



wwPDB EM Validation Summary Report ⓘ

Aug 4, 2026 – 04:42 PM JST

PDB ID : 9XJ1 / pdb_00009xj1
EMDB ID : EMD-66925
Title : In situ structure of the PSI-LHCI supercomplex from *Oryza sativa*
Authors : Li, J.; Elias, E.; Zhang, K.; Croce, R.; Zhu, J.
Deposited on : 2025-11-04
Resolution : 2.38 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

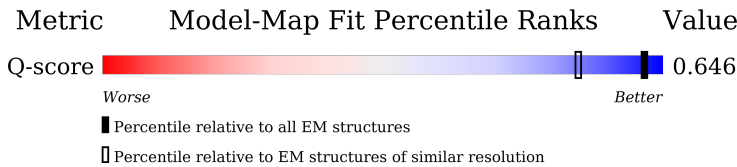
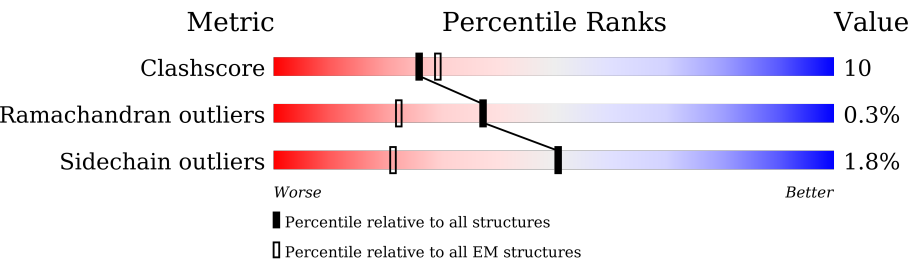
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.38 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	4811 (1.88 - 2.88)

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	200	78% 22%
2	2	208	85% 13% .
3	3	223	82% 18%
4	4	198	80% 18% .

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Mol	Chain	Length	Quality of chain
5	A	744	 87% 12%
6	B	734	 87% 13%
7	C	81	 94% 5% .
8	D	143	 87% 13%
9	E	68	 85% 10% .
10	F	158	 91% 9% .
11	G	97	 78% 22%
12	H	93	 88% 9% ..
13	I	30	 90% 7% .
14	J	44	 80% 20%
15	K	88	 92% 8%
16	L	163	 91% 8% .
17	N	84	 95% 5%
18	O	92	 97% .

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
19	CHL	2	318	X	-	-	-
20	CLA	1	303	X	-	-	-
20	CLA	1	304	X	-	-	-
20	CLA	1	307	X	-	-	-
20	CLA	1	318	X	-	-	-
20	CLA	1	319	X	-	-	-
20	CLA	2	304	X	-	-	-
20	CLA	2	305	X	-	-	-
20	CLA	2	307	X	-	-	-
20	CLA	2	319	X	-	-	-
20	CLA	3	307	X	-	-	-
20	CLA	3	308	X	-	-	-
20	CLA	3	309	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	3	311	X	-	-	-
20	CLA	3	315	X	-	-	-
20	CLA	3	317	X	-	-	-
20	CLA	4	302	X	-	-	-
20	CLA	4	310	X	-	-	-
20	CLA	4	312	X	-	-	-
20	CLA	4	316	X	-	-	-
20	CLA	A	801	X	-	-	-
20	CLA	A	802	X	-	-	-
20	CLA	A	806	X	-	-	-
20	CLA	A	807	X	-	-	-
20	CLA	A	808	X	-	-	-
20	CLA	A	809	X	-	-	-
20	CLA	A	811	X	-	-	-
20	CLA	A	812	X	-	-	-
20	CLA	A	825	X	-	-	-
20	CLA	A	826	X	-	-	-
20	CLA	A	827	X	-	-	-
20	CLA	A	829	X	-	-	-
20	CLA	A	830	X	-	-	-
20	CLA	A	832	X	-	-	-
20	CLA	A	833	X	-	-	-
20	CLA	A	834	X	-	-	-
20	CLA	A	835	X	-	-	-
20	CLA	A	837	X	-	-	-
20	CLA	A	841	X	-	-	-
20	CLA	A	842	X	-	-	-
20	CLA	A	843	X	-	-	-
20	CLA	A	845	X	-	-	-
20	CLA	A	847	X	-	-	-
20	CLA	A	848	X	-	-	-
20	CLA	A	849	X	-	-	-
20	CLA	A	850	X	-	-	-
20	CLA	A	851	X	-	-	-
20	CLA	A	852	X	-	-	-
20	CLA	A	853	X	-	-	-
20	CLA	A	854	X	-	-	-
20	CLA	A	855	X	-	-	-
20	CLA	A	856	X	-	-	-
20	CLA	B	801	X	-	-	-
20	CLA	B	803	X	-	-	-
20	CLA	B	804	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	806	X	-	-	-
20	CLA	B	807	X	-	-	-
20	CLA	B	808	X	-	-	-
20	CLA	B	809	X	-	-	-
20	CLA	B	811	X	-	-	-
20	CLA	B	812	X	-	-	-
20	CLA	B	813	X	-	-	-
20	CLA	B	814	X	-	-	-
20	CLA	B	815	X	-	-	-
20	CLA	B	816	X	-	-	-
20	CLA	B	817	X	-	-	-
20	CLA	B	818	X	-	-	-
20	CLA	B	819	X	-	-	-
20	CLA	B	820	X	-	-	-
20	CLA	B	821	X	-	-	-
20	CLA	B	822	X	-	-	-
20	CLA	B	823	X	-	-	-
20	CLA	B	824	X	-	-	-
20	CLA	B	827	X	-	-	-
20	CLA	B	829	X	-	-	-
20	CLA	B	830	X	-	-	-
20	CLA	B	831	X	-	-	-
20	CLA	B	833	X	-	-	-
20	CLA	B	844	X	-	-	-
20	CLA	B	845	X	-	-	-
20	CLA	B	847	X	-	-	-
20	CLA	B	848	X	-	-	-
20	CLA	B	850	X	-	-	-
20	CLA	B	851	X	-	-	-
20	CLA	B	852	X	-	-	-
20	CLA	B	853	X	-	-	-
20	CLA	F	304	X	-	-	-
20	CLA	H	201	X	-	-	-
20	CLA	K	204	X	-	-	-
20	CLA	N	202	X	-	-	-
20	CLA	O	206	X	-	-	-
20	CLA	O	207	X	-	-	-
22	XAT	1	311	-	-	X	-
28	CL0	A	824	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 39160 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, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	200	Total	C	N	O	S	0	0
			1560	1013	258	283	6		

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	207	Total	C	N	O	S	0	0
			1612	1055	263	289	5		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	223	Total	C	N	O	S	0	0
			1731	1138	277	310	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	198	Total	C	N	O	S	0	0
			1570	1024	257	284	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	742	Total	C	N	O	S	0	0
			5833	3819	991	1005	18		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	LEU	TRP	conflict	UNP P0C353

- 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
			5865	3848	995	1009	13		

- 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
			602	371	104	116	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	143	Total	C	N	O	S	0	0
			1128	726	197	202	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	65	Total	C	N	O	0	0
			518	329	92	97		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	158	Total	C	N	O	S	0	0
			1236	806	210	217	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	97	Total	C	N	O	S	0	0
			760	492	128	139	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	H	93	Total	C	N	O	0	0
			709	465	112	132		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	30	Total	C	N	O	S	0	0
			232	160	35	36	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	44	Total	C	N	O	S	0	0
			353	241	53	58	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	88	Total	C	N	O	S	0	0
			620	392	107	117	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	163	Total	C	N	O	S	0	0
			1223	809	194	218	2		

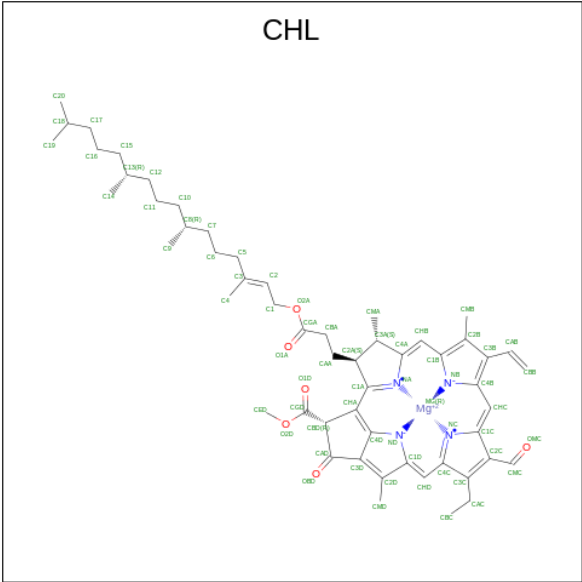
- Molecule 17 is a protein called Photosystem I reaction center subunit N, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	84	Total	C	N	O	S	0	0
			685	439	112	130	4		

- Molecule 18 is a protein called Os04g0414700 protein.

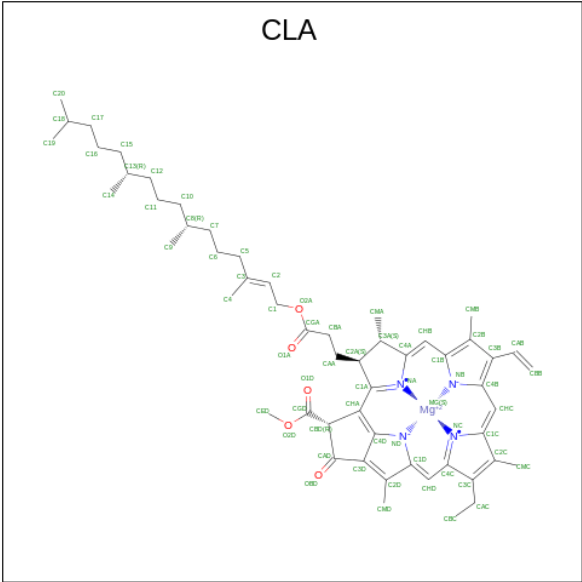
Mol	Chain	Residues	Atoms				AltConf	Trace
18	O	92	Total	C	N	O	0	0
			733	491	118	124		

- Molecule 19 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
19	1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
19	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
19	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
19	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
19	2	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
19	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
19	3	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
19	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
19	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
19	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
19	4	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			59	51	1	4	3	
20	3	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
20	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	4	1	Total 54	C 44	Mg 1	N 4	O 5	0
20	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 63	C 53	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
20	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	A	1	Total 64	C 54	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	A	1	Total 59	C 49	Mg 1	N 4	O 5	0
20	A	1	Total 61	C 51	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 58	C 48	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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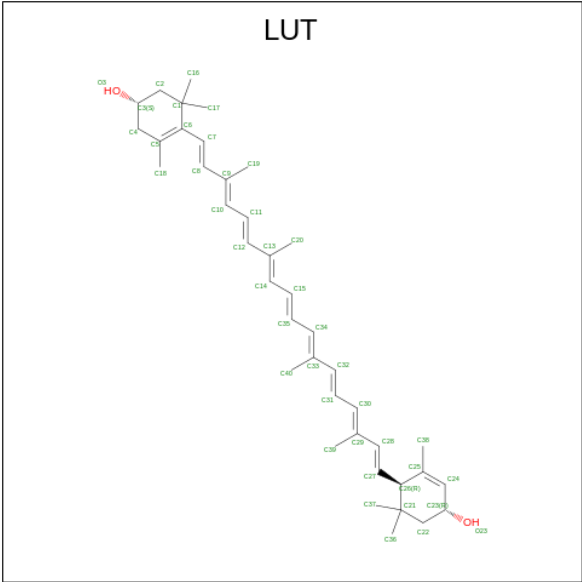
Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	H	1	Total 59	C 49	Mg 1	N 4	O 5	0

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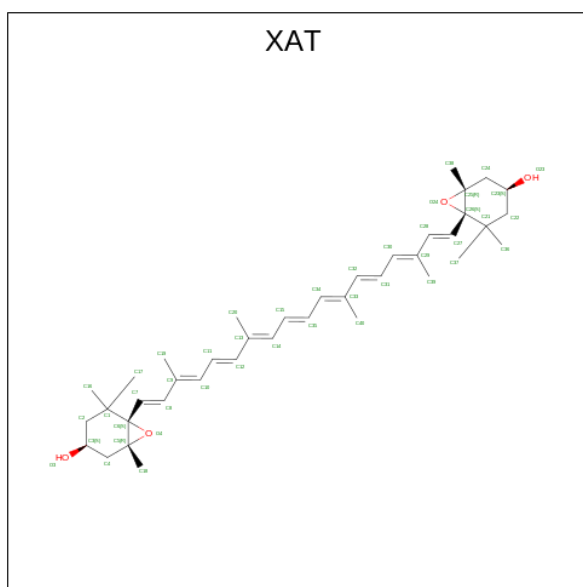
Mol	Chain	Residues	Atoms					AltConf
20	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
20	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	N	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	O	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
20	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 21 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



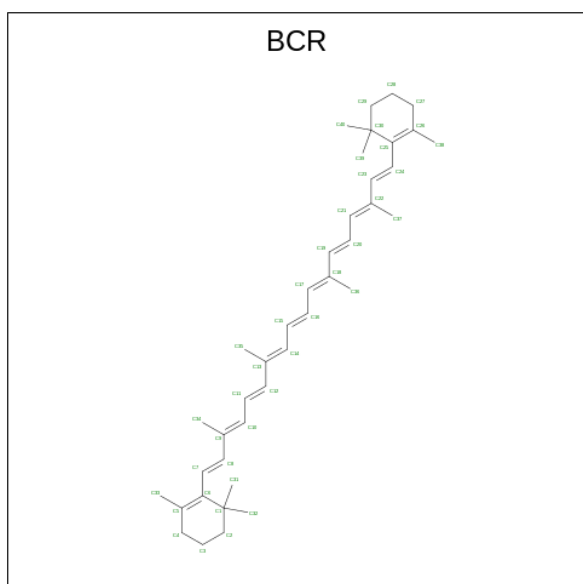
Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			42	40	2	
21	1	1	Total	C	O	0
			42	40	2	
21	2	1	Total	C	O	0
			42	40	2	
21	3	1	Total	C	O	0
			42	40	2	
21	4	1	Total	C	O	0
			42	40	2	

- Molecule 22 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
22	1	1	Total	C	O	0
			44	40	4	
22	2	1	Total	C	O	0
			44	40	4	
22	3	1	Total	C	O	0
			44	40	4	
22	4	1	Total	C	O	0
			44	40	4	

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



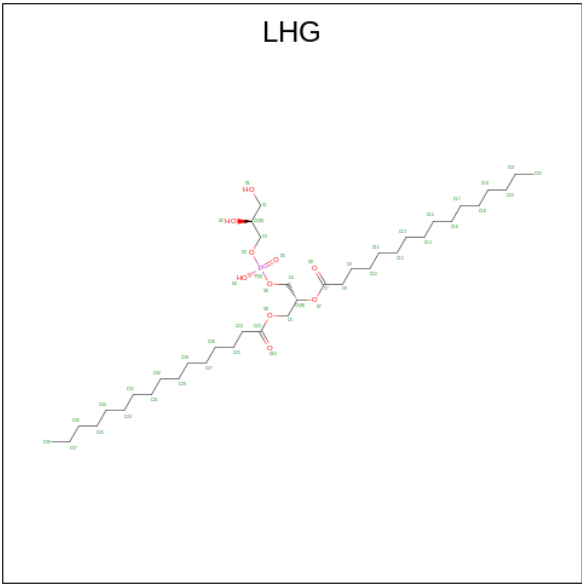
Mol	Chain	Residues	Atoms	AltConf
23	1	1	Total C 40 40	0
23	2	1	Total C 40 40	0
23	3	1	Total C 40 40	0
23	4	1	Total C 40 40	0
23	4	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 39 39	0
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 30 30	0
23	F	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	I	1	Total C 40 40	0

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

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



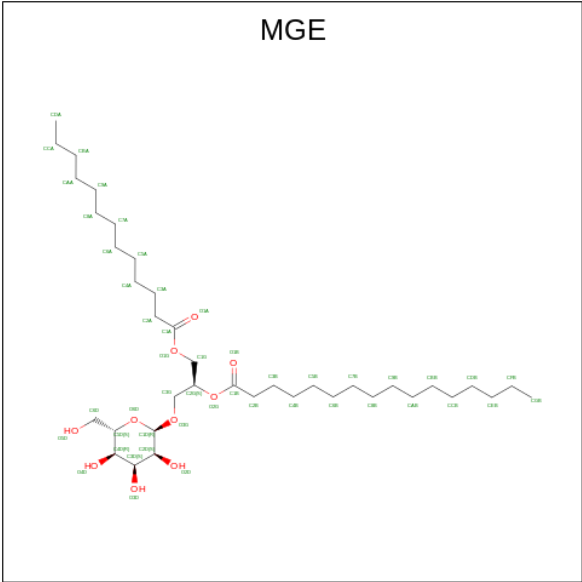
Mol	Chain	Residues	Atoms				AltConf
24	1	1	Total	C	O	P	0
			49	38	10	1	
24	1	1	Total	C	O		0
			33	28	5		

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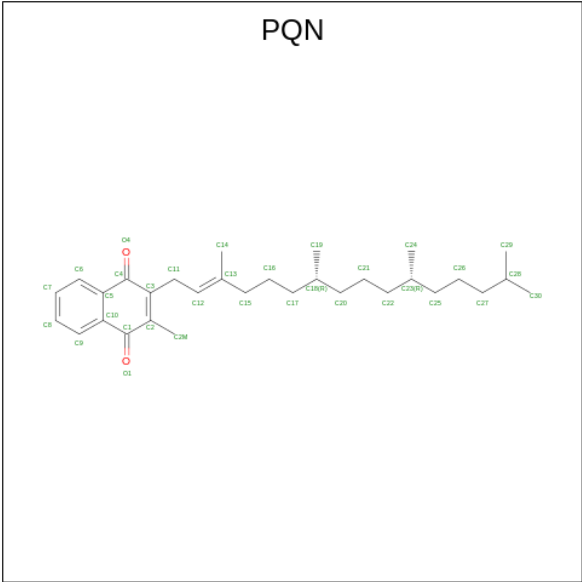
Mol	Chain	Residues	Atoms				AltConf
24	2	1	Total	C	O	P	0
			41	30	10	1	
24	2	1	Total	C	O	P	0
			40	30	9	1	
24	2	1	Total	C	O	P	0
			32	21	10	1	
24	2	1	Total	C	O	P	0
			37	28	8	1	
24	4	1	Total	C	O	P	0
			33	22	10	1	
24	4	1	Total	C	O	P	0
			49	38	10	1	
24	A	1	Total	C	O	P	0
			49	38	10	1	
24	A	1	Total	C	O	P	0
			27	18	8	1	
24	A	1	Total	C	O	P	0
			47	36	10	1	
24	A	1	Total	C	O	P	0
			42	33	8	1	
24	B	1	Total	C	O	P	0
			32	21	10	1	
24	B	1	Total	C	O	P	0
			32	23	8	1	
24	B	1	Total	C	O	P	0
			28	19	8	1	
24	I	1	Total	C	O		0
			37	33	4		
24	O	1	Total	C	O	P	0
			25	16	8	1	
24	O	1	Total	C	O	P	0
			42	33	8	1	

- Molecule 25 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: MGE) (formula: C₃₈H₇₂O₁₀) (labeled as "Ligand of Interest" by depositor).



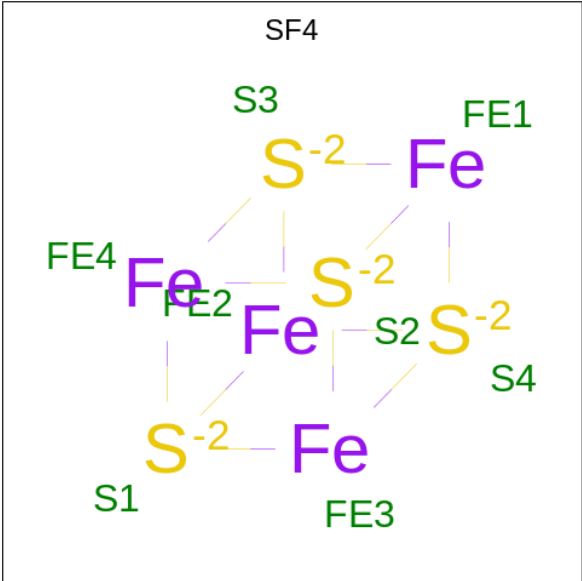
Mol	Chain	Residues	Atoms			AltConf
25	1	1	Total	C	O	0
			37	27	10	
25	1	1	Total	C	O	0
			40	30	10	
25	1	1	Total	C	O	0
			48	38	10	
25	3	1	Total	C	O	0
			33	23	10	
25	3	1	Total	C	O	0
			34	24	10	
25	3	1	Total	C	O	0
			38	28	10	
25	4	1	Total	C	O	0
			40	30	10	
25	A	1	Total	C	O	0
			34	24	10	
25	F	1	Total	C	O	0
			28	18	10	
25	G	1	Total	C	O	0
			48	38	10	
25	J	1	Total	C	O	0
			42	32	10	
25	N	1	Total	C	O	0
			40	30	10	

- Molecule 26 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Lig- and of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			33	31	2	
26	B	1	Total	C	O	0
			30	28	2	

- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



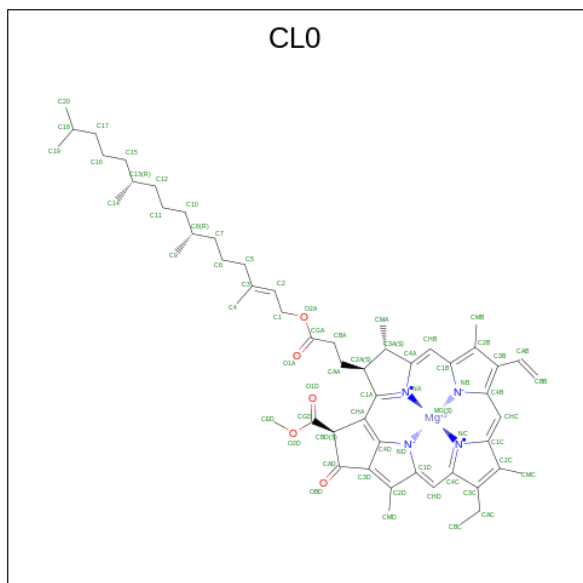
Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	Fe	S	0
			8	4	4	

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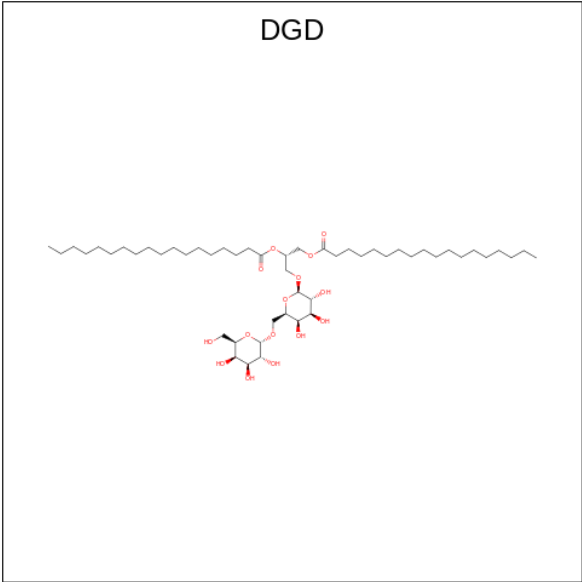
Mol	Chain	Residues	Atoms			AltConf
27	C	1	Total	Fe	S	0
			8	4	4	
27	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 28 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).

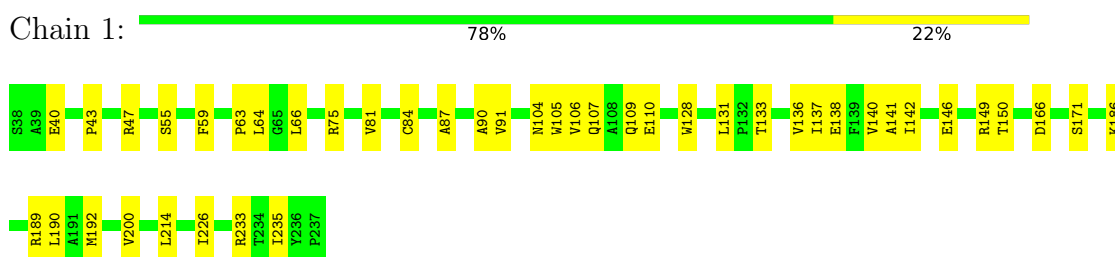


Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	C	O	0
			59	44	15	
29	G	1	Total	C	O	0
			40	31	9	
29	J	1	Total	C	O	0
			66	51	15	
29	O	1	Total	C	O	0
			53	38	15	

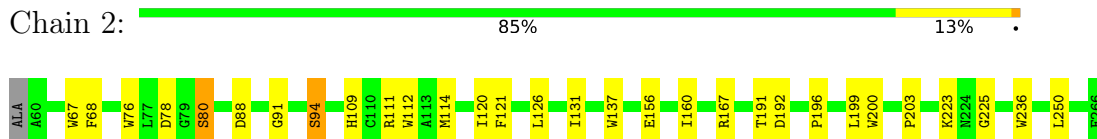
3 Residue-property plots

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.

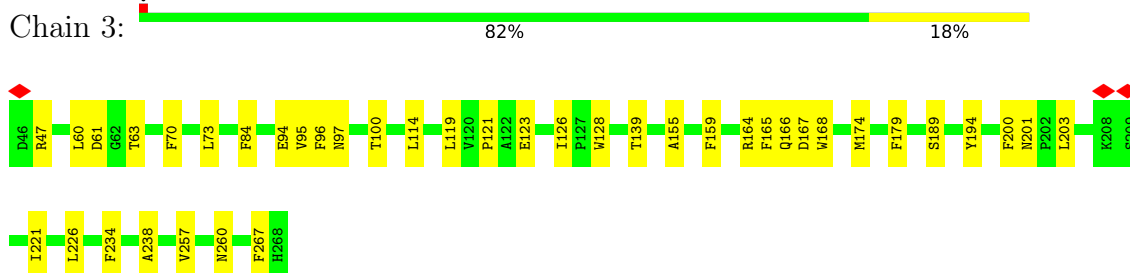
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



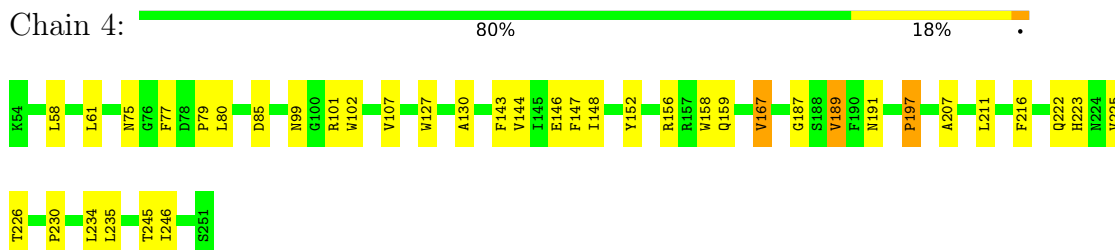
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



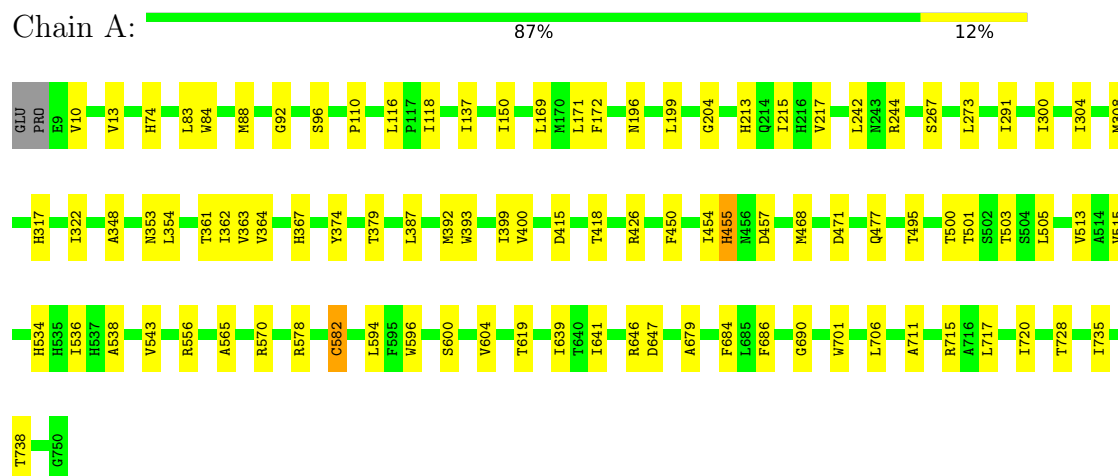
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



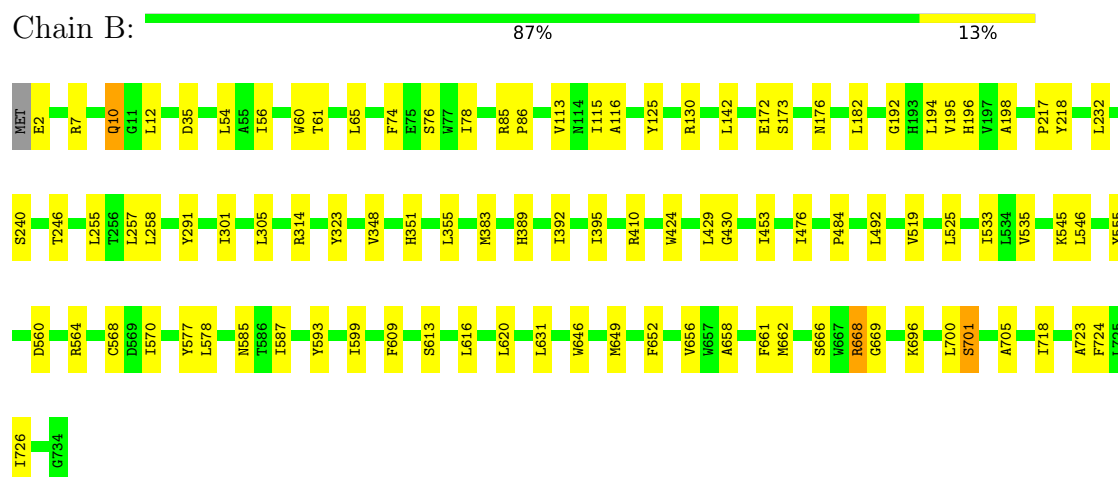
- Molecule 4: Chlorophyll a-b binding protein, chloroplastic



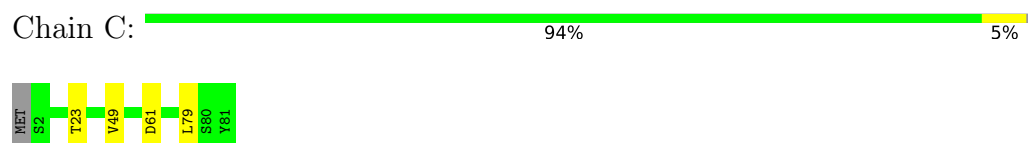
- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1



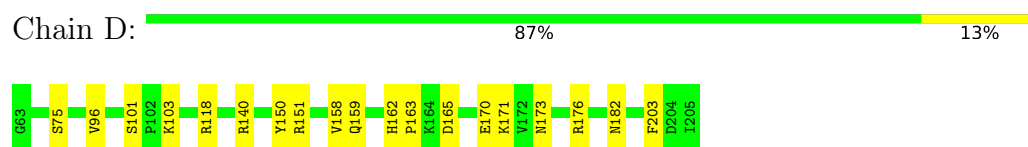
- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2



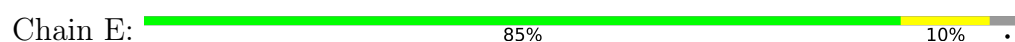
- Molecule 7: Photosystem I iron-sulfur center



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



- Molecule 9: Photosystem I reaction center subunit IV





- Molecule 10: Photosystem I reaction center subunit III

Chain F: 91% 9% .



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

Chain G: 78% 22%



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

Chain H: 88% 9% ..



- Molecule 13: Photosystem I reaction center subunit VIII

Chain I: 90% 7% .



- Molecule 14: Photosystem I reaction center subunit IX

Chain J: 80% 20%



- Molecule 15: Photosystem I reaction center subunit psaK, chloroplastic

Chain K: 92% 8%

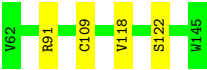


- Molecule 16: Photosystem I reaction center subunit XI, chloroplastic

Chain L: 91% 8% .



- Molecule 17: Photosystem I reaction center subunit N, chloroplastic



- Molecule 18: Os04g0414700 protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	182666	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.375	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.786	Depositor
Minimum map value	-0.971	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.14	Depositor
Map size ($\text{\AA}$)	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	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: PQN, MGE, XAT, DGD, BCR, CHL, LHG, CLA, CL0, SF4, LUT

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	0.18	0/1614	0.37	0/2203
2	2	0.23	0/1670	0.44	0/2286
3	3	0.20	0/1787	0.39	0/2430
4	4	0.27	1/1621 (0.1%)	0.48	1/2214 (0.0%)
5	A	0.20	0/6029	0.39	0/8222
6	B	0.20	0/6076	0.38	0/8297
7	C	0.16	0/613	0.35	0/830
8	D	0.16	0/1157	0.39	0/1564
9	E	0.16	0/530	0.38	0/722
10	F	0.17	0/1265	0.35	0/1710
11	G	0.32	0/780	0.52	0/1057
12	H	0.59	1/732 (0.1%)	0.67	2/996 (0.2%)
13	I	0.16	0/238	0.33	0/324
14	J	0.46	0/364	0.44	0/495
15	K	0.18	0/626	0.35	0/847
16	L	0.30	1/1261 (0.1%)	0.42	0/1726
17	N	0.15	0/701	0.36	0/939
18	O	0.18	0/762	0.39	0/1041
All	All	0.23	3/27826 (0.0%)	0.41	3/37903 (0.0%)

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
8	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	77	SER	CA-C	-7.09	1.45	1.53
16	L	91	SER	CA-C	-6.46	1.46	1.53
4	4	197	PRO	CB-CG	5.27	1.76	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	83	GLN	N-CA-C	-8.56	92.56	110.80
4	4	197	PRO	N-CD-CG	-7.50	91.95	103.20
12	H	78	PRO	N-CA-C	-6.87	98.32	112.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	D	162	HIS	Peptide

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	1560	0	1507	49	0
2	2	1612	0	1554	32	0
3	3	1731	0	1692	41	0
4	4	1570	0	1528	46	0
5	A	5833	0	5688	88	0
6	B	5865	0	5641	81	0
7	C	602	0	585	3	0
8	D	1128	0	1135	9	0
9	E	518	0	517	4	0
10	F	1236	0	1274	12	0
11	G	760	0	734	19	0
12	H	709	0	704	12	0
13	I	232	0	252	2	0
14	J	353	0	363	9	0
15	K	620	0	647	4	0
16	L	1223	0	1228	8	0
17	N	685	0	658	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	O	733	0	710	4	0
19	1	94	0	66	16	0
19	2	241	0	173	26	0
19	3	50	0	37	11	0
19	4	184	0	121	26	0
20	1	653	0	537	37	0
20	2	565	0	469	22	0
20	3	675	0	589	17	0
20	4	577	0	497	19	0
20	A	2551	0	2555	98	0
20	B	2510	0	2547	104	0
20	F	157	0	138	9	0
20	G	142	0	104	8	0
20	H	59	0	58	2	0
20	J	46	0	33	0	0
20	K	196	0	160	5	0
20	L	144	0	109	5	0
20	N	56	0	51	4	0
20	O	169	0	163	2	0
21	1	84	0	112	27	0
21	2	42	0	56	19	0
21	3	42	0	56	15	0
21	4	42	0	56	17	0
22	1	44	0	56	25	0
22	2	44	0	56	8	0
22	3	44	0	54	12	0
22	4	44	0	56	11	0
23	1	40	0	56	4	0
23	2	40	0	56	6	0
23	3	40	0	56	2	0
23	4	80	0	112	12	0
23	A	239	0	333	24	0
23	B	230	0	319	29	0
23	F	80	0	112	10	0
23	G	80	0	112	10	0
23	I	40	0	56	2	0
23	J	40	0	56	6	0
23	K	80	0	112	6	0
23	L	160	0	224	15	0
23	O	80	0	112	8	0
24	1	82	0	121	3	0
24	2	150	0	185	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	4	82	0	110	1	0
24	A	165	0	228	7	0
24	B	92	0	100	0	0
24	I	37	0	58	0	0
24	O	67	0	83	2	0
25	1	125	0	166	32	0
25	3	105	0	123	25	0
25	4	40	0	53	6	0
25	A	34	0	38	15	0
25	F	28	0	26	5	0
25	G	48	0	72	9	0
25	J	42	0	57	13	0
25	N	40	0	50	15	0
26	A	33	0	46	11	0
26	B	30	0	37	16	0
27	A	8	0	0	0	0
27	C	16	0	0	0	0
28	A	64	0	69	13	0
29	B	59	0	79	1	0
29	G	40	0	49	13	0
29	J	66	0	96	0	0
29	O	53	0	64	0	0
All	All	39160	0	38952	800	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 10.

The worst 5 of 800 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)
4:4:197:PRO:CB	4:4:197:PRO:CG	1.76	1.40
21:1:310:LUT:H171	21:1:310:LUT:H8	1.55	0.89
21:3:301:LUT:H8	21:3:301:LUT:H171	1.53	0.89
12:H:78:PRO:HB2	20:L:305:CLA:HMD2	1.52	0.89
19:2:318:CHL:HAA2	19:2:318:CHL:HED2	1.55	0.88

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	198/200 (99%)	194 (98%)	4 (2%)	0	100	100
2	2	205/208 (99%)	194 (95%)	11 (5%)	0	100	100
3	3	221/223 (99%)	210 (95%)	11 (5%)	0	100	100
4	4	196/198 (99%)	189 (96%)	7 (4%)	0	100	100
5	A	740/744 (100%)	707 (96%)	30 (4%)	3 (0%)	30	40
6	B	731/734 (100%)	709 (97%)	22 (3%)	0	100	100
7	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
8	D	141/143 (99%)	132 (94%)	7 (5%)	2 (1%)	9	11
9	E	63/68 (93%)	61 (97%)	2 (3%)	0	100	100
10	F	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
11	G	95/97 (98%)	88 (93%)	6 (6%)	1 (1%)	11	16
12	H	91/93 (98%)	81 (89%)	7 (8%)	3 (3%)	3	2
13	I	28/30 (93%)	28 (100%)	0	0	100	100
14	J	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
15	K	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
16	L	161/163 (99%)	154 (96%)	5 (3%)	2 (1%)	10	14
17	N	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
18	O	90/92 (98%)	81 (90%)	9 (10%)	0	100	100
All	All	3404/3448 (99%)	3264 (96%)	129 (4%)	11 (0%)	37	48

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	13	VAL
5	A	348	ALA
5	A	720	ILE
8	D	163	PRO

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Mol	Chain	Res	Type
16	L	57	ILE

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	162/162 (100%)	159 (98%)	3 (2%)	50	69
2	2	165/165 (100%)	163 (99%)	2 (1%)	63	79
3	3	177/177 (100%)	174 (98%)	3 (2%)	53	72
4	4	169/169 (100%)	164 (97%)	5 (3%)	36	56
5	A	602/604 (100%)	595 (99%)	7 (1%)	63	79
6	B	599/601 (100%)	584 (98%)	15 (2%)	42	61
7	C	69/71 (97%)	69 (100%)	0	100	100
8	D	121/121 (100%)	120 (99%)	1 (1%)	73	85
9	E	57/60 (95%)	54 (95%)	3 (5%)	20	33
10	F	127/127 (100%)	124 (98%)	3 (2%)	43	63
11	G	81/81 (100%)	79 (98%)	2 (2%)	42	61
12	H	76/76 (100%)	75 (99%)	1 (1%)	61	78
13	I	26/26 (100%)	25 (96%)	1 (4%)	29	46
14	J	38/38 (100%)	38 (100%)	0	100	100
15	K	64/64 (100%)	63 (98%)	1 (2%)	55	74
16	L	126/126 (100%)	123 (98%)	3 (2%)	43	63
17	N	73/73 (100%)	73 (100%)	0	100	100
18	O	77/77 (100%)	77 (100%)	0	100	100
All	All	2809/2818 (100%)	2759 (98%)	50 (2%)	51	71

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	429	LEU

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Mol	Chain	Res	Type
8	D	150	TYR
16	L	166	ARG
6	B	476	ILE
6	B	599	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
12	H	83	GLN
18	O	68	ASN
16	L	123	HIS
6	B	95	HIS
11	G	126	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

244 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	4	302	4	64,68,73	2.22	21 (32%)	77,107,113	2.97	29 (37%)
20	CLA	K	204	-	65,69,73	2.22	21 (32%)	78,108,113	2.97	29 (37%)
20	CLA	3	307	-	62,67,73	2.14	19 (30%)	76,105,113	3.06	34 (44%)
20	CLA	B	816	6	69,73,73	2.13	20 (28%)	83,113,113	2.93	34 (40%)
19	CHL	2	302	-	51,55,74	2.20	17 (33%)	57,91,114	3.10	24 (42%)
20	CLA	B	814	-	69,73,73	2.05	19 (27%)	83,113,113	3.02	32 (38%)
20	CLA	A	801	5	67,71,73	2.10	20 (29%)	83,110,113	2.84	31 (37%)
20	CLA	G	206	-	54,58,73	2.43	20 (37%)	63,94,113	3.30	29 (46%)
19	CHL	2	322	-	50,54,74	2.25	18 (36%)	56,90,114	3.18	22 (39%)
23	BCR	G	203	-	41,41,41	1.93	8 (19%)	56,56,56	1.90	15 (26%)
20	CLA	A	838	5	49,53,73	2.50	21 (42%)	59,89,113	3.27	27 (45%)
19	CHL	4	315	4	48,53,74	2.26	17 (35%)	53,89,114	3.13	21 (39%)
20	CLA	A	807	5	59,63,73	2.29	20 (33%)	71,101,113	3.12	30 (42%)
22	XAT	3	302	-	39,47,47	0.85	0	54,74,74	7.29	26 (48%)
23	BCR	L	301	-	41,41,41	1.71	7 (17%)	56,56,56	1.54	7 (12%)
26	PQN	A	810	-	34,34,34	0.38	0	42,45,45	0.41	0
20	CLA	A	840	-	50,54,73	2.48	20 (40%)	60,90,113	3.29	27 (45%)
20	CLA	L	305	16	50,54,73	2.52	21 (42%)	60,90,113	3.23	29 (48%)
20	CLA	1	319	-	59,63,73	2.31	21 (35%)	71,101,113	3.12	30 (42%)
20	CLA	B	815	-	60,64,73	2.30	20 (33%)	72,102,113	3.04	29 (40%)
20	CLA	4	311	-	50,54,73	2.52	20 (40%)	60,90,113	3.30	26 (43%)
24	LHG	4	301	-	32,32,48	0.34	0	35,38,54	0.46	0
20	CLA	G	205	-	50,54,73	2.48	20 (40%)	60,90,113	3.26	27 (45%)
21	LUT	3	301	-	42,43,43	1.59	8 (19%)	51,60,60	1.57	11 (21%)
20	CLA	B	809	-	69,73,73	2.15	20 (28%)	83,113,113	2.64	26 (31%)
20	CLA	A	806	5	69,73,73	2.12	20 (28%)	83,113,113	2.77	29 (34%)
20	CLA	4	316	-	69,73,73	2.15	20 (28%)	83,113,113	2.94	31 (37%)
23	BCR	4	320	-	41,41,41	1.87	8 (19%)	56,56,56	1.81	17 (30%)
19	CHL	1	301	1	47,51,74	2.22	16 (34%)	52,86,114	3.21	22 (42%)
21	LUT	1	323	-	42,43,43	1.66	8 (19%)	51,60,60	2.22	13 (25%)
20	CLA	G	207	11	50,54,73	2.50	20 (40%)	60,90,113	3.28	26 (43%)
20	CLA	A	805	5	58,62,73	2.37	18 (31%)	69,99,113	3.15	29 (42%)
19	CHL	4	306	-	50,54,74	2.24	16 (32%)	56,90,114	3.18	21 (37%)
20	CLA	B	817	6	62,66,73	2.21	20 (32%)	74,104,113	3.07	30 (40%)
20	CLA	4	314	4	54,58,73	2.40	20 (37%)	65,95,113	3.22	30 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	813	6	61,65,73	2.27	18 (29%)	73,103,113	2.98	29 (39%)
20	CLA	B	823	6	66,70,73	2.15	20 (30%)	79,109,113	2.87	29 (36%)
24	LHG	A	819	-	48,48,48	0.30	0	51,54,54	0.38	0
20	CLA	4	312	4	59,63,73	2.34	20 (33%)	71,101,113	3.05	29 (40%)
20	CLA	O	207	-	63,67,73	2.25	20 (31%)	75,105,113	2.94	30 (40%)
19	CHL	2	309	2	47,51,74	2.25	16 (34%)	52,86,114	3.30	22 (42%)
29	DGD	O	201	-	54,54,67	0.96	2 (3%)	68,68,81	0.76	3 (4%)
20	CLA	A	855	5	59,63,73	2.27	19 (32%)	71,101,113	2.98	29 (40%)
20	CLA	4	304	-	49,53,73	2.58	20 (40%)	59,89,113	3.22	26 (44%)
19	CHL	4	307	-	50,54,74	2.22	17 (34%)	56,90,114	3.06	23 (41%)
24	LHG	1	313	20	48,48,48	0.27	0	51,54,54	0.40	0
23	BCR	1	312	-	41,41,41	1.83	8 (19%)	56,56,56	1.58	13 (23%)
20	CLA	B	806	6	61,65,73	2.28	19 (31%)	73,103,113	3.11	30 (41%)
20	CLA	4	308	4	50,54,73	2.42	21 (42%)	60,90,113	3.21	29 (48%)
20	CLA	L	306	16	56,60,73	2.34	19 (33%)	67,97,113	3.16	30 (44%)
20	CLA	2	306	-	49,53,73	2.55	19 (38%)	59,89,113	3.38	26 (44%)
23	BCR	L	303	-	41,41,41	1.96	8 (19%)	56,56,56	1.63	13 (23%)
20	CLA	2	303	2	49,53,73	2.49	19 (38%)	59,89,113	3.15	29 (49%)
20	CLA	B	805	-	49,53,73	2.52	20 (40%)	59,89,113	3.29	28 (47%)
20	CLA	A	839	5	49,53,73	2.54	21 (42%)	59,89,113	3.35	29 (49%)
20	CLA	L	307	-	50,54,73	2.50	21 (42%)	60,90,113	3.28	28 (46%)
20	CLA	1	302	-	54,58,73	2.40	19 (35%)	65,95,113	3.22	29 (44%)
24	LHG	O	204	-	24,24,48	0.49	0	28,29,54	0.65	1 (3%)
25	MGE	1	315	-	37,37,48	0.25	0	45,45,56	0.48	0
20	CLA	A	848	5	69,73,73	2.13	20 (28%)	83,113,113	2.84	32 (38%)
20	CLA	1	322	1	50,54,73	2.52	20 (40%)	60,90,113	3.27	27 (45%)
20	CLA	B	851	6	69,73,73	2.07	19 (27%)	83,113,113	2.73	28 (33%)
19	CHL	4	305	-	51,55,74	2.21	18 (35%)	57,91,114	3.09	23 (40%)
20	CLA	A	826	-	69,73,73	2.05	20 (28%)	83,113,113	2.59	27 (32%)
20	CLA	1	321	-	50,54,73	2.47	21 (42%)	60,90,113	3.24	28 (46%)
20	CLA	1	303	1	57,62,73	2.34	19 (33%)	68,100,113	2.94	28 (41%)
20	CLA	F	306	-	50,54,73	2.49	19 (38%)	60,90,113	3.25	26 (43%)
20	CLA	A	852	5	69,73,73	2.12	19 (27%)	83,113,113	2.80	27 (32%)
23	BCR	L	304	-	41,41,41	1.88	8 (19%)	56,56,56	2.15	16 (28%)
24	LHG	A	821	20	46,46,48	0.29	0	49,52,54	0.38	0
25	MGE	N	201	-	40,40,48	0.23	0	48,48,56	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	842	5	65,69,73	2.22	19 (29%)	78,108,113	2.97	31 (39%)
23	BCR	A	857	-	41,41,41	1.80	7 (17%)	56,56,56	1.67	12 (21%)
20	CLA	3	315	3	59,63,73	2.31	20 (33%)	71,101,113	3.01	29 (40%)
20	CLA	3	317	3	62,66,73	2.25	20 (32%)	74,104,113	2.99	31 (41%)
24	LHG	2	315	20	31,31,48	0.33	0	34,37,54	0.41	0
20	CLA	B	811	6	61,65,73	2.29	19 (31%)	73,103,113	3.00	29 (39%)
20	CLA	1	304	1	59,63,73	2.33	20 (33%)	71,101,113	3.02	28 (39%)
20	CLA	A	804	5	55,59,73	2.34	19 (34%)	66,96,113	3.20	31 (46%)
20	CLA	A	841	5	63,67,73	2.25	20 (31%)	75,105,113	2.95	28 (37%)
20	CLA	F	304	-	69,73,73	2.09	19 (27%)	83,113,113	2.83	29 (34%)
23	BCR	F	301	-	41,41,41	1.89	8 (19%)	56,56,56	1.74	12 (21%)
23	BCR	K	201	-	41,41,41	1.76	8 (19%)	56,56,56	1.54	9 (16%)
20	CLA	3	311	-	69,73,73	2.13	21 (30%)	83,113,113	2.85	31 (37%)
24	LHG	2	316	-	36,36,48	0.40	0	40,41,54	0.51	1 (2%)
20	CLA	B	801	-	69,73,73	2.14	21 (30%)	83,113,113	2.85	31 (37%)
20	CLA	B	825	-	49,53,73	2.52	19 (38%)	59,89,113	3.10	27 (45%)
22	XAT	1	311	-	39,47,47	0.86	1 (2%)	54,74,74	3.66	25 (46%)
20	CLA	1	305	24	50,54,73	2.54	20 (40%)	60,90,113	3.24	28 (46%)
20	CLA	2	320	2	51,55,73	2.61	23 (45%)	61,91,113	3.41	27 (44%)
25	MGE	J	102	-	42,42,48	0.23	0	50,50,56	0.27	0
20	CLA	4	309	4	58,62,73	2.36	19 (32%)	69,99,113	3.11	29 (42%)
20	CLA	B	827	6	69,73,73	2.14	19 (27%)	83,113,113	2.82	30 (36%)
20	CLA	3	318	3	45,49,73	2.64	20 (44%)	54,84,113	3.43	27 (50%)
20	CLA	A	827	5	69,73,73	2.14	21 (30%)	83,113,113	2.87	30 (36%)
20	CLA	1	309	-	45,49,73	2.65	19 (42%)	54,84,113	3.51	27 (50%)
20	CLA	3	312	3	49,53,73	2.54	21 (42%)	59,89,113	3.28	27 (45%)
20	CLA	A	809	5	69,73,73	2.14	20 (28%)	83,113,113	2.87	27 (32%)
20	CLA	1	320	-	53,57,73	2.46	20 (37%)	62,93,113	3.22	28 (45%)
24	LHG	B	843	-	27,27,48	0.46	0	31,32,54	0.59	1 (3%)
27	SF4	C	102	7	0,12,12	-	-	-	-	-
29	DGD	J	104	-	67,67,67	0.87	2 (2%)	81,81,81	1.04	5 (6%)
20	CLA	B	830	6	69,73,73	2.12	20 (28%)	83,113,113	2.86	29 (34%)
20	CLA	A	837	5	69,73,73	2.15	19 (27%)	83,113,113	2.96	29 (34%)
20	CLA	A	846	5	50,54,73	2.47	20 (40%)	60,90,113	3.28	27 (45%)
24	LHG	B	841	-	31,31,48	0.32	0	34,37,54	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	847	5	60,64,73	2.28	19 (31%)	72,102,113	3.07	30 (41%)
20	CLA	A	825	-	69,73,73	2.08	19 (27%)	83,113,113	2.74	29 (34%)
20	CLA	A	803	5	64,68,73	2.16	18 (28%)	76,106,113	2.87	30 (39%)
20	CLA	B	812	6	69,73,73	2.12	19 (27%)	83,113,113	2.76	31 (37%)
20	CLA	2	308	2	55,59,73	2.43	20 (36%)	66,96,113	3.19	29 (43%)
20	CLA	K	203	15	51,55,73	2.51	21 (41%)	61,91,113	3.29	29 (47%)
23	BCR	A	817	-	41,41,41	1.67	10 (24%)	56,56,56	1.55	9 (16%)
20	CLA	A	802	5	69,73,73	2.14	21 (30%)	83,113,113	2.84	32 (38%)
20	CLA	A	836	5	56,60,73	2.39	20 (35%)	67,97,113	3.19	28 (41%)
23	BCR	G	201	-	41,41,41	1.72	8 (19%)	56,56,56	1.61	11 (19%)
24	LHG	B	842	-	31,31,48	0.46	0	35,36,54	1.37	3 (8%)
23	BCR	A	818	-	40,40,41	1.58	6 (15%)	54,54,56	1.74	9 (16%)
20	CLA	A	833	5	69,73,73	2.10	20 (28%)	83,113,113	2.78	29 (34%)
20	CLA	F	305	-	50,54,73	2.49	19 (38%)	60,90,113	3.21	26 (43%)
20	CLA	J	103	14	50,54,73	2.52	20 (40%)	60,90,113	3.26	27 (45%)
20	CLA	A	829	5	68,72,73	2.13	19 (27%)	81,111,113	2.76	28 (34%)
20	CLA	B	846	6	49,53,73	2.55	21 (42%)	59,89,113	3.33	28 (47%)
23	BCR	B	837	-	41,41,41	1.77	8 (19%)	56,56,56	1.59	12 (21%)
23	BCR	B	838	-	41,41,41	1.85	8 (19%)	56,56,56	1.63	10 (17%)
27	SF4	A	813	5,6	0,12,12	-	-	-	-	-
20	CLA	2	307	2	66,70,73	2.20	21 (31%)	79,109,113	2.90	29 (36%)
20	CLA	4	303	-	50,54,73	2.50	20 (40%)	60,90,113	3.31	27 (45%)
20	CLA	A	811	24	59,63,73	2.32	19 (32%)	71,101,113	3.06	30 (42%)
20	CLA	B	810	6	52,56,73	2.43	18 (34%)	62,92,113	3.17	28 (45%)
20	CLA	A	856	5	60,64,73	2.30	21 (35%)	72,102,113	3.09	30 (41%)
20	CLA	B	802	6	49,53,73	2.54	20 (40%)	59,89,113	3.35	28 (47%)
20	CLA	B	831	-	69,73,73	2.13	19 (27%)	83,113,113	2.92	31 (37%)
23	BCR	O	202	-	41,41,41	1.73	6 (14%)	56,56,56	2.05	13 (23%)
20	CLA	B	829	-	69,73,73	2.14	19 (27%)	83,113,113	2.80	27 (32%)
20	CLA	3	316	-	50,54,73	2.50	19 (38%)	60,90,113	3.29	27 (45%)
29	DGD	G	202	-	40,40,67	1.04	2 (5%)	48,48,81	1.12	3 (6%)
20	CLA	A	845	-	69,73,73	2.13	20 (28%)	83,113,113	2.67	30 (36%)
20	CLA	B	849	6	56,60,73	2.37	20 (35%)	67,97,113	3.21	32 (47%)
23	BCR	A	814	-	41,41,41	1.72	8 (19%)	56,56,56	1.46	9 (16%)
20	CLA	A	854	5	69,73,73	2.05	17 (24%)	83,113,113	2.62	33 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	828	6	51,55,73	2.42	19 (37%)	61,91,113	3.23	26 (42%)
23	BCR	L	302	-	41,41,41	1.76	9 (21%)	56,56,56	1.58	10 (17%)
24	LHG	A	820	-	26,26,48	0.48	0	30,31,54	1.39	4 (13%)
20	CLA	1	308	1	50,54,73	2.51	21 (42%)	60,90,113	3.29	28 (46%)
20	CLA	3	319	-	50,54,73	2.51	20 (40%)	60,90,113	3.25	26 (43%)
23	BCR	A	815	-	41,41,41	1.68	7 (17%)	56,56,56	1.57	8 (14%)
21	LUT	1	310	-	42,43,43	1.60	8 (19%)	51,60,60	1.57	11 (21%)
19	CHL	1	317	1	55,59,74	2.13	16 (29%)	62,96,114	3.08	26 (41%)
20	CLA	K	205	15	50,54,73	2.57	20 (40%)	60,90,113	3.20	23 (38%)
20	CLA	A	850	-	62,66,73	2.25	20 (32%)	74,104,113	2.95	30 (40%)
23	BCR	3	303	-	41,41,41	1.73	9 (21%)	56,56,56	1.50	11 (19%)
23	BCR	K	202	-	41,41,41	1.86	6 (14%)	56,56,56	1.56	9 (16%)
26	PQN	B	832	-	31,31,34	0.39	0	38,41,45	0.40	0
20	CLA	O	208	-	49,53,73	2.55	21 (42%)	59,89,113	3.27	28 (47%)
20	CLA	B	822	6	69,73,73	2.09	20 (28%)	83,113,113	2.78	30 (36%)
28	CL0	A	824	5	67,72,73	2.01	19 (28%)	80,112,113	2.77	31 (38%)
20	CLA	1	318	1	69,73,73	2.19	20 (28%)	83,113,113	2.86	30 (36%)
23	BCR	B	834	-	41,41,41	1.72	7 (17%)	56,56,56	1.66	10 (17%)
19	CHL	2	318	2	62,66,74	1.99	17 (27%)	70,104,114	2.93	24 (34%)
23	BCR	4	319	-	41,41,41	1.78	8 (19%)	56,56,56	1.76	10 (17%)
22	XAT	2	311	-	39,47,47	1.01	1 (2%)	54,74,74	5.69	24 (44%)
20	CLA	B	821	6	60,64,73	2.27	19 (31%)	72,102,113	3.04	30 (41%)
20	CLA	3	309	-	64,68,73	2.23	20 (31%)	77,107,113	2.94	27 (35%)
23	BCR	J	101	-	41,41,41	1.82	9 (21%)	56,56,56	1.62	12 (21%)
20	CLA	A	808	5	69,73,73	2.12	20 (28%)	83,113,113	2.82	30 (36%)
20	CLA	B	850	6	69,73,73	2.07	18 (26%)	83,113,113	2.75	29 (34%)
20	CLA	A	851	5	69,73,73	2.14	20 (28%)	83,113,113	2.88	30 (36%)
25	MGE	4	322	-	40,40,48	0.22	0	48,48,56	0.43	0
25	MGE	A	823	-	34,34,48	0.25	0	42,42,56	0.55	0
19	CHL	2	301	-	51,55,74	2.20	15 (29%)	57,91,114	3.14	23 (40%)
20	CLA	H	201	12	63,67,73	2.25	20 (31%)	75,105,113	2.98	30 (40%)
20	CLA	N	202	17	60,64,73	2.32	20 (33%)	72,102,113	3.02	28 (38%)
20	CLA	B	826	6	54,58,73	2.40	20 (37%)	65,95,113	3.21	31 (47%)
23	BCR	B	835	-	41,41,41	1.79	7 (17%)	56,56,56	1.68	12 (21%)
20	CLA	B	852	-	69,73,73	2.15	20 (28%)	83,113,113	2.85	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	3	310	-	53,57,73	2.45	20 (37%)	62,93,113	3.20	28 (45%)
25	MGE	1	316	-	40,40,48	0.23	0	48,48,56	0.32	0
20	CLA	A	831	5	56,60,73	2.35	20 (35%)	67,97,113	3.19	32 (47%)
20	CLA	A	849	-	69,73,73	2.10	21 (30%)	83,113,113	2.92	29 (34%)
25	MGE	G	204	-	48,48,48	0.23	0	56,56,56	0.40	0
20	CLA	B	845	-	69,73,73	2.06	17 (24%)	83,113,113	2.75	28 (33%)
20	CLA	A	812	-	69,73,73	2.07	20 (28%)	83,113,113	2.75	31 (37%)
20	CLA	B	847	6	69,73,73	2.14	19 (27%)	83,113,113	2.92	29 (34%)
23	BCR	2	312	-	41,41,41	1.81	7 (17%)	56,56,56	1.77	12 (21%)
24	LHG	A	822	-	41,41,48	0.38	0	45,46,54	0.53	1 (2%)
21	LUT	2	310	-	42,43,43	1.64	8 (19%)	51,60,60	1.65	12 (23%)
20	CLA	A	835	5,20	69,73,73	2.13	19 (27%)	83,113,113	2.86	31 (37%)
20	CLA	1	307	1	59,63,73	2.32	20 (33%)	71,101,113	3.09	30 (42%)
20	CLA	2	321	-	54,58,73	2.44	20 (37%)	65,95,113	3.17	30 (46%)
25	MGE	1	324	-	48,48,48	0.22	0	56,56,56	0.59	1 (1%)
25	MGE	3	304	-	33,33,48	0.25	0	41,41,56	0.26	0
20	CLA	2	304	2	59,63,73	2.32	20 (33%)	71,101,113	2.90	27 (38%)
24	LHG	O	205	-	41,41,48	0.39	0	45,46,54	0.57	1 (2%)
20	CLA	A	853	5	69,73,73	2.07	20 (28%)	83,113,113	2.69	29 (34%)
20	CLA	2	317	-	51,55,73	2.53	20 (39%)	61,91,113	3.22	27 (44%)
20	CLA	B	818	6	69,73,73	2.12	18 (26%)	83,113,113	2.77	28 (33%)
20	CLA	B	844	6	69,73,73	2.07	19 (27%)	83,113,113	2.94	32 (38%)
20	CLA	B	819	6	69,73,73	2.08	18 (26%)	83,113,113	2.55	28 (33%)
27	SF4	C	101	7	0,12,12	-	-	-	-	-
20	CLA	B	848	6	69,73,73	2.12	19 (27%)	83,113,113	2.91	29 (34%)
20	CLA	A	843	5	69,73,73	2.12	20 (28%)	83,113,113	2.74	28 (33%)
25	MGE	3	305	-	34,34,48	0.25	0	42,42,56	0.41	0
24	LHG	1	314	-	32,32,48	0.29	0	34,34,54	0.48	0
20	CLA	B	833	-	65,69,73	2.24	20 (30%)	78,108,113	3.01	30 (38%)
20	CLA	3	308	3	65,69,73	2.26	20 (30%)	78,108,113	2.96	31 (39%)
24	LHG	I	101	-	36,36,48	0.25	0	38,38,54	0.28	0
20	CLA	A	828	5,20	56,60,73	2.37	20 (35%)	67,97,113	3.12	30 (44%)
23	BCR	B	839	-	30,30,41	1.92	7 (23%)	39,39,56	2.04	10 (25%)
20	CLA	B	824	6	64,68,73	2.21	20 (31%)	77,107,113	2.95	28 (36%)
20	CLA	B	803	6	69,73,73	2.12	21 (30%)	83,113,113	2.91	31 (37%)
25	MGE	F	303	-	28,28,48	0.26	0	36,36,56	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	2	319	2	66,70,73	2.19	21 (31%)	79,109,113	2.96	30 (37%)
20	CLA	B	853	6	59,63,73	2.33	21 (35%)	71,101,113	3.01	28 (39%)
20	CLA	B	807	6	69,73,73	2.15	19 (27%)	83,113,113	2.93	30 (36%)
20	CLA	B	820	6	63,67,73	2.16	20 (31%)	75,105,113	2.94	30 (40%)
20	CLA	K	206	15	46,50,73	2.57	20 (43%)	55,85,113	3.40	27 (49%)
20	CLA	B	804	6	69,73,73	2.09	21 (30%)	83,113,113	2.77	28 (33%)
20	CLA	3	320	3	49,53,73	2.54	21 (42%)	59,89,113	3.26	27 (45%)
20	CLA	4	310	-	64,68,73	2.22	20 (31%)	77,107,113	2.92	29 (37%)
19	CHL	3	313	-	54,58,74	2.14	17 (31%)	59,94,114	3.04	23 (38%)
20	CLA	3	314	3	49,53,73	2.48	19 (38%)	59,89,113	3.18	27 (45%)
23	BCR	A	816	-	41,41,41	1.94	9 (21%)	56,56,56	1.77	12 (21%)
23	BCR	I	102	-	41,41,41	1.76	8 (19%)	56,56,56	1.66	11 (19%)
23	BCR	O	203	-	41,41,41	1.92	6 (14%)	56,56,56	2.41	15 (26%)
23	BCR	B	836	-	41,41,41	1.89	6 (14%)	56,56,56	1.74	15 (26%)
20	CLA	1	306	-	49,53,73	2.55	20 (40%)	59,89,113	3.30	28 (47%)
20	CLA	O	206	18	69,73,73	2.15	21 (30%)	83,113,113	2.81	29 (34%)
25	MGE	3	306	-	38,38,48	0.25	0	46,46,56	0.41	0
20	CLA	A	832	5	69,73,73	2.13	19 (27%)	83,113,113	2.76	30 (36%)
24	LHG	2	313	-	40,40,48	0.33	0	43,46,54	0.50	0
24	LHG	4	321	-	48,48,48	0.27	0	51,54,54	0.32	0
20	CLA	A	834	5	59,63,73	2.25	19 (32%)	71,101,113	3.06	27 (38%)
29	DGD	B	840	-	60,60,67	0.89	2 (3%)	74,74,81	0.93	3 (4%)
20	CLA	2	323	4	50,54,73	2.51	20 (40%)	60,90,113	3.31	28 (46%)
20	CLA	4	313	4	54,58,73	2.45	20 (37%)	65,95,113	3.19	27 (41%)
21	LUT	4	317	-	42,43,43	1.61	8 (19%)	51,60,60	1.51	10 (19%)
22	XAT	4	318	-	39,47,47	0.87	0	54,74,74	2.73	20 (37%)
23	BCR	F	302	-	41,41,41	1.71	9 (21%)	56,56,56	1.59	11 (19%)
20	CLA	A	830	5	69,73,73	2.12	20 (28%)	83,113,113	2.84	30 (36%)
20	CLA	A	844	5	50,54,73	2.44	20 (40%)	60,90,113	3.35	30 (50%)
20	CLA	2	305	24	59,63,73	2.35	20 (33%)	71,101,113	3.09	29 (40%)
24	LHG	2	314	-	38,39,48	0.31	0	41,45,54	0.48	0
20	CLA	B	808	6	69,73,73	2.14	20 (28%)	83,113,113	2.86	32 (38%)

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
20	CLA	4	302	4	1/1/14/20	5/33/109/115	-
20	CLA	K	204	-	1/1/14/20	8/35/111/115	-
20	CLA	3	307	-	1/1/13/20	7/30/106/115	-
20	CLA	B	816	6	1/1/15/20	12/39/115/115	-
20	CLA	B	814	-	1/1/15/20	10/39/115/115	-
19	CHL	2	302	-	-	8/19/95/117	-
20	CLA	A	801	5	1/1/14/20	6/35/111/115	-
20	CLA	G	206	-	-	5/21/97/115	-
19	CHL	2	322	-	-	7/17/93/117	-
23	BCR	G	203	-	-	7/29/63/63	0/2/2/2
20	CLA	A	838	5	-	7/15/91/115	-
19	CHL	4	315	4	-	5/15/91/117	-
20	CLA	A	807	5	1/1/13/20	11/27/103/115	-
22	XAT	3	302	-	-	10/31/93/93	0/4/4/4
23	BCR	L	301	-	-	7/29/63/63	0/2/2/2
26	PQN	A	810	-	-	6/23/43/43	0/2/2/2
20	CLA	A	840	-	-	1/17/93/115	-
20	CLA	L	305	16	-	1/17/93/115	-
20	CLA	1	319	-	1/1/13/20	8/27/103/115	-
20	CLA	B	815	-	1/1/13/20	6/29/105/115	-
20	CLA	4	311	-	-	2/17/93/115	-
24	LHG	4	301	-	-	6/37/37/53	-
20	CLA	G	205	-	-	3/17/93/115	-
21	LUT	3	301	-	-	0/29/67/67	0/2/2/2
20	CLA	B	809	-	1/1/15/20	14/39/115/115	-
20	CLA	A	806	5	1/1/15/20	12/39/115/115	-
20	CLA	4	316	-	1/1/15/20	16/39/115/115	-
23	BCR	4	320	-	-	6/29/63/63	0/2/2/2
19	CHL	1	301	1	-	9/14/90/117	-
21	LUT	1	323	-	-	7/29/67/67	0/2/2/2
20	CLA	G	207	11	-	4/17/93/115	-
20	CLA	A	805	5	-	7/26/102/115	-
19	CHL	4	306	-	-	14/17/93/117	-
20	CLA	B	817	6	1/1/13/20	7/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	314	4	-	8/21/97/115	-
20	CLA	B	813	6	1/1/13/20	10/30/106/115	-
20	CLA	B	823	6	1/1/14/20	11/36/112/115	-
24	LHG	A	819	-	-	5/53/53/53	-
20	CLA	4	312	4	1/1/13/20	7/27/103/115	-
20	CLA	O	207	-	1/1/13/20	8/32/108/115	-
19	CHL	2	309	2	-	5/14/90/117	-
29	DGD	O	201	-	-	9/42/82/95	0/2/2/2
20	CLA	A	855	5	1/1/13/20	4/27/103/115	-
20	CLA	4	304	-	-	8/15/91/115	-
19	CHL	4	307	-	-	7/17/93/117	-
24	LHG	1	313	20	-	8/53/53/53	-
23	BCR	1	312	-	-	8/29/63/63	0/2/2/2
20	CLA	B	806	6	1/1/13/20	12/30/106/115	-
20	CLA	4	308	4	-	2/17/93/115	-
20	CLA	L	306	16	-	3/24/100/115	-
20	CLA	2	306	-	-	2/15/91/115	-
23	BCR	L	303	-	-	7/29/63/63	0/2/2/2
20	CLA	2	303	2	-	3/15/91/115	-
20	CLA	B	805	-	-	2/15/91/115	-
20	CLA	A	839	5	-	8/15/91/115	-
20	CLA	L	307	-	-	3/17/93/115	-
20	CLA	1	302	-	-	3/21/97/115	-
24	LHG	O	204	-	-	1/26/26/53	-
25	MGE	1	315	-	-	3/32/52/63	0/1/1/1
20	CLA	A	848	5	1/1/15/20	8/39/115/115	-
20	CLA	B	851	6	1/1/15/20	11/39/115/115	-
20	CLA	1	322	1	-	3/17/93/115	-
20	CLA	A	826	-	1/1/15/20	13/39/115/115	-
19	CHL	4	305	-	-	16/19/95/117	-
20	CLA	1	321	-	-	0/17/93/115	-
20	CLA	1	303	1	1/1/13/20	8/25/101/115	-
20	CLA	F	306	-	-	6/17/93/115	-
20	CLA	A	852	5	1/1/15/20	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	L	304	-	-	9/29/63/63	0/2/2/2
24	LHG	A	821	20	-	8/51/51/53	-
25	MGE	N	201	-	-	8/35/55/63	0/1/1/1
20	CLA	A	842	5	1/1/14/20	10/35/111/115	-
23	BCR	A	857	-	-	6/29/63/63	0/2/2/2
20	CLA	3	317	3	1/1/13/20	9/31/107/115	-
20	CLA	3	315	3	1/1/13/20	7/27/103/115	-
24	LHG	2	315	20	-	8/36/36/53	-
20	CLA	B	811	6	1/1/13/20	8/30/106/115	-
20	CLA	1	304	1	1/1/13/20	6/27/103/115	-
20	CLA	A	841	5	1/1/13/20	7/31/107/115	-
20	CLA	A	804	5	-	10/23/99/115	-
20	CLA	F	304	-	1/1/15/20	17/39/115/115	-
23	BCR	F	301	-	-	3/29/63/63	0/2/2/2
23	BCR	K	201	-	-	4/29/63/63	0/2/2/2
20	CLA	3	311	-	1/1/15/20	11/39/115/115	-
24	LHG	2	316	-	-	3/38/38/53	-
20	CLA	B	801	-	1/1/15/20	15/39/115/115	-
20	CLA	B	825	-	-	4/15/91/115	-
22	XAT	1	311	-	-	14/31/93/93	0/4/4/4
20	CLA	1	305	24	-	5/17/93/115	-
20	CLA	2	320	2	-	6/17/93/115	-
25	MGE	J	102	-	-	3/37/57/63	0/1/1/1
20	CLA	B	827	6	1/1/15/20	11/39/115/115	-
20	CLA	4	309	4	-	9/26/102/115	-
20	CLA	3	318	3	-	0/10/86/115	-
20	CLA	A	827	5	1/1/15/20	10/39/115/115	-
20	CLA	1	309	-	-	4/10/86/115	-
20	CLA	3	312	3	-	1/15/91/115	-
20	CLA	A	809	5	1/1/15/20	16/39/115/115	-
20	CLA	1	320	-	-	7/20/96/115	-
24	LHG	B	843	-	-	5/29/29/53	-
27	SF4	C	102	7	-	-	0/6/5/5
29	DGD	J	104	-	-	14/55/95/95	0/2/2/2
20	CLA	B	830	6	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	837	5	1/1/15/20	13/39/115/115	-
20	CLA	A	846	5	-	6/17/93/115	-
24	LHG	B	841	-	-	8/36/36/53	-
20	CLA	A	847	5	1/1/13/20	6/29/105/115	-
20	CLA	A	825	-	1/1/15/20	11/39/115/115	-
20	CLA	A	803	5	-	4/33/109/115	-
20	CLA	B	812	6	1/1/15/20	15/39/115/115	-
20	CLA	2	308	2	-	6/23/99/115	-
20	CLA	K	203	15	-	9/18/94/115	-
23	BCR	A	817	-	-	1/29/63/63	0/2/2/2
20	CLA	A	802	5	1/1/15/20	18/39/115/115	-
20	CLA	A	836	5	-	9/24/100/115	-
23	BCR	G	201	-	-	5/29/63/63	0/2/2/2
24	LHG	B	842	-	-	6/33/33/53	-
23	BCR	A	818	-	-	6/27/61/63	0/2/2/2
20	CLA	A	833	5	1/1/15/20	11/39/115/115	-
20	CLA	F	305	-	-	0/17/93/115	-
20	CLA	J	103	14	-	4/17/93/115	-
20	CLA	A	829	5	1/1/14/20	17/38/114/115	-
20	CLA	B	846	6	-	3/15/91/115	-
23	BCR	B	837	-	-	2/29/63/63	0/2/2/2
23	BCR	B	838	-	-	5/29/63/63	0/2/2/2
27	SF4	A	813	5,6	-	-	0/6/5/5
20	CLA	2	307	2	1/1/14/20	16/36/112/115	-
20	CLA	A	811	24	1/1/13/20	14/27/103/115	-
20	CLA	4	303	-	-	3/17/93/115	-
20	CLA	B	810	6	-	4/19/95/115	-
20	CLA	A	856	5	1/1/13/20	5/29/105/115	-
20	CLA	B	802	6	-	5/15/91/115	-
20	CLA	B	831	-	1/1/15/20	8/39/115/115	-
23	BCR	O	202	-	-	8/29/63/63	0/2/2/2
20	CLA	B	829	-	1/1/15/20	10/39/115/115	-
20	CLA	3	316	-	-	2/17/93/115	-
29	DGD	G	202	-	-	8/34/54/95	0/1/1/2
20	CLA	A	845	-	1/1/15/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	849	6	-	7/24/100/115	-
23	BCR	A	814	-	-	2/29/63/63	0/2/2/2
20	CLA	A	854	5	1/1/15/20	15/39/115/115	-
20	CLA	B	828	6	-	8/18/94/115	-
23	BCR	L	302	-	-	2/29/63/63	0/2/2/2
24	LHG	A	820	-	-	5/28/28/53	-
20	CLA	1	308	1	-	3/17/93/115	-
20	CLA	3	319	-	-	7/17/93/115	-
23	BCR	A	815	-	-	2/29/63/63	0/2/2/2
21	LUT	1	310	-	-	1/29/67/67	0/2/2/2
19	CHL	1	317	1	-	9/23/99/117	-
20	CLA	K	205	15	-	3/17/93/115	-
20	CLA	A	850	-	1/1/13/20	11/31/107/115	-
23	BCR	3	303	-	-	4/29/63/63	0/2/2/2
28	CL0	A	824	5	1/1/15/20	5/37/113/115	-
23	BCR	K	202	-	-	2/29/63/63	0/2/2/2
20	CLA	O	208	-	-	5/15/91/115	-
20	CLA	B	822	6	1/1/15/20	9/39/115/115	-
26	PQN	B	832	-	-	4/20/40/43	0/2/2/2
20	CLA	1	318	1	1/1/15/20	8/39/115/115	-
23	BCR	B	834	-	-	6/29/63/63	0/2/2/2
19	CHL	2	318	2	1/1/13/21	14/32/108/117	-
23	BCR	4	319	-	-	6/29/63/63	0/2/2/2
22	XAT	2	311	-	-	7/31/93/93	0/4/4/4
20	CLA	B	821	6	1/1/13/20	5/29/105/115	-
20	CLA	3	309	-	1/1/14/20	15/33/109/115	-
23	BCR	J	101	-	-	4/29/63/63	0/2/2/2
20	CLA	A	808	5	1/1/15/20	11/39/115/115	-
20	CLA	B	850	6	1/1/15/20	14/39/115/115	-
20	CLA	A	851	5	1/1/15/20	20/39/115/115	-
25	MGE	4	322	-	-	5/35/55/63	0/1/1/1
25	MGE	A	823	-	-	3/29/49/63	0/1/1/1
19	CHL	2	301	-	-	9/19/95/117	-
20	CLA	H	201	12	1/1/13/20	10/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	N	202	17	1/1/13/20	5/29/105/115	-
20	CLA	B	826	6	-	5/21/97/115	-
23	BCR	B	835	-	-	4/29/63/63	0/2/2/2
20	CLA	B	852	-	1/1/15/20	11/39/115/115	-
20	CLA	3	310	-	-	6/20/96/115	-
25	MGE	1	316	-	-	4/35/55/63	0/1/1/1
20	CLA	A	849	-	1/1/15/20	15/39/115/115	-
20	CLA	A	831	5	-	7/24/100/115	-
25	MGE	G	204	-	-	6/43/63/63	0/1/1/1
20	CLA	B	845	-	1/1/15/20	9/39/115/115	-
20	CLA	A	812	-	1/1/15/20	6/39/115/115	-
20	CLA	B	847	6	1/1/15/20	15/39/115/115	-
23	BCR	2	312	-	-	8/29/63/63	0/2/2/2
24	LHG	A	822	-	-	8/43/43/53	-
21	LUT	2	310	-	-	3/29/67/67	0/2/2/2
20	CLA	A	835	5,20	1/1/15/20	10/39/115/115	-
20	CLA	1	307	1	1/1/13/20	6/27/103/115	-
20	CLA	2	321	-	-	10/21/97/115	-
25	MGE	1	324	-	-	12/43/63/63	0/1/1/1
25	MGE	3	304	-	-	1/28/48/63	0/1/1/1
20	CLA	2	304	2	1/1/13/20	4/27/103/115	-
24	LHG	O	205	-	-	16/43/43/53	-
20	CLA	A	853	5	1/1/15/20	16/39/115/115	-
20	CLA	2	317	-	-	6/18/94/115	-
20	CLA	B	818	6	1/1/15/20	7/39/115/115	-
20	CLA	B	844	6	1/1/15/20	10/39/115/115	-
20	CLA	B	819	6	1/1/15/20	13/39/115/115	-
27	SF4	C	101	7	-	-	0/6/5/5
20	CLA	B	848	6	1/1/15/20	11/39/115/115	-
20	CLA	A	843	5	1/1/15/20	7/39/115/115	-
25	MGE	3	305	-	-	7/29/49/63	0/1/1/1
24	LHG	1	314	-	-	8/34/34/53	-
20	CLA	B	833	-	1/1/14/20	13/35/111/115	-
20	CLA	3	308	3	1/1/14/20	8/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LHG	I	101	-	-	6/37/37/53	-
20	CLA	A	828	5,20	-	7/24/100/115	-
23	BCR	B	839	-	-	10/24/41/63	0/1/1/2
20	CLA	B	824	6	1/1/14/20	10/33/109/115	-
20	CLA	B	803	6	1/1/15/20	17/39/115/115	-
25	MGE	F	303	-	-	8/23/43/63	0/1/1/1
20	CLA	2	319	2	1/1/14/20	10/36/112/115	-
20	CLA	B	853	6	1/1/13/20	7/27/103/115	-
20	CLA	B	807	6	1/1/15/20	13/39/115/115	-
20	CLA	B	820	6	1/1/13/20	7/32/108/115	-
20	CLA	K	206	15	-	2/12/88/115	-
20	CLA	B	804	6	1/1/15/20	13/39/115/115	-
20	CLA	3	320	3	-	2/15/91/115	-
20	CLA	4	310	-	1/1/14/20	9/33/109/115	-
19	CHL	3	313	-	-	12/22/98/117	-
20	CLA	3	314	3	-	2/15/91/115	-
23	BCR	A	816	-	-	9/29/63/63	0/2/2/2
23	BCR	I	102	-	-	4/29/63/63	0/2/2/2
23	BCR	O	203	-	-	2/29/63/63	0/2/2/2
23	BCR	B	836	-	-	5/29/63/63	0/2/2/2
20	CLA	1	306	-	-	4/15/91/115	-
20	CLA	O	206	18	1/1/15/20	11/39/115/115	-
25	MGE	3	306	-	-	5/33/53/63	0/1/1/1
20	CLA	A	832	5	1/1/15/20	11/39/115/115	-
24	LHG	2	313	-	-	15/45/45/53	-
24	LHG	4	321	-	-	5/53/53/53	-
20	CLA	A	834	5	1/1/13/20	11/27/103/115	-
29	DGD	B	840	-	-	17/48/88/95	0/2/2/2
20	CLA	2	323	4	-	5/17/93/115	-
20	CLA	4	313	4	-	4/21/97/115	-
21	LUT	4	317	-	-	2/29/67/67	0/2/2/2
22	XAT	4	318	-	-	1/31/93/93	0/4/4/4
23	BCR	F	302	-	-	4/29/63/63	0/2/2/2
20	CLA	A	830	5	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	844	5	-	6/17/93/115	-
20	CLA	2	305	24	1/1/13/20	7/27/103/115	-
24	LHG	2	314	-	-	14/43/43/53	-
20	CLA	B	808	6	1/1/15/20	11/39/115/115	-

The worst 5 of 3517 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	805	CLA	C1D-ND	8.79	1.48	1.37
20	K	205	CLA	C1D-ND	8.65	1.48	1.37
20	1	309	CLA	C1D-ND	8.63	1.48	1.37
20	1	305	CLA	C1D-ND	8.62	1.48	1.37
20	2	308	CLA	C1D-ND	8.61	1.48	1.37

The worst 5 of 5231 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	302	XAT	C40-C33-C34	-33.63	75.82	122.92
22	3	302	XAT	C40-C33-C32	-26.40	76.48	118.08
22	2	311	XAT	O4-C5-C4	-23.89	95.43	113.38
22	3	302	XAT	C32-C33-C34	21.58	152.06	118.94
22	2	311	XAT	O4-C5-C18	-18.69	92.66	115.06

5 of 93 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	2	318	CHL	C8
20	1	303	CLA	C8
20	1	304	CLA	C8
20	1	307	CLA	C8
20	1	318	CLA	C8

5 of 1804 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	1	301	CHL	C1A-C2A-CAA-CBA
19	1	317	CHL	C2B-C3B-CAB-CBB
19	1	317	CHL	C4B-C3B-CAB-CBB
19	1	317	CHL	C3C-C2C-CMC-OMC
19	2	301	CHL	C3A-C2A-CAA-CBA

There are no ring outliers.

199 monomers are involved in 678 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	4	302	CLA	3	0
20	K	204	CLA	2	0
20	B	816	CLA	6	0
19	2	302	CHL	7	0
20	B	814	CLA	12	0
20	A	801	CLA	5	0
20	G	206	CLA	1	0
19	2	322	CHL	3	0
23	G	203	BCR	4	0
20	A	838	CLA	2	0
19	4	315	CHL	5	0
22	3	302	XAT	12	0
23	L	301	BCR	3	0
26	A	810	PQN	11	0
20	A	840	CLA	2	0
20	L	305	CLA	2	0
20	1	319	CLA	5	0
20	B	815	CLA	3	0
20	G	205	CLA	6	0
21	3	301	LUT	15	0
20	B	809	CLA	5	0
20	A	806	CLA	6	0
20	4	316	CLA	1	0
23	4	320	BCR	6	0
19	1	301	CHL	6	0
21	1	323	LUT	15	0
20	G	207	CLA	1	0
20	A	805	CLA	4	0
19	4	306	CHL	7	0
20	B	817	CLA	4	0
20	4	314	CLA	2	0
20	B	813	CLA	1	0
20	B	823	CLA	2	0
24	A	819	LHG	3	0
20	4	312	CLA	2	0
20	O	207	CLA	1	0
19	2	309	CHL	4	0
20	A	855	CLA	2	0
20	4	304	CLA	4	0
19	4	307	CHL	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	1	313	LHG	2	0
23	1	312	BCR	4	0
20	4	308	CLA	2	0
20	L	306	CLA	2	0
20	2	306	CLA	1	0
23	L	303	BCR	4	0
20	2	303	CLA	3	0
20	B	805	CLA	4	0
20	A	839	CLA	2	0
20	L	307	CLA	1	0
20	1	302	CLA	2	0
25	1	315	MGE	12	0
20	A	848	CLA	2	0
20	1	322	CLA	4	0
20	B	851	CLA	1	0
19	4	305	CHL	12	0
20	A	826	CLA	5	0
20	1	321	CLA	1	0
20	1	303	CLA	6	0
20	F	306	CLA	5	0
20	A	852	CLA	4	0
23	L	304	BCR	3	0
25	N	201	MGE	15	0
20	A	842	CLA	1	0
23	A	857	BCR	6	0
20	3	315	CLA	1	0
20	3	317	CLA	3	0
20	1	304	CLA	2	0
20	A	841	CLA	1	0
20	F	304	CLA	4	0
23	F	301	BCR	7	0
23	K	201	BCR	4	0
20	3	311	CLA	4	0
20	B	801	CLA	3	0
20	B	825	CLA	4	0
22	1	311	XAT	25	0
25	J	102	MGE	13	0
20	4	309	CLA	2	0
20	B	827	CLA	3	0
20	A	827	CLA	1	0
20	1	309	CLA	2	0
20	3	312	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	809	CLA	4	0
20	1	320	CLA	2	0
20	B	830	CLA	5	0
20	A	837	CLA	1	0
20	A	846	CLA	3	0
20	A	847	CLA	3	0
20	A	825	CLA	4	0
20	B	812	CLA	7	0
20	2	308	CLA	2	0
23	A	817	BCR	3	0
20	A	802	CLA	3	0
20	A	836	CLA	2	0
23	G	201	BCR	6	0
23	A	818	BCR	2	0
20	A	833	CLA	5	0
20	A	829	CLA	1	0
20	B	846	CLA	3	0
23	B	837	BCR	6	0
23	B	838	BCR	10	0
20	2	307	CLA	6	0
20	4	303	CLA	1	0
20	B	810	CLA	3	0
20	B	802	CLA	1	0
23	O	202	BCR	3	0
20	B	829	CLA	6	0
29	G	202	DGD	13	0
20	A	845	CLA	4	0
23	A	814	BCR	4	0
20	A	854	CLA	3	0
20	B	828	CLA	7	0
23	L	302	BCR	6	0
24	A	820	LHG	4	0
20	1	308	CLA	3	0
23	A	815	BCR	3	0
21	1	310	LUT	12	0
19	1	317	CHL	10	0
20	K	205	CLA	3	0
20	A	850	CLA	1	0
23	3	303	BCR	2	0
23	K	202	BCR	2	0
26	B	832	PQN	16	0
20	B	822	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	A	824	CL0	13	0
20	1	318	CLA	8	0
23	B	834	BCR	4	0
19	2	318	CHL	12	0
23	4	319	BCR	6	0
22	2	311	XAT	8	0
20	B	821	CLA	5	0
20	3	309	CLA	2	0
23	J	101	BCR	6	0
20	B	850	CLA	1	0
25	4	322	MGE	6	0
25	A	823	MGE	15	0
19	2	301	CHL	4	0
20	H	201	CLA	2	0
20	N	202	CLA	4	0
20	B	826	CLA	1	0
23	B	835	BCR	3	0
20	B	852	CLA	1	0
20	3	310	CLA	3	0
25	1	316	MGE	11	0
20	A	831	CLA	6	0
20	A	849	CLA	4	0
25	G	204	MGE	9	0
20	B	845	CLA	6	0
20	A	812	CLA	11	0
20	B	847	CLA	2	0
23	2	312	BCR	6	0
21	2	310	LUT	19	0
20	1	307	CLA	4	0
20	2	321	CLA	2	0
25	1	324	MGE	9	0
25	3	304	MGE	10	0
20	2	304	CLA	2	0
24	O	205	LHG	2	0
20	A	853	CLA	5	0
20	B	818	CLA	2	0
20	B	844	CLA	9	0
20	B	819	CLA	1	0
20	A	843	CLA	3	0
25	3	305	MGE	8	0
24	1	314	LHG	1	0
20	B	833	CLA	1	0

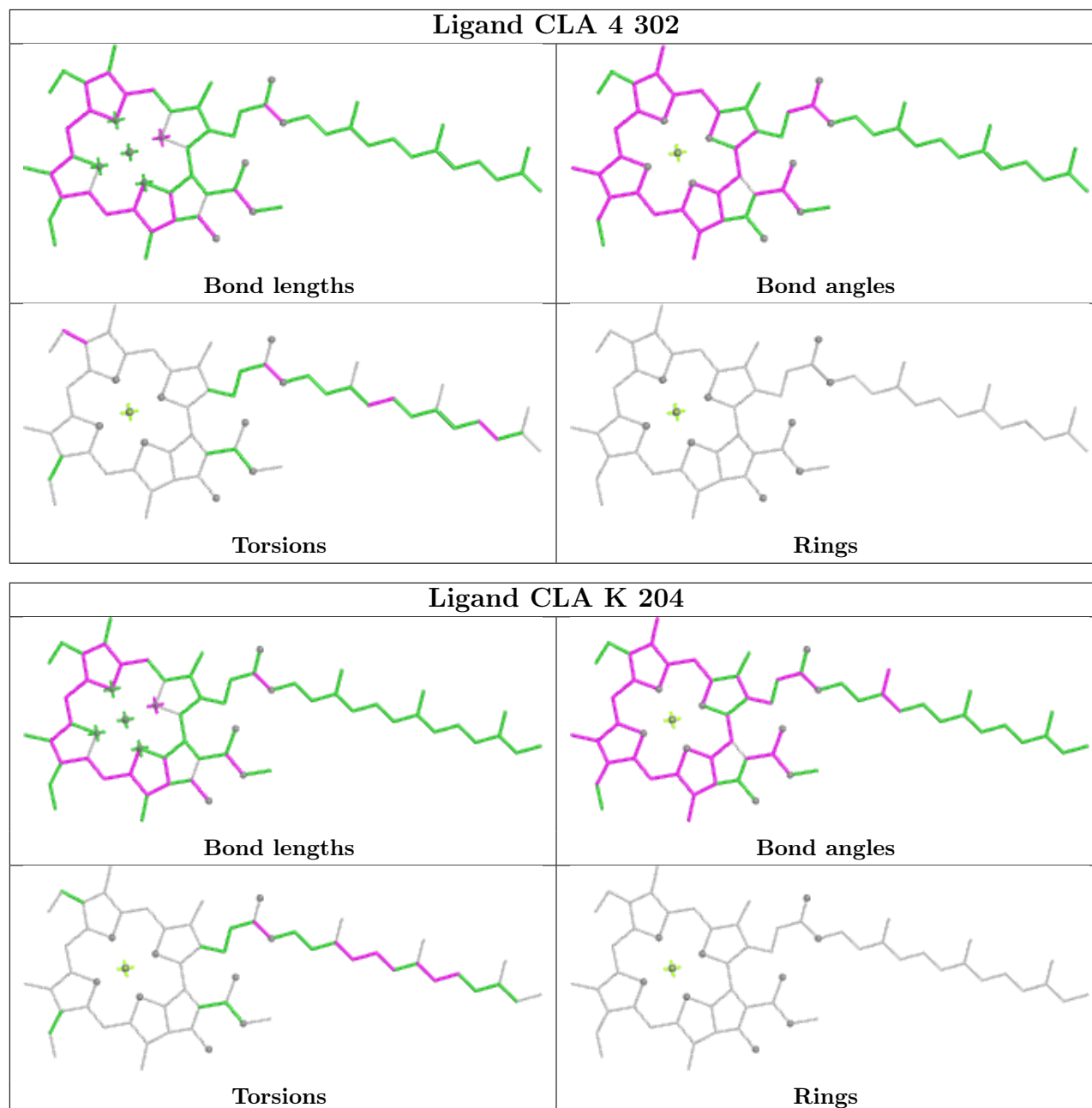
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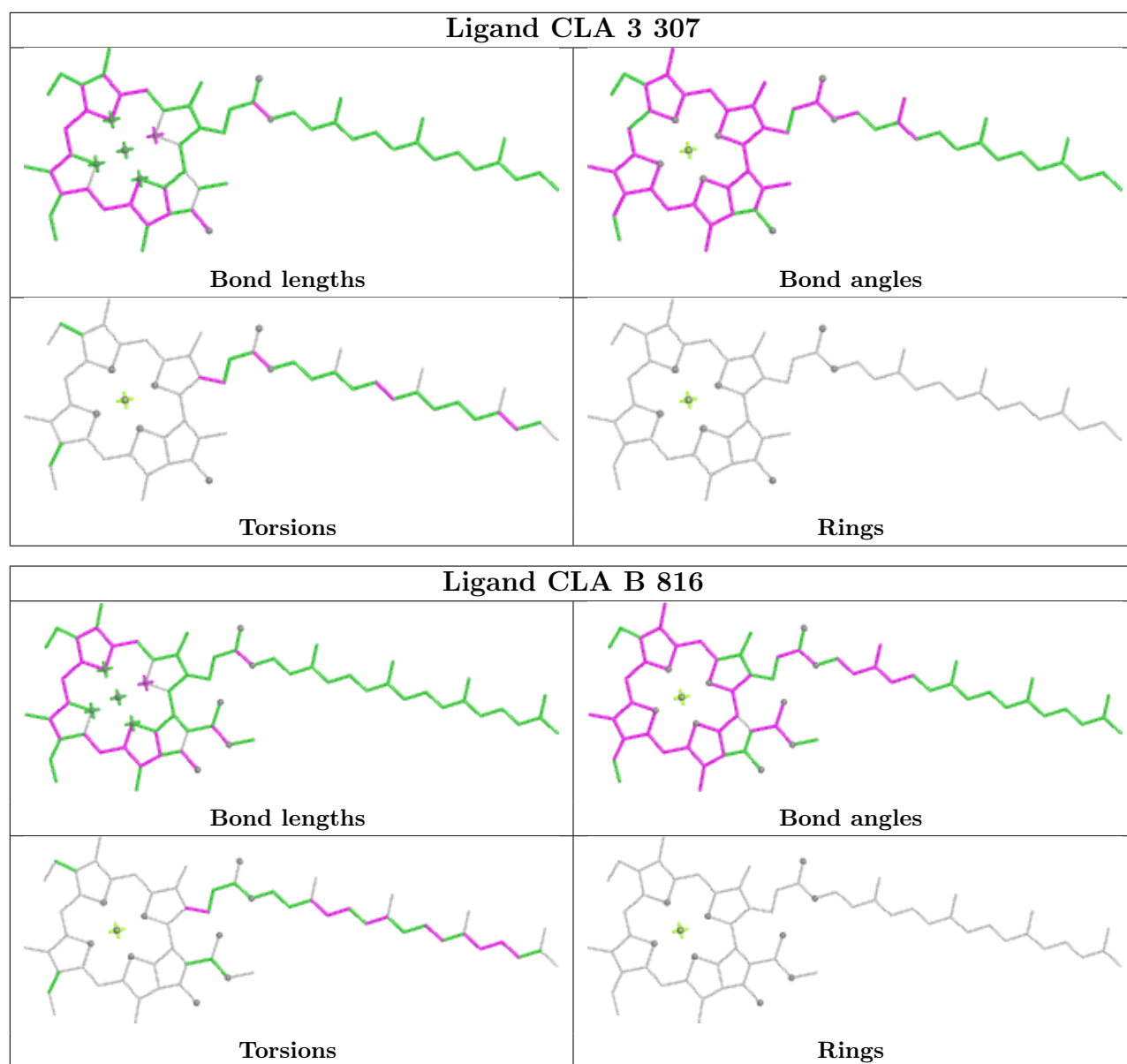
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	3	308	CLA	1	0
23	B	839	BCR	3	0
20	B	824	CLA	1	0
20	B	803	CLA	4	0
25	F	303	MGE	5	0
20	2	319	CLA	4	0
20	B	853	CLA	1	0
20	B	807	CLA	6	0
20	B	820	CLA	1	0
20	B	804	CLA	1	0
20	3	320	CLA	1	0
20	4	310	CLA	1	0
19	3	313	CHL	11	0
20	3	314	CLA	1	0
23	A	816	BCR	6	0
23	I	102	BCR	2	0
23	O	203	BCR	5	0
23	B	836	BCR	5	0
20	O	206	CLA	1	0
25	3	306	MGE	10	0
20	A	832	CLA	2	0
24	4	321	LHG	1	0
20	A	834	CLA	2	0
29	B	840	DGD	1	0
20	2	323	CLA	1	0
20	4	313	CLA	1	0
21	4	317	LUT	17	0
22	4	318	XAT	11	0
23	F	302	BCR	3	0
20	A	830	CLA	2	0
20	A	844	CLA	1	0
20	2	305	CLA	1	0
20	B	808	CLA	5	0

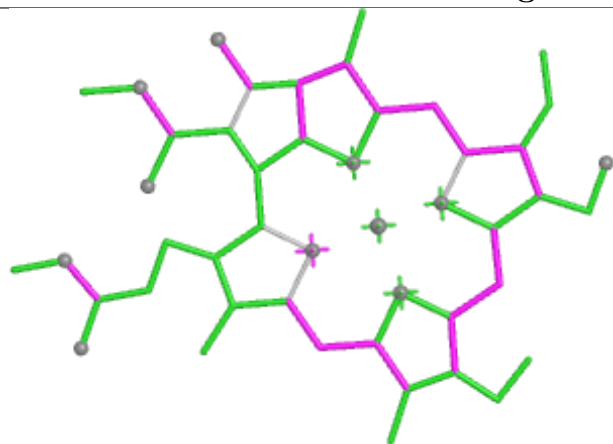
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

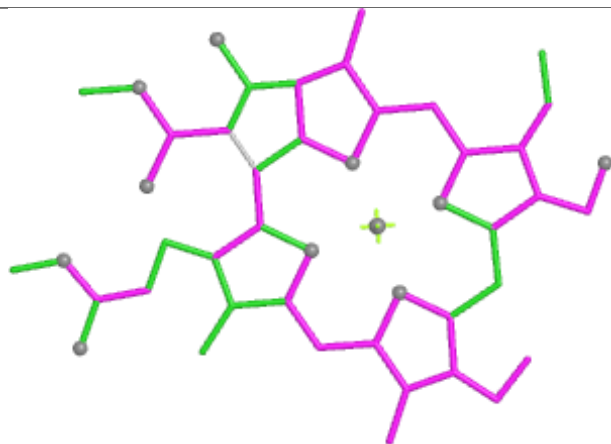




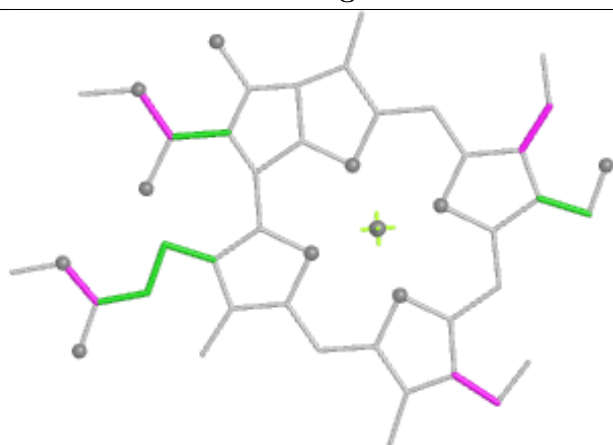
Ligand CHL 2 302



Bond lengths



Bond angles

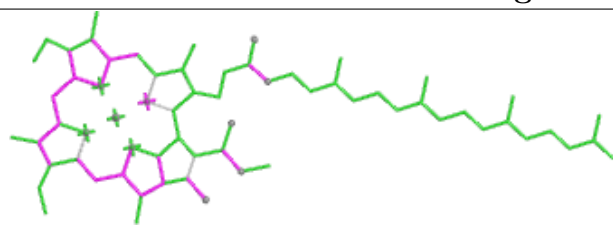


Torsions

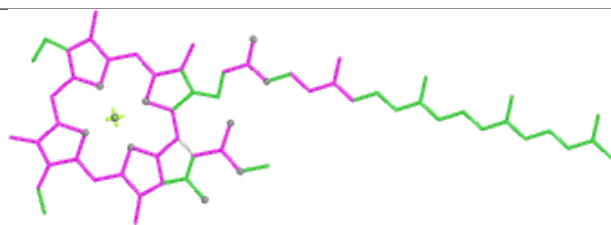


Rings

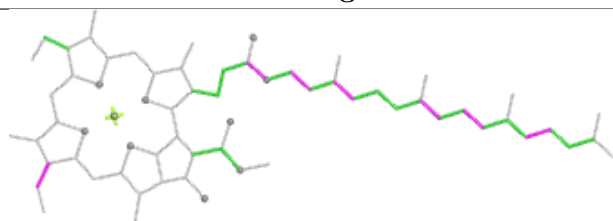
Ligand CLA B 814



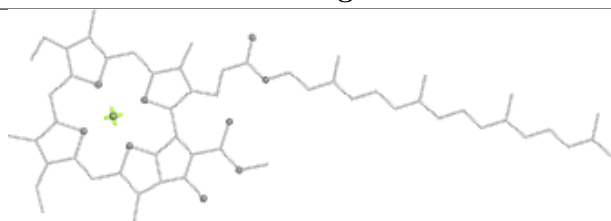
Bond lengths



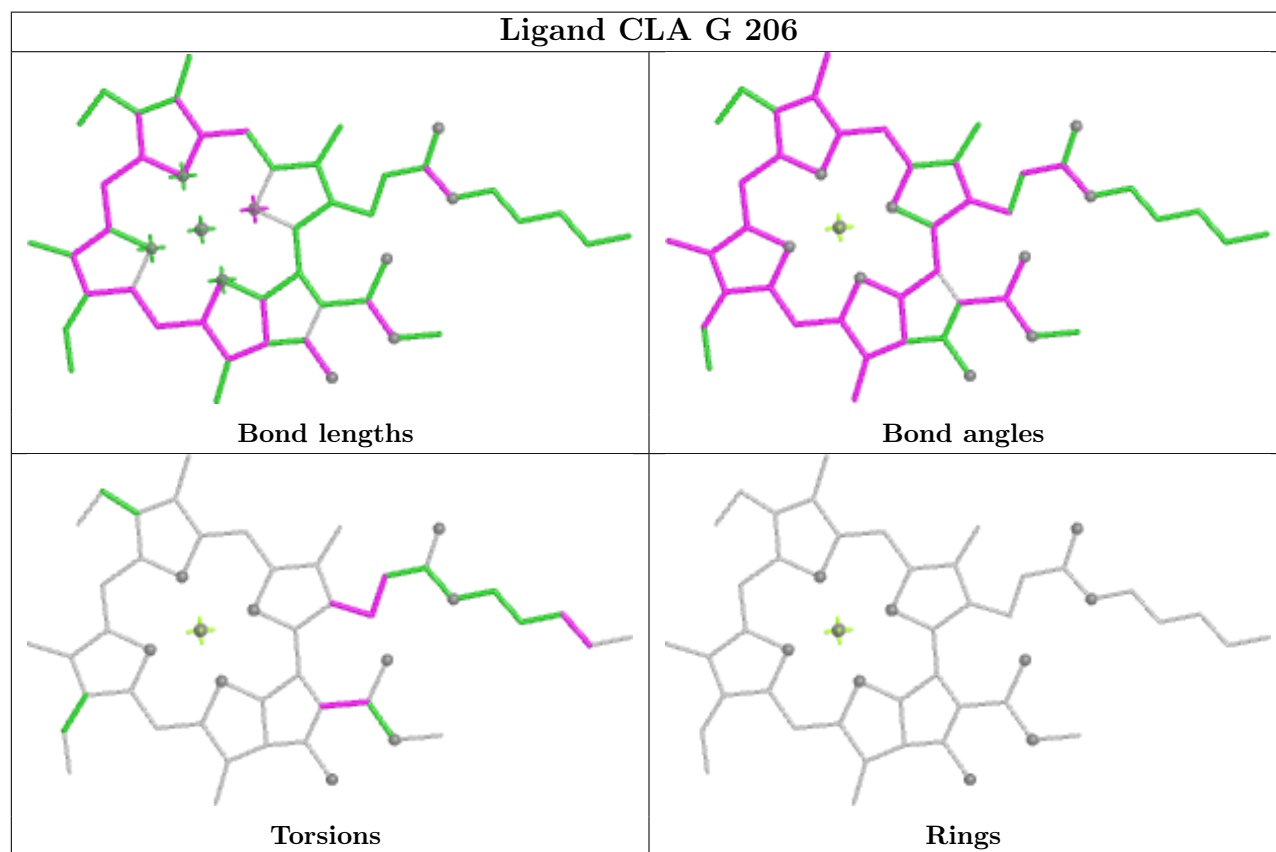
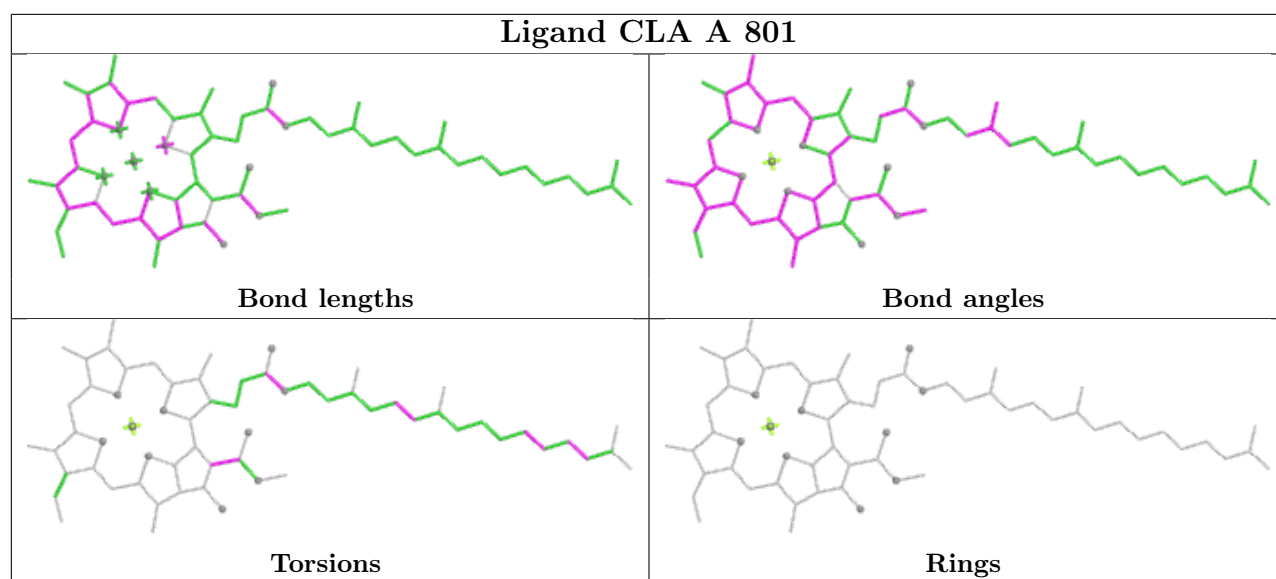
Bond angles



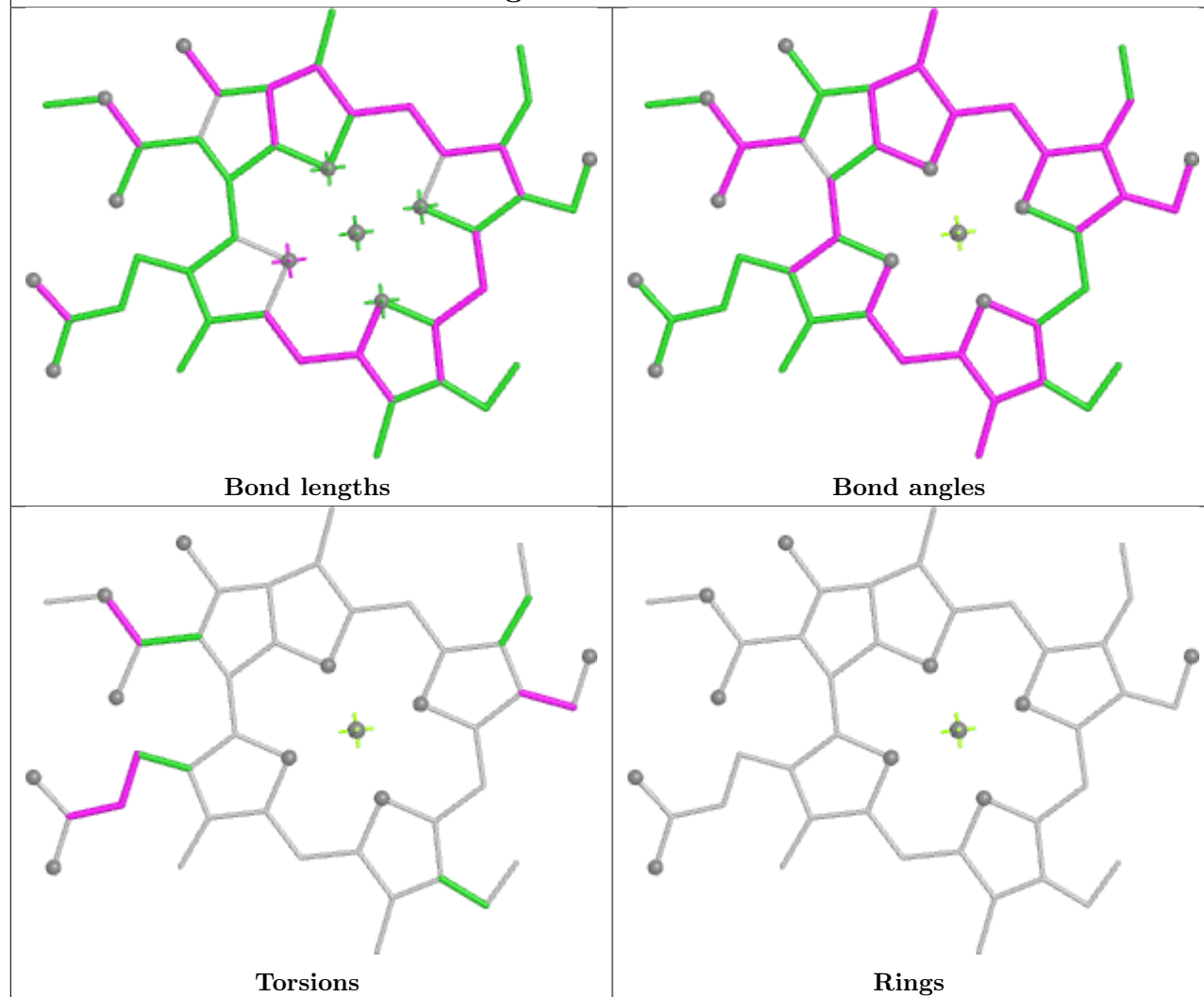
Torsions



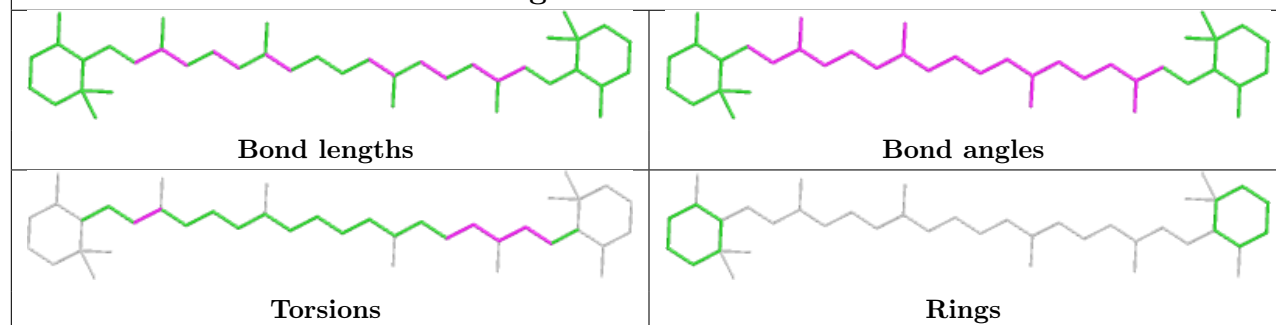
Rings



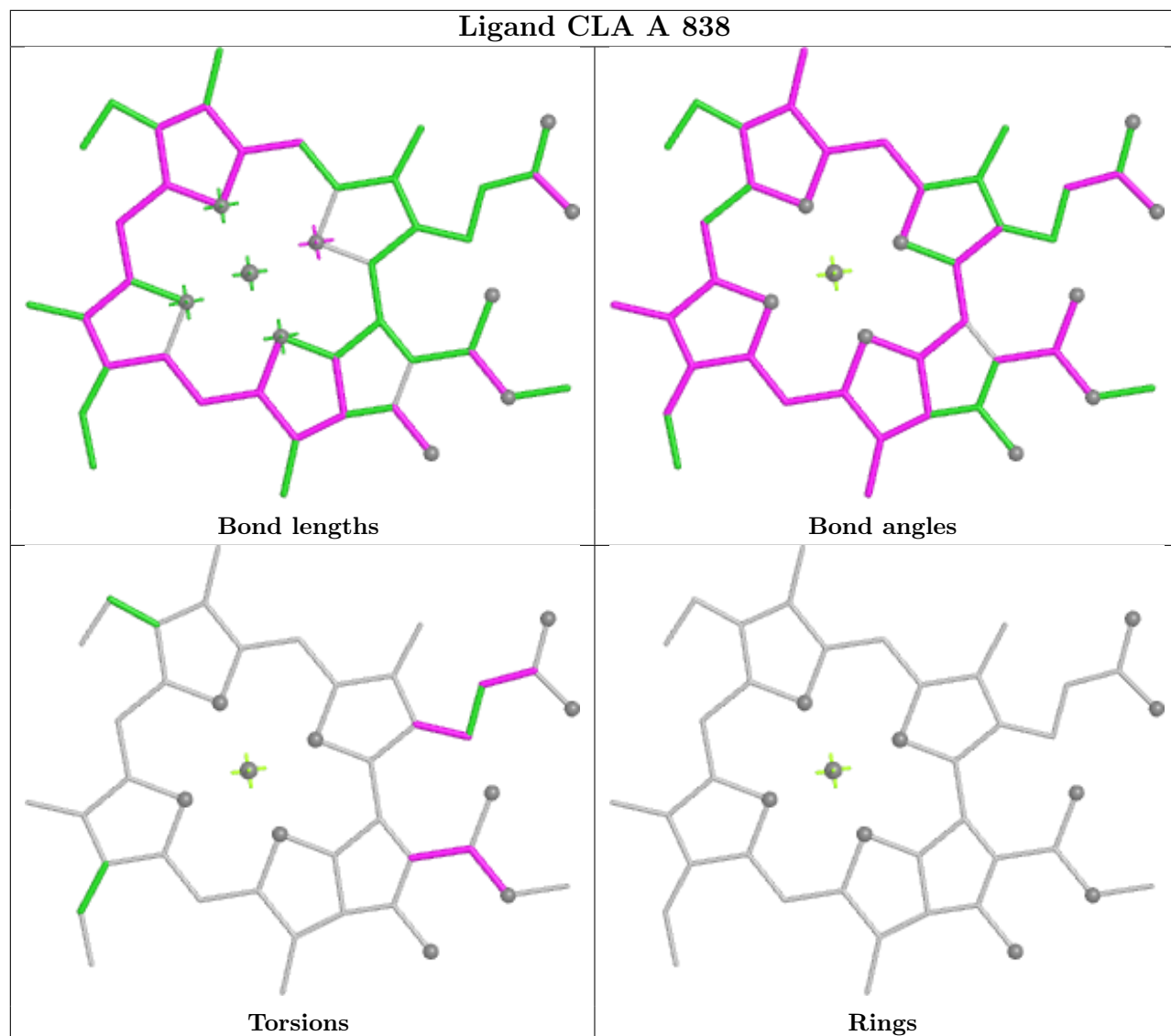
Ligand CHL 2 322



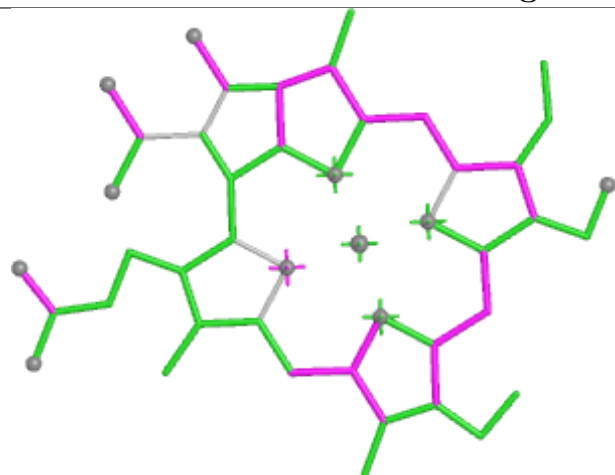
Ligand BCR G 203



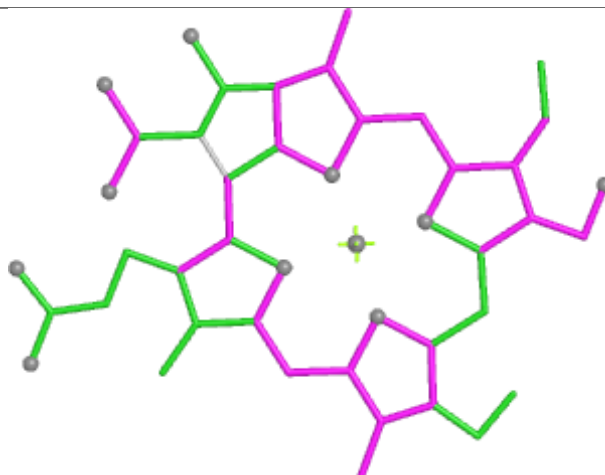
Ligand CLA A 838



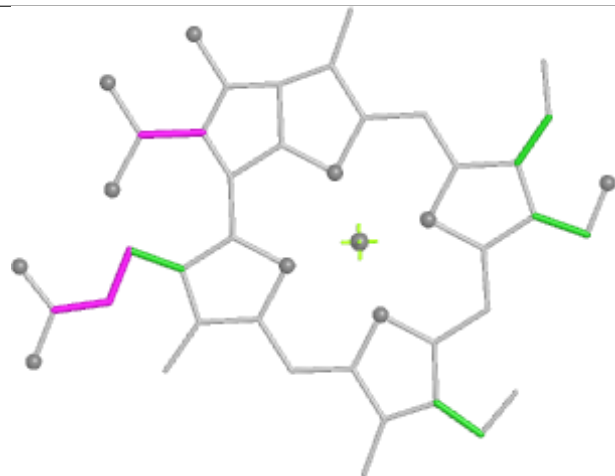
Ligand CHL 4 315



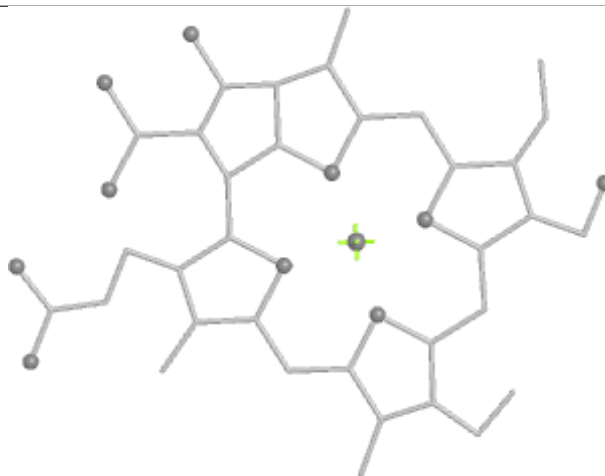
Bond lengths



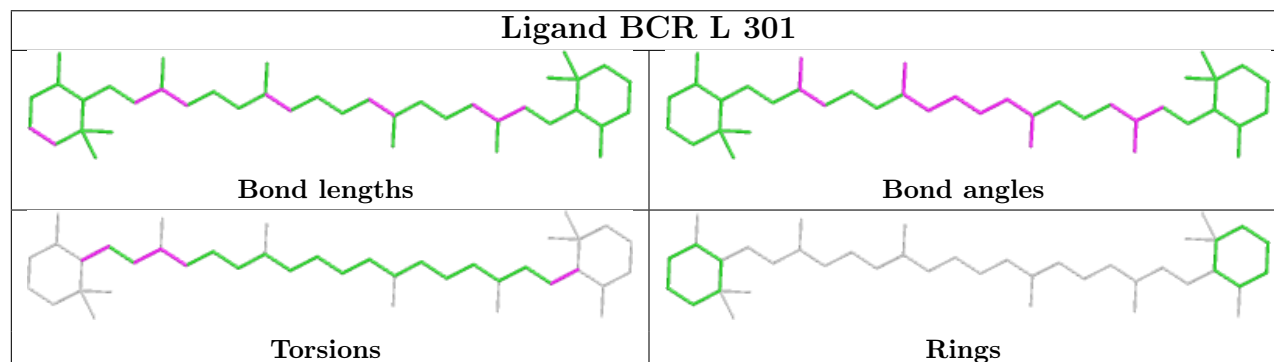
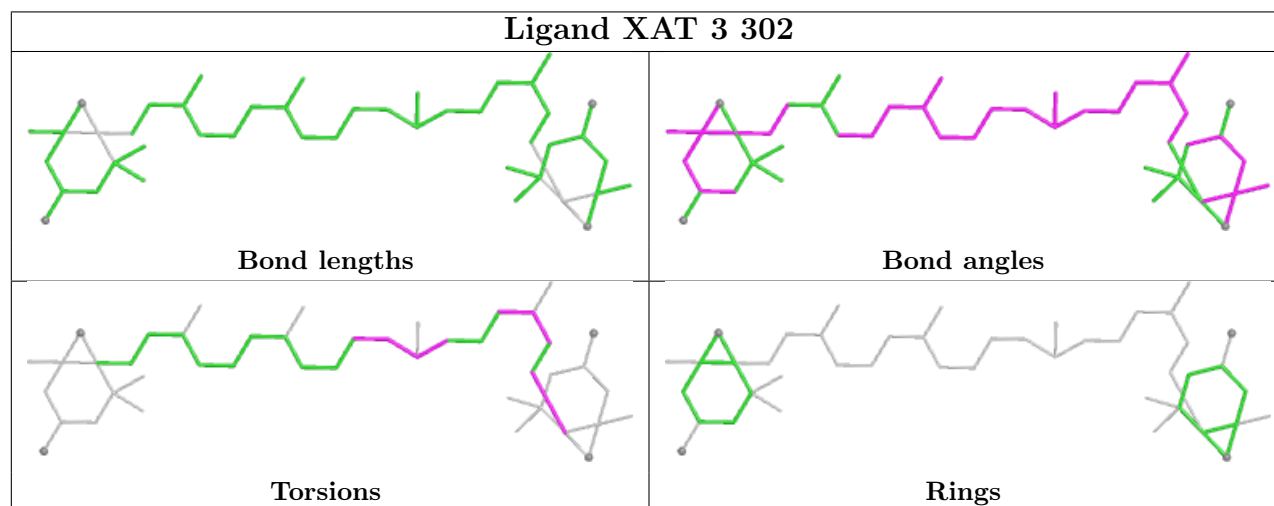
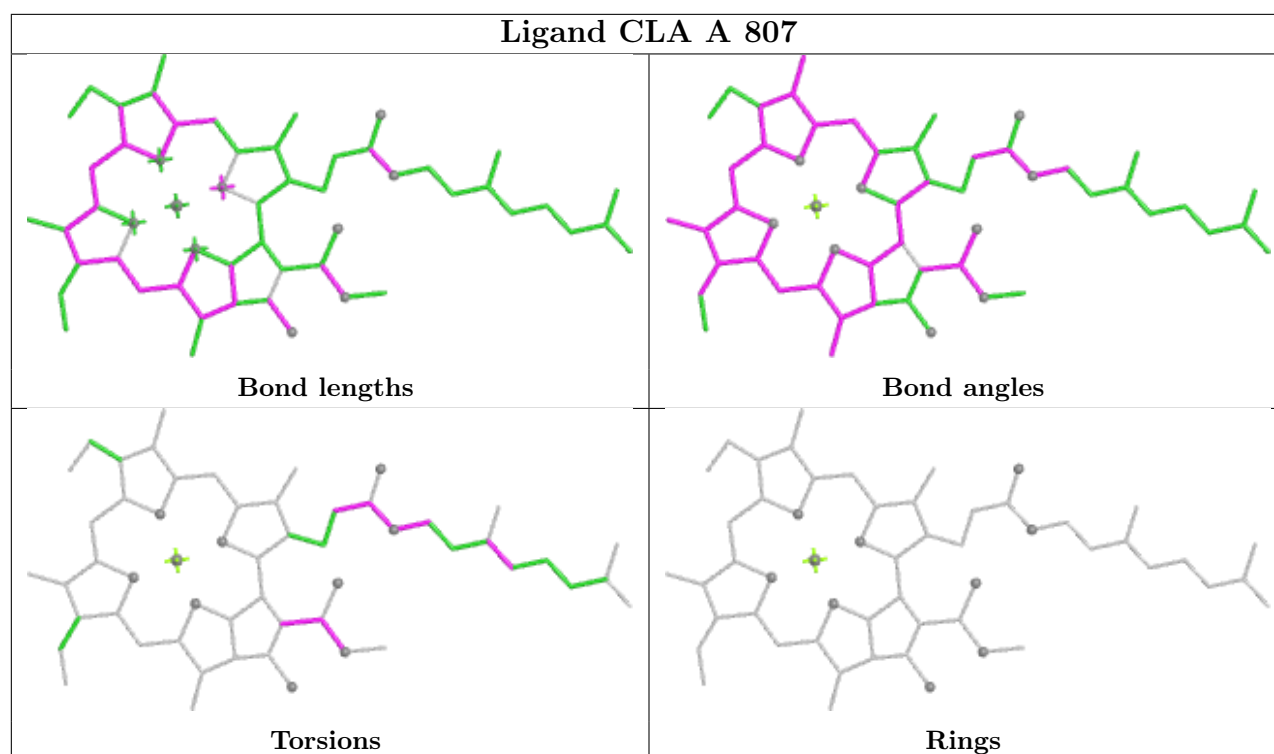
Bond angles

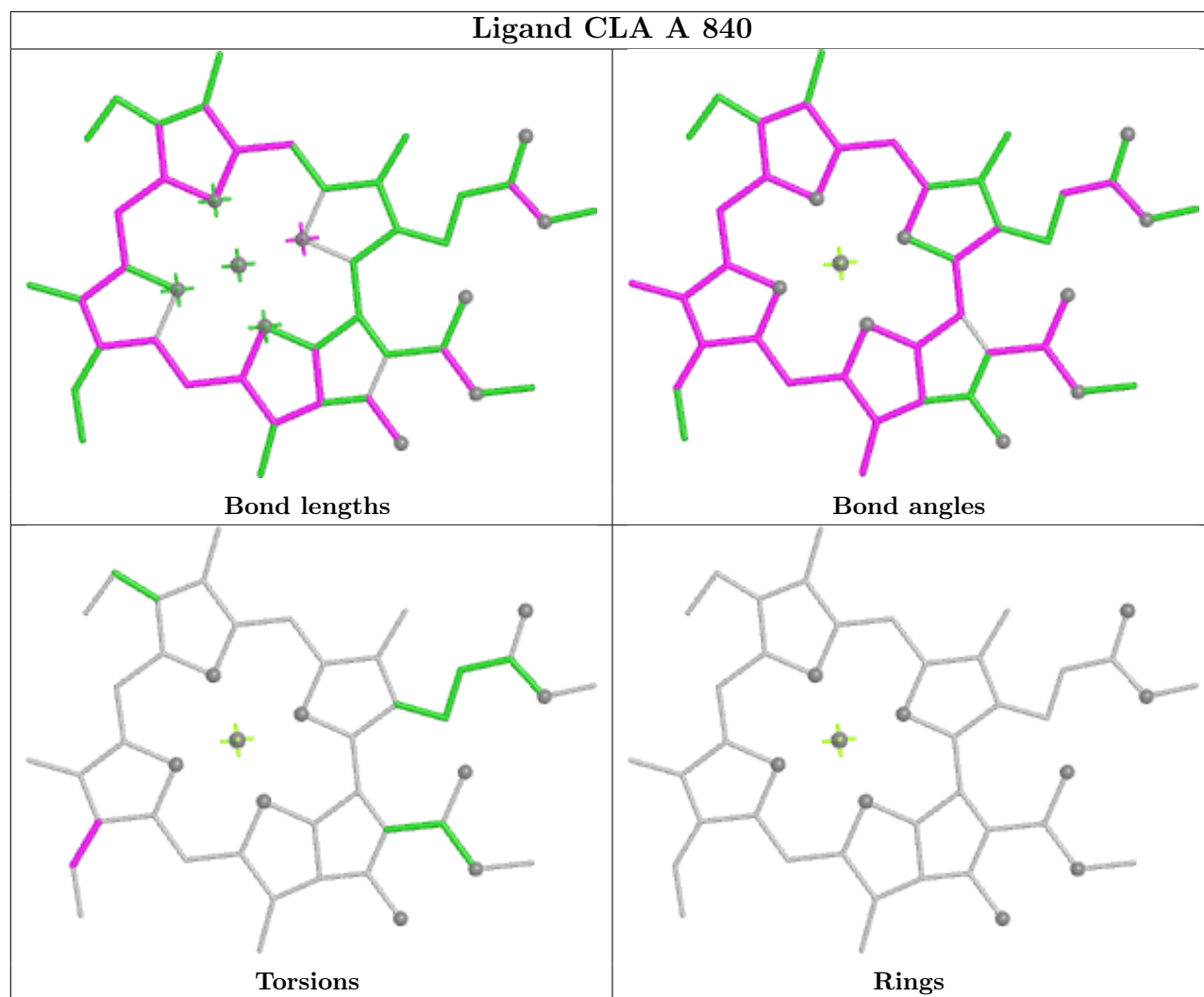
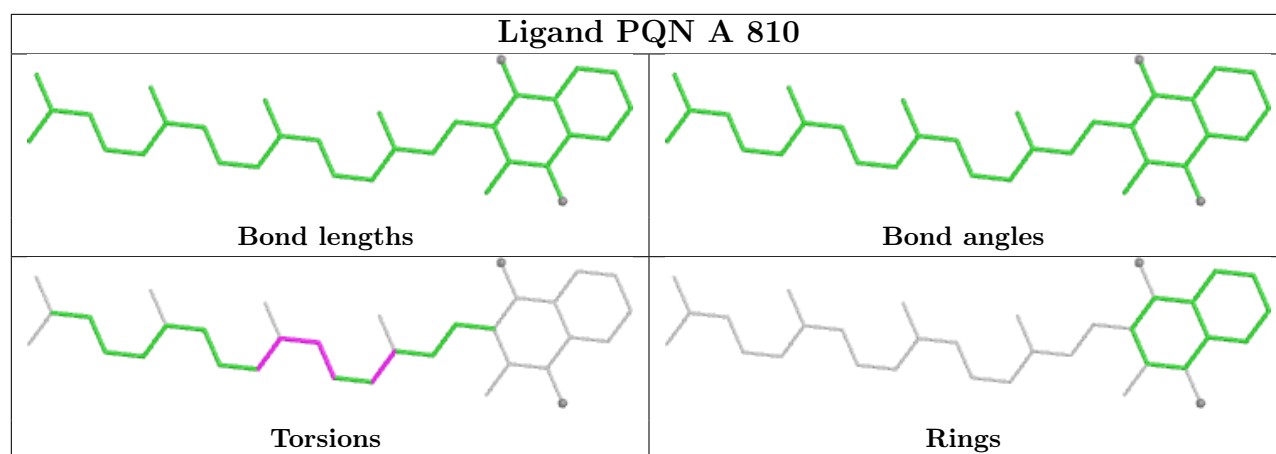


Torsions

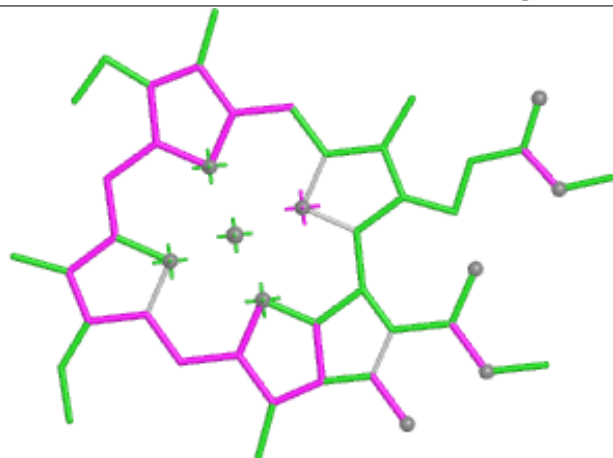


Rings

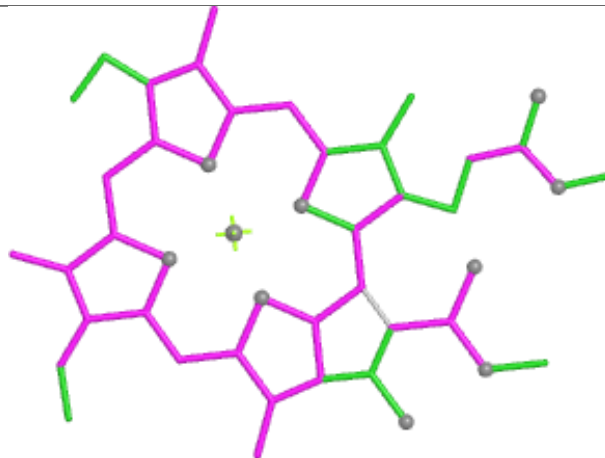




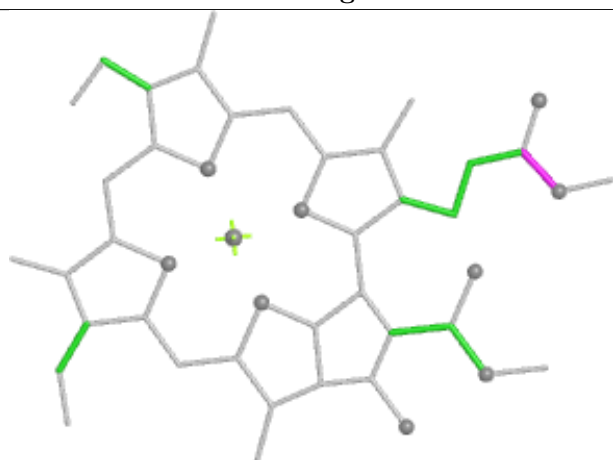
Ligand CLA L 305



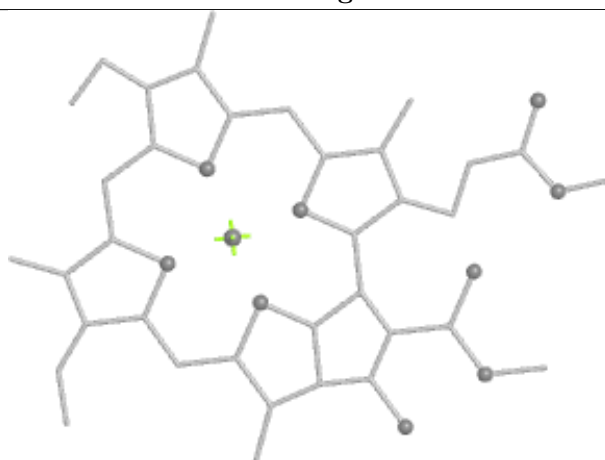
Bond lengths



Bond angles

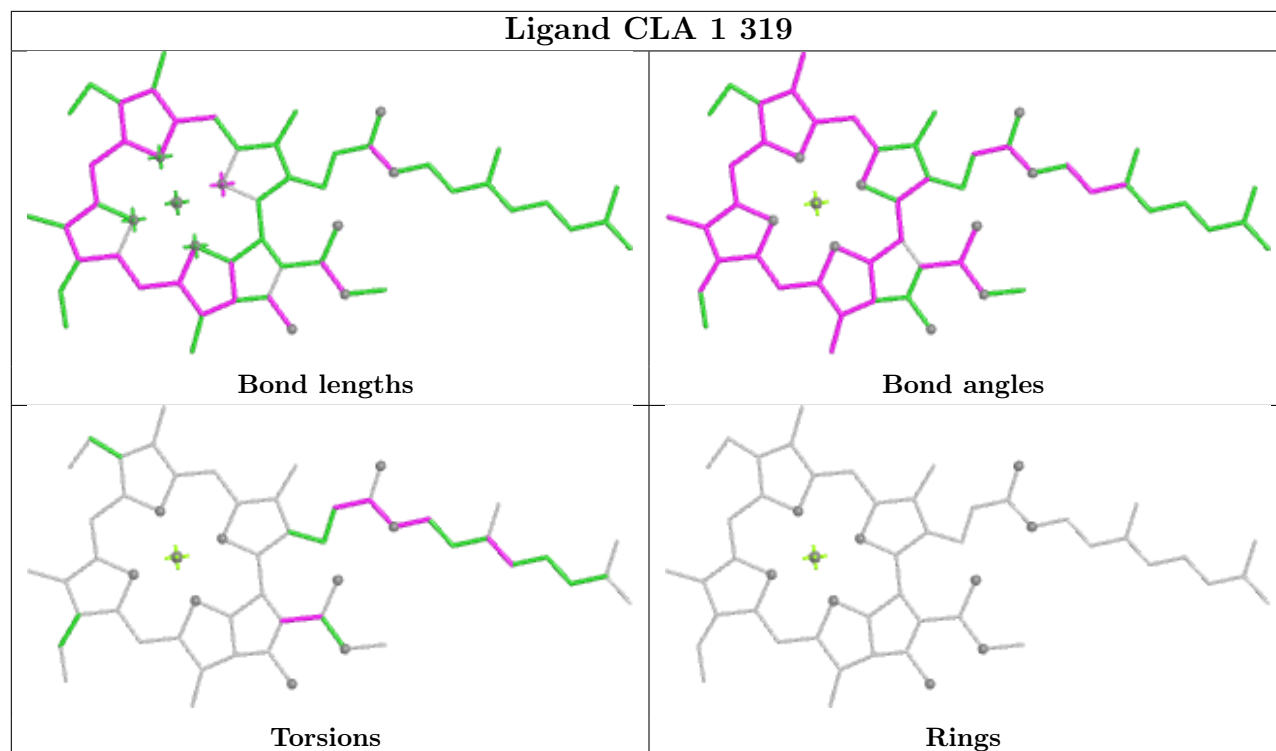


Torsions

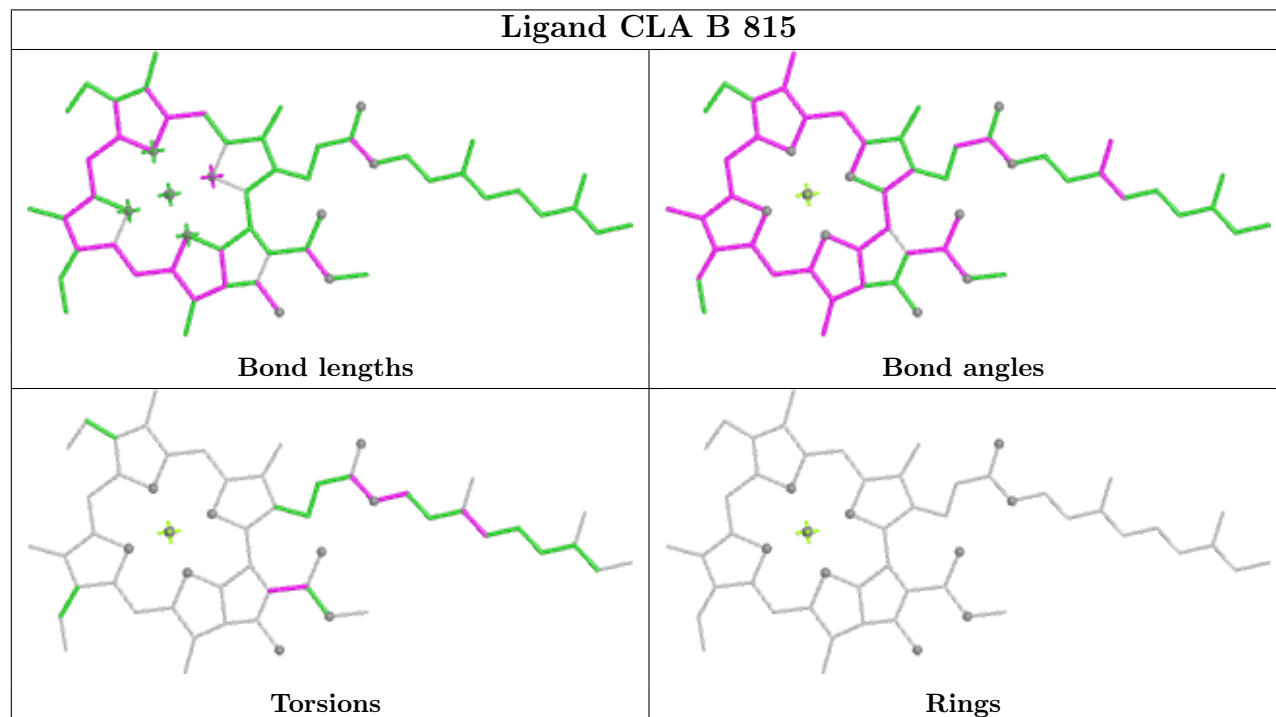


Rings

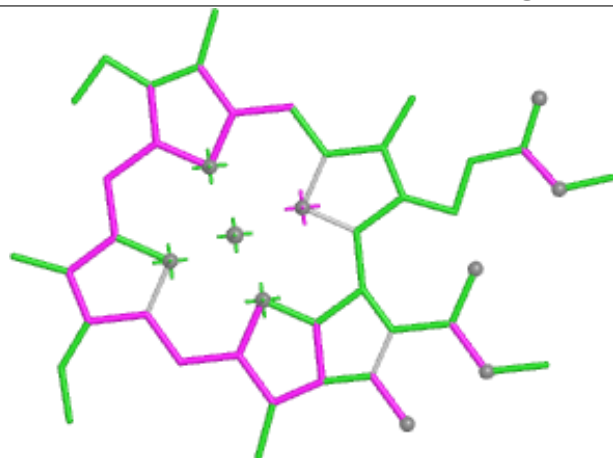
Ligand CLA 1 319



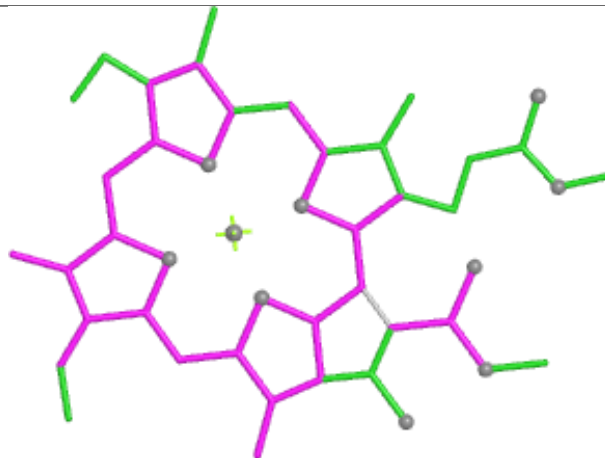
Ligand CLA B 815



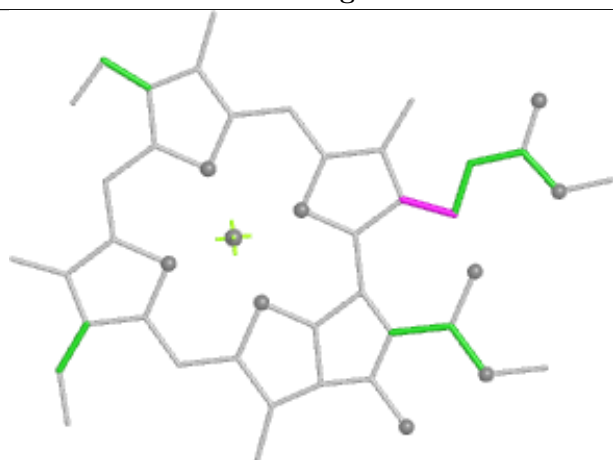
Ligand CLA 4 311



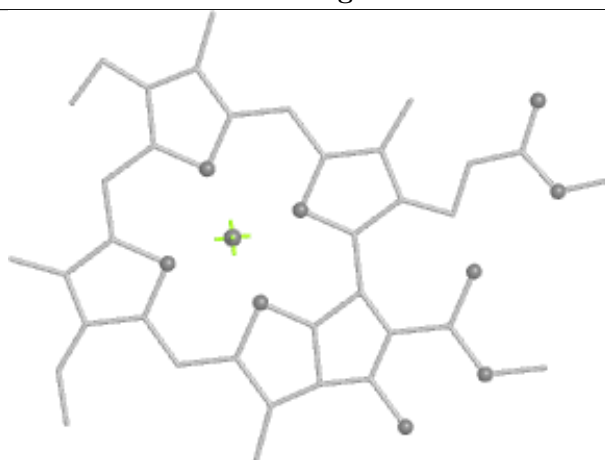
Bond lengths



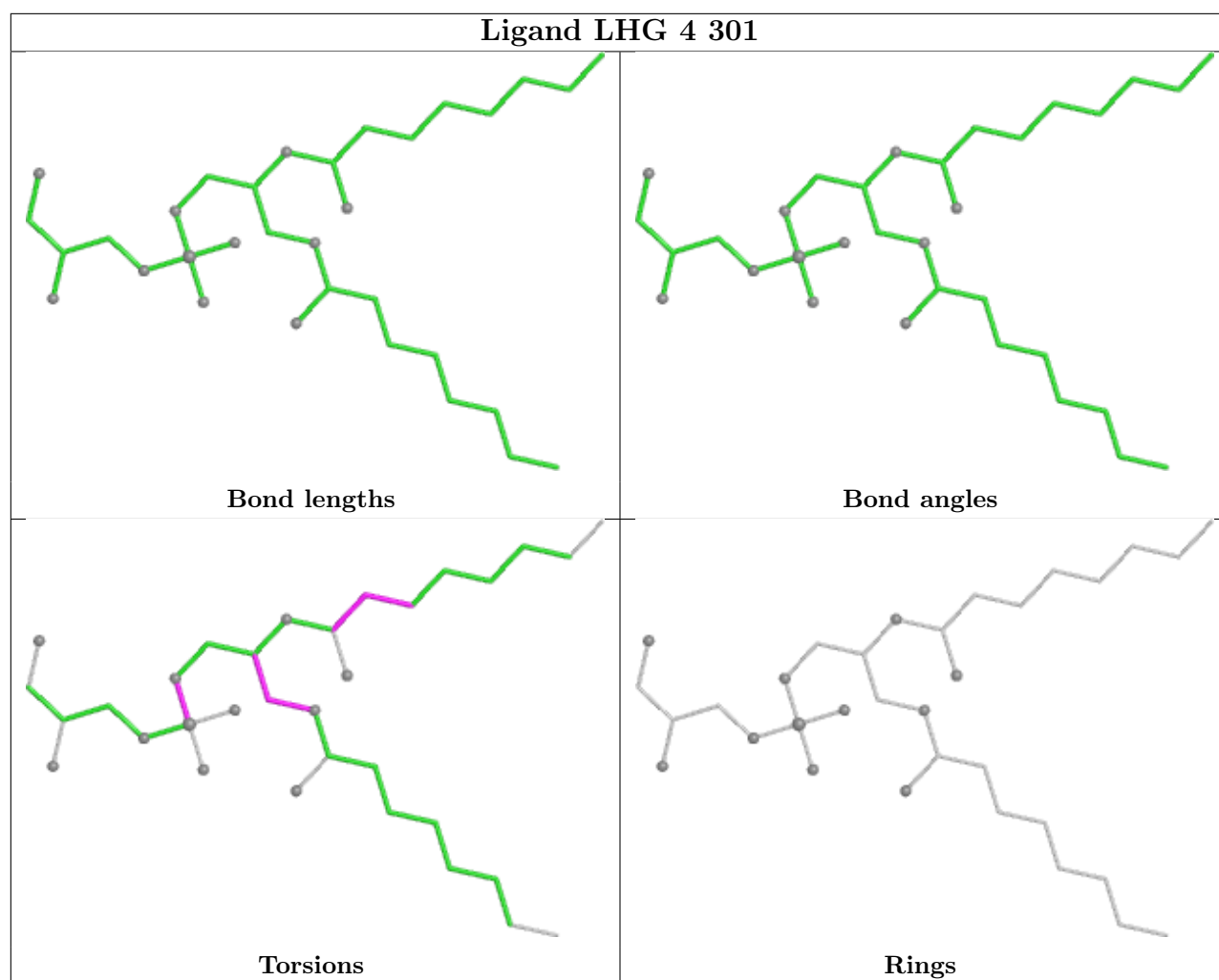
Bond angles

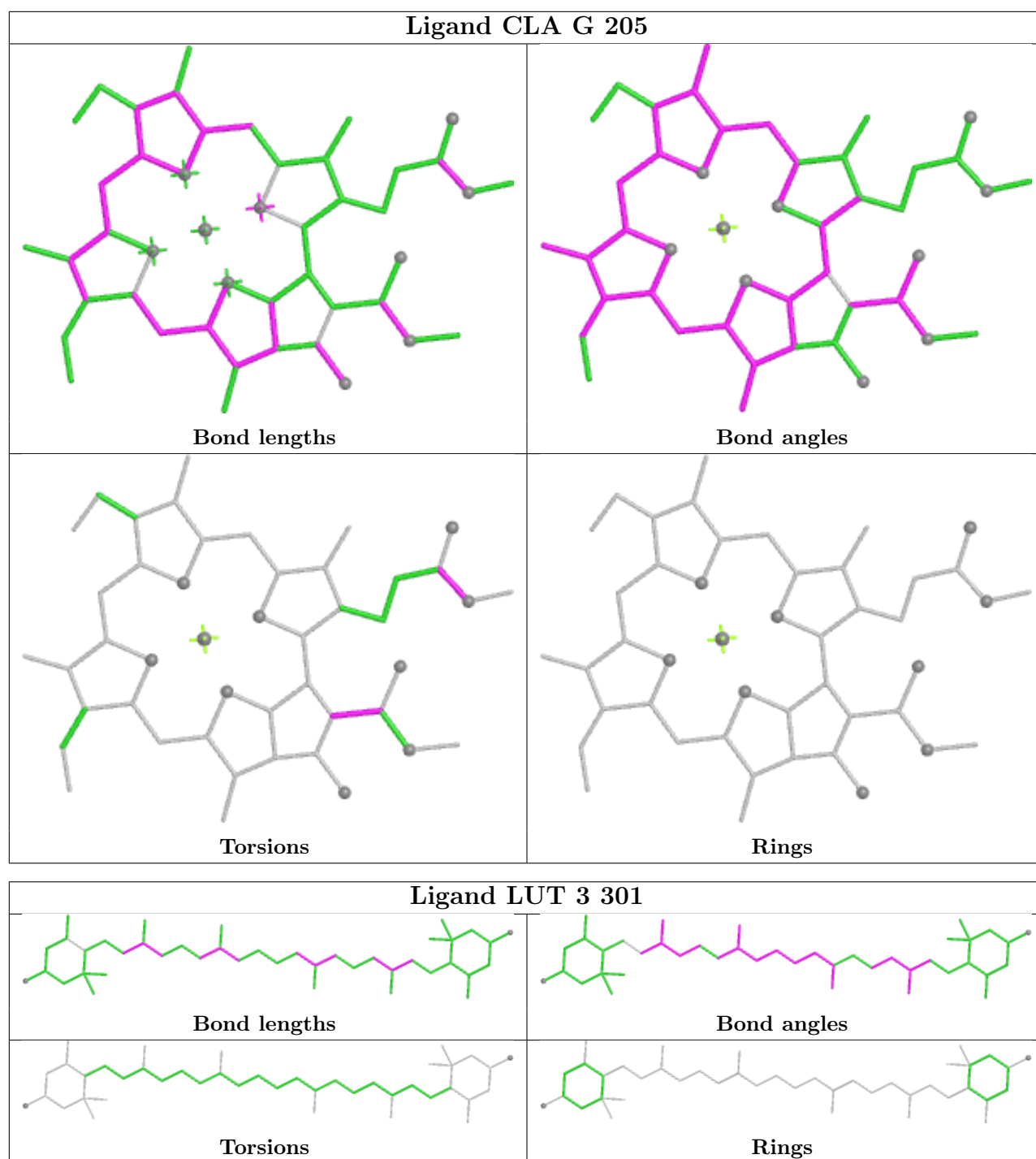


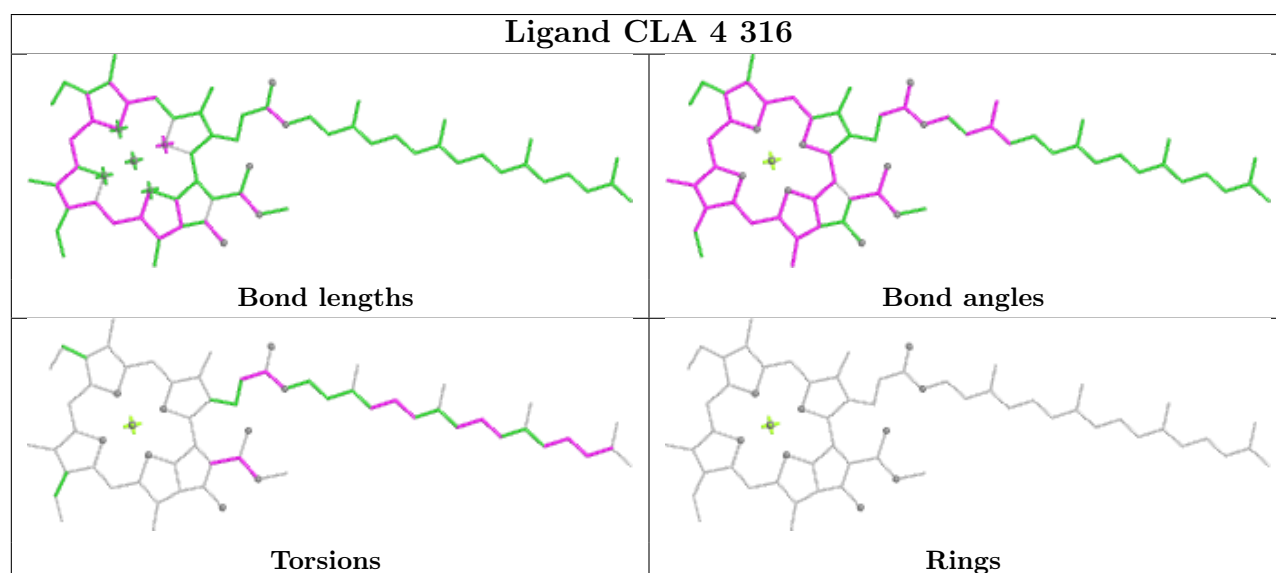
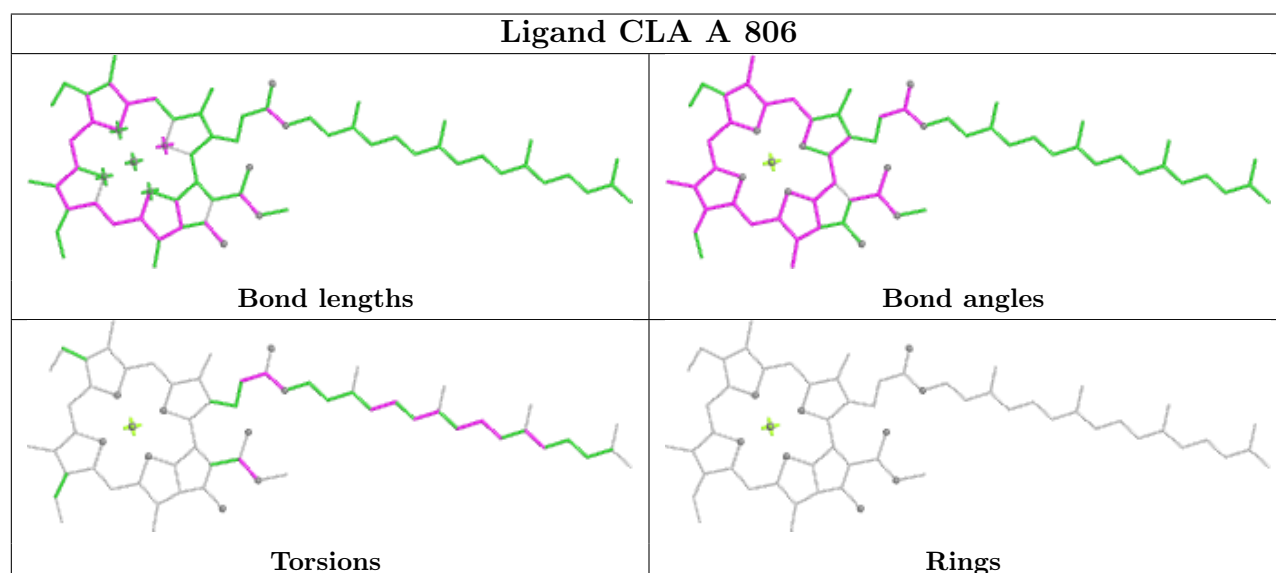
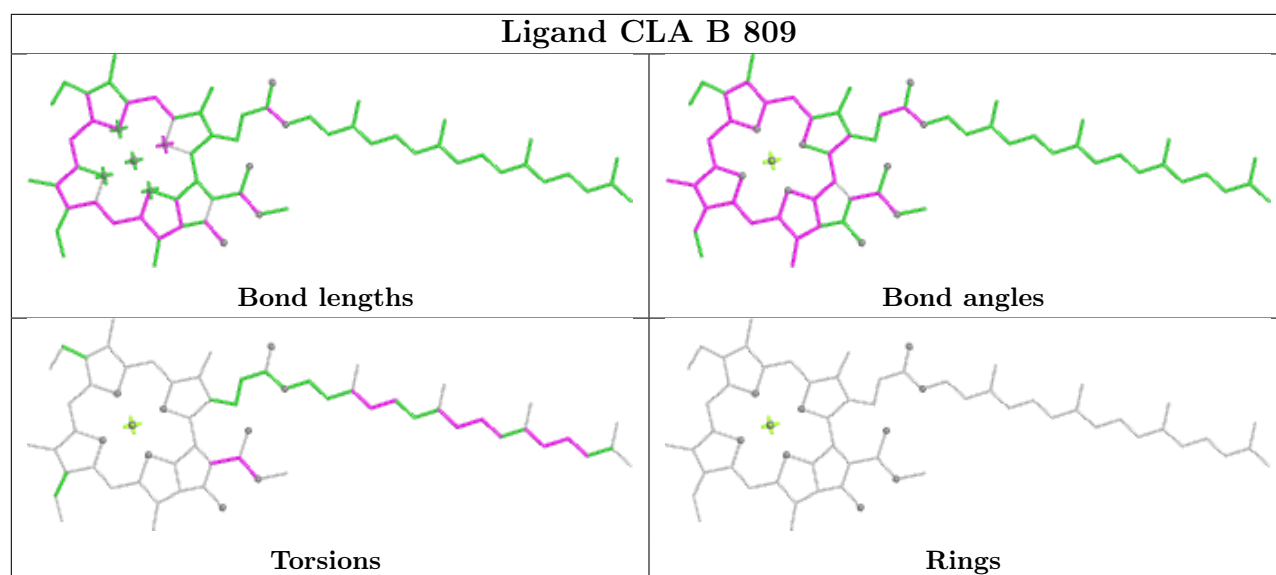
Torsions

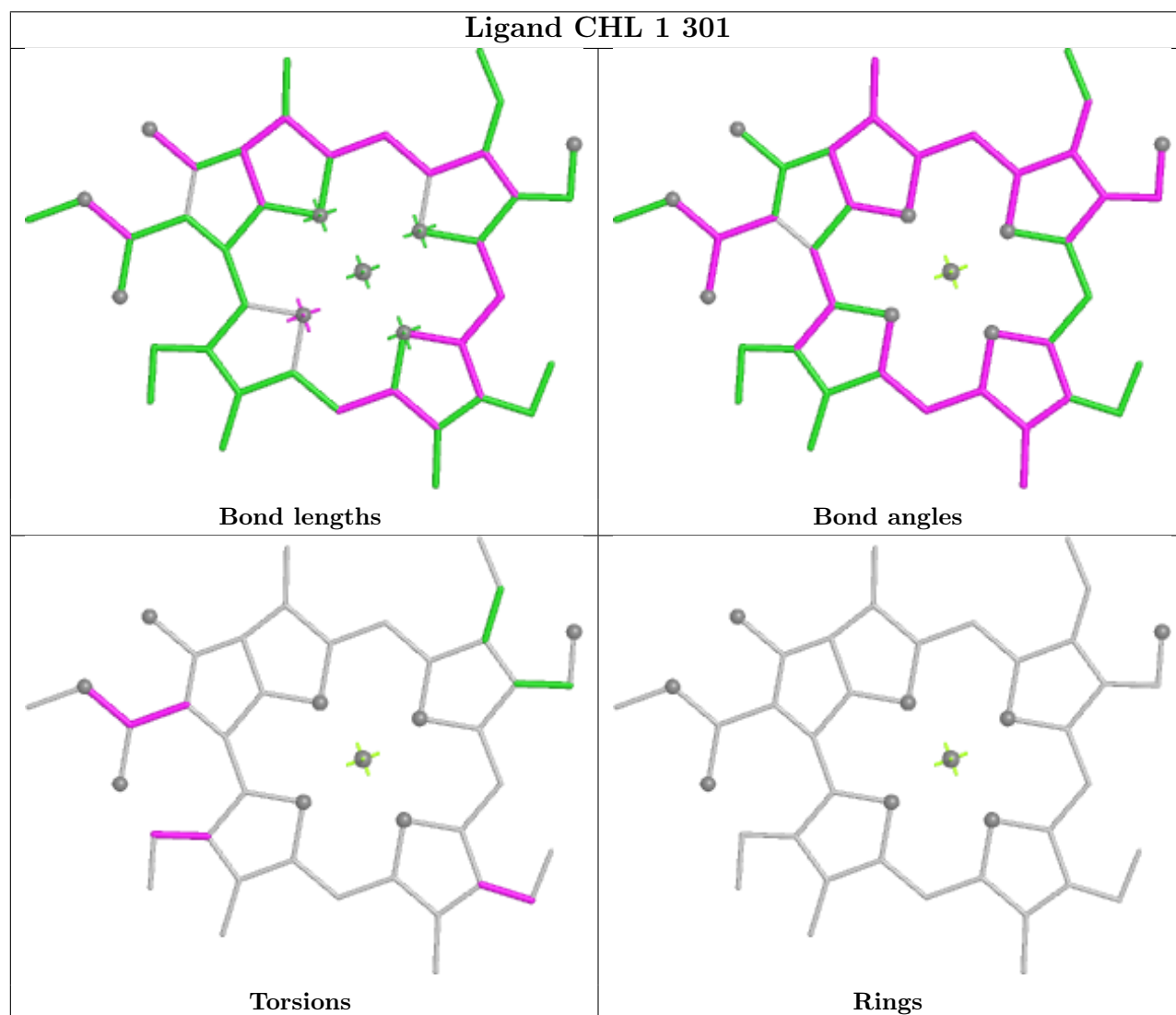
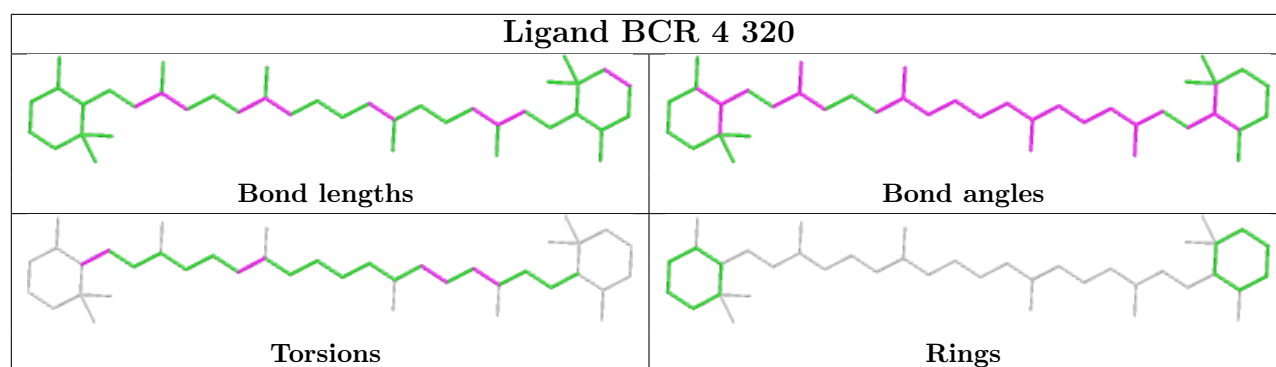


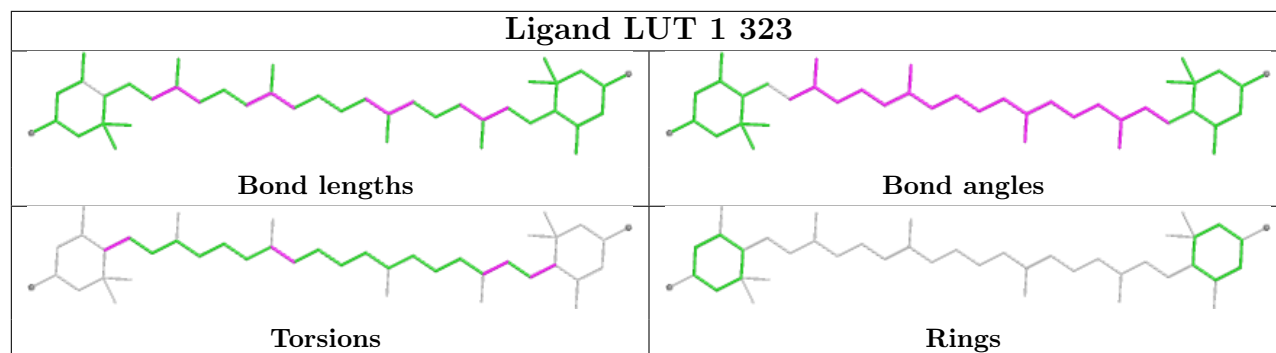
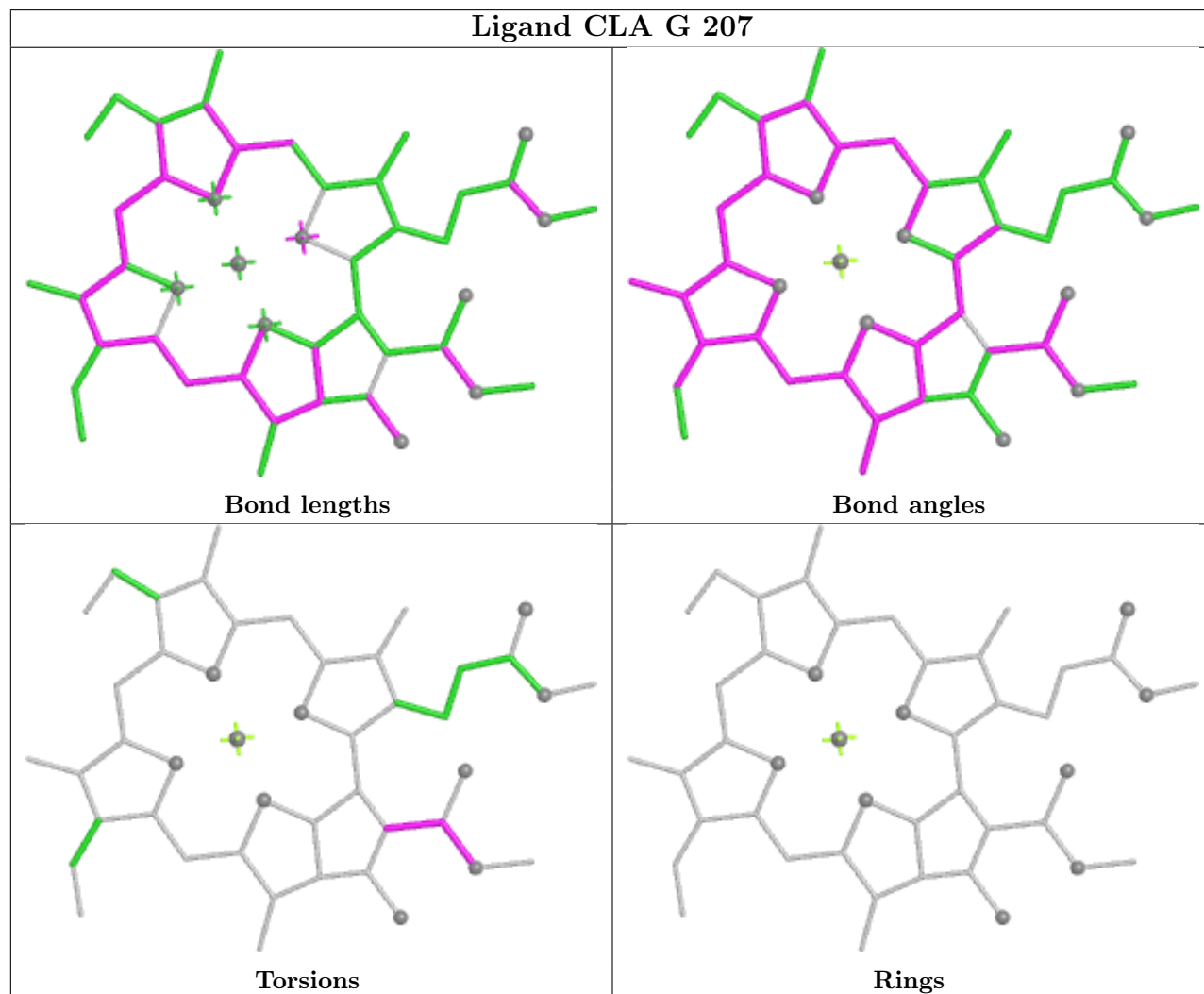
Rings

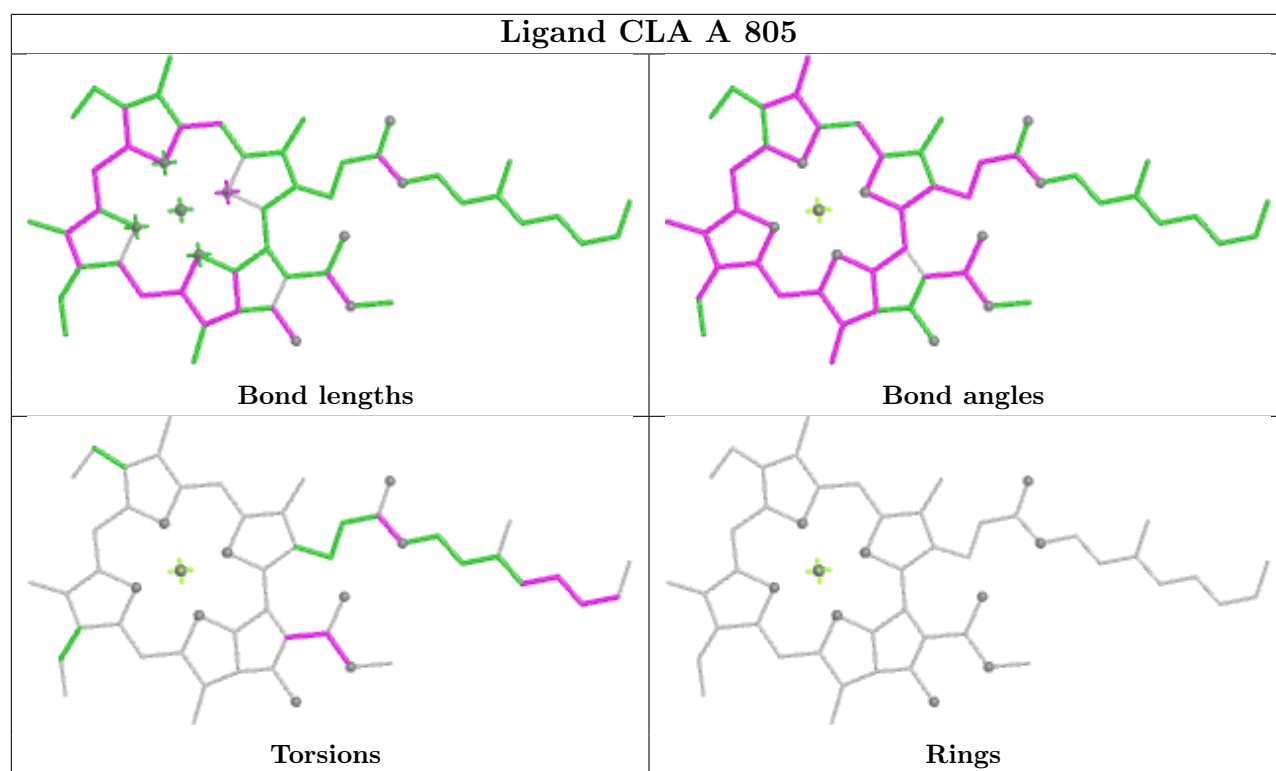




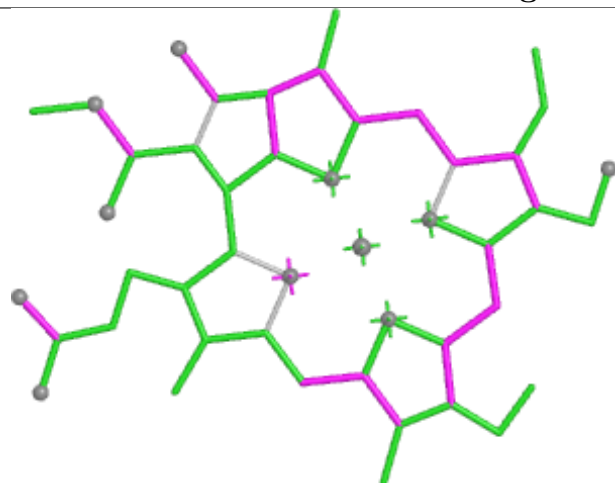




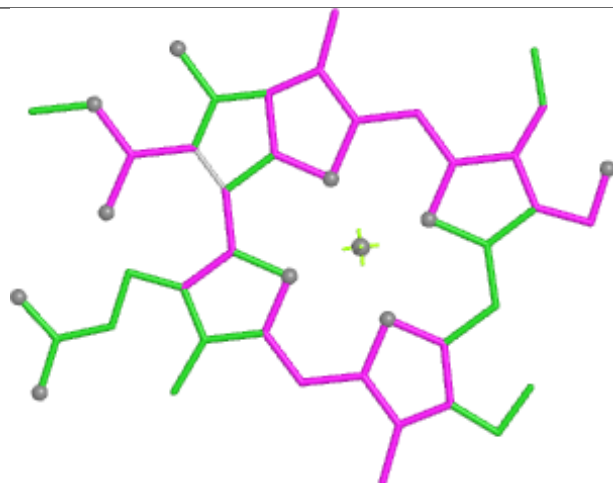
Ligand LUT 1 323**Ligand CLA G 207**



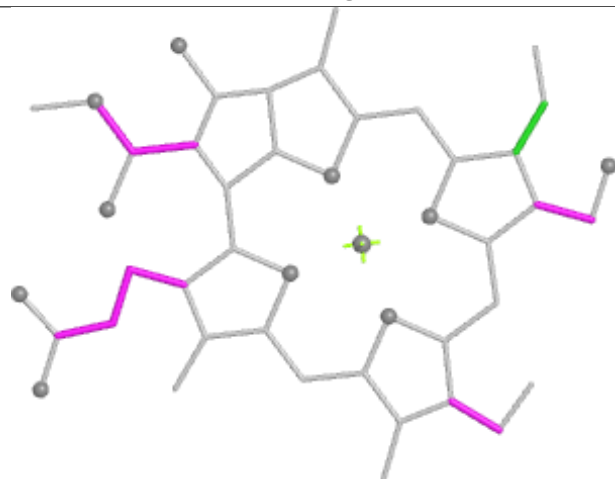
Ligand CHL 4 306



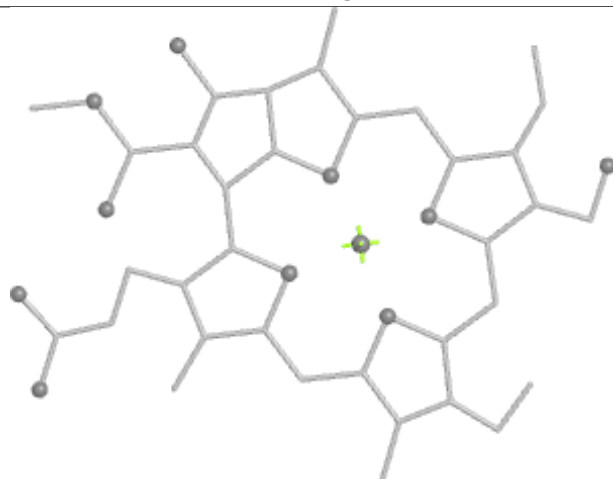
Bond lengths



Bond angles

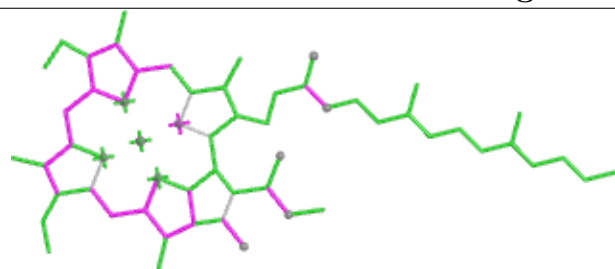


Torsions

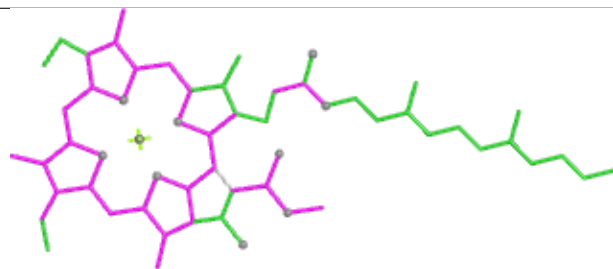


Rings

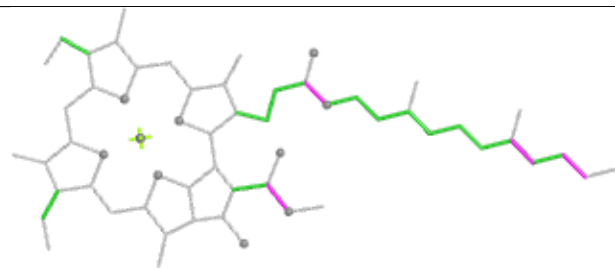
Ligand CLA B 817



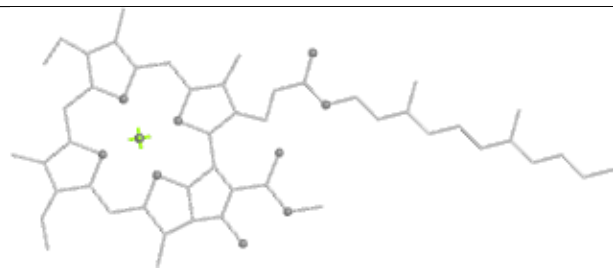
Bond lengths



Bond angles

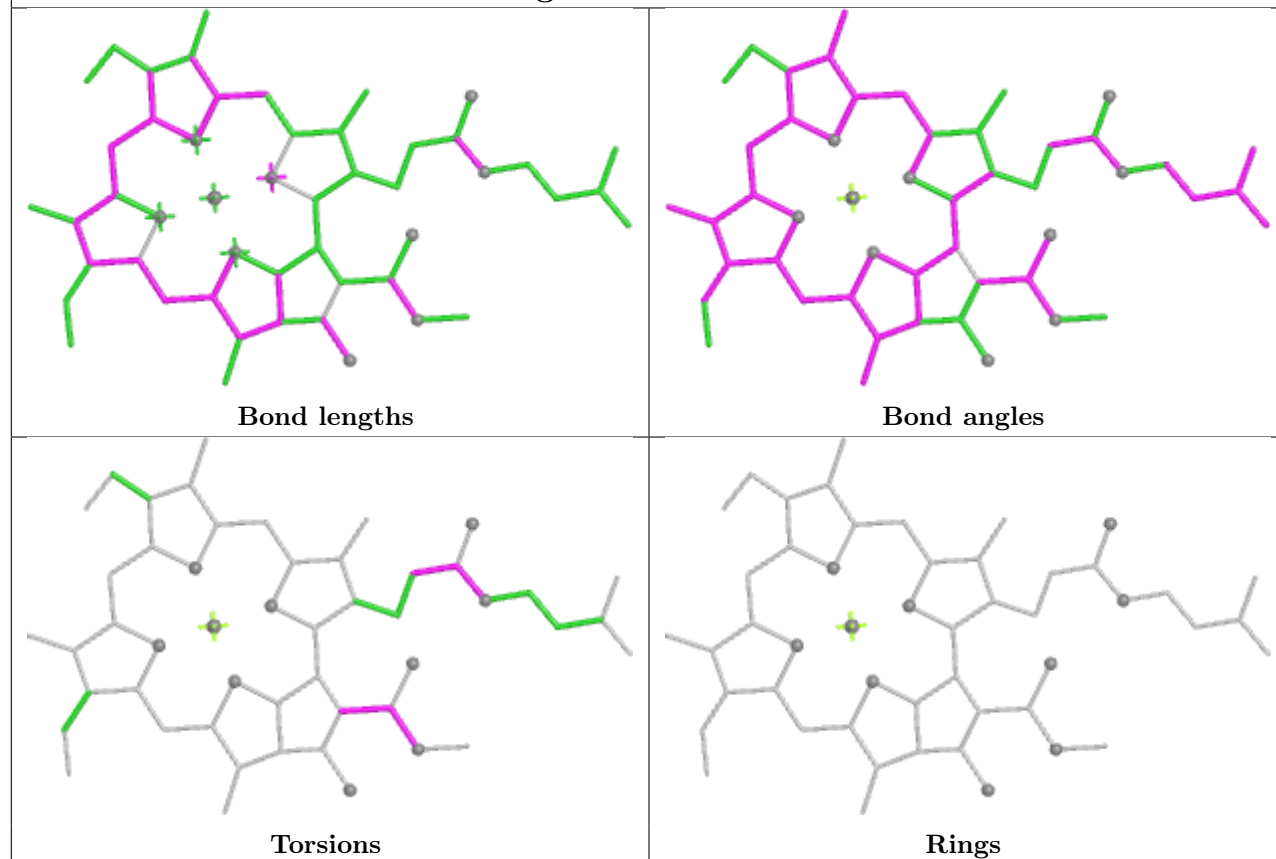


Torsions

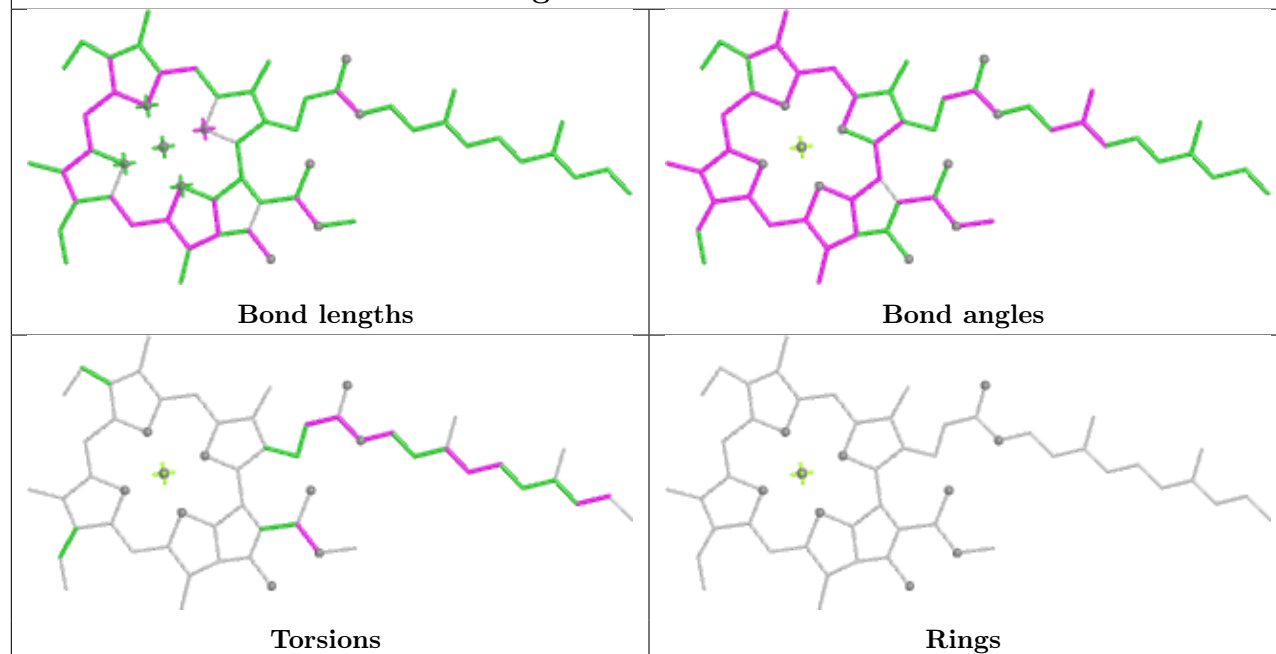


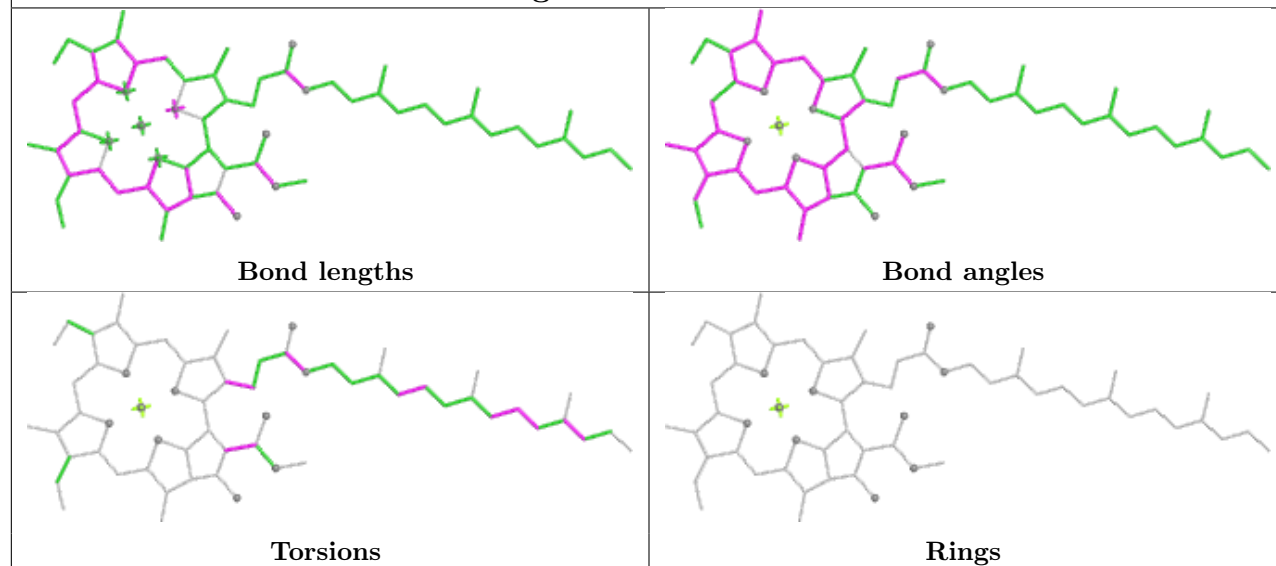
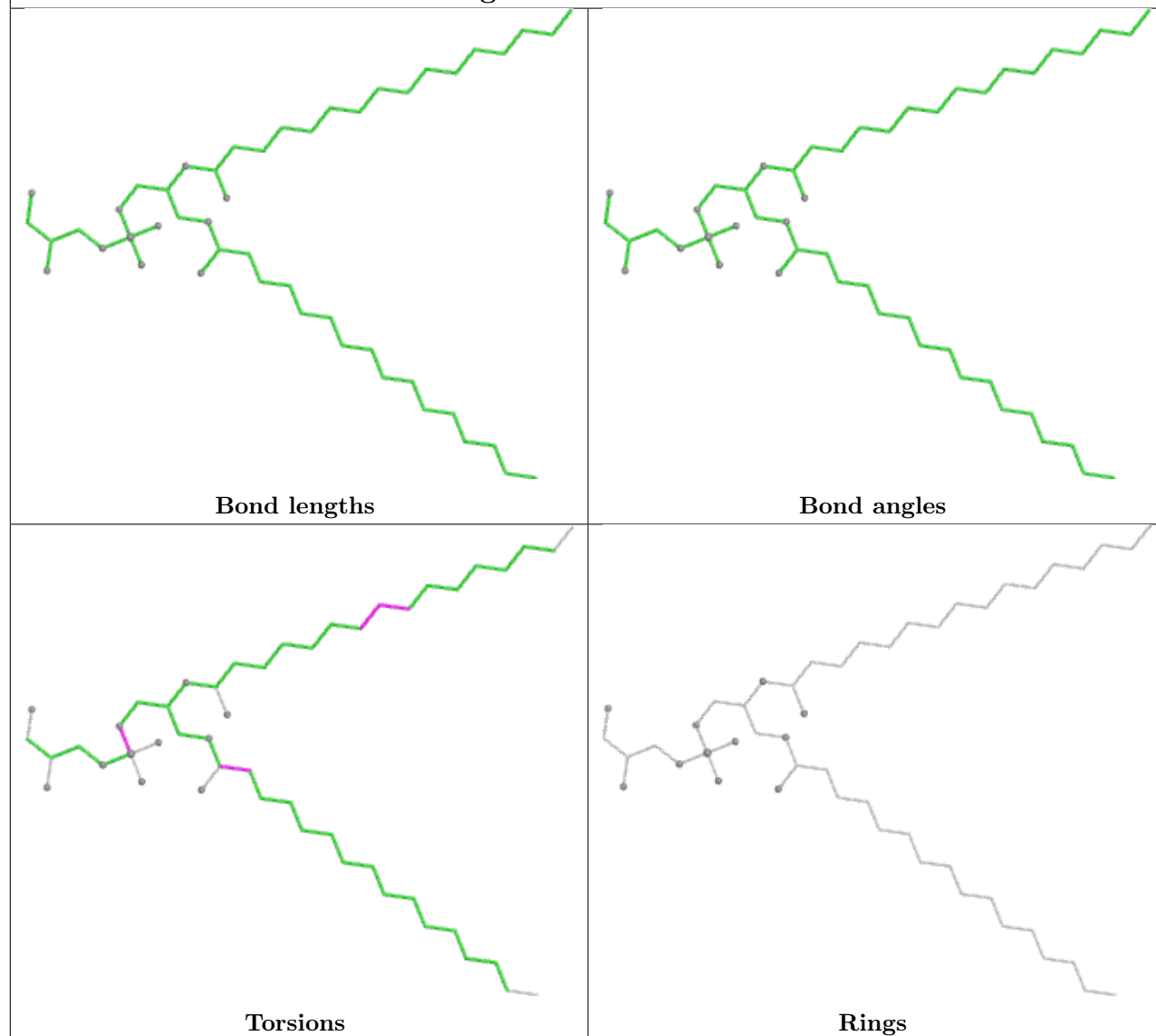
Rings

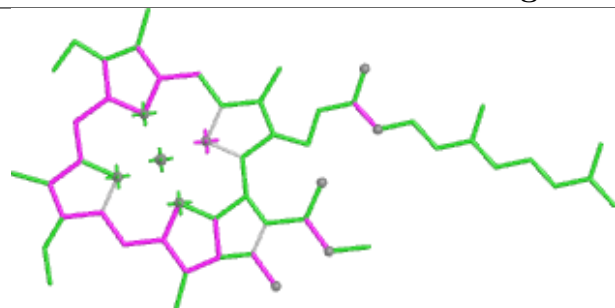
Ligand CLA 4 314



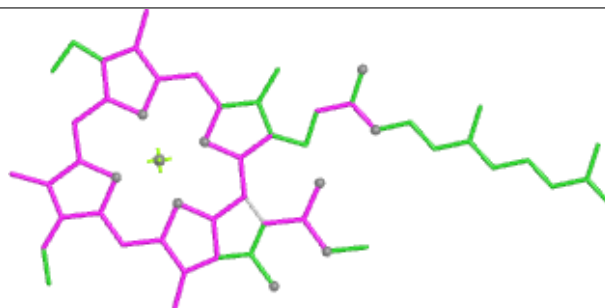
Ligand CLA B 813



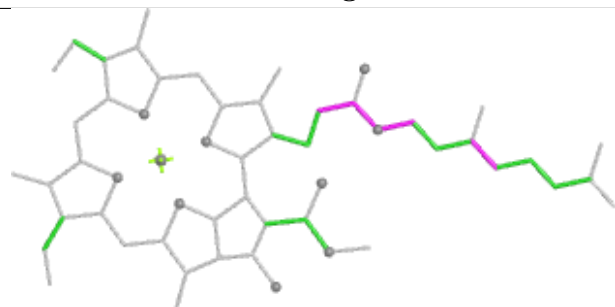
Ligand CLA B 823**Ligand LHG A 819**

Ligand CLA 4 312

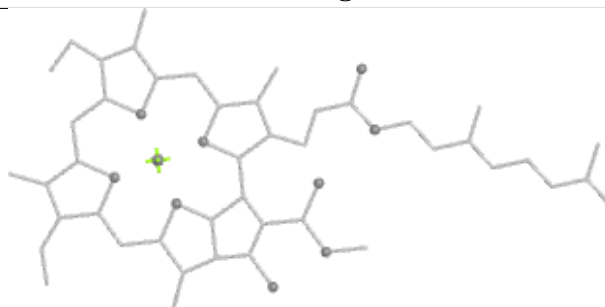
Bond lengths



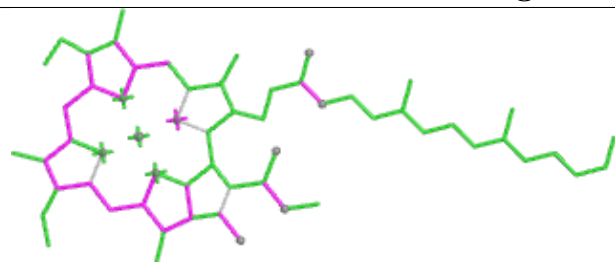
Bond angles



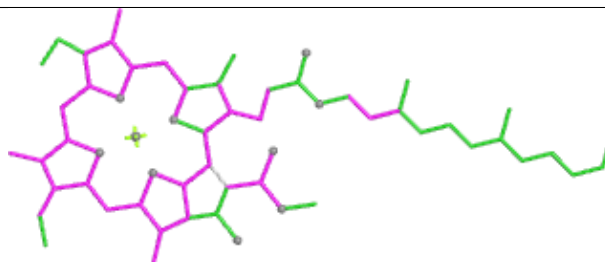
Torsions



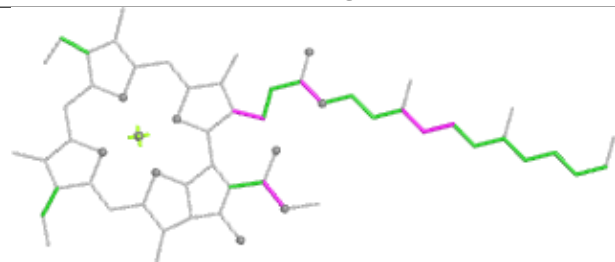
Rings

Ligand CLA O 207

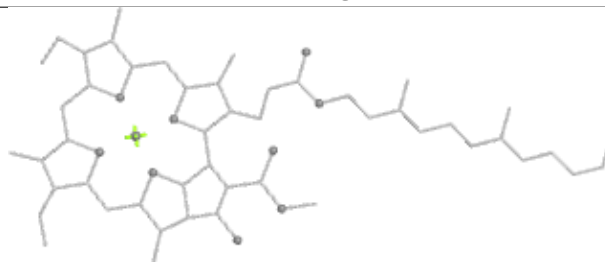
Bond lengths



Bond angles

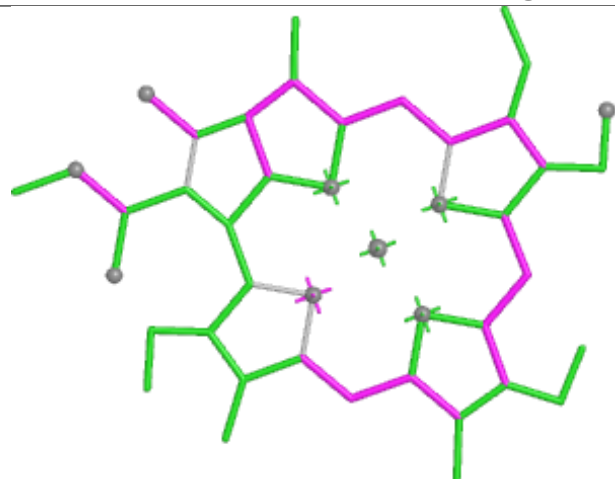


Torsions

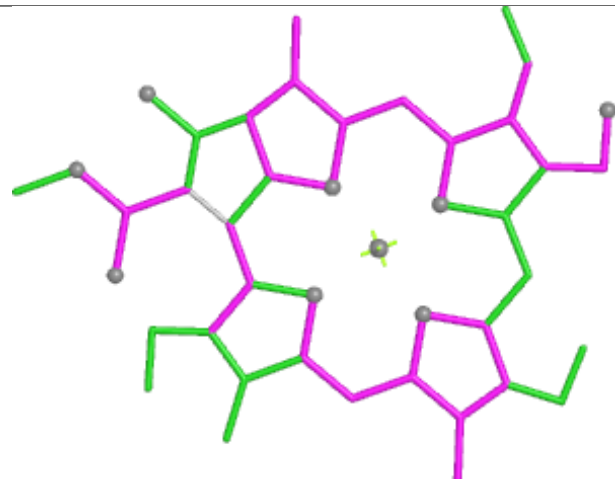


Rings

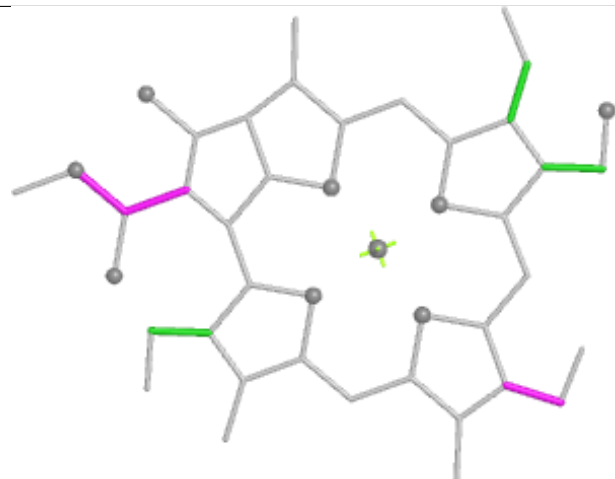
Ligand CHL 2 309



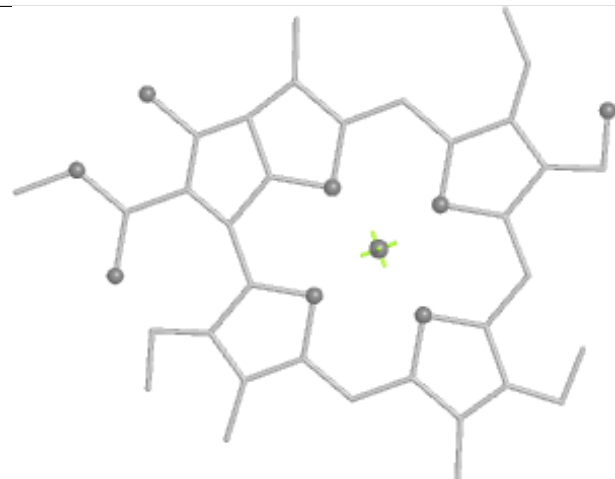
Bond lengths



Bond angles

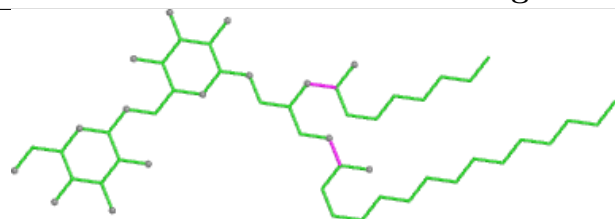


Torsions

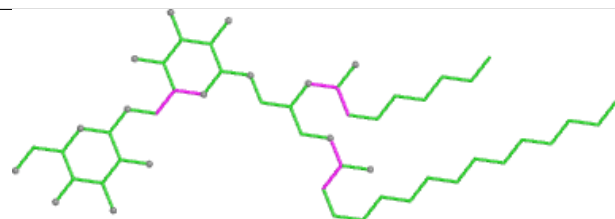


Rings

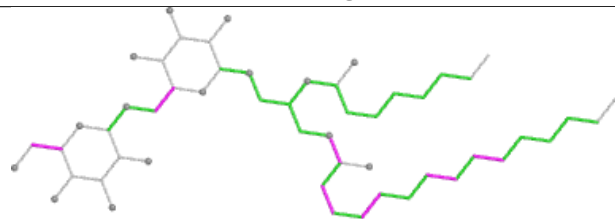
Ligand DGD O 201



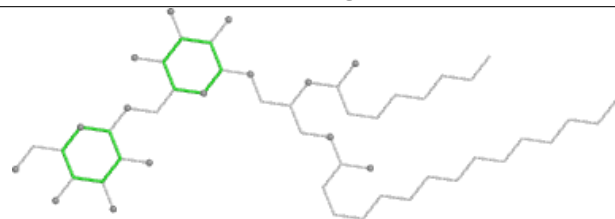
Bond lengths



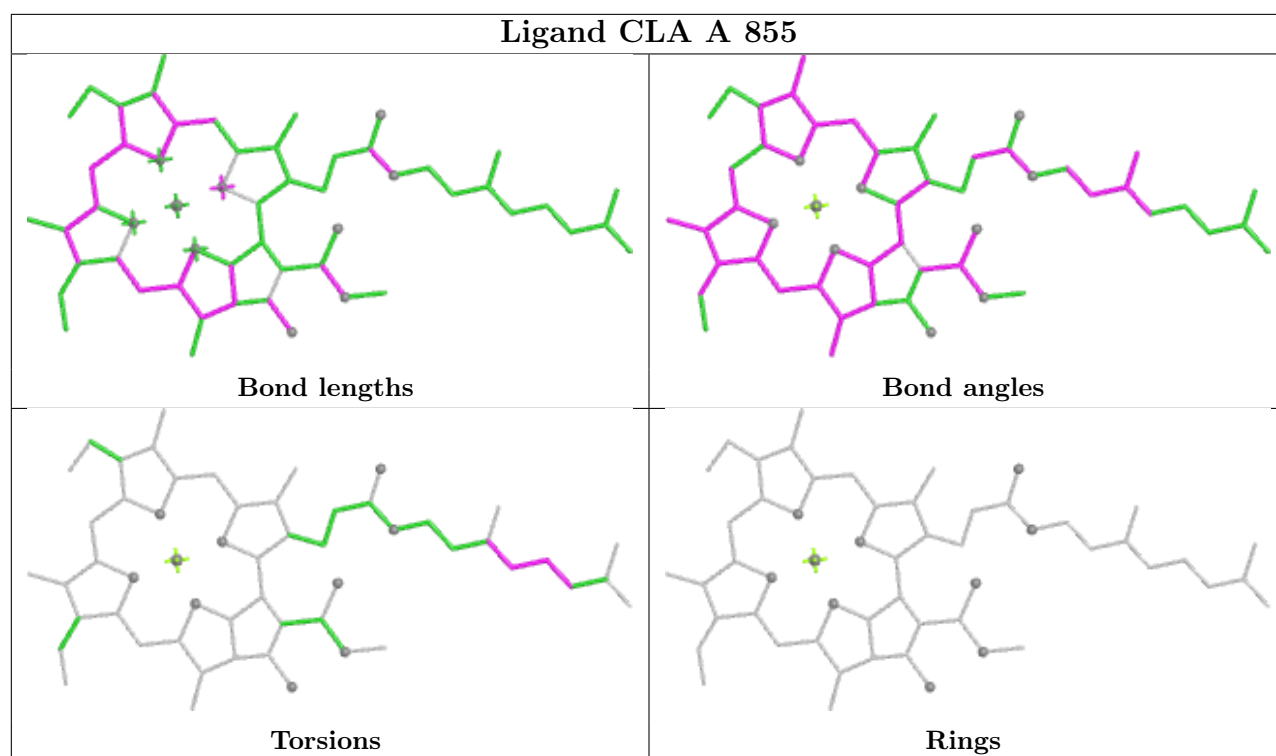
Bond angles

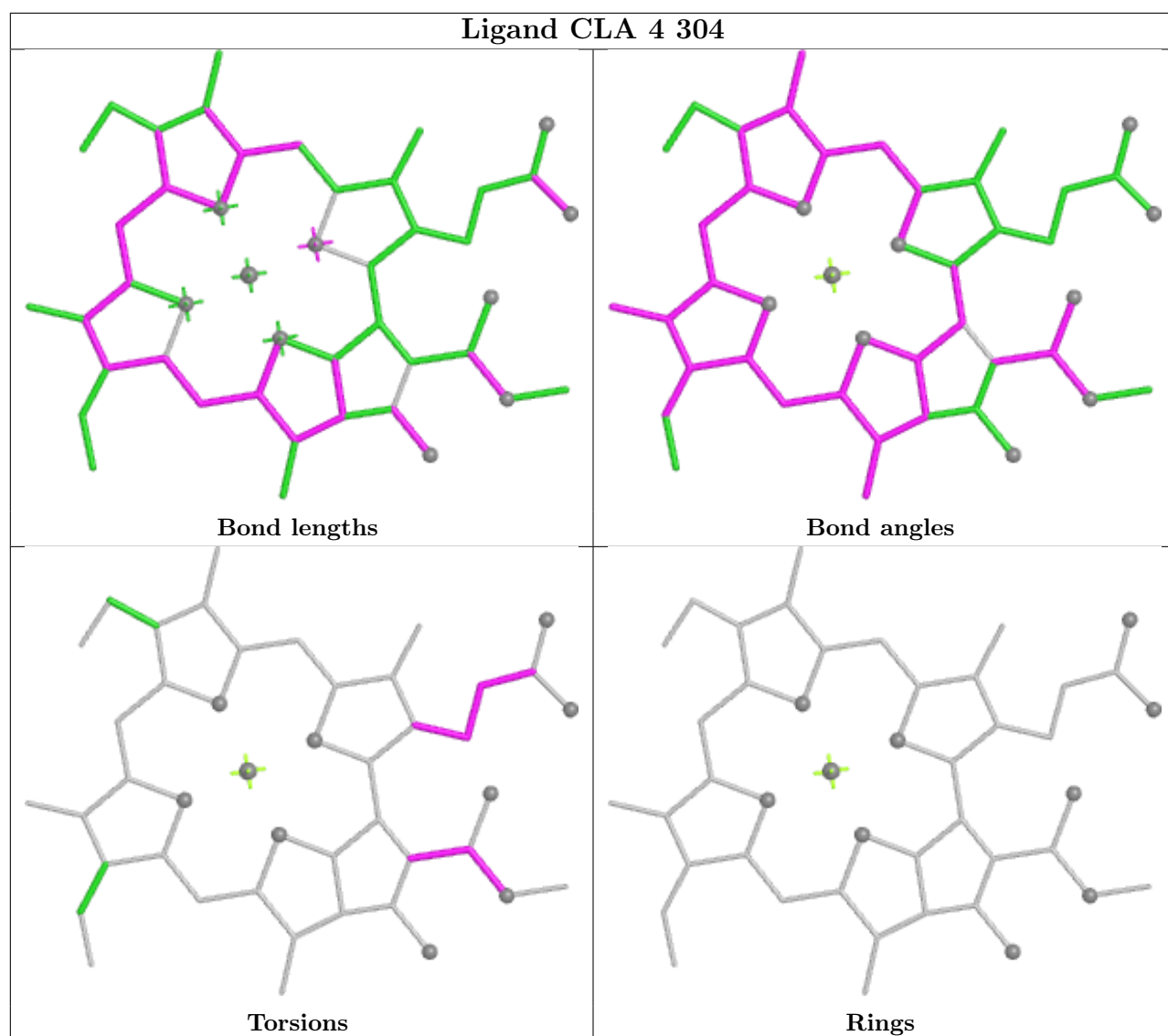


Torsions

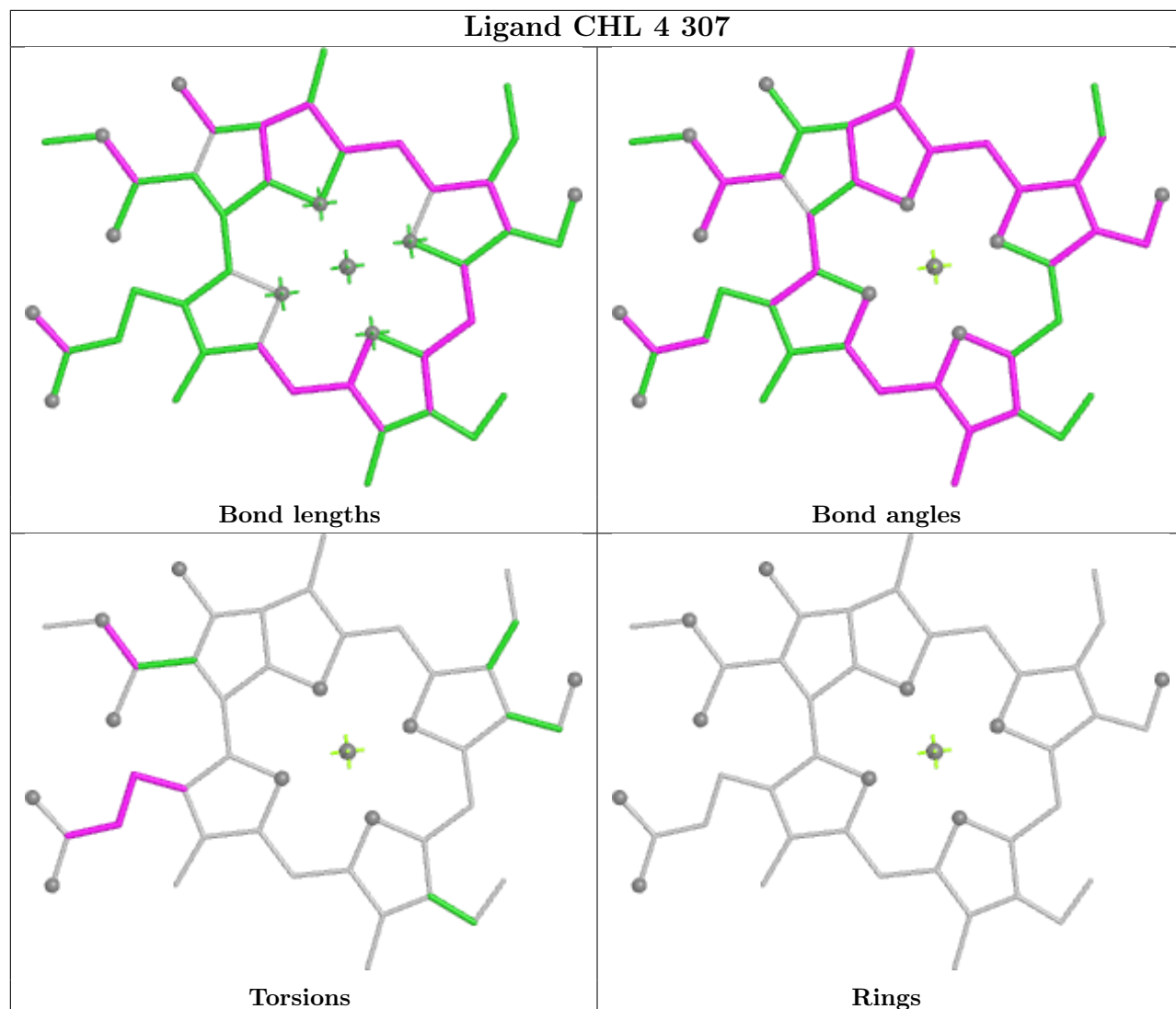


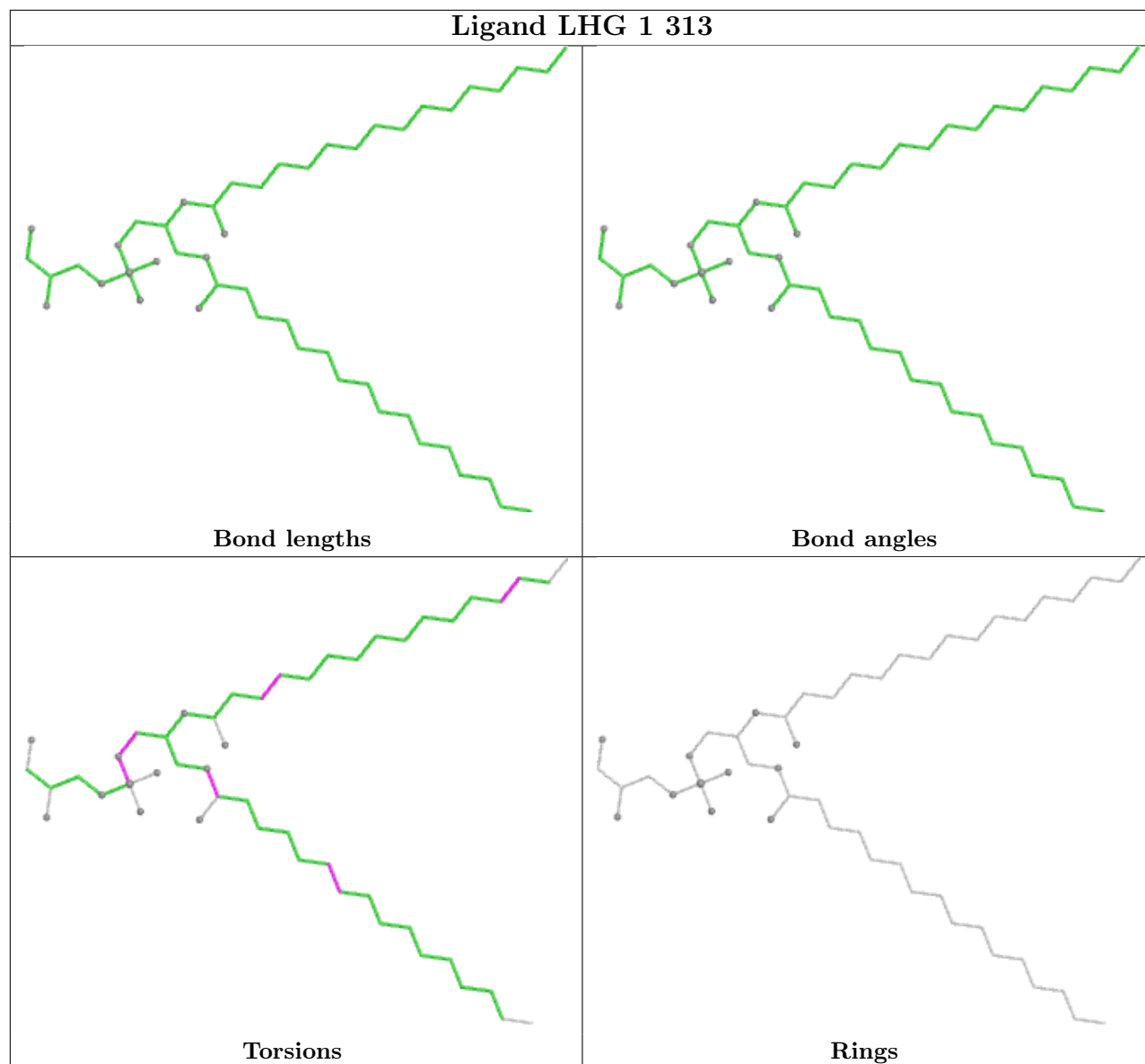
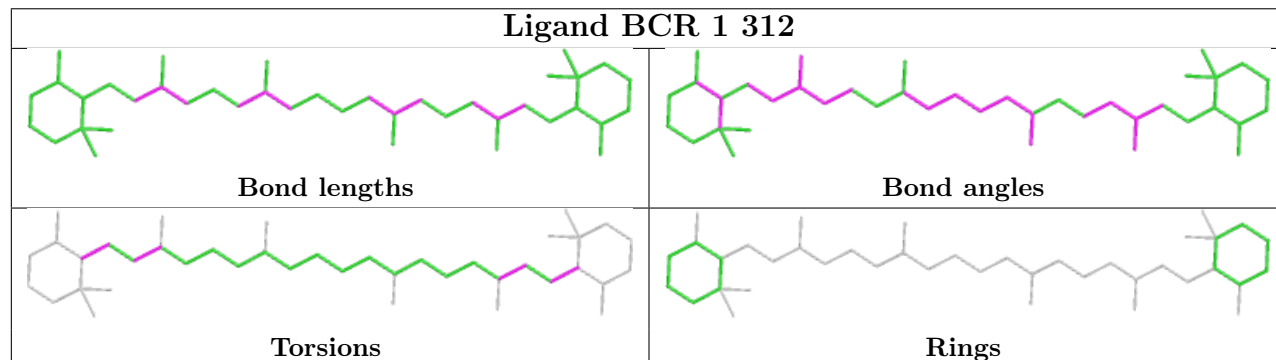
Rings



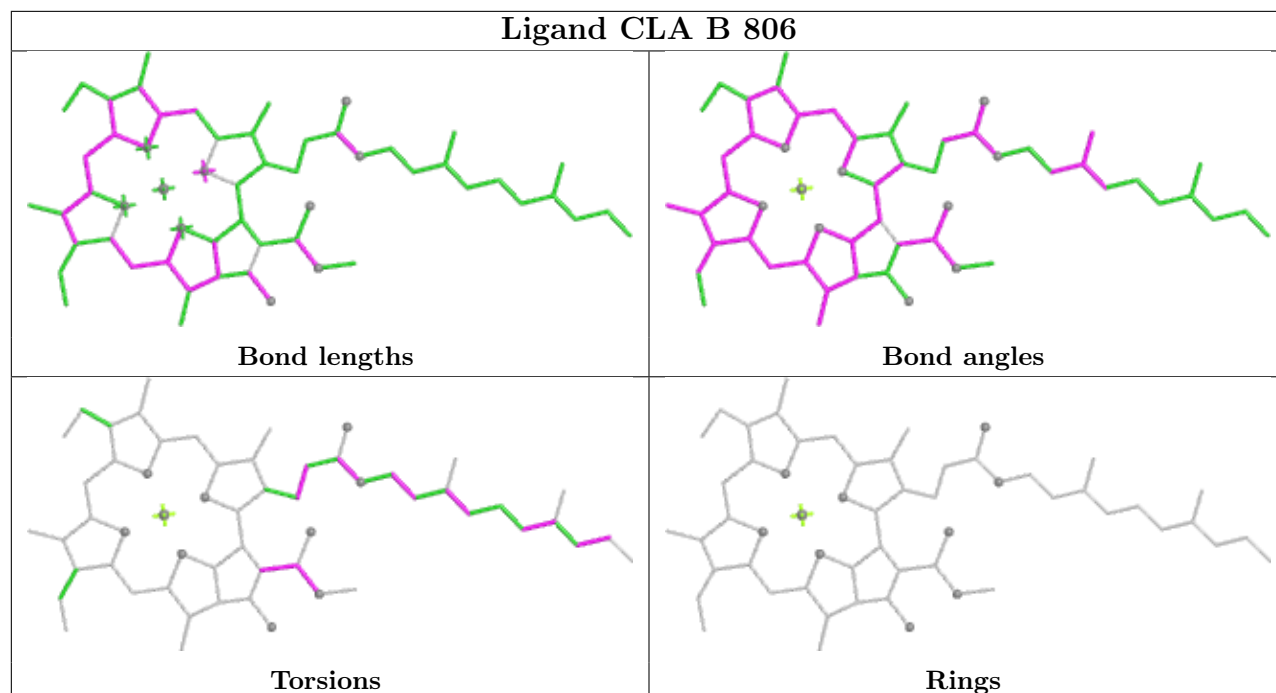


Ligand CHL 4 307

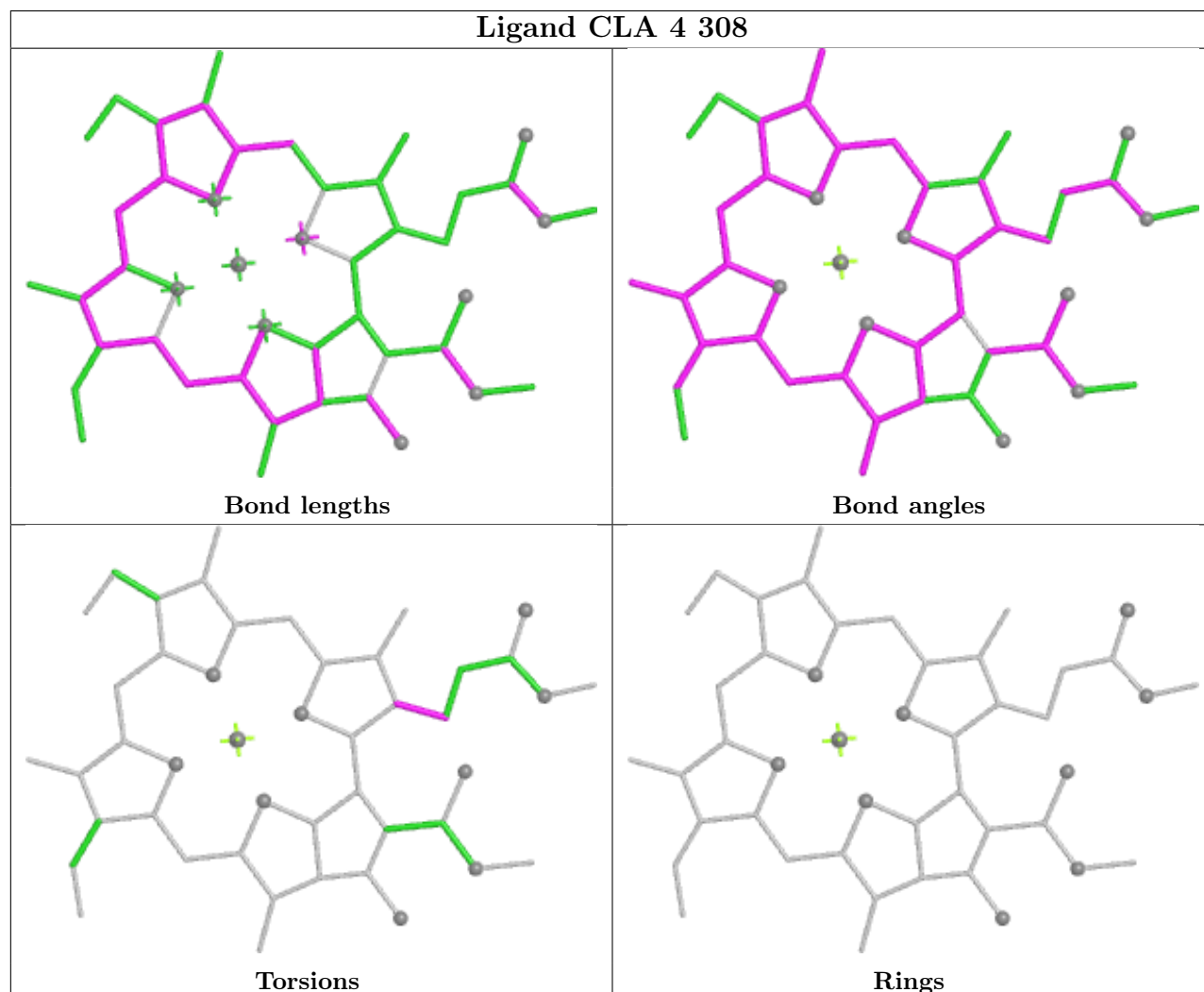


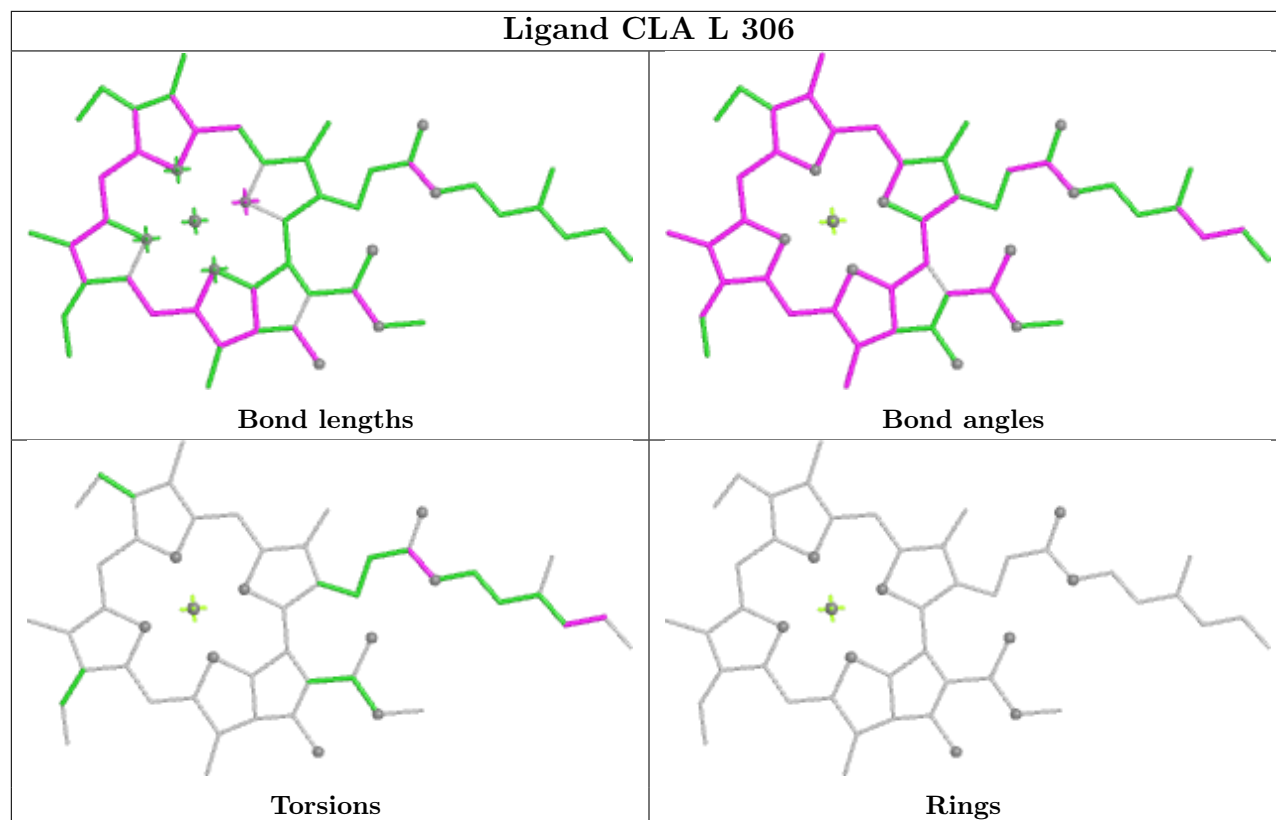
Ligand LHG 1 313**Ligand BCR 1 312**

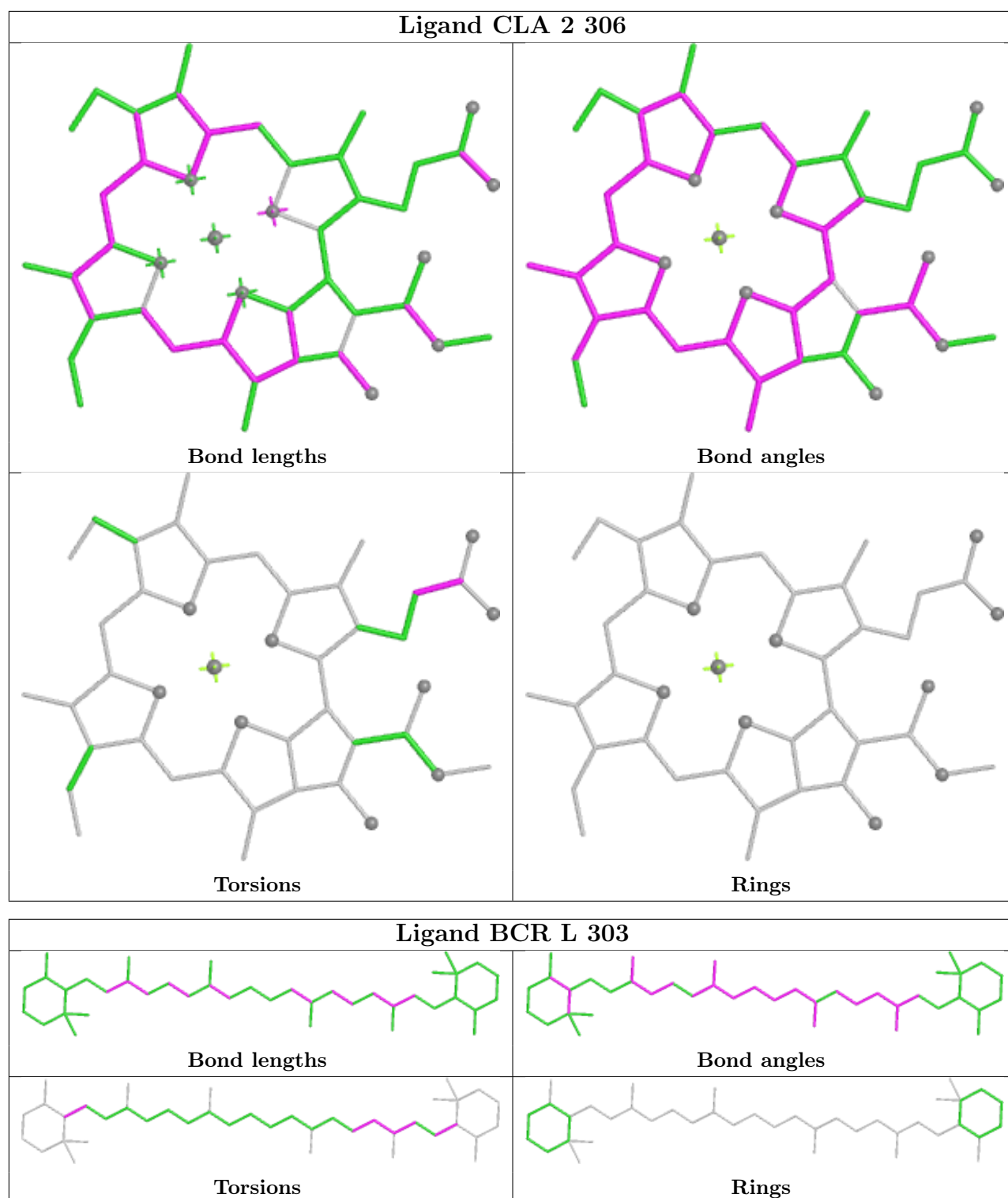
Ligand CLA B 806

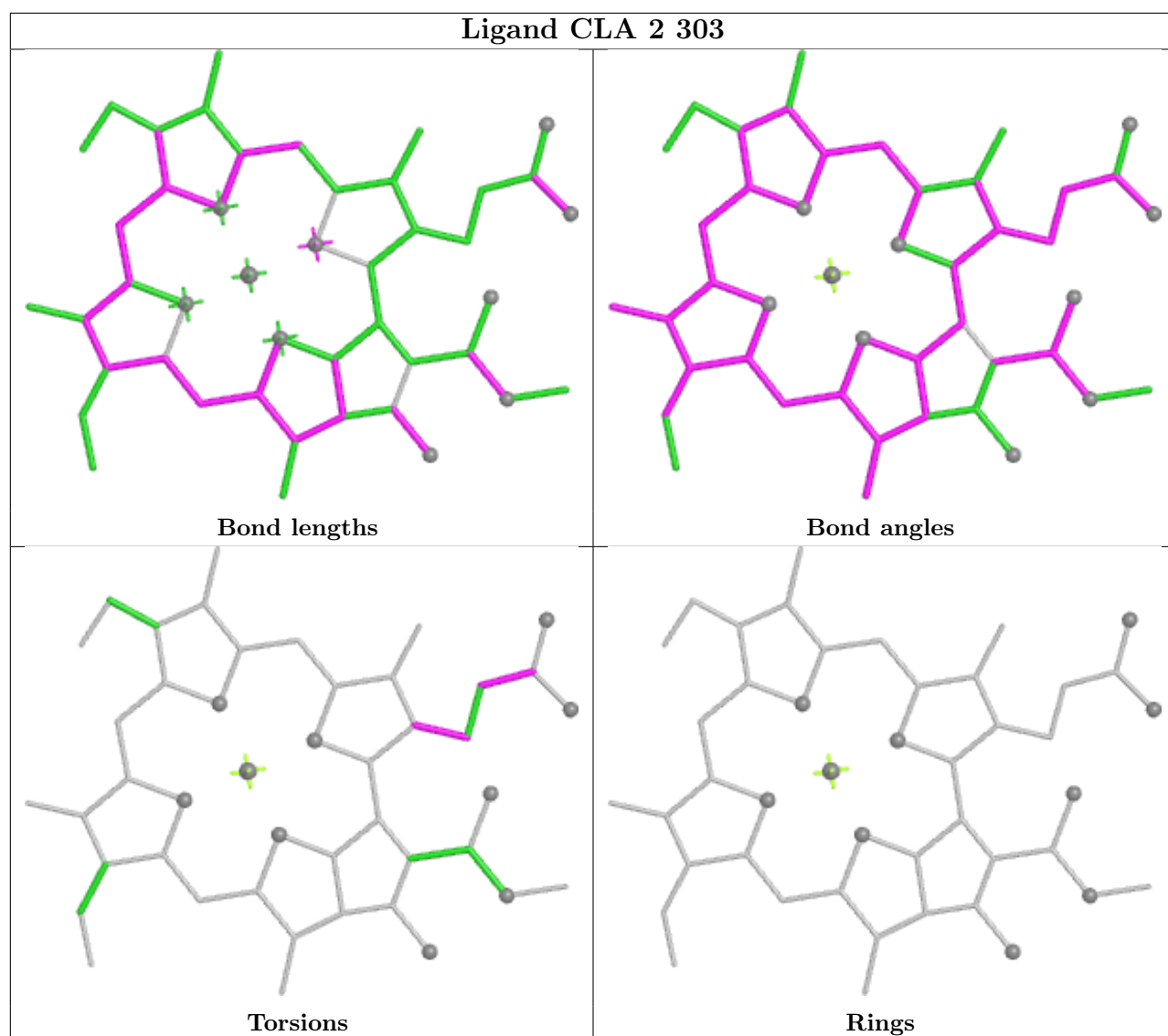


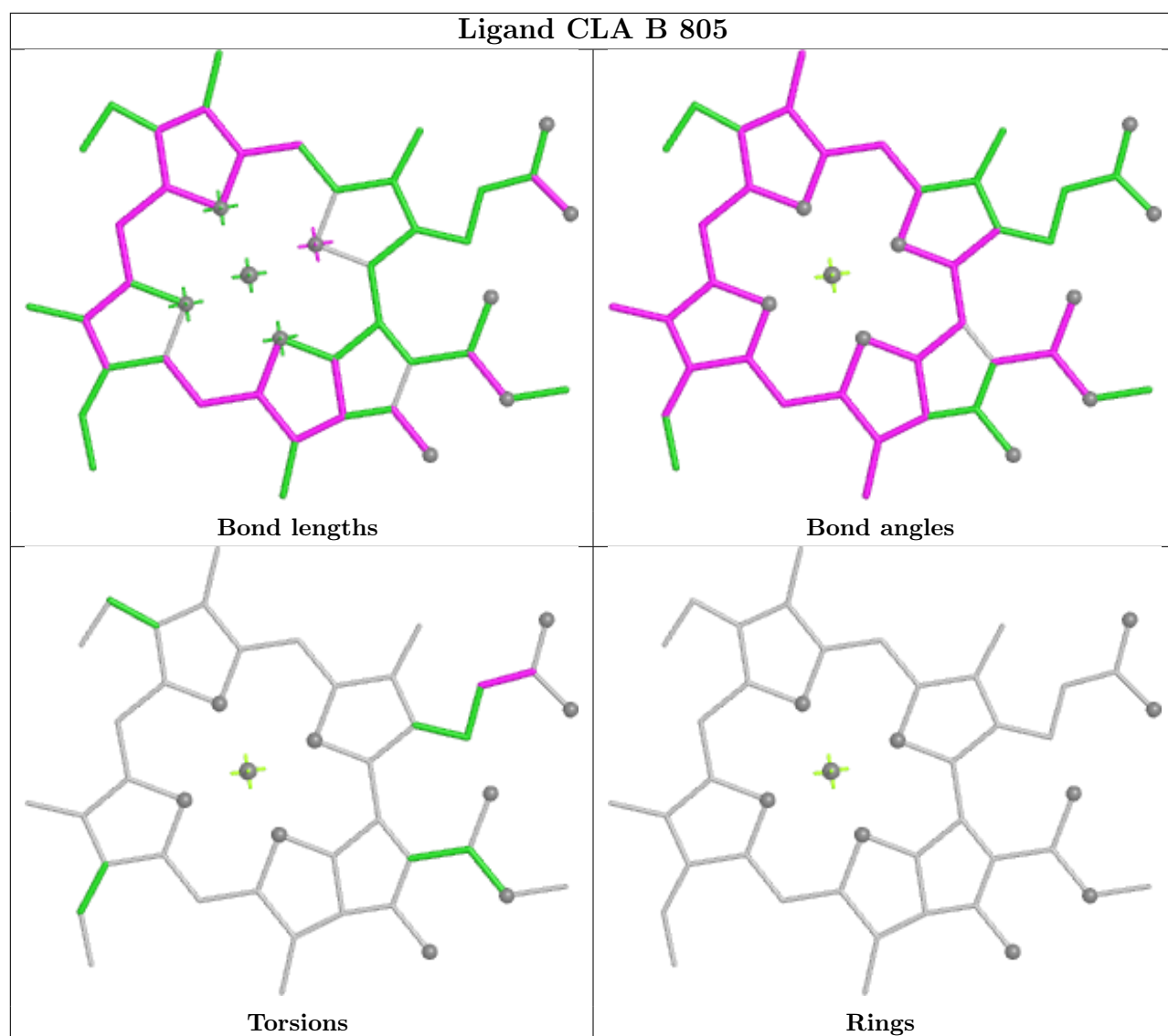
Ligand CLA 4 308

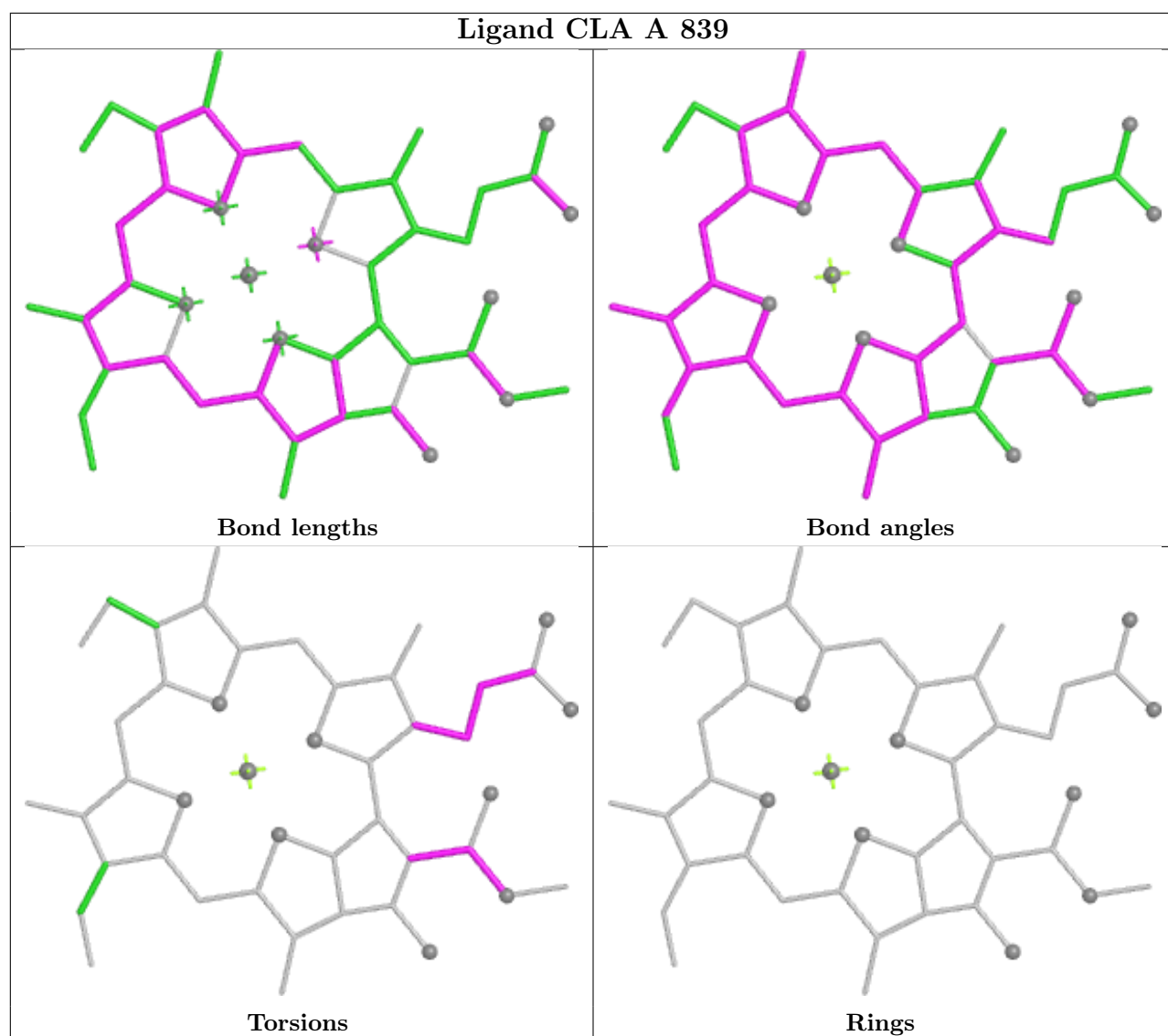




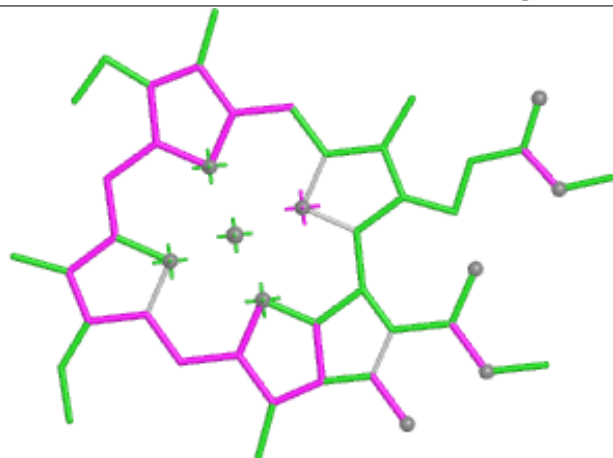




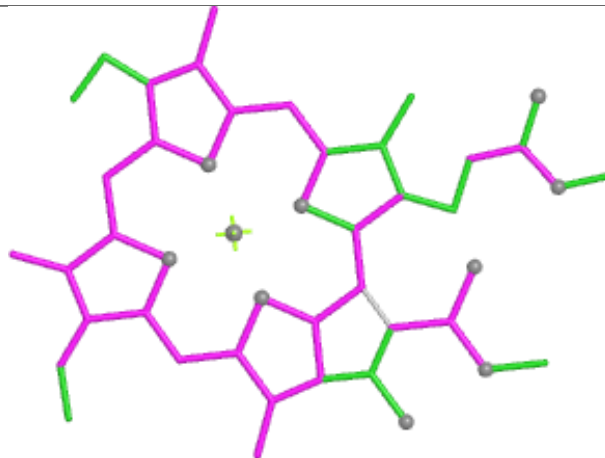




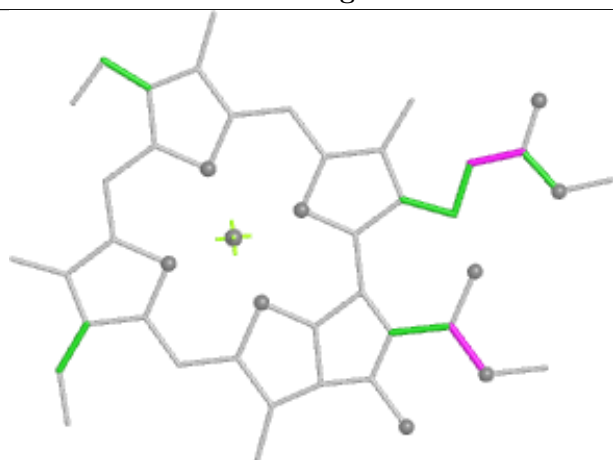
Ligand CLA L 307



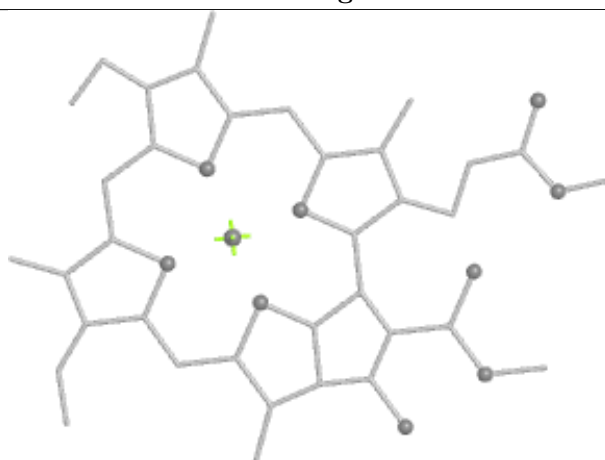
Bond lengths



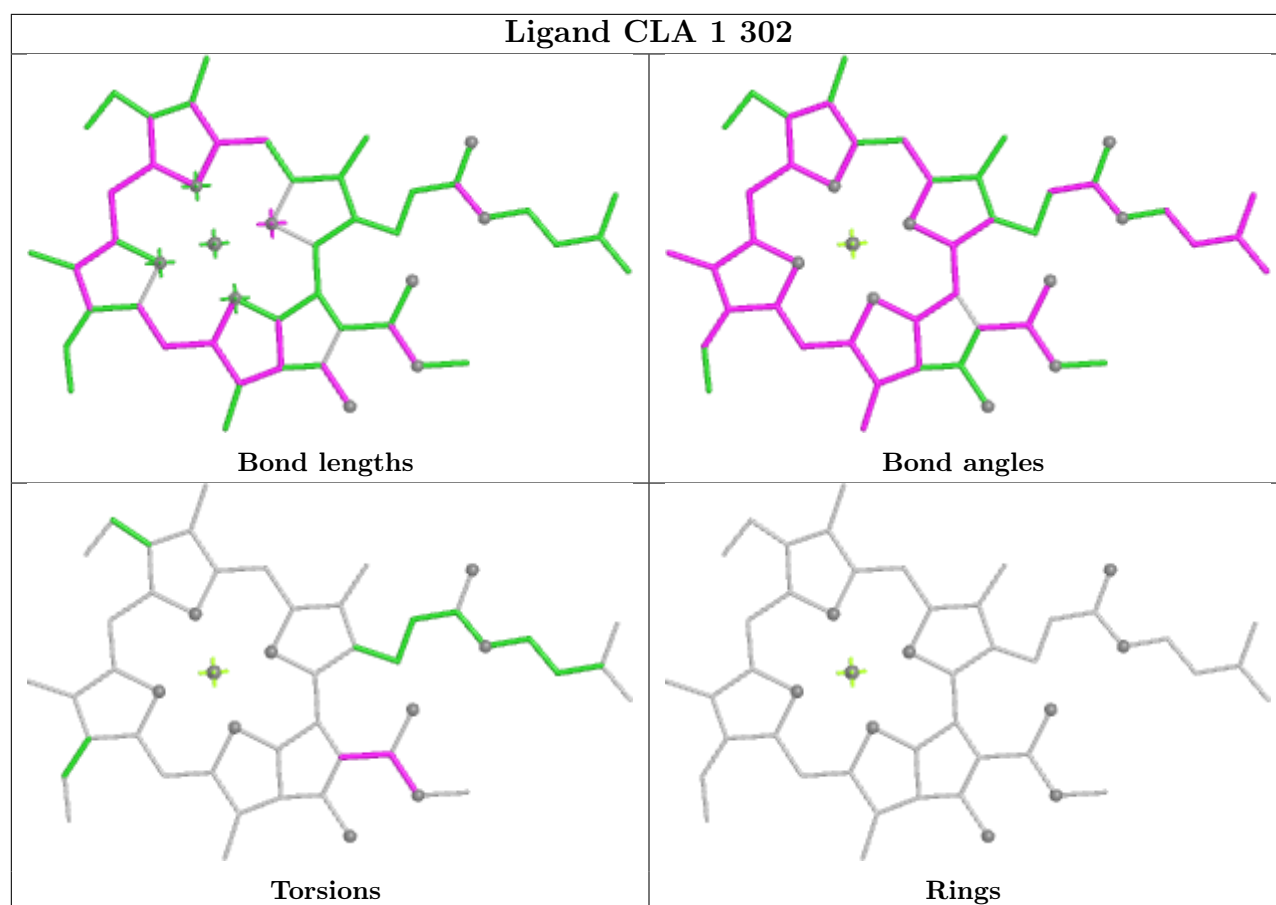
Bond angles

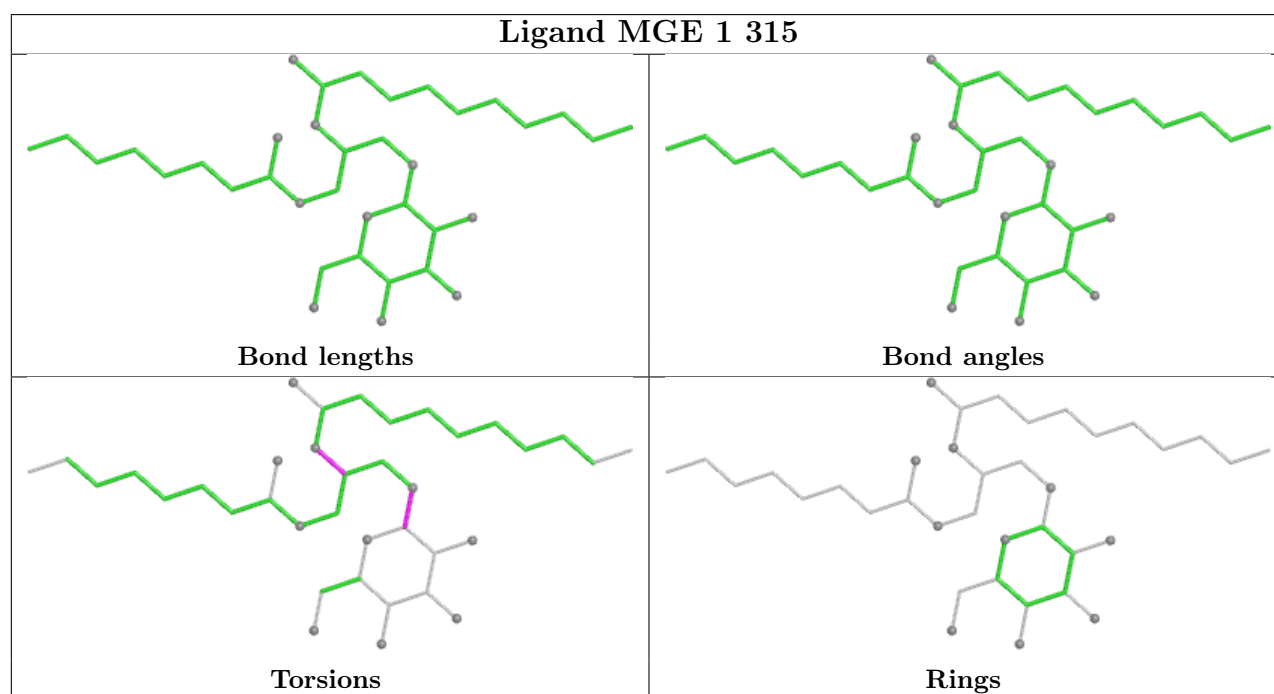
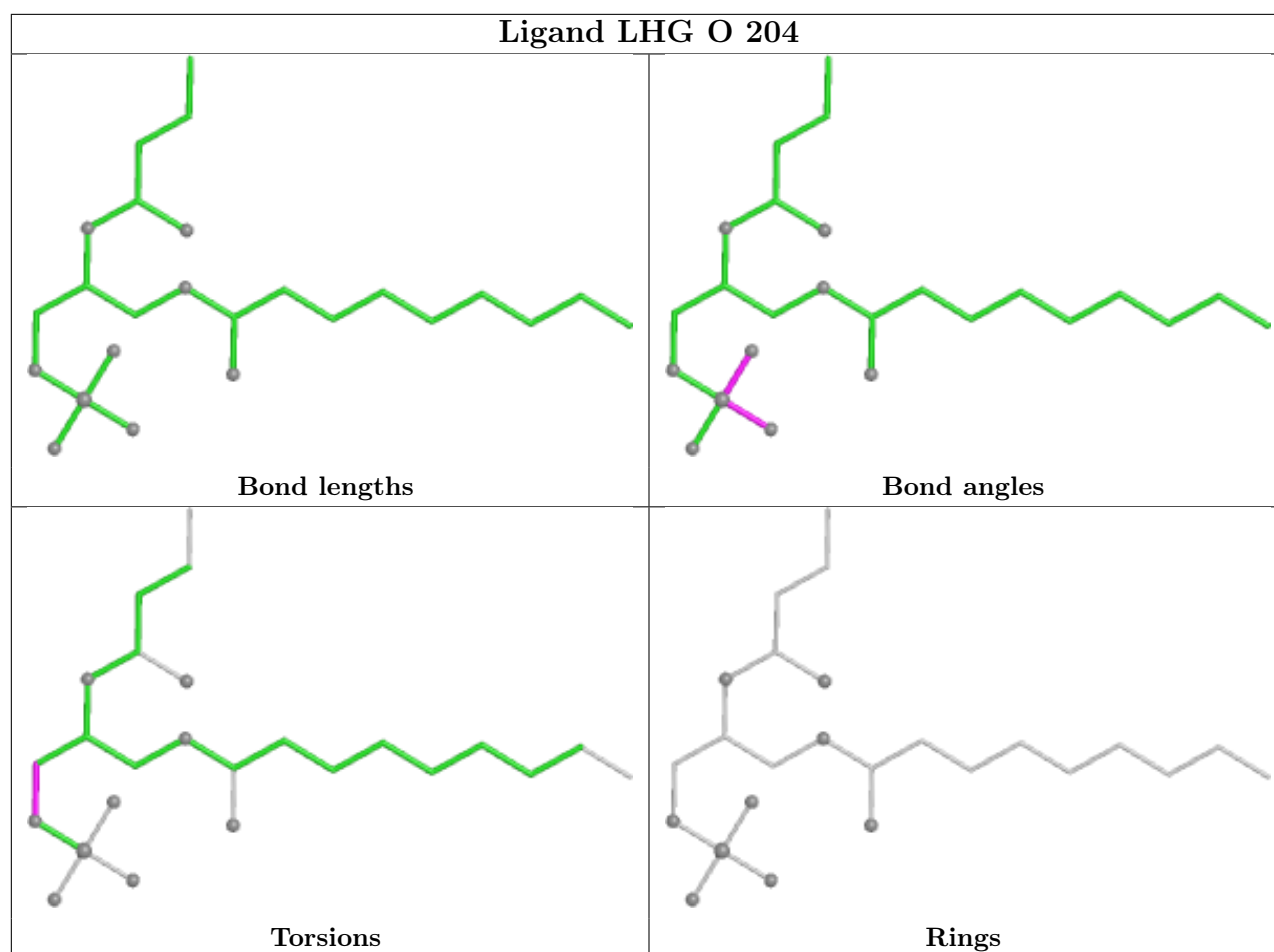


Torsions

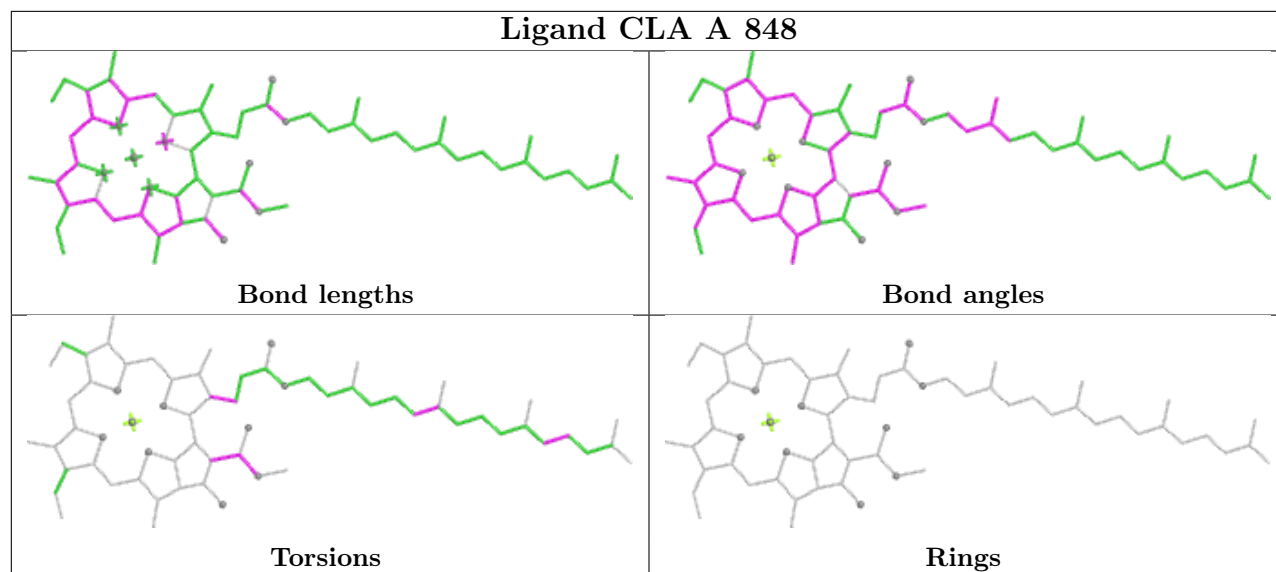


Rings

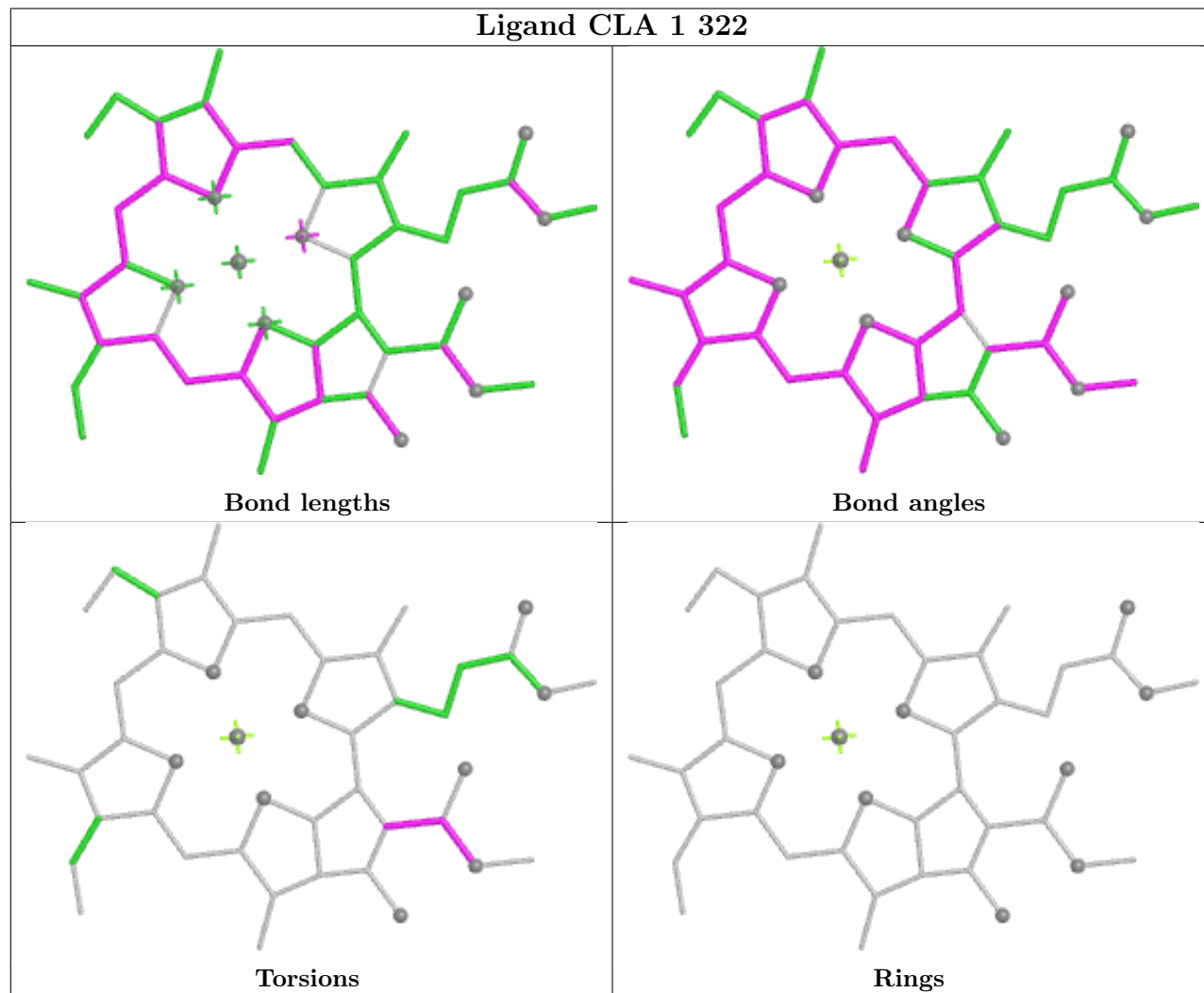


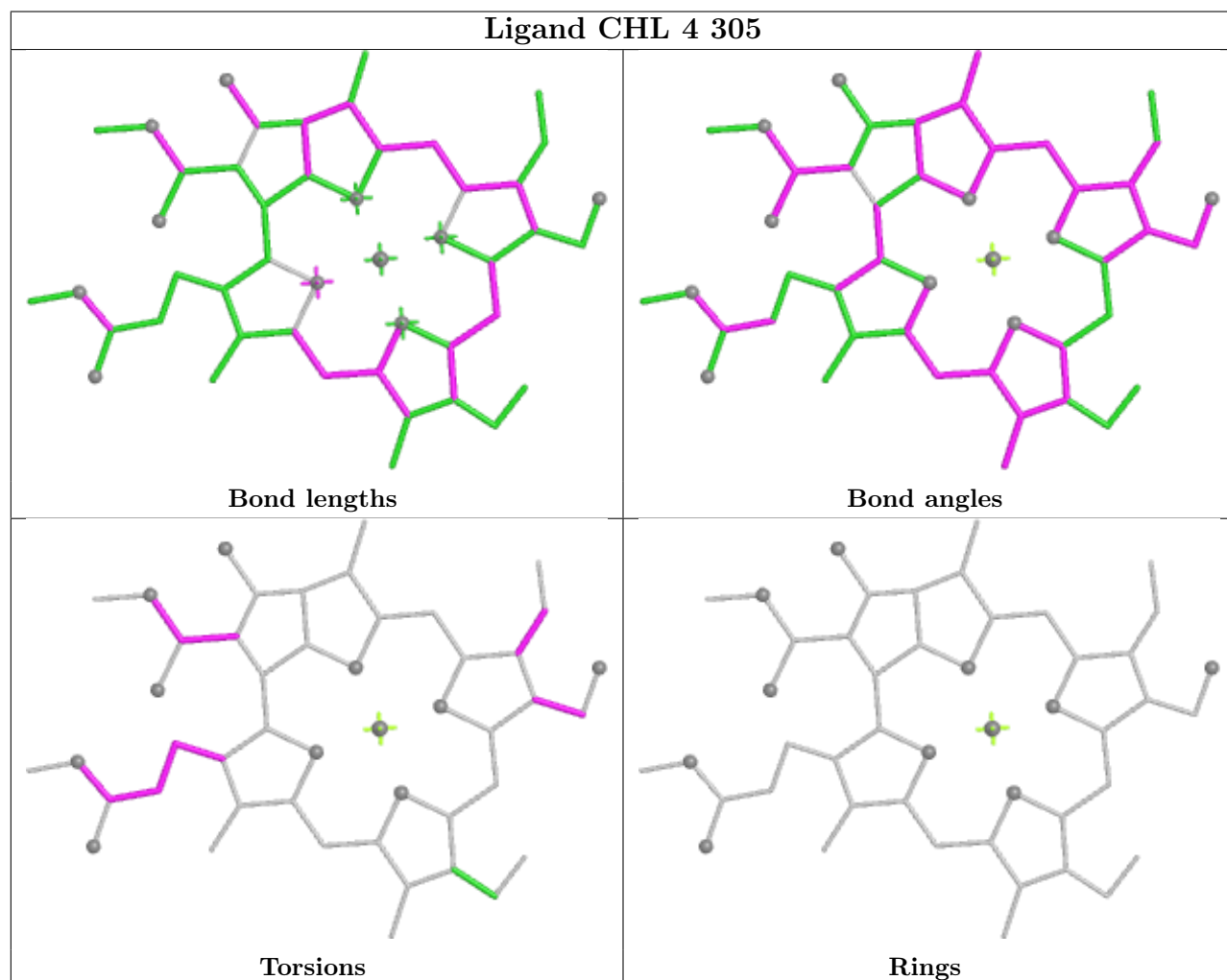
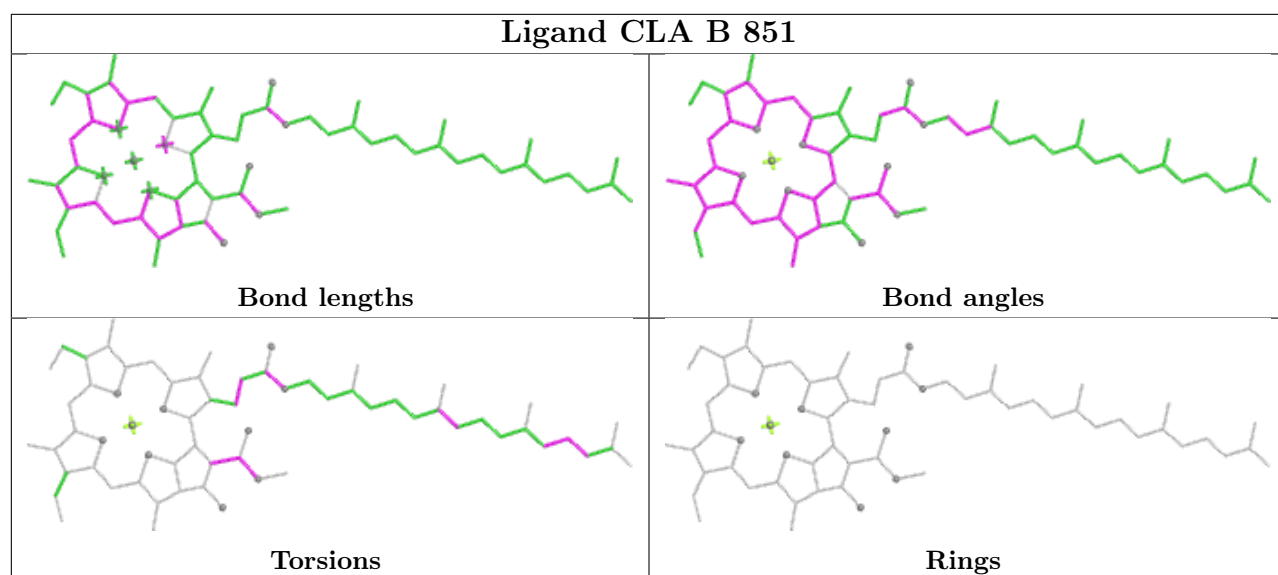


Ligand CLA A 848

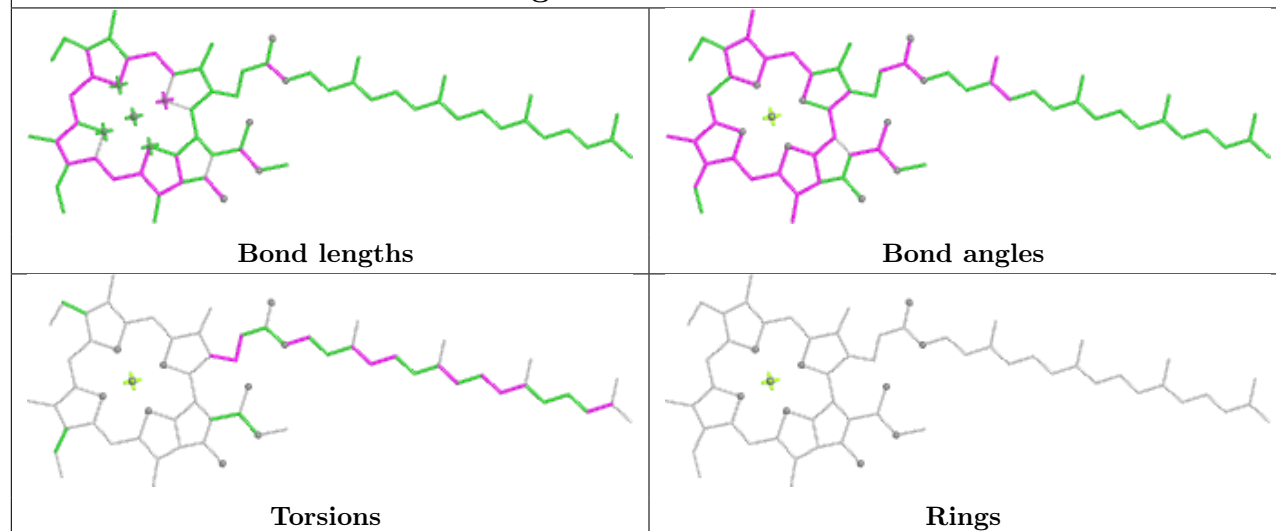


Ligand CLA 1 322

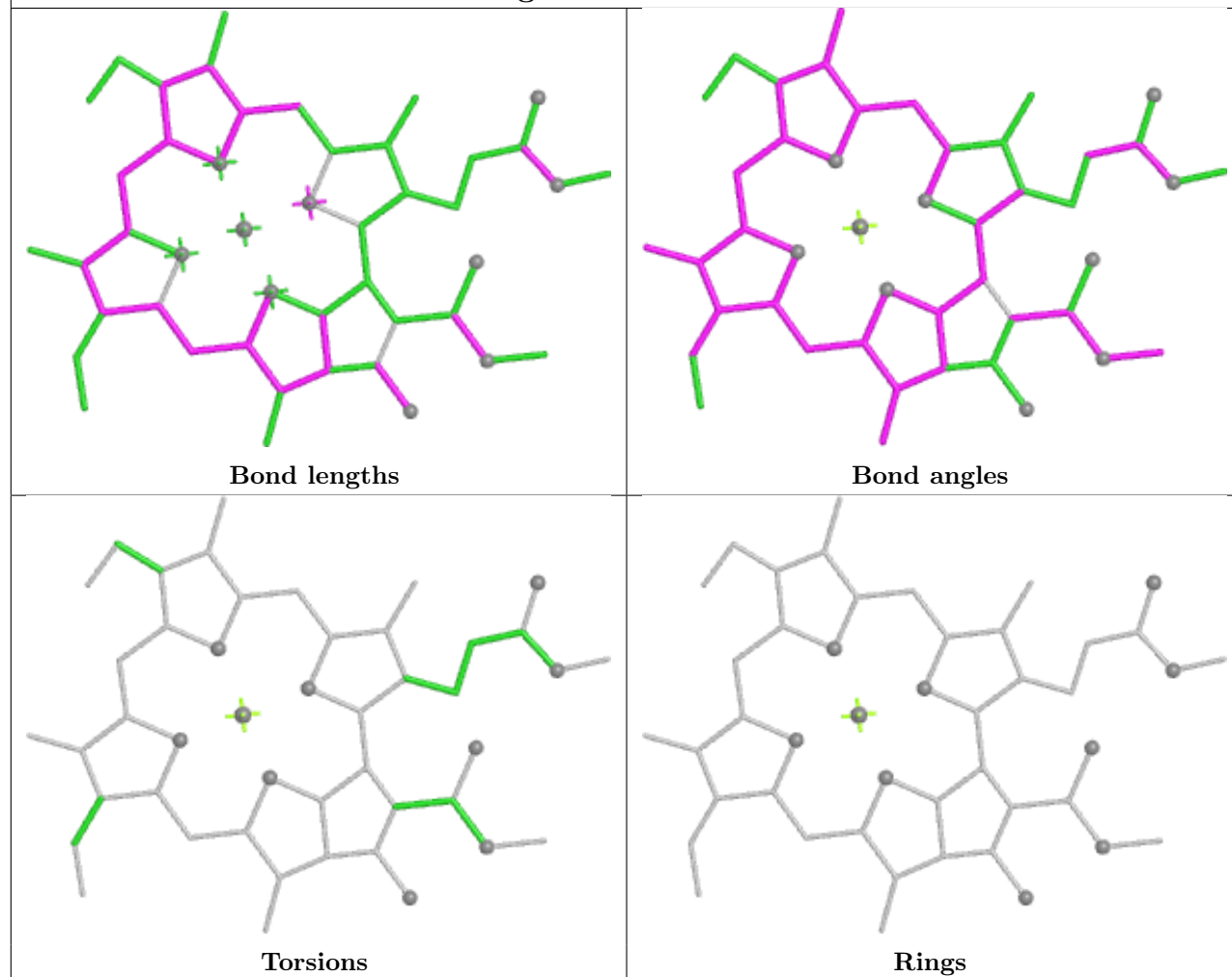


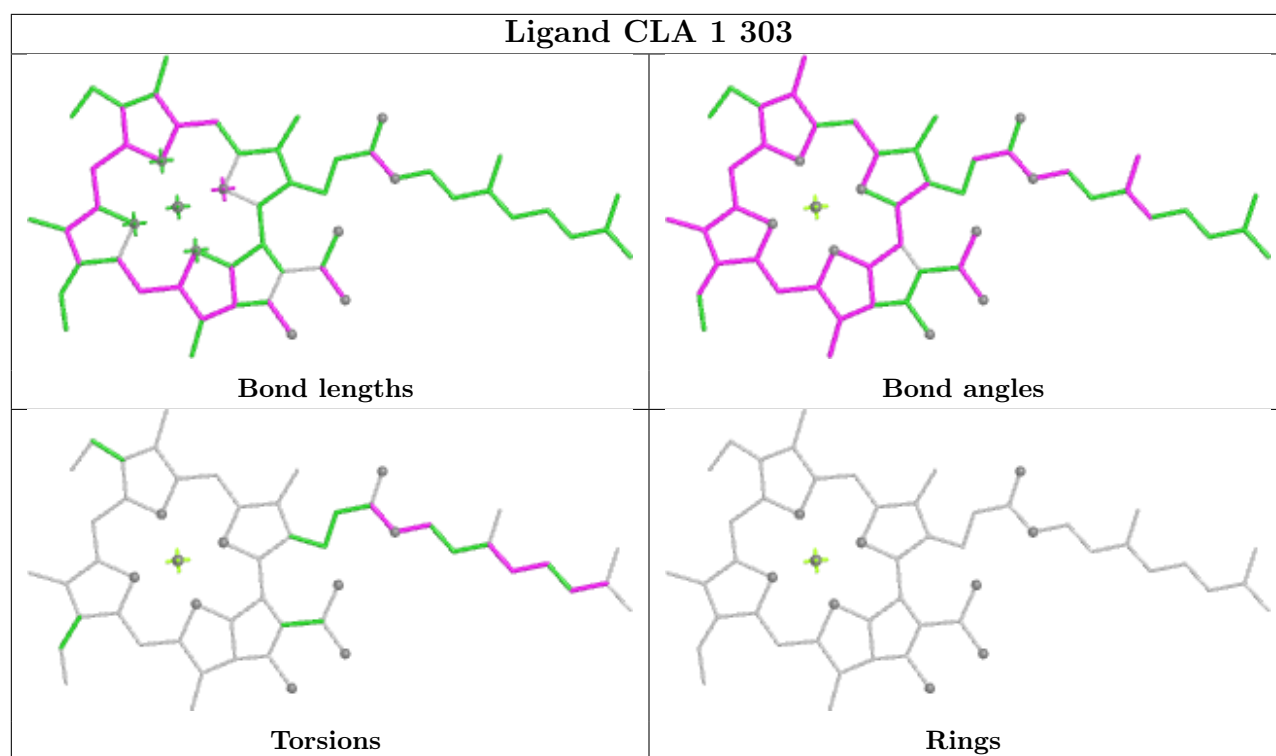


Ligand CLA A 826

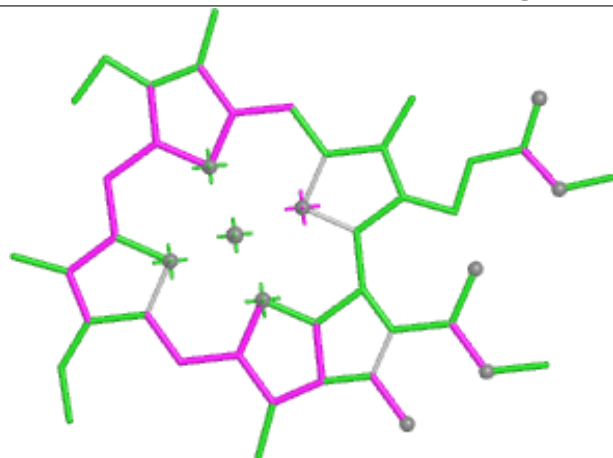


Ligand CLA 1 321

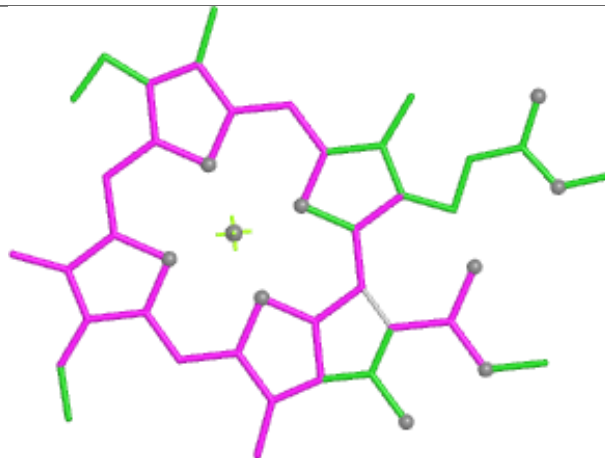




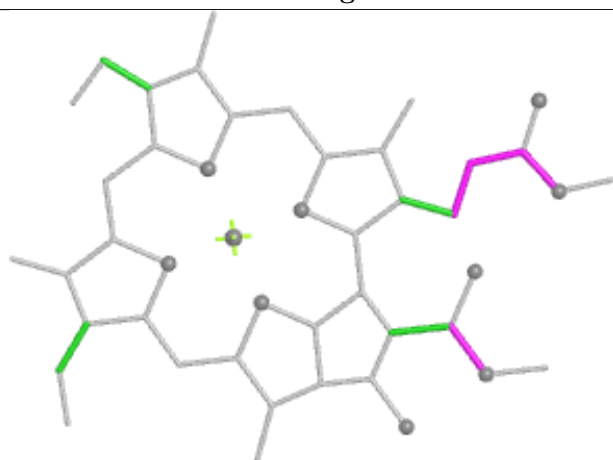
Ligand CLA F 306



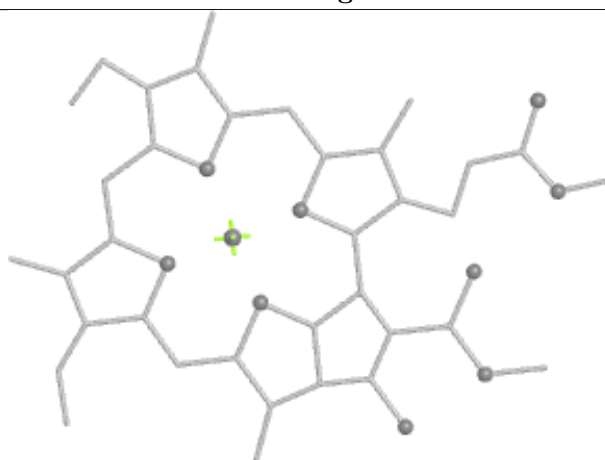
Bond lengths



Bond angles

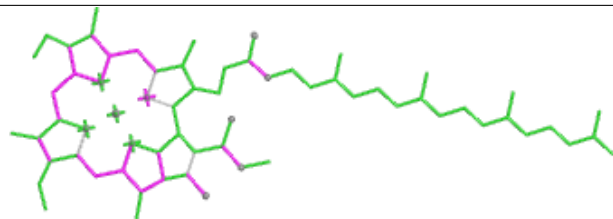


Torsions

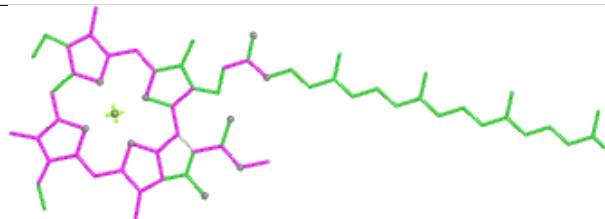


Rings

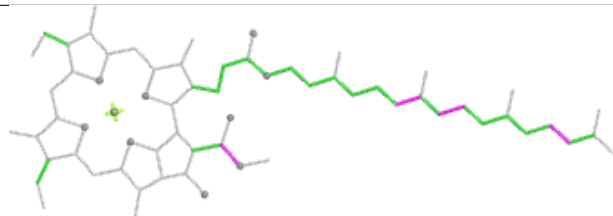
Ligand CLA A 852



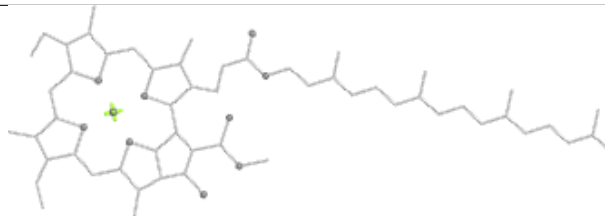
Bond lengths



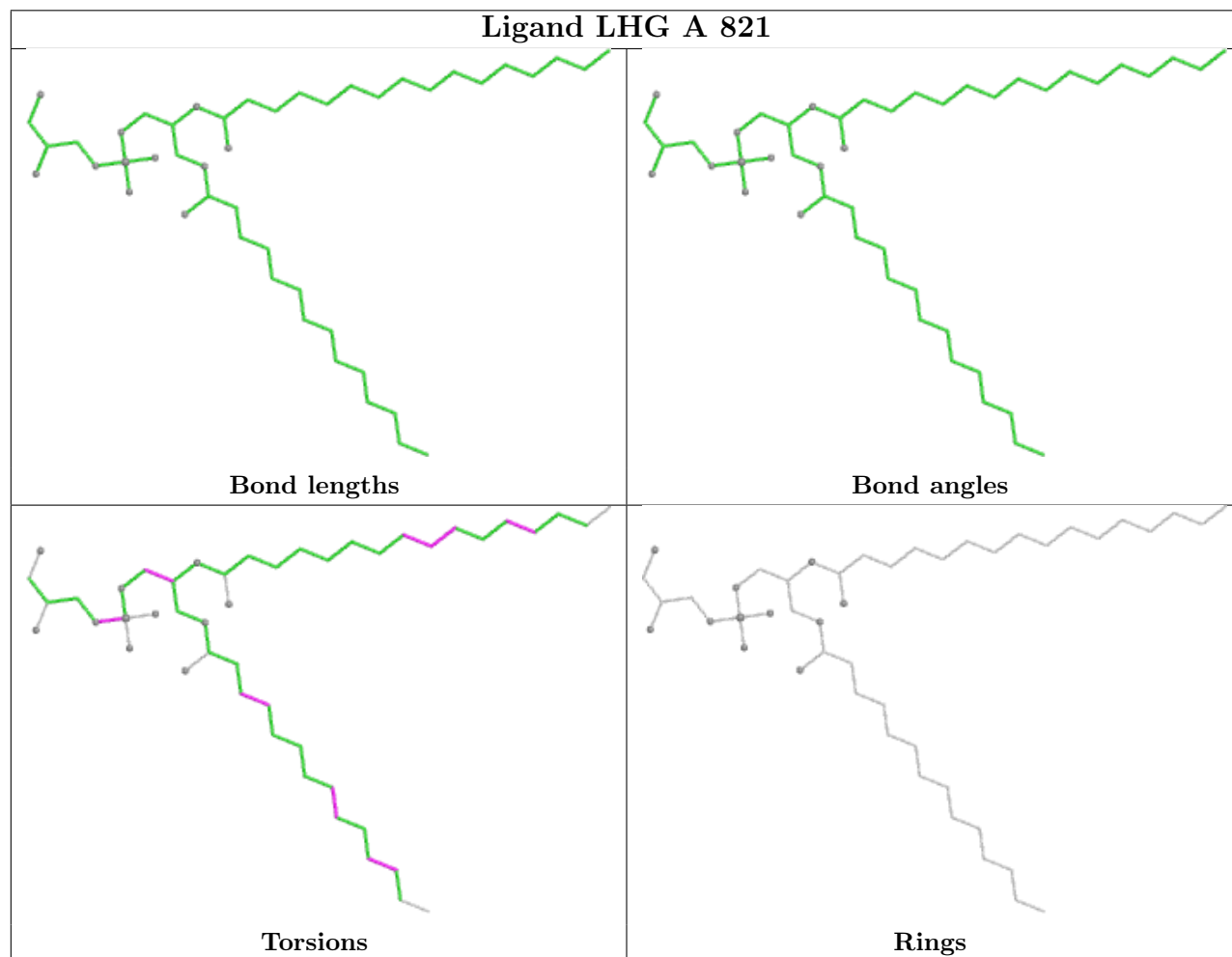
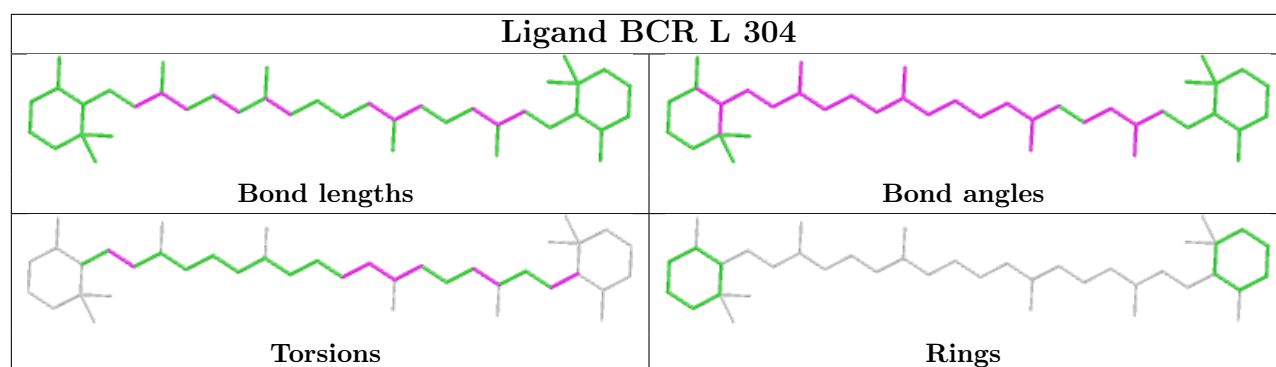
Bond angles

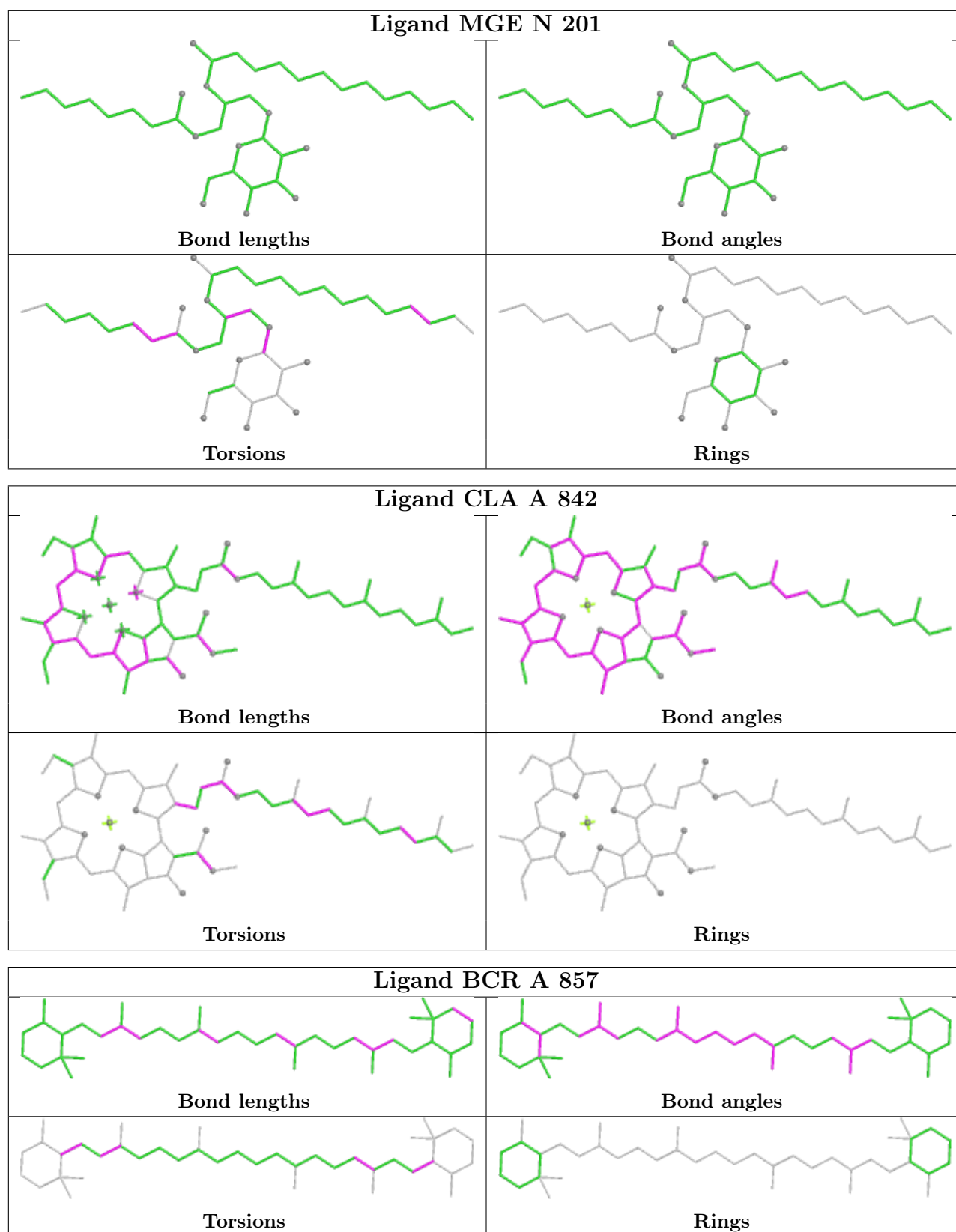


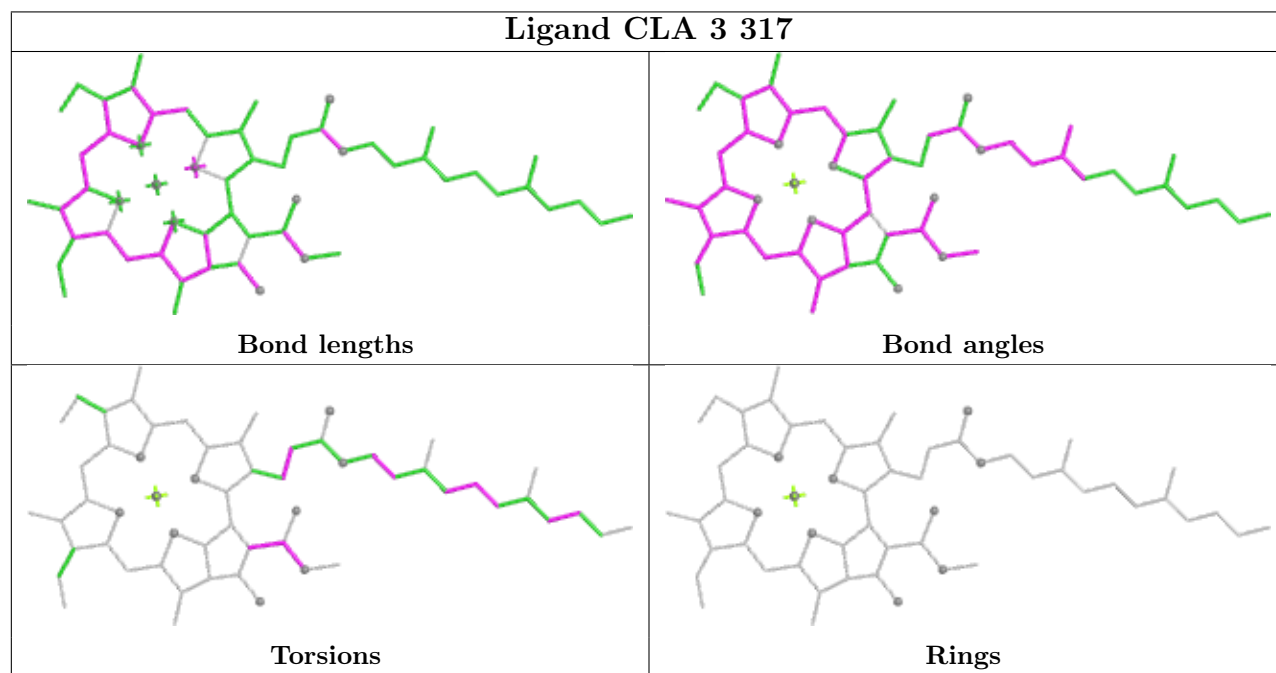
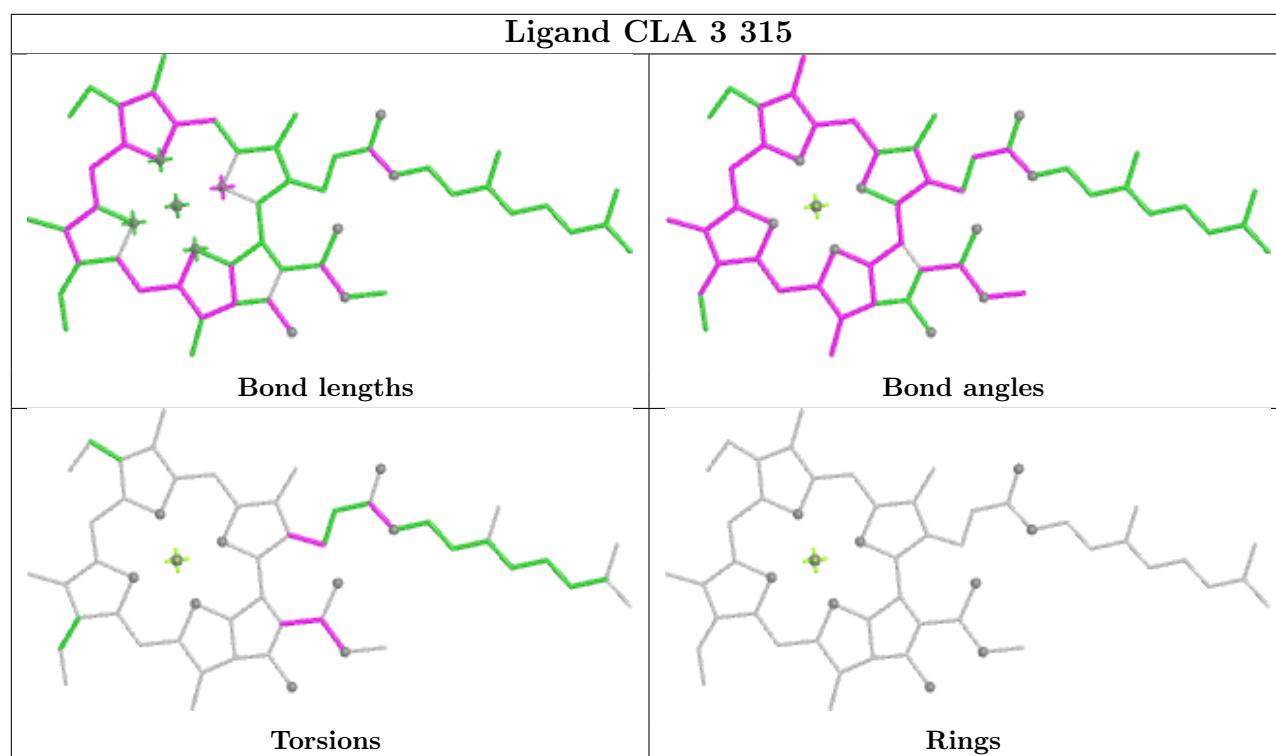
Torsions



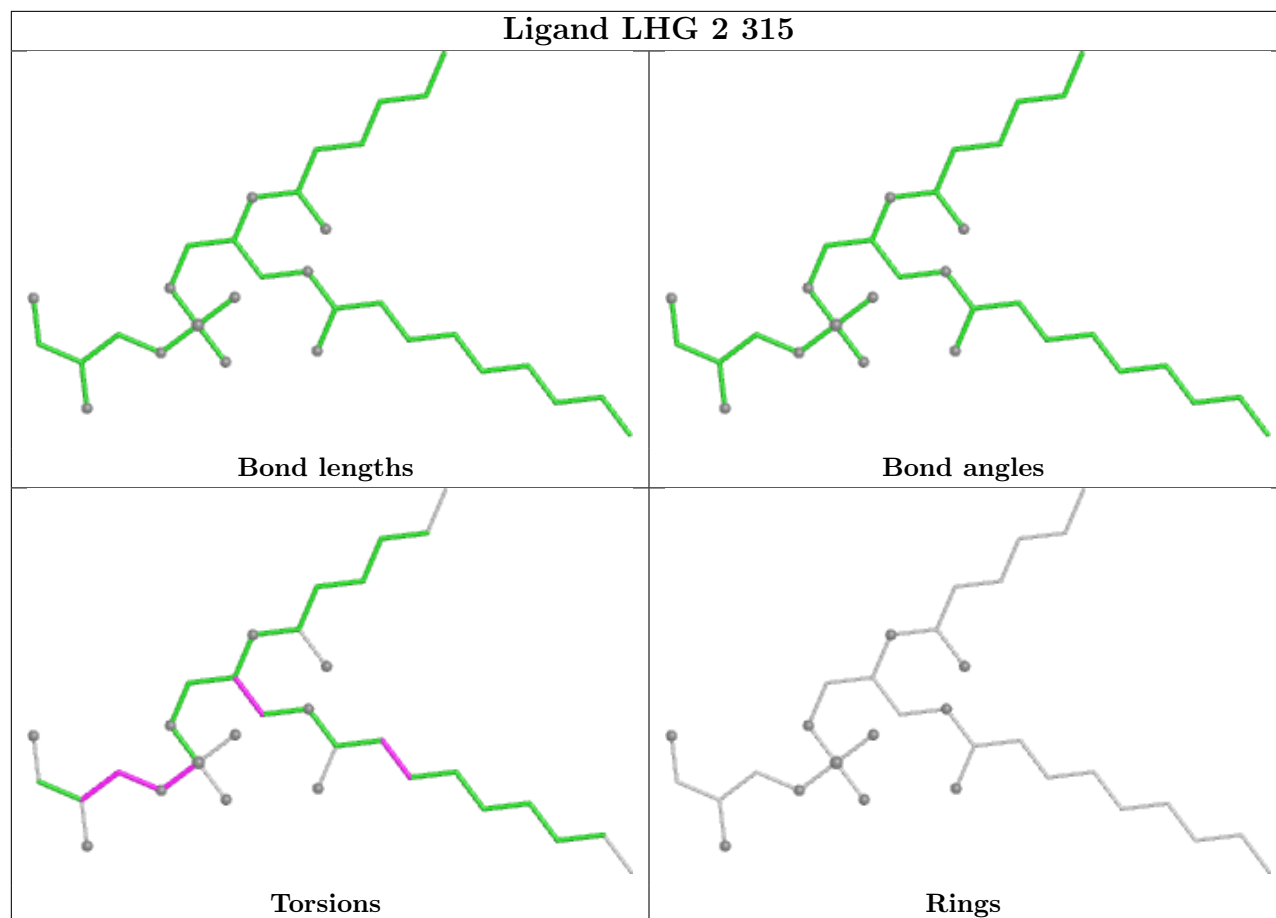
Rings



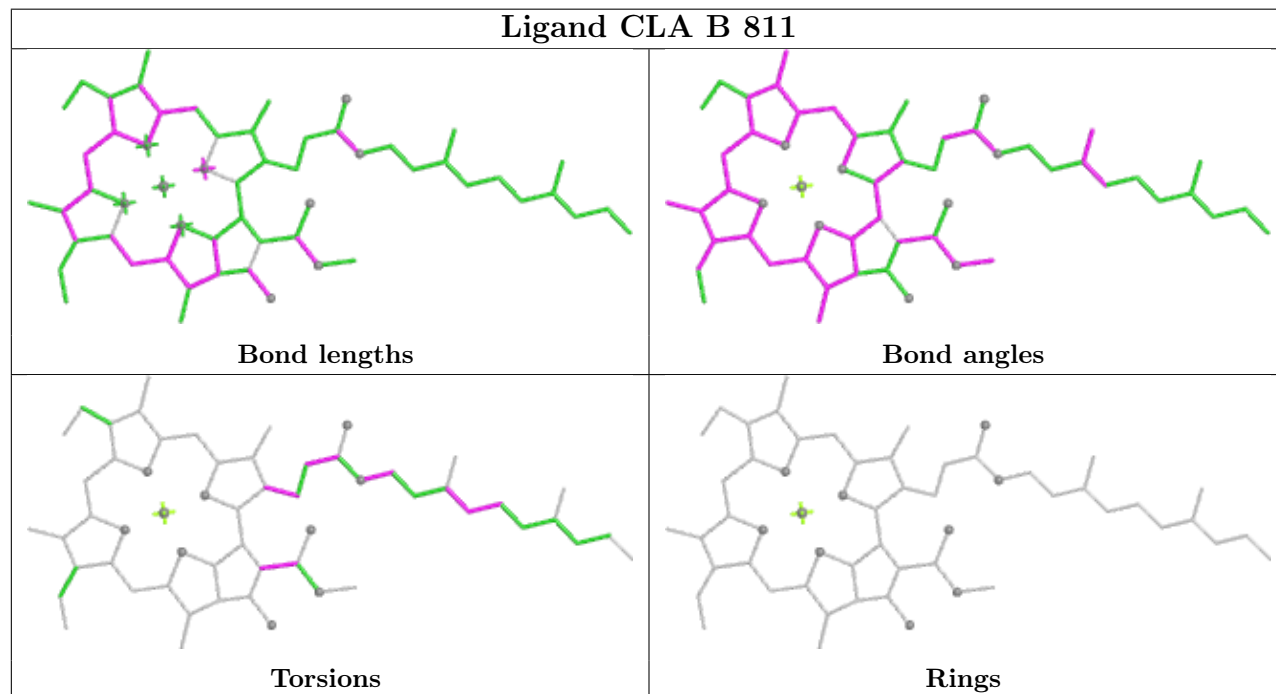




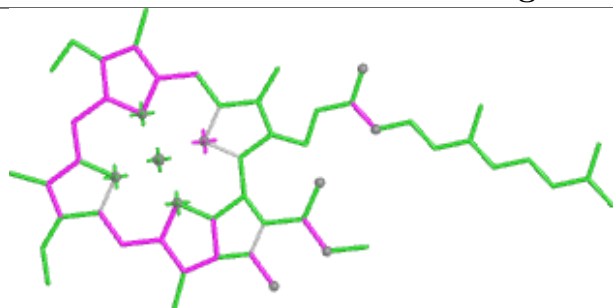
Ligand LHG 2 315



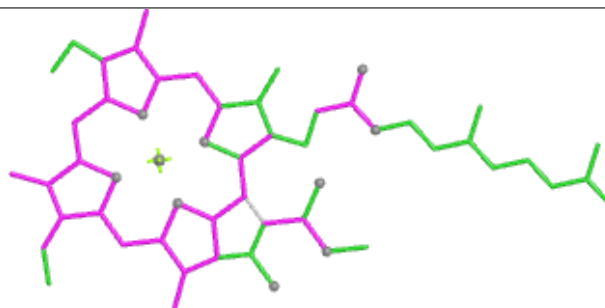
Ligand CLA B 811



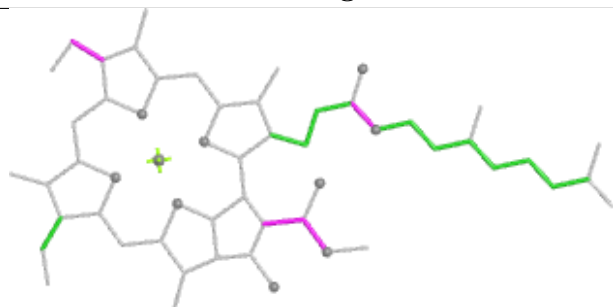
Ligand CLA 1 304



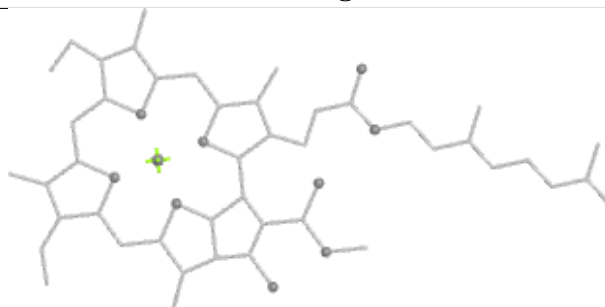
Bond lengths



Bond angles

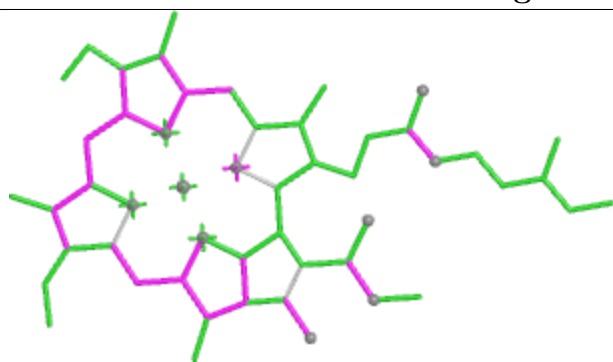


Torsions

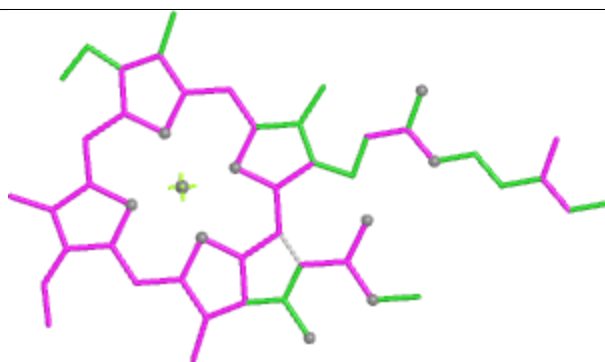


Rings

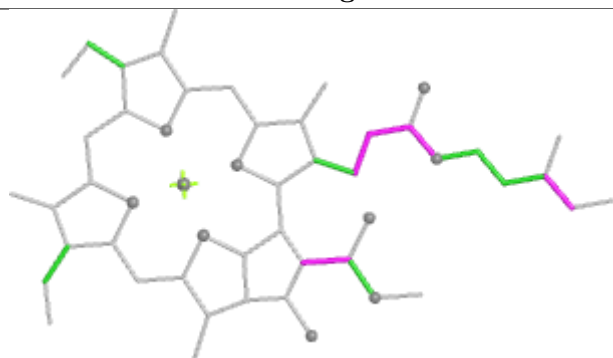
Ligand CLA A 804



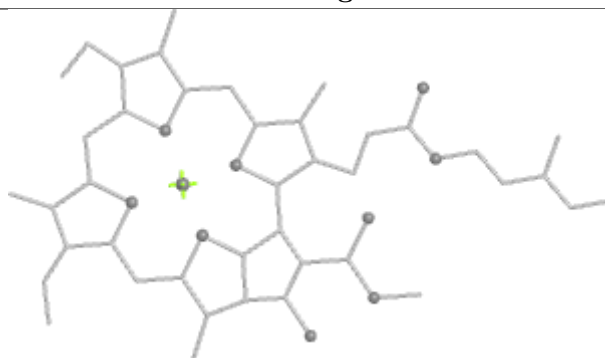
Bond lengths



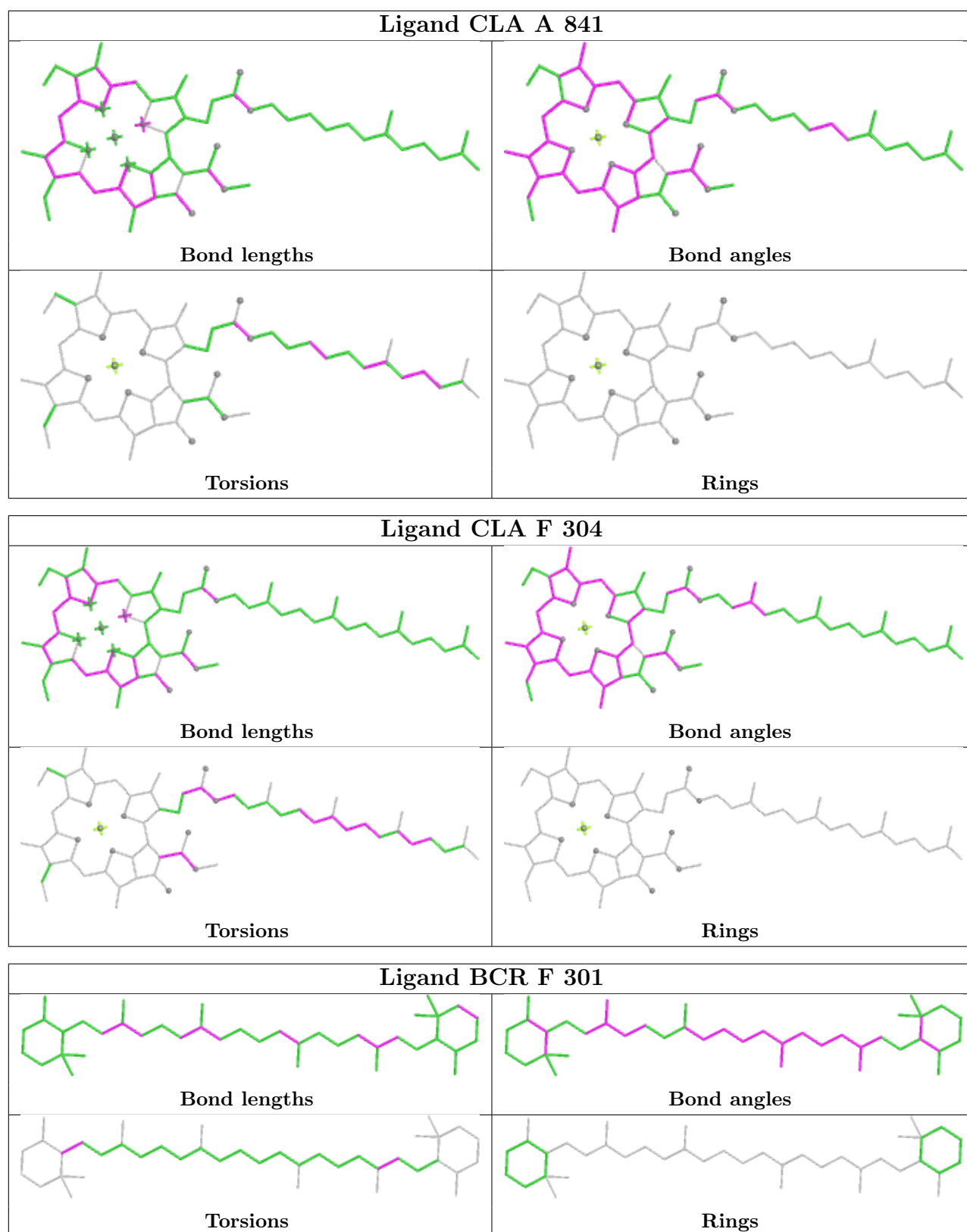
Bond angles

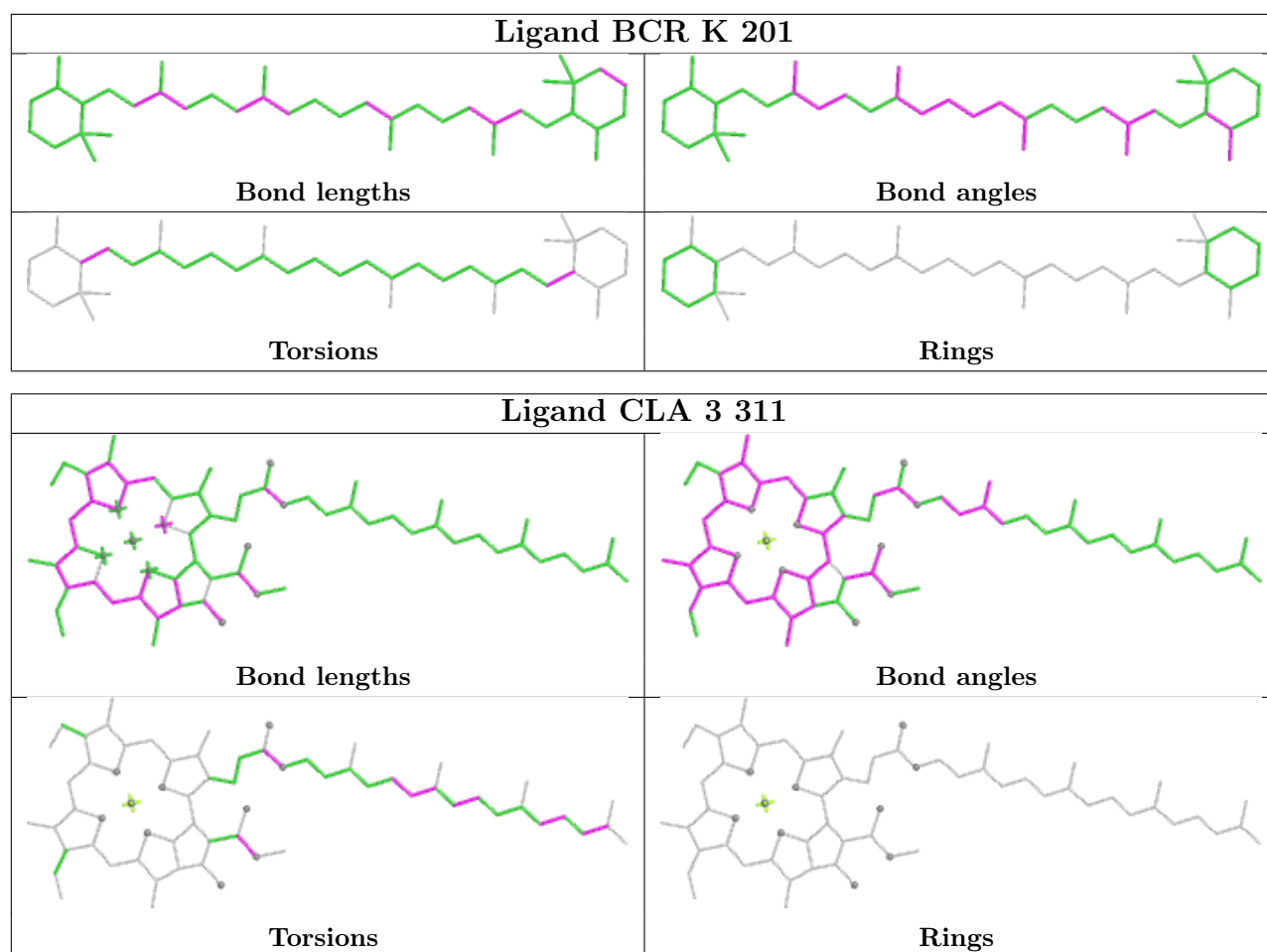


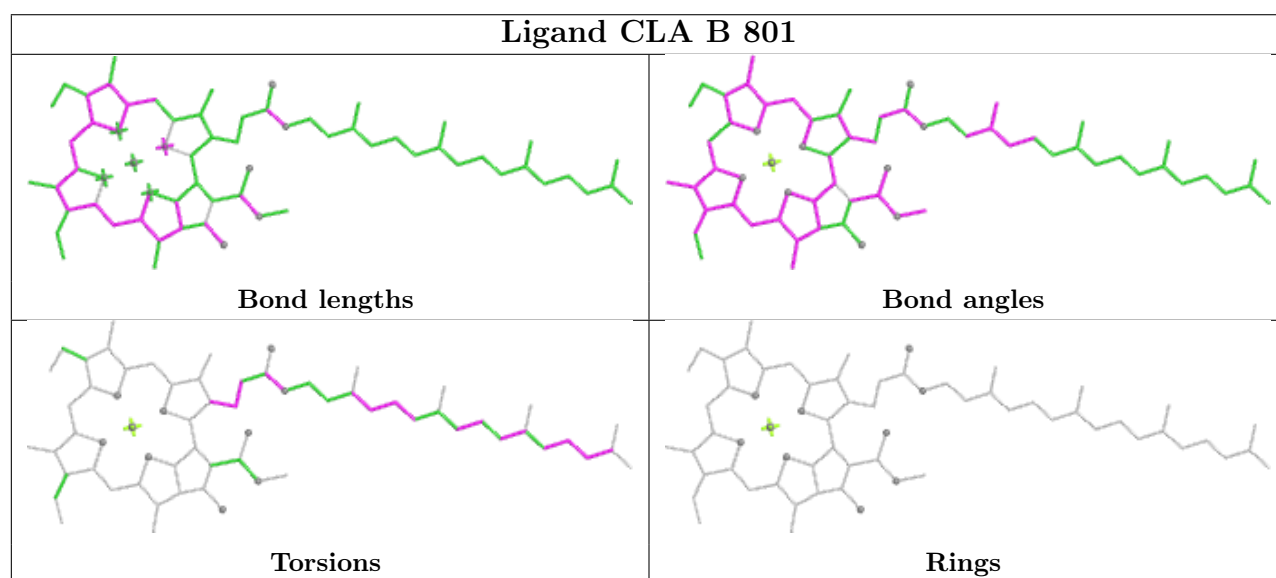
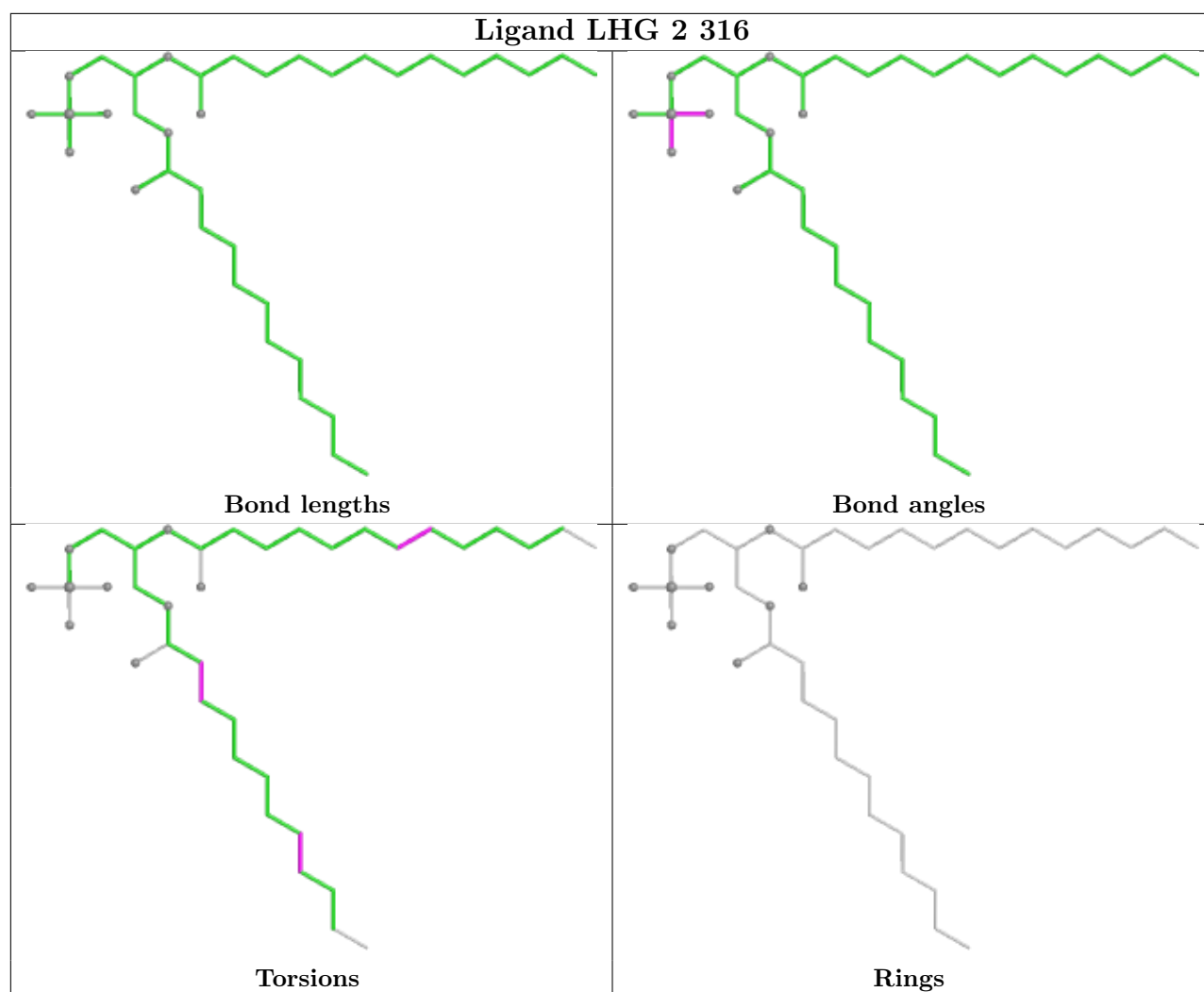
Torsions

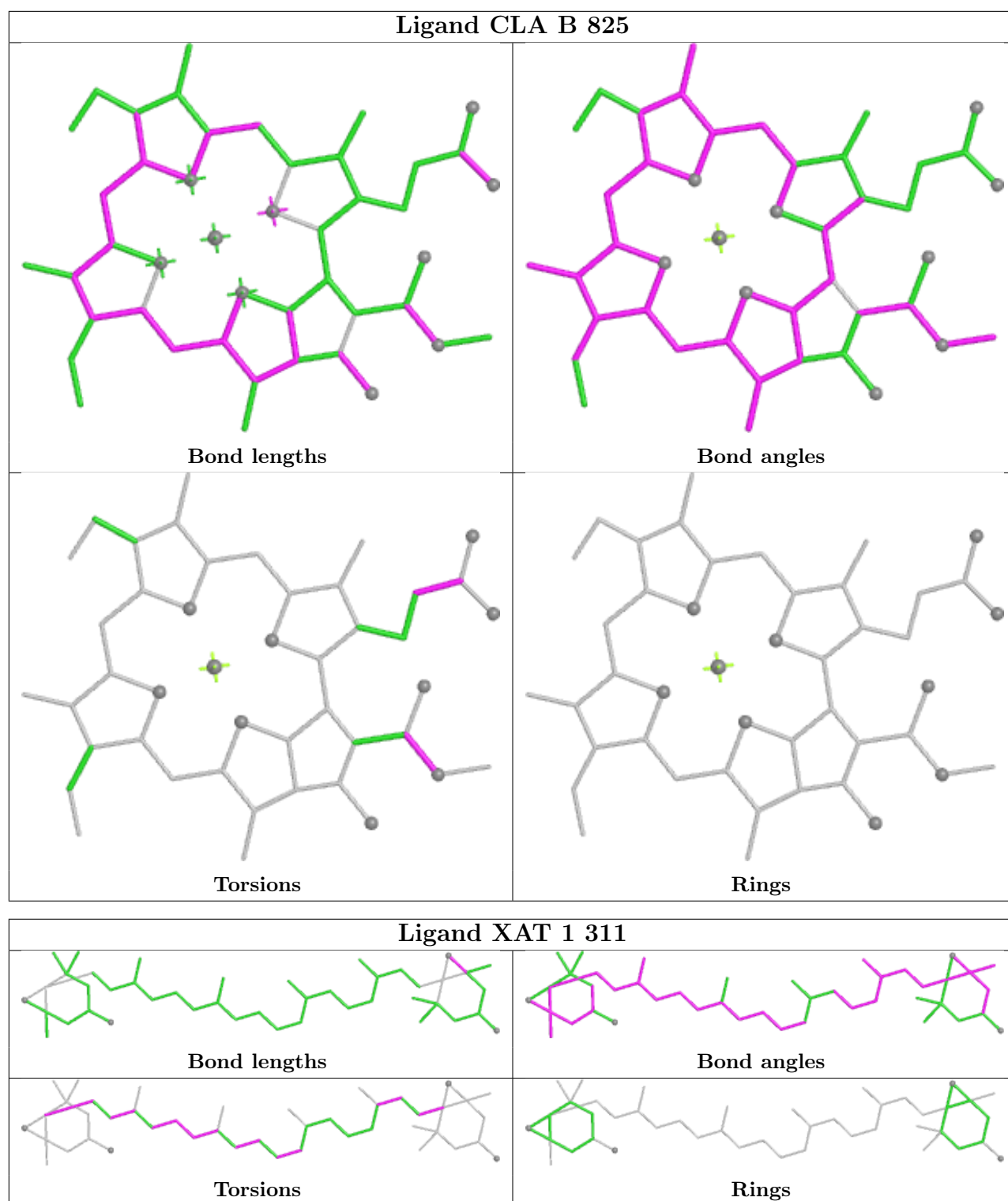


Rings

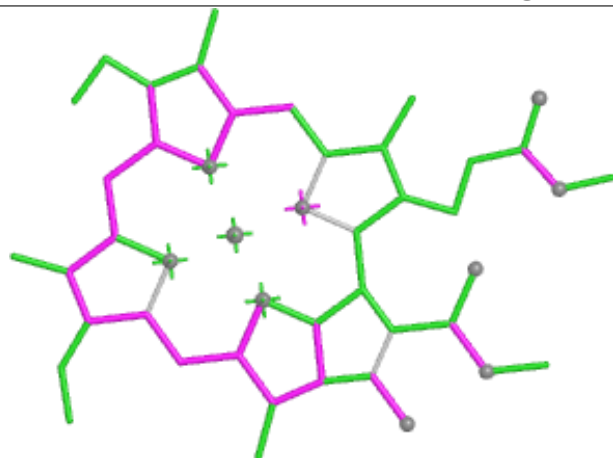




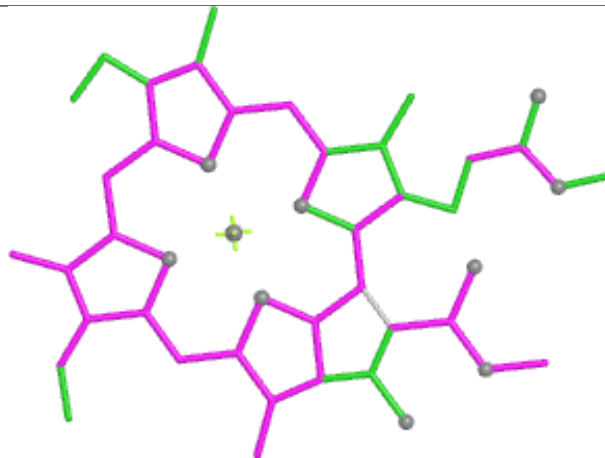




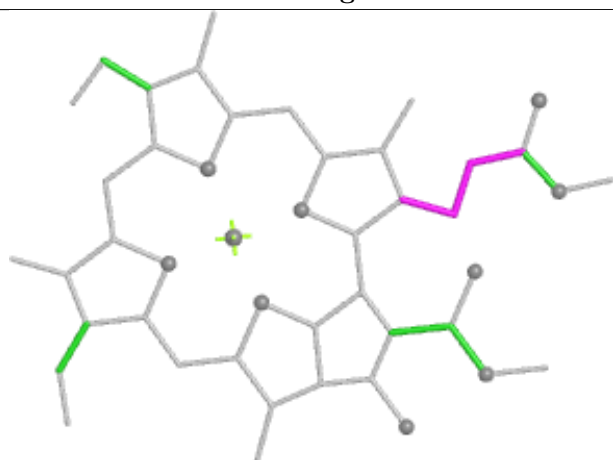
Ligand CLA 1 305



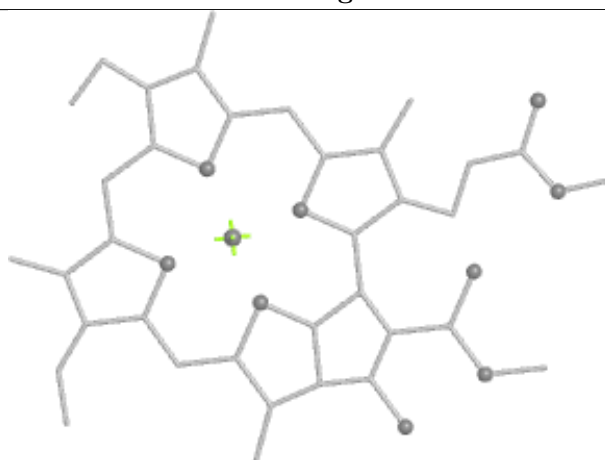
Bond lengths



Bond angles

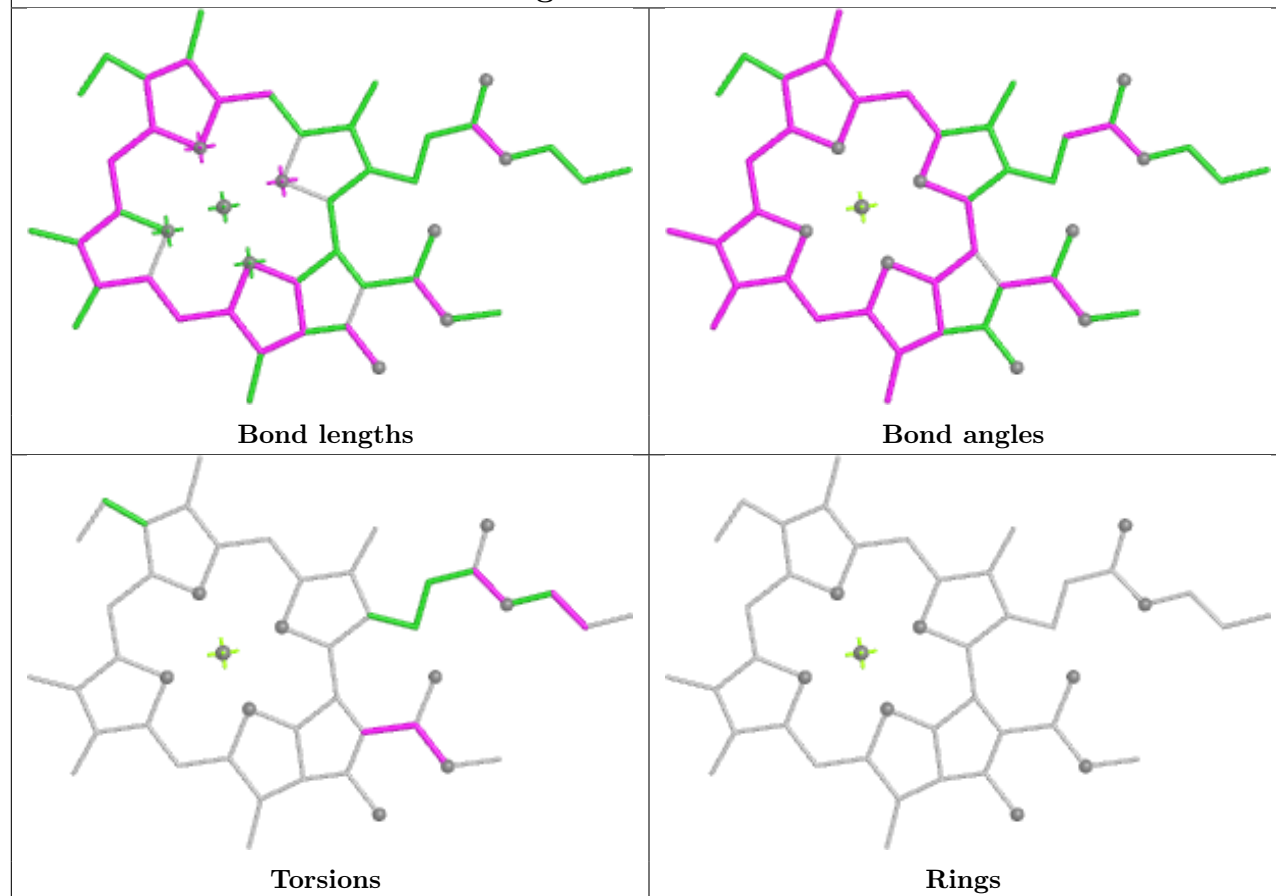


Torsions

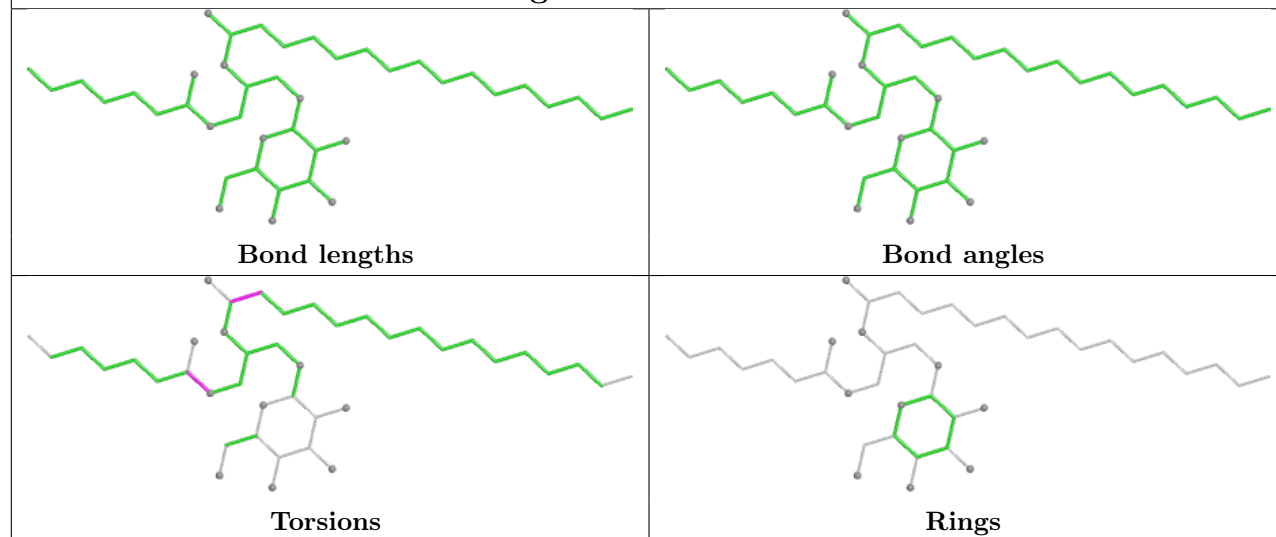


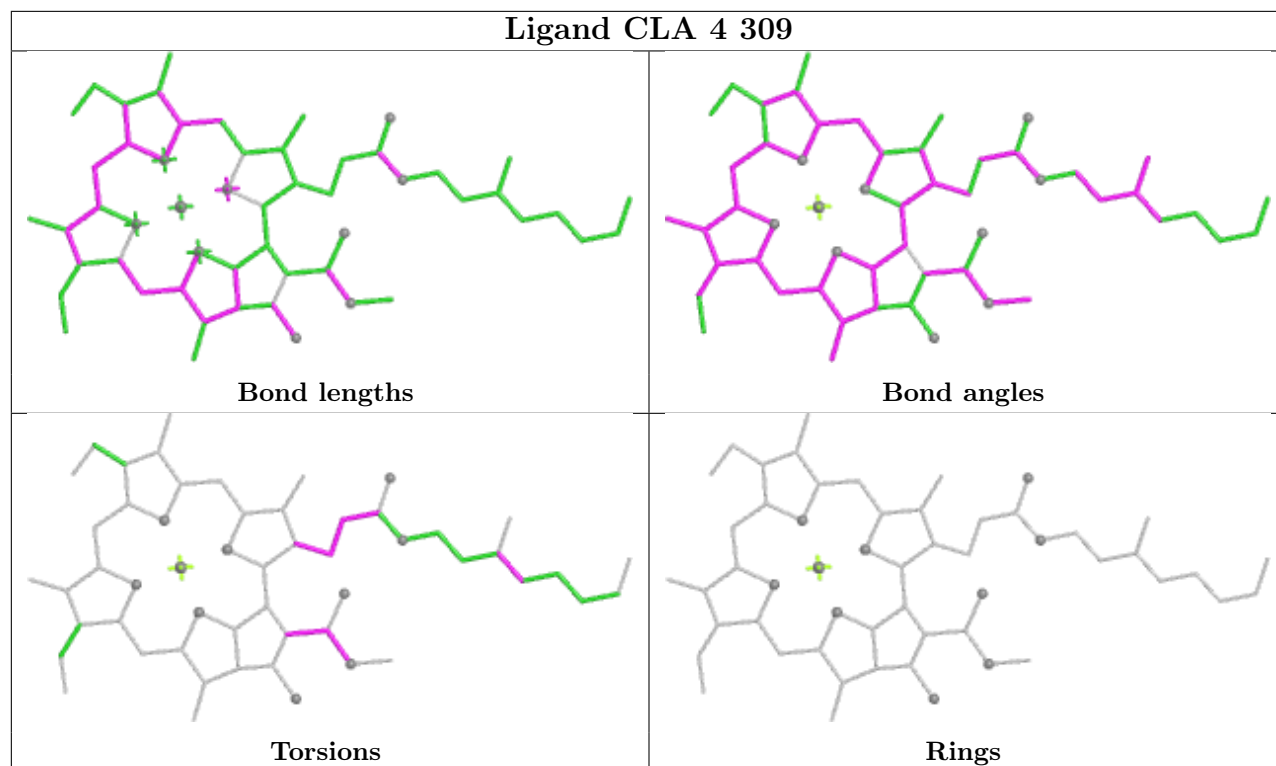
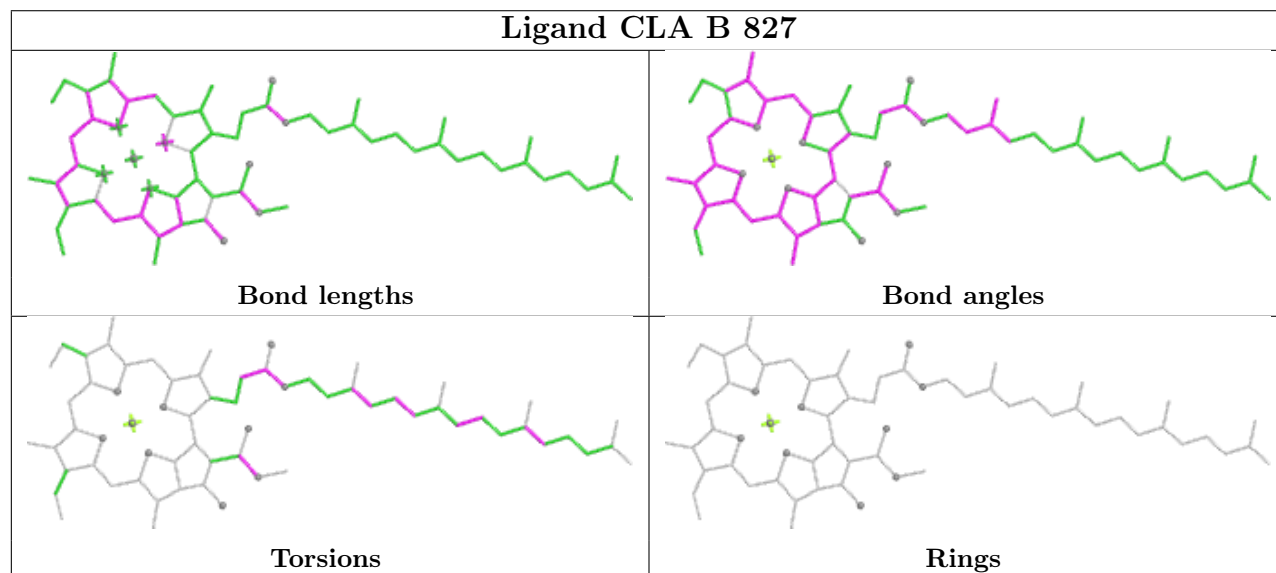
Rings

Ligand CLA 2 320

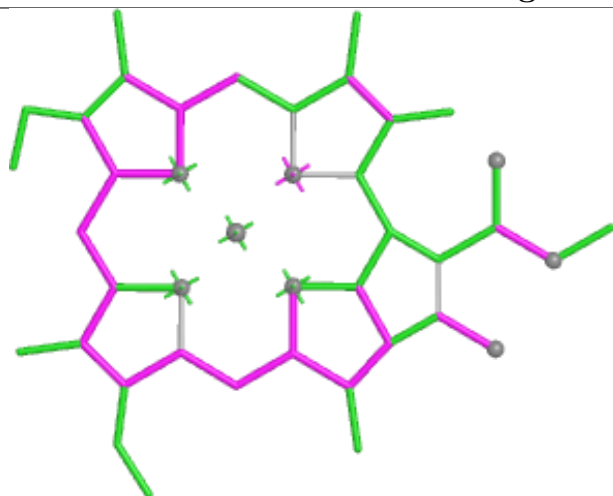


Ligand MGE J 102



Ligand CLA 4 309**Ligand CLA B 827**

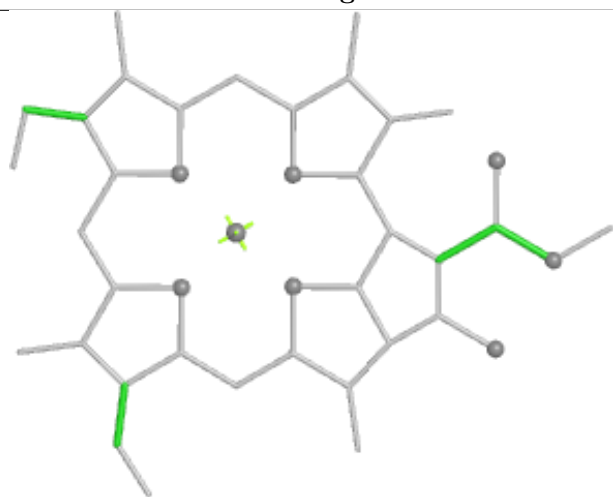
Ligand CLA 3 318



Bond lengths



Bond angles

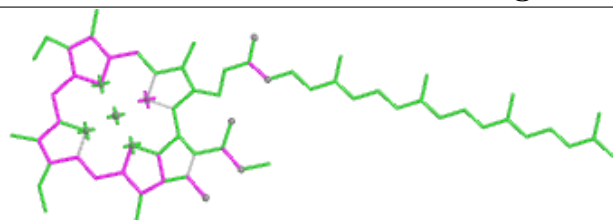


Torsions

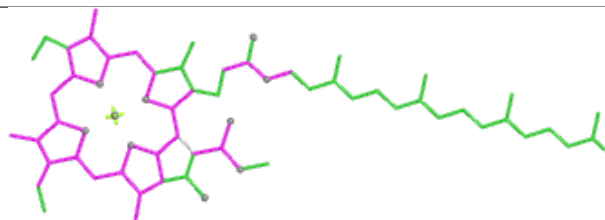


Rings

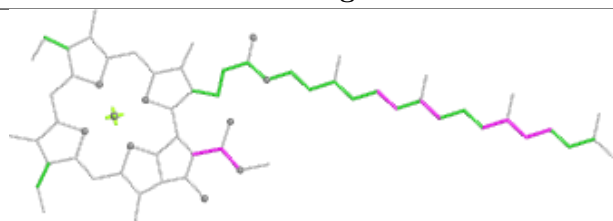
Ligand CLA A 827



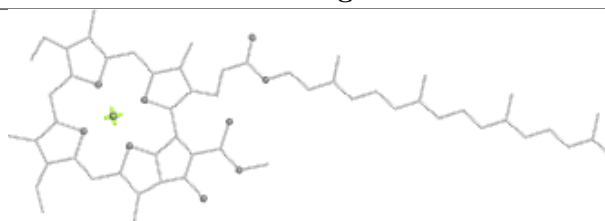
Bond lengths



Bond angles

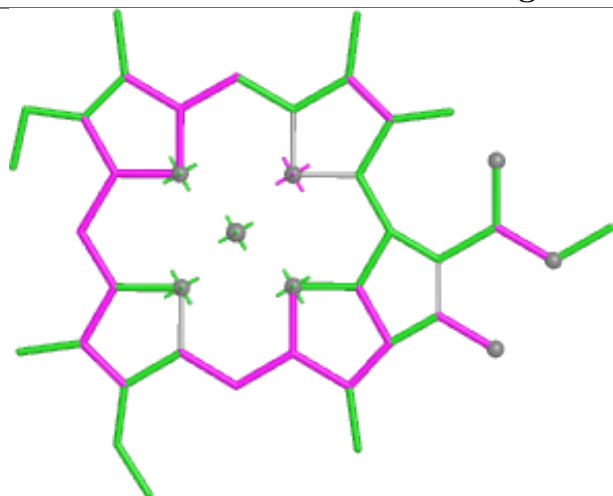


Torsions



Rings

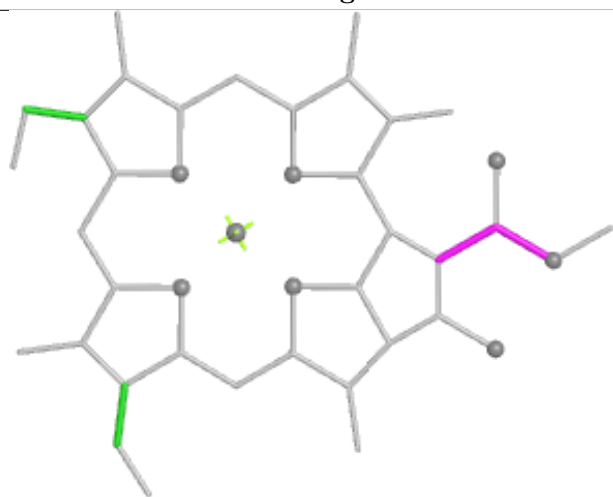
Ligand CLA 1 309



Bond lengths



Bond angles

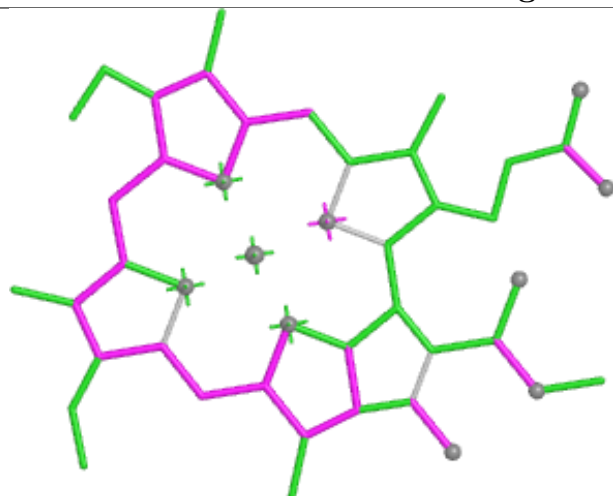


Torsions

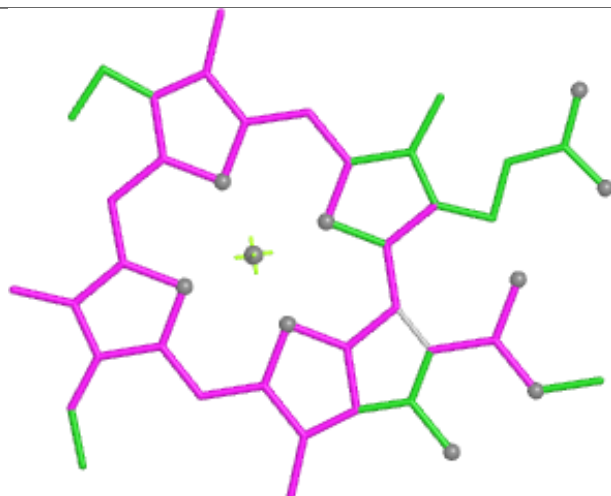


Rings

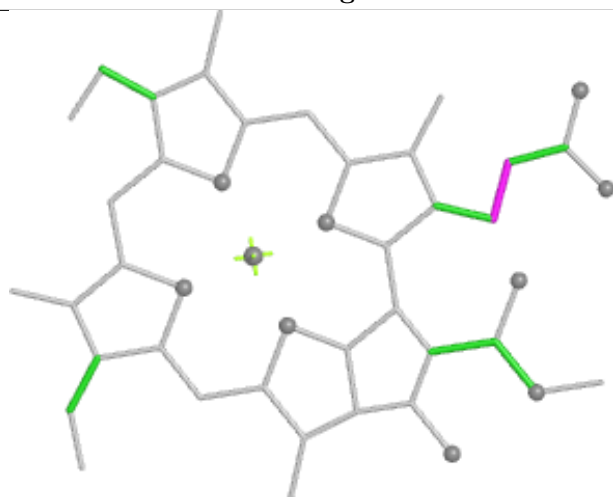
Ligand CLA 3 312



Bond lengths



Bond angles

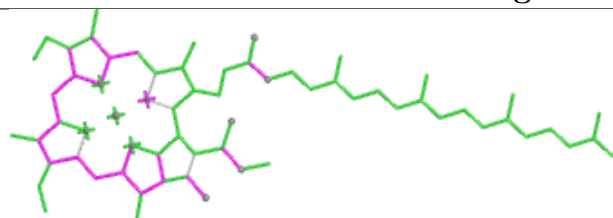


Torsions

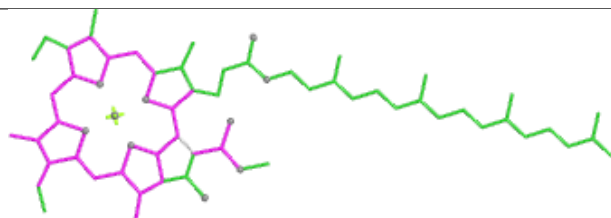


Rings

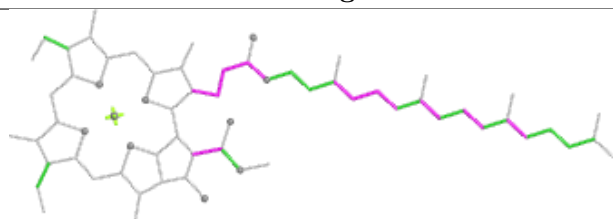
Ligand CLA A 809



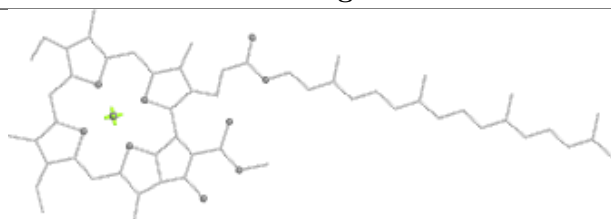
Bond lengths



Bond angles

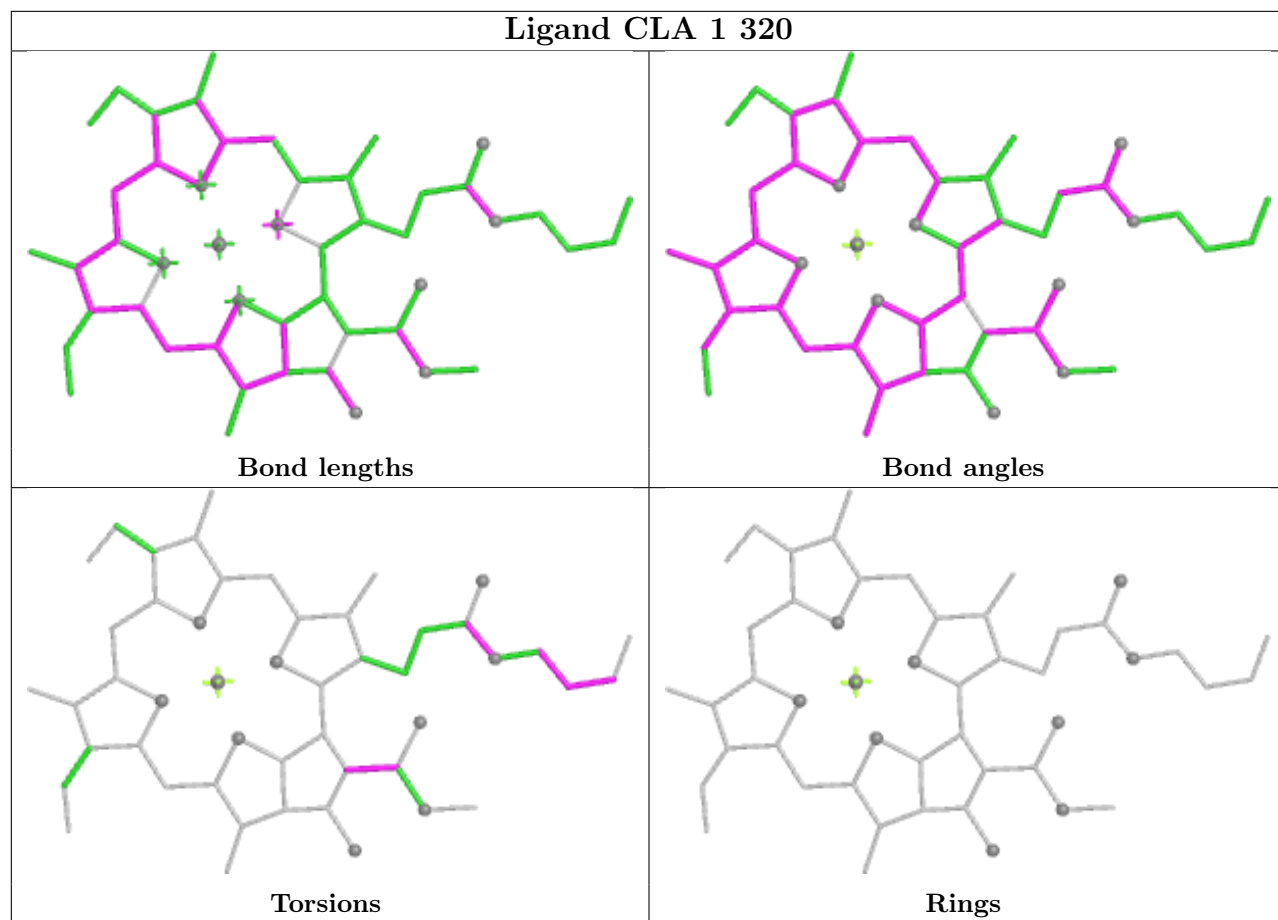


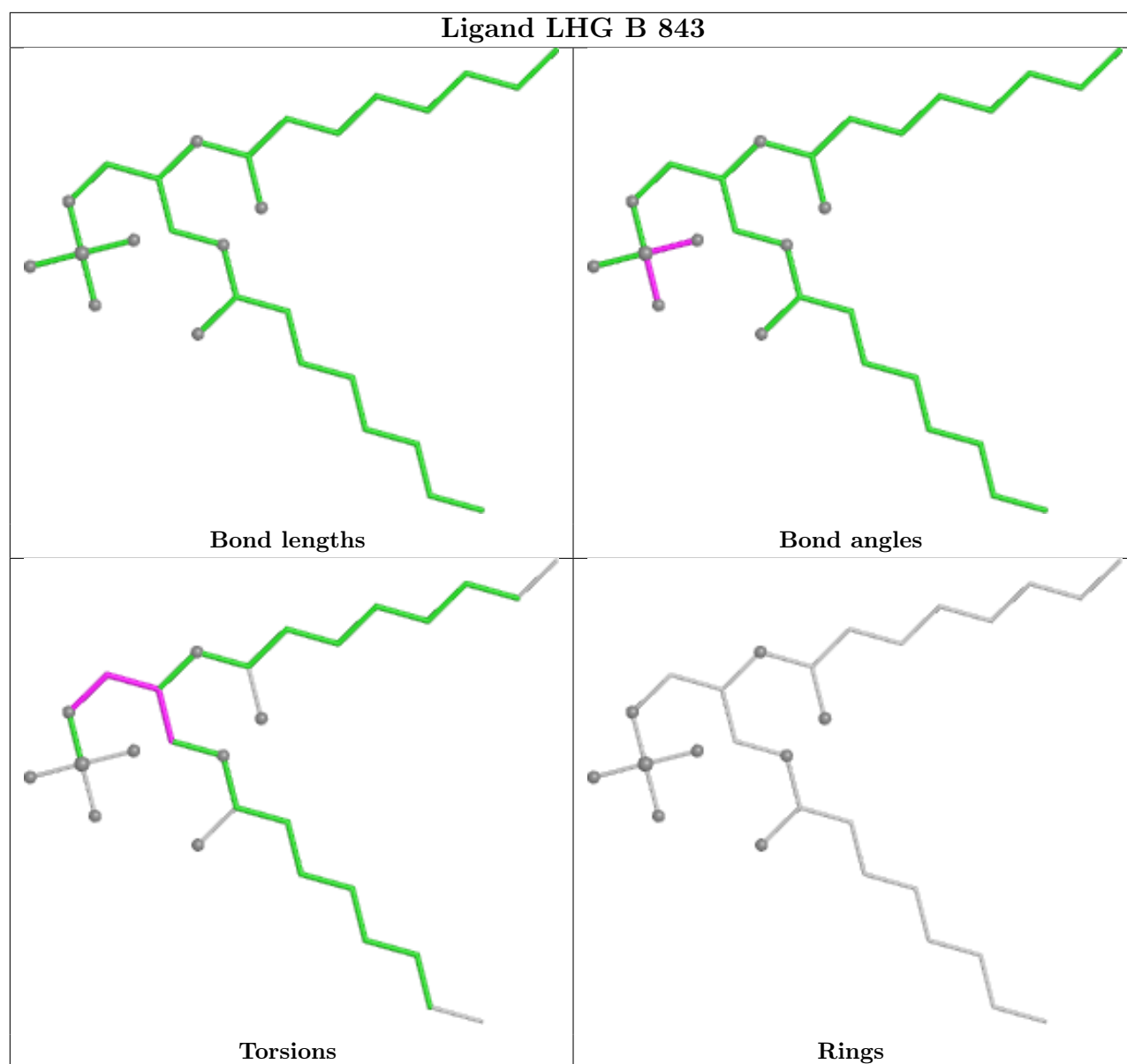
Torsions

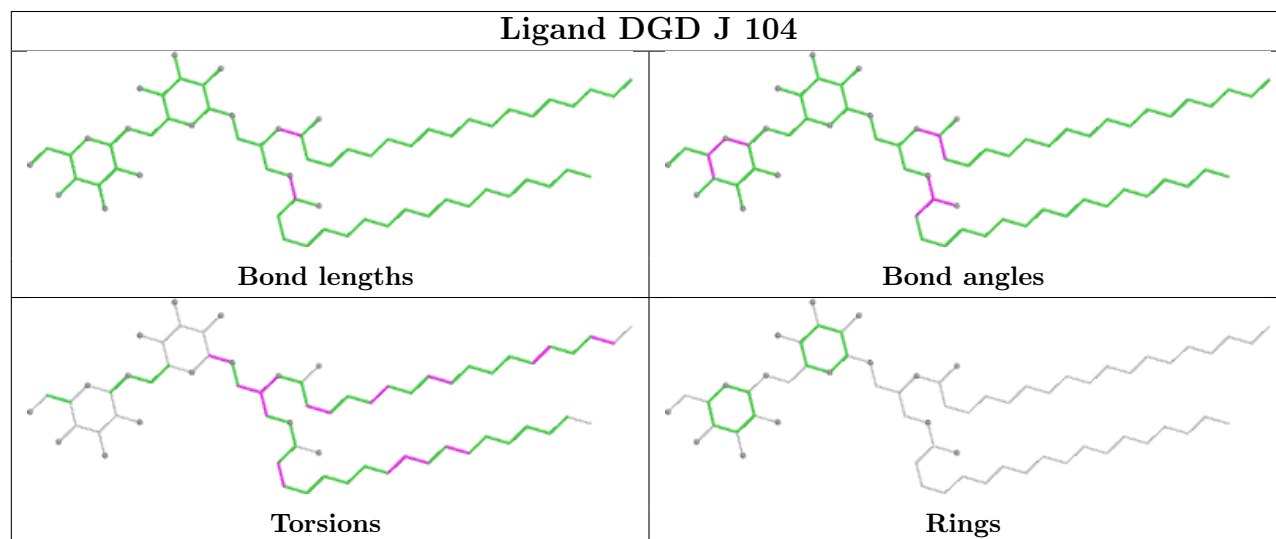
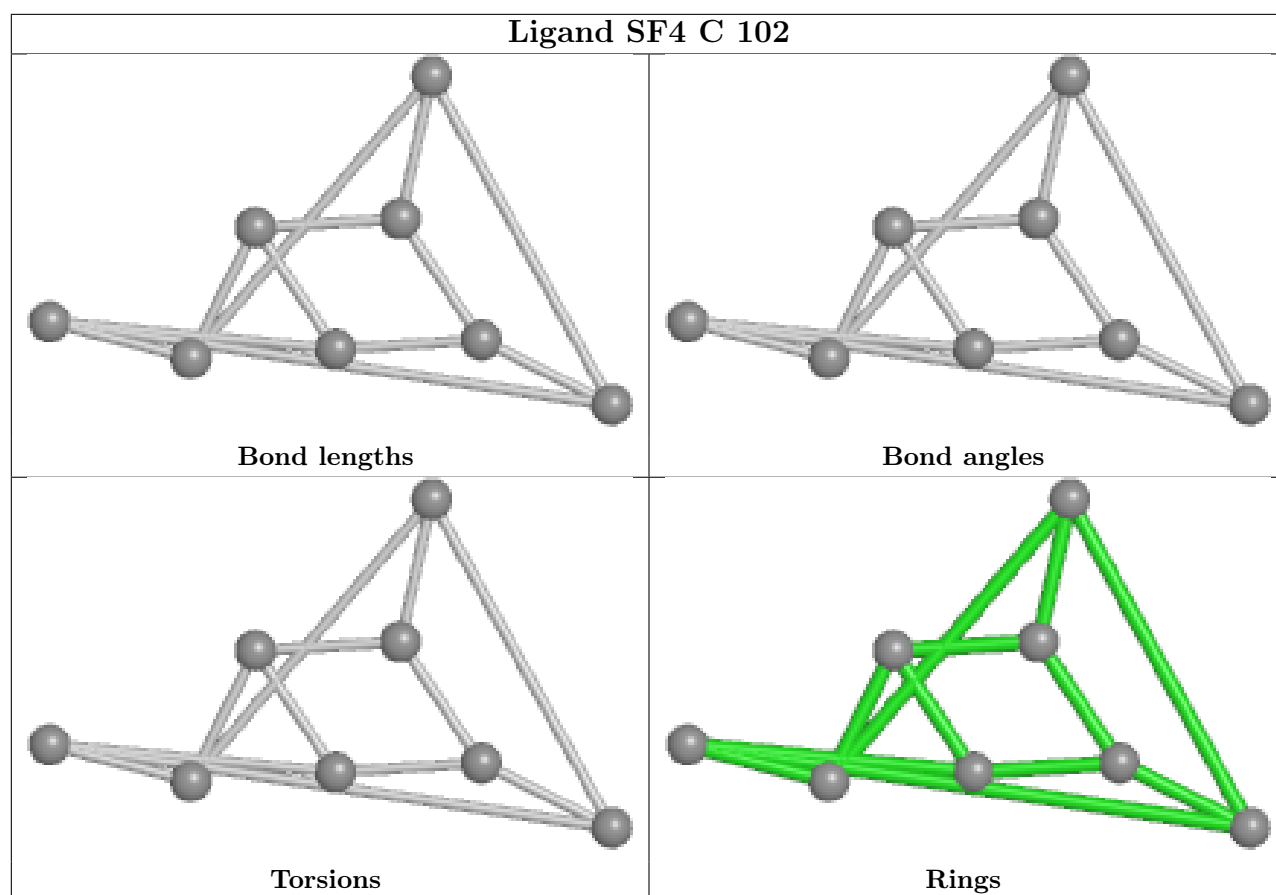


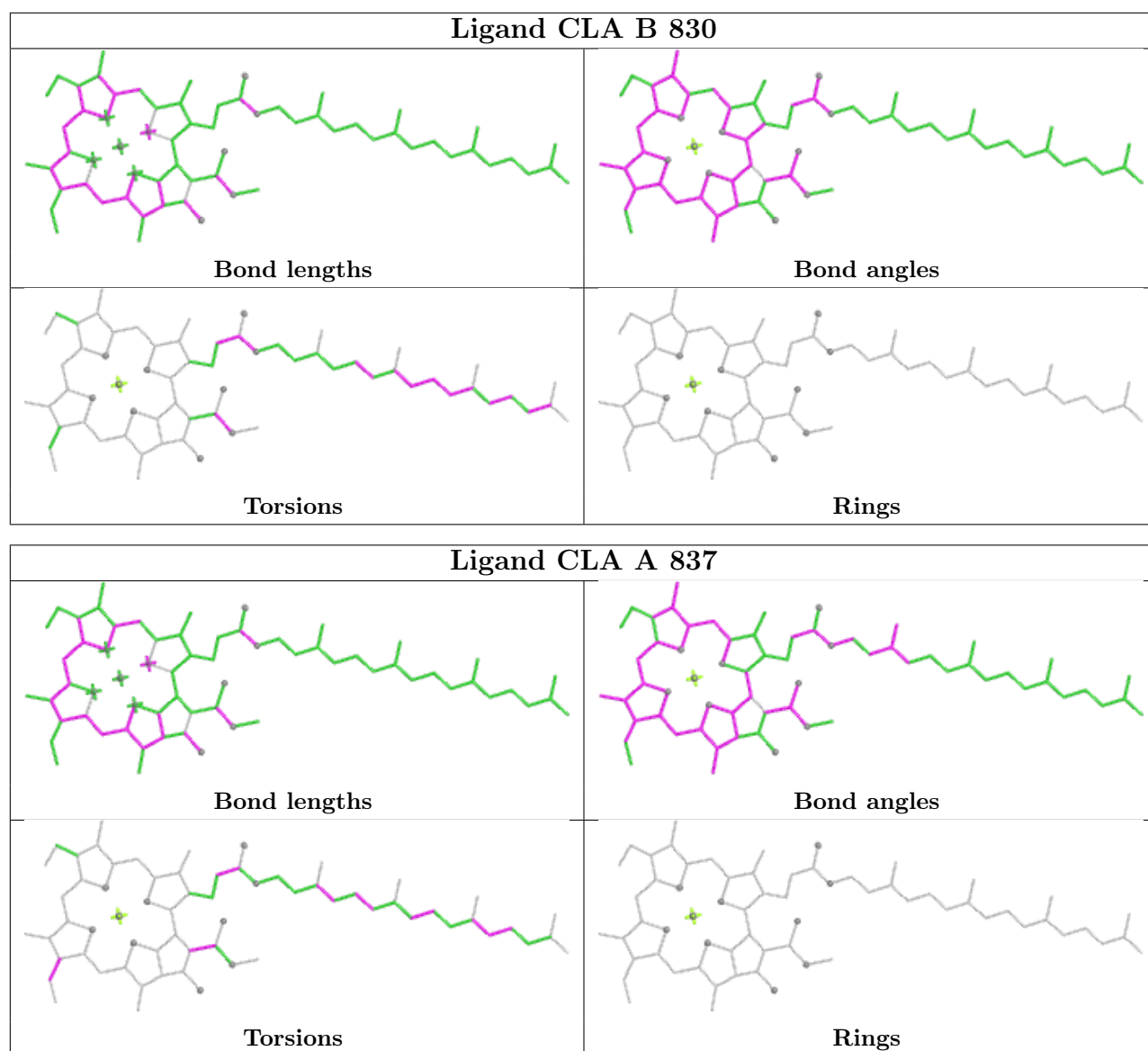
Rings

Ligand CLA 1 320

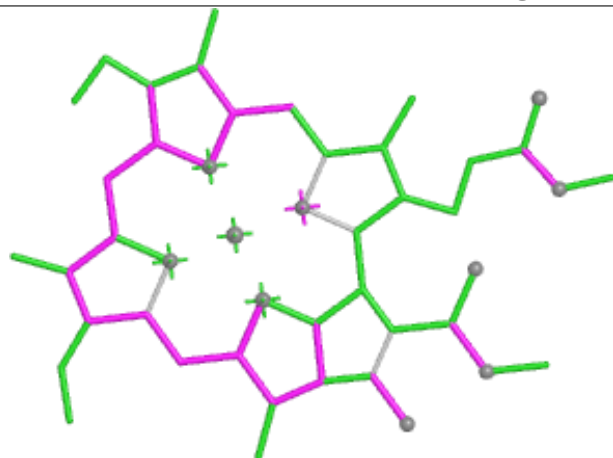




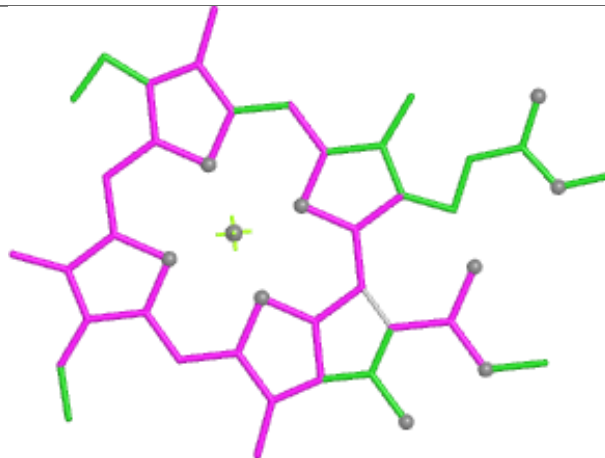




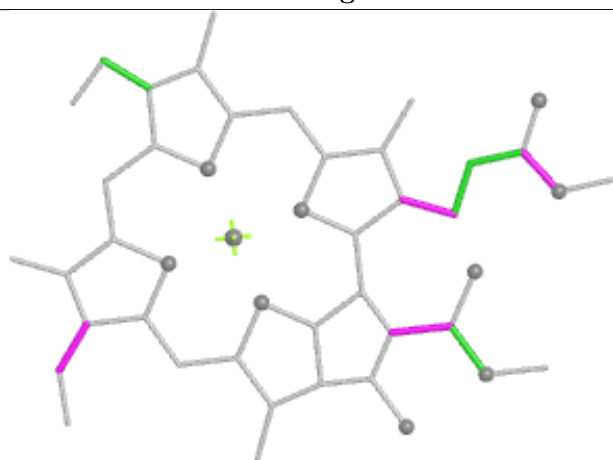
Ligand CLA A 846



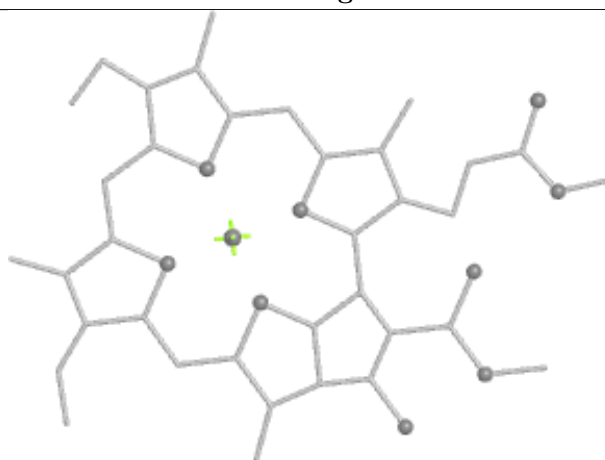
Bond lengths



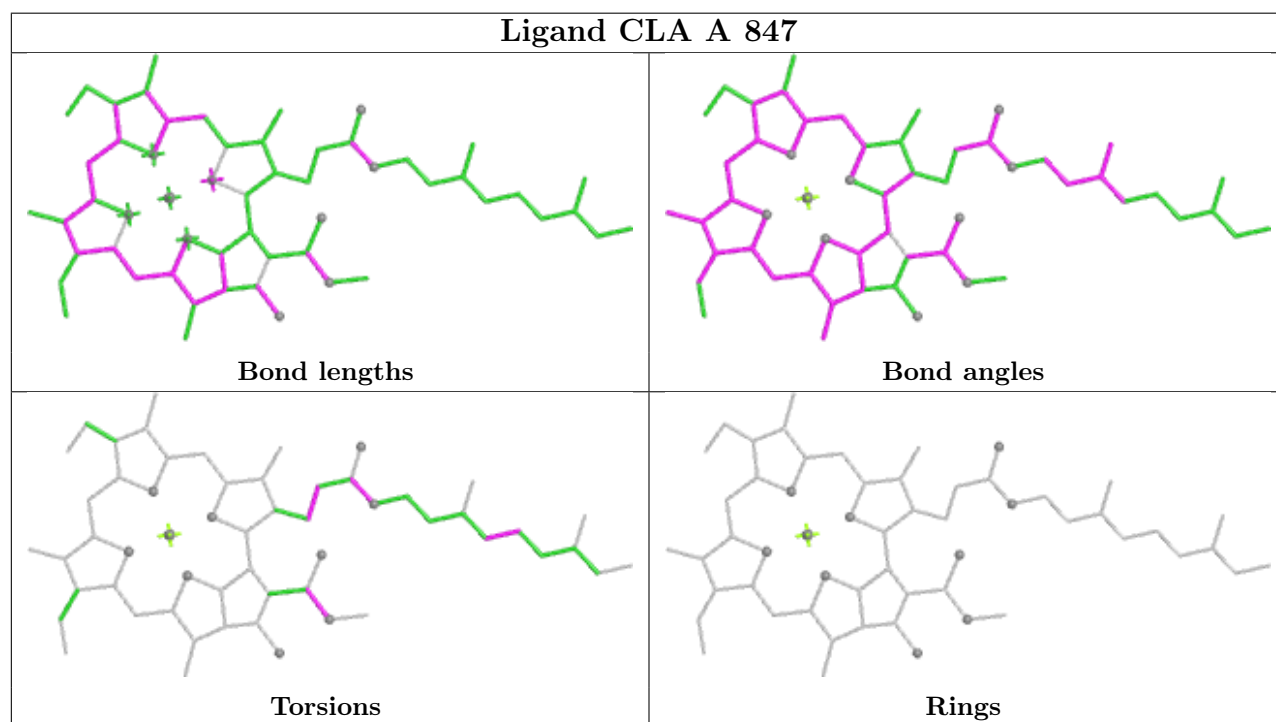
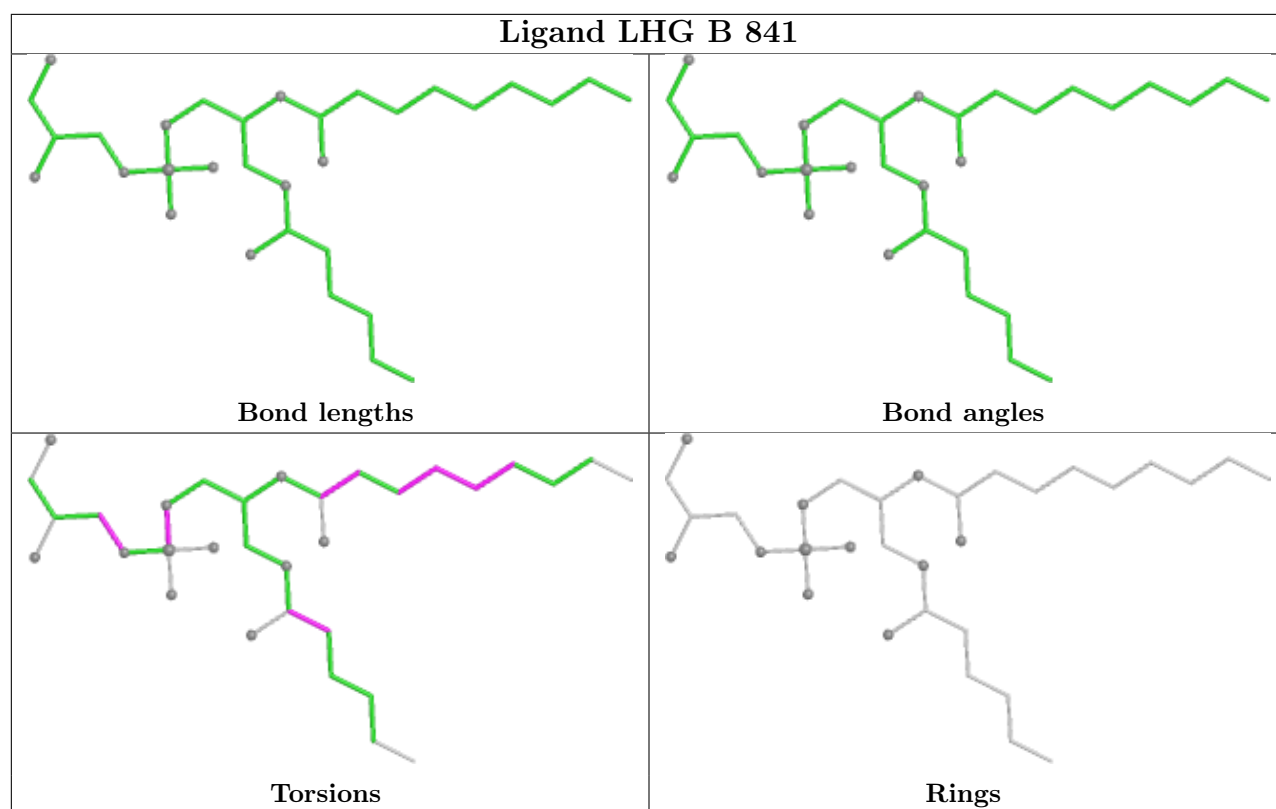
Bond angles

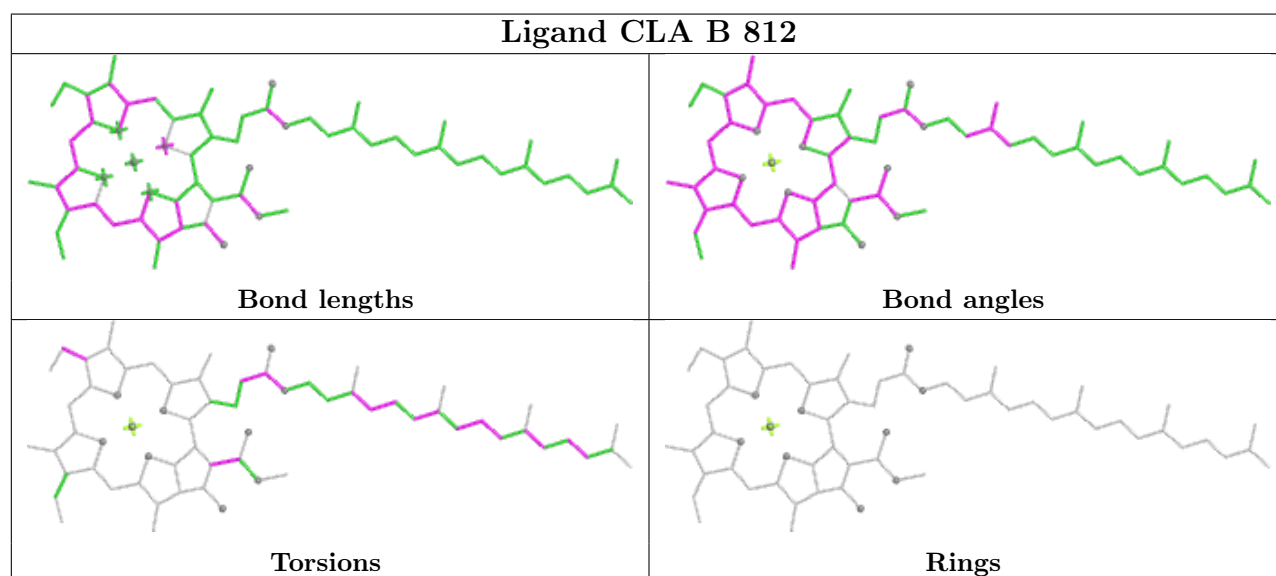
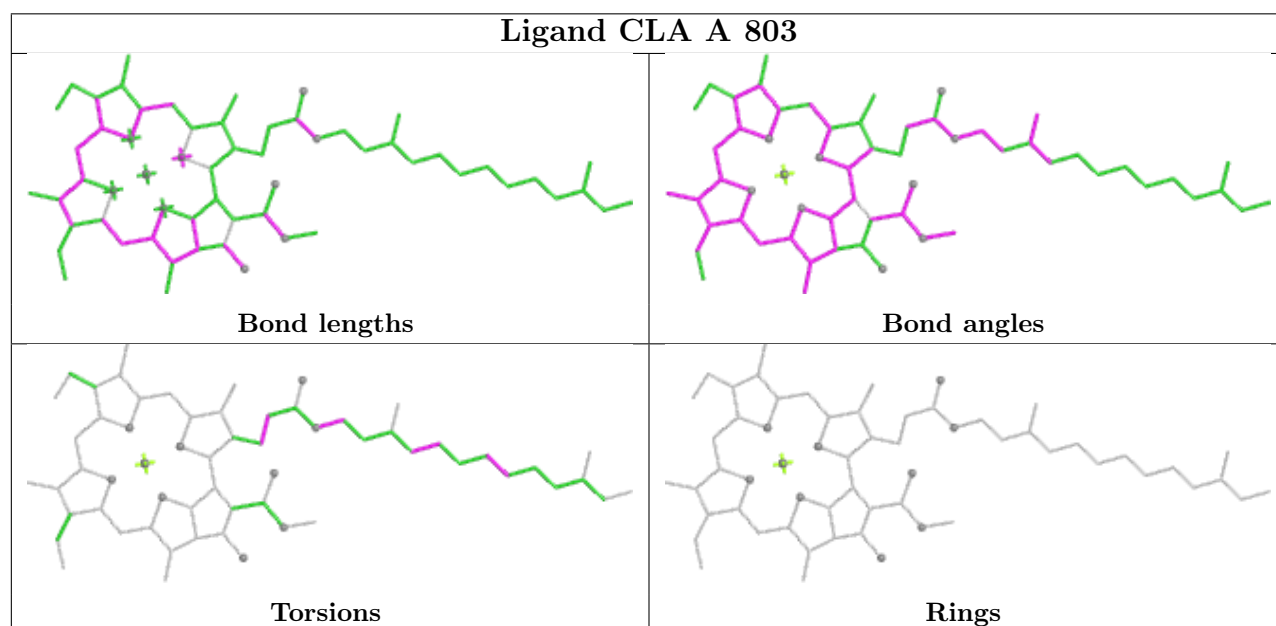
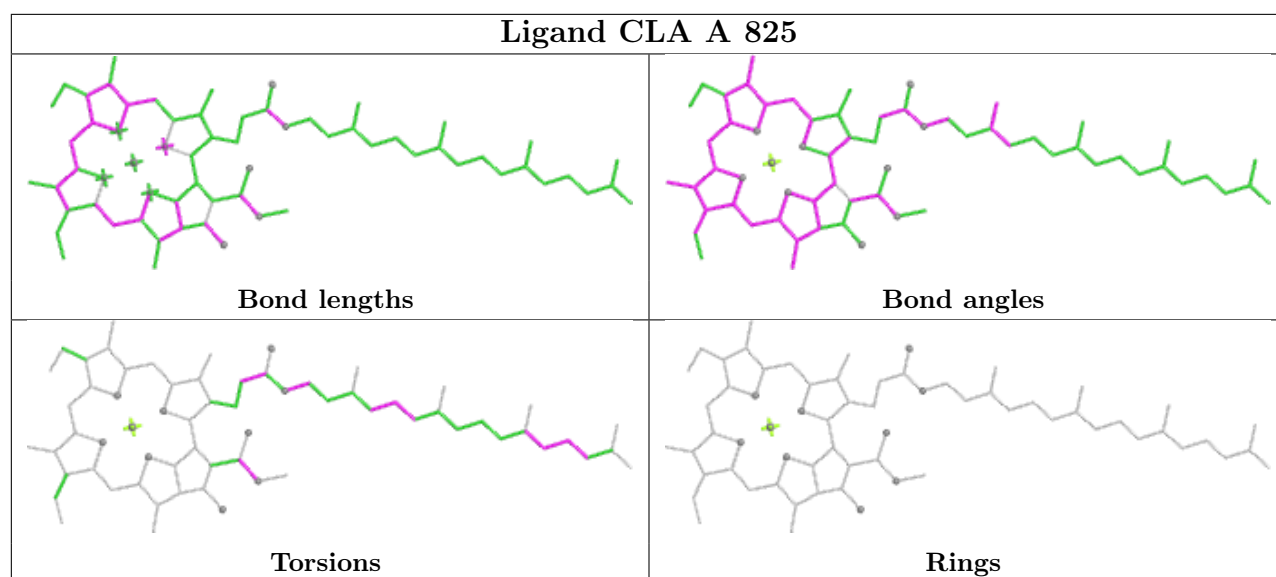


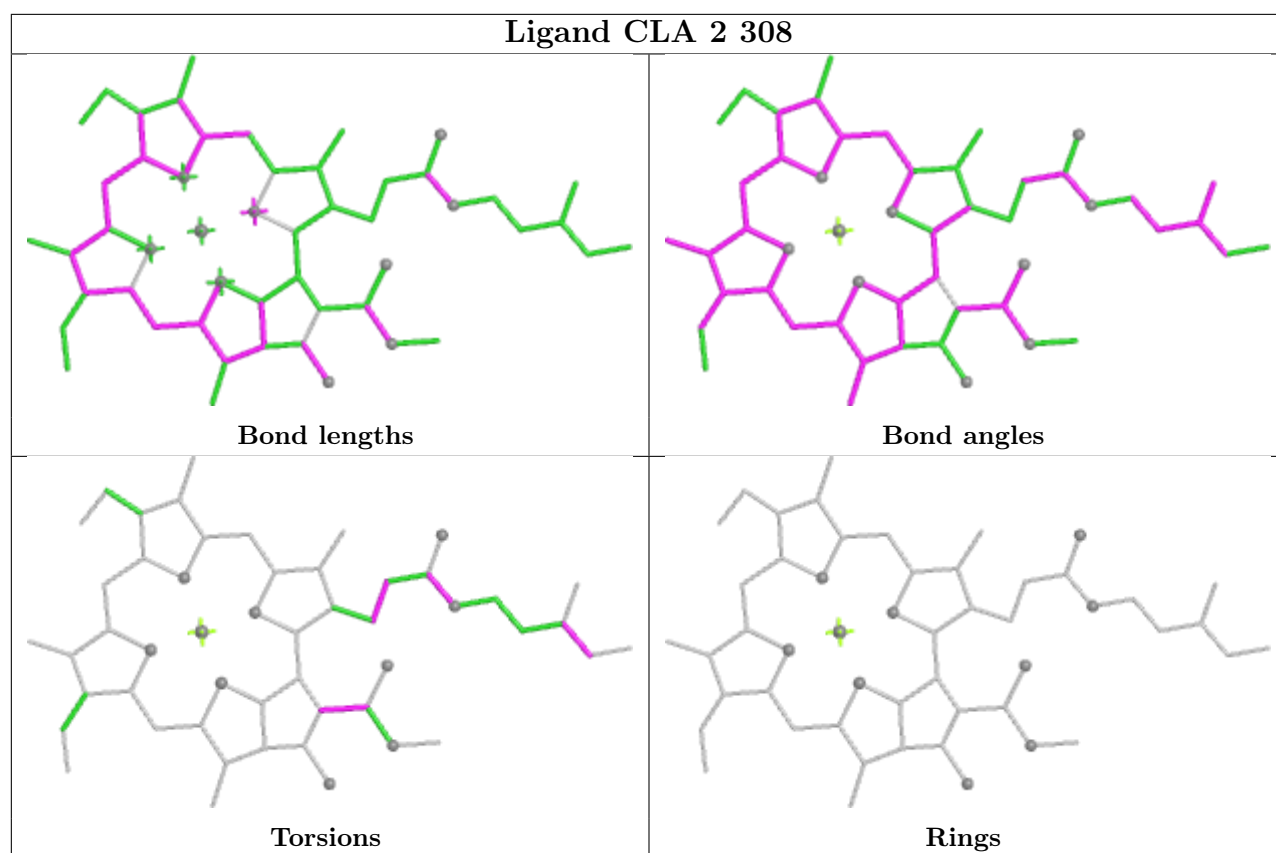
Torsions



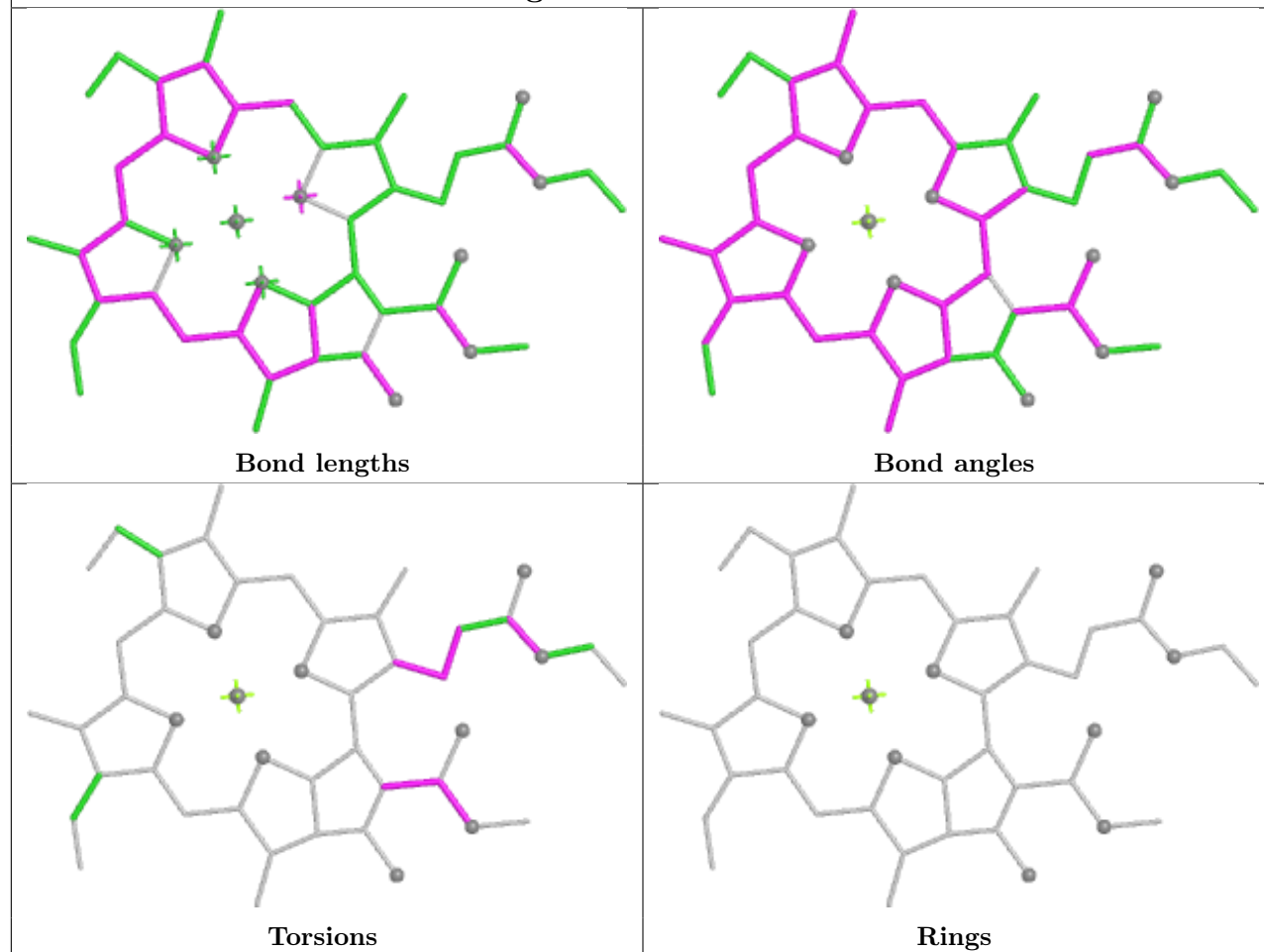
Rings



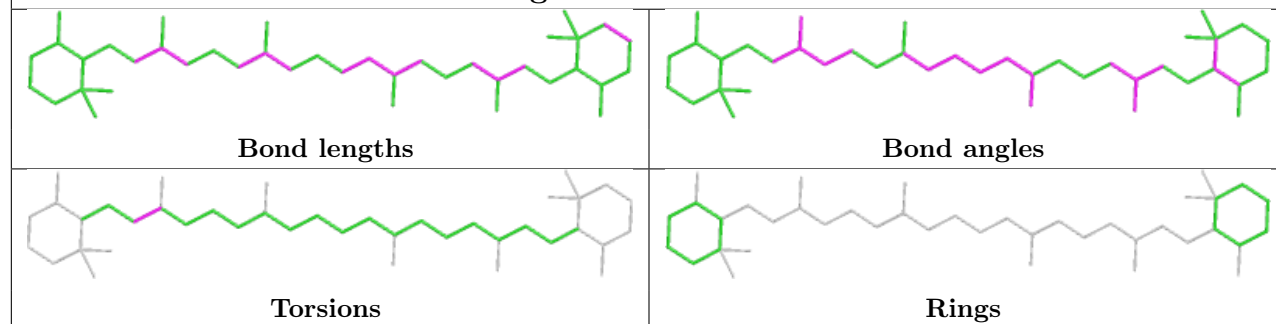


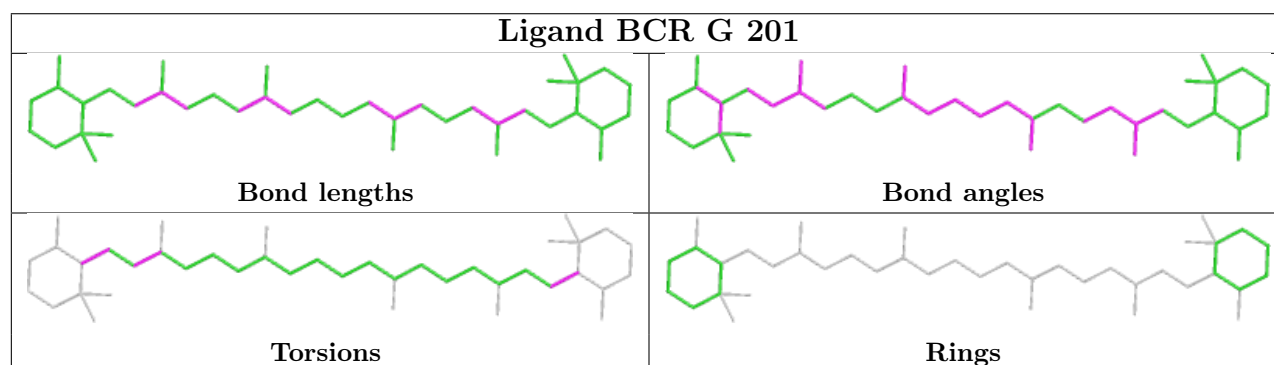
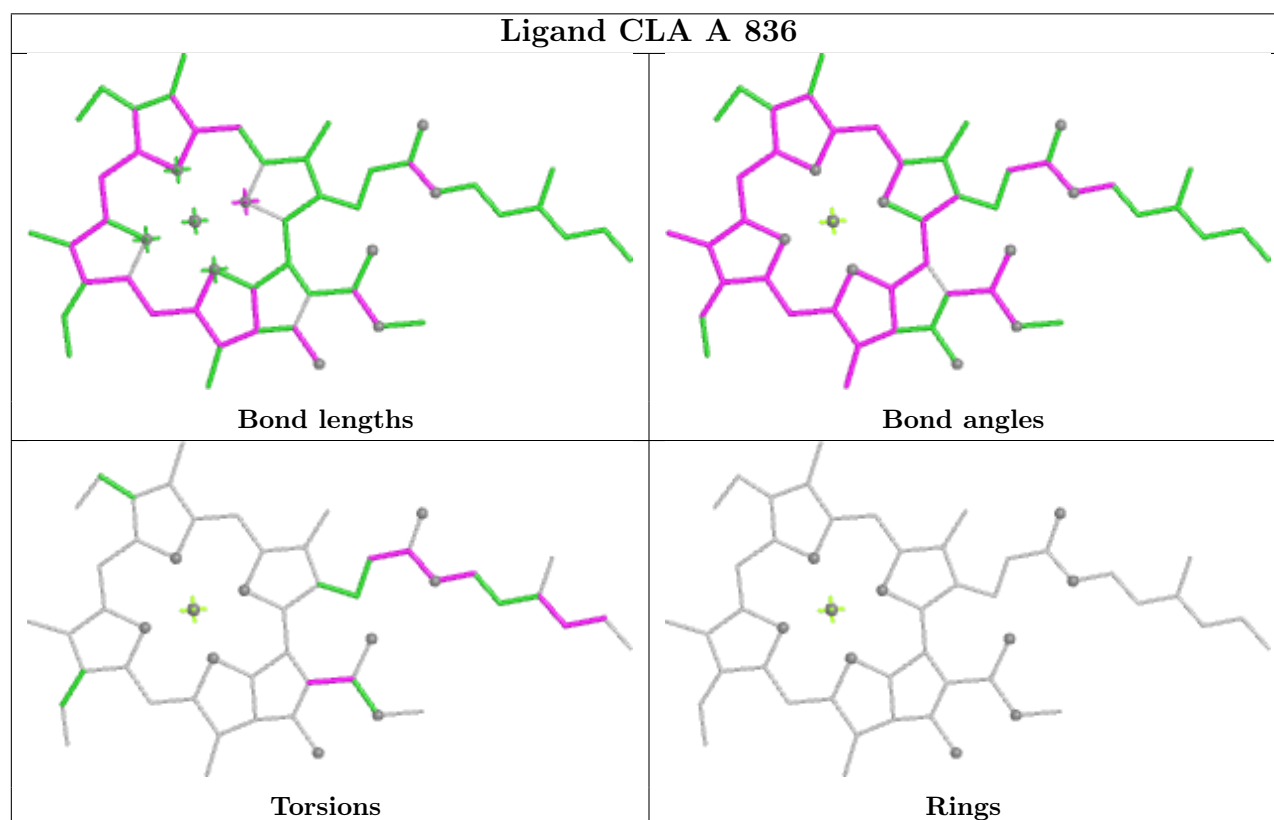
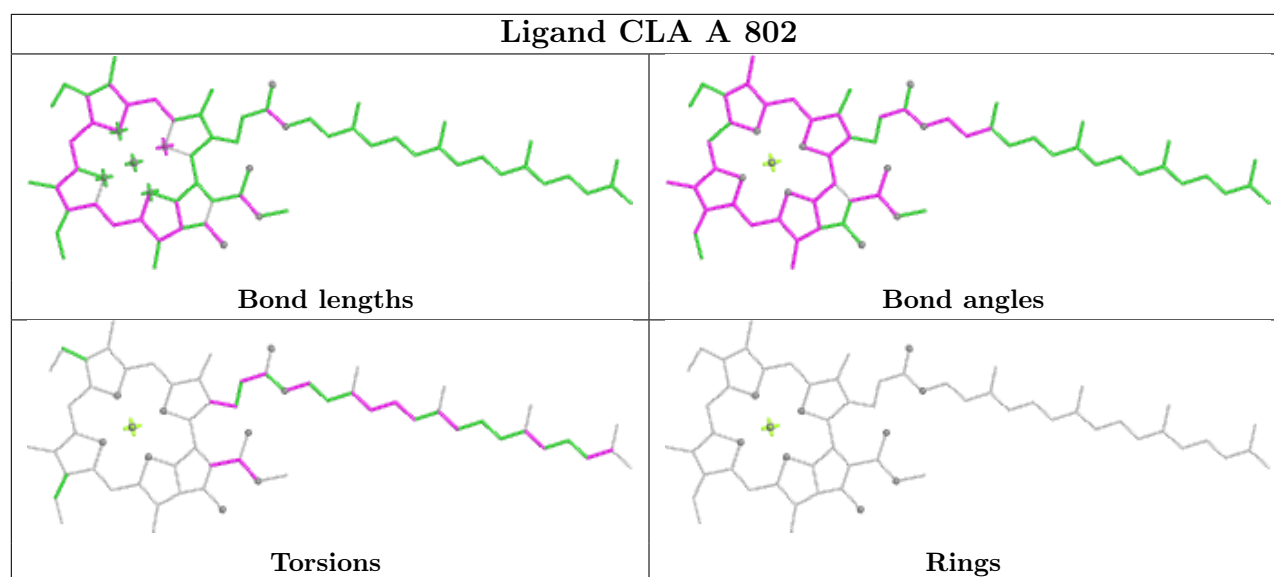


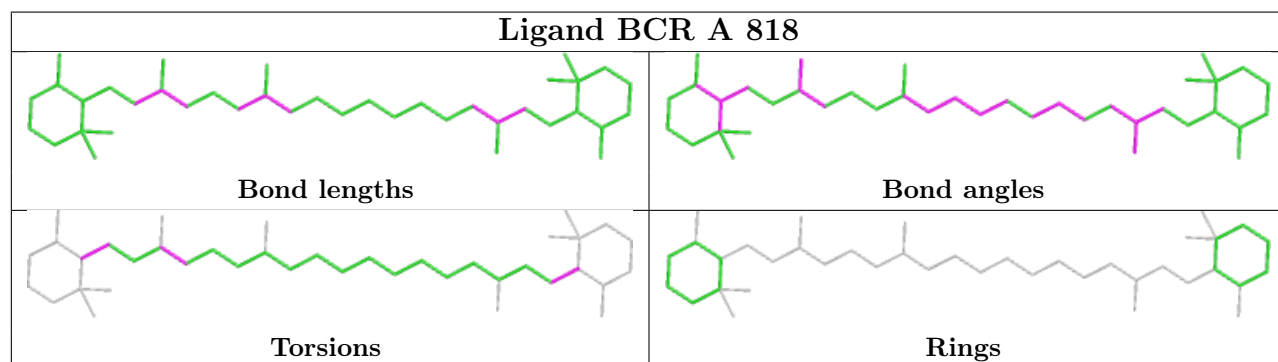
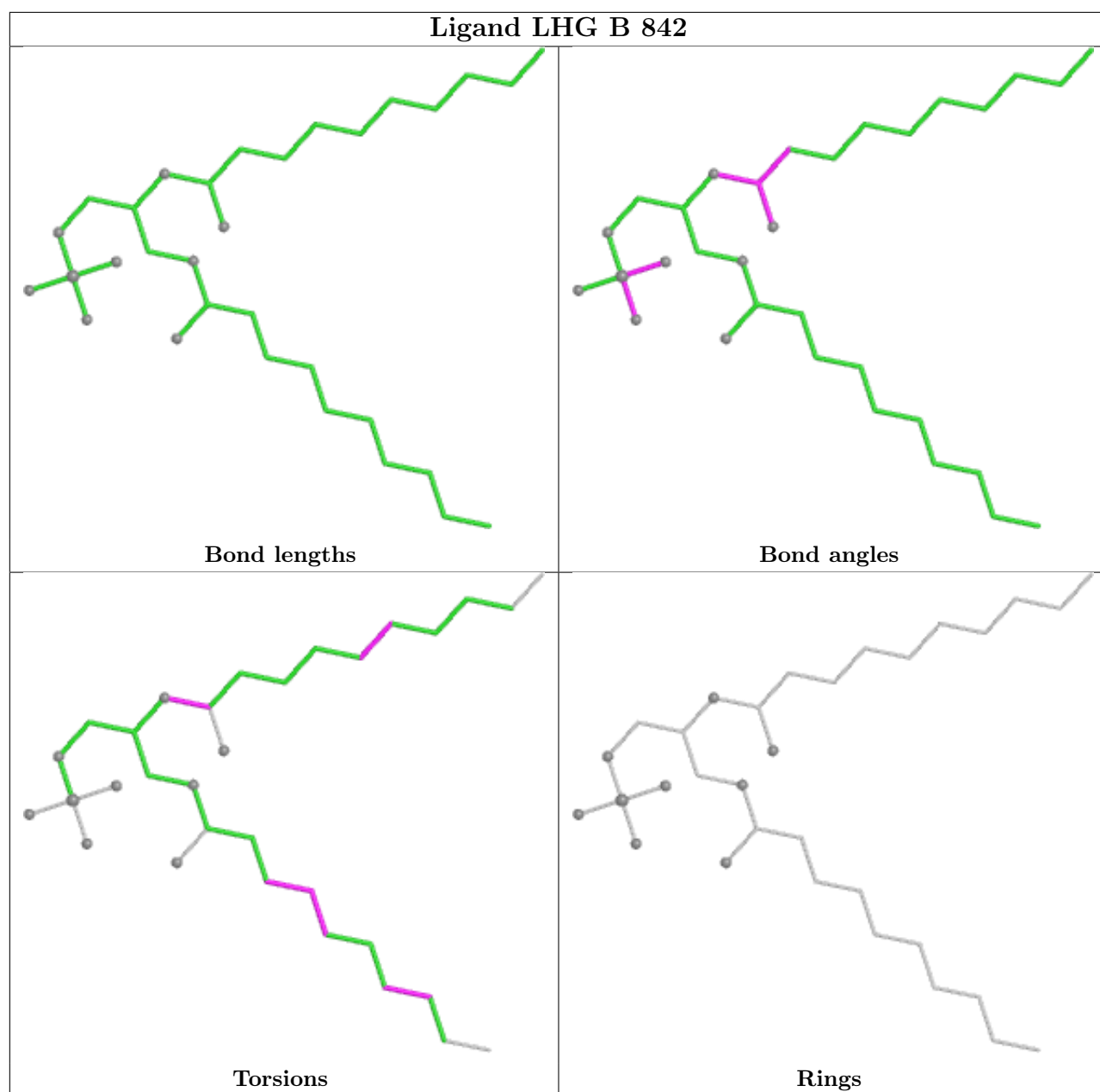
Ligand CLA K 203

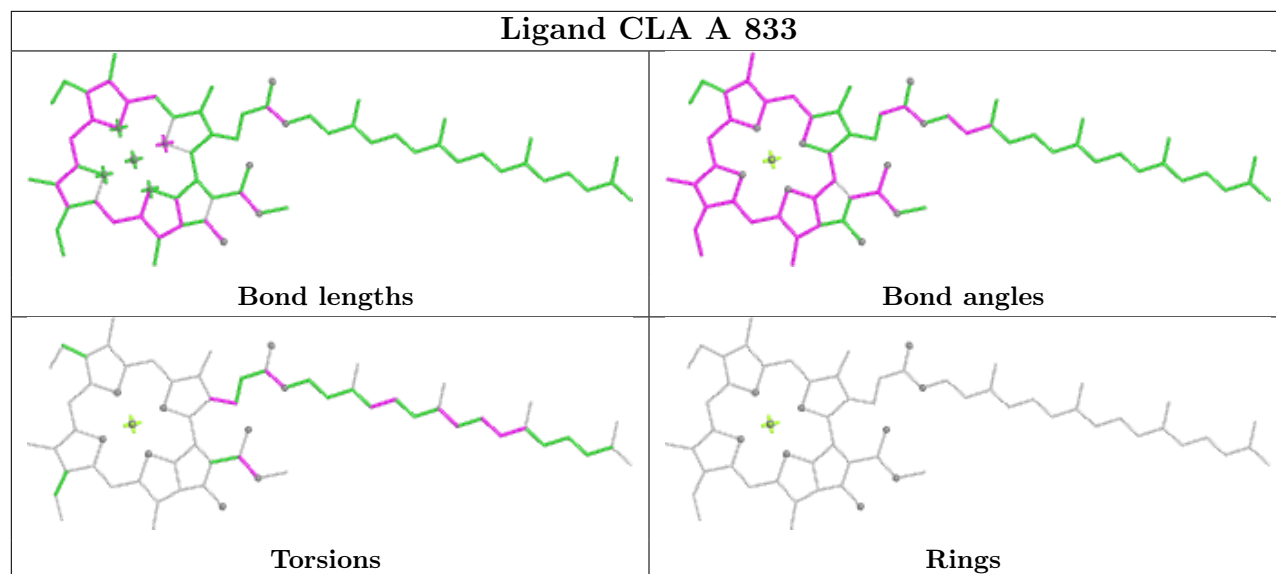
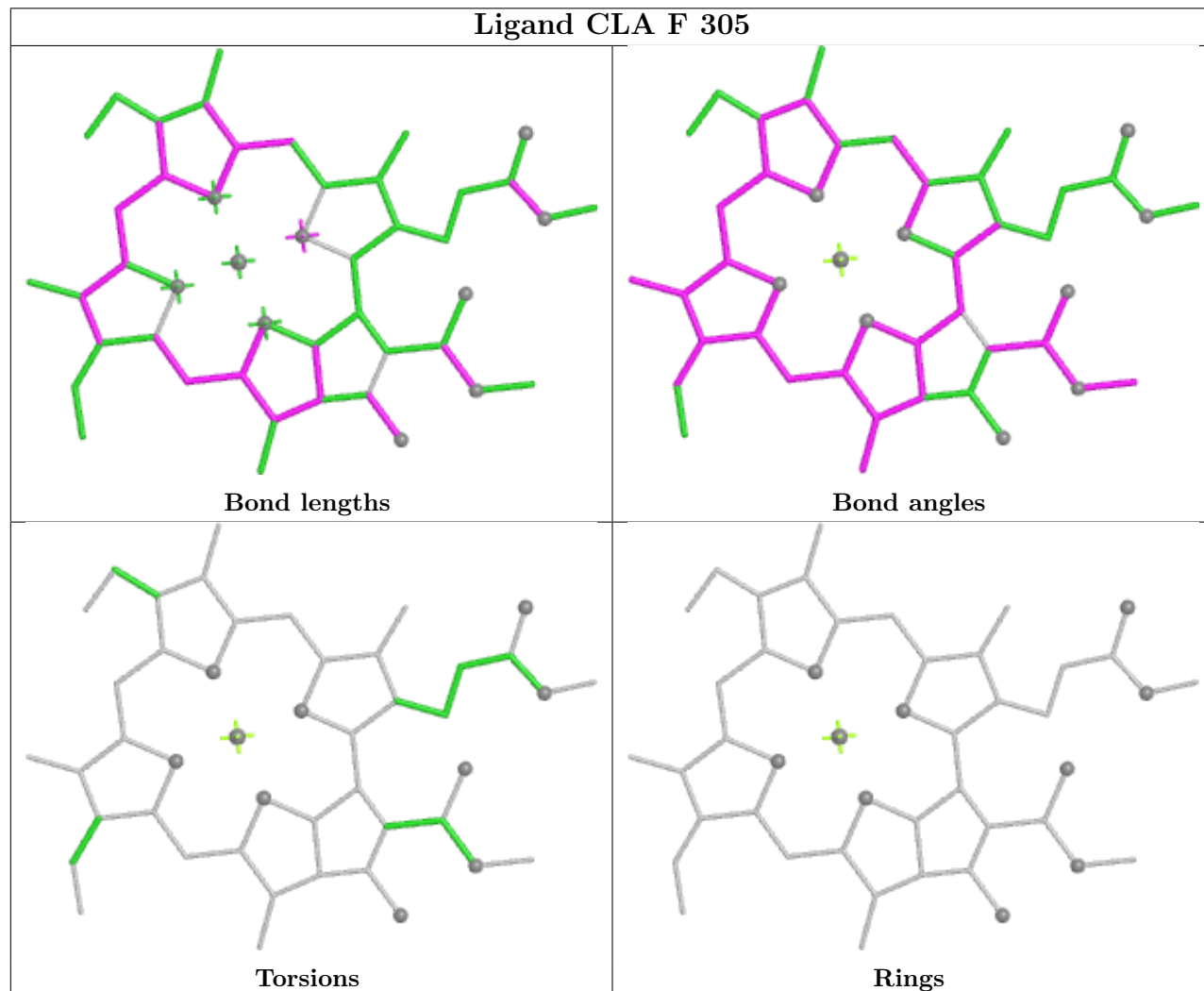


Ligand BCR A 817

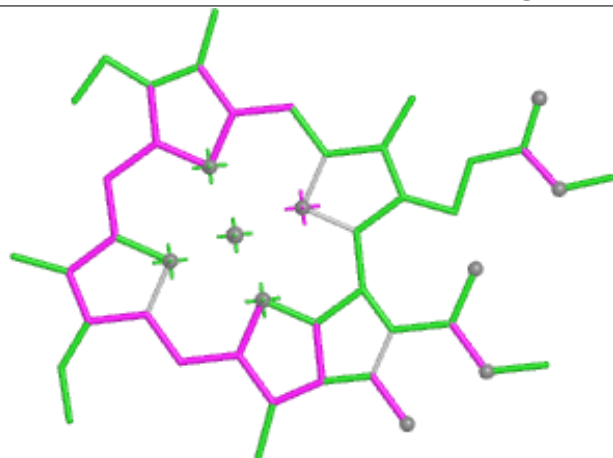




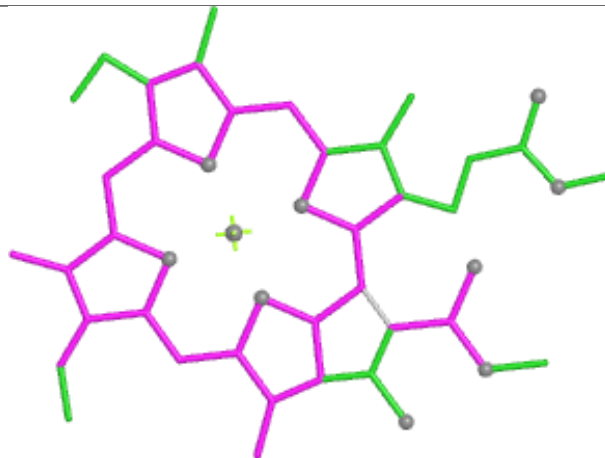


Ligand CLA A 833**Ligand CLA F 305**

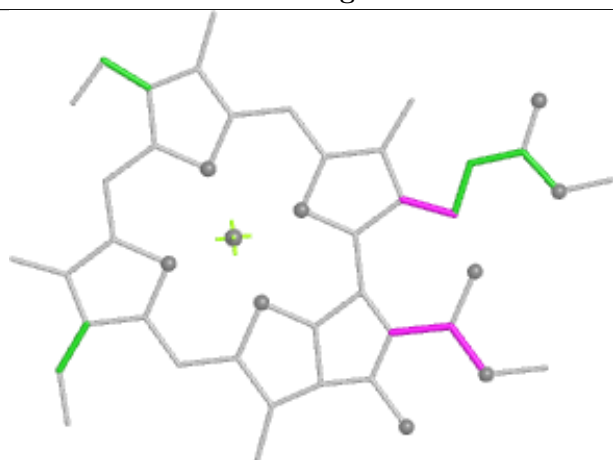
Ligand CLA J 103



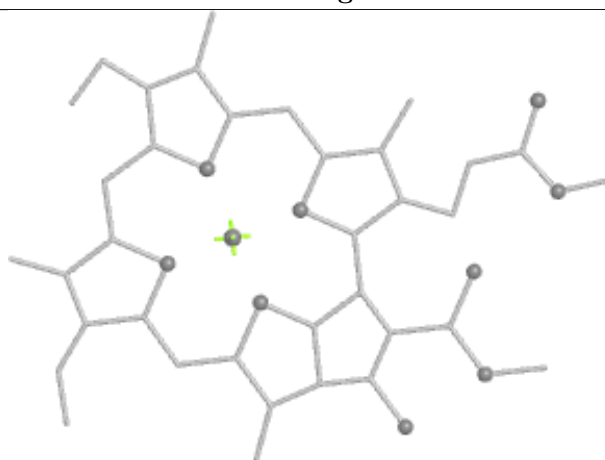
Bond lengths



Bond angles

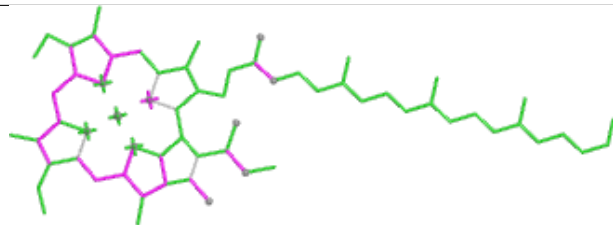


Torsions

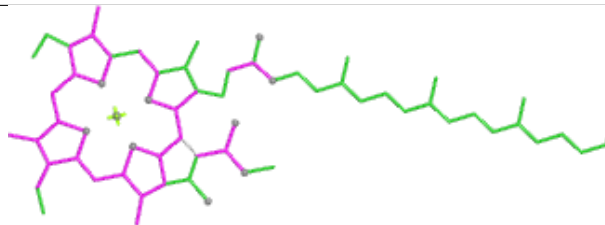


Rings

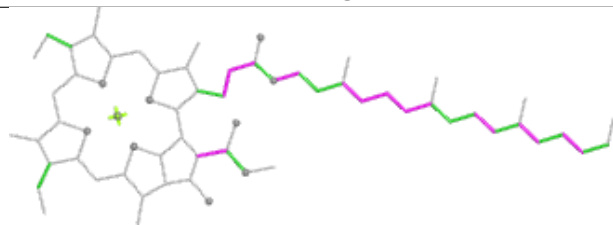
Ligand CLA A 829



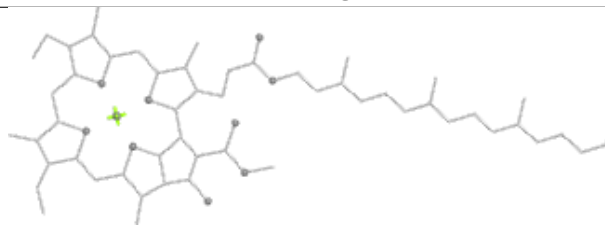
Bond lengths



Bond angles

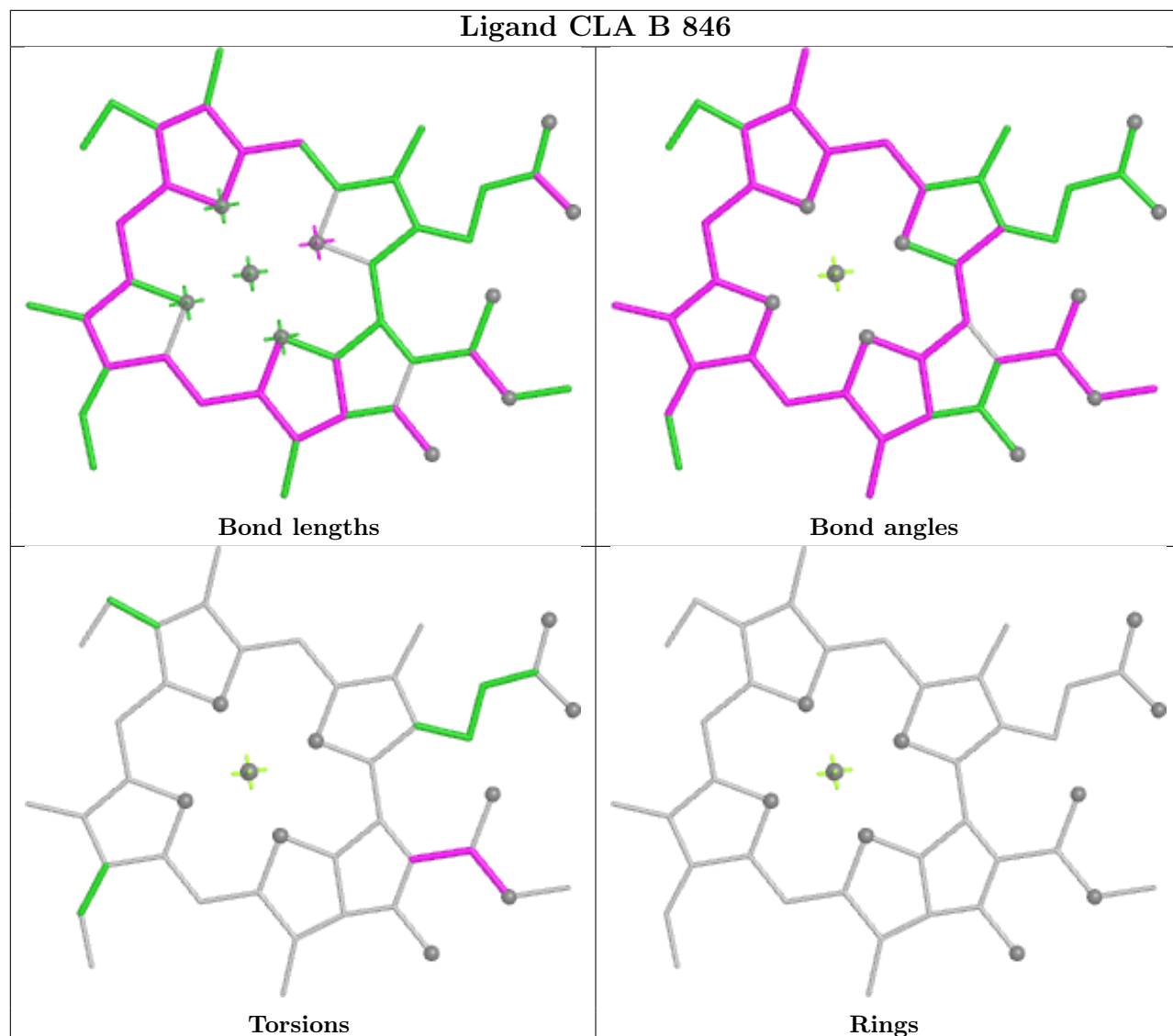


Torsions

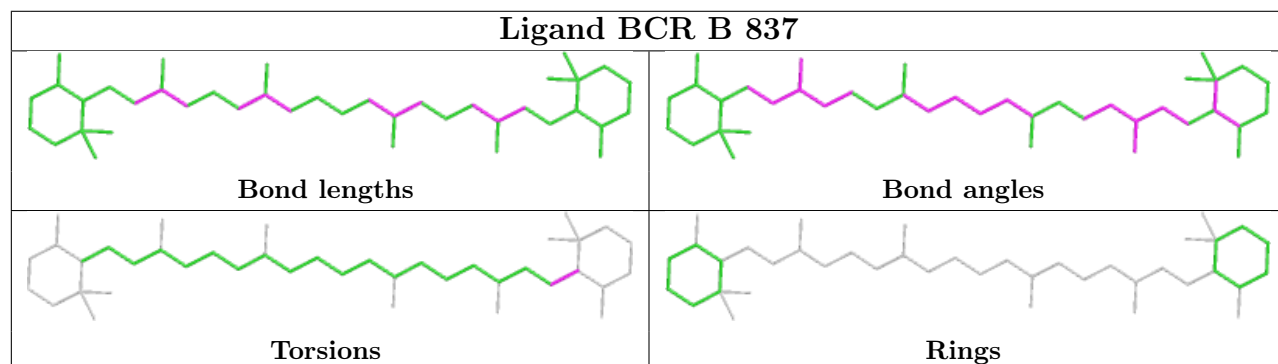


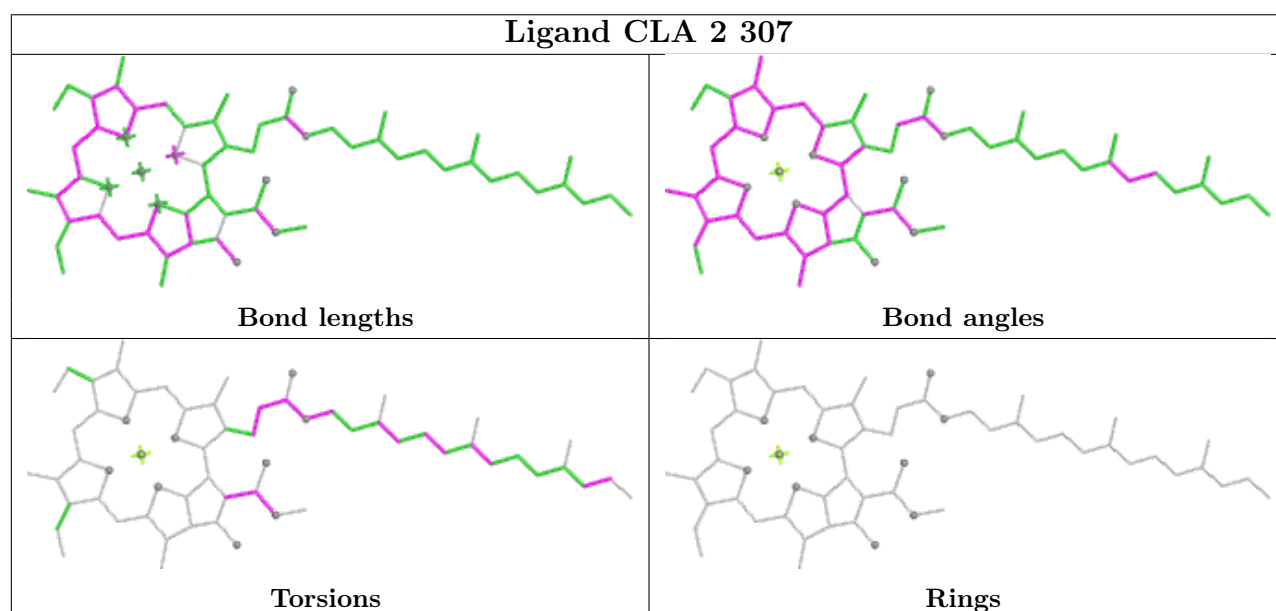
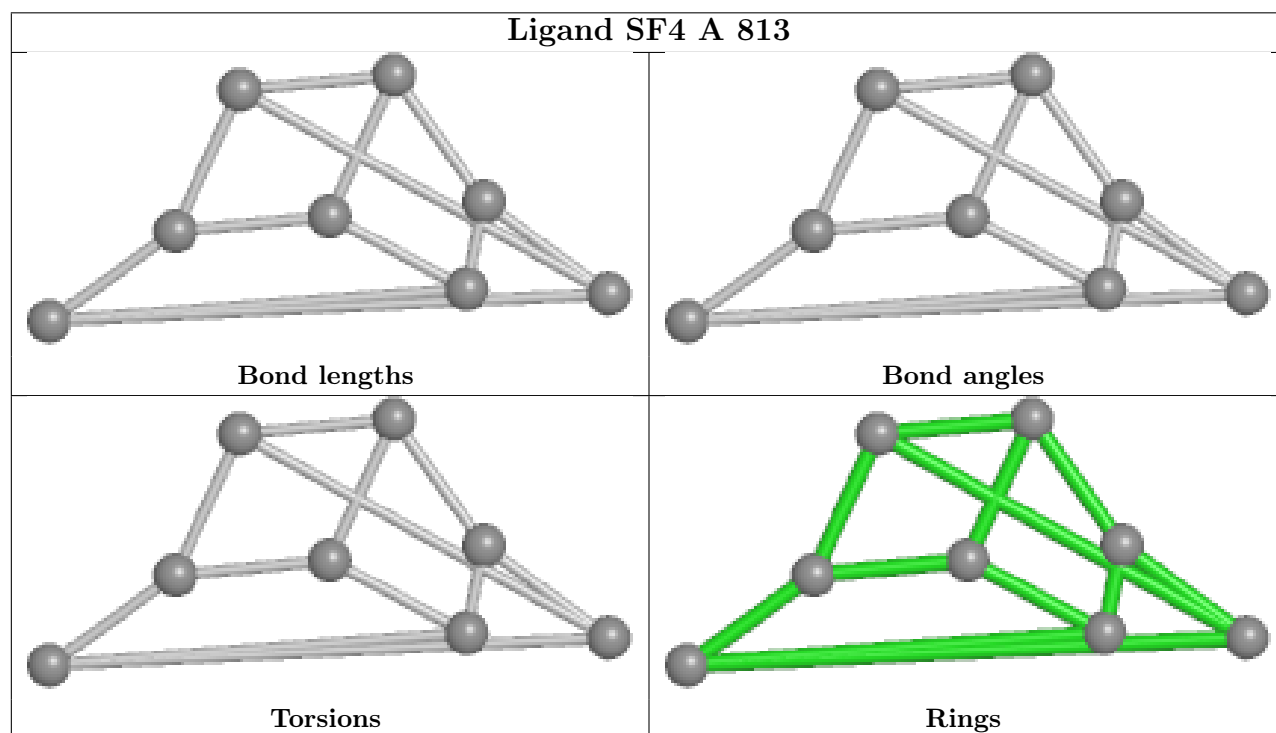
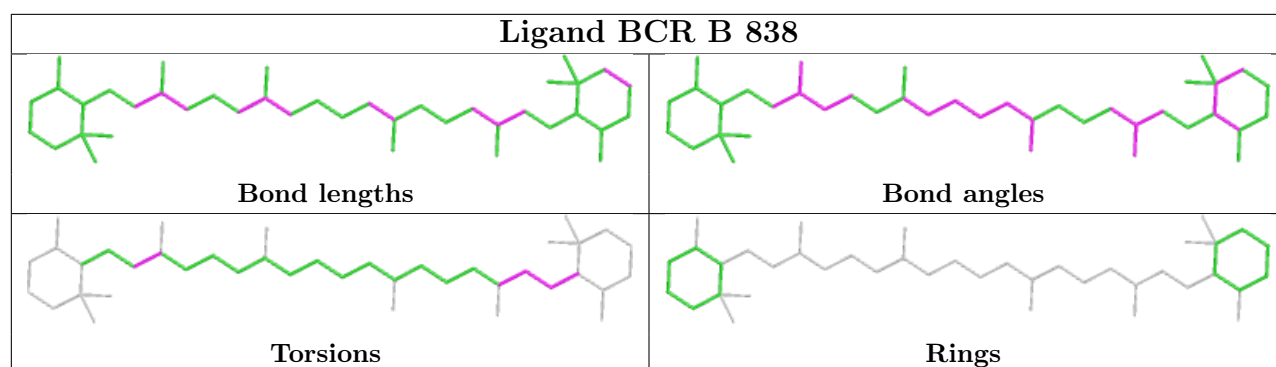
Rings

Ligand CLA B 846

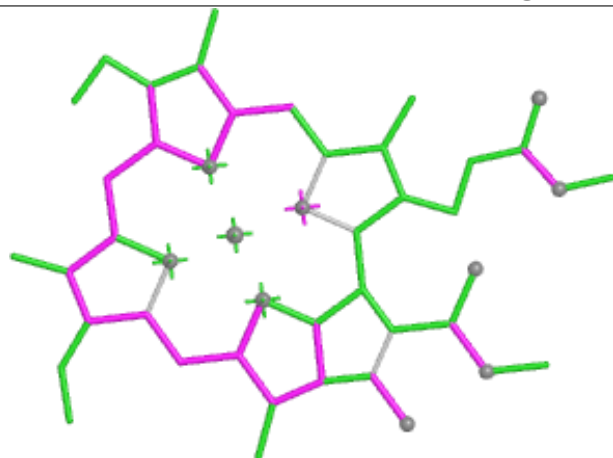


Ligand BCR B 837

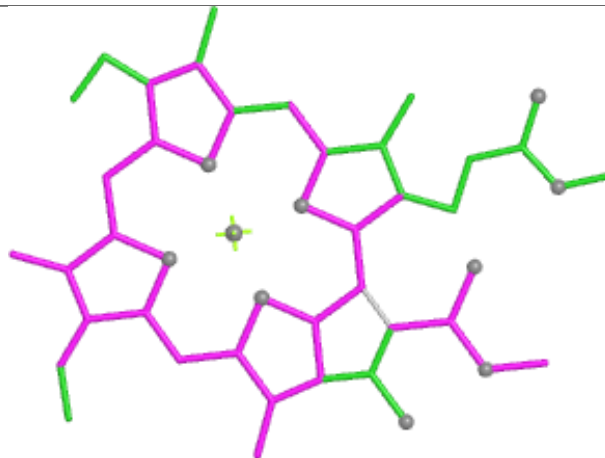




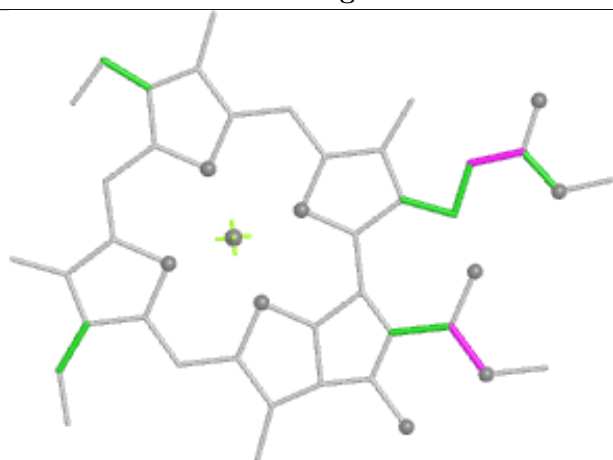
Ligand CLA 4 303



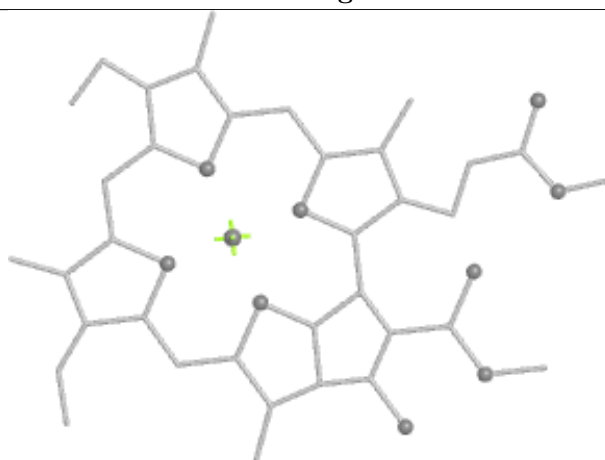
Bond lengths



Bond angles

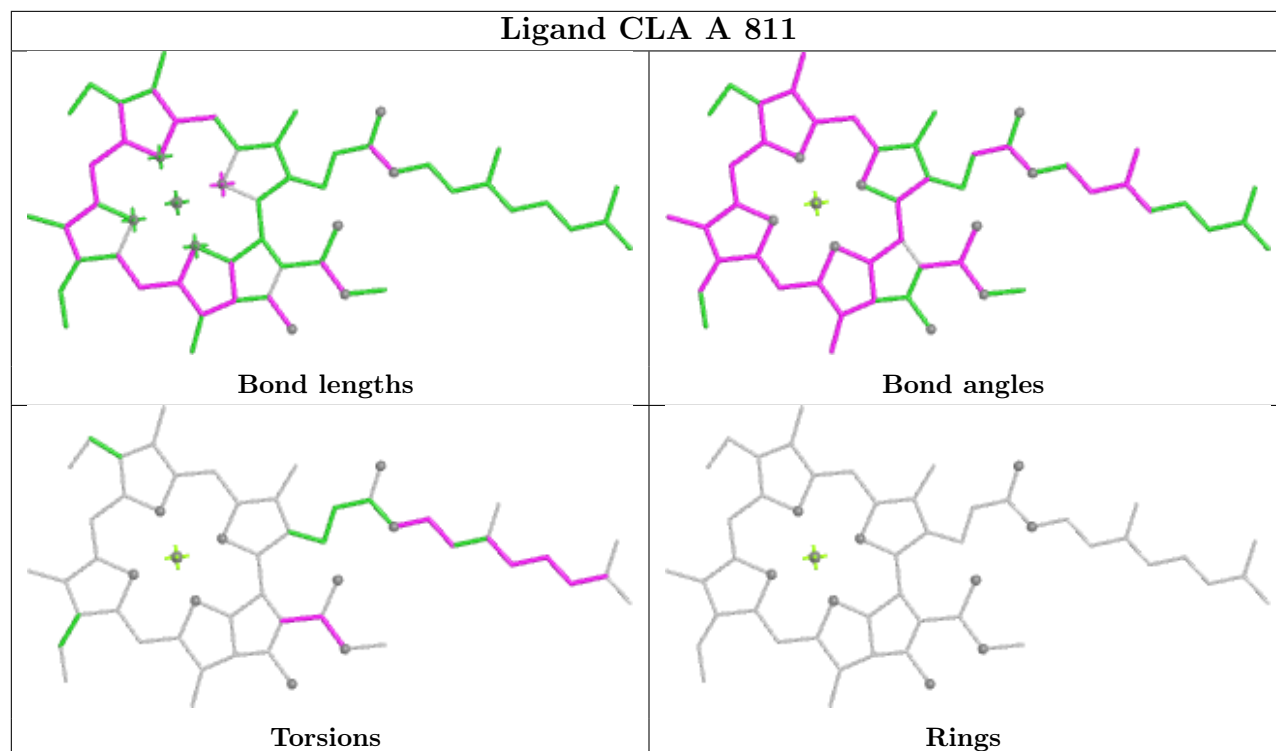


Torsions

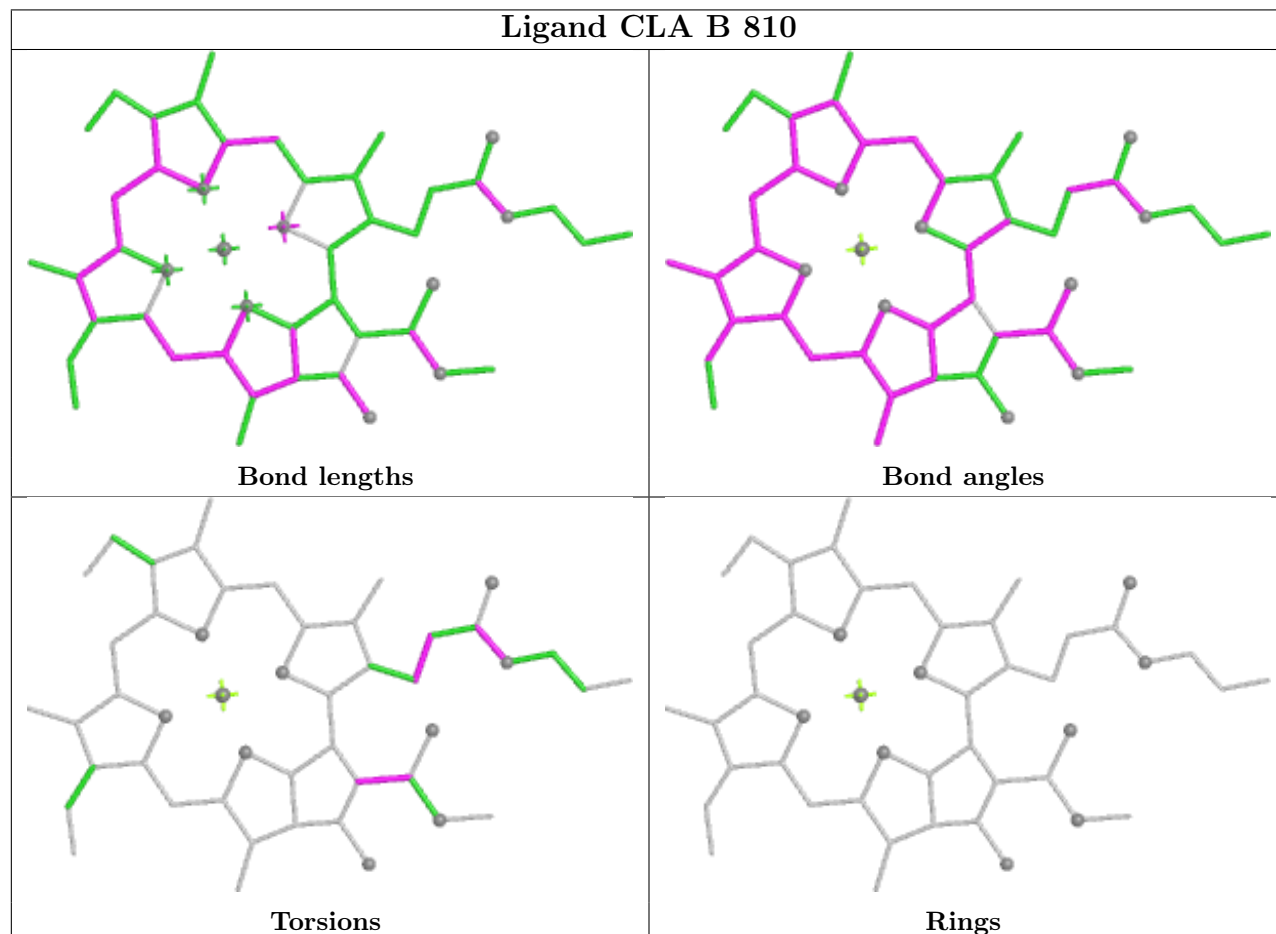


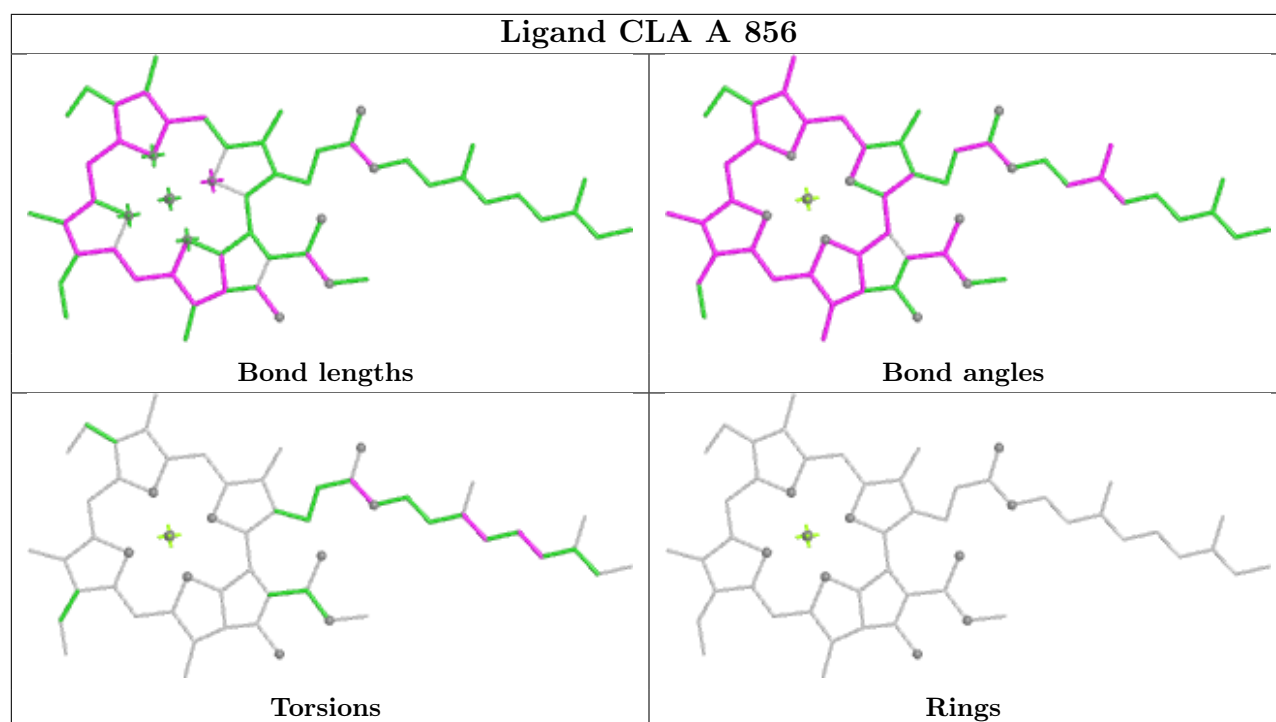
Rings

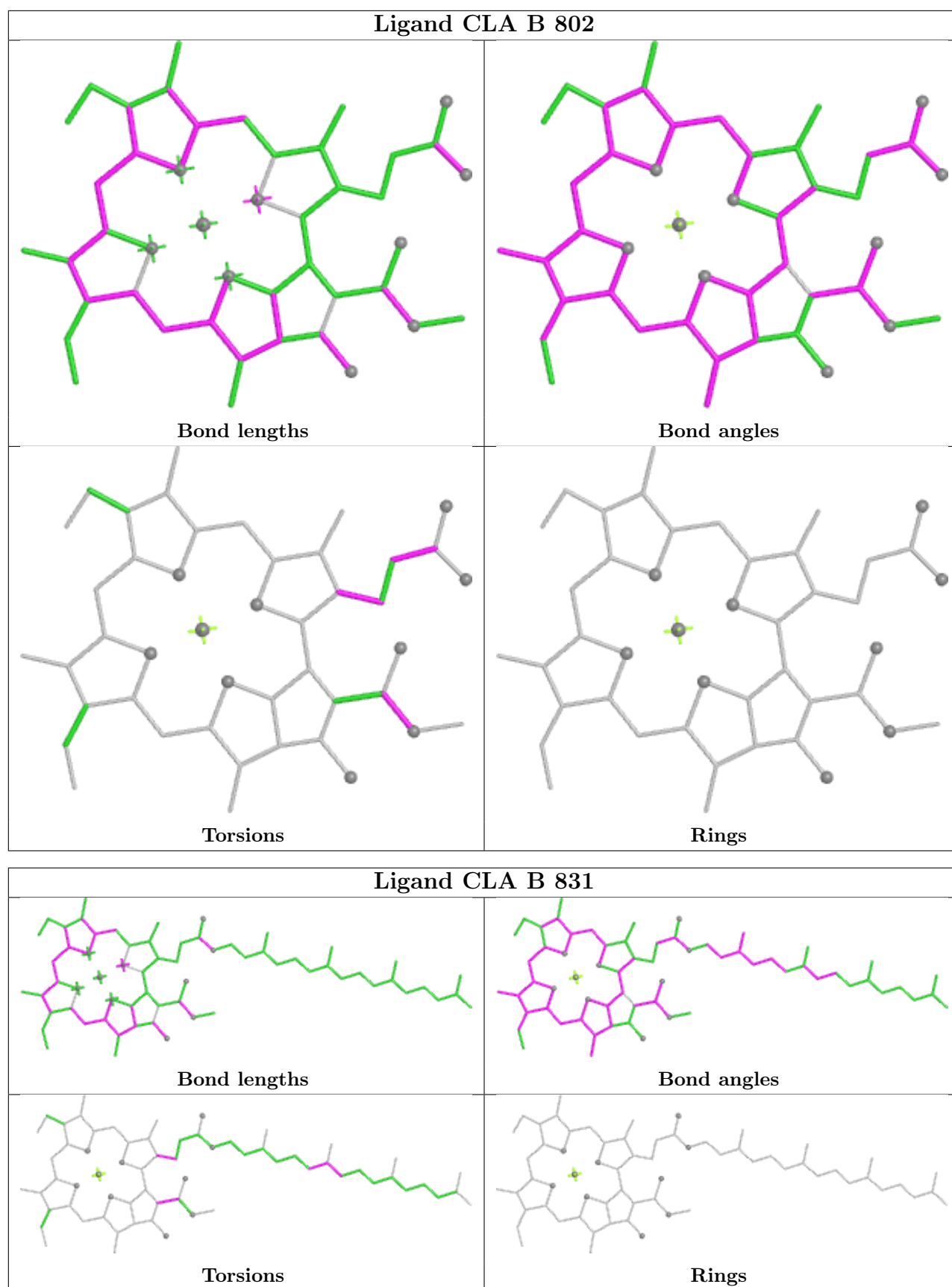
Ligand CLA A 811

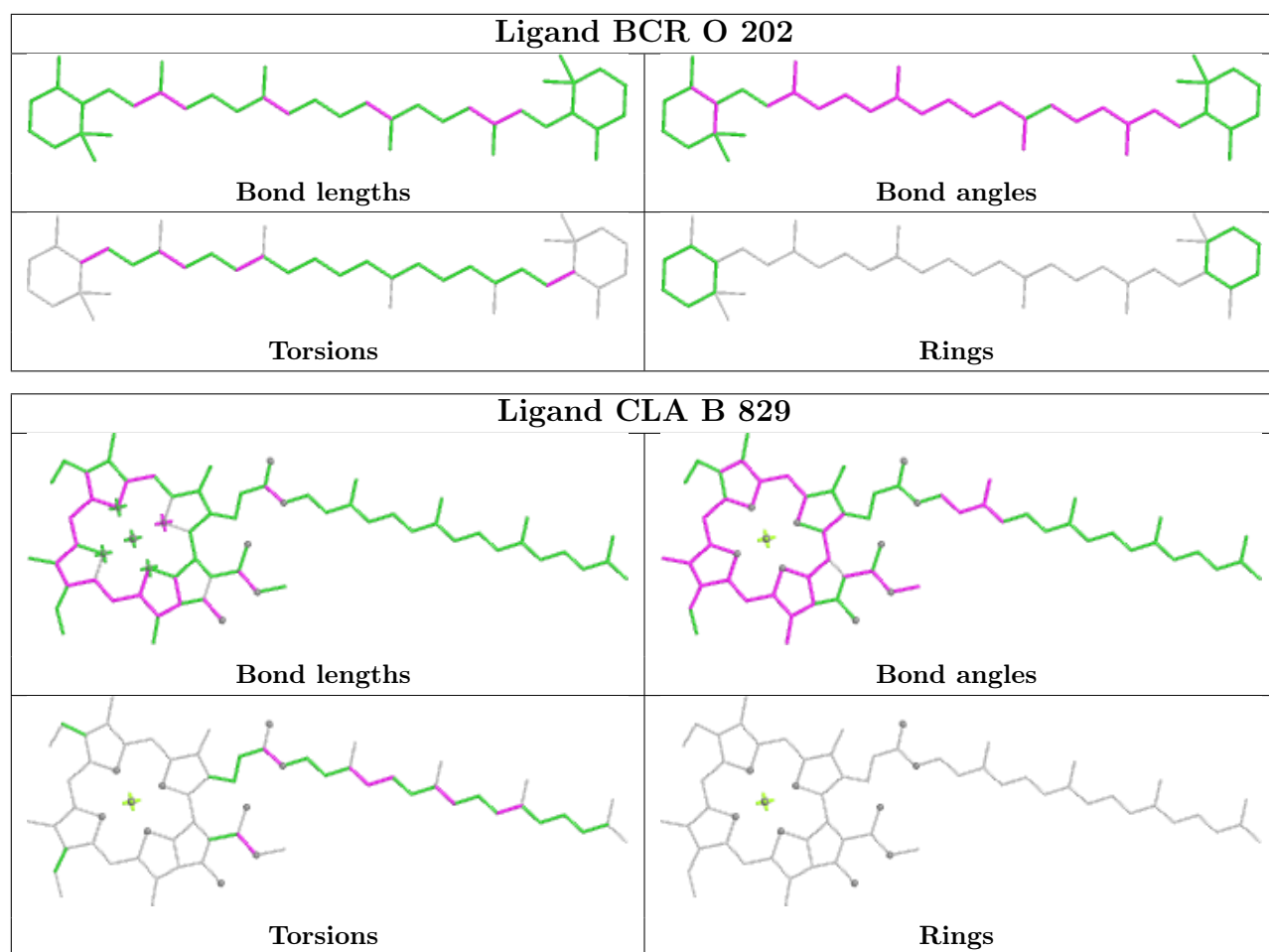


Ligand CLA B 810

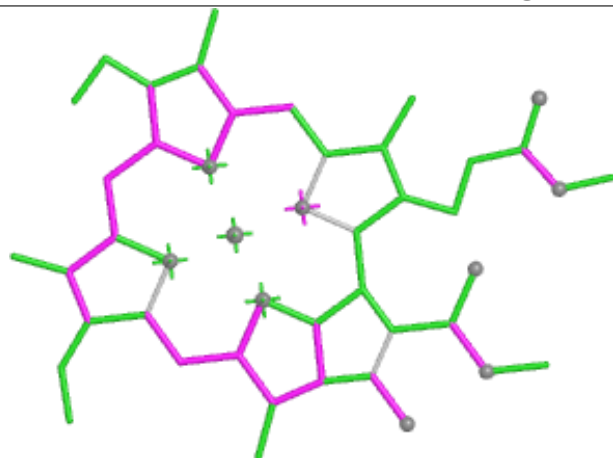




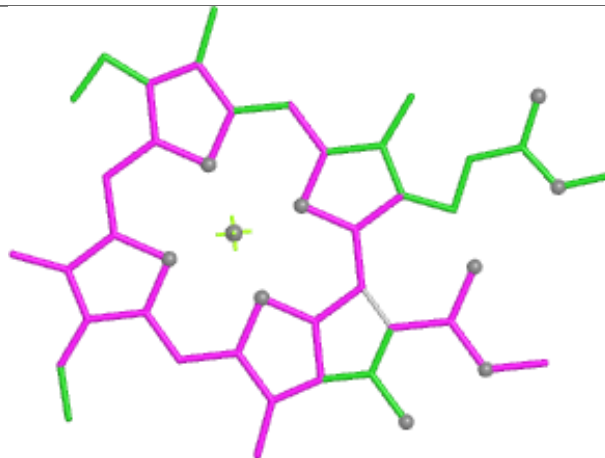




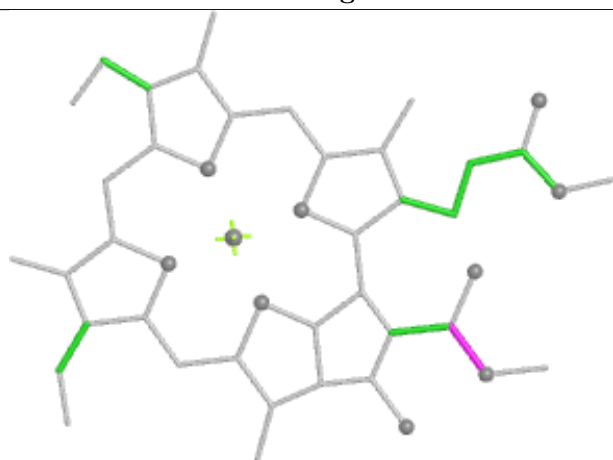
Ligand CLA 3 316



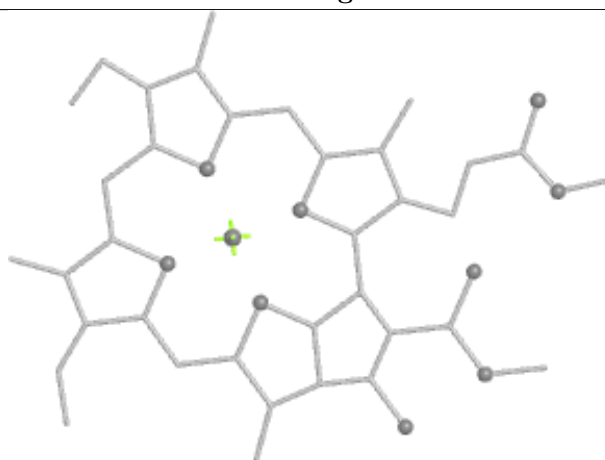
Bond lengths



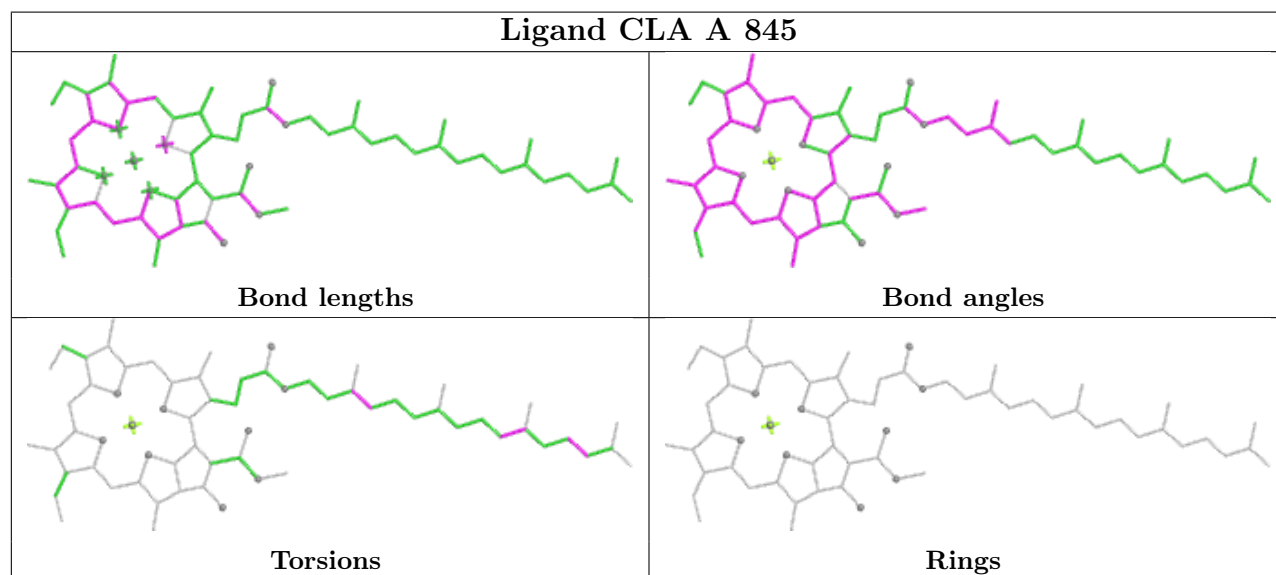
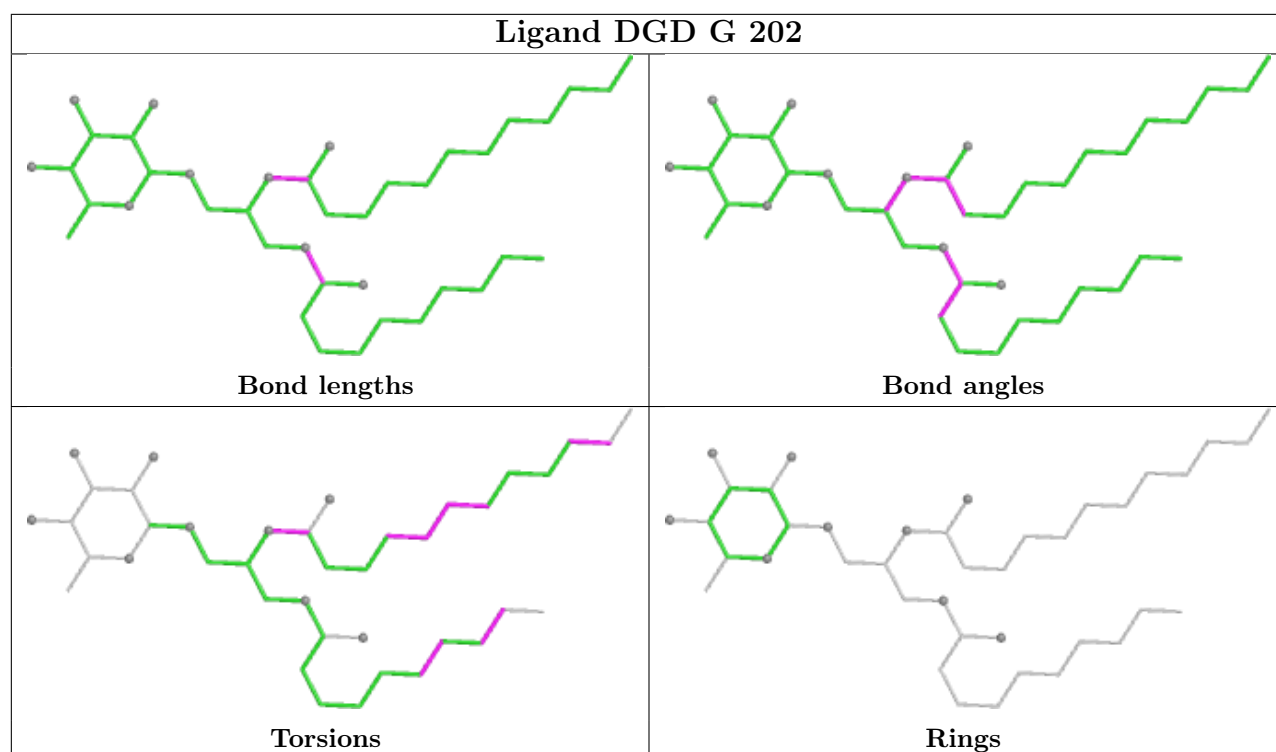
Bond angles

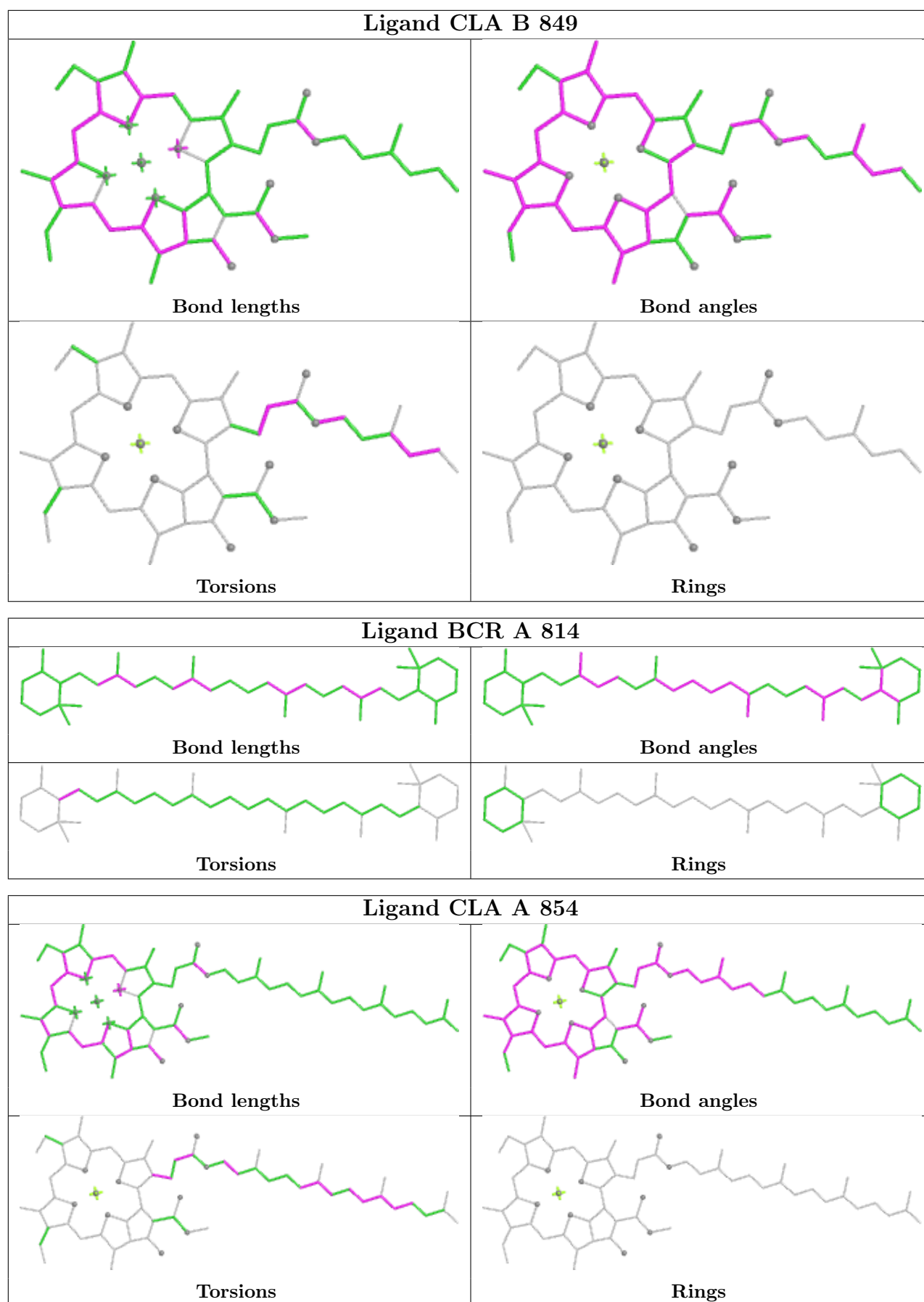


Torsions

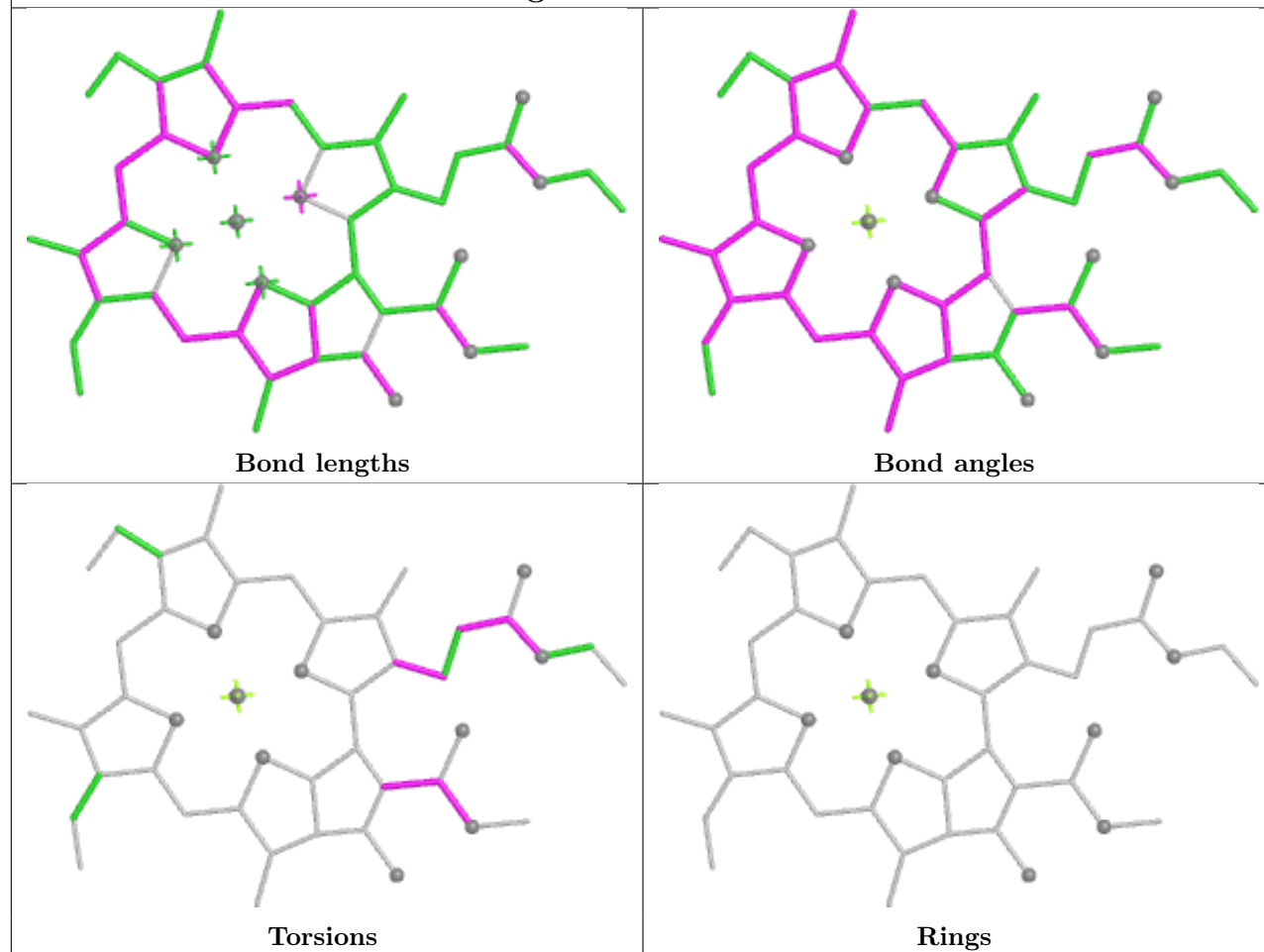


Rings

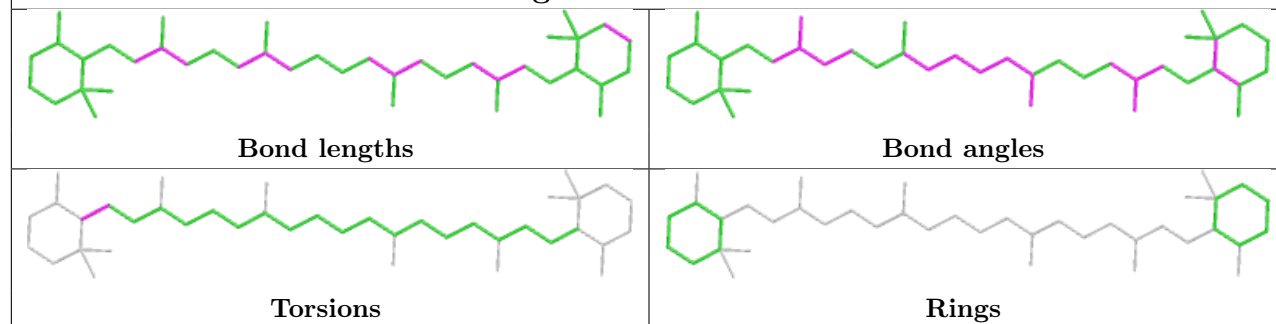


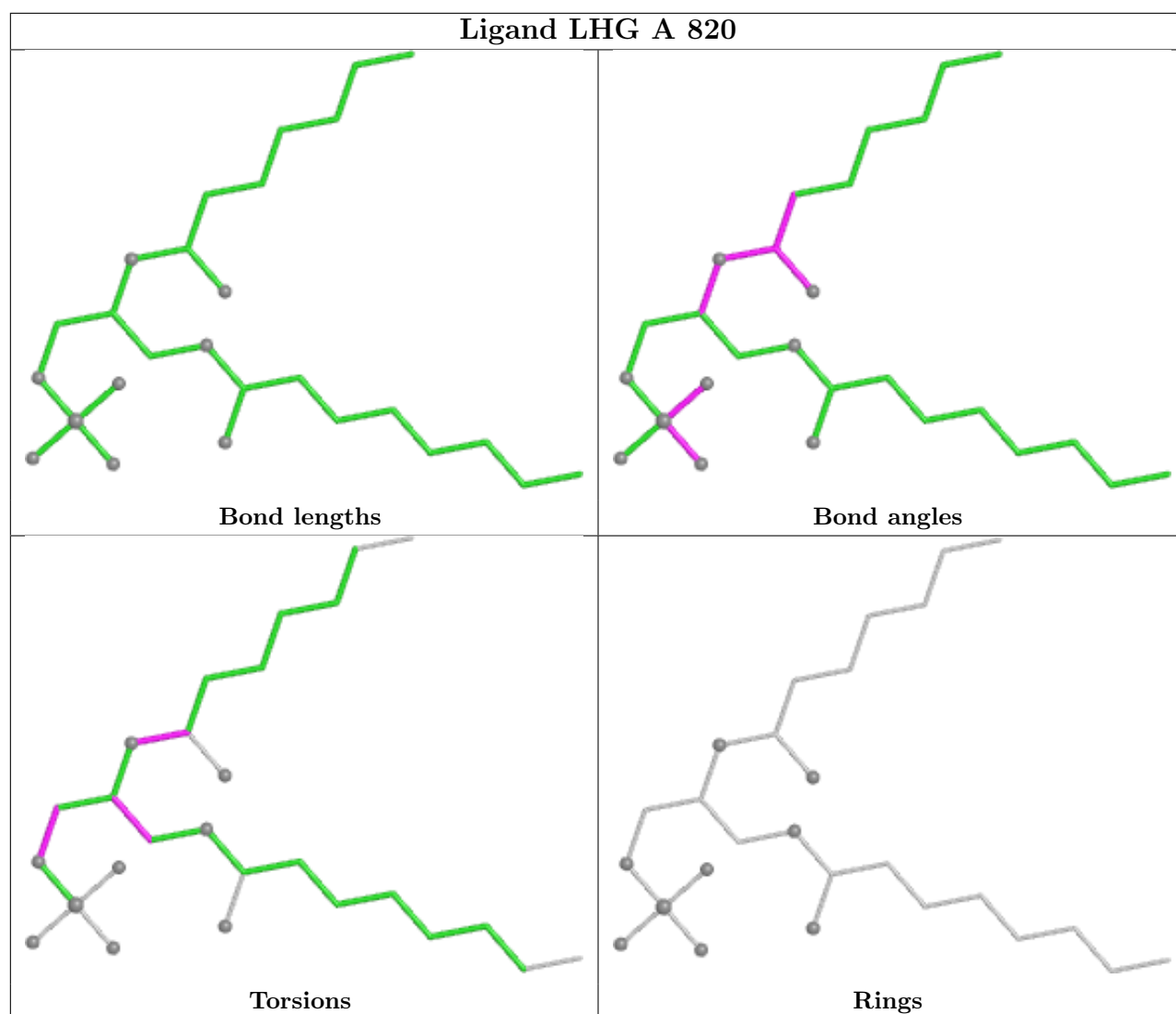


Ligand CLA B 828

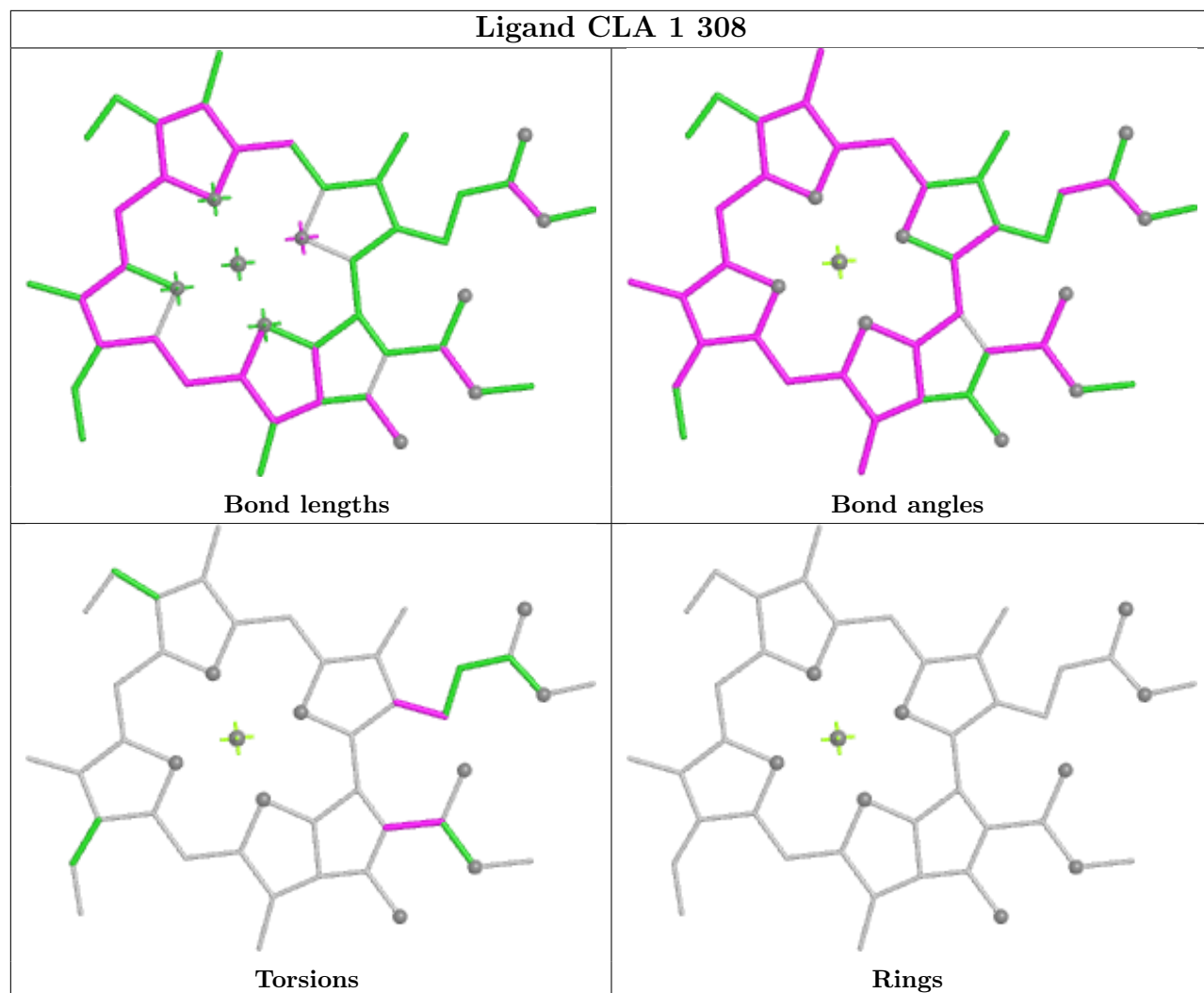


Ligand BCR L 302

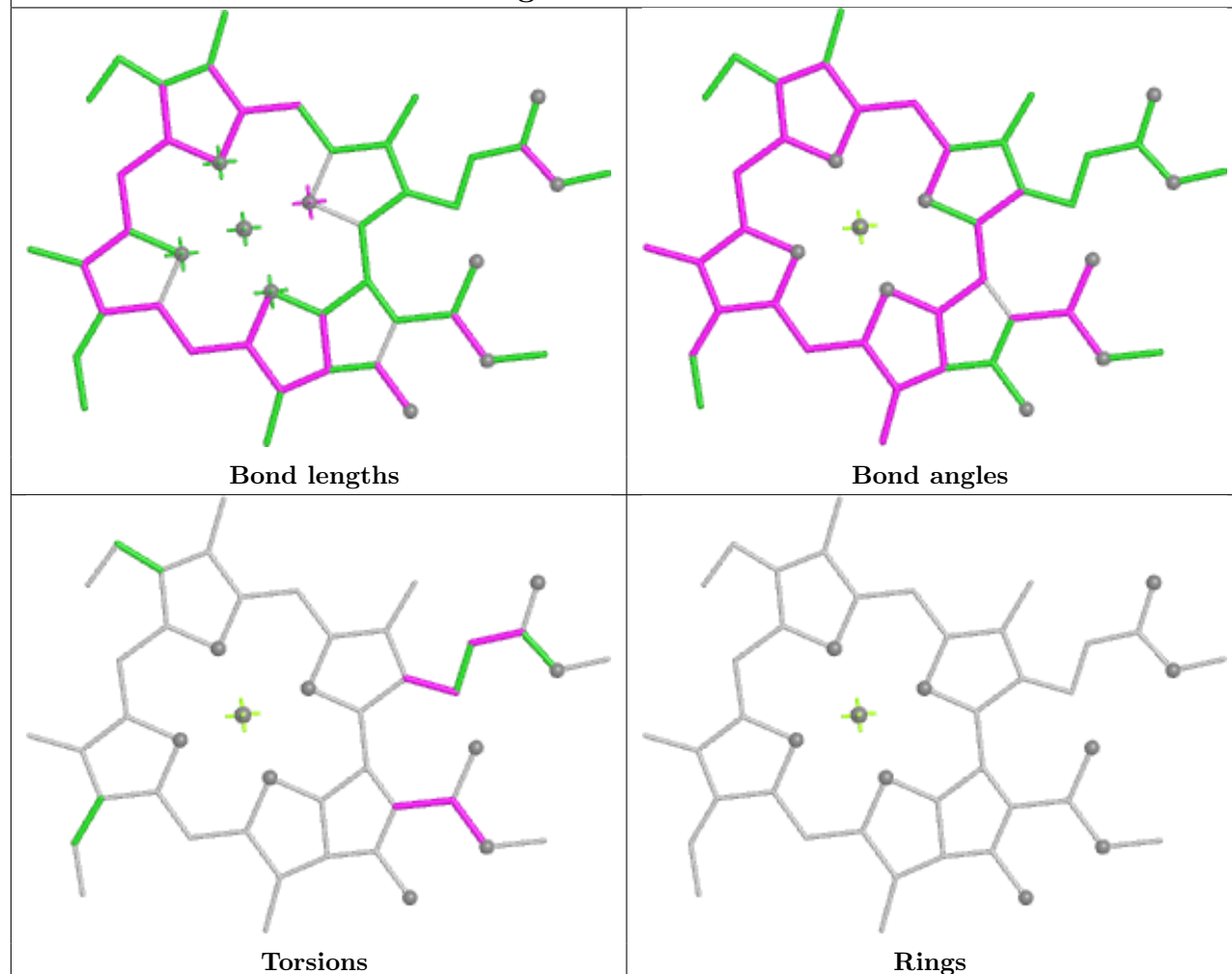




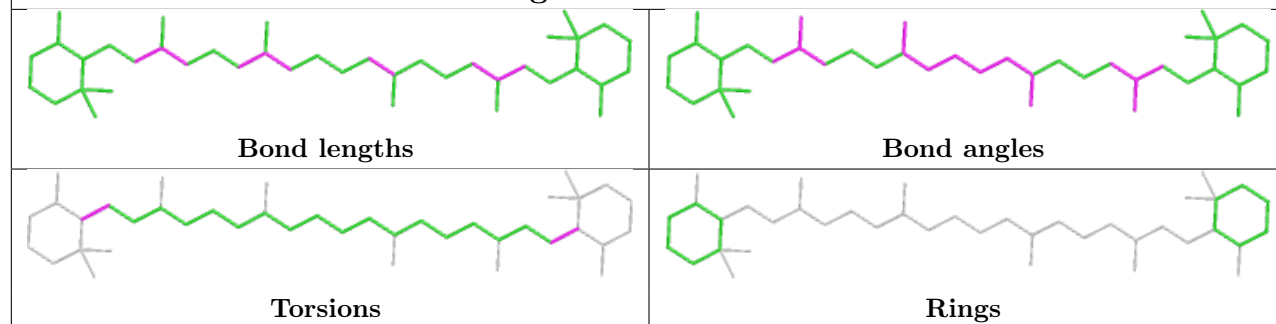
Ligand CLA 1 308



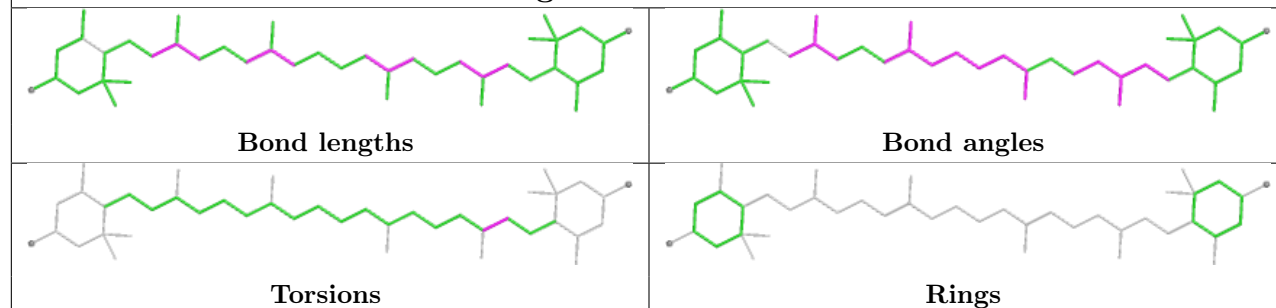
Ligand CLA 3 319

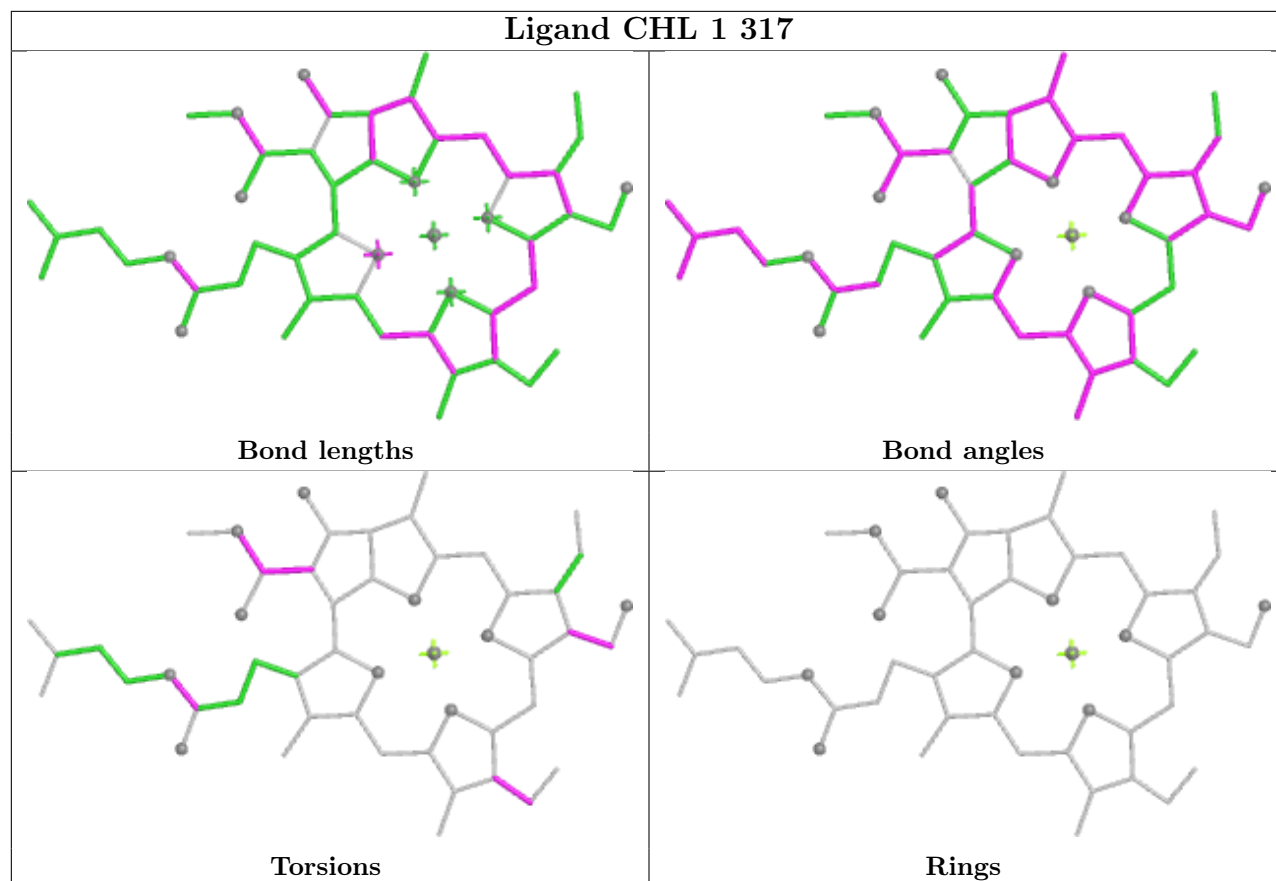


Ligand BCR A 815

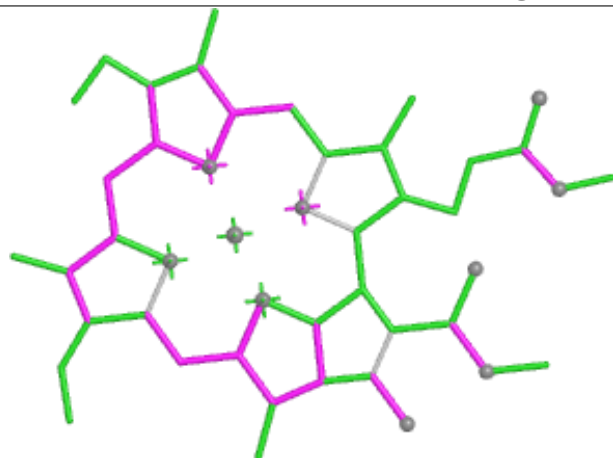


Ligand LUT 1 310

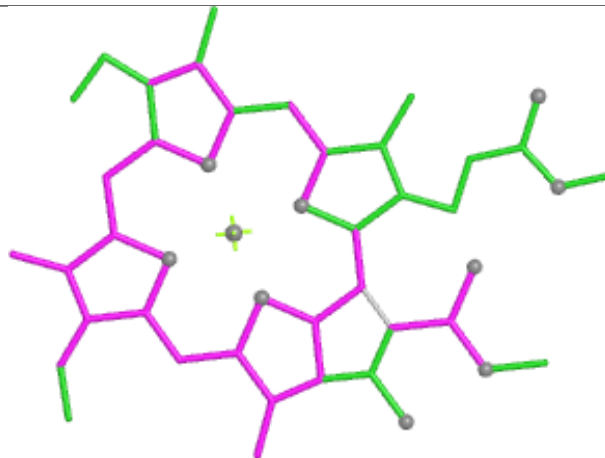




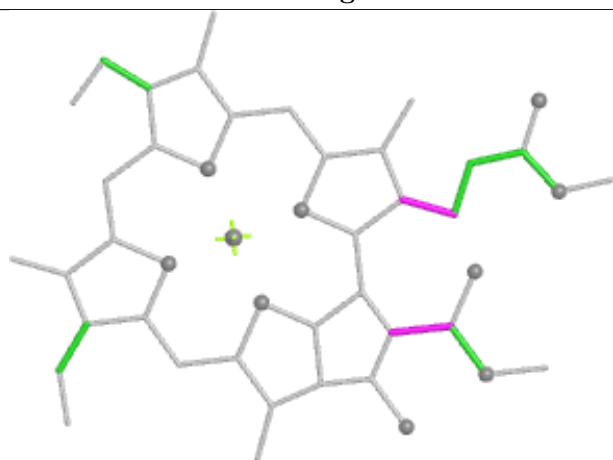
Ligand CLA K 205



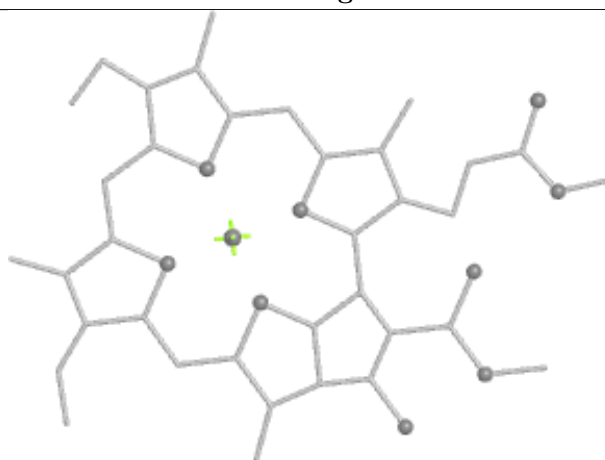
Bond lengths



Bond angles

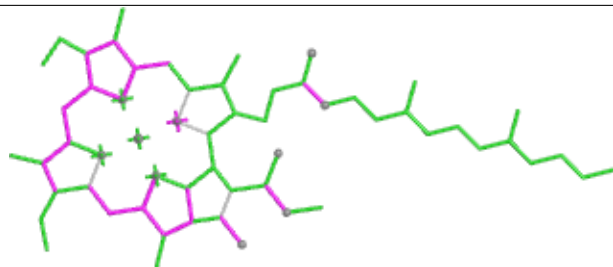


Torsions

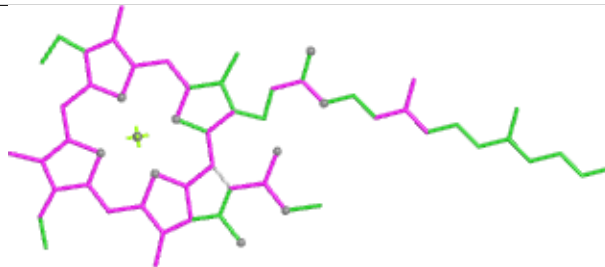


Rings

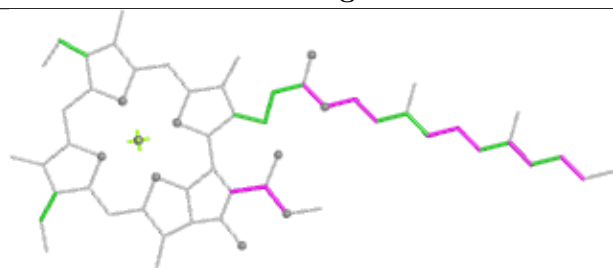
Ligand CLA A 850



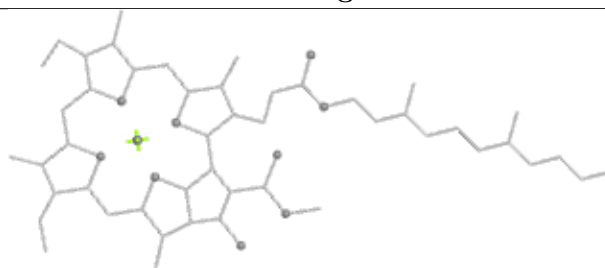
Bond lengths



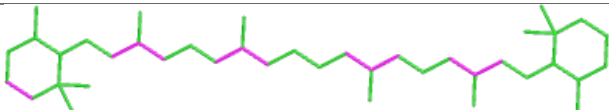
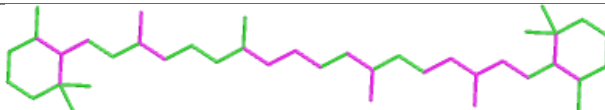
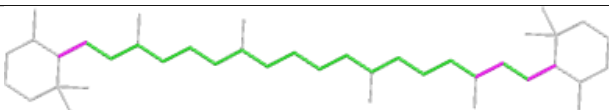
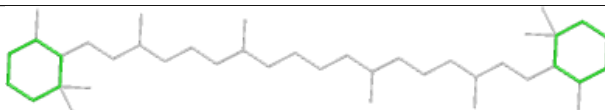
Bond angles

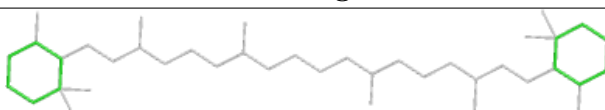


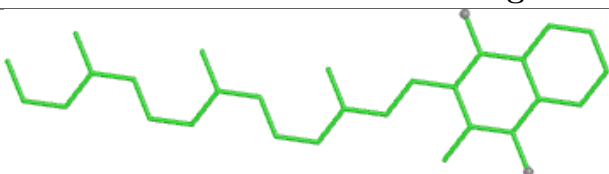
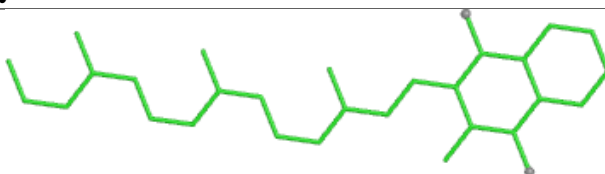
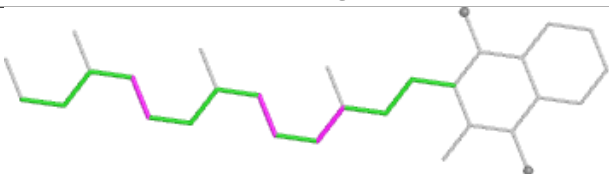
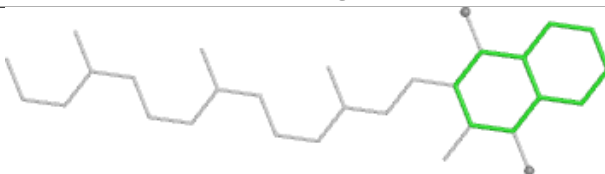
Torsions



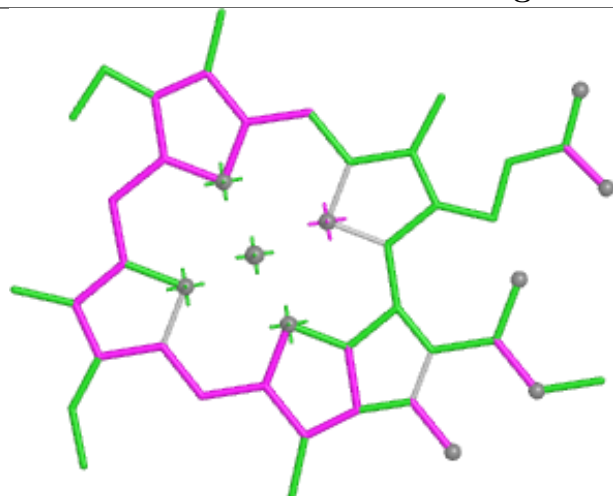
Rings

Ligand BCR 3 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

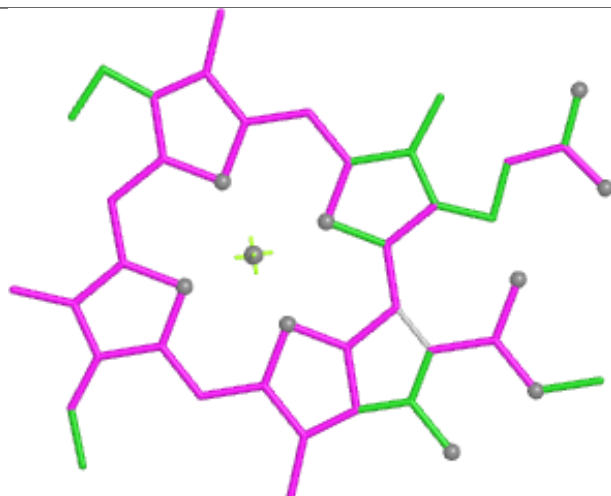
Ligand BCR K 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PQN B 832	
	
Bond lengths	Bond angles
	
Torsions	Rings

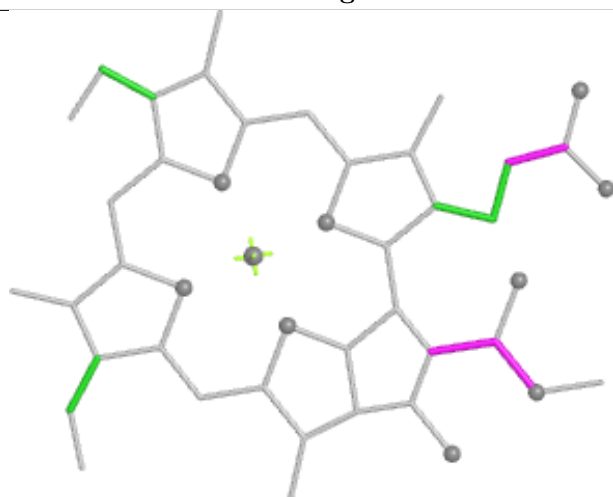
Ligand CLA O 208



Bond lengths



Bond angles

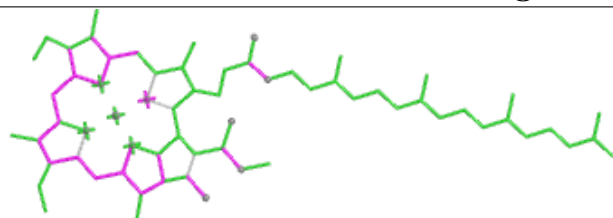


Torsions

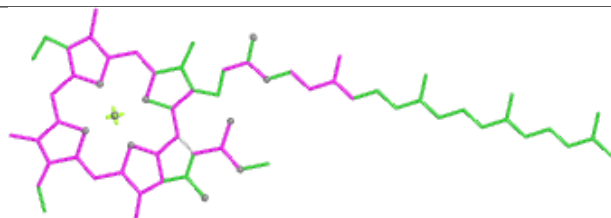


Rings

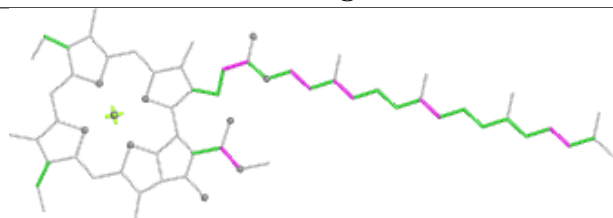
Ligand CLA B 822



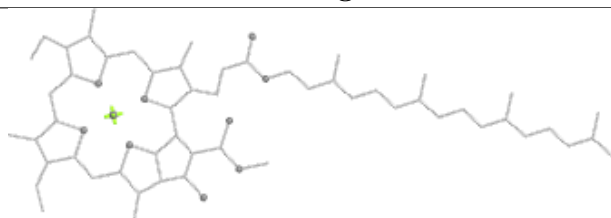
Bond lengths



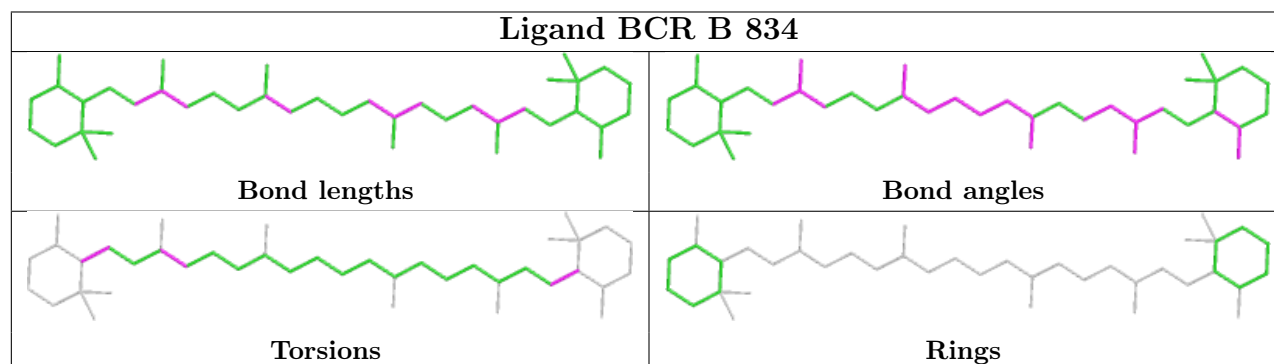
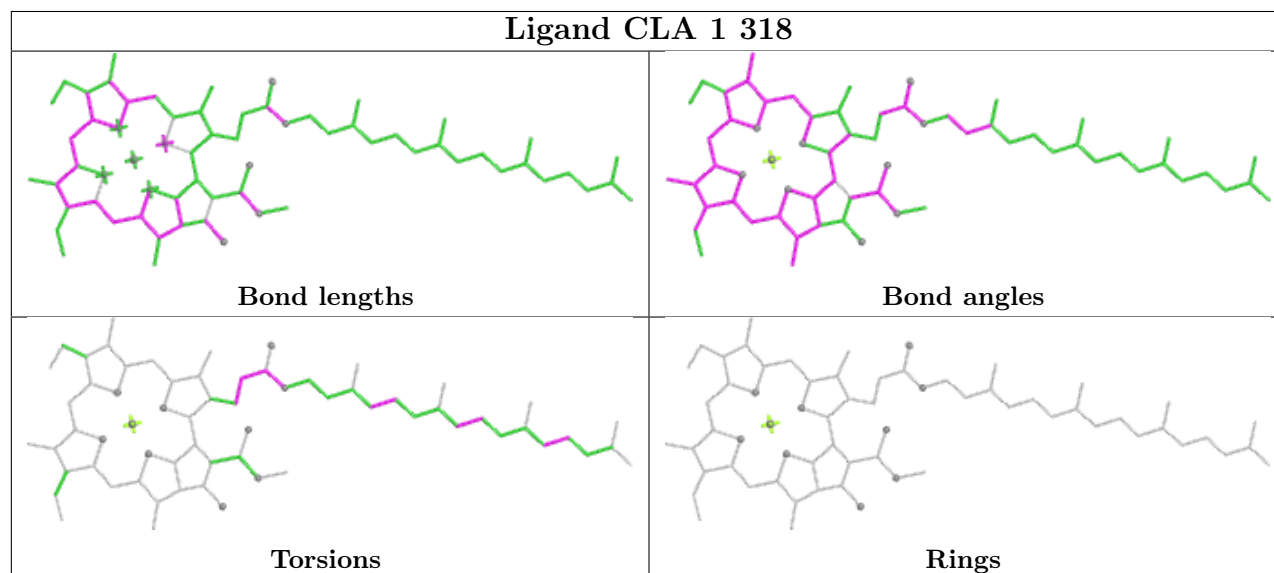
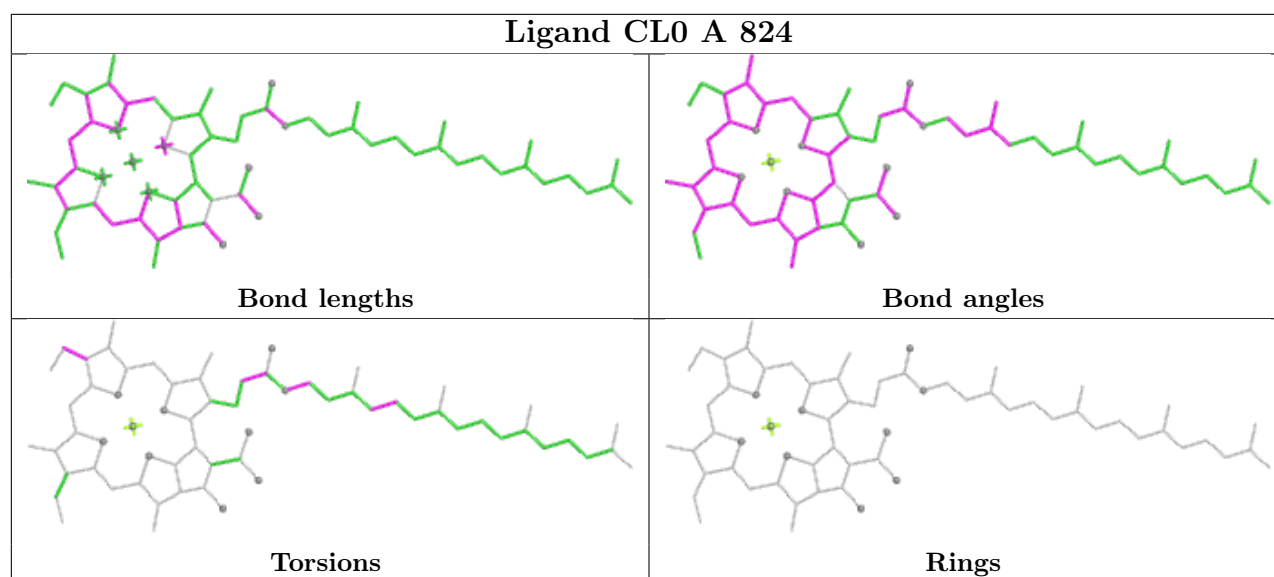
Bond angles

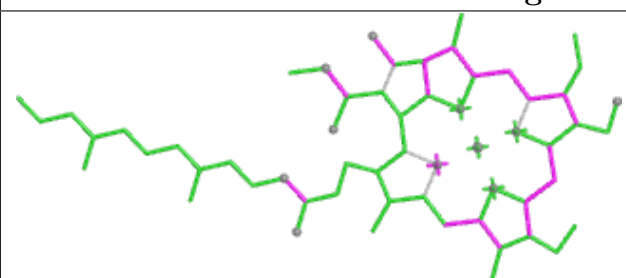
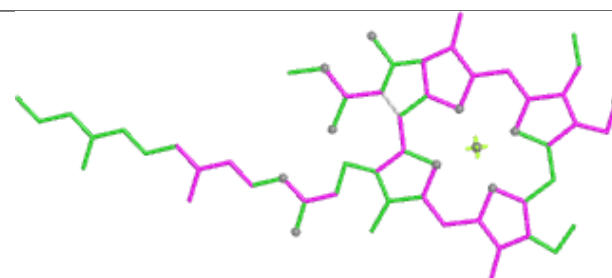
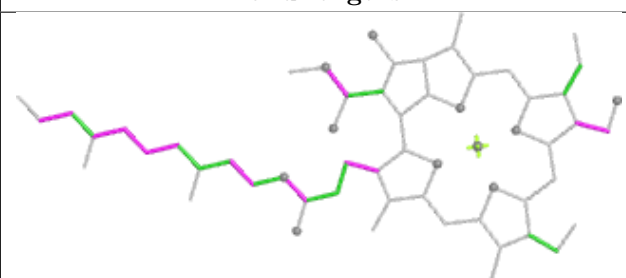
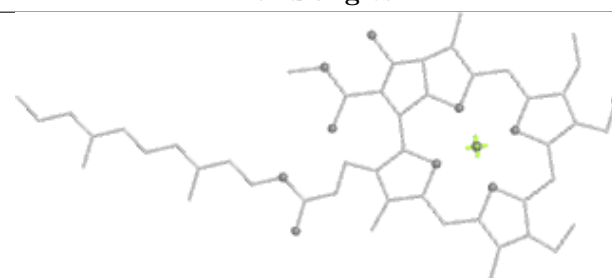


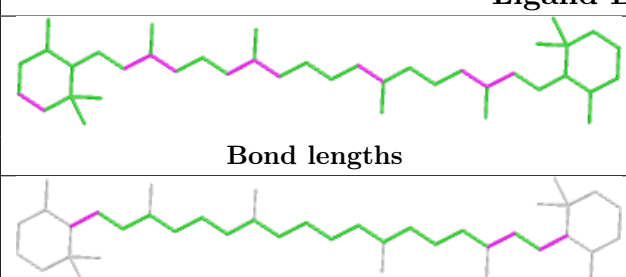
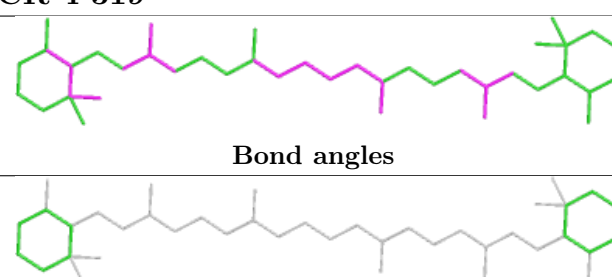
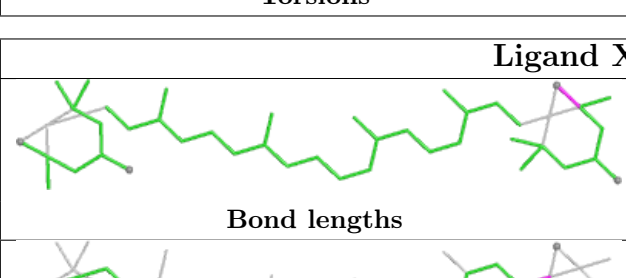
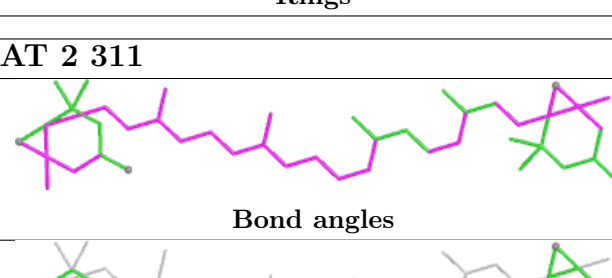
Torsions

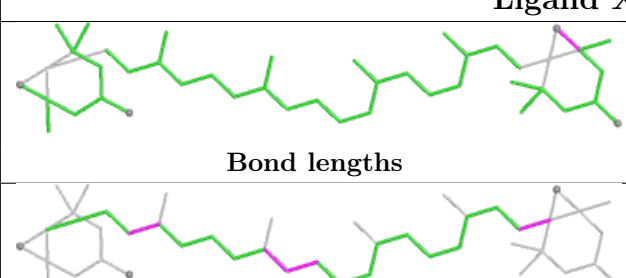
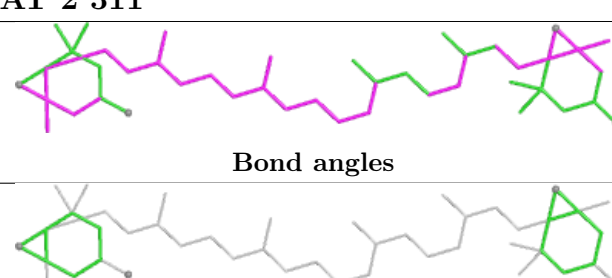
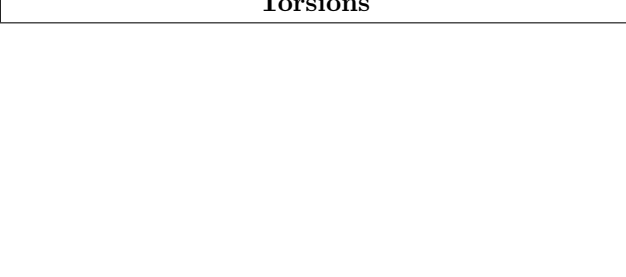
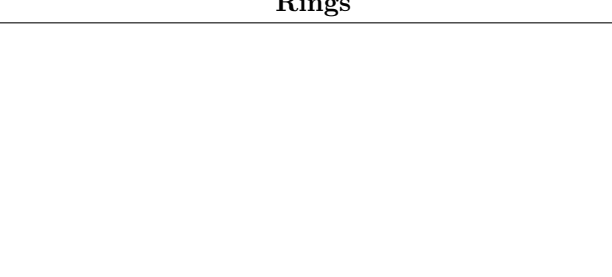


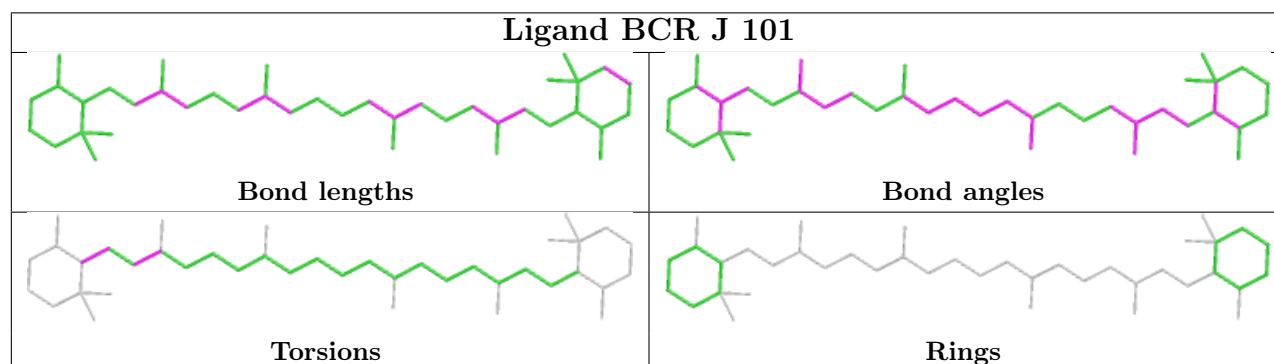
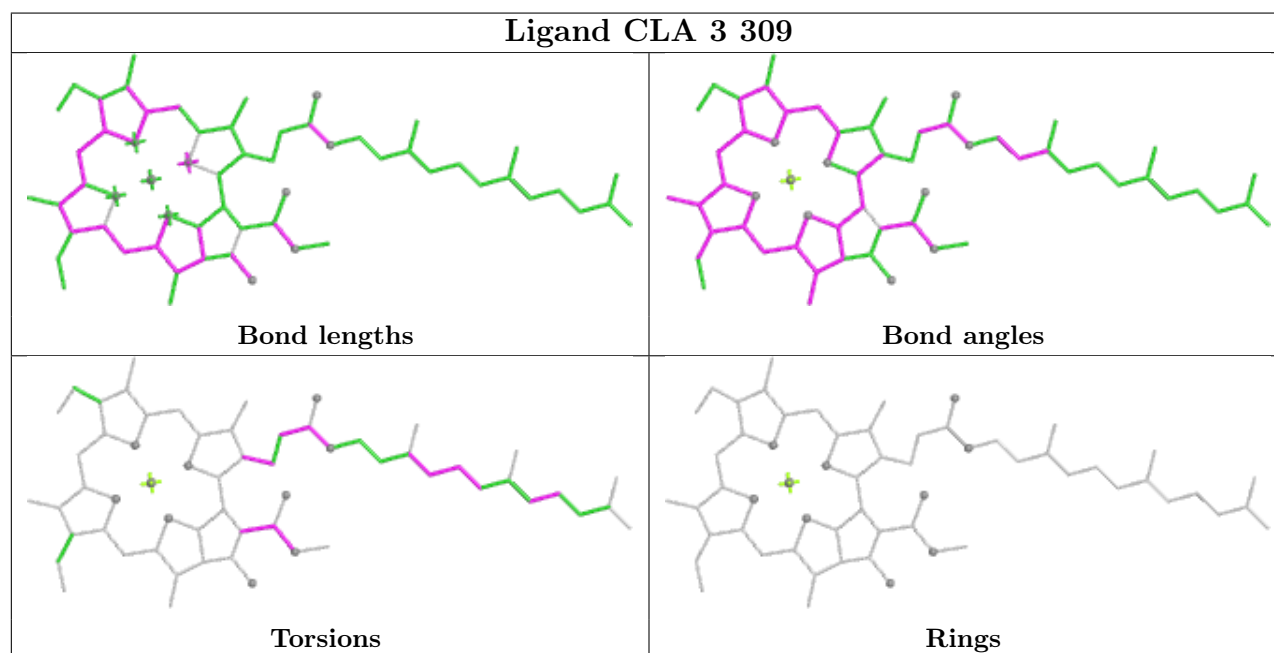
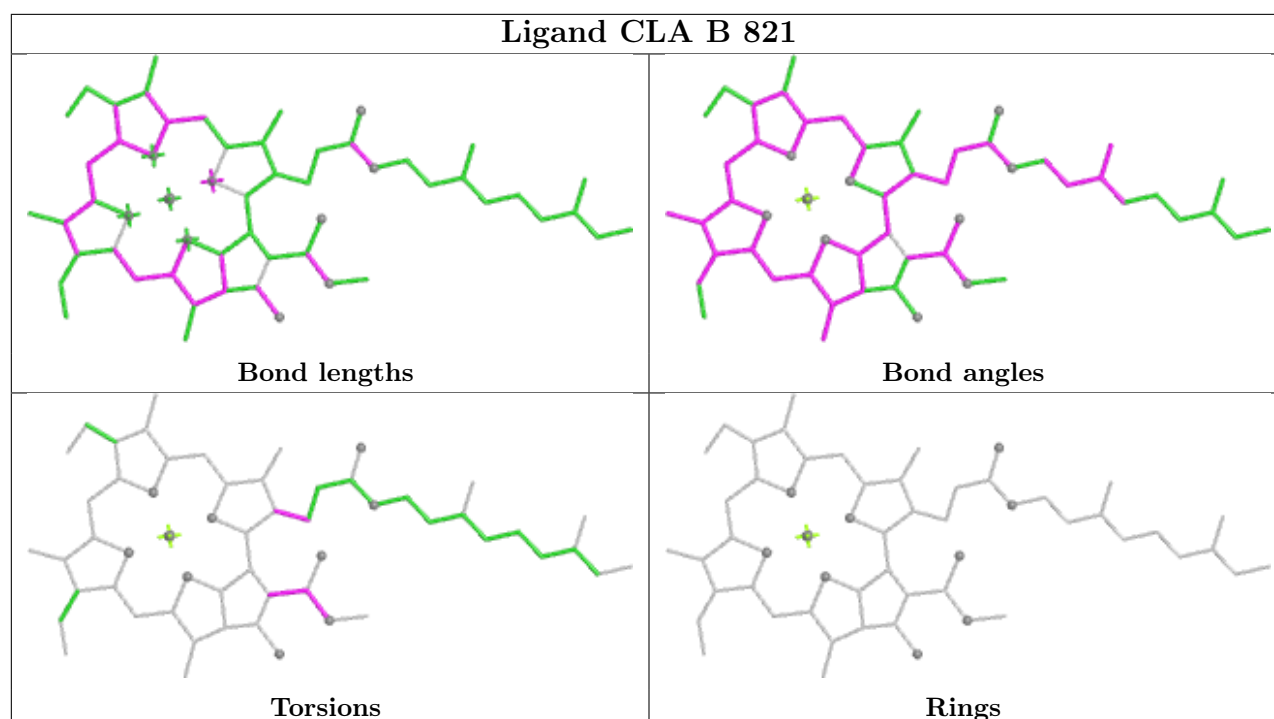
Rings

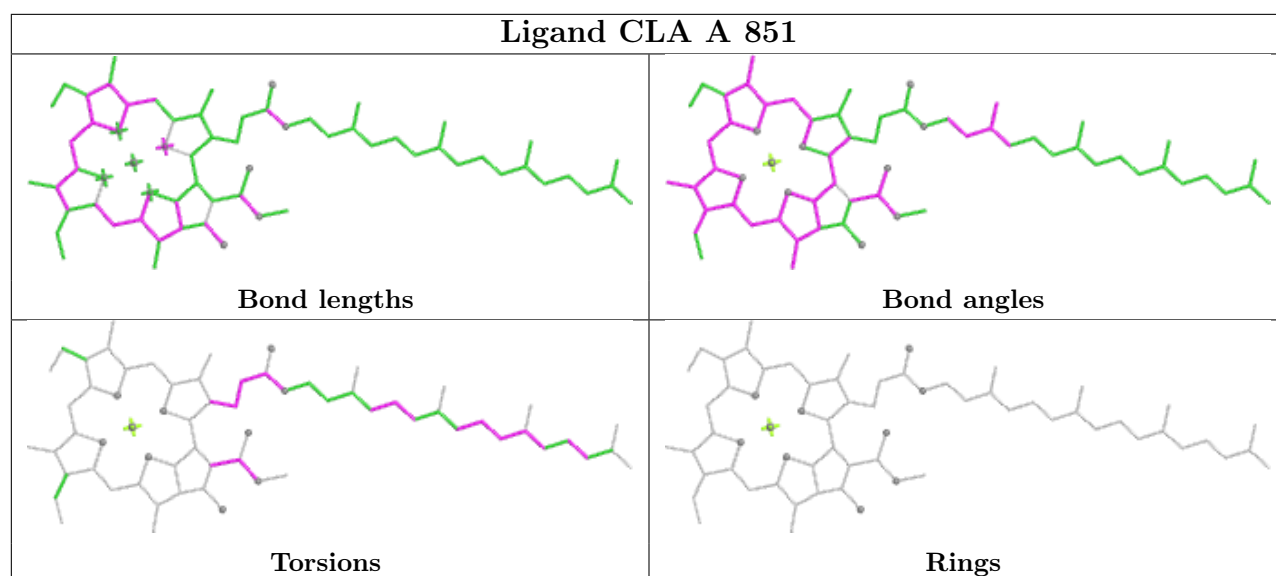
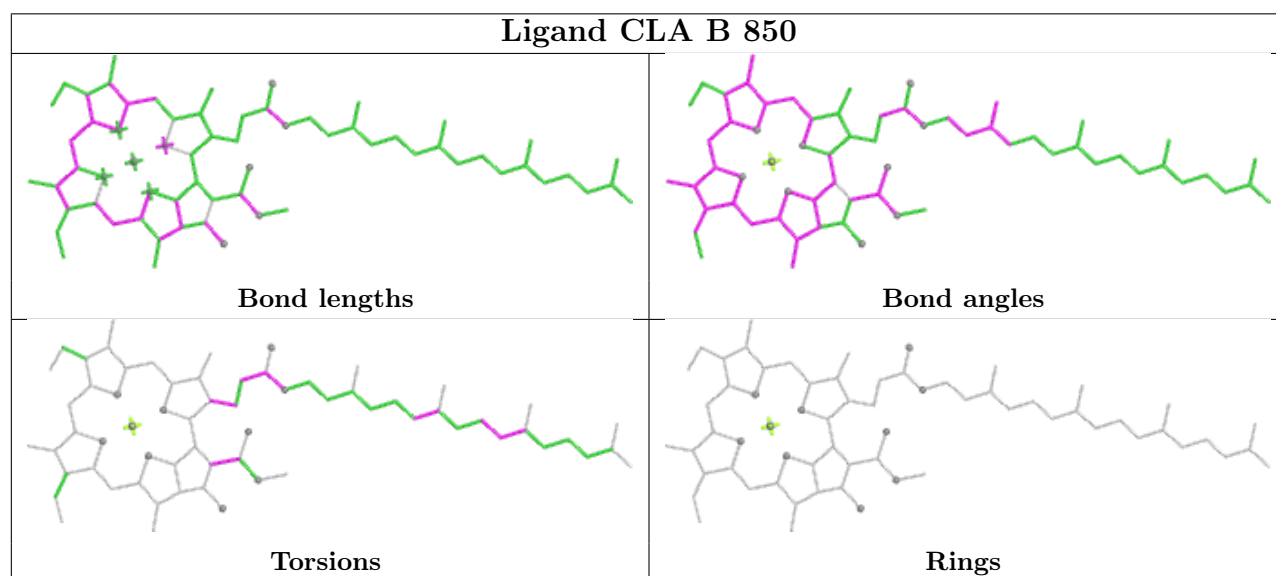
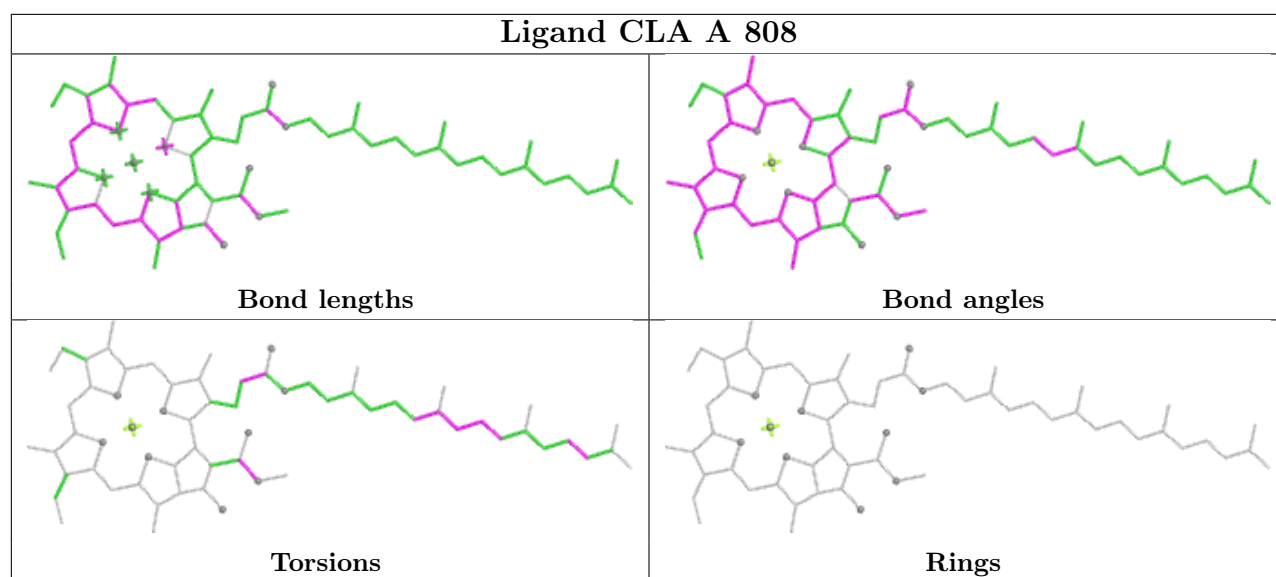


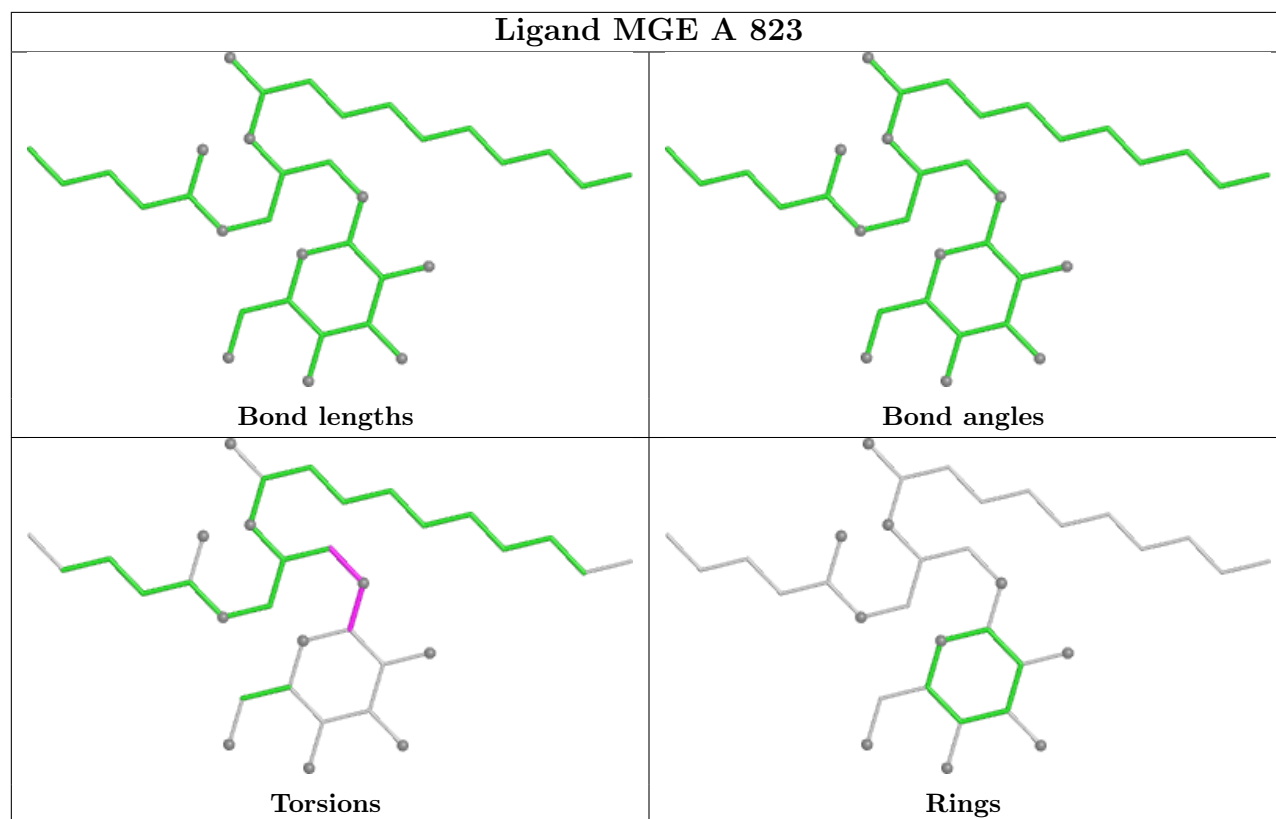
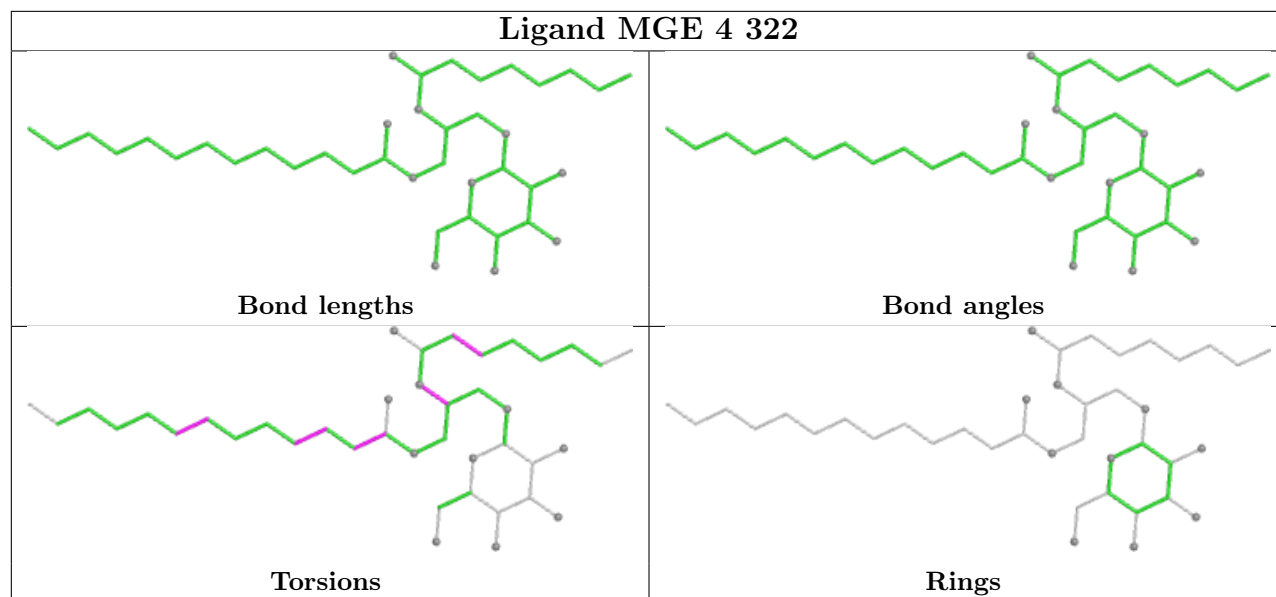
Ligand CHL 2 318	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 4 319	
	
Bond lengths	Bond angles
	
Torsions	Rings

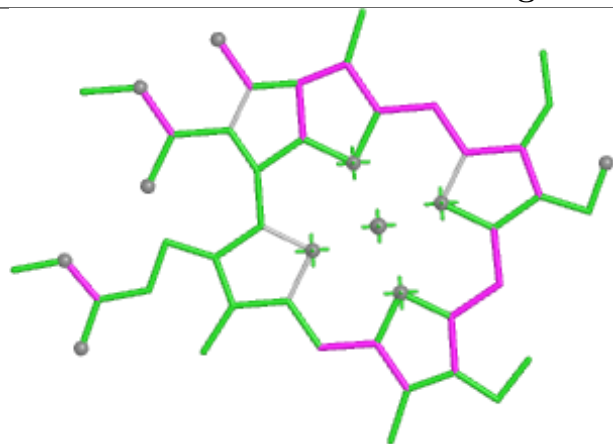
Ligand XAT 2 311	
	
Bond lengths	Bond angles
	
Torsions	Rings



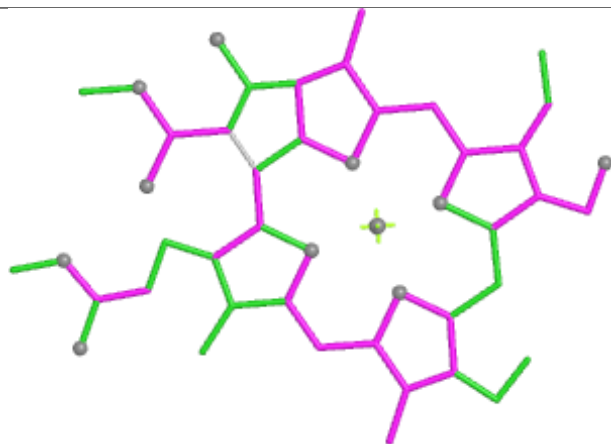




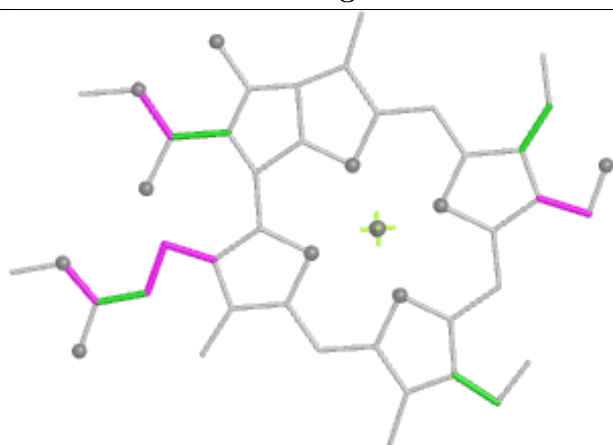
Ligand CHL 2 301



Bond lengths



Bond angles

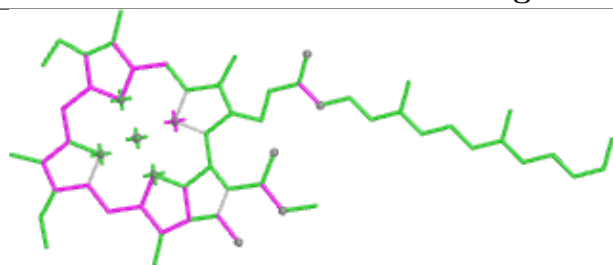


Torsions

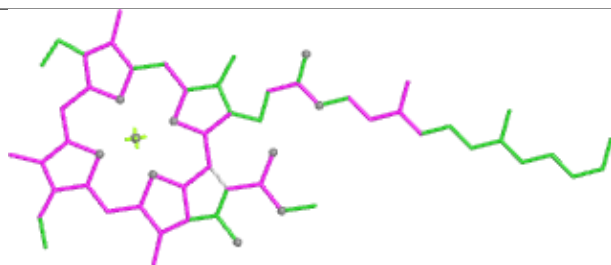


Rings

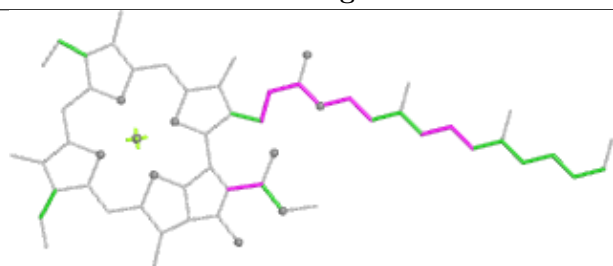
Ligand CLA H 201



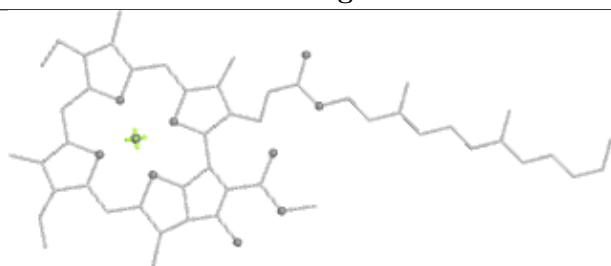
Bond lengths



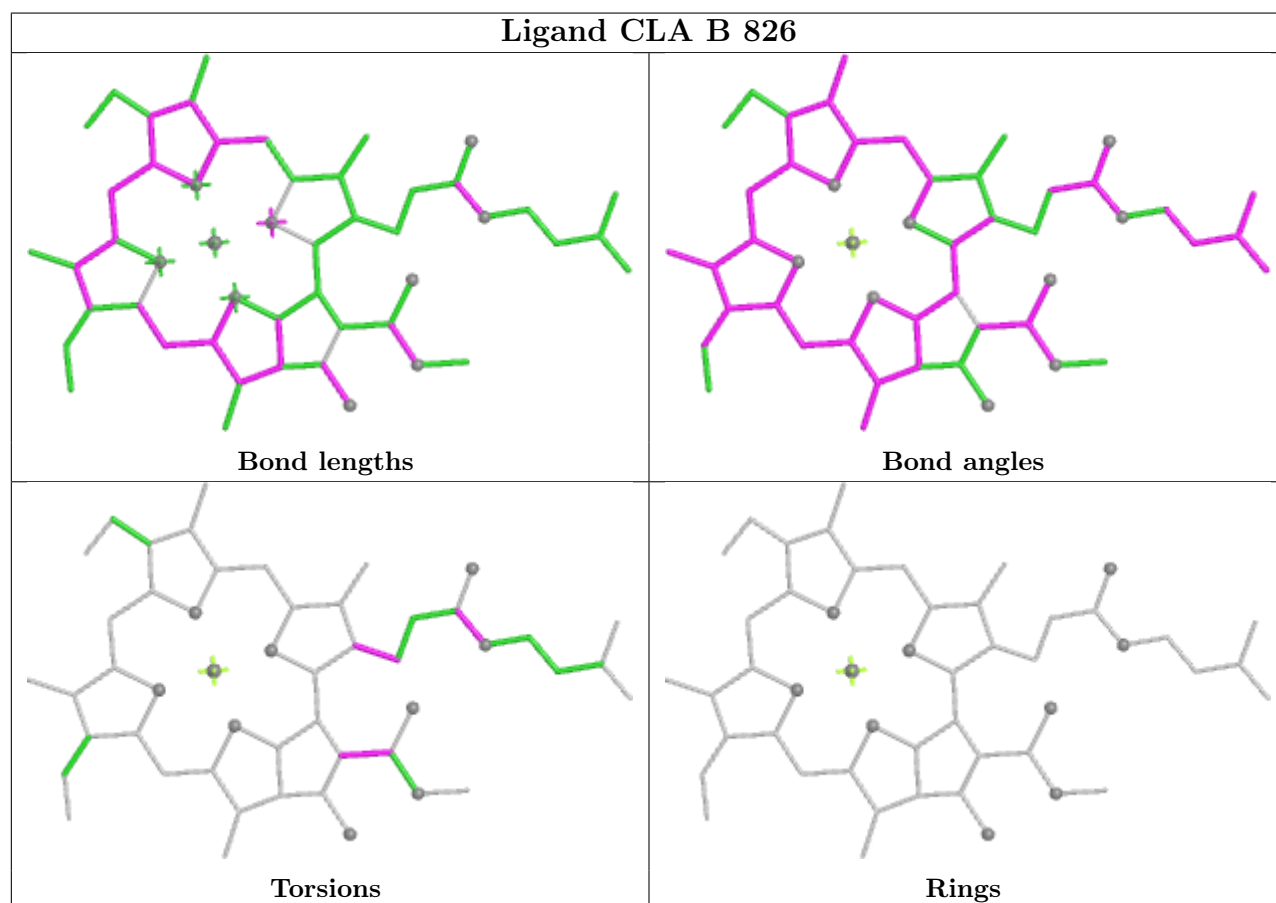
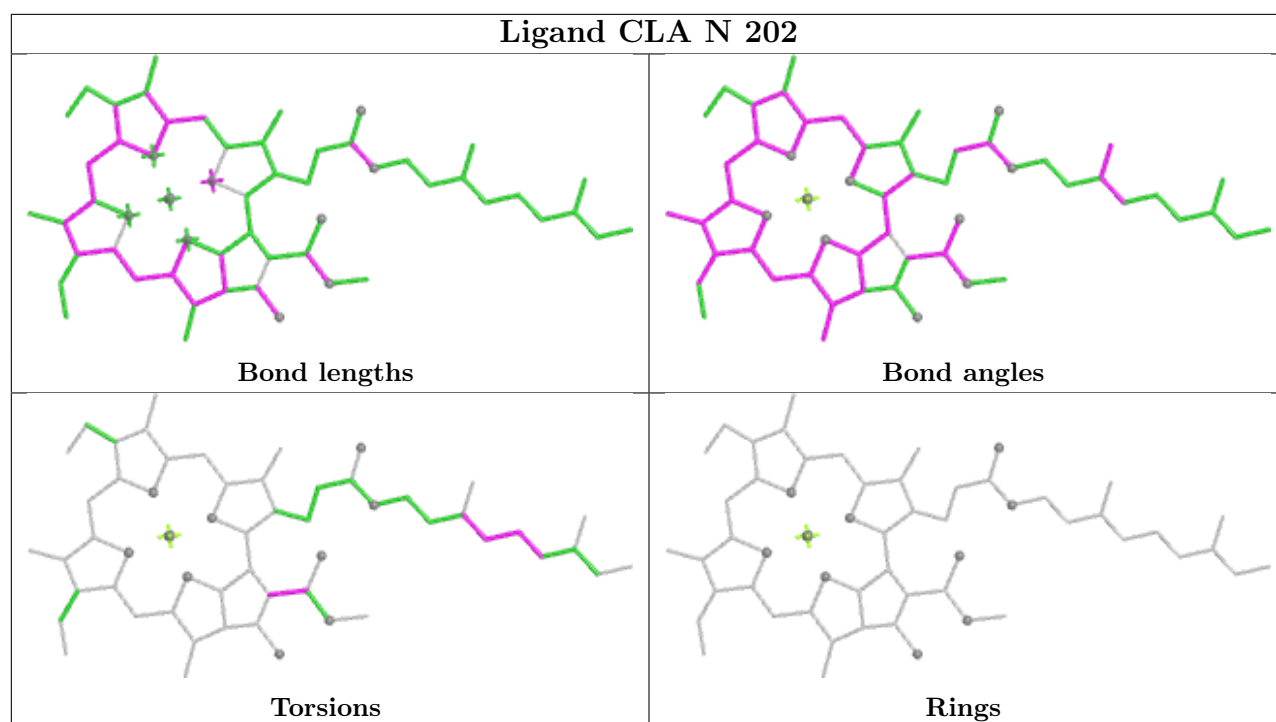
Bond angles

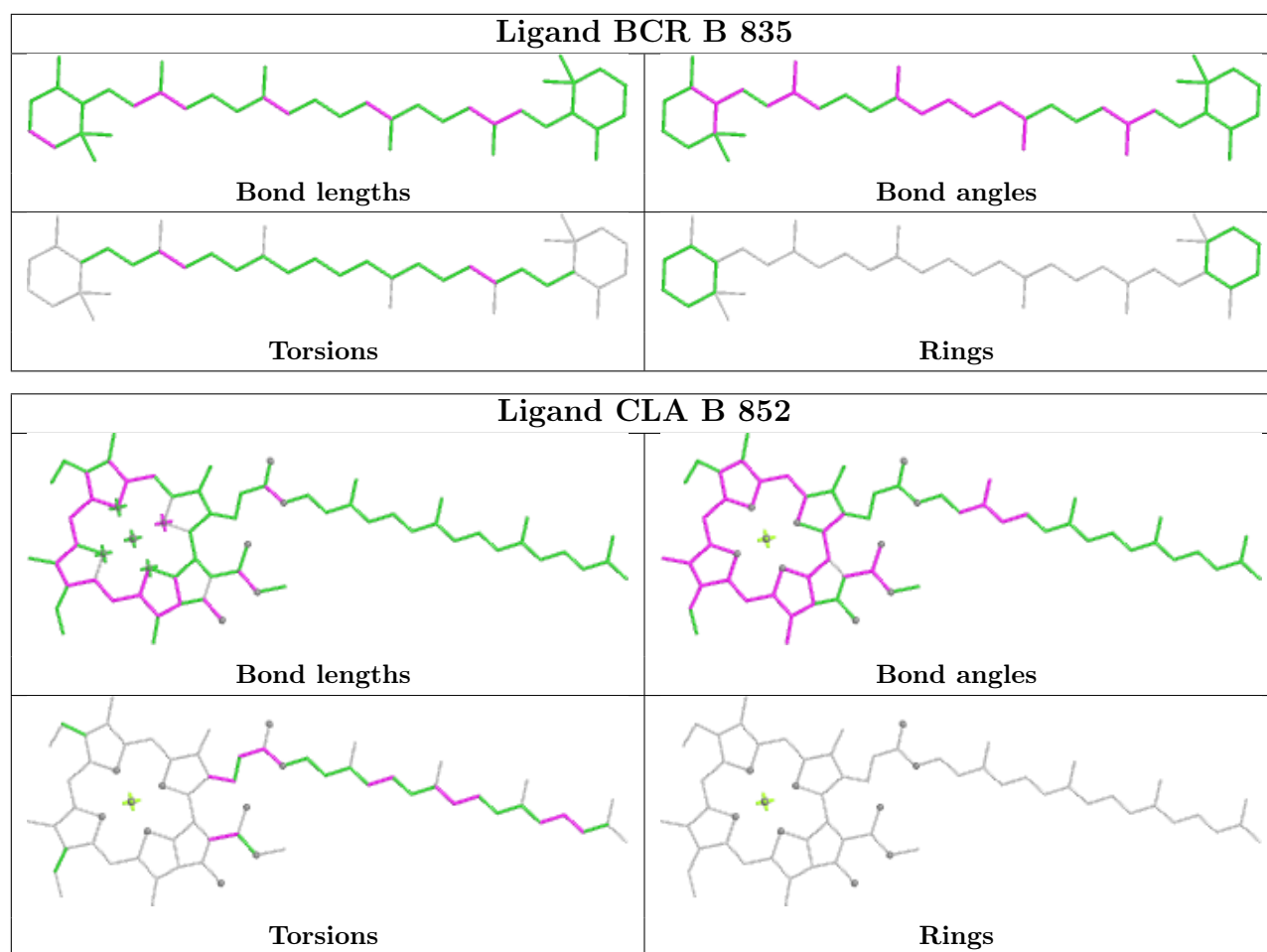


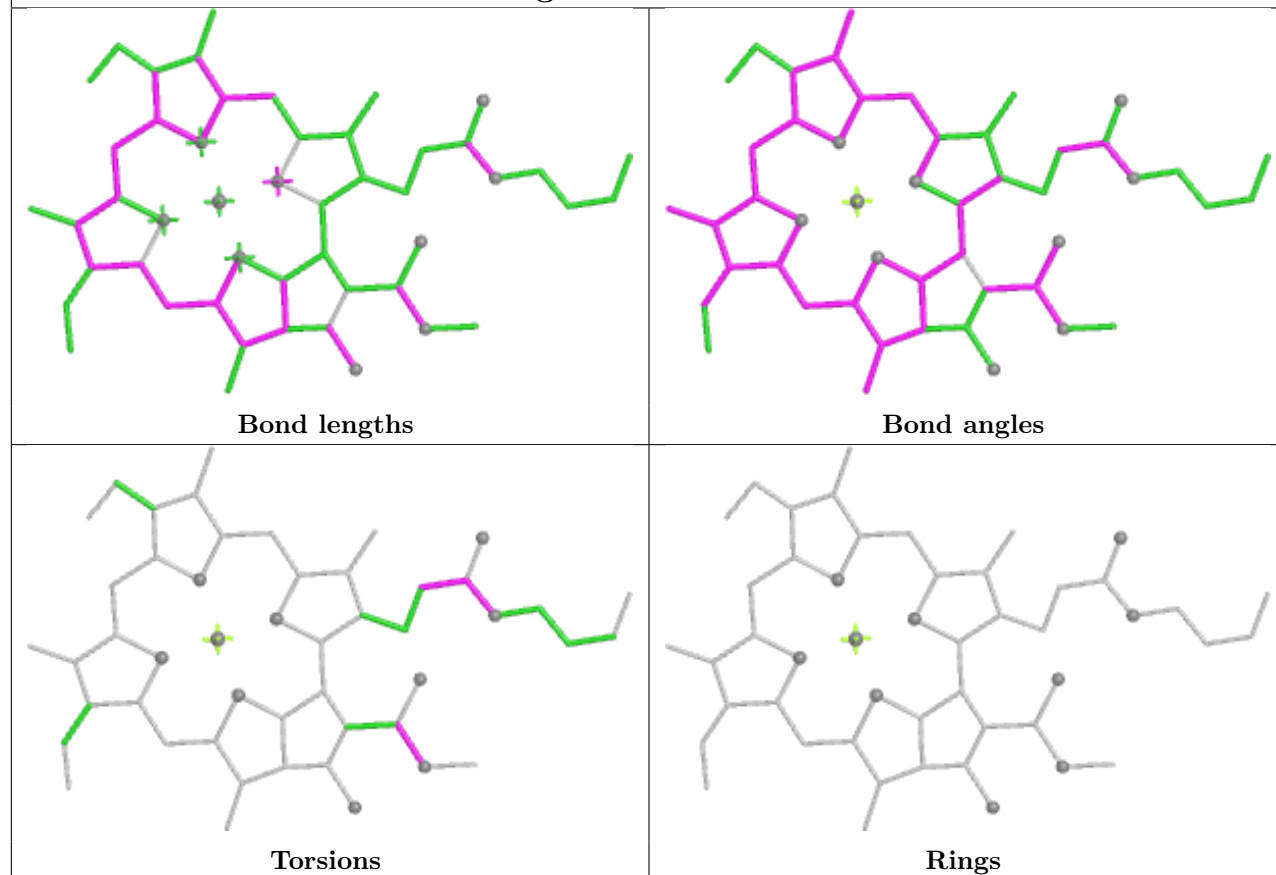
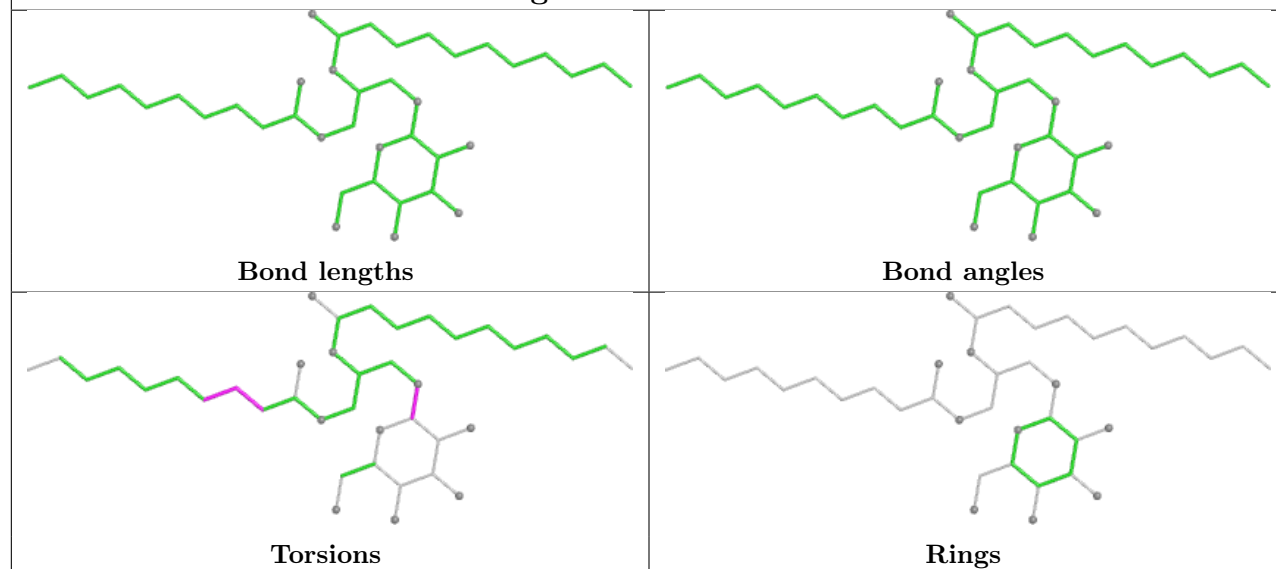
Torsions



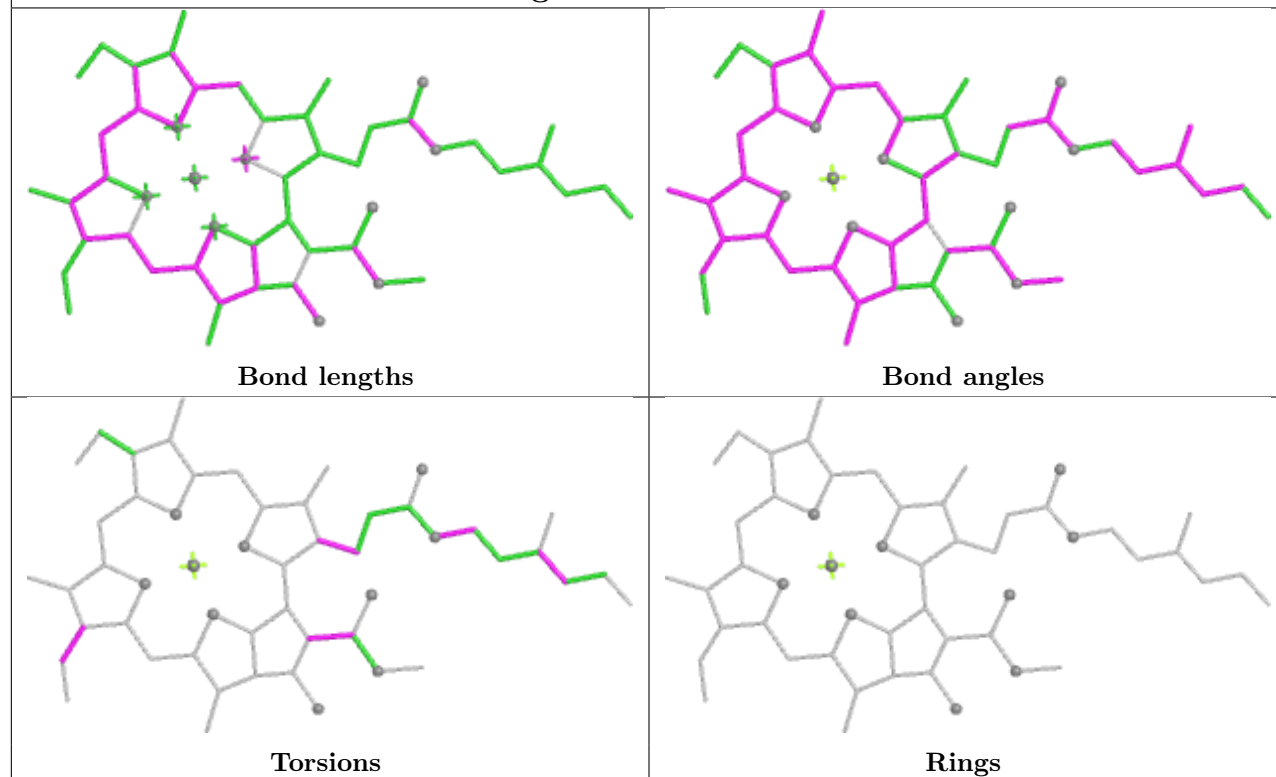
Rings



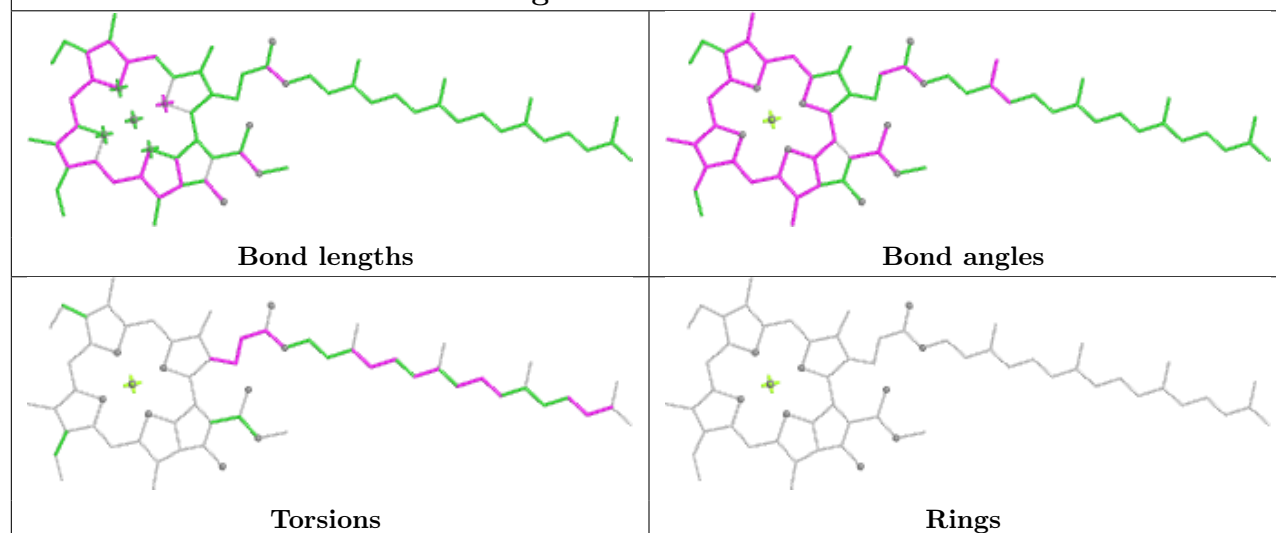


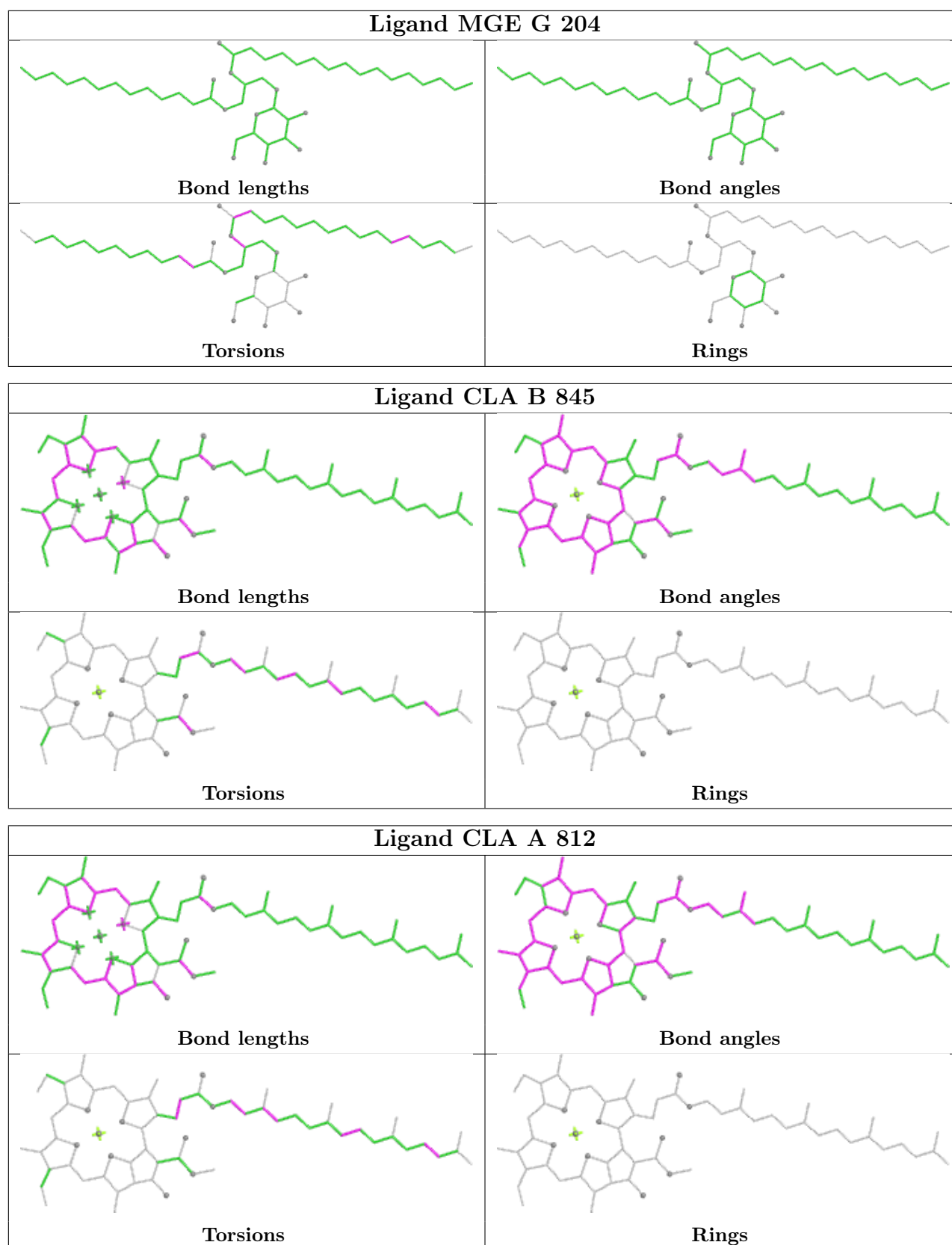
Ligand CLA 3 310**Ligand MGE 1 316**

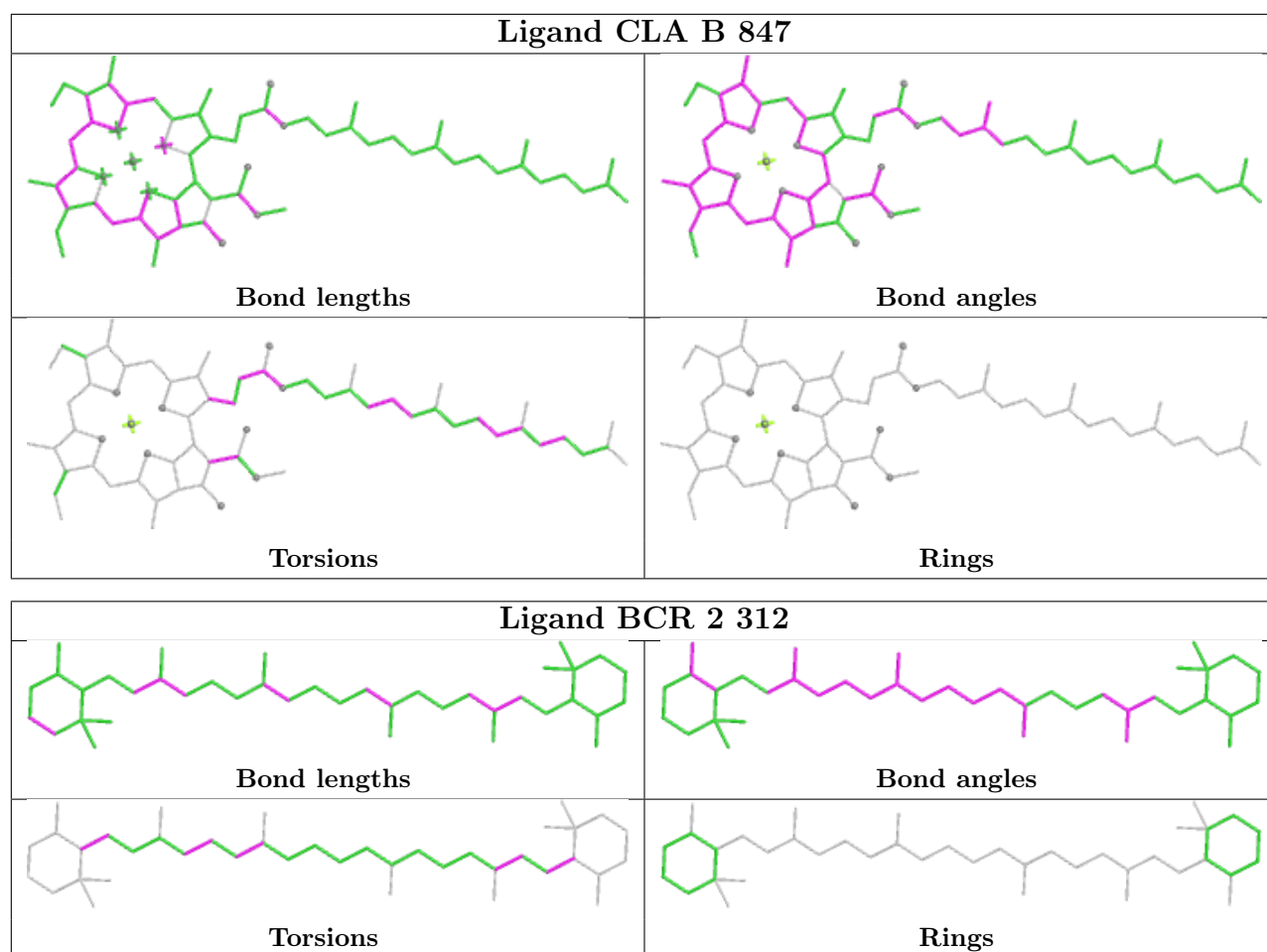
Ligand CLA A 831

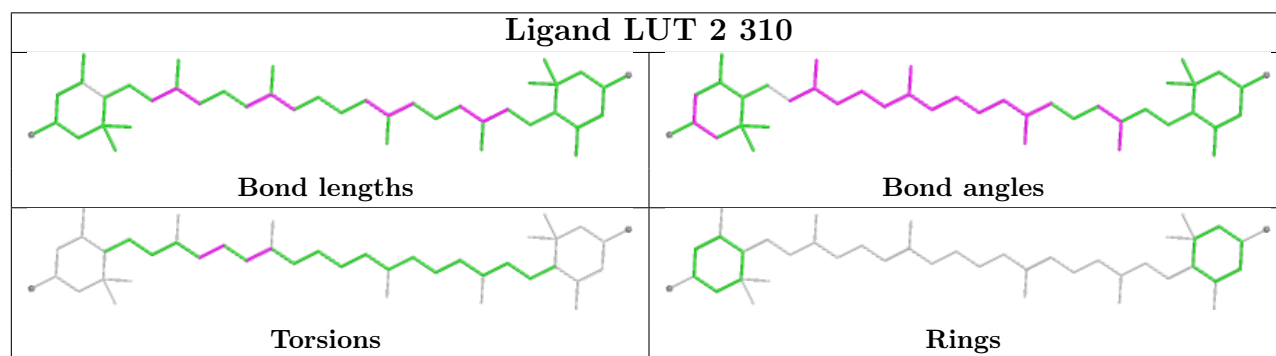
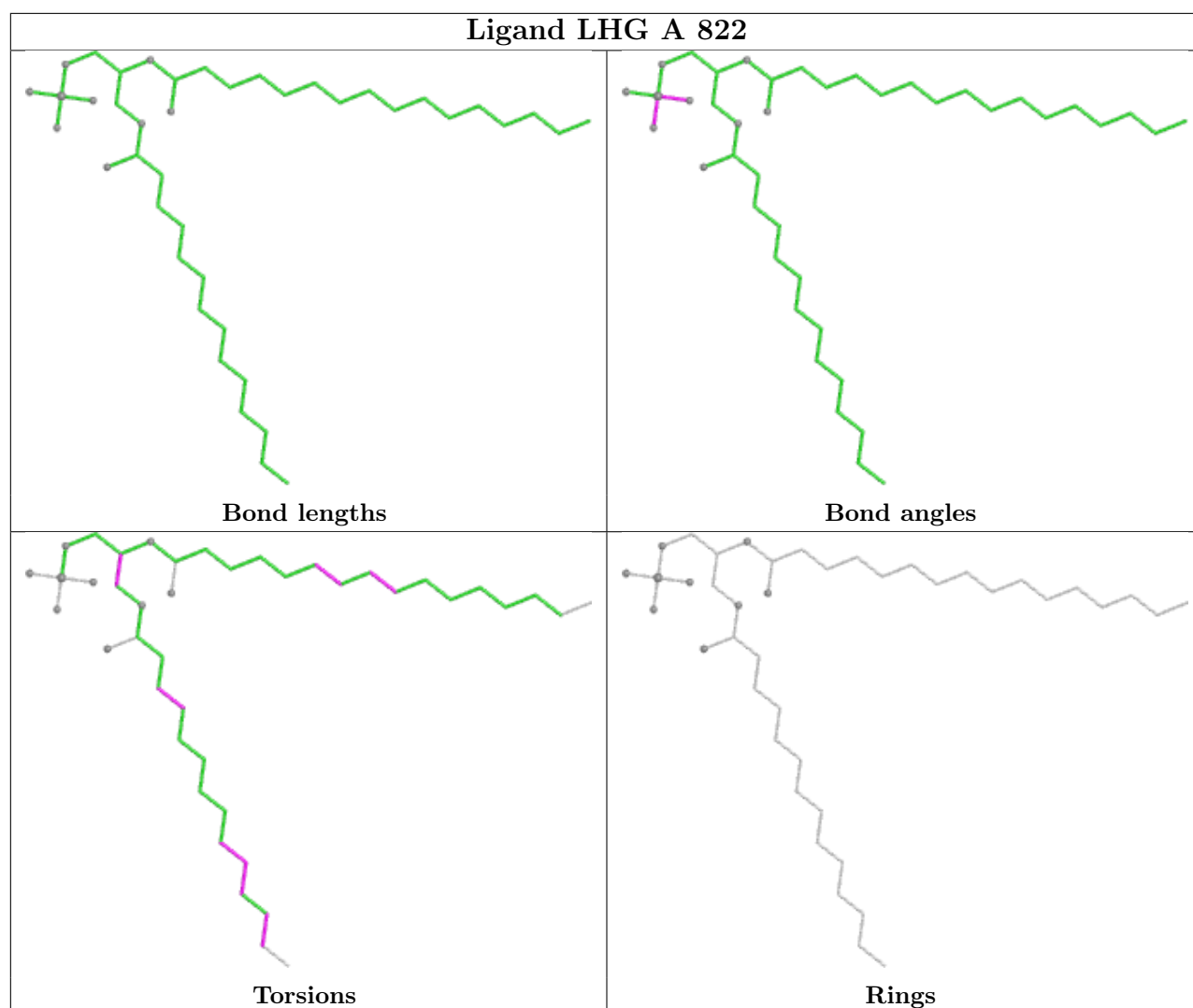


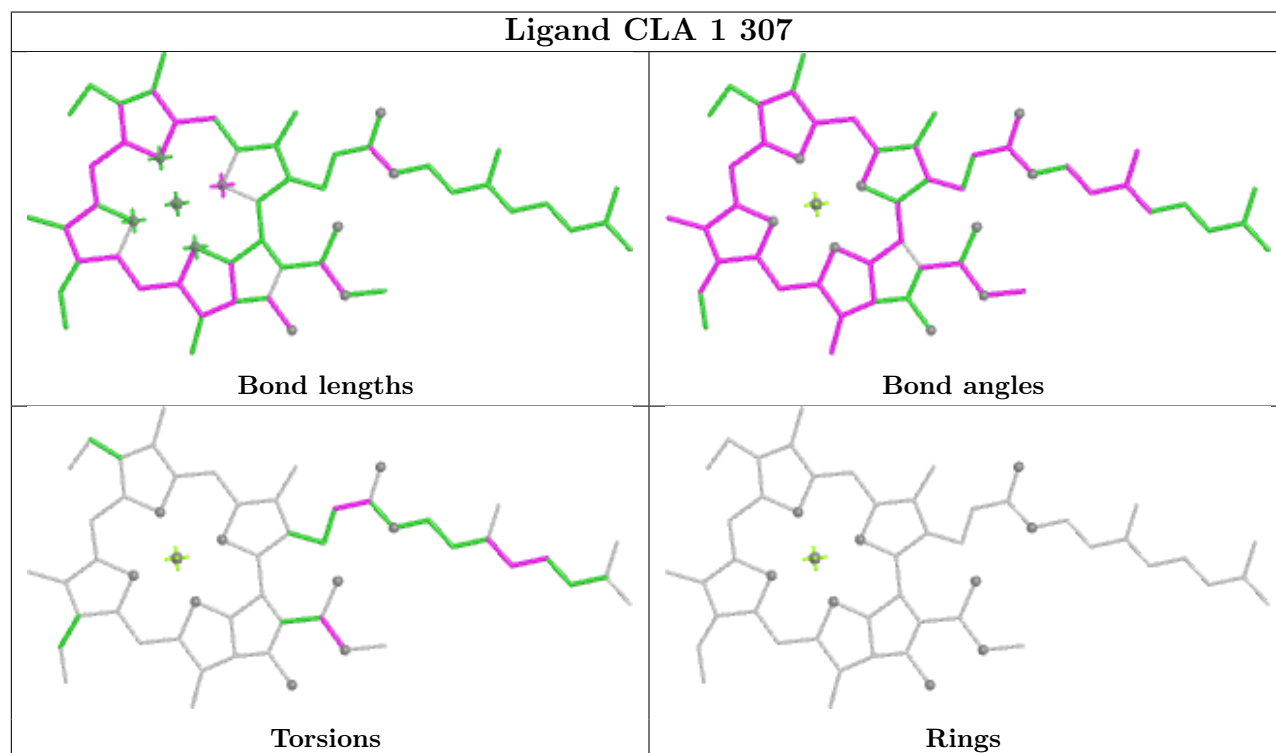
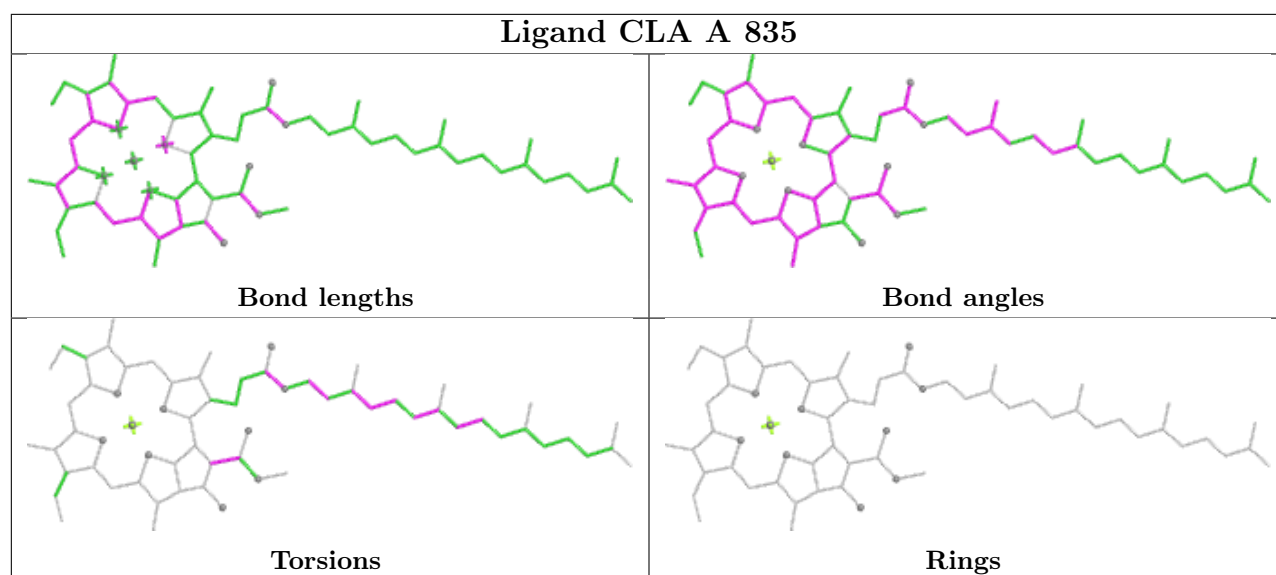
Ligand CLA A 849



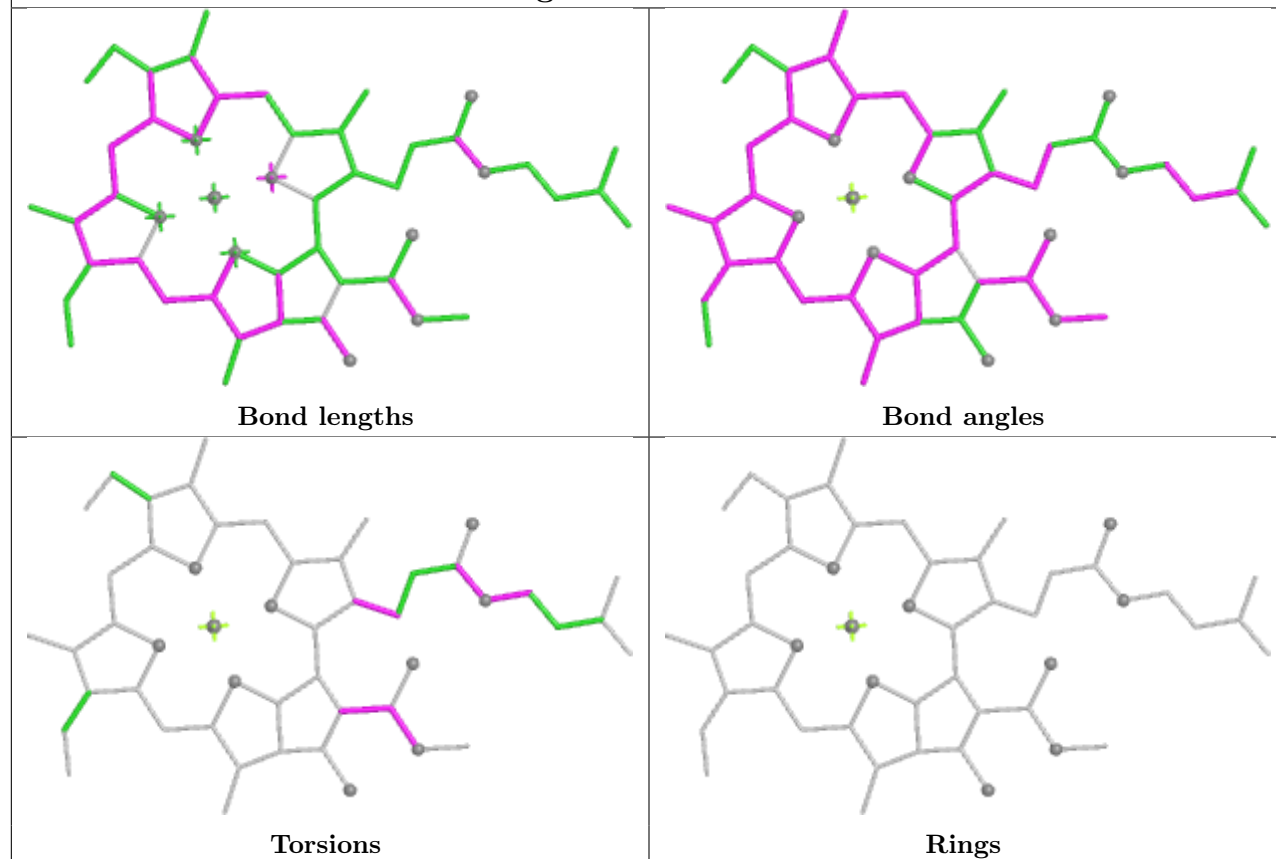




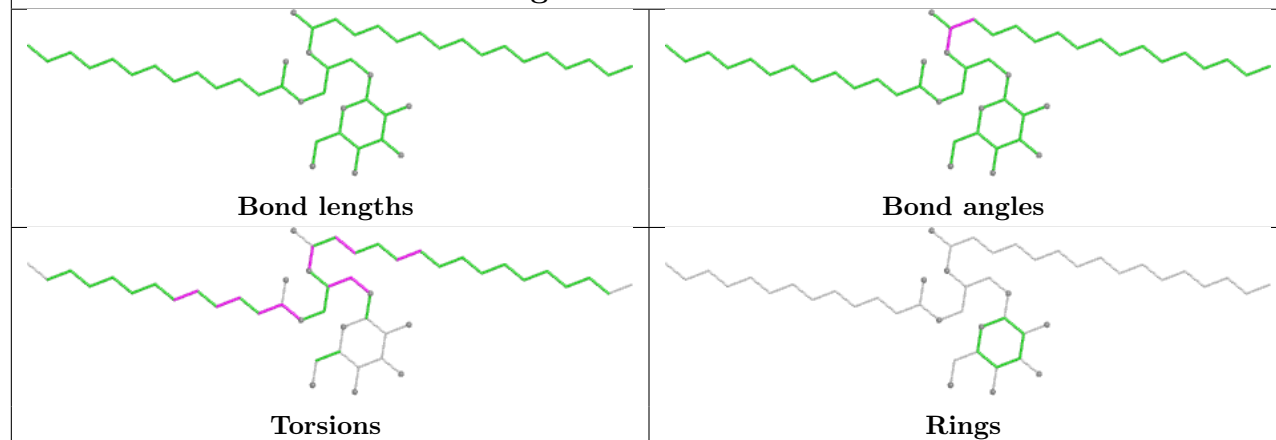


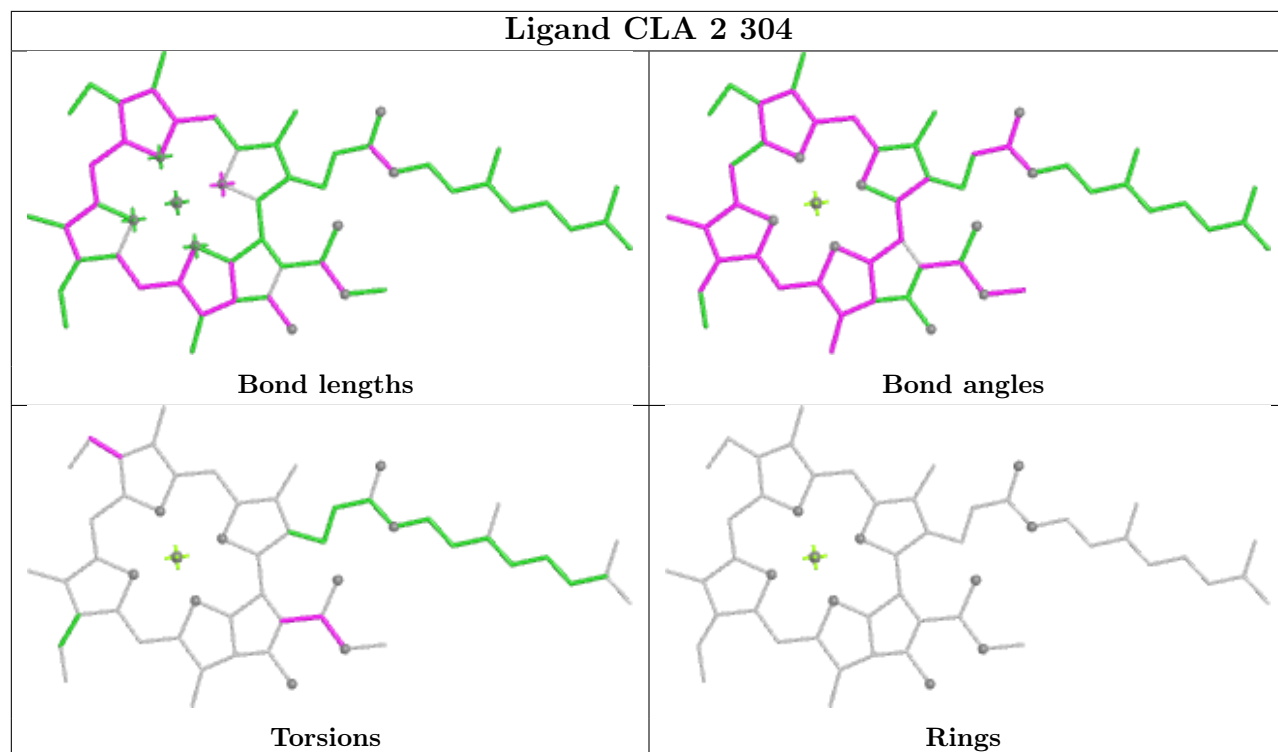
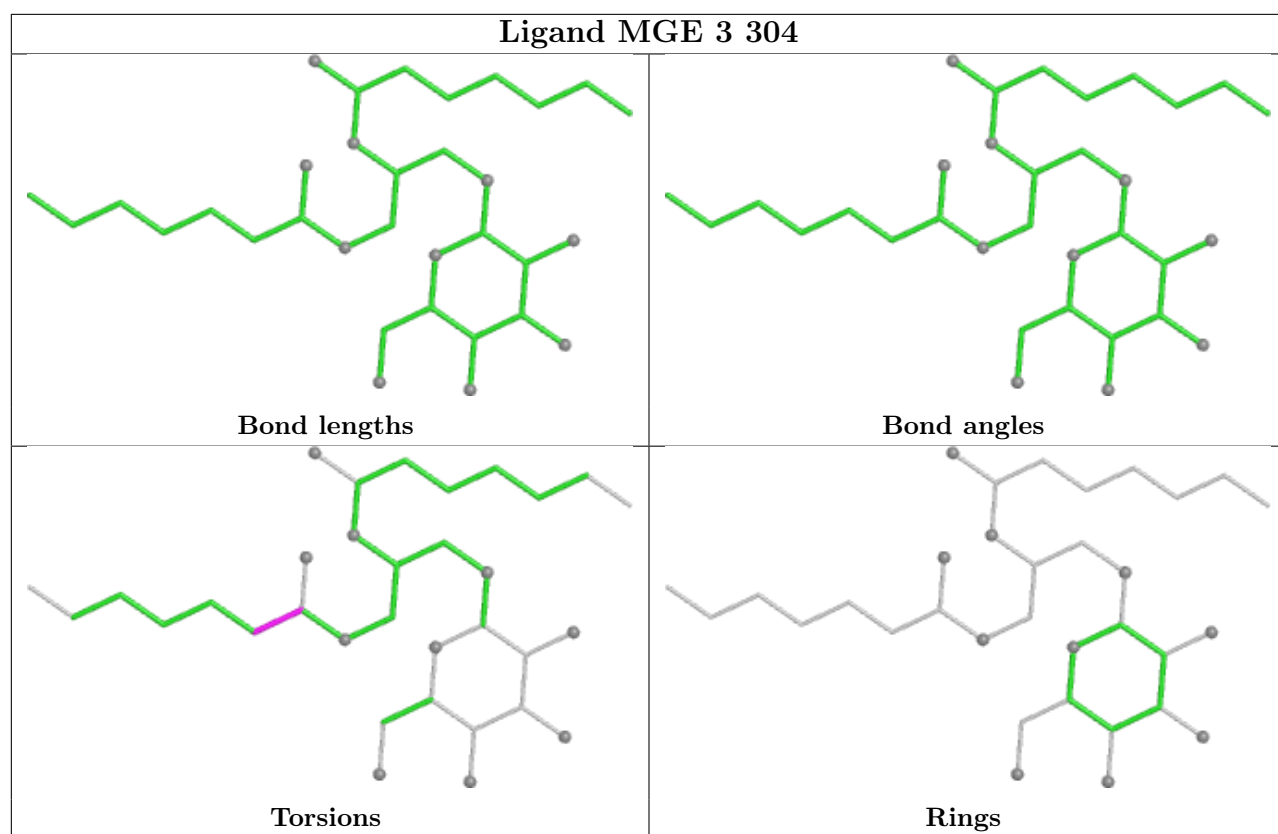


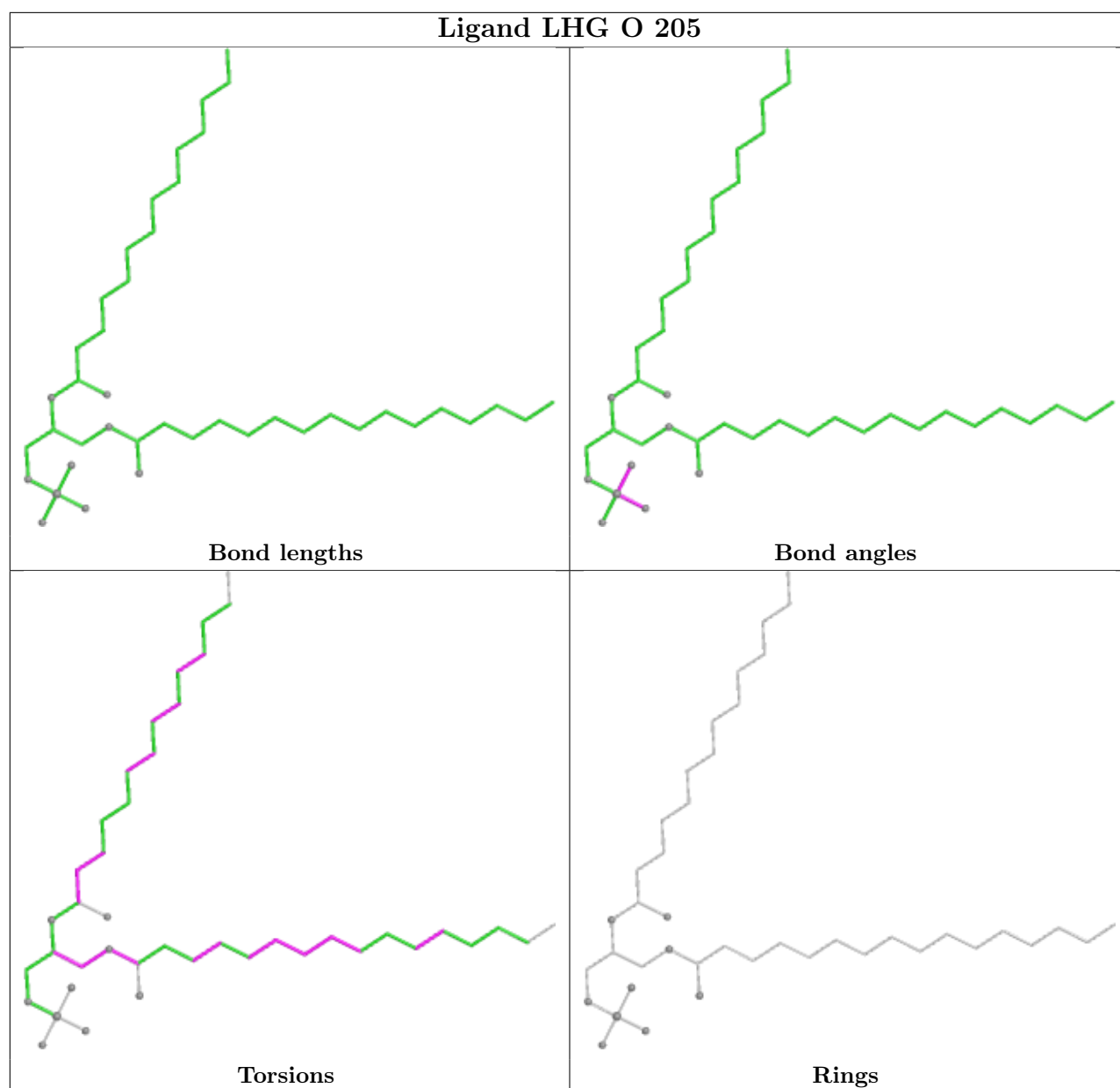
Ligand CLA 2 321



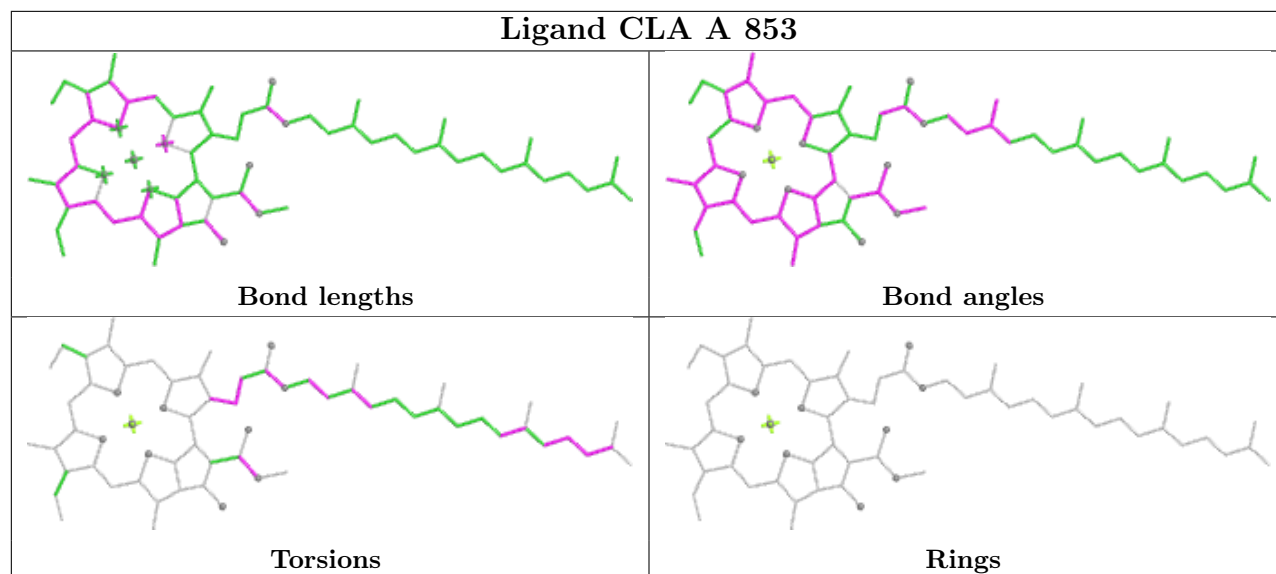
Ligand MGE 1 324



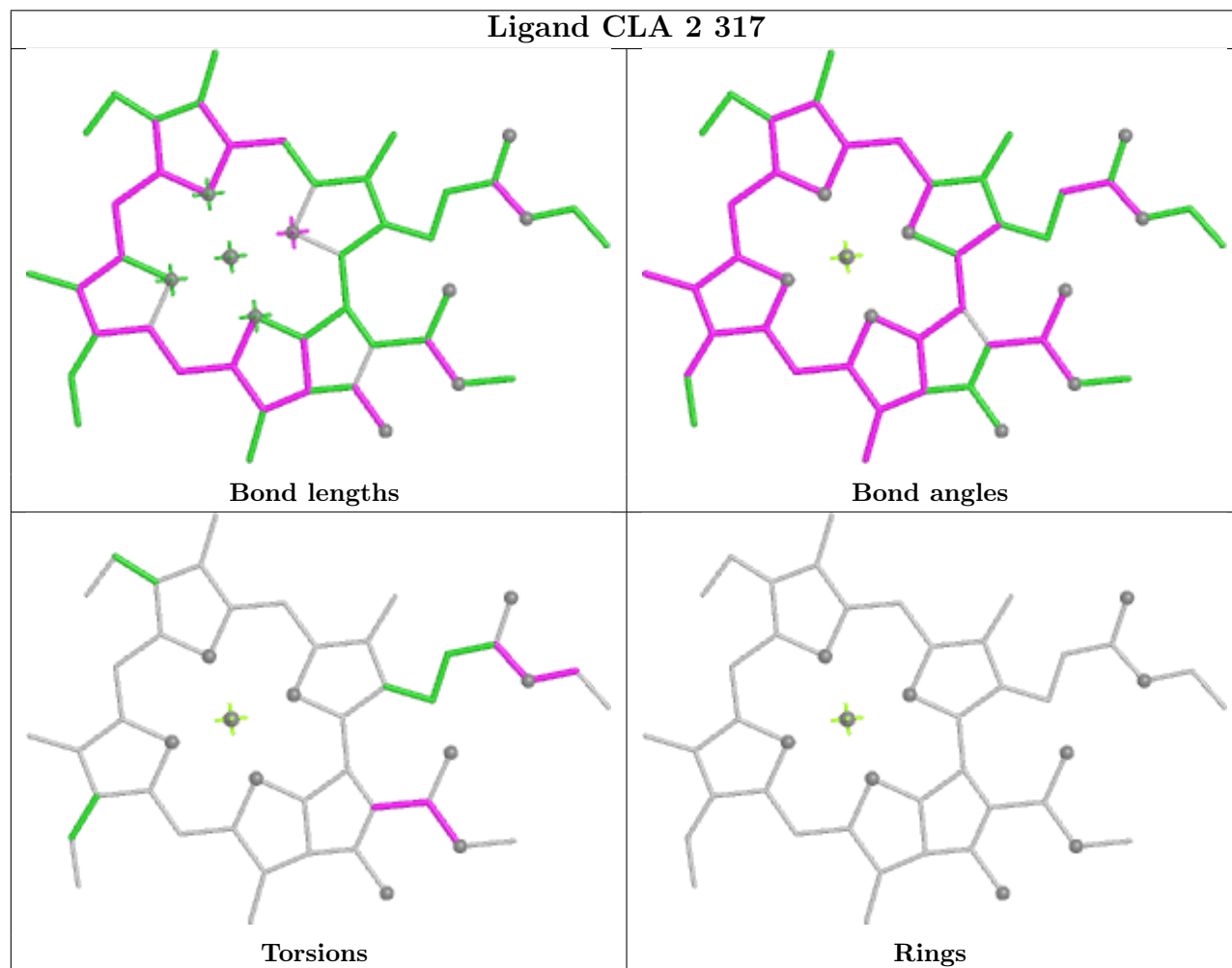


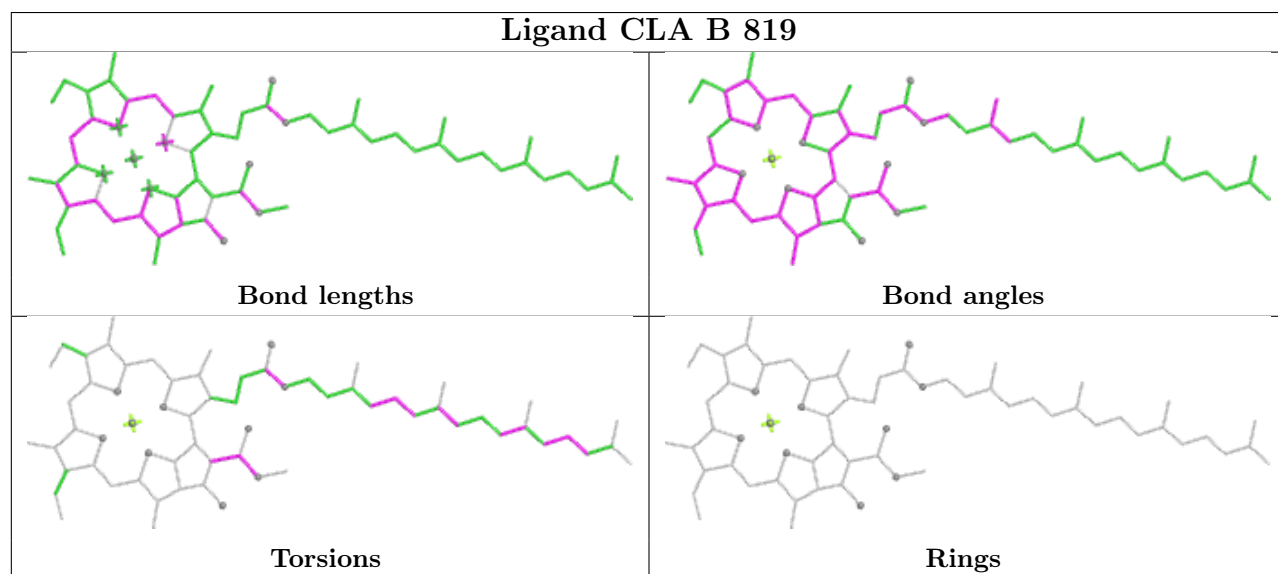
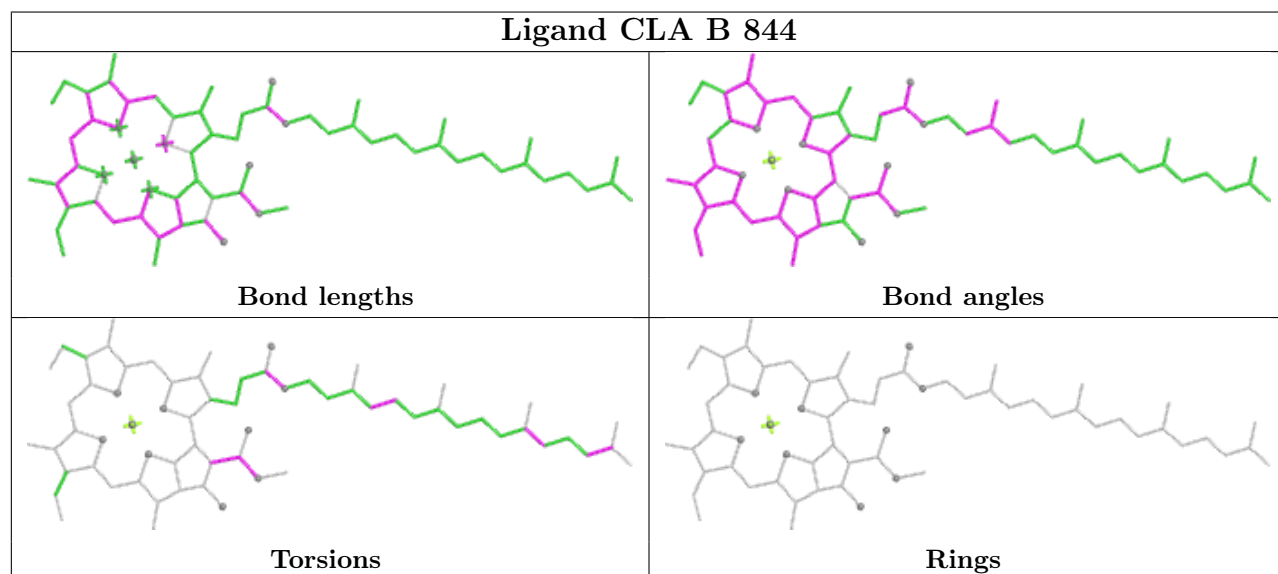
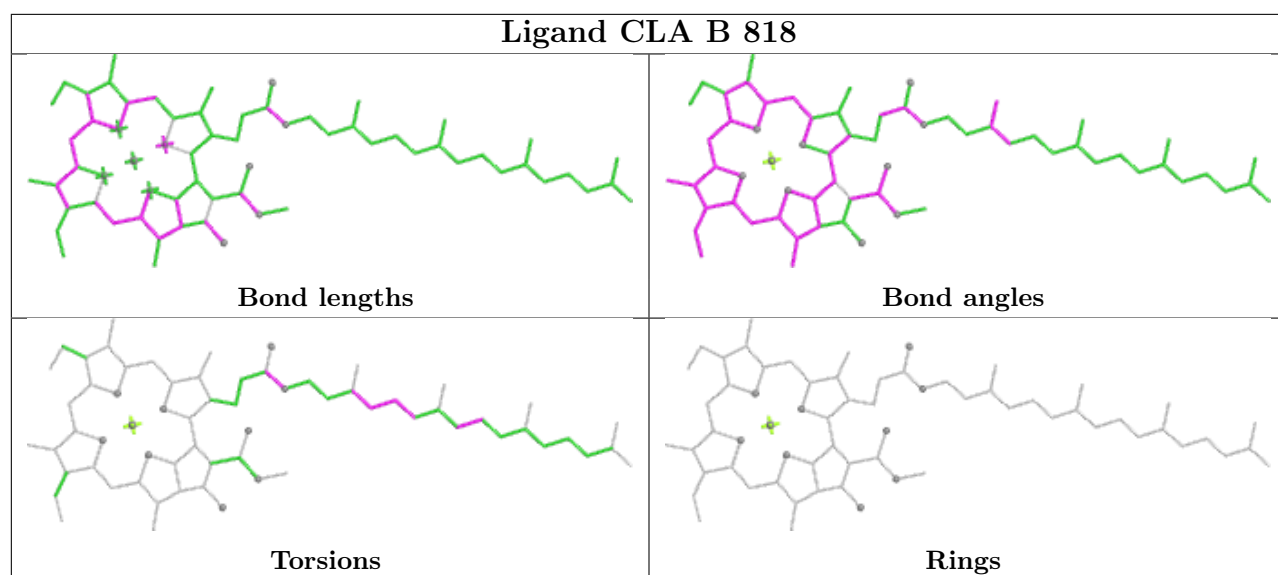


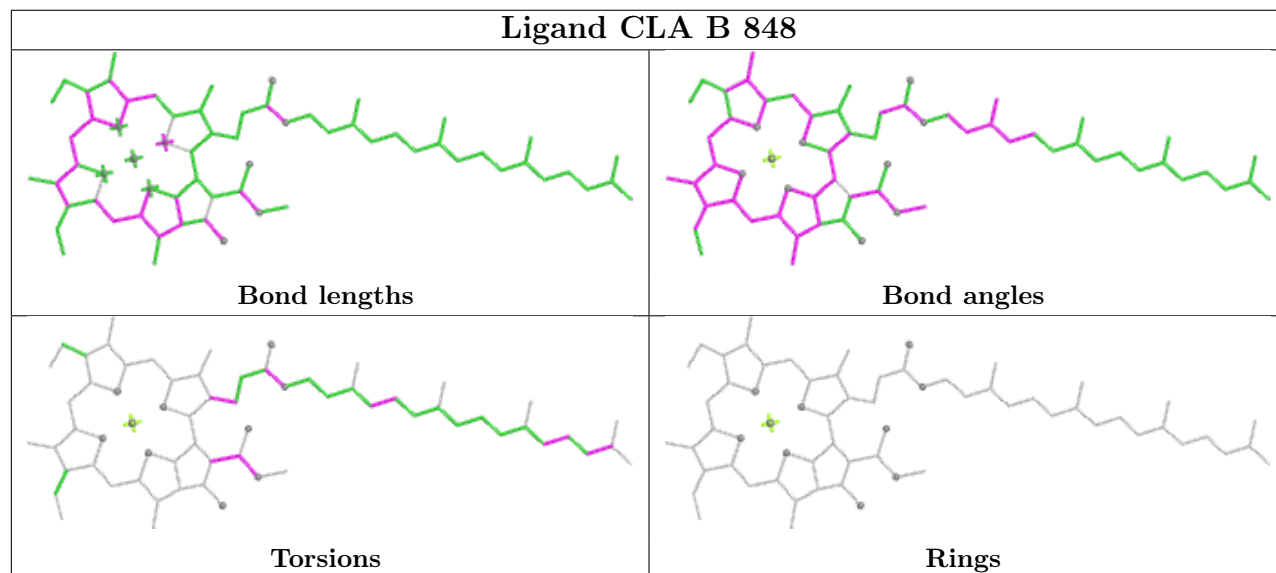
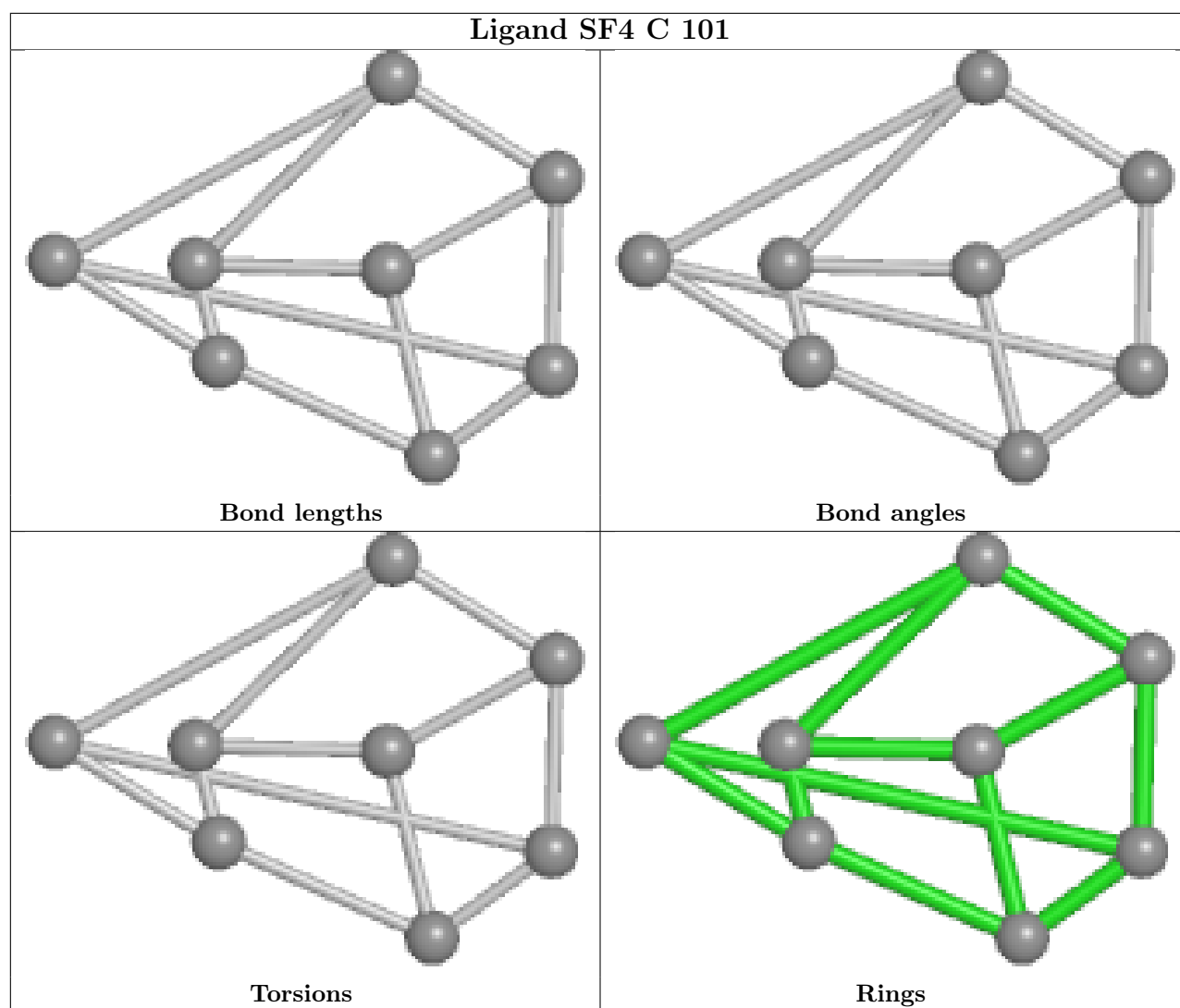
Ligand CLA A 853

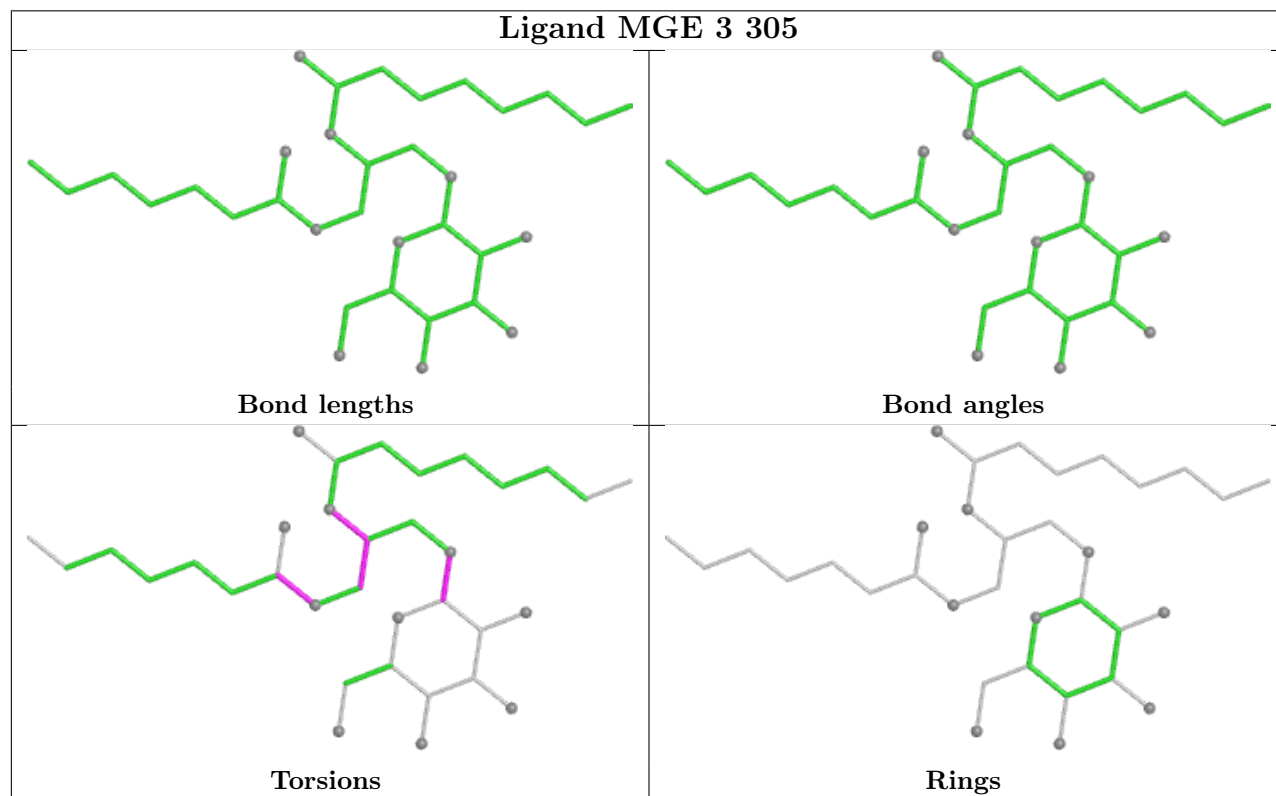
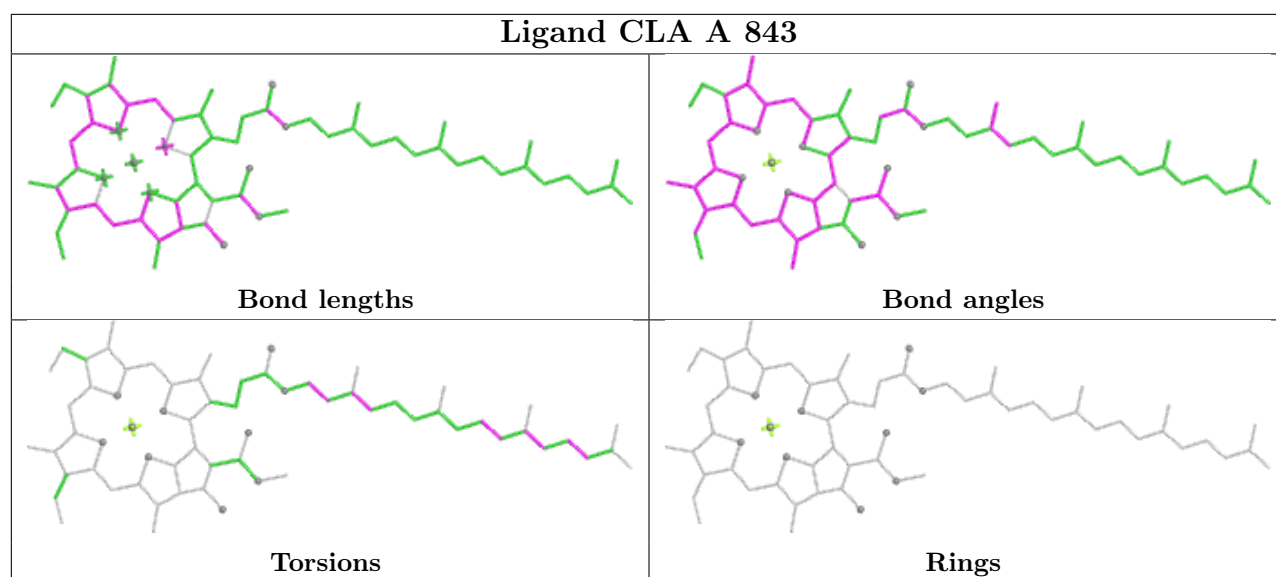


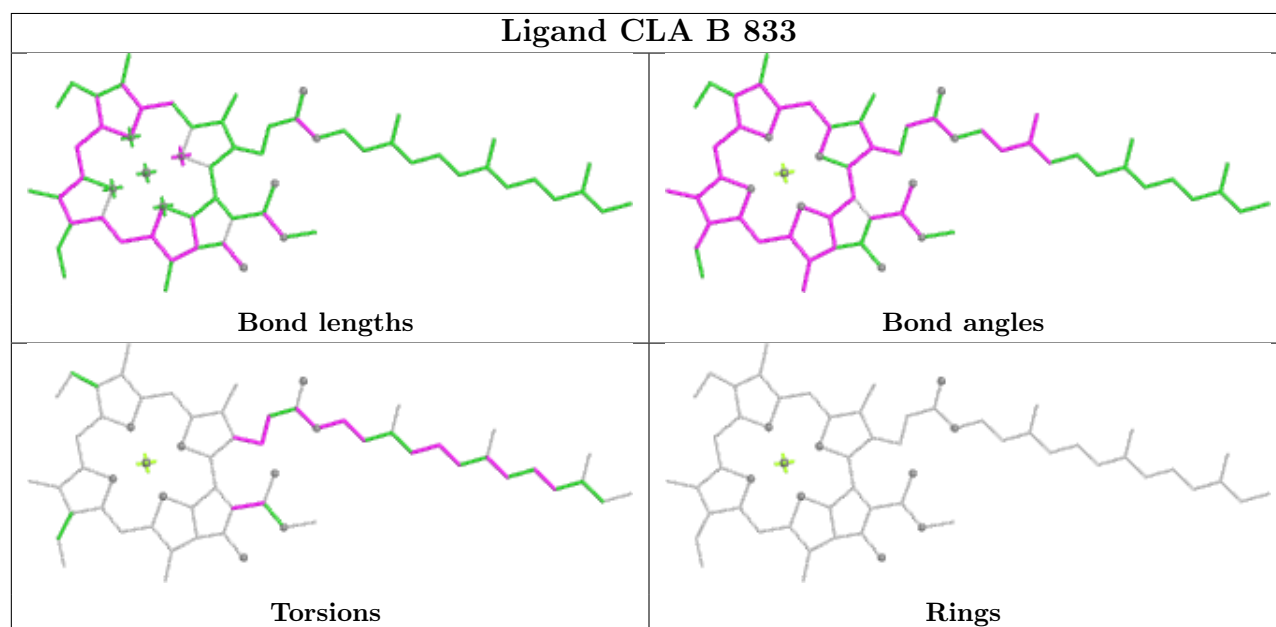
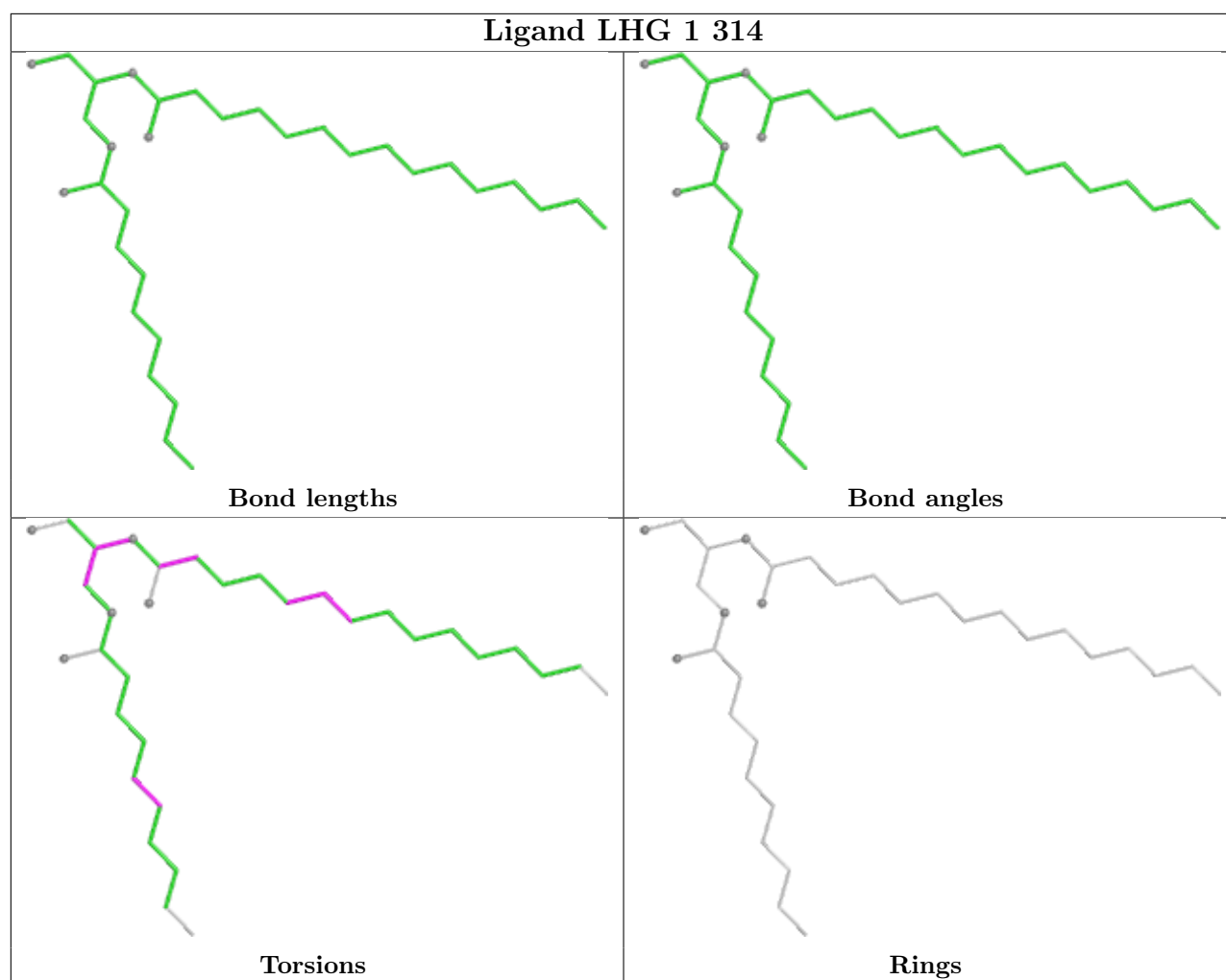
Ligand CLA 2 317

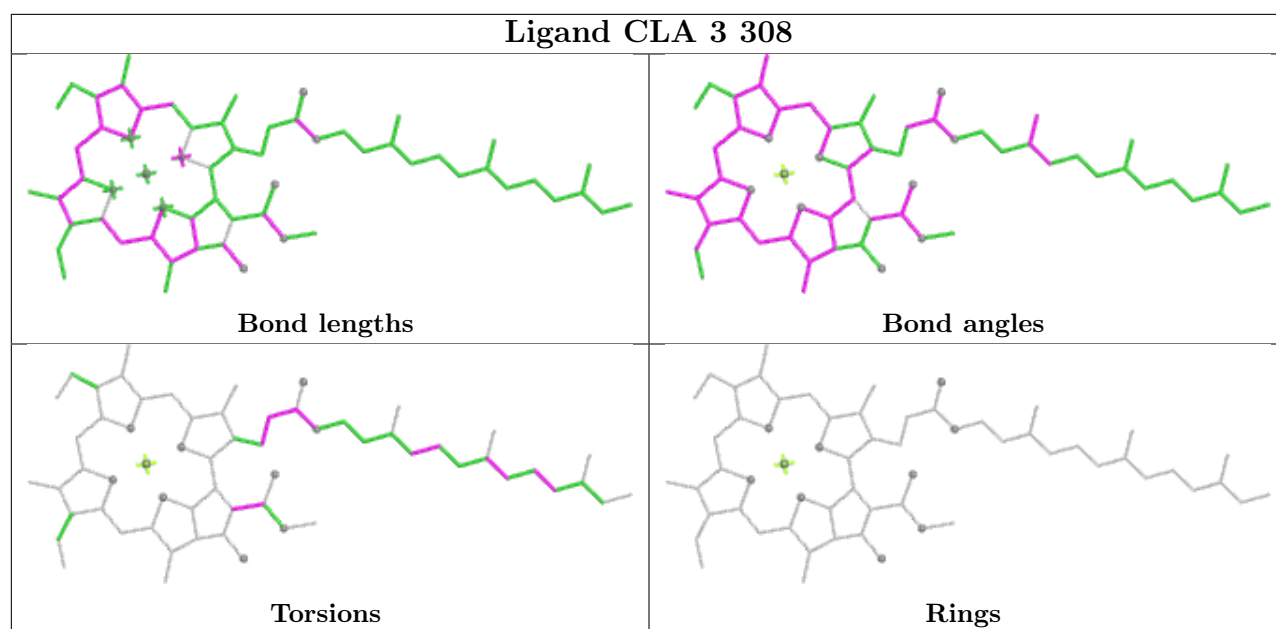


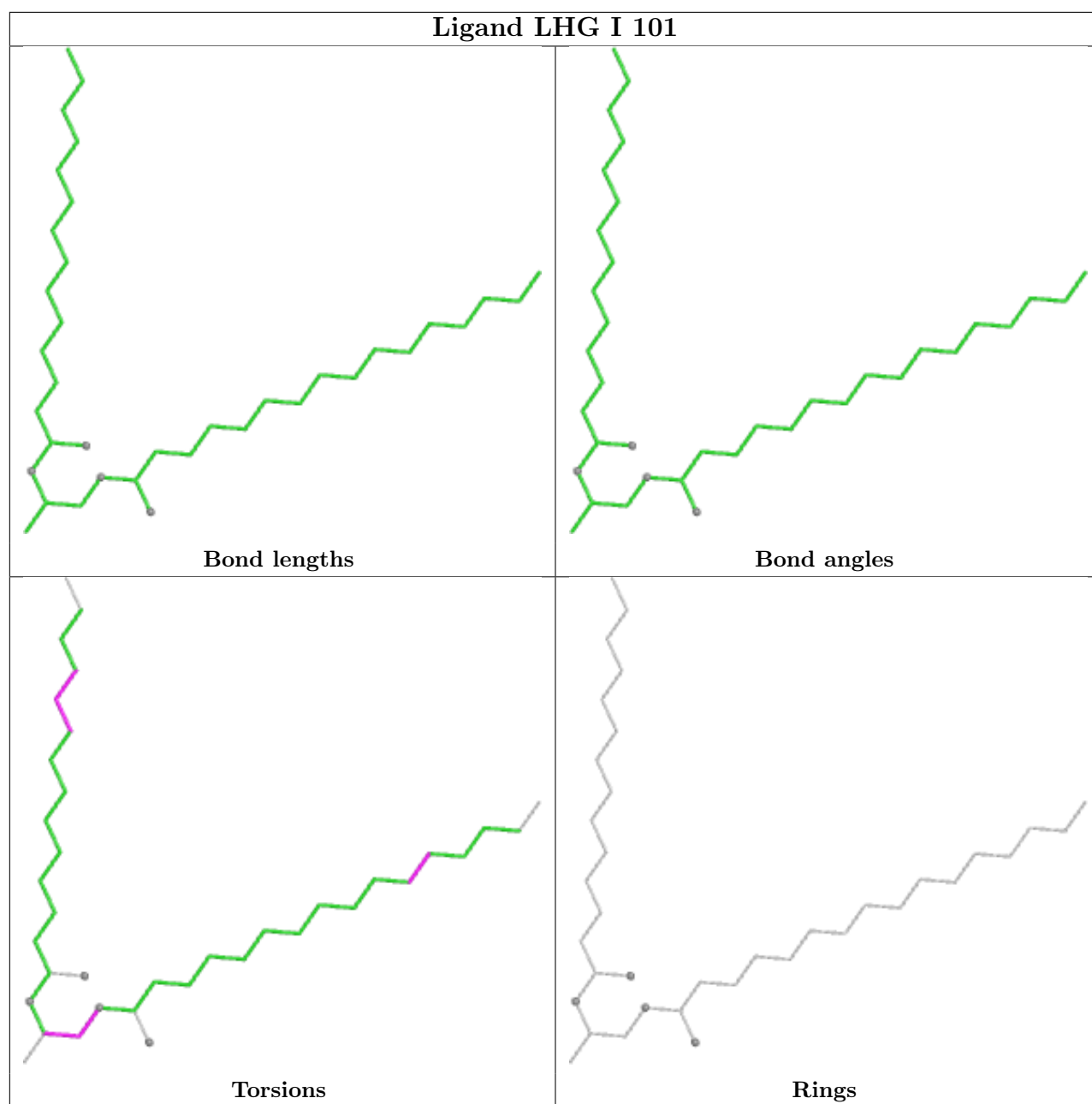


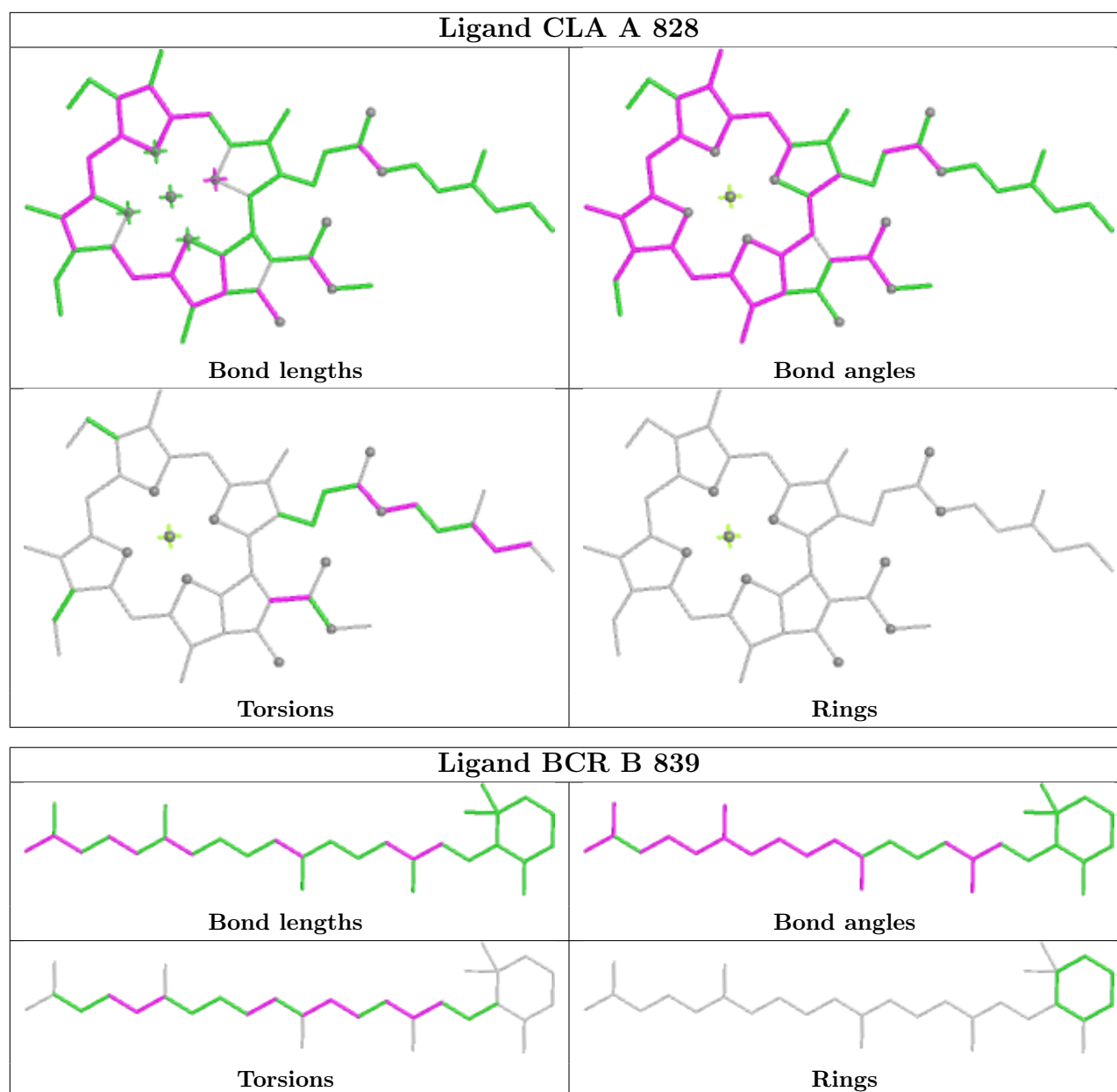


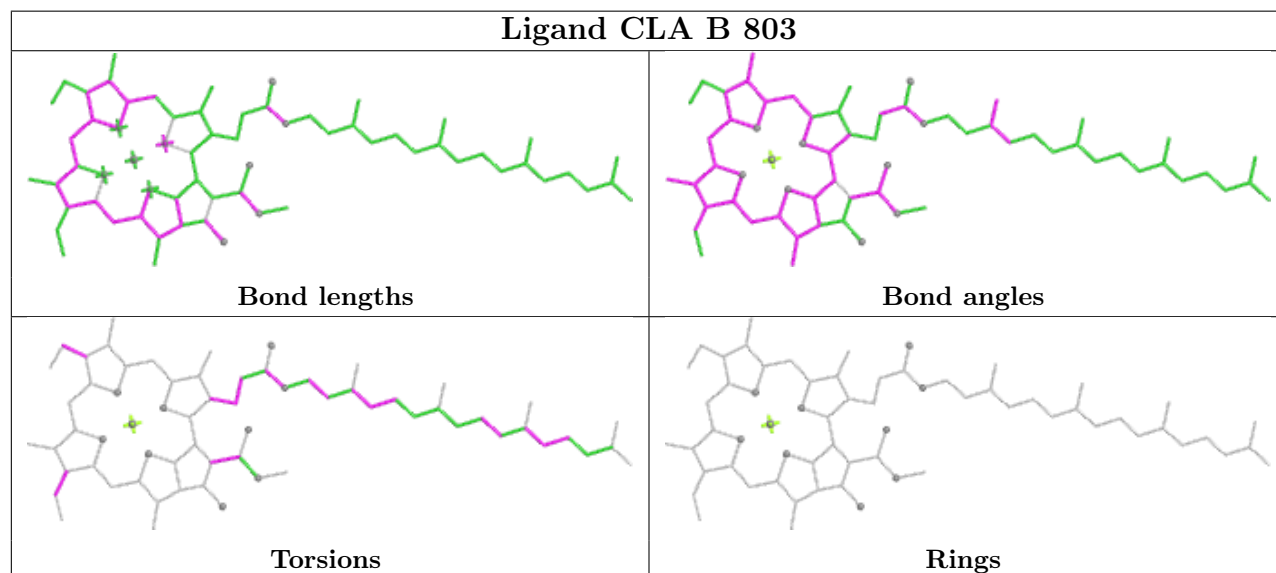
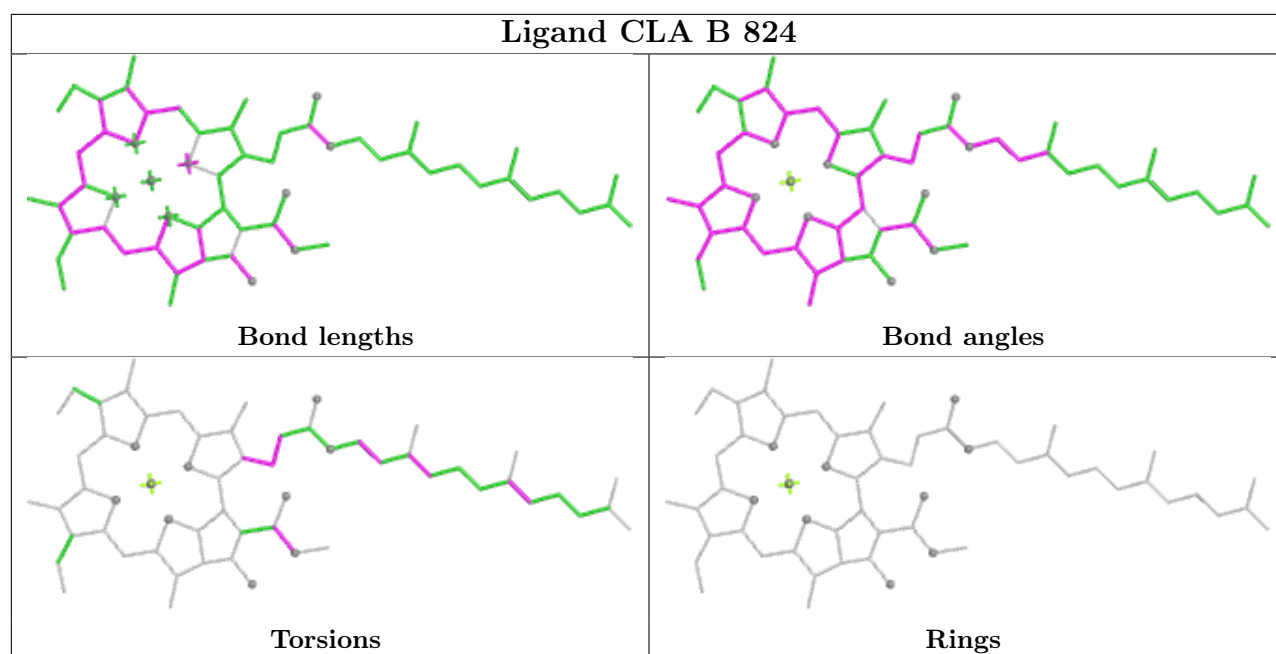


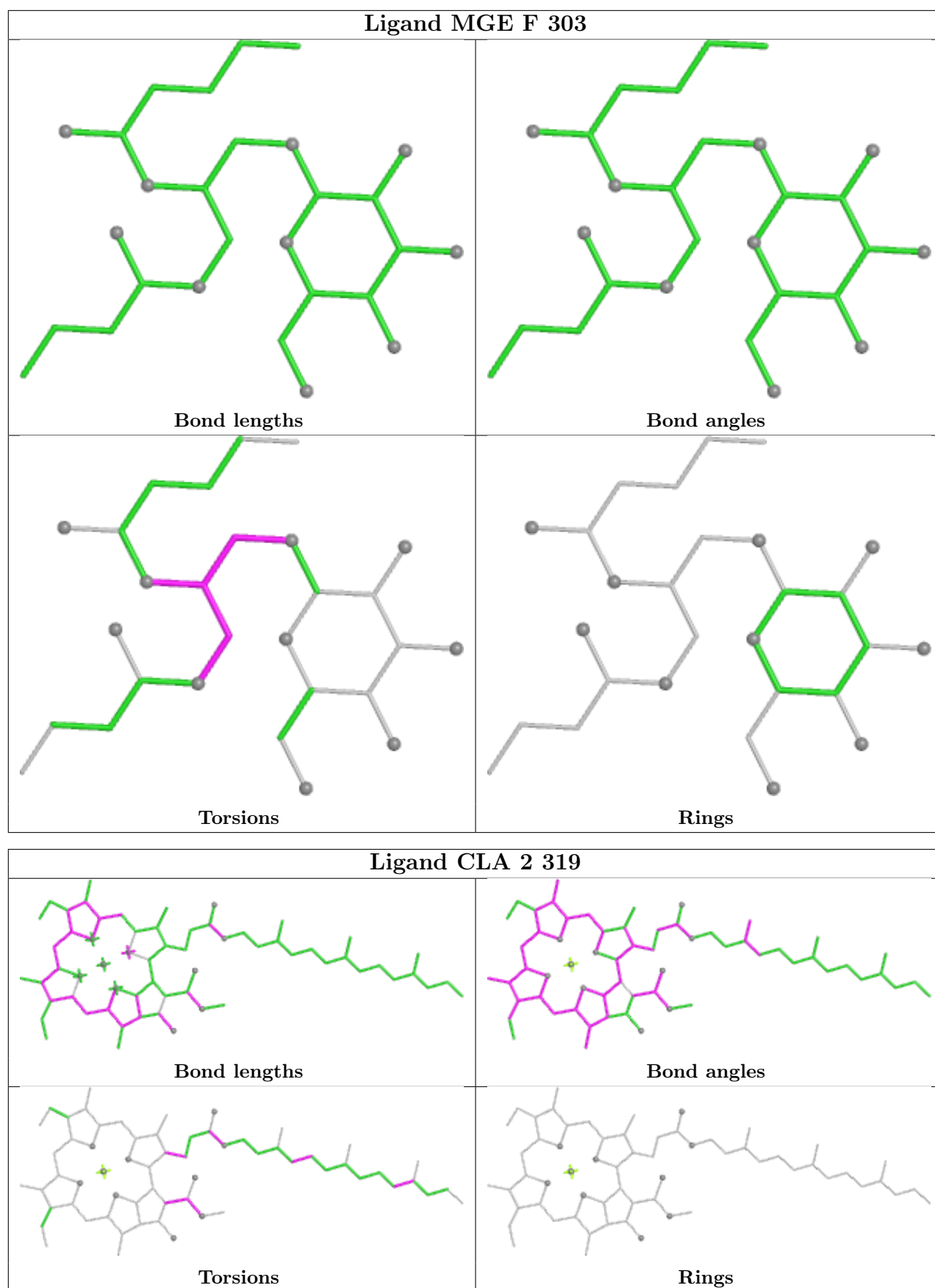


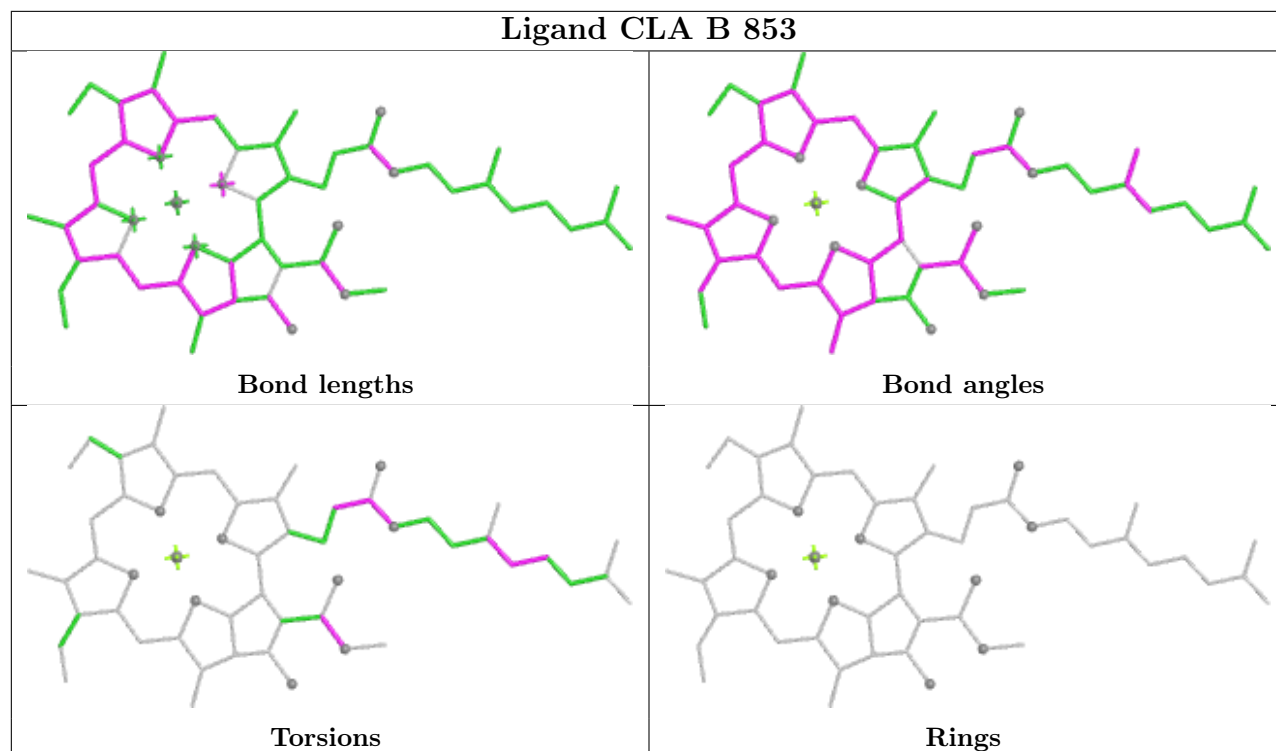
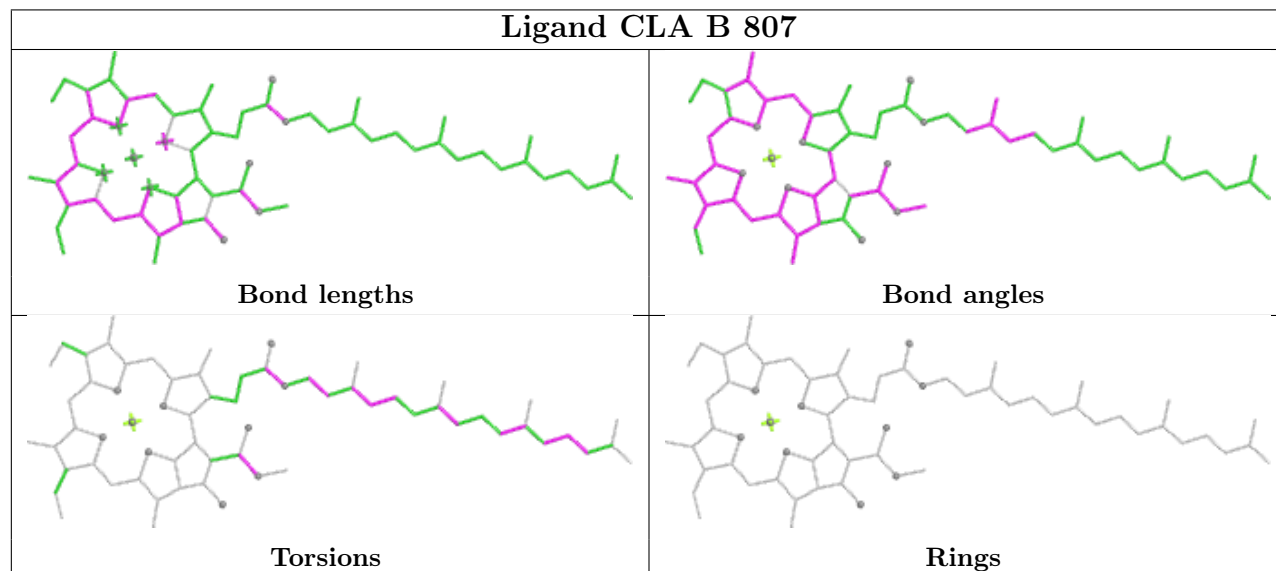




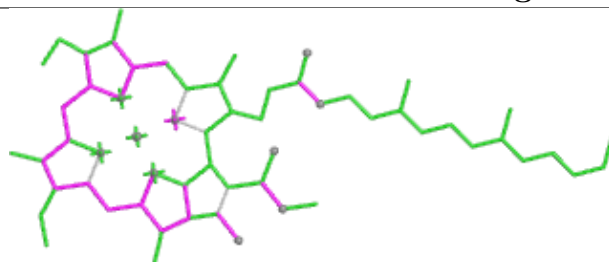




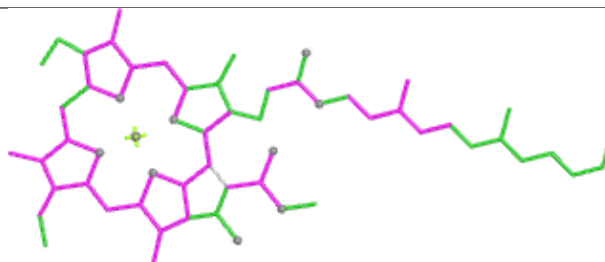


Ligand CLA B 853**Ligand CLA B 807**

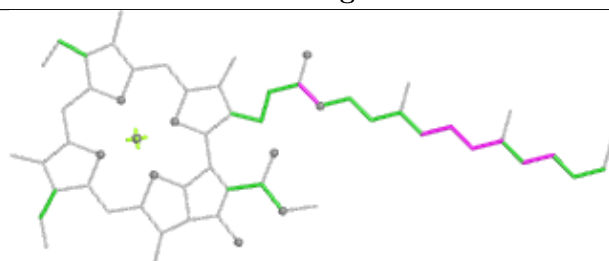
Ligand CLA B 820



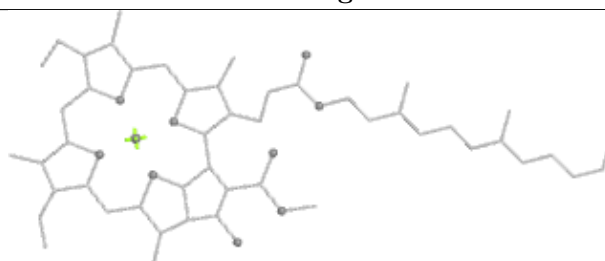
Bond lengths



Bond angles

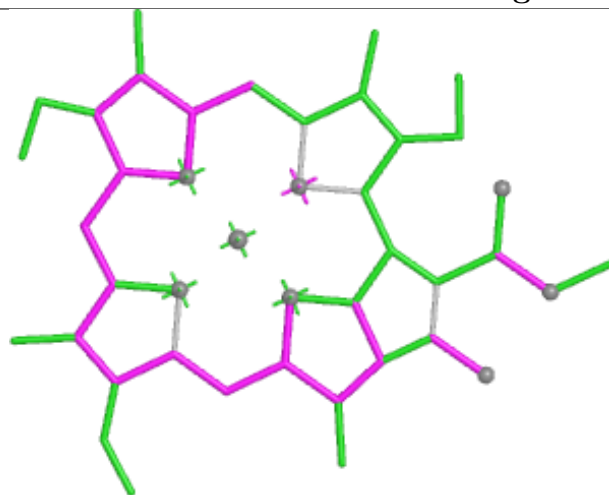


Torsions



Rings

Ligand CLA K 206



Bond lengths



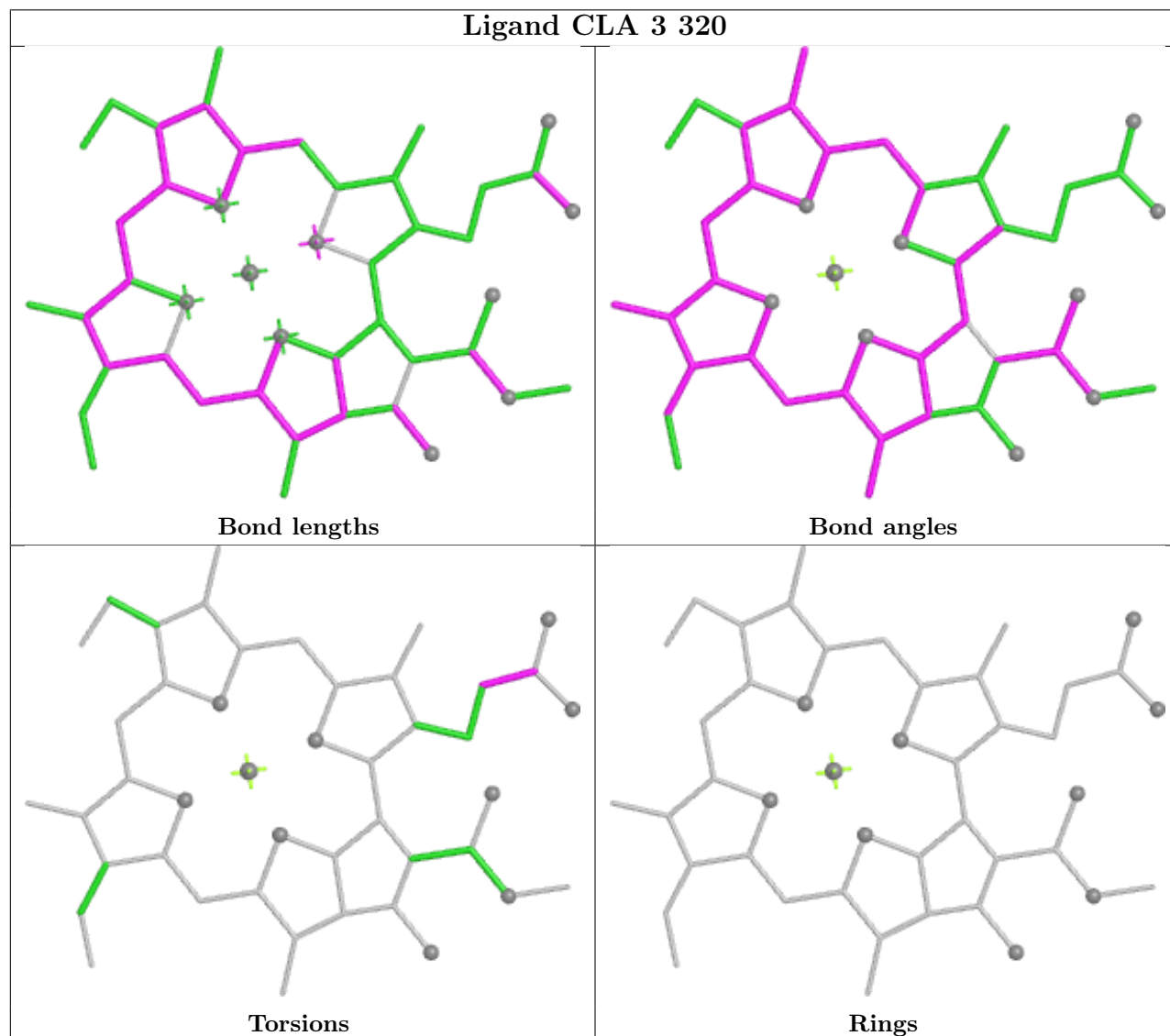
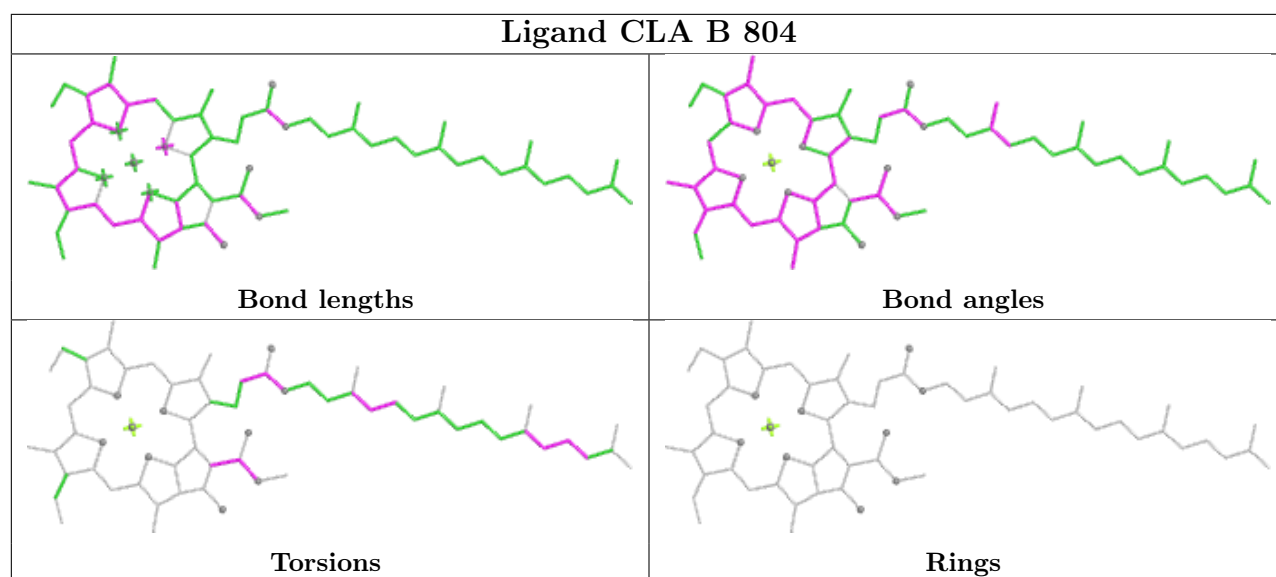
Bond angles

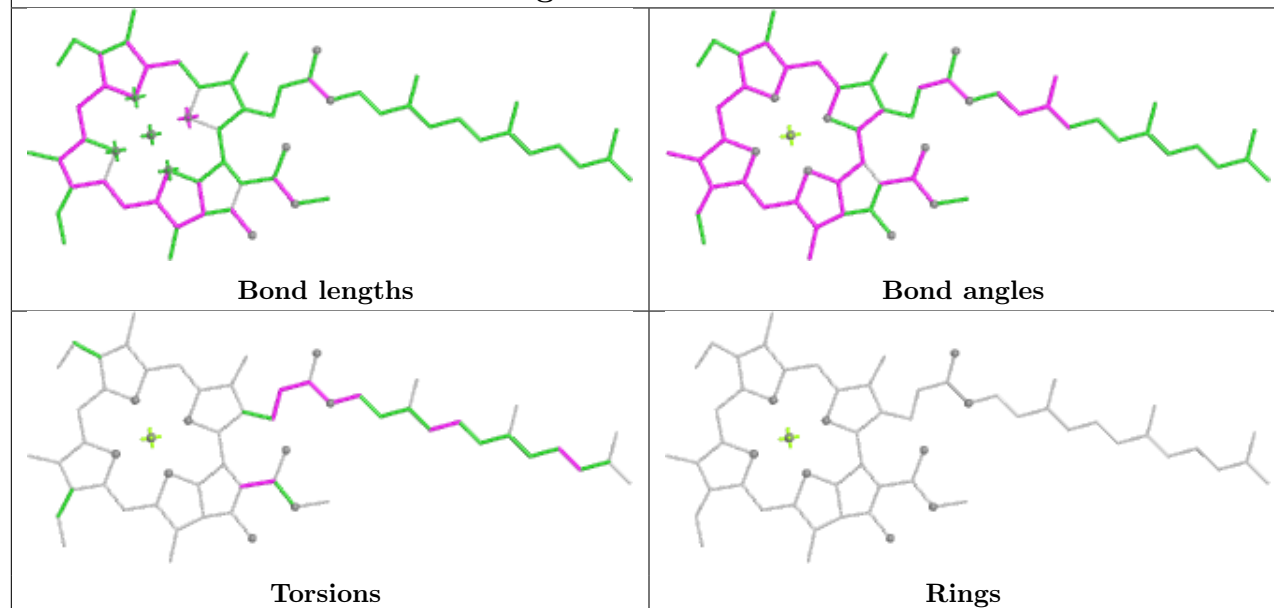
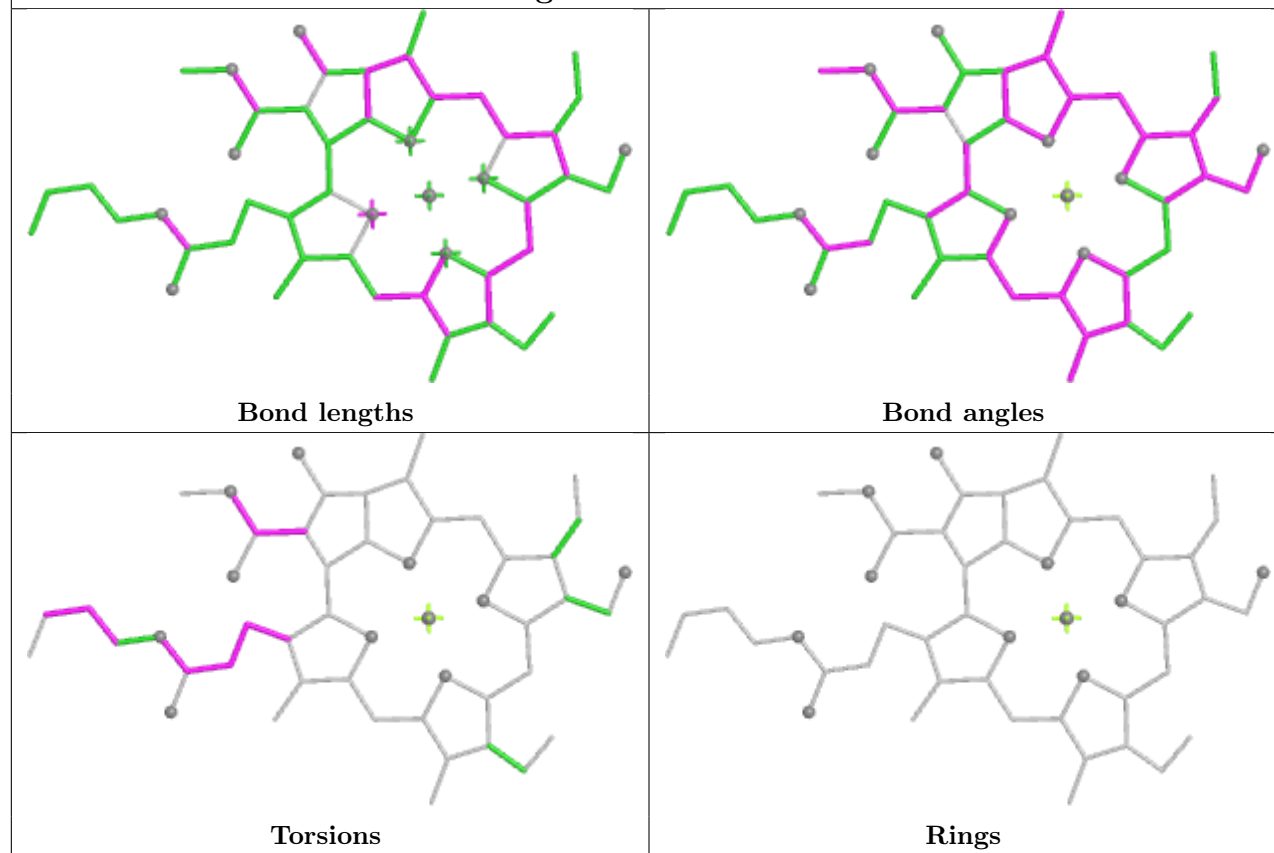


Torsions

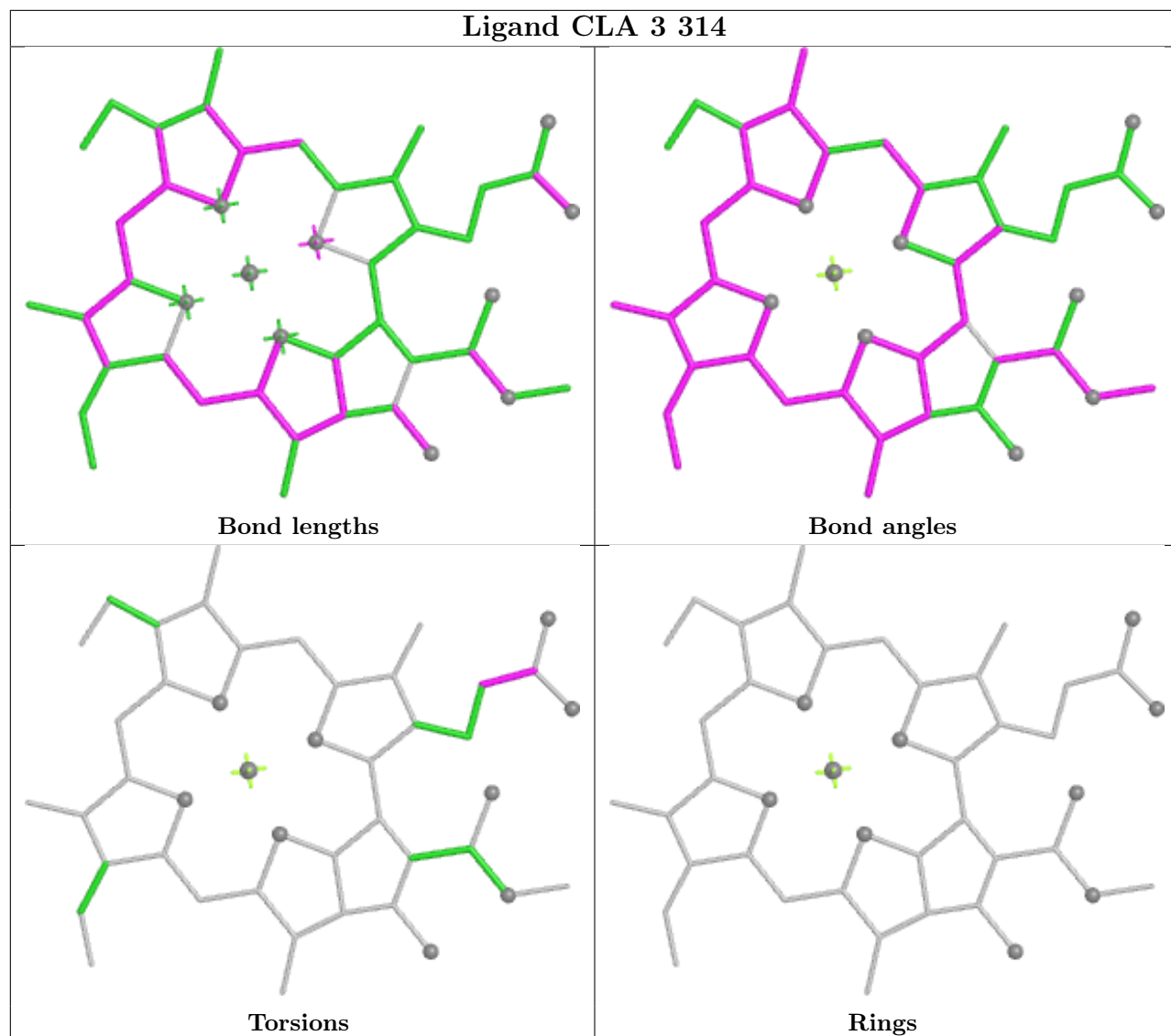


Rings

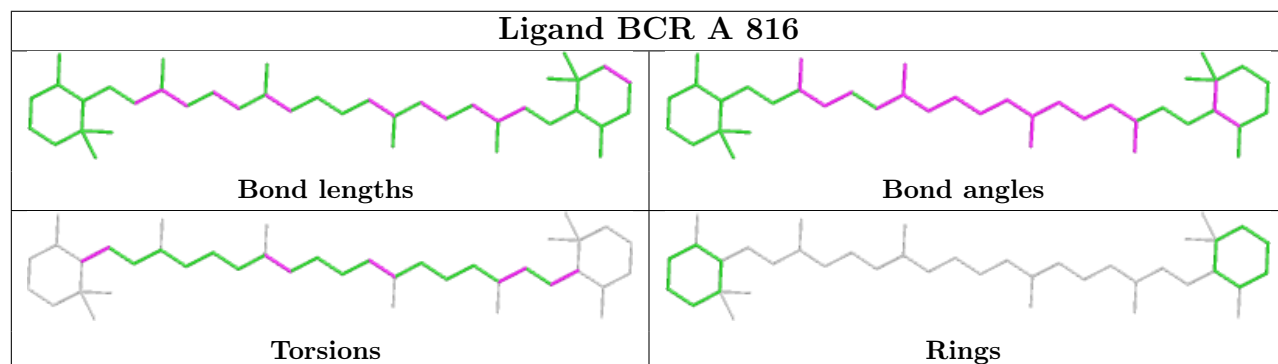


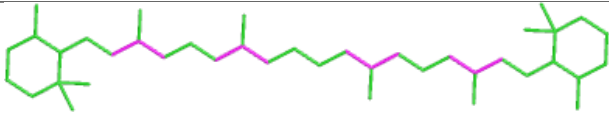
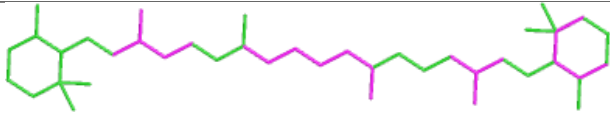
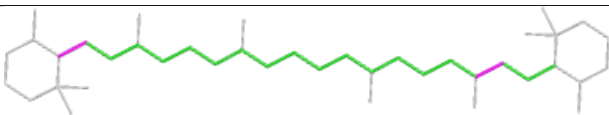
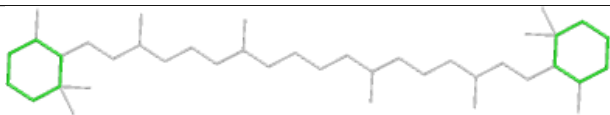
Ligand CLA 4 310**Ligand CHL 3 313**

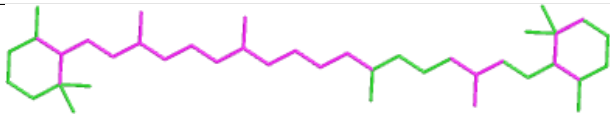
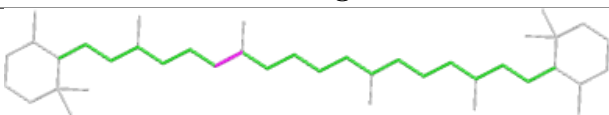
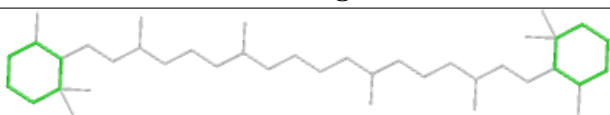
Ligand CLA 3 314

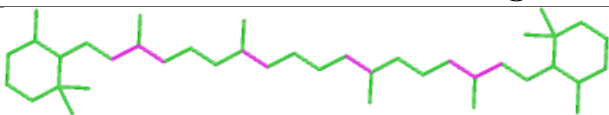
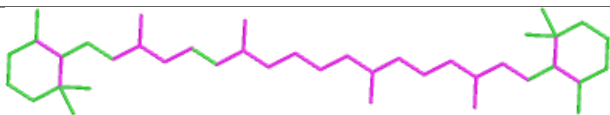
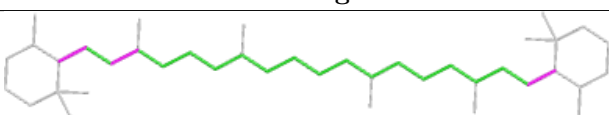
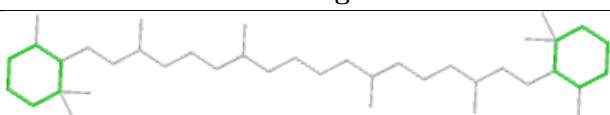


Ligand BCR A 816

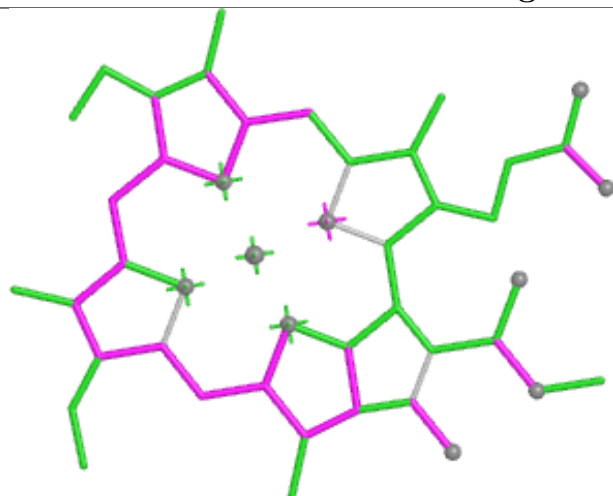


Ligand BCR I 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

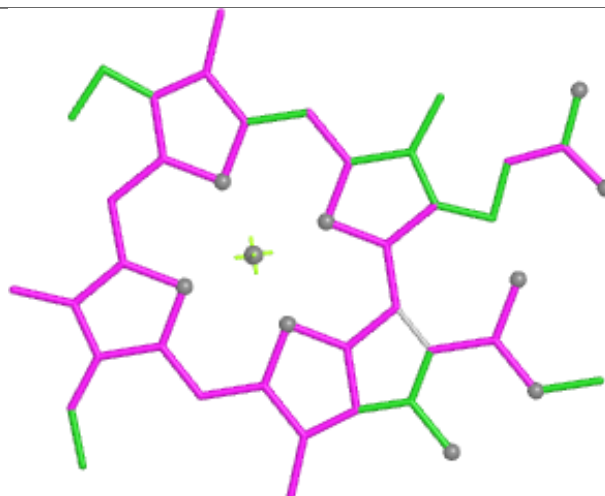
Ligand BCR O 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 836	
	
Bond lengths	Bond angles
	
Torsions	Rings

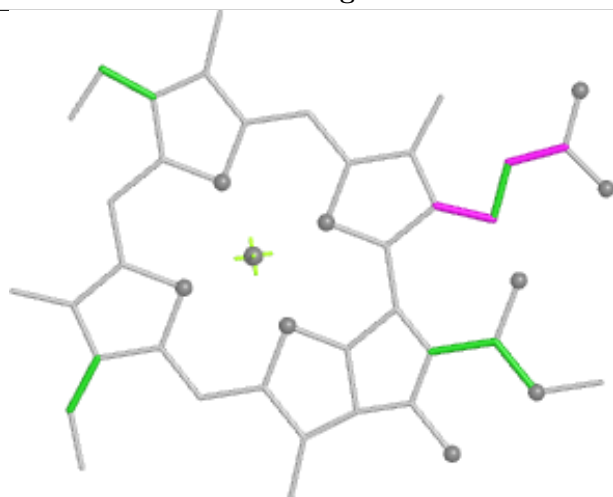
Ligand CLA 1 306



Bond lengths



Bond angles

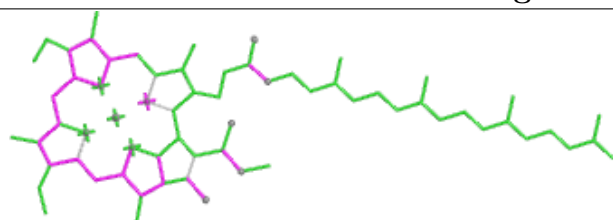


Torsions

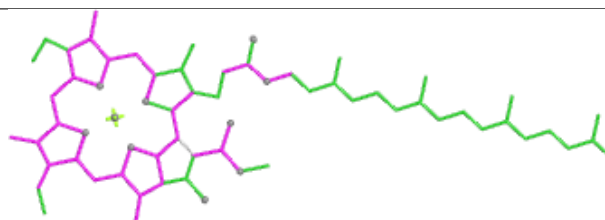


Rings

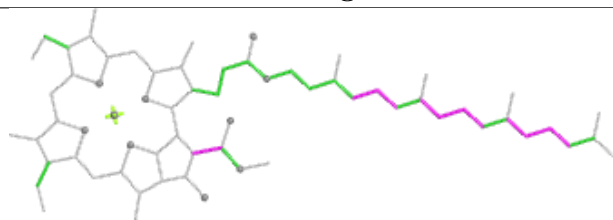
Ligand CLA O 206



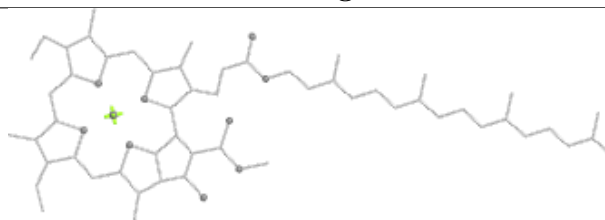
Bond lengths



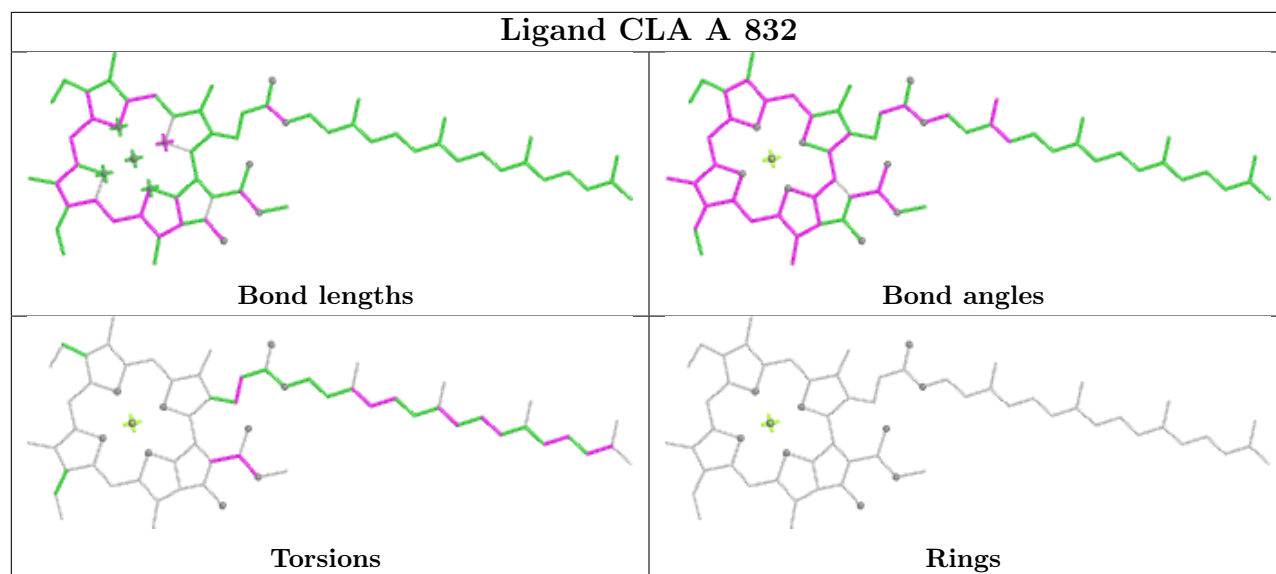
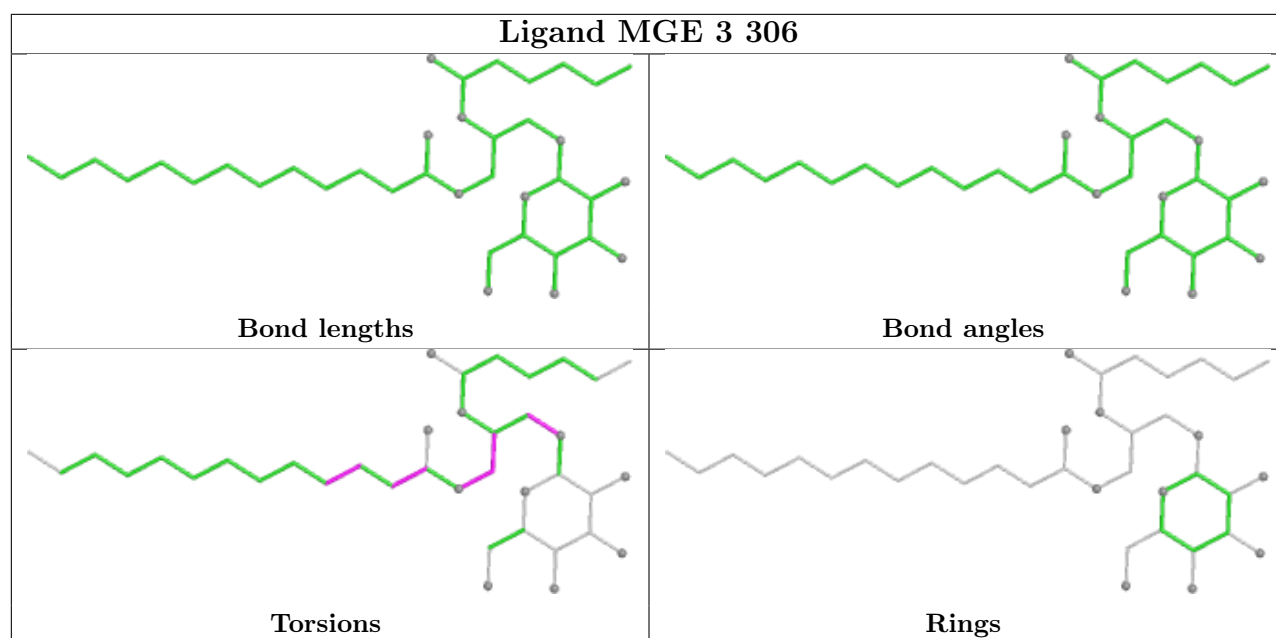
Bond angles

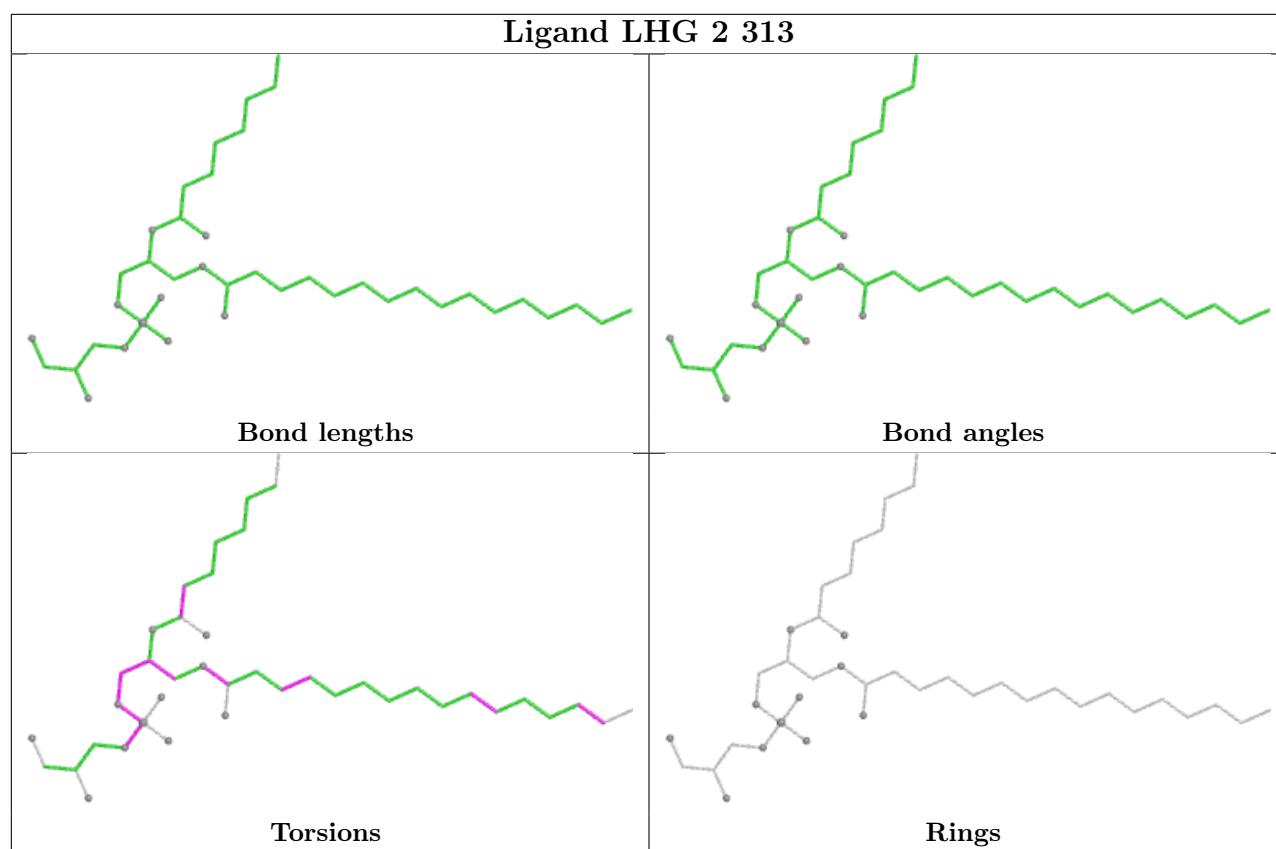


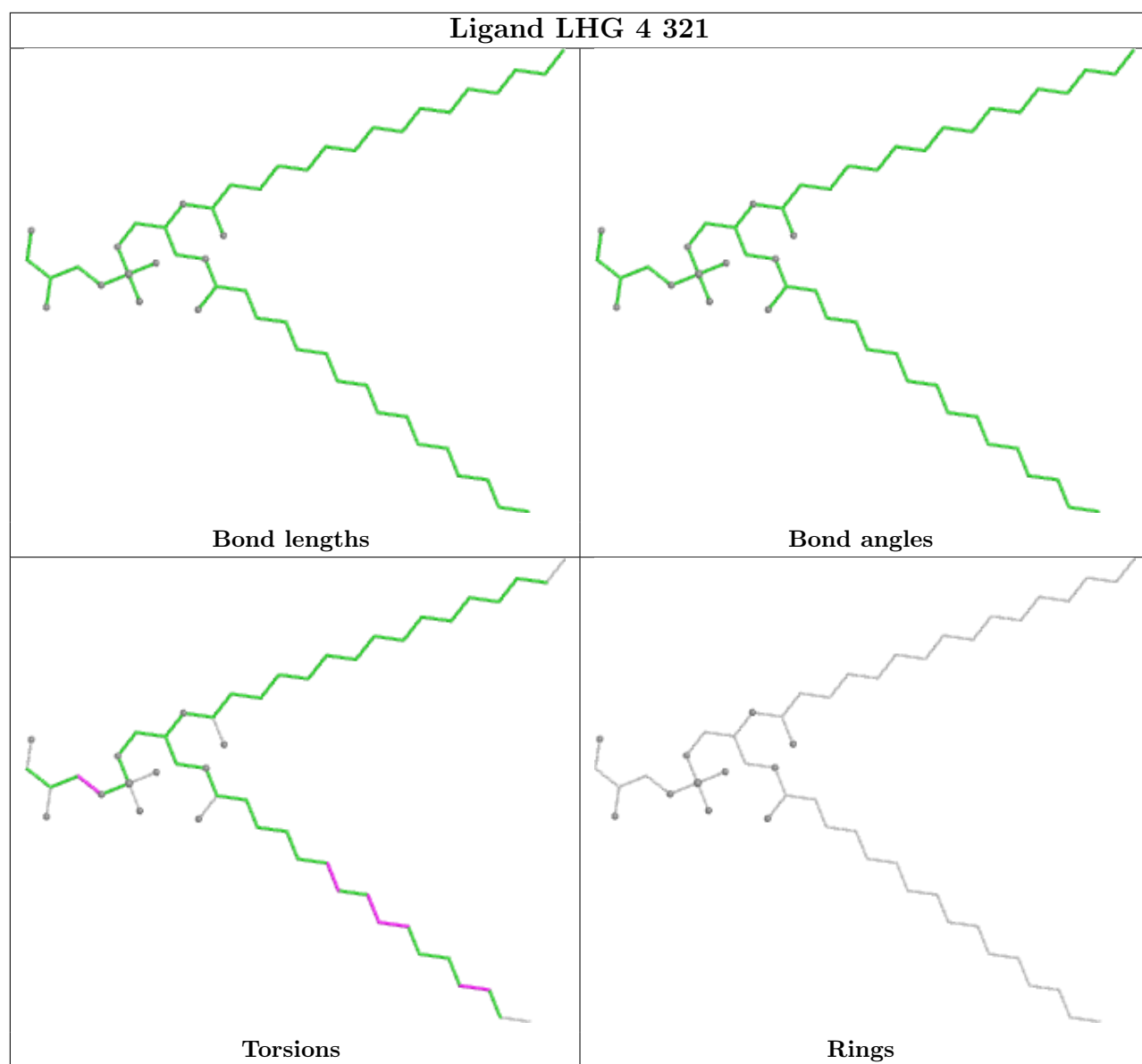
Torsions

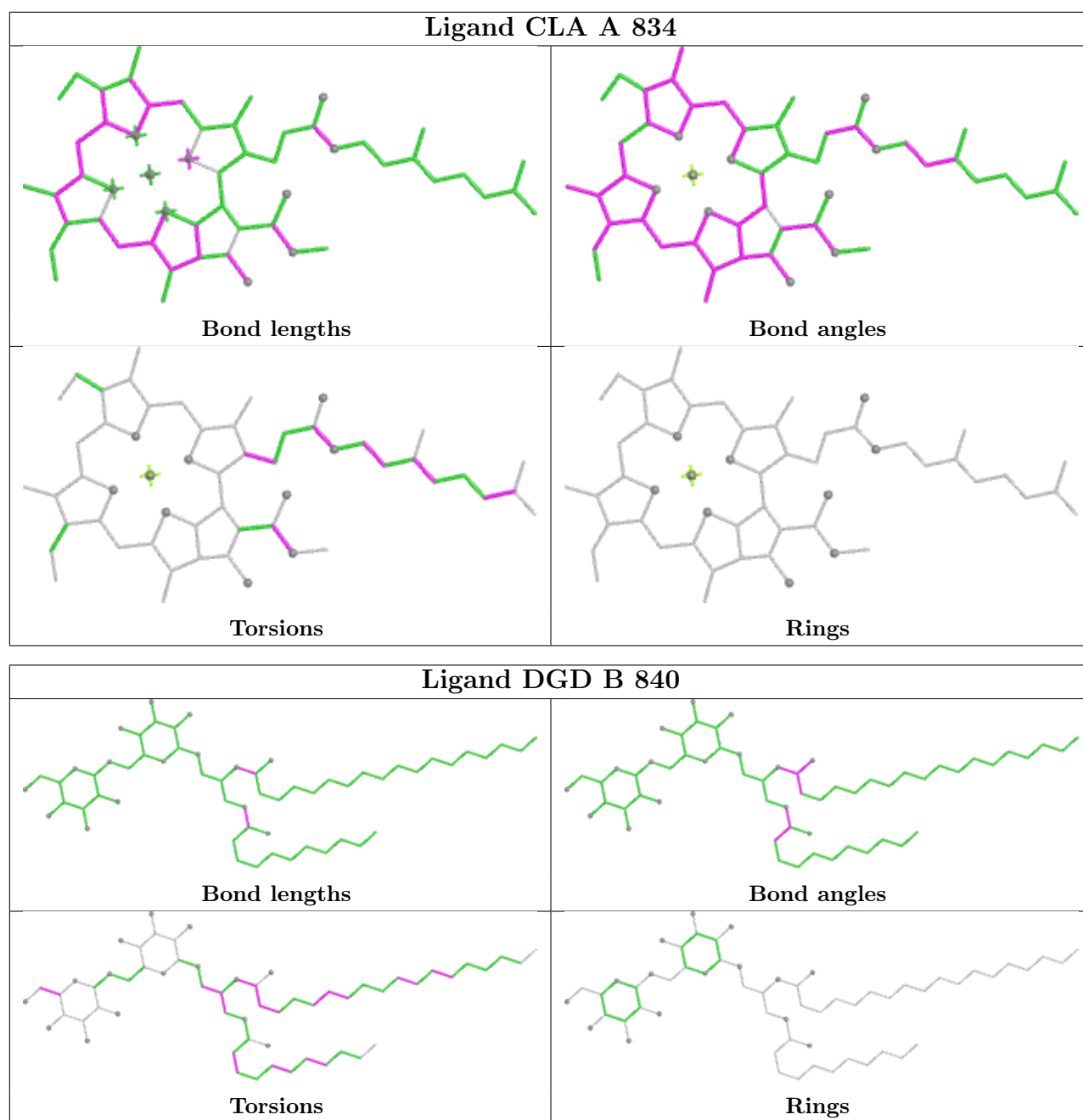


Rings

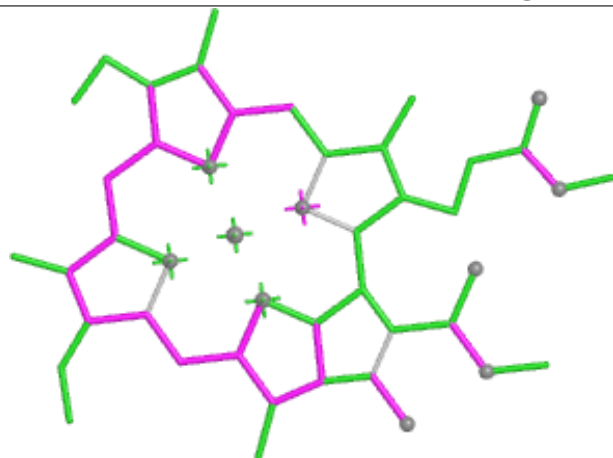




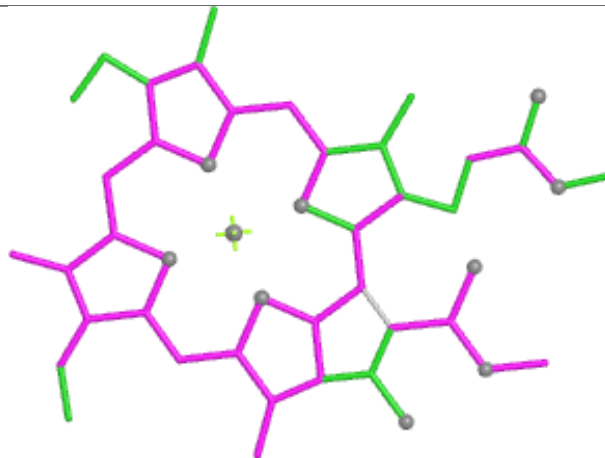




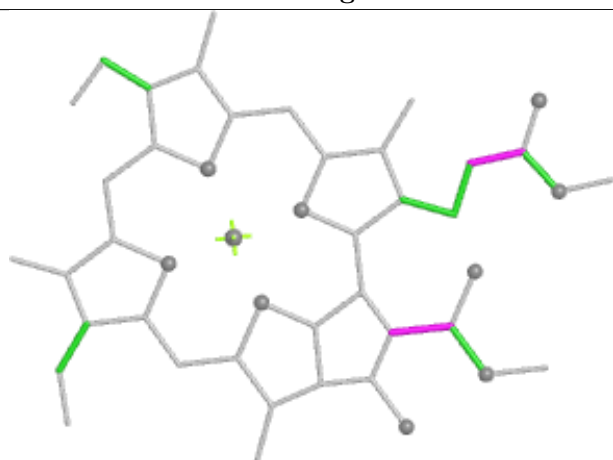
Ligand CLA 2 323



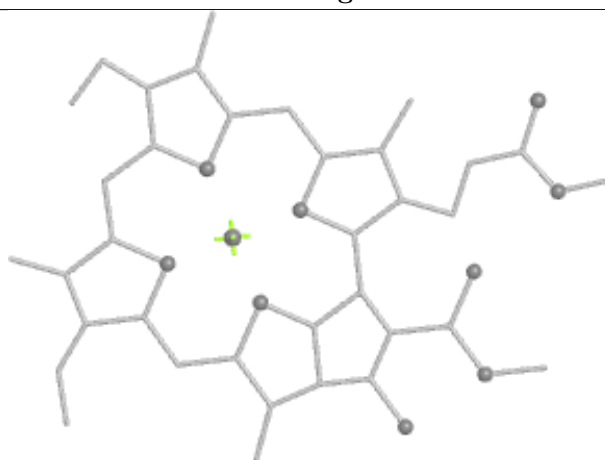
Bond lengths



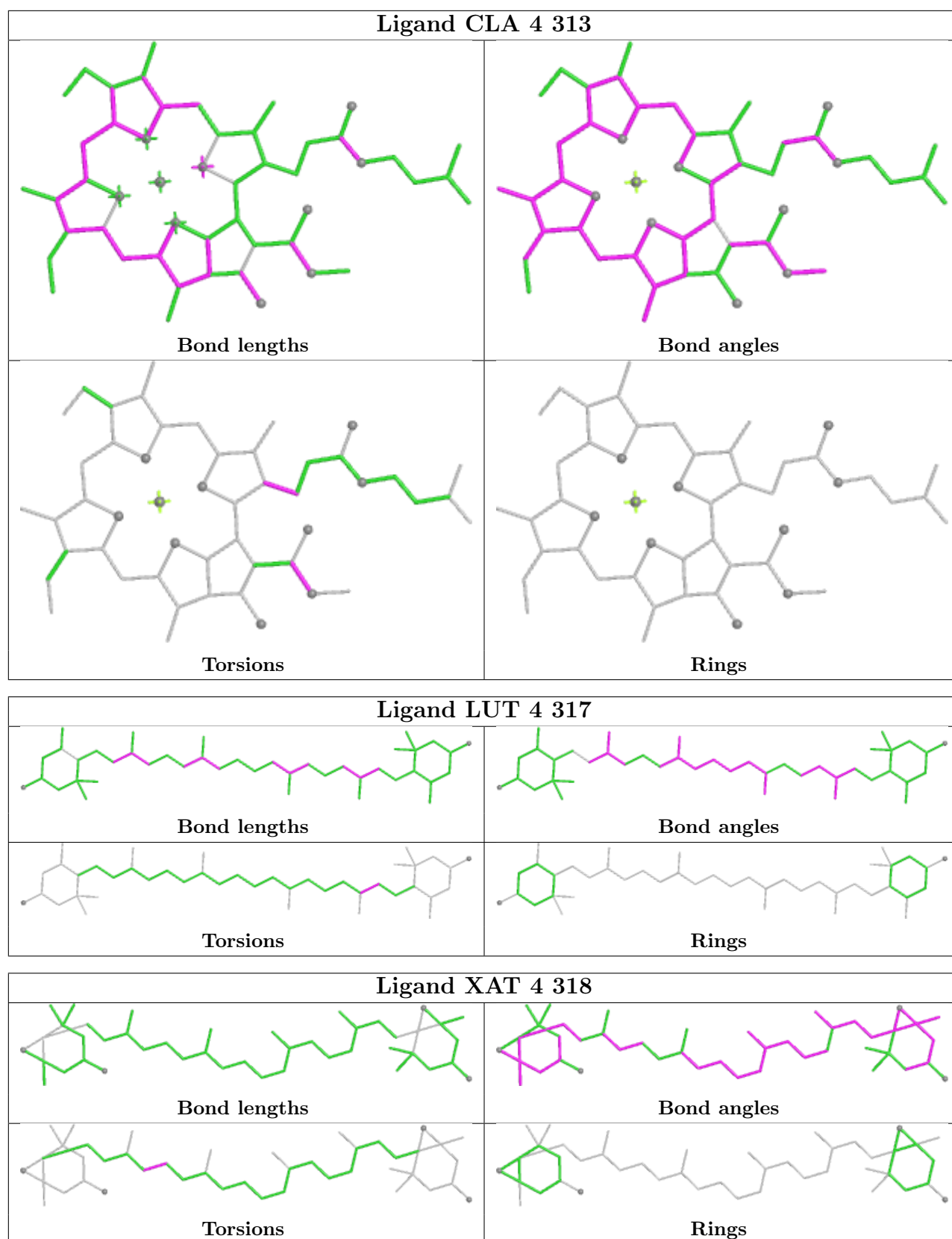
Bond angles

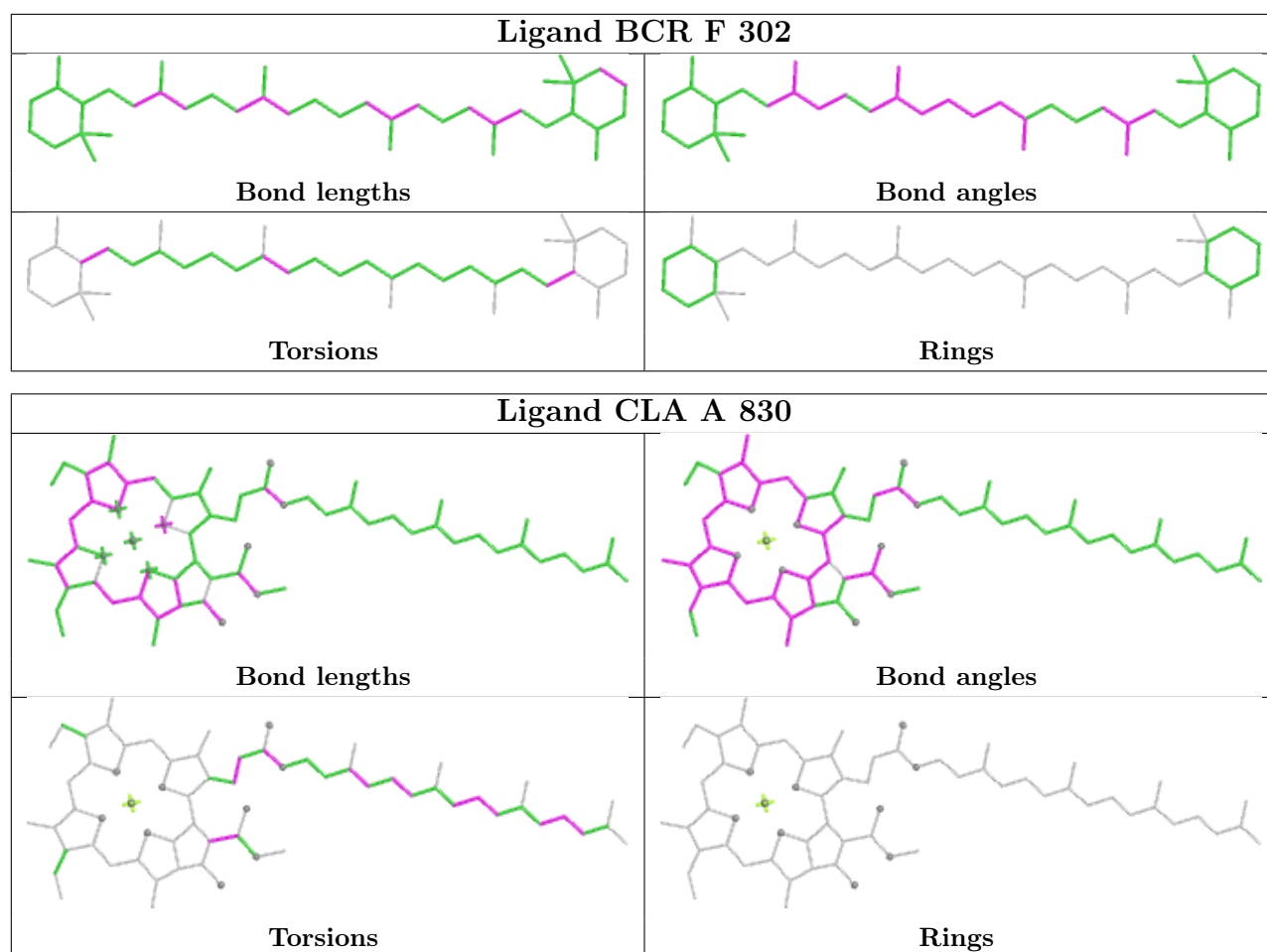


Torsions

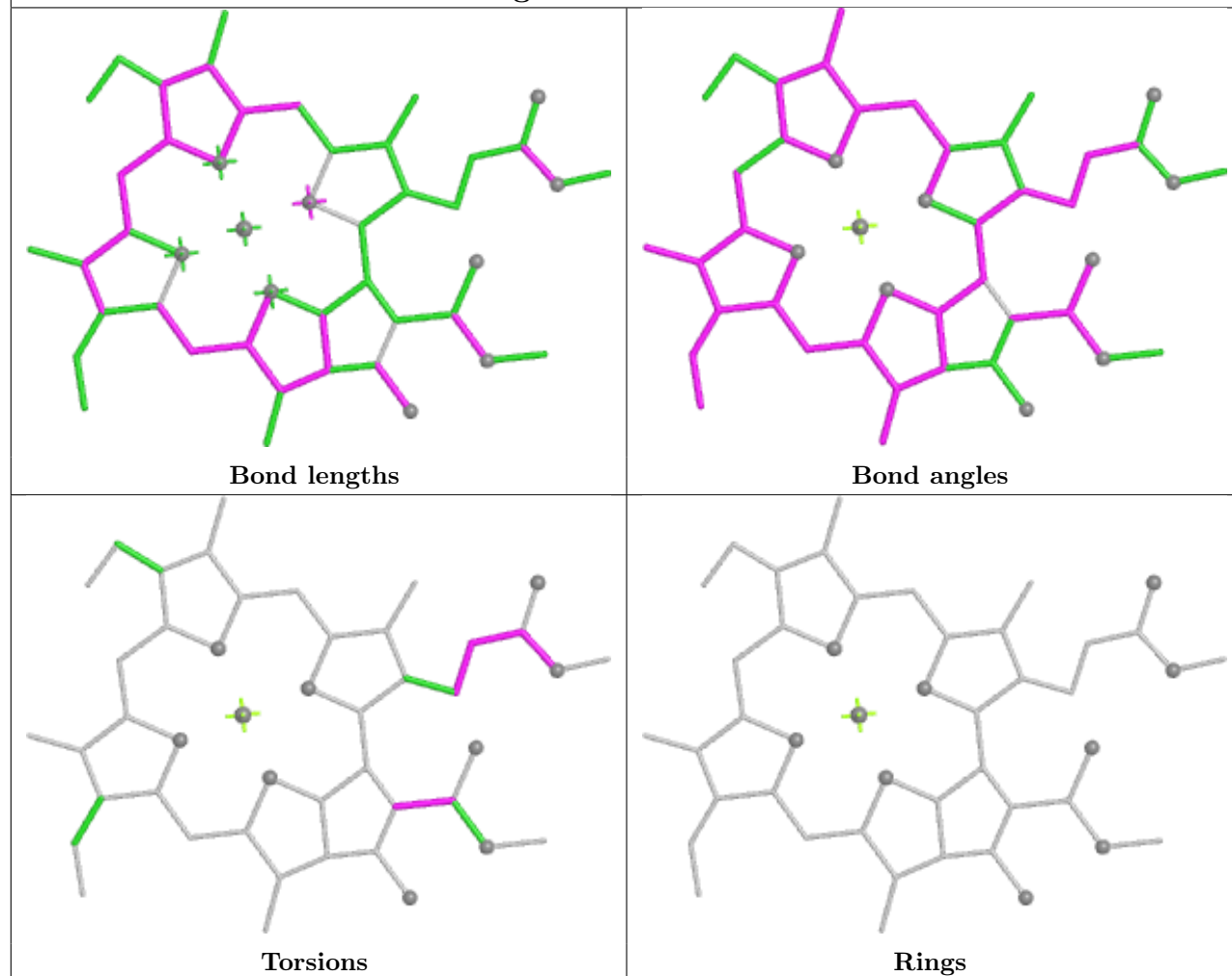


Rings

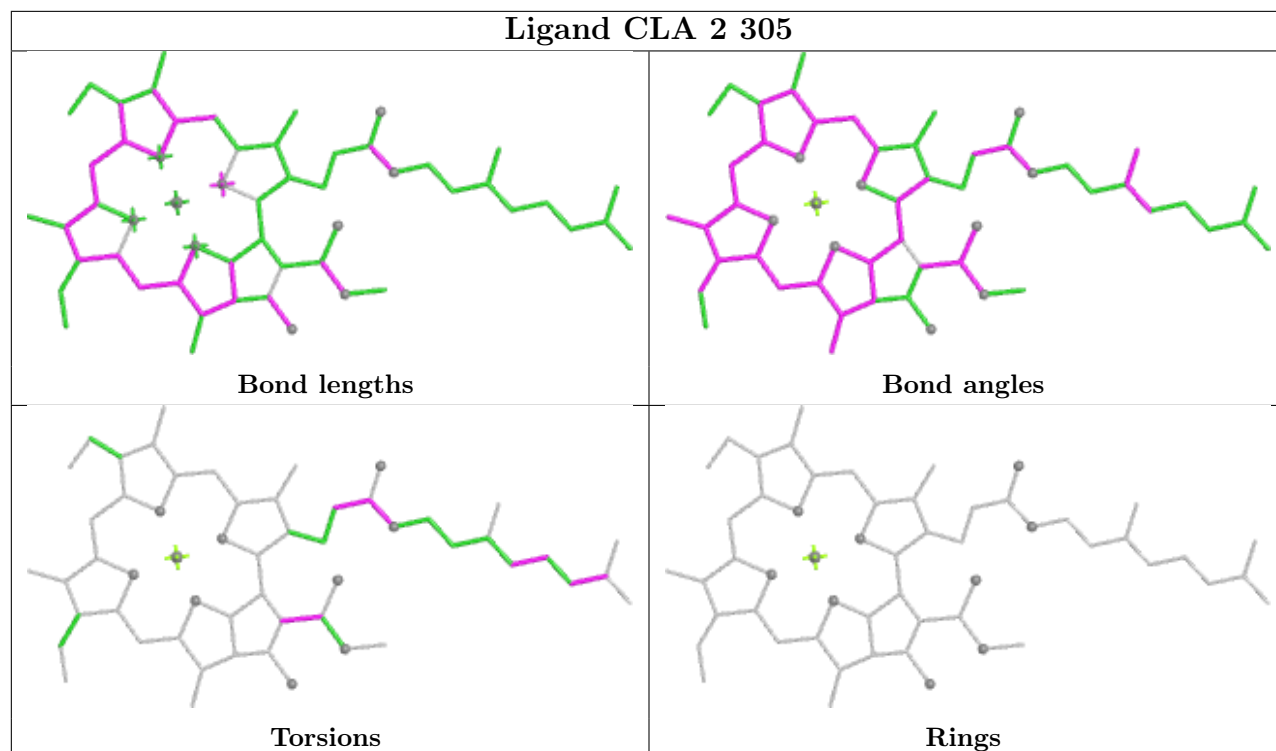




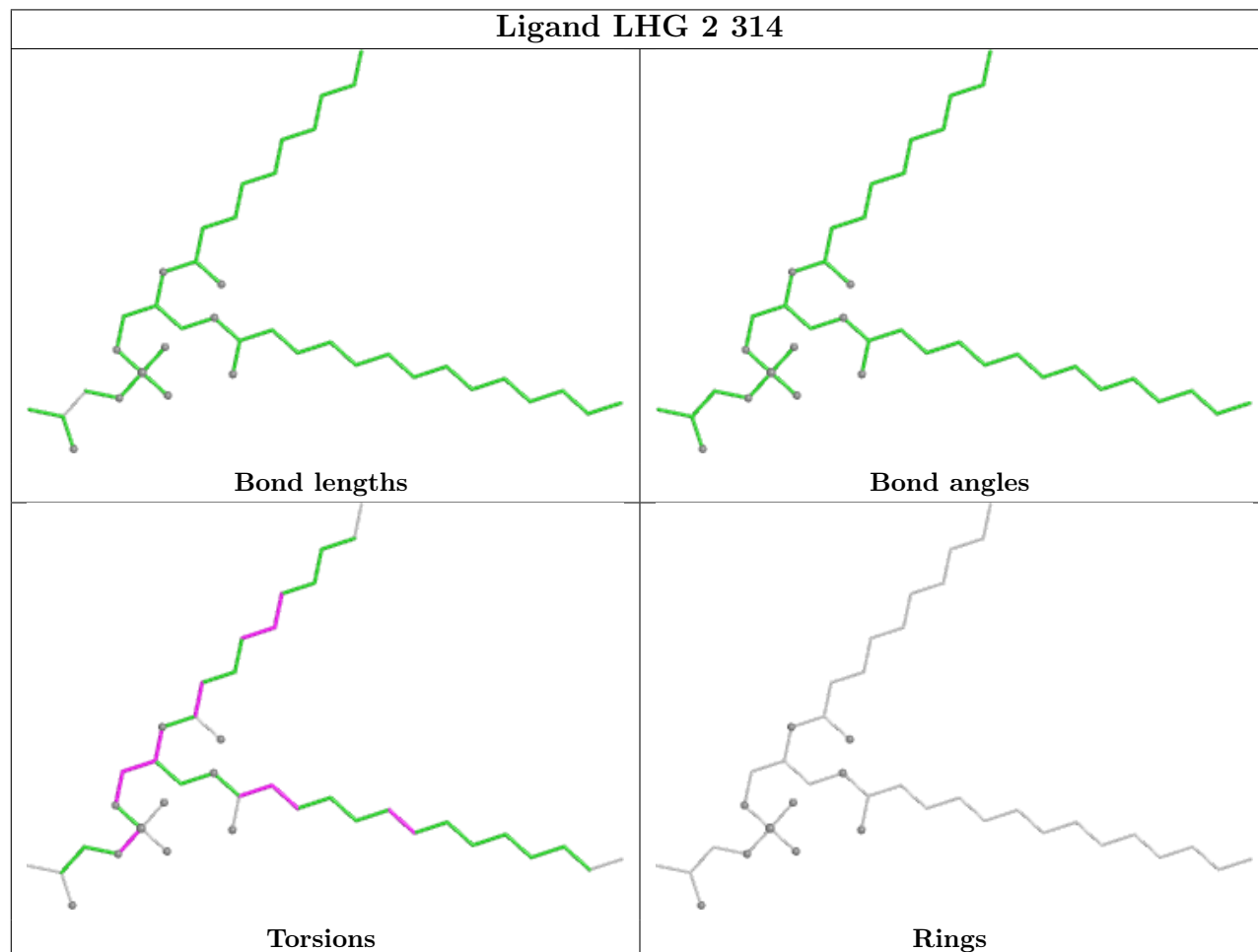
Ligand CLA A 844

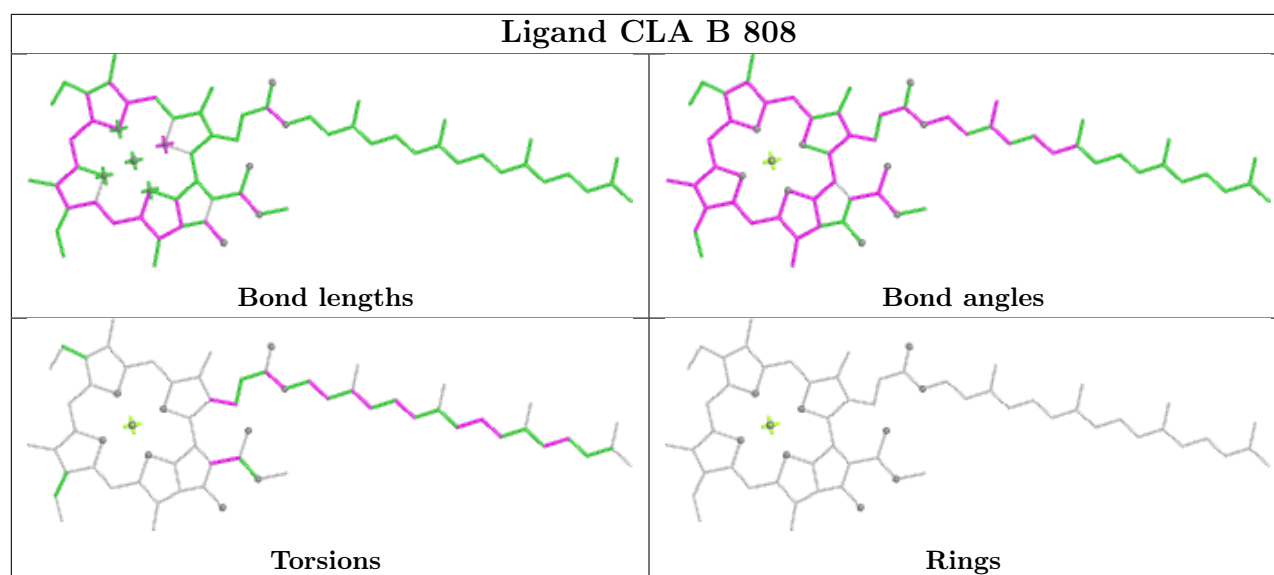


Ligand CLA 2 305



Ligand LHG 2 314





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.

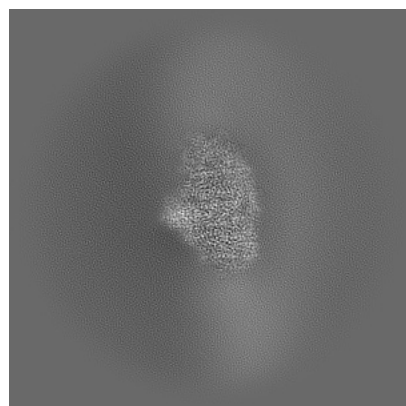
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66925. These allow visual inspection of the internal detail of the map and identification of artifacts.

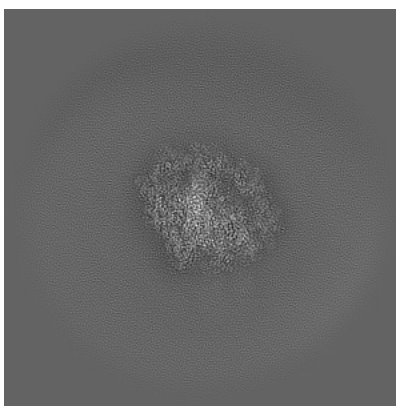
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

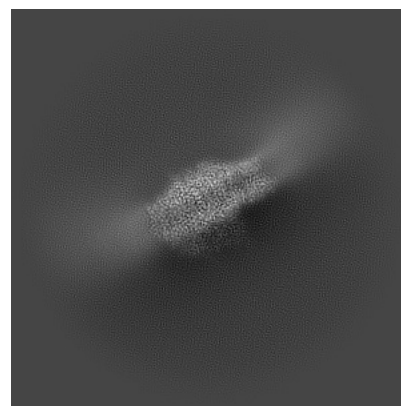
6.1.1 Primary map



X



Y

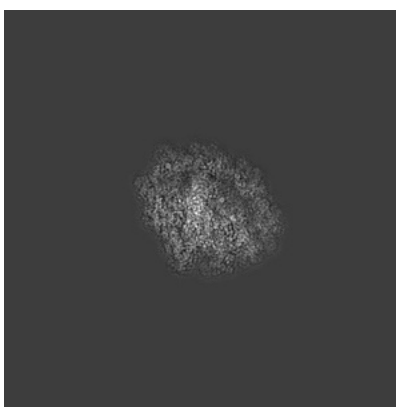


Z

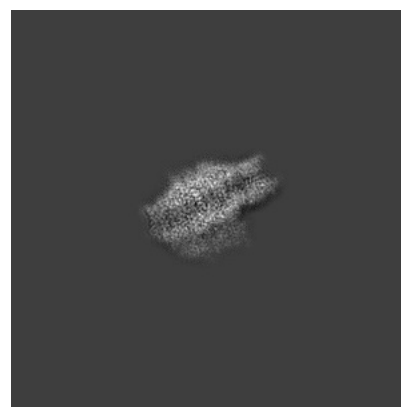
6.1.2 Raw map



X



Y

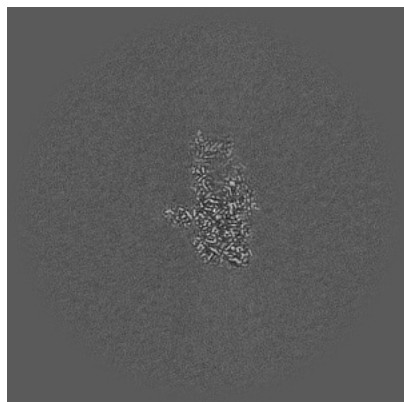


Z

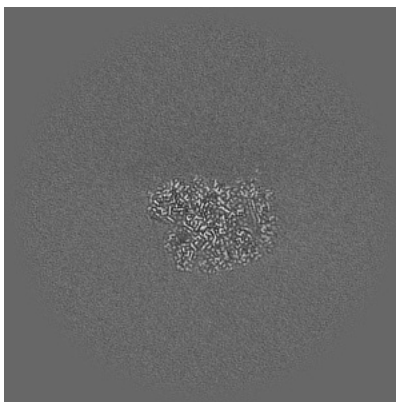
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

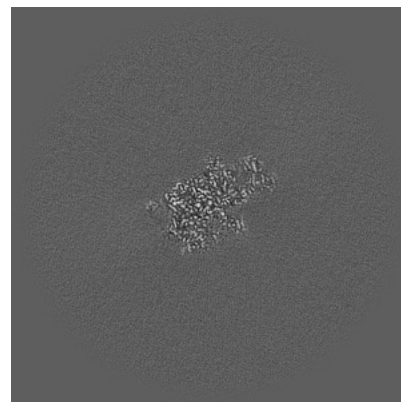
6.2.1 Primary map



X Index: 256

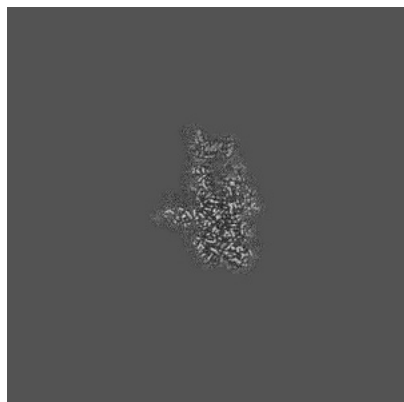


Y Index: 256

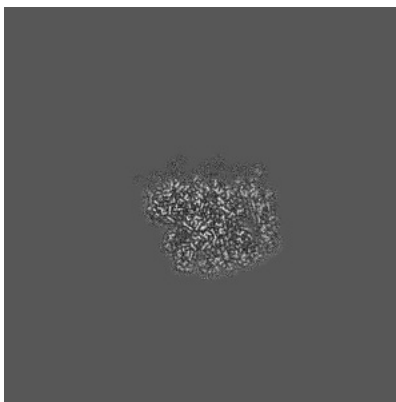


Z Index: 256

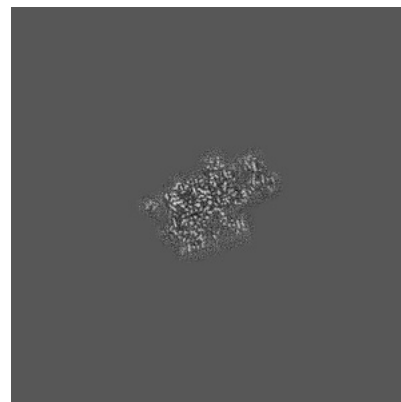
6.2.2 Raw map



X Index: 256



Y Index: 256

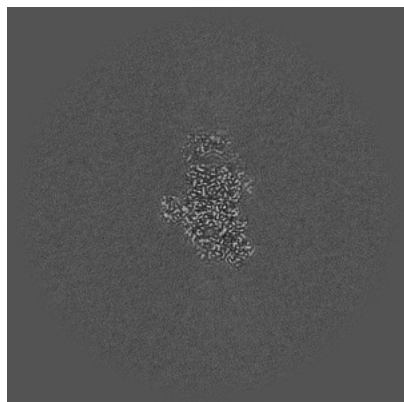


Z Index: 256

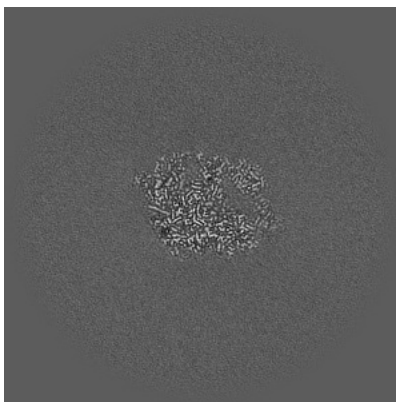
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

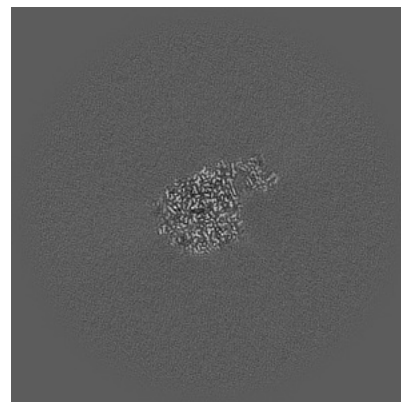
6.3.1 Primary map



X Index: 240

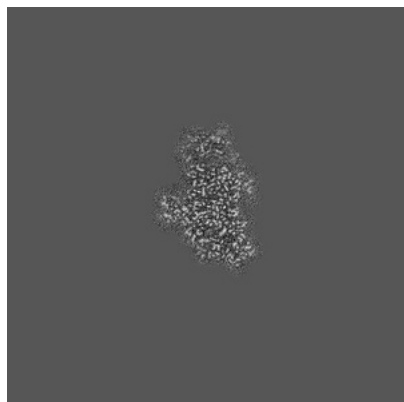


Y Index: 274

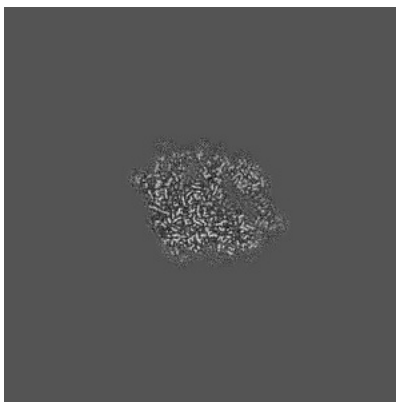


Z Index: 245

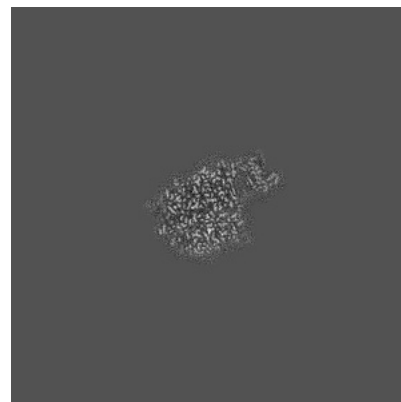
6.3.2 Raw map



X Index: 240



Y Index: 274

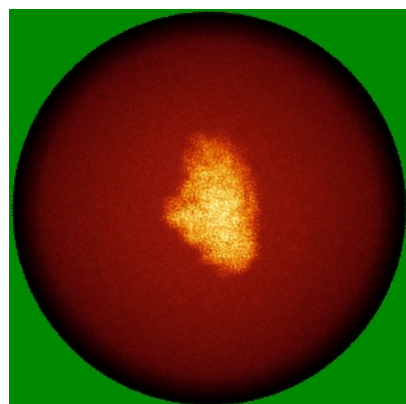


Z Index: 245

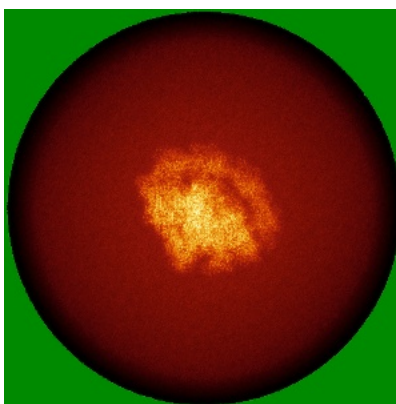
The images above show the largest variance slices of the map in three orthogonal directions.

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

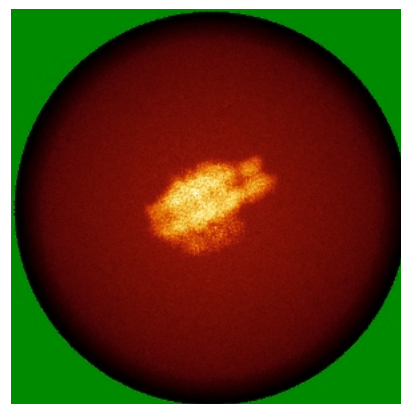
6.4.1 Primary map



X

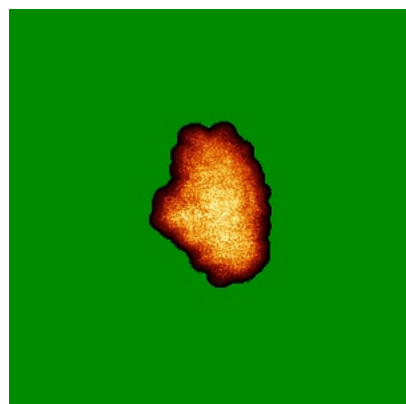


Y

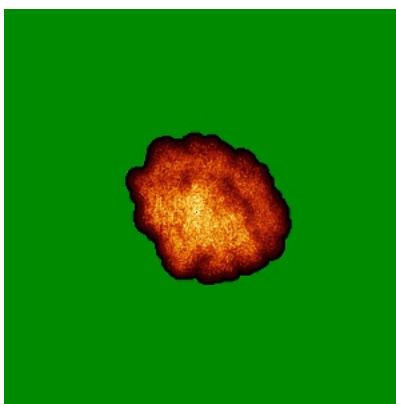


Z

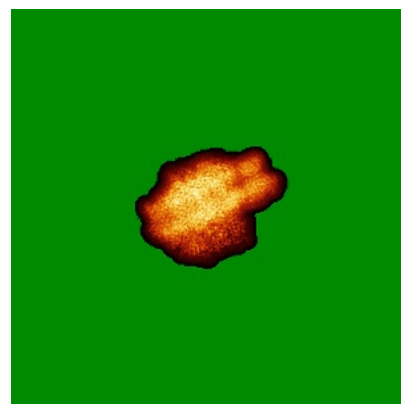
6.4.2 Raw map



X



Y

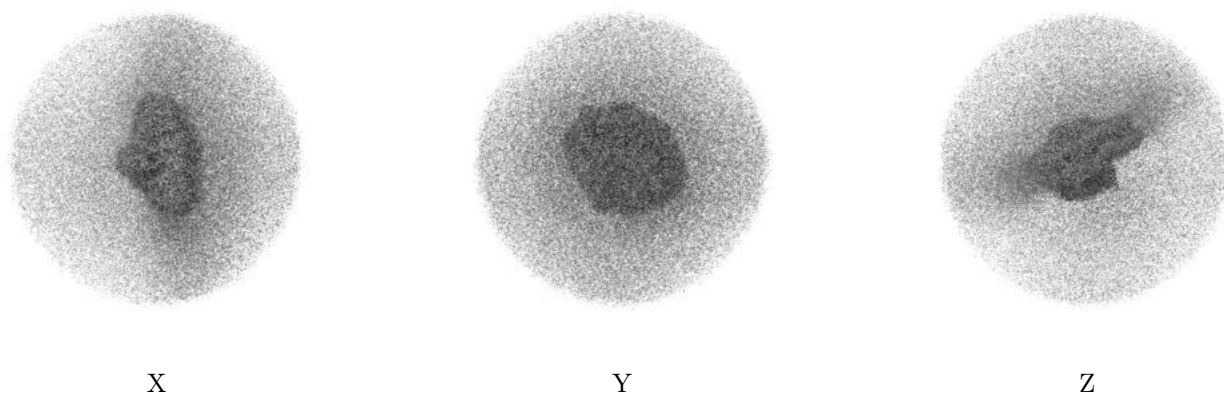


Z

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.

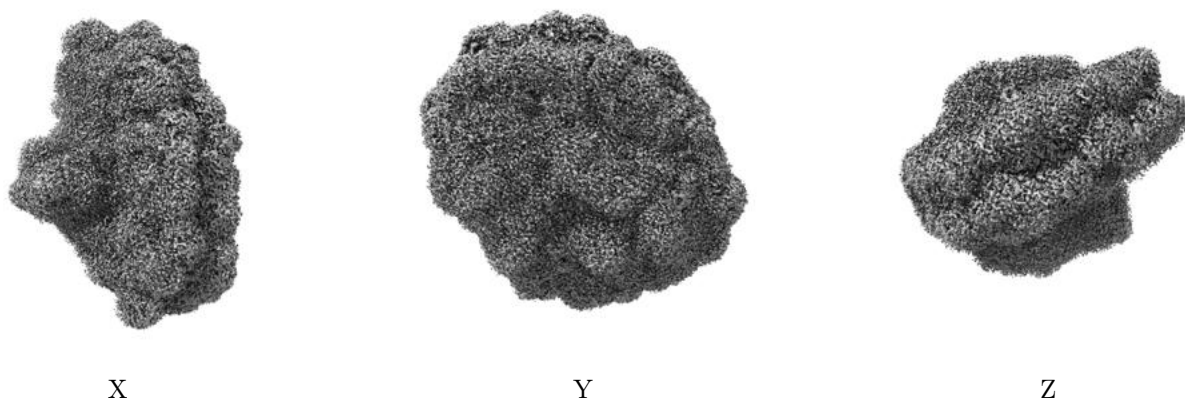
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

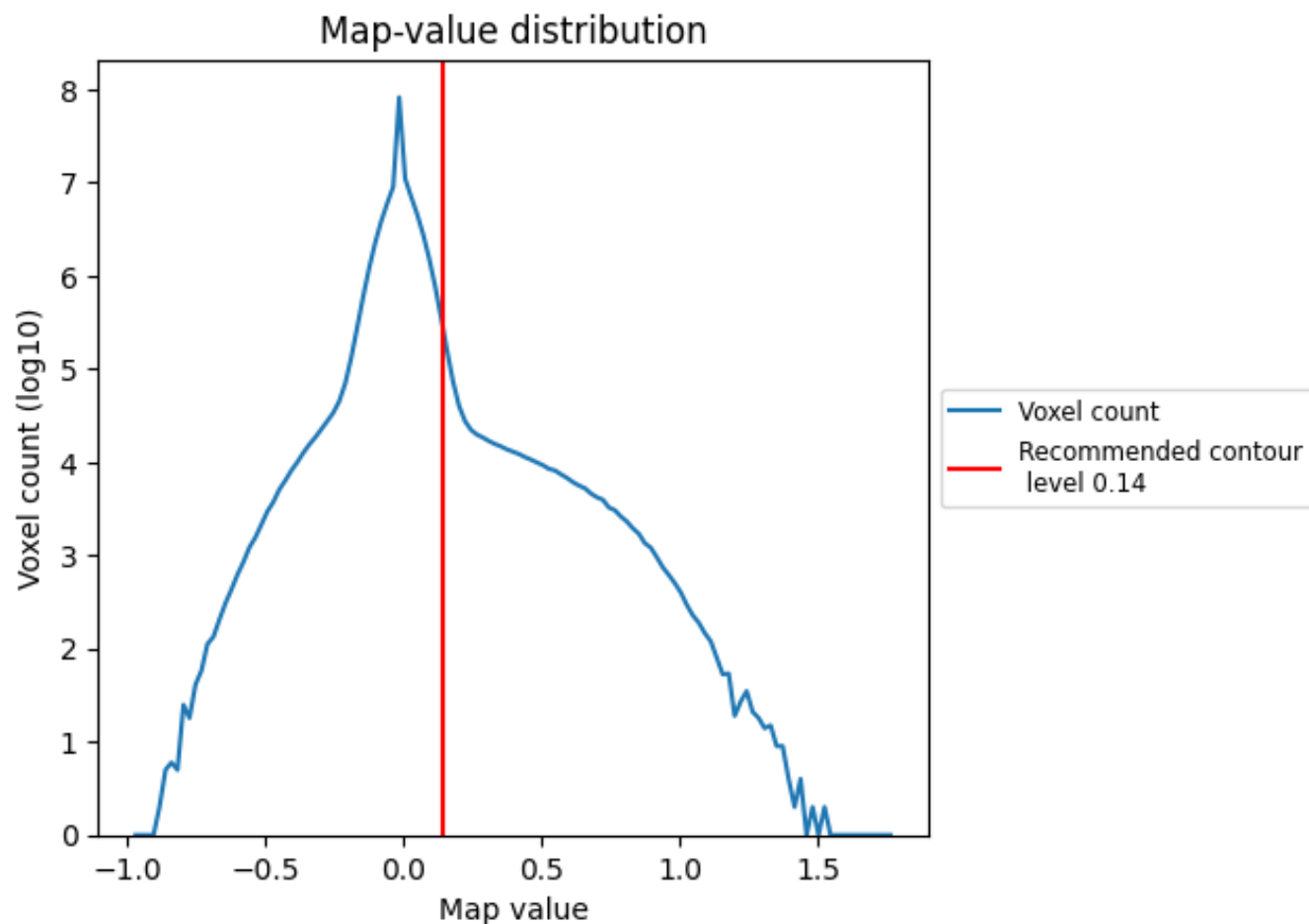
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

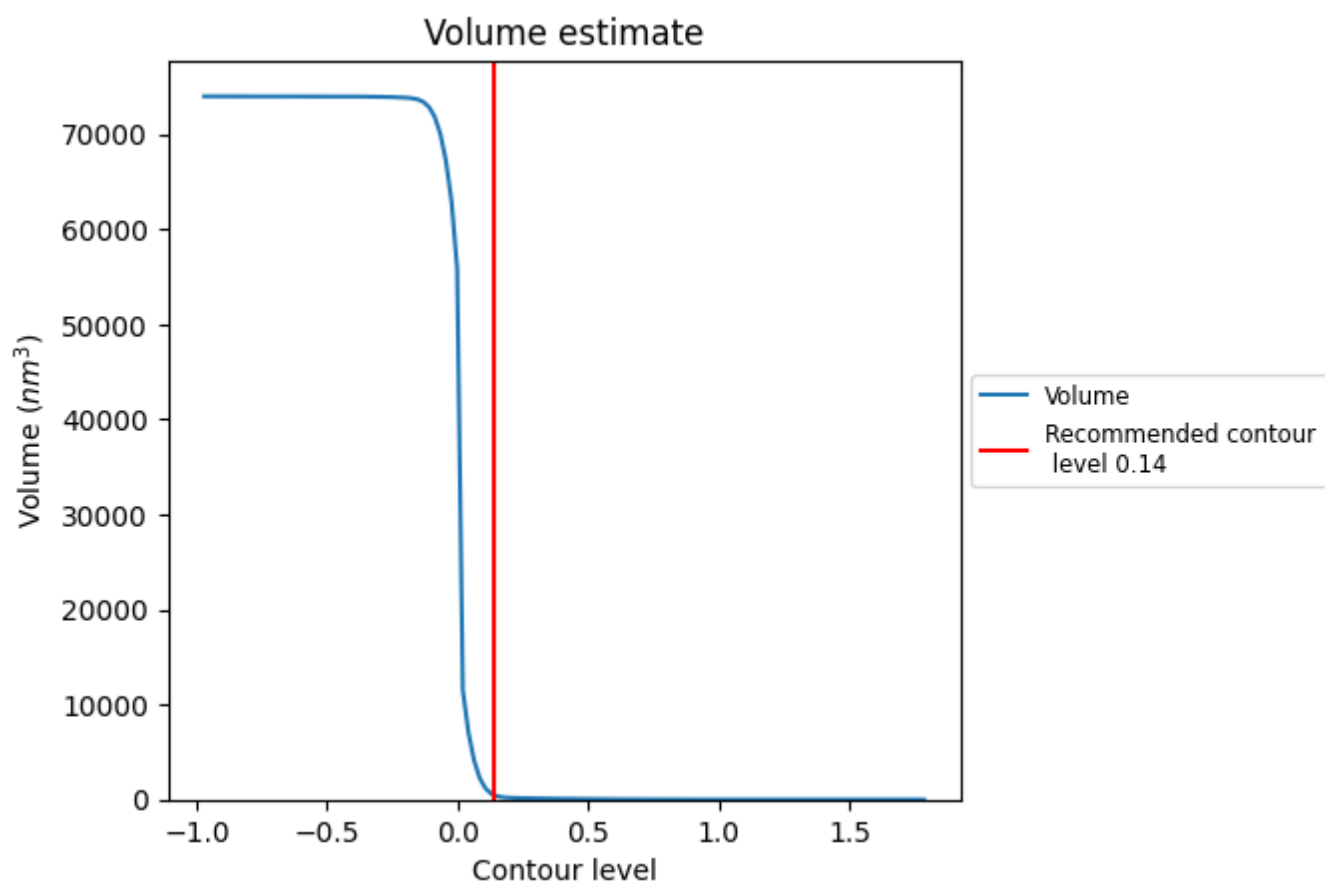
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

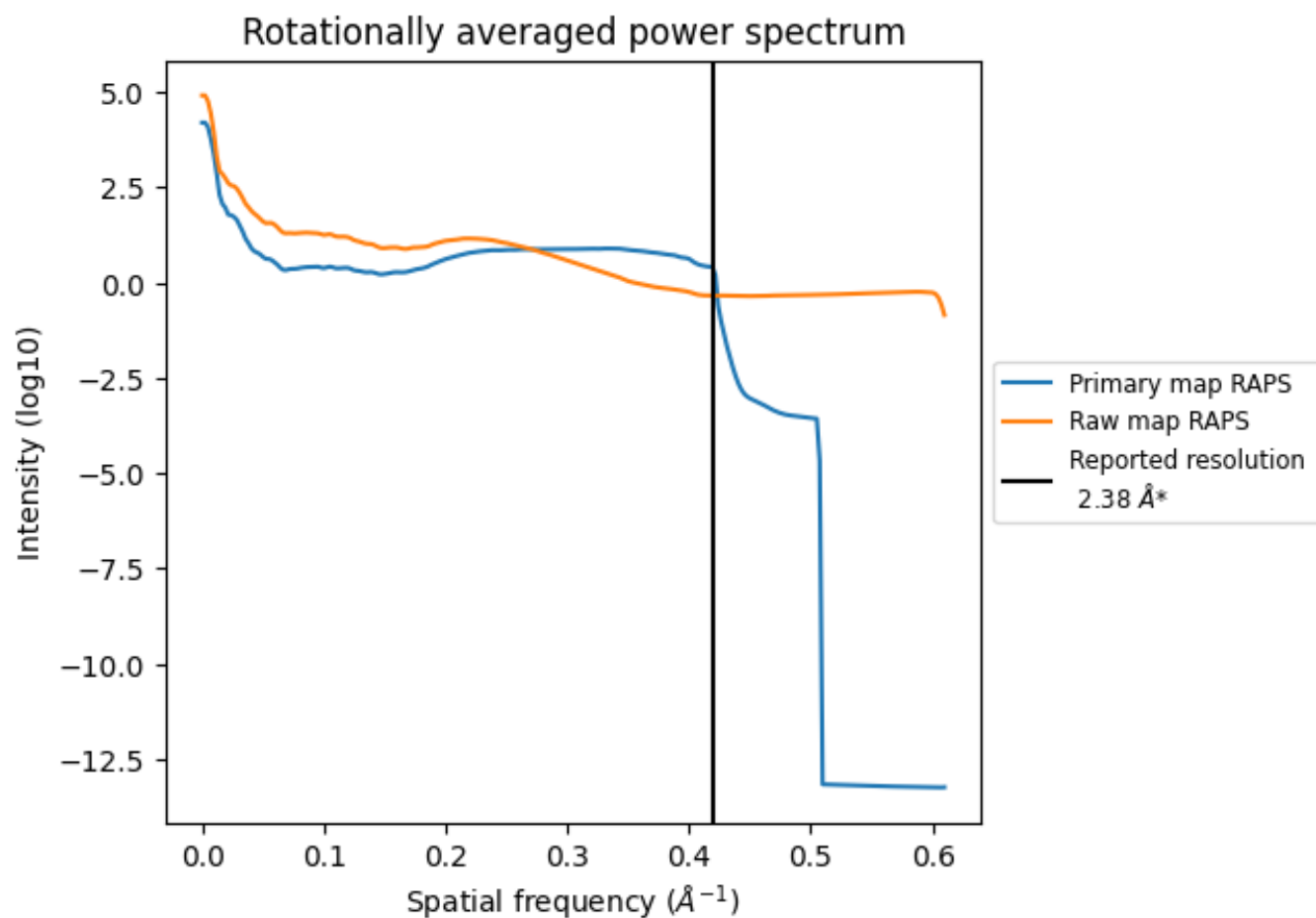
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 489 nm³; this corresponds to an approximate mass of 442 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 ⓘ

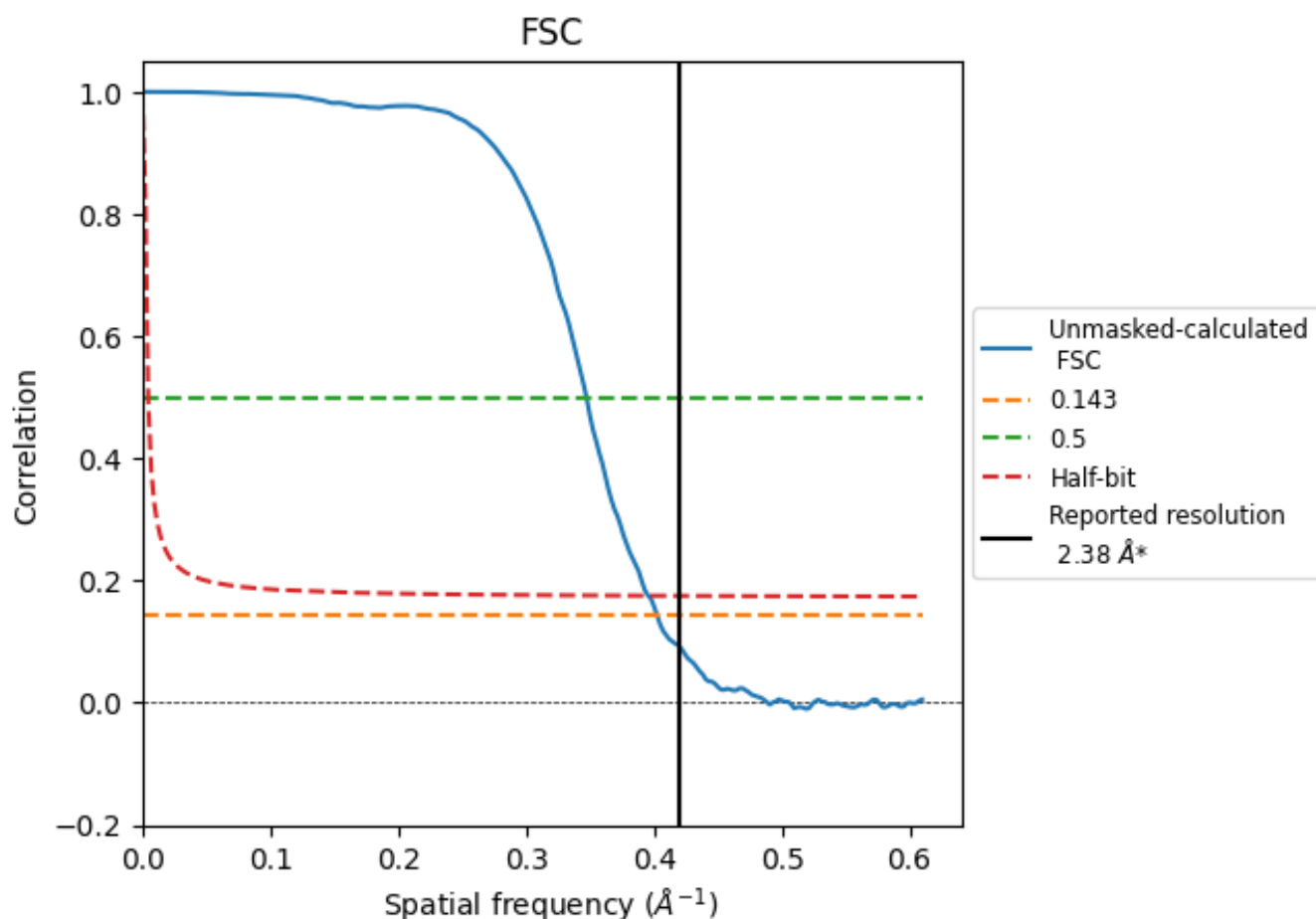


*Reported resolution corresponds to spatial frequency of 0.420 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.420 Å⁻¹

8.2 Resolution estimates [i](#)

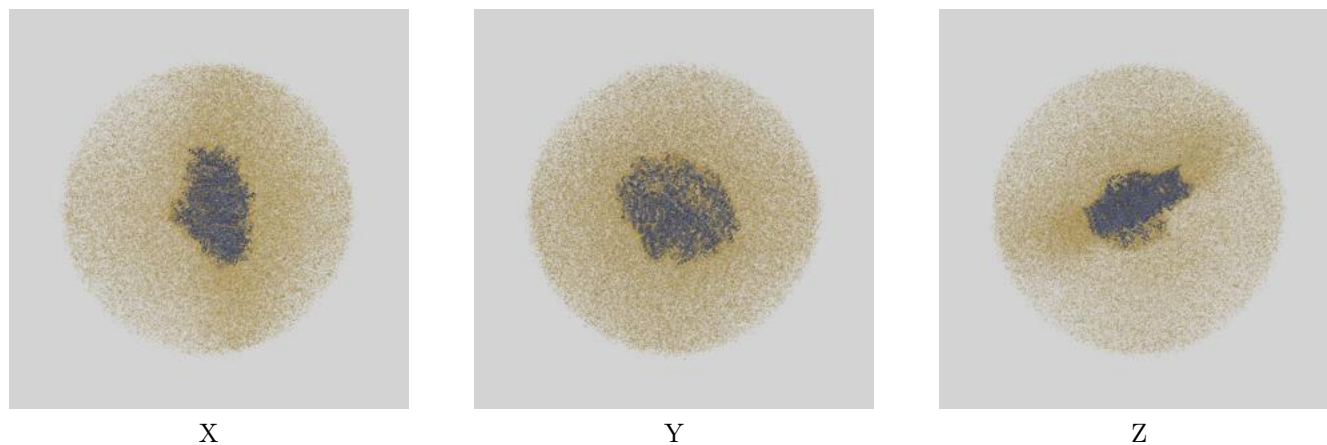
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.38	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.48	2.88	2.53

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

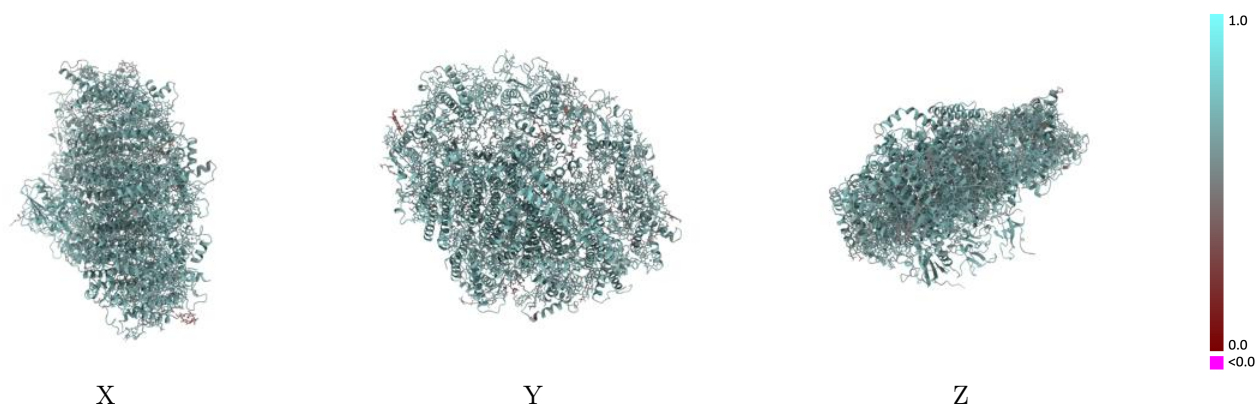
This section contains information regarding the fit between EMDB map EMD-66925 and PDB model 9XJ1. Per-residue inclusion information can be found in [section 3](#) on [page 27](#).

9.1 Map-model overlay [i](#)



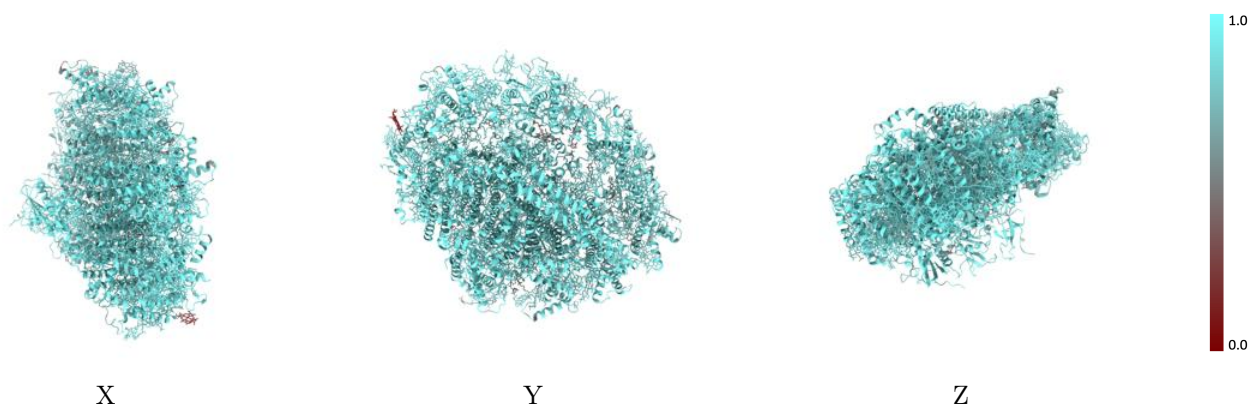
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



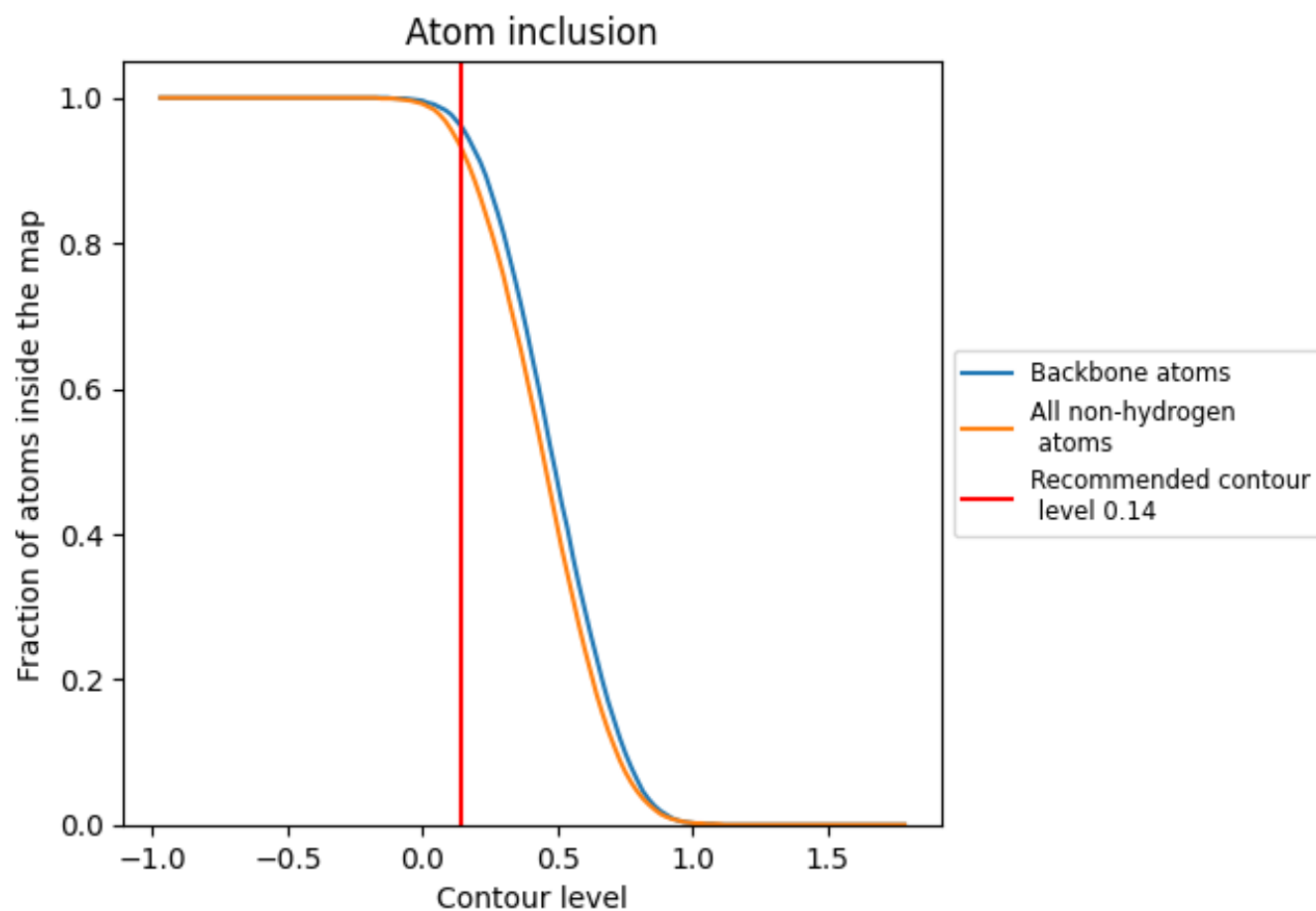
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.14).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9340	 0.6460
1	 0.8930	 0.6190
2	 0.8810	 0.6200
3	 0.8790	 0.6140
4	 0.8840	 0.6100
A	 0.9710	 0.6700
B	 0.9650	 0.6670
C	 0.9800	 0.6720
D	 0.9630	 0.6590
E	 0.9480	 0.6500
F	 0.9590	 0.6630
G	 0.9080	 0.6330
H	 0.9100	 0.6240
I	 0.9250	 0.6310
J	 0.9270	 0.6330
K	 0.9070	 0.6240
L	 0.9570	 0.6550
N	 0.8210	 0.6040
O	 0.8780	 0.6070

