



# wwPDB EM Validation Summary Report ⓘ

Jun 8, 2026 – 02:30 PM JST

PDB ID : 9WLS / pdb\_00009wls  
EMDB ID : EMD-66073  
Title : PSI complex of A.thaliana isolated using DOC based Clear-Native-PAGE method  
Authors : Kawamoto, A.; Seki, S.; Kurisu, G.  
Deposited on : 2025-09-02  
Resolution : 2.18 Å(reported)  
Based on initial model : 8J7B

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev132  
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) : 2.49

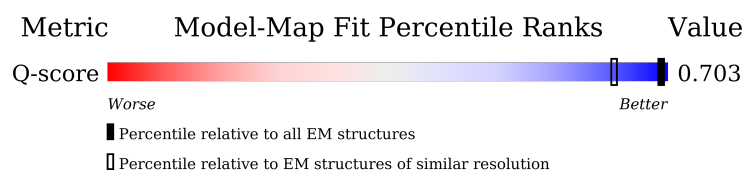
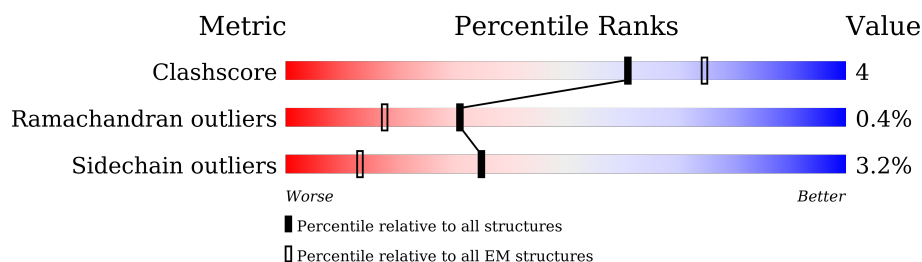
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.18 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	2701 ( 1.70 - 2.68 )

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  $\geq 3$ , 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	1	241	<div> <div>16%</div> <div> <div></div> <div>71%</div> <div>9%</div> <div>20%</div> </div> </div>
2	2	257	<div> <div>25%</div> <div> <div></div> <div>72%</div> <div>9%</div> <div>19%</div> </div> </div>
3	3	273	<div> <div>8%</div> <div> <div></div> <div>73%</div> <div>7%</div> <div>19%</div> </div> </div>
4	4	251	<div> <div>19%</div> <div> <div></div> <div>74%</div> <div>5%</div> <div>22%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	A	750	
6	B	734	
7	C	81	
8	D	204	
9	E	143	
10	F	221	
11	G	160	
12	H	145	
13	I	37	
14	J	44	
15	K	130	
16	L	219	
17	N	171	

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
18	CHL	1	601	X	-	-	-
18	CHL	2	316	X	-	-	-
18	CHL	3	303	X	-	-	-
19	CLA	1	602	X	-	-	-
19	CLA	1	603	X	-	-	-
19	CLA	1	608	X	-	-	-
19	CLA	1	612	X	-	-	-
19	CLA	2	310	X	-	-	-
19	CLA	2	312	X	-	-	-
19	CLA	3	301	X	-	-	-
19	CLA	3	304	X	-	-	-
19	CLA	3	314	X	-	-	-
19	CLA	4	317	X	-	-	-
19	CLA	A	801	X	-	-	-
19	CLA	A	802	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	808	X	-	-	-
19	CLA	A	809	X	-	-	-
19	CLA	A	811	X	-	-	-
19	CLA	A	812	X	-	-	-
19	CLA	A	813	X	-	-	-
19	CLA	A	814	X	-	-	-
19	CLA	A	818	X	-	-	-
19	CLA	A	819	X	-	-	-
19	CLA	A	824	X	-	-	-
19	CLA	A	826	X	-	-	-
19	CLA	A	827	X	-	-	-
19	CLA	A	828	X	-	-	-
19	CLA	A	829	X	-	-	-
19	CLA	A	831	X	-	-	-
19	CLA	A	833	X	-	-	-
19	CLA	A	834	X	-	-	-
19	CLA	A	837	X	-	-	-
19	CLA	A	840	X	-	-	-
19	CLA	A	842	X	-	-	-
19	CLA	A	846	X	-	-	-
19	CLA	A	850	X	-	-	-
19	CLA	A	851	X	-	-	-
19	CLA	B	801	X	-	-	-
19	CLA	B	802	X	-	-	-
19	CLA	B	806	X	-	-	-
19	CLA	B	808	X	-	-	-
19	CLA	B	809	X	-	-	-
19	CLA	B	810	X	-	-	-
19	CLA	B	818	X	-	-	-
19	CLA	B	819	X	-	-	-
19	CLA	B	820	X	-	-	-
19	CLA	B	822	X	-	-	-
19	CLA	B	823	X	-	-	-
19	CLA	B	825	X	-	-	-
19	CLA	B	826	X	-	-	-
19	CLA	B	827	X	-	-	-
19	CLA	B	830	X	-	-	-
19	CLA	B	831	X	-	-	-
19	CLA	B	833	X	-	-	-
19	CLA	B	834	X	-	-	-
19	CLA	B	835	X	-	-	-
19	CLA	B	836	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	841	X	-	-	-
19	CLA	B	843	X	-	-	-
19	CLA	B	844	X	-	-	-
19	CLA	B	845	X	-	-	-
19	CLA	B	846	X	-	-	-
19	CLA	H	201	X	-	-	-
19	CLA	J	101	X	-	-	-
19	CLA	L	304	X	-	-	-

## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 36141 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 Chlorophyll a-b binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	194	Total	C	N	O	S	0	0
			1501	978	249	269	5		

- Molecule 2 is a protein called Photosystem I chlorophyll a/b-binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	209	Total	C	N	O	S	0	0
			1622	1061	264	293	4		

- Molecule 3 is a protein called Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	221	Total	C	N	O	S	0	0
			1699	1112	276	306	5		

- Molecule 4 is a protein called Chlorophyll a-b binding protein 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	197	Total	C	N	O	S	0	0
			1550	1012	252	283	3		

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	743	Total	C	N	O	S	0	0
			5851	3836	993	1004	18		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	733	Total	C	N	O	S	0	0
			5858	3845	998	1001	14		

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			615	381	107	116	11		

- Molecule 8 is a protein called Photosystem I reaction center subunit II-2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	143	Total	C	N	O	S	0	0
			1128	723	195	206	4		

- Molecule 9 is a protein called Photosystem I reaction center subunit IV A, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	64	Total	C	N	O	S	0	0
			517	331	92	94			

- Molecule 10 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	153	Total	C	N	O	S	0	0
			1211	791	207	210	3		

- Molecule 11 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	98	Total	C	N	O	S	0	0
			763	495	125	143			

- Molecule 12 is a protein called Photosystem I reaction center subunit VI-2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	95	Total	C	N	O	S	0	0
			735	478	119	138			

- Molecule 13 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	31	Total	C	N	O	S	0	0
			239	162	39	37	1		

- Molecule 14 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	42	Total	C	N	O	S	0	0
			338	230	51	56	1		

- Molecule 15 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	64	Total	C	N	O	S	0	0
			447	286	73	85	3		

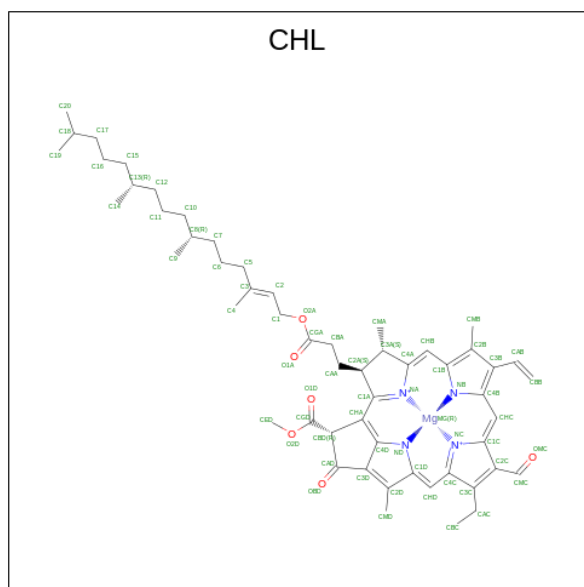
- Molecule 16 is a protein called Photosystem I reaction center subunit XI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	150	Total	C	N	O	S	0	0
			1119	737	179	201	2		

- Molecule 17 is a protein called Photosystem I reaction center subunit N, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	50	Total	C	N	O	S	0	0
			394	246	70	76	2		

- Molecule 18 is CHLOROPHYLL B (CCD ID: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



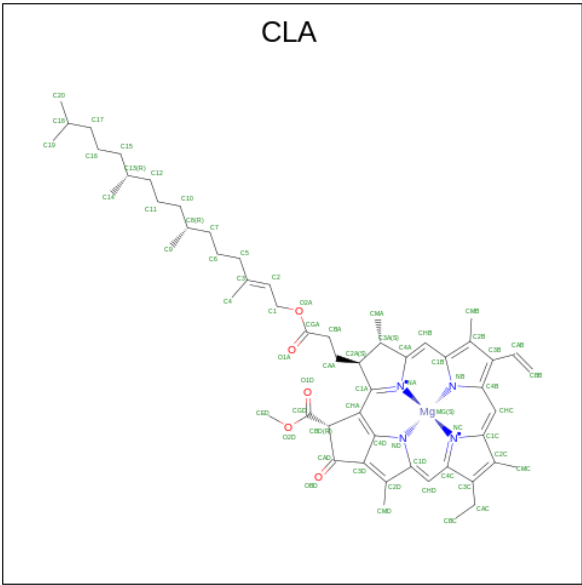
Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total	C	Mg	N	O	0
			59	48	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
18	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
18	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
18	2	1	Total	C	Mg	N	O	0
			59	48	1	4	6	
18	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
18	3	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
18	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
18	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	1	1	Total 57	C 47	Mg 1	N 4	O 5	0
19	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	2	1	Total 62	C 52	Mg 1	N 4	O 5	0
19	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	3	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	3	1	Total 48	C 38	Mg 1	N 4	O 5	0
19	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
19	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	4	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	4	1	Total 57	C 47	Mg 1	N 4	O 5	0
19	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 58	C 48	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	A	1	Total 53	C 43	Mg 1	N 4	O 5	0
19	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	B	1	Total 43	C 35	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
19	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	F	1	Total 42	C 34	Mg 1	N 4	O 3	0
19	F	1	Total 48	C 38	Mg 1	N 4	O 5	0

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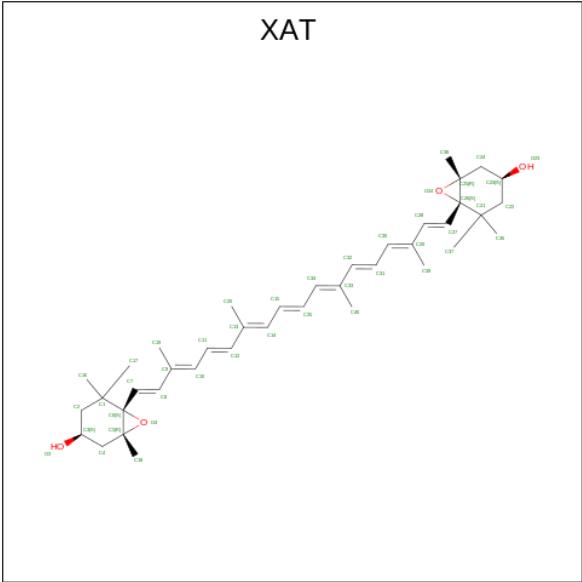
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Mol	Chain	Residues	Atoms					AltConf
19	G	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 20 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ) (labeled as "Ligand of Interest" by depositor).

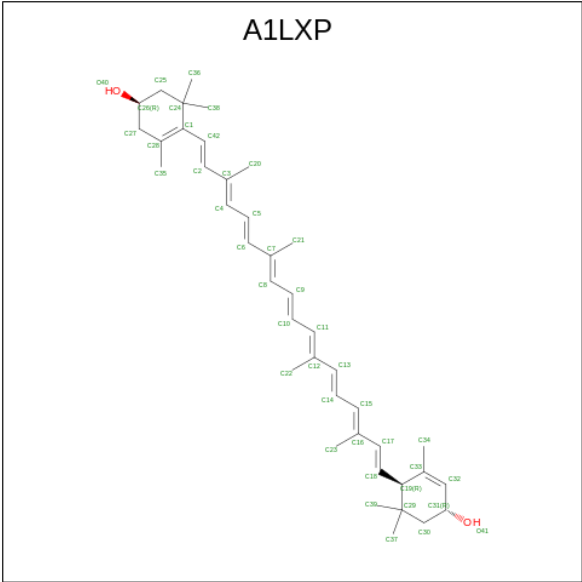
Mol	Chain	Residues	Atoms					AltConf
20	1	6	Total	C	Mg	N	O	0
			274	220	6	24	24	
20	2	7	Total	C	Mg	N	O	0
			291	234	7	28	22	
20	3	4	Total	C	Mg	N	O	0
			163	133	4	16	10	
20	4	8	Total	C	Mg	N	O	0
			354	284	8	32	30	
20	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
20	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
20	N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 21 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: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



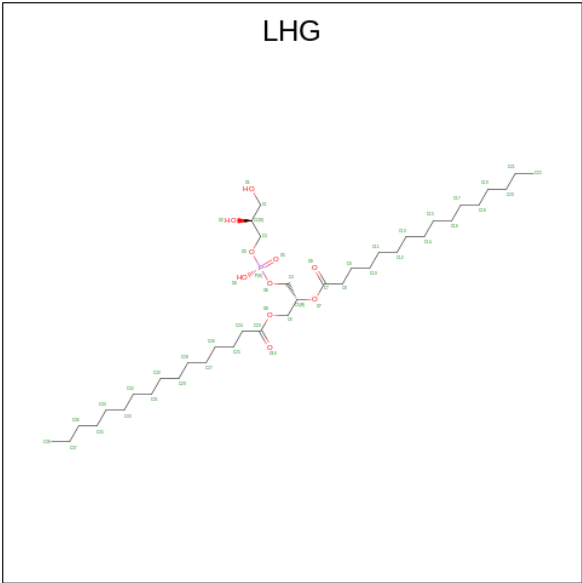
Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			44	40	4	
21	1	1	Total	C	O	0
			28	26	2	
21	2	1	Total	C	O	0
			44	40	4	

- Molecule 22 is Lutein (CCD ID: A1LXP) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
22	1	1	Total	C	O	0
			42	40	2	
22	1	1	Total	C	O	0
			42	40	2	
22	2	1	Total	C	O	0
			42	40	2	
22	3	1	Total	C	O	0
			42	40	2	
22	3	1	Total	C	O	0
			42	40	2	
22	4	1	Total	C	O	0
			42	40	2	
22	4	1	Total	C	O	0
			42	40	2	
22	J	1	Total	C	O	0
			42	40	2	

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



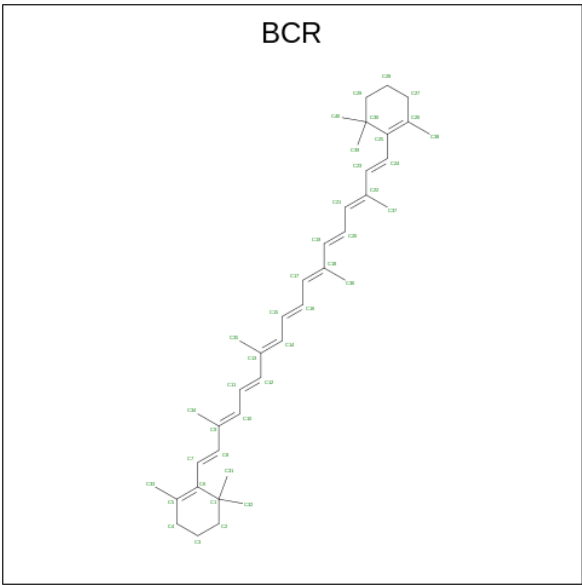
Mol	Chain	Residues	Atoms				AltConf
23	1	1	Total	C	O	P	0
			49	38	10	1	
23	1	1	Total	C	O	P	0
			21	10	10	1	
23	2	1	Total	C	O	P	0
			45	34	10	1	

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

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).



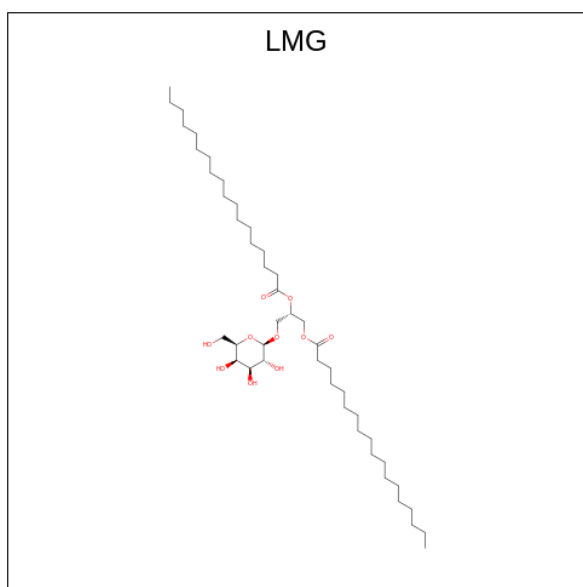
Mol	Chain	Residues	Atoms		AltConf
24	3	1	Total	C	0
			40	40	
24	4	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			25	25	
24	A	1	Total	C	0
			40	40	
24	B	1	Total	C	0
			40	40	
24	B	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	I	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	K	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	L	1	Total C 40 40	0

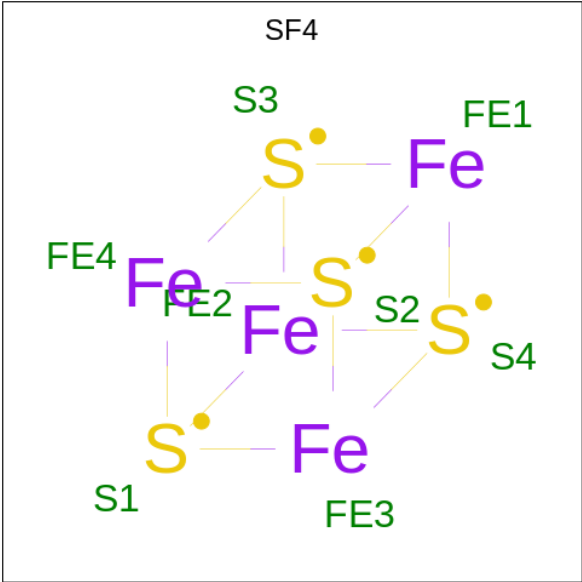
- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
25	4	1	Total	C	O	0
			34	24	10	
25	F	1	Total	C	O	0
			30	20	10	
25	F	1	Total	C	O	0
			30	20	10	
25	G	1	Total	C	O	0
			35	25	10	
25	J	1	Total	C	O	0
			41	31	10	
25	N	1	Total	C	O	0
			27	18	9	

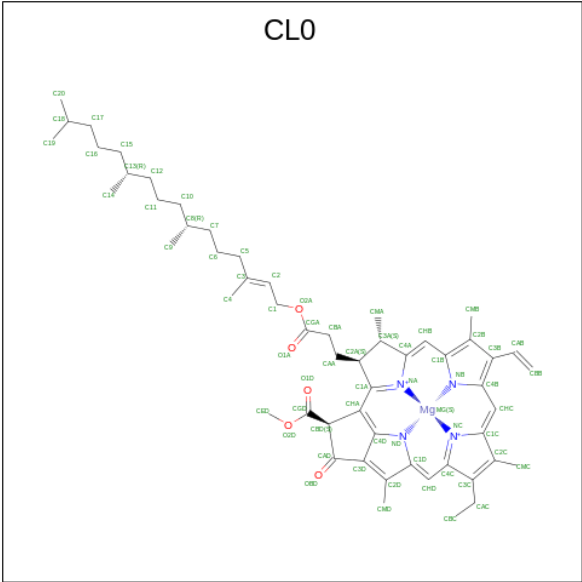
- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).





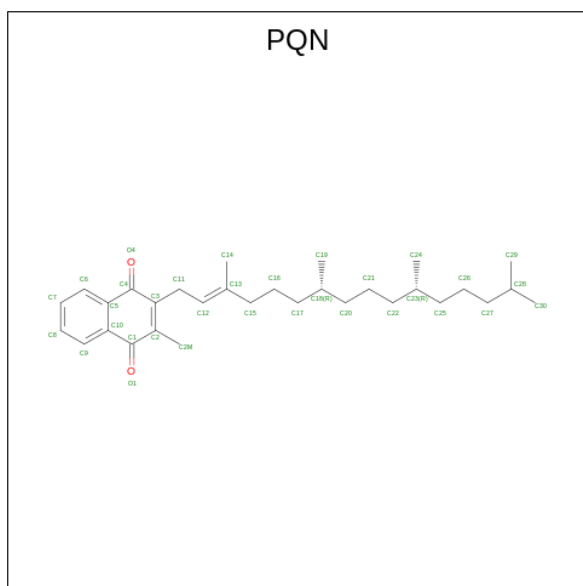
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 27 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



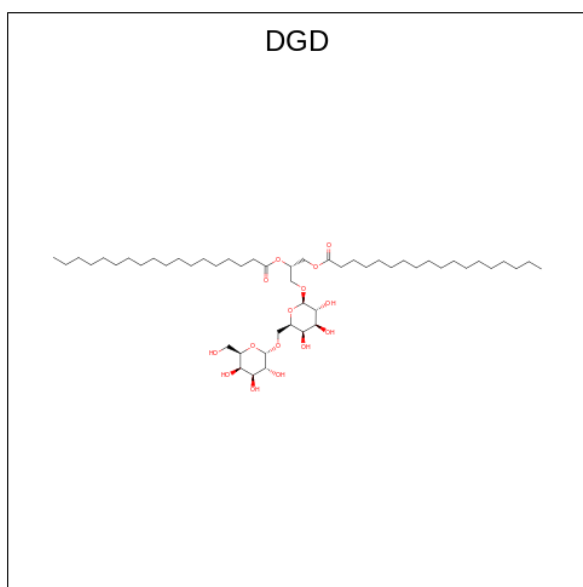
Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 28 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 29 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
29	B	1	Total	C	O	0
			60	45	15	

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		AltConf
30	1	6	Total	O	0
			6	6	
30	2	12	Total	O	0
			12	12	
30	3	11	Total	O	0
			11	11	
30	4	3	Total	O	0
			3	3	
30	A	137	Total	O	0
			137	137	
30	B	177	Total	O	0
			177	177	
30	C	43	Total	O	0
			43	43	
30	D	29	Total	O	0
			29	29	
30	E	16	Total	O	0
			16	16	
30	F	6	Total	O	0
			6	6	
30	G	4	Total	O	0
			4	4	

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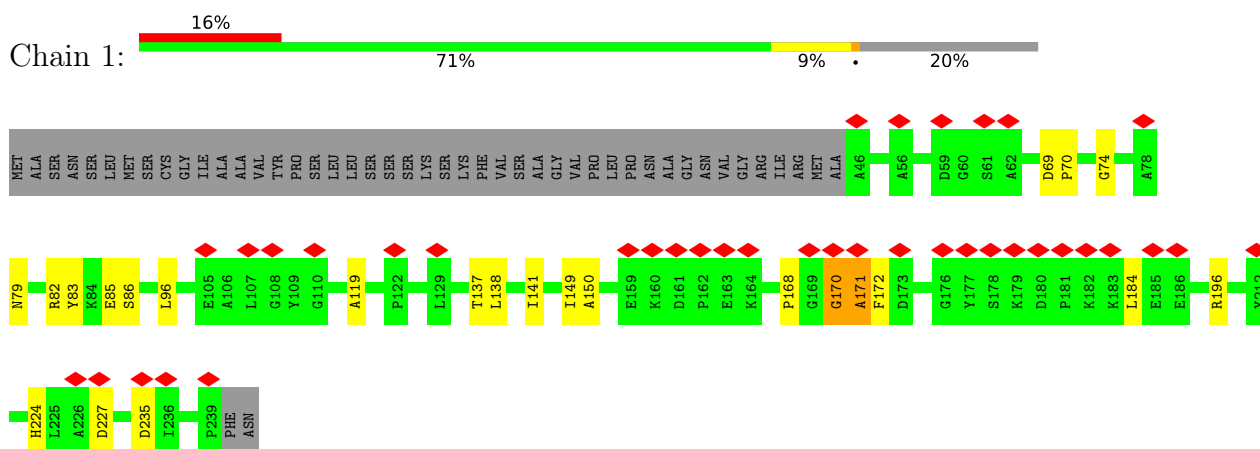
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Mol	Chain	Residues	Atoms		AltConf
30	H	7	Total 7	O 7	0
30	I	1	Total 1	O 1	0
30	J	6	Total 6	O 6	0
30	K	2	Total 2	O 2	0
30	L	16	Total 16	O 16	0
30	N	4	Total 4	O 4	0

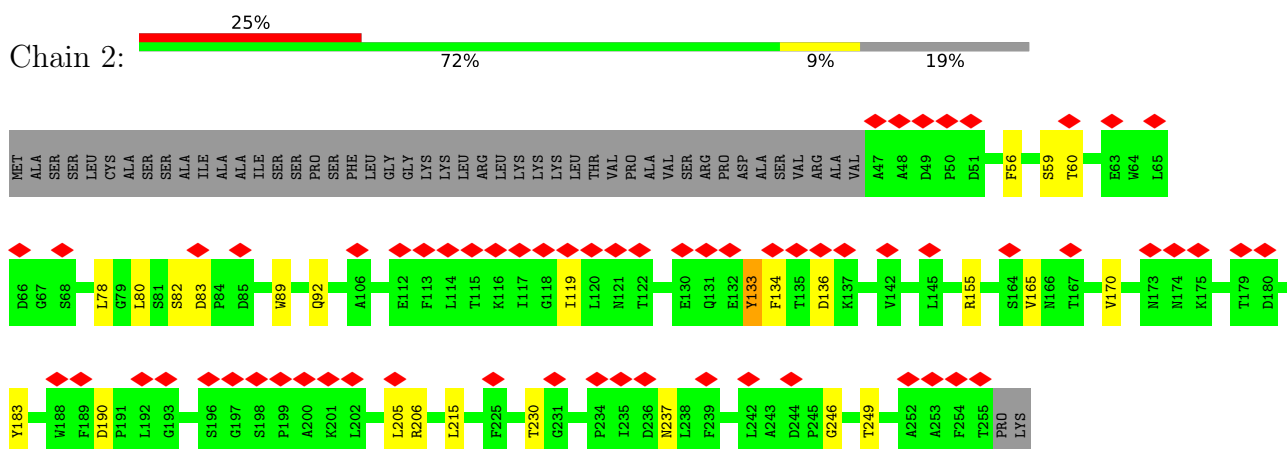
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

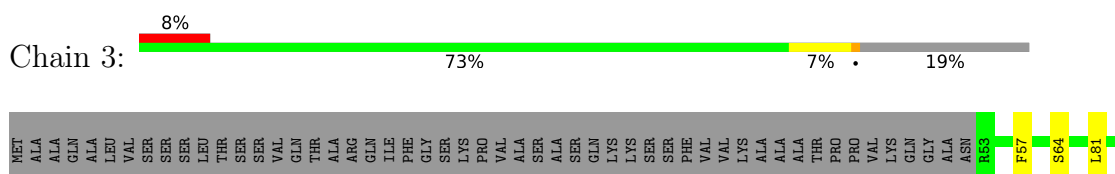
- Molecule 1: Chlorophyll a-b binding protein 6, chloroplastic

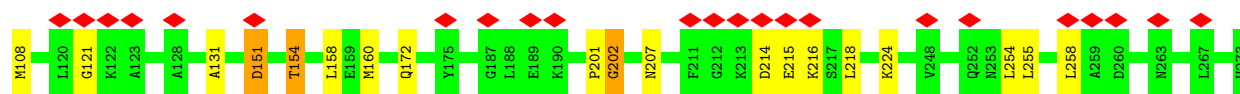


- Molecule 2: Photosystem I chlorophyll a/b-binding protein 2, chloroplastic

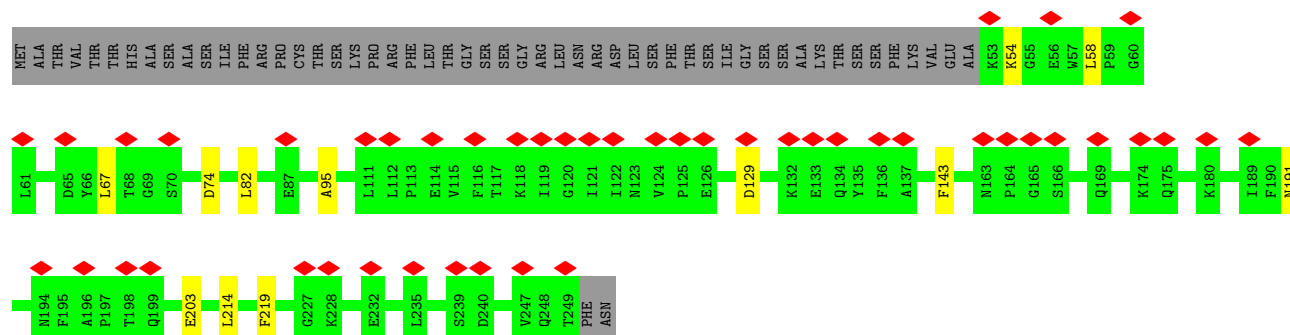
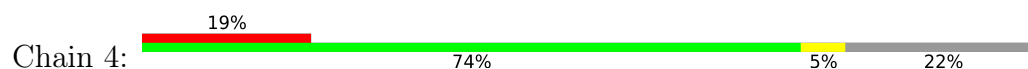


- Molecule 3: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic

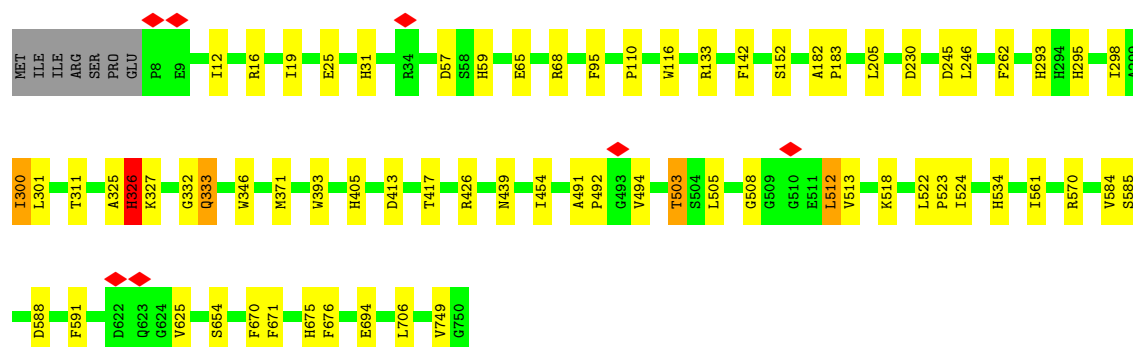
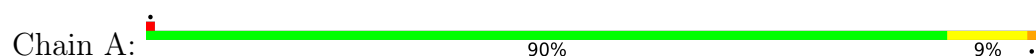




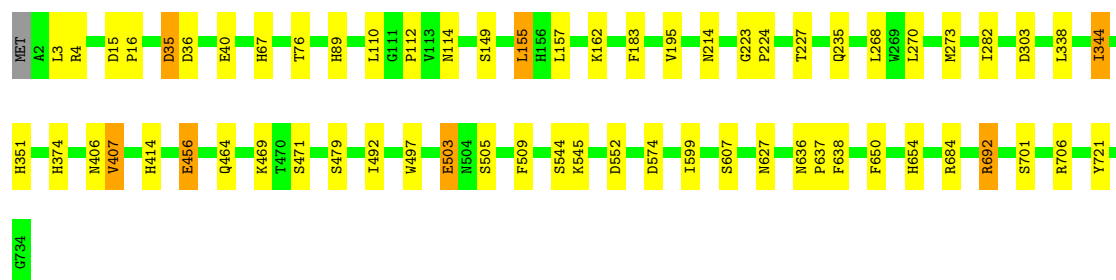
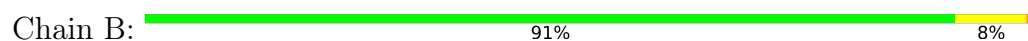
- Molecule 4: Chlorophyll a-b binding protein 4, chloroplastic



- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 7: Photosystem I iron-sulfur center





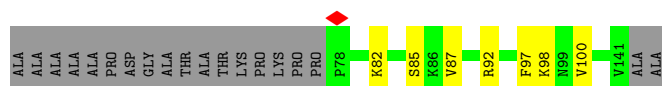
- Molecule 8: Photosystem I reaction center subunit II-2, chloroplastic

Chain D: 63% 6% 30%



- Molecule 9: Photosystem I reaction center subunit IV A, chloroplastic

Chain E: 40% 5% 55%



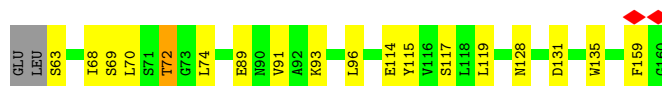
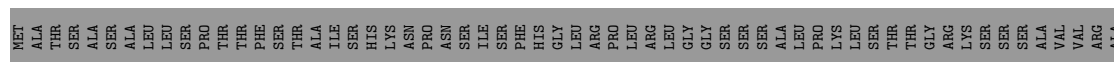
- Molecule 10: Photosystem I reaction center subunit III, chloroplastic

Chain F: 62% 7% 31%



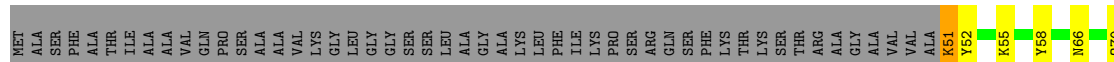
- Molecule 11: Photosystem I reaction center subunit V, chloroplastic

Chain G: 50% 11% 39%



- Molecule 12: Photosystem I reaction center subunit VI-2, chloroplastic

Chain H: 57% 8% 34%







C134	ASP
C135	LEU
Q136	ALA
	LYS
	GLN
	LYS
	LYS
	VAL
	PRO
	PHE
	ILE
	SER
	GLU
	ASP
	ILE
	ALA
	LEU
	GLU
	CYS
	GLU
	GLY
	LYS
	LYS
	ASP
	LYS
	TYR
	LYS
	CYS
	GLY
	SER
	ASN
	VAL
	PHE
	TRP
	LYS
	TRP

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	148985	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.101	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00994	Depositor
Map size ( $\text{\AA}$ )	264.6, 264.6, 264.6	wwPDB
Map dimensions	392, 392, 392	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.675, 0.675, 0.675	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: UNL, LHG, XAT, CLA, CL0, CHL, PQN, LMG, BCR, SF4, A1LXP, DGD

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	1	0.55	0/1551	1.08	1/2117 (0.0%)
2	2	0.55	0/1680	1.14	2/2299 (0.1%)
3	3	0.55	0/1752	1.06	2/2382 (0.1%)
4	4	0.54	0/1598	1.08	2/2179 (0.1%)
5	A	0.89	0/6050	1.16	13/8254 (0.2%)
6	B	0.90	0/6069	1.22	24/8286 (0.3%)
7	C	0.88	0/628	1.46	7/852 (0.8%)
8	D	0.72	0/1157	1.24	4/1563 (0.3%)
9	E	0.67	0/528	1.05	0/715
10	F	0.72	0/1241	1.22	2/1675 (0.1%)
11	G	0.68	0/783	1.21	4/1061 (0.4%)
12	H	0.66	0/756	1.23	4/1024 (0.4%)
13	I	0.76	0/245	1.09	1/333 (0.3%)
14	J	0.69	0/348	1.20	5/474 (1.1%)
15	K	0.60	0/451	1.18	3/608 (0.5%)
16	L	0.74	0/1152	1.18	2/1572 (0.1%)
17	N	0.49	0/400	1.19	0/534
All	All	0.77	0/26389	1.18	76/35928 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	0	1
5	A	0	5
7	C	0	2
9	E	0	1
10	F	0	1
14	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	L	0	1
All	All	0	12

There are no bond length outliers.

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	326	HIS	CA-CB-CG	-10.49	103.31	113.80
6	B	4	ARG	N-CA-CB	-10.39	95.15	111.56
7	C	23	THR	OG1-CB-CG2	-9.60	90.10	109.30
6	B	407	VAL	N-CA-CB	-9.10	95.09	110.65
7	C	23	THR	CA-C-N	-8.74	109.78	123.24

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	133	TYR	Peptide
5	A	16	ARG	Sidechain
5	A	326	HIS	Peptide
5	A	426	ARG	Sidechain
5	A	68	ARG	Sidechain

## 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	1	1501	0	1476	14	0
2	2	1622	0	1562	8	0
3	3	1699	0	1665	8	0
4	4	1550	0	1490	9	0
5	A	5851	0	5706	41	0
6	B	5858	0	5649	24	0
7	C	615	0	592	3	0
8	D	1128	0	1134	6	0
9	E	517	0	526	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	F	1211	0	1239	5	0
11	G	763	0	738	9	0
12	H	735	0	732	8	0
13	I	239	0	258	2	0
14	J	338	0	351	5	0
15	K	447	0	460	4	0
16	L	1119	0	1124	9	0
17	N	394	0	381	5	0
18	1	102	0	82	4	0
18	2	147	0	111	0	0
18	3	117	0	107	1	0
18	4	92	0	62	2	0
19	1	325	0	288	9	0
19	2	212	0	184	2	0
19	3	404	0	335	4	0
19	4	244	0	195	6	0
19	A	2378	0	2287	57	0
19	B	2326	0	2257	56	0
19	F	90	0	67	2	0
19	G	87	0	64	5	0
19	H	55	0	49	0	0
19	J	65	0	72	1	0
19	K	90	0	66	2	0
19	L	155	0	138	2	0
20	1	274	0	0	4	0
20	2	291	0	0	1	0
20	3	163	0	0	1	0
20	4	354	0	0	1	0
20	G	45	0	0	0	0
20	J	42	0	0	1	0
20	K	42	0	0	0	0
20	N	41	0	0	0	0
21	1	72	0	90	6	0
21	2	44	0	56	1	0
22	1	84	0	0	0	0
22	2	42	0	0	1	0
22	3	84	0	0	1	0
22	4	84	0	0	1	0
22	J	42	0	0	0	0
23	1	70	0	86	0	0
23	2	45	0	63	0	0
23	A	49	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	3	40	0	56	0	0
24	4	40	0	56	3	0
24	A	225	0	313	25	0
24	B	200	0	280	11	0
24	F	80	0	112	5	0
24	G	80	0	112	6	0
24	I	40	0	56	1	0
24	J	40	0	56	0	0
24	K	40	0	56	2	0
24	L	120	0	168	4	0
25	4	34	0	38	0	0
25	F	60	0	60	2	0
25	G	35	0	40	0	0
25	J	41	0	55	0	0
25	N	27	0	30	3	0
26	A	8	0	0	0	0
26	C	16	0	0	0	0
27	A	65	0	72	0	0
28	A	33	0	46	0	0
28	B	33	0	46	0	0
29	B	60	0	81	1	0
30	1	6	0	0	0	0
30	2	12	0	0	0	0
30	3	11	0	0	0	0
30	4	3	0	0	0	0
30	A	137	0	0	1	0
30	B	177	0	0	0	0
30	C	43	0	0	0	0
30	D	29	0	0	1	0
30	E	16	0	0	0	0
30	F	6	0	0	0	0
30	G	4	0	0	0	0
30	H	7	0	0	0	0
30	I	1	0	0	0	0
30	J	6	0	0	0	0
30	K	2	0	0	0	0
30	L	16	0	0	0	0
30	N	4	0	0	0	0
All	All	36141	0	33549	303	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 4.

The worst 5 of 303 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)
12:H:51:LYS:HA	12:H:66:ASN:HB3	1.43	0.99
16:L:65:ILE:HB	16:L:73:SER:OG	1.66	0.95
19:1:602:CLA:O1A	21:1:615:XAT:H241	1.72	0.88
19:G:203:CLA:HBB1	24:G:205:BCR:H352	1.67	0.77
4:4:54:LYS:NZ	4:4:74:ASP:OD1	2.16	0.76

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	192/241 (80%)	182 (95%)	8 (4%)	2 (1%)	12	10
2	2	207/257 (80%)	192 (93%)	13 (6%)	2 (1%)	12	10
3	3	219/273 (80%)	208 (95%)	9 (4%)	2 (1%)	14	12
4	4	195/251 (78%)	183 (94%)	12 (6%)	0	100	100
5	A	741/750 (99%)	713 (96%)	24 (3%)	4 (0%)	24	25
6	B	731/734 (100%)	712 (97%)	18 (2%)	1 (0%)	48	55
7	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
8	D	141/204 (69%)	139 (99%)	2 (1%)	0	100	100
9	E	62/143 (43%)	61 (98%)	1 (2%)	0	100	100
10	F	151/221 (68%)	147 (97%)	4 (3%)	0	100	100
11	G	96/160 (60%)	94 (98%)	2 (2%)	0	100	100
12	H	93/145 (64%)	91 (98%)	2 (2%)	0	100	100
13	I	29/37 (78%)	27 (93%)	2 (7%)	0	100	100
14	J	40/44 (91%)	38 (95%)	1 (2%)	1 (2%)	4	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	K	60/130 (46%)	55 (92%)	5 (8%)	0	100	100
16	L	148/219 (68%)	142 (96%)	6 (4%)	0	100	100
17	N	48/171 (28%)	45 (94%)	3 (6%)	0	100	100
All	All	3231/4061 (80%)	3103 (96%)	116 (4%)	12 (0%)	31	31

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	171	ALA
3	3	202	GLY
1	1	170	GLY
5	A	31	HIS
5	A	503	THR

### 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	1	153/190 (80%)	148 (97%)	5 (3%)	33	42
2	2	166/205 (81%)	155 (93%)	11 (7%)	15	16
3	3	171/211 (81%)	160 (94%)	11 (6%)	16	16
4	4	161/210 (77%)	160 (99%)	1 (1%)	78	87
5	A	603/610 (99%)	592 (98%)	11 (2%)	51	65
6	B	599/600 (100%)	582 (97%)	17 (3%)	38	49
7	C	70/71 (99%)	68 (97%)	2 (3%)	37	47
8	D	121/170 (71%)	118 (98%)	3 (2%)	42	53
9	E	57/114 (50%)	57 (100%)	0	100	100
10	F	124/185 (67%)	118 (95%)	6 (5%)	23	27
11	G	82/133 (62%)	77 (94%)	5 (6%)	17	18
12	H	79/113 (70%)	76 (96%)	3 (4%)	29	37
13	I	27/33 (82%)	27 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	J	37/39 (95%)	36 (97%)	1 (3%)	39	50
15	K	47/95 (50%)	46 (98%)	1 (2%)	47	59
16	L	116/174 (67%)	109 (94%)	7 (6%)	17	19
17	N	42/138 (30%)	42 (100%)	0	100	100
All	All	2655/3291 (81%)	2571 (97%)	84 (3%)	35	43

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	C	65	VAL
11	G	117	SER
8	D	105	ILE
10	F	167	VAL
14	J	41	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	210	ASN
9	E	127	ASN
7	C	38	GLN
10	F	137	HIS
3	3	252	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 206 ligands modelled in this entry, 29 are unknown - leaving 177 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
19	CLA	A	836	5	49,53,73	1.62	7 (14%)	59,89,113	1.70	10 (16%)
24	BCR	F	302	-	41,41,41	0.59	0	56,56,56	0.76	0
19	CLA	J	101	5	69,73,73	1.75	8 (11%)	83,113,113	1.20	7 (8%)
19	CLA	B	822	6	69,73,73	1.62	8 (11%)	83,113,113	1.22	7 (8%)
24	BCR	F	304	-	41,41,41	0.47	0	56,56,56	0.58	0
25	LMG	F	305	-	30,30,55	0.34	0	38,38,63	0.68	1 (2%)
19	CLA	B	804	30	49,53,73	1.82	5 (10%)	59,89,113	1.44	10 (16%)
19	CLA	3	306	3	51,55,73	2.17	8 (15%)	61,91,113	1.51	9 (14%)
19	CLA	B	839	6	47,51,73	1.85	9 (19%)	56,86,113	1.64	8 (14%)
19	CLA	A	848	5	54,58,73	1.72	9 (16%)	65,95,113	1.81	13 (20%)
24	BCR	A	852	-	41,41,41	0.70	1 (2%)	56,56,56	0.73	1 (1%)
19	CLA	B	807	6	49,53,73	1.33	7 (14%)	59,89,113	1.44	6 (10%)
19	CLA	A	810	5	54,58,73	2.02	8 (14%)	65,95,113	1.69	11 (16%)
19	CLA	B	830	6	69,73,73	1.46	6 (8%)	83,113,113	1.61	9 (10%)
24	BCR	L	302	-	41,41,41	0.63	0	56,56,56	0.57	1 (1%)
19	CLA	A	825	5	46,50,73	2.01	8 (17%)	55,85,113	1.45	9 (16%)
26	SF4	C	102	7	0,12,12	-	-	-	-	-
19	CLA	B	844	6	63,67,73	1.76	11 (17%)	75,105,113	1.55	10 (13%)
19	CLA	B	826	6	69,73,73	1.15	5 (7%)	83,113,113	1.38	9 (10%)
19	CLA	B	818	30	69,73,73	1.28	6 (8%)	83,113,113	1.83	16 (19%)
19	CLA	3	308	30	49,53,73	1.43	7 (14%)	59,89,113	1.26	8 (13%)
19	CLA	3	301	3	64,68,73	1.65	9 (14%)	77,107,113	1.36	10 (12%)
24	BCR	G	201	-	41,41,41	0.83	2 (4%)	56,56,56	0.54	0
18	CHL	2	313	30	41,50,74	3.11	9 (21%)	30,85,114	2.91	10 (33%)
22	A1LXP	2	309	-	42,43,43	0.27	0	51,60,60	0.65	0
28	PQN	A	839	-	34,34,34	0.41	0	42,45,45	0.74	1 (2%)
19	CLA	B	834	6	69,73,73	1.10	4 (5%)	83,113,113	1.46	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CHL	1	601	1	58,67,74	2.73	7 (12%)	50,105,114	2.22	9 (18%)
19	CLA	A	816	5	54,58,73	1.82	7 (12%)	65,95,113	1.28	9 (13%)
24	BCR	B	813	-	41,41,41	0.75	1 (2%)	56,56,56	0.69	1 (1%)
22	A1LXP	4	306	-	42,43,43	0.38	0	51,60,60	0.66	0
19	CLA	3	314	3	59,63,73	1.93	6 (10%)	71,101,113	1.37	9 (12%)
19	CLA	2	312	2	66,70,73	2.01	7 (10%)	79,109,113	1.36	9 (11%)
26	SF4	C	101	7	0,12,12	-	-	-	-	-
19	CLA	A	824	5	69,73,73	1.33	6 (8%)	83,113,113	1.23	5 (6%)
23	LHG	1	617	20	48,48,48	0.35	0	51,54,54	0.79	2 (3%)
19	CLA	B	808	30	69,73,73	1.19	7 (10%)	83,113,113	1.53	11 (13%)
19	CLA	A	801	30	59,63,73	1.84	10 (16%)	71,101,113	1.73	14 (19%)
19	CLA	3	312	3	46,50,73	1.90	9 (19%)	55,85,113	1.49	5 (9%)
19	CLA	B	847	6	54,58,73	1.46	9 (16%)	65,95,113	1.51	5 (7%)
19	CLA	A	802	5,19	60,64,73	1.23	5 (8%)	72,102,113	1.65	12 (16%)
19	CLA	1	602	1	64,68,73	1.67	9 (14%)	77,107,113	1.66	15 (19%)
22	A1LXP	1	619	-	42,43,43	0.44	0	51,60,60	0.57	0
19	CLA	2	311	2	49,53,73	2.06	9 (18%)	59,89,113	1.47	8 (13%)
19	CLA	A	815	5	49,53,73	1.75	9 (18%)	59,89,113	1.87	12 (20%)
19	CLA	A	831	5	69,73,73	1.44	7 (10%)	83,113,113	1.37	10 (12%)
19	CLA	A	806	5	46,50,73	2.21	9 (19%)	55,85,113	1.56	7 (12%)
19	CLA	A	833	-	69,73,73	1.58	10 (14%)	83,113,113	1.20	5 (6%)
18	CHL	4	313	30	45,54,74	3.09	10 (22%)	35,90,114	2.50	9 (25%)
25	LMG	G	206	-	35,35,55	0.37	0	43,43,63	0.51	0
27	CL0	A	830	5	63,73,73	1.65	8 (12%)	61,113,113	2.65	14 (22%)
18	CHL	2	315	30	45,54,74	3.25	10 (22%)	35,90,114	2.40	9 (25%)
24	BCR	B	814	-	41,41,41	0.52	0	56,56,56	0.58	0
19	CLA	3	302	3	56,60,73	1.89	8 (14%)	67,97,113	1.34	5 (7%)
19	CLA	B	810	23	69,73,73	1.44	8 (11%)	83,113,113	1.22	6 (7%)
19	CLA	B	821	6	46,50,73	1.64	6 (13%)	55,85,113	2.04	10 (18%)
19	CLA	A	808	30	69,73,73	1.37	6 (8%)	83,113,113	1.47	9 (10%)
19	CLA	B	803	6	49,53,73	1.74	9 (18%)	59,89,113	1.78	12 (20%)
23	LHG	A	835	-	48,48,48	0.80	1 (2%)	51,54,54	1.43	7 (13%)
19	CLA	A	837	5	69,73,73	1.64	10 (14%)	83,113,113	1.66	10 (12%)
24	BCR	B	812	-	41,41,41	0.59	0	56,56,56	0.79	1 (1%)
19	CLA	B	838	6	49,53,73	1.65	11 (22%)	59,89,113	1.30	6 (10%)
24	BCR	3	316	-	41,41,41	0.46	0	56,56,56	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	H	201	12	59,63,73	1.61	10 (16%)	71,101,113	1.39	9 (12%)
19	CLA	B	848	6	49,53,73	2.21	10 (20%)	59,89,113	2.16	6 (10%)
19	CLA	B	820	-	69,73,73	1.75	9 (13%)	83,113,113	1.19	8 (9%)
25	LMG	4	304	-	34,34,55	0.34	0	42,42,63	0.59	1 (2%)
23	LHG	1	620	19	20,20,48	0.59	0	23,26,54	0.81	0
19	CLA	F	306	30	52,56,73	1.59	7 (13%)	62,92,113	1.38	8 (12%)
22	A1LXP	3	310	-	42,43,43	0.62	1 (2%)	51,60,60	1.02	3 (5%)
19	CLA	A	812	5	69,73,73	1.40	9 (13%)	83,113,113	1.25	10 (12%)
24	BCR	B	816	-	41,41,41	0.55	0	56,56,56	0.74	1 (1%)
19	CLA	B	824	6	56,60,73	1.70	6 (10%)	67,97,113	1.70	10 (14%)
19	CLA	F	303	10	46,50,73	1.82	8 (17%)	55,85,113	1.72	9 (16%)
19	CLA	1	605	30	49,53,73	1.92	9 (18%)	59,89,113	1.36	8 (13%)
19	CLA	A	849	5	54,58,73	1.58	10 (18%)	65,95,113	1.54	7 (10%)
24	BCR	A	838	-	41,41,41	0.63	1 (2%)	56,56,56	0.54	0
19	CLA	A	842	5	64,68,73	1.55	7 (10%)	77,107,113	1.69	15 (19%)
25	LMG	N	201	-	27,27,55	0.46	0	34,34,63	0.83	2 (5%)
19	CLA	A	813	5	64,68,73	1.60	12 (18%)	77,107,113	1.85	10 (12%)
19	CLA	B	843	6	69,73,73	1.43	8 (11%)	83,113,113	1.36	10 (12%)
19	CLA	A	850	30	69,73,73	1.13	6 (8%)	83,113,113	1.27	4 (4%)
19	CLA	1	608	1	61,65,73	1.74	7 (11%)	73,103,113	1.17	7 (9%)
21	XAT	2	306	-	39,47,47	0.31	0	54,74,74	1.02	2 (3%)
19	CLA	A	822	5	57,61,73	1.64	8 (14%)	68,98,113	1.42	9 (13%)
24	BCR	4	308	-	41,41,41	0.35	0	56,56,56	0.56	0
24	BCR	L	306	-	41,41,41	0.53	0	56,56,56	0.46	0
19	CLA	B	841	30	60,64,73	1.42	10 (16%)	72,102,113	1.75	14 (19%)
19	CLA	A	840	5,19	69,73,73	1.57	8 (11%)	83,113,113	1.49	10 (12%)
19	CLA	1	603	1	61,65,73	1.83	8 (13%)	73,103,113	1.53	9 (12%)
19	CLA	4	307	4	49,53,73	2.37	5 (10%)	59,89,113	1.59	8 (13%)
19	CLA	A	832	5	49,53,73	2.07	7 (14%)	59,89,113	1.82	11 (18%)
18	CHL	3	303	3	65,74,74	2.27	6 (9%)	59,114,114	2.22	11 (18%)
24	BCR	A	804	-	41,41,41	0.65	0	56,56,56	0.70	2 (3%)
19	CLA	A	821	5	56,60,73	1.45	9 (16%)	67,97,113	1.42	8 (11%)
24	BCR	A	841	-	41,41,41	0.66	0	56,56,56	0.63	0
19	CLA	B	828	6	55,59,73	1.73	6 (10%)	66,96,113	1.69	12 (18%)
26	SF4	A	803	5,6	0,12,12	-	-	-	-	-
24	BCR	K	201	-	41,41,41	0.42	0	56,56,56	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CHL	2	316	2	58,67,74	2.78	12 (20%)	50,105,114	2.14	7 (14%)
22	A1LXP	4	303	-	42,43,43	0.78	3 (7%)	51,60,60	0.89	1 (1%)
25	LMG	F	301	-	30,30,55	0.36	0	38,38,63	0.48	0
19	CLA	4	314	4	56,60,73	2.17	7 (12%)	67,97,113	1.39	10 (14%)
19	CLA	B	835	6	61,65,73	1.50	6 (9%)	73,103,113	1.72	18 (24%)
19	CLA	4	317	4	61,65,73	1.90	9 (14%)	73,103,113	1.44	9 (12%)
19	CLA	A	827	5	62,66,73	1.89	9 (14%)	74,104,113	1.38	11 (14%)
19	CLA	L	305	16	49,53,73	2.38	6 (12%)	59,89,113	1.45	7 (11%)
19	CLA	L	303	30	49,53,73	1.70	7 (14%)	59,89,113	1.41	7 (11%)
19	CLA	B	845	6	69,73,73	1.49	8 (11%)	83,113,113	1.51	11 (13%)
19	CLA	A	807	30	49,53,73	1.89	9 (18%)	59,89,113	1.42	10 (16%)
19	CLA	B	819	6	69,73,73	1.18	7 (10%)	83,113,113	1.11	6 (7%)
18	CHL	1	606	1	42,51,74	3.29	7 (16%)	31,86,114	2.75	7 (22%)
23	LHG	2	302	20	44,44,48	0.36	0	47,50,54	0.56	0
19	CLA	B	806	6	69,73,73	1.37	5 (7%)	83,113,113	1.86	9 (10%)
19	CLA	3	307	30	52,56,73	1.71	9 (17%)	62,92,113	1.21	8 (12%)
19	CLA	B	805	6	54,58,73	1.40	5 (9%)	65,95,113	1.55	5 (7%)
19	CLA	A	805	5	51,55,73	1.89	9 (17%)	61,91,113	1.47	7 (11%)
19	CLA	A	829	5	69,73,73	1.38	8 (11%)	83,113,113	1.53	11 (13%)
19	CLA	B	829	6	47,51,73	1.78	7 (14%)	56,86,113	1.60	9 (16%)
19	CLA	B	837	6	51,55,73	1.66	8 (15%)	61,91,113	1.59	12 (19%)
19	CLA	B	823	6	69,73,73	1.14	7 (10%)	83,113,113	1.23	8 (9%)
19	CLA	K	202	15	49,53,73	1.82	10 (20%)	59,89,113	2.05	7 (11%)
19	CLA	4	311	4	49,53,73	2.24	10 (20%)	59,89,113	1.58	11 (18%)
19	CLA	A	817	30	53,57,73	1.41	7 (13%)	62,93,113	1.87	11 (17%)
24	BCR	J	105	-	41,41,41	0.58	0	56,56,56	0.56	0
24	BCR	B	815	-	41,41,41	0.59	1 (2%)	56,56,56	0.75	1 (1%)
29	DGD	B	817	-	61,61,67	0.42	0	75,75,81	0.88	3 (4%)
19	CLA	1	612	1	59,63,73	2.04	8 (13%)	71,101,113	1.28	10 (14%)
19	CLA	B	802	6	64,68,73	1.35	8 (12%)	77,107,113	1.40	8 (10%)
19	CLA	A	828	5	69,73,73	1.57	10 (14%)	83,113,113	1.70	16 (19%)
19	CLA	B	846	6	69,73,73	1.44	9 (13%)	83,113,113	1.42	9 (10%)
28	PQN	B	811	-	34,34,34	0.60	0	42,45,45	0.96	2 (4%)
24	BCR	A	845	-	41,41,41	0.51	0	56,56,56	0.65	0
24	BCR	I	101	-	41,41,41	0.59	0	56,56,56	0.58	0
19	CLA	A	826	5	69,73,73	1.17	6 (8%)	83,113,113	1.55	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	A1LXP	3	305	-	42,43,43	0.42	0	51,60,60	0.70	1 (1%)
19	CLA	4	318	4	49,53,73	2.34	7 (14%)	59,89,113	1.55	9 (15%)
22	A1LXP	J	102	-	42,43,43	0.41	0	51,60,60	0.80	1 (1%)
19	CLA	A	843	5	57,61,73	1.72	9 (15%)	68,98,113	1.73	12 (17%)
19	CLA	A	846	5	69,73,73	1.36	10 (14%)	83,113,113	1.60	15 (18%)
19	CLA	A	818	5	69,73,73	1.54	9 (13%)	83,113,113	1.56	13 (15%)
19	CLA	K	203	30	49,53,73	2.01	10 (20%)	59,89,113	1.55	6 (10%)
19	CLA	A	823	30	69,73,73	1.57	8 (11%)	83,113,113	1.66	13 (15%)
18	CHL	4	319	4	45,54,74	3.26	8 (17%)	35,90,114	2.59	9 (25%)
18	CHL	3	315	30	50,59,74	2.80	9 (18%)	41,96,114	2.48	8 (19%)
19	CLA	A	814	5	69,73,73	1.52	6 (8%)	83,113,113	1.64	17 (20%)
19	CLA	B	836	30	60,64,73	1.76	8 (13%)	72,102,113	1.23	8 (11%)
19	CLA	A	834	5	69,73,73	1.40	6 (8%)	83,113,113	1.42	7 (8%)
19	CLA	3	304	3	59,63,73	1.77	8 (13%)	71,101,113	1.46	10 (14%)
19	CLA	L	304	16	69,73,73	1.29	6 (8%)	83,113,113	1.25	8 (9%)
24	BCR	A	847	-	25,25,41	0.51	0	33,33,56	0.84	1 (3%)
19	CLA	B	833	6	64,68,73	2.41	7 (10%)	77,107,113	1.51	11 (14%)
19	CLA	B	825	6	69,73,73	1.55	5 (7%)	83,113,113	1.60	9 (10%)
19	CLA	B	840	6	49,53,73	2.00	8 (16%)	59,89,113	1.93	12 (20%)
21	XAT	1	618	-	25,29,47	0.42	0	33,43,74	1.54	2 (6%)
22	A1LXP	1	616	-	42,43,43	0.58	1 (2%)	51,60,60	0.71	0
19	CLA	G	203	11	49,53,73	1.73	11 (22%)	59,89,113	2.06	10 (16%)
25	LMG	J	103	-	41,41,55	0.45	0	49,49,63	0.68	1 (2%)
19	CLA	2	301	2	54,58,73	2.12	8 (14%)	65,95,113	1.34	9 (13%)
19	CLA	B	842	30	54,58,73	1.71	10 (18%)	65,95,113	1.66	10 (15%)
19	CLA	A	844	5	46,50,73	2.23	8 (17%)	55,85,113	1.52	9 (16%)
19	CLA	2	310	2	59,63,73	2.12	6 (10%)	71,101,113	1.51	14 (19%)
19	CLA	B	831	6	69,73,73	1.41	8 (11%)	83,113,113	1.49	9 (10%)
19	CLA	1	607	-	55,59,73	1.91	8 (14%)	66,96,113	1.33	4 (6%)
19	CLA	B	809	6	69,73,73	1.21	10 (14%)	83,113,113	1.37	11 (13%)
24	BCR	G	205	-	41,41,41	0.54	0	56,56,56	0.52	0
19	CLA	A	820	5	46,50,73	1.60	5 (10%)	55,85,113	1.50	8 (14%)
19	CLA	A	811	5	59,63,73	2.13	8 (13%)	71,101,113	1.31	9 (12%)
21	XAT	1	615	-	39,47,47	0.44	0	54,74,74	1.65	5 (9%)
19	CLA	A	819	5	69,73,73	1.38	8 (11%)	83,113,113	1.58	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	B	832	6	49,53,73	1.92	7 (14%)	59,89,113	2.13	14 (23%)
19	CLA	A	809	5	69,73,73	1.11	4 (5%)	83,113,113	1.71	15 (18%)
19	CLA	B	801	6	69,73,73	1.62	8 (11%)	83,113,113	1.48	9 (10%)
19	CLA	G	202	30	46,50,73	1.96	10 (21%)	55,85,113	1.54	7 (12%)
19	CLA	B	827	6	69,73,73	1.91	11 (15%)	83,113,113	1.52	11 (13%)
19	CLA	A	851	30	66,70,73	1.53	7 (10%)	79,109,113	1.62	13 (16%)
24	BCR	L	301	-	41,41,41	0.53	0	56,56,56	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	836	5	-	5/15/91/115	-
24	BCR	F	302	-	-	0/29/63/63	0/2/2/2
19	CLA	J	101	5	1/1/15/20	9/39/115/115	-
19	CLA	B	822	6	1/1/15/20	13/39/115/115	-
24	BCR	F	304	-	-	2/29/63/63	0/2/2/2
25	LMG	F	305	-	-	7/24/44/70	0/1/1/1
19	CLA	B	804	30	-	0/15/91/115	-
19	CLA	3	306	3	-	3/18/94/115	-
19	CLA	B	839	6	-	2/13/89/115	-
19	CLA	A	848	5	-	2/21/97/115	-
24	BCR	A	852	-	-	2/29/63/63	0/2/2/2
19	CLA	B	807	6	-	2/15/91/115	-
19	CLA	B	830	6	1/1/15/20	20/39/115/115	-
19	CLA	A	810	5	-	0/21/97/115	-
24	BCR	L	302	-	-	0/29/63/63	0/2/2/2
19	CLA	A	825	5	-	10/12/88/115	-
26	SF4	C	102	7	-	-	0/6/5/5
19	CLA	B	844	6	1/1/13/20	7/32/108/115	-
19	CLA	B	826	6	1/1/15/20	14/39/115/115	-
19	CLA	B	818	30	1/1/15/20	17/39/115/115	-
19	CLA	3	308	30	-	0/15/91/115	-
19	CLA	3	301	3	1/1/14/20	7/33/109/115	-
24	BCR	G	201	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CHL	2	313	30	-	5/10/108/137	-
22	A1LXP	2	309	-	-	2/29/67/67	0/2/2/2
28	PQN	A	839	-	-	4/23/43/43	0/2/2/2
19	CLA	B	834	6	1/1/15/20	9/39/115/115	-
18	CHL	1	601	1	1/1/18/26	11/31/129/137	-
19	CLA	A	816	5	-	2/21/97/115	-
24	BCR	B	813	-	-	6/29/63/63	0/2/2/2
22	A1LXP	4	306	-	-	2/29/67/67	0/2/2/2
19	CLA	3	314	3	1/1/13/20	2/27/103/115	-
19	CLA	2	312	2	1/1/14/20	15/36/112/115	-
26	SF4	C	101	7	-	-	0/6/5/5
19	CLA	A	824	5	1/1/15/20	11/39/115/115	-
23	LHG	1	617	20	-	25/53/53/53	-
19	CLA	B	808	30	1/1/15/20	10/39/115/115	-
19	CLA	A	801	30	1/1/13/20	2/27/103/115	-
19	CLA	3	312	3	-	3/12/88/115	-
19	CLA	B	847	6	-	3/21/97/115	-
19	CLA	A	802	5,19	1/1/13/20	6/29/105/115	-
19	CLA	1	602	1	1/1/14/20	15/33/109/115	-
22	A1LXP	1	619	-	-	2/29/67/67	0/2/2/2
19	CLA	2	311	2	-	0/15/91/115	-
19	CLA	A	815	5	-	3/15/91/115	-
19	CLA	A	831	5	1/1/15/20	12/39/115/115	-
19	CLA	A	833	-	1/1/15/20	6/39/115/115	-
19	CLA	A	806	5	-	7/12/88/115	-
18	CHL	4	313	30	-	2/15/113/137	-
25	LMG	G	206	-	-	7/30/50/70	0/1/1/1
27	CL0	A	830	5	-	4/37/135/135	-
18	CHL	2	315	30	-	11/15/113/137	-
24	BCR	B	814	-	-	2/29/63/63	0/2/2/2
19	CLA	3	302	3	-	9/24/100/115	-
19	CLA	B	810	23	1/1/15/20	14/39/115/115	-
19	CLA	B	821	6	-	4/12/88/115	-
19	CLA	A	808	30	1/1/15/20	7/39/115/115	-
19	CLA	B	803	6	-	0/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LHG	A	835	-	-	17/53/53/53	-
19	CLA	A	837	5	1/1/15/20	12/39/115/115	-
24	BCR	B	812	-	-	4/29/63/63	0/2/2/2
19	CLA	B	838	6	-	3/15/91/115	-
24	BCR	3	316	-	-	4/29/63/63	0/2/2/2
19	CLA	H	201	12	1/1/13/20	8/27/103/115	-
19	CLA	B	848	6	-	1/15/91/115	-
19	CLA	B	820	-	1/1/15/20	9/39/115/115	-
25	LMG	4	304	-	-	7/29/49/70	0/1/1/1
23	LHG	1	620	19	-	2/23/23/53	-
19	CLA	F	306	30	-	3/19/95/115	-
22	A1LXP	3	310	-	-	0/29/67/67	0/2/2/2
19	CLA	A	812	5	1/1/15/20	10/39/115/115	-
24	BCR	B	816	-	-	0/29/63/63	0/2/2/2
19	CLA	B	824	6	-	1/24/100/115	-
19	CLA	F	303	10	-	2/12/88/115	-
19	CLA	1	605	30	-	8/15/91/115	-
19	CLA	A	849	5	-	1/21/97/115	-
24	BCR	A	838	-	-	2/29/63/63	0/2/2/2
19	CLA	A	842	5	1/1/14/20	8/33/109/115	-
25	LMG	N	201	-	-	5/20/40/70	0/1/1/1
19	CLA	A	813	5	1/1/14/20	6/33/109/115	-
19	CLA	B	843	6	1/1/15/20	7/39/115/115	-
19	CLA	A	850	30	1/1/15/20	6/39/115/115	-
19	CLA	1	608	1	1/1/13/20	10/30/106/115	-
21	XAT	2	306	-	-	1/31/93/93	0/4/4/4
19	CLA	A	822	5	-	10/25/101/115	-
24	BCR	4	308	-	-	6/29/63/63	0/2/2/2
24	BCR	L	306	-	-	3/29/63/63	0/2/2/2
19	CLA	B	841	30	1/1/13/20	5/29/105/115	-
19	CLA	A	840	5,19	1/1/15/20	12/39/115/115	-
19	CLA	1	603	1	1/1/13/20	12/30/106/115	-
19	CLA	4	307	4	-	5/15/91/115	-
19	CLA	A	832	5	-	0/15/91/115	-
18	CHL	3	303	3	1/1/20/26	13/39/137/137	-
24	BCR	A	804	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	821	5	-	7/24/100/115	-
24	BCR	A	841	-	-	4/29/63/63	0/2/2/2
19	CLA	B	828	6	-	10/23/99/115	-
26	SF4	A	803	5,6	-	-	0/6/5/5
24	BCR	K	201	-	-	4/29/63/63	0/2/2/2
18	CHL	2	316	2	1/1/18/26	9/31/129/137	-
22	A1LXP	4	303	-	-	0/29/67/67	0/2/2/2
25	LMG	F	301	-	-	2/25/45/70	0/1/1/1
19	CLA	4	314	4	-	2/24/100/115	-
19	CLA	B	835	6	1/1/13/20	3/30/106/115	-
19	CLA	4	317	4	1/1/13/20	4/30/106/115	-
19	CLA	A	827	5	1/1/13/20	4/31/107/115	-
19	CLA	L	305	16	-	0/15/91/115	-
19	CLA	L	303	30	-	2/15/91/115	-
19	CLA	B	845	6	1/1/15/20	4/39/115/115	-
19	CLA	A	807	30	-	0/15/91/115	-
19	CLA	B	819	6	1/1/15/20	9/39/115/115	-
18	CHL	1	606	1	-	6/12/110/137	-
23	LHG	2	302	20	-	20/49/49/53	-
19	CLA	B	806	6	1/1/15/20	9/39/115/115	-
19	CLA	3	307	30	-	3/19/95/115	-
19	CLA	B	805	6	-	1/21/97/115	-
19	CLA	A	829	5	1/1/15/20	6/39/115/115	-
19	CLA	A	805	5	-	1/18/94/115	-
19	CLA	B	829	6	-	3/13/89/115	-
19	CLA	B	837	6	-	1/18/94/115	-
19	CLA	B	823	6	1/1/15/20	9/39/115/115	-
19	CLA	K	202	15	-	7/15/91/115	-
19	CLA	4	311	4	-	2/15/91/115	-
19	CLA	A	817	30	-	5/20/96/115	-
24	BCR	J	105	-	-	2/29/63/63	0/2/2/2
24	BCR	B	815	-	-	4/29/63/63	0/2/2/2
29	DGD	B	817	-	-	16/49/89/95	0/2/2/2
19	CLA	1	612	1	1/1/13/20	4/27/103/115	-
19	CLA	B	802	6	1/1/14/20	7/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	828	5	1/1/15/20	17/39/115/115	-
19	CLA	B	846	6	1/1/15/20	12/39/115/115	-
28	PQN	B	811	-	-	5/23/43/43	0/2/2/2
24	BCR	A	845	-	-	4/29/63/63	0/2/2/2
24	BCR	I	101	-	-	0/29/63/63	0/2/2/2
19	CLA	A	826	5	1/1/15/20	9/39/115/115	-
22	A1LXP	3	305	-	-	2/29/67/67	0/2/2/2
19	CLA	4	318	4	-	5/15/91/115	-
22	A1LXP	J	102	-	-	3/29/67/67	0/2/2/2
19	CLA	A	843	5	-	1/25/101/115	-
19	CLA	A	846	5	1/1/15/20	8/39/115/115	-
19	CLA	A	818	5	1/1/15/20	14/39/115/115	-
19	CLA	K	203	30	-	6/15/91/115	-
19	CLA	A	823	30	-	8/39/115/115	-
18	CHL	4	319	4	-	3/15/113/137	-
19	CLA	A	814	5	1/1/15/20	12/39/115/115	-
19	CLA	B	836	30	1/1/13/20	1/29/105/115	-
18	CHL	3	315	30	-	8/21/119/137	-
19	CLA	A	834	5	1/1/15/20	8/39/115/115	-
19	CLA	3	304	3	1/1/13/20	5/27/103/115	-
19	CLA	L	304	16	1/1/15/20	9/39/115/115	-
24	BCR	A	847	-	-	2/18/35/63	0/1/1/2
19	CLA	B	833	6	1/1/14/20	7/33/109/115	-
19	CLA	B	825	6	1/1/15/20	12/39/115/115	-
19	CLA	B	840	6	-	2/15/91/115	-
21	XAT	1	618	-	-	0/21/52/93	0/2/2/4
22	A1LXP	1	616	-	-	0/29/67/67	0/2/2/2
19	CLA	G	203	11	-	7/15/91/115	-
25	LMG	J	103	-	-	16/36/56/70	0/1/1/1
19	CLA	2	301	2	-	7/21/97/115	-
19	CLA	B	842	30	-	4/21/97/115	-
19	CLA	A	844	5	-	2/12/88/115	-
19	CLA	2	310	2	1/1/13/20	8/27/103/115	-
19	CLA	B	831	6	1/1/15/20	15/39/115/115	-
19	CLA	1	607	-	-	7/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	809	6	1/1/15/20	7/39/115/115	-
24	BCR	G	205	-	-	4/29/63/63	0/2/2/2
19	CLA	A	820	5	-	4/12/88/115	-
19	CLA	A	811	5	1/1/13/20	2/27/103/115	-
21	XAT	1	615	-	-	0/31/93/93	0/4/4/4
19	CLA	A	819	5	1/1/15/20	7/39/115/115	-
19	CLA	B	832	6	-	6/15/91/115	-
19	CLA	A	809	5	1/1/15/20	7/39/115/115	-
19	CLA	B	801	6	1/1/15/20	10/39/115/115	-
19	CLA	G	202	30	-	3/12/88/115	-
19	CLA	B	827	6	1/1/15/20	10/39/115/115	-
19	CLA	A	851	30	1/1/14/20	12/36/112/115	-
24	BCR	L	301	-	-	1/29/63/63	0/2/2/2

The worst 5 of 1017 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	315	CHL	C4C-NC	18.17	1.51	1.35
18	1	606	CHL	C4C-NC	16.75	1.50	1.35
18	2	316	CHL	C4C-NC	16.62	1.50	1.35
18	4	313	CHL	C4C-NC	15.90	1.49	1.35
18	2	313	CHL	C4C-NC	15.77	1.49	1.35

The worst 5 of 1261 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	830	CL0	C1B-CHB-C4A	16.50	131.50	121.39
19	G	203	CLA	C4A-NA-C1A	-12.86	100.92	106.71
18	3	315	CHL	C1B-CHB-C4A	12.46	129.03	121.39
18	3	303	CHL	C1B-CHB-C4A	12.46	129.03	121.39
19	K	202	CLA	C4A-NA-C1A	-12.13	101.25	106.71

5 of 65 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	1	601	CHL	C8
18	2	316	CHL	C8
18	3	303	CHL	C8
19	1	602	CLA	C8

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Mol	Chain	Res	Type	Atom
19	1	603	CLA	C8

5 of 1021 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	1	601	CHL	C1C-C2C-CMC-OMC
18	1	601	CHL	C3C-C2C-CMC-OMC
18	1	606	CHL	C1C-C2C-CMC-OMC
18	1	606	CHL	C3C-C2C-CMC-OMC
18	1	606	CHL	C4C-C3C-CAC-CBC

There are no ring outliers.

112 monomers are involved in 203 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	F	302	BCR	3	0
19	J	101	CLA	1	0
19	B	822	CLA	2	0
24	F	304	BCR	2	0
25	F	305	LMG	2	0
19	B	804	CLA	1	0
24	A	852	BCR	8	0
19	A	810	CLA	2	0
19	B	830	CLA	2	0
24	L	302	BCR	2	0
19	B	844	CLA	5	0
19	B	818	CLA	5	0
19	3	308	CLA	1	0
19	3	301	CLA	1	0
24	G	201	BCR	4	0
22	2	309	A1LXP	1	0
19	B	834	CLA	4	0
18	1	601	CHL	2	0
24	B	813	BCR	5	0
22	4	306	A1LXP	1	0
19	2	312	CLA	1	0
19	B	808	CLA	3	0
19	A	802	CLA	3	0
19	1	602	CLA	3	0
19	2	311	CLA	1	0
19	A	815	CLA	1	0
19	A	831	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	806	CLA	2	0
19	A	833	CLA	3	0
18	4	313	CHL	1	0
24	B	814	BCR	1	0
19	B	810	CLA	2	0
19	A	808	CLA	4	0
19	B	803	CLA	1	0
24	B	812	BCR	4	0
19	B	848	CLA	1	0
19	B	820	CLA	2	0
19	A	812	CLA	1	0
24	B	816	BCR	2	0
19	B	824	CLA	1	0
19	F	303	CLA	2	0
19	1	605	CLA	1	0
19	A	849	CLA	2	0
24	A	838	BCR	2	0
19	A	842	CLA	3	0
25	N	201	LMG	3	0
19	A	813	CLA	4	0
19	B	843	CLA	1	0
19	A	850	CLA	1	0
19	1	608	CLA	1	0
21	2	306	XAT	1	0
24	4	308	BCR	3	0
19	B	841	CLA	1	0
19	A	840	CLA	5	0
19	1	603	CLA	3	0
18	3	303	CHL	1	0
24	A	804	BCR	5	0
19	A	821	CLA	4	0
24	A	841	BCR	1	0
24	K	201	BCR	2	0
19	4	317	CLA	3	0
19	A	827	CLA	1	0
19	L	303	CLA	1	0
19	B	845	CLA	2	0
19	A	807	CLA	1	0
19	B	819	CLA	1	0
18	1	606	CHL	2	0
19	B	806	CLA	3	0
19	B	805	CLA	1	0

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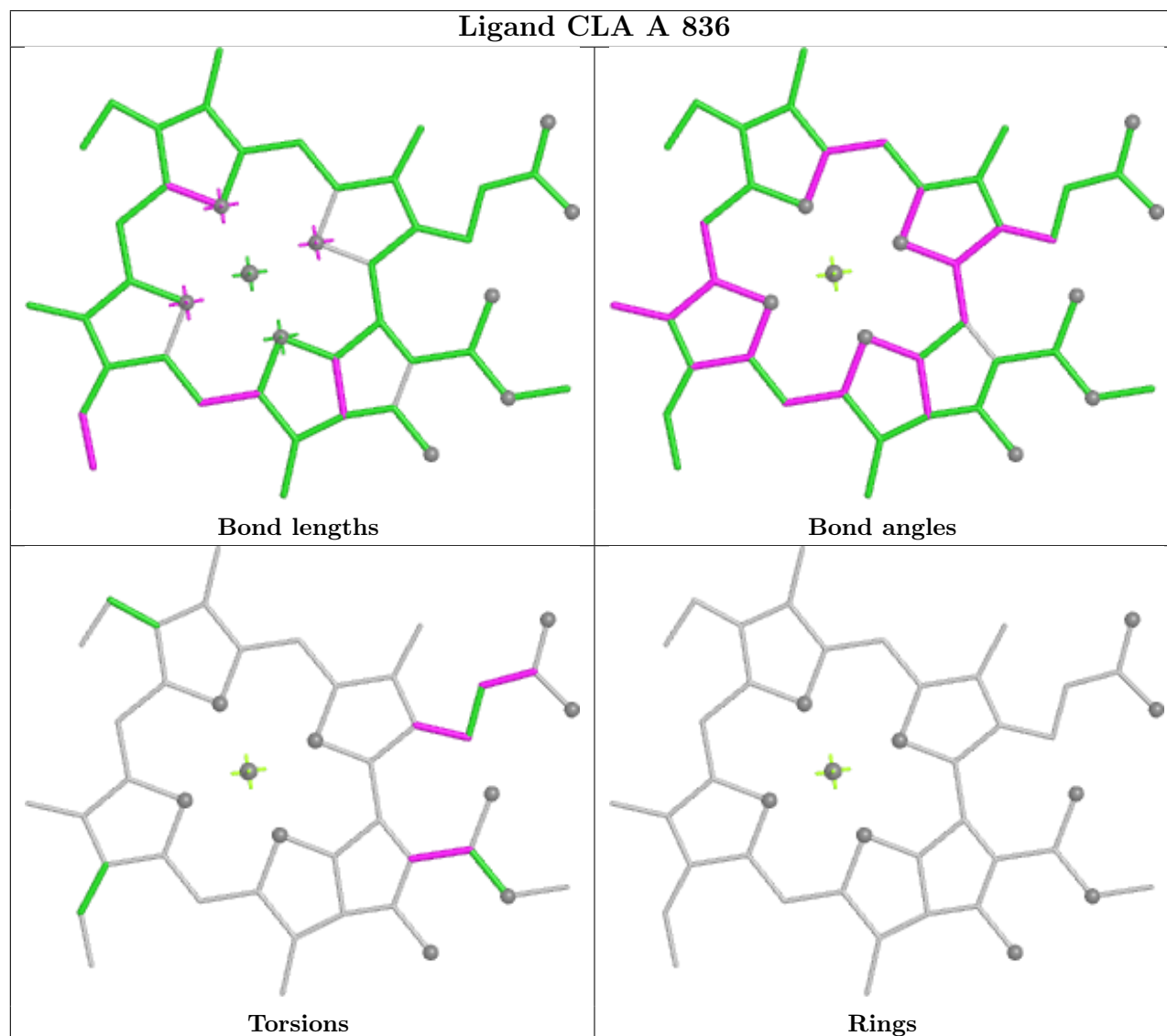
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	805	CLA	2	0
19	A	829	CLA	2	0
19	B	829	CLA	2	0
19	B	837	CLA	1	0
19	4	311	CLA	2	0
24	B	815	BCR	1	0
29	B	817	DGD	1	0
19	1	612	CLA	1	0
19	B	802	CLA	1	0
19	A	828	CLA	1	0
19	B	846	CLA	1	0
24	A	845	BCR	7	0
24	I	101	BCR	1	0
19	A	826	CLA	2	0
22	3	305	A1LXP	1	0
19	4	318	CLA	1	0
19	A	843	CLA	2	0
19	A	818	CLA	1	0
19	K	203	CLA	2	0
19	A	823	CLA	1	0
18	4	319	CHL	1	0
19	A	814	CLA	2	0
19	A	834	CLA	1	0
19	3	304	CLA	2	0
19	L	304	CLA	1	0
24	A	847	BCR	2	0
19	B	833	CLA	4	0
19	B	825	CLA	2	0
19	B	840	CLA	1	0
21	1	618	XAT	3	0
19	G	203	CLA	5	0
19	B	842	CLA	1	0
19	1	607	CLA	1	0
19	B	809	CLA	1	0
24	G	205	BCR	3	0
21	1	615	XAT	3	0
19	A	819	CLA	3	0
19	B	832	CLA	2	0
19	A	809	CLA	3	0
19	B	801	CLA	2	0
19	B	827	CLA	3	0
19	A	851	CLA	5	0

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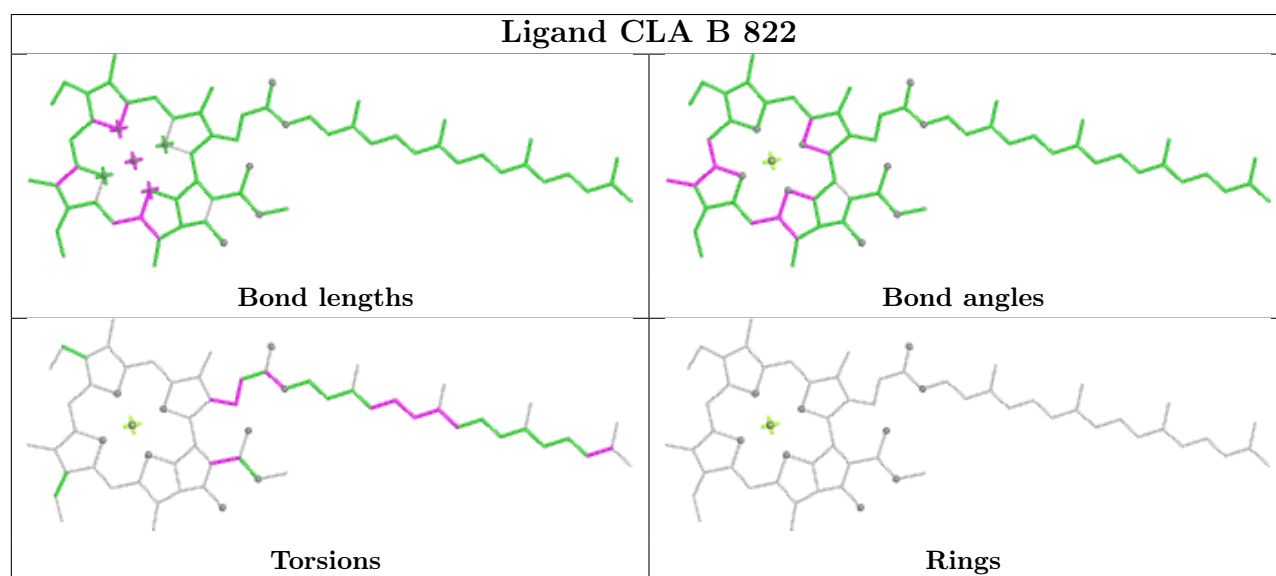
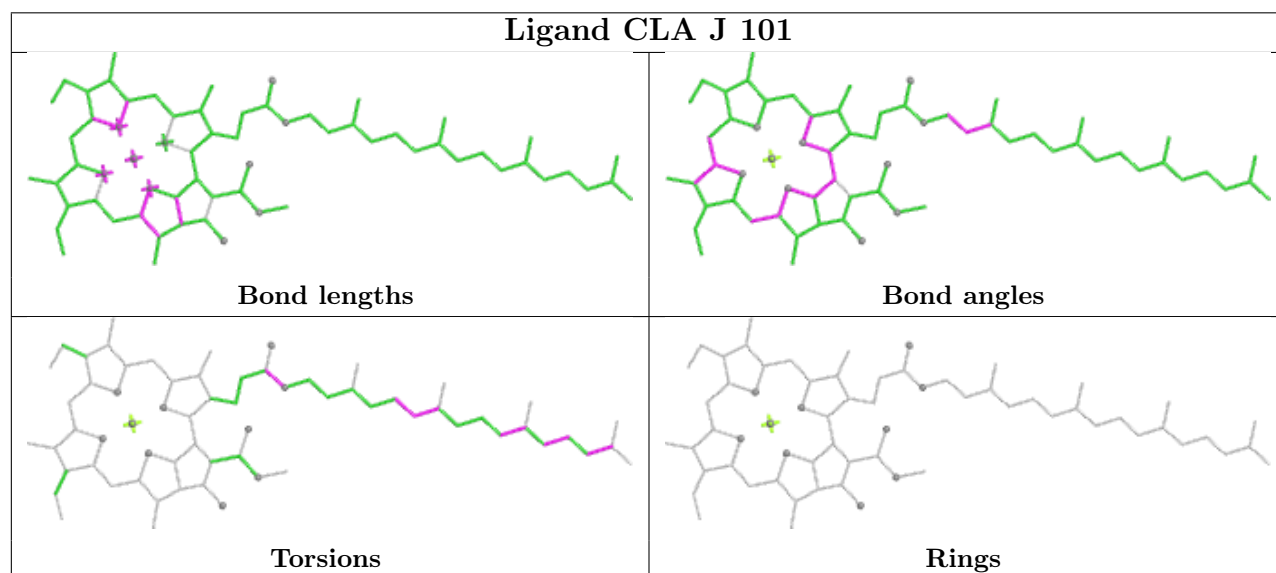
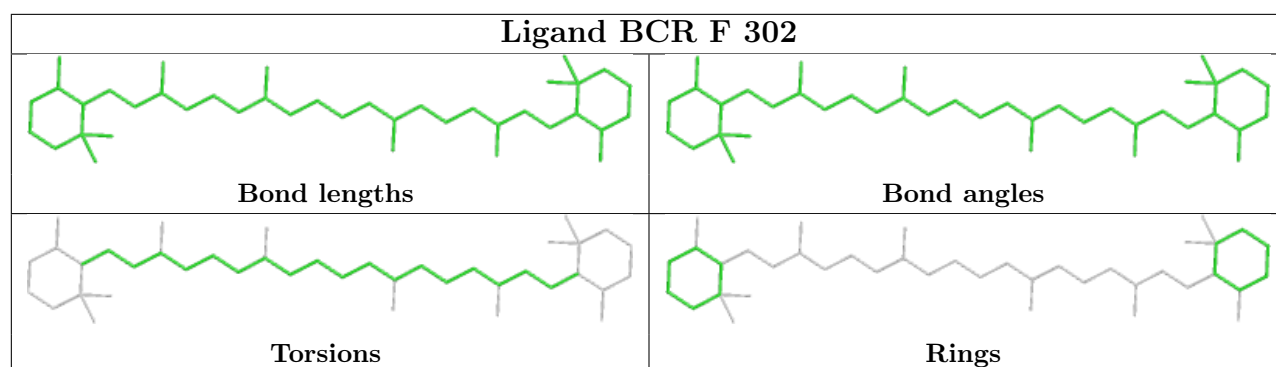
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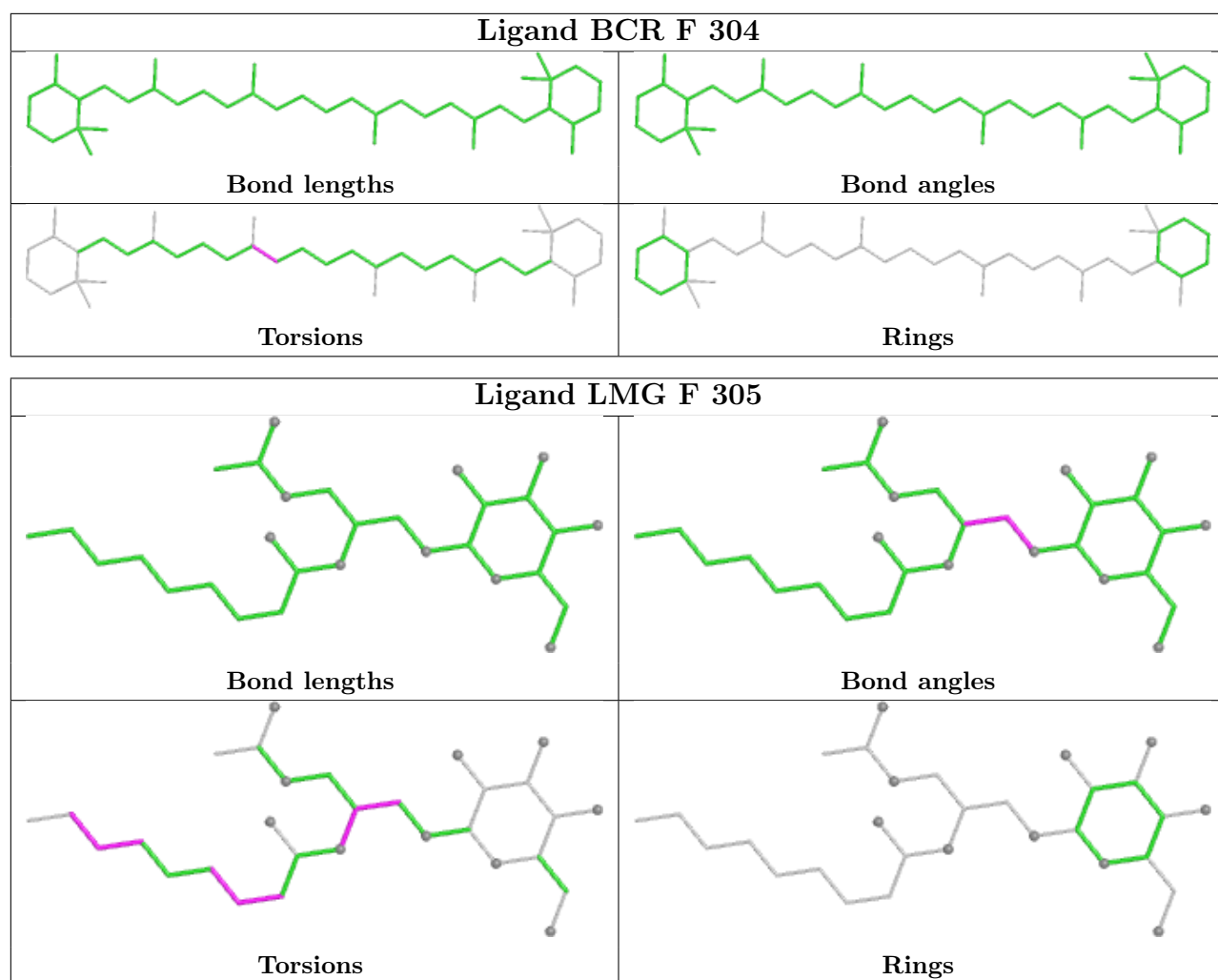
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	L	301	BCR	2	0

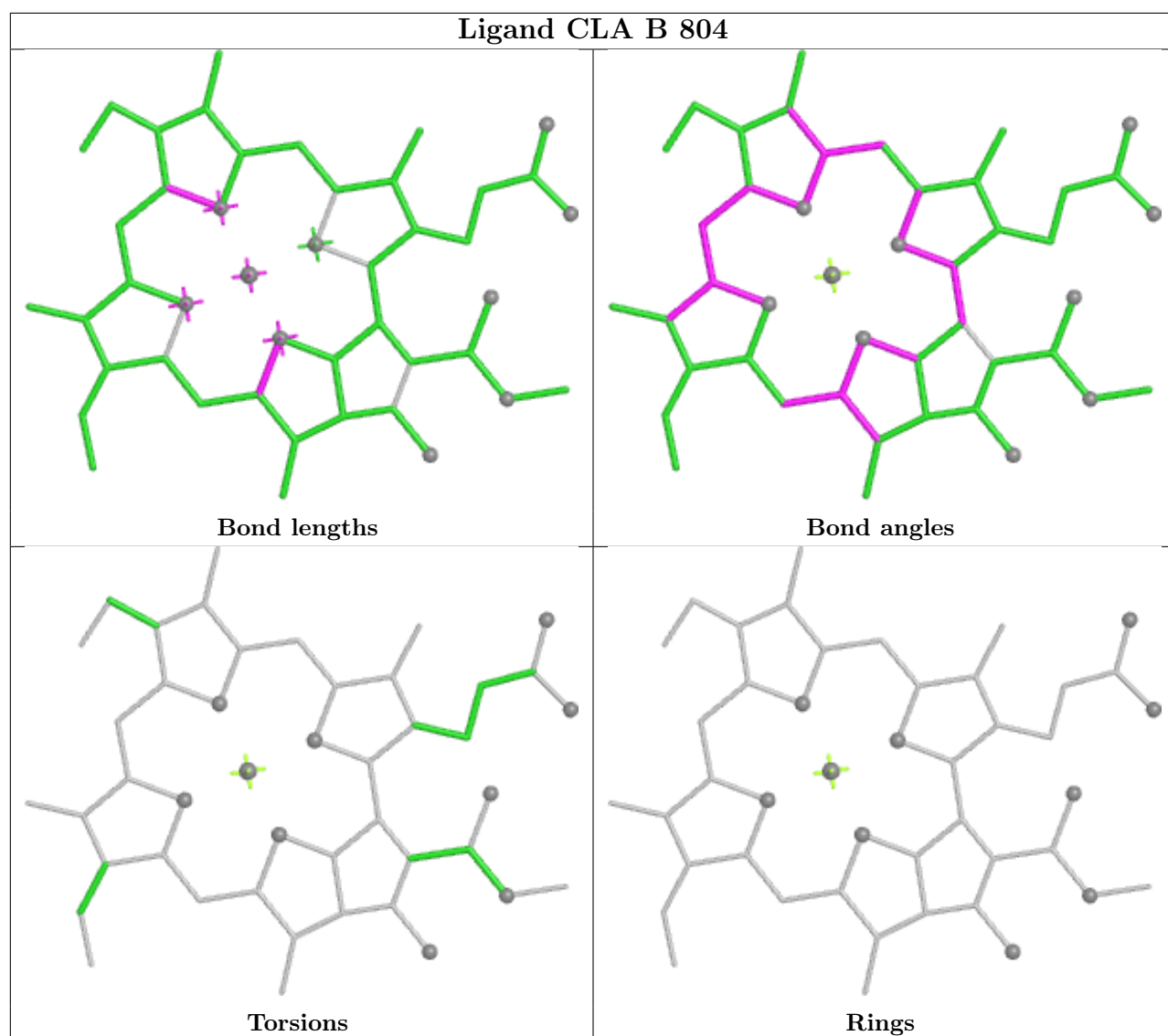
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



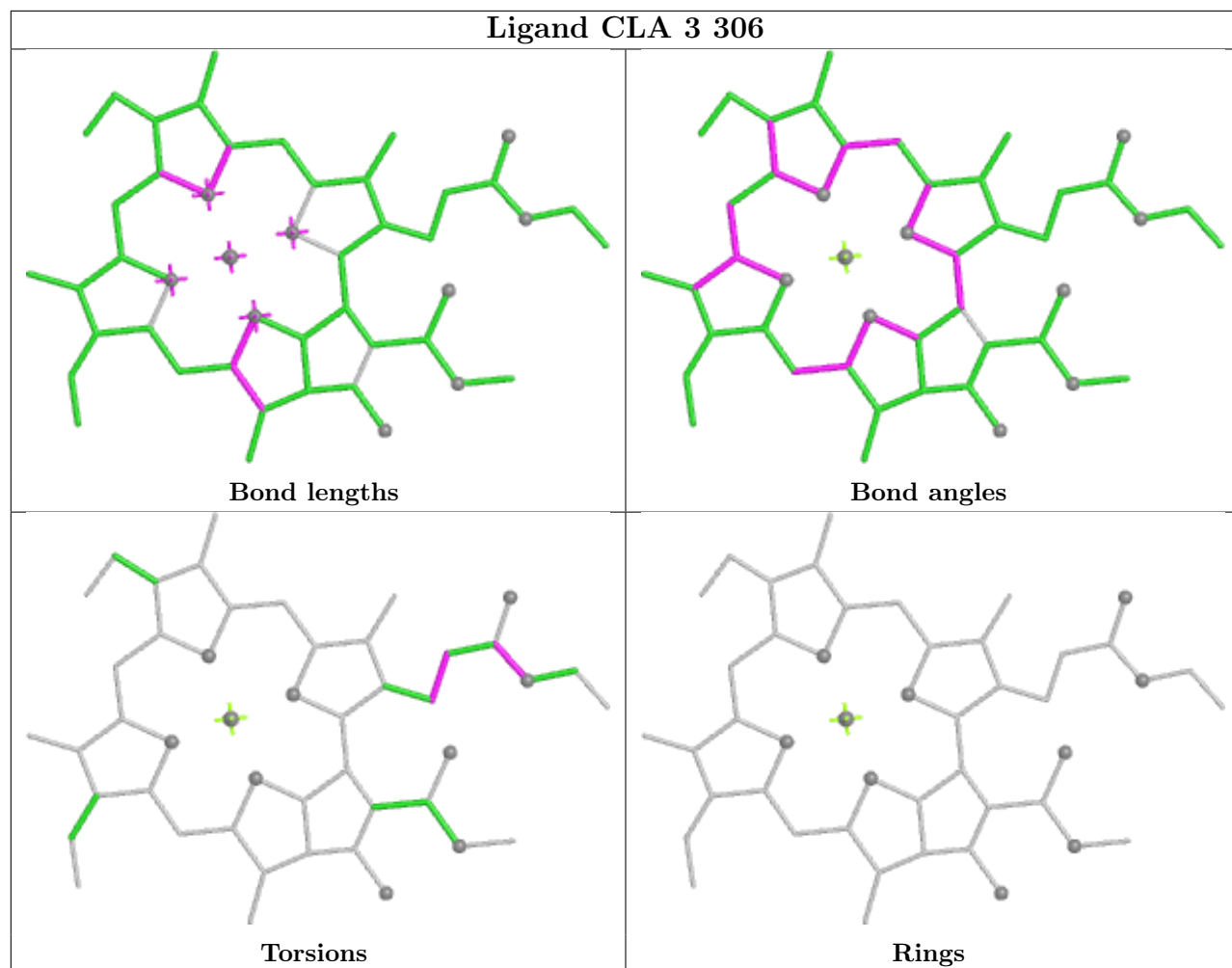




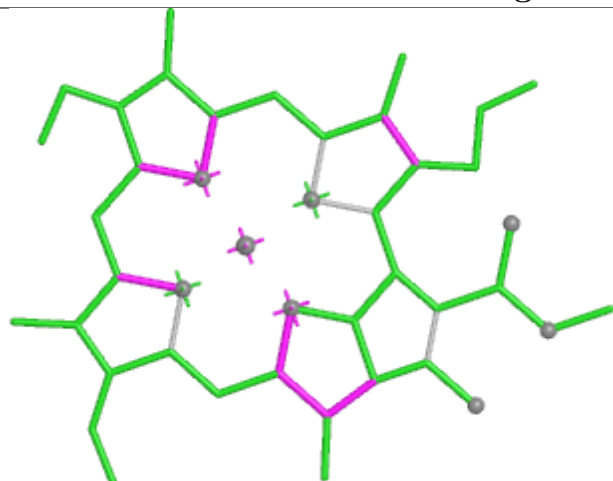




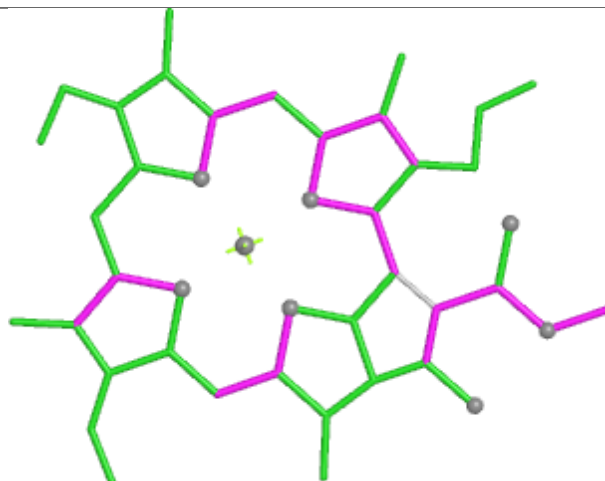
## Ligand CLA 3 306



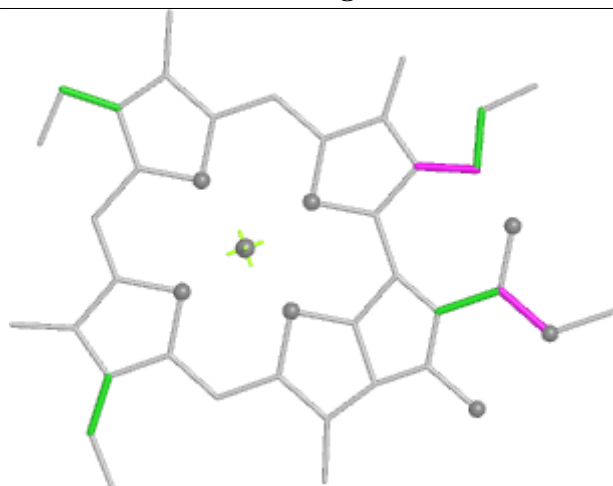
## Ligand CLA B 839



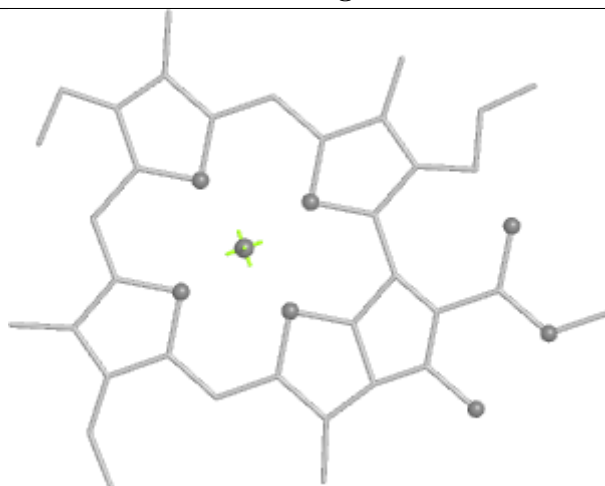
Bond lengths



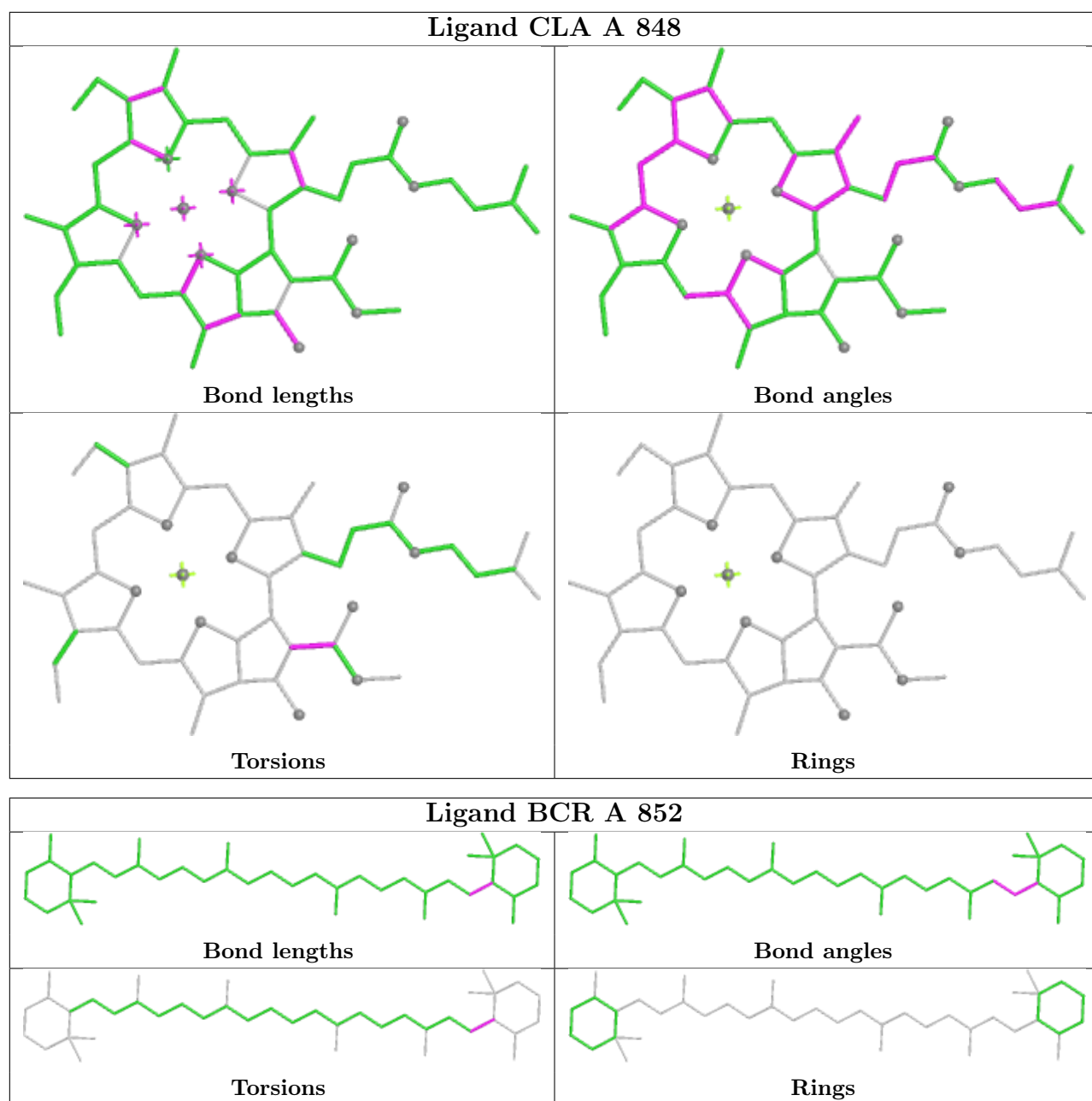
Bond angles



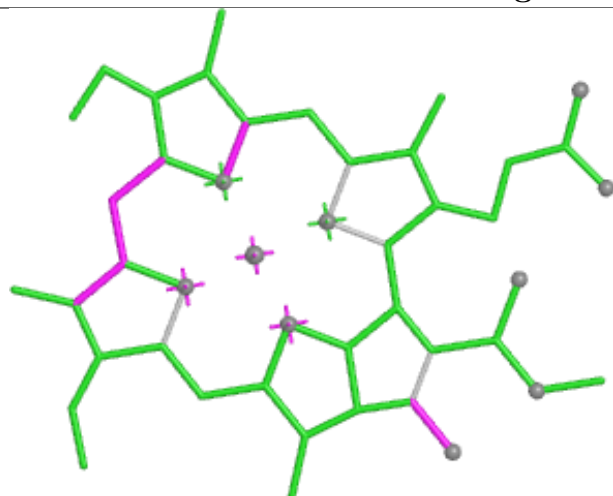
Torsions



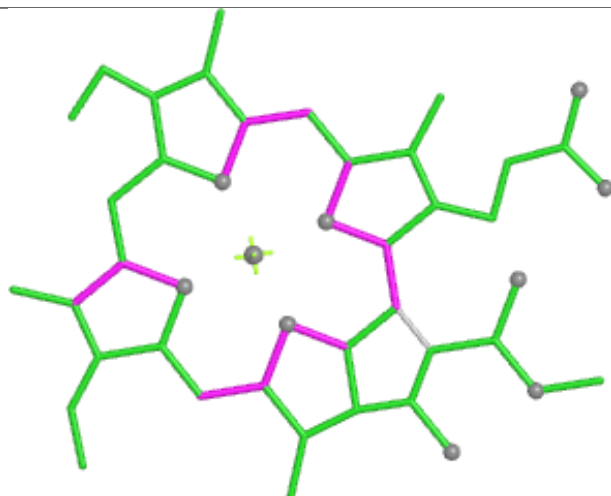
Rings



## Ligand CLA B 807



Bond lengths



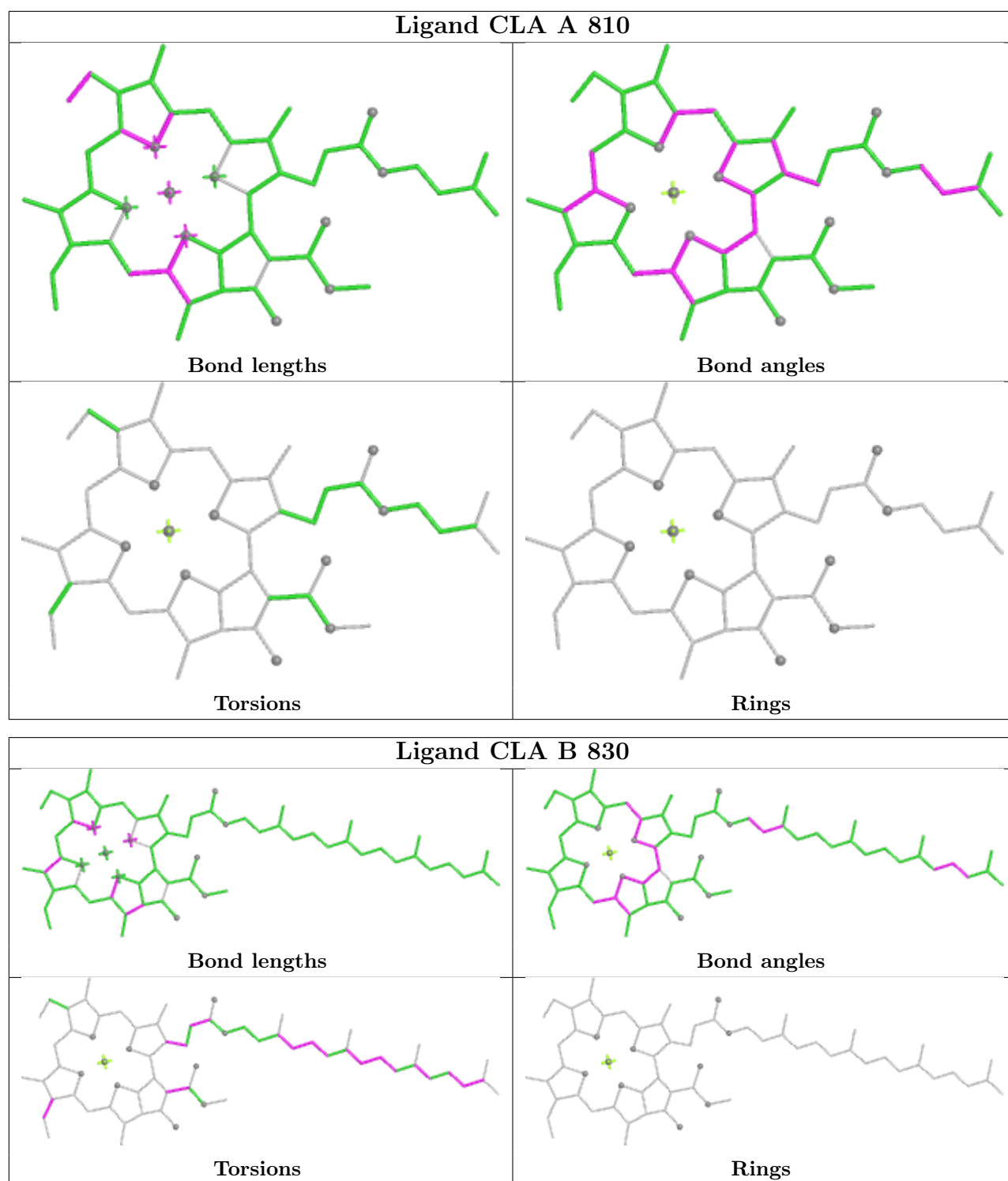
Bond angles



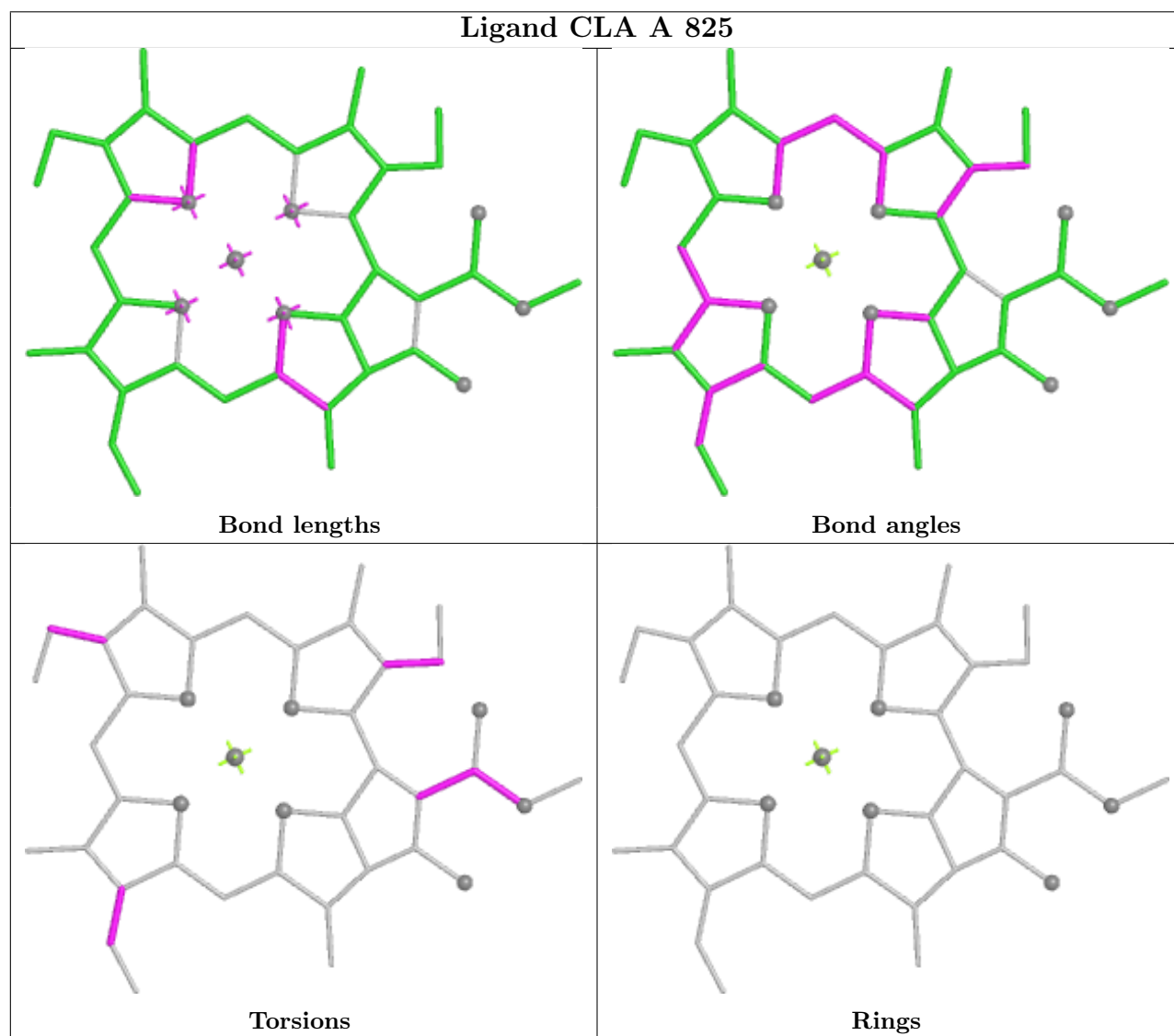
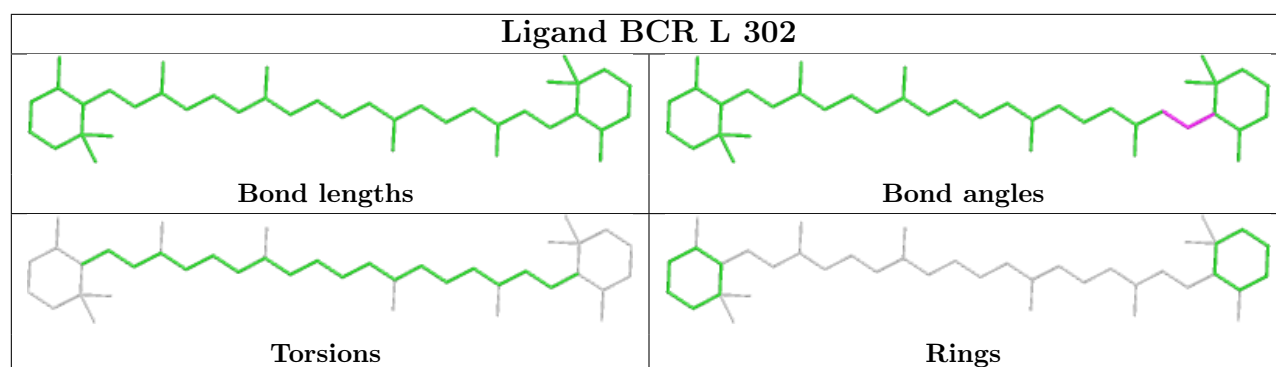
Torsions

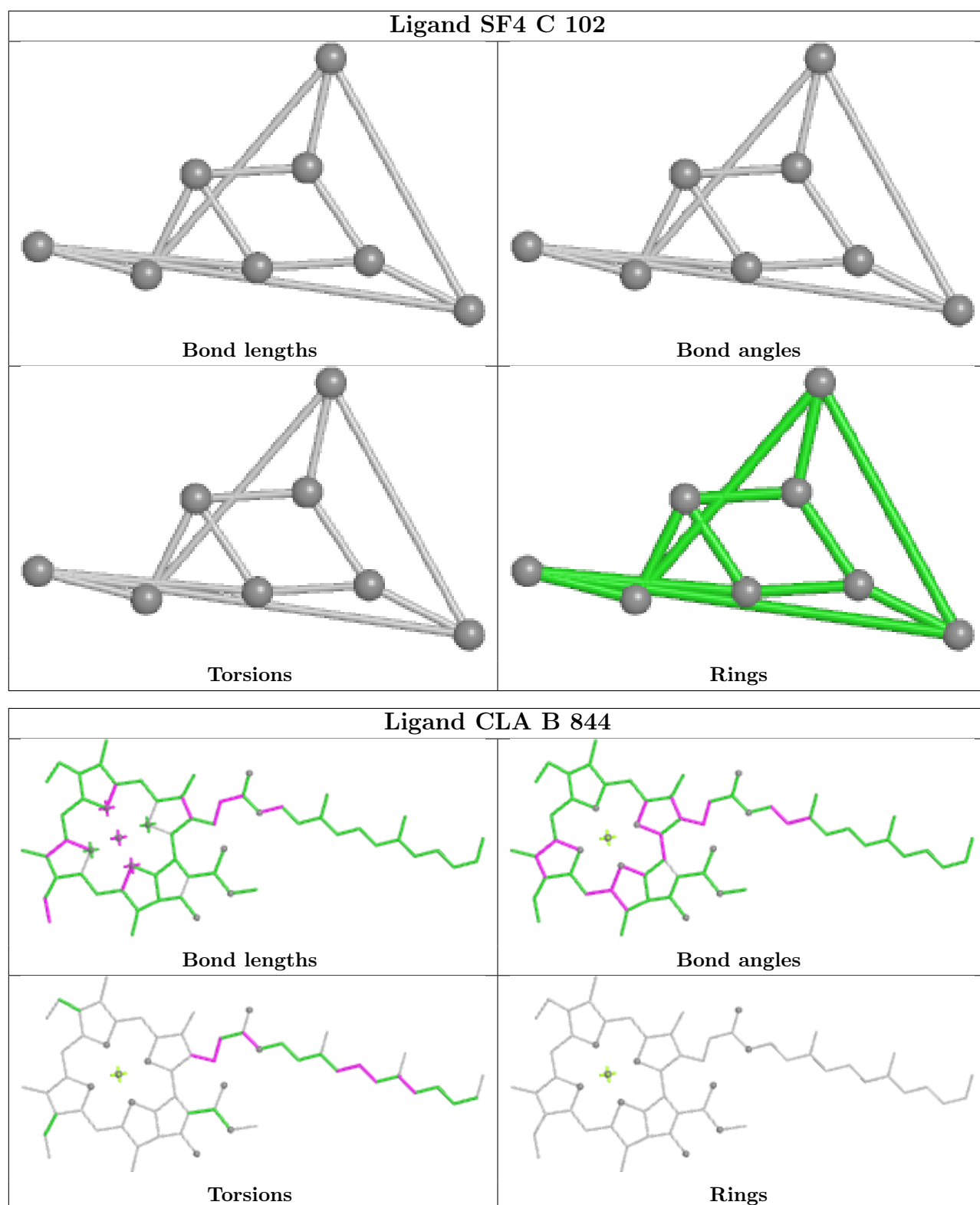


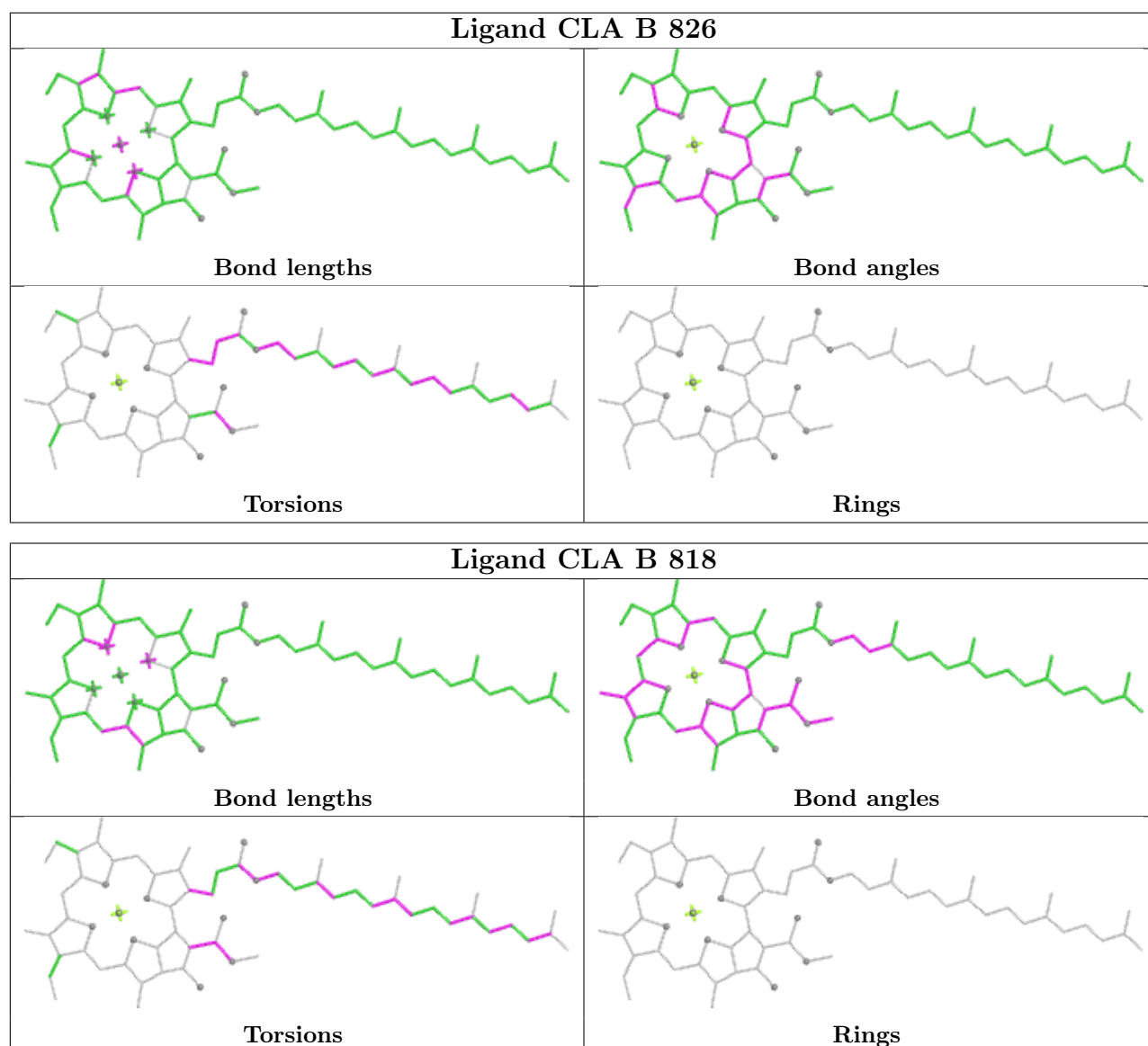
Rings



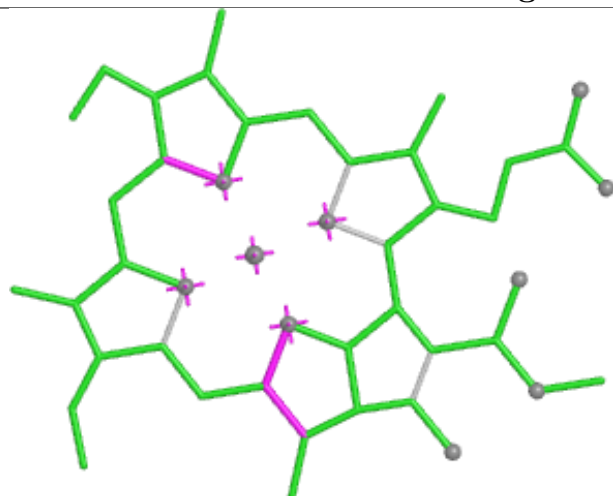




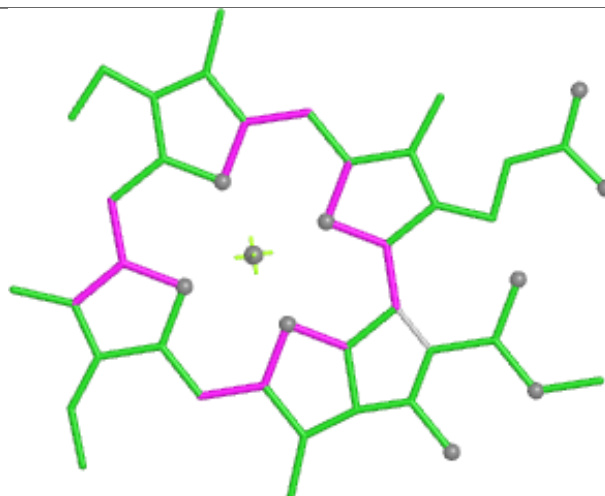




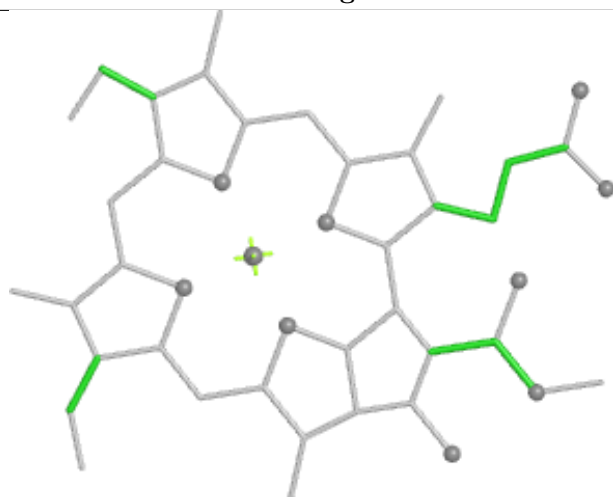
## Ligand CLA 3 308



Bond lengths



Bond angles

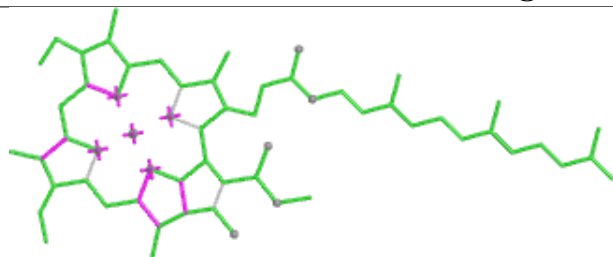


Torsions

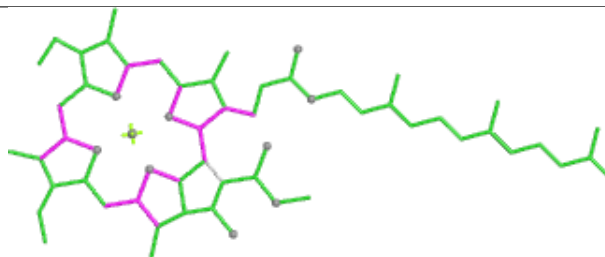


Rings

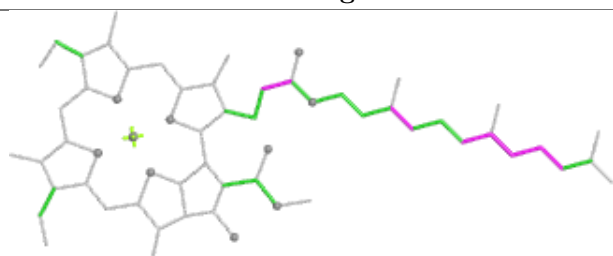
## Ligand CLA 3 301



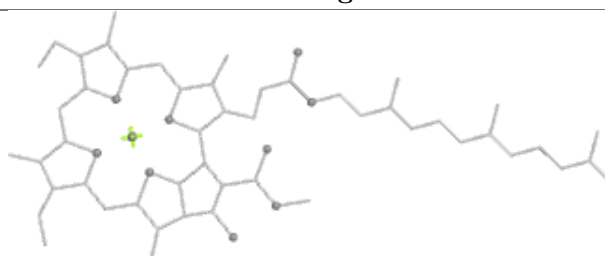
Bond lengths



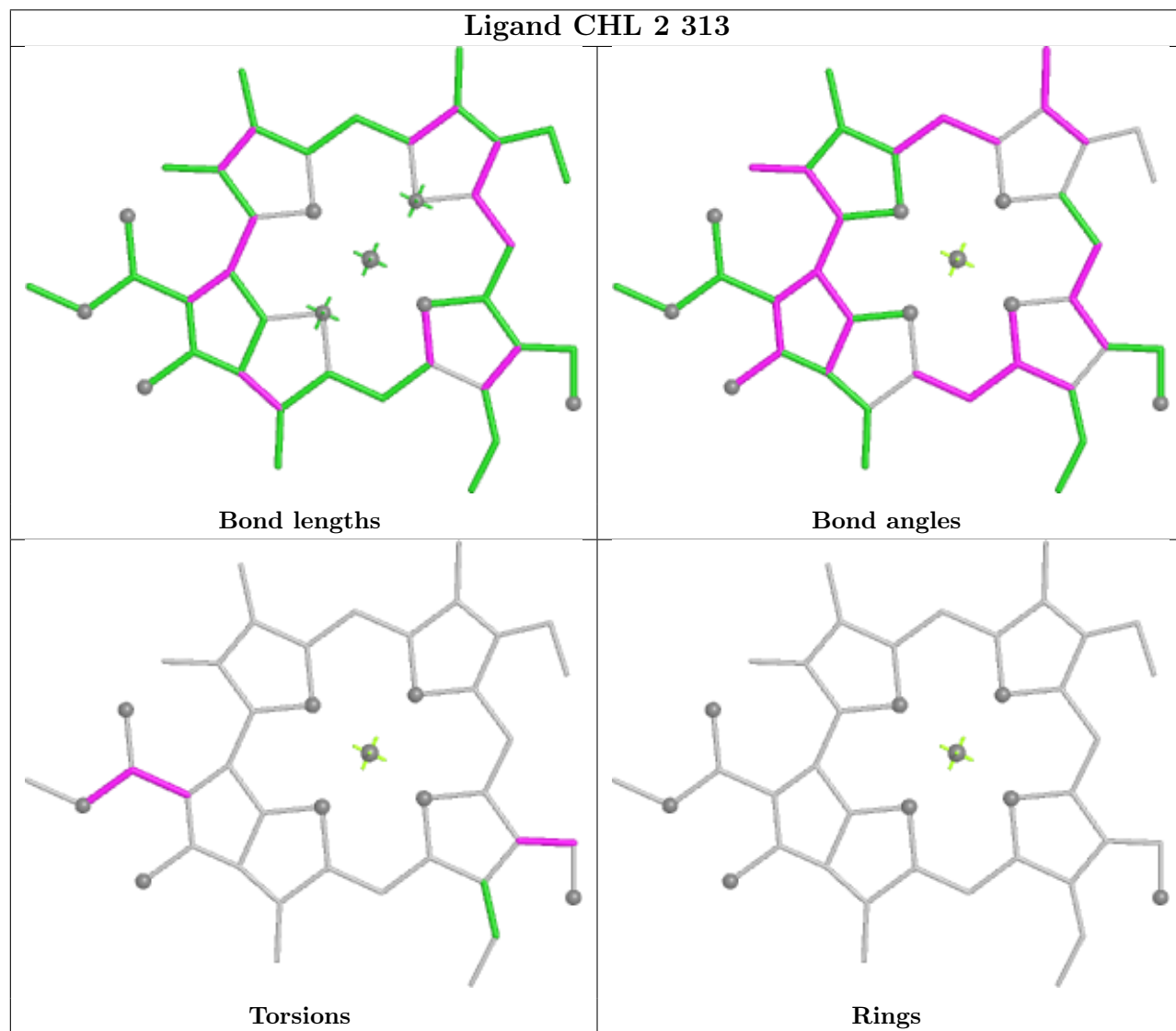
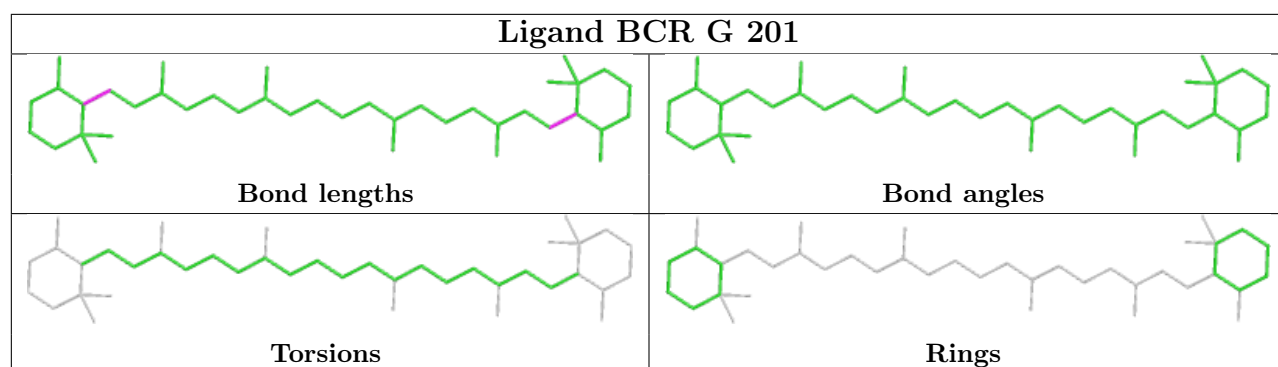
Bond angles

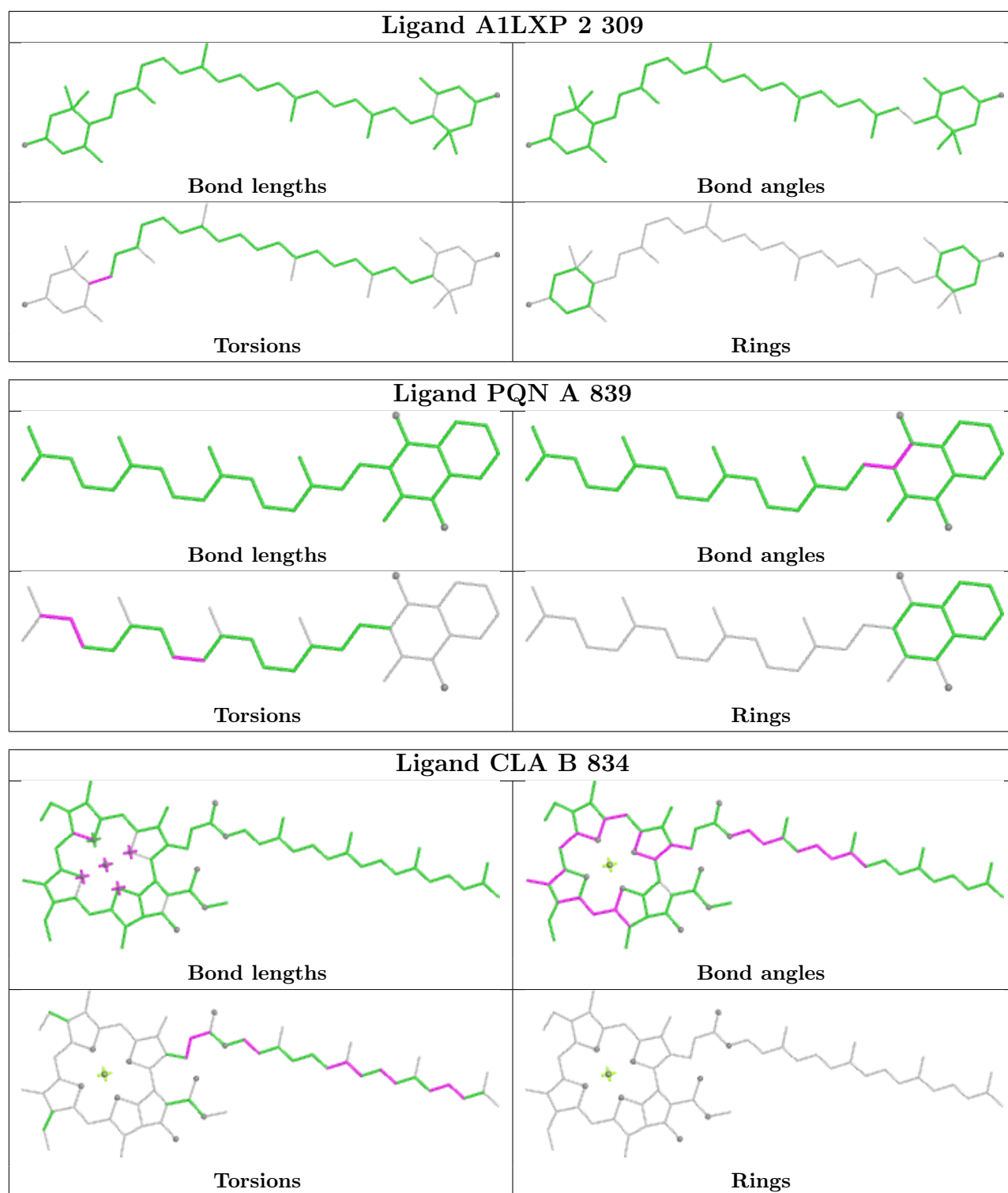


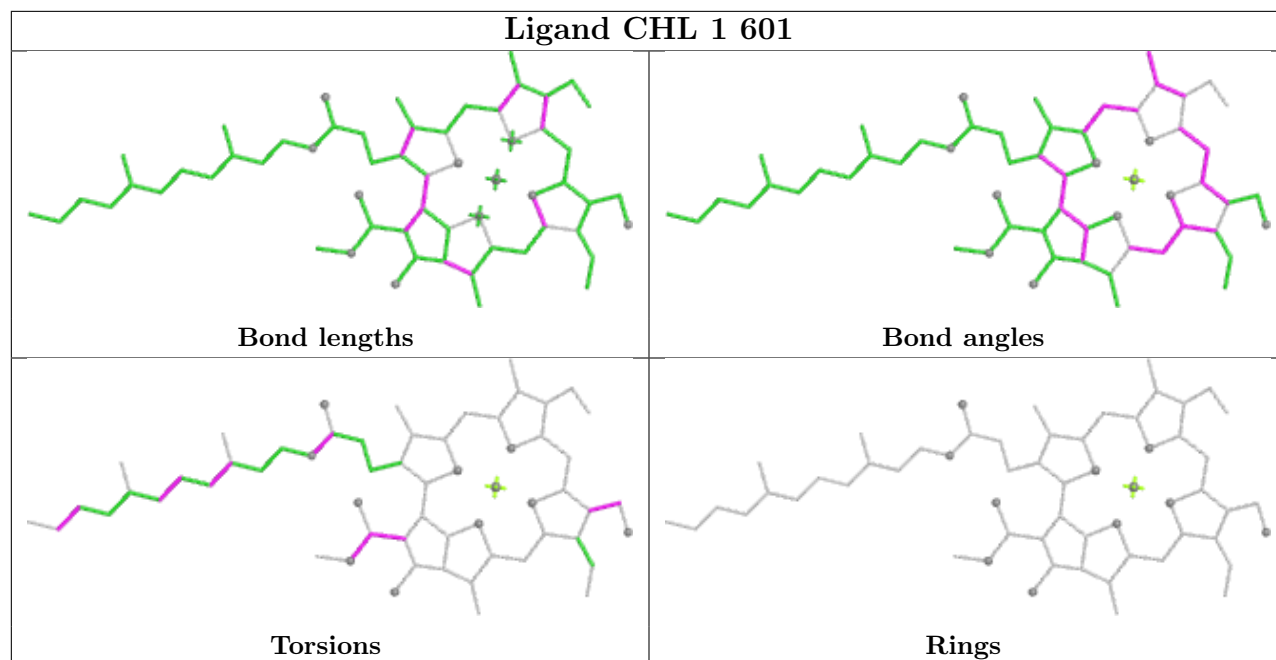
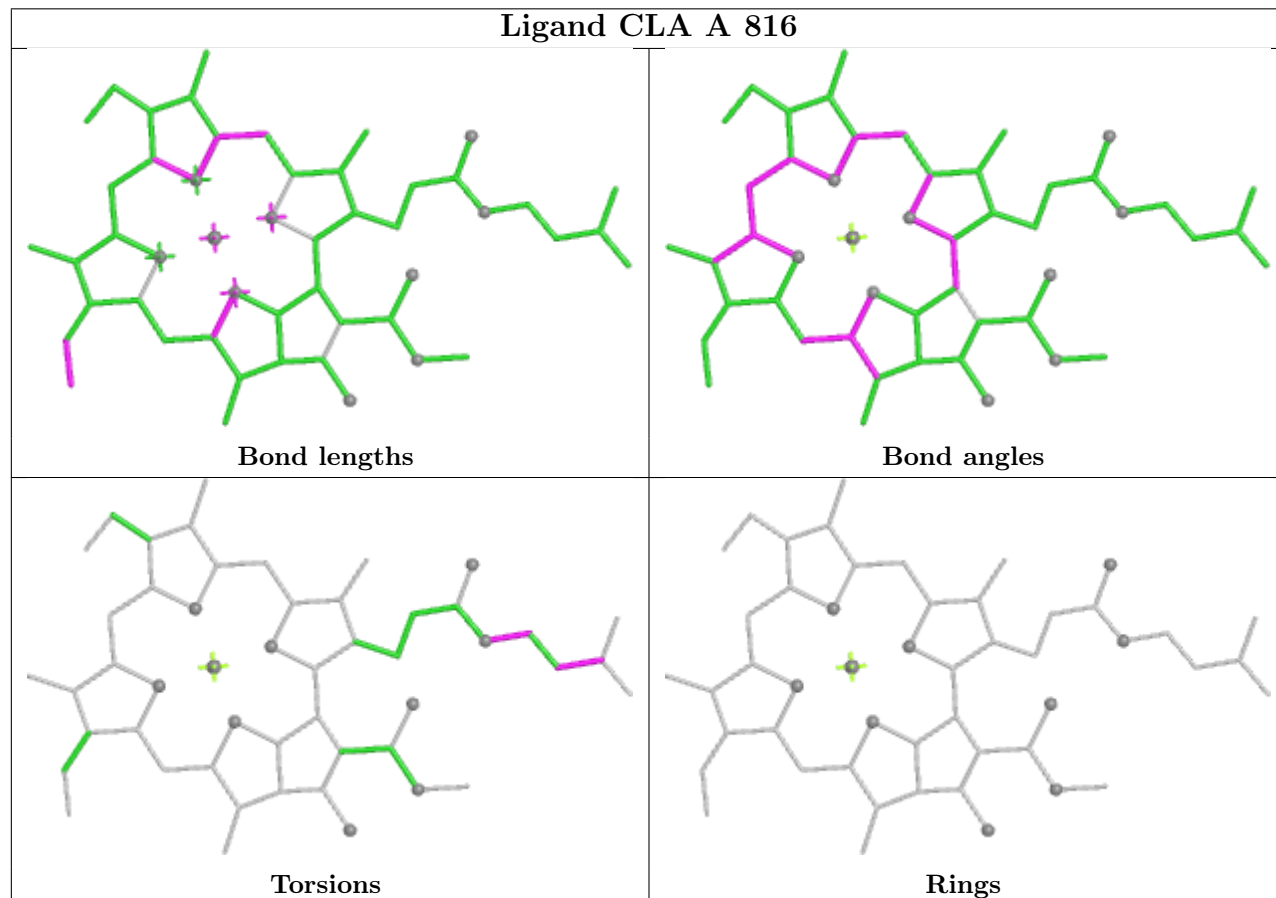
Torsions

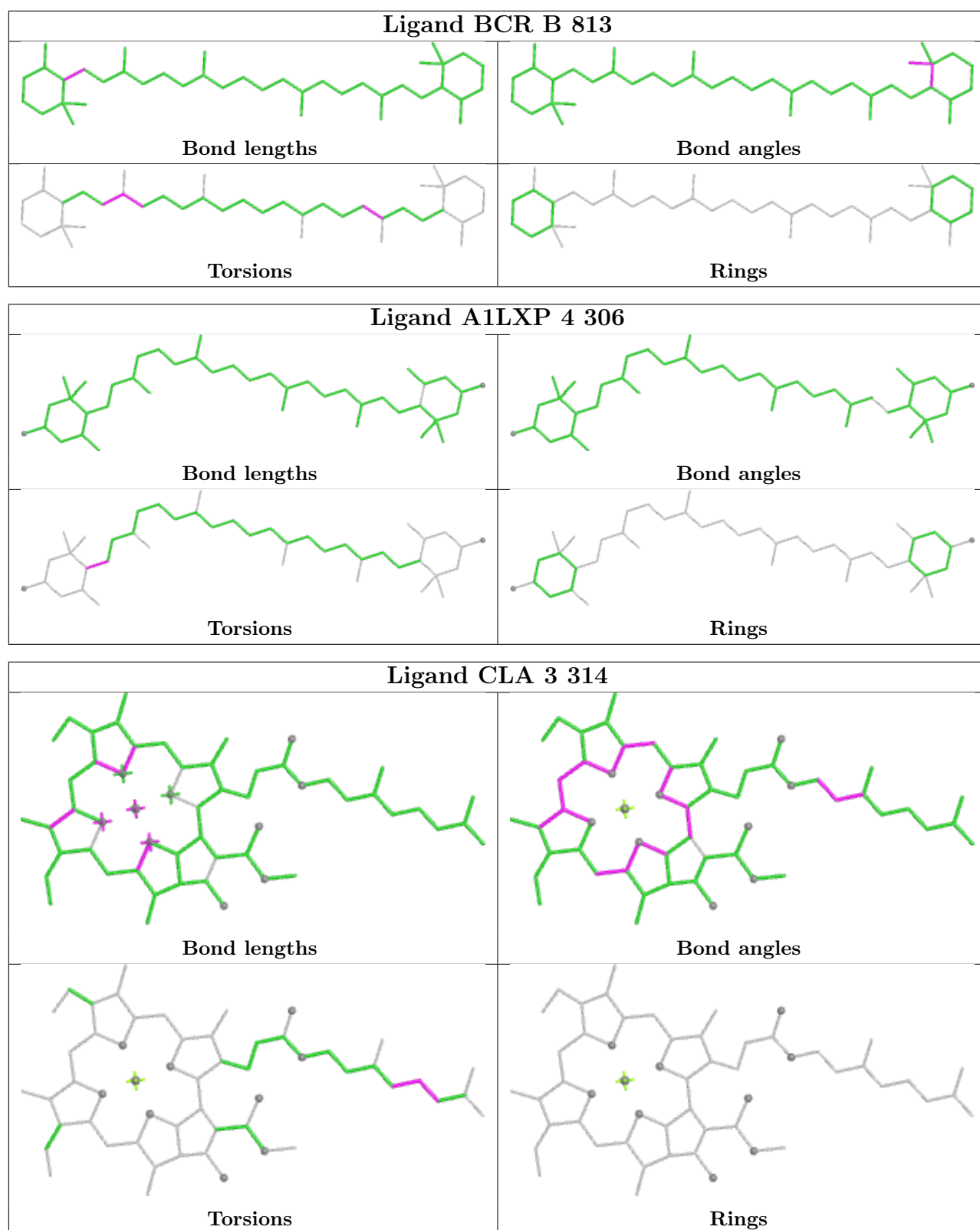


Rings



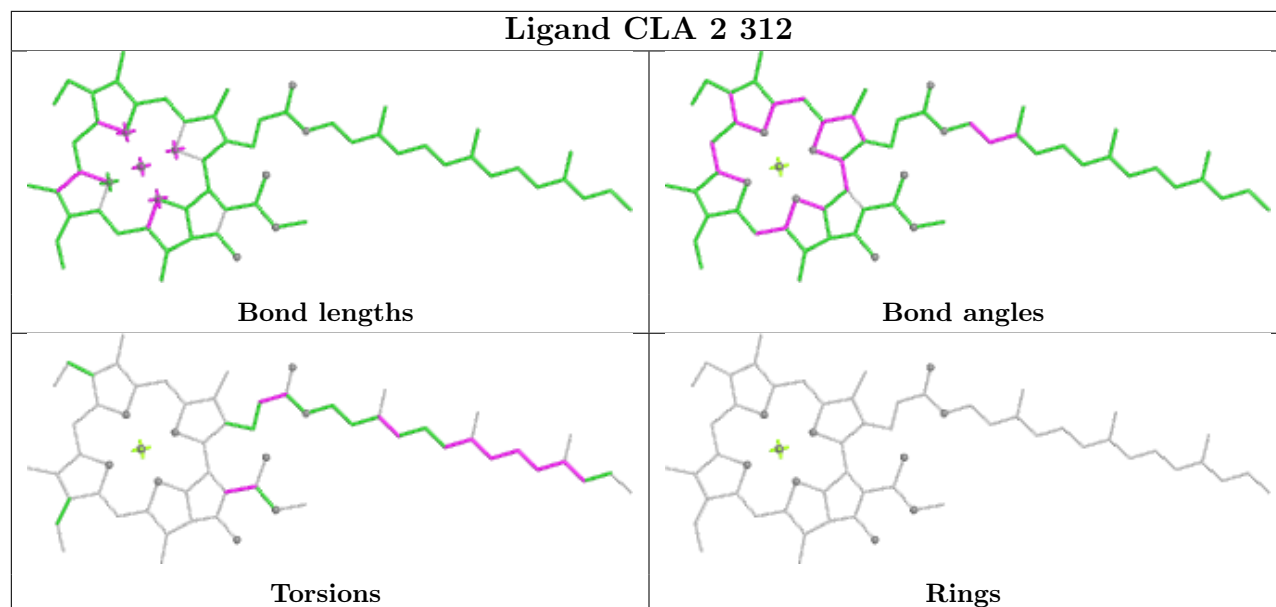


**Ligand CHL 1 601****Ligand CLA A 816**

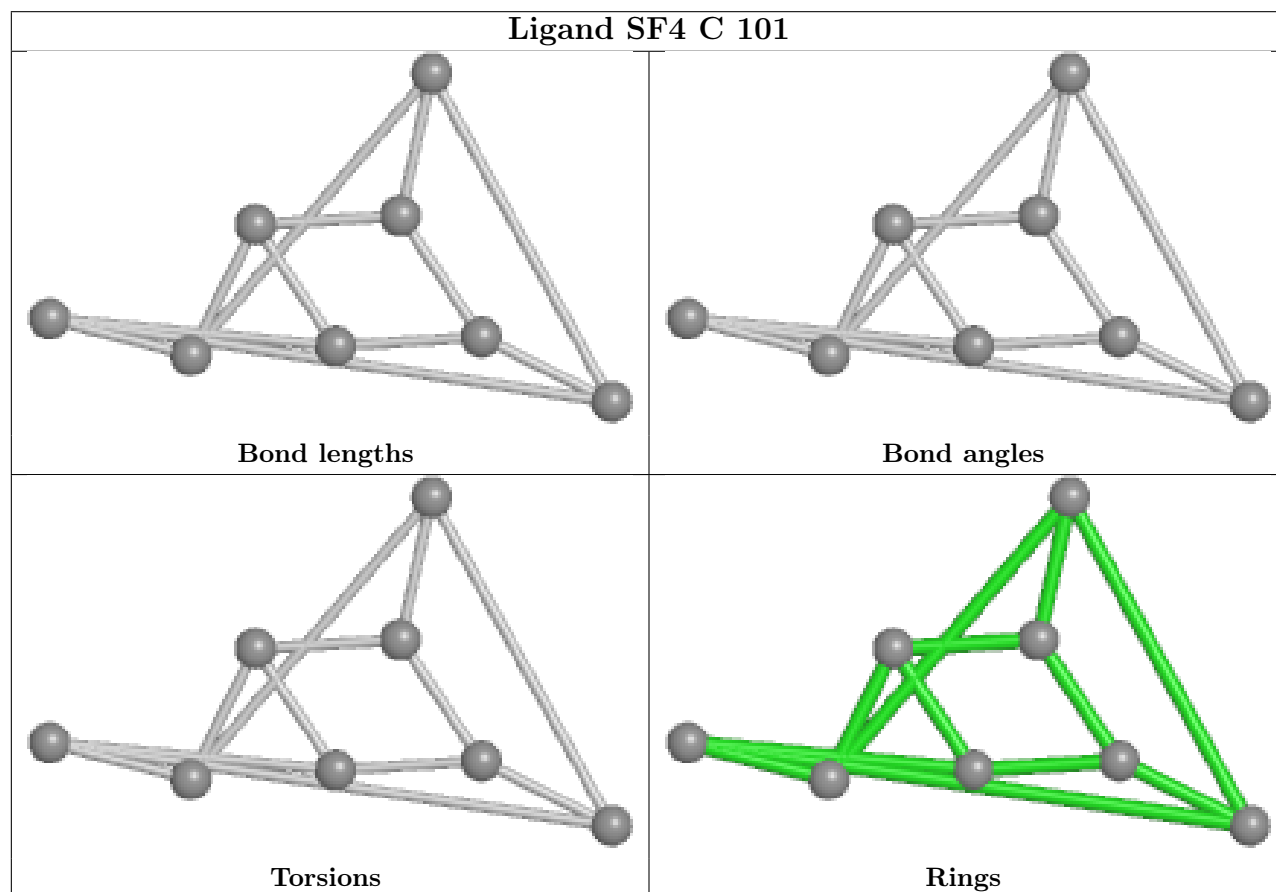


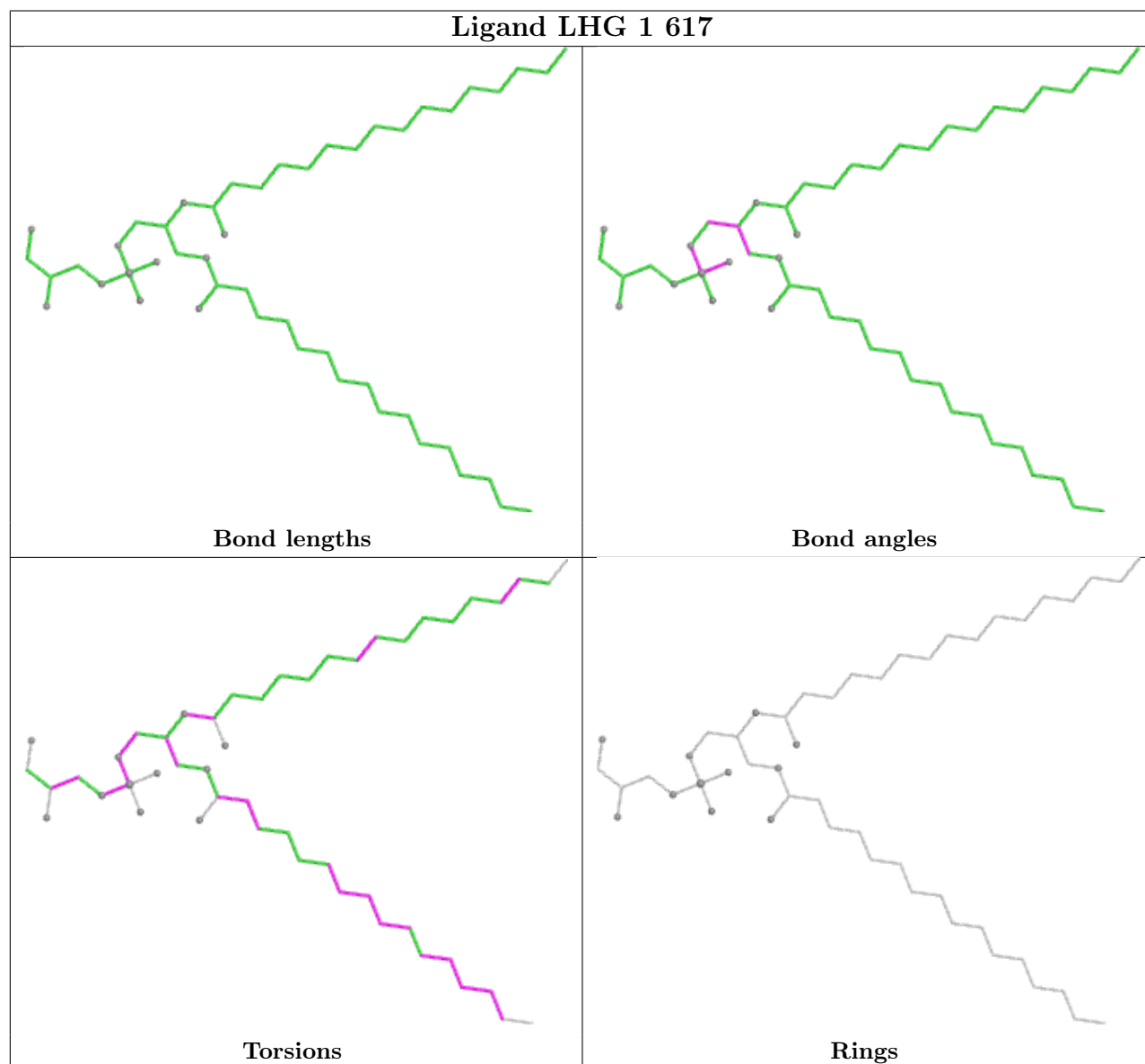
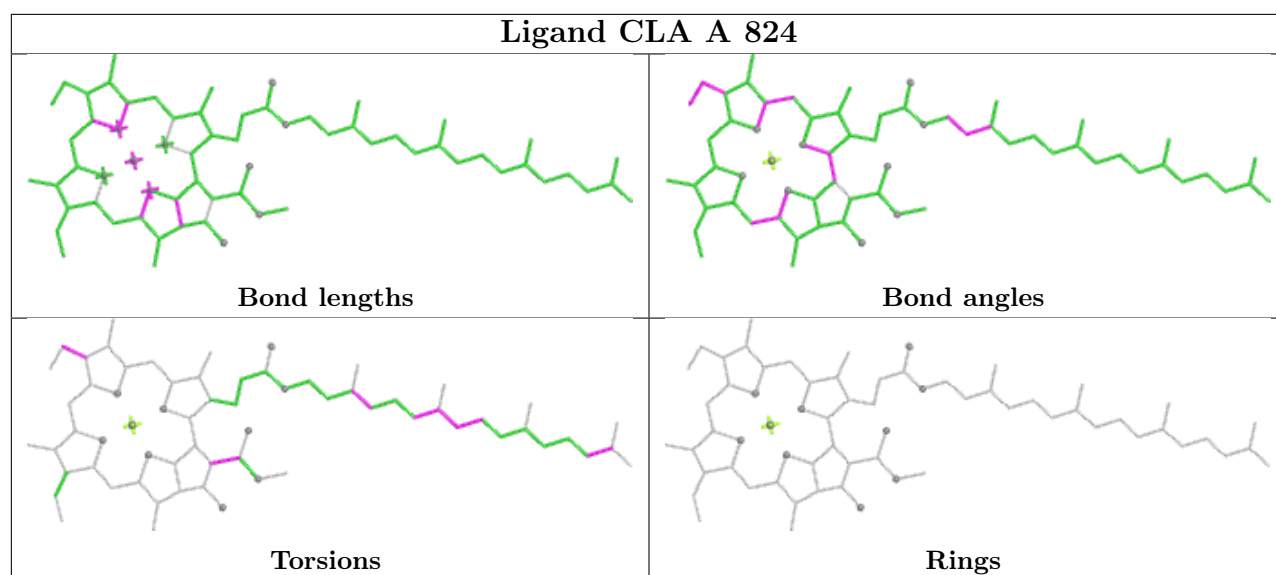


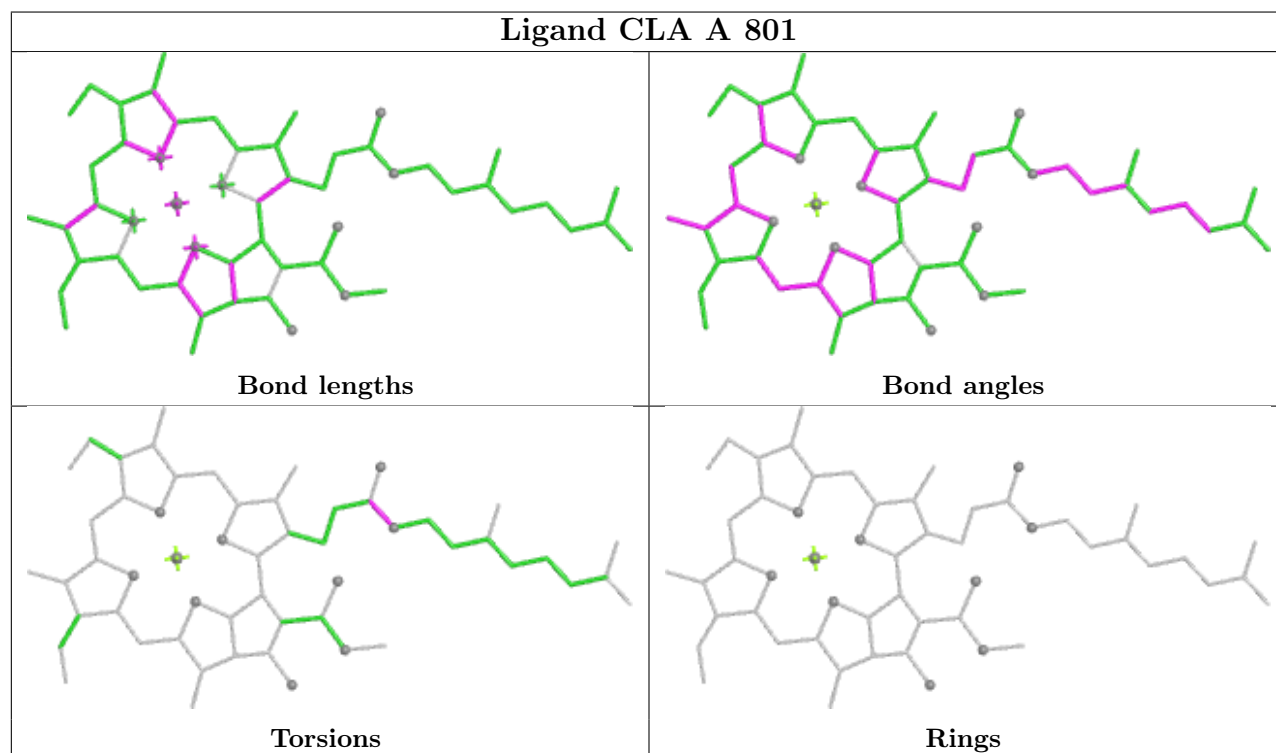
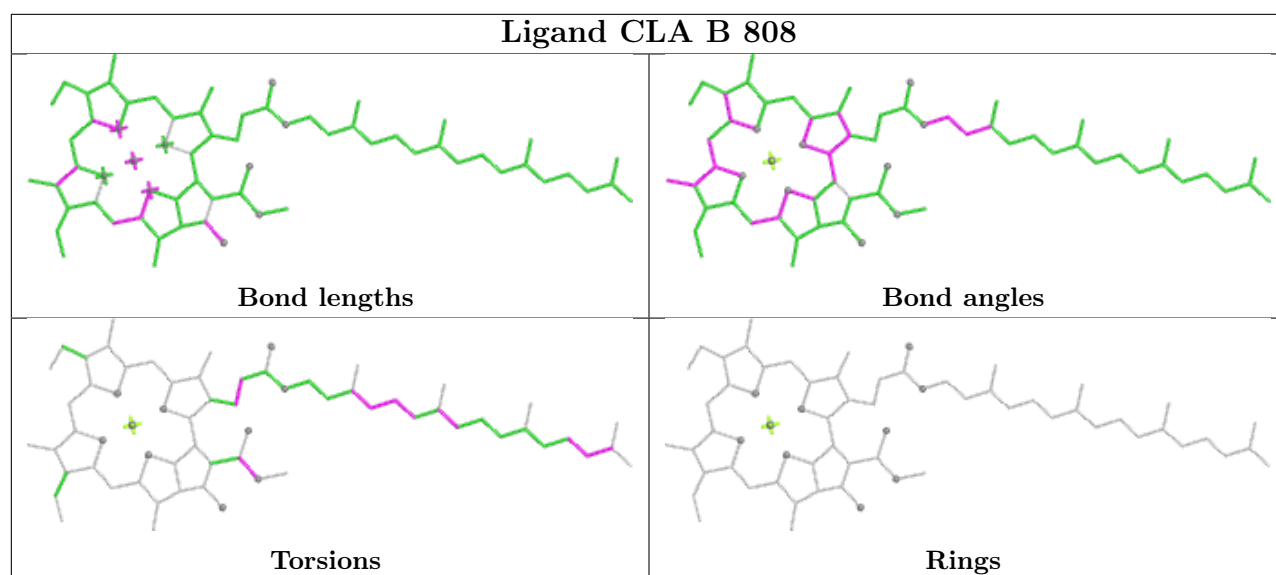
## Ligand CLA 2 312



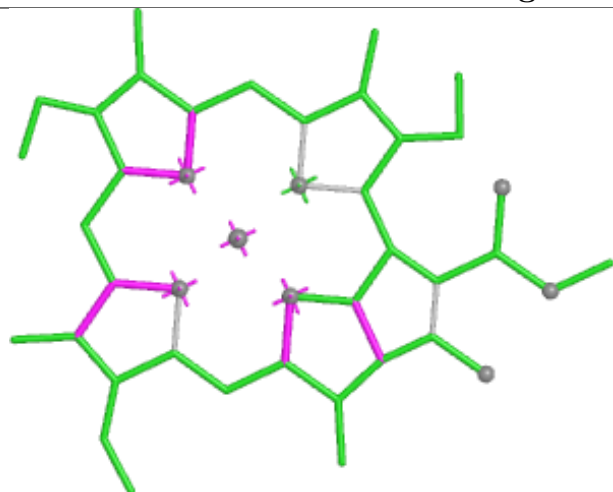
## Ligand SF4 C 101



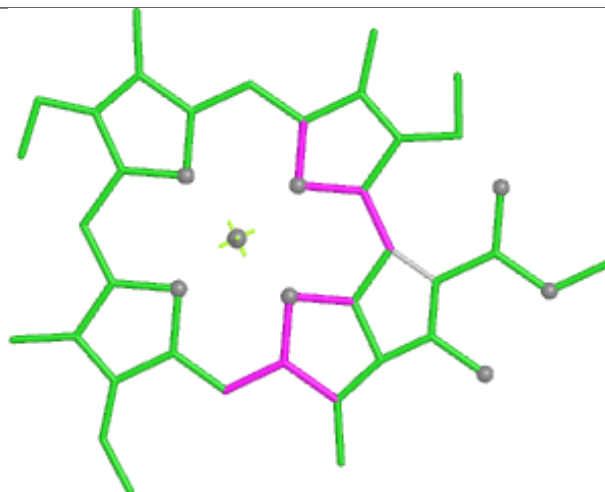




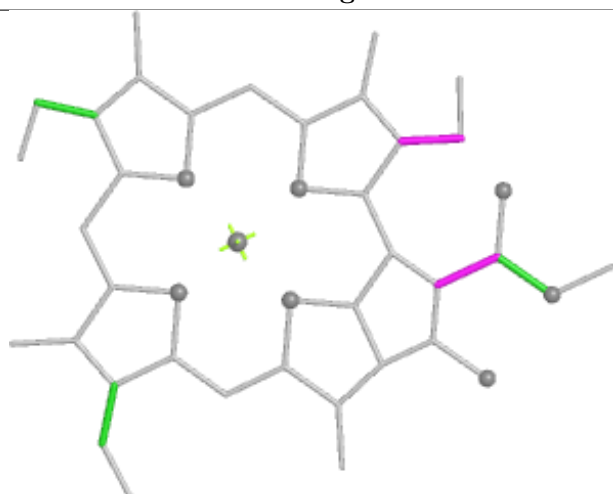
## Ligand CLA 3 312



Bond lengths



Bond angles

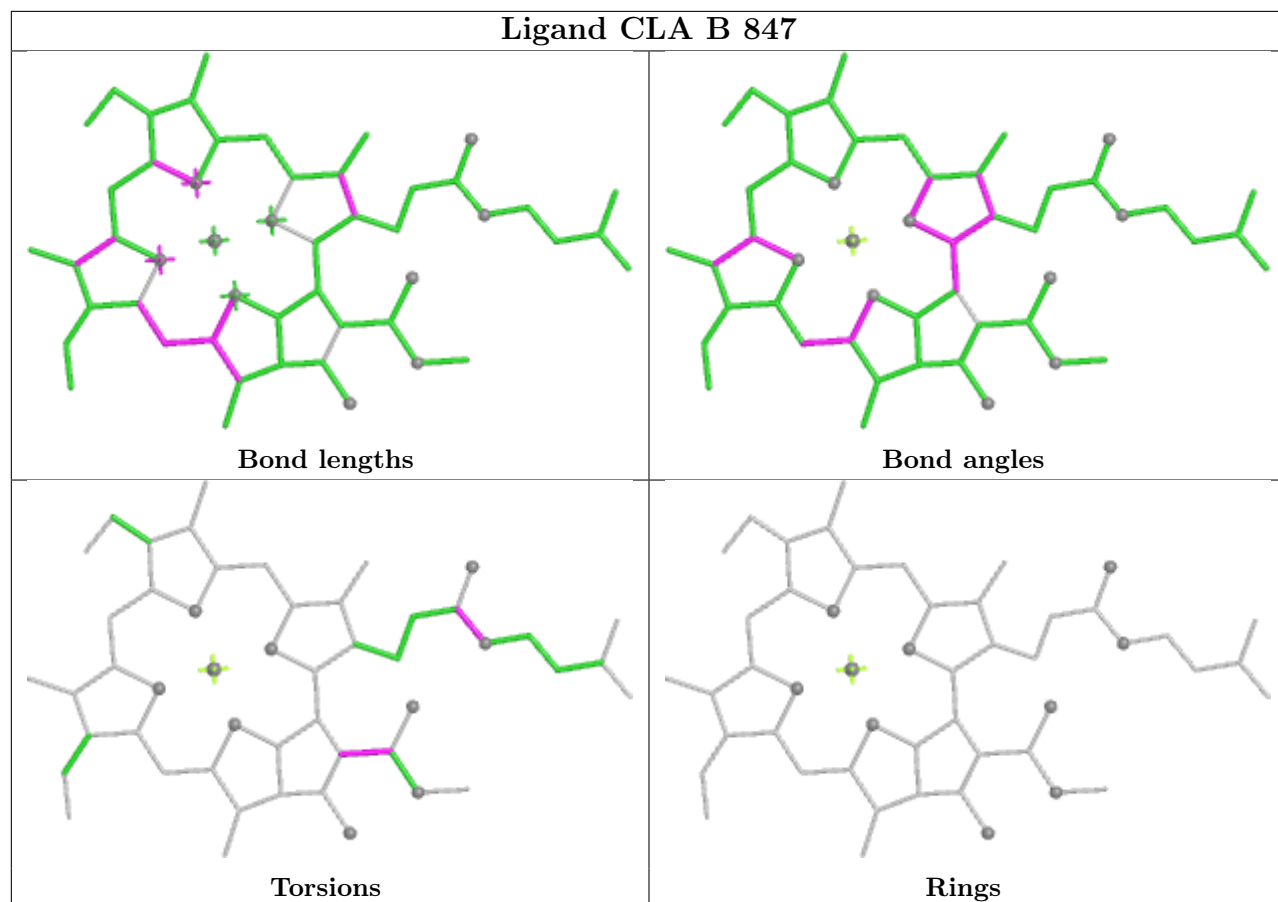


Torsions

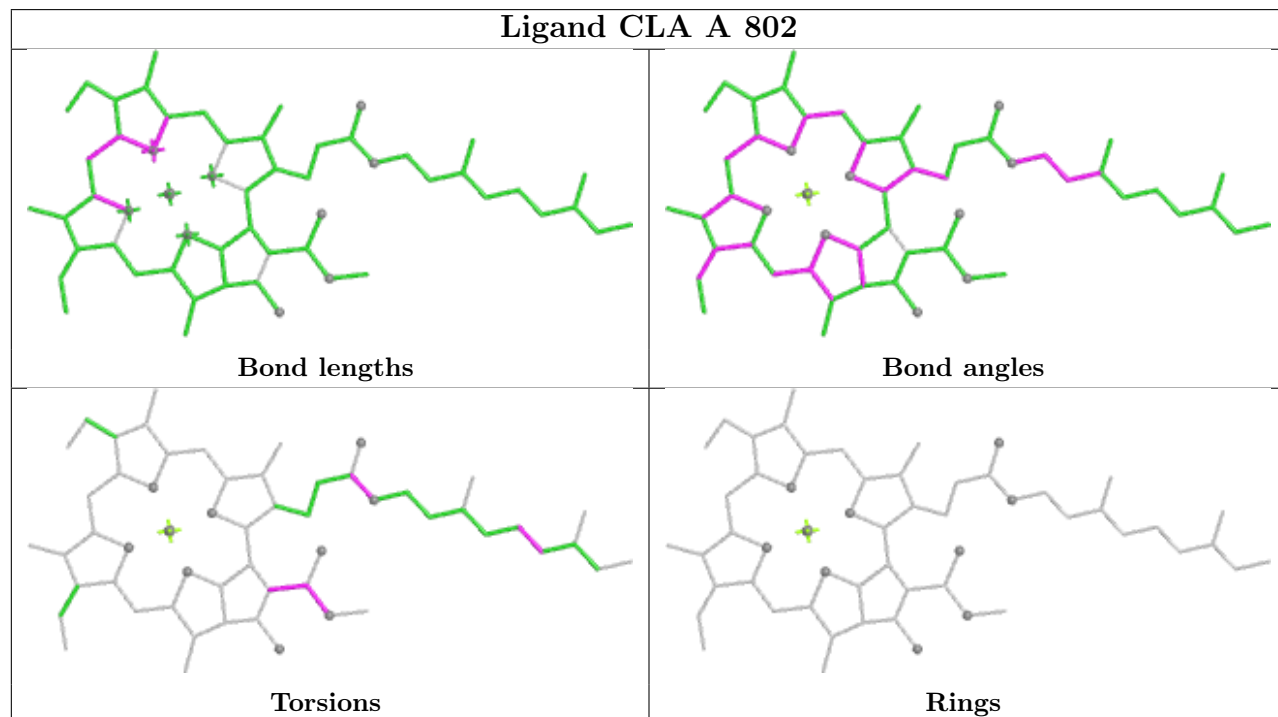


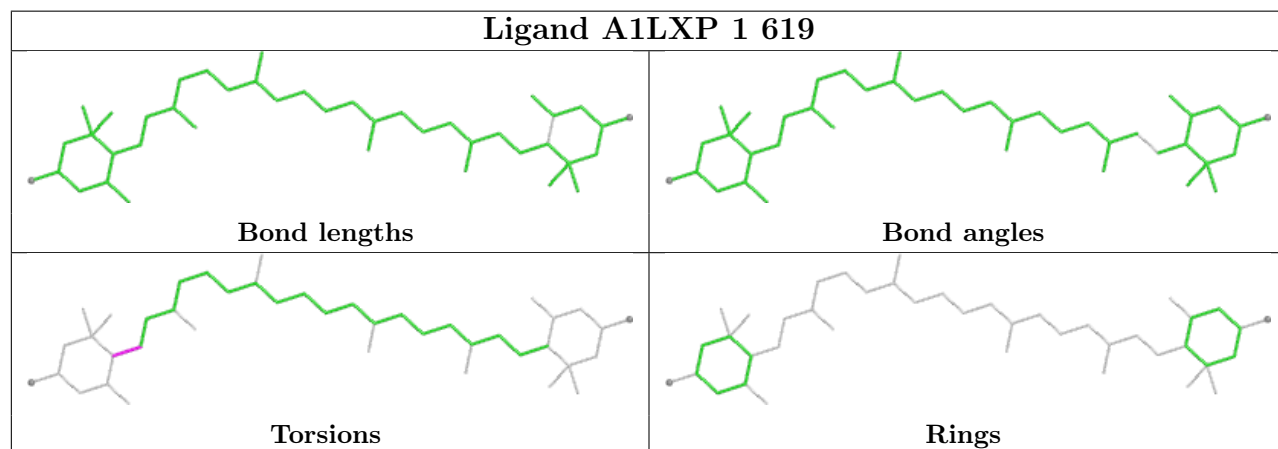
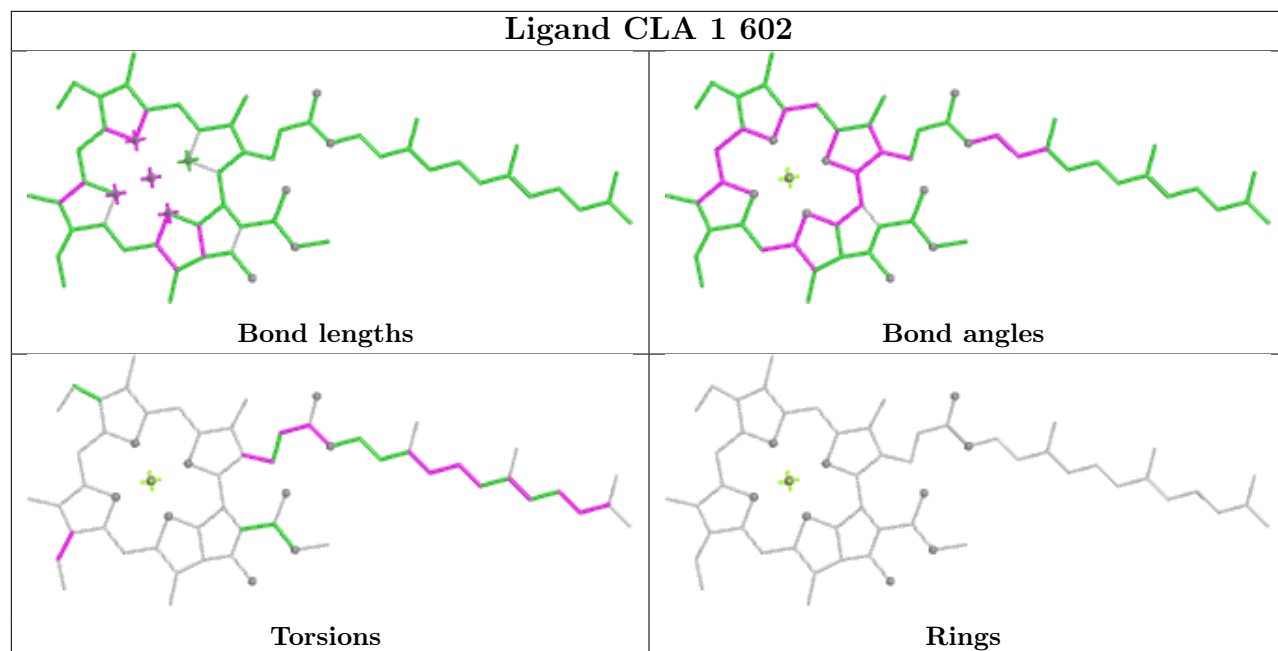
Rings

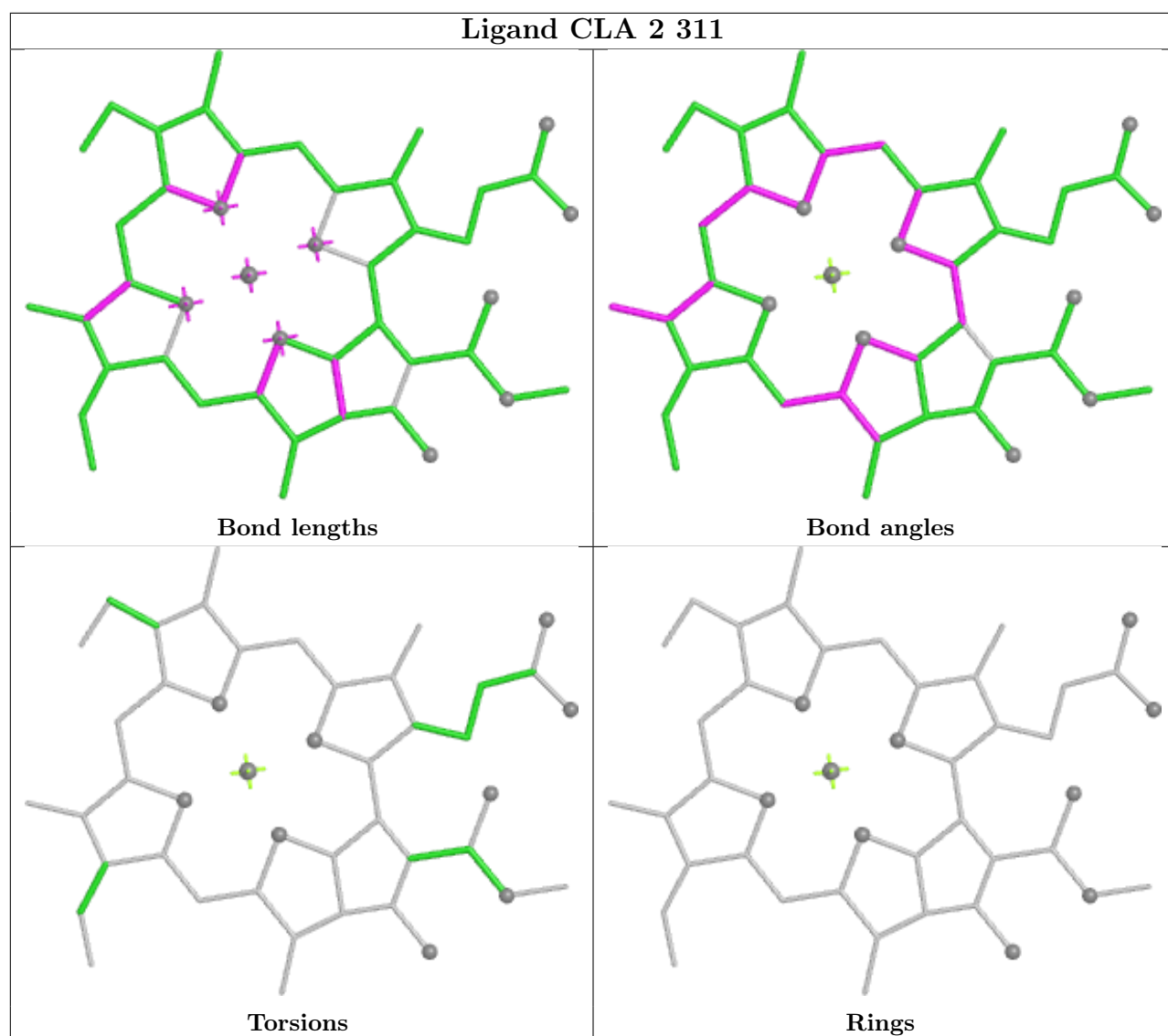
## Ligand CLA B 847

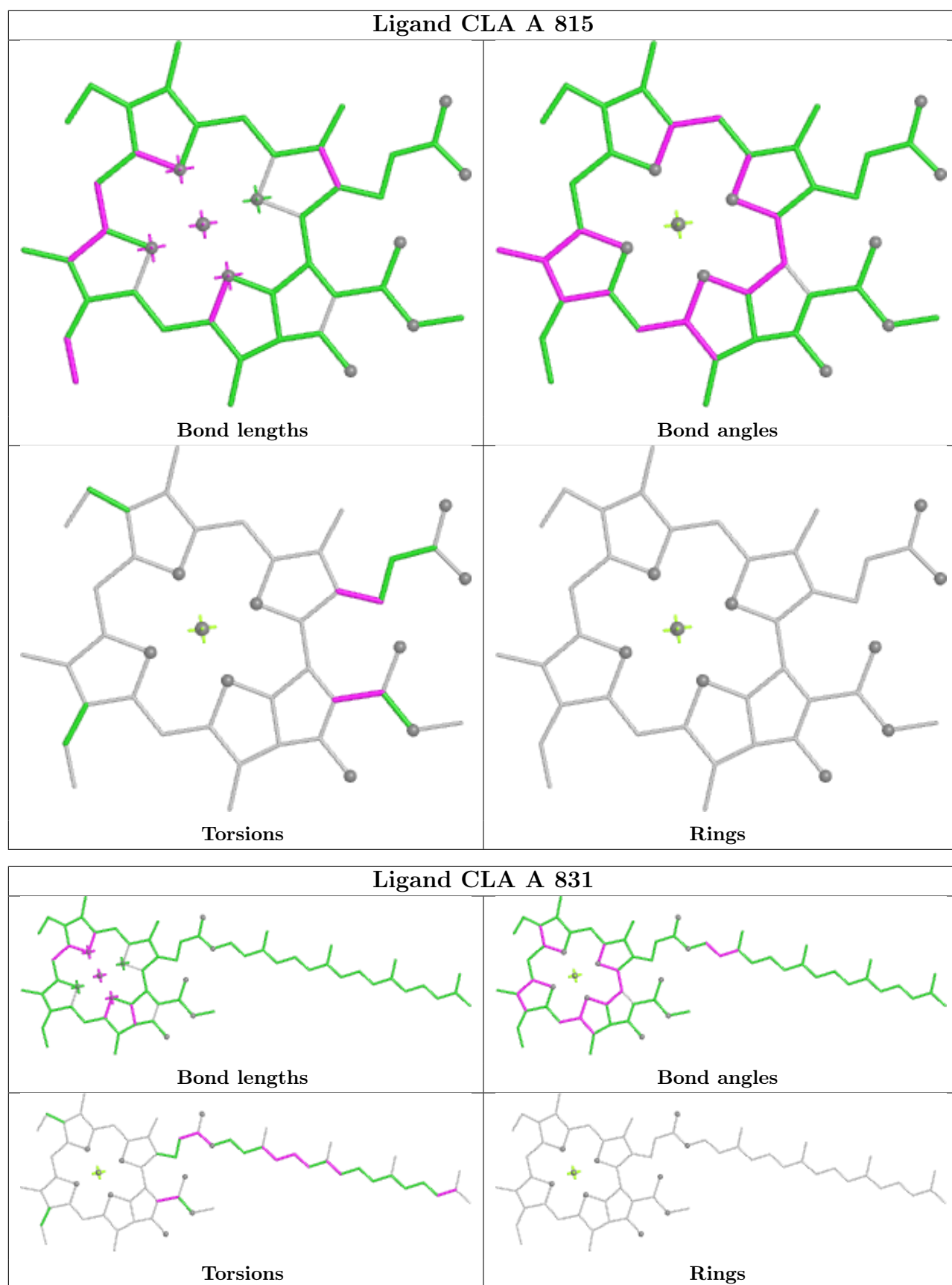


## Ligand CLA A 802



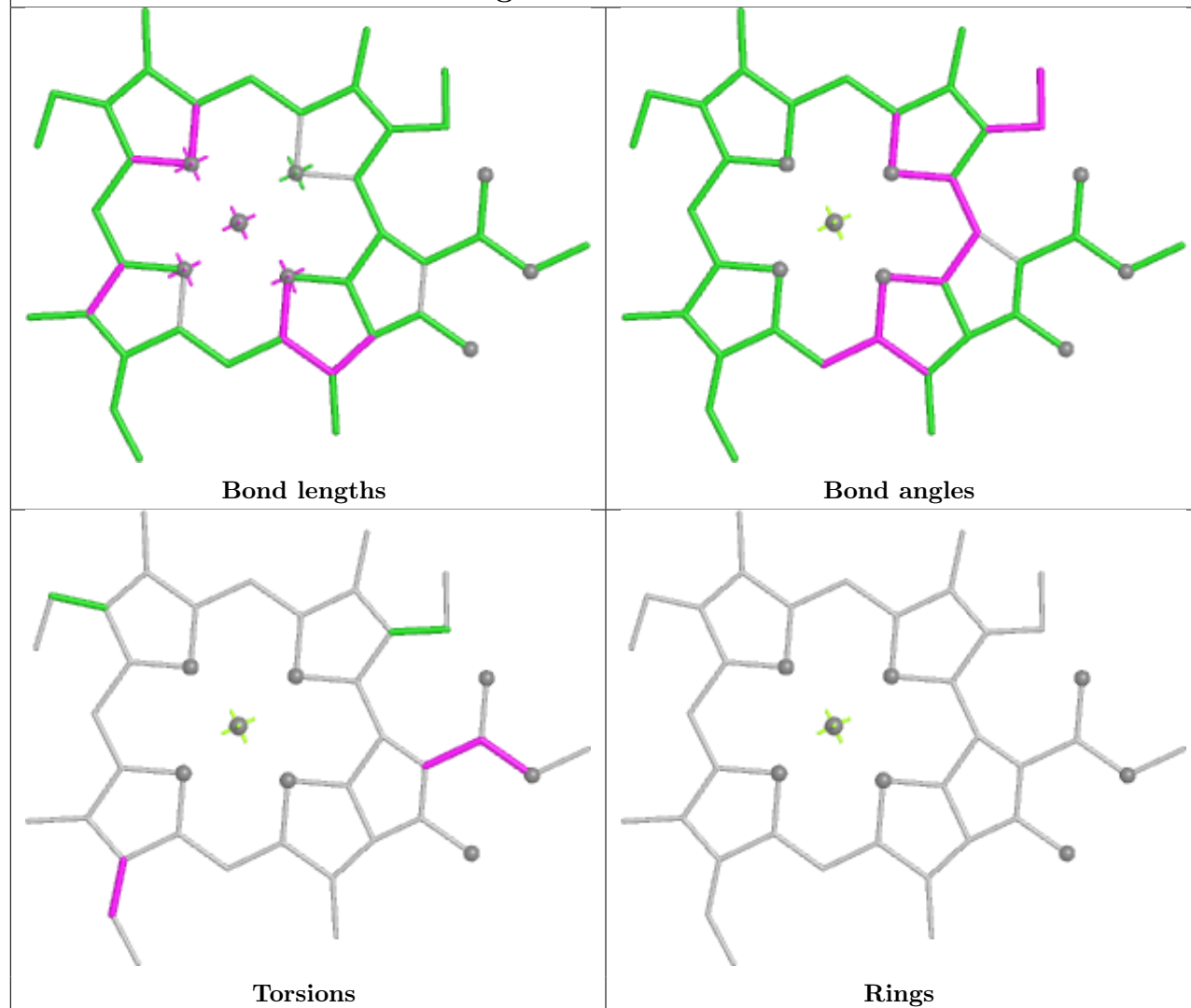




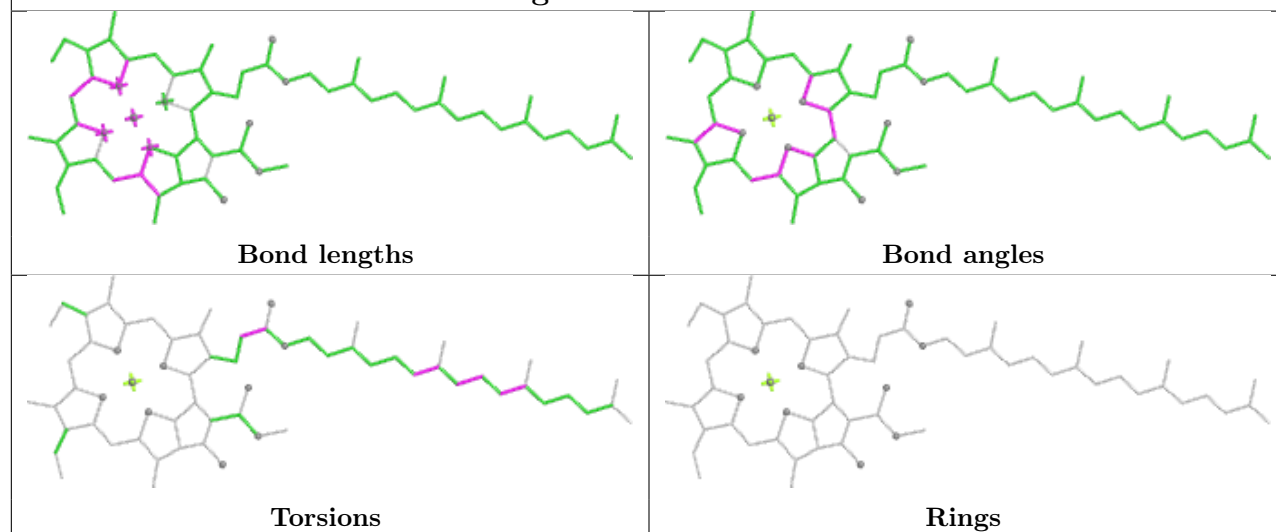




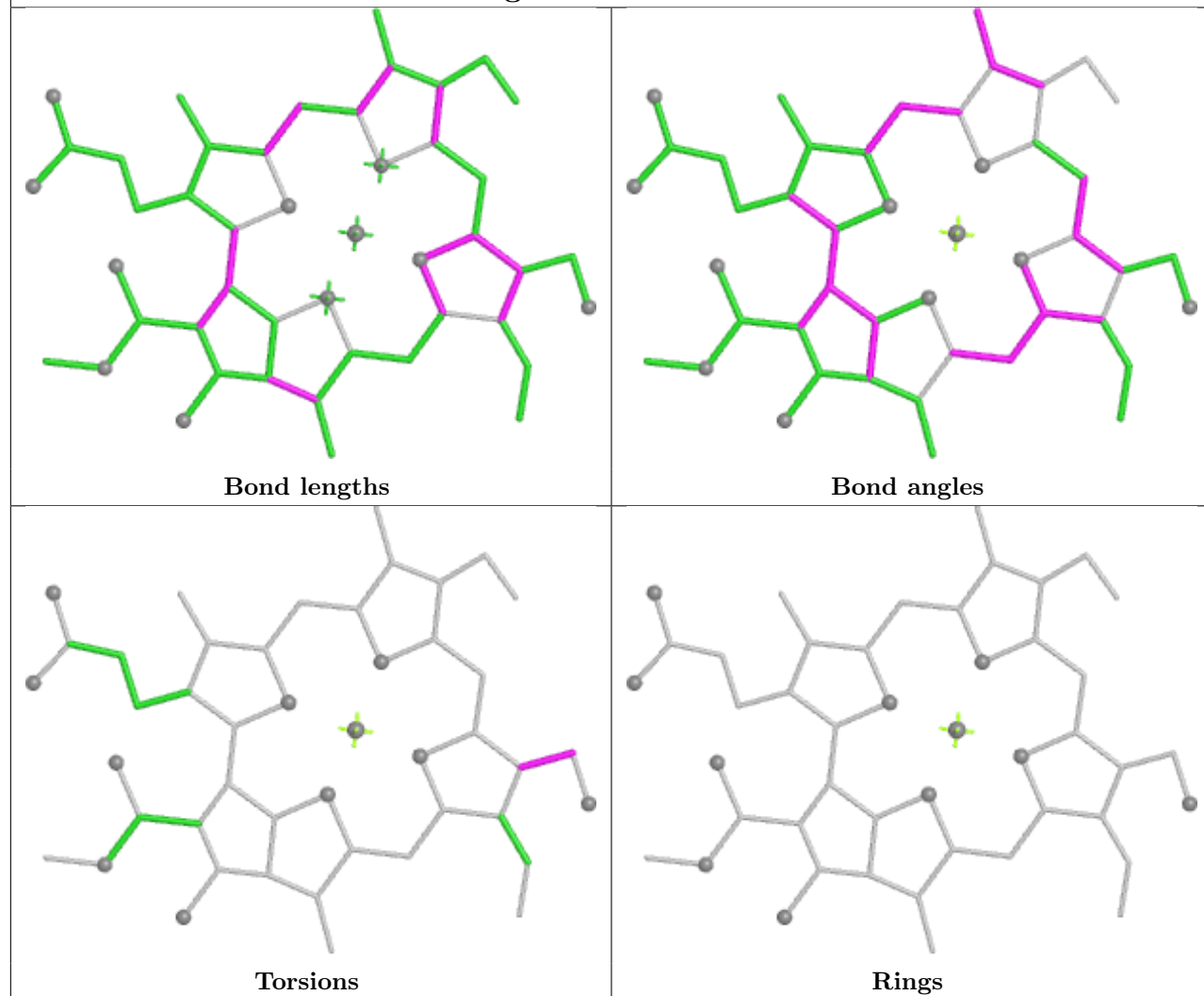
## Ligand CLA A 806



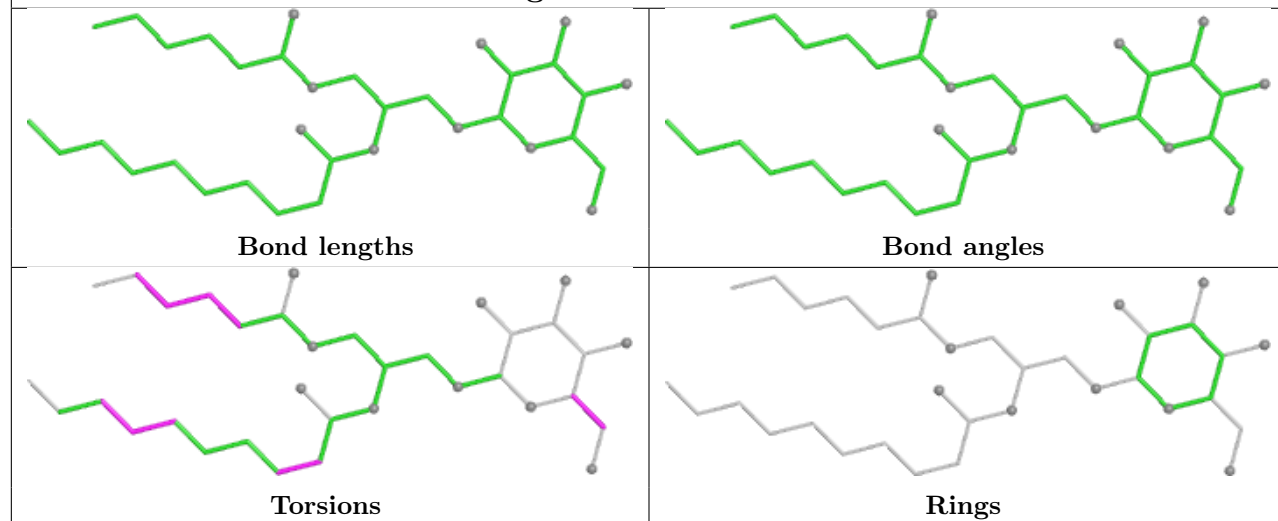
## Ligand CLA A 833

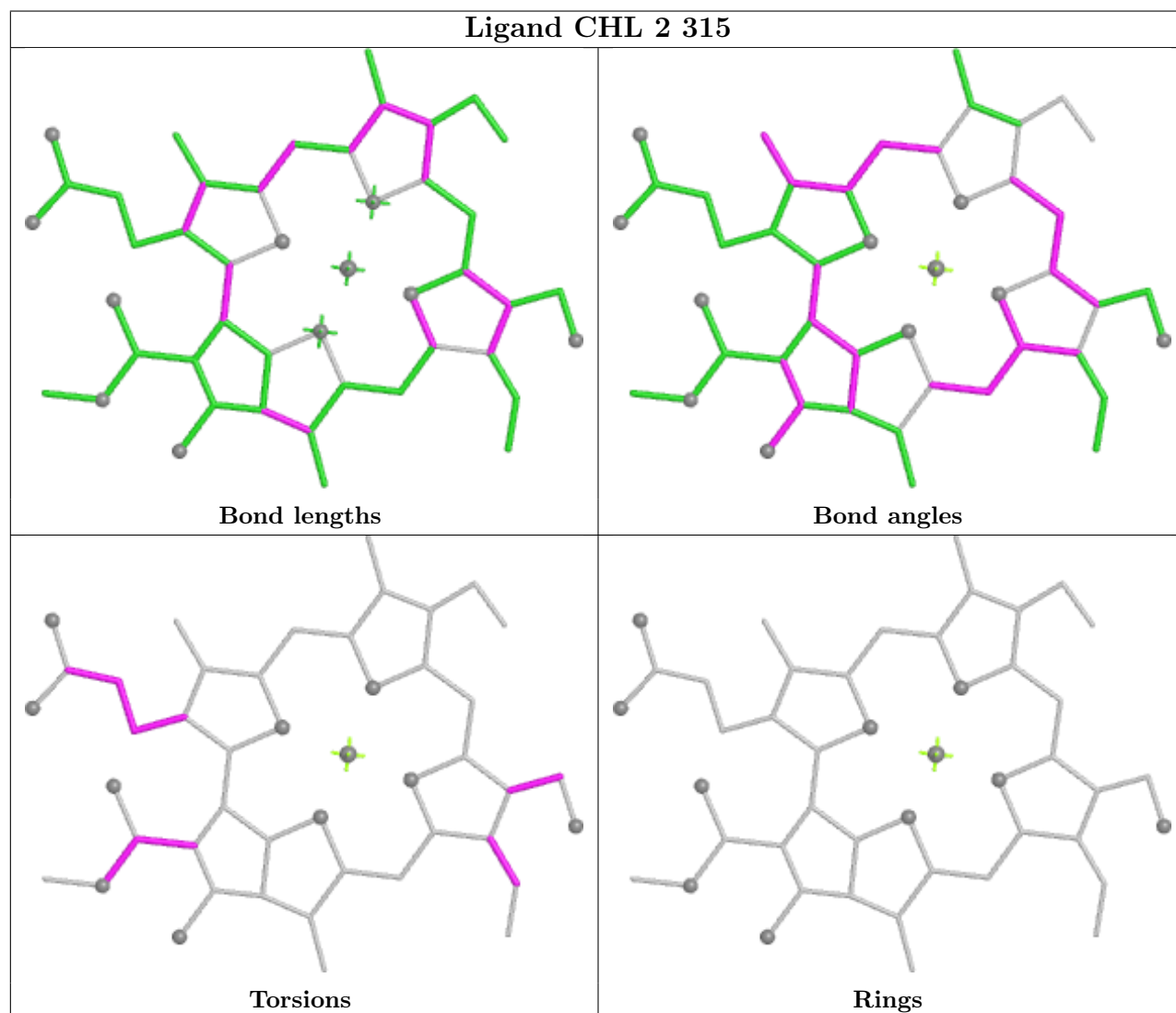
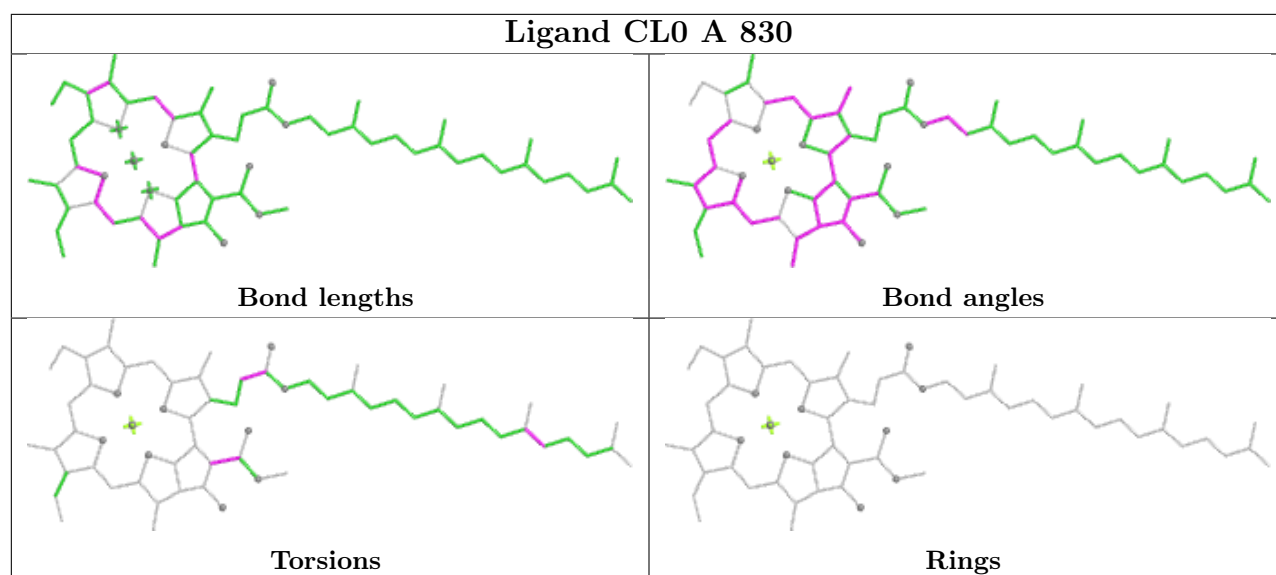


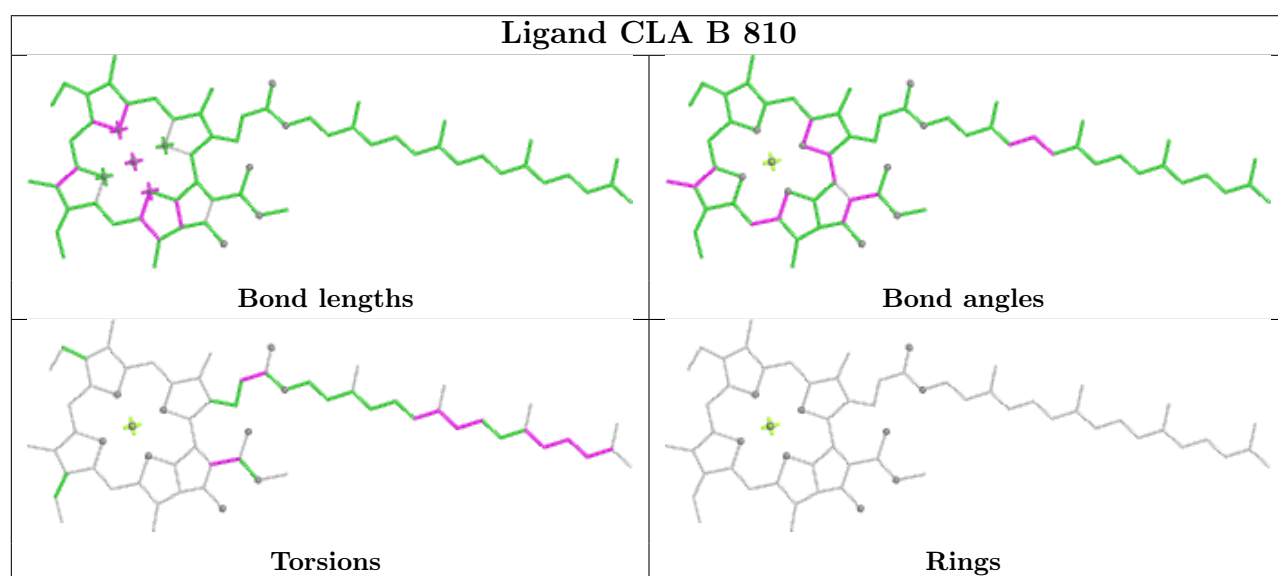
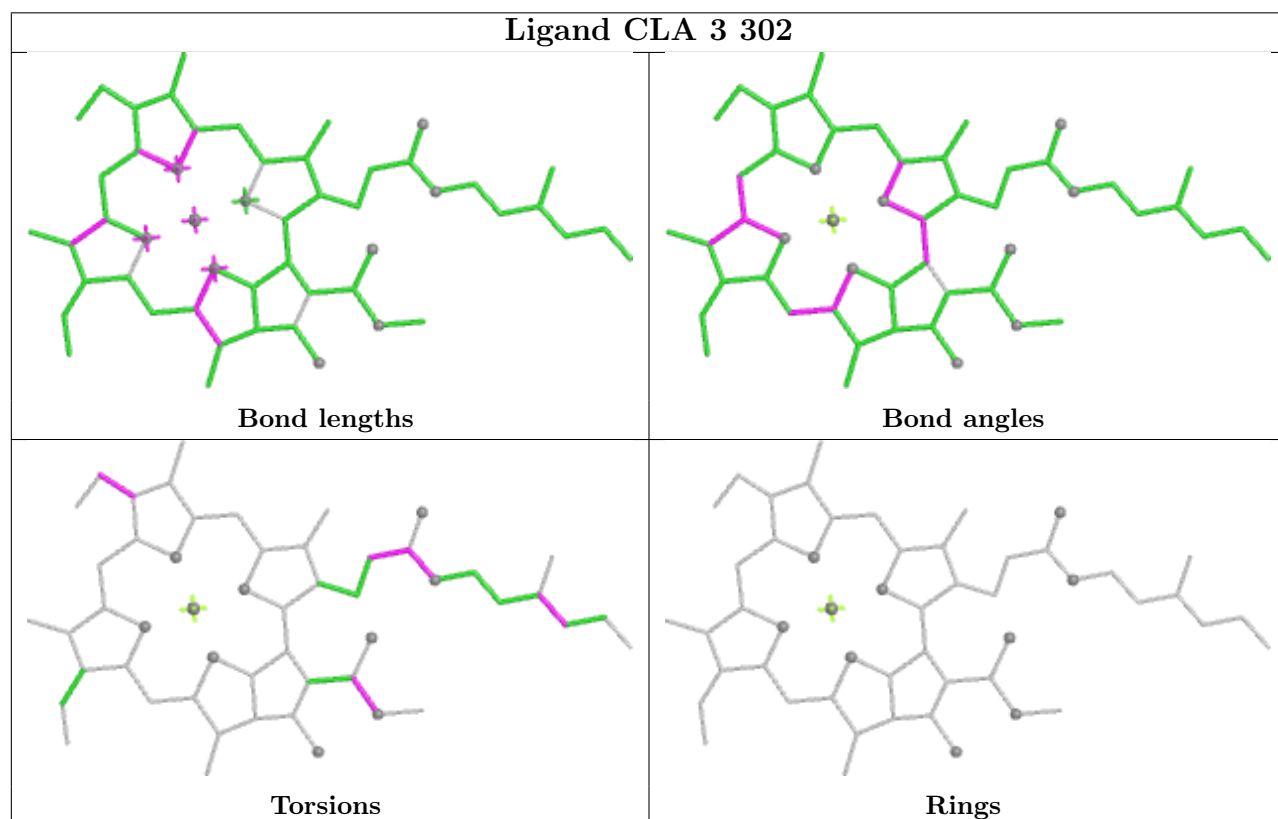
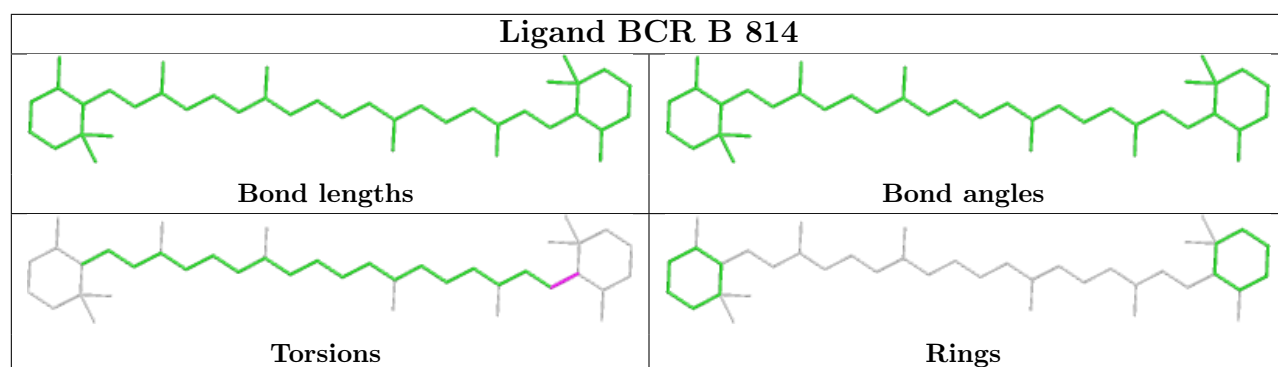
## Ligand CHL 4 313

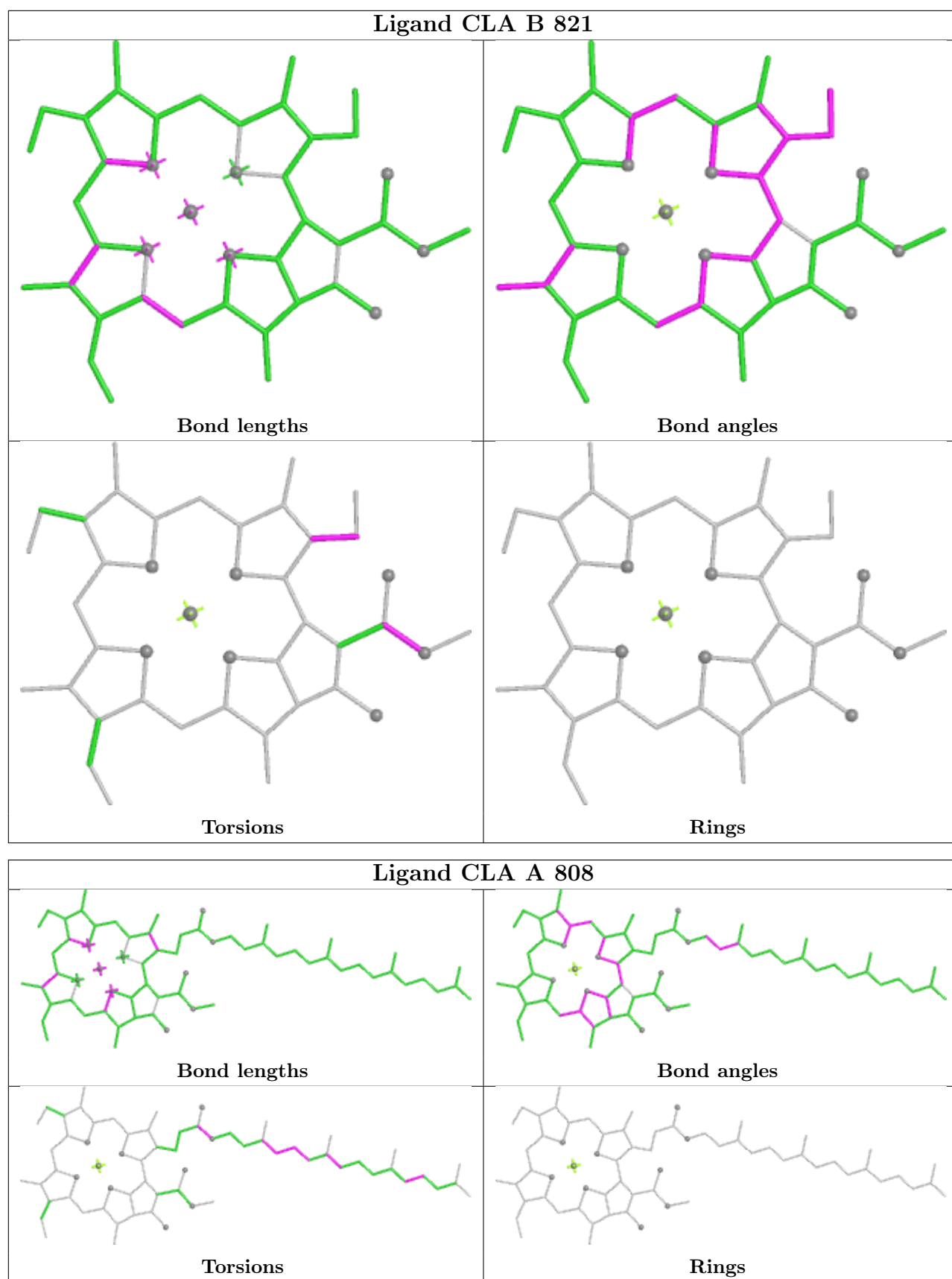


## Ligand LMG G 206

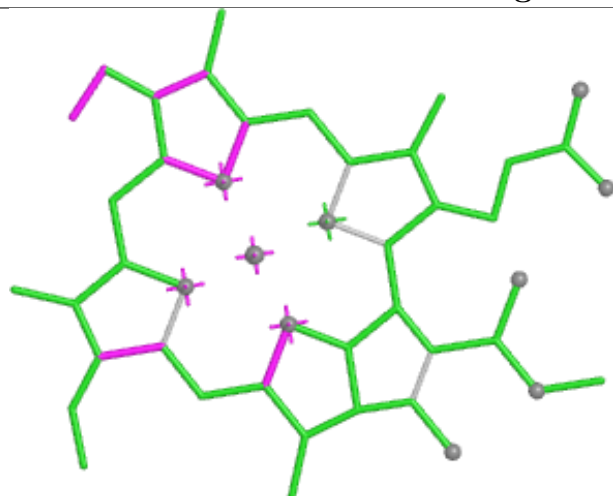




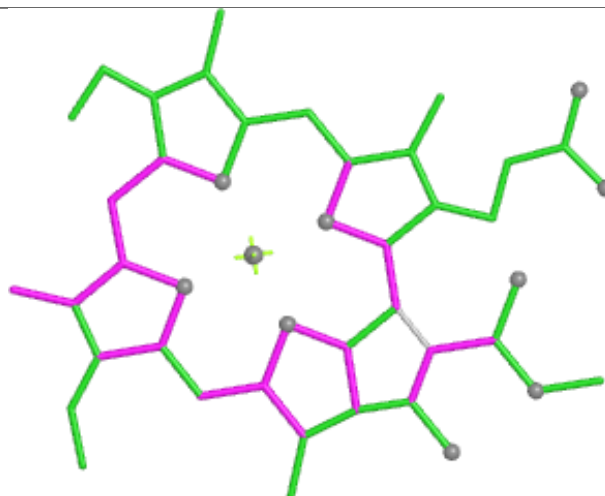




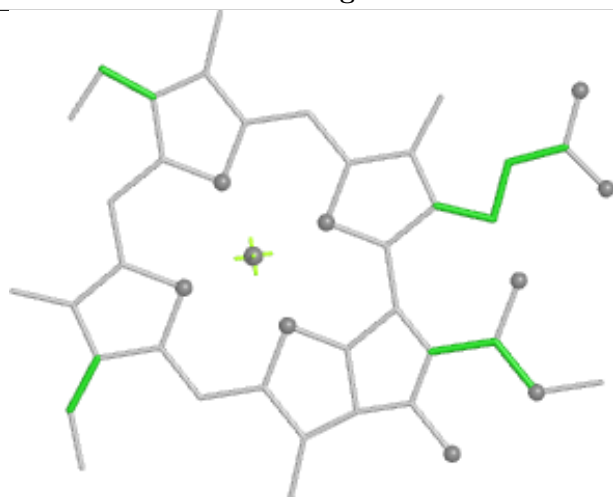
## Ligand CLA B 803



Bond lengths



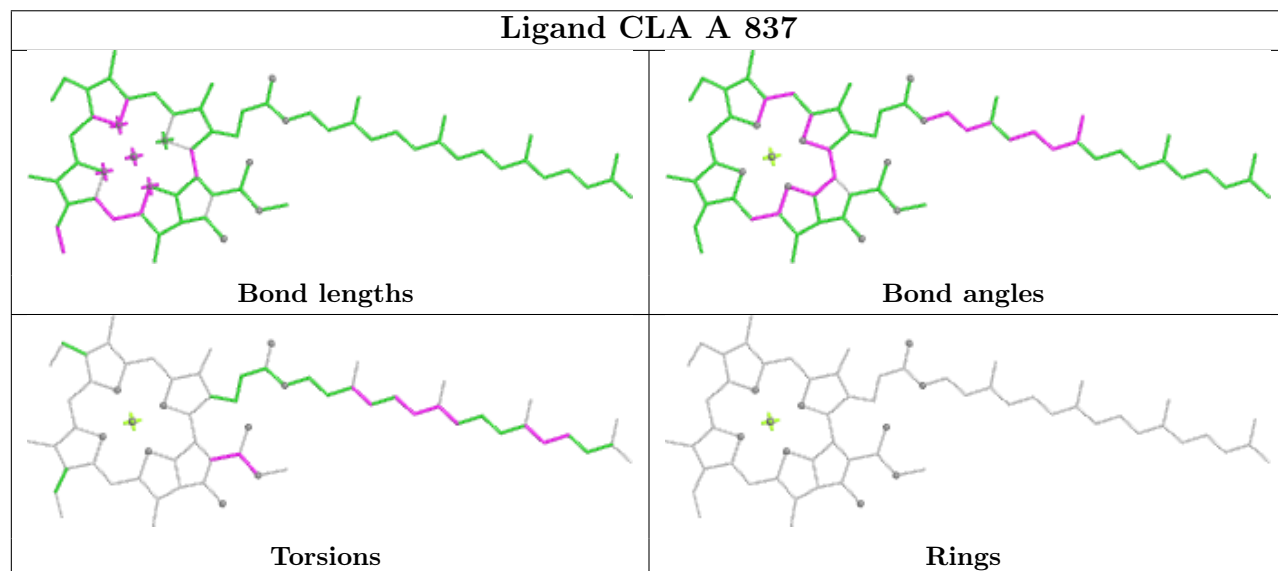
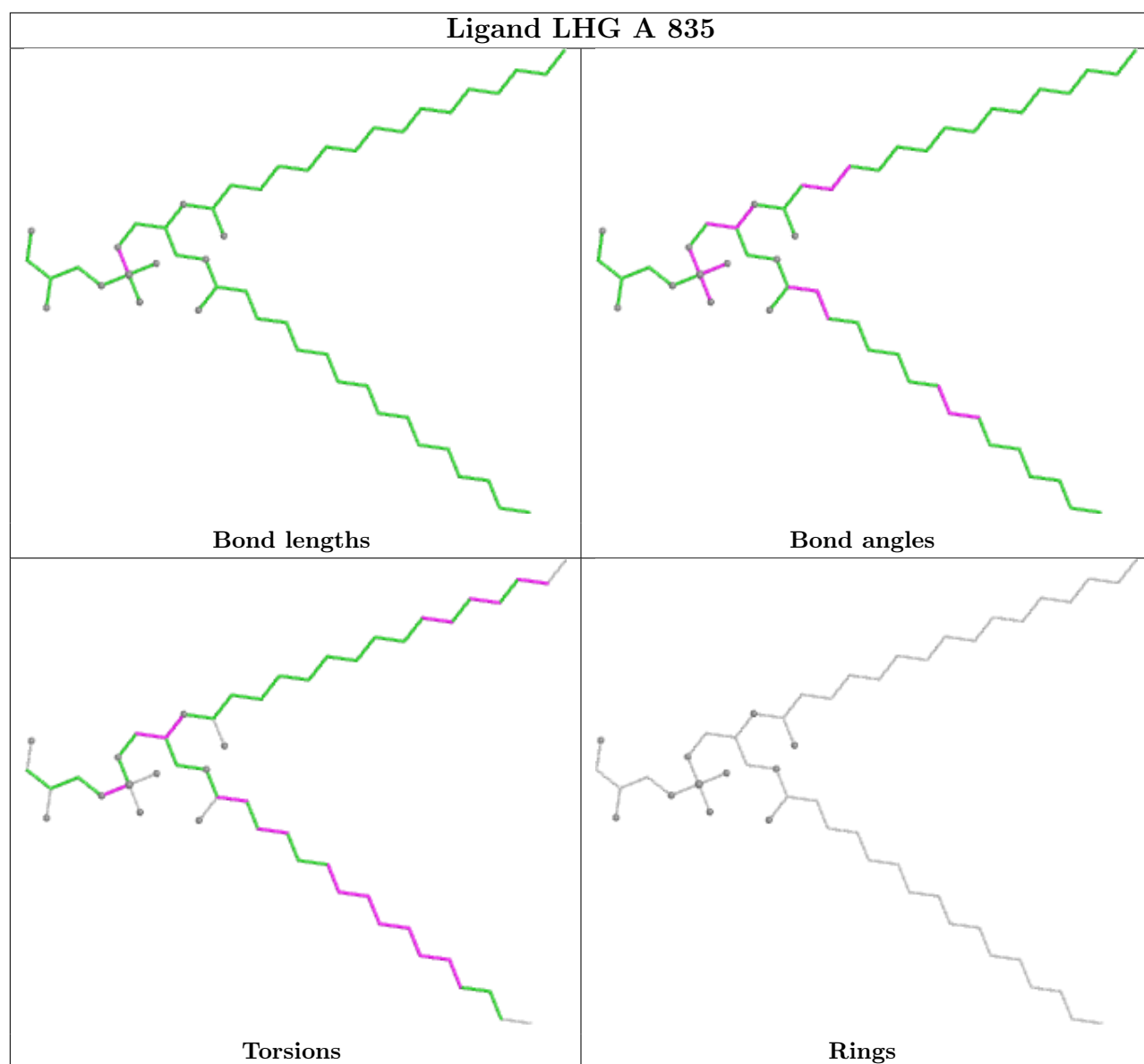
Bond angles

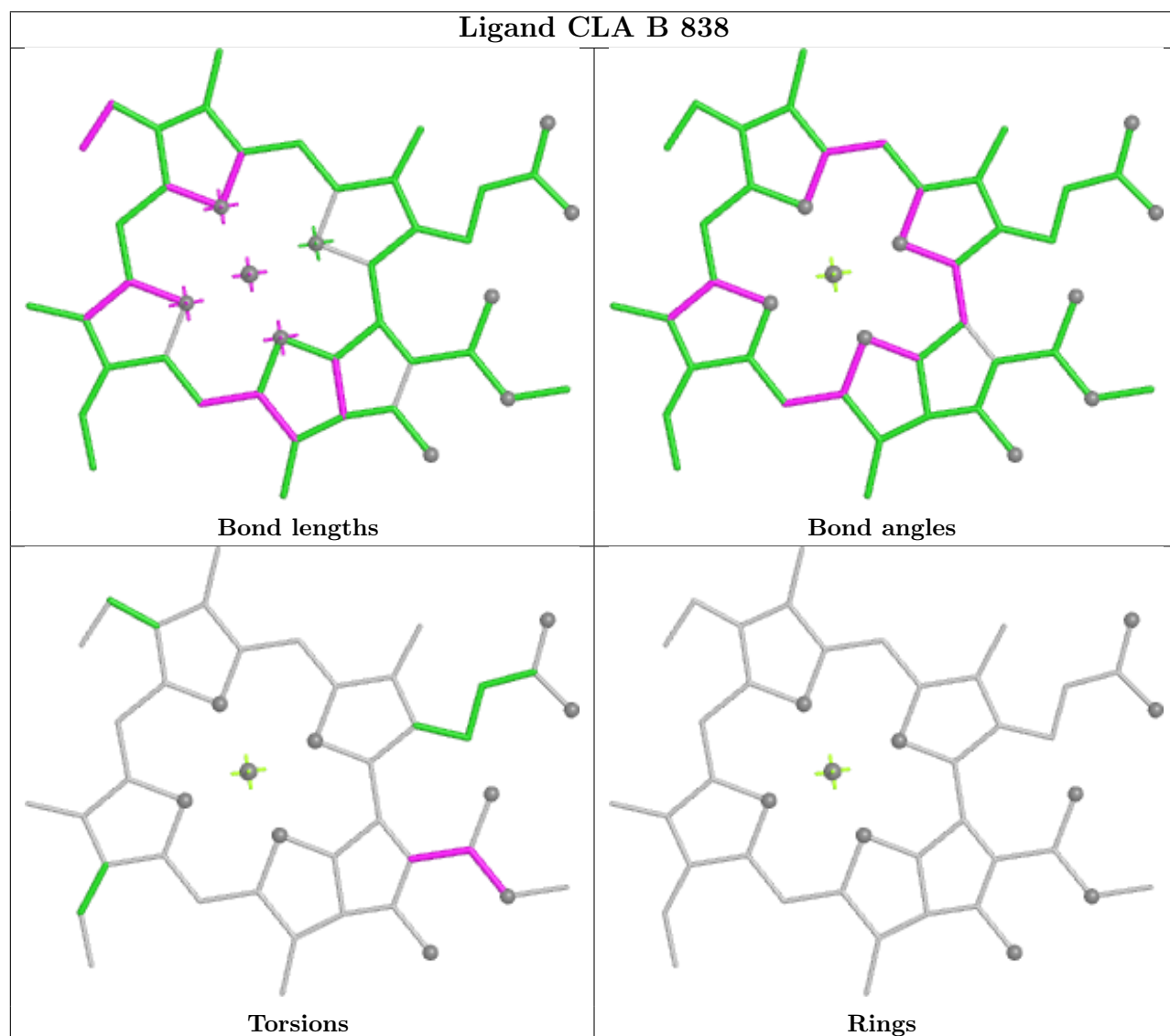
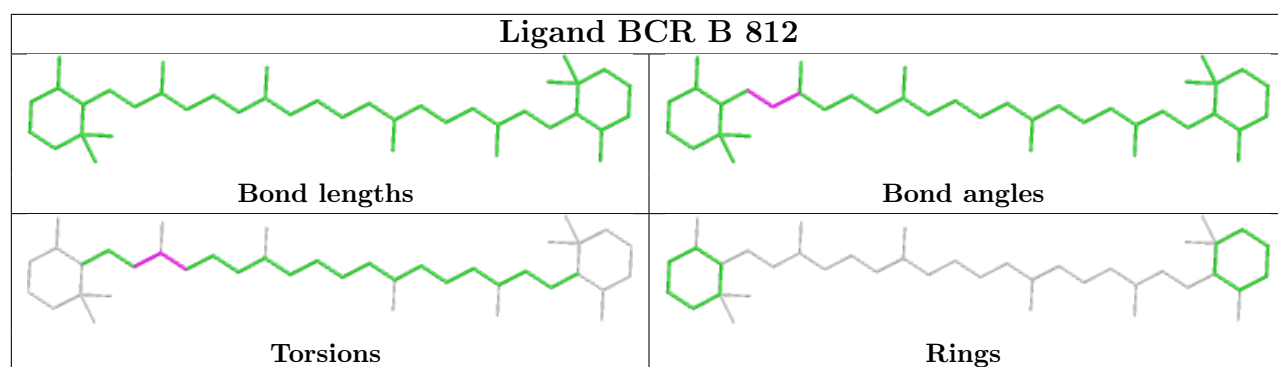


Torsions

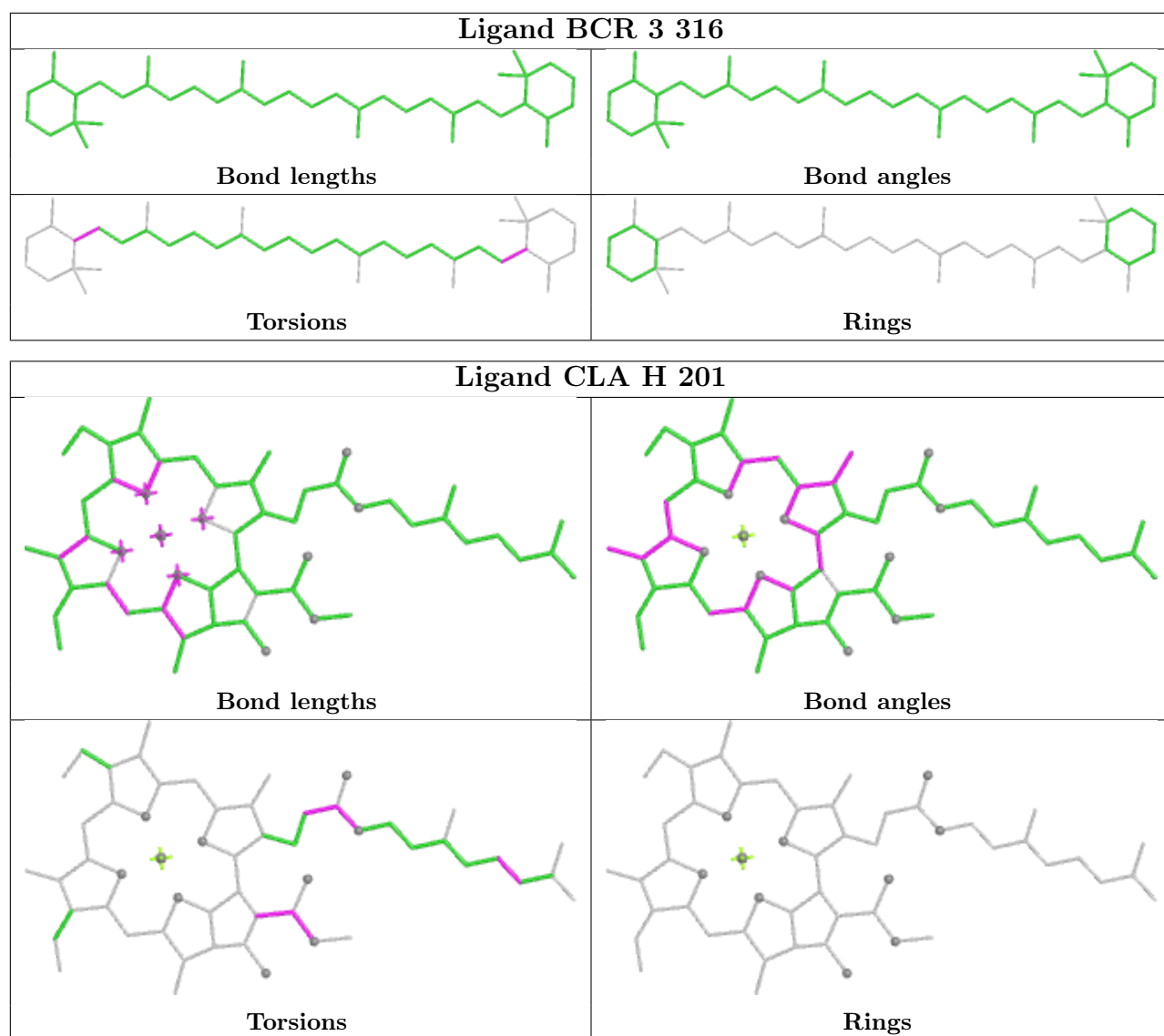


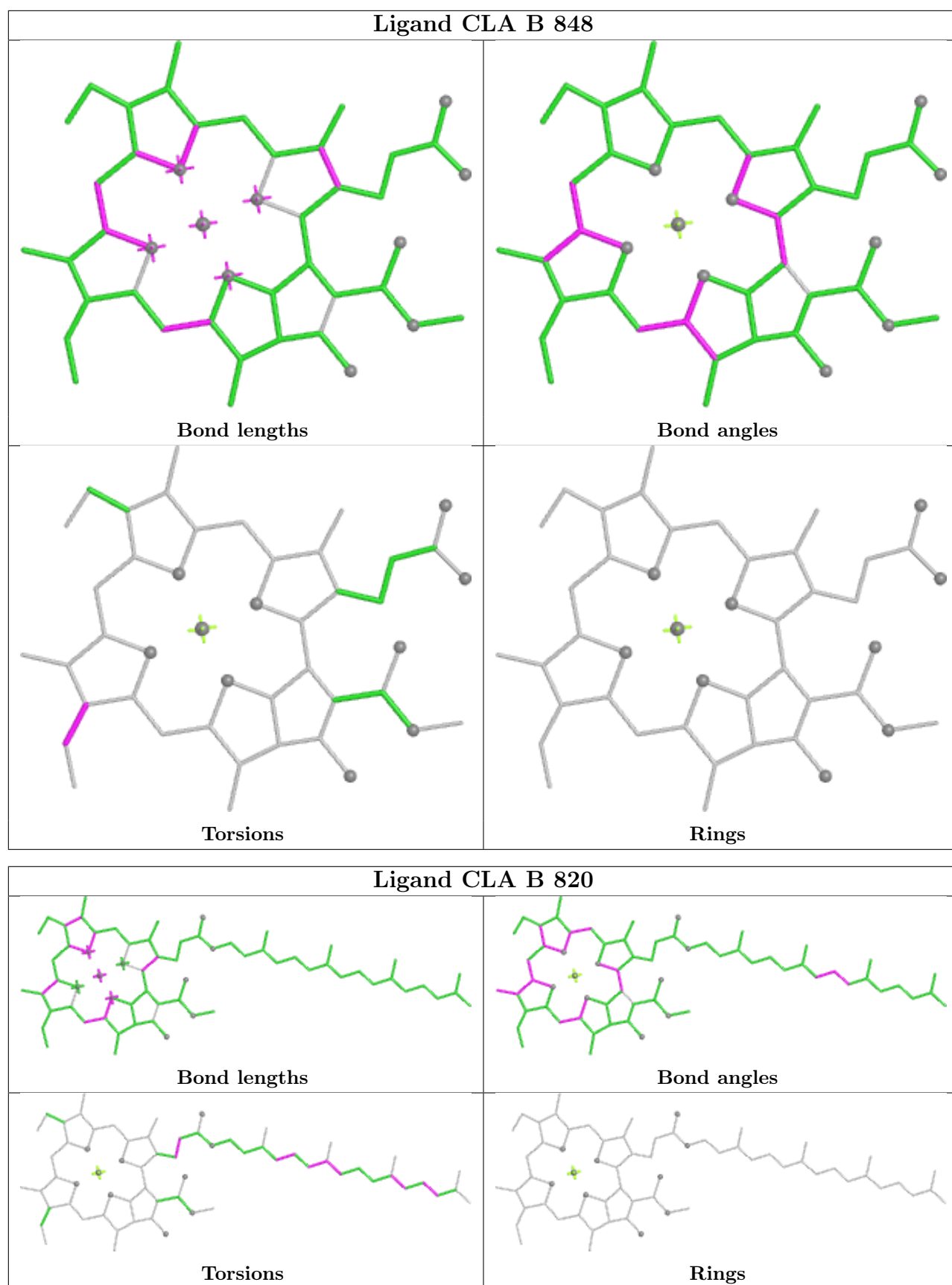
Rings

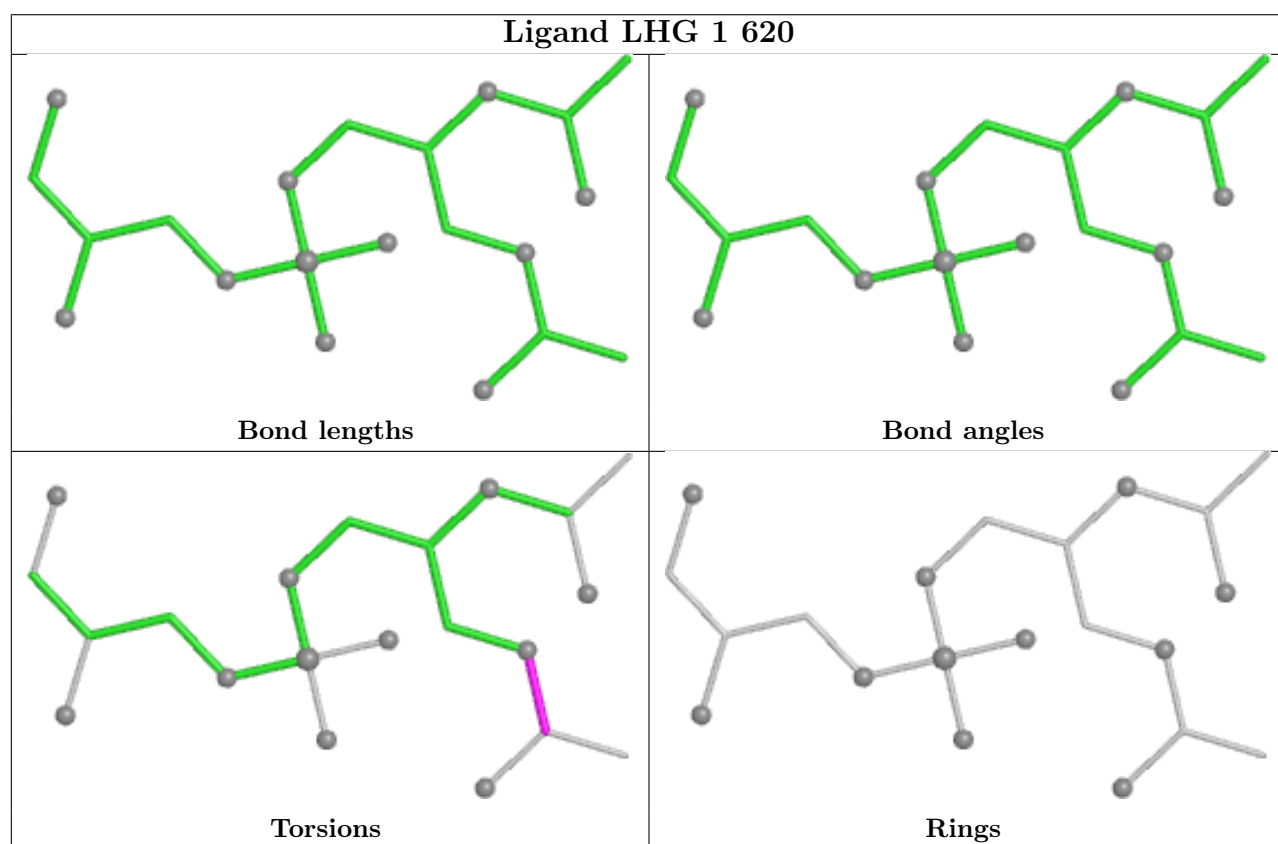
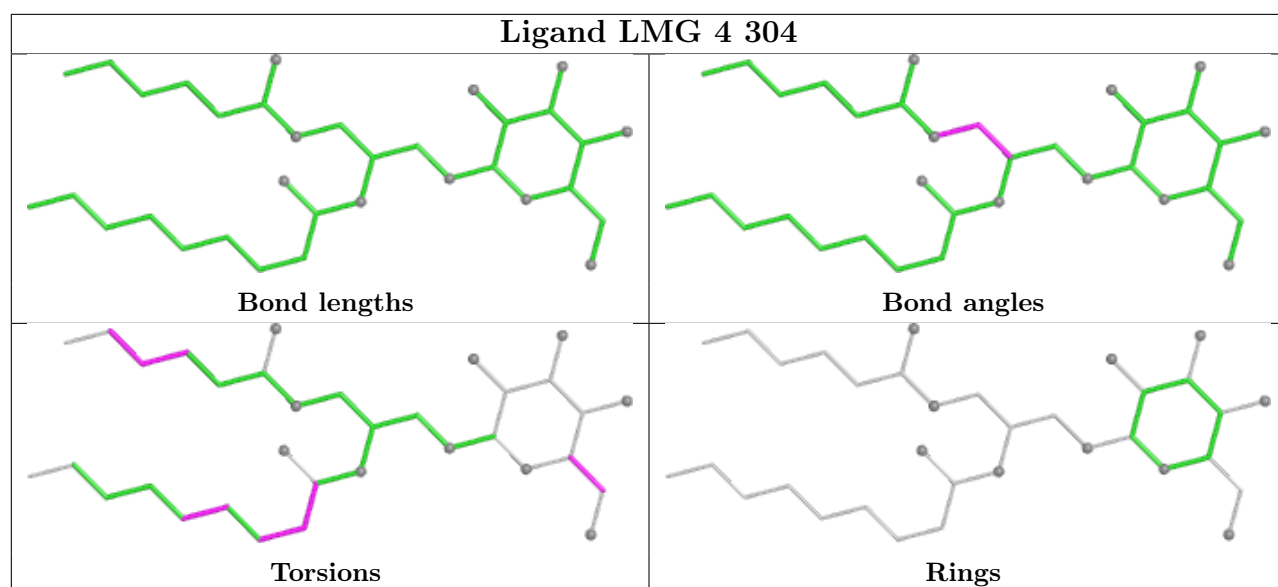


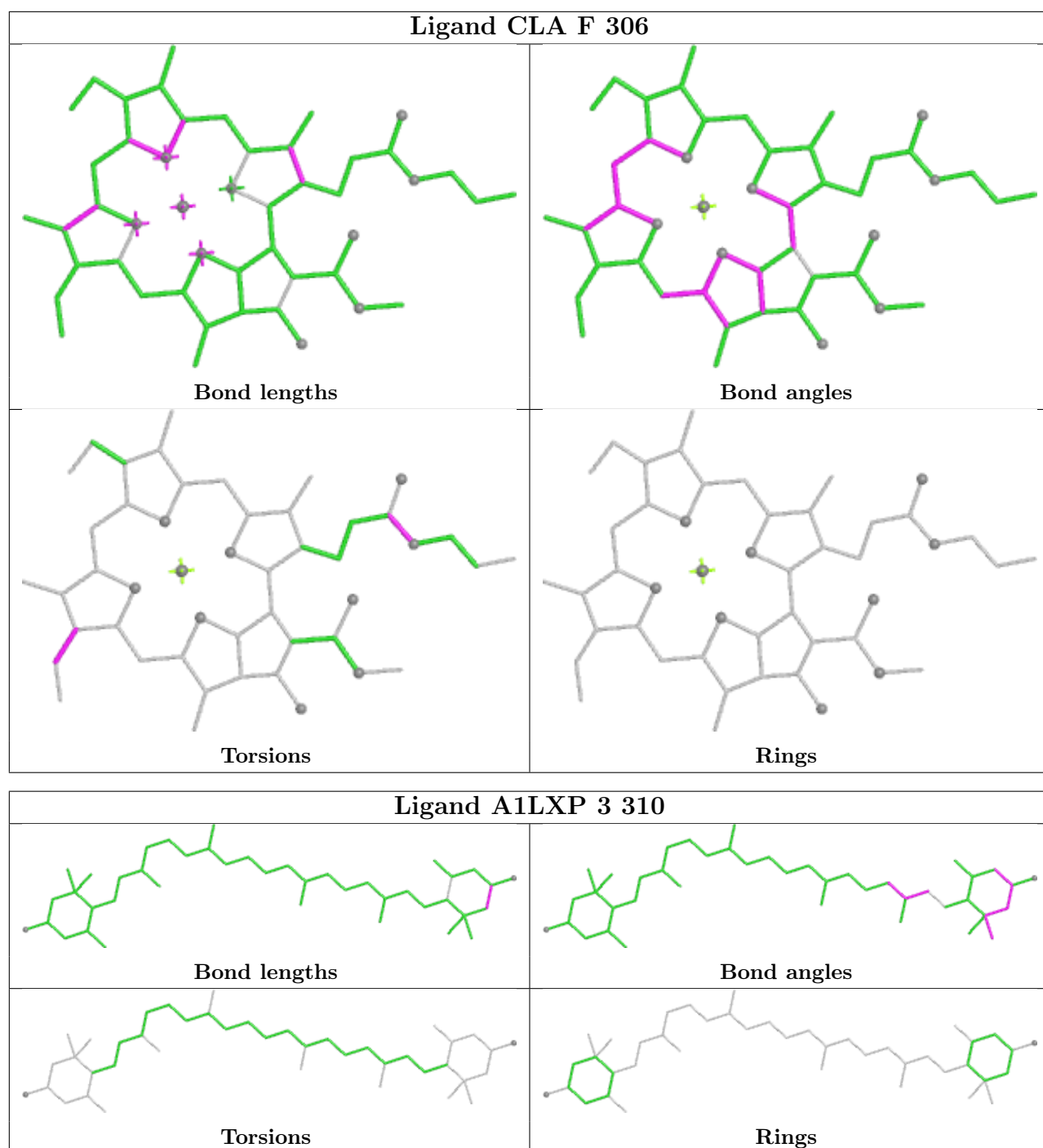


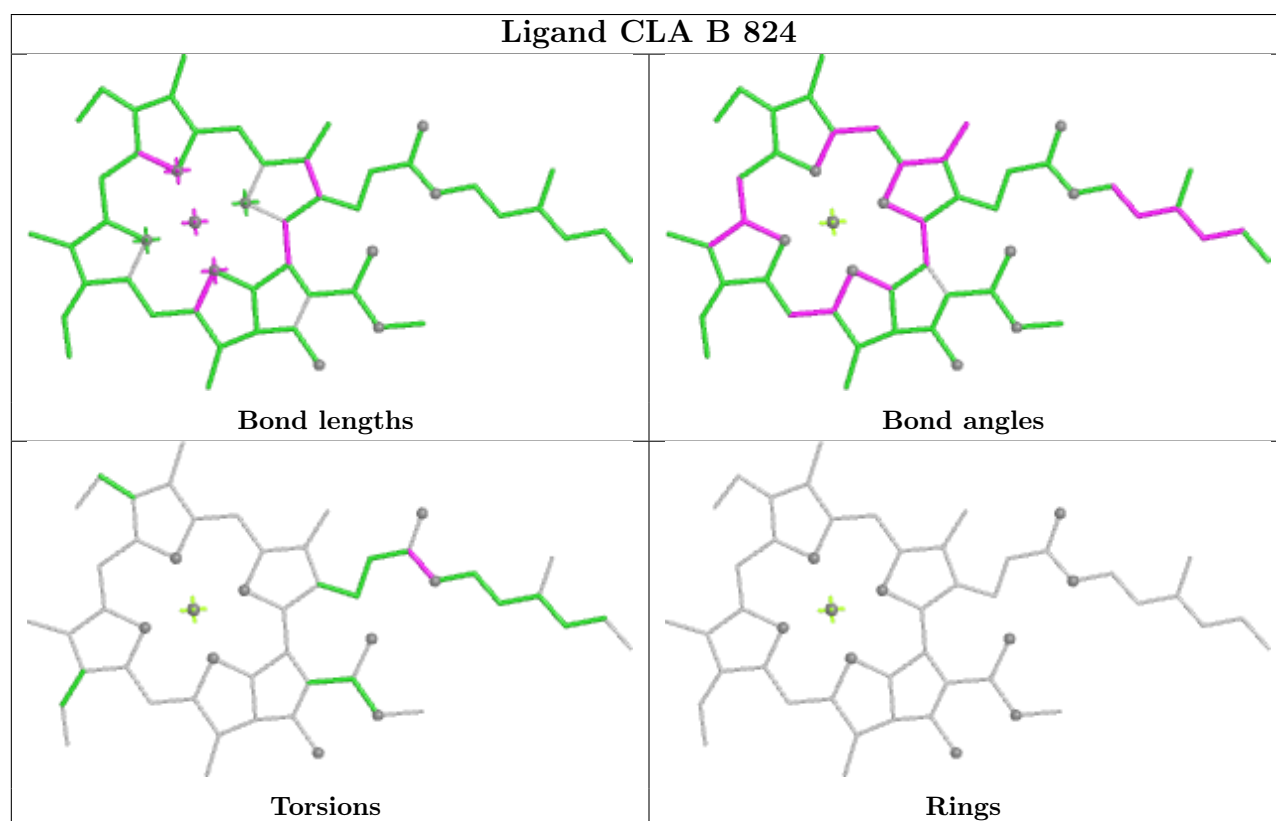
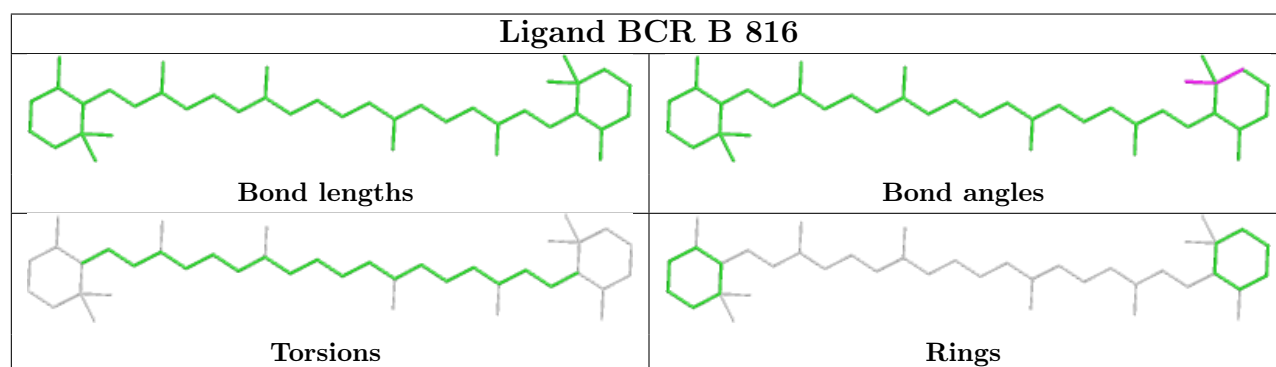
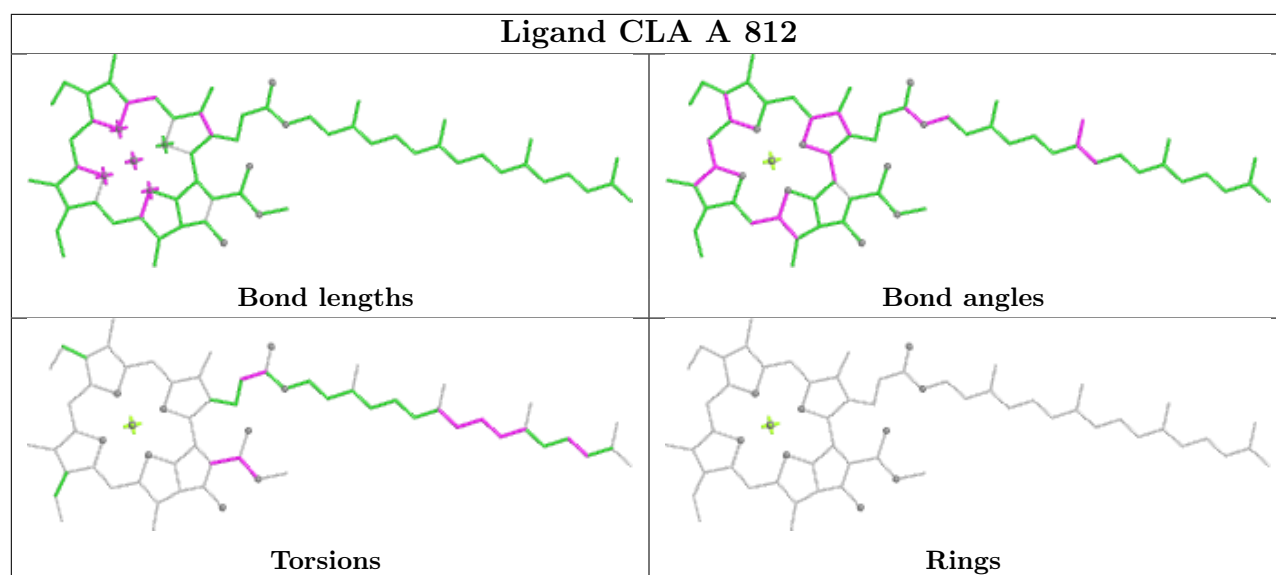




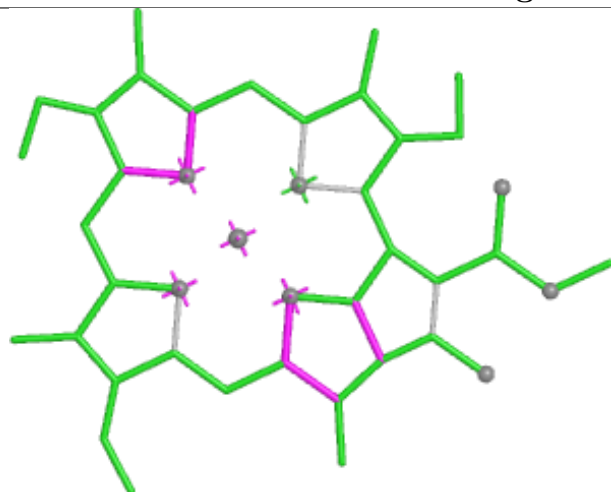




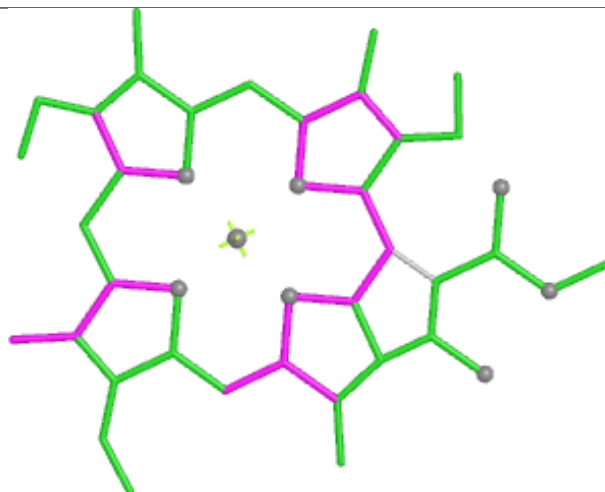




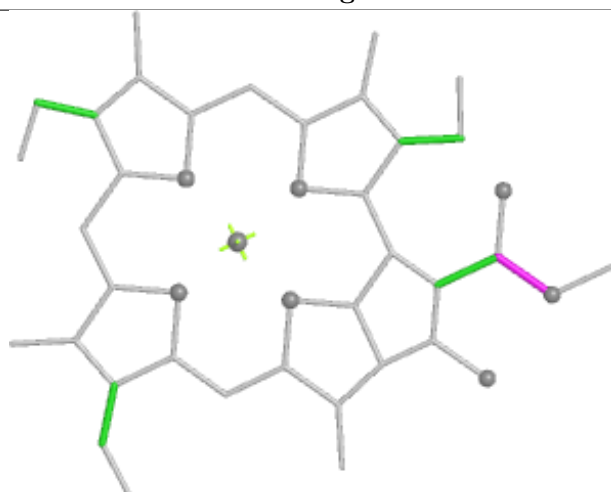
## Ligand CLA F 303



Bond lengths



Bond angles

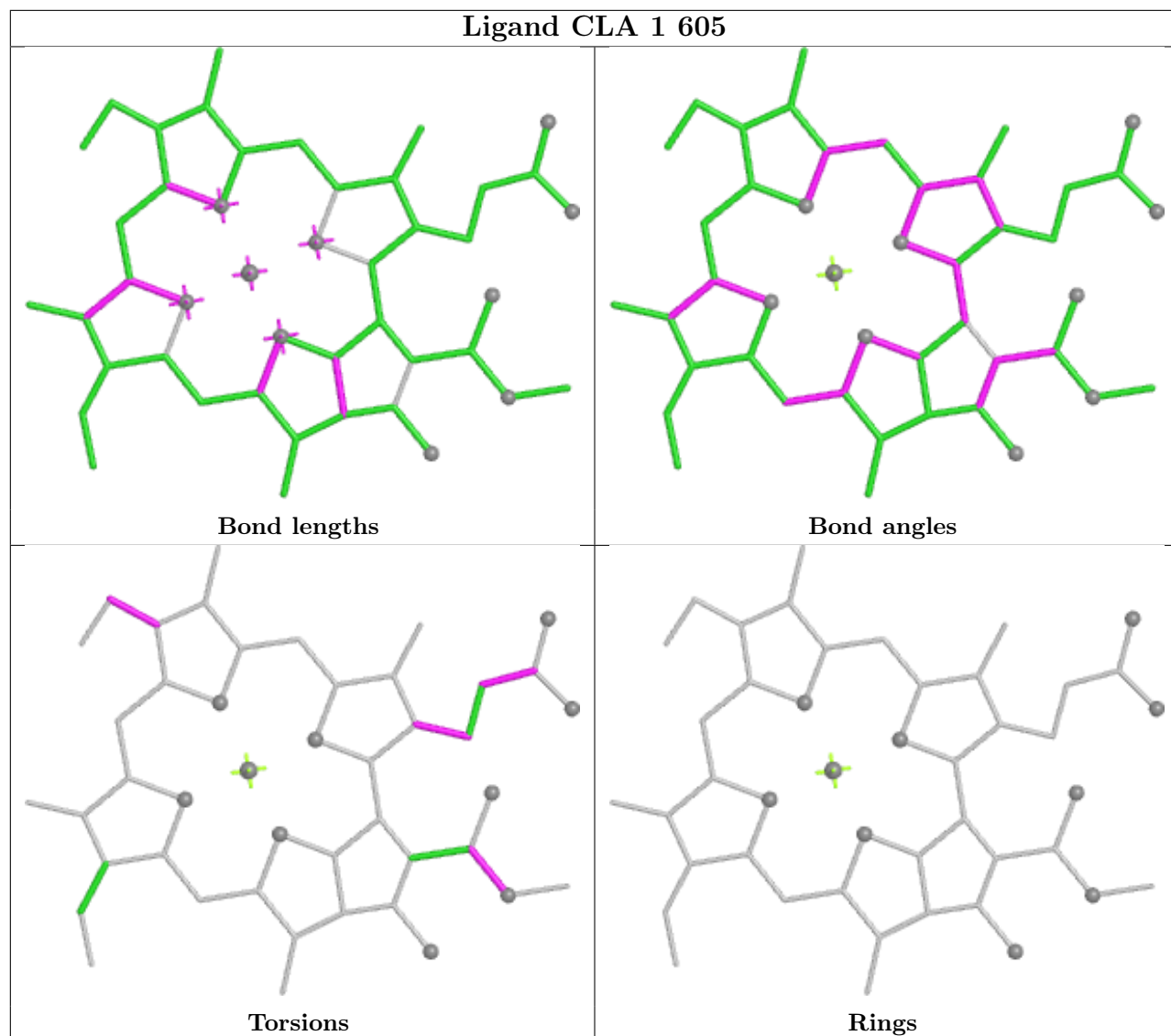


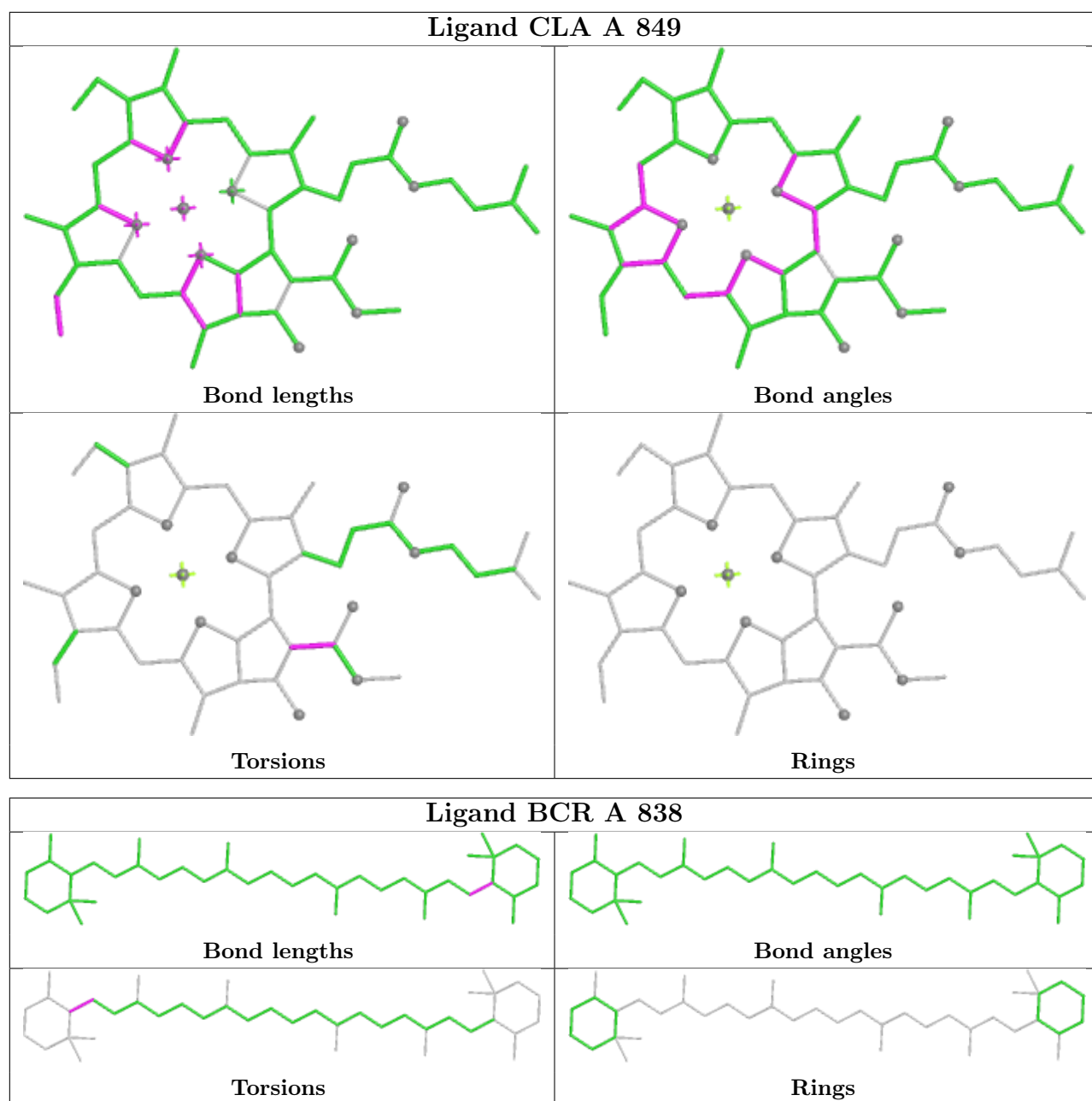
Torsions



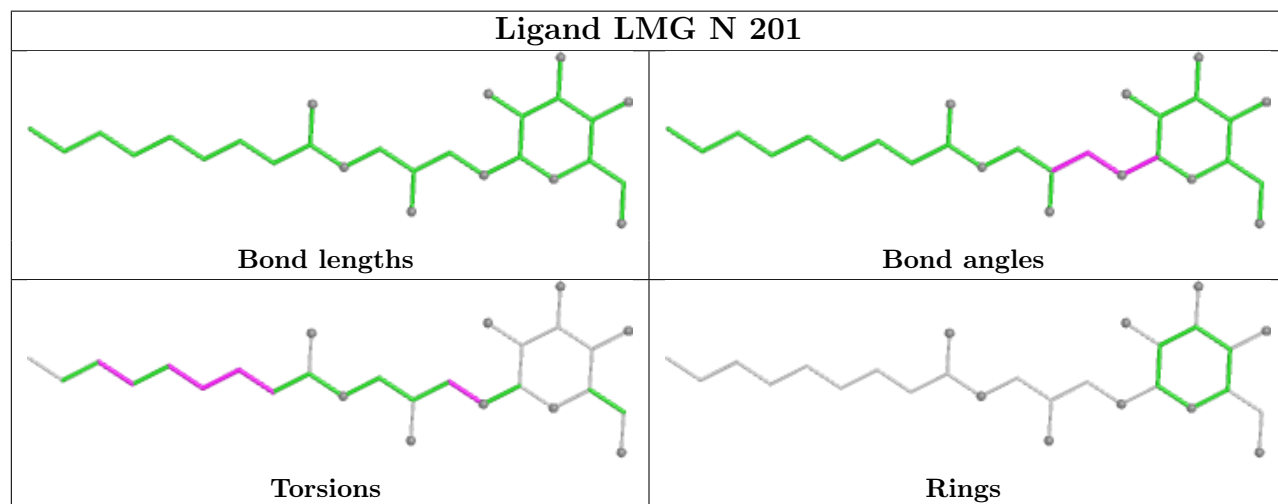
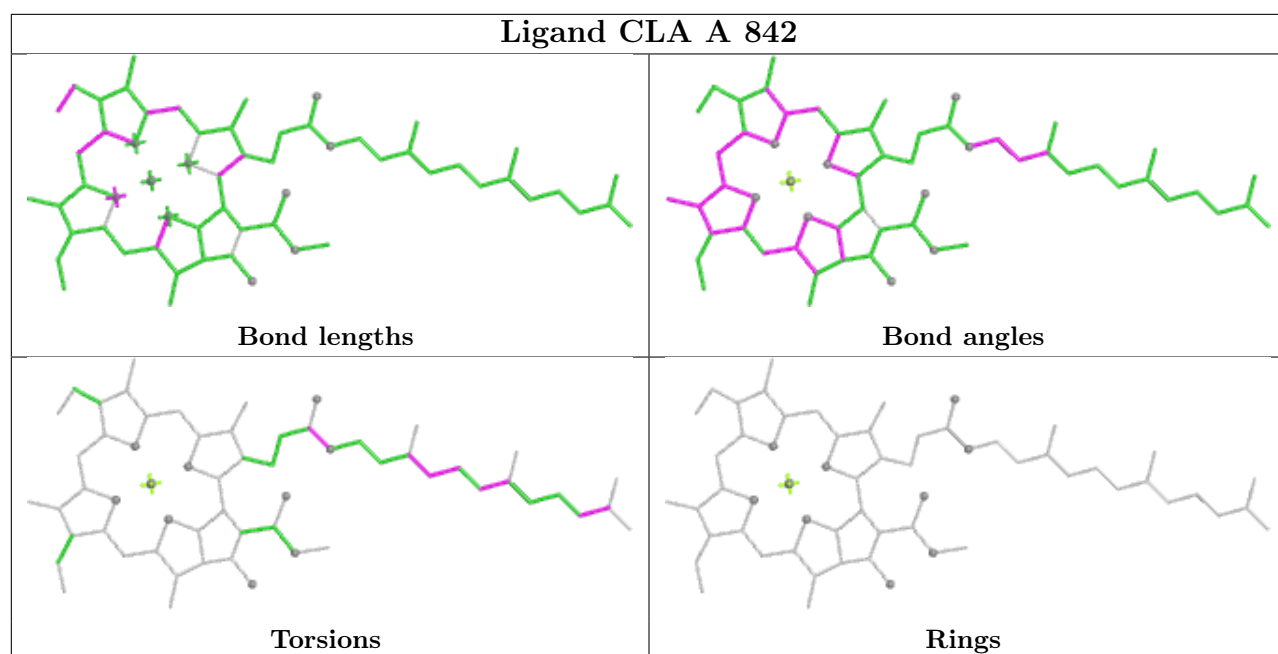
Rings

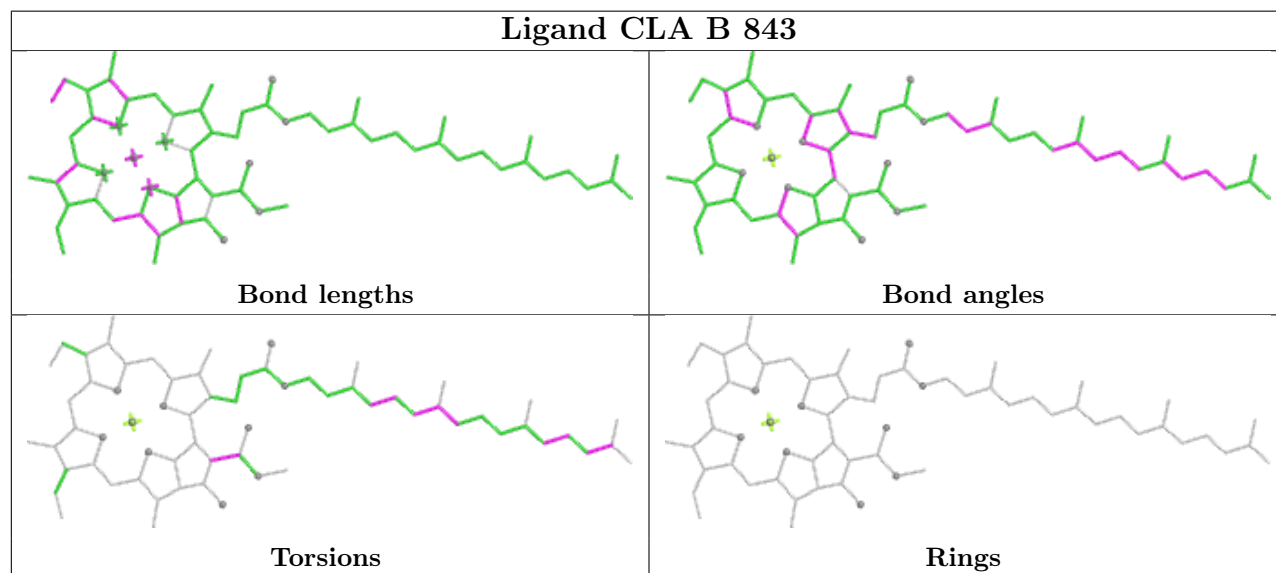
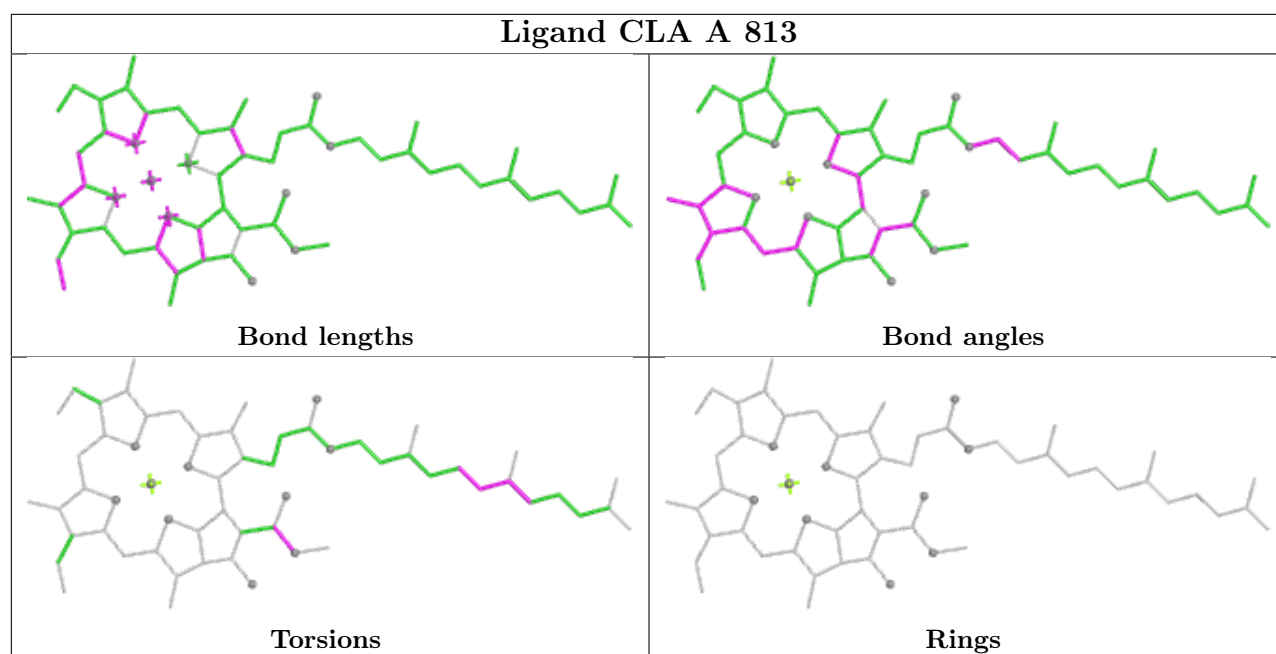
## Ligand CLA 1 605

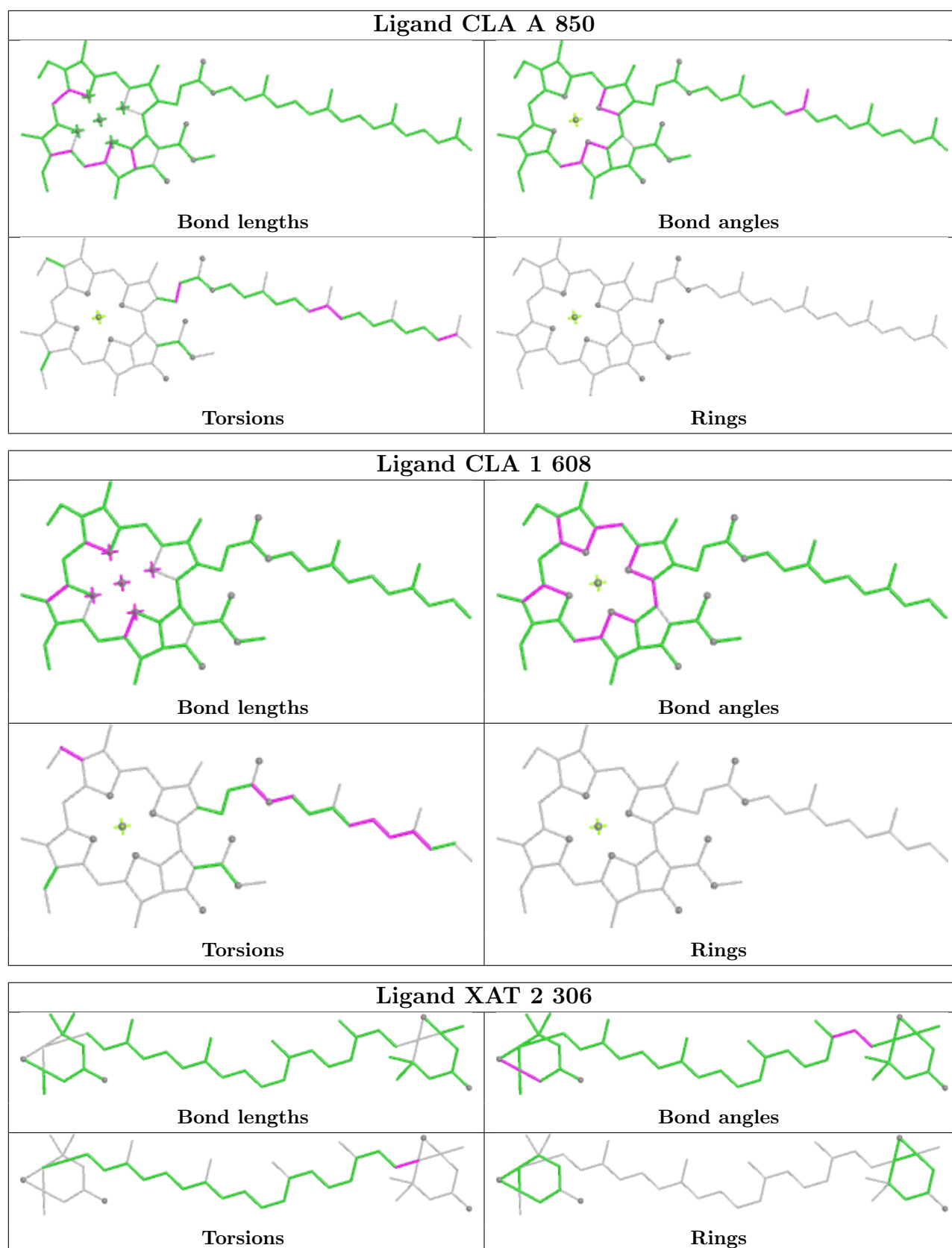


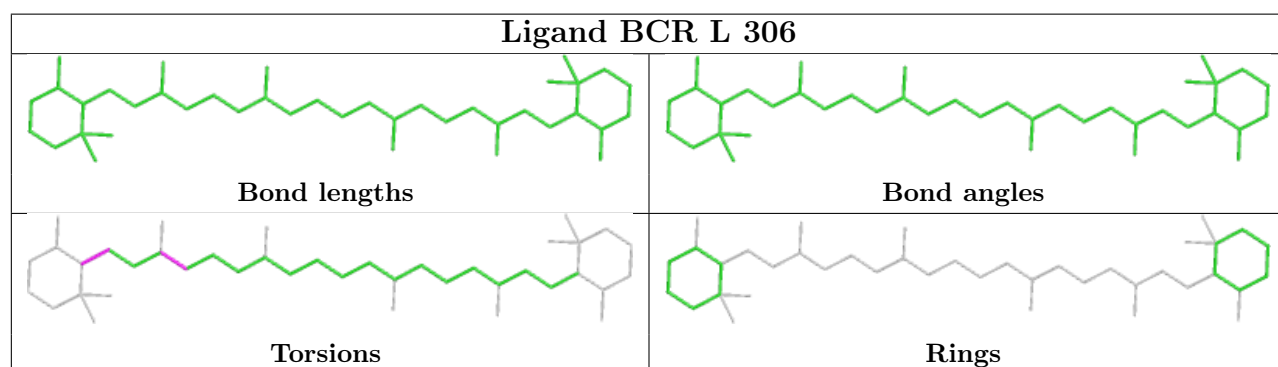
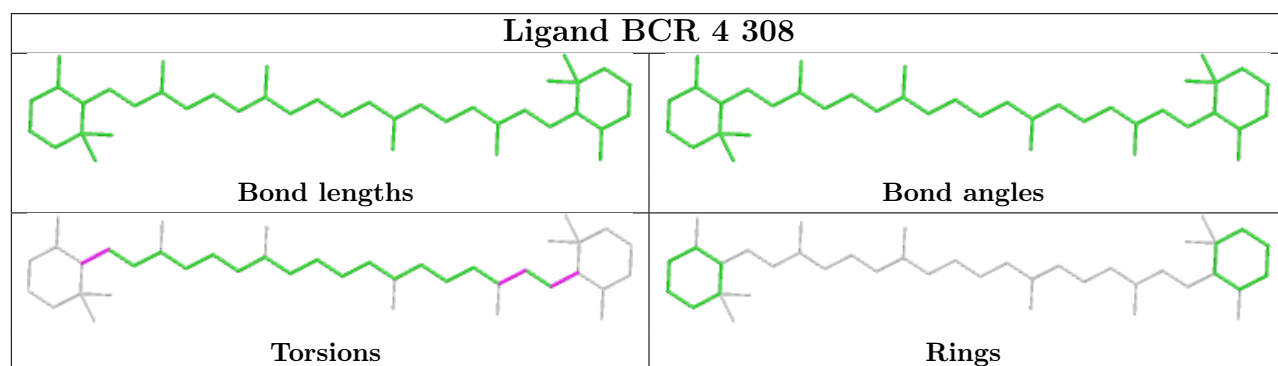
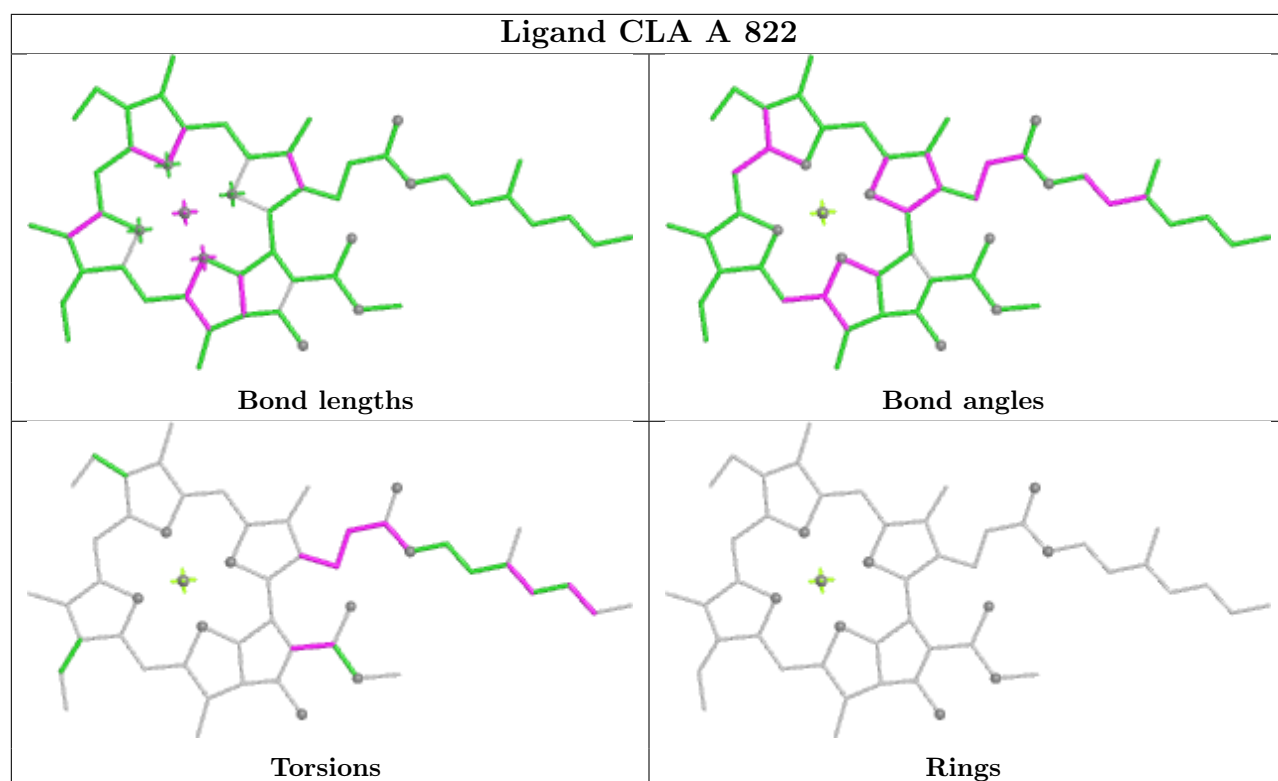


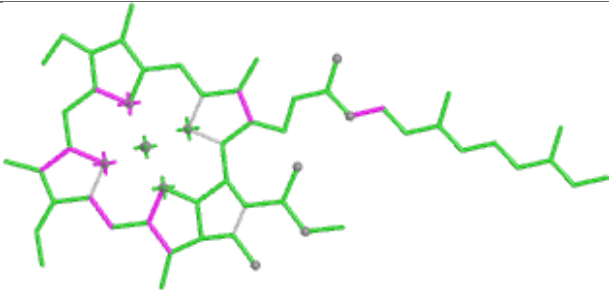
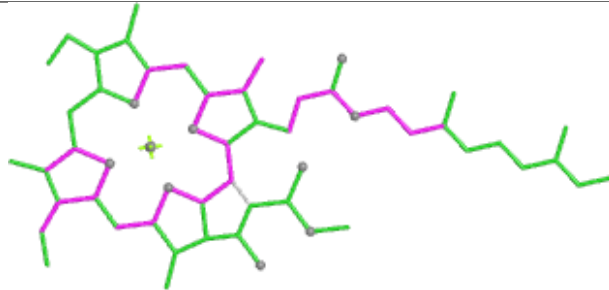
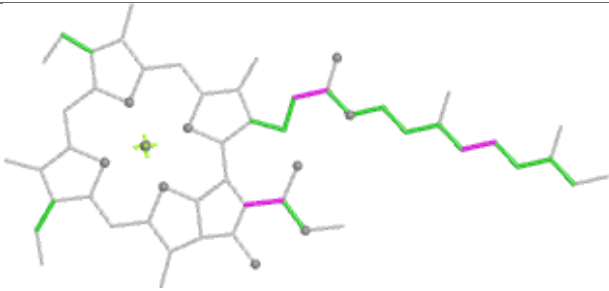
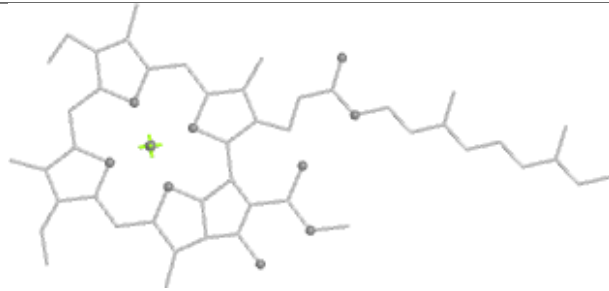


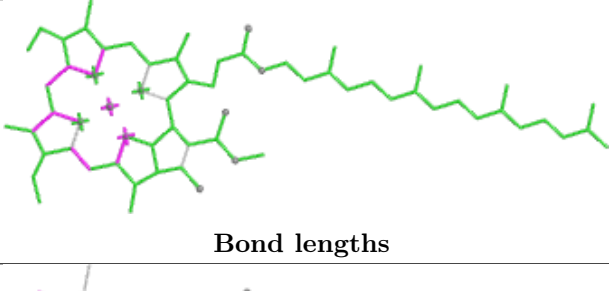
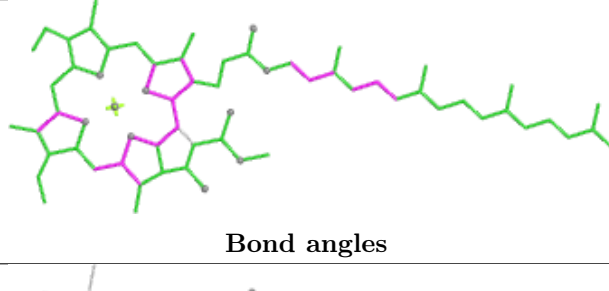
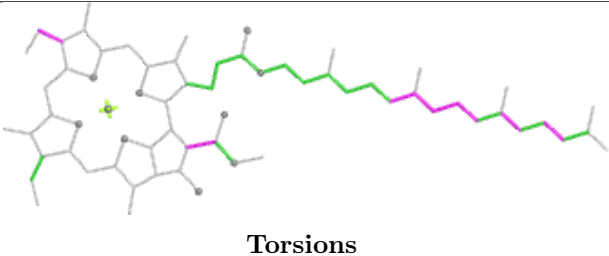
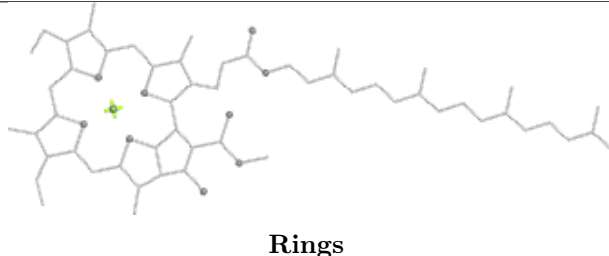


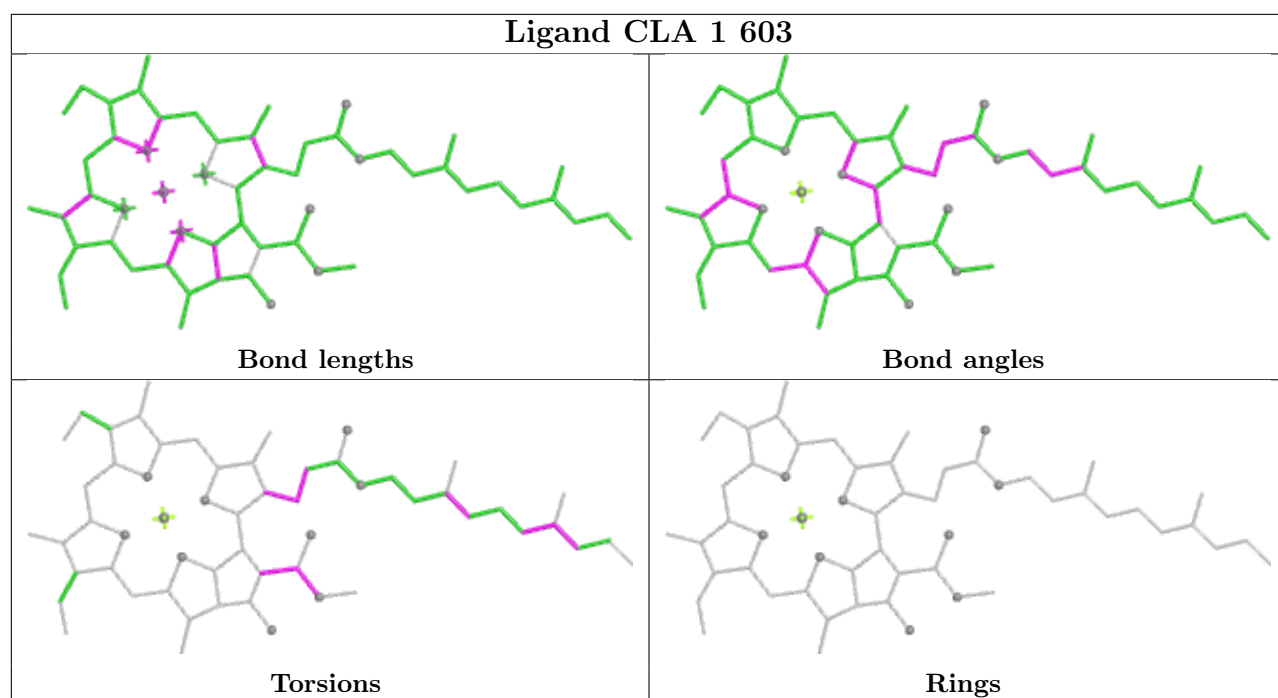




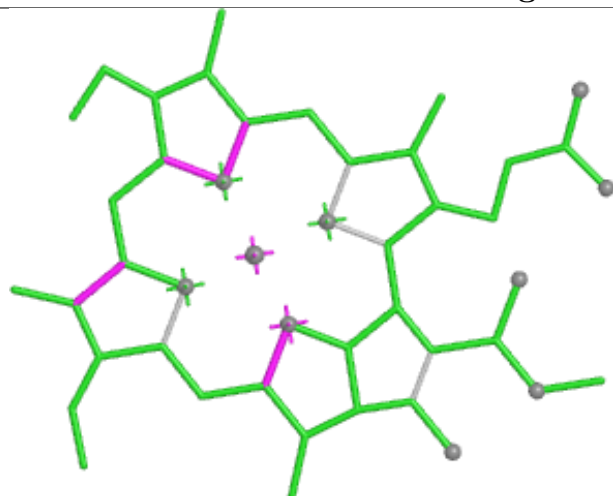


Ligand CLA B 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

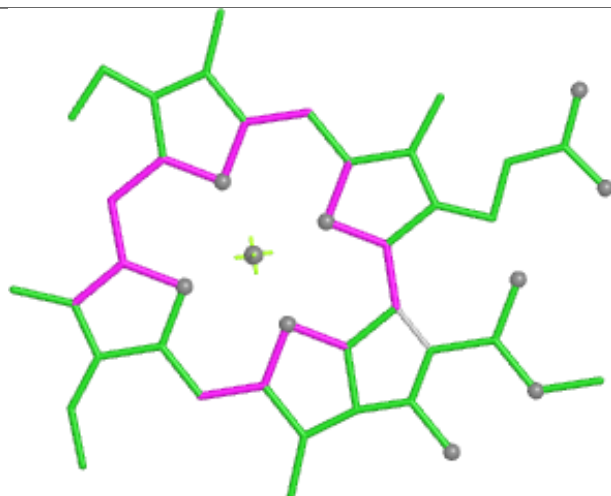
Ligand CLA A 840	
	
Bond lengths	Bond angles
	
Torsions	Rings



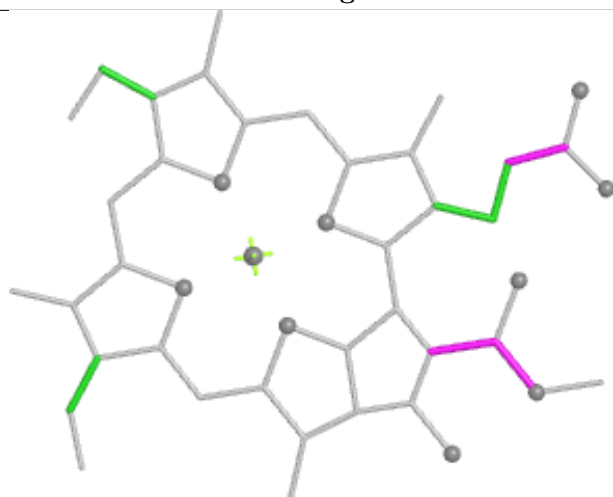
## Ligand CLA 4 307



Bond lengths



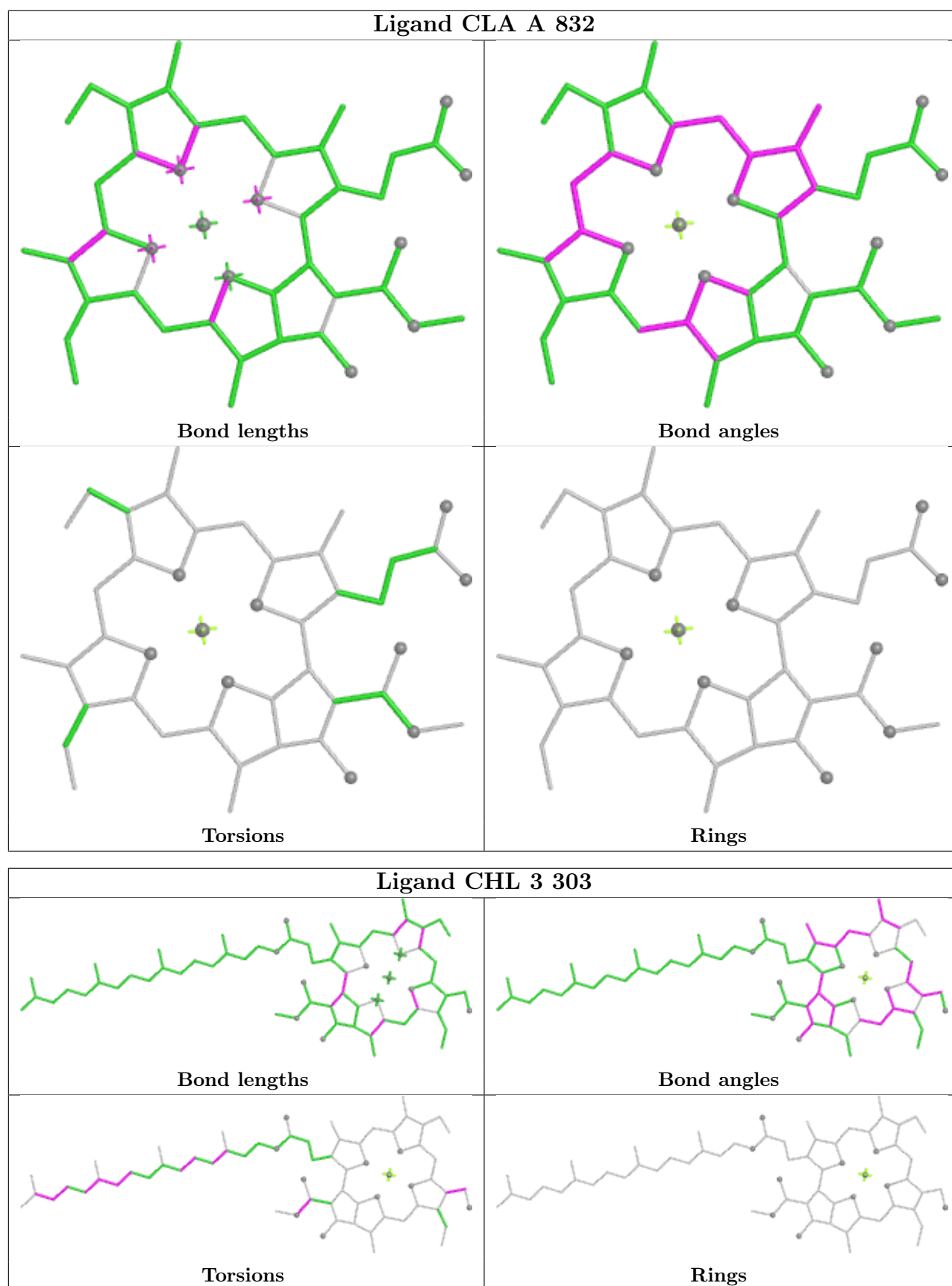
Bond angles



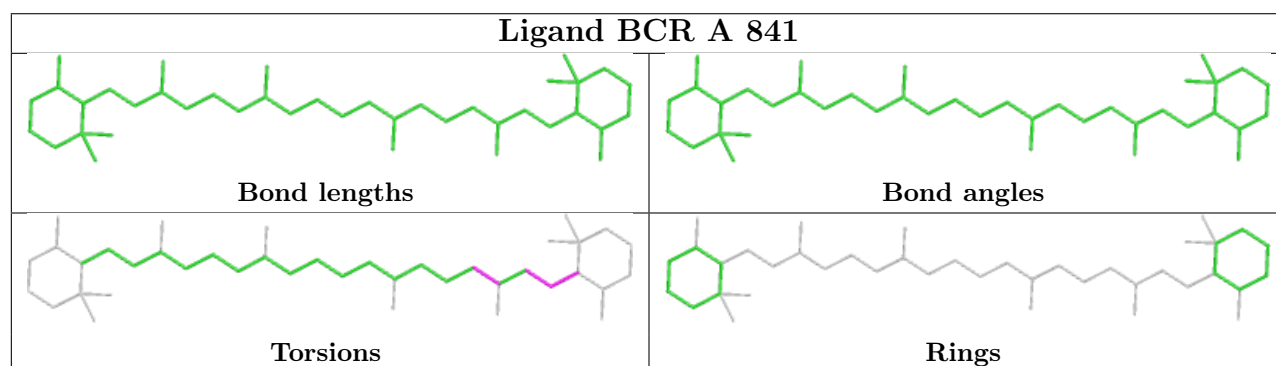
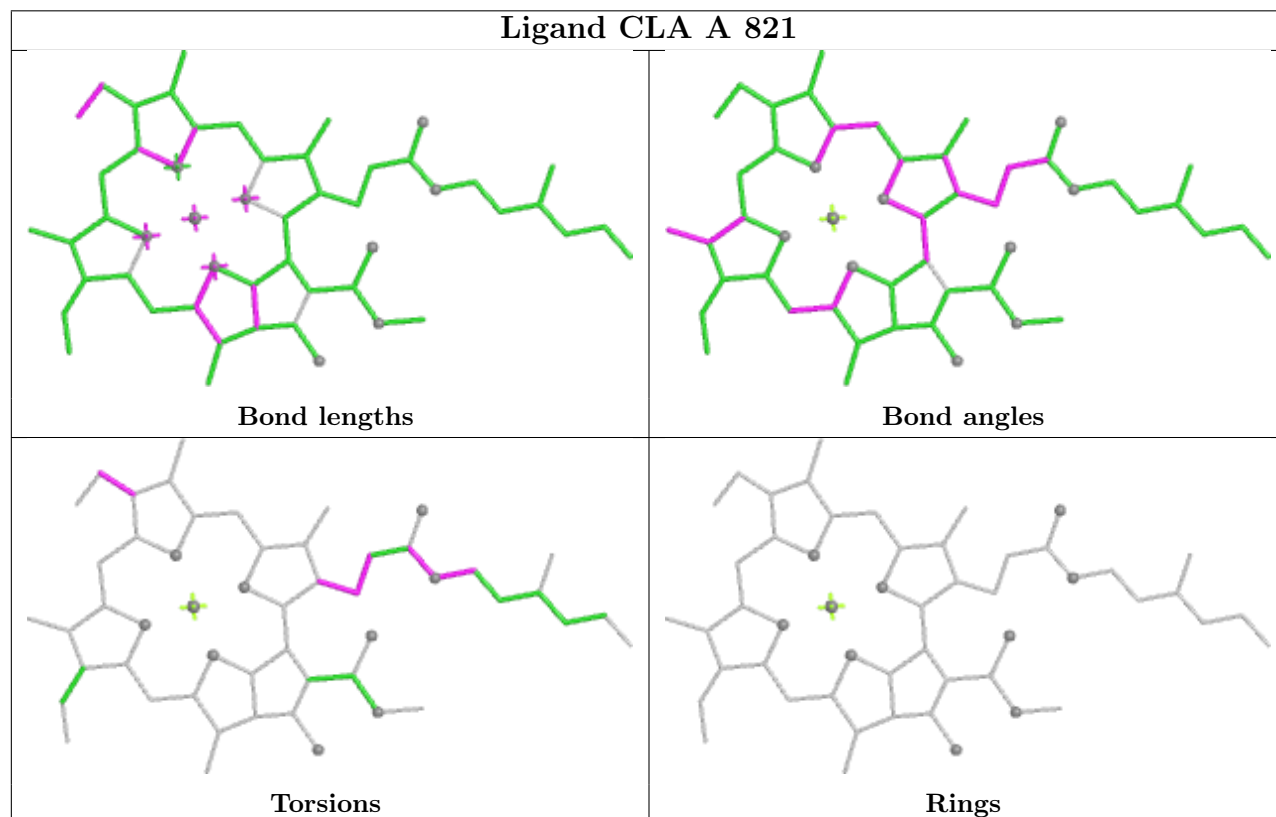
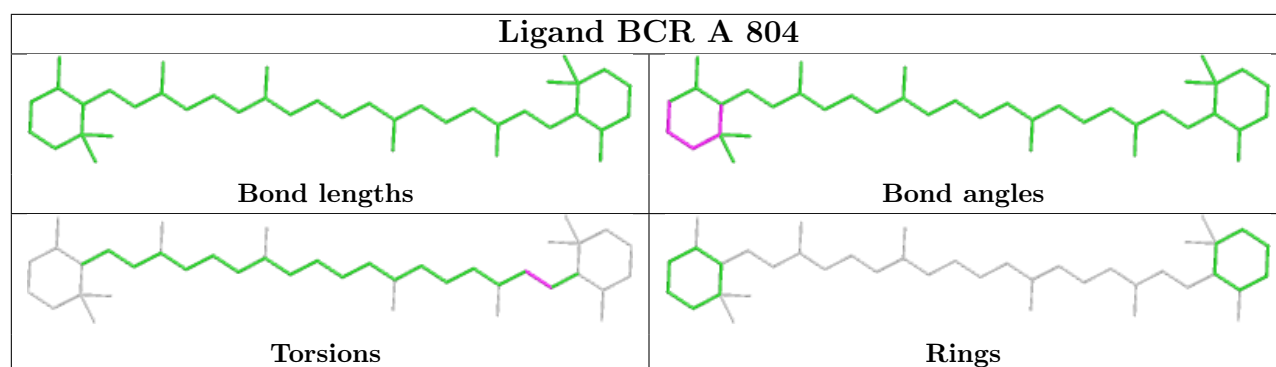
Torsions



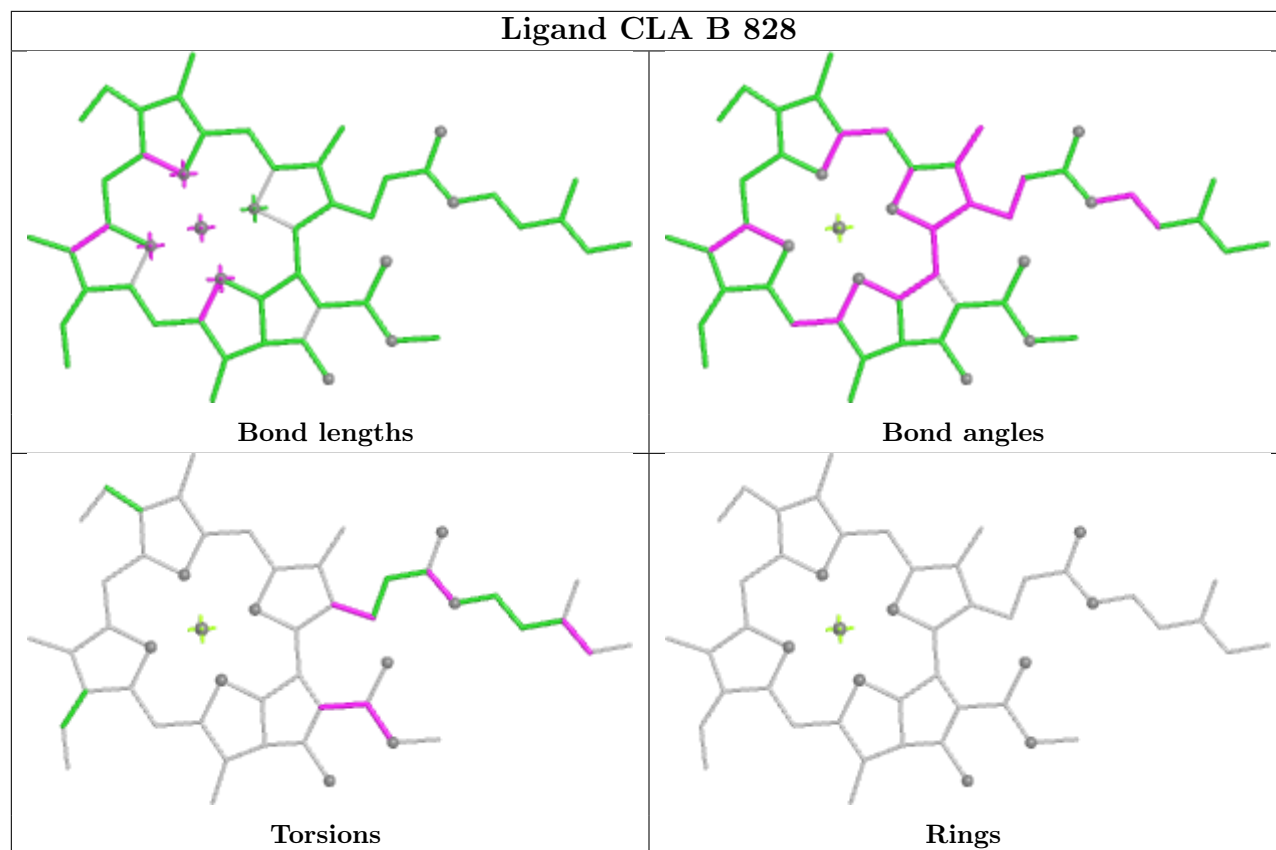
Rings



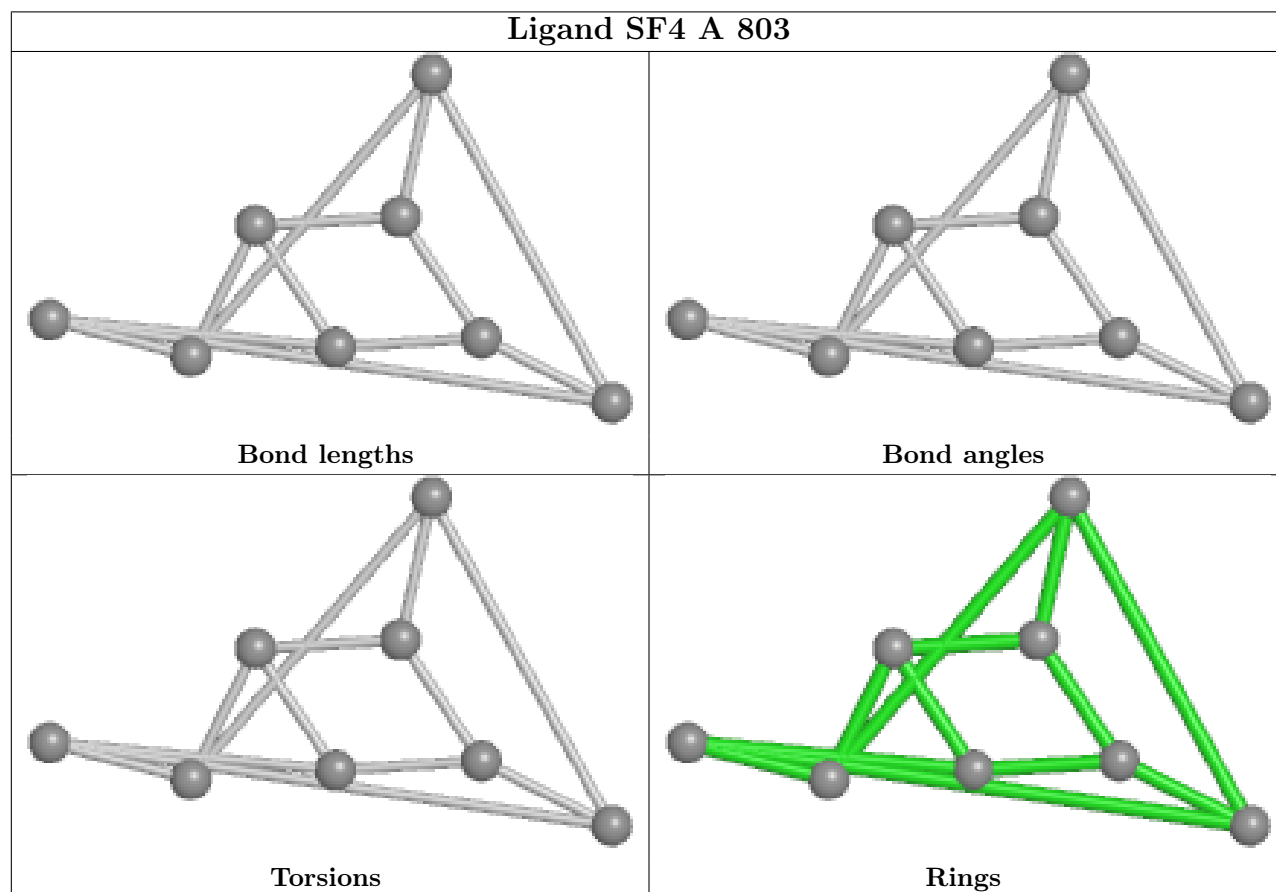


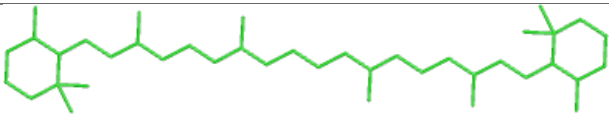
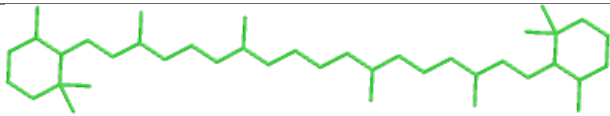
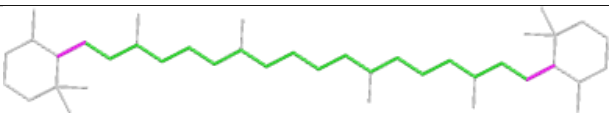
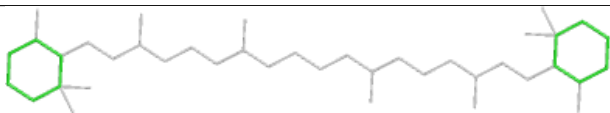


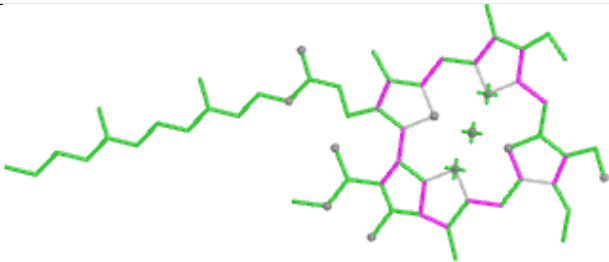
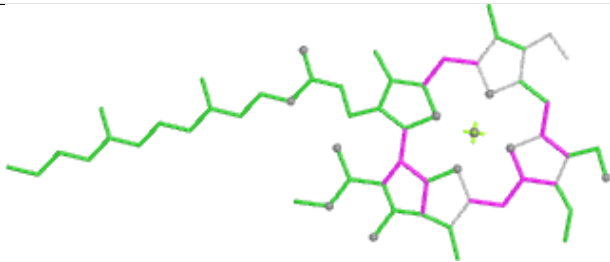
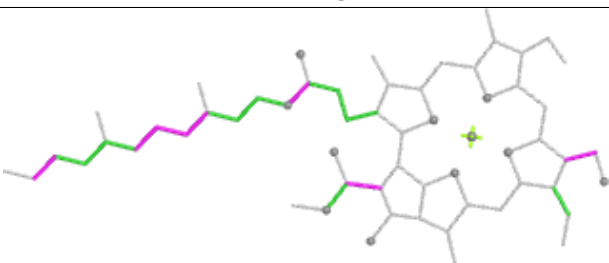
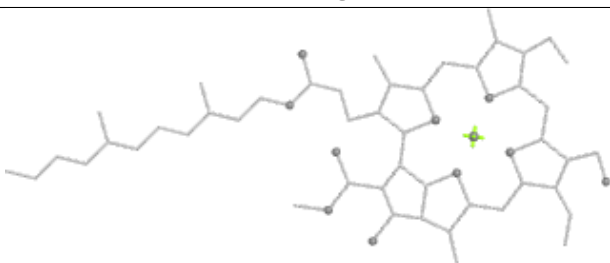
## Ligand CLA B 828

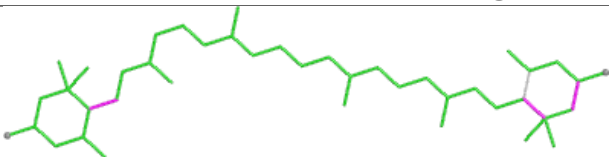
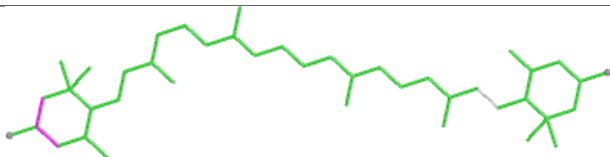
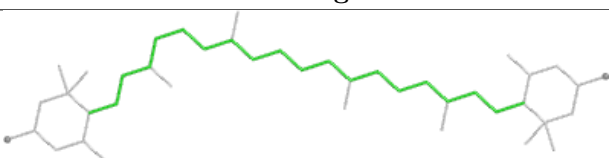
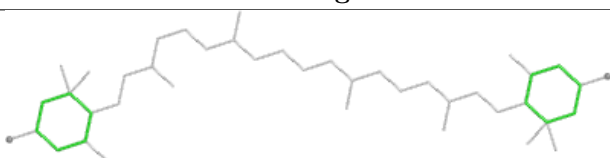


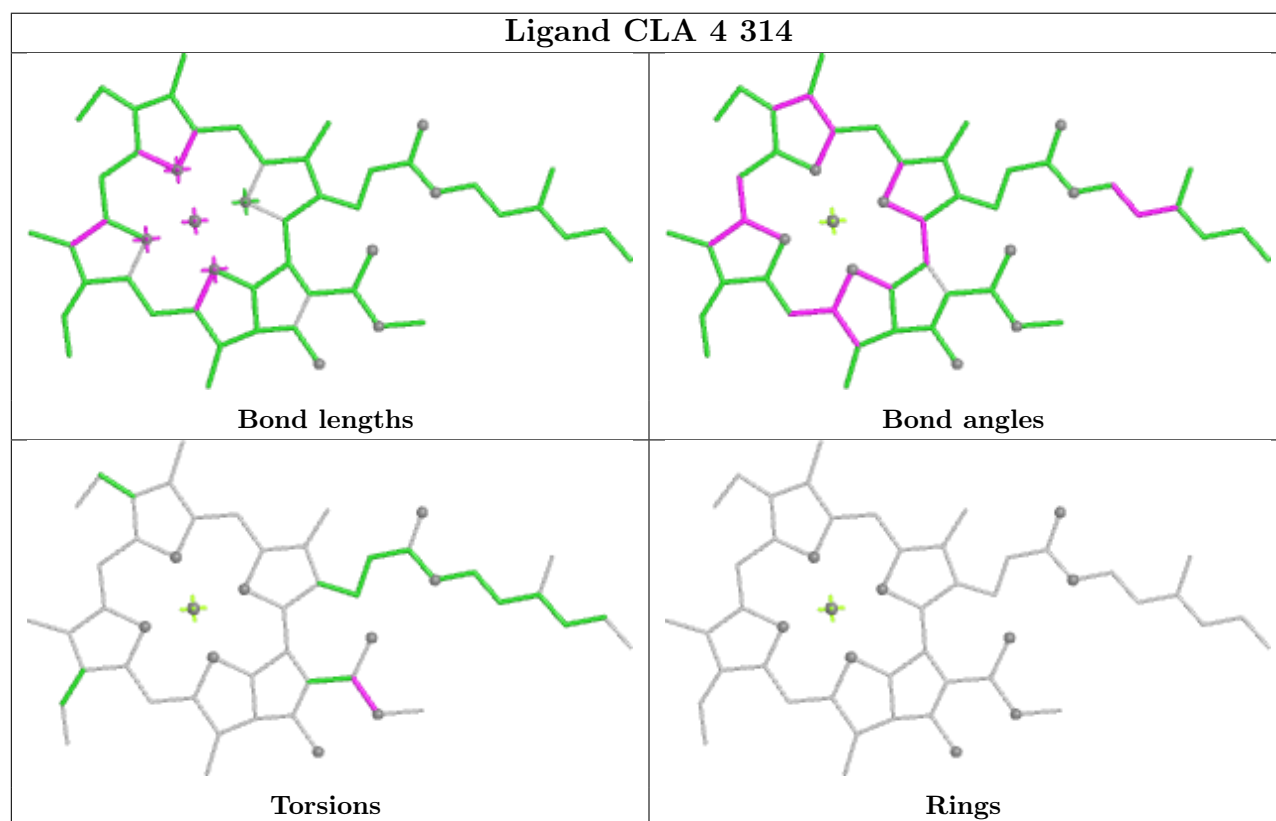
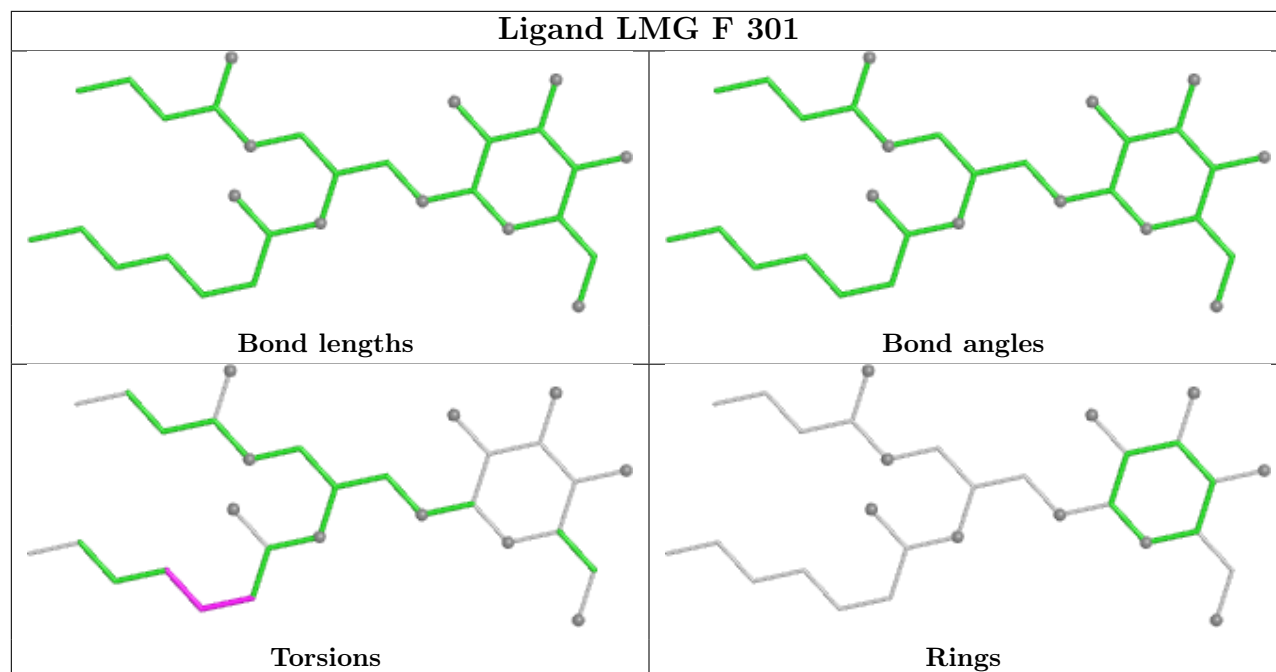
## Ligand SF4 A 803

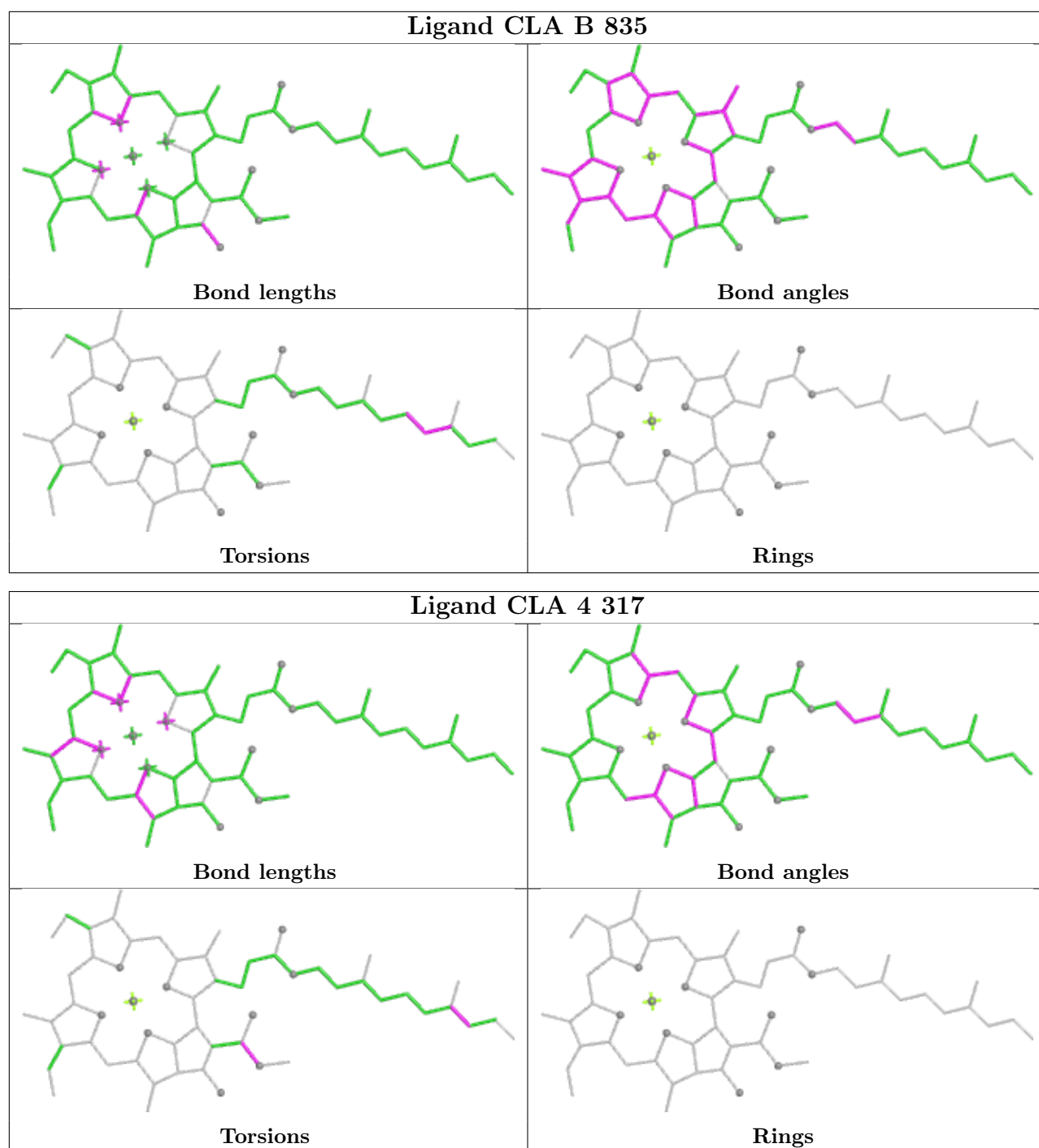


Ligand BCR K 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

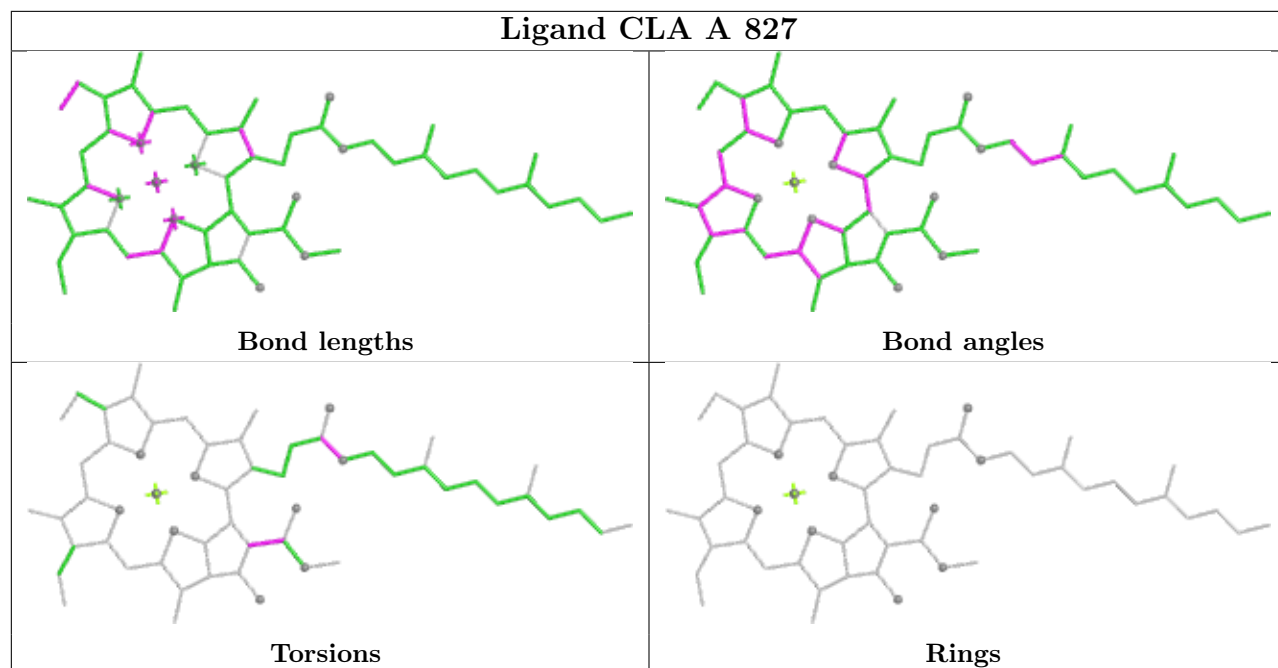
Ligand CHL 2 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand A1LXP 4 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

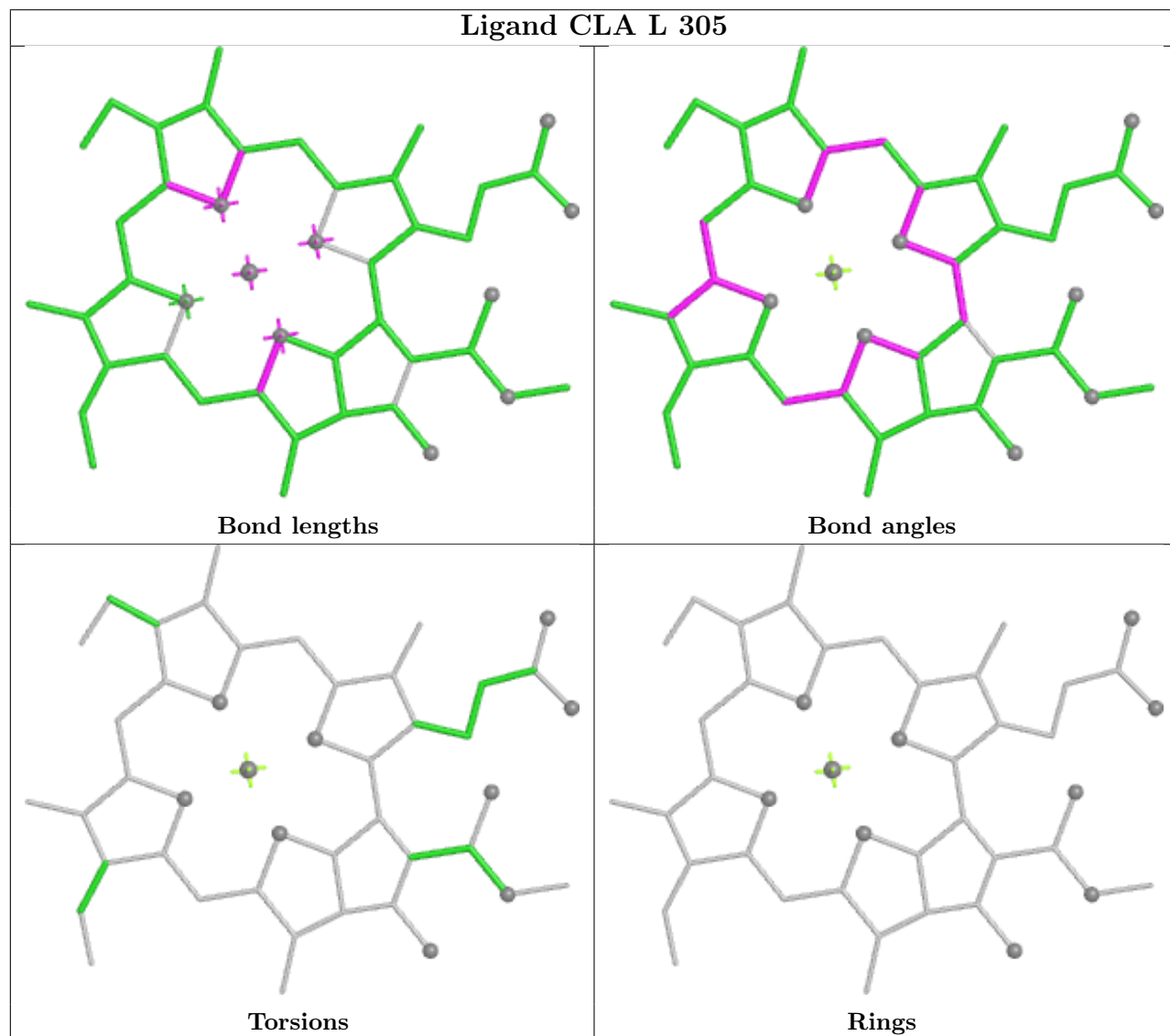




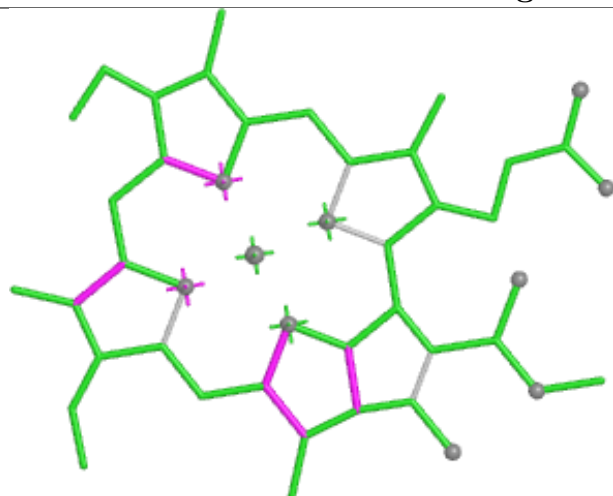
## Ligand CLA A 827



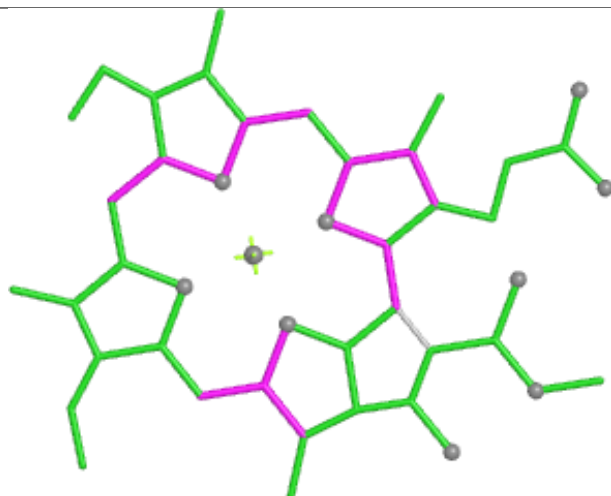
## Ligand CLA L 305



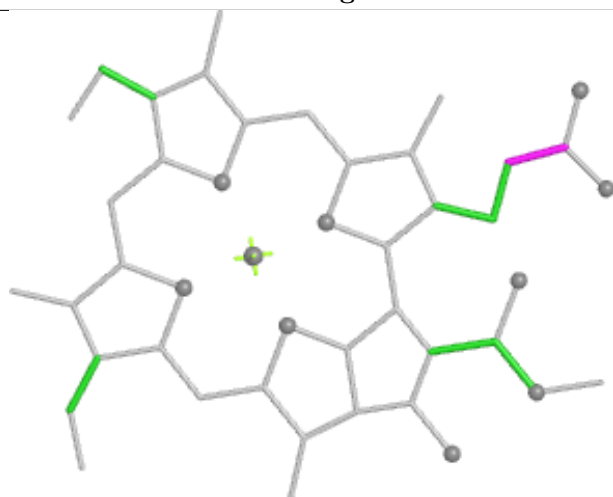
## Ligand CLA L 303



Bond lengths



Bond angles

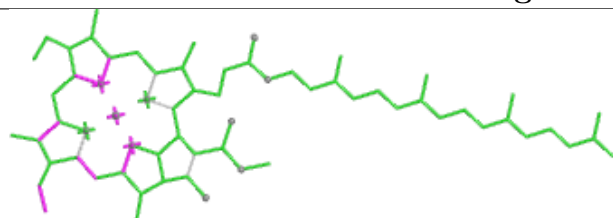


Torsions

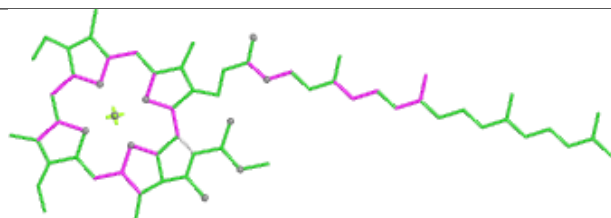


Rings

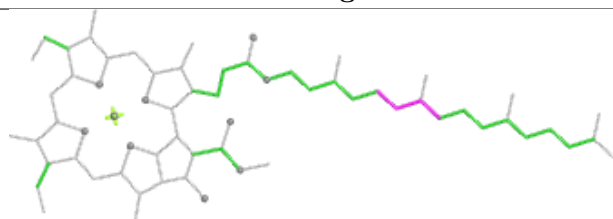
## Ligand CLA B 845



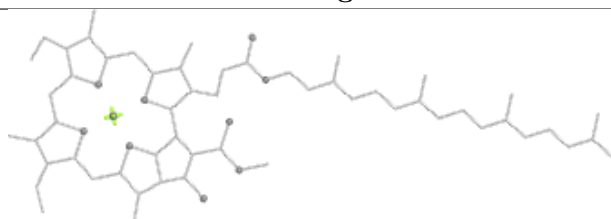
Bond lengths



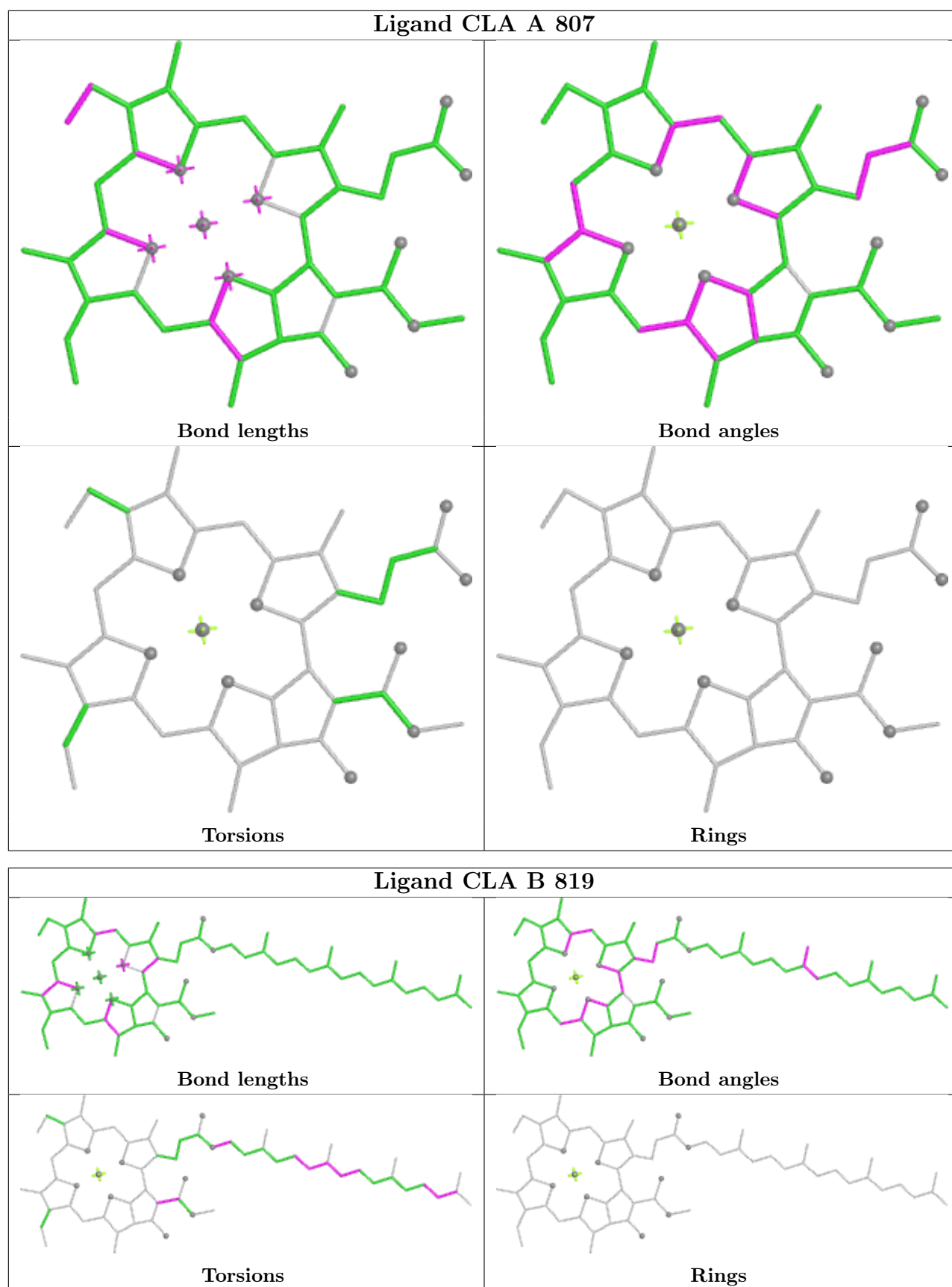
Bond angles



Torsions

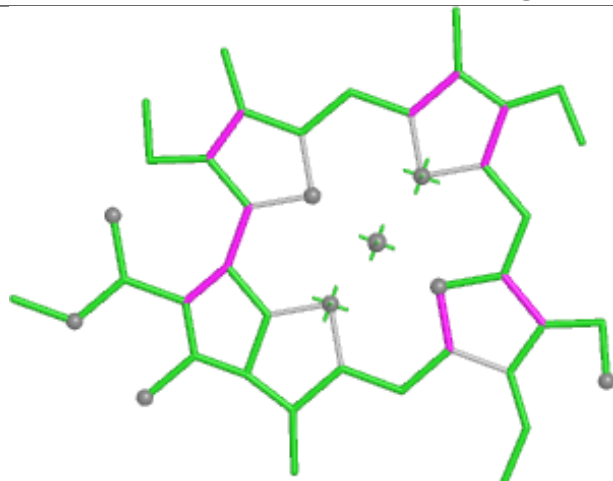


Rings

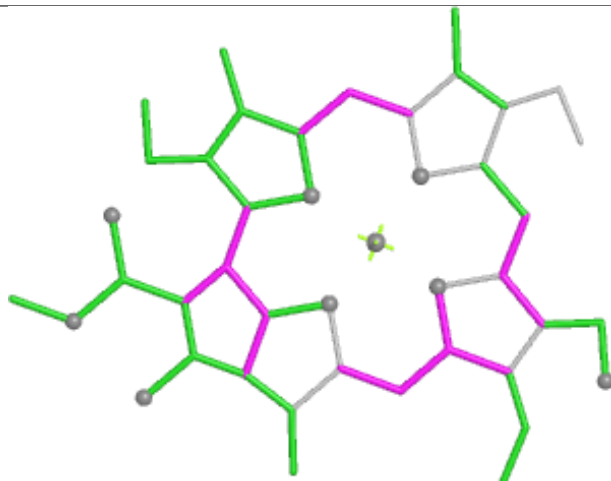




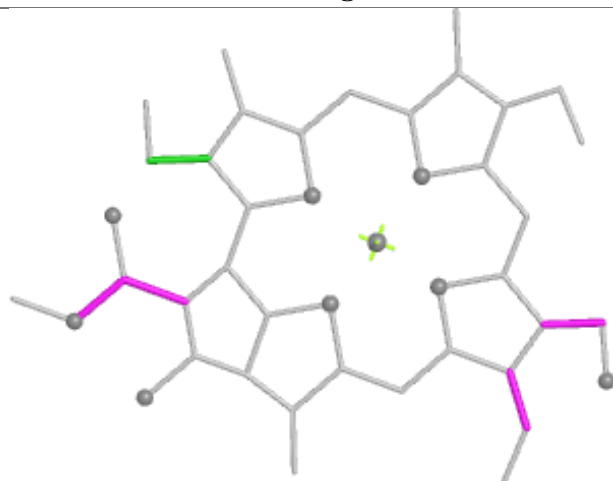
## Ligand CHL 1 606



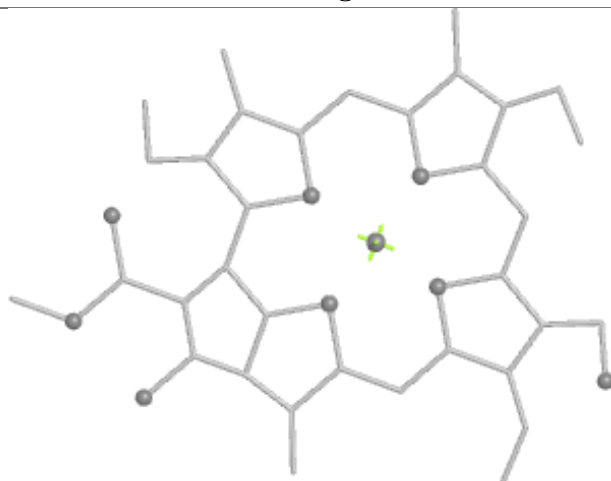
Bond lengths



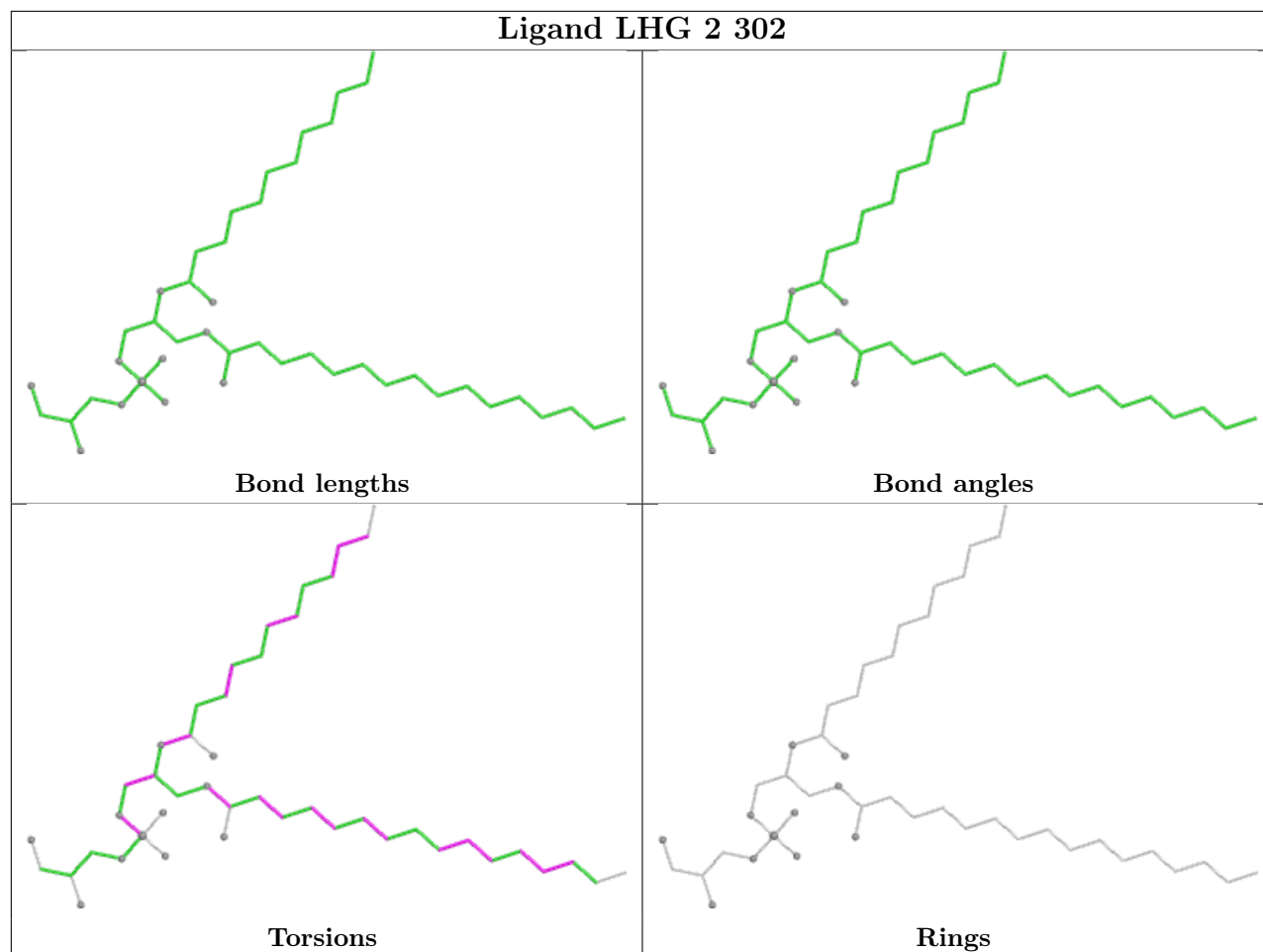
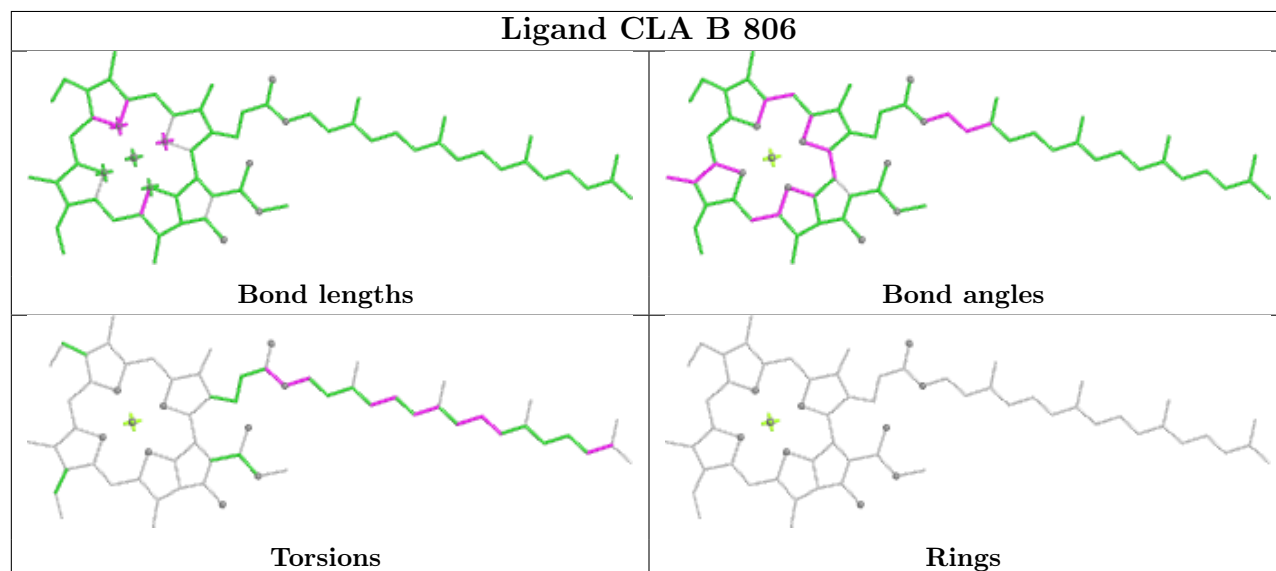
Bond angles



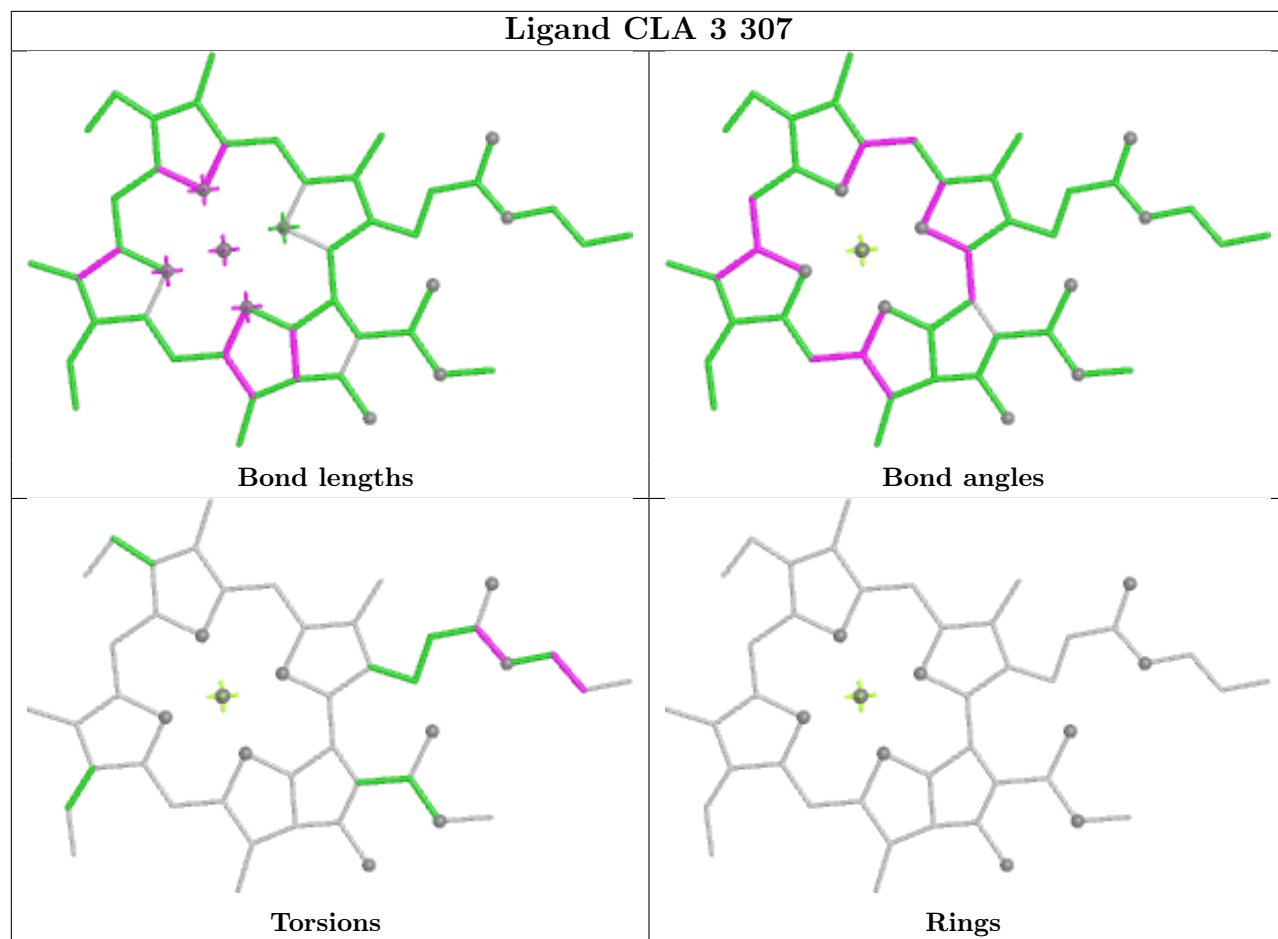
Torsions

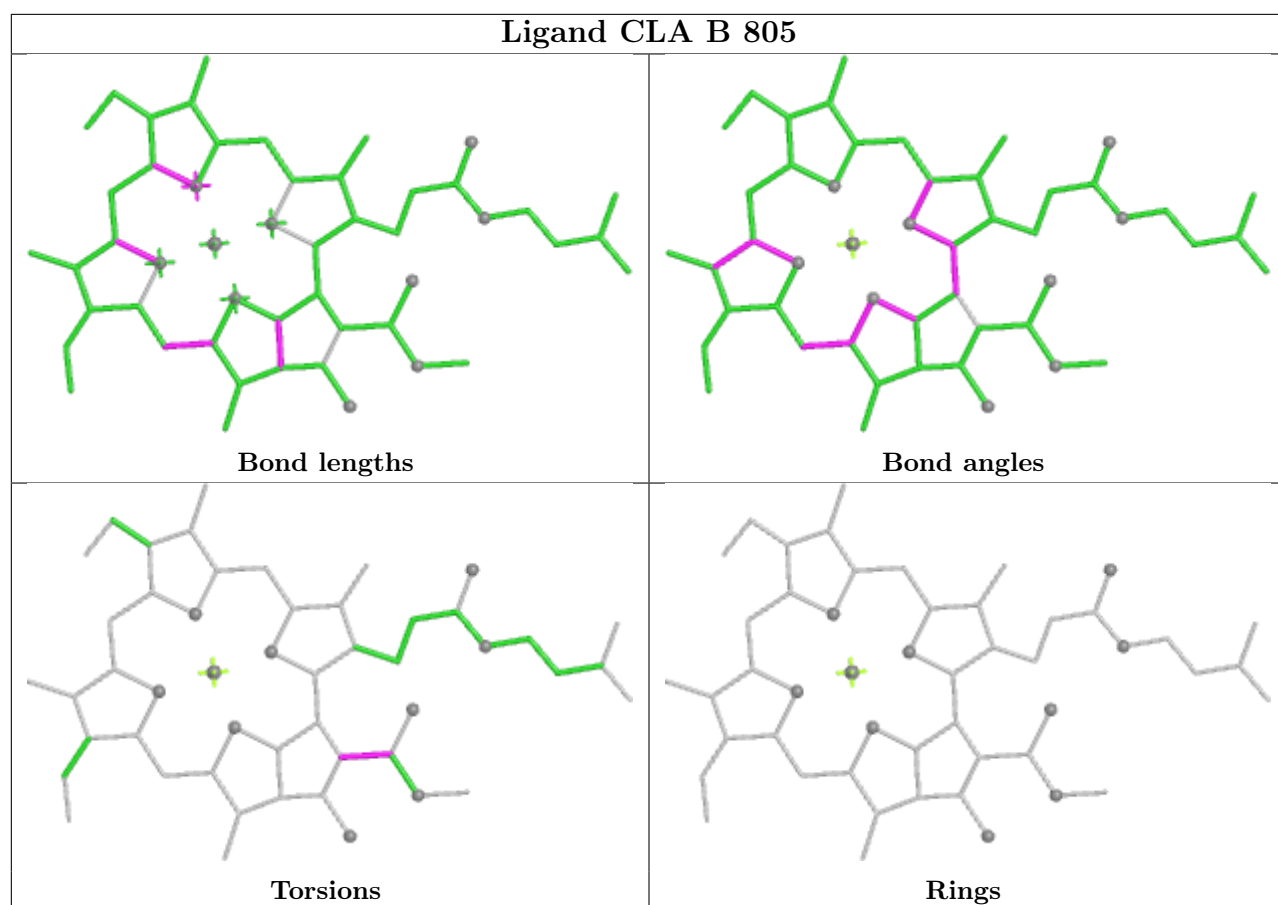


Rings

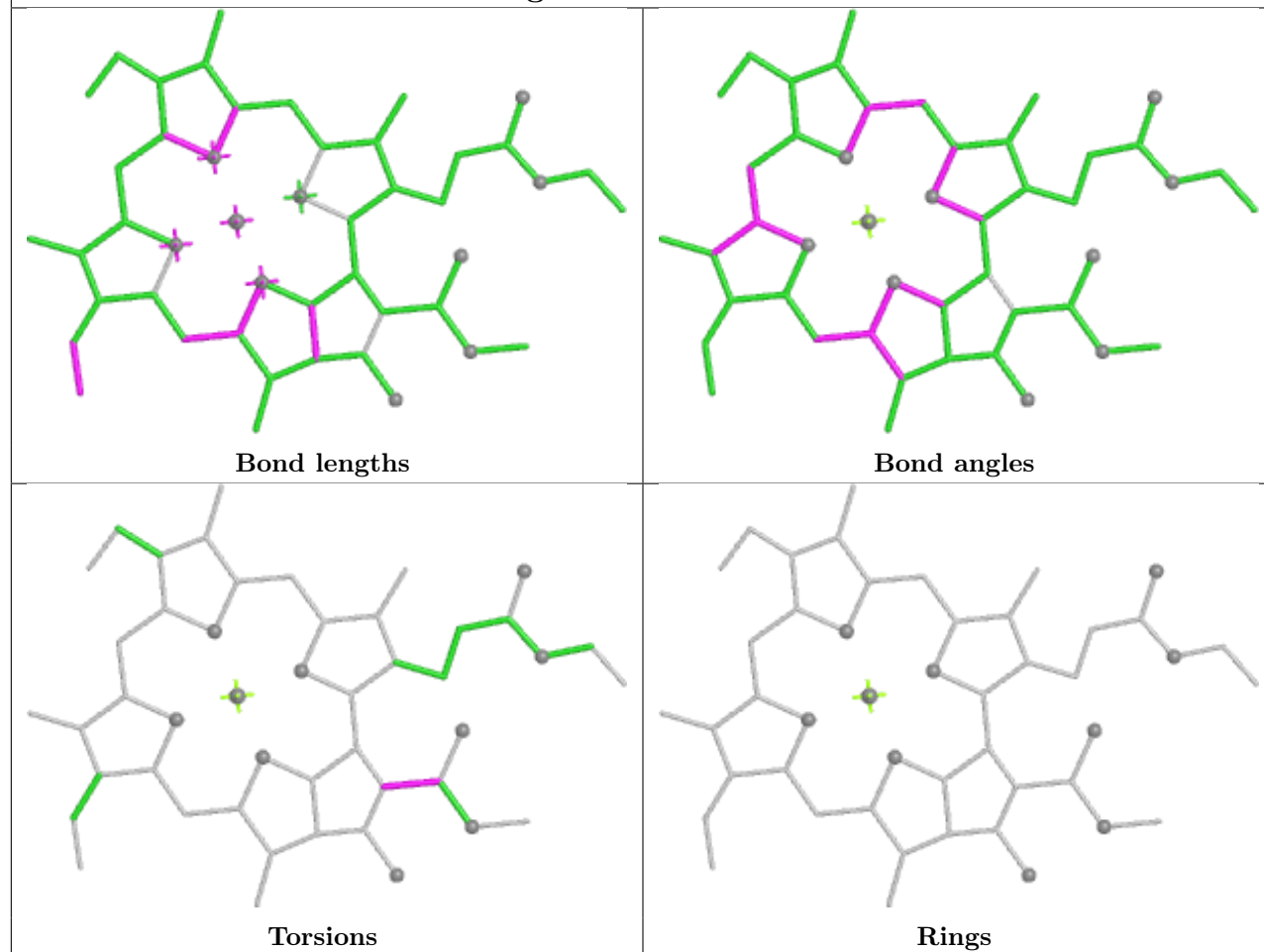
**Ligand LHG 2 302****Ligand CLA B 806**

## Ligand CLA 3 307

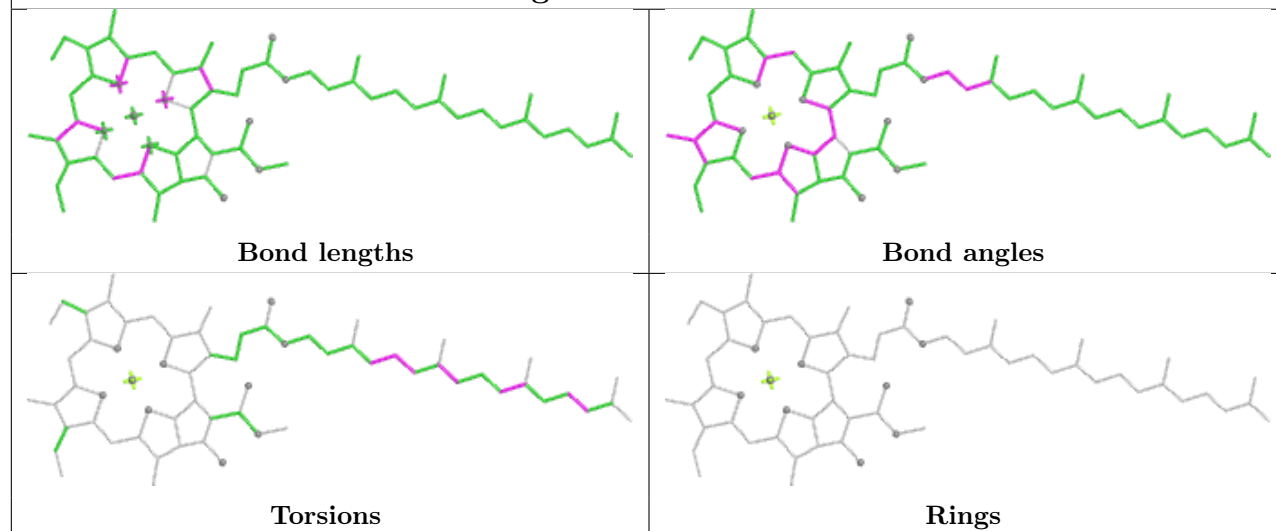




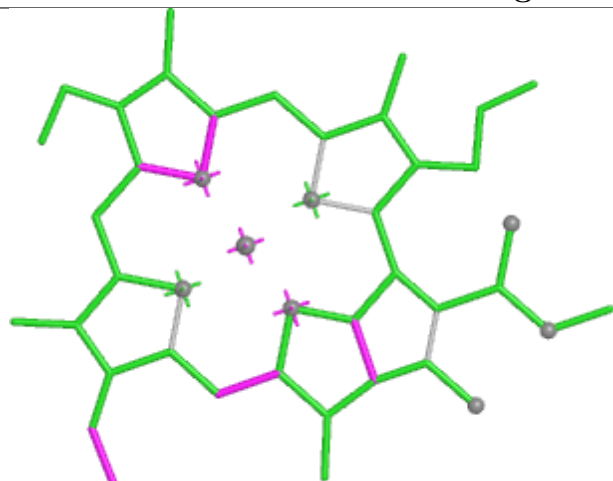
## Ligand CLA A 805



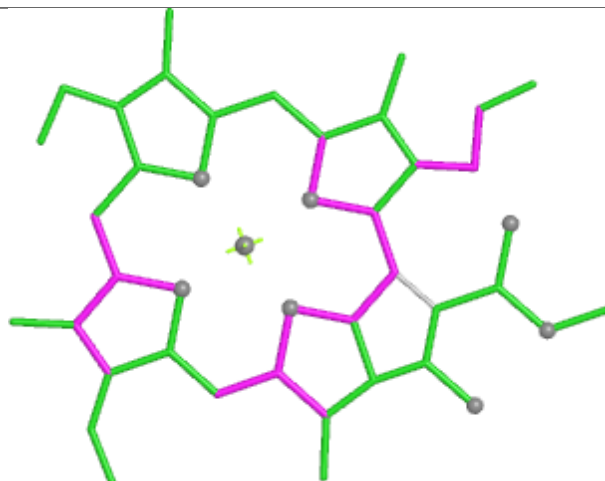
## Ligand CLA A 829



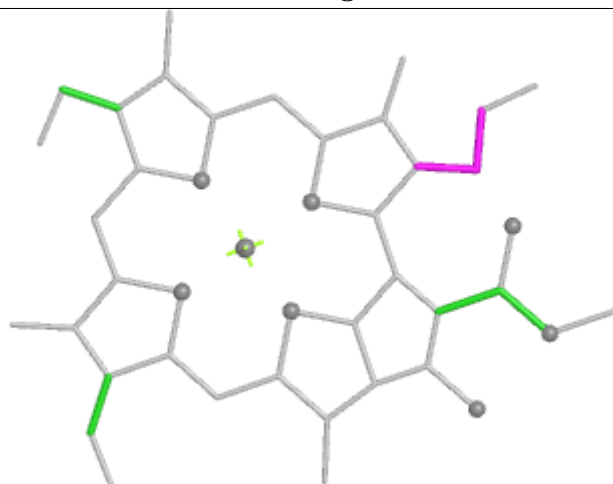
## Ligand CLA B 829



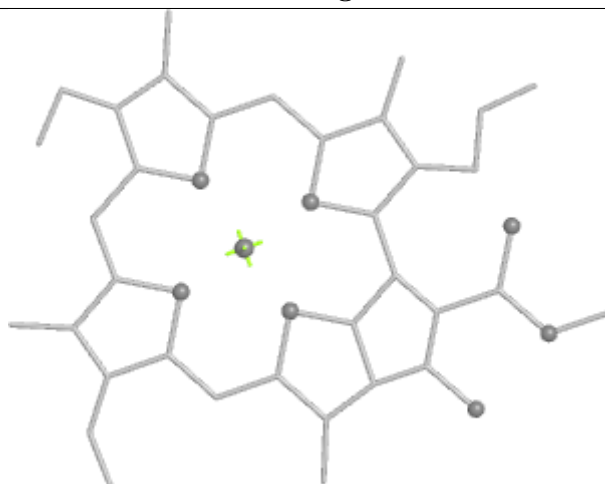
Bond lengths



Bond angles

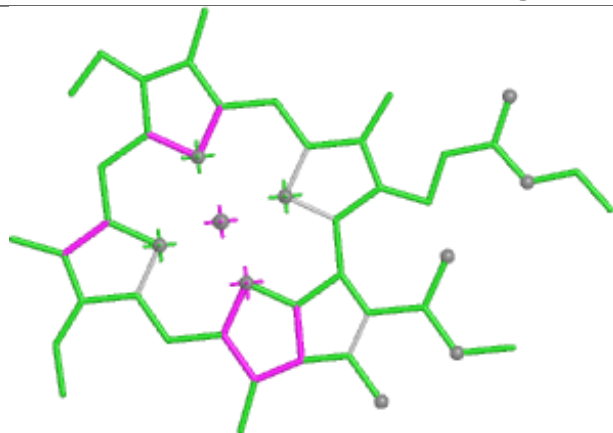


Torsions

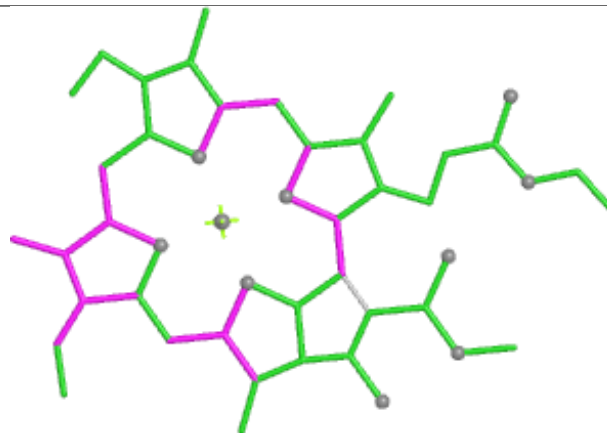


Rings

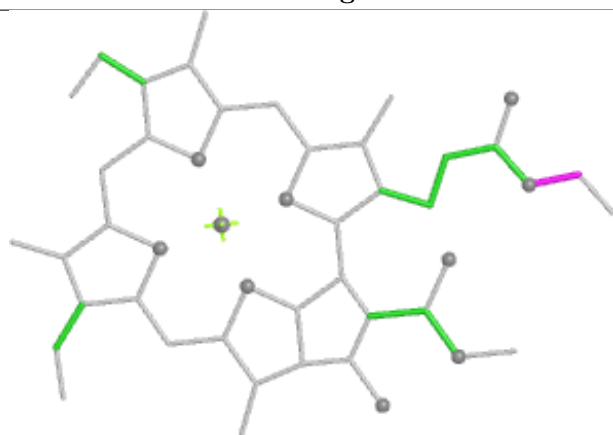
## Ligand CLA B 837



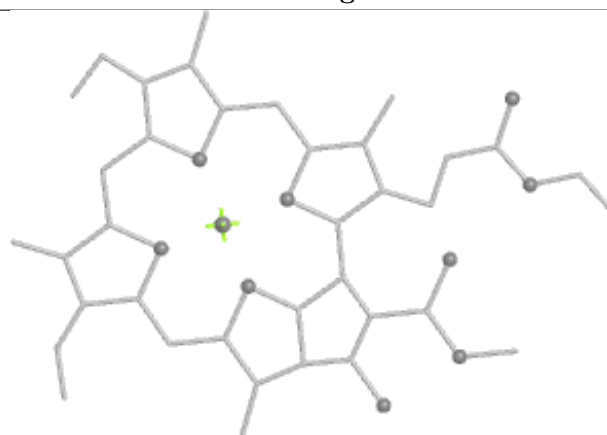
Bond lengths



Bond angles

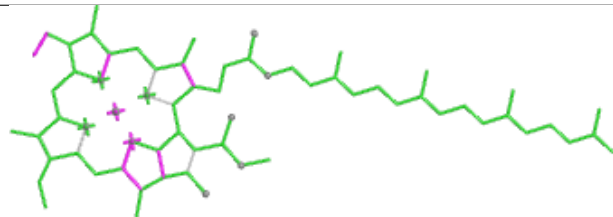


Torsions

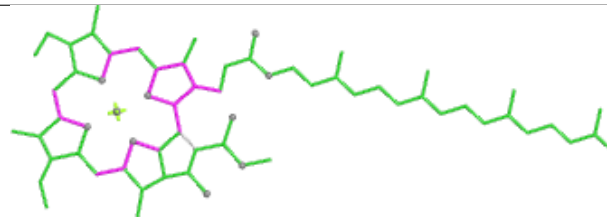


Rings

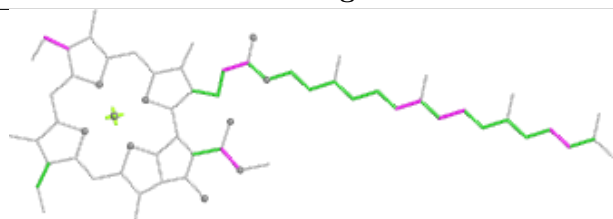
## Ligand CLA B 823



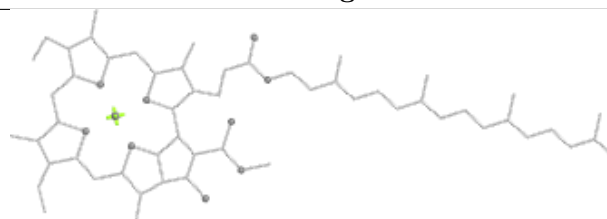
Bond lengths



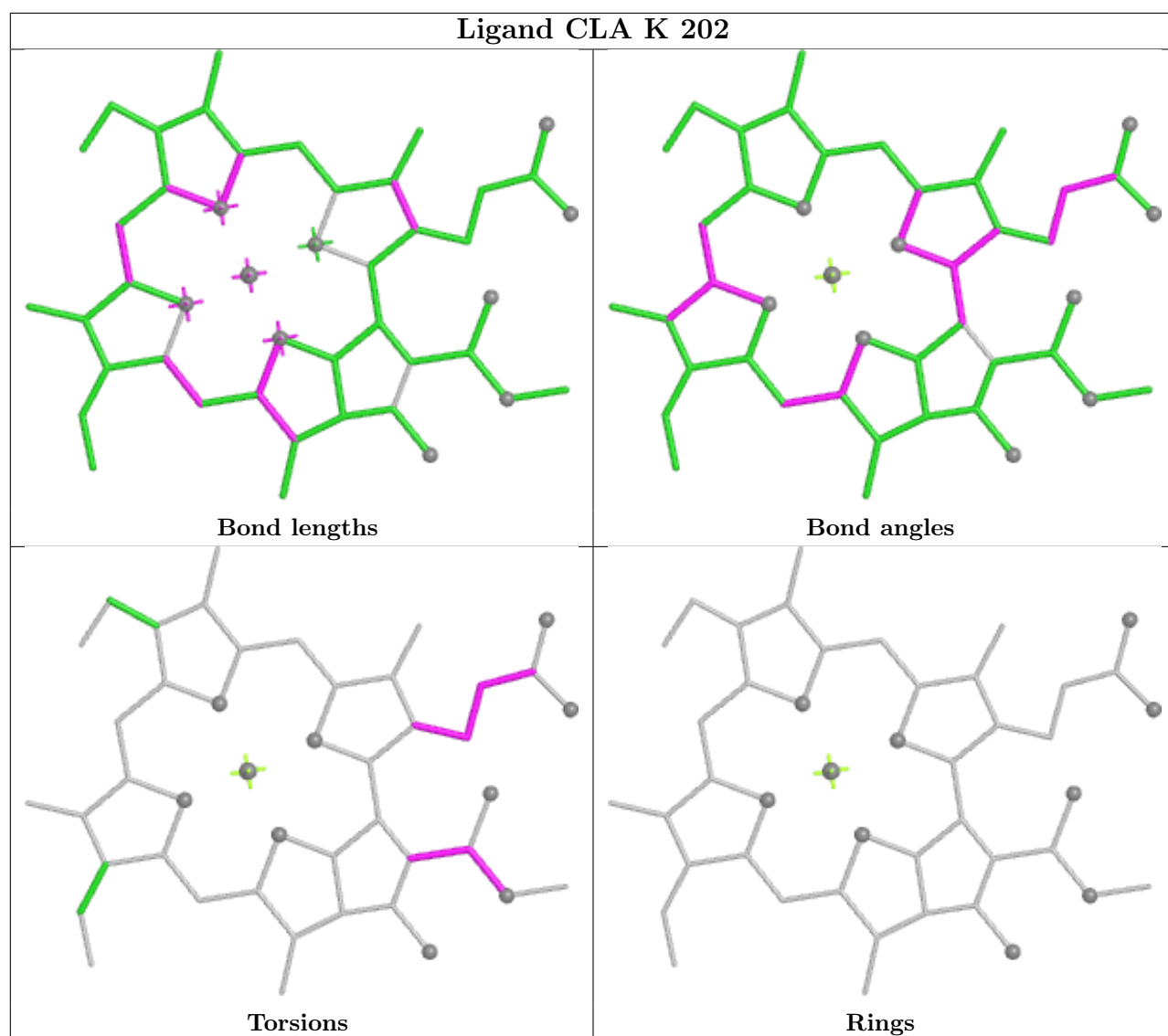
Bond angles



Torsions

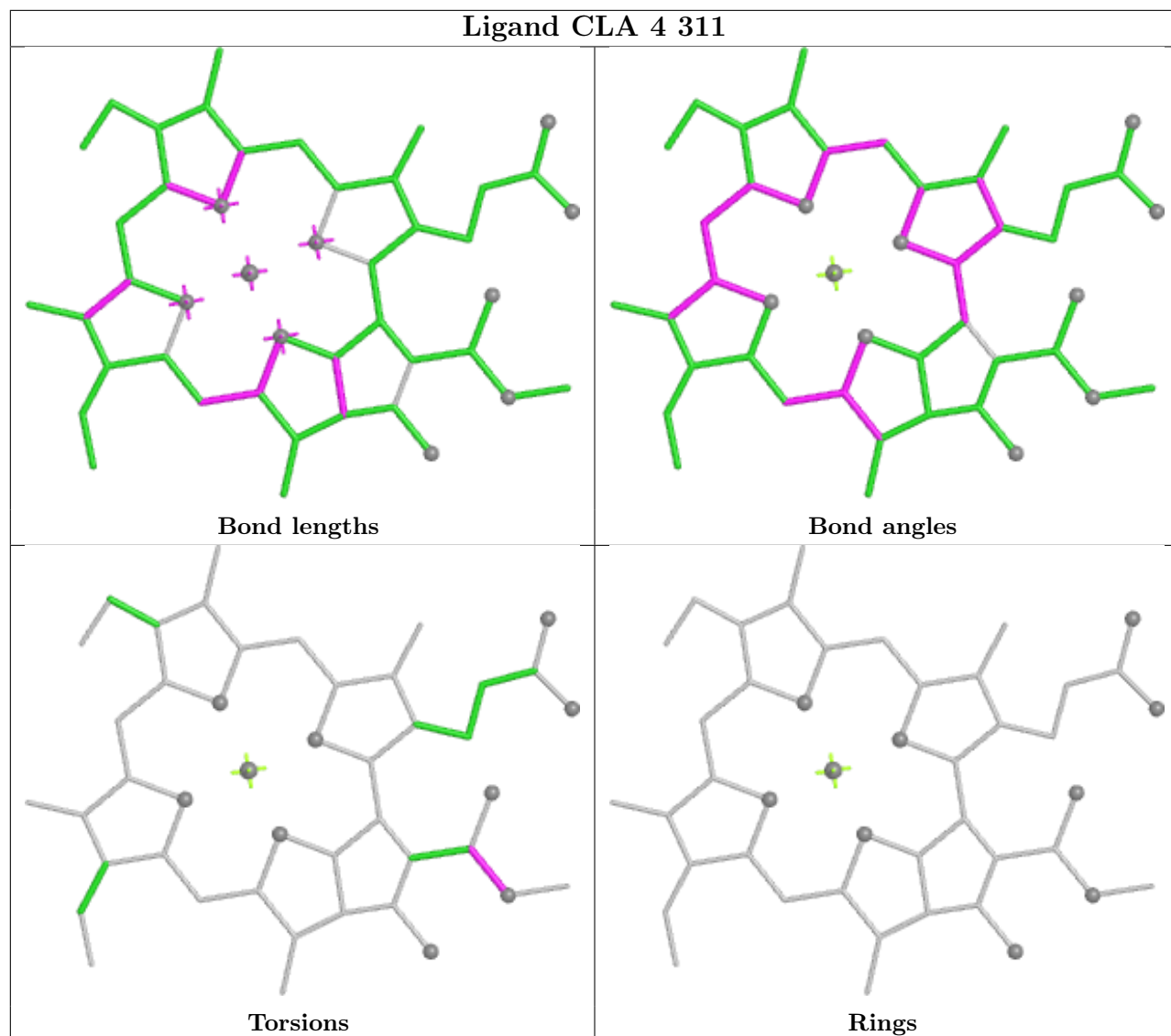


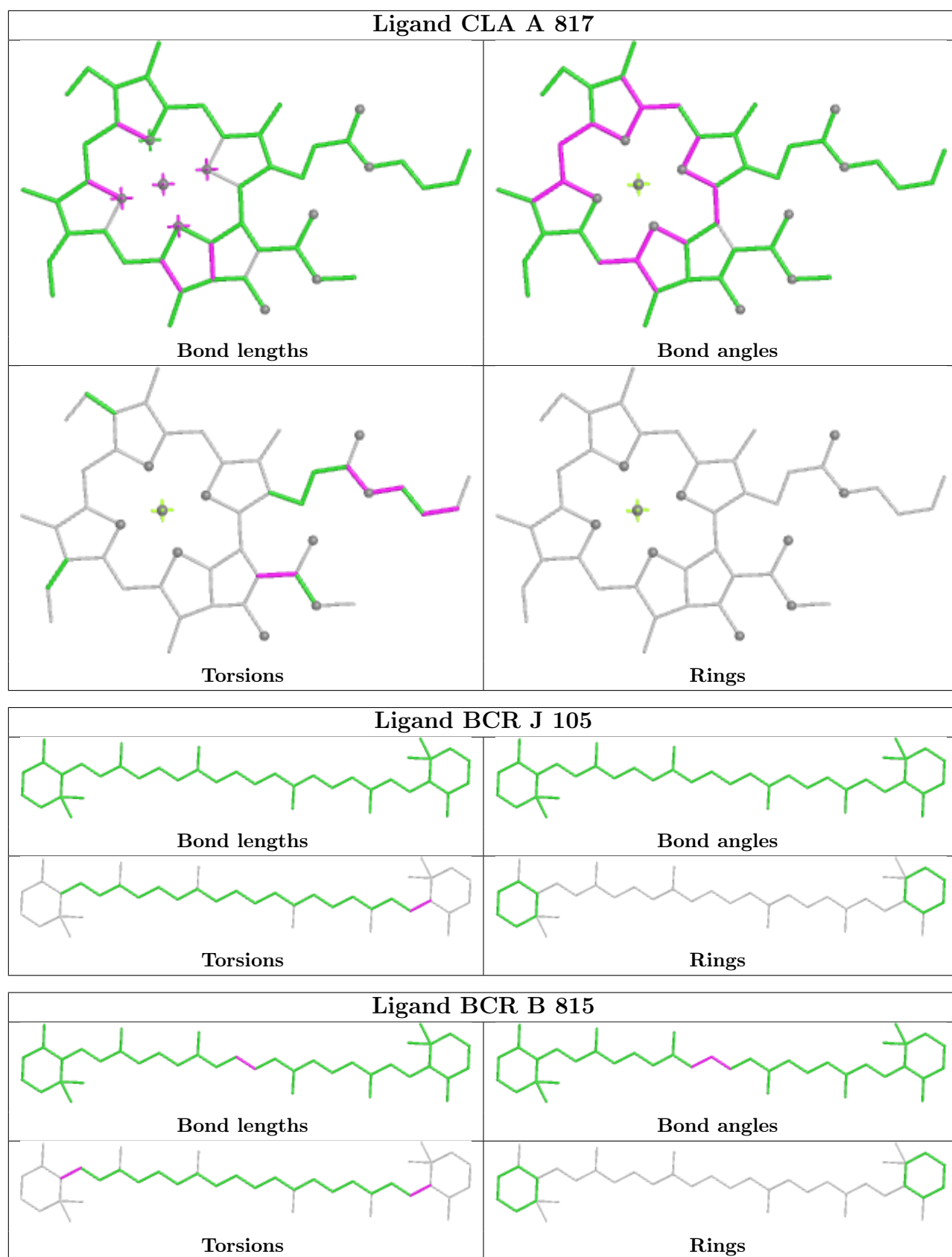
Rings

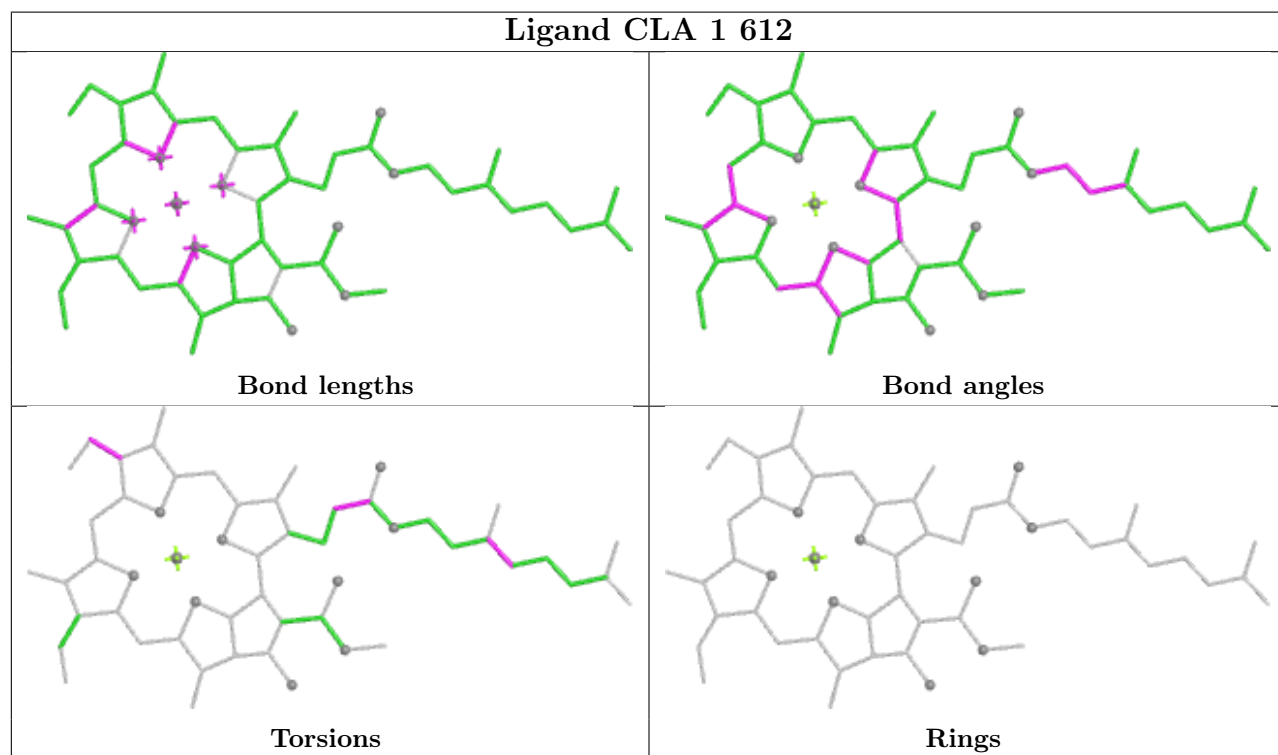
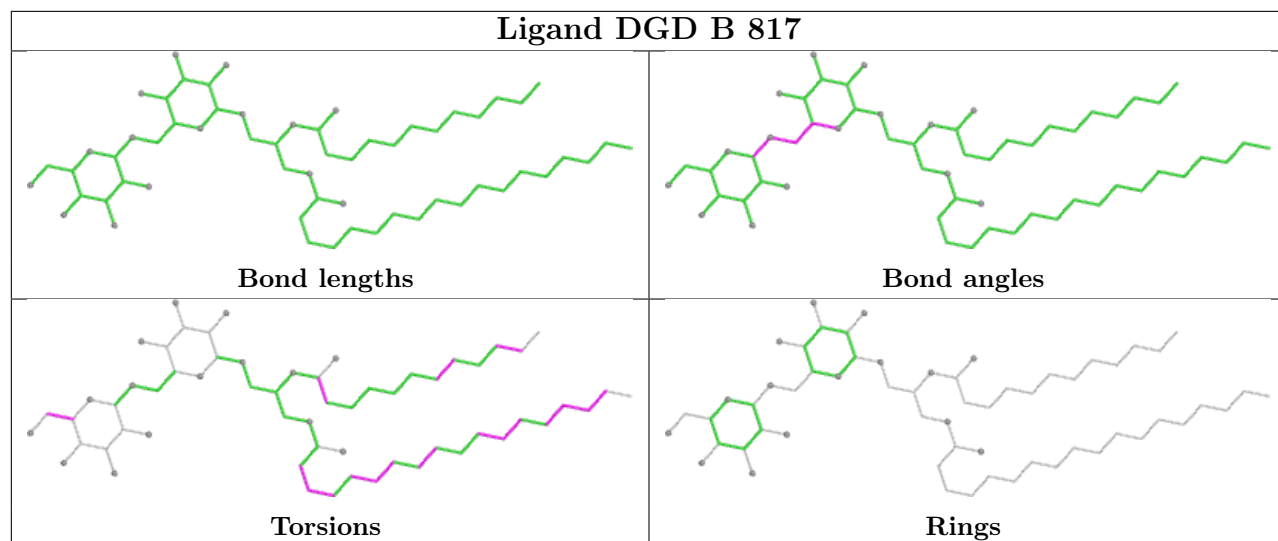


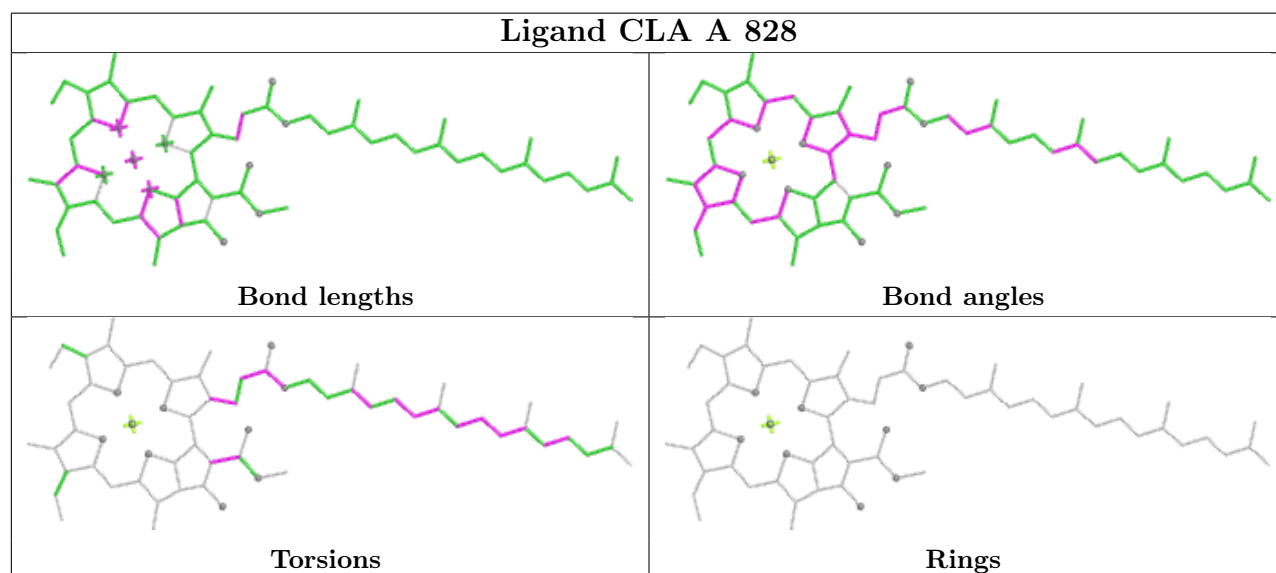
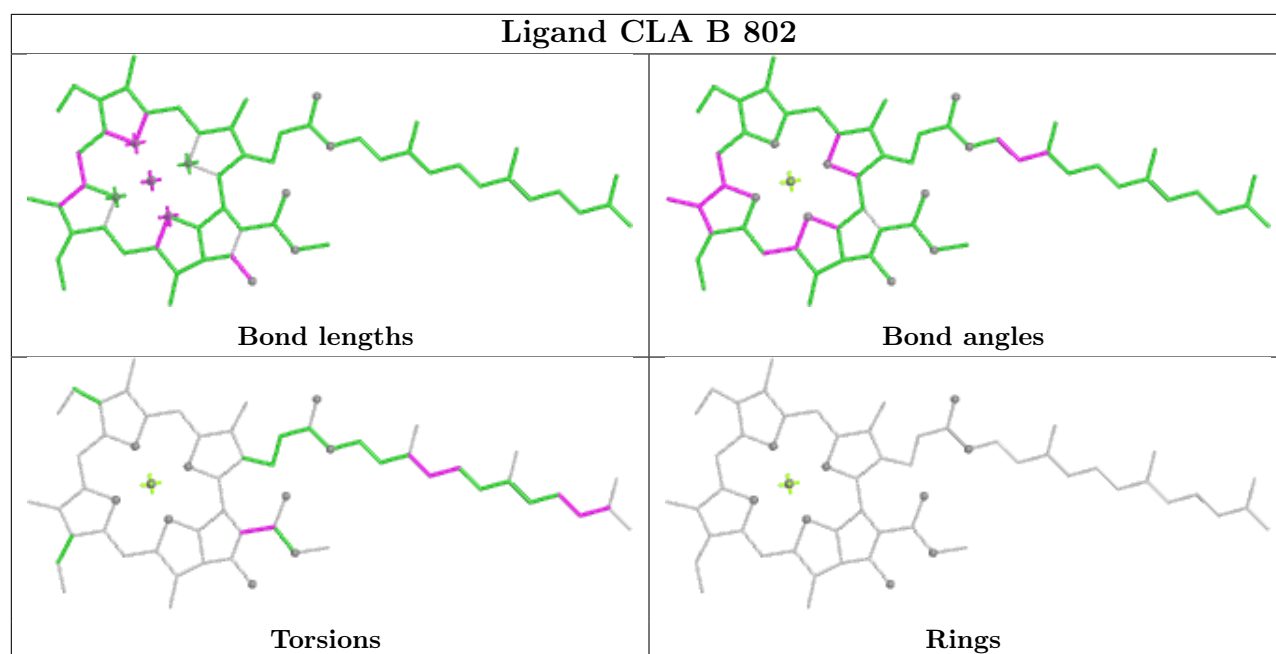


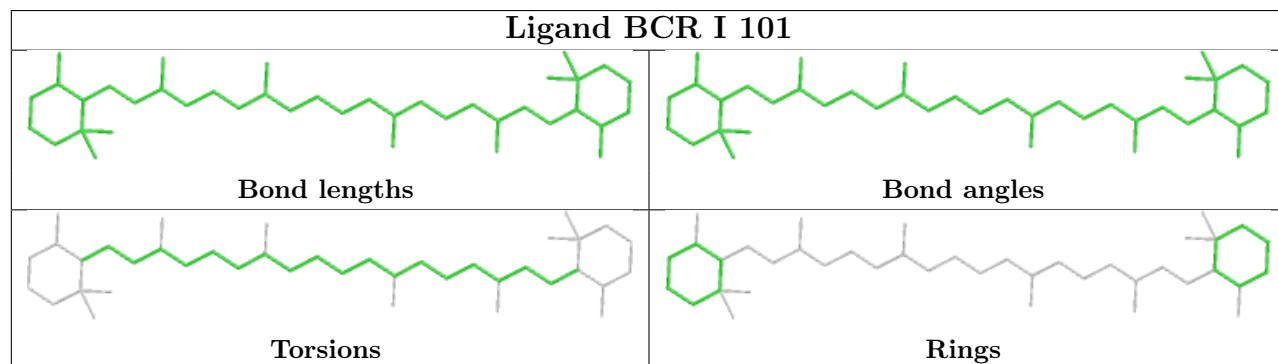
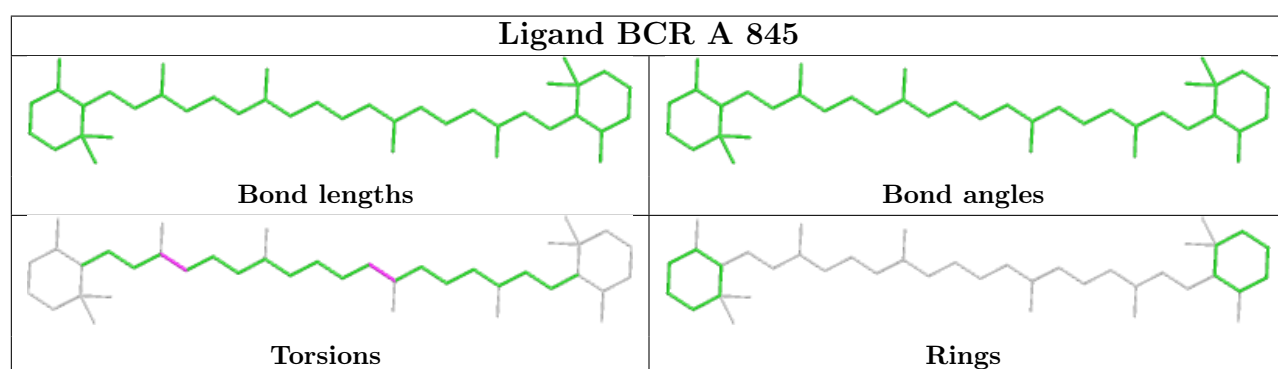
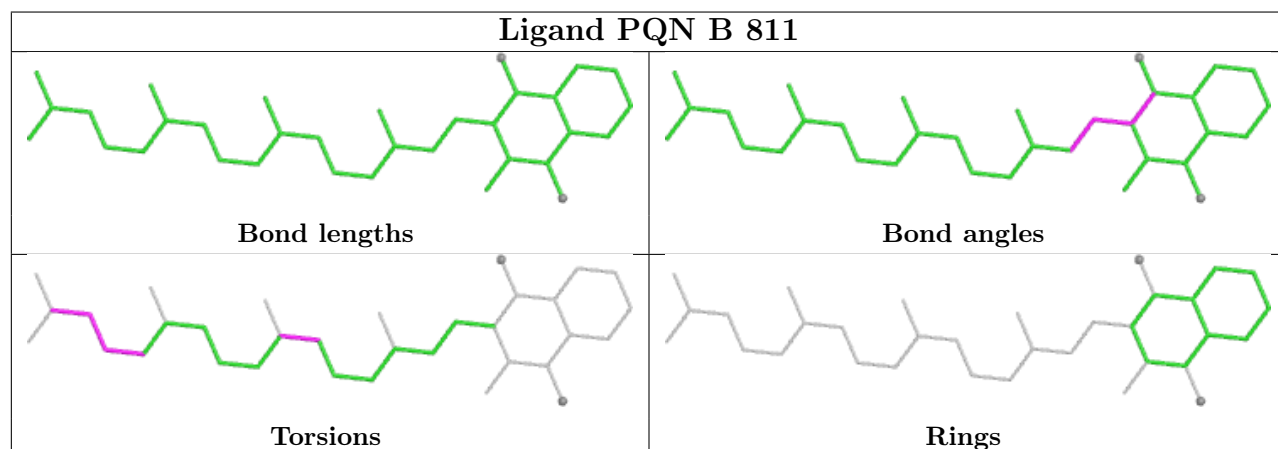
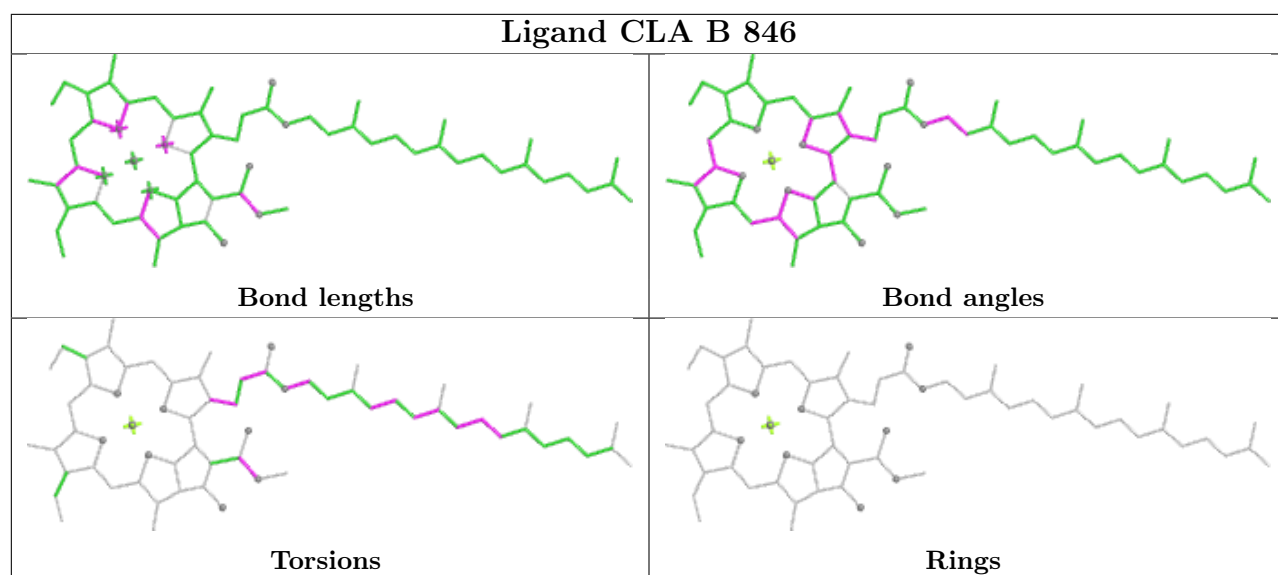
## Ligand CLA 4 311

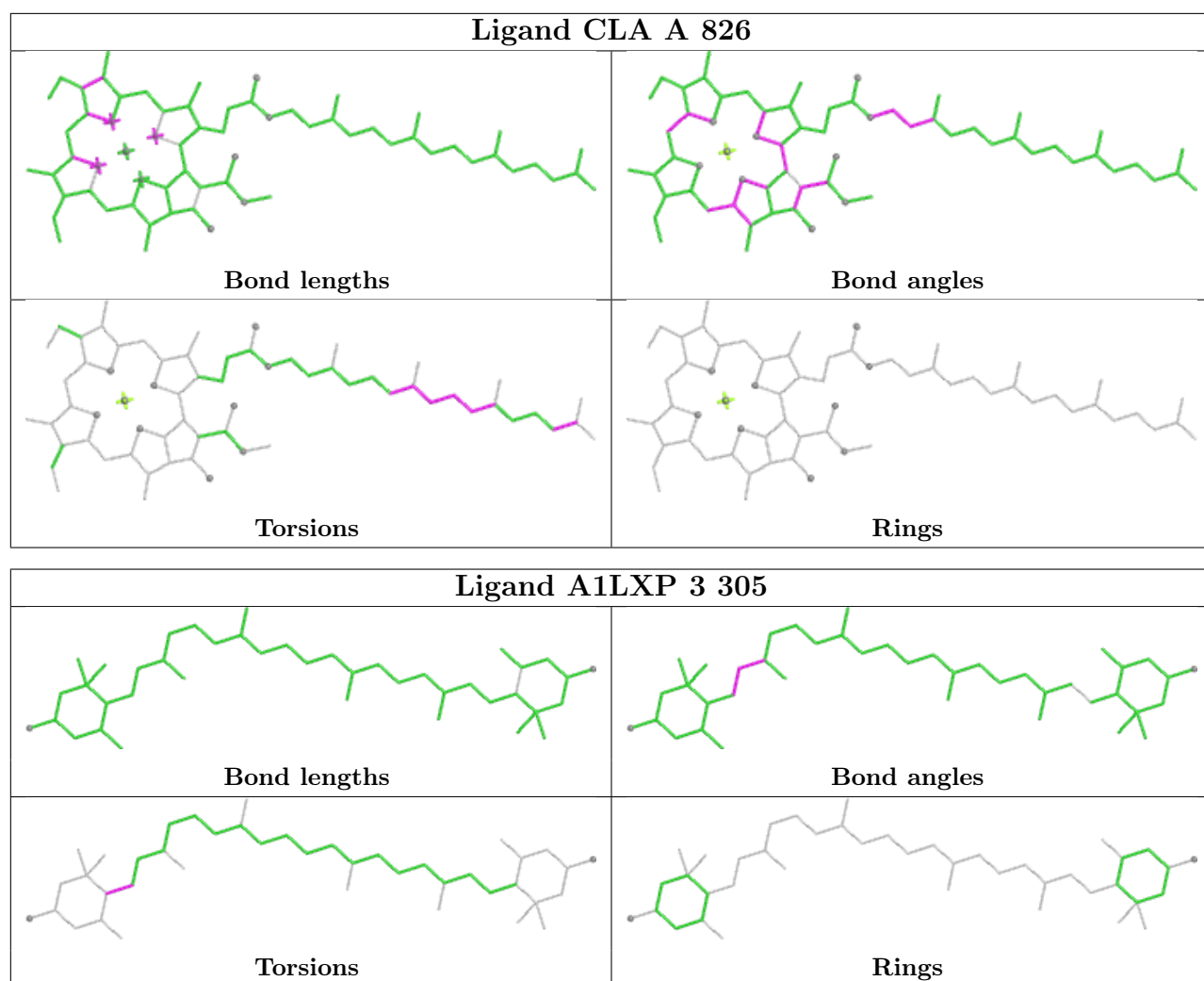




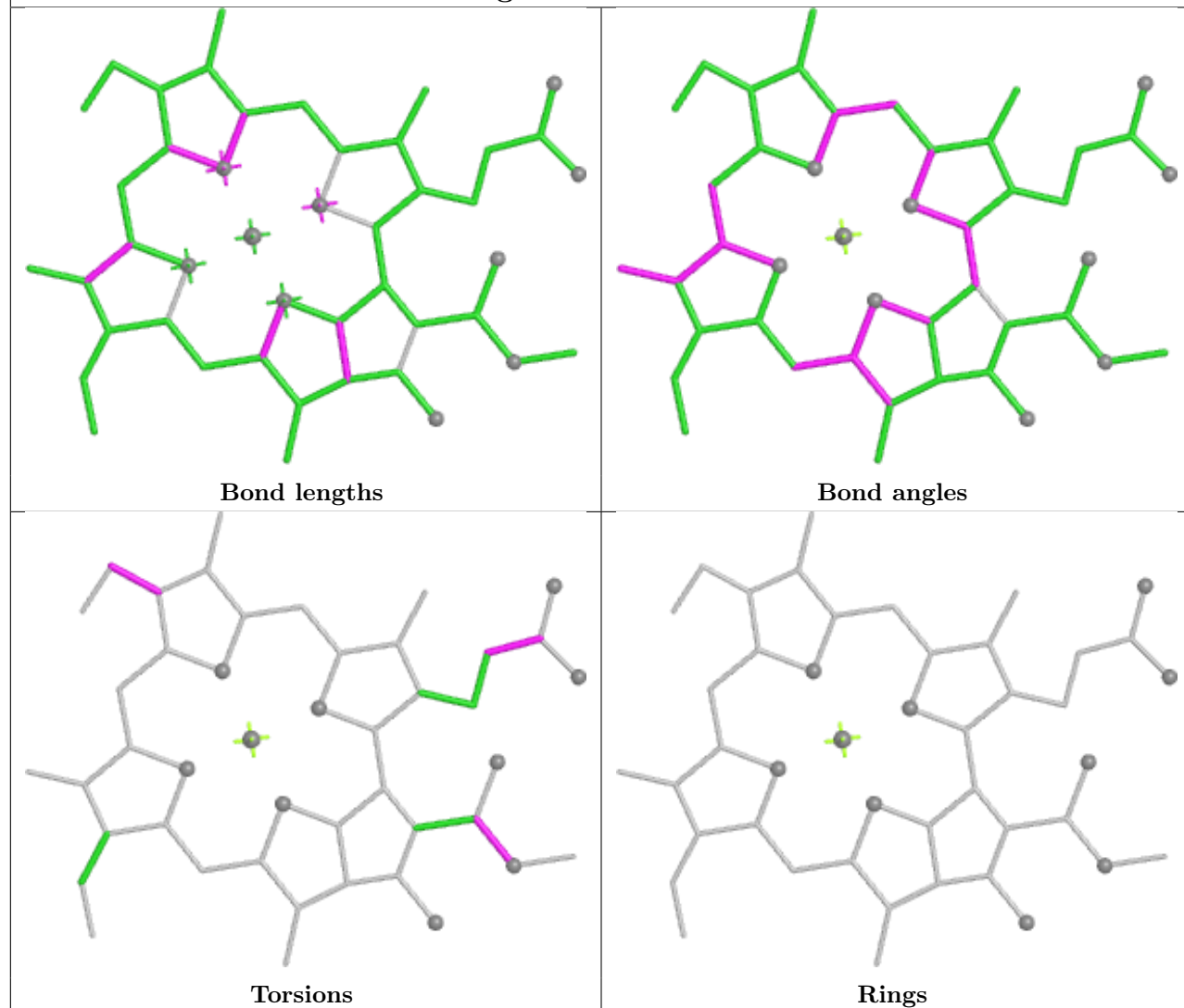




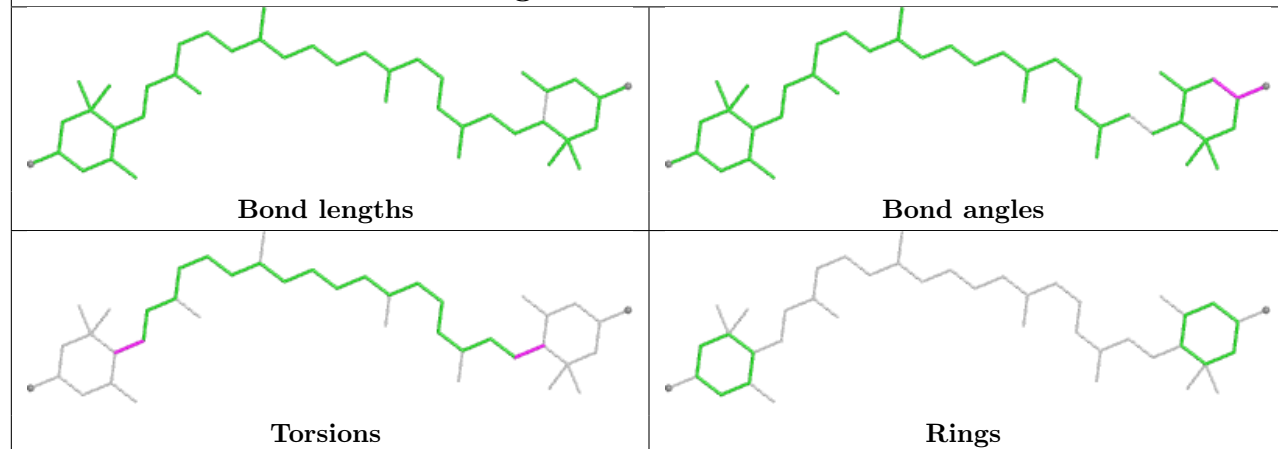


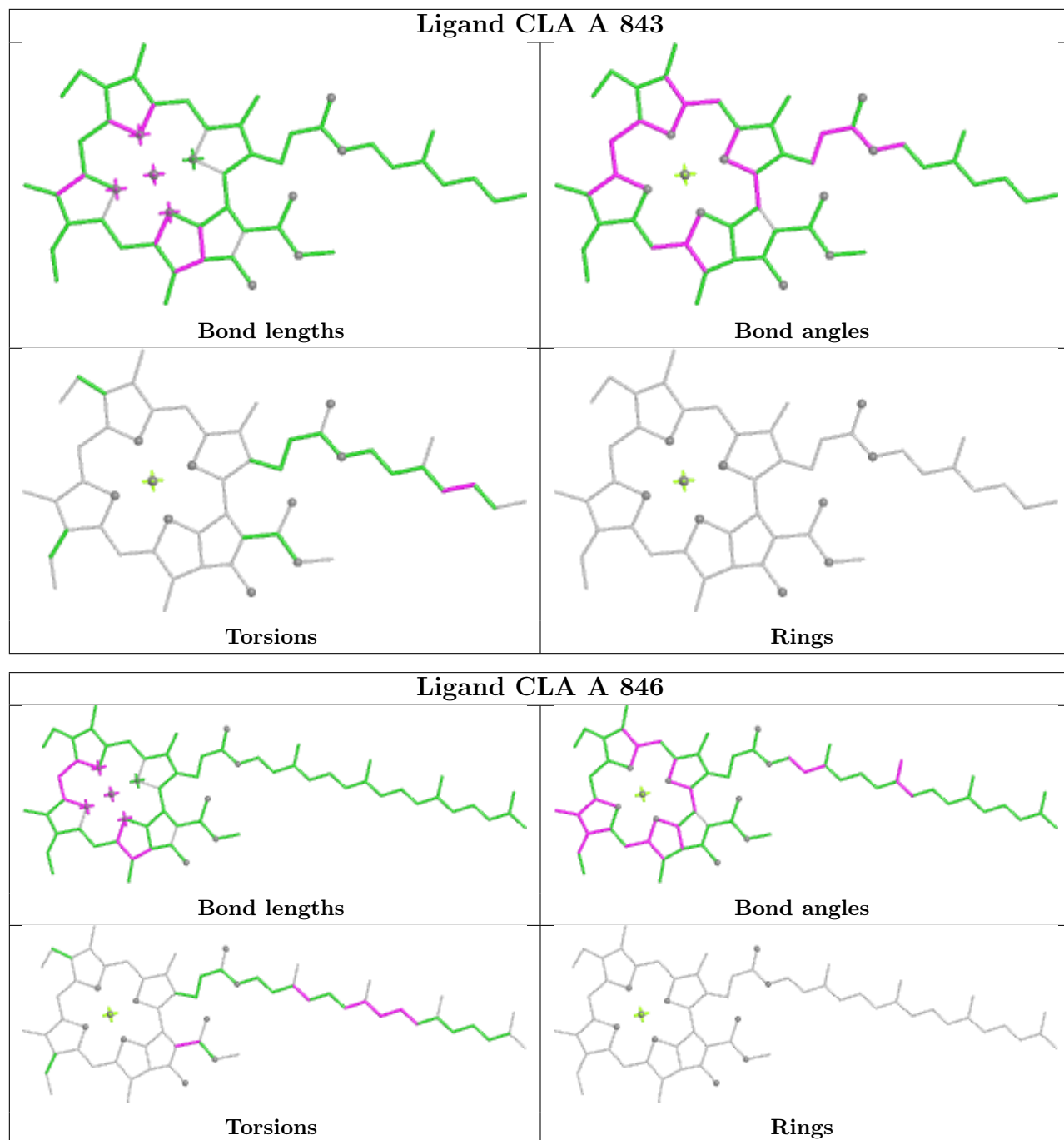


## Ligand CLA 4 318

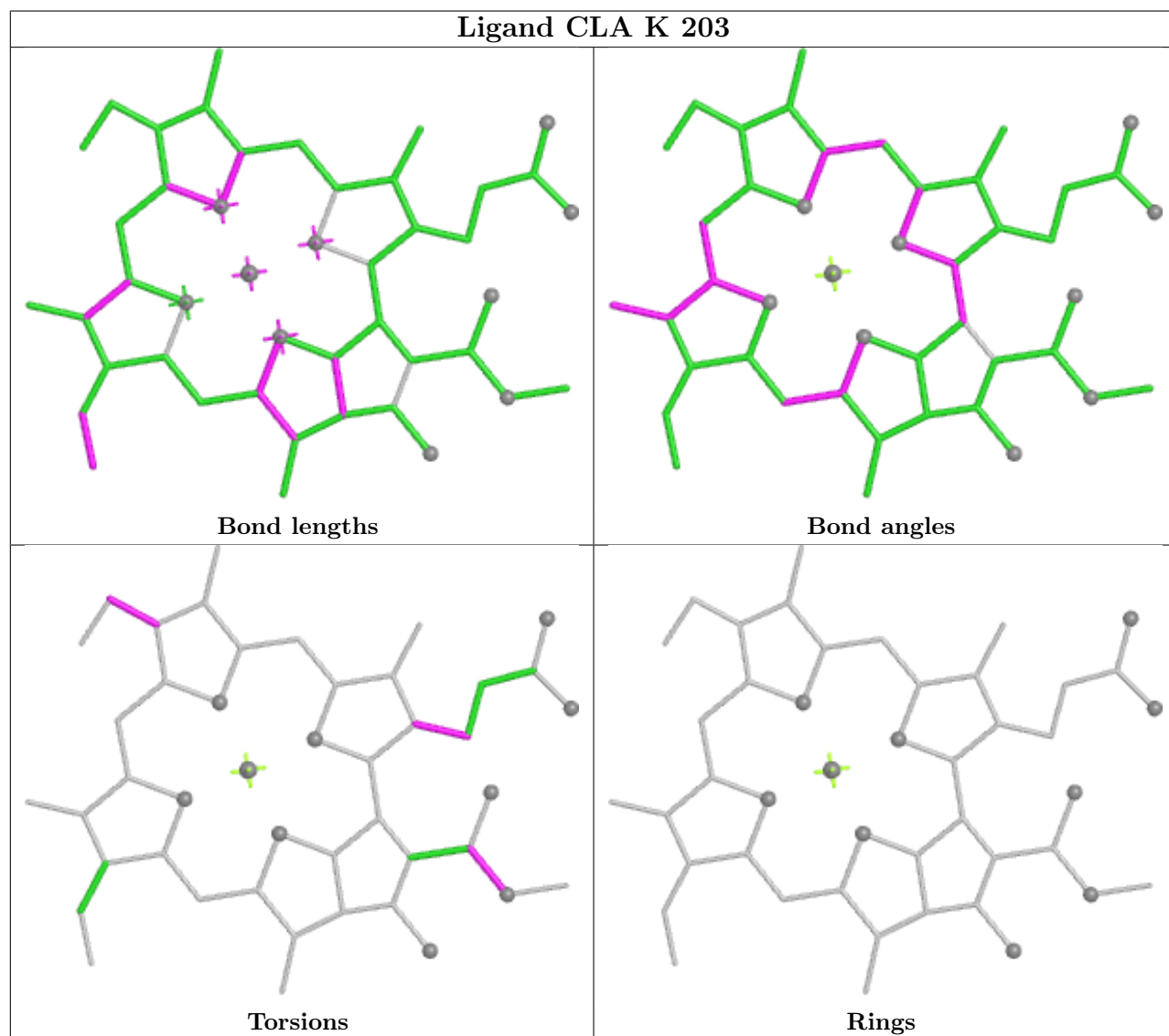
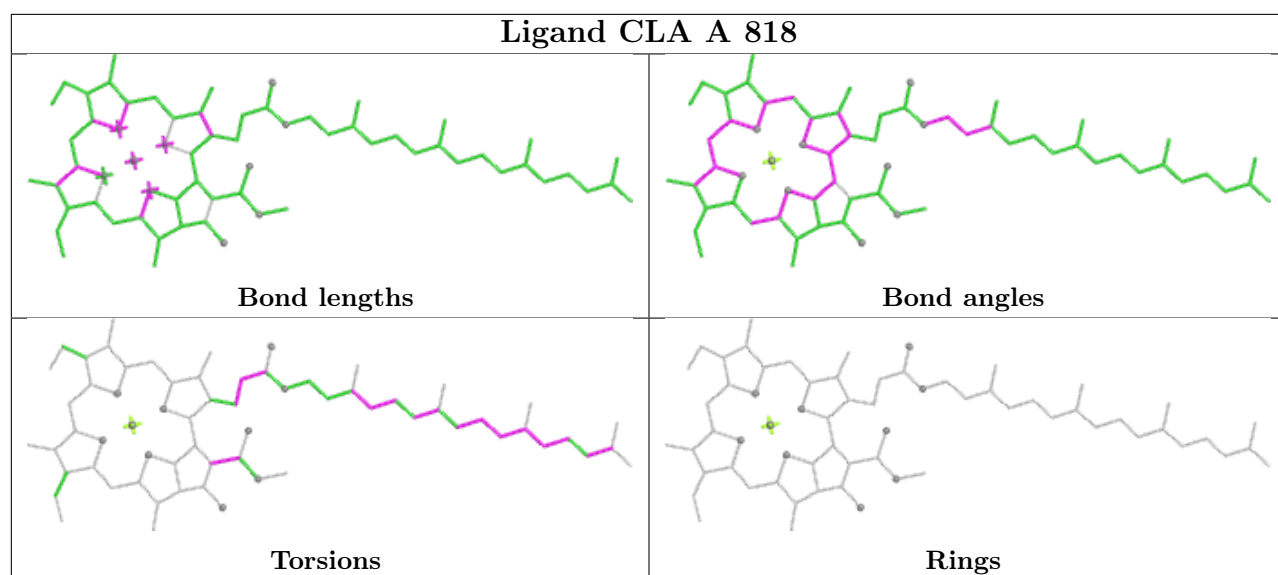


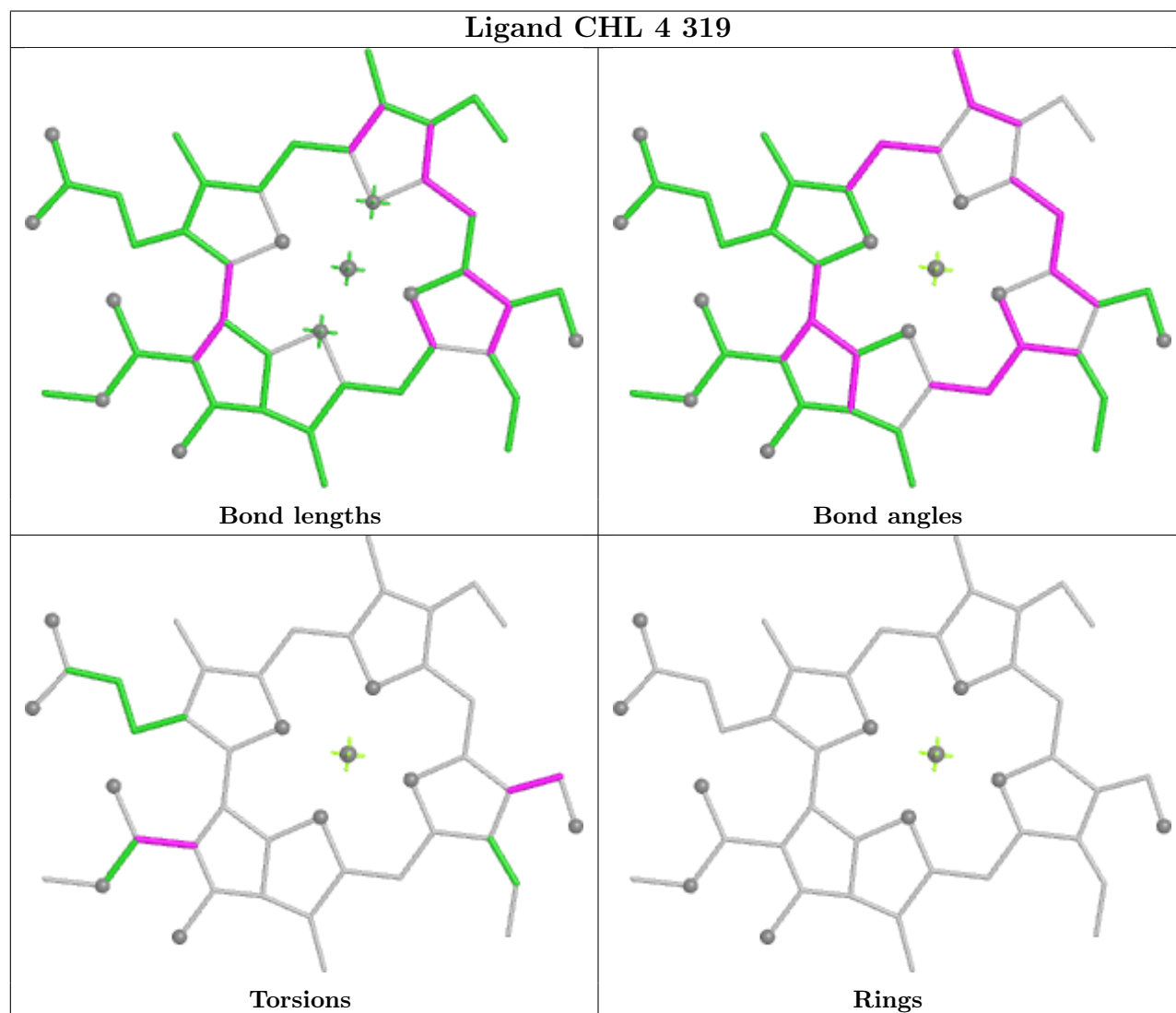
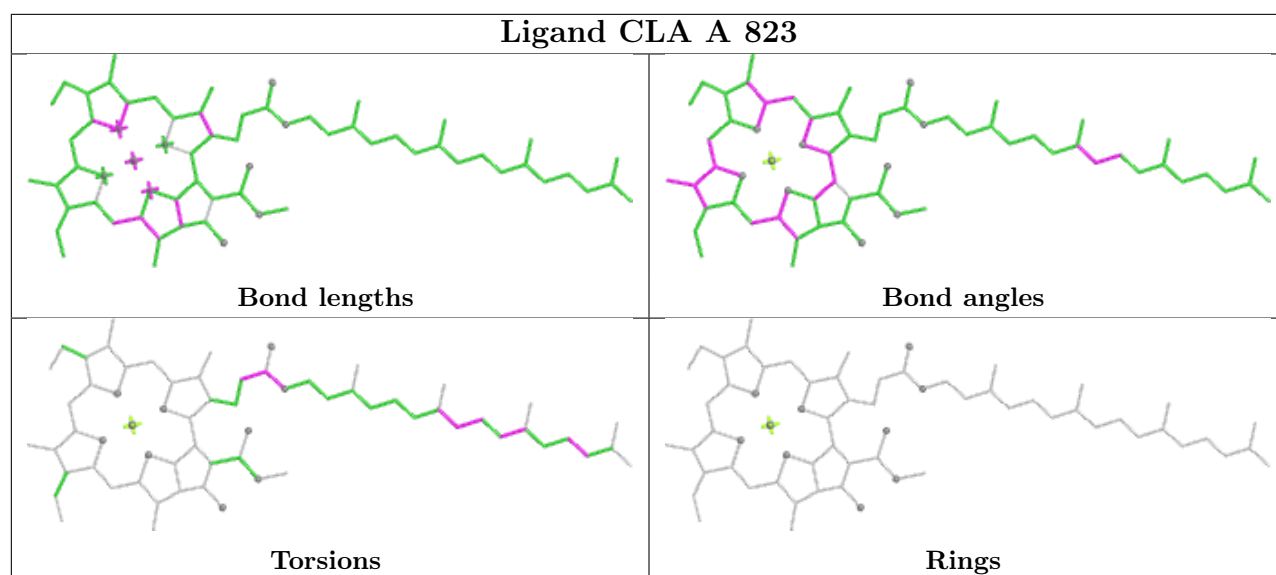
## Ligand A1LXP J 102



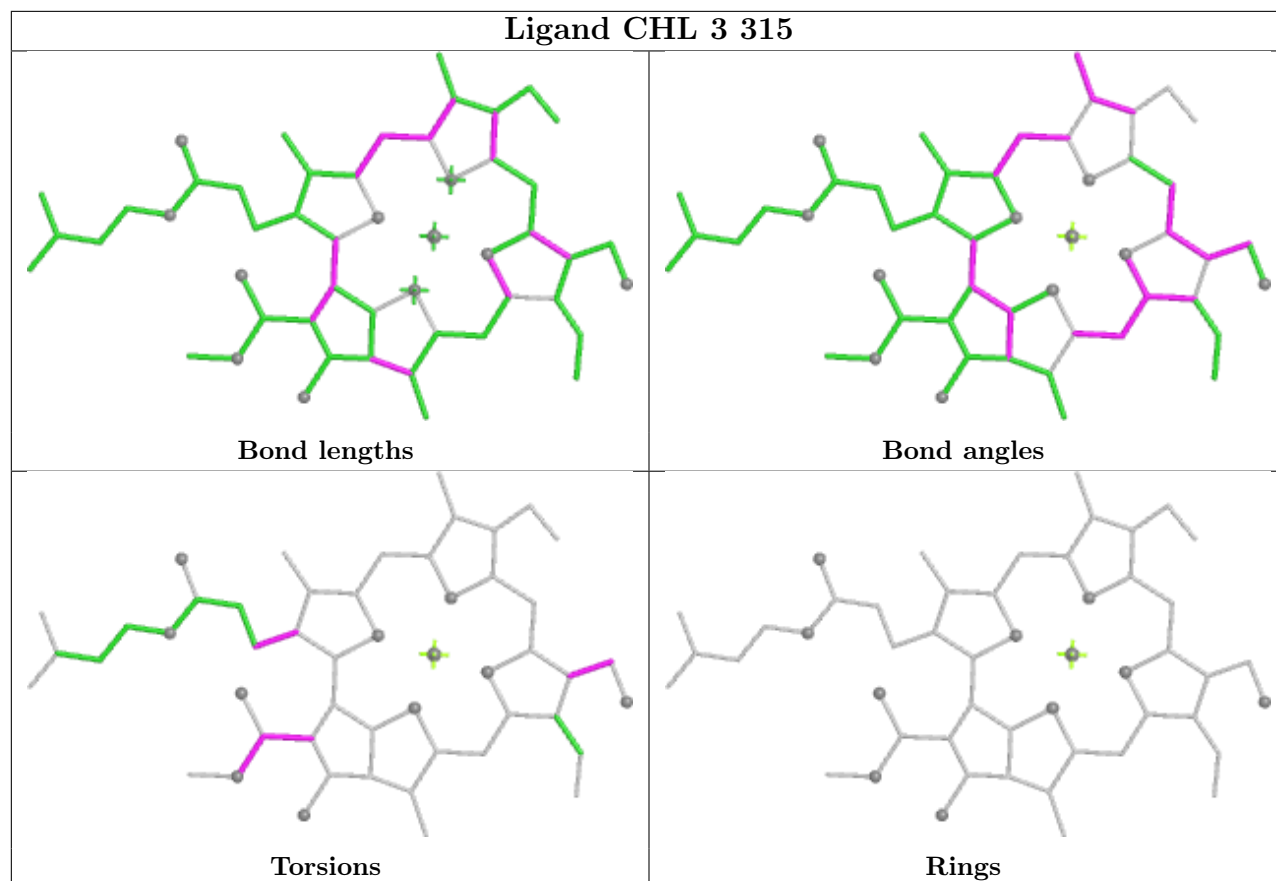




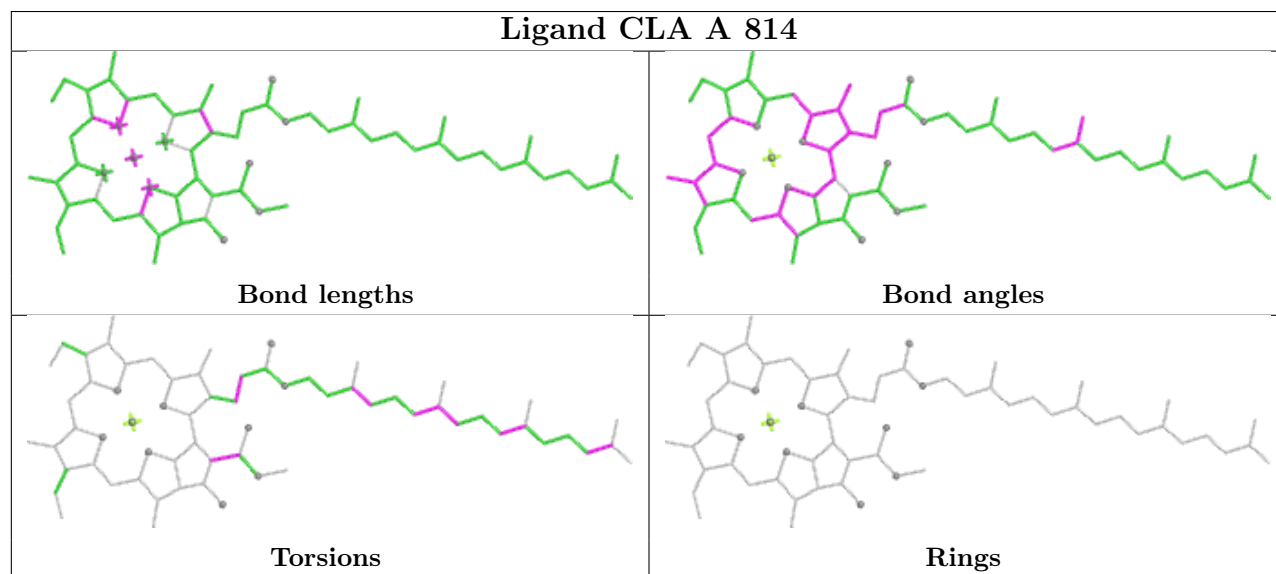


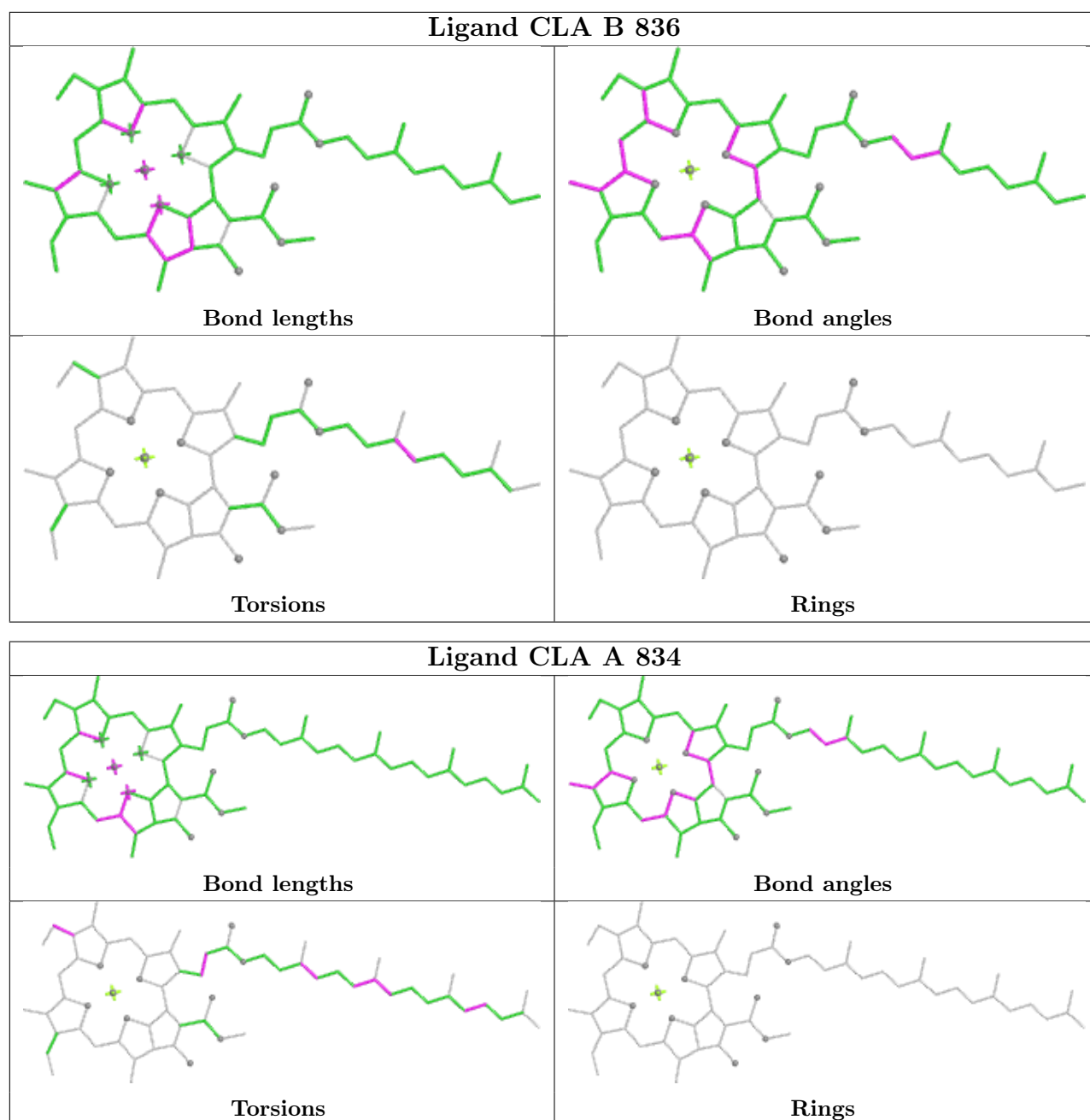


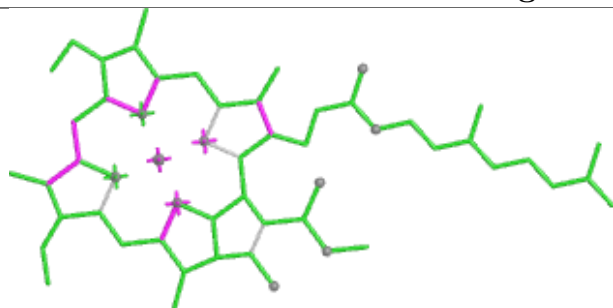
## Ligand CHL 3 315



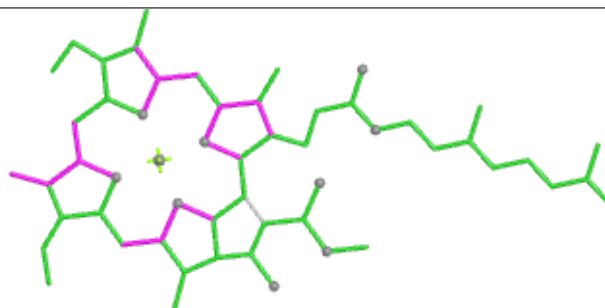
## Ligand CLA A 814



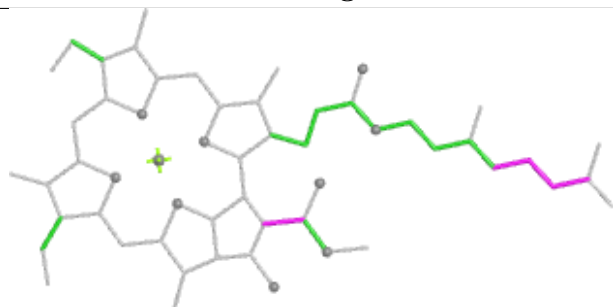


**Ligand CLA 3 304**

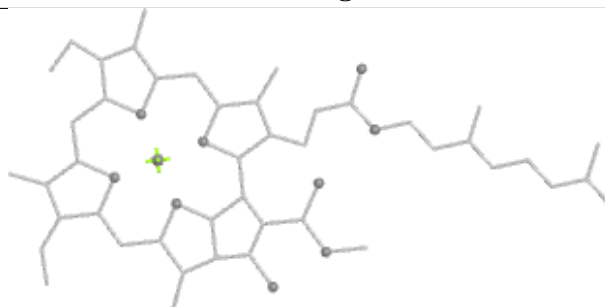
Bond lengths



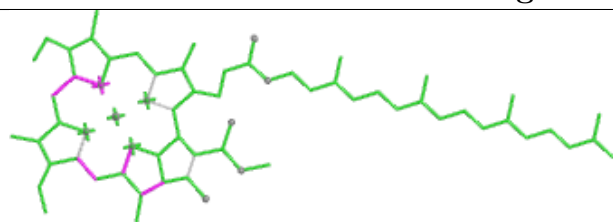
Bond angles



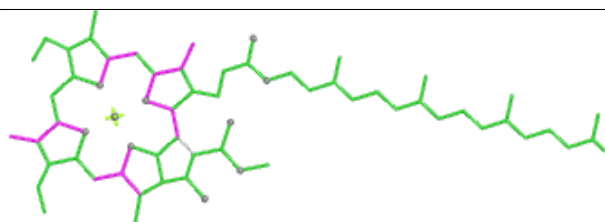
Torsions



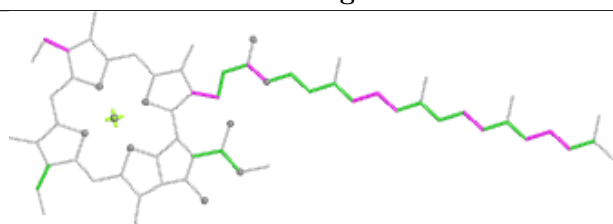
Rings

**Ligand CLA L 304**

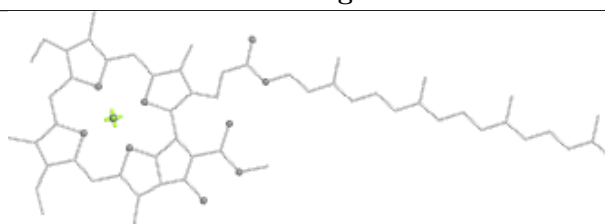
Bond lengths



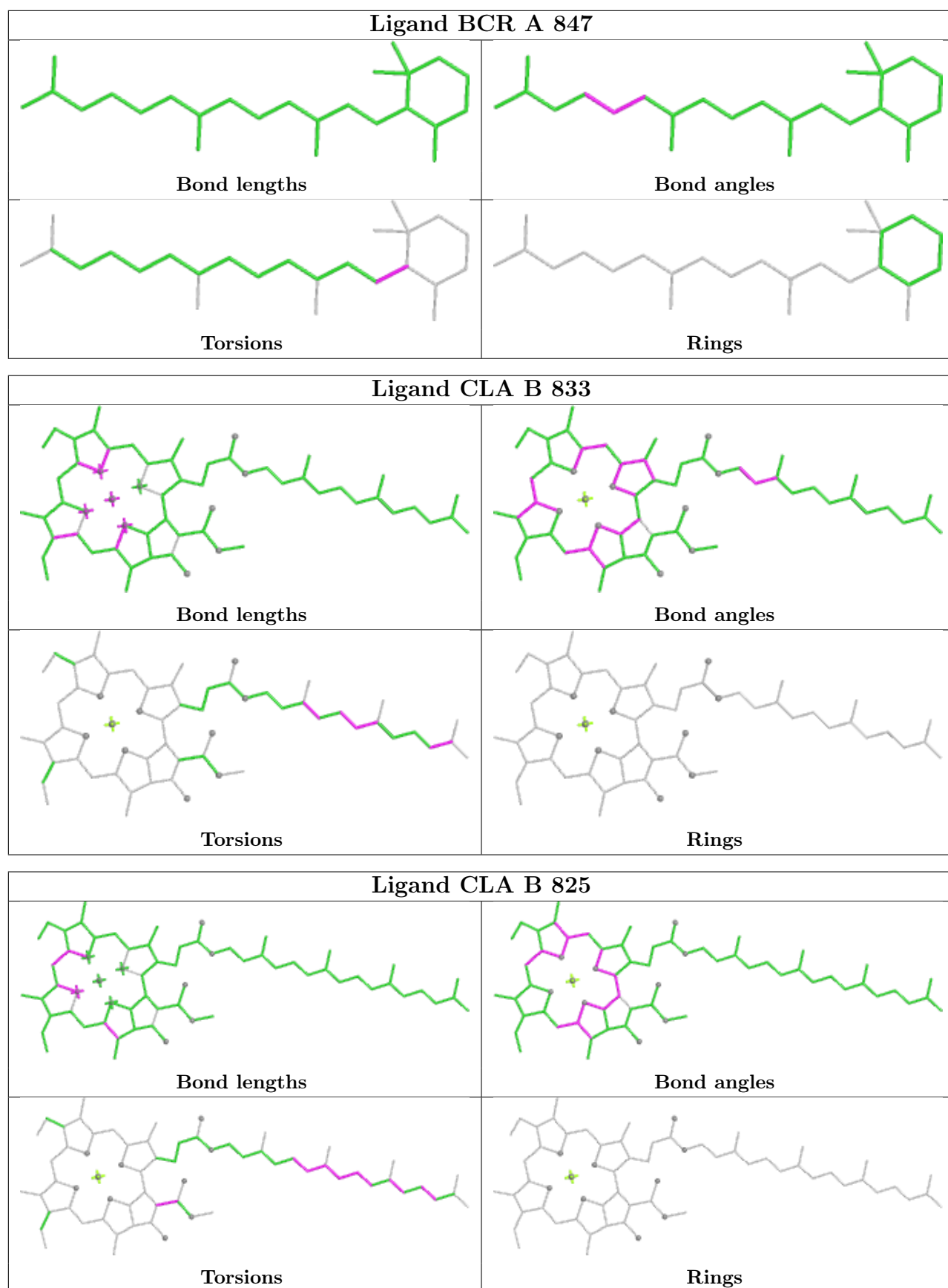
Bond angles

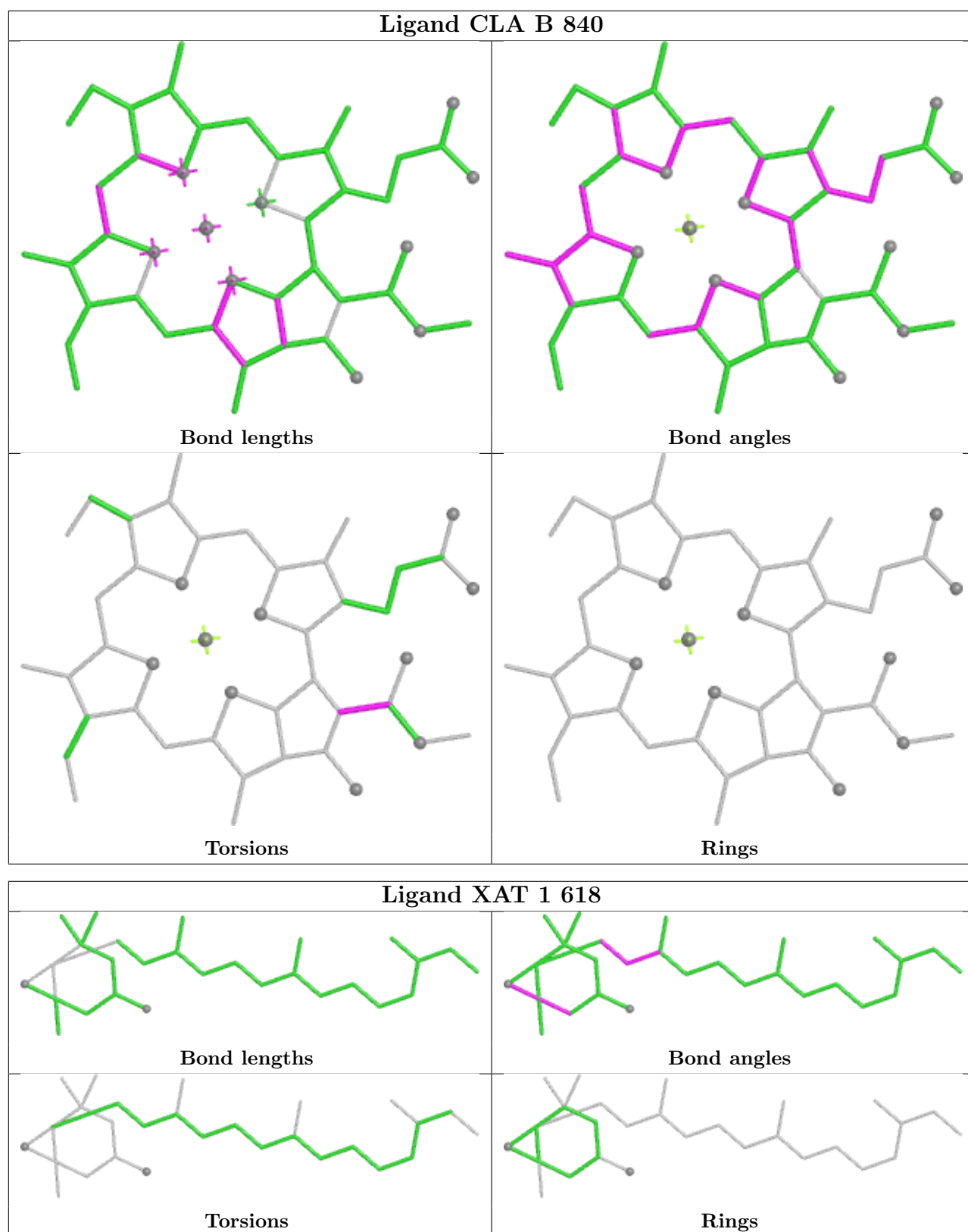


Torsions

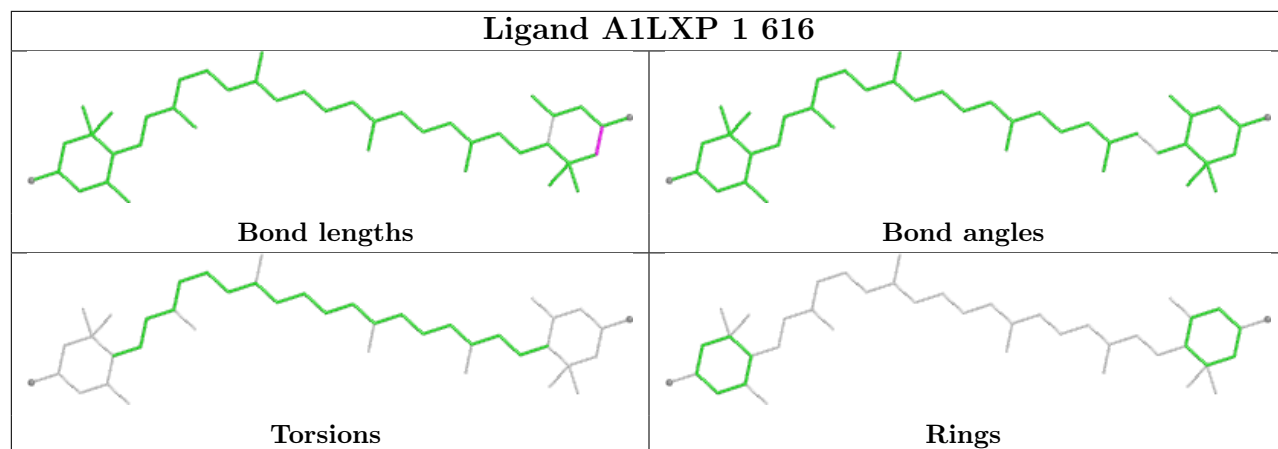


Rings

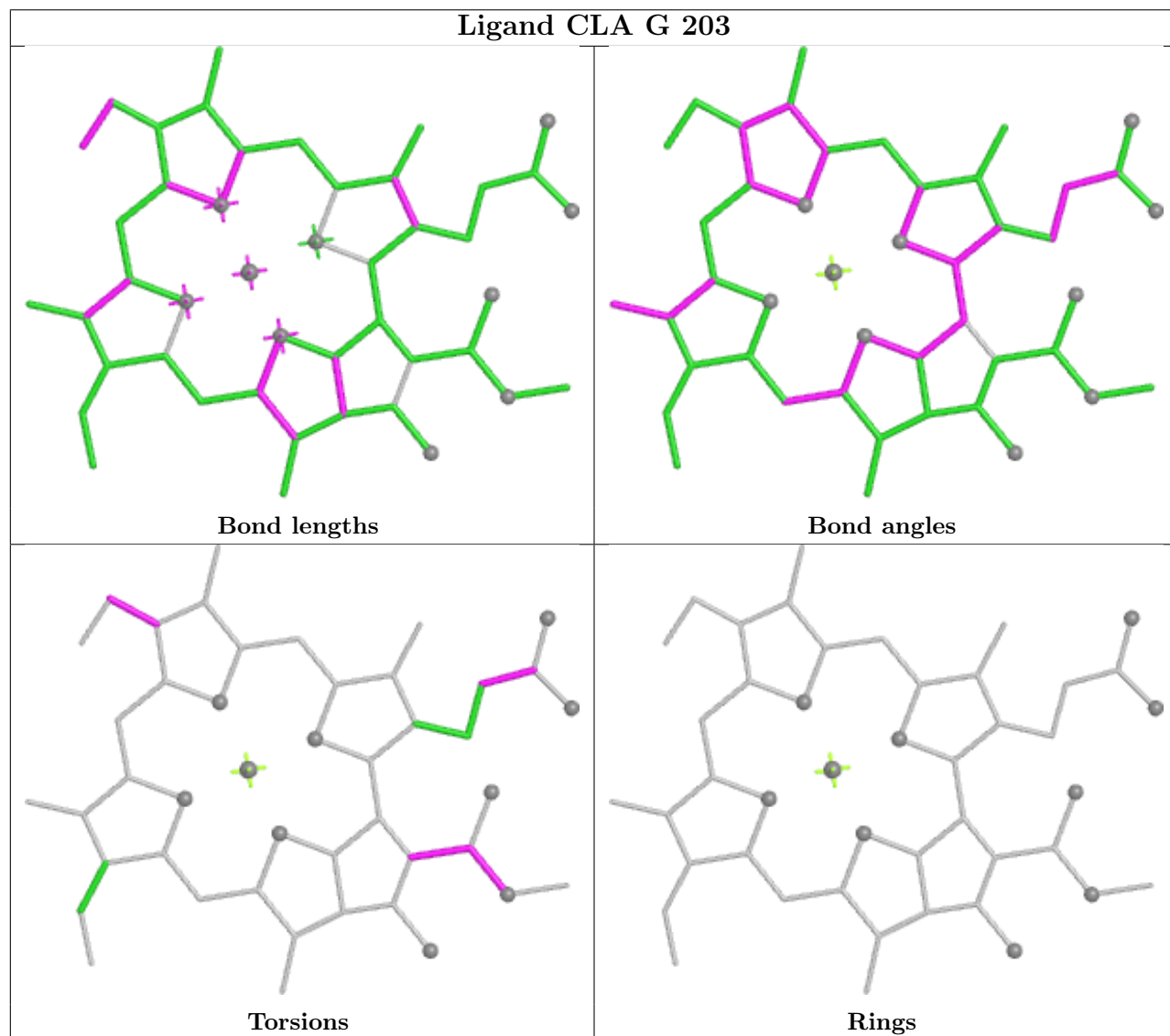




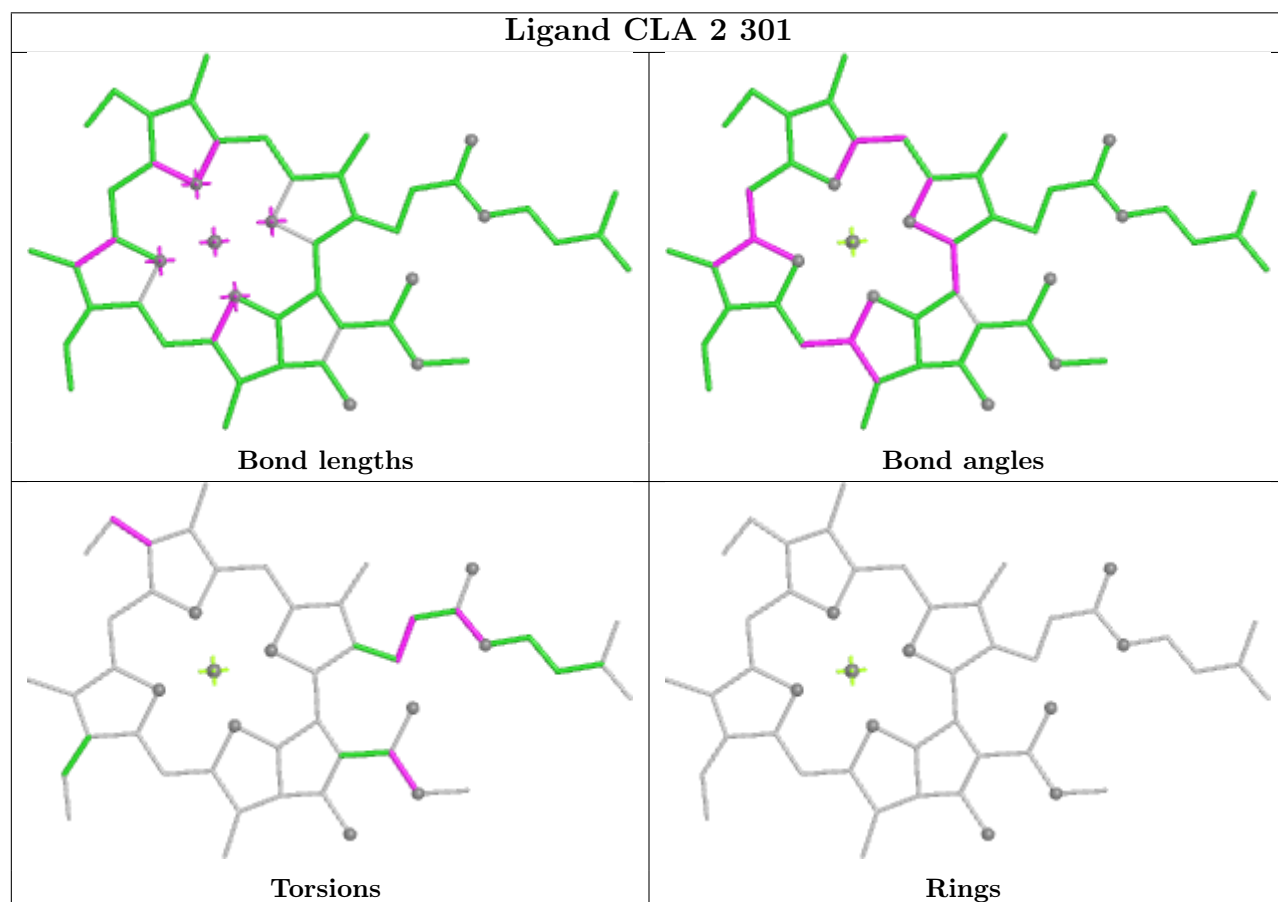
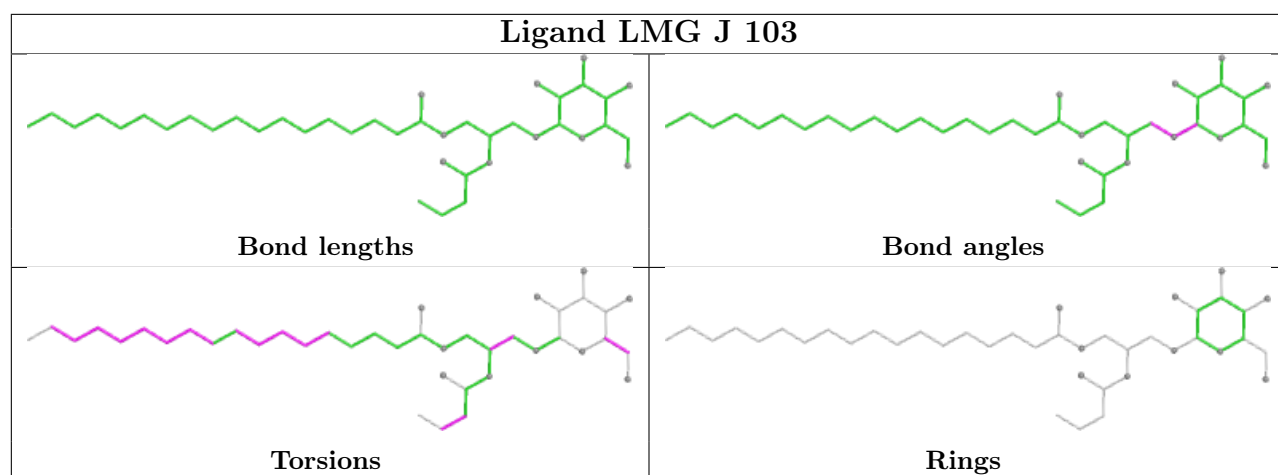
## Ligand A1LXP 1 616

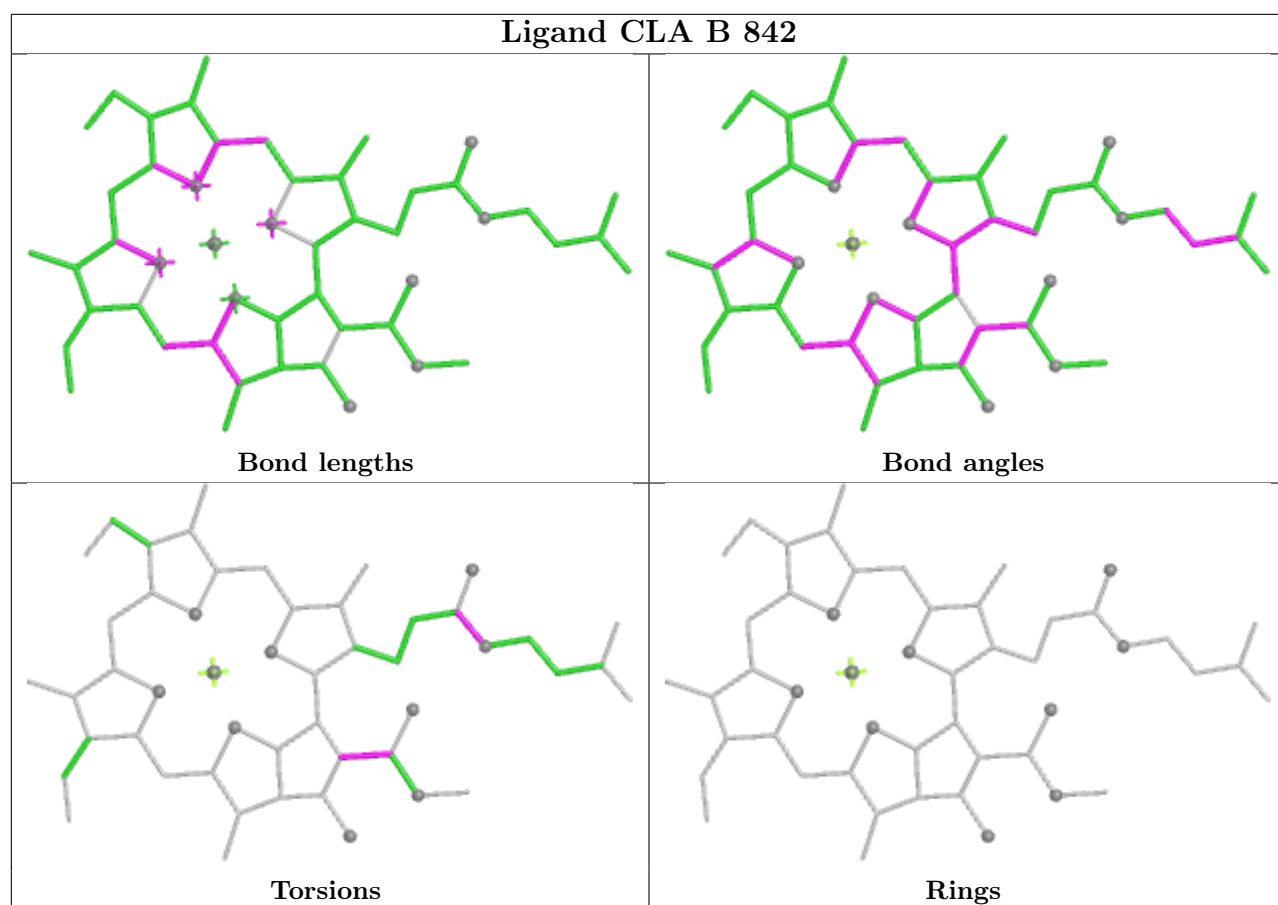


## Ligand CLA G 203

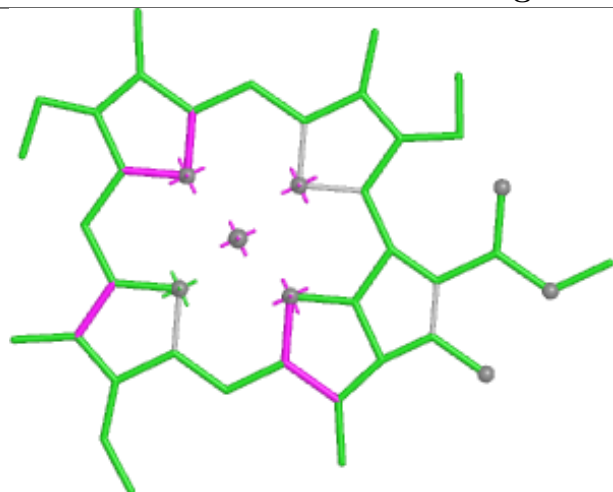




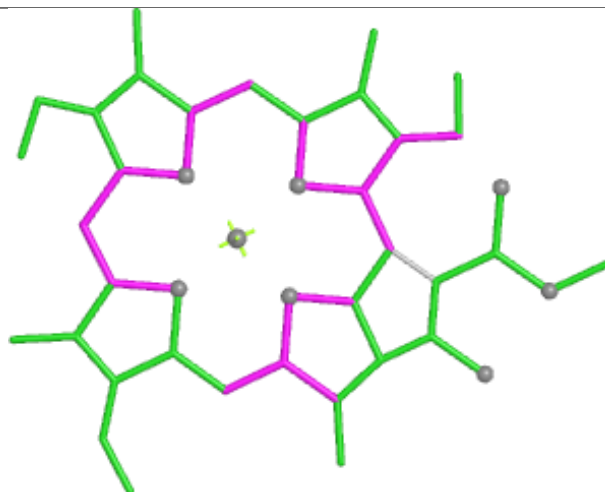




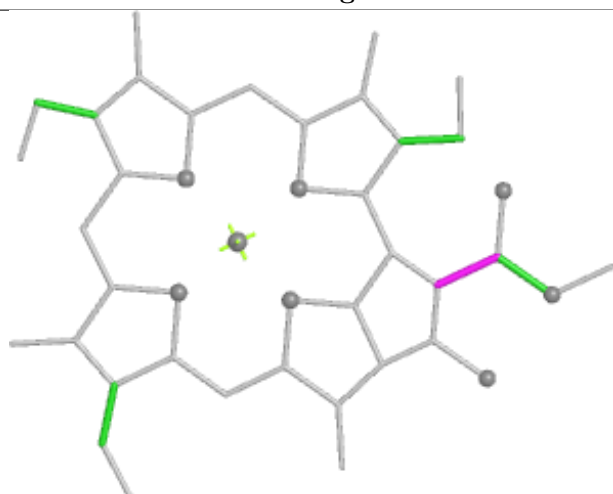
## Ligand CLA A 844



Bond lengths



Bond angles

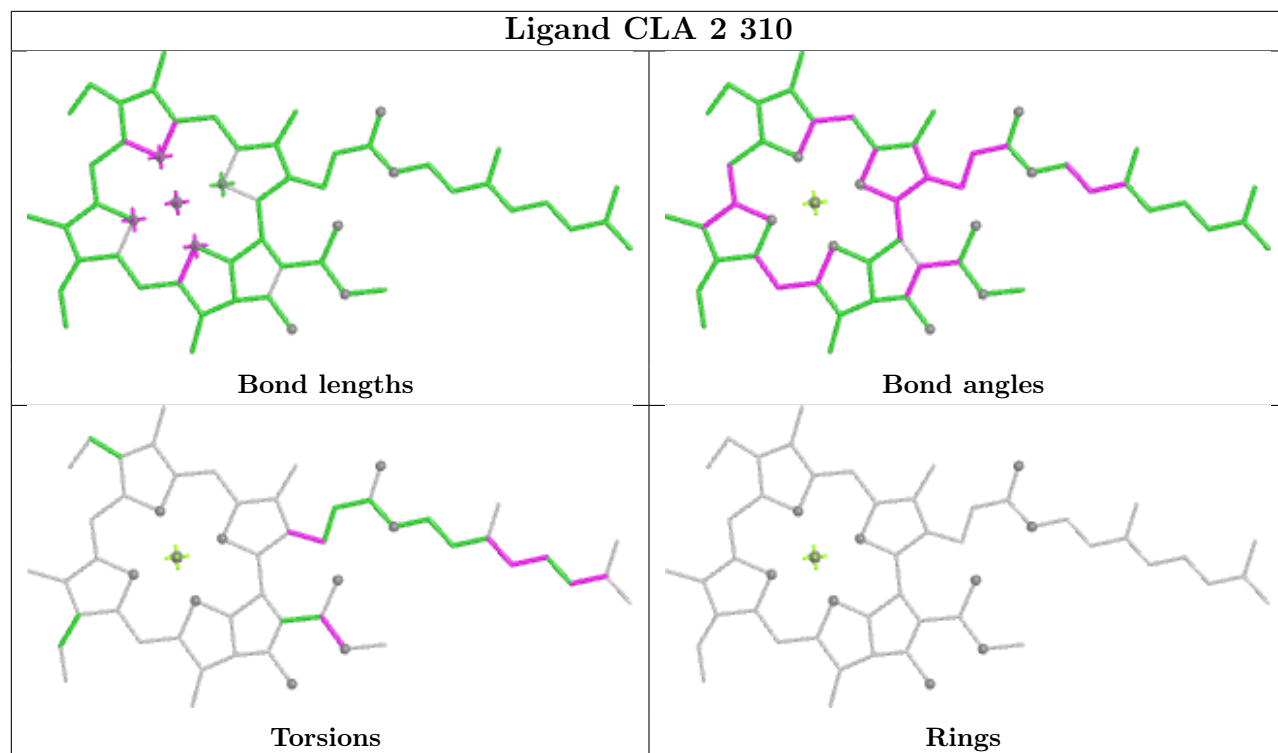


Torsions

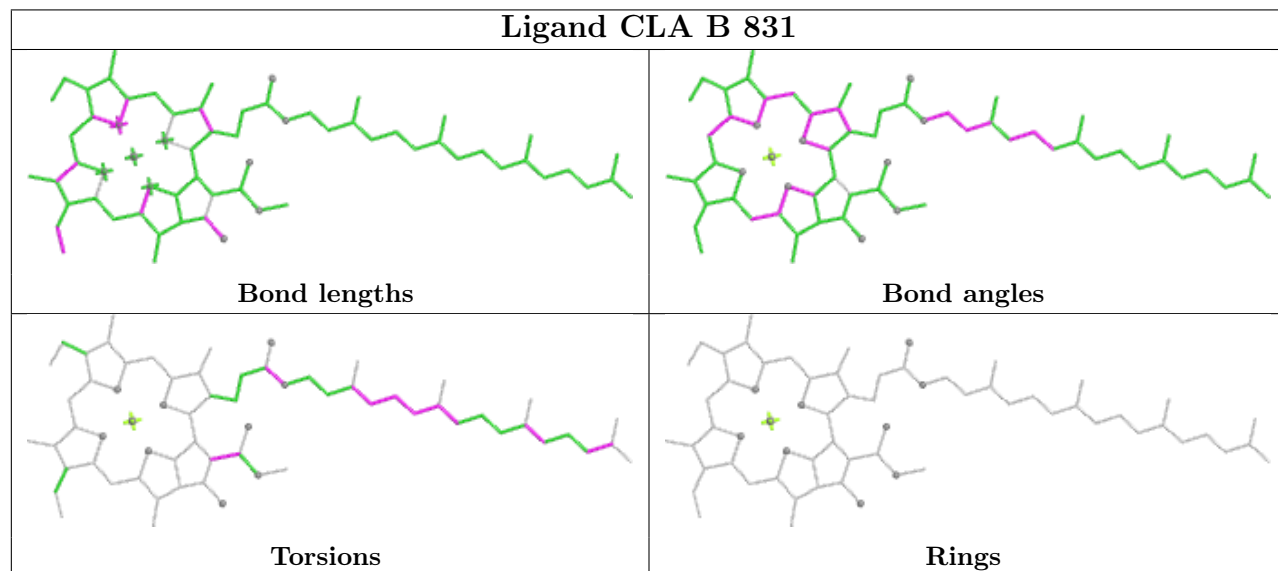


Rings

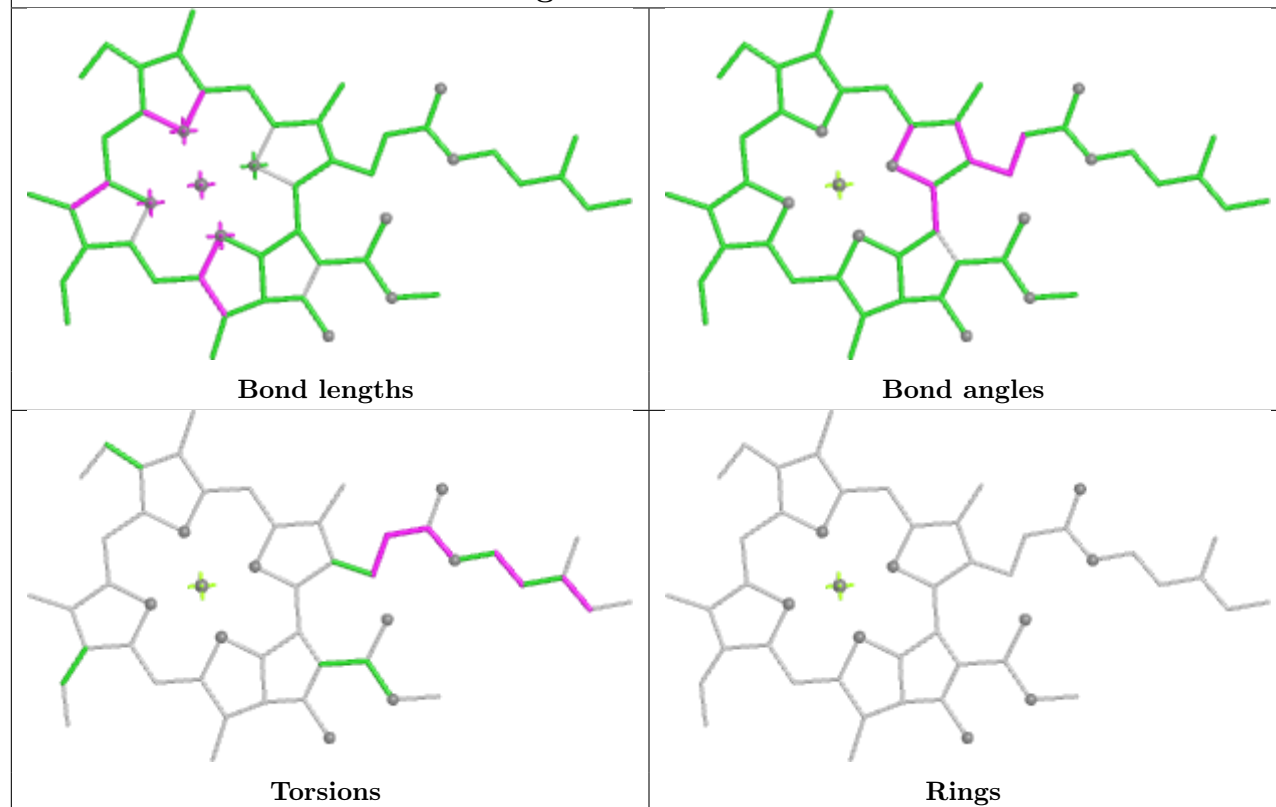
## Ligand CLA 2 310



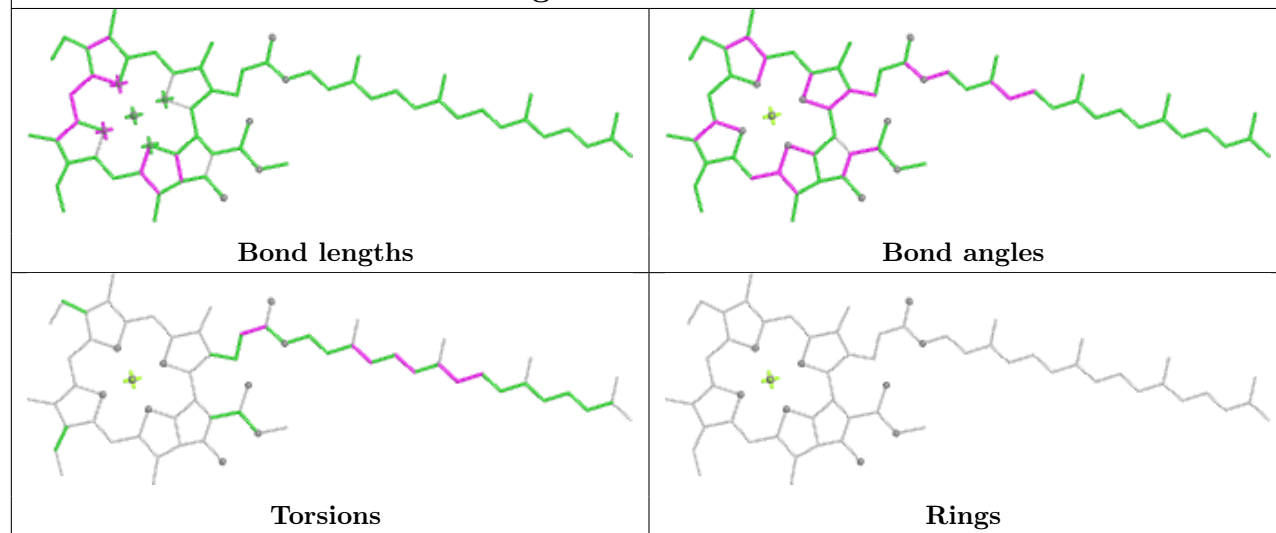
## Ligand CLA B 831

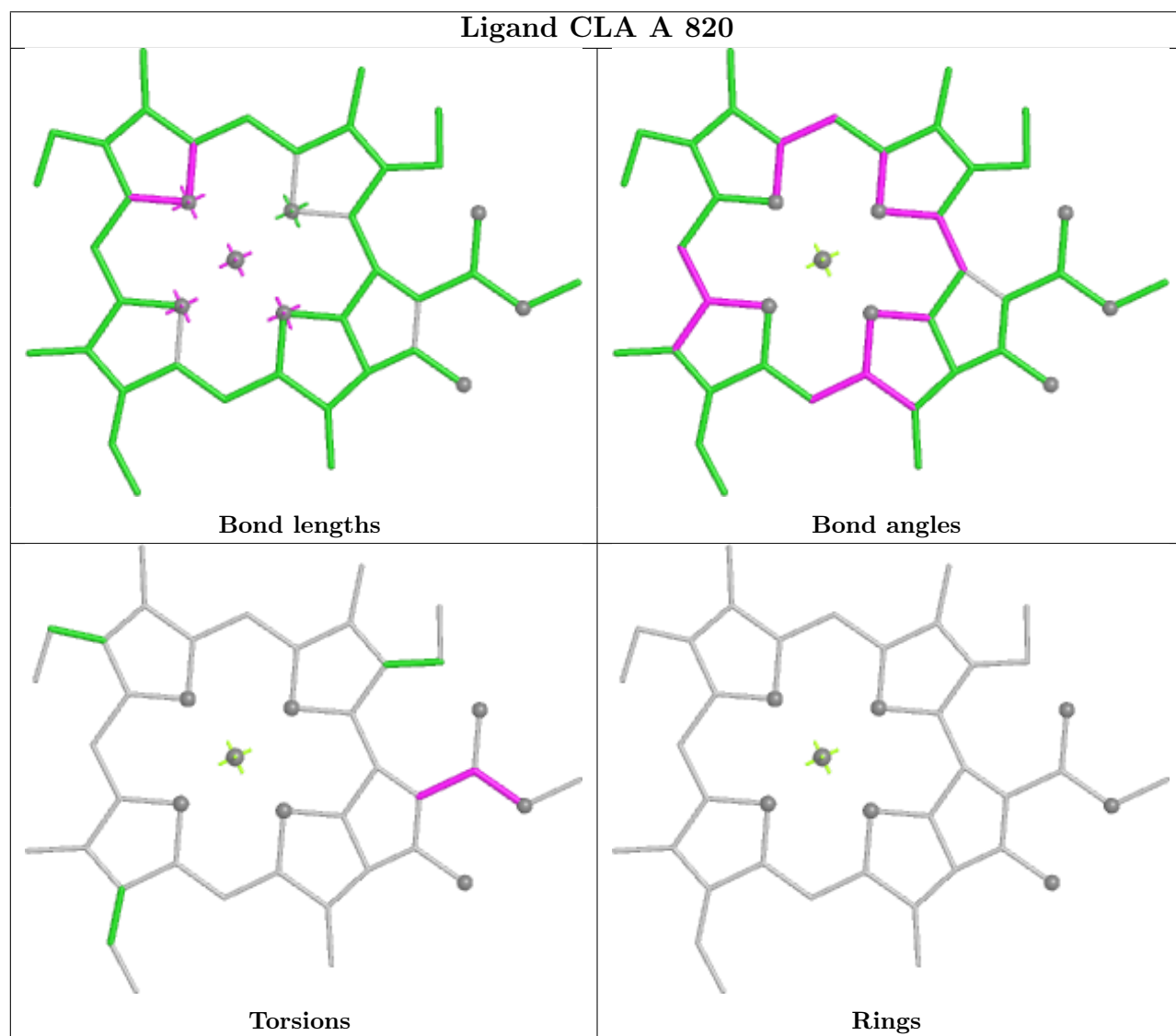
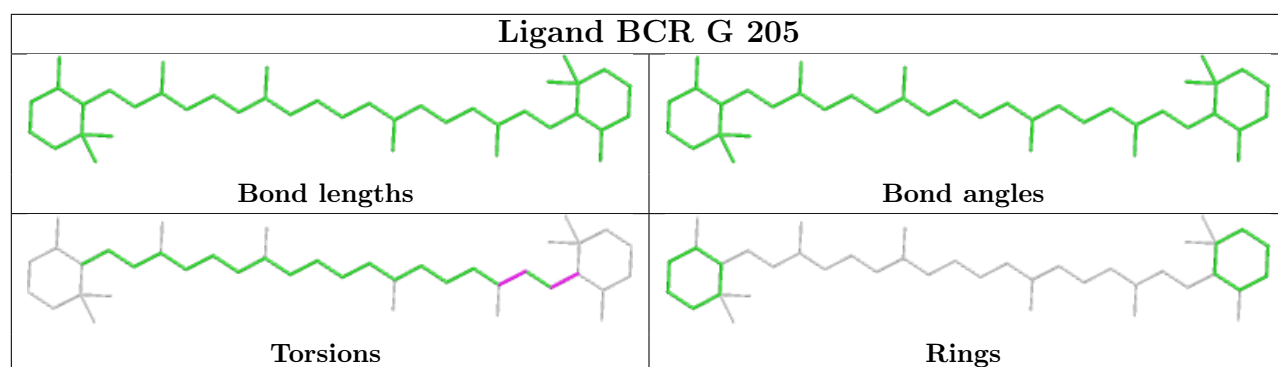


## Ligand CLA 1 607

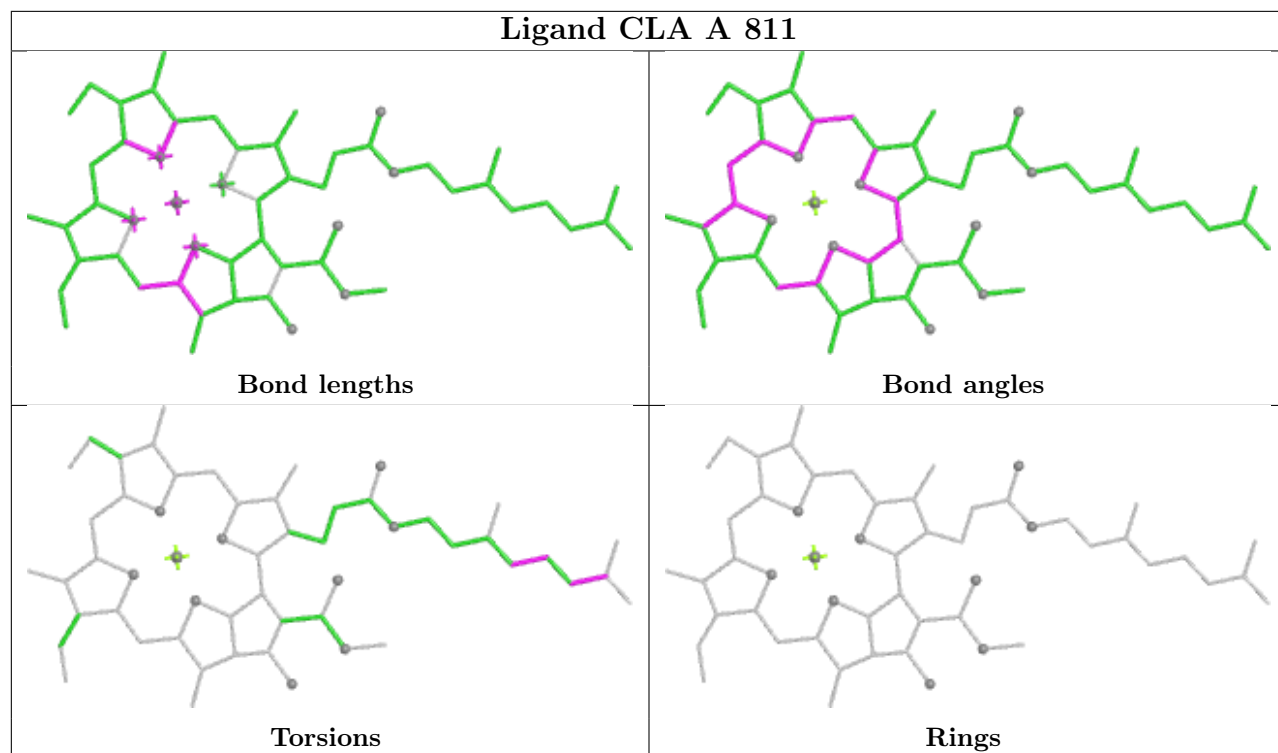


## Ligand CLA B 809

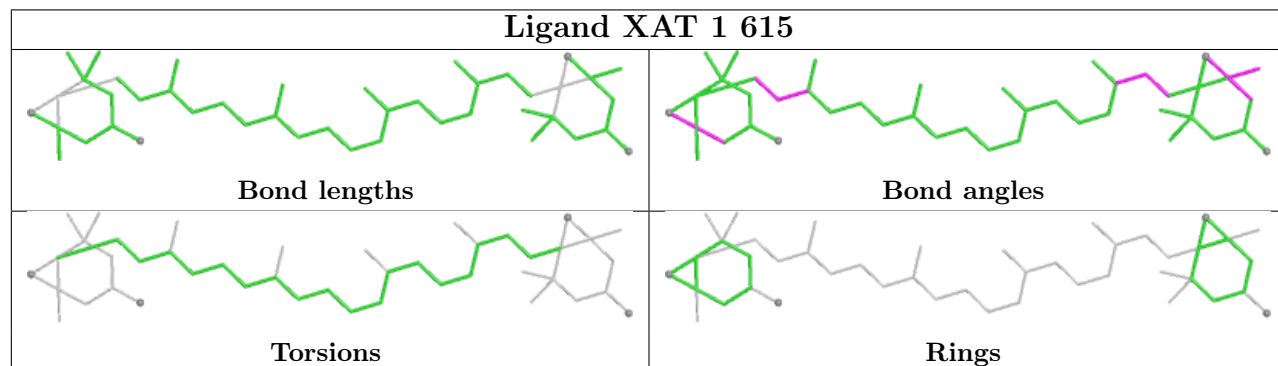




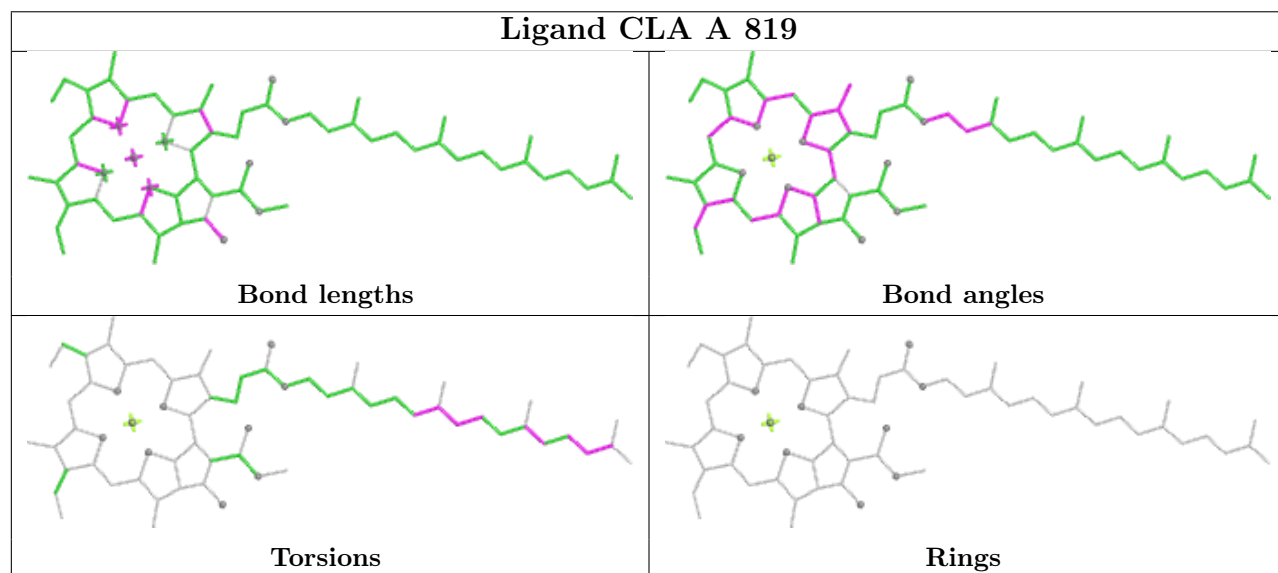
## Ligand CLA A 811



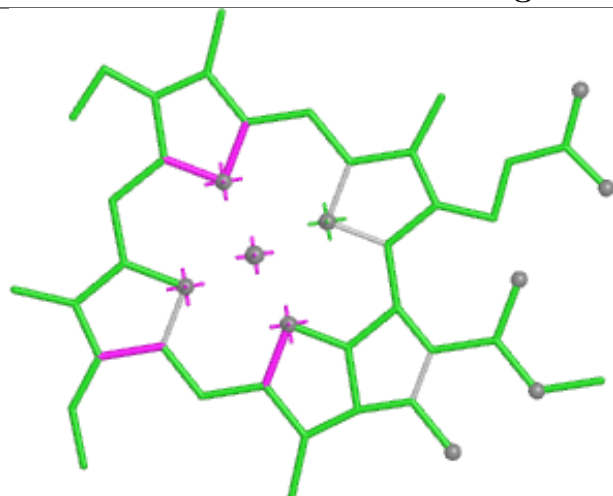
## Ligand XAT 1 615



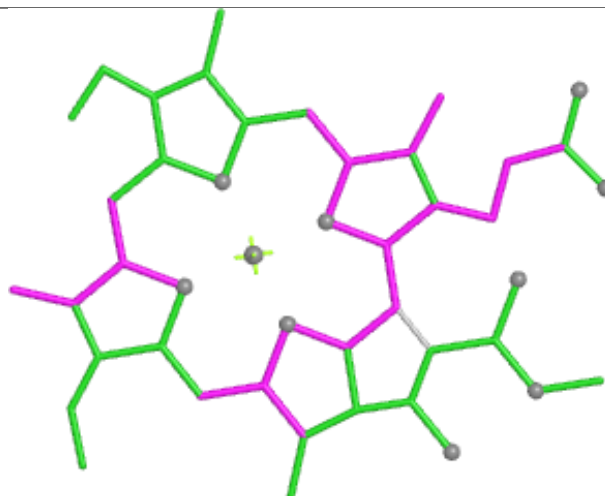
## Ligand CLA A 819



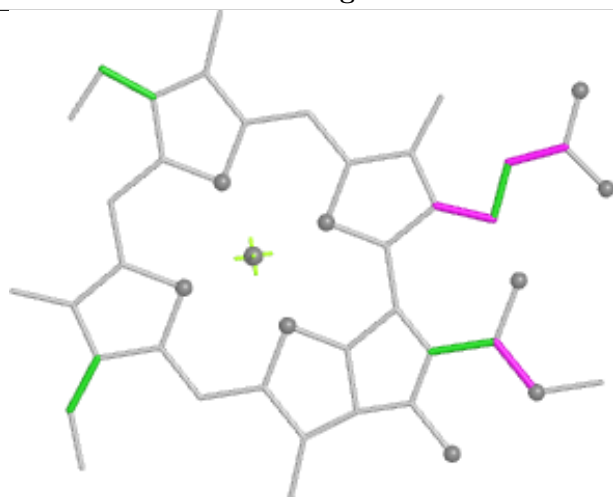
## Ligand CLA B 832



Bond lengths



Bond angles

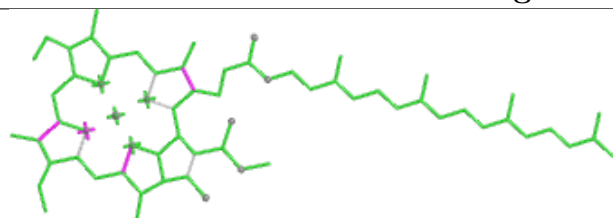


Torsions

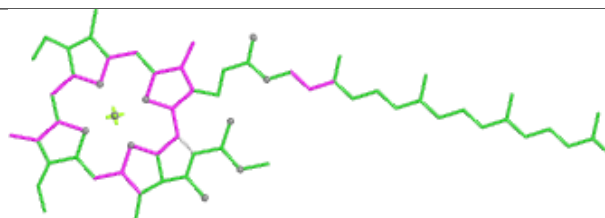


Rings

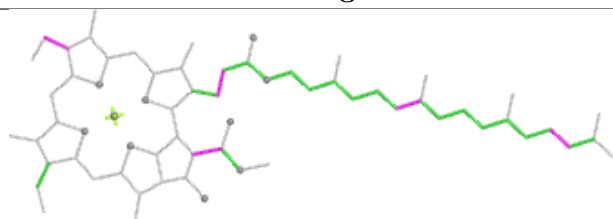
## Ligand CLA A 809



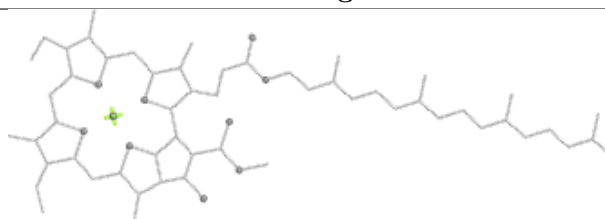
Bond lengths



Bond angles

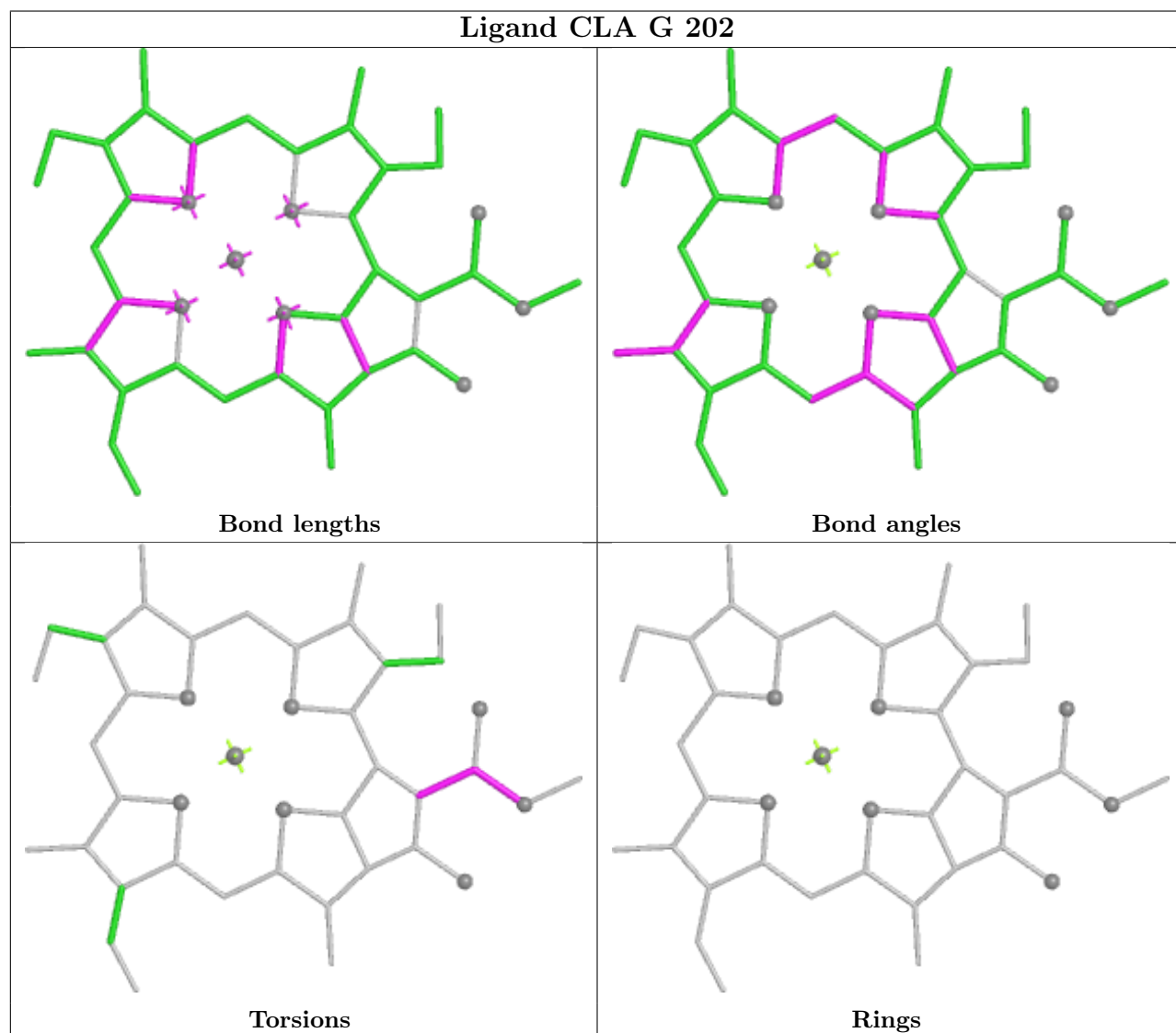
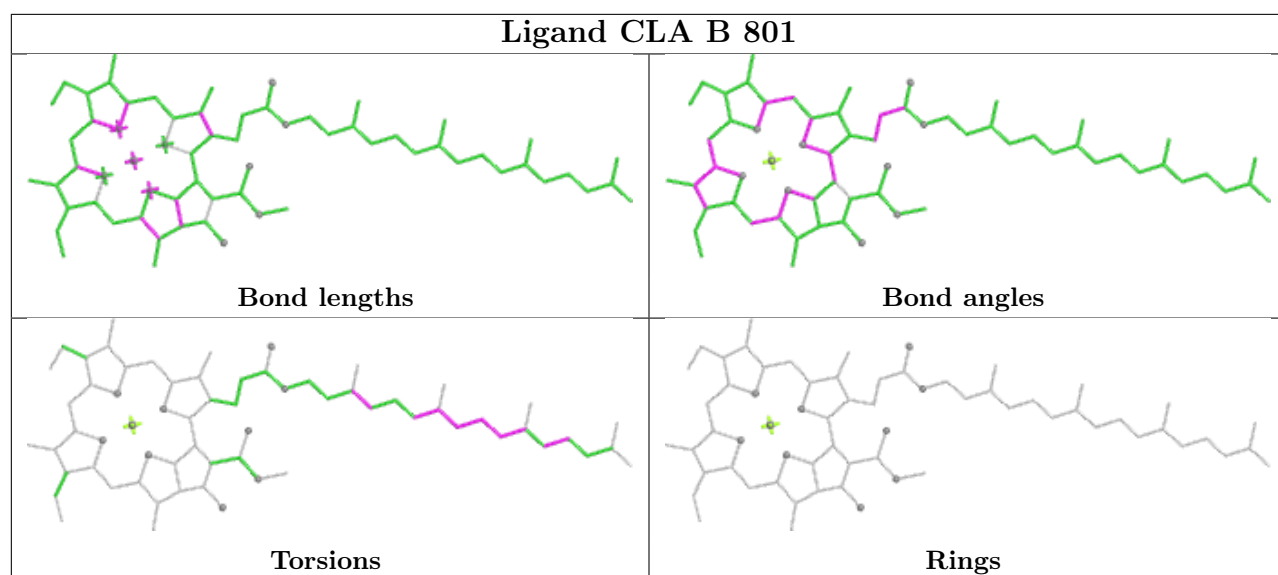


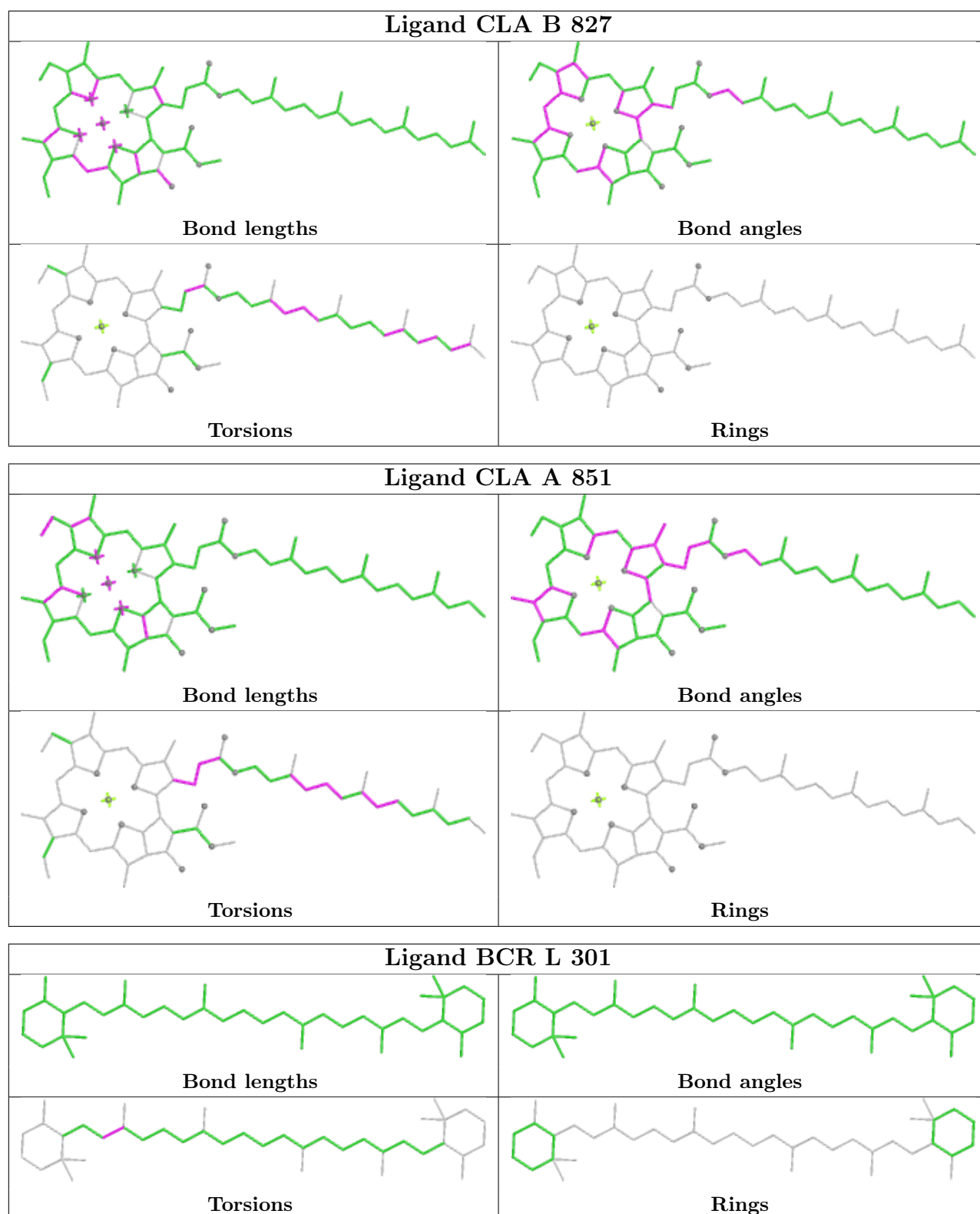
Torsions



Rings







## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

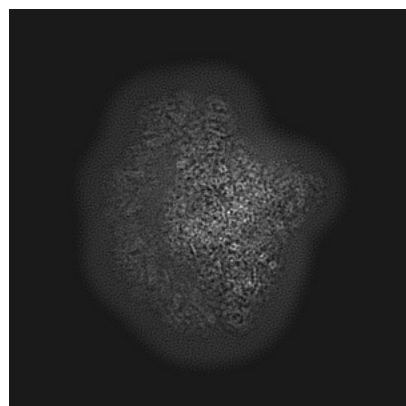
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66073. These allow visual inspection of the internal detail of the map and identification of artifacts.

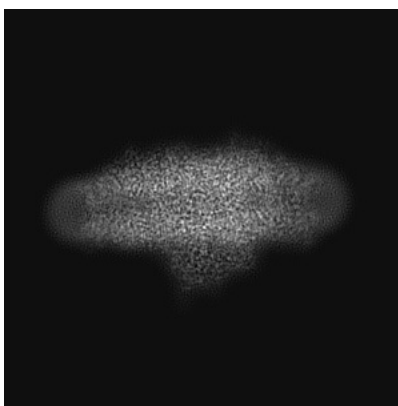
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

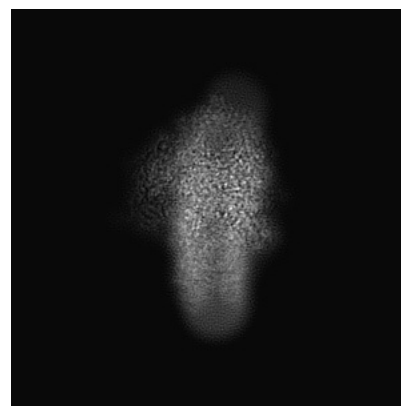
#### 6.1.1 Primary map



X

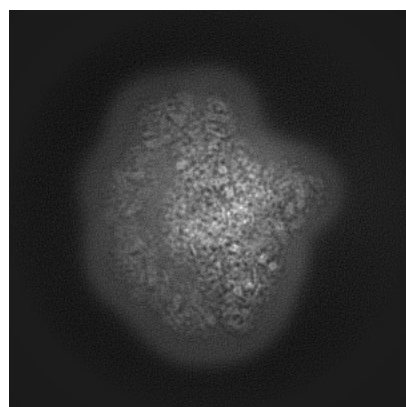


Y

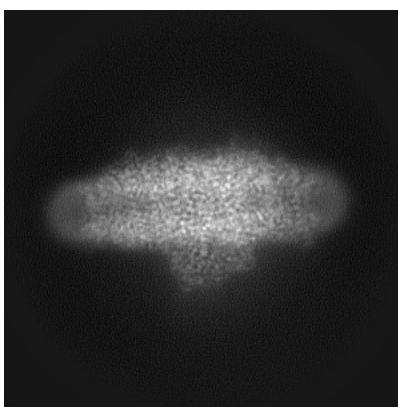


Z

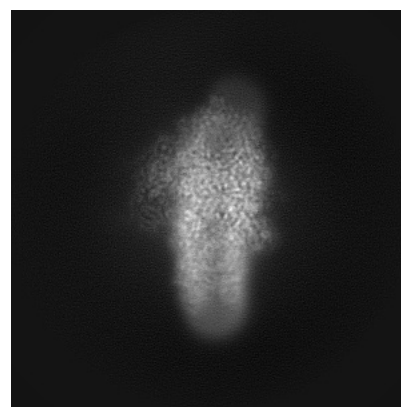
#### 6.1.2 Raw map



X



Y

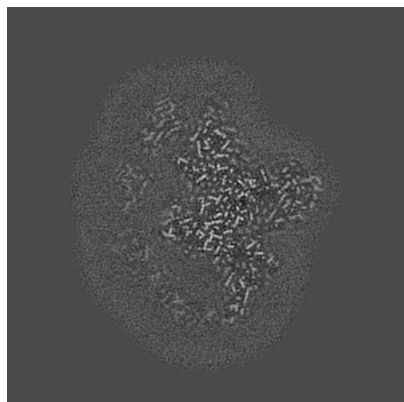


Z

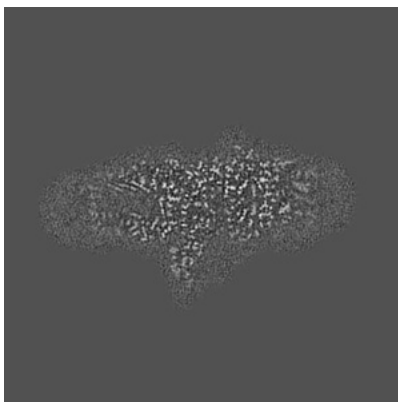
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

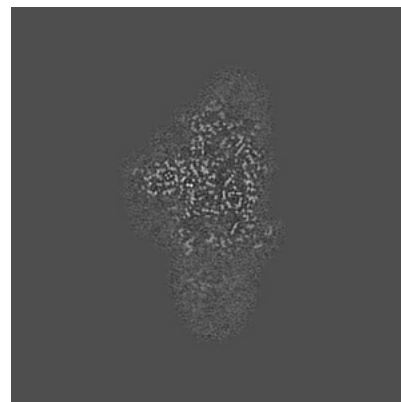
### 6.2.1 Primary map



X Index: 196

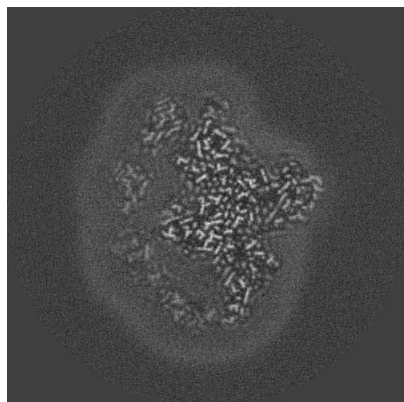


Y Index: 196

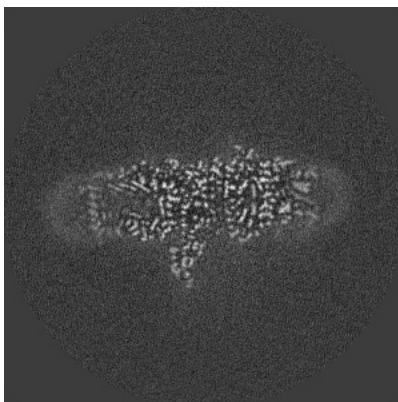


Z Index: 196

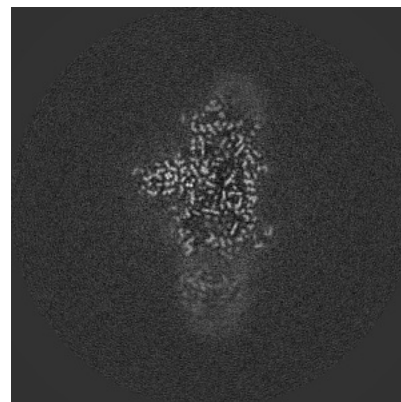
### 6.2.2 Raw map



X Index: 196



Y Index: 196

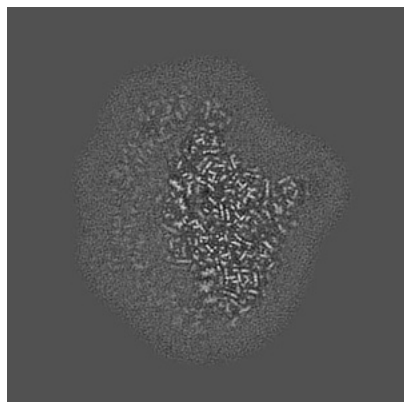


Z Index: 196

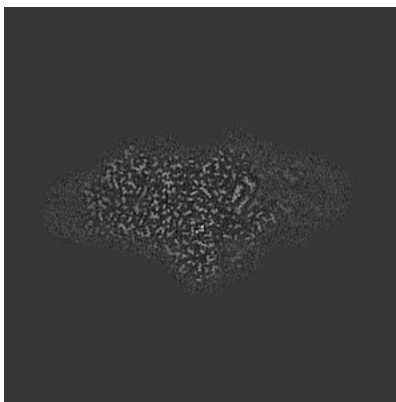
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

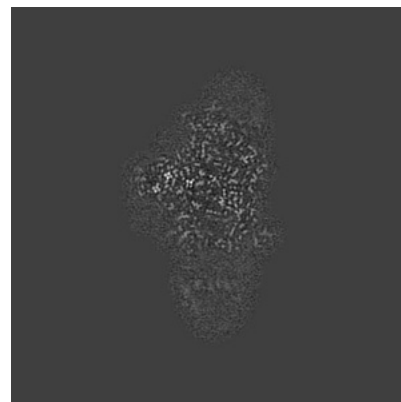
### 6.3.1 Primary map



X Index: 217

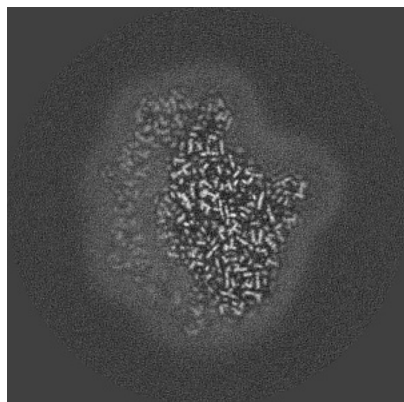


Y Index: 220

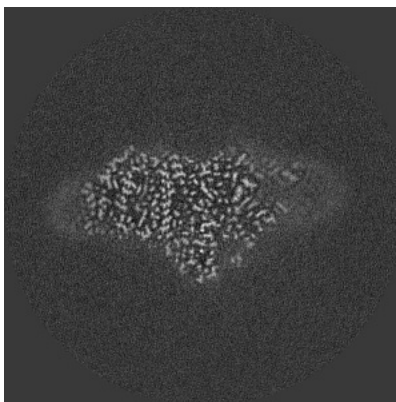


Z Index: 194

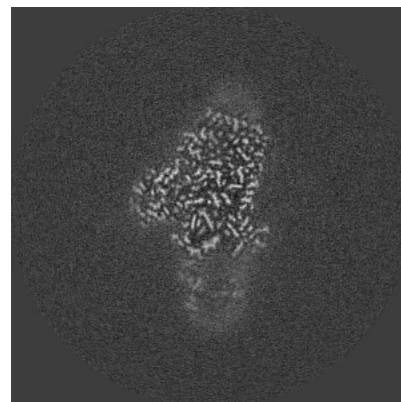
### 6.3.2 Raw map



X Index: 220



Y Index: 221



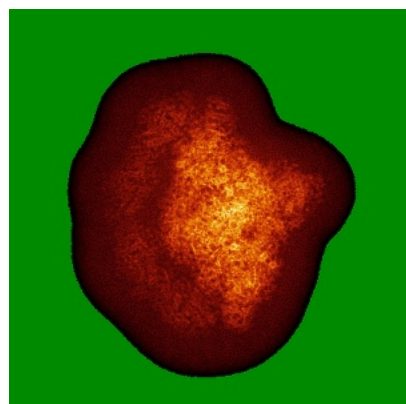
Z Index: 183

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

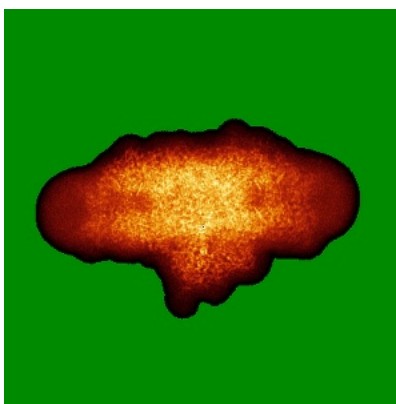


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

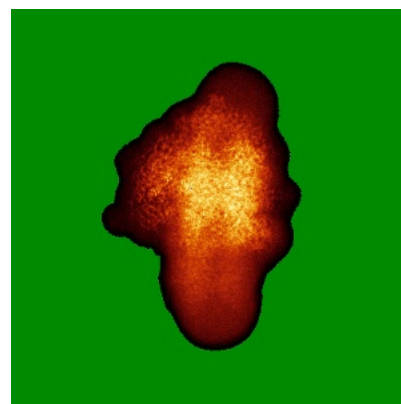
### 6.4.1 Primary map



X

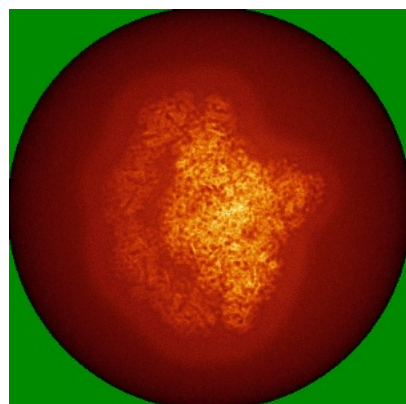


Y

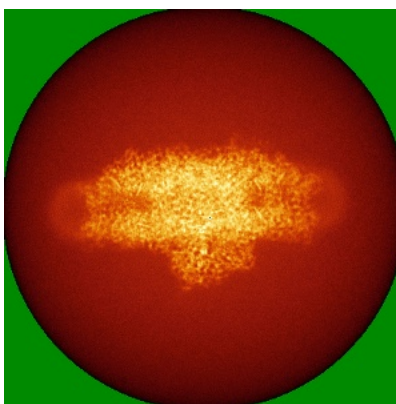


Z

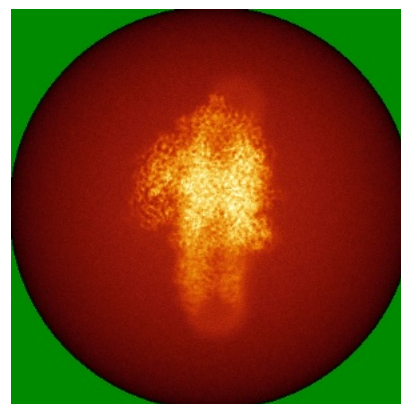
### 6.4.2 Raw map



X



Y

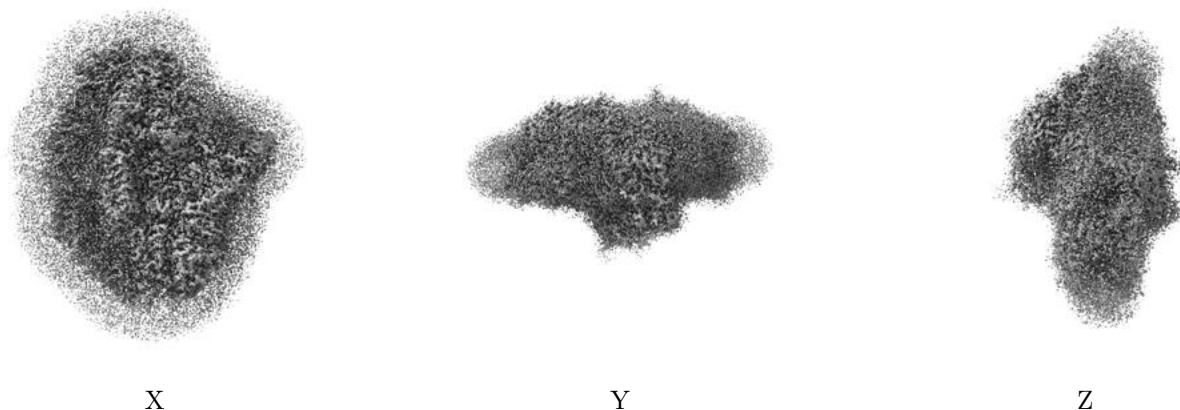


Z

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.

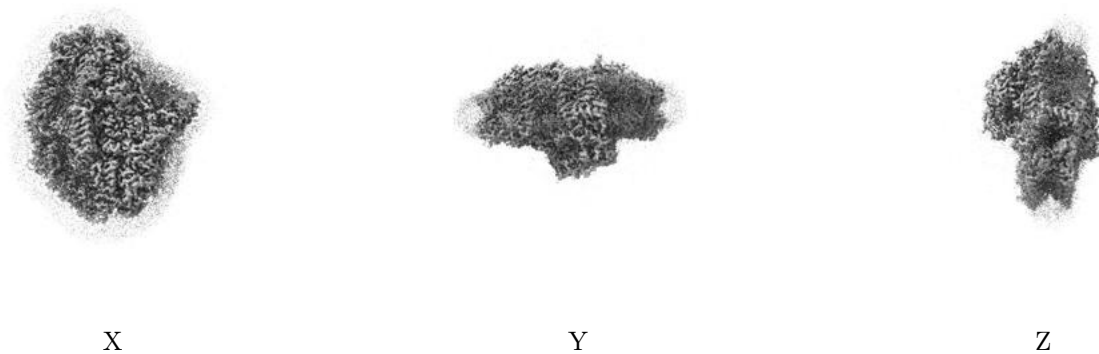
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00994. 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.



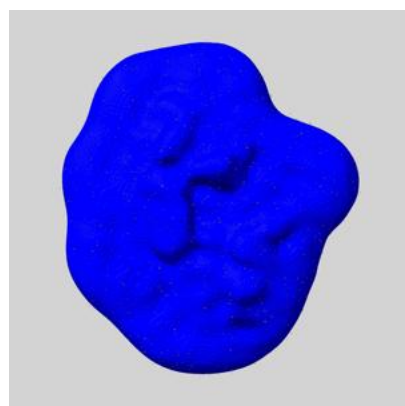
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

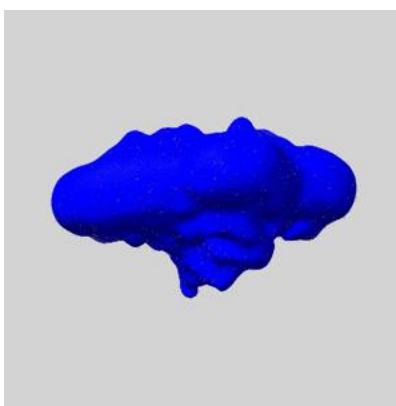
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

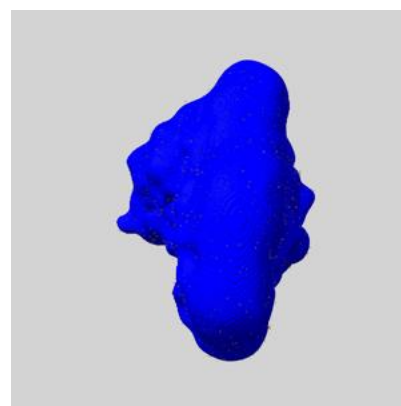
### 6.6.1 emd\_66073\_msk\_1.map [i](#)



X



Y

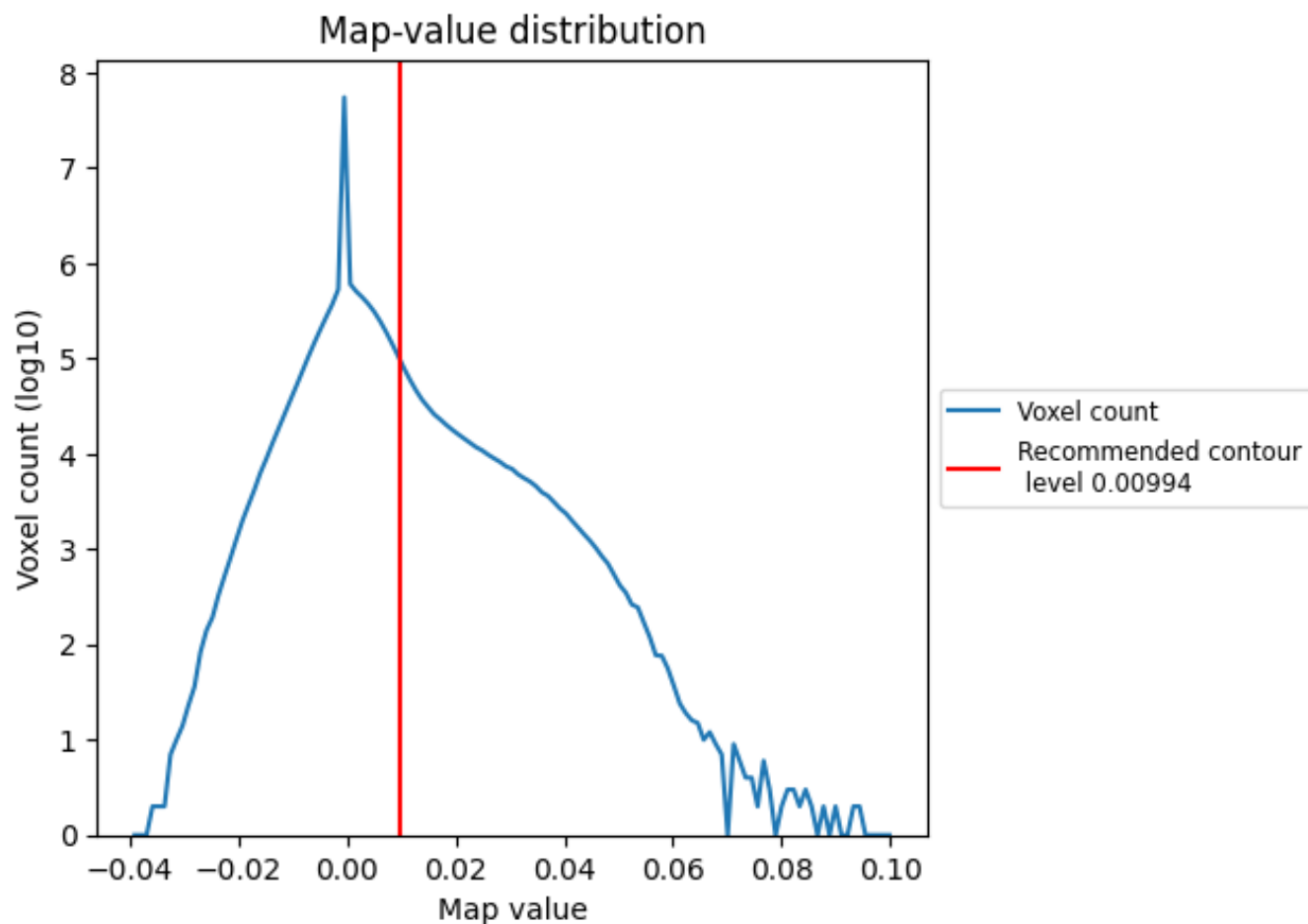


Z

## 7 Map analysis [i](#)

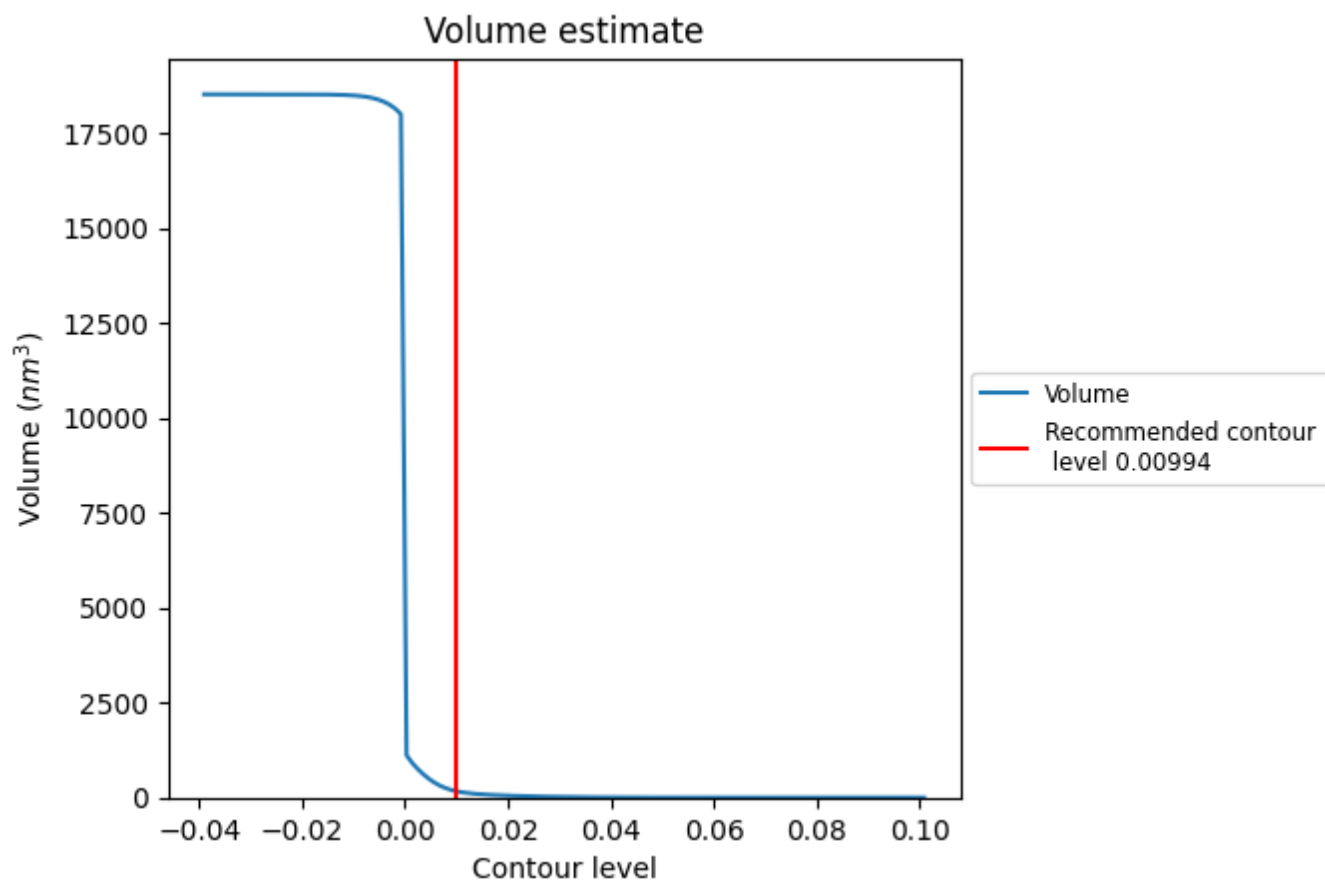
This section contains the results of statistical analysis of the map.

### 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.

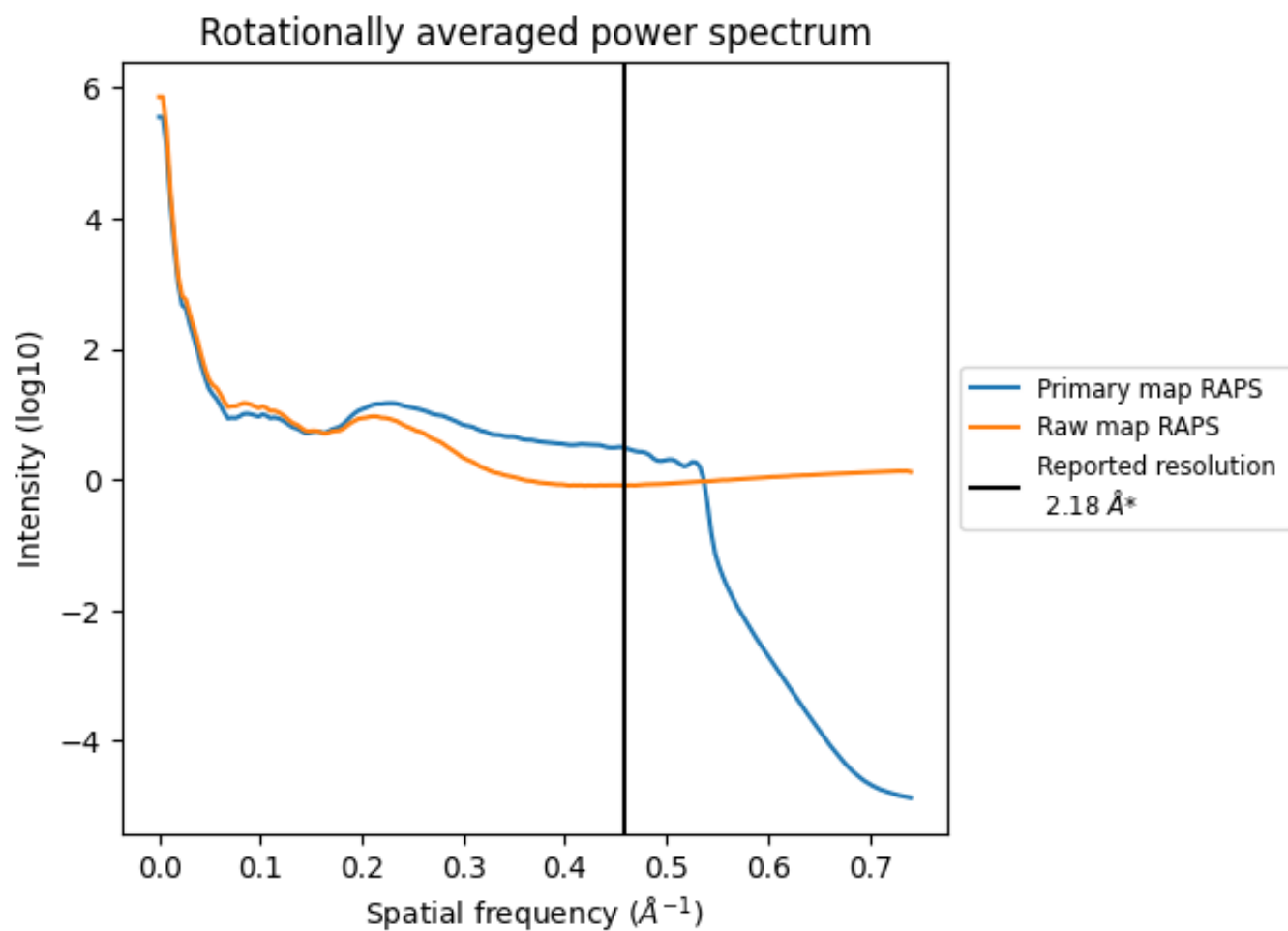
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 169 nm<sup>3</sup>; this corresponds to an approximate mass of 153 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

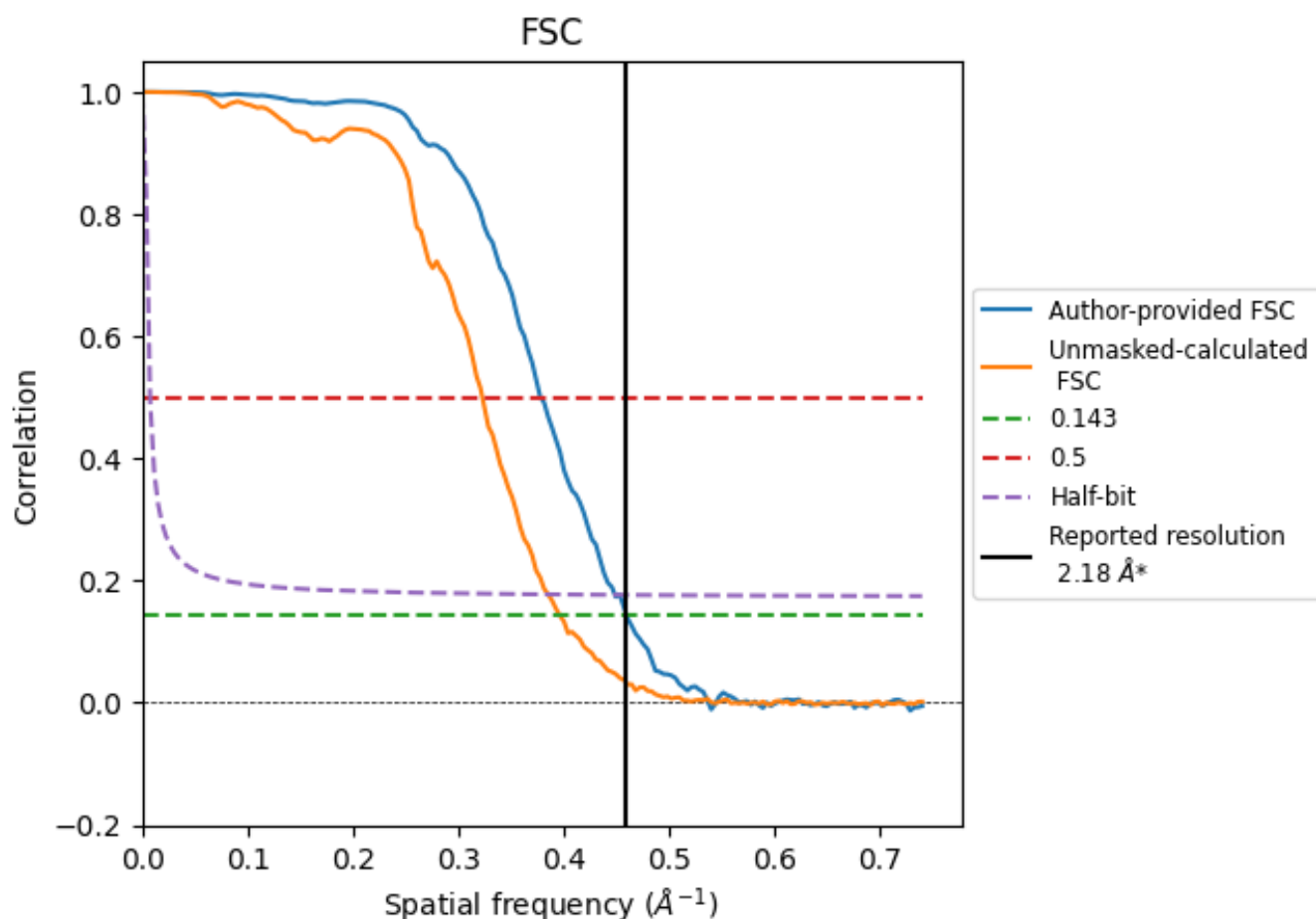


\*Reported resolution corresponds to spatial frequency of 0.459 Å<sup>-1</sup>

## 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  $0.459 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

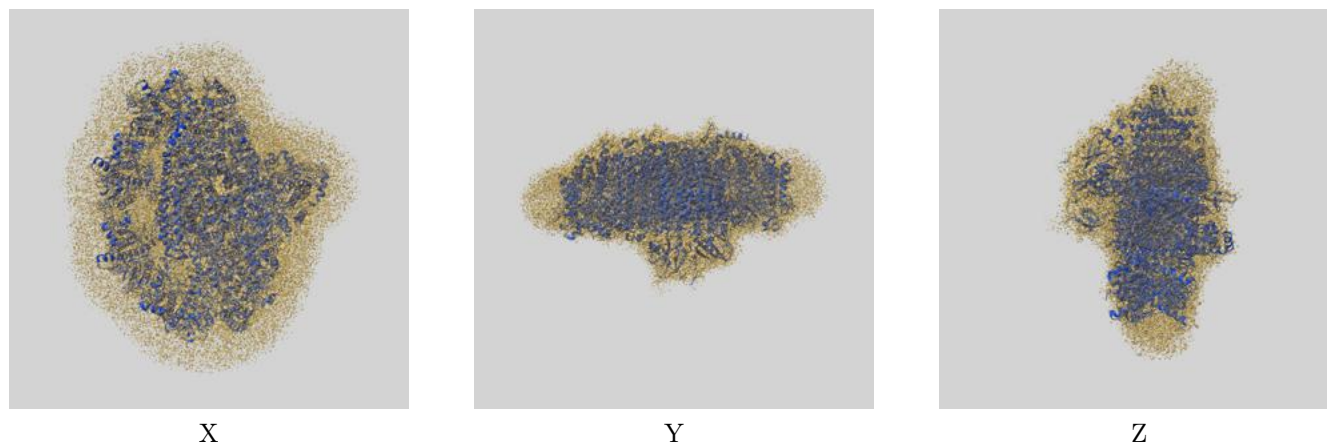
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.18	-	-
Author-provided FSC curve	2.17	2.64	2.23
Unmasked-calculated*	2.52	3.10	2.59

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.52 differs from the reported value 2.18 by more than 10 %

## 9 Map-model fit [i](#)

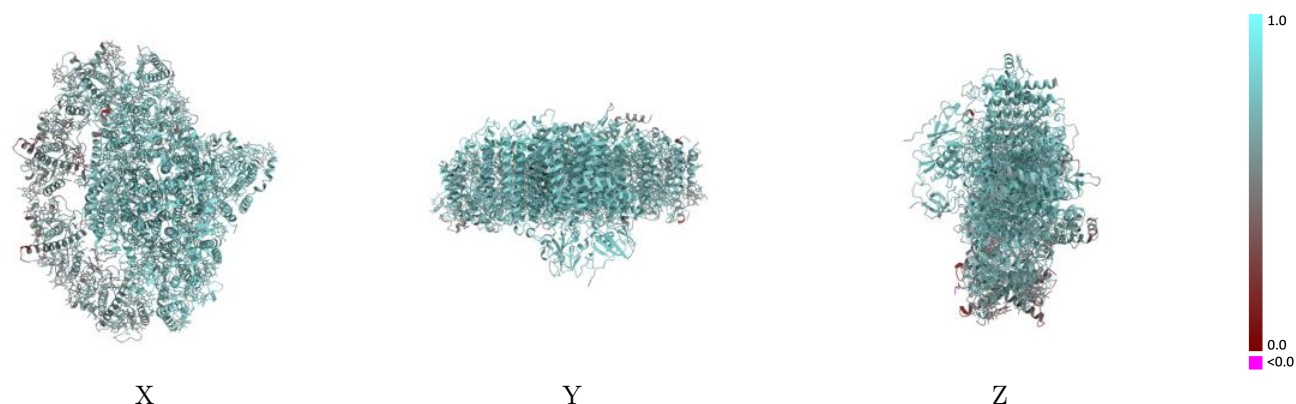
This section contains information regarding the fit between EMDB map EMD-66073 and PDB model 9WLS. Per-residue inclusion information can be found in section [3](#) on page [25](#).

### 9.1 Map-model overlay [i](#)



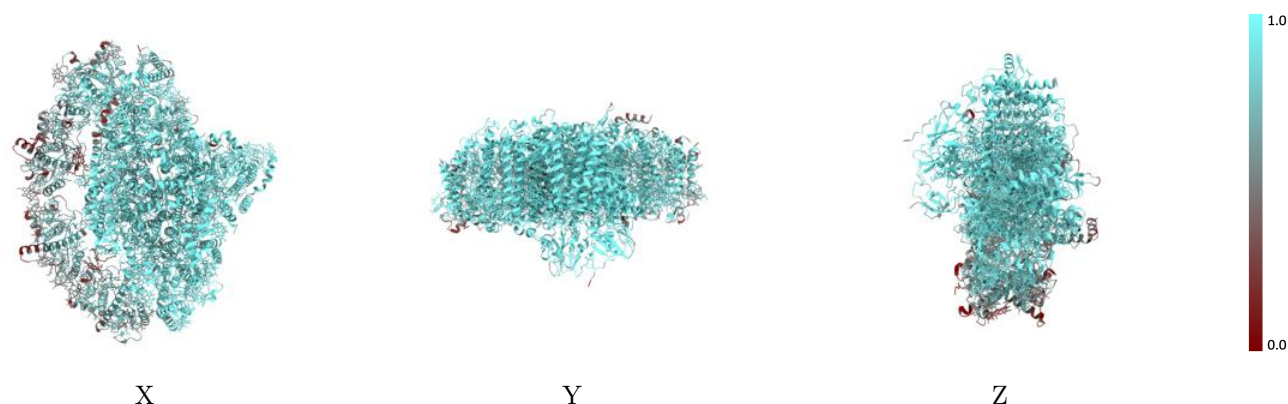
The images above show the 3D surface view of the map at the recommended contour level 0.00994 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

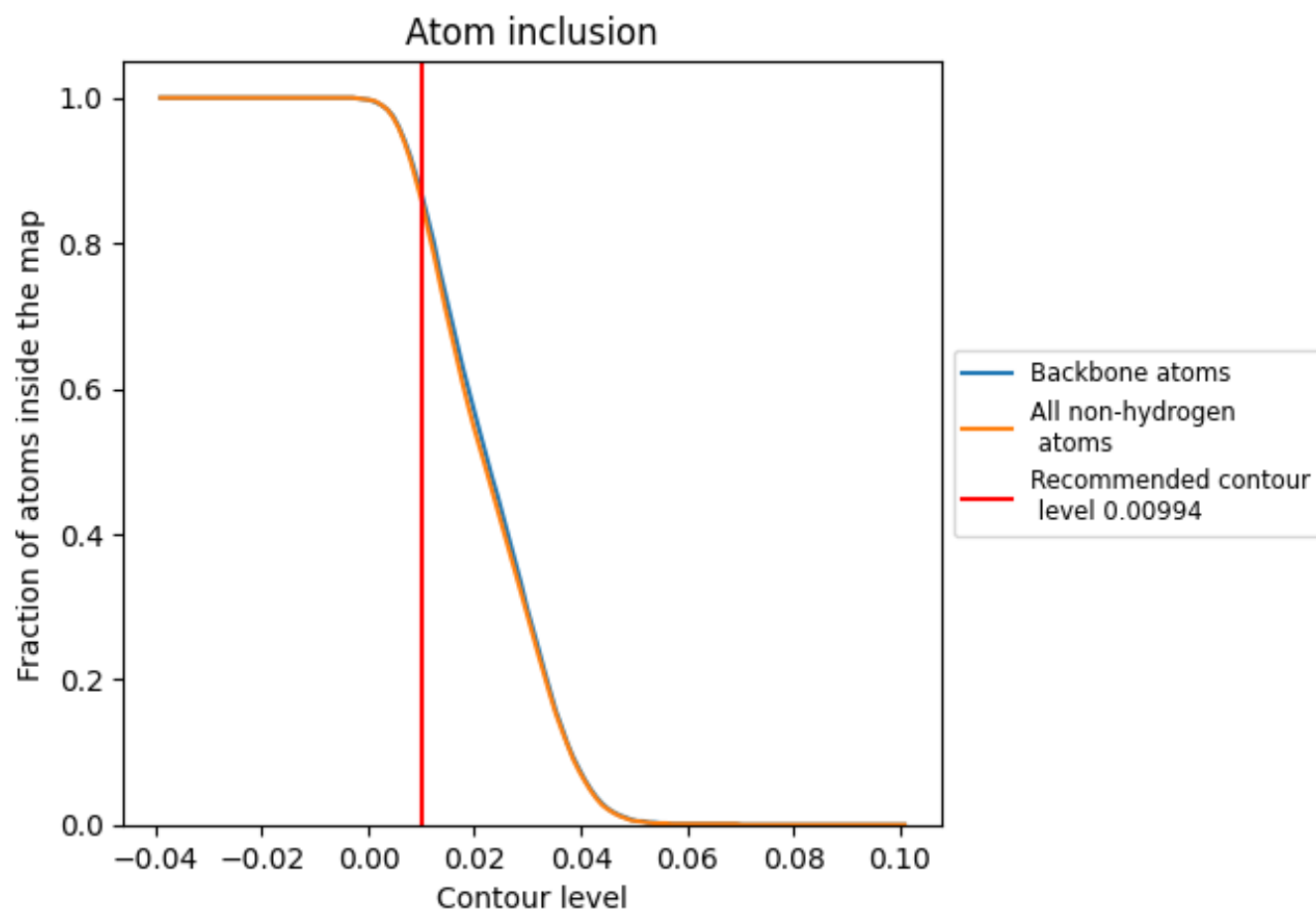
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.00994).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% 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 (0.00994) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8620	<div></div> 0.7030
1	<div></div> 0.6550	<div></div> 0.5890
2	<div></div> 0.5750	<div></div> 0.5450
3	<div></div> 0.7660	<div></div> 0.6300
4	<div></div> 0.6500	<div></div> 0.5830
A	<div></div> 0.9600	<div></div> 0.7640
B	<div></div> 0.9750	<div></div> 0.7760
C	<div></div> 0.9890	<div></div> 0.7860
D	<div></div> 0.9340	<div></div> 0.7360
E	<div></div> 0.8860	<div></div> 0.7000
F	<div></div> 0.9000	<div></div> 0.7110
G	<div></div> 0.8870	<div></div> 0.6960
H	<div></div> 0.8800	<div></div> 0.6930
I	<div></div> 0.9390	<div></div> 0.7420
J	<div></div> 0.9080	<div></div> 0.7040
K	<div></div> 0.7440	<div></div> 0.6090
L	<div></div> 0.9300	<div></div> 0.7300
N	<div></div> 0.4520	<div></div> 0.5040

1.0

0.0

<0.0