



wwPDB EM Validation Summary Report ⓘ

Aug 9, 2026 – 03:18 AM JST

PDB ID : 8ZOF / pdb_00008zof
EMDB ID : EMD-60291
Title : Structure of the canthaxanthin mutant PSI-3VCPI supercomplex in *Nanochloropsis oceanica*
Authors : Shen, L.L.; Li, Z.H.; Shen, J.R.; Wang, W.D.
Deposited on : 2024-05-28
Resolution : 3.06 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:

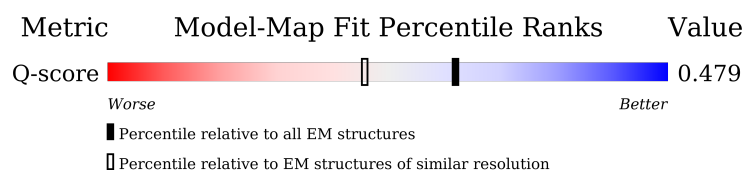
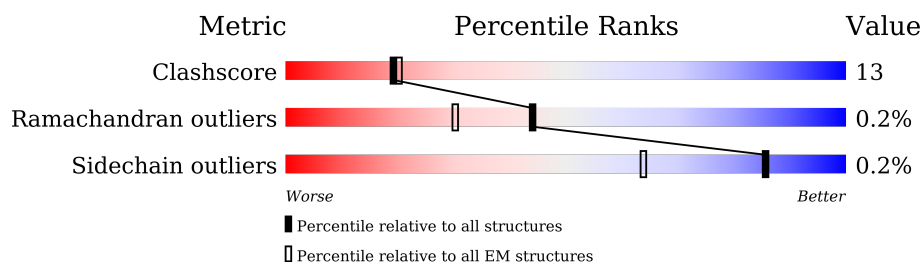
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 3.06 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.



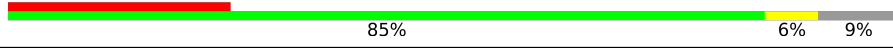
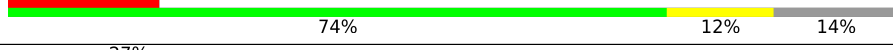
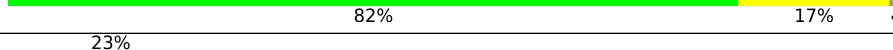
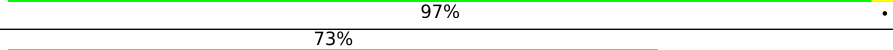
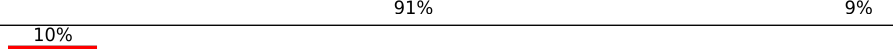
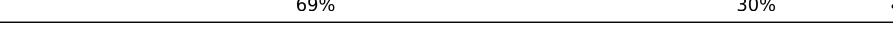
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13976 (2.56 - 3.56)

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	5	244	65% 52% 18% 31%
2	4	202	82% 72% 11% 17%
3	1	208	20% 51% 27% 22%
4	a	745	75% 24%

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Mol	Chain	Length	Quality of chain
5	b	737	
6	d	136	
7	e	67	
8	f	185	
9	i	45	
10	j	41	
11	l	172	
12	m	30	
13	g	55	
14	c	81	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	SF4	c	102	-	-	X	-

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 30455 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 VCPI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	169	Total	C	N	O	S	0	0
			1317	867	222	222	6		

- Molecule 2 is a protein called VCPI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	168	Total	C	N	O	S	0	0
			1268	822	211	229	6		

- Molecule 3 is a protein called VCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	162	Total	C	N	O	S	0	0
			1262	816	209	234	3		

- Molecule 4 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	739	Total	C	N	O	S	0	0
			5827	3828	982	1000	17		

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	b	735	Total	C	N	O	S	0	0
			5865	3874	985	989	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	130	Total	C	N	O	S	0	0
			1014	652	175	184	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	e	61	Total	C	N	O	0	0
			494	314	86	94		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	f	160	Total	C	N	O	S	0	0
			1266	815	213	235	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	34	Total	C	N	O	S	0	0
			271	189	36	45	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	41	Total	C	N	O	S	0	0
			339	233	48	57	1		

- Molecule 11 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	l	171	Total	C	N	O	0	0
			1283	848	203	232		

- Molecule 12 is a protein called PsaM.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	m	30	Total	C	N	O	0	0
			210	137	35	38		

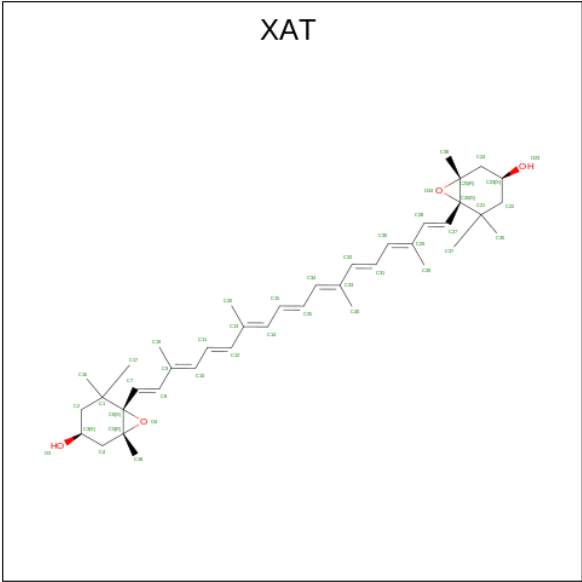
- Molecule 13 is a protein called PsaS.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	g	55	Total	C	N	O	0	0
			275	165	55	55		

- Molecule 14 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	c	80	Total	C	N	O	S	0	0
			596	366	103	117	10		

- Molecule 15 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



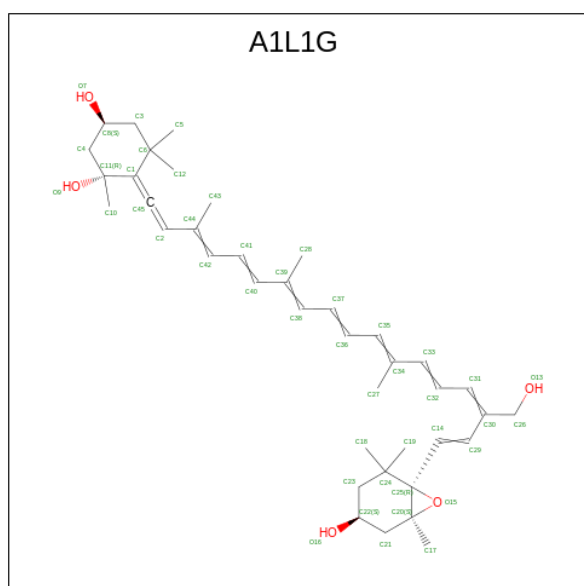
Mol	Chain	Residues	Atoms			AltConf
15	5	1	Total	C	O	0
			44	40	4	
15	5	1	Total	C	O	0
			44	40	4	
15	5	1	Total	C	O	0
			44	40	4	
15	4	1	Total	C	O	0
			44	40	4	
15	4	1	Total	C	O	0
			44	40	4	
15	4	1	Total	C	O	0
			44	40	4	
15	4	1	Total	C	O	0
			44	40	4	
15	4	1	Total	C	O	0
			44	40	4	
15	1	1	Total	C	O	0
			44	40	4	

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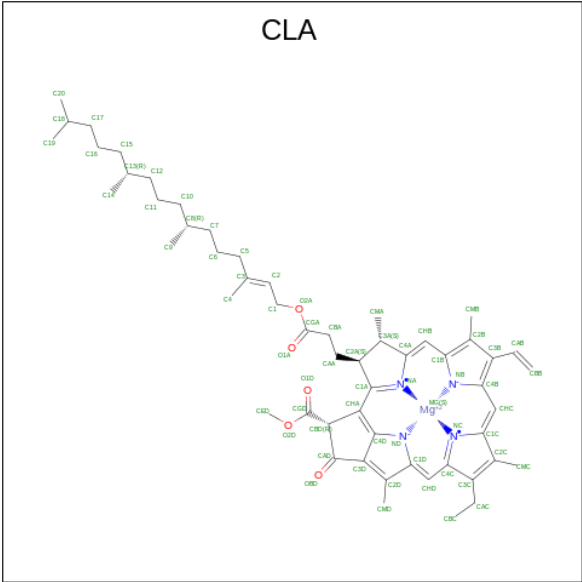
Mol	Chain	Residues	Atoms			AltConf
15	1	1	Total	C	O	0
			44	40	4	
15	a	1	Total	C	O	0
			44	40	4	
15	j	1	Total	C	O	0
			44	40	4	

- Molecule 16 is (1 {R},3 {S})-6-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {Z},17 {E})-16-(hydroxymethyl)-3,7,12-trimethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]-1,5,5-trimethyl-cyclohexane-1,3-diol (CCD ID: A1L1G) (formula: C₄₀H₅₆O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
16	5	1	Total	C	O	0
			45	40	5	
16	1	1	Total	C	O	0
			45	40	5	

- Molecule 17 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
17	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	4	1	Total 53	C 43	Mg 1	N 4	O 5	0
17	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
17	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	1	1	Total 54	C 44	Mg 1	N 4	O 5	0
17	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	1	1	Total 53	C 43	Mg 1	N 4	O 5	0
17	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
17	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	a	1	Total 58	C 48	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	a	1	Total 62	C 52	Mg 1	N 4	O 5	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
17	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	b	1	Total 59	C 49	Mg 1	N 4	O 5	0
17	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	b	1	Total 50	C 40	Mg 1	N 4	O 5	0

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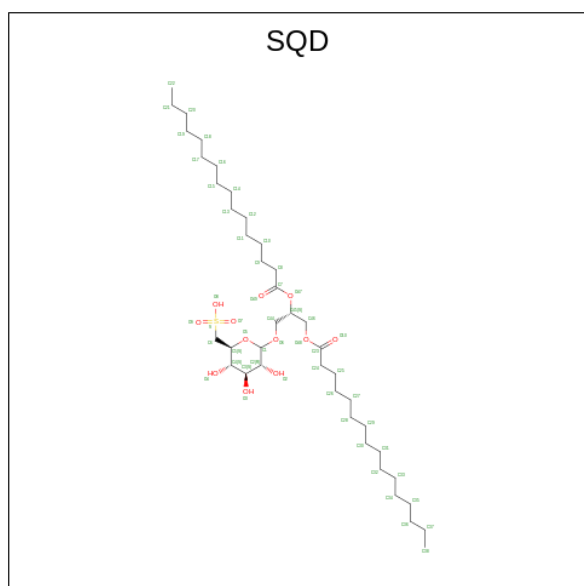
Mol	Chain	Residues	Atoms					AltConf
17	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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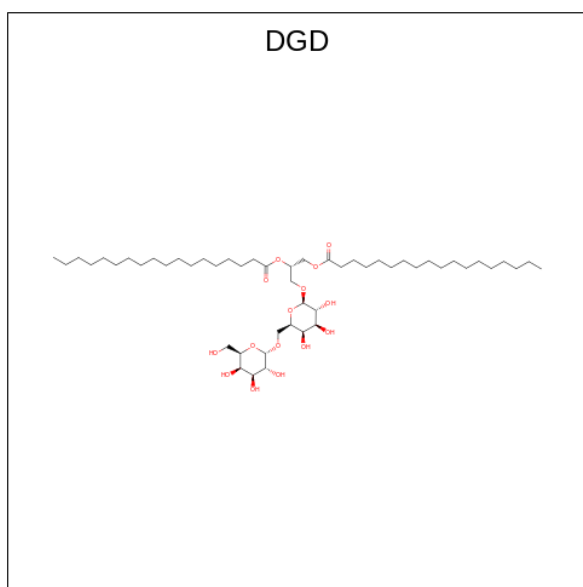
Mol	Chain	Residues	Atoms					AltConf
17	f	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	i	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
17	j	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
17	j	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	l	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	l	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 18 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



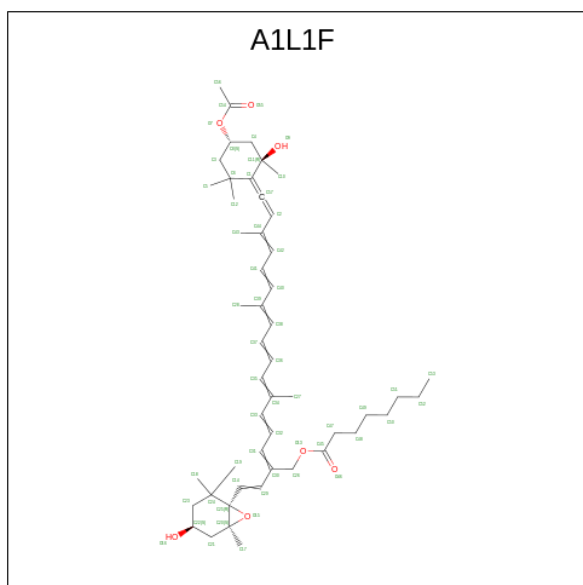
Mol	Chain	Residues	Atoms				AltConf
18	5	1	Total	C	O	S	0
			35	22	12	1	
18	1	1	Total	C	O	S	0
			45	32	12	1	

- Molecule 19 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



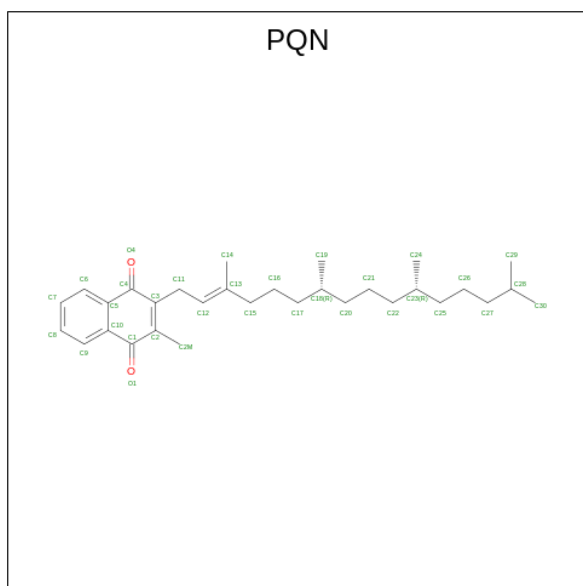
Mol	Chain	Residues	Atoms			AltConf
19	4	1	Total	C	O	0
			40	25	15	
19	b	1	Total	C	O	0
			57	42	15	

- Molecule 20 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-17-[(4 {S},6 {R})-4-acetyloxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]-6,11,15-trimethyl-2-[({E})-2-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]ethenyl]heptadeca-2,4,6,8,10,12,14,16-octaenyl] octanoate (CCD ID: A1L1F) (formula: C₅₀H₇₂O₇) (labeled as "Ligand of Interest" by depositor).



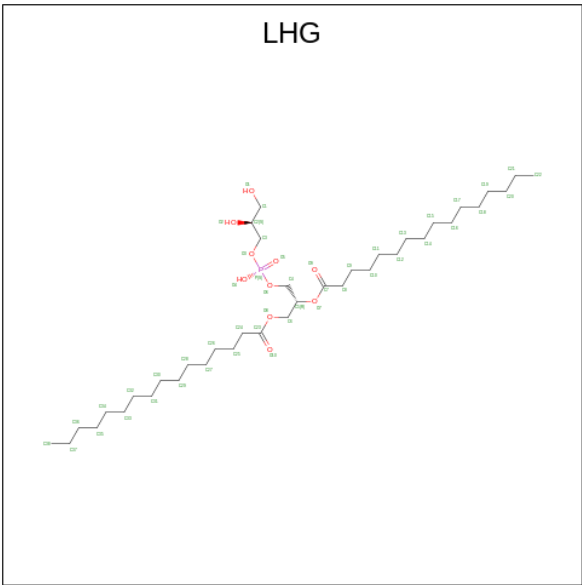
Mol	Chain	Residues	Atoms			AltConf
20	1	1	Total	C	O	0
			57	50	7	

- Molecule 21 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



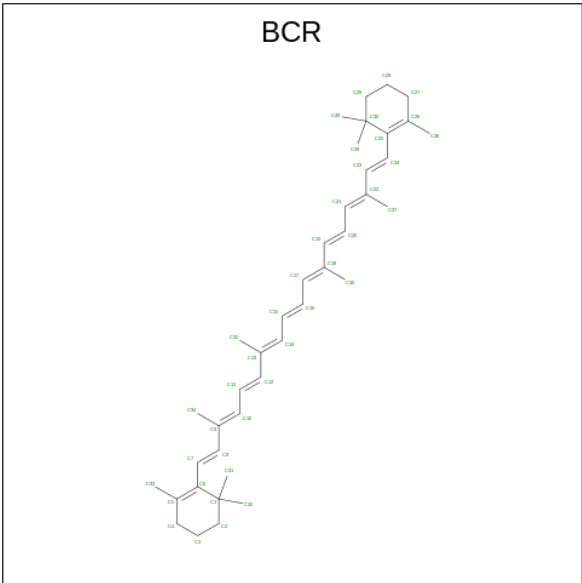
Mol	Chain	Residues	Atoms			AltConf
21	a	1	Total	C	O	0
			33	31	2	
21	b	1	Total	C	O	0
			33	31	2	

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



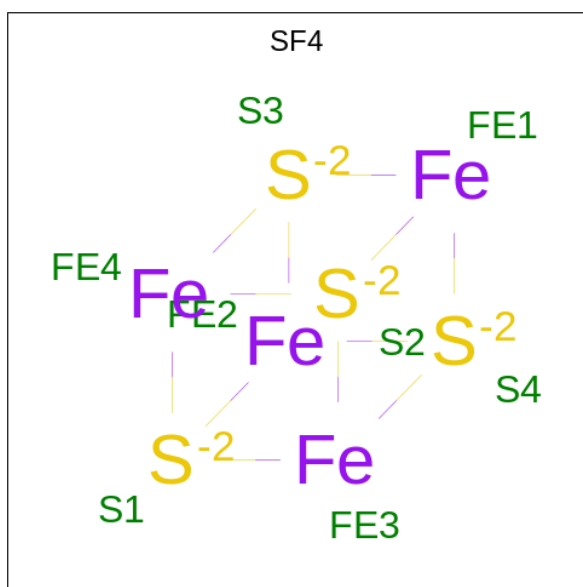
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
22	a	1	48	37	10	1	0
22	a	1	27	16	10	1	0
22	b	1	31	20	10	1	0
22	m	1	46	35	10	1	0

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



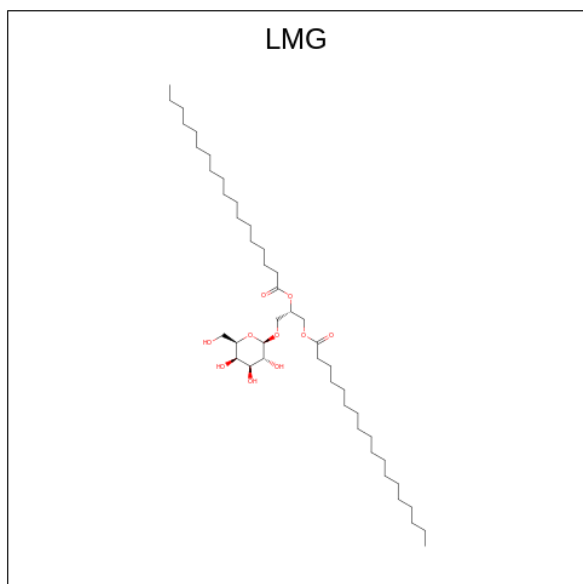
Mol	Chain	Residues	Atoms	AltConf
23	a	1	Total C 40 40	0
23	a	1	Total C 40 40	0
23	a	1	Total C 40 40	0
23	a	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	f	1	Total C 40 40	0
23	f	1	Total C 40 40	0
23	i	1	Total C 40 40	0
23	j	1	Total C 40 40	0
23	l	1	Total C 40 40	0
23	l	1	Total C 40 40	0
23	m	1	Total C 40 40	0

- Molecule 24 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
24	a	1	Total	Fe	S	0
			8	4	4	
24	c	1	Total	Fe	S	0
			8	4	4	
24	c	1	Total	Fe	S	0
			8	4	4	

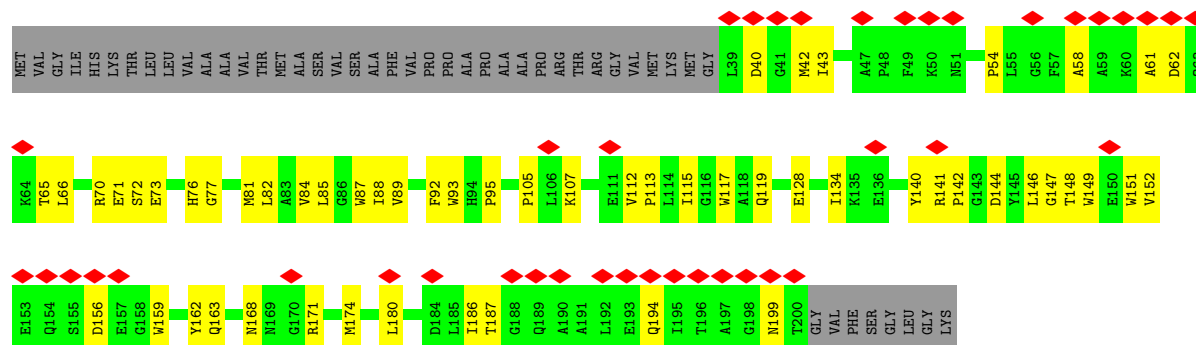
- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



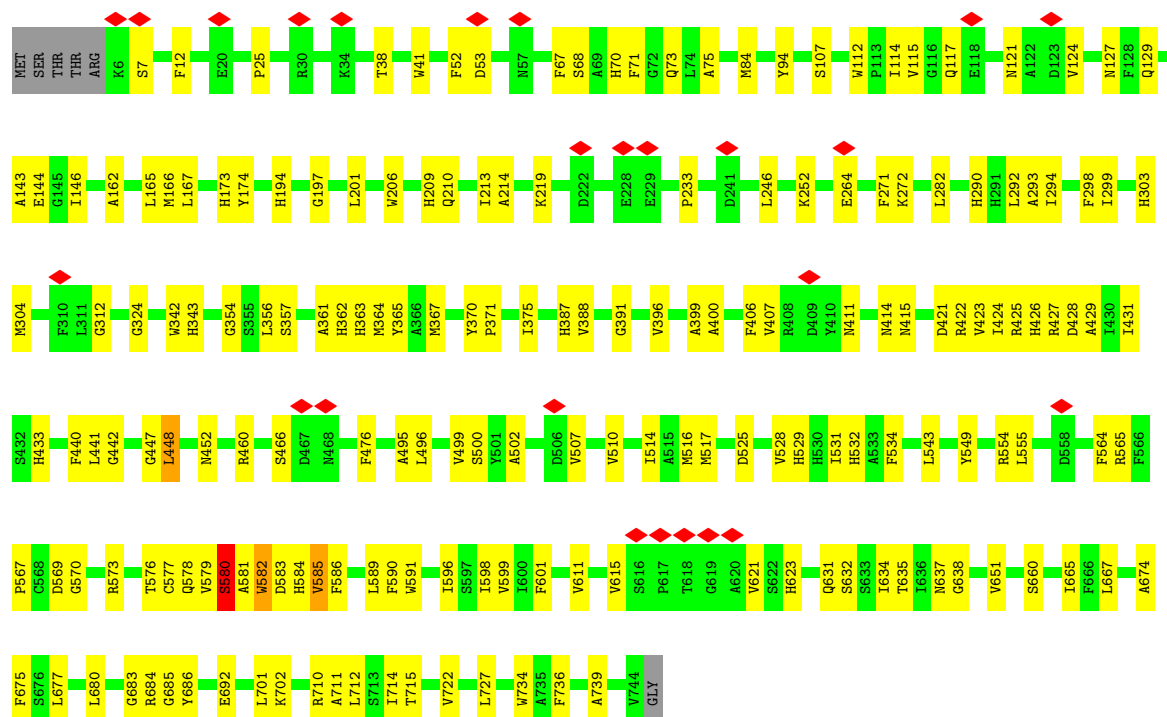
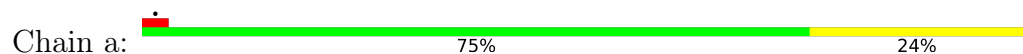
Mol	Chain	Residues	Atoms			AltConf
25	a	1	Total 34	C 24	O 10	0
25	j	1	Total 32	C 22	O 10	0



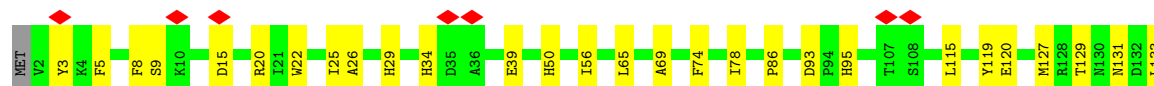
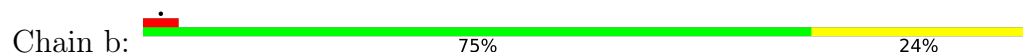
• Molecule 3: VCPI-1

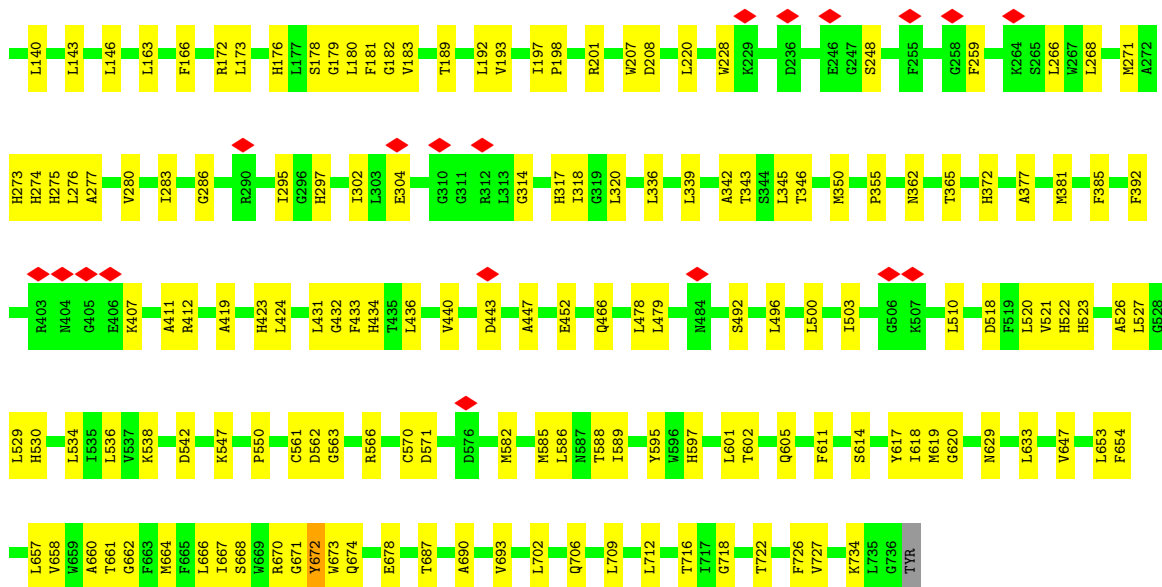


• Molecule 4: Photosystem I P700 chlorophyll a apoprotein A1

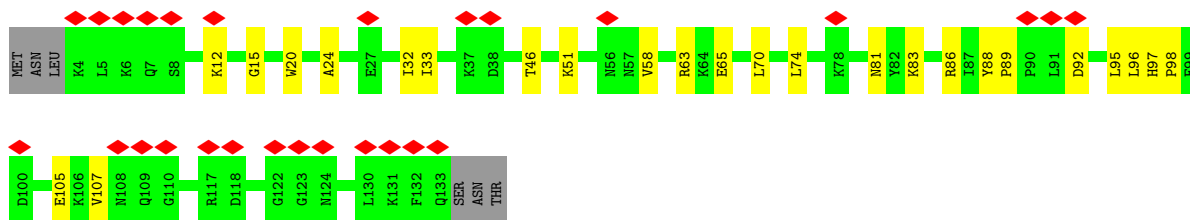
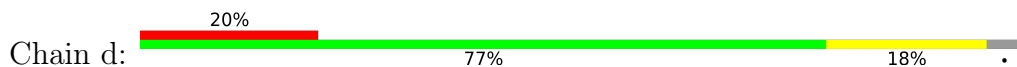


• Molecule 5: Photosystem I P700 chlorophyll a apoprotein A2

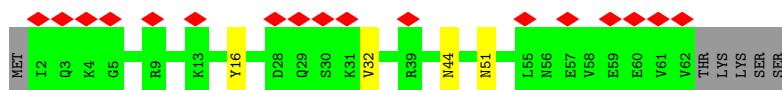
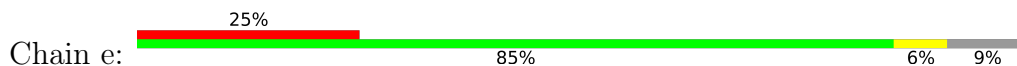




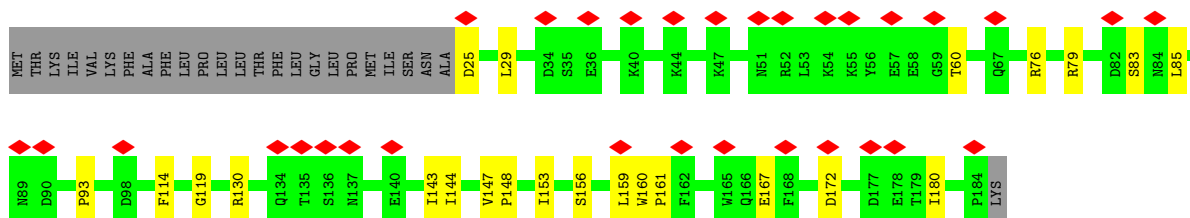
• Molecule 6: Photosystem I reaction center subunit II



• Molecule 7: Photosystem I reaction center subunit IV



• Molecule 8: Photosystem I reaction center subunit III



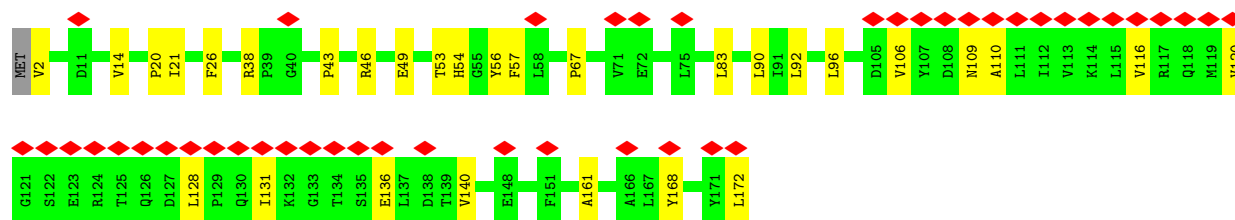
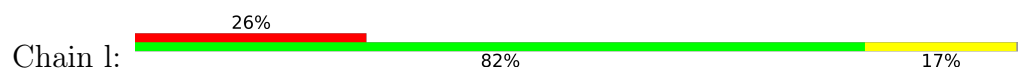
• Molecule 9: Photosystem I reaction center subunit VIII



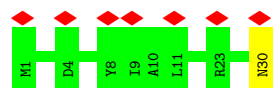
• Molecule 10: Photosystem I reaction center subunit IX



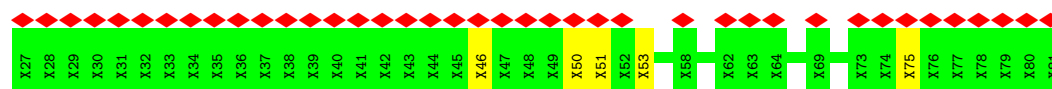
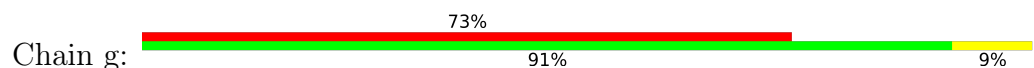
• Molecule 11: PSI subunit V



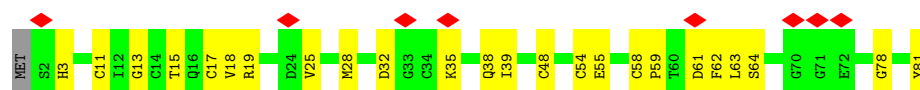
• Molecule 12: PsaM



• Molecule 13: PsaS



• Molecule 14: Photosystem I iron-sulfur center



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35610	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.594	Depositor
Minimum map value	-0.417	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.345	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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: LMG, SF4, LHG, PQN, BCR, XAT, A1L1F, DGD, CLA, A1L1G, SQD

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	5	0.14	0/1353	0.29	0/1823
2	4	0.17	0/1298	0.32	0/1761
3	1	0.14	0/1293	0.33	0/1759
4	a	0.28	3/6024 (0.0%)	0.33	4/8219 (0.0%)
5	b	0.20	0/6080	0.32	1/8302 (0.0%)
6	d	0.12	0/1040	0.32	0/1402
7	e	0.09	0/502	0.20	0/681
8	f	0.14	0/1297	0.31	0/1762
9	i	0.14	0/278	0.33	0/378
10	j	0.16	0/351	0.36	0/478
11	l	0.14	0/1315	0.31	0/1796
12	m	0.09	0/210	0.28	0/288
14	c	0.13	0/606	0.34	0/822
All	All	0.21	3/21647 (0.0%)	0.32	5/29471 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	a	580	SER	CA-C	-7.08	1.43	1.52
4	a	581	ALA	CA-C	-5.48	1.45	1.52
4	a	582	TRP	CA-C	-5.05	1.45	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	a	581	ALA	N-CA-C	-8.63	102.50	113.72
4	a	448	LEU	N-CA-C	-6.10	104.19	111.69
4	a	584	HIS	N-CA-C	-5.83	106.51	113.97
5	b	672	TYR	N-CA-C	-5.56	106.33	113.23
4	a	585	VAL	N-CA-C	-5.07	105.45	112.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5	1317	0	1318	37	0
2	4	1268	0	1288	23	0
3	1	1262	0	1237	41	0
4	a	5827	0	5697	141	0
5	b	5865	0	5710	145	0
6	d	1014	0	1015	19	0
7	e	494	0	495	4	0
8	f	1266	0	1262	20	0
9	i	271	0	292	11	0
10	j	339	0	342	21	0
11	l	1283	0	1278	21	0
12	m	210	0	226	1	0
13	g	275	0	62	3	0
14	c	596	0	583	20	0
15	1	88	0	112	7	0
15	4	264	0	336	27	0
15	5	132	0	168	20	0
15	a	44	0	56	5	0
15	j	44	0	56	5	0
16	1	45	0	0	1	0
16	5	45	0	0	1	0
17	1	547	0	508	15	0
17	4	613	0	522	33	0
17	5	563	0	472	23	0
17	a	2579	0	2562	144	0
17	b	2475	0	2536	126	0
17	f	117	0	115	1	0
17	i	62	0	63	4	0
17	j	100	0	86	7	0
17	l	148	0	123	3	0
18	1	45	0	54	3	0
18	5	35	0	34	1	0
19	4	40	0	38	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	b	57	0	72	6	0
20	l	57	0	0	2	0
21	a	33	0	46	3	0
21	b	33	0	46	2	0
22	a	75	0	93	6	0
22	b	31	0	32	0	0
22	m	46	0	65	1	0
23	a	160	0	224	12	0
23	b	320	0	448	29	0
23	f	80	0	112	14	0
23	i	40	0	56	2	0
23	j	40	0	56	8	0
23	l	80	0	112	16	0
23	m	40	0	56	3	0
24	a	8	0	0	0	0
24	c	16	0	0	3	0
25	a	34	0	38	11	0
25	j	32	0	34	7	0
All	All	30455	0	30136	767	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 13.

The worst 5 of 767 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)
2:4:193:ALA:HB1	19:4:319:DGD:HE62	1.13	1.12
2:4:193:ALA:HB1	19:4:319:DGD:C6E	1.85	1.07
19:4:319:DGD:O5E	19:4:319:DGD:O4E	1.61	0.95
15:5:302:XAT:H12	17:5:307:CLA:HAB	1.53	0.90
17:a:806:CLA:O1A	17:a:814:CLA:HBA1	1.81	0.81

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	5	167/244 (68%)	158 (95%)	9 (5%)	0	100	100
2	4	166/202 (82%)	149 (90%)	16 (10%)	1 (1%)	21	48
3	1	160/208 (77%)	149 (93%)	11 (7%)	0	100	100
4	a	737/745 (99%)	713 (97%)	23 (3%)	1 (0%)	48	75
5	b	733/737 (100%)	702 (96%)	31 (4%)	0	100	100
6	d	128/136 (94%)	113 (88%)	15 (12%)	0	100	100
7	e	59/67 (88%)	54 (92%)	5 (8%)	0	100	100
8	f	158/185 (85%)	151 (96%)	7 (4%)	0	100	100
9	i	32/45 (71%)	30 (94%)	2 (6%)	0	100	100
10	j	39/41 (95%)	39 (100%)	0	0	100	100
11	l	169/172 (98%)	154 (91%)	13 (8%)	2 (1%)	10	32
12	m	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
All	All	2654/2893 (92%)	2513 (95%)	137 (5%)	4 (0%)	44	70

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	l	120	VAL
4	a	580	SER
11	l	131	ILE
2	4	146	SER

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	5	133/182 (73%)	133 (100%)	0	100	100
2	4	133/159 (84%)	133 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1	128/165 (78%)	128 (100%)	0	100	100
4	a	607/613 (99%)	603 (99%)	4 (1%)	76	80
5	b	599/602 (100%)	599 (100%)	0	100	100
6	d	107/113 (95%)	107 (100%)	0	100	100
7	e	56/62 (90%)	56 (100%)	0	100	100
8	f	138/162 (85%)	138 (100%)	0	100	100
9	i	32/43 (74%)	32 (100%)	0	100	100
10	j	36/36 (100%)	36 (100%)	0	100	100
11	l	130/141 (92%)	130 (100%)	0	100	100
12	m	21/24 (88%)	21 (100%)	0	100	100
14	c	67/68 (98%)	67 (100%)	0	100	100
All	All	2187/2370 (92%)	2183 (100%)	4 (0%)	85	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	a	428	ASP
4	a	448	LEU
4	a	579	VAL
4	a	580	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
5	b	629	ASN
8	f	166	GLN
4	a	435	ASN
5	b	80	ASN
5	b	112	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](#)

176 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	$\# Z > 2$
17	CLA	a	809	4	69,73,73	1.23	7 (10%)	83,113,113	1.31	8 (9%)
17	CLA	b	809	5	69,73,73	1.24	10 (14%)	83,113,113	1.34	6 (7%)
17	CLA	5	313	1	49,53,73	1.51	6 (12%)	59,89,113	1.44	5 (8%)
17	CLA	1	309	3	50,54,73	1.47	8 (16%)	60,90,113	1.36	5 (8%)
22	LHG	m	101	-	45,45,48	1.15	6 (13%)	48,51,54	0.95	2 (4%)
17	CLA	a	811	4	60,64,73	1.35	7 (11%)	72,102,113	1.36	6 (8%)
17	CLA	a	818	4	60,64,73	1.36	8 (13%)	72,102,113	1.33	7 (9%)
24	SF4	a	851	-	0,12,12	-	-	-	-	-
15	XAT	4	301	-	39,47,47	0.94	2 (5%)	54,74,74	2.63	19 (35%)
17	CLA	b	836	5	62,66,73	1.33	7 (11%)	74,104,113	1.39	8 (10%)
17	CLA	a	819	4	58,62,73	1.37	7 (12%)	69,99,113	1.34	5 (7%)
17	CLA	i	102	-	66,70,73	1.29	8 (12%)	79,109,113	1.29	7 (8%)
17	CLA	a	844	22	69,73,73	1.25	7 (10%)	83,113,113	1.27	8 (9%)
17	CLA	b	840	5	69,73,73	1.26	7 (10%)	83,113,113	1.33	6 (7%)
18	SQD	5	316	17	34,35,54	1.47	4 (11%)	43,46,65	1.34	7 (16%)
17	CLA	5	311	-	55,59,73	1.40	7 (12%)	66,96,113	1.38	8 (12%)
17	CLA	b	819	5	64,68,73	1.31	8 (12%)	77,107,113	1.31	5 (6%)
15	XAT	a	852	-	39,47,47	0.95	2 (5%)	54,74,74	2.69	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	b	831	5	45,49,73	1.51	9 (20%)	54,84,113	1.50	7 (12%)
17	CLA	b	804	-	69,73,73	1.22	7 (10%)	83,113,113	1.47	11 (13%)
23	BCR	a	847	-	41,41,41	0.69	0	56,56,56	1.94	16 (28%)
17	CLA	1	313	3	45,49,73	1.51	7 (15%)	54,84,113	1.50	5 (9%)
17	CLA	l	203	-	64,68,73	1.30	9 (14%)	77,107,113	1.36	6 (7%)
17	CLA	a	806	4	69,73,73	1.32	11 (15%)	83,113,113	1.58	13 (15%)
17	CLA	a	804	4	59,63,73	1.36	8 (13%)	71,101,113	1.41	9 (12%)
15	XAT	5	301	-	39,47,47	0.94	1 (2%)	54,74,74	2.57	19 (35%)
17	CLA	b	816	5	49,53,73	1.49	8 (16%)	59,89,113	1.45	6 (10%)
17	CLA	b	837	-	69,73,73	1.25	7 (10%)	83,113,113	1.31	6 (7%)
17	CLA	a	813	4	58,62,73	1.38	6 (10%)	69,99,113	1.34	6 (8%)
17	CLA	a	840	4	69,73,73	1.27	8 (11%)	83,113,113	1.28	7 (8%)
17	CLA	b	833	5	69,73,73	1.25	7 (10%)	83,113,113	1.28	6 (7%)
24	SF4	c	102	-	0,12,12	-	-	-	-	-
17	CLA	a	808	-	55,59,73	1.42	8 (14%)	66,96,113	1.39	7 (10%)
17	CLA	b	826	-	68,72,73	1.26	8 (11%)	81,111,113	1.32	8 (9%)
20	A1L1F	1	304	-	50,59,59	1.30	5 (10%)	62,85,85	2.30	17 (27%)
17	CLA	4	313	-	50,54,73	1.47	7 (14%)	60,90,113	1.41	6 (10%)
17	CLA	4	314	-	57,61,73	1.39	8 (14%)	68,98,113	1.34	8 (11%)
17	CLA	a	803	-	69,73,73	1.25	9 (13%)	83,113,113	1.24	7 (8%)
18	SQD	1	315	-	44,45,54	1.29	4 (9%)	53,56,65	1.16	5 (9%)
23	BCR	i	101	-	41,41,41	0.75	0	56,56,56	2.13	14 (25%)
17	CLA	b	829	-	69,73,73	1.27	9 (13%)	83,113,113	1.22	5 (6%)
23	BCR	b	850	-	41,41,41	0.73	0	56,56,56	1.88	17 (30%)
17	CLA	5	306	18	49,53,73	1.49	6 (12%)	59,89,113	1.43	5 (8%)
15	XAT	4	305	-	39,47,47	0.89	1 (2%)	54,74,74	2.56	16 (29%)
17	CLA	4	317	-	50,54,73	1.46	6 (12%)	60,90,113	1.45	6 (10%)
17	CLA	b	830	5	69,73,73	1.28	8 (11%)	83,113,113	1.32	9 (10%)
17	CLA	a	801	4	69,73,73	1.26	10 (14%)	83,113,113	1.30	5 (6%)
17	CLA	4	315	2	49,53,73	1.50	7 (14%)	59,89,113	1.44	6 (10%)
23	BCR	b	844	-	41,41,41	0.71	0	56,56,56	1.91	16 (28%)
17	CLA	a	820	4	69,73,73	1.26	8 (11%)	83,113,113	1.32	9 (10%)
15	XAT	5	302	-	39,47,47	0.93	1 (2%)	54,74,74	2.58	20 (37%)
17	CLA	5	314	1	56,60,73	1.39	7 (12%)	67,97,113	1.41	7 (10%)
17	CLA	a	836	4	54,58,73	1.41	7 (12%)	65,95,113	1.40	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	a	824	4	50,54,73	1.47	9 (18%)	60,90,113	1.38	5 (8%)
23	BCR	a	848	-	41,41,41	0.74	0	56,56,56	1.94	18 (32%)
17	CLA	1	306	-	69,73,73	1.25	7 (10%)	83,113,113	1.32	7 (8%)
16	A1L1G	5	303	-	38,47,47	1.41	6 (15%)	49,71,71	1.46	7 (14%)
15	XAT	5	304	-	39,47,47	0.90	0	54,74,74	2.86	22 (40%)
17	CLA	1	314	3	49,53,73	1.49	7 (14%)	59,89,113	1.42	4 (6%)
17	CLA	a	831	4	69,73,73	1.26	8 (11%)	83,113,113	1.36	7 (8%)
17	CLA	a	829	4	66,70,73	1.29	7 (10%)	79,109,113	1.26	8 (10%)
17	CLA	a	835	-	69,73,73	1.24	8 (11%)	83,113,113	1.33	7 (8%)
17	CLA	5	308	-	59,63,73	1.37	8 (13%)	71,101,113	1.37	6 (8%)
17	CLA	4	316	2	45,49,73	1.53	6 (13%)	54,84,113	1.50	7 (12%)
17	CLA	a	807	-	69,73,73	1.25	8 (11%)	83,113,113	1.29	6 (7%)
17	CLA	b	817	-	59,63,73	1.36	7 (11%)	71,101,113	1.34	8 (11%)
23	BCR	f	801	-	41,41,41	0.69	0	56,56,56	2.14	16 (28%)
23	BCR	m	102	-	41,41,41	1.18	2 (4%)	56,56,56	1.24	6 (10%)
17	CLA	b	805	5	69,73,73	1.25	6 (8%)	83,113,113	1.30	6 (7%)
17	CLA	1	308	3	69,73,73	1.25	7 (10%)	83,113,113	1.30	6 (7%)
17	CLA	5	305	1	50,54,73	1.47	8 (16%)	60,90,113	1.40	5 (8%)
17	CLA	a	816	4	54,58,73	1.42	8 (14%)	65,95,113	1.43	8 (12%)
17	CLA	a	825	4	59,63,73	1.36	7 (11%)	71,101,113	1.35	7 (9%)
17	CLA	b	825	-	69,73,73	1.26	7 (10%)	83,113,113	1.31	5 (6%)
17	CLA	4	318	-	59,63,73	1.37	8 (13%)	71,101,113	1.36	6 (8%)
17	CLA	l	204	-	50,54,73	1.46	8 (16%)	60,90,113	1.41	4 (6%)
17	CLA	b	834	-	69,73,73	1.26	7 (10%)	83,113,113	1.26	5 (6%)
17	CLA	b	806	5	69,73,73	1.25	7 (10%)	83,113,113	1.31	6 (7%)
17	CLA	b	812	5	58,62,73	1.42	9 (15%)	73,100,113	1.39	7 (9%)
25	LMG	a	853	-	34,34,55	1.13	2 (5%)	42,42,63	1.16	3 (7%)
17	CLA	b	801	-	69,73,73	1.27	9 (13%)	83,113,113	1.28	6 (7%)
17	CLA	a	830	4	69,73,73	1.27	9 (13%)	83,113,113	1.27	6 (7%)
17	CLA	a	834	-	69,73,73	1.26	7 (10%)	83,113,113	1.27	7 (8%)
17	CLA	b	808	5	69,73,73	1.24	8 (11%)	83,113,113	1.25	7 (8%)
17	CLA	a	842	4	69,73,73	1.27	8 (11%)	83,113,113	1.29	5 (6%)
15	XAT	4	304	-	39,47,47	0.88	0	54,74,74	2.58	18 (33%)
17	CLA	a	833	4	59,63,73	1.34	7 (11%)	71,101,113	1.40	7 (9%)
17	CLA	f	802	-	69,73,73	1.26	7 (10%)	83,113,113	1.29	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	j	102	5	62,66,73	1.34	7 (11%)	74,104,113	1.32	7 (9%)
17	CLA	b	803	5	69,73,73	1.24	8 (11%)	83,113,113	1.25	5 (6%)
23	BCR	b	843	-	41,41,41	0.71	0	56,56,56	2.28	19 (33%)
17	CLA	f	803	8	56,60,73	1.39	7 (12%)	67,97,113	1.39	7 (10%)
23	BCR	b	852	-	41,41,41	0.73	0	56,56,56	2.05	15 (26%)
17	CLA	b	807	5	69,73,73	1.26	7 (10%)	83,113,113	1.29	6 (7%)
17	CLA	b	827	-	69,73,73	1.27	7 (10%)	83,113,113	1.25	3 (3%)
17	CLA	a	814	4	69,73,73	1.26	8 (11%)	83,113,113	1.30	7 (8%)
17	CLA	b	815	-	59,63,73	1.36	7 (11%)	71,101,113	1.42	8 (11%)
17	CLA	a	841	4	69,73,73	1.24	6 (8%)	83,113,113	1.31	8 (9%)
25	LMG	j	105	-	32,32,55	1.12	2 (6%)	40,40,63	1.14	3 (7%)
15	XAT	4	303	-	39,47,47	0.91	0	54,74,74	2.57	20 (37%)
17	CLA	b	835	-	57,61,73	1.40	9 (15%)	68,98,113	1.39	7 (10%)
17	CLA	b	820	-	59,63,73	1.36	9 (15%)	71,101,113	1.34	7 (9%)
17	CLA	b	814	-	69,73,73	1.26	7 (10%)	83,113,113	1.28	7 (8%)
17	CLA	4	311	-	69,73,73	1.25	7 (10%)	83,113,113	1.34	6 (7%)
17	CLA	1	312	3	56,60,73	1.42	7 (12%)	67,97,113	1.36	7 (10%)
23	BCR	a	849	-	41,41,41	0.73	0	56,56,56	2.17	20 (35%)
17	CLA	5	310	-	50,54,73	1.47	7 (14%)	60,90,113	1.42	6 (10%)
23	BCR	b	848	-	41,41,41	0.75	0	56,56,56	1.78	15 (26%)
15	XAT	4	302	-	39,47,47	0.90	2 (5%)	54,74,74	2.55	18 (33%)
23	BCR	l	205	-	41,41,41	0.70	0	56,56,56	2.03	13 (23%)
23	BCR	j	104	-	41,41,41	0.73	0	56,56,56	2.08	18 (32%)
17	CLA	b	818	5	63,67,73	1.32	9 (14%)	75,105,113	1.39	10 (13%)
17	CLA	a	854	-	69,73,73	1.26	7 (10%)	83,113,113	1.27	7 (8%)
22	LHG	a	845	-	47,47,48	1.11	6 (12%)	50,53,54	0.97	2 (4%)
22	LHG	a	846	17	26,26,48	1.27	5 (19%)	29,32,54	1.21	2 (6%)
17	CLA	a	837	4	49,53,73	1.49	9 (18%)	59,89,113	1.44	6 (10%)
17	CLA	1	310	3	69,73,73	1.26	7 (10%)	83,113,113	1.25	7 (8%)
23	BCR	b	847	-	41,41,41	0.76	0	56,56,56	2.19	21 (37%)
17	CLA	a	839	4	69,73,73	1.25	7 (10%)	83,113,113	1.31	8 (9%)
23	BCR	b	846	-	41,41,41	0.70	0	56,56,56	1.97	21 (37%)
22	LHG	b	849	17	30,30,48	1.33	6 (20%)	33,36,54	1.15	2 (6%)
17	CLA	b	821	5	54,58,73	1.42	8 (14%)	65,95,113	1.46	8 (12%)
17	CLA	1	307	3	58,62,73	1.37	7 (12%)	69,99,113	1.38	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	XAT	1	303	-	39,47,47	0.90	0	54,74,74	2.52	19 (35%)
17	CLA	a	838	4	55,59,73	1.40	8 (14%)	66,96,113	1.41	6 (9%)
17	CLA	b	811	5	69,73,73	1.25	7 (10%)	83,113,113	1.31	8 (9%)
17	CLA	4	308	-	60,64,73	1.35	7 (11%)	72,102,113	1.34	6 (8%)
17	CLA	b	810	-	69,73,73	1.25	8 (11%)	83,113,113	1.30	5 (6%)
17	CLA	5	312	-	56,60,73	1.41	7 (12%)	67,97,113	1.41	7 (10%)
17	CLA	1	311	-	57,61,73	1.39	7 (12%)	68,98,113	1.38	7 (10%)
17	CLA	a	815	-	49,53,73	1.48	7 (14%)	59,89,113	1.44	6 (10%)
17	CLA	b	824	-	57,61,73	1.38	8 (14%)	68,98,113	1.37	7 (10%)
15	XAT	j	101	-	39,47,47	0.88	0	54,74,74	2.72	18 (33%)
17	CLA	5	315	1	50,54,73	1.46	7 (14%)	60,90,113	1.41	6 (10%)
17	CLA	a	832	4	54,58,73	1.42	9 (16%)	65,95,113	1.42	7 (10%)
23	BCR	a	850	-	41,41,41	0.73	0	56,56,56	2.17	15 (26%)
17	CLA	b	832	5	53,57,73	1.43	7 (13%)	62,93,113	1.40	7 (11%)
17	CLA	a	823	-	53,57,73	1.42	8 (15%)	62,93,113	1.44	6 (9%)
17	CLA	b	822	5	55,59,73	1.39	7 (12%)	66,96,113	1.41	8 (12%)
17	CLA	b	828	5	69,73,73	1.25	8 (11%)	83,113,113	1.26	5 (6%)
23	BCR	f	804	-	41,41,41	0.72	0	56,56,56	2.04	16 (28%)
17	CLA	4	309	-	69,73,73	1.25	8 (11%)	83,113,113	1.24	7 (8%)
21	PQN	a	843	-	34,34,34	1.58	2 (5%)	42,45,45	1.09	3 (7%)
15	XAT	1	302	-	39,47,47	0.91	1 (2%)	54,74,74	2.59	17 (31%)
17	CLA	4	310	2	54,58,73	1.41	7 (12%)	65,95,113	1.41	7 (10%)
17	CLA	a	805	17,4	59,63,73	1.35	6 (10%)	71,101,113	1.38	7 (9%)
17	CLA	a	826	-	69,73,73	1.26	8 (11%)	83,113,113	1.32	6 (7%)
17	CLA	a	828	4	69,73,73	1.26	8 (11%)	83,113,113	1.29	5 (6%)
17	CLA	5	309	1	69,73,73	1.26	7 (10%)	83,113,113	1.27	6 (7%)
17	CLA	a	812	17,4	66,70,73	1.27	8 (12%)	79,109,113	1.33	6 (7%)
16	A1L1G	1	301	-	38,47,47	1.45	6 (15%)	49,71,71	1.58	11 (22%)
17	CLA	4	307	2	49,53,73	1.48	6 (12%)	59,89,113	1.43	5 (8%)
23	BCR	b	845	-	41,41,41	0.69	0	56,56,56	2.10	16 (28%)
24	SF4	c	101	-	0,12,12	-	-	-	-	-
21	PQN	b	842	-	34,34,34	1.56	2 (5%)	42,45,45	1.20	4 (9%)
17	CLA	1	305	-	65,69,73	1.30	7 (10%)	78,108,113	1.30	5 (6%)
17	CLA	j	103	10	46,50,73	1.51	7 (15%)	55,85,113	1.50	4 (7%)
17	CLA	b	838	5	69,73,73	1.26	8 (11%)	83,113,113	1.24	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	a	822	-	69,73,73	1.26	8 (11%)	83,113,113	1.28	7 (8%)
17	CLA	b	813	5	57,61,73	1.39	7 (12%)	68,98,113	1.37	6 (8%)
17	CLA	b	823	5	64,68,73	1.30	8 (12%)	77,107,113	1.28	6 (7%)
17	CLA	5	307	1	64,68,73	1.31	7 (10%)	77,107,113	1.29	7 (9%)
17	CLA	a	802	-	62,66,73	1.31	9 (14%)	74,104,113	1.35	8 (10%)
19	DGD	b	851	-	58,58,67	1.15	7 (12%)	72,72,81	1.53	10 (13%)
17	CLA	4	312	-	50,54,73	1.48	9 (18%)	60,90,113	1.44	5 (8%)
17	CLA	l	202	-	46,50,73	1.52	9 (19%)	55,85,113	1.47	5 (9%)
17	CLA	b	839	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	7 (8%)
17	CLA	a	810	4	69,73,73	1.26	9 (13%)	83,113,113	1.33	6 (7%)
15	XAT	4	306	-	39,47,47	0.91	1 (2%)	54,74,74	2.75	19 (35%)
17	CLA	b	802	-	69,73,73	1.25	7 (10%)	83,113,113	1.20	4 (4%)
17	CLA	a	827	-	69,73,73	1.26	8 (11%)	83,113,113	1.34	7 (8%)
23	BCR	l	201	-	41,41,41	0.71	0	56,56,56	1.96	17 (30%)
17	CLA	b	841	22	69,73,73	1.27	7 (10%)	83,113,113	1.28	7 (8%)
17	CLA	a	821	4	49,53,73	1.48	8 (16%)	59,89,113	1.49	4 (6%)
19	DGD	4	319	-	41,41,67	1.07	2 (4%)	55,55,81	1.82	6 (10%)
17	CLA	a	817	-	49,53,73	1.49	8 (16%)	59,89,113	1.45	5 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	a	809	4	-	15/39/115/115	-
17	CLA	b	809	5	-	13/39/115/115	-
17	CLA	5	313	1	-	4/15/91/115	-
17	CLA	l	309	3	-	8/17/93/115	-
22	LHG	m	101	-	-	28/50/50/53	-
17	CLA	a	811	4	-	8/29/105/115	-
17	CLA	a	818	4	-	11/29/105/115	-
24	SF4	a	851	-	-	-	0/6/5/5
15	XAT	4	301	-	-	4/31/93/93	0/4/4/4
17	CLA	b	836	5	-	11/31/107/115	-
17	CLA	a	819	4	-	6/26/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	i	102	-	-	11/36/112/115	-
17	CLA	a	844	22	-	16/39/115/115	-
17	CLA	b	840	5	-	17/39/115/115	-
18	SQD	5	316	17	-	11/30/50/69	0/1/1/1
17	CLA	5	311	-	-	8/23/99/115	-
17	CLA	b	819	5	-	16/33/109/115	-
15	XAT	a	852	-	-	7/31/93/93	0/4/4/4
17	CLA	b	831	5	-	3/10/86/115	-
17	CLA	b	804	-	-	10/39/115/115	-
23	BCR	a	847	-	-	0/29/63/63	0/2/2/2
17	CLA	1	313	3	-	5/10/86/115	-
17	CLA	l	203	-	-	6/33/109/115	-
17	CLA	a	806	4	-	12/39/115/115	-
17	CLA	a	804	4	-	10/27/103/115	-
15	XAT	5	301	-	-	3/31/93/93	0/4/4/4
17	CLA	b	816	5	-	3/15/91/115	-
17	CLA	b	837	-	-	8/39/115/115	-
17	CLA	a	813	4	-	11/26/102/115	-
17	CLA	a	840	4	-	9/39/115/115	-
17	CLA	b	833	5	-	13/39/115/115	-
24	SF4	c	102	-	-	-	0/6/5/5
17	CLA	a	808	-	-	5/23/99/115	-
17	CLA	b	826	-	-	6/38/114/115	-
20	A1L1F	1	304	-	-	12/43/99/99	0/3/3/3
17	CLA	4	313	-	-	6/17/93/115	-
17	CLA	4	314	-	-	6/25/101/115	-
17	CLA	a	803	-	-	3/39/115/115	-
18	SQD	1	315	-	-	19/40/60/69	0/1/1/1
23	BCR	i	101	-	-	3/29/63/63	0/2/2/2
17	CLA	b	829	-	-	13/39/115/115	-
23	BCR	b	850	-	-	2/29/63/63	0/2/2/2
17	CLA	5	306	18	-	9/15/91/115	-
15	XAT	4	305	-	-	0/31/93/93	0/4/4/4
17	CLA	4	317	-	-	8/17/93/115	-
17	CLA	b	830	5	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	a	801	4	-	24/39/115/115	-
17	CLA	4	315	2	-	5/15/91/115	-
23	BCR	b	844	-	-	2/29/63/63	0/2/2/2
17	CLA	a	820	4	-	15/39/115/115	-
15	XAT	5	302	-	-	3/31/93/93	0/4/4/4
17	CLA	5	314	1	-	4/24/100/115	-
17	CLA	a	836	4	-	8/21/97/115	-
17	CLA	a	824	4	-	6/17/93/115	-
23	BCR	a	848	-	-	0/29/63/63	0/2/2/2
17	CLA	1	306	-	-	15/39/115/115	-
16	A1L1G	5	303	-	-	9/29/85/85	0/3/3/3
15	XAT	5	304	-	-	1/31/93/93	0/4/4/4
17	CLA	1	314	3	-	7/15/91/115	-
17	CLA	a	831	4	-	11/39/115/115	-
17	CLA	a	829	4	-	15/36/112/115	-
17	CLA	a	835	-	-	12/39/115/115	-
17	CLA	5	308	-	-	6/27/103/115	-
17	CLA	4	316	2	-	7/10/86/115	-
17	CLA	a	807	-	-	20/39/115/115	-
17	CLA	b	817	-	-	4/27/103/115	-
23	BCR	f	801	-	-	3/29/63/63	0/2/2/2
23	BCR	m	102	-	-	9/29/63/63	0/2/2/2
17	CLA	b	805	5	-	12/39/115/115	-
17	CLA	1	308	3	-	13/39/115/115	-
17	CLA	5	305	1	-	6/17/93/115	-
17	CLA	a	816	4	-	5/21/97/115	-
17	CLA	a	825	4	-	10/27/103/115	-
17	CLA	b	825	-	-	14/39/115/115	-
17	CLA	4	318	-	-	9/27/103/115	-
17	CLA	l	204	-	-	4/17/93/115	-
17	CLA	b	834	-	-	14/39/115/115	-
17	CLA	b	806	5	-	16/39/115/115	-
17	CLA	b	812	5	-	5/25/101/115	-
25	LMG	a	853	-	-	13/29/49/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	b	801	-	-	22/39/115/115	-
17	CLA	a	830	4	-	15/39/115/115	-
17	CLA	a	834	-	-	9/39/115/115	-
17	CLA	b	808	5	-	12/39/115/115	-
17	CLA	a	842	4	-	9/39/115/115	-
15	XAT	4	304	-	-	3/31/93/93	0/4/4/4
17	CLA	a	833	4	-	2/27/103/115	-
17	CLA	f	802	-	-	13/39/115/115	-
17	CLA	j	102	5	-	18/31/107/115	-
17	CLA	b	803	5	-	19/39/115/115	-
23	BCR	b	843	-	-	2/29/63/63	0/2/2/2
17	CLA	f	803	8	-	4/24/100/115	-
23	BCR	b	852	-	-	5/29/63/63	0/2/2/2
17	CLA	b	807	5	-	19/39/115/115	-
17	CLA	b	827	-	-	5/39/115/115	-
17	CLA	a	814	4	-	20/39/115/115	-
17	CLA	b	815	-	-	13/27/103/115	-
17	CLA	a	841	4	-	17/39/115/115	-
25	LMG	j	105	-	-	11/27/47/70	0/1/1/1
15	XAT	4	303	-	-	0/31/93/93	0/4/4/4
17	CLA	b	835	-	-	10/25/101/115	-
17	CLA	b	820	-	-	5/27/103/115	-
17	CLA	b	814	-	-	14/39/115/115	-
17	CLA	4	311	-	-	17/39/115/115	-
17	CLA	1	312	3	-	3/24/100/115	-
23	BCR	a	849	-	-	0/29/63/63	0/2/2/2
17	CLA	5	310	-	-	8/17/93/115	-
23	BCR	b	848	-	-	2/29/63/63	0/2/2/2
15	XAT	4	302	-	-	3/31/93/93	0/4/4/4
23	BCR	l	205	-	-	8/29/63/63	0/2/2/2
23	BCR	j	104	-	-	4/29/63/63	0/2/2/2
17	CLA	b	818	5	-	12/32/108/115	-
17	CLA	a	854	-	-	15/39/115/115	-
22	LHG	a	845	-	-	27/52/52/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LHG	a	846	17	-	16/31/31/53	-
17	CLA	a	837	4	-	6/15/91/115	-
17	CLA	1	310	3	-	18/39/115/115	-
23	BCR	b	847	-	-	1/29/63/63	0/2/2/2
17	CLA	a	839	4	-	15/39/115/115	-
23	BCR	b	846	-	-	0/29/63/63	0/2/2/2
22	LHG	b	849	17	-	20/35/35/53	-
17	CLA	b	821	5	-	7/21/97/115	-
17	CLA	1	307	3	-	6/26/102/115	-
15	XAT	1	303	-	-	0/31/93/93	0/4/4/4
17	CLA	a	838	4	-	6/23/99/115	-
17	CLA	b	811	5	-	17/39/115/115	-
17	CLA	4	308	-	-	9/29/105/115	-
17	CLA	b	810	-	-	16/39/115/115	-
17	CLA	5	312	-	-	0/24/100/115	-
17	CLA	1	311	-	-	6/25/101/115	-
17	CLA	a	815	-	-	2/15/91/115	-
17	CLA	b	824	-	-	10/25/101/115	-
15	XAT	j	101	-	-	5/31/93/93	0/4/4/4
17	CLA	5	315	1	-	5/17/93/115	-
17	CLA	a	832	4	-	7/21/97/115	-
23	BCR	a	850	-	-	4/29/63/63	0/2/2/2
17	CLA	b	832	5	-	6/20/96/115	-
17	CLA	a	823	-	-	7/20/96/115	-
17	CLA	b	822	5	-	2/23/99/115	-
17	CLA	b	828	5	-	14/39/115/115	-
23	BCR	f	804	-	-	4/29/63/63	0/2/2/2
17	CLA	4	309	-	-	14/39/115/115	-
21	PQN	a	843	-	-	5/23/43/43	0/2/2/2
15	XAT	1	302	-	-	0/31/93/93	0/4/4/4
17	CLA	4	310	2	-	7/21/97/115	-
17	CLA	a	805	17,4	-	6/27/103/115	-
17	CLA	a	826	-	-	10/39/115/115	-
17	CLA	a	828	4	-	9/39/115/115	-
17	CLA	5	309	1	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	a	812	17,4	-	9/36/112/115	-
16	A1L1G	1	301	-	-	11/29/85/85	0/3/3/3
17	CLA	4	307	2	-	9/15/91/115	-
23	BCR	b	845	-	-	6/29/63/63	0/2/2/2
24	SF4	c	101	-	-	-	0/6/5/5
21	PQN	b	842	-	-	1/23/43/43	0/2/2/2
17	CLA	1	305	-	-	12/35/111/115	-
17	CLA	j	103	10	-	7/12/88/115	-
17	CLA	b	838	5	-	10/39/115/115	-
17	CLA	a	822	-	-	5/39/115/115	-
17	CLA	b	813	5	-	6/25/101/115	-
17	CLA	b	823	5	-	7/33/109/115	-
17	CLA	5	307	1	-	7/33/109/115	-
17	CLA	a	802	-	-	7/31/107/115	-
19	DGD	b	851	-	-	20/46/86/95	0/2/2/2
17	CLA	4	312	-	-	10/17/93/115	-
17	CLA	l	202	-	-	2/12/88/115	-
17	CLA	b	839	-	-	15/39/115/115	-
17	CLA	a	810	4	-	15/39/115/115	-
15	XAT	4	306	-	-	4/31/93/93	0/4/4/4
17	CLA	b	802	-	-	17/39/115/115	-
17	CLA	a	827	-	-	8/39/115/115	-
23	BCR	l	201	-	-	4/29/63/63	0/2/2/2
17	CLA	b	841	22	-	11/39/115/115	-
17	CLA	a	821	4	-	2/15/91/115	-
19	DGD	4	319	-	-	10/29/69/95	0/2/2/2
17	CLA	a	817	-	-	8/15/91/115	-

The worst 5 of 1037 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	843	PQN	C3-C2	7.56	1.49	1.35
21	b	842	PQN	C3-C2	7.38	1.48	1.35
21	a	843	PQN	C10-C5	4.85	1.48	1.40
21	b	842	PQN	C10-C5	4.83	1.48	1.40
18	5	316	SQD	O8-S	4.62	1.63	1.47

The worst 5 of 1457 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	319	DGD	C6E-C5E-C4E	-9.40	91.00	113.00
20	1	304	A1L1F	C17-C20-C25	-8.11	108.66	122.26
17	a	806	CLA	C4A-NA-C1A	7.41	110.04	106.71
20	1	304	A1L1F	O15-C20-C21	7.29	118.86	113.38
17	b	840	CLA	C4A-NA-C1A	7.29	109.98	106.71

There are no chirality outliers.

5 of 1540 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	5	302	XAT	O4-C6-C7-C8
15	5	302	XAT	C7-C8-C9-C10
15	5	302	XAT	C7-C8-C9-C19
15	4	301	XAT	C27-C28-C29-C30
15	4	301	XAT	C27-C28-C29-C39

There are no ring outliers.

158 monomers are involved in 480 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	a	809	CLA	3	0
17	b	809	CLA	4	0
22	m	101	LHG	1	0
17	a	818	CLA	10	0
15	4	301	XAT	4	0
17	b	836	CLA	4	0
17	a	819	CLA	6	0
17	i	102	CLA	4	0
17	a	844	CLA	5	0
17	b	840	CLA	3	0
18	5	316	SQD	1	0
17	5	311	CLA	1	0
17	b	819	CLA	3	0
15	a	852	XAT	5	0
17	b	831	CLA	5	0
17	b	804	CLA	4	0
23	a	847	BCR	2	0
17	l	203	CLA	2	0
17	a	806	CLA	7	0
17	a	804	CLA	4	0
15	5	301	XAT	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	b	837	CLA	6	0
17	a	813	CLA	1	0
17	a	840	CLA	6	0
17	b	833	CLA	3	0
24	c	102	SF4	3	0
17	a	808	CLA	1	0
17	b	826	CLA	3	0
20	1	304	A1L1F	2	0
17	4	313	CLA	1	0
17	4	314	CLA	4	0
17	a	803	CLA	4	0
18	1	315	SQD	3	0
23	i	101	BCR	2	0
17	b	829	CLA	3	0
23	b	850	BCR	4	0
15	4	305	XAT	4	0
17	4	317	CLA	1	0
17	b	830	CLA	4	0
17	a	801	CLA	6	0
17	4	315	CLA	1	0
23	b	844	BCR	2	0
17	a	820	CLA	6	0
15	5	302	XAT	10	0
17	5	314	CLA	1	0
17	a	824	CLA	1	0
23	a	848	BCR	5	0
17	1	306	CLA	6	0
16	5	303	A1L1G	1	0
15	5	304	XAT	5	0
17	a	831	CLA	6	0
17	a	829	CLA	6	0
17	a	835	CLA	5	0
17	5	308	CLA	2	0
17	4	316	CLA	1	0
17	a	807	CLA	4	0
17	b	817	CLA	4	0
23	f	801	BCR	9	0
23	m	102	BCR	3	0
17	b	805	CLA	3	0
17	1	308	CLA	4	0
17	5	305	CLA	2	0
17	a	816	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	a	825	CLA	4	0
17	b	825	CLA	6	0
17	4	318	CLA	5	0
17	b	834	CLA	5	0
17	b	806	CLA	2	0
17	b	812	CLA	2	0
25	a	853	LMG	11	0
17	b	801	CLA	4	0
17	a	830	CLA	7	0
17	a	834	CLA	7	0
17	b	808	CLA	1	0
17	a	842	CLA	5	0
15	4	304	XAT	9	0
17	a	833	CLA	2	0
17	f	802	CLA	1	0
17	j	102	CLA	5	0
17	b	803	CLA	2	0
23	b	843	BCR	3	0
23	b	852	BCR	5	0
17	b	807	CLA	7	0
17	b	827	CLA	4	0
17	a	814	CLA	3	0
17	b	815	CLA	3	0
17	a	841	CLA	7	0
25	j	105	LMG	7	0
15	4	303	XAT	3	0
17	b	835	CLA	1	0
17	b	820	CLA	2	0
17	b	814	CLA	7	0
17	4	311	CLA	6	0
17	1	312	CLA	2	0
23	a	849	BCR	2	0
17	5	310	CLA	2	0
23	b	848	BCR	2	0
15	4	302	XAT	5	0
23	l	205	BCR	11	0
23	j	104	BCR	8	0
17	b	818	CLA	7	0
17	a	854	CLA	3	0
22	a	845	LHG	3	0
22	a	846	LHG	3	0
17	a	837	CLA	1	0

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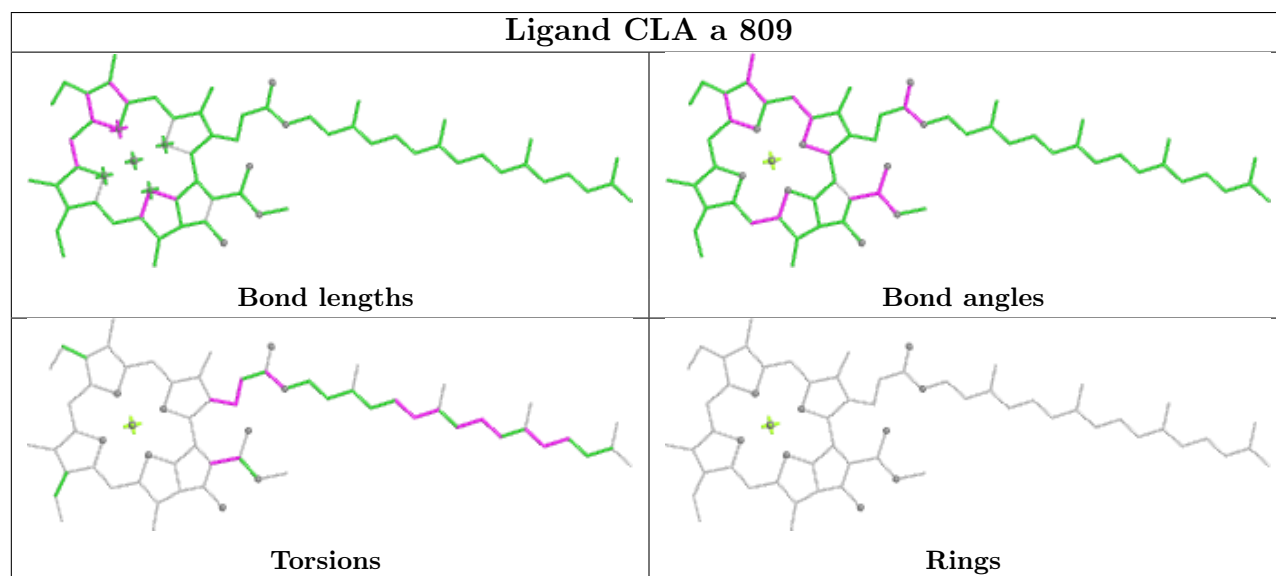
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	1	310	CLA	1	0
23	b	847	BCR	7	0
17	a	839	CLA	6	0
23	b	846	BCR	2	0
17	b	821	CLA	2	0
15	1	303	XAT	3	0
17	a	838	CLA	1	0
17	b	811	CLA	6	0
17	4	308	CLA	2	0
17	b	810	CLA	1	0
17	5	312	CLA	3	0
17	1	311	CLA	2	0
17	a	815	CLA	1	0
17	b	824	CLA	6	0
15	j	101	XAT	5	0
17	5	315	CLA	2	0
17	a	832	CLA	2	0
23	a	850	BCR	4	0
17	b	832	CLA	2	0
17	a	823	CLA	3	0
17	b	822	CLA	3	0
17	b	828	CLA	4	0
23	f	804	BCR	5	0
17	4	309	CLA	8	0
21	a	843	PQN	3	0
15	1	302	XAT	4	0
17	4	310	CLA	3	0
17	a	805	CLA	3	0
17	a	826	CLA	6	0
17	a	828	CLA	5	0
17	5	309	CLA	4	0
16	1	301	A1L1G	1	0
17	4	307	CLA	2	0
23	b	845	BCR	5	0
21	b	842	PQN	2	0
17	j	103	CLA	2	0
17	b	838	CLA	5	0
17	a	822	CLA	5	0
17	b	813	CLA	4	0
17	b	823	CLA	5	0
17	5	307	CLA	7	0
17	a	802	CLA	5	0

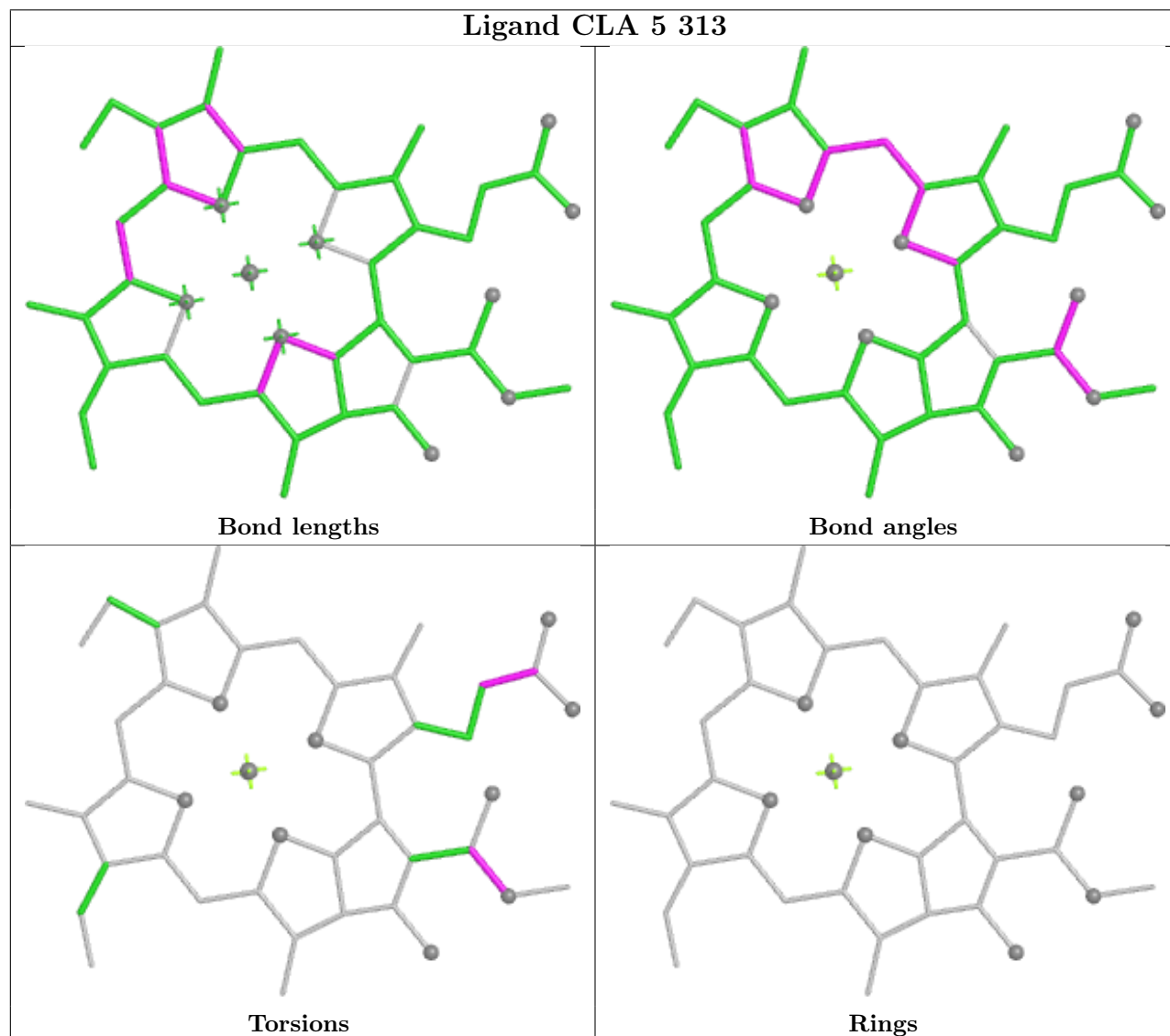
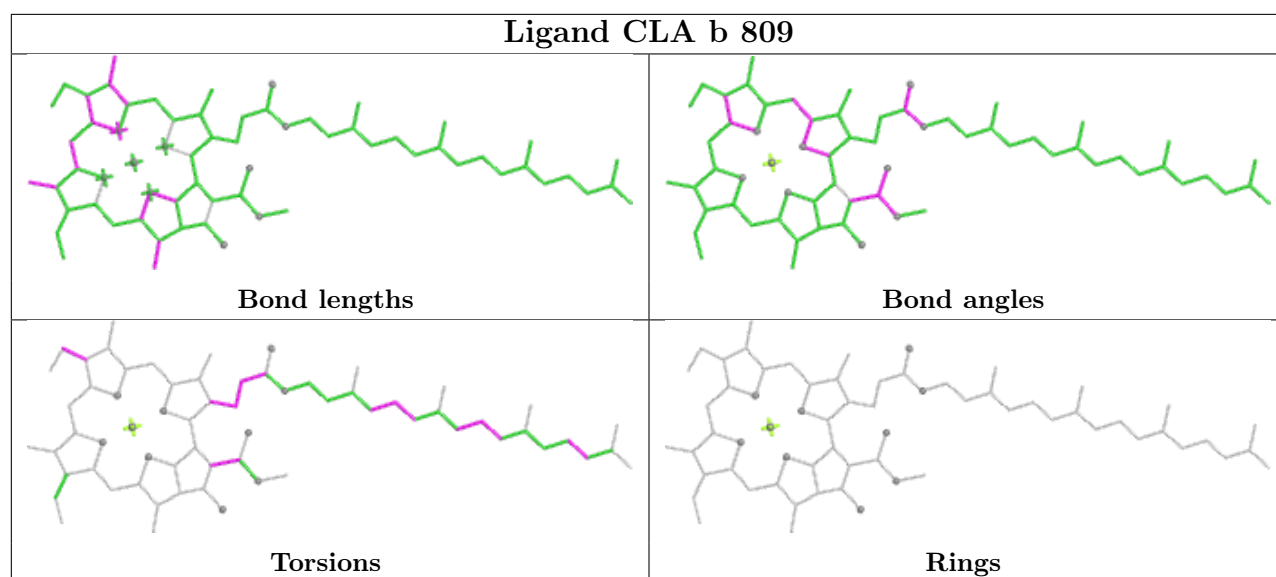
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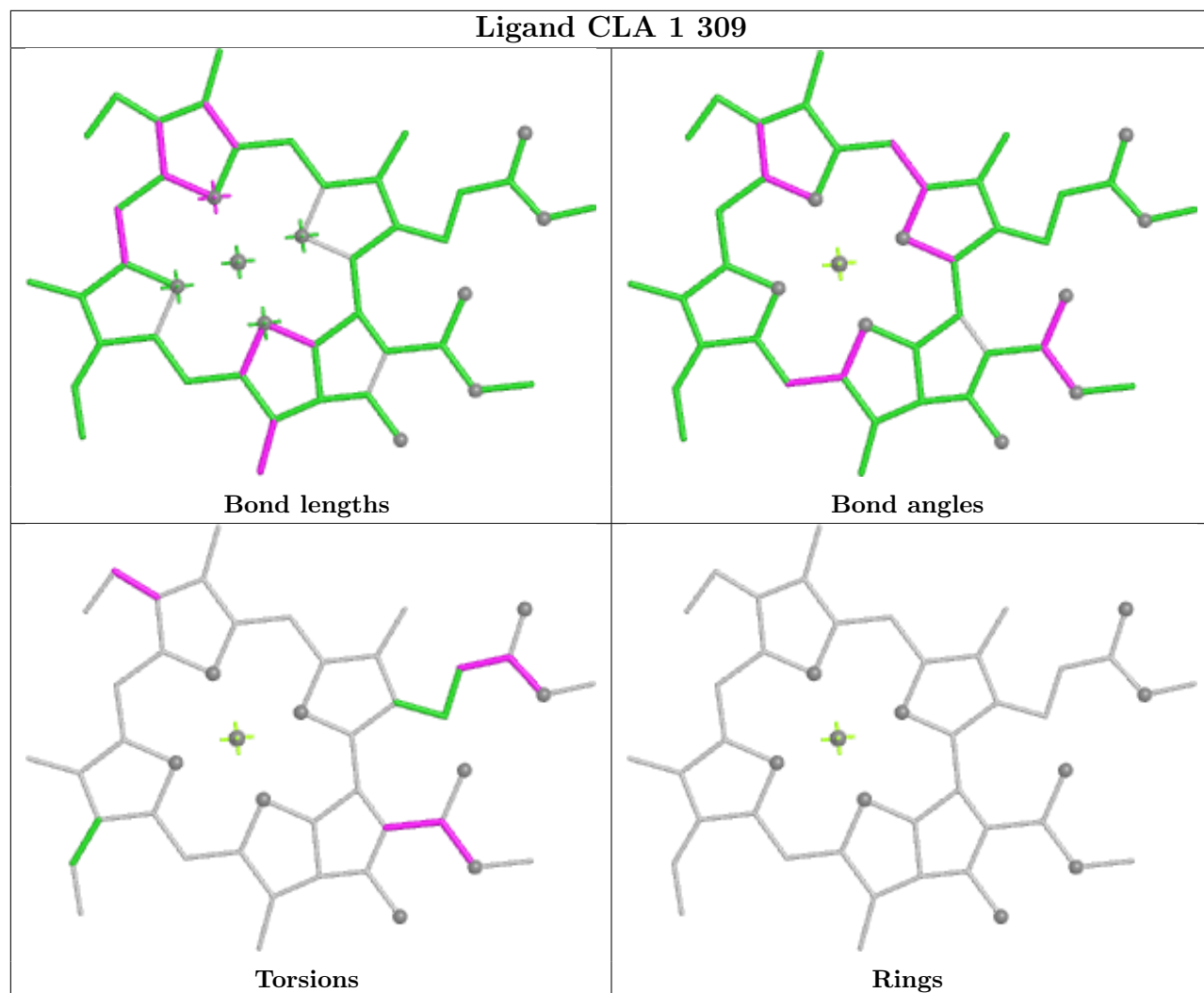
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19	b	851	DGD	6	0
17	4	312	CLA	1	0
17	l	202	CLA	1	0
17	b	839	CLA	5	0
17	a	810	CLA	4	0
15	4	306	XAT	4	0
17	b	802	CLA	3	0
17	a	827	CLA	3	0
23	l	201	BCR	5	0
17	b	841	CLA	4	0
19	4	319	DGD	11	0

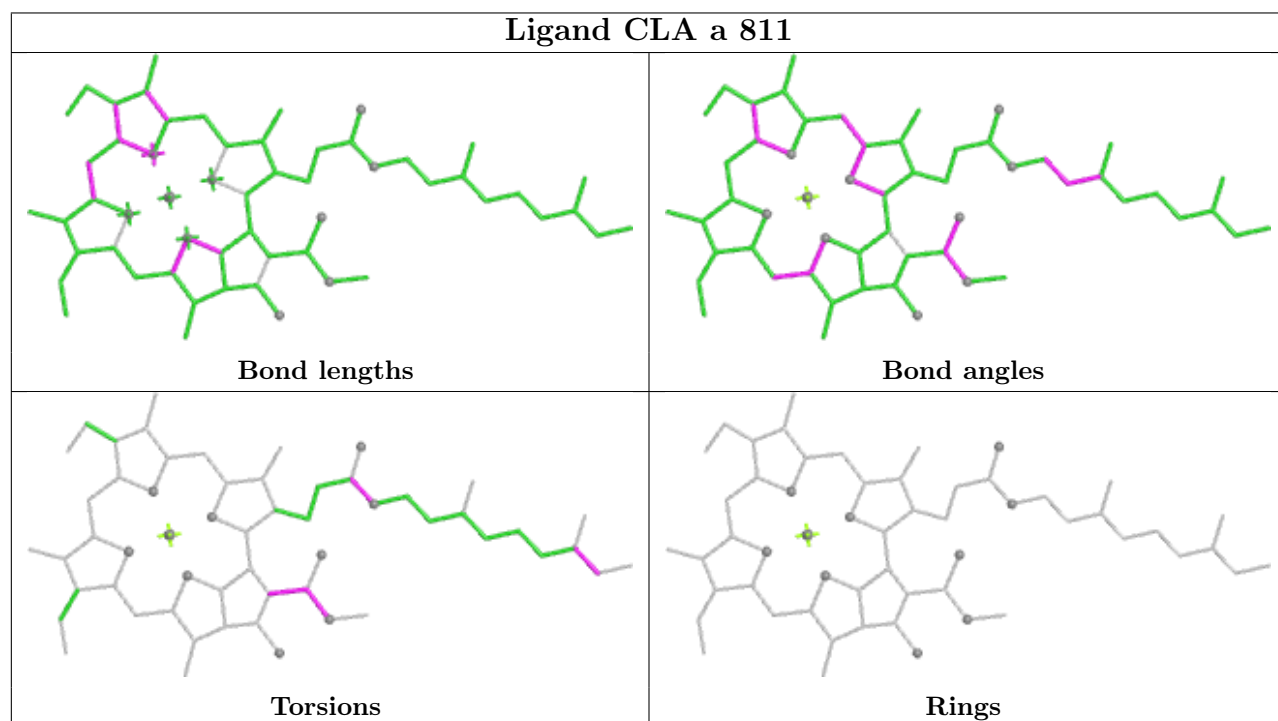
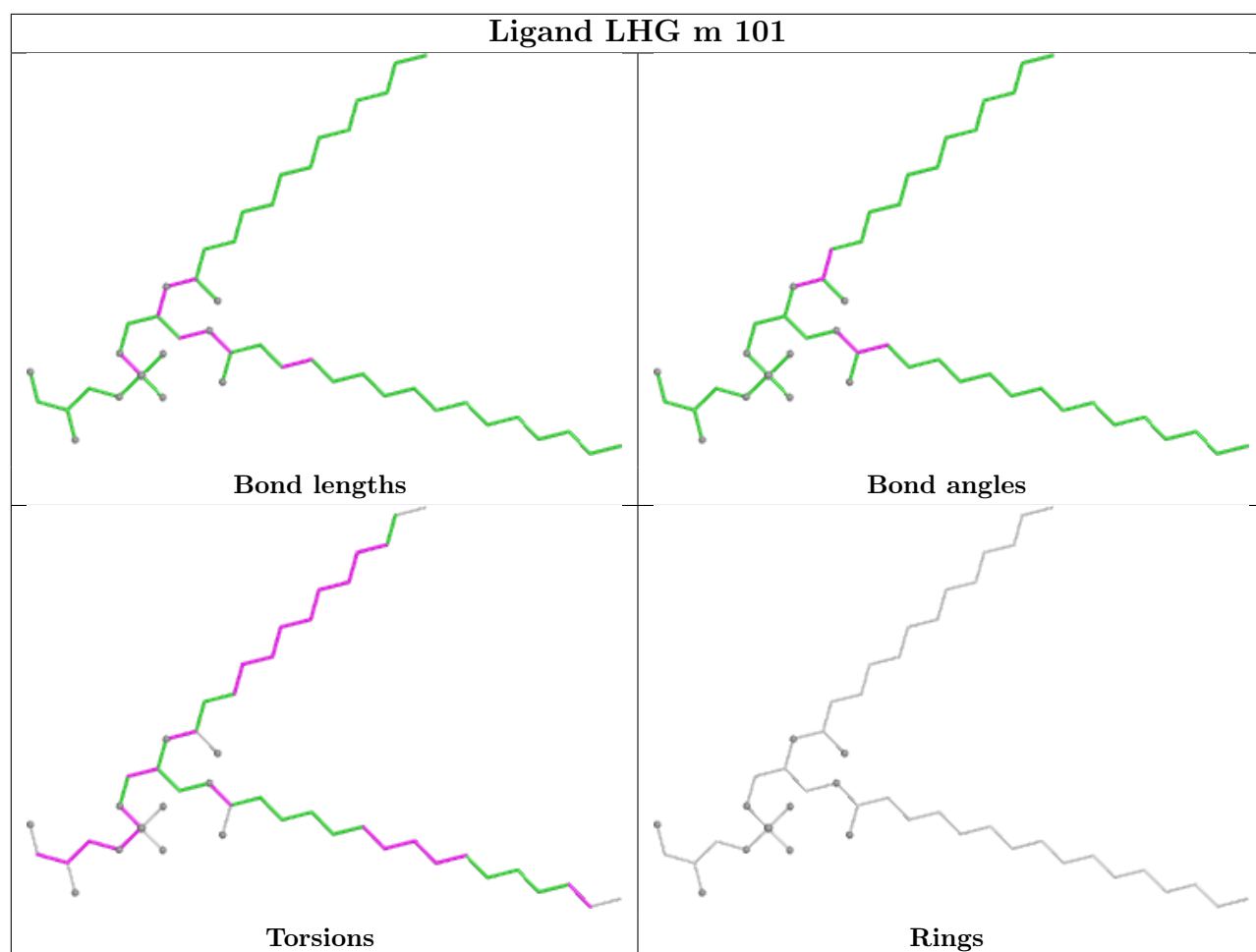
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



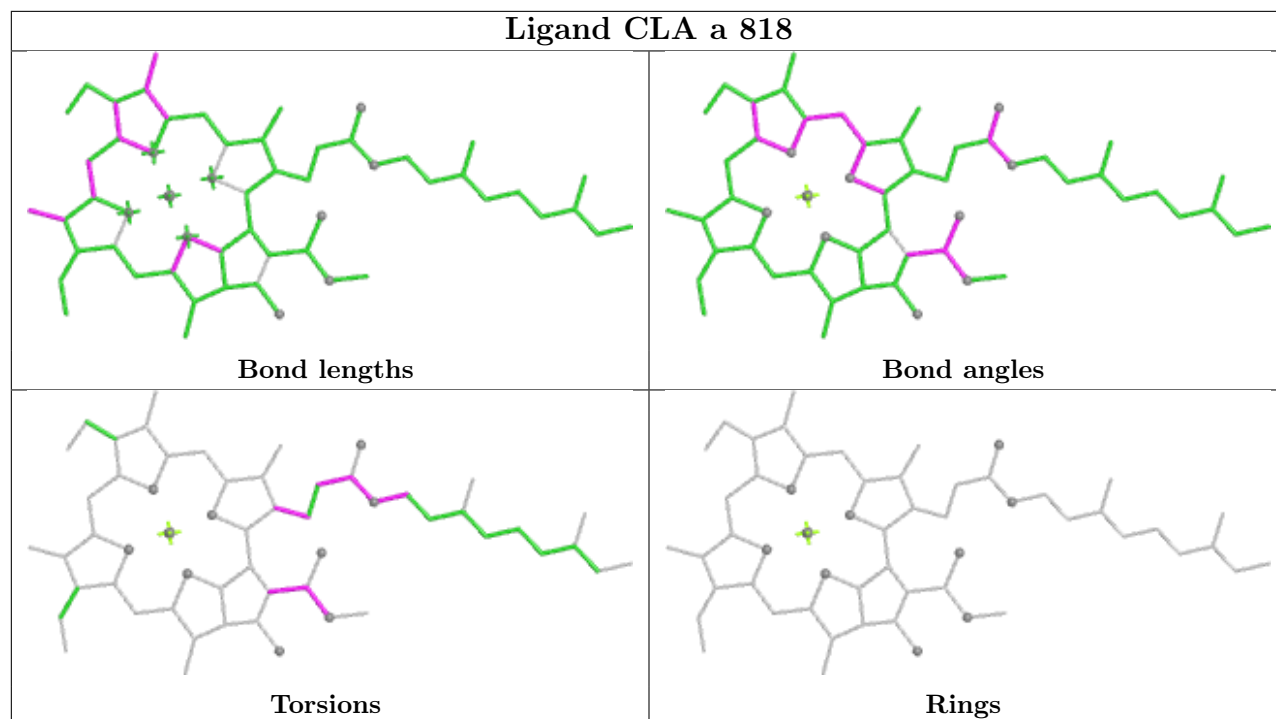


Ligand CLA 1 309

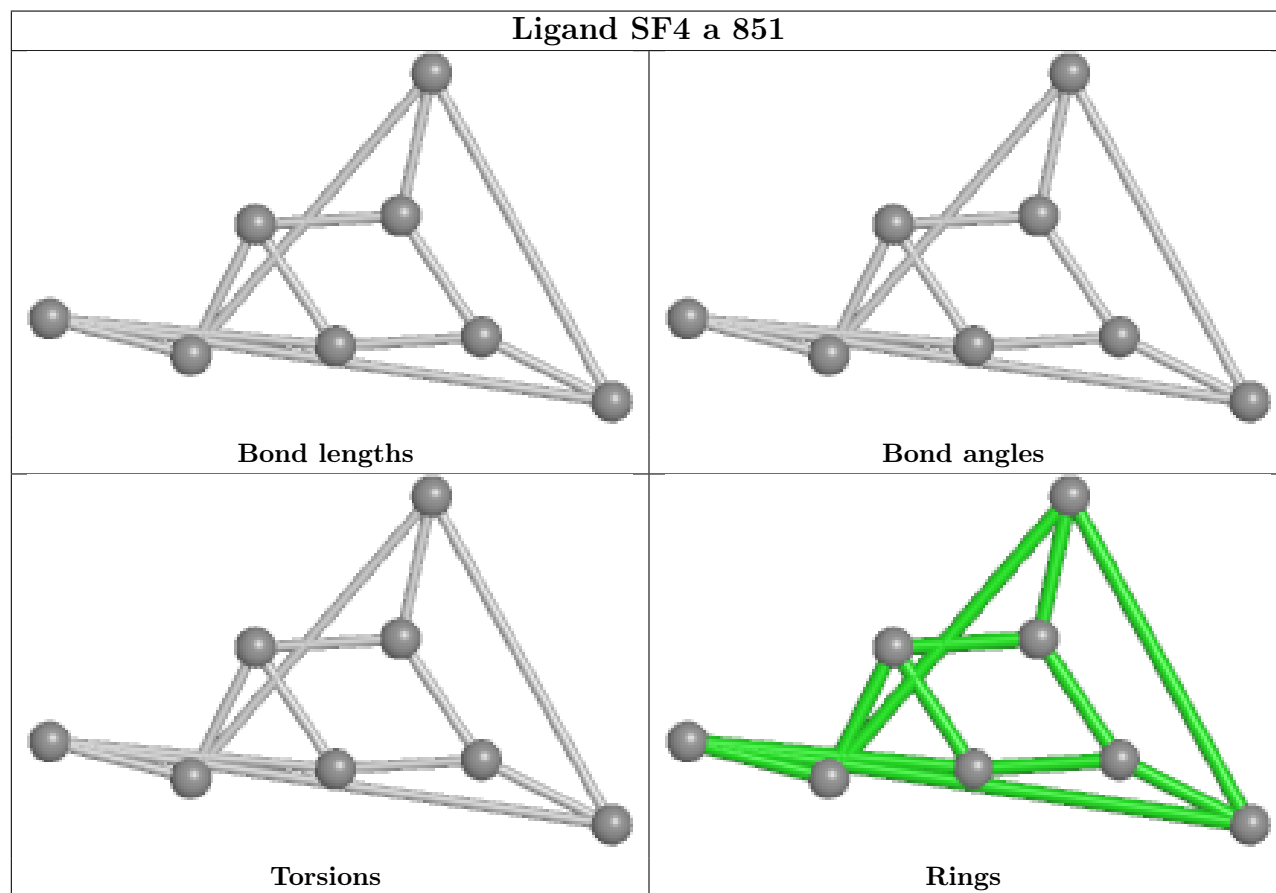


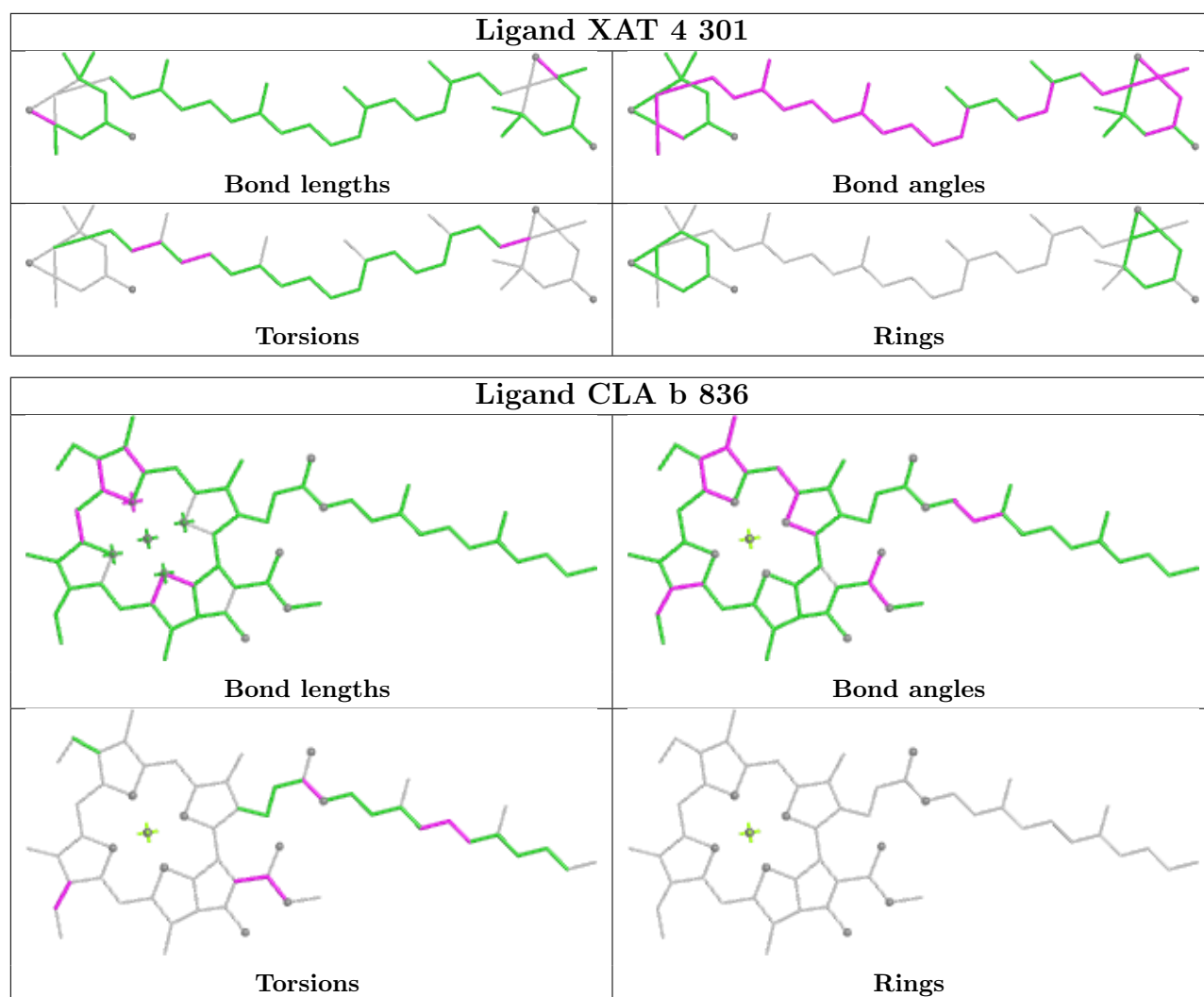


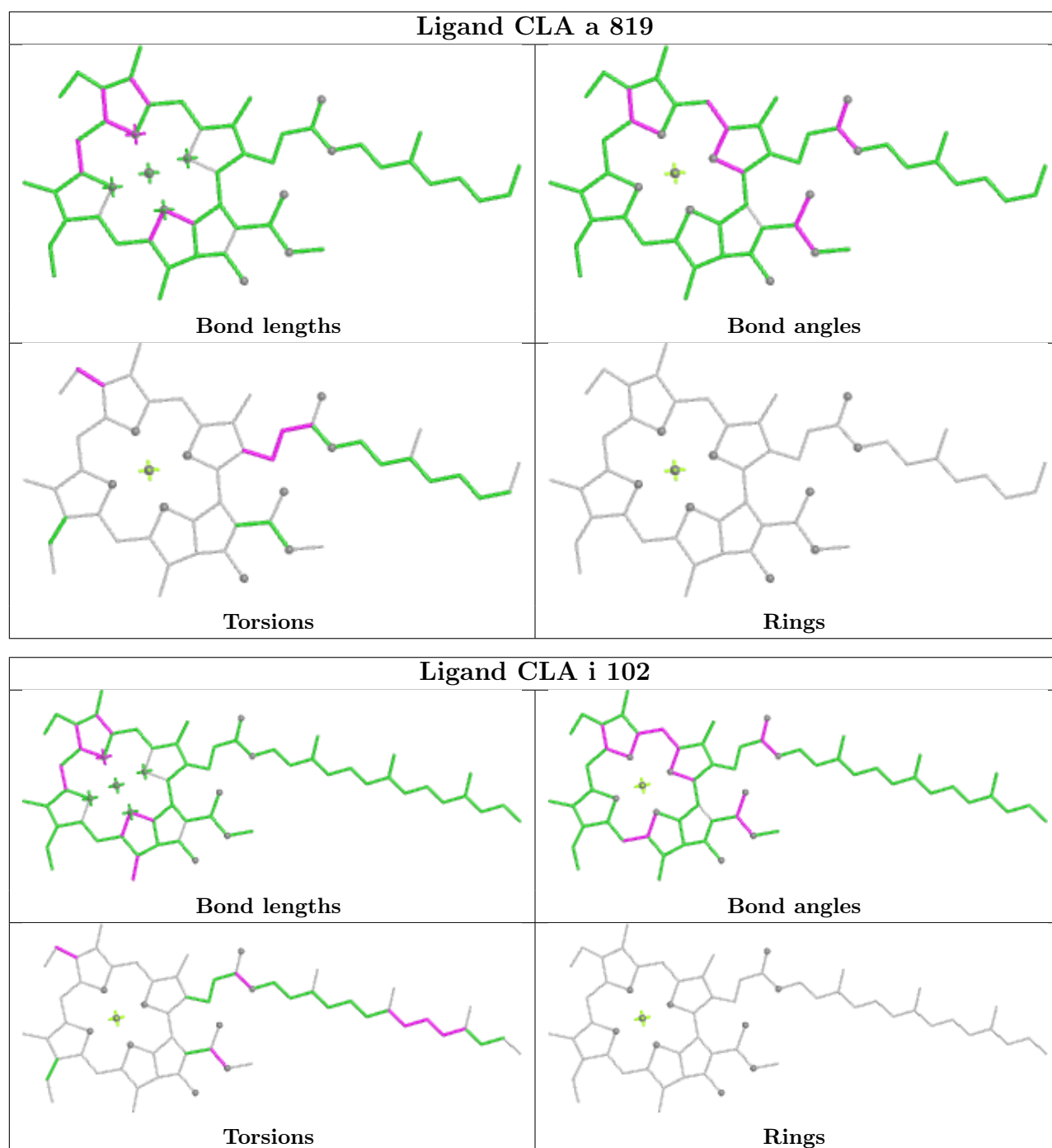
Ligand CLA a 818

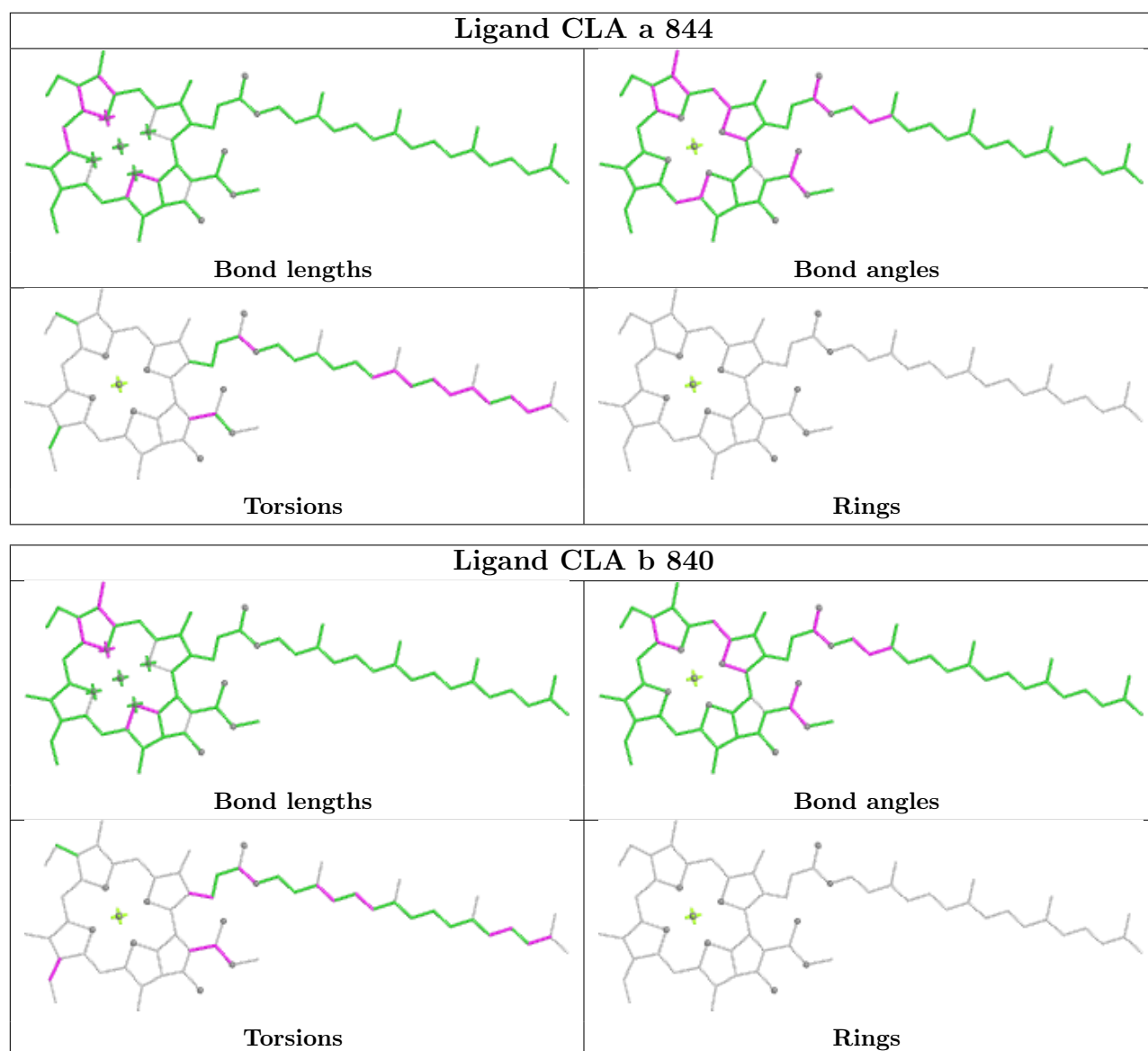


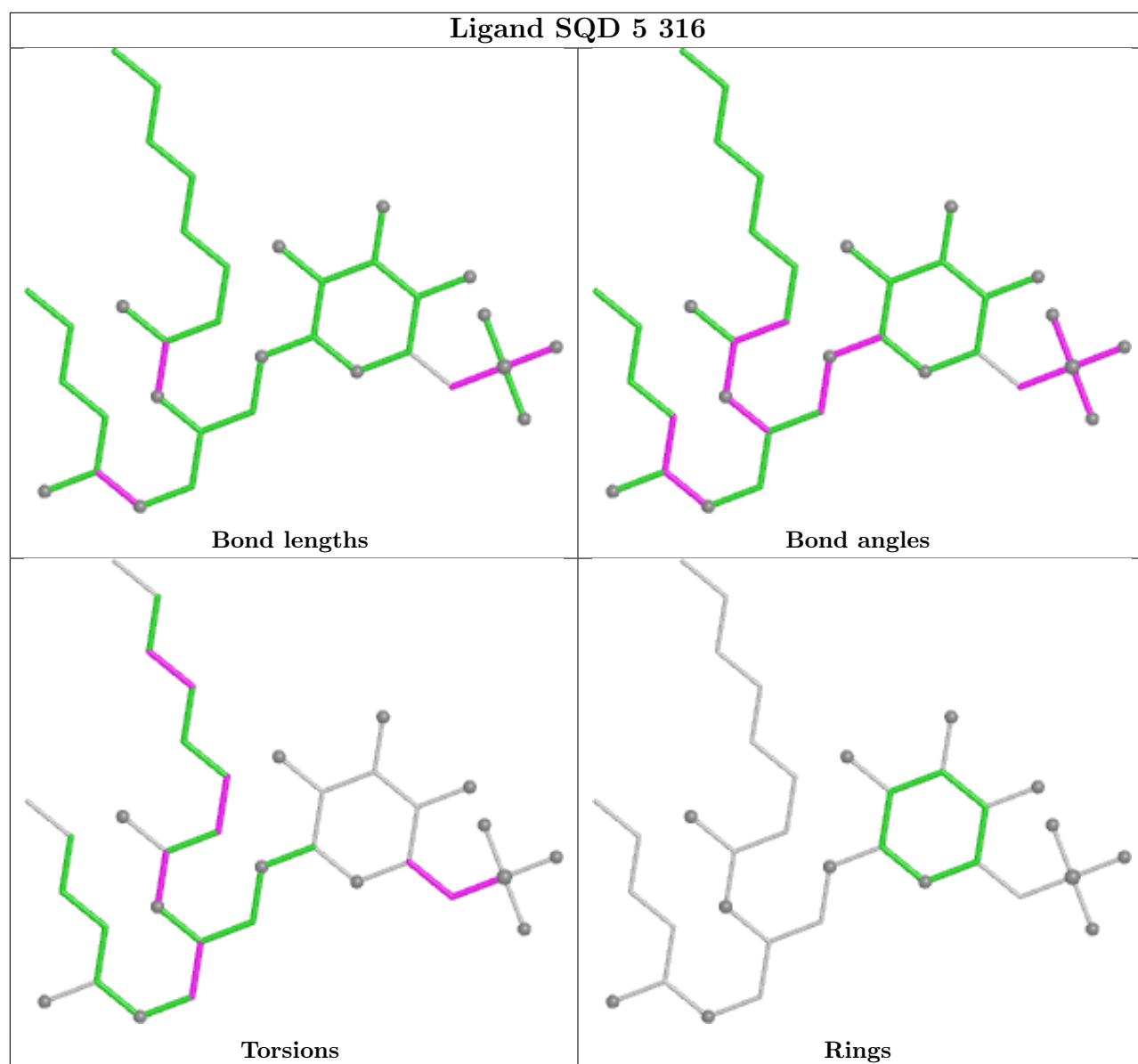
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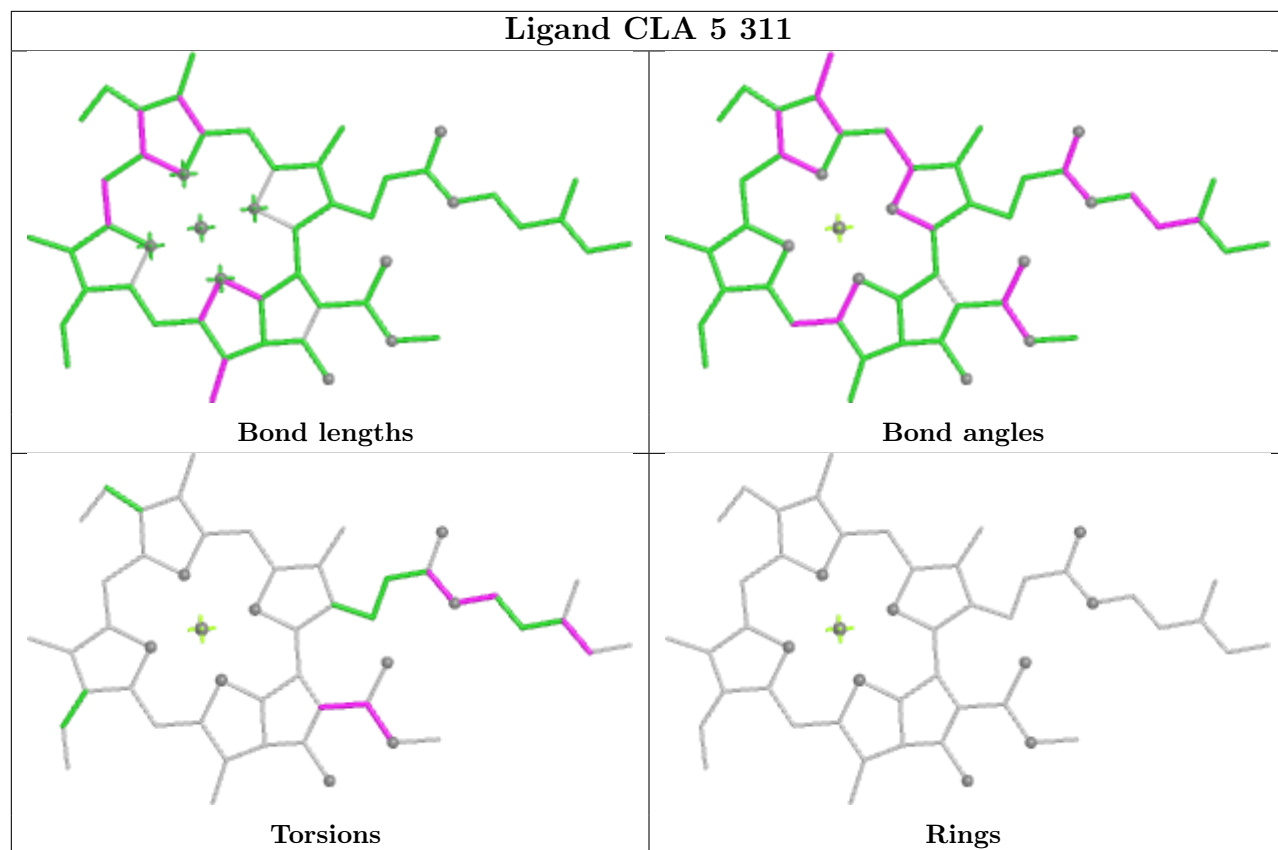




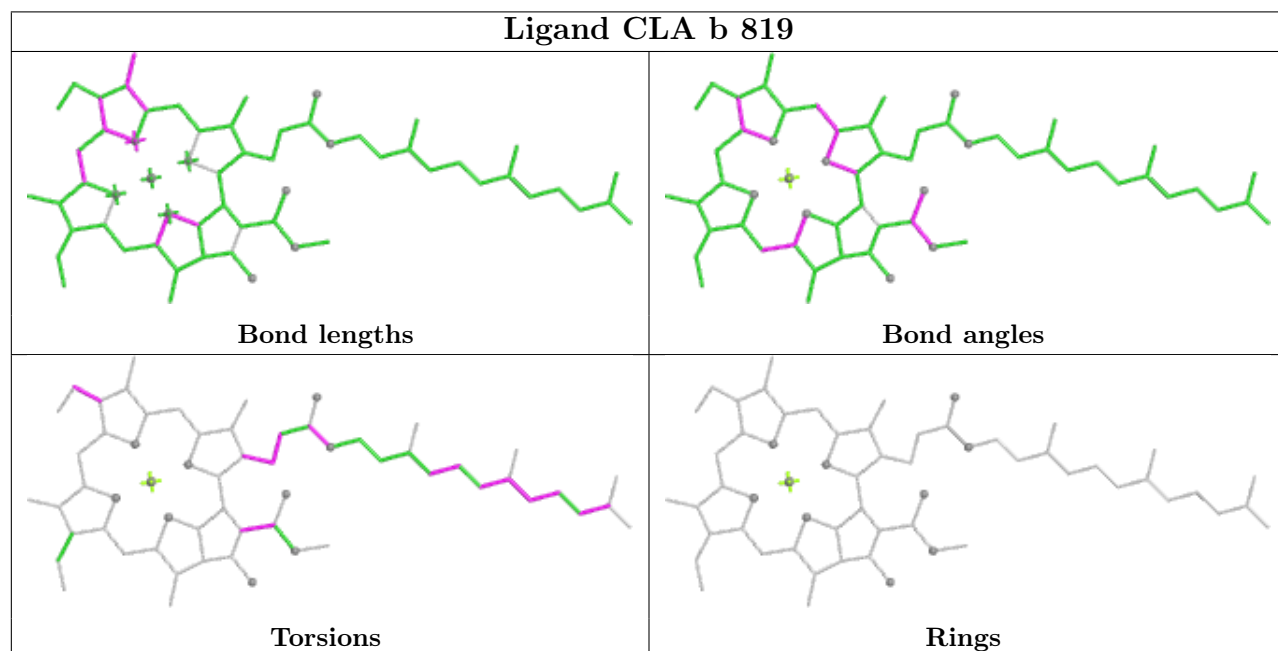


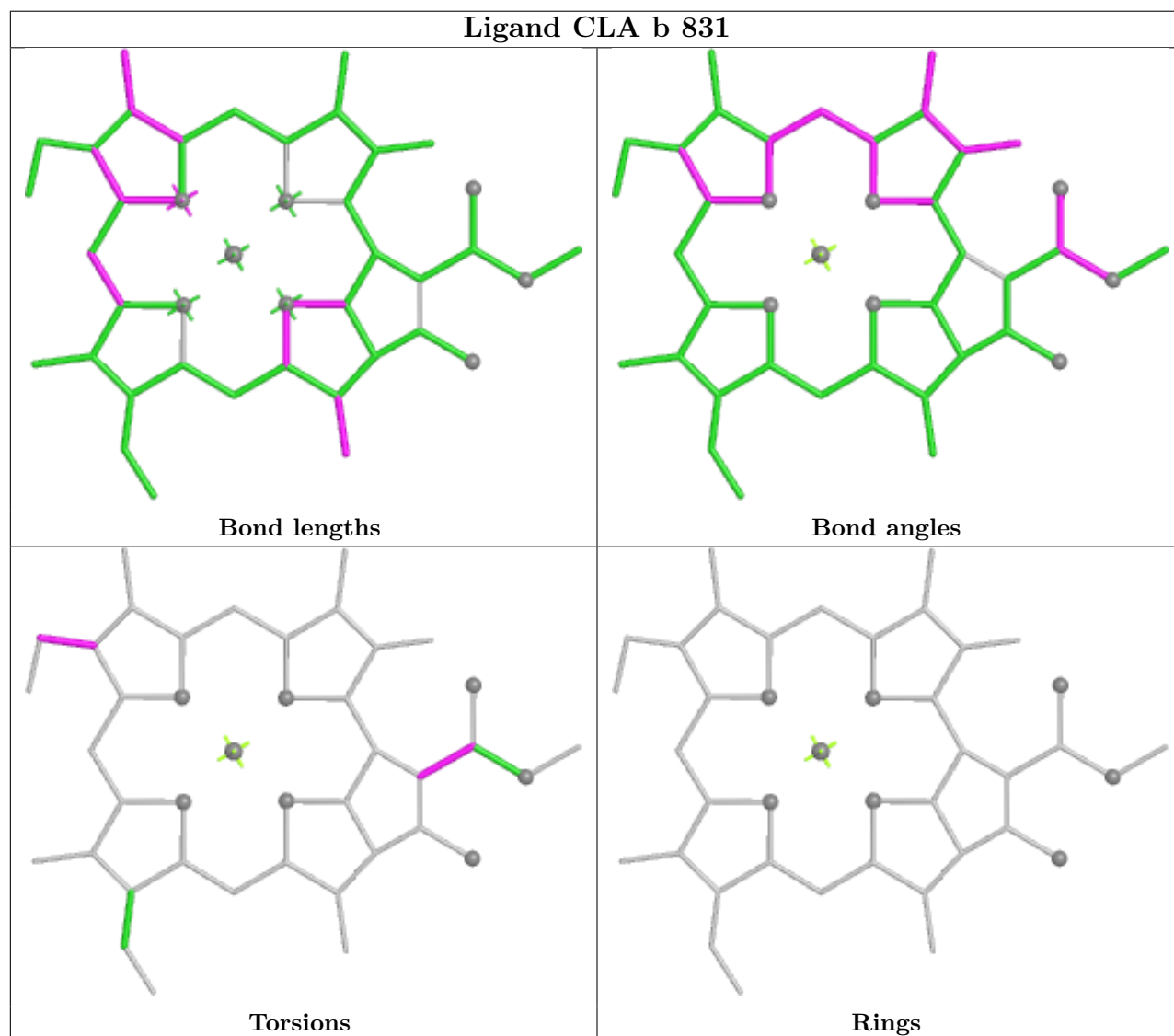
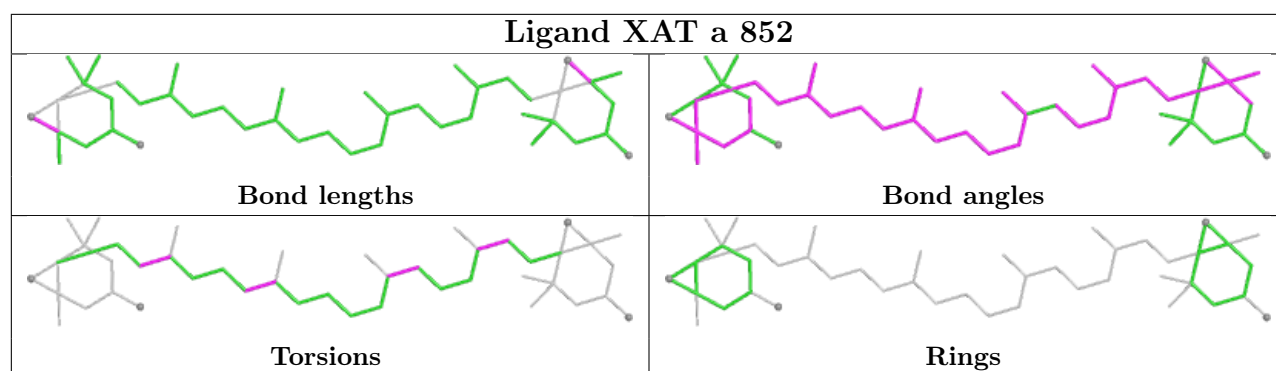


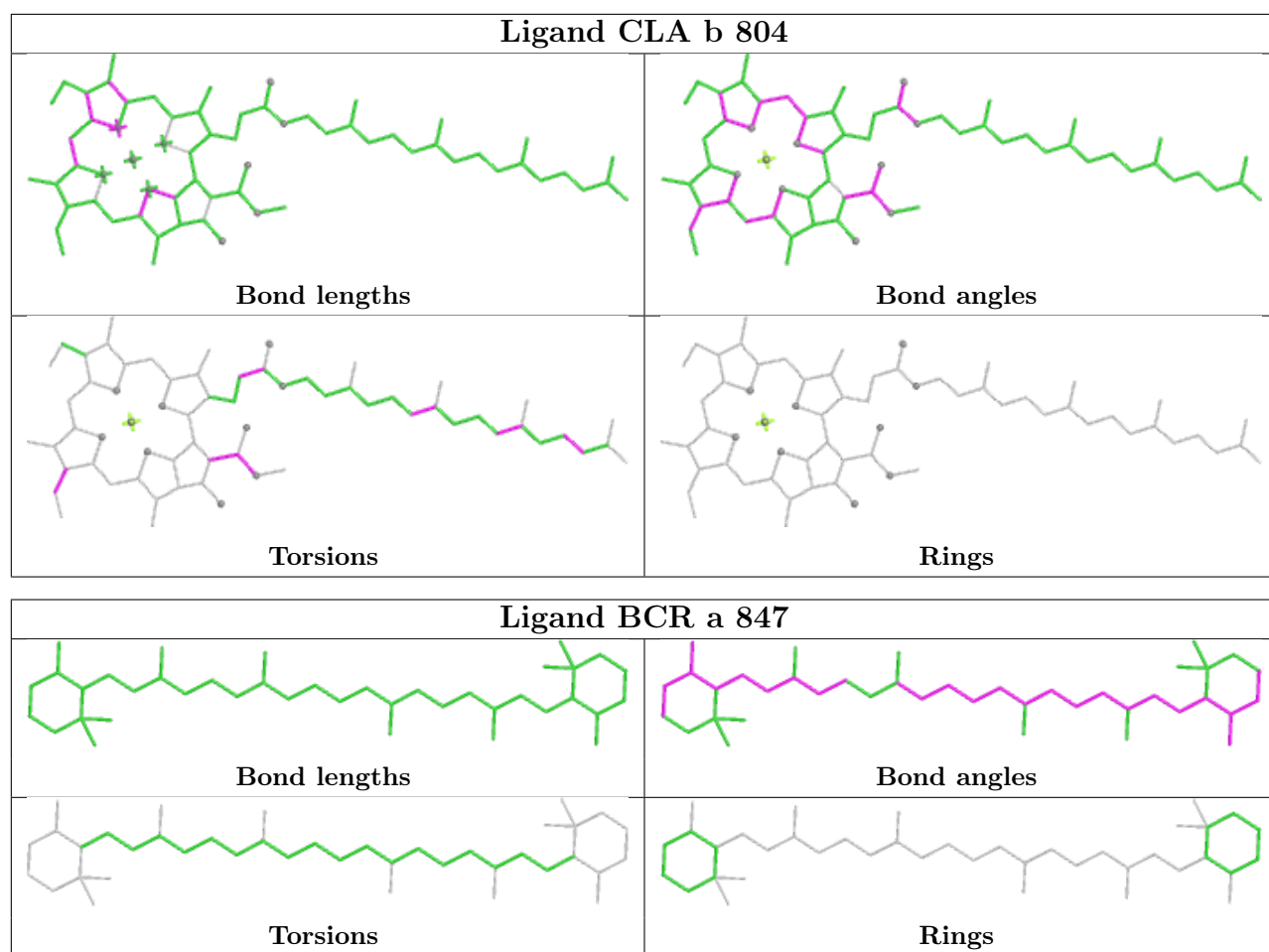
Ligand CLA 5 311



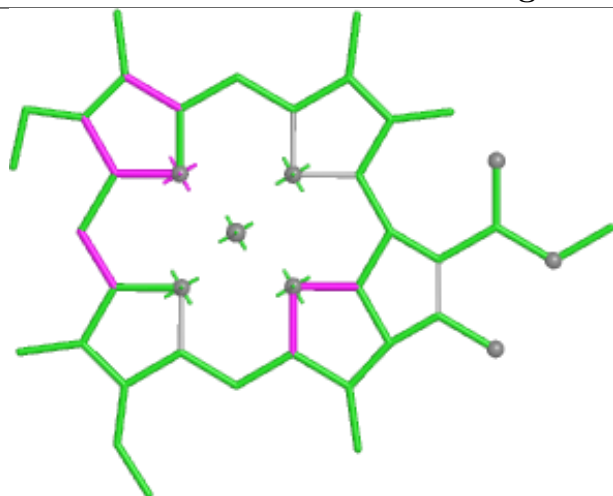
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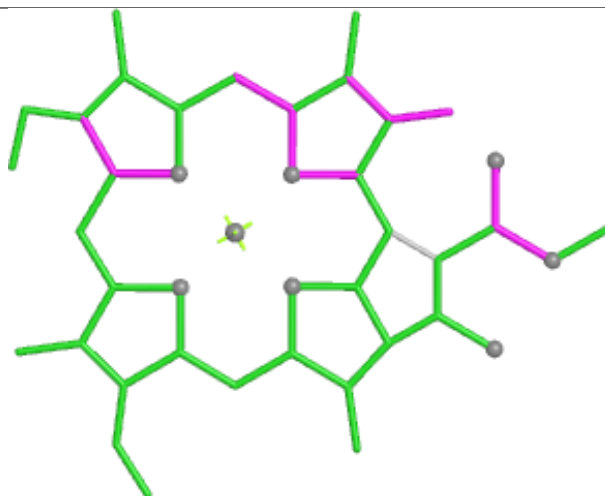




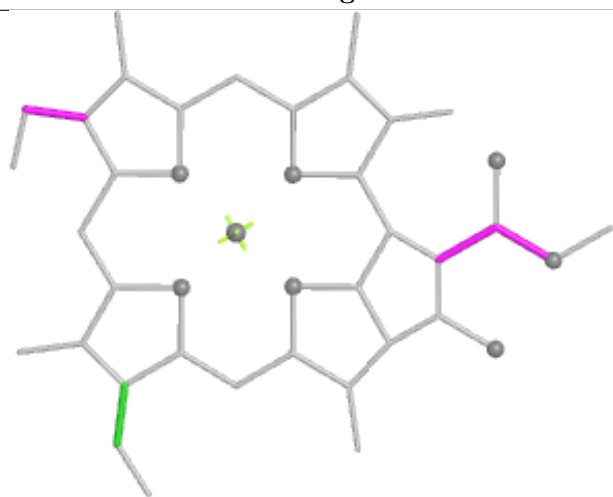
Ligand CLA 1 313



Bond lengths



Bond angles

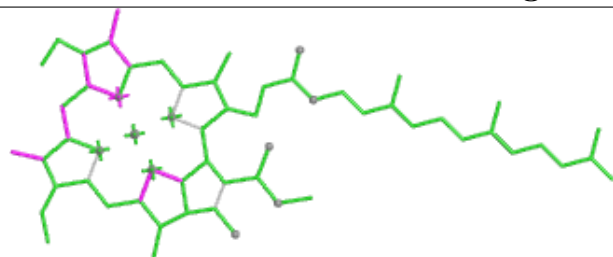


Torsions

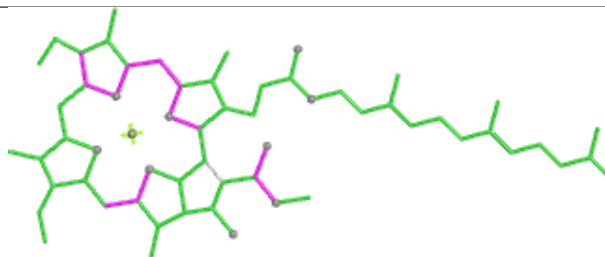


Rings

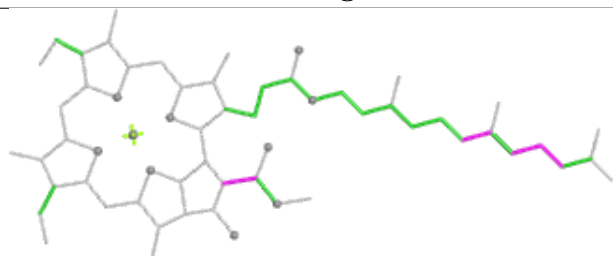
Ligand CLA 1 203



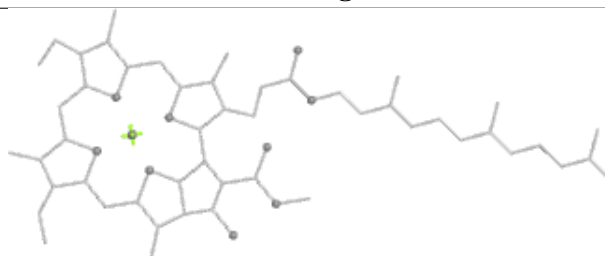
Bond lengths



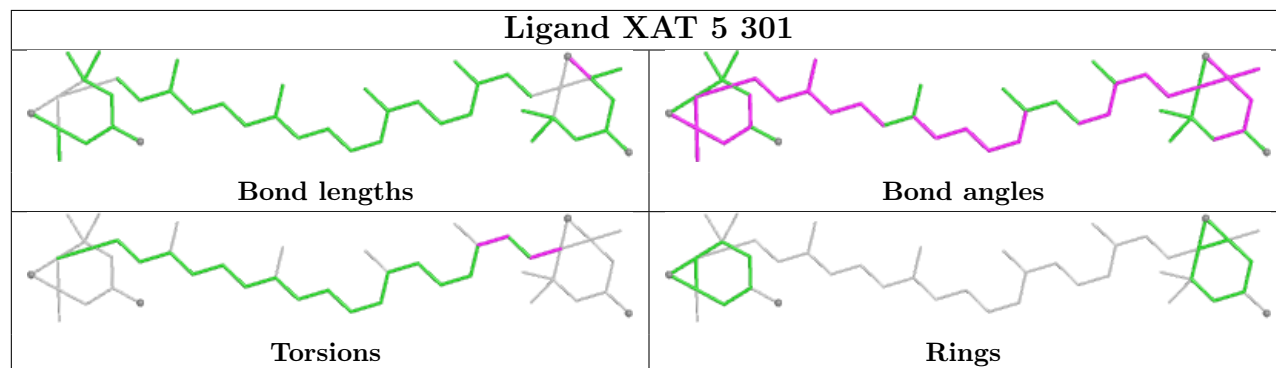
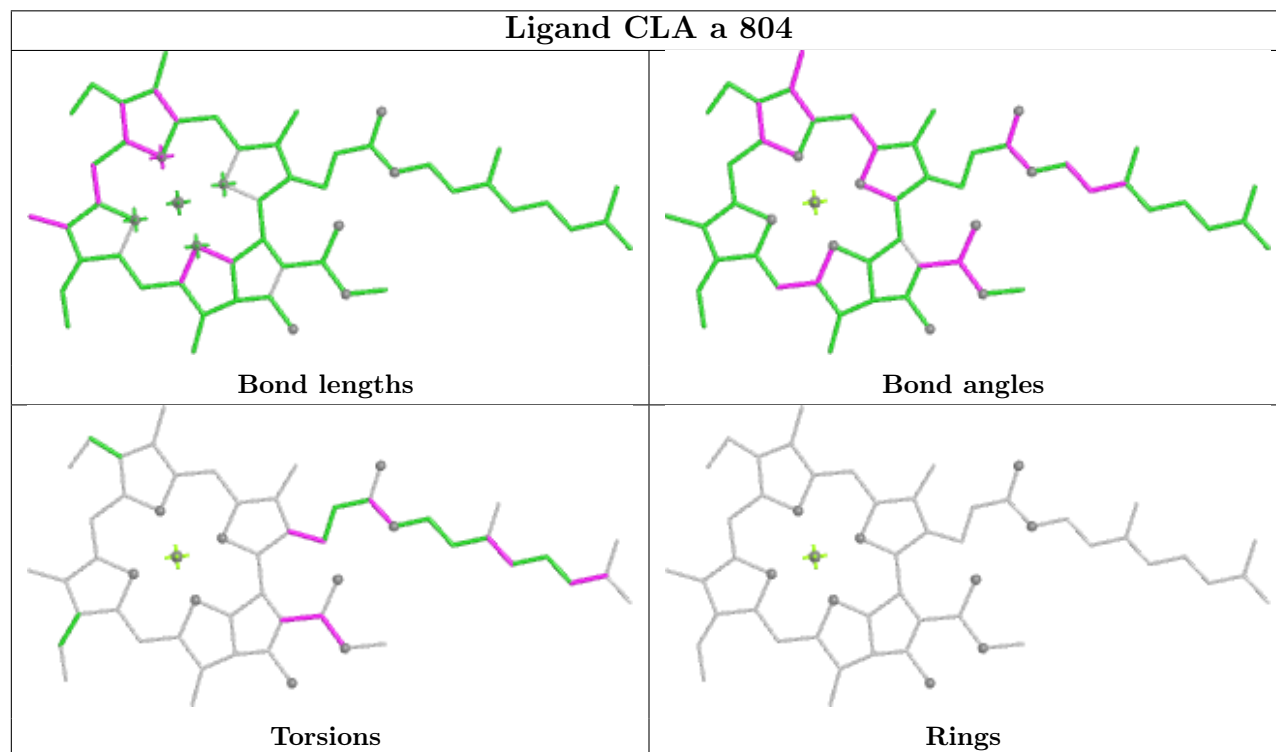
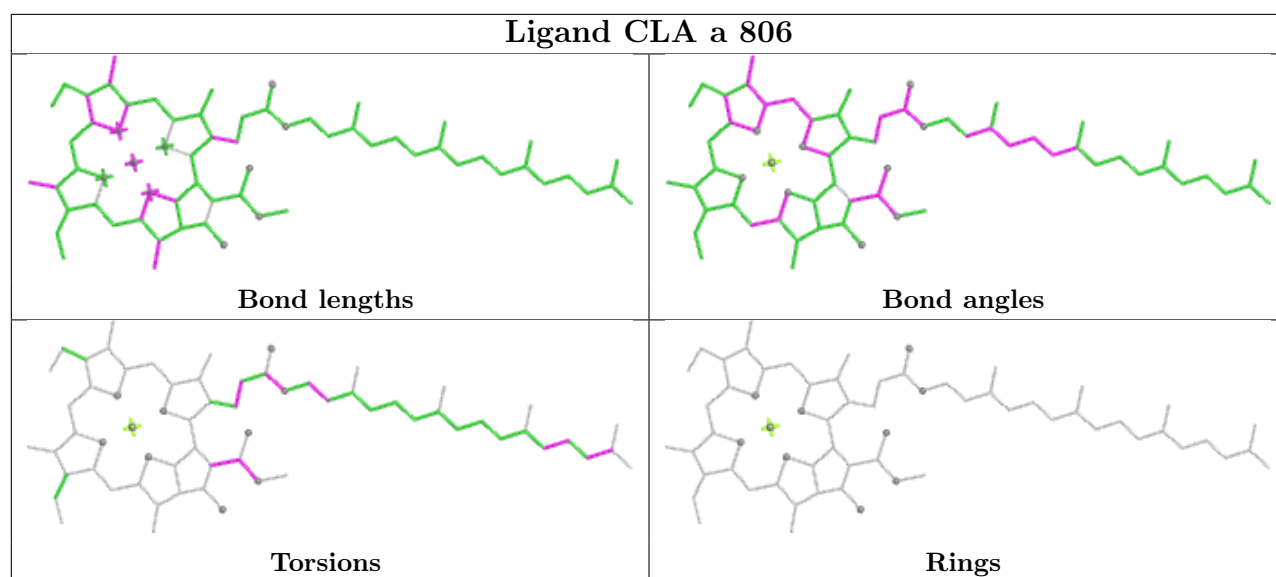
Bond angles



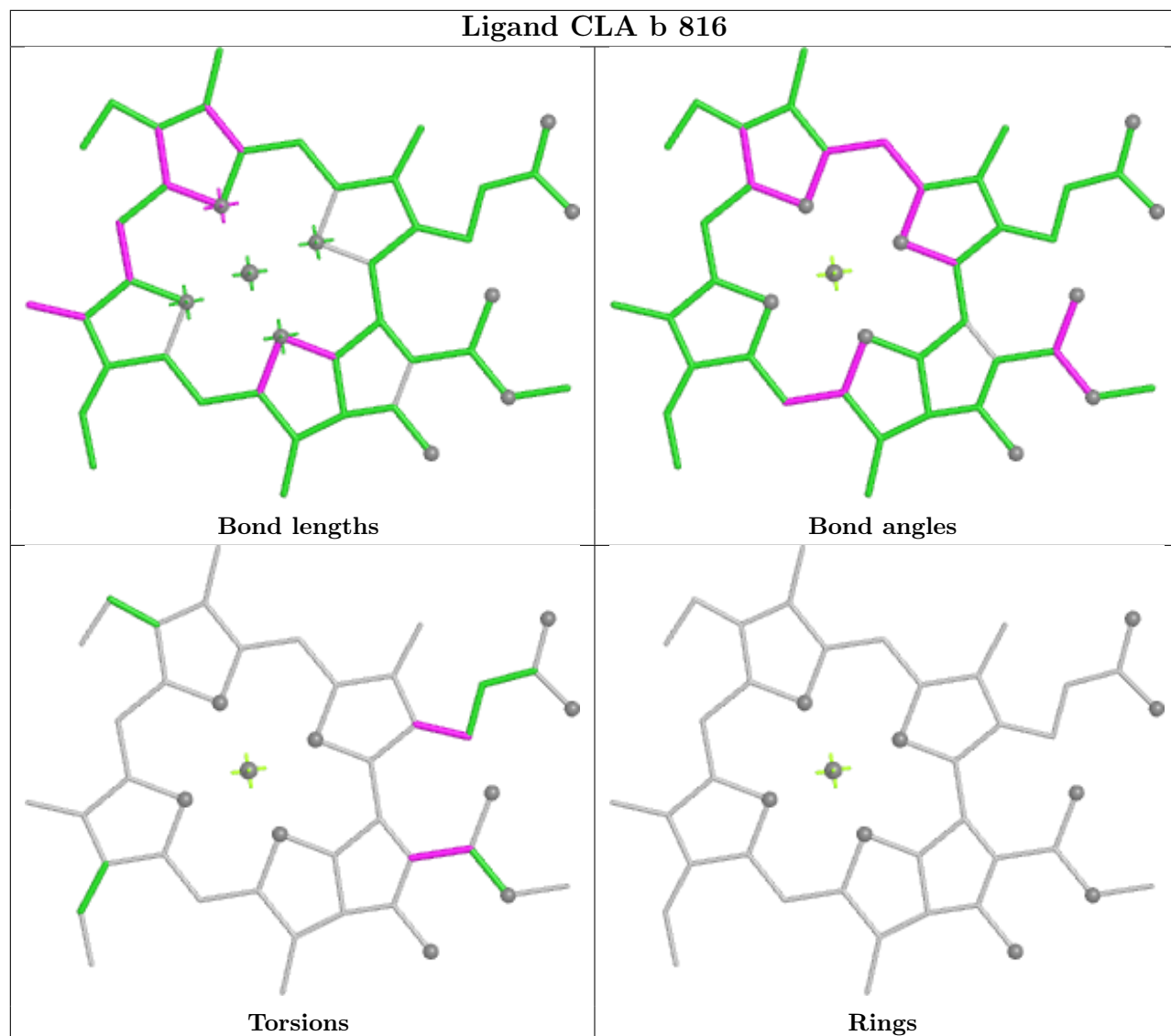
Torsions



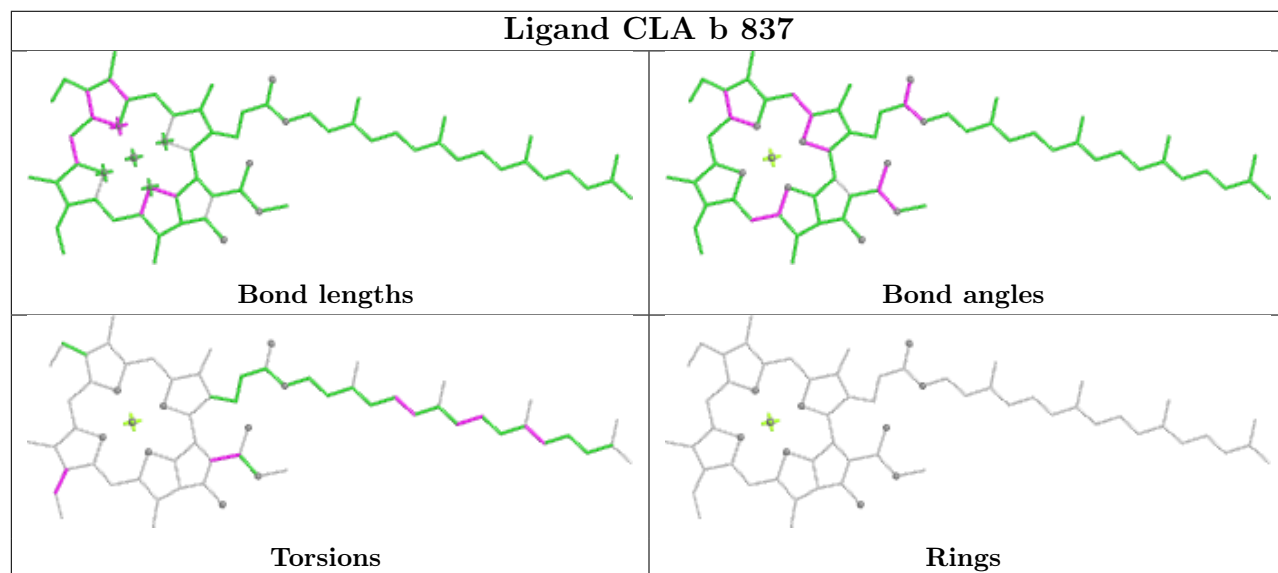
Rings

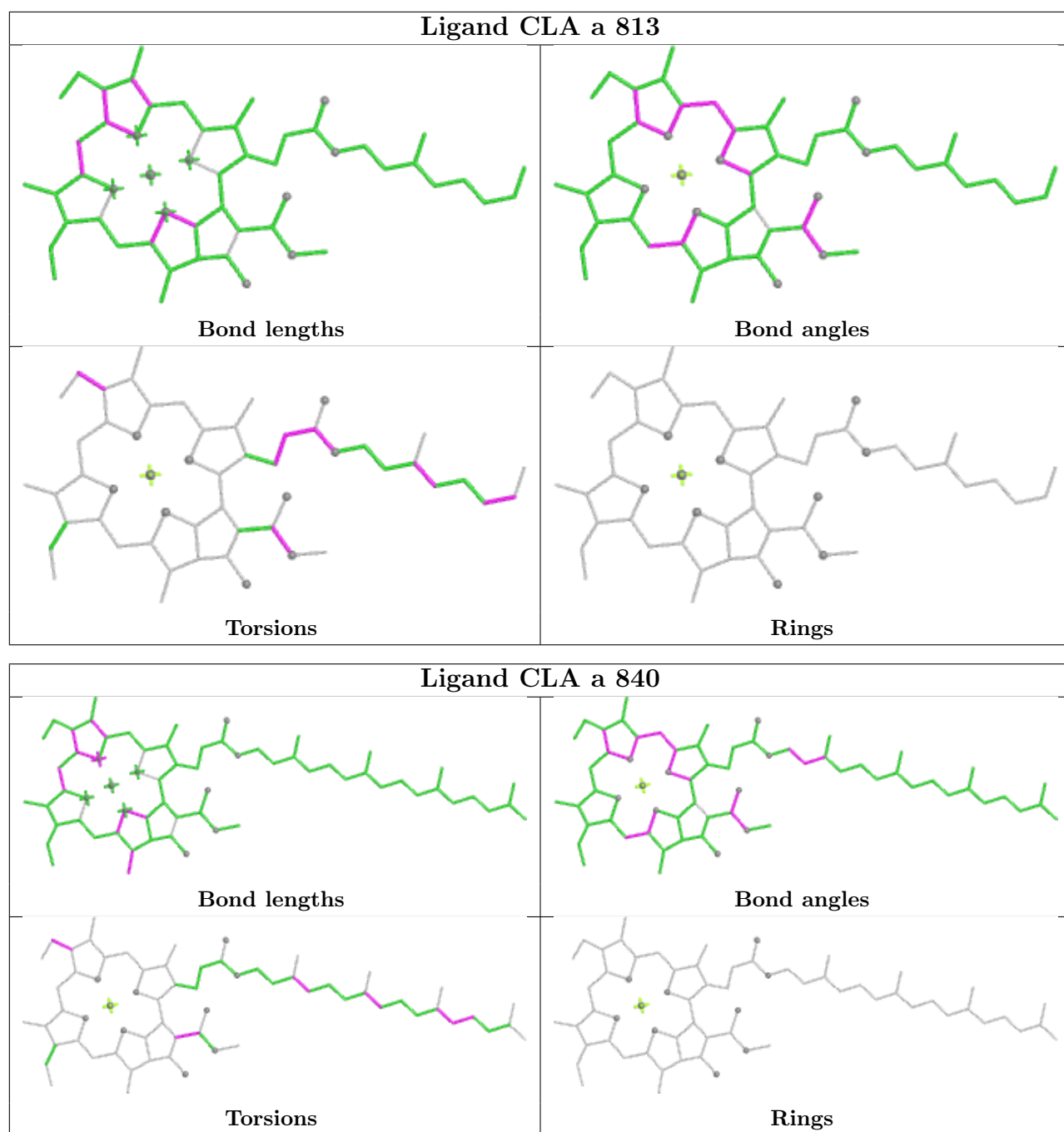


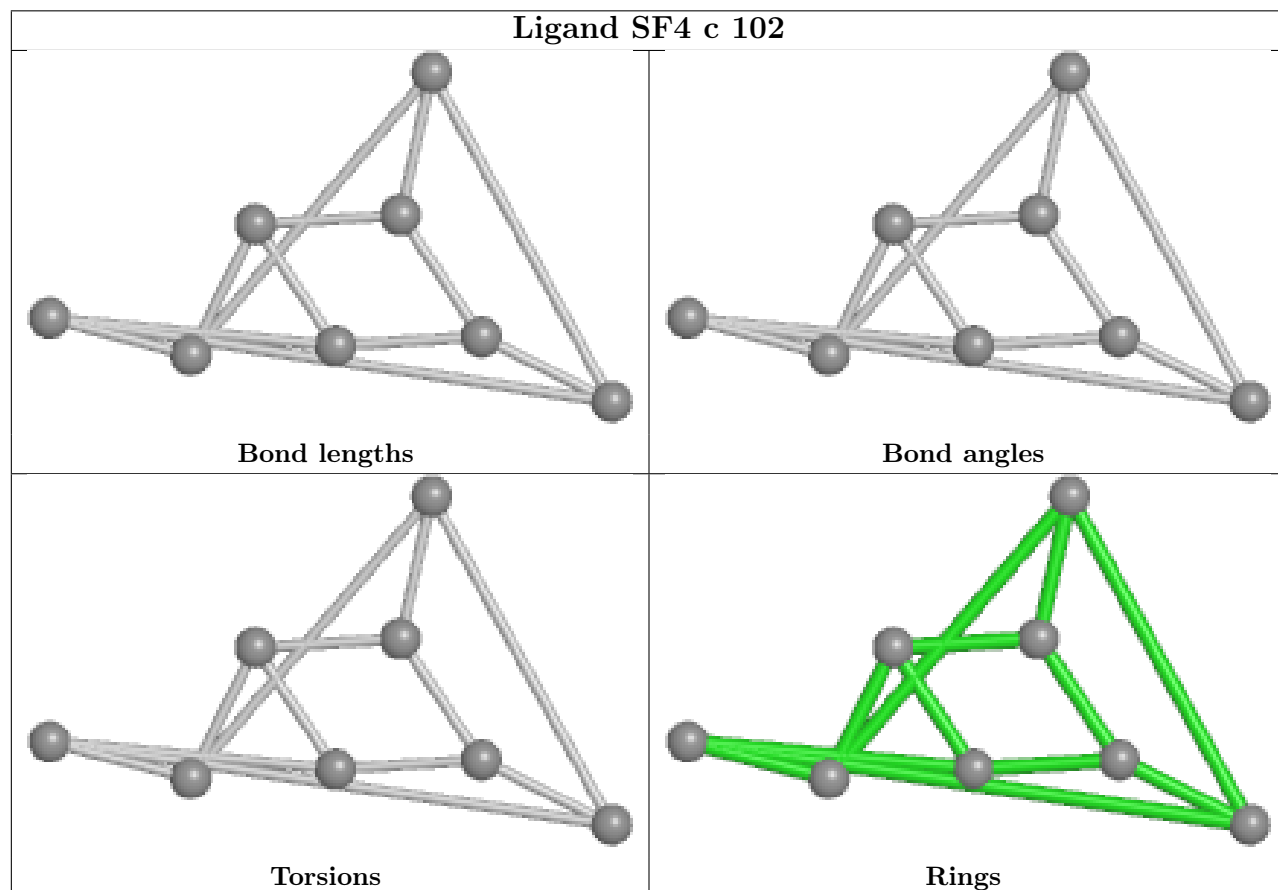
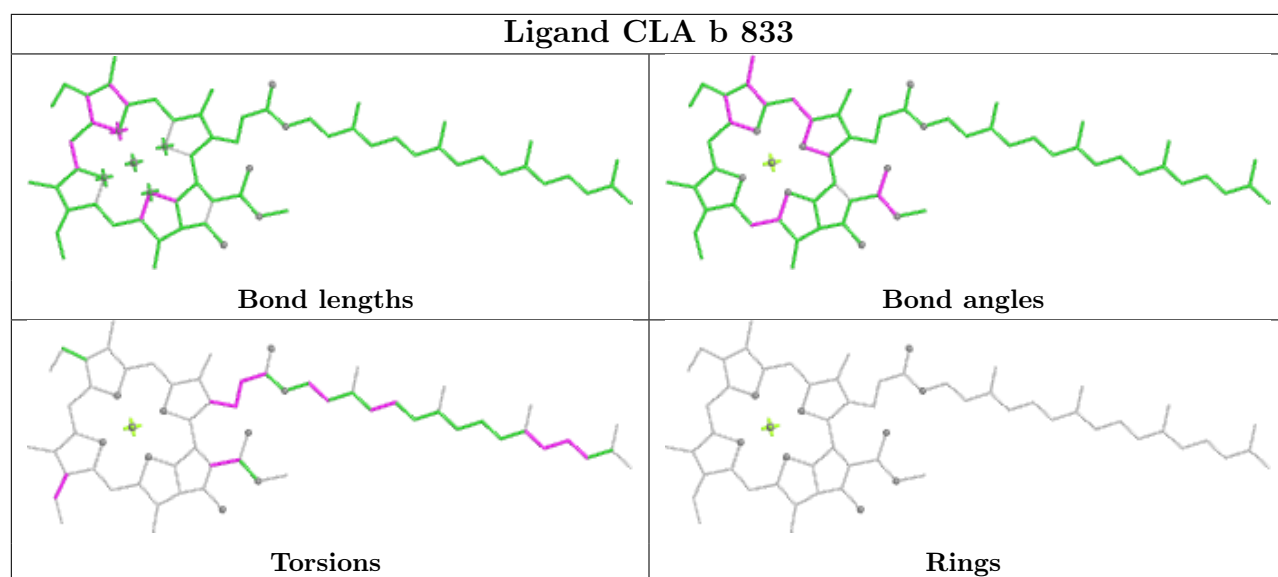
Ligand CLA b 816

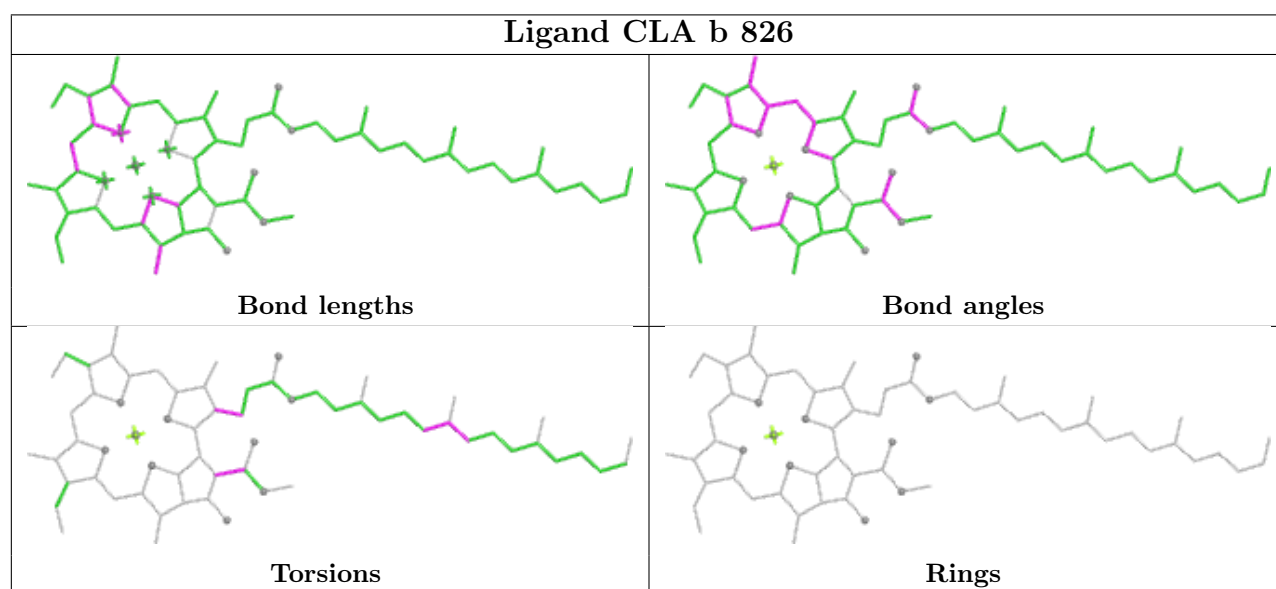
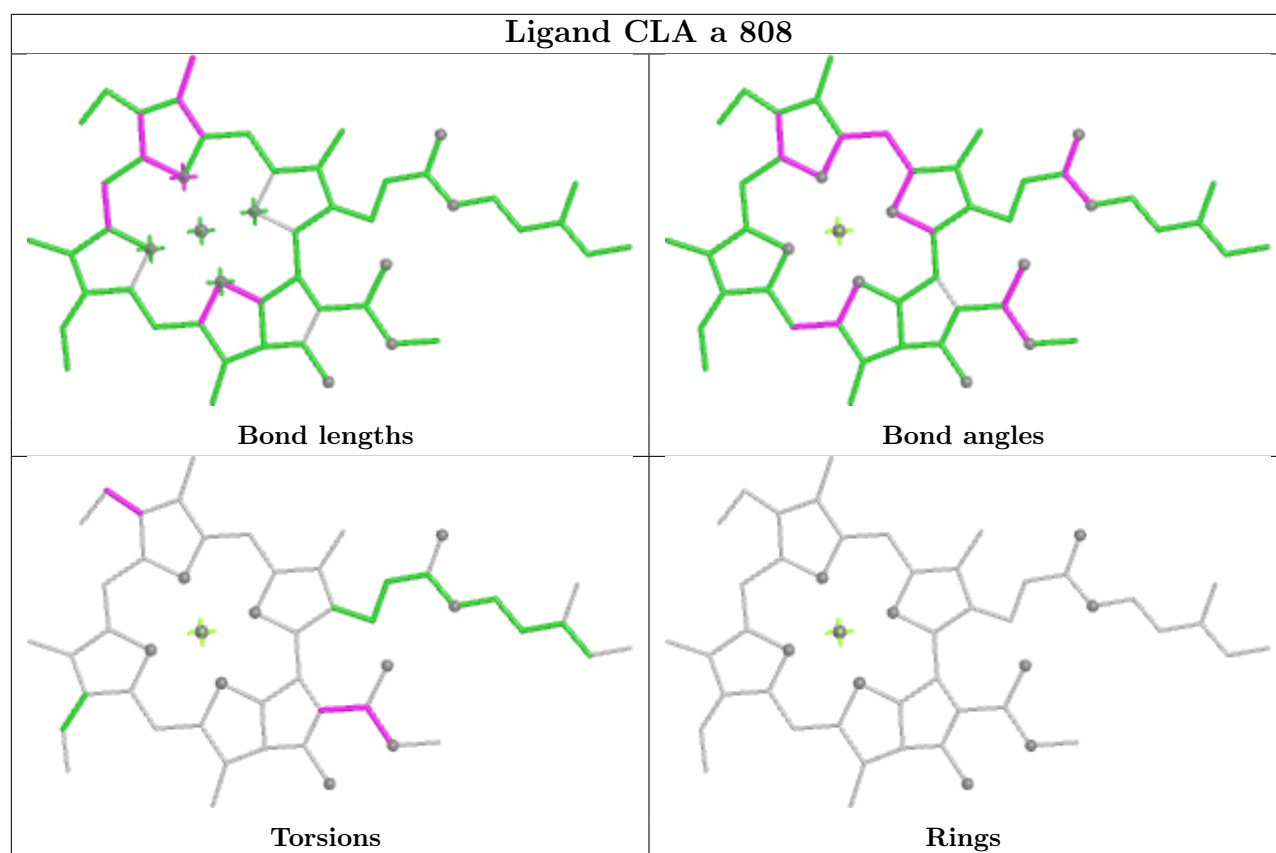


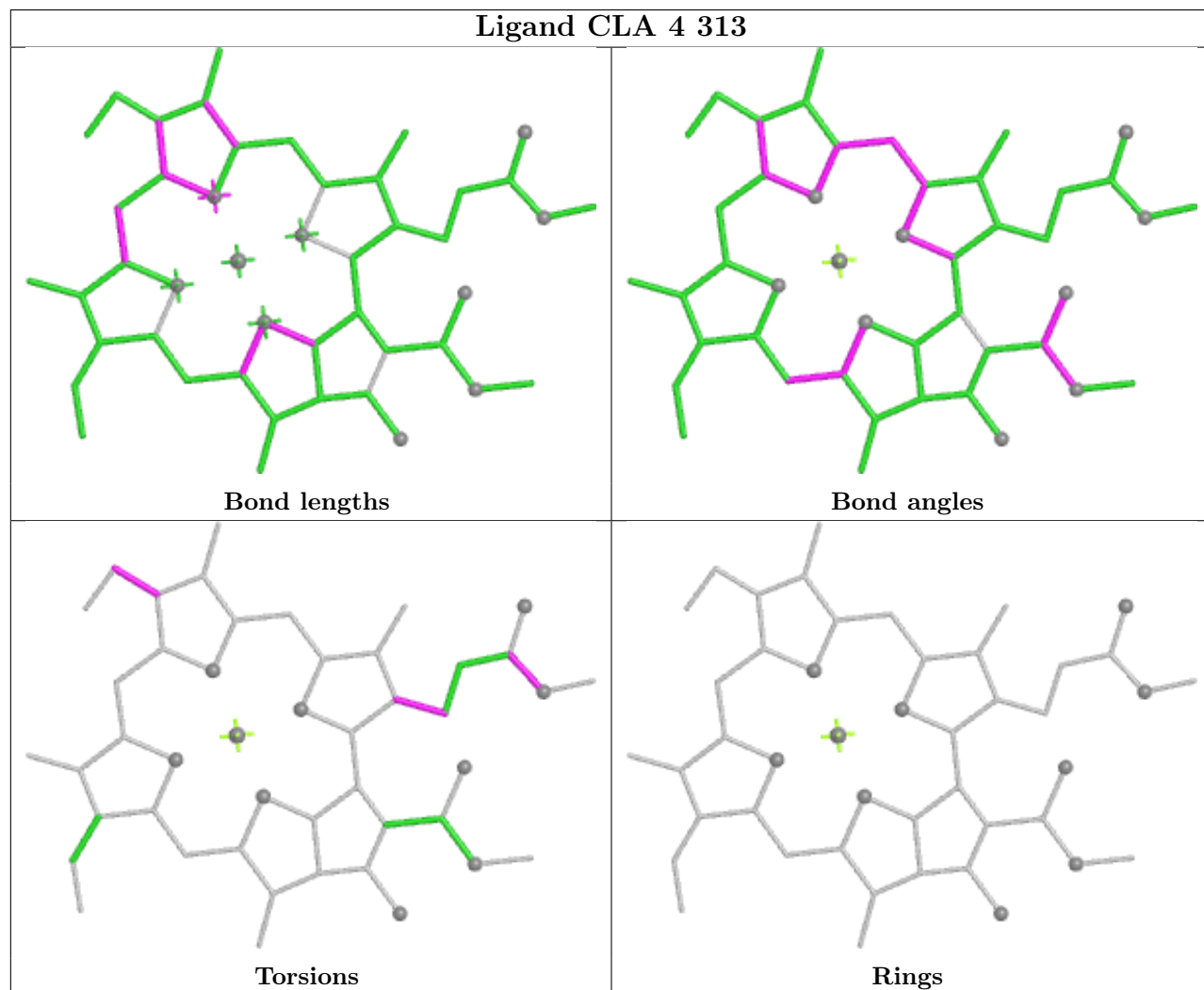
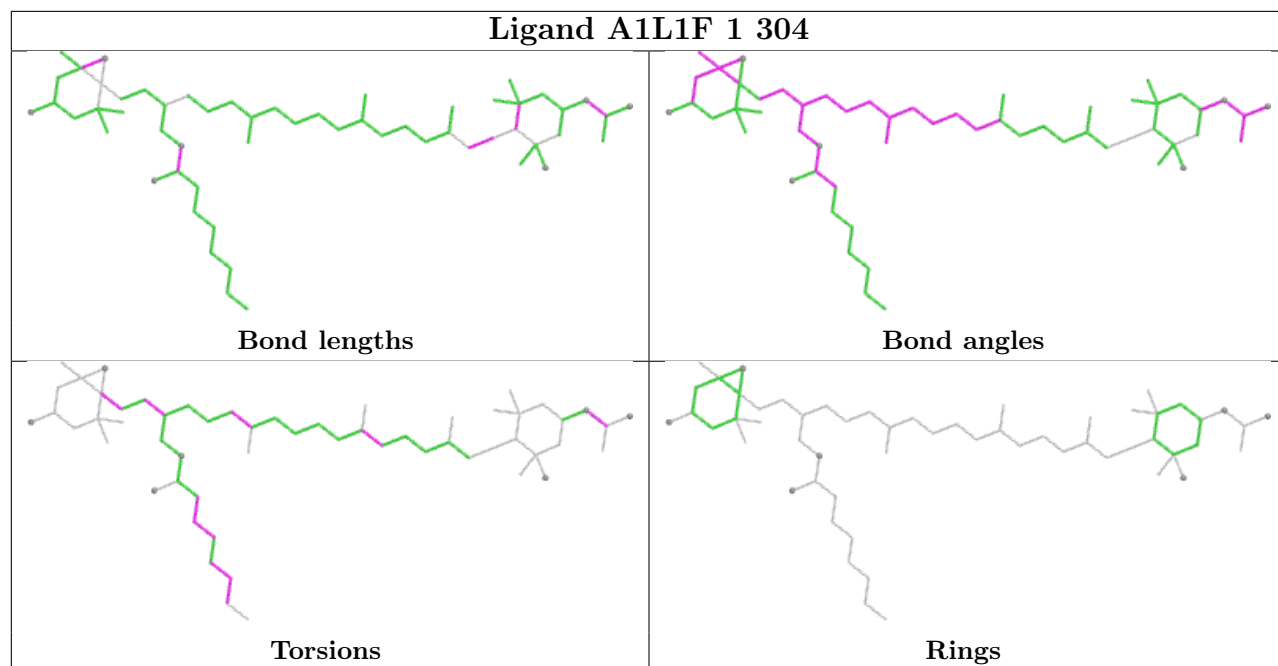
Ligand CLA b 837

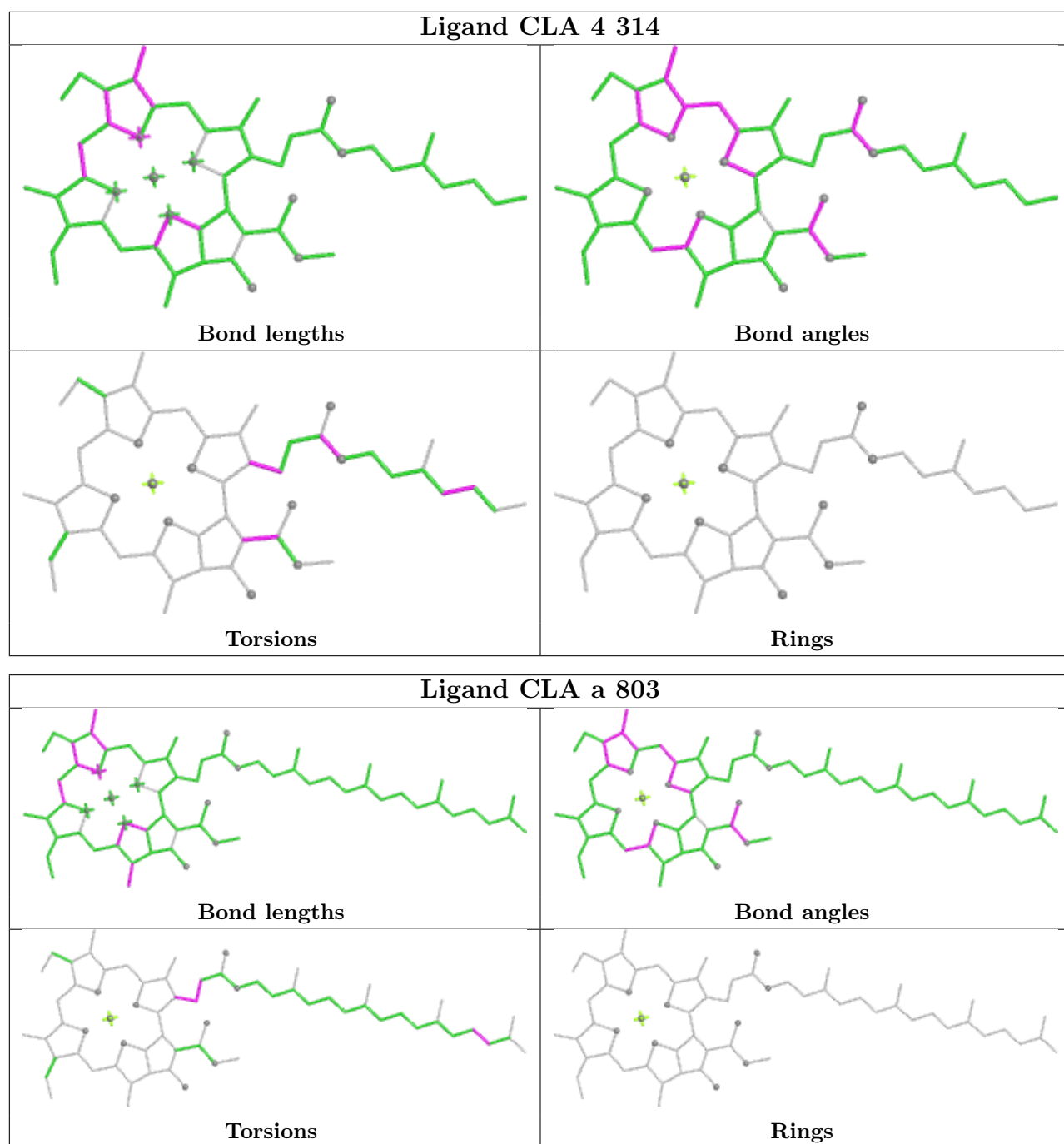


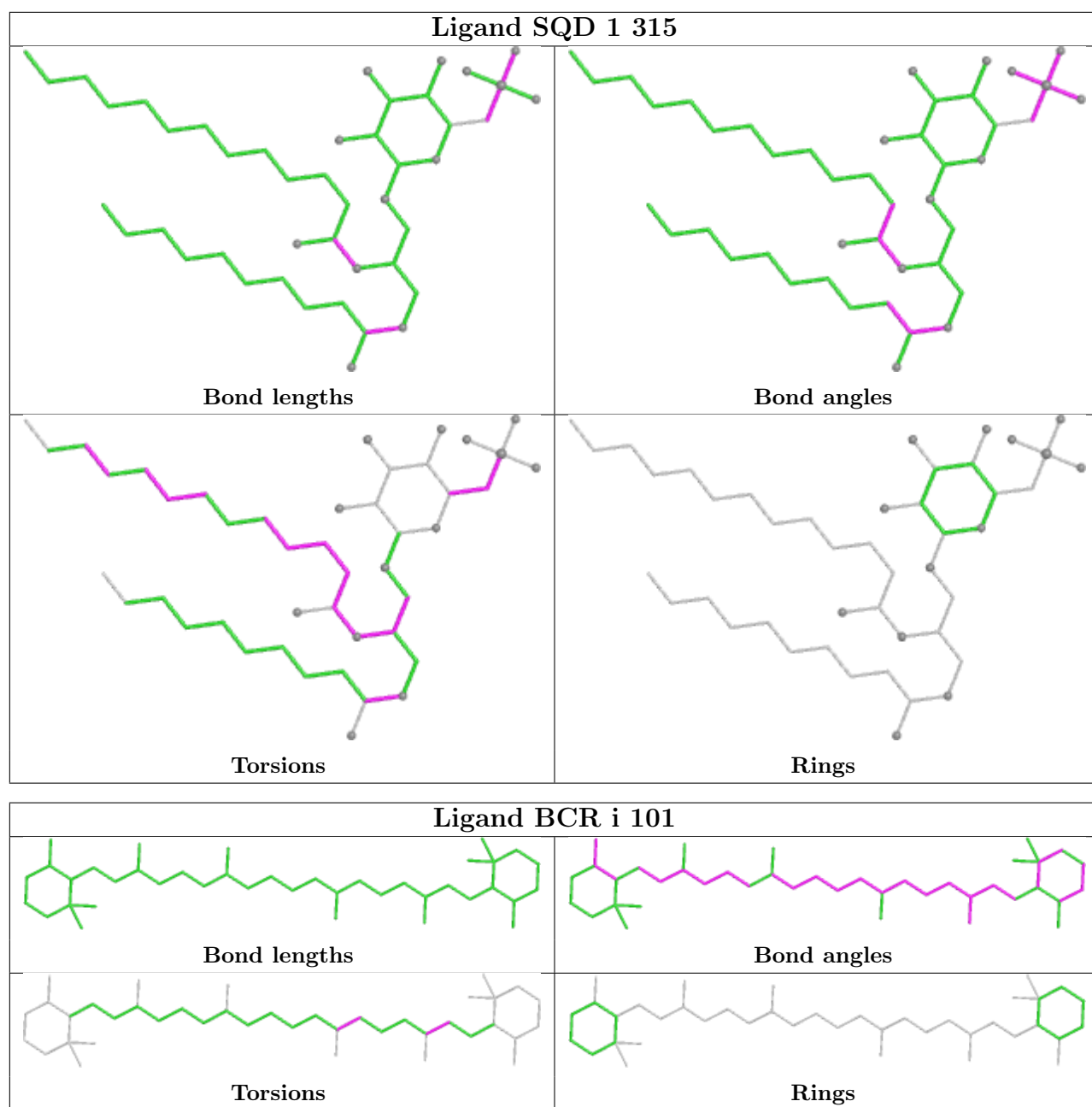


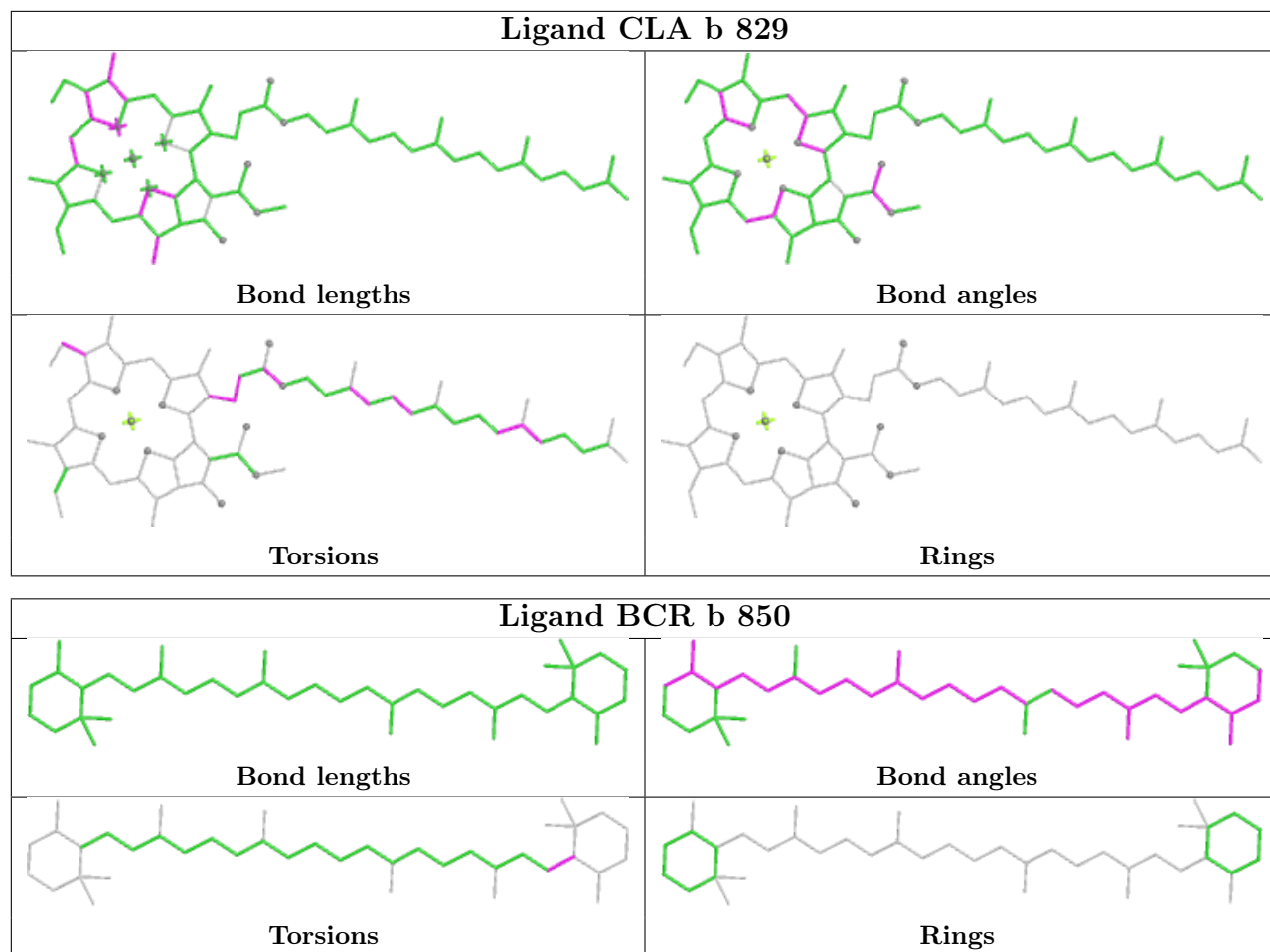




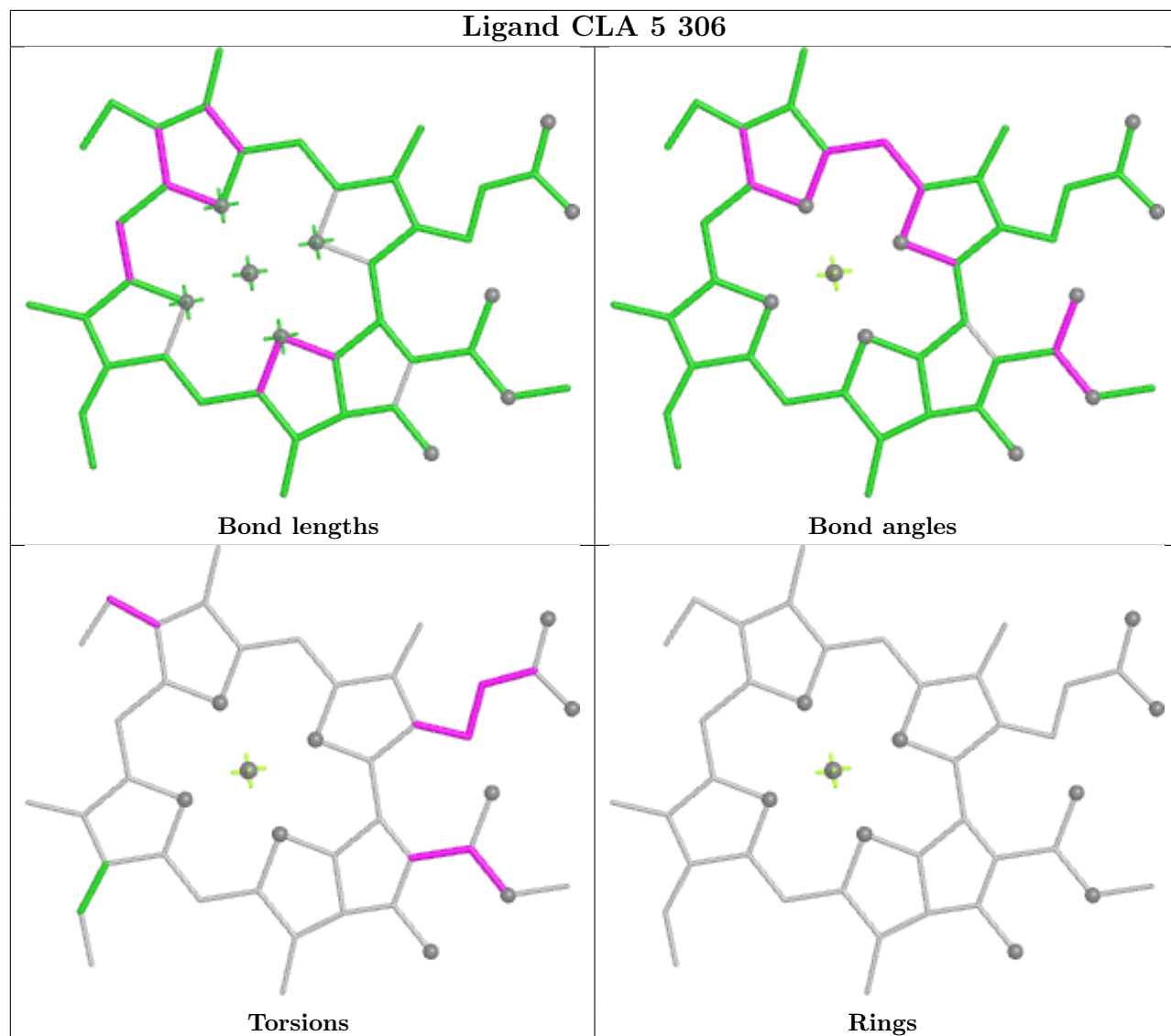




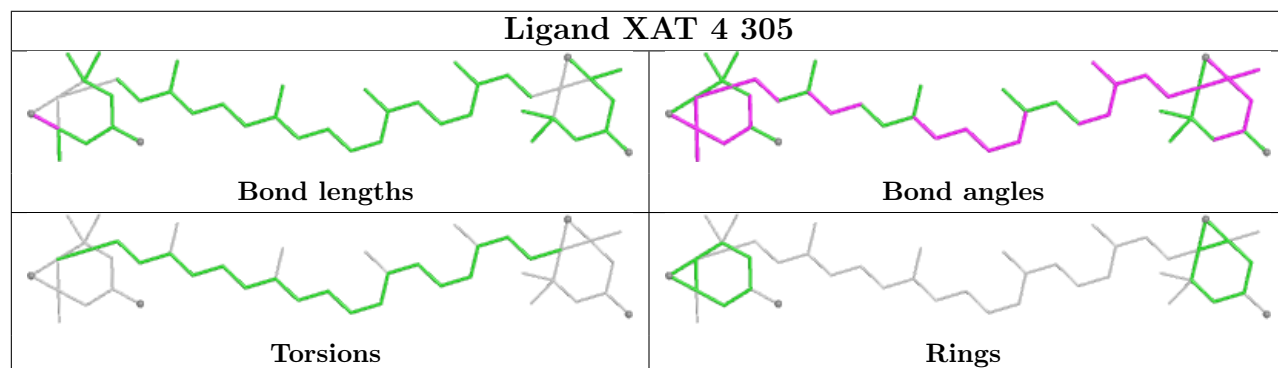




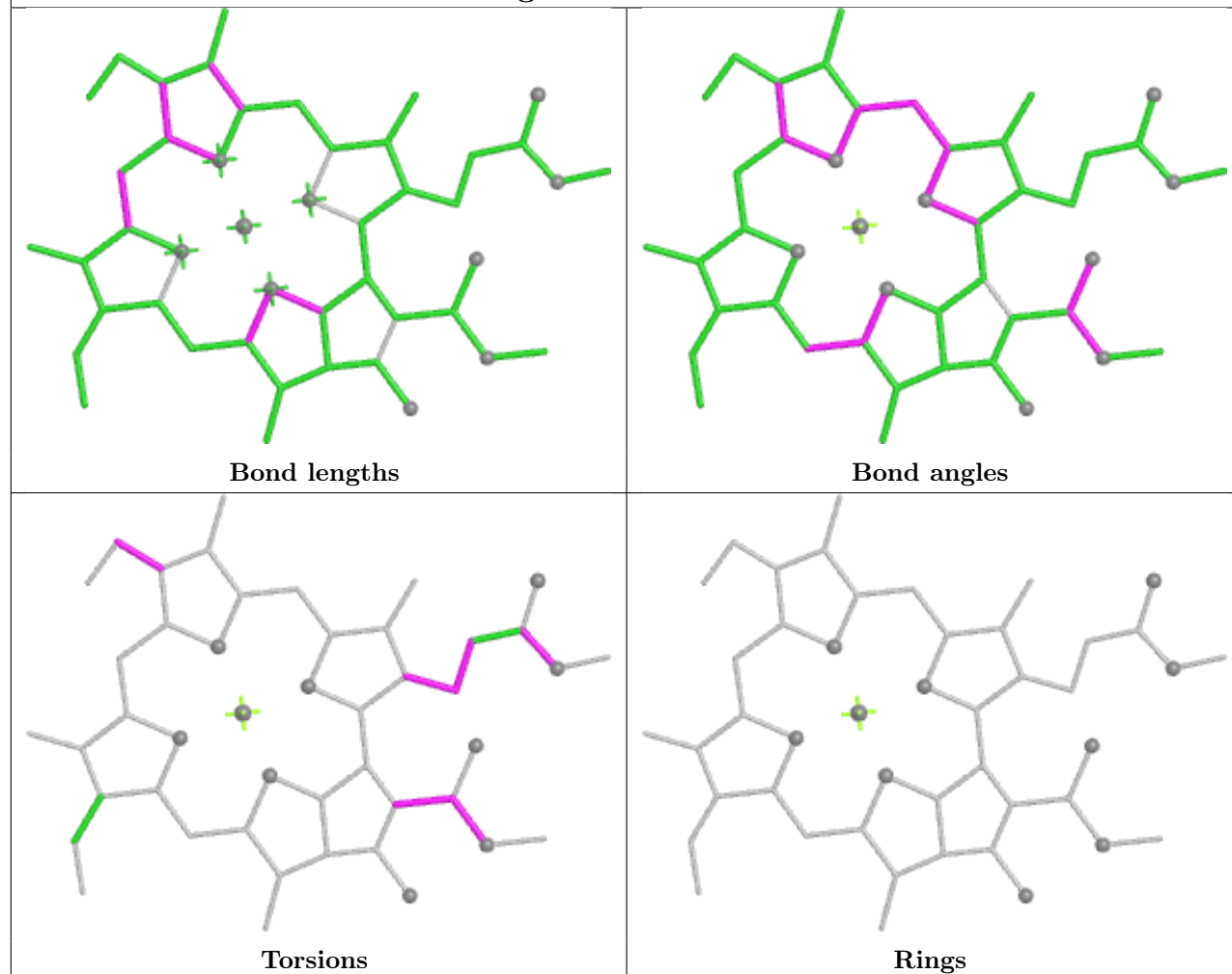
Ligand CLA 5 306



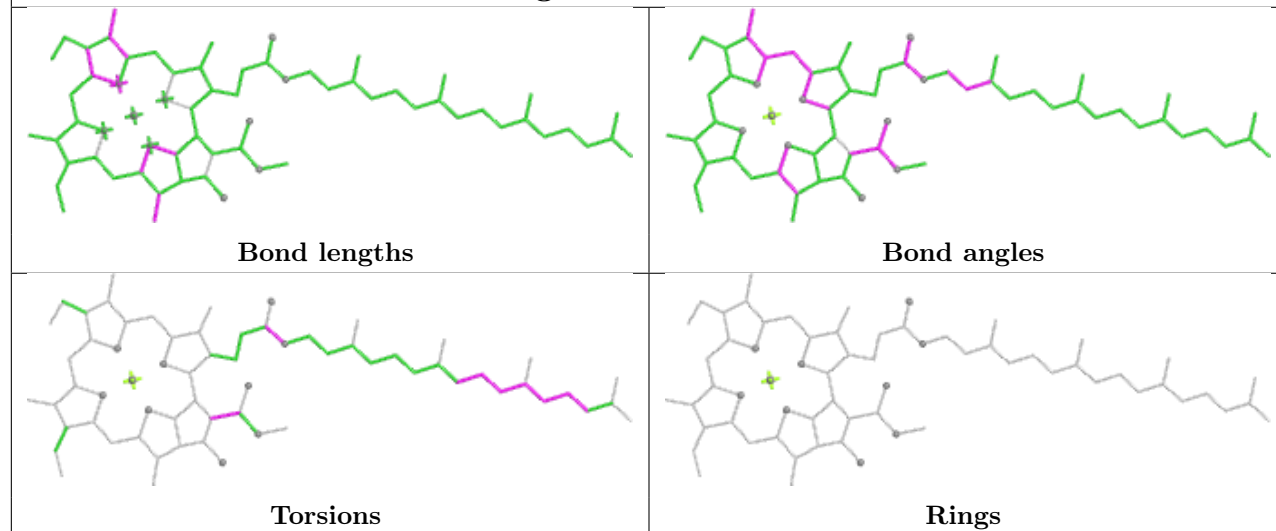
Ligand XAT 4 305

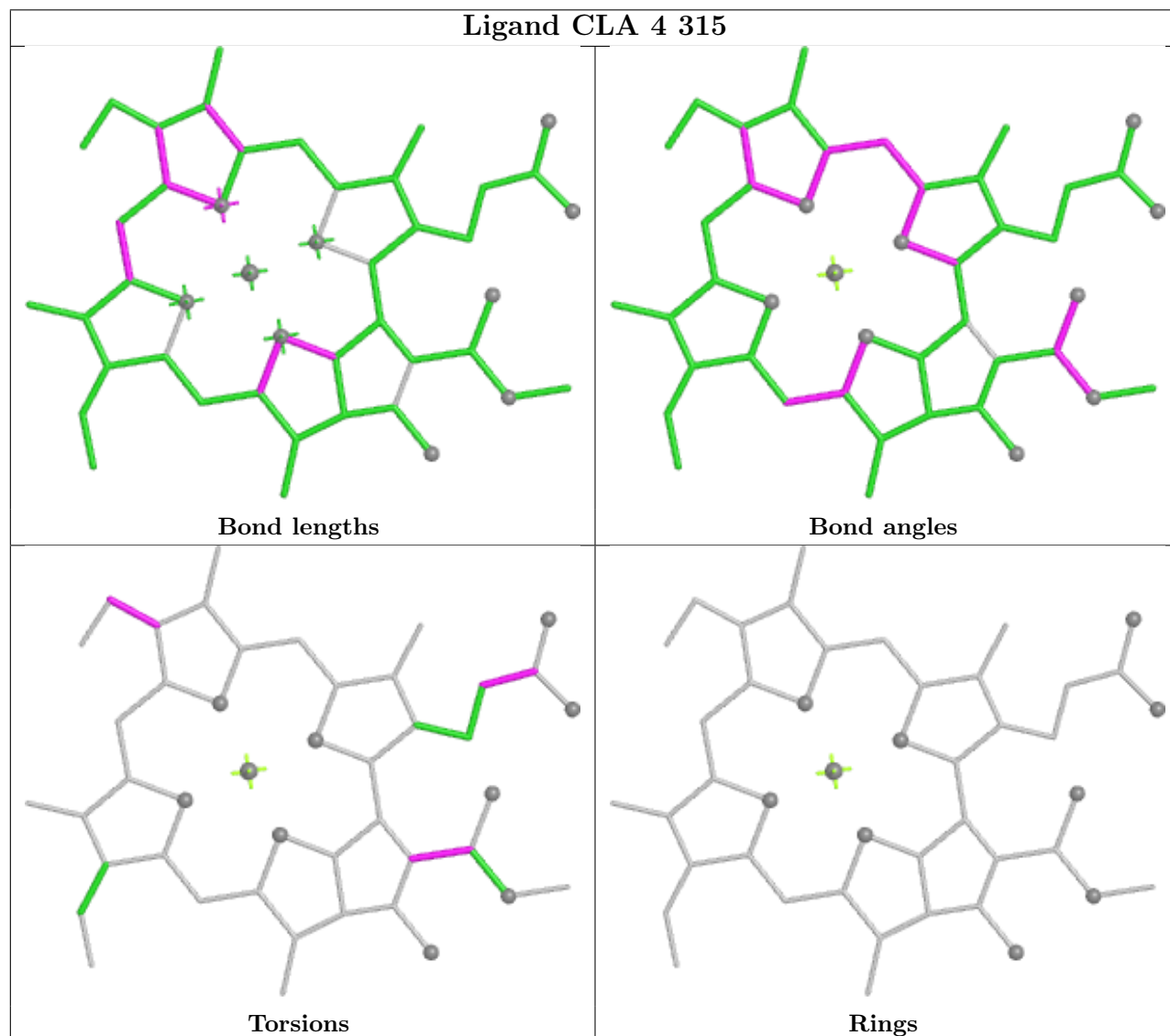
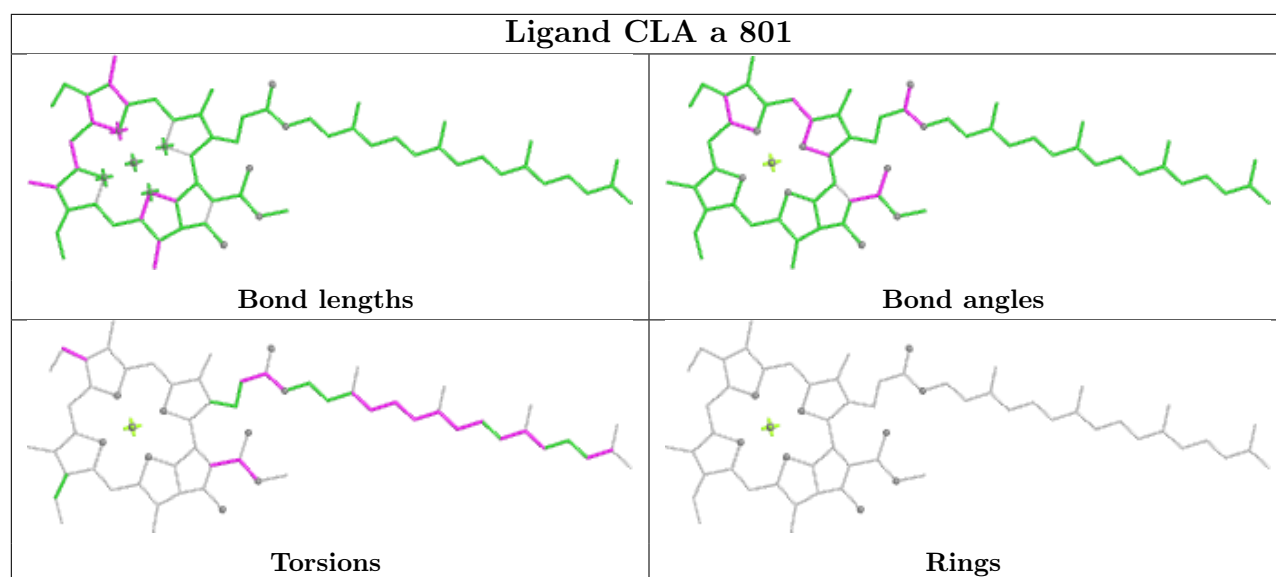


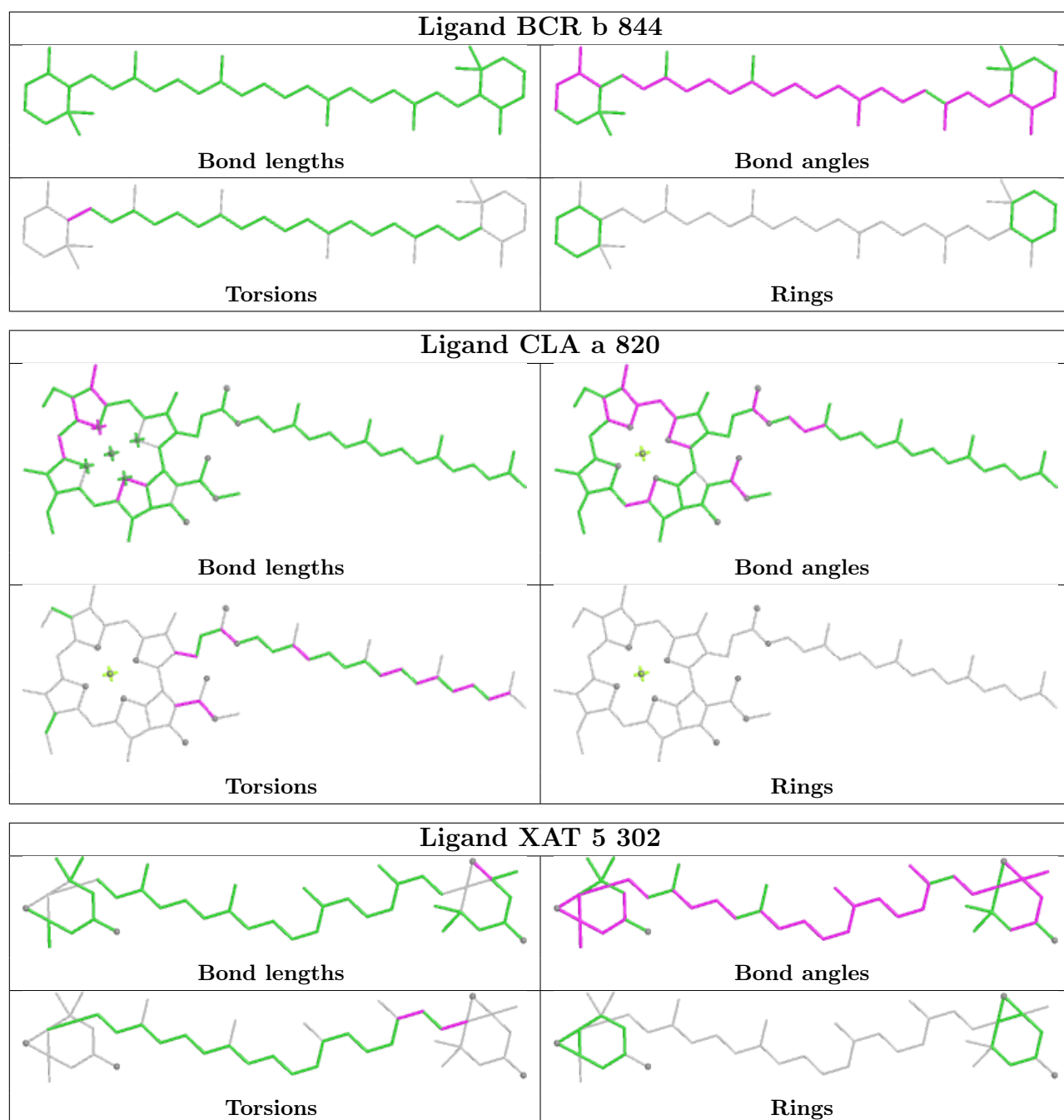
Ligand CLA 4 317



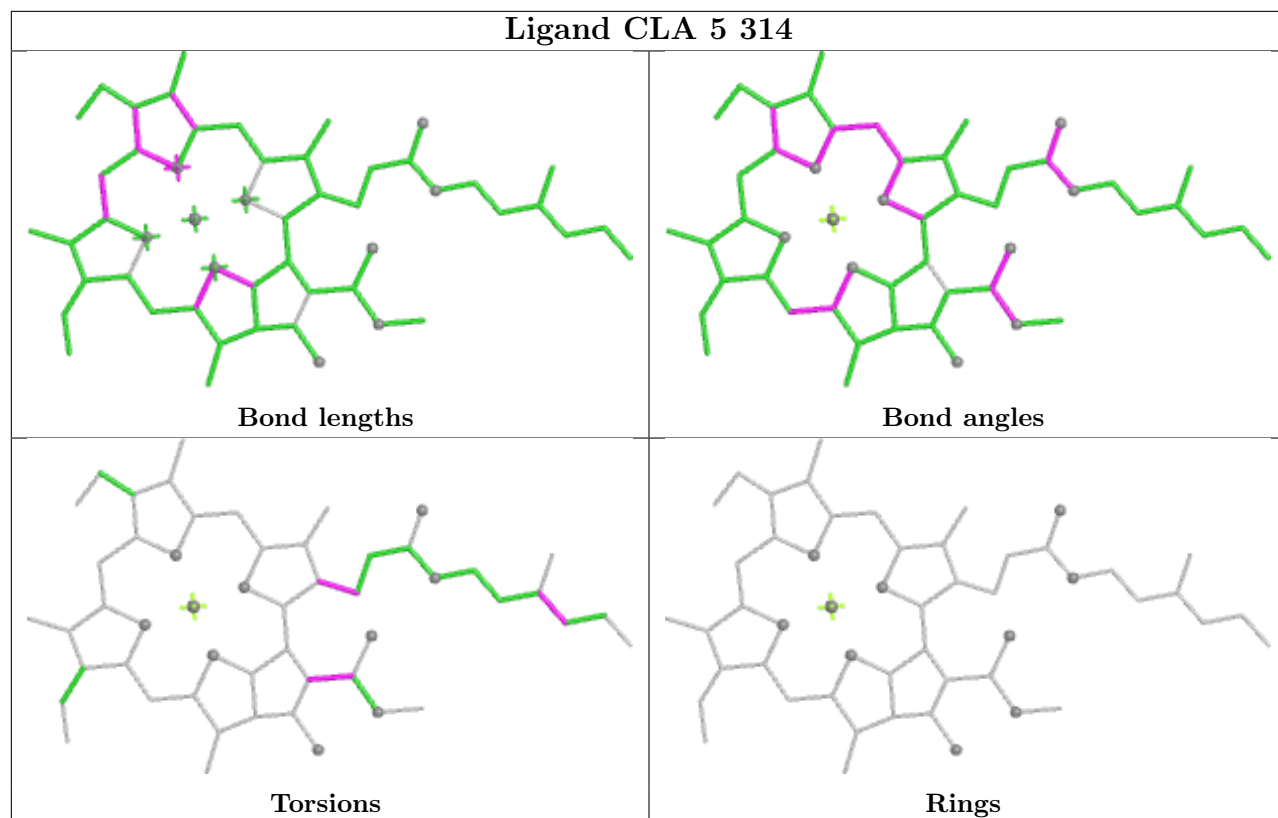
Ligand CLA b 830



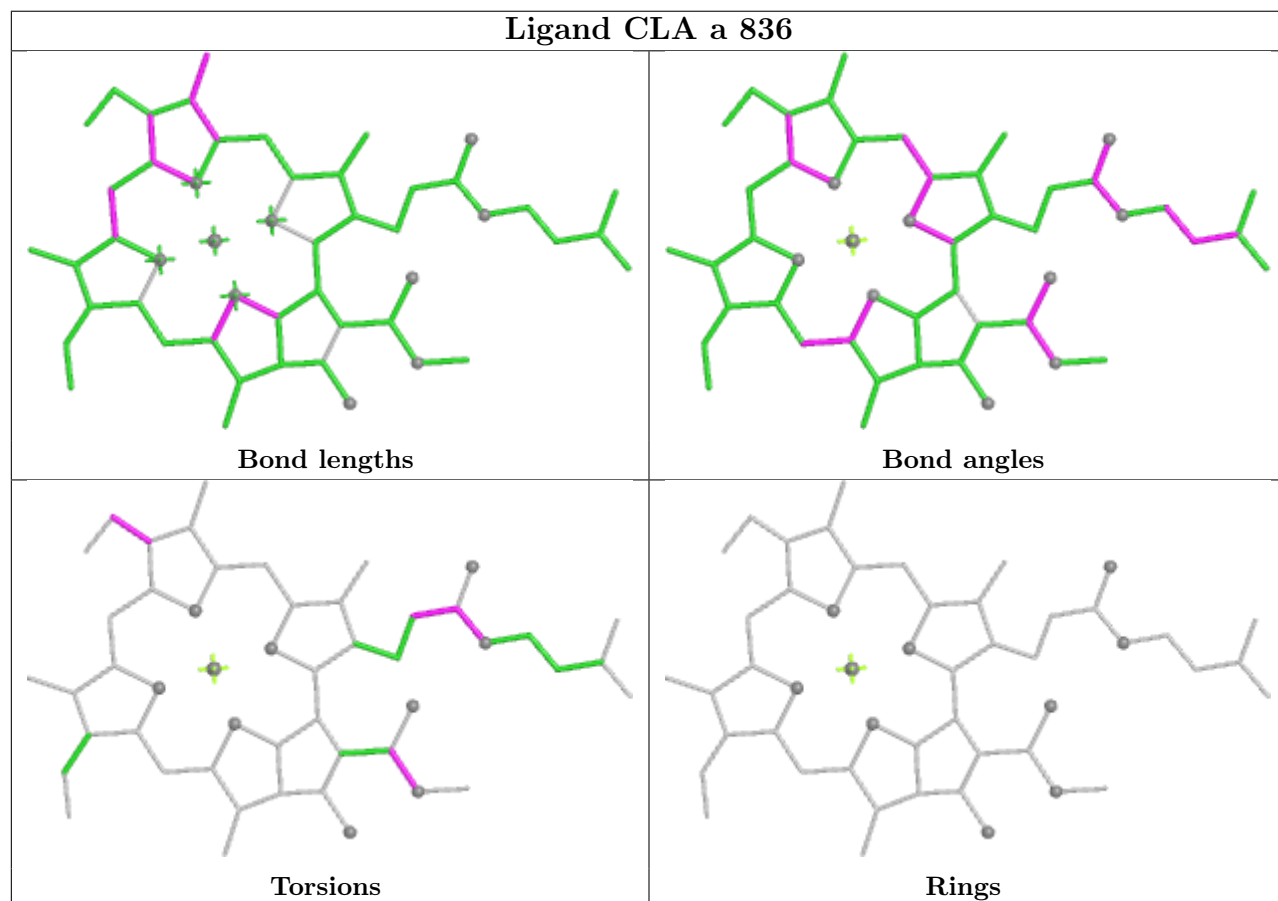


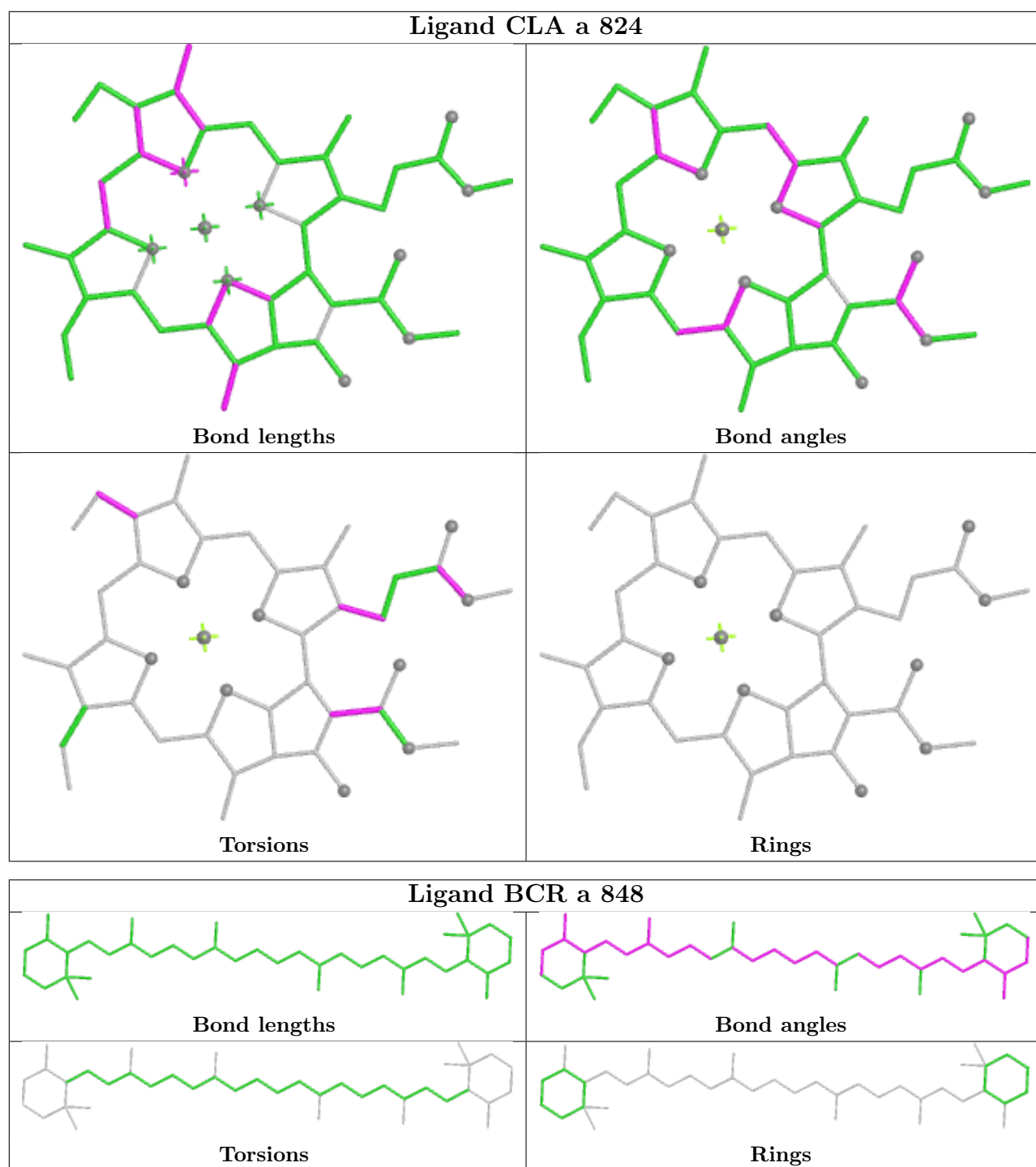


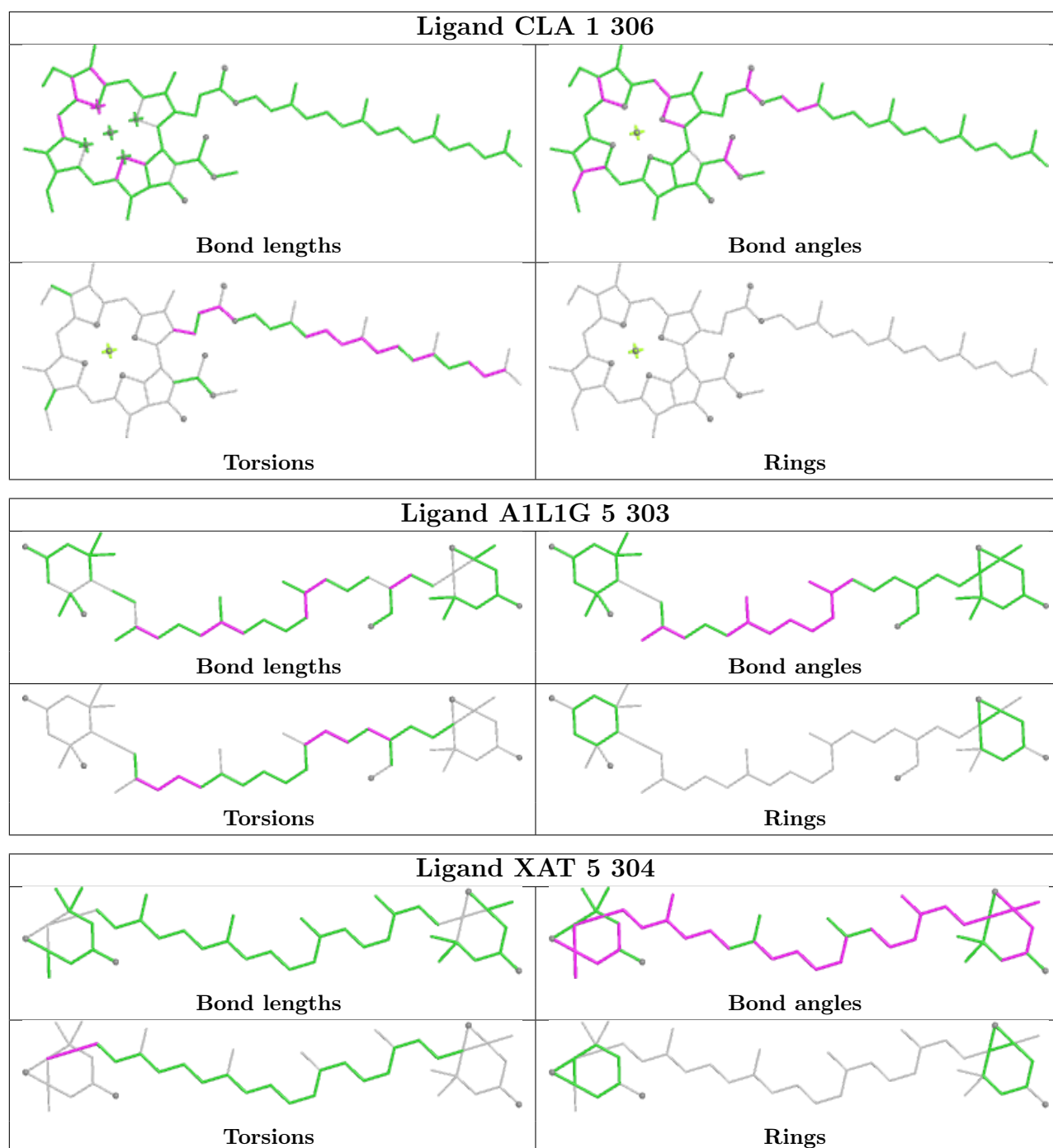
Ligand CLA 5 314

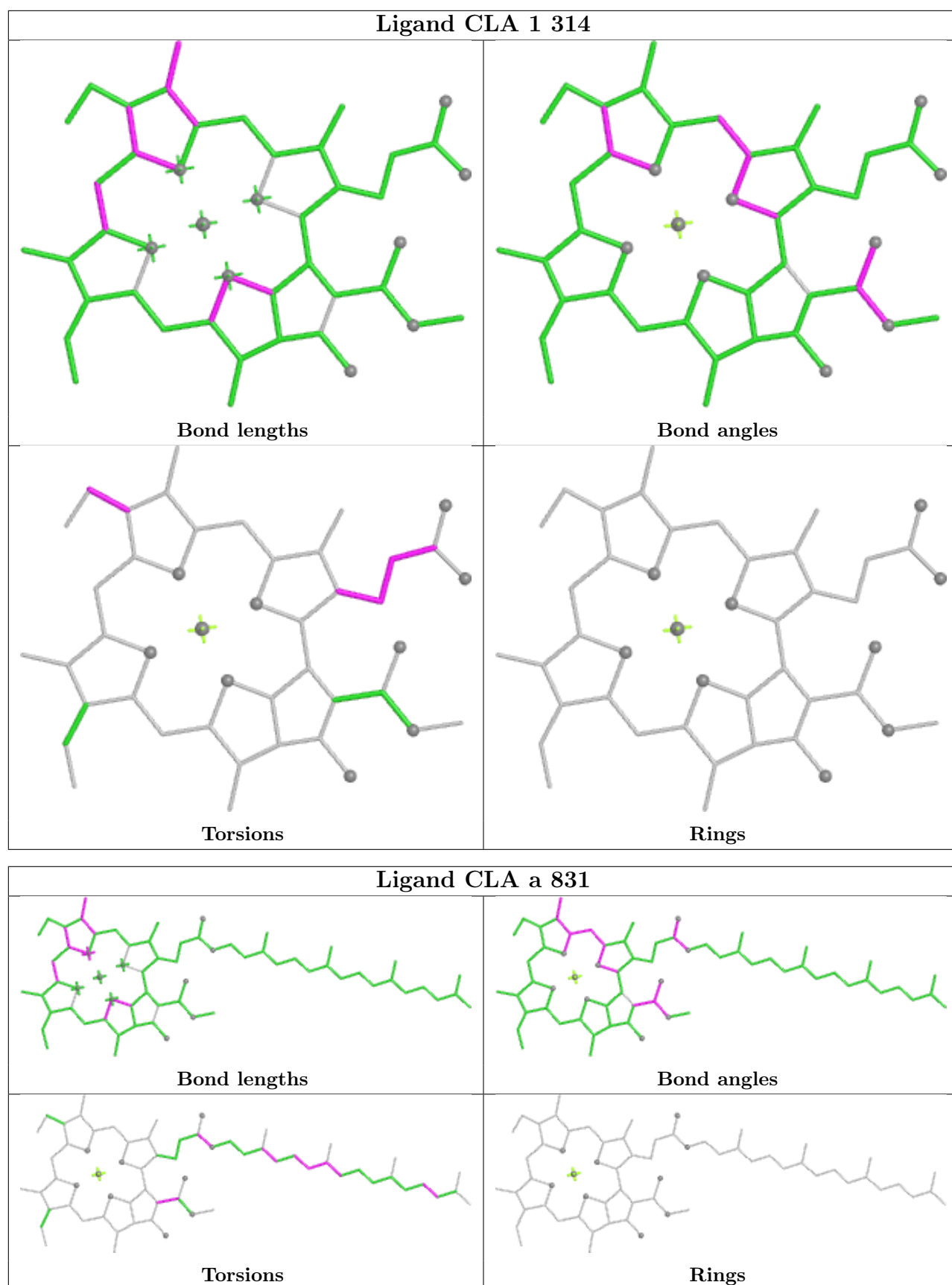


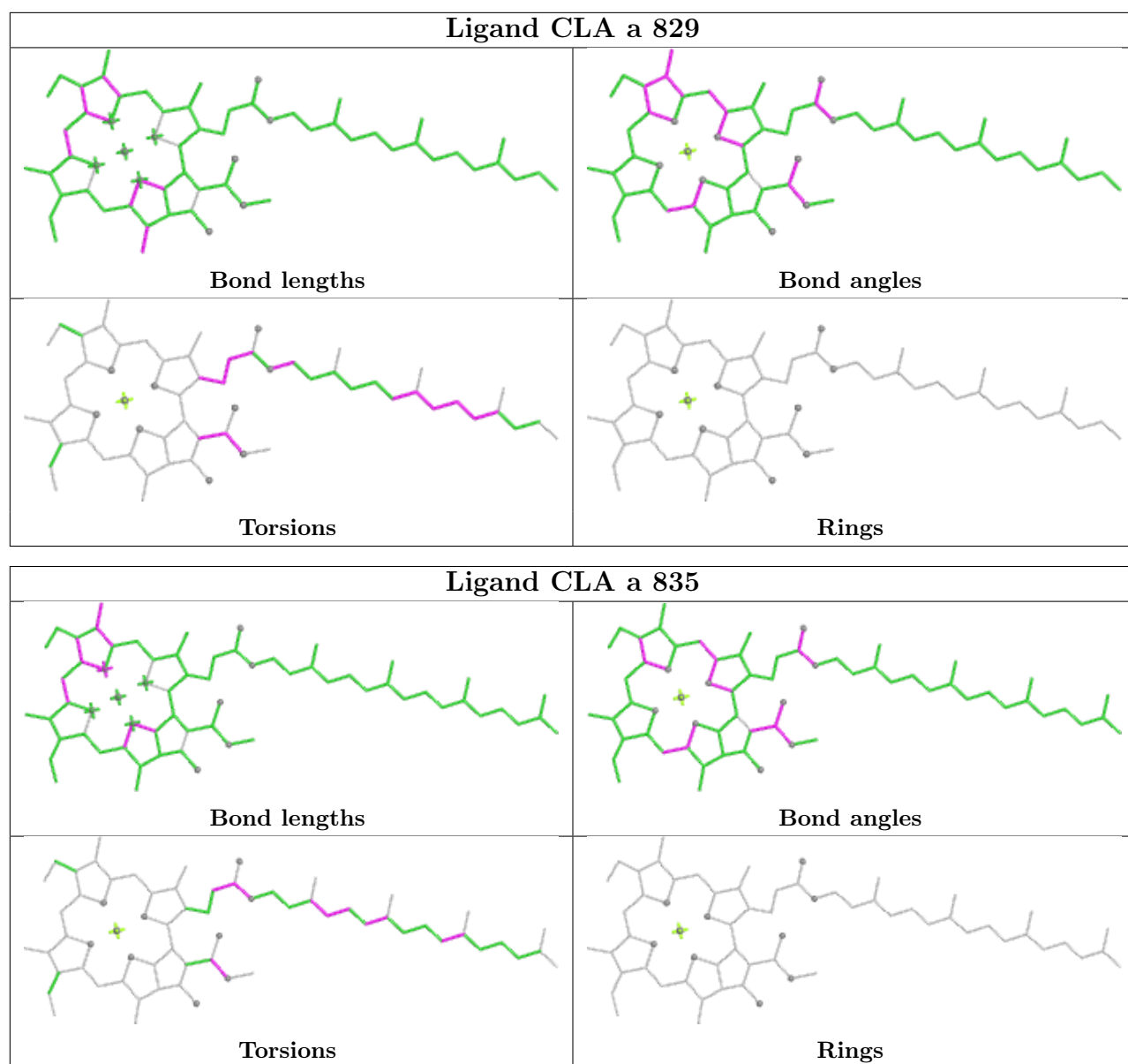
Ligand CLA a 836

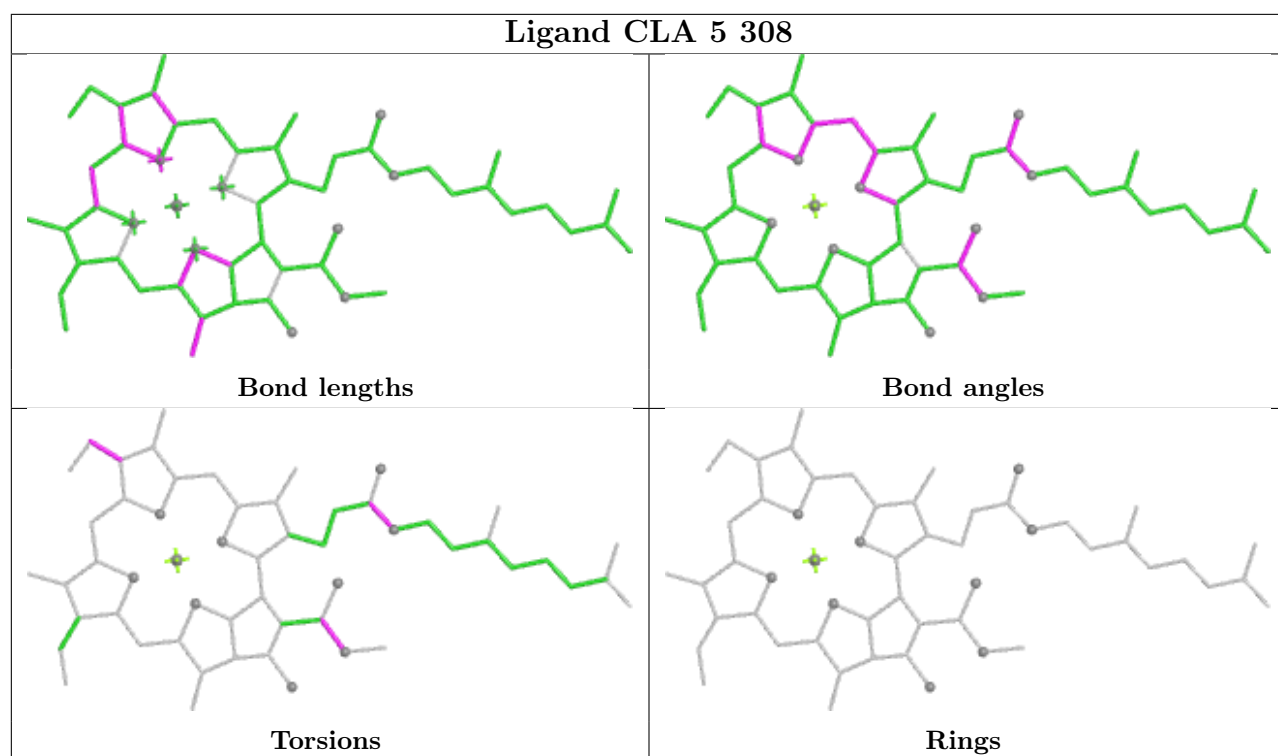




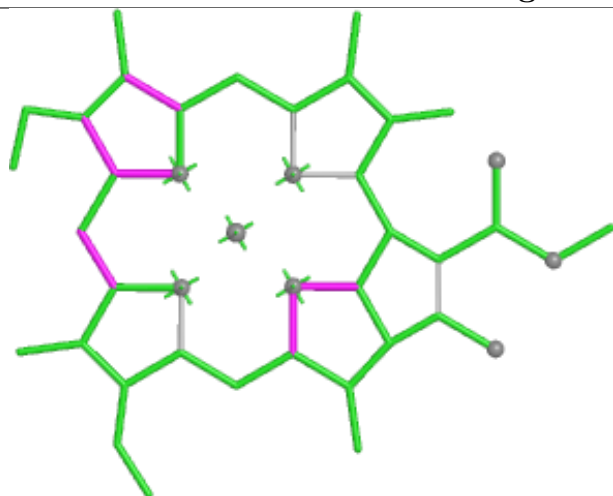




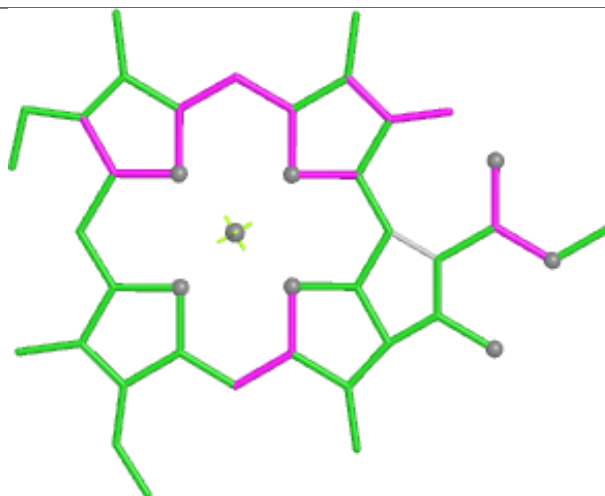




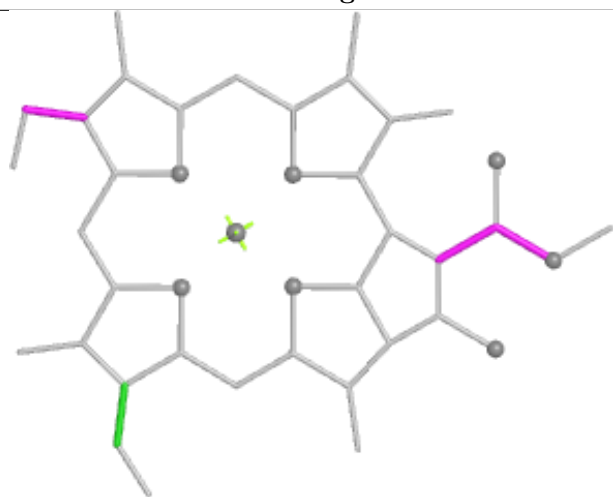
Ligand CLA 4 316



Bond lengths



Bond angles

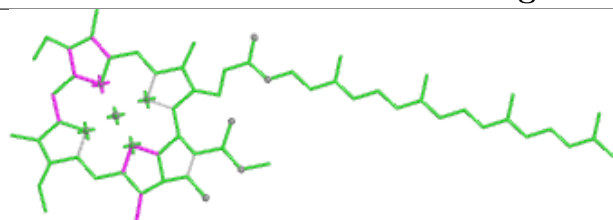


Torsions

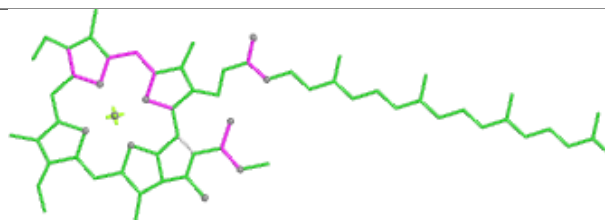


Rings

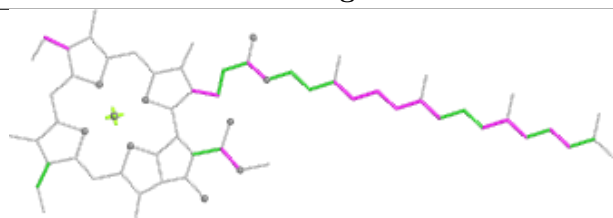
Ligand CLA a 807



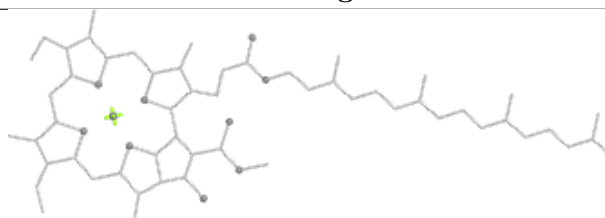
Bond lengths



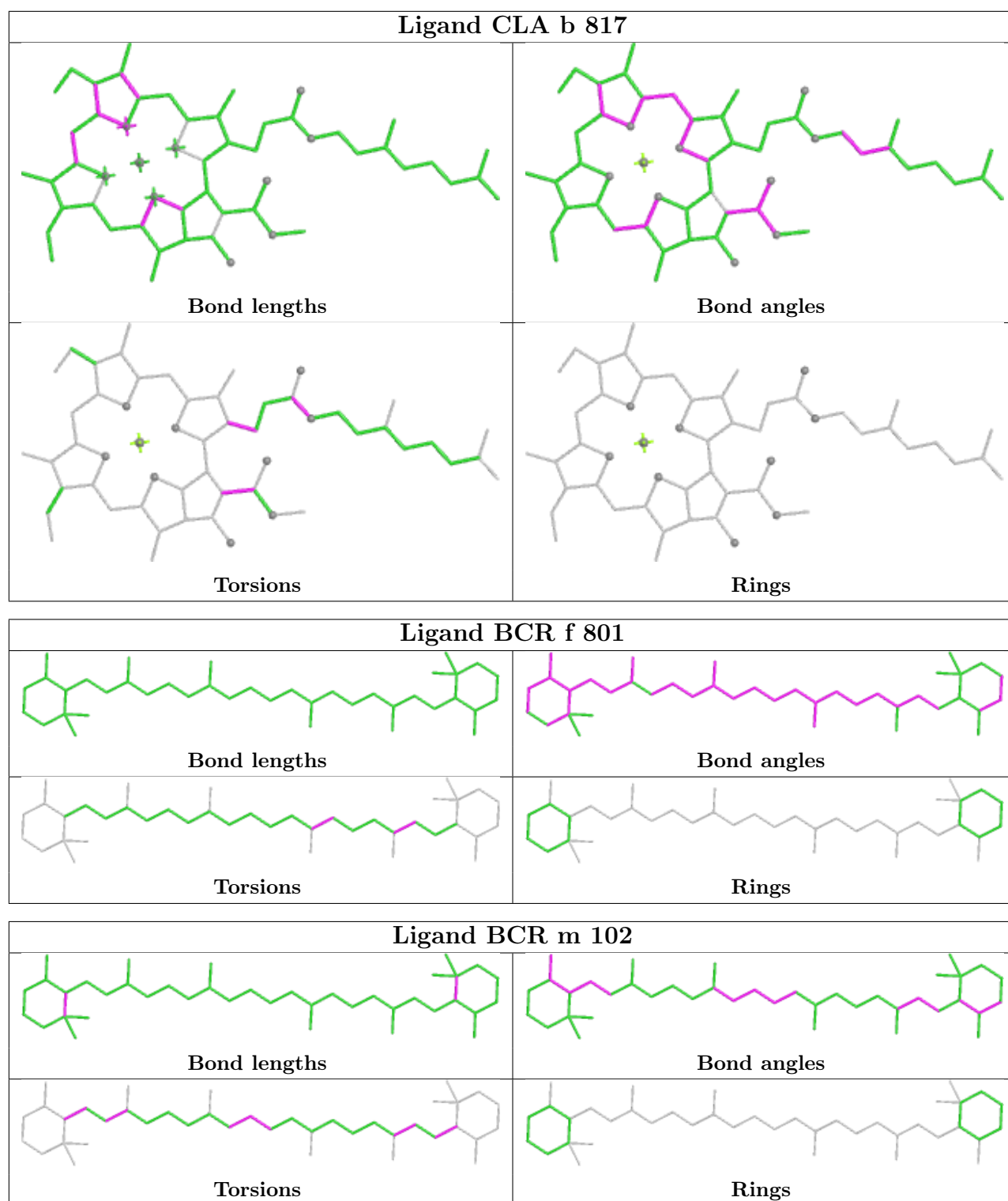
Bond angles

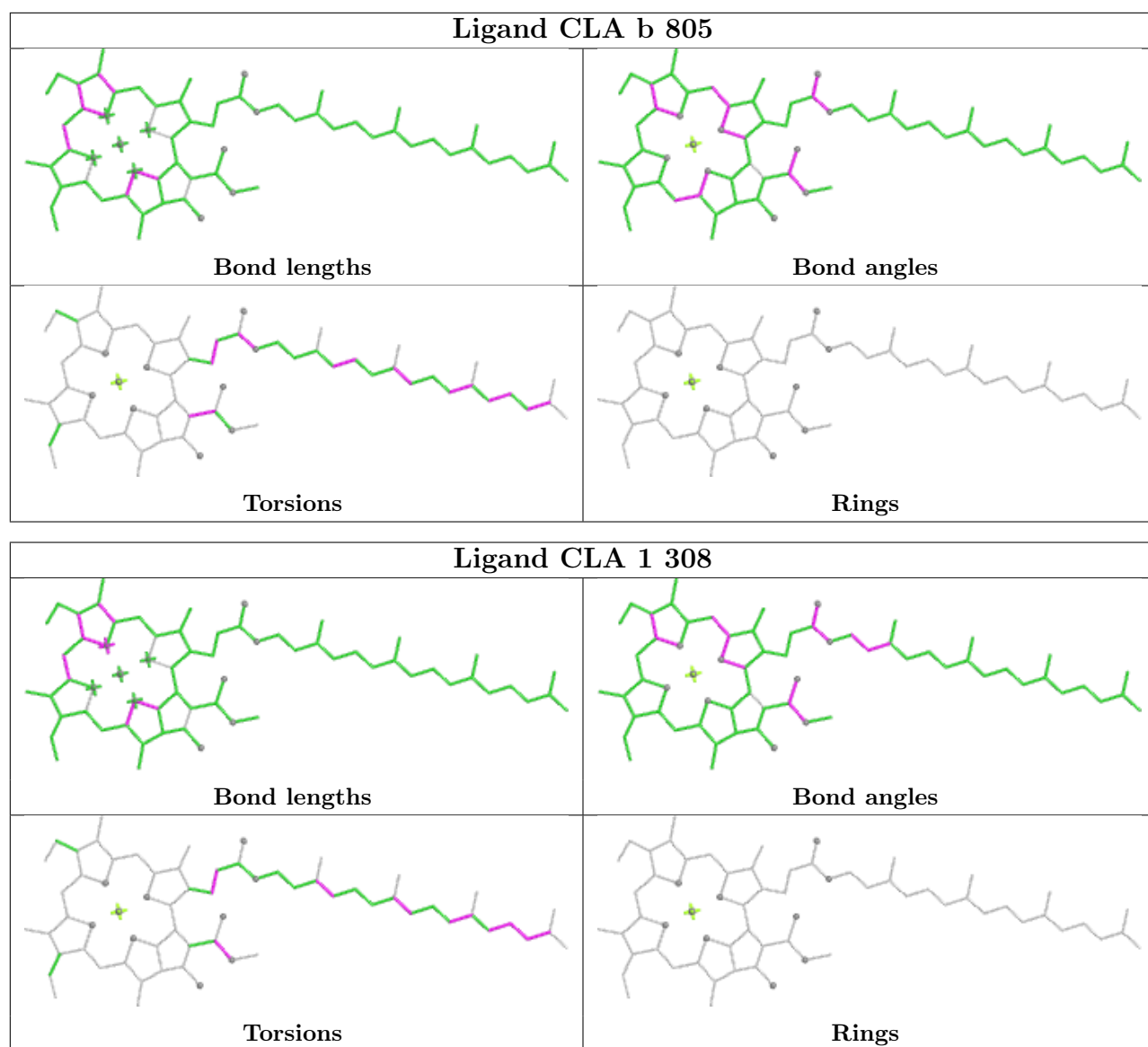


Torsions

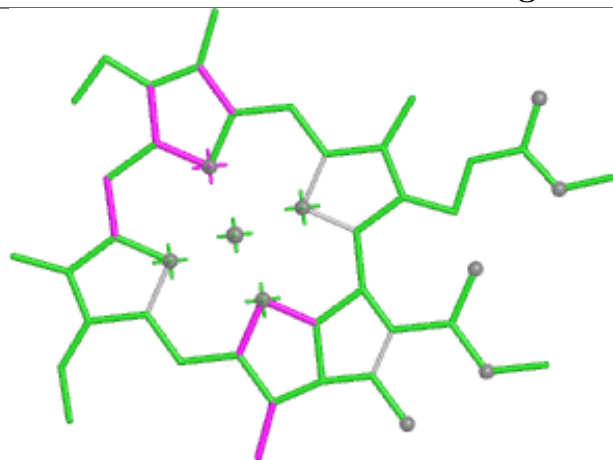


Rings

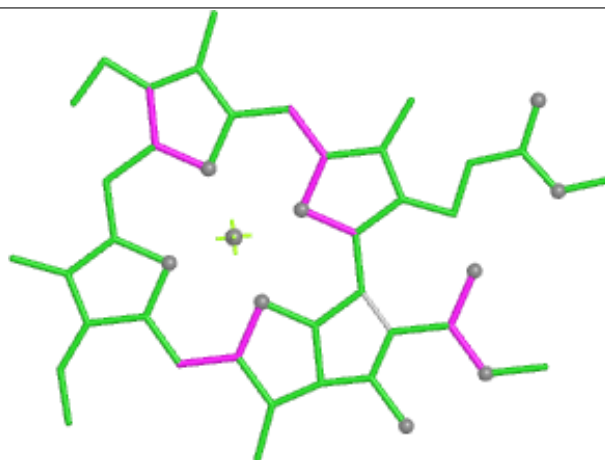




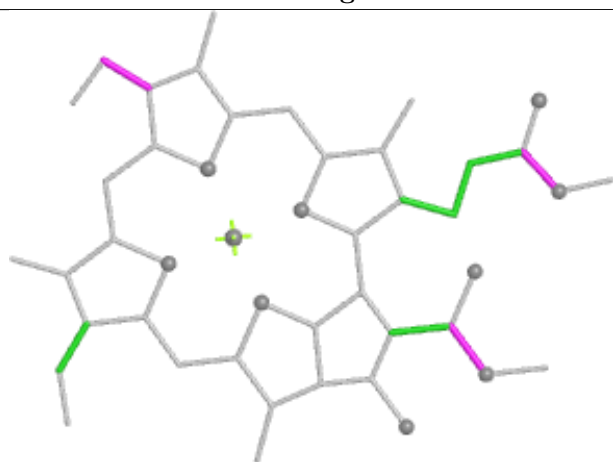
Ligand CLA 5 305



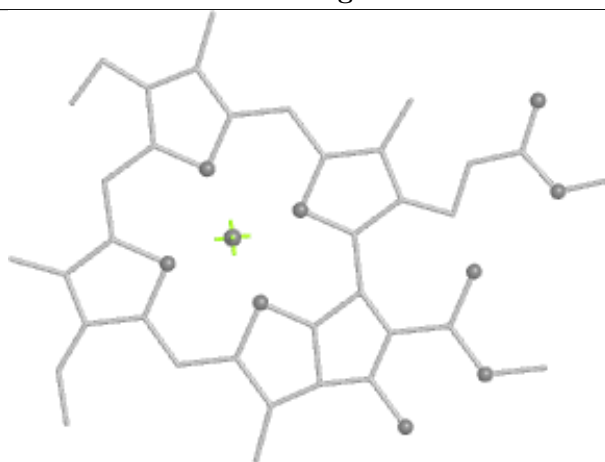
Bond lengths



Bond angles

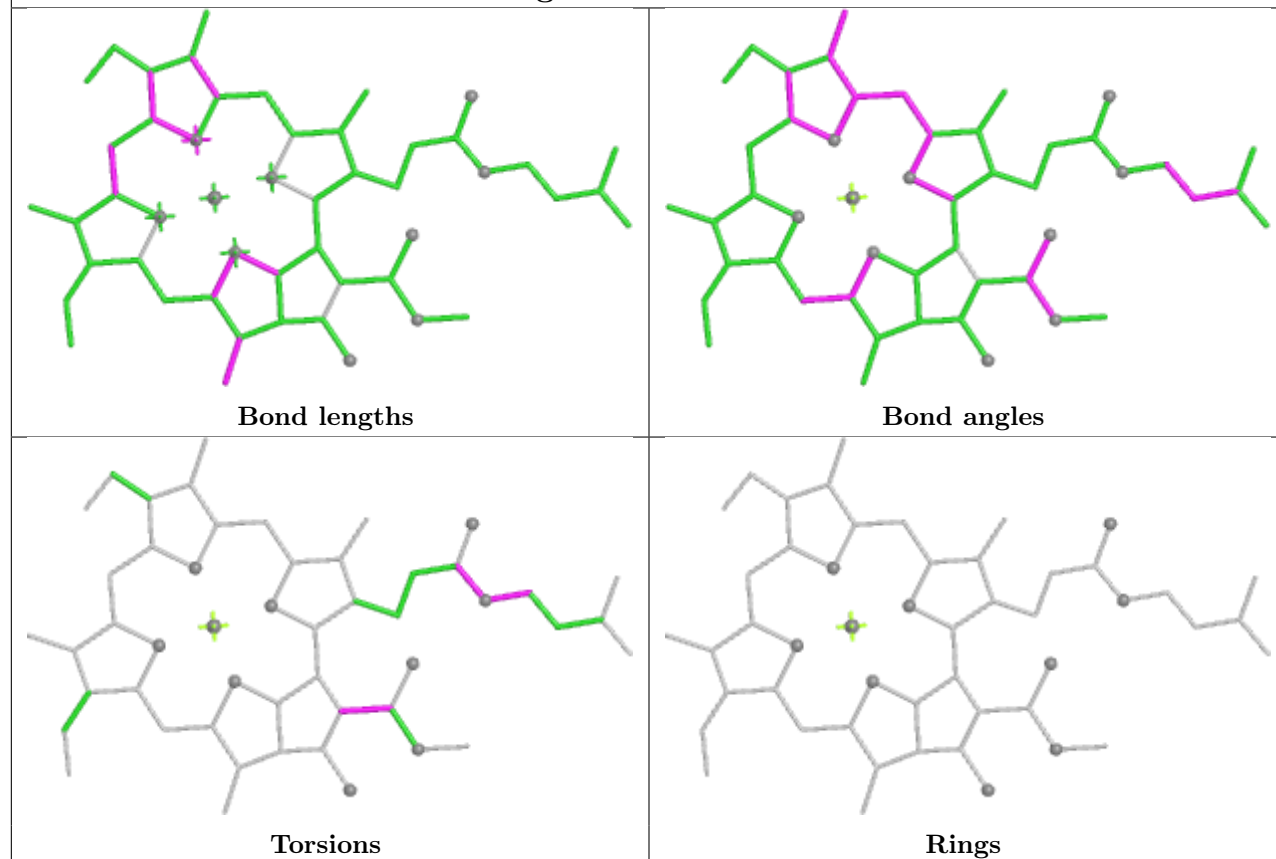


Torsions

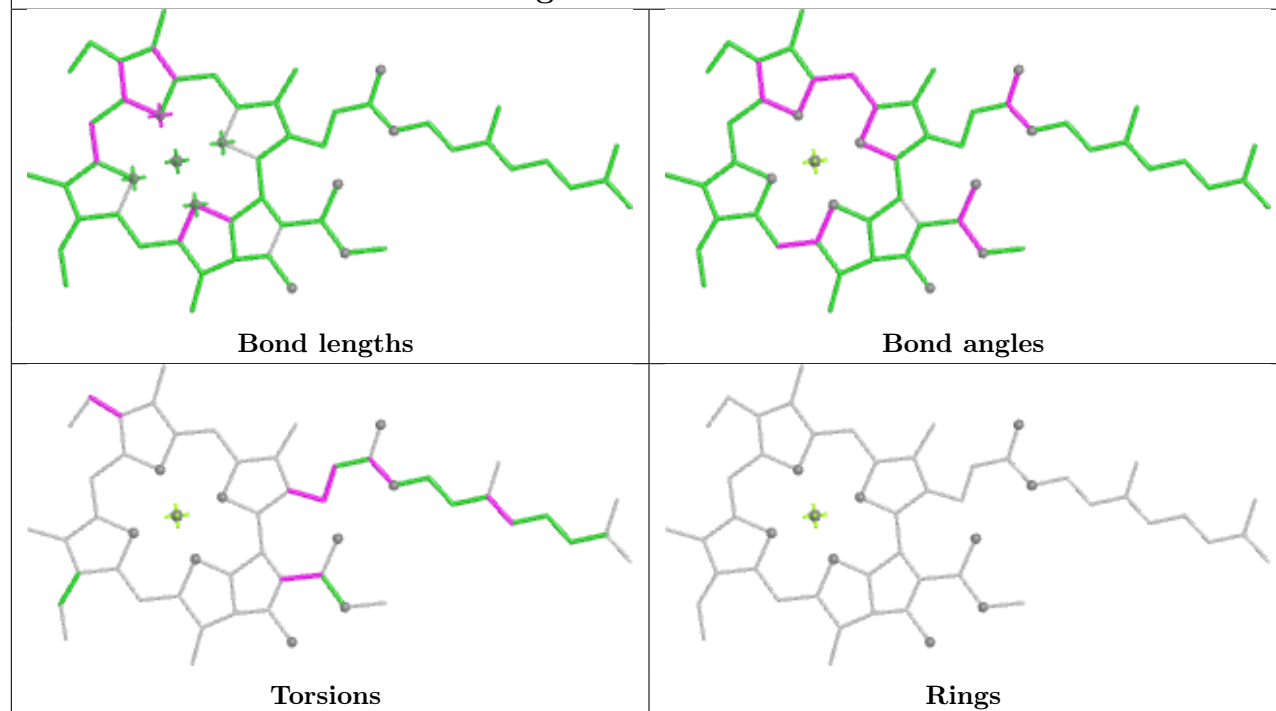


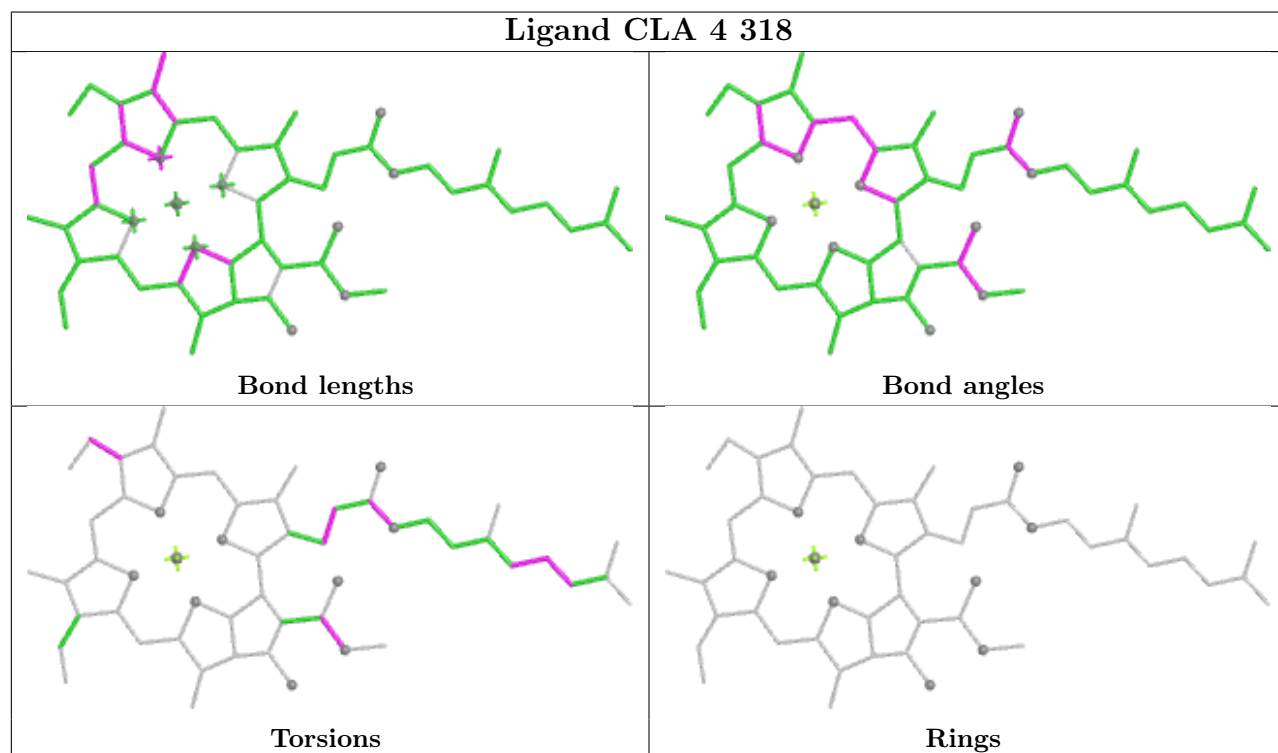
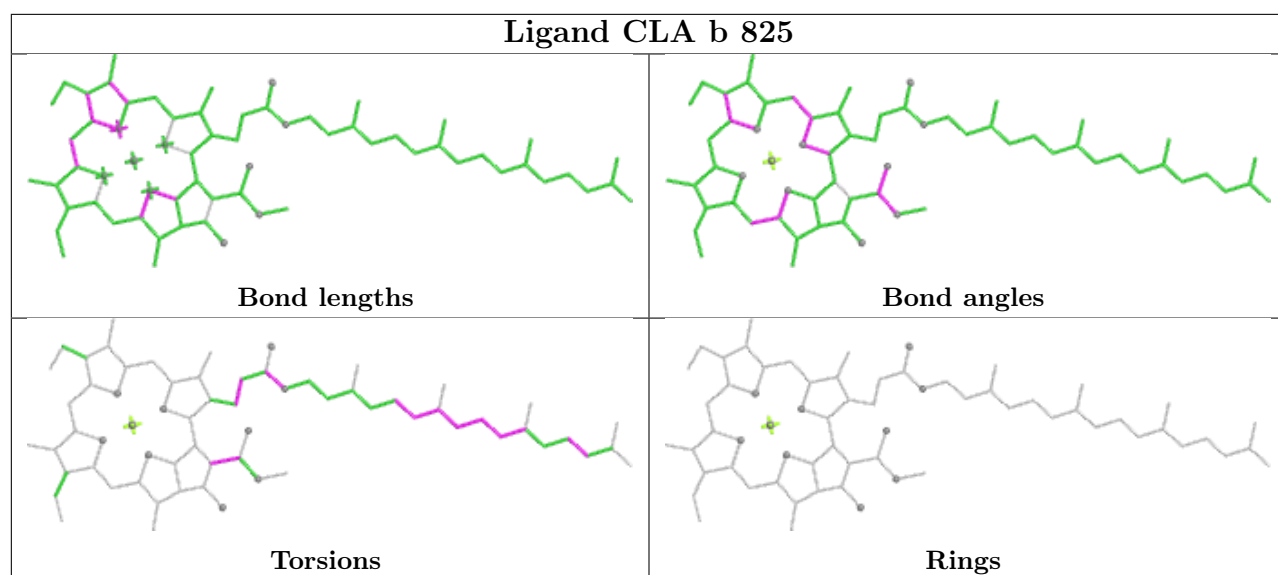
Rings

Ligand CLA a 816

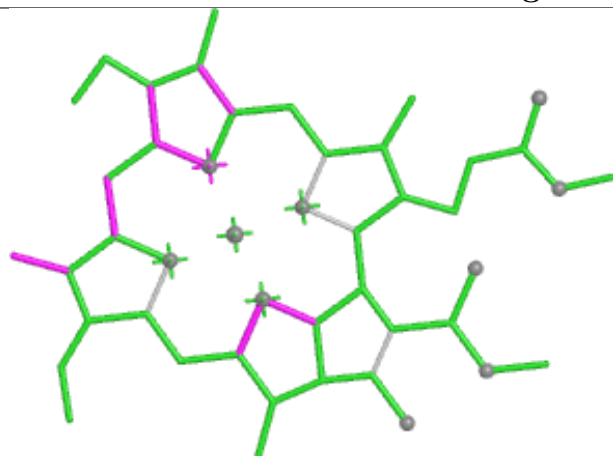


Ligand CLA a 825

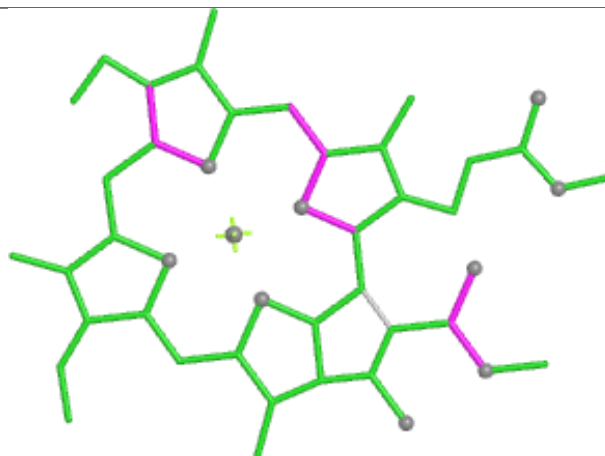




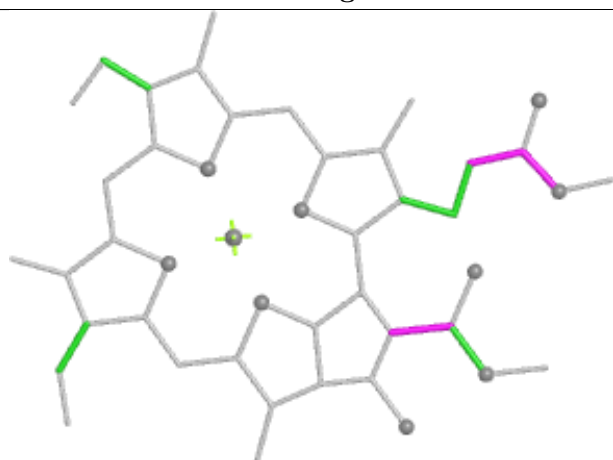
Ligand CLA l 204



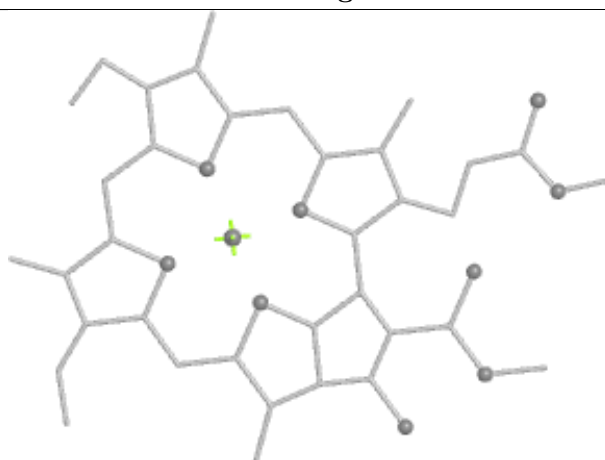
Bond lengths



Bond angles

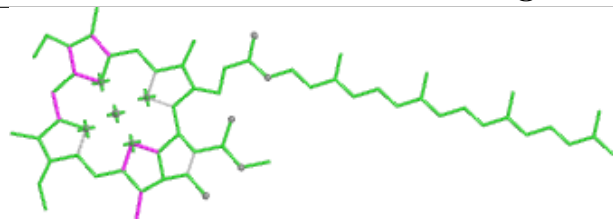


Torsions

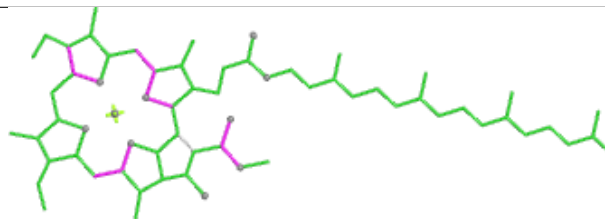


Rings

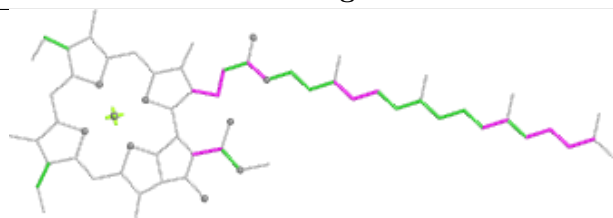
Ligand CLA b 834



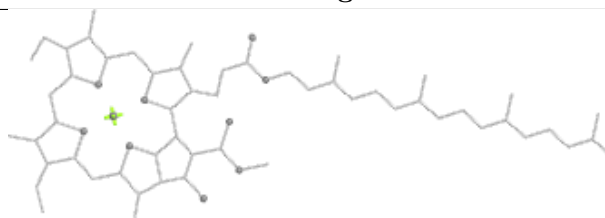
Bond lengths



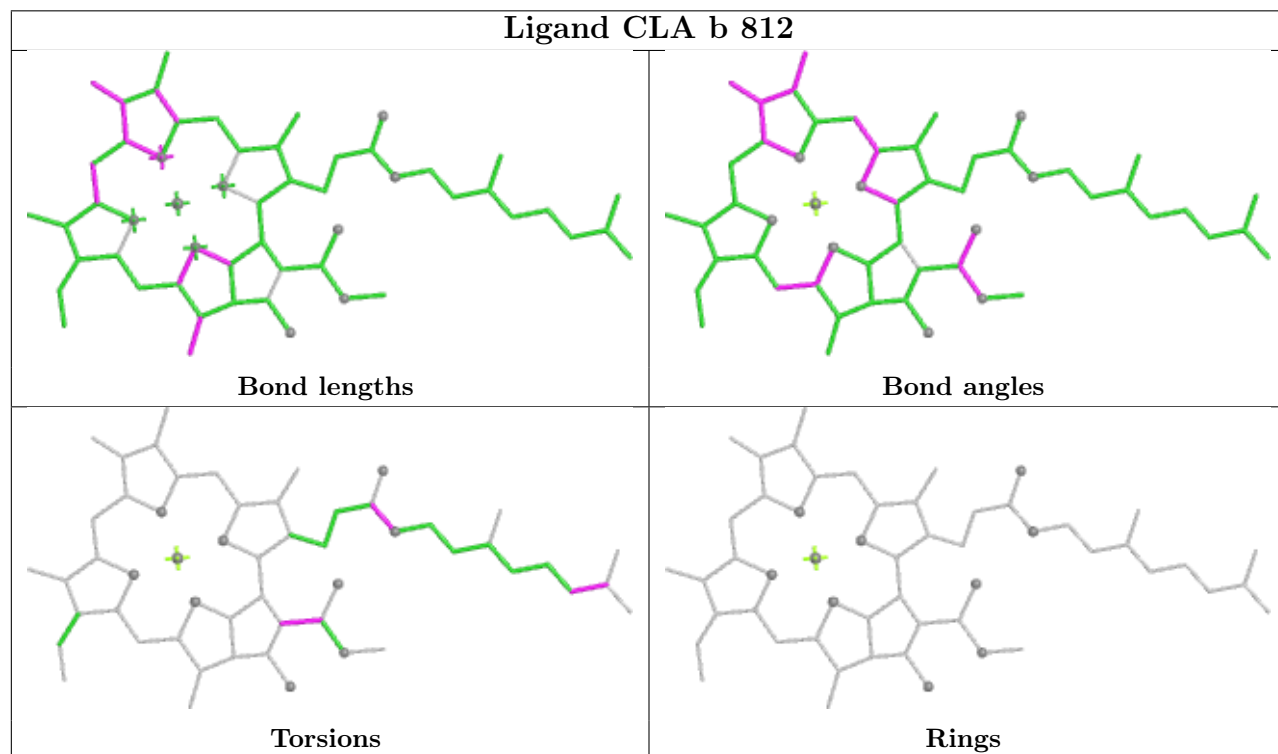
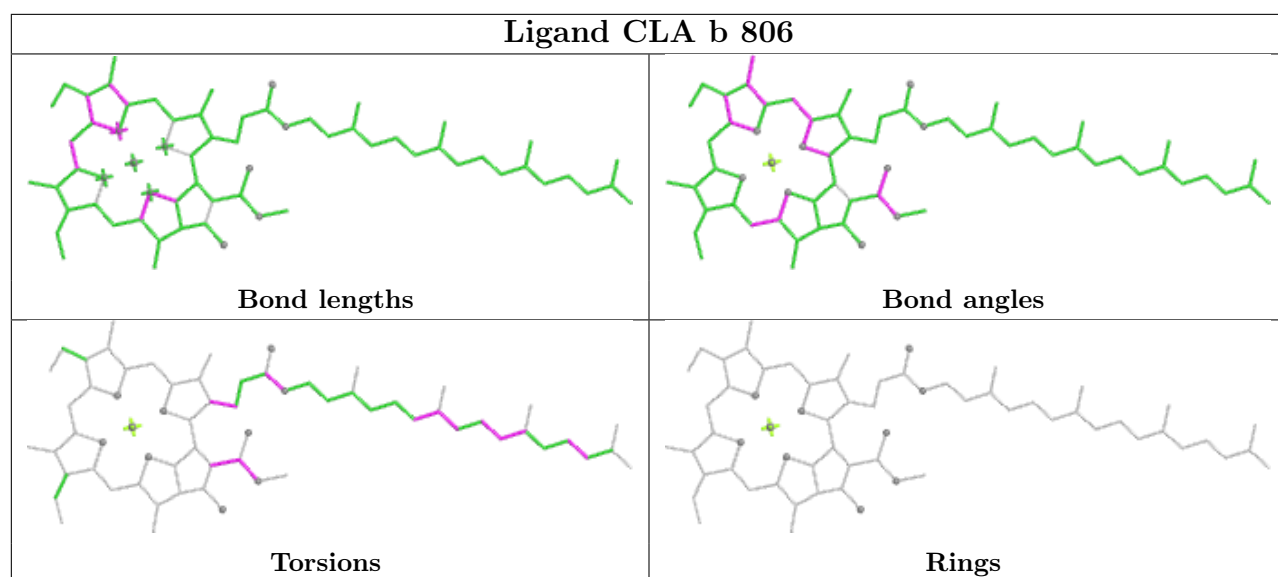
Bond angles

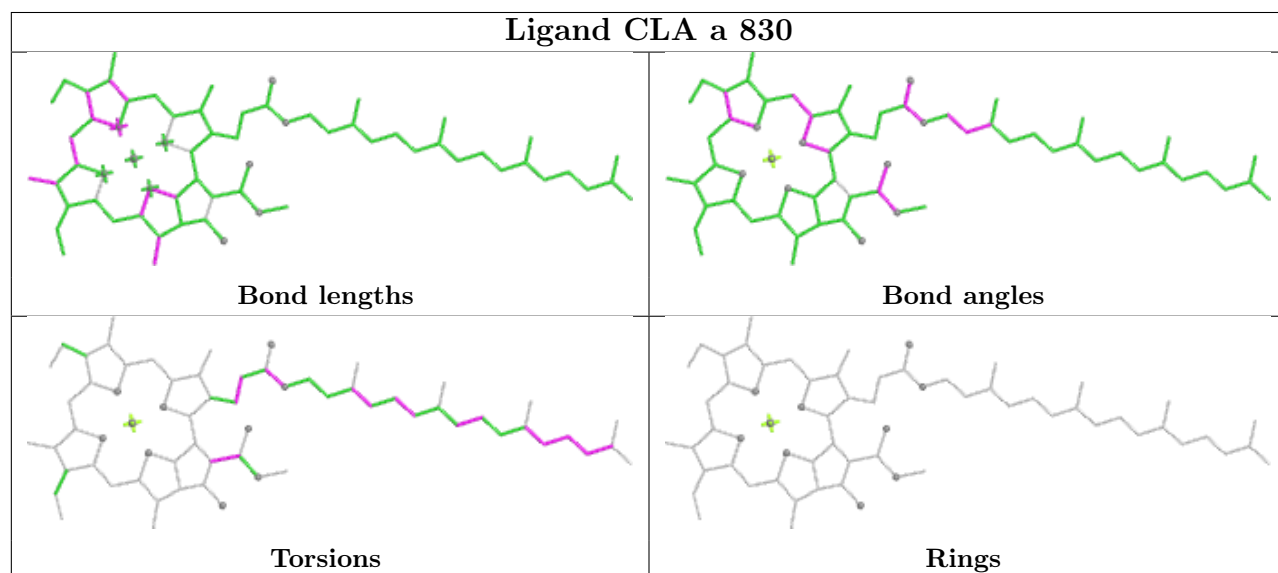
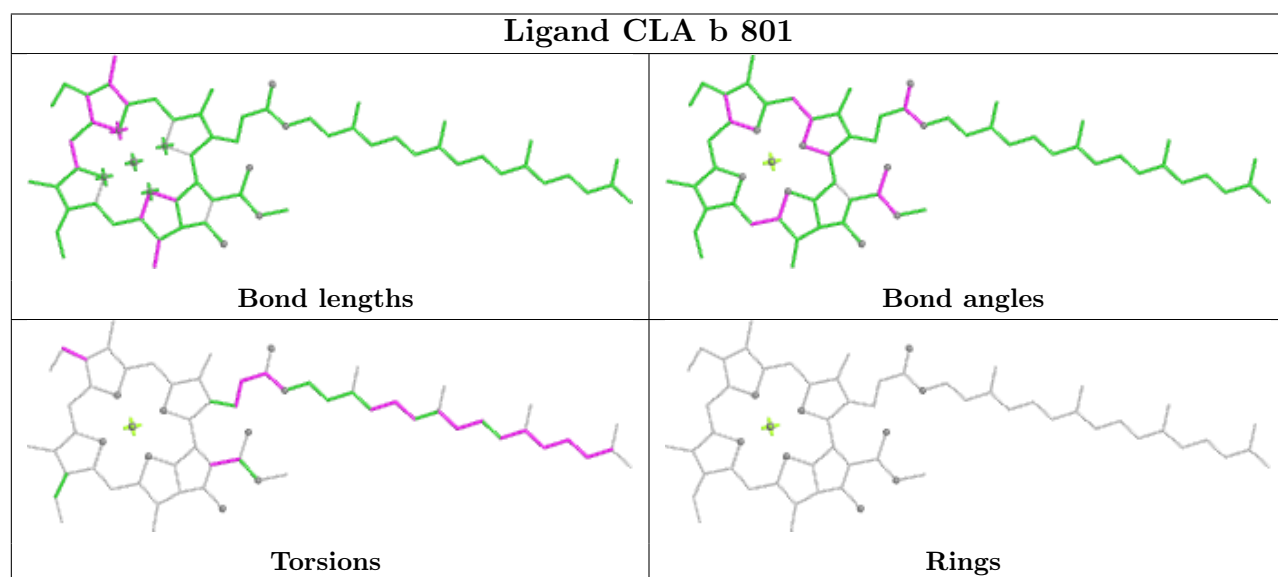
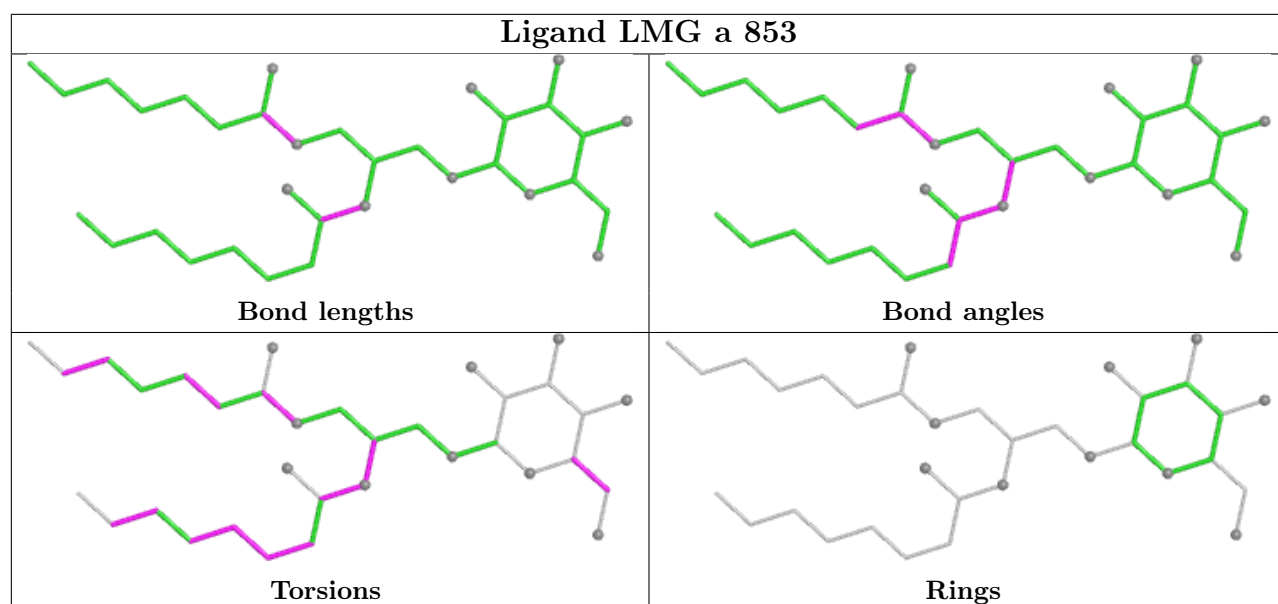


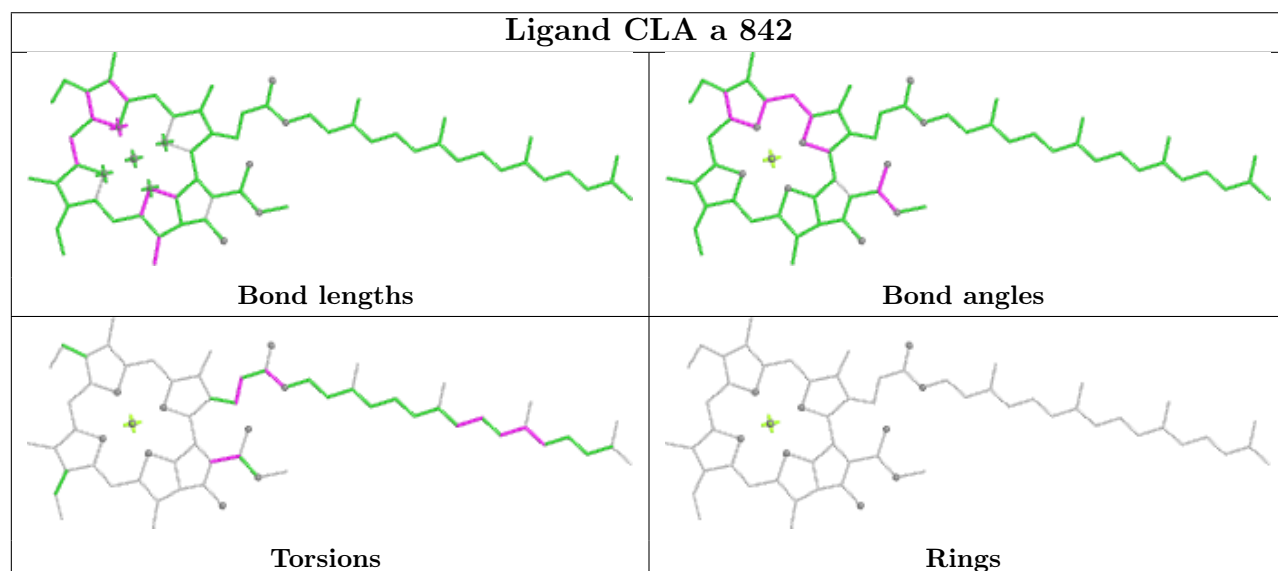
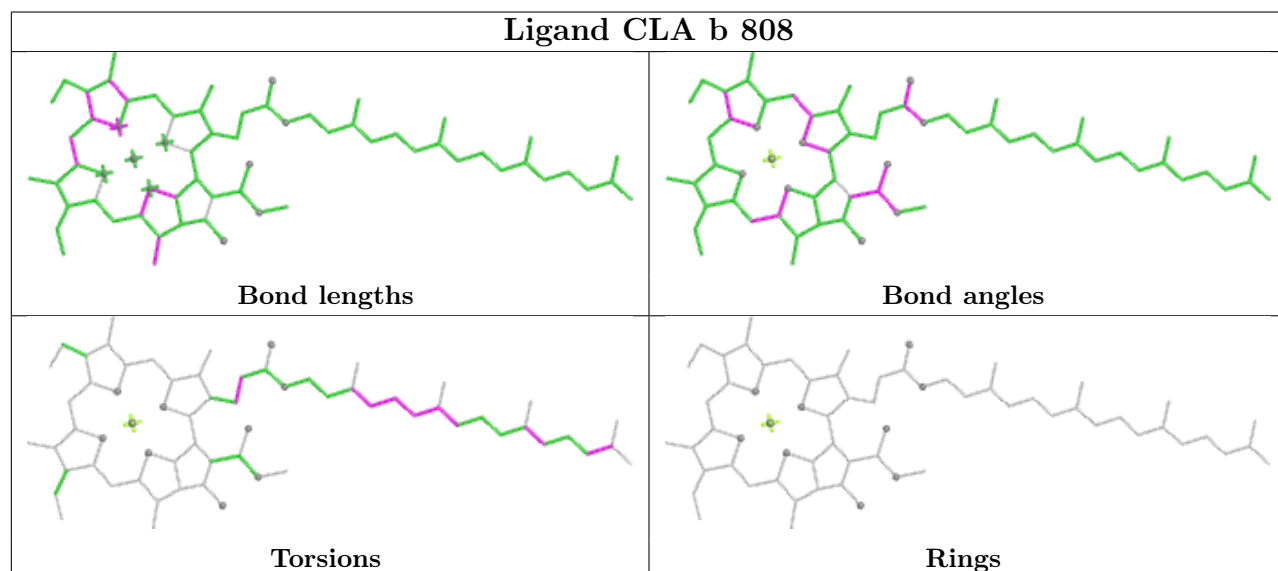
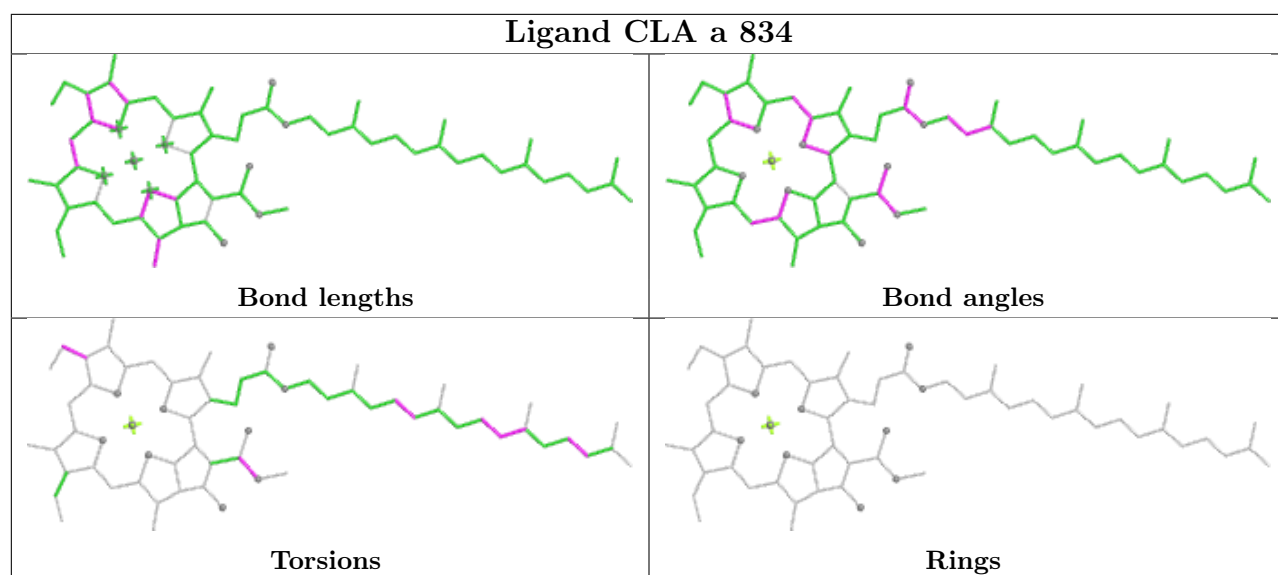
Torsions

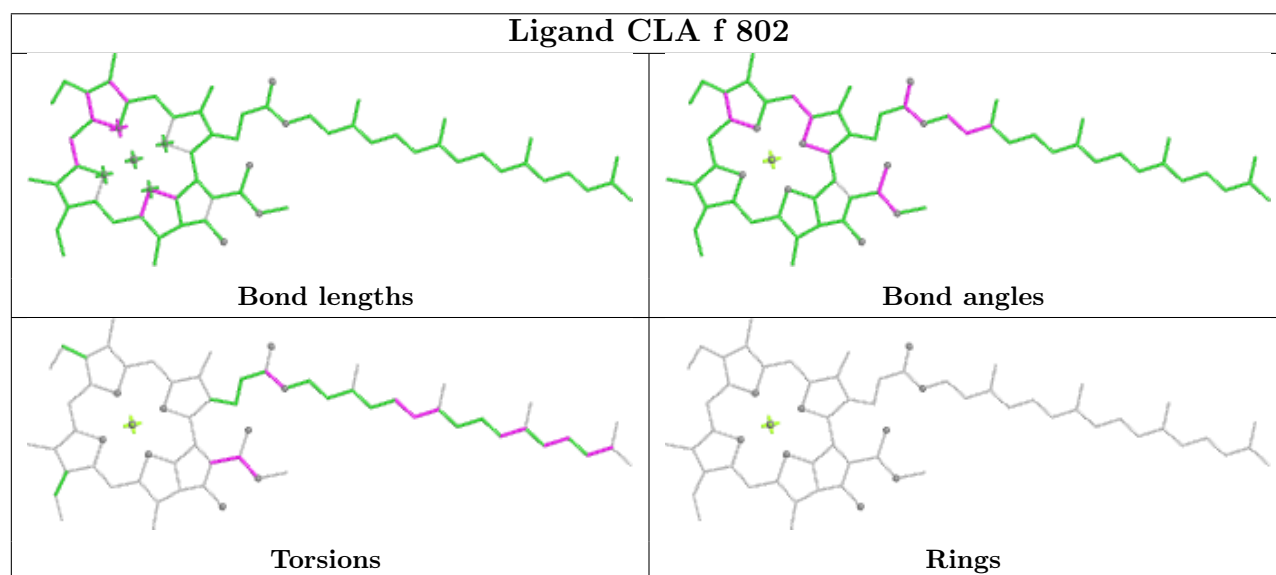
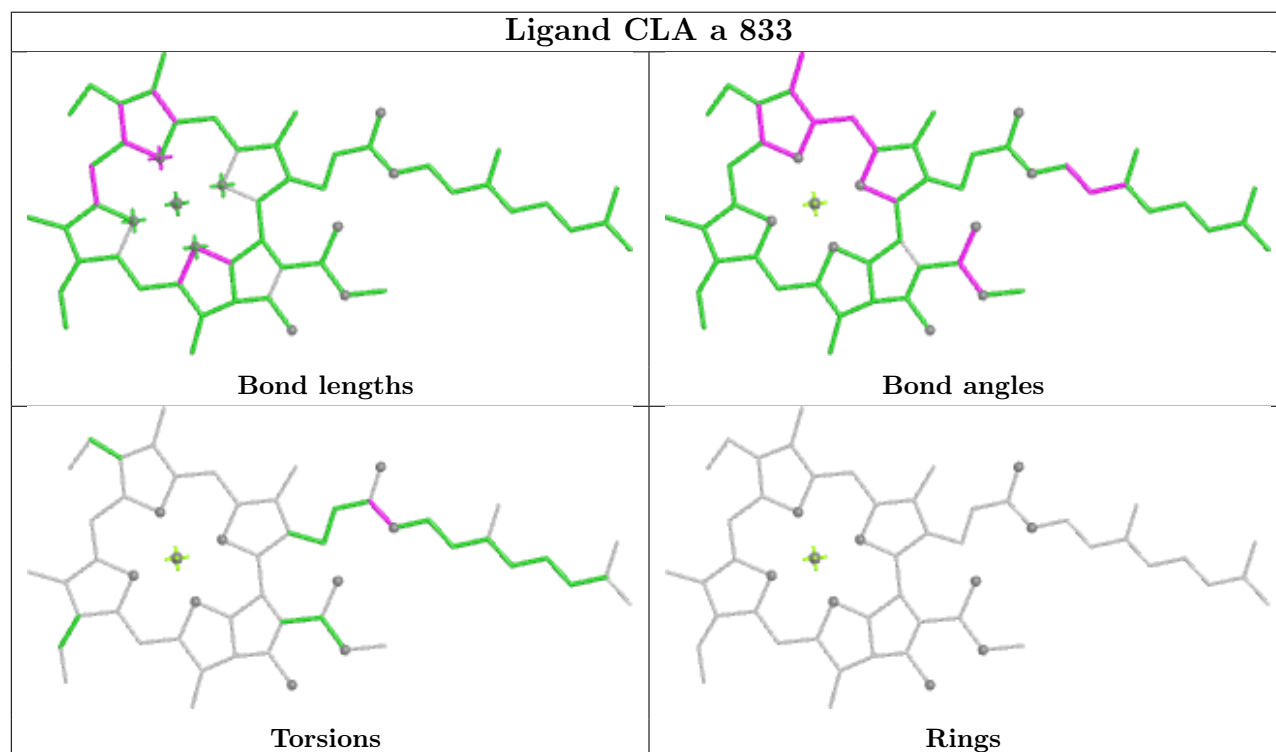
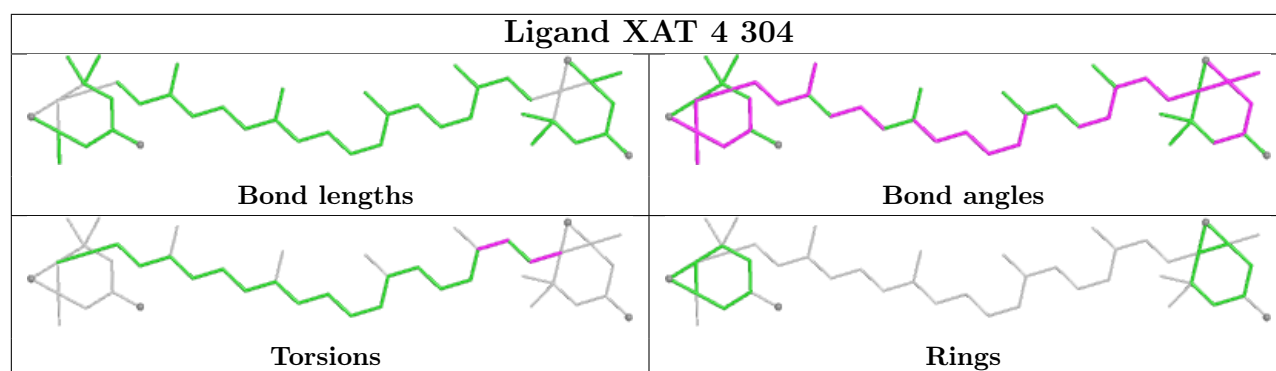


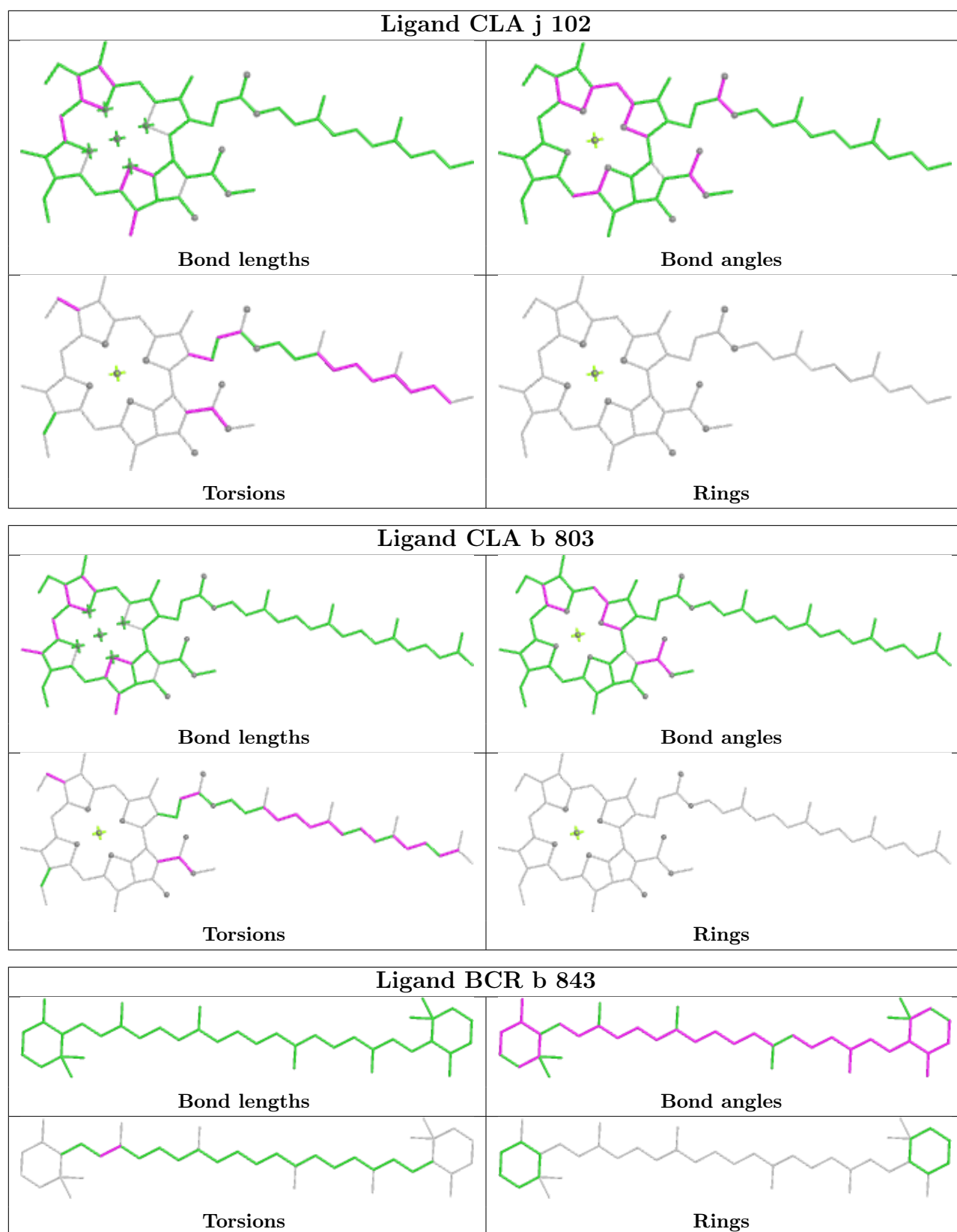
Rings

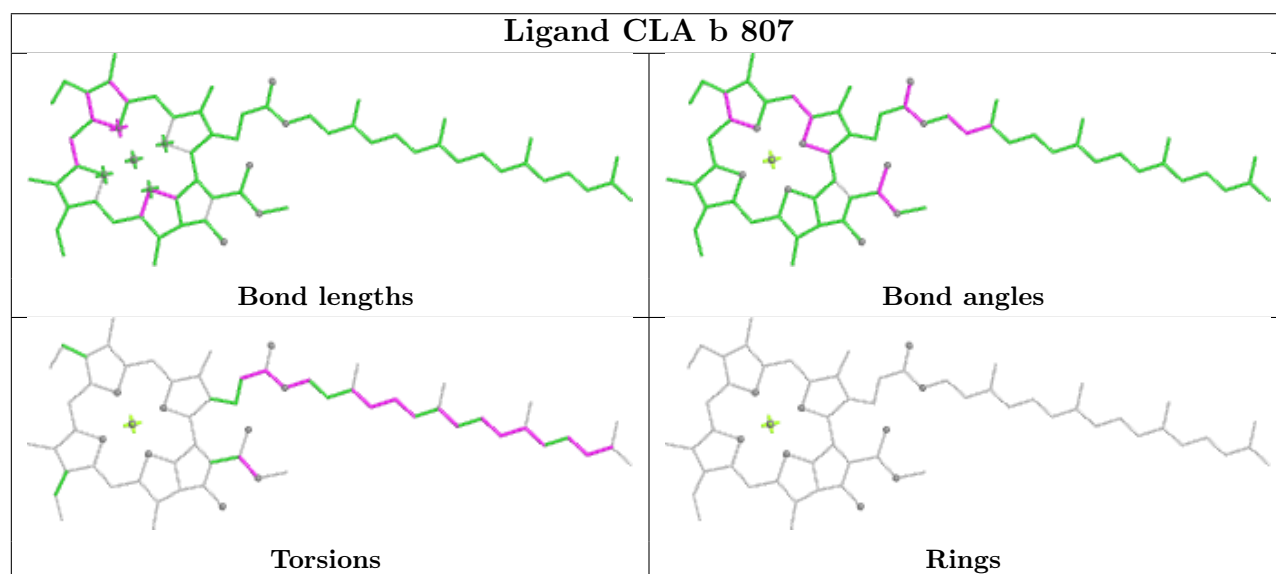
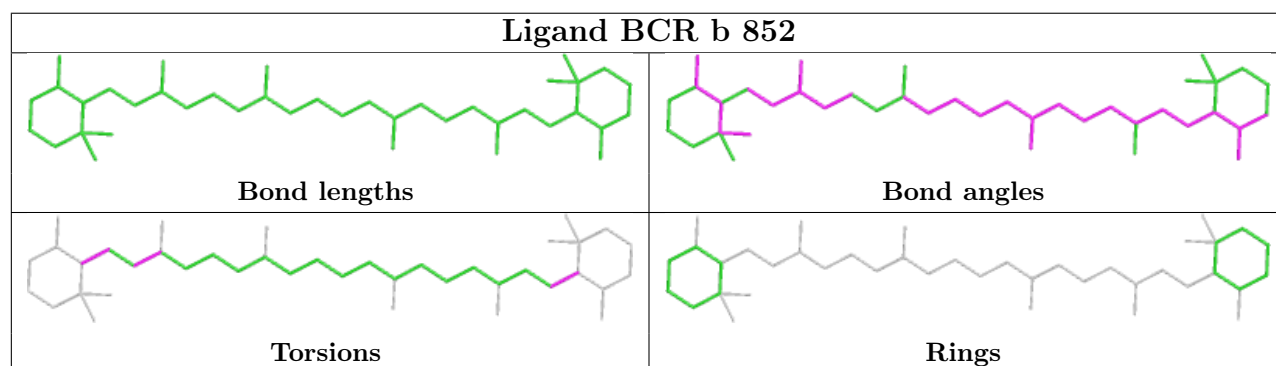
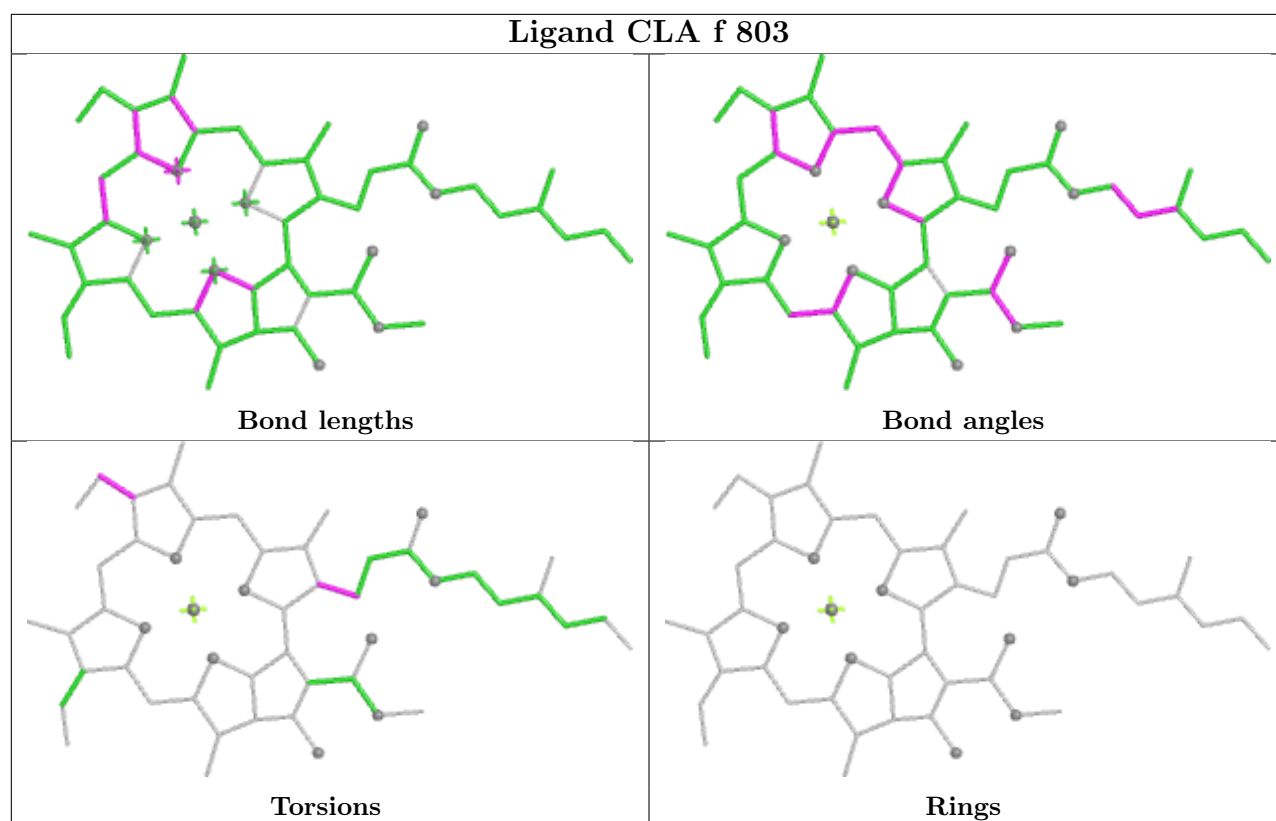


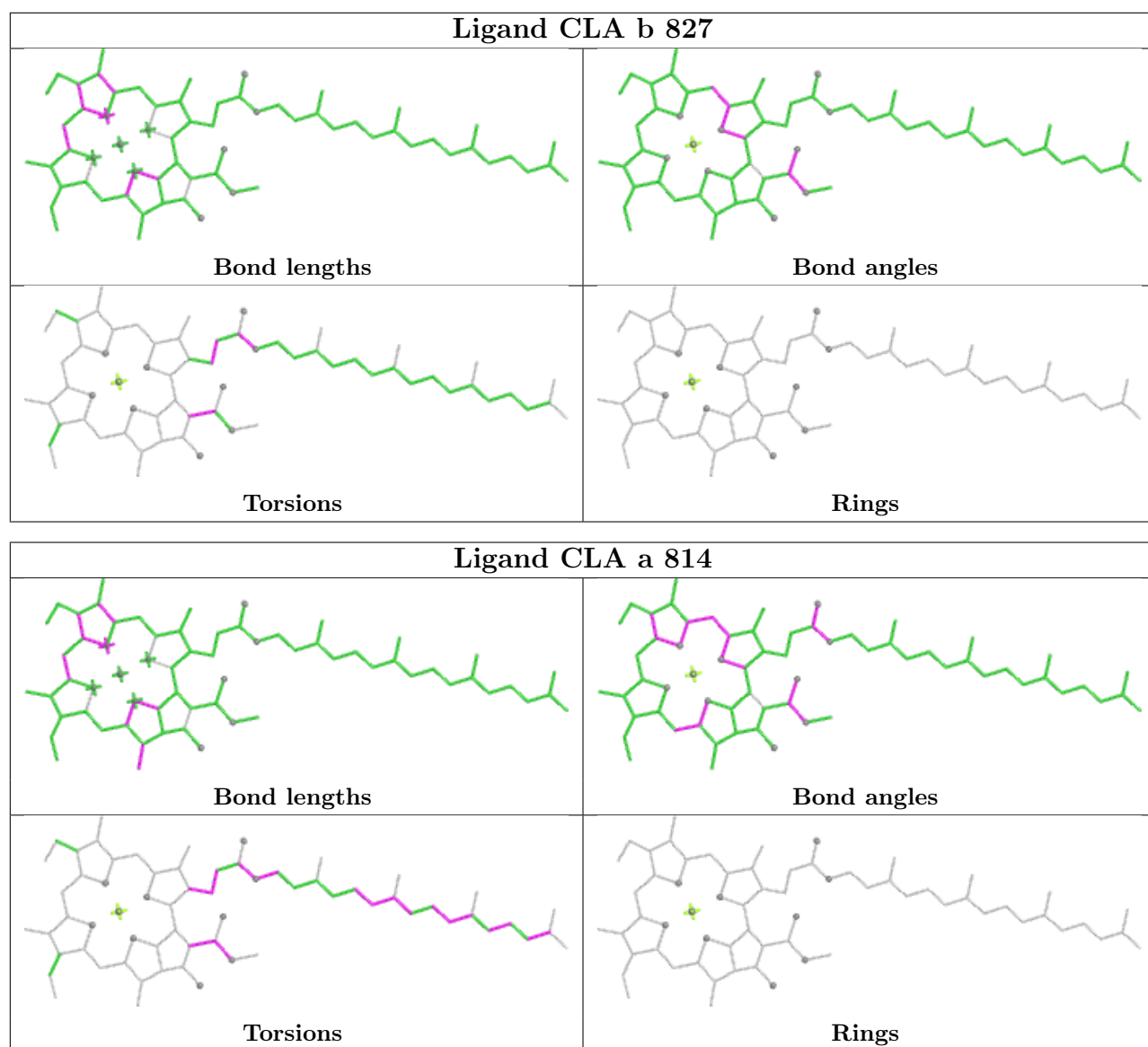




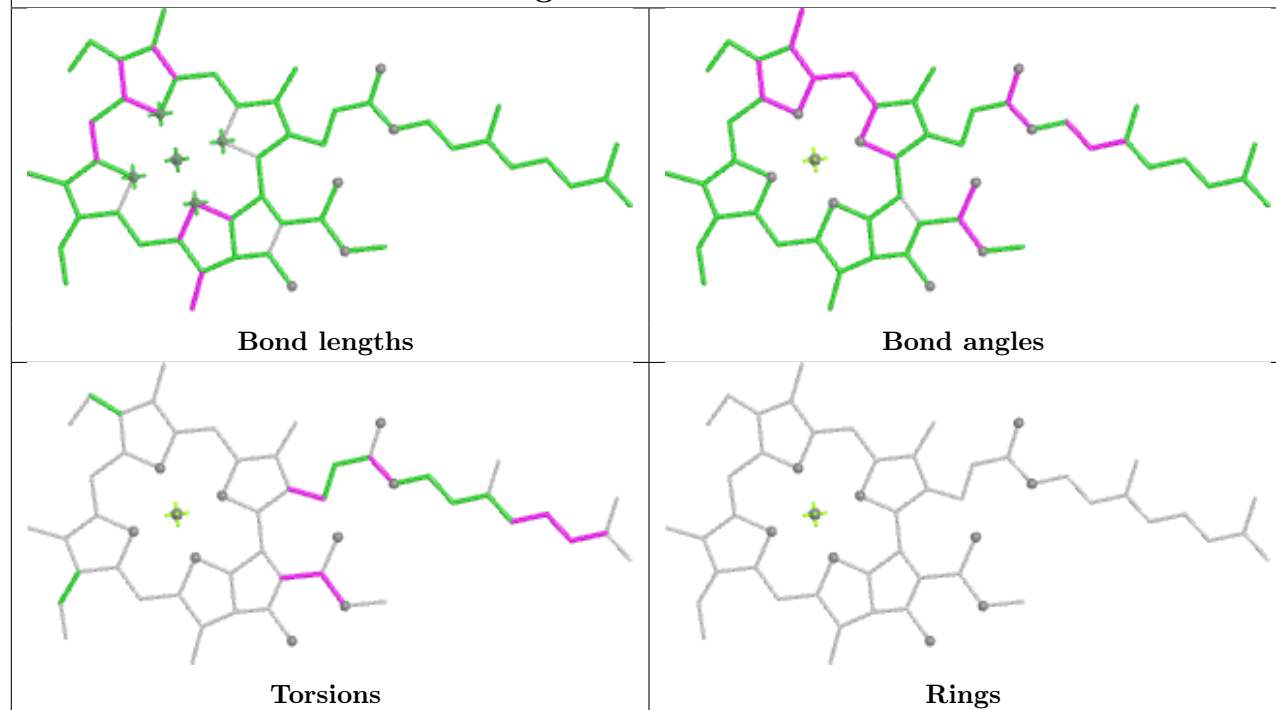




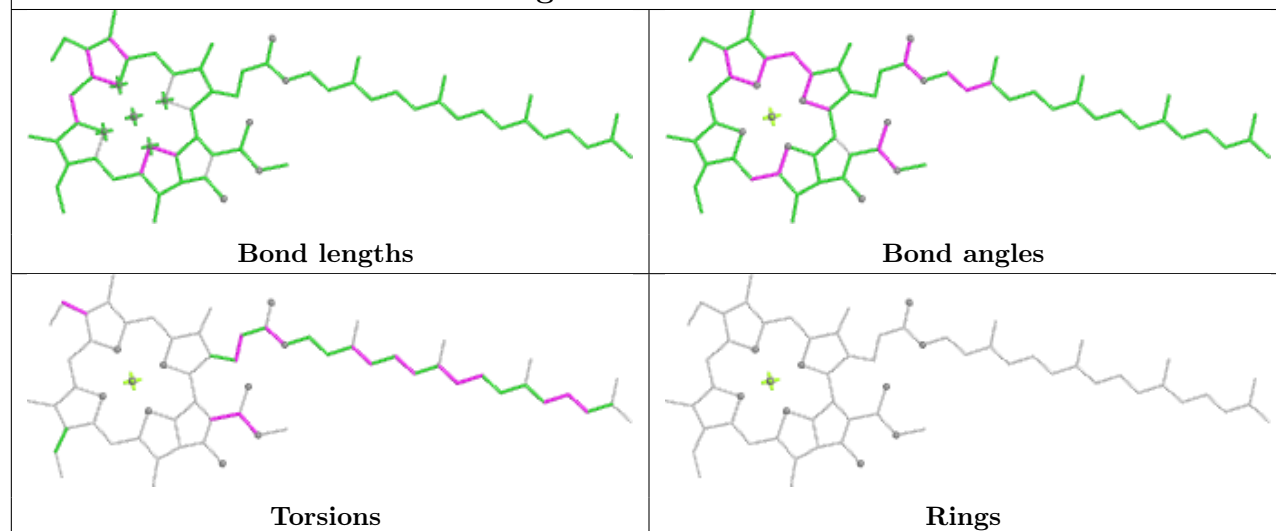


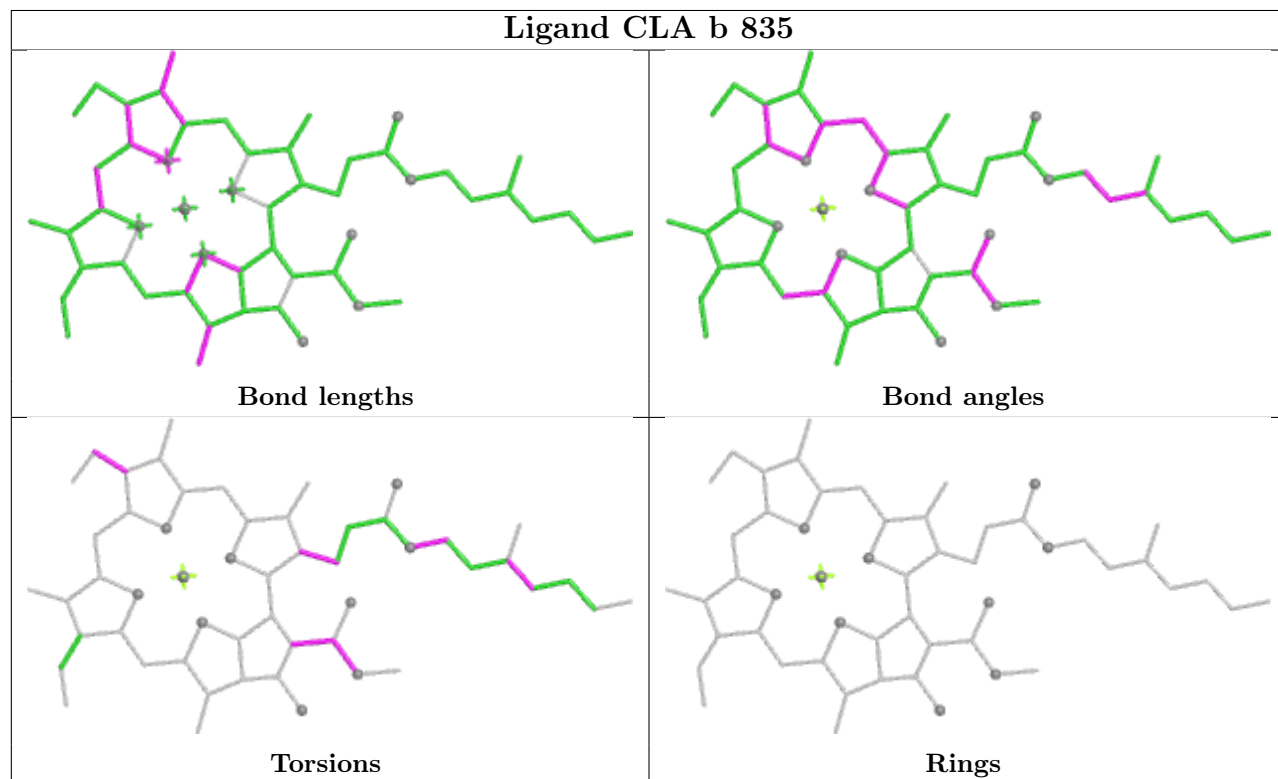
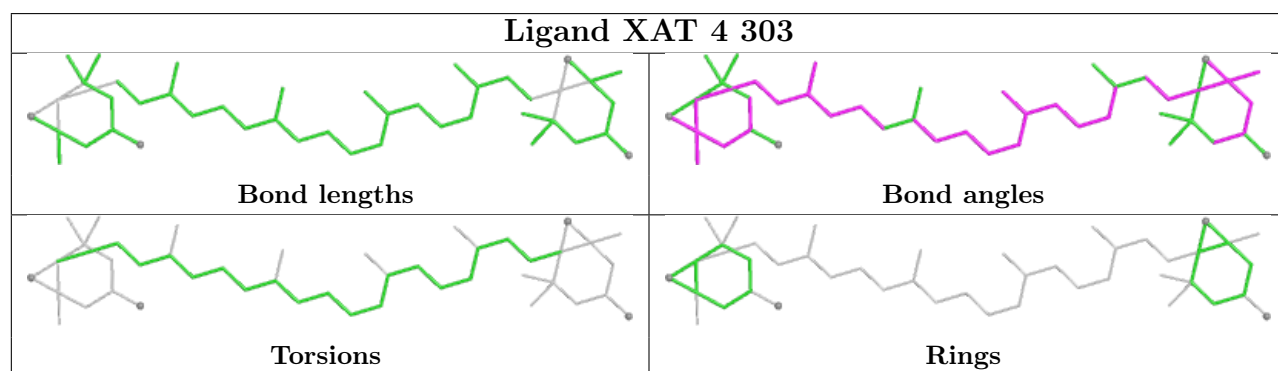
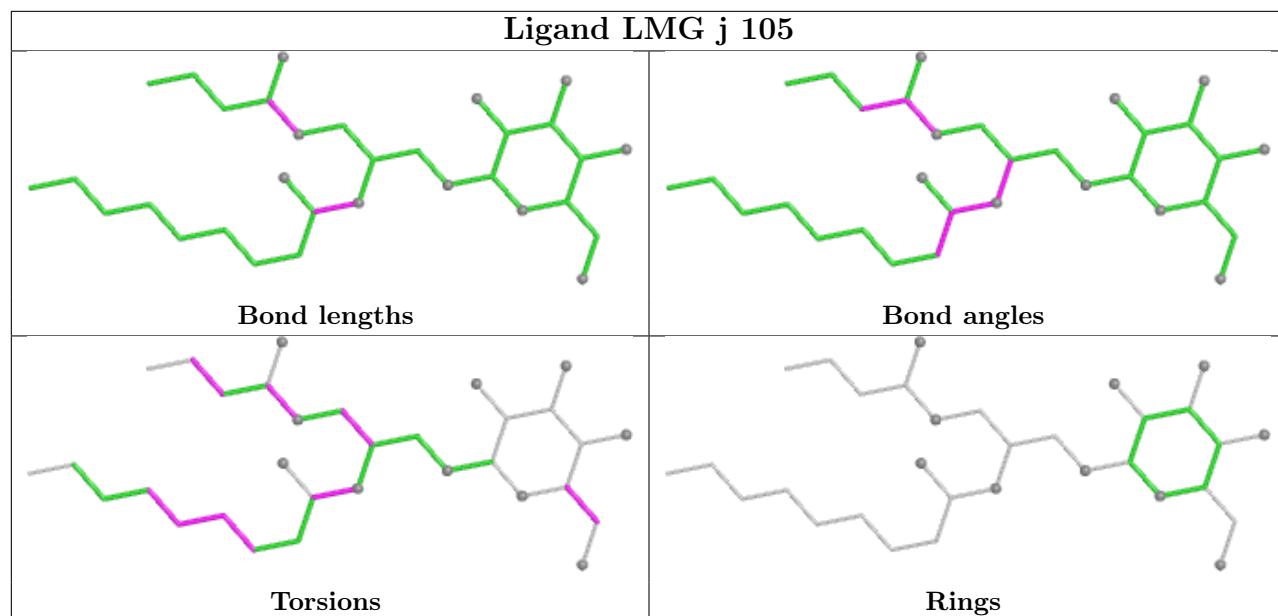


Ligand CLA b 815

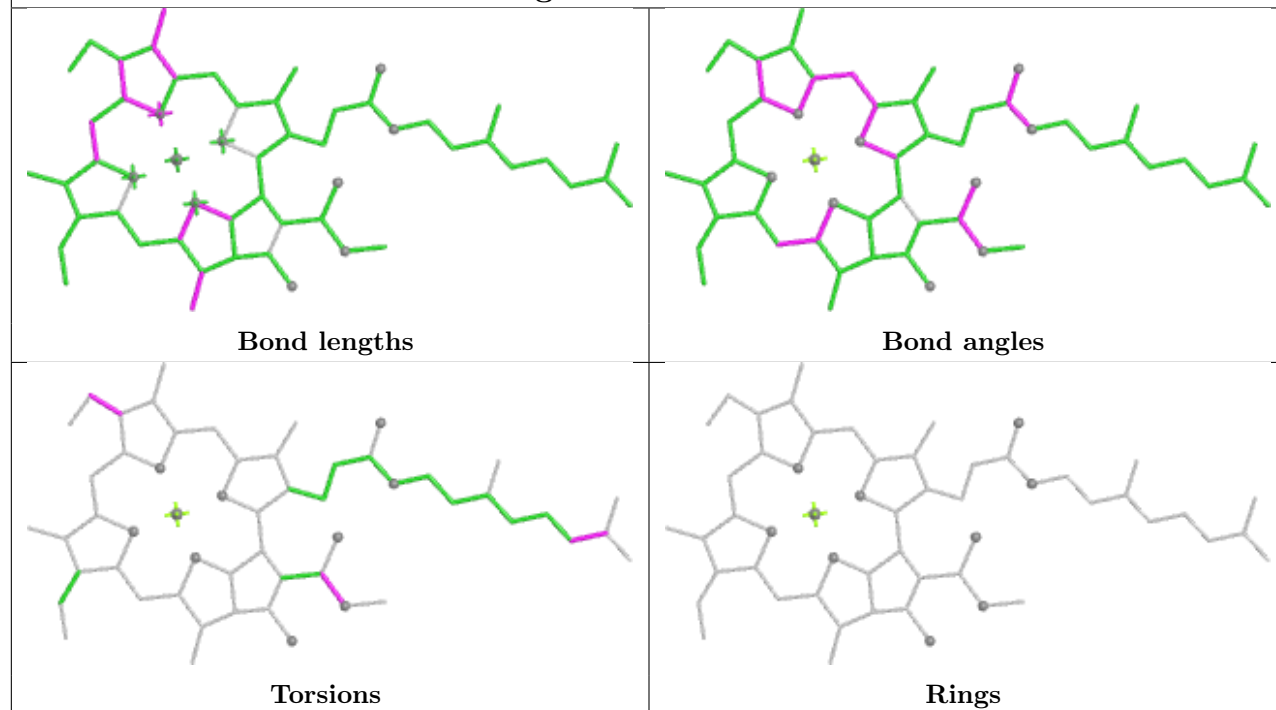


Ligand CLA a 841

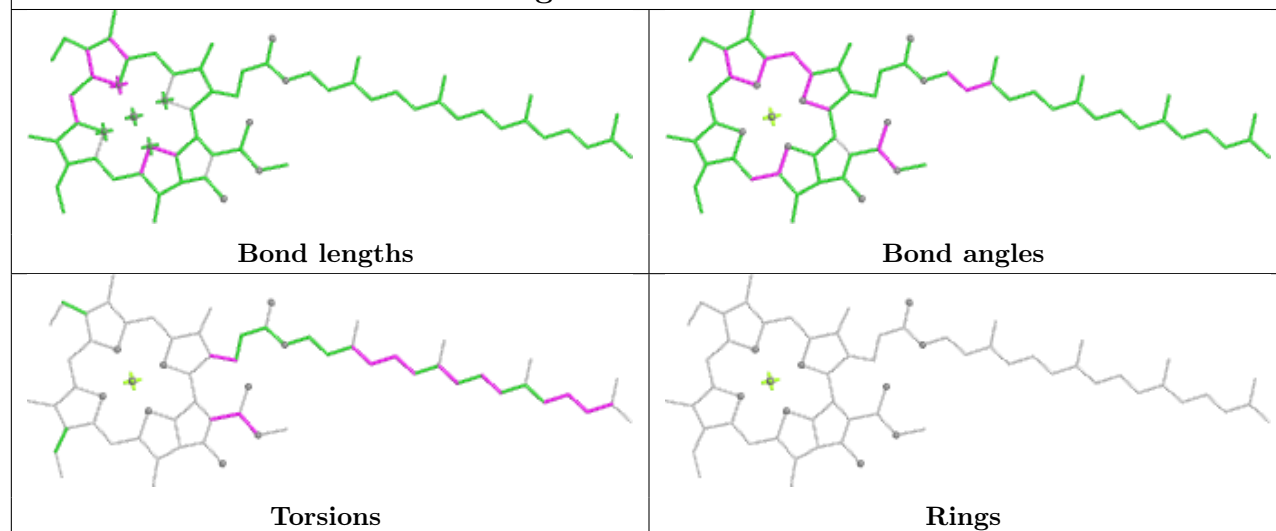


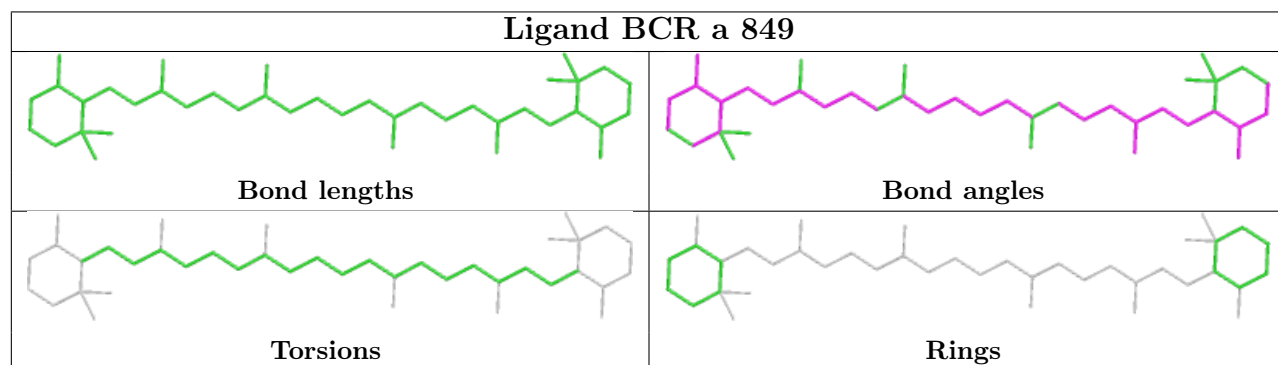
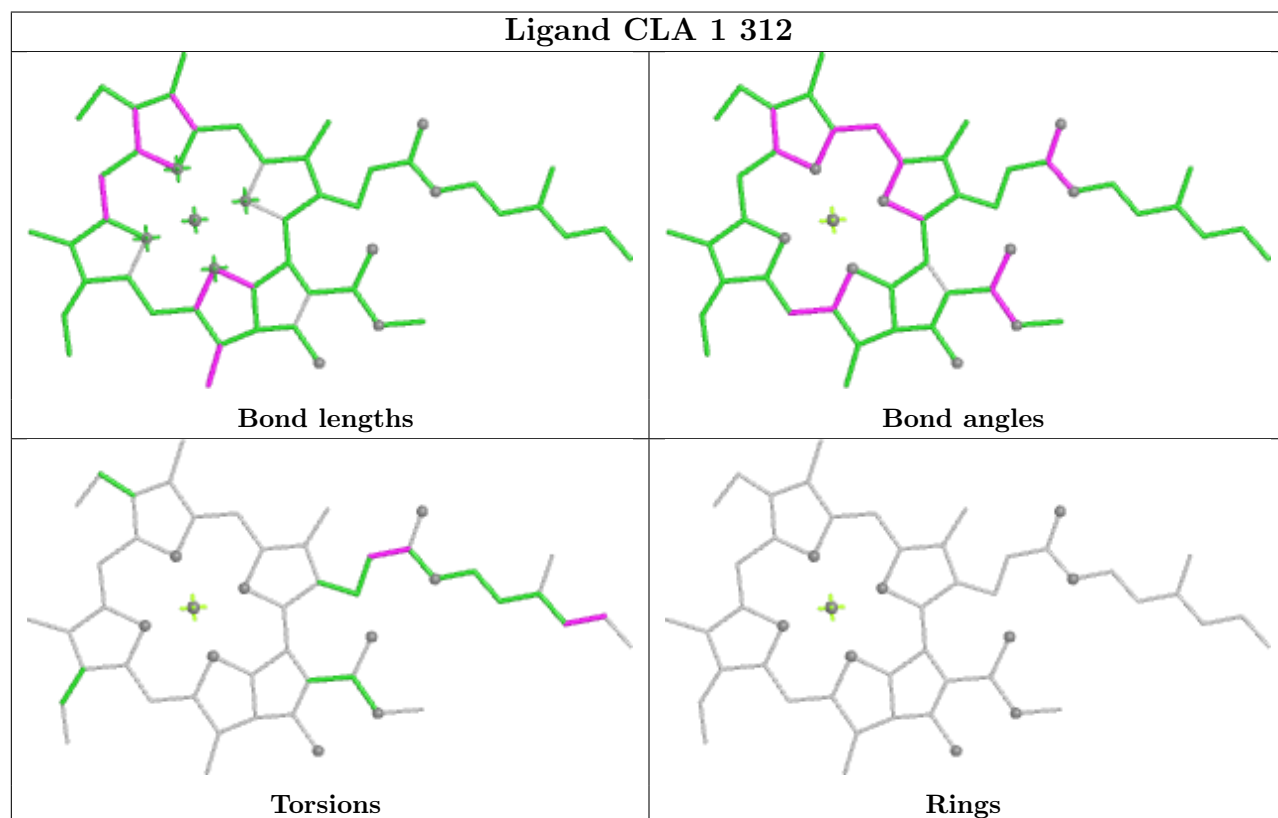
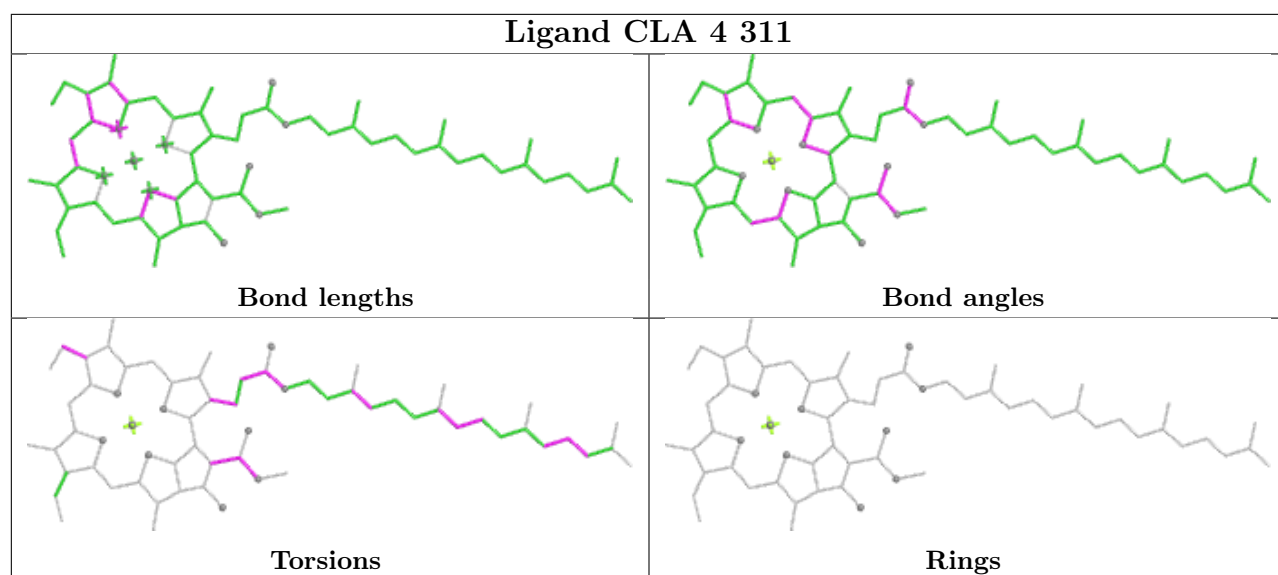


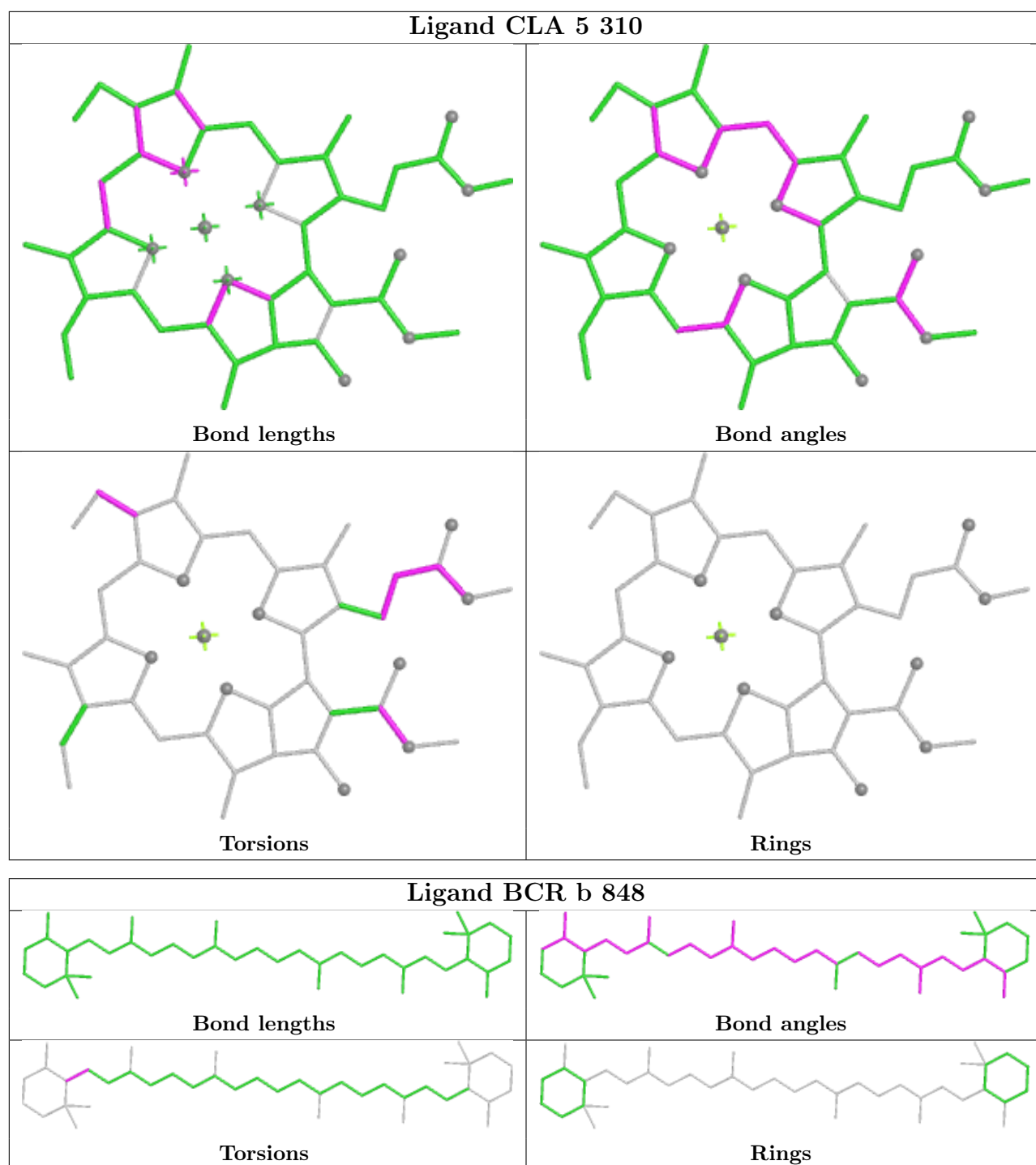
Ligand CLA b 820

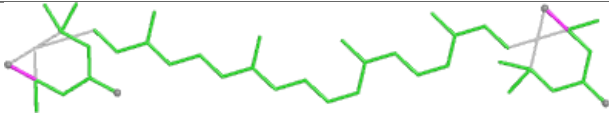
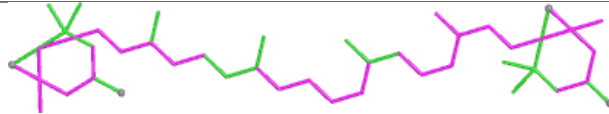
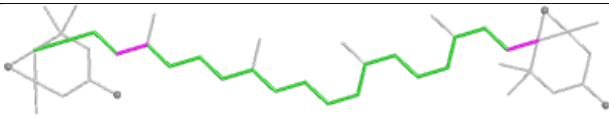
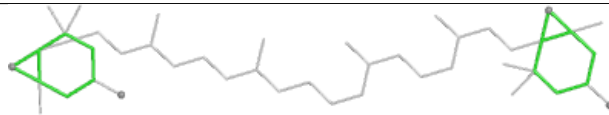


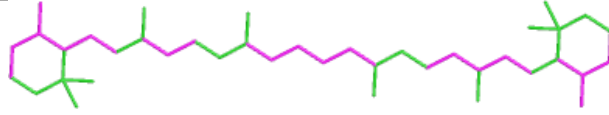
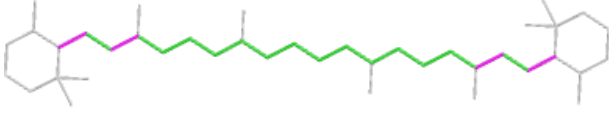
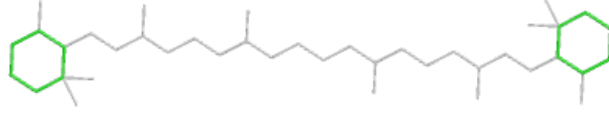
Ligand CLA b 814

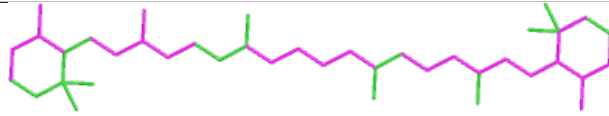
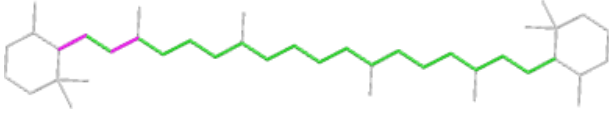
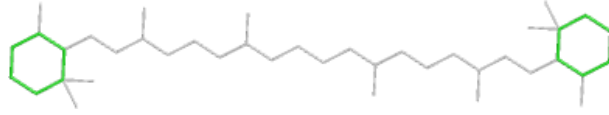


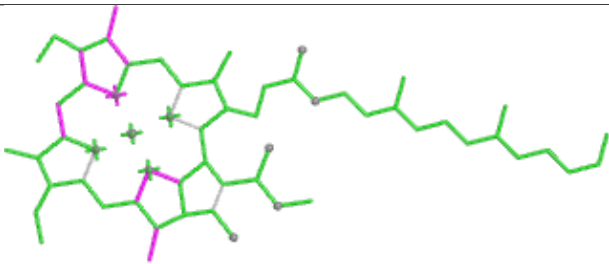
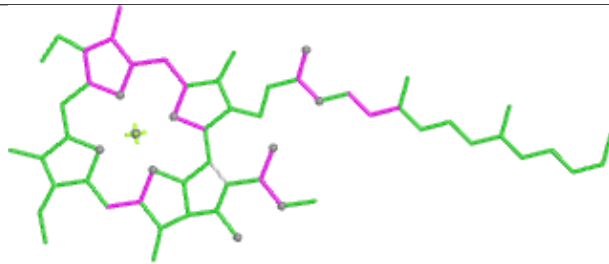
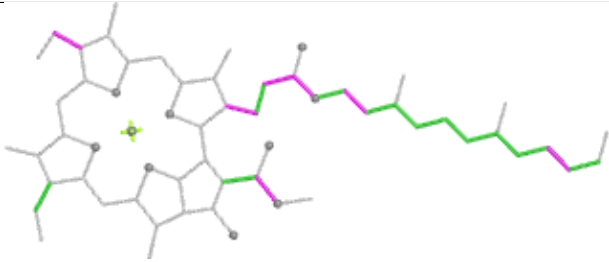
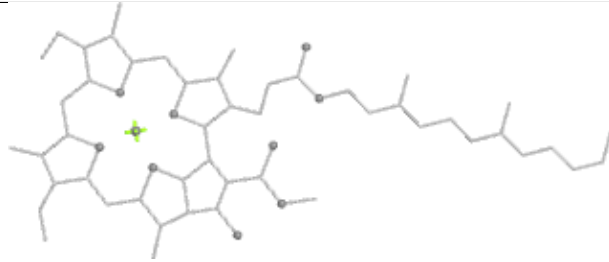


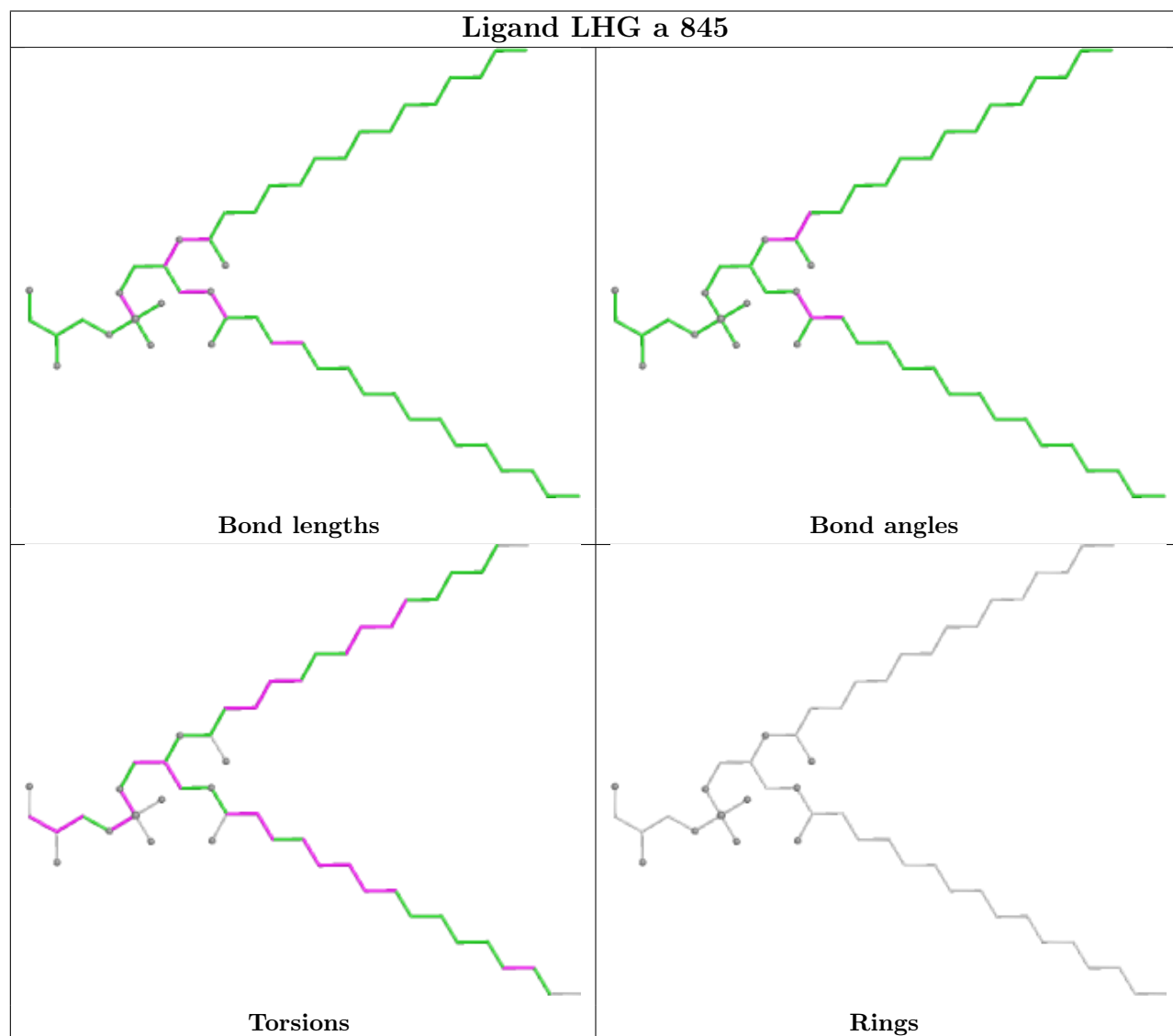
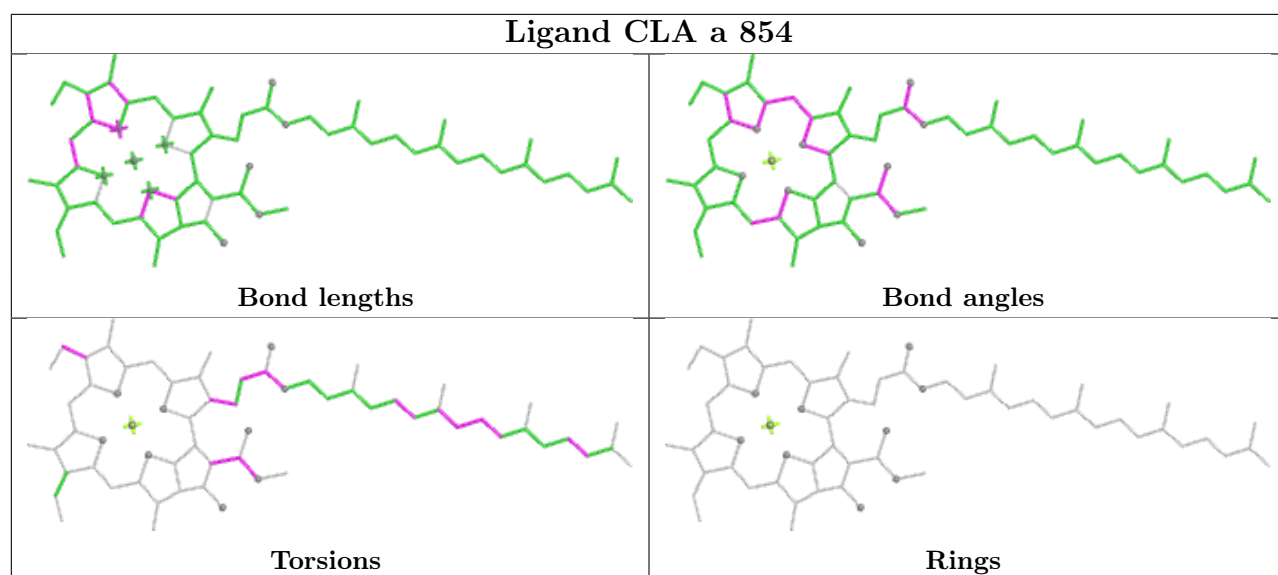


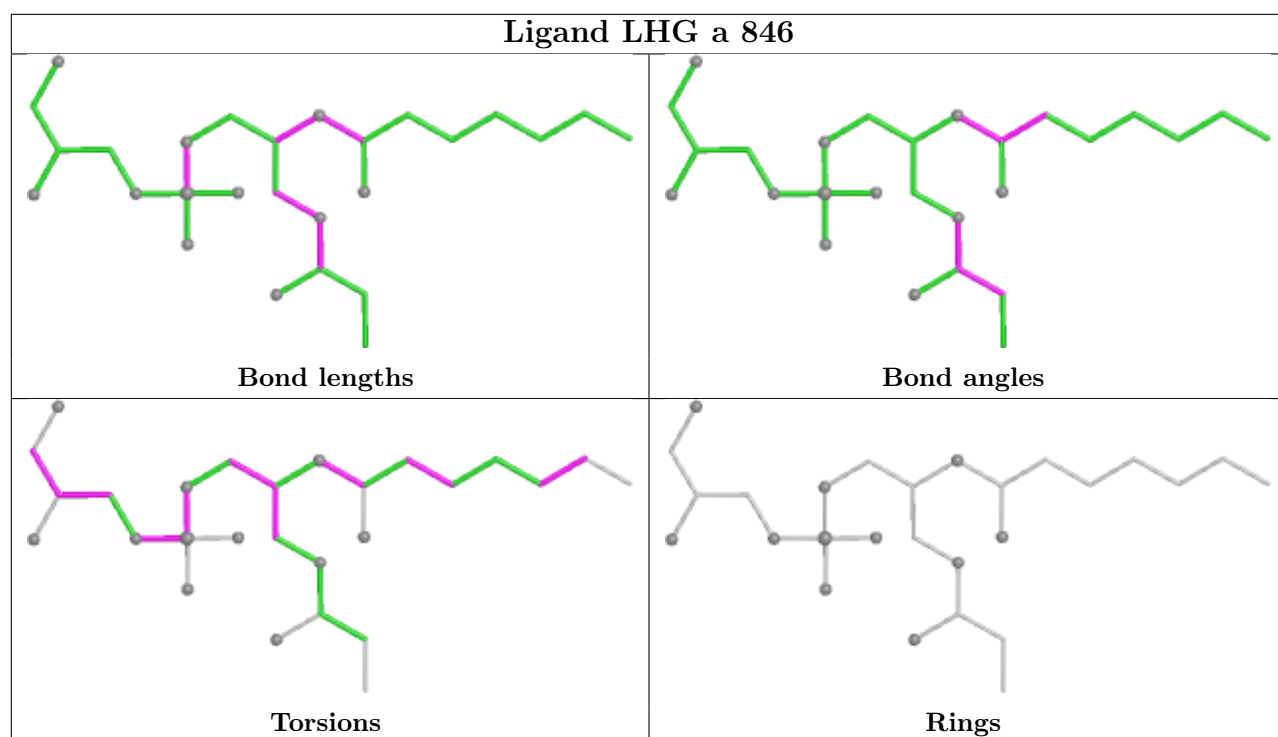
Ligand XAT 4 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 1 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

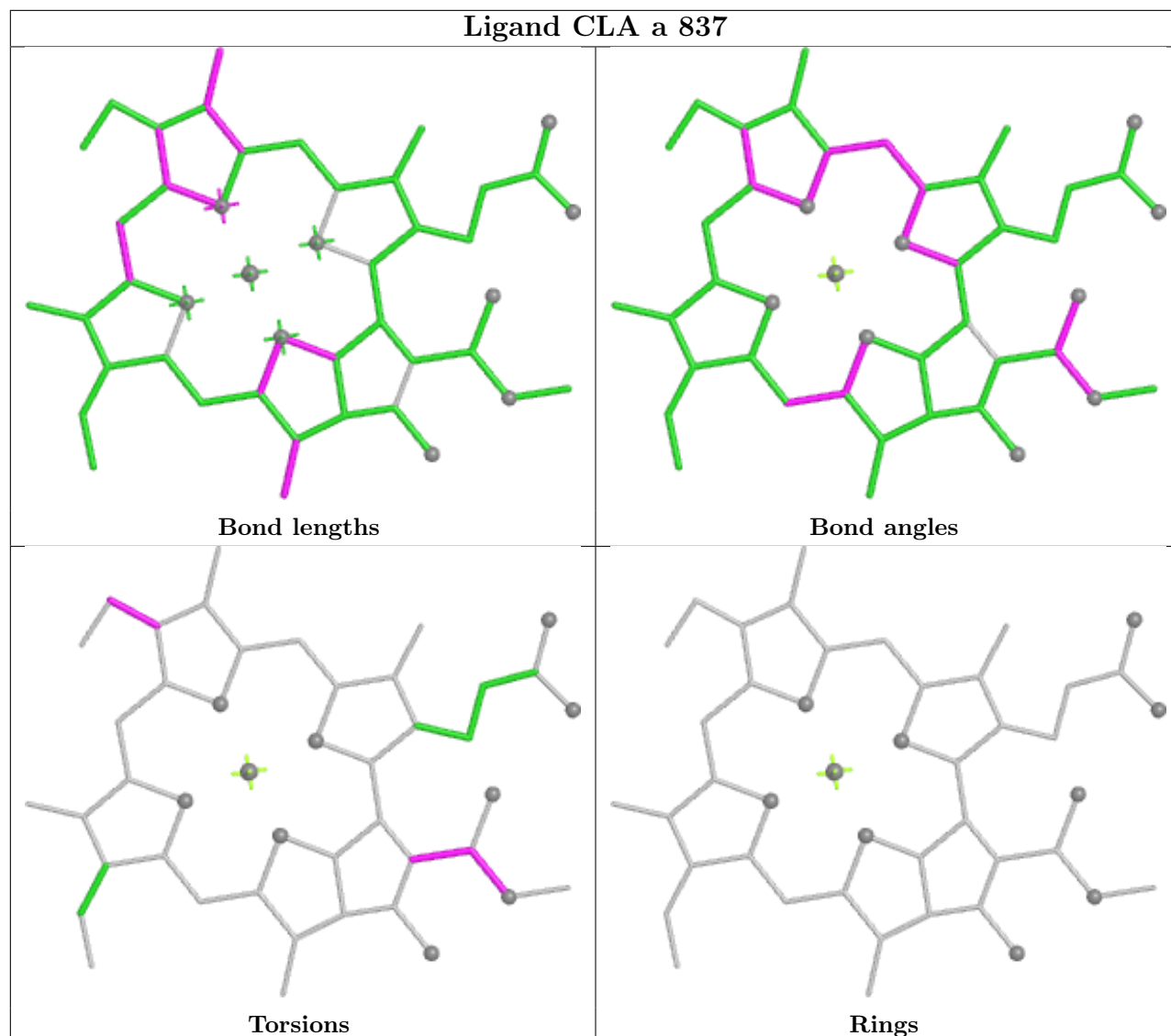
Ligand BCR j 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 818	
	
Bond lengths	Bond angles
	
Torsions	Rings

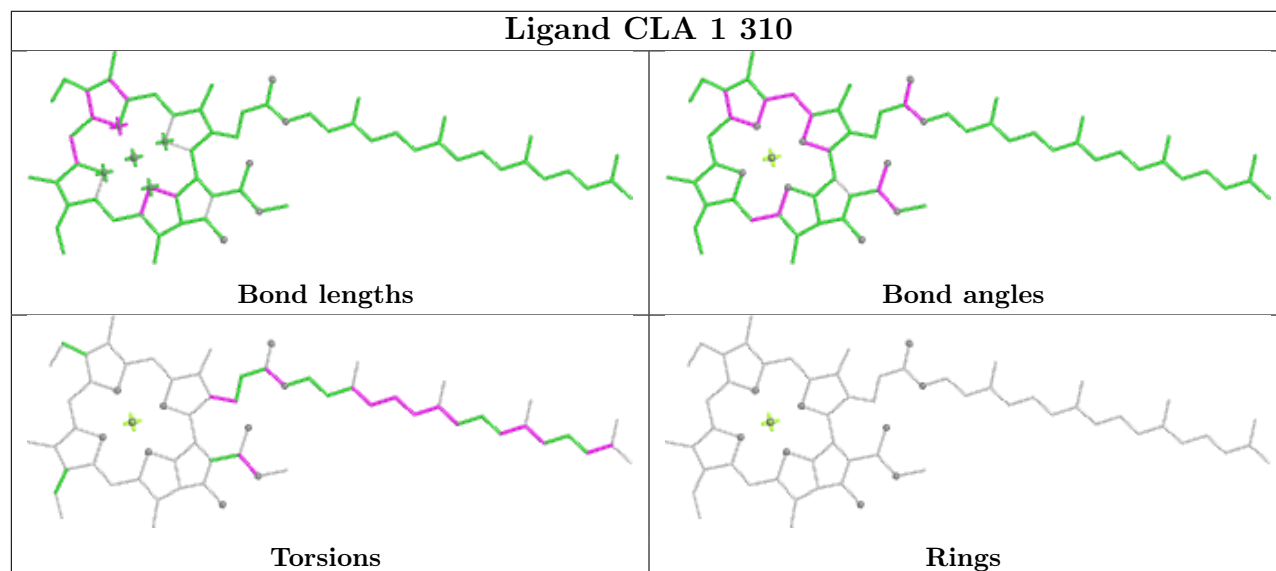


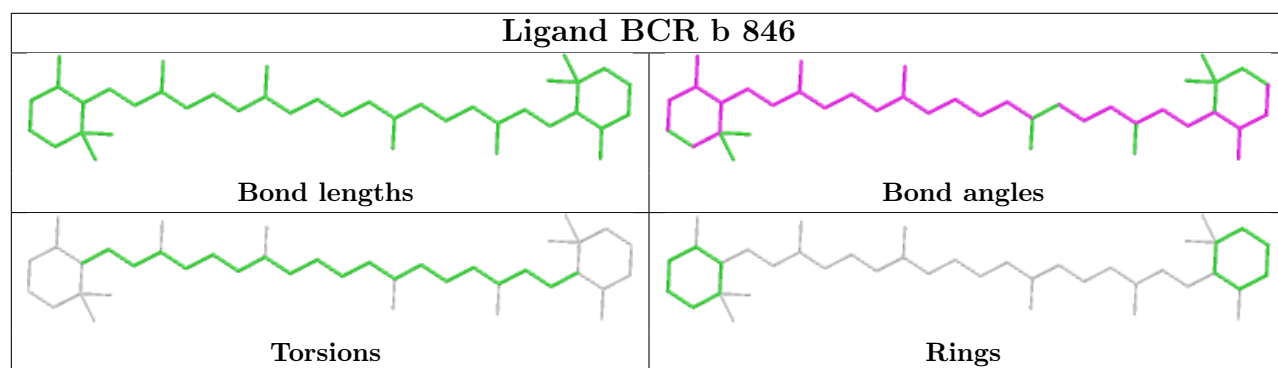
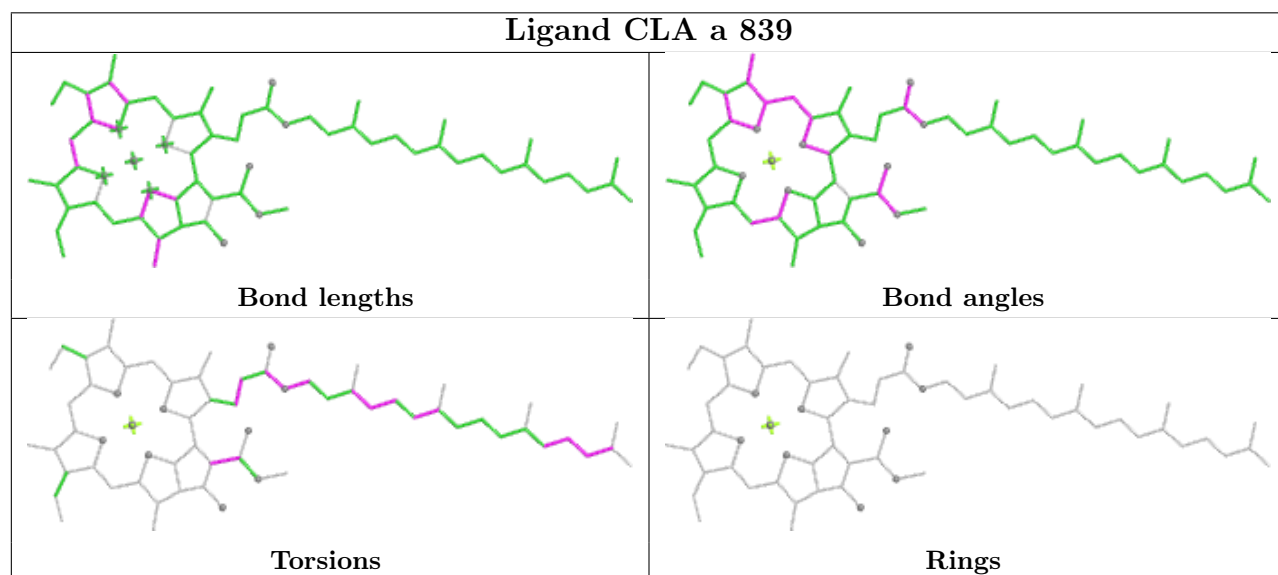
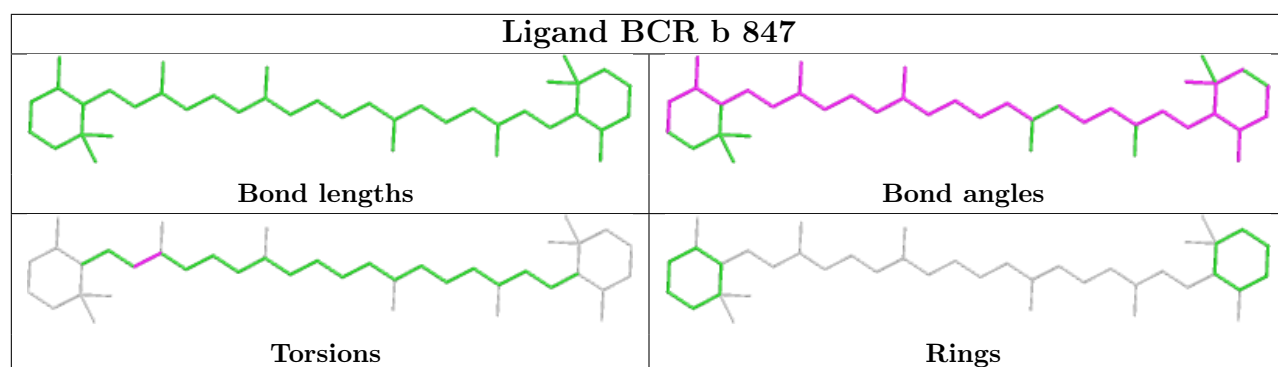


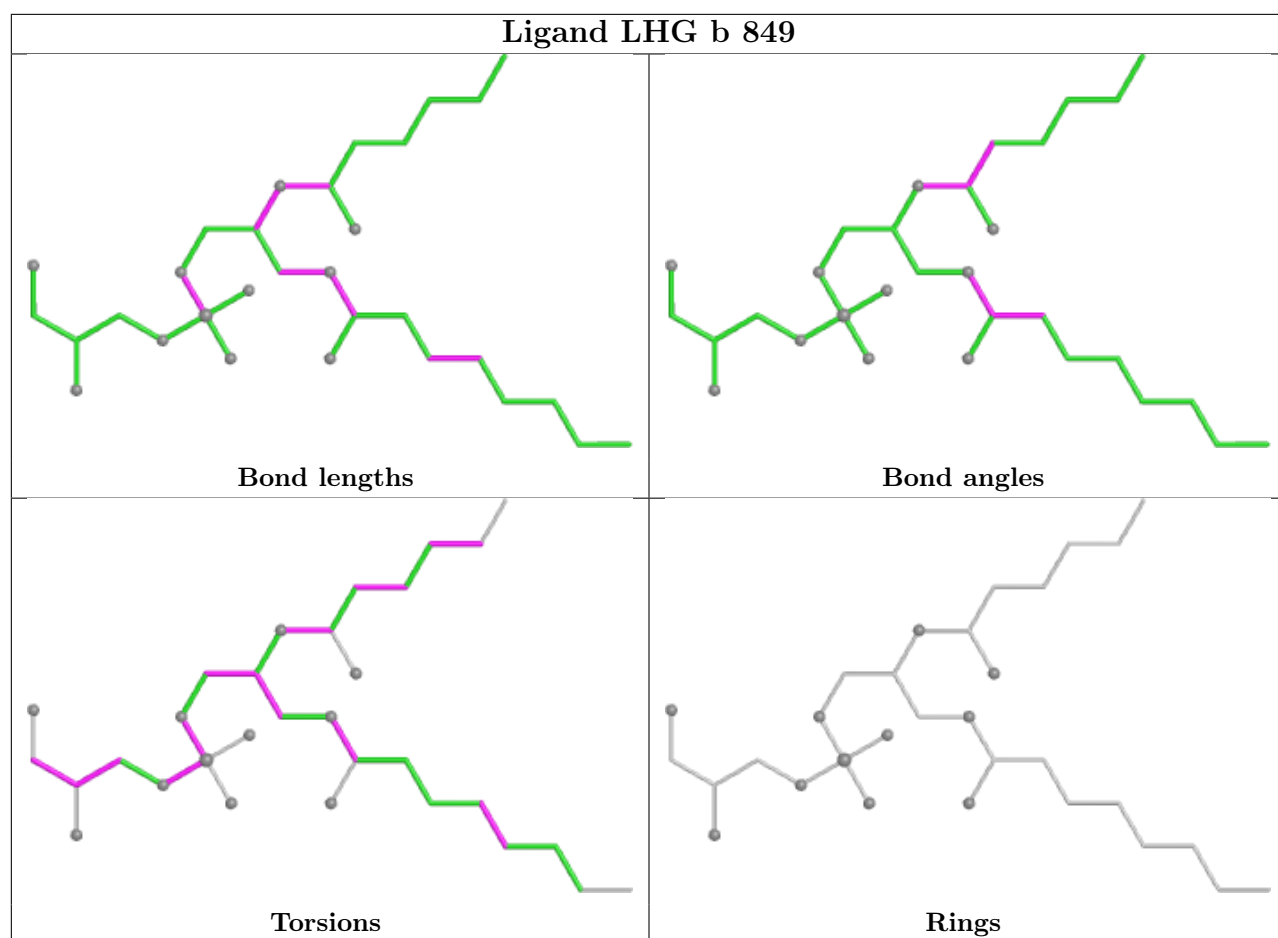
Ligand CLA a 837



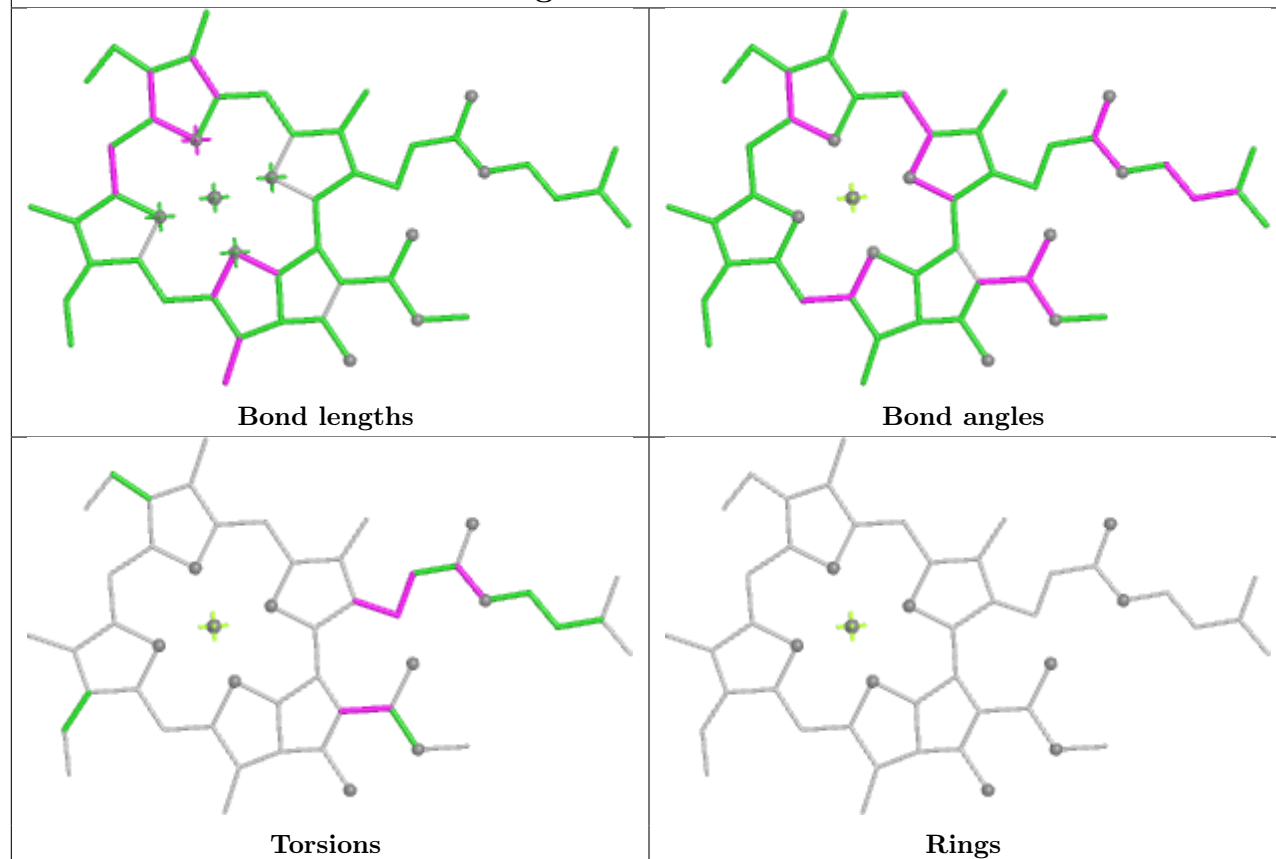
Ligand CLA 1 310



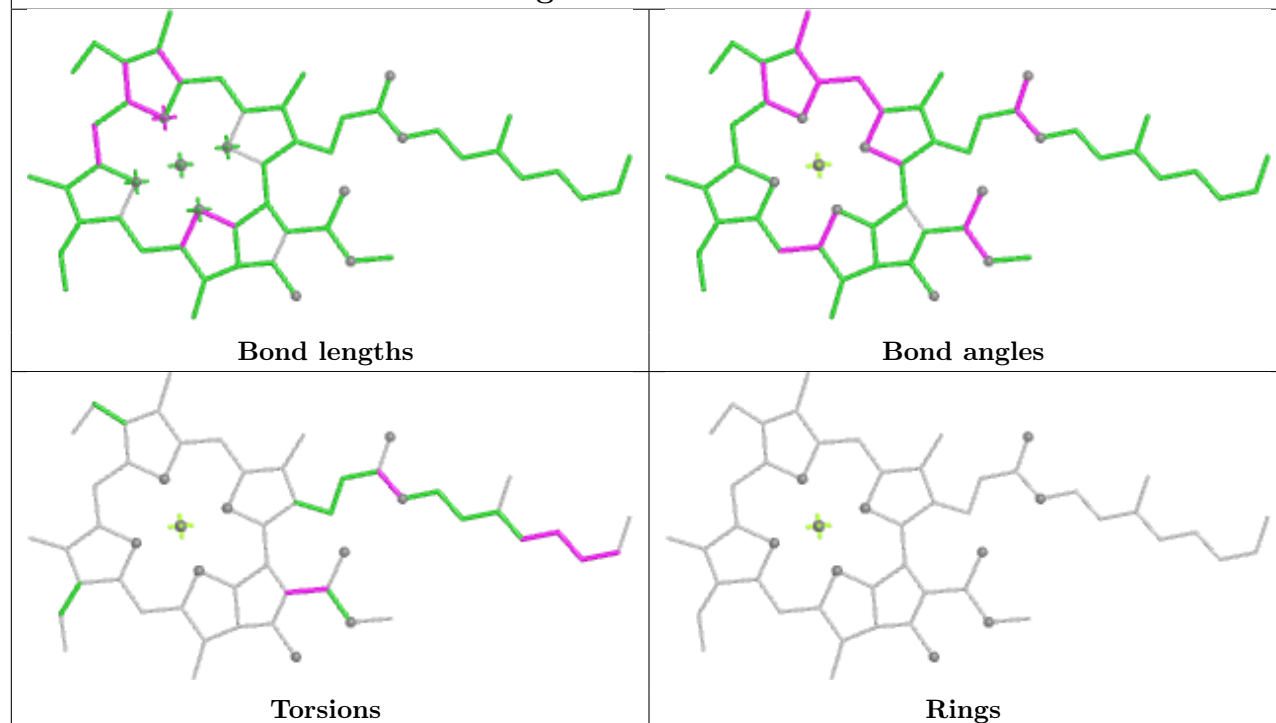


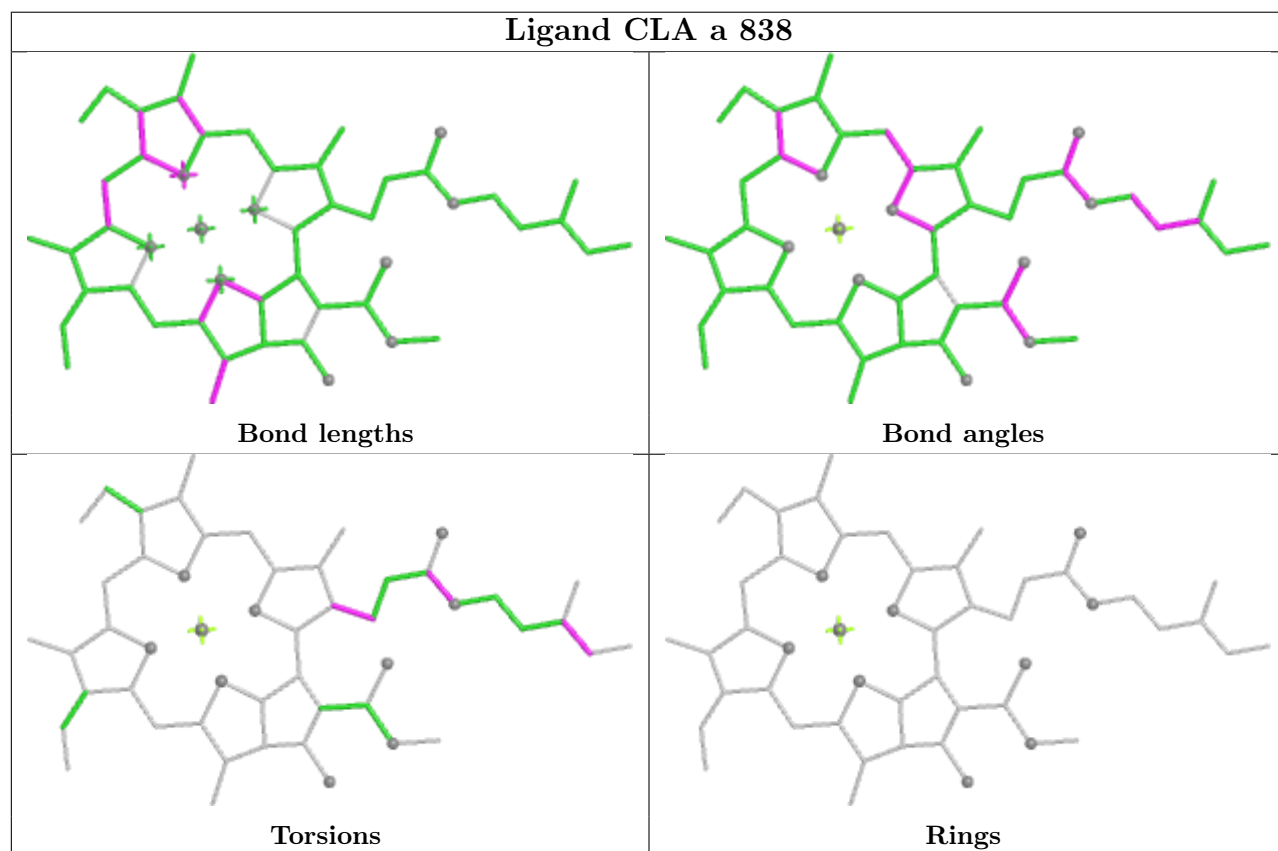
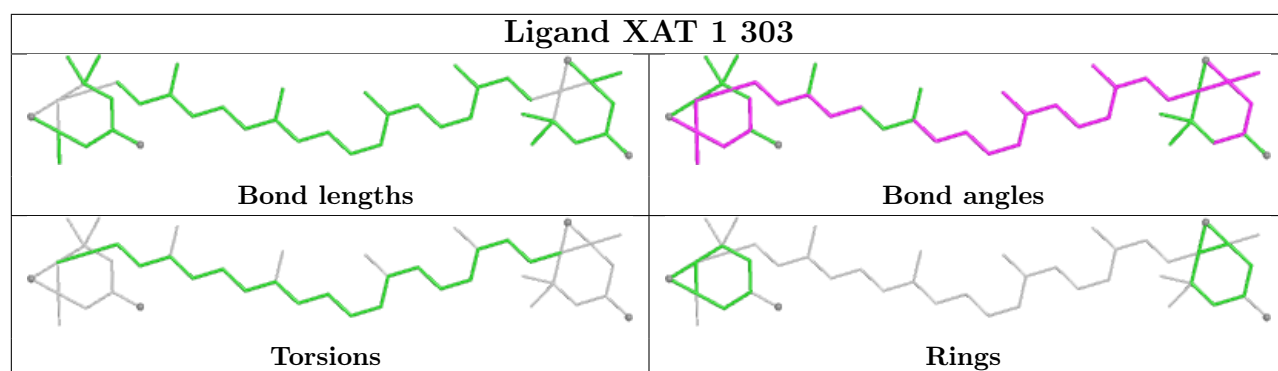


Ligand CLA b 821

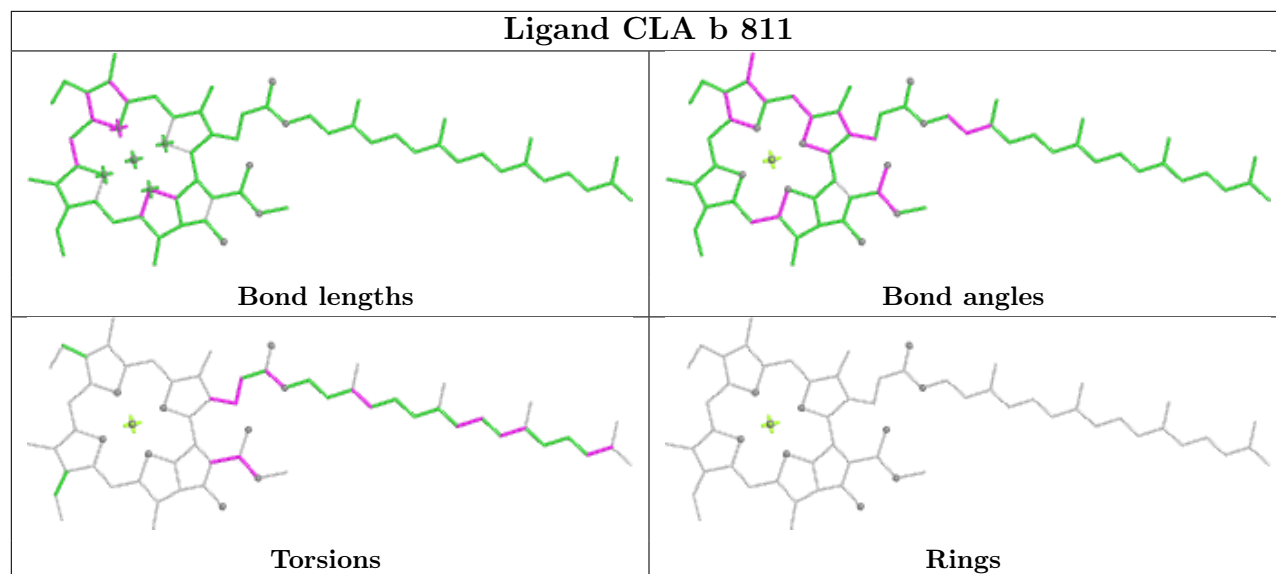


Ligand CLA 1 307

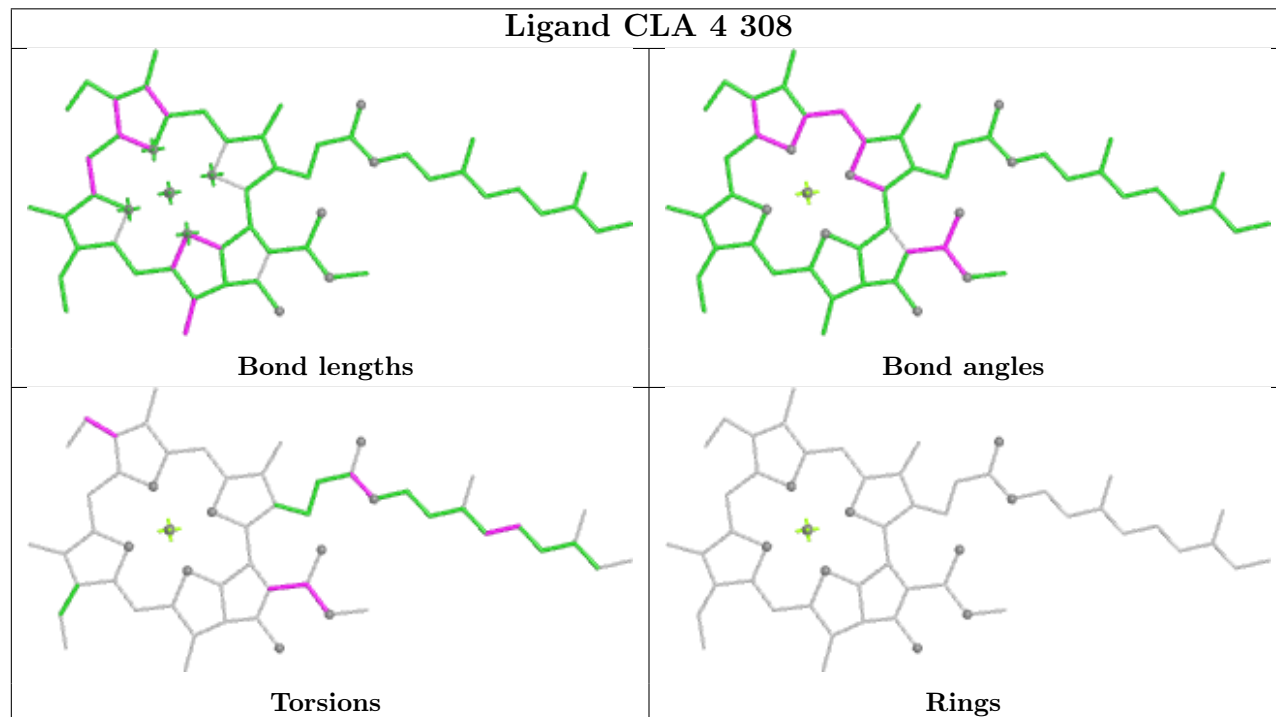


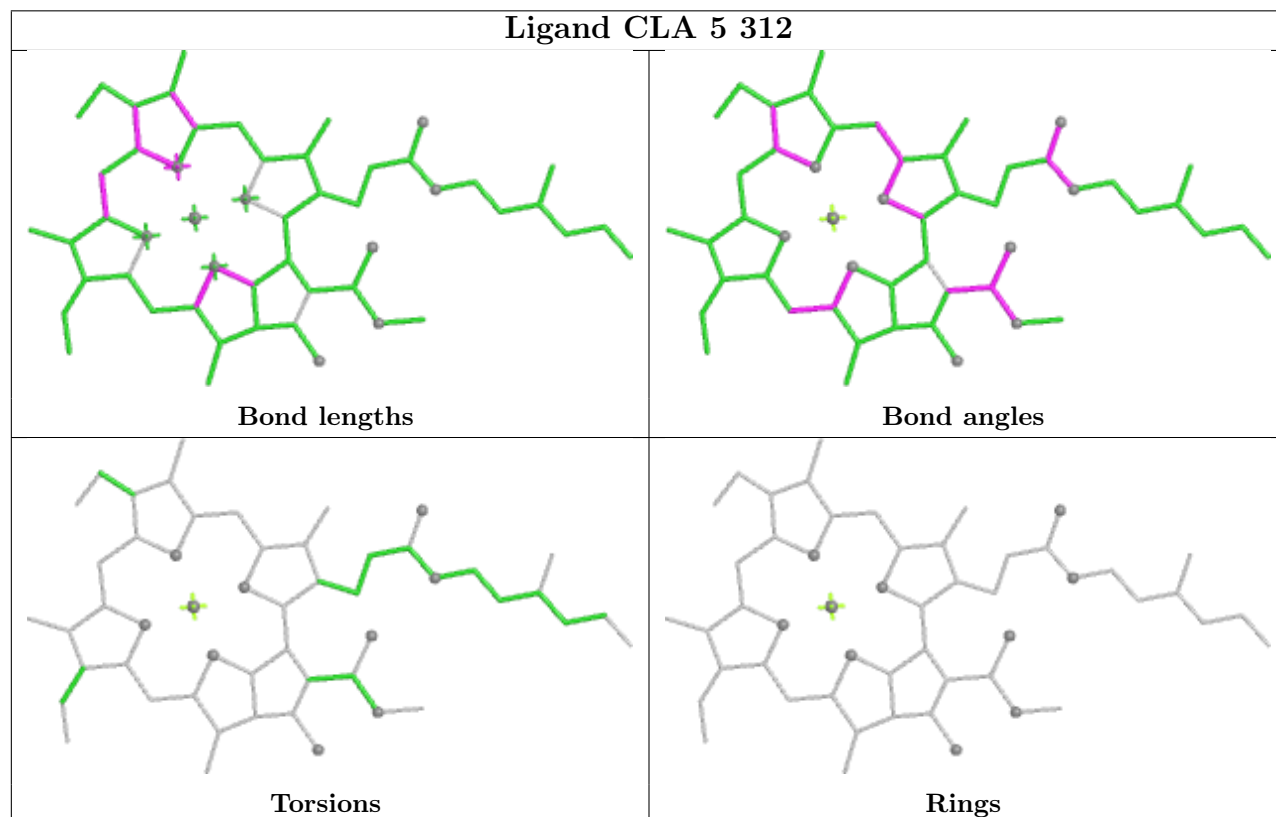
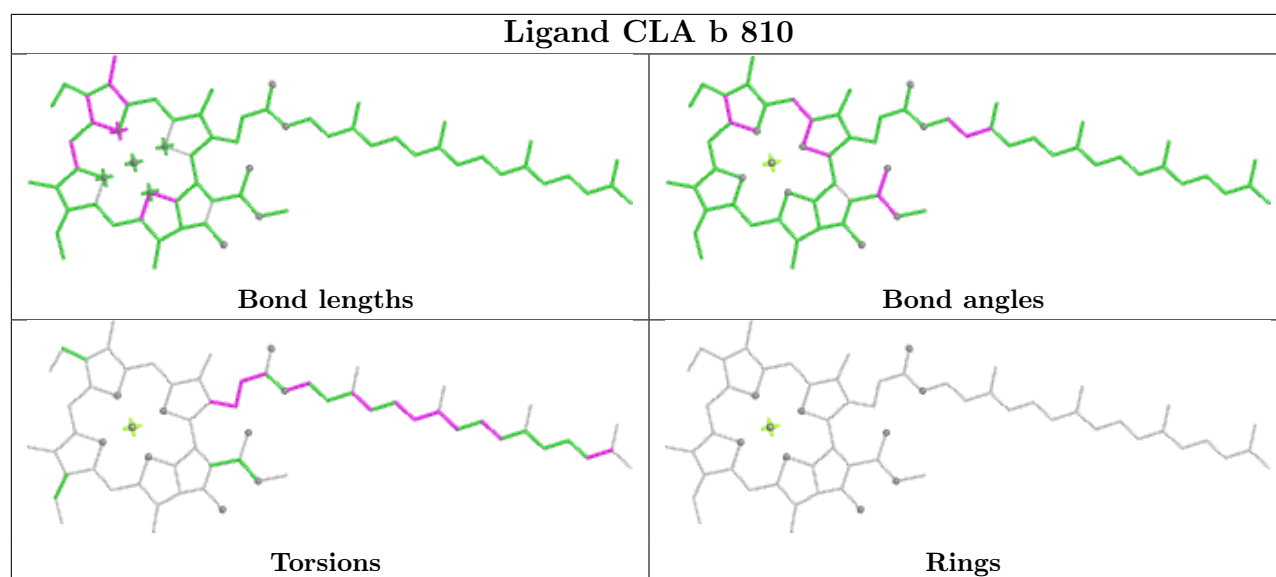


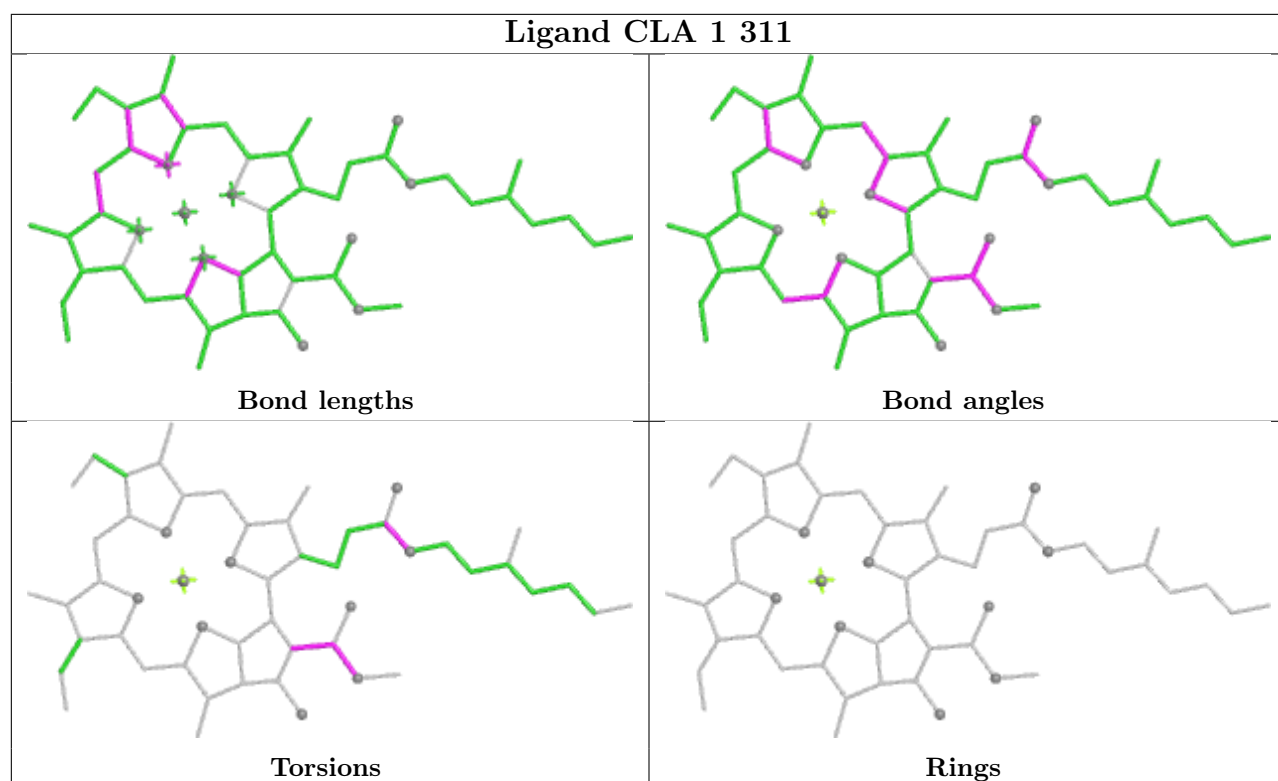
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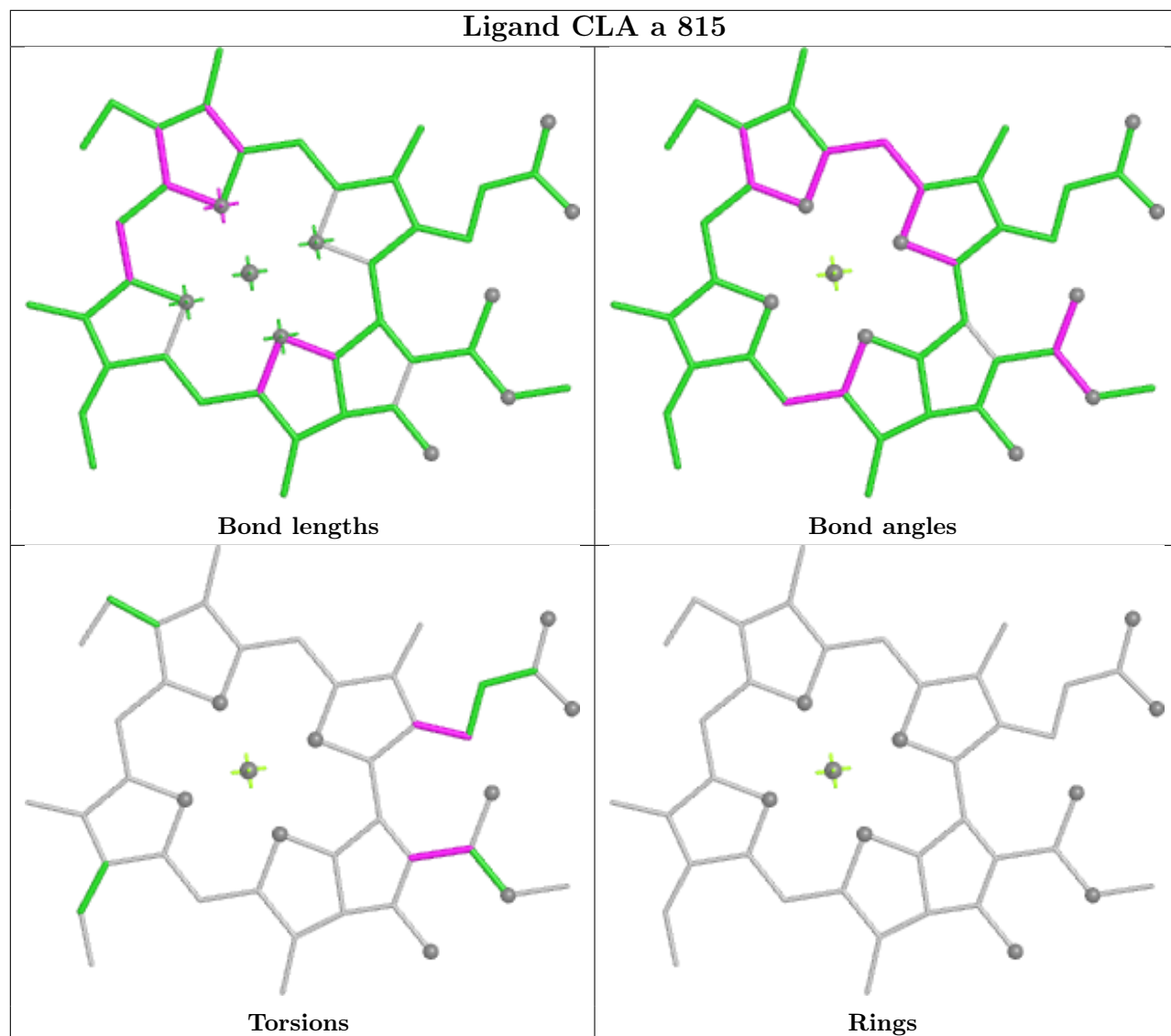
Ligand CLA 4 308

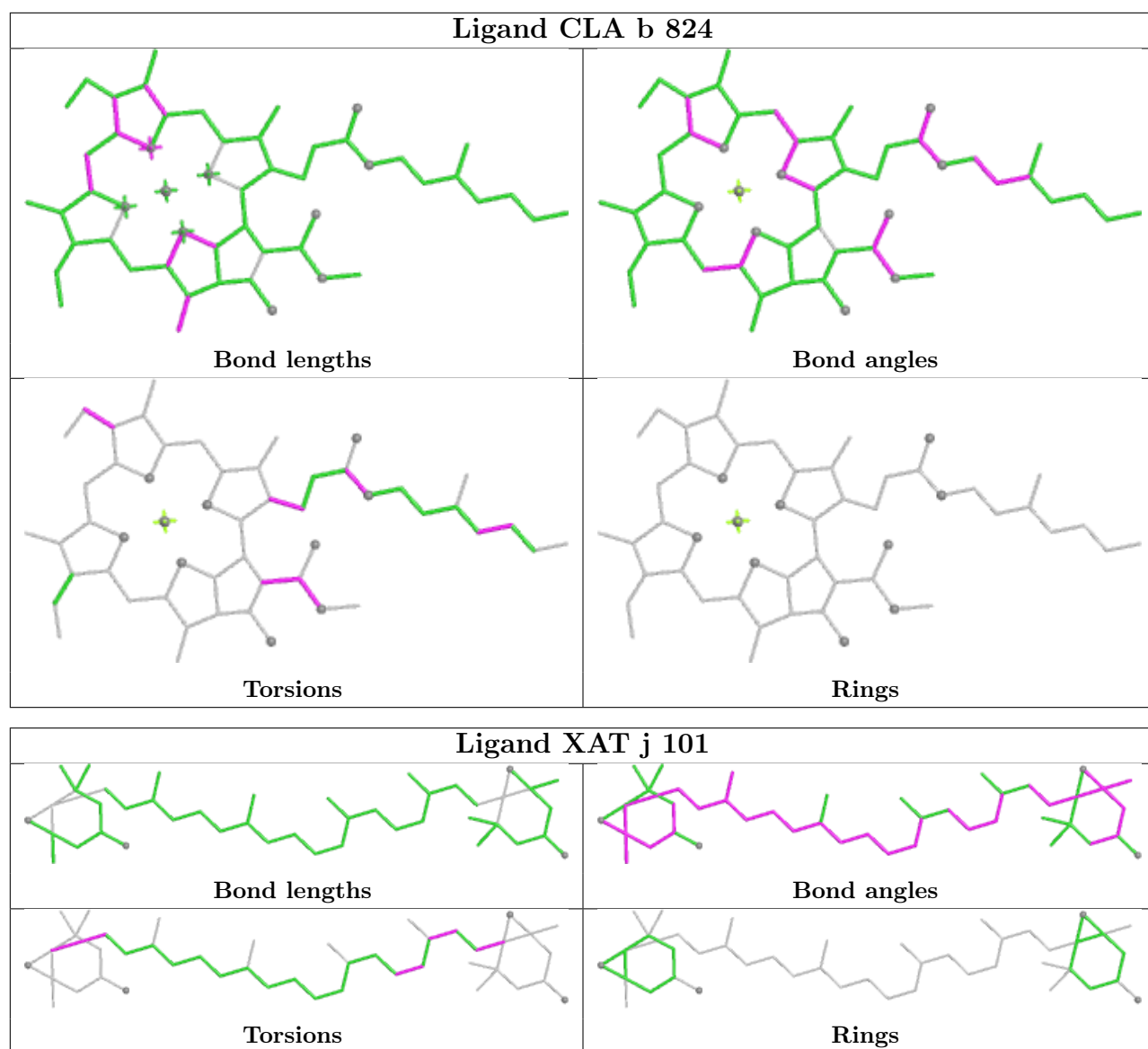




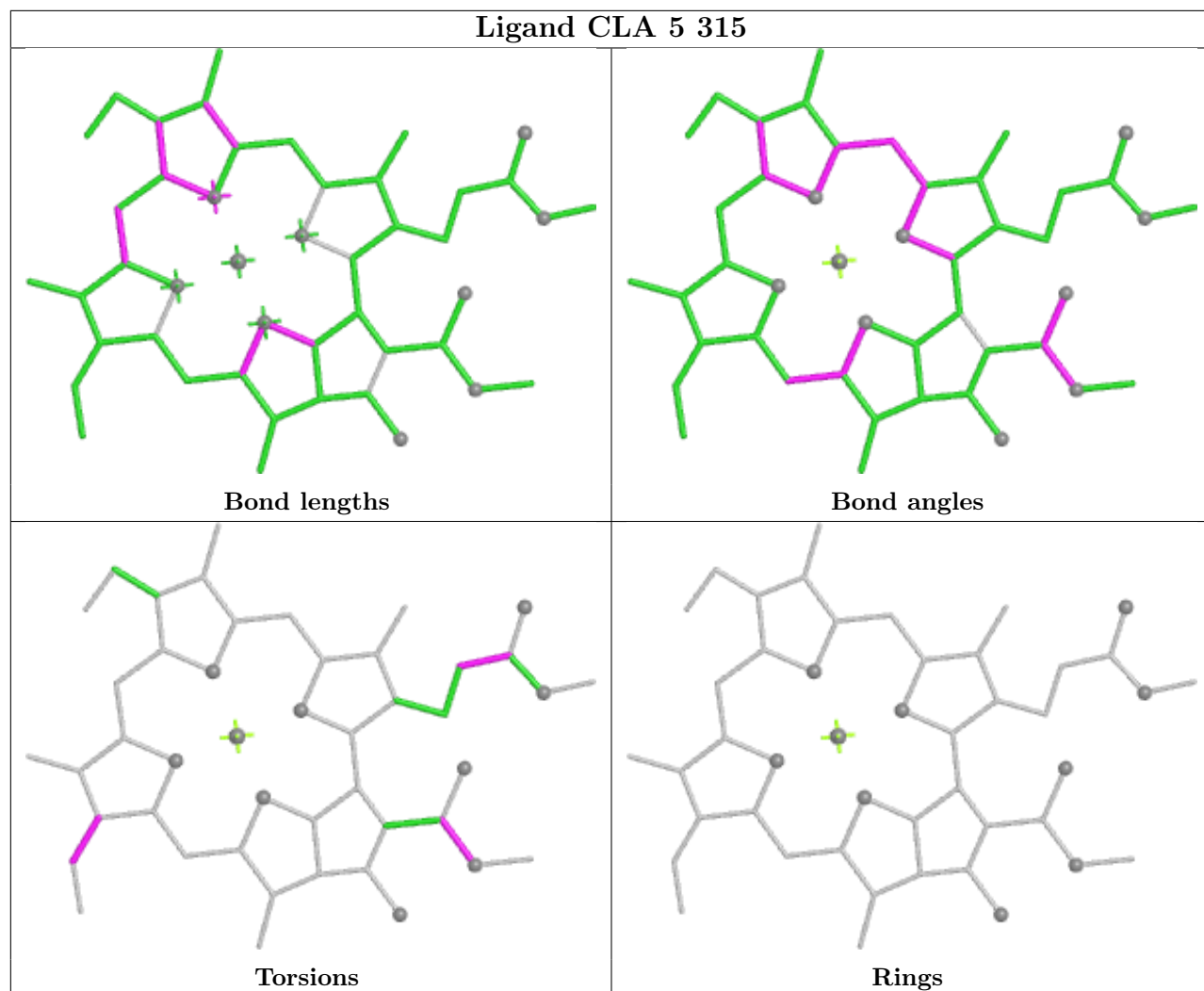


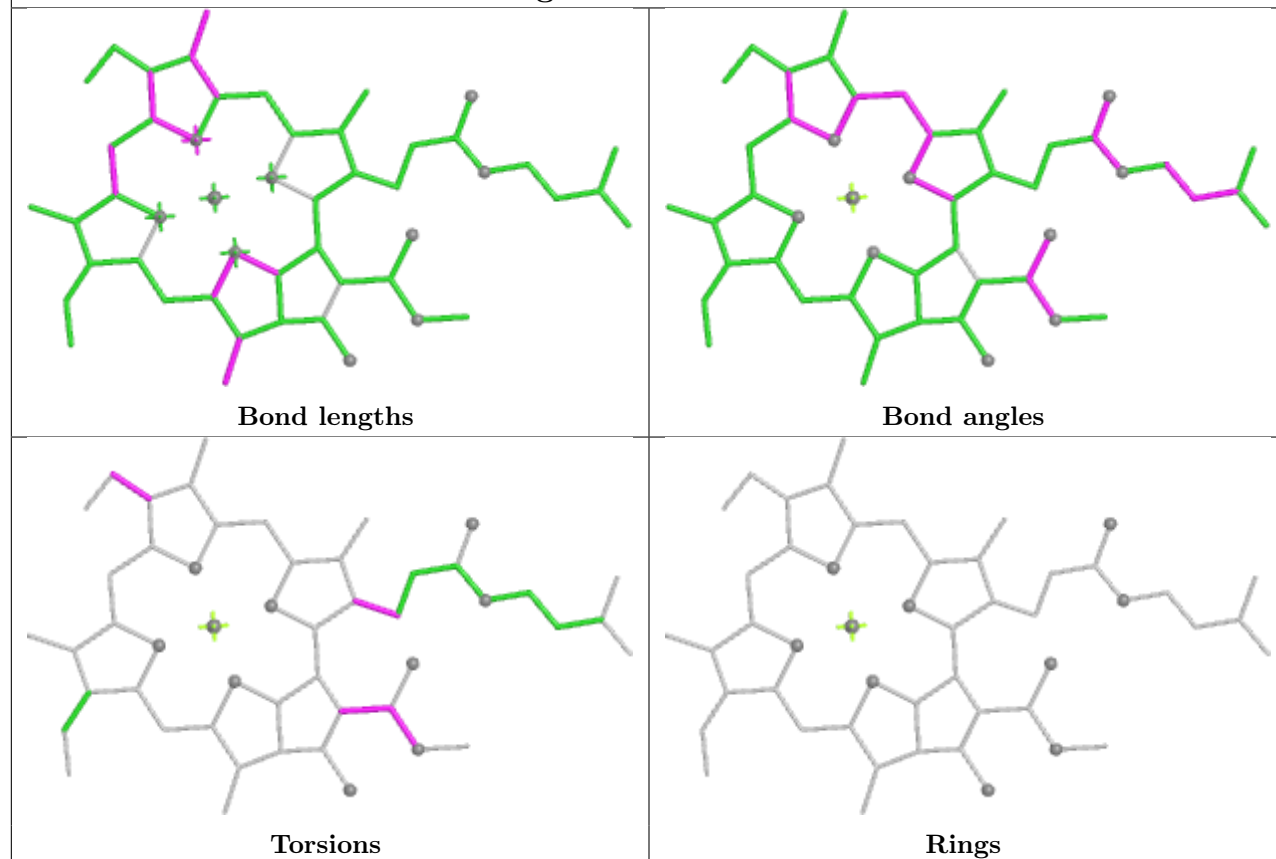
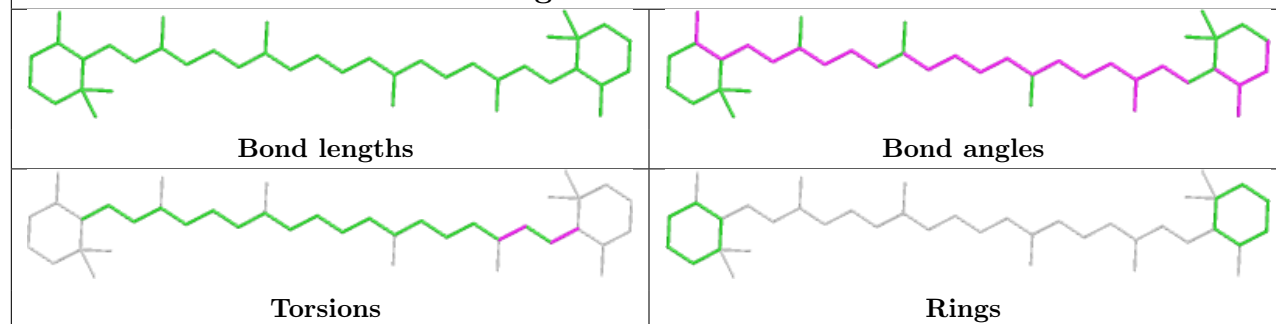
Ligand CLA a 815



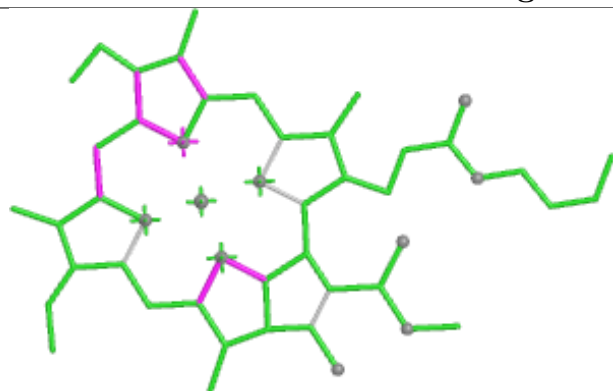


Ligand CLA 5 315

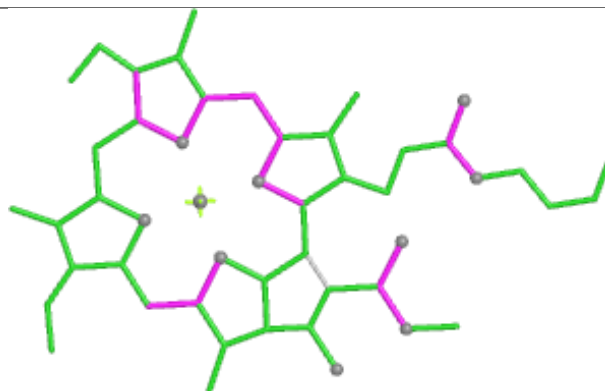


Ligand CLA a 832**Ligand BCR a 850**

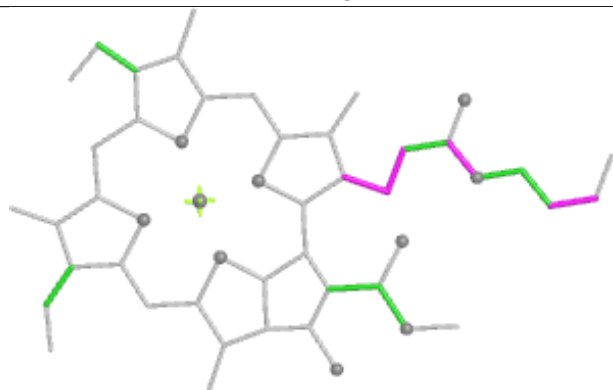
Ligand CLA b 832



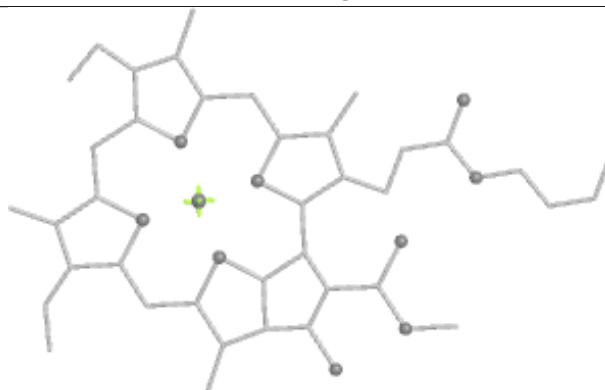
Bond lengths



Bond angles

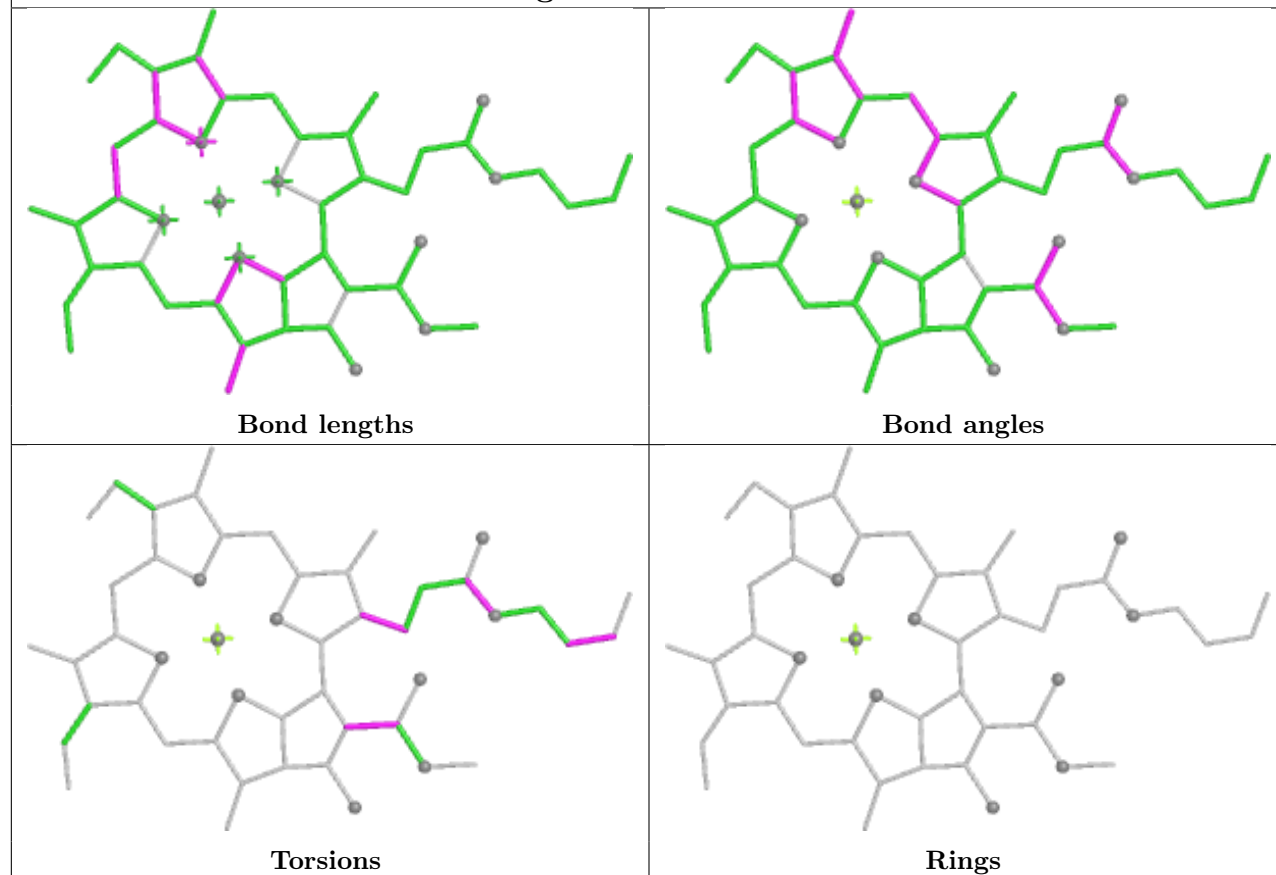


Torsions

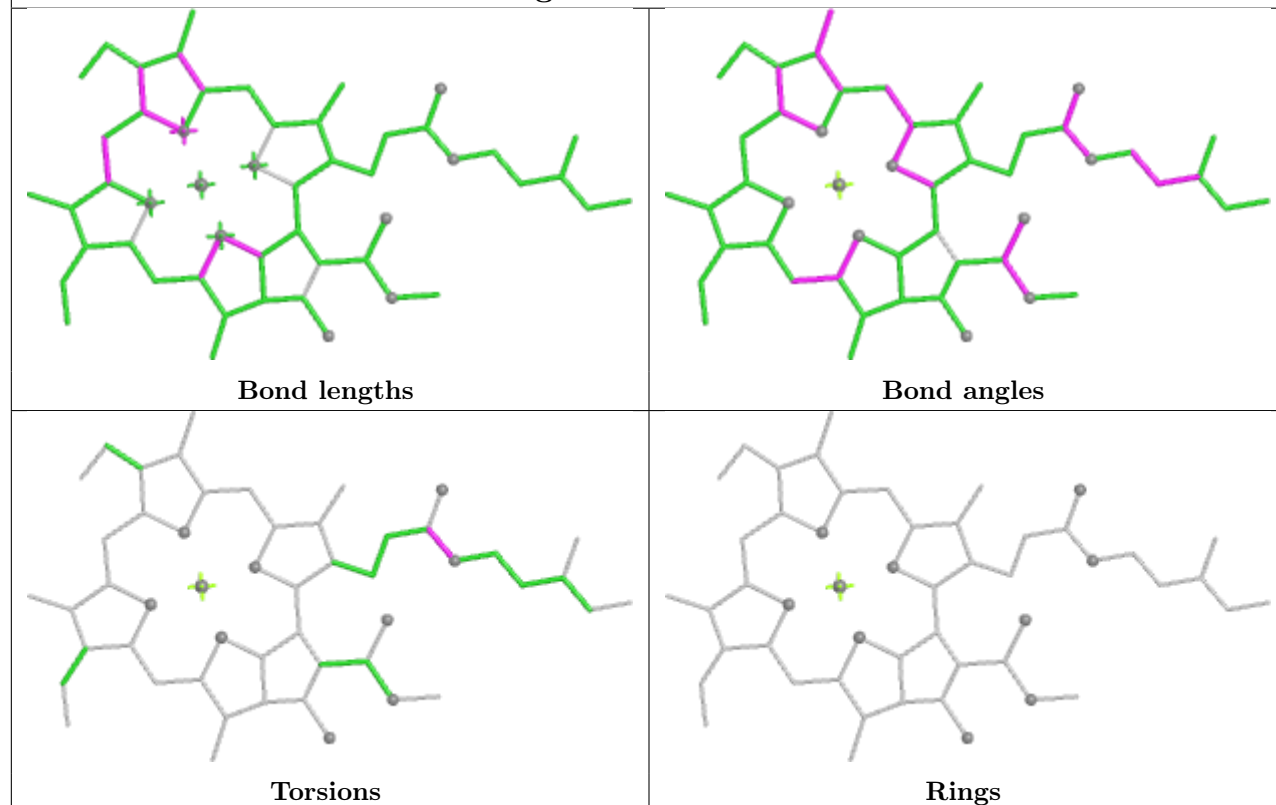


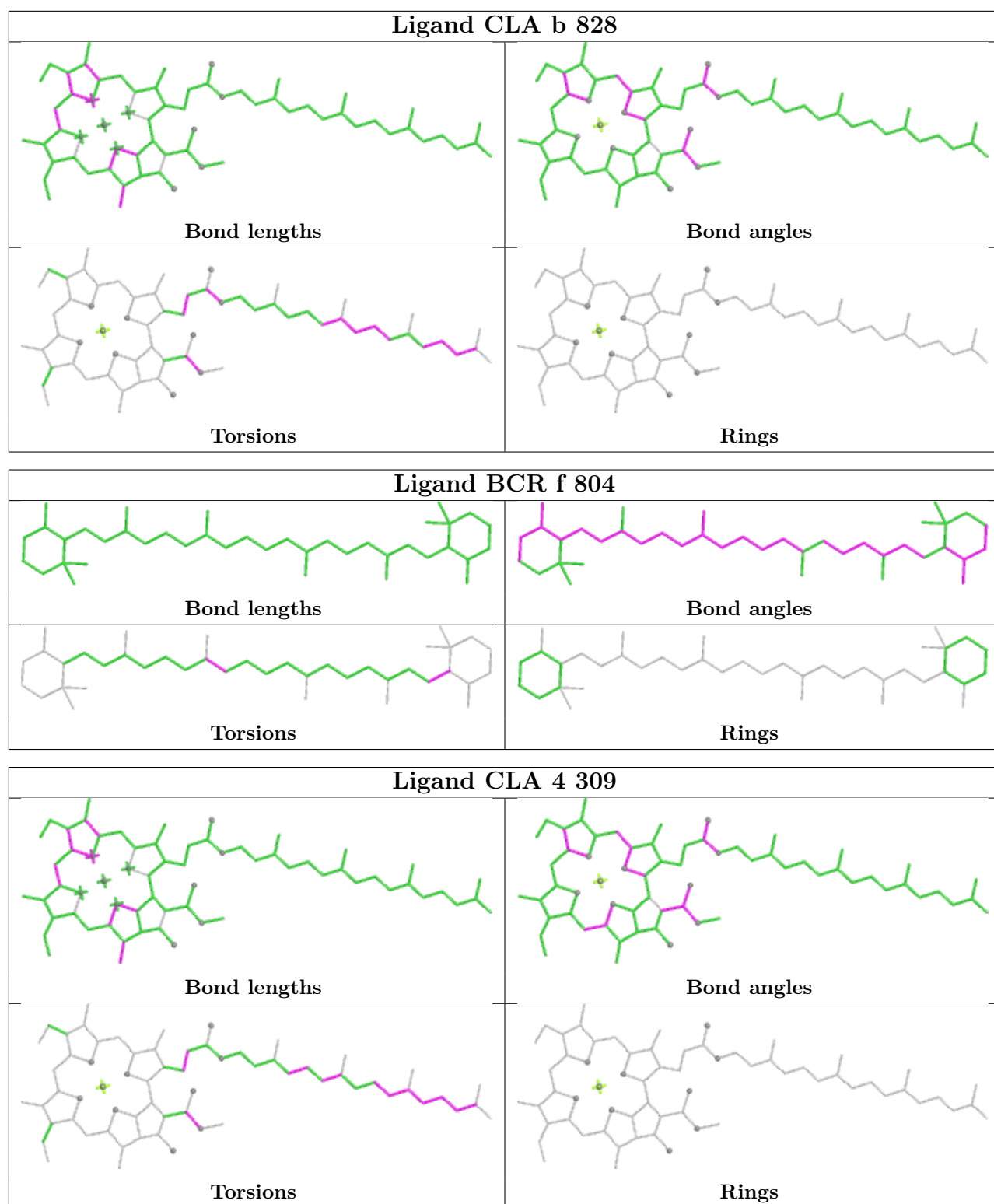
Rings

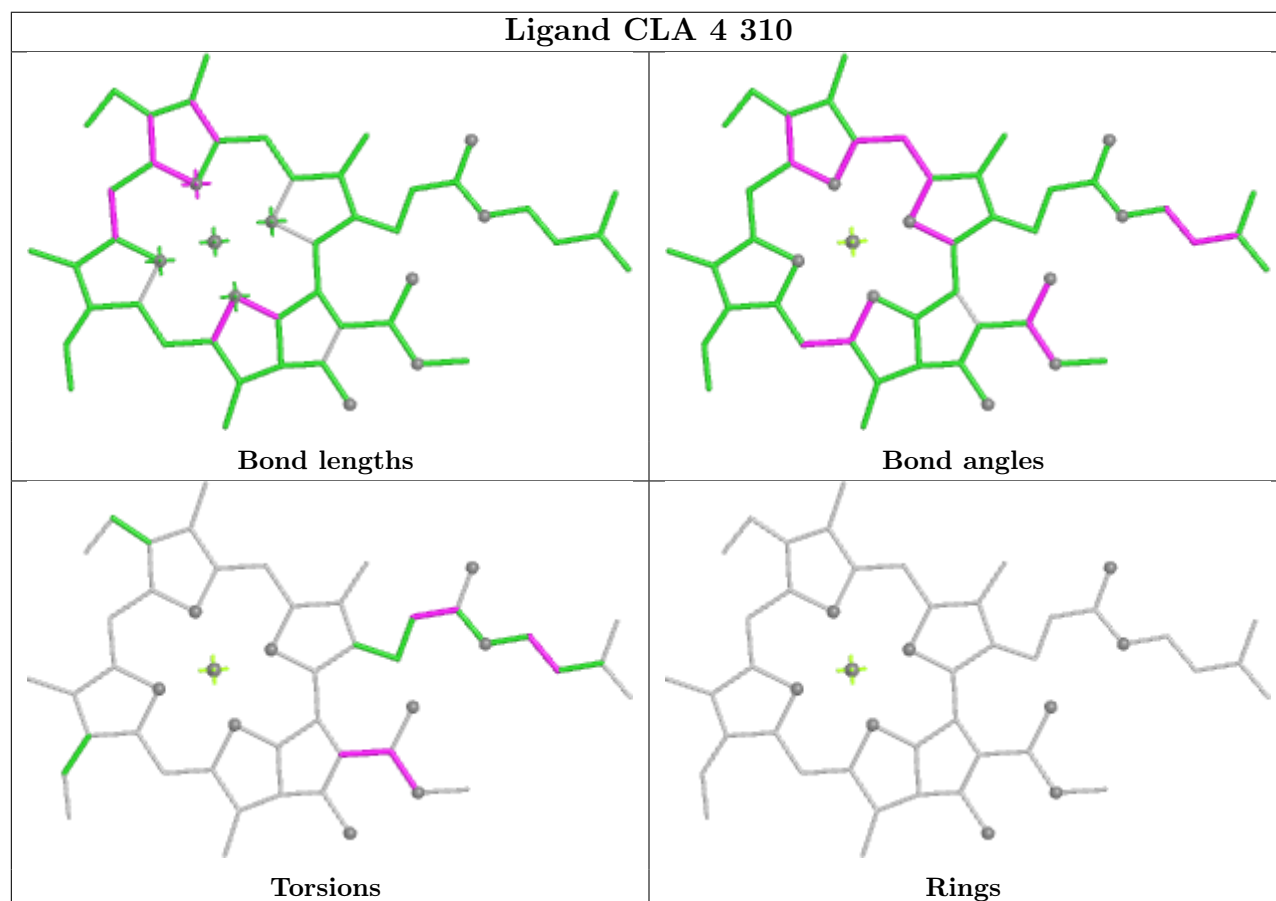
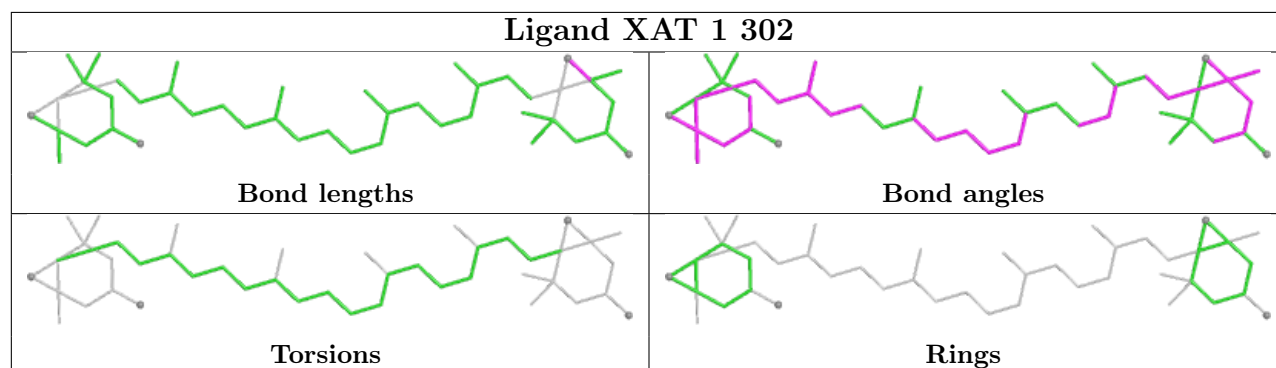
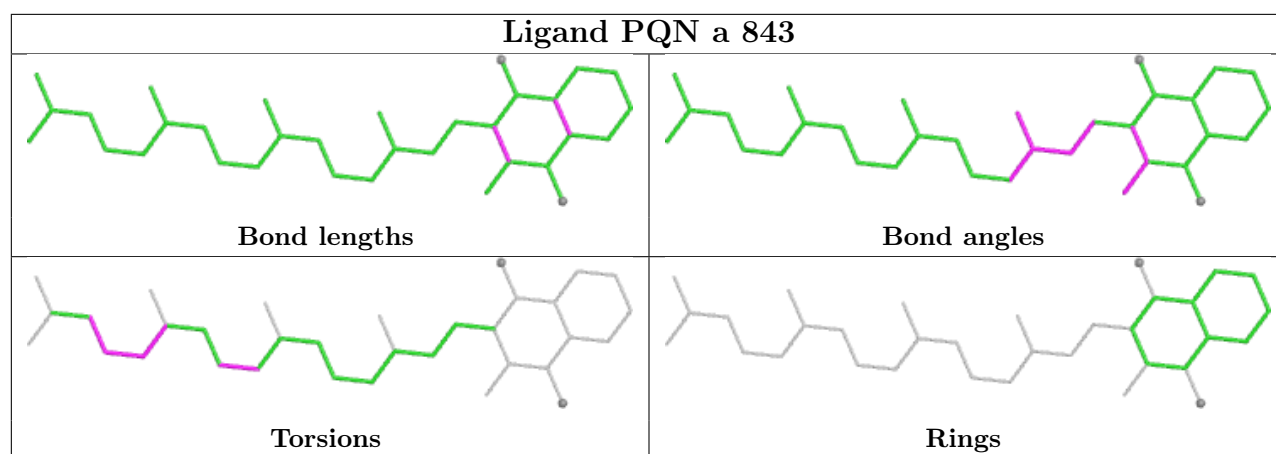
Ligand CLA a 823

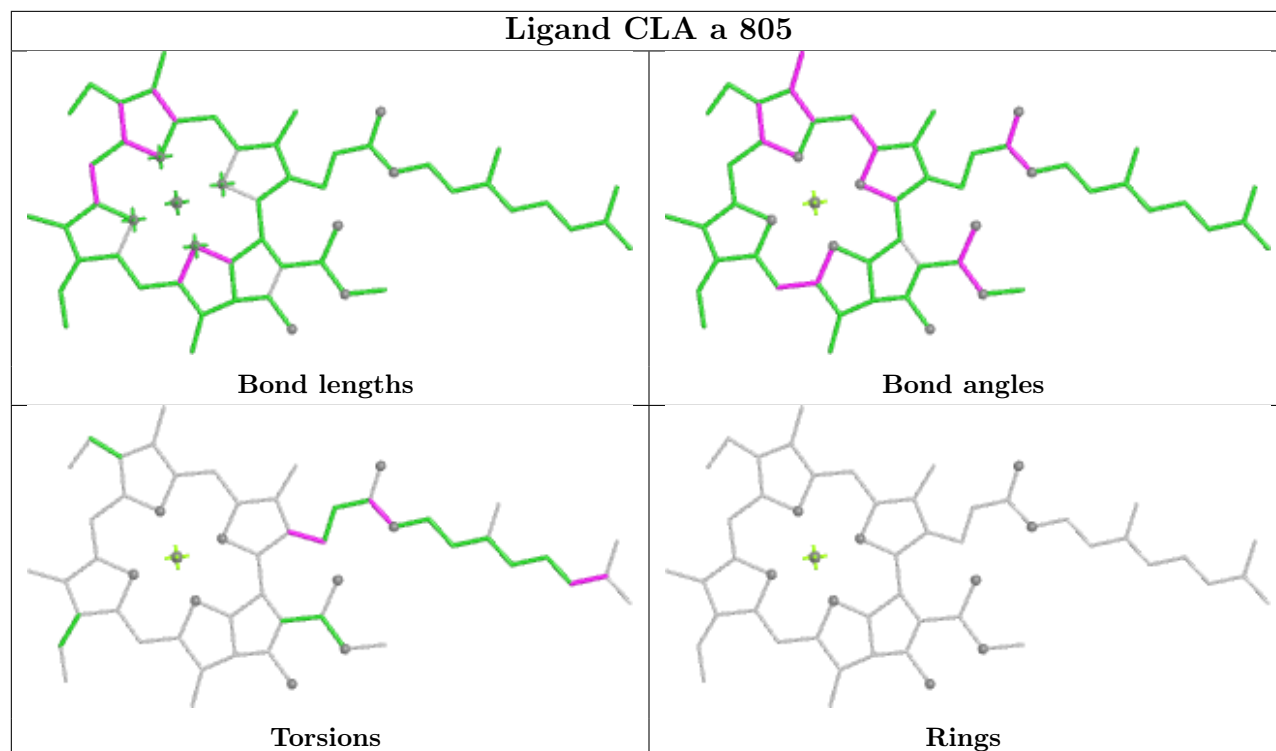
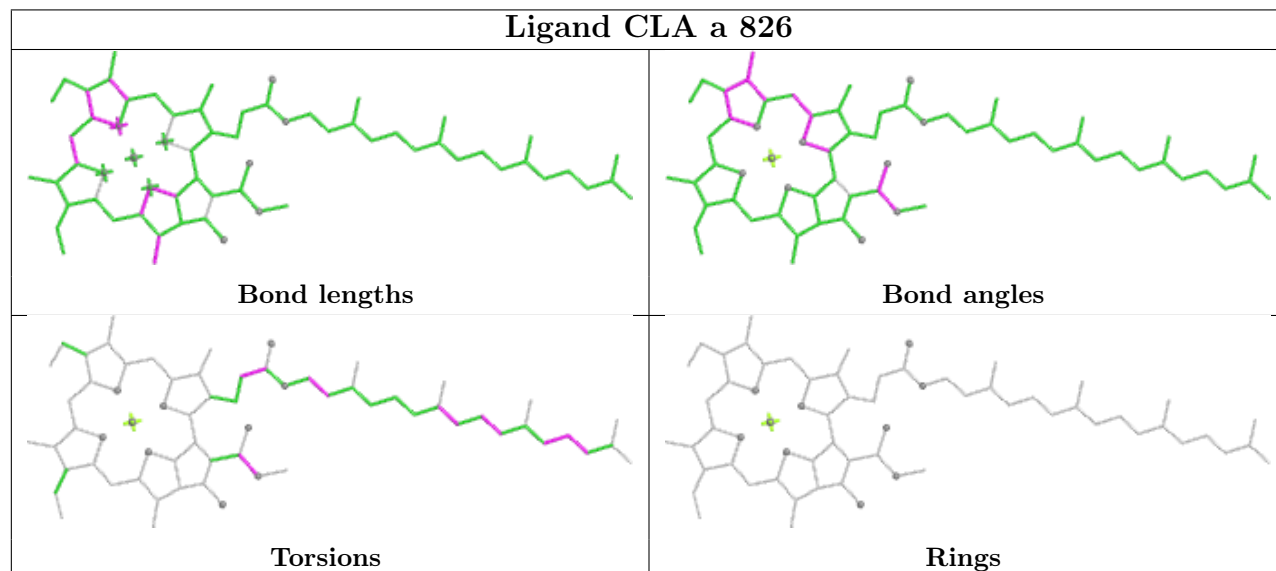


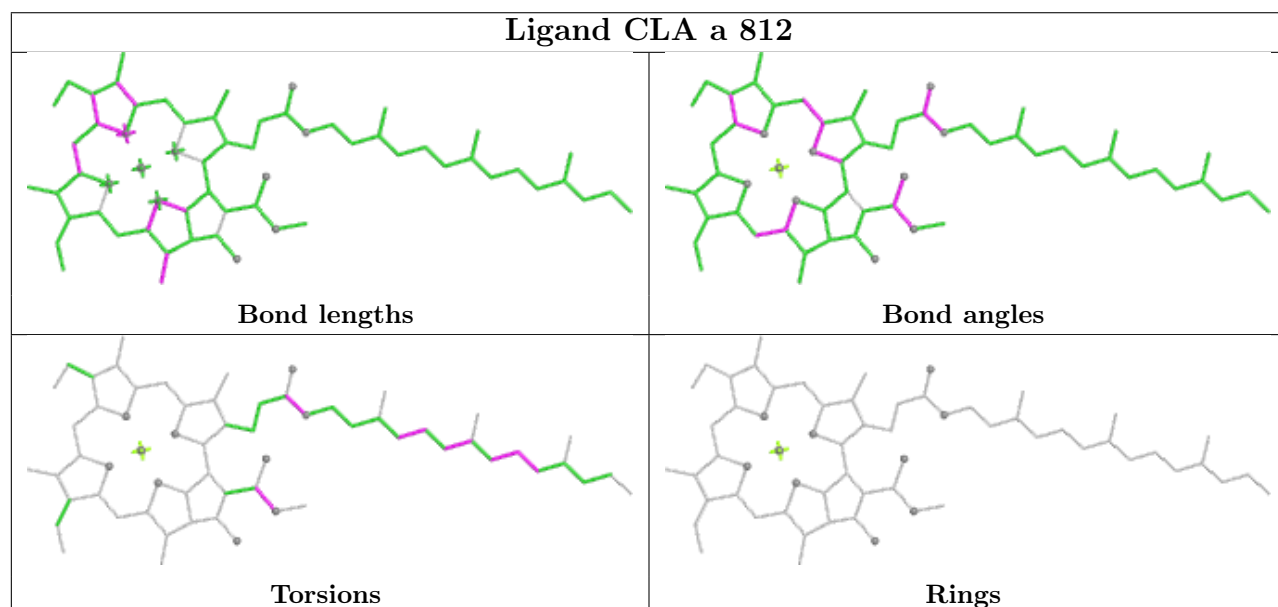
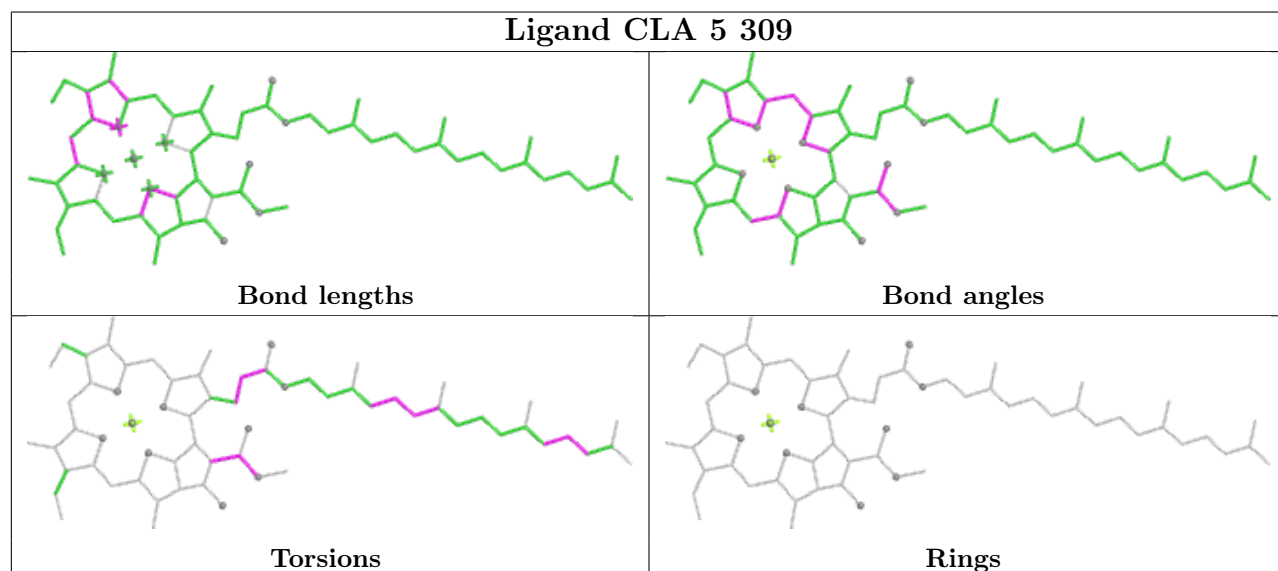
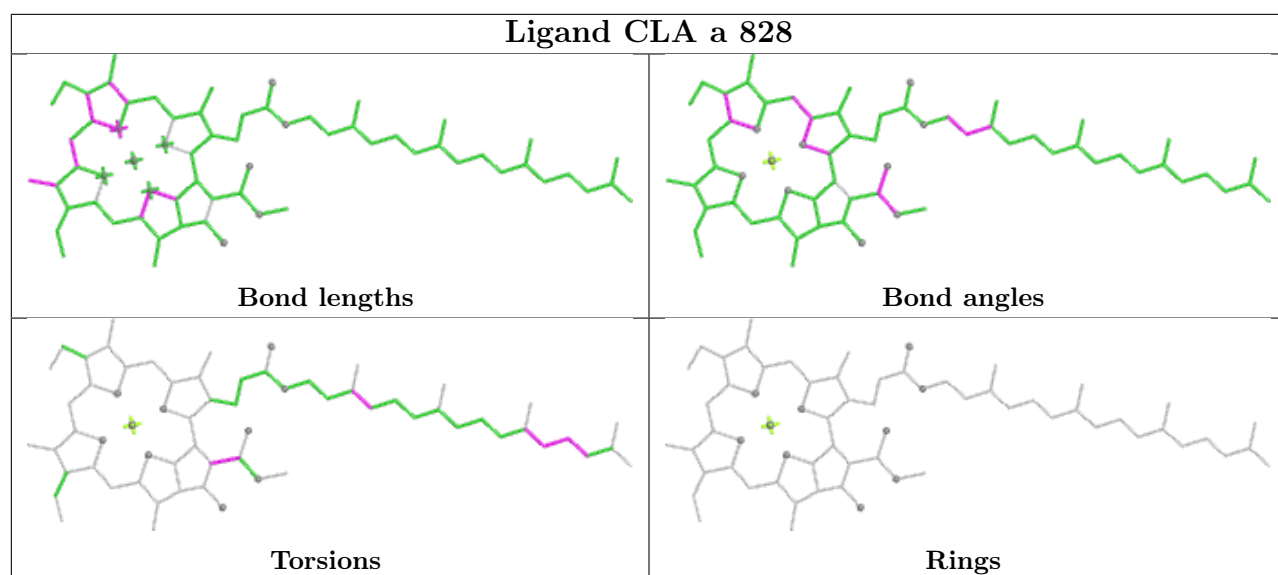
Ligand CLA b 822

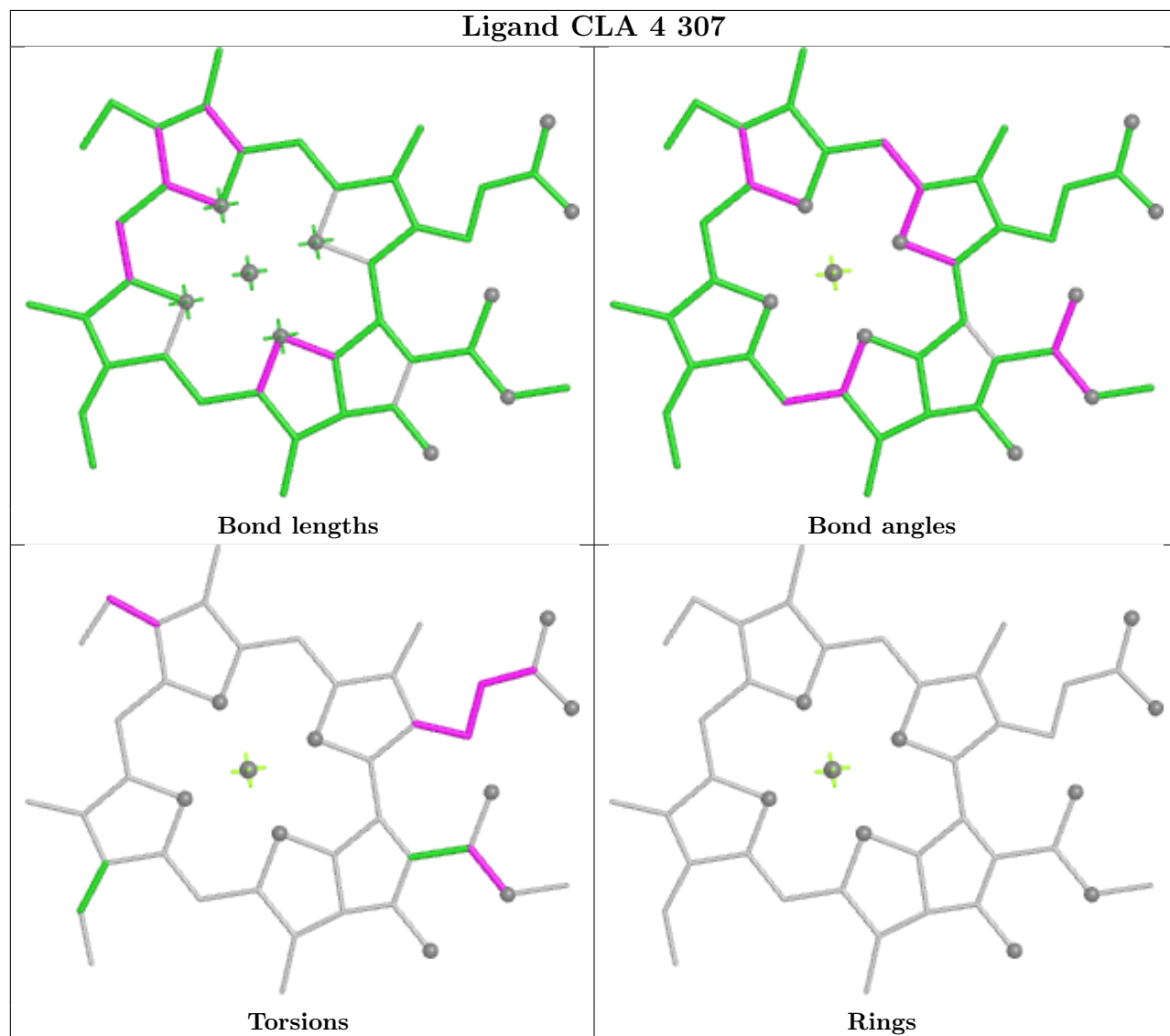
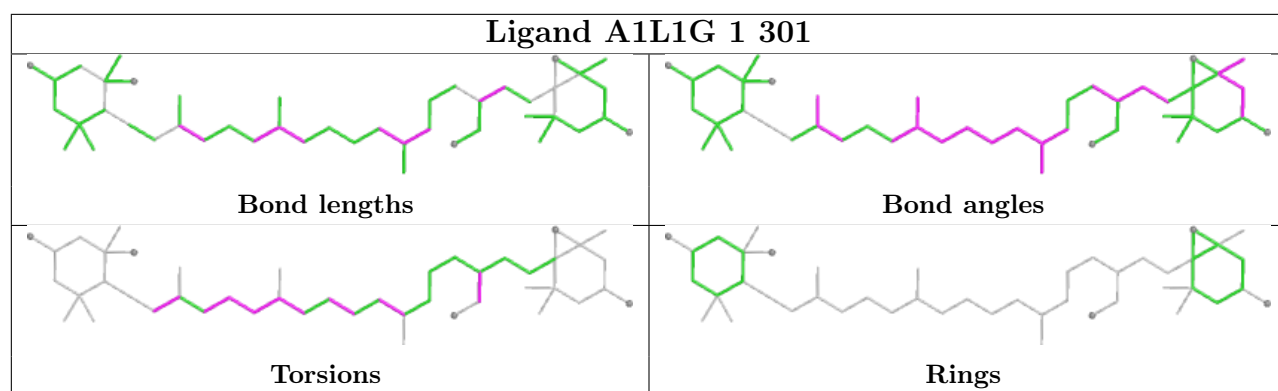


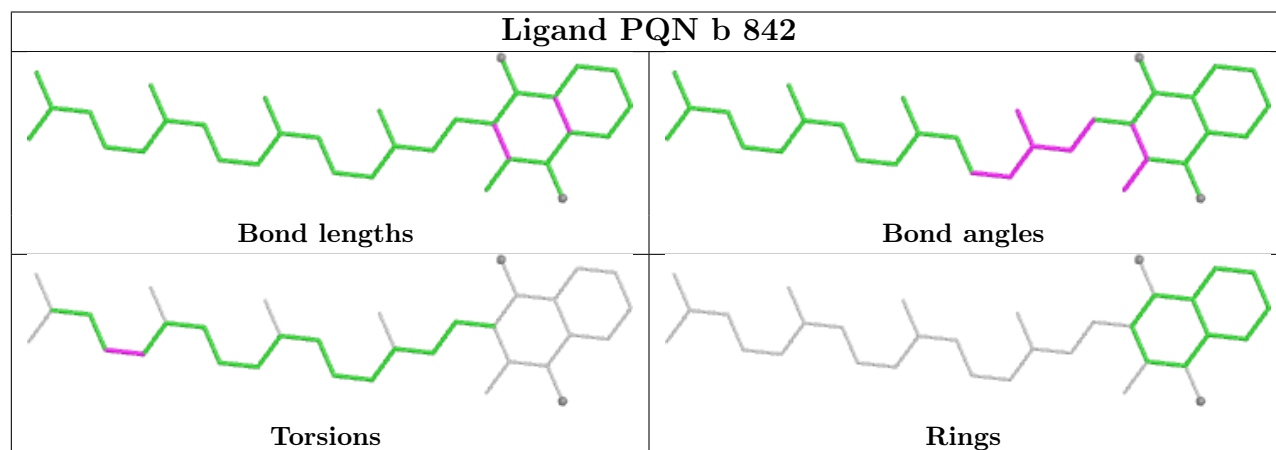
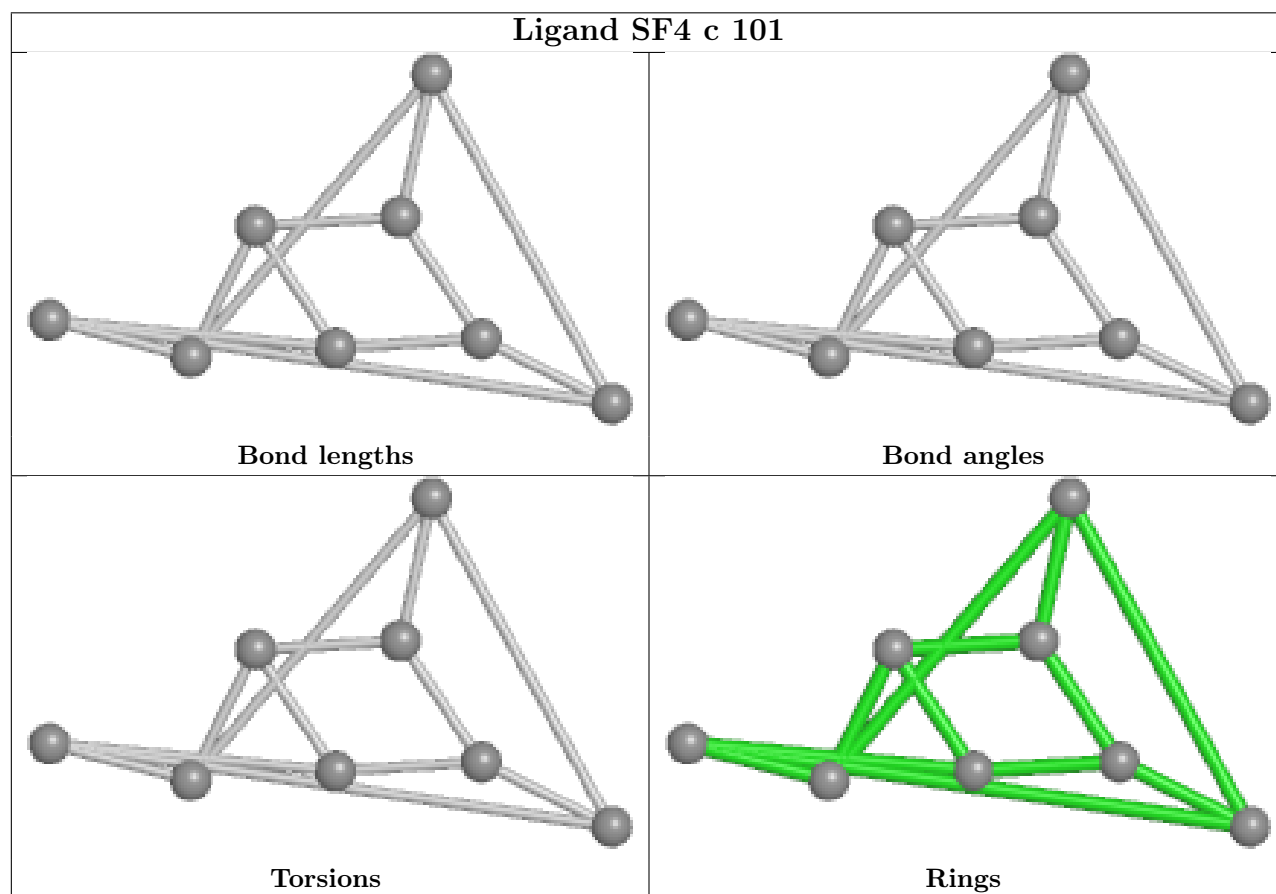
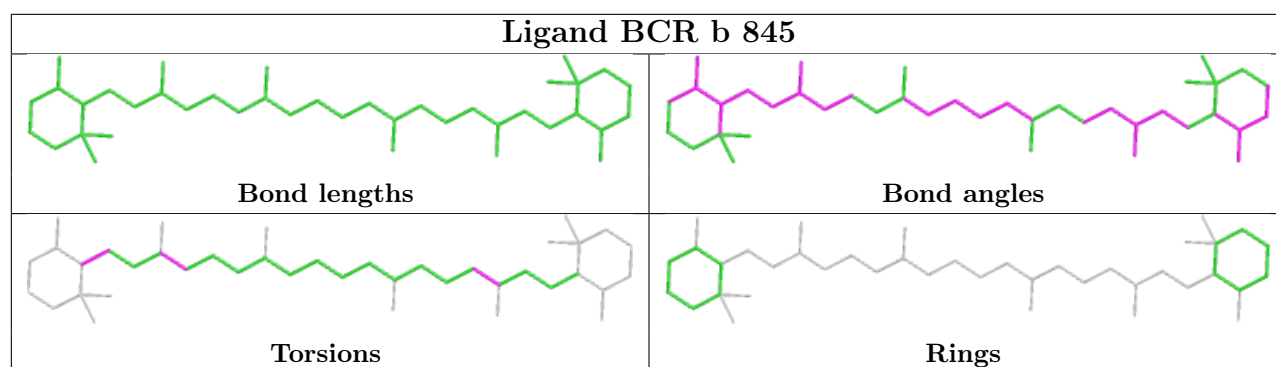




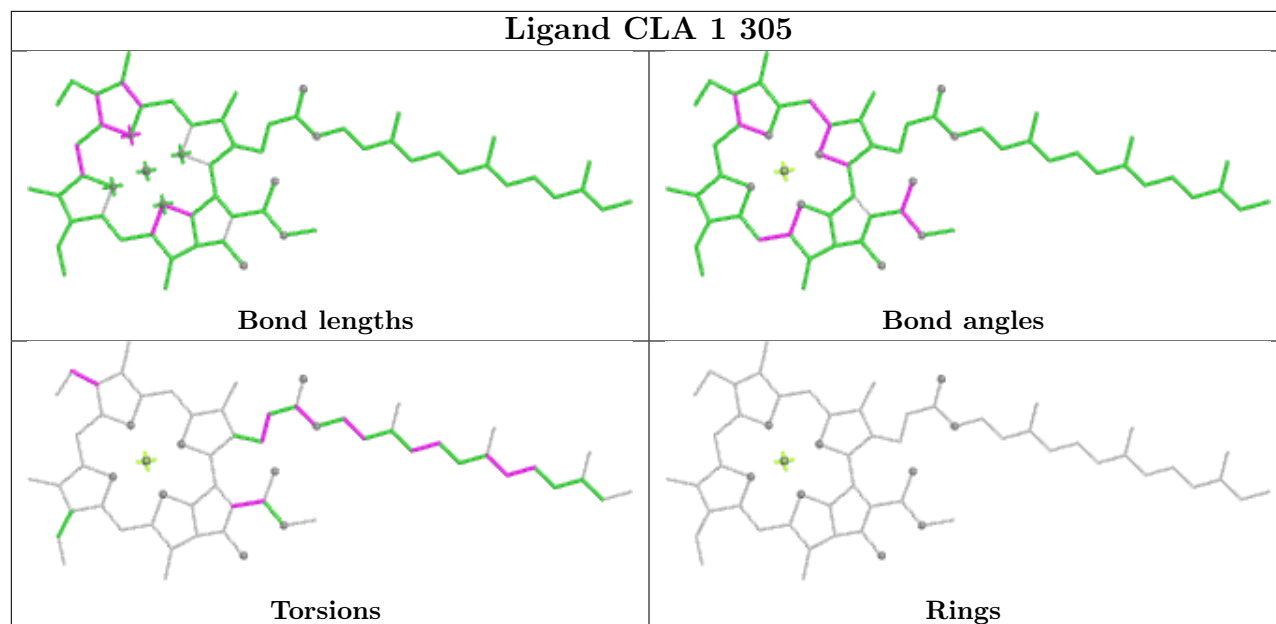
Ligand CLA a 805**Ligand CLA a 826**



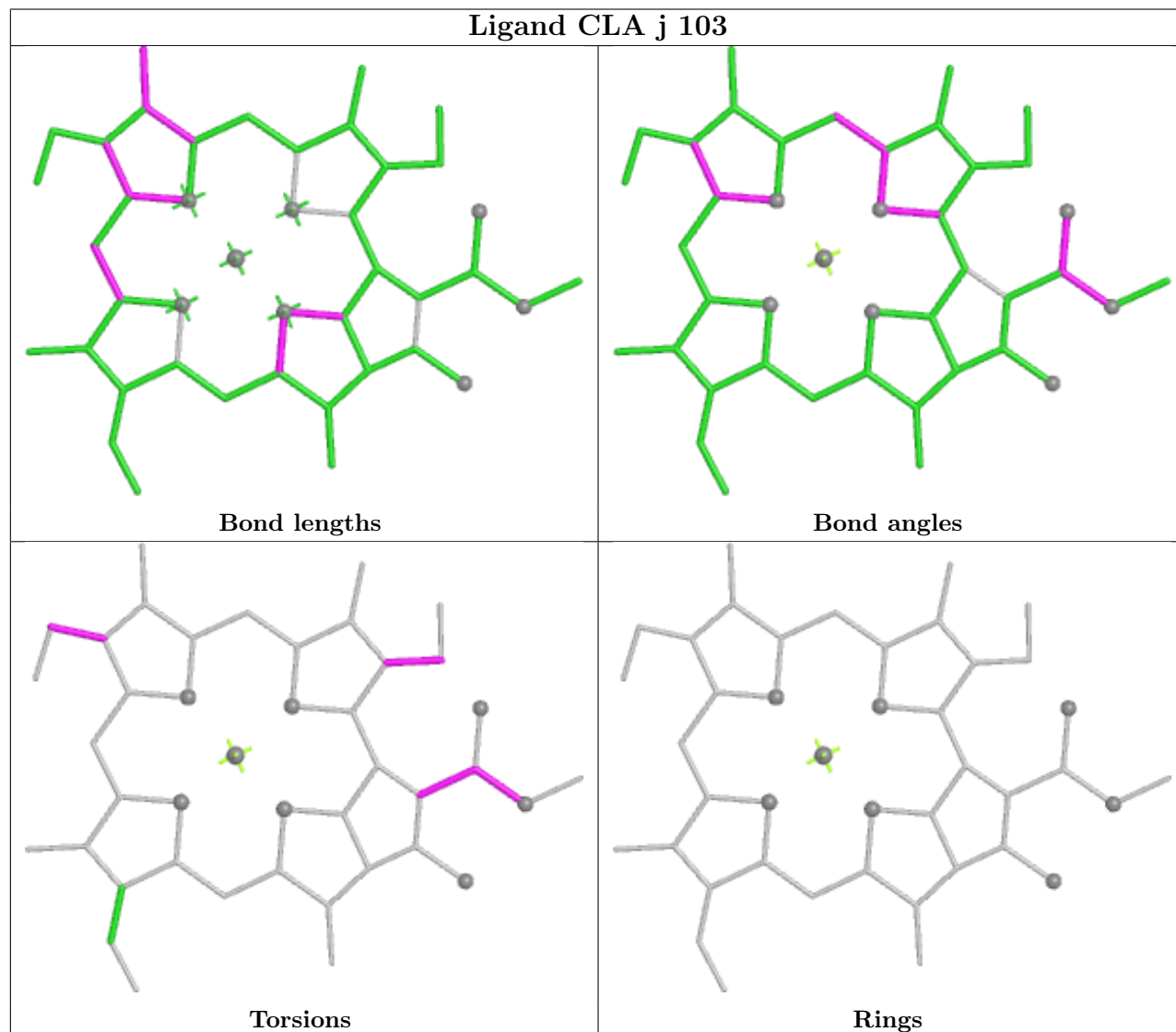


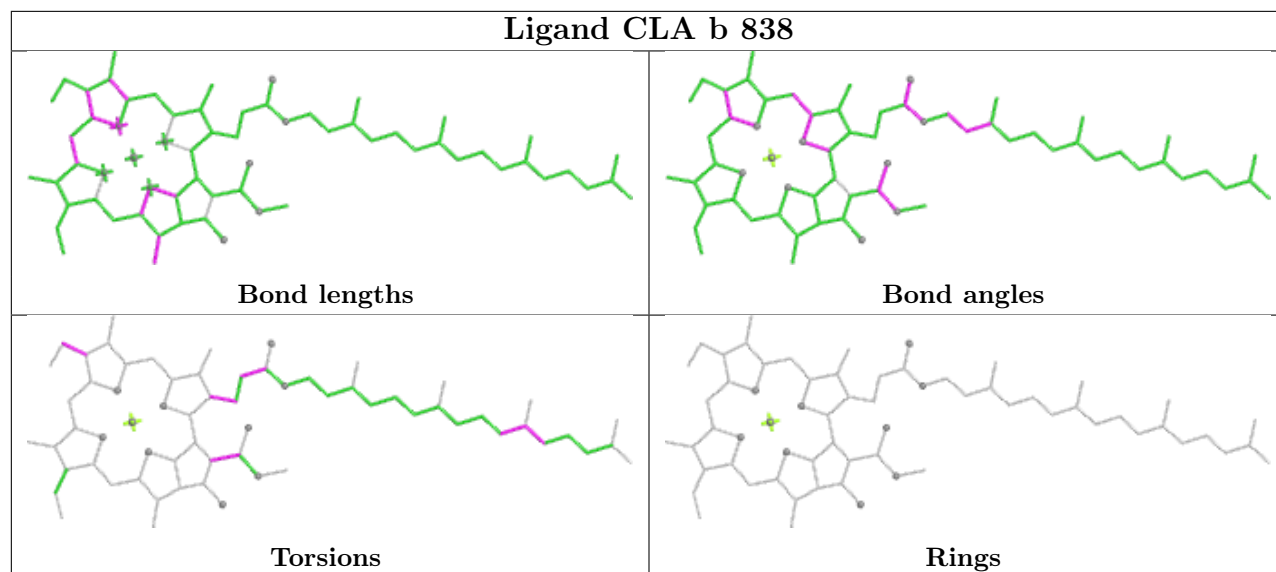
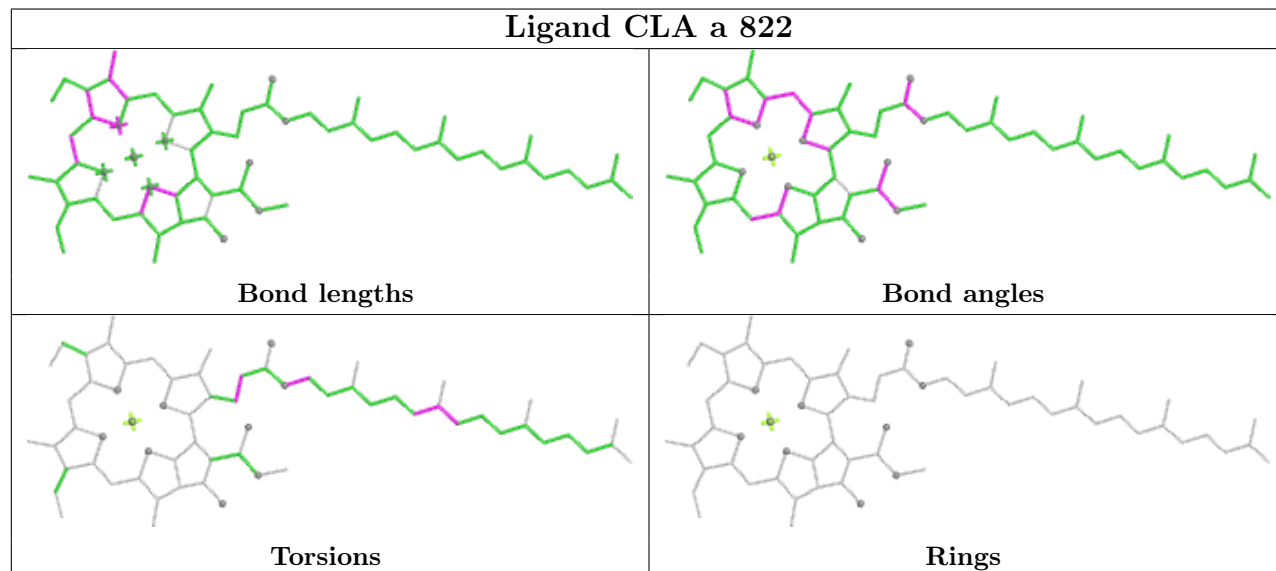


Ligand CLA 1 305

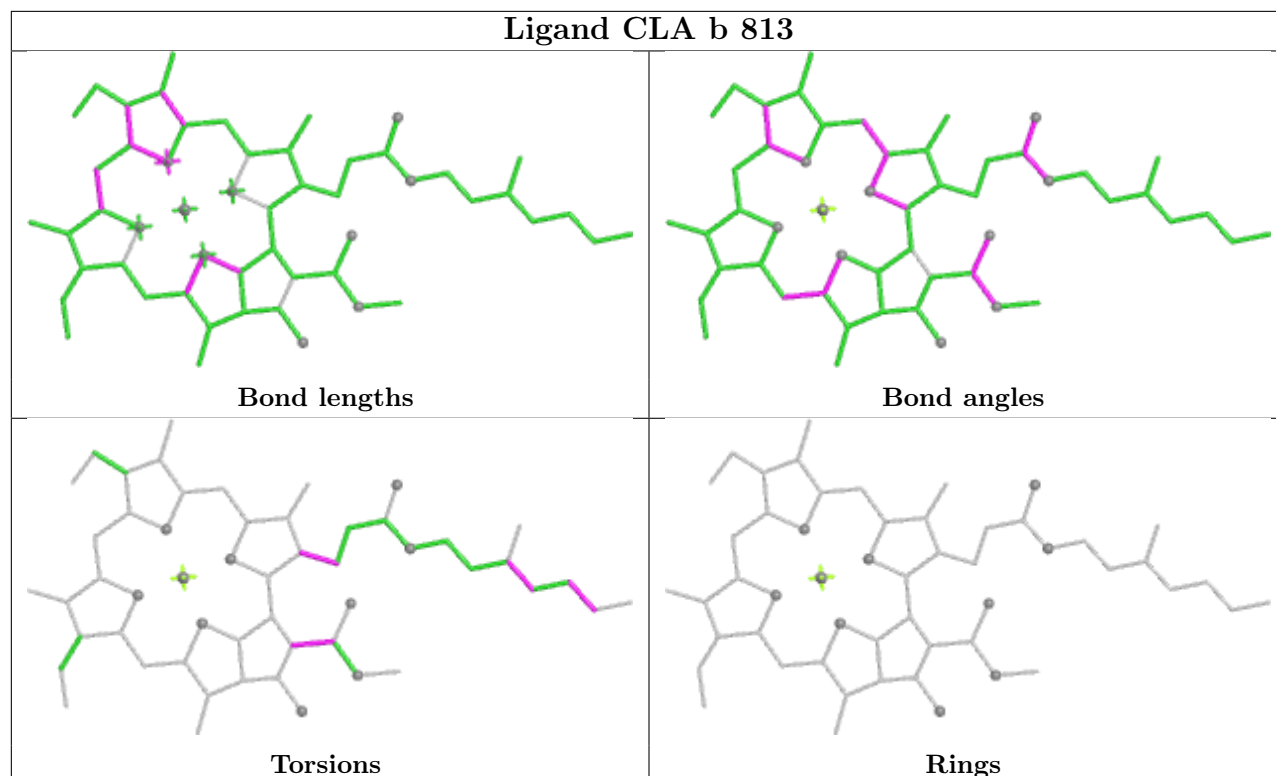


Ligand CLA j 103

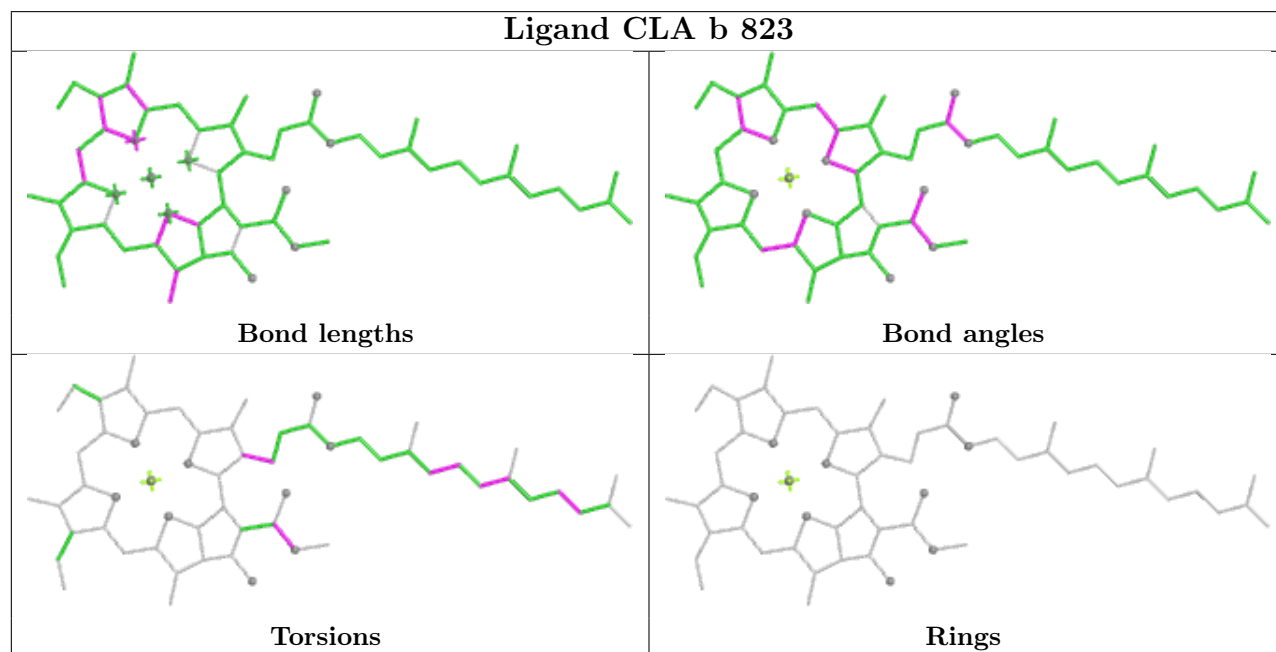


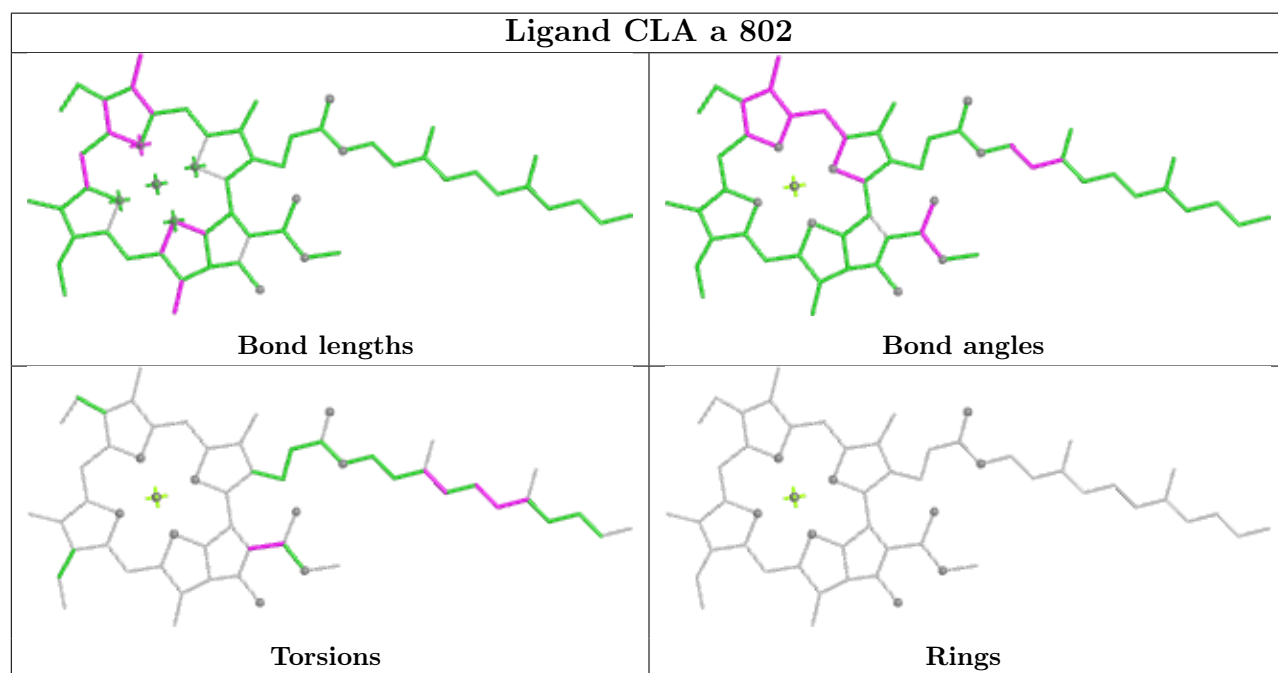
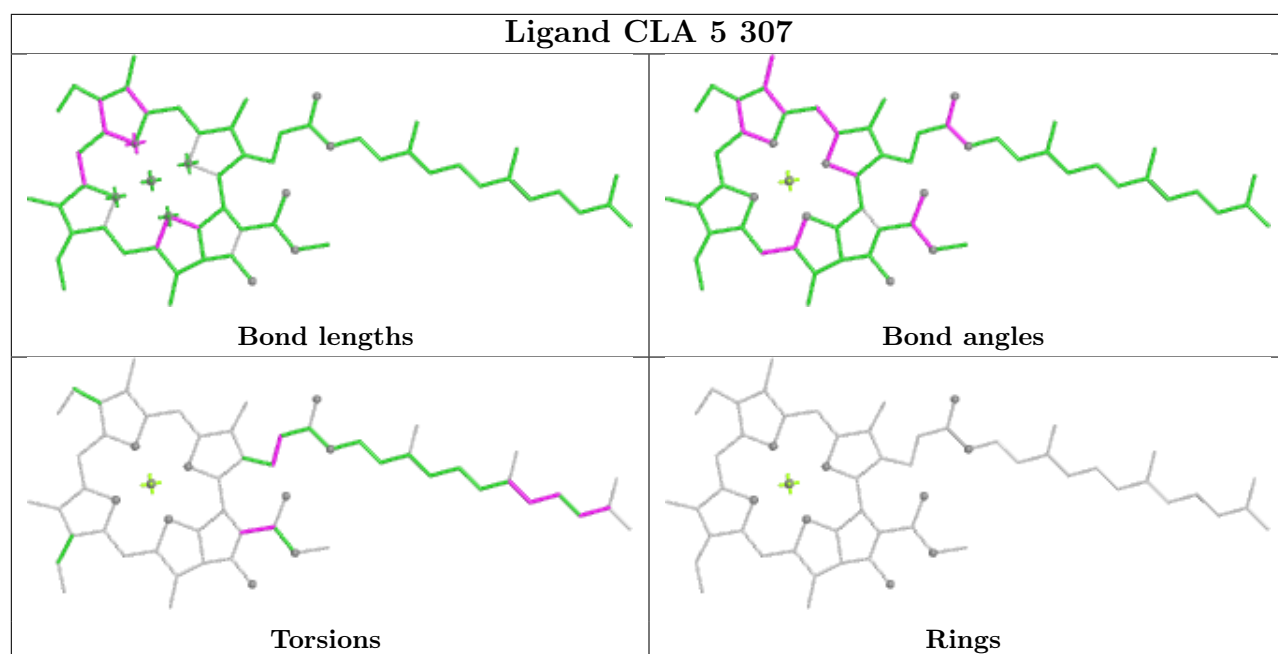
Ligand CLA b 838**Ligand CLA a 822**

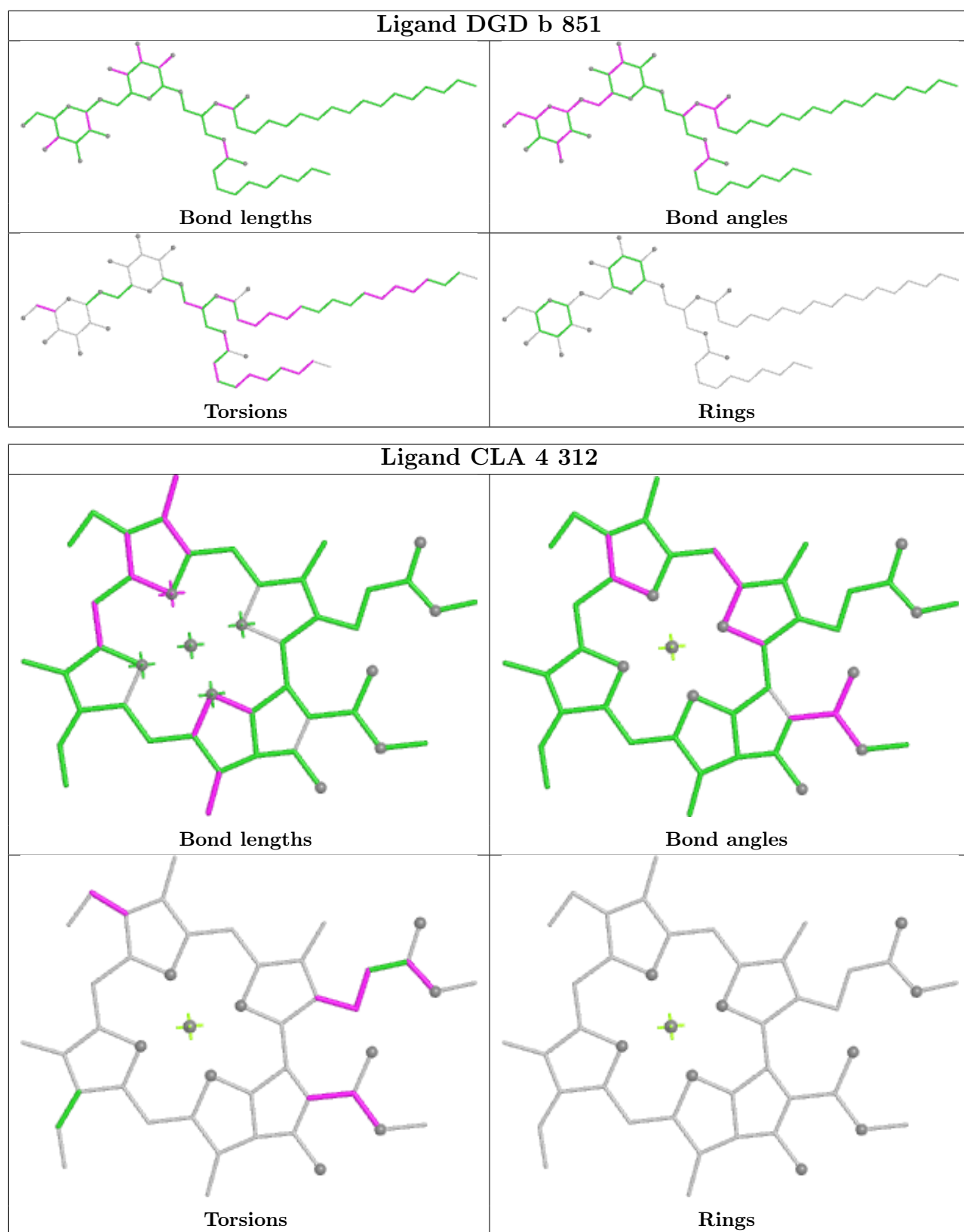
Ligand CLA b 813



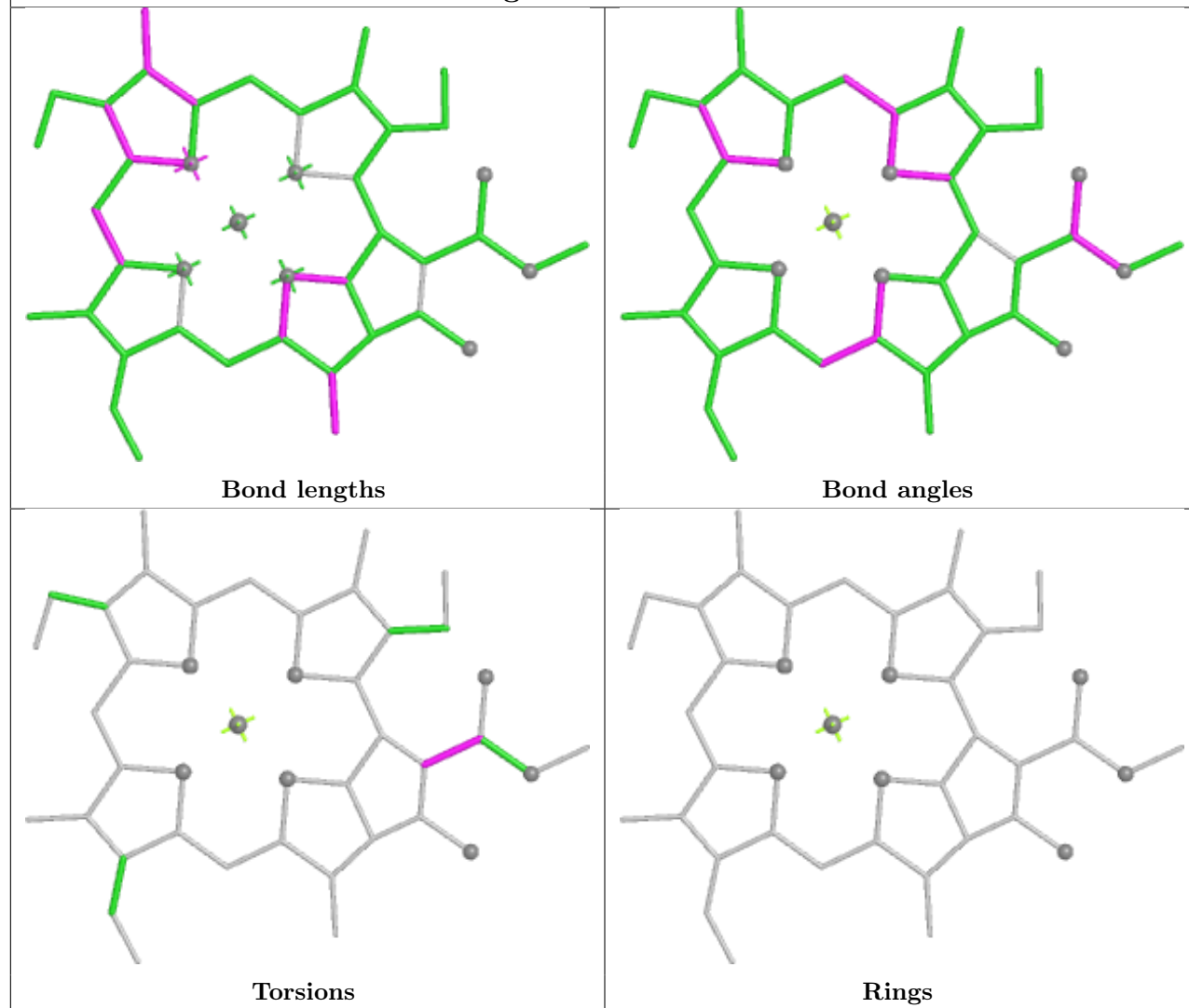
Ligand CLA b 823



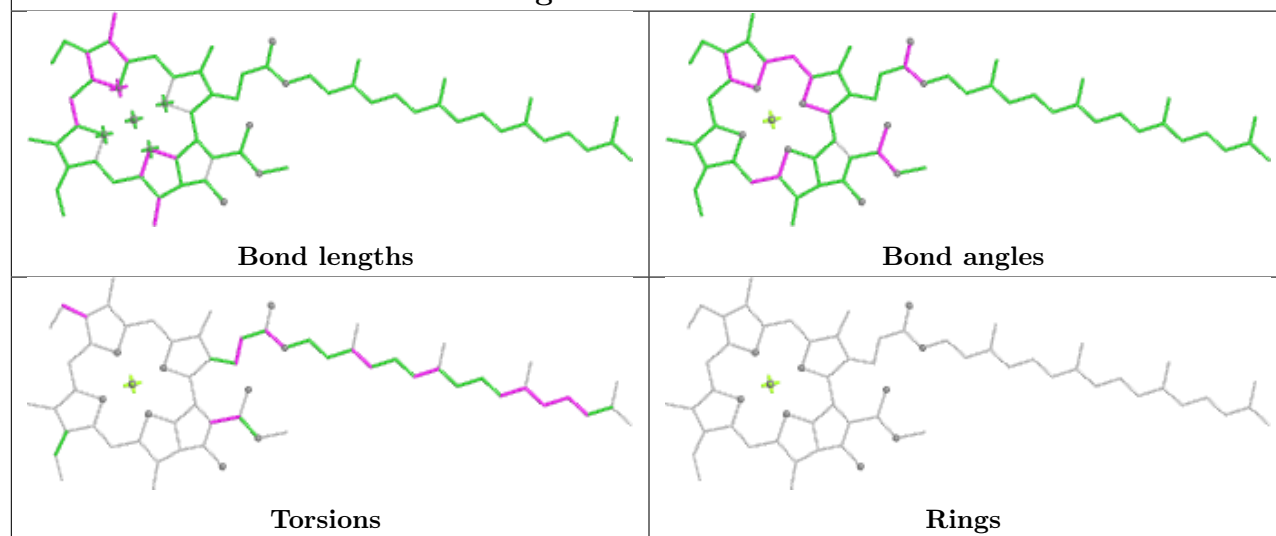


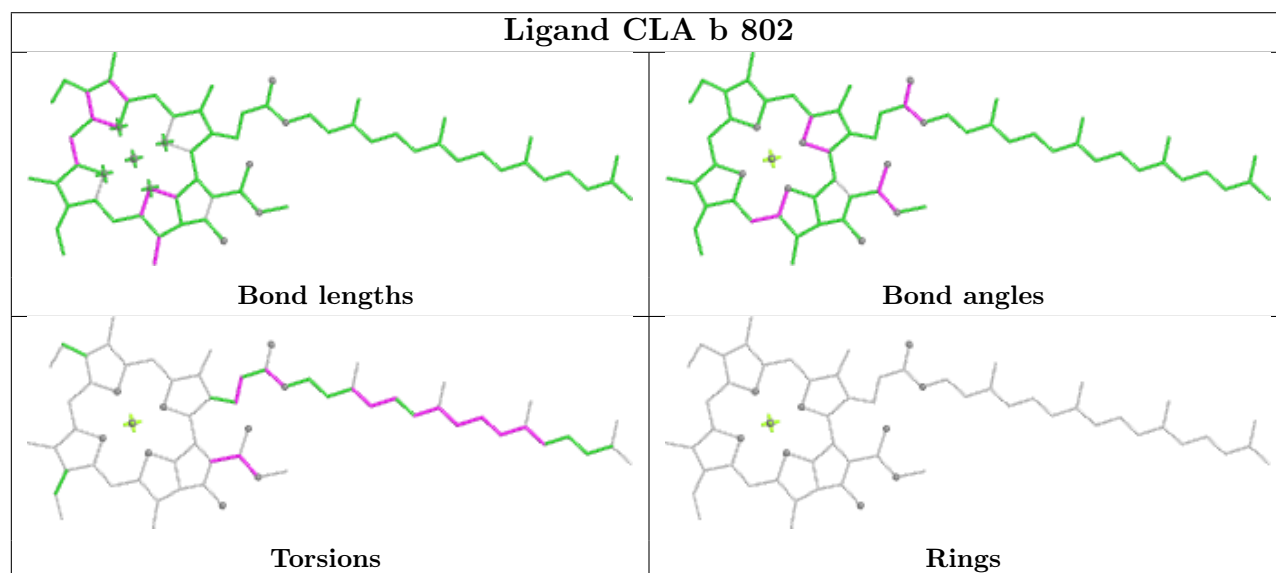
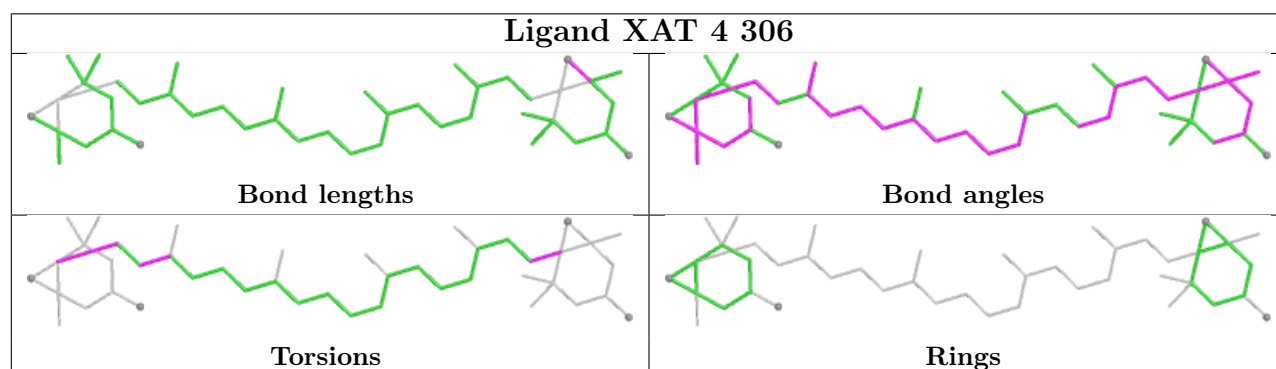
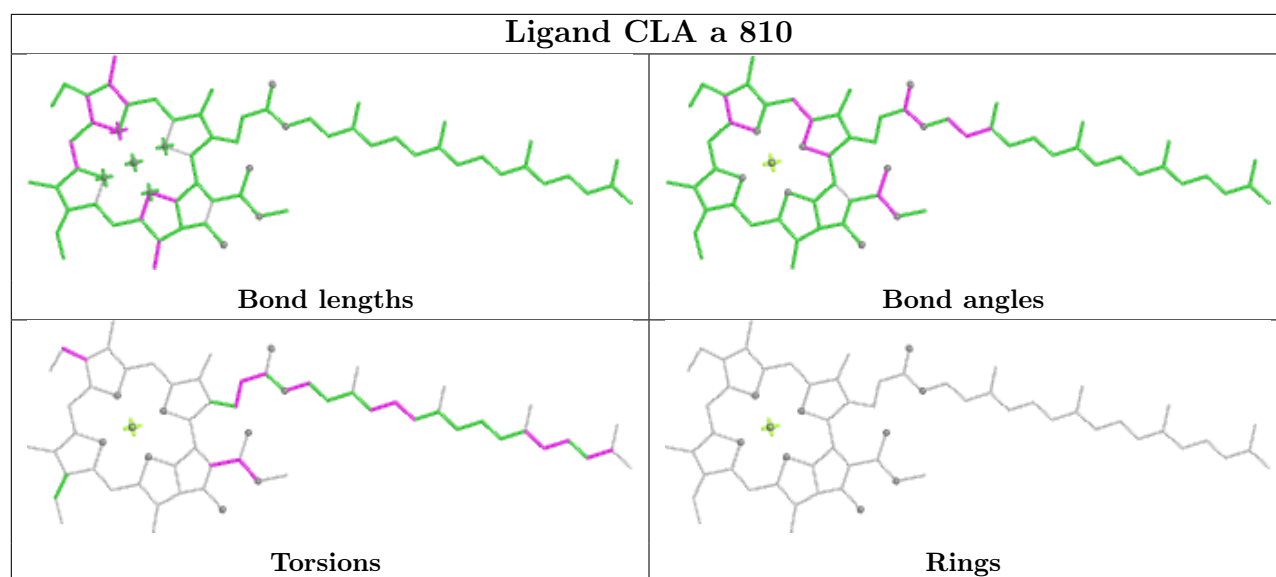


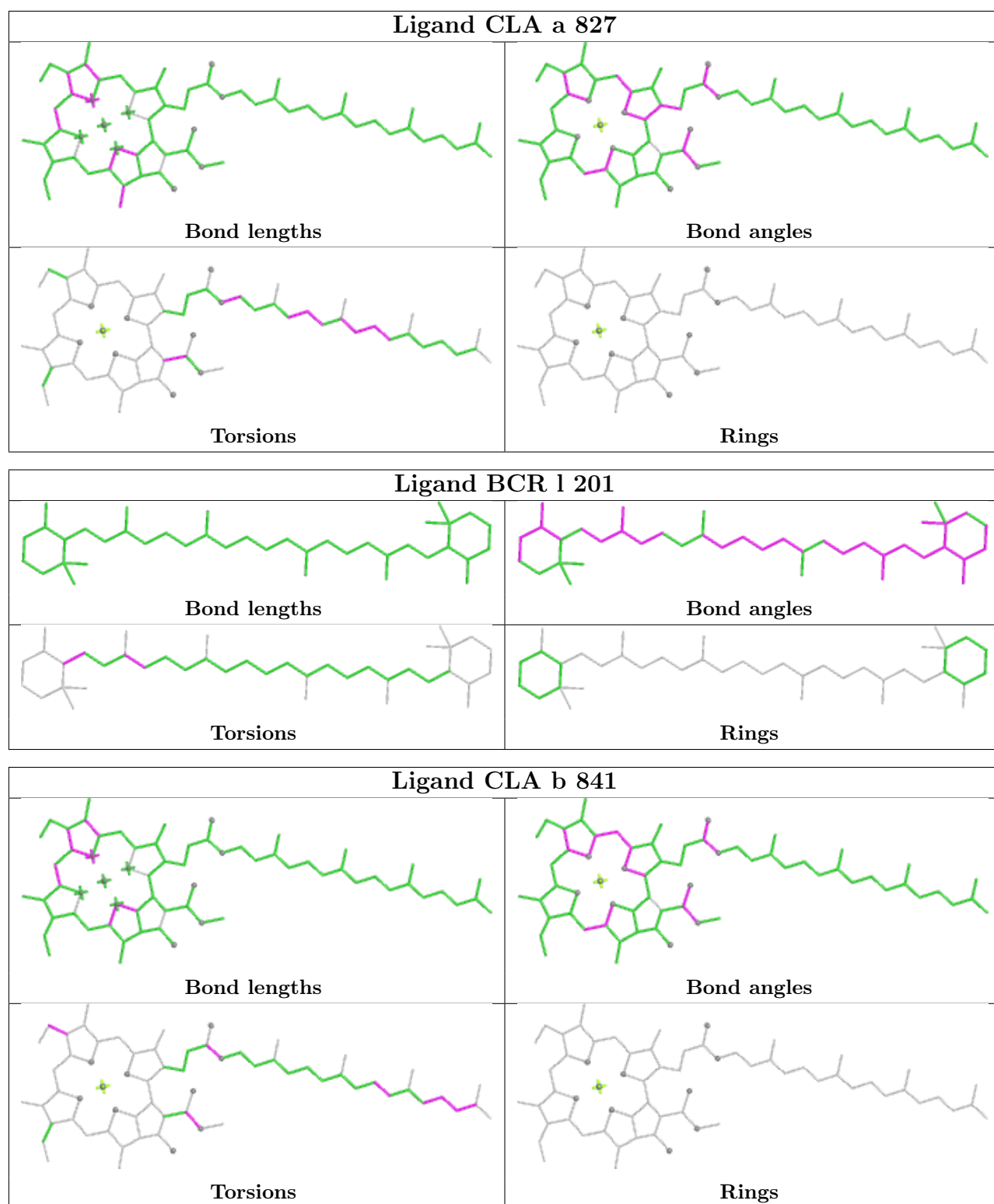
Ligand CLA 1 202



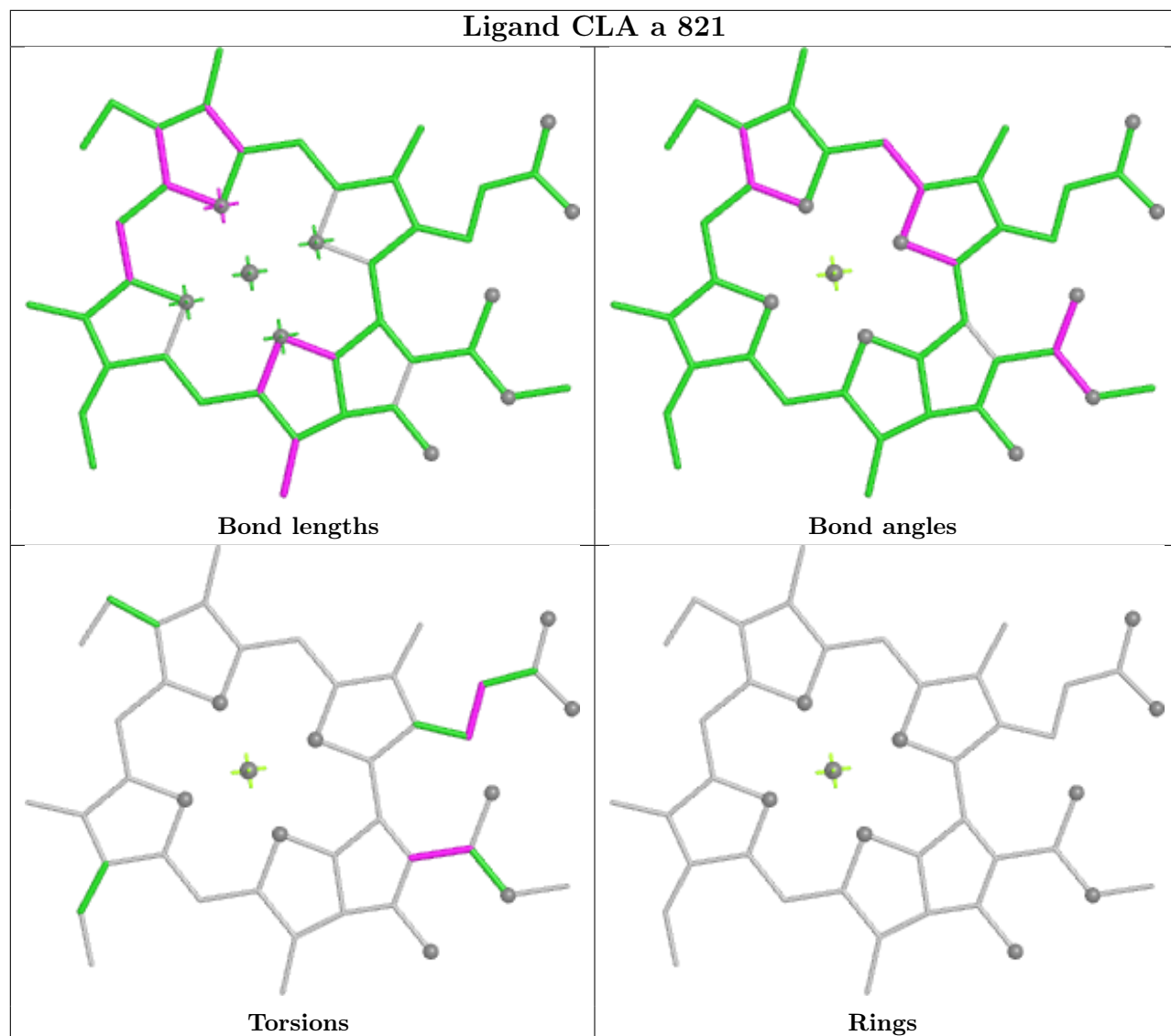
Ligand CLA b 839

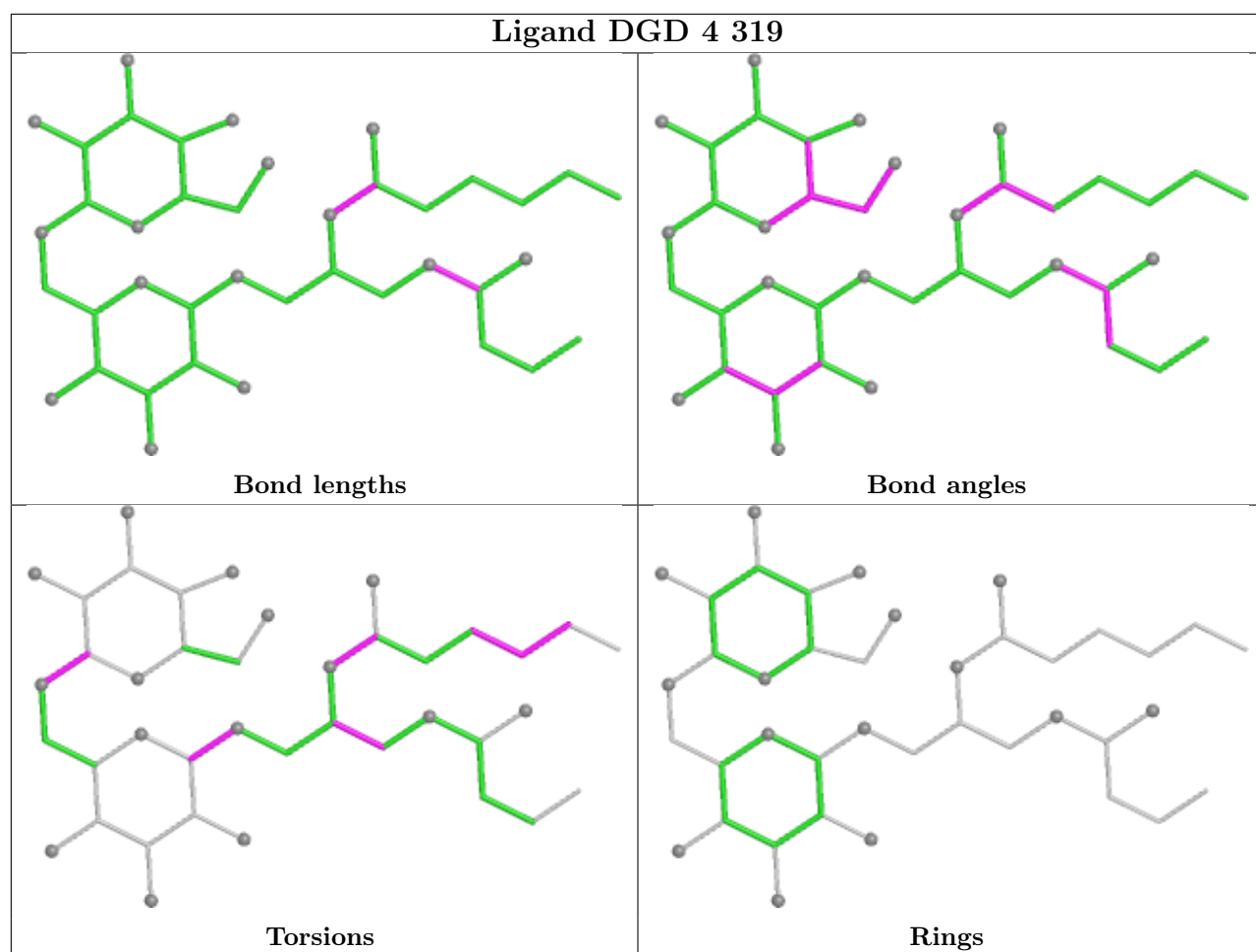


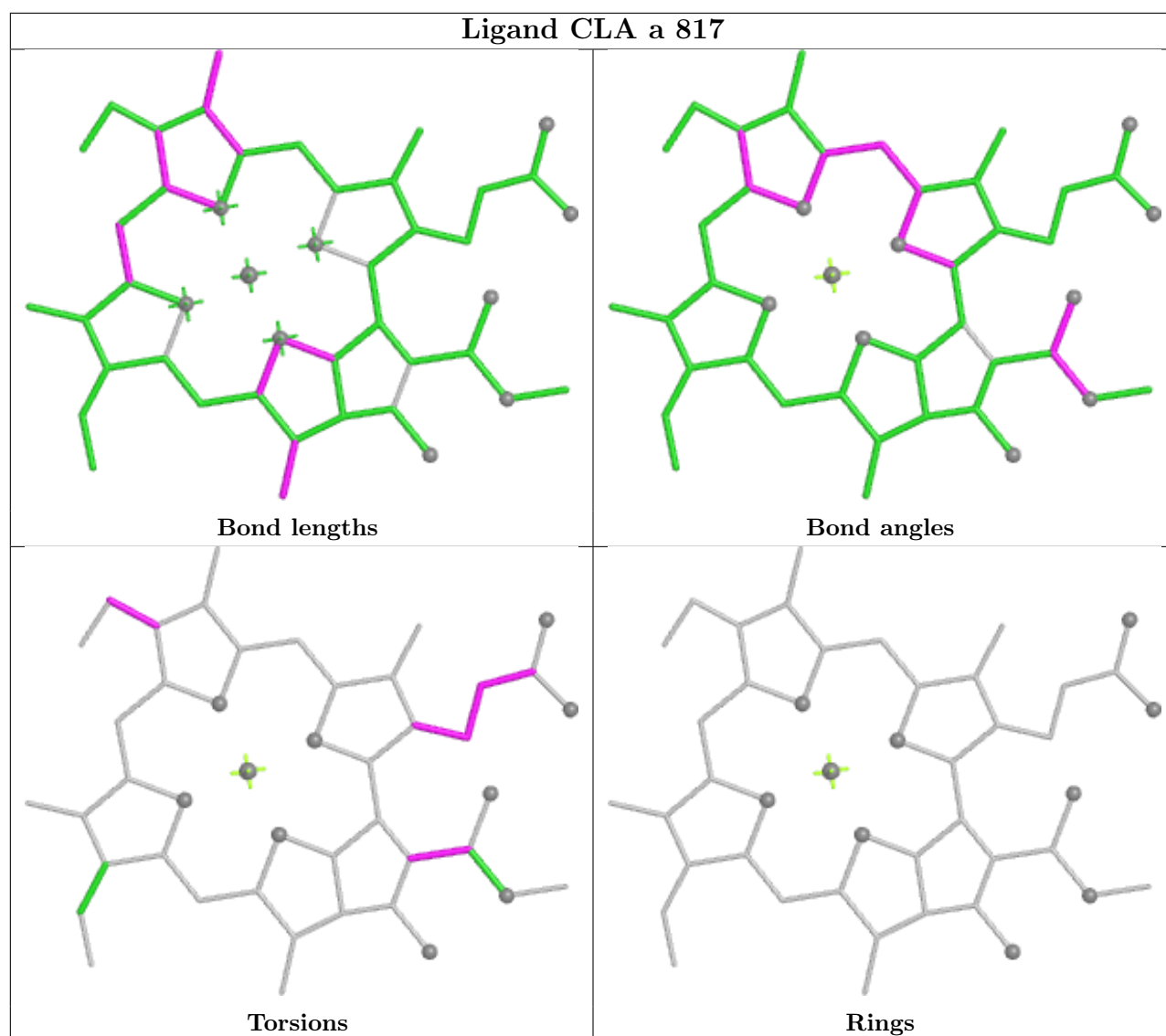




Ligand CLA a 821







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.

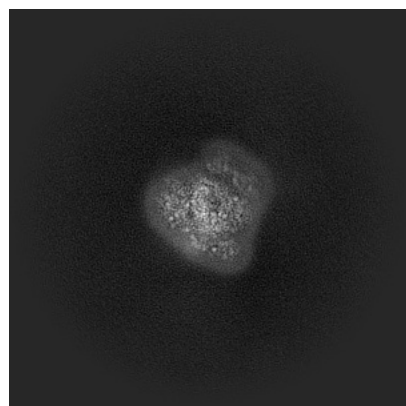
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60291. These allow visual inspection of the internal detail of the map and identification of artifacts.

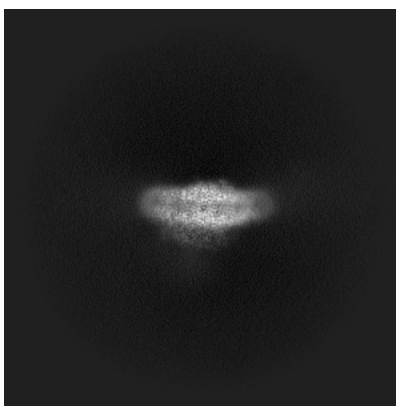
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

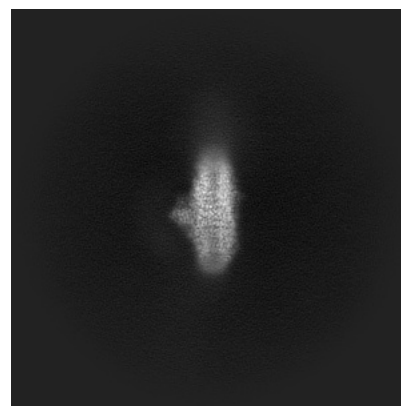
6.1.1 Primary map



X

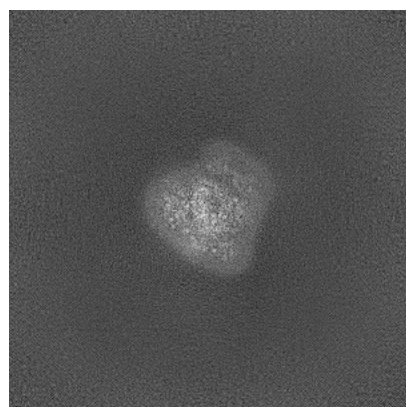


Y

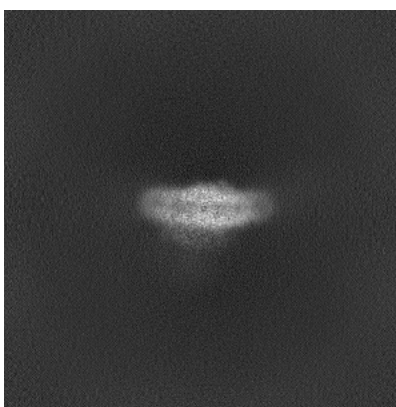


Z

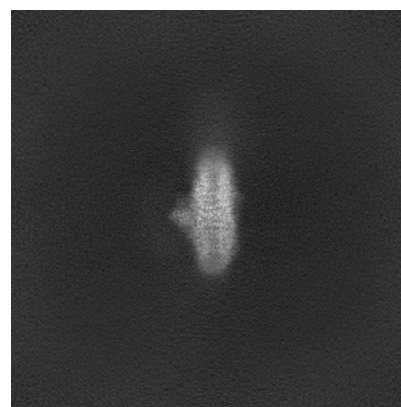
6.1.2 Raw map



X



Y

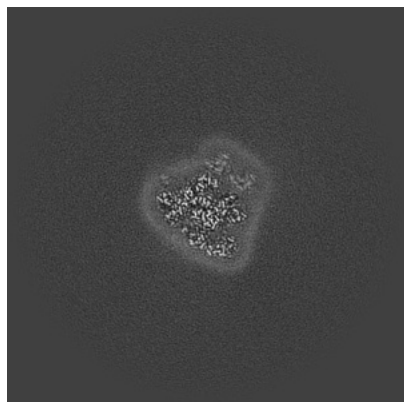


Z

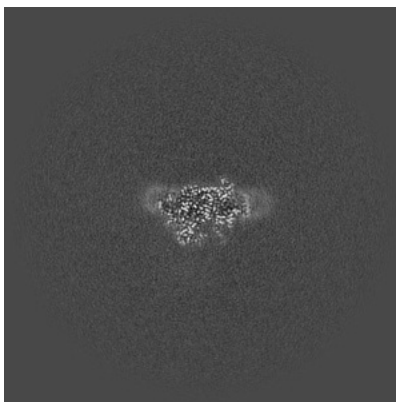
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

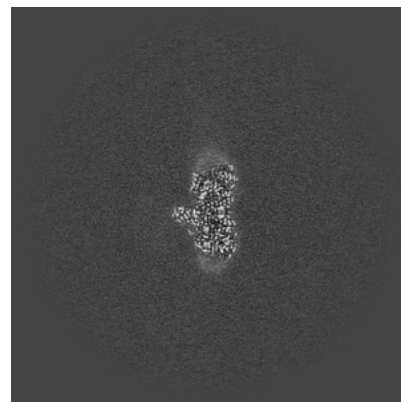
6.2.1 Primary map



X Index: 256

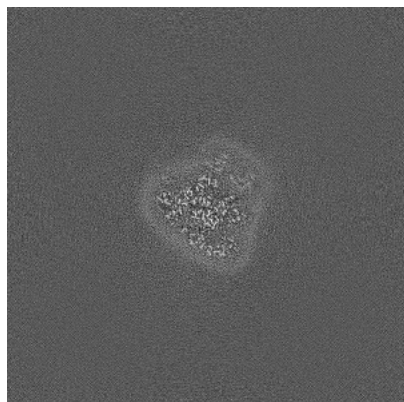


Y Index: 256

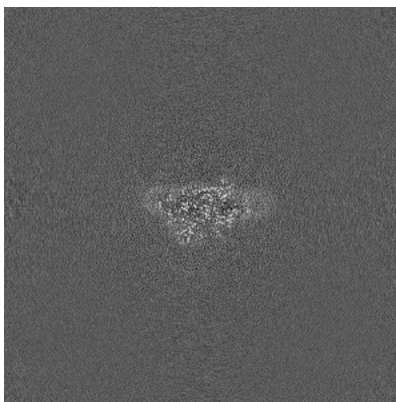


Z Index: 256

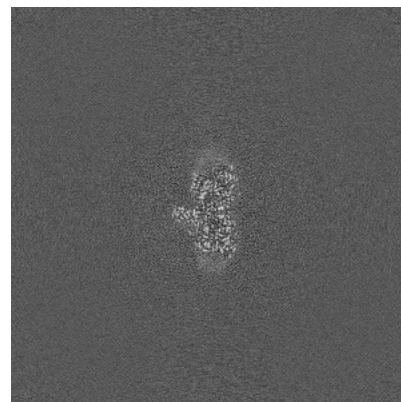
6.2.2 Raw map



X Index: 256



Y Index: 256

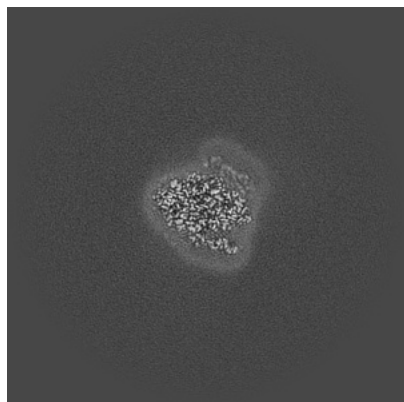


Z Index: 256

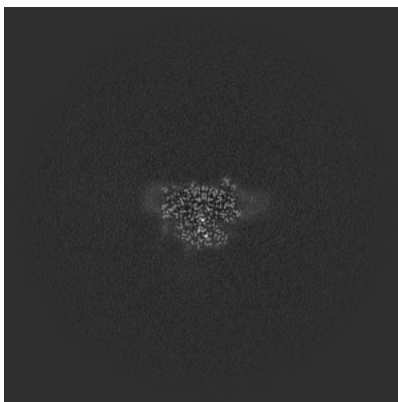
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

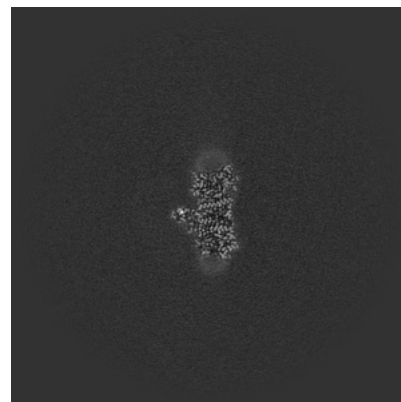
6.3.1 Primary map



X Index: 269

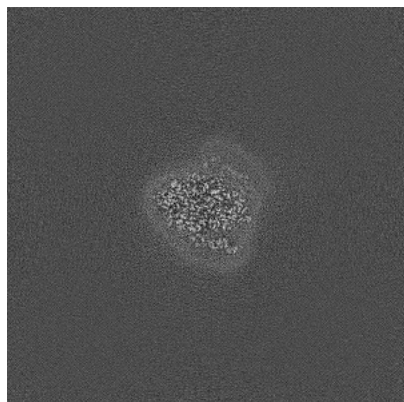


Y Index: 249

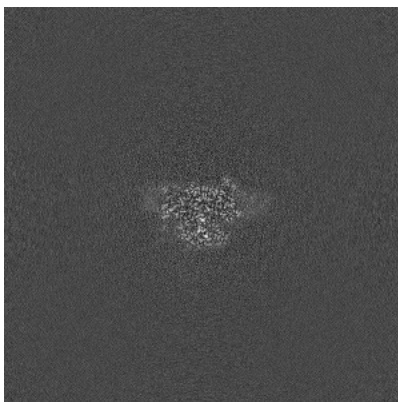


Z Index: 259

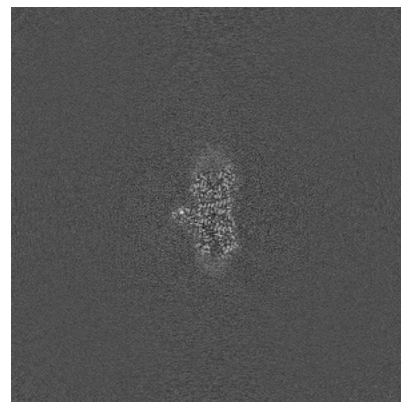
6.3.2 Raw map



X Index: 269



Y Index: 249

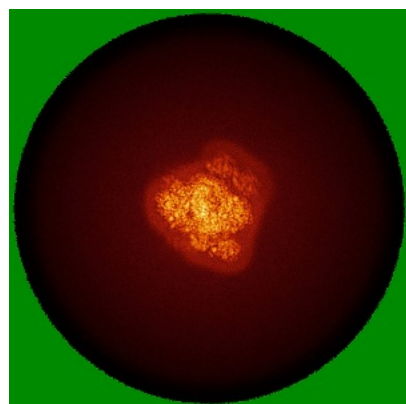


Z Index: 258

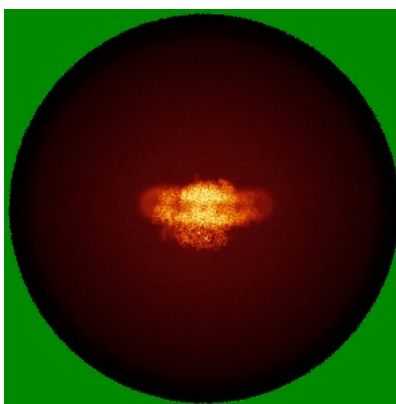
The images above show the largest variance slices of the map in three orthogonal directions.

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

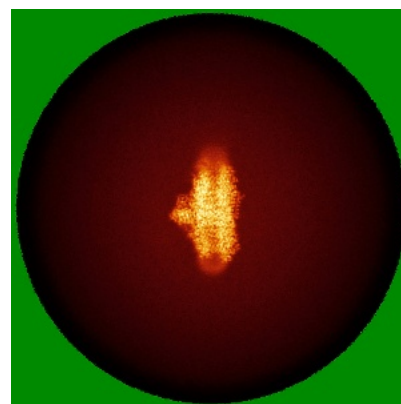
6.4.1 Primary map



X

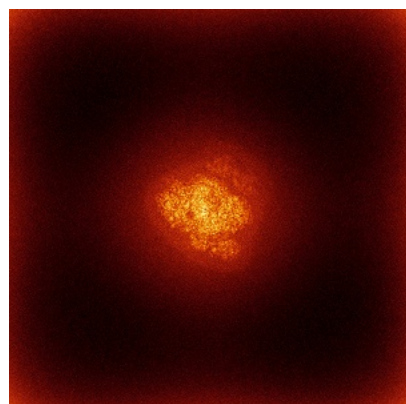


Y

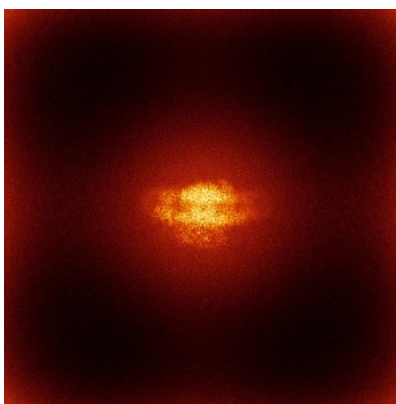


Z

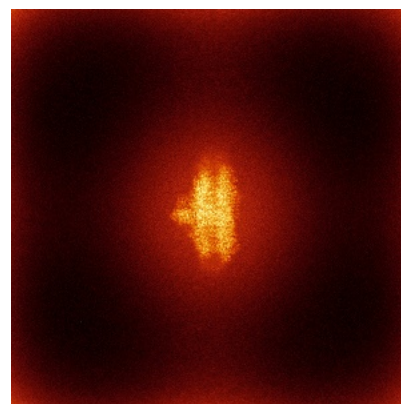
6.4.2 Raw map



X



Y

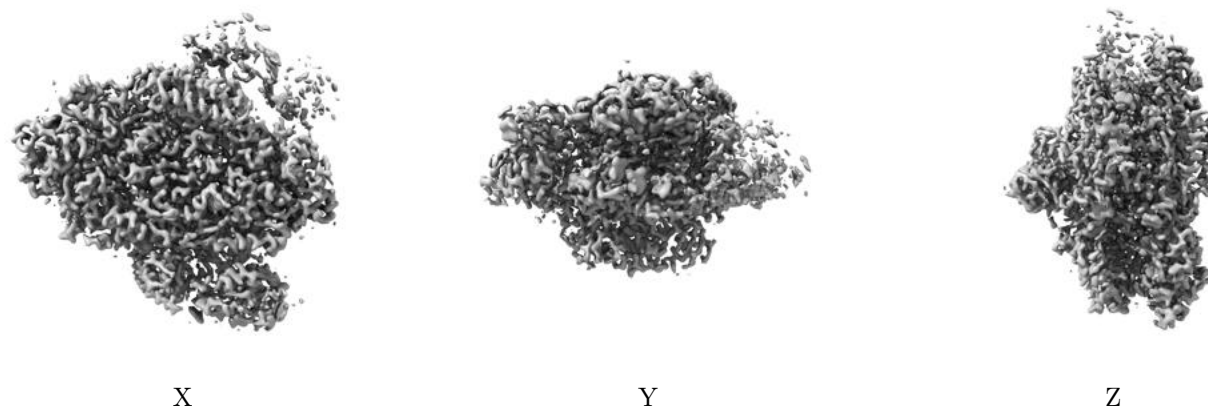


Z

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.

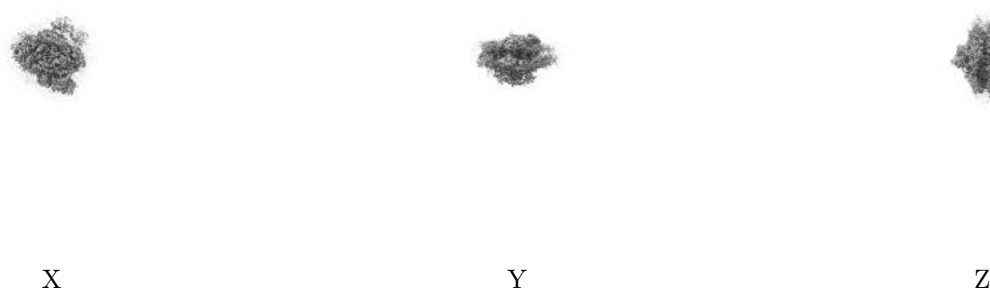
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.345. 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.

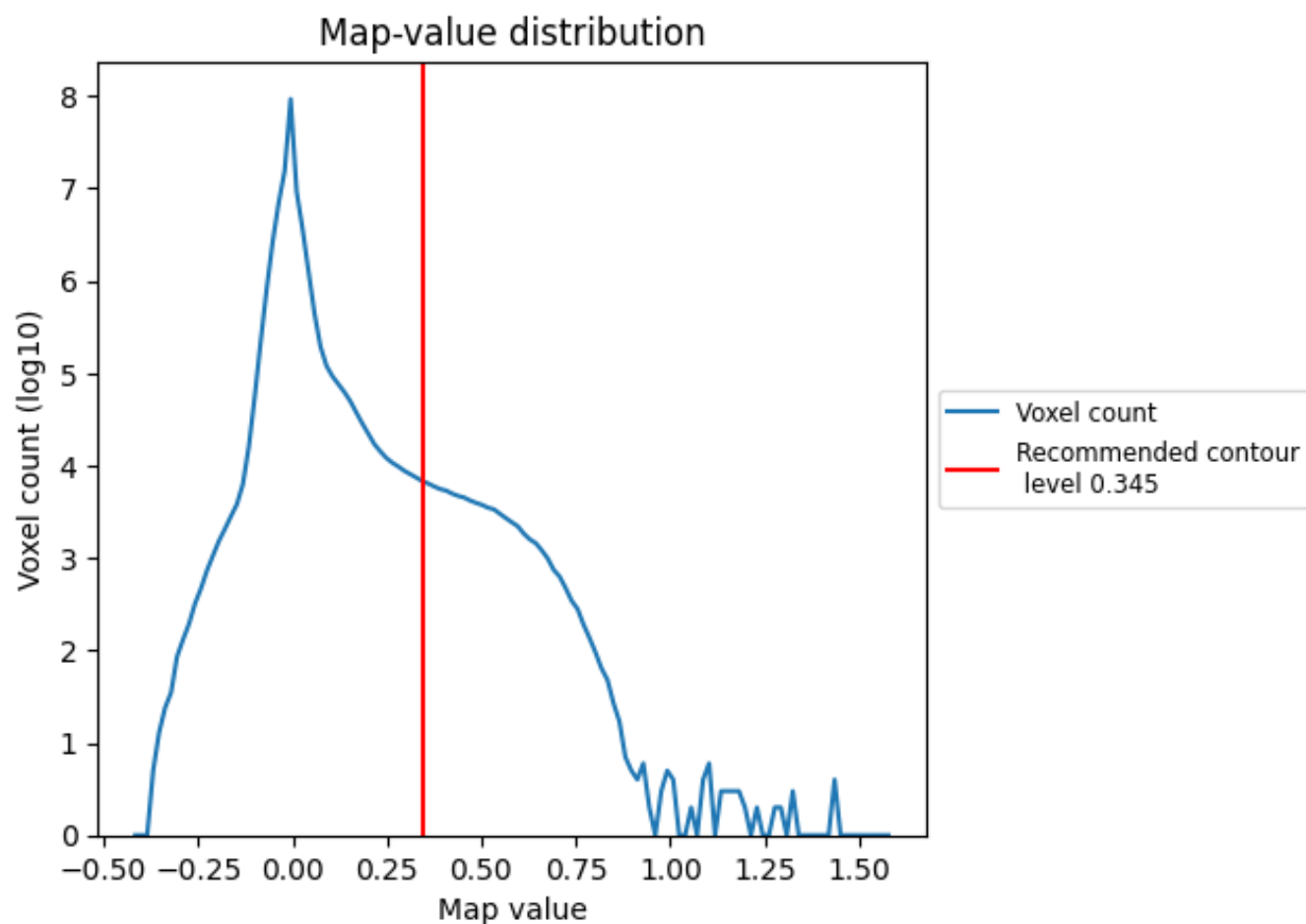
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

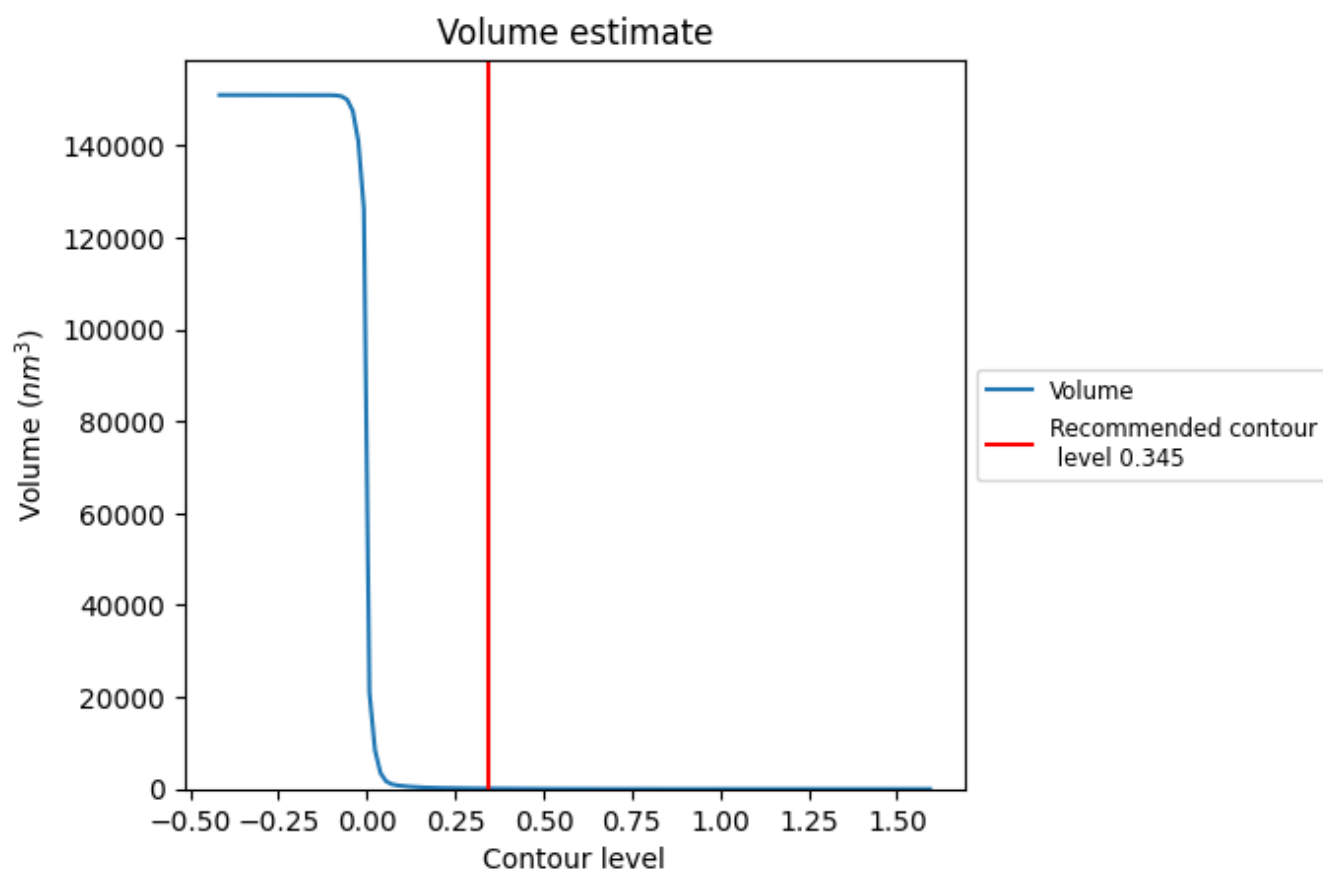
This section contains the results of statistical analysis of the map.

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.

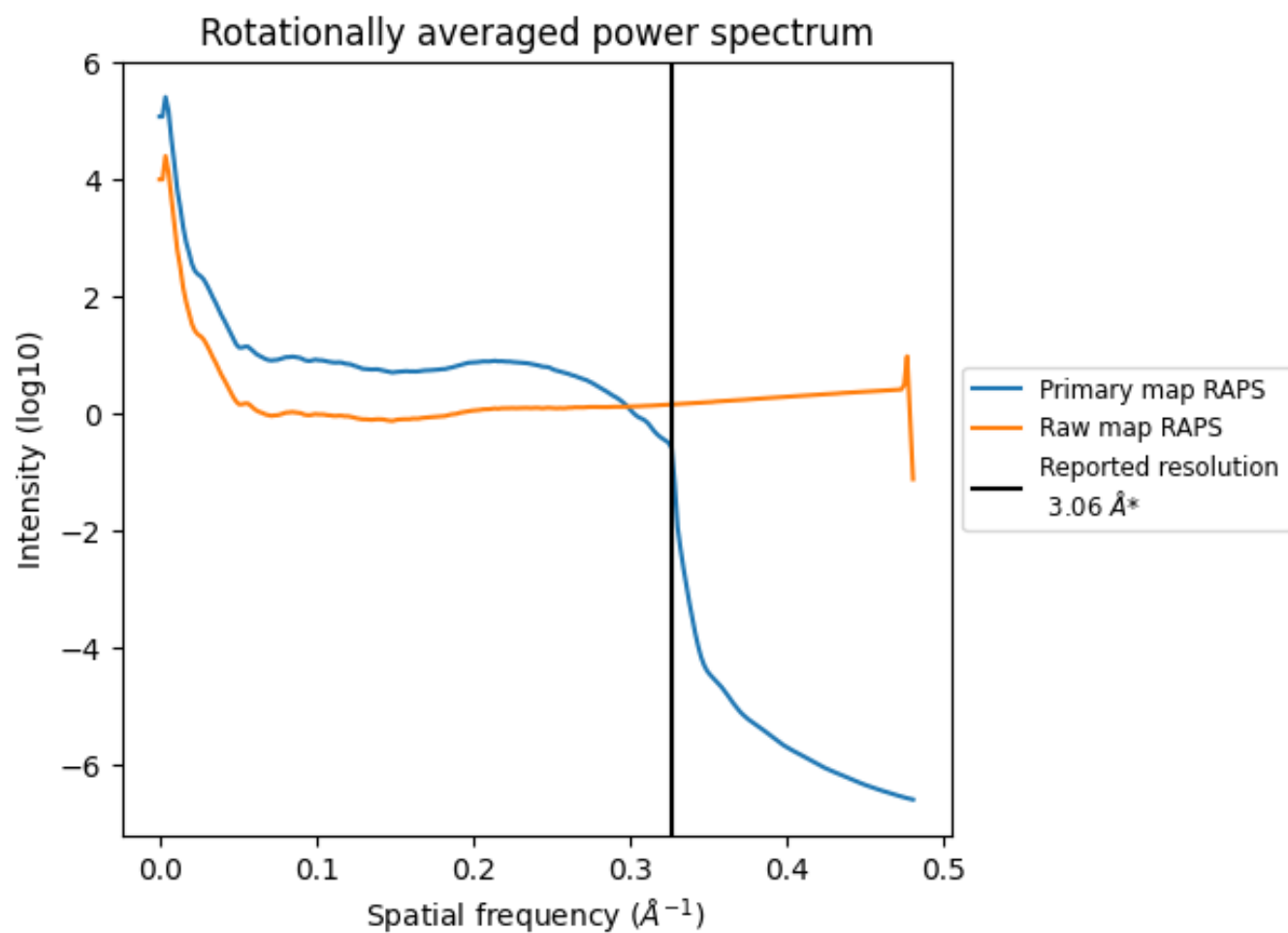
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 93 nm^3 ; this corresponds to an approximate mass of 84 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 [i](#)

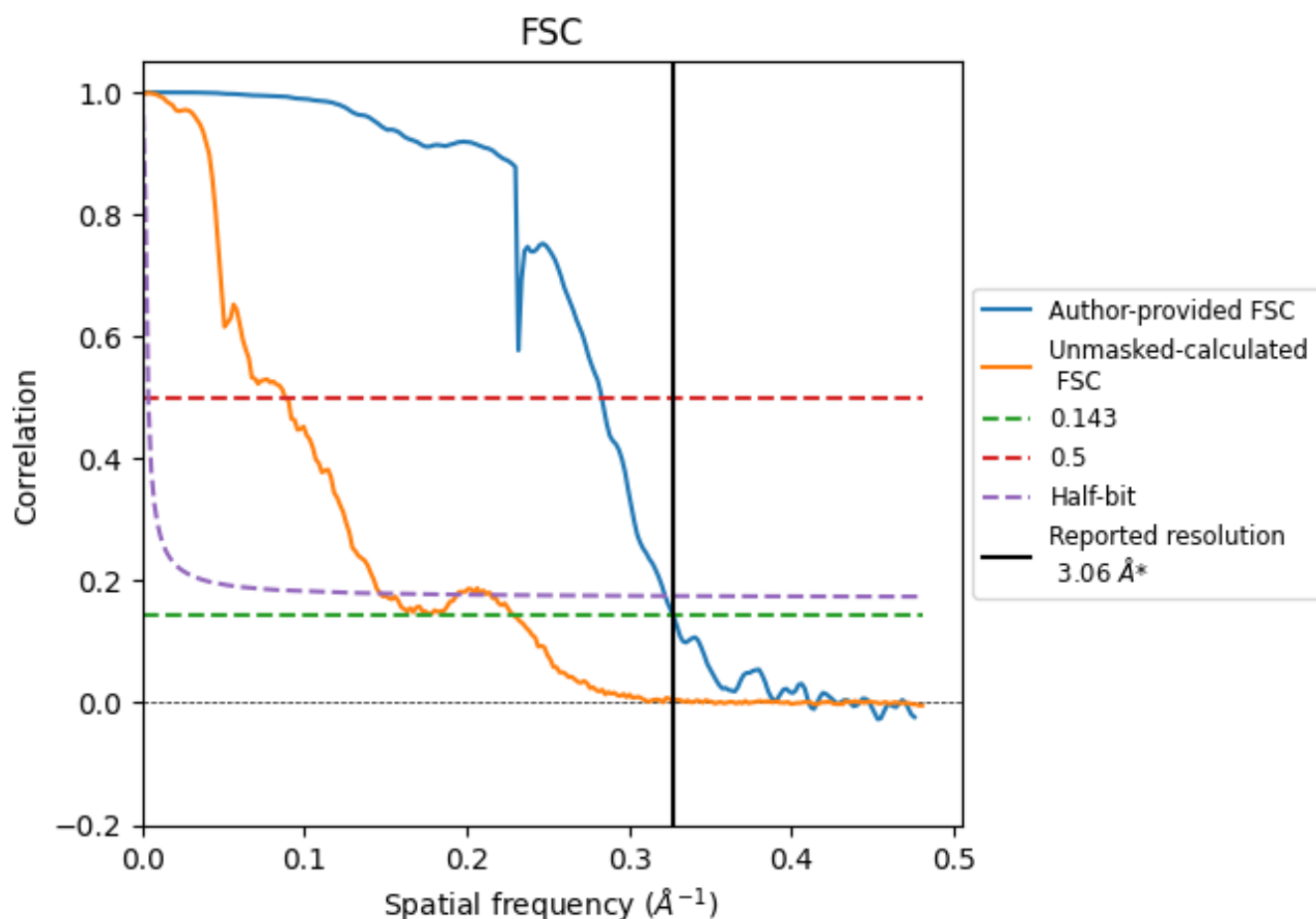


*Reported resolution corresponds to spatial frequency of 0.327 Å⁻¹

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 $0.327 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

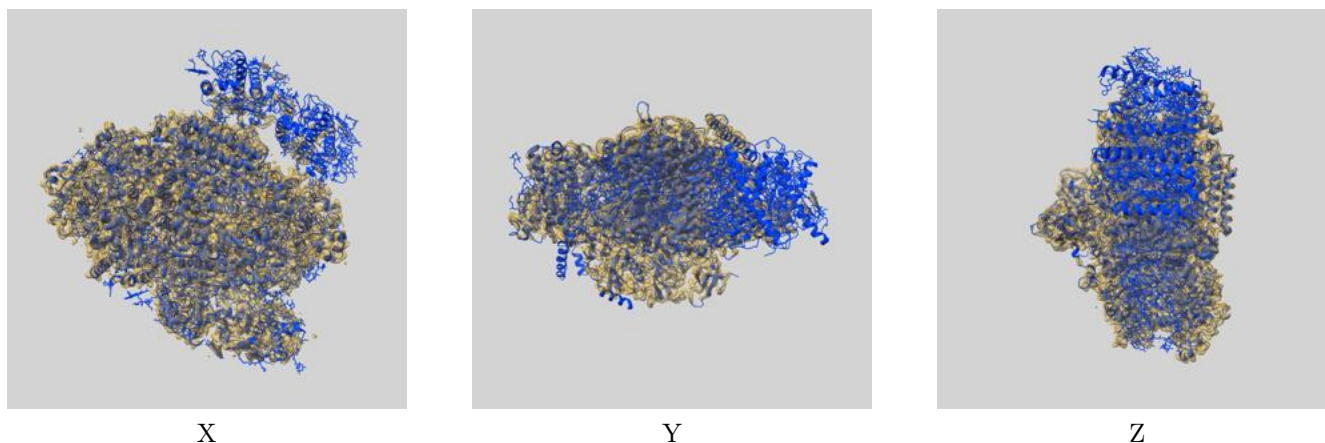
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	3.06	3.53	3.10
Unmasked-calculated*	4.37	11.36	6.82

*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 4.37 differs from the reported value 3.06 by more than 10 %

9 Map-model fit [i](#)

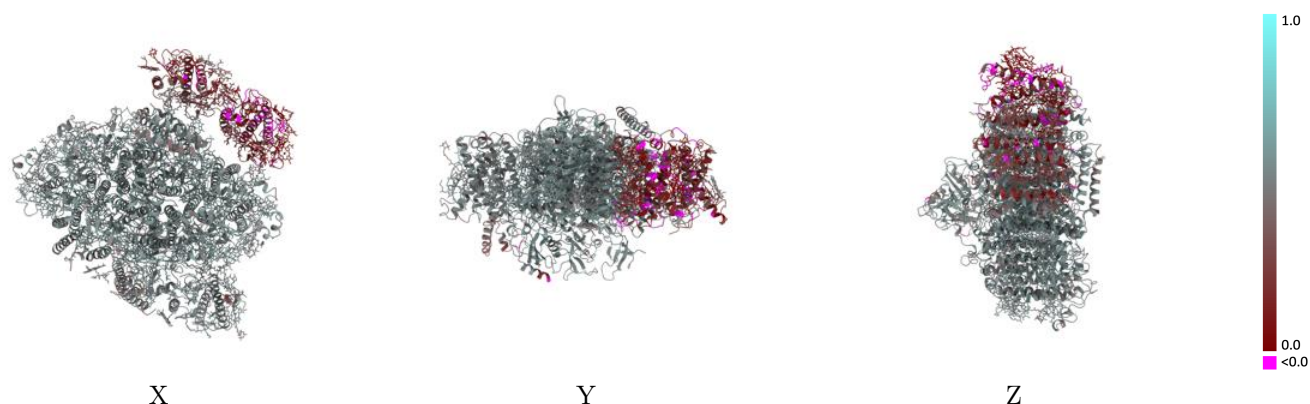
This section contains information regarding the fit between EMDB map EMD-60291 and PDB model 8ZOF. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



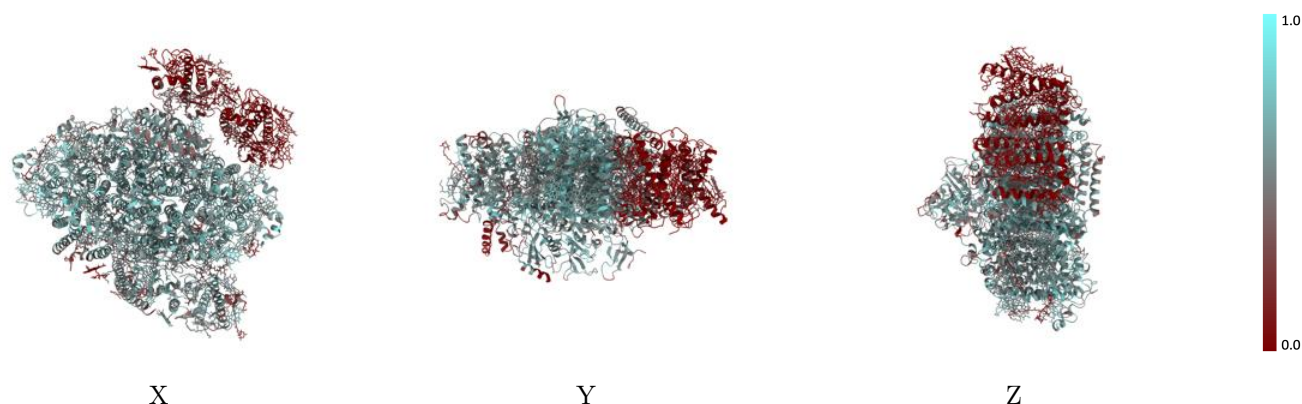
The images above show the 3D surface view of the map at the recommended contour level 0.345 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



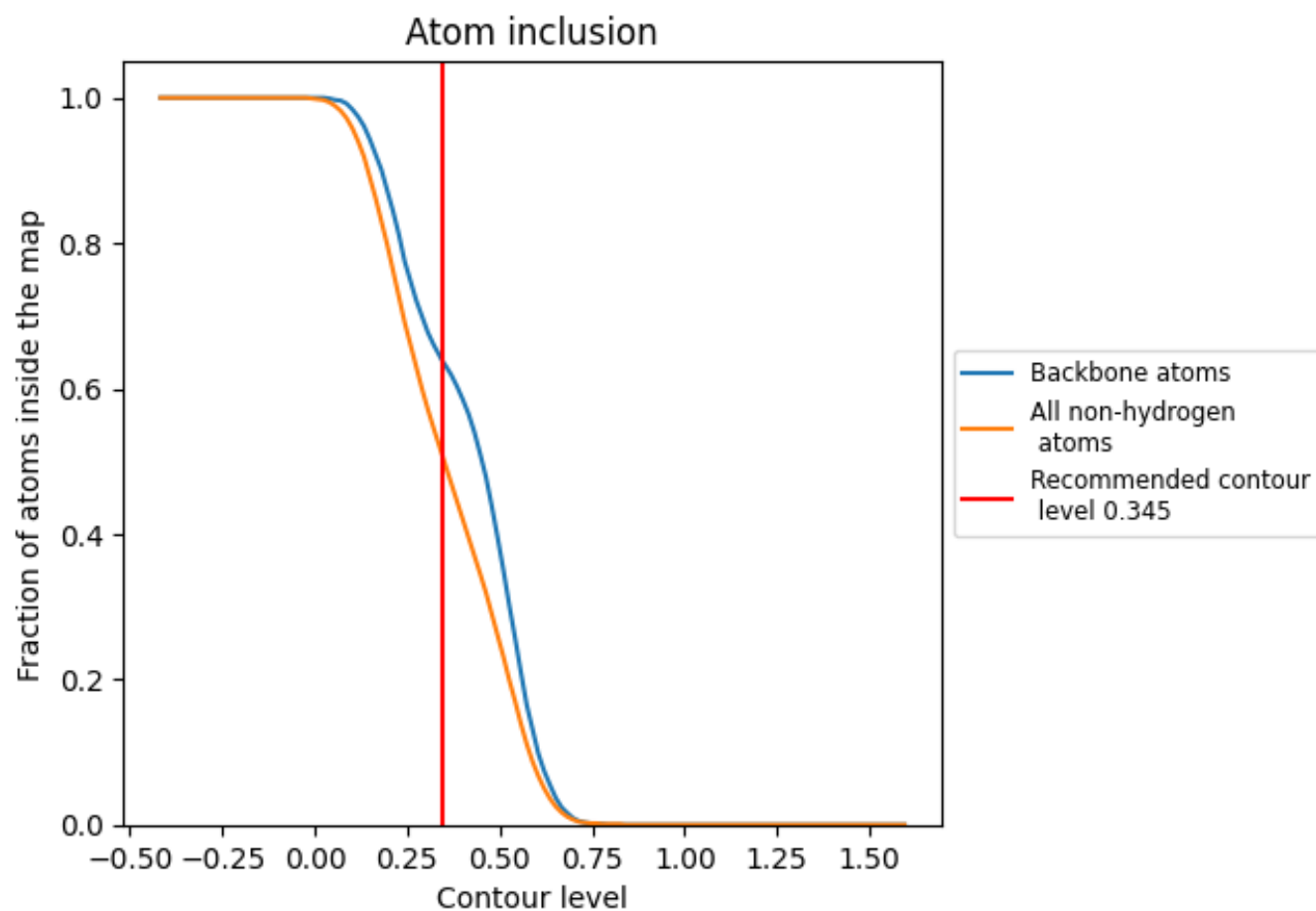
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.345).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 51% 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 (0.345) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5080	0.4790
1	0.5060	0.5080
4	0.0350	0.1180
5	0.0900	0.2380
a	0.6210	0.5430
b	0.6110	0.5390
c	0.6540	0.5300
d	0.5410	0.5250
e	0.5380	0.5150
f	0.5300	0.4960
g	0.2360	0.3820
i	0.3780	0.4890
j	0.5110	0.5320
l	0.5020	0.4900
m	0.4330	0.4670

