



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 01:08 AM UTC

PDB ID : 8ZET / pdb_00008zet
EMDB ID : EMD-60044
Title : Tp-PSI-FCPI-S in Thalassiosira pseudonana
Authors : Feng, Y.; Li, Z.; Shen, J.R.; Wang, W.
Deposited on : 2024-05-06
Resolution : 3.20 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:

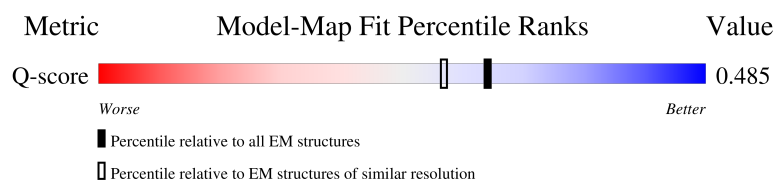
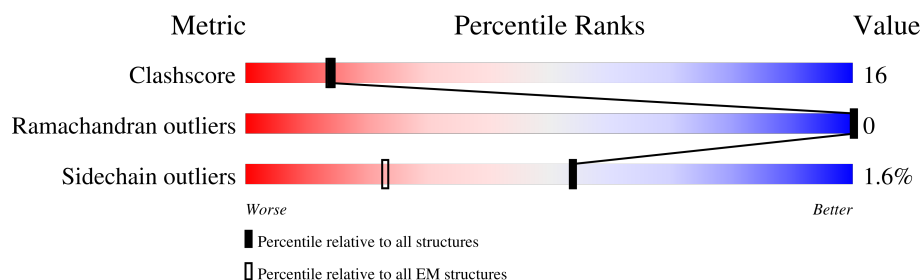
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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.



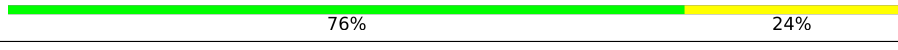
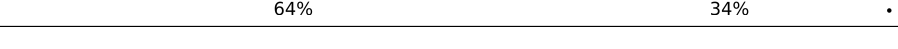
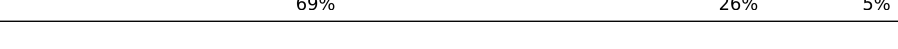
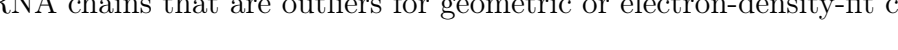
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a	743	 80% 20%
2	b	732	 77% 23% .
3	c	80	 78% 22%
4	d	132	 73% 27%

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Mol	Chain	Length	Quality of chain
5	e	62	
6	f	160	
7	g	131	
8	i	33	
9	j	40	
10	l	146	
11	m	29	
12	r	89	
13	B	165	
14	C	170	
15	D	164	
16	E	185	
17	H	168	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	306	X	-	-	-
18	CLA	B	307	X	-	-	-
18	CLA	B	308	X	-	-	-
18	CLA	B	309	X	-	-	-
18	CLA	B	310	X	-	-	-
18	CLA	B	311	X	-	-	-
18	CLA	B	312	X	-	-	-
18	CLA	B	314	X	-	-	-
18	CLA	C	306	X	-	-	-
18	CLA	C	307	X	-	-	-
18	CLA	C	309	X	-	-	-
18	CLA	C	310	X	-	-	-
18	CLA	C	311	X	-	-	-
18	CLA	C	312	X	-	-	-
18	CLA	C	314	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	C	315	X	-	-	-
18	CLA	C	316	X	-	-	-
18	CLA	C	317	X	-	-	-
18	CLA	C	318	X	-	-	-
18	CLA	D	207	X	-	-	-
18	CLA	D	208	X	-	-	-
18	CLA	D	209	X	-	-	-
18	CLA	D	210	X	-	-	-
18	CLA	D	211	X	-	-	-
18	CLA	D	212	X	-	-	-
18	CLA	D	213	X	-	-	-
18	CLA	D	214	X	-	-	-
18	CLA	D	215	X	-	-	-
18	CLA	D	216	X	-	-	-
18	CLA	D	217	X	-	-	-
18	CLA	E	309	X	-	-	-
18	CLA	E	310	X	-	-	-
18	CLA	E	311	X	-	-	-
18	CLA	E	312	X	-	-	-
18	CLA	E	313	X	-	-	-
18	CLA	E	314	X	-	-	-
18	CLA	E	315	X	-	-	-
18	CLA	E	316	X	-	-	-
18	CLA	H	305	X	-	-	-
18	CLA	H	306	X	-	-	-
18	CLA	H	307	X	-	-	-
18	CLA	H	308	X	-	-	-
18	CLA	H	309	X	-	-	-
18	CLA	H	310	X	-	-	-
18	CLA	H	311	X	-	-	-
18	CLA	H	313	X	-	-	-
18	CLA	H	314	X	-	-	-
18	CLA	H	315	X	-	-	-
18	CLA	a	801	X	-	-	-
18	CLA	a	802	X	-	-	-
18	CLA	a	803	X	-	-	-
18	CLA	a	804	X	-	-	-
18	CLA	a	805	X	-	-	-
18	CLA	a	806	X	-	-	-
18	CLA	a	807	X	-	-	-
18	CLA	a	808	X	-	-	-
18	CLA	a	809	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	a	810	X	-	-	-
18	CLA	a	811	X	-	-	-
18	CLA	a	812	X	-	-	-
18	CLA	a	813	X	-	-	-
18	CLA	a	814	X	-	-	-
18	CLA	a	815	X	-	-	-
18	CLA	a	816	X	-	-	-
18	CLA	a	817	X	-	-	-
18	CLA	a	818	X	-	-	-
18	CLA	a	819	X	-	-	-
18	CLA	a	820	X	-	-	-
18	CLA	a	821	X	-	-	-
18	CLA	a	822	X	-	-	-
18	CLA	a	823	X	-	-	-
18	CLA	a	824	X	-	-	-
18	CLA	a	825	X	-	-	-
18	CLA	a	826	X	-	-	-
18	CLA	a	827	X	-	-	-
18	CLA	a	828	X	-	-	-
18	CLA	a	830	X	-	-	-
18	CLA	a	836	X	-	-	-
18	CLA	a	837	X	-	-	-
18	CLA	a	838	X	-	-	-
18	CLA	a	839	X	-	-	-
18	CLA	a	840	X	-	-	-
18	CLA	a	841	X	-	-	-
18	CLA	a	842	X	-	-	-
18	CLA	a	843	X	-	-	-
18	CLA	a	844	X	-	-	-
18	CLA	a	846	X	-	-	-
18	CLA	a	847	X	-	-	-
18	CLA	a	848	X	-	-	-
18	CLA	a	853	X	-	-	-
18	CLA	a	854	X	-	-	-
18	CLA	a	855	X	-	-	-
18	CLA	b	801	X	-	-	-
18	CLA	b	803	X	-	-	-
18	CLA	b	804	X	-	-	-
18	CLA	b	805	X	-	-	-
18	CLA	b	806	X	-	-	-
18	CLA	b	807	X	-	-	-
18	CLA	b	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	b	809	X	-	-	-
18	CLA	b	810	X	-	-	-
18	CLA	b	811	X	-	-	-
18	CLA	b	812	X	-	-	-
18	CLA	b	813	X	-	-	-
18	CLA	b	814	X	-	-	-
18	CLA	b	815	X	-	-	-
18	CLA	b	816	X	-	-	-
18	CLA	b	817	X	-	-	-
18	CLA	b	818	X	-	-	-
18	CLA	b	819	X	-	-	-
18	CLA	b	820	X	-	-	-
18	CLA	b	821	X	-	-	-
18	CLA	b	822	X	-	-	-
18	CLA	b	823	X	-	-	-
18	CLA	b	824	X	-	-	-
18	CLA	b	825	X	-	-	-
18	CLA	b	826	X	-	-	-
18	CLA	b	827	X	-	-	-
18	CLA	b	828	X	-	-	-
18	CLA	b	829	X	-	-	-
18	CLA	b	830	X	-	-	-
18	CLA	b	837	X	-	-	-
18	CLA	b	838	X	-	-	-
18	CLA	b	840	X	-	-	-
18	CLA	b	841	X	-	-	-
18	CLA	b	842	X	-	-	-
18	CLA	b	843	X	-	-	-
18	CLA	b	844	X	-	-	-
18	CLA	b	845	X	-	-	-
18	CLA	b	846	X	-	-	-
18	CLA	b	848	X	-	-	-
18	CLA	b	849	X	-	-	-
18	CLA	b	850	X	-	-	-
18	CLA	f	202	X	-	-	-
18	CLA	f	203	X	-	-	-
18	CLA	f	204	X	-	-	-
18	CLA	i	101	X	-	-	-
18	CLA	j	104	X	-	-	-
18	CLA	l	202	X	-	-	-
18	CLA	l	203	X	-	-	-
18	CLA	l	205	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	r	202	X	-	-	-
24	SF4	b	802	-	-	X	-
24	SF4	c	101	-	-	X	-
24	SF4	c	102	-	-	X	-

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 36577 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	743	Total	C	N	O	S	0	0
			5852	3822	992	1009	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	732	Total	C	N	O	S	0	0
			5824	3827	982	996	19		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	80	Total	C	N	O	S	0	0
			599	368	103	118	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	132	Total	C	N	O	S	0	0
			1040	665	177	195	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	62	Total	C	N	O	S	0	0
			503	317	89	96	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	160	Total	C	N	O	S	0	0
			1242	795	211	233	3		

- Molecule 7 is a protein called Photosystem I reaction center subunit Psa29.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	131	Total	C	N	O	S	0	0
			981	619	154	204	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	i	33	Total	C	N	O	S	0	0
			256	177	34	44	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	j	40	Total	C	N	O	S	0	0
			332	224	48	57	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	146	Total	C	N	O	S	0	0
			1095	722	178	193	2		

- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	m	29	Total	C	N	O	S	0	0
			220	147	33	38	2		

- Molecule 12 is a protein called Tp-PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	r	89	Total	C	N	O	S	0	0
			683	443	112	121	7		

- Molecule 13 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	165	Total	C	N	O	S	0	0
			1285	833	204	240	8		

- Molecule 14 is a protein called Fucoxanthin chl a/c light-harvesting protein, major type.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	170	Total	C	N	O	S	0	0
			1302	841	213	240	8		

- Molecule 15 is a protein called Pt17531-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	D	164	Total	C	N	O	S	0	0
			1271	819	208	234	10		

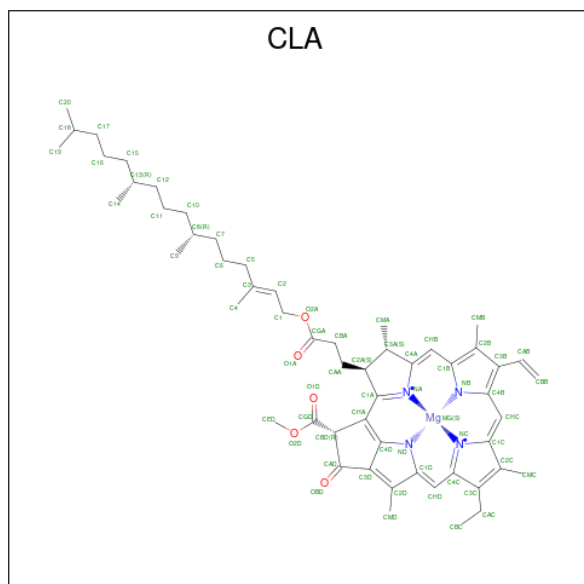
- Molecule 16 is a protein called Tp-RedCAP.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E	185	Total	C	N	O	S	0	0
			1413	902	235	262	14		

- Molecule 17 is a protein called Fucoxanthin chl a/c light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	168	Total	C	N	O	S	0	0
			1300	834	214	242	10		

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

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

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

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Mol	Chain	Residues	Atoms					AltConf
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	b	1	Total 59	C 49	Mg 1	N 4	O 5	0
18	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 58	C 48	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 61	C 51	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 62	C 52	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	i	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	j	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	l	1	Total 49	C 39	Mg 1	N 4	O 5	0
18	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	l	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 57	C 49	Mg 1	N 4	O 3	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 62	C 52	Mg 1	N 4	O 5	0
18	C	1	Total 46	C 36	Mg 1	N 4	O 5	0

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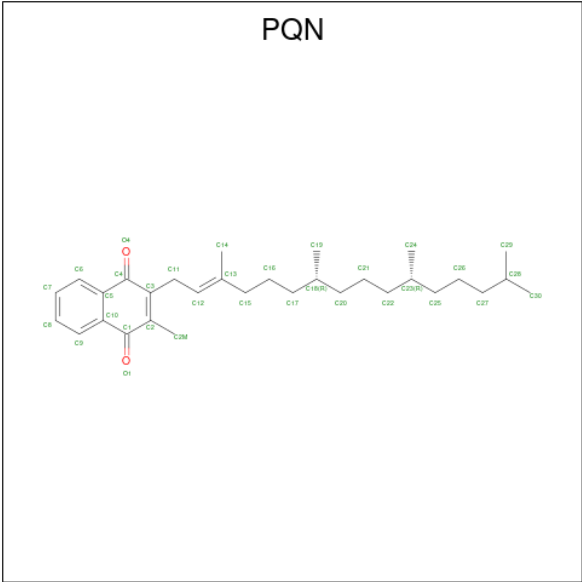
Mol	Chain	Residues	Atoms					AltConf
18	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	C	1	Total 61	C 51	Mg 1	N 4	O 5	0
18	C	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	C	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	C	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	C	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	C	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	D	1	Total 61	C 51	Mg 1	N 4	O 5	0
18	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	D	1	Total 49	C 39	Mg 1	N 4	O 5	0
18	D	1	Total 56	C 46	Mg 1	N 4	O 5	0
18	D	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	D	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	D	1	Total 56	C 46	Mg 1	N 4	O 5	0
18	D	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	D	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	D	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	E	1	Total 46	C 36	Mg 1	N 4	O 5	0

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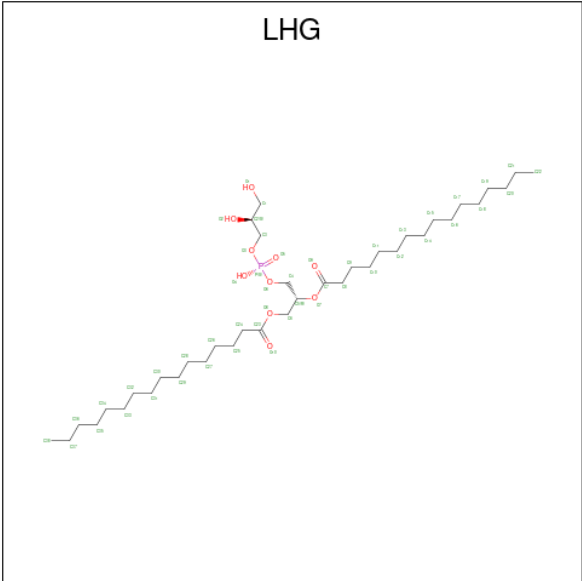
Mol	Chain	Residues	Atoms					AltConf
18	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	E	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	E	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	E	1	Total 56	C 46	Mg 1	N 4	O 5	0
18	H	1	Total 54	C 44	Mg 1	N 4	O 5	0
18	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	H	1	Total 57	C 47	Mg 1	N 4	O 5	0
18	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	H	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 19 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



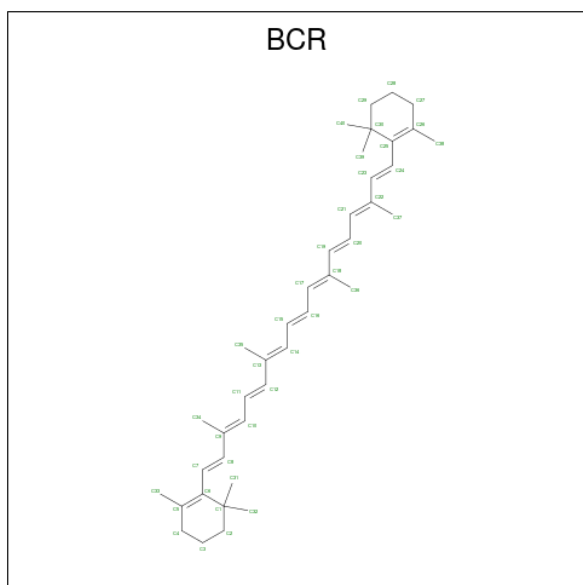
Mol	Chain	Residues	Atoms				AltConf
20	a	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
20	a	1	Total	C	O	P	0
			27	16	10	1	
20	a	1	Total	C	O	P	0
			33	22	10	1	
20	b	1	Total	C	O	P	0
			49	38	10	1	
20	j	1	Total	C	O	P	0
			49	38	10	1	
20	B	1	Total	C	O	P	0
			42	31	10	1	
20	D	1	Total	C	O	P	0
			49	38	10	1	
20	E	1	Total	C	O	P	0
			49	38	10	1	
20	E	1	Total	C	O	P	0
			42	31	10	1	
20	H	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



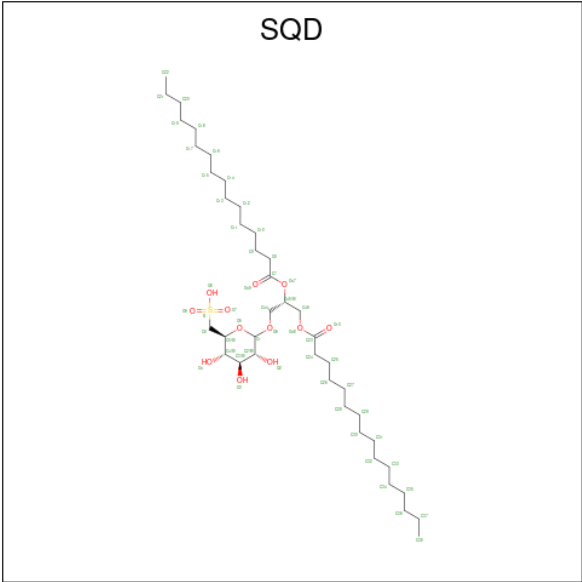
Mol	Chain	Residues	Atoms		AltConf
21	a	1	Total	C	0
			40	40	
21	a	1	Total	C	0
			40	40	

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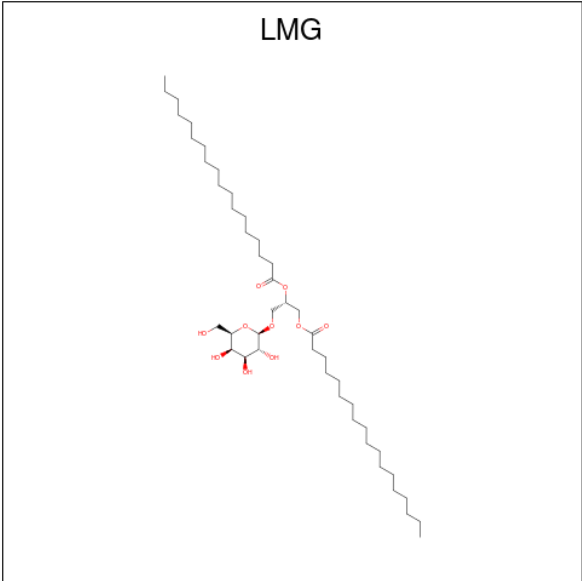
Mol	Chain	Residues	Atoms	AltConf
21	a	1	Total C 40 40	0
21	a	1	Total C 40 40	0
21	a	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	f	1	Total C 40 40	0
21	f	1	Total C 40 40	0
21	i	1	Total C 40 40	0
21	i	1	Total C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

- Molecule 22 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
22	a	1	33	23	9	1	0

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



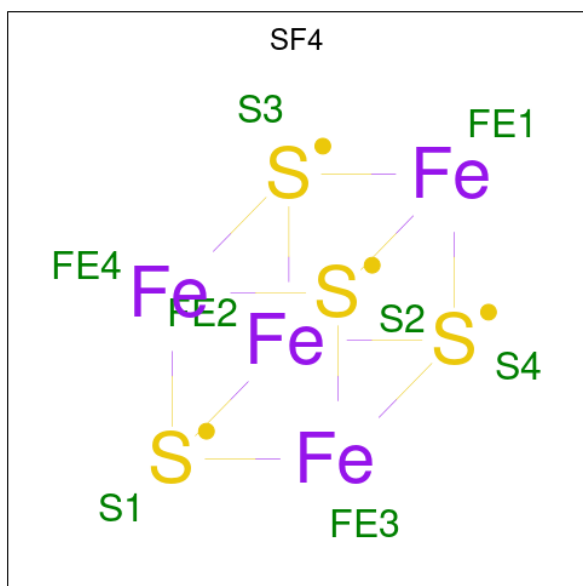
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	a	1	33	23	10	0
23	j	1	37	27	10	0

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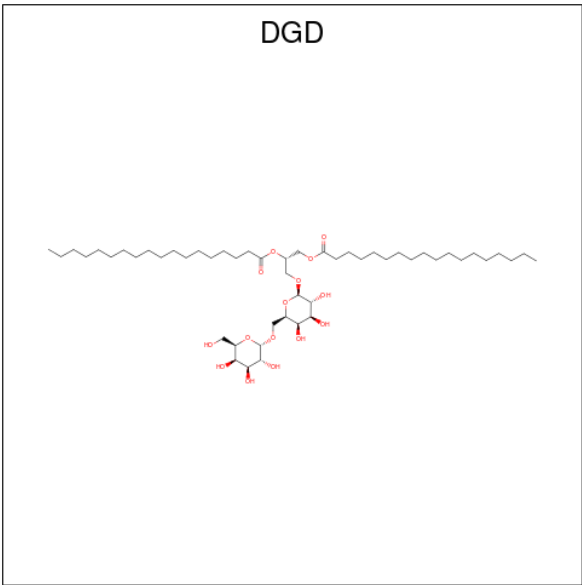
Mol	Chain	Residues	Atoms			AltConf
23	l	1	Total	C	O	0
			40	30	10	
23	C	1	Total	C	O	0
			31	21	10	
23	C	1	Total	C	O	0
			44	34	10	
23	D	1	Total	C	O	0
			46	36	10	
23	E	1	Total	C	O	0
			43	33	10	

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



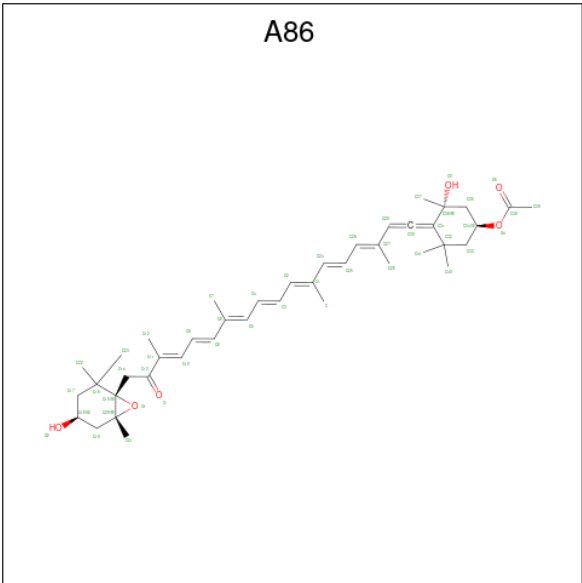
Mol	Chain	Residues	Atoms			AltConf
24	b	1	Total	Fe	S	0
			8	4	4	
24	c	1	Total	Fe	S	0
			8	4	4	
24	c	1	Total	Fe	S	0
			8	4	4	

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $\text{C}_{51}\text{H}_{96}\text{O}_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
25	b	1	Total	C	O	0
			60	45	15	

- Molecule 26 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'- yl acetate (CCD ID: A86) (formula: C₄₂H₅₈O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
26	b	1	Total	C	O	0
			48	42	6	
26	m	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
26	r	1	Total	C	O	0
			48	42	6	
26	B	1	Total	C	O	0
			48	42	6	
26	B	1	Total	C	O	0
			48	42	6	
26	B	1	Total	C	O	0
			48	42	6	
26	B	1	Total	C	O	0
			48	42	6	
26	C	1	Total	C	O	0
			48	42	6	
26	C	1	Total	C	O	0
			48	42	6	
26	C	1	Total	C	O	0
			48	42	6	
26	D	1	Total	C	O	0
			48	42	6	
26	D	1	Total	C	O	0
			48	42	6	
26	D	1	Total	C	O	0
			48	42	6	
26	E	1	Total	C	O	0
			48	42	6	
26	H	1	Total	C	O	0
			48	42	6	
26	H	1	Total	C	O	0
			48	42	6	
26	H	1	Total	C	O	0
			48	42	6	

- Molecule 27 is (1 {R})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15-octaen-17-ynyl]cyclohex-3-en-1-ol (CCD ID: ET4) (formula: C₄₀H₅₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			42	40	2	

- Molecule 28 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: C₄₀H₅₄O₃) (labeled as "Ligand of Interest" by depositor).



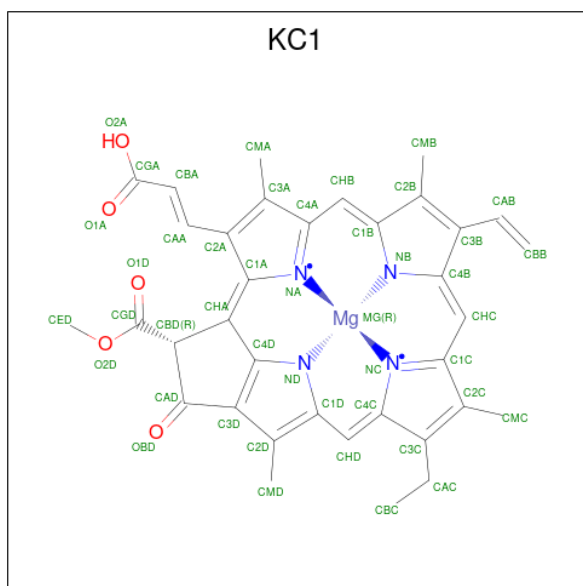
Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	C	O	0
			43	40	3	
28	C	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms			AltConf
28	D	1	Total	C	O	0
			43	40	3	
28	E	1	Total	C	O	0
			43	40	3	
28	E	1	Total	C	O	0
			43	40	3	
28	E	1	Total	C	O	0
			43	40	3	
28	E	1	Total	C	O	0
			43	40	3	
28	H	1	Total	C	O	0
			43	40	3	

- Molecule 29 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).

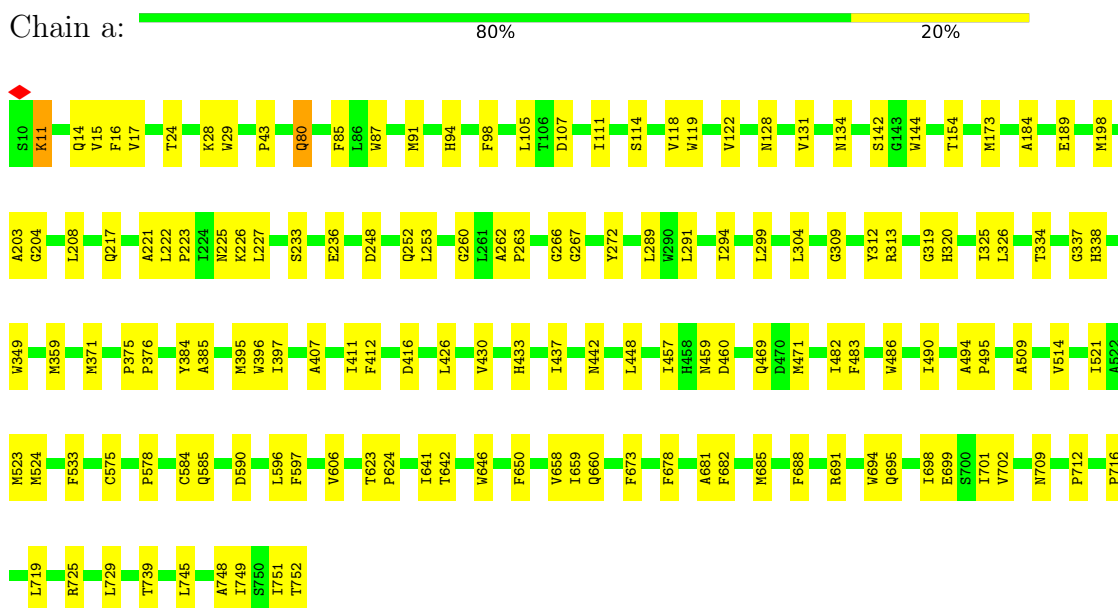


Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

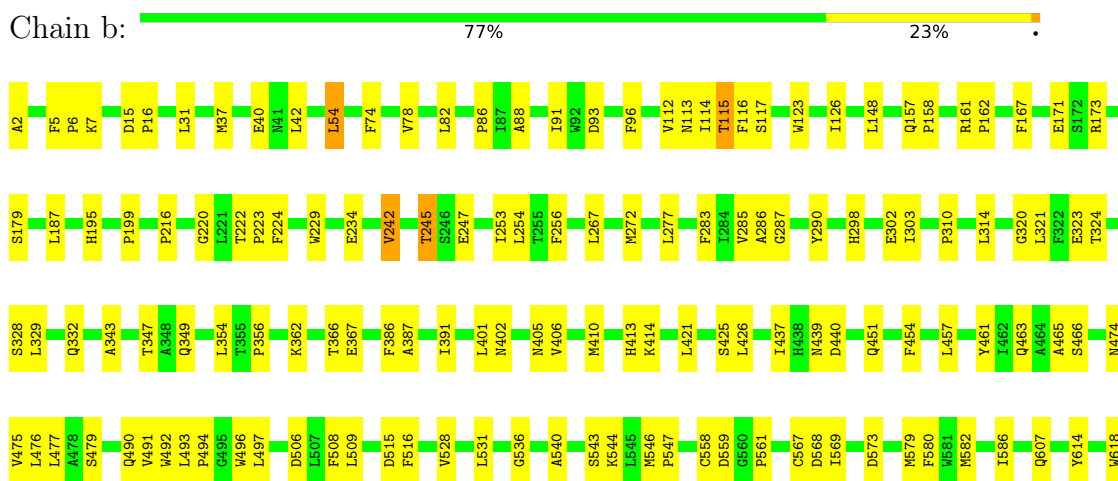
3 Residue-property plots

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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

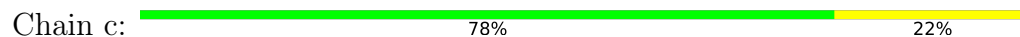


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





- Molecule 3: Photosystem I iron-sulfur center



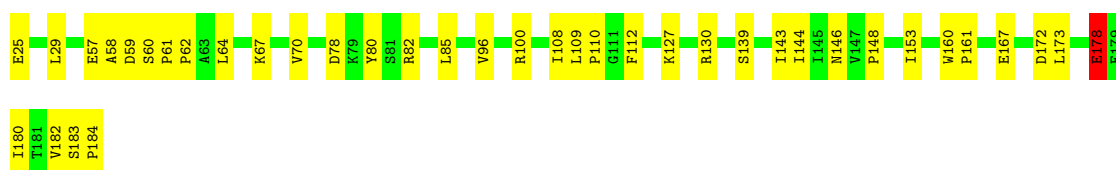
- Molecule 4: Photosystem I reaction center subunit II



- Molecule 5: Photosystem I reaction center subunit IV



- Molecule 6: Photosystem I reaction center subunit III



- Molecule 7: Photosystem I reaction center subunit Psa29



- Molecule 8: Photosystem I reaction center subunit VIII





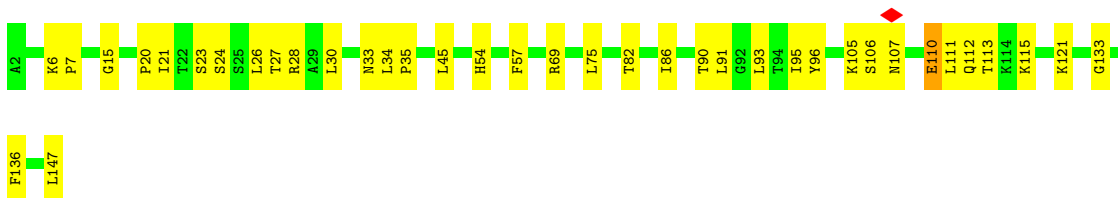
- Molecule 9: Photosystem I reaction center subunit IX

Chain j: 70% 22% 8%



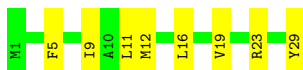
- Molecule 10: Photosystem I reaction center subunit XI

Chain l: 74% 25%



- Molecule 11: Photosystem I reaction center subunit XII

Chain m: 72% 28%



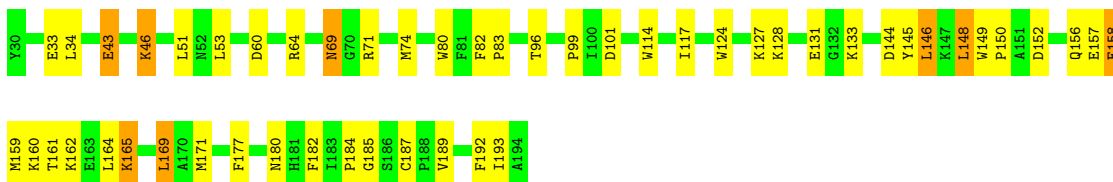
- Molecule 12: Tp-PsaR

Chain r: 67% 33%



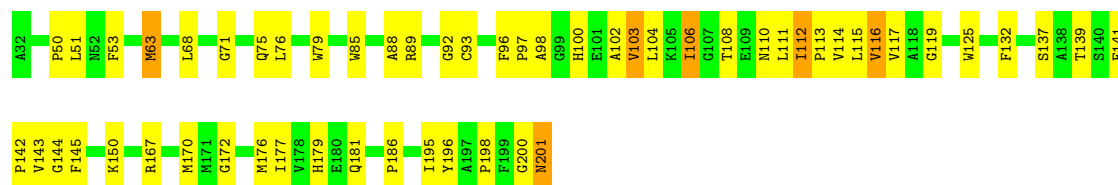
- Molecule 13: Fucoxanthin chlorophyll a/c-binding protein Lhcq8

Chain B: 69% 26% 5%



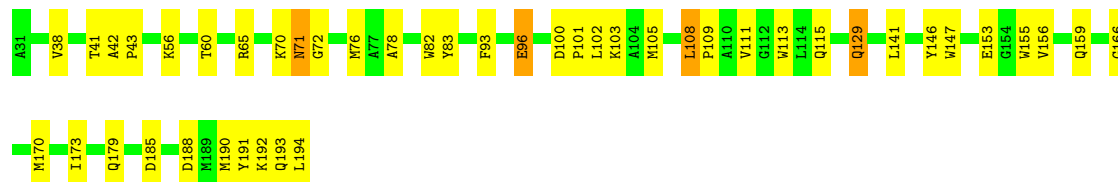
- Molecule 14: Fucoxanthin chl a/c light-harvesting protein, major type

Chain C: 68% 29%



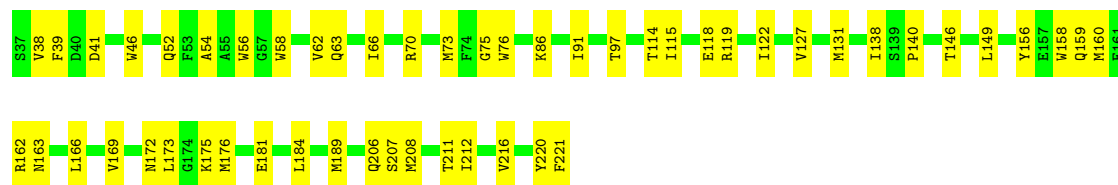
- Molecule 15: Pt17531-like protein

Chain D: 73% 25%



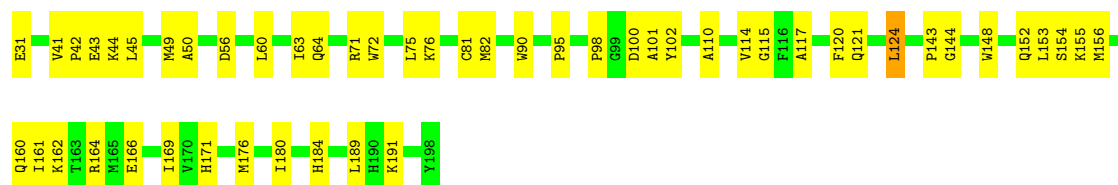
- Molecule 16: Tp-RedCAP

Chain E: 72% 28%



- Molecule 17: Fucoxanthin chl a/c light-harvesting protein

Chain H: 70% 30%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52772	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.370	Depositor
Minimum map value	-0.381	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	563.2, 563.2, 563.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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: CLA, LHG, LMG, BCR, A86, SQD, PQN, ET4, KC1, SF4, DD6, DGD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.53	0/6049	0.67	2/8234 (0.0%)
2	b	0.53	0/6034	0.66	1/8236 (0.0%)
3	c	0.52	0/609	0.80	1/826 (0.1%)
4	d	0.47	0/1067	0.72	0/1441
5	e	0.43	0/511	0.72	0/690
6	f	0.53	0/1271	0.73	3/1727 (0.2%)
7	g	0.43	0/1003	0.68	1/1354 (0.1%)
8	i	0.51	0/264	0.73	0/360
9	j	0.52	0/342	0.78	2/463 (0.4%)
10	l	0.54	0/1123	0.67	1/1523 (0.1%)
11	m	0.56	0/222	0.56	0/300
12	r	0.48	0/704	0.60	0/957
13	B	0.53	0/1324	0.66	0/1804
14	C	0.50	0/1339	0.68	1/1813 (0.1%)
15	D	0.51	0/1304	0.64	0/1771
16	E	0.52	0/1450	0.67	0/1974
17	H	0.51	0/1334	0.65	1/1809 (0.1%)
All	All	0.52	0/25950	0.67	13/35282 (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
4	d	0	1

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	667	ARG	N-CA-C	8.65	120.33	111.07
7	g	156	GLY	N-CA-C	-8.09	103.12	112.50
6	f	58	ALA	CB-CA-C	-6.27	109.33	116.54
1	a	266	GLY	N-CA-C	-6.25	102.80	112.85
1	a	122	VAL	N-CA-C	6.09	122.02	109.34

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	d	96	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	5852	0	5682	113	0
2	b	5824	0	5643	144	0
3	c	599	0	582	19	0
4	d	1040	0	1027	26	0
5	e	503	0	500	18	0
6	f	1242	0	1239	34	0
7	g	981	0	922	40	0
8	i	256	0	259	13	0
9	j	332	0	331	19	0
10	l	1095	0	1116	37	0
11	m	220	0	241	8	0
12	r	683	0	675	26	0
13	B	1285	0	1239	61	0
14	C	1302	0	1243	69	0
15	D	1271	0	1227	41	0
16	E	1413	0	1365	47	0
17	H	1300	0	1262	44	0
18	B	469	0	479	33	0
18	C	547	0	472	60	0
18	D	568	0	501	34	0
18	E	462	0	454	21	0
18	H	587	0	583	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	a	2671	0	2759	134	0
18	b	2492	0	2569	138	0
18	f	175	0	177	3	0
18	i	60	0	59	1	0
18	j	41	0	29	1	0
18	l	159	0	144	10	0
18	r	45	0	33	2	0
19	a	33	0	46	1	0
19	b	33	0	46	4	0
20	B	42	0	54	3	0
20	D	49	0	74	6	0
20	E	91	0	131	5	0
20	H	35	0	43	0	0
20	a	109	0	134	6	0
20	b	49	0	74	5	0
20	j	49	0	74	5	0
21	E	80	0	112	9	0
21	a	200	0	280	31	0
21	b	160	0	224	19	0
21	f	80	0	112	6	0
21	i	80	0	112	14	0
21	j	80	0	112	17	0
21	l	80	0	112	11	0
21	m	40	0	56	5	0
21	r	40	0	56	2	0
22	a	33	0	39	7	0
23	C	75	0	88	1	0
23	D	46	0	61	1	0
23	E	43	0	55	5	0
23	a	33	0	33	2	0
23	j	37	0	42	0	0
23	l	40	0	49	1	0
24	b	8	0	0	2	0
24	c	16	0	0	7	0
25	b	60	0	81	0	0
26	B	192	0	0	7	0
26	C	144	0	0	5	0
26	D	144	0	0	3	0
26	E	48	0	0	0	0
26	H	144	0	0	17	0
26	b	48	0	0	4	0
26	m	48	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	r	48	0	0	1	0
27	l	42	0	0	0	0
28	B	43	0	0	0	0
28	C	43	0	0	1	0
28	D	43	0	0	3	0
28	E	172	0	0	2	0
28	H	43	0	0	3	0
29	B	45	0	0	5	0
29	C	90	0	0	4	0
29	H	45	0	0	1	0
All	All	36577	0	35112	1120	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 16.

The worst 5 of 1120 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)
26:H:302:A86:C1	18:H:309:CLA:CMD	2.27	1.12
26:H:302:A86:C1	18:H:309:CLA:HMD1	1.82	1.10
18:a:807:CLA:H202	21:j:105:BCR:H392	1.33	1.05
13:B:165:LYS:CB	18:B:306:CLA:HMD2	1.86	1.05
13:B:165:LYS:HB3	18:B:306:CLA:CMD	1.88	1.02

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	741/743 (100%)	723 (98%)	18 (2%)	0	100	100
2	b	730/732 (100%)	713 (98%)	17 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
4	d	130/132 (98%)	126 (97%)	4 (3%)	0	100	100
5	e	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
6	f	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
7	g	129/131 (98%)	121 (94%)	8 (6%)	0	100	100
8	i	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
9	j	38/40 (95%)	36 (95%)	2 (5%)	0	100	100
10	l	144/146 (99%)	138 (96%)	6 (4%)	0	100	100
11	m	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
12	r	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
13	B	163/165 (99%)	157 (96%)	6 (4%)	0	100	100
14	C	168/170 (99%)	165 (98%)	3 (2%)	0	100	100
15	D	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
16	E	183/185 (99%)	180 (98%)	3 (2%)	0	100	100
17	H	166/168 (99%)	162 (98%)	4 (2%)	0	100	100
All	All	3195/3229 (99%)	3103 (97%)	92 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	603/603 (100%)	598 (99%)	5 (1%)	73	82
2	b	597/597 (100%)	591 (99%)	6 (1%)	68	80
3	c	69/69 (100%)	68 (99%)	1 (1%)	59	77
4	d	111/111 (100%)	111 (100%)	0	100	100
5	e	55/55 (100%)	52 (94%)	3 (6%)	19	52
6	f	132/132 (100%)	130 (98%)	2 (2%)	57	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	g	98/98 (100%)	95 (97%)	3 (3%)	35	66
8	i	28/28 (100%)	28 (100%)	0	100	100
9	j	36/36 (100%)	34 (94%)	2 (6%)	19	52
10	l	113/113 (100%)	113 (100%)	0	100	100
11	m	22/22 (100%)	22 (100%)	0	100	100
12	r	72/72 (100%)	72 (100%)	0	100	100
13	B	133/133 (100%)	124 (93%)	9 (7%)	14	46
14	C	129/130 (99%)	123 (95%)	6 (5%)	23	57
15	D	128/128 (100%)	124 (97%)	4 (3%)	35	66
16	E	144/144 (100%)	144 (100%)	0	100	100
17	H	136/136 (100%)	135 (99%)	1 (1%)	76	83
All	All	2606/2607 (100%)	2564 (98%)	42 (2%)	54	75

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	B	164	LEU
14	C	116	VAL
13	B	165	LYS
14	C	68	LEU
15	D	71	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
9	j	2	ASN
14	C	52	ASN
10	l	9	ASN
13	B	69	ASN
15	D	71	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

217 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	$\# Z > 2$
18	CLA	a	809	18,1	66,70,73	1.18	7 (10%)	78,109,113	1.27	4 (5%)
26	A86	D	206	-	47,50,50	1.70	9 (19%)	51,76,76	3.31	21 (41%)
21	BCR	i	103	-	41,41,41	0.67	0	56,56,56	2.05	13 (23%)
21	BCR	f	201	-	41,41,41	0.94	2 (4%)	56,56,56	1.94	17 (30%)
26	A86	b	847	-	47,50,50	1.63	9 (19%)	51,76,76	2.69	18 (35%)
18	CLA	b	849	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)
18	CLA	C	312	14	65,69,73	1.20	9 (13%)	77,108,113	1.38	7 (9%)
18	CLA	D	217	-	45,49,73	1.39	8 (17%)	54,84,113	1.47	6 (11%)
18	CLA	b	814	-	69,73,73	1.18	9 (13%)	82,113,113	1.30	7 (8%)
18	CLA	a	815	1	69,73,73	1.16	8 (11%)	82,113,113	1.26	7 (8%)
18	CLA	a	816	1	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)
20	LHG	b	835	18	48,48,48	1.14	3 (6%)	51,54,54	1.04	3 (5%)
18	CLA	E	311	16	50,54,73	1.36	9 (18%)	59,90,113	1.38	5 (8%)
18	CLA	a	825	1	64,68,73	1.24	11 (17%)	76,107,113	1.47	10 (13%)
28	DD6	B	303	-	40,45,45	2.06	7 (17%)	51,67,67	2.92	18 (35%)
18	CLA	a	828	1	69,73,73	1.16	8 (11%)	82,113,113	1.26	6 (7%)
21	BCR	m	101	-	41,41,41	0.66	0	56,56,56	2.14	15 (26%)
18	CLA	b	817	2	64,68,73	1.21	9 (14%)	76,107,113	1.29	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	311	13	69,73,73	1.16	8 (11%)	82,113,113	1.27	6 (7%)
26	A86	m	102	-	47,50,50	1.56	9 (19%)	51,76,76	3.32	25 (49%)
18	CLA	a	814	1	69,73,73	1.16	9 (13%)	82,113,113	1.27	6 (7%)
18	CLA	E	310	16	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
18	CLA	a	802	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
23	LMG	l	207	-	40,40,55	1.23	4 (10%)	48,48,63	1.79	4 (8%)
18	CLA	b	846	2	69,73,73	1.16	8 (11%)	82,113,113	1.24	5 (6%)
18	CLA	H	314	17	69,73,73	1.17	9 (13%)	82,113,113	1.38	8 (9%)
18	CLA	a	838	1	69,73,73	1.16	7 (10%)	82,113,113	1.27	6 (7%)
18	CLA	b	830	20	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
18	CLA	H	310	-	64,68,73	1.21	8 (12%)	76,107,113	1.45	7 (9%)
18	CLA	a	824	1	55,59,73	1.29	8 (14%)	64,96,113	1.43	8 (12%)
21	BCR	r	201	-	41,41,41	0.67	0	56,56,56	1.77	15 (26%)
18	CLA	a	844	1	69,73,73	1.17	7 (10%)	82,113,113	1.28	5 (6%)
23	LMG	E	318	-	43,43,55	2.00	7 (16%)	51,51,63	1.99	7 (13%)
20	LHG	B	315	-	41,41,48	0.99	2 (4%)	44,47,54	1.10	3 (6%)
18	CLA	B	308	13	69,73,73	1.17	9 (13%)	82,113,113	1.27	5 (6%)
18	CLA	a	823	1	49,53,73	1.37	8 (16%)	58,89,113	1.42	4 (6%)
18	CLA	a	817	1	53,57,73	1.32	8 (15%)	61,93,113	1.42	5 (8%)
29	KC1	B	313	-	49,53,53	1.55	8 (16%)	61,89,89	1.89	13 (21%)
18	CLA	a	839	1	69,73,73	1.14	9 (13%)	82,113,113	1.30	5 (6%)
18	CLA	D	207	-	65,69,73	1.20	10 (15%)	77,108,113	1.39	7 (9%)
18	CLA	b	818	2	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
18	CLA	B	312	13	69,73,73	1.15	8 (11%)	82,113,113	1.27	4 (4%)
18	CLA	B	307	13	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
18	CLA	b	811	2	64,68,73	1.20	8 (12%)	76,107,113	1.40	6 (7%)
18	CLA	l	202	10	53,57,73	1.33	9 (16%)	61,93,113	1.49	8 (13%)
18	CLA	b	828	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	6 (7%)
18	CLA	a	808	1	69,73,73	1.17	9 (13%)	82,113,113	1.28	5 (6%)
18	CLA	b	805	2	69,73,73	1.16	8 (11%)	82,113,113	1.34	6 (7%)
21	BCR	E	306	-	41,41,41	0.69	0	56,56,56	2.02	15 (26%)
23	LMG	C	319	18	44,44,55	1.32	7 (15%)	52,52,63	1.85	4 (7%)
18	CLA	H	306	17	69,73,73	1.17	9 (13%)	82,113,113	1.29	6 (7%)
18	CLA	a	807	1	69,73,73	1.19	9 (13%)	82,113,113	1.46	9 (10%)
20	LHG	D	201	-	48,48,48	1.12	4 (8%)	51,54,54	1.05	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	KC1	C	313	-	49,53,53	1.36	6 (12%)	61,89,89	1.76	13 (21%)
25	DGD	b	834	-	61,61,67	0.86	2 (3%)	75,75,81	1.11	4 (5%)
18	CLA	b	816	2	59,63,73	1.25	8 (13%)	70,101,113	1.31	4 (5%)
18	CLA	a	822	1	54,58,73	1.30	7 (12%)	64,95,113	1.41	6 (9%)
21	BCR	a	852	-	41,41,41	0.71	0	56,56,56	2.15	17 (30%)
18	CLA	a	806	1	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
18	CLA	b	838	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	5 (6%)
18	CLA	E	314	16	49,53,73	1.38	11 (22%)	58,89,113	1.47	6 (10%)
18	CLA	a	801	1	69,73,73	1.22	9 (13%)	82,113,113	1.34	8 (9%)
18	CLA	D	214	15	60,64,73	1.25	9 (15%)	71,102,113	1.38	7 (9%)
21	BCR	j	105	-	41,41,41	0.73	0	56,56,56	2.09	11 (19%)
18	CLA	B	309	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	5 (6%)
18	CLA	a	805	1	69,73,73	1.15	8 (11%)	82,113,113	1.31	6 (7%)
26	A86	H	302	-	47,50,50	1.80	10 (21%)	51,76,76	3.56	24 (47%)
21	BCR	b	832	-	41,41,41	0.68	0	56,56,56	1.92	14 (25%)
18	CLA	C	316	14	45,49,73	1.40	10 (22%)	54,84,113	1.52	5 (9%)
18	CLA	a	846	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	5 (6%)
18	CLA	b	825	-	49,53,73	1.40	8 (16%)	58,89,113	1.42	5 (8%)
18	CLA	b	824	-	69,73,73	1.20	8 (11%)	82,113,113	1.48	7 (8%)
21	BCR	j	101	-	41,41,41	0.69	0	56,56,56	2.06	13 (23%)
24	SF4	c	101	3	0,12,12	-	-	-	-	-
18	CLA	b	844	2	66,70,73	1.18	8 (12%)	78,109,113	1.32	5 (6%)
18	CLA	a	843	-	69,73,73	1.16	8 (11%)	82,113,113	1.32	7 (8%)
18	CLA	B	314	13	45,49,73	1.41	9 (20%)	54,84,113	1.49	7 (12%)
18	CLA	E	315	16	69,73,73	1.18	9 (13%)	82,113,113	1.27	5 (6%)
18	CLA	D	215	-	45,49,73	1.41	9 (20%)	54,84,113	1.46	5 (9%)
26	A86	H	301	-	47,50,50	1.74	10 (21%)	51,76,76	3.37	25 (49%)
18	CLA	H	307	17	69,73,73	1.18	8 (11%)	82,113,113	1.48	12 (14%)
18	CLA	a	830	20	56,60,73	1.30	9 (16%)	65,97,113	1.37	5 (7%)
18	CLA	b	829	2	69,73,73	1.20	9 (13%)	82,113,113	1.44	8 (9%)
18	CLA	a	812	-	49,53,73	1.39	9 (18%)	58,89,113	1.45	4 (6%)
21	BCR	a	833	-	41,41,41	0.89	1 (2%)	56,56,56	1.93	21 (37%)
18	CLA	a	841	-	69,73,73	1.20	9 (13%)	82,113,113	1.34	8 (9%)
18	CLA	b	812	2	63,67,73	1.22	9 (14%)	74,105,113	1.31	6 (8%)
26	A86	C	304	-	47,50,50	1.67	9 (19%)	51,76,76	2.83	16 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	C	310	14	50,54,73	1.31	8 (16%)	59,90,113	1.41	5 (8%)
18	CLA	a	854	-	69,73,73	1.20	7 (10%)	82,113,113	1.43	6 (7%)
26	A86	D	203	-	47,50,50	1.58	7 (14%)	51,76,76	3.56	20 (39%)
18	CLA	a	847	1	69,73,73	1.17	9 (13%)	82,113,113	1.28	5 (6%)
20	LHG	a	831	-	48,48,48	1.16	3 (6%)	51,54,54	1.02	3 (5%)
21	BCR	b	839	-	41,41,41	1.01	2 (4%)	56,56,56	2.04	20 (35%)
18	CLA	b	823	2	62,66,73	1.22	8 (12%)	73,104,113	1.36	6 (8%)
18	CLA	f	202	-	69,73,73	1.16	7 (10%)	82,113,113	1.30	7 (8%)
28	DD6	E	308	-	40,45,45	1.54	2 (5%)	51,67,67	1.77	12 (23%)
24	SF4	c	102	3	0,12,12	-	-	-	-	-
18	CLA	a	811	1	54,58,73	1.29	8 (14%)	64,95,113	1.43	7 (10%)
18	CLA	H	309	17	50,54,73	1.35	8 (16%)	59,90,113	1.40	4 (6%)
18	CLA	a	804	18,1	59,63,73	1.27	9 (15%)	70,101,113	1.34	6 (8%)
18	CLA	b	806	2	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
18	CLA	b	821	2	54,58,73	1.31	9 (16%)	64,95,113	1.36	6 (9%)
18	CLA	b	826	2	64,68,73	1.21	8 (12%)	76,107,113	1.36	7 (9%)
21	BCR	E	305	-	41,41,41	0.67	0	56,56,56	1.88	17 (30%)
18	CLA	a	820	1	69,73,73	1.17	8 (11%)	82,113,113	1.31	7 (8%)
18	CLA	b	815	2	50,54,73	1.36	9 (18%)	59,90,113	1.45	4 (6%)
24	SF4	b	802	2	0,12,12	-	-	-	-	-
18	CLA	a	848	1	60,64,73	1.26	8 (13%)	71,102,113	1.31	5 (7%)
18	CLA	C	306	23	49,53,73	1.39	9 (18%)	58,89,113	1.44	4 (6%)
18	CLA	a	837	1	64,68,73	1.25	8 (12%)	76,107,113	1.52	8 (10%)
26	A86	B	304	-	47,50,50	1.70	9 (19%)	51,76,76	3.02	19 (37%)
18	CLA	E	309	16	69,73,73	1.16	8 (11%)	82,113,113	1.28	7 (8%)
21	BCR	f	205	-	41,41,41	0.71	0	56,56,56	1.96	15 (26%)
28	DD6	D	205	-	40,45,45	1.98	7 (17%)	51,67,67	3.21	24 (47%)
19	PQN	a	829	-	34,34,34	1.63	2 (5%)	43,45,45	1.10	3 (6%)
23	LMG	D	202	-	46,46,55	1.80	7 (15%)	54,54,63	1.37	5 (9%)
18	CLA	H	313	17	69,73,73	1.17	9 (13%)	82,113,113	1.44	7 (8%)
27	ET4	l	206	-	41,43,43	1.45	8 (19%)	52,60,60	2.23	18 (34%)
18	CLA	b	841	2	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
18	CLA	a	819	1	69,73,73	1.16	8 (11%)	82,113,113	1.30	6 (7%)
28	DD6	H	303	-	40,45,45	2.16	11 (27%)	51,67,67	2.44	19 (37%)
29	KC1	H	312	17	49,53,53	1.63	8 (16%)	61,89,89	1.80	13 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	A86	B	305	-	47,50,50	1.72	12 (25%)	51,76,76	3.43	27 (52%)
21	BCR	l	201	-	41,41,41	0.96	2 (4%)	56,56,56	2.05	16 (28%)
18	CLA	C	317	-	46,50,73	1.44	8 (17%)	53,85,113	1.60	5 (9%)
18	CLA	b	827	2	51,55,73	1.35	9 (17%)	60,91,113	1.40	5 (8%)
18	CLA	D	211	15	50,54,73	1.37	9 (18%)	59,90,113	1.41	4 (6%)
18	CLA	b	843	2	69,73,73	1.17	8 (11%)	82,113,113	1.35	6 (7%)
18	CLA	b	804	2	49,53,73	1.38	9 (18%)	58,89,113	1.52	6 (10%)
20	LHG	j	102	-	48,48,48	1.15	6 (12%)	51,54,54	0.93	2 (3%)
26	A86	C	305	-	47,50,50	1.76	10 (21%)	51,76,76	3.40	26 (50%)
18	CLA	H	311	17	61,65,73	1.24	7 (11%)	72,103,113	1.40	6 (8%)
18	CLA	l	203	10	69,73,73	1.18	8 (11%)	82,113,113	1.45	7 (8%)
18	CLA	b	813	2	59,63,73	1.26	8 (13%)	70,101,113	1.35	5 (7%)
18	CLA	C	307	14	69,73,73	1.17	7 (10%)	82,113,113	1.35	8 (9%)
18	CLA	b	837	2	64,68,73	1.20	8 (12%)	76,107,113	1.44	6 (7%)
19	PQN	b	831	-	34,34,34	1.61	2 (5%)	43,45,45	1.21	4 (9%)
26	A86	r	203	-	47,50,50	1.78	10 (21%)	51,76,76	3.90	27 (52%)
29	KC1	C	308	14	49,53,53	1.35	6 (12%)	61,89,89	1.78	13 (21%)
20	LHG	H	316	-	34,34,48	1.15	4 (11%)	37,40,54	0.98	2 (5%)
28	DD6	E	303	-	40,45,45	1.53	2 (5%)	51,67,67	1.88	8 (15%)
18	CLA	b	820	2	69,73,73	1.16	9 (13%)	82,113,113	1.48	7 (8%)
18	CLA	a	853	1	59,63,73	1.27	8 (13%)	70,101,113	1.37	6 (8%)
18	CLA	B	306	13	61,65,73	1.23	9 (14%)	73,102,113	1.25	3 (4%)
18	CLA	H	305	-	58,62,73	1.27	8 (13%)	68,99,113	1.48	6 (8%)
18	CLA	b	803	2	69,73,73	1.22	9 (13%)	82,113,113	1.33	8 (9%)
18	CLA	b	840	2	65,69,73	1.19	9 (13%)	77,108,113	1.34	6 (7%)
18	CLA	b	848	2	58,62,73	1.27	8 (13%)	68,99,113	1.31	4 (5%)
28	DD6	C	303	-	40,45,45	1.70	3 (7%)	51,67,67	2.28	17 (33%)
18	CLA	b	850	2	69,73,73	1.16	7 (10%)	82,113,113	1.28	5 (6%)
21	BCR	b	836	-	41,41,41	0.74	0	56,56,56	2.00	17 (30%)
18	CLA	b	808	2	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
18	CLA	D	208	15	69,73,73	1.20	11 (15%)	82,113,113	1.46	9 (10%)
18	CLA	a	810	1	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
18	CLA	H	308	17	69,73,73	1.17	9 (13%)	82,113,113	1.43	7 (8%)
21	BCR	b	833	-	41,41,41	0.69	0	56,56,56	3.34	20 (35%)
18	CLA	b	809	2	59,63,73	1.28	9 (15%)	70,101,113	1.36	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	f	204	6	49,53,73	1.39	8 (16%)	58,89,113	1.43	4 (6%)
18	CLA	E	316	-	60,64,73	1.25	8 (13%)	71,102,113	1.34	5 (7%)
18	CLA	j	104	9	45,49,73	1.41	8 (17%)	54,84,113	1.51	5 (9%)
18	CLA	a	818	1	55,59,73	1.31	8 (14%)	64,96,113	1.55	7 (10%)
18	CLA	a	840	-	69,73,73	1.21	8 (11%)	82,113,113	1.36	6 (7%)
18	CLA	D	209	15	53,57,73	1.33	9 (16%)	61,93,113	1.40	5 (8%)
20	LHG	E	301	-	48,48,48	1.15	6 (12%)	51,54,54	1.05	3 (5%)
18	CLA	D	212	15	46,50,73	1.39	8 (17%)	53,85,113	1.41	4 (7%)
18	CLA	C	315	14	46,50,73	1.41	7 (15%)	53,85,113	1.41	4 (7%)
21	BCR	a	834	-	41,41,41	0.70	0	56,56,56	1.98	15 (26%)
23	LMG	C	301	-	31,31,55	1.60	6 (19%)	39,39,63	3.05	7 (17%)
18	CLA	b	842	2	69,73,73	1.16	8 (11%)	82,113,113	1.28	5 (6%)
26	A86	E	302	-	47,50,50	1.68	9 (19%)	51,76,76	3.04	24 (47%)
18	CLA	C	314	14	45,49,73	1.41	11 (24%)	54,84,113	1.49	6 (11%)
22	SQD	a	849	-	31,32,54	3.13	8 (25%)	33,36,65	2.78	8 (24%)
18	CLA	b	819	2	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
18	CLA	i	101	-	64,68,73	1.21	8 (12%)	76,107,113	1.32	7 (9%)
18	CLA	b	822	2	69,73,73	1.16	8 (11%)	82,113,113	1.30	6 (7%)
18	CLA	f	203	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	5 (6%)
18	CLA	a	842	-	69,73,73	1.17	7 (10%)	82,113,113	1.39	6 (7%)
21	BCR	a	850	-	41,41,41	1.05	2 (4%)	56,56,56	1.80	11 (19%)
18	CLA	l	205	-	49,53,73	1.38	8 (16%)	58,89,113	1.44	6 (10%)
28	DD6	E	307	-	40,45,45	1.71	3 (7%)	51,67,67	2.90	20 (39%)
18	CLA	a	836	1	69,73,73	1.15	7 (10%)	82,113,113	1.24	5 (6%)
18	CLA	b	810	2	69,73,73	1.17	9 (13%)	82,113,113	1.29	5 (6%)
18	CLA	a	821	1	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
21	BCR	l	204	-	41,41,41	0.87	0	56,56,56	2.06	15 (26%)
18	CLA	C	318	14	46,50,73	1.38	8 (17%)	53,85,113	1.48	3 (5%)
20	LHG	a	832	18	26,26,48	1.31	5 (19%)	29,32,54	1.17	2 (6%)
26	A86	D	204	-	47,50,50	1.73	10 (21%)	51,76,76	3.96	24 (47%)
21	BCR	i	102	-	41,41,41	0.73	1 (2%)	56,56,56	1.96	17 (30%)
26	A86	B	302	-	47,50,50	1.81	10 (21%)	51,76,76	3.58	24 (47%)
18	CLA	b	845	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	5 (6%)
18	CLA	a	827	1	69,73,73	1.15	8 (11%)	82,113,113	1.31	6 (7%)
26	A86	H	304	-	47,50,50	1.71	9 (19%)	51,76,76	3.22	23 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	D	210	-	60,64,73	1.25	8 (13%)	71,102,113	1.43	6 (8%)
20	LHG	a	835	-	32,32,48	1.33	5 (15%)	35,38,54	1.20	2 (5%)
23	LMG	a	851	-	33,33,55	1.59	5 (15%)	41,41,63	3.67	7 (17%)
18	CLA	b	807	2	69,73,73	1.16	8 (11%)	82,113,113	1.23	5 (6%)
18	CLA	a	813	1	69,73,73	1.16	9 (13%)	82,113,113	1.47	10 (12%)
18	CLA	a	826	1	69,73,73	1.18	8 (11%)	82,113,113	1.30	6 (7%)
26	A86	C	302	-	47,50,50	1.74	11 (23%)	51,76,76	3.28	24 (47%)
18	CLA	C	309	-	66,70,73	1.19	9 (13%)	78,109,113	1.48	8 (10%)
23	LMG	j	103	-	37,37,55	1.57	5 (13%)	45,45,63	3.67	7 (15%)
18	CLA	C	311	14	64,68,73	1.22	9 (14%)	76,107,113	1.35	6 (7%)
18	CLA	D	216	15	50,54,73	1.34	8 (16%)	59,90,113	1.41	5 (8%)
18	CLA	E	313	16	59,63,73	1.26	9 (15%)	70,101,113	1.39	6 (8%)
18	CLA	b	801	-	69,73,73	1.20	10 (14%)	82,113,113	1.45	7 (8%)
18	CLA	r	202	12	49,53,73	1.37	8 (16%)	58,89,113	1.40	5 (8%)
18	CLA	a	855	1	69,73,73	1.16	8 (11%)	82,113,113	1.31	7 (8%)
18	CLA	B	310	13	50,54,73	1.36	9 (18%)	59,90,113	1.39	4 (6%)
18	CLA	E	312	16	69,73,73	1.22	9 (13%)	82,113,113	1.34	7 (8%)
18	CLA	H	315	17	49,53,73	1.38	9 (18%)	58,89,113	1.45	4 (6%)
21	BCR	a	845	-	41,41,41	0.93	2 (4%)	56,56,56	1.96	20 (35%)
18	CLA	D	213	15	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
20	LHG	E	317	-	41,41,48	1.00	2 (4%)	44,47,54	1.22	5 (11%)
28	DD6	E	304	-	40,45,45	2.17	8 (20%)	51,67,67	3.34	15 (29%)
18	CLA	a	803	1	69,73,73	1.18	9 (13%)	82,113,113	1.49	7 (8%)
26	A86	B	301	-	47,50,50	1.50	7 (14%)	51,76,76	2.88	17 (33%)

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
18	CLA	a	809	18,1	1/1/14/20	13/36/112/115	-
26	A86	D	206	-	-	7/34/90/90	0/3/3/3
21	BCR	i	103	-	-	4/29/63/63	0/2/2/2
21	BCR	f	201	-	-	8/29/63/63	0/2/2/2
26	A86	b	847	-	-	15/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	b	849	-	1/1/15/20	16/39/115/115	-
18	CLA	C	312	14	1/1/14/20	12/35/111/115	-
18	CLA	D	217	-	1/1/10/20	4/10/86/115	-
18	CLA	b	814	-	1/1/15/20	11/39/115/115	-
18	CLA	a	815	1	1/1/15/20	15/39/115/115	-
18	CLA	a	816	1	1/1/11/20	10/15/91/115	-
20	LHG	b	835	18	-	32/53/53/53	-
18	CLA	E	311	16	1/1/11/20	6/17/93/115	-
18	CLA	a	825	1	1/1/14/20	13/33/109/115	-
28	DD6	B	303	-	-	0/26/80/80	0/3/3/3
18	CLA	a	828	1	1/1/15/20	10/39/115/115	-
21	BCR	m	101	-	-	7/29/63/63	0/2/2/2
18	CLA	b	817	2	1/1/14/20	17/33/109/115	-
18	CLA	B	311	13	1/1/15/20	12/39/115/115	-
26	A86	m	102	-	-	7/34/90/90	0/3/3/3
18	CLA	a	814	1	1/1/15/20	8/39/115/115	-
18	CLA	E	310	16	1/1/15/20	13/39/115/115	-
18	CLA	a	802	-	1/1/15/20	8/39/115/115	-
23	LMG	l	207	-	-	16/35/55/70	0/1/1/1
18	CLA	b	846	2	1/1/15/20	14/39/115/115	-
18	CLA	H	314	17	1/1/15/20	12/39/115/115	-
18	CLA	a	838	1	1/1/15/20	12/39/115/115	-
18	CLA	b	830	20	1/1/15/20	9/39/115/115	-
18	CLA	H	310	-	1/1/14/20	9/33/109/115	-
18	CLA	a	824	1	1/1/12/20	9/23/99/115	-
21	BCR	r	201	-	-	4/29/63/63	0/2/2/2
18	CLA	a	844	1	1/1/15/20	16/39/115/115	-
23	LMG	E	318	-	-	21/38/58/70	0/1/1/1
20	LHG	B	315	-	-	25/46/46/53	-
18	CLA	B	308	13	1/1/15/20	11/39/115/115	-
18	CLA	a	823	1	1/1/11/20	9/15/91/115	-
18	CLA	a	817	1	1/1/11/20	11/20/96/115	-
29	KC1	B	313	-	-	6/15/71/71	-
18	CLA	a	839	1	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	D	207	-	1/1/14/20	11/35/111/115	-
18	CLA	b	818	2	1/1/15/20	7/39/115/115	-
18	CLA	B	312	13	1/1/15/20	12/39/115/115	-
18	CLA	B	307	13	1/1/15/20	8/39/115/115	-
18	CLA	b	811	2	1/1/14/20	8/33/109/115	-
18	CLA	l	202	10	1/1/11/20	7/20/96/115	-
18	CLA	b	828	-	1/1/15/20	10/39/115/115	-
18	CLA	a	808	1	1/1/15/20	12/39/115/115	-
18	CLA	b	805	2	1/1/15/20	13/39/115/115	-
21	BCR	E	306	-	-	0/29/63/63	0/2/2/2
23	LMG	C	319	18	-	20/39/59/70	0/1/1/1
18	CLA	H	306	17	1/1/15/20	12/39/115/115	-
18	CLA	a	807	1	1/1/15/20	9/39/115/115	-
20	LHG	D	201	-	-	32/53/53/53	-
29	KC1	C	313	-	-	5/15/71/71	-
25	DGD	b	834	-	-	28/49/89/95	0/2/2/2
18	CLA	b	816	2	1/1/13/20	6/27/103/115	-
18	CLA	a	822	1	1/1/12/20	7/21/97/115	-
21	BCR	a	852	-	-	8/29/63/63	0/2/2/2
18	CLA	a	806	1	1/1/15/20	13/39/115/115	-
18	CLA	b	838	-	1/1/15/20	8/39/115/115	-
18	CLA	E	314	16	1/1/11/20	4/15/91/115	-
18	CLA	a	801	1	1/1/15/20	15/39/115/115	-
18	CLA	D	214	15	1/1/13/20	9/29/105/115	-
21	BCR	j	105	-	-	5/29/63/63	0/2/2/2
18	CLA	B	309	-	1/1/15/20	9/39/115/115	-
18	CLA	a	805	1	1/1/15/20	12/39/115/115	-
26	A86	H	302	-	-	5/34/90/90	0/3/3/3
21	BCR	b	832	-	-	0/29/63/63	0/2/2/2
18	CLA	C	316	14	1/1/10/20	4/10/86/115	-
18	CLA	a	846	-	1/1/15/20	8/39/115/115	-
18	CLA	b	825	-	1/1/11/20	4/15/91/115	-
18	CLA	b	824	-	1/1/15/20	17/39/115/115	-
21	BCR	j	101	-	-	2/29/63/63	0/2/2/2
28	DD6	E	308	-	-	1/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	b	844	2	1/1/14/20	10/36/112/115	-
18	CLA	a	843	-	1/1/15/20	10/39/115/115	-
18	CLA	B	314	13	1/1/10/20	2/10/86/115	-
18	CLA	E	315	16	1/1/15/20	11/39/115/115	-
18	CLA	D	215	-	1/1/10/20	4/10/86/115	-
26	A86	H	301	-	-	5/34/90/90	0/3/3/3
18	CLA	H	307	17	1/1/15/20	15/39/115/115	-
18	CLA	a	830	20	1/1/12/20	6/24/100/115	-
18	CLA	b	829	2	1/1/15/20	13/39/115/115	-
18	CLA	a	812	-	1/1/11/20	6/15/91/115	-
21	BCR	a	833	-	-	0/29/63/63	0/2/2/2
18	CLA	a	841	-	1/1/15/20	20/39/115/115	-
18	CLA	b	812	2	1/1/13/20	9/32/108/115	-
26	A86	C	304	-	-	4/34/90/90	0/3/3/3
18	CLA	C	310	14	1/1/11/20	8/17/93/115	-
18	CLA	a	854	-	1/1/15/20	16/39/115/115	-
26	A86	D	203	-	-	10/34/90/90	0/3/3/3
18	CLA	a	847	1	1/1/15/20	14/39/115/115	-
20	LHG	a	831	-	-	25/53/53/53	-
21	BCR	b	839	-	-	6/29/63/63	0/2/2/2
18	CLA	b	823	2	1/1/13/20	13/31/107/115	-
18	CLA	f	202	-	1/1/15/20	7/39/115/115	-
24	SF4	c	102	3	-	-	0/6/5/5
18	CLA	a	811	1	1/1/12/20	6/21/97/115	-
18	CLA	H	309	17	1/1/11/20	9/17/93/115	-
18	CLA	a	804	18,1	1/1/13/20	5/27/103/115	-
18	CLA	b	806	2	1/1/15/20	15/39/115/115	-
18	CLA	b	821	2	1/1/12/20	9/21/97/115	-
18	CLA	b	826	2	1/1/14/20	9/33/109/115	-
21	BCR	E	305	-	-	2/29/63/63	0/2/2/2
18	CLA	a	820	1	1/1/15/20	8/39/115/115	-
18	CLA	b	815	2	1/1/11/20	6/17/93/115	-
24	SF4	b	802	2	-	-	0/6/5/5
18	CLA	a	848	1	1/1/13/20	11/29/105/115	-
18	CLA	C	306	23	1/1/11/20	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	a	837	1	1/1/14/20	14/33/109/115	-
26	A86	B	304	-	-	3/34/90/90	0/3/3/3
18	CLA	E	309	16	1/1/15/20	13/39/115/115	-
21	BCR	f	205	-	-	2/29/63/63	0/2/2/2
28	DD6	D	205	-	-	3/26/80/80	0/3/3/3
19	PQN	a	829	-	-	2/23/43/43	0/2/2/2
23	LMG	D	202	-	-	17/41/61/70	0/1/1/1
18	CLA	H	313	17	1/1/15/20	18/39/115/115	-
27	ET4	l	206	-	-	3/25/67/67	0/2/2/2
18	CLA	b	841	2	1/1/15/20	7/39/115/115	-
18	CLA	a	819	1	1/1/15/20	4/39/115/115	-
28	DD6	H	303	-	-	3/26/80/80	0/3/3/3
29	KC1	H	312	17	-	9/15/71/71	-
26	A86	B	305	-	-	4/34/90/90	0/3/3/3
21	BCR	l	201	-	-	4/29/63/63	0/2/2/2
18	CLA	C	317	-	1/1/10/20	8/12/88/115	-
18	CLA	b	827	2	1/1/11/20	5/18/94/115	-
18	CLA	D	211	15	1/1/11/20	10/17/93/115	-
18	CLA	b	843	2	1/1/15/20	17/39/115/115	-
18	CLA	b	804	2	1/1/11/20	3/15/91/115	-
20	LHG	j	102	-	-	18/53/53/53	-
26	A86	C	305	-	-	4/34/90/90	0/3/3/3
18	CLA	H	311	17	1/1/13/20	8/30/106/115	-
18	CLA	l	203	10	1/1/15/20	16/39/115/115	-
18	CLA	b	813	2	1/1/13/20	12/27/103/115	-
18	CLA	C	307	14	1/1/15/20	5/39/115/115	-
18	CLA	b	837	2	1/1/14/20	13/33/109/115	-
19	PQN	b	831	-	-	3/23/43/43	0/2/2/2
26	A86	r	203	-	-	6/34/90/90	0/3/3/3
29	KC1	C	308	14	-	7/15/71/71	-
20	LHG	H	316	-	-	19/38/38/53	-
28	DD6	E	303	-	-	3/26/80/80	0/3/3/3
18	CLA	b	820	2	1/1/15/20	15/39/115/115	-
18	CLA	a	853	1	1/1/13/20	10/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	306	13	1/1/12/20	18/29/101/115	-
18	CLA	H	305	-	1/1/12/20	10/26/102/115	-
24	SF4	c	101	3	-	-	0/6/5/5
18	CLA	b	803	2	1/1/15/20	17/39/115/115	-
18	CLA	b	840	2	1/1/14/20	12/35/111/115	-
18	CLA	b	848	2	1/1/12/20	10/26/102/115	-
28	DD6	C	303	-	-	5/26/80/80	0/3/3/3
18	CLA	b	850	2	1/1/15/20	11/39/115/115	-
21	BCR	b	836	-	-	5/29/63/63	0/2/2/2
18	CLA	b	808	2	1/1/15/20	10/39/115/115	-
18	CLA	D	208	15	1/1/15/20	15/39/115/115	-
18	CLA	a	810	1	1/1/15/20	8/39/115/115	-
18	CLA	H	308	17	1/1/15/20	10/39/115/115	-
21	BCR	b	833	-	-	6/29/63/63	0/2/2/2
18	CLA	b	809	2	1/1/13/20	4/27/103/115	-
18	CLA	f	204	6	1/1/11/20	5/15/91/115	-
18	CLA	E	316	-	1/1/13/20	4/29/105/115	-
18	CLA	j	104	9	1/1/10/20	4/10/86/115	-
18	CLA	a	818	1	1/1/12/20	4/23/99/115	-
18	CLA	a	840	-	1/1/15/20	13/39/115/115	-
18	CLA	D	209	15	1/1/11/20	11/20/96/115	-
20	LHG	E	301	-	-	33/53/53/53	-
18	CLA	D	212	15	1/1/10/20	2/12/88/115	-
18	CLA	C	315	14	1/1/10/20	6/12/88/115	-
21	BCR	a	834	-	-	4/29/63/63	0/2/2/2
23	LMG	C	301	-	-	14/26/46/70	0/1/1/1
18	CLA	b	842	2	1/1/15/20	15/39/115/115	-
26	A86	E	302	-	-	5/34/90/90	0/3/3/3
18	CLA	C	314	14	1/1/10/20	4/10/86/115	-
22	SQD	a	849	-	-	19/33/33/69	-
18	CLA	b	819	2	1/1/15/20	14/39/115/115	-
18	CLA	i	101	-	1/1/14/20	10/33/109/115	-
18	CLA	b	822	2	1/1/15/20	15/39/115/115	-
18	CLA	f	203	-	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	a	842	-	1/1/15/20	9/39/115/115	-
21	BCR	a	850	-	-	4/29/63/63	0/2/2/2
18	CLA	l	205	-	1/1/11/20	3/15/91/115	-
28	DD6	E	307	-	-	11/26/80/80	0/3/3/3
18	CLA	a	836	1	1/1/15/20	12/39/115/115	-
18	CLA	b	810	2	1/1/15/20	7/39/115/115	-
18	CLA	a	821	1	1/1/15/20	13/39/115/115	-
21	BCR	l	204	-	-	8/29/63/63	0/2/2/2
18	CLA	C	318	14	1/1/10/20	6/12/88/115	-
20	LHG	a	832	18	-	13/31/31/53	-
26	A86	D	204	-	-	4/34/90/90	0/3/3/3
21	BCR	i	102	-	-	0/29/63/63	0/2/2/2
26	A86	B	302	-	-	5/34/90/90	0/3/3/3
18	CLA	b	845	-	1/1/15/20	13/39/115/115	-
18	CLA	a	827	1	1/1/15/20	7/39/115/115	-
26	A86	H	304	-	-	4/34/90/90	0/3/3/3
18	CLA	D	210	-	1/1/13/20	6/29/105/115	-
20	LHG	a	835	-	-	19/36/36/53	-
23	LMG	a	851	-	-	16/28/48/70	0/1/1/1
18	CLA	b	807	2	1/1/15/20	9/39/115/115	-
18	CLA	a	813	1	1/1/15/20	24/39/115/115	-
18	CLA	a	826	1	1/1/15/20	11/39/115/115	-
26	A86	C	302	-	-	5/34/90/90	0/3/3/3
18	CLA	C	309	-	1/1/14/20	14/36/112/115	-
23	LMG	j	103	-	-	16/32/52/70	0/1/1/1
18	CLA	C	311	14	1/1/14/20	13/33/109/115	-
18	CLA	D	216	15	1/1/11/20	5/17/93/115	-
18	CLA	E	313	16	1/1/13/20	9/27/103/115	-
18	CLA	b	801	-	1/1/15/20	8/39/115/115	-
18	CLA	r	202	12	1/1/11/20	11/15/91/115	-
18	CLA	a	855	1	1/1/15/20	12/39/115/115	-
18	CLA	B	310	13	1/1/11/20	6/17/93/115	-
18	CLA	E	312	16	1/1/15/20	10/39/115/115	-
18	CLA	H	315	17	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	a	845	-	-	2/29/63/63	0/2/2/2
18	CLA	D	213	15	1/1/15/20	10/39/115/115	-
20	LHG	E	317	-	-	5/46/46/53	-
28	DD6	E	304	-	-	6/26/80/80	0/3/3/3
18	CLA	a	803	1	1/1/15/20	13/39/115/115	-
26	A86	B	301	-	-	10/34/90/90	0/3/3/3

The worst 5 of 1547 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	849	SQD	C6-S	-12.69	1.59	1.77
23	E	318	LMG	O2-C2	-10.20	1.17	1.43
28	E	307	DD6	C30-C31	-9.01	1.25	1.42
28	E	304	DD6	C30-C31	-8.98	1.25	1.42
28	C	303	DD6	C30-C31	-8.95	1.25	1.42

The worst 5 of 1840 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	j	103	LMG	O2-C2-C1	-21.74	58.28	110.08
23	a	851	LMG	O2-C2-C1	-19.19	64.35	110.08
28	E	304	DD6	C21-C20-C15	-16.50	95.14	122.30
23	C	301	LMG	O2-C2-C1	15.53	147.09	110.08
21	b	833	BCR	C32-C1-C6	-14.58	87.39	110.24

5 of 142 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	a	801	CLA	ND
18	a	802	CLA	ND
18	a	803	CLA	ND
18	a	804	CLA	ND
18	a	805	CLA	ND

5 of 2059 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	a	801	CLA	CBD-CGD-O2D-CED
18	a	801	CLA	O1D-CGD-O2D-CED
18	a	803	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	a	803	CLA	CHA-CBD-CGD-O2D
18	a	804	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

188 monomers are involved in 611 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	a	809	CLA	4	0
21	i	103	BCR	5	0
21	f	201	BCR	4	0
26	b	847	A86	4	0
18	b	849	CLA	5	0
18	C	312	CLA	10	0
18	D	217	CLA	3	0
18	b	814	CLA	7	0
18	a	815	CLA	6	0
18	a	816	CLA	1	0
20	b	835	LHG	5	0
18	E	311	CLA	1	0
18	a	825	CLA	5	0
18	a	828	CLA	2	0
21	m	101	BCR	5	0
18	b	817	CLA	6	0
18	B	311	CLA	4	0
26	m	102	A86	5	0
18	a	814	CLA	2	0
18	E	310	CLA	1	0
18	a	802	CLA	12	0
23	l	207	LMG	1	0
18	b	846	CLA	2	0
18	H	314	CLA	5	0
18	a	838	CLA	2	0
18	b	830	CLA	1	0
18	H	310	CLA	3	0
21	r	201	BCR	2	0
18	a	844	CLA	5	0
23	E	318	LMG	5	0
20	B	315	LHG	3	0
18	B	308	CLA	1	0
18	a	823	CLA	1	0
18	a	817	CLA	1	0
29	B	313	KC1	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	a	839	CLA	1	0
18	D	207	CLA	3	0
18	b	818	CLA	3	0
18	B	312	CLA	7	0
18	B	307	CLA	4	0
18	b	811	CLA	1	0
18	l	202	CLA	4	0
18	b	828	CLA	1	0
18	a	808	CLA	5	0
18	b	805	CLA	4	0
21	E	306	BCR	7	0
23	C	319	LMG	1	0
18	H	306	CLA	8	0
18	a	807	CLA	14	0
20	D	201	LHG	6	0
21	a	852	BCR	14	0
18	a	806	CLA	4	0
18	b	838	CLA	4	0
18	a	801	CLA	3	0
18	D	214	CLA	5	0
21	j	105	BCR	11	0
18	B	309	CLA	2	0
18	a	805	CLA	2	0
26	H	302	A86	17	0
21	b	832	BCR	3	0
18	C	316	CLA	10	0
18	a	846	CLA	1	0
18	b	825	CLA	3	0
18	b	824	CLA	5	0
21	j	101	BCR	6	0
24	c	101	SF4	2	0
18	b	844	CLA	2	0
18	B	314	CLA	3	0
18	E	315	CLA	3	0
18	D	215	CLA	5	0
18	H	307	CLA	4	0
18	a	830	CLA	3	0
18	b	829	CLA	6	0
21	a	833	BCR	17	0
18	a	841	CLA	7	0
18	b	812	CLA	2	0
26	C	304	A86	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	C	310	CLA	3	0
18	a	854	CLA	3	0
26	D	203	A86	3	0
18	a	847	CLA	3	0
20	a	831	LHG	2	0
21	b	839	BCR	9	0
18	b	823	CLA	7	0
18	f	202	CLA	1	0
24	c	102	SF4	5	0
18	a	811	CLA	1	0
18	H	309	CLA	16	0
18	a	804	CLA	7	0
18	b	806	CLA	3	0
18	b	821	CLA	3	0
21	E	305	BCR	2	0
18	a	820	CLA	2	0
24	b	802	SF4	2	0
18	a	848	CLA	5	0
18	a	837	CLA	5	0
26	B	304	A86	2	0
18	E	309	CLA	5	0
21	f	205	BCR	2	0
28	D	205	DD6	3	0
19	a	829	PQN	1	0
23	D	202	LMG	1	0
18	H	313	CLA	6	0
18	b	841	CLA	3	0
18	a	819	CLA	1	0
28	H	303	DD6	3	0
29	H	312	KC1	1	0
21	l	201	BCR	3	0
18	C	317	CLA	8	0
18	b	827	CLA	2	0
18	D	211	CLA	2	0
18	b	843	CLA	5	0
18	b	804	CLA	1	0
20	j	102	LHG	5	0
26	C	305	A86	4	0
18	H	311	CLA	6	0
18	l	203	CLA	6	0
18	b	813	CLA	18	0
18	C	307	CLA	6	0

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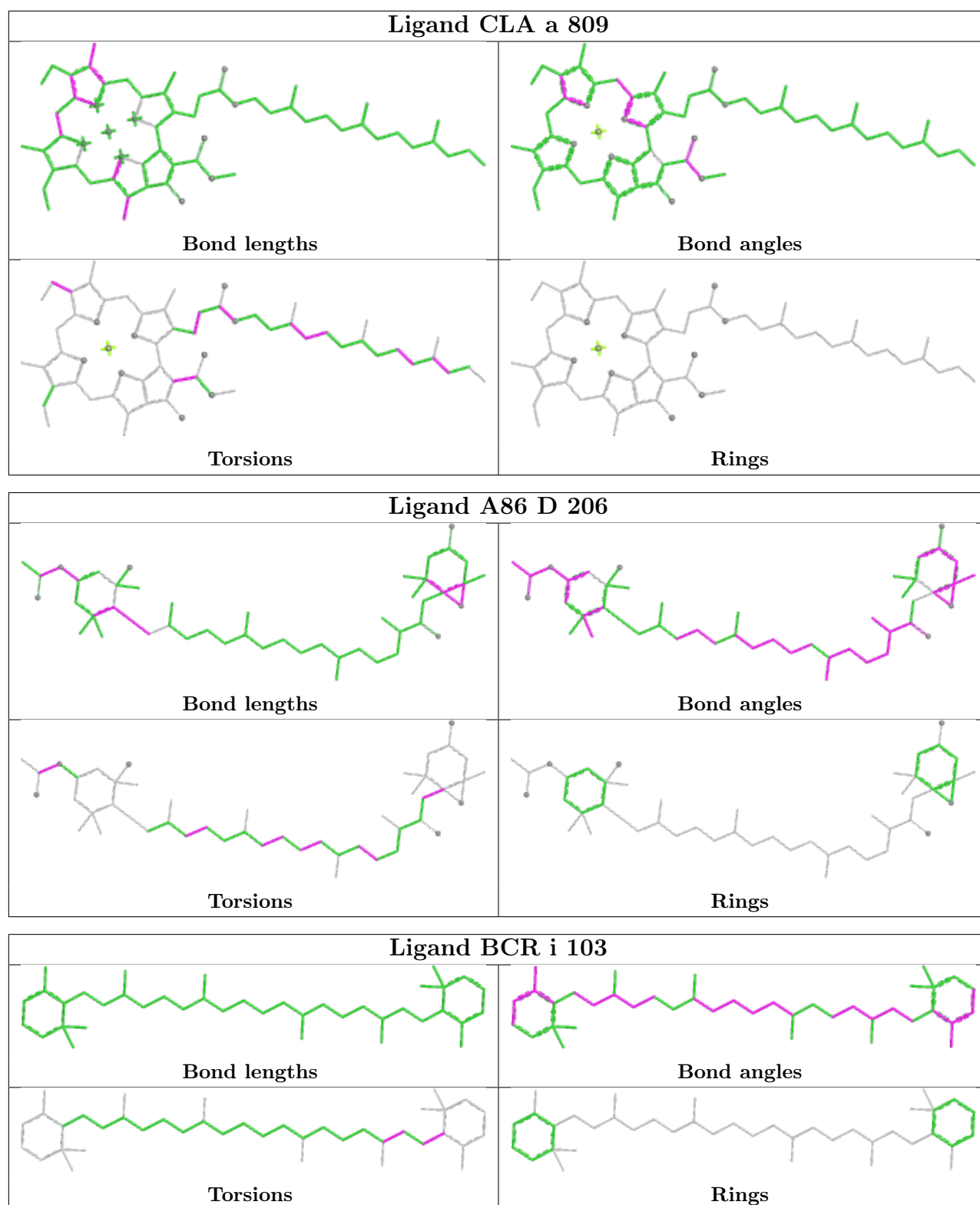
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	b	837	CLA	2	0
19	b	831	PQN	4	0
26	r	203	A86	1	0
29	C	308	KC1	4	0
18	b	820	CLA	5	0
18	B	306	CLA	13	0
18	H	305	CLA	3	0
18	b	803	CLA	4	0
18	b	840	CLA	3	0
18	b	848	CLA	3	0
28	C	303	DD6	1	0
18	b	850	CLA	6	0
21	b	836	BCR	4	0
18	b	808	CLA	2	0
18	D	208	CLA	9	0
18	a	810	CLA	3	0
18	H	308	CLA	4	0
21	b	833	BCR	3	0
18	b	809	CLA	2	0
18	f	204	CLA	1	0
18	E	316	CLA	6	0
18	j	104	CLA	1	0
18	a	818	CLA	2	0
18	a	840	CLA	2	0
18	D	209	CLA	3	0
20	E	301	LHG	3	0
18	D	212	CLA	1	0
18	C	315	CLA	2	0
21	a	834	BCR	4	0
18	b	842	CLA	6	0
18	C	314	CLA	3	0
22	a	849	SQD	7	0
18	b	819	CLA	4	0
18	i	101	CLA	1	0
18	b	822	CLA	3	0
18	f	203	CLA	1	0
18	a	842	CLA	5	0
21	a	850	BCR	4	0
28	E	307	DD6	1	0
18	a	836	CLA	3	0
18	b	810	CLA	2	0
18	a	821	CLA	1	0

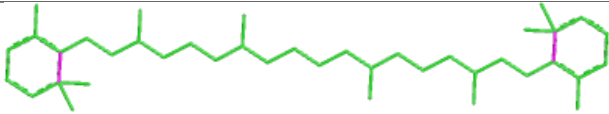
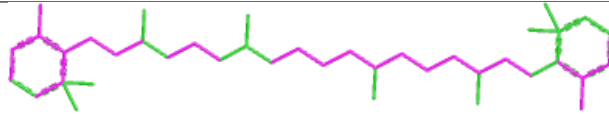
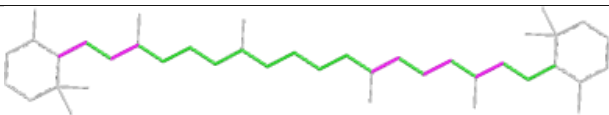
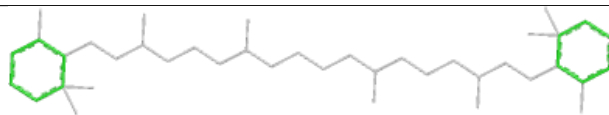
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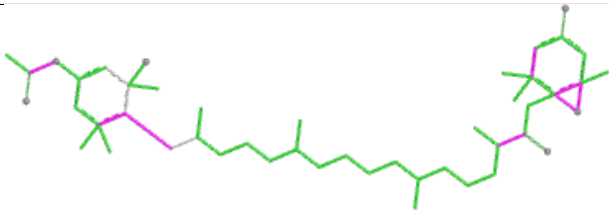
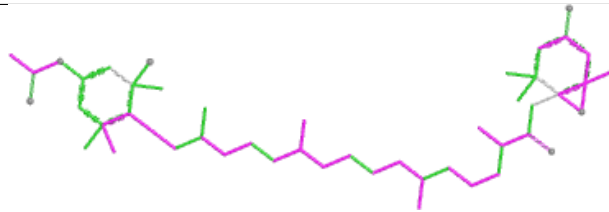
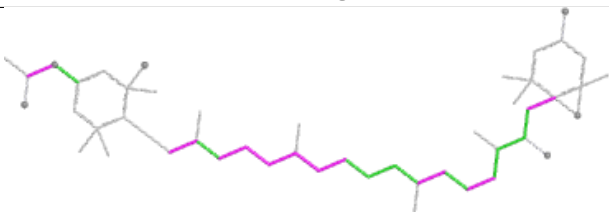
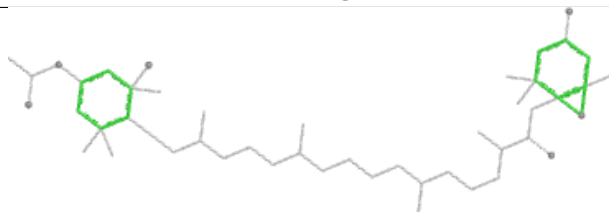
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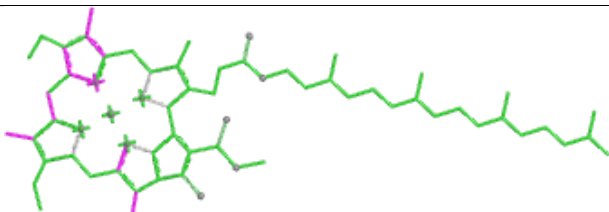
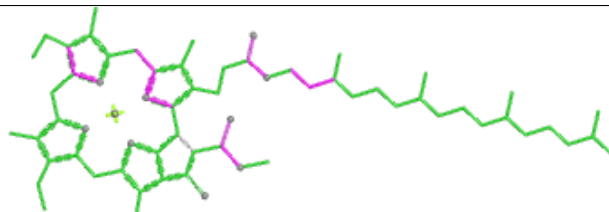
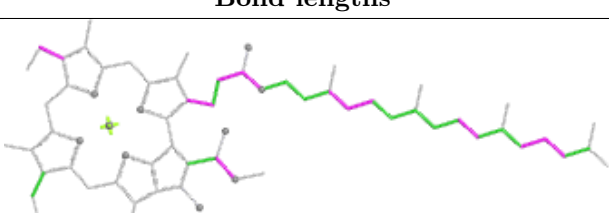
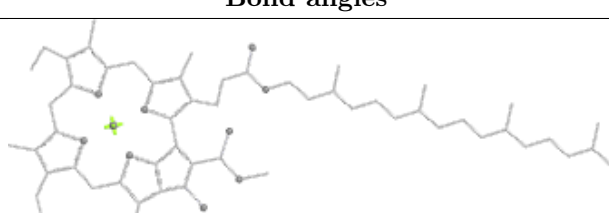
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	l	204	BCR	8	0
18	C	318	CLA	11	0
20	a	832	LHG	3	0
21	i	102	BCR	9	0
26	B	302	A86	3	0
18	b	845	CLA	7	0
18	a	827	CLA	3	0
18	D	210	CLA	1	0
20	a	835	LHG	1	0
23	a	851	LMG	2	0
18	b	807	CLA	3	0
18	a	813	CLA	8	0
18	a	826	CLA	1	0
18	C	309	CLA	6	0
18	C	311	CLA	6	0
18	D	216	CLA	4	0
18	E	313	CLA	2	0
18	b	801	CLA	10	0
18	r	202	CLA	2	0
18	a	855	CLA	5	0
18	E	312	CLA	7	0
21	a	845	BCR	4	0
18	D	213	CLA	2	0
20	E	317	LHG	2	0
28	E	304	DD6	1	0
18	a	803	CLA	12	0
26	B	301	A86	2	0

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

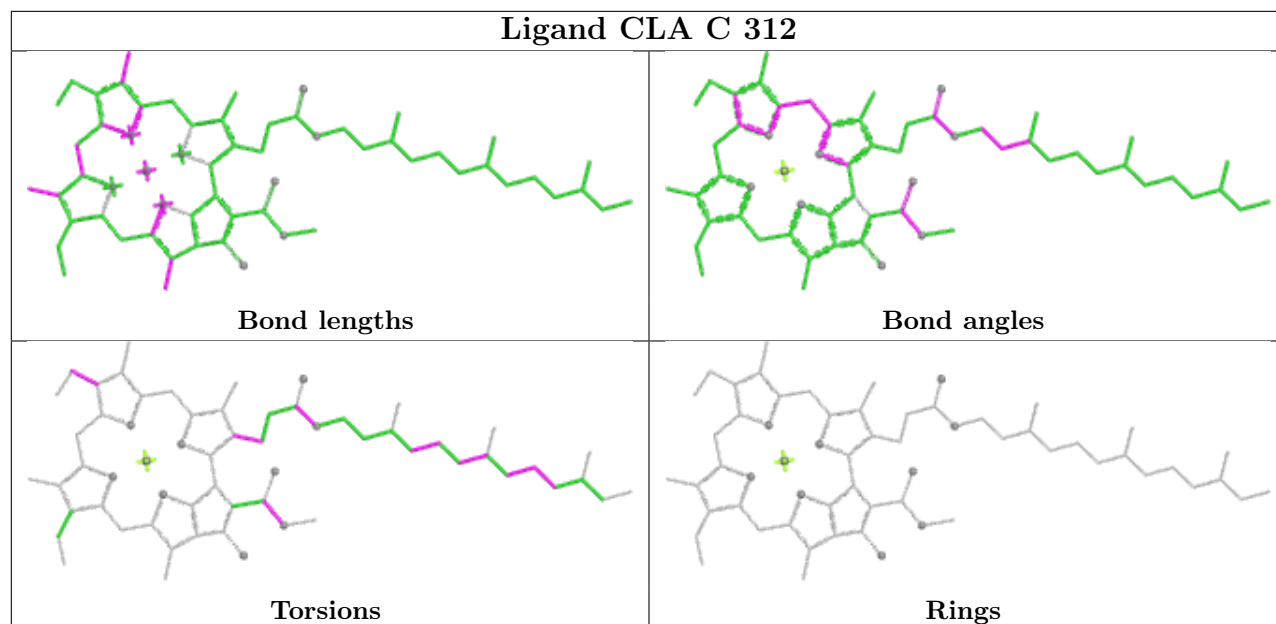


Ligand BCR f 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

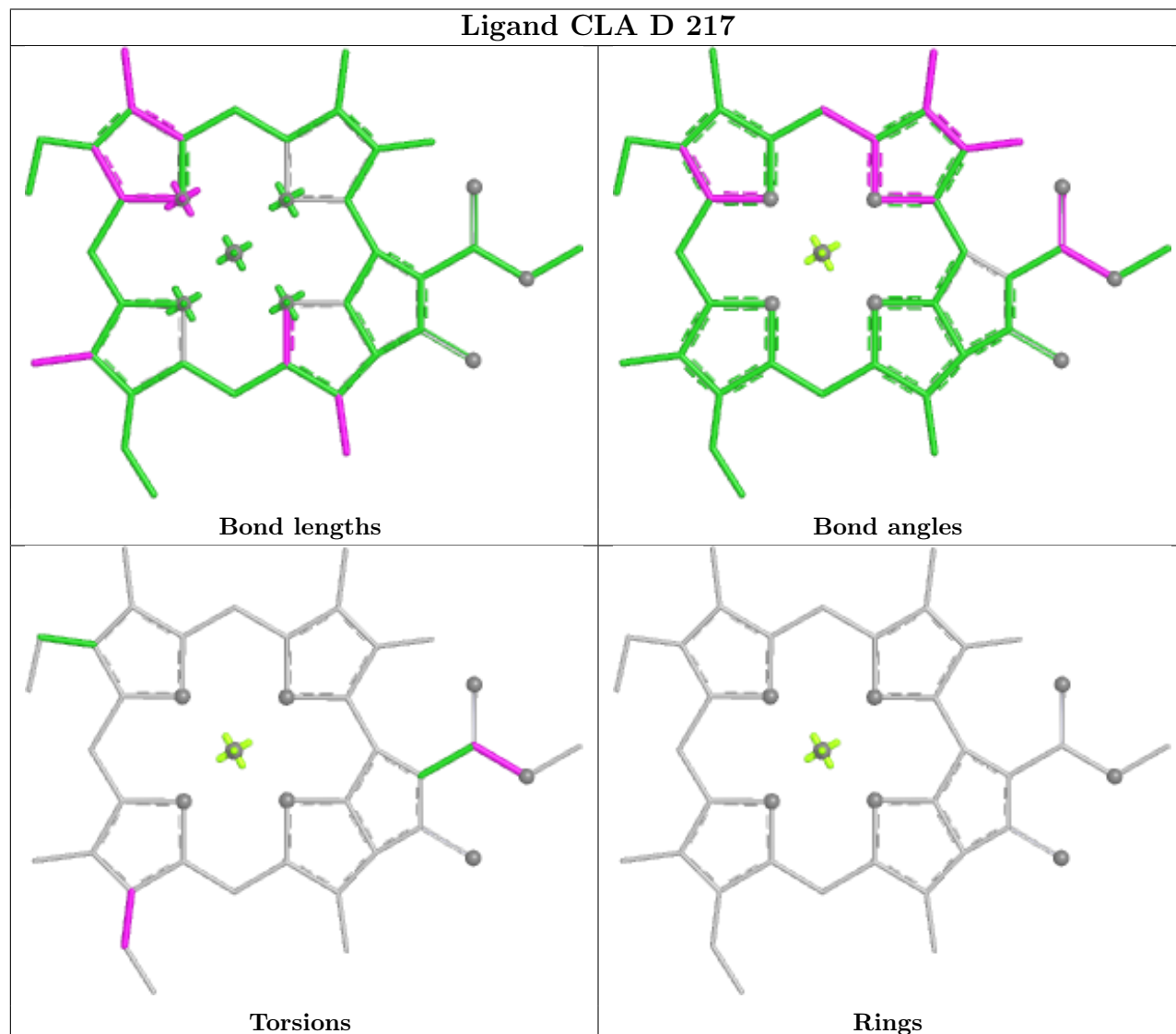
Ligand A86 b 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

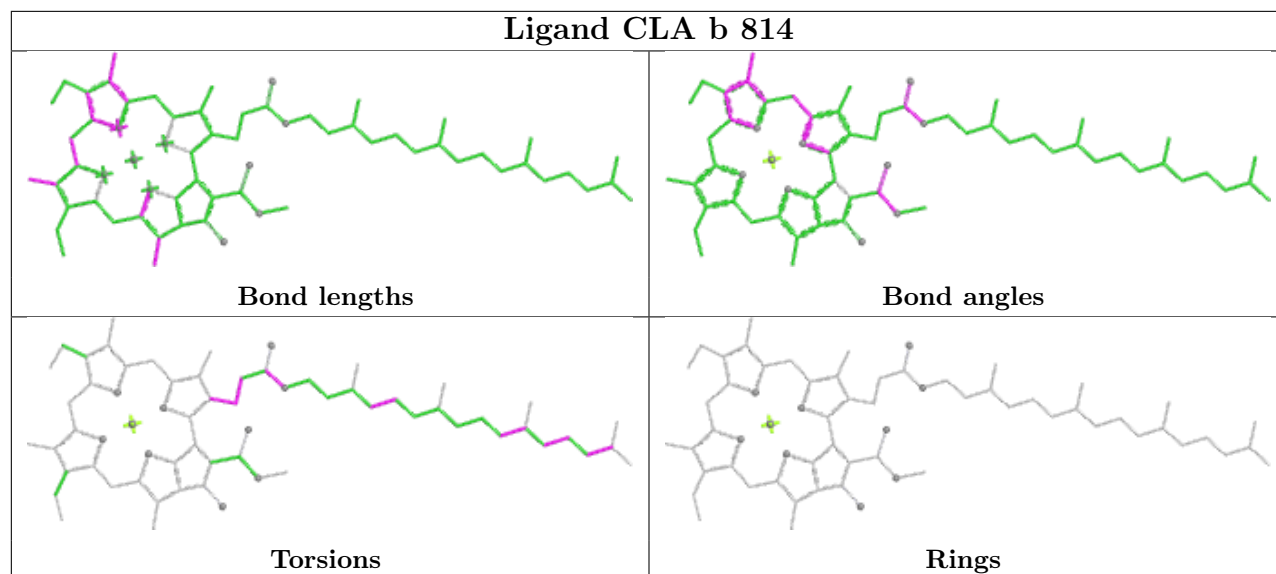
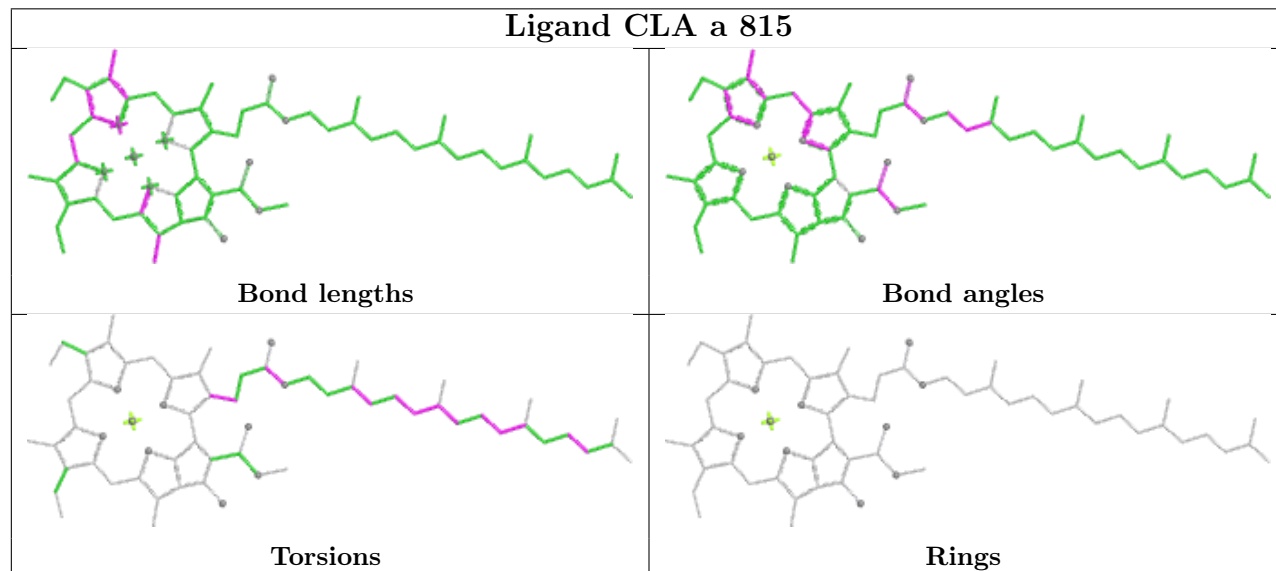
Ligand CLA b 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 312

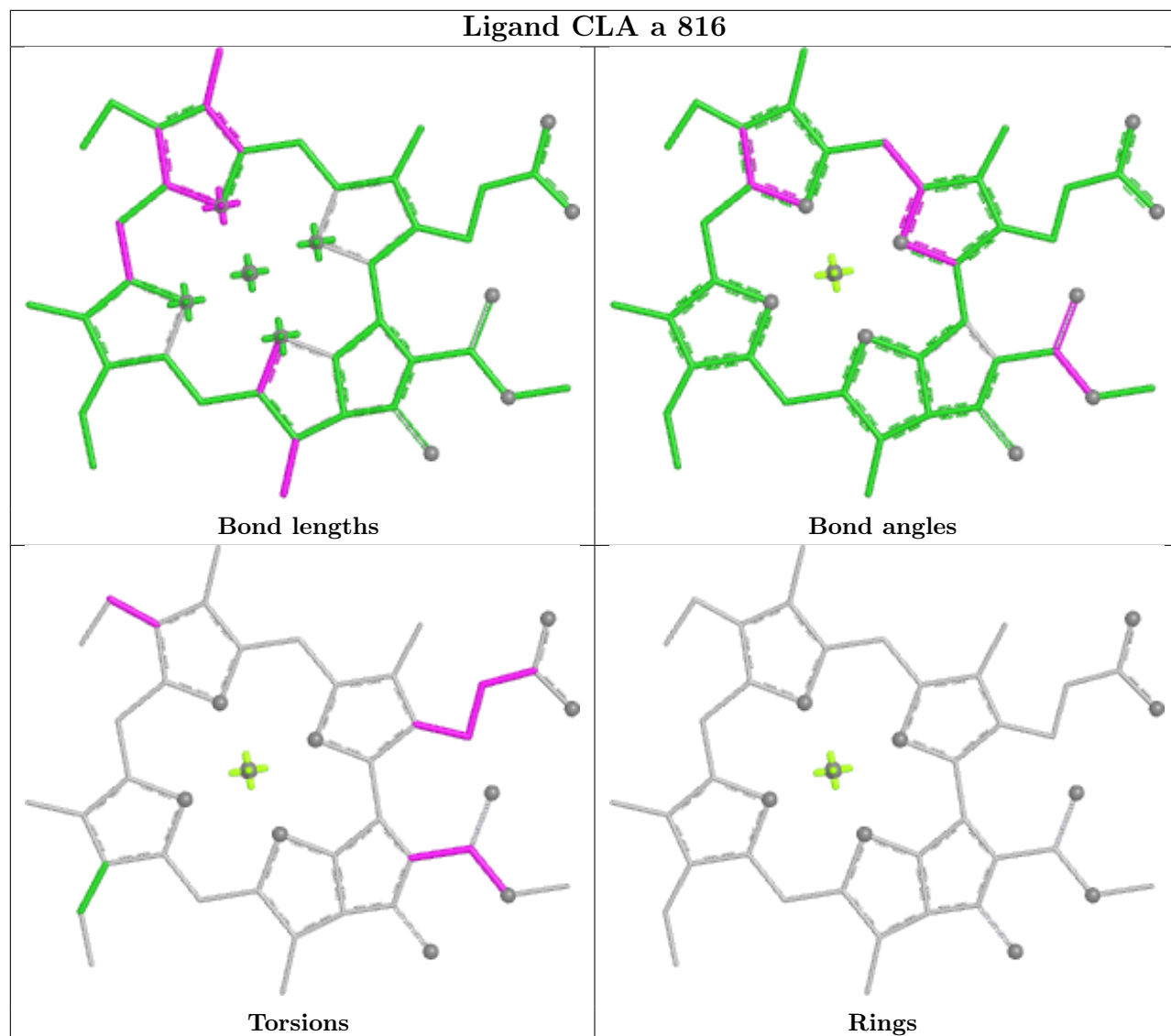


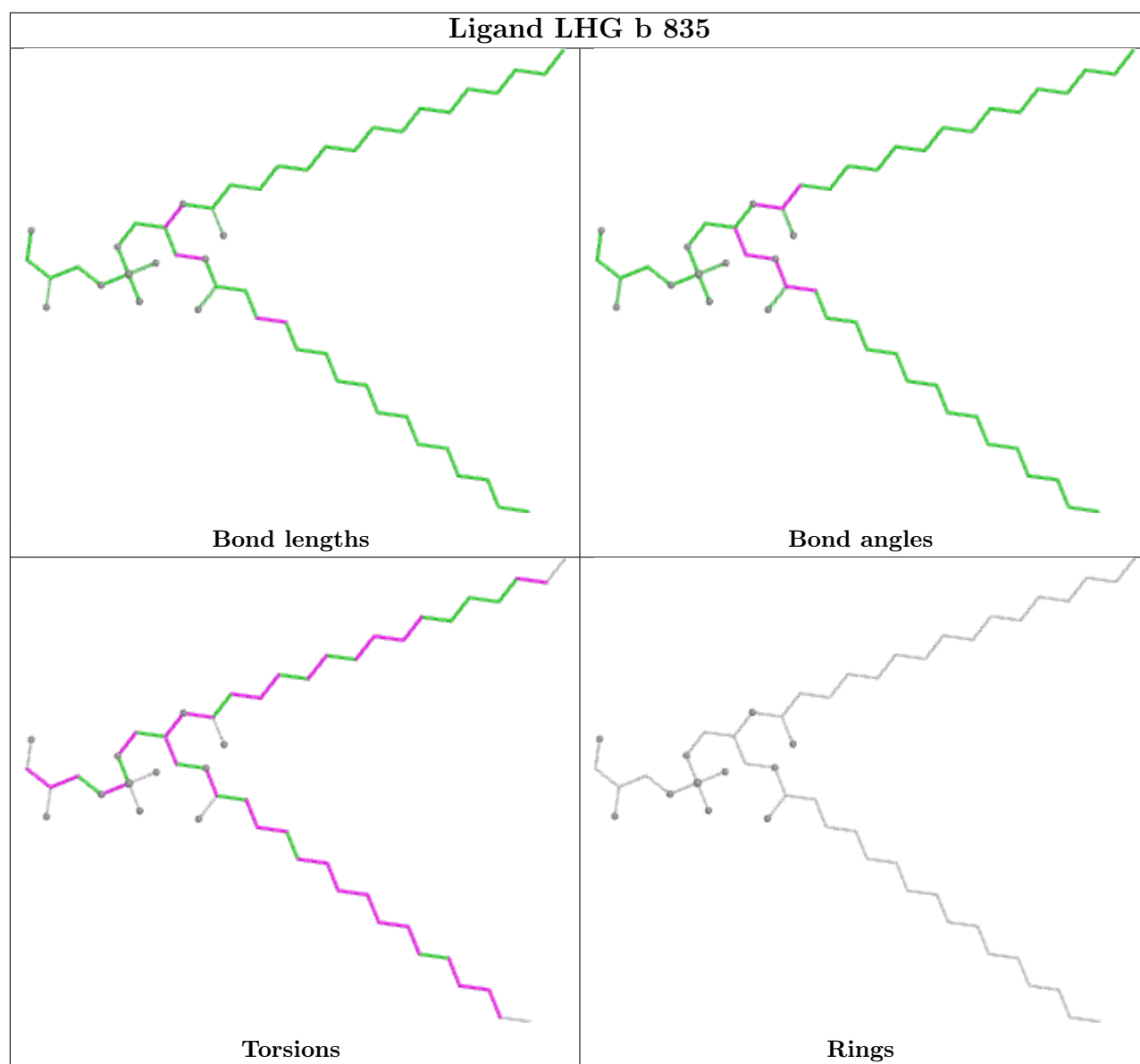
Ligand CLA D 217



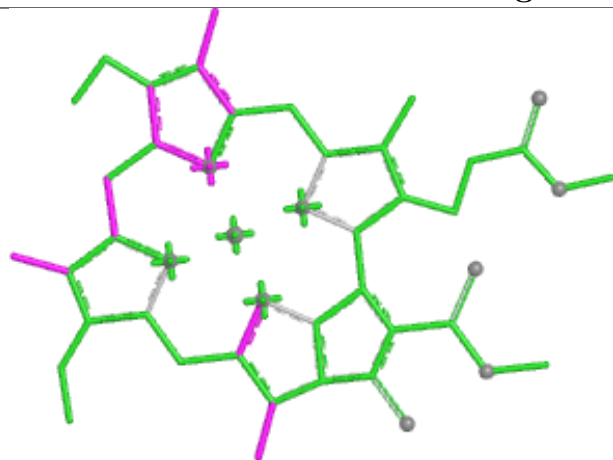
Ligand CLA b 814**Ligand CLA a 815**

Ligand CLA a 816

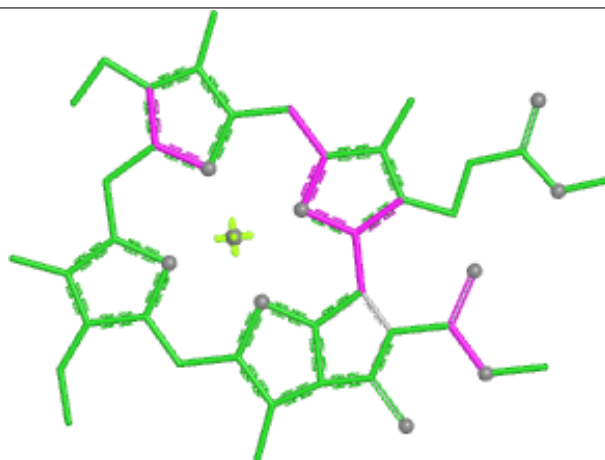




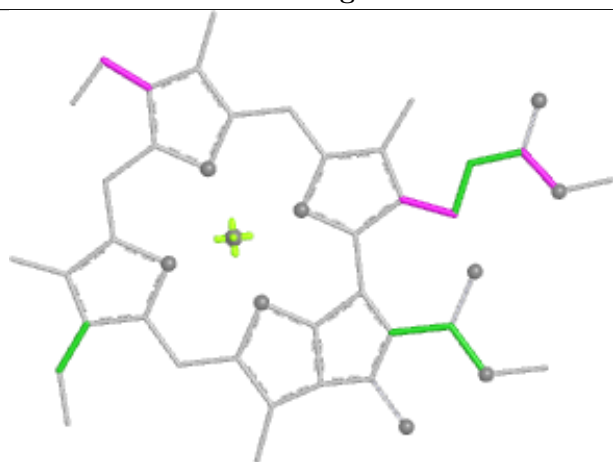
Ligand CLA E 311



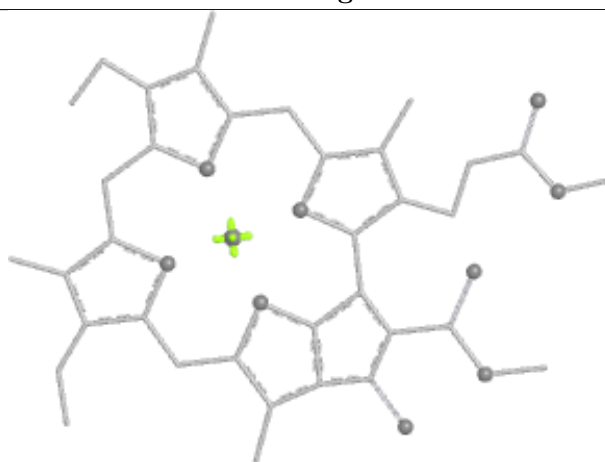
Bond lengths



Bond angles

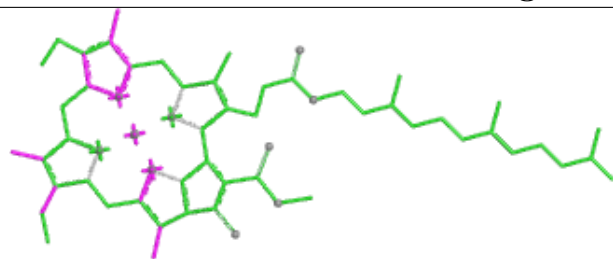


Torsions

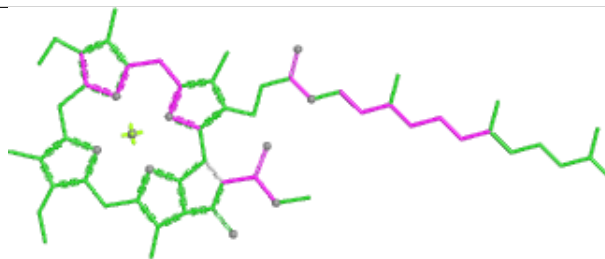


Rings

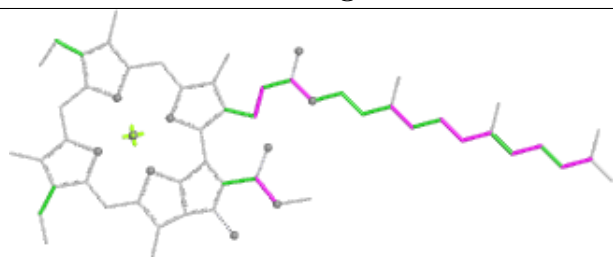
Ligand CLA a 825



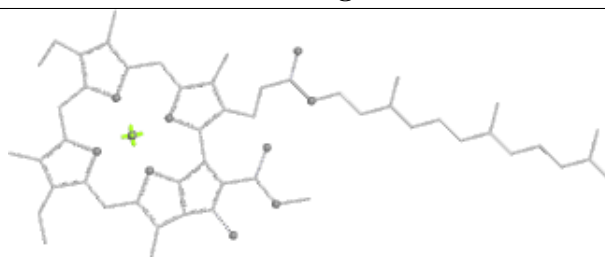
Bond lengths



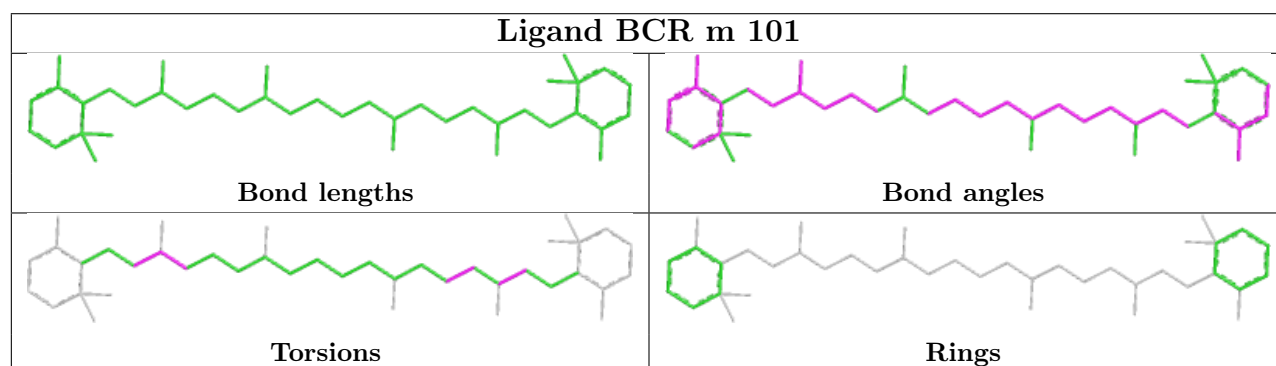
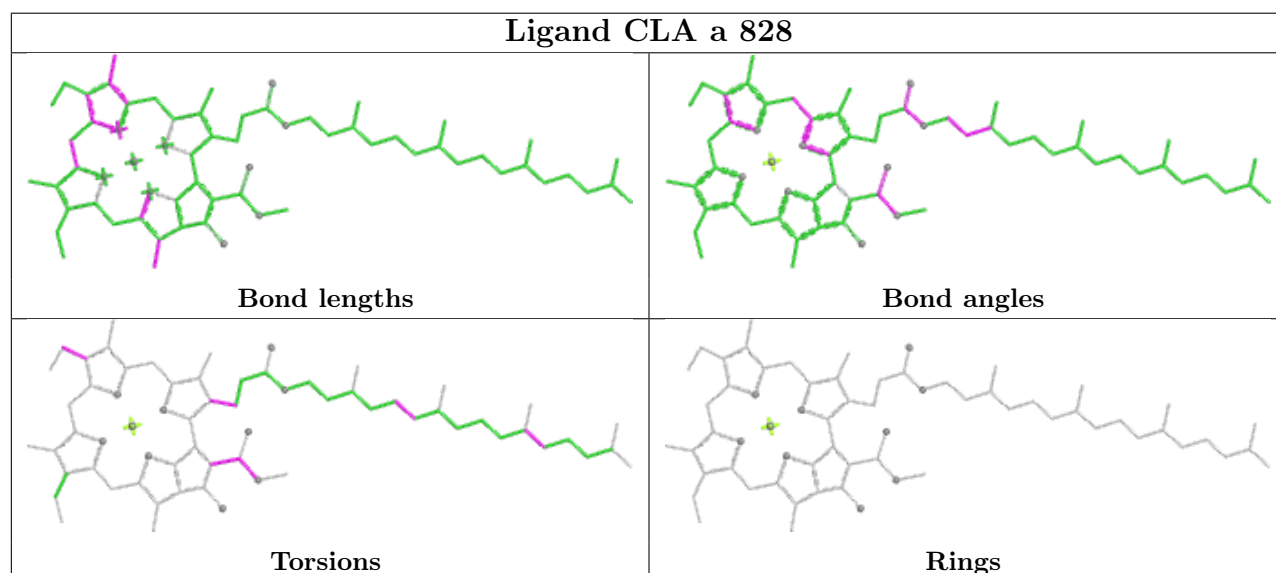
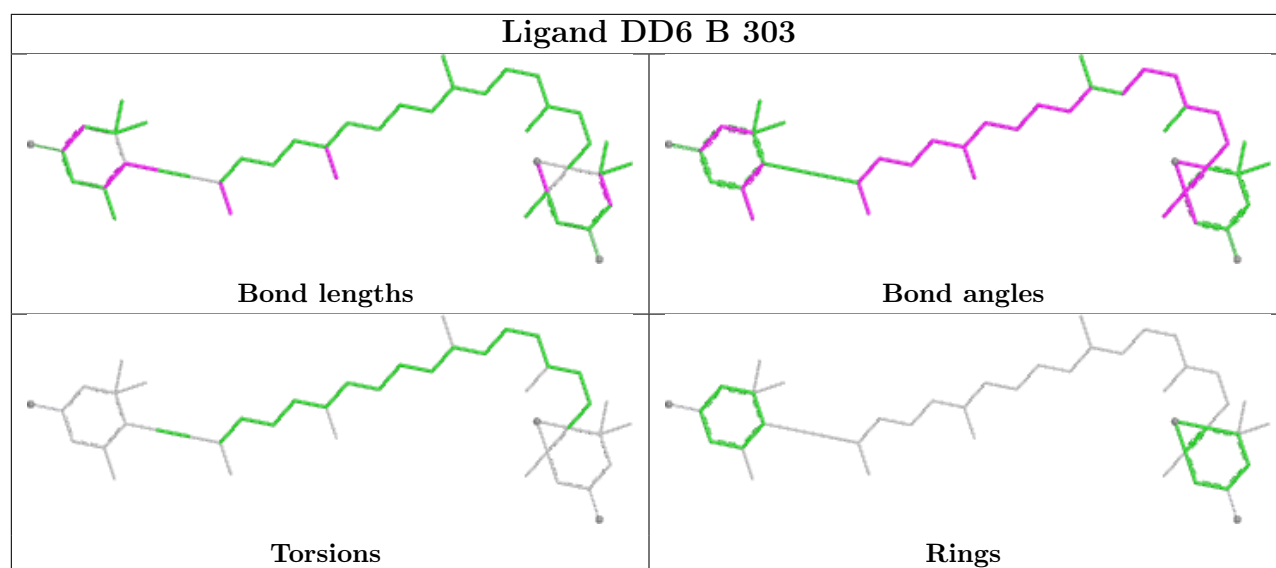
Bond angles

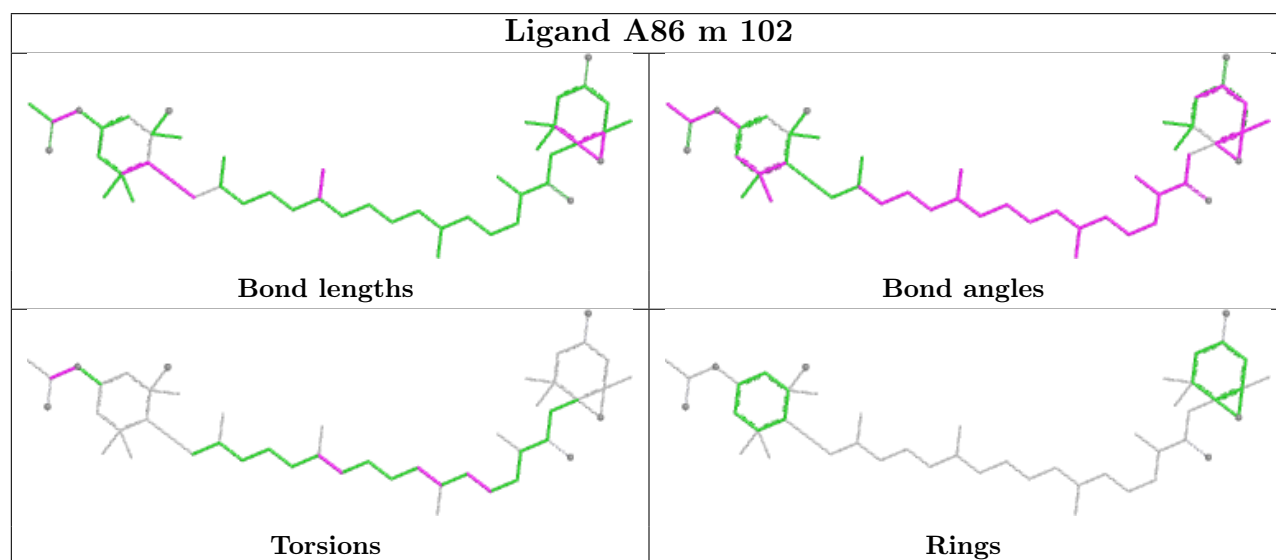
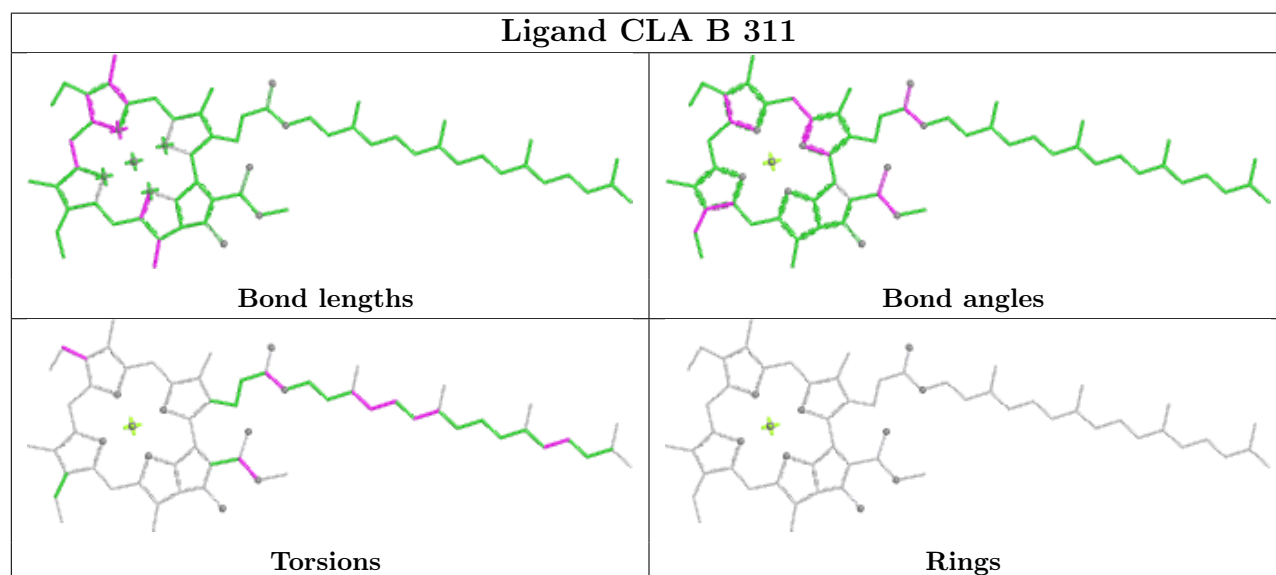
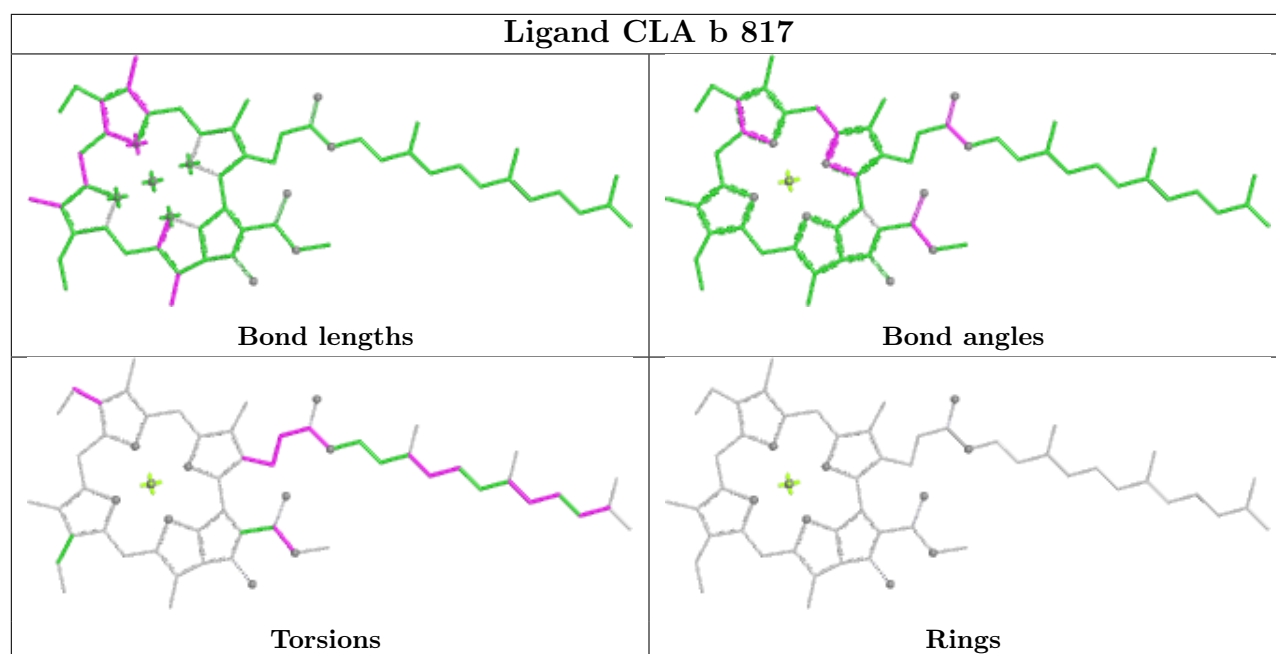


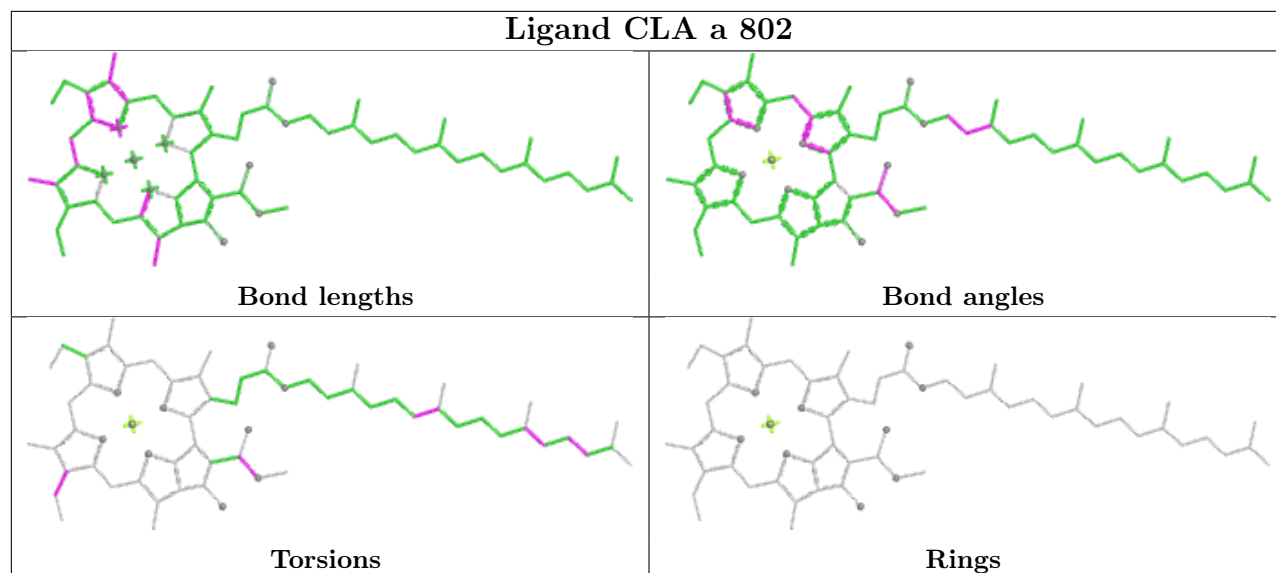
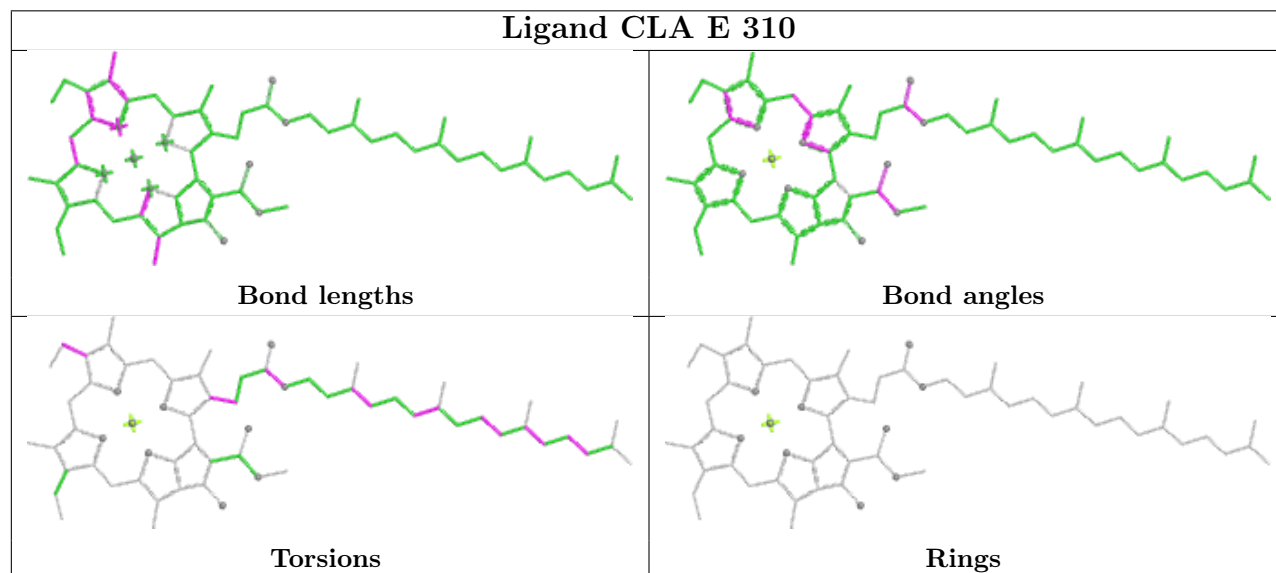
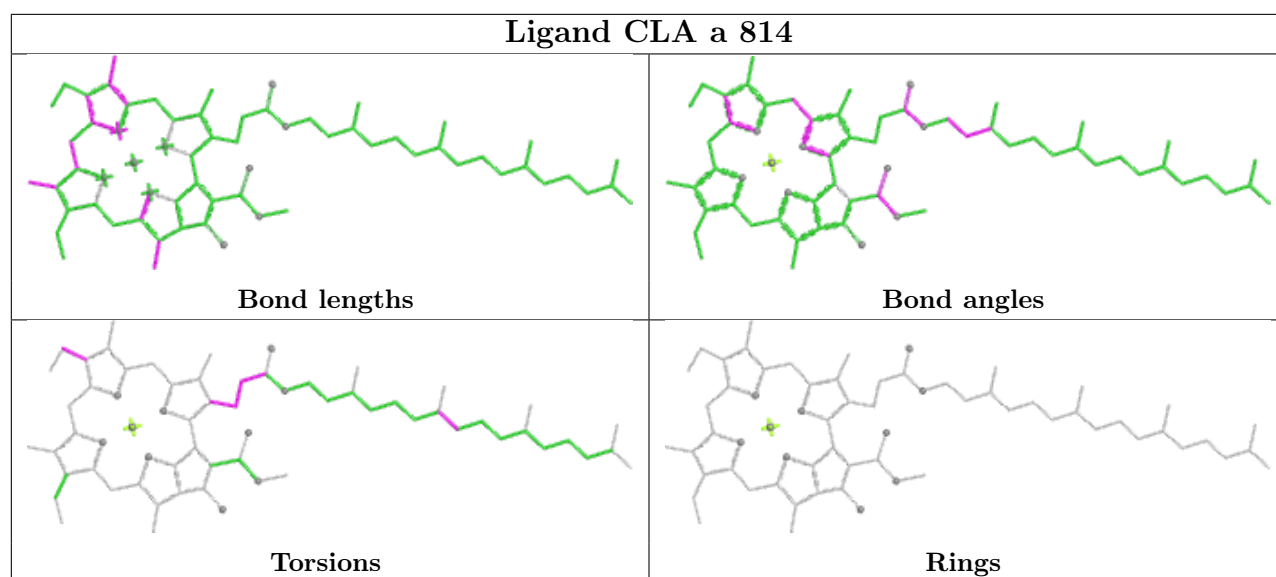
Torsions

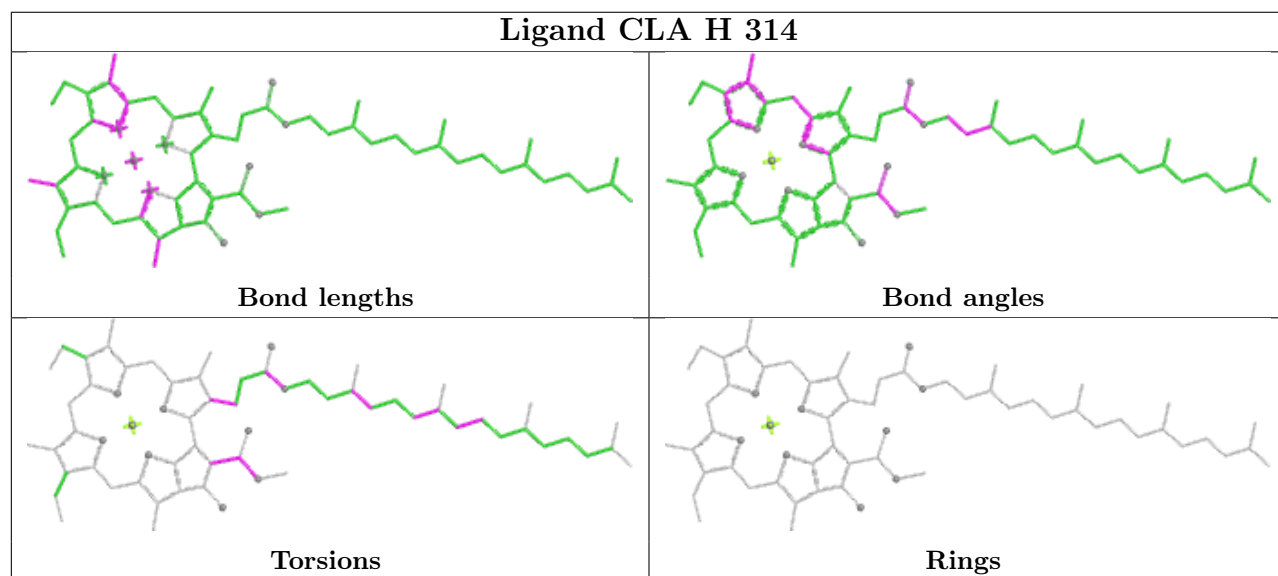
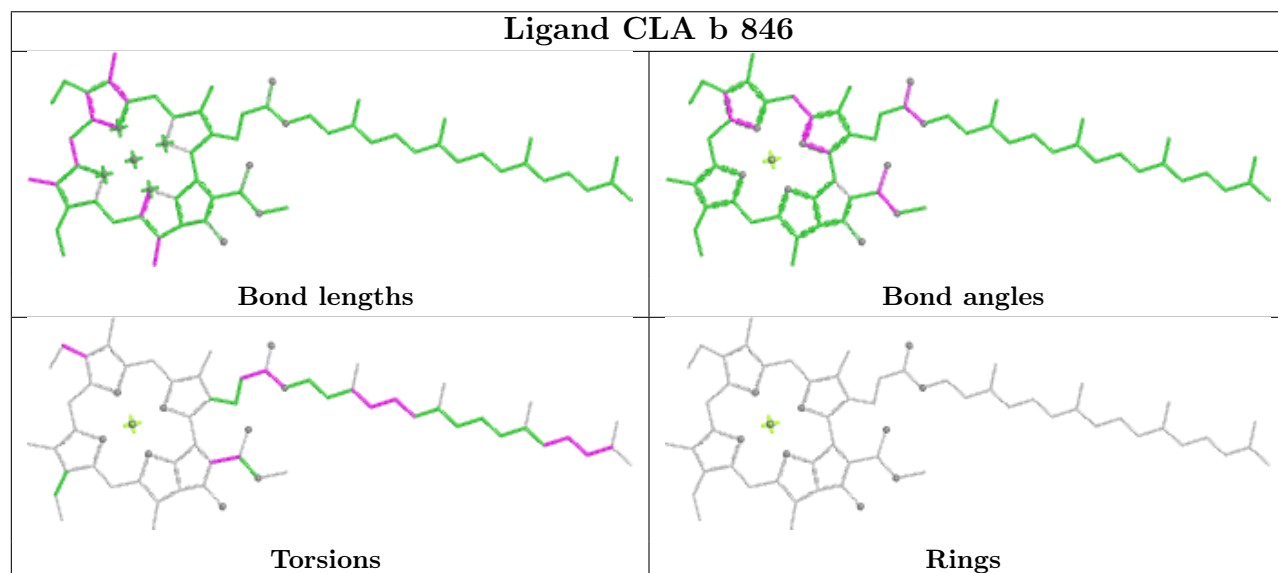
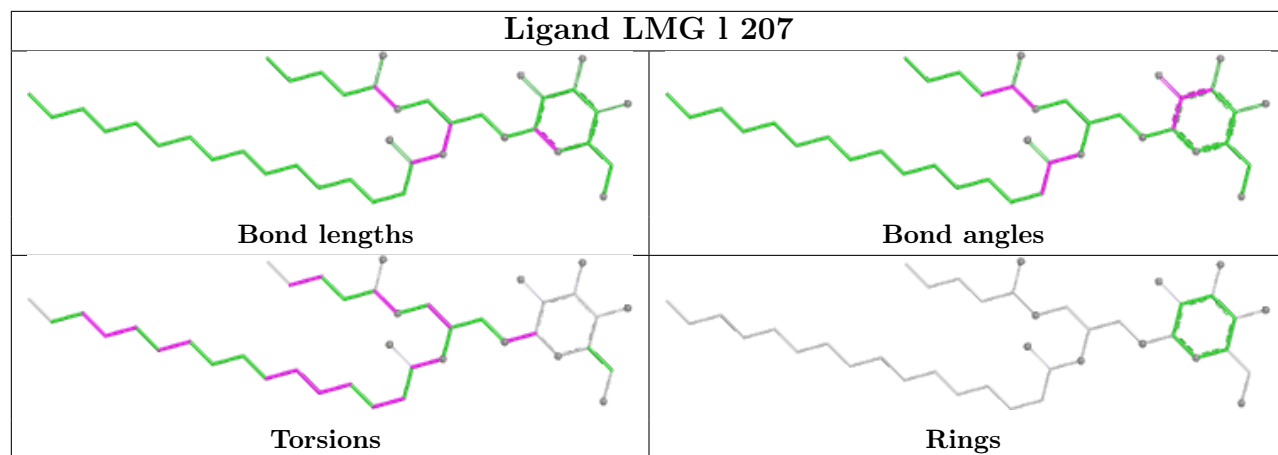


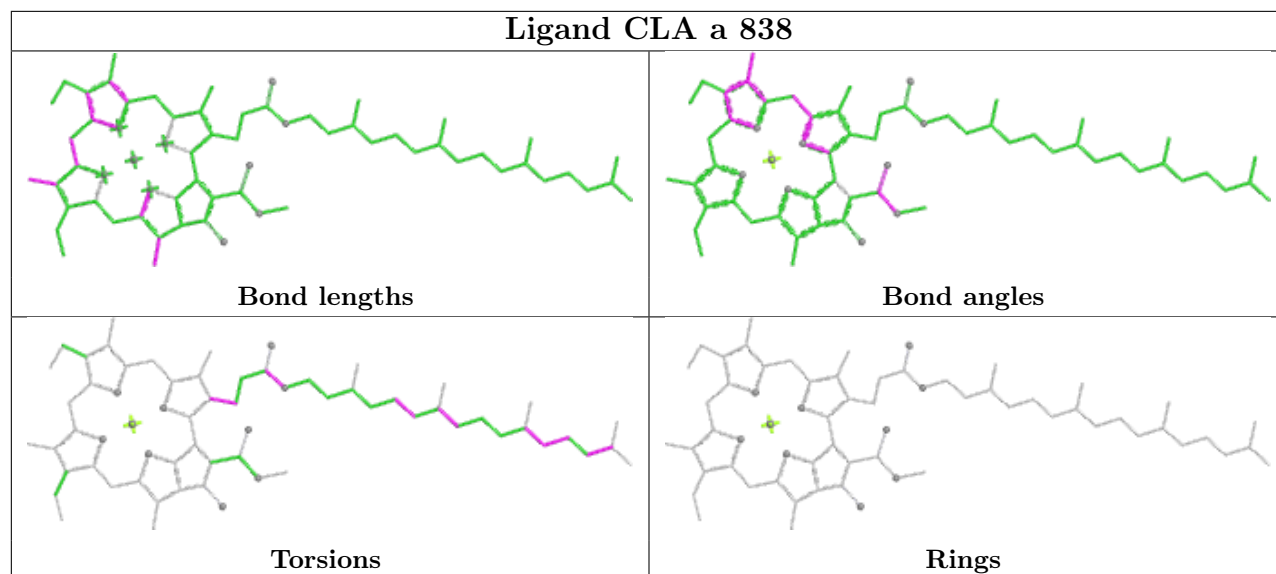
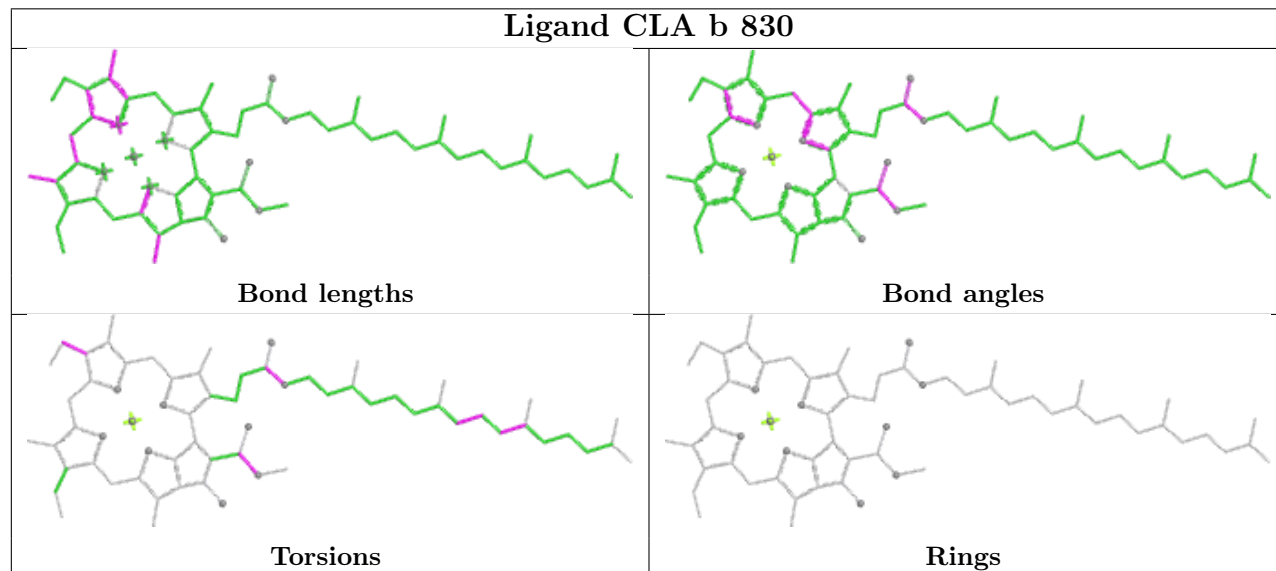
Rings

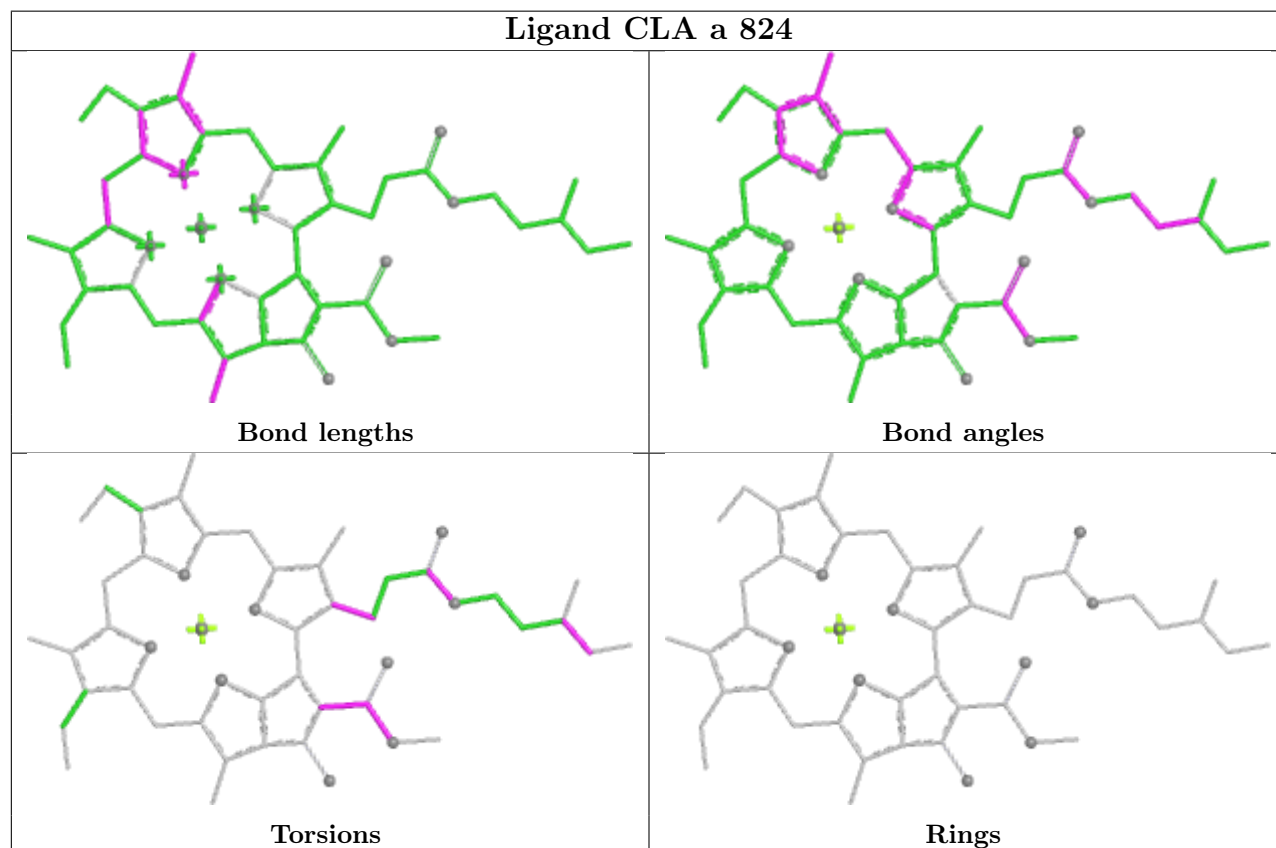
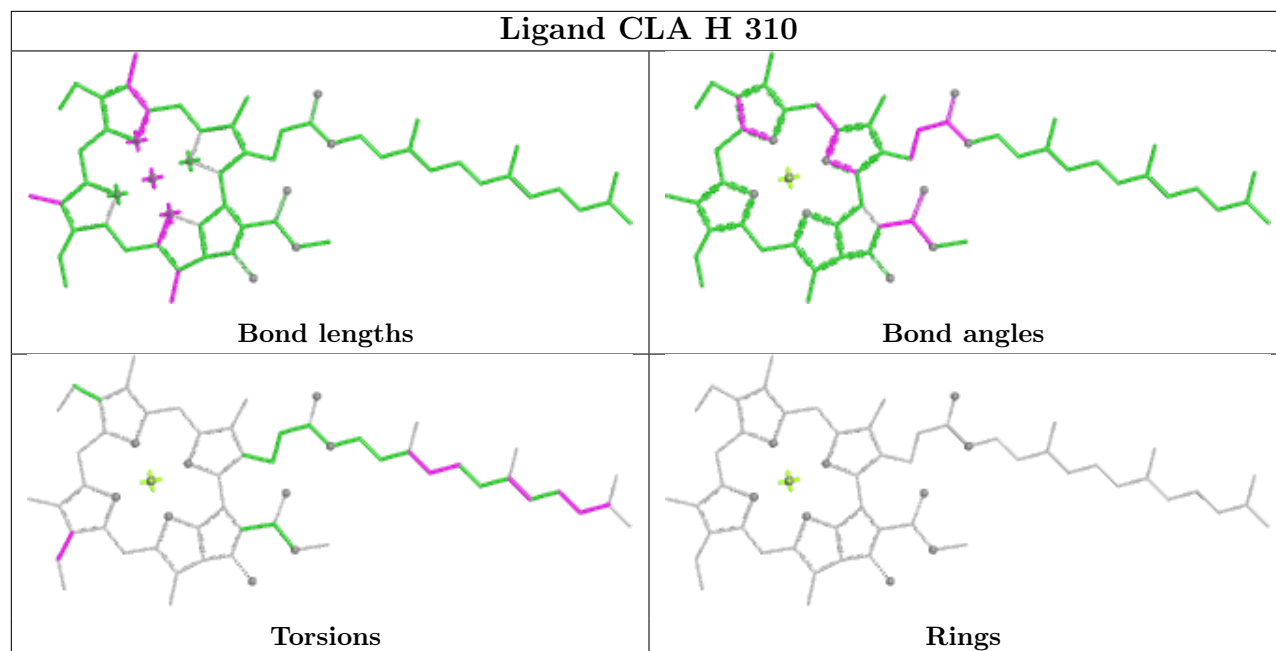


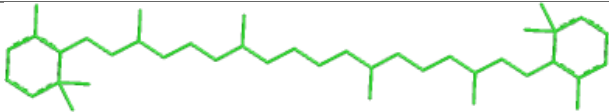
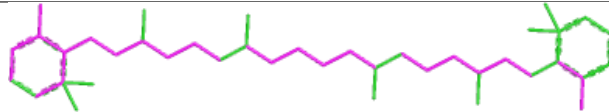
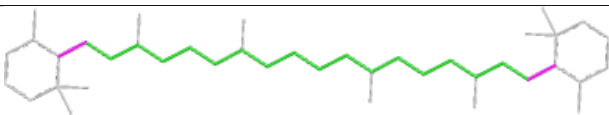
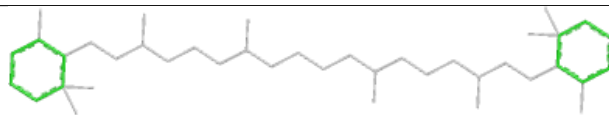


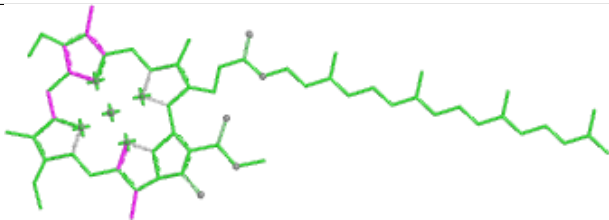
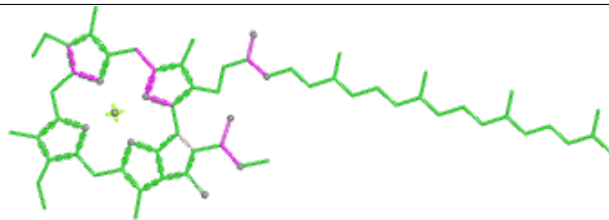
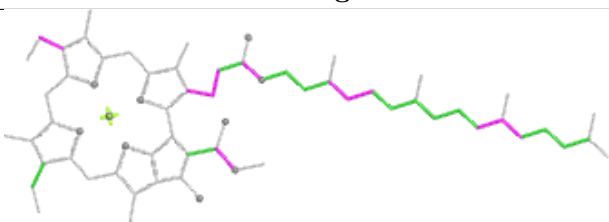
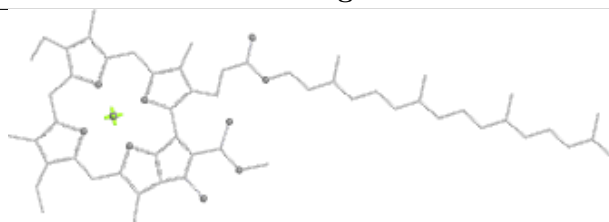


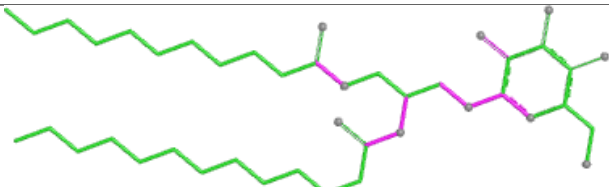
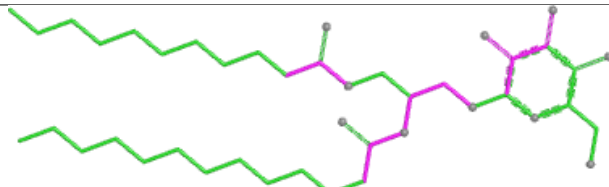
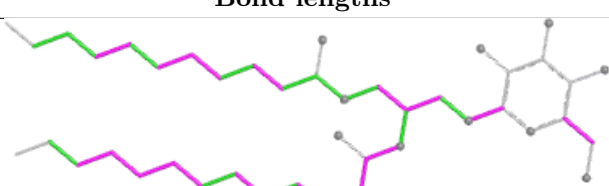
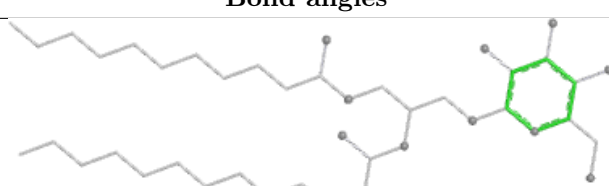


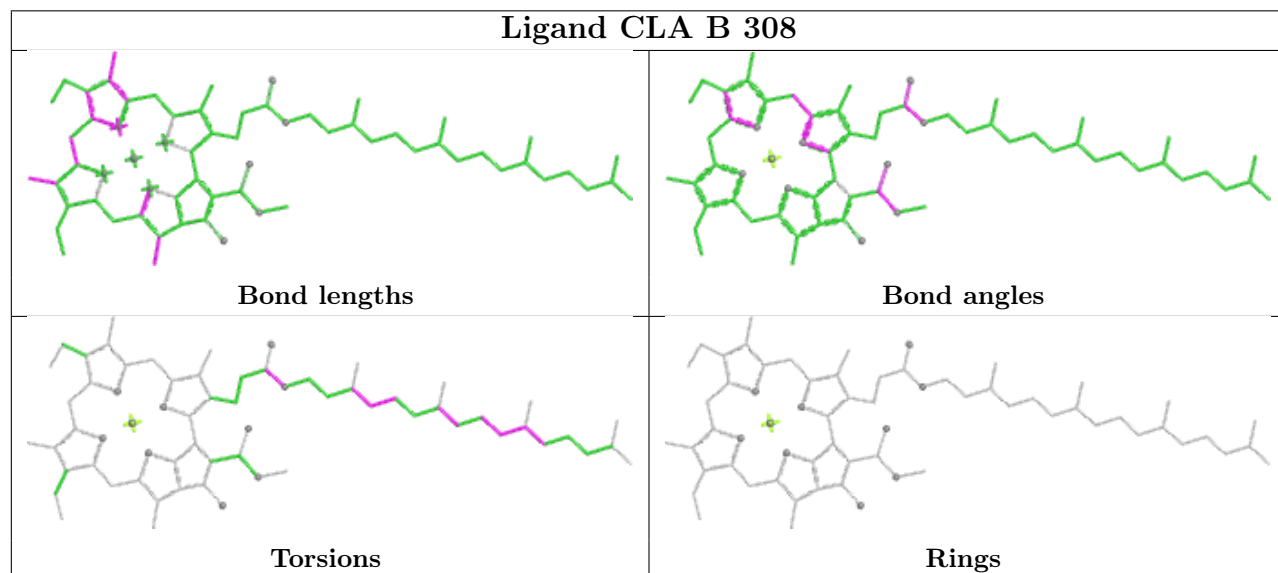
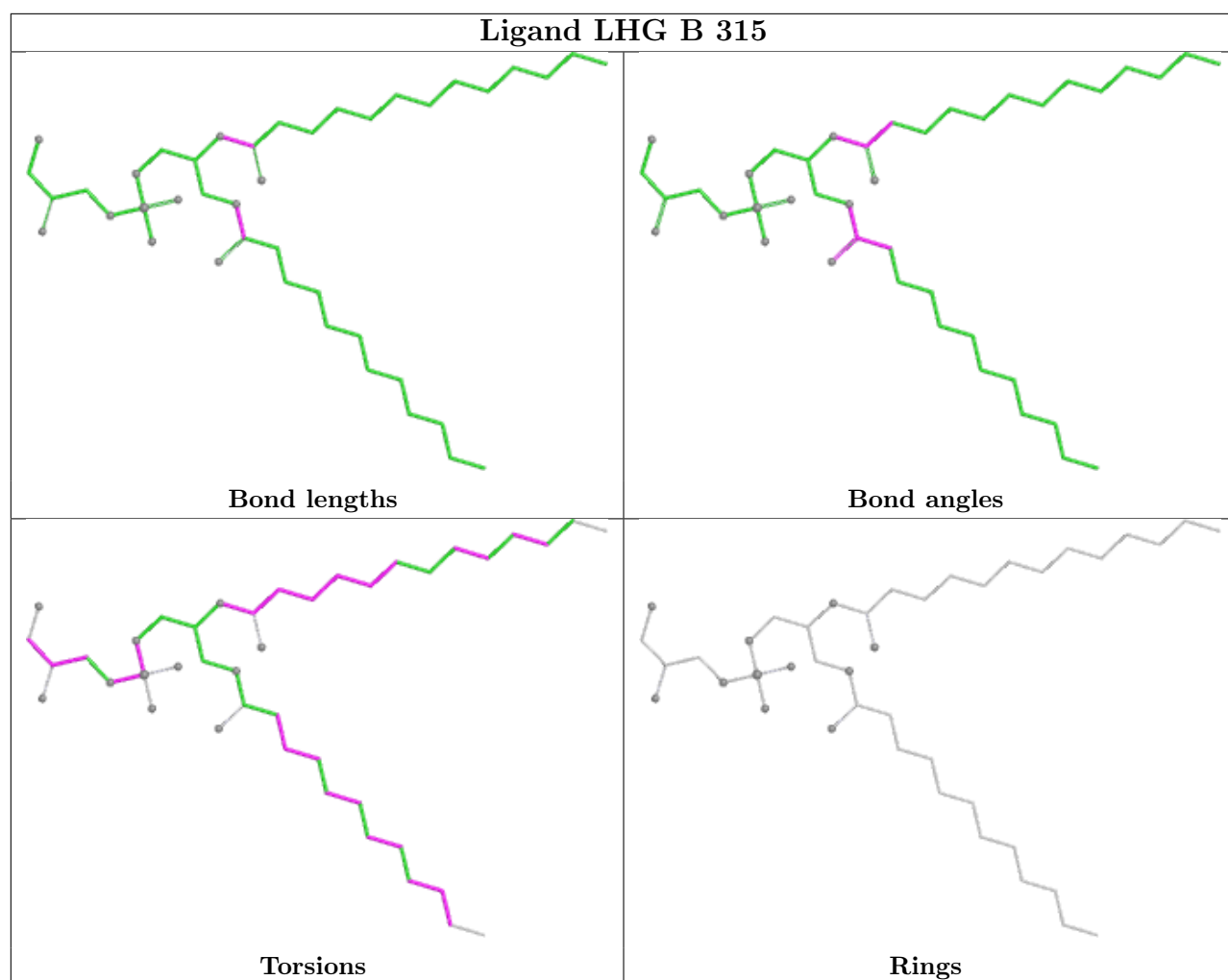
Ligand CLA a 838**Ligand CLA b 830**



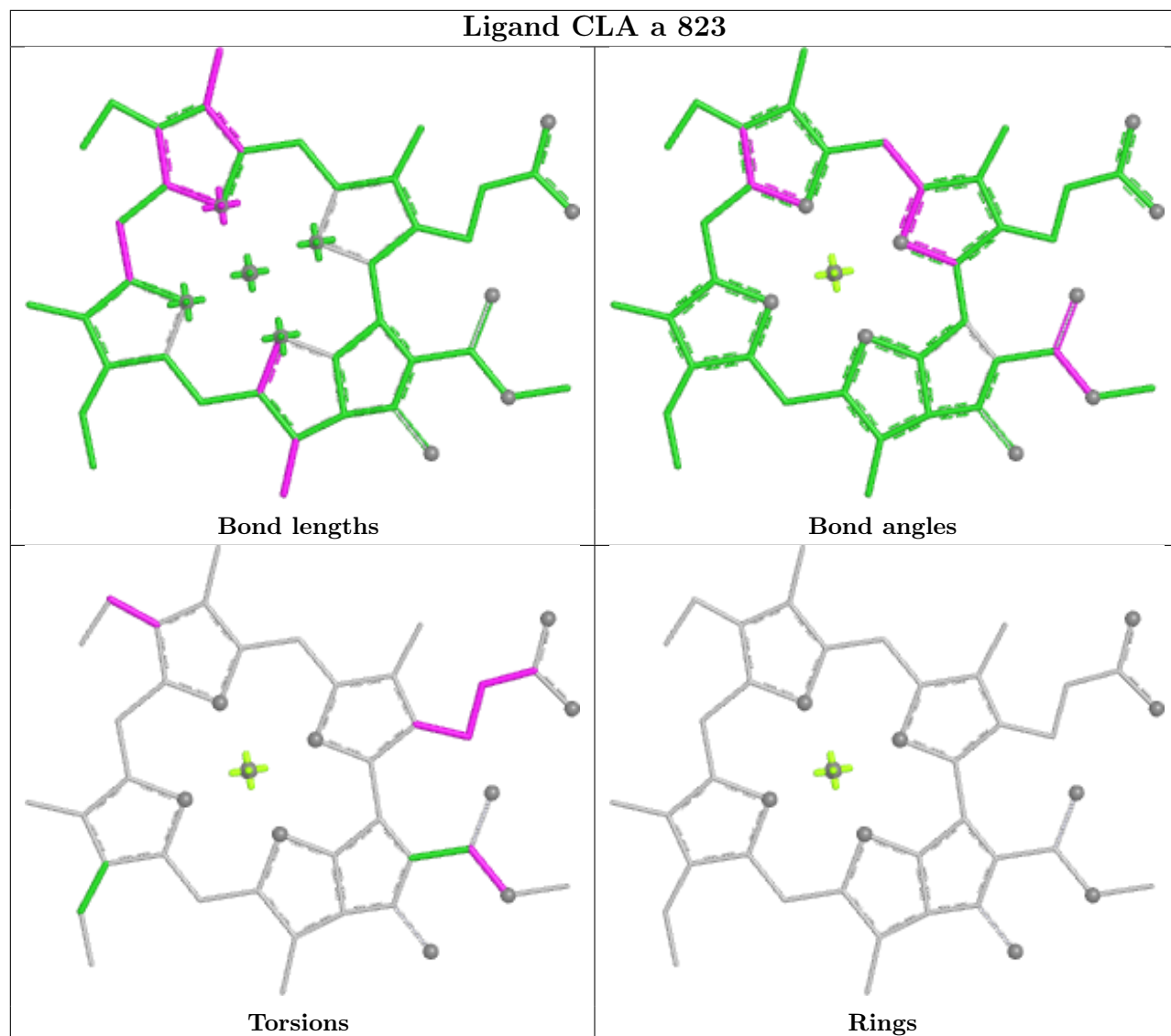
Ligand BCR r 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

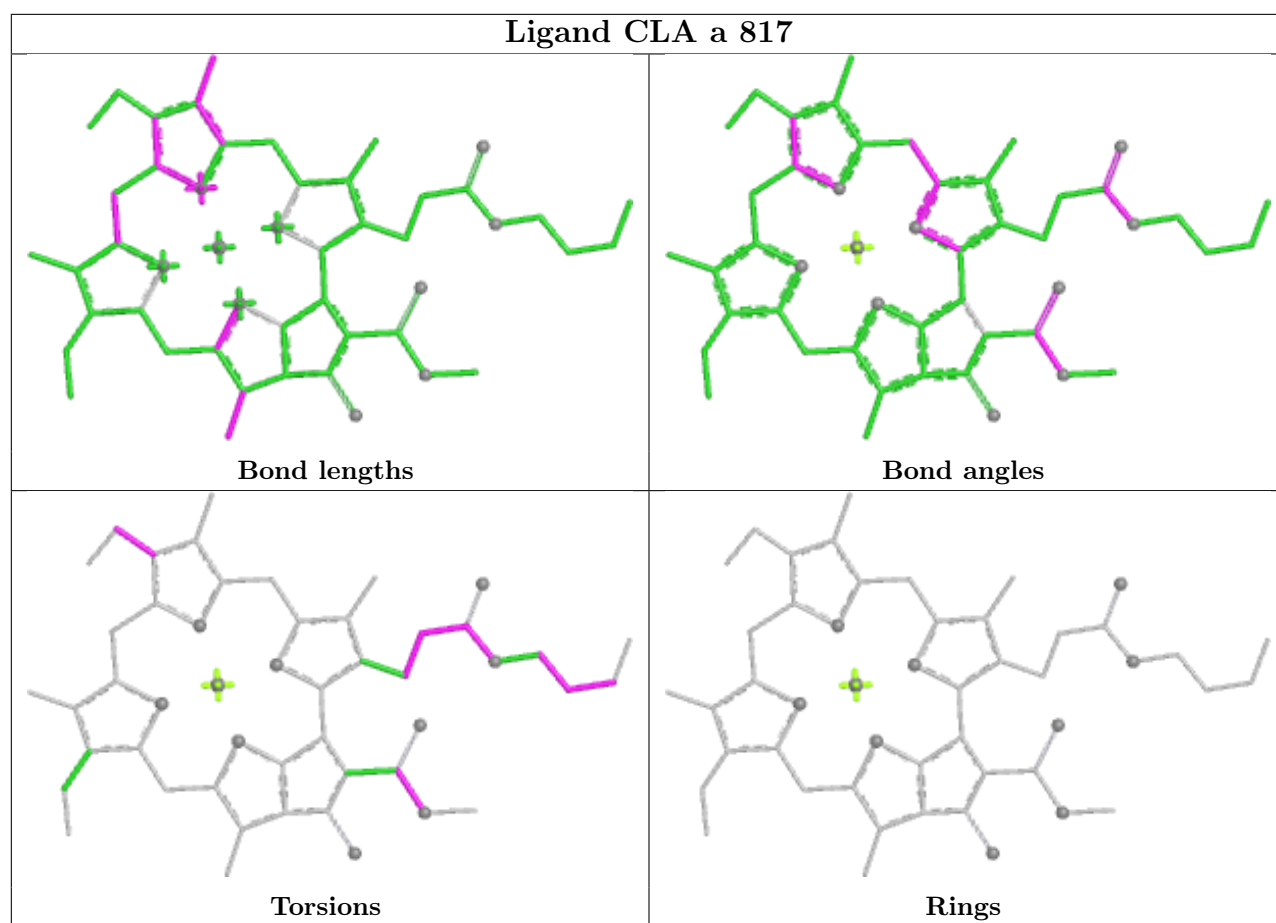
Ligand CLA a 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG E 318	
	
Bond lengths	Bond angles
	
Torsions	Rings

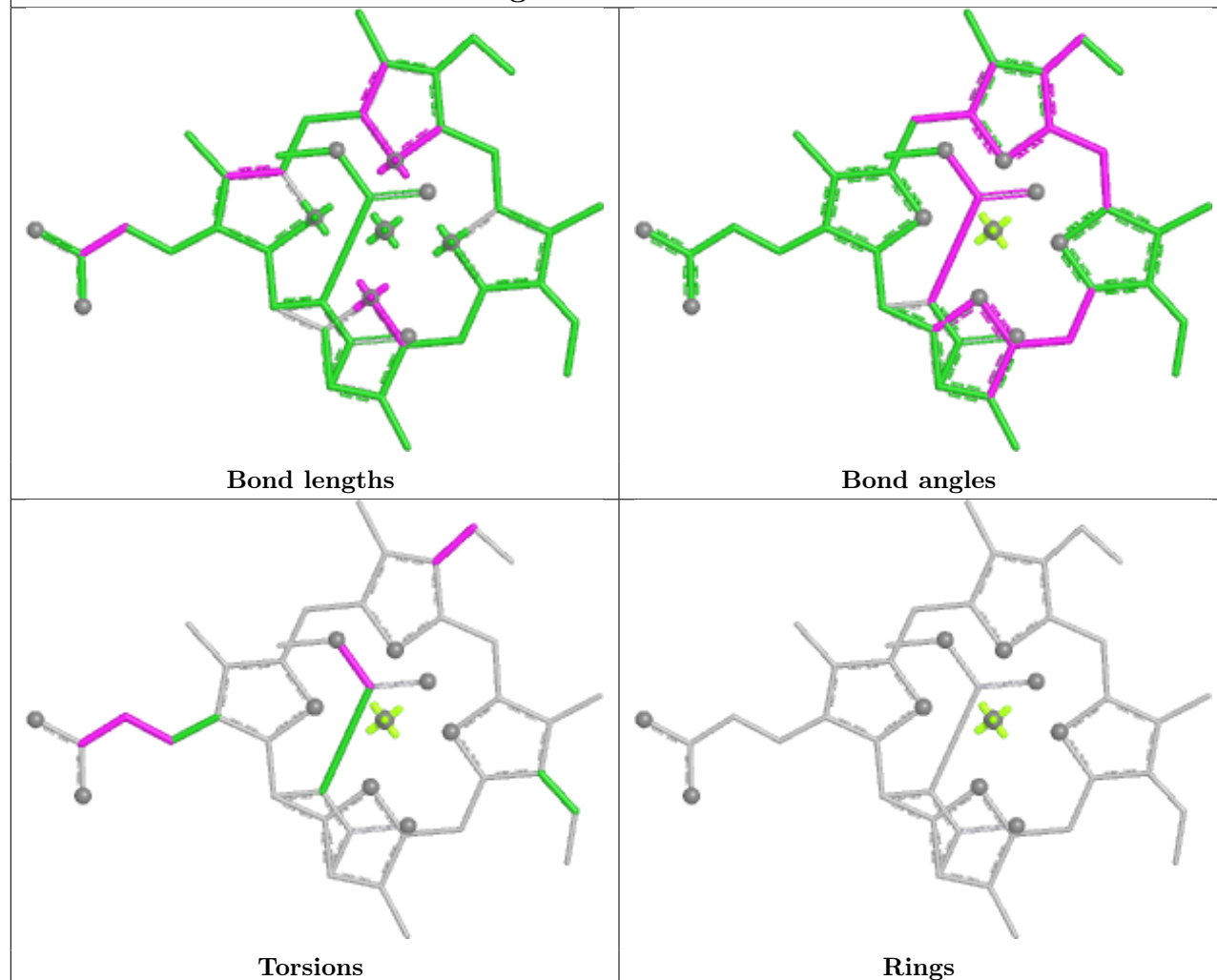


Ligand CLA a 823

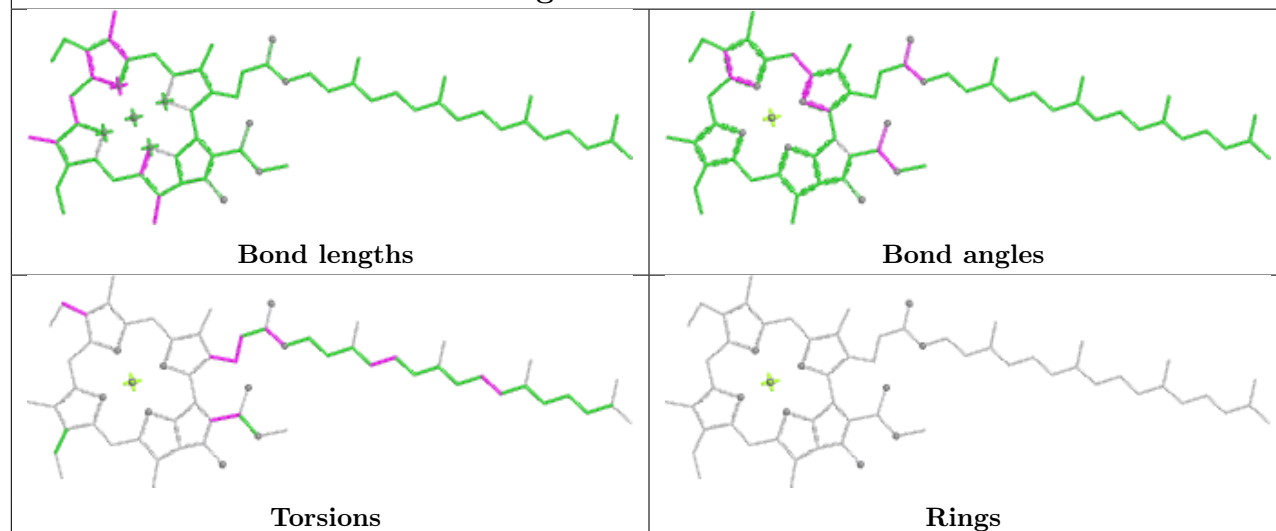


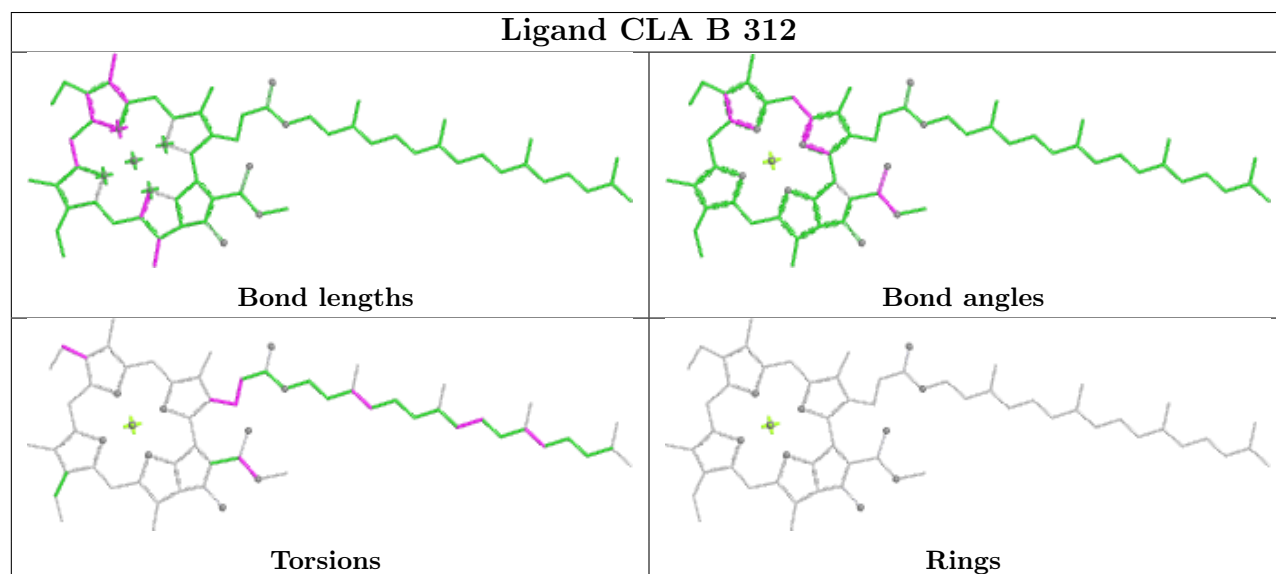
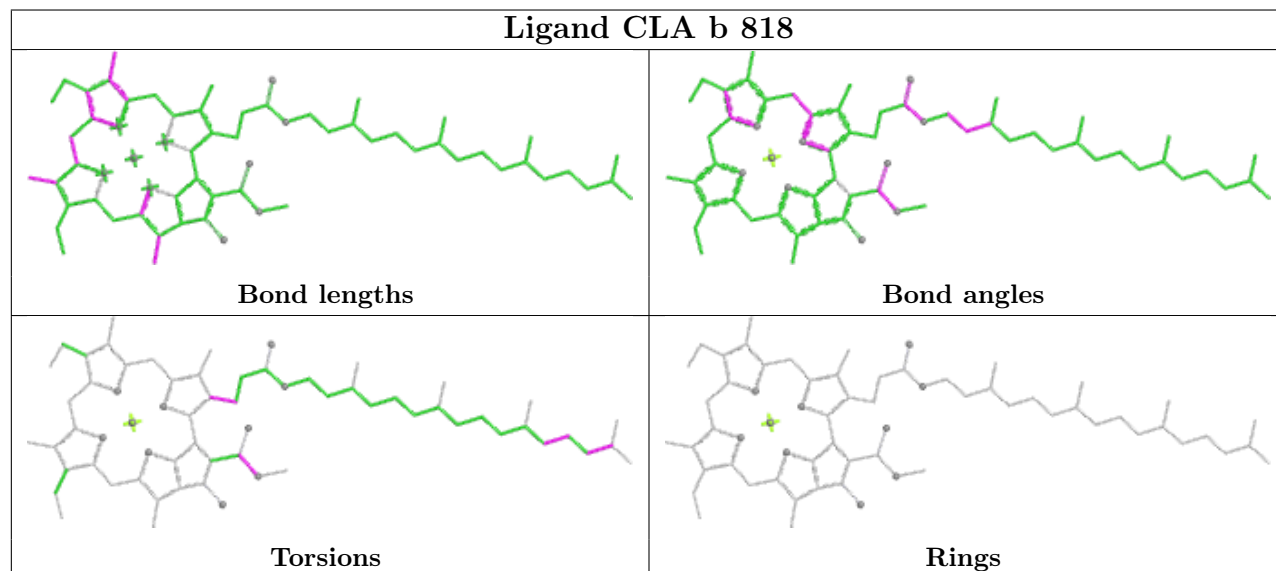
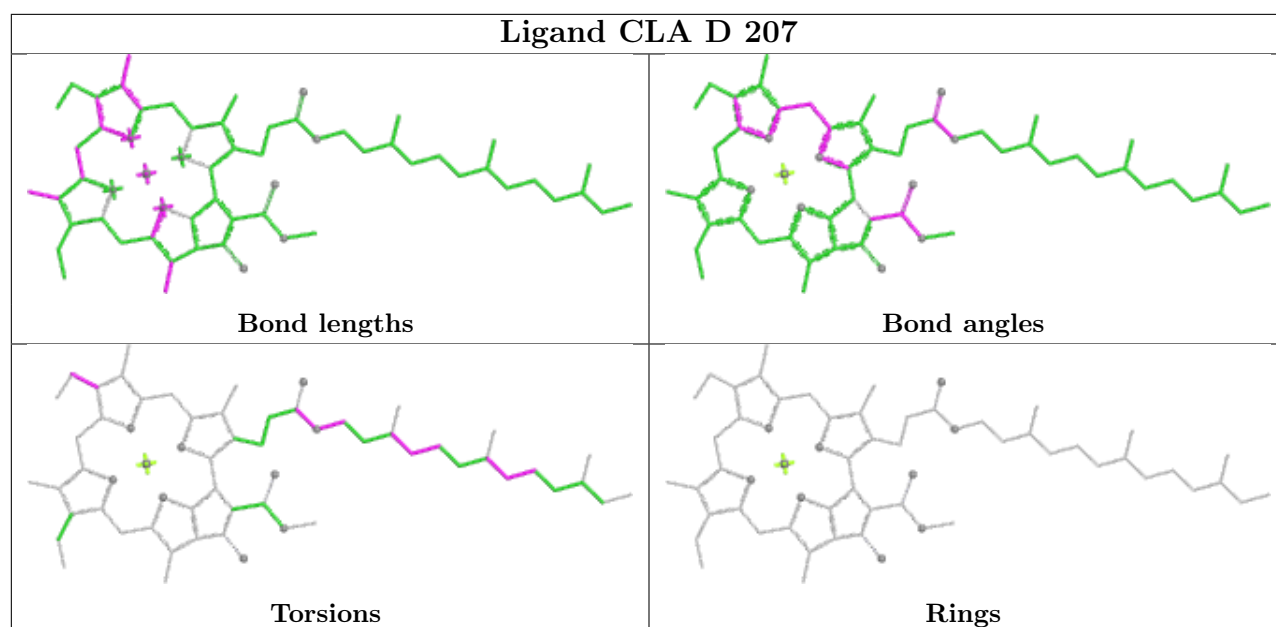


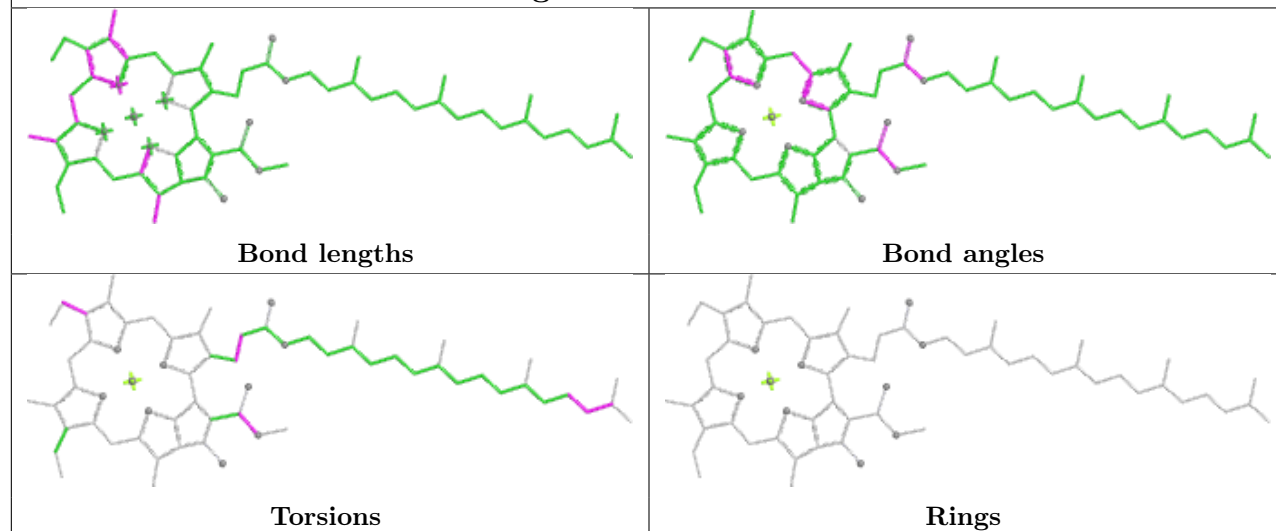
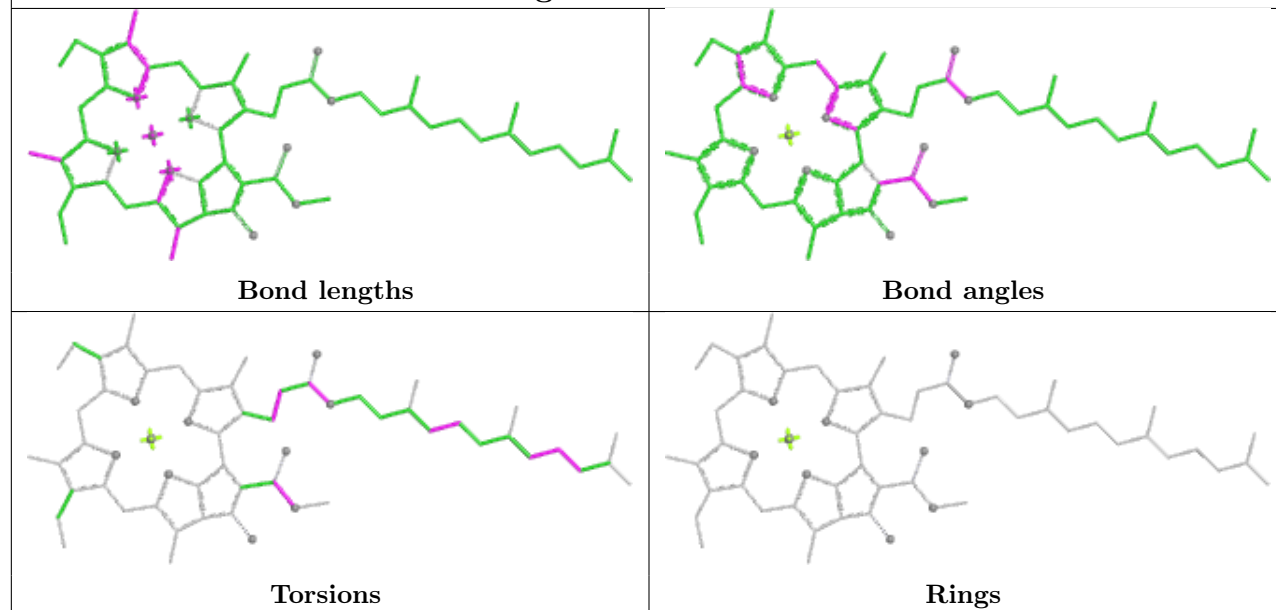
Ligand KC1 B 313



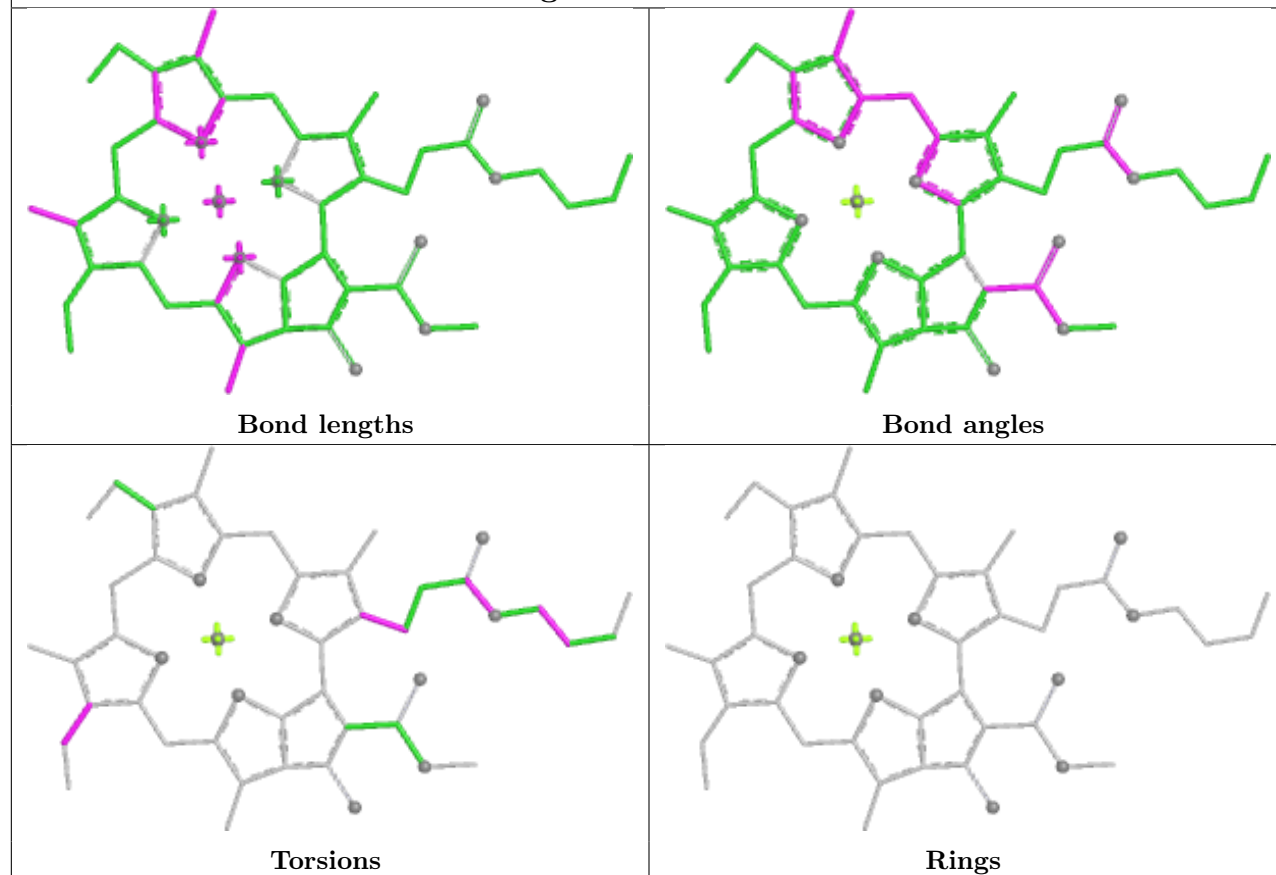
Ligand CLA a 839



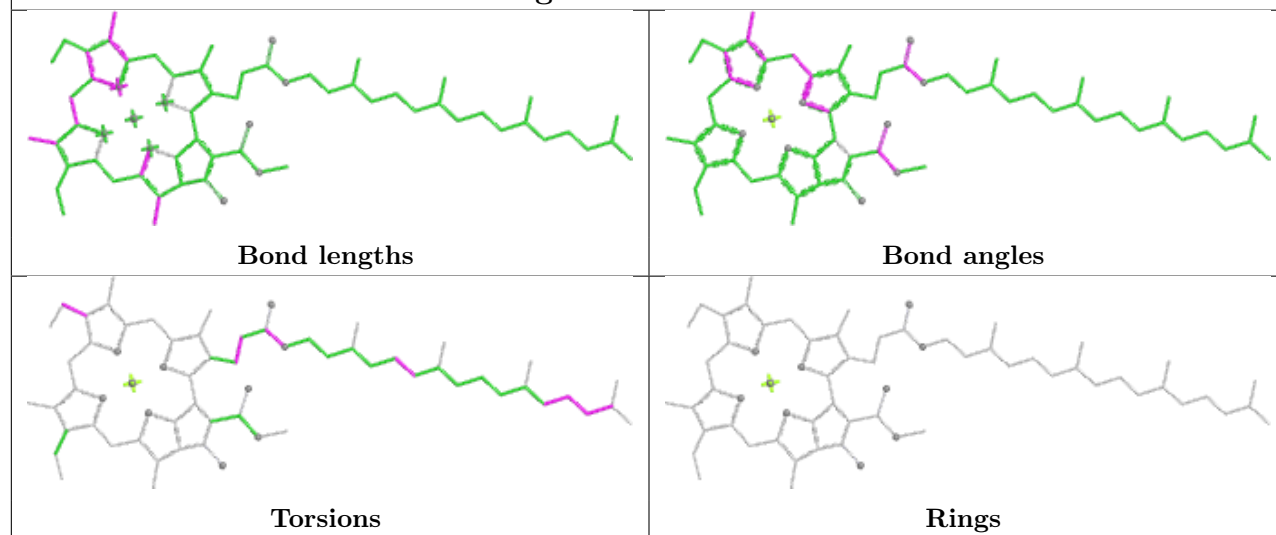


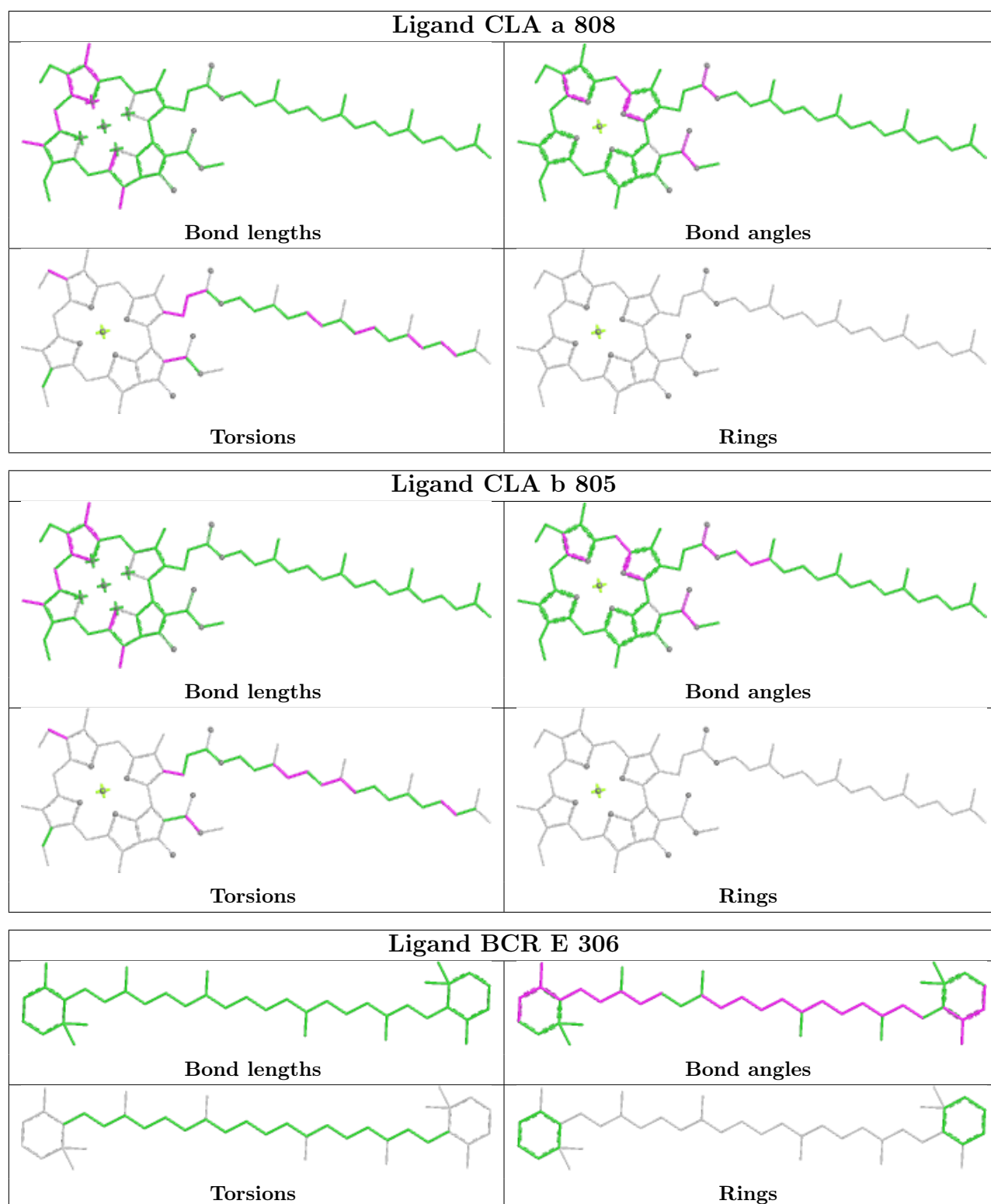
Ligand CLA B 307**Ligand CLA b 811**

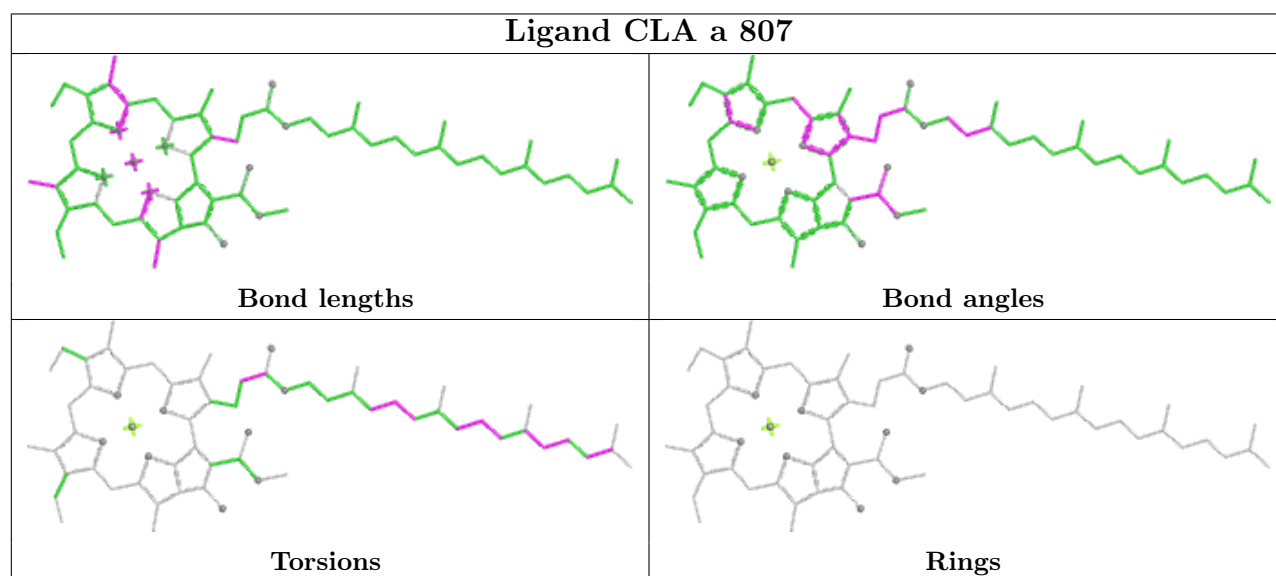
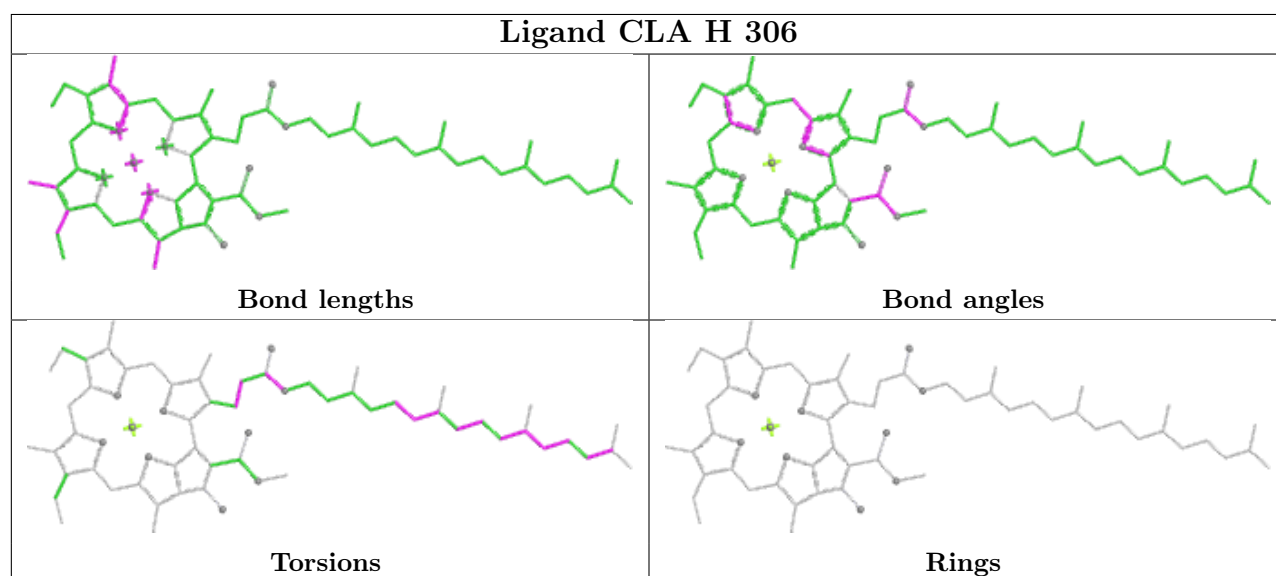
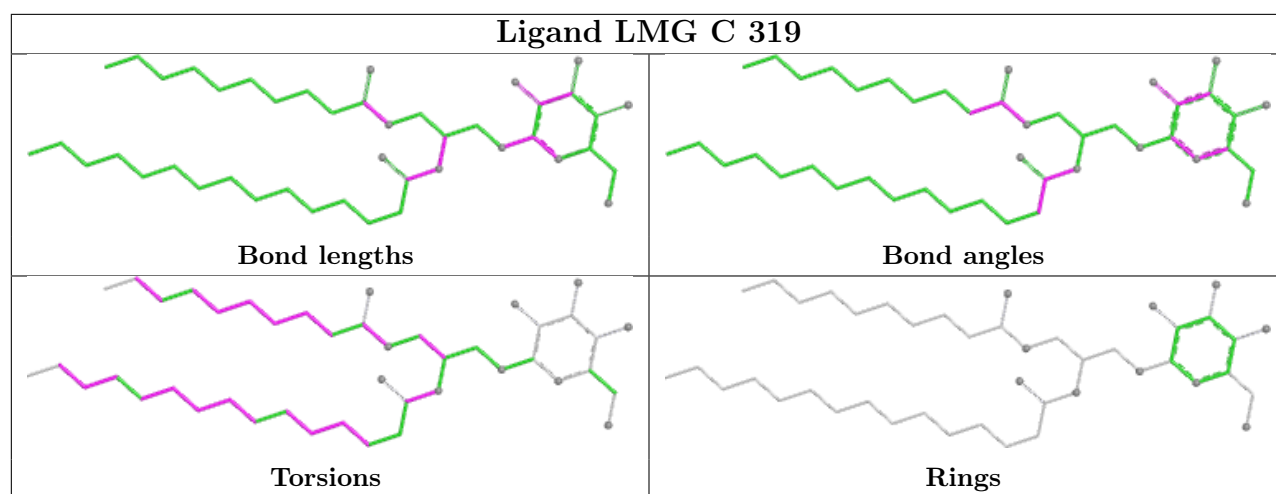
Ligand CLA 1 202

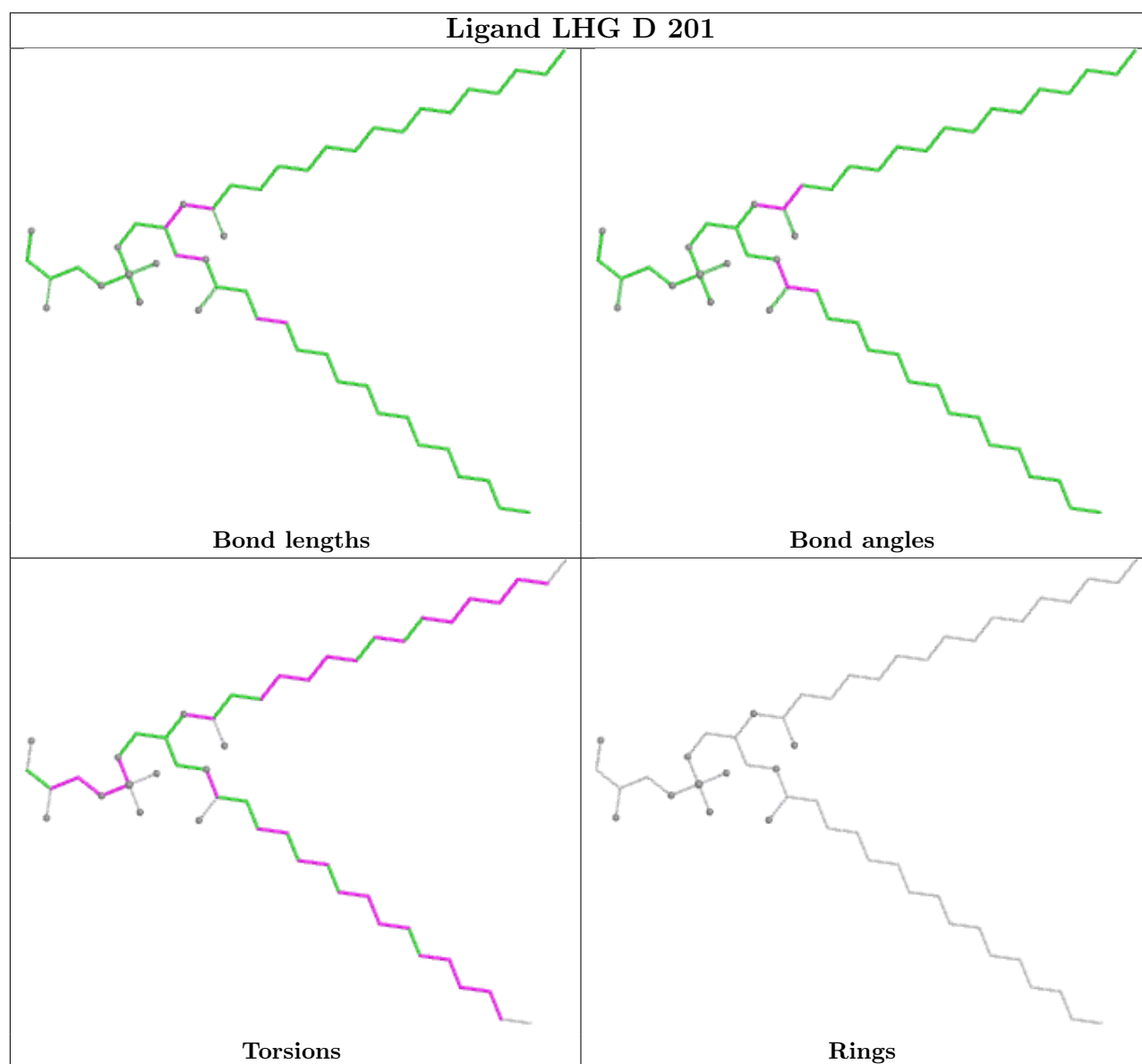


Ligand CLA b 828

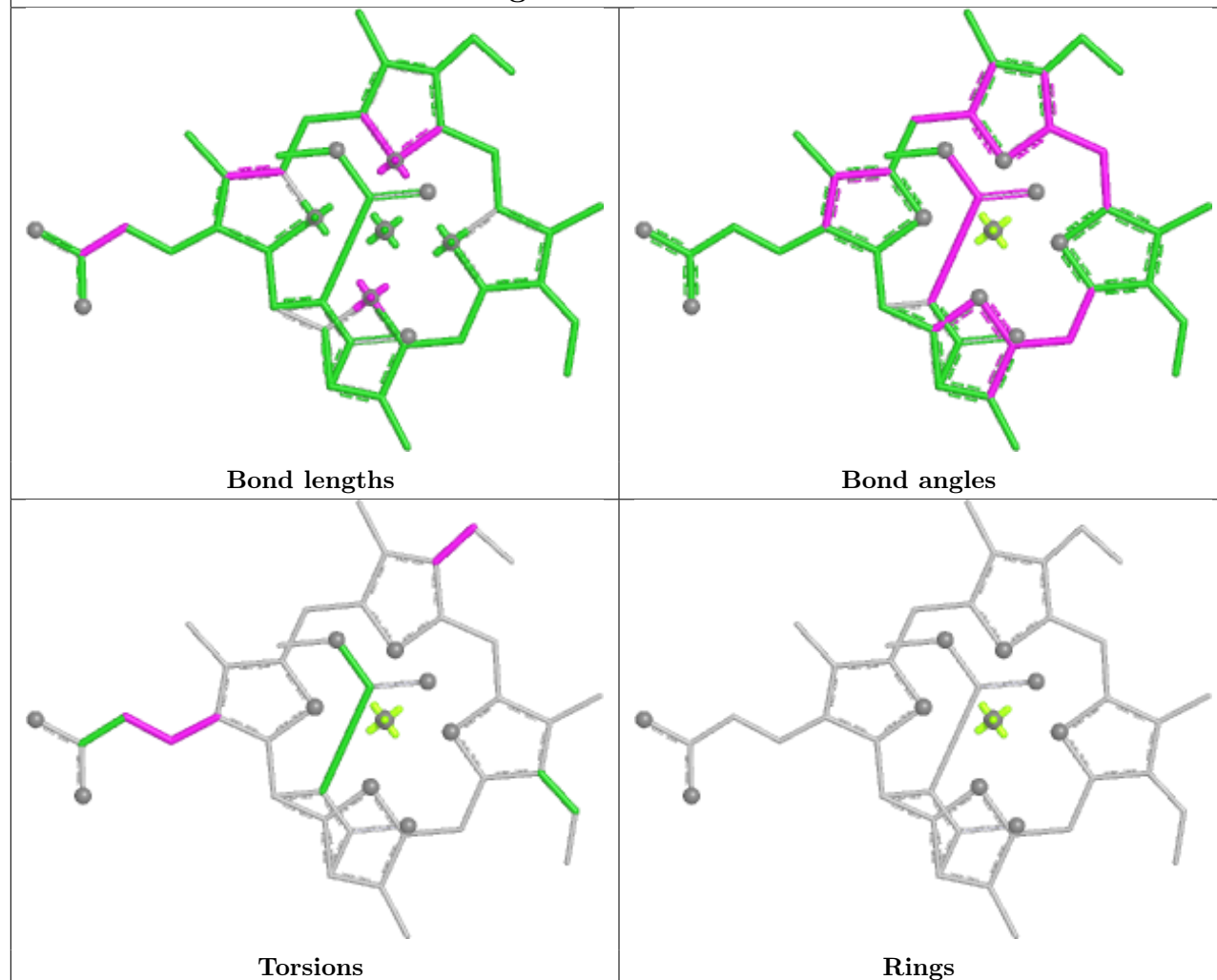




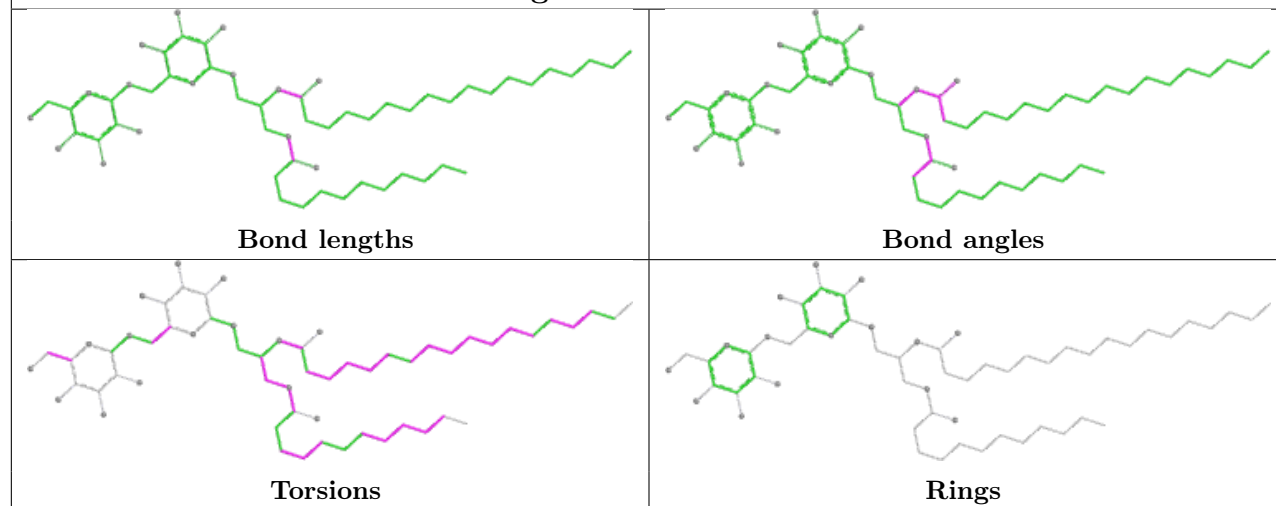




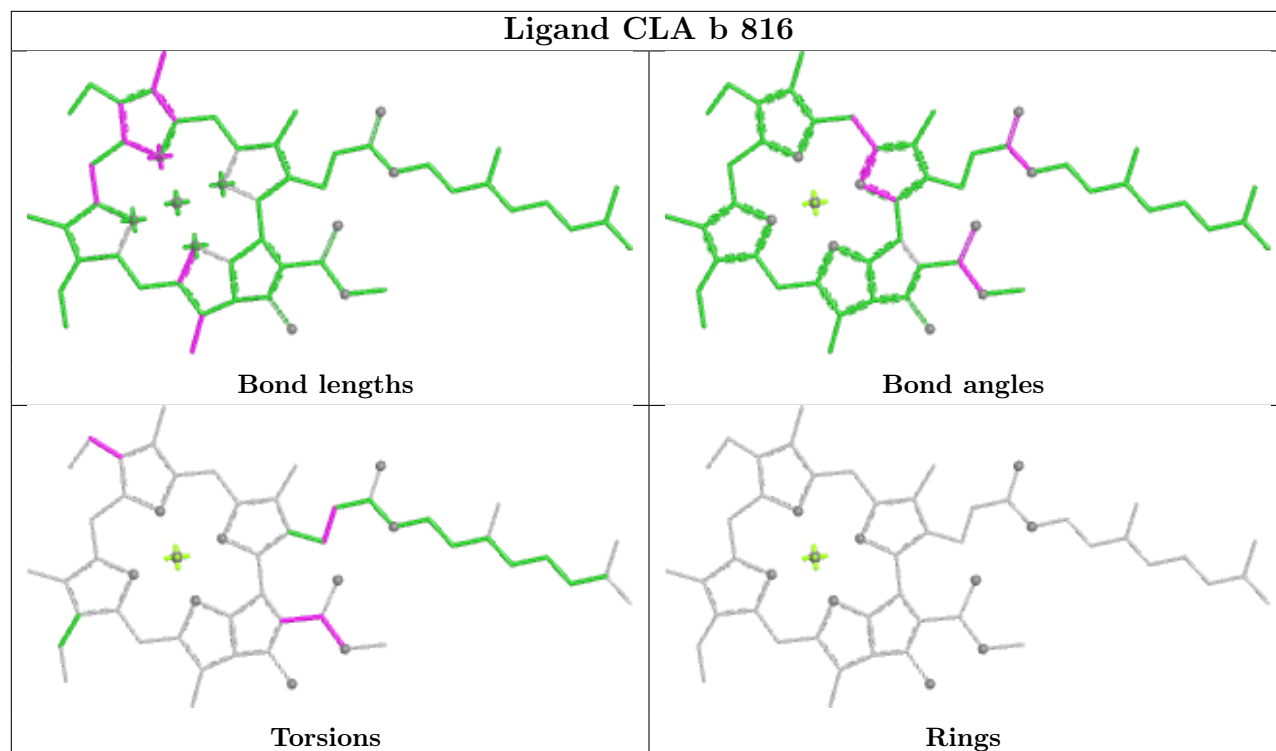
Ligand KC1 C 313



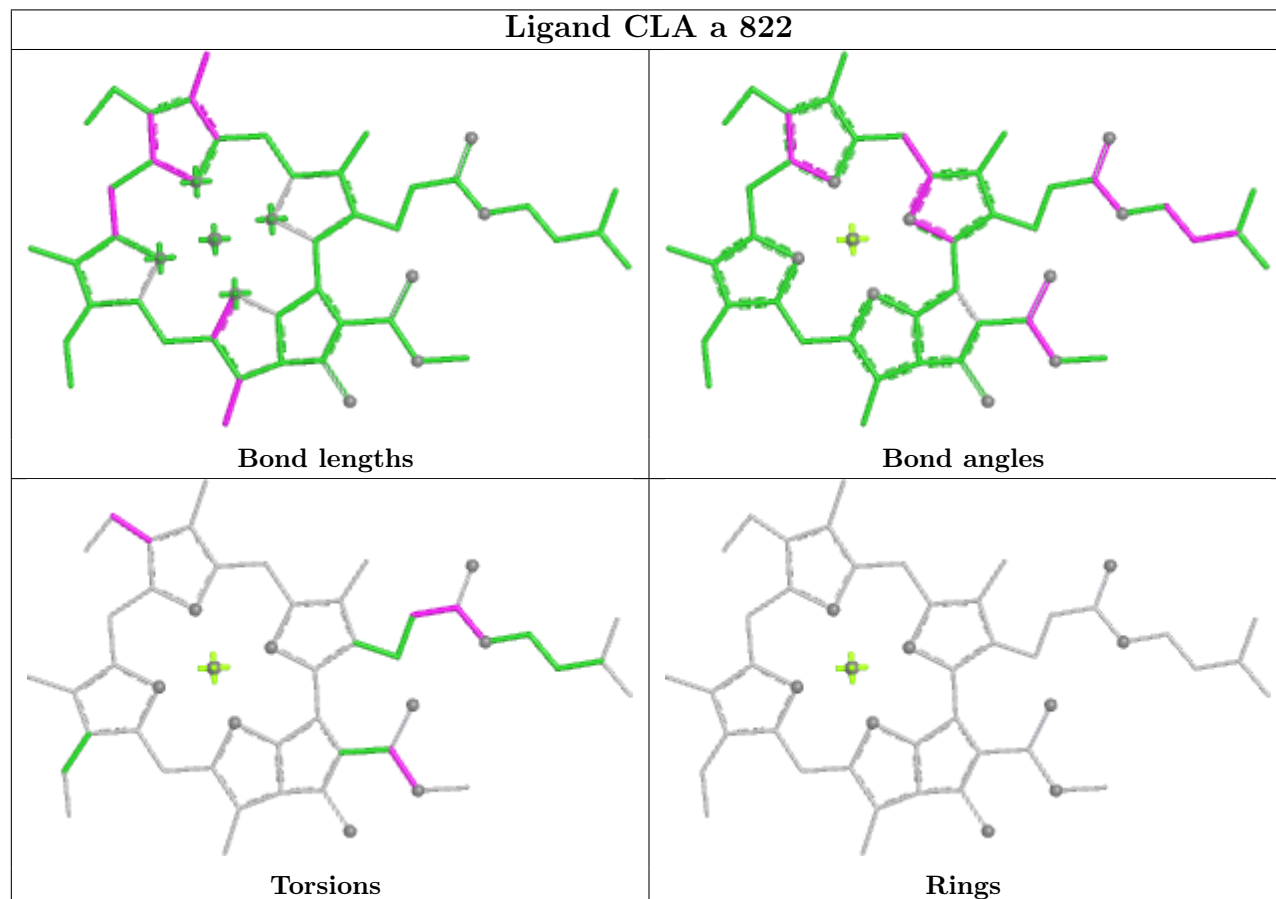
Ligand DGD b 834

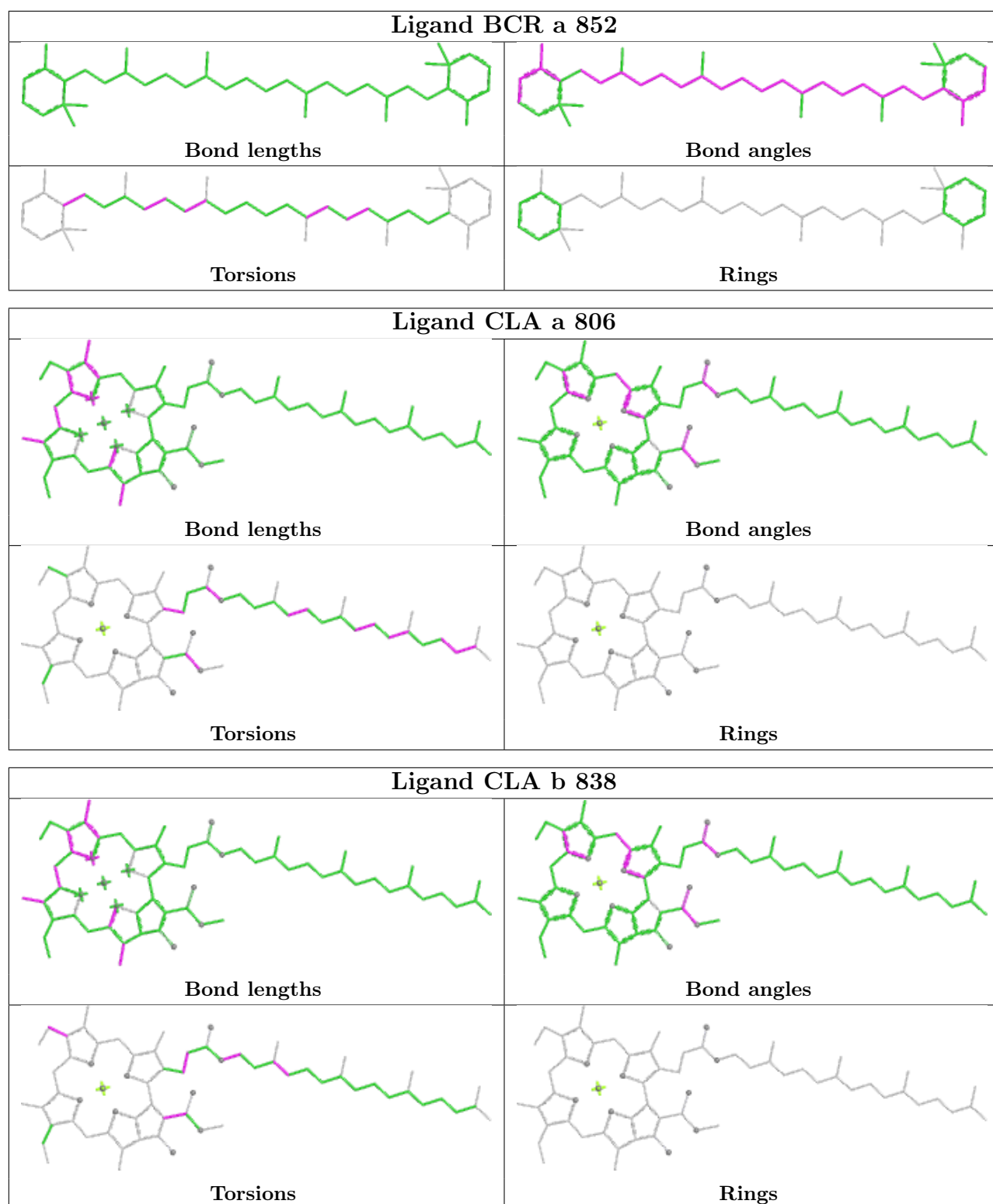


Ligand CLA b 816

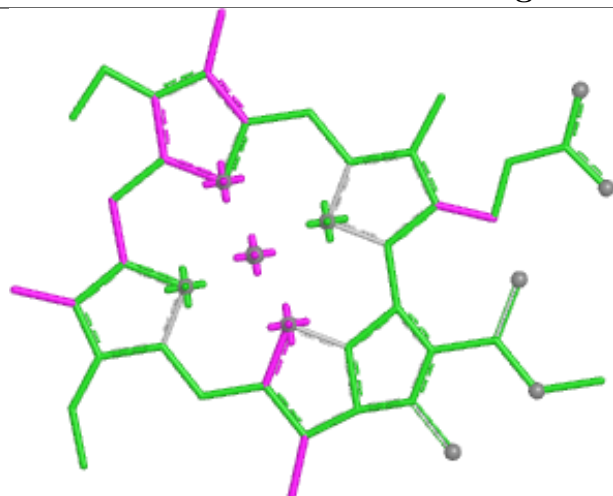


Ligand CLA a 822

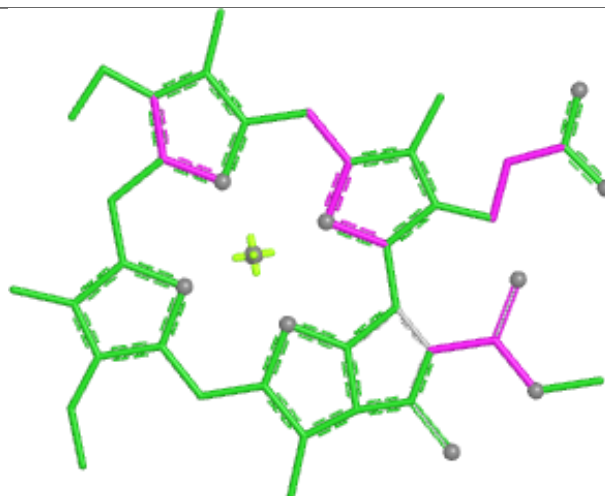




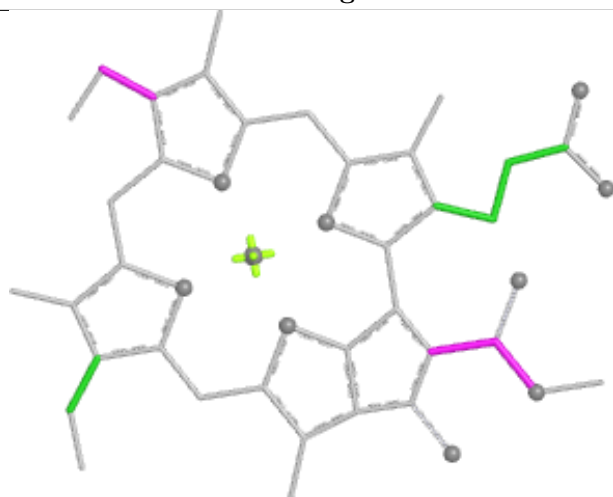
Ligand CLA E 314



Bond lengths



Bond angles

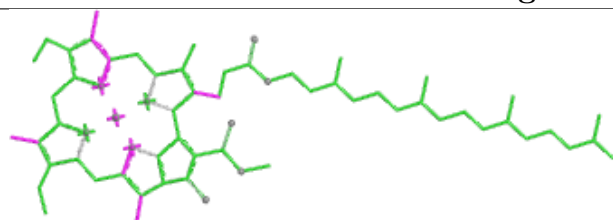


Torsions

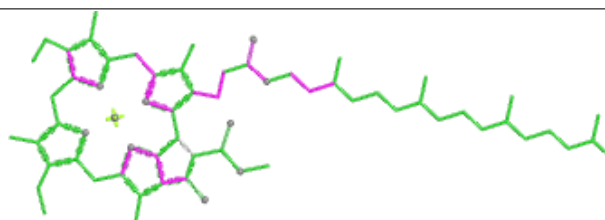


Rings

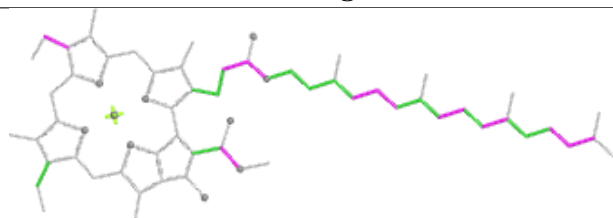
Ligand CLA a 801



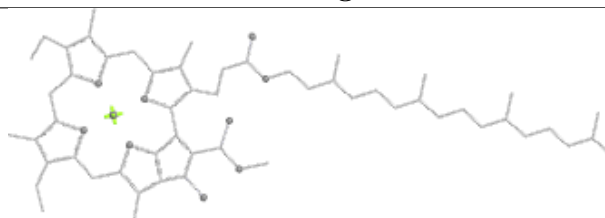
Bond lengths



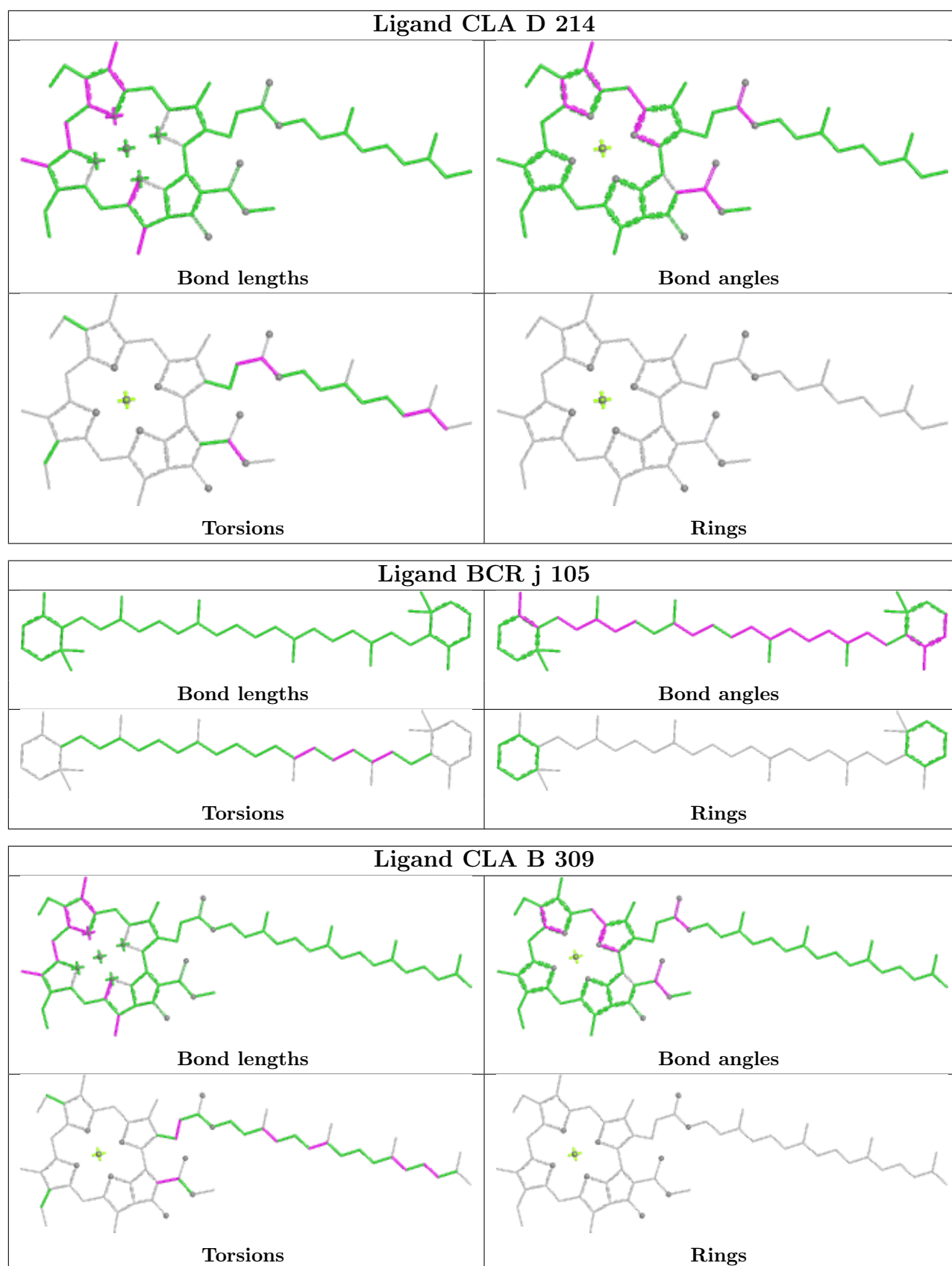
Bond angles

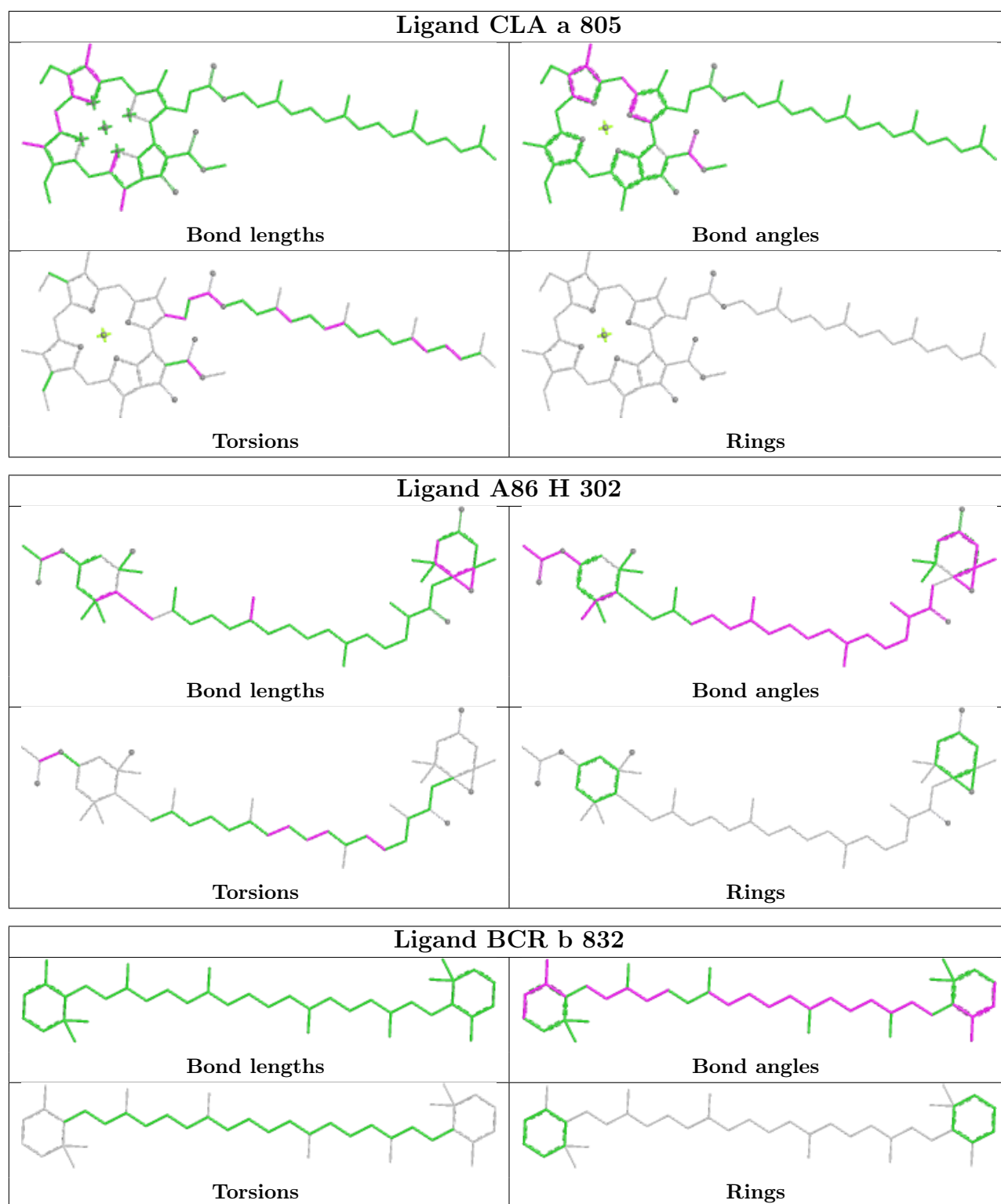


Torsions

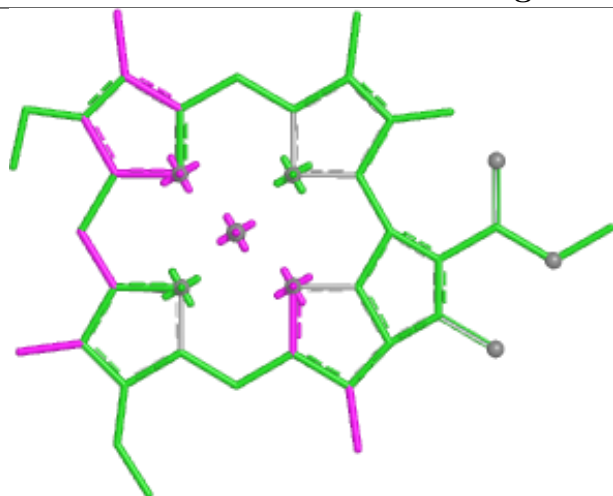


Rings

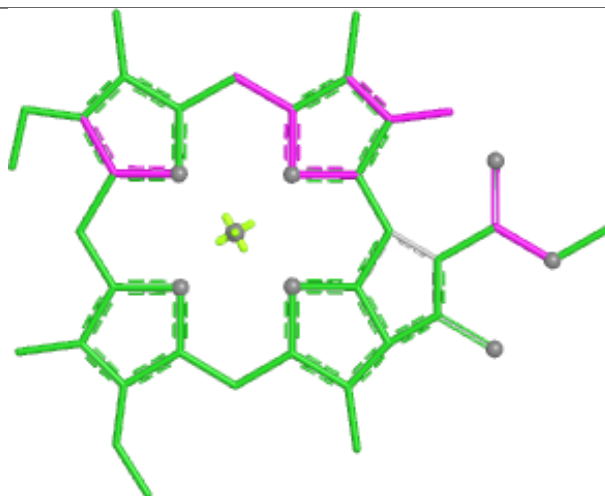




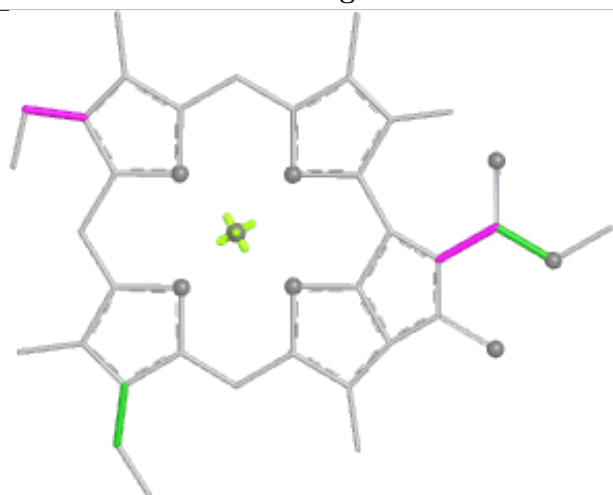
Ligand CLA C 316



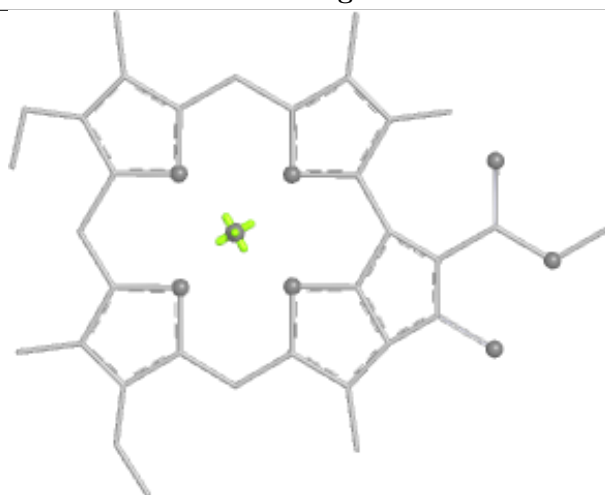
Bond lengths



Bond angles

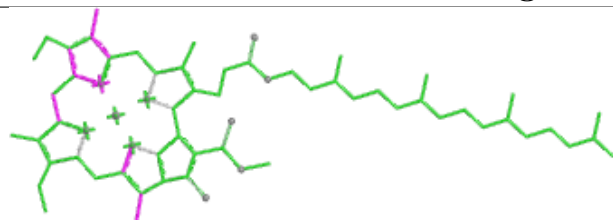


Torsions

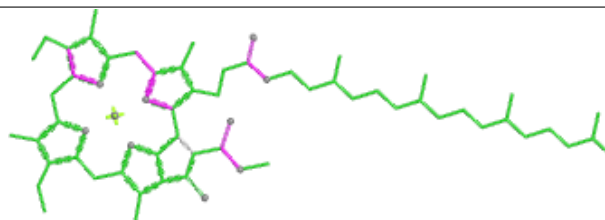


Rings

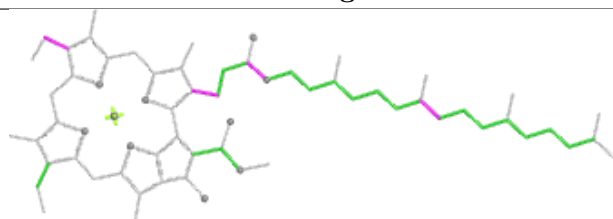
Ligand CLA a 846



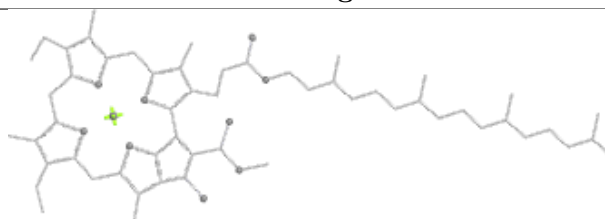
Bond lengths



Bond angles

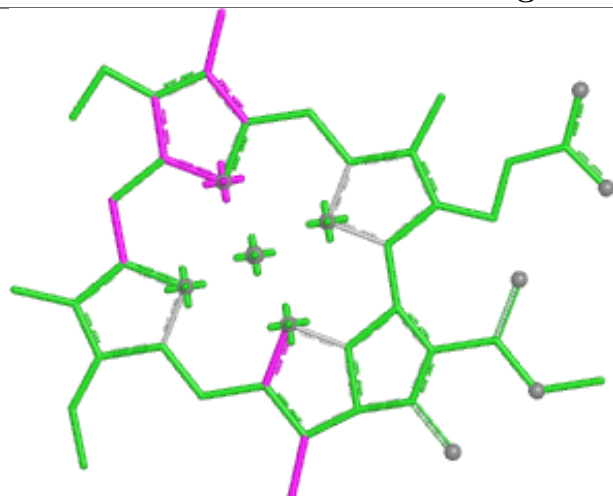


Torsions

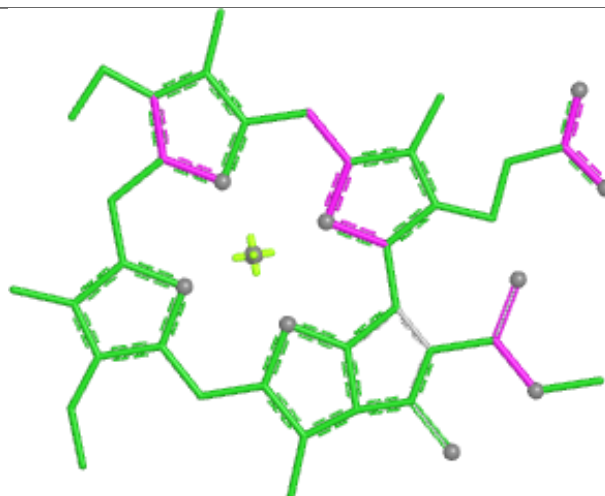


Rings

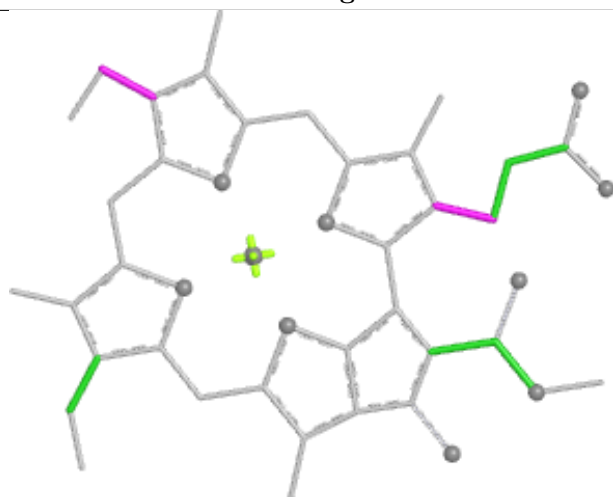
Ligand CLA b 825



Bond lengths



Bond angles

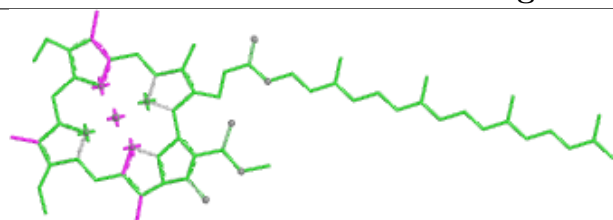


Torsions

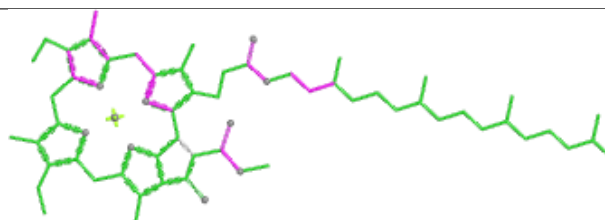


Rings

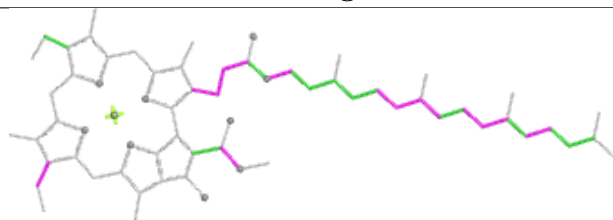
Ligand CLA b 824



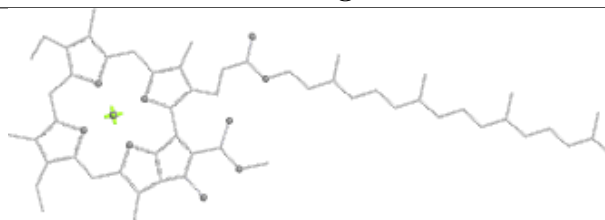
Bond lengths



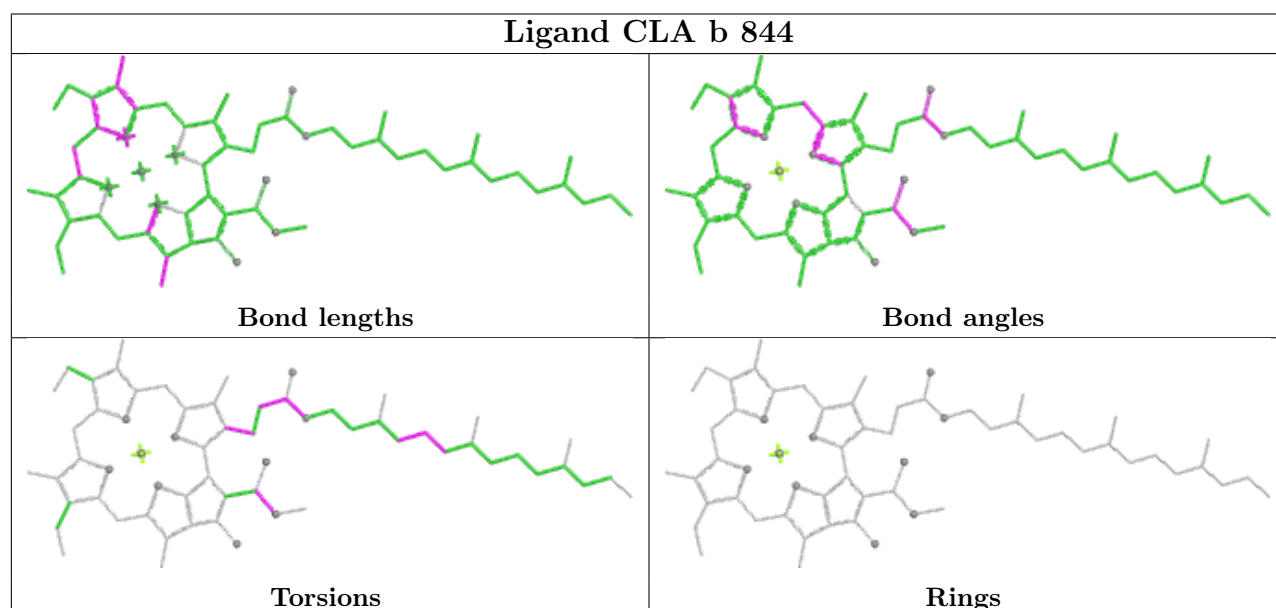
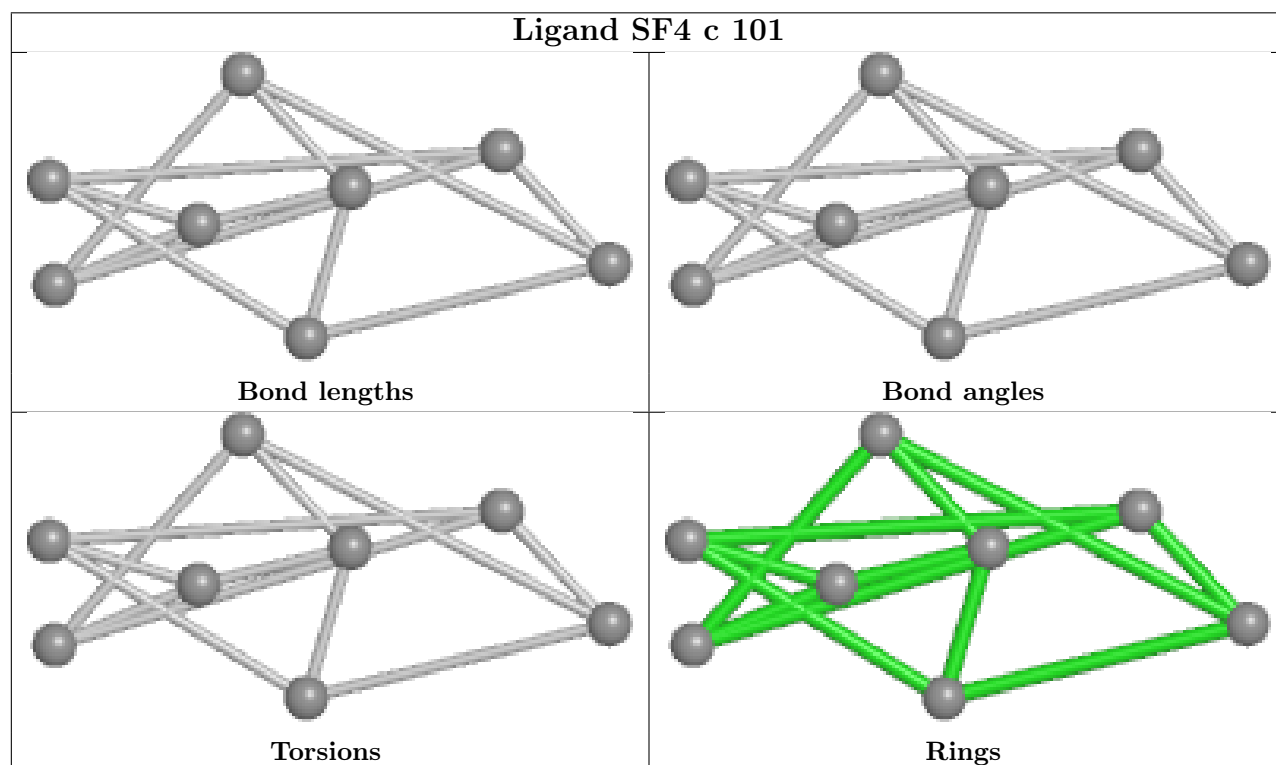
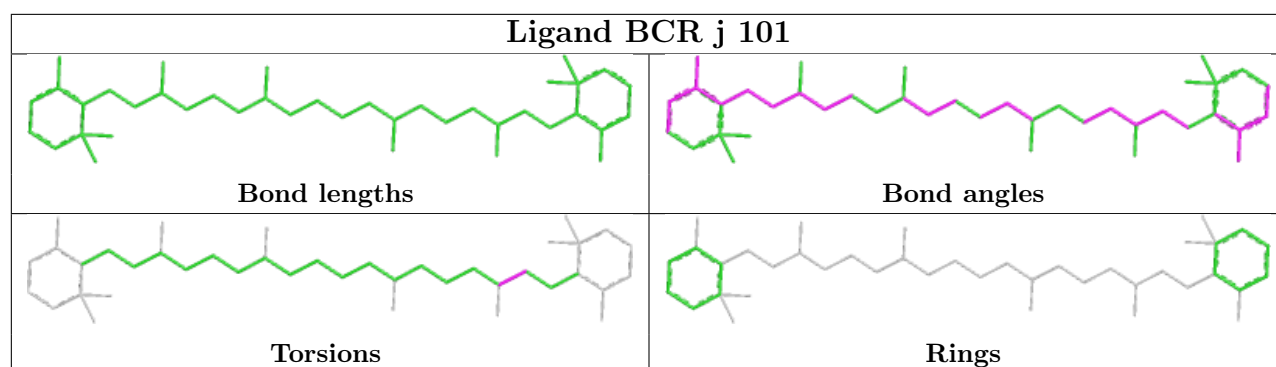
Bond angles



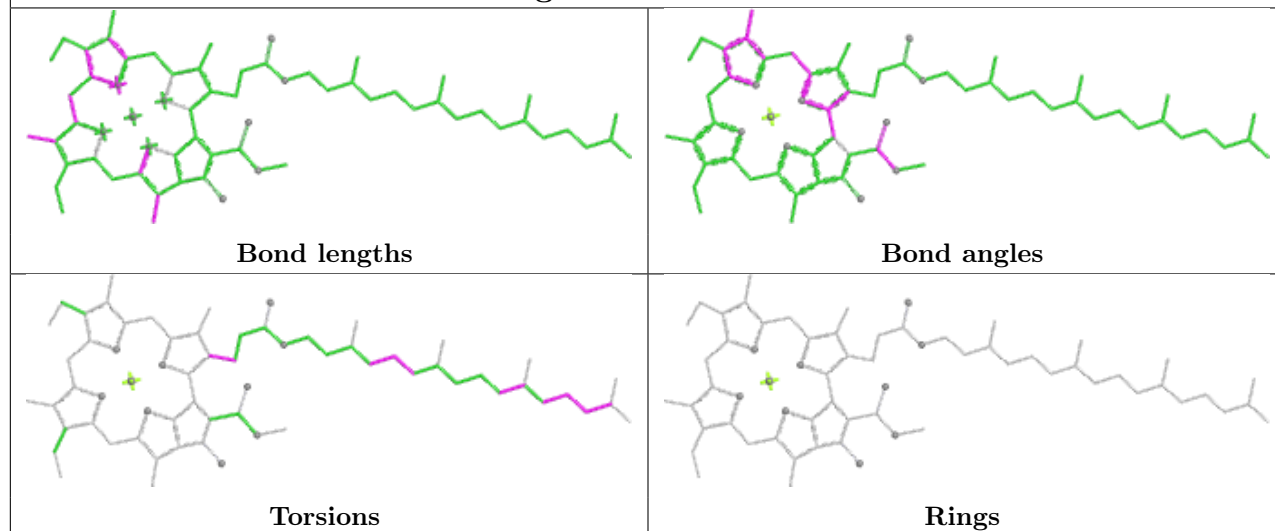
Torsions



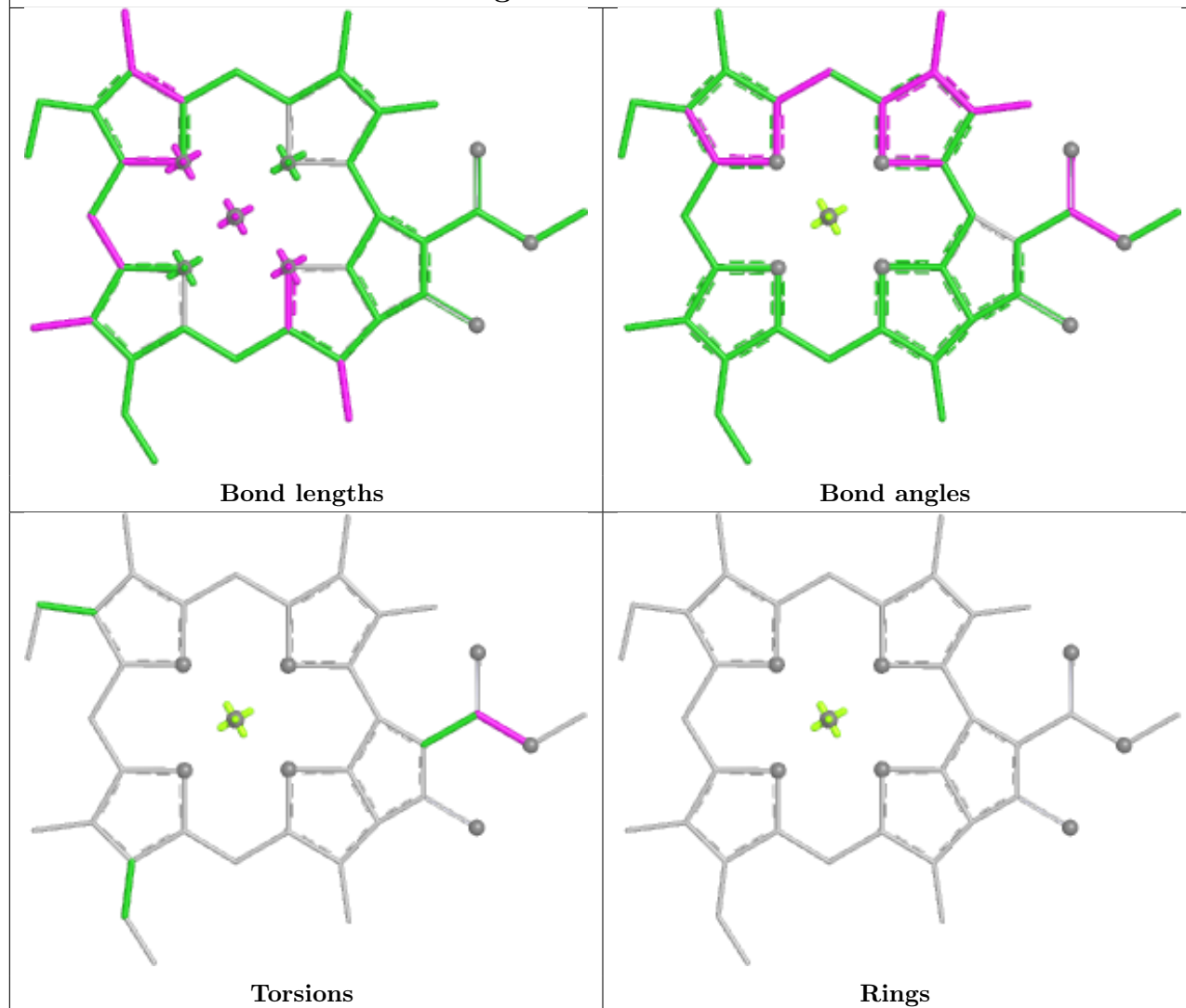
Rings



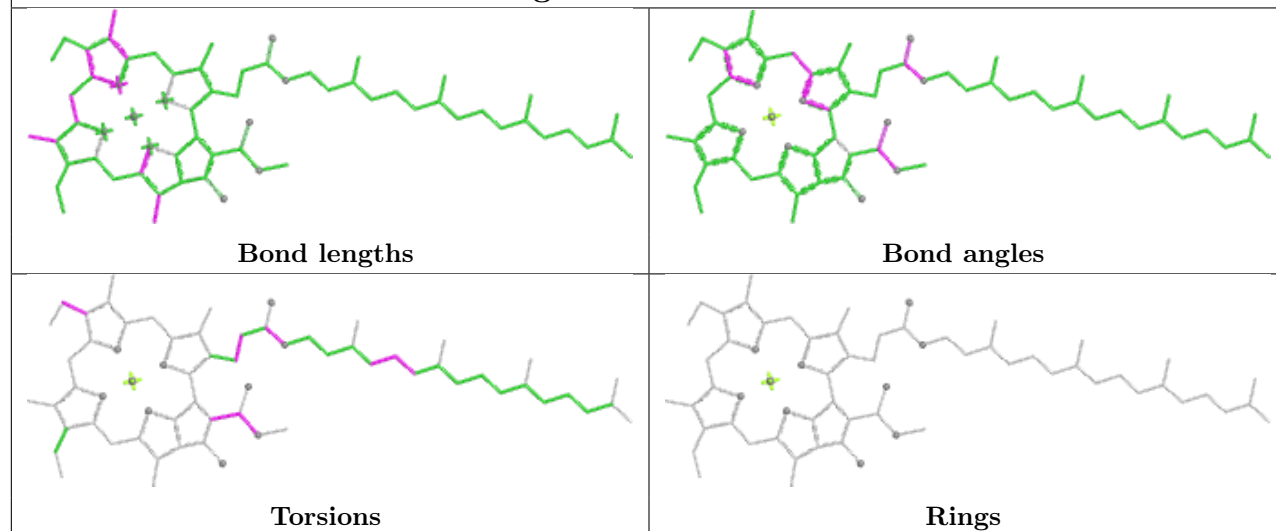
Ligand CLA a 843



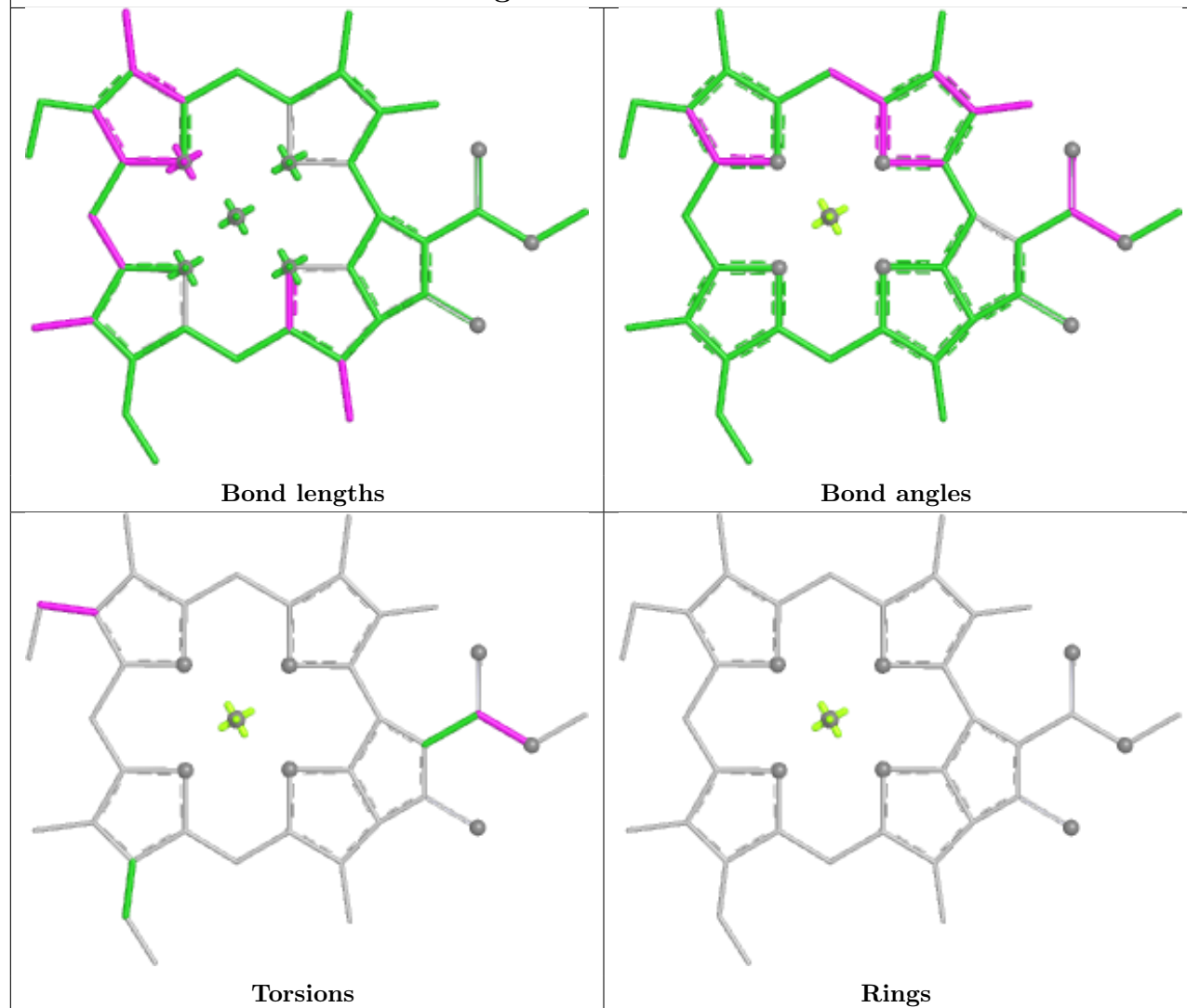
Ligand CLA B 314

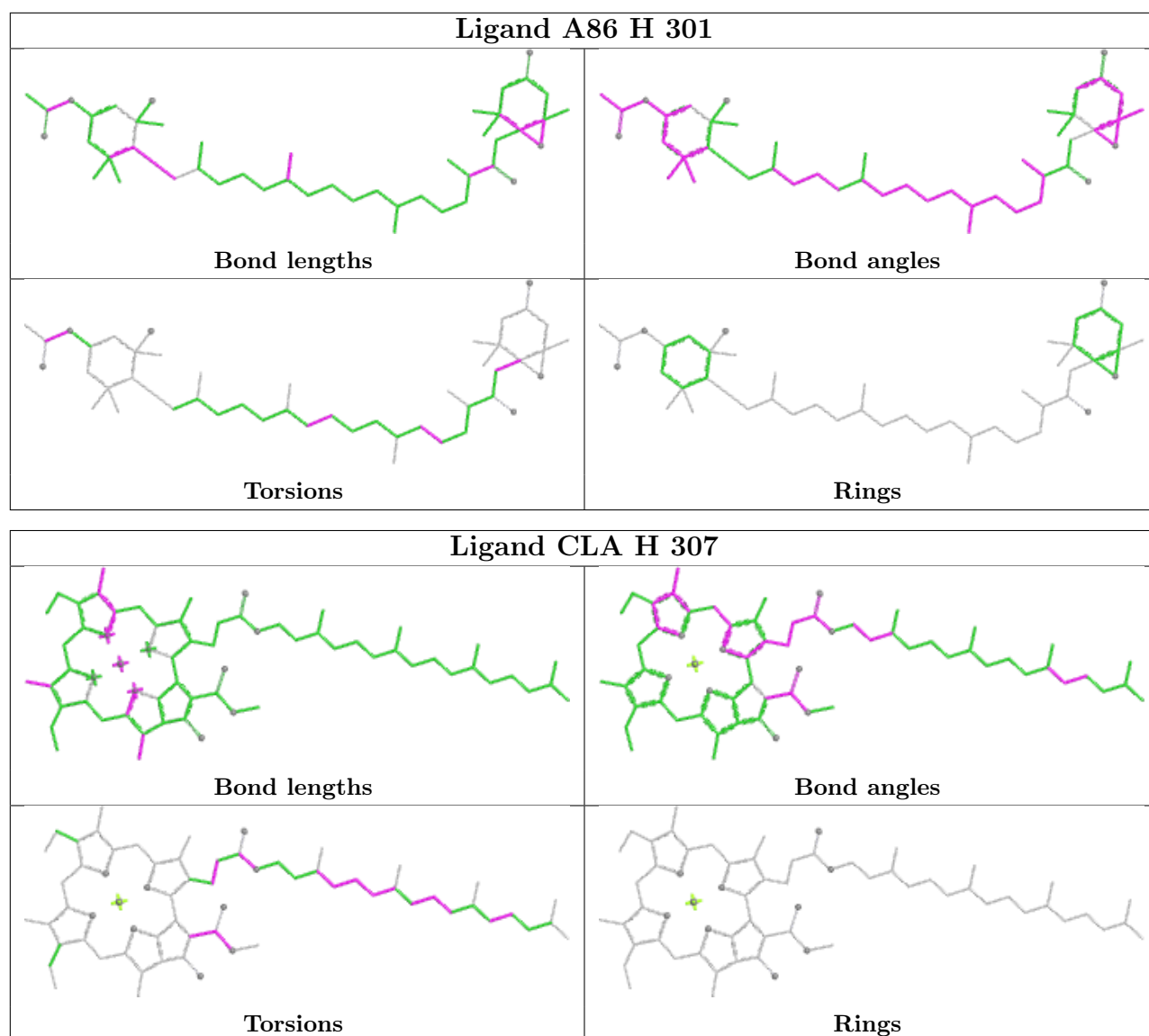


Ligand CLA E 315

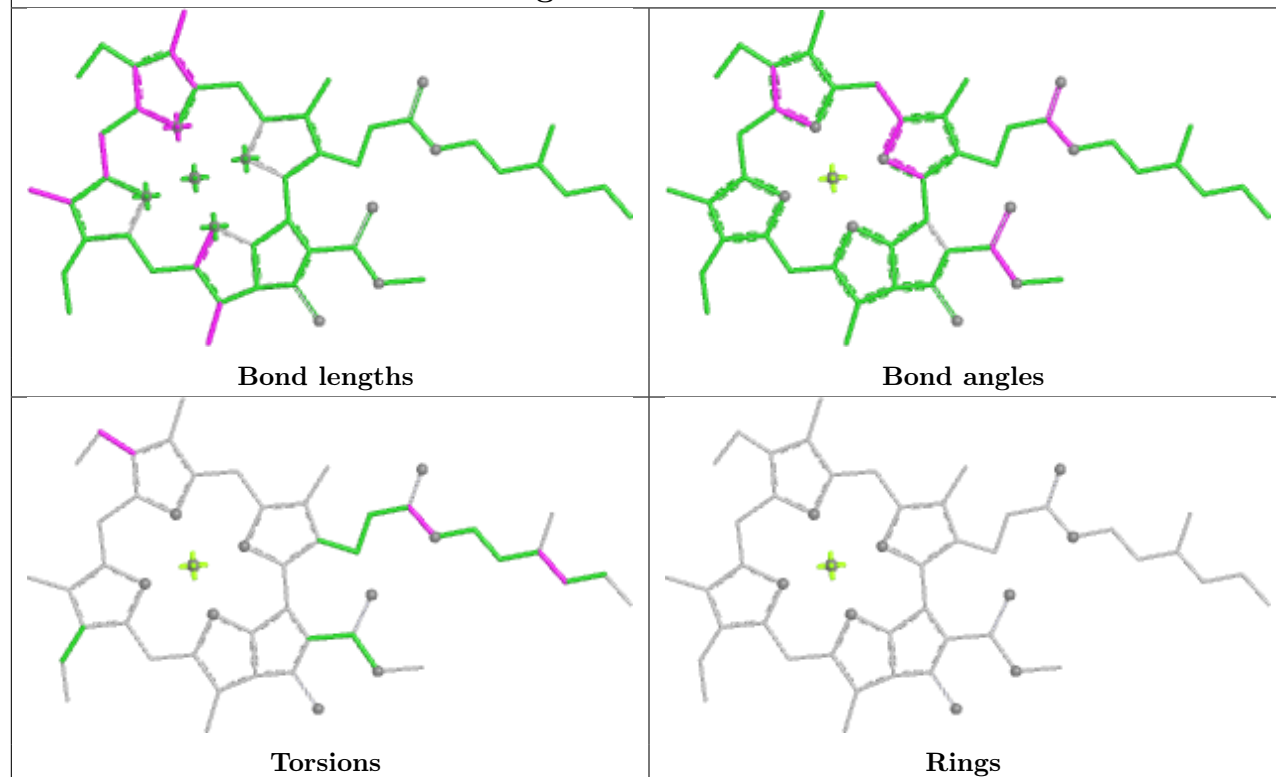


Ligand CLA D 215

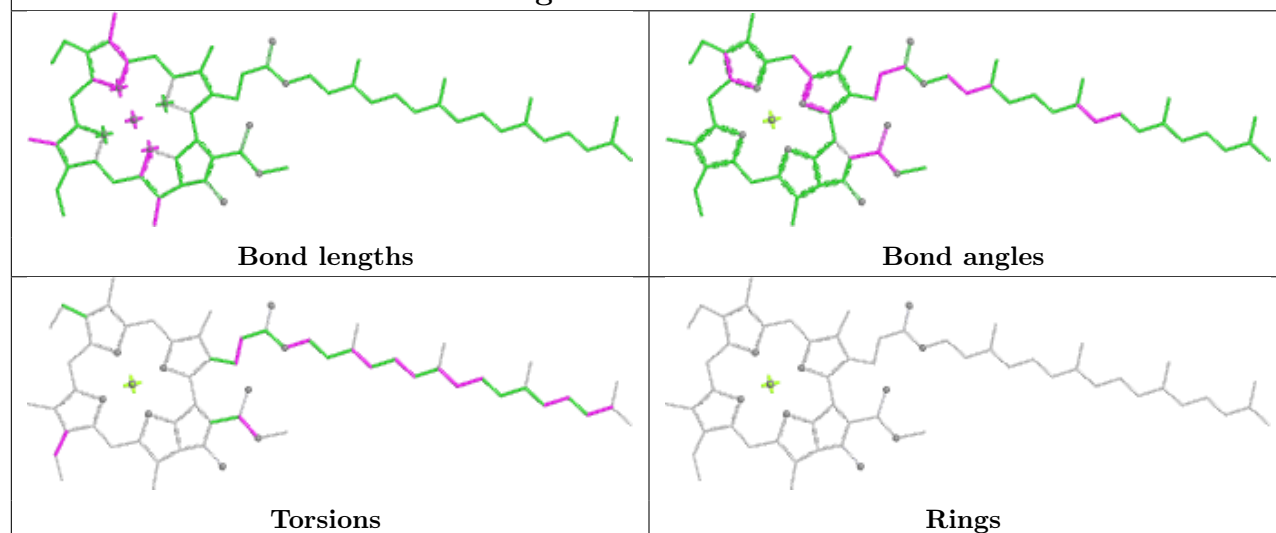


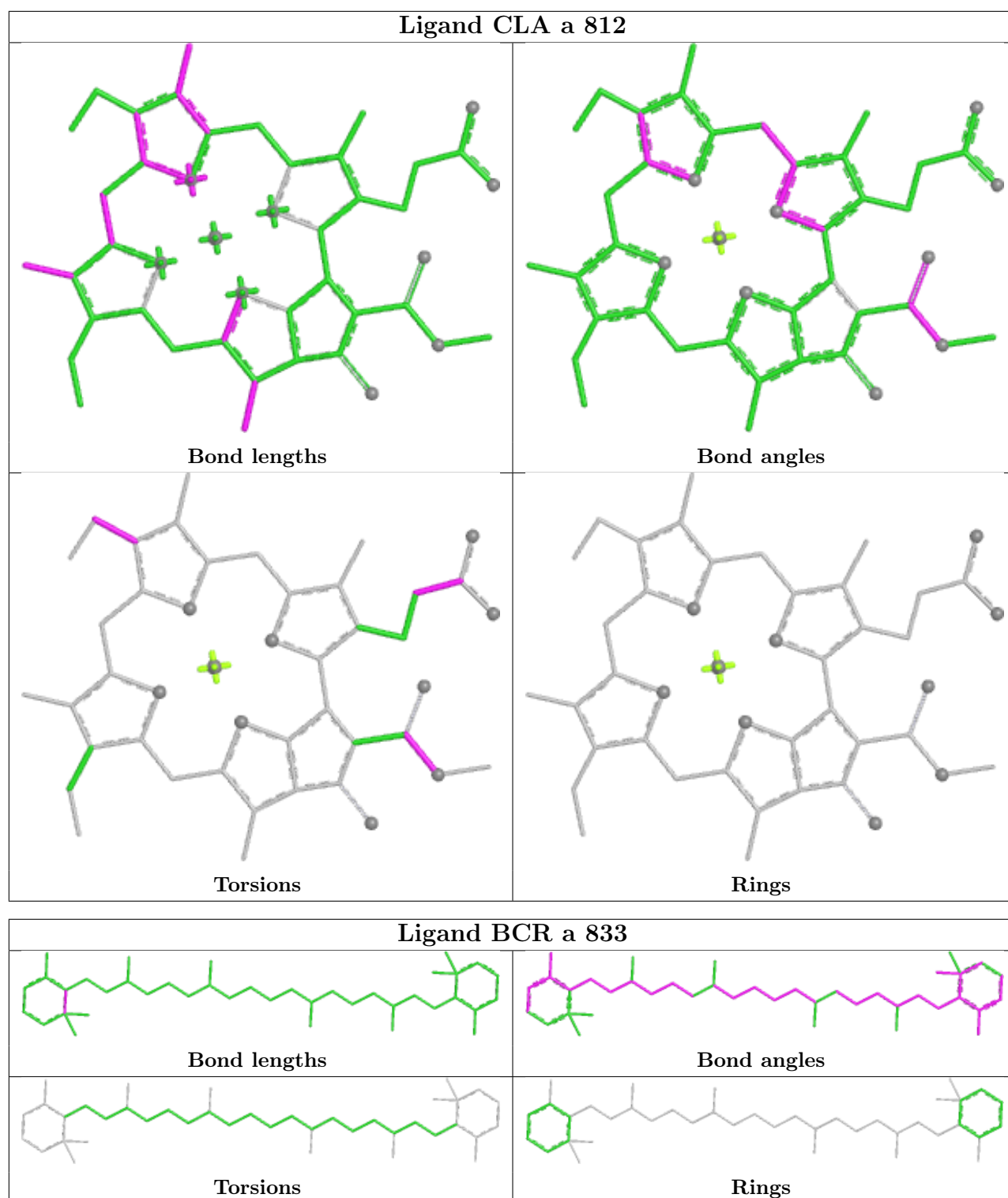


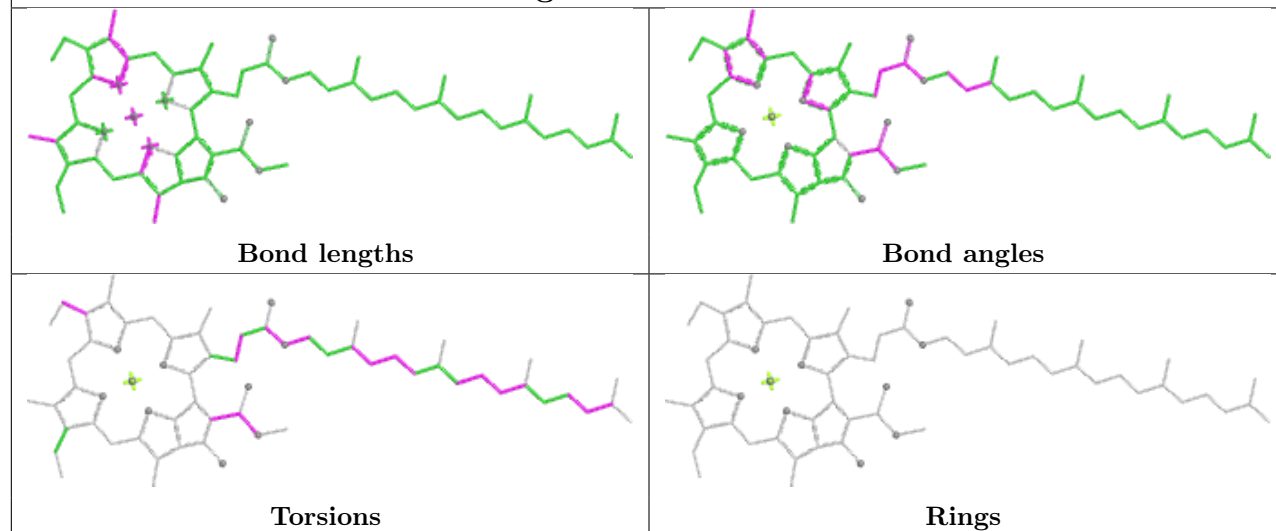
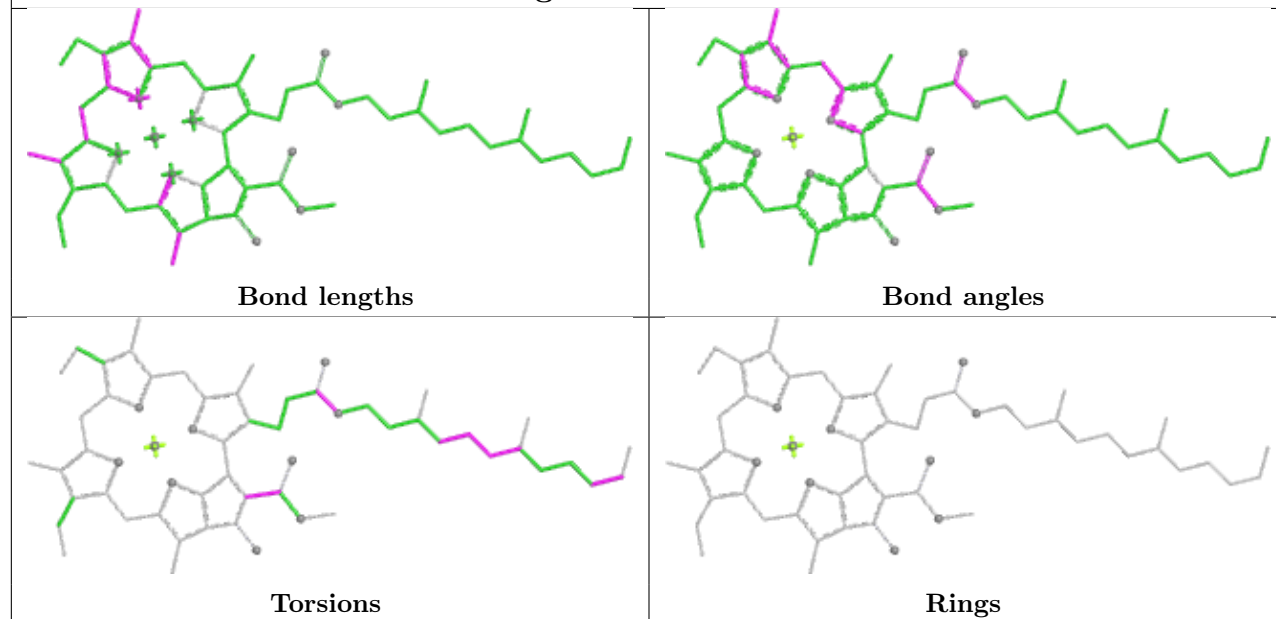
Ligand CLA a 830

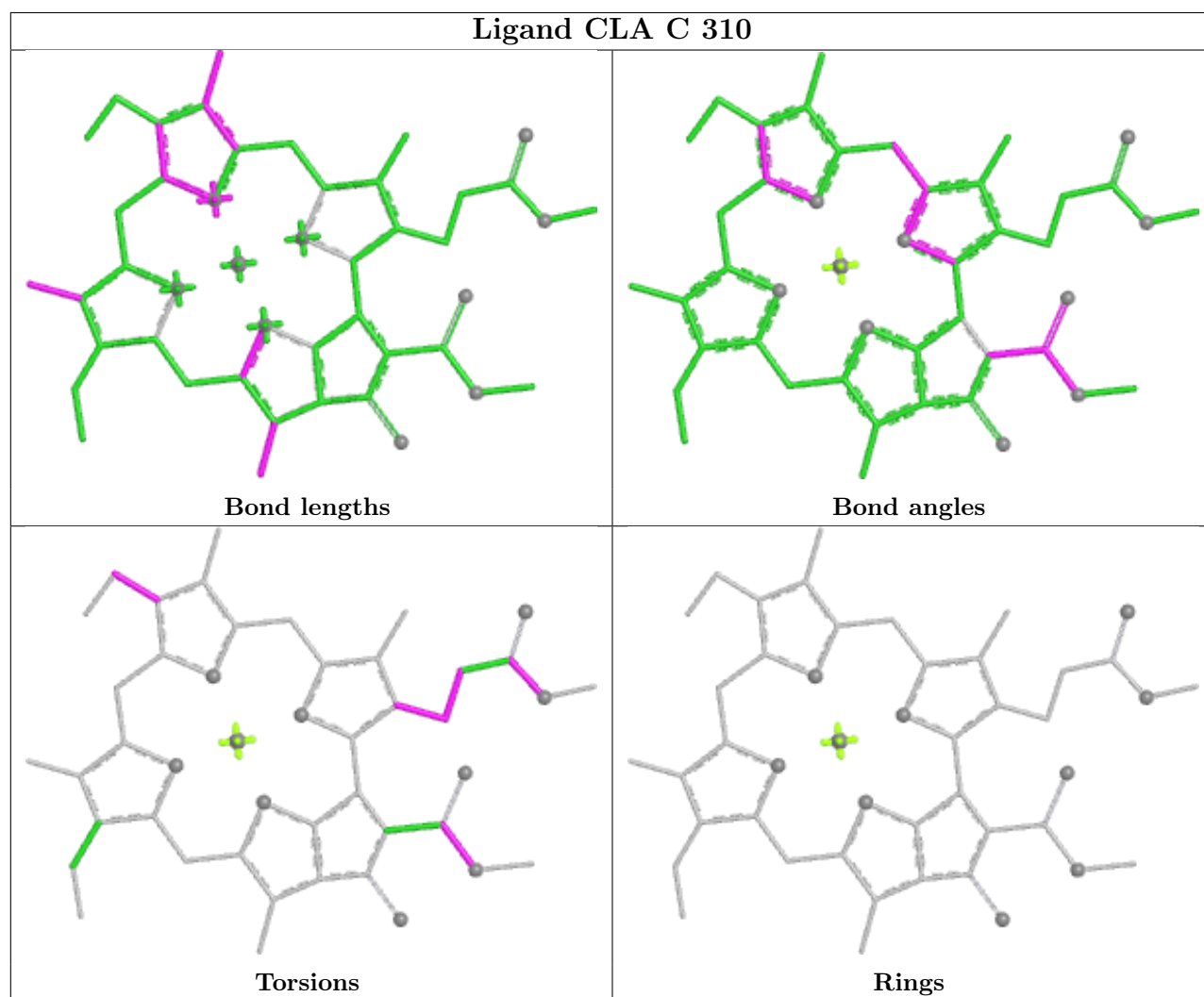
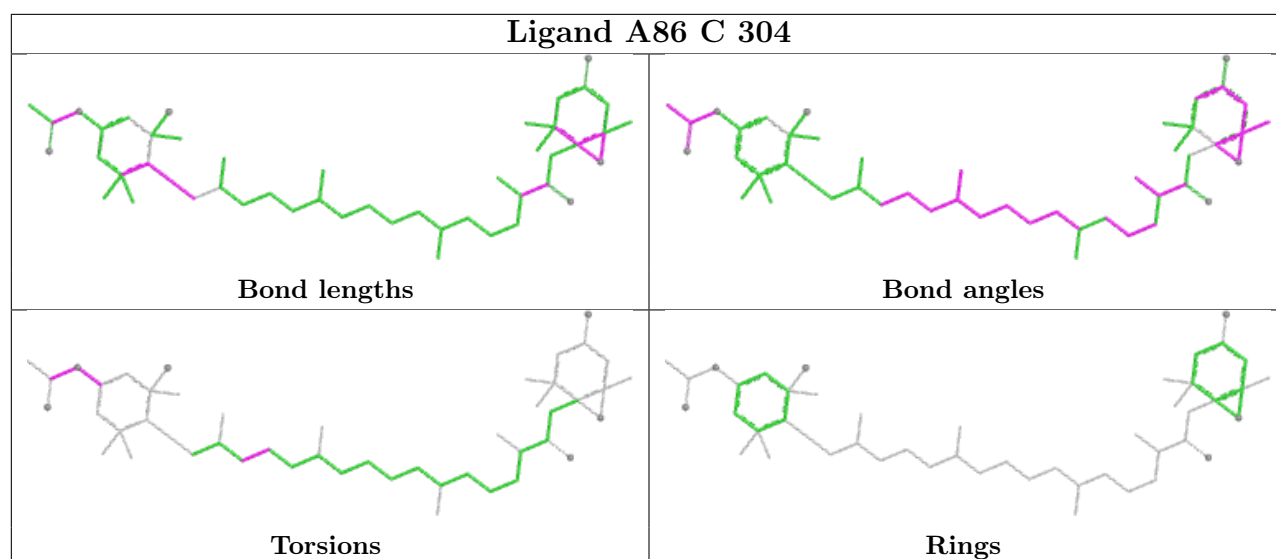


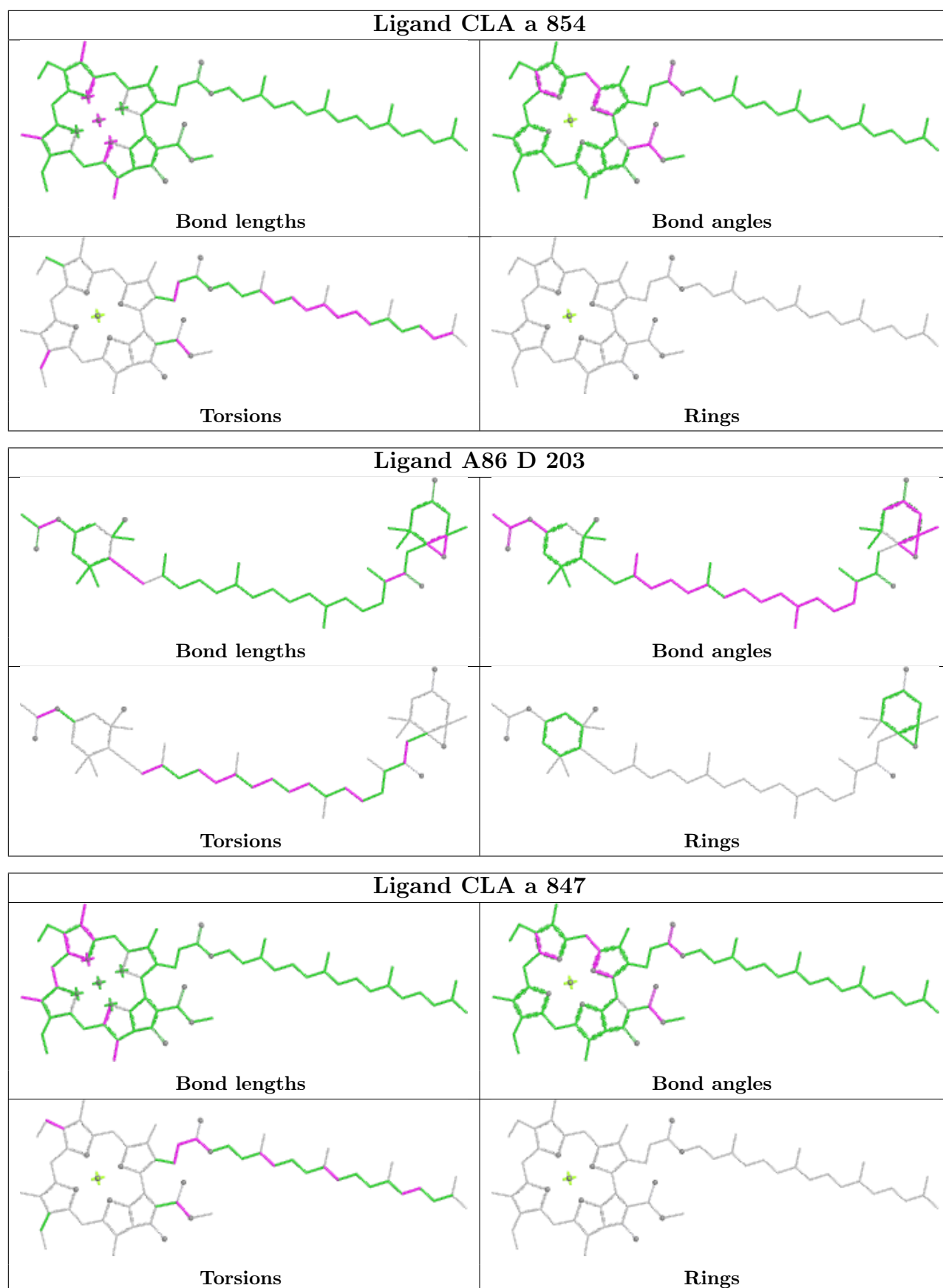
Ligand CLA b 829

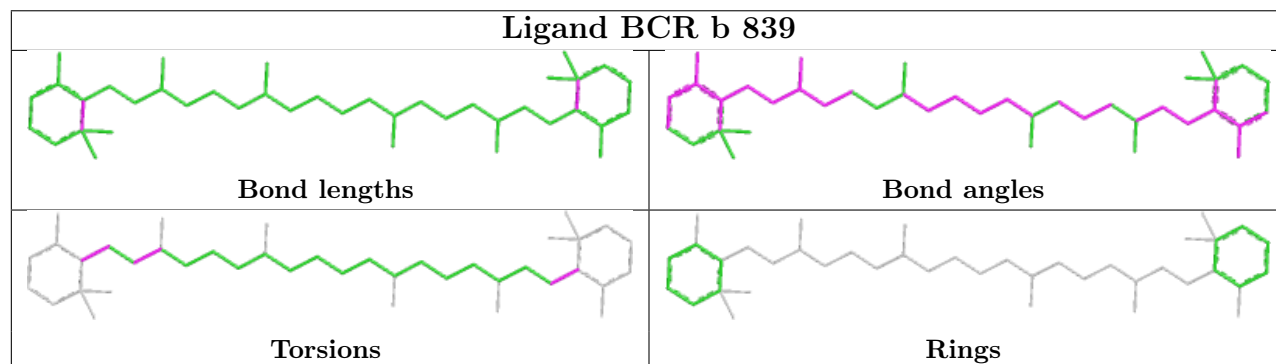
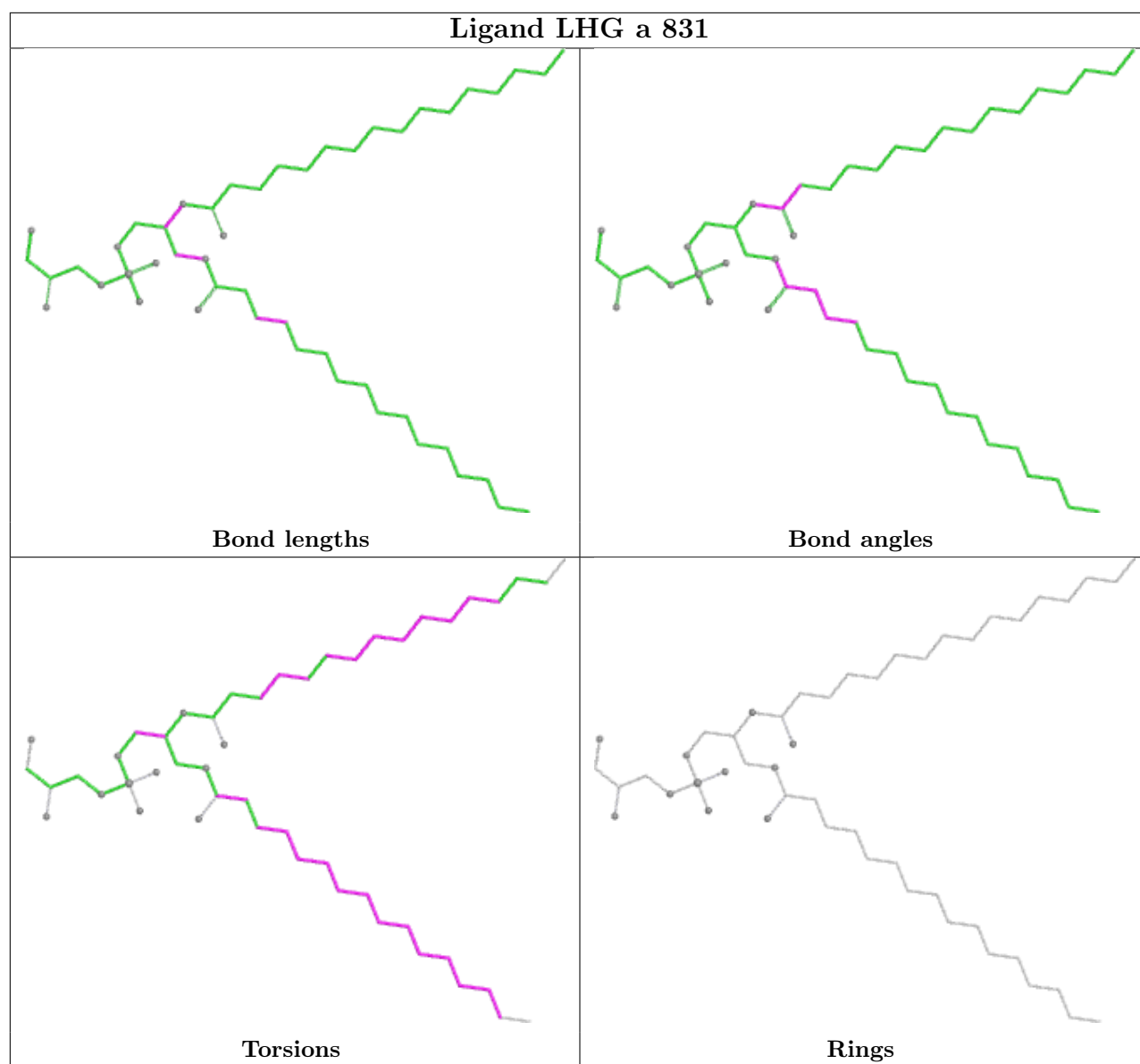


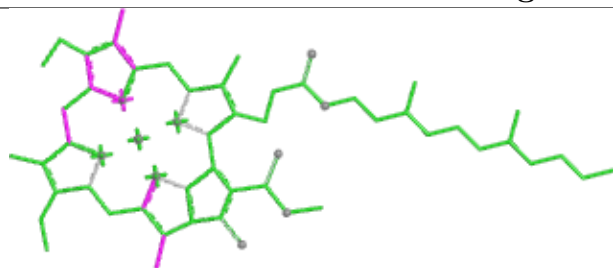


Ligand CLA a 841**Ligand CLA b 812**

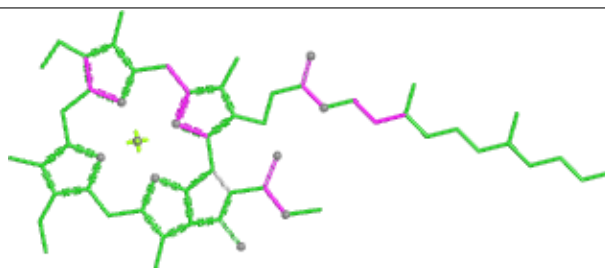




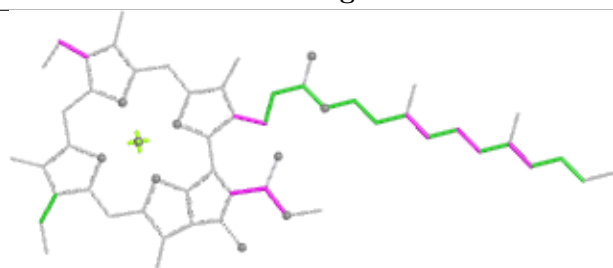


Ligand CLA b 823

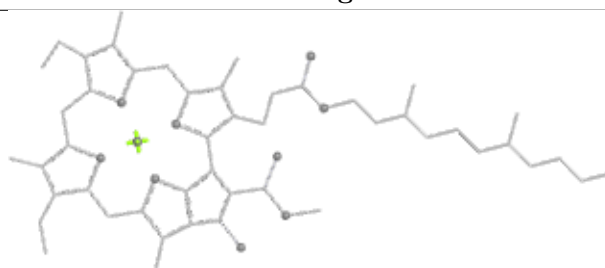
Bond lengths



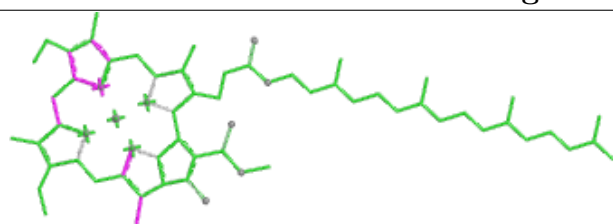
Bond angles



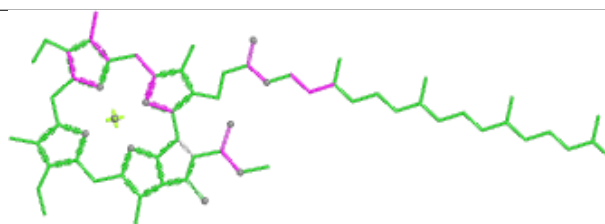
Torsions



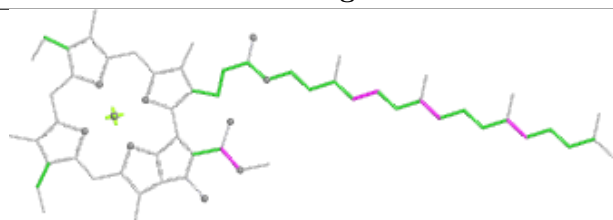
Rings

Ligand CLA f 202

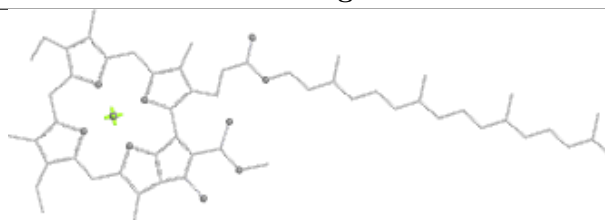
Bond lengths



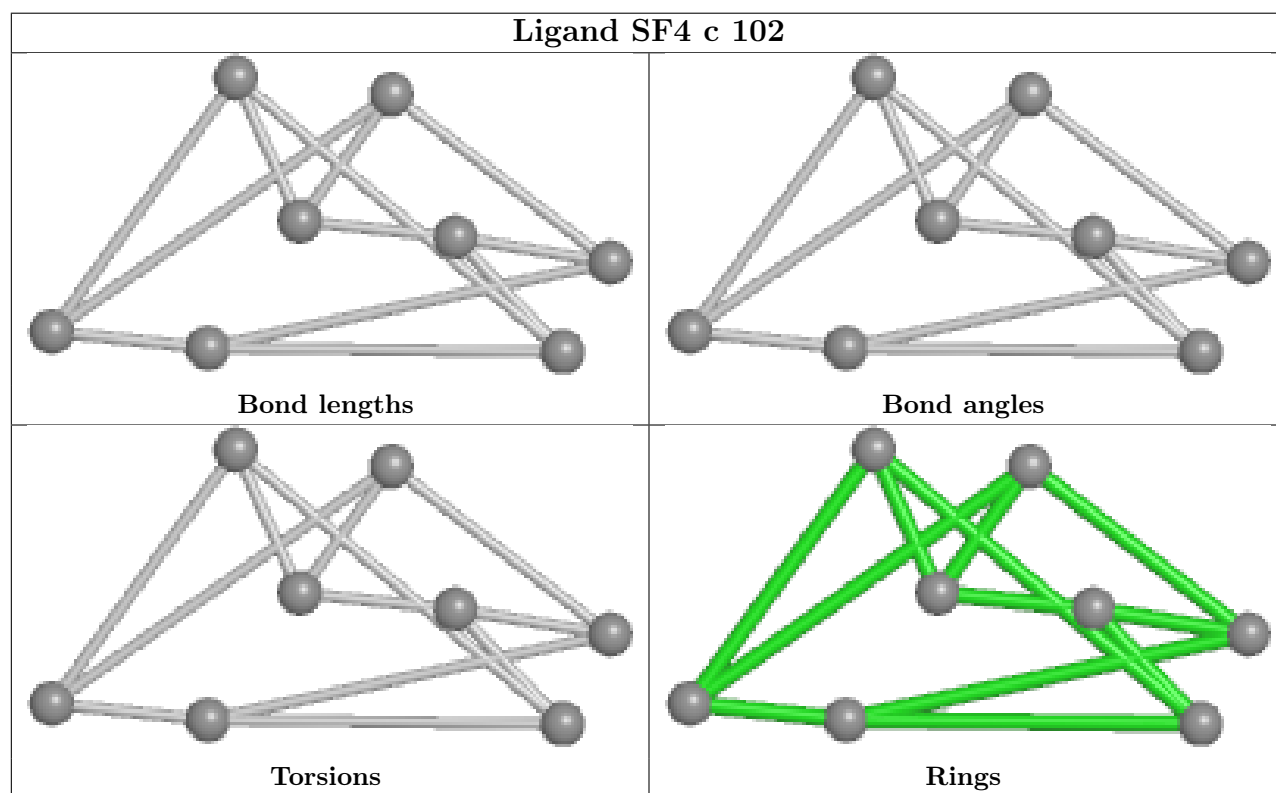
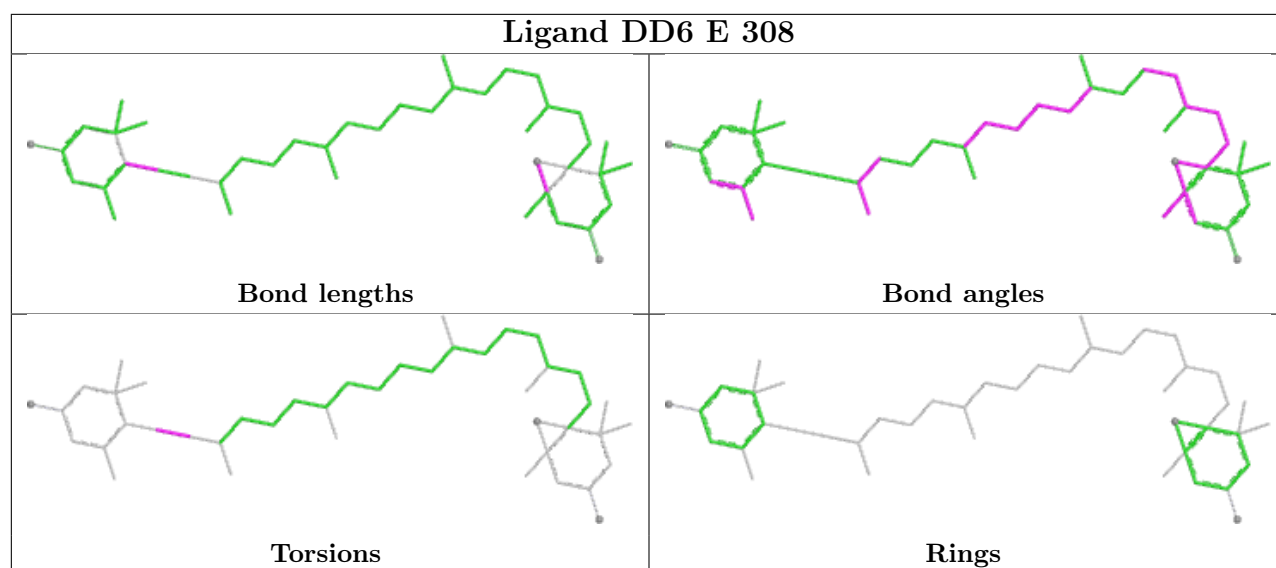
Bond angles



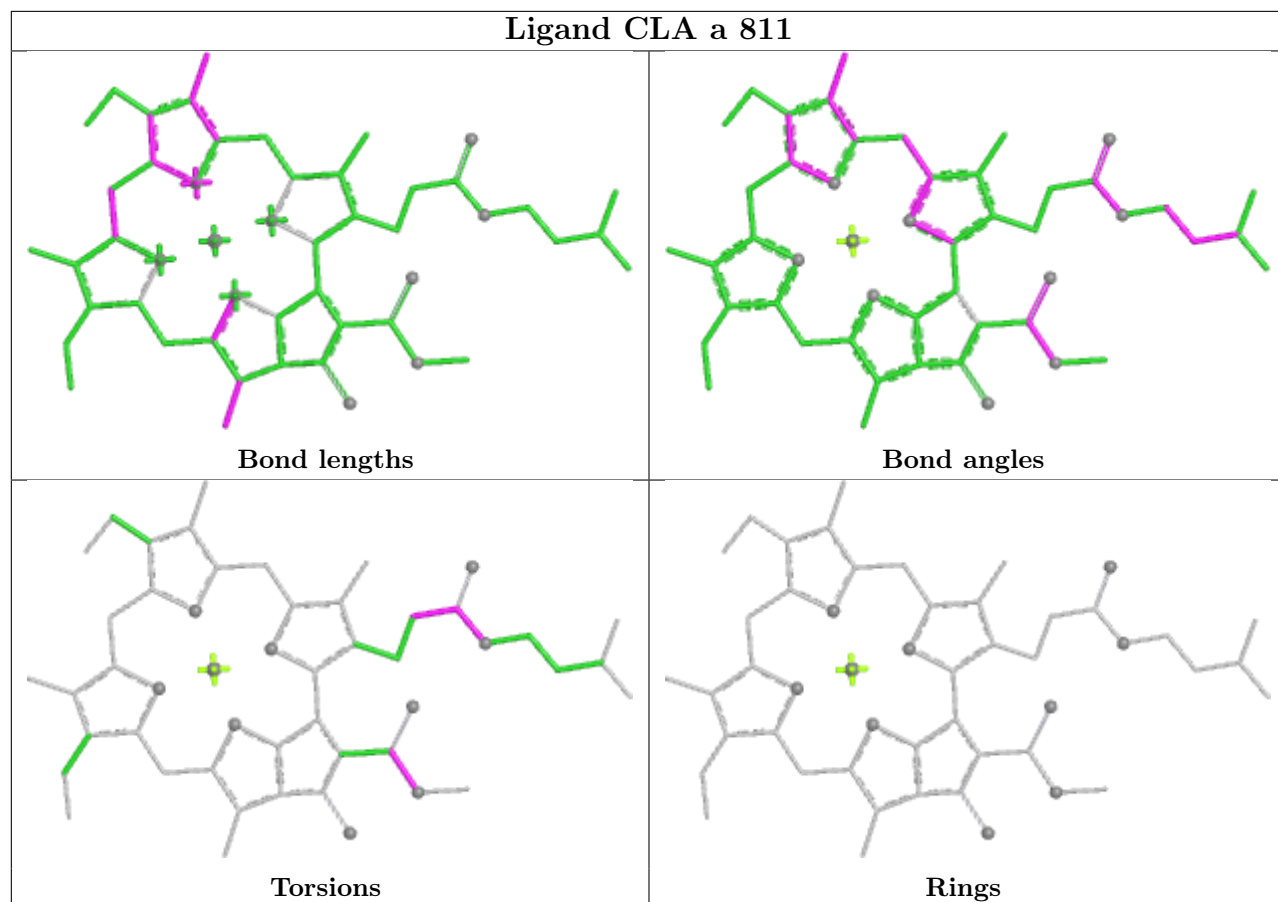
Torsions



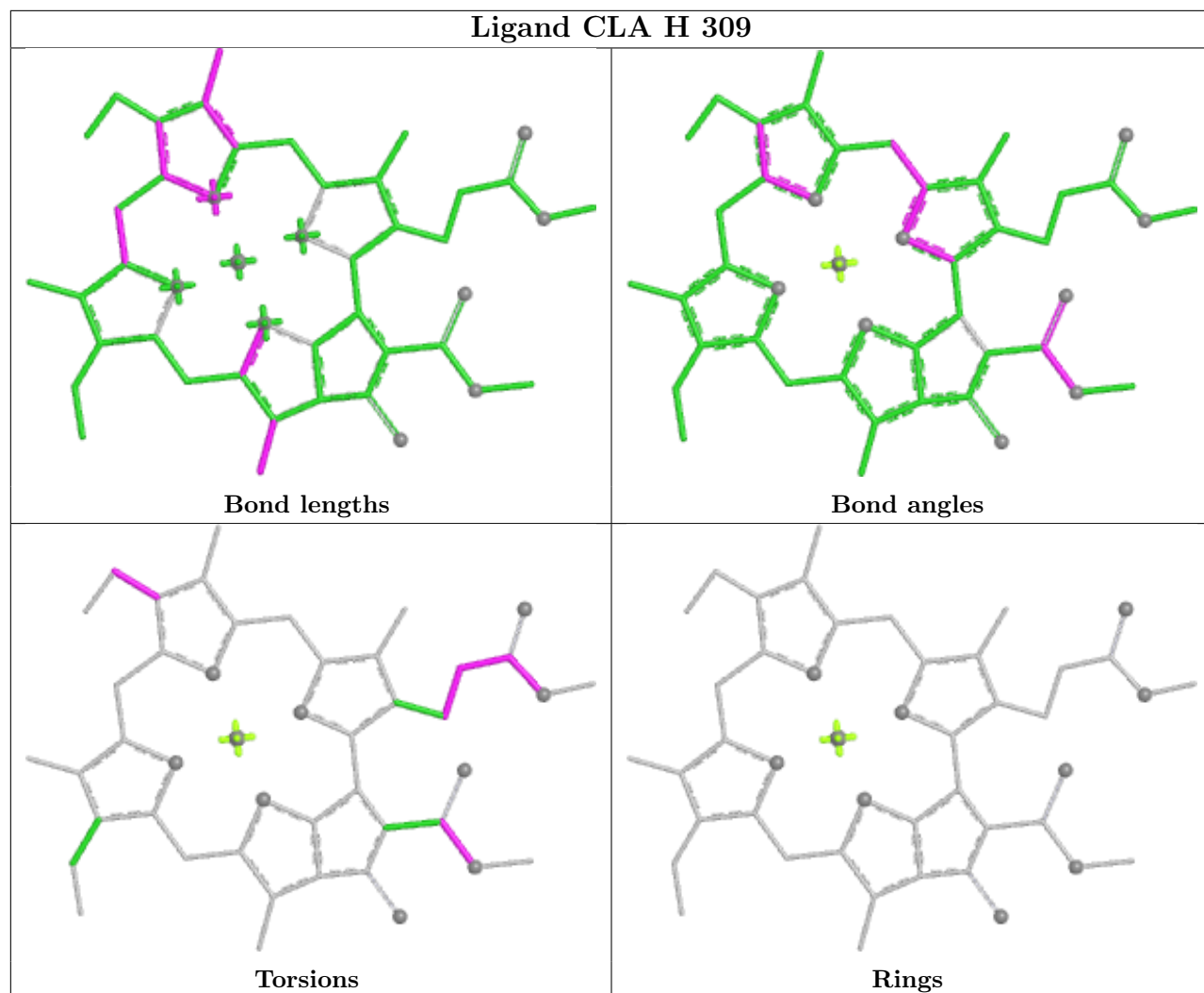
Rings



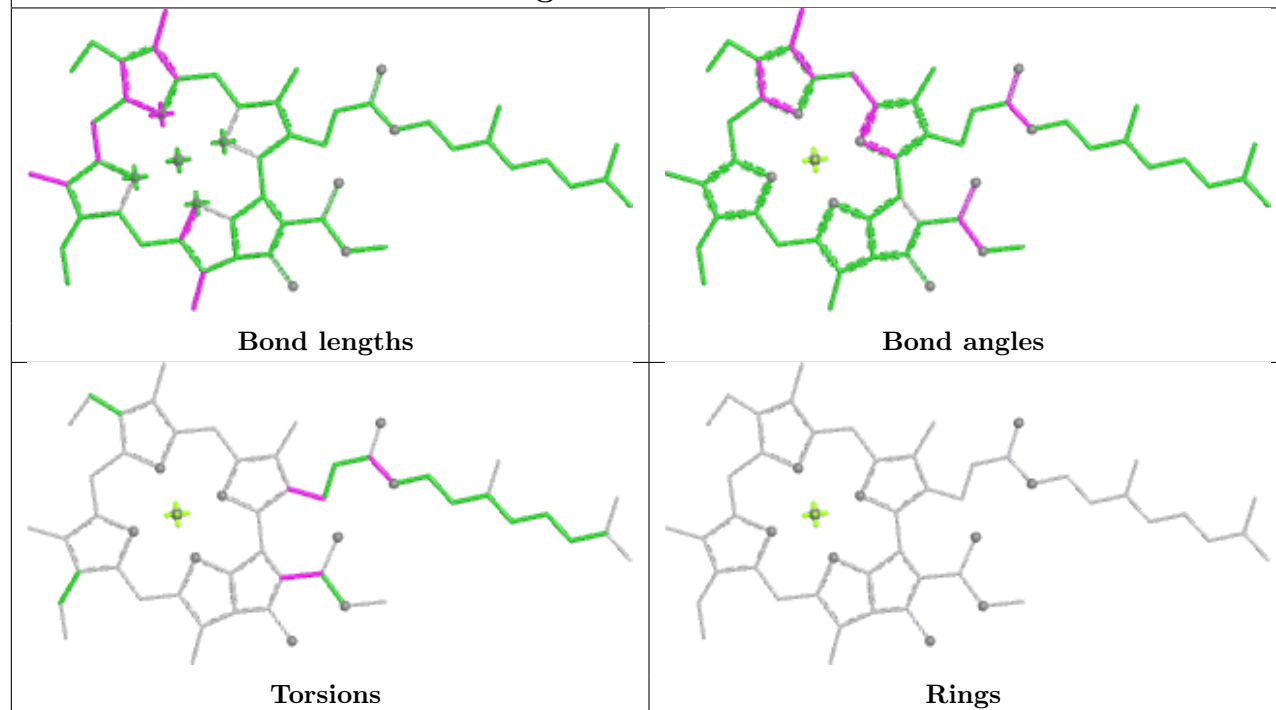
Ligand CLA a 811



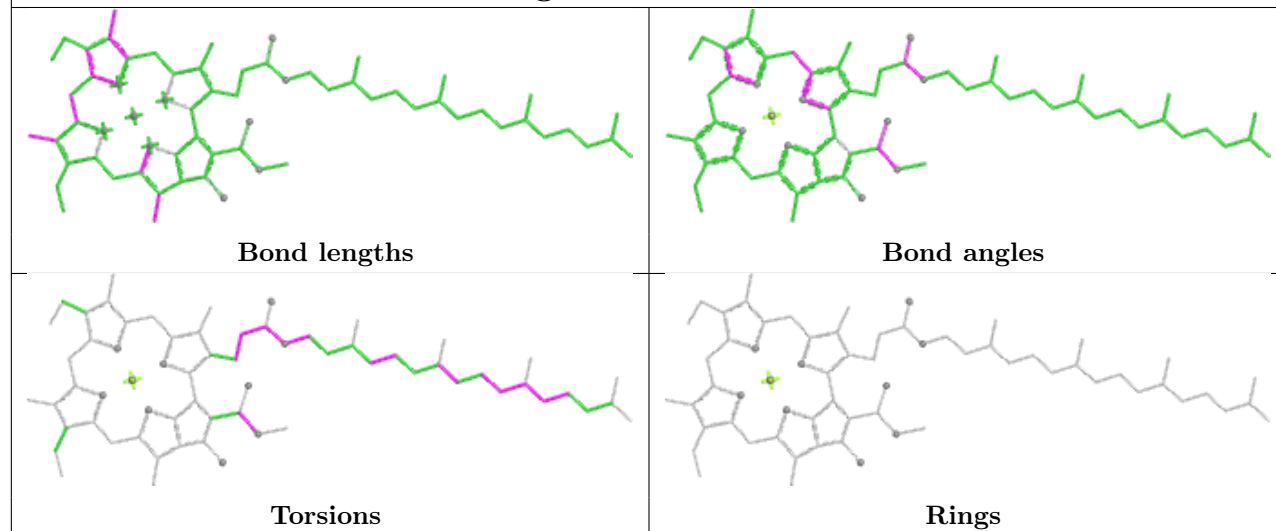
Ligand CLA H 309



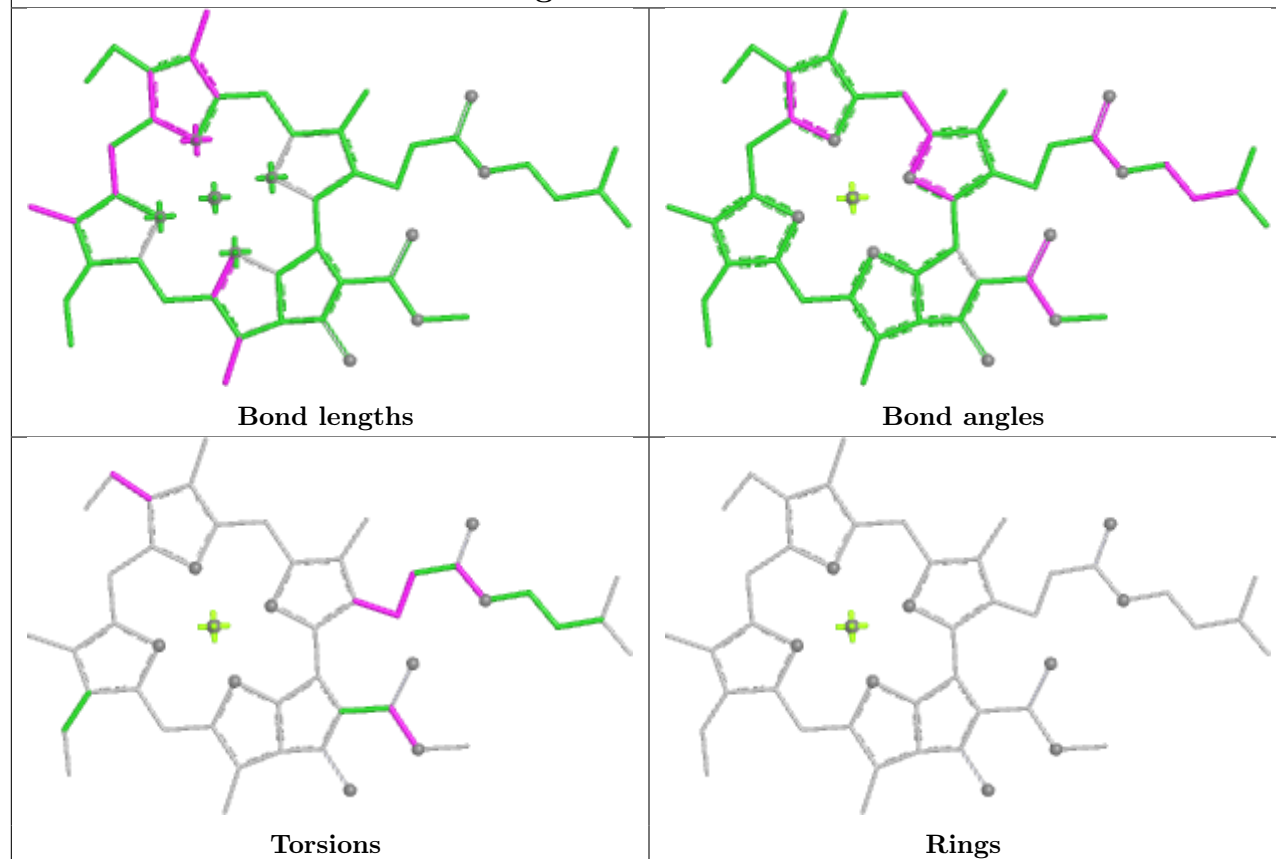
Ligand CLA a 804



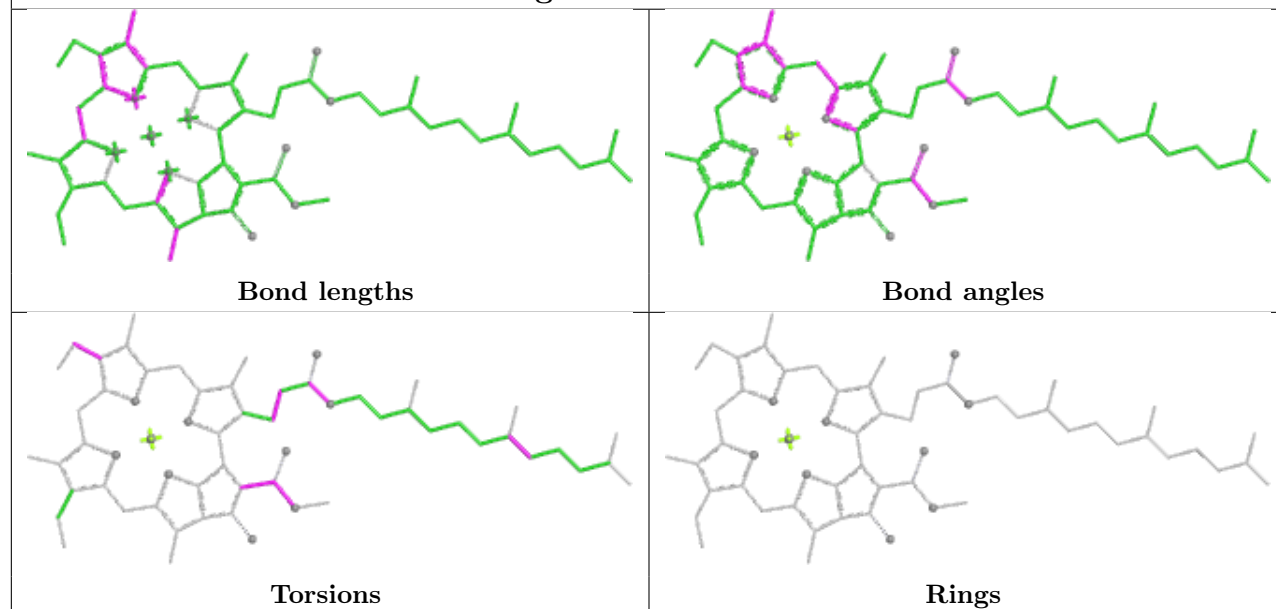
Ligand CLA b 806

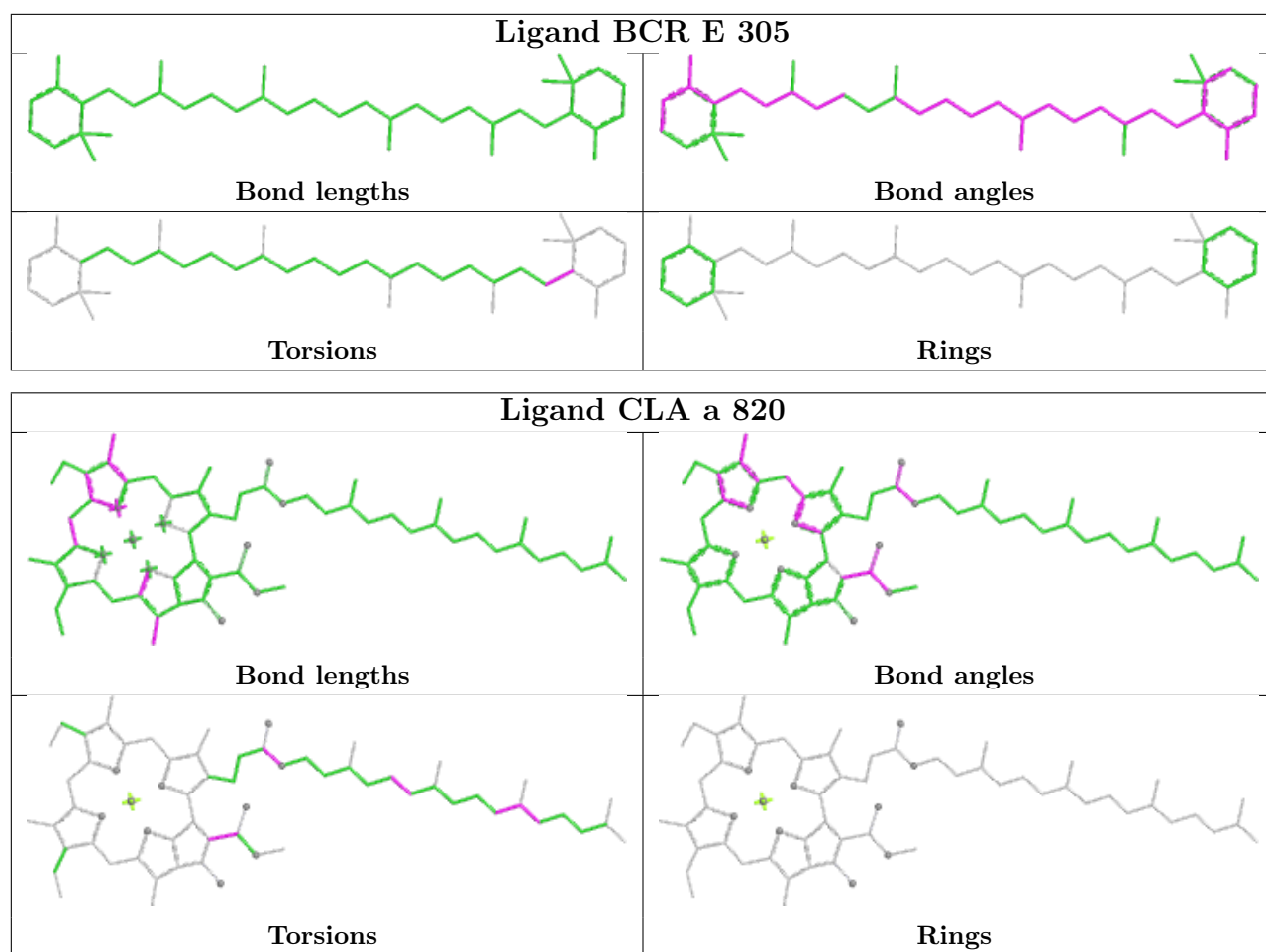


Ligand CLA b 821

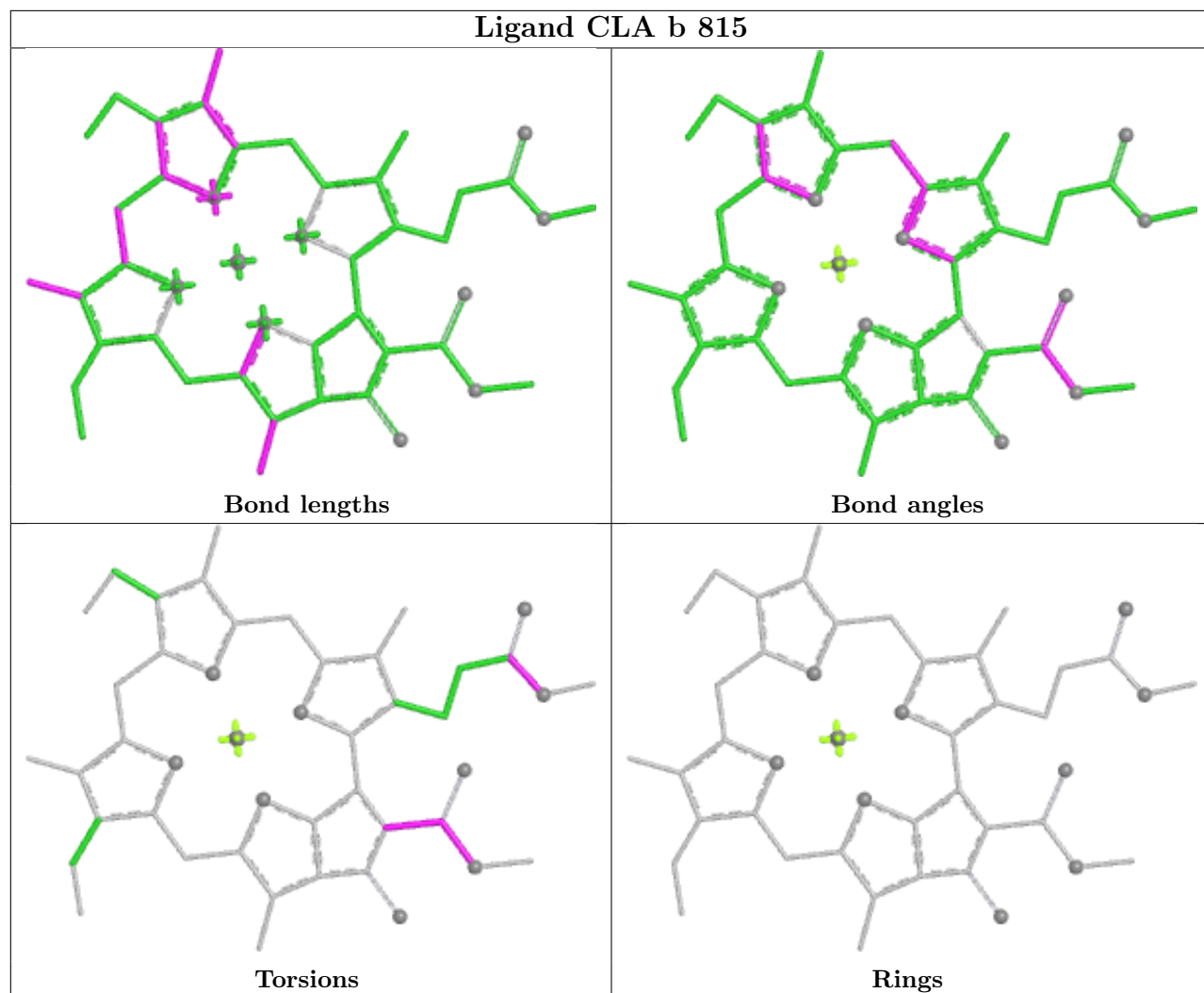


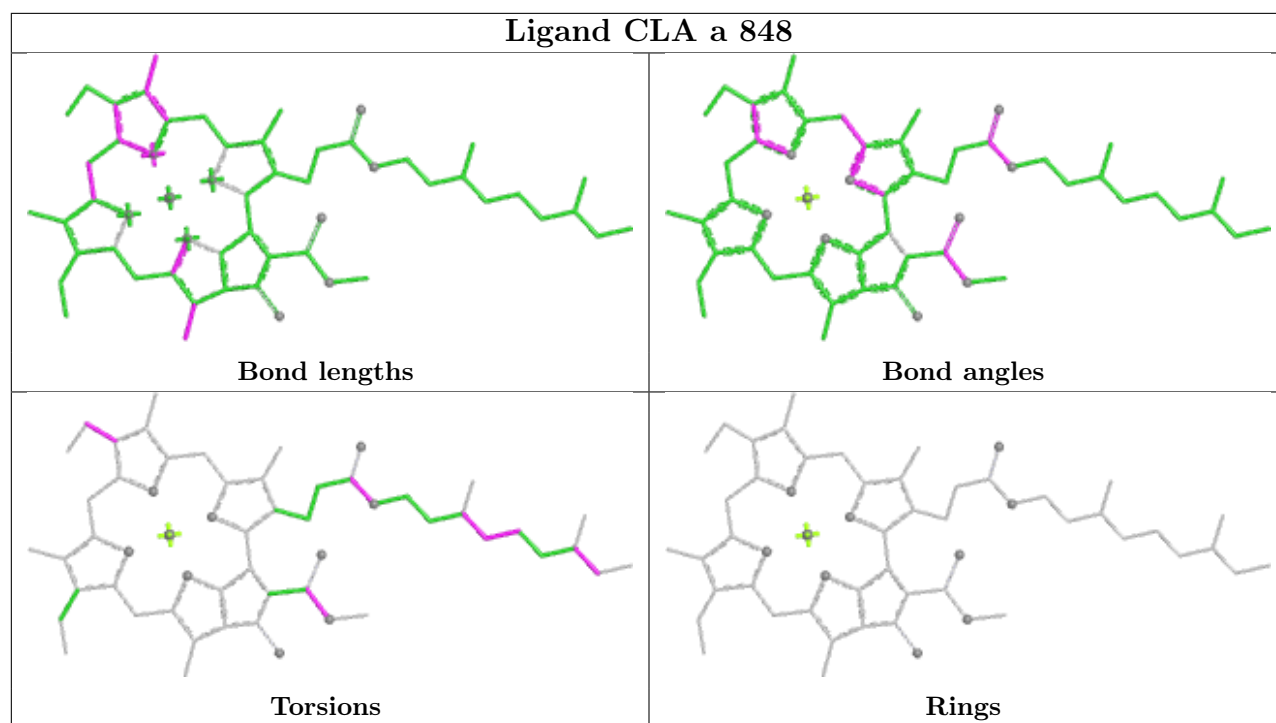
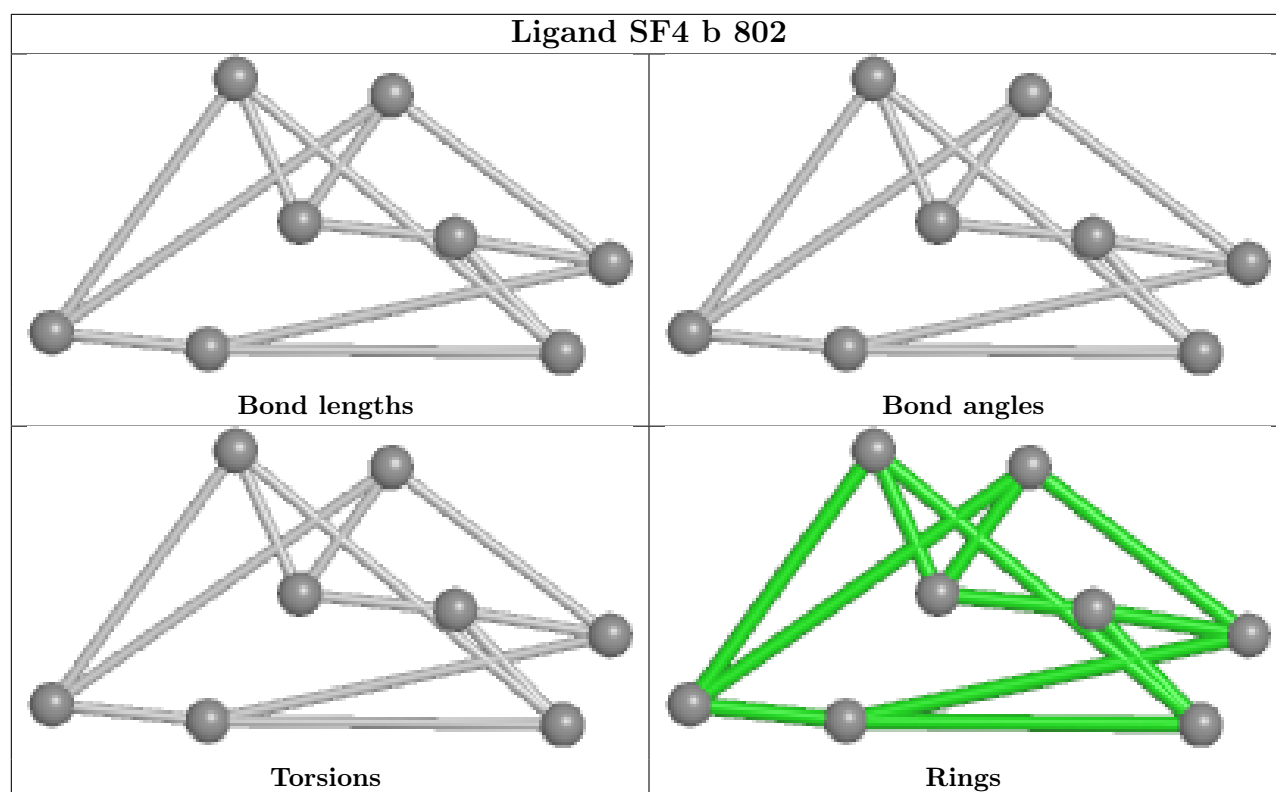
Ligand CLA b 826



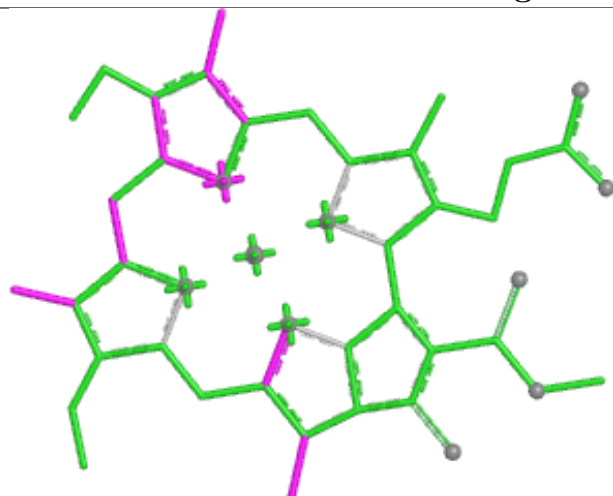


Ligand CLA b 815

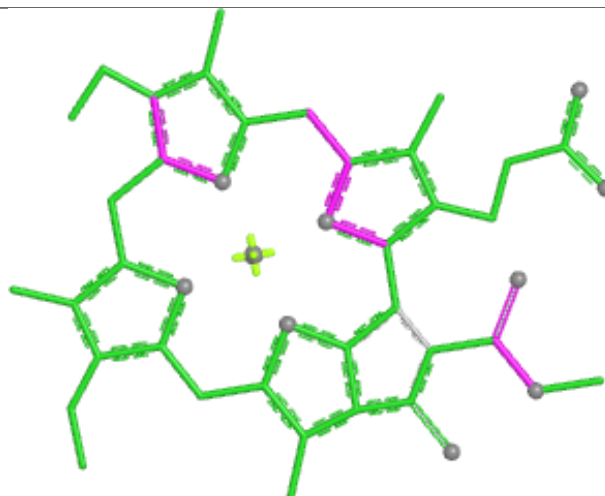




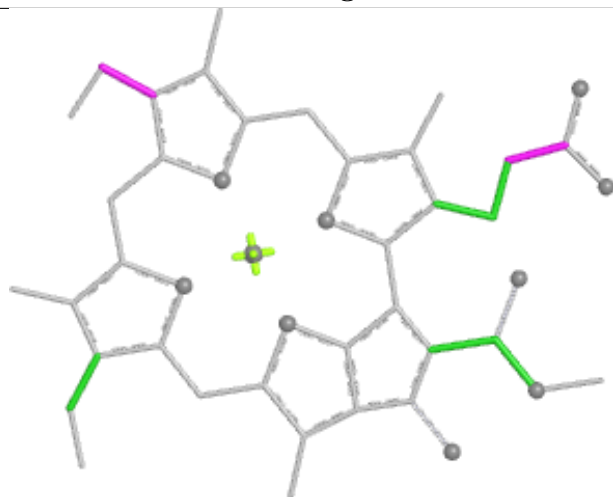
Ligand CLA C 306



Bond lengths



Bond angles

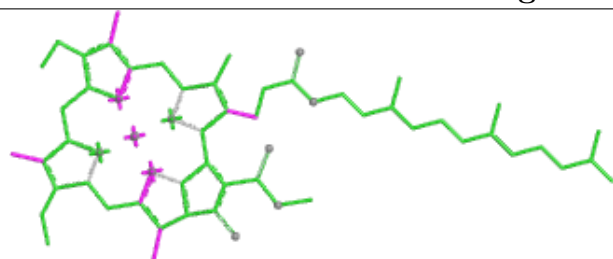


Torsions

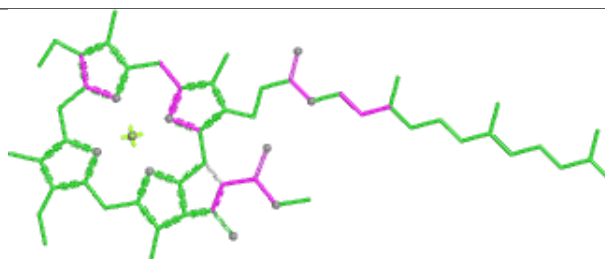


Rings

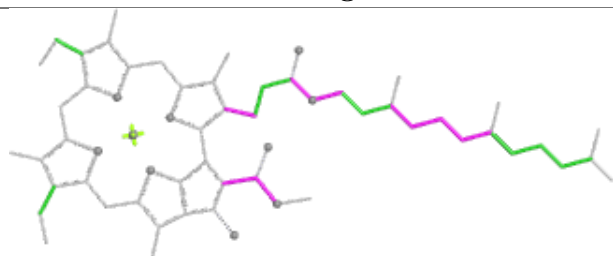
Ligand CLA a 837



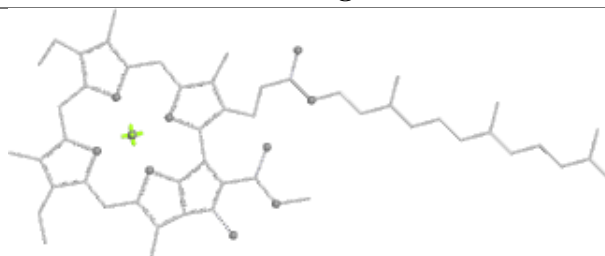
Bond lengths



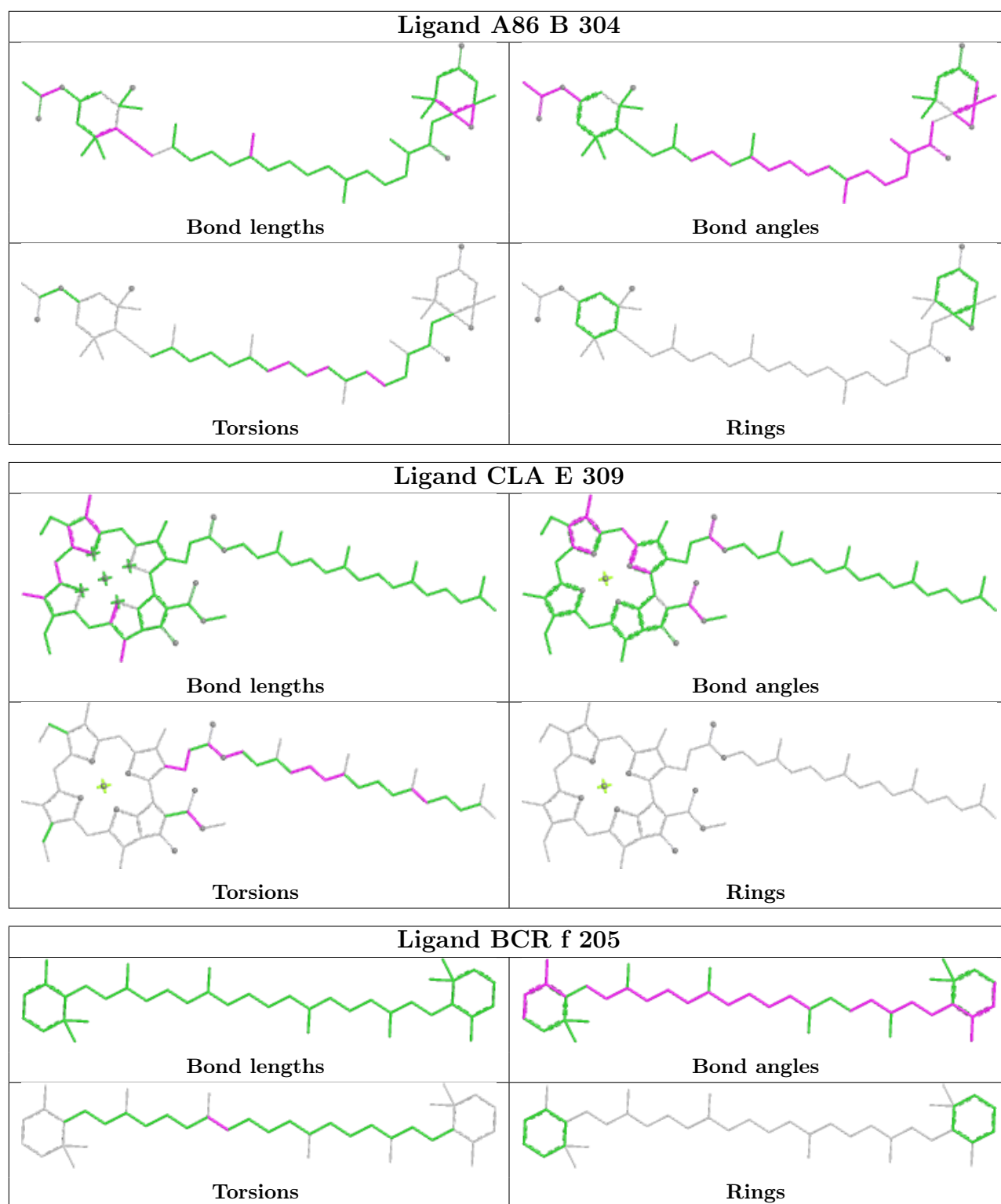
Bond angles

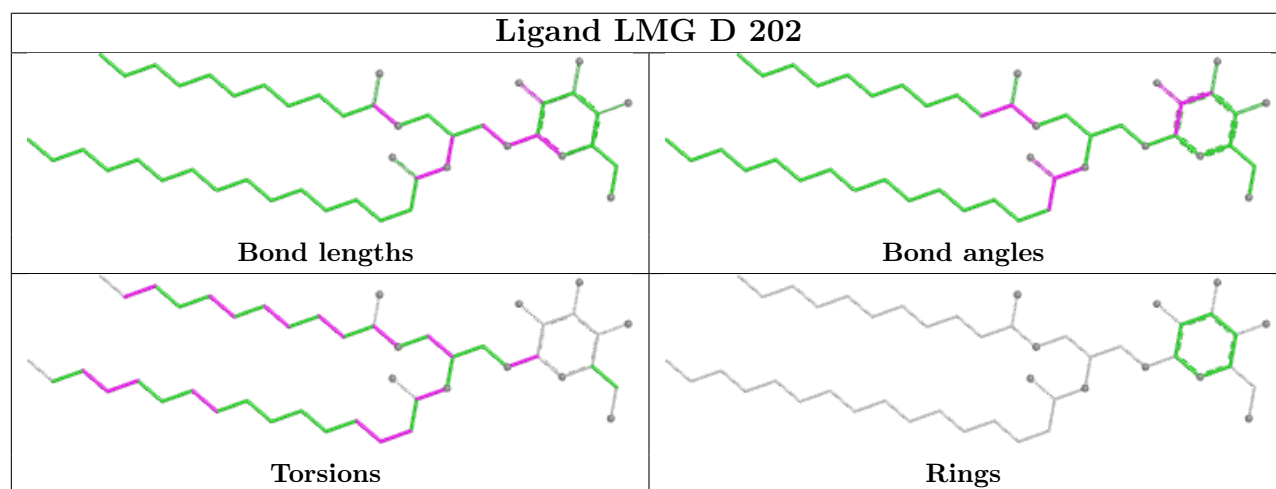
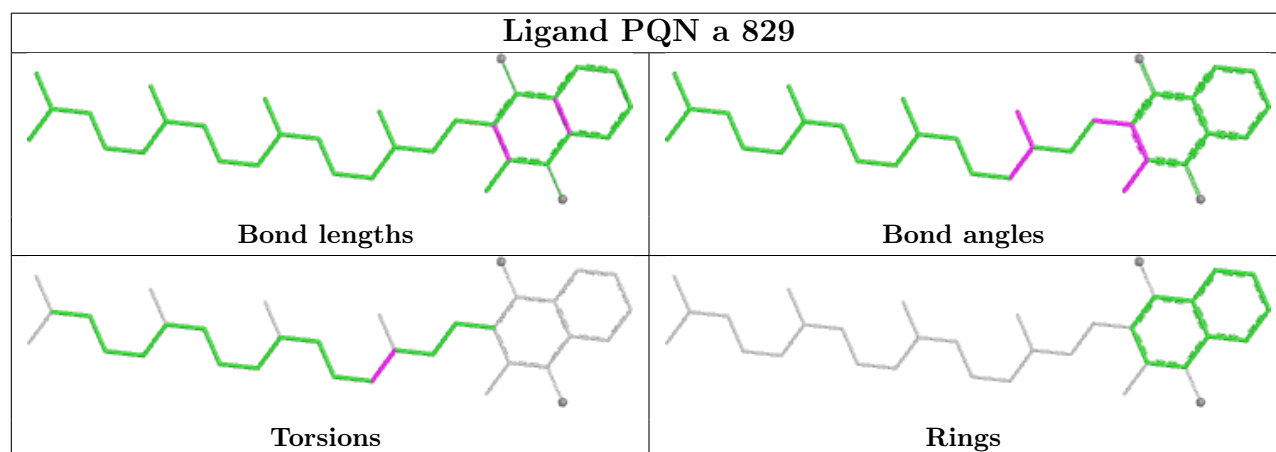
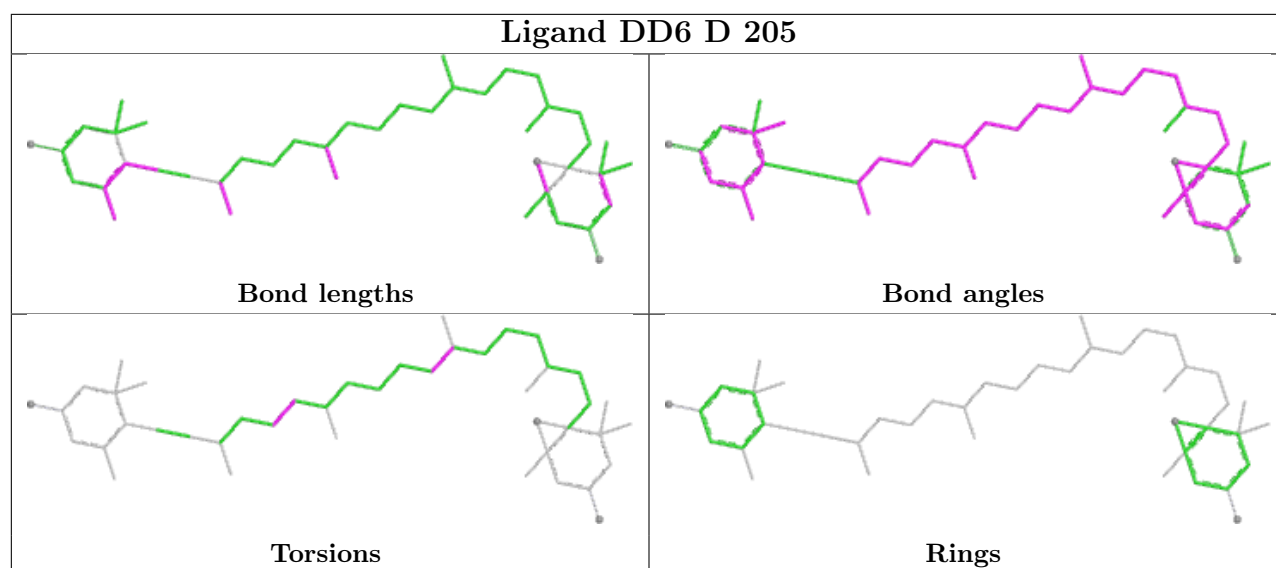


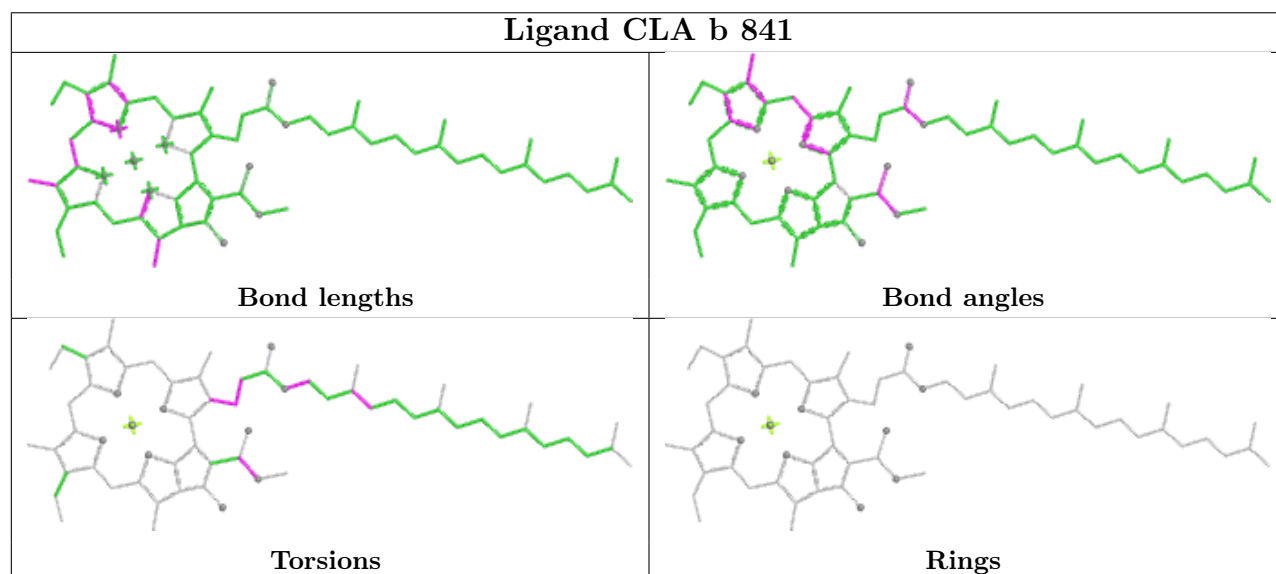
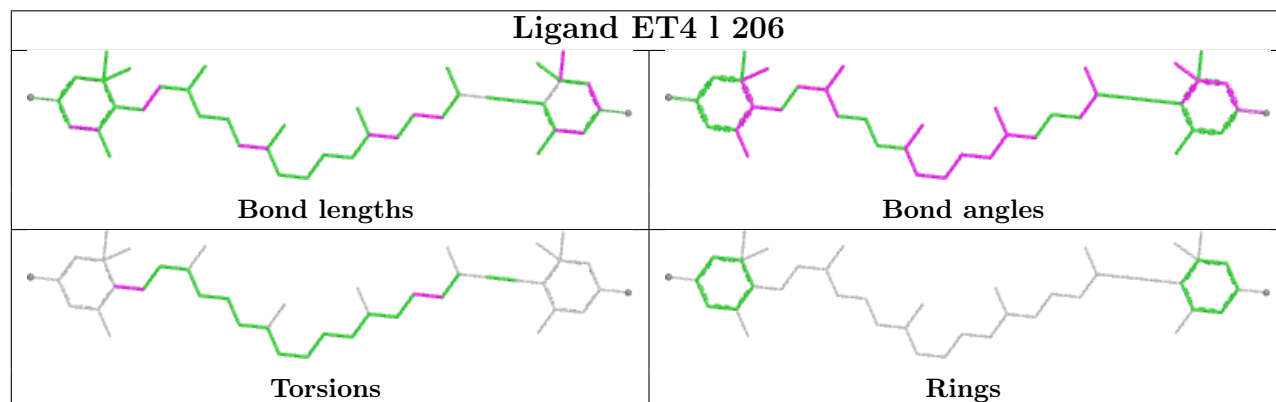
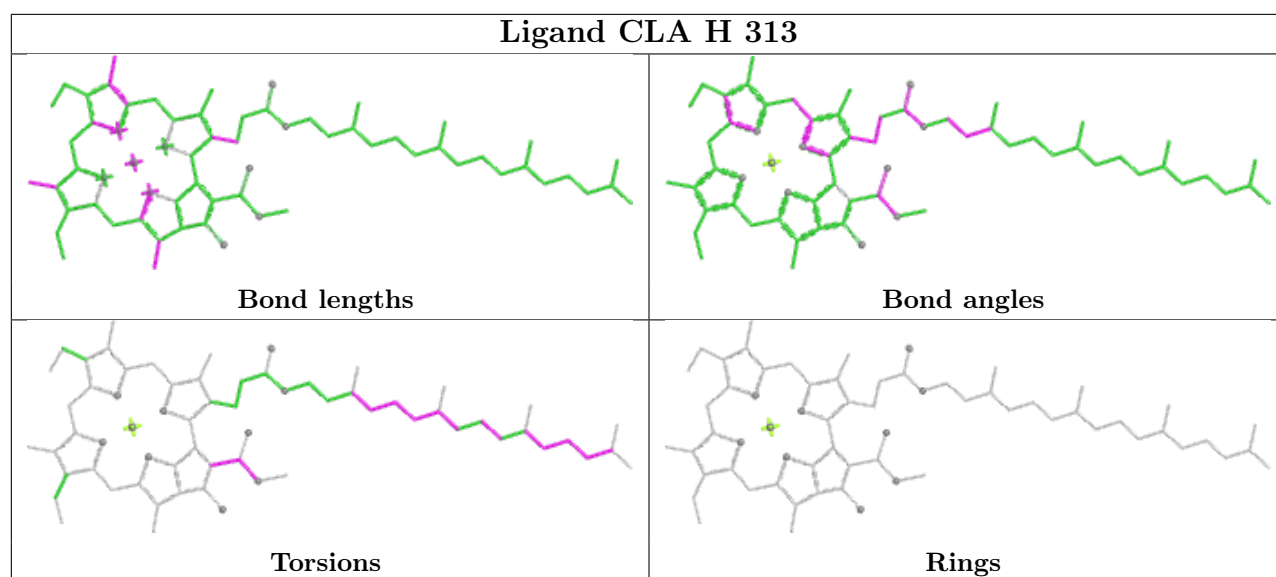
Torsions

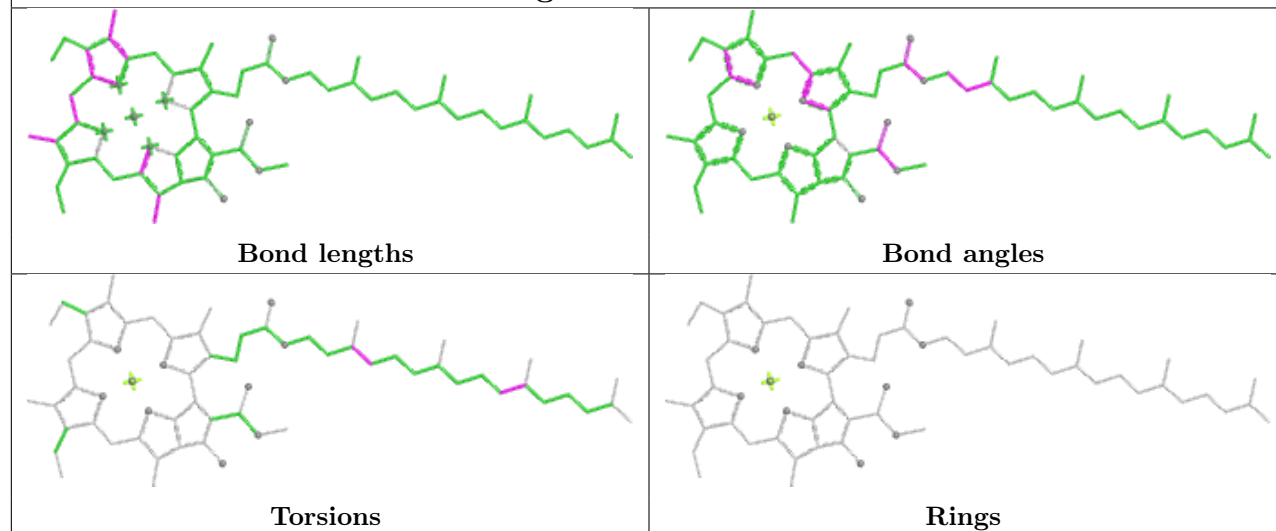
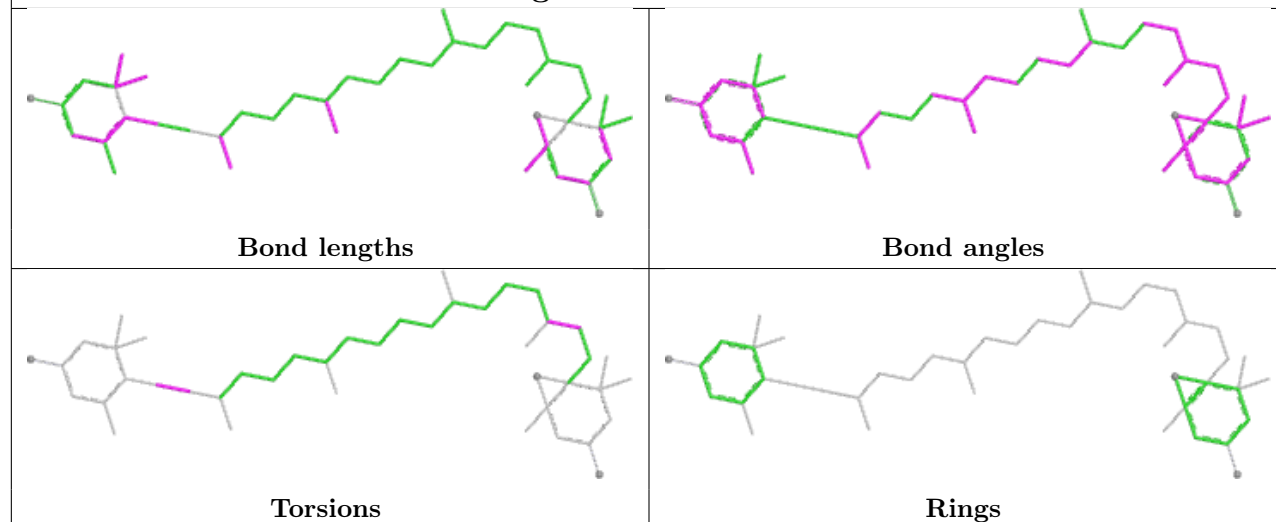


Rings

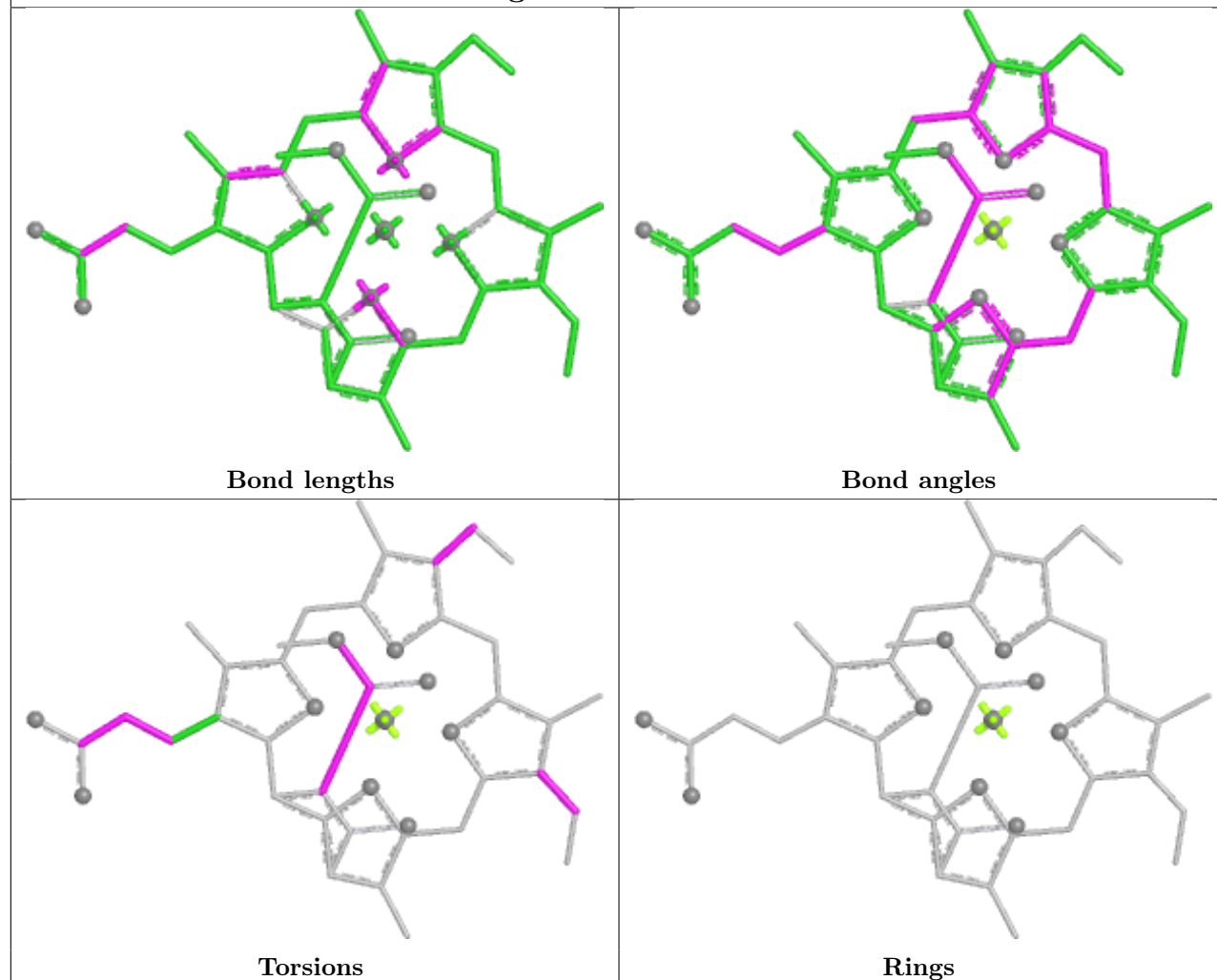




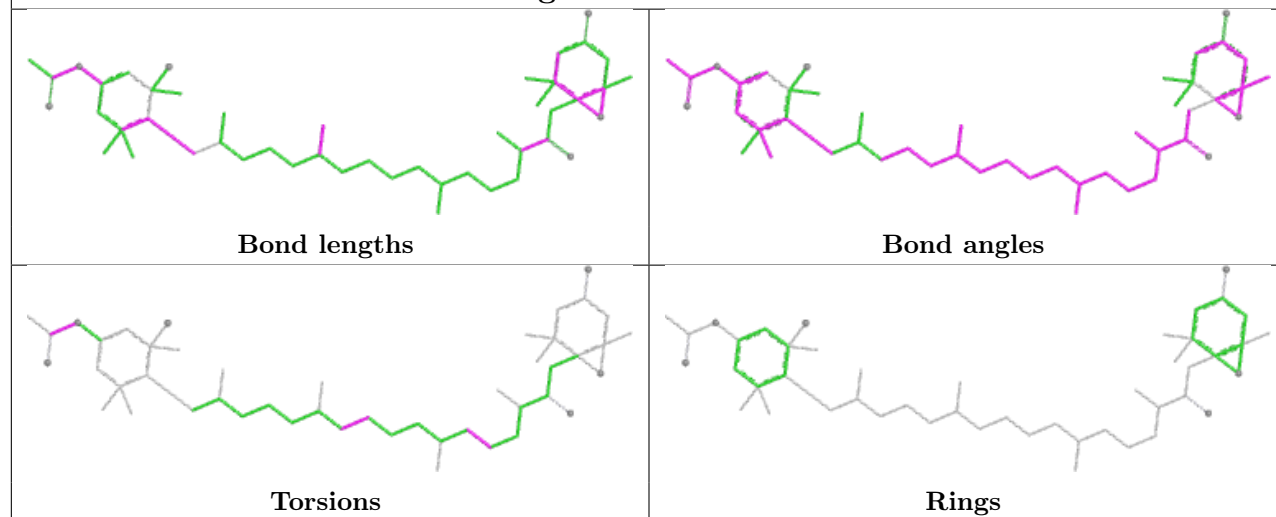


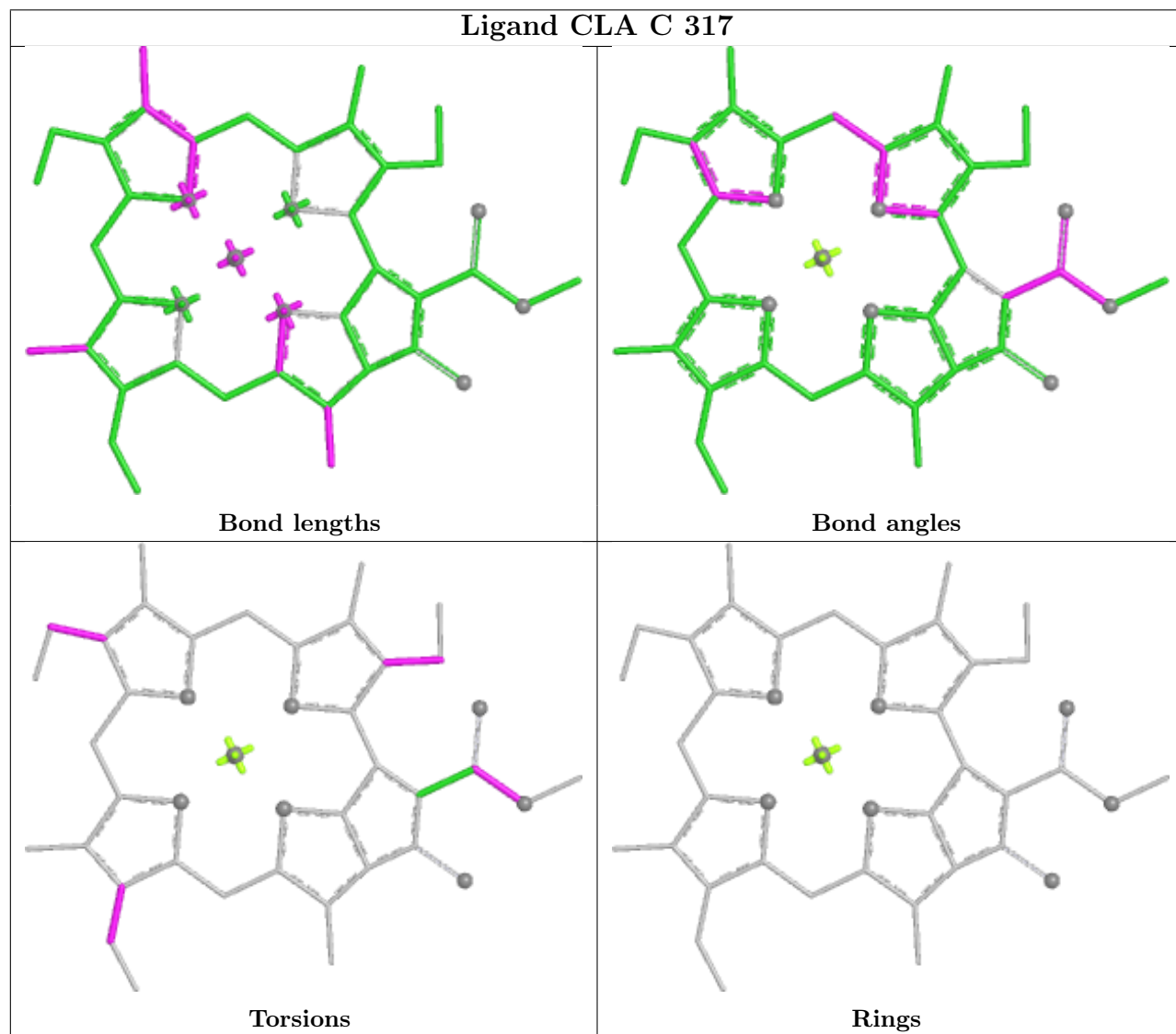
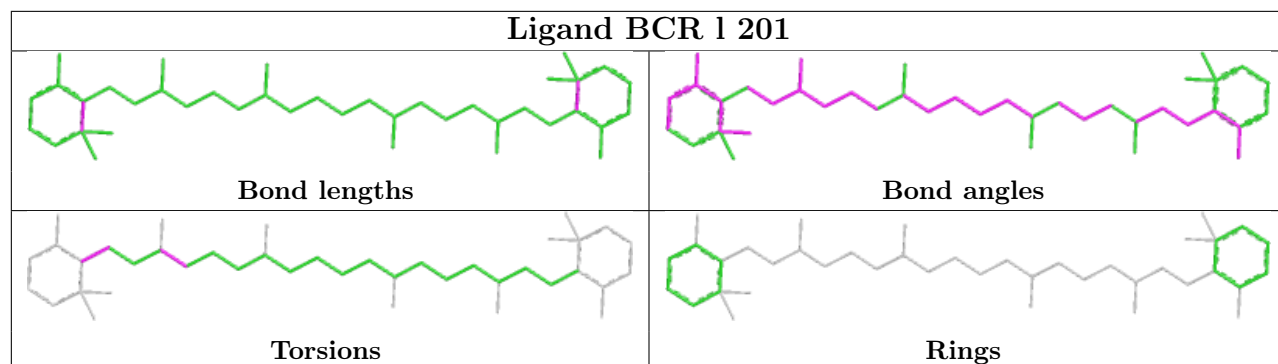
Ligand CLA a 819**Ligand DD6 H 303**

Ligand KC1 H 312

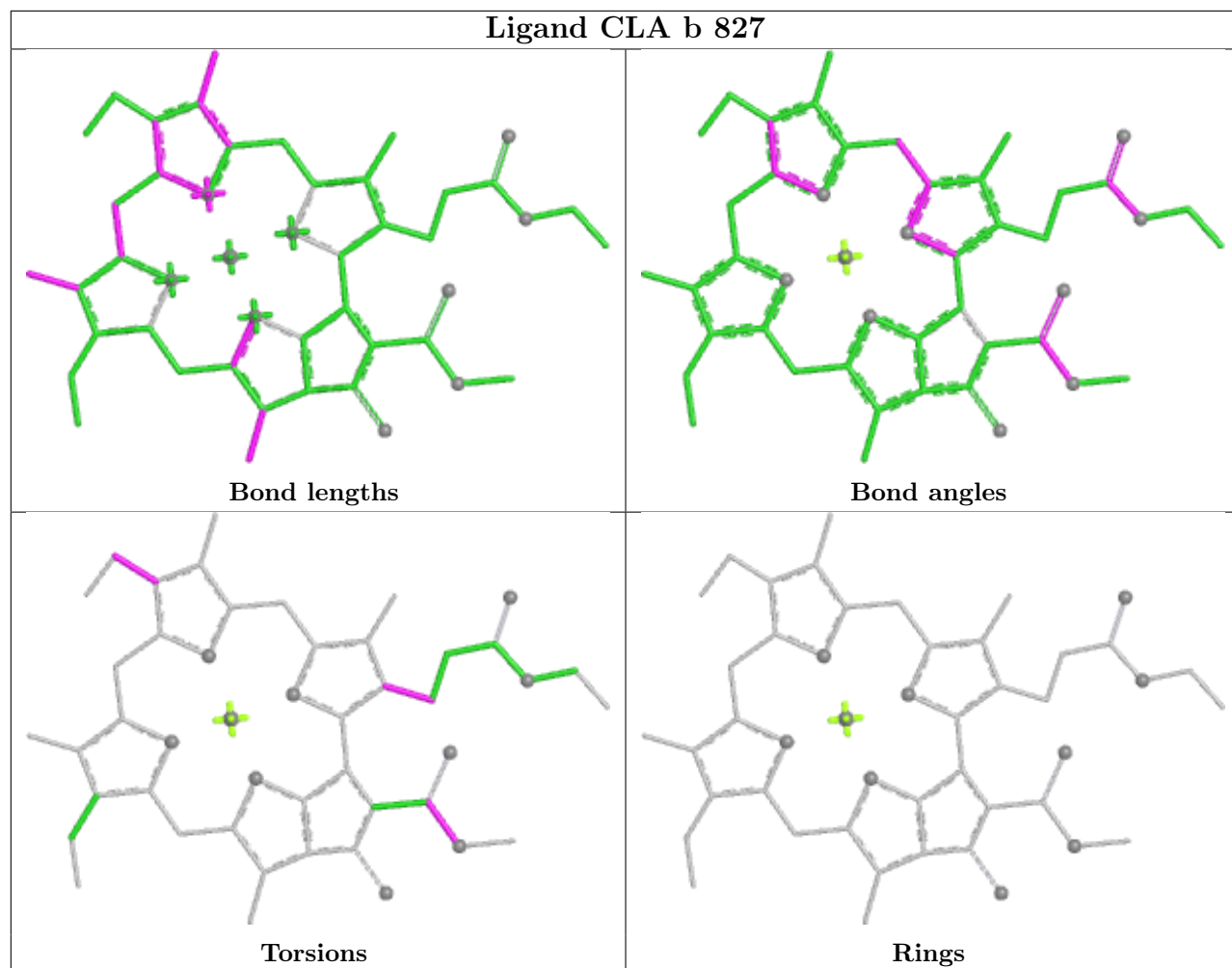


Ligand A86 B 305

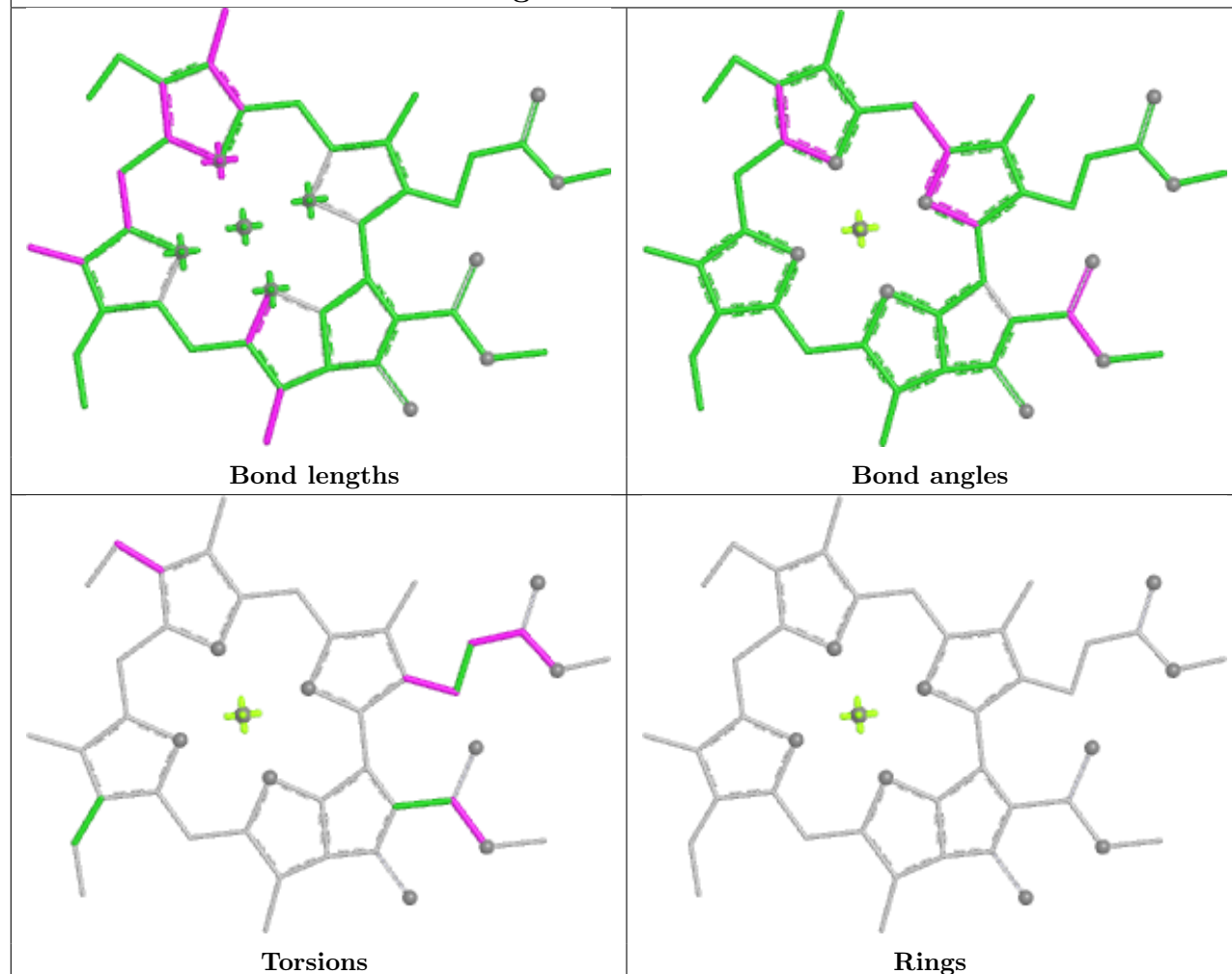




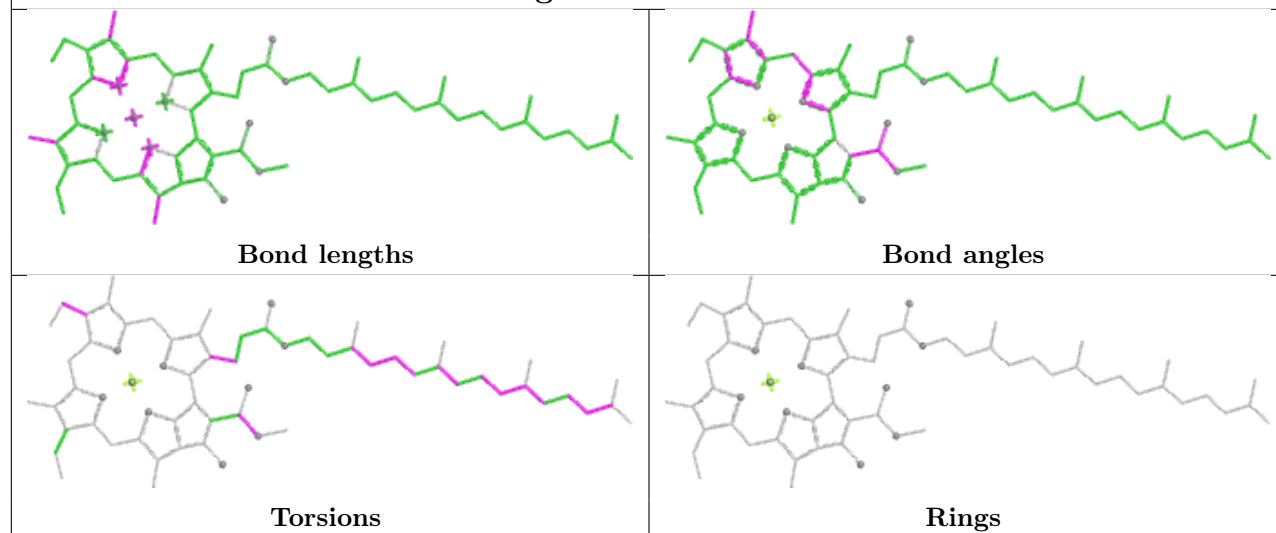
Ligand CLA b 827



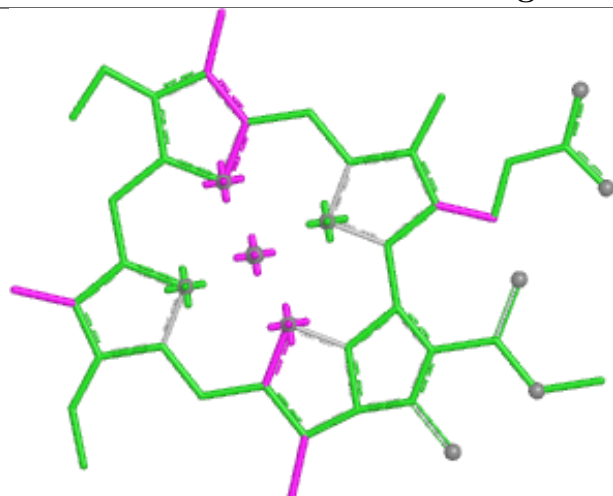
Ligand CLA D 211



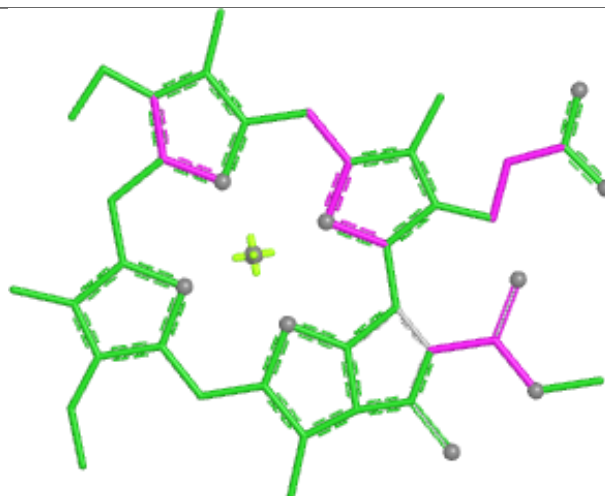
Ligand CLA b 843



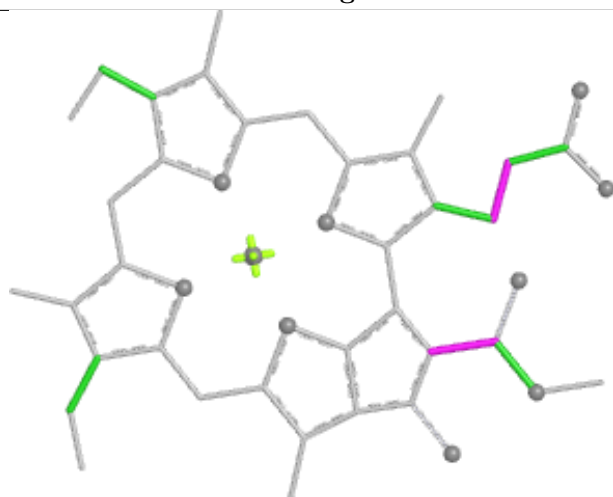
Ligand CLA b 804



Bond lengths



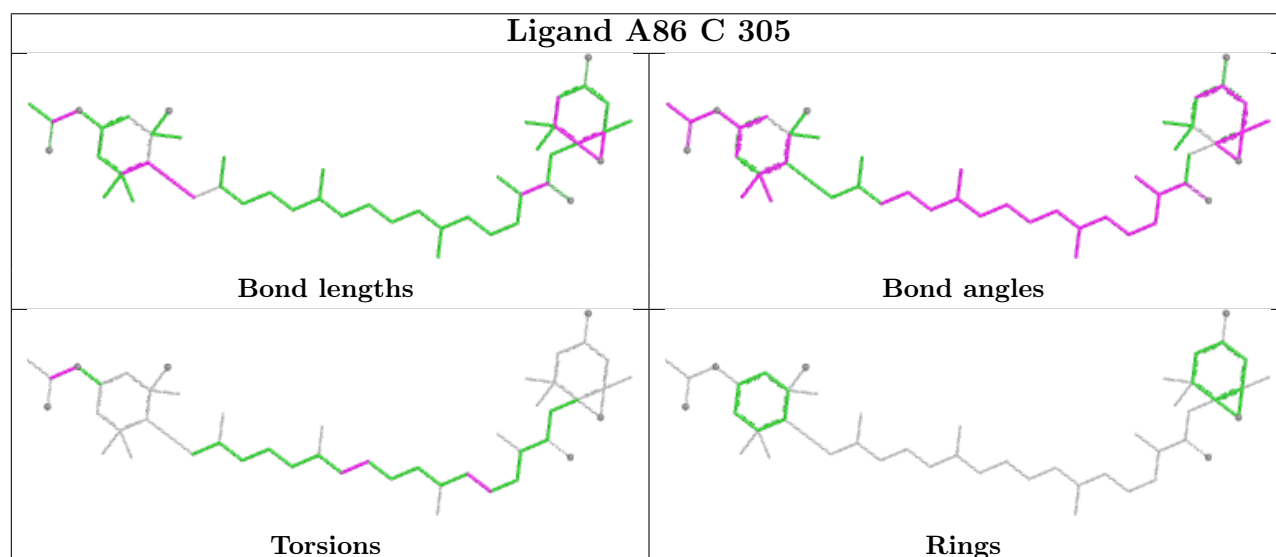
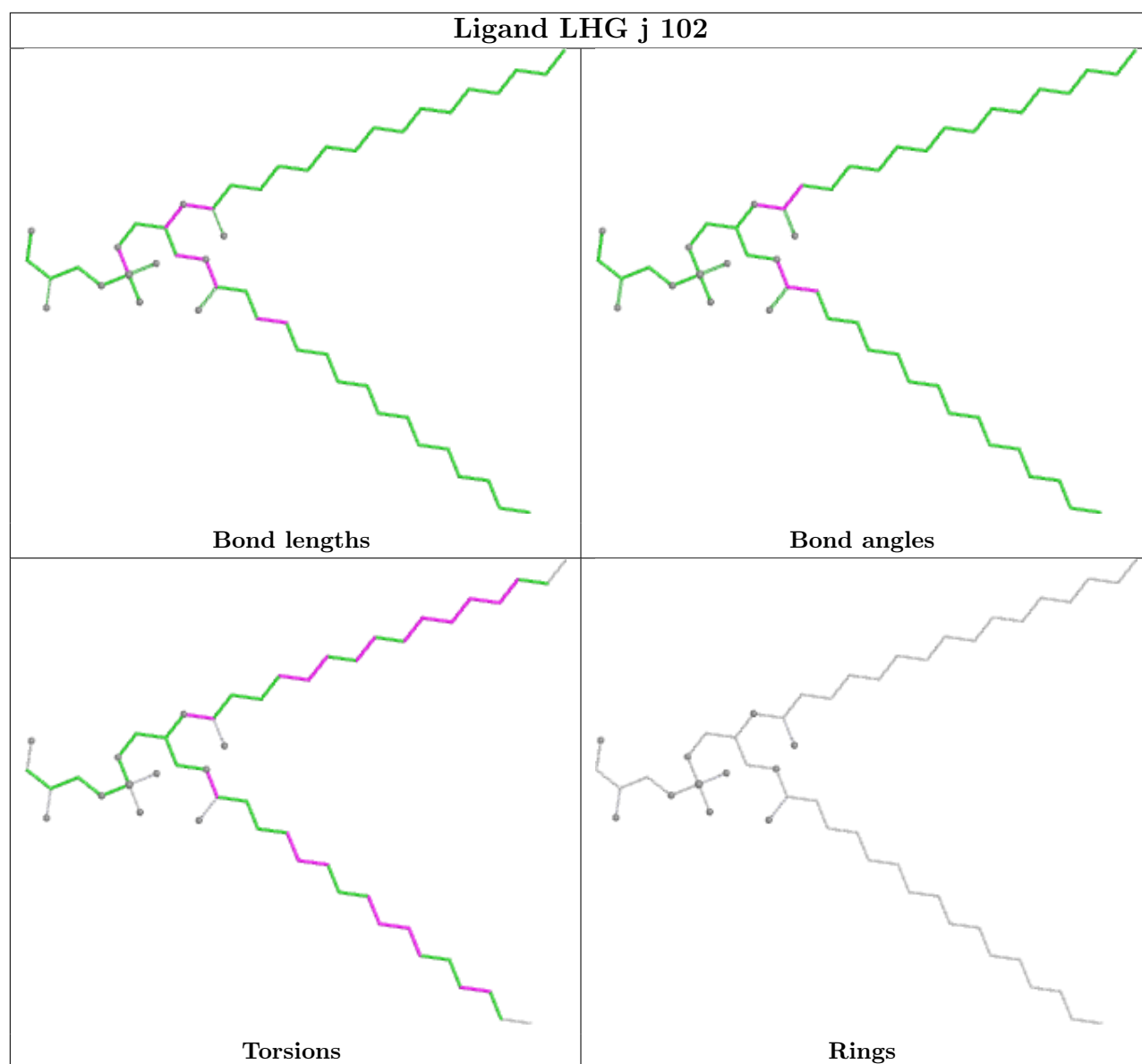
Bond angles



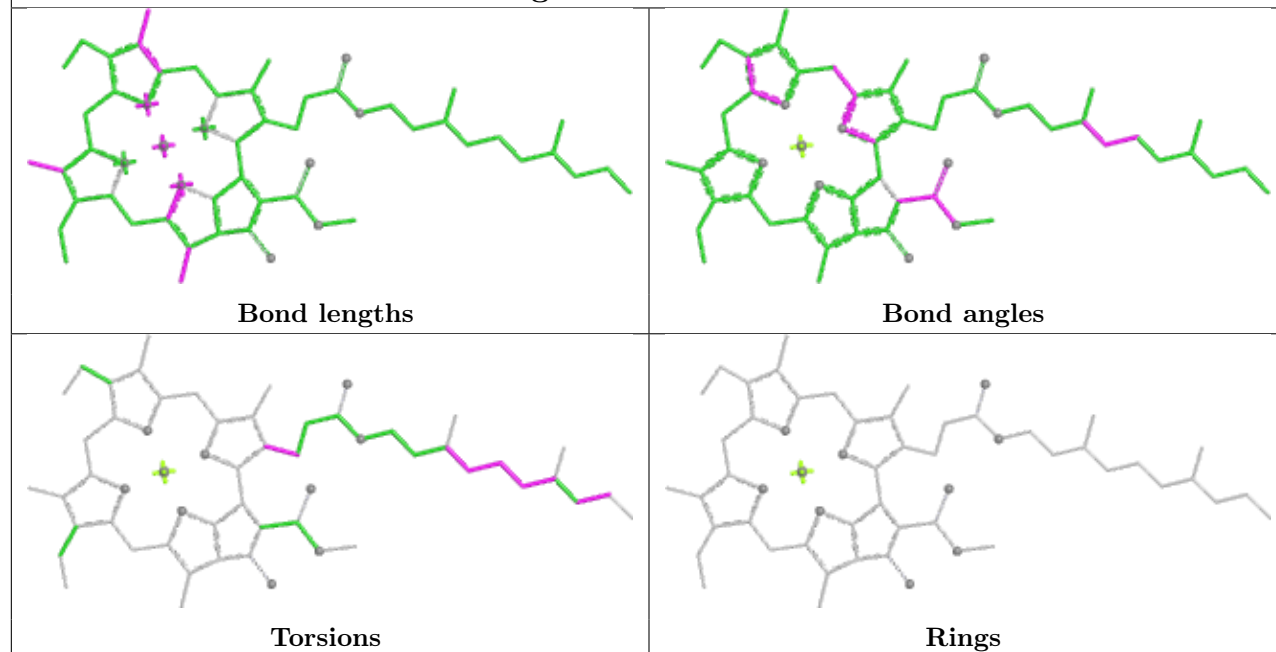
Torsions



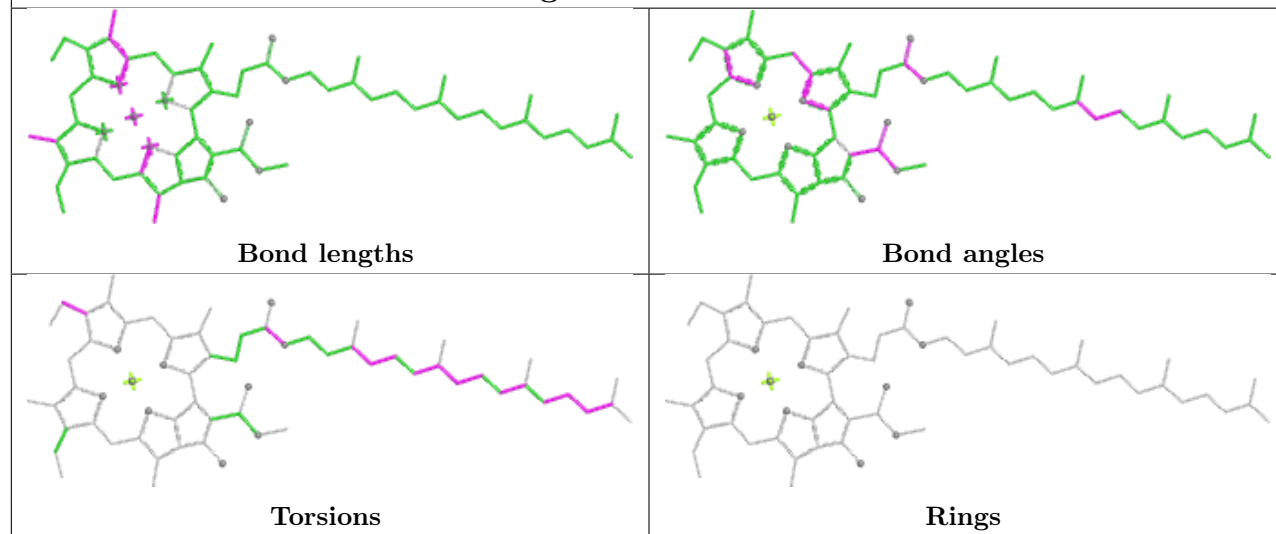
Rings

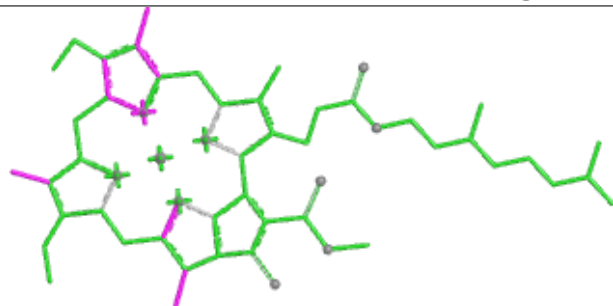


Ligand CLA H 311

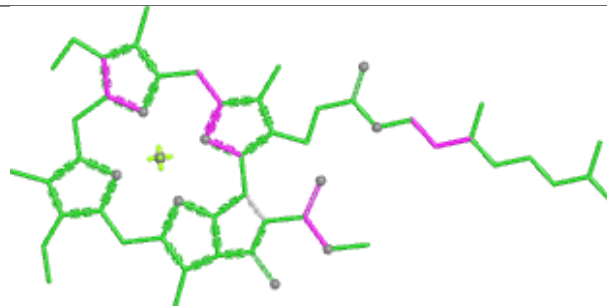


Ligand CLA I 203

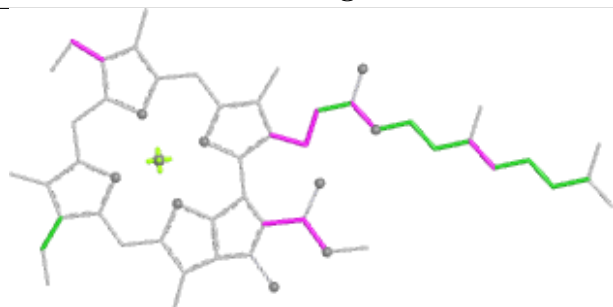


Ligand CLA b 813

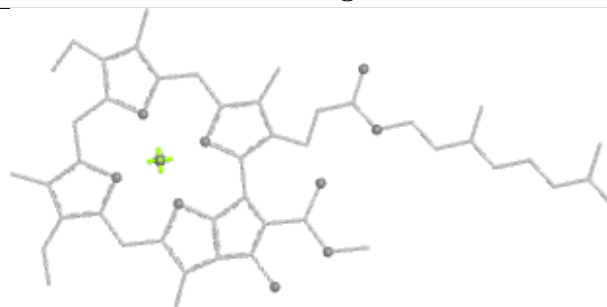
Bond lengths



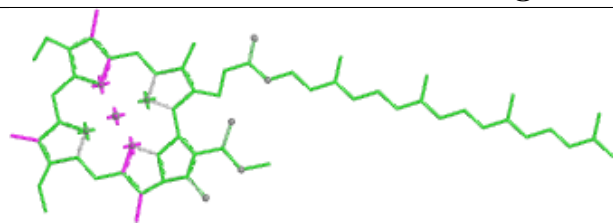
Bond angles



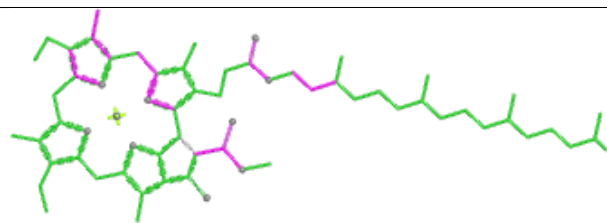
Torsions



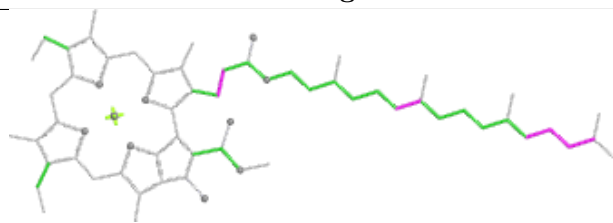
Rings

Ligand CLA C 307

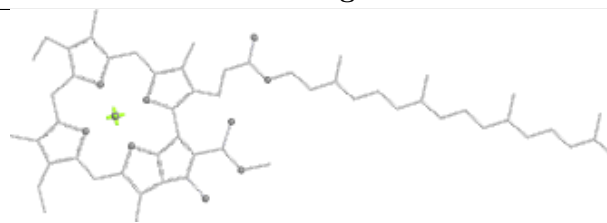
Bond lengths



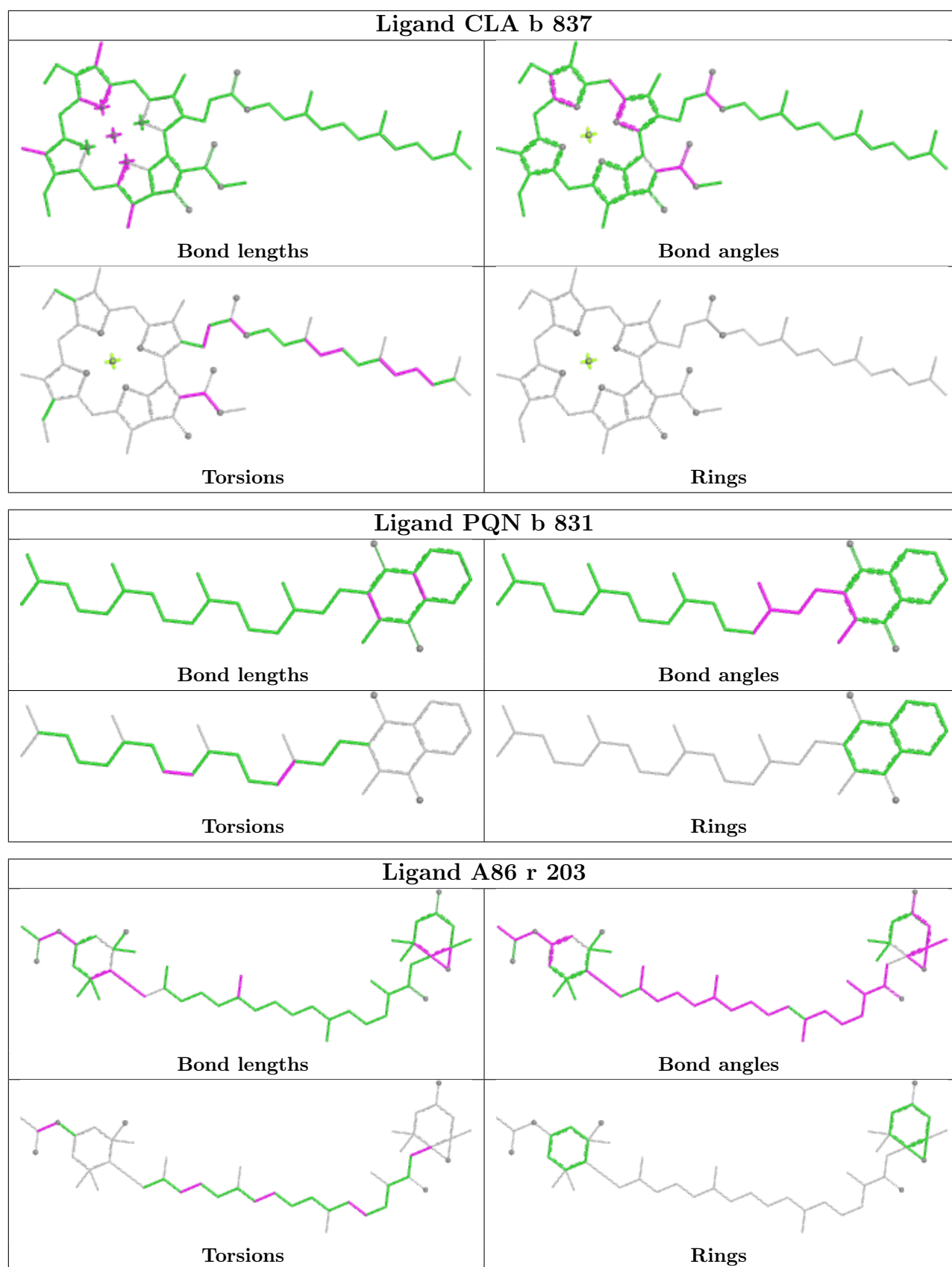
Bond angles



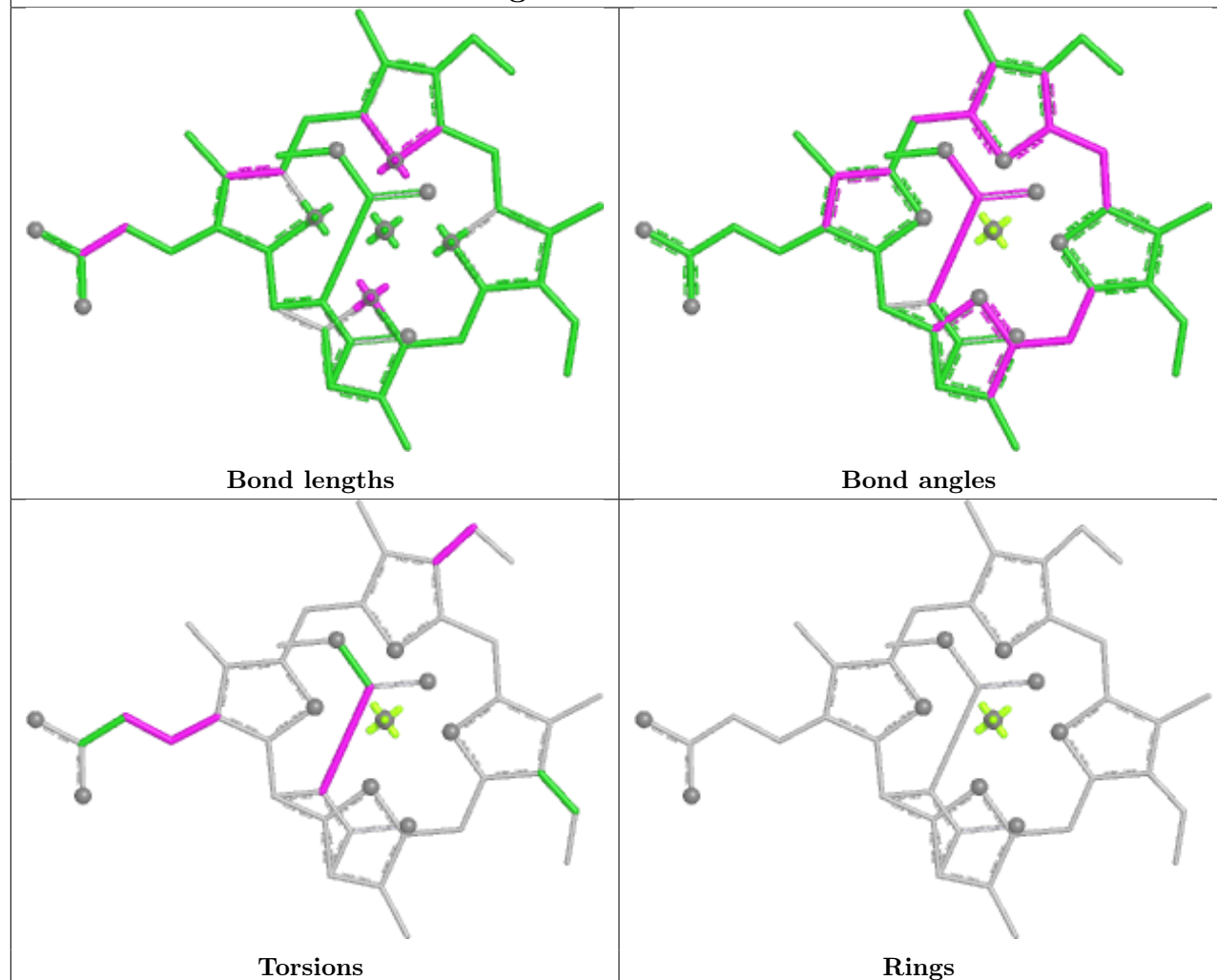
Torsions



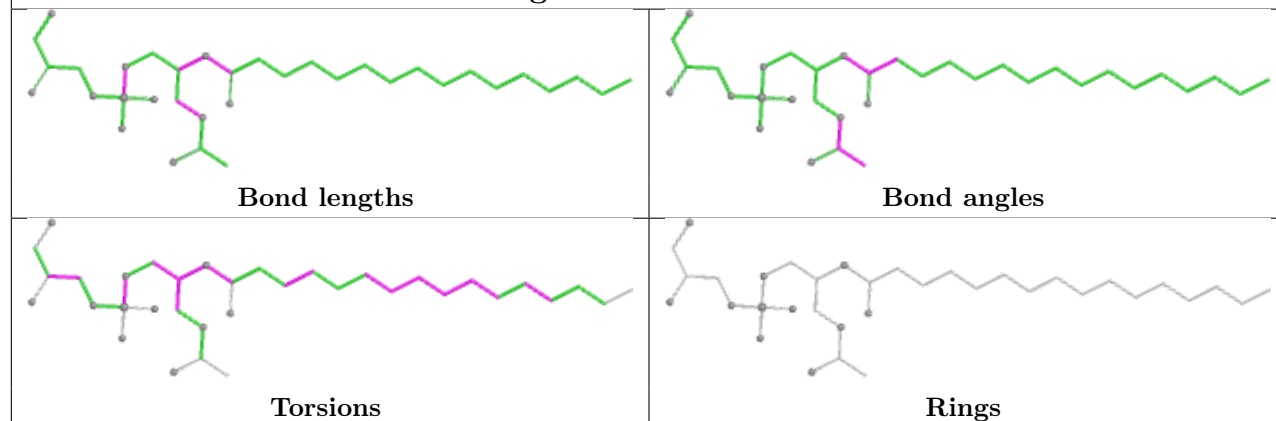
Rings

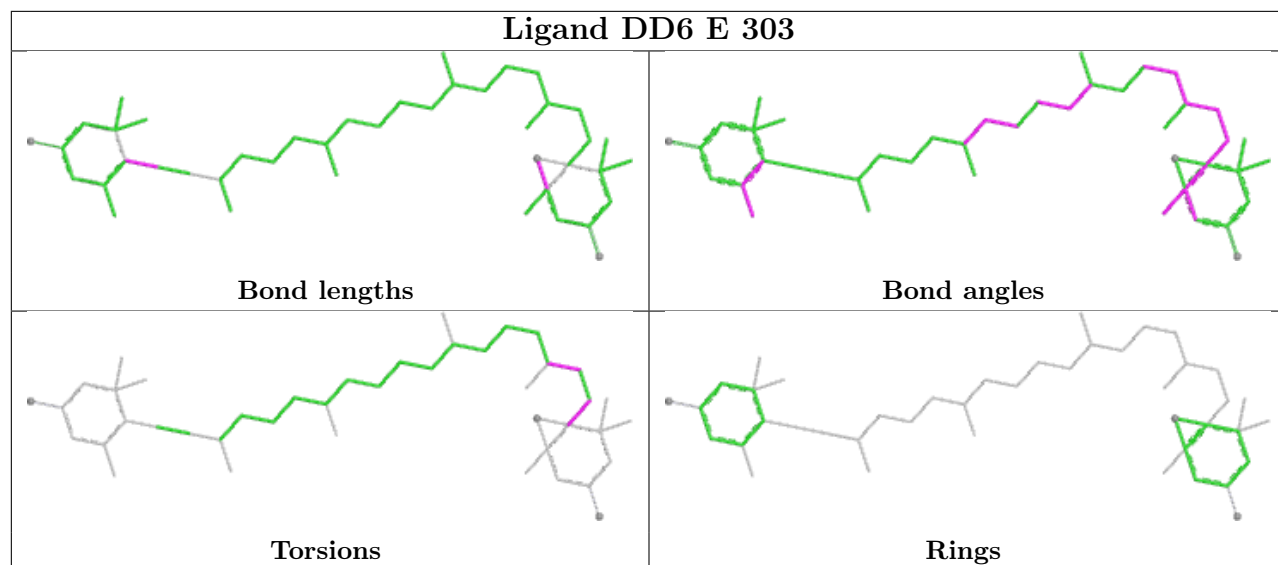
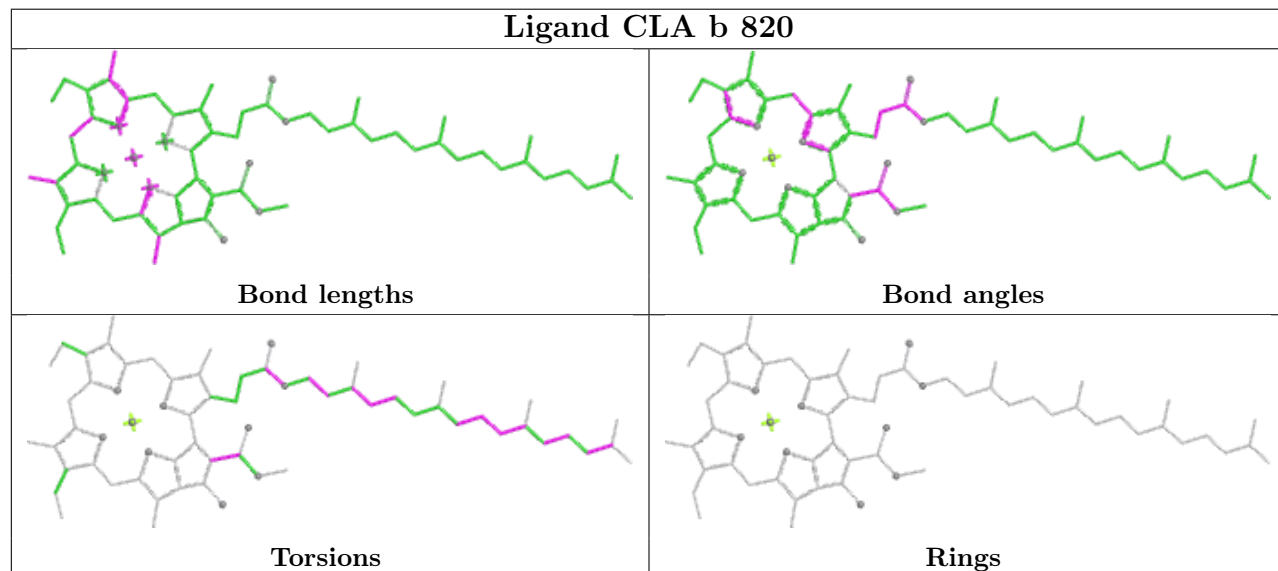


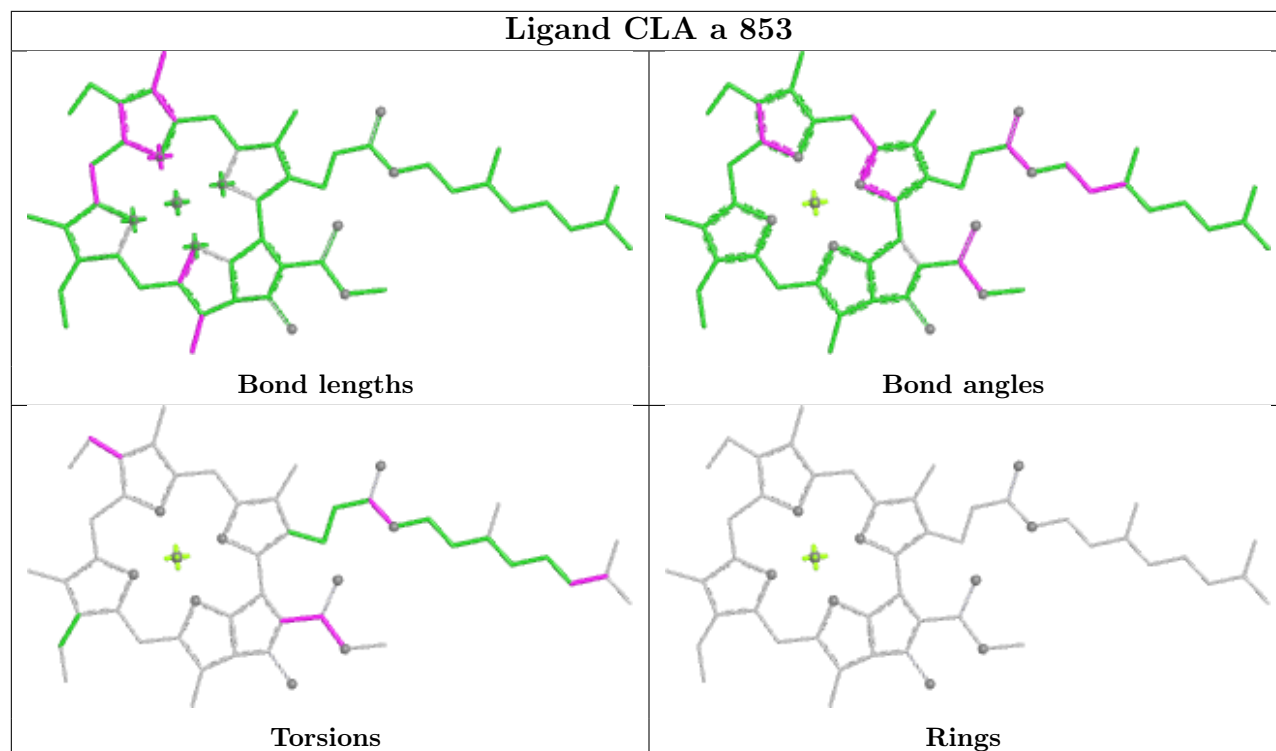
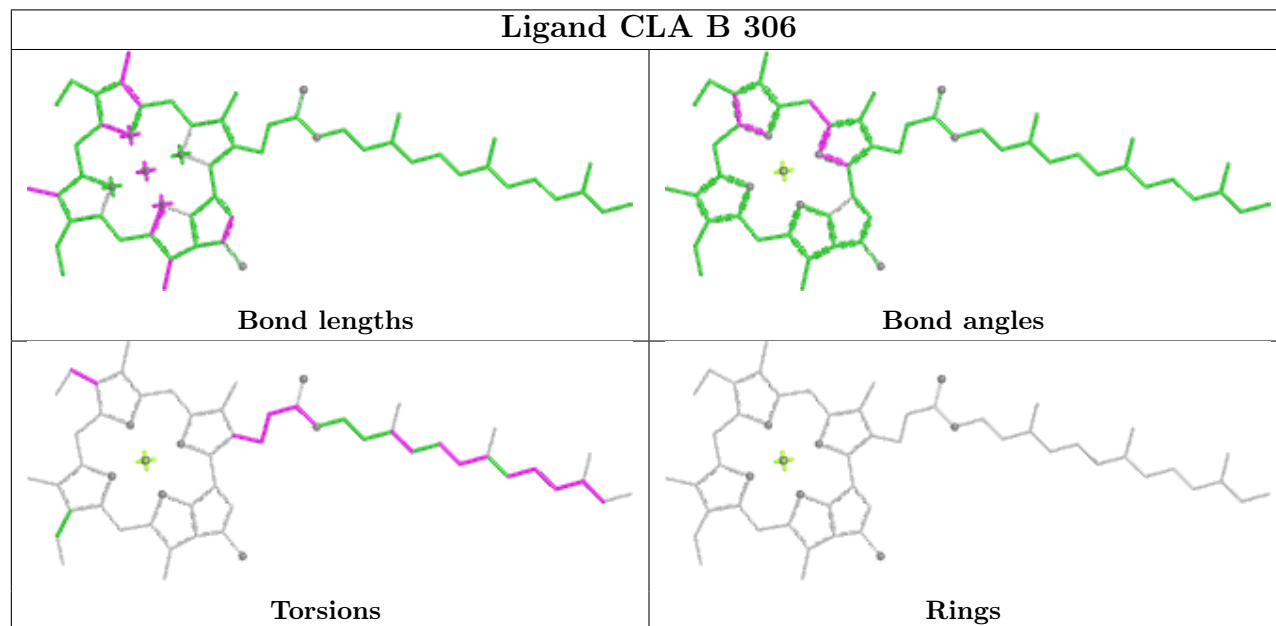
Ligand KC1 C 308



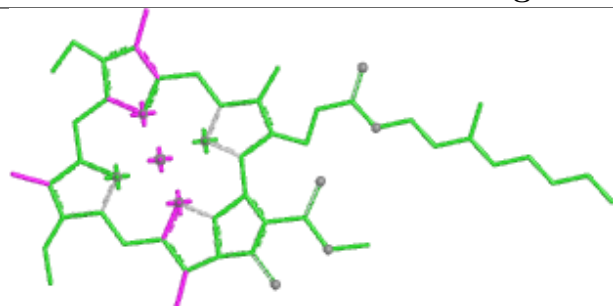
Ligand LHG H 316



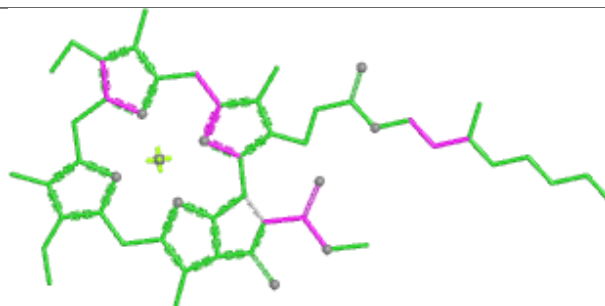
Ligand DD6 E 303**Ligand CLA b 820**

Ligand CLA a 853**Ligand CLA B 306**

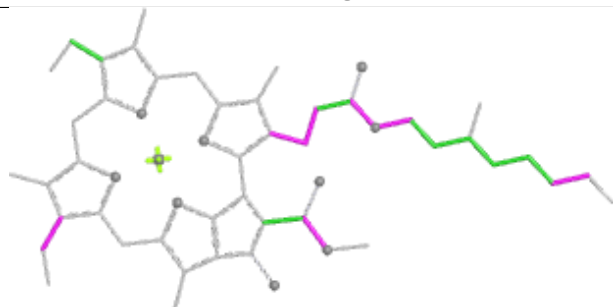
Ligand CLA H 305



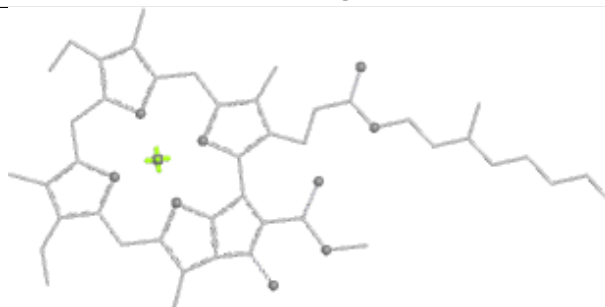
Bond lengths



Bond angles

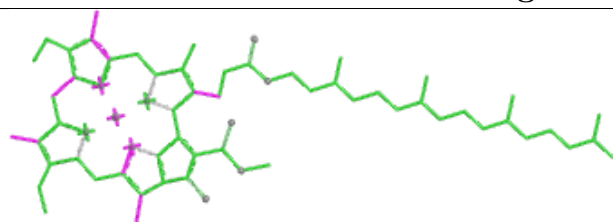


Torsions

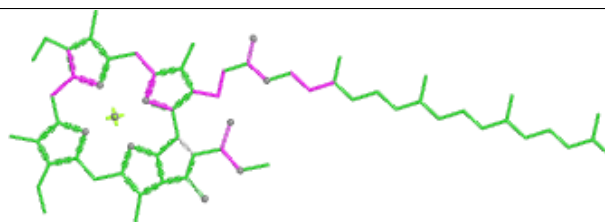


Rings

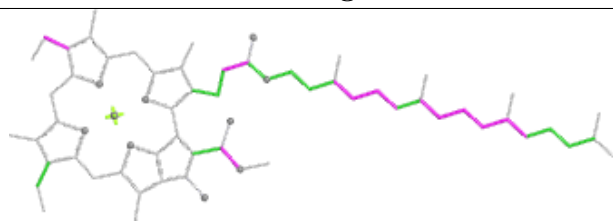
Ligand CLA b 803



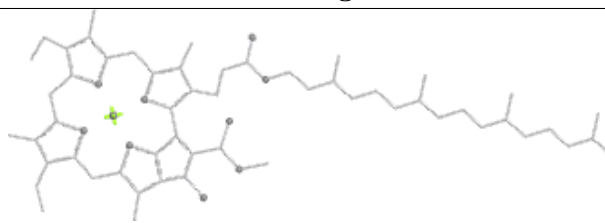
Bond lengths



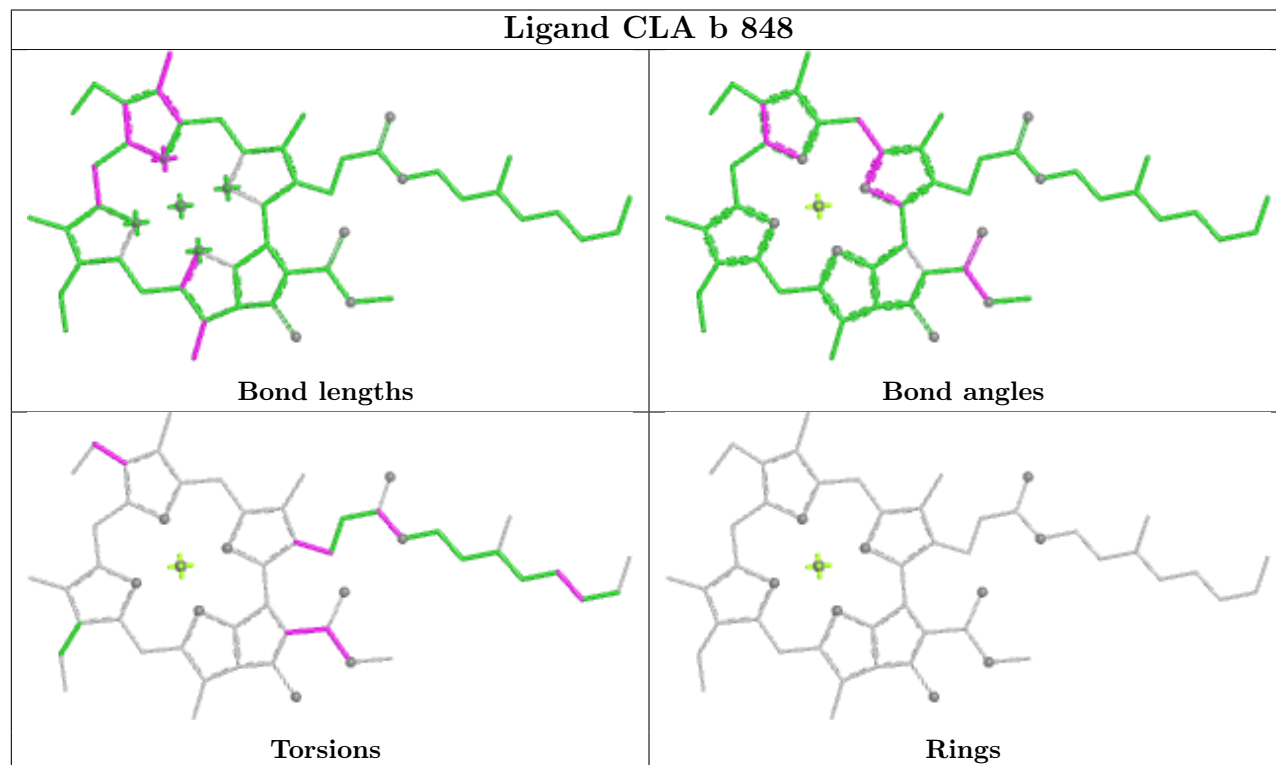
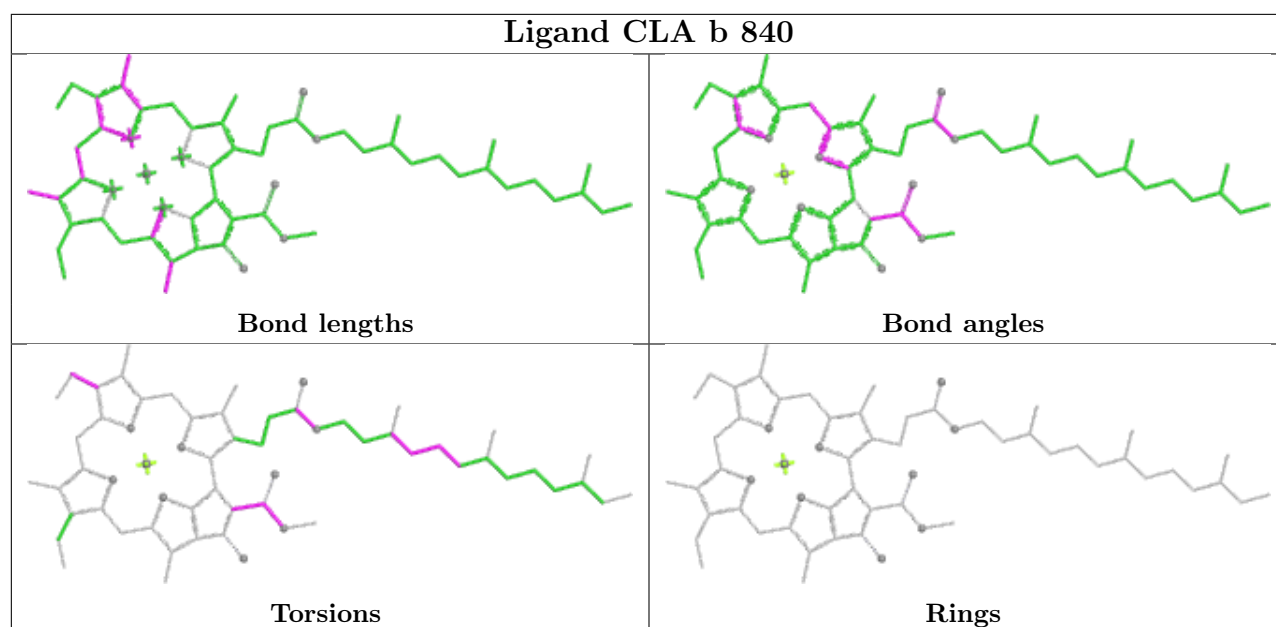
Bond angles

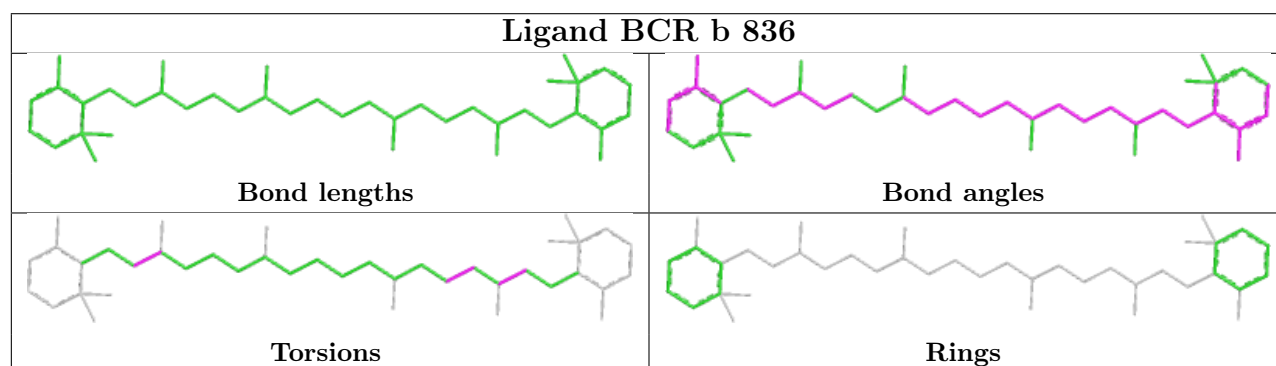
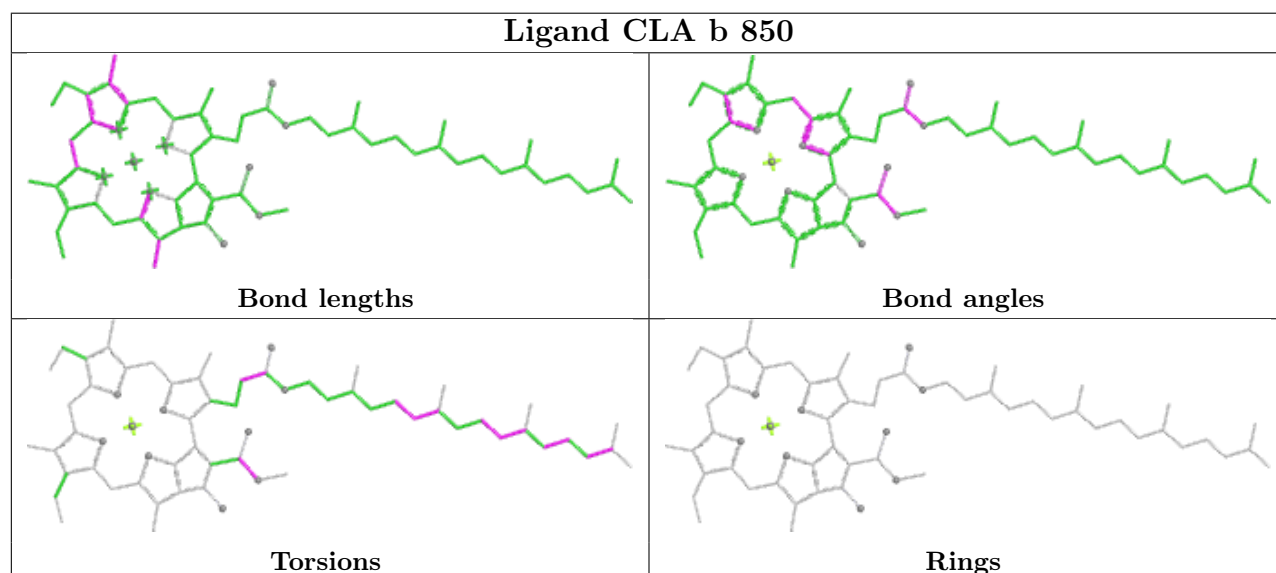
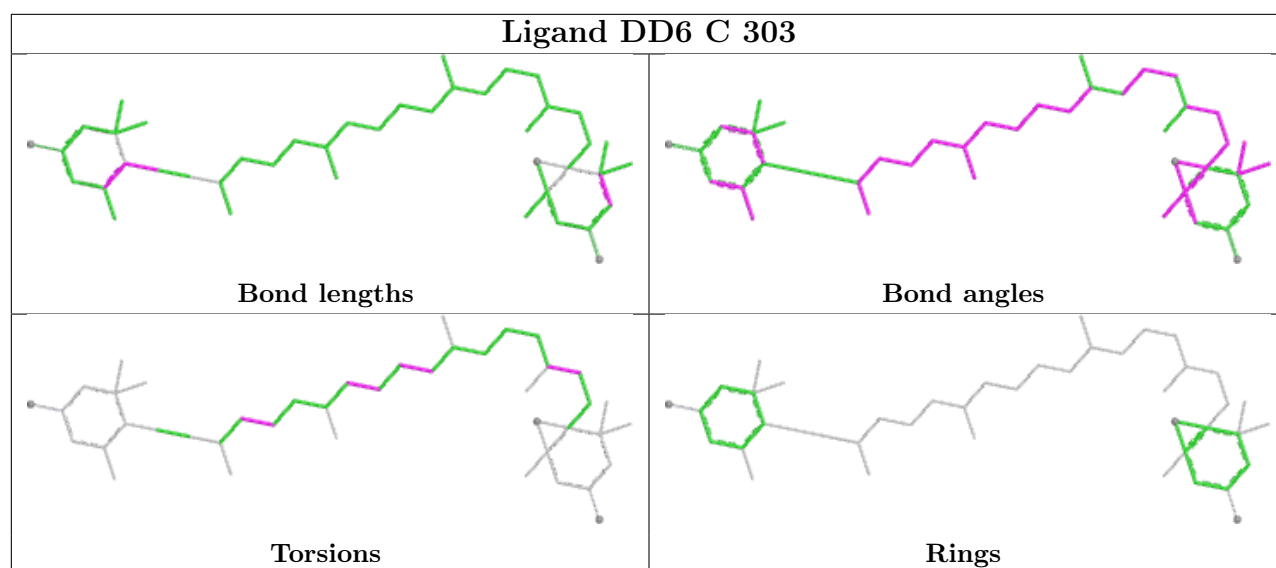


Torsions

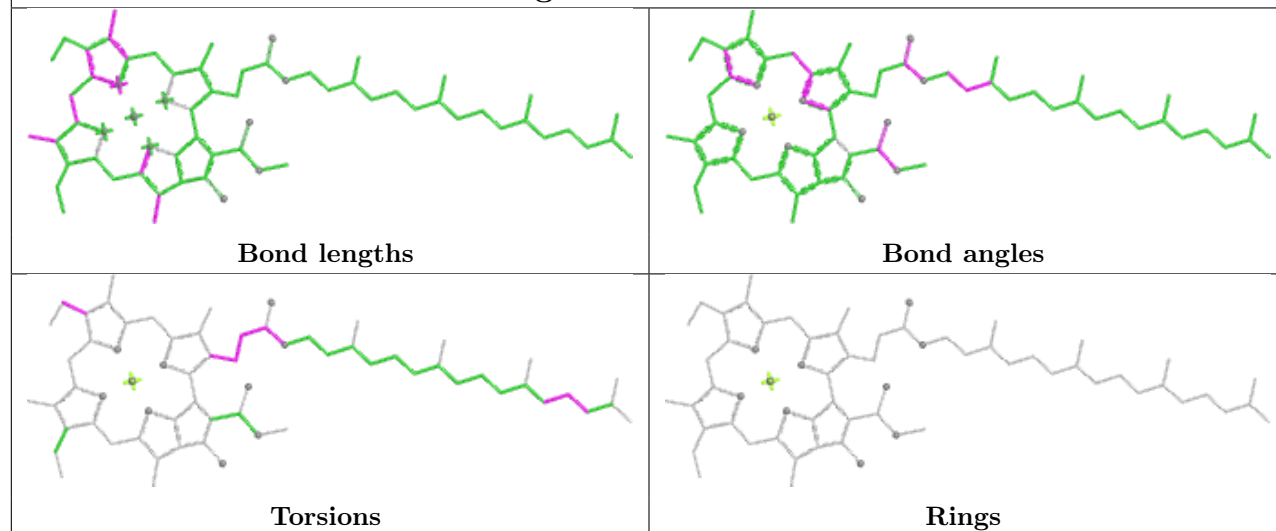


Rings

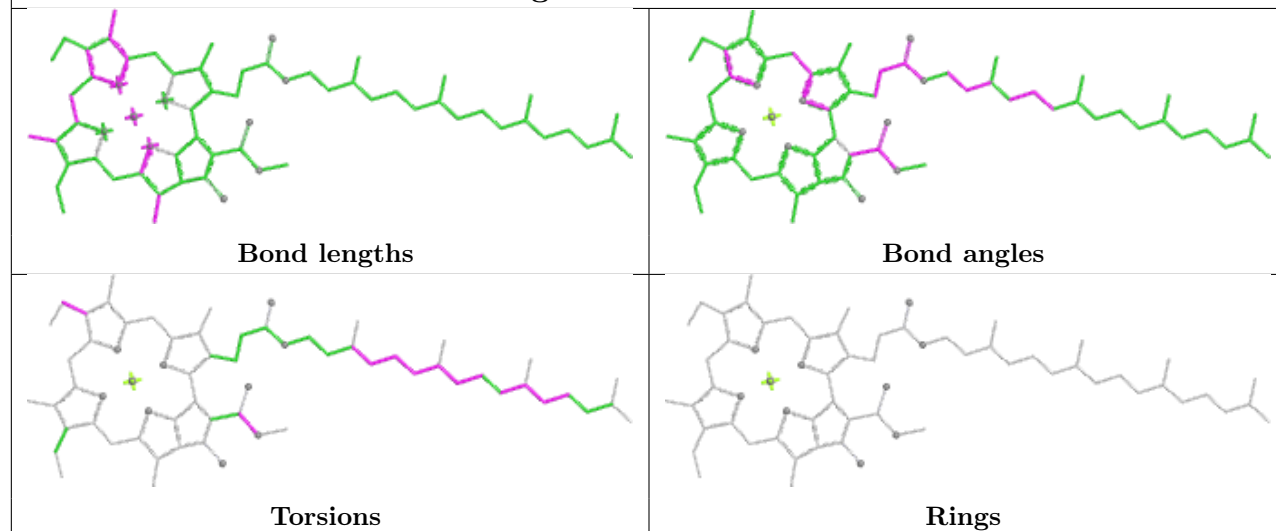




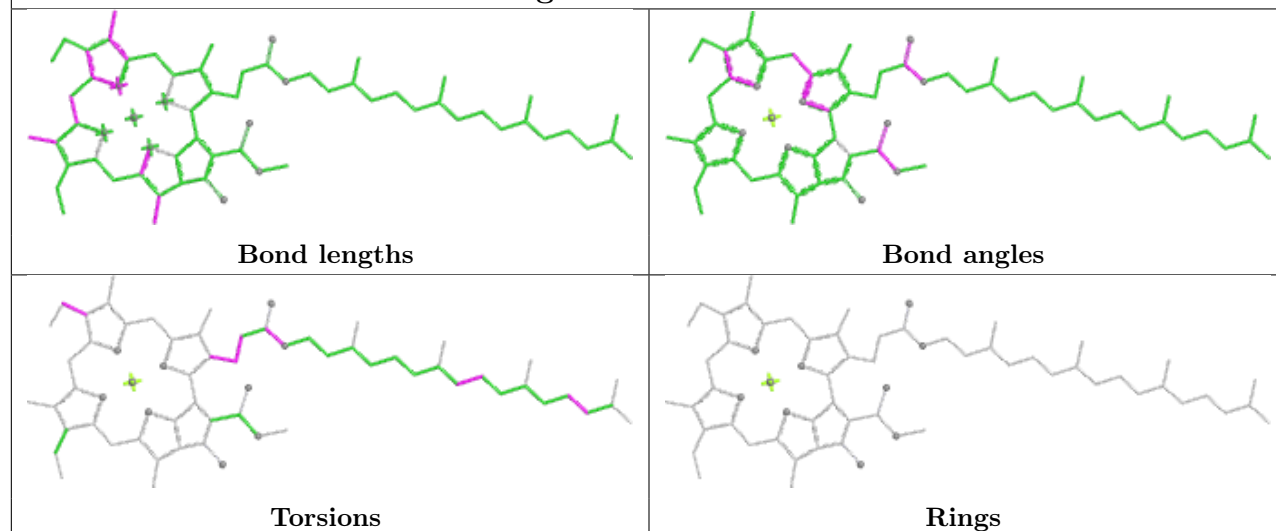
Ligand CLA b 808

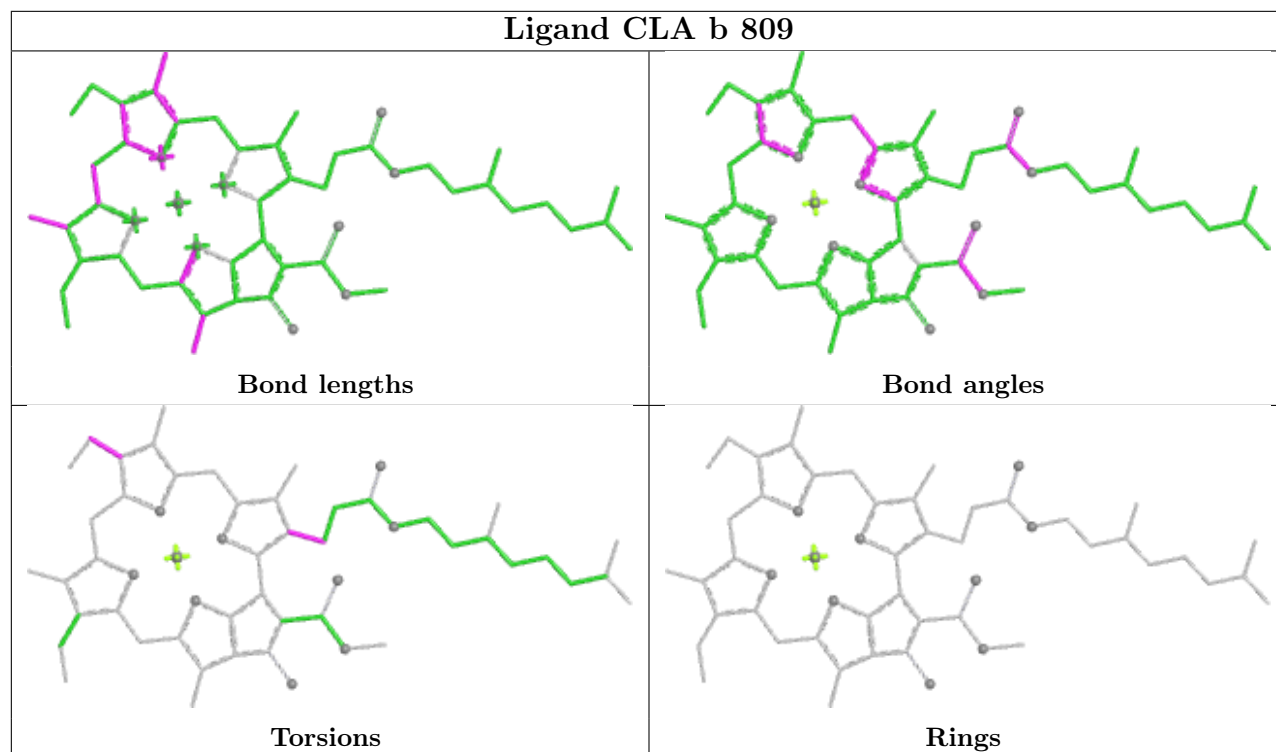
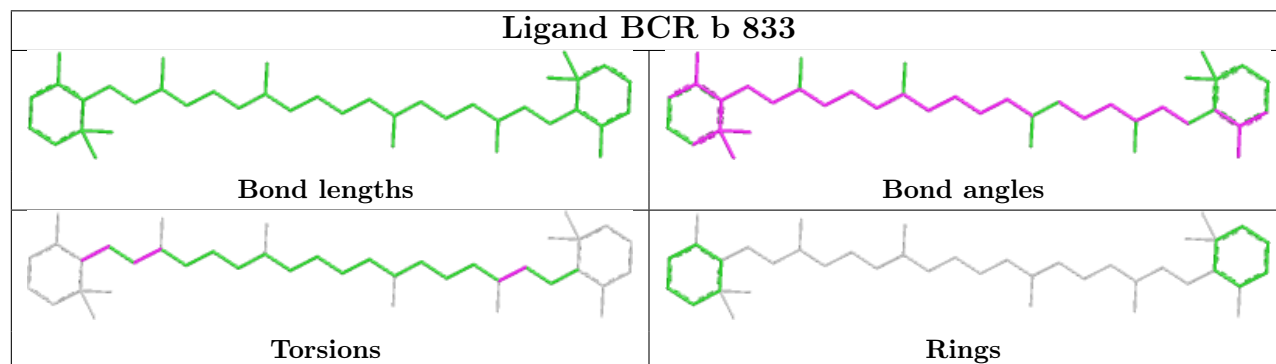
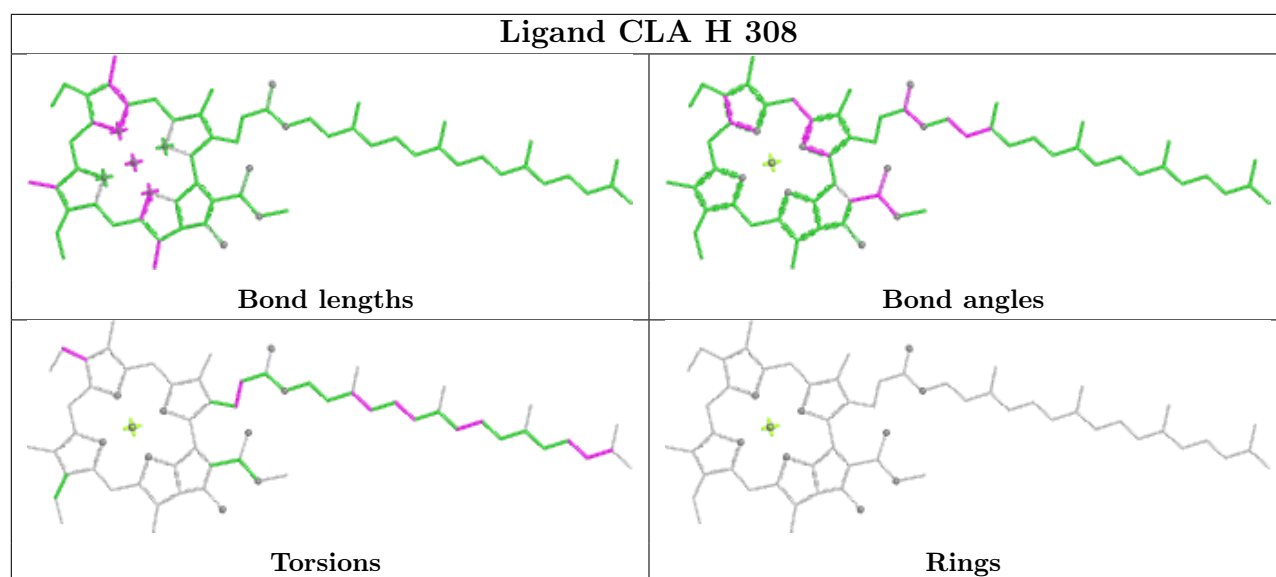


Ligand CLA D 208

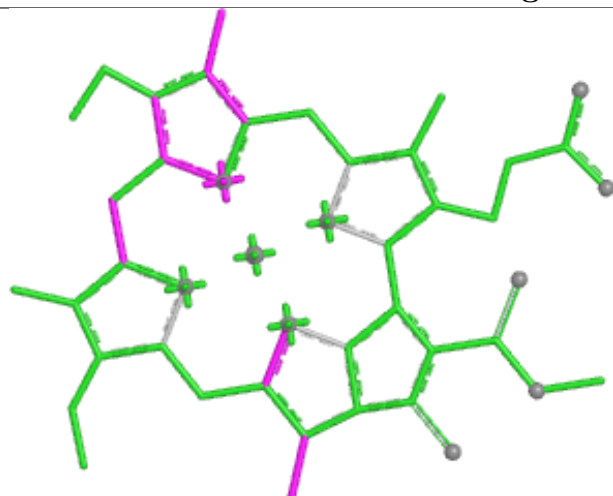


Ligand CLA a 810

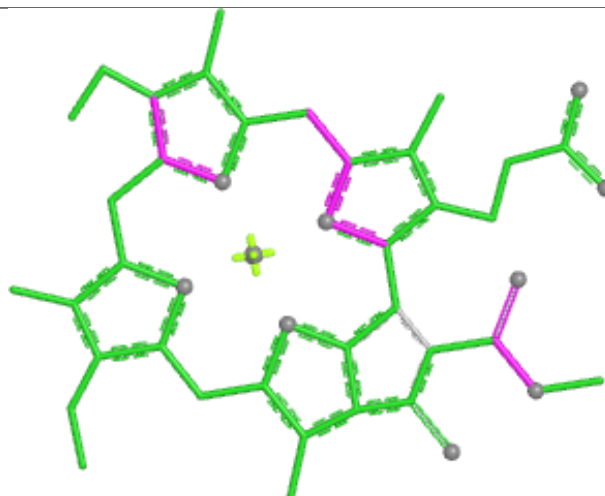




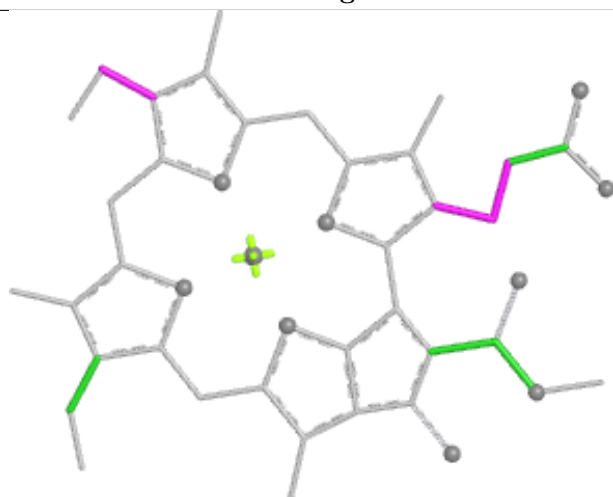
Ligand CLA f 204



Bond lengths



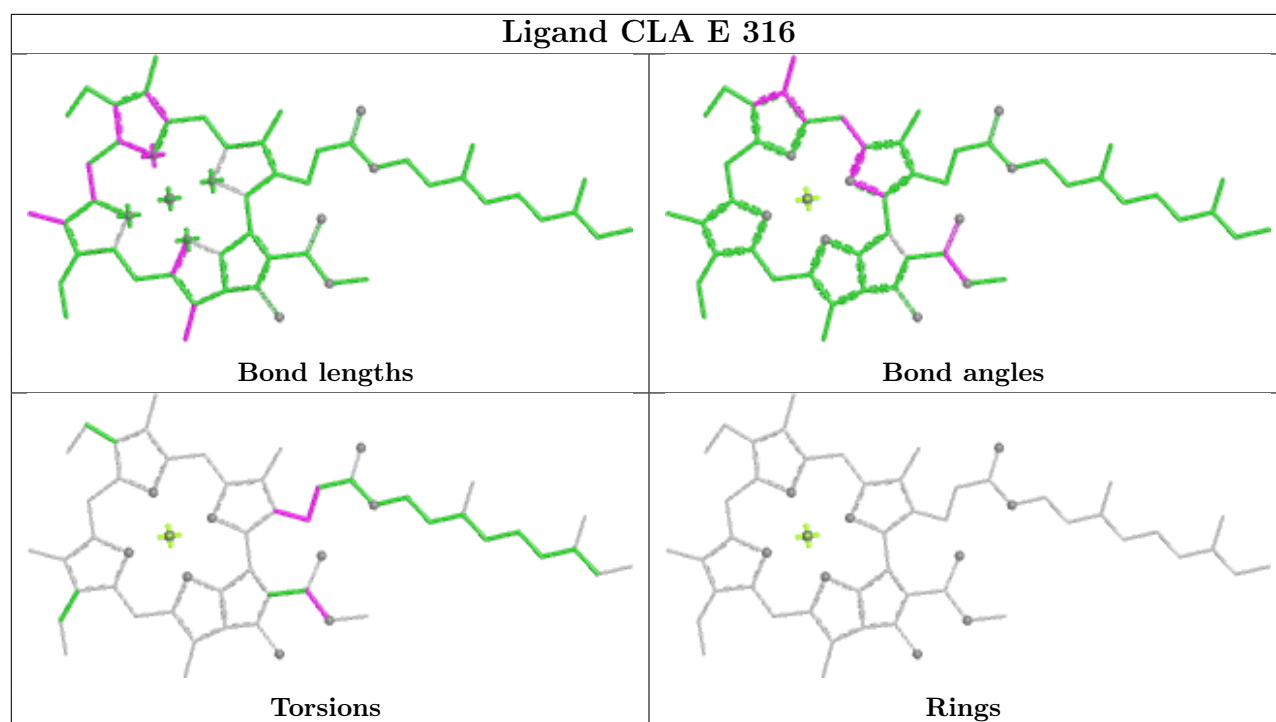
Bond angles



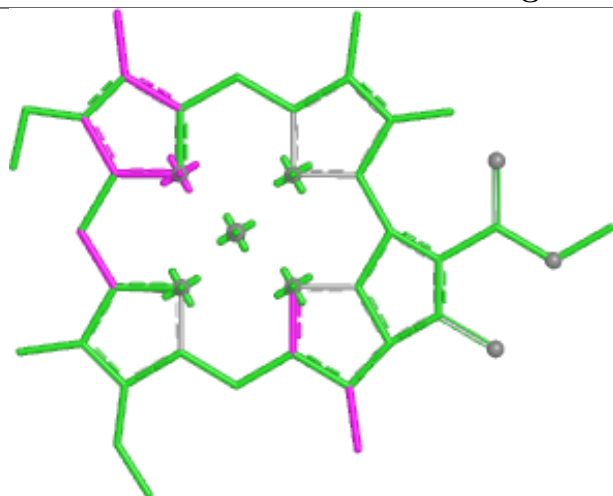
Torsions



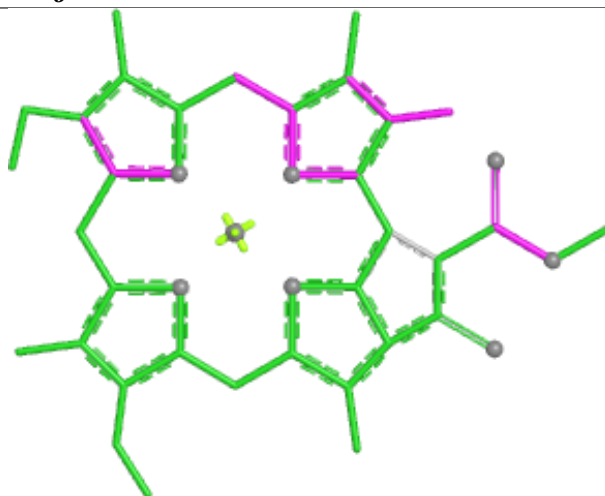
Rings



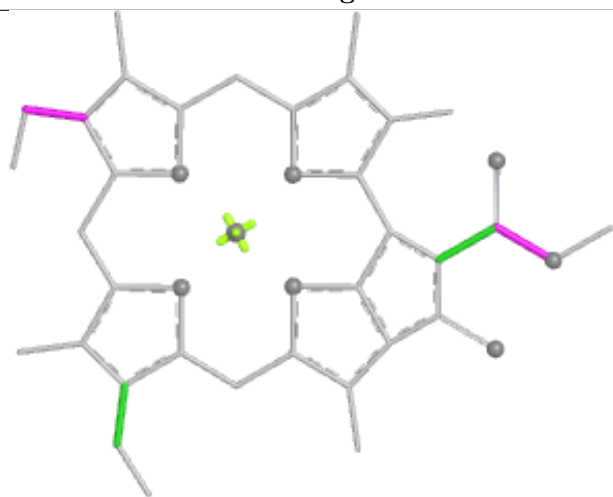
Ligand CLA j 104



Bond lengths



Bond angles

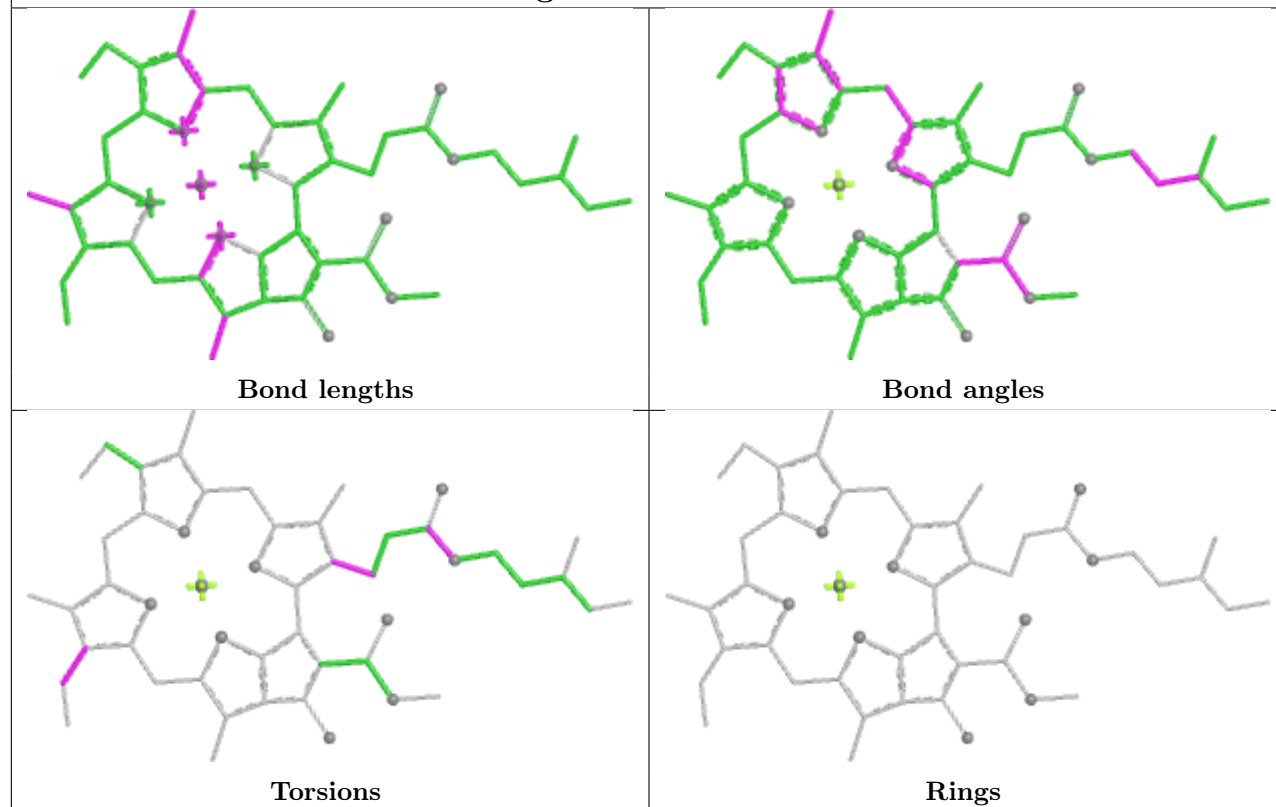


Torsions

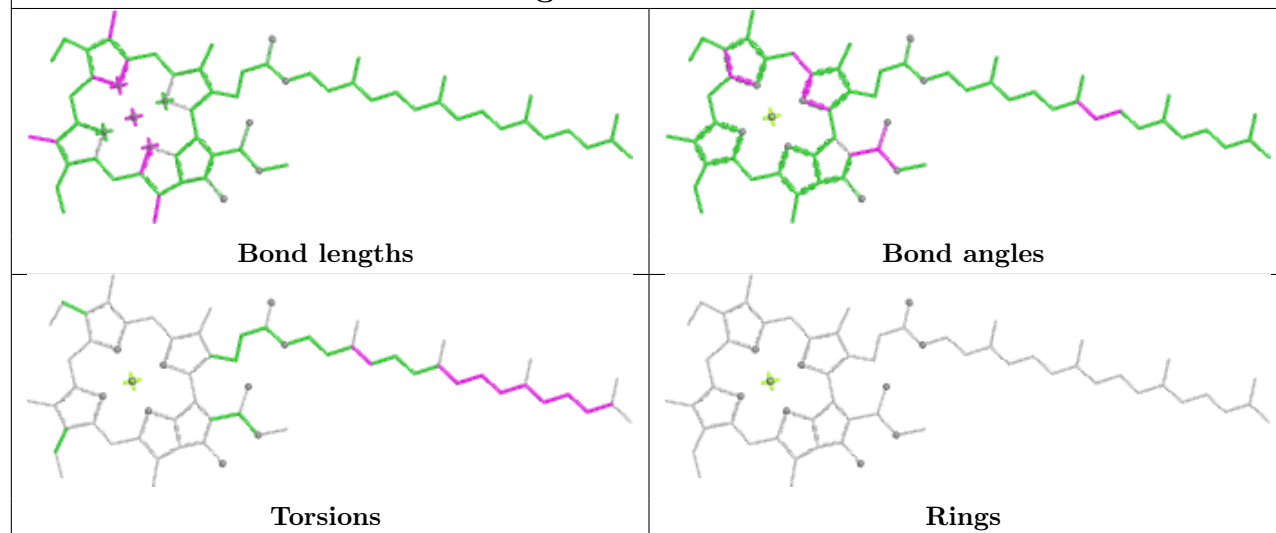


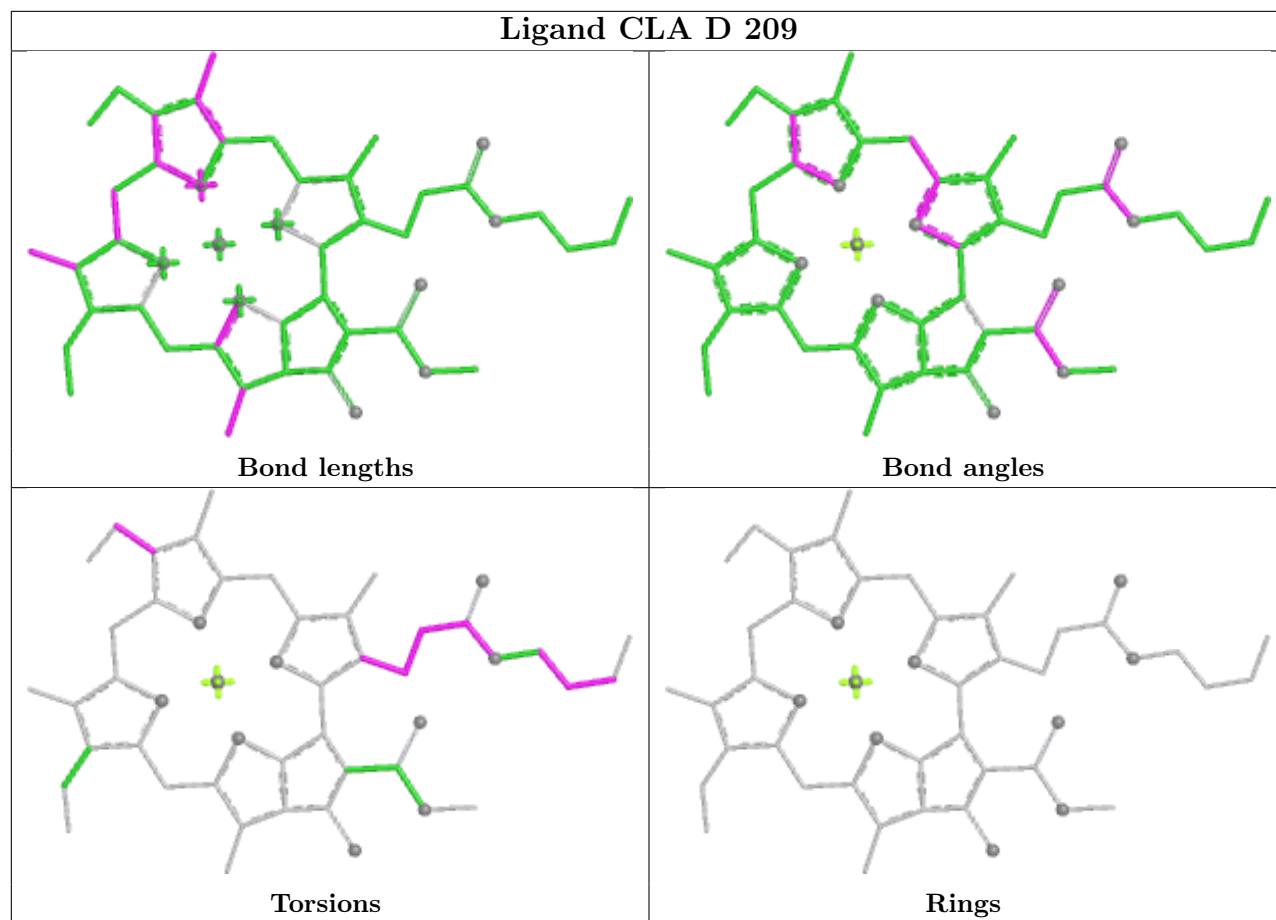
Rings

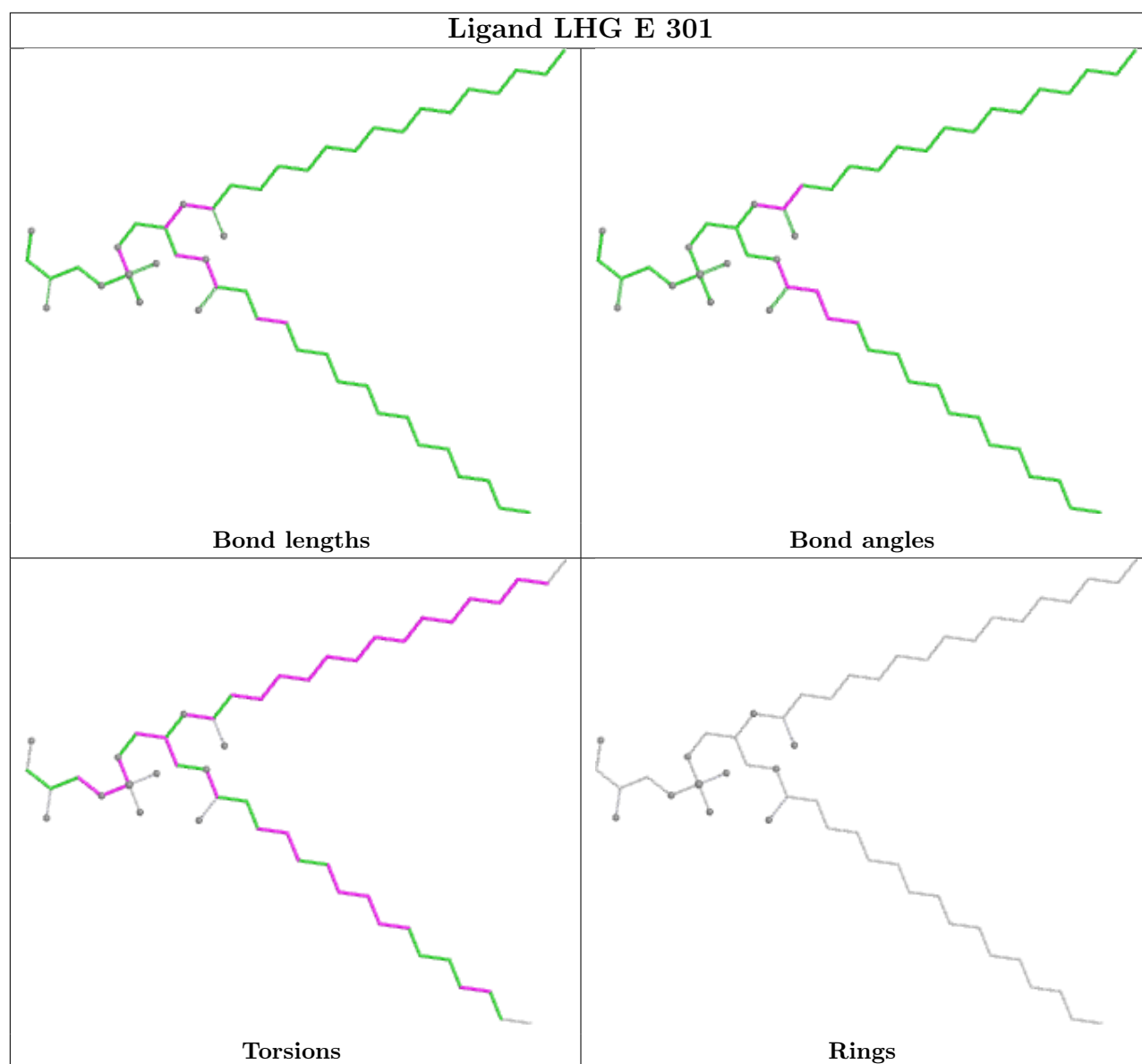
Ligand CLA a 818



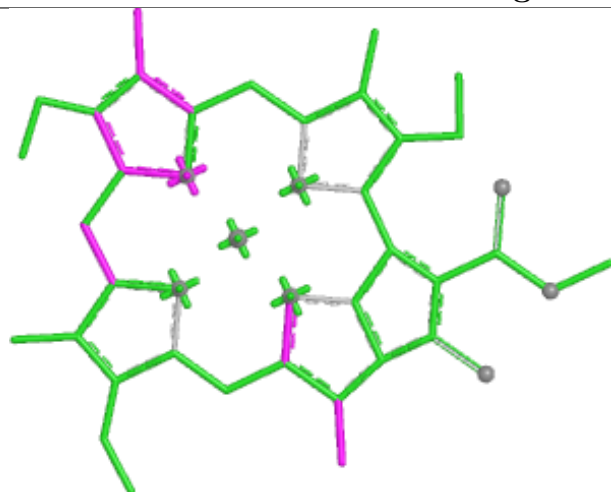
Ligand CLA a 840



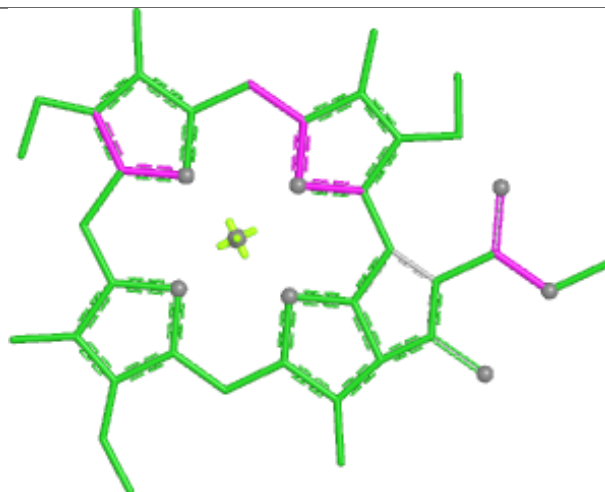




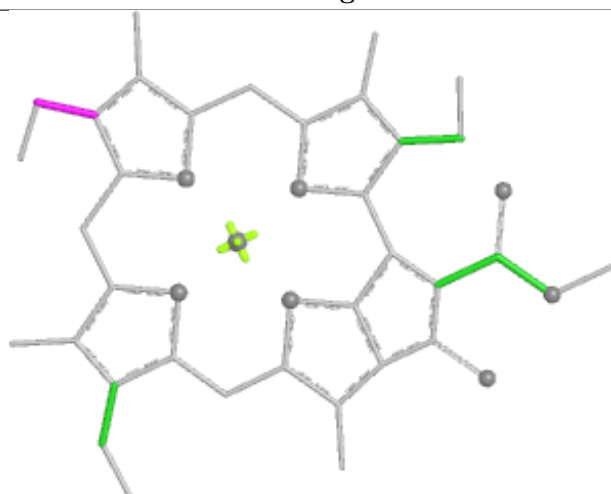
Ligand CLA D 212



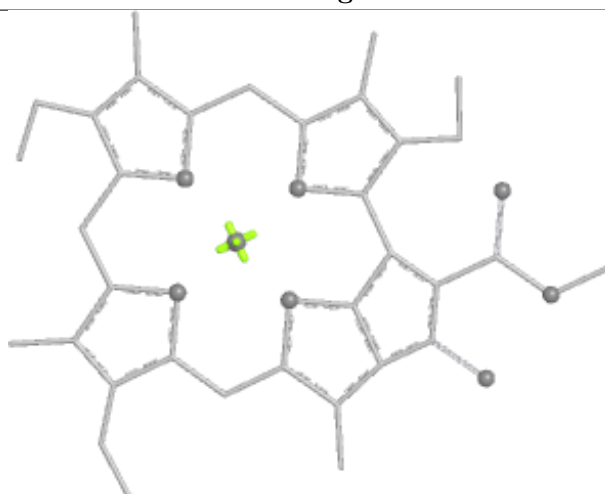
Bond lengths



Bond angles

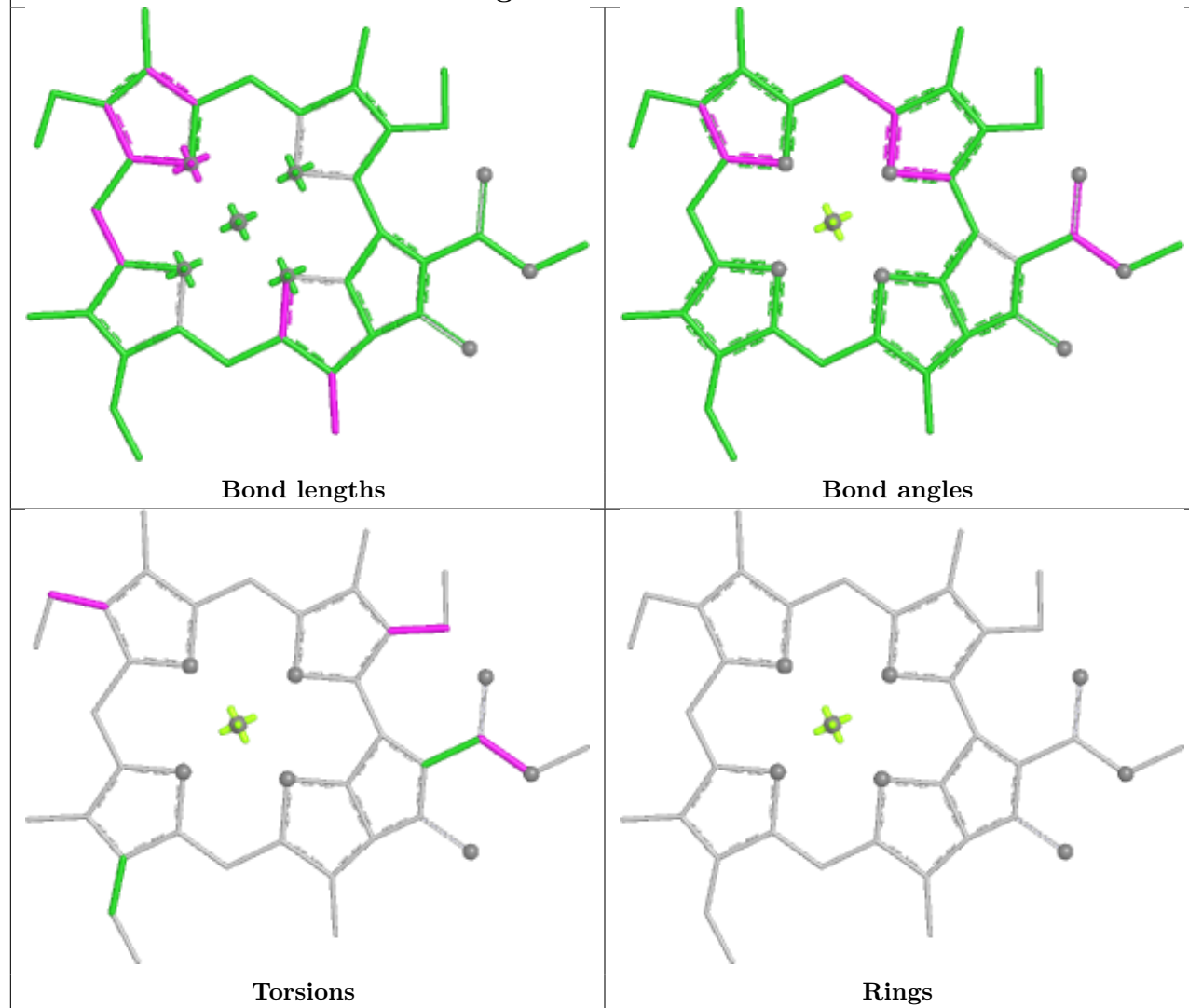


Torsions

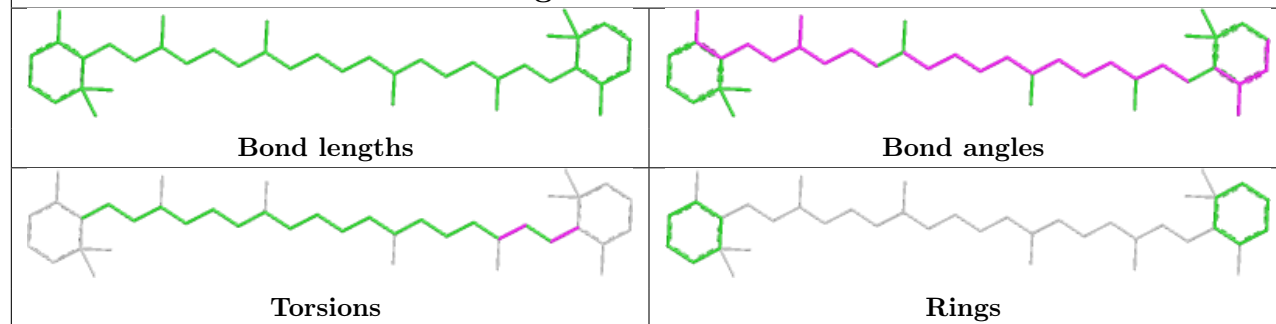


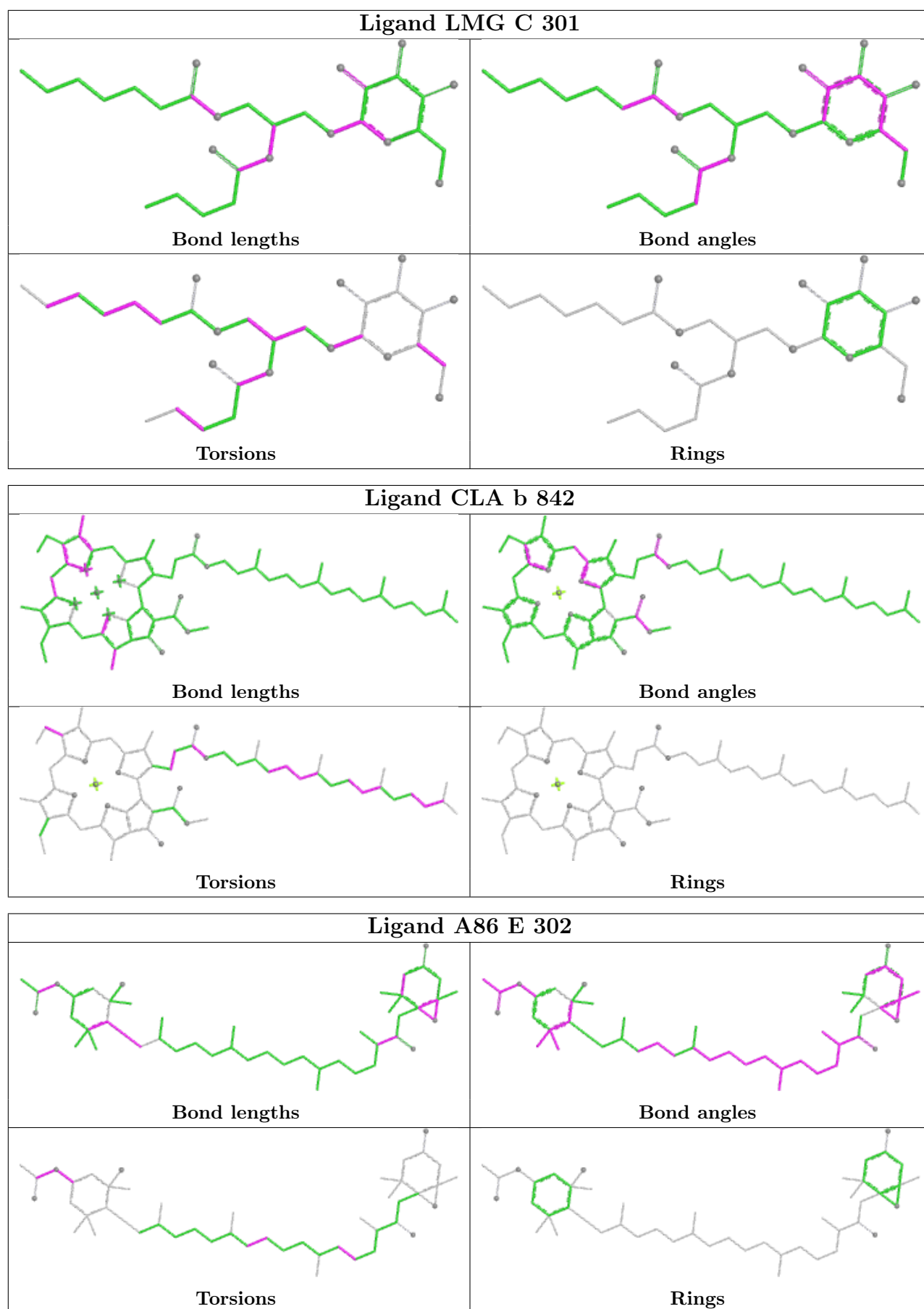
Rings

Ligand CLA C 315

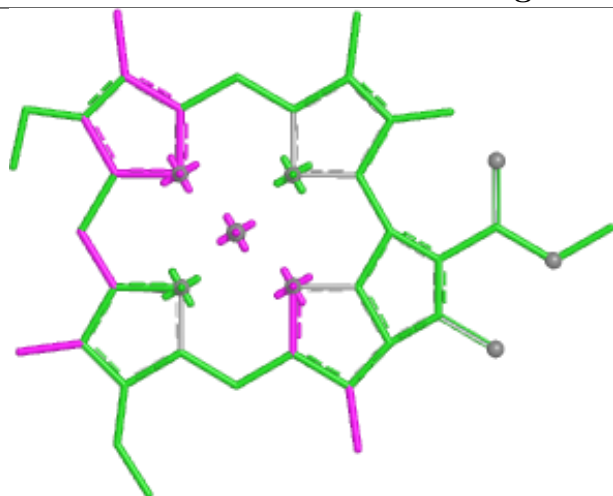


Ligand BCR a 834

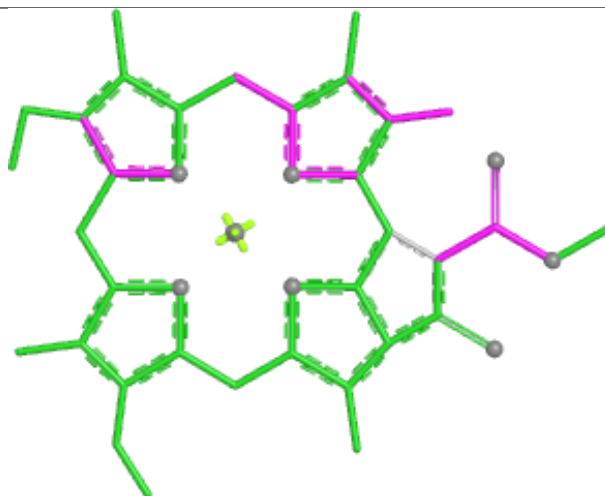




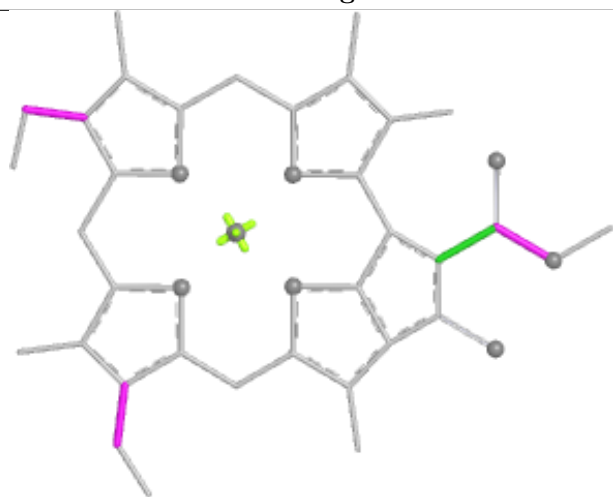
Ligand CLA C 314



Bond lengths



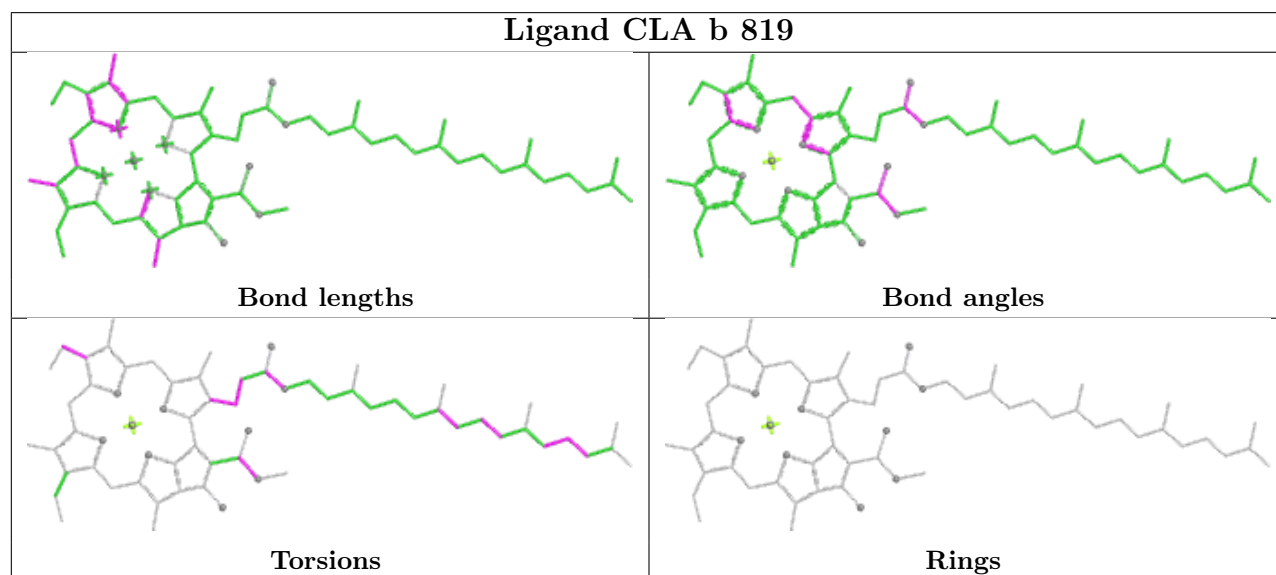
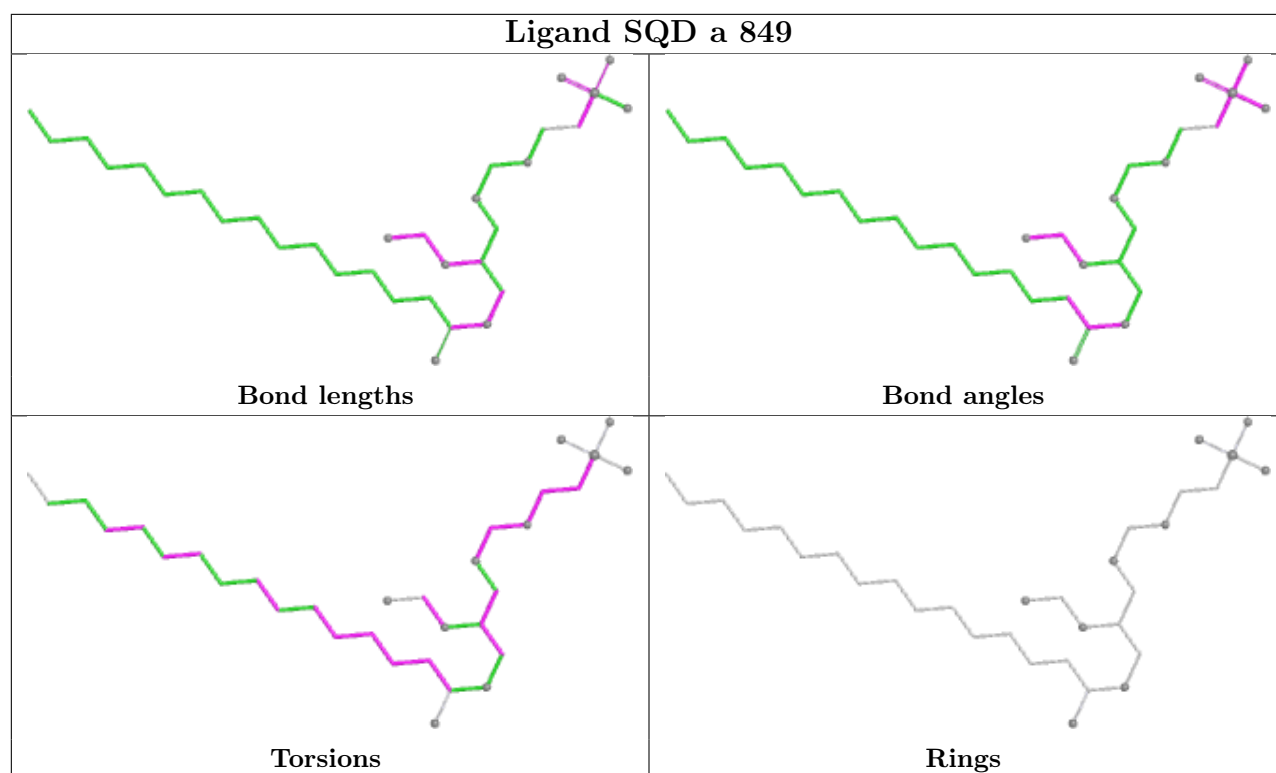
Bond angles

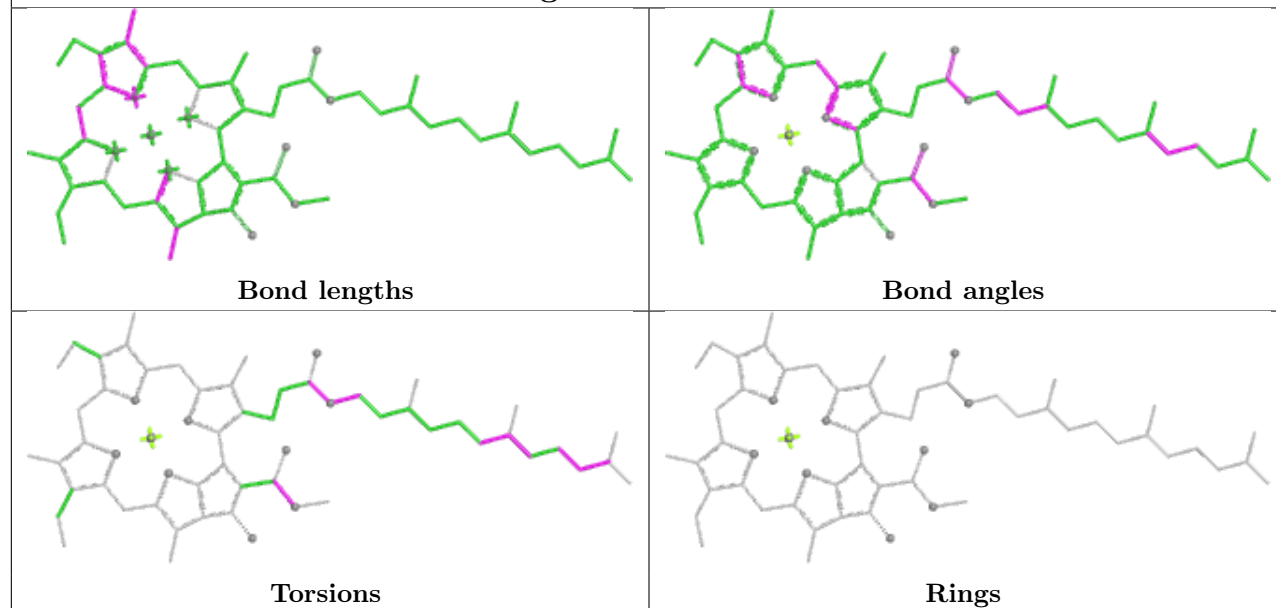
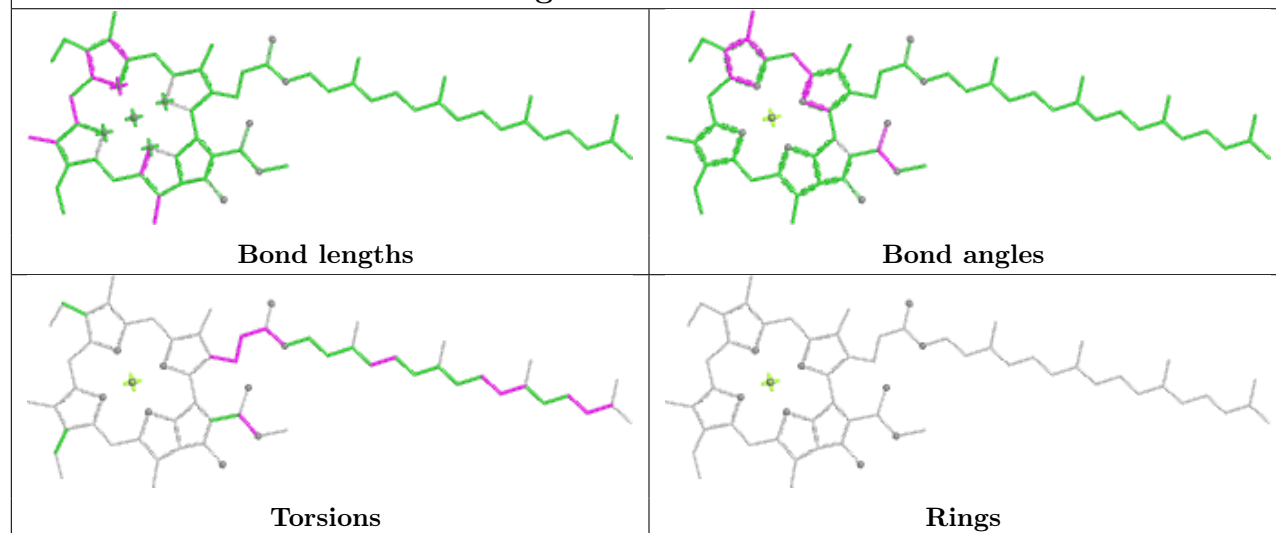


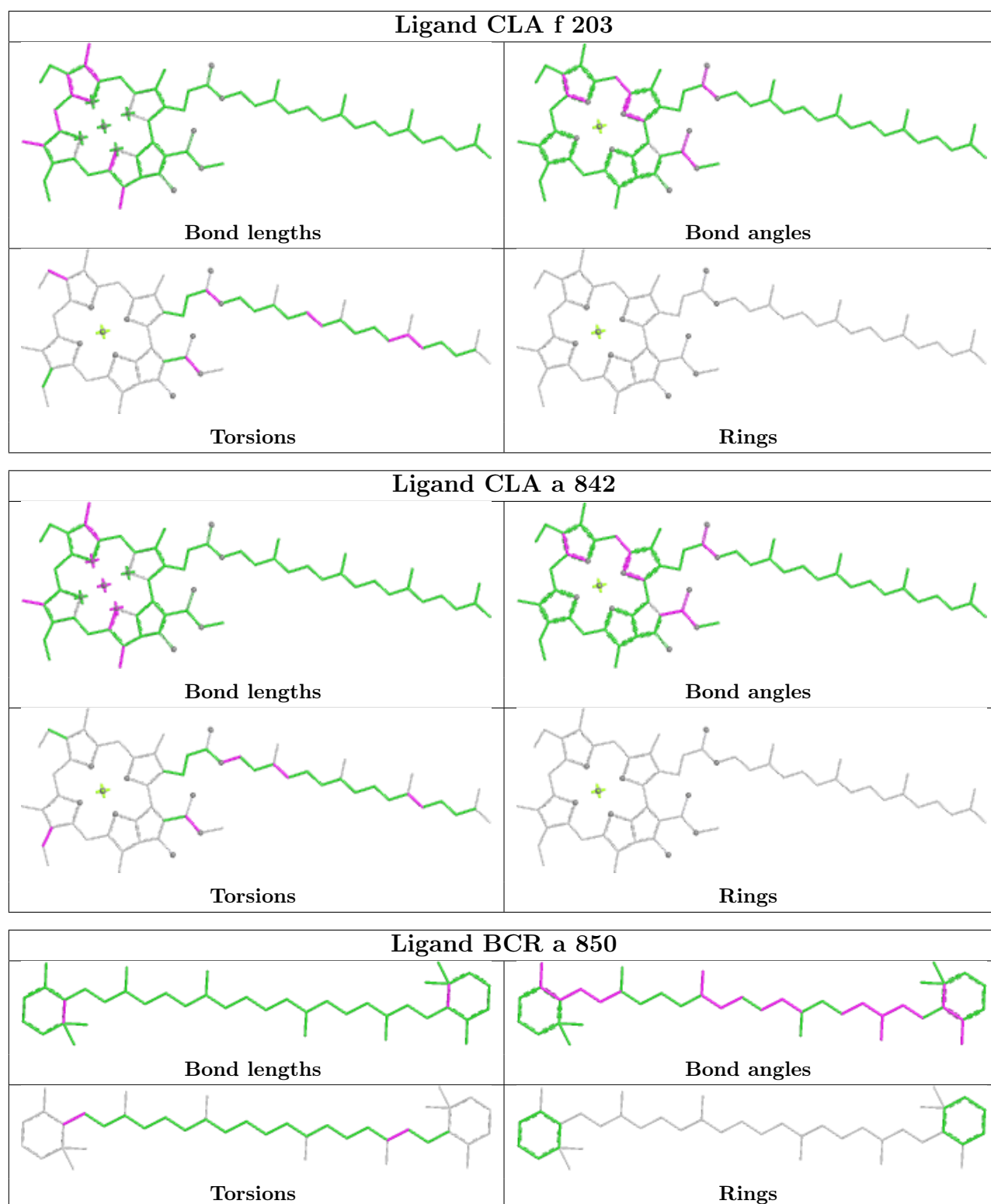
Torsions



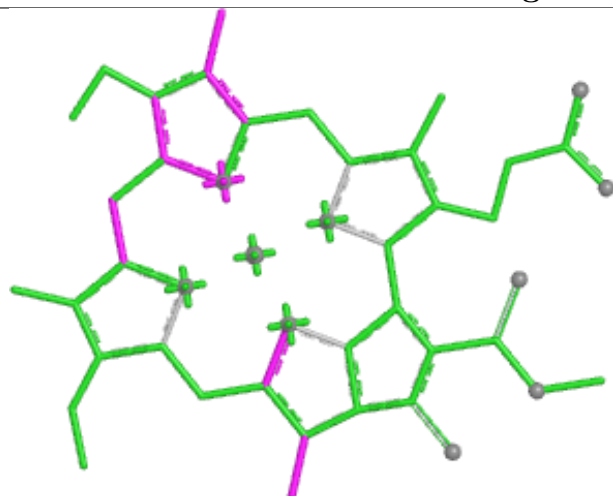
Rings



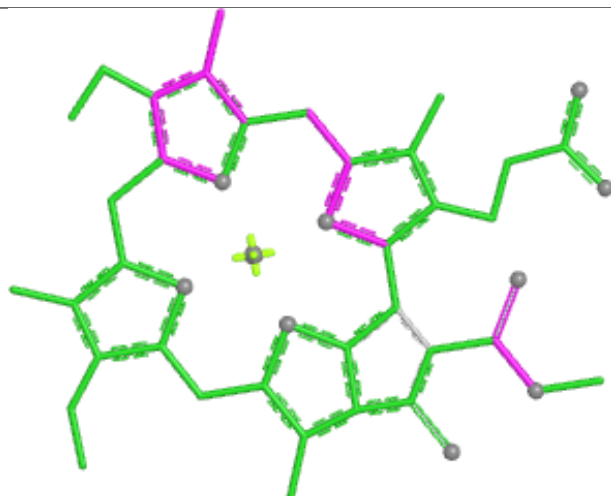
Ligand CLA i 101**Ligand CLA b 822**



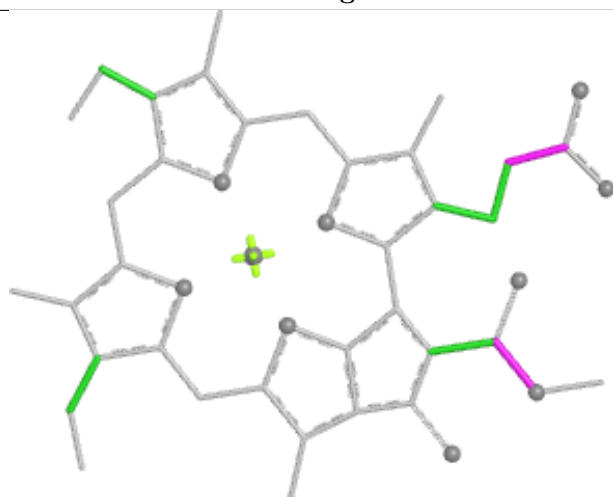
Ligand CLA 1 205



Bond lengths



Bond angles

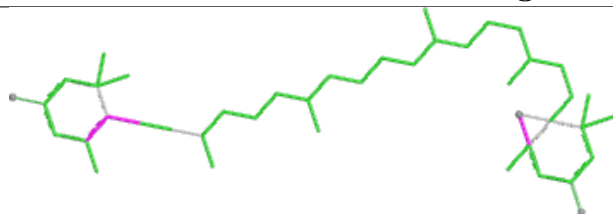


Torsions

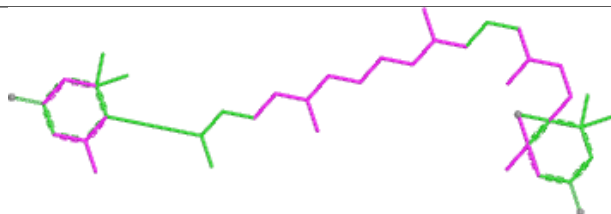


Rings

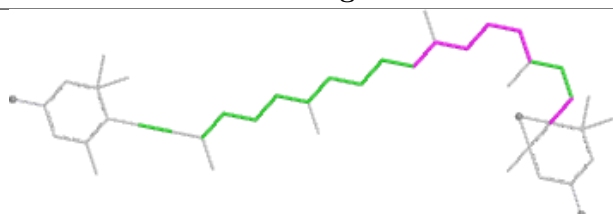
Ligand DD6 E 307



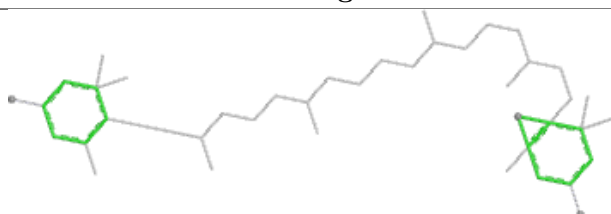
Bond lengths



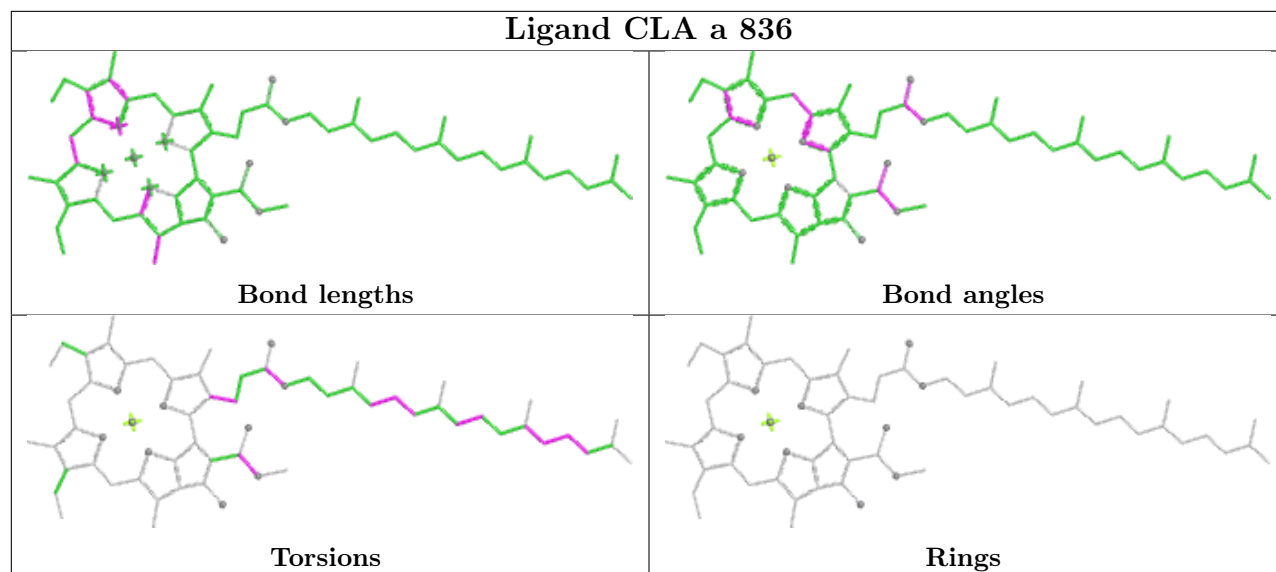
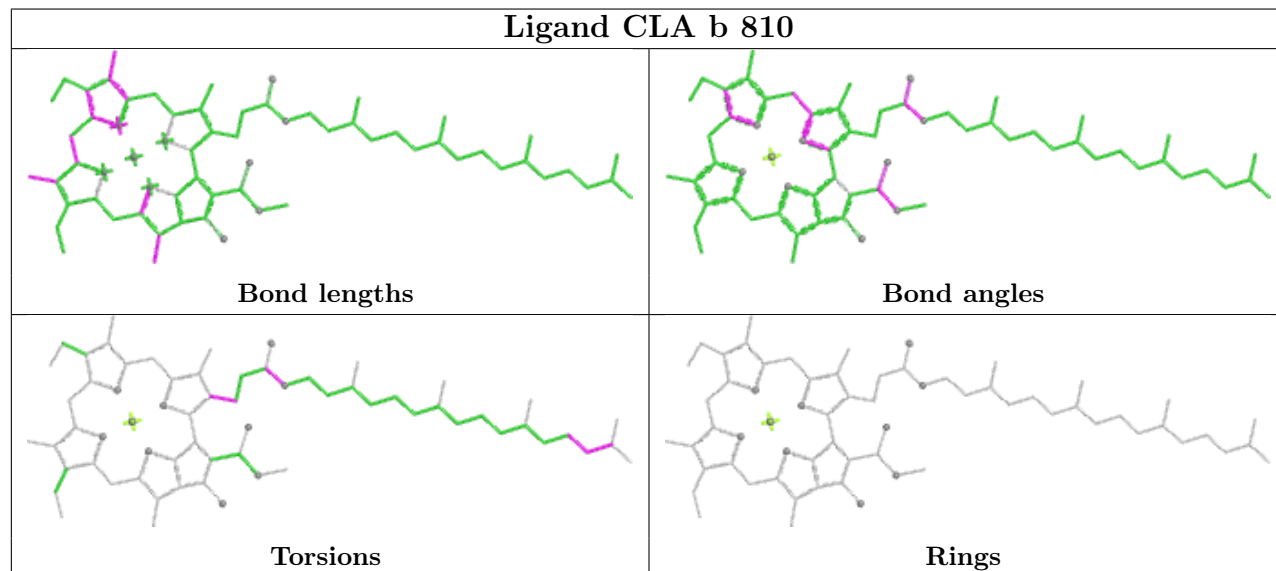
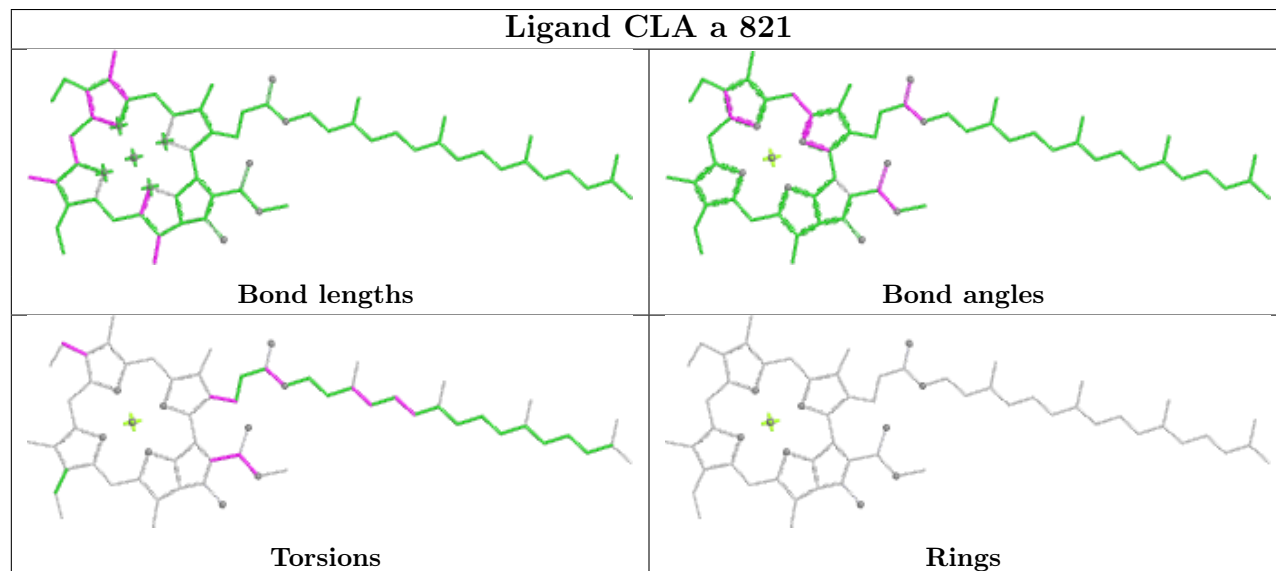
Bond angles

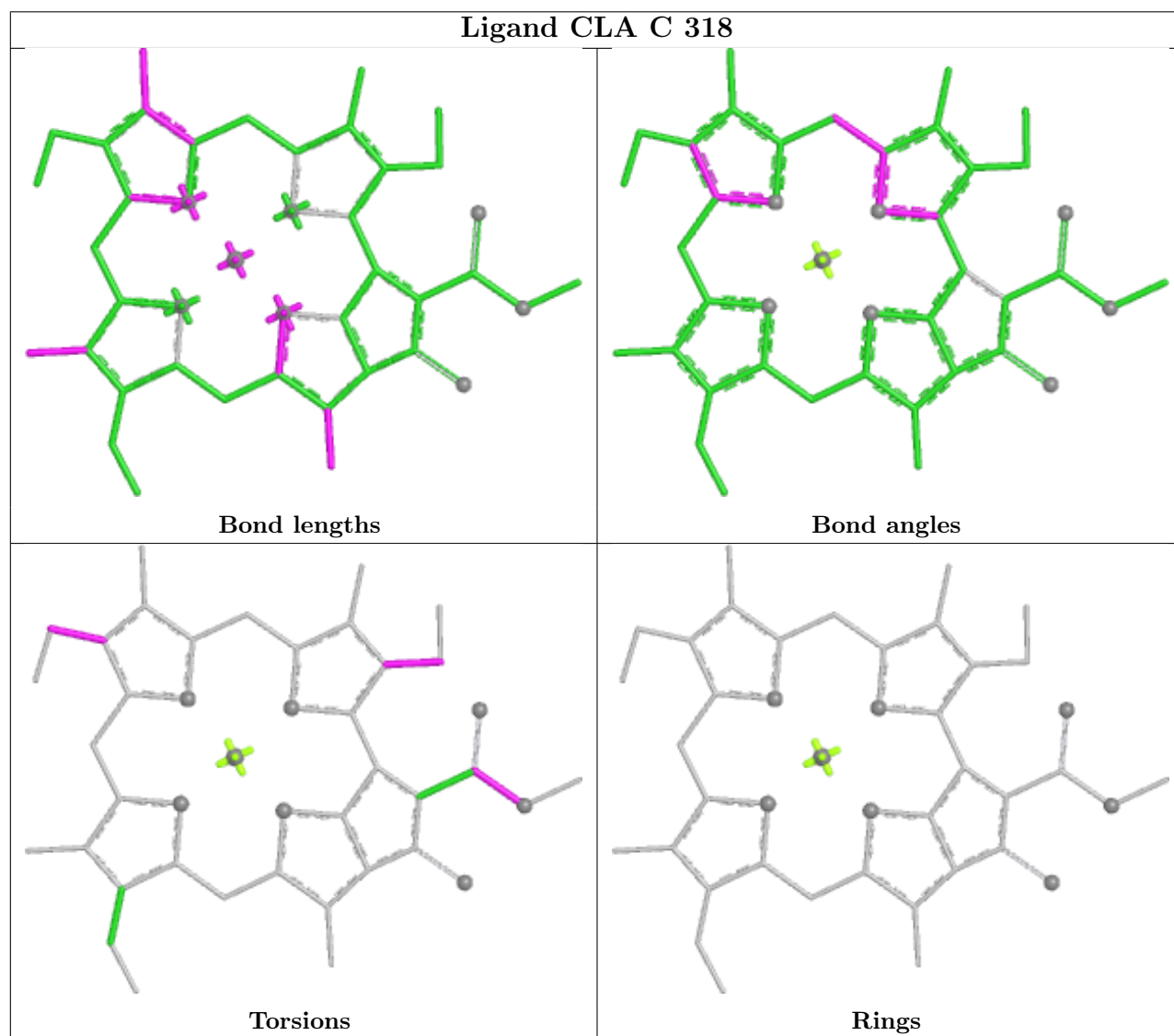
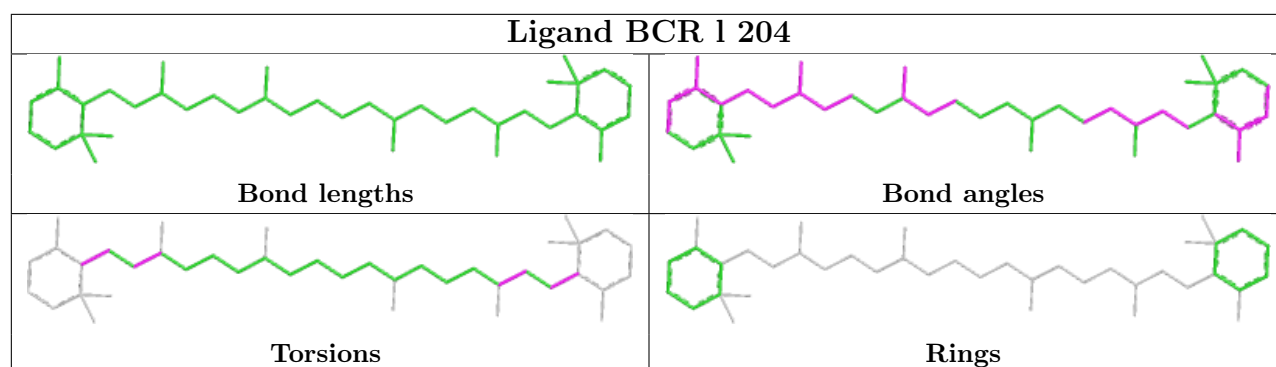


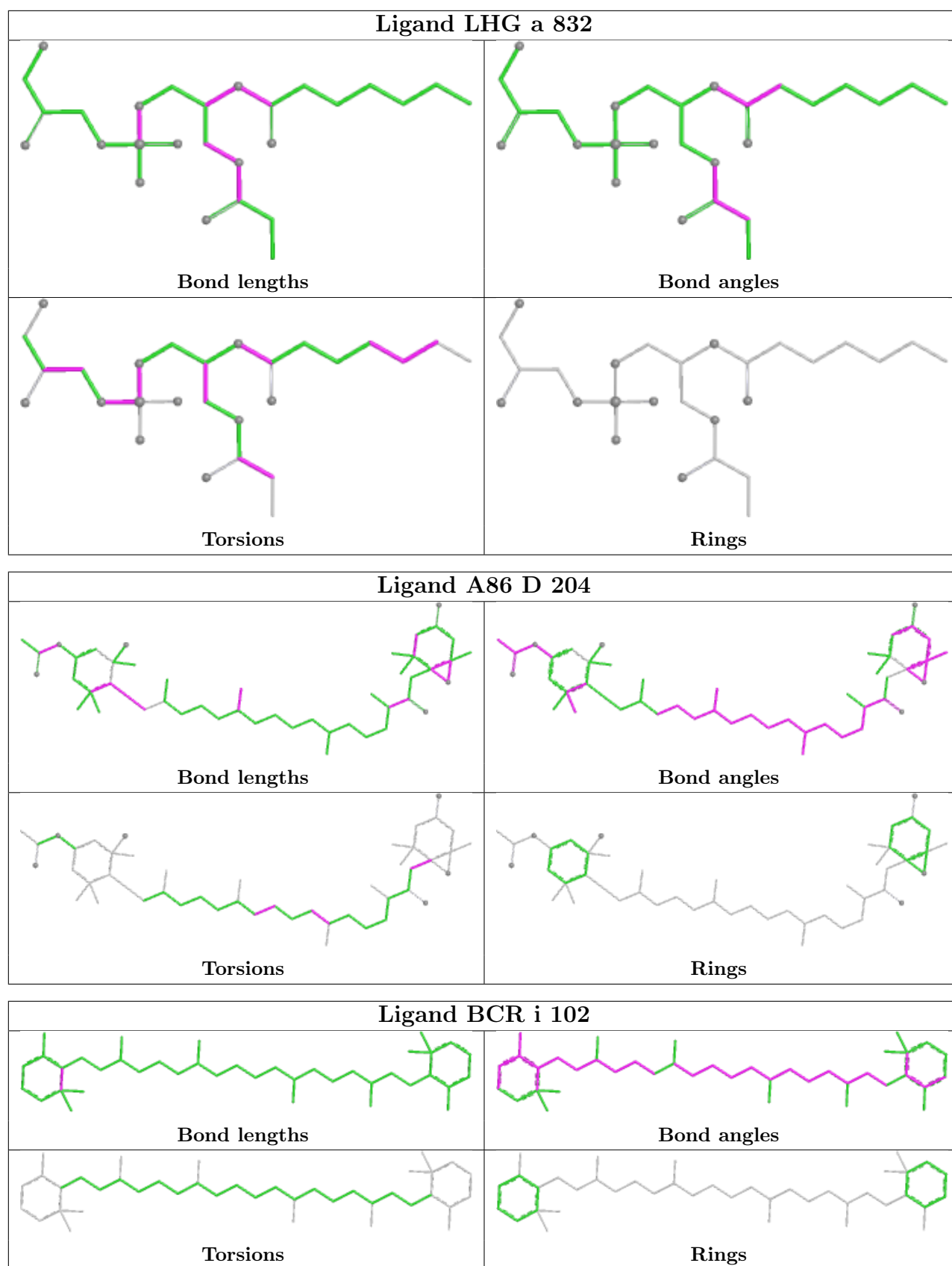
Torsions

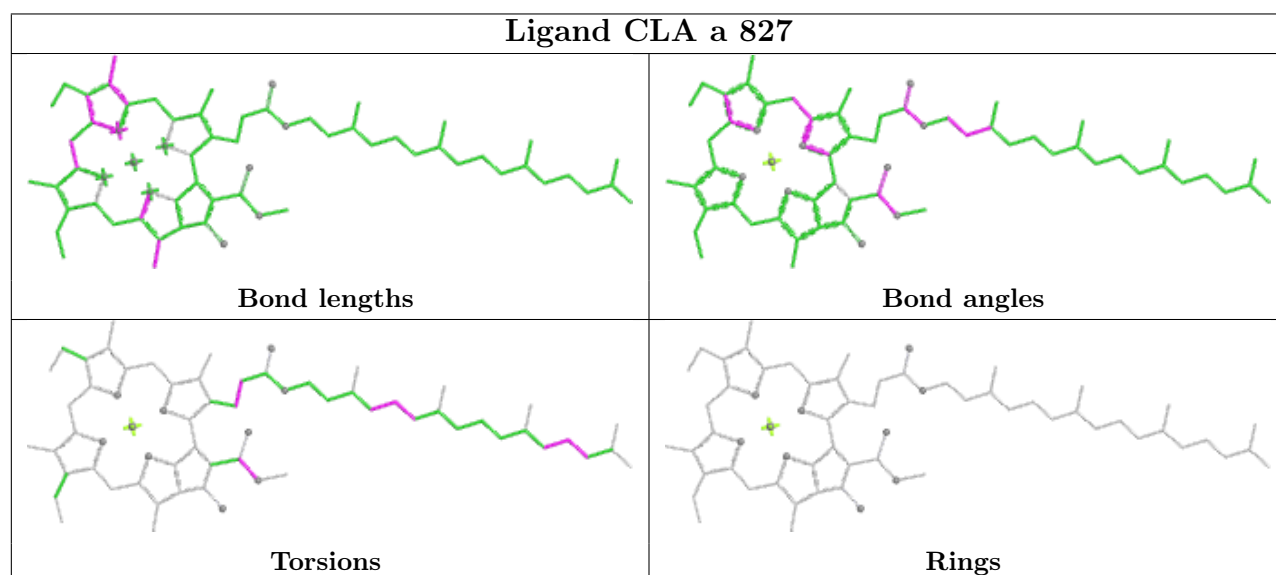
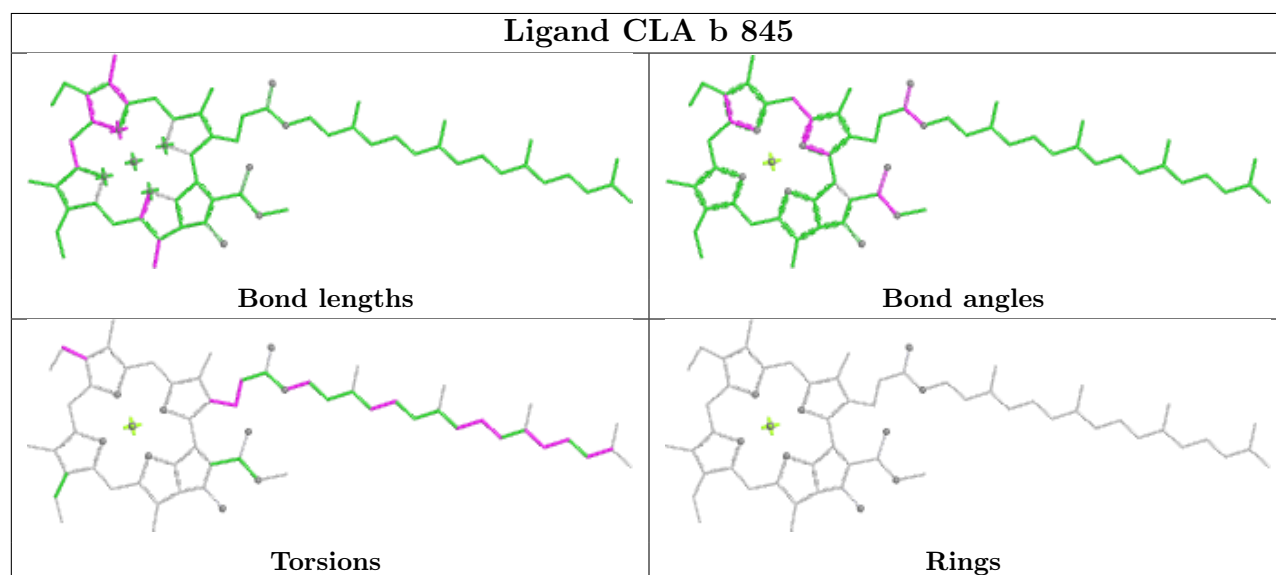
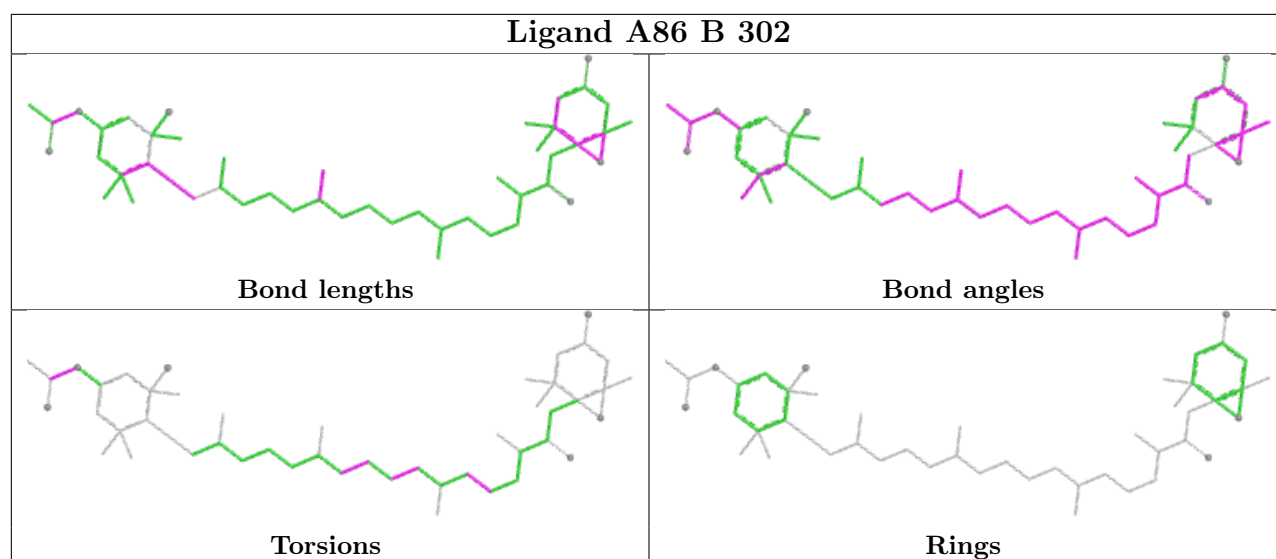


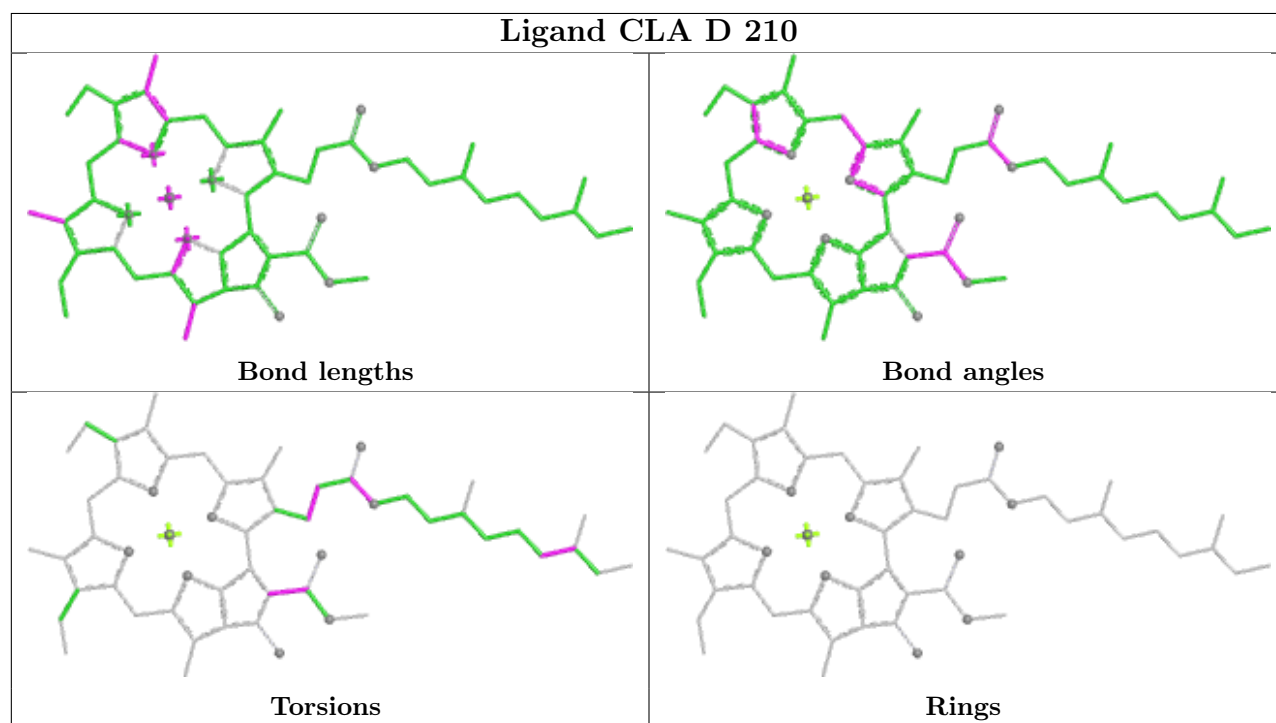
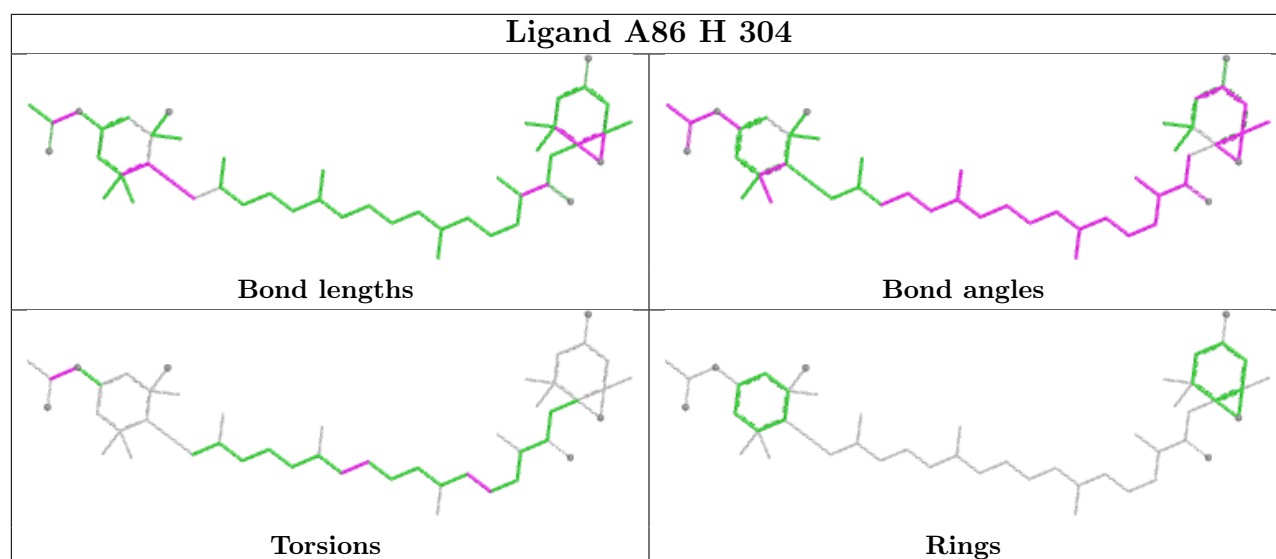
Rings

Ligand CLA a 836**Ligand CLA b 810****Ligand CLA a 821**

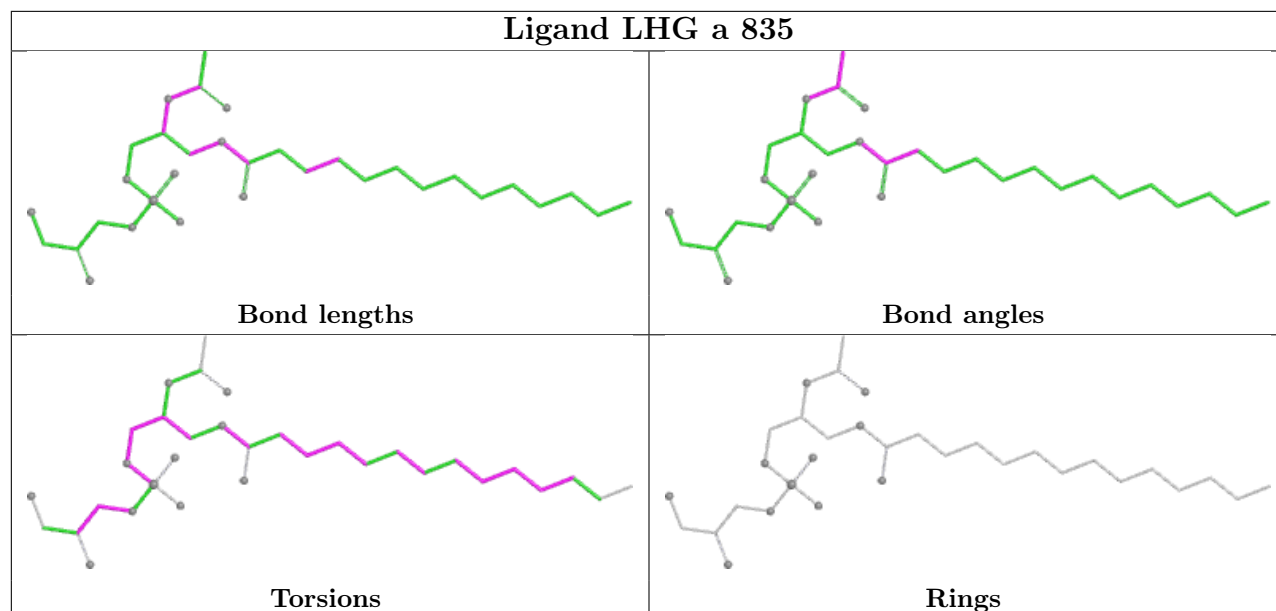




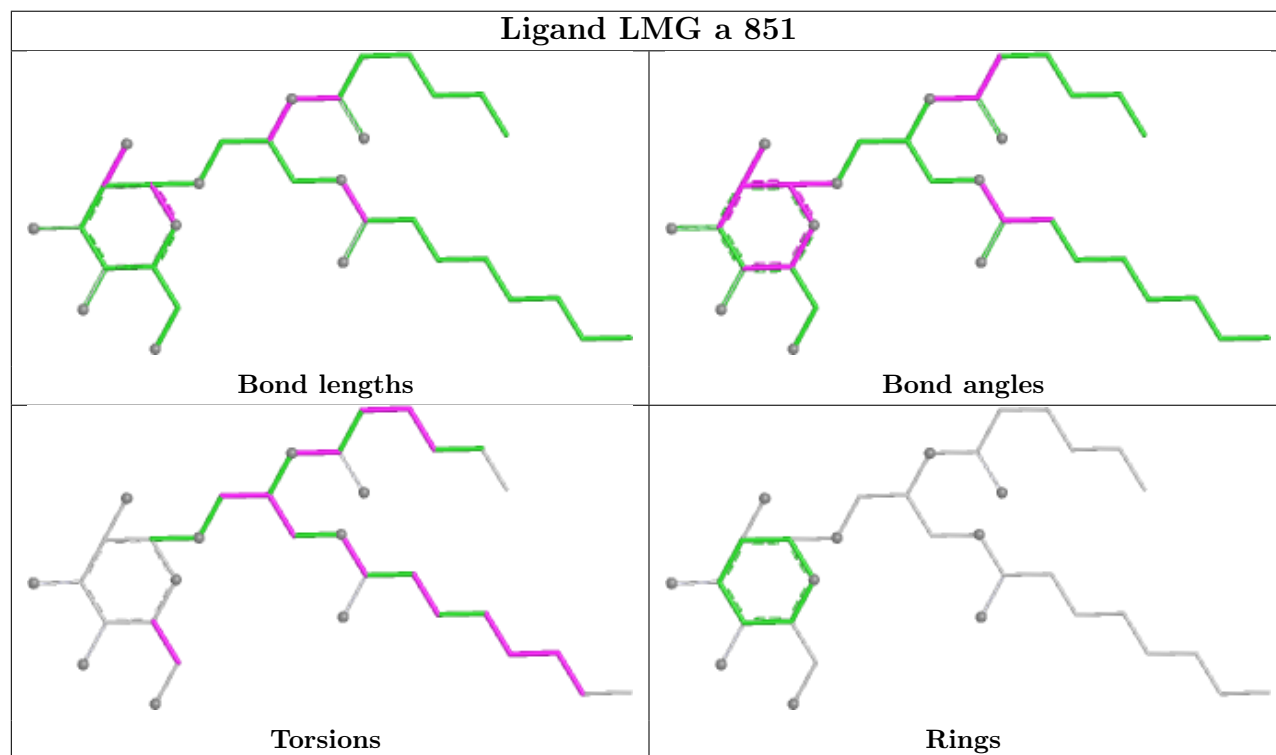


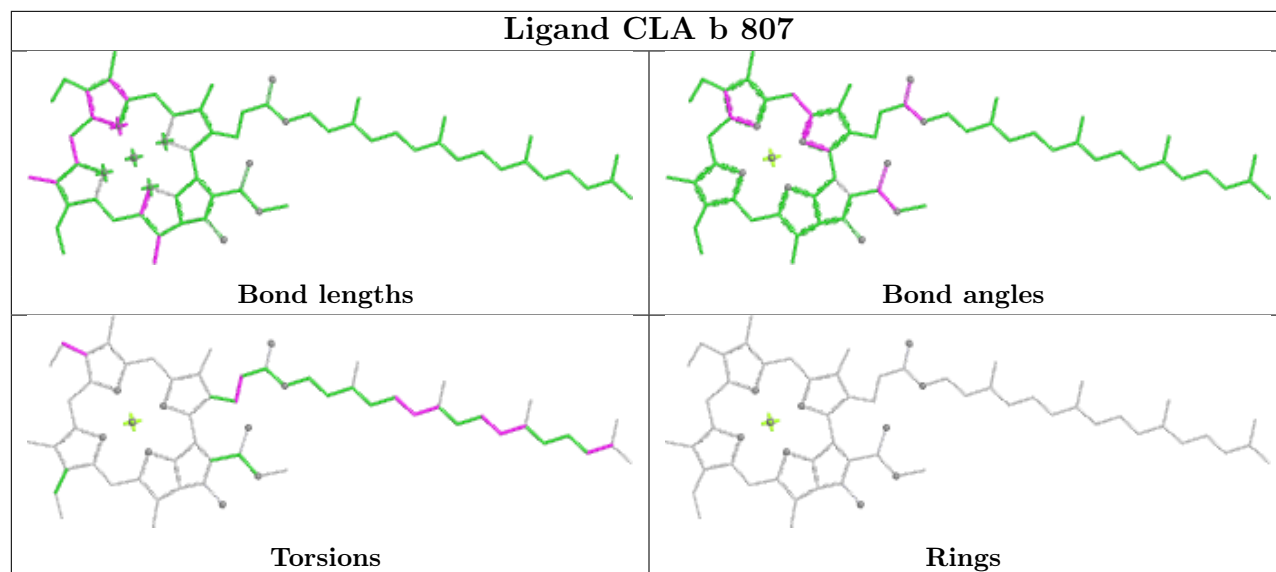
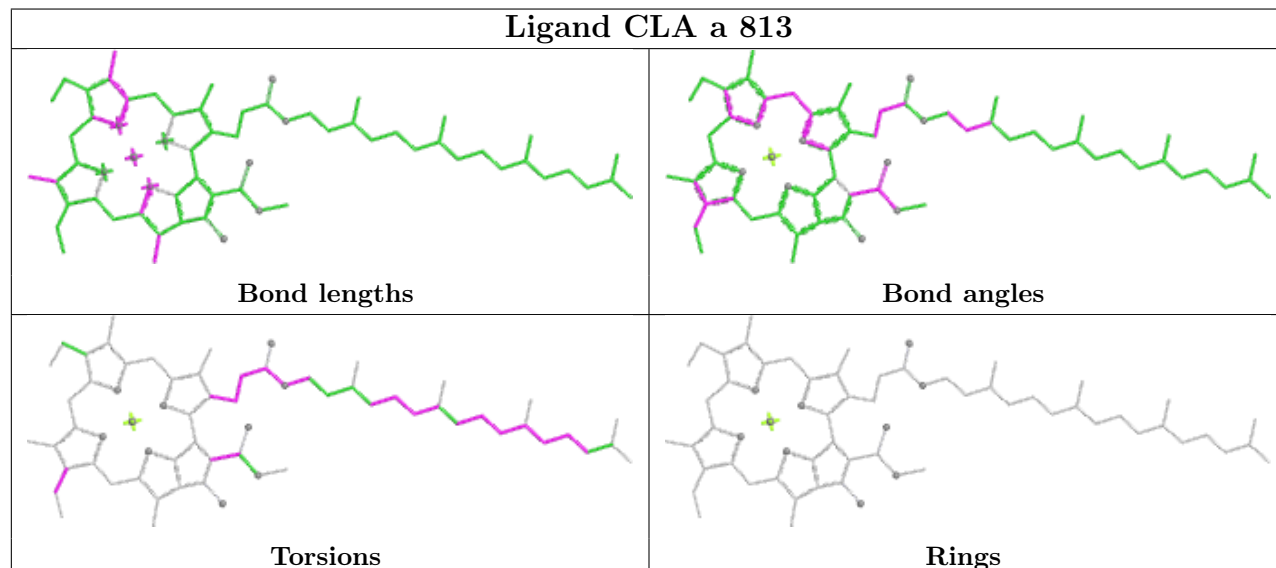
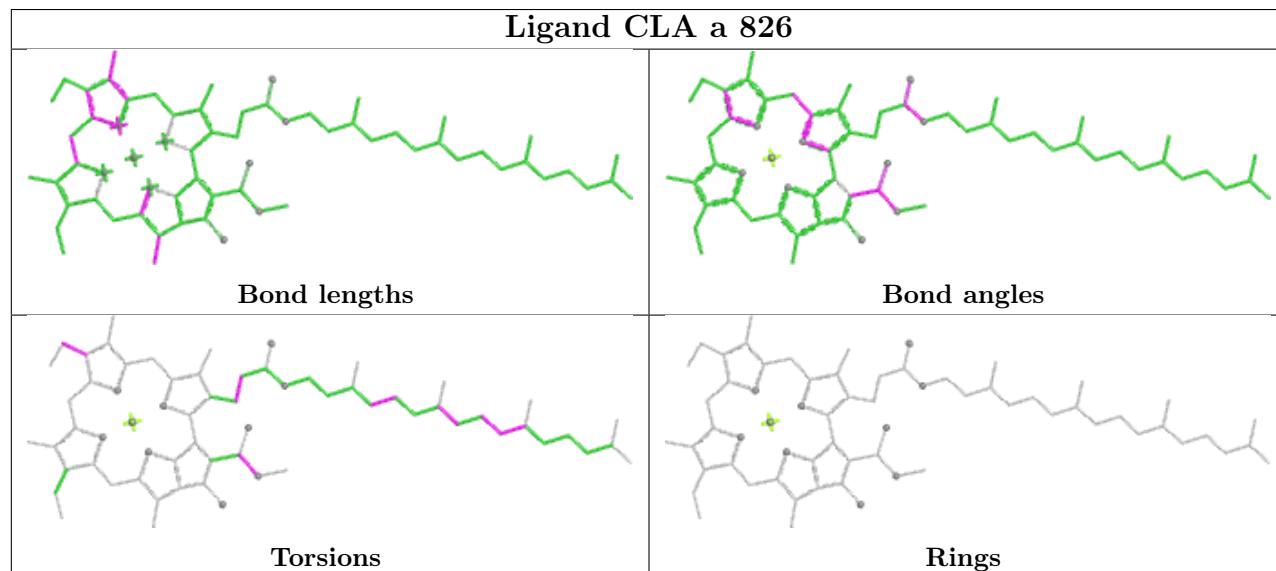


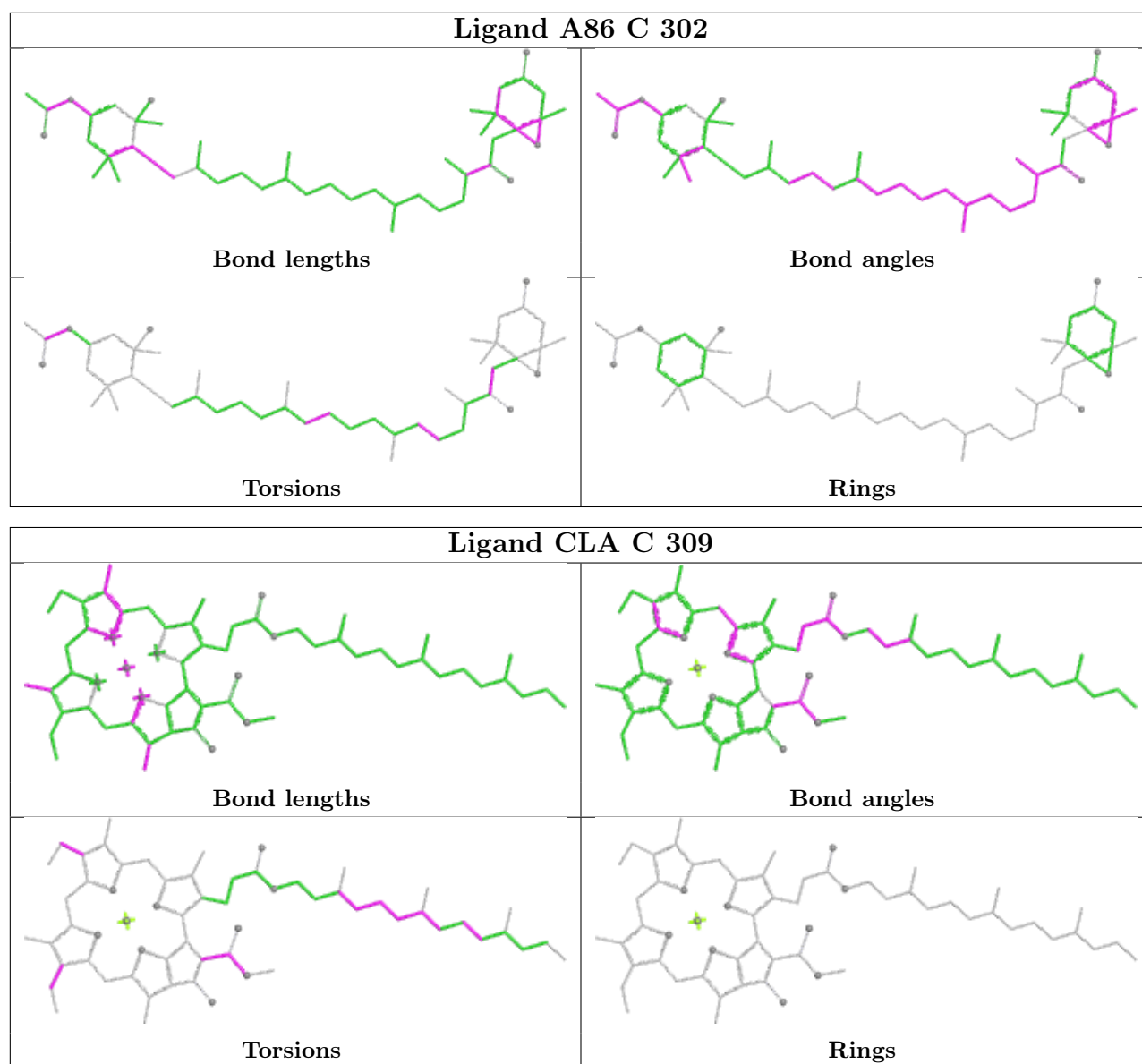
Ligand LHG a 835

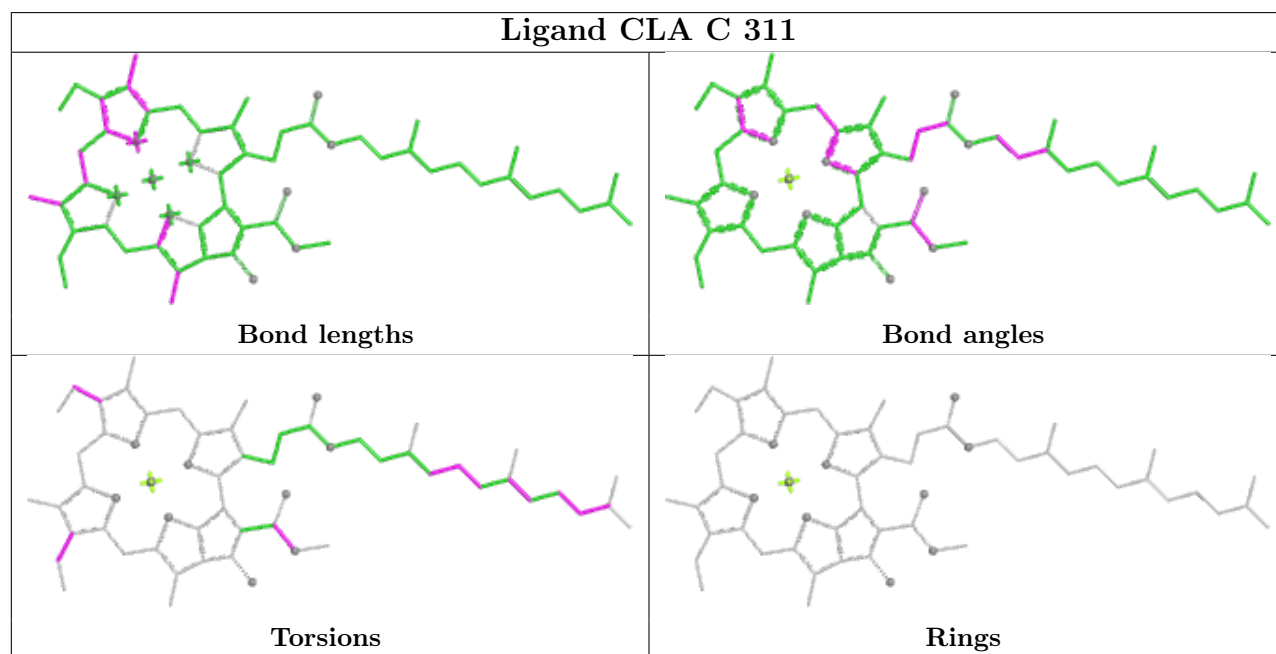
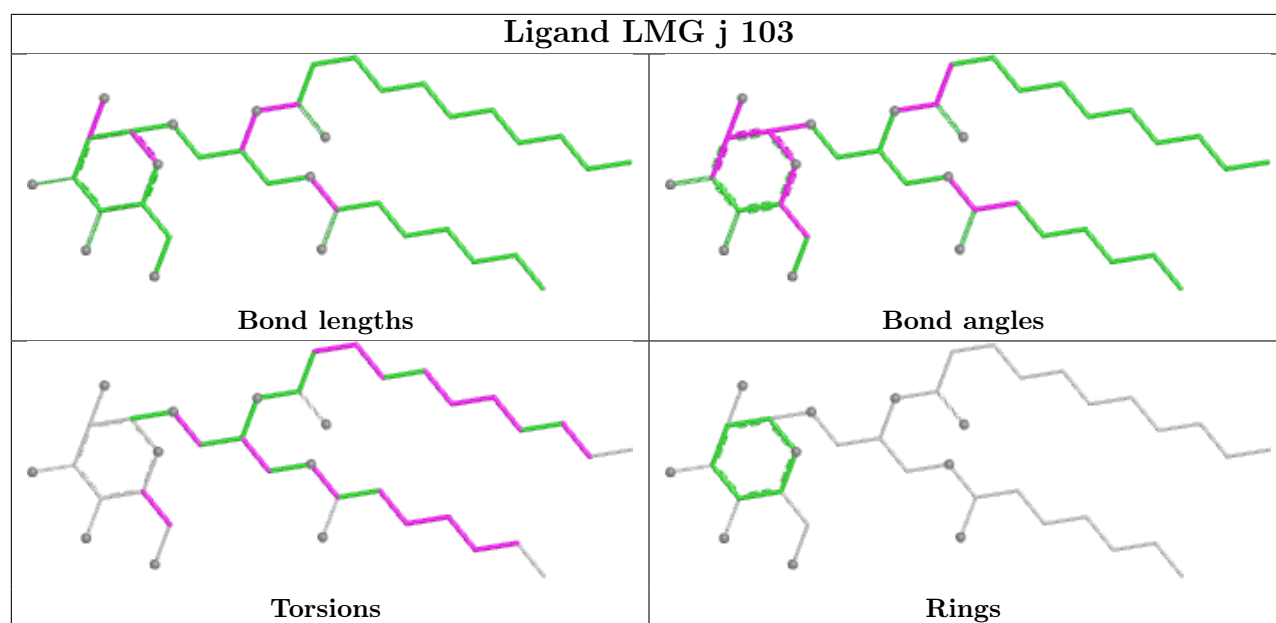


Ligand LMG a 851

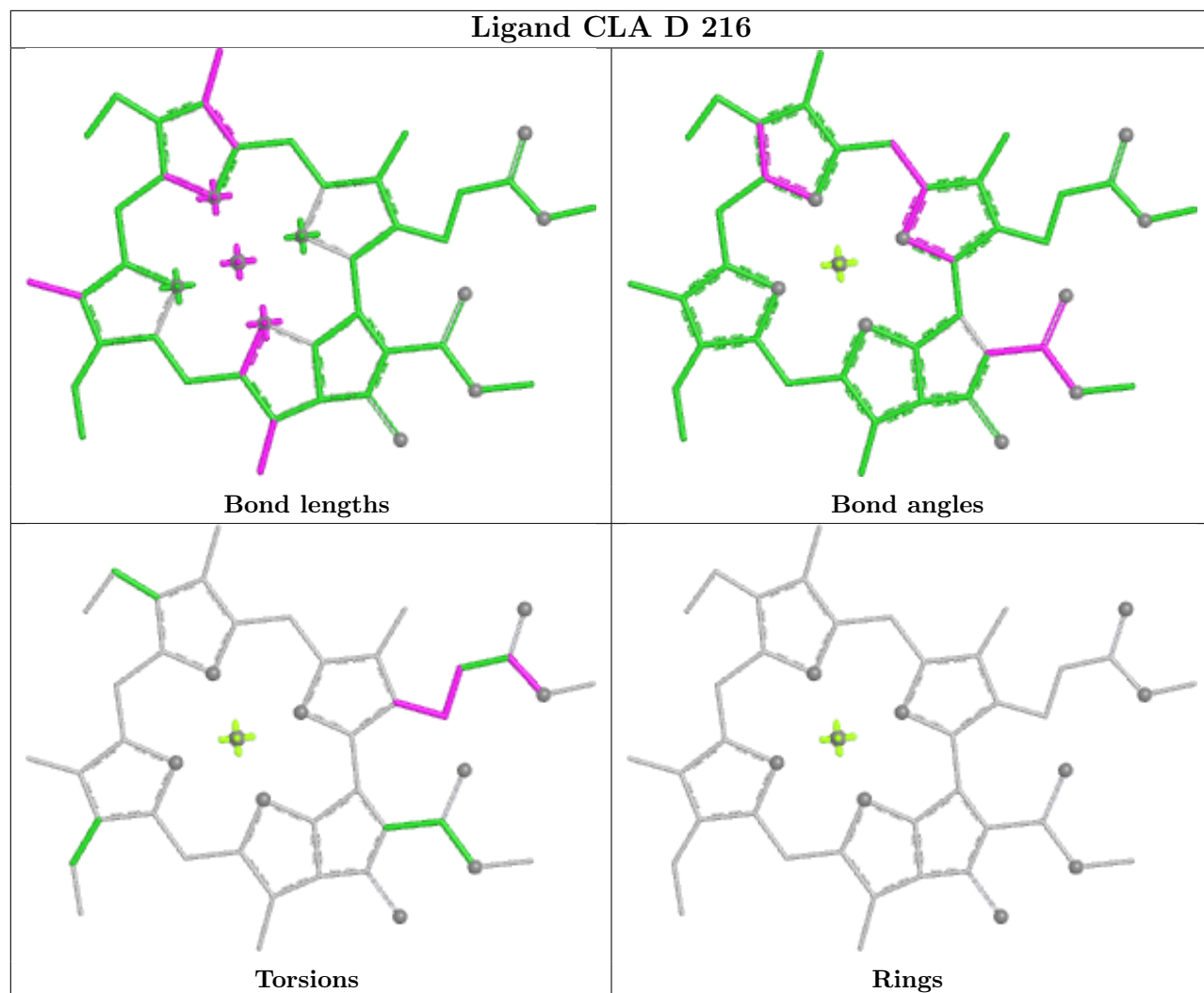


Ligand CLA b 807**Ligand CLA a 813****Ligand CLA a 826**

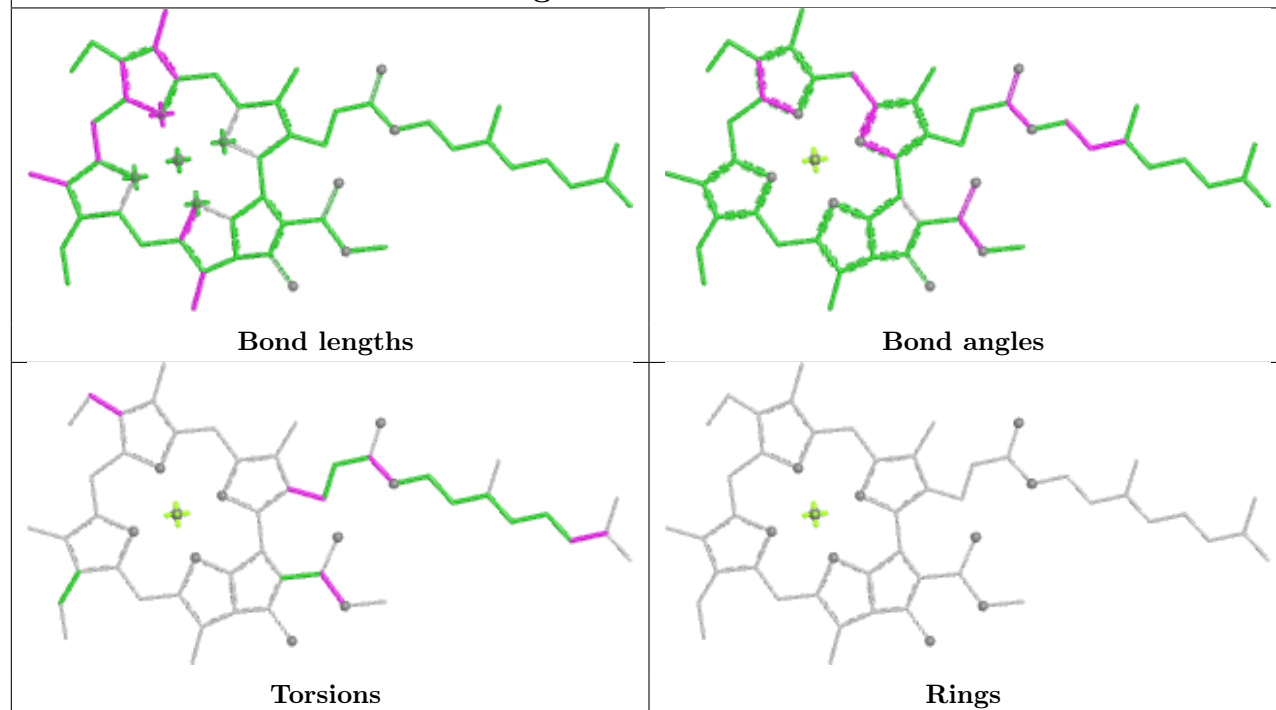




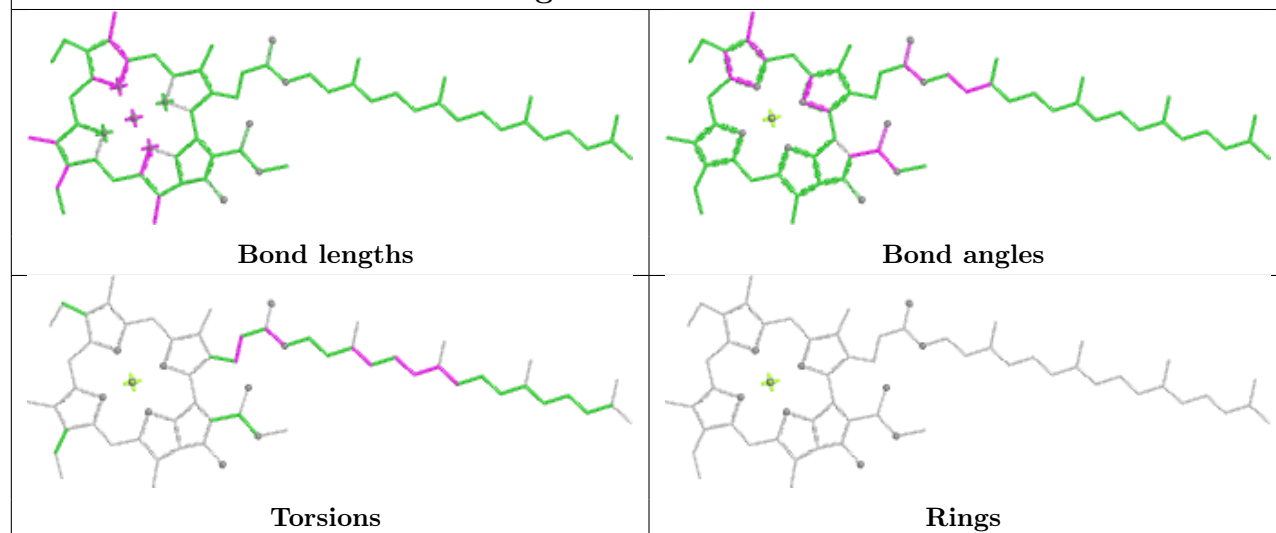
Ligand CLA D 216



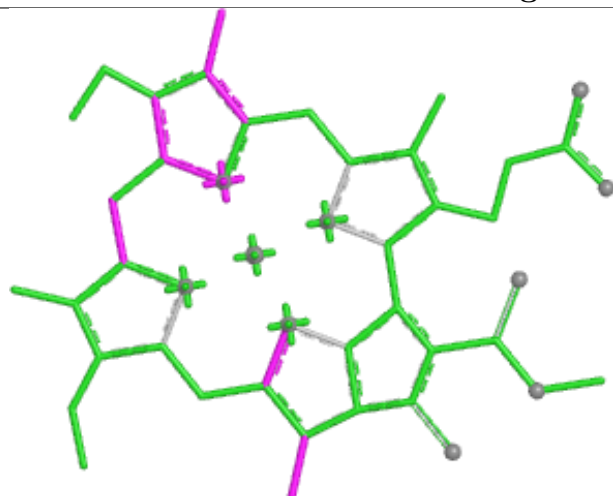
Ligand CLA E 313



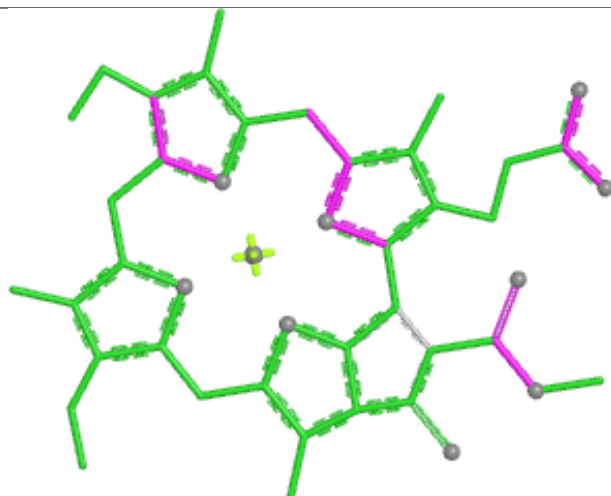
Ligand CLA b 801



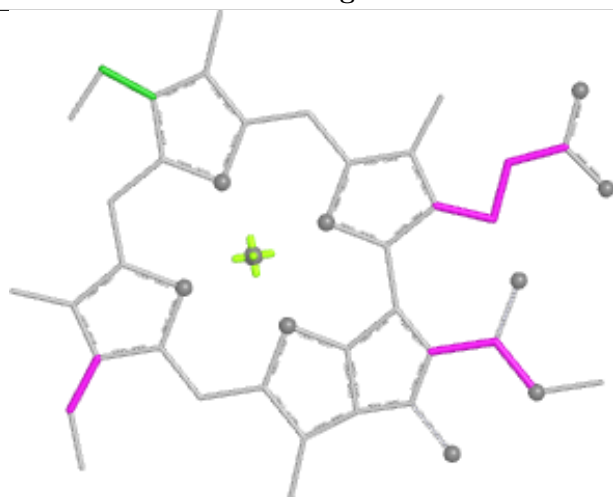
Ligand CLA r 202



Bond lengths



Bond angles

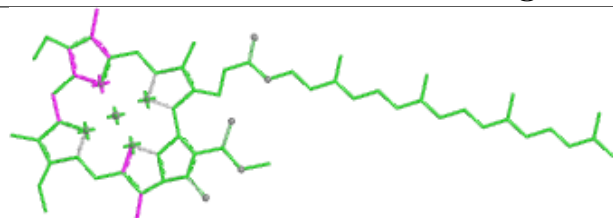


Torsions

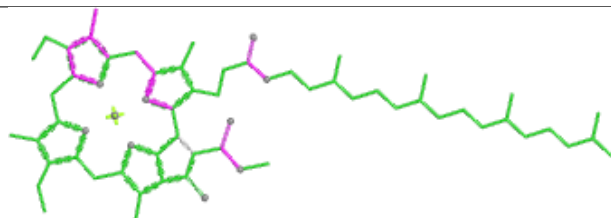


Rings

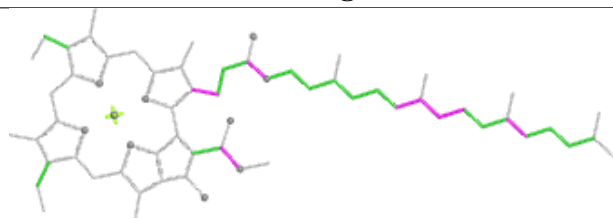
Ligand CLA a 855



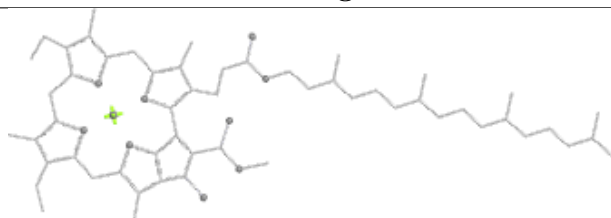
Bond lengths



Bond angles

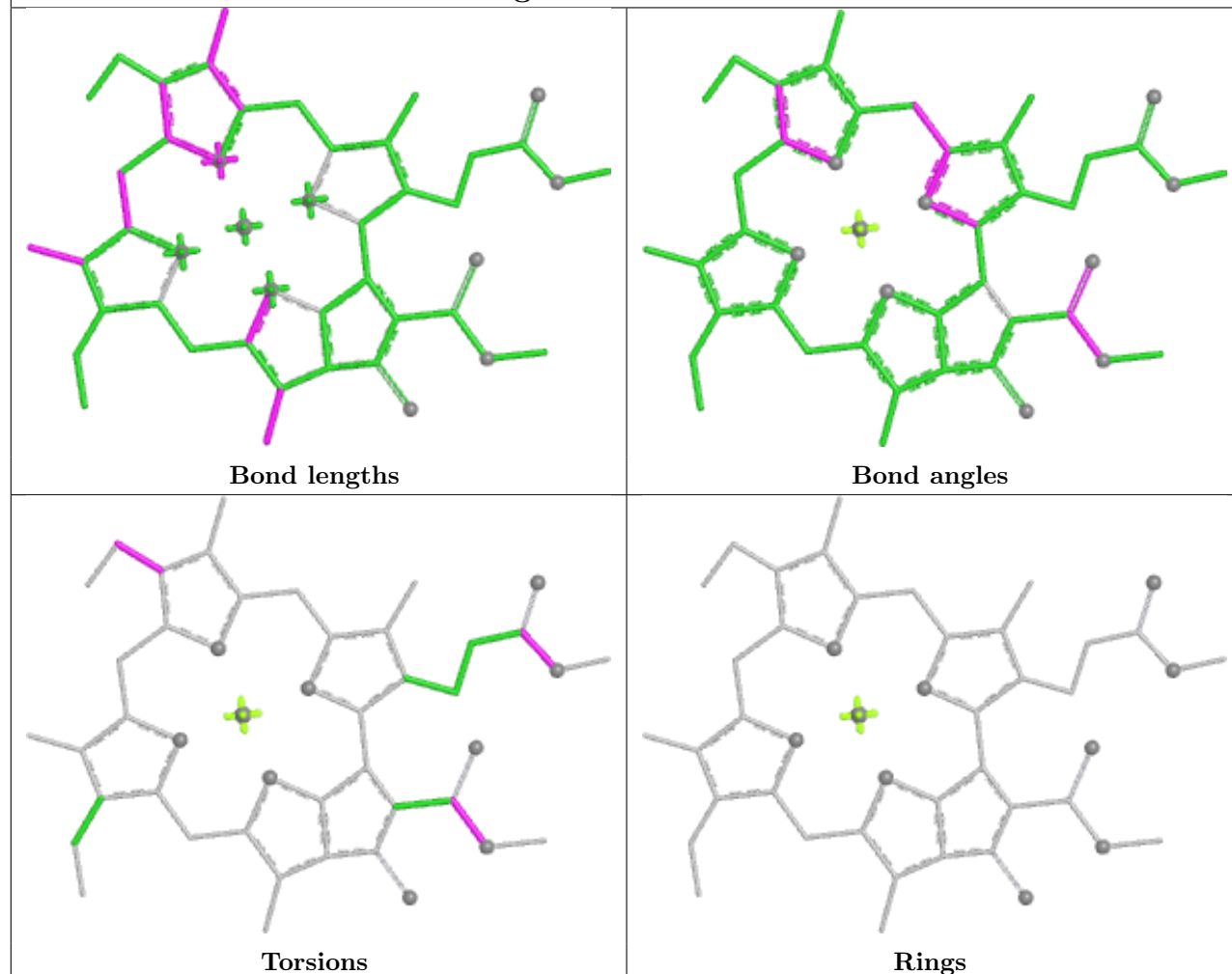


Torsions

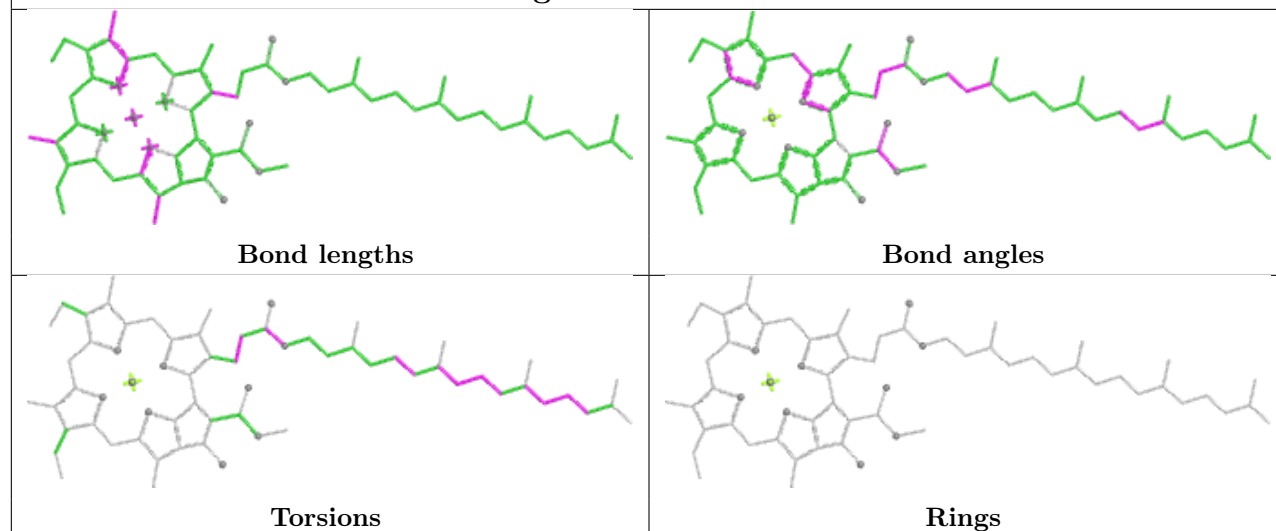


Rings

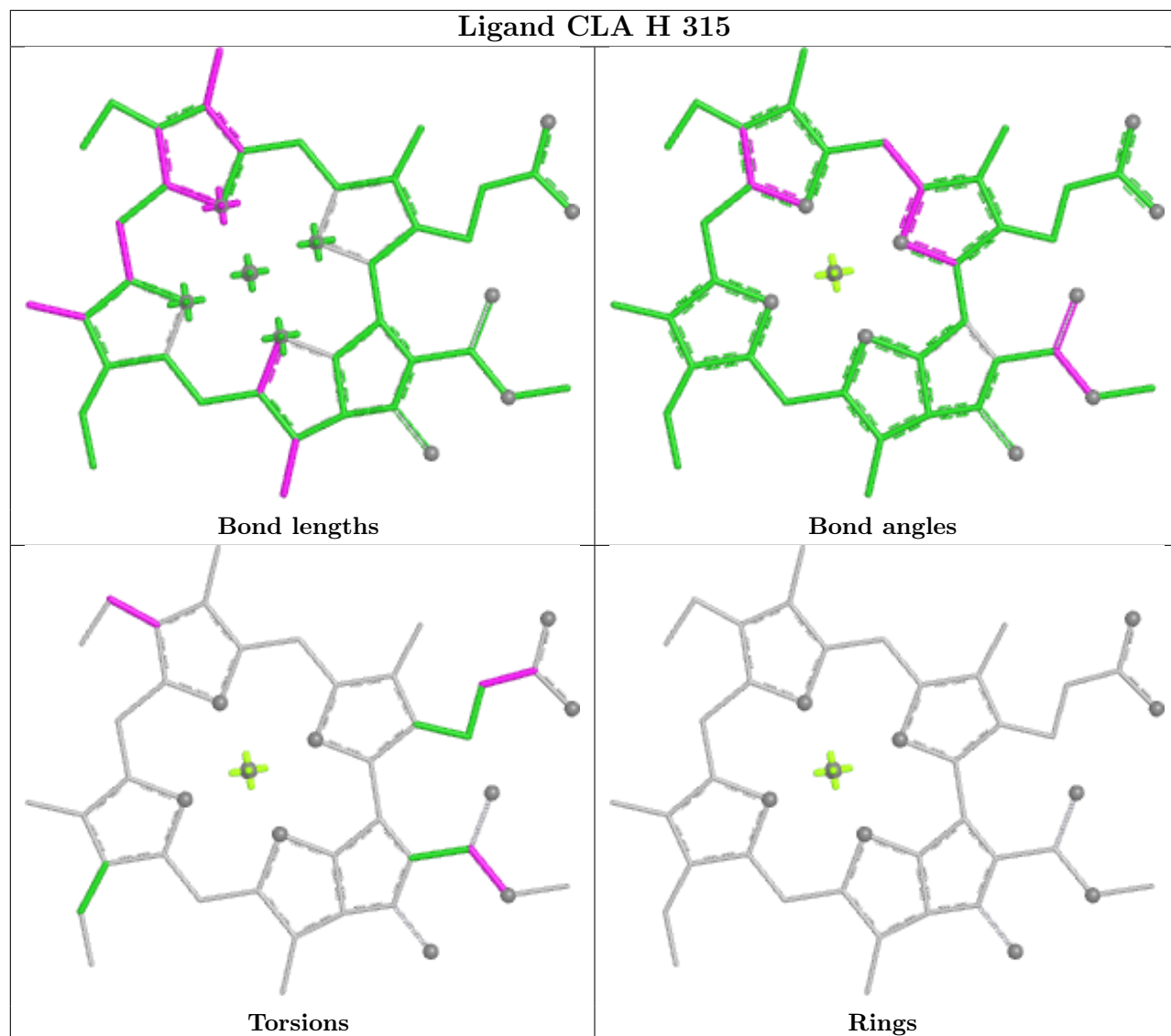
Ligand CLA B 310



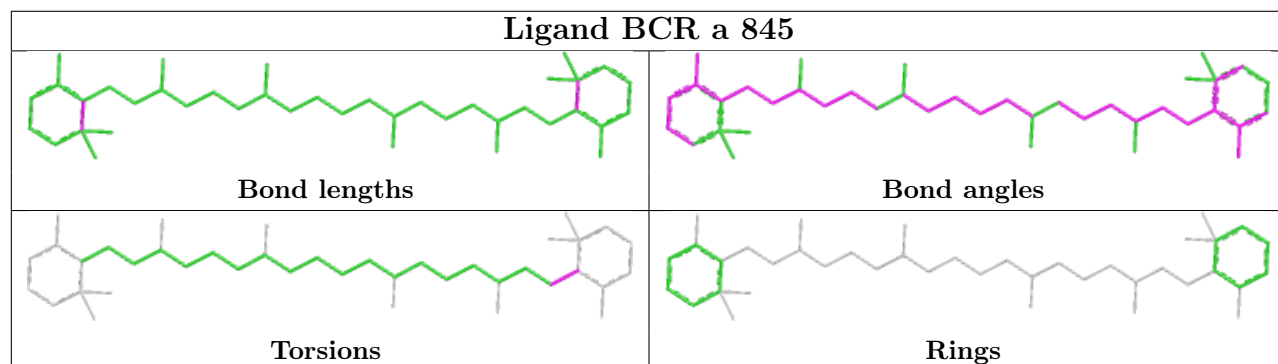
Ligand CLA E 312

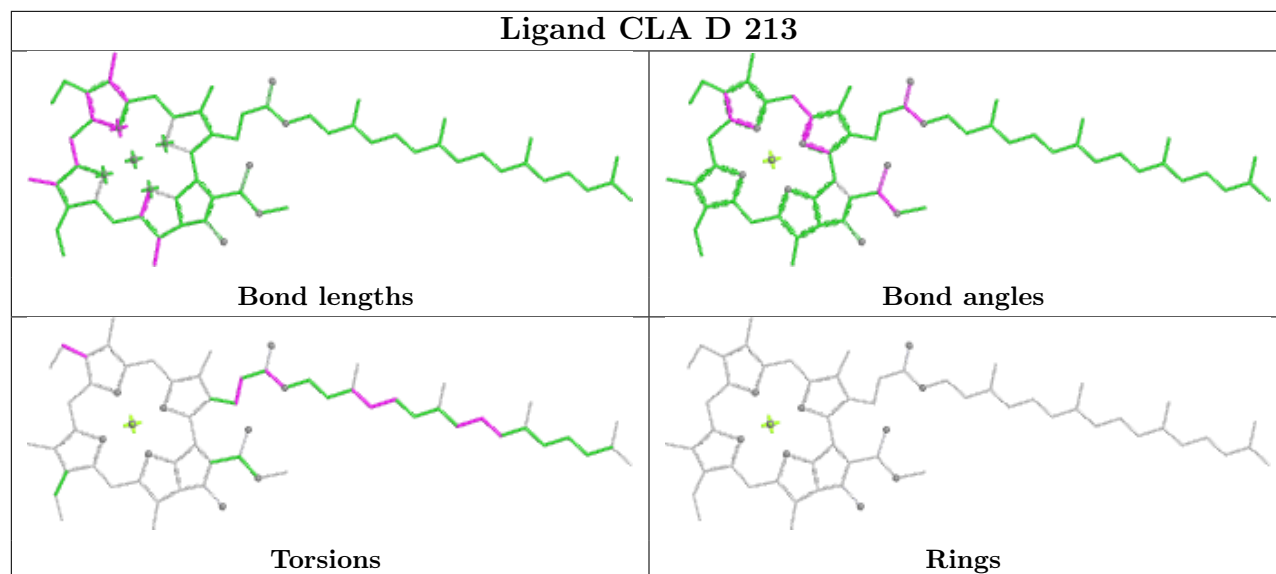
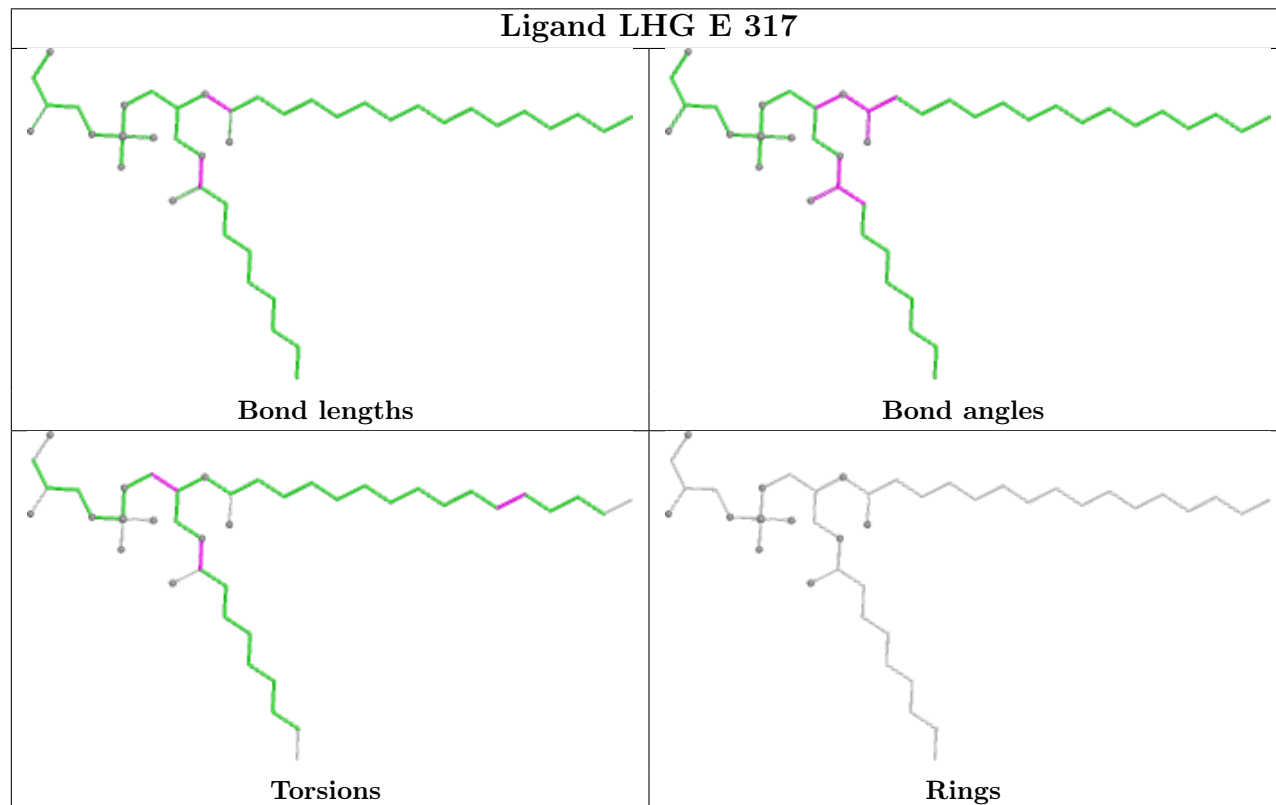


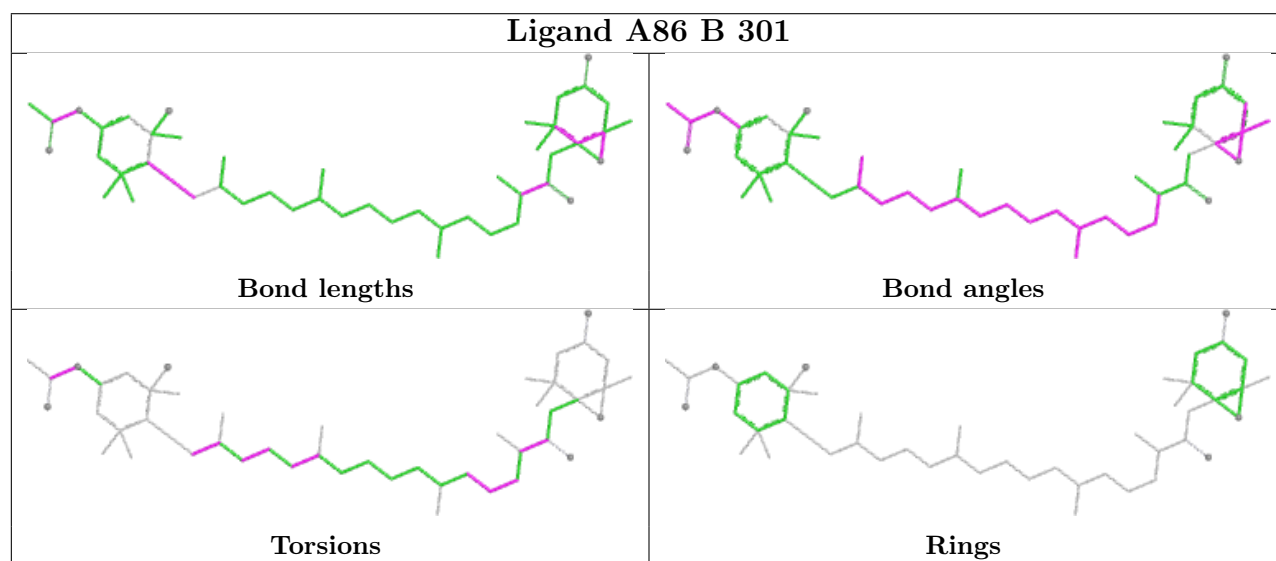
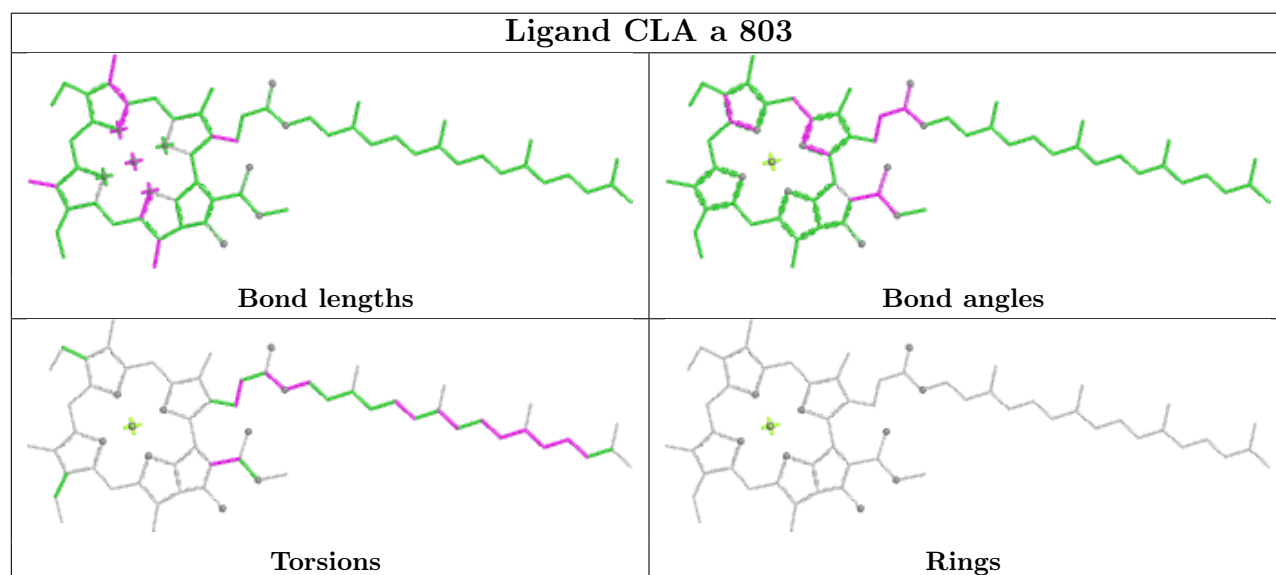
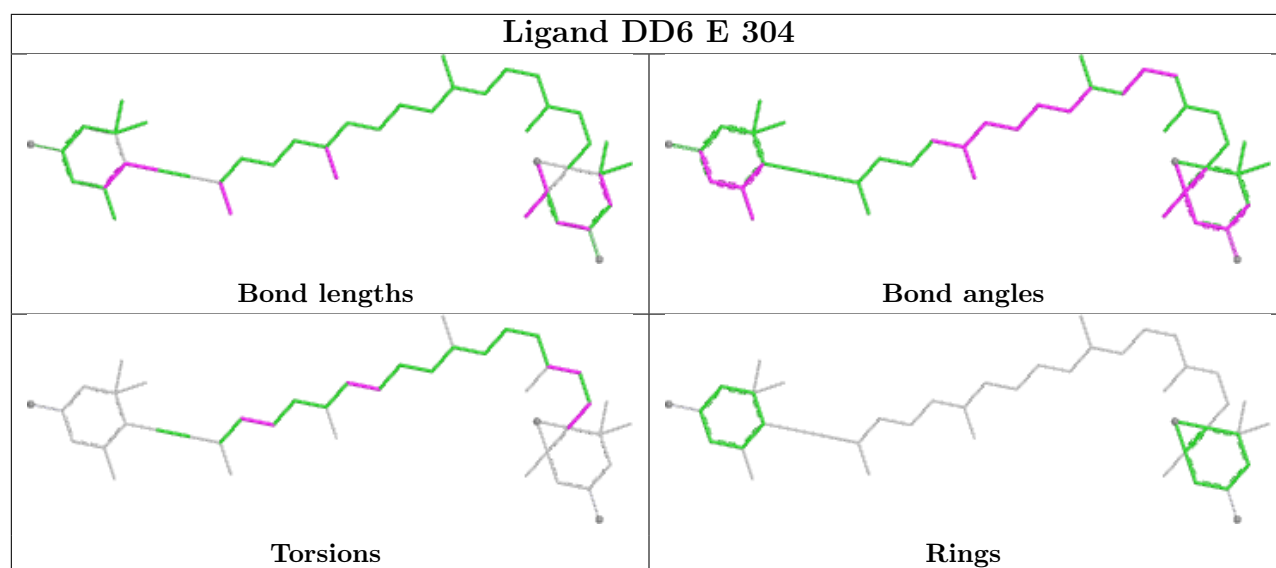
Ligand CLA H 315



Ligand BCR a 845



Ligand CLA D 213**Ligand LHG E 317**



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.

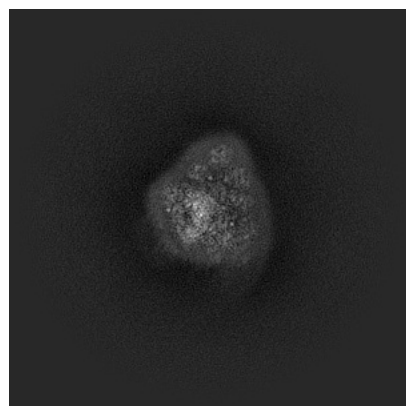
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60044. These allow visual inspection of the internal detail of the map and identification of artifacts.

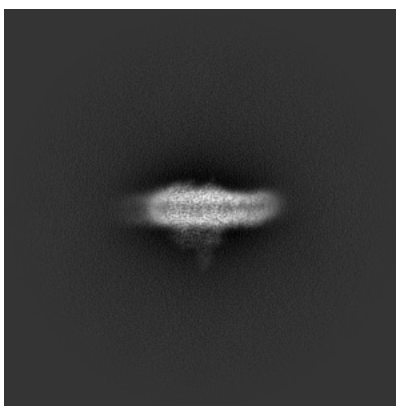
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

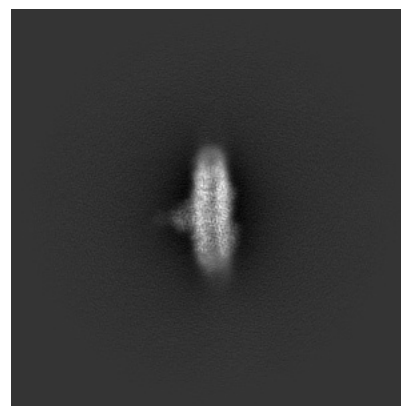
6.1.1 Primary map



X

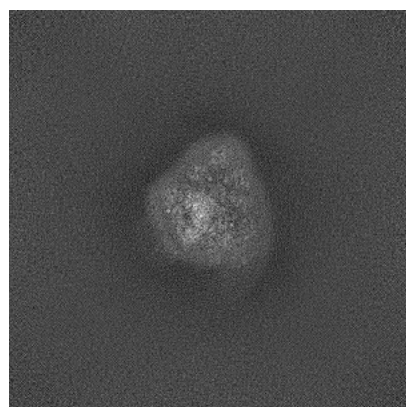


Y

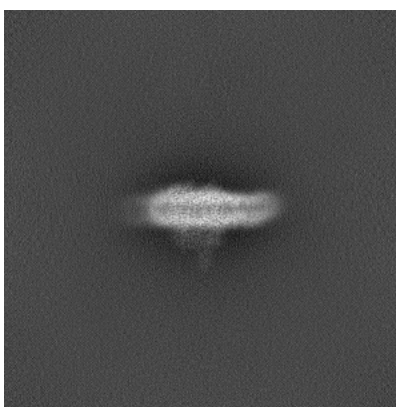


Z

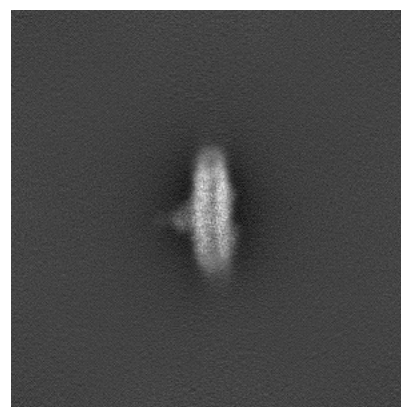
6.1.2 Raw map



X



Y

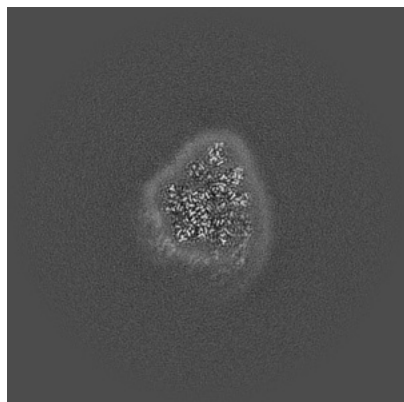


Z

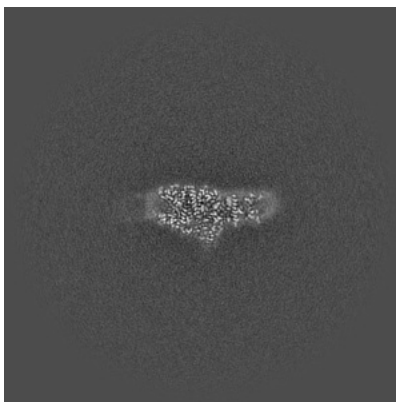
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

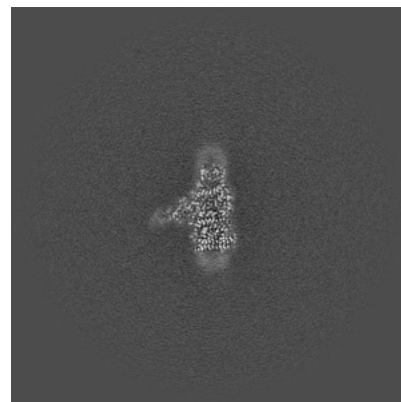
6.2.1 Primary map



X Index: 256

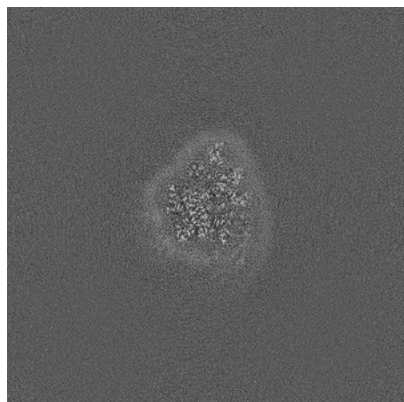


Y Index: 256

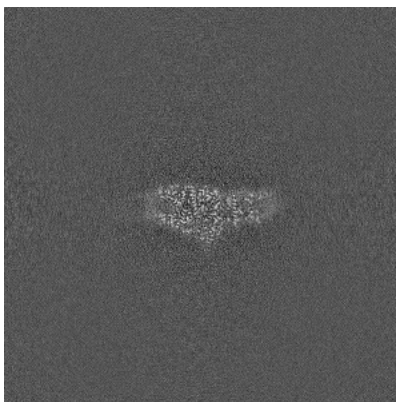


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

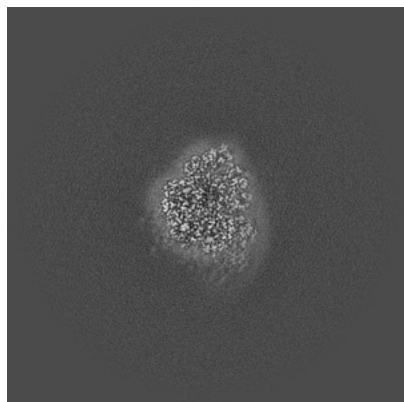


Z Index: 256

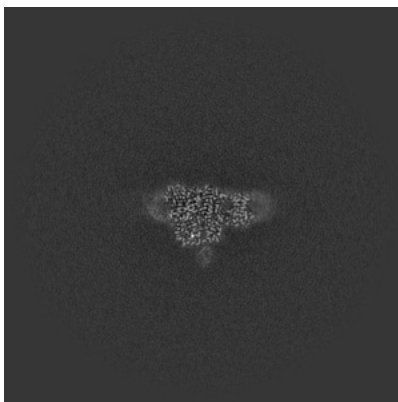
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

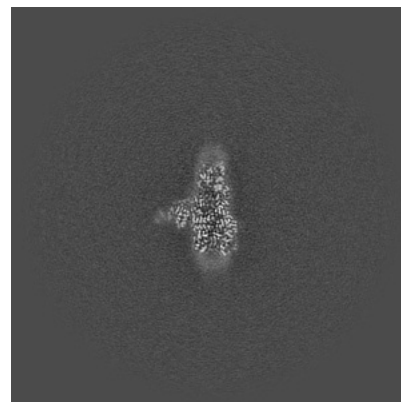
6.3.1 Primary map



X Index: 244

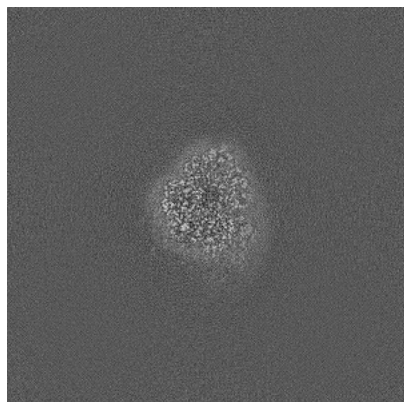


Y Index: 240

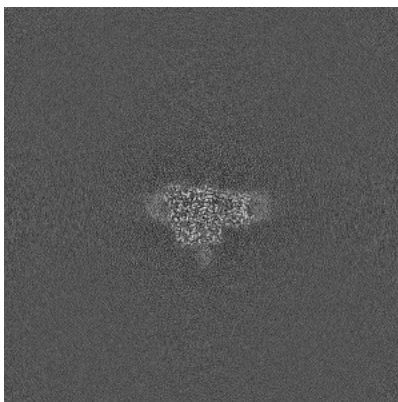


Z Index: 262

6.3.2 Raw map



X Index: 244



Y Index: 239

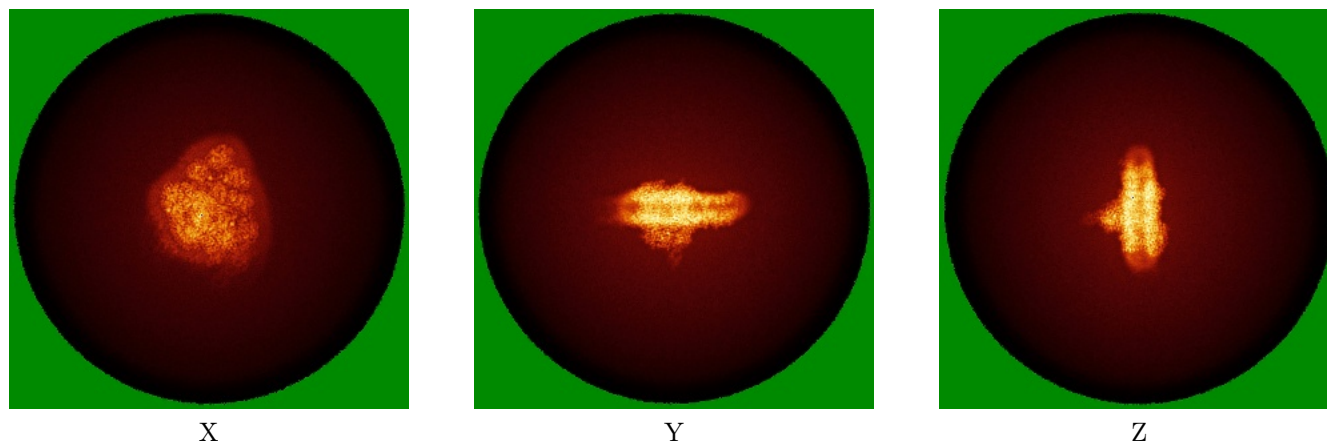


Z Index: 262

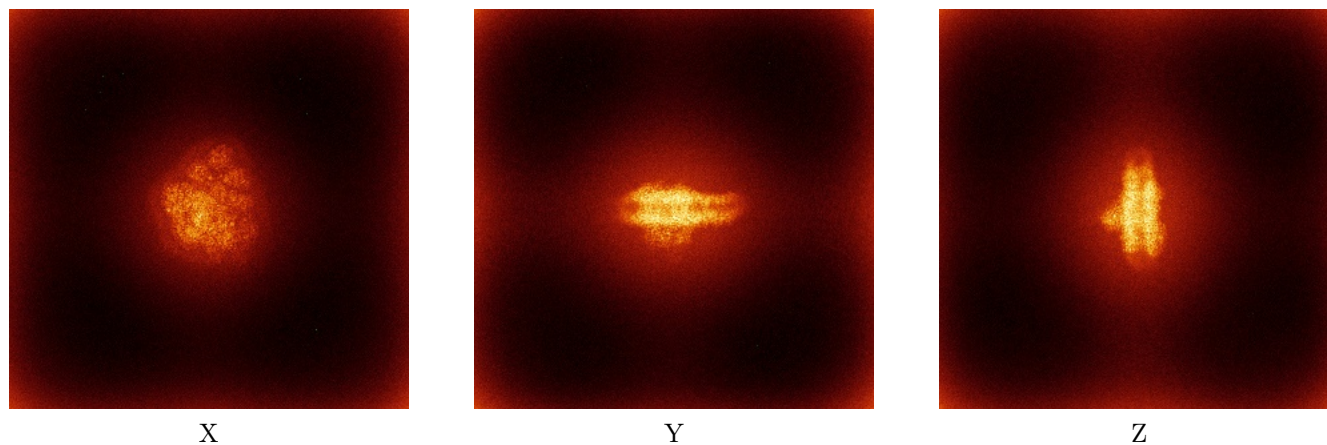
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



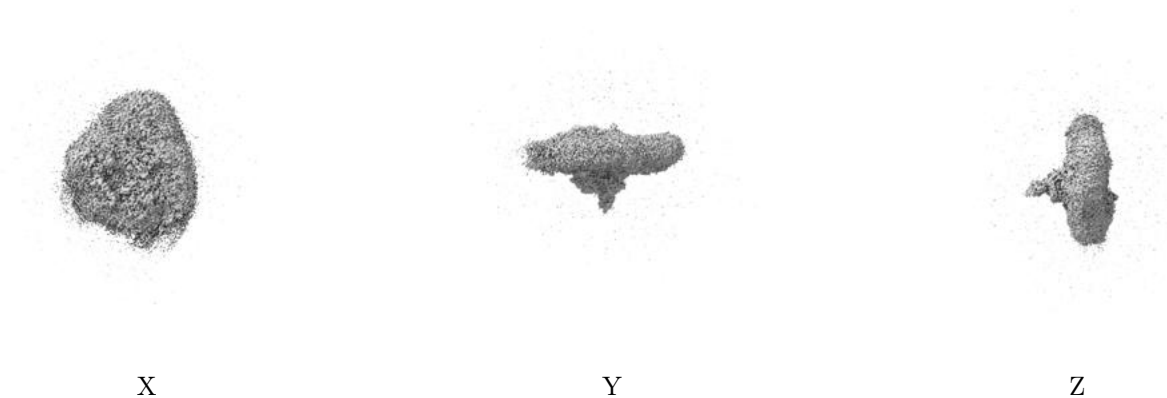
6.4.2 Raw map



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.

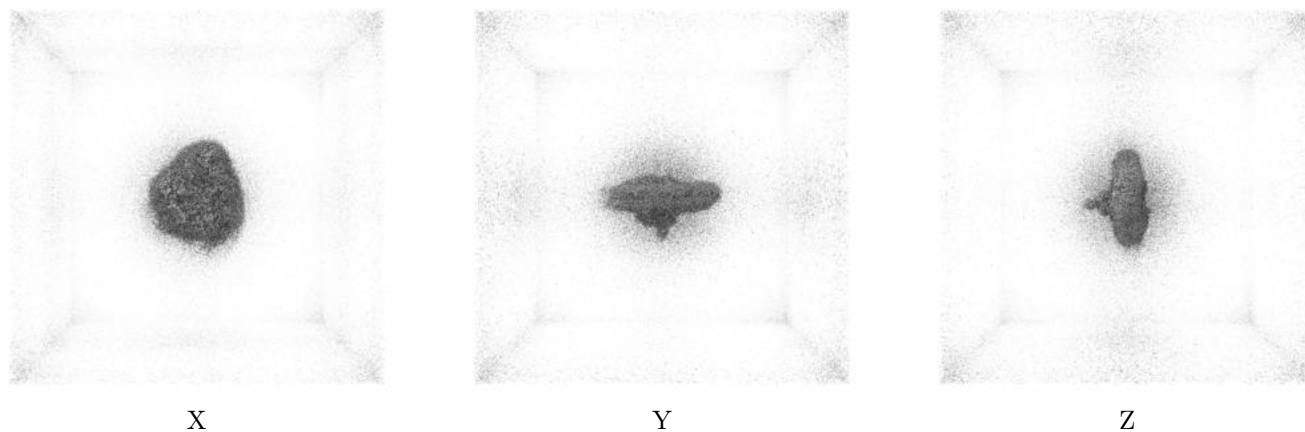
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

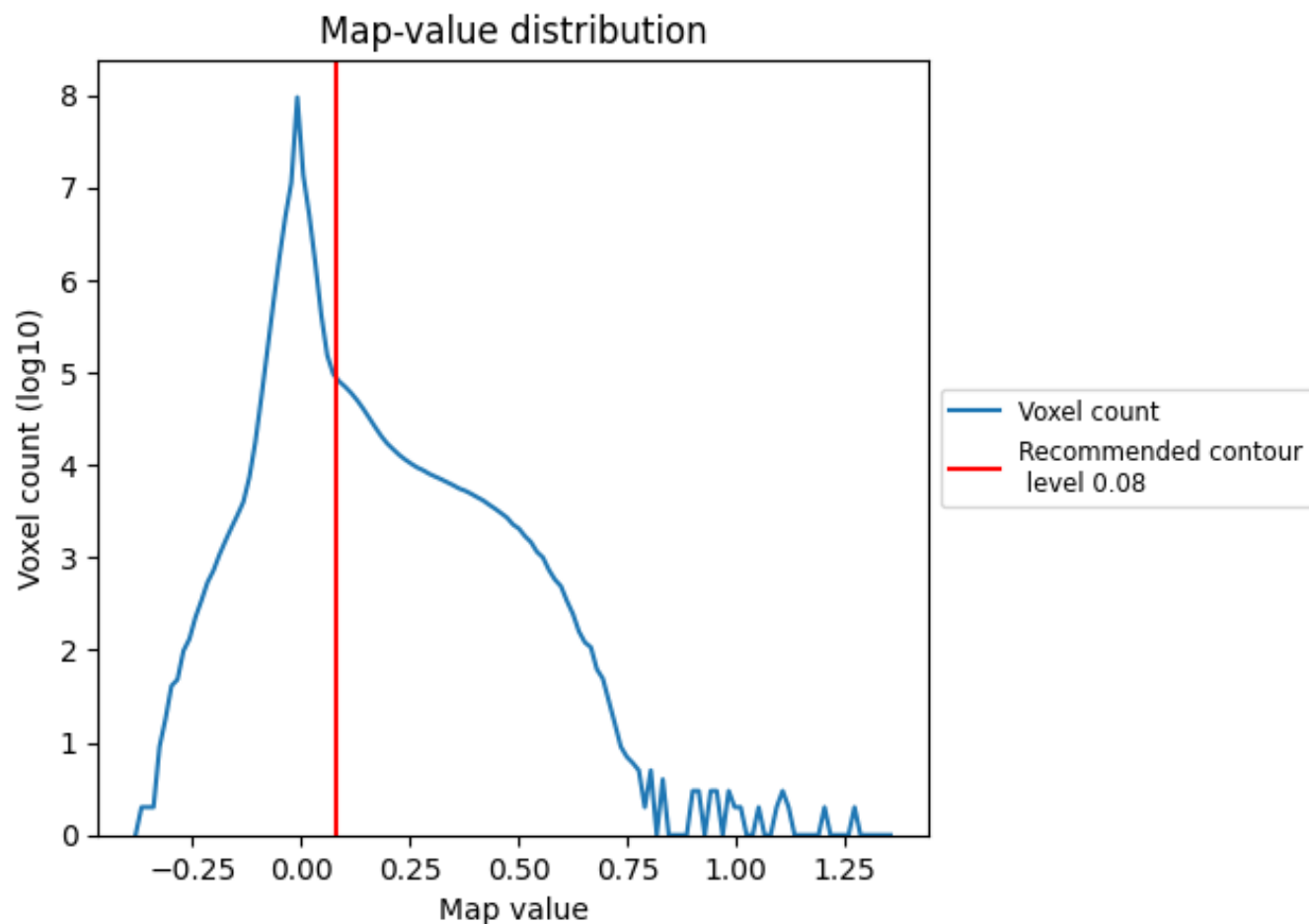
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

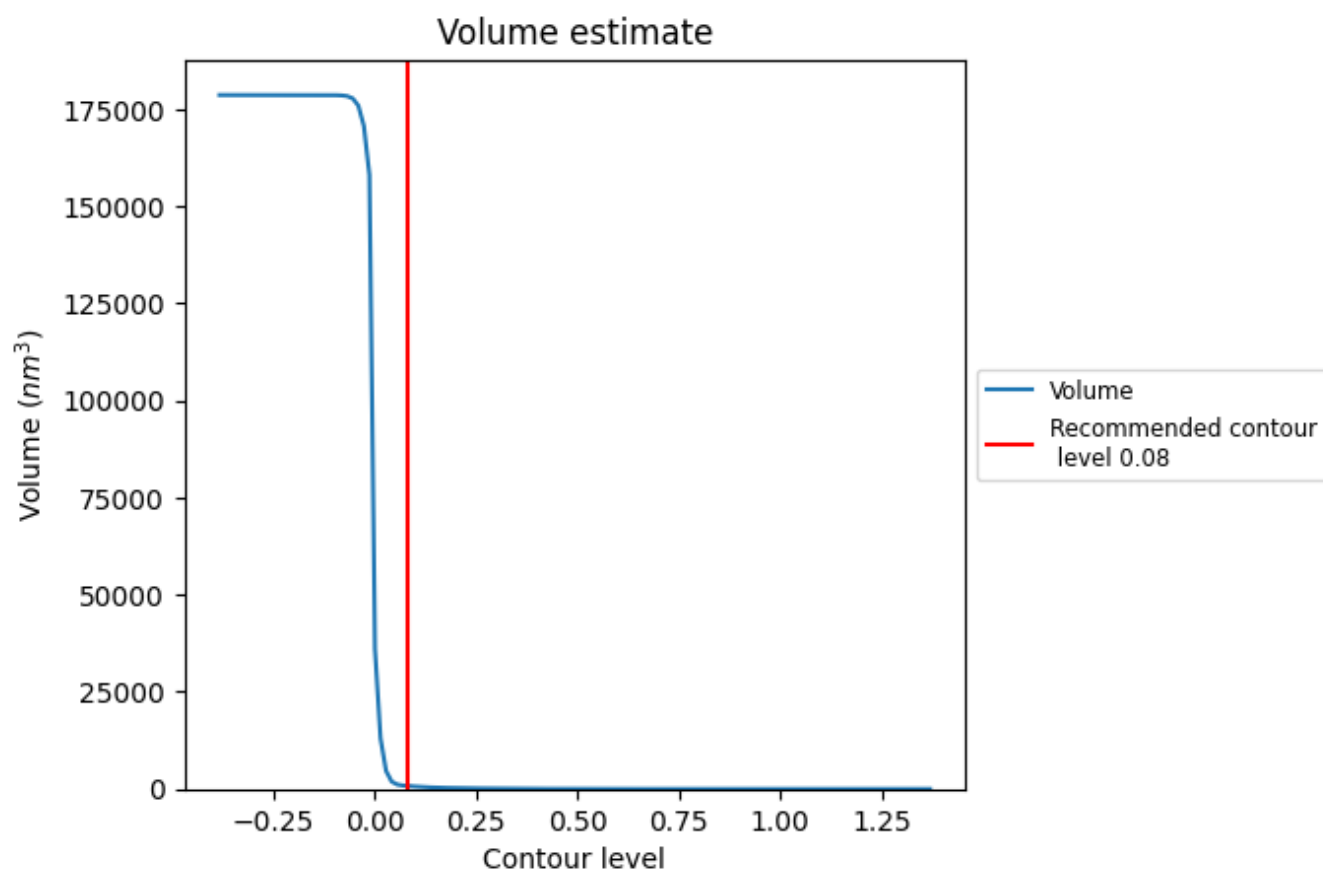
This section contains the results of statistical analysis of the map.

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.

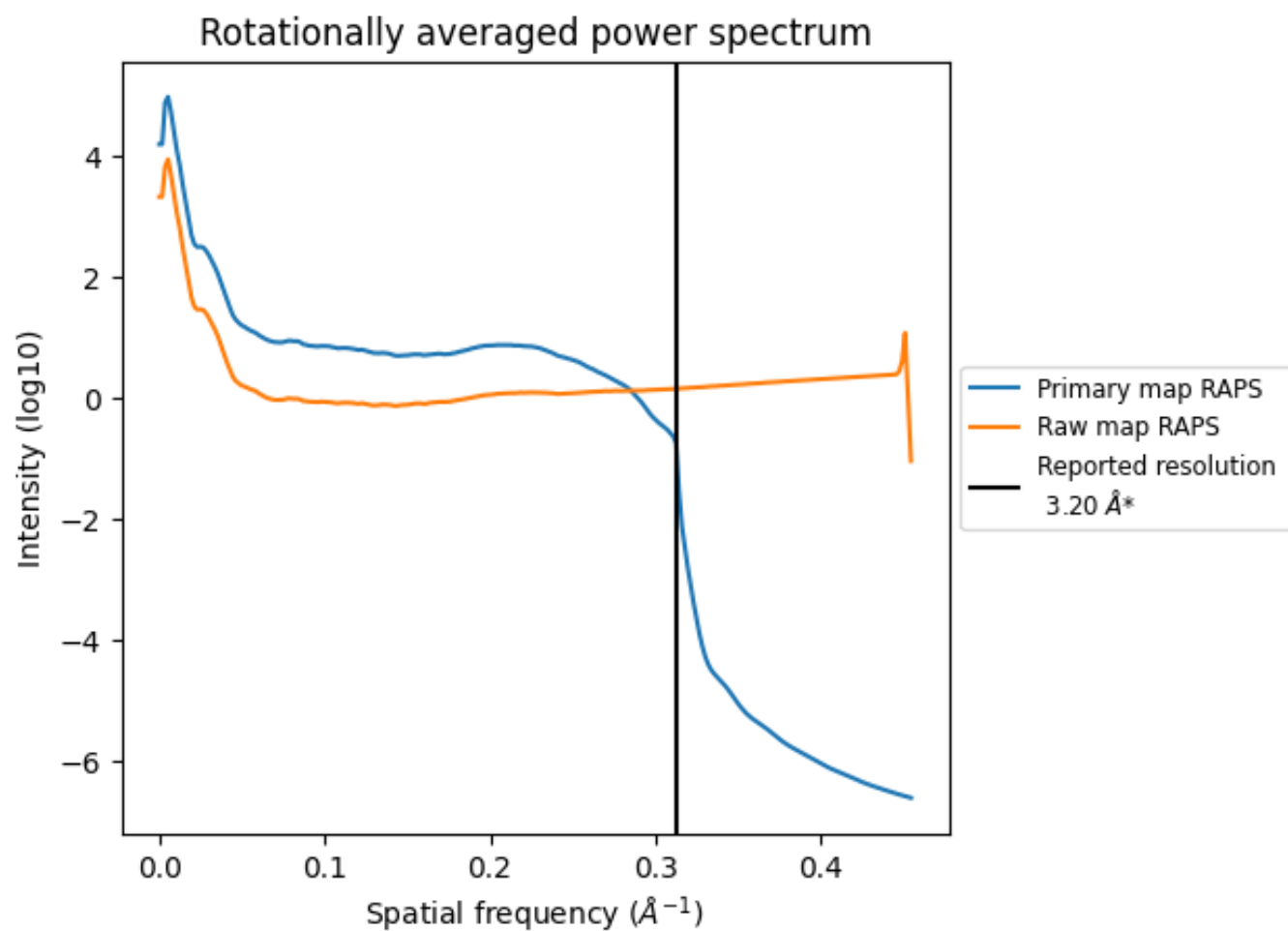
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 799 nm^3 ; this corresponds to an approximate mass of 722 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 ⓘ

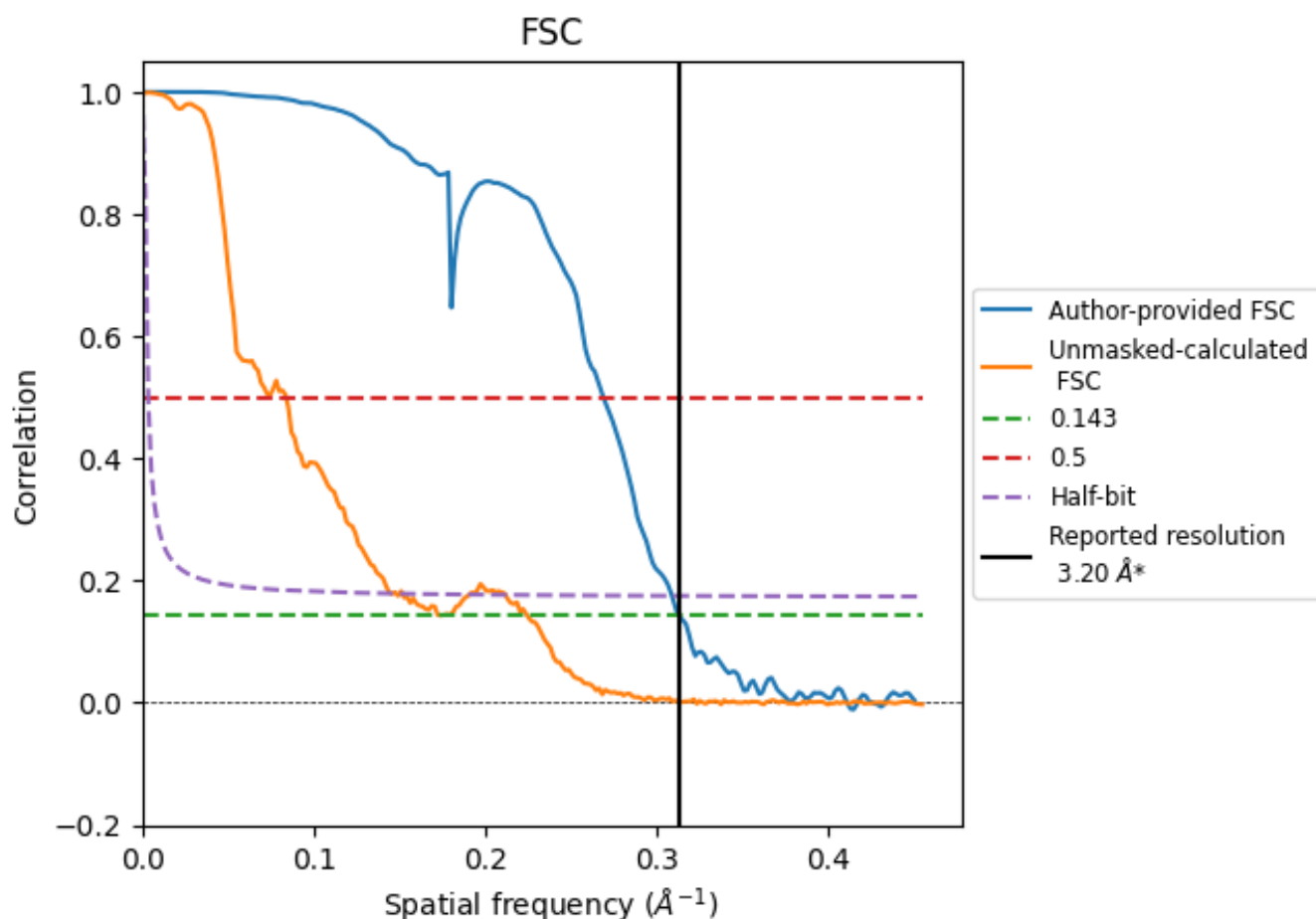


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

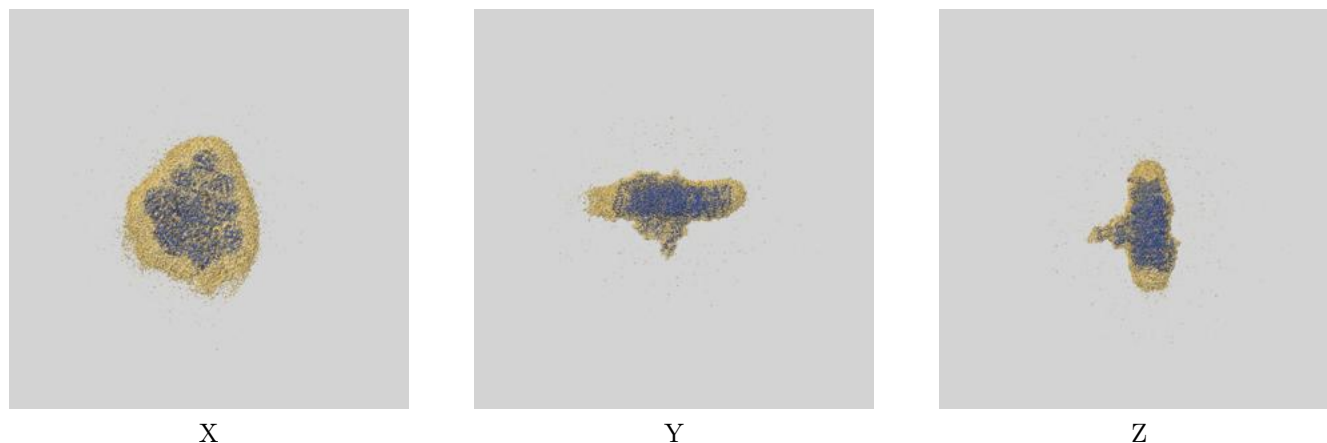
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.72	3.24
Unmasked-calculated*	5.75	11.93	6.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.75 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

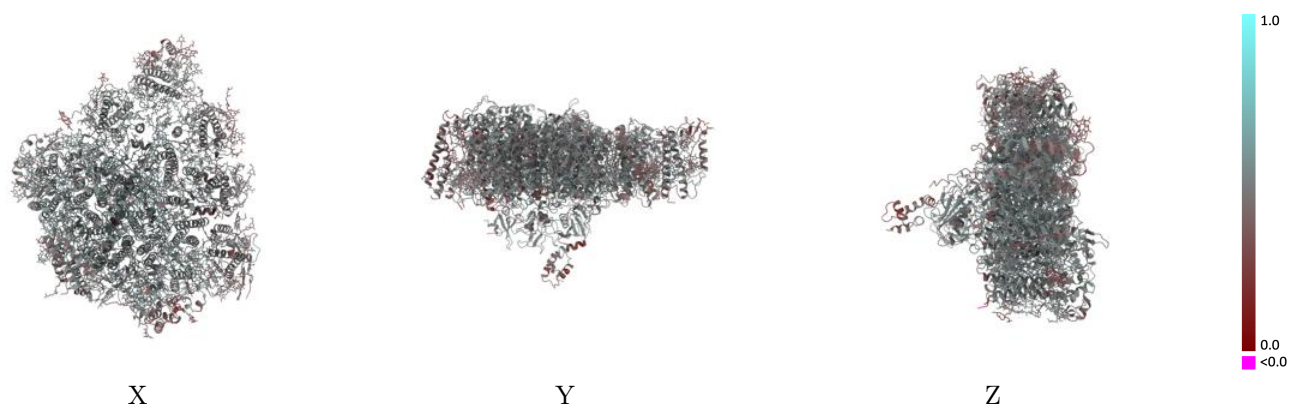
This section contains information regarding the fit between EMDB map EMD-60044 and PDB model 8ZET. Per-residue inclusion information can be found in [section 3](#) on [page 27](#).

9.1 Map-model overlay [i](#)



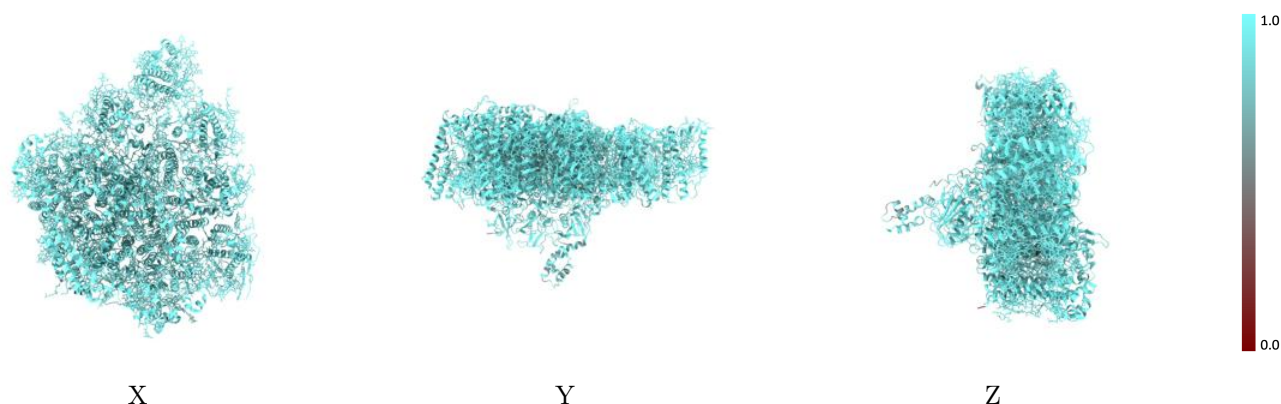
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



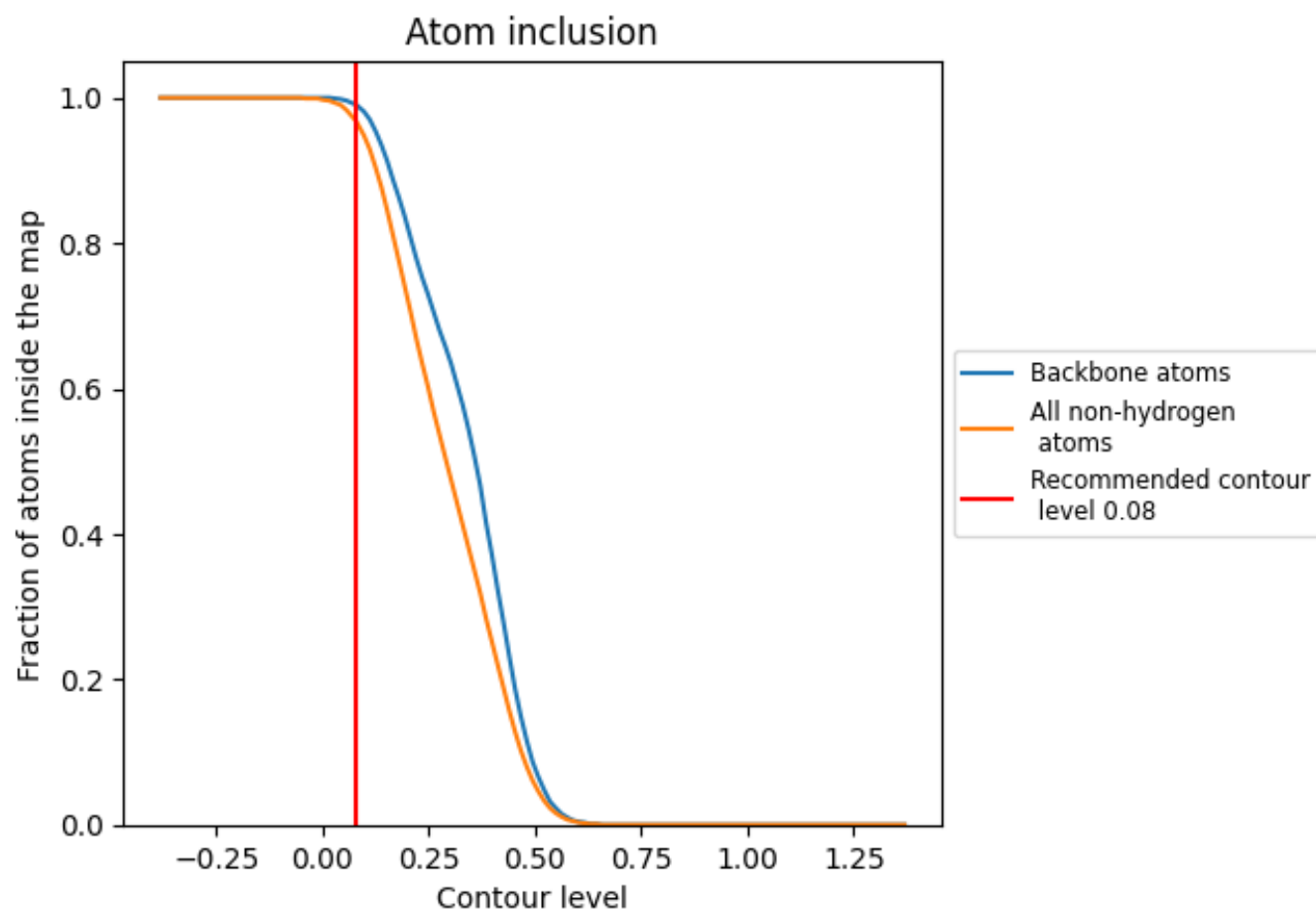
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 97% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9670	0.4850
B	0.9740	0.4570
C	0.9780	0.4520
D	0.9670	0.4720
E	0.9700	0.4710
H	0.9600	0.4360
a	0.9740	0.5120
b	0.9690	0.5060
c	0.9880	0.5100
d	0.9790	0.5070
e	0.9510	0.4720
f	0.9650	0.4760
g	0.8680	0.4000
i	0.9640	0.5130
j	0.9490	0.4710
l	0.9770	0.5060
m	0.9440	0.4770
r	0.9330	0.3970

