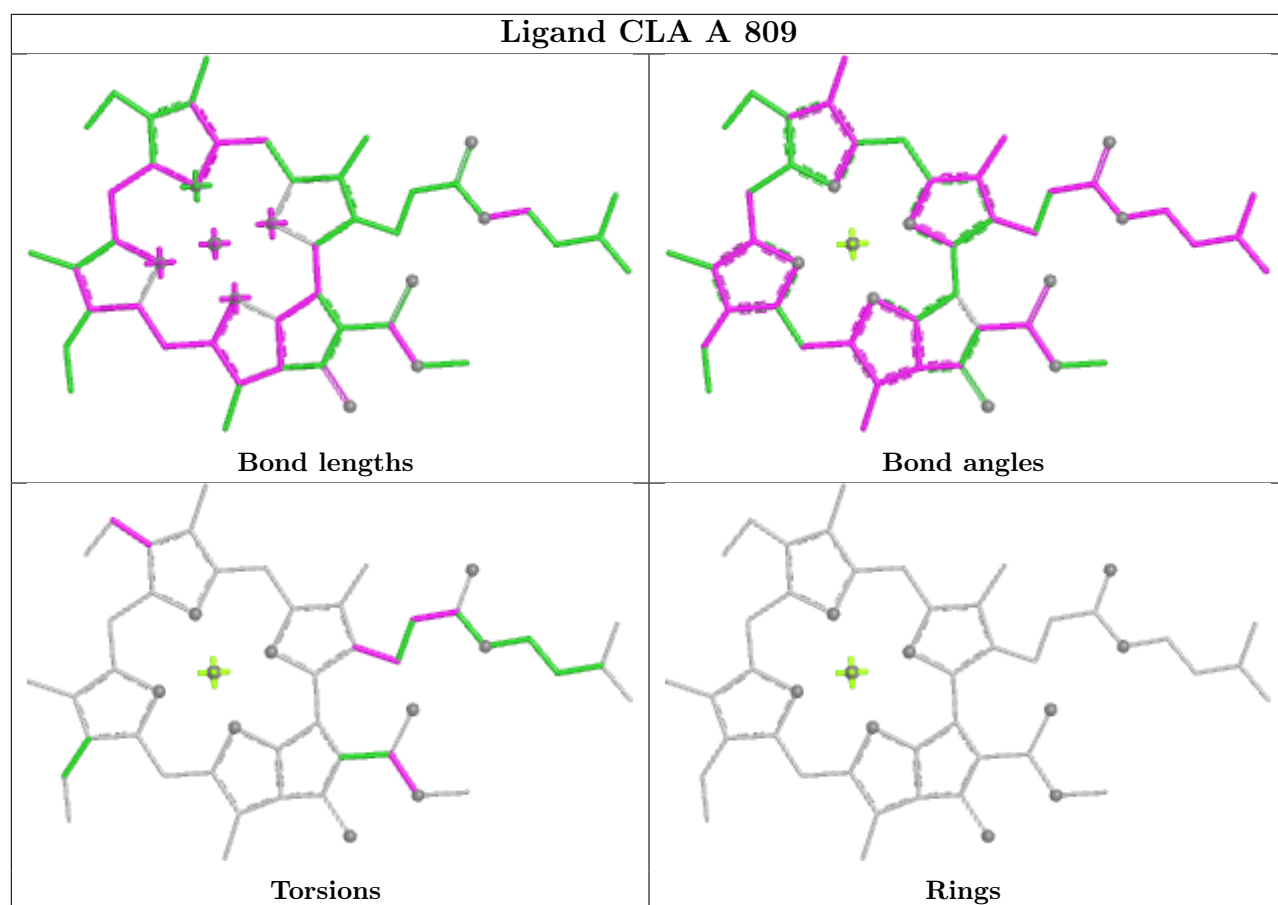


Rings

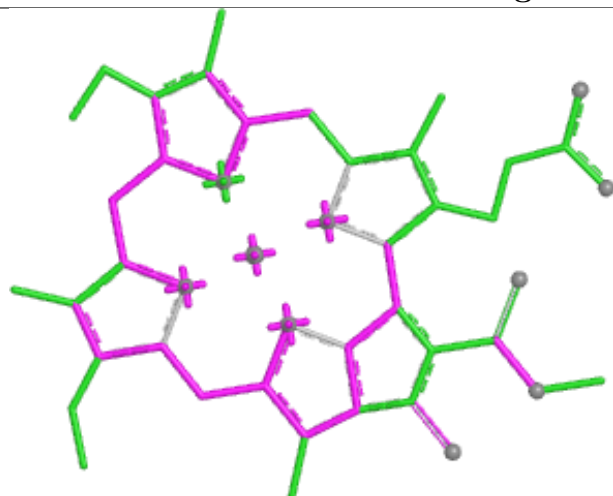




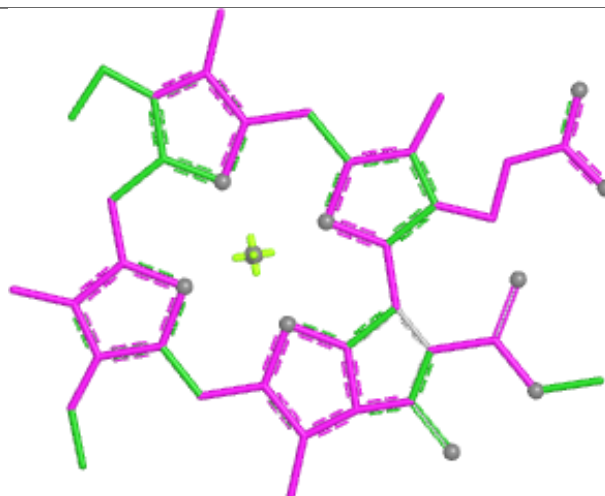




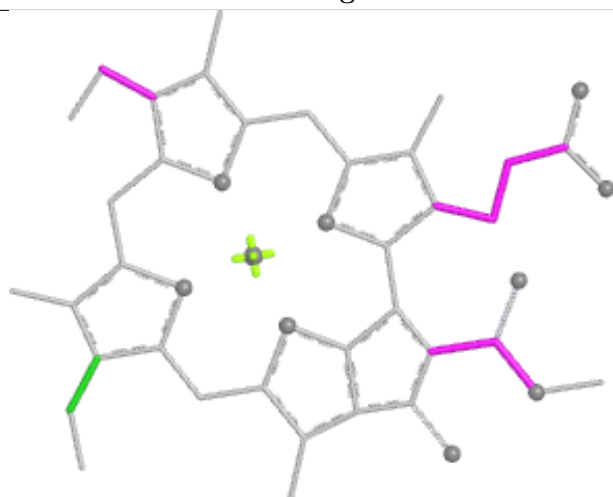
Ligand CLA B 830



Bond lengths



Bond angles

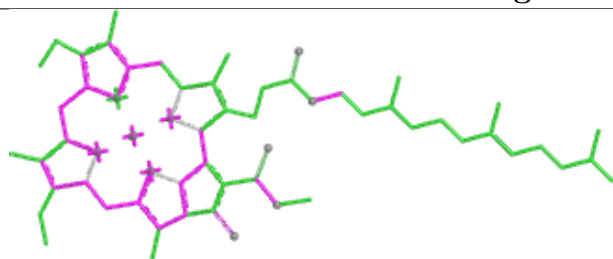


Torsions

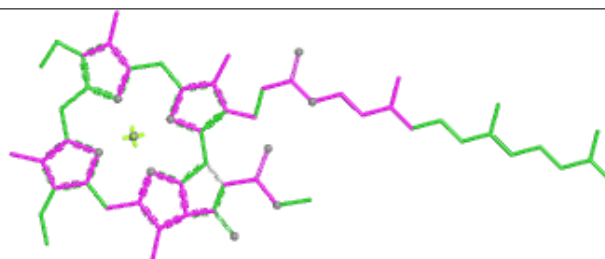


Rings

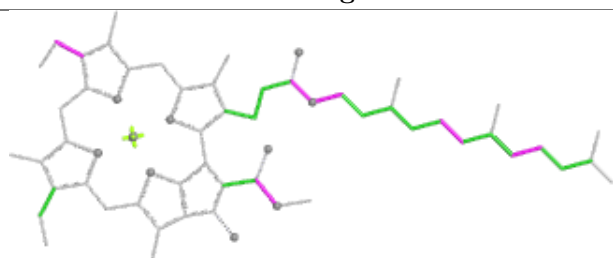
Ligand CLA A 826



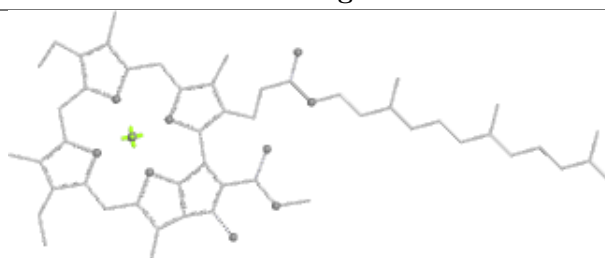
Bond lengths



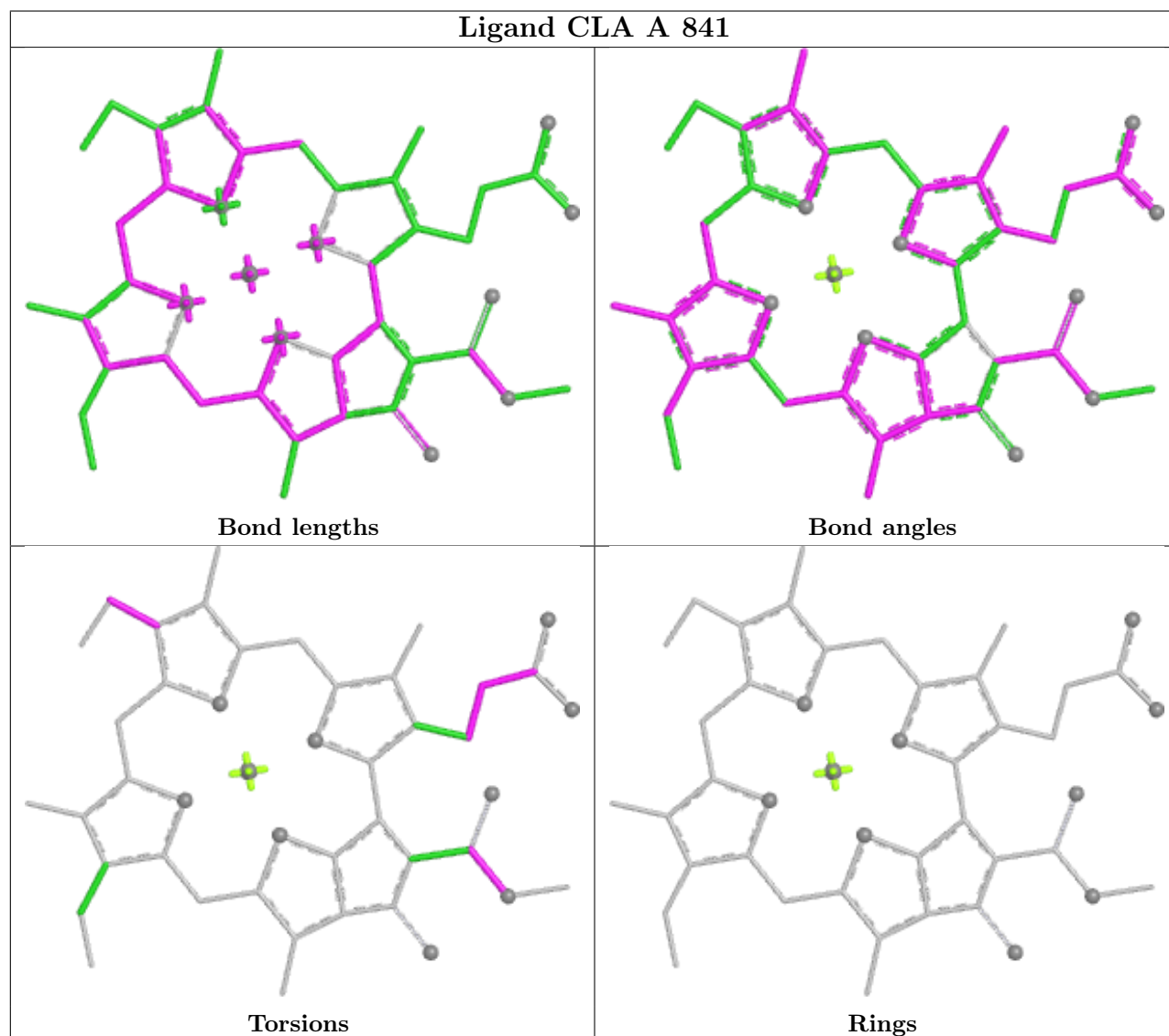
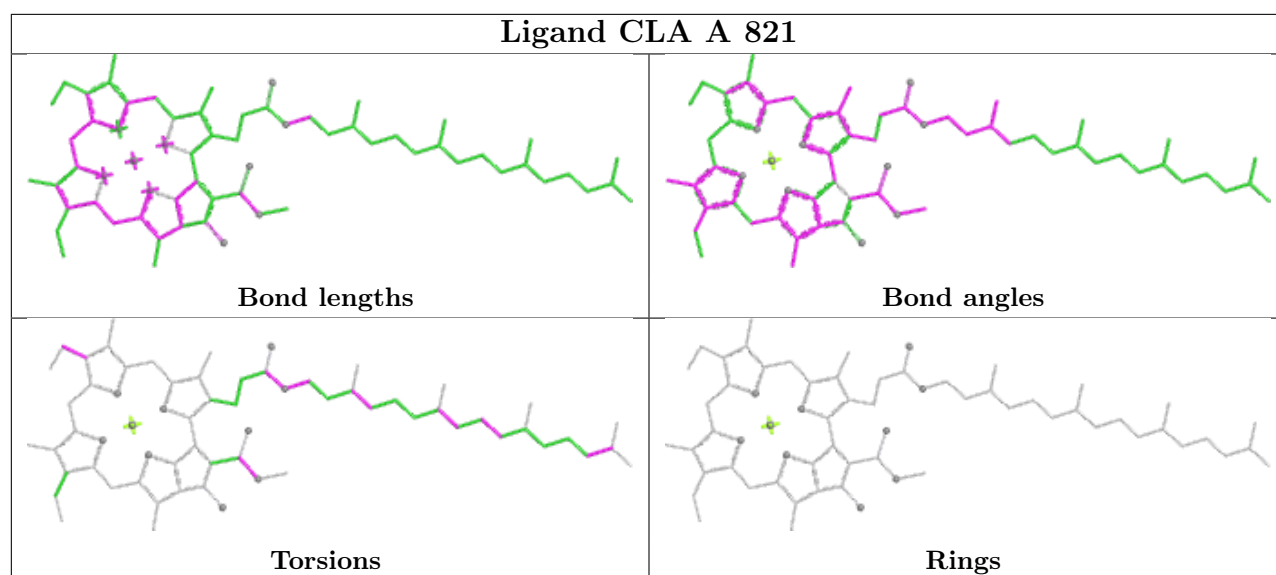
Bond angles



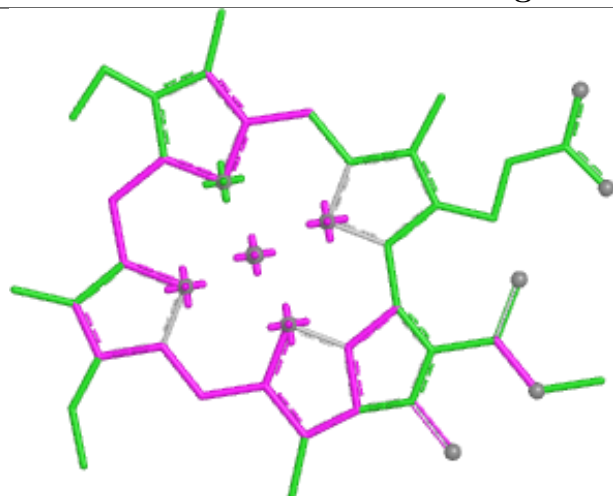
Torsions



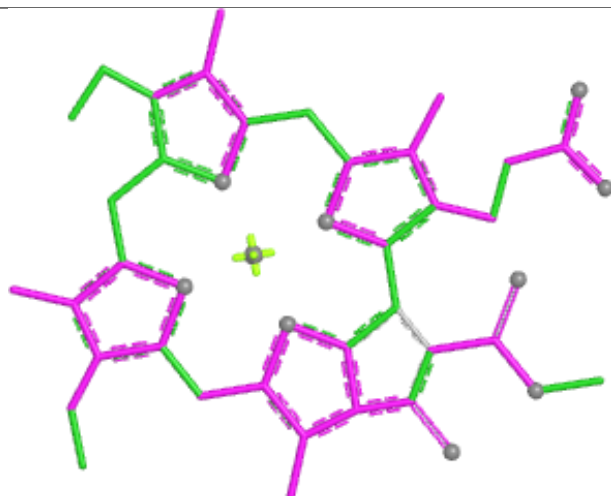
Rings



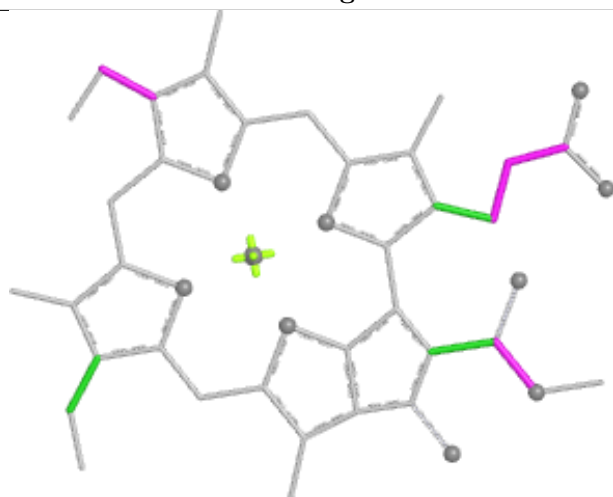
Ligand CLA B 808



Bond lengths



Bond angles

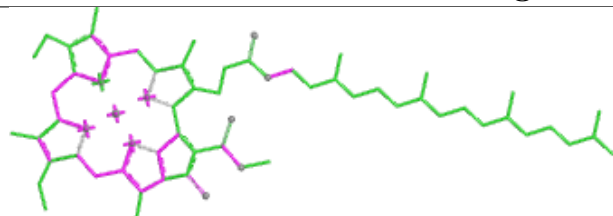


Torsions

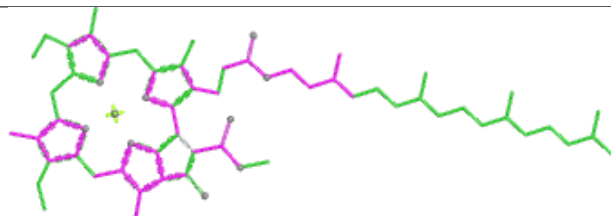


Rings

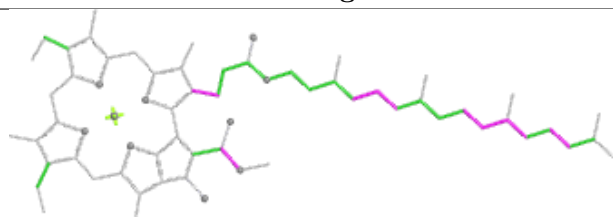
Ligand CLA A 806



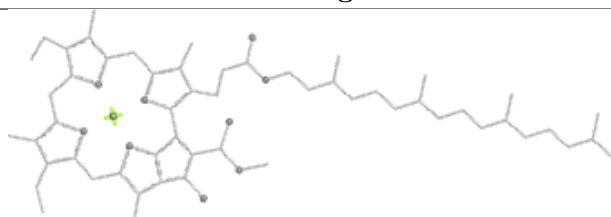
Bond lengths



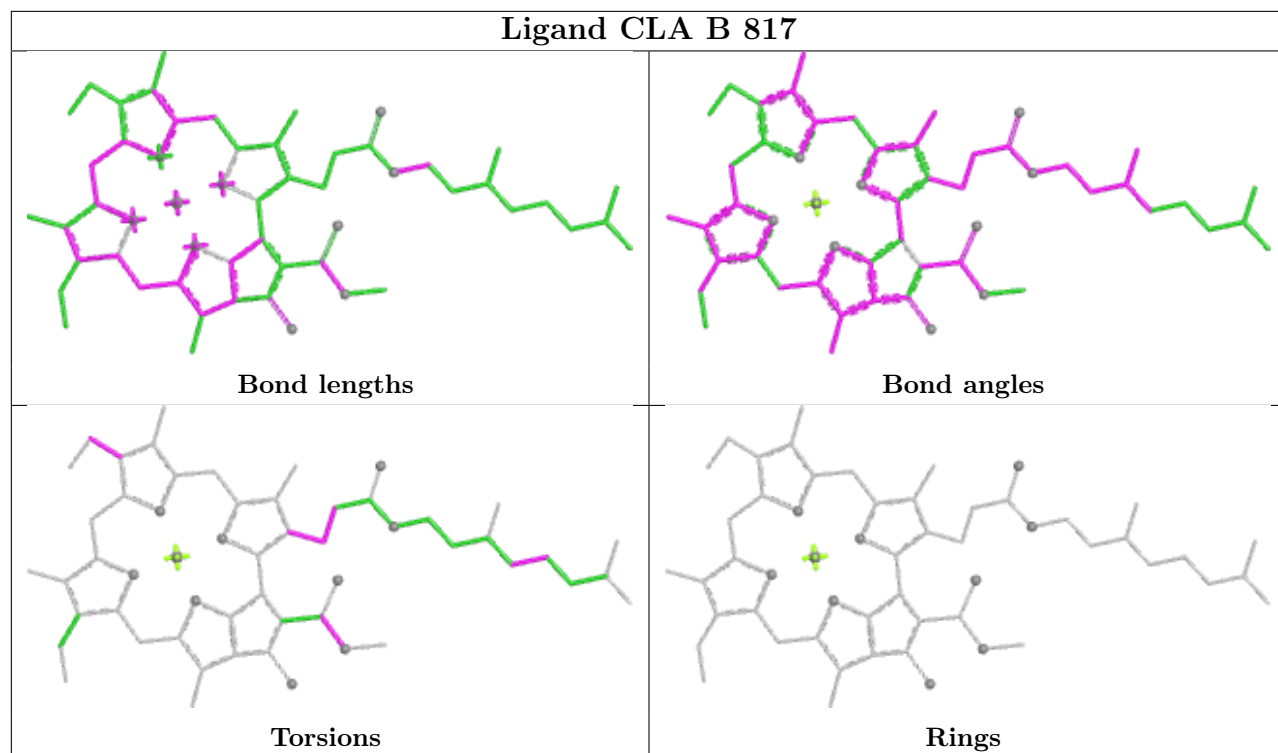
Bond angles



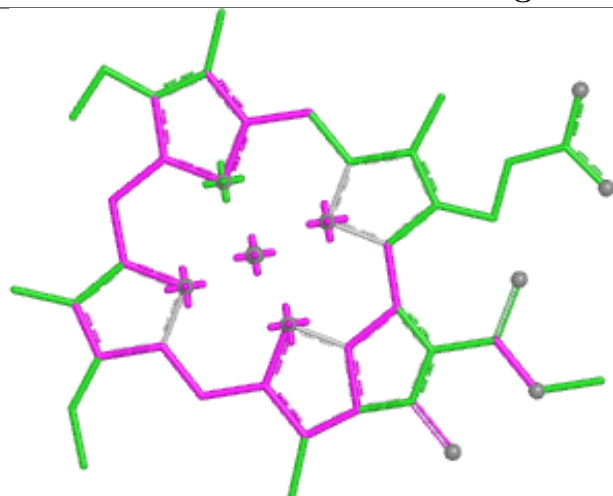
Torsions



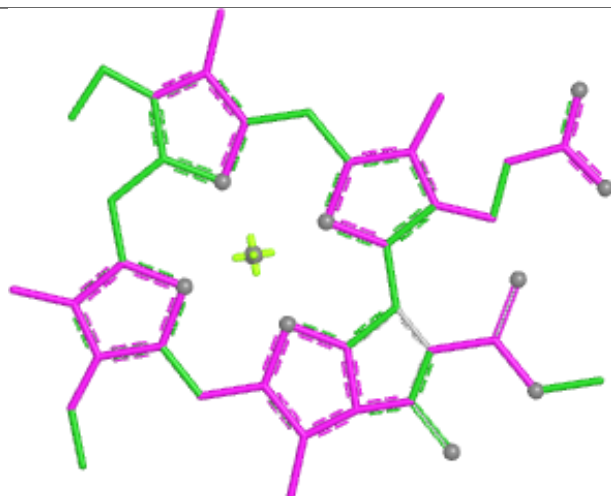
Rings



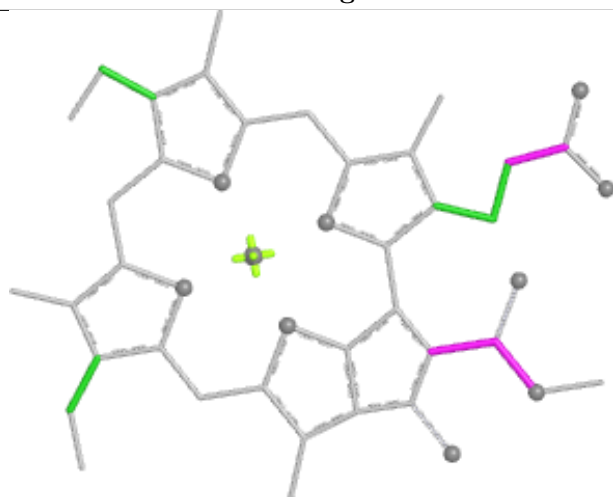
Ligand CLA B 833



Bond lengths



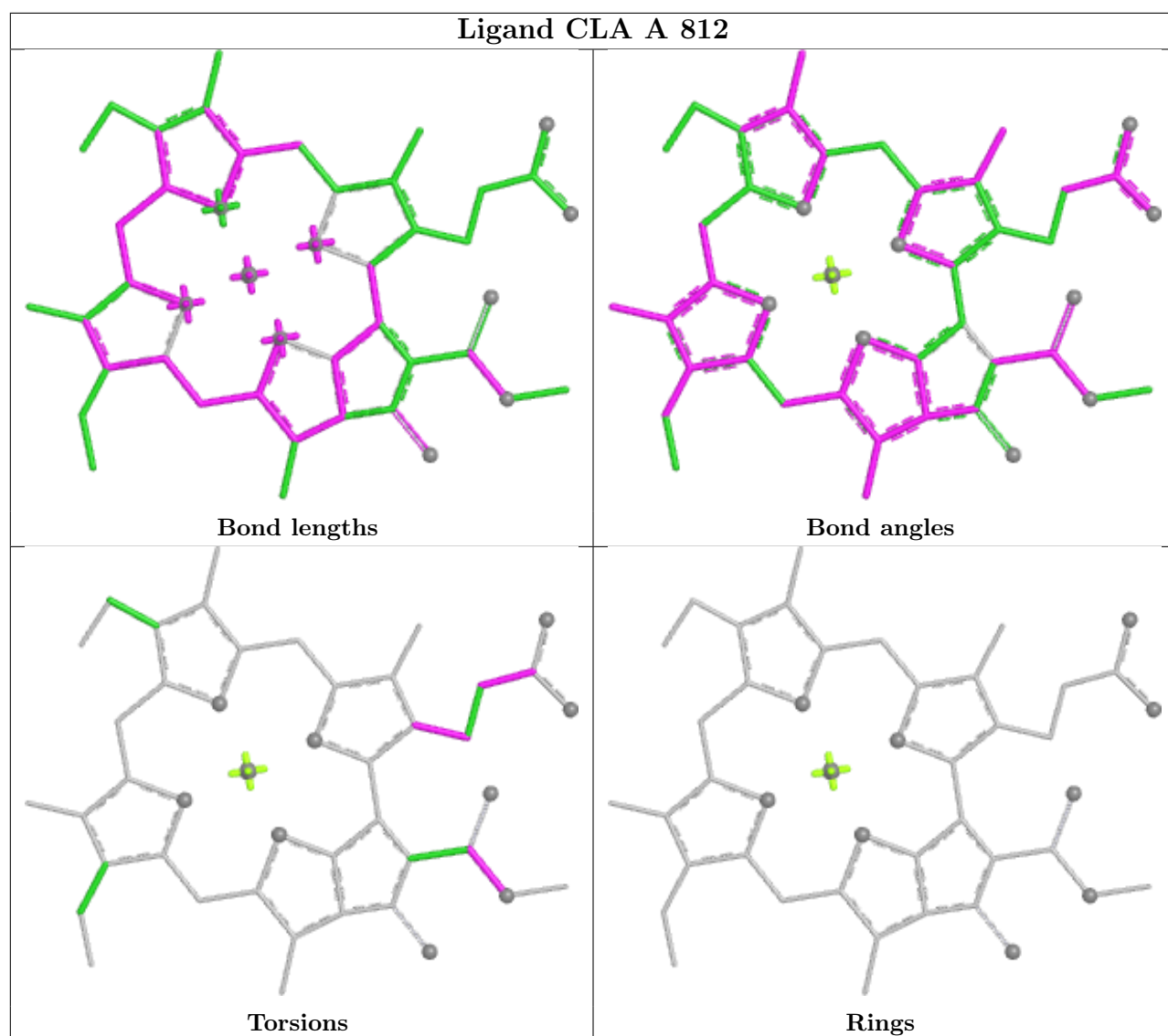
Bond angles

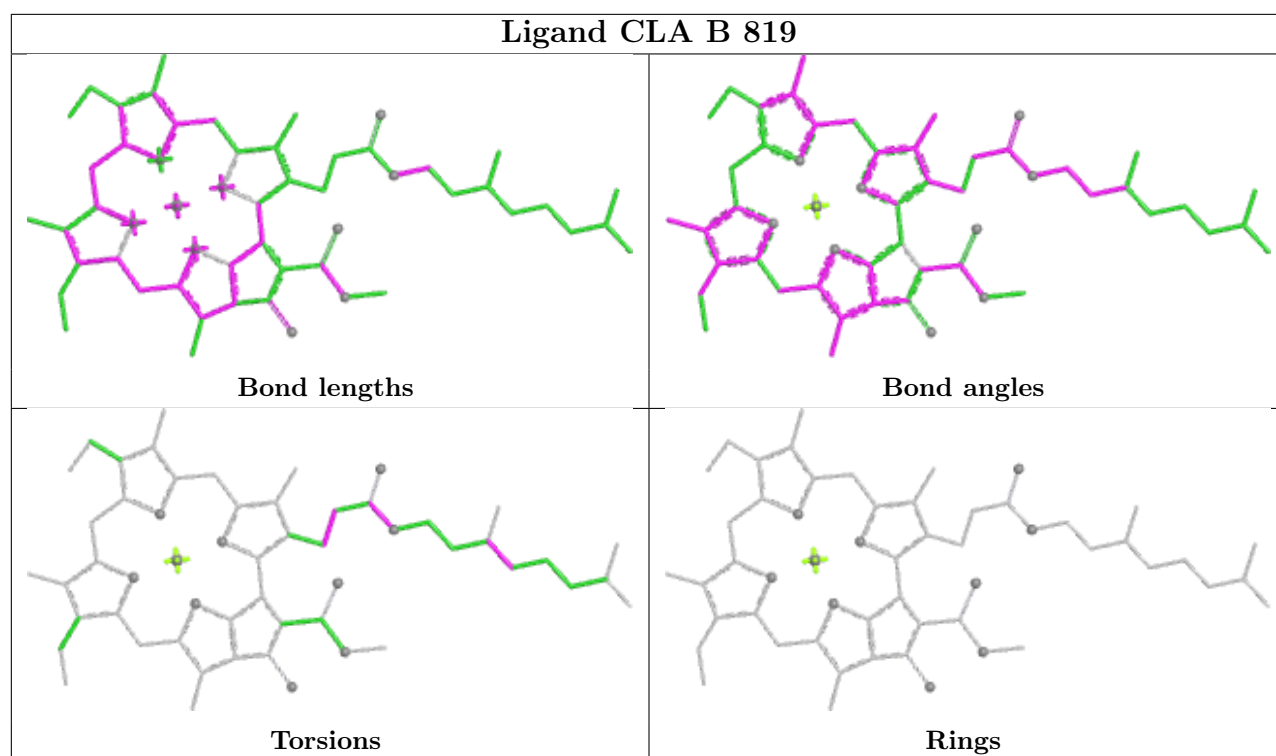


Torsions

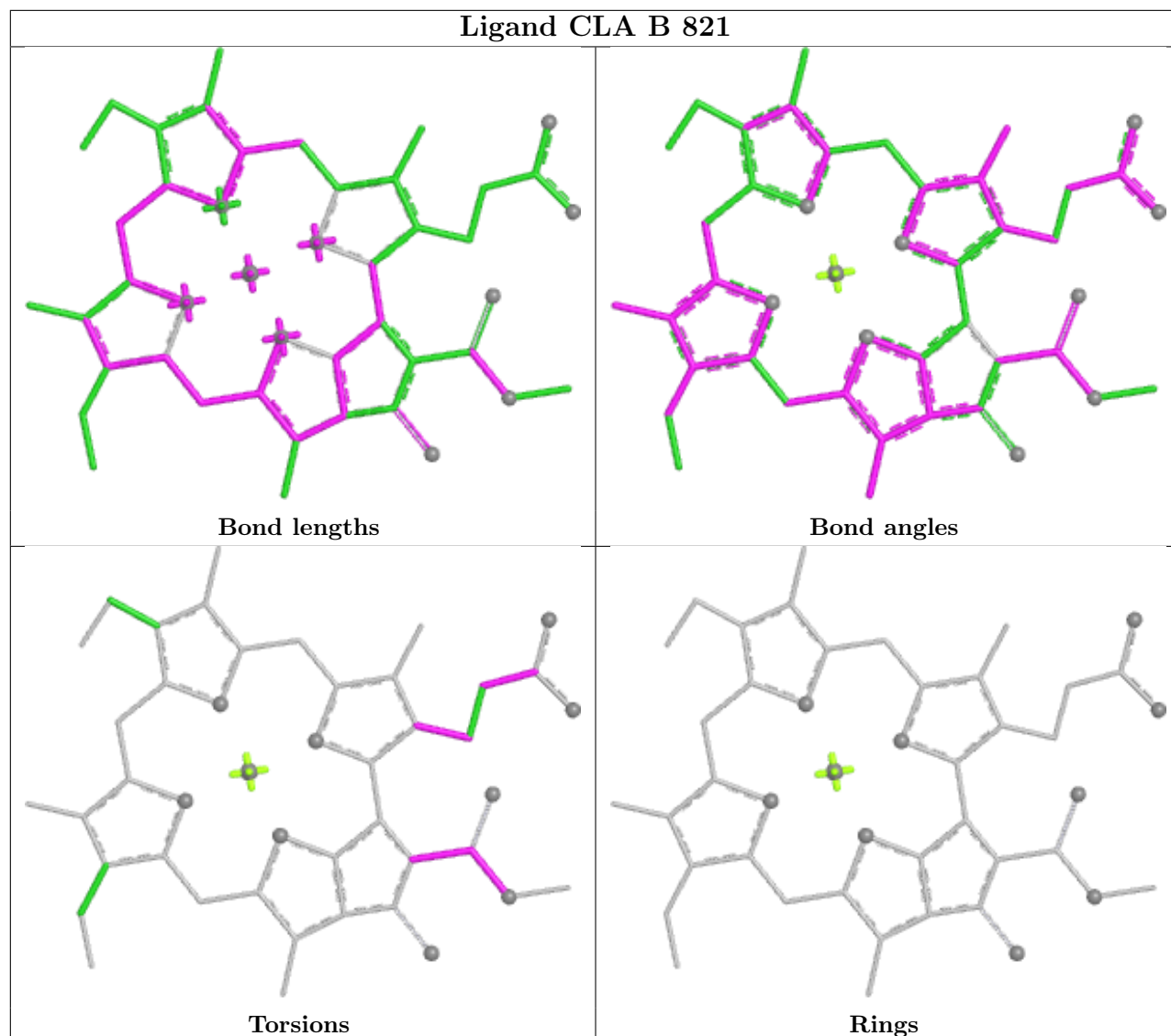


Rings

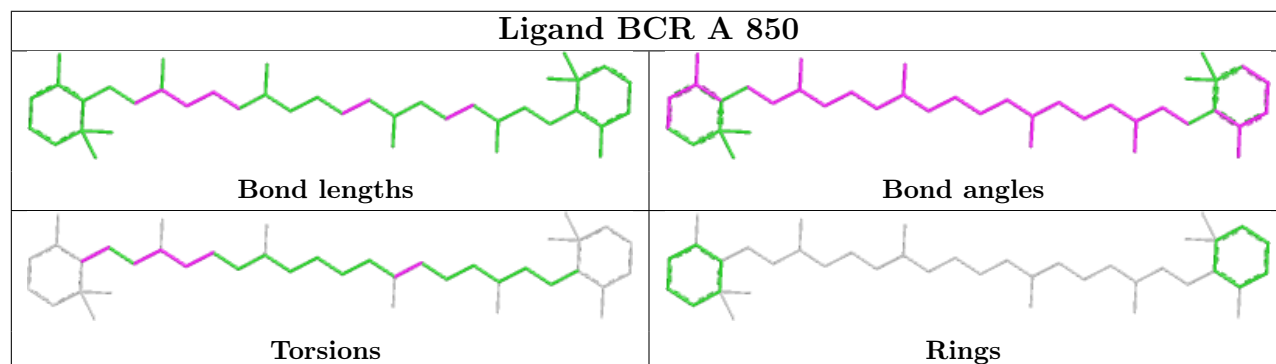


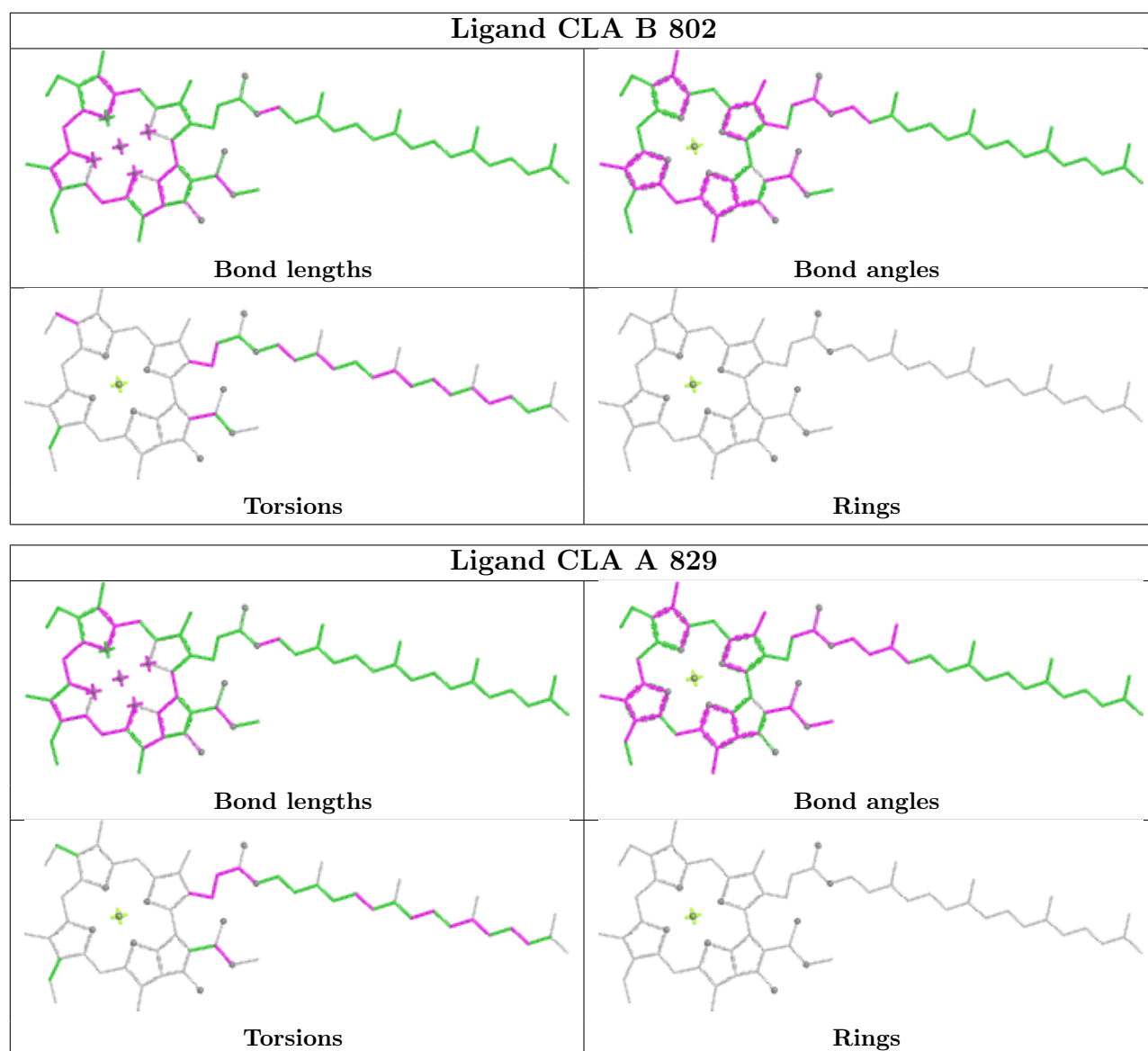


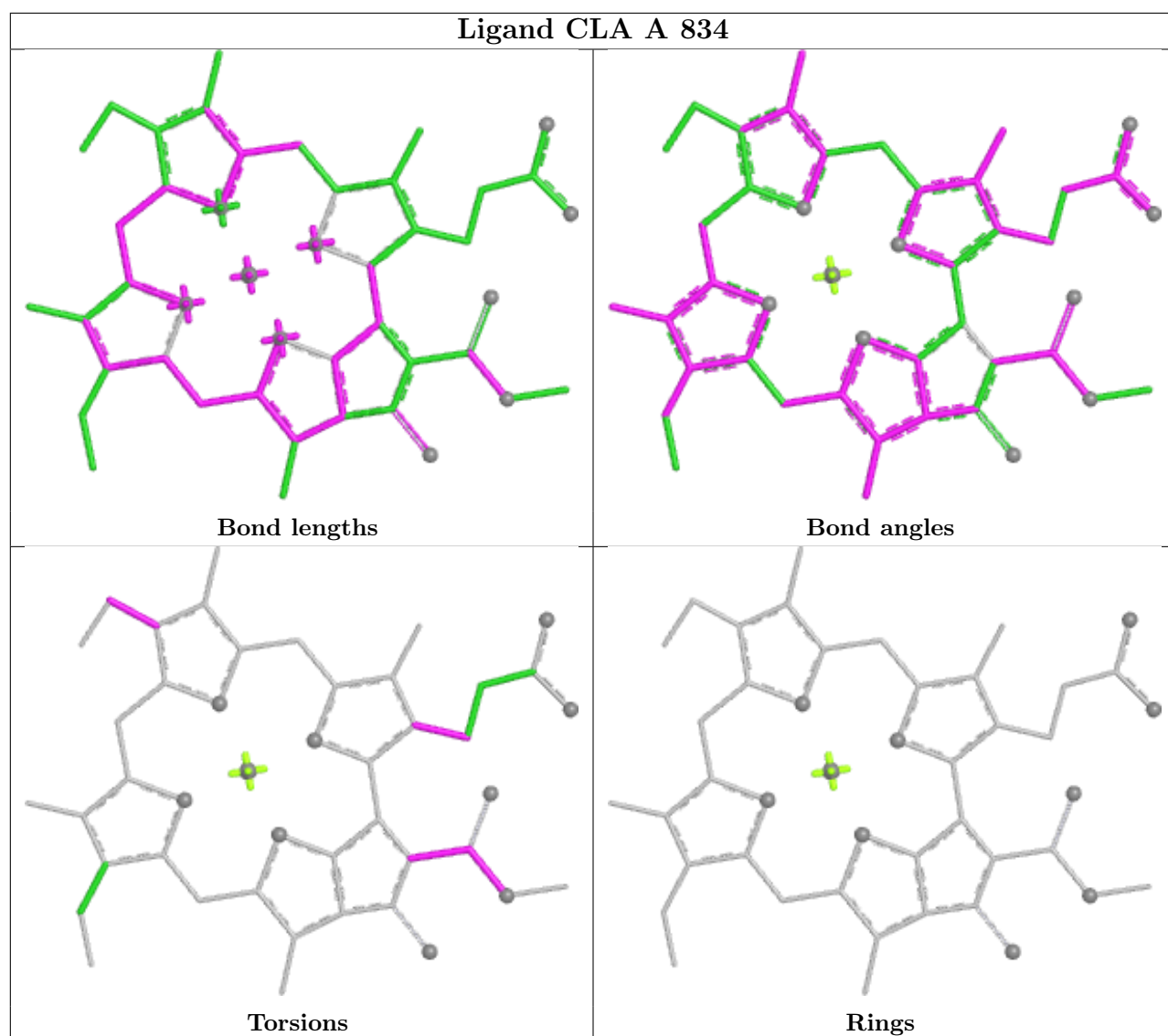
Ligand CLA B 821



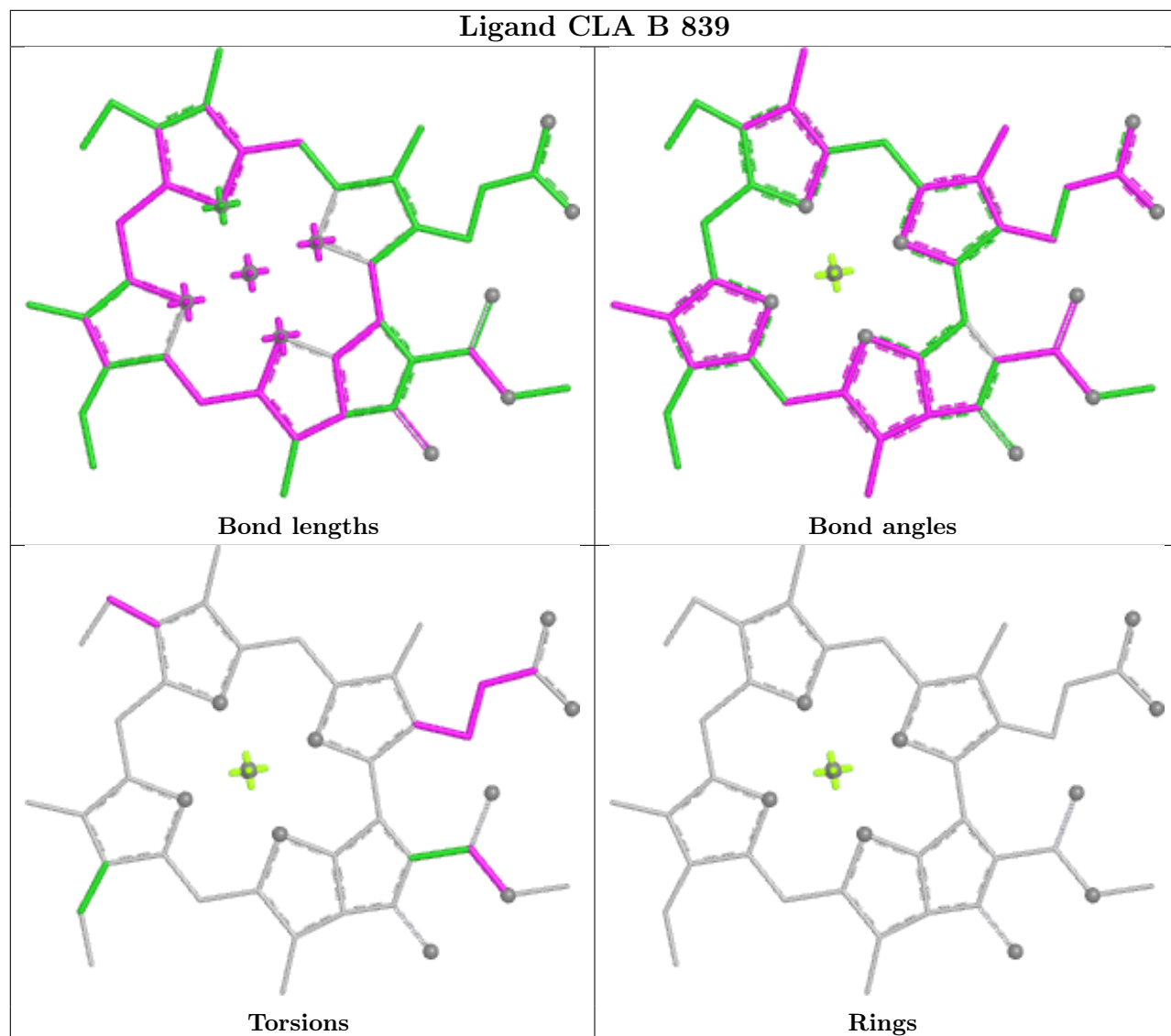
Ligand BCR A 850



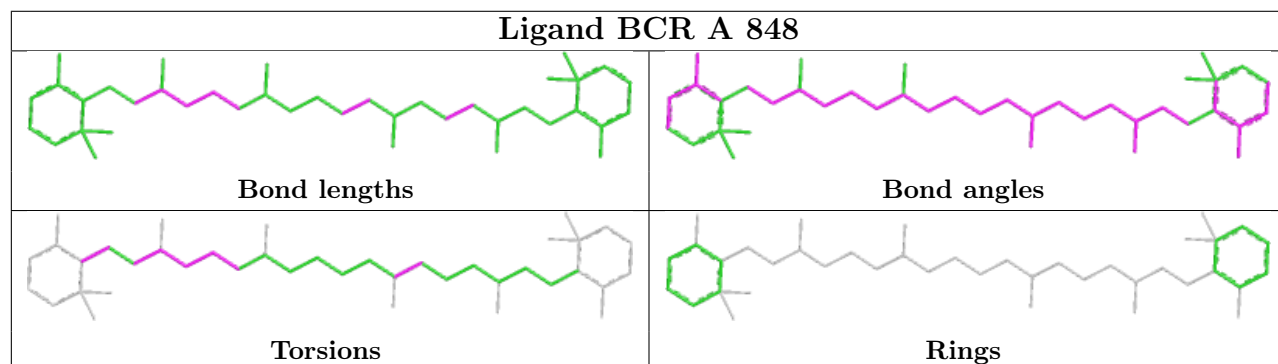


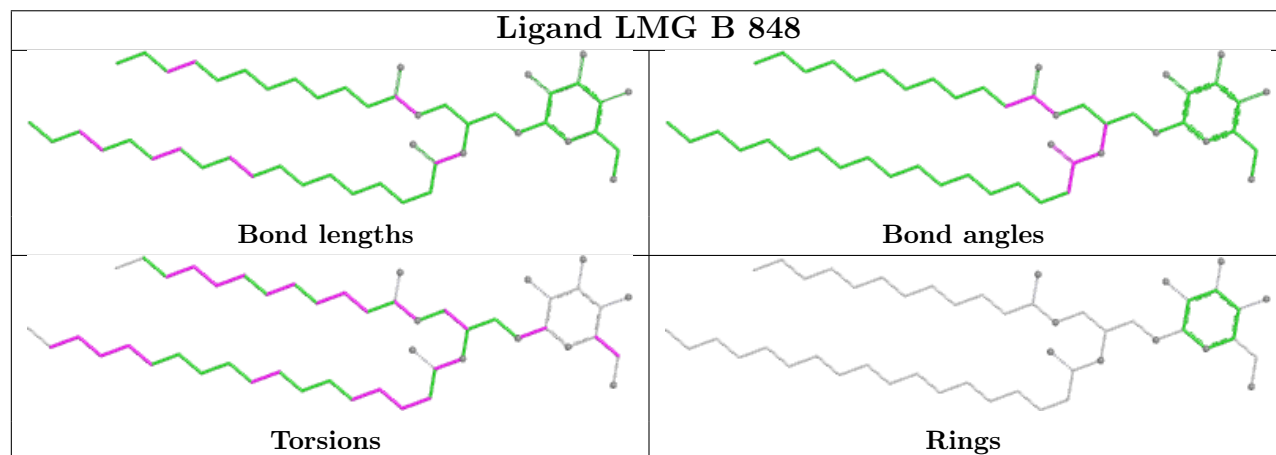
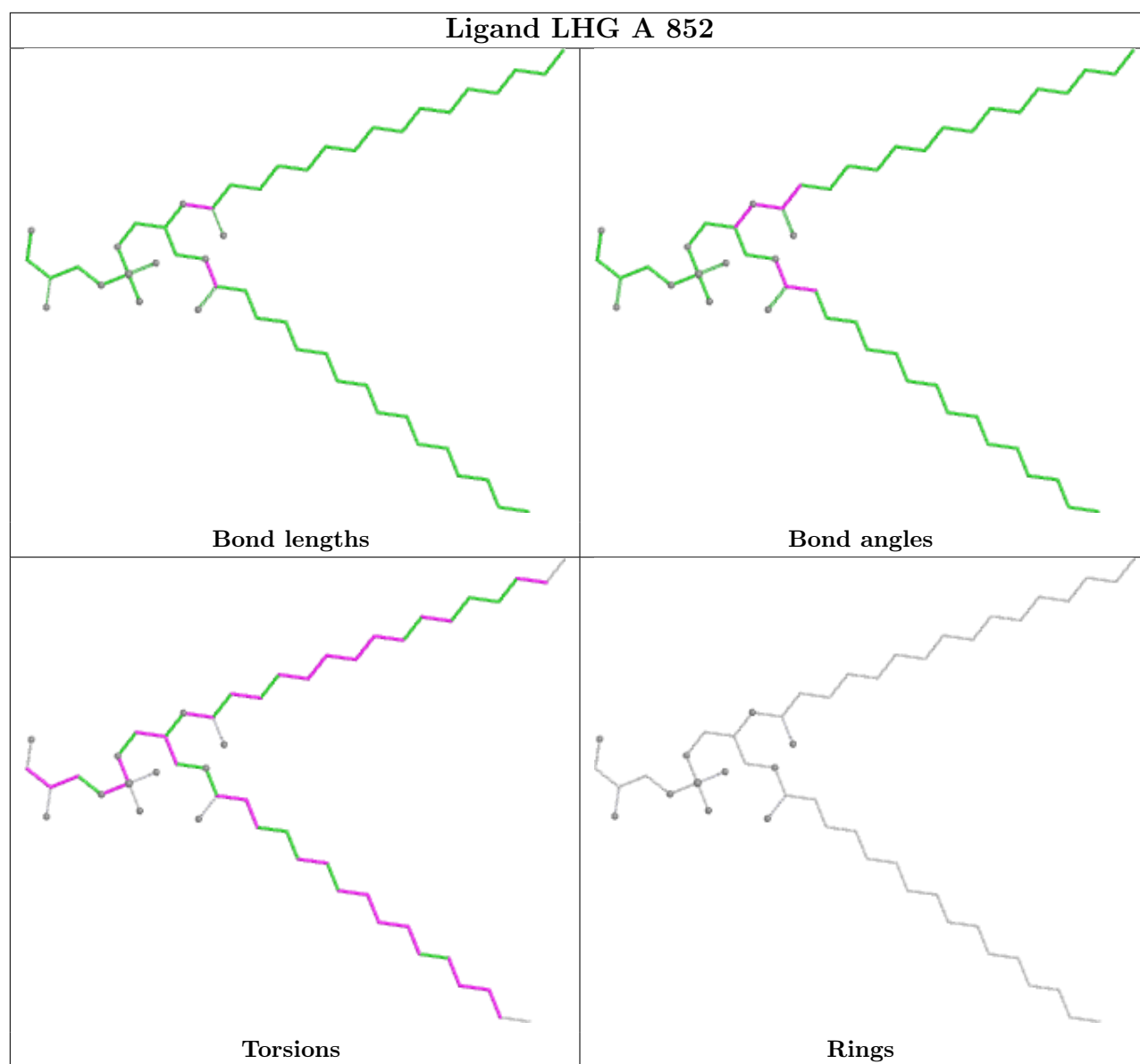


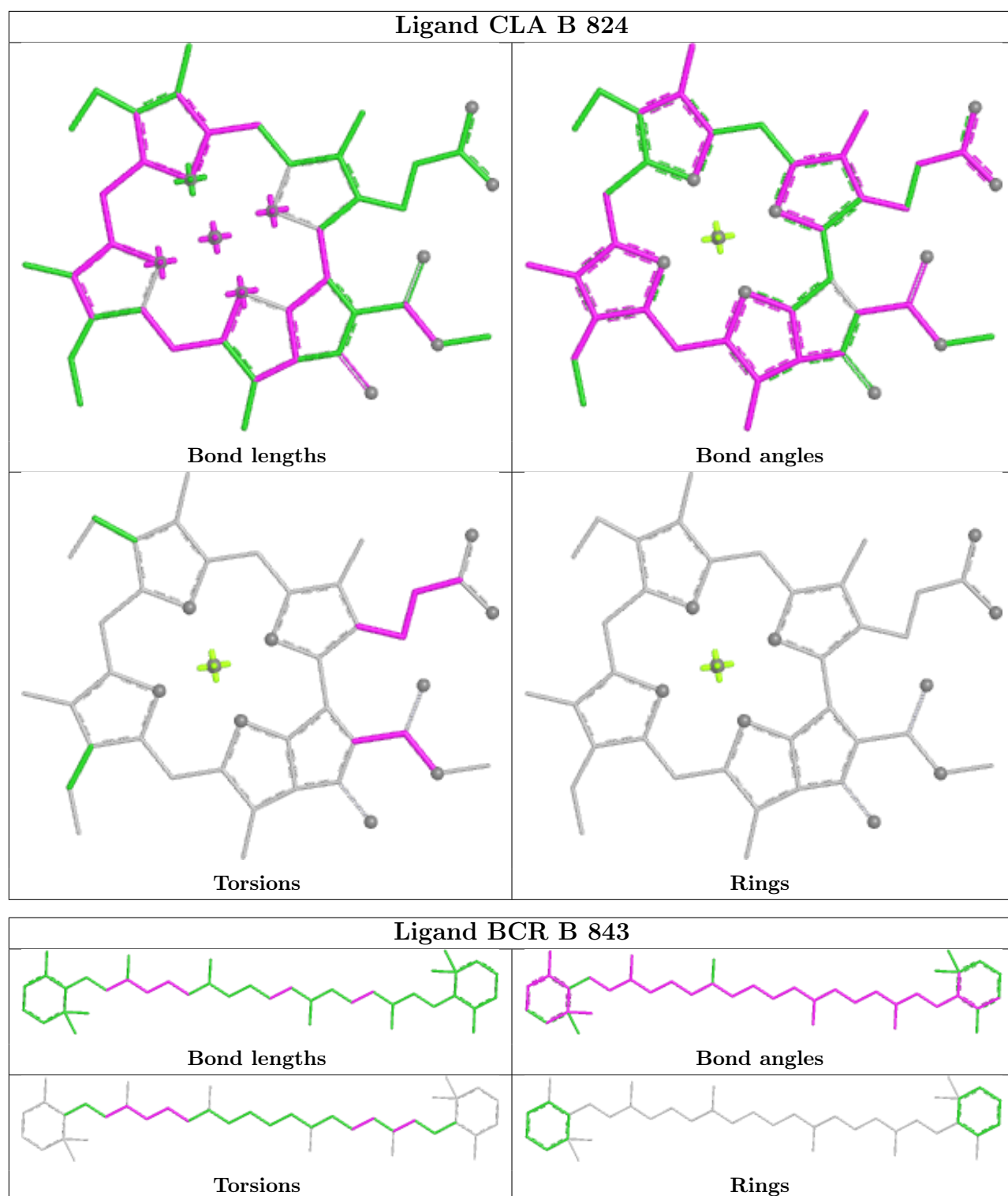
Ligand CLA B 839

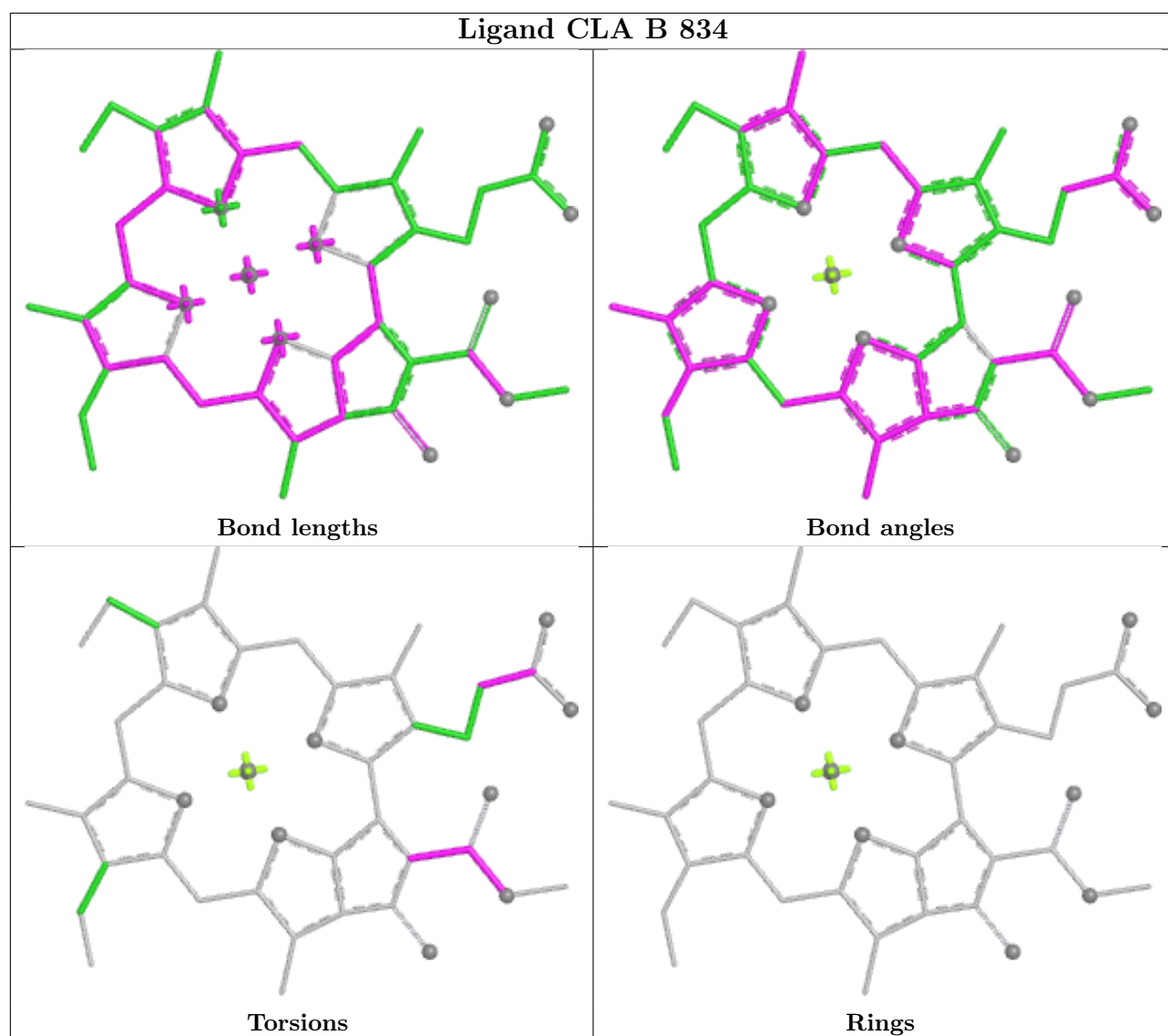


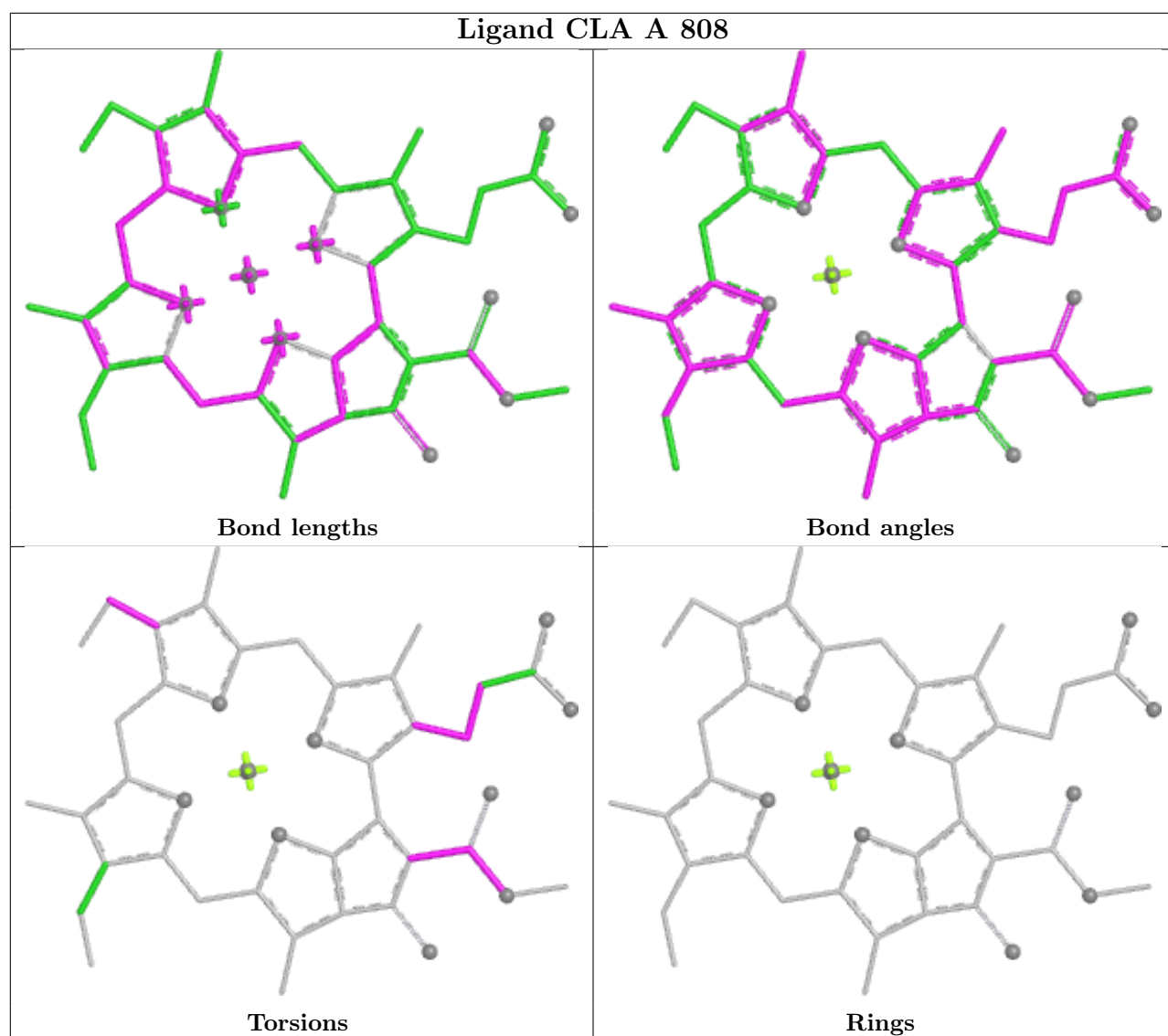
Ligand BCR A 848



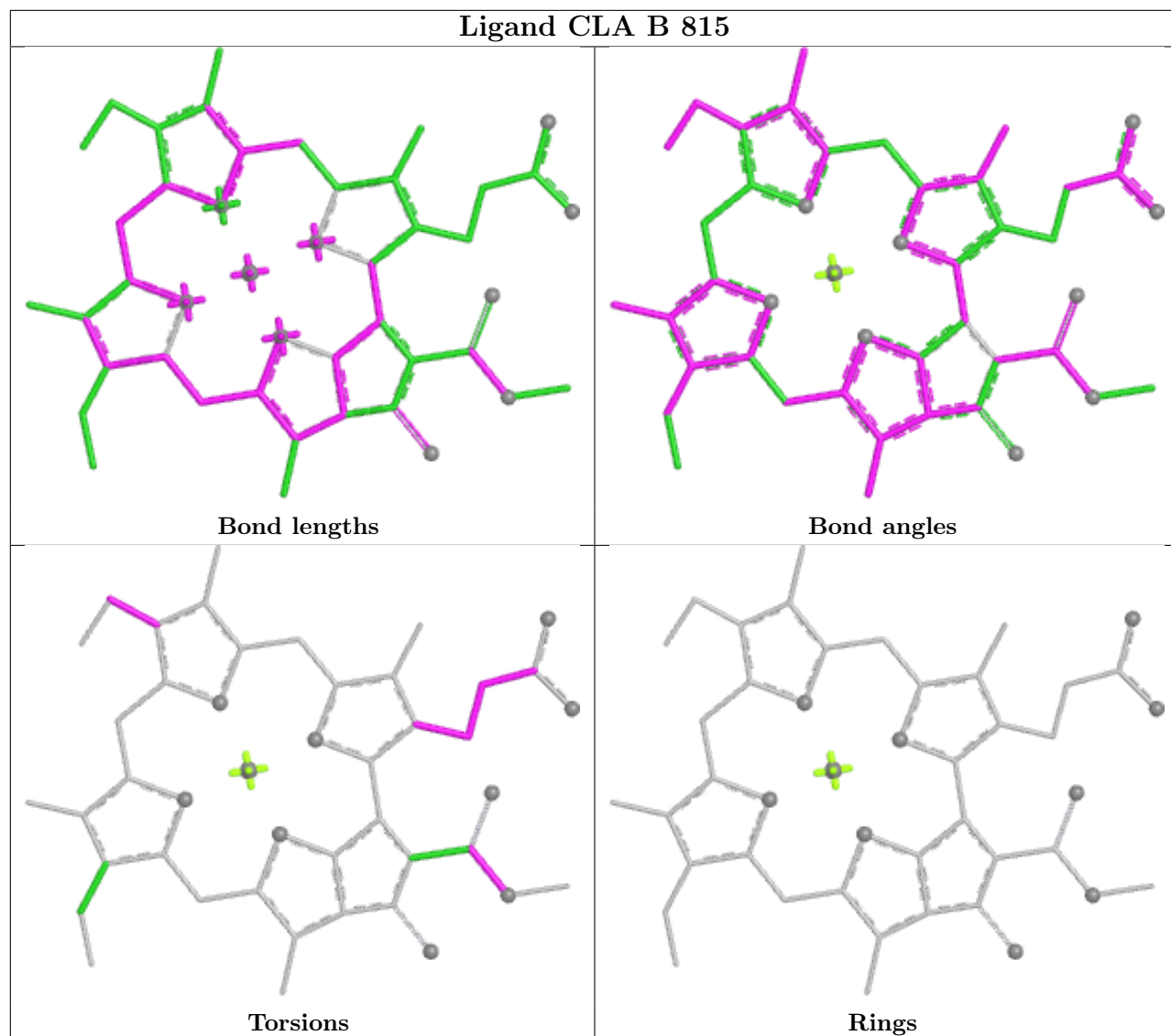




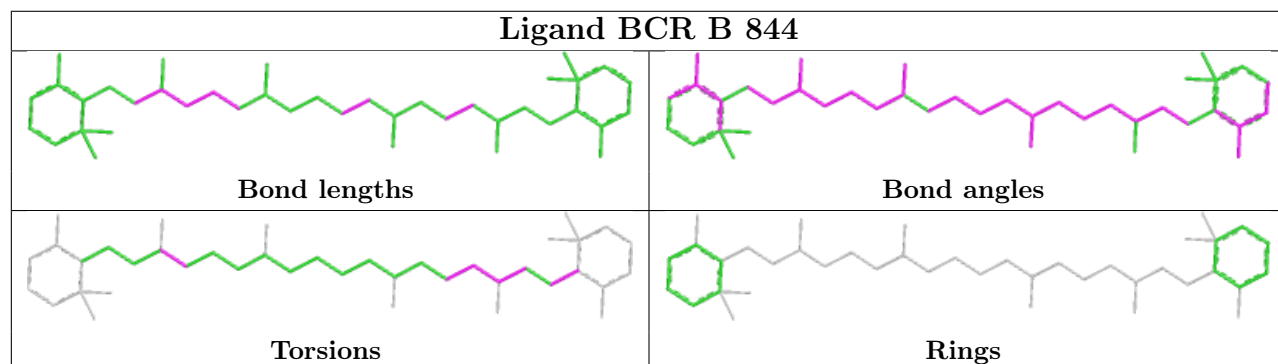


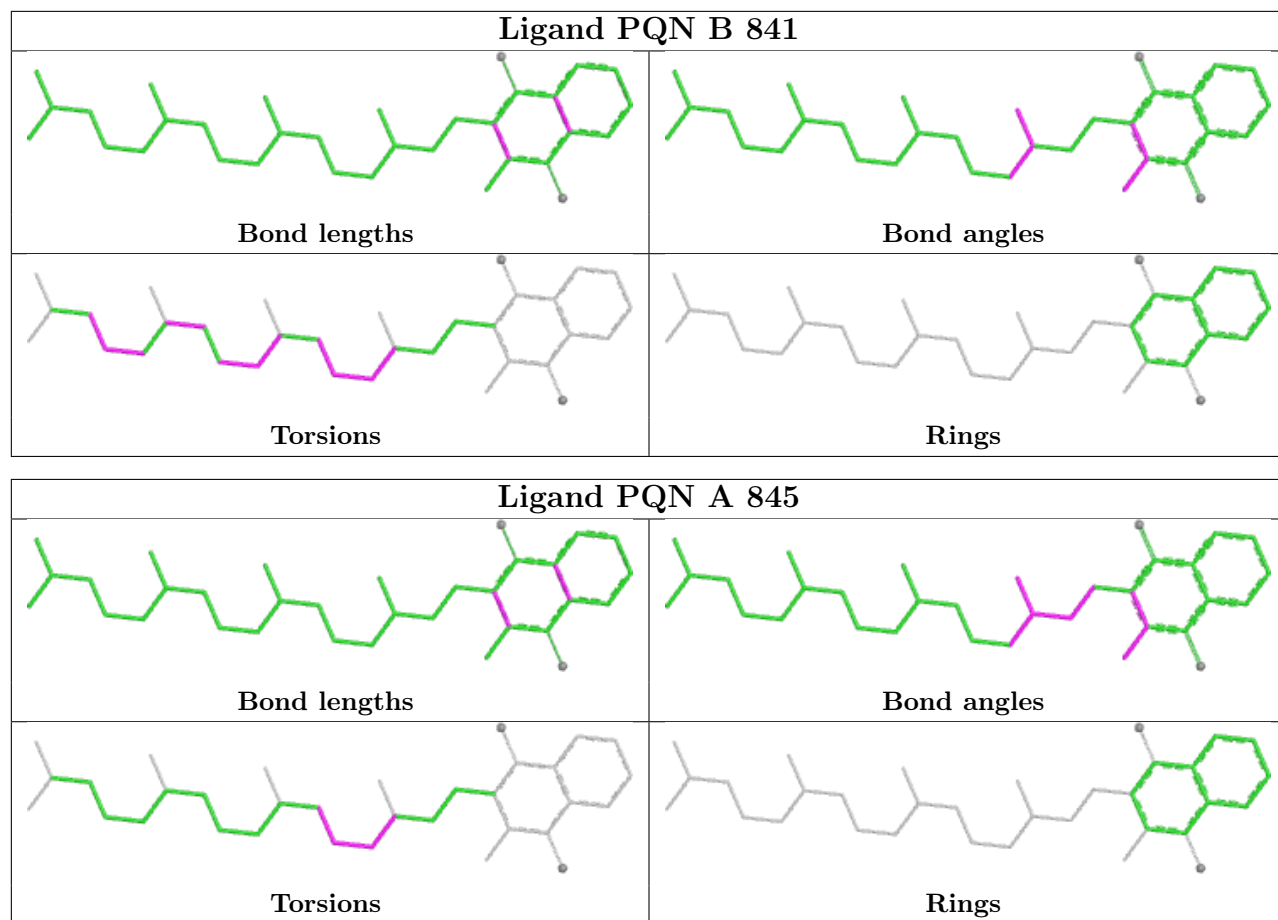


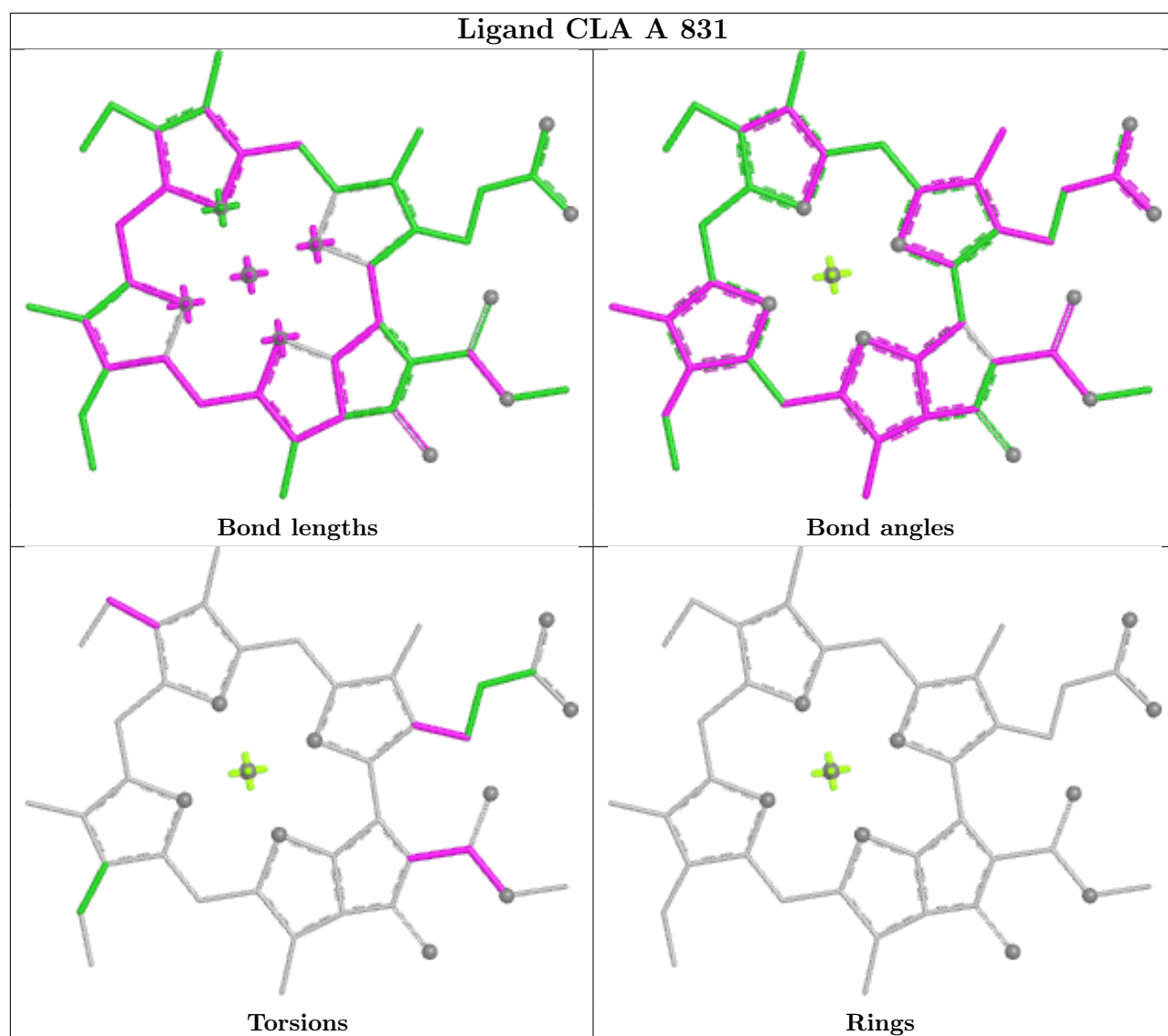
Ligand CLA B 815



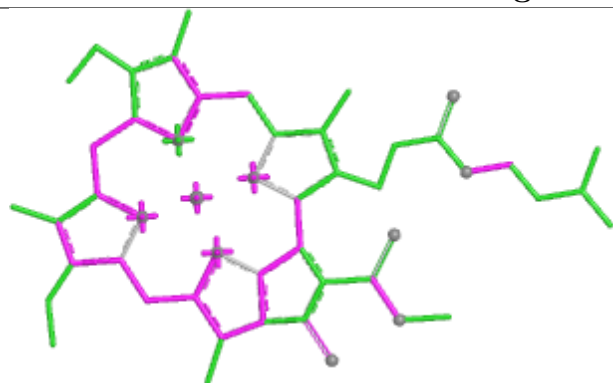
Ligand BCR B 844



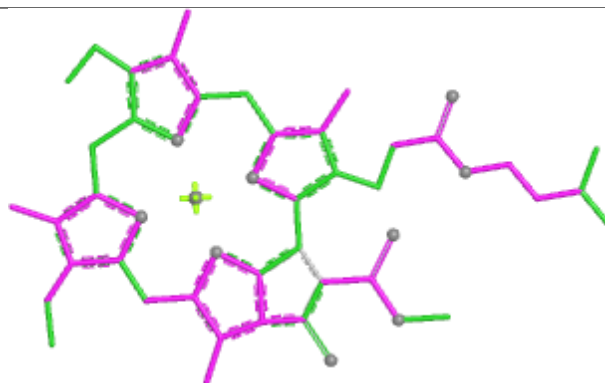




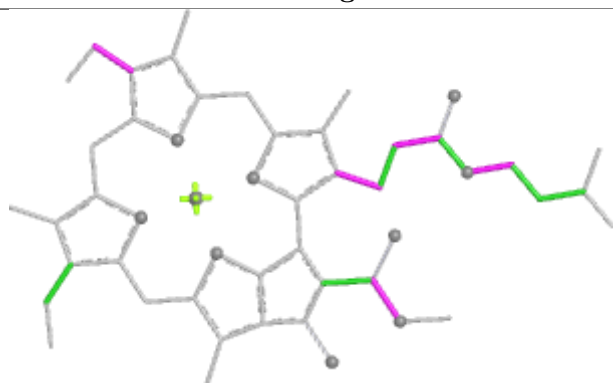
Ligand CLA A 842



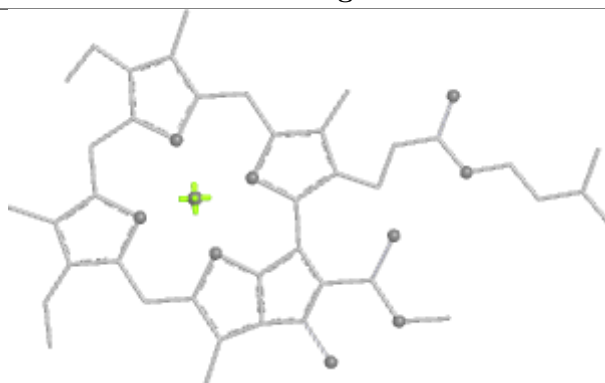
Bond lengths



Bond angles

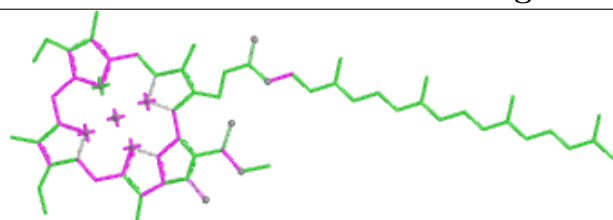


Torsions

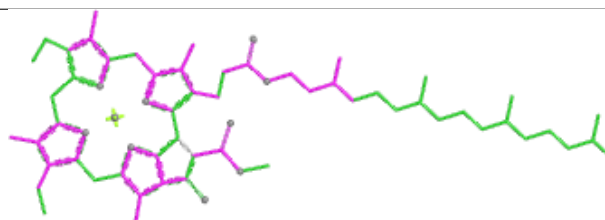


Rings

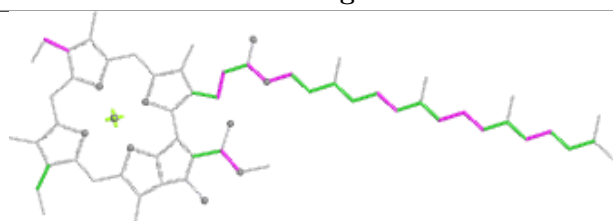
Ligand CLA B 804



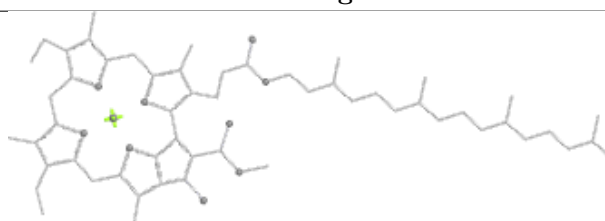
Bond lengths



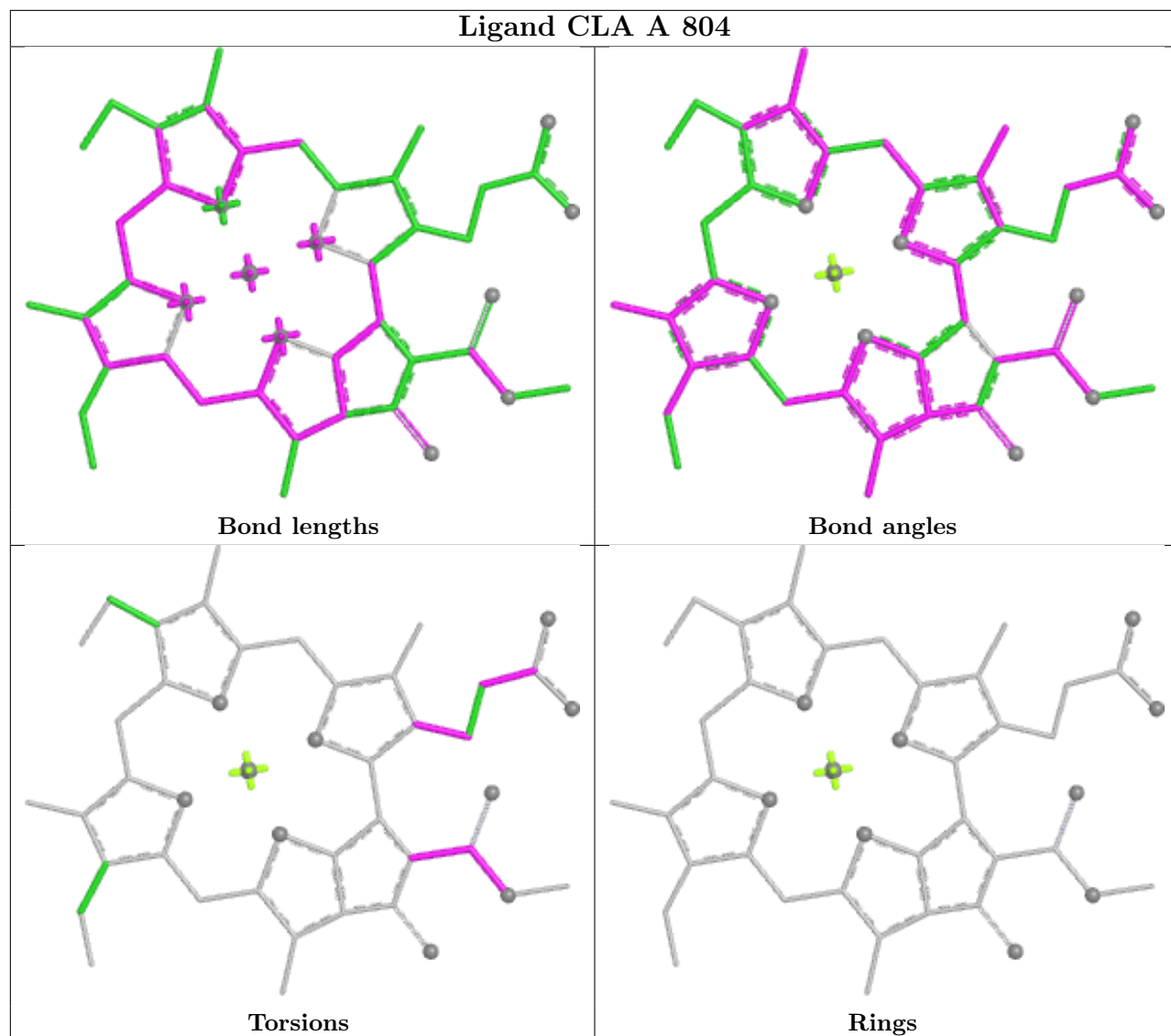
Bond angles

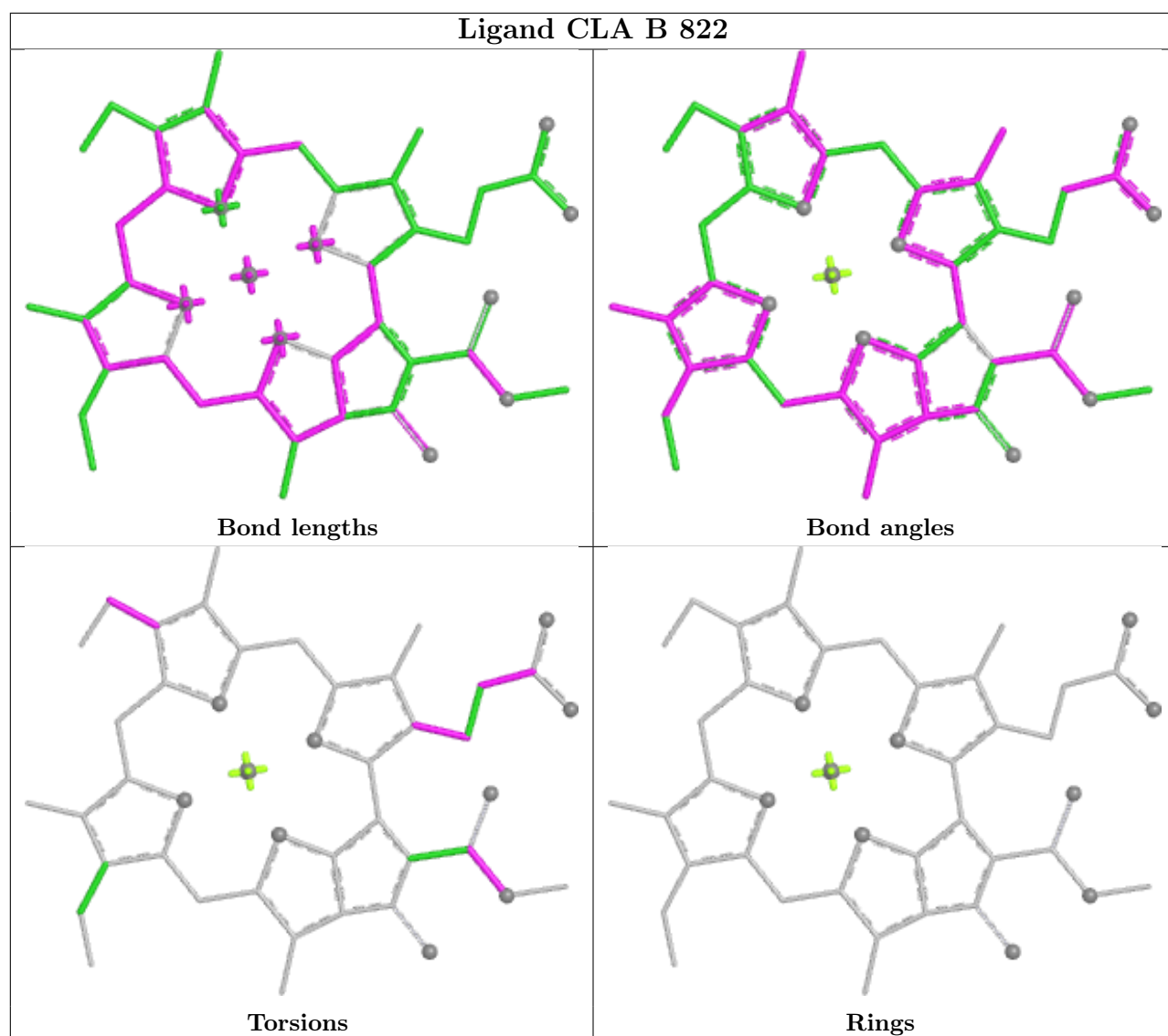


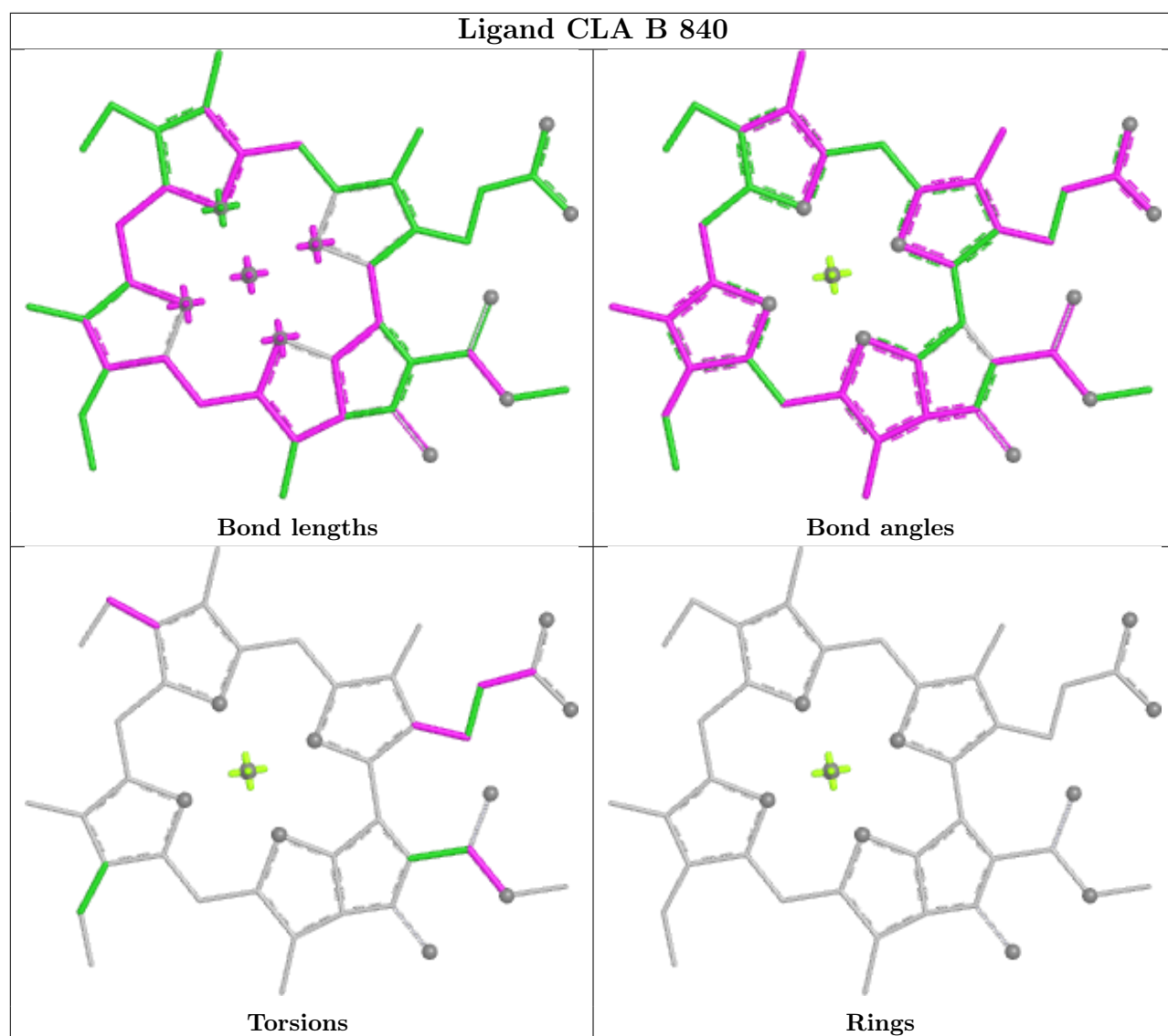
Torsions



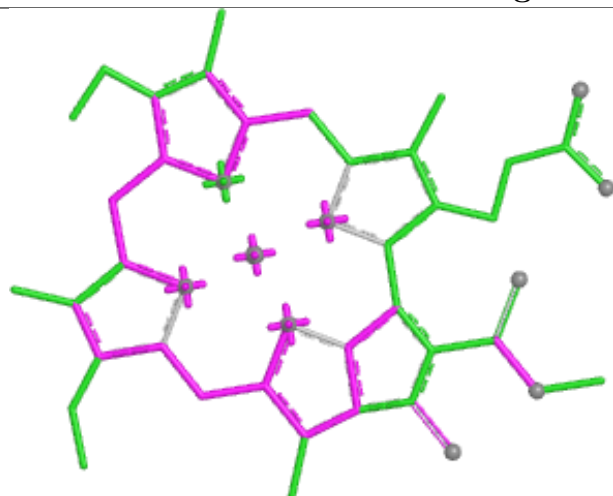
Rings



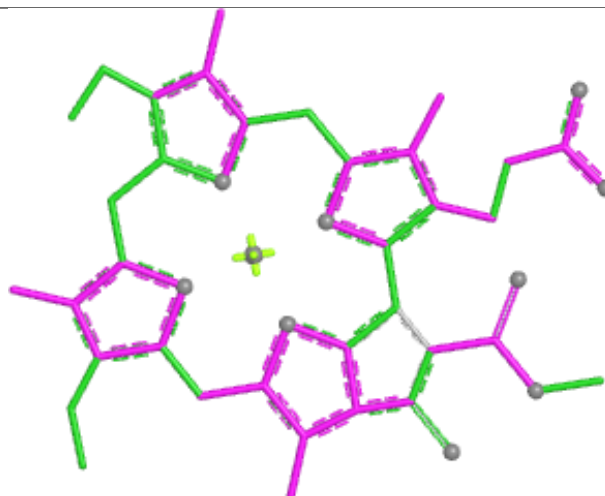




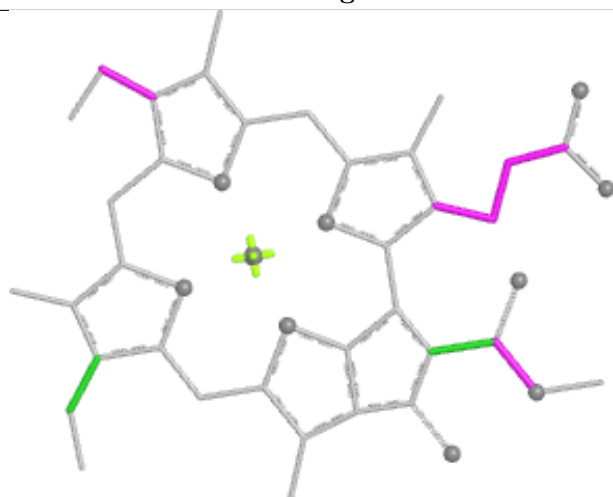
Ligand CLA A 816



Bond lengths



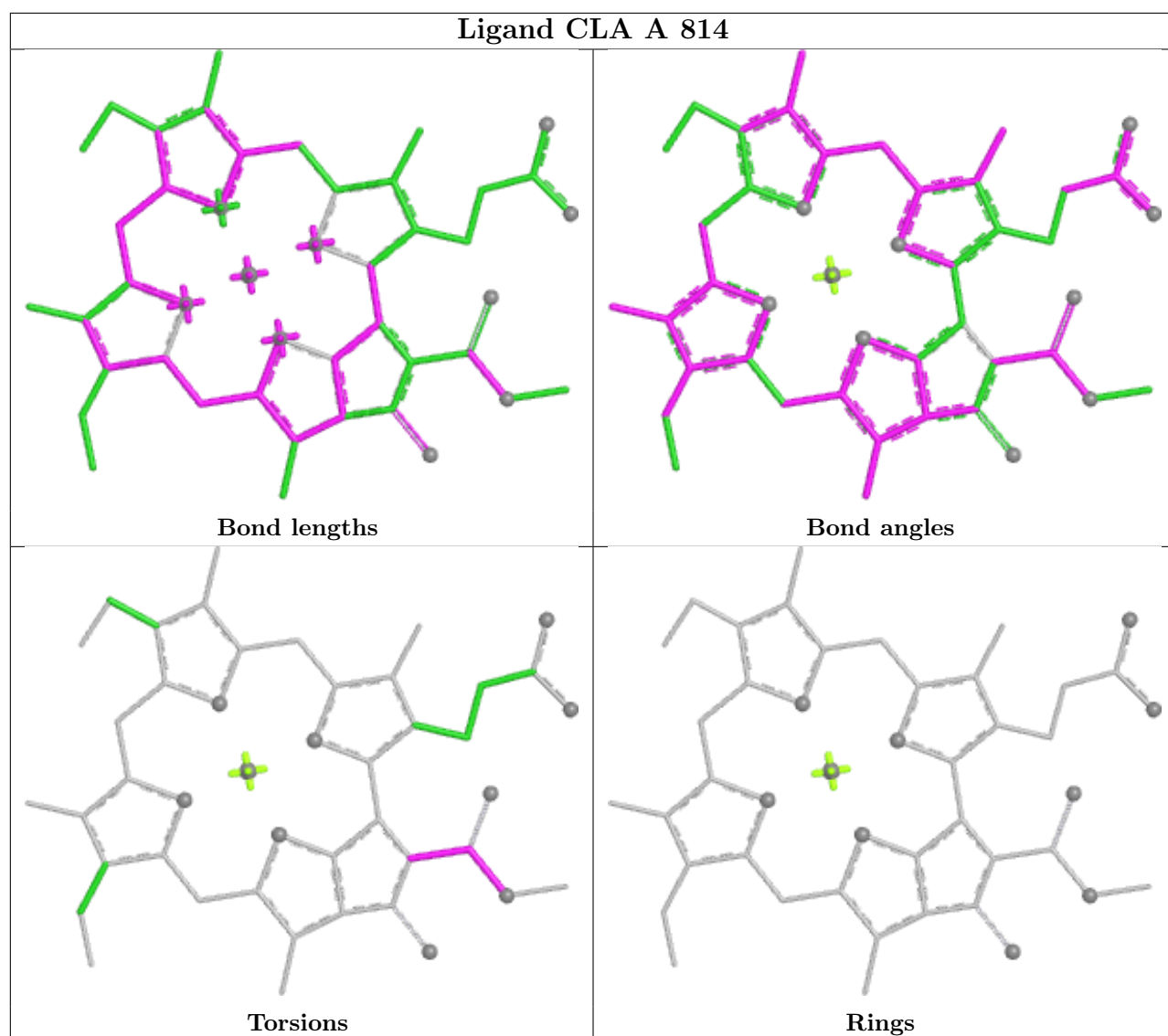
Bond angles



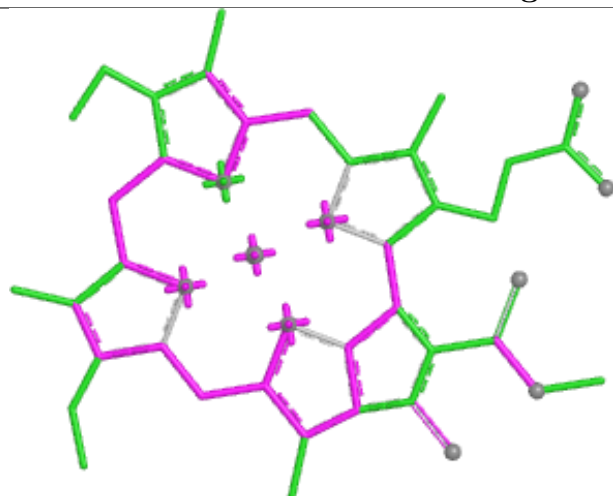
Torsions



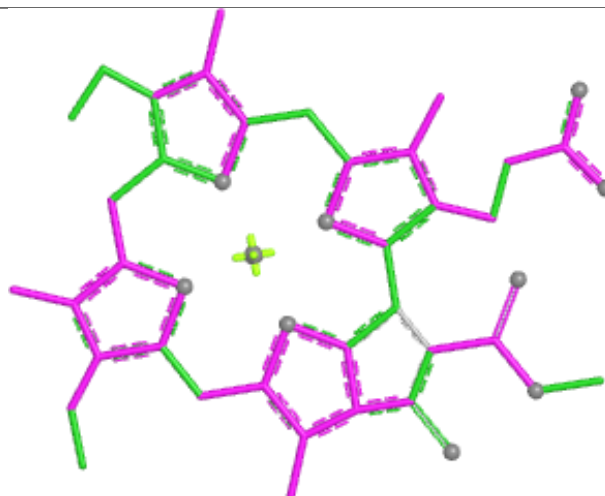
Rings



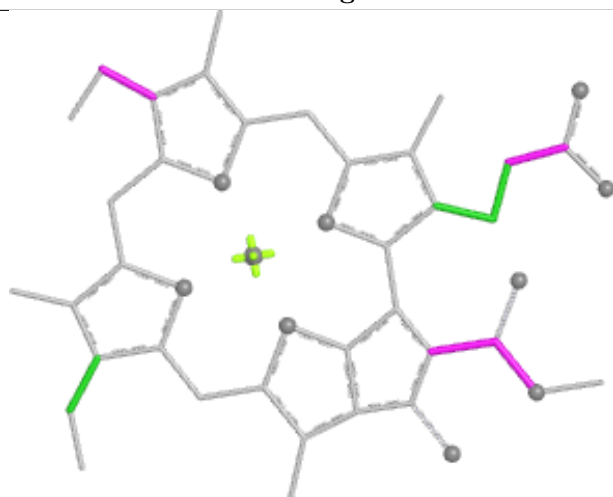
Ligand CLA I 101



Bond lengths



Bond angles

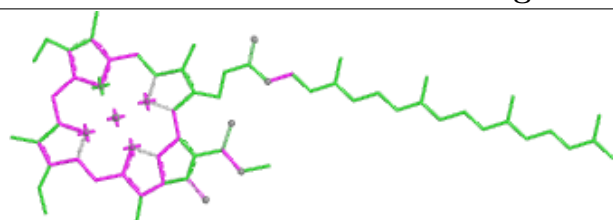


Torsions

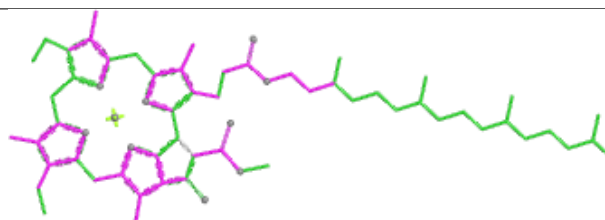


Rings

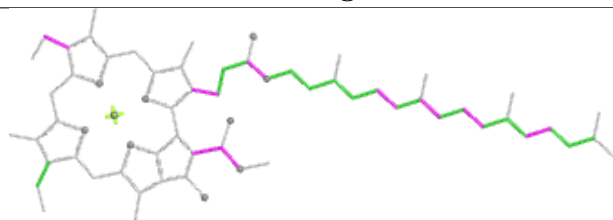
Ligand CLA A 830



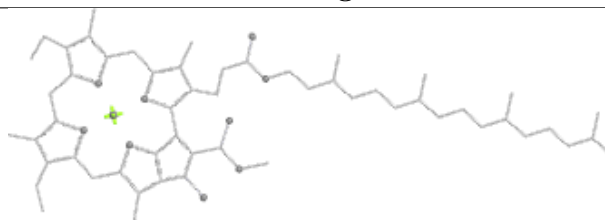
Bond lengths



Bond angles

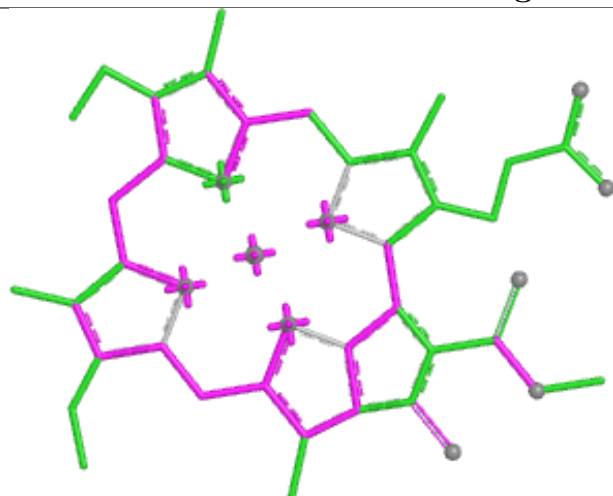


Torsions

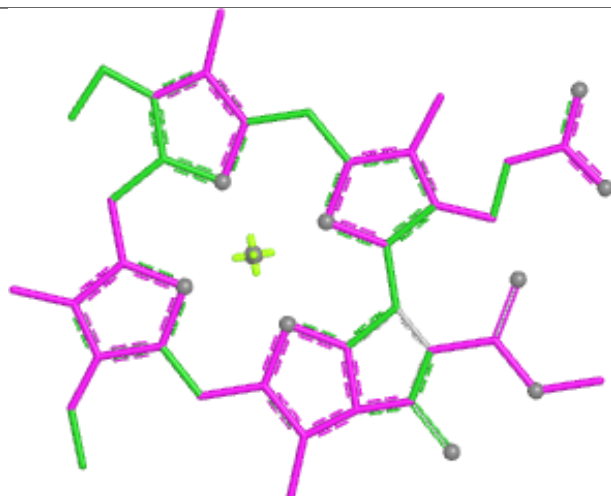


Rings

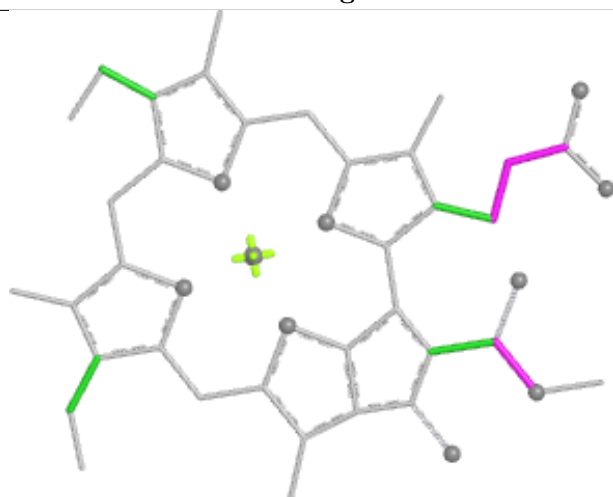
Ligand CLA B 812



Bond lengths



Bond angles

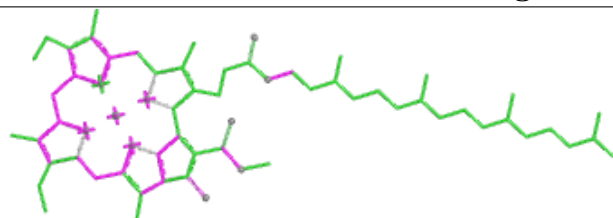


Torsions

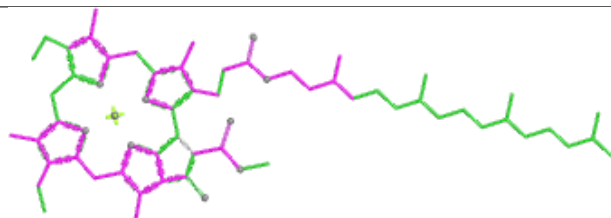


Rings

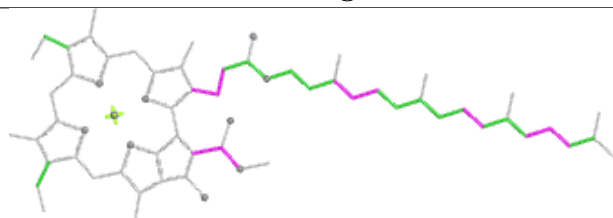
Ligand CLA A 827



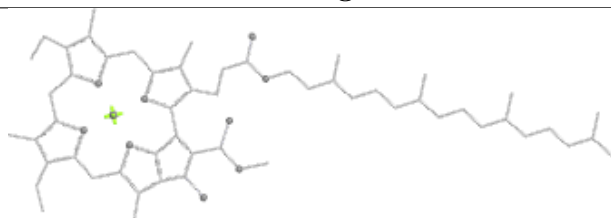
Bond lengths



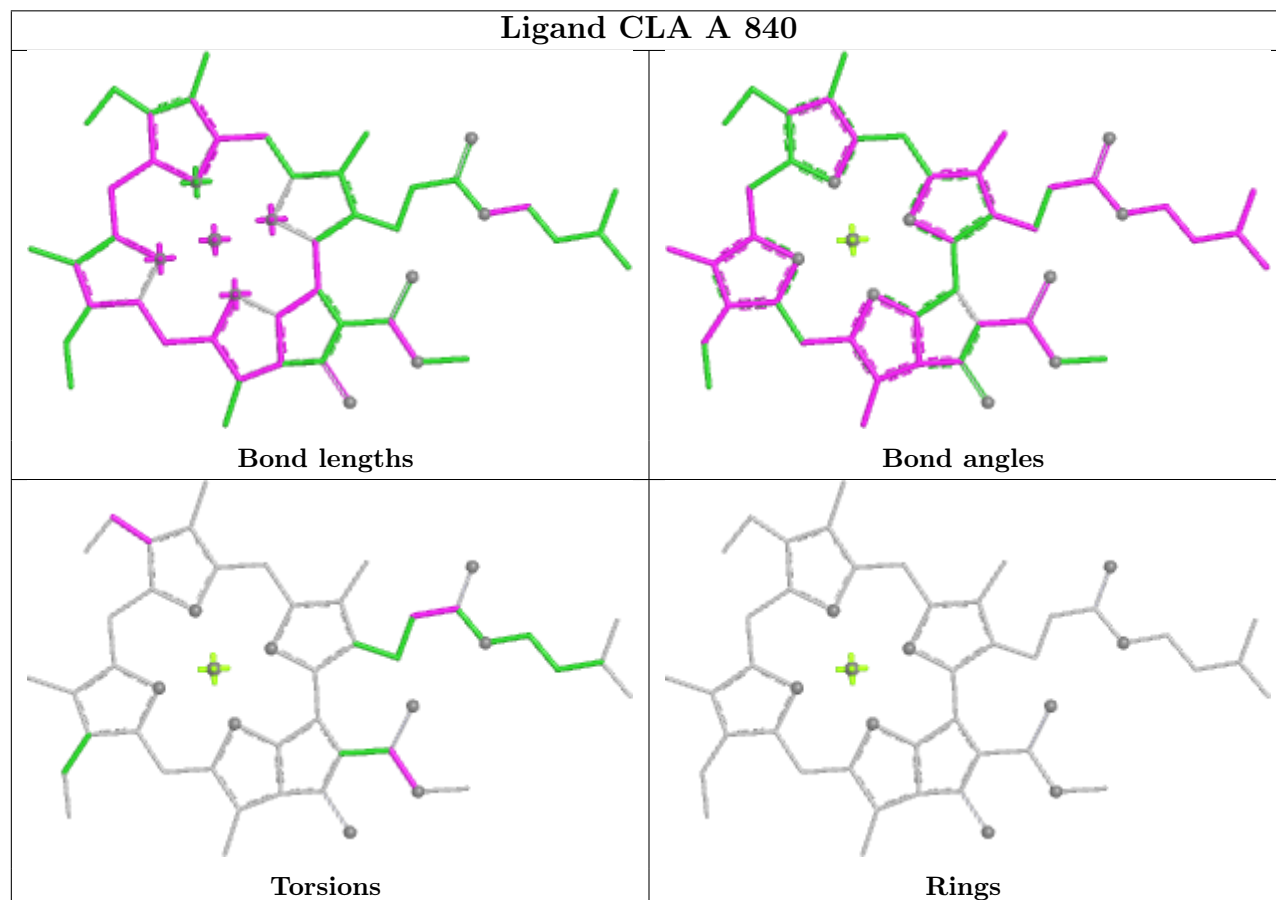
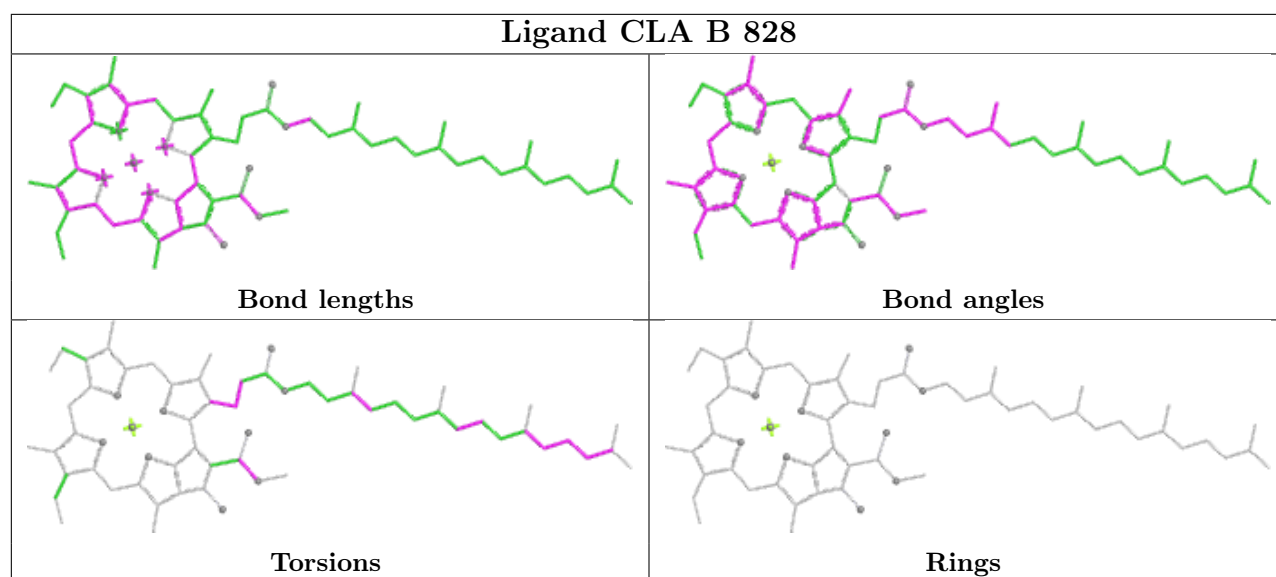
Bond angles



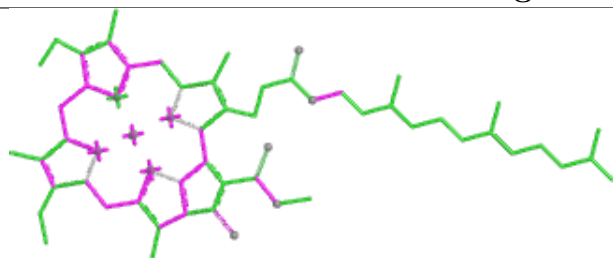
Torsions



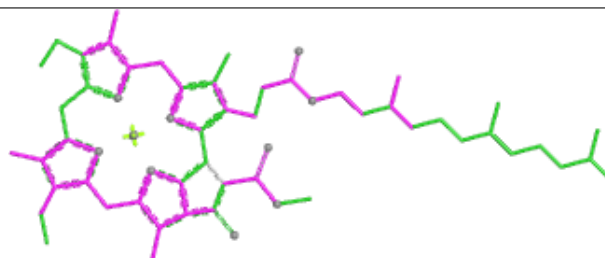
Rings



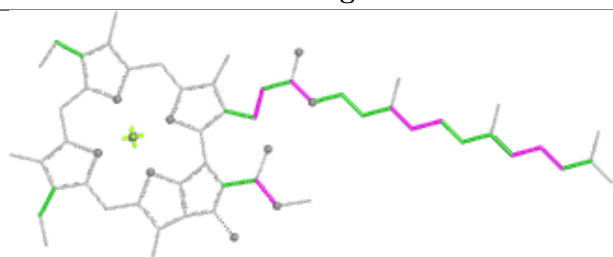
Ligand CLA B 801



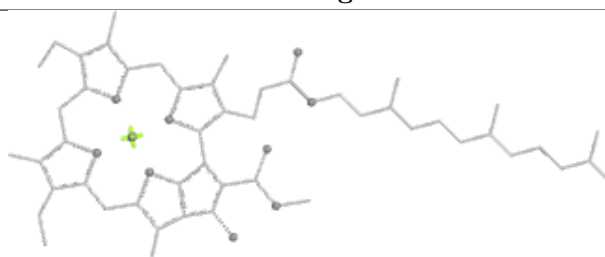
Bond lengths



Bond angles

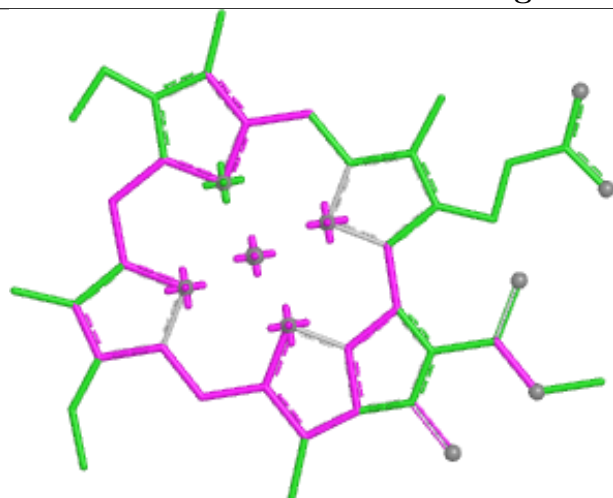


Torsions

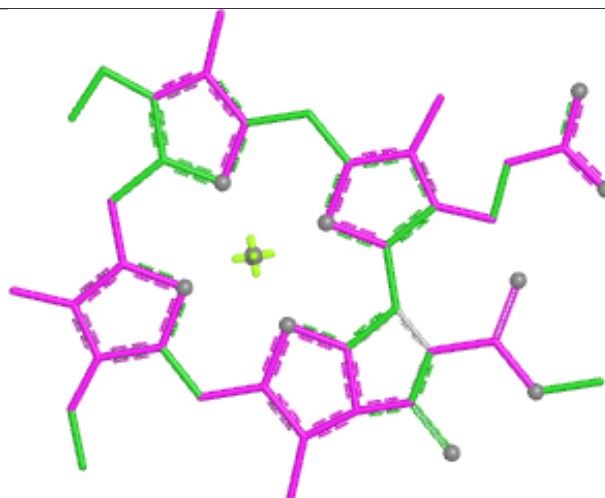


Rings

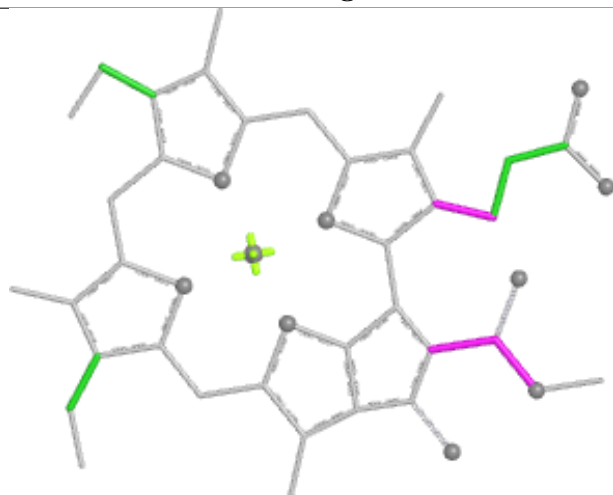
Ligand CLA B 829



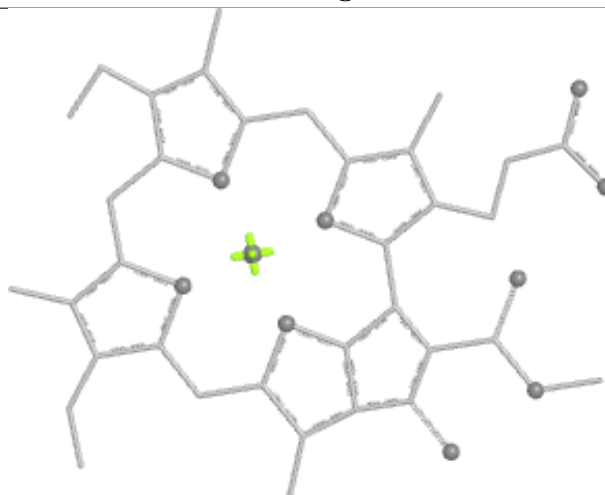
Bond lengths



Bond angles

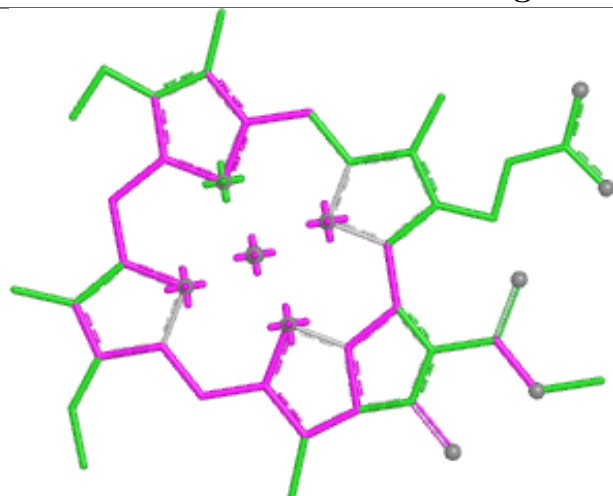


Torsions

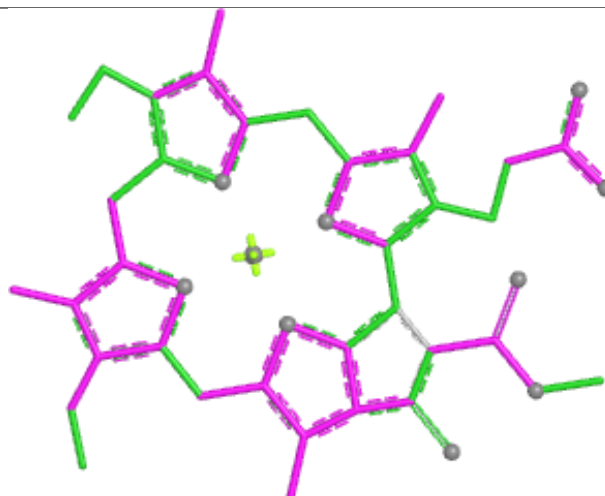


Rings

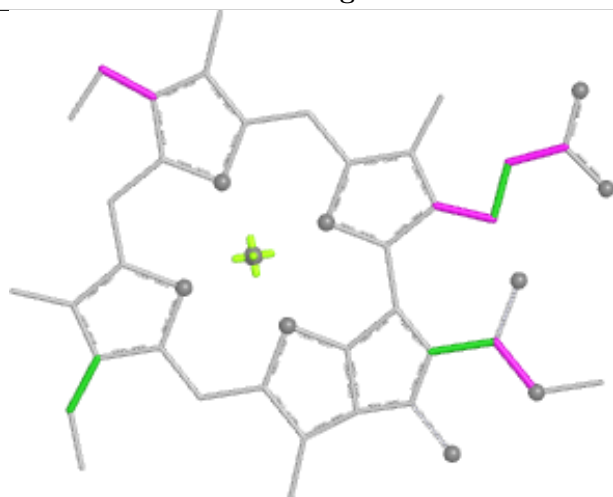
Ligand CLA A 823



Bond lengths



Bond angles

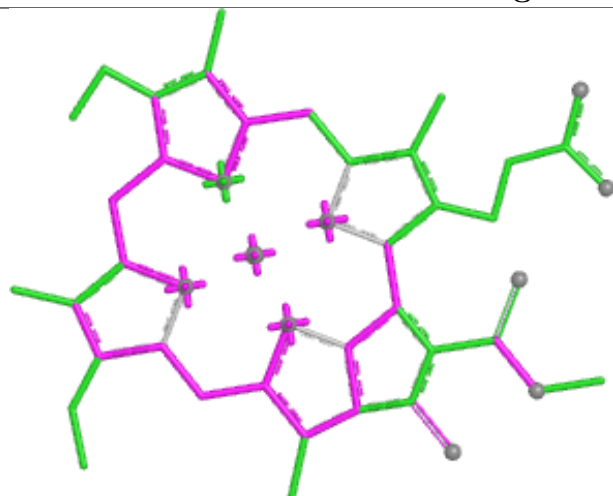


Torsions

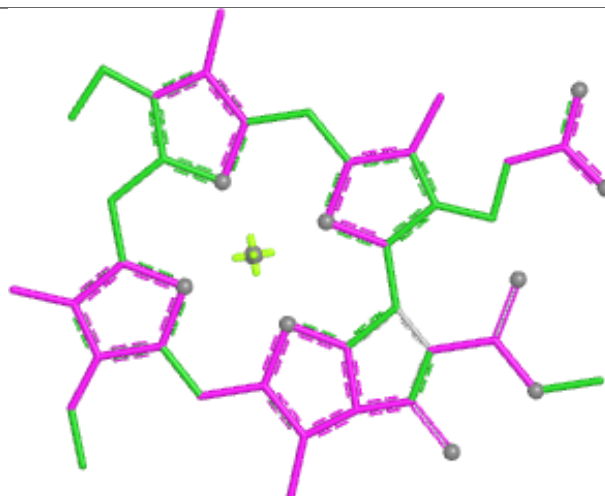


Rings

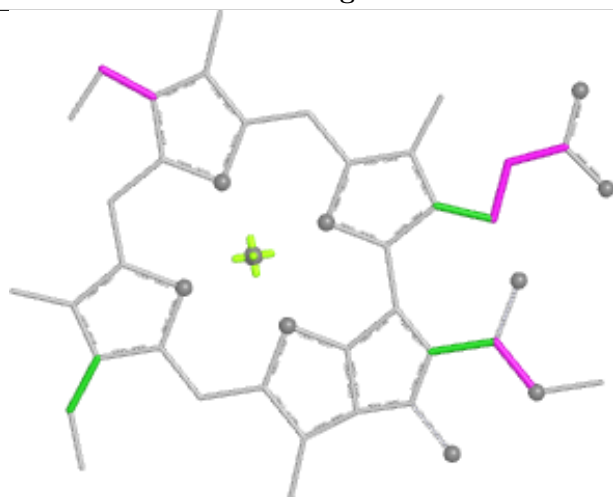
Ligand CLA A 811



Bond lengths



Bond angles

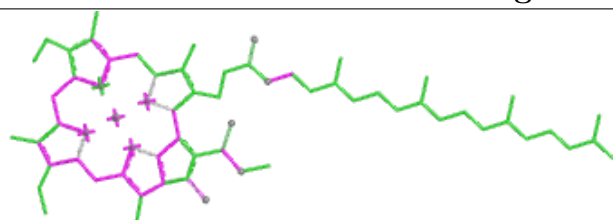


Torsions

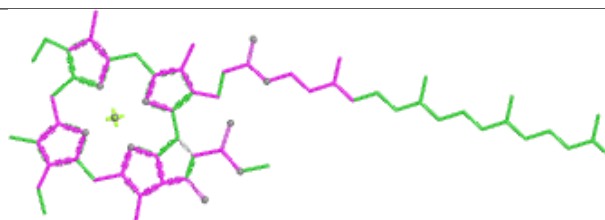


Rings

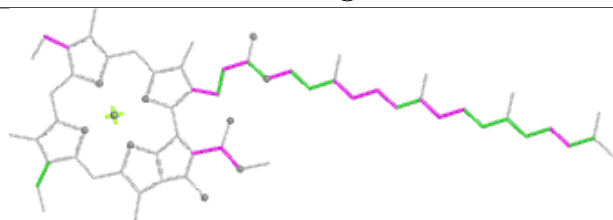
Ligand CLA B 826



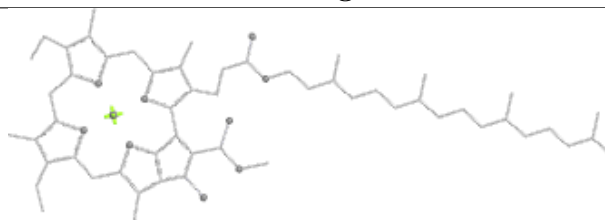
Bond lengths



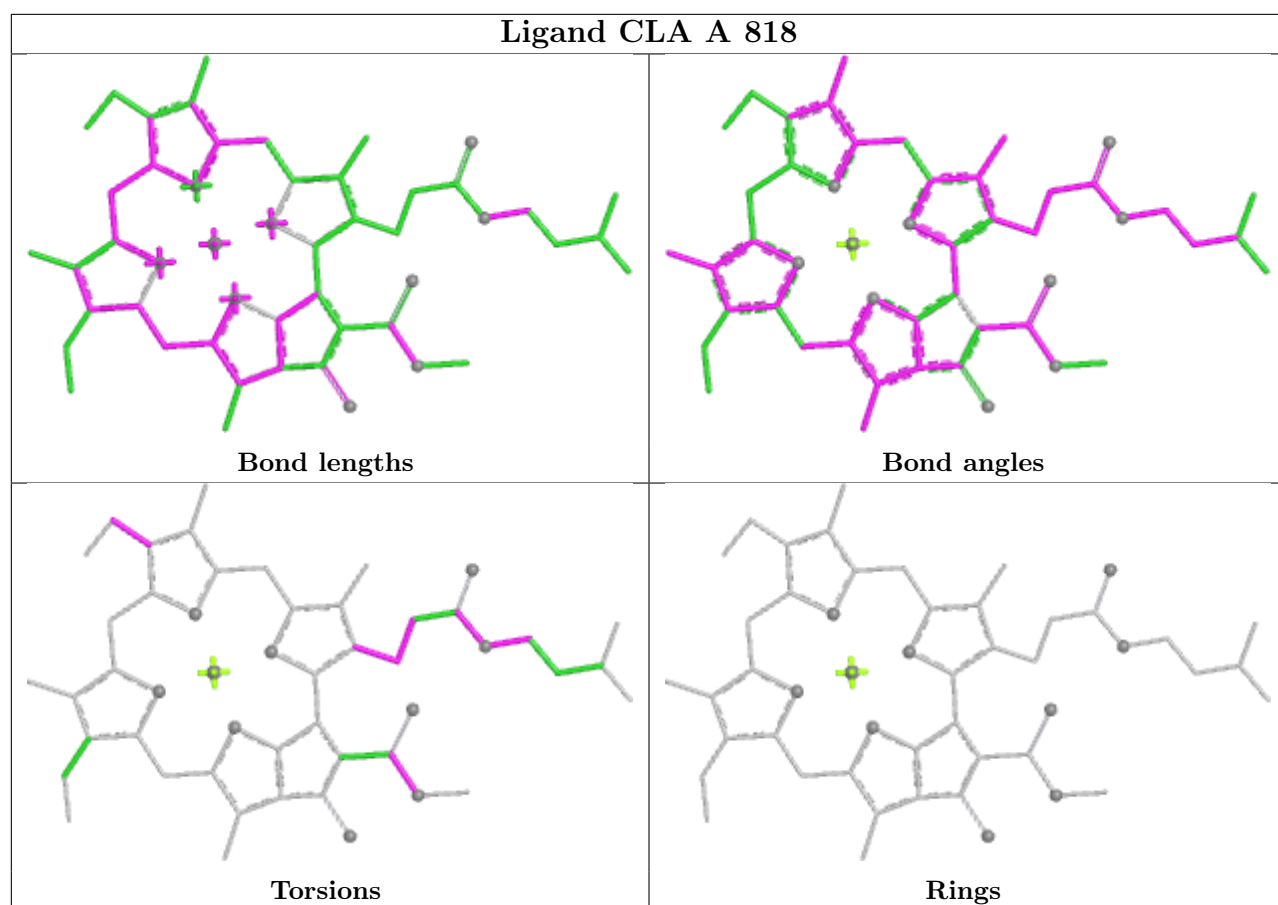
Bond angles

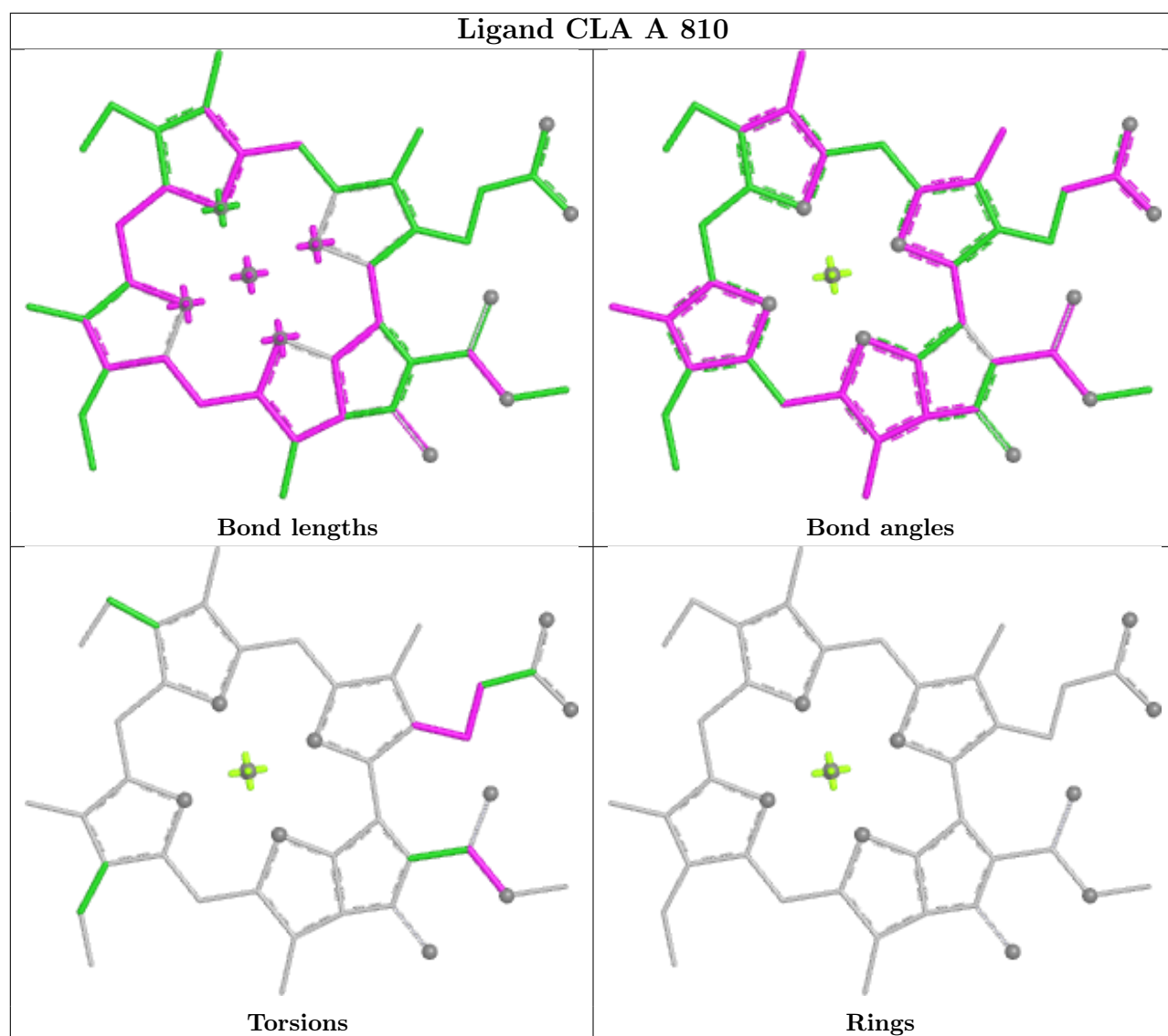


Torsions

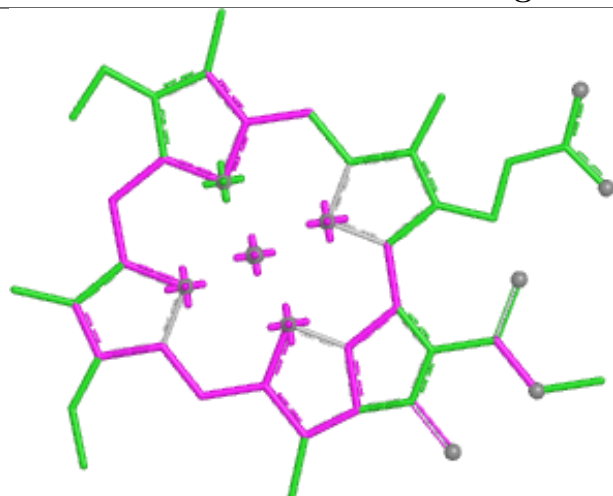


Rings

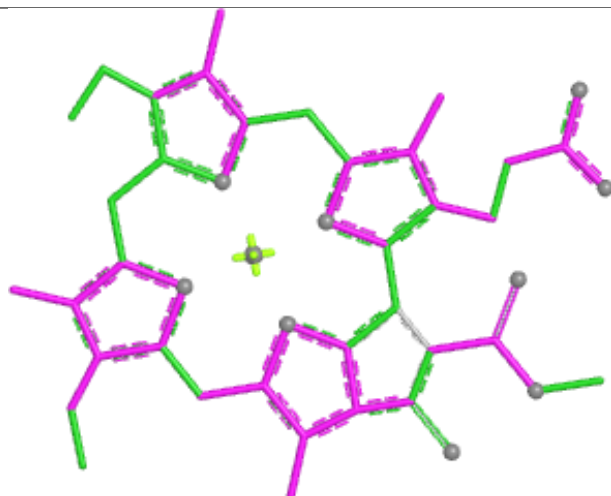




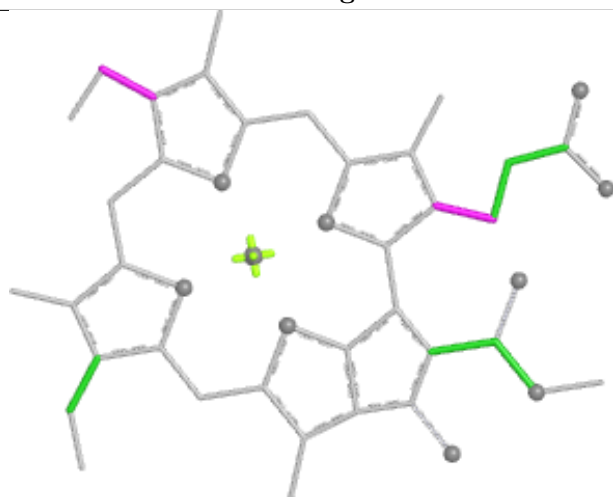
Ligand CLA B 832



Bond lengths



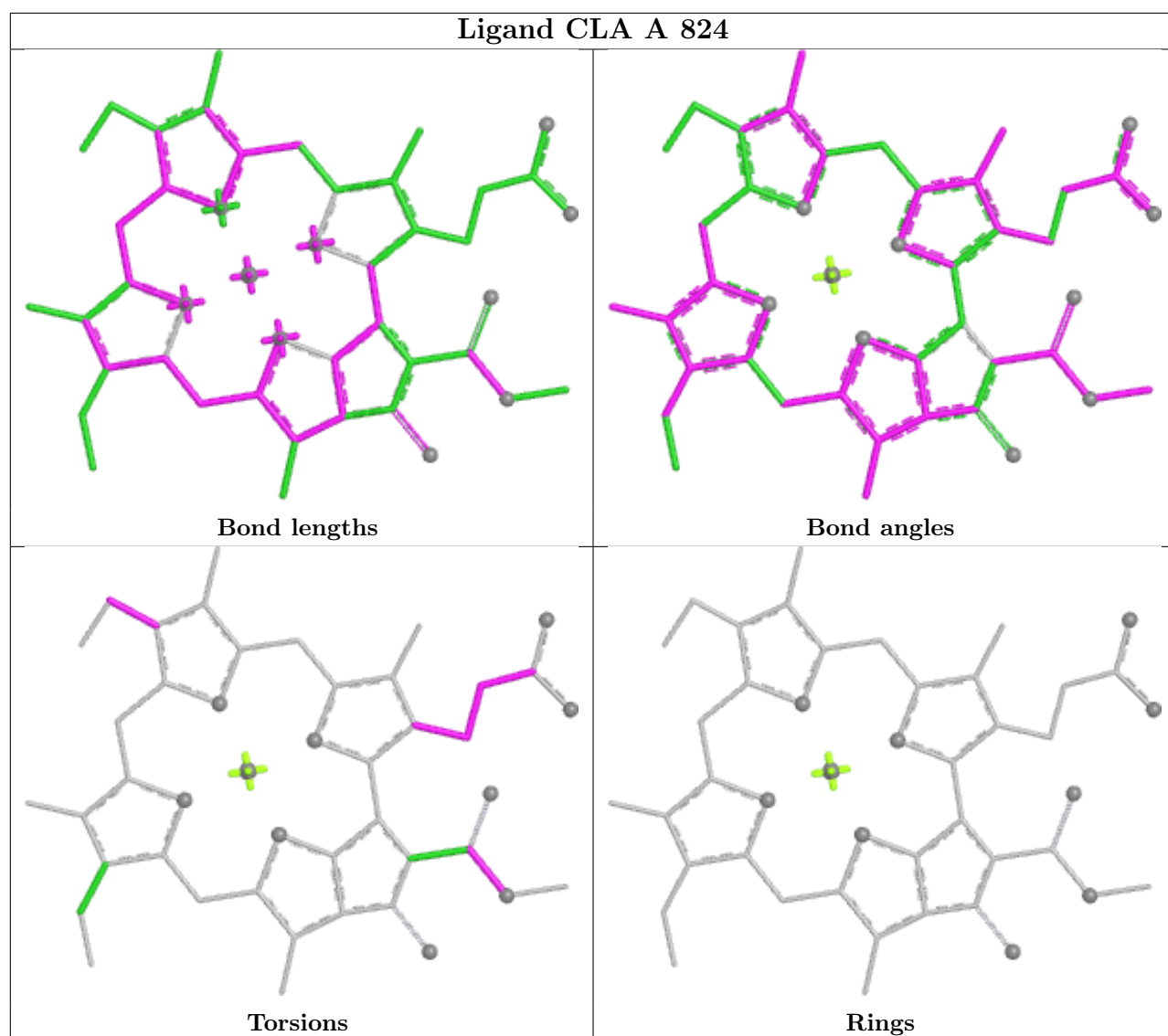
Bond angles



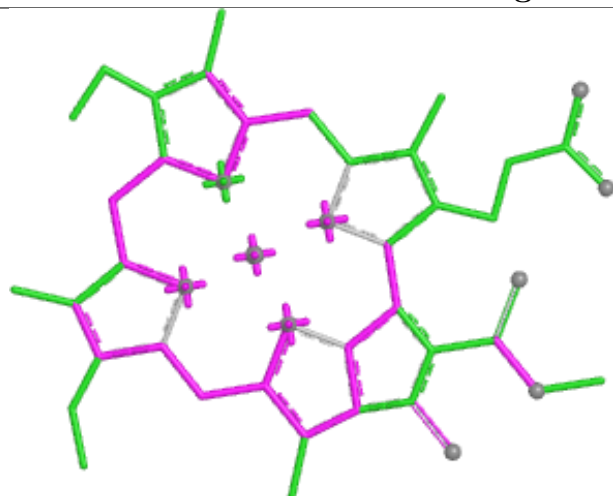
Torsions



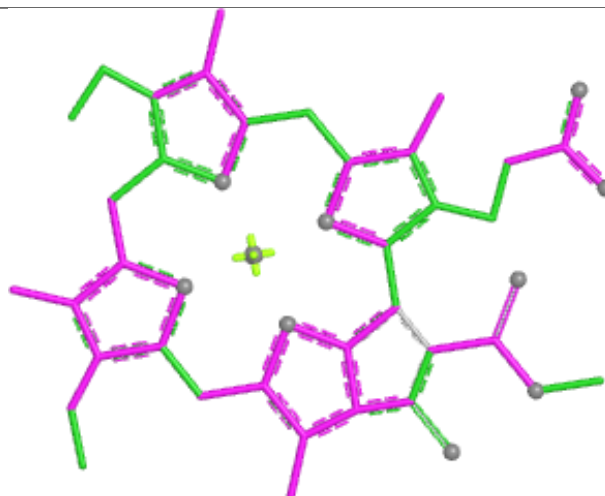
Rings



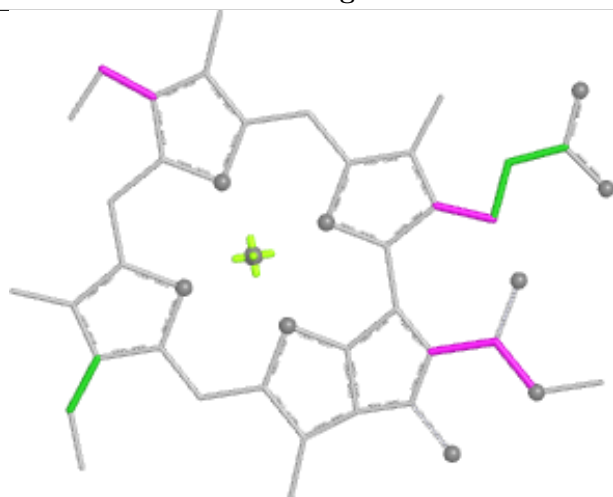
Ligand CLA B 820



Bond lengths



Bond angles

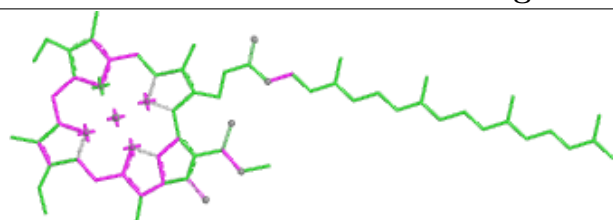


Torsions

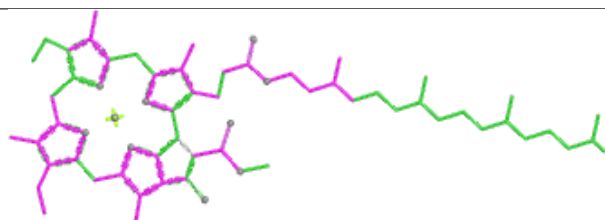


Rings

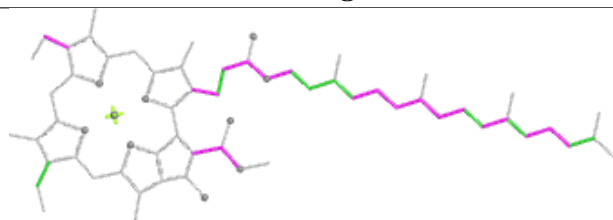
Ligand CLA A 805



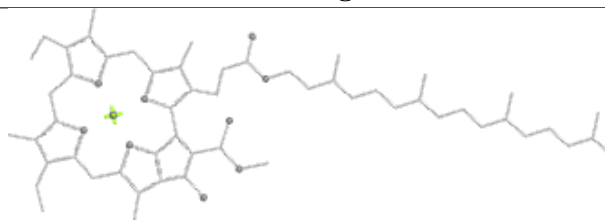
Bond lengths



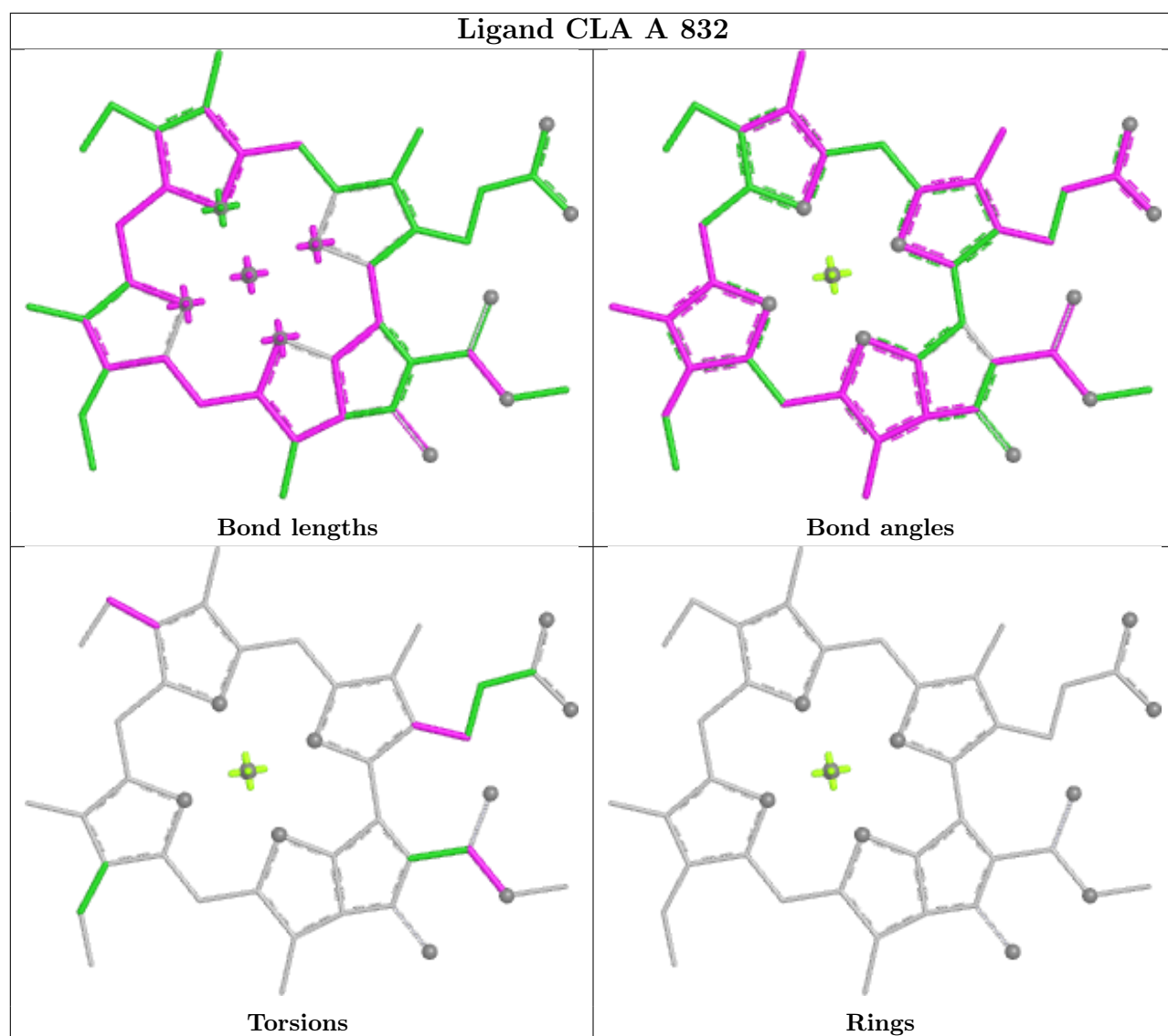
Bond angles

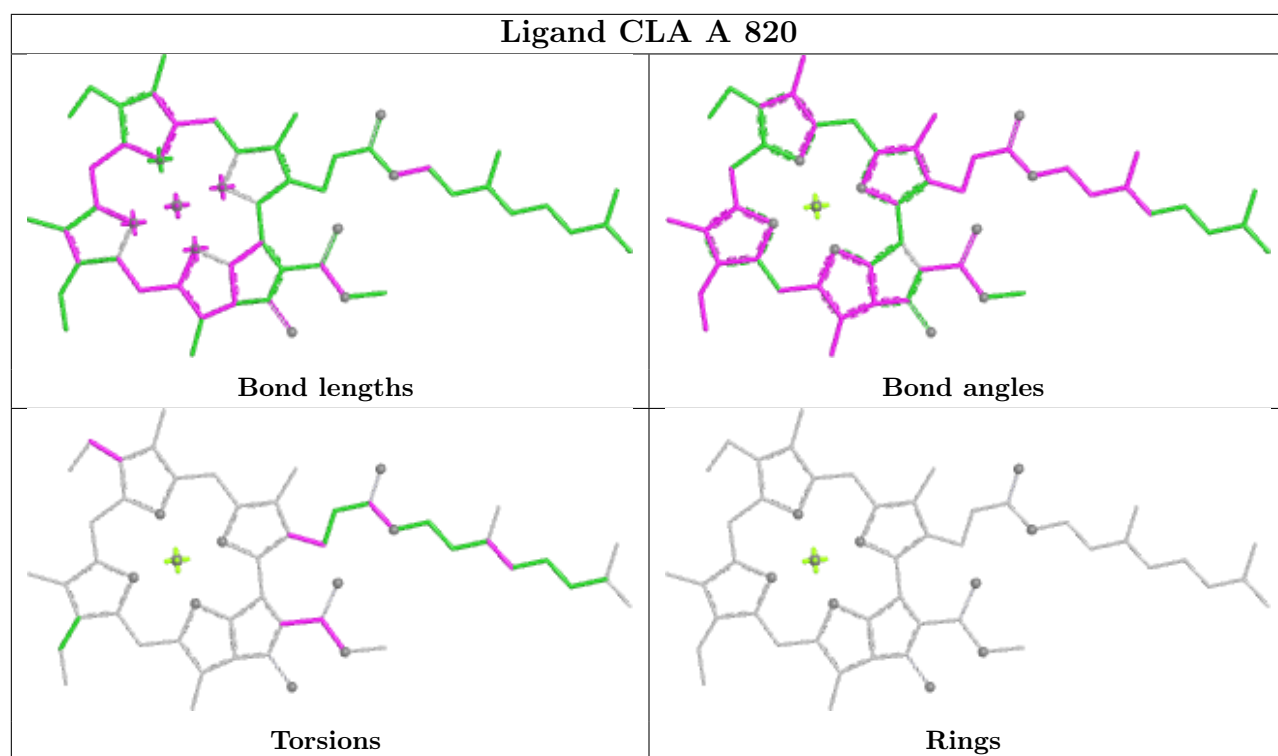


Torsions

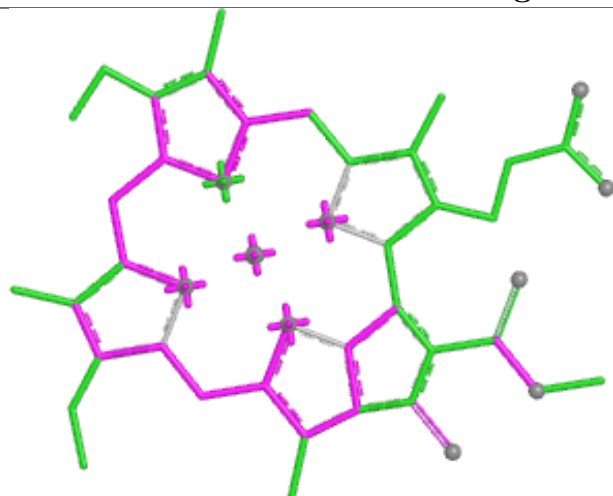


Rings

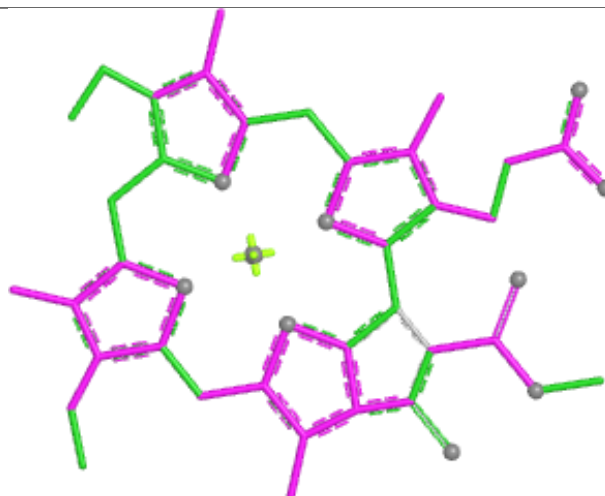




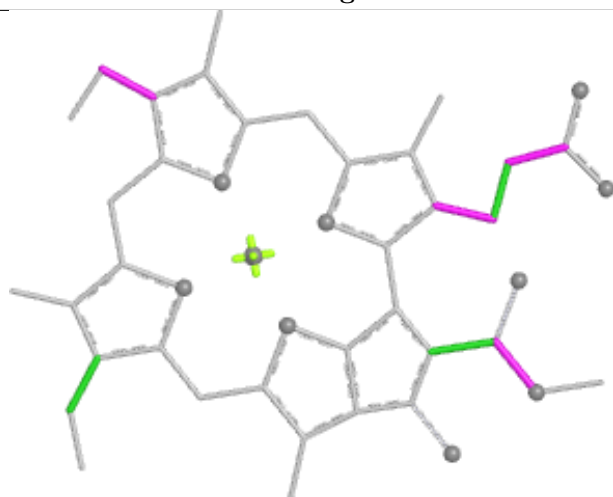
Ligand CLA A 839



Bond lengths



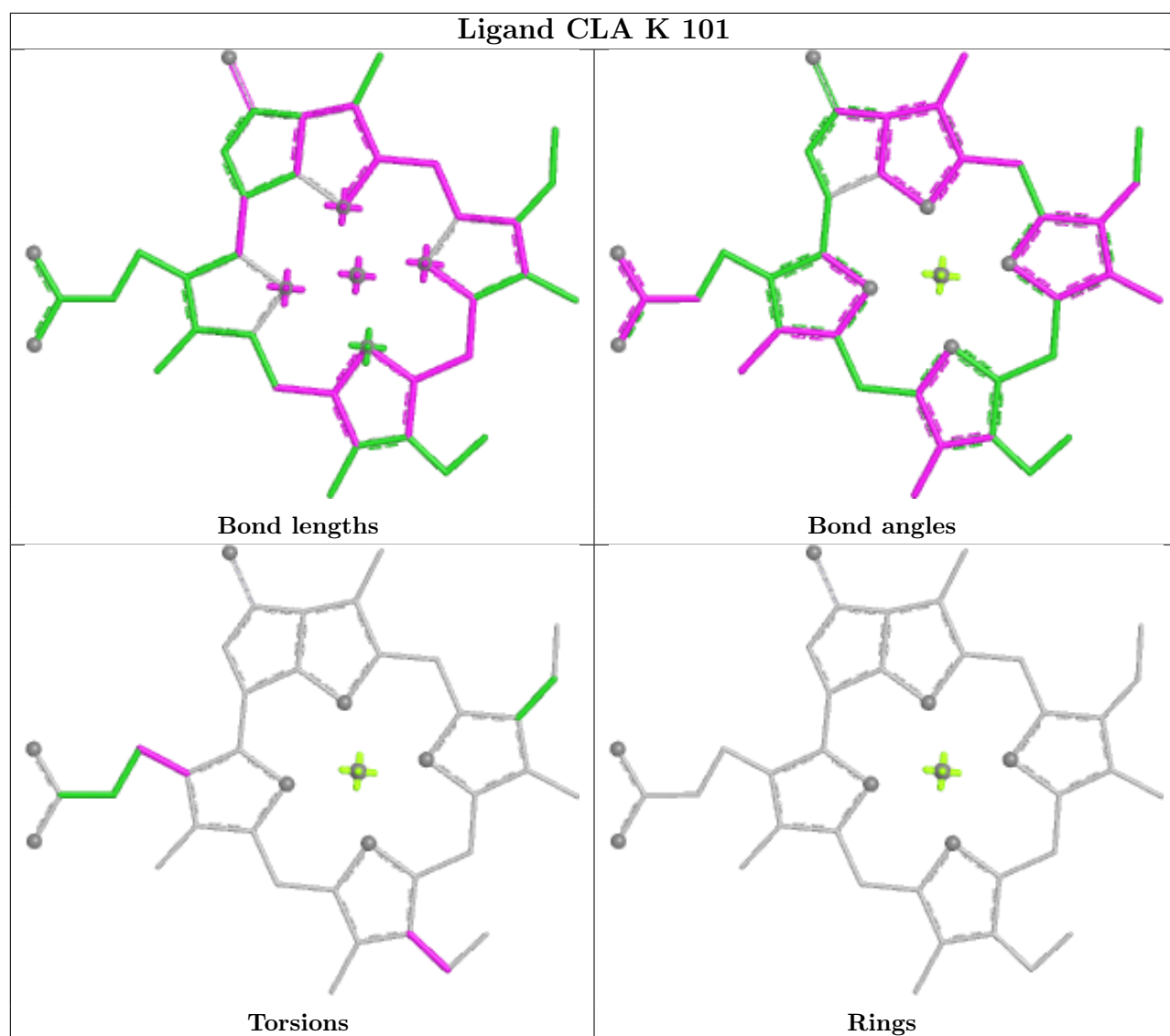
Bond angles

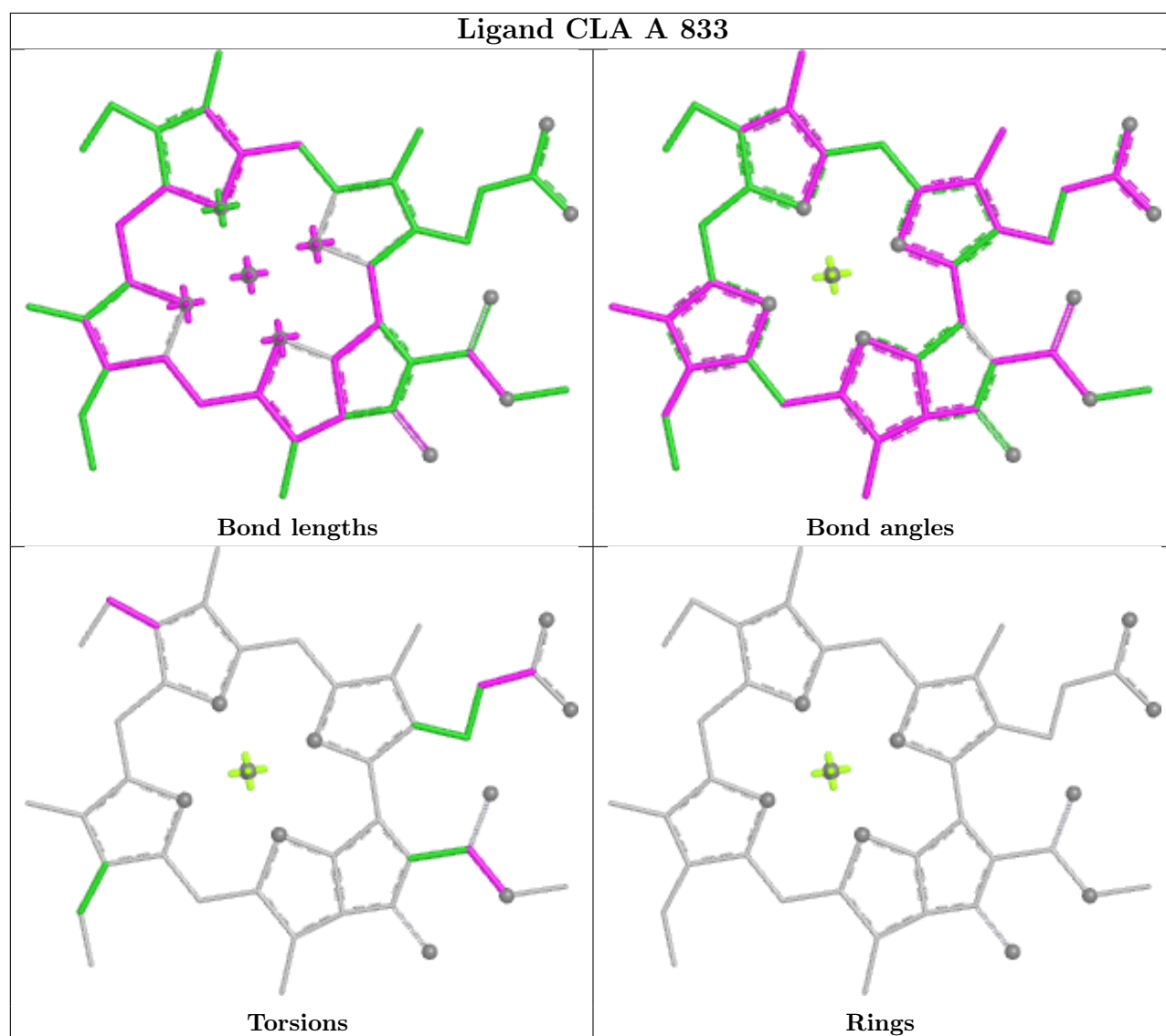


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

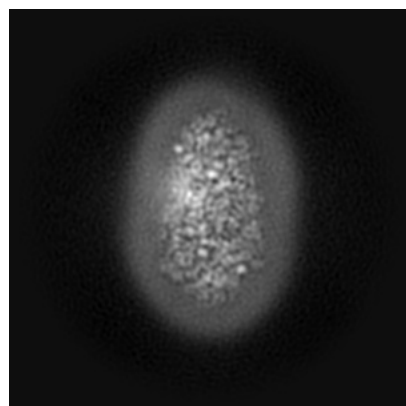
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75232. These allow visual inspection of the internal detail of the map and identification of artifacts.

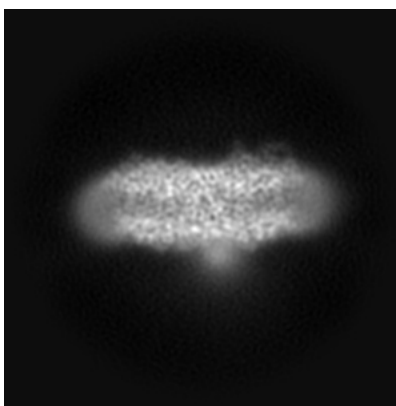
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

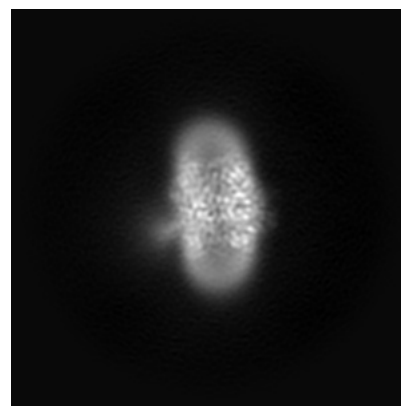
6.1.1 Primary map



X

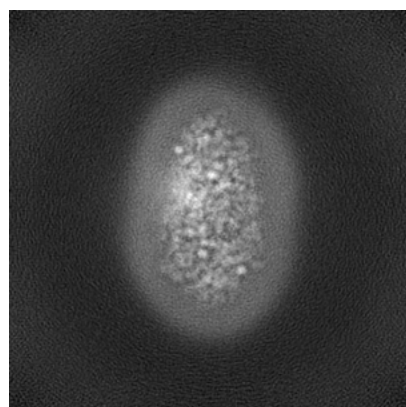


Y

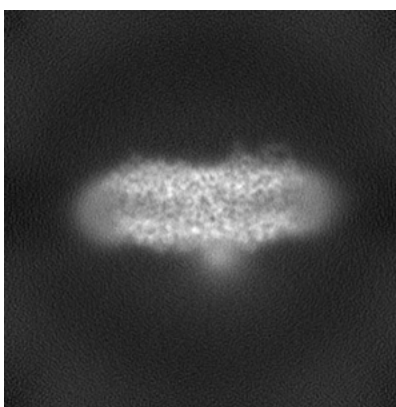


Z

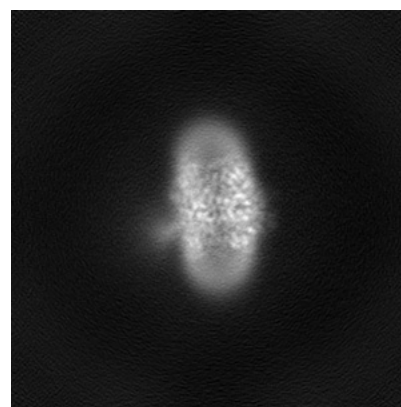
6.1.2 Raw map



X



Y

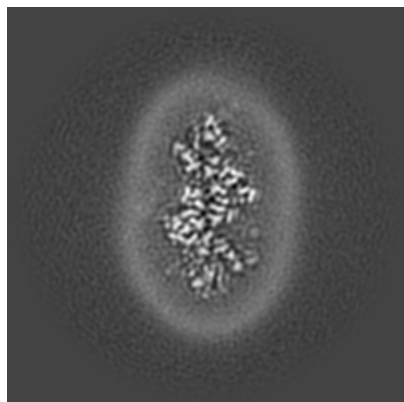


Z

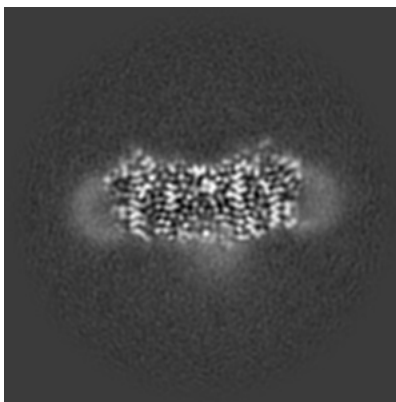
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

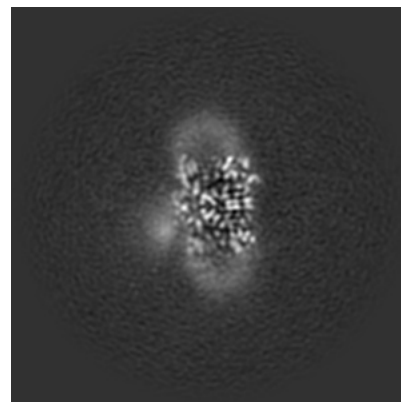
6.2.1 Primary map



X Index: 128

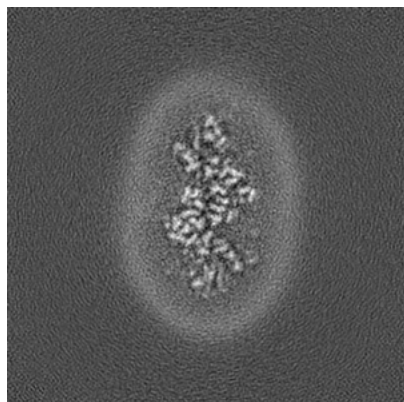


Y Index: 128

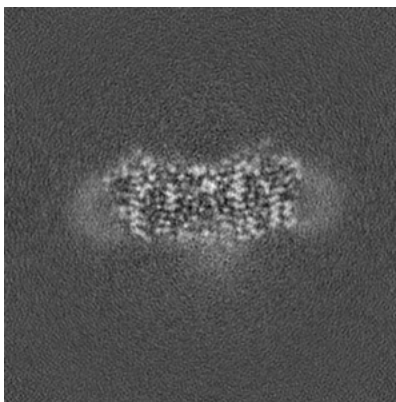


Z Index: 128

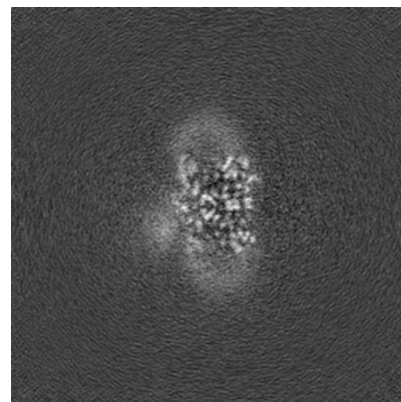
6.2.2 Raw map



X Index: 128



Y Index: 128

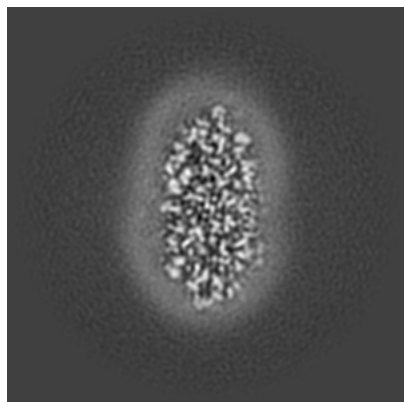


Z Index: 128

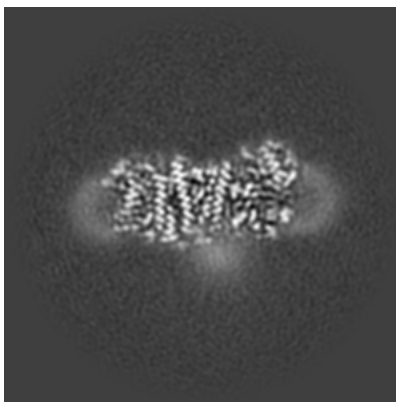
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

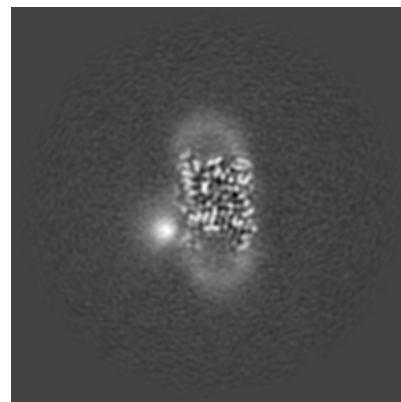
6.3.1 Primary map



X Index: 144

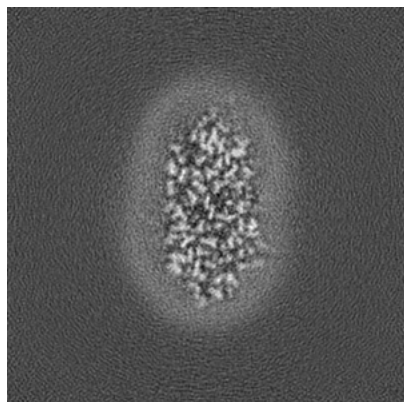


Y Index: 123

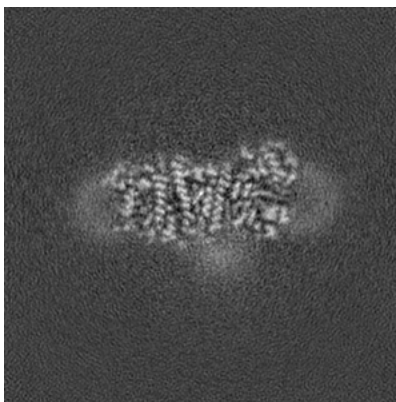


Z Index: 135

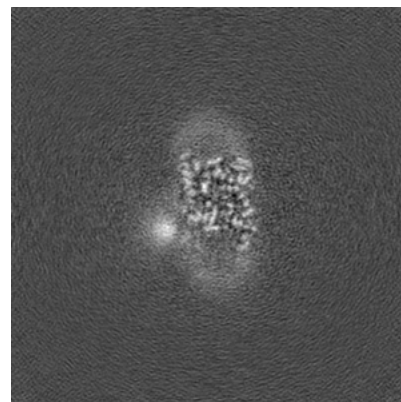
6.3.2 Raw map



X Index: 142



Y Index: 122

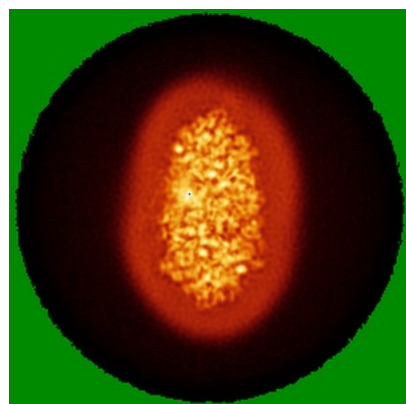


Z Index: 135

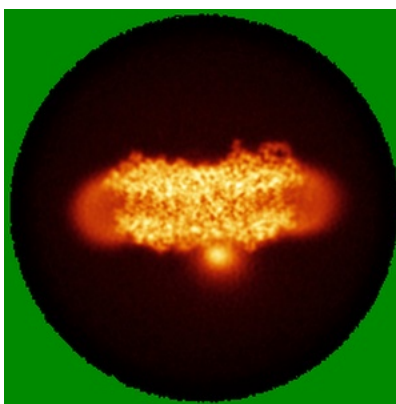
The images above show the largest variance slices of the map in three orthogonal directions.

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

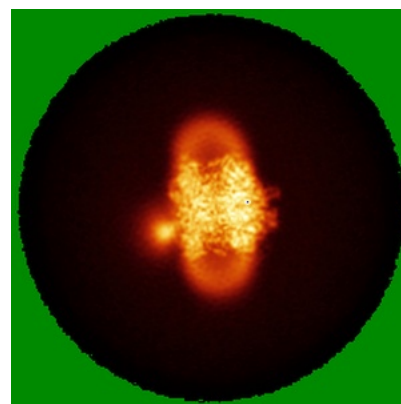
6.4.1 Primary map



X

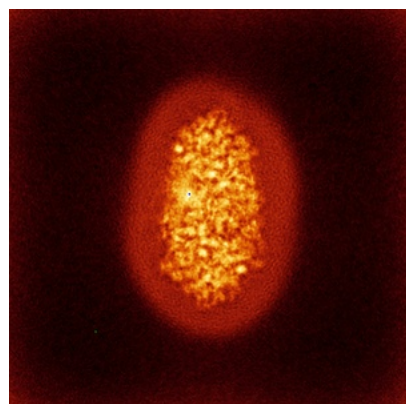


Y

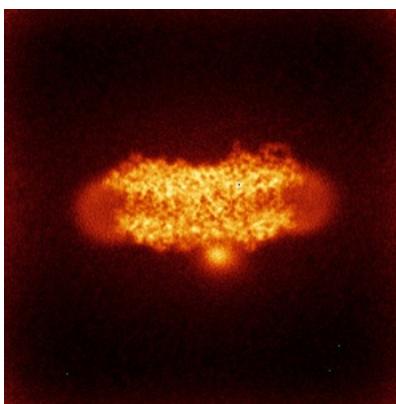


Z

6.4.2 Raw map



X



Y

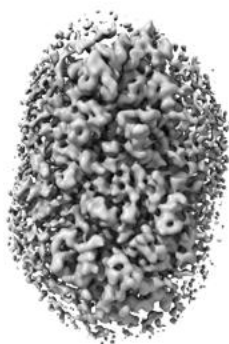


Z

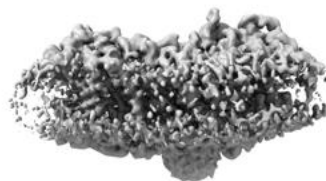
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

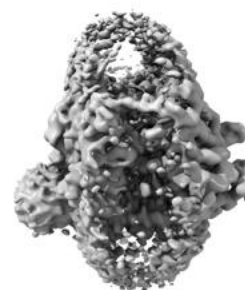
6.5.1 Primary map



X



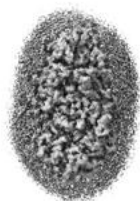
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.164. 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



X



Y



Z

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.

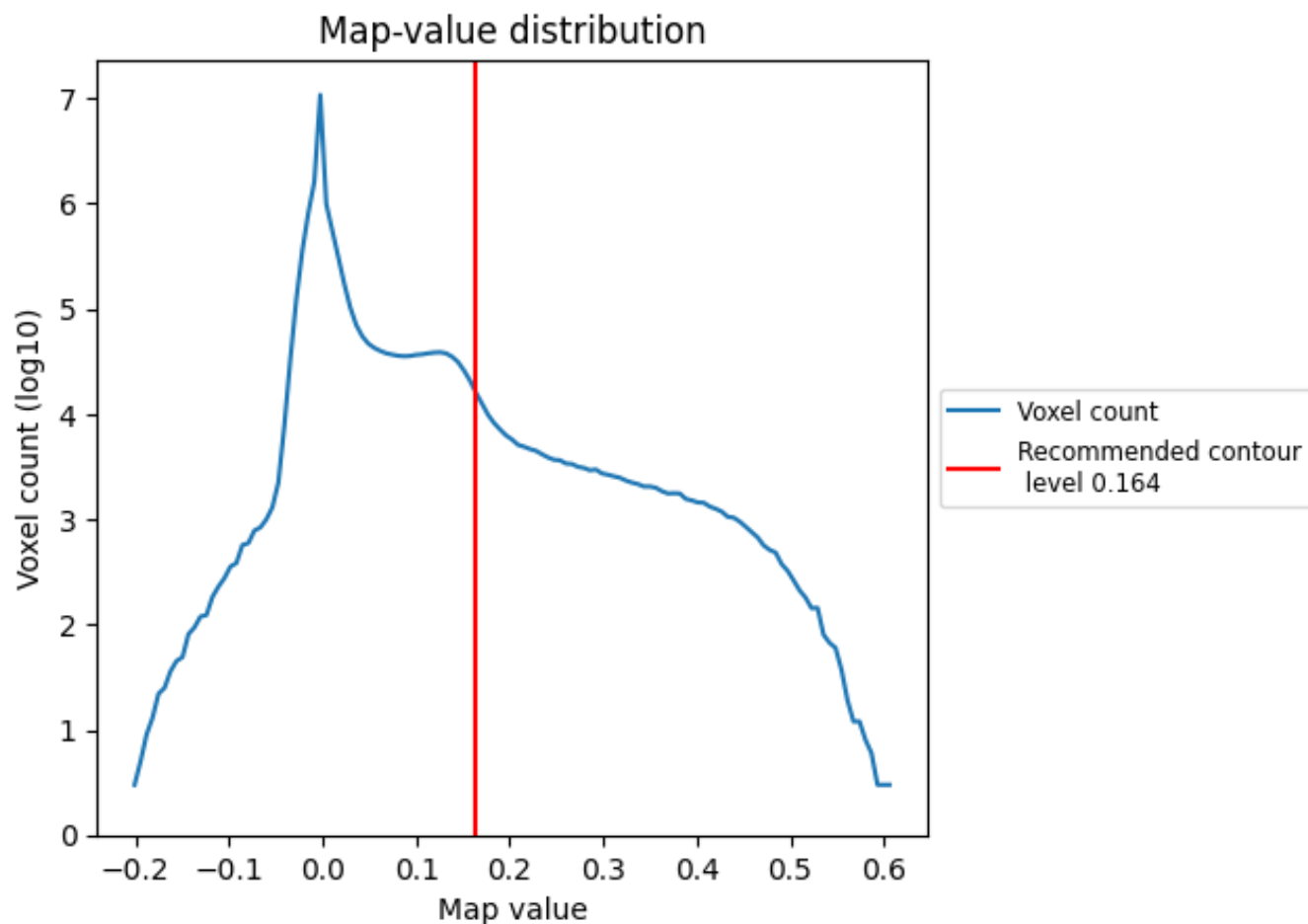
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

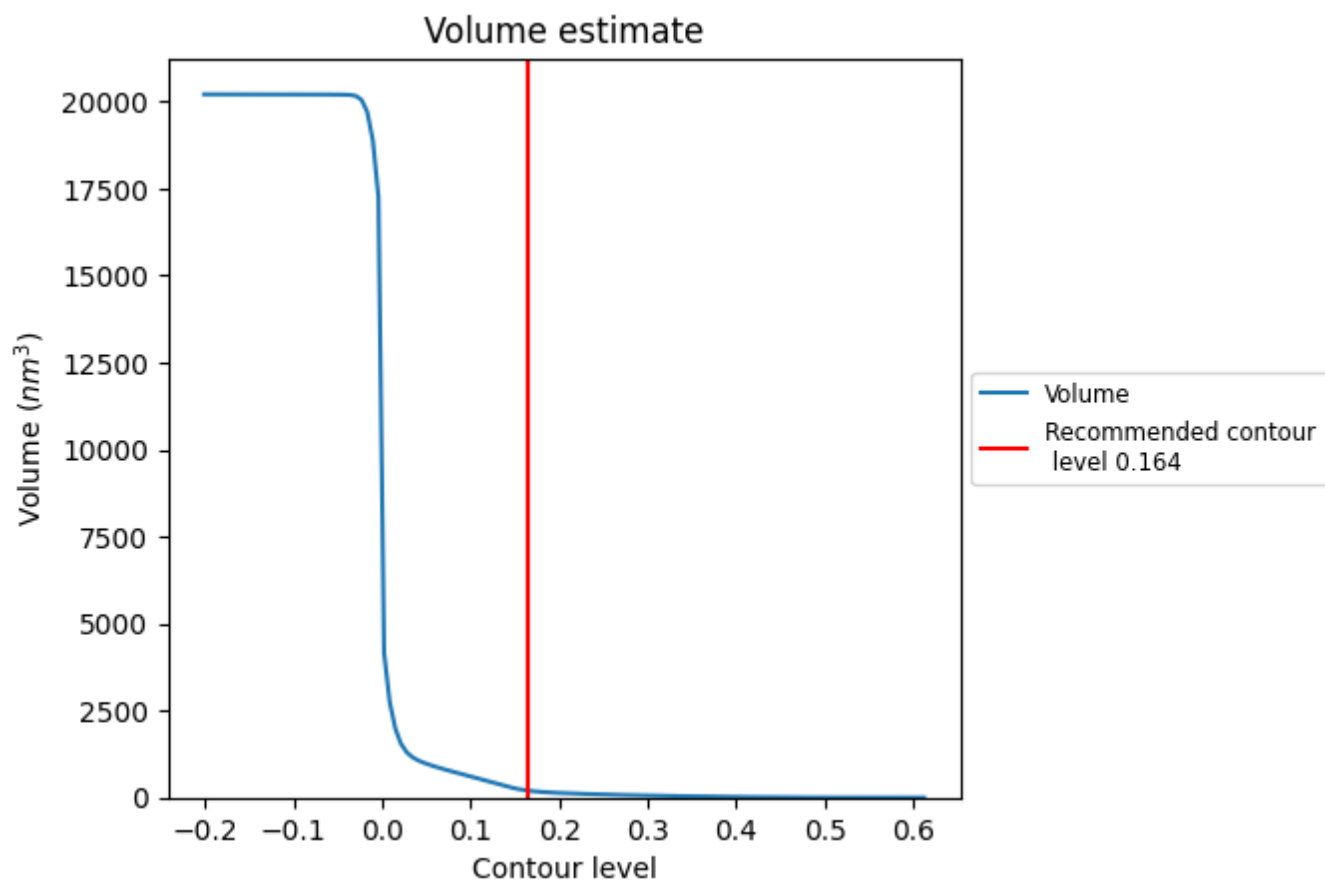
This section contains the results of statistical analysis of the map.

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.

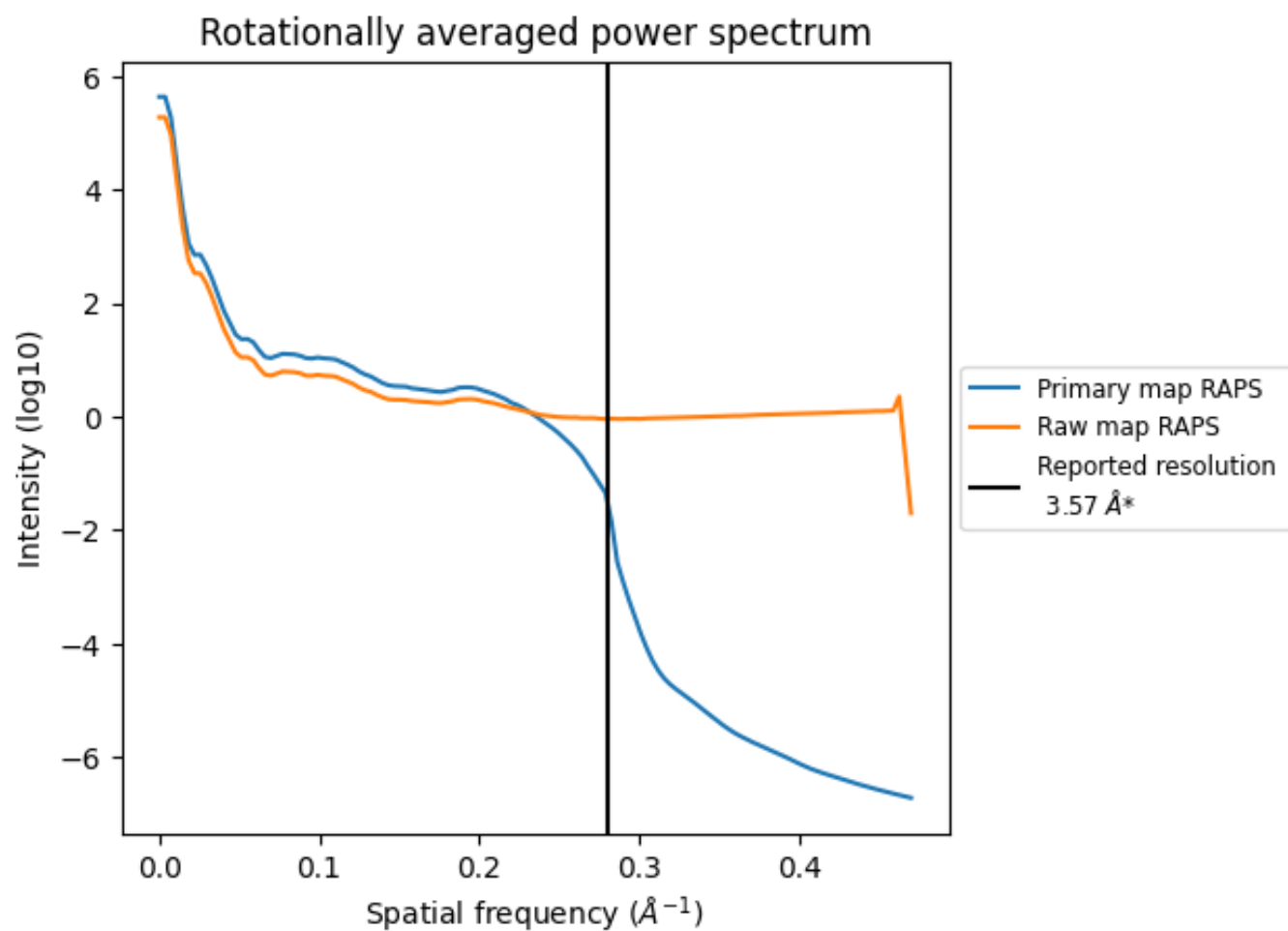
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 203 nm³; this corresponds to an approximate mass of 184 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 ⓘ

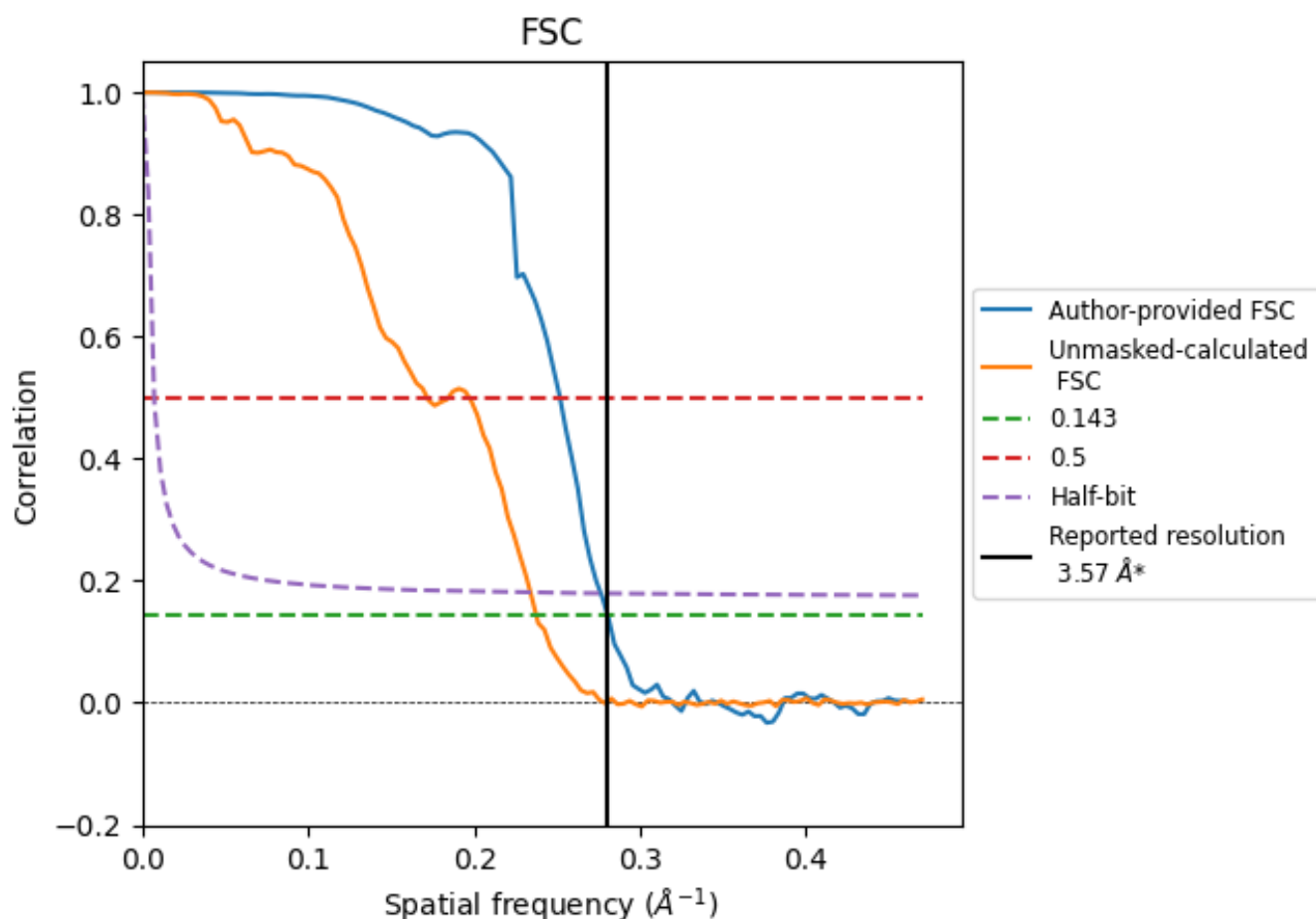


*Reported resolution corresponds to spatial frequency of 0.280 $\text{\AA}^{-1}$

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 0.280 Å⁻¹

8.2 Resolution estimates [i](#)

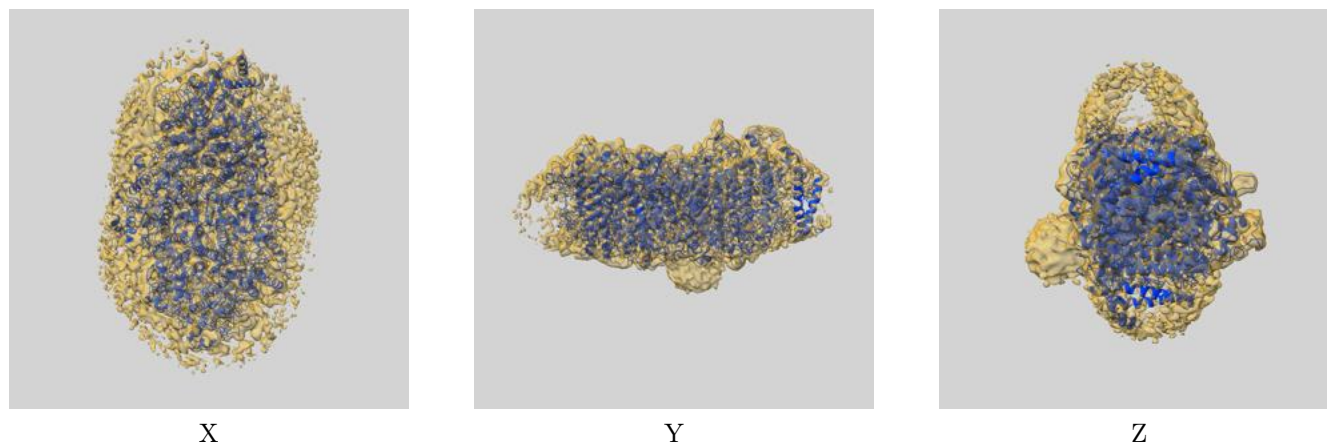
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.57	-	-
Author-provided FSC curve	3.57	3.97	3.62
Unmasked-calculated*	4.21	5.82	4.28

*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 4.21 differs from the reported value 3.57 by more than 10 %

9 Map-model fit [i](#)

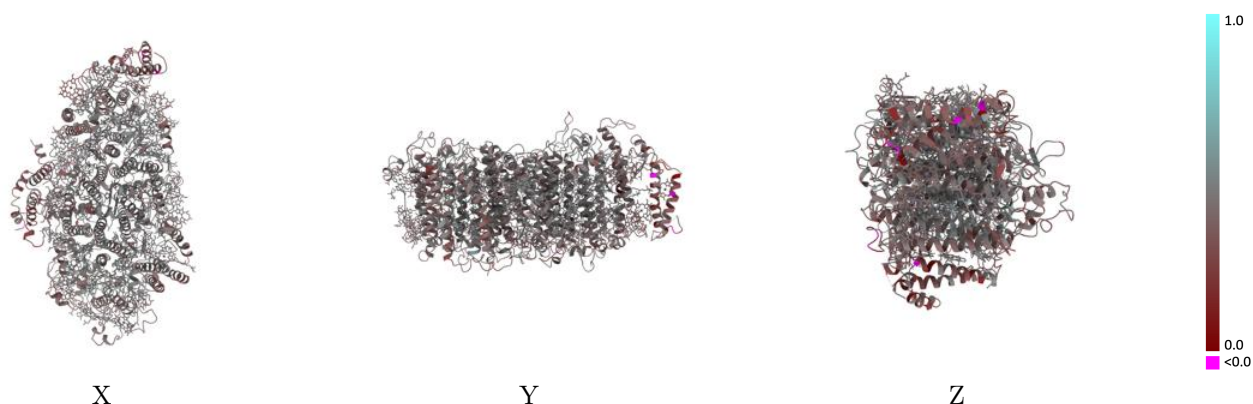
This section contains information regarding the fit between EMDB map EMD-75232 and PDB model 10KF. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



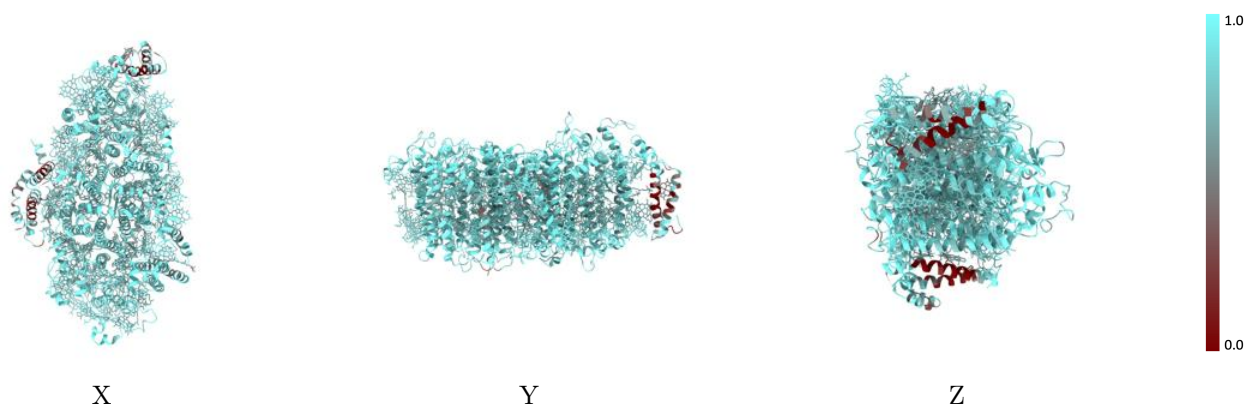
The images above show the 3D surface view of the map at the recommended contour level 0.164 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



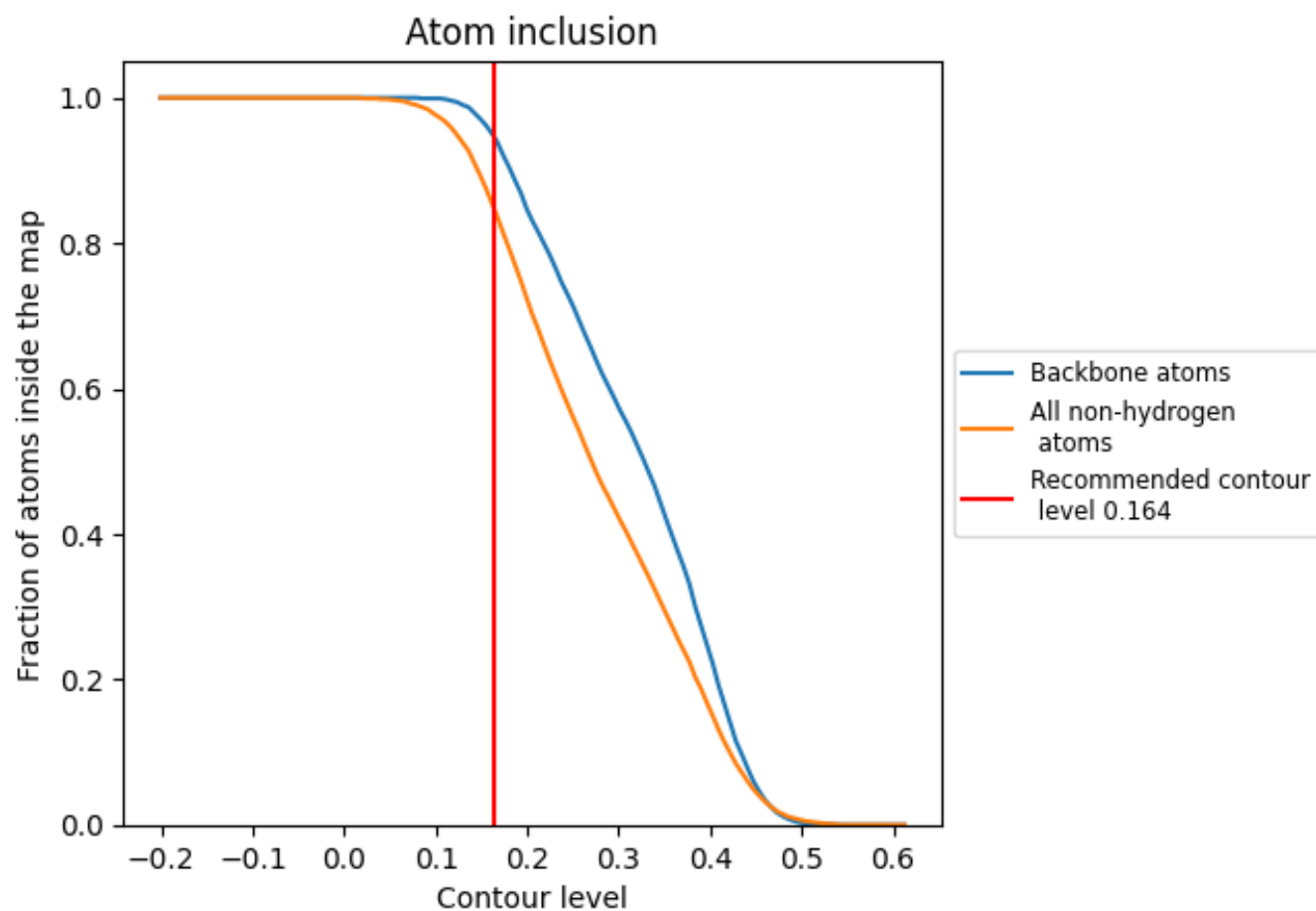
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.164).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 85% 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 (0.164) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8470	0.4230
A	0.8660	0.4280
B	0.8690	0.4340
F	0.5850	0.3130
I	0.7780	0.3760
J	0.5740	0.3120
K	0.5210	0.2990
M	0.7710	0.3930

1.0

0.0

<0.0