



wwPDB EM Validation Summary Report ⓘ

Sep 15, 2026 – 05:06 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

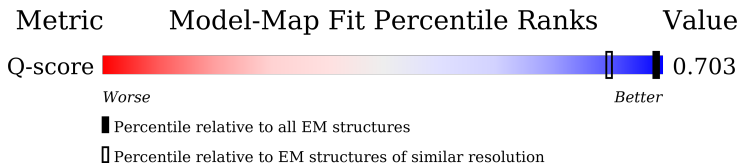
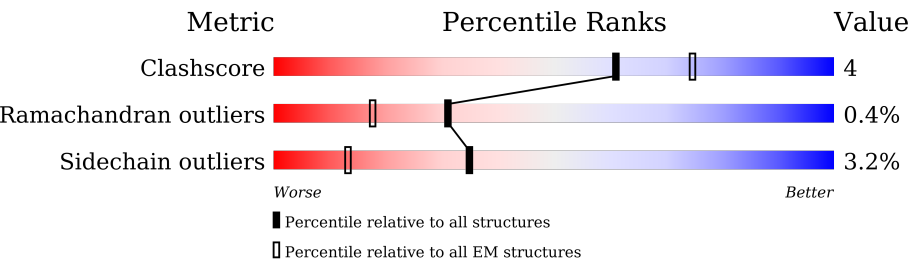
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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.



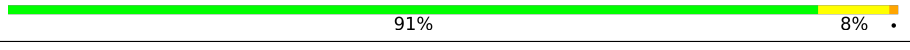
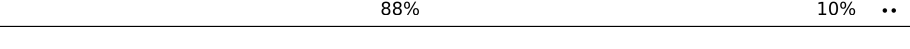
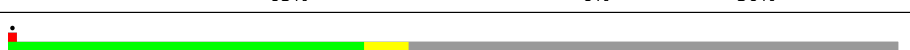
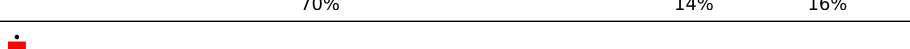
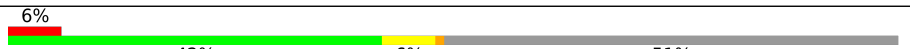
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2701 (1.70 - 2.68)

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 ≥ 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	16% 71% 9% • 20%
2	2	257	25% 72% 9% 19%
3	3	273	8% 73% 7% • 19%
4	4	251	19% 74% 5% 22%

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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		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		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		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		

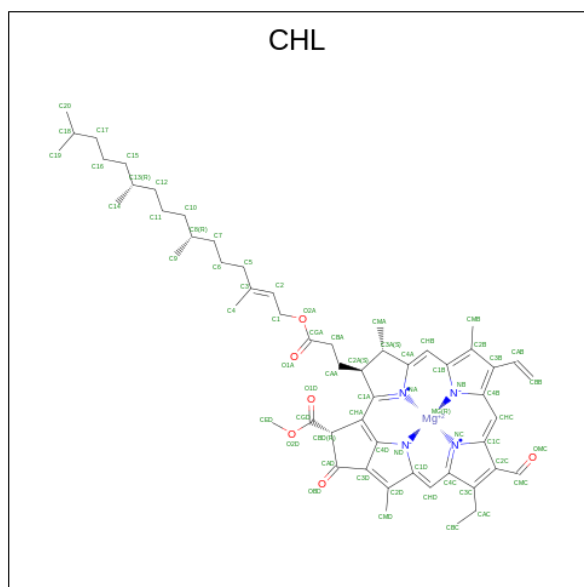
- Molecule 16 is a protein called Photosystem I reaction center subunit XI, chloroplastic.

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).



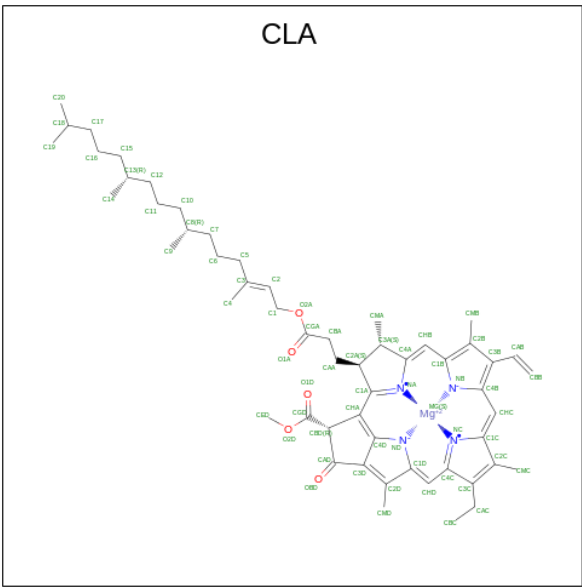
Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total	C	Mg	N	O	0
			59	48	1	4	6	

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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: C₅₅H₇₂MgN₄O₅) (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 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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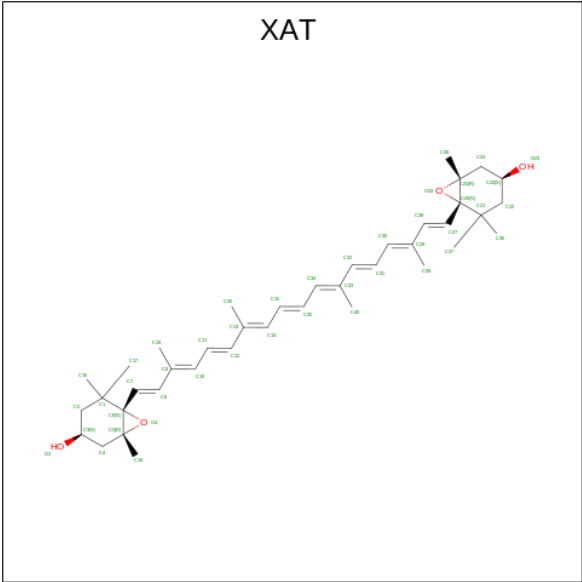
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Mol	Chain	Residues	Atoms					AltConf
19	G	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	K	1	Total	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).

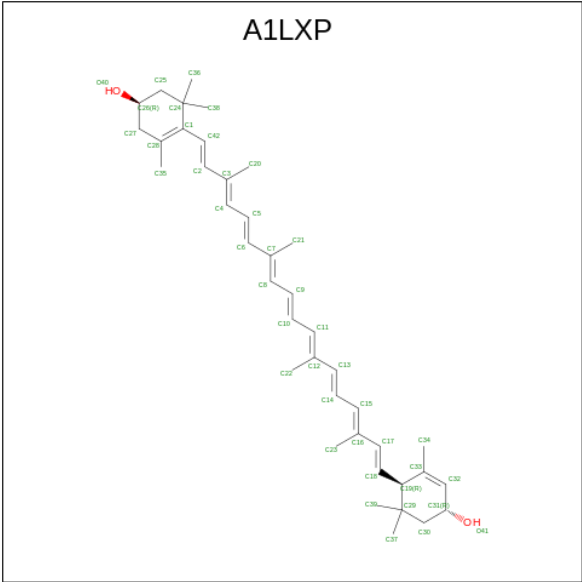
Mol	Chain	Residues	Atoms					AltConf
20	1	6	Total	C	Mg	N	O	0
			274	220	6	24	24	
20	2	7	Total	C	Mg	N	O	0
			291	234	7	28	22	
20	3	4	Total	C	Mg	N	O	0
			163	133	4	16	10	
20	4	8	Total	C	Mg	N	O	0
			354	284	8	32	30	
20	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
20	K	1	Total	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: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



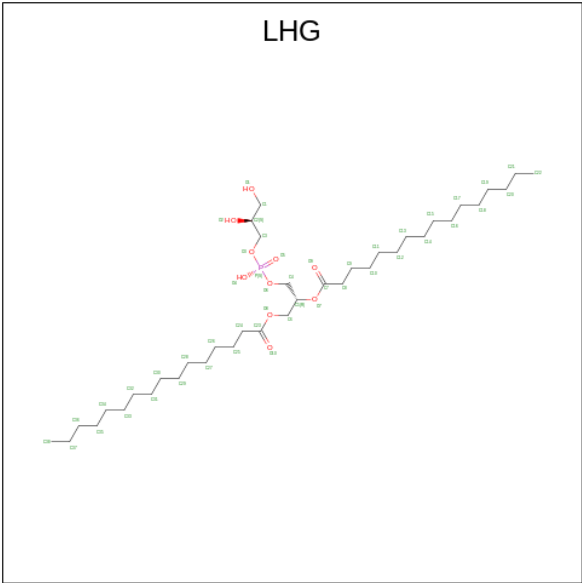
Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			44	40	4	
21	1	1	Total	C	O	0
			28	26	2	
21	2	1	Total	C	O	0
			44	40	4	

- Molecule 22 is Lutein (CCD ID: A1LXP) (formula: C₄₀H₅₆O₂) (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: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



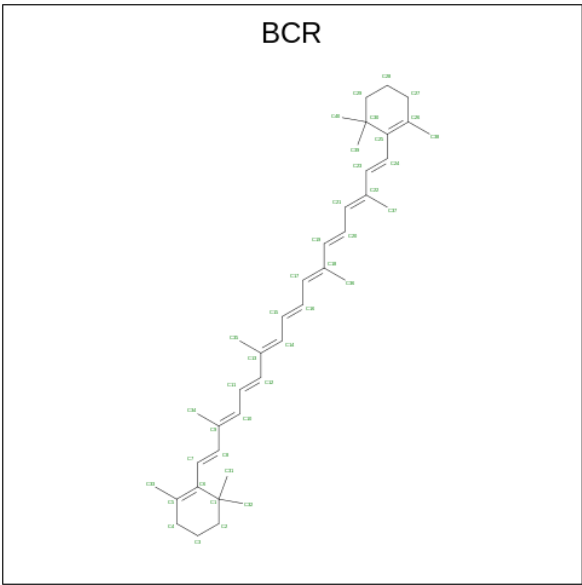
Mol	Chain	Residues	Atoms				AltConf
23	1	1	Total	C	O	P	0
			49	38	10	1	
23	1	1	Total	C	O	P	0
			21	10	10	1	
23	2	1	Total	C	O	P	0
			45	34	10	1	

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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: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



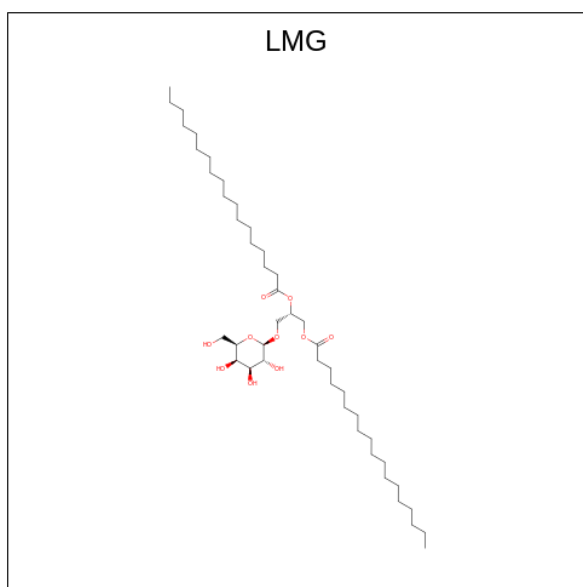
Mol	Chain	Residues	Atoms		AltConf
24	3	1	Total	C	0
			40	40	
24	4	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			25	25	
24	A	1	Total	C	0
			40	40	
24	B	1	Total	C	0
			40	40	
24	B	1	Total	C	0
			40	40	

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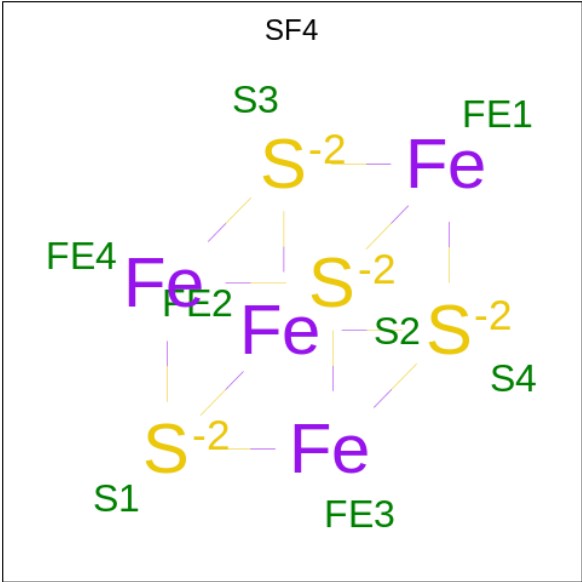
Mol	Chain	Residues	Atoms	AltConf
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	I	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	K	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	L	1	Total C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

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



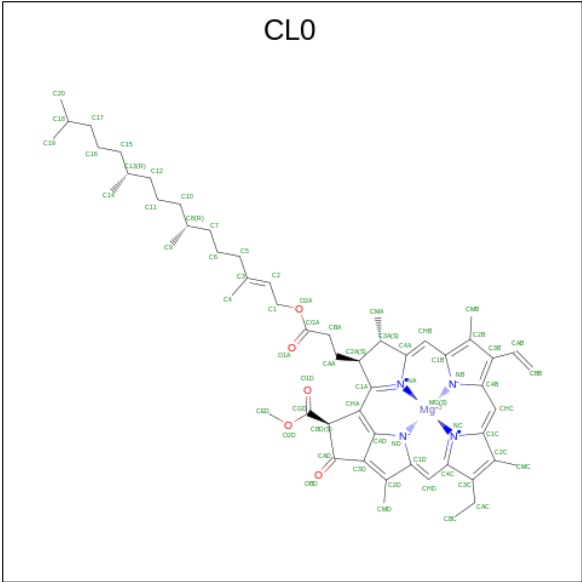
Mol	Chain	Residues	Atoms			AltConf
25	4	1	Total	C	O	0
			34	24	10	
25	F	1	Total	C	O	0
			30	20	10	
25	F	1	Total	C	O	0
			30	20	10	
25	G	1	Total	C	O	0
			35	25	10	
25	J	1	Total	C	O	0
			41	31	10	
25	N	1	Total	C	O	0
			27	18	9	

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



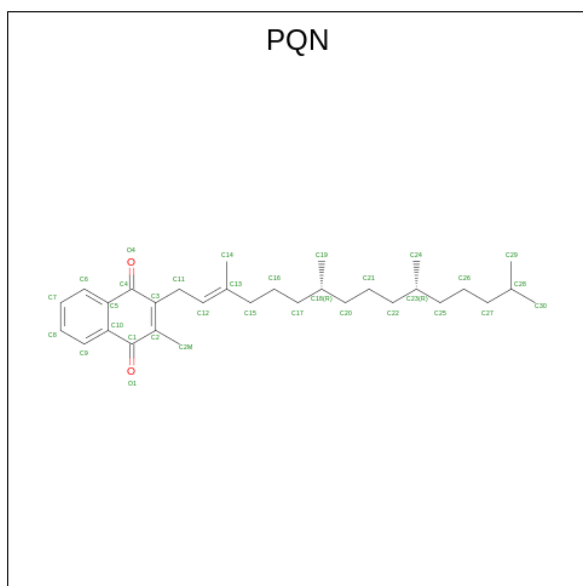
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 27 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



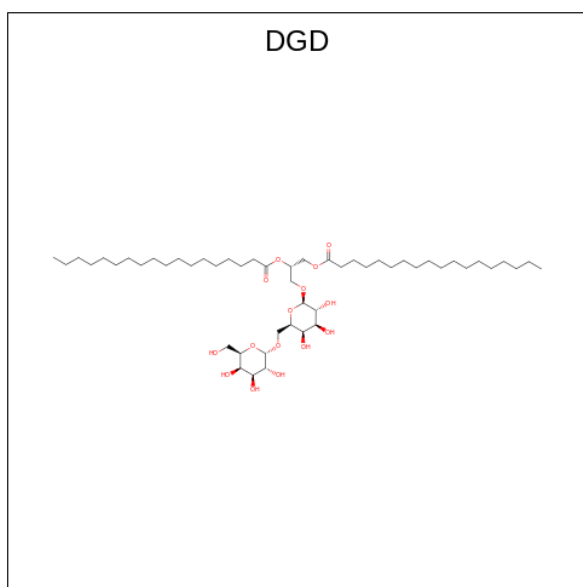
Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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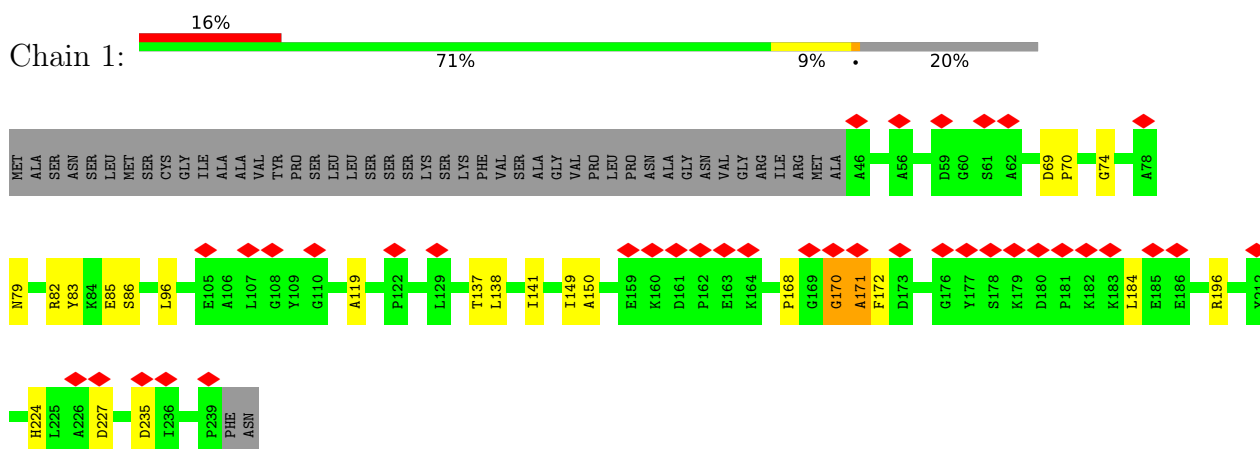
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Mol	Chain	Residues	Atoms		AltConf
30	H	7	Total 7	O 7	0
30	I	1	Total 1	O 1	0
30	J	6	Total 6	O 6	0
30	K	2	Total 2	O 2	0
30	L	16	Total 16	O 16	0
30	N	4	Total 4	O 4	0

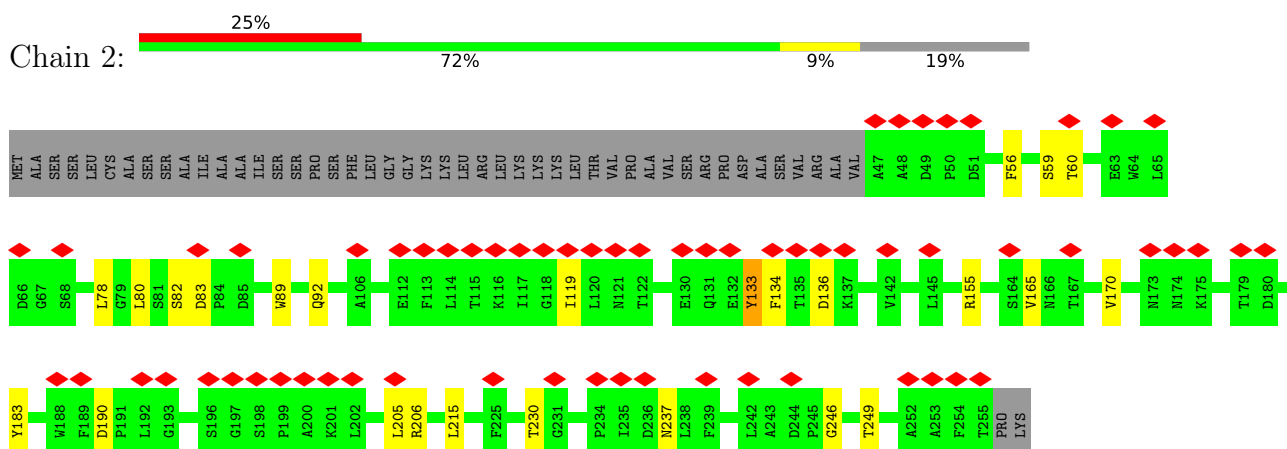
3 Residue-property plots

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.

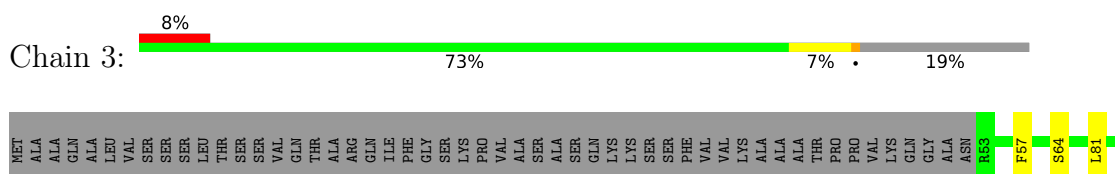
- Molecule 1: Chlorophyll a-b binding protein 6, chloroplastic

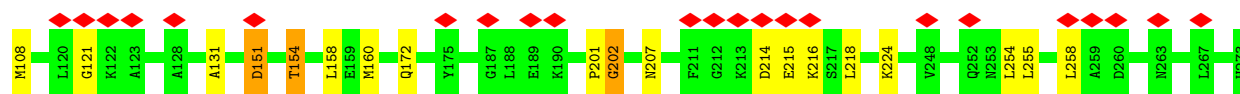


- Molecule 2: Photosystem I chlorophyll a/b-binding protein 2, chloroplastic

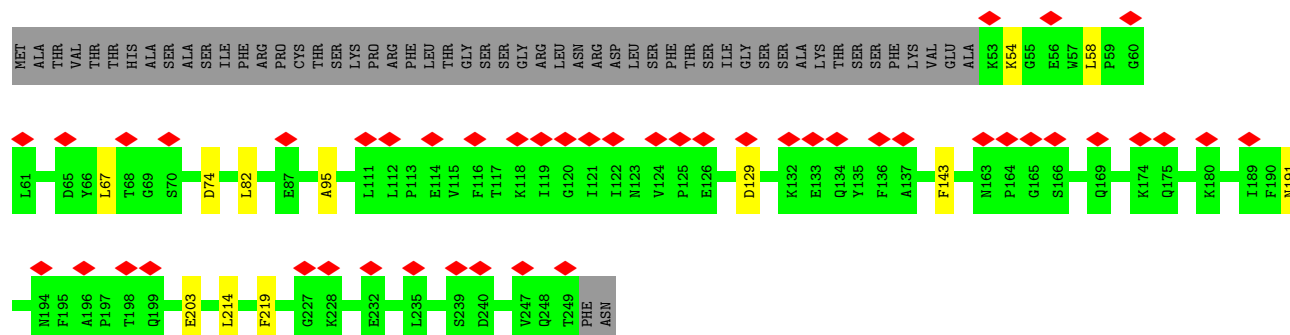
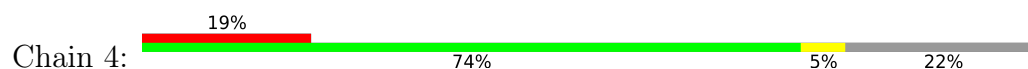


- Molecule 3: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic

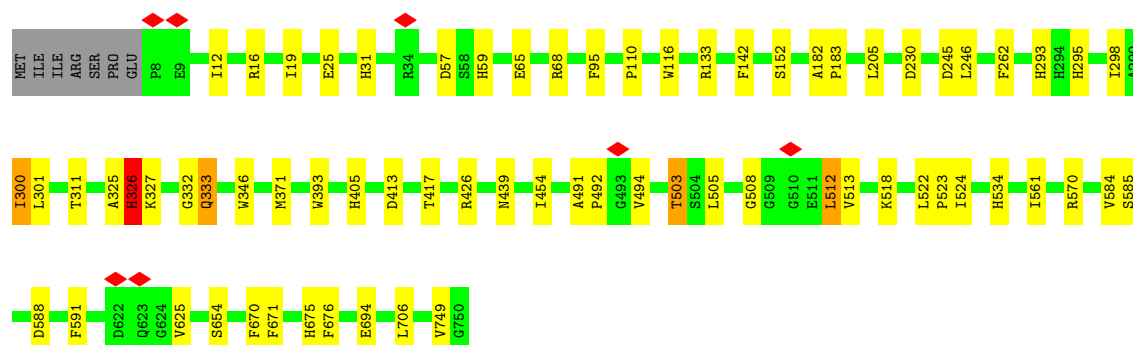
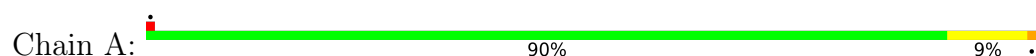




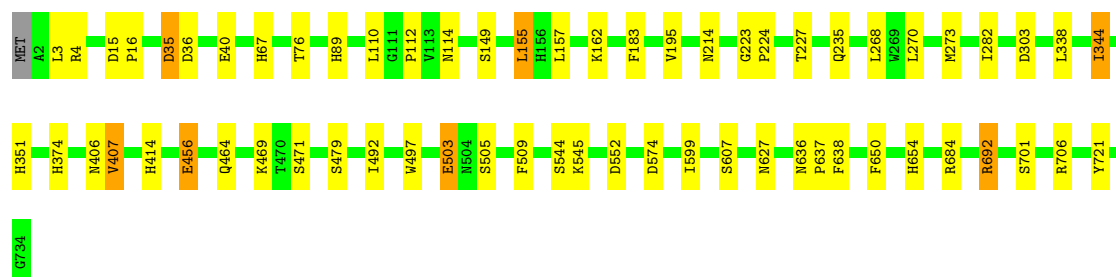
- Molecule 4: Chlorophyll a-b binding protein 4, chloroplastic



- 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



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: XAT, A1LXP, SF4, CHL, UNL, BCR, LMG, CL0, DGD, LHG, CLA, PQN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	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	807	30	49,53,73	1.89	9 (18%)	59,89,113	1.42	10 (16%)
19	CLA	A	837	5	69,73,73	1.64	10 (14%)	83,113,113	1.66	10 (12%)
24	BCR	F	302	-	41,41,41	0.59	0	56,56,56	0.76	0
19	CLA	A	814	5	69,73,73	1.52	6 (8%)	83,113,113	1.64	17 (20%)
19	CLA	A	805	5	51,55,73	1.89	9 (17%)	61,91,113	1.47	7 (11%)
19	CLA	B	803	6	49,53,73	1.74	9 (18%)	59,89,113	1.78	12 (20%)
19	CLA	G	202	30	46,50,73	1.96	10 (21%)	55,85,113	1.54	7 (12%)
19	CLA	3	312	3	46,50,73	1.90	9 (19%)	55,85,113	1.49	5 (9%)
19	CLA	A	823	30	69,73,73	1.57	8 (11%)	83,113,113	1.66	13 (15%)
22	A1LXP	J	102	-	42,43,43	0.41	0	51,60,60	0.80	1 (1%)
19	CLA	B	832	6	49,53,73	1.92	7 (14%)	59,89,113	2.13	14 (23%)
19	CLA	B	827	6	69,73,73	1.91	11 (15%)	83,113,113	1.52	11 (13%)
19	CLA	A	826	5	69,73,73	1.17	6 (8%)	83,113,113	1.55	9 (10%)
18	CHL	2	315	30	50,54,74	1.18	6 (12%)	56,90,114	1.97	12 (21%)
19	CLA	B	825	6	69,73,73	1.55	5 (7%)	83,113,113	1.60	9 (10%)
22	A1LXP	3	305	-	42,43,43	0.42	0	51,60,60	0.70	1 (1%)
24	BCR	G	205	-	41,41,41	0.54	0	56,56,56	0.52	0
19	CLA	B	830	6	69,73,73	1.46	6 (8%)	83,113,113	1.61	9 (10%)
19	CLA	H	201	12	59,63,73	1.61	10 (16%)	71,101,113	1.39	9 (12%)
19	CLA	B	836	30	60,64,73	1.76	8 (13%)	72,102,113	1.23	8 (11%)
27	CL0	A	830	5	69,73,73	1.65	6 (8%)	83,113,113	1.55	8 (9%)
19	CLA	3	302	3	56,60,73	1.89	8 (14%)	67,97,113	1.34	5 (7%)
19	CLA	A	815	5	49,53,73	1.75	9 (18%)	59,89,113	1.87	12 (20%)
19	CLA	A	840	19,5	69,73,73	1.57	8 (11%)	83,113,113	1.49	10 (12%)
19	CLA	B	823	6	69,73,73	1.14	7 (10%)	83,113,113	1.23	8 (9%)
19	CLA	B	838	6	49,53,73	1.65	11 (22%)	59,89,113	1.30	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	4	318	4	49,53,73	2.34	7 (14%)	59,89,113	1.55	9 (15%)
24	BCR	K	201	-	41,41,41	0.42	0	56,56,56	0.51	0
19	CLA	A	816	5	54,58,73	1.82	7 (12%)	65,95,113	1.28	9 (13%)
19	CLA	A	825	5	46,50,73	2.01	8 (17%)	55,85,113	1.45	9 (16%)
19	CLA	A	828	5	69,73,73	1.57	10 (14%)	83,113,113	1.70	16 (19%)
19	CLA	A	832	5	49,53,73	2.07	7 (14%)	59,89,113	1.82	11 (18%)
19	CLA	F	303	10	46,50,73	1.82	8 (17%)	55,85,113	1.72	9 (16%)
18	CHL	1	606	1	47,51,74	1.45	4 (8%)	52,86,114	2.47	10 (19%)
24	BCR	B	816	-	41,41,41	0.55	0	56,56,56	0.74	1 (1%)
19	CLA	B	843	6	69,73,73	1.43	8 (11%)	83,113,113	1.36	10 (12%)
19	CLA	B	822	6	69,73,73	1.62	8 (11%)	83,113,113	1.22	7 (8%)
18	CHL	2	313	30	46,50,74	1.31	3 (6%)	51,85,114	2.16	14 (27%)
19	CLA	A	821	5	56,60,73	1.45	9 (16%)	67,97,113	1.42	8 (11%)
24	BCR	3	316	-	41,41,41	0.46	0	56,56,56	0.65	0
19	CLA	B	844	6	63,67,73	1.76	11 (17%)	75,105,113	1.55	10 (13%)
19	CLA	4	307	4	49,53,73	2.37	5 (10%)	59,89,113	1.59	8 (13%)
19	CLA	B	847	6	54,58,73	1.46	9 (16%)	65,95,113	1.51	5 (7%)
19	CLA	1	612	1	59,63,73	2.04	8 (13%)	71,101,113	1.28	10 (14%)
28	PQN	A	839	-	34,34,34	0.41	0	42,45,45	0.74	1 (2%)
19	CLA	1	608	1	61,65,73	1.74	7 (11%)	73,103,113	1.17	7 (9%)
19	CLA	B	807	6	49,53,73	1.33	7 (14%)	59,89,113	1.44	6 (10%)
19	CLA	1	607	-	55,59,73	1.91	8 (14%)	66,96,113	1.33	4 (6%)
19	CLA	3	306	3	51,55,73	2.17	8 (15%)	61,91,113	1.51	9 (14%)
19	CLA	A	818	5	69,73,73	1.54	9 (13%)	83,113,113	1.56	13 (15%)
23	LHG	A	835	-	48,48,48	0.80	1 (2%)	51,54,54	1.43	7 (13%)
22	A1LXP	2	309	-	42,43,43	0.27	0	51,60,60	0.65	0
25	LMG	J	103	-	41,41,55	0.45	0	49,49,63	0.68	1 (2%)
26	SF4	A	803	6,5	0,12,12	-	-	-	-	-
19	CLA	B	826	6	69,73,73	1.15	5 (7%)	83,113,113	1.38	9 (10%)
19	CLA	A	836	5	49,53,73	1.62	7 (14%)	59,89,113	1.70	10 (16%)
19	CLA	B	834	6	69,73,73	1.10	4 (5%)	83,113,113	1.46	13 (15%)
24	BCR	B	813	-	41,41,41	0.75	1 (2%)	56,56,56	0.69	1 (1%)
21	XAT	2	306	-	39,47,47	0.31	0	54,74,74	1.02	2 (3%)
19	CLA	B	819	6	69,73,73	1.18	7 (10%)	83,113,113	1.11	6 (7%)
19	CLA	B	833	6	64,68,73	2.41	7 (10%)	77,107,113	1.51	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	839	6	47,51,73	1.85	9 (19%)	56,86,113	1.64	8 (14%)
19	CLA	3	304	3	59,63,73	1.77	8 (13%)	71,101,113	1.46	10 (14%)
19	CLA	A	811	5	59,63,73	2.13	8 (13%)	71,101,113	1.31	9 (12%)
19	CLA	B	840	6	49,53,73	2.00	8 (16%)	59,89,113	1.93	12 (20%)
19	CLA	B	801	6	69,73,73	1.62	8 (11%)	83,113,113	1.48	9 (10%)
19	CLA	1	603	1	61,65,73	1.83	8 (13%)	73,103,113	1.53	9 (12%)
24	BCR	B	812	-	41,41,41	0.59	0	56,56,56	0.79	1 (1%)
19	CLA	B	818	30	69,73,73	1.28	6 (8%)	83,113,113	1.83	16 (19%)
19	CLA	F	306	30	52,56,73	1.59	7 (13%)	62,92,113	1.38	8 (12%)
19	CLA	A	833	-	69,73,73	1.58	10 (14%)	83,113,113	1.20	5 (6%)
24	BCR	A	838	-	41,41,41	0.63	1 (2%)	56,56,56	0.54	0
19	CLA	B	802	6	64,68,73	1.35	8 (12%)	77,107,113	1.40	8 (10%)
18	CHL	4	313	30	50,54,74	1.44	5 (10%)	56,90,114	2.02	11 (19%)
24	BCR	F	304	-	41,41,41	0.47	0	56,56,56	0.58	0
19	CLA	B	842	30	54,58,73	1.71	10 (18%)	65,95,113	1.66	10 (15%)
19	CLA	B	845	6	69,73,73	1.49	8 (11%)	83,113,113	1.51	11 (13%)
19	CLA	B	806	6	69,73,73	1.37	5 (7%)	83,113,113	1.86	9 (10%)
19	CLA	B	828	6	55,59,73	1.73	6 (10%)	66,96,113	1.69	12 (18%)
24	BCR	A	845	-	41,41,41	0.51	0	56,56,56	0.65	0
24	BCR	A	804	-	41,41,41	0.65	0	56,56,56	0.70	2 (3%)
18	CHL	3	303	3	70,74,74	0.99	5 (7%)	80,114,114	1.95	13 (16%)
19	CLA	B	846	6	69,73,73	1.44	9 (13%)	83,113,113	1.42	9 (10%)
19	CLA	A	802	19,5	60,64,73	1.23	5 (8%)	72,102,113	1.65	12 (16%)
24	BCR	A	841	-	41,41,41	0.66	0	56,56,56	0.63	0
25	LMG	F	305	-	30,30,55	0.34	0	38,38,63	0.68	1 (2%)
22	A1LXP	4	303	-	42,43,43	0.78	3 (7%)	51,60,60	0.89	1 (1%)
19	CLA	4	317	4	61,65,73	1.90	9 (14%)	73,103,113	1.44	9 (12%)
19	CLA	2	310	2	59,63,73	2.12	6 (10%)	71,101,113	1.51	14 (19%)
19	CLA	G	203	11	49,53,73	1.73	11 (22%)	59,89,113	2.06	10 (16%)
19	CLA	1	602	1	64,68,73	1.67	9 (14%)	77,107,113	1.66	15 (19%)
26	SF4	C	101	7	0,12,12	-	-	-	-	-
19	CLA	A	829	5	69,73,73	1.38	8 (11%)	83,113,113	1.53	11 (13%)
23	LHG	1	617	20	48,48,48	0.35	0	51,54,54	0.79	2 (3%)
19	CLA	B	831	6	69,73,73	1.41	8 (11%)	83,113,113	1.49	9 (10%)
19	CLA	4	311	4	49,53,73	2.24	10 (20%)	59,89,113	1.58	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CHL	2	316	2	63,67,74	1.17	5 (7%)	71,105,114	2.04	10 (14%)
19	CLA	B	810	23	69,73,73	1.44	8 (11%)	83,113,113	1.22	6 (7%)
19	CLA	B	824	6	56,60,73	1.70	6 (10%)	67,97,113	1.70	10 (14%)
23	LHG	2	302	20	44,44,48	0.36	0	47,50,54	0.56	0
24	BCR	J	105	-	41,41,41	0.58	0	56,56,56	0.56	0
25	LMG	N	201	-	27,27,55	0.46	0	34,34,63	0.83	2 (5%)
19	CLA	B	808	30	69,73,73	1.19	7 (10%)	83,113,113	1.53	11 (13%)
18	CHL	3	315	30	55,59,74	1.29	7 (12%)	62,96,114	1.84	10 (16%)
19	CLA	B	809	6	69,73,73	1.21	10 (14%)	83,113,113	1.37	11 (13%)
22	A1LXP	4	306	-	42,43,43	0.38	0	51,60,60	0.66	0
19	CLA	A	817	30	53,57,73	1.41	7 (13%)	62,93,113	1.87	11 (17%)
23	LHG	1	620	19	20,20,48	0.59	0	23,26,54	0.81	0
19	CLA	L	303	30	49,53,73	1.70	7 (14%)	59,89,113	1.41	7 (11%)
22	A1LXP	1	619	-	42,43,43	0.44	0	51,60,60	0.57	0
19	CLA	B	848	6	49,53,73	2.21	10 (20%)	59,89,113	2.16	6 (10%)
22	A1LXP	1	616	-	42,43,43	0.58	1 (2%)	51,60,60	0.71	0
24	BCR	L	301	-	41,41,41	0.53	0	56,56,56	0.50	0
19	CLA	A	843	5	57,61,73	1.72	9 (15%)	68,98,113	1.73	12 (17%)
19	CLA	2	311	2	49,53,73	2.06	9 (18%)	59,89,113	1.47	8 (13%)
19	CLA	A	827	5	62,66,73	1.89	9 (14%)	74,104,113	1.38	11 (14%)
19	CLA	A	834	5	69,73,73	1.40	6 (8%)	83,113,113	1.42	7 (8%)
22	A1LXP	3	310	-	42,43,43	0.62	1 (2%)	51,60,60	1.02	3 (5%)
19	CLA	1	605	30	49,53,73	1.92	9 (18%)	59,89,113	1.36	8 (13%)
19	CLA	3	314	3	59,63,73	1.93	6 (10%)	71,101,113	1.37	9 (12%)
19	CLA	A	813	5	64,68,73	1.60	12 (18%)	77,107,113	1.85	10 (12%)
19	CLA	A	820	5	46,50,73	1.60	5 (10%)	55,85,113	1.50	8 (14%)
19	CLA	A	824	5	69,73,73	1.33	6 (8%)	83,113,113	1.23	5 (6%)
19	CLA	A	810	5	54,58,73	2.02	8 (14%)	65,95,113	1.69	11 (16%)
19	CLA	3	301	3	64,68,73	1.65	9 (14%)	77,107,113	1.36	10 (12%)
19	CLA	A	831	5	69,73,73	1.44	7 (10%)	83,113,113	1.37	10 (12%)
25	LMG	4	304	-	34,34,55	0.34	0	42,42,63	0.59	1 (2%)
24	BCR	4	308	-	41,41,41	0.35	0	56,56,56	0.56	0
19	CLA	A	819	5	69,73,73	1.38	8 (11%)	83,113,113	1.58	12 (14%)
19	CLA	A	848	5	54,58,73	1.72	9 (16%)	65,95,113	1.81	13 (20%)
19	CLA	A	849	5	54,58,73	1.58	10 (18%)	65,95,113	1.54	7 (10%)
28	PQN	B	811	-	34,34,34	0.60	0	42,45,45	0.96	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LMG	G	206	-	35,35,55	0.37	0	43,43,63	0.51	0
24	BCR	I	101	-	41,41,41	0.59	0	56,56,56	0.58	0
24	BCR	A	847	-	25,25,41	0.51	0	33,33,56	0.84	1 (3%)
19	CLA	A	801	30	59,63,73	1.84	10 (16%)	71,101,113	1.73	14 (19%)
19	CLA	B	835	6	61,65,73	1.50	6 (9%)	73,103,113	1.72	18 (24%)
19	CLA	L	304	16	69,73,73	1.29	6 (8%)	83,113,113	1.25	8 (9%)
19	CLA	A	850	30	69,73,73	1.13	6 (8%)	83,113,113	1.27	4 (4%)
19	CLA	3	308	30	49,53,73	1.43	7 (14%)	59,89,113	1.26	8 (13%)
19	CLA	B	841	30	60,64,73	1.42	10 (16%)	72,102,113	1.75	14 (19%)
19	CLA	A	822	5	57,61,73	1.64	8 (14%)	68,98,113	1.42	9 (13%)
19	CLA	J	101	5	69,73,73	1.75	8 (11%)	83,113,113	1.20	7 (8%)
19	CLA	K	203	30	49,53,73	2.01	10 (20%)	59,89,113	1.55	6 (10%)
25	LMG	F	301	-	30,30,55	0.36	0	38,38,63	0.48	0
18	CHL	4	319	4	50,54,74	1.27	6 (12%)	56,90,114	2.06	9 (16%)
19	CLA	2	312	2	66,70,73	2.01	7 (10%)	79,109,113	1.36	9 (11%)
19	CLA	L	305	16	49,53,73	2.38	6 (12%)	59,89,113	1.45	7 (11%)
26	SF4	C	102	7	0,12,12	-	-	-	-	-
24	BCR	G	201	-	41,41,41	0.83	2 (4%)	56,56,56	0.54	0
24	BCR	L	306	-	41,41,41	0.53	0	56,56,56	0.46	0
18	CHL	1	601	1	63,67,74	1.12	6 (9%)	71,105,114	1.93	8 (11%)
24	BCR	A	852	-	41,41,41	0.70	1 (2%)	56,56,56	0.73	1 (1%)
24	BCR	B	814	-	41,41,41	0.52	0	56,56,56	0.58	0
19	CLA	A	851	30	66,70,73	1.53	7 (10%)	79,109,113	1.62	13 (16%)
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	A	812	5	69,73,73	1.40	9 (13%)	83,113,113	1.25	10 (12%)
19	CLA	B	805	6	54,58,73	1.40	5 (9%)	65,95,113	1.55	5 (7%)
19	CLA	B	804	30	49,53,73	1.82	5 (10%)	59,89,113	1.44	10 (16%)
24	BCR	L	302	-	41,41,41	0.63	0	56,56,56	0.57	1 (1%)
24	BCR	B	815	-	41,41,41	0.59	1 (2%)	56,56,56	0.75	1 (1%)
19	CLA	3	307	30	52,56,73	1.71	9 (17%)	62,92,113	1.21	8 (12%)
19	CLA	B	820	-	69,73,73	1.75	9 (13%)	83,113,113	1.19	8 (9%)
21	XAT	1	615	-	39,47,47	0.44	0	54,74,74	1.65	5 (9%)
19	CLA	B	821	6	46,50,73	1.64	6 (13%)	55,85,113	2.04	10 (18%)
19	CLA	A	842	5	64,68,73	1.55	7 (10%)	77,107,113	1.69	15 (19%)
19	CLA	A	846	5	69,73,73	1.36	10 (14%)	83,113,113	1.60	15 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	DGD	B	817	-	61,61,67	0.42	0	75,75,81	0.88	3 (4%)
19	CLA	A	806	5	46,50,73	2.21	9 (19%)	55,85,113	1.56	7 (12%)
19	CLA	K	202	15	49,53,73	1.82	10 (20%)	59,89,113	2.05	7 (11%)
19	CLA	4	314	4	56,60,73	2.17	7 (12%)	67,97,113	1.39	10 (14%)
19	CLA	A	808	30	69,73,73	1.37	6 (8%)	83,113,113	1.47	9 (10%)
21	XAT	1	618	-	25,29,47	0.42	0	33,43,74	1.54	2 (6%)
19	CLA	A	809	5	69,73,73	1.11	4 (5%)	83,113,113	1.71	15 (18%)
19	CLA	A	844	5	46,50,73	2.23	8 (17%)	55,85,113	1.52	9 (16%)
19	CLA	2	301	2	54,58,73	2.12	8 (14%)	65,95,113	1.34	9 (13%)

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	807	30	-	0/15/91/115	-
19	CLA	A	837	5	1/1/15/20	12/39/115/115	-
24	BCR	F	302	-	-	0/29/63/63	0/2/2/2
19	CLA	A	814	5	1/1/15/20	12/39/115/115	-
19	CLA	A	805	5	-	1/18/94/115	-
19	CLA	B	803	6	-	0/15/91/115	-
19	CLA	A	809	5	1/1/15/20	7/39/115/115	-
19	CLA	G	202	30	-	3/12/88/115	-
19	CLA	3	312	3	-	3/12/88/115	-
19	CLA	A	823	30	-	8/39/115/115	-
22	A1LXP	J	102	-	-	3/29/67/67	0/2/2/2
19	CLA	B	832	6	-	6/15/91/115	-
19	CLA	B	827	6	1/1/15/20	10/39/115/115	-
19	CLA	A	826	5	1/1/15/20	9/39/115/115	-
18	CHL	2	315	30	-	10/17/93/117	-
19	CLA	B	825	6	1/1/15/20	12/39/115/115	-
22	A1LXP	3	305	-	-	2/29/67/67	0/2/2/2
24	BCR	G	205	-	-	4/29/63/63	0/2/2/2
19	CLA	B	830	6	1/1/15/20	20/39/115/115	-
19	CLA	H	201	12	1/1/13/20	8/27/103/115	-
19	CLA	B	836	30	1/1/13/20	1/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CL0	A	830	5	-	2/39/115/115	-
19	CLA	A	840	19,5	1/1/15/20	12/39/115/115	-
19	CLA	3	302	3	-	9/24/100/115	-
19	CLA	A	815	5	-	3/15/91/115	-
19	CLA	B	838	6	-	3/15/91/115	-
19	CLA	4	318	4	-	5/15/91/115	-
24	BCR	K	201	-	-	4/29/63/63	0/2/2/2
19	CLA	A	828	5	1/1/15/20	17/39/115/115	-
19	CLA	A	816	5	-	2/21/97/115	-
19	CLA	A	825	5	-	10/12/88/115	-
19	CLA	A	832	5	-	0/15/91/115	-
19	CLA	F	303	10	-	2/12/88/115	-
18	CHL	1	606	1	-	5/14/90/117	-
24	BCR	B	816	-	-	0/29/63/63	0/2/2/2
19	CLA	B	843	6	1/1/15/20	7/39/115/115	-
19	CLA	B	822	6	1/1/15/20	13/39/115/115	-
18	CHL	2	313	30	-	6/12/88/117	-
19	CLA	A	821	5	-	7/24/100/115	-
24	BCR	3	316	-	-	4/29/63/63	0/2/2/2
19	CLA	B	844	6	1/1/13/20	7/32/108/115	-
19	CLA	4	307	4	-	5/15/91/115	-
19	CLA	B	847	6	-	3/21/97/115	-
19	CLA	1	612	1	1/1/13/20	4/27/103/115	-
28	PQN	A	839	-	-	4/23/43/43	0/2/2/2
19	CLA	1	608	1	1/1/13/20	10/30/106/115	-
19	CLA	B	807	6	-	2/15/91/115	-
19	CLA	1	607	-	-	7/23/99/115	-
19	CLA	A	818	5	1/1/15/20	14/39/115/115	-
19	CLA	3	306	3	-	3/18/94/115	-
23	LHG	A	835	-	-	17/53/53/53	-
22	A1LXP	2	309	-	-	2/29/67/67	0/2/2/2
25	LMG	J	103	-	-	16/36/56/70	0/1/1/1
26	SF4	A	803	6,5	-	-	0/6/5/5
19	CLA	B	826	6	1/1/15/20	14/39/115/115	-
19	CLA	A	836	5	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	834	6	1/1/15/20	9/39/115/115	-
24	BCR	B	813	-	-	6/29/63/63	0/2/2/2
21	XAT	2	306	-	-	1/31/93/93	0/4/4/4
19	CLA	B	819	6	1/1/15/20	9/39/115/115	-
19	CLA	B	833	6	1/1/14/20	7/33/109/115	-
19	CLA	B	839	6	-	2/13/89/115	-
19	CLA	3	304	3	1/1/13/20	5/27/103/115	-
19	CLA	A	811	5	1/1/13/20	2/27/103/115	-
19	CLA	B	840	6	-	2/15/91/115	-
19	CLA	B	801	6	1/1/15/20	10/39/115/115	-
19	CLA	1	603	1	1/1/13/20	12/30/106/115	-
24	BCR	B	812	-	-	4/29/63/63	0/2/2/2
19	CLA	B	818	30	1/1/15/20	17/39/115/115	-
19	CLA	F	306	30	-	3/19/95/115	-
19	CLA	A	833	-	1/1/15/20	6/39/115/115	-
24	BCR	A	838	-	-	2/29/63/63	0/2/2/2
19	CLA	B	802	6	1/1/14/20	7/33/109/115	-
18	CHL	4	313	30	-	4/17/93/117	-
24	BCR	F	304	-	-	2/29/63/63	0/2/2/2
19	CLA	B	842	30	-	4/21/97/115	-
19	CLA	B	845	6	1/1/15/20	4/39/115/115	-
19	CLA	B	806	6	1/1/15/20	9/39/115/115	-
19	CLA	B	828	6	-	10/23/99/115	-
24	BCR	A	845	-	-	4/29/63/63	0/2/2/2
24	BCR	A	804	-	-	1/29/63/63	0/2/2/2
18	CHL	3	303	3	1/1/15/21	14/41/117/117	-
19	CLA	B	846	6	1/1/15/20	12/39/115/115	-
19	CLA	A	802	19,5	1/1/13/20	6/29/105/115	-
24	BCR	A	841	-	-	4/29/63/63	0/2/2/2
25	LMG	F	305	-	-	7/24/44/70	0/1/1/1
22	A1LXP	4	303	-	-	0/29/67/67	0/2/2/2
19	CLA	4	317	4	1/1/13/20	4/30/106/115	-
19	CLA	2	310	2	1/1/13/20	8/27/103/115	-
19	CLA	G	203	11	-	7/15/91/115	-
19	CLA	1	602	1	1/1/14/20	15/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SF4	C	101	7	-	-	0/6/5/5
19	CLA	A	829	5	1/1/15/20	6/39/115/115	-
23	LHG	1	617	20	-	25/53/53/53	-
19	CLA	B	831	6	1/1/15/20	15/39/115/115	-
19	CLA	4	311	4	-	2/15/91/115	-
18	CHL	2	316	2	1/1/13/21	10/33/109/117	-
19	CLA	B	810	23	1/1/15/20	14/39/115/115	-
19	CLA	B	824	6	-	1/24/100/115	-
23	LHG	2	302	20	-	20/49/49/53	-
24	BCR	J	105	-	-	2/29/63/63	0/2/2/2
25	LMG	N	201	-	-	5/20/40/70	0/1/1/1
19	CLA	B	808	30	1/1/15/20	10/39/115/115	-
18	CHL	3	315	30	-	8/23/99/117	-
19	CLA	B	809	6	1/1/15/20	7/39/115/115	-
22	A1LXP	4	306	-	-	2/29/67/67	0/2/2/2
19	CLA	A	817	30	-	5/20/96/115	-
23	LHG	1	620	19	-	2/23/23/53	-
19	CLA	L	303	30	-	2/15/91/115	-
22	A1LXP	1	619	-	-	2/29/67/67	0/2/2/2
19	CLA	B	848	6	-	1/15/91/115	-
22	A1LXP	1	616	-	-	0/29/67/67	0/2/2/2
24	BCR	L	301	-	-	1/29/63/63	0/2/2/2
19	CLA	A	843	5	-	1/25/101/115	-
19	CLA	2	311	2	-	0/15/91/115	-
19	CLA	A	827	5	1/1/13/20	4/31/107/115	-
19	CLA	A	834	5	1/1/15/20	8/39/115/115	-
22	A1LXP	3	310	-	-	0/29/67/67	0/2/2/2
19	CLA	1	605	30	-	8/15/91/115	-
19	CLA	3	314	3	1/1/13/20	2/27/103/115	-
19	CLA	A	813	5	1/1/14/20	6/33/109/115	-
19	CLA	A	824	5	1/1/15/20	11/39/115/115	-
19	CLA	A	820	5	-	4/12/88/115	-
19	CLA	A	810	5	-	0/21/97/115	-
19	CLA	3	301	3	1/1/14/20	7/33/109/115	-
19	CLA	A	831	5	1/1/15/20	12/39/115/115	-
25	LMG	4	304	-	-	7/29/49/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	4	308	-	-	6/29/63/63	0/2/2/2
19	CLA	A	819	5	1/1/15/20	7/39/115/115	-
19	CLA	A	848	5	-	2/21/97/115	-
19	CLA	A	849	5	-	1/21/97/115	-
28	PQN	B	811	-	-	5/23/43/43	0/2/2/2
25	LMG	G	206	-	-	7/30/50/70	0/1/1/1
24	BCR	I	101	-	-	0/29/63/63	0/2/2/2
24	BCR	A	847	-	-	2/18/35/63	0/1/1/2
19	CLA	A	801	30	1/1/13/20	2/27/103/115	-
19	CLA	B	835	6	1/1/13/20	3/30/106/115	-
19	CLA	L	304	16	1/1/15/20	9/39/115/115	-
19	CLA	A	850	30	1/1/15/20	6/39/115/115	-
19	CLA	3	308	30	-	0/15/91/115	-
19	CLA	B	841	30	1/1/13/20	5/29/105/115	-
19	CLA	J	101	5	1/1/15/20	9/39/115/115	-
19	CLA	A	822	5	-	10/25/101/115	-
19	CLA	K	203	30	-	6/15/91/115	-
25	LMG	F	301	-	-	2/25/45/70	0/1/1/1
18	CHL	4	319	4	-	7/17/93/117	-
19	CLA	2	312	2	1/1/14/20	15/36/112/115	-
19	CLA	L	305	16	-	0/15/91/115	-
26	SF4	C	102	7	-	-	0/6/5/5
24	BCR	G	201	-	-	0/29/63/63	0/2/2/2
24	BCR	L	306	-	-	3/29/63/63	0/2/2/2
18	CHL	1	601	1	1/1/13/21	11/33/109/117	-
24	BCR	A	852	-	-	2/29/63/63	0/2/2/2
24	BCR	B	814	-	-	2/29/63/63	0/2/2/2
19	CLA	A	851	30	1/1/14/20	12/36/112/115	-
19	CLA	B	829	6	-	3/13/89/115	-
19	CLA	B	837	6	-	1/18/94/115	-
19	CLA	A	812	5	1/1/15/20	10/39/115/115	-
19	CLA	B	805	6	-	1/21/97/115	-
19	CLA	B	804	30	-	0/15/91/115	-
24	BCR	L	302	-	-	0/29/63/63	0/2/2/2
24	BCR	B	815	-	-	4/29/63/63	0/2/2/2
19	CLA	3	307	30	-	3/19/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	820	-	1/1/15/20	9/39/115/115	-
21	XAT	1	615	-	-	0/31/93/93	0/4/4/4
19	CLA	B	821	6	-	4/12/88/115	-
19	CLA	A	842	5	1/1/14/20	8/33/109/115	-
19	CLA	A	846	5	1/1/15/20	8/39/115/115	-
29	DGD	B	817	-	-	16/49/89/95	0/2/2/2
19	CLA	A	806	5	-	7/12/88/115	-
19	CLA	K	202	15	-	7/15/91/115	-
19	CLA	4	314	4	-	2/24/100/115	-
19	CLA	A	808	30	1/1/15/20	7/39/115/115	-
21	XAT	1	618	-	-	0/21/52/93	0/2/2/4
19	CLA	B	823	6	1/1/15/20	9/39/115/115	-
19	CLA	A	844	5	-	2/12/88/115	-
19	CLA	2	301	2	-	7/21/97/115	-

The worst 5 of 984 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	312	CLA	C4B-NB	12.65	1.53	1.37
19	4	307	CLA	C4B-NB	11.36	1.51	1.37
19	A	844	CLA	C4B-NB	10.87	1.51	1.37
19	3	314	CLA	C4B-NB	10.35	1.50	1.37
19	B	833	CLA	C1B-NB	10.34	1.50	1.37

The worst 5 of 1273 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	606	CHL	C4A-NA-C1A	13.18	112.63	106.71
19	G	203	CLA	C4A-NA-C1A	-12.86	100.92	106.71
18	2	316	CHL	C4A-NA-C1A	12.82	112.47	106.71
19	K	202	CLA	C4A-NA-C1A	-12.13	101.25	106.71
19	A	813	CLA	C4A-NA-C1A	-12.08	101.28	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

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Mol	Chain	Res	Type	Atom
19	1	602	CLA	C8
19	1	603	CLA	C8

5 of 1026 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	2	313	CHL	C1C-C2C-CMC-OMC

There are no ring outliers.

112 monomers are involved in 203 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	807	CLA	1	0
24	F	302	BCR	3	0
19	A	814	CLA	2	0
19	A	805	CLA	2	0
19	B	803	CLA	1	0
19	A	823	CLA	1	0
19	B	832	CLA	2	0
19	B	827	CLA	3	0
19	A	826	CLA	2	0
19	B	825	CLA	2	0
22	3	305	A1LXP	1	0
24	G	205	BCR	3	0
19	B	830	CLA	2	0
19	A	815	CLA	1	0
19	A	840	CLA	5	0
19	4	318	CLA	1	0
24	K	201	BCR	2	0
19	A	828	CLA	1	0
19	F	303	CLA	2	0
18	1	606	CHL	2	0
24	B	816	BCR	2	0
19	B	843	CLA	1	0
19	B	822	CLA	2	0
19	A	821	CLA	4	0
19	B	844	CLA	5	0
19	1	612	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	608	CLA	1	0
19	1	607	CLA	1	0
19	A	818	CLA	1	0
22	2	309	A1LXP	1	0
19	B	834	CLA	4	0
24	B	813	BCR	5	0
21	2	306	XAT	1	0
19	B	819	CLA	1	0
19	B	833	CLA	4	0
19	3	304	CLA	2	0
19	B	840	CLA	1	0
19	B	801	CLA	2	0
19	1	603	CLA	3	0
24	B	812	BCR	4	0
19	B	818	CLA	5	0
19	A	833	CLA	3	0
24	A	838	BCR	2	0
19	B	802	CLA	1	0
18	4	313	CHL	1	0
24	F	304	BCR	2	0
19	B	842	CLA	1	0
19	B	845	CLA	2	0
19	B	806	CLA	3	0
24	A	845	BCR	7	0
24	A	804	BCR	5	0
18	3	303	CHL	1	0
19	B	846	CLA	1	0
19	A	802	CLA	3	0
24	A	841	BCR	1	0
25	F	305	LMG	2	0
19	4	317	CLA	3	0
19	G	203	CLA	5	0
19	1	602	CLA	3	0
19	A	829	CLA	2	0
19	4	311	CLA	2	0
19	B	810	CLA	2	0
19	B	824	CLA	1	0
25	N	201	LMG	3	0
19	B	808	CLA	3	0
19	B	809	CLA	1	0
22	4	306	A1LXP	1	0
19	L	303	CLA	1	0

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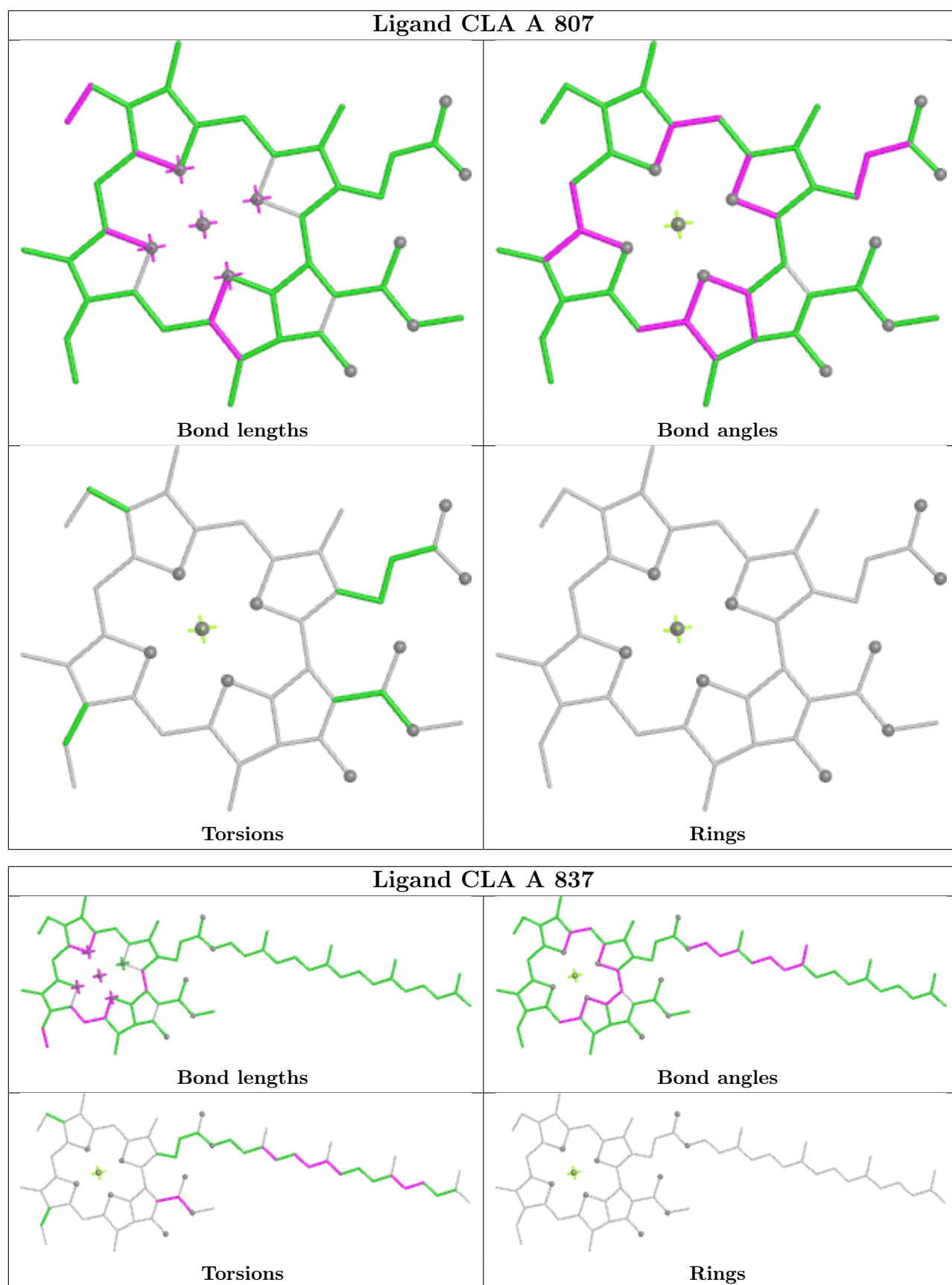
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	848	CLA	1	0
24	L	301	BCR	2	0
19	A	843	CLA	2	0
19	2	311	CLA	1	0
19	A	827	CLA	1	0
19	A	834	CLA	1	0
19	1	605	CLA	1	0
19	A	813	CLA	4	0
19	A	810	CLA	2	0
19	3	301	CLA	1	0
19	A	831	CLA	5	0
24	4	308	BCR	3	0
19	A	819	CLA	3	0
19	A	849	CLA	2	0
24	I	101	BCR	1	0
24	A	847	BCR	2	0
19	L	304	CLA	1	0
19	A	850	CLA	1	0
19	3	308	CLA	1	0
19	B	841	CLA	1	0
19	J	101	CLA	1	0
19	K	203	CLA	2	0
18	4	319	CHL	1	0
19	2	312	CLA	1	0
24	G	201	BCR	4	0
18	1	601	CHL	2	0
24	A	852	BCR	8	0
24	B	814	BCR	1	0
19	A	851	CLA	5	0
19	B	829	CLA	2	0
19	B	837	CLA	1	0
19	A	812	CLA	1	0
19	B	805	CLA	1	0
19	B	804	CLA	1	0
24	L	302	BCR	2	0
24	B	815	BCR	1	0
19	B	820	CLA	2	0
21	1	615	XAT	3	0
19	A	842	CLA	3	0
29	B	817	DGD	1	0
19	A	806	CLA	2	0
19	A	808	CLA	4	0

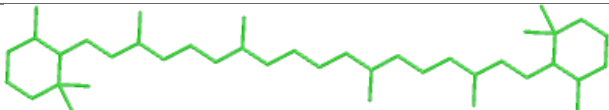
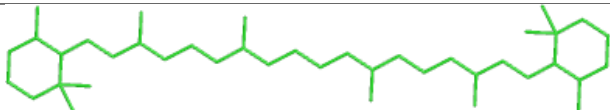
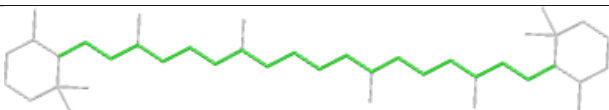
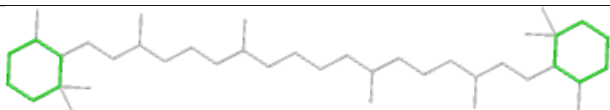
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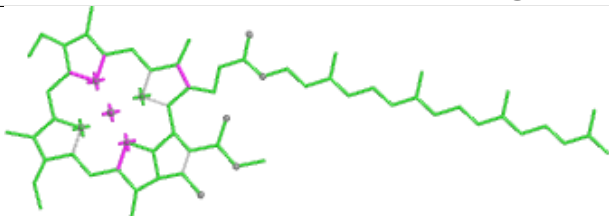
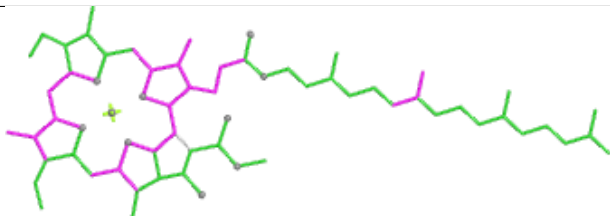
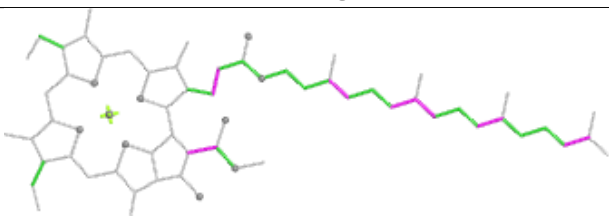
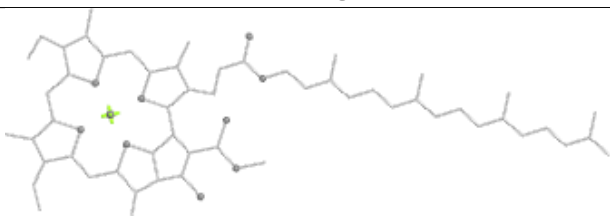
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	1	618	XAT	3	0
19	A	809	CLA	3	0

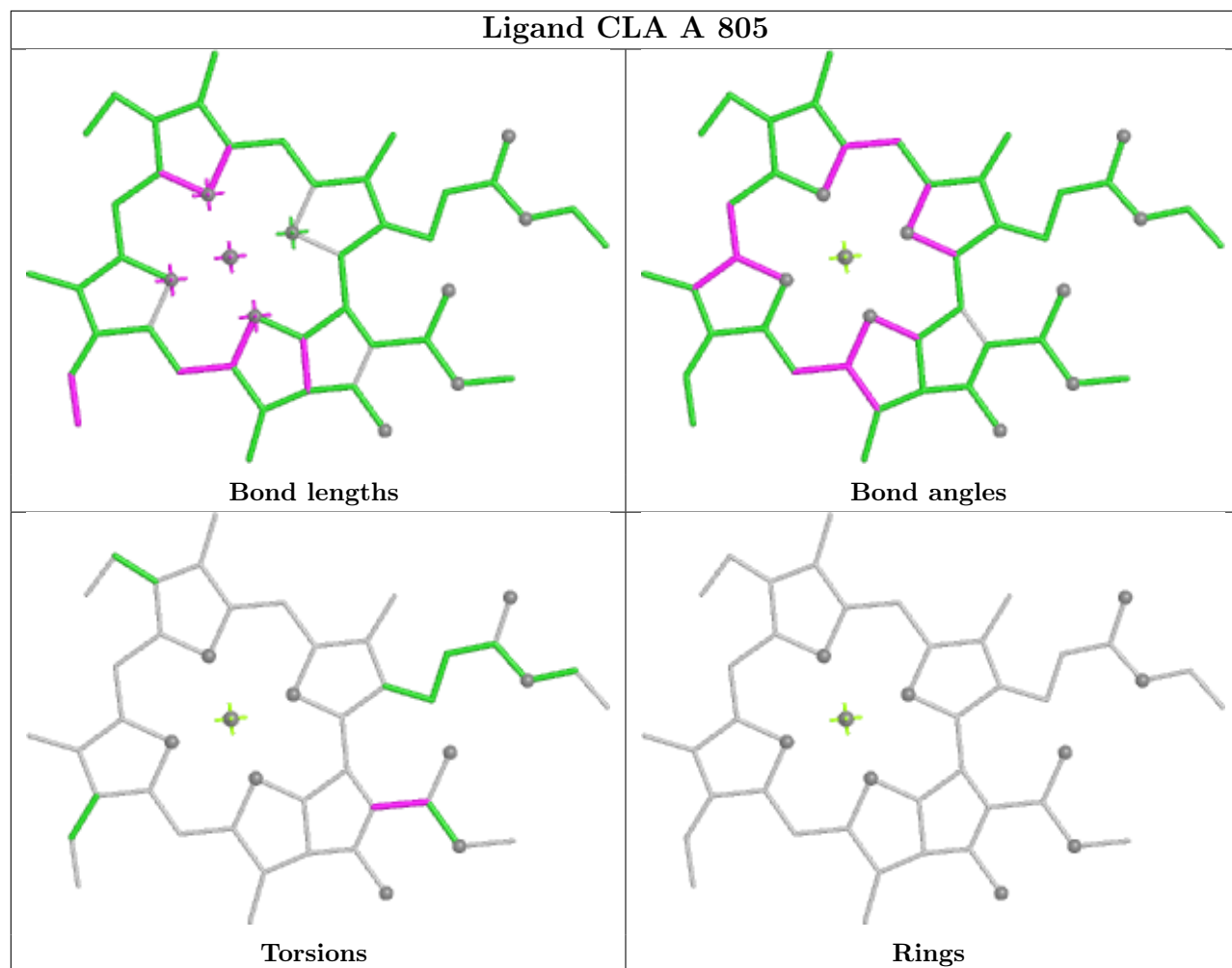
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



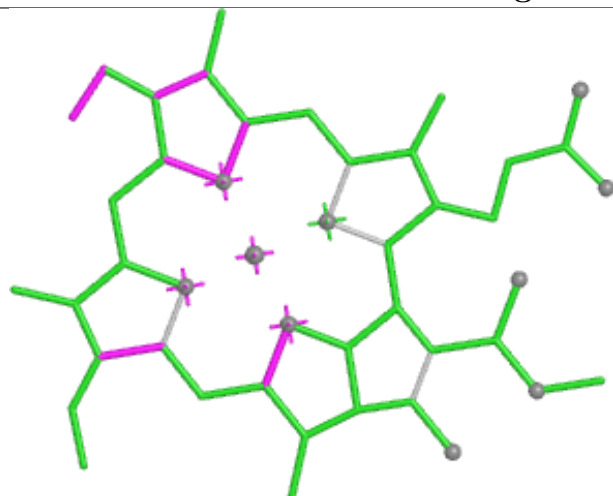
Ligand BCR F 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

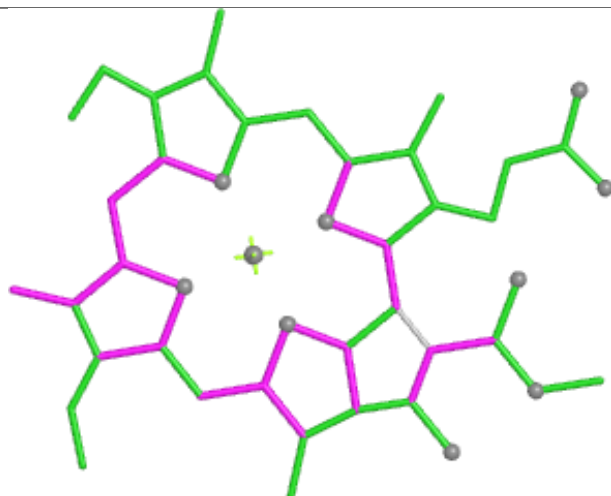
Ligand CLA A 805



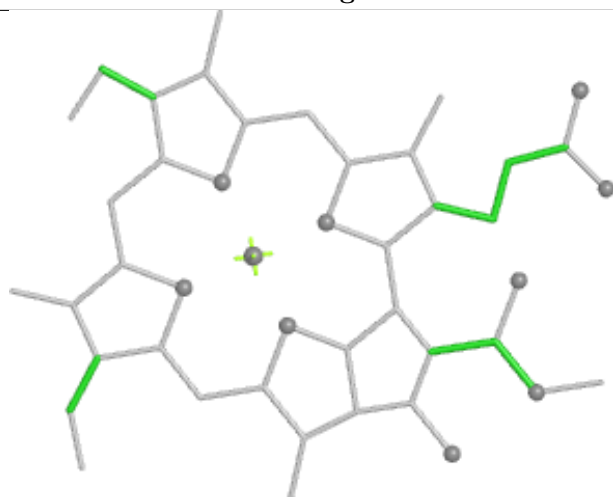
Ligand CLA B 803



Bond lengths



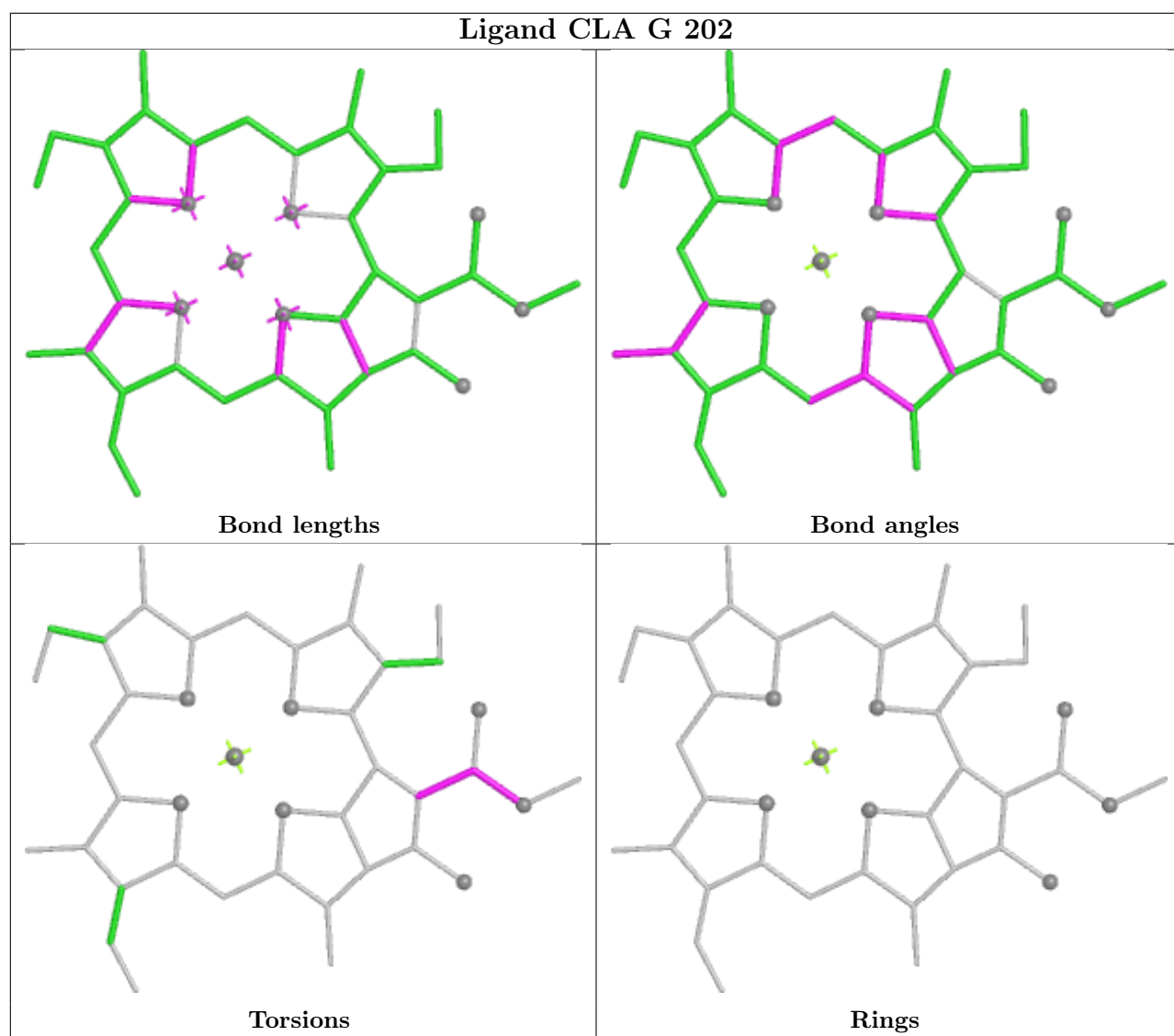
Bond angles



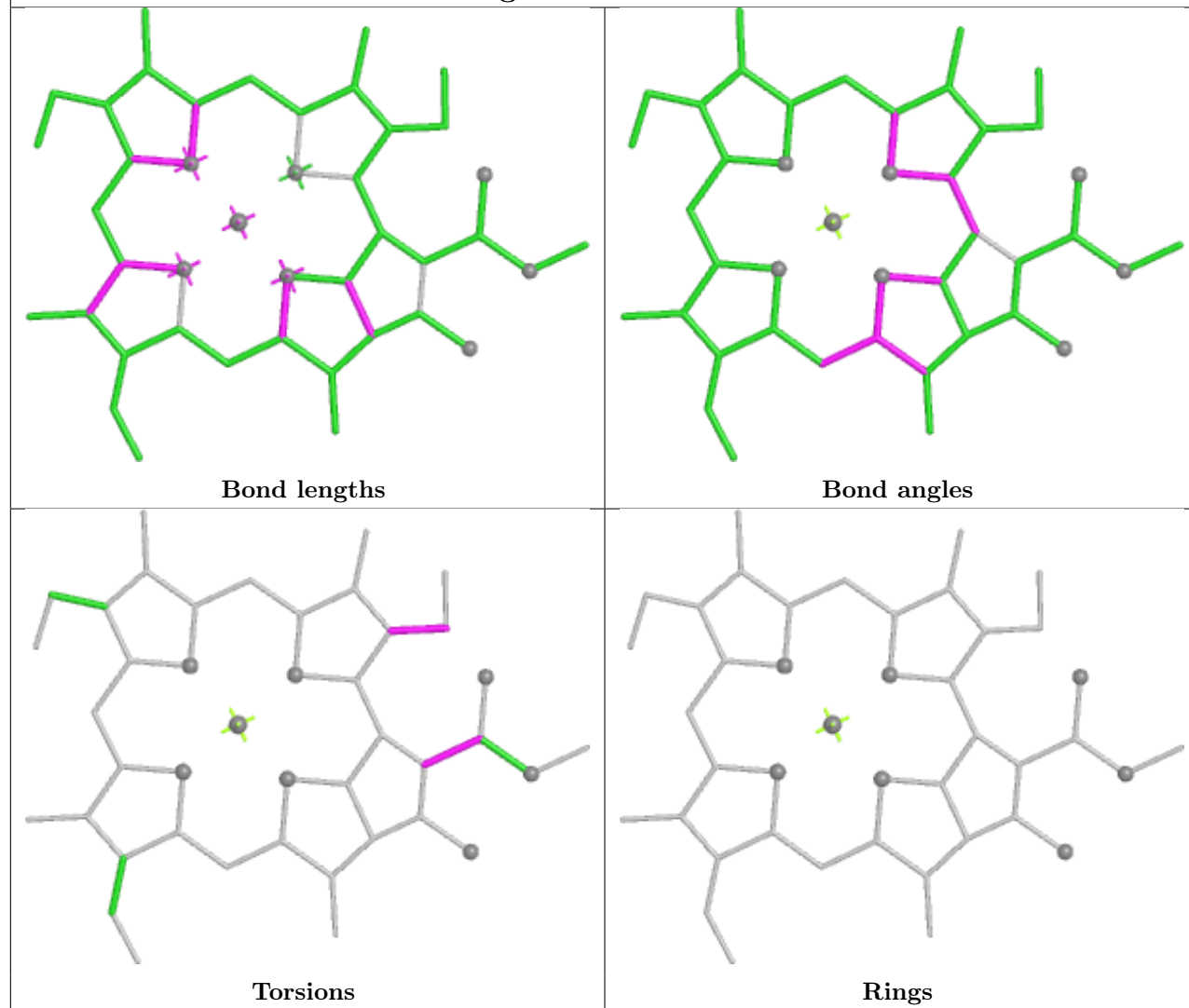
Torsions



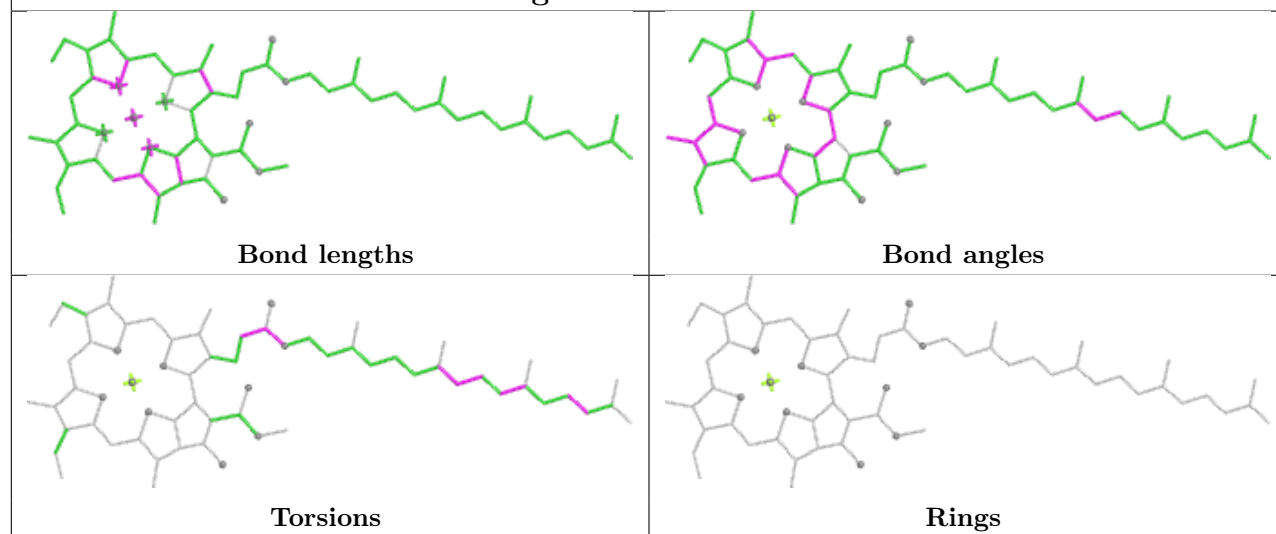
Rings



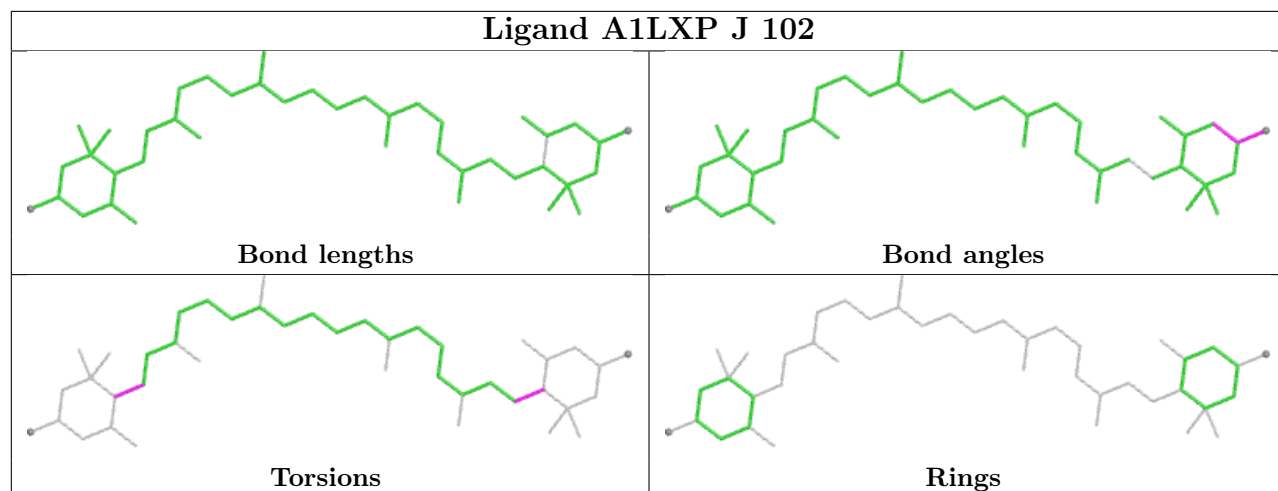
Ligand CLA 3 312



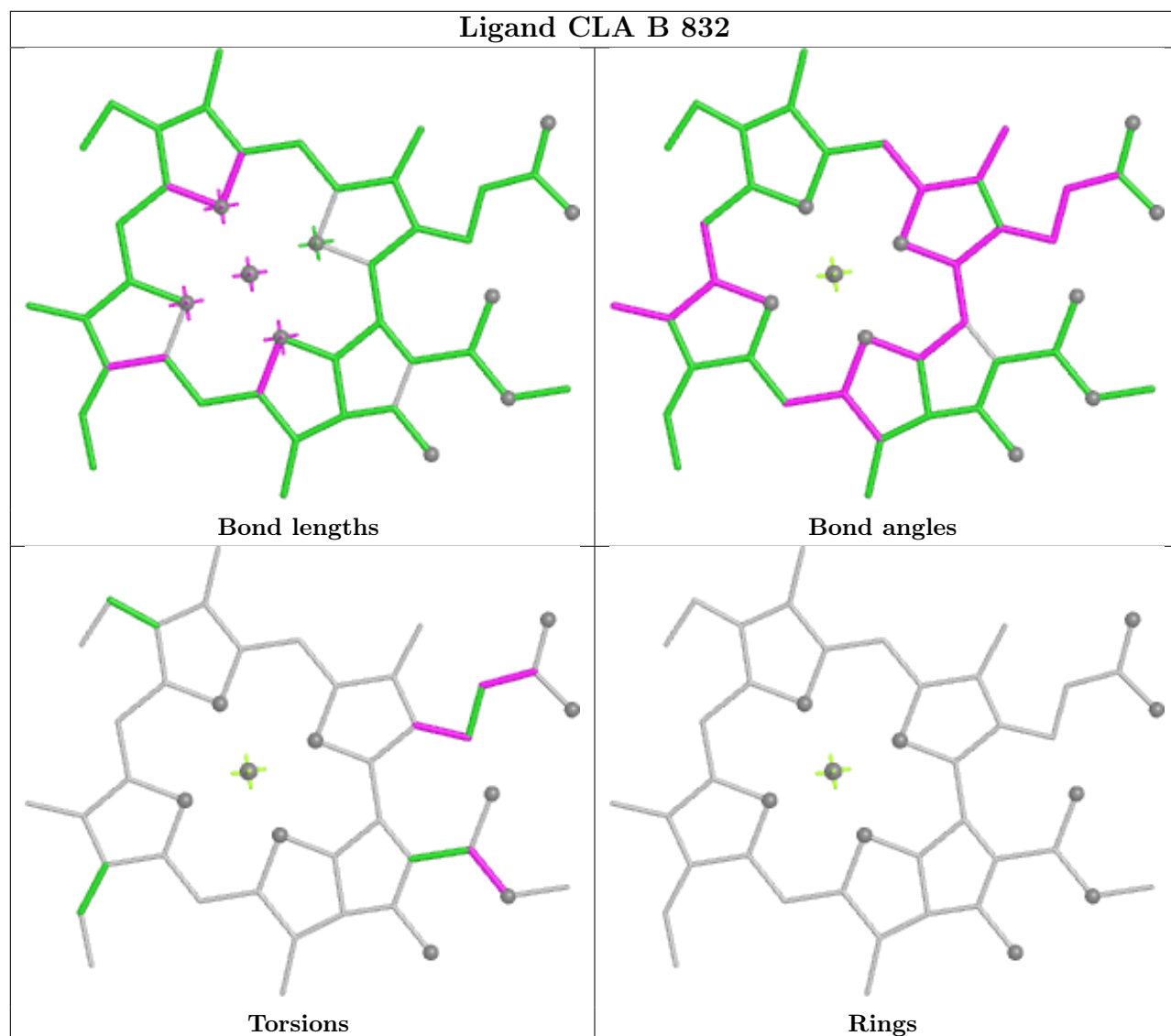
Ligand CLA A 823

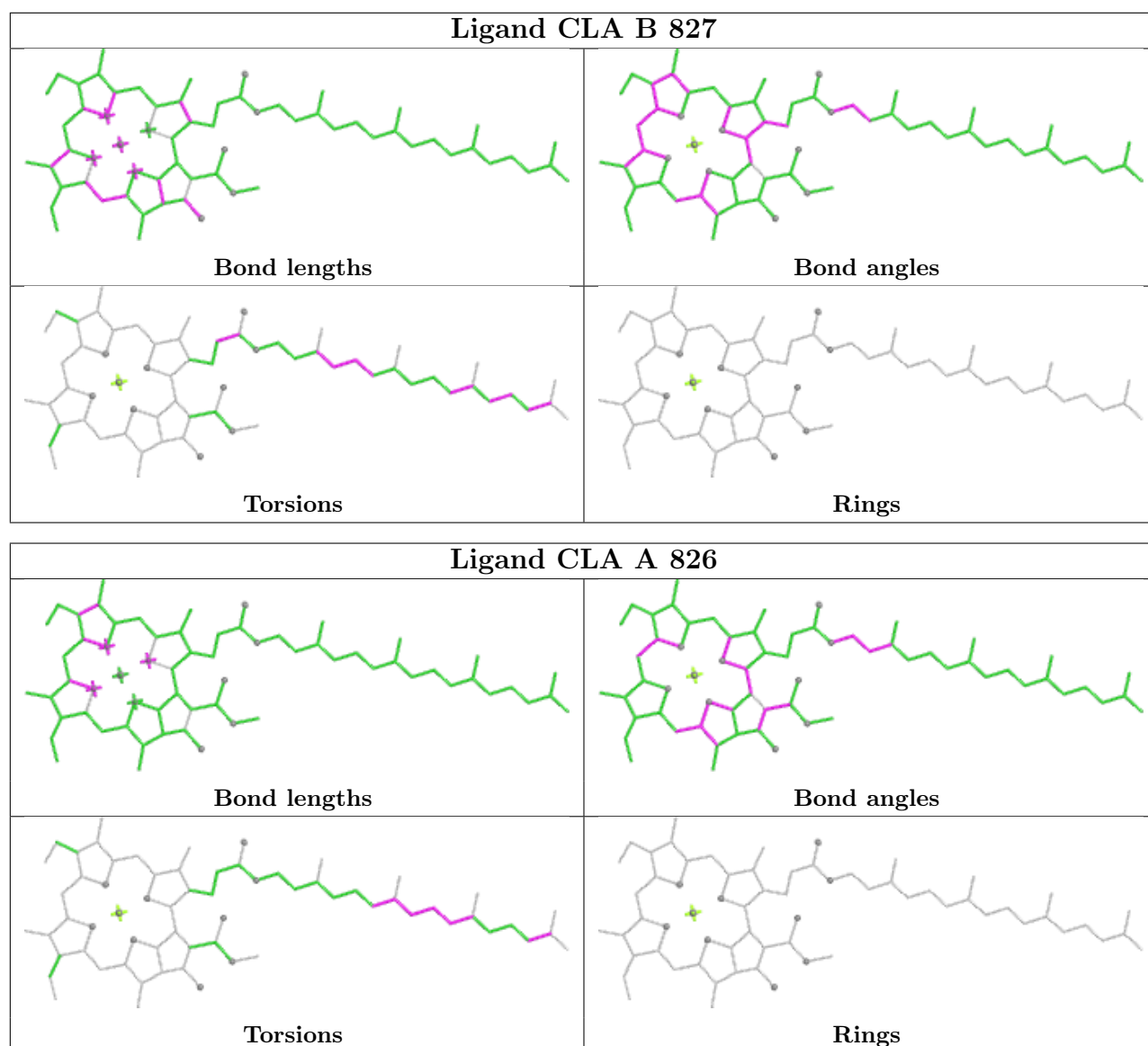


Ligand A1LXP J 102

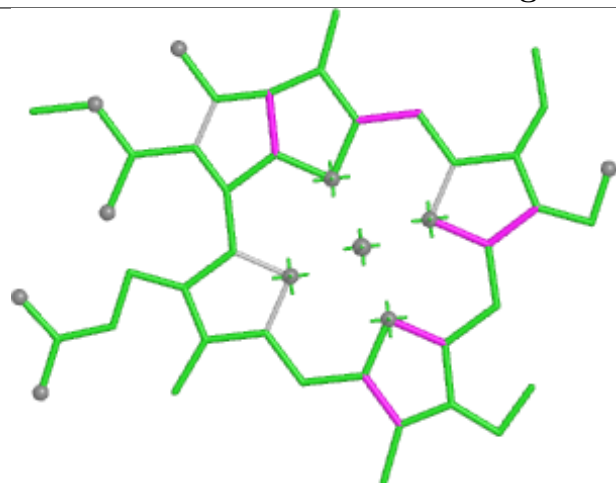


Ligand CLA B 832

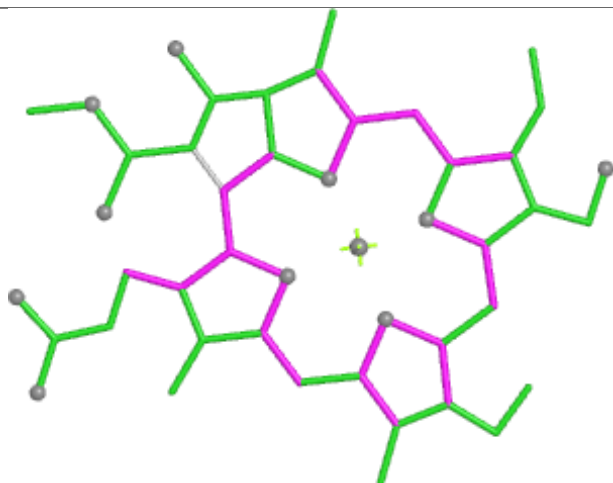




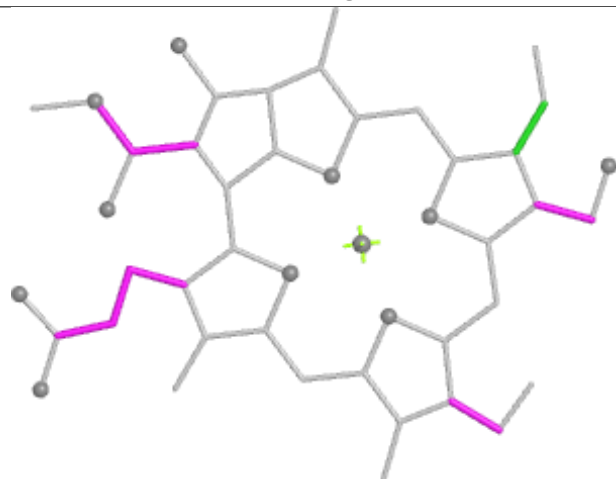
Ligand CHL 2 315



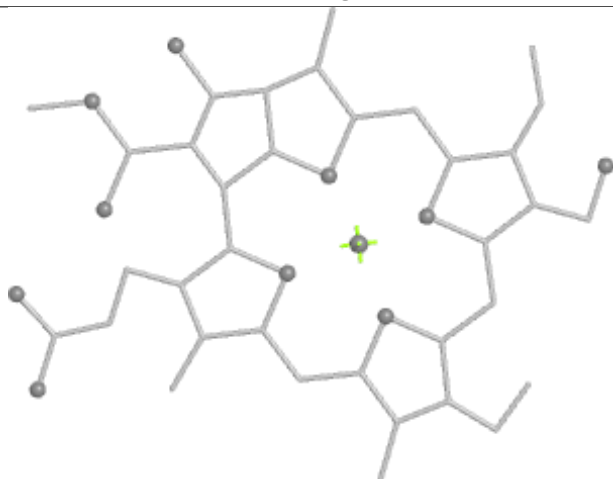
Bond lengths



Bond angles

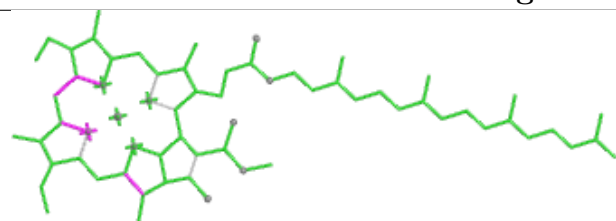


Torsions

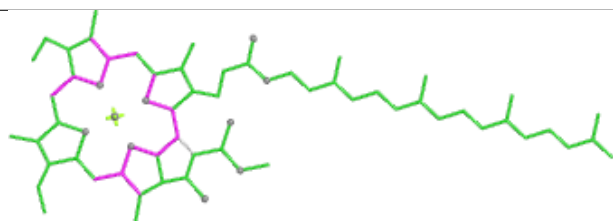


Rings

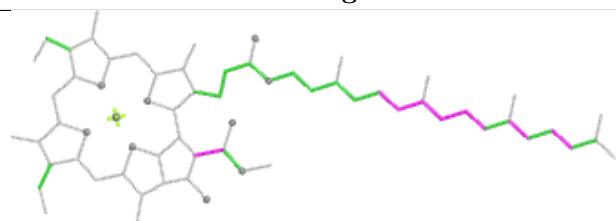
Ligand CLA B 825



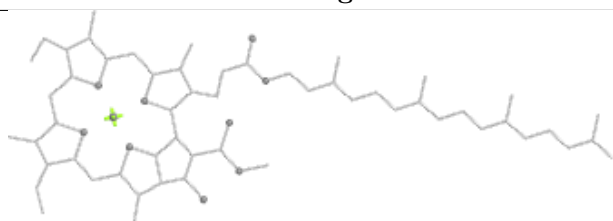
Bond lengths



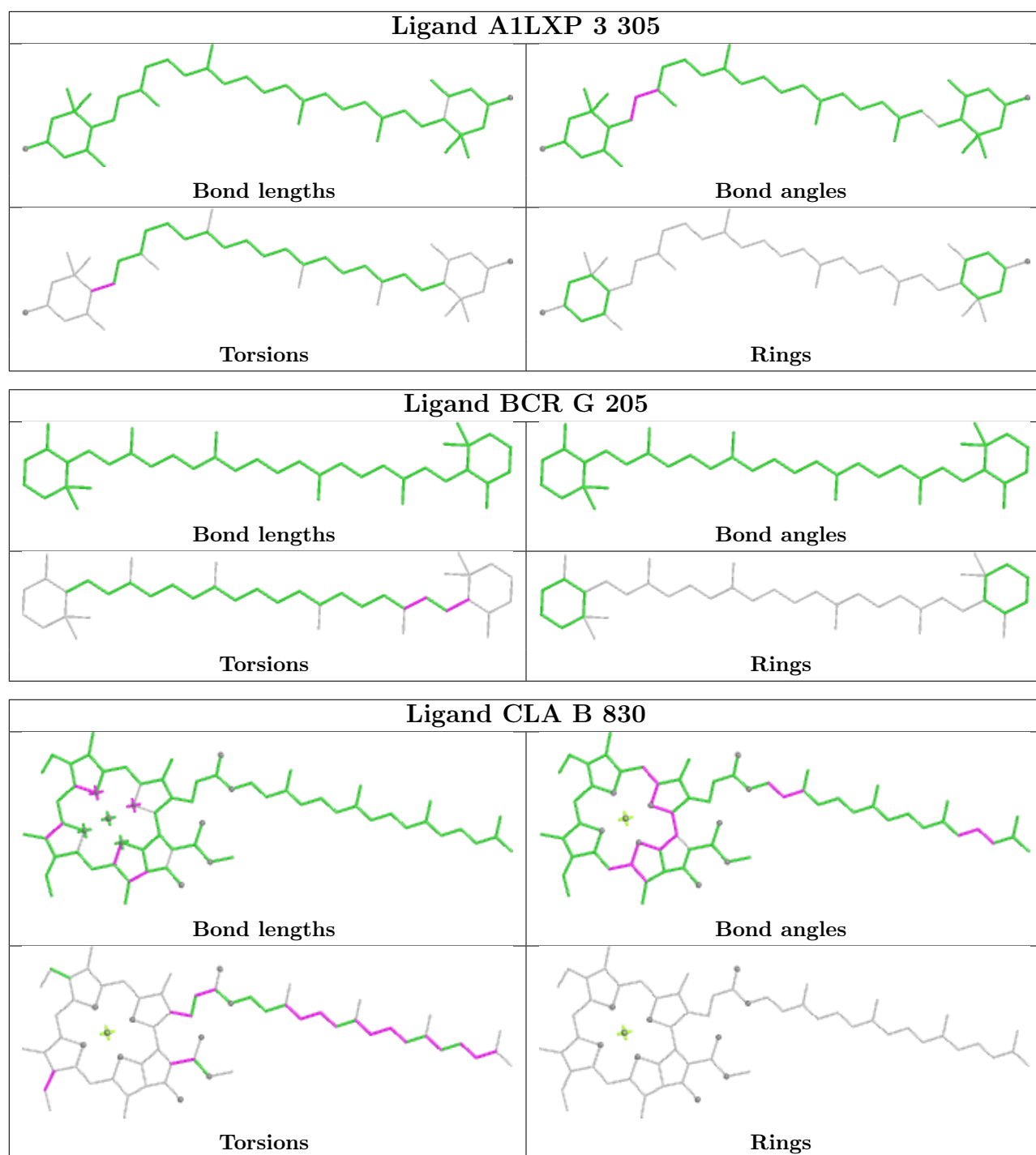
Bond angles



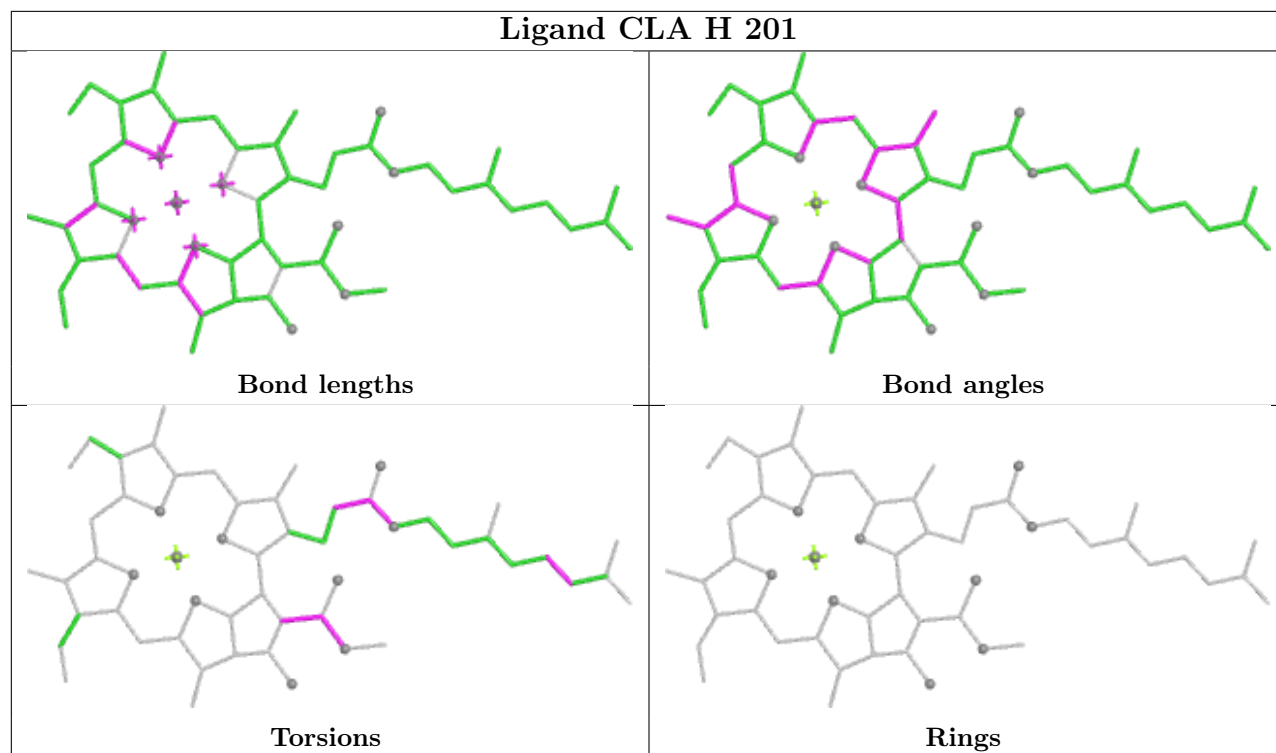
Torsions



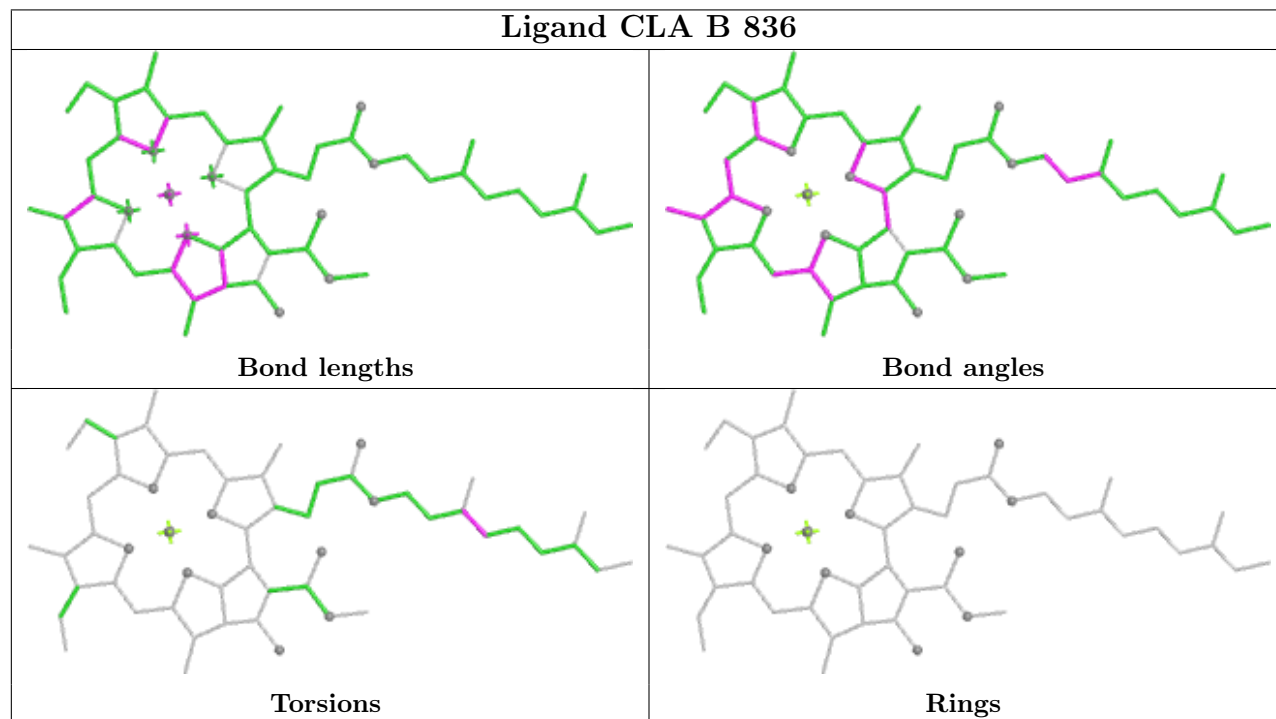
Rings

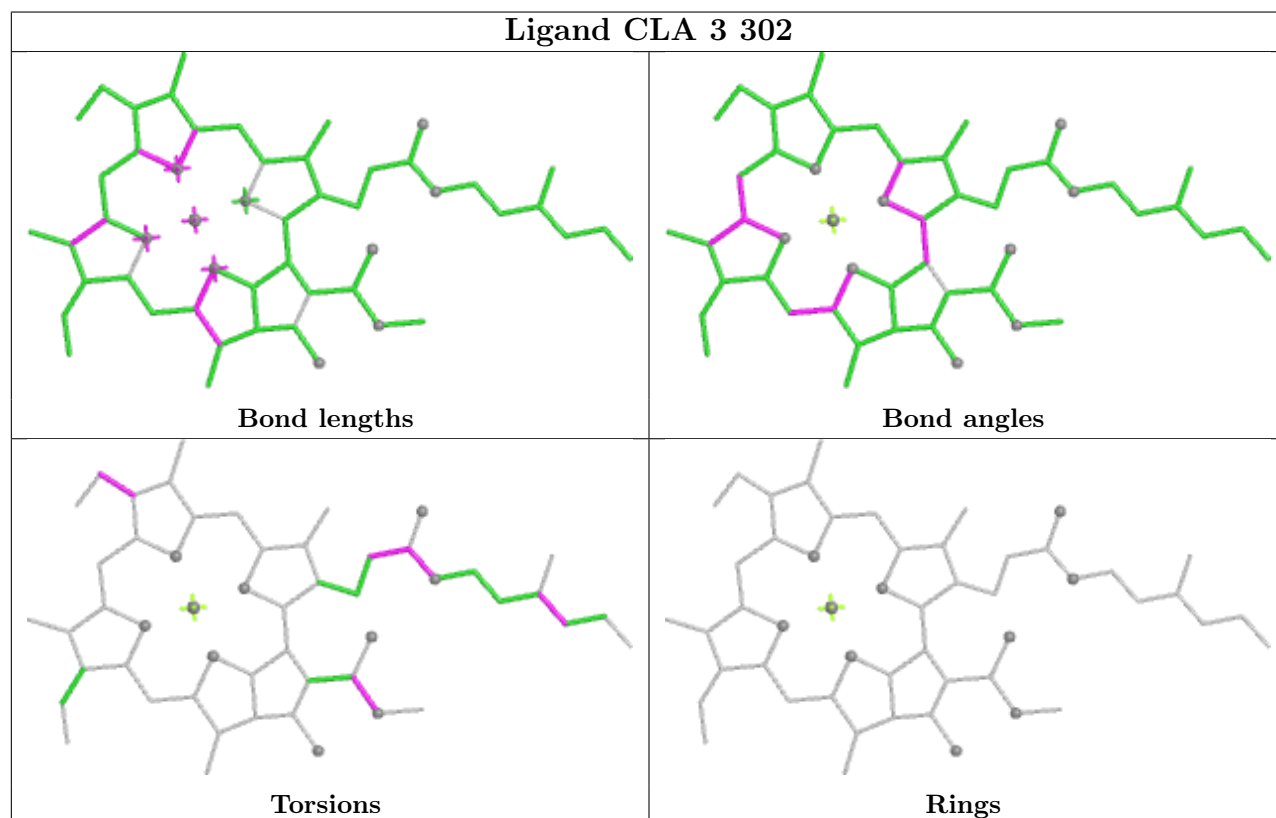
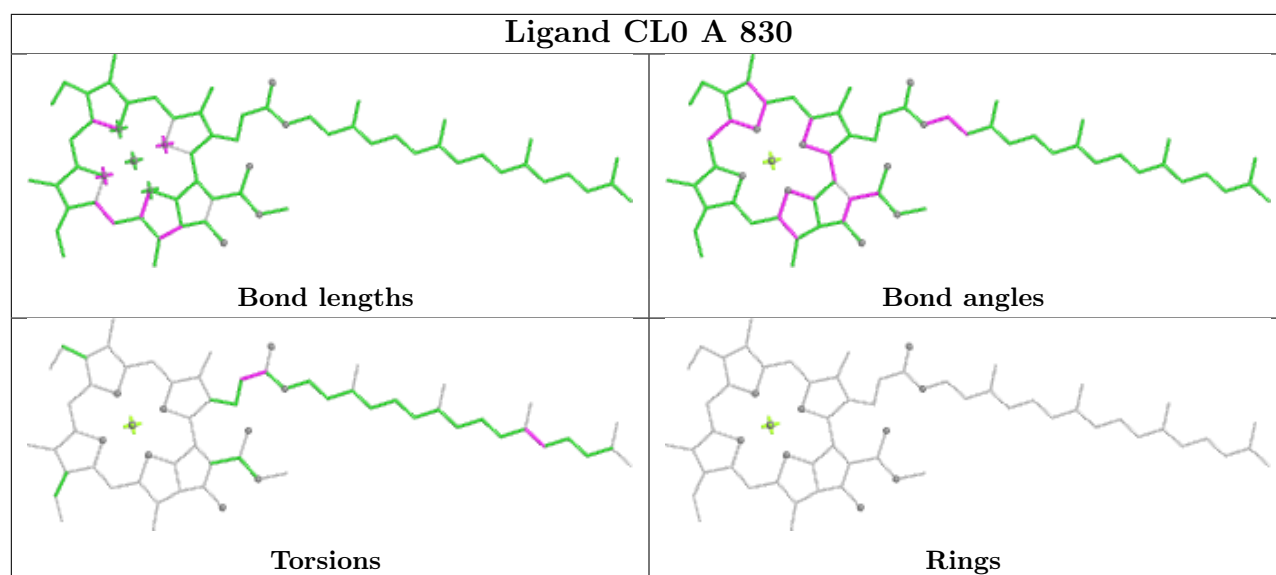


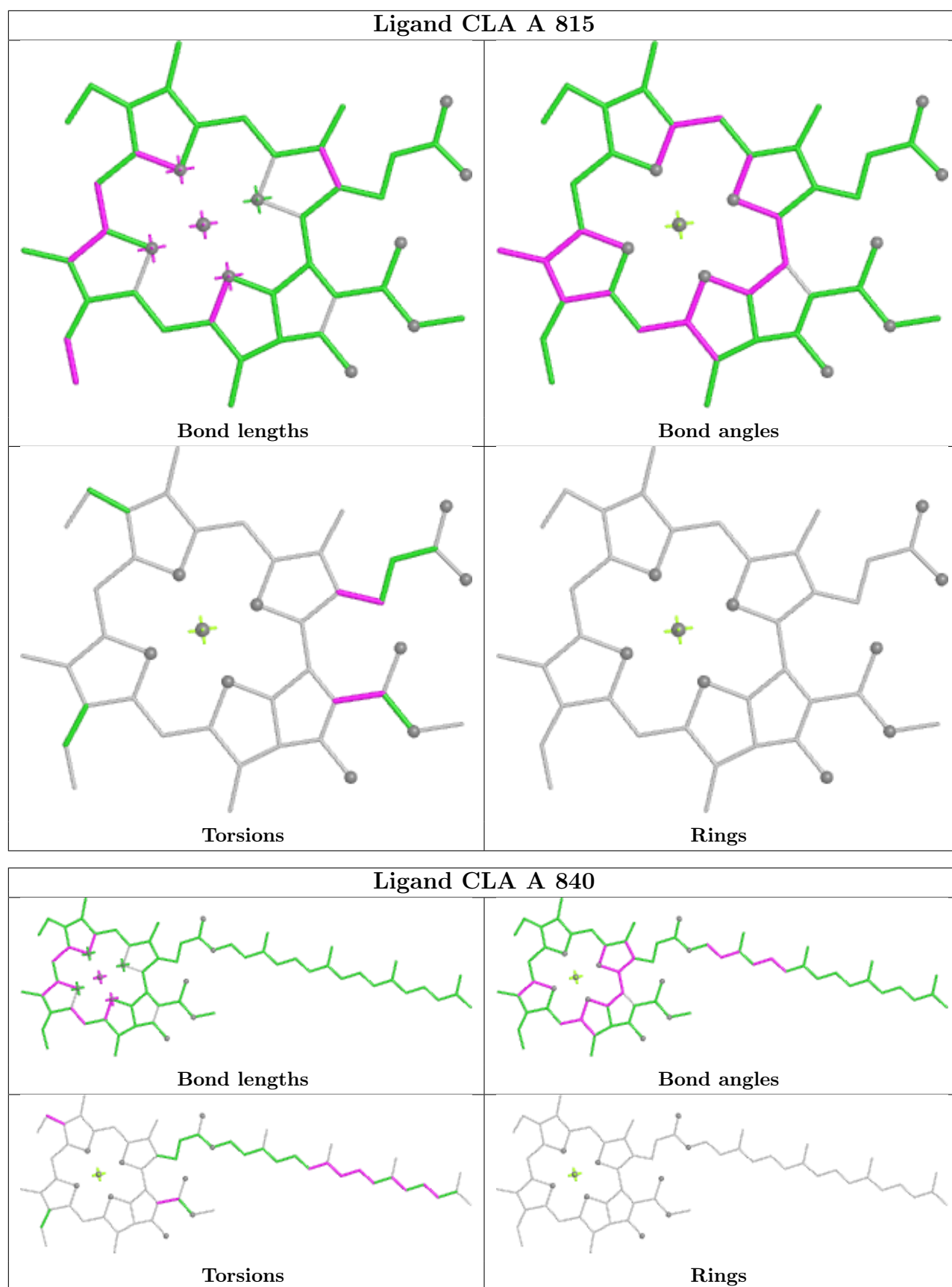
Ligand CLA H 201

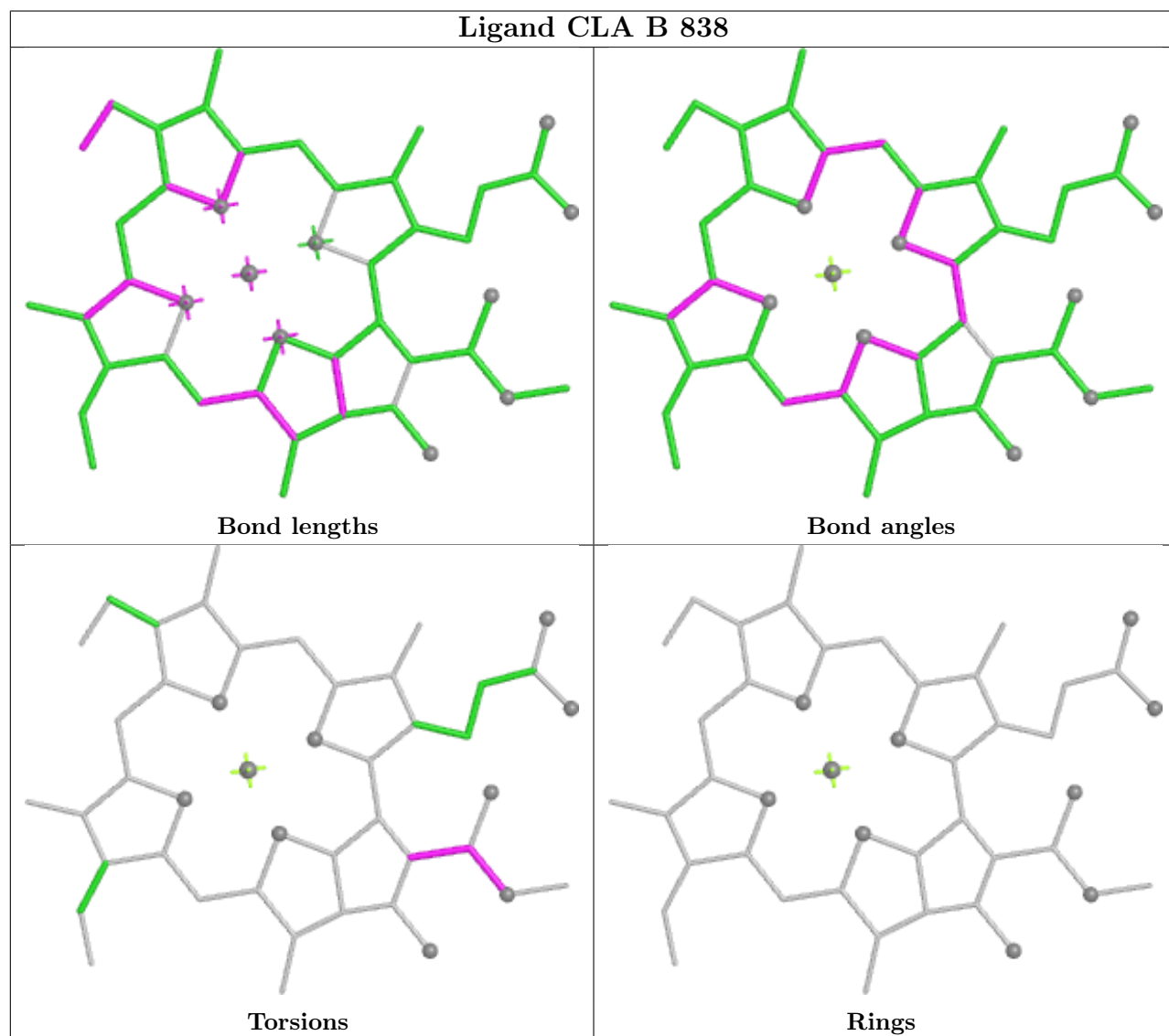
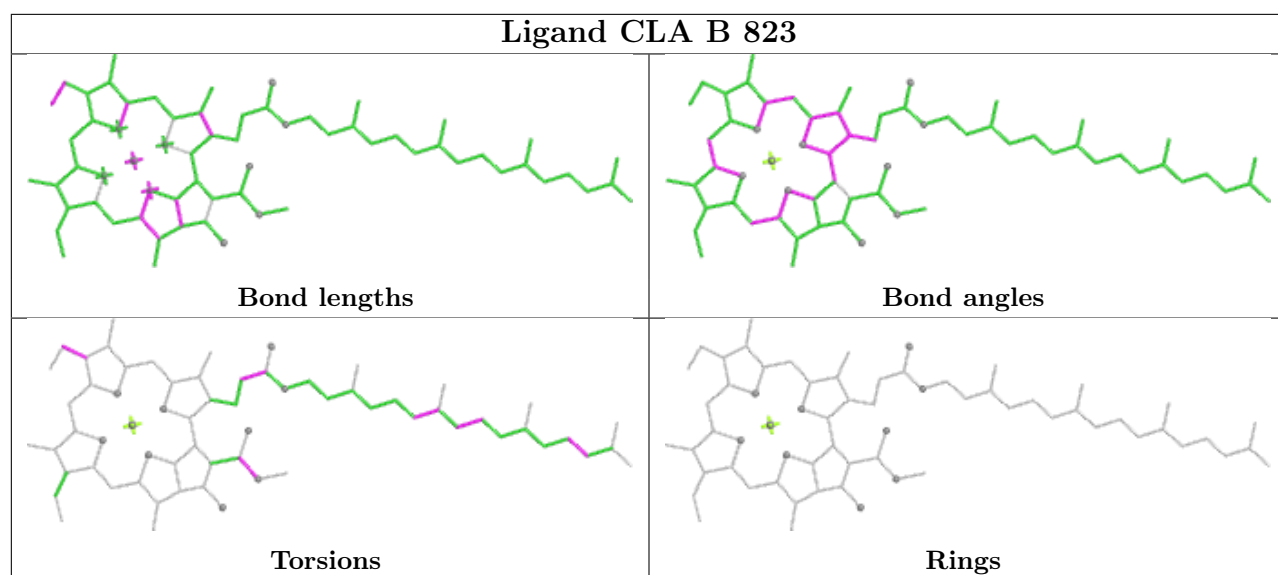


Ligand CLA B 836

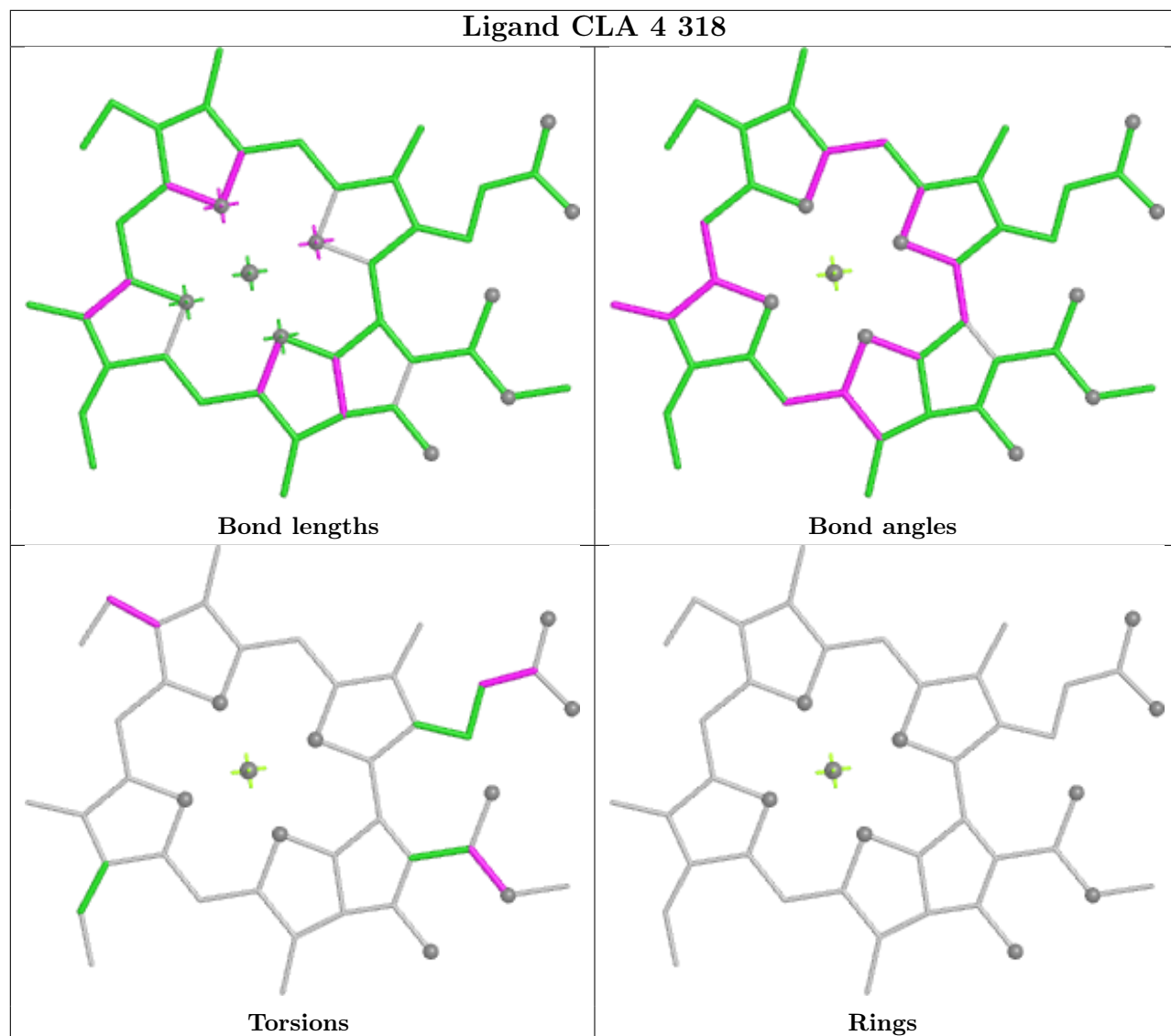




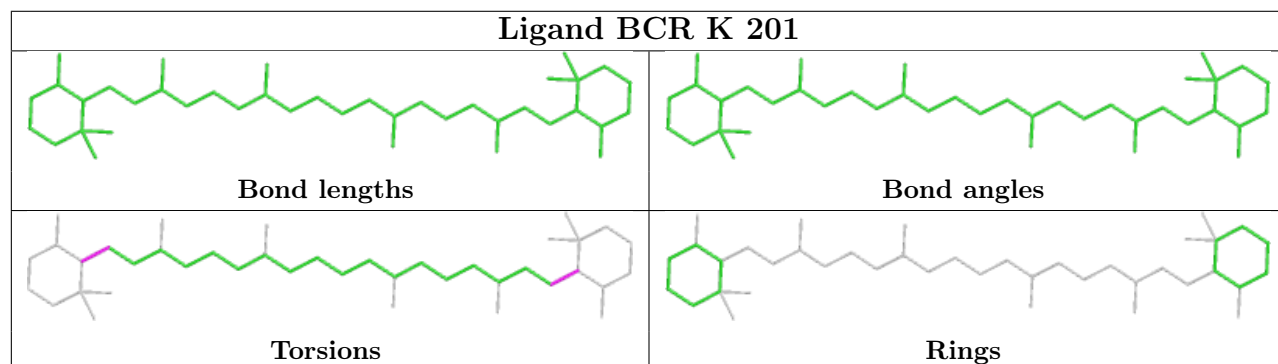


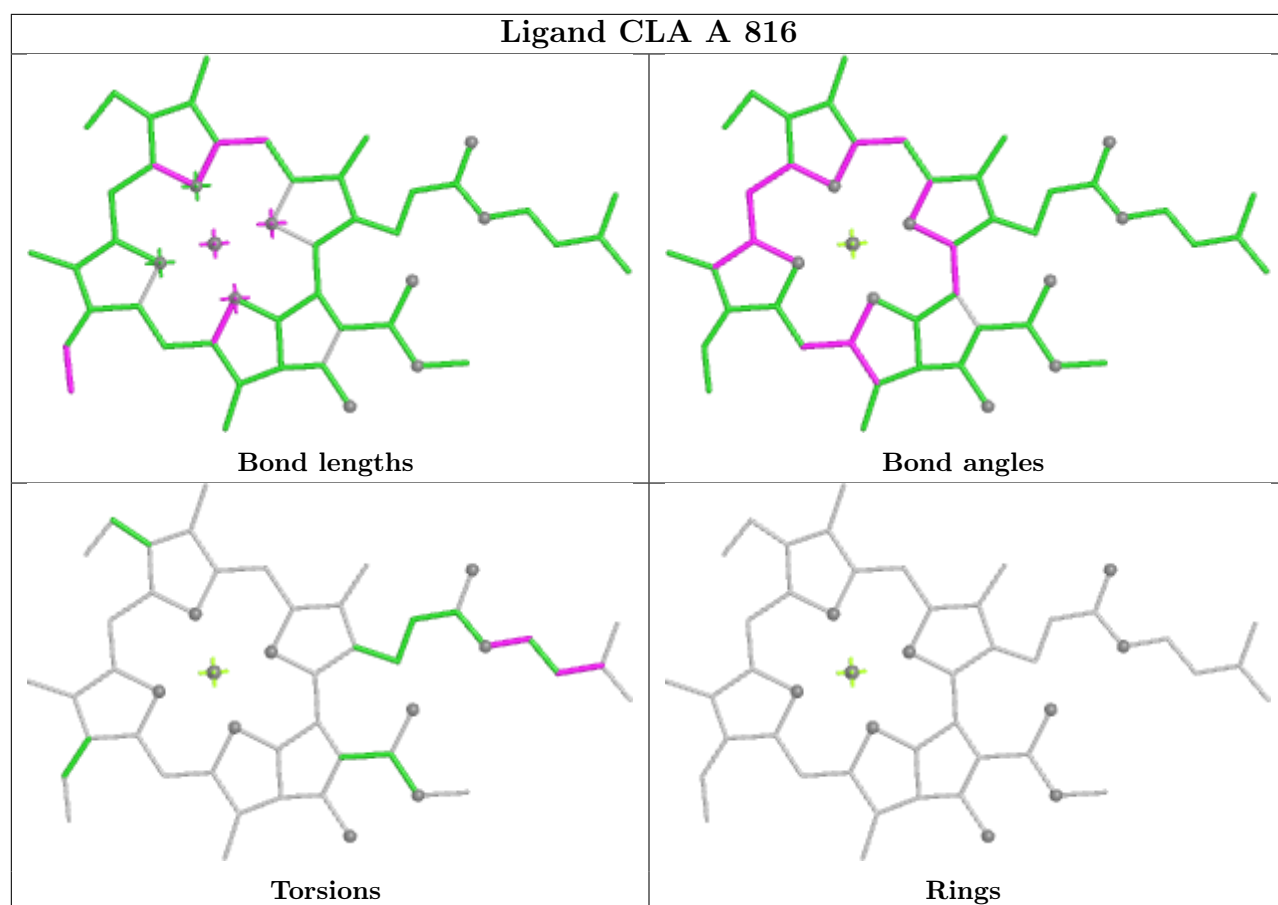


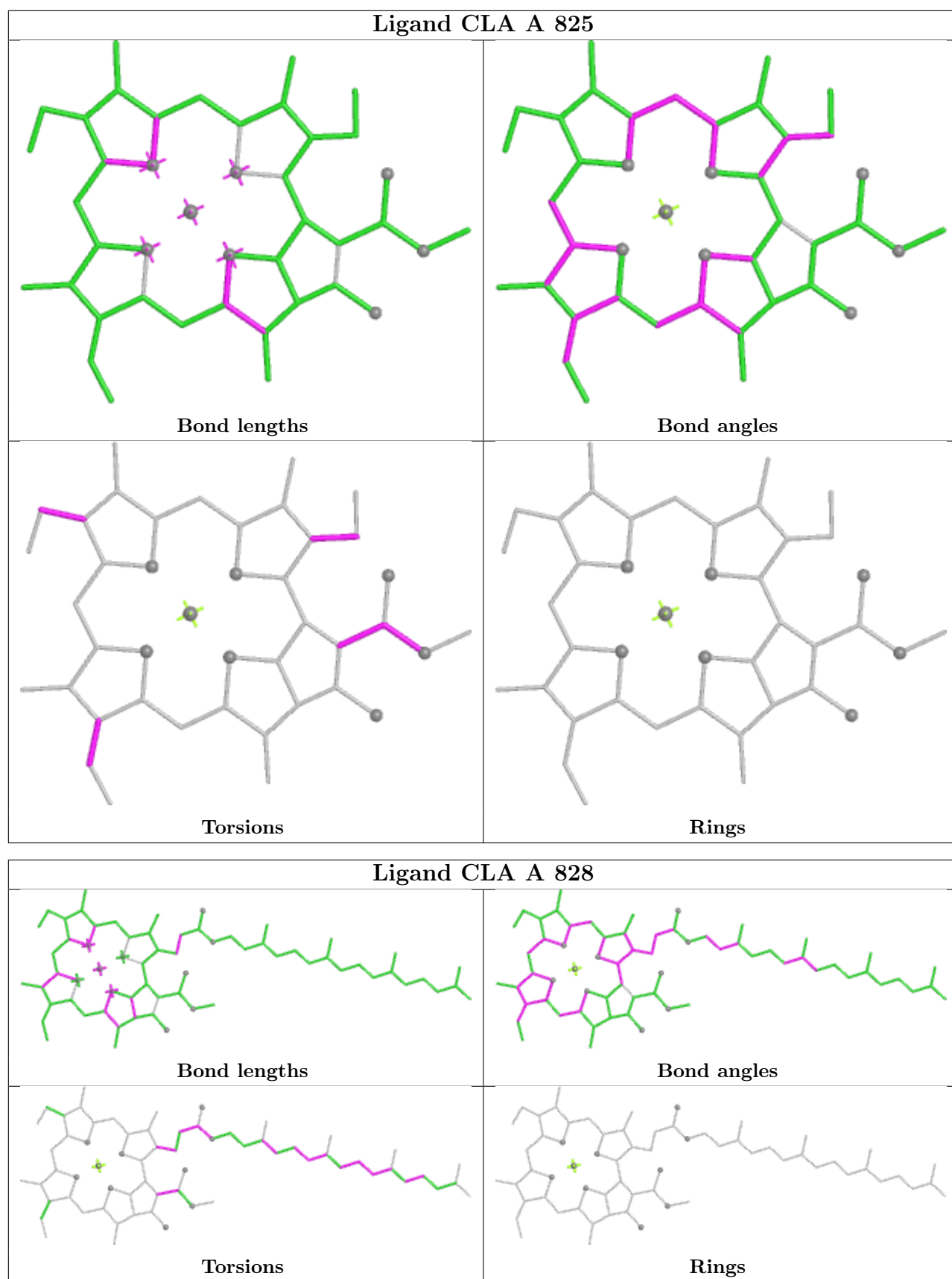
Ligand CLA 4 318



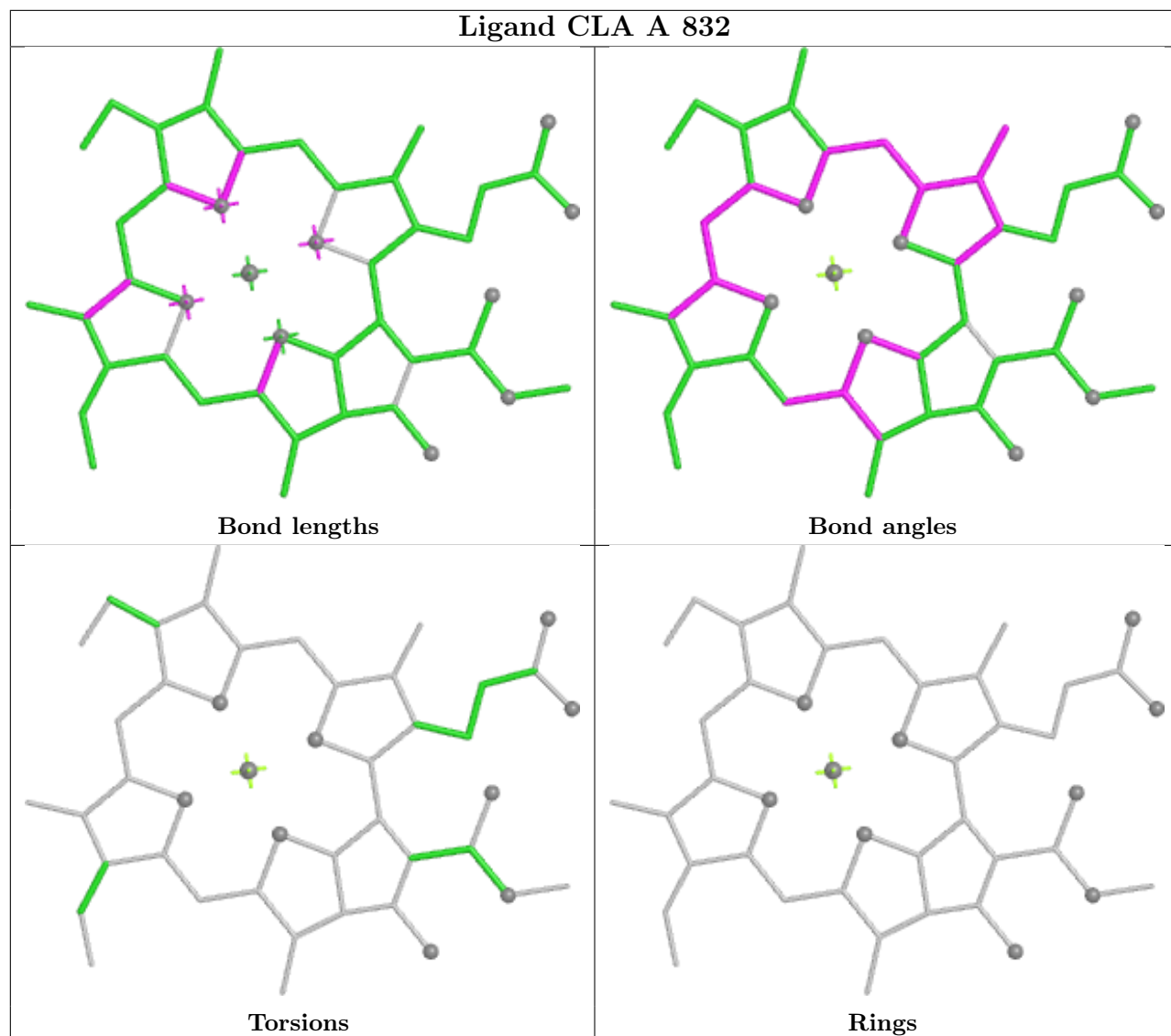
Ligand BCR K 201



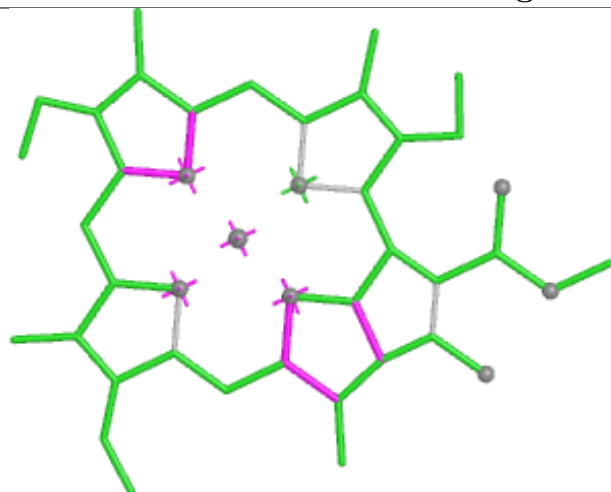




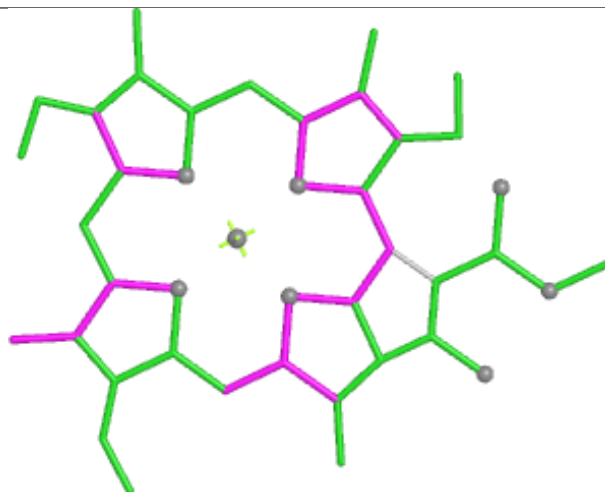
Ligand CLA A 832



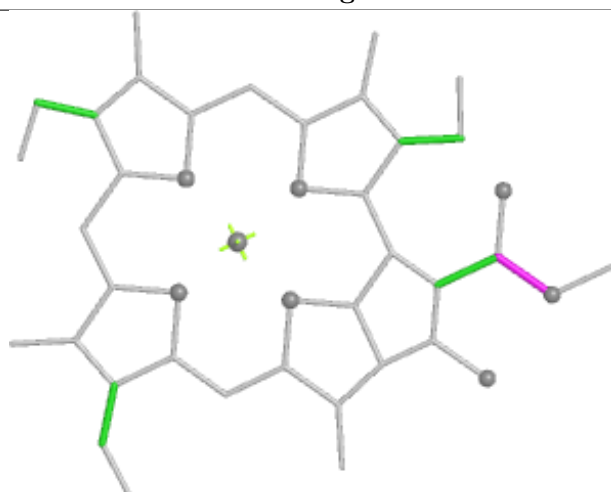
Ligand CLA F 303



Bond lengths



Bond angles

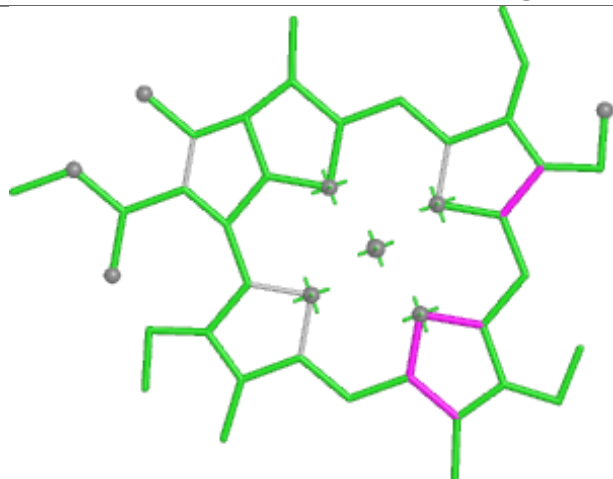


Torsions

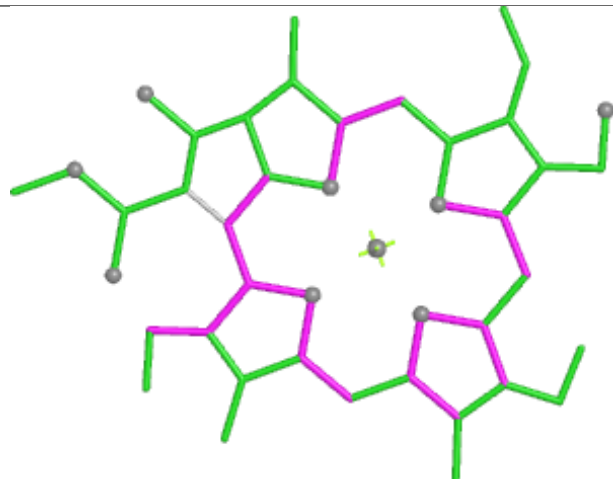


Rings

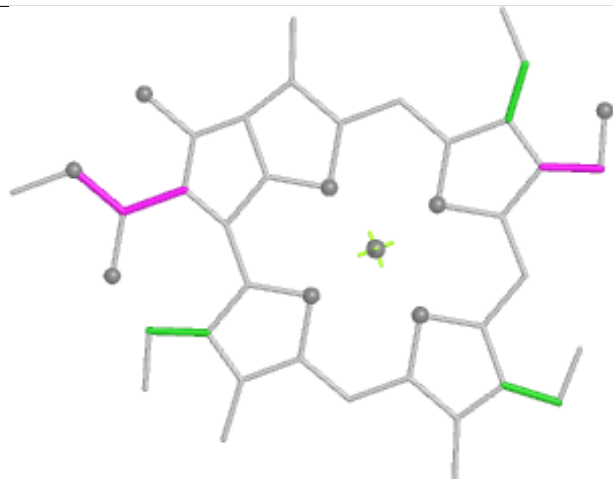
Ligand CHL 1 606



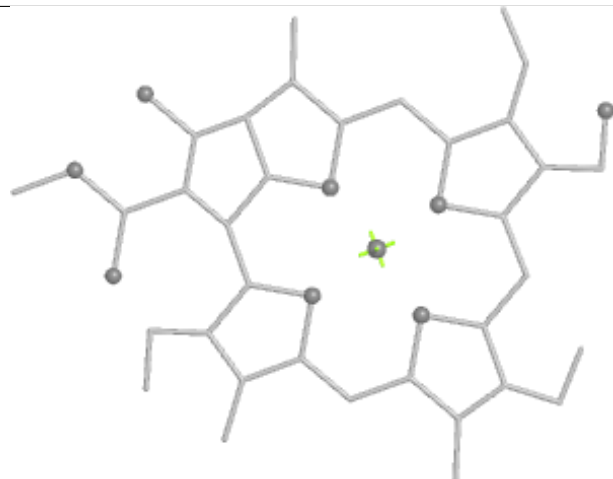
Bond lengths



Bond angles



Torsions



Rings

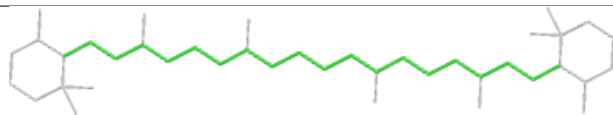
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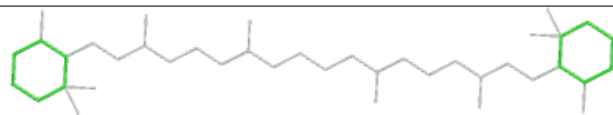
Bond lengths



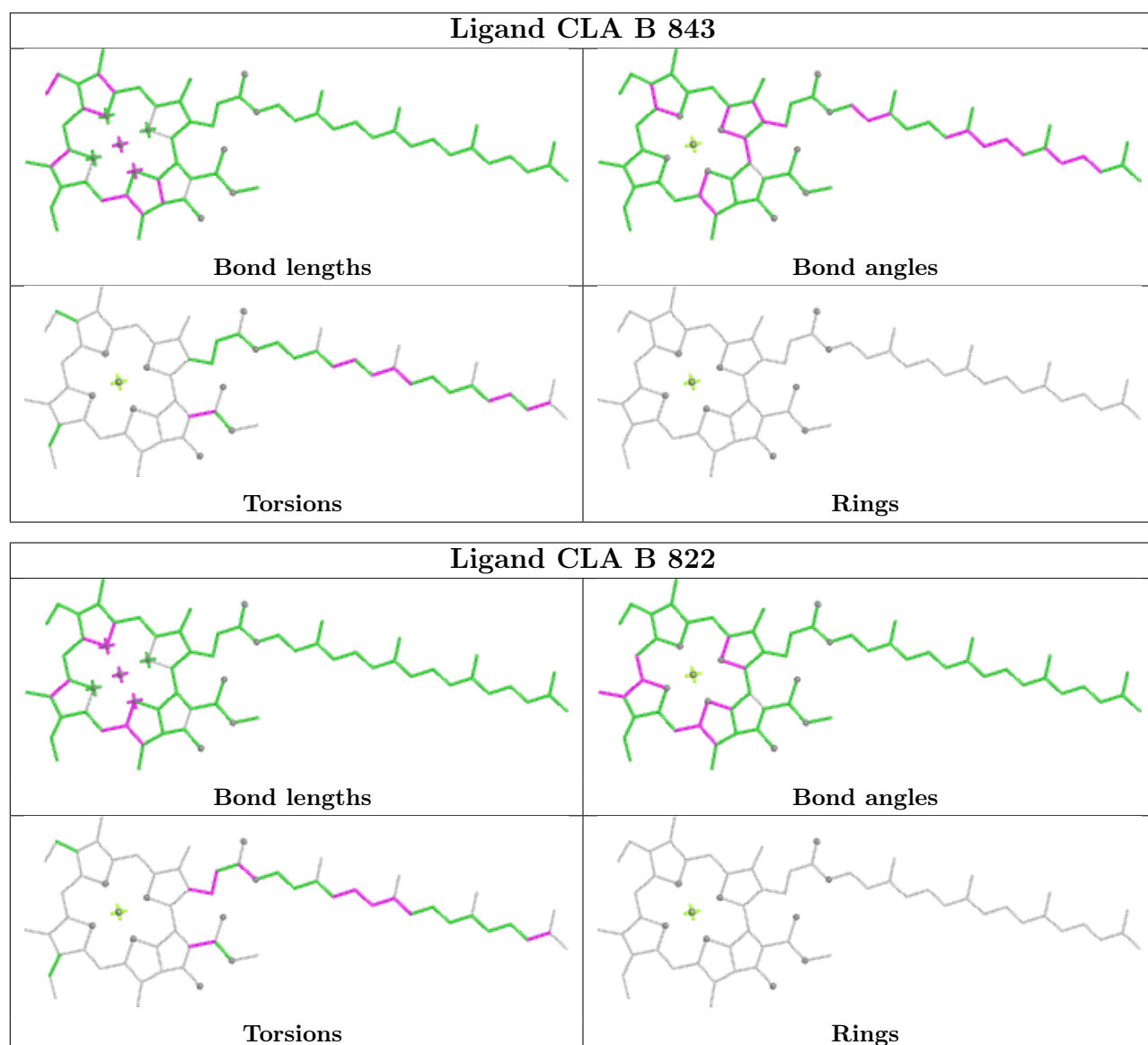
Bond angles



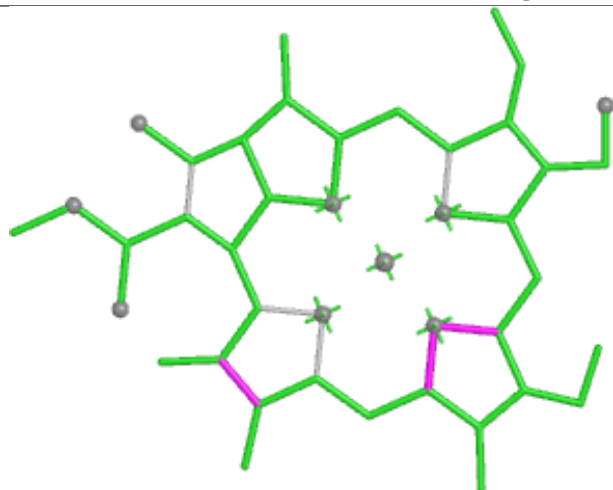
Torsions



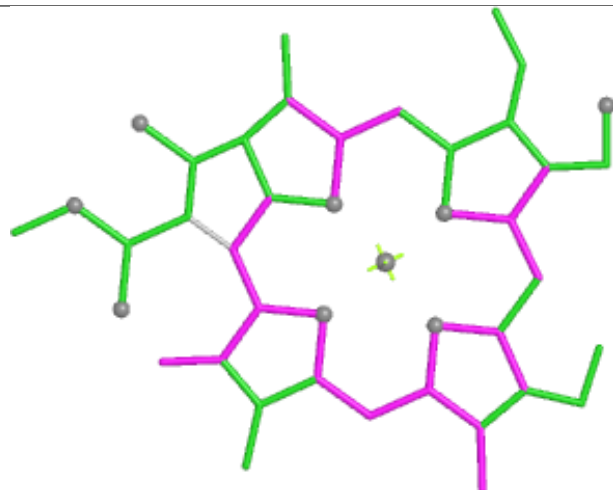
Rings



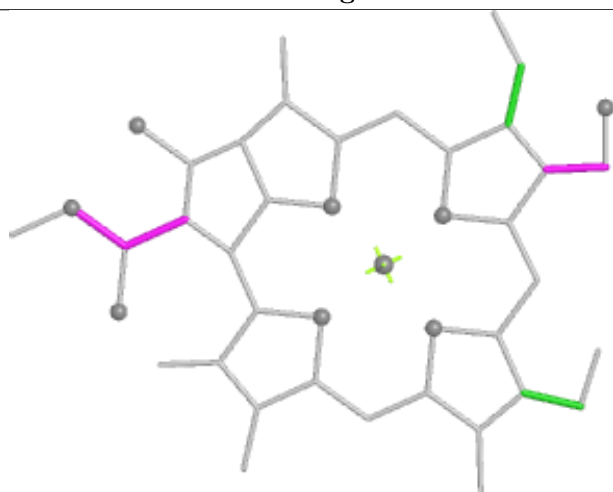
Ligand CHL 2 313



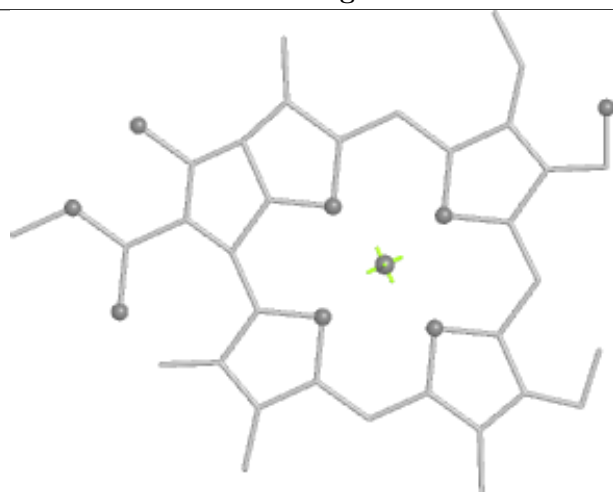
Bond lengths



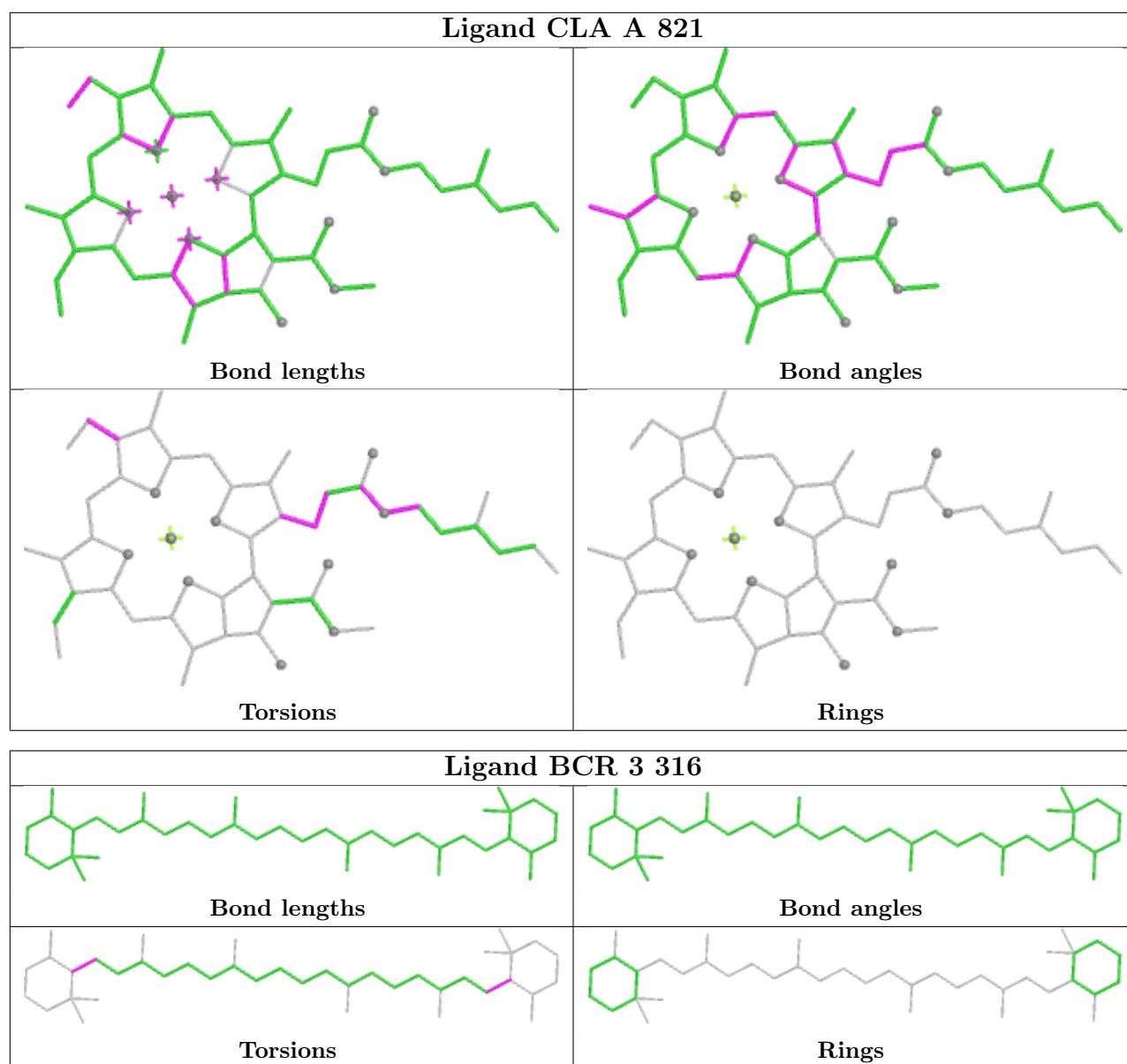
Bond angles



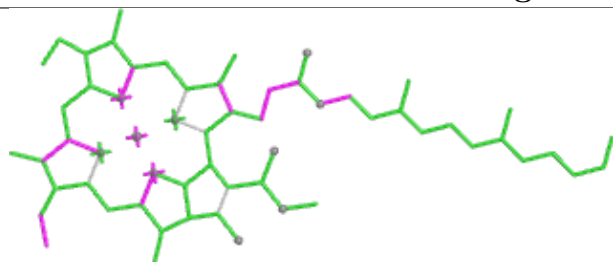
Torsions



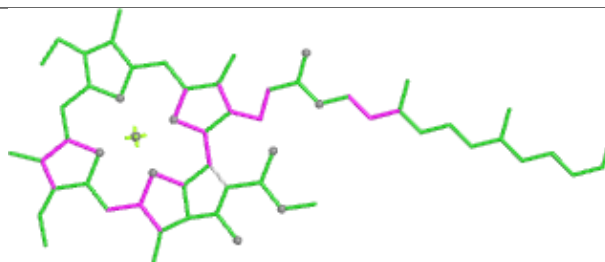
Rings



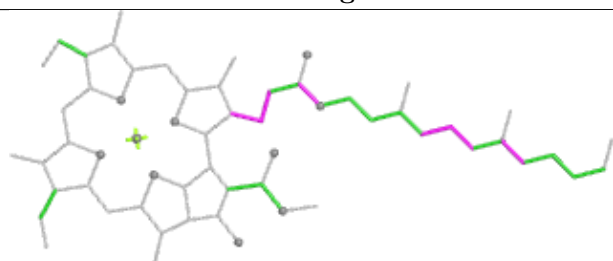
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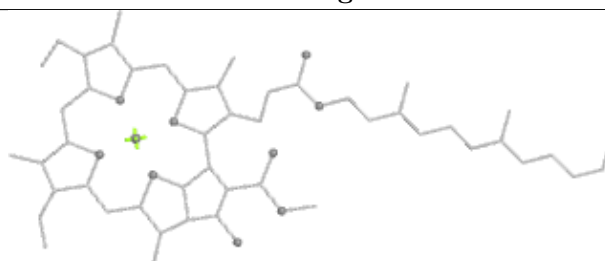
Bond lengths



Bond angles

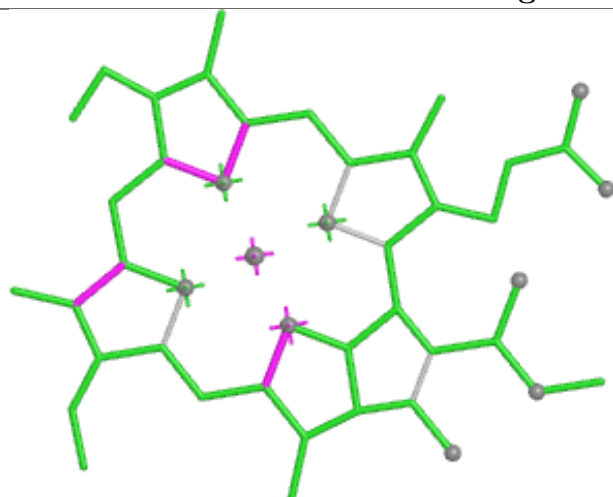


Torsions

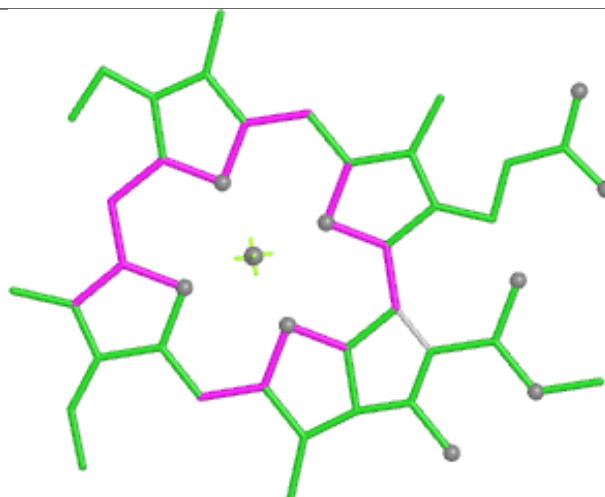


Rings

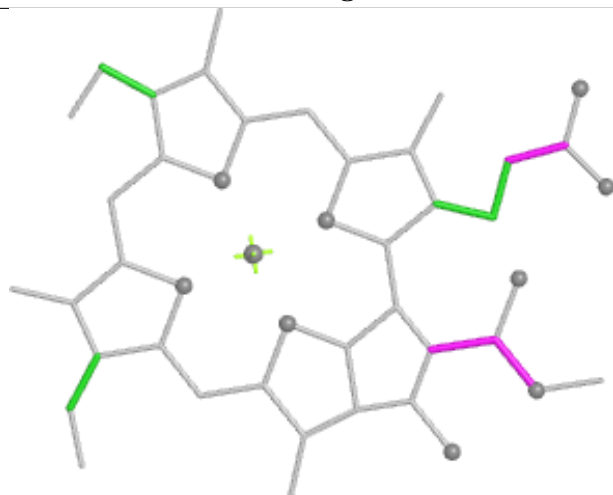
Ligand CLA 4 307



Bond lengths



Bond angles

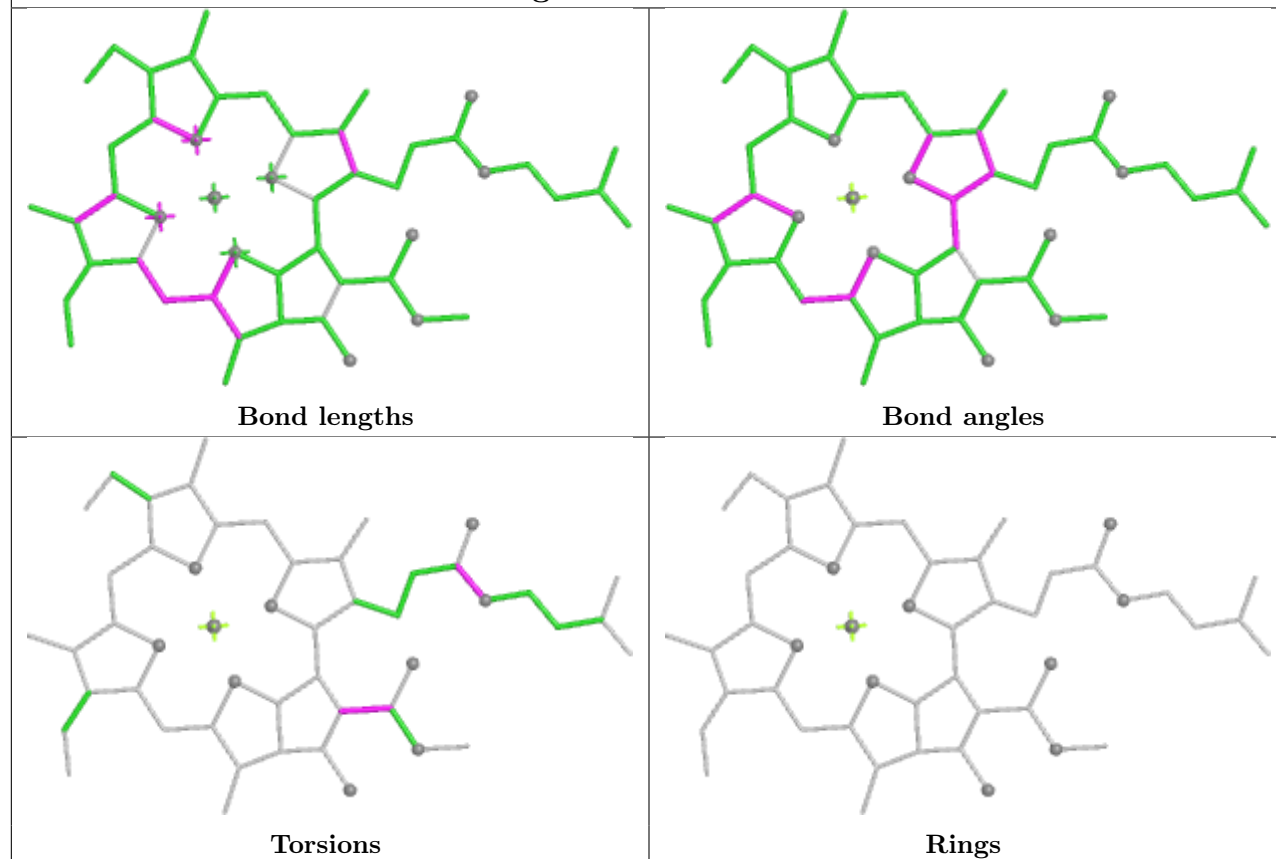


Torsions

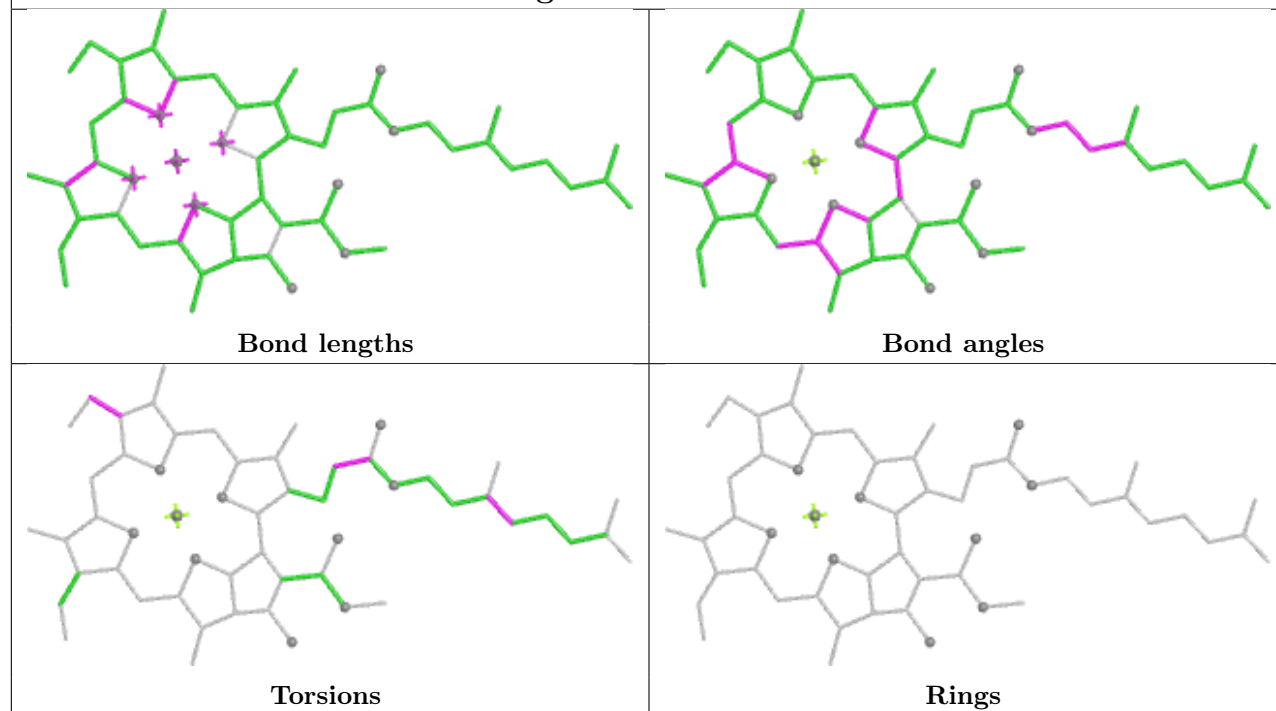


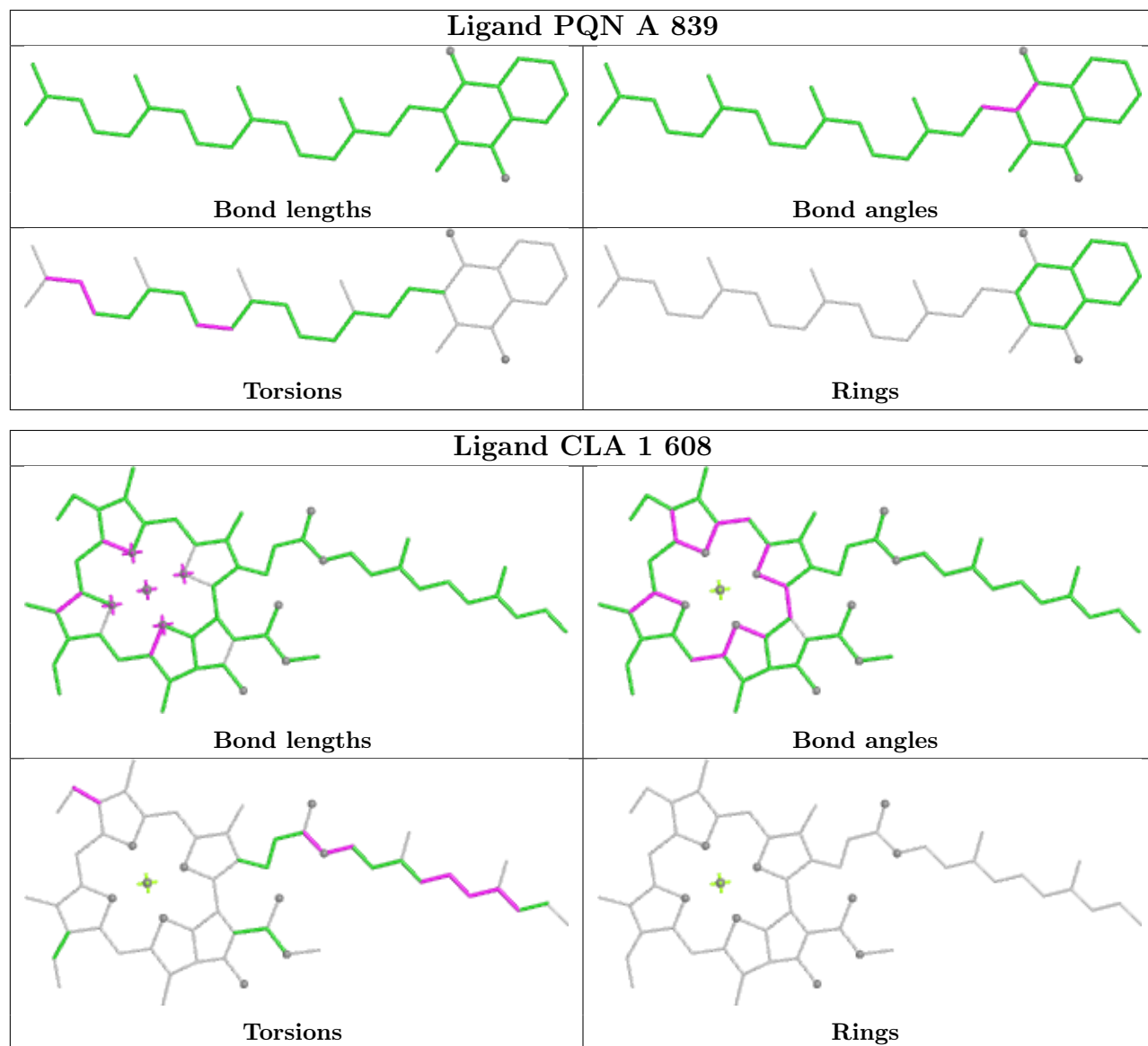
Rings

Ligand CLA B 847

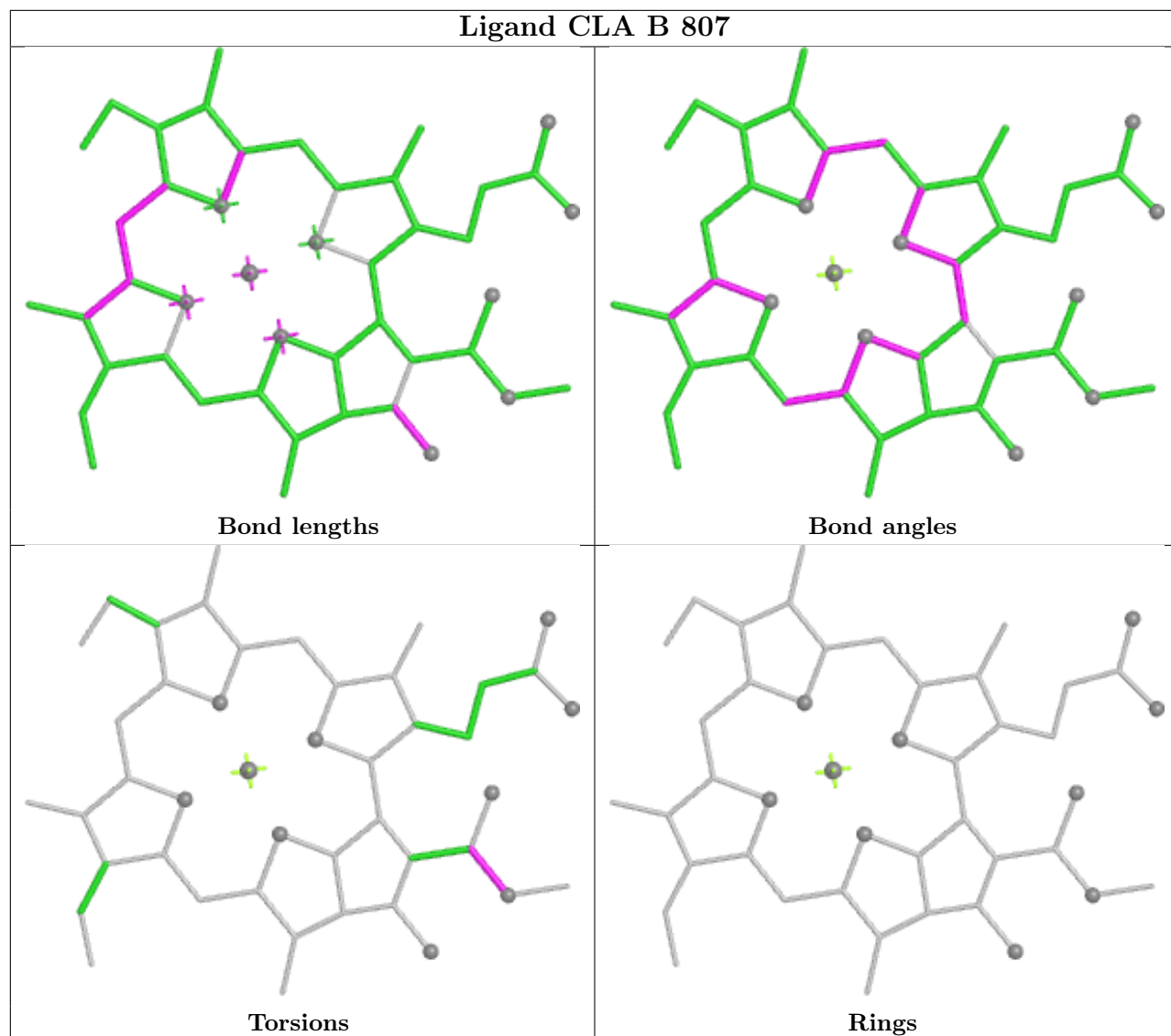


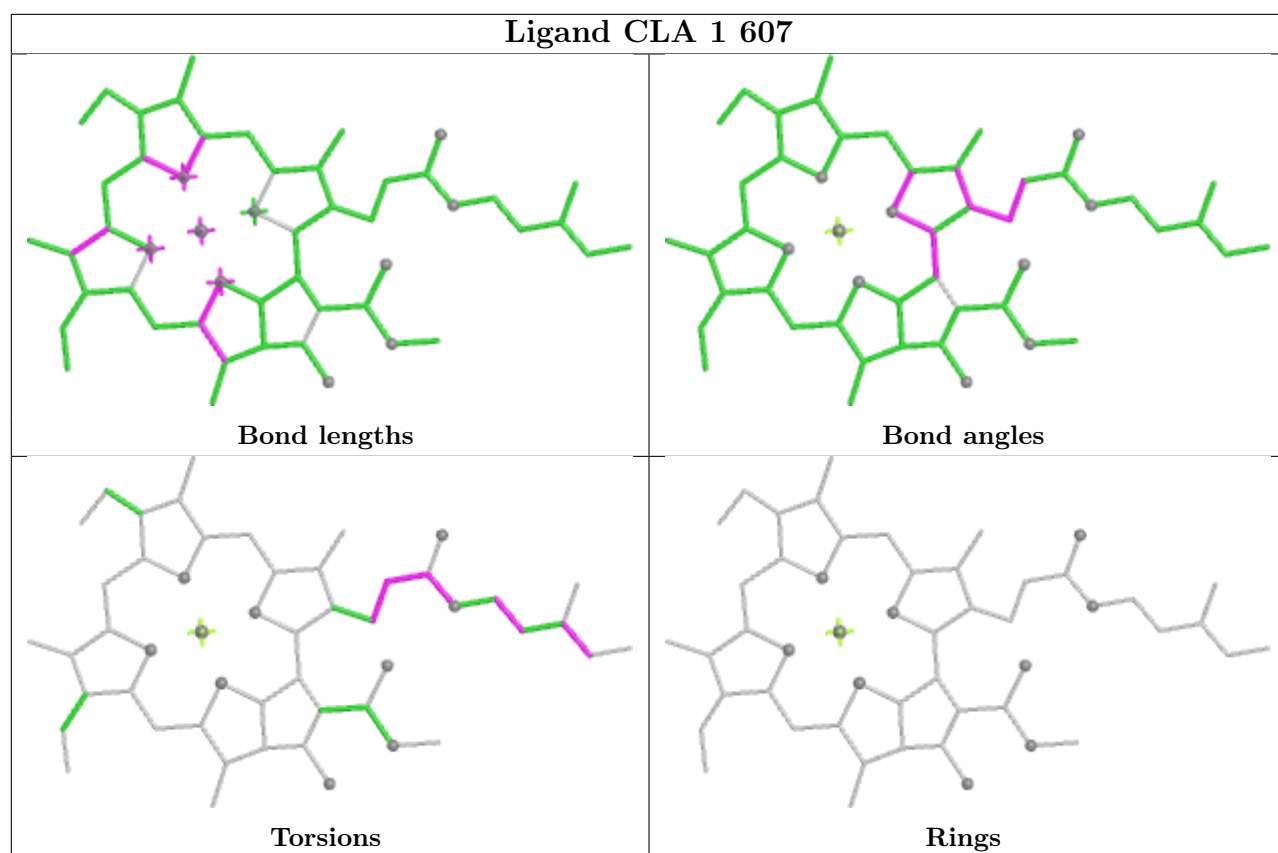
Ligand CLA 1 612



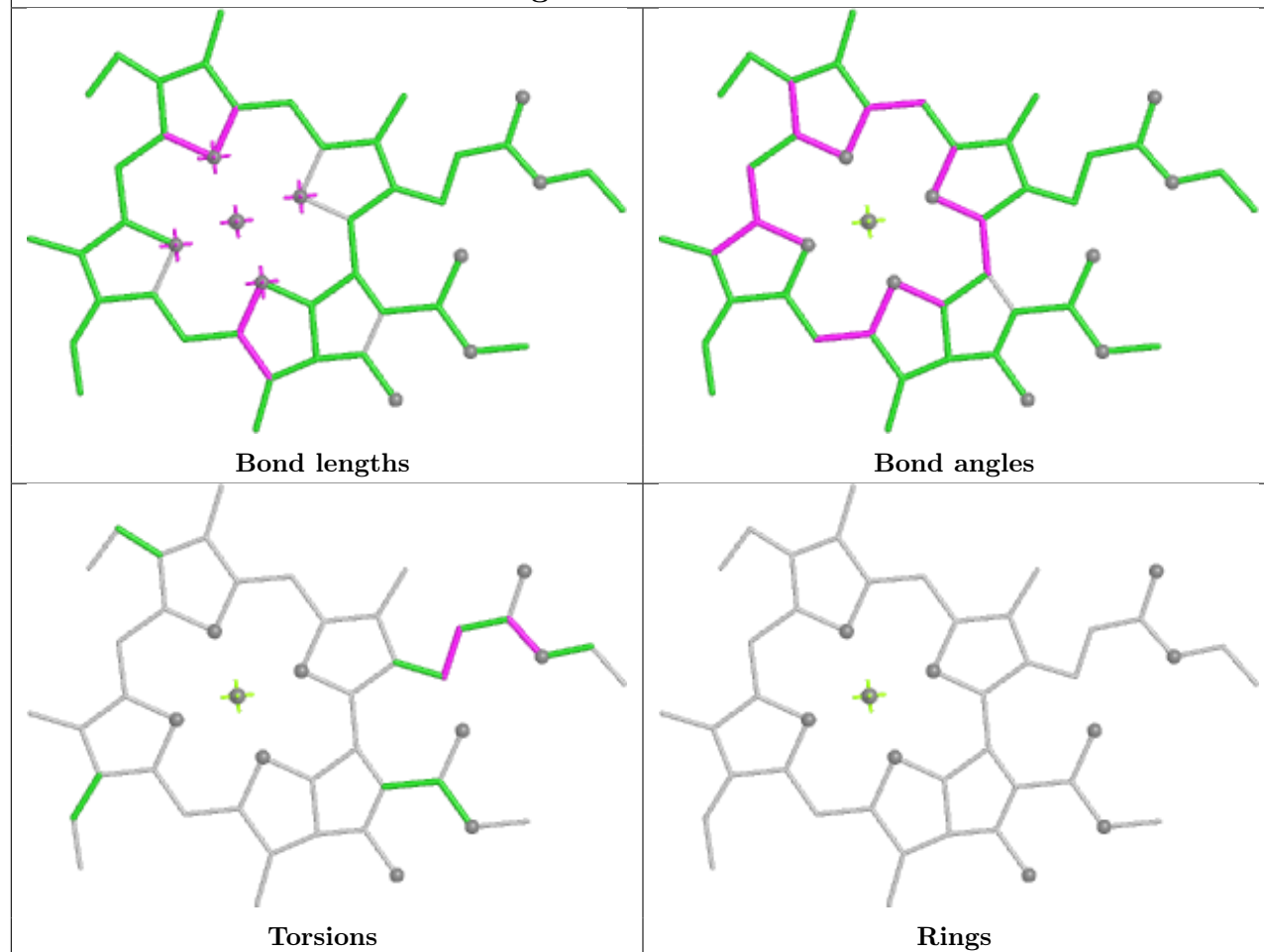


Ligand CLA B 807

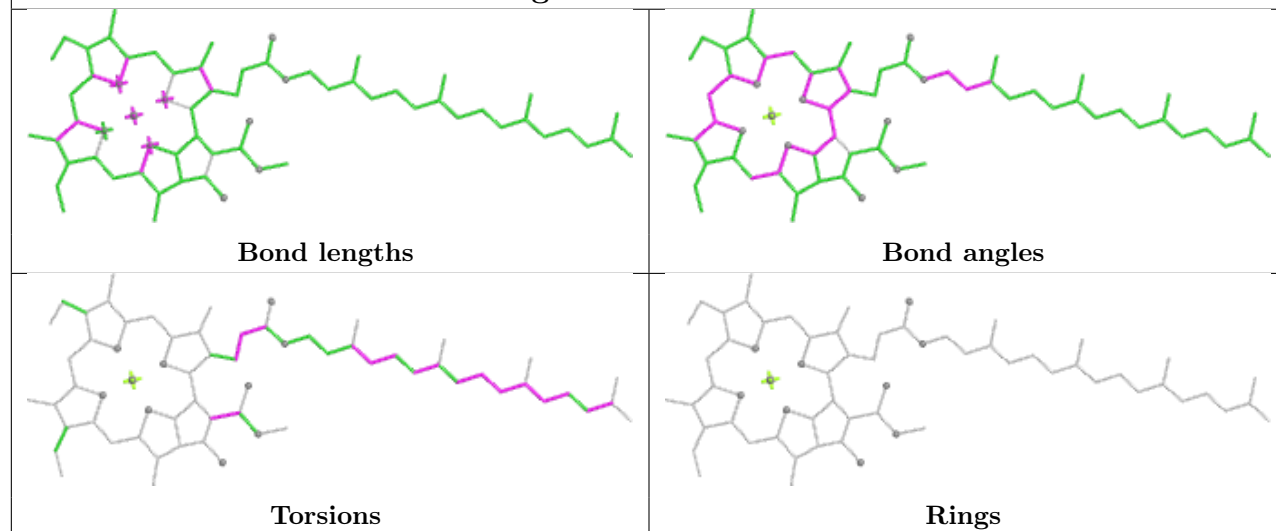


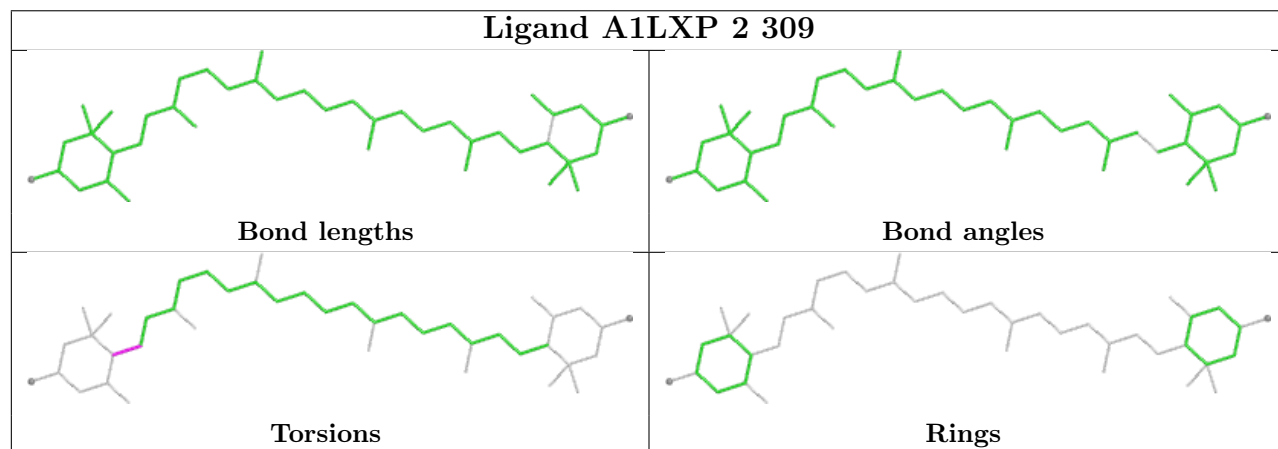
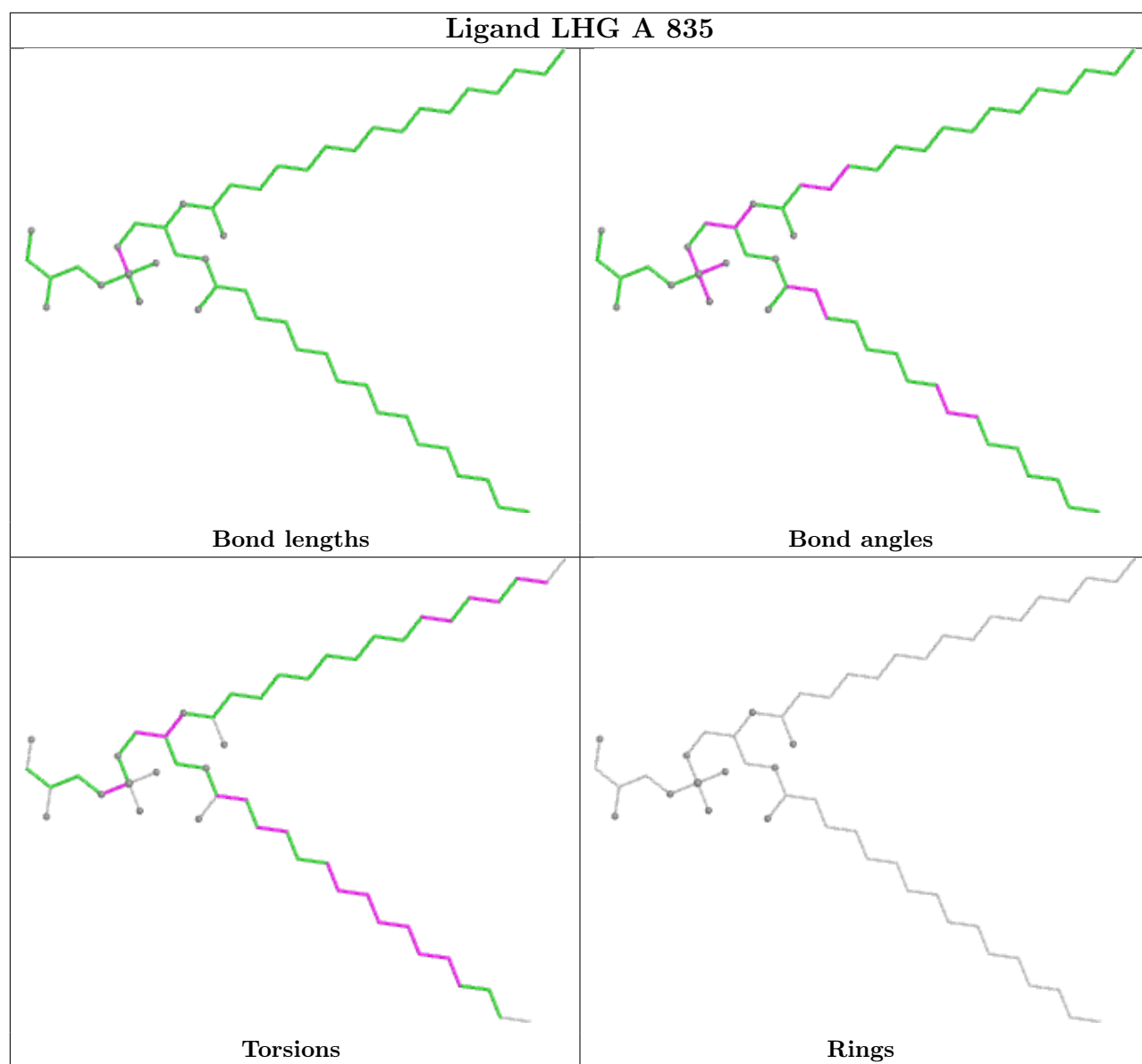


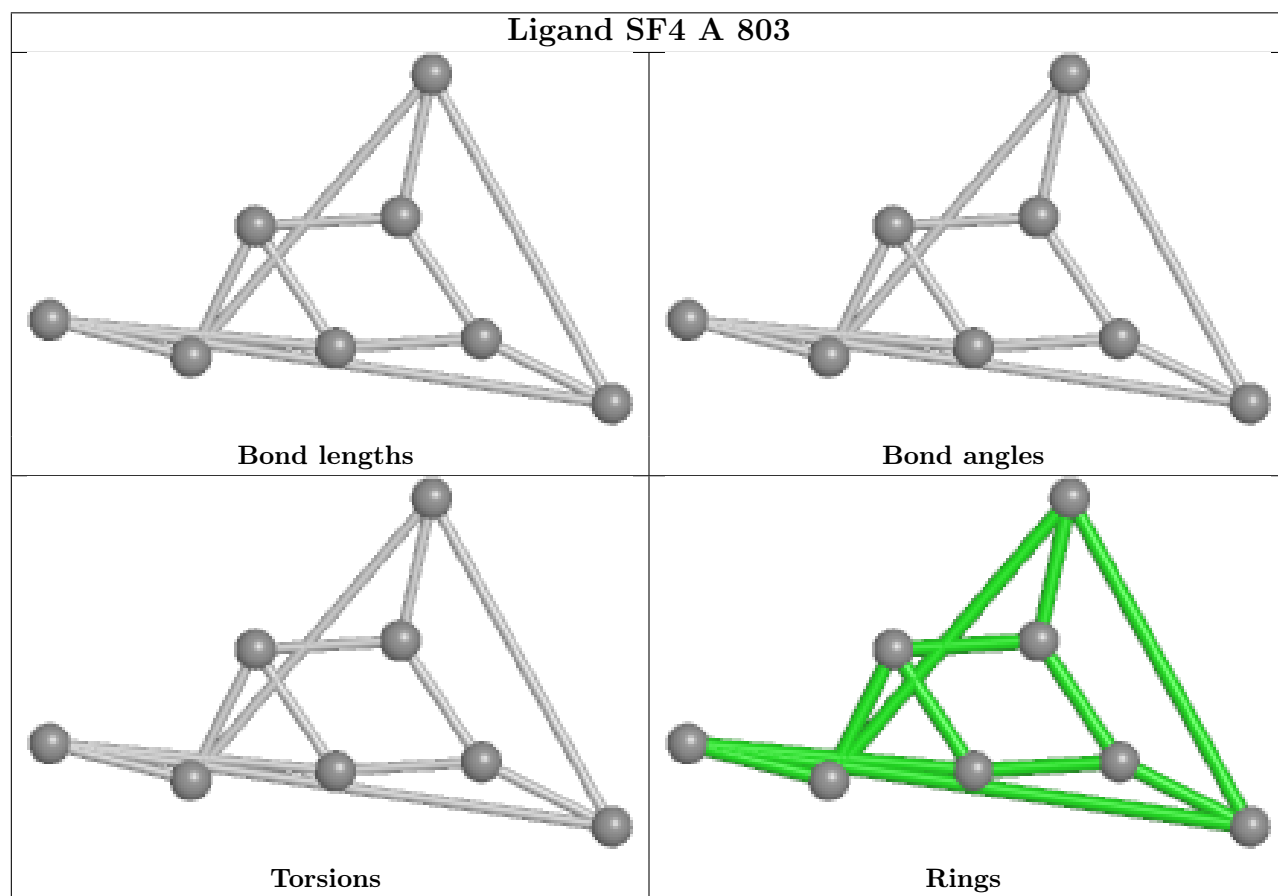
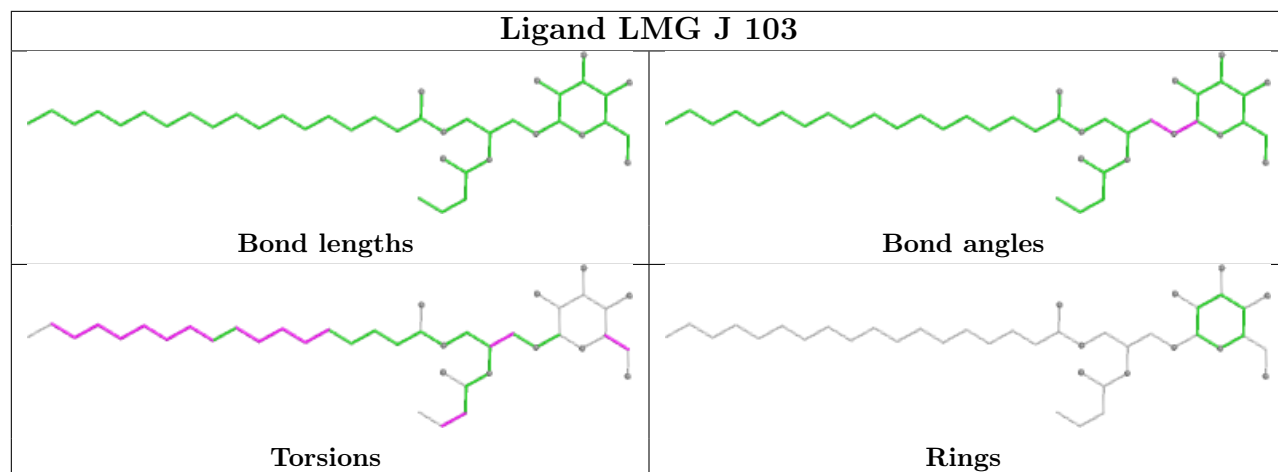
Ligand CLA 3 306

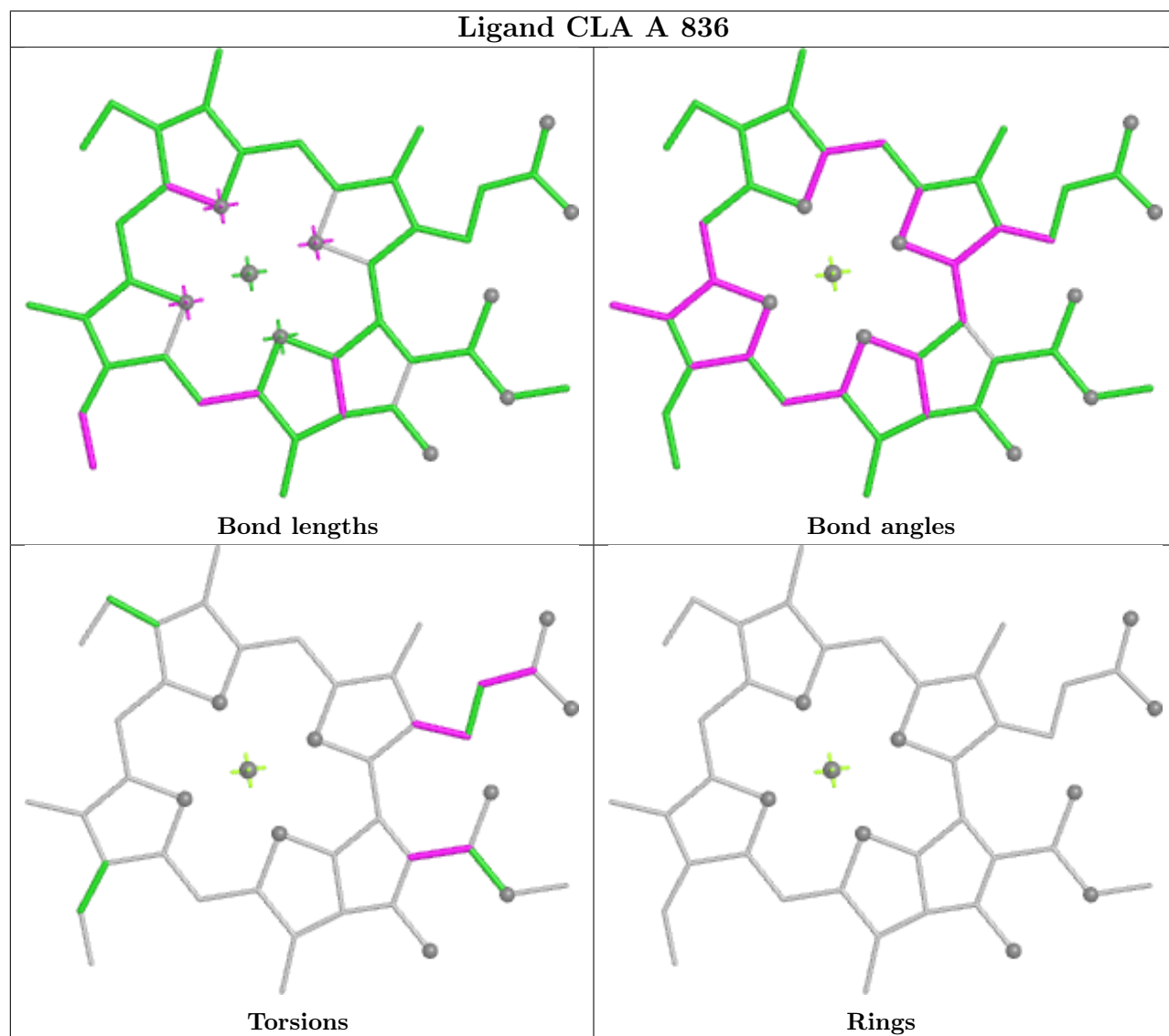
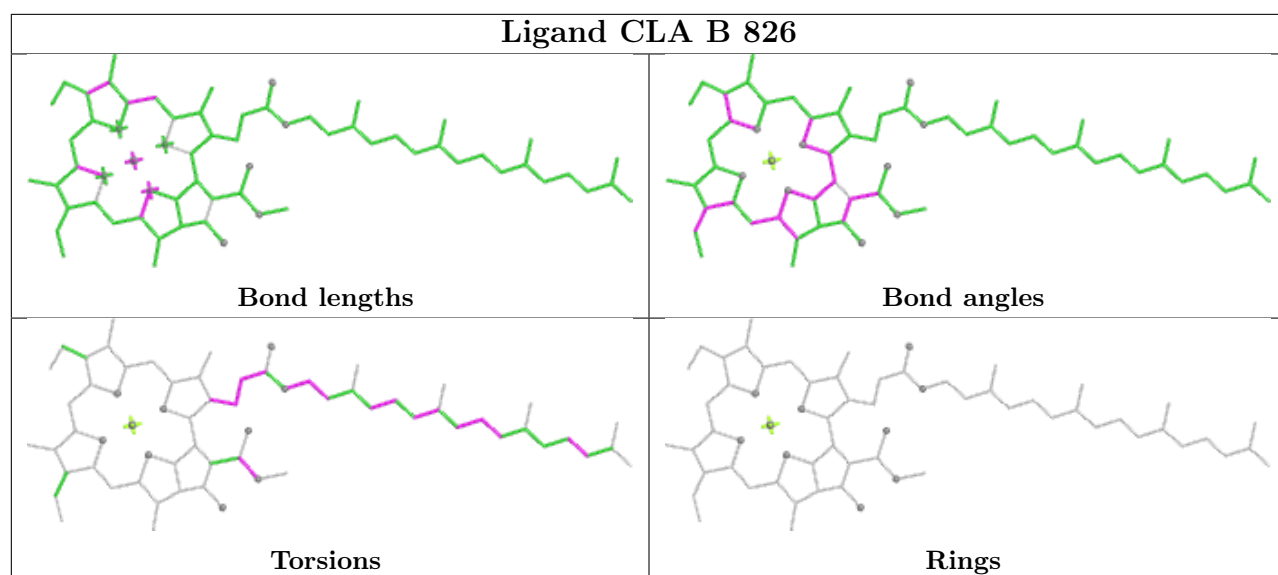


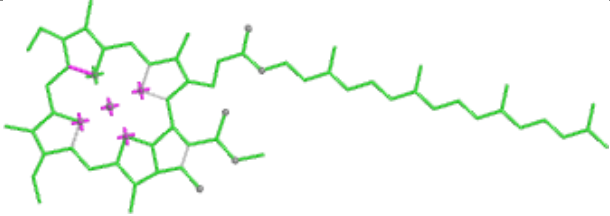
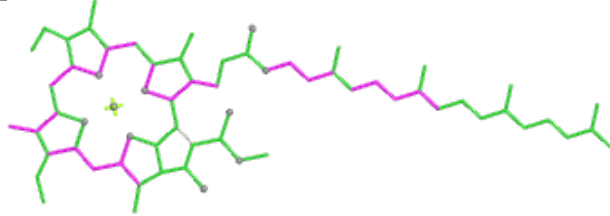
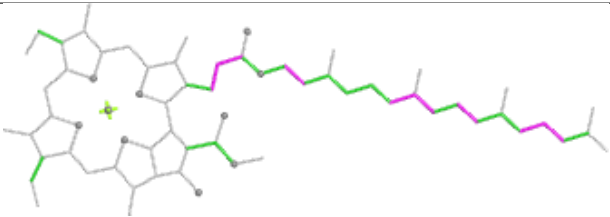
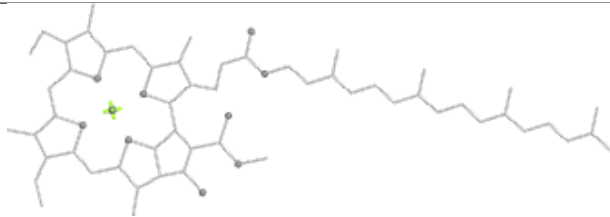
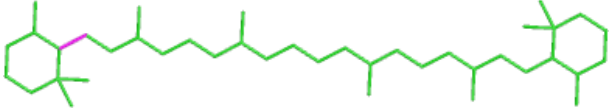
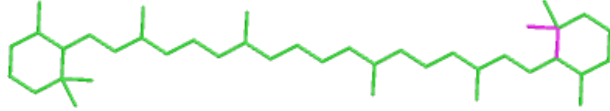
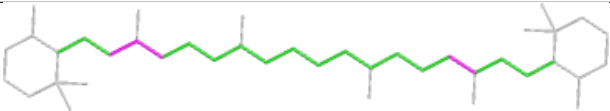
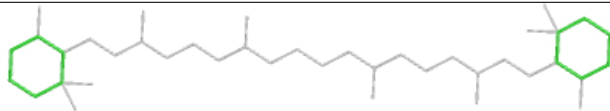
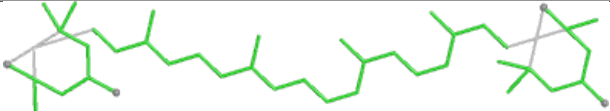
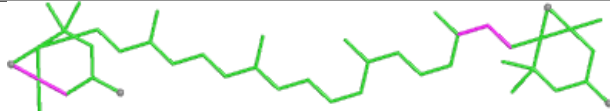
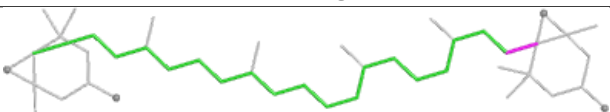
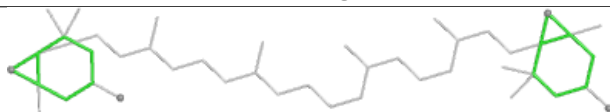
Ligand CLA A 818

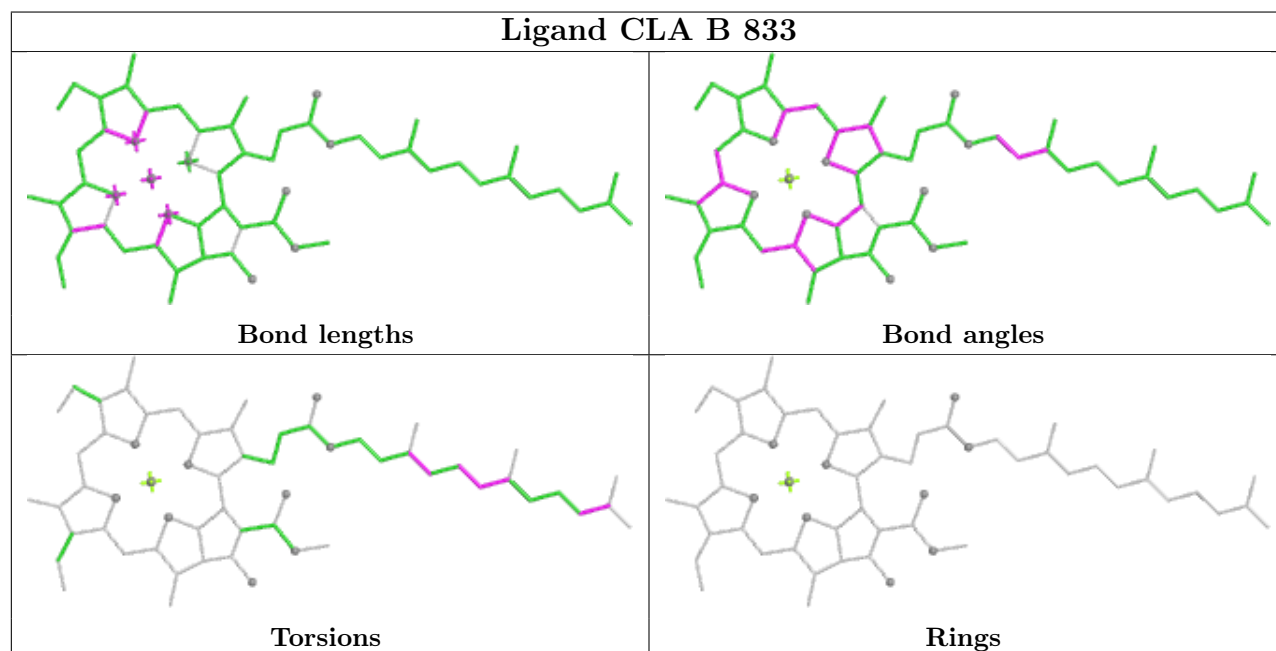
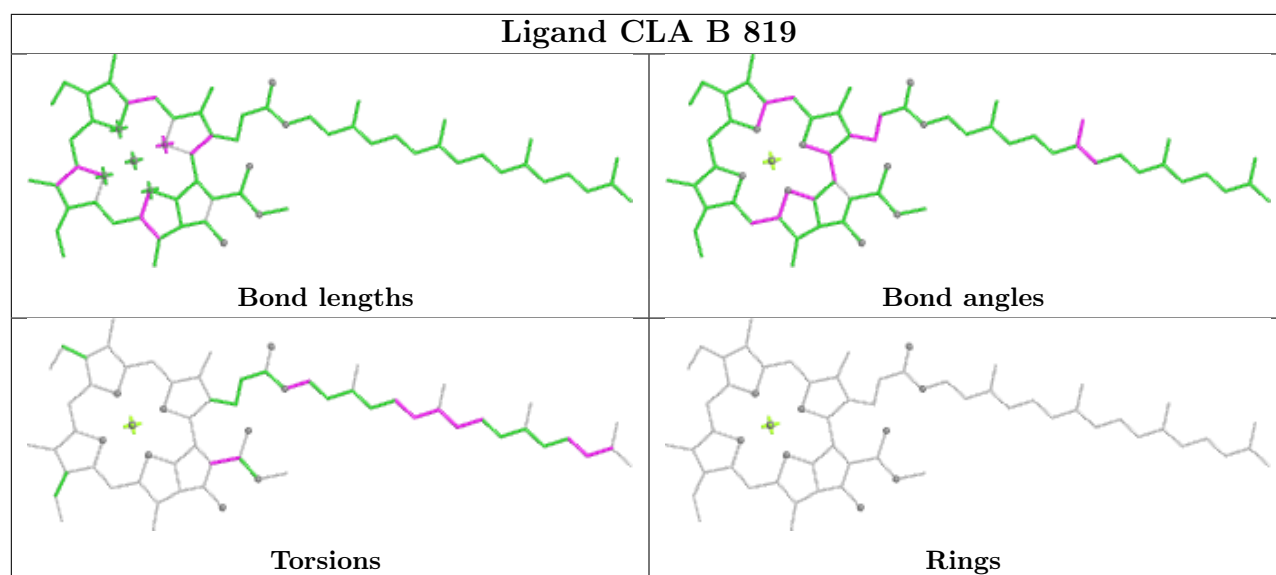




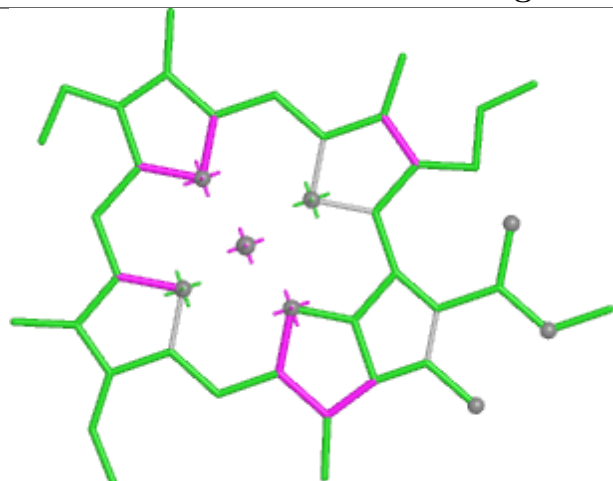




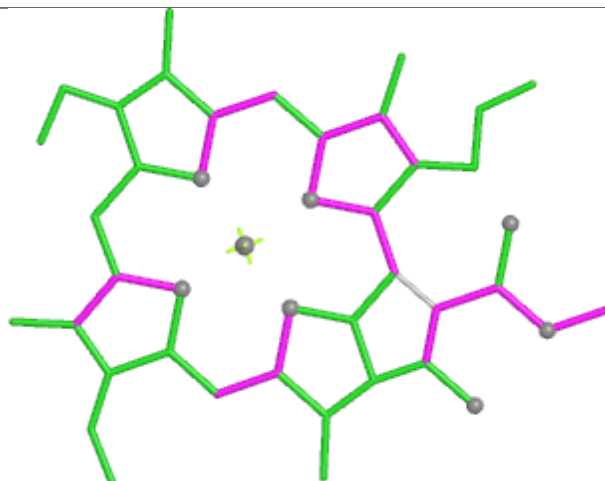
Ligand CLA B 834	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 813	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand XAT 2 306	
 Bond lengths	 Bond angles
 Torsions	 Rings



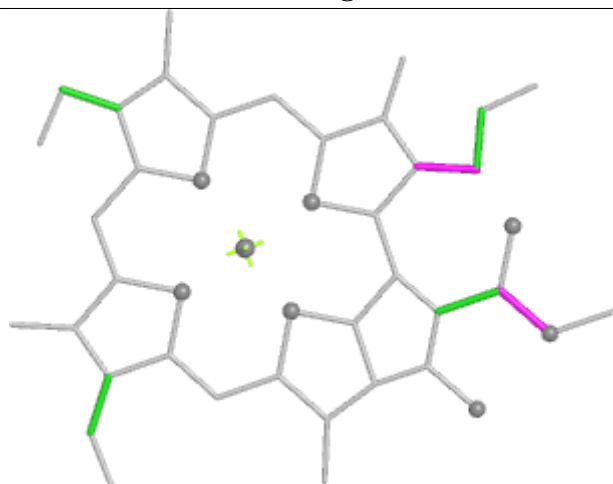
Ligand CLA B 839



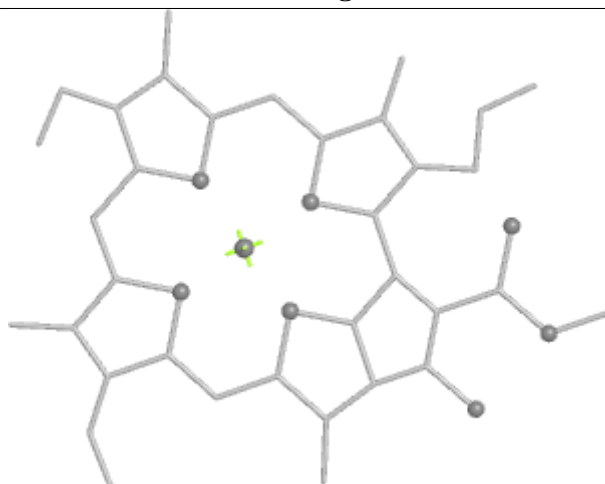
Bond lengths



Bond angles

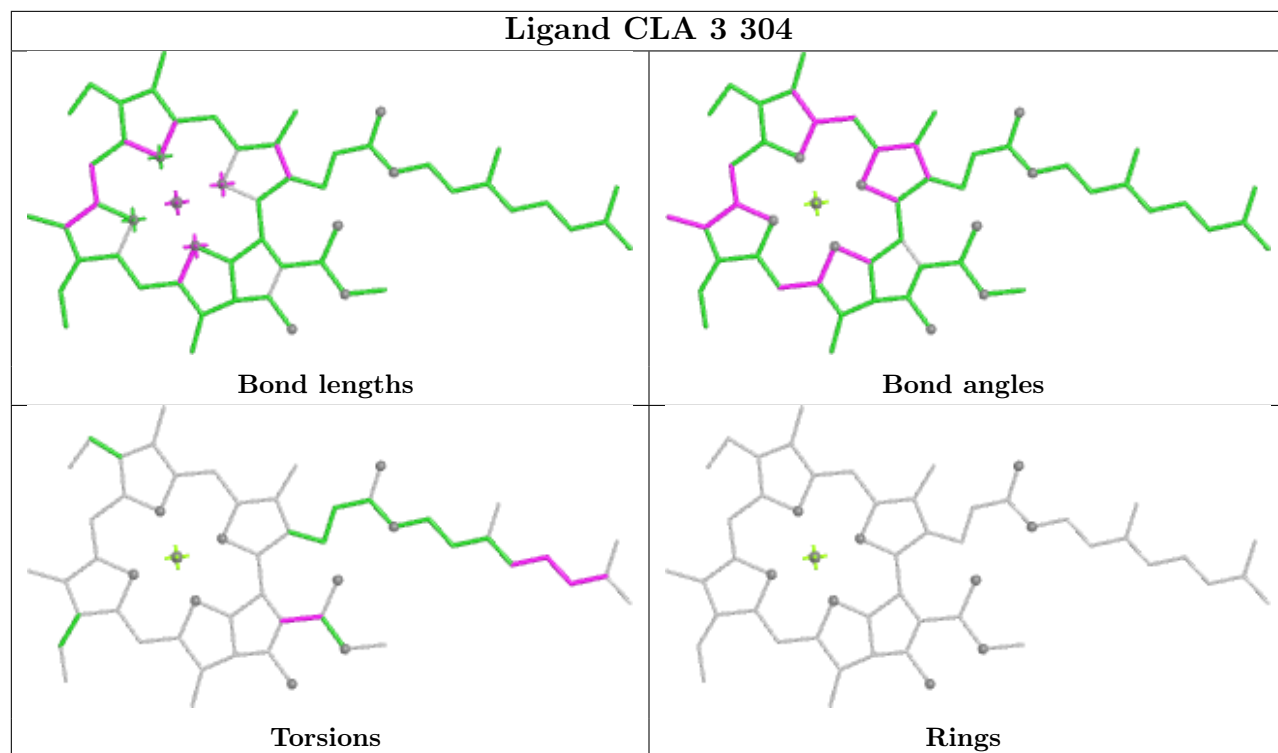


Torsions

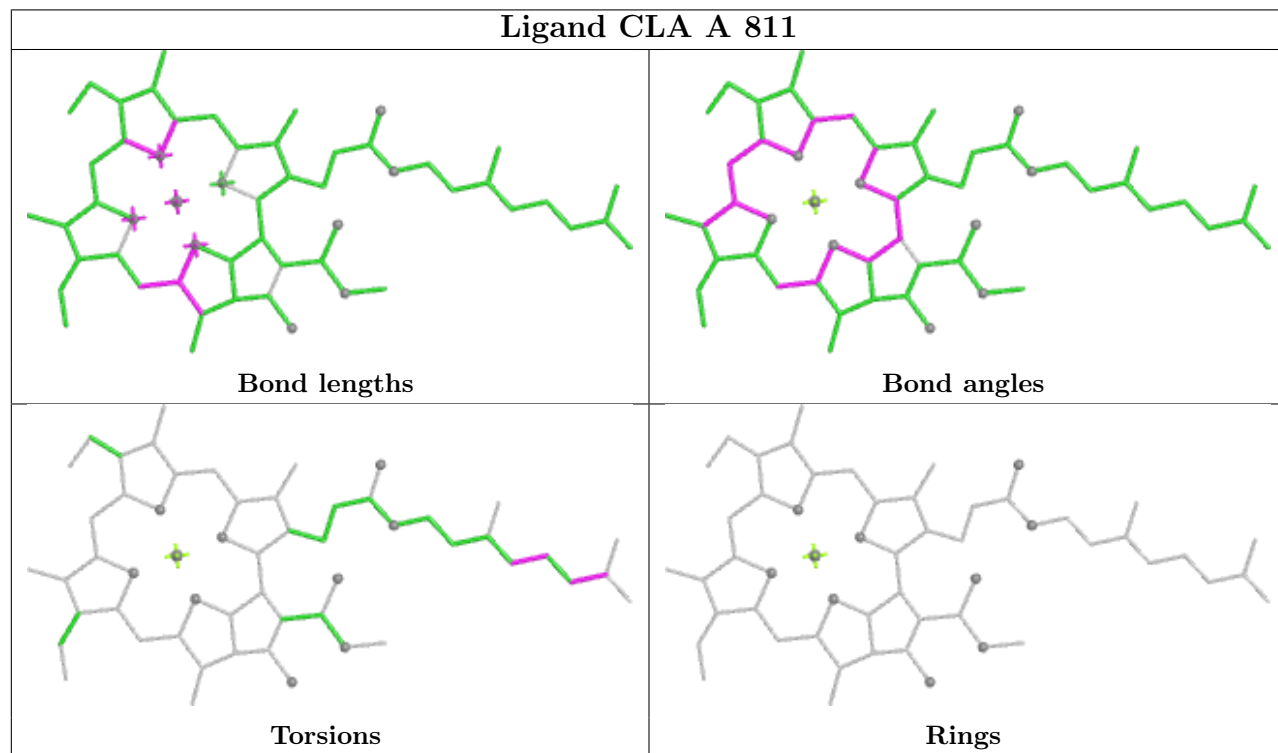


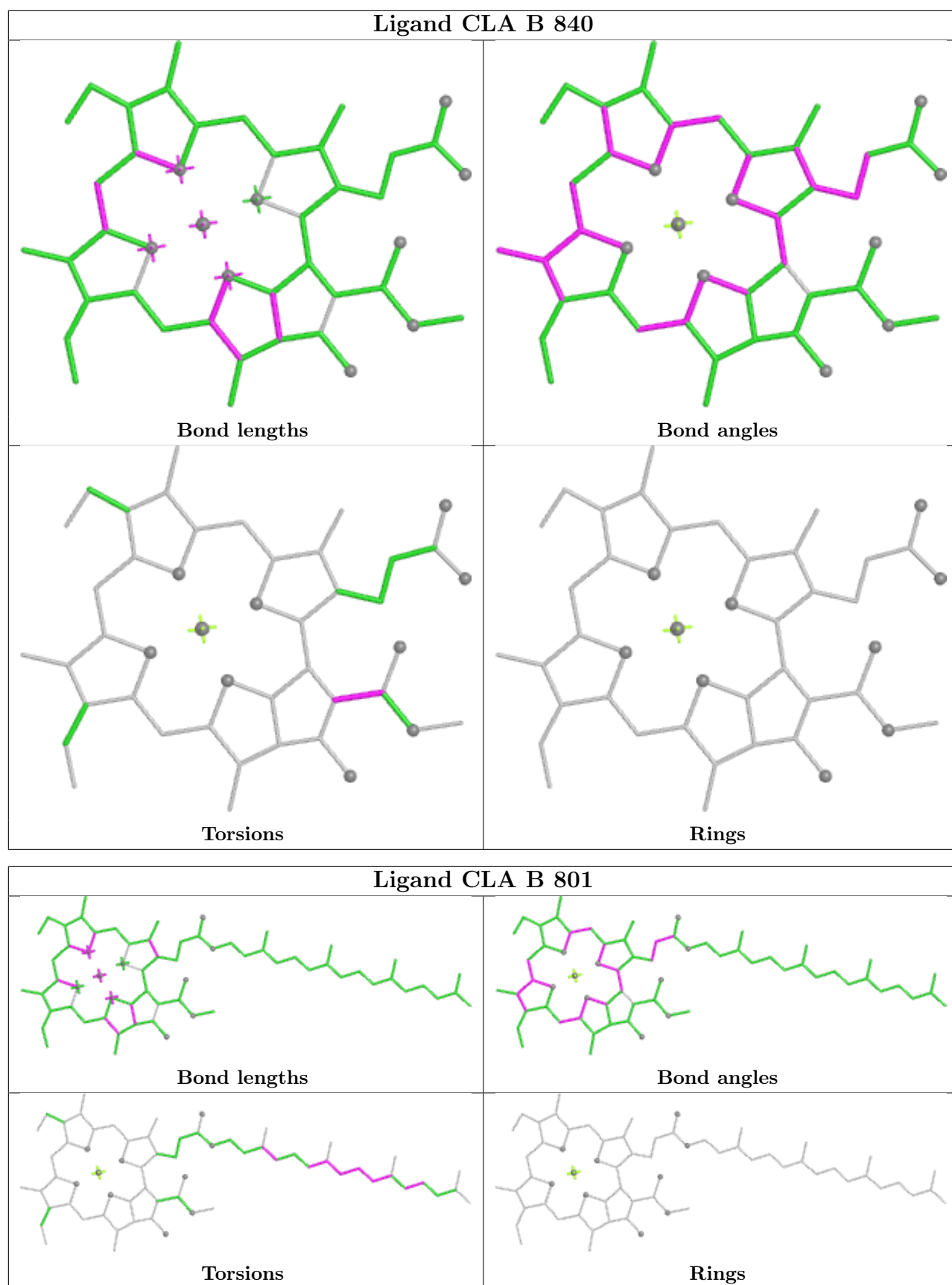
Rings

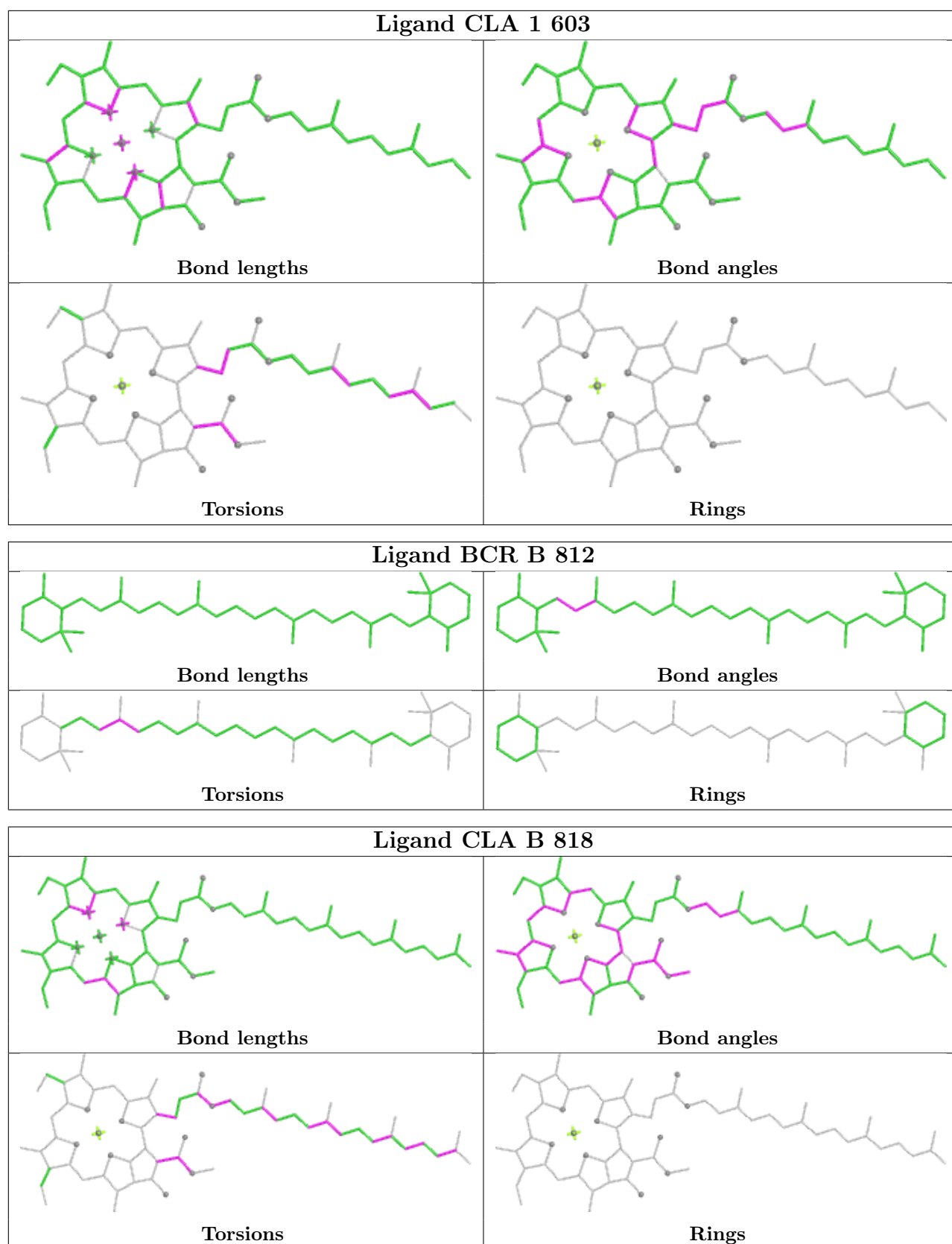
Ligand CLA 3 304



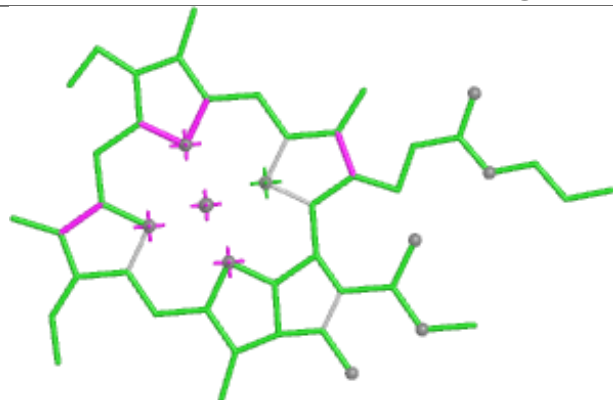
Ligand CLA A 811



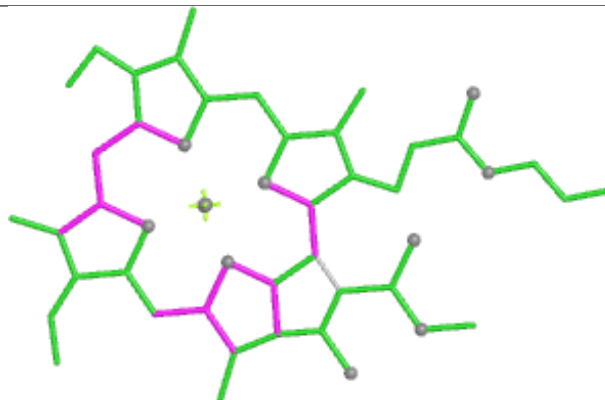




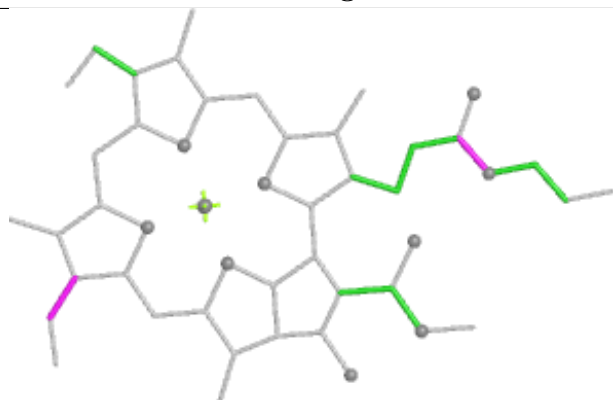
Ligand CLA F 306



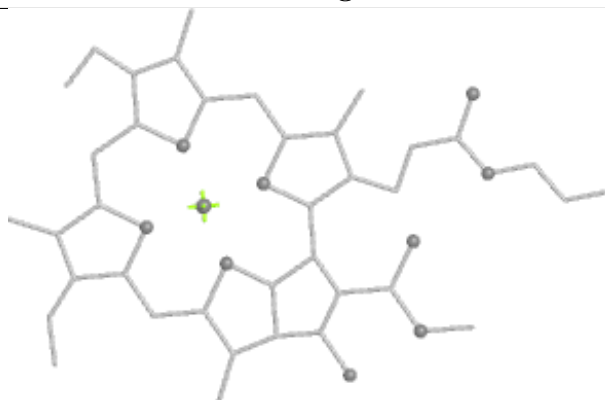
Bond lengths



Bond angles

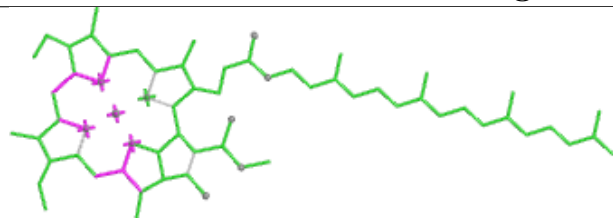


Torsions

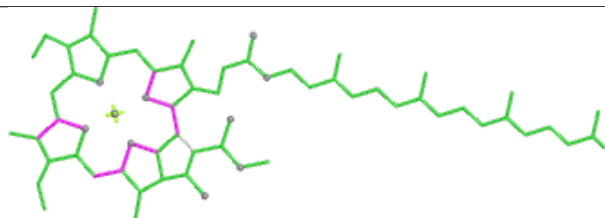


Rings

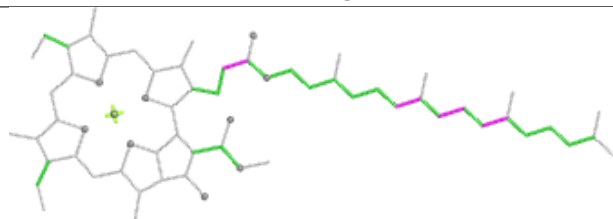
Ligand CLA A 833



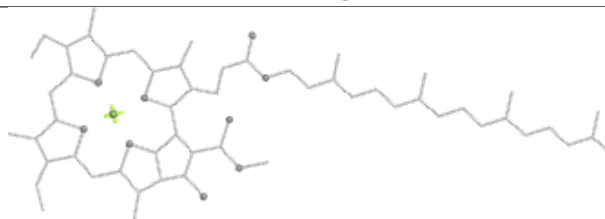
Bond lengths



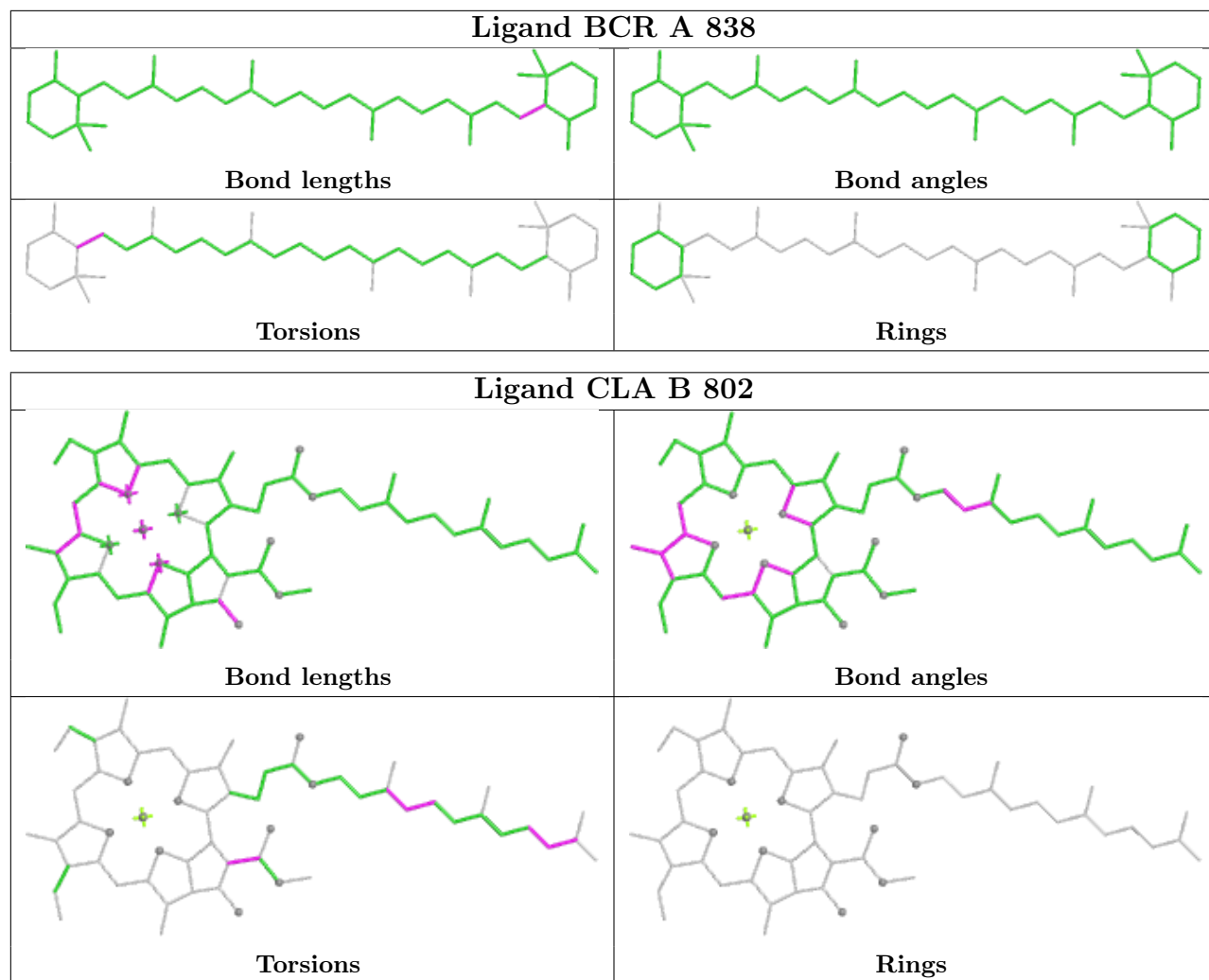
Bond angles



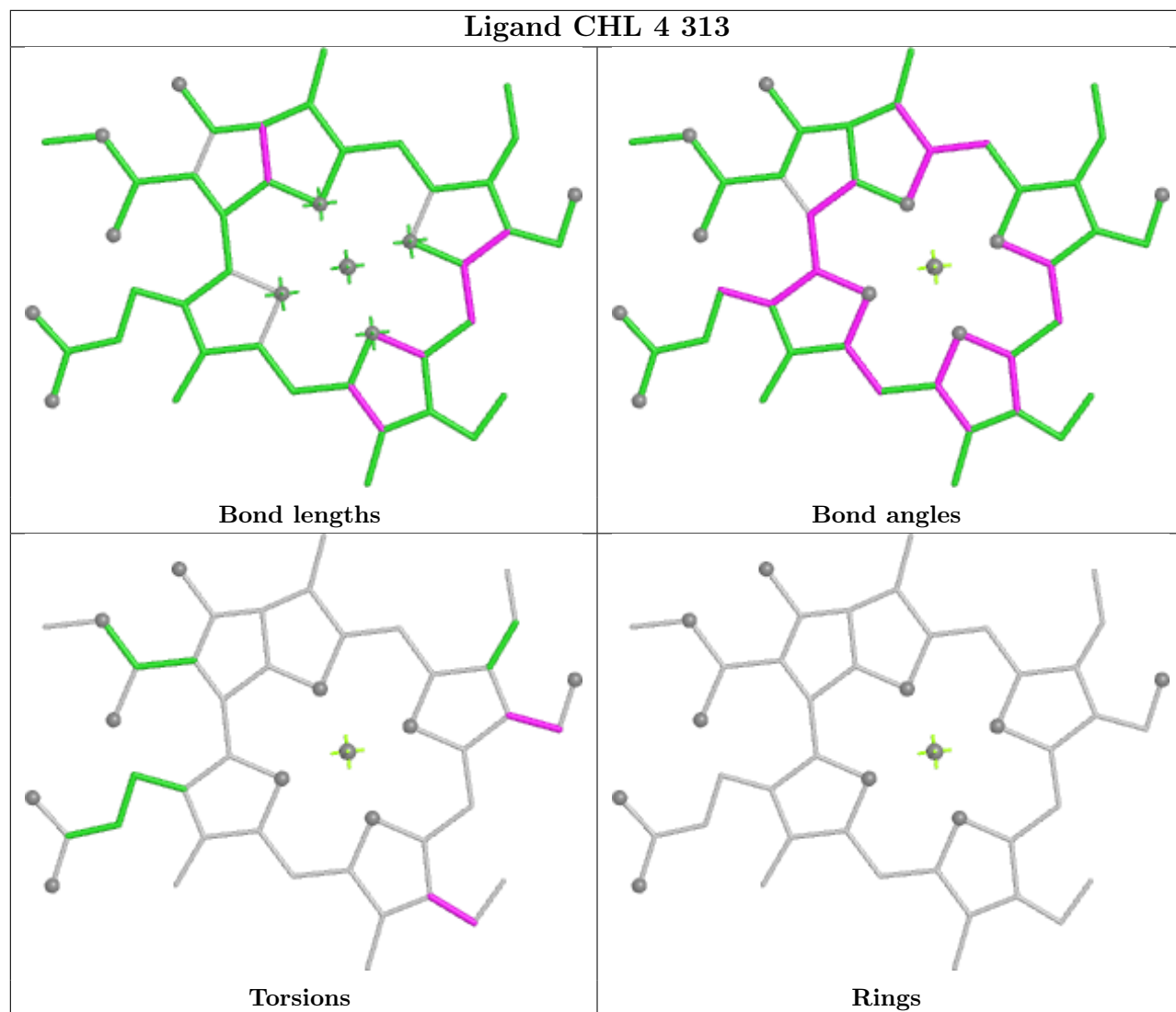
Torsions



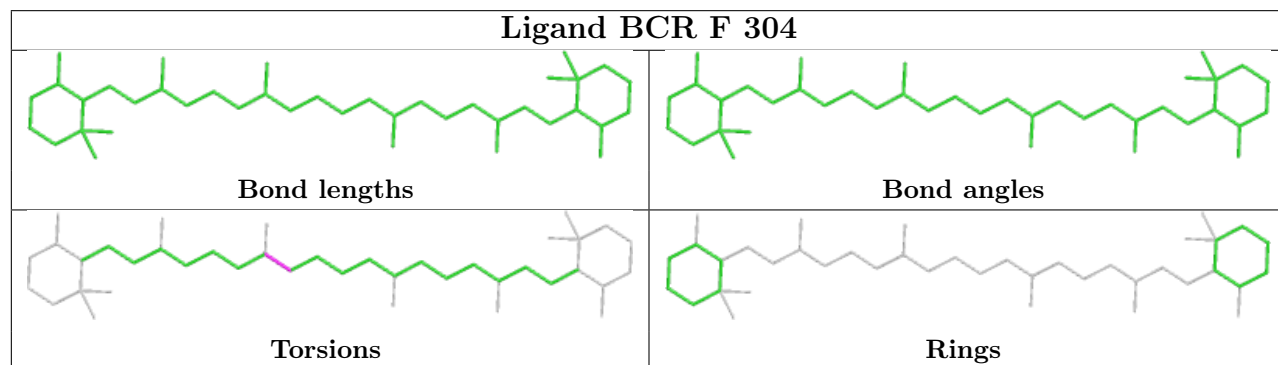
Rings

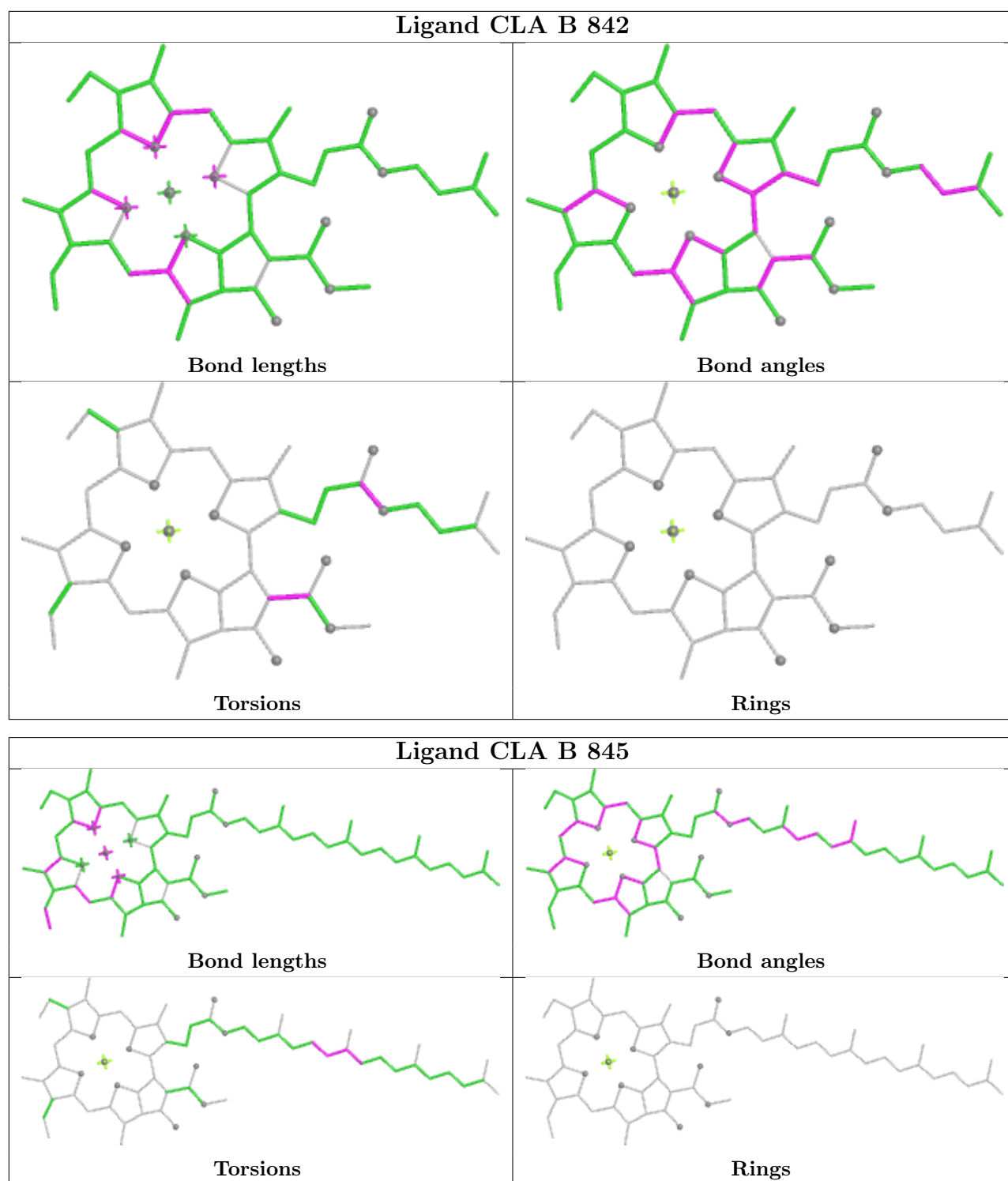


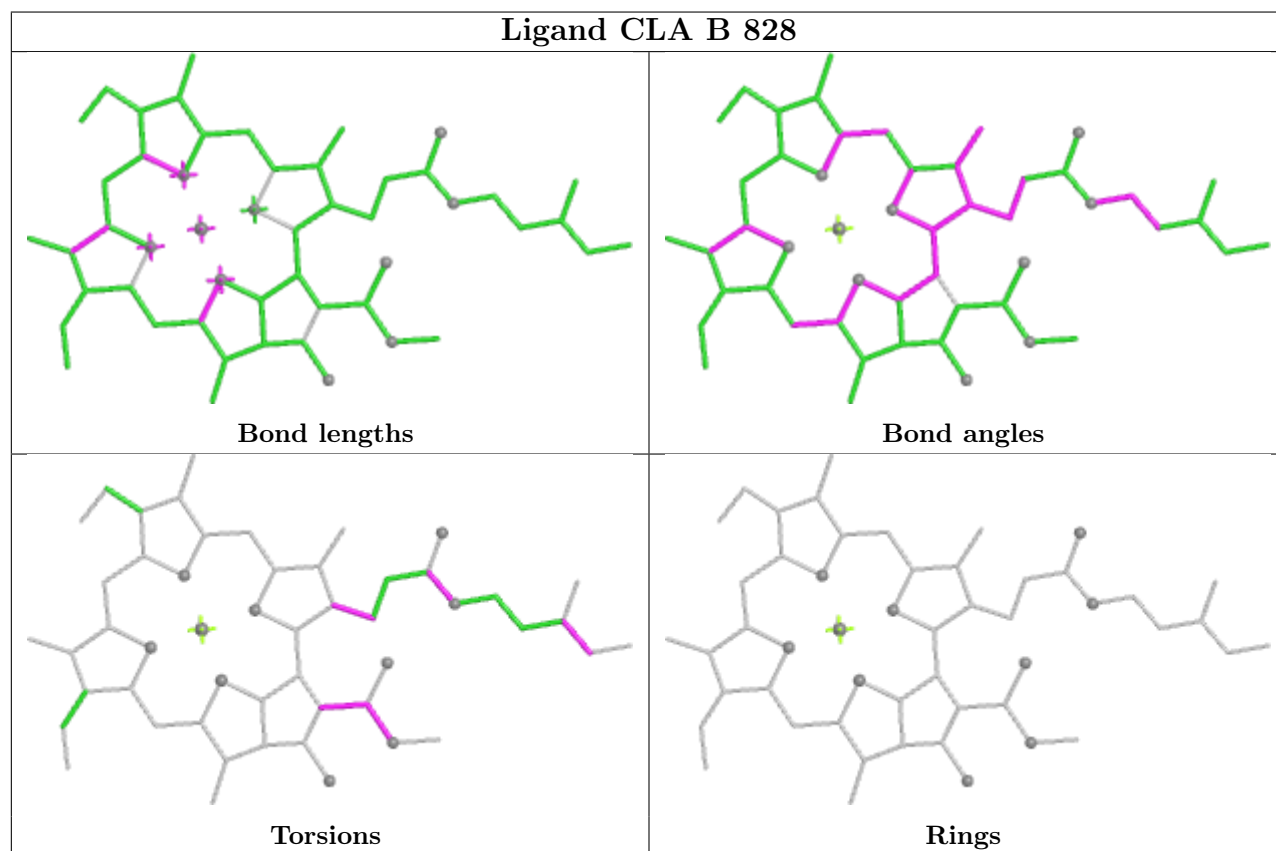
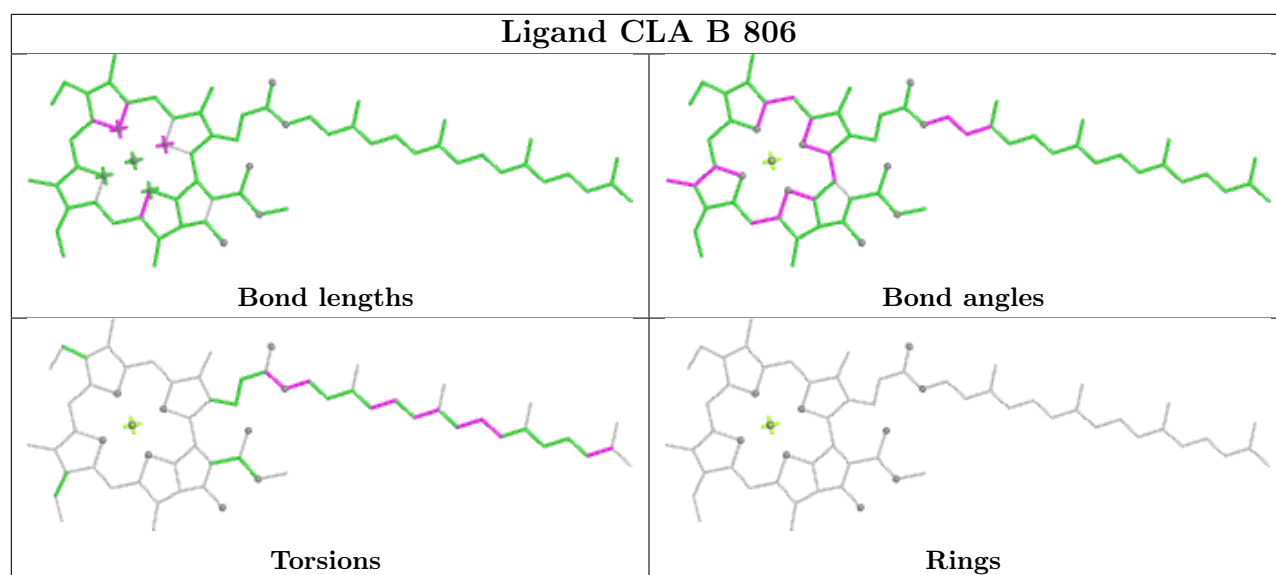
Ligand CHL 4 313

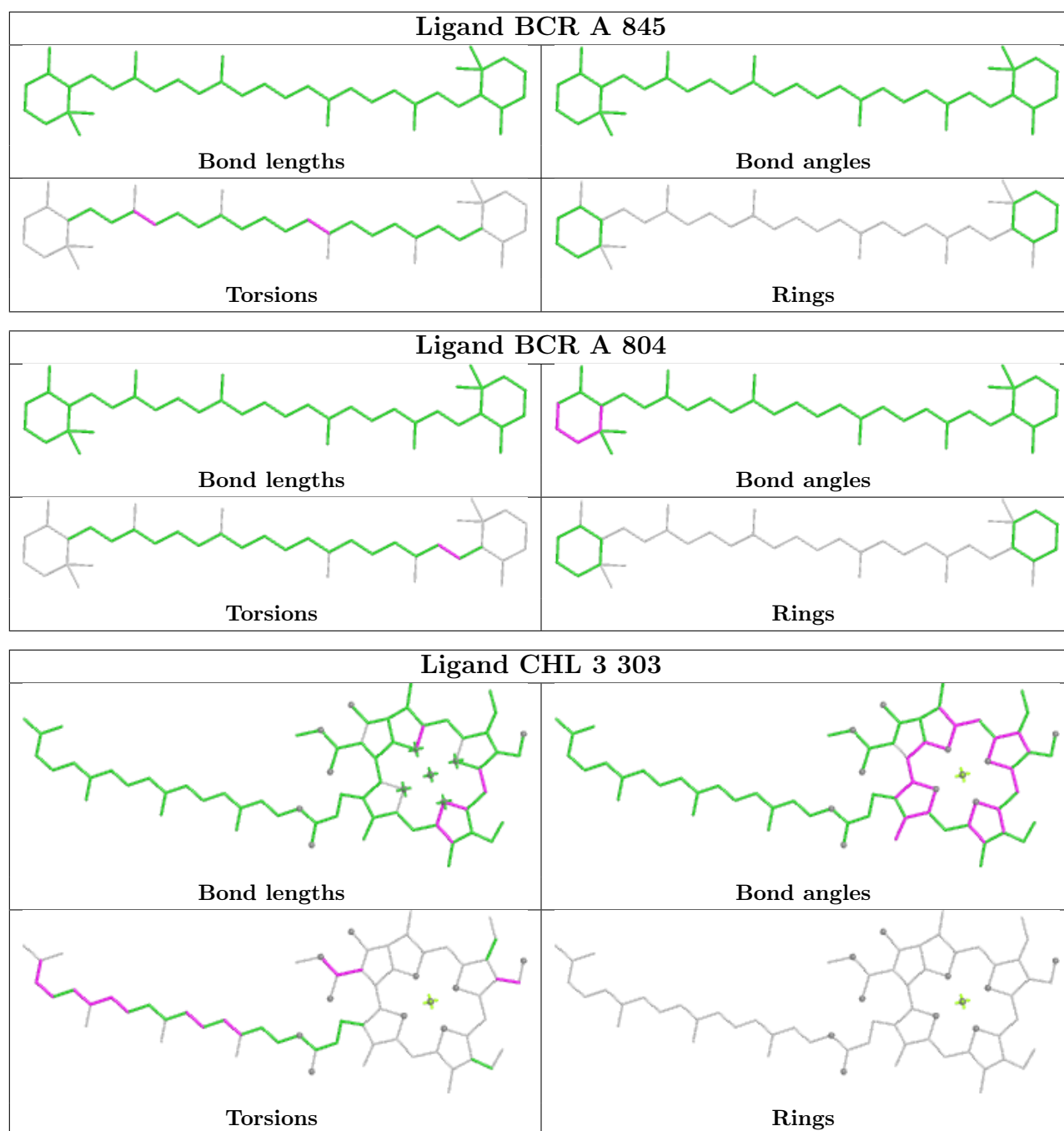


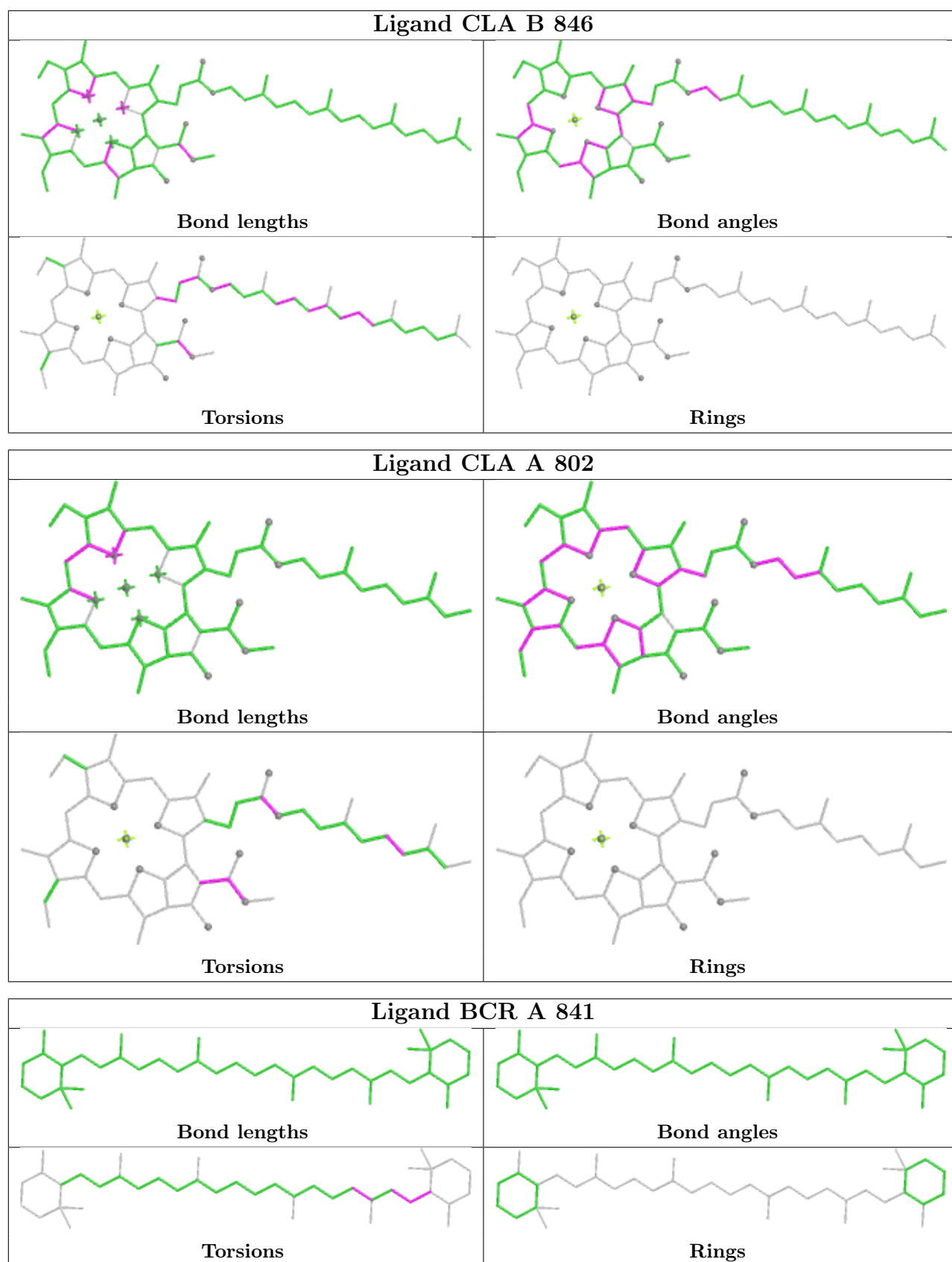
Ligand BCR F 304

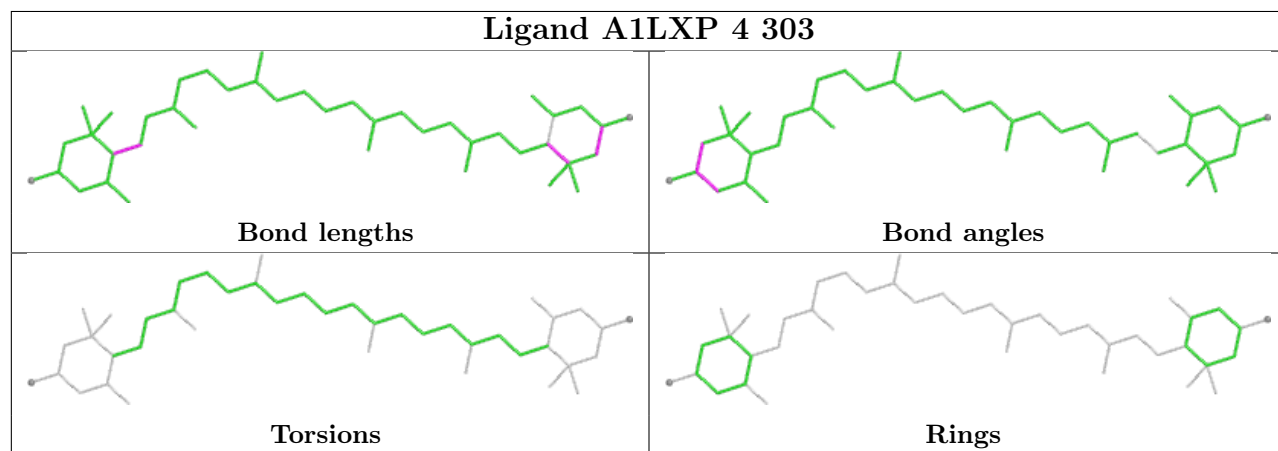
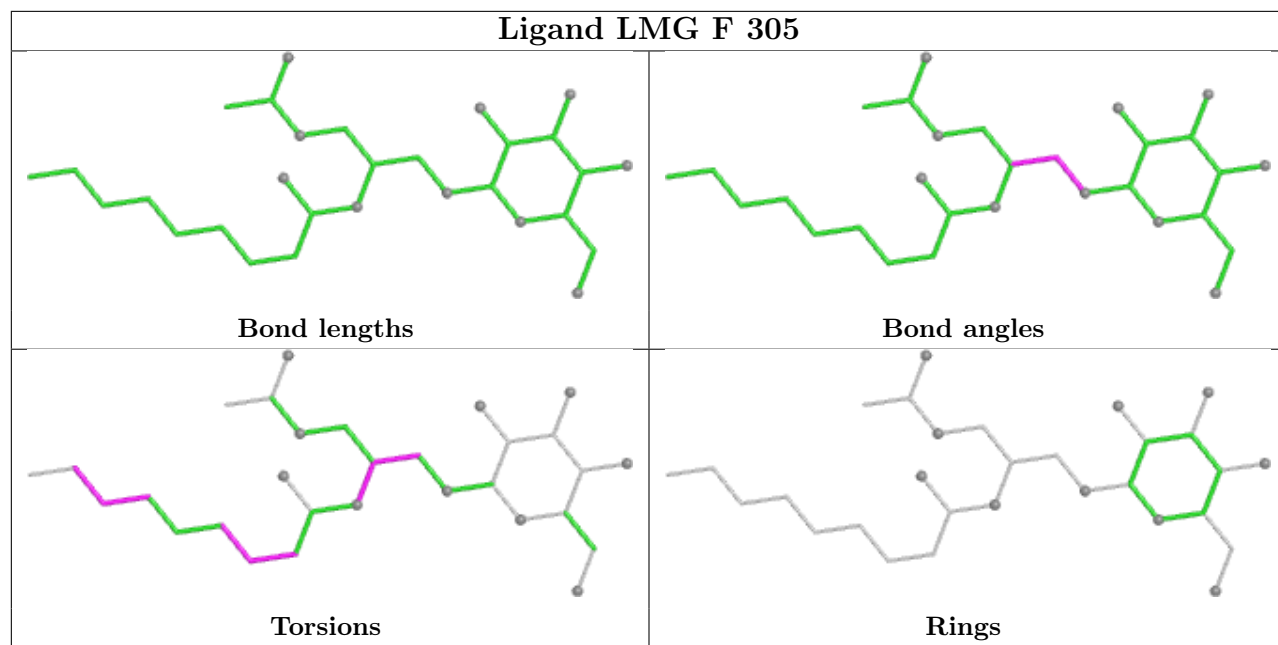


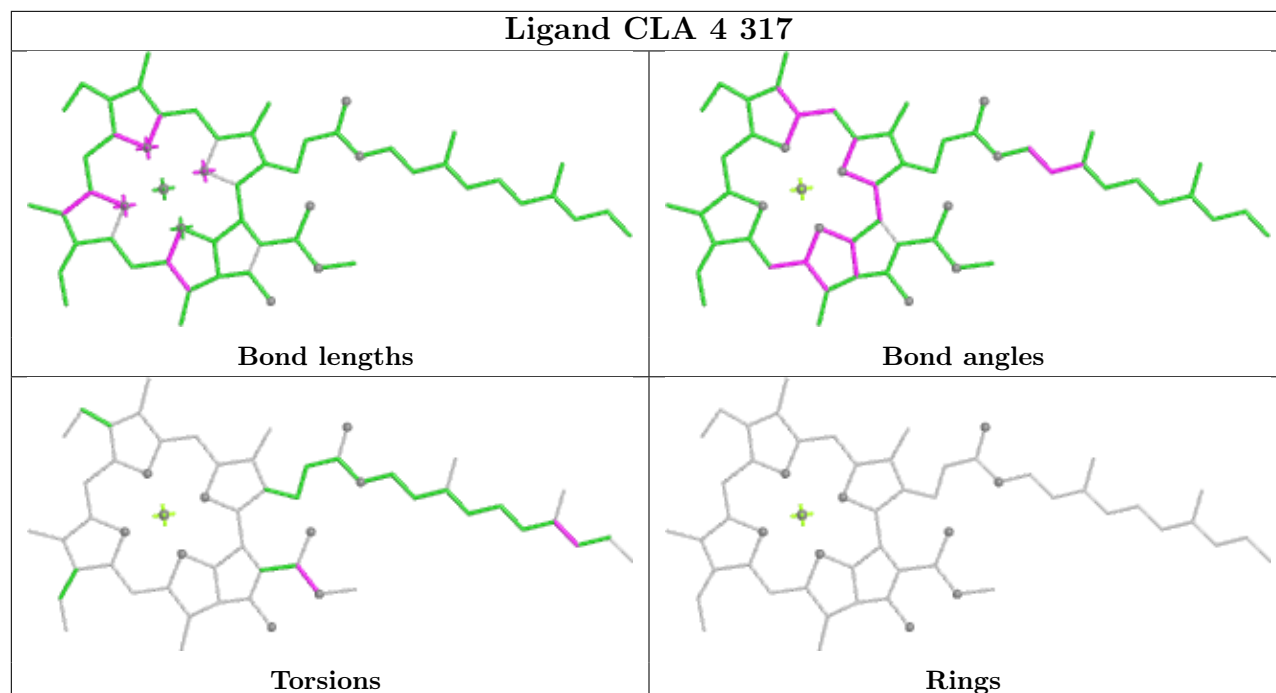
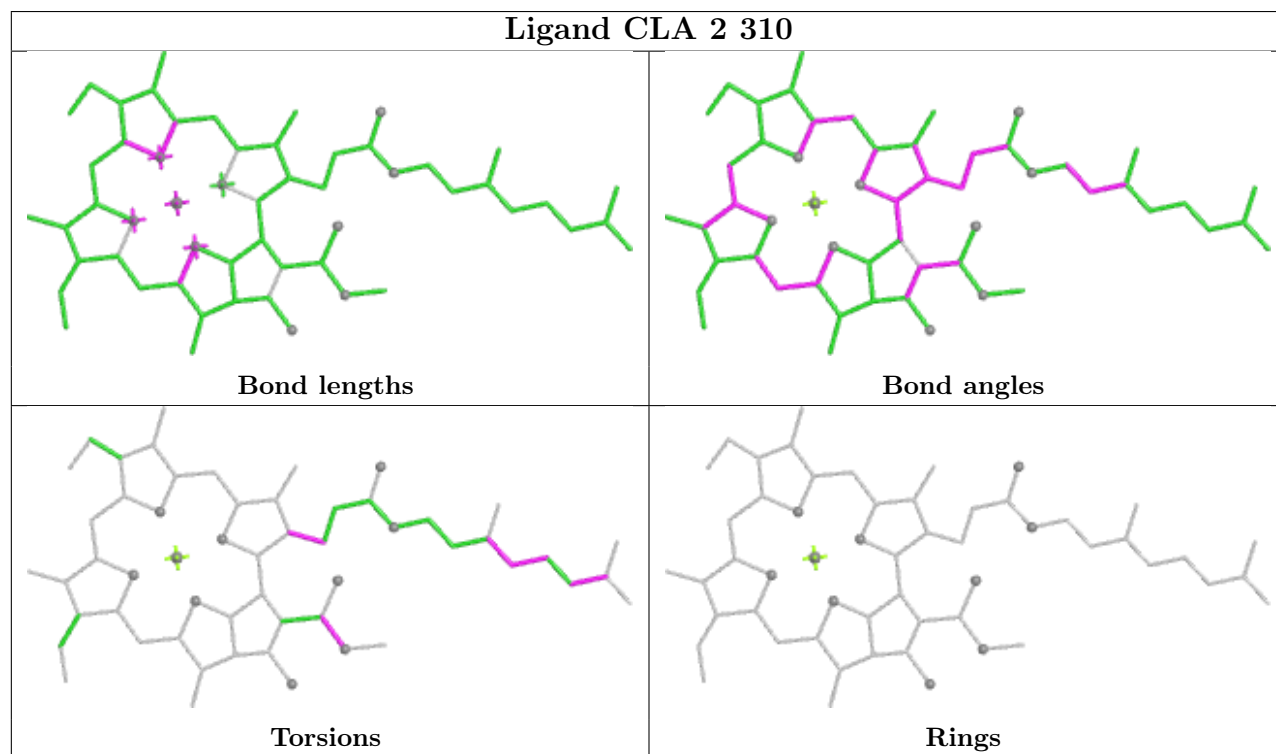




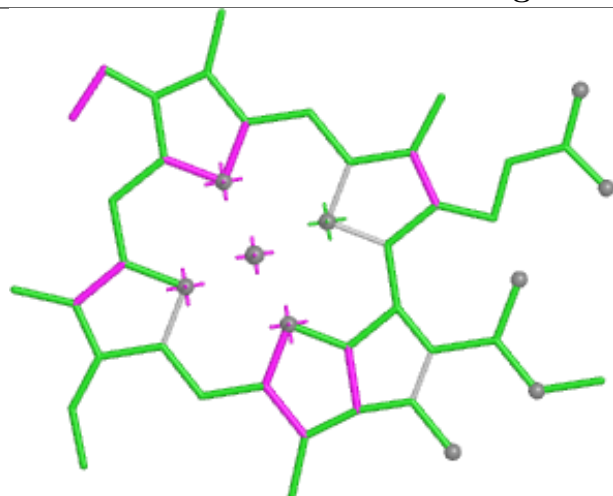




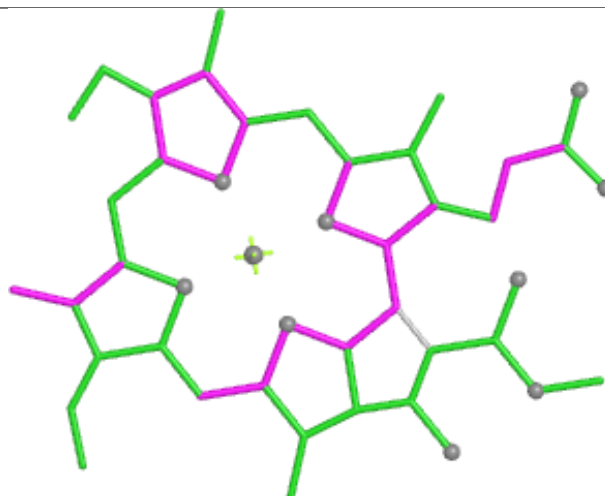


Ligand CLA 4 317**Ligand CLA 2 310**

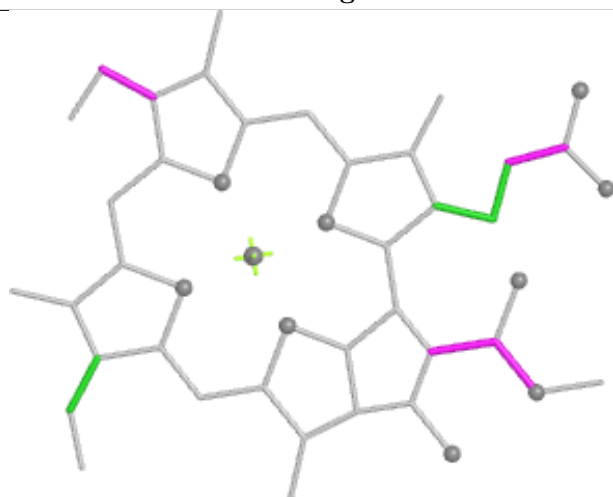
Ligand CLA G 203



Bond lengths



Bond angles

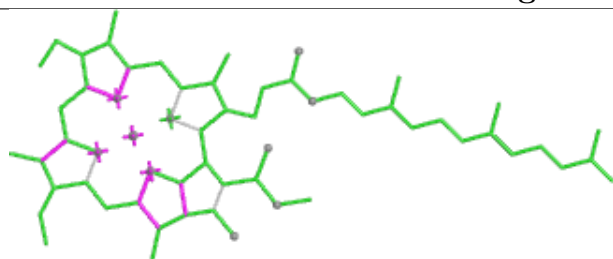


Torsions

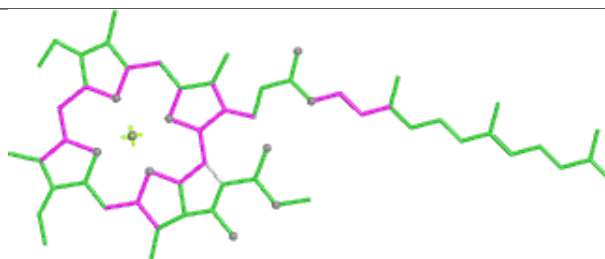


Rings

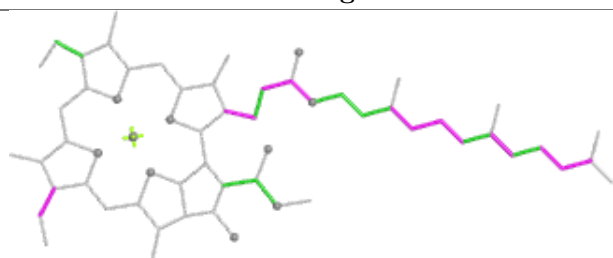
Ligand CLA 1 602



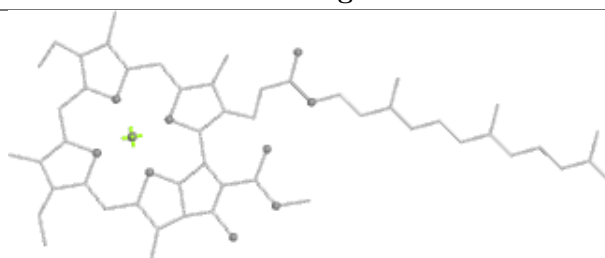
Bond lengths



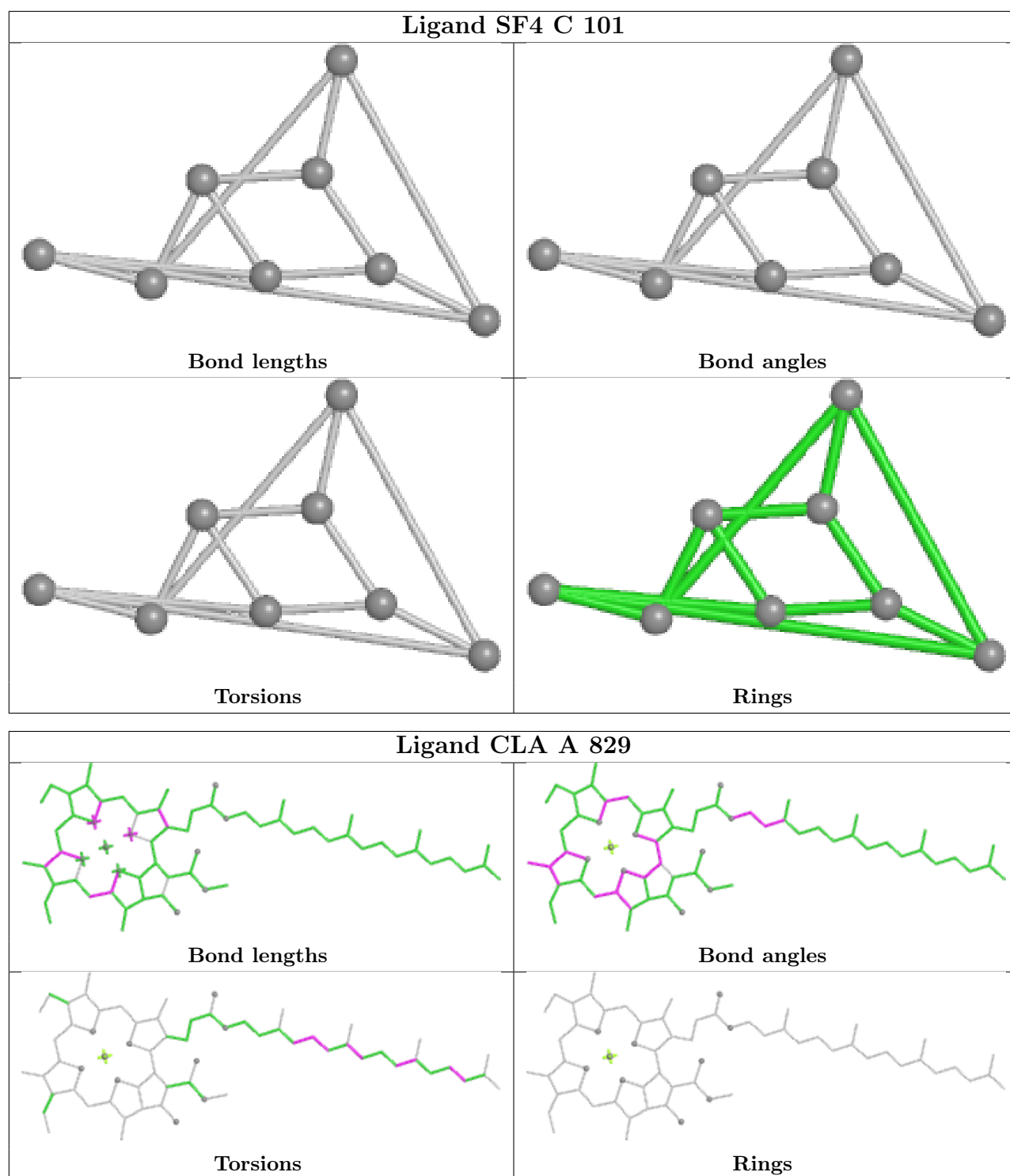
Bond angles

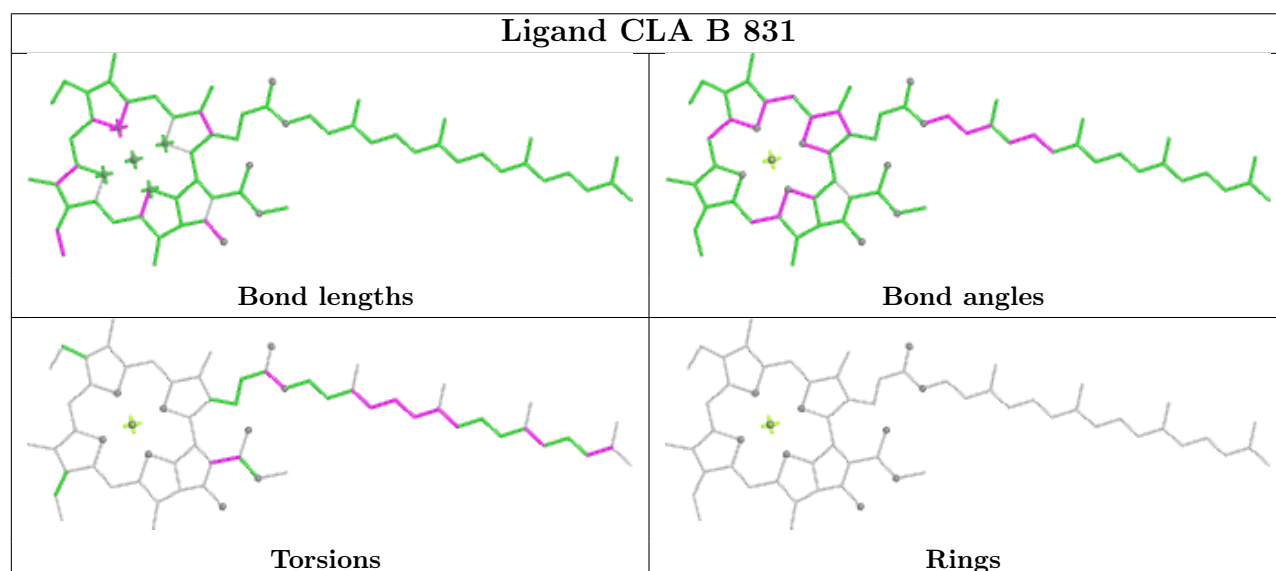
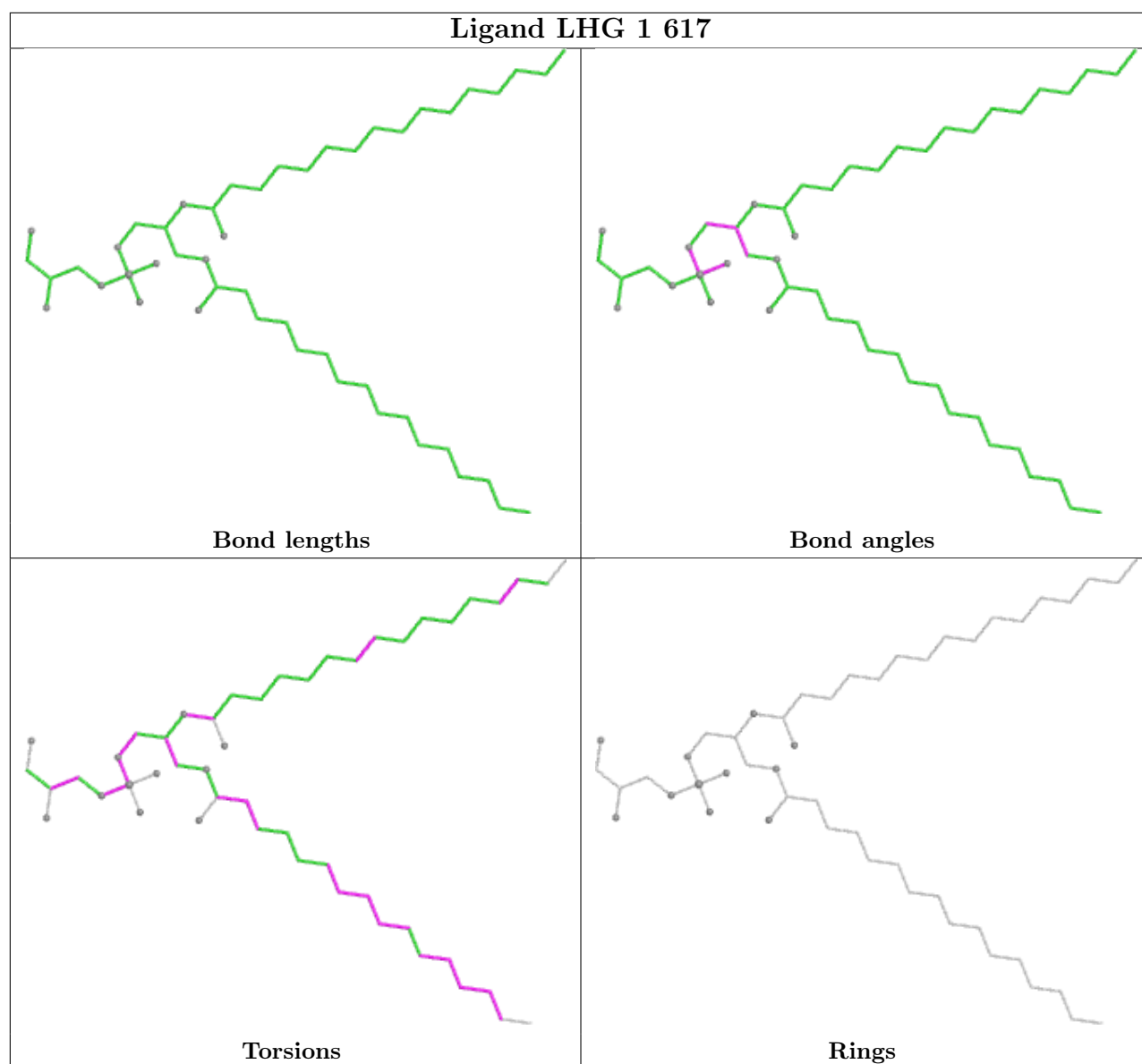


Torsions

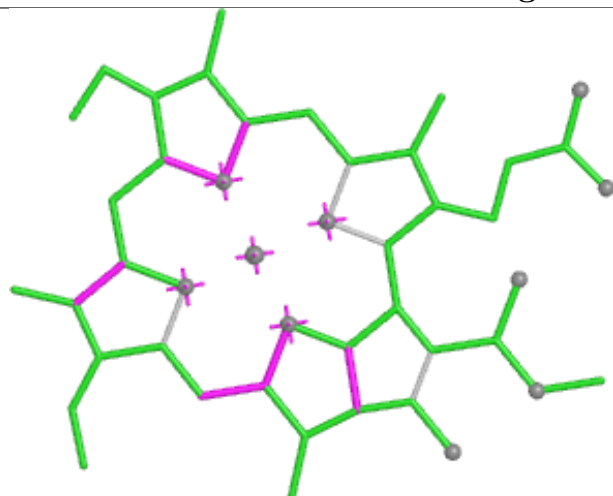


Rings

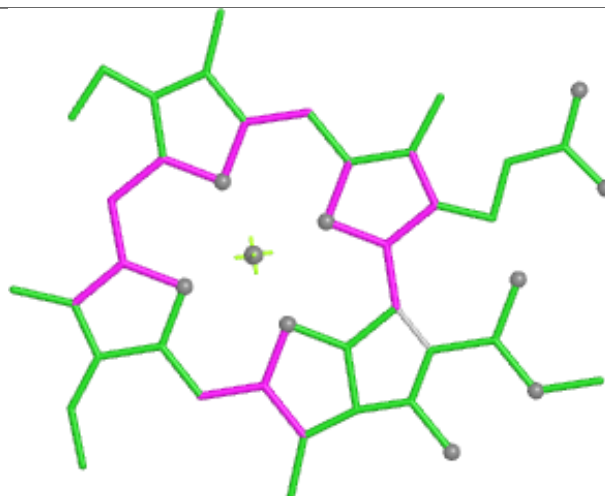




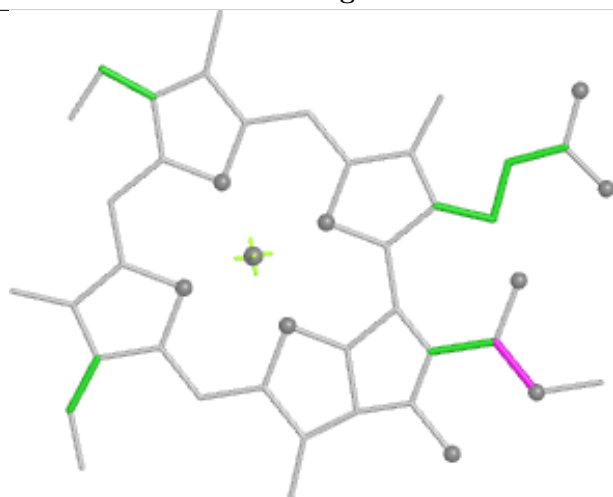
Ligand CLA 4 311



Bond lengths



Bond angles

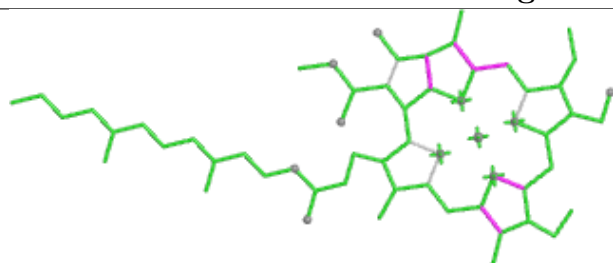


Torsions

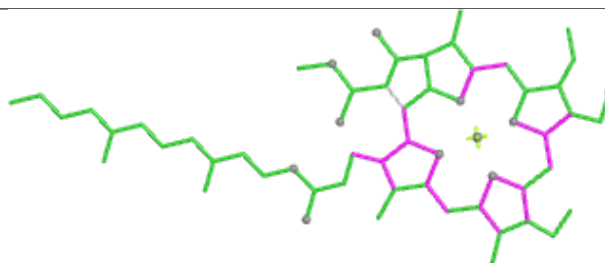


Rings

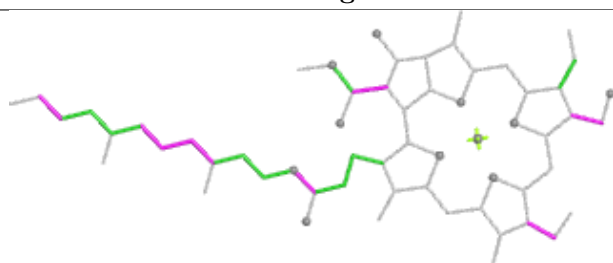
Ligand CHL 2 316



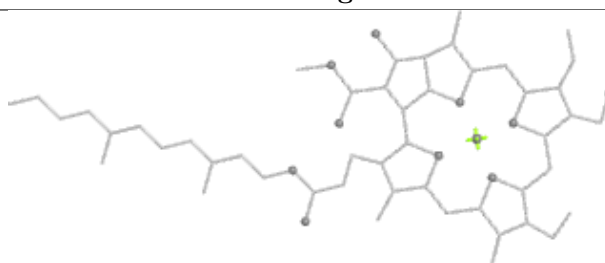
Bond lengths



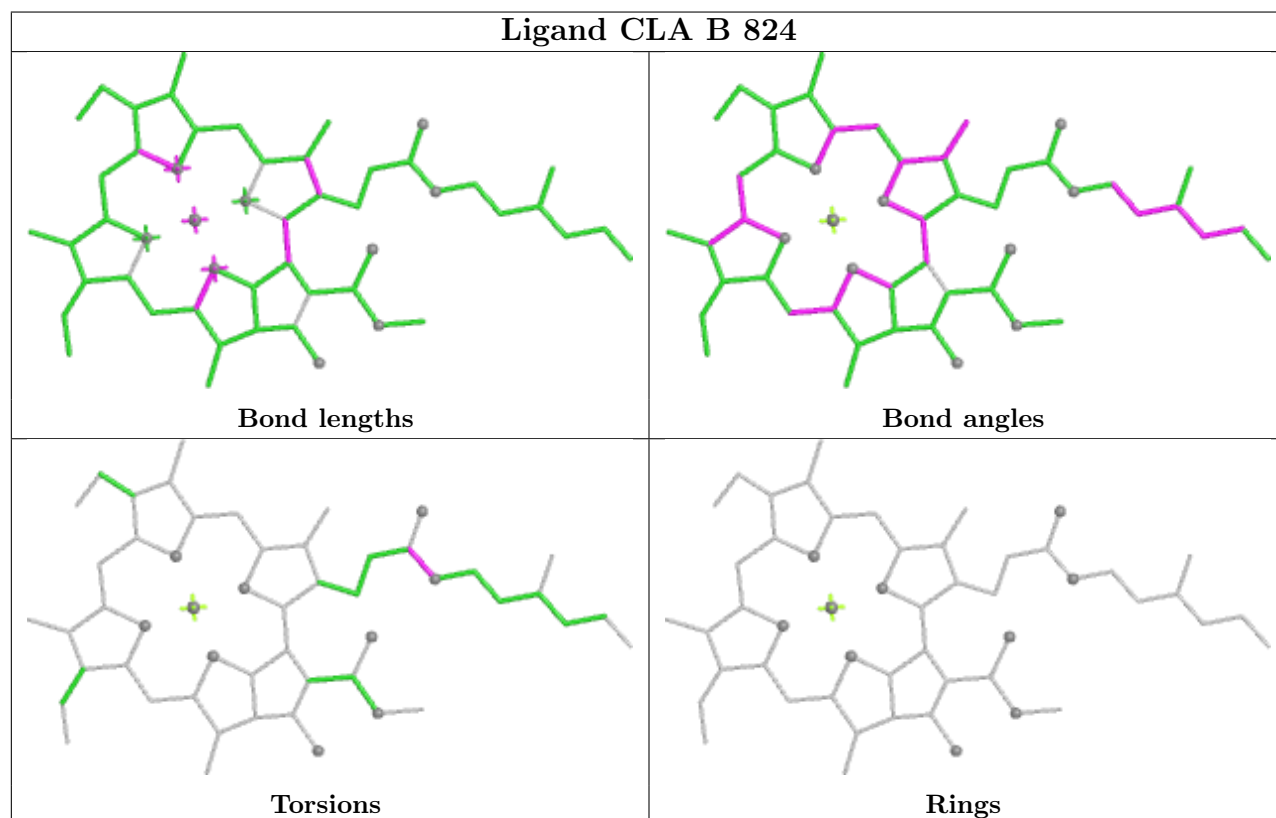
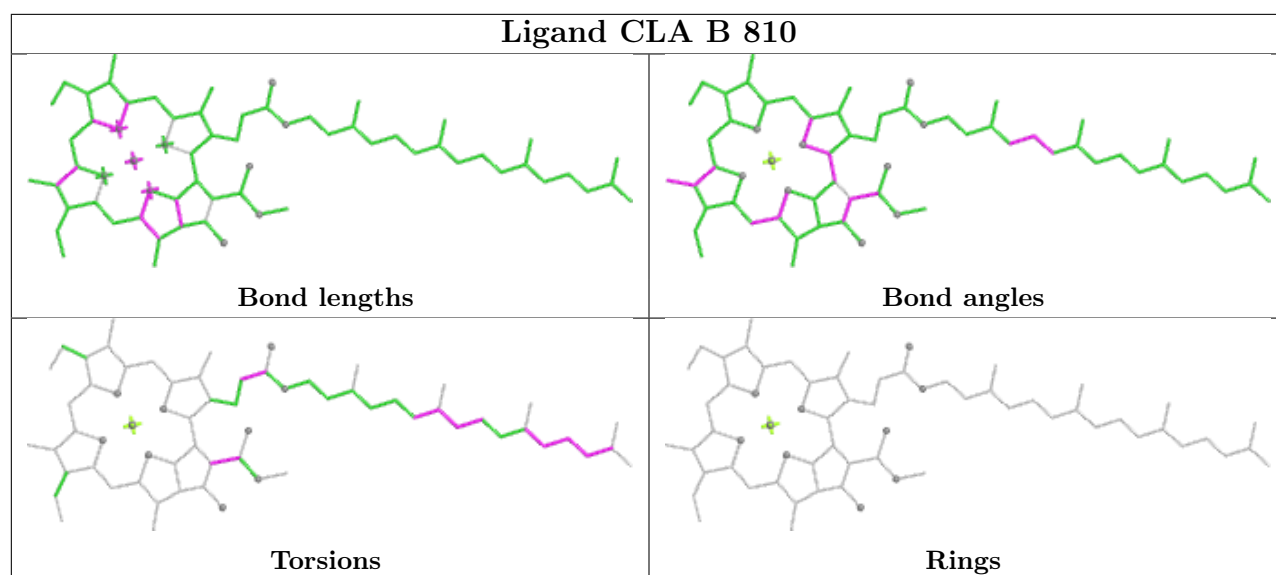
Bond angles

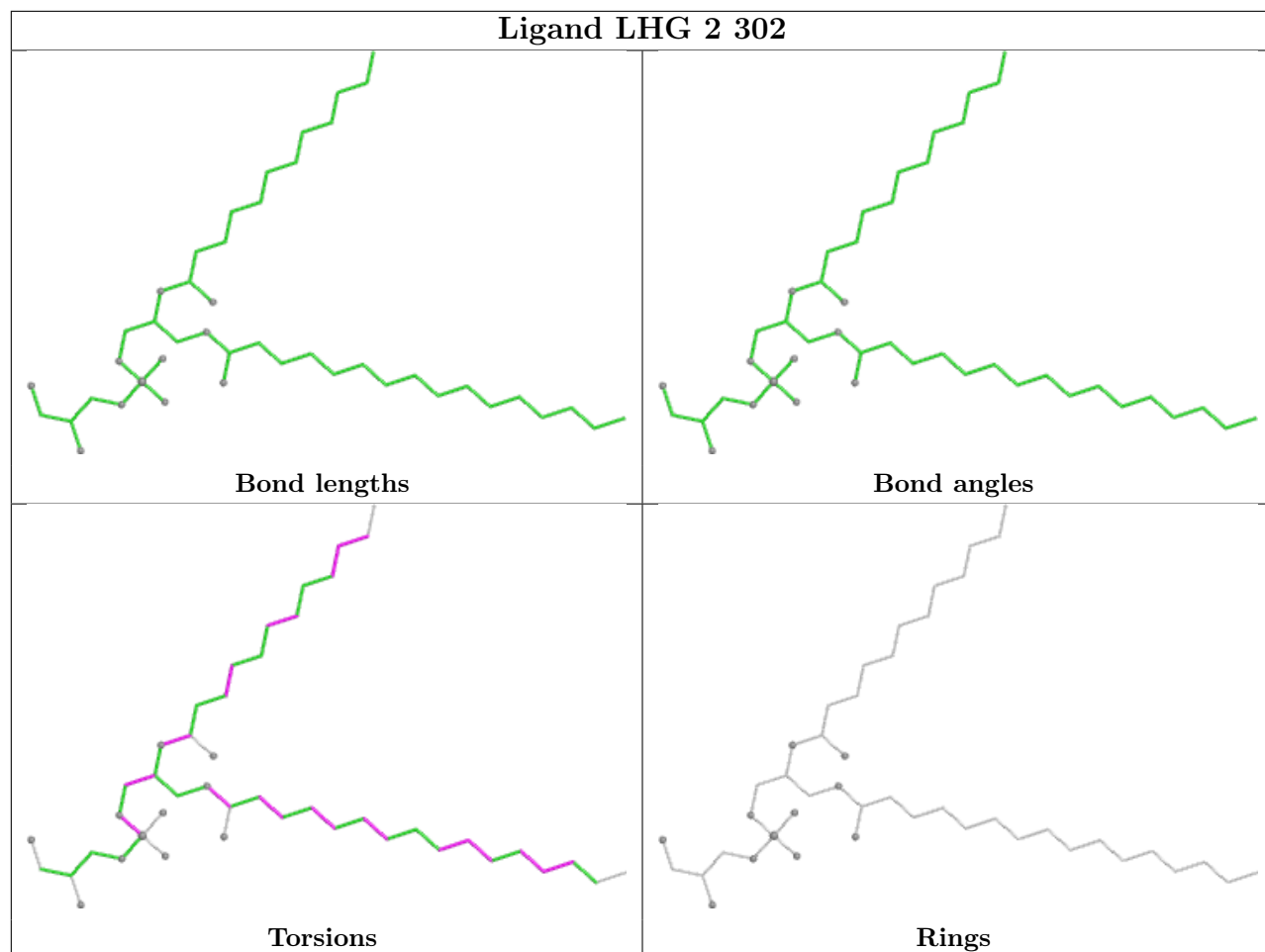
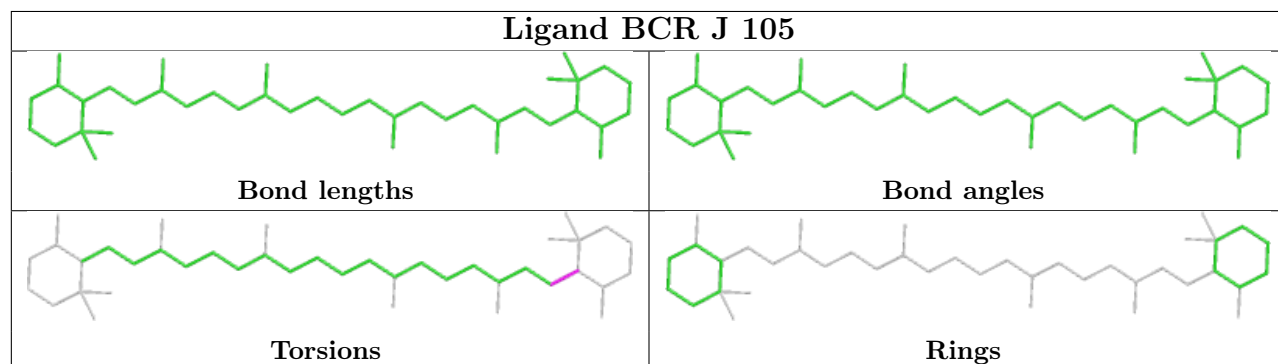


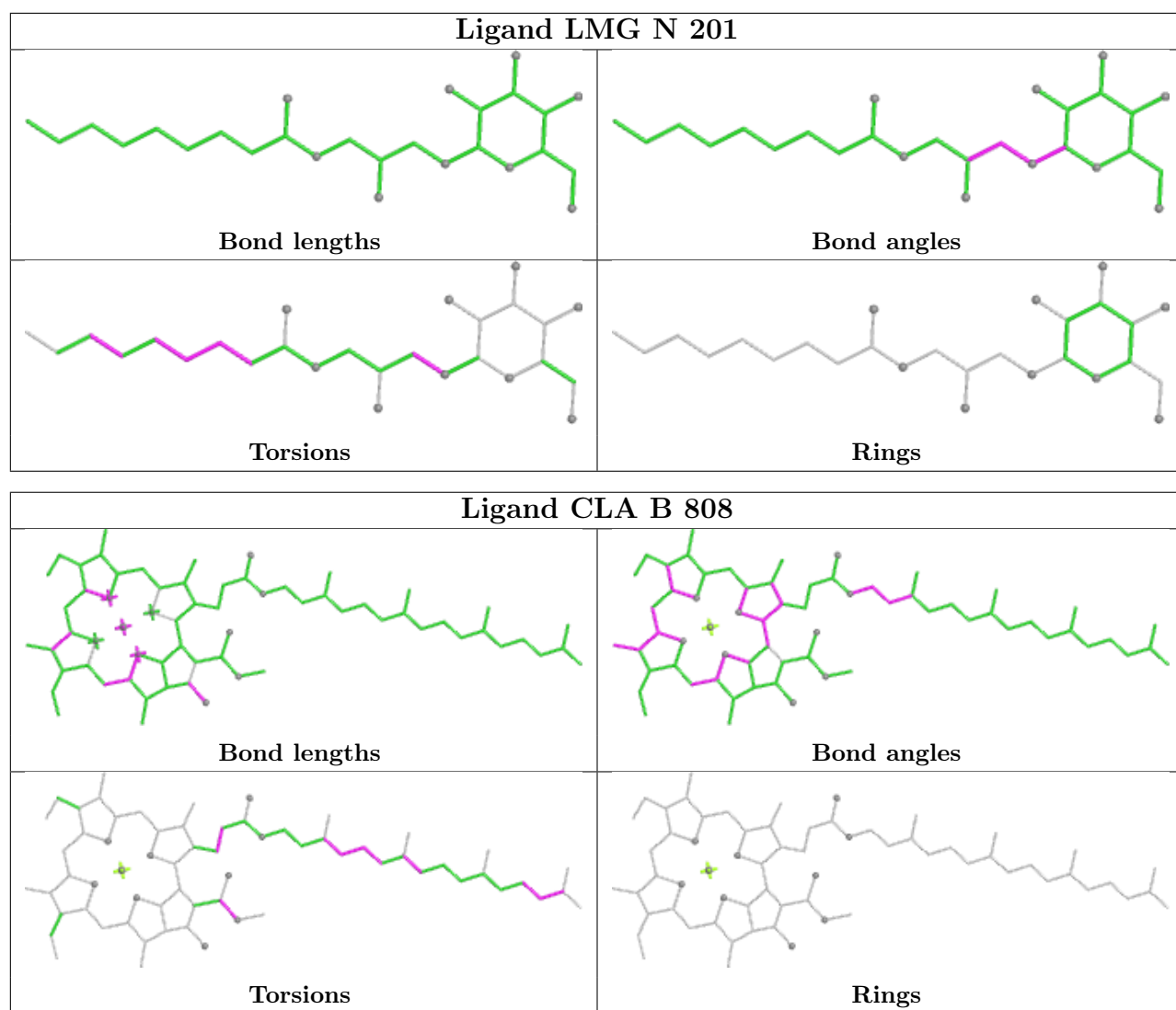
Torsions



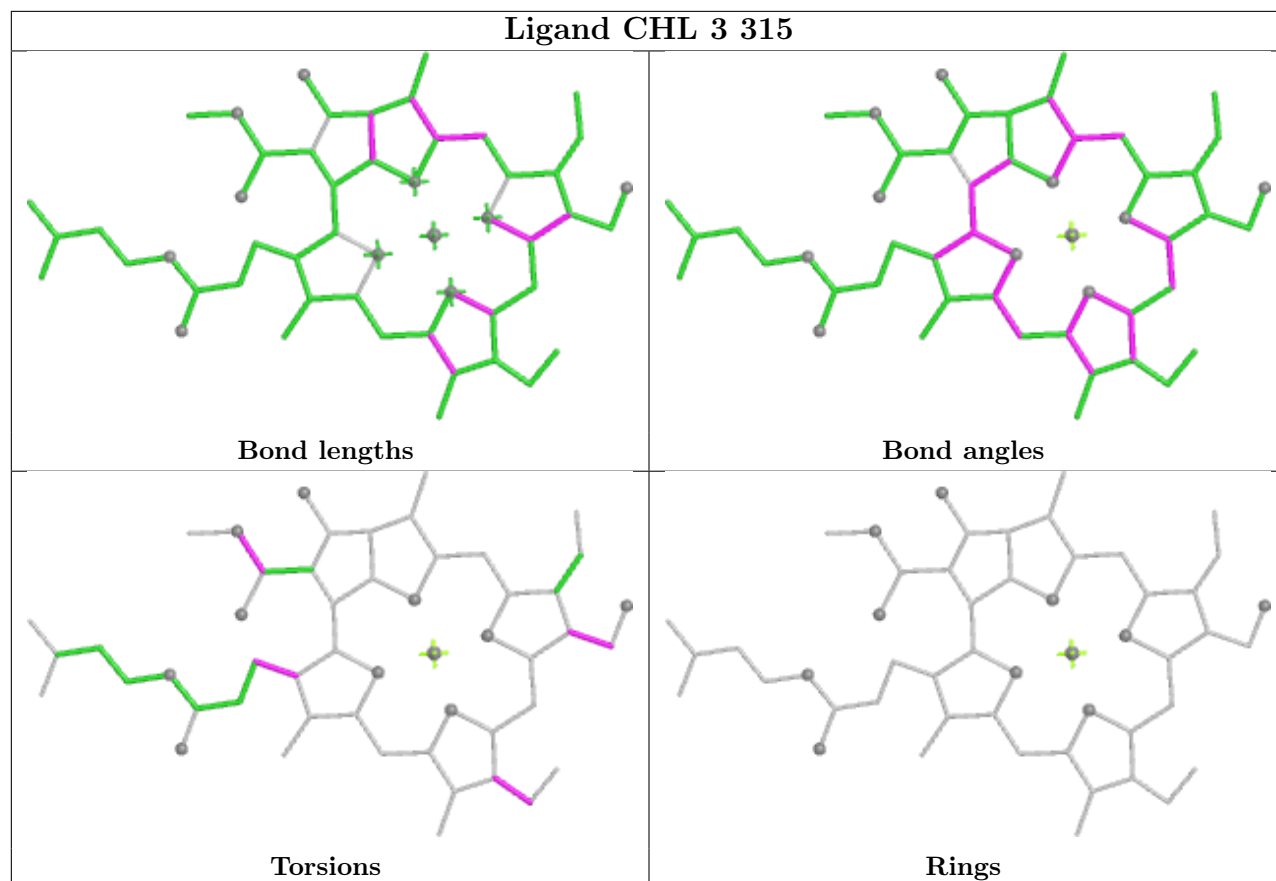
Rings



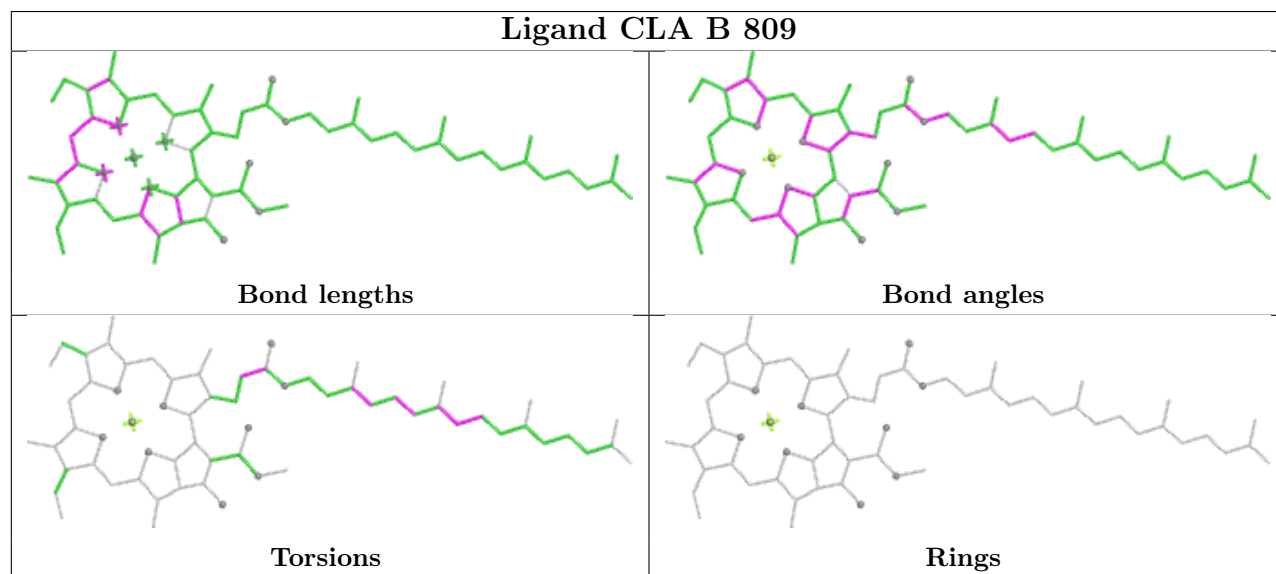
Ligand LHG 2 302**Ligand BCR J 105**

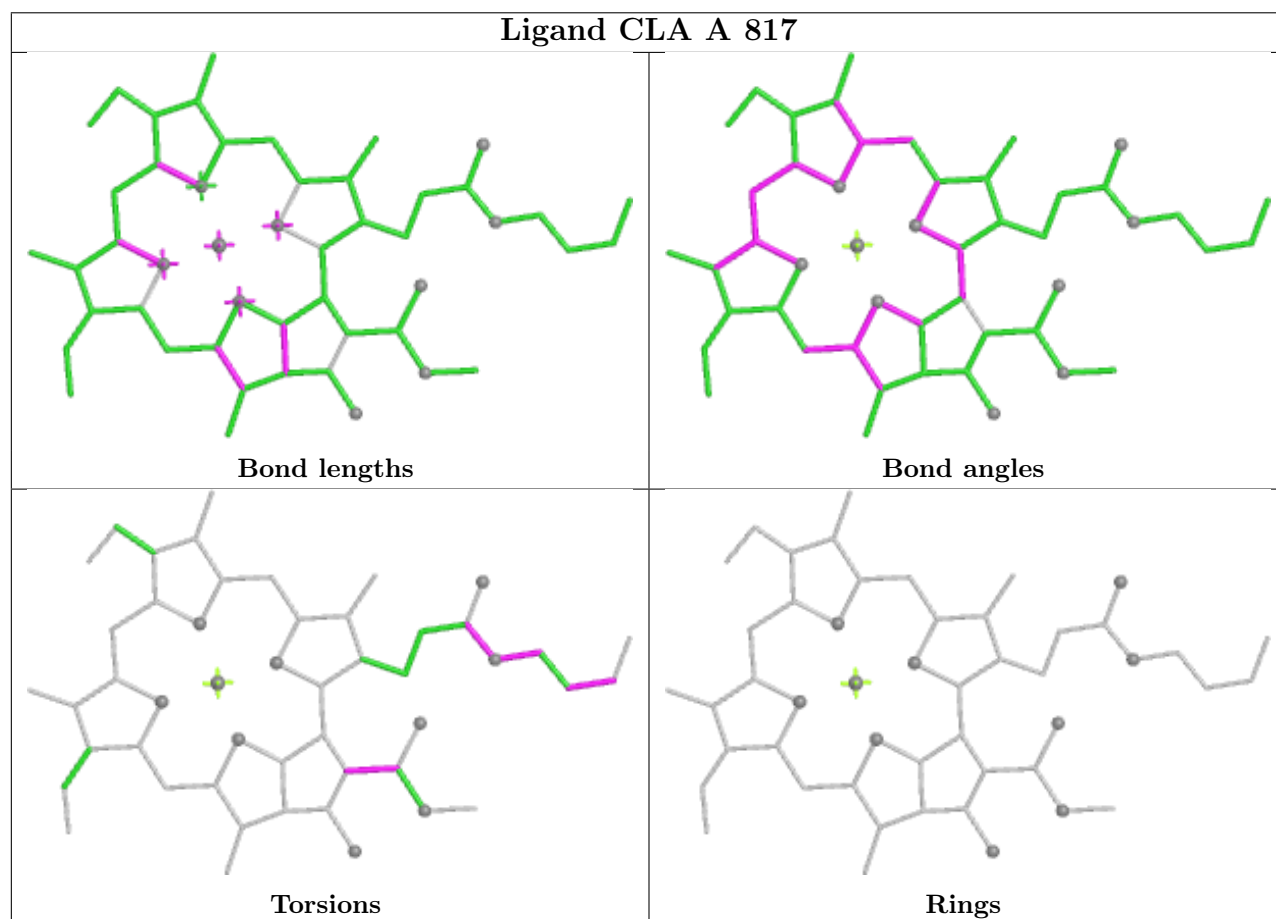
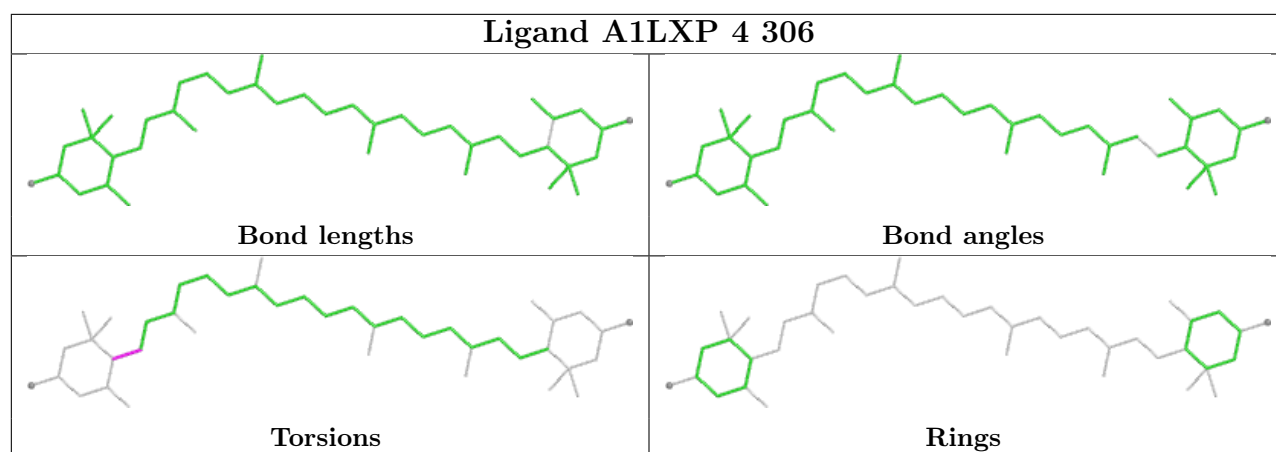


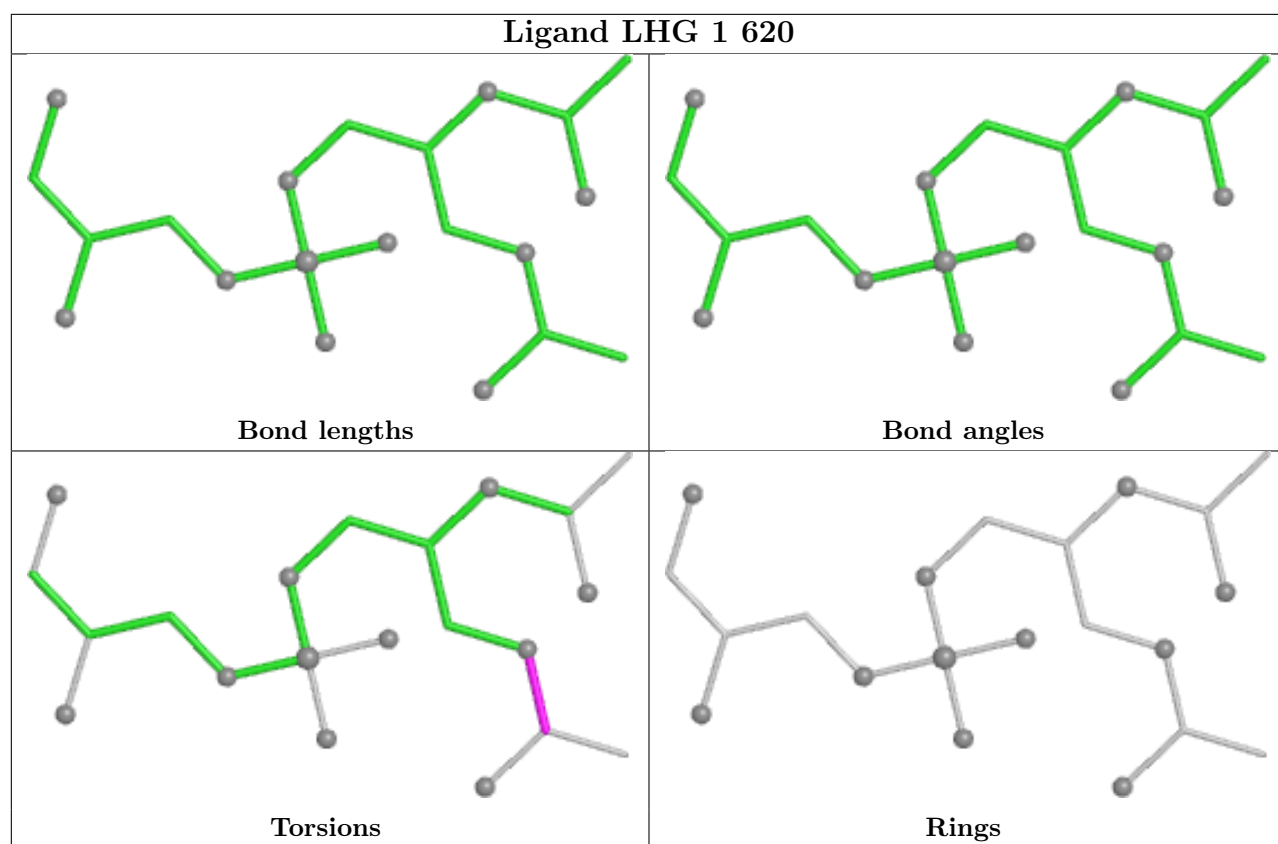
Ligand CHL 3 315



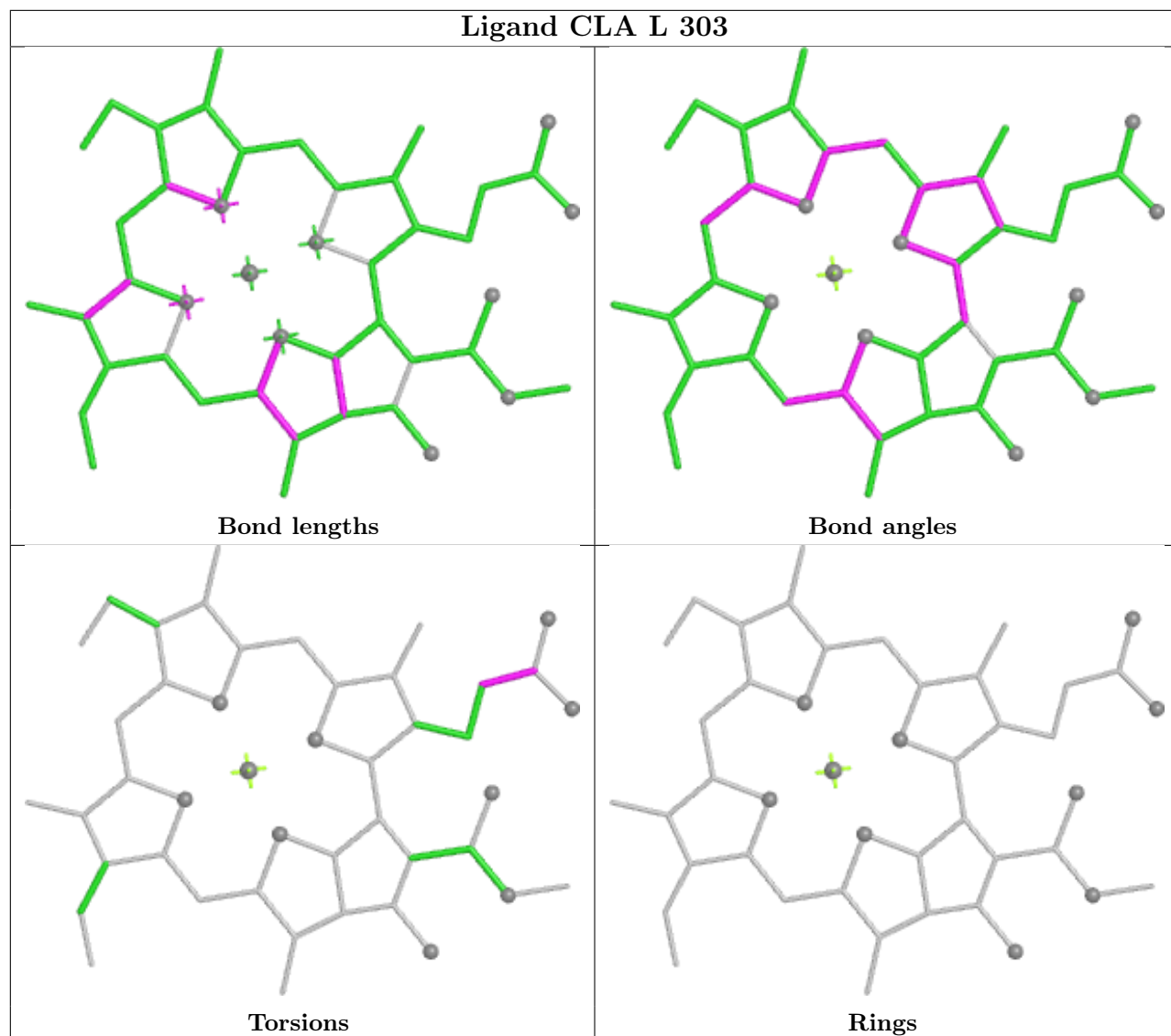
Ligand CLA B 809



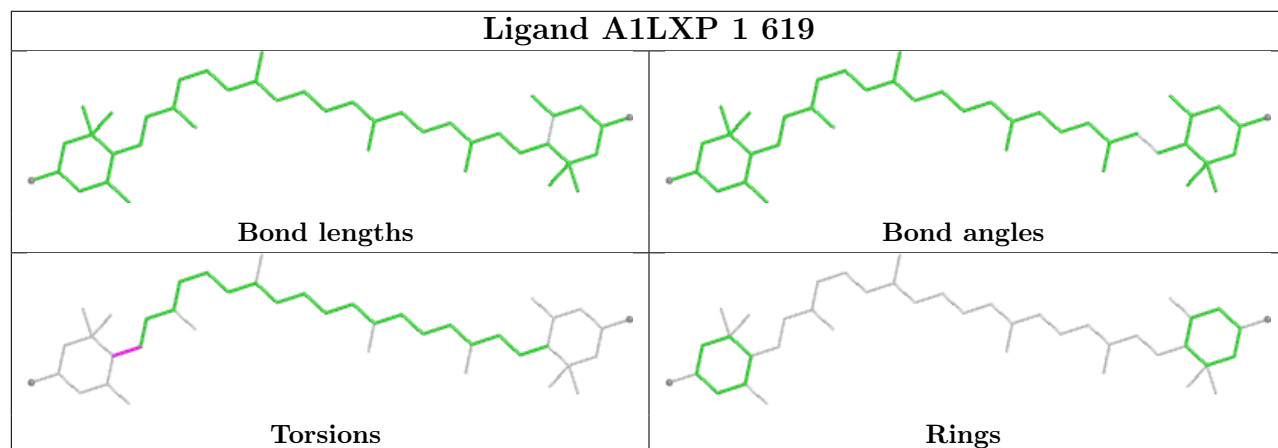




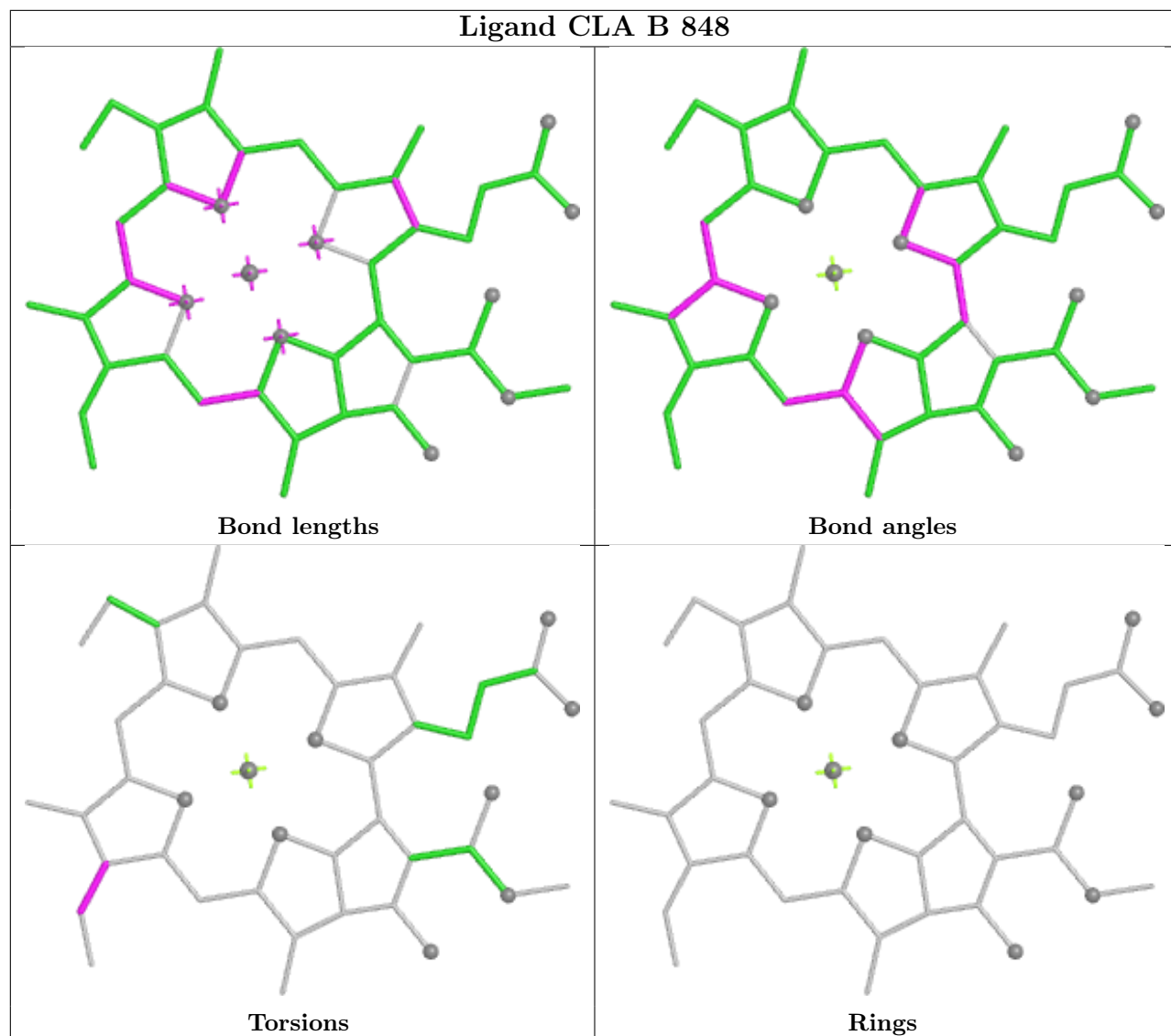
Ligand CLA L 303



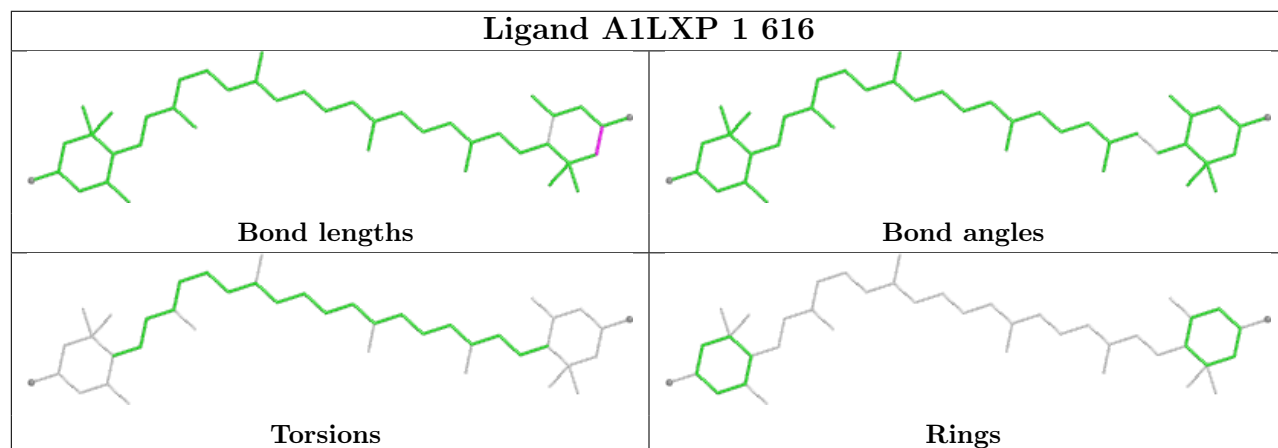
Ligand A1LXP 1 619

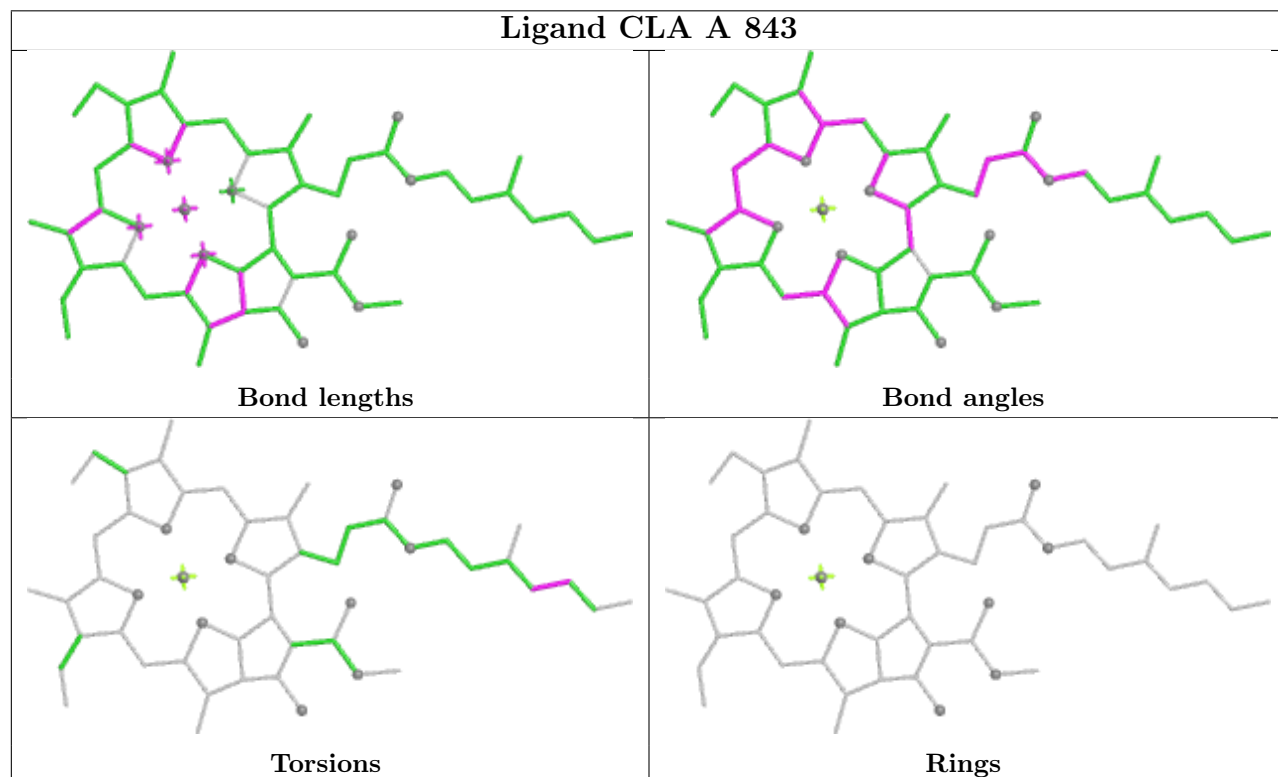
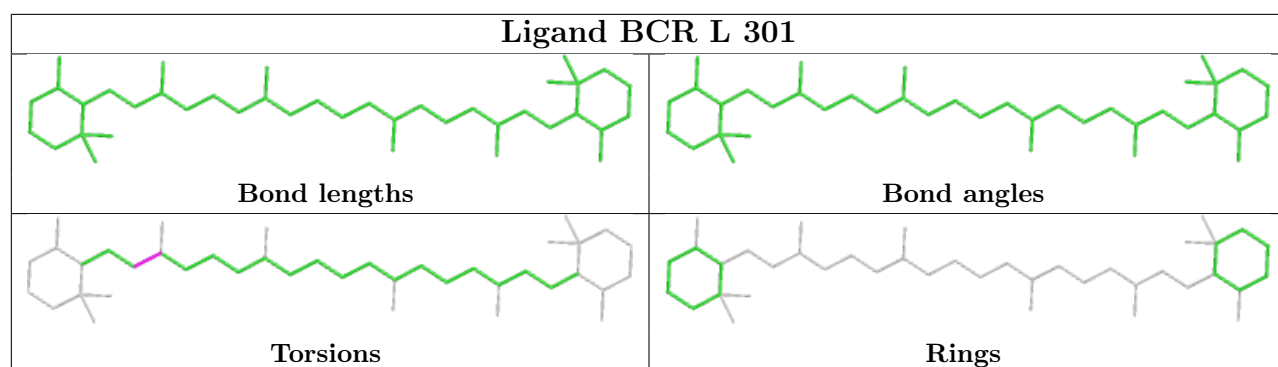


Ligand CLA B 848

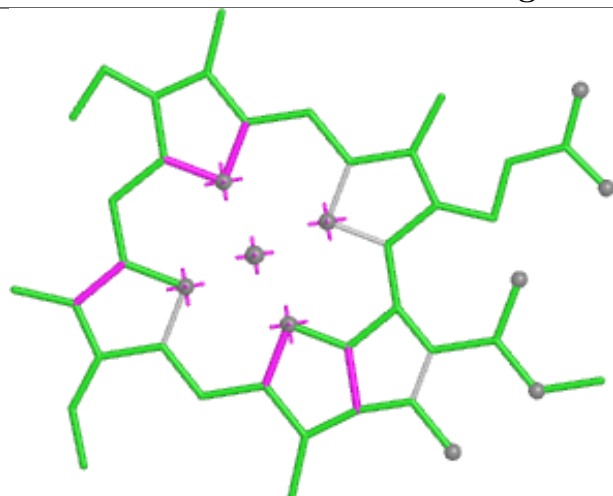


Ligand A1LXP 1 616

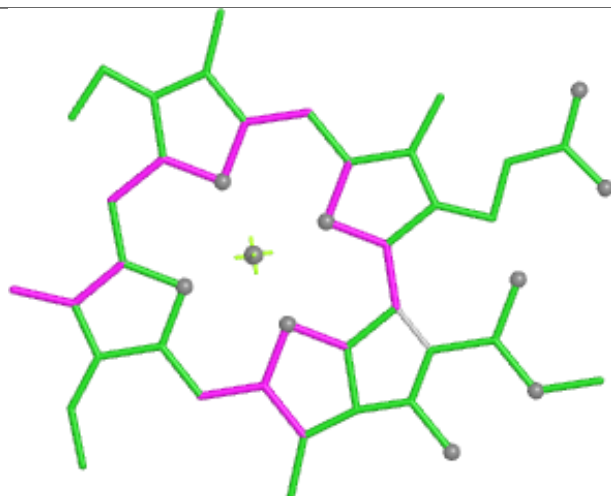




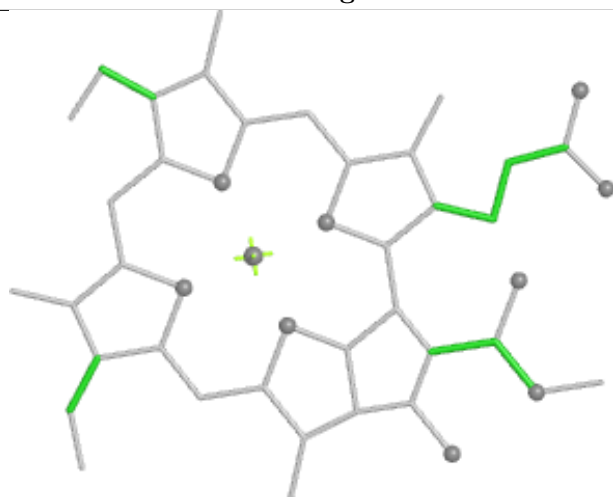
Ligand CLA 2 311



Bond lengths



Bond angles

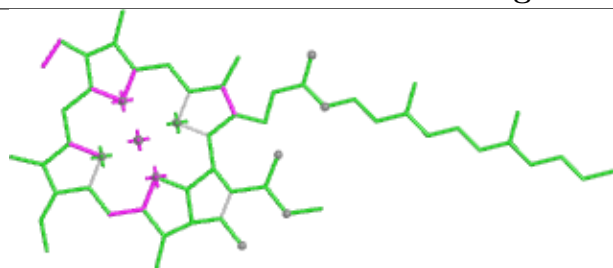


Torsions

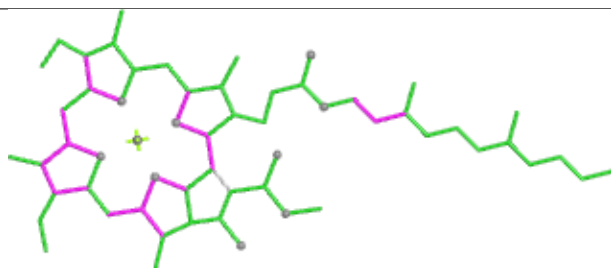


Rings

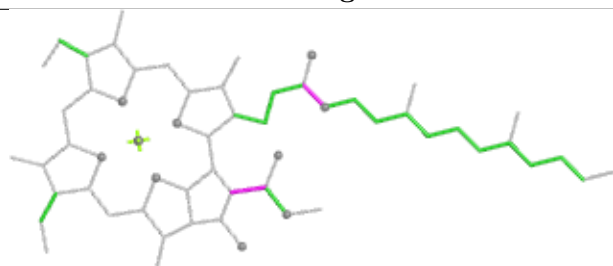
Ligand CLA A 827



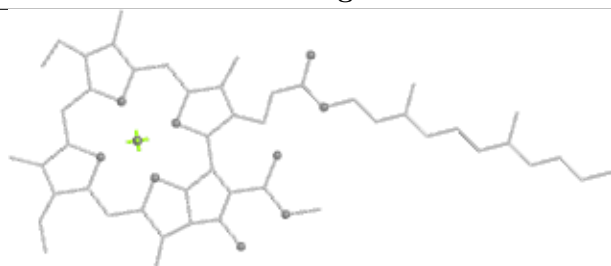
Bond lengths



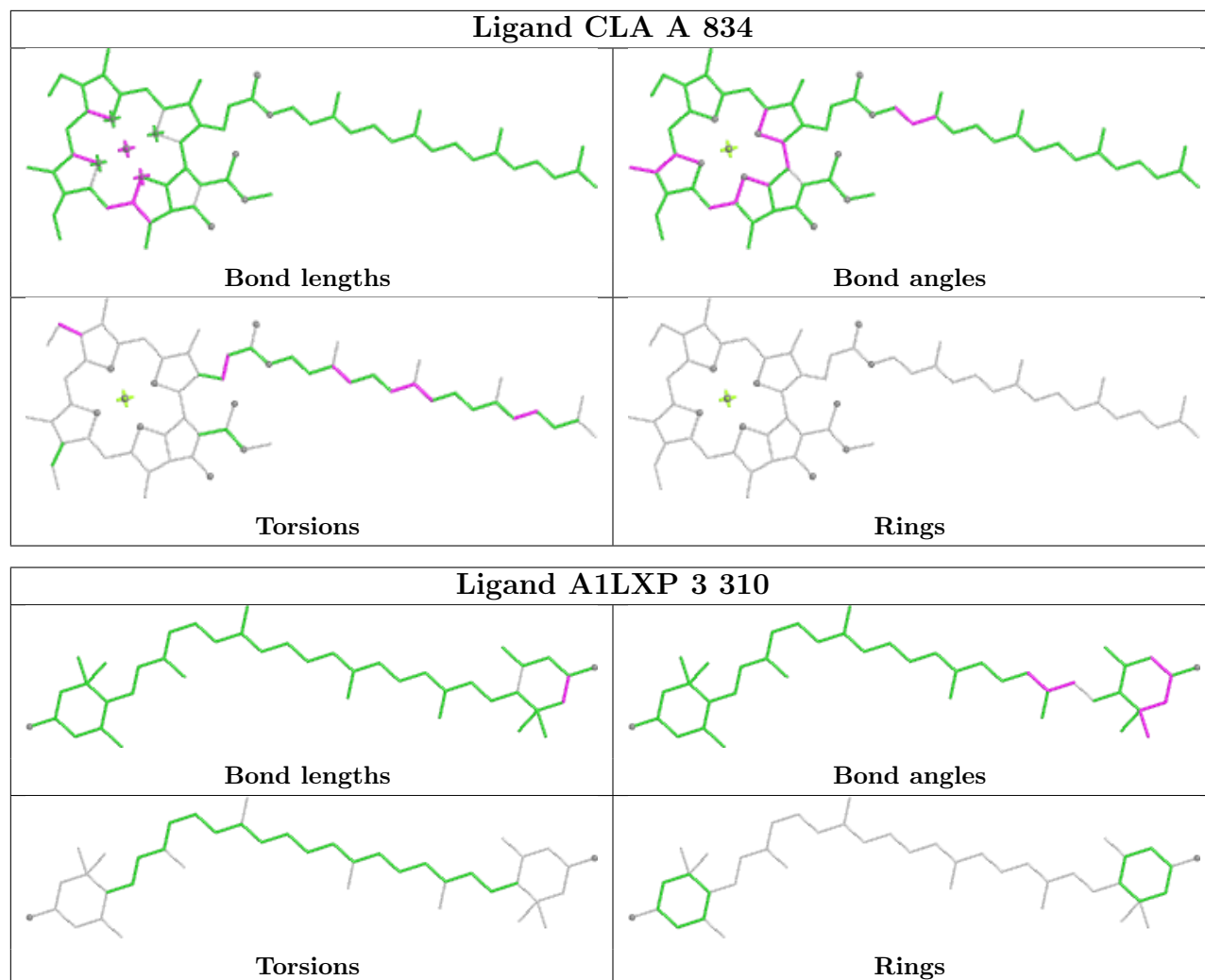
Bond angles



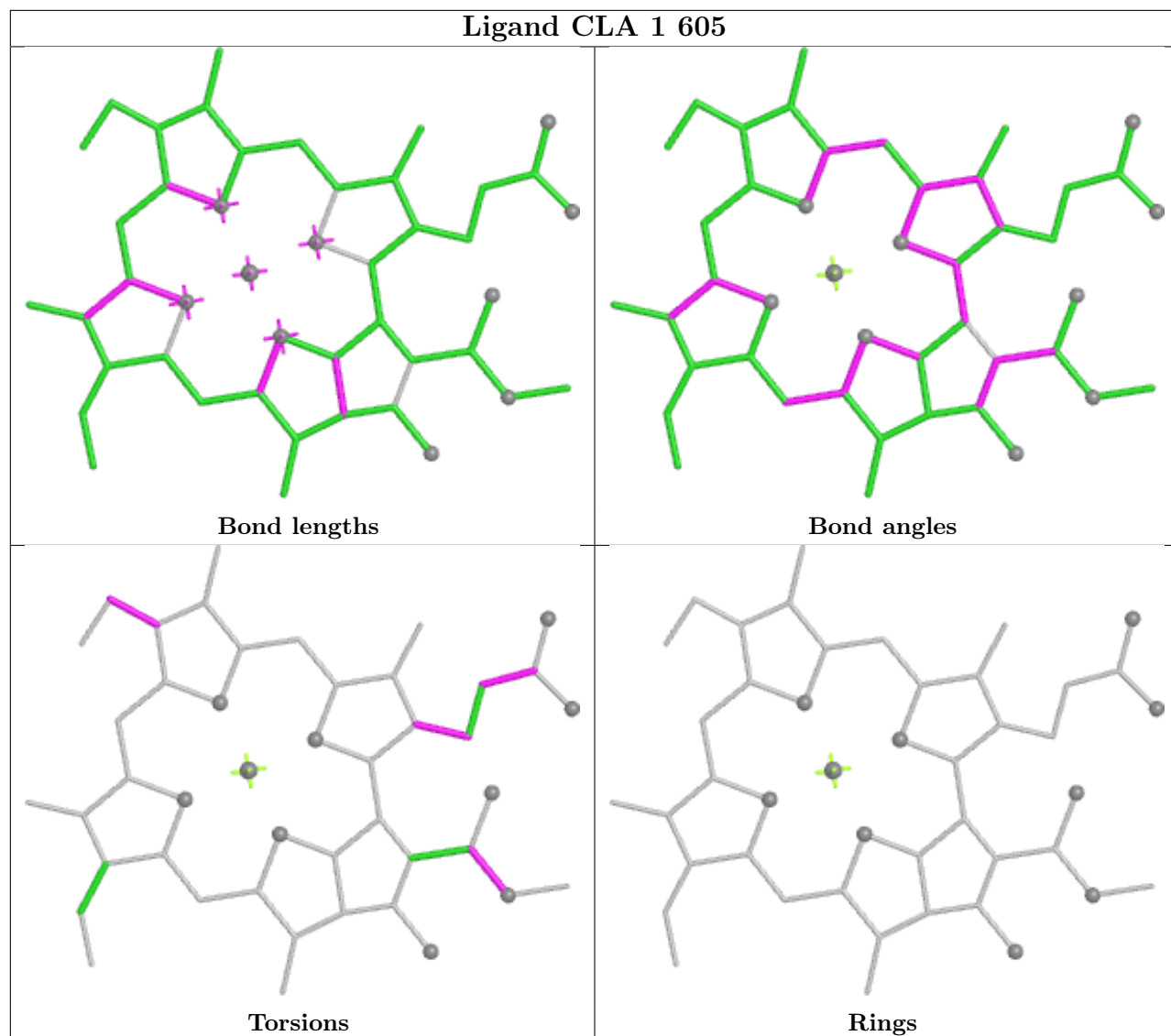
Torsions

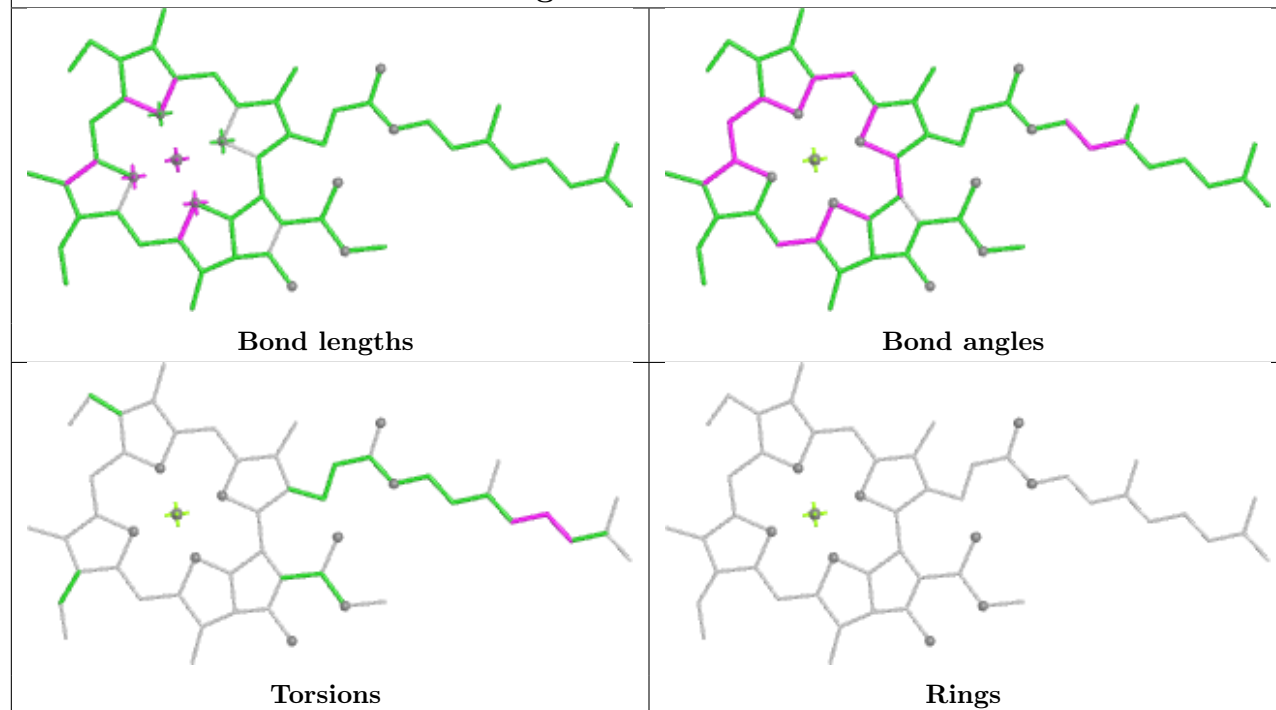
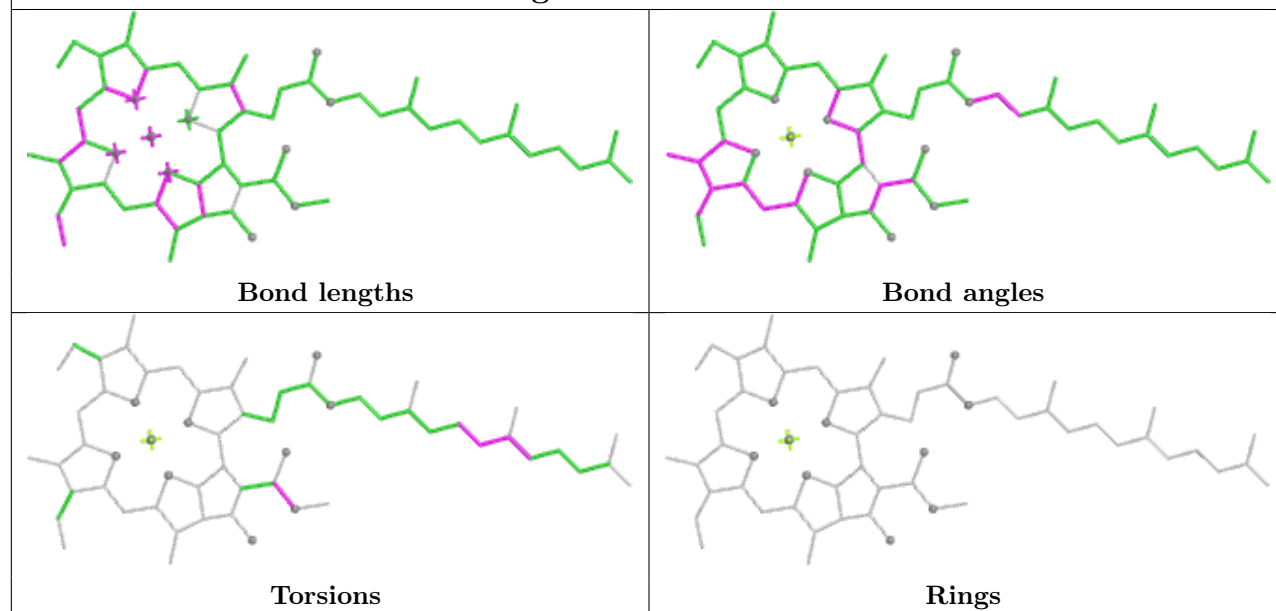


Rings

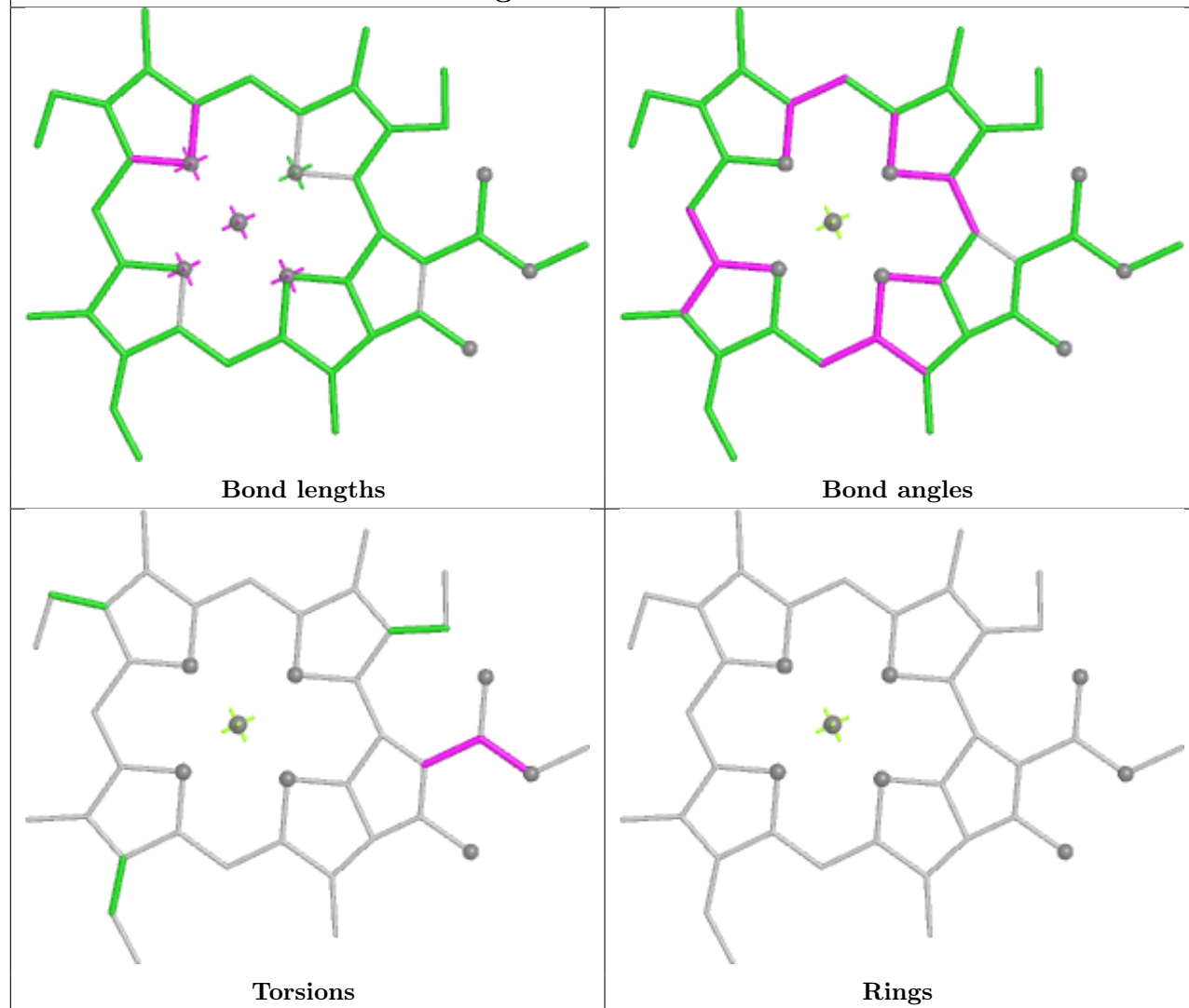


Ligand CLA 1 605

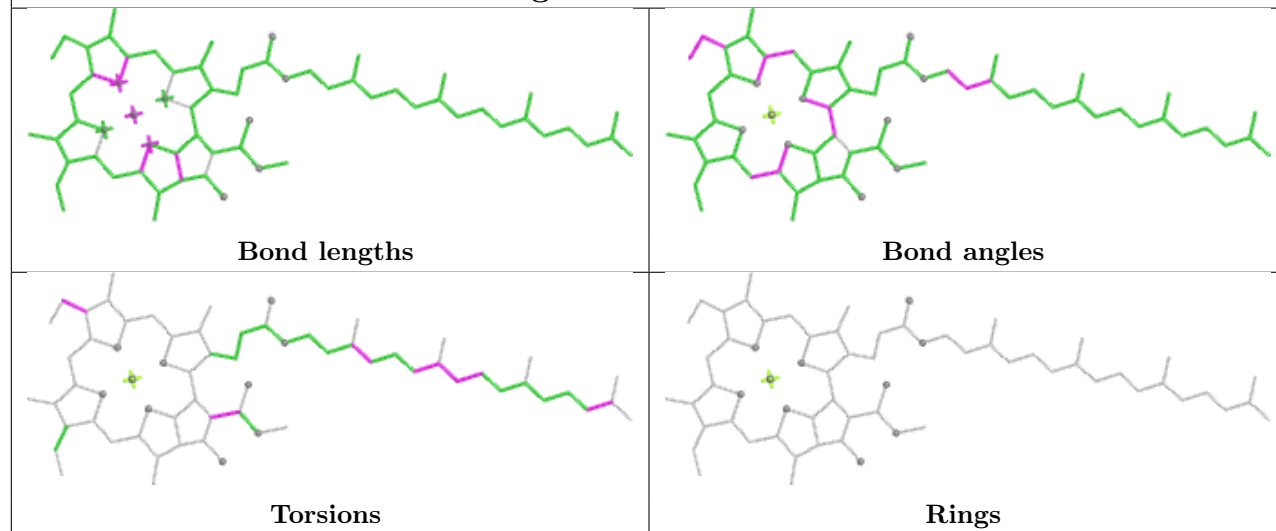


Ligand CLA 3 314**Ligand CLA A 813**

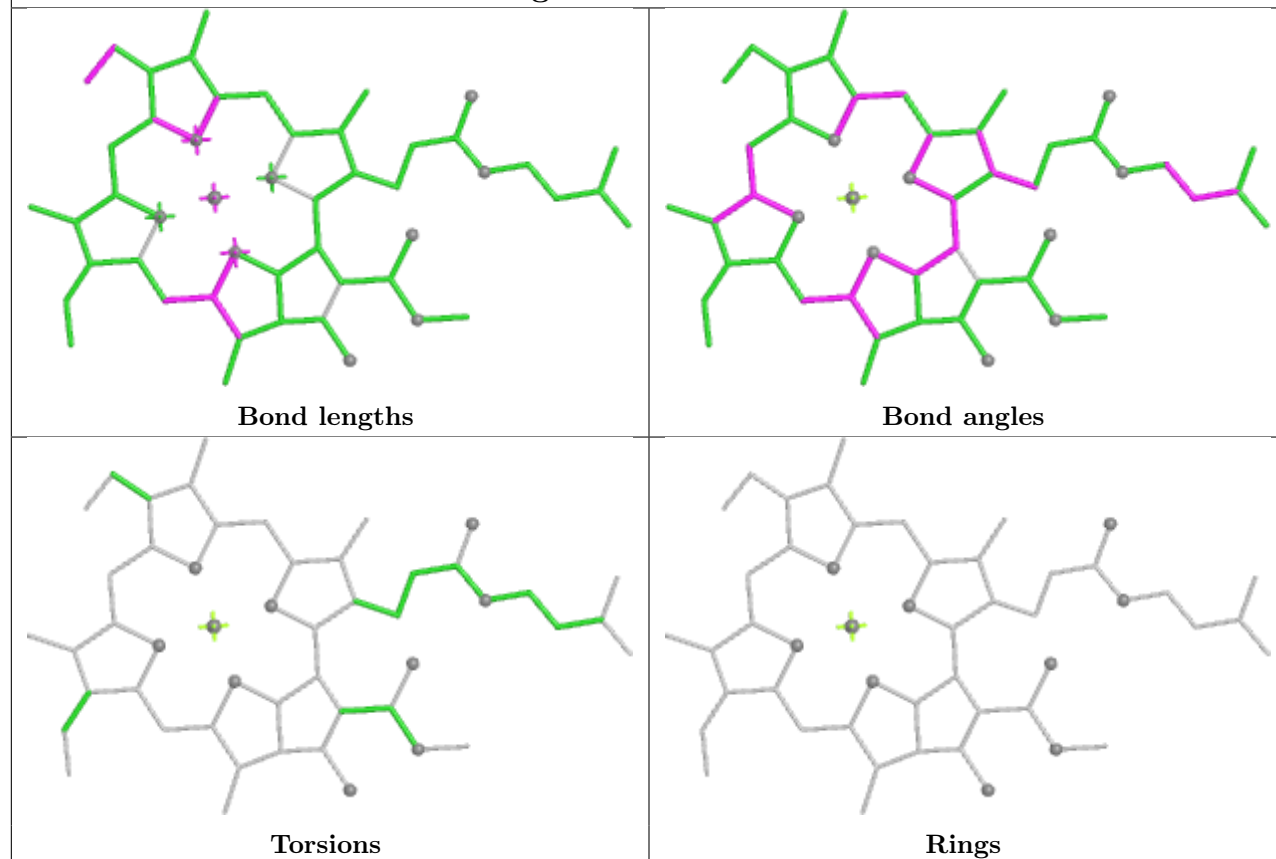
Ligand CLA A 820



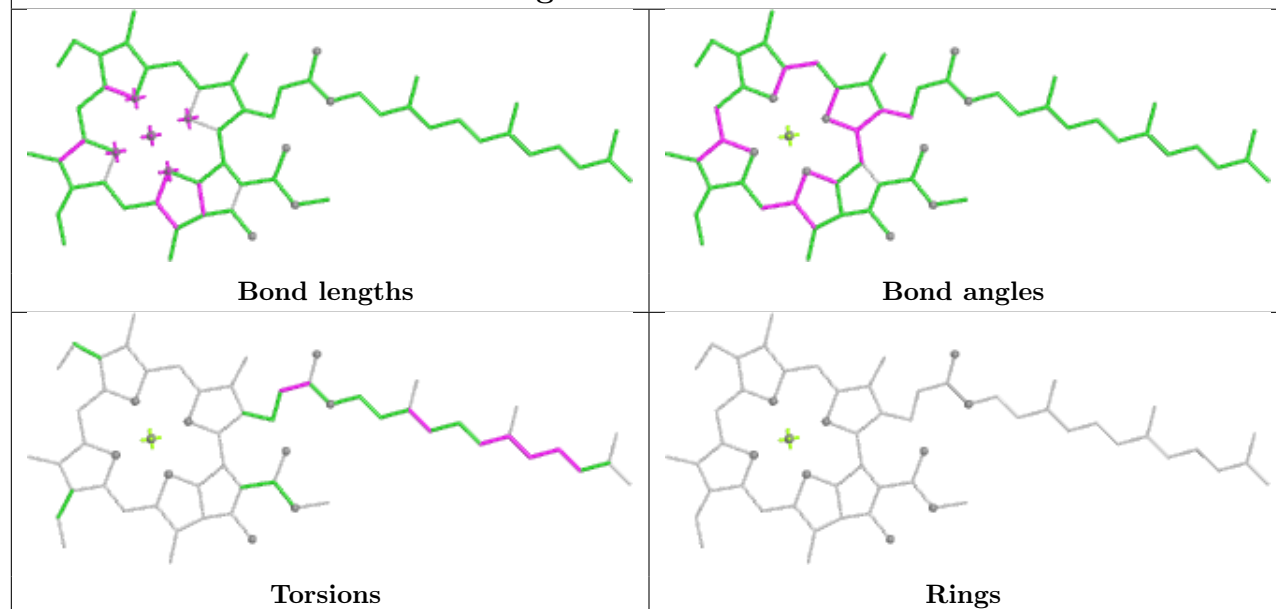
Ligand CLA A 824

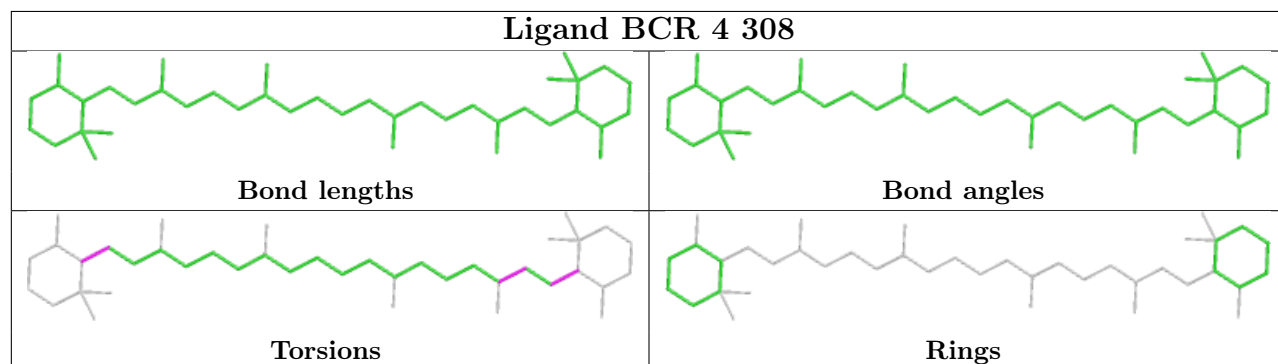
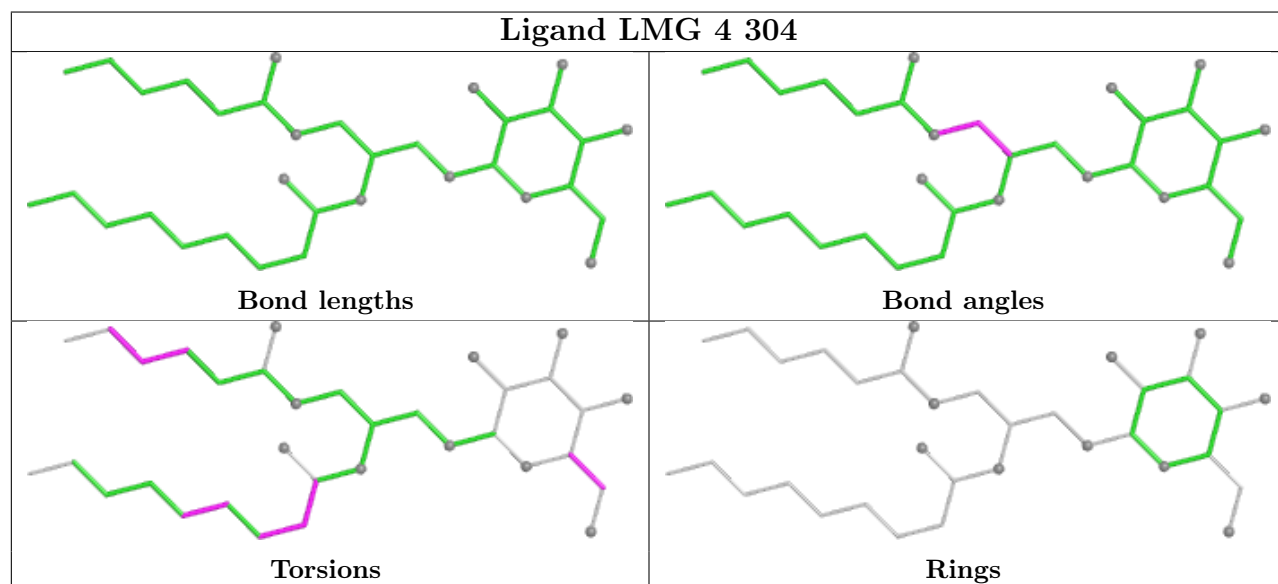
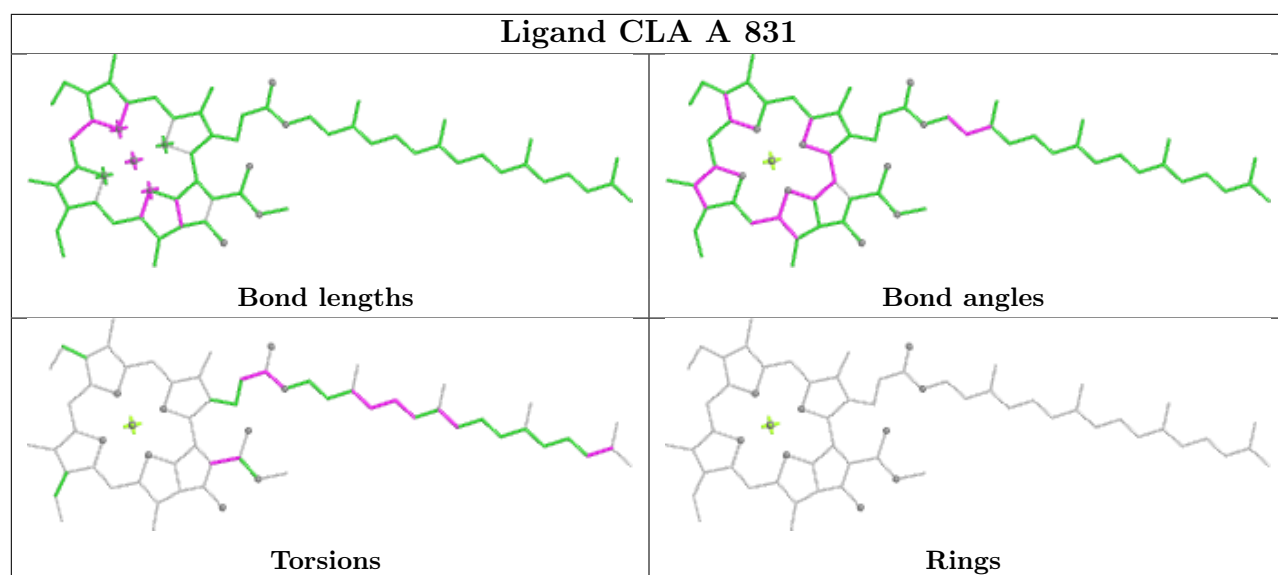


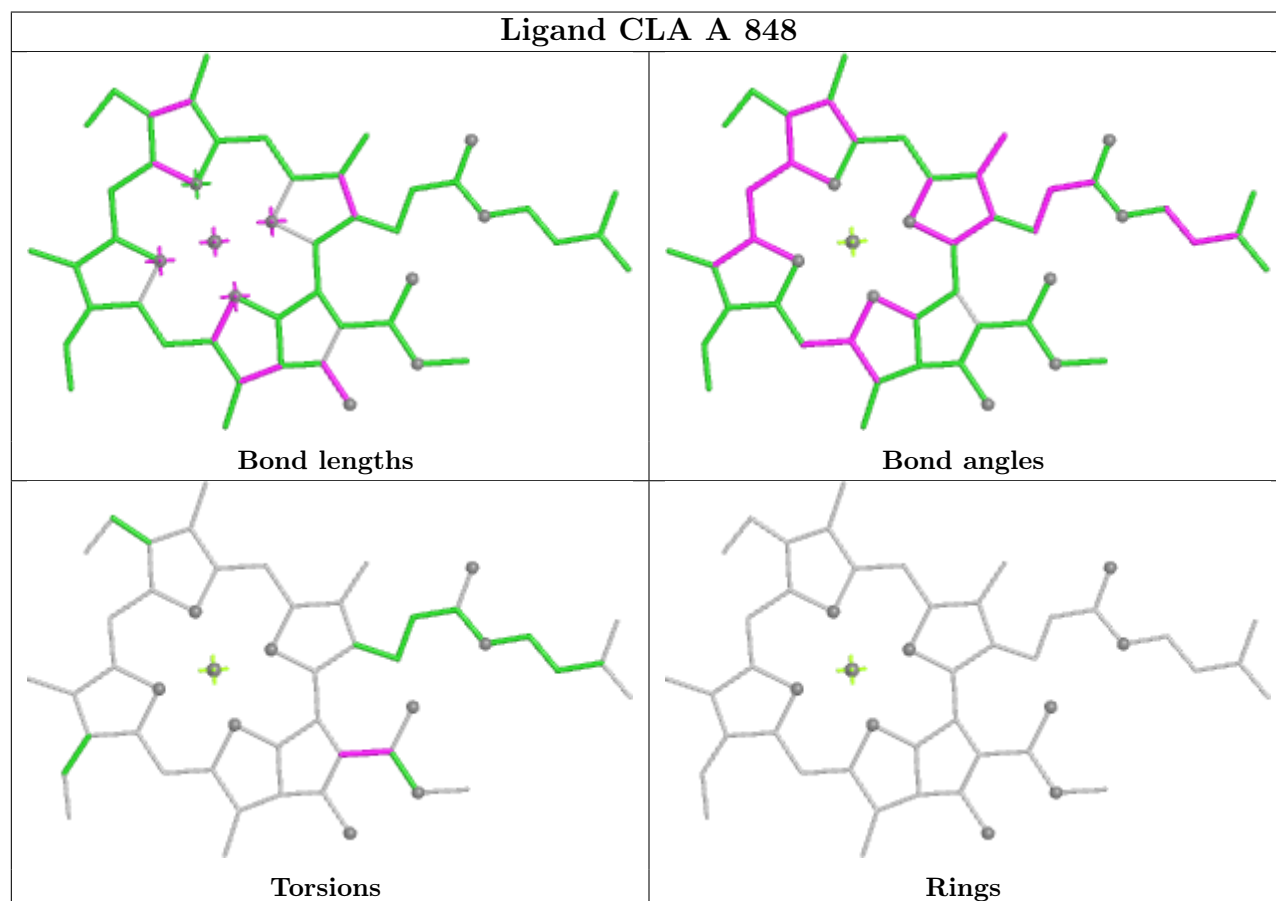
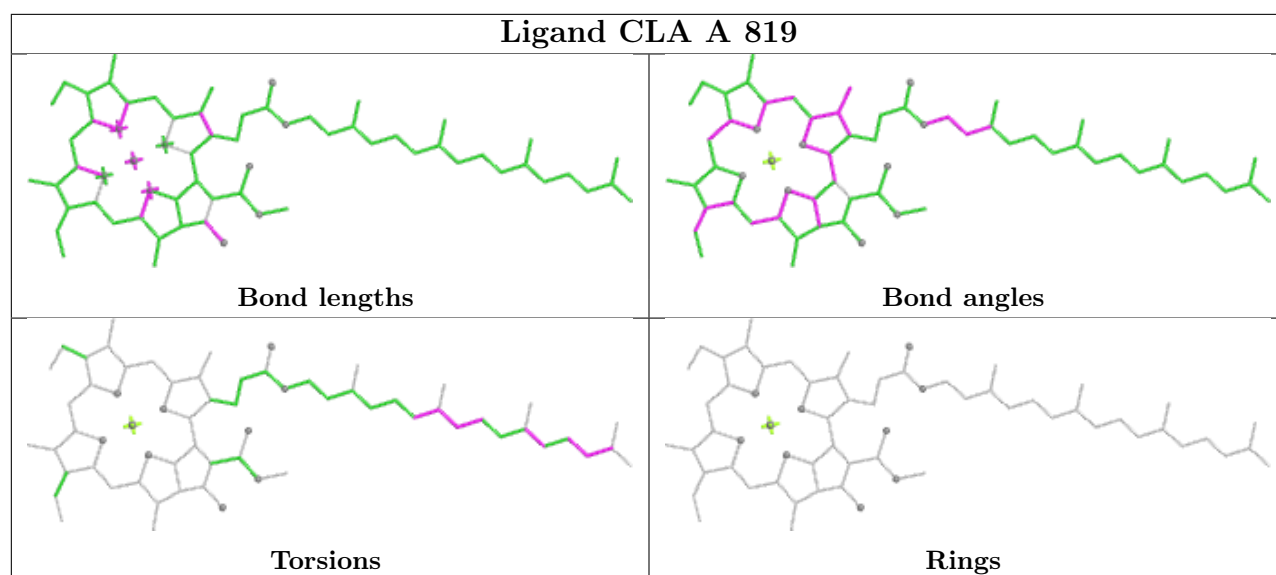
Ligand CLA A 810

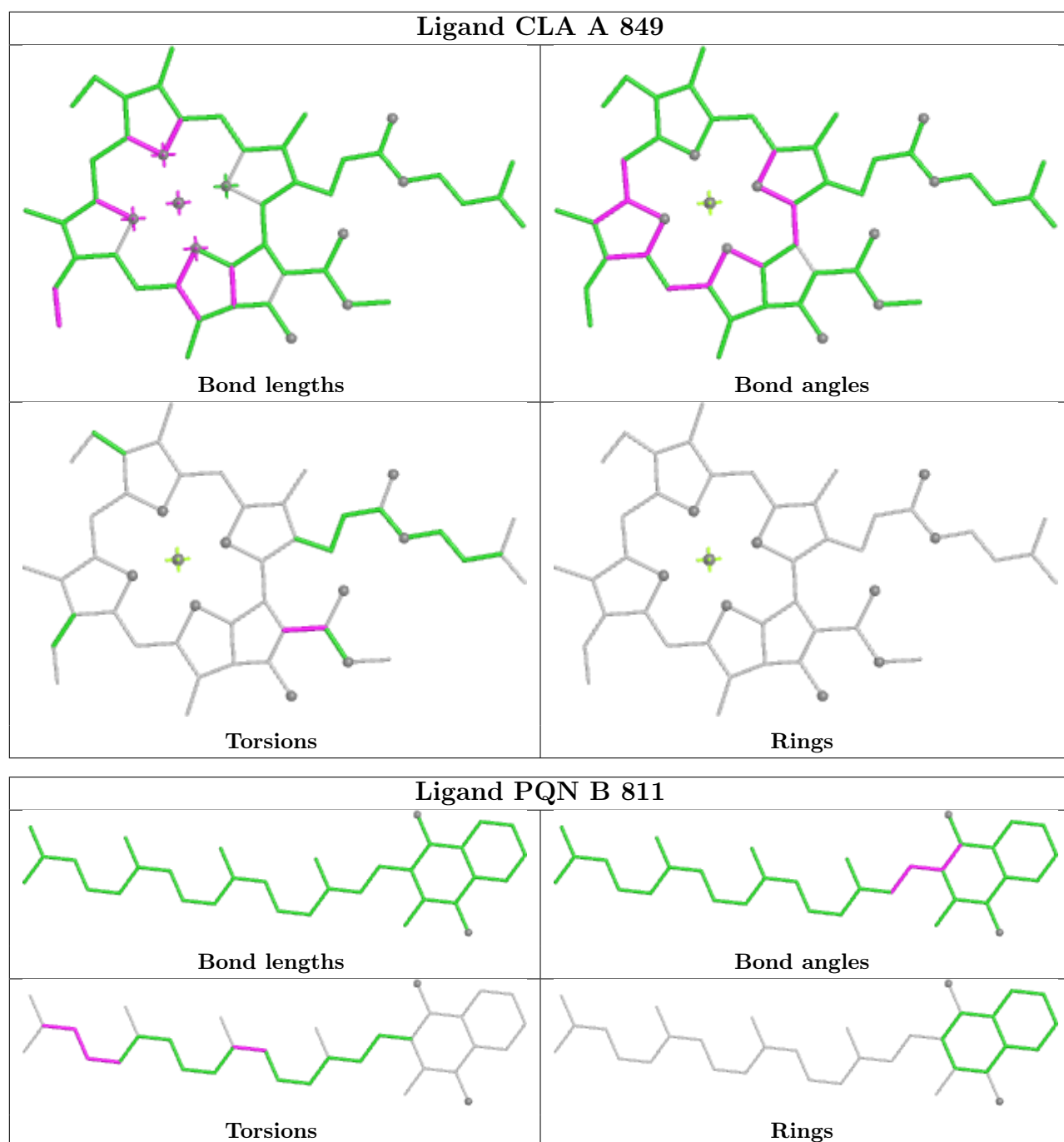


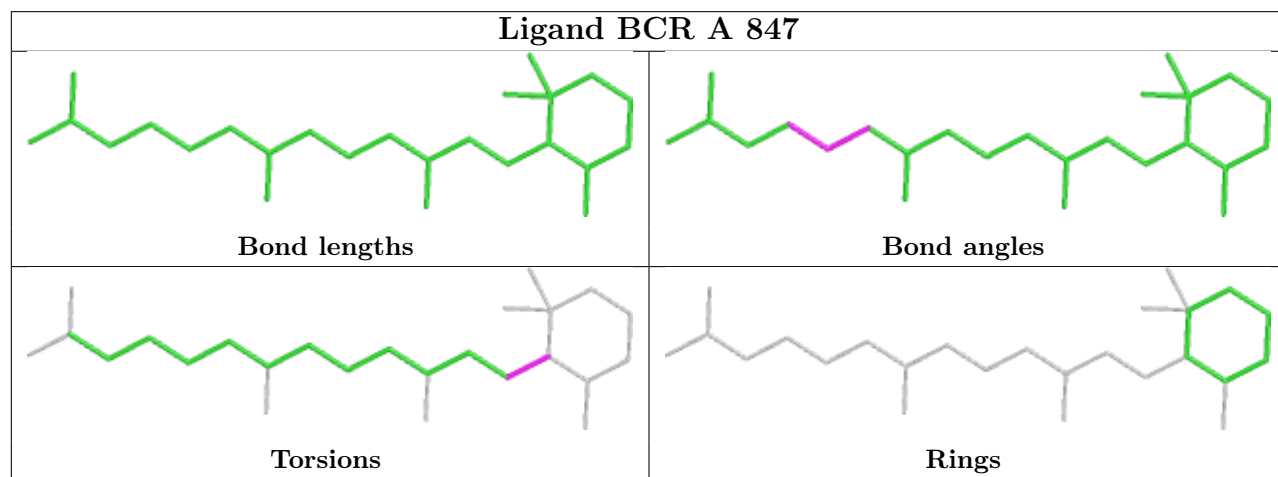
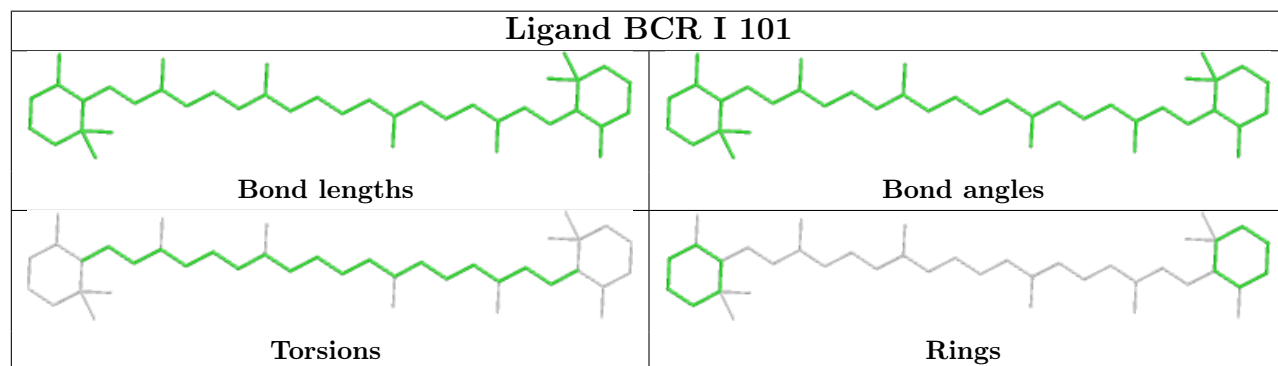
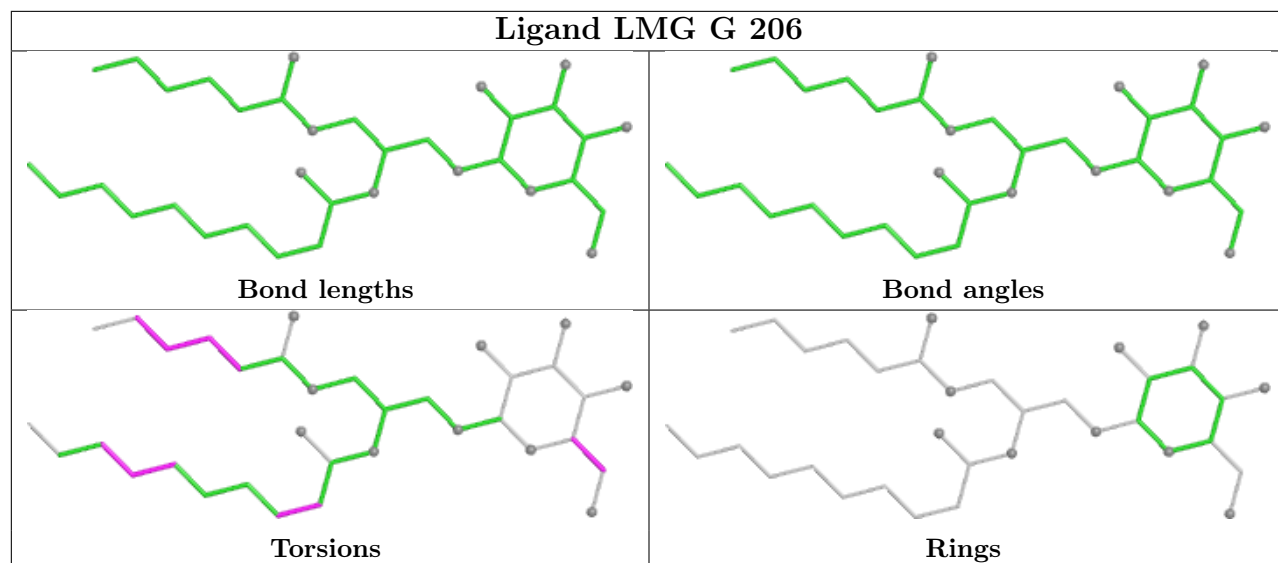
Ligand CLA 3 301



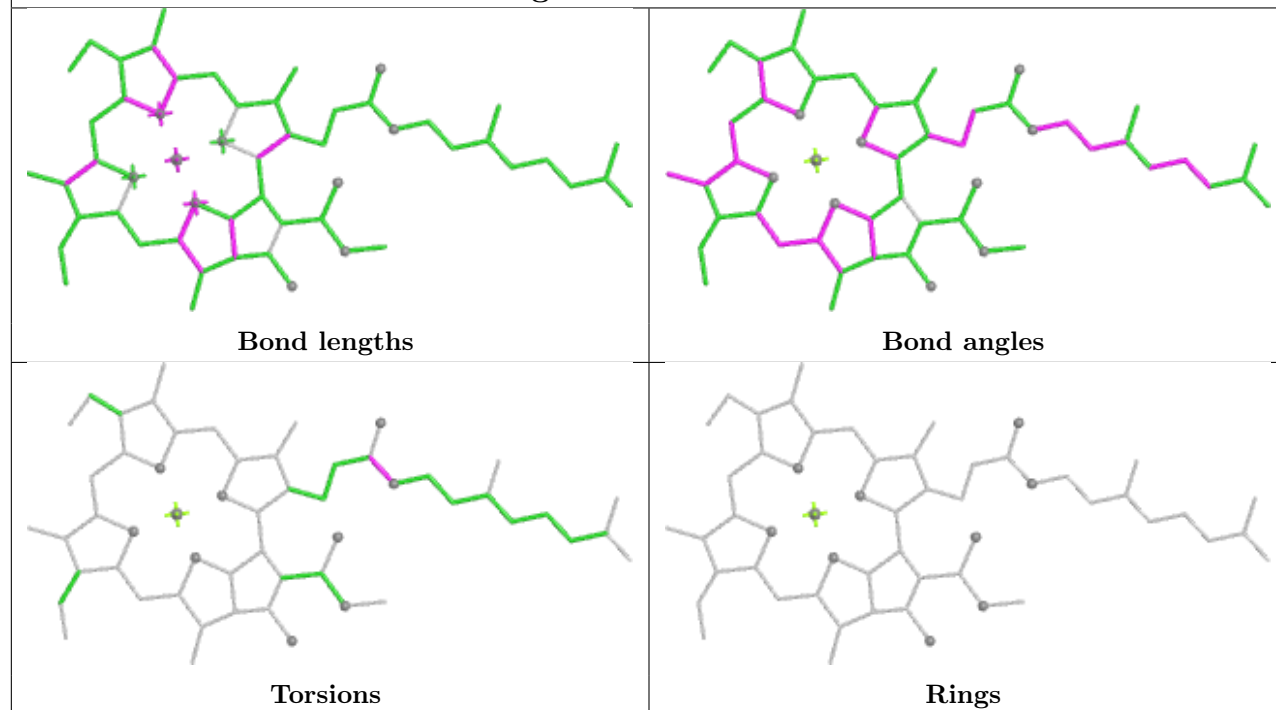




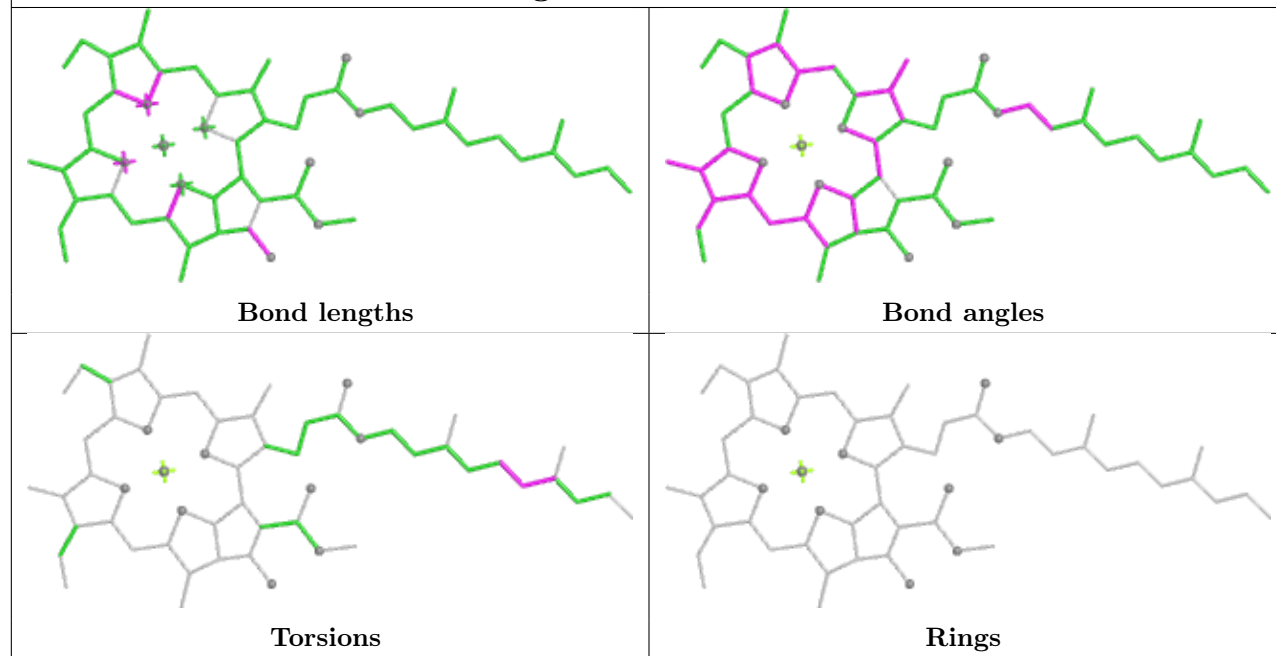


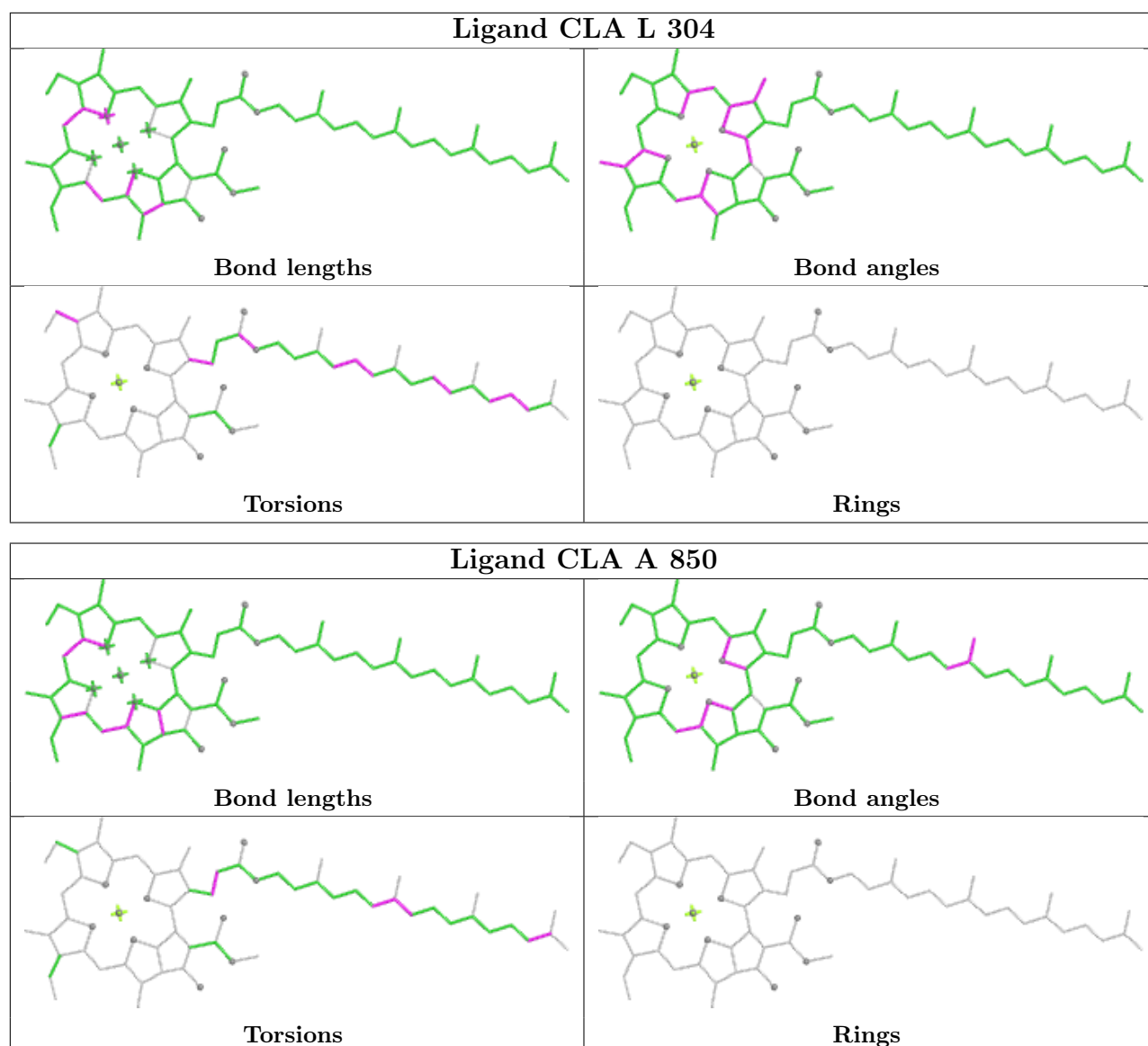


Ligand CLA A 801

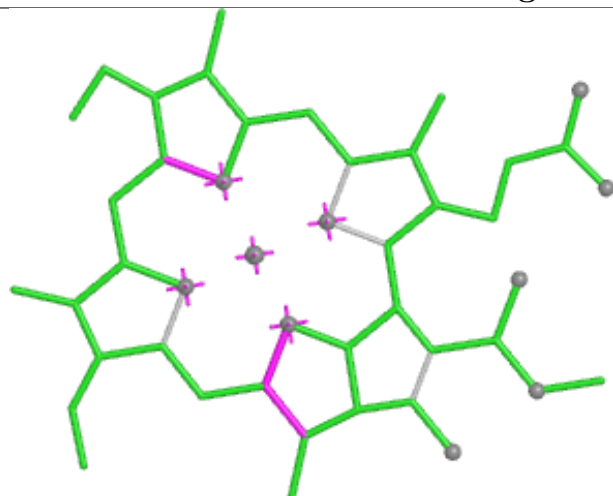


Ligand CLA B 835

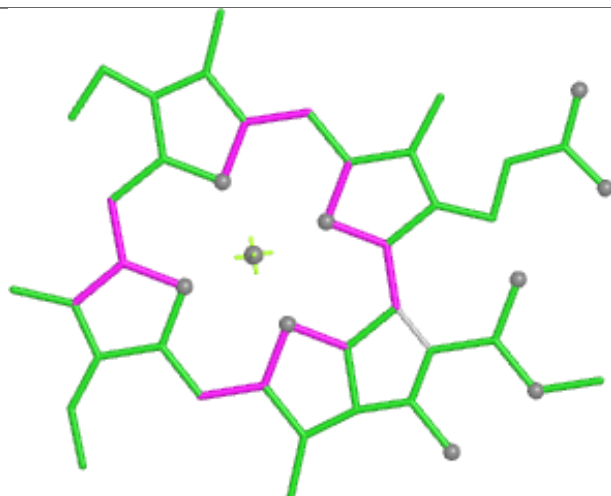




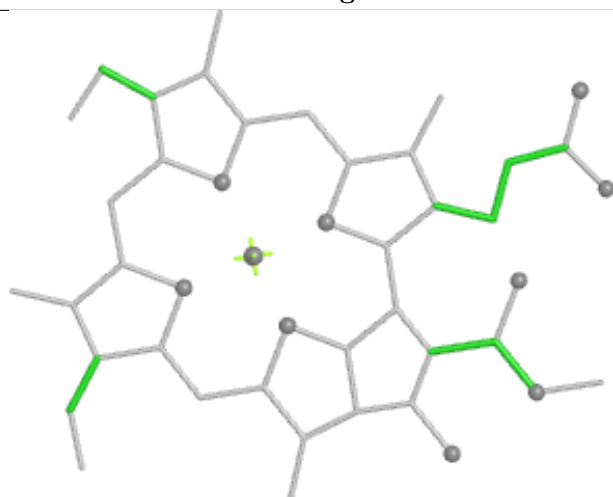
Ligand CLA 3 308



Bond lengths



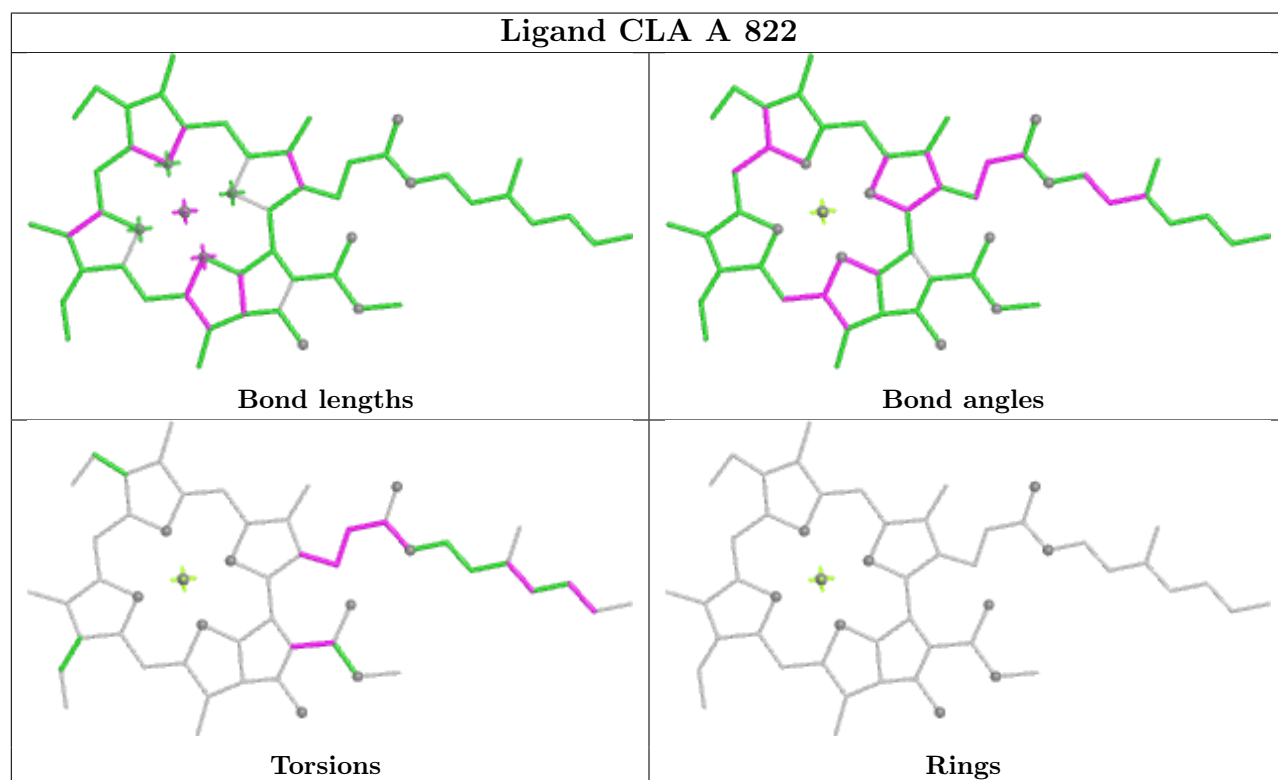
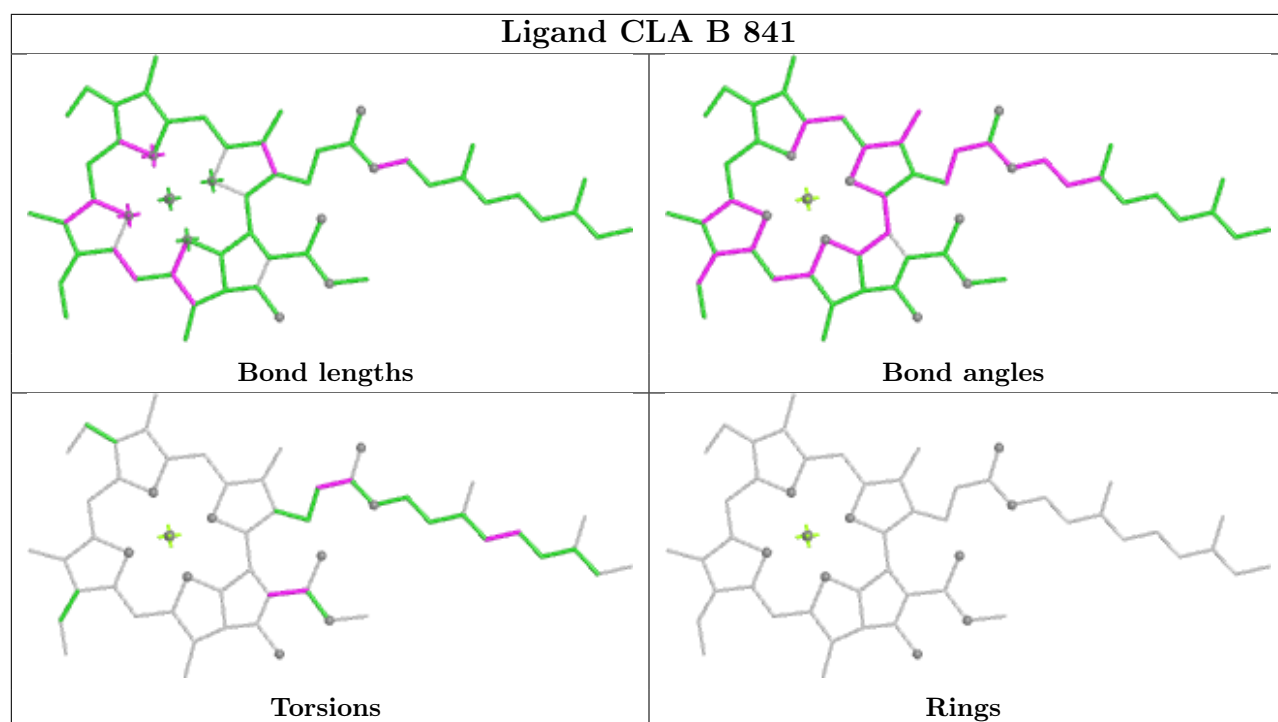
Bond angles

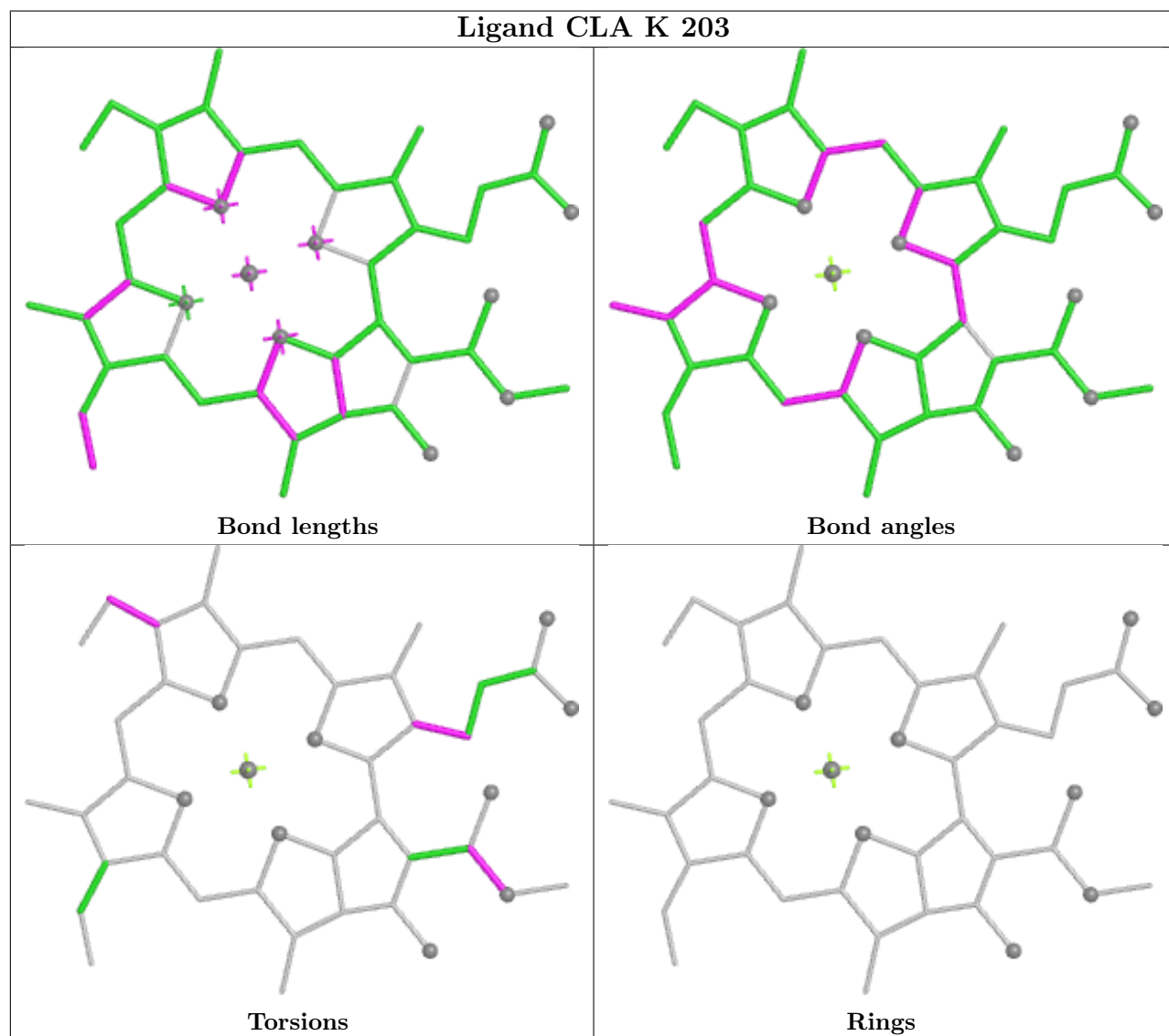
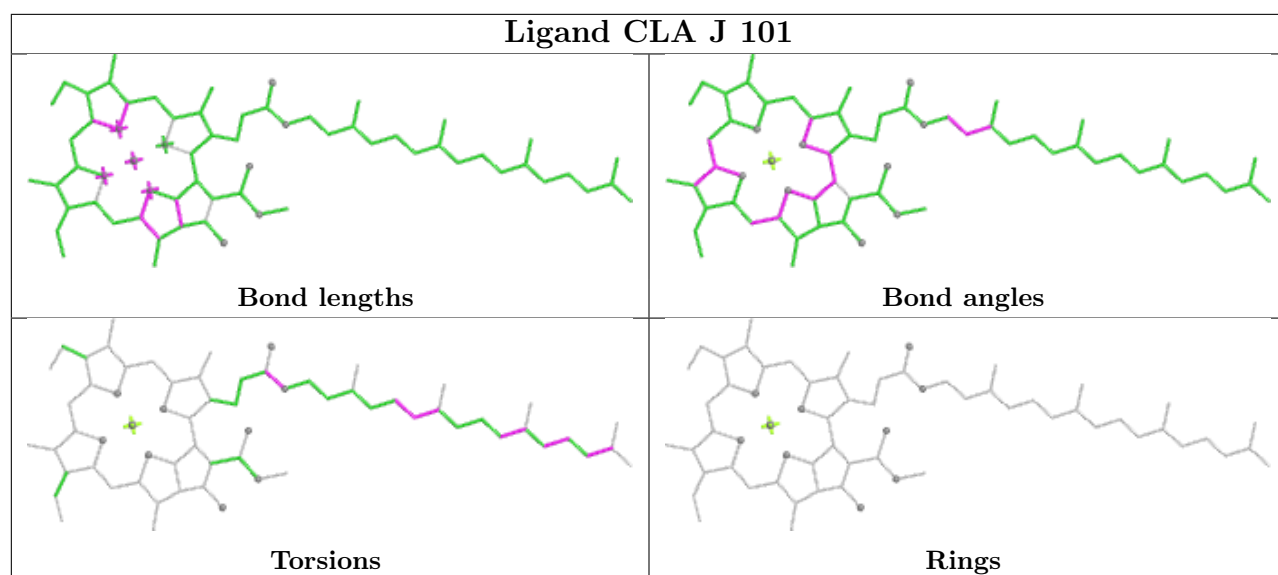


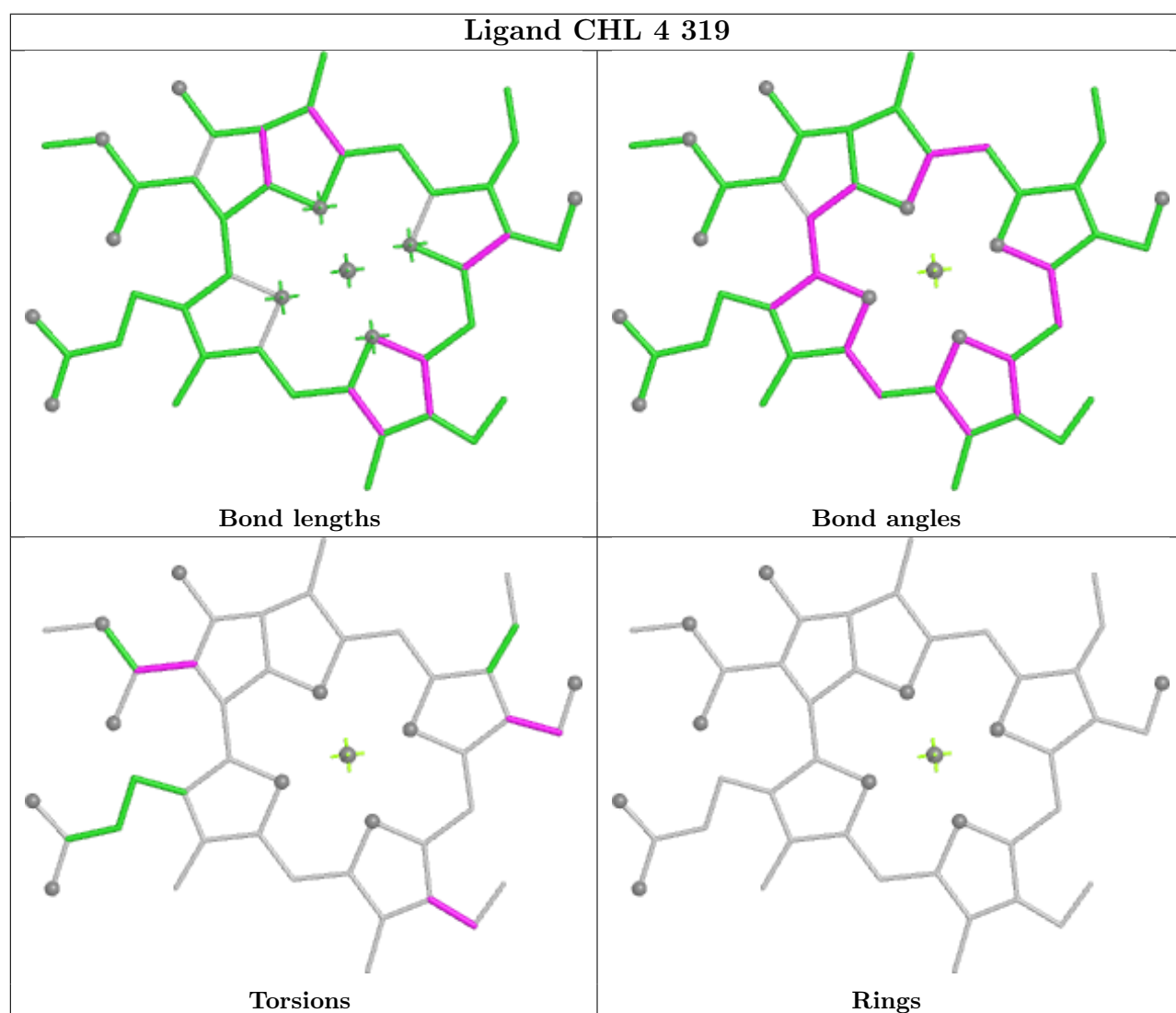
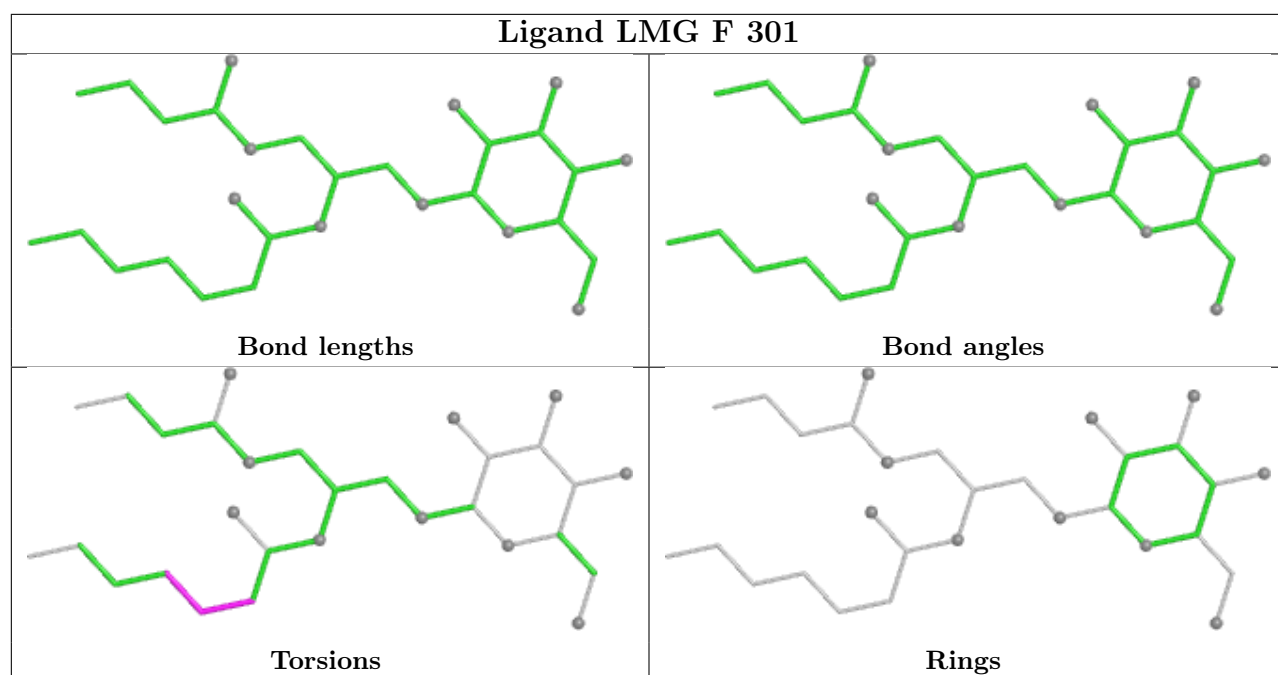
Torsions



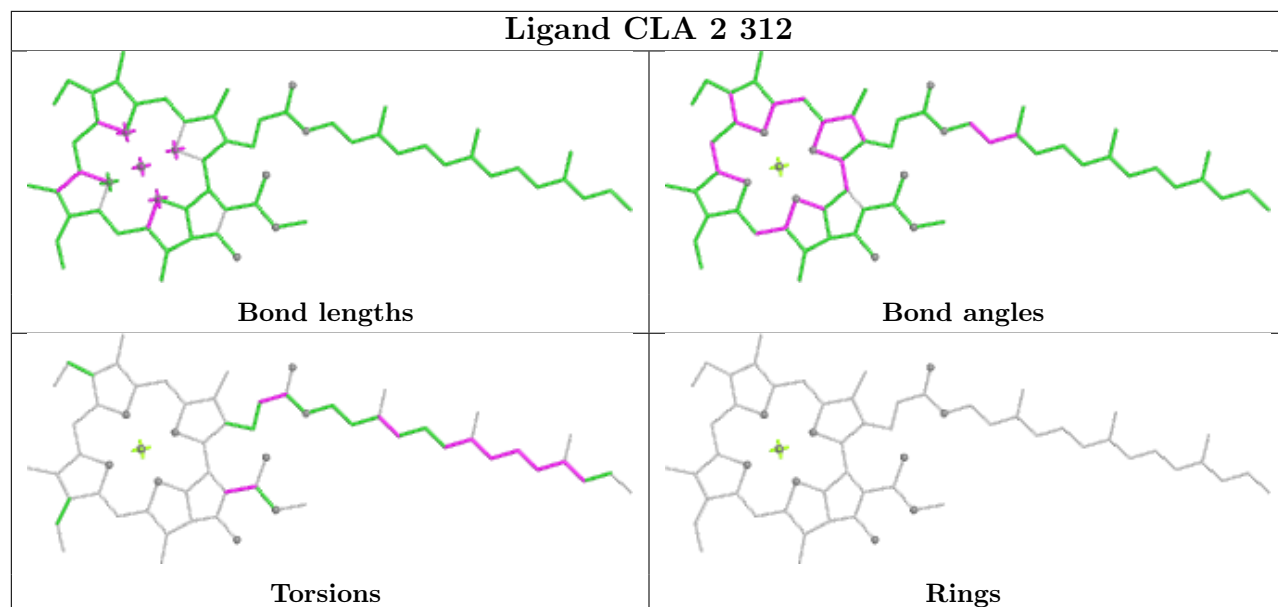
Rings



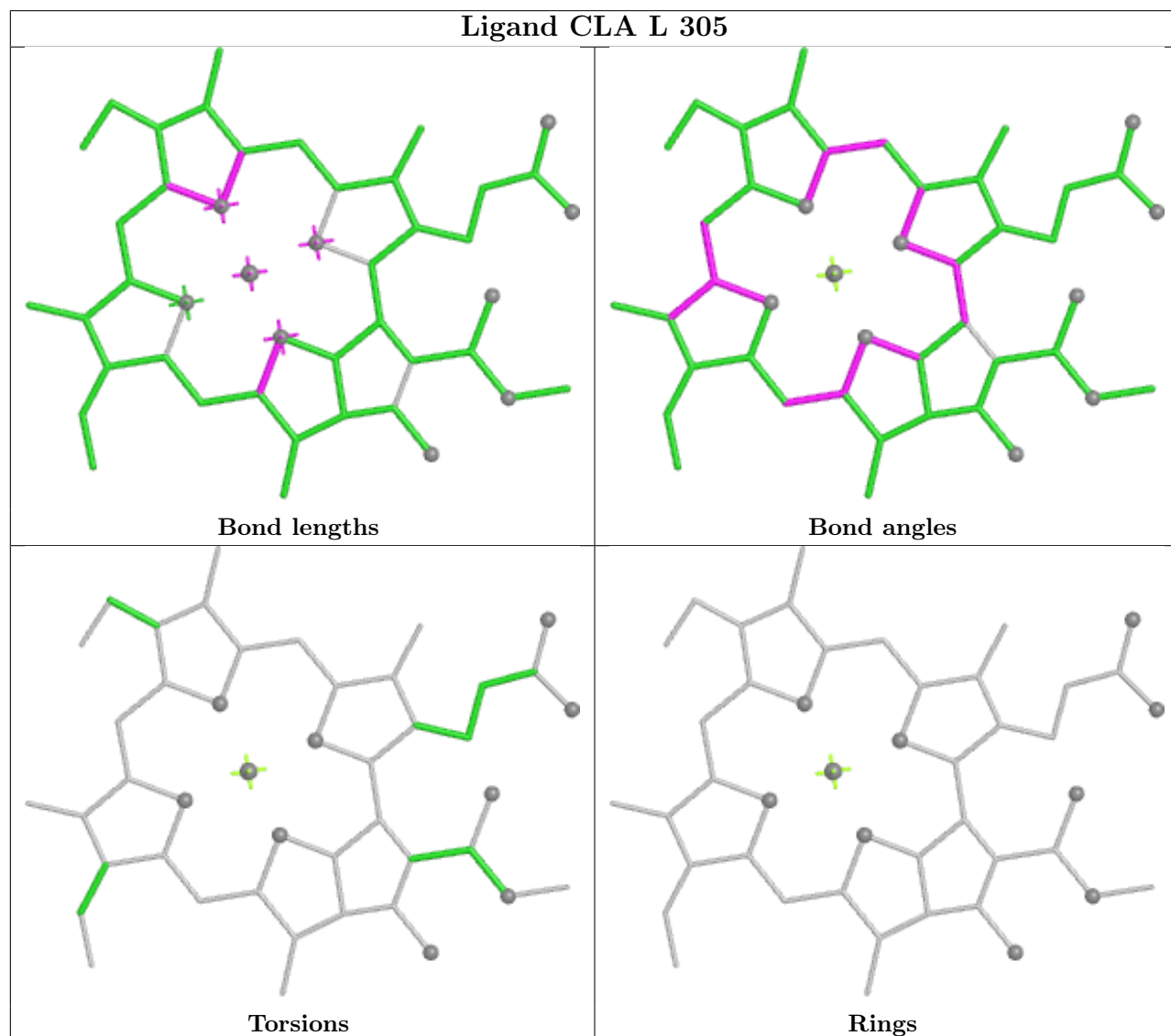


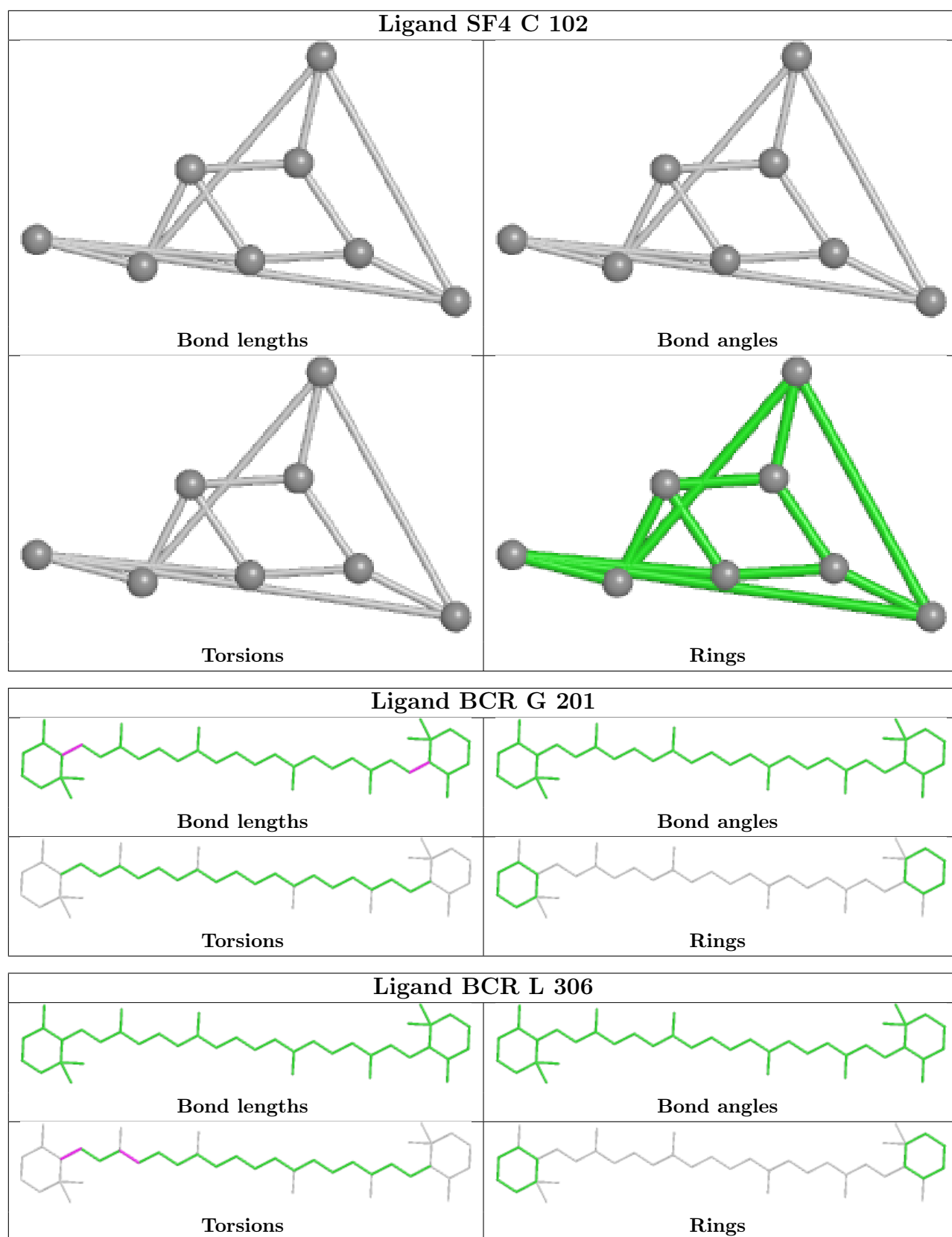


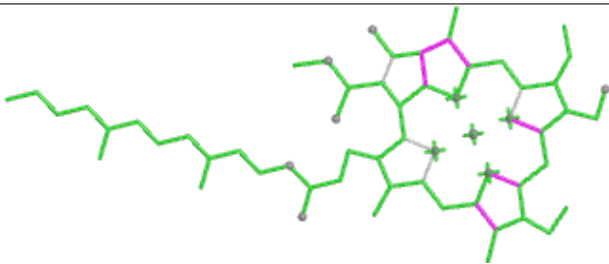
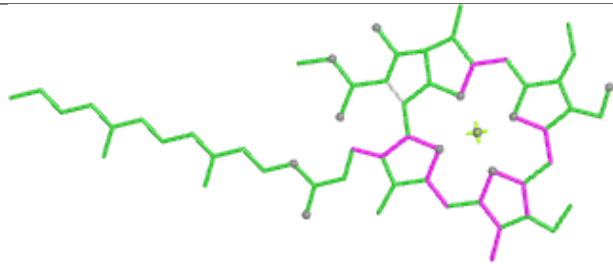
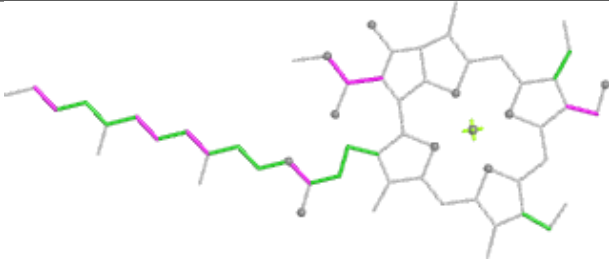
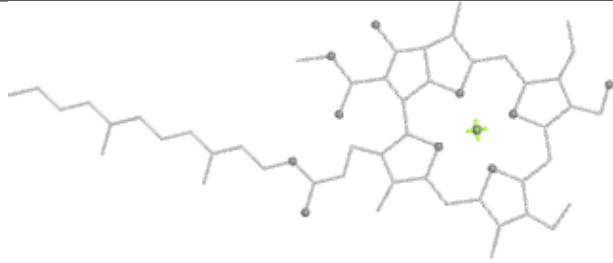
Ligand CLA 2 312

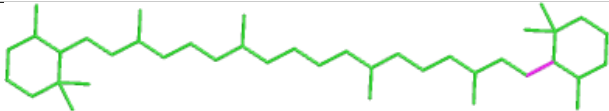
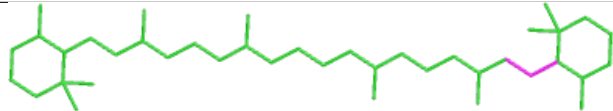
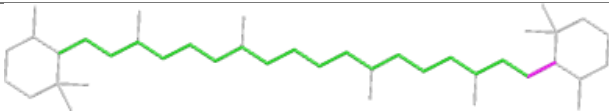
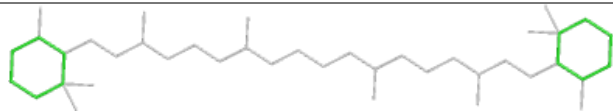


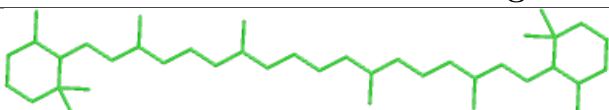
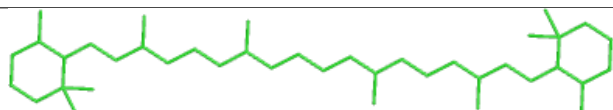
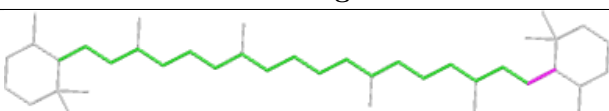
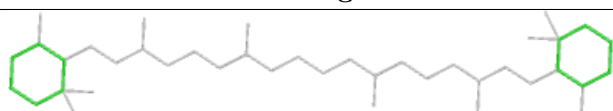
Ligand CLA L 305

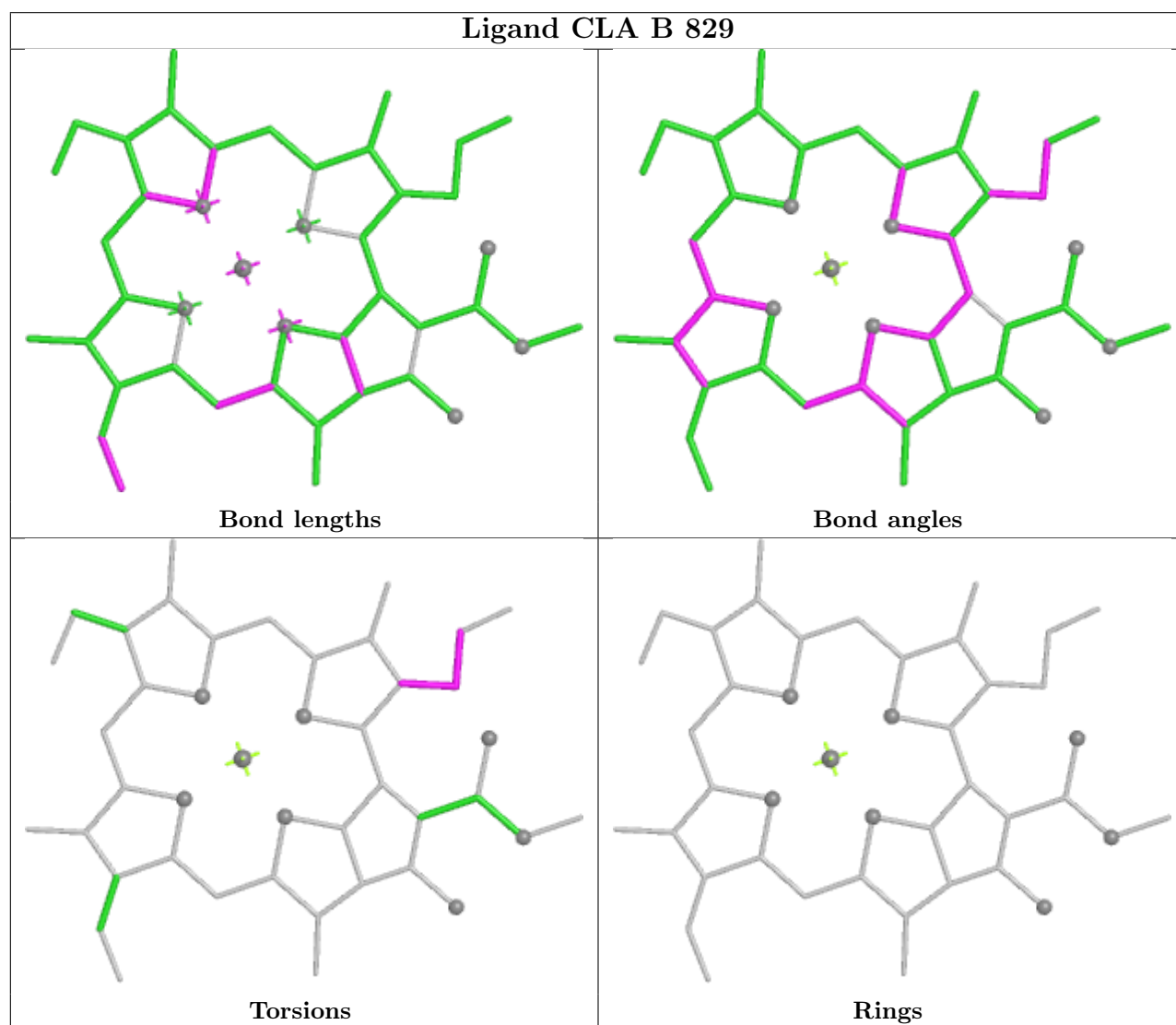
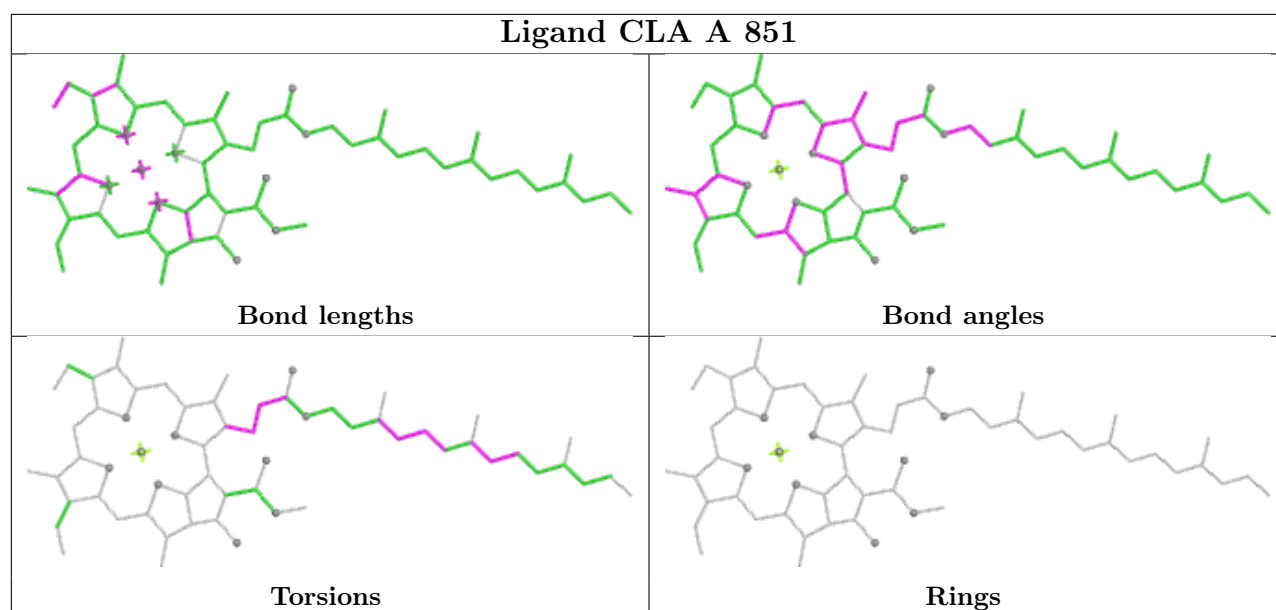




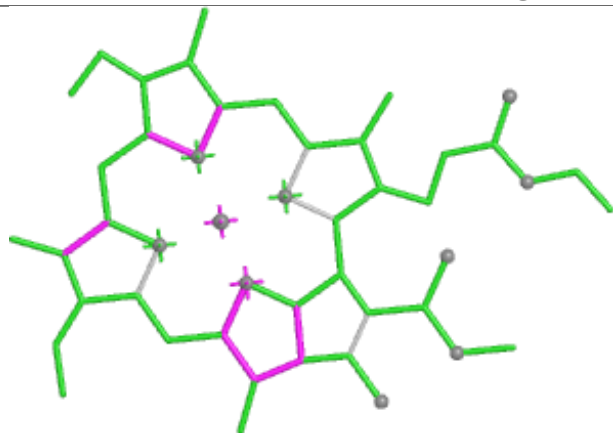
Ligand CHL 1 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 852	
	
Bond lengths	Bond angles
	
Torsions	Rings

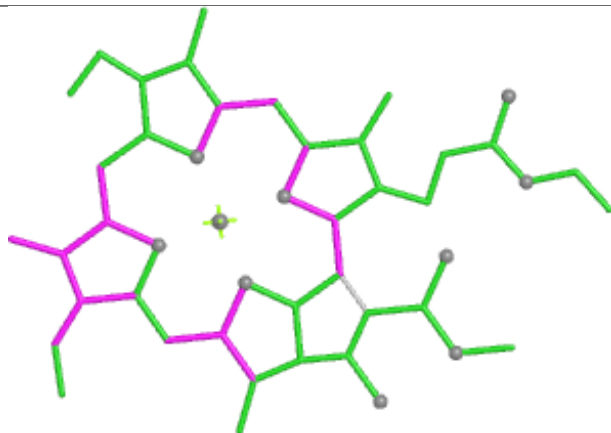
Ligand BCR B 814	
	
Bond lengths	Bond angles
	
Torsions	Rings



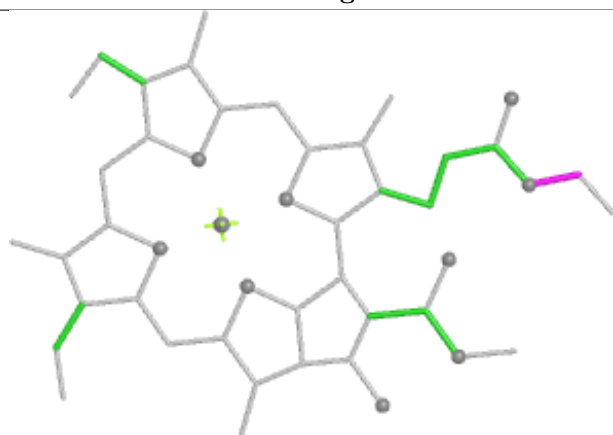
Ligand CLA B 837



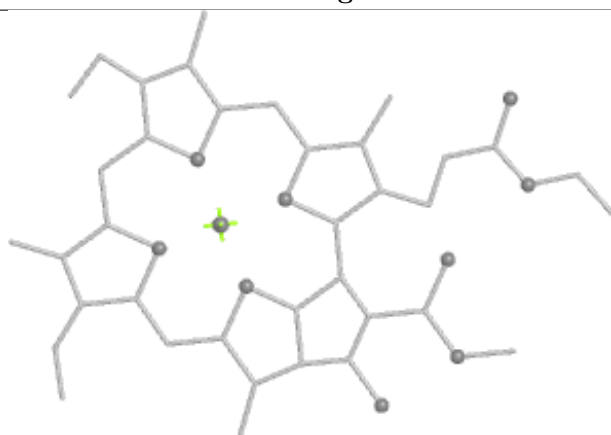
Bond lengths



Bond angles

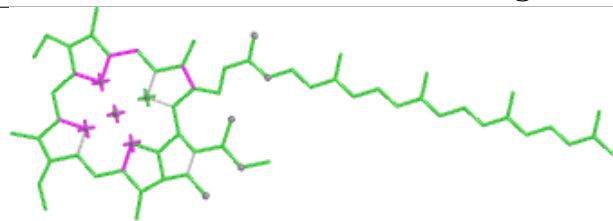


Torsions

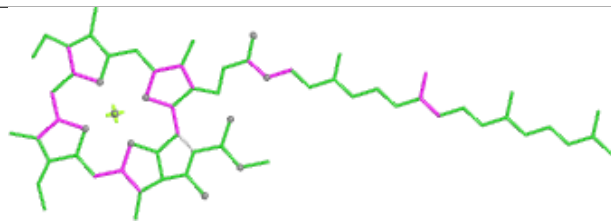


Rings

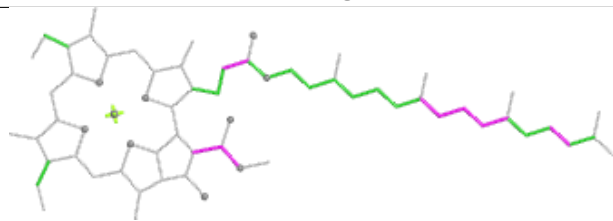
Ligand CLA A 812



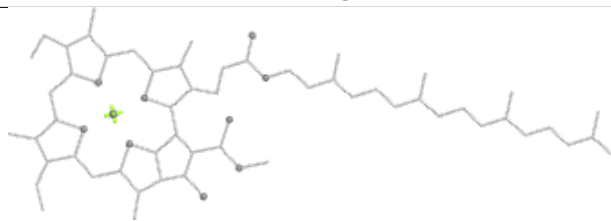
Bond lengths



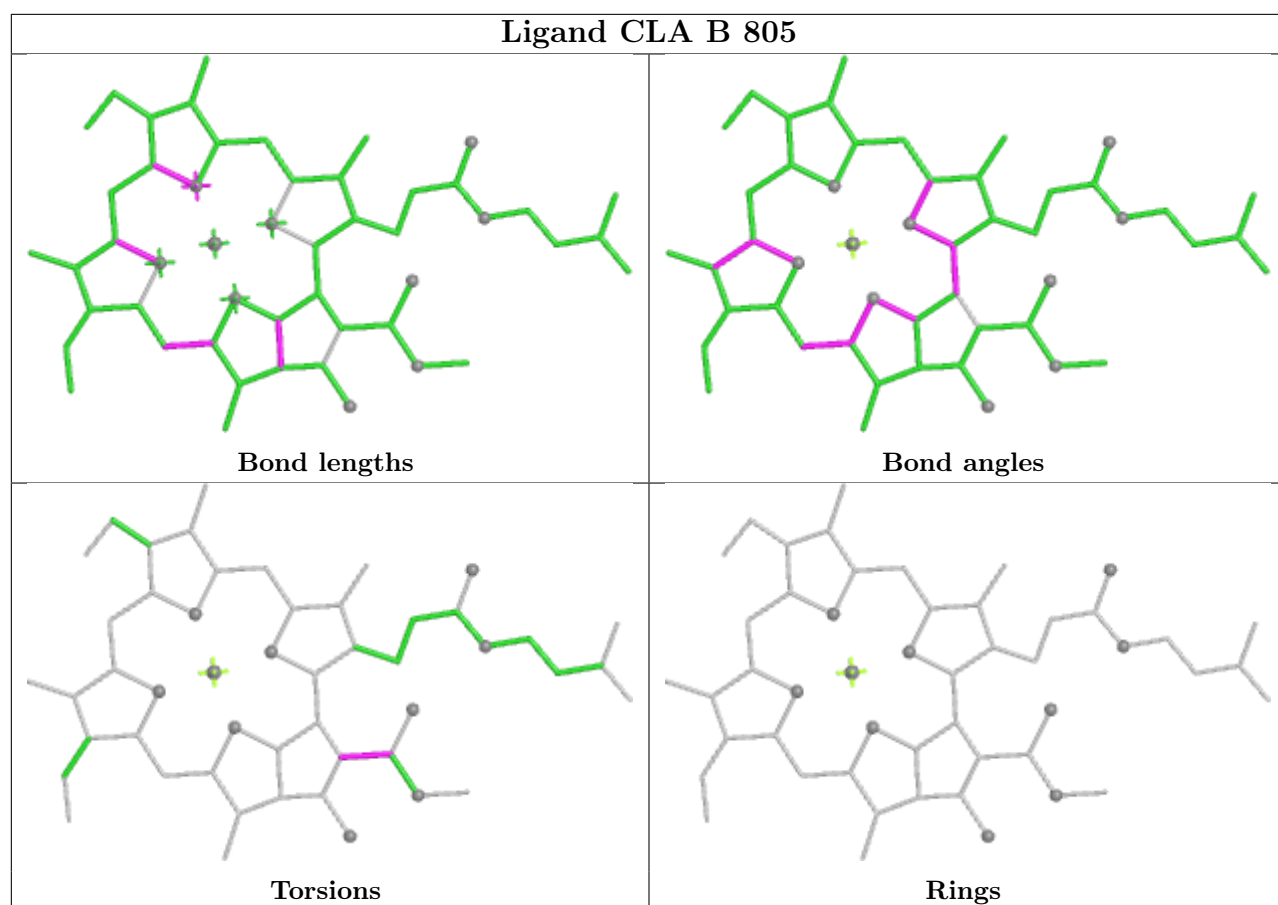
Bond angles

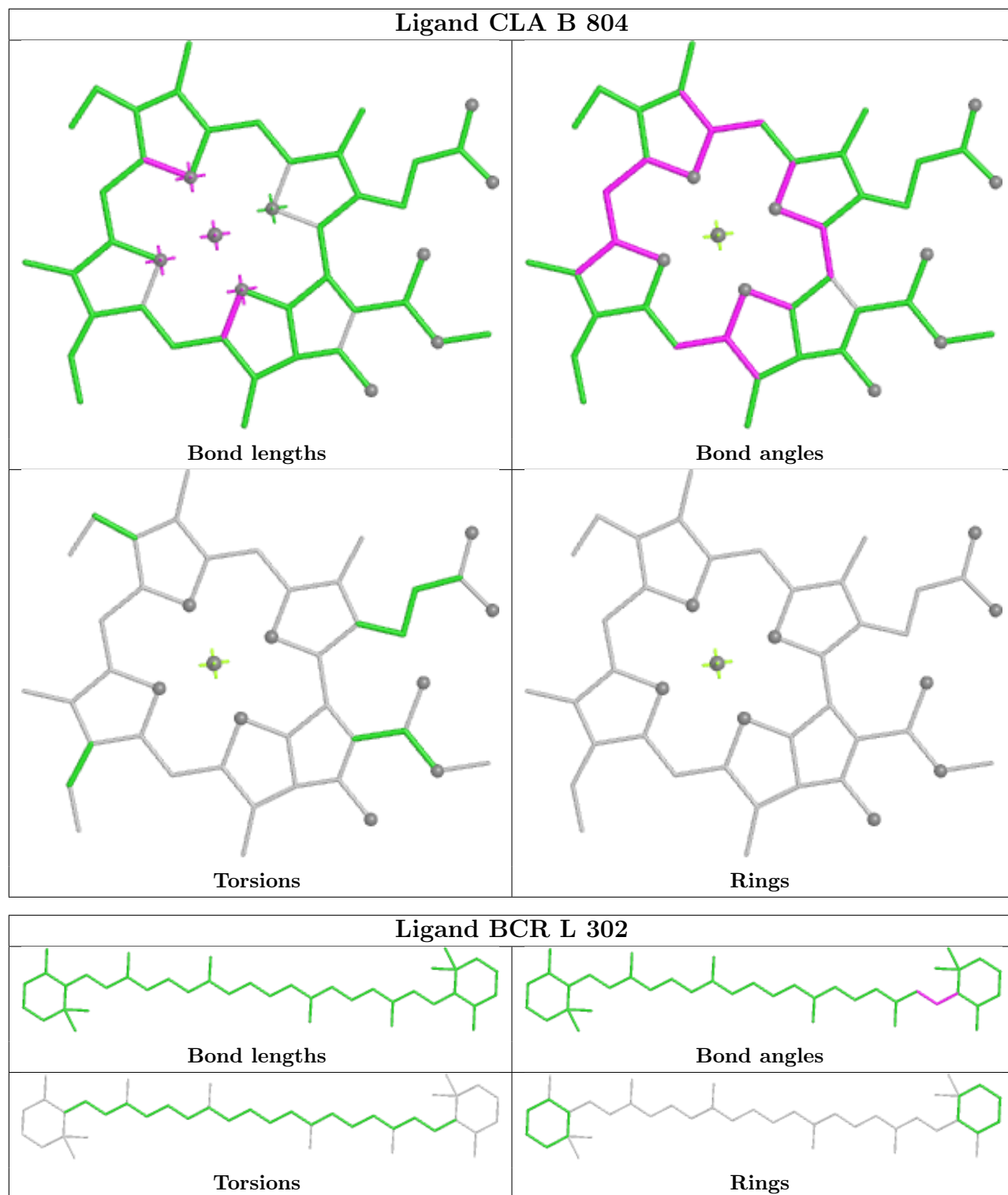


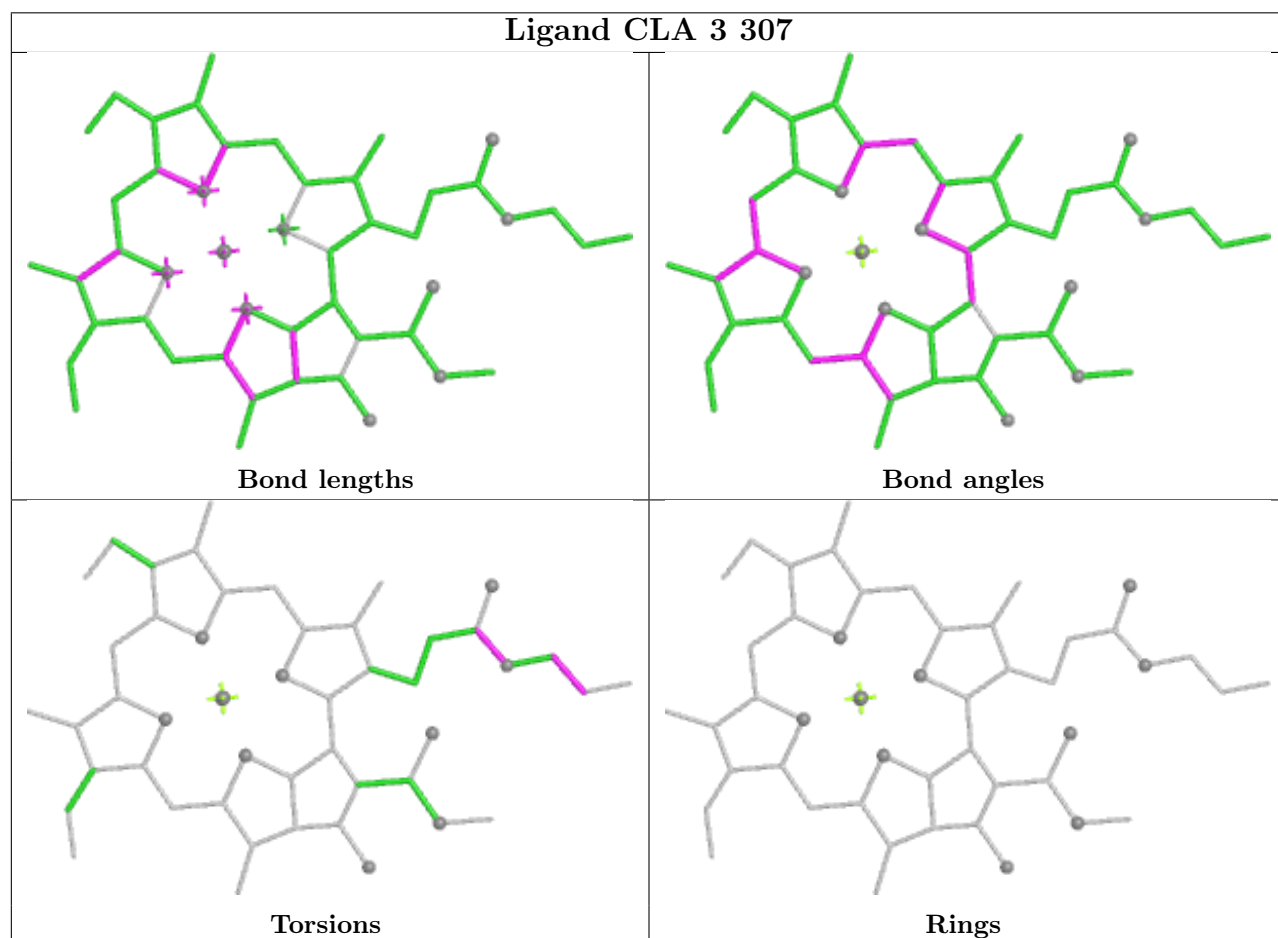
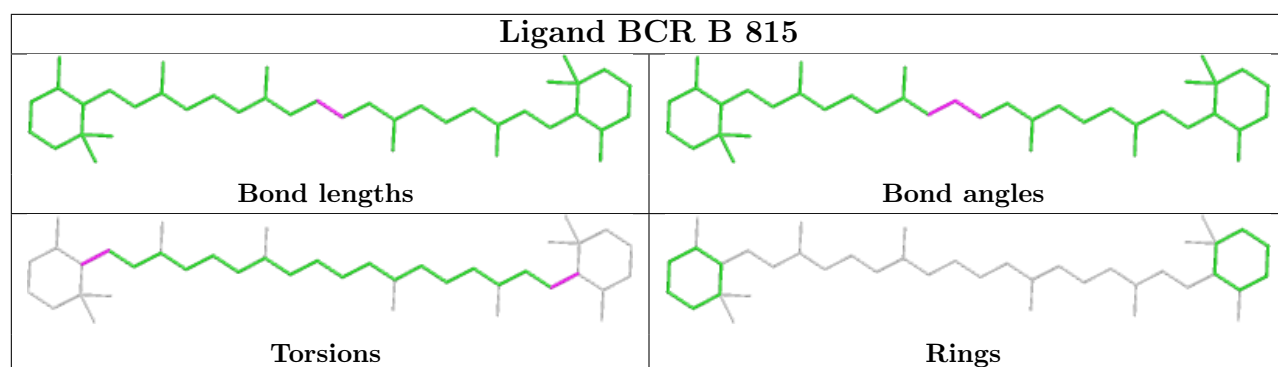
Torsions

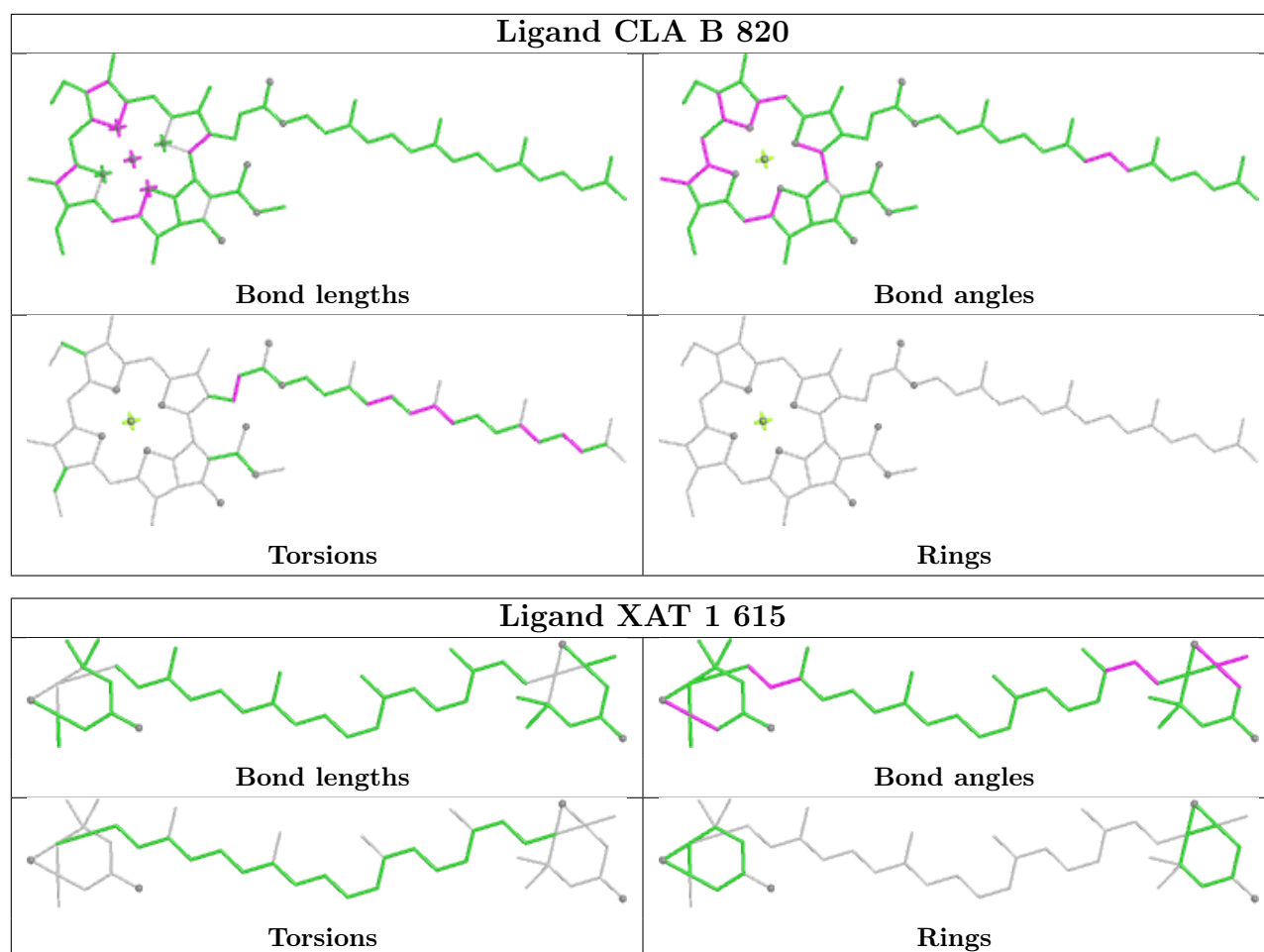


Rings

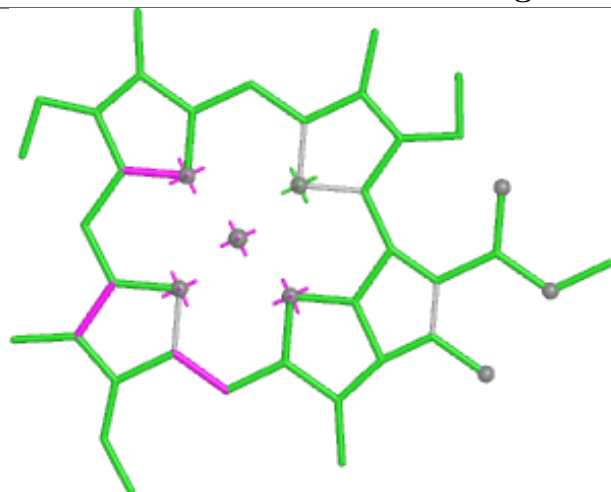




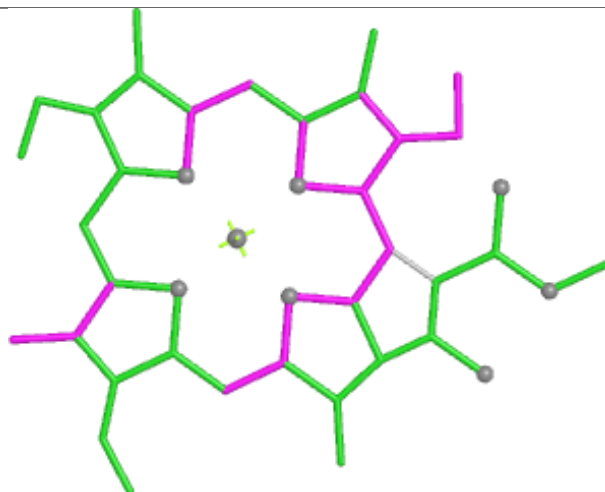




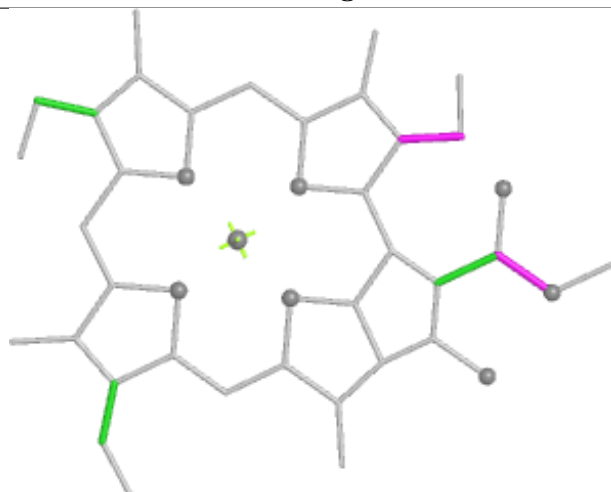
Ligand CLA B 821



Bond lengths



Bond angles

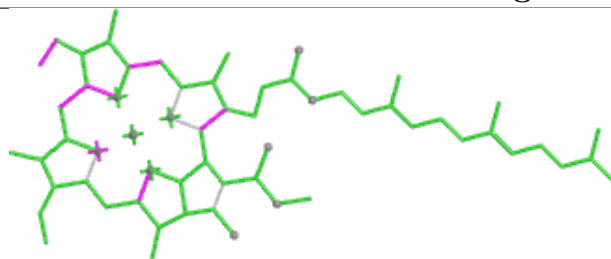


Torsions

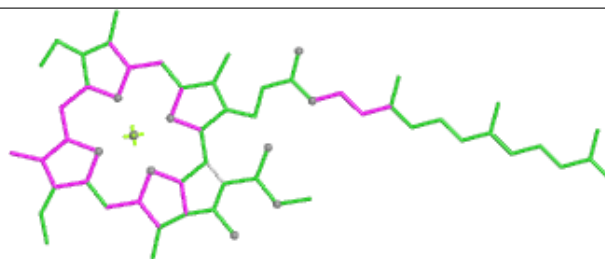


Rings

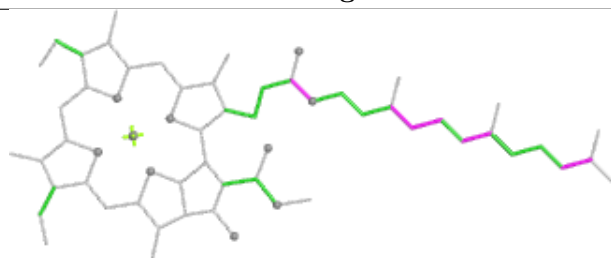
Ligand CLA A 842



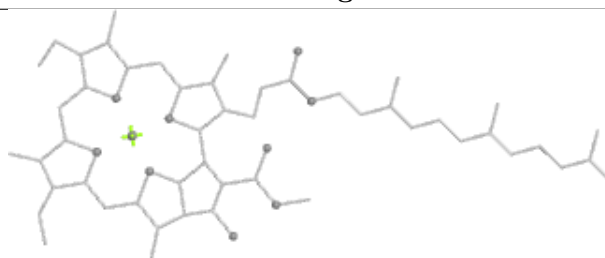
Bond lengths



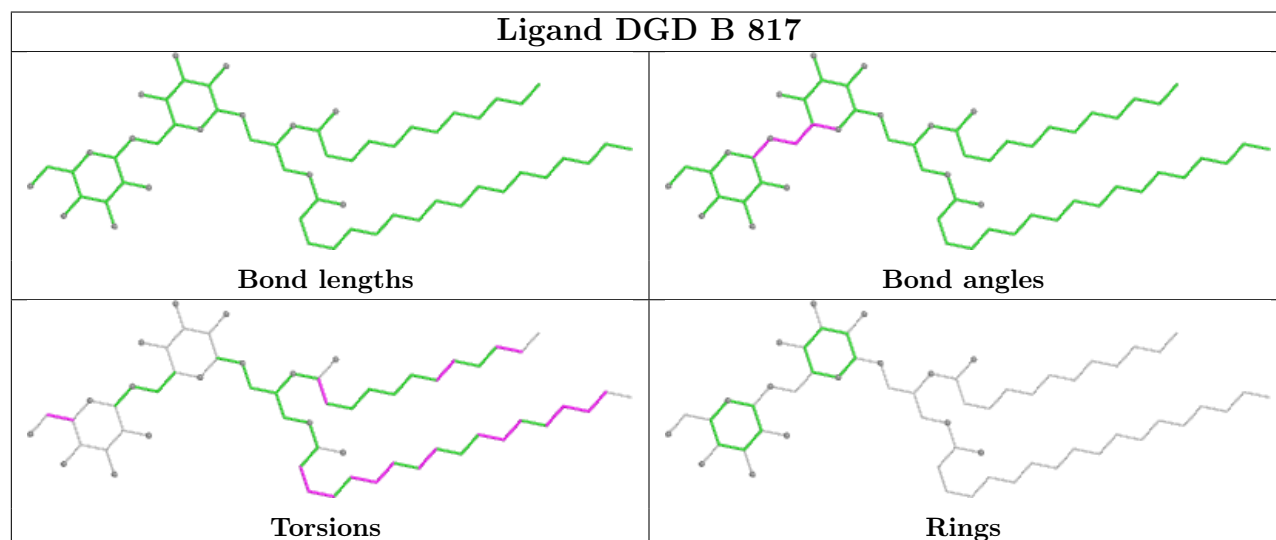
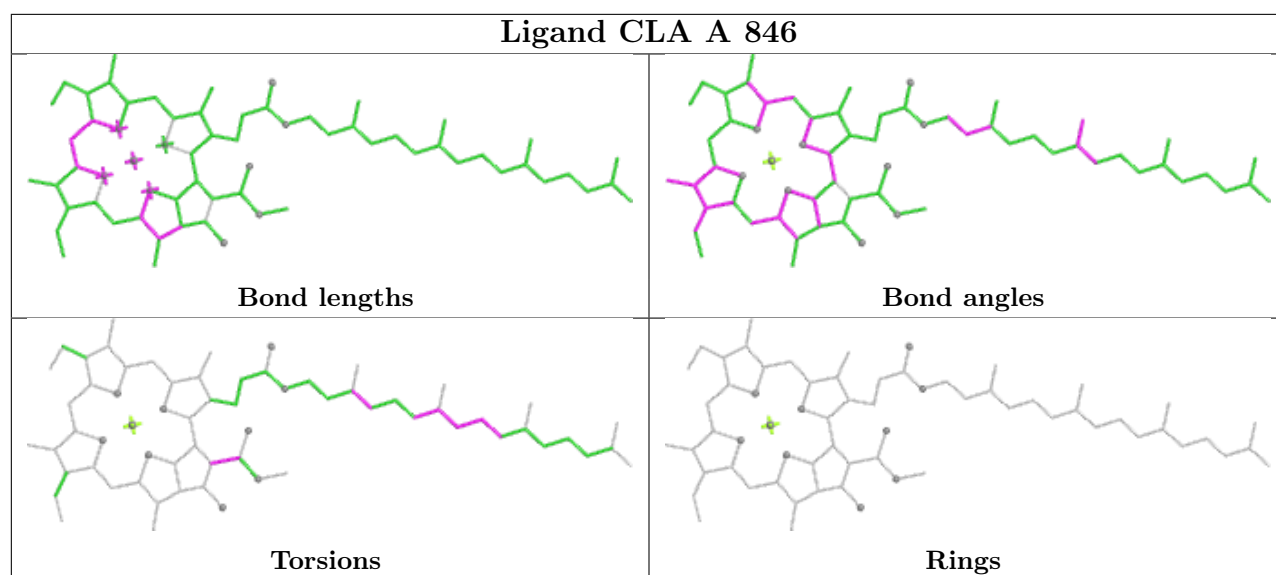
Bond angles



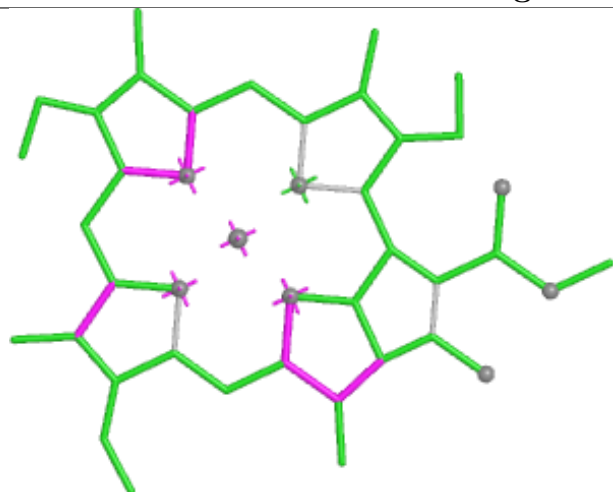
Torsions



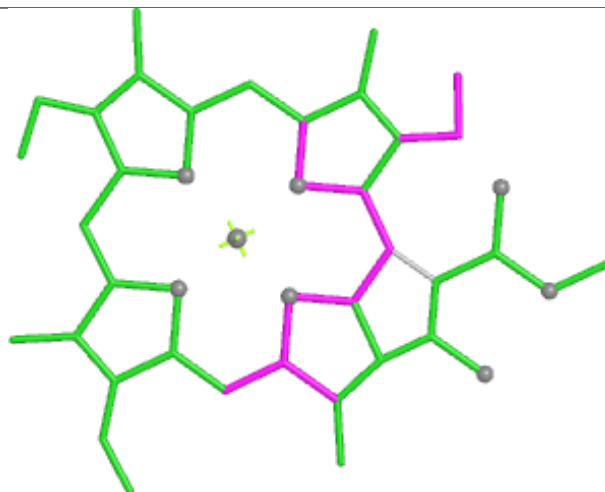
Rings



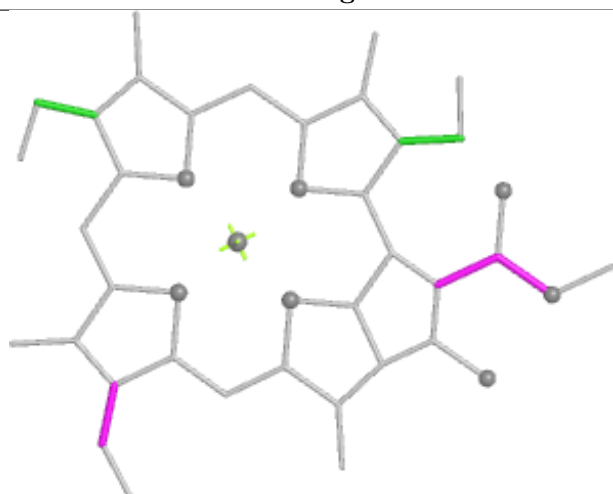
Ligand CLA A 806



Bond lengths



Bond angles

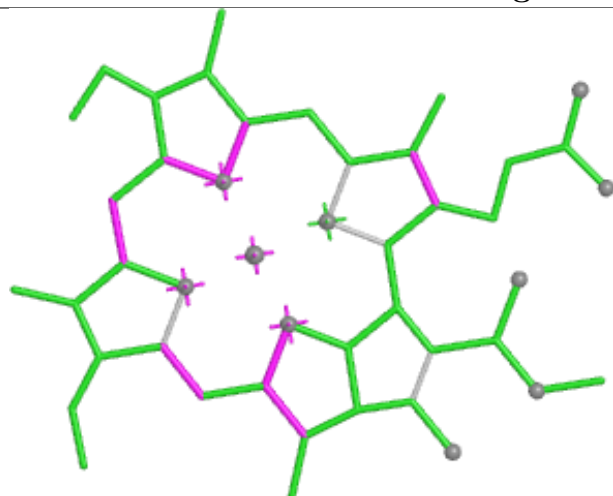


Torsions

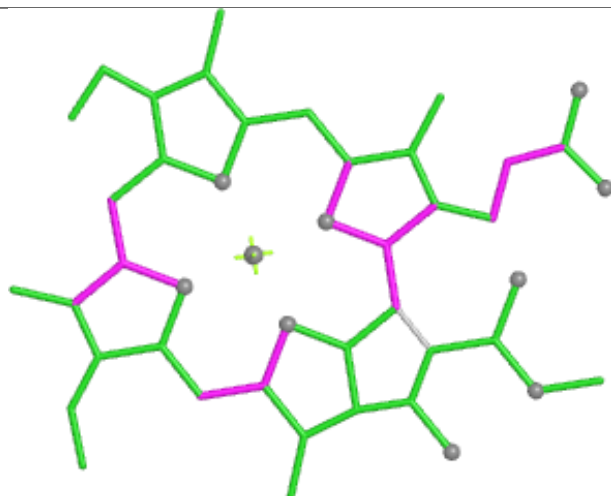


Rings

Ligand CLA K 202



Bond lengths



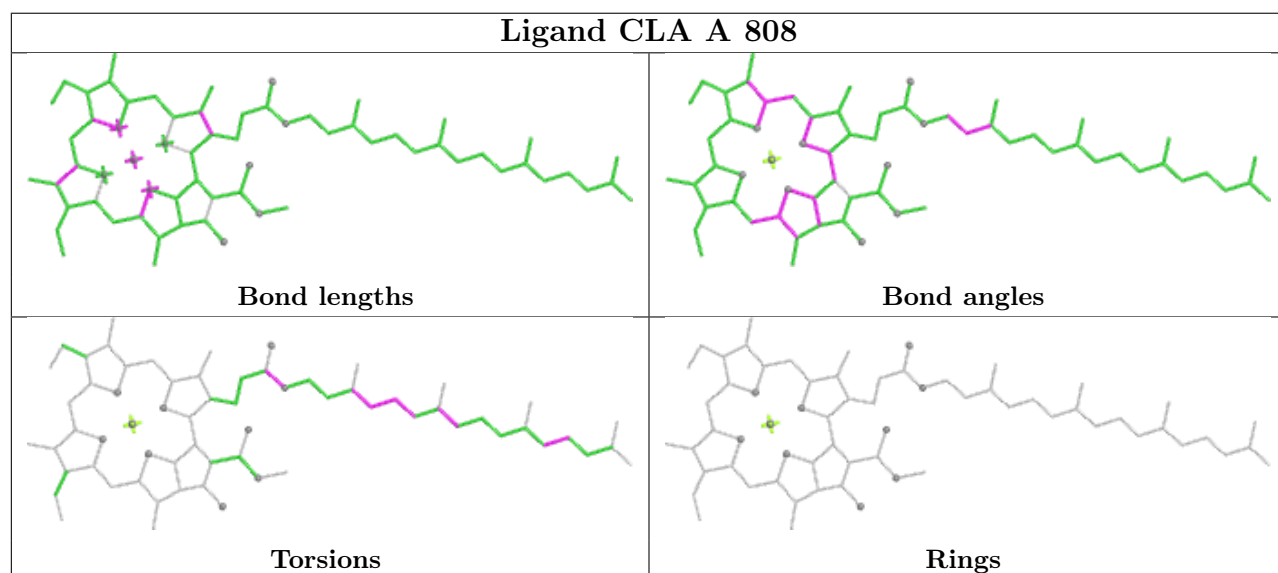
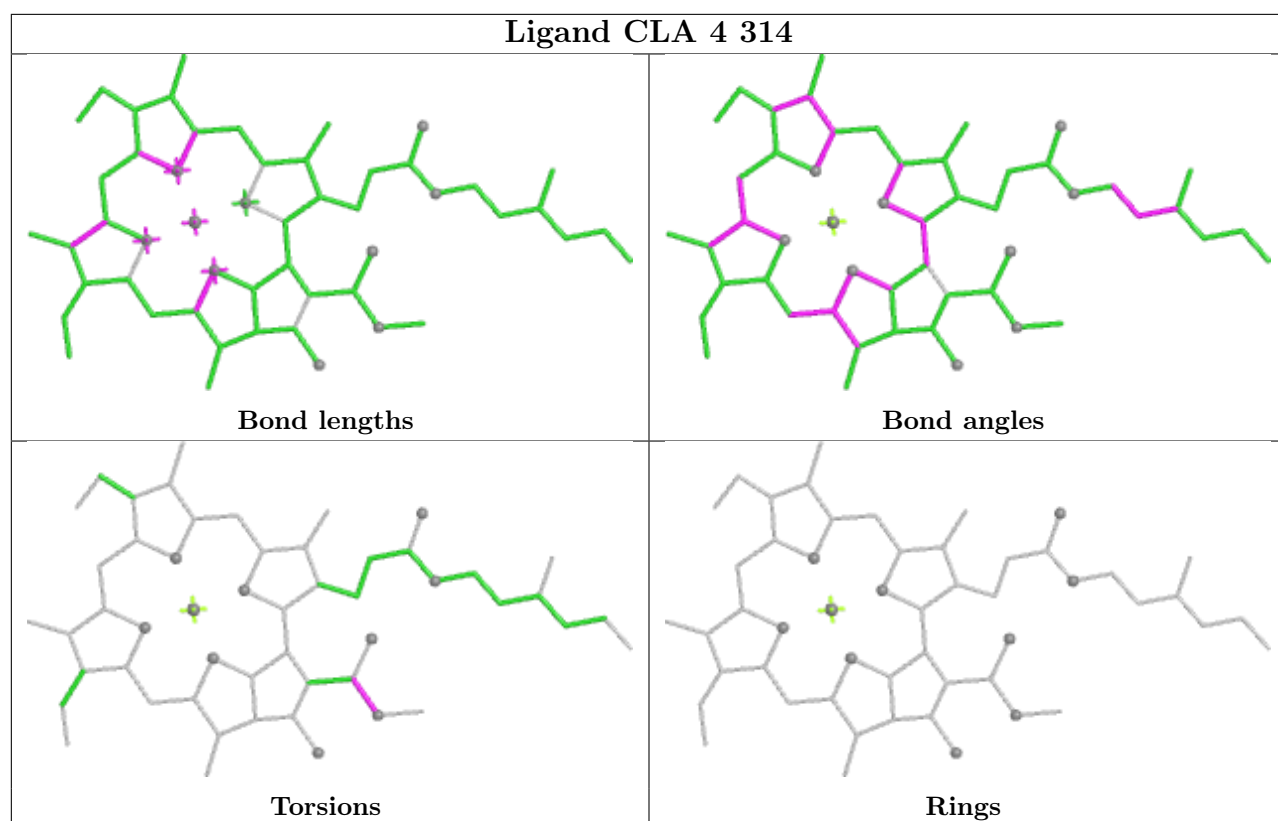
Bond angles

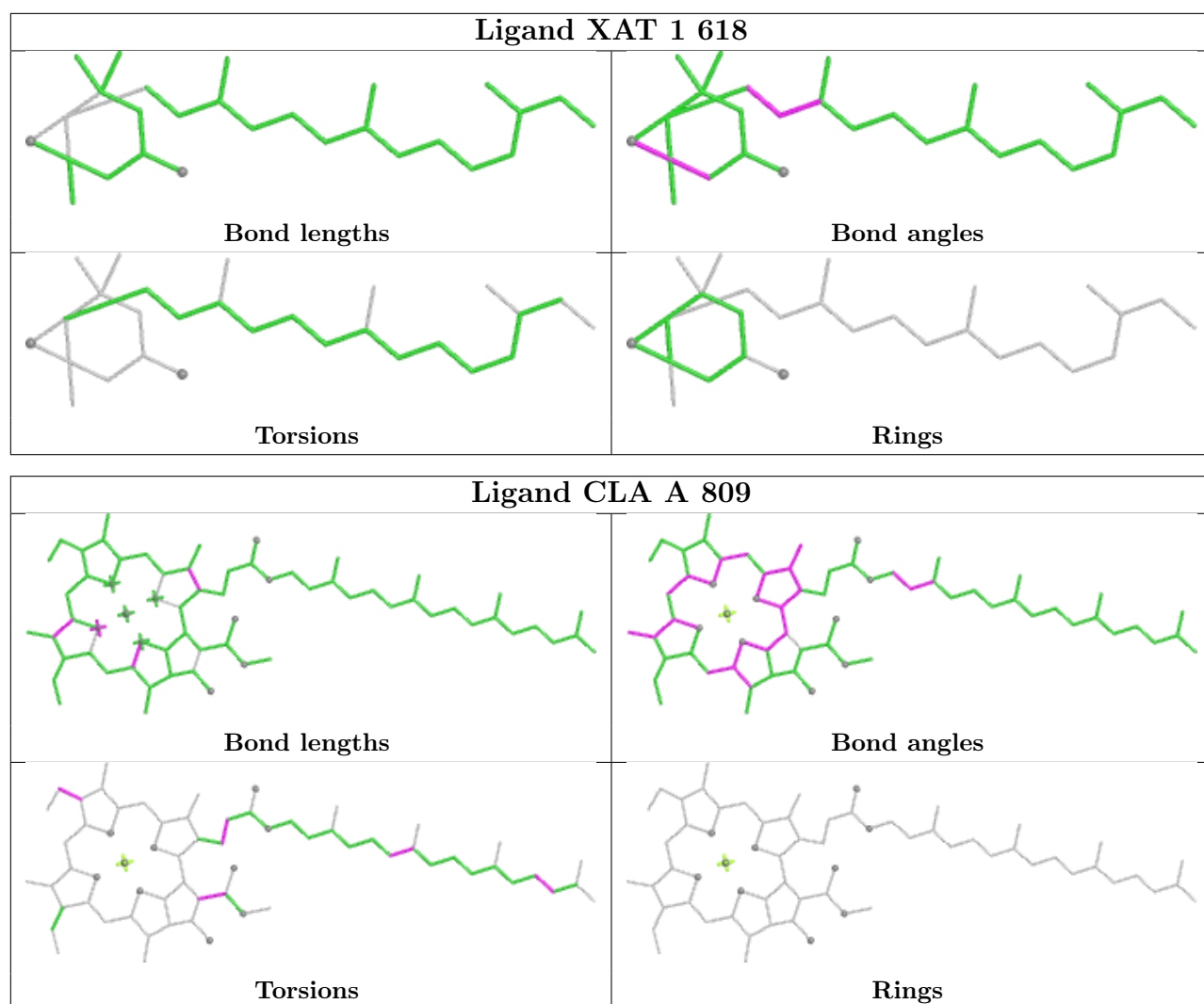


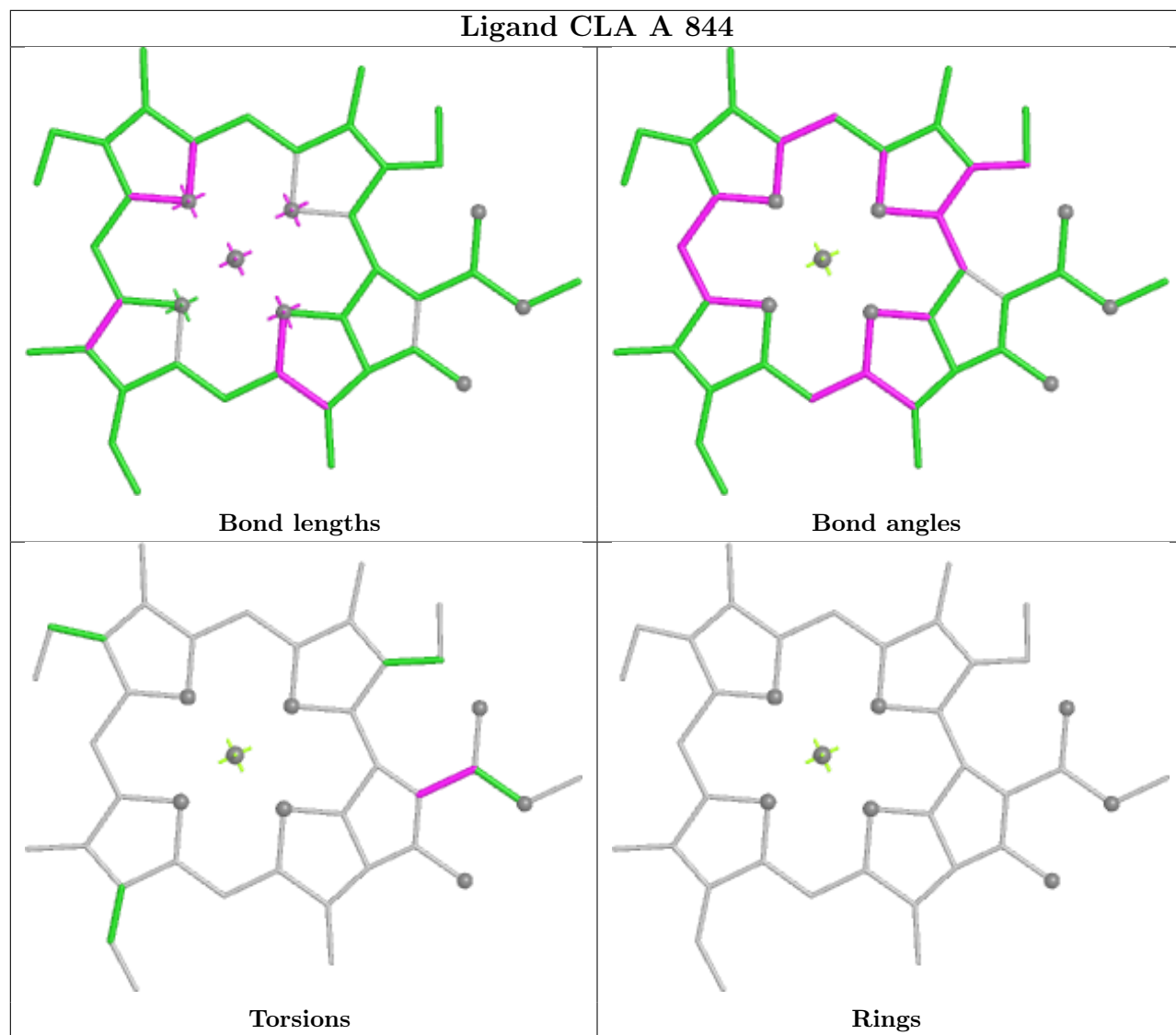
Torsions

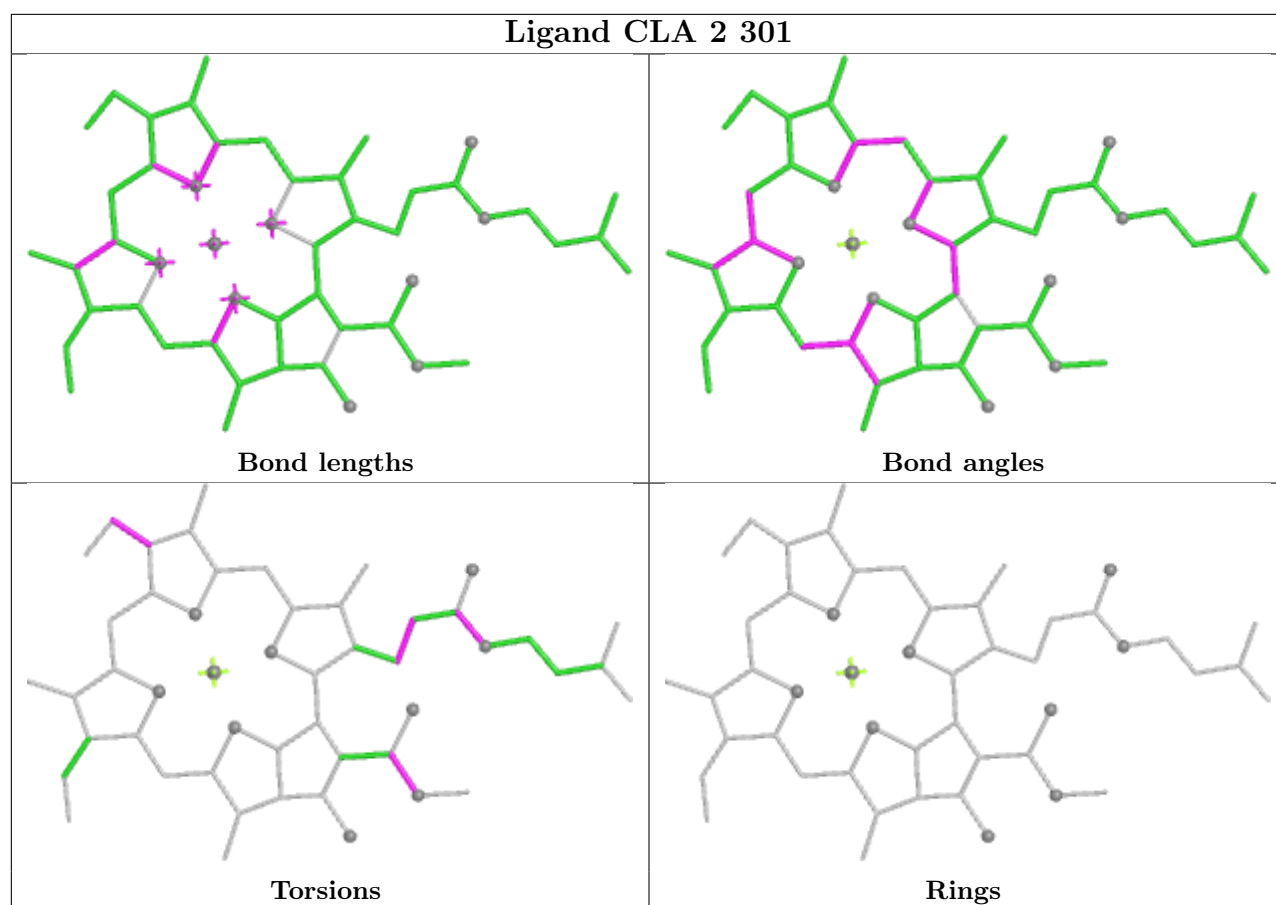


Rings









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

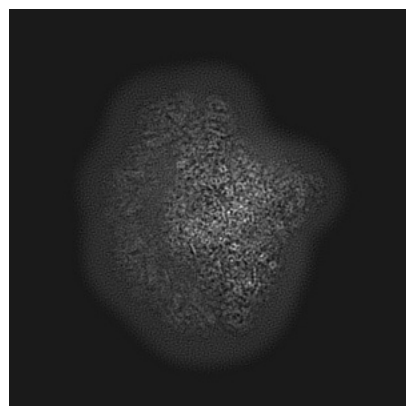
6 Map visualisation [i](#)

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

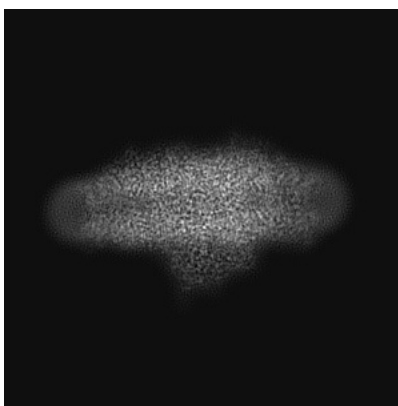
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

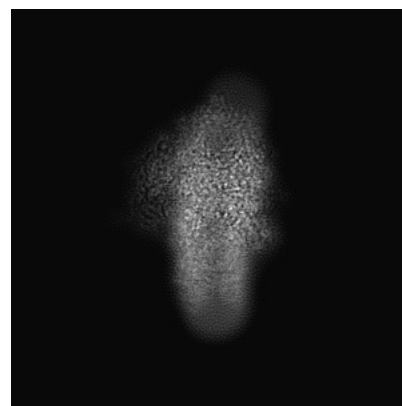
6.1.1 Primary map



X

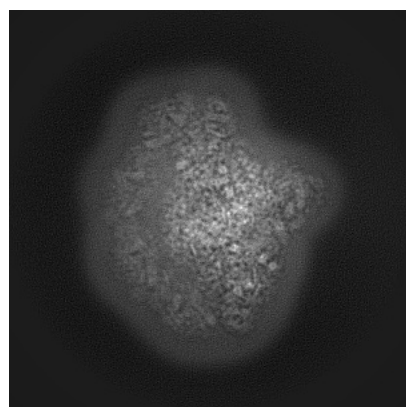


Y

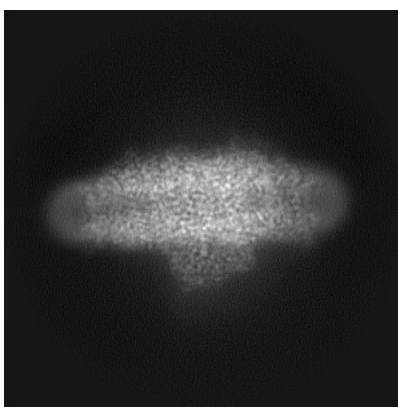


Z

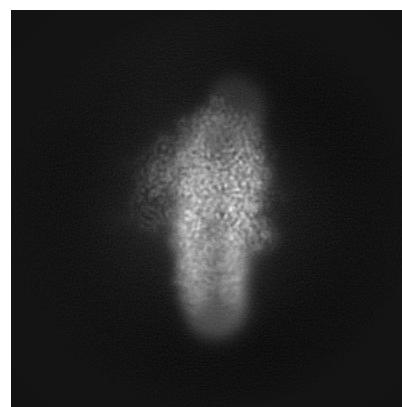
6.1.2 Raw map



X



Y

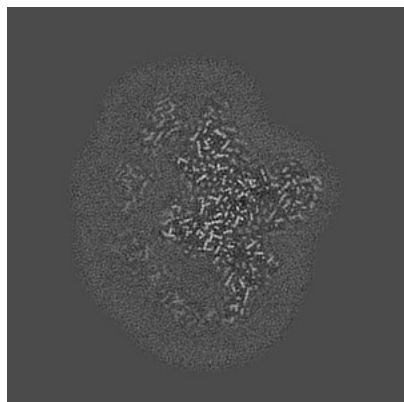


Z

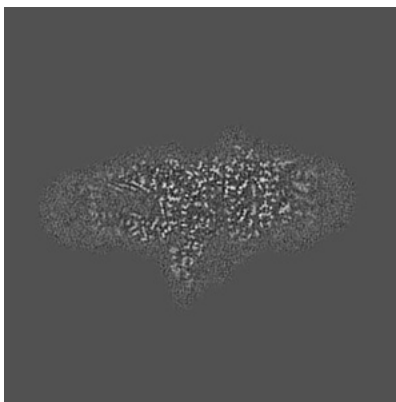
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

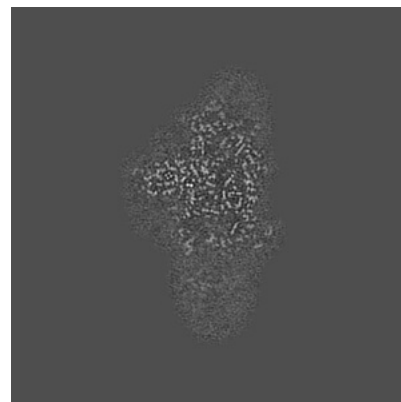
6.2.1 Primary map



X Index: 196

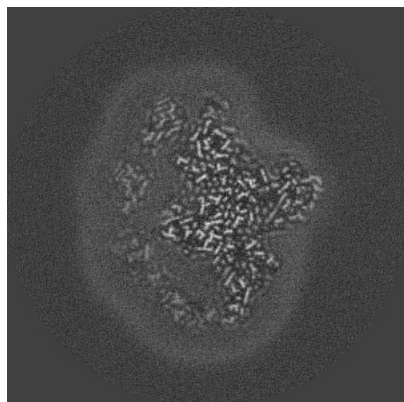


Y Index: 196

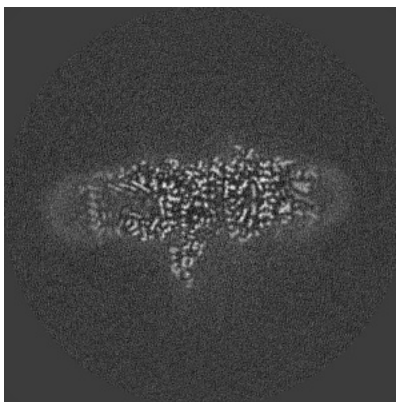


Z Index: 196

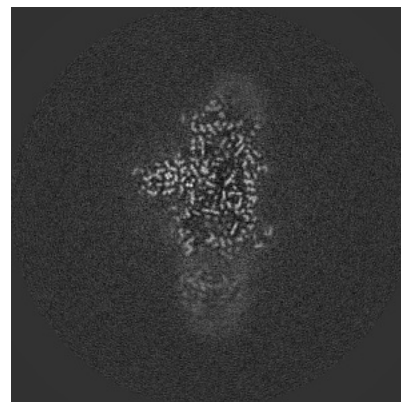
6.2.2 Raw map



X Index: 196



Y Index: 196

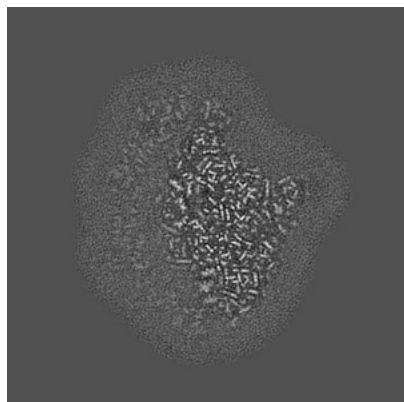


Z Index: 196

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

6.3 Largest variance slices [i](#)

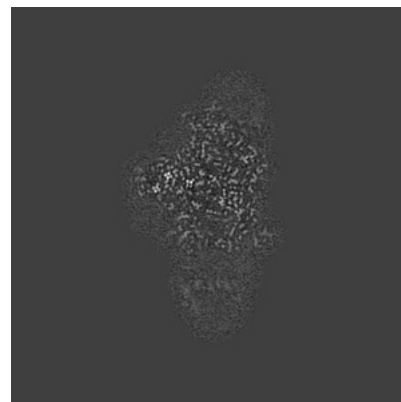
6.3.1 Primary map



X Index: 217

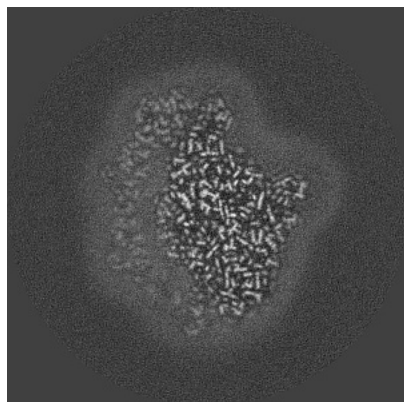


Y Index: 220

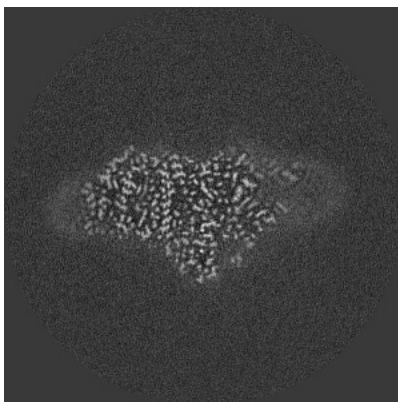


Z Index: 194

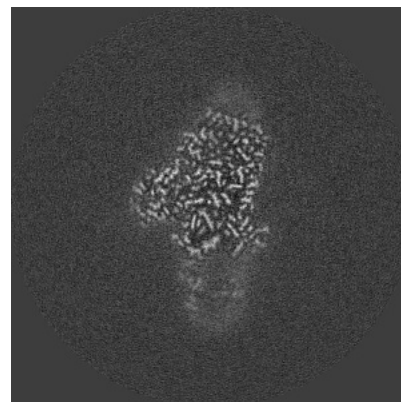
6.3.2 Raw map



X Index: 220



Y Index: 221

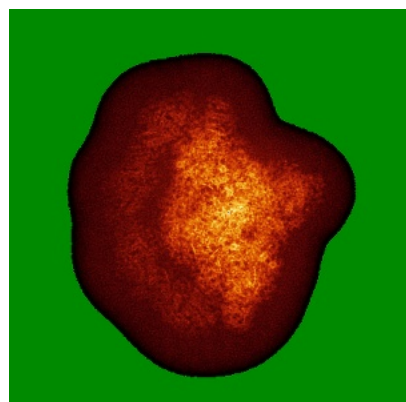


Z Index: 183

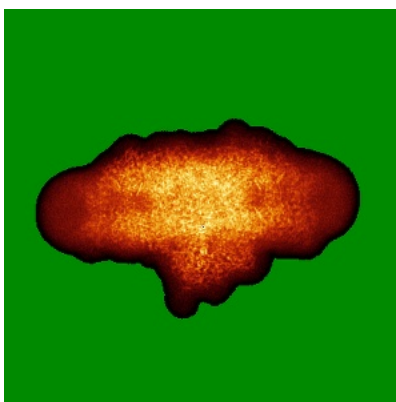
The images above show the largest variance slices of the map in three orthogonal directions.

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

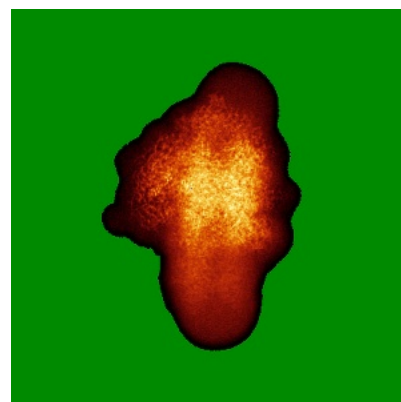
6.4.1 Primary map



X

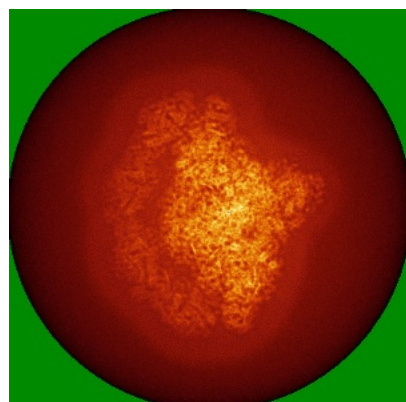


Y

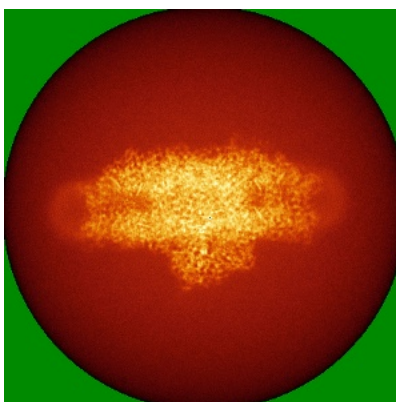


Z

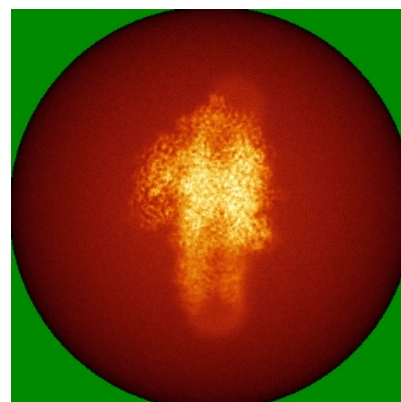
6.4.2 Raw map



X



Y

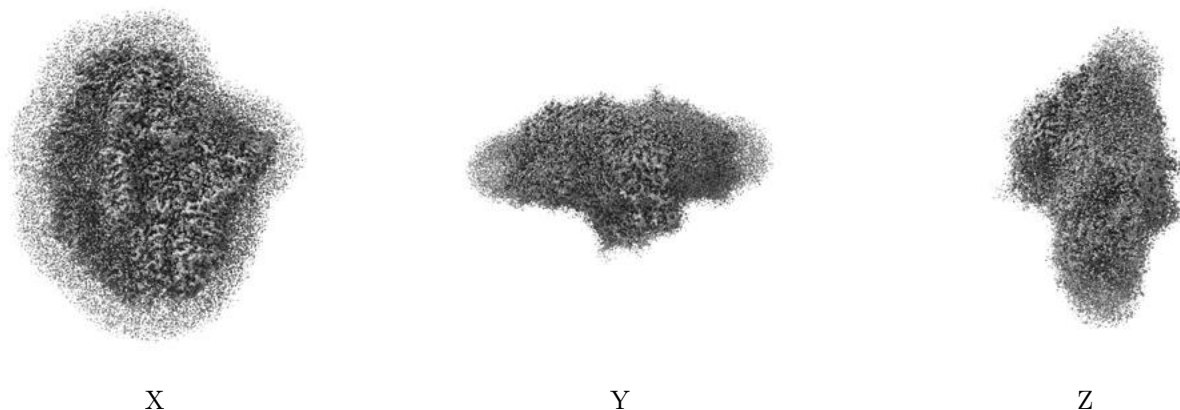


Z

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.

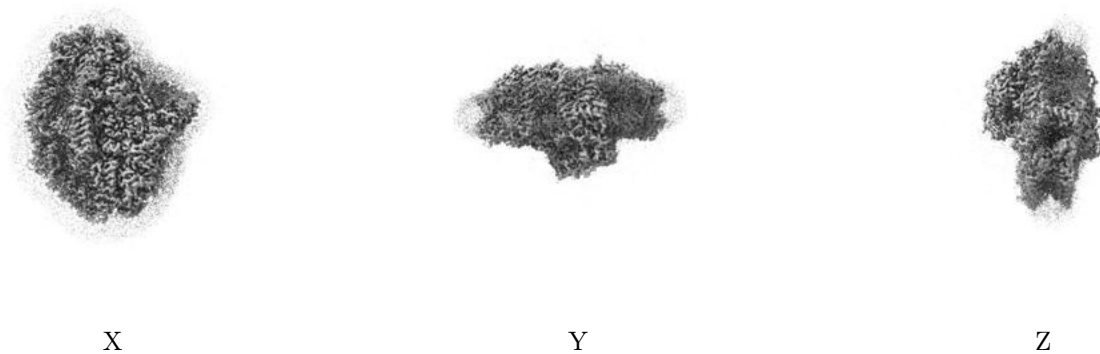
6.5 Orthogonal surface views [i](#)

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.

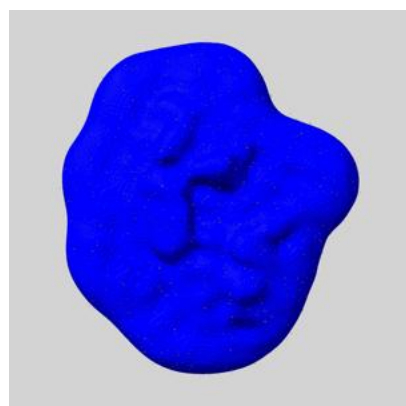
6.6 Mask visualisation [i](#)

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

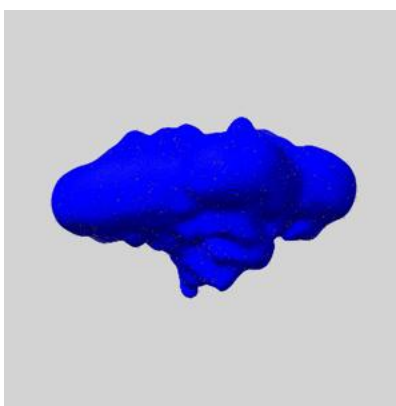
A mask typically either:

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

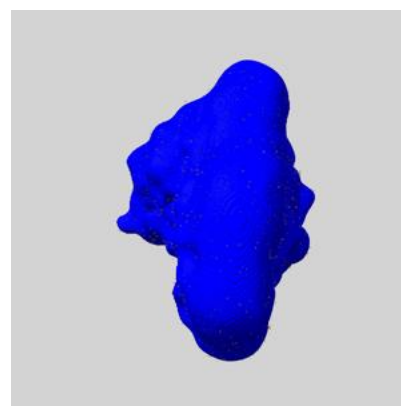
6.6.1 emd_66073_msk_1.map [i](#)



X



Y

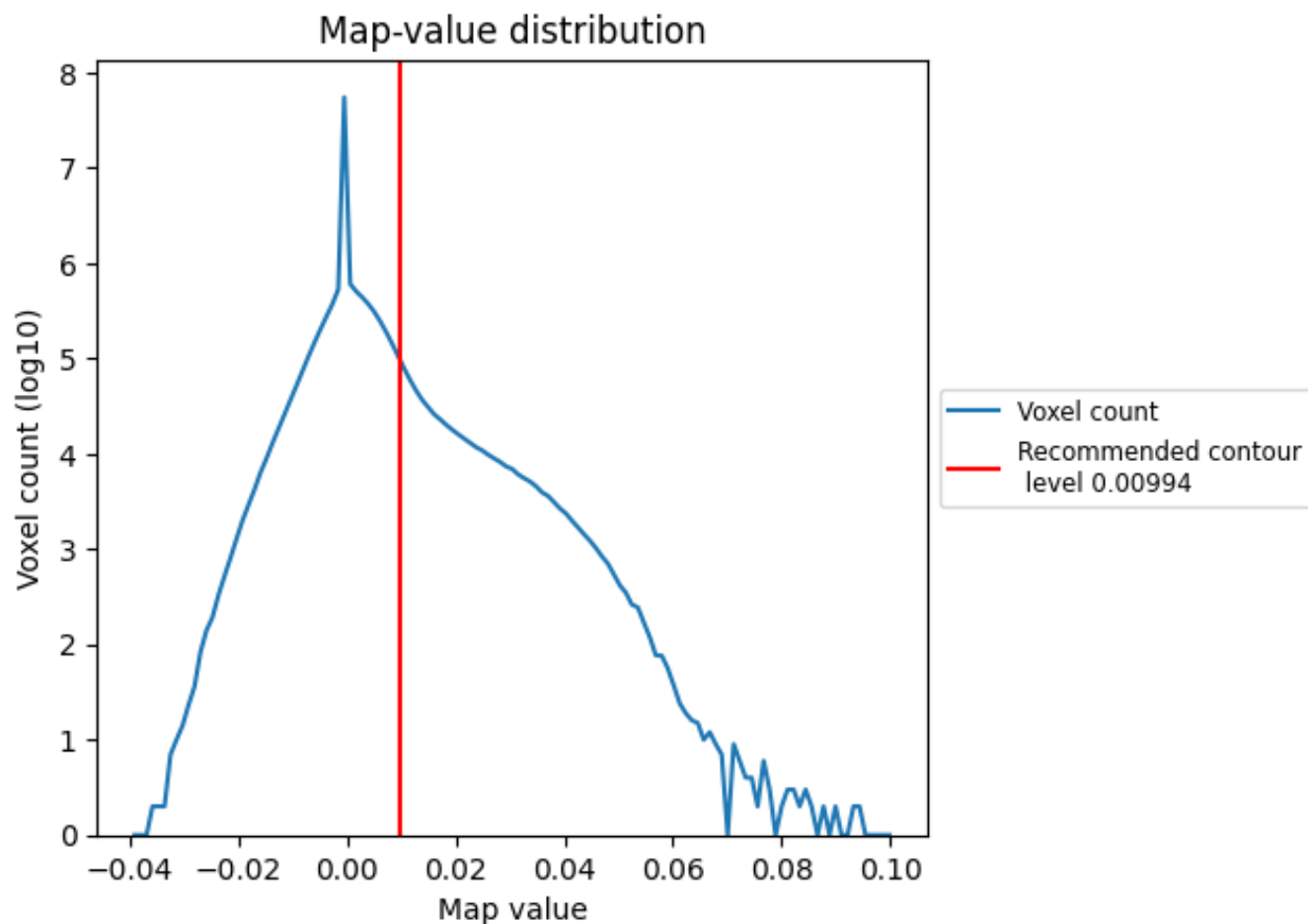


Z

7 Map analysis [i](#)

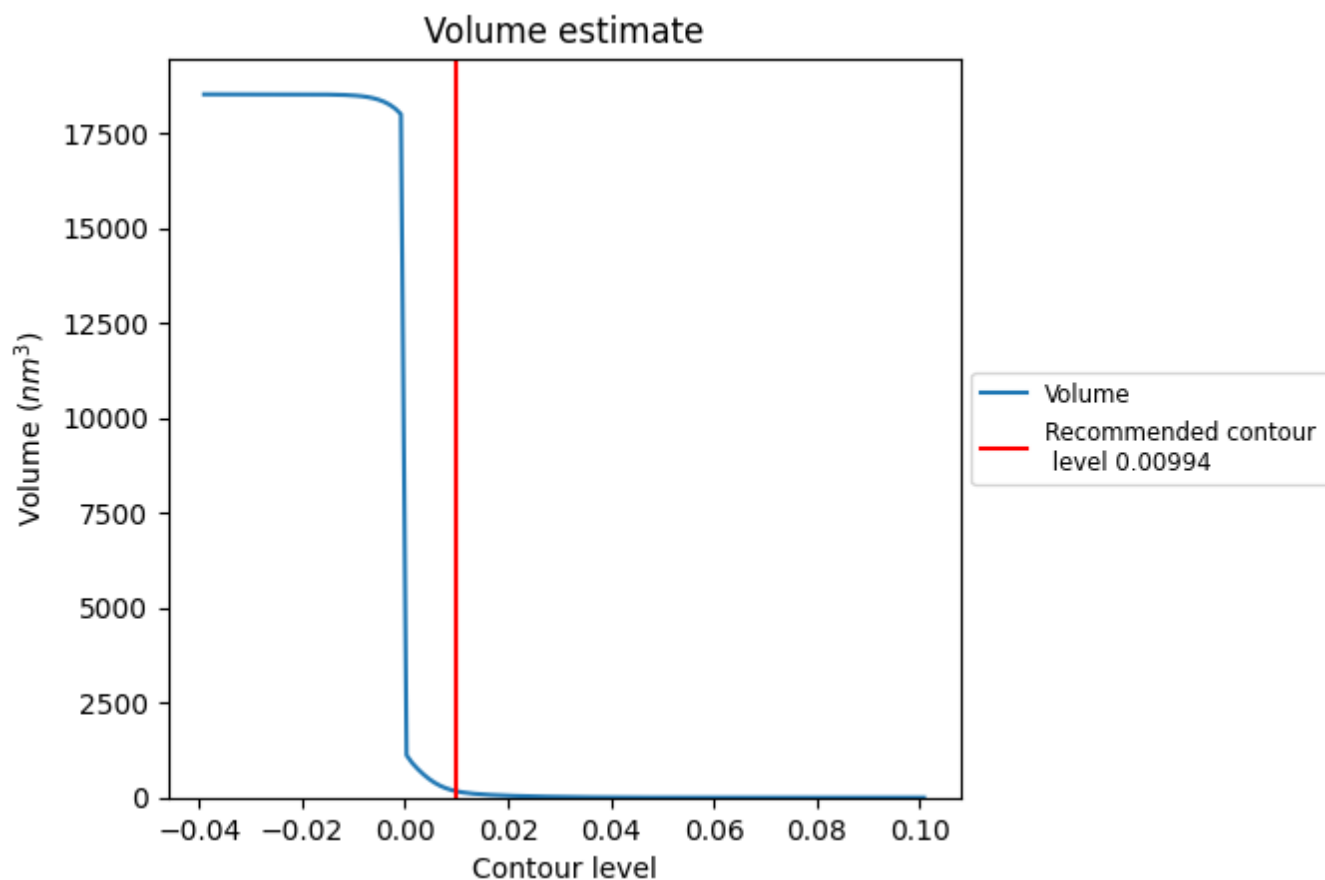
This section contains the results of statistical analysis of the map.

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.

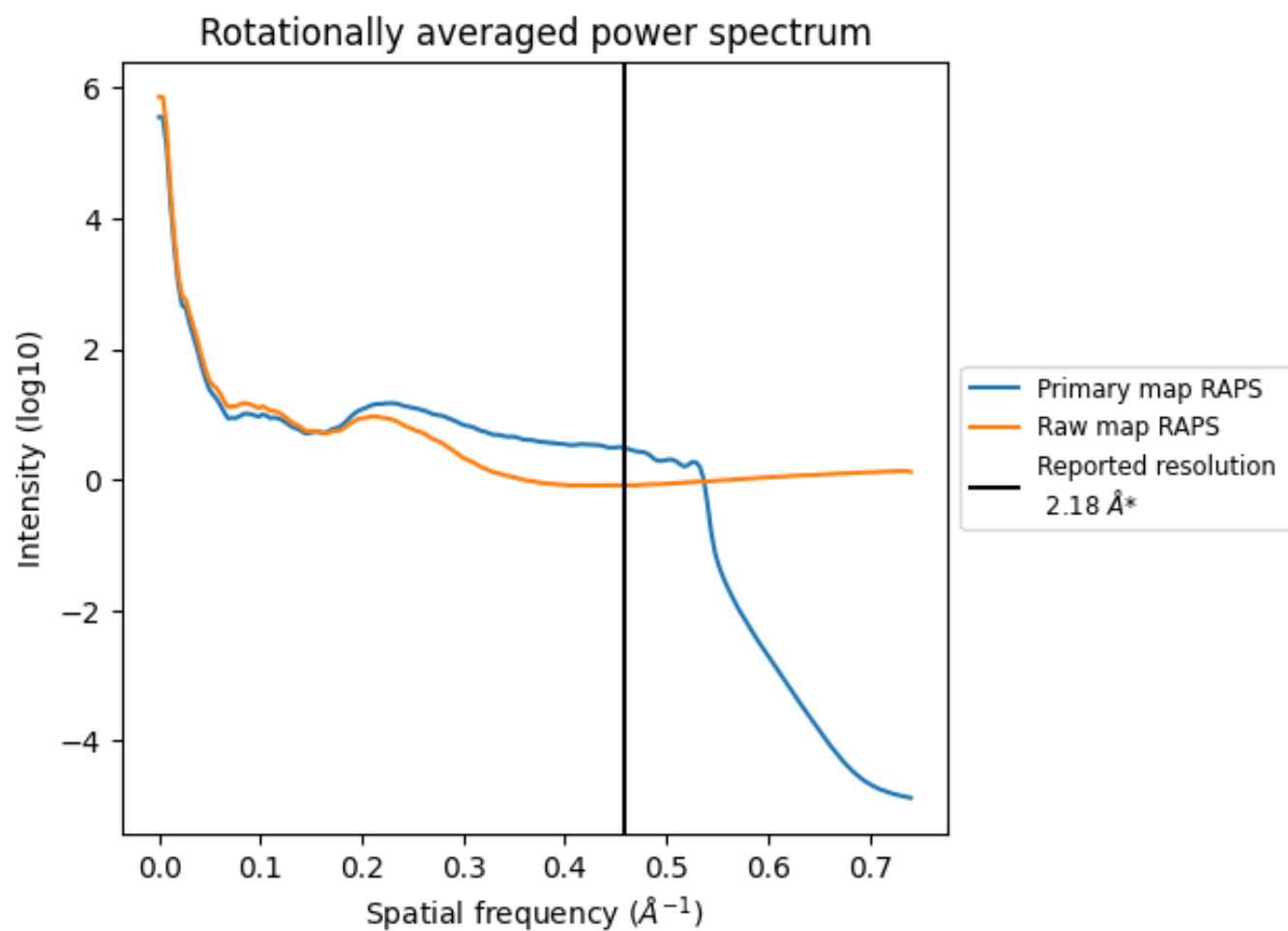
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 169 nm^3 ; 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 ⓘ

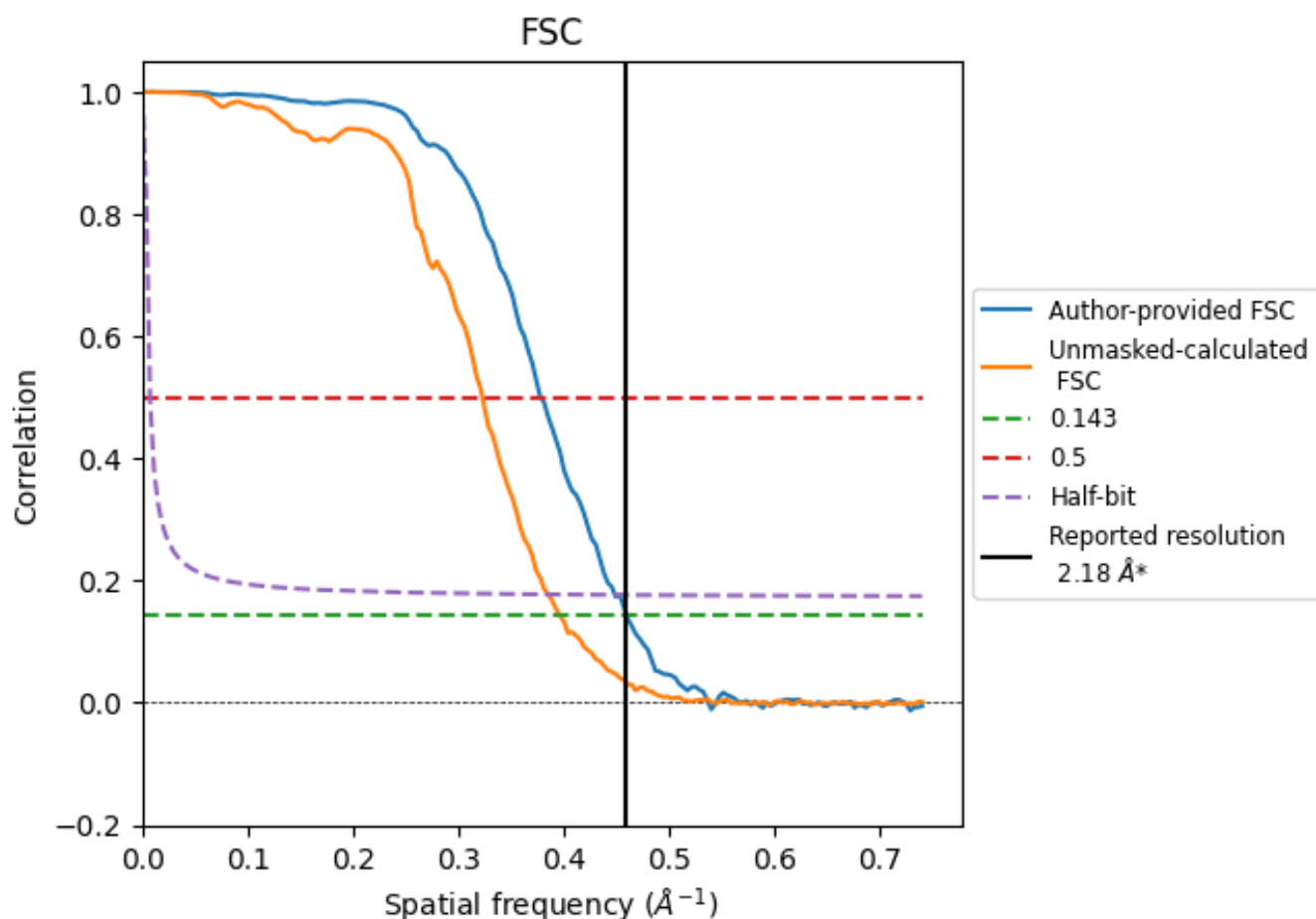


*Reported resolution corresponds to spatial frequency of 0.459 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.459 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

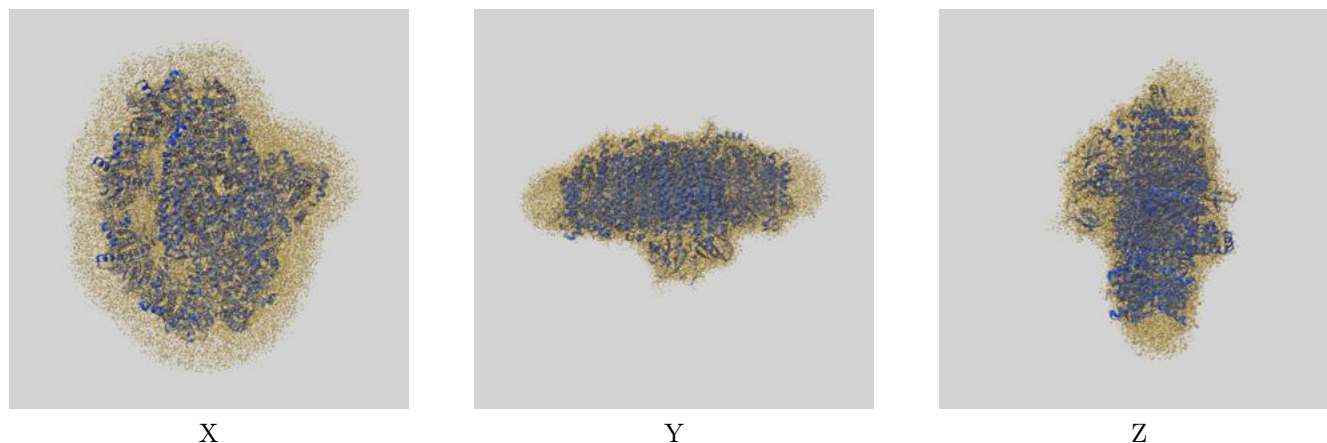
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.18	-	-
Author-provided FSC curve	2.17	2.64	2.23
Unmasked-calculated*	2.52	3.10	2.59

*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](#)

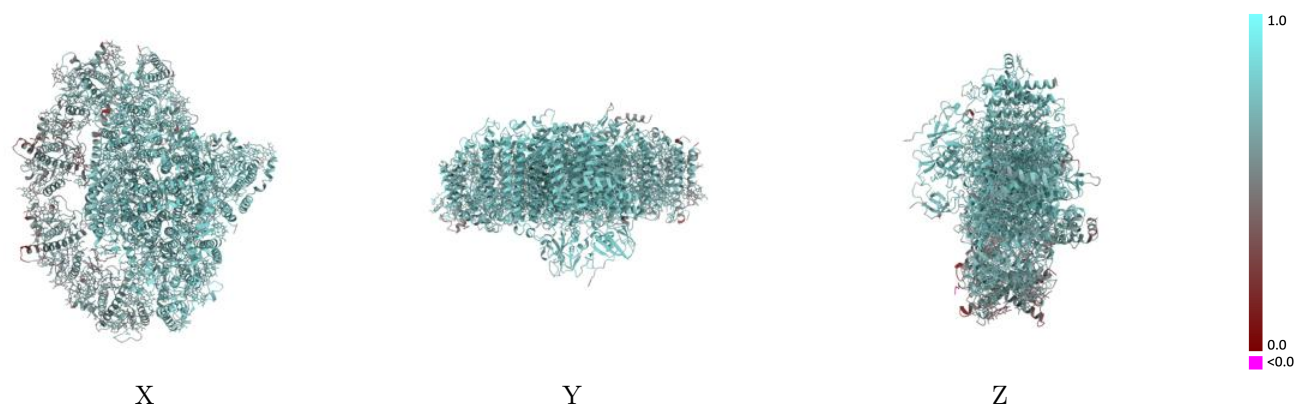
This section contains information regarding the fit between EMDB map EMD-66073 and PDB model 9WLS. Per-residue inclusion information can be found in section [3](#) on page [25](#).

9.1 Map-model overlay [i](#)



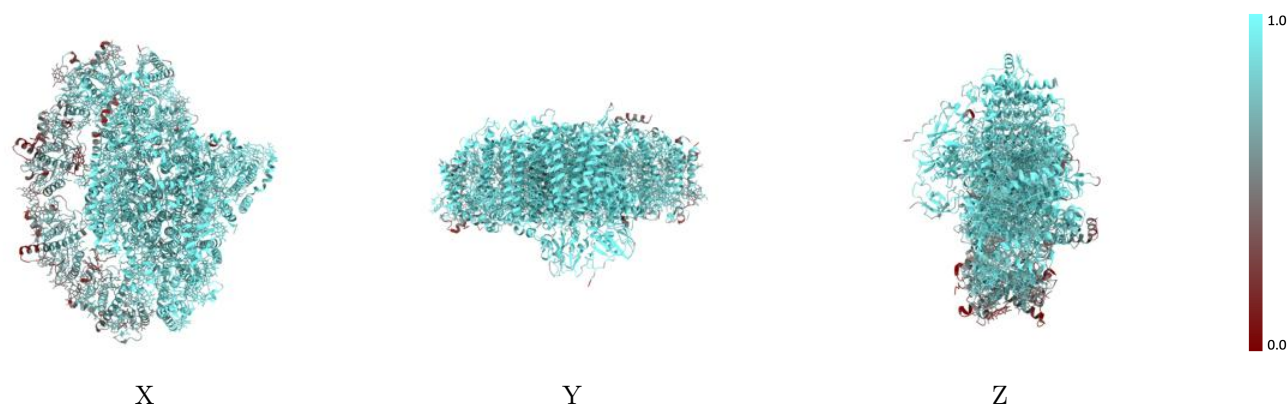
The images above show the 3D surface view of the map at the recommended contour level 0.00994 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



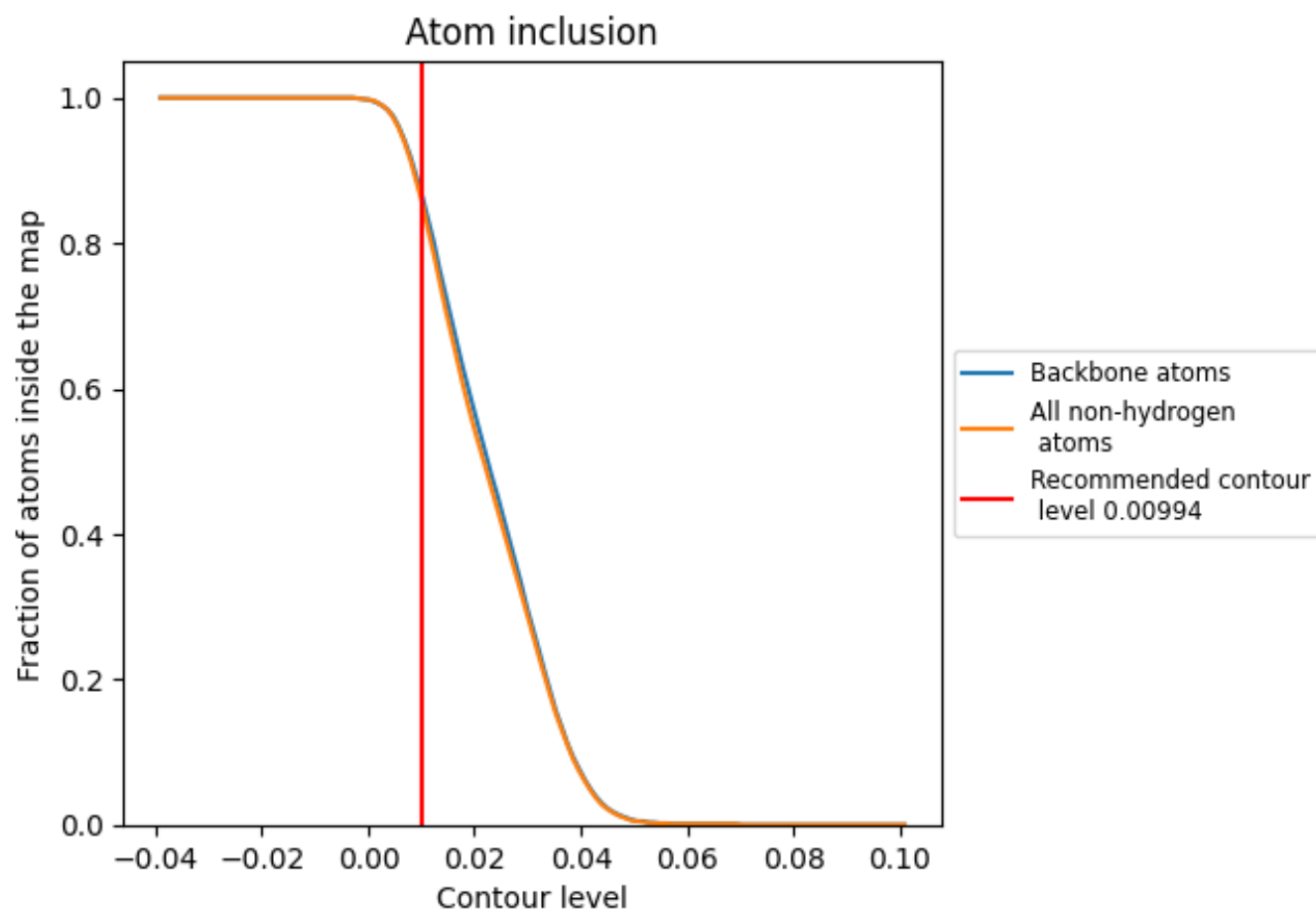
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.8620	0.7030
1	0.6550	0.5890
2	0.5750	0.5450
3	0.7660	0.6300
4	0.6500	0.5830
A	0.9600	0.7640
B	0.9750	0.7760
C	0.9890	0.7860
D	0.9340	0.7360
E	0.8860	0.7000
F	0.9000	0.7110
G	0.8870	0.6960
H	0.8800	0.6930
I	0.9390	0.7420
J	0.9080	0.7040
K	0.7440	0.6090
L	0.9300	0.7300
N	0.4520	0.5040

