



wwPDB EM Validation Summary Report ⓘ

Apr 24, 2025 – 12:34 PM JST

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.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

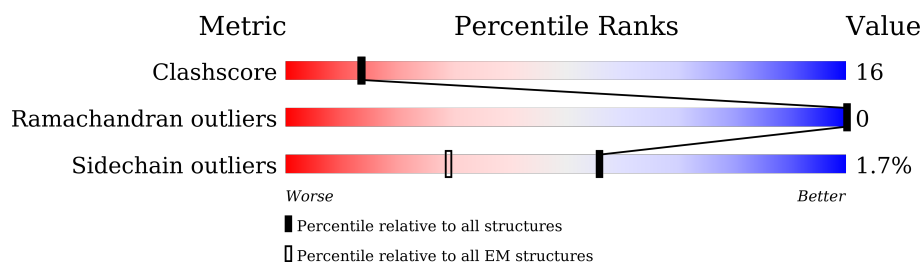
1 Overall quality at a glance

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.




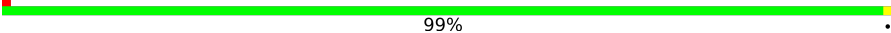
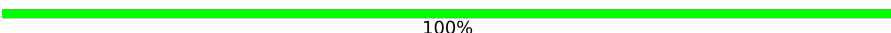
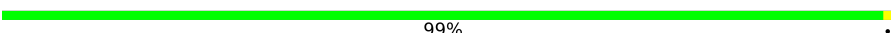





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	99% .
2	b	732	99% .
3	c	80	100%
4	d	132	98% .
5	e	62	95% 5%
6	f	160	99% .
7	g	131	97% .
8	i	33	100%

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Mol	Chain	Length	Quality of chain
9	j	40	 92% 8%
10	l	146	 99%
11	m	29	 100%
12	r	89	 99%
13	B	165	 68% 27% 5%
14	C	170	 67% 32%
15	D	164	 74% 24%
16	E	185	 74% 26%
17	H	168	 72% 28%

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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
18	CLA	r	202	X	-	-	-

2 Entry composition

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		

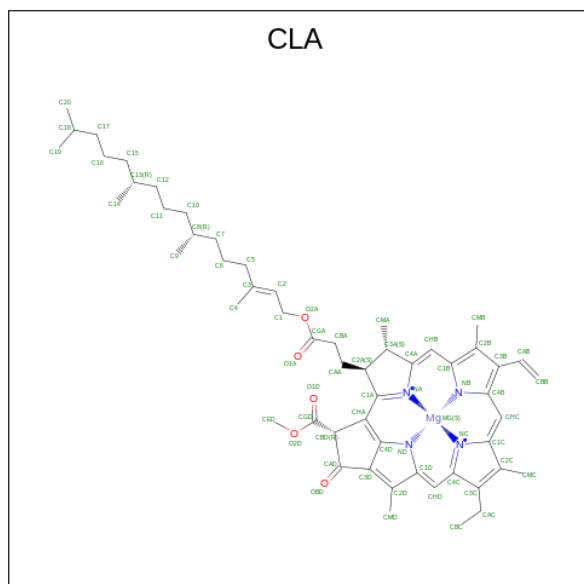
- Molecule 16 is a protein called Tp-RedCAP.

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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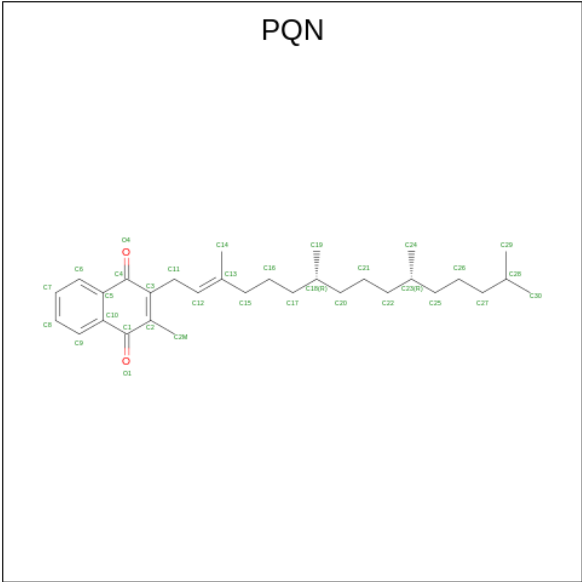
Mol	Chain	Residues	Atoms					AltConf
18	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	C	1	Total 61	C 51	Mg 1	N 4	O 5	0
18	C	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	C	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	C	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	C	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	C	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	D	1	Total 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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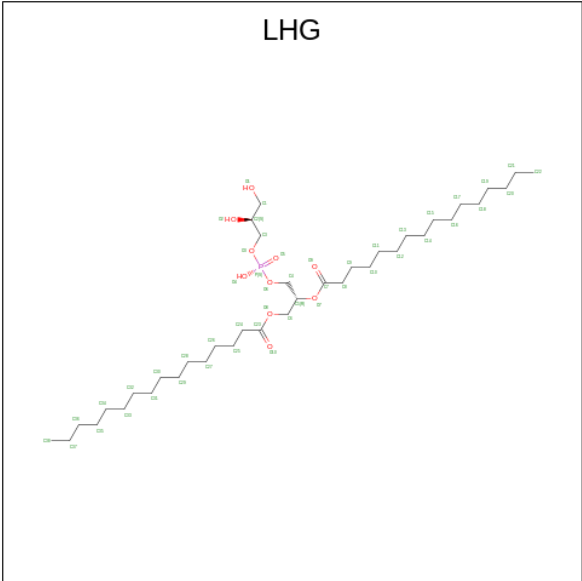
Mol	Chain	Residues	Atoms					AltConf
18	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	E	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	E	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	E	1	Total 56	C 46	Mg 1	N 4	O 5	0
18	H	1	Total 54	C 44	Mg 1	N 4	O 5	0
18	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	H	1	Total 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).



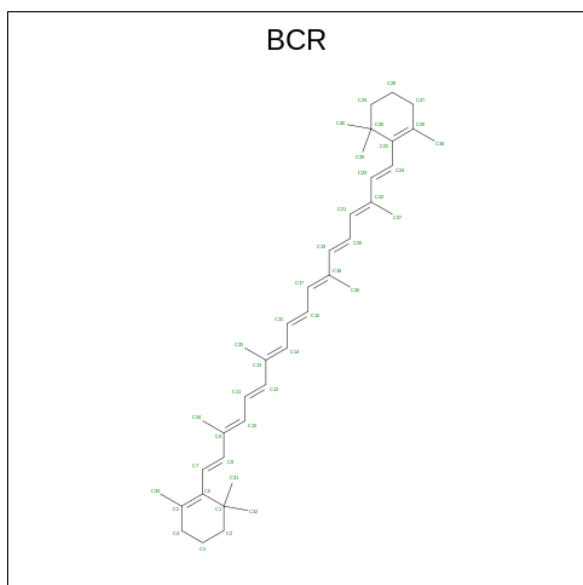
Mol	Chain	Residues	Atoms				AltConf
20	a	1	Total	C	O	P	0
			49	38	10	1	

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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).



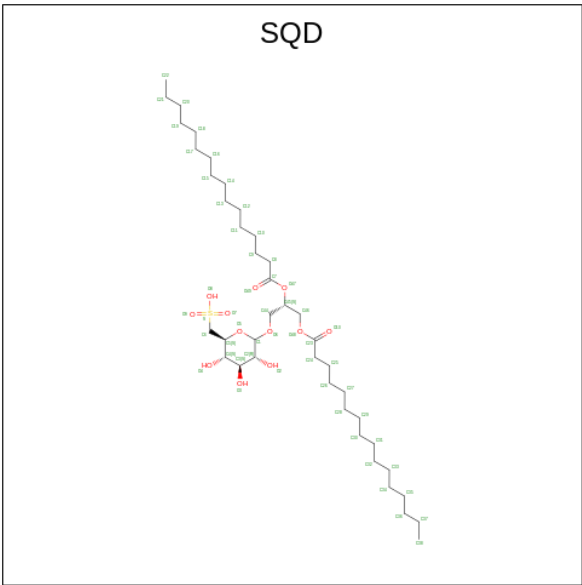
Mol	Chain	Residues	Atoms		AltConf
21	a	1	Total	C	0
			40	40	
21	a	1	Total	C	0
			40	40	

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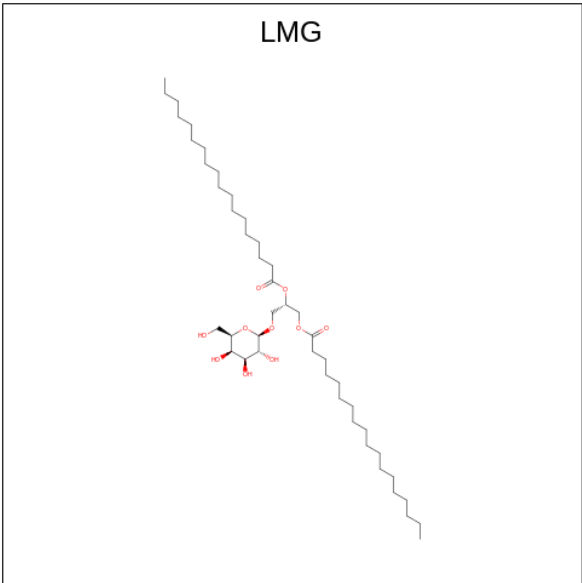
Mol	Chain	Residues	Atoms	AltConf
21	a	1	Total C 40 40	0
21	a	1	Total C 40 40	0
21	a	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	f	1	Total C 40 40	0
21	f	1	Total C 40 40	0
21	i	1	Total C 40 40	0
21	i	1	Total C 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).



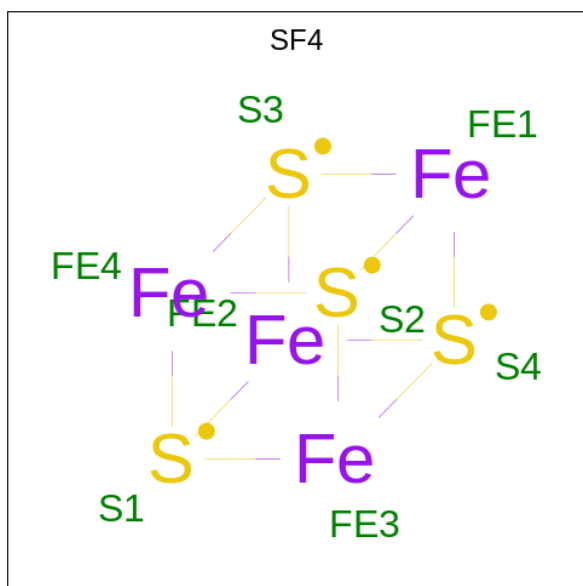
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	a	1	33	23	10	0
23	j	1	37	27	10	0

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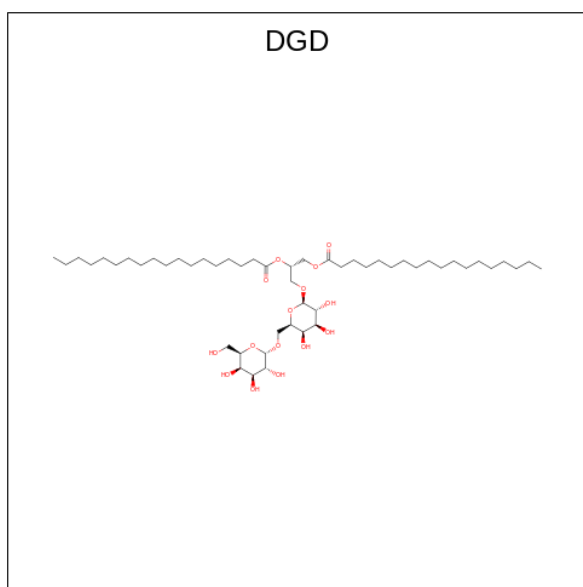
Mol	Chain	Residues	Atoms			AltConf
23	l	1	Total	C	O	0
			40	30	10	
23	C	1	Total	C	O	0
			31	21	10	
23	C	1	Total	C	O	0
			44	34	10	
23	D	1	Total	C	O	0
			46	36	10	
23	E	1	Total	C	O	0
			43	33	10	

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



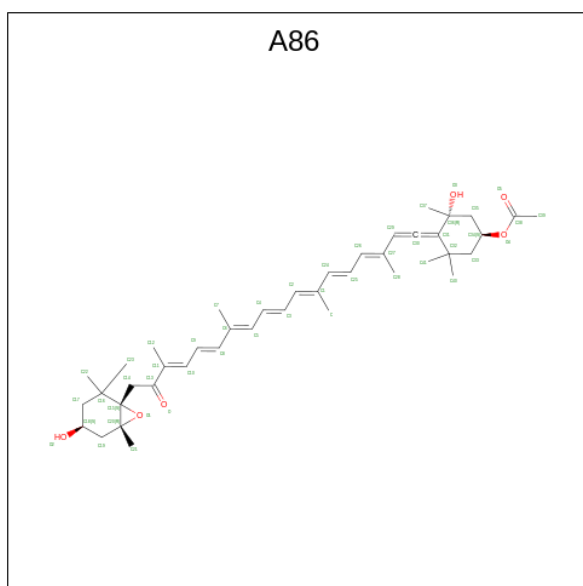
Mol	Chain	Residues	Atoms			AltConf
24	b	1	Total	Fe	S	0
			8	4	4	
24	c	1	Total	Fe	S	0
			8	4	4	
24	c	1	Total	Fe	S	0
			8	4	4	

- 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: $C_{42}H_{58}O_6$) (labeled as "Ligand of Interest" by depositor).



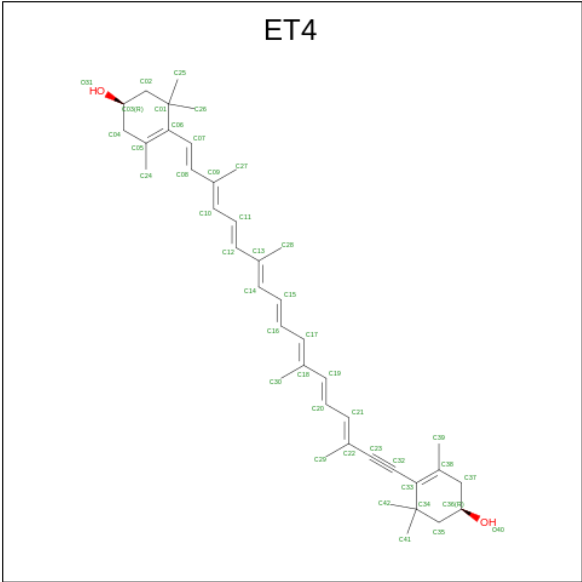
Mol	Chain	Residues	Atoms			AltConf
26	b	1	Total	C	O	0
			48	42	6	
26	m	1	Total	C	O	0
			48	42	6	

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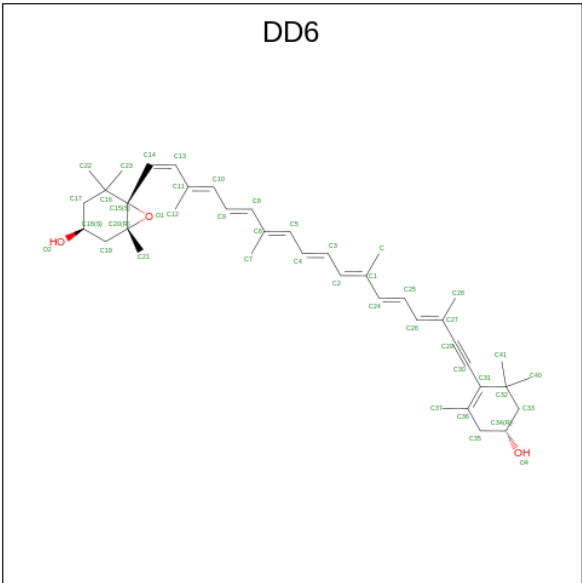
Mol	Chain	Residues	Atoms			AltConf
26	r	1	Total	C	O	0
			48	42	6	
26	B	1	Total	C	O	0
			48	42	6	
26	B	1	Total	C	O	0
			48	42	6	
26	B	1	Total	C	O	0
			48	42	6	
26	B	1	Total	C	O	0
			48	42	6	
26	C	1	Total	C	O	0
			48	42	6	
26	C	1	Total	C	O	0
			48	42	6	
26	C	1	Total	C	O	0
			48	42	6	
26	D	1	Total	C	O	0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



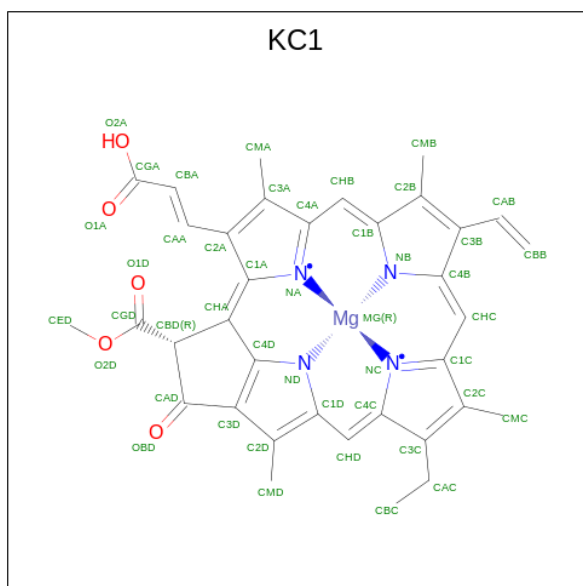
Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	C	O	0
			43	40	3	
28	C	1	Total	C	O	0
			43	40	3	

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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

Chain a:  99%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:  99%



- Molecule 3: Photosystem I iron-sulfur center

Chain c:  100%

There are no outlier residues recorded for this chain.

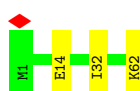
- Molecule 4: Photosystem I reaction center subunit II

Chain d:  98%

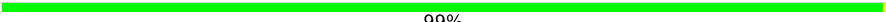


- Molecule 5: Photosystem I reaction center subunit IV

Chain e:  95% 5%



- Molecule 6: Photosystem I reaction center subunit III

Chain f:  99%



- Molecule 7: Photosystem I reaction center subunit Psa29

Chain g:  97%




- Molecule 8: Photosystem I reaction center subunit VIII

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Photosystem I reaction center subunit IX

Chain j:  92% 8%



- Molecule 10: Photosystem I reaction center subunit XI

Chain l:  99%



- Molecule 11: Photosystem I reaction center subunit XII

Chain m:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: Tp-PsaR

Chain r:  99%



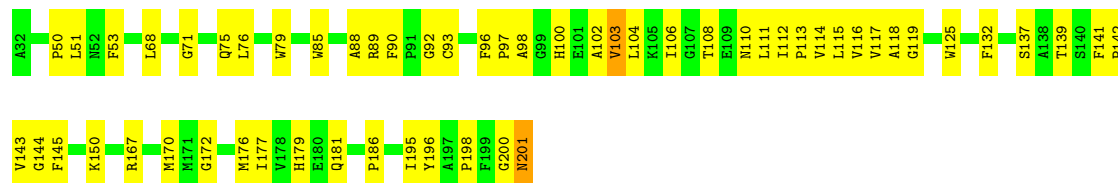
- Molecule 13: Fucoxanthin chlorophyll a/c-binding protein Lhcq8

Chain B:  68% 27% 5%



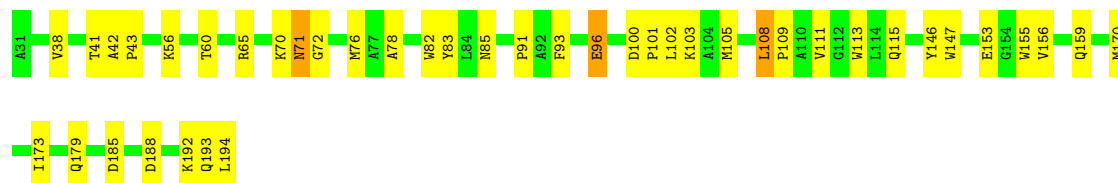
- Molecule 14: Fucoxanthin chl a/c light-harvesting protein, major type

Chain C: 67% 32%



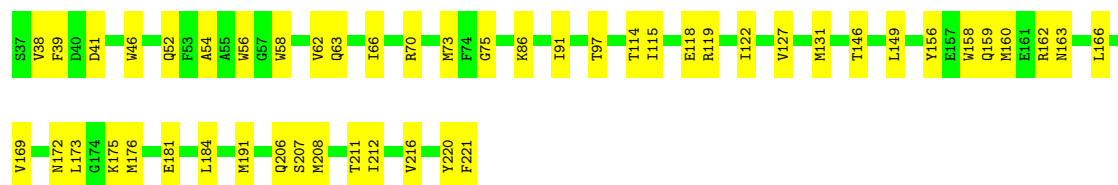
- Molecule 15: Pt17531-like protein

Chain D: 74% 24%



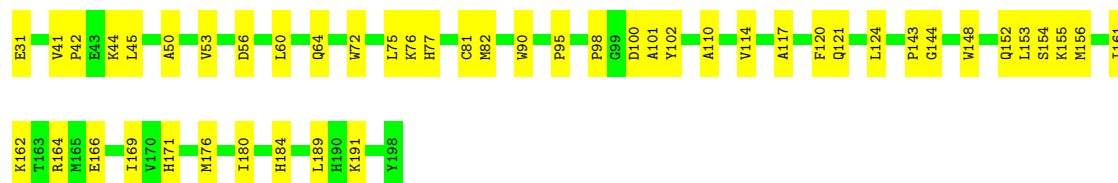
- Molecule 16: Tp-RedCAP

Chain E: 74% 26%



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

Chain H: 72% 28%



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 (\AA)	563.2, 563.2, 563.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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: BCR, A86, KC1, CLA, SQD, DD6, SF4, LMG, ET4, PQN, LHG, 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	0.34	0/6049	0.41	0/8234
2	b	0.34	0/6034	0.41	0/8236
3	c	0.33	0/609	0.44	0/826
4	d	0.32	0/1067	0.41	0/1441
5	e	0.31	0/511	0.41	0/690
6	f	0.33	0/1271	0.42	0/1727
7	g	0.30	0/1003	0.41	0/1354
8	i	0.33	0/264	0.40	0/360
9	j	0.34	0/342	0.50	0/463
10	l	0.35	0/1123	0.44	0/1523
11	m	0.35	0/222	0.38	0/300
12	r	0.31	0/704	0.38	0/957
13	B	0.34	0/1324	0.39	0/1804
14	C	0.33	0/1339	0.40	0/1813
15	D	0.32	0/1304	0.39	0/1771
16	E	0.33	0/1450	0.40	0/1974
17	H	0.33	0/1334	0.41	0/1809
All	All	0.33	0/25950	0.41	0/35282

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.

There are no bond angle outliers.

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	0	0
2	b	5824	0	5643	0	0
3	c	599	0	582	0	0
4	d	1040	0	1027	0	0
5	e	503	0	500	0	0
6	f	1242	0	1239	0	0
7	g	981	0	922	0	0
8	i	256	0	259	0	0
9	j	332	0	331	0	0
10	l	1095	0	1116	0	0
11	m	220	0	241	0	0
12	r	683	0	675	0	0
13	B	1285	0	1239	66	0
14	C	1302	0	1243	70	0
15	D	1271	0	1227	33	0
16	E	1413	0	1365	41	0
17	H	1300	0	1262	44	0
18	B	469	0	479	39	0
18	C	547	0	472	64	0
18	D	568	0	501	37	0
18	E	462	0	454	23	0
18	H	587	0	583	56	0
18	a	2671	0	2759	0	0
18	b	2492	0	2569	0	0
18	f	175	0	177	0	0
18	i	60	0	59	0	0
18	j	41	0	29	0	0
18	l	159	0	144	0	0
18	r	45	0	33	0	0
19	a	33	0	46	0	0
19	b	33	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	B	42	0	54	2	0
20	D	49	0	74	6	0
20	E	91	0	131	2	0
20	H	35	0	43	0	0
20	a	109	0	134	0	0
20	b	49	0	74	0	0
20	j	49	0	74	0	0
21	E	80	0	112	5	0
21	a	200	0	280	0	0
21	b	160	0	224	0	0
21	f	80	0	112	0	0
21	i	80	0	112	0	0
21	j	80	0	112	0	0
21	l	80	0	112	0	0
21	m	40	0	56	0	0
21	r	40	0	56	0	0
22	a	33	0	39	0	0
23	C	75	0	88	2	0
23	D	46	0	61	0	0
23	E	43	0	55	3	0
23	a	33	0	33	0	0
23	j	37	0	42	0	0
23	l	40	0	49	0	0
24	b	8	0	0	0	0
24	c	16	0	0	0	0
25	b	60	0	81	0	0
26	B	192	0	0	8	0
26	C	144	0	0	5	0
26	D	144	0	0	6	0
26	E	48	0	0	0	0
26	H	144	0	0	14	0
26	b	48	0	0	0	0
26	m	48	0	0	0	0
26	r	48	0	0	0	0
27	l	42	0	0	0	0
28	B	43	0	0	1	0
28	C	43	0	0	1	0
28	D	43	0	0	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	H	45	0	0	1	0
All	All	36577	0	35112	398	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 398 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:HMD2	1.45	1.46
26:H:302:A86:C2	18:H:309:CLA:HMD2	1.73	1.17
26:H:302:A86:C1	18:H:309:CLA:CMD	2.27	1.12
13:B:165:LYS:HB3	18:B:306:CLA:HMD3	1.32	1.06
26:H:302:A86:C	18:H:309:CLA:HMD2	1.87	1.03

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	597 (99%)	6 (1%)	73	87
2	b	597/597 (100%)	589 (99%)	8 (1%)	65	83
3	c	69/69 (100%)	69 (100%)	0	100	100
4	d	111/111 (100%)	110 (99%)	1 (1%)	75	89
5	e	55/55 (100%)	52 (94%)	3 (6%)	18	51
6	f	132/132 (100%)	130 (98%)	2 (2%)	60	81
7	g	98/98 (100%)	94 (96%)	4 (4%)	26	59
8	i	28/28 (100%)	28 (100%)	0	100	100
9	j	36/36 (100%)	33 (92%)	3 (8%)	9	35
10	l	113/113 (100%)	112 (99%)	1 (1%)	75	89
11	m	22/22 (100%)	22 (100%)	0	100	100
12	r	72/72 (100%)	71 (99%)	1 (1%)	62	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	B	133/133 (100%)	124 (93%)	9 (7%)	13	43
14	C	129/130 (99%)	126 (98%)	3 (2%)	45	72
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%)	136 (100%)	0	100	100
All	All	2606/2607 (100%)	2561 (98%)	45 (2%)	56	78

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	r	113	TYR
13	B	164	LEU
13	B	43	GLU
13	B	146	LEU
13	B	180	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
14	C	52	ASN
17	H	185	GLN
14	C	201	ASN
15	D	179	GLN
2	b	330	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	814	1	65,73,73	1.49	6 (9%)	76,113,113	1.38	8 (10%)
21	BCR	j	101	-	41,41,41	0.70	0	56,56,56	2.06	14 (25%)
28	DD6	E	304	-	39,45,45	2.53	8 (20%)	52,67,67	3.42	16 (30%)
26	A86	D	203	-	44,50,50	1.34	4 (9%)	51,76,76	3.58	21 (41%)
18	CLA	D	213	15	65,73,73	1.48	7 (10%)	76,113,113	1.39	7 (9%)
29	KC1	B	313	-	48,53,53	1.72	8 (16%)	55,89,89	1.99	10 (18%)
18	CLA	a	842	-	65,73,73	1.43	11 (16%)	76,113,113	1.50	9 (11%)
18	CLA	b	823	2	58,66,73	1.56	6 (10%)	67,104,113	1.48	8 (11%)
18	CLA	C	307	14	65,73,73	1.45	10 (15%)	76,113,113	1.45	9 (11%)
18	CLA	C	310	14	46,54,73	1.66	8 (17%)	53,90,113	1.56	7 (13%)
18	CLA	D	212	15	42,50,73	1.79	6 (14%)	48,85,113	1.59	6 (12%)
21	BCR	f	201	-	41,41,41	0.94	1 (2%)	56,56,56	1.94	18 (32%)
22	SQD	a	849	-	31,32,54	3.14	8 (25%)	34,36,65	2.91	9 (26%)
18	CLA	a	813	1	65,73,73	1.45	10 (15%)	76,113,113	1.56	12 (15%)
18	CLA	B	312	13	65,73,73	1.46	5 (7%)	76,113,113	1.39	7 (9%)
18	CLA	E	310	16	65,73,73	1.49	6 (9%)	76,113,113	1.36	7 (9%)
21	BCR	a	833	-	41,41,41	0.93	1 (2%)	56,56,56	1.92	20 (35%)
20	LHG	b	835	18	48,48,48	1.09	3 (6%)	51,54,54	1.03	3 (5%)
21	BCR	m	101	-	41,41,41	0.67	0	56,56,56	2.14	16 (28%)
21	BCR	r	201	-	41,41,41	0.71	0	56,56,56	1.75	15 (26%)
23	LMG	a	851	-	33,33,55	1.62	5 (15%)	41,41,63	3.61	8 (19%)
18	CLA	a	807	1	65,73,73	1.47	11 (16%)	76,113,113	1.56	11 (14%)
18	CLA	b	816	2	55,63,73	1.61	6 (10%)	64,101,113	1.46	7 (10%)
18	CLA	H	313	17	65,73,73	1.46	11 (16%)	76,113,113	1.53	9 (11%)
18	CLA	b	845	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	8 (10%)
18	CLA	b	809	2	55,63,73	1.64	6 (10%)	64,101,113	1.48	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	BCR	a	852	-	41,41,41	0.71	0	56,56,56	2.16	19 (33%)
28	DD6	E	303	-	39,45,45	1.99	2 (5%)	52,67,67	1.91	10 (19%)
23	LMG	C	319	18	44,44,55	1.32	7 (15%)	52,52,63	1.86	4 (7%)
18	CLA	a	811	1	50,58,73	1.64	6 (12%)	58,95,113	1.60	7 (12%)
28	DD6	E	307	-	39,45,45	2.13	3 (7%)	52,67,67	3.02	23 (44%)
21	BCR	l	201	-	41,41,41	1.00	2 (4%)	56,56,56	2.04	16 (28%)
18	CLA	i	101	-	60,68,73	1.55	6 (10%)	70,107,113	1.43	10 (14%)
18	CLA	l	205	-	45,53,73	1.75	6 (13%)	52,89,113	1.62	6 (11%)
26	A86	B	305	-	44,50,50	1.49	7 (15%)	51,76,76	3.13	26 (50%)
18	CLA	b	827	2	47,55,73	1.76	8 (17%)	54,91,113	1.57	7 (12%)
18	CLA	b	822	2	65,73,73	1.47	6 (9%)	76,113,113	1.45	6 (7%)
28	DD6	C	303	-	39,45,45	2.20	5 (12%)	52,67,67	2.32	18 (34%)
18	CLA	a	836	1	65,73,73	1.45	6 (9%)	76,113,113	1.38	7 (9%)
18	CLA	a	816	1	45,53,73	1.81	6 (13%)	52,89,113	1.58	6 (11%)
18	CLA	H	315	17	45,53,73	1.76	5 (11%)	52,89,113	1.62	6 (11%)
20	LHG	a	832	18	26,26,48	1.29	5 (19%)	29,32,54	1.19	2 (6%)
26	A86	H	301	-	44,50,50	1.51	8 (18%)	51,76,76	3.17	24 (47%)
26	A86	D	204	-	44,50,50	1.54	8 (18%)	51,76,76	3.73	22 (43%)
25	DGD	b	834	-	61,61,67	0.85	2 (3%)	75,75,81	1.10	4 (5%)
23	LMG	C	301	-	31,31,55	1.61	6 (19%)	39,39,63	3.02	7 (17%)
18	CLA	B	311	13	65,73,73	1.49	6 (9%)	76,113,113	1.37	8 (10%)
18	CLA	E	314	16	45,53,73	1.76	11 (24%)	52,89,113	1.62	9 (17%)
18	CLA	H	306	17	65,73,73	1.43	11 (16%)	76,113,113	1.40	9 (11%)
18	CLA	B	309	-	65,73,73	1.45	6 (9%)	76,113,113	1.42	6 (7%)
18	CLA	E	315	16	65,73,73	1.48	6 (9%)	76,113,113	1.38	7 (9%)
18	CLA	H	314	17	65,73,73	1.44	11 (16%)	76,113,113	1.50	10 (13%)
26	A86	b	847	-	44,50,50	1.41	6 (13%)	51,76,76	2.22	13 (25%)
18	CLA	b	818	2	65,73,73	1.48	7 (10%)	76,113,113	1.39	7 (9%)
18	CLA	a	803	1	65,73,73	1.44	11 (16%)	76,113,113	1.59	10 (13%)
18	CLA	b	819	2	65,73,73	1.47	6 (9%)	76,113,113	1.37	7 (9%)
18	CLA	a	853	1	55,63,73	1.61	6 (10%)	64,101,113	1.49	9 (14%)
26	A86	E	302	-	44,50,50	1.45	6 (13%)	51,76,76	2.82	23 (45%)
18	CLA	H	305	-	54,62,73	1.60	10 (18%)	62,99,113	1.60	6 (9%)
18	CLA	b	812	2	59,67,73	1.53	5 (8%)	68,105,113	1.46	7 (10%)
18	CLA	b	840	2	61,69,73	1.52	7 (11%)	71,108,113	1.46	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	DD6	H	303	-	39,45,45	2.48	11 (28%)	52,67,67	2.56	20 (38%)
18	CLA	b	814	-	65,73,73	1.49	6 (9%)	76,113,113	1.43	8 (10%)
18	CLA	D	217	-	41,49,73	1.80	6 (14%)	47,84,113	1.64	8 (17%)
26	A86	H	304	-	44,50,50	1.46	5 (11%)	51,76,76	2.89	24 (47%)
18	CLA	C	315	14	42,50,73	1.83	5 (11%)	48,85,113	1.60	6 (12%)
18	CLA	a	824	1	51,59,73	1.63	6 (11%)	59,96,113	1.58	7 (11%)
21	BCR	i	102	-	41,41,41	0.75	0	56,56,56	1.94	17 (30%)
21	BCR	j	105	-	41,41,41	0.72	0	56,56,56	2.09	13 (23%)
26	A86	D	206	-	44,50,50	1.46	6 (13%)	51,76,76	3.10	21 (41%)
20	LHG	E	301	-	48,48,48	1.11	6 (12%)	51,54,54	1.04	3 (5%)
18	CLA	E	311	16	46,54,73	1.76	6 (13%)	53,90,113	1.52	7 (13%)
18	CLA	B	310	13	46,54,73	1.77	6 (13%)	53,90,113	1.54	6 (11%)
18	CLA	a	809	18,1	62,70,73	1.50	6 (9%)	72,109,113	1.39	6 (8%)
18	CLA	b	829	2	65,73,73	1.47	10 (15%)	76,113,113	1.51	11 (14%)
18	CLA	B	314	13	41,49,73	1.83	10 (24%)	47,84,113	1.62	8 (17%)
18	CLA	C	317	-	42,50,73	1.81	10 (23%)	48,85,113	1.69	8 (16%)
18	CLA	a	820	1	65,73,73	1.48	6 (9%)	76,113,113	1.41	8 (10%)
18	CLA	H	309	17	46,54,73	1.75	6 (13%)	53,90,113	1.57	6 (11%)
18	CLA	C	318	14	42,50,73	1.77	10 (23%)	48,85,113	1.59	6 (12%)
18	CLA	a	825	1	60,68,73	1.55	11 (18%)	70,107,113	1.54	9 (12%)
18	CLA	a	812	-	45,53,73	1.80	6 (13%)	52,89,113	1.59	6 (11%)
26	A86	C	304	-	44,50,50	1.44	5 (11%)	51,76,76	2.68	16 (31%)
26	A86	C	302	-	44,50,50	1.50	6 (13%)	51,76,76	2.99	22 (43%)
18	CLA	a	846	-	65,73,73	1.45	6 (9%)	76,113,113	1.38	8 (10%)
18	CLA	D	209	15	49,57,73	1.71	7 (14%)	55,93,113	1.56	7 (12%)
18	CLA	C	311	14	60,68,73	1.54	9 (15%)	70,107,113	1.45	9 (12%)
18	CLA	B	306	13	58,65,73	1.54	10 (17%)	67,102,113	1.39	5 (7%)
18	CLA	a	838	1	65,73,73	1.49	6 (9%)	76,113,113	1.44	7 (9%)
18	CLA	a	808	1	65,73,73	1.49	8 (12%)	76,113,113	1.37	7 (9%)
18	CLA	D	216	15	46,54,73	1.71	10 (21%)	53,90,113	1.54	7 (13%)
18	CLA	b	801	-	65,73,73	1.49	12 (18%)	76,113,113	1.58	8 (10%)
18	CLA	a	844	1	65,73,73	1.49	6 (9%)	76,113,113	1.39	7 (9%)
18	CLA	a	848	1	56,64,73	1.59	6 (10%)	65,102,113	1.45	6 (9%)
18	CLA	b	821	2	50,58,73	1.69	6 (12%)	58,95,113	1.49	8 (13%)
23	LMG	D	202	-	46,46,55	1.84	7 (15%)	54,54,63	1.36	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	SF4	c	102	3	0,12,12	-	-	-		
23	LMG	l	207	-	40,40,55	1.22	4 (10%)	48,48,63	1.76	4 (8%)
20	LHG	B	315	-	41,41,48	0.98	2 (4%)	44,47,54	1.08	3 (6%)
28	DD6	B	303	-	39,45,45	2.32	7 (17%)	52,67,67	2.91	20 (38%)
18	CLA	l	202	10	49,57,73	1.66	10 (20%)	55,93,113	1.62	8 (14%)
18	CLA	a	839	1	65,73,73	1.44	6 (9%)	76,113,113	1.42	7 (9%)
21	BCR	E	306	-	41,41,41	0.71	0	56,56,56	2.02	16 (28%)
18	CLA	b	837	2	60,68,73	1.52	10 (16%)	70,107,113	1.55	8 (11%)
18	CLA	b	830	20	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
18	CLA	D	208	15	65,73,73	1.48	10 (15%)	76,113,113	1.52	11 (14%)
27	ET4	l	206	-	41,43,43	1.45	7 (17%)	54,60,60	2.28	19 (35%)
18	CLA	a	801	1	65,73,73	1.53	11 (16%)	76,113,113	1.44	10 (13%)
18	CLA	a	804	18,1	55,63,73	1.64	7 (12%)	64,101,113	1.49	8 (12%)
18	CLA	b	838	-	65,73,73	1.47	7 (10%)	76,113,113	1.41	7 (9%)
18	CLA	a	826	1	65,73,73	1.53	6 (9%)	76,113,113	1.40	7 (9%)
18	CLA	E	316	-	56,64,73	1.56	6 (10%)	65,102,113	1.51	6 (9%)
21	BCR	f	205	-	41,41,41	0.72	0	56,56,56	1.96	16 (28%)
18	CLA	b	817	2	60,68,73	1.55	7 (11%)	70,107,113	1.41	7 (10%)
18	CLA	H	310	-	60,68,73	1.46	10 (16%)	70,107,113	1.59	9 (12%)
18	CLA	D	215	-	41,49,73	1.84	5 (12%)	47,84,113	1.66	7 (14%)
20	LHG	a	835	-	32,32,48	1.28	5 (15%)	35,38,54	1.17	2 (5%)
18	CLA	E	312	16	65,73,73	1.47	11 (16%)	76,113,113	1.45	9 (11%)
18	CLA	b	804	2	45,53,73	1.74	11 (24%)	52,89,113	1.69	8 (15%)
18	CLA	C	314	14	41,49,73	1.80	10 (24%)	47,84,113	1.63	8 (17%)
19	PQN	b	831	-	34,34,34	1.58	2 (5%)	42,45,45	1.17	3 (7%)
18	CLA	a	843	-	65,73,73	1.45	6 (9%)	76,113,113	1.46	7 (9%)
18	CLA	b	841	2	65,73,73	1.50	6 (9%)	76,113,113	1.41	7 (9%)
18	CLA	E	309	16	65,73,73	1.47	7 (10%)	76,113,113	1.41	7 (9%)
18	CLA	b	807	2	65,73,73	1.48	6 (9%)	76,113,113	1.36	7 (9%)
18	CLA	a	817	1	49,57,73	1.68	6 (12%)	55,93,113	1.58	7 (12%)
21	BCR	i	103	-	41,41,41	0.70	0	56,56,56	2.04	13 (23%)
24	SF4	b	802	2	0,12,12	-	-	-		
18	CLA	a	810	1	65,73,73	1.46	7 (10%)	76,113,113	1.39	7 (9%)
26	A86	r	203	-	44,50,50	1.50	7 (15%)	51,76,76	3.78	27 (52%)
18	CLA	H	308	17	65,73,73	1.45	10 (15%)	76,113,113	1.50	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	BCR	a	834	-	41,41,41	0.73	0	56,56,56	1.97	14 (25%)
18	CLA	f	202	-	65,73,73	1.46	6 (9%)	76,113,113	1.42	8 (10%)
18	CLA	C	312	14	61,69,73	1.52	10 (16%)	71,108,113	1.47	7 (9%)
18	CLA	f	203	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	7 (9%)
26	A86	B	302	-	44,50,50	1.62	9 (20%)	51,76,76	3.40	23 (45%)
18	CLA	C	306	23	45,53,73	1.79	6 (13%)	52,89,113	1.59	6 (11%)
18	CLA	a	841	-	65,73,73	1.47	10 (15%)	76,113,113	1.47	8 (10%)
19	PQN	a	829	-	34,34,34	1.59	2 (5%)	42,45,45	1.07	2 (4%)
18	CLA	a	806	1	65,73,73	1.46	6 (9%)	76,113,113	1.40	6 (7%)
18	CLA	b	828	-	65,73,73	1.49	6 (9%)	76,113,113	1.41	8 (10%)
18	CLA	b	813	2	55,63,73	1.62	7 (12%)	64,101,113	1.49	6 (9%)
28	DD6	E	308	-	39,45,45	1.99	3 (7%)	52,67,67	1.78	13 (25%)
26	A86	H	302	-	44,50,50	1.61	8 (18%)	51,76,76	3.41	23 (45%)
18	CLA	H	311	17	57,65,73	1.54	10 (17%)	66,103,113	1.49	7 (10%)
18	CLA	B	307	13	65,73,73	1.48	7 (10%)	76,113,113	1.37	7 (9%)
23	LMG	j	103	-	37,37,55	1.59	5 (13%)	45,45,63	3.61	8 (17%)
18	CLA	b	806	2	65,73,73	1.49	6 (9%)	76,113,113	1.39	7 (9%)
18	CLA	a	830	20	52,60,73	1.67	7 (13%)	60,97,113	1.51	7 (11%)
18	CLA	b	808	2	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
18	CLA	a	840	-	65,73,73	1.50	10 (15%)	76,113,113	1.46	9 (11%)
18	CLA	b	805	2	65,73,73	1.49	6 (9%)	76,113,113	1.46	7 (9%)
20	LHG	H	316	-	34,34,48	1.12	3 (8%)	37,40,54	0.97	2 (5%)
23	LMG	E	318	-	43,43,55	2.06	7 (16%)	51,51,63	1.98	7 (13%)
29	KC1	C	313	-	48,53,53	1.53	7 (14%)	55,89,89	1.87	11 (20%)
18	CLA	a	854	-	65,73,73	1.45	11 (16%)	76,113,113	1.54	10 (13%)
26	A86	B	301	-	44,50,50	1.30	4 (9%)	51,76,76	2.80	18 (35%)
21	BCR	a	850	-	41,41,41	1.03	2 (4%)	56,56,56	1.82	13 (23%)
18	CLA	a	837	1	60,68,73	1.53	12 (20%)	70,107,113	1.62	10 (14%)
18	CLA	D	207	-	61,69,73	1.53	10 (16%)	71,108,113	1.48	8 (11%)
18	CLA	a	855	1	65,73,73	1.45	6 (9%)	76,113,113	1.45	7 (9%)
18	CLA	r	202	12	45,53,73	1.77	5 (11%)	52,89,113	1.57	8 (15%)
18	CLA	a	823	1	45,53,73	1.78	6 (13%)	52,89,113	1.60	6 (11%)
18	CLA	B	308	13	65,73,73	1.47	7 (10%)	76,113,113	1.39	7 (9%)
21	BCR	b	832	-	41,41,41	0.70	0	56,56,56	1.92	14 (25%)
29	KC1	C	308	14	48,53,53	1.51	7 (14%)	55,89,89	1.92	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	a	847	1	65,73,73	1.48	7 (10%)	76,113,113	1.39	6 (7%)
18	CLA	f	204	6	45,53,73	1.77	6 (13%)	52,89,113	1.59	6 (11%)
18	CLA	b	826	2	60,68,73	1.51	6 (10%)	70,107,113	1.53	7 (10%)
21	BCR	E	305	-	41,41,41	0.70	0	56,56,56	1.87	17 (30%)
18	CLA	D	211	15	46,54,73	1.76	7 (15%)	53,90,113	1.55	6 (11%)
29	KC1	H	312	17	48,53,53	1.82	8 (16%)	55,89,89	1.96	11 (20%)
18	CLA	a	805	1	65,73,73	1.46	7 (10%)	76,113,113	1.46	6 (7%)
18	CLA	a	822	1	50,58,73	1.68	6 (12%)	58,95,113	1.55	7 (12%)
18	CLA	b	844	2	62,70,73	1.50	6 (9%)	72,109,113	1.45	7 (9%)
18	CLA	a	821	1	65,73,73	1.50	7 (10%)	76,113,113	1.39	8 (10%)
18	CLA	b	848	2	54,62,73	1.61	6 (11%)	62,99,113	1.44	6 (9%)
18	CLA	D	214	15	56,64,73	1.60	7 (12%)	65,102,113	1.52	7 (10%)
20	LHG	j	102	-	48,48,48	1.11	6 (12%)	51,54,54	0.91	2 (3%)
26	A86	B	304	-	44,50,50	1.52	7 (15%)	51,76,76	2.80	18 (35%)
18	CLA	b	849	-	65,73,73	1.49	7 (10%)	76,113,113	1.40	7 (9%)
18	CLA	a	828	1	65,73,73	1.47	6 (9%)	76,113,113	1.38	7 (9%)
18	CLA	b	811	2	60,68,73	1.49	10 (16%)	70,107,113	1.51	8 (11%)
20	LHG	a	831	-	48,48,48	1.11	3 (6%)	51,54,54	1.00	3 (5%)
21	BCR	b	836	-	41,41,41	0.74	0	56,56,56	2.00	18 (32%)
18	CLA	b	843	2	65,73,73	1.45	10 (15%)	76,113,113	1.46	8 (10%)
18	CLA	H	307	17	65,73,73	1.43	11 (16%)	76,113,113	1.62	13 (17%)
26	A86	m	102	-	44,50,50	1.36	4 (9%)	51,76,76	3.28	25 (49%)
18	CLA	a	827	1	65,73,73	1.47	5 (7%)	76,113,113	1.43	7 (9%)
18	CLA	j	104	9	41,49,73	1.84	6 (14%)	47,84,113	1.68	7 (14%)
20	LHG	E	317	-	41,41,48	1.00	2 (4%)	44,47,54	1.20	4 (9%)
21	BCR	a	845	-	41,41,41	0.98	2 (4%)	56,56,56	1.94	20 (35%)
18	CLA	l	203	10	65,73,73	1.45	11 (16%)	76,113,113	1.56	10 (13%)
18	CLA	b	810	2	65,73,73	1.48	7 (10%)	76,113,113	1.41	7 (9%)
18	CLA	C	316	14	41,49,73	1.81	11 (26%)	47,84,113	1.69	9 (19%)
18	CLA	b	825	-	45,53,73	1.81	6 (13%)	52,89,113	1.58	7 (13%)
20	LHG	D	201	-	48,48,48	1.08	4 (8%)	51,54,54	1.03	2 (3%)
28	DD6	D	205	-	39,45,45	2.22	6 (15%)	52,67,67	3.22	26 (50%)
18	CLA	b	846	2	65,73,73	1.47	7 (10%)	76,113,113	1.34	7 (9%)
18	CLA	a	818	1	51,59,73	1.63	11 (21%)	59,96,113	1.69	7 (11%)
18	CLA	E	313	16	55,63,73	1.59	6 (10%)	64,101,113	1.52	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	b	850	2	65,73,73	1.47	6 (9%)	76,113,113	1.39	6 (7%)
18	CLA	a	819	1	65,73,73	1.47	7 (10%)	76,113,113	1.42	7 (9%)
18	CLA	b	842	2	65,73,73	1.47	5 (7%)	76,113,113	1.40	8 (10%)
18	CLA	a	802	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	8 (10%)
21	BCR	b	839	-	41,41,41	1.01	2 (4%)	56,56,56	2.04	21 (37%)
21	BCR	l	204	-	41,41,41	0.86	0	56,56,56	2.07	15 (26%)
26	A86	C	305	-	44,50,50	1.53	7 (15%)	51,76,76	3.11	24 (47%)
18	CLA	D	210	-	56,64,73	1.57	10 (17%)	65,102,113	1.55	9 (13%)
24	SF4	c	101	3	0,12,12	-	-	-	-	-
18	CLA	b	815	2	46,54,73	1.73	6 (13%)	53,90,113	1.62	6 (11%)
18	CLA	b	824	-	65,73,73	1.48	10 (15%)	76,113,113	1.57	7 (9%)
21	BCR	b	833	-	41,41,41	0.71	0	56,56,56	3.25	21 (37%)
18	CLA	b	820	2	65,73,73	1.44	11 (16%)	76,113,113	1.58	9 (11%)
18	CLA	b	803	2	65,73,73	1.45	12 (18%)	76,113,113	1.41	9 (11%)
18	CLA	C	309	-	62,70,73	1.49	10 (16%)	72,109,113	1.59	10 (13%)
18	CLA	a	815	1	65,73,73	1.48	6 (9%)	76,113,113	1.39	9 (11%)

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	814	1	1/1/15/20	7/37/115/115	-
21	BCR	j	101	-	-	4/29/63/63	0/2/2/2
28	DD6	E	304	-	-	6/26/80/80	0/3/3/3
26	A86	D	203	-	-	9/34/90/90	0/3/3/3
18	CLA	D	213	15	1/1/15/20	8/37/115/115	-
29	KC1	B	313	-	-	8/15/71/71	-
18	CLA	a	842	-	1/1/15/20	10/37/115/115	-
18	CLA	b	823	2	1/1/13/20	11/29/107/115	-
18	CLA	C	307	14	1/1/15/20	8/37/115/115	-
18	CLA	C	310	14	1/1/11/20	6/15/93/115	-
18	CLA	D	212	15	1/1/10/20	1/10/88/115	-
21	BCR	f	201	-	-	9/29/63/63	0/2/2/2
22	SQD	a	849	-	-	18/33/33/69	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	a	813	1	1/1/15/20	24/37/115/115	-
18	CLA	B	312	13	1/1/15/20	11/37/115/115	-
18	CLA	E	310	16	1/1/15/20	12/37/115/115	-
21	BCR	a	833	-	-	0/29/63/63	0/2/2/2
20	LHG	b	835	18	-	32/53/53/53	-
21	BCR	m	101	-	-	7/29/63/63	0/2/2/2
21	BCR	r	201	-	-	4/29/63/63	0/2/2/2
23	LMG	a	851	-	-	16/28/48/70	0/1/1/1
18	CLA	a	807	1	1/1/15/20	9/37/115/115	-
18	CLA	b	816	2	1/1/13/20	3/25/103/115	-
18	CLA	H	313	17	1/1/15/20	18/37/115/115	-
18	CLA	b	845	-	1/1/15/20	12/37/115/115	-
18	CLA	b	809	2	1/1/13/20	3/25/103/115	-
21	BCR	a	852	-	-	8/29/63/63	0/2/2/2
28	DD6	E	303	-	-	3/26/80/80	0/3/3/3
23	LMG	C	319	18	-	19/39/59/70	0/1/1/1
18	CLA	a	811	1	1/1/12/20	8/19/97/115	-
28	DD6	E	307	-	-	10/26/80/80	0/3/3/3
21	BCR	l	201	-	-	6/29/63/63	0/2/2/2
18	CLA	i	101	-	1/1/14/20	11/31/109/115	-
18	CLA	l	205	-	1/1/11/20	4/13/91/115	-
26	A86	B	305	-	-	4/34/90/90	0/3/3/3
18	CLA	b	827	2	1/1/11/20	5/16/94/115	-
18	CLA	b	822	2	1/1/15/20	18/37/115/115	-
28	DD6	C	303	-	-	5/26/80/80	0/3/3/3
18	CLA	a	836	1	1/1/15/20	13/37/115/115	-
18	CLA	a	816	1	1/1/11/20	7/13/91/115	-
18	CLA	H	315	17	1/1/11/20	4/13/91/115	-
20	LHG	a	832	18	-	12/31/31/53	-
26	A86	H	301	-	-	5/34/90/90	0/3/3/3
26	A86	D	204	-	-	4/34/90/90	0/3/3/3
25	DGD	b	834	-	-	27/49/89/95	0/2/2/2
23	LMG	C	301	-	-	14/26/46/70	0/1/1/1
18	CLA	B	311	13	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	E	314	16	1/1/11/20	3/13/91/115	-
18	CLA	H	306	17	1/1/15/20	12/37/115/115	-
18	CLA	B	309	-	1/1/15/20	12/37/115/115	-
18	CLA	E	315	16	1/1/15/20	10/37/115/115	-
18	CLA	H	314	17	1/1/15/20	15/37/115/115	-
26	A86	b	847	-	-	17/34/90/90	0/3/3/3
18	CLA	b	818	2	1/1/15/20	9/37/115/115	-
18	CLA	a	803	1	1/1/15/20	13/37/115/115	-
18	CLA	b	819	2	1/1/15/20	14/37/115/115	-
18	CLA	a	853	1	1/1/13/20	10/25/103/115	-
26	A86	E	302	-	-	5/34/90/90	0/3/3/3
18	CLA	H	305	-	1/1/12/20	10/24/102/115	-
18	CLA	b	812	2	1/1/13/20	9/30/108/115	-
18	CLA	b	840	2	1/1/14/20	10/33/111/115	-
28	DD6	H	303	-	-	3/26/80/80	0/3/3/3
18	CLA	b	814	-	1/1/15/20	11/37/115/115	-
18	CLA	D	217	-	1/1/10/20	5/8/86/115	-
26	A86	H	304	-	-	4/34/90/90	0/3/3/3
18	CLA	C	315	14	1/1/10/20	4/10/88/115	-
18	CLA	a	824	1	1/1/12/20	10/21/99/115	-
21	BCR	i	102	-	-	0/29/63/63	0/2/2/2
21	BCR	j	105	-	-	5/29/63/63	0/2/2/2
26	A86	D	206	-	-	6/34/90/90	0/3/3/3
20	LHG	E	301	-	-	35/53/53/53	-
18	CLA	E	311	16	1/1/11/20	6/15/93/115	-
18	CLA	B	310	13	1/1/11/20	5/15/93/115	-
18	CLA	a	809	18,1	1/1/14/20	12/34/112/115	-
18	CLA	b	829	2	1/1/15/20	14/37/115/115	-
18	CLA	B	314	13	1/1/10/20	2/8/86/115	-
18	CLA	C	317	-	1/1/10/20	8/10/88/115	-
18	CLA	a	820	1	1/1/15/20	8/37/115/115	-
18	CLA	H	309	17	1/1/11/20	8/15/93/115	-
18	CLA	C	318	14	1/1/10/20	5/10/88/115	-
18	CLA	a	825	1	1/1/14/20	14/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	a	812	-	1/1/11/20	4/13/91/115	-
26	A86	C	304	-	-	3/34/90/90	0/3/3/3
26	A86	C	302	-	-	5/34/90/90	0/3/3/3
18	CLA	a	846	-	1/1/15/20	8/37/115/115	-
18	CLA	D	209	15	1/1/11/20	9/18/96/115	-
18	CLA	C	311	14	1/1/14/20	12/31/109/115	-
18	CLA	B	306	13	1/1/12/20	17/27/101/115	-
18	CLA	a	838	1	1/1/15/20	12/37/115/115	-
18	CLA	a	808	1	1/1/15/20	10/37/115/115	-
18	CLA	D	216	15	1/1/11/20	5/15/93/115	-
18	CLA	b	801	-	1/1/15/20	9/37/115/115	-
18	CLA	a	844	1	1/1/15/20	17/37/115/115	-
18	CLA	a	848	1	1/1/13/20	9/27/105/115	-
18	CLA	b	821	2	1/1/12/20	8/19/97/115	-
23	LMG	D	202	-	-	17/41/61/70	0/1/1/1
24	SF4	c	102	3	-	-	0/6/5/5
23	LMG	l	207	-	-	16/35/55/70	0/1/1/1
20	LHG	B	315	-	-	25/46/46/53	-
28	DD6	B	303	-	-	0/26/80/80	0/3/3/3
18	CLA	l	202	10	1/1/11/20	8/18/96/115	-
18	CLA	a	839	1	1/1/15/20	9/37/115/115	-
21	BCR	E	306	-	-	0/29/63/63	0/2/2/2
18	CLA	b	837	2	1/1/14/20	14/31/109/115	-
18	CLA	b	830	20	1/1/15/20	7/37/115/115	-
18	CLA	D	208	15	1/1/15/20	13/37/115/115	-
27	ET4	l	206	-	-	3/25/67/67	0/2/2/2
18	CLA	a	801	1	1/1/15/20	15/37/115/115	-
18	CLA	a	804	18,1	1/1/13/20	6/25/103/115	-
18	CLA	b	838	-	1/1/15/20	5/37/115/115	-
18	CLA	a	826	1	1/1/15/20	12/37/115/115	-
18	CLA	E	316	-	1/1/13/20	7/27/105/115	-
21	BCR	f	205	-	-	2/29/63/63	0/2/2/2
18	CLA	b	817	2	1/1/14/20	17/31/109/115	-
18	CLA	H	310	-	1/1/14/20	9/31/109/115	-
18	CLA	D	215	-	1/1/10/20	2/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LHG	a	835	-	-	20/36/36/53	-
18	CLA	E	312	16	1/1/15/20	11/37/115/115	-
18	CLA	b	804	2	1/1/11/20	3/13/91/115	-
18	CLA	C	314	14	1/1/10/20	4/8/86/115	-
19	PQN	b	831	-	-	3/23/43/43	0/2/2/2
18	CLA	a	843	-	1/1/15/20	12/37/115/115	-
18	CLA	b	841	2	1/1/15/20	9/37/115/115	-
18	CLA	E	309	16	1/1/15/20	14/37/115/115	-
18	CLA	b	807	2	1/1/15/20	10/37/115/115	-
18	CLA	a	817	1	1/1/11/20	10/18/96/115	-
21	BCR	i	103	-	-	4/29/63/63	0/2/2/2
24	SF4	b	802	2	-	-	0/6/5/5
18	CLA	a	810	1	1/1/15/20	7/37/115/115	-
26	A86	r	203	-	-	6/34/90/90	0/3/3/3
18	CLA	H	308	17	1/1/15/20	10/37/115/115	-
21	BCR	a	834	-	-	4/29/63/63	0/2/2/2
18	CLA	f	202	-	1/1/15/20	10/37/115/115	-
18	CLA	C	312	14	1/1/14/20	10/33/111/115	-
18	CLA	f	203	-	1/1/15/20	10/37/115/115	-
26	A86	B	302	-	-	5/34/90/90	0/3/3/3
18	CLA	C	306	23	1/1/11/20	4/13/91/115	-
18	CLA	a	841	-	1/1/15/20	21/37/115/115	-
19	PQN	a	829	-	-	2/23/43/43	0/2/2/2
18	CLA	a	806	1	1/1/15/20	13/37/115/115	-
18	CLA	b	828	-	1/1/15/20	9/37/115/115	-
18	CLA	b	813	2	1/1/13/20	12/25/103/115	-
28	DD6	E	308	-	-	1/26/80/80	0/3/3/3
26	A86	H	302	-	-	5/34/90/90	0/3/3/3
18	CLA	H	311	17	1/1/13/20	8/28/106/115	-
18	CLA	B	307	13	1/1/15/20	7/37/115/115	-
23	LMG	j	103	-	-	16/32/52/70	0/1/1/1
18	CLA	b	806	2	1/1/15/20	17/37/115/115	-
18	CLA	a	830	20	1/1/12/20	6/22/100/115	-
18	CLA	b	808	2	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	a	840	-	1/1/15/20	13/37/115/115	-
18	CLA	b	805	2	1/1/15/20	13/37/115/115	-
20	LHG	H	316	-	-	19/38/38/53	-
23	LMG	E	318	-	-	21/38/58/70	0/1/1/1
29	KC1	C	313	-	-	7/15/71/71	-
18	CLA	a	854	-	1/1/15/20	16/37/115/115	-
26	A86	B	301	-	-	12/34/90/90	0/3/3/3
21	BCR	a	850	-	-	4/29/63/63	0/2/2/2
18	CLA	a	837	1	1/1/14/20	14/31/109/115	-
18	CLA	D	207	-	1/1/14/20	10/33/111/115	-
18	CLA	a	855	1	1/1/15/20	14/37/115/115	-
18	CLA	r	202	12	1/1/11/20	12/13/91/115	-
18	CLA	a	823	1	1/1/11/20	9/13/91/115	-
18	CLA	B	308	13	1/1/15/20	11/37/115/115	-
21	BCR	b	832	-	-	0/29/63/63	0/2/2/2
29	KC1	C	308	14	-	7/15/71/71	-
18	CLA	a	847	1	1/1/15/20	13/37/115/115	-
18	CLA	f	204	6	1/1/11/20	3/13/91/115	-
18	CLA	b	826	2	1/1/14/20	8/31/109/115	-
21	BCR	E	305	-	-	2/29/63/63	0/2/2/2
18	CLA	D	211	15	1/1/11/20	9/15/93/115	-
29	KC1	H	312	17	-	9/15/71/71	-
18	CLA	a	805	1	1/1/15/20	15/37/115/115	-
18	CLA	a	822	1	1/1/12/20	5/19/97/115	-
18	CLA	b	844	2	1/1/14/20	10/34/112/115	-
18	CLA	a	821	1	1/1/15/20	10/37/115/115	-
18	CLA	b	848	2	1/1/12/20	8/24/102/115	-
18	CLA	D	214	15	1/1/13/20	9/27/105/115	-
20	LHG	j	102	-	-	20/53/53/53	-
26	A86	B	304	-	-	3/34/90/90	0/3/3/3
18	CLA	b	849	-	1/1/15/20	14/37/115/115	-
18	CLA	a	828	1	1/1/15/20	11/37/115/115	-
18	CLA	b	811	2	1/1/14/20	9/31/109/115	-
20	LHG	a	831	-	-	26/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	b	836	-	-	5/29/63/63	0/2/2/2
18	CLA	b	843	2	1/1/15/20	17/37/115/115	-
18	CLA	H	307	17	1/1/15/20	15/37/115/115	-
26	A86	m	102	-	-	7/34/90/90	0/3/3/3
18	CLA	a	827	1	1/1/15/20	10/37/115/115	-
18	CLA	j	104	9	1/1/10/20	2/8/86/115	-
20	LHG	E	317	-	-	6/46/46/53	-
21	BCR	a	845	-	-	2/29/63/63	0/2/2/2
18	CLA	l	203	10	1/1/15/20	16/37/115/115	-
18	CLA	b	810	2	1/1/15/20	10/37/115/115	-
18	CLA	C	316	14	1/1/10/20	3/8/86/115	-
18	CLA	b	825	-	1/1/11/20	4/13/91/115	-
20	LHG	D	201	-	-	32/53/53/53	-
28	DD6	D	205	-	-	3/26/80/80	0/3/3/3
18	CLA	b	846	2	1/1/15/20	12/37/115/115	-
18	CLA	a	818	1	1/1/12/20	5/21/99/115	-
18	CLA	E	313	16	1/1/13/20	9/25/103/115	-
18	CLA	b	850	2	1/1/15/20	12/37/115/115	-
18	CLA	a	819	1	1/1/15/20	4/37/115/115	-
18	CLA	b	842	2	1/1/15/20	14/37/115/115	-
18	CLA	a	802	-	1/1/15/20	10/37/115/115	-
21	BCR	b	839	-	-	6/29/63/63	0/2/2/2
21	BCR	l	204	-	-	8/29/63/63	0/2/2/2
26	A86	C	305	-	-	4/34/90/90	0/3/3/3
18	CLA	D	210	-	1/1/13/20	6/27/105/115	-
24	SF4	c	101	3	-	-	0/6/5/5
18	CLA	b	815	2	1/1/11/20	5/15/93/115	-
18	CLA	b	824	-	1/1/15/20	17/37/115/115	-
21	BCR	b	833	-	-	6/29/63/63	0/2/2/2
18	CLA	b	820	2	1/1/15/20	17/37/115/115	-
18	CLA	b	803	2	1/1/15/20	16/37/115/115	-
18	CLA	C	309	-	1/1/14/20	12/34/112/115	-
18	CLA	a	815	1	1/1/15/20	15/37/115/115	-

The worst 5 of 1371 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	849	SQD	C6-S	-12.47	1.59	1.77
23	E	318	LMG	O2-C2	-10.74	1.17	1.43
23	D	202	LMG	O2-C2	-9.35	1.21	1.43
28	H	303	DD6	C29-C27	-9.22	1.24	1.42
28	C	303	DD6	C29-C27	-9.14	1.25	1.42

The worst 5 of 2085 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	j	103	LMG	O2-C2-C1	-21.31	58.28	110.05
23	a	851	LMG	O2-C2-C1	-18.81	64.35	110.05
28	E	304	DD6	C21-C20-C15	-16.18	95.14	122.26
26	r	203	A86	O1-C20-C19	-15.79	101.52	113.38
23	C	301	LMG	O2-C2-C1	15.25	147.09	110.05

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 2052 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	802	CLA	CHA-CBD-CGD-O1D
18	a	802	CLA	CHA-CBD-CGD-O2D
18	a	803	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

68 monomers are involved in 244 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	E	304	DD6	1	0
26	D	203	A86	4	0
29	B	313	KC1	5	0
18	C	307	CLA	5	0
18	C	310	CLA	4	0

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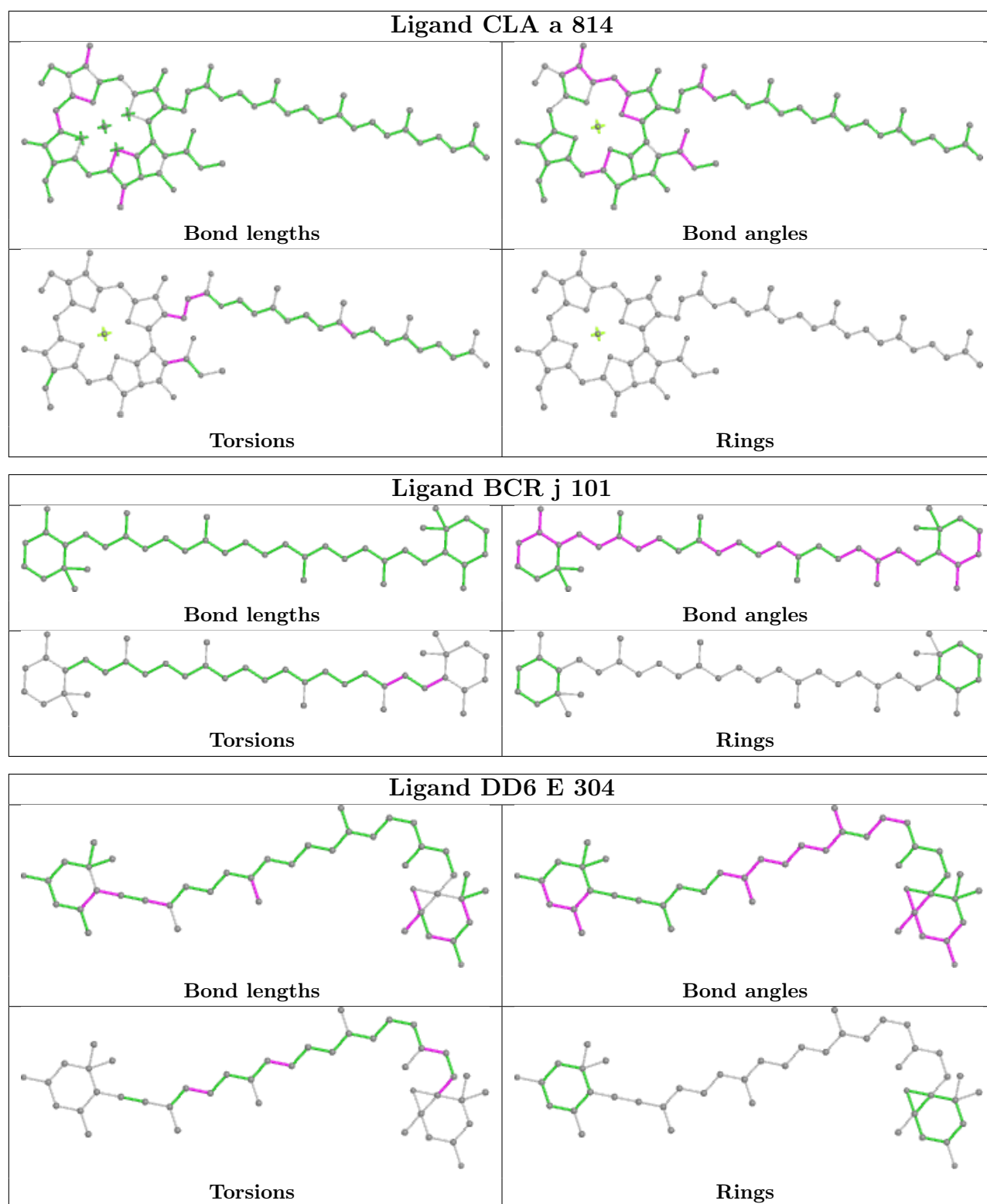
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	D	212	CLA	2	0
18	B	312	CLA	8	0
18	E	310	CLA	1	0
18	H	313	CLA	7	0
23	C	319	LMG	2	0
28	E	307	DD6	1	0
28	C	303	DD6	1	0
26	D	204	A86	2	0
18	B	311	CLA	6	0
18	H	306	CLA	10	0
18	B	309	CLA	2	0
18	E	315	CLA	3	0
18	H	314	CLA	4	0
18	H	305	CLA	5	0
28	H	303	DD6	3	0
18	D	217	CLA	3	0
18	C	315	CLA	2	0
20	E	301	LHG	2	0
18	E	311	CLA	1	0
18	B	314	CLA	2	0
18	C	317	CLA	9	0
18	H	309	CLA	13	0
18	C	318	CLA	12	0
26	C	304	A86	1	0
18	D	209	CLA	4	0
18	C	311	CLA	7	0
18	B	306	CLA	16	0
18	D	216	CLA	4	0
20	B	315	LHG	2	0
28	B	303	DD6	1	0
21	E	306	BCR	4	0
18	D	208	CLA	9	0
18	E	316	CLA	6	0
18	H	310	CLA	4	0
18	D	215	CLA	6	0
18	E	312	CLA	8	0
18	C	314	CLA	3	0
18	E	309	CLA	6	0
18	H	308	CLA	5	0
18	C	312	CLA	10	0
26	B	302	A86	4	0
18	C	306	CLA	1	0

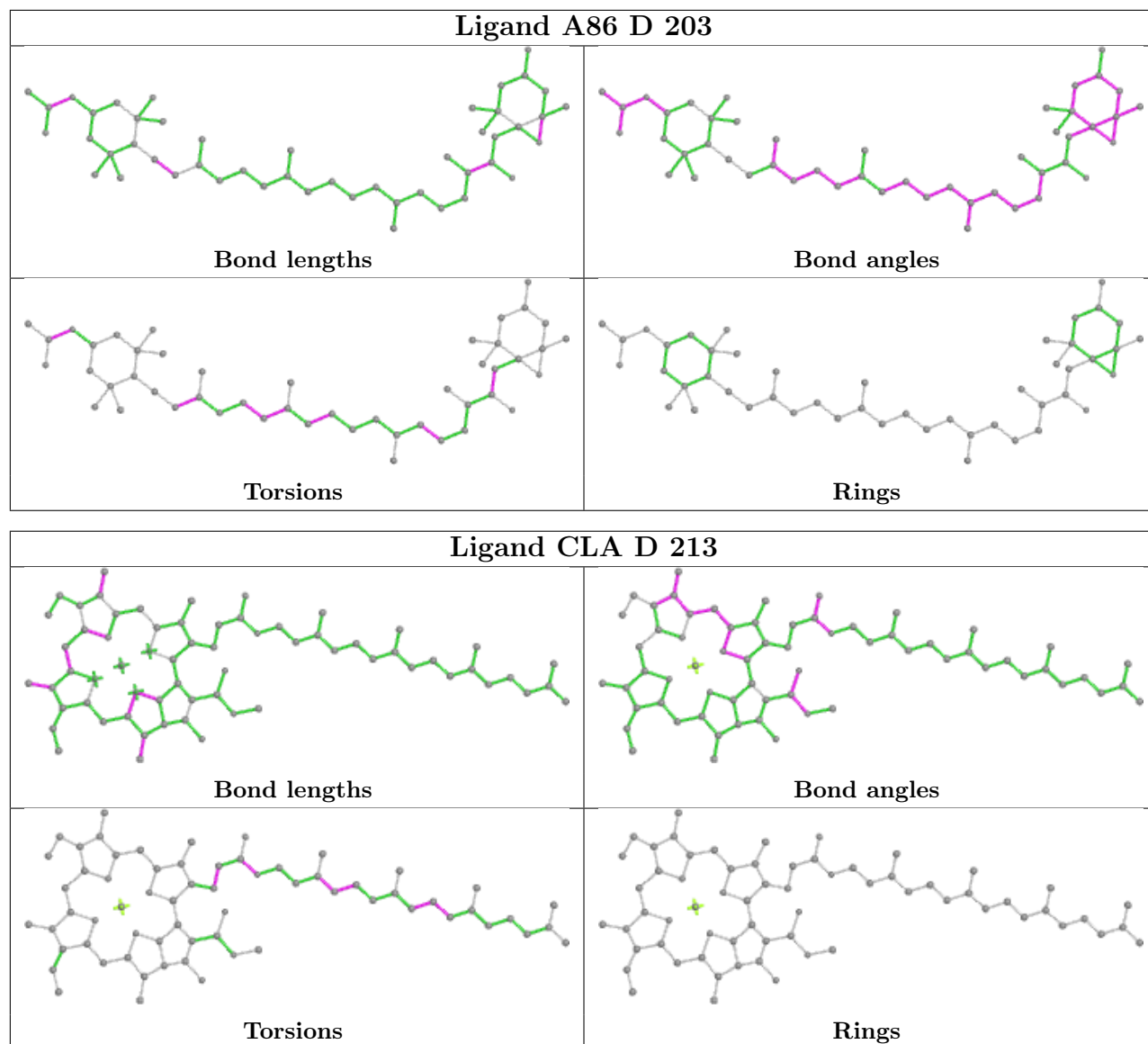
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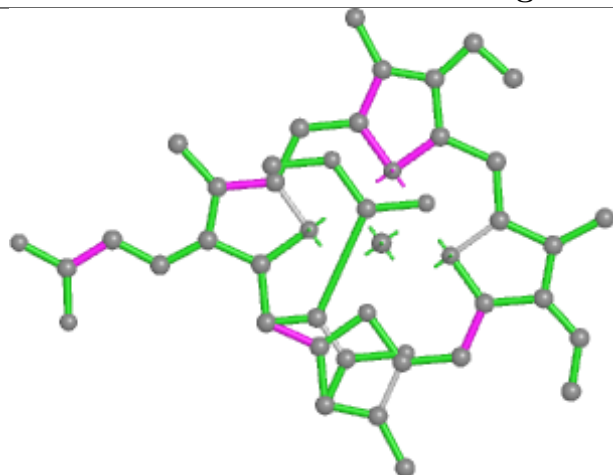
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	H	302	A86	14	0
18	H	311	CLA	7	0
18	B	307	CLA	5	0
23	E	318	LMG	3	0
26	B	301	A86	2	0
18	D	207	CLA	3	0
18	B	308	CLA	2	0
29	C	308	KC1	4	0
21	E	305	BCR	1	0
18	D	211	CLA	2	0
29	H	312	KC1	1	0
18	D	214	CLA	5	0
26	B	304	A86	2	0
18	H	307	CLA	3	0
18	C	316	CLA	10	0
20	D	201	LHG	6	0
28	D	205	DD6	2	0
18	E	313	CLA	3	0
26	C	305	A86	4	0
18	D	210	CLA	3	0
18	C	309	CLA	6	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.

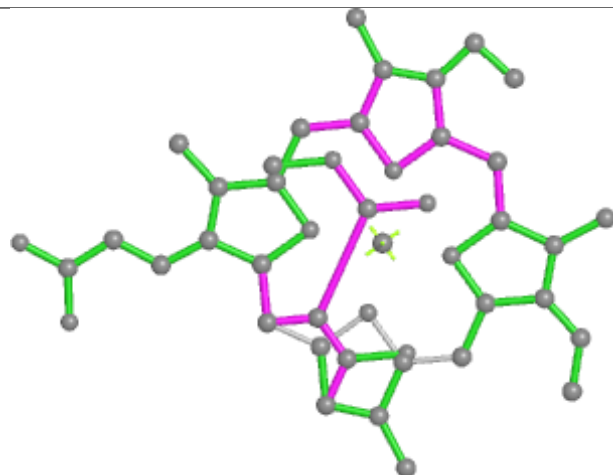




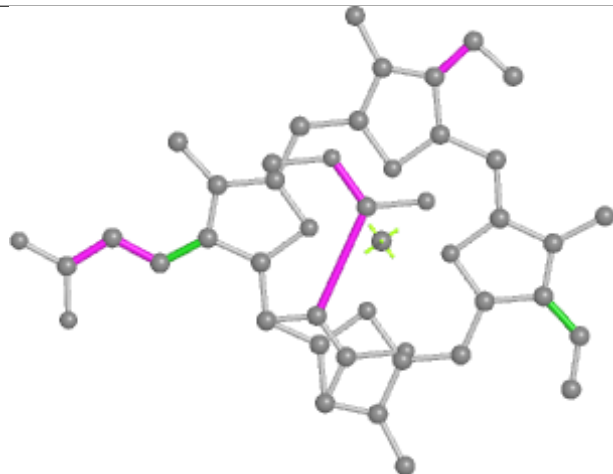
Ligand KC1 B 313



Bond lengths



Bond angles

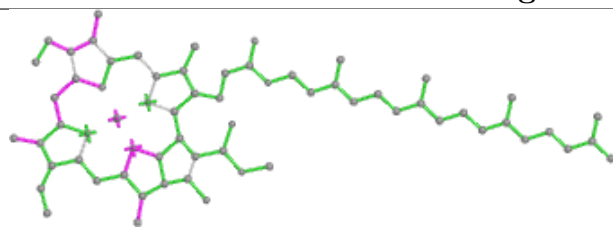


Torsions

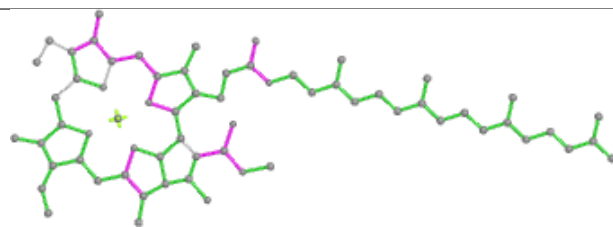


Rings

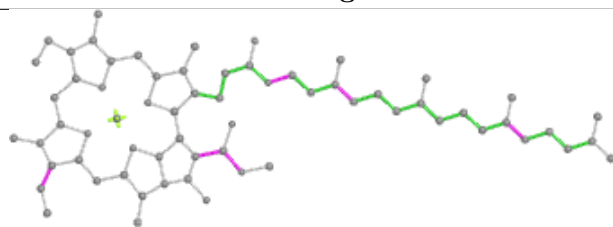
Ligand CLA a 842



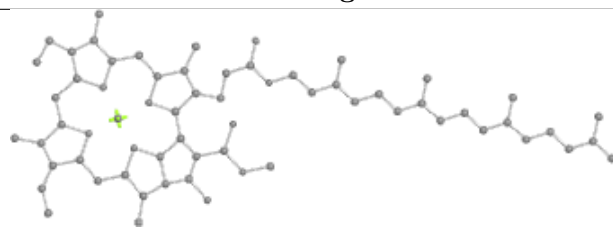
Bond lengths



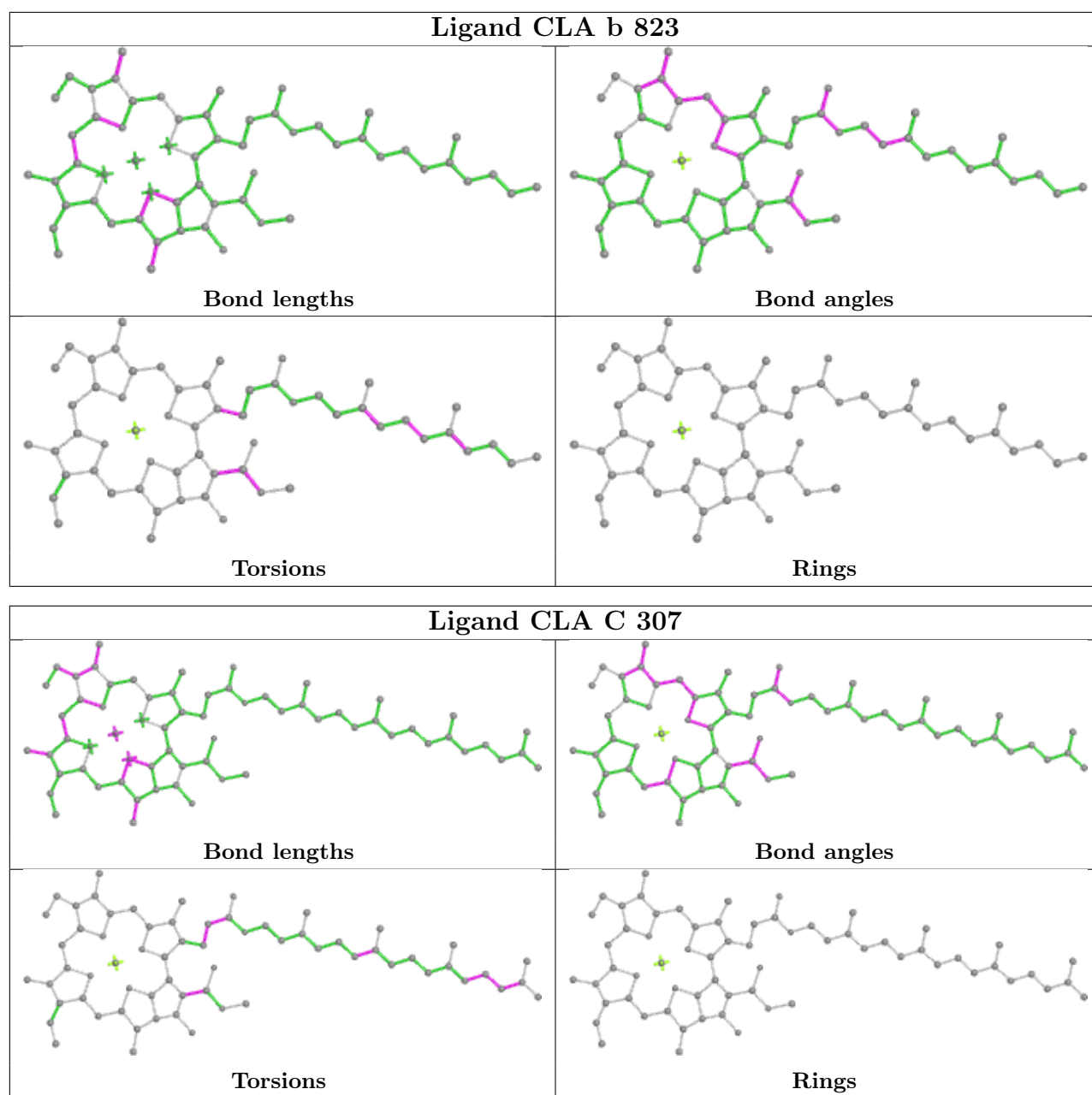
Bond angles



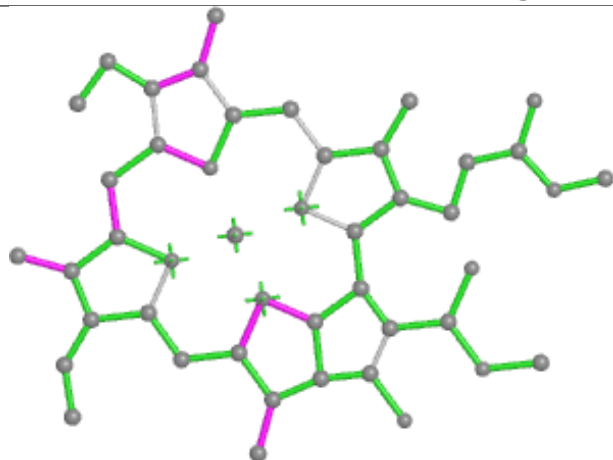
Torsions



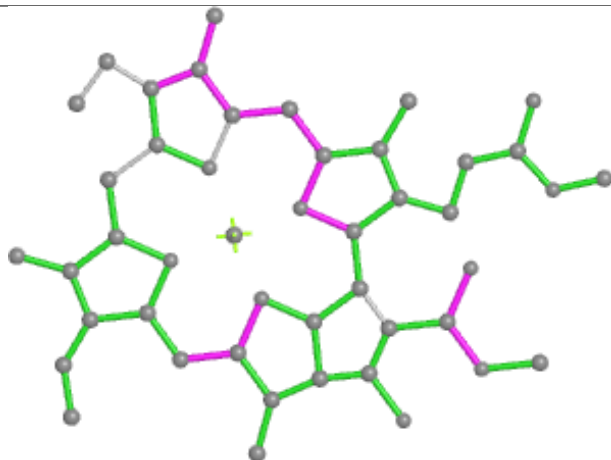
Rings



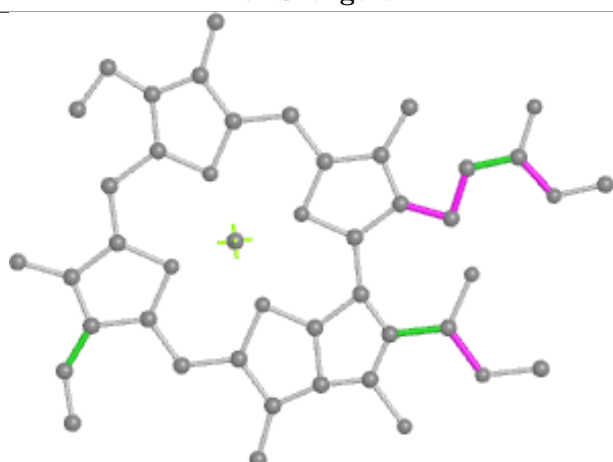
Ligand CLA C 310



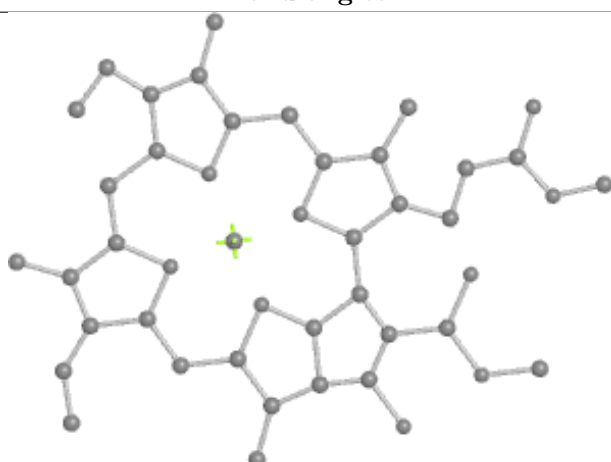
Bond lengths



Bond angles

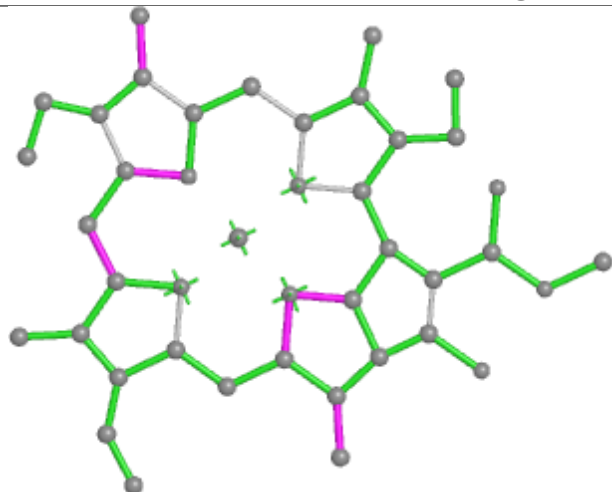


Torsions

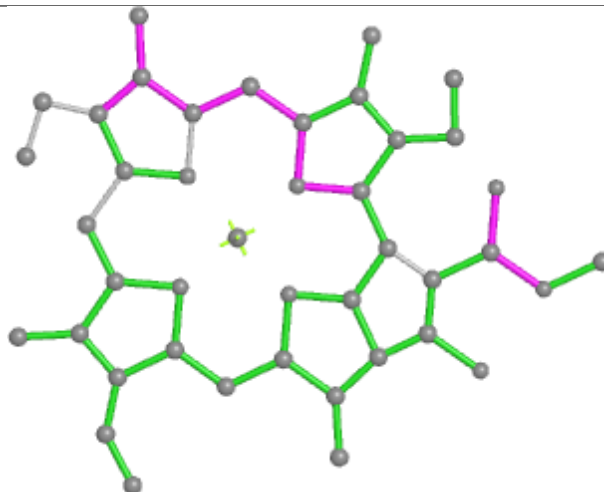


Rings

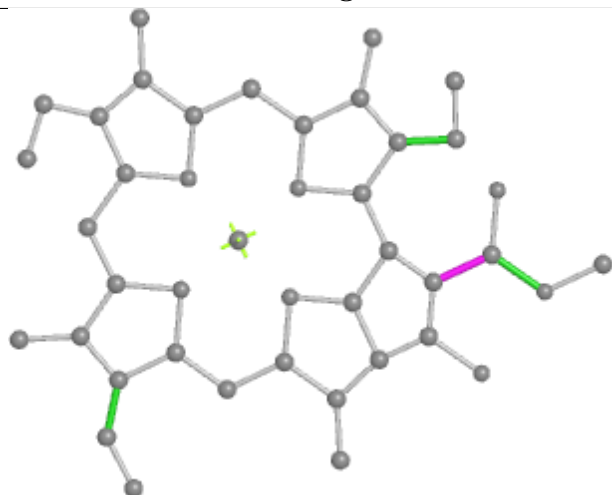
Ligand CLA D 212



Bond lengths



Bond angles

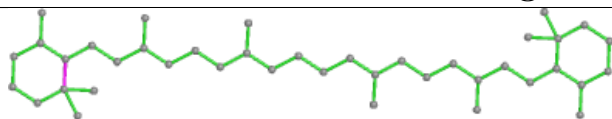


Torsions

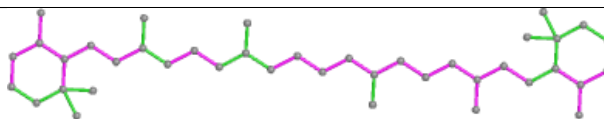


Rings

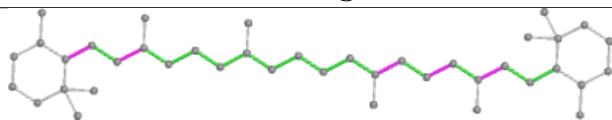
Ligand BCR f 201



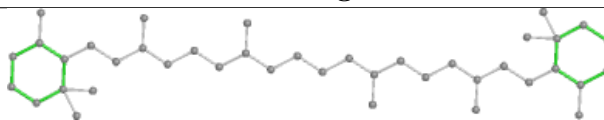
Bond lengths



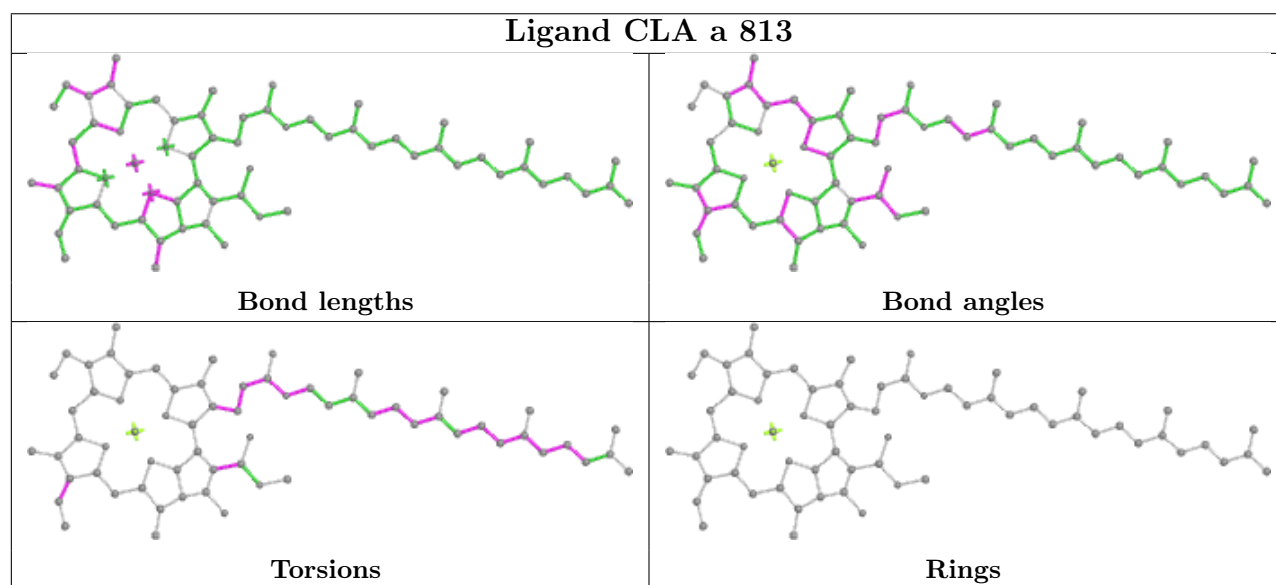
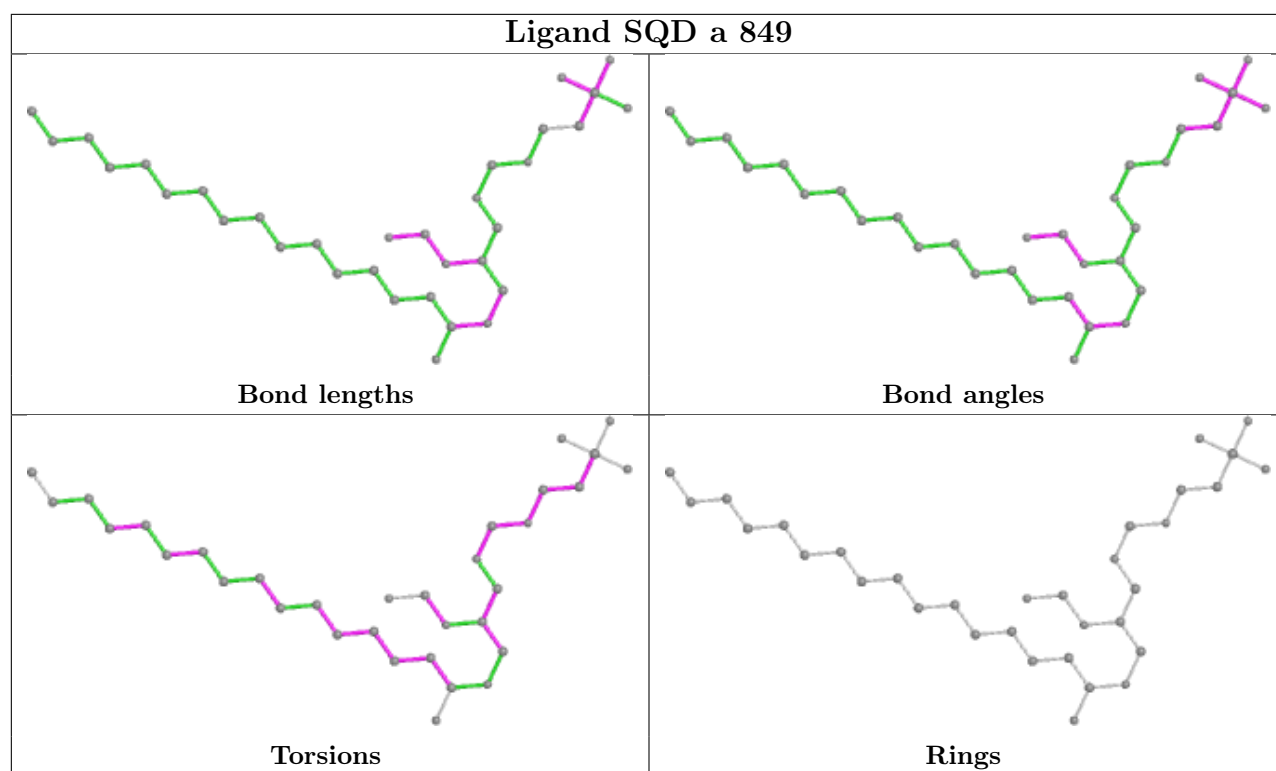
Bond angles

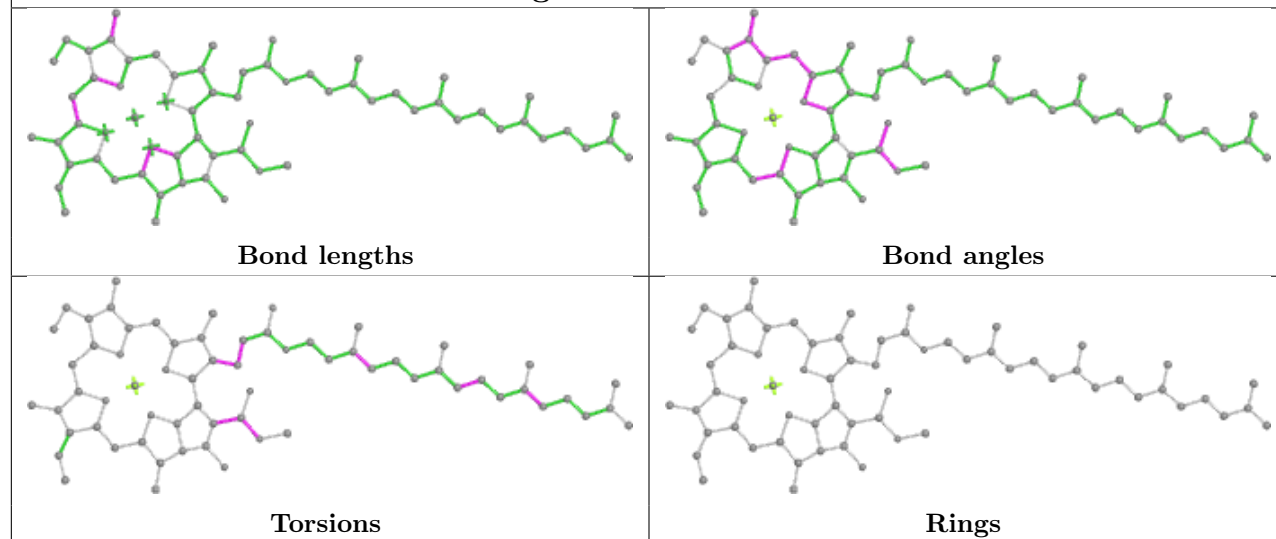
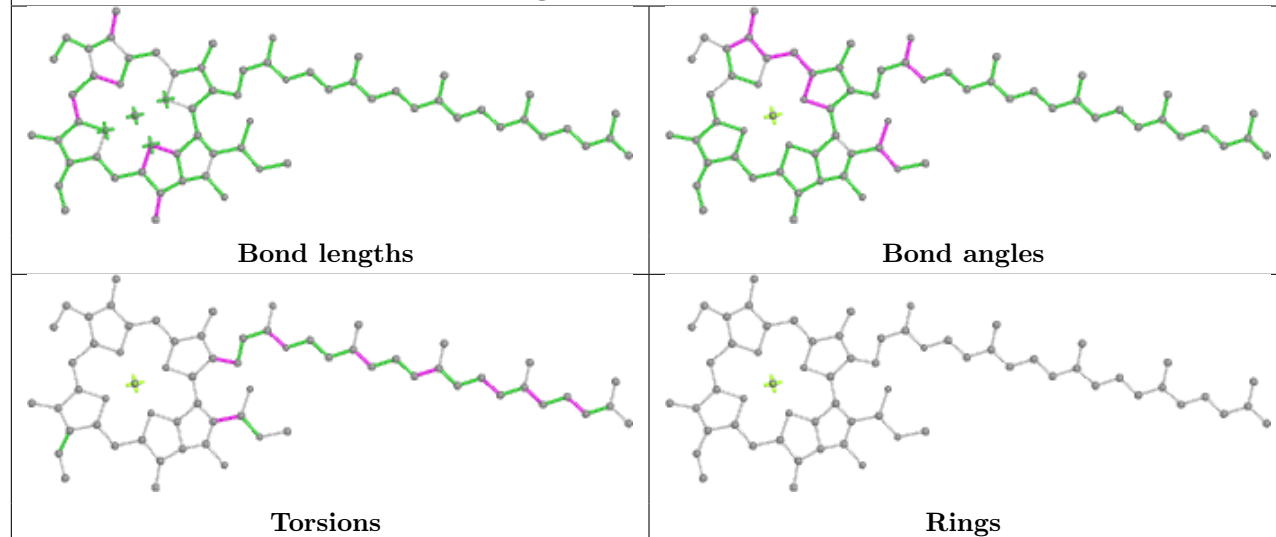
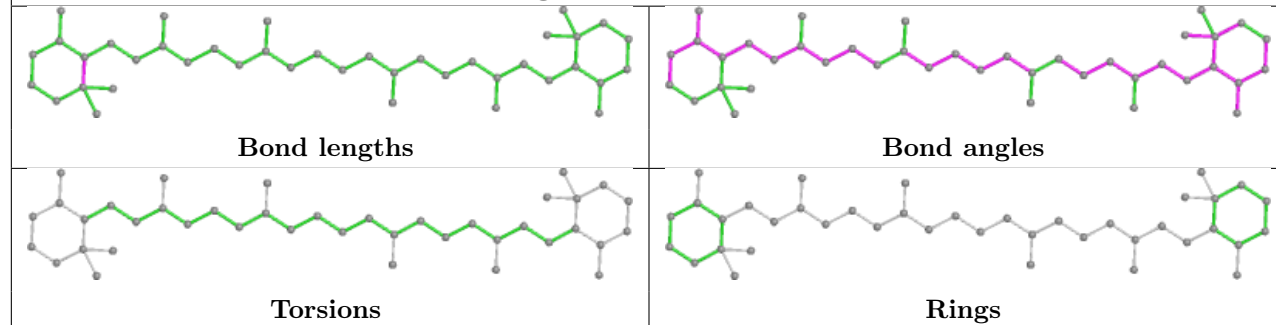


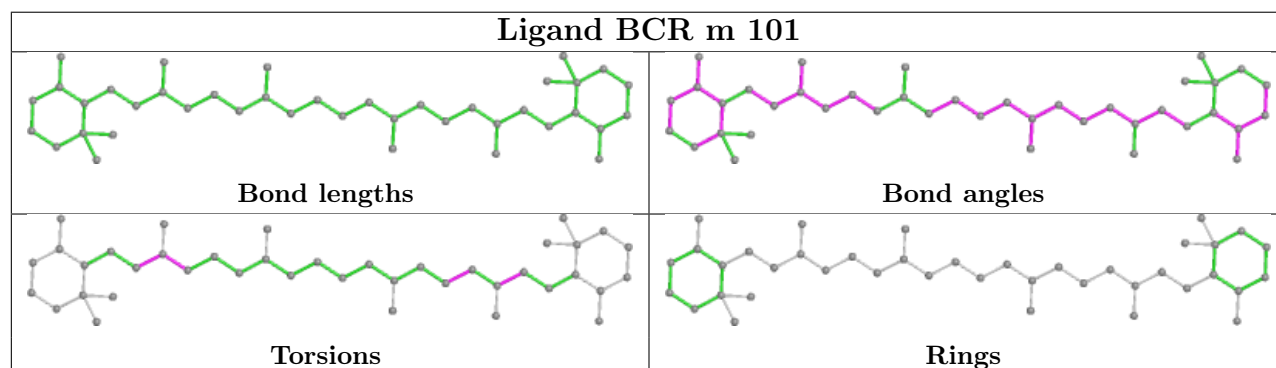
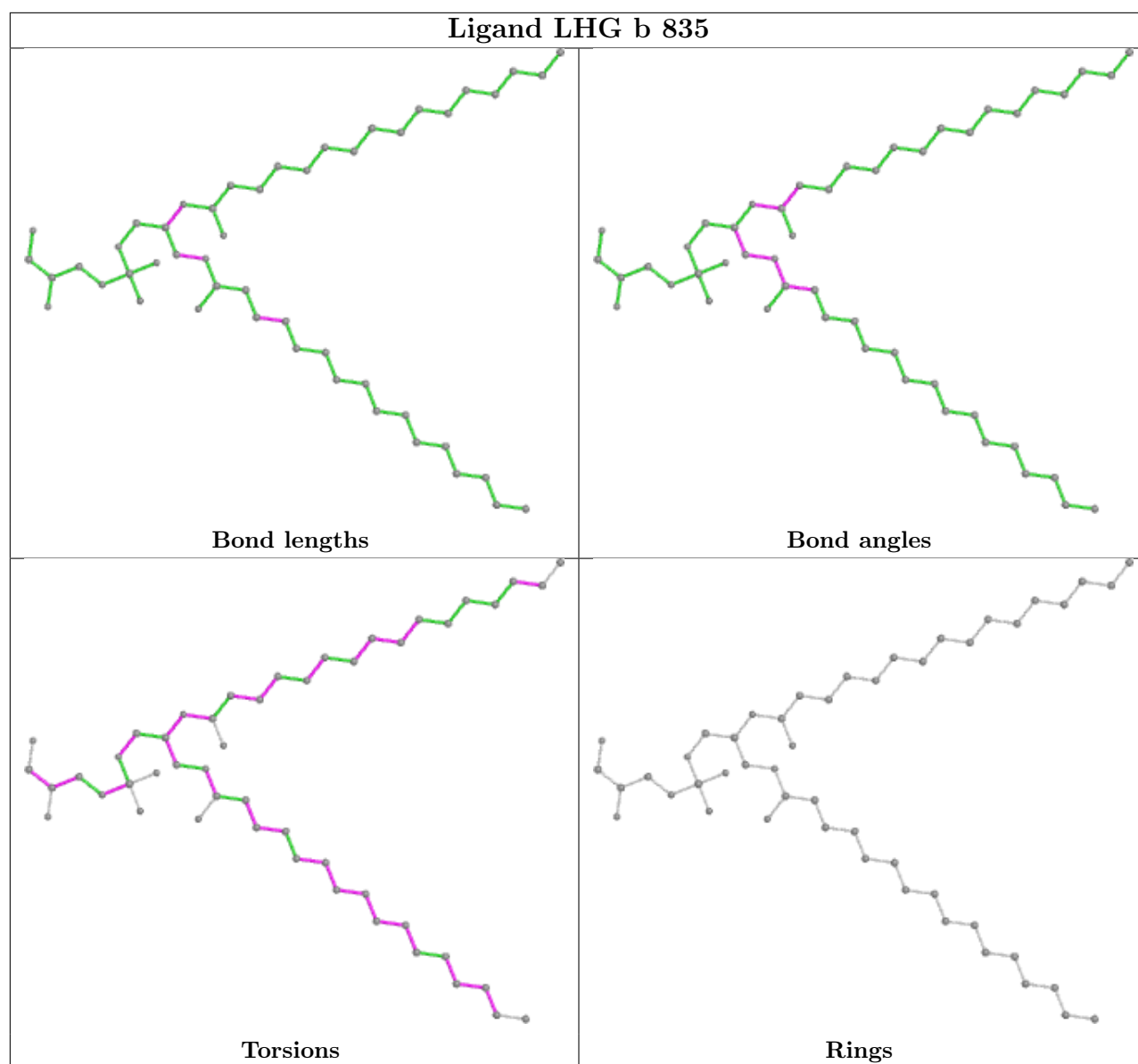
Torsions

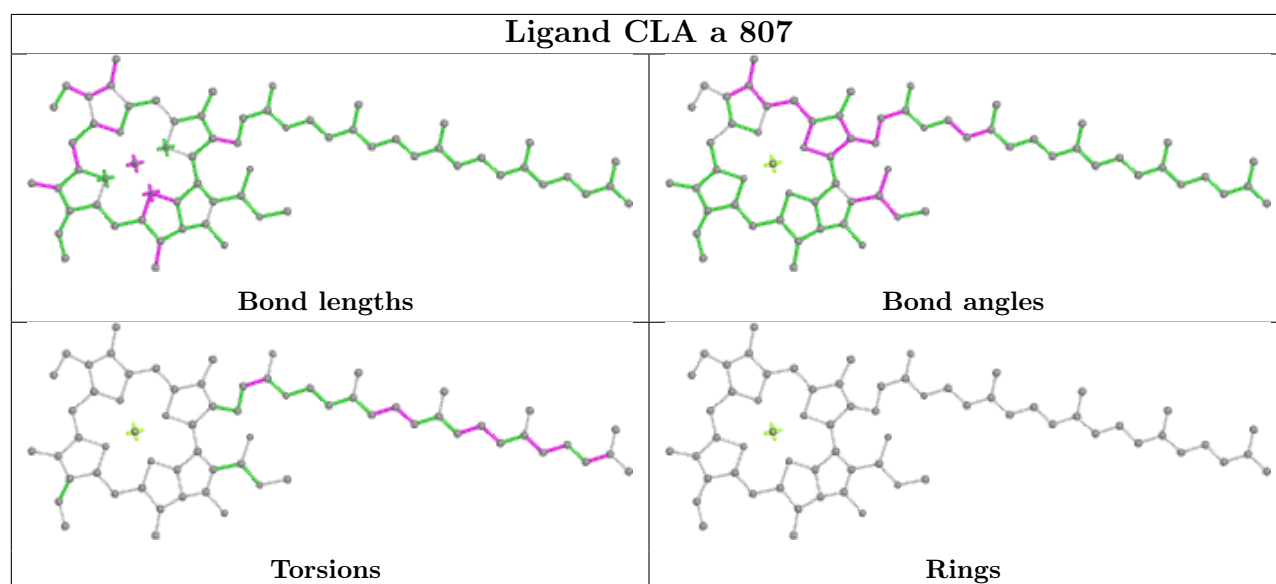
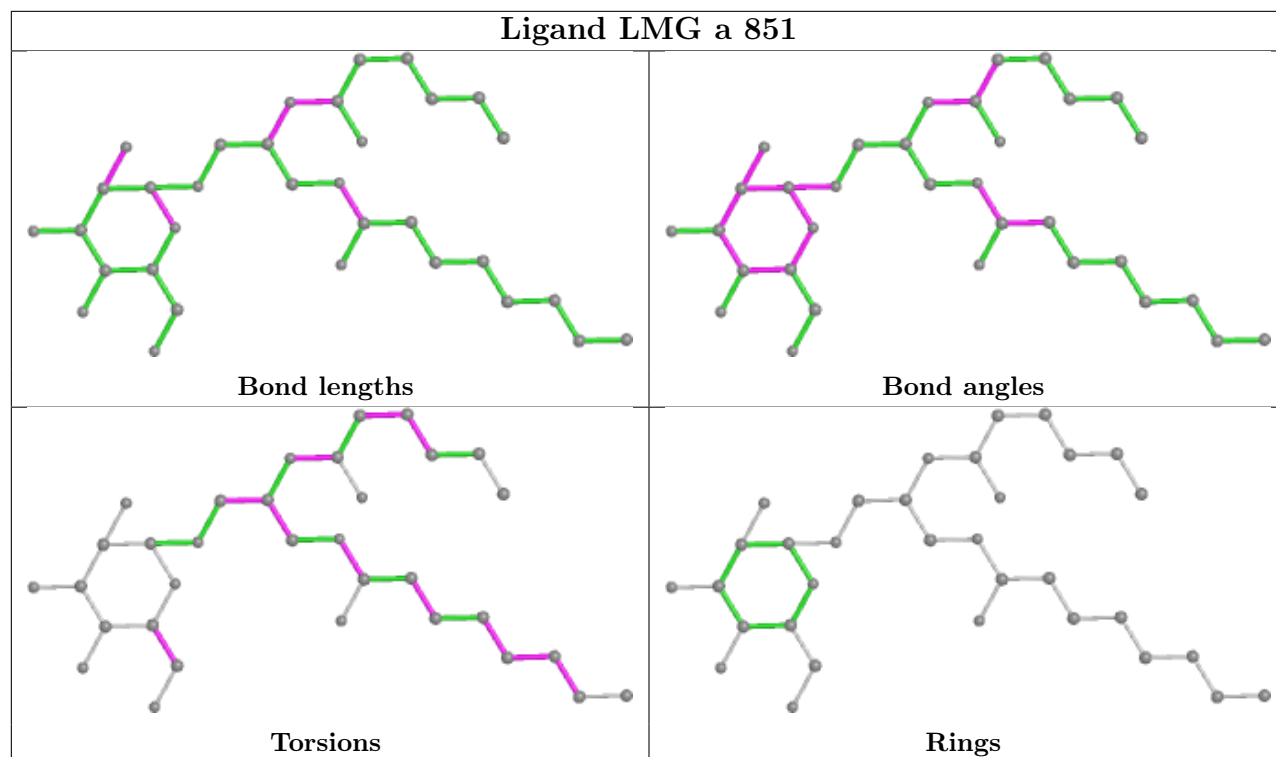
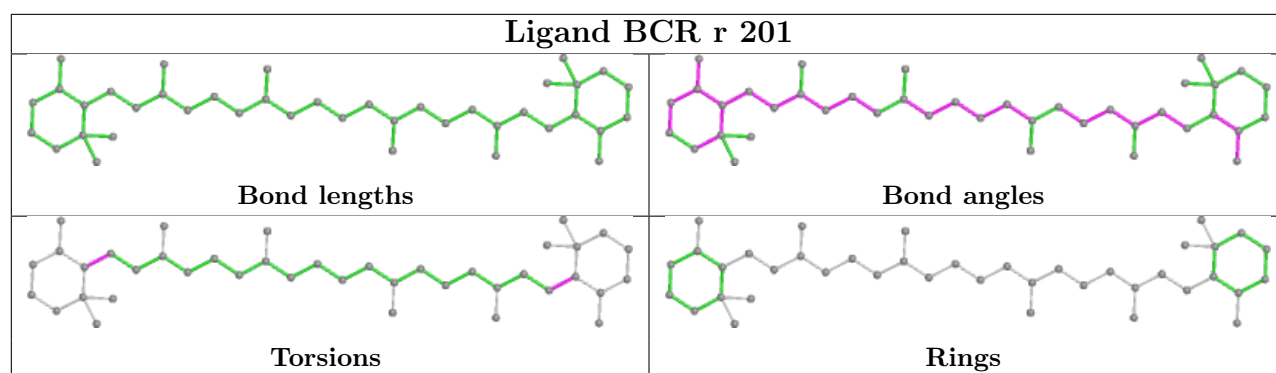


Rings

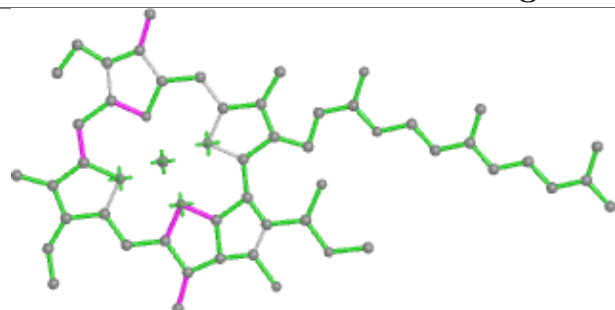


Ligand CLA B 312**Ligand CLA E 310****Ligand BCR a 833**

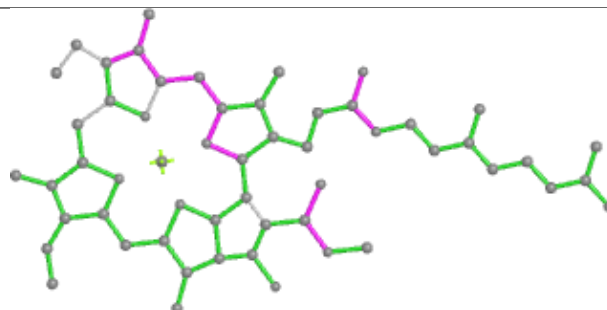




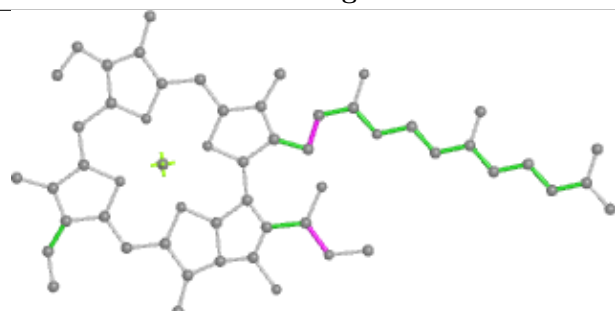
Ligand CLA b 816



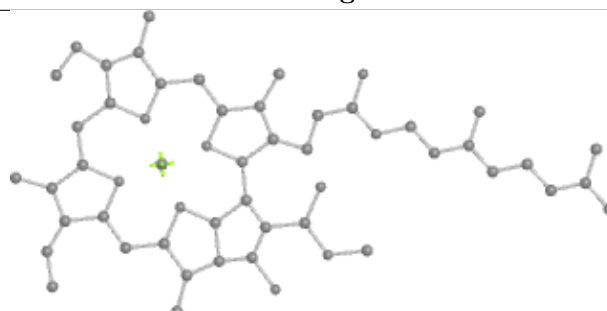
Bond lengths



Bond angles

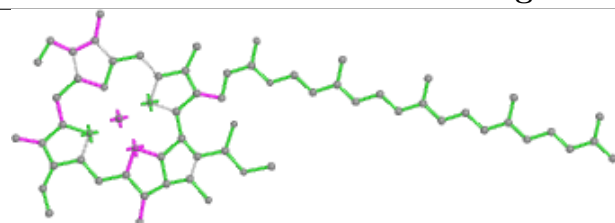


Torsions

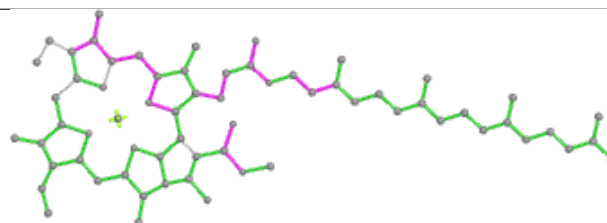


Rings

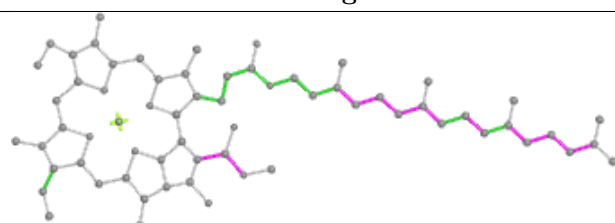
Ligand CLA H 313



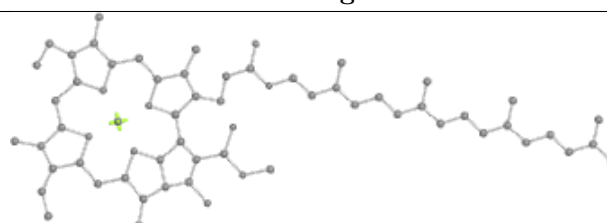
Bond lengths



Bond angles

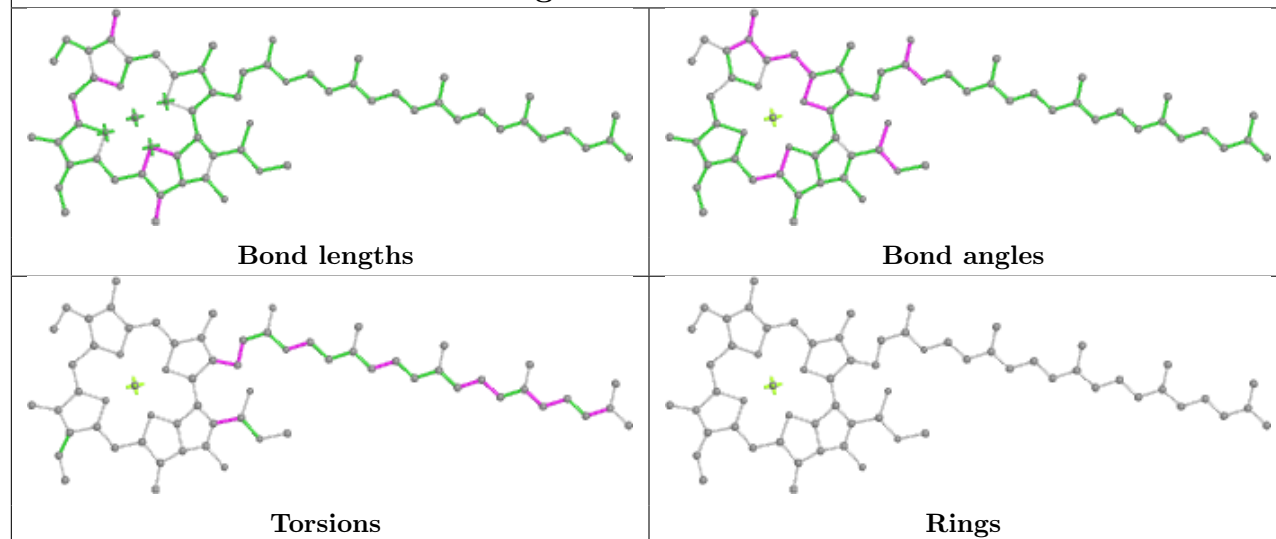


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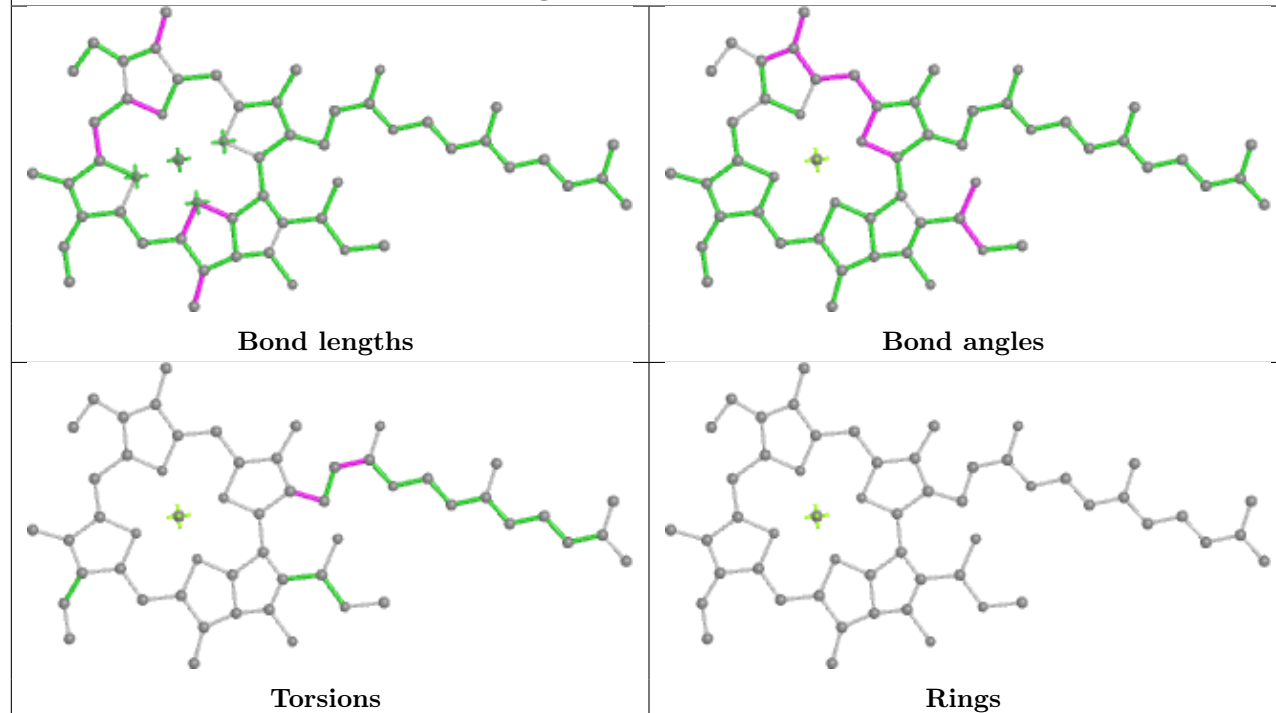


Rings

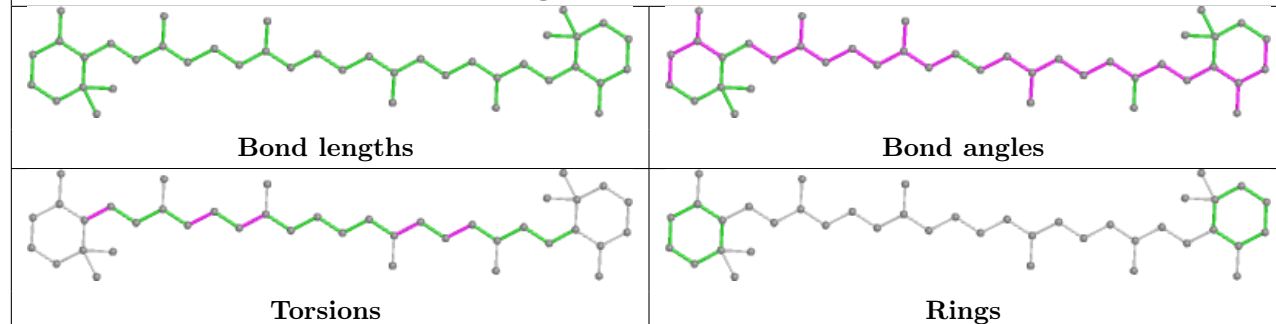
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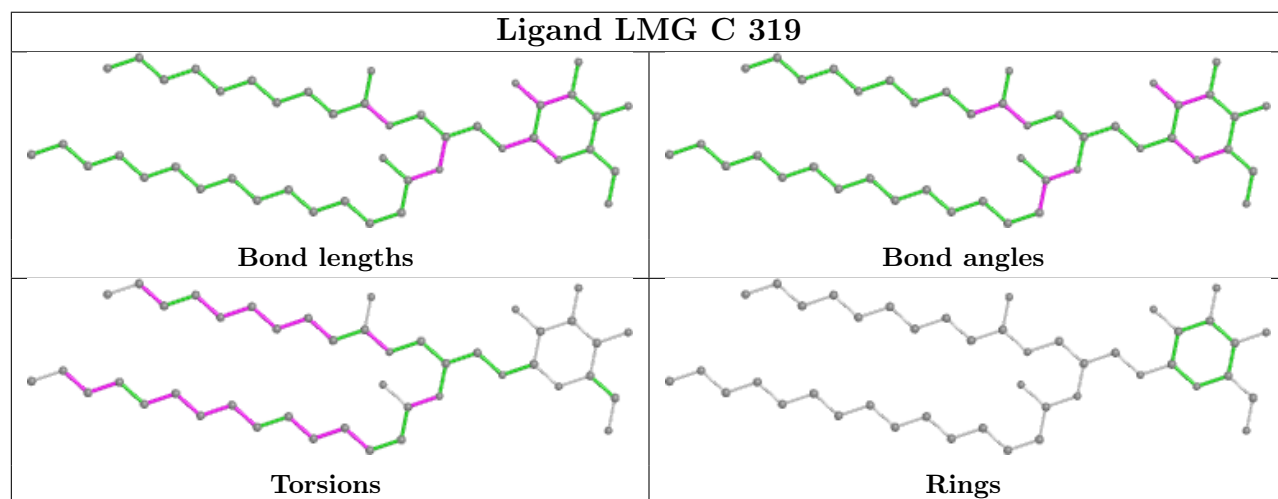
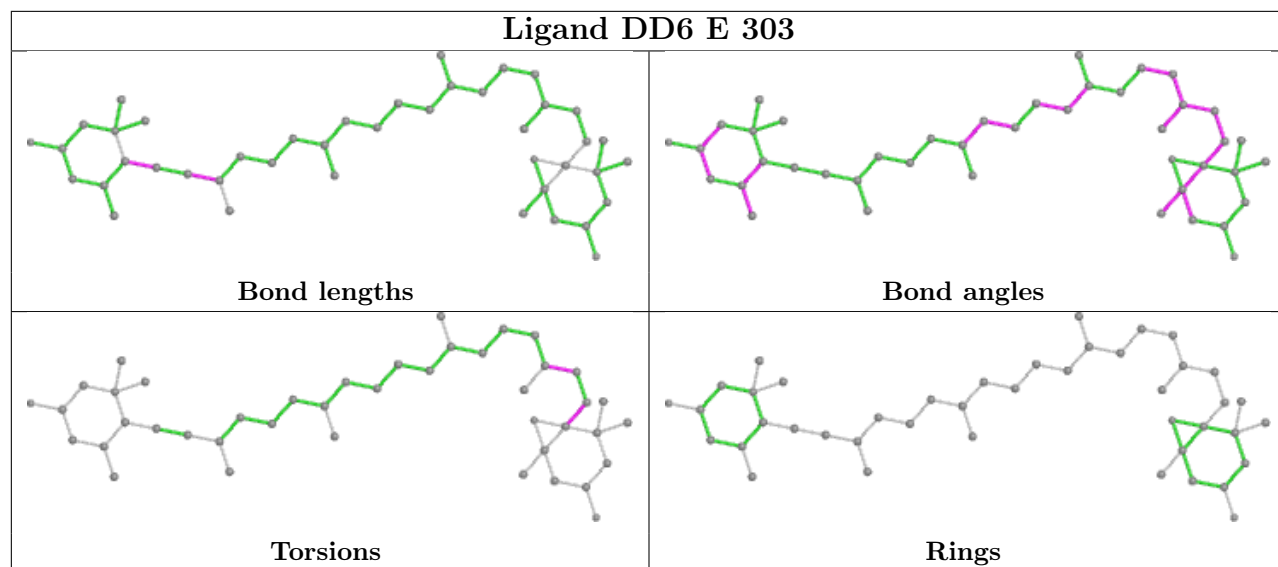


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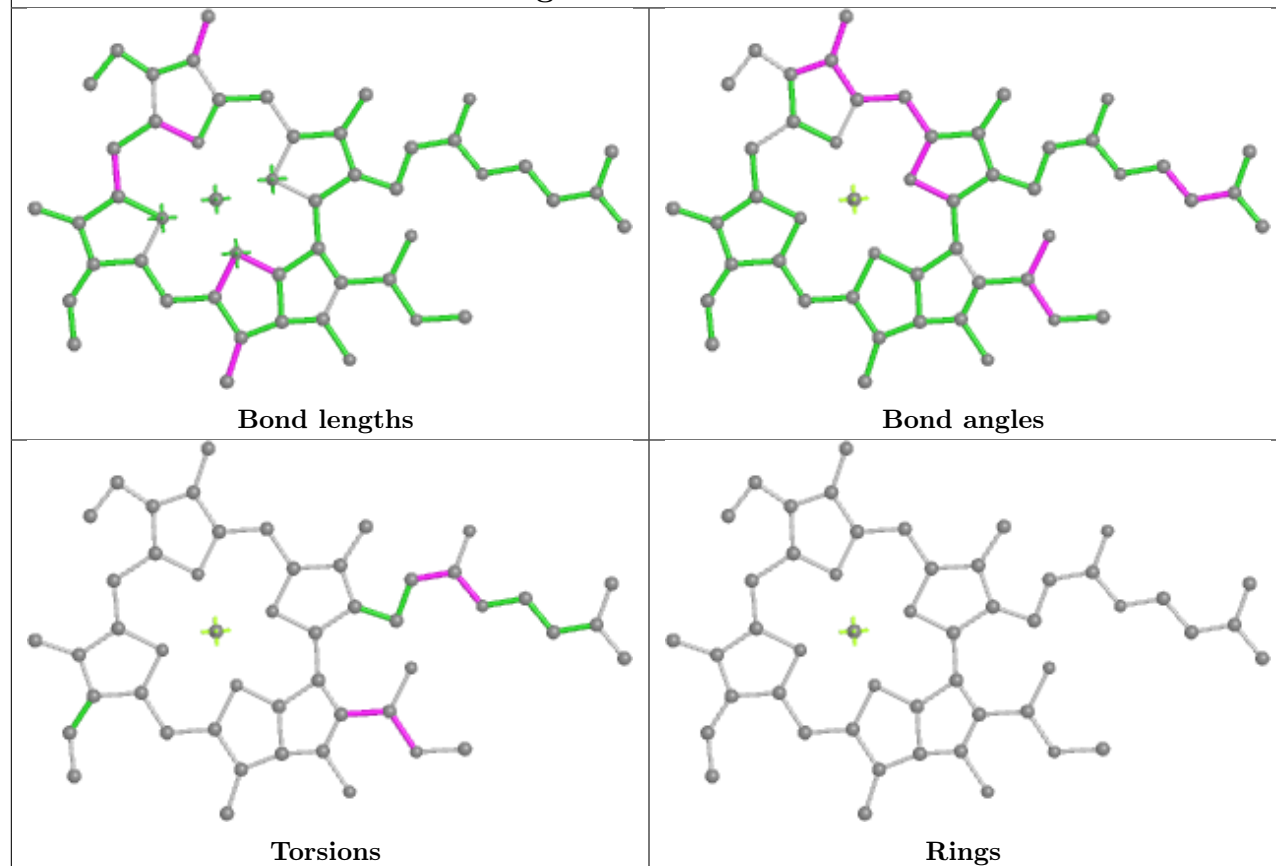


Ligand BCR a 852

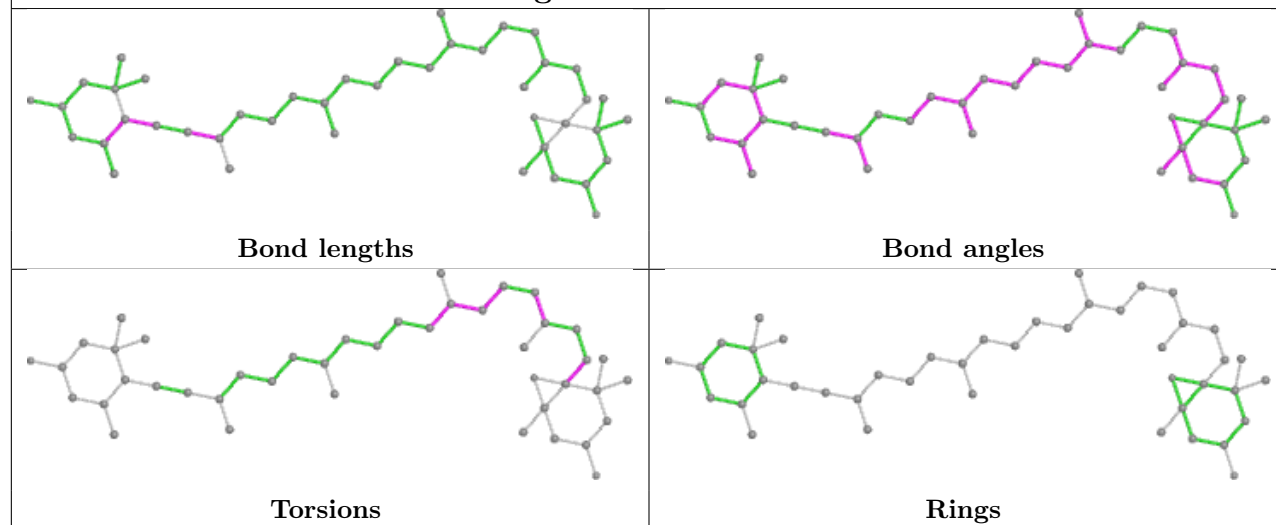


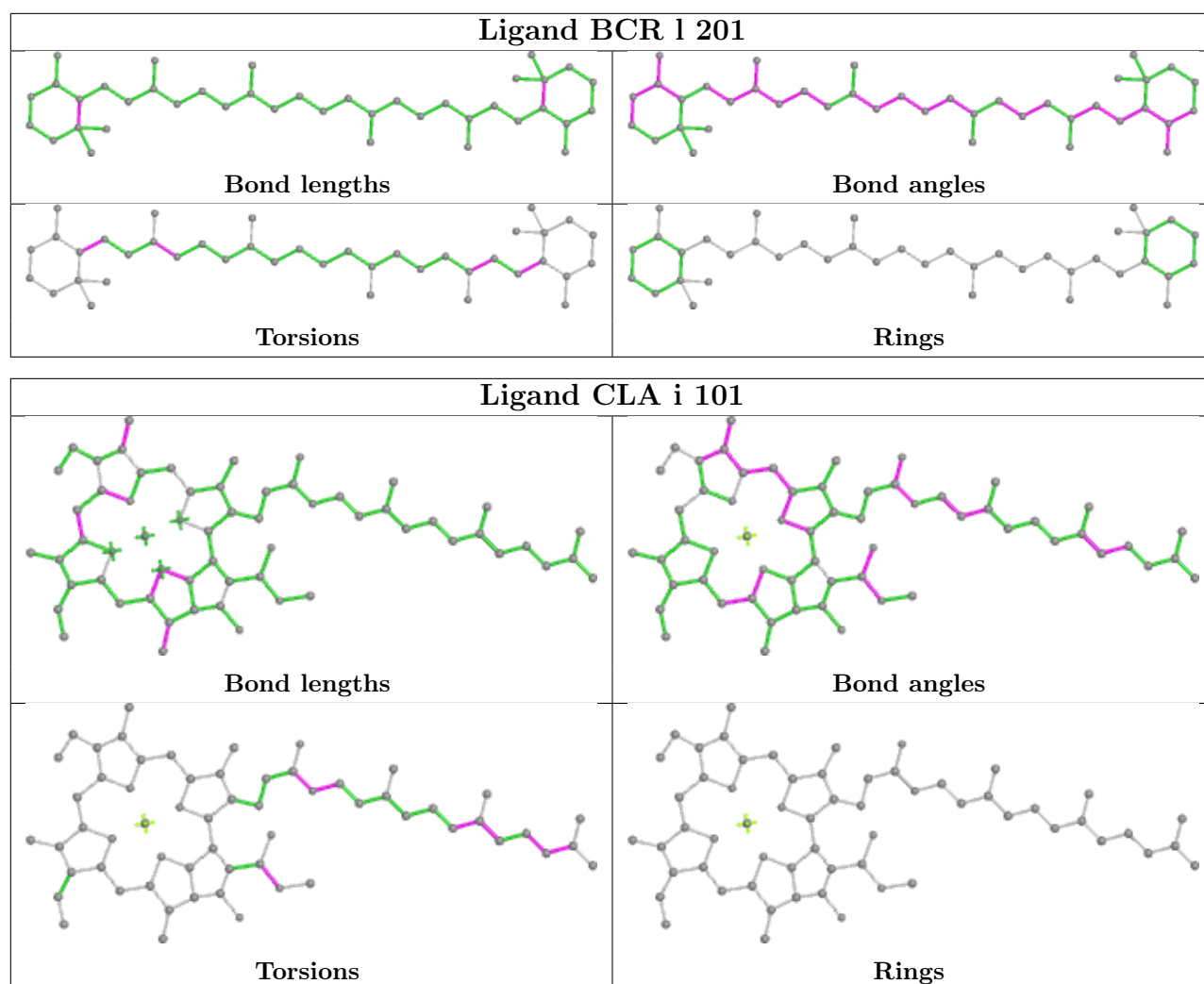


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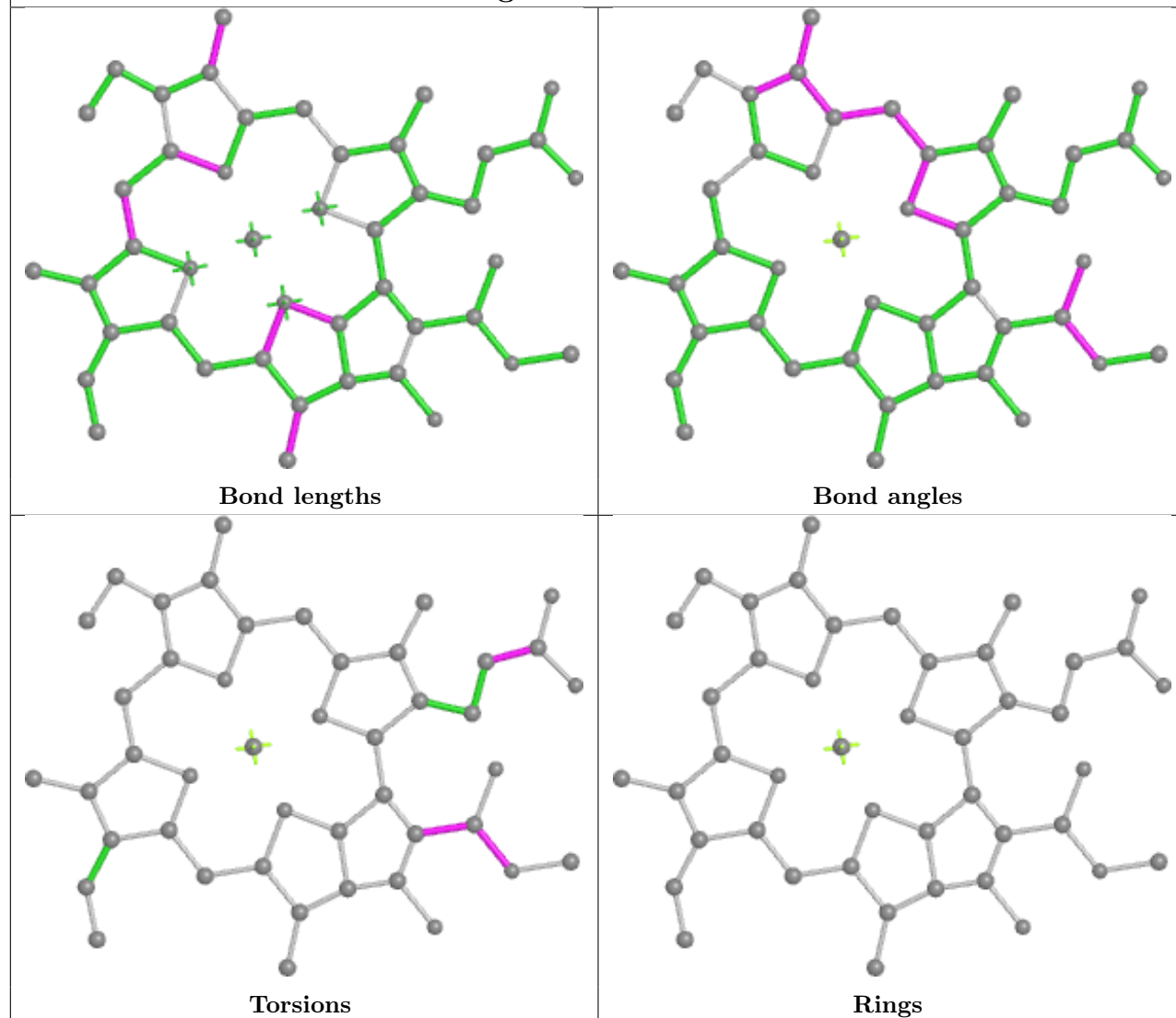


Ligand DD6 E 307

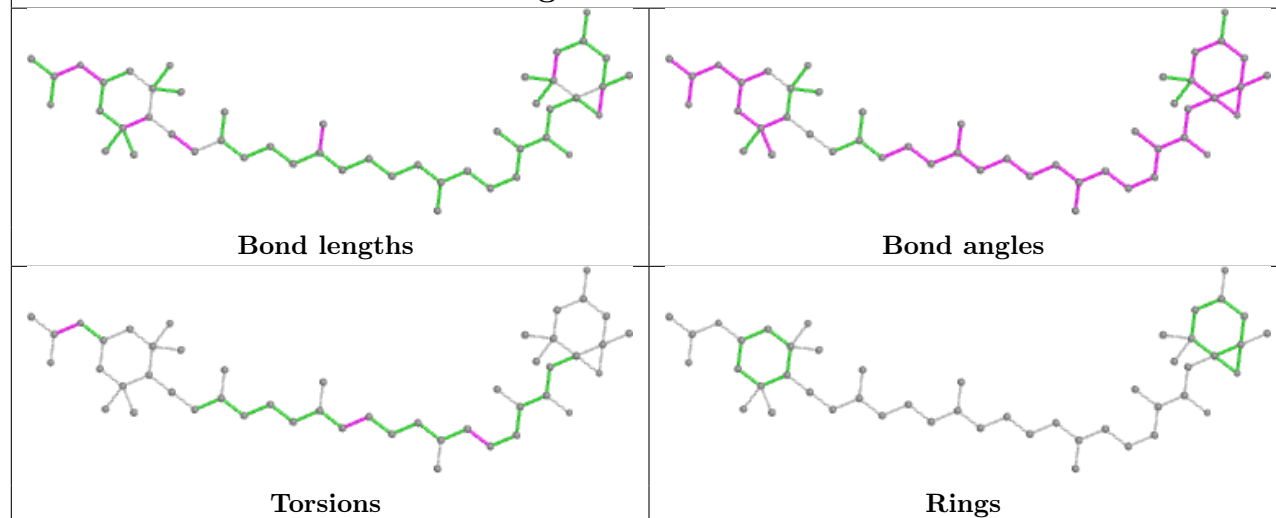




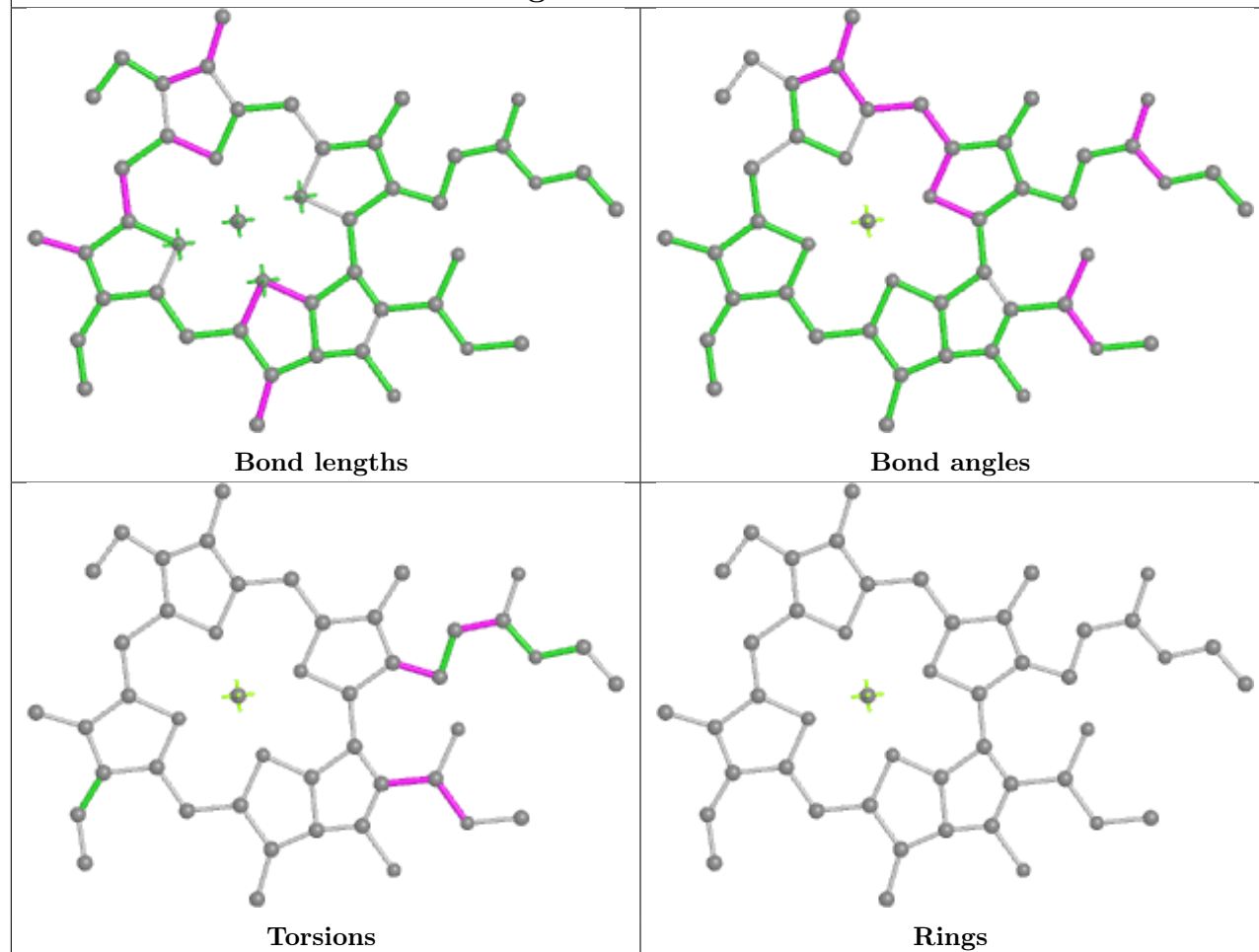
Ligand CLA 1 205



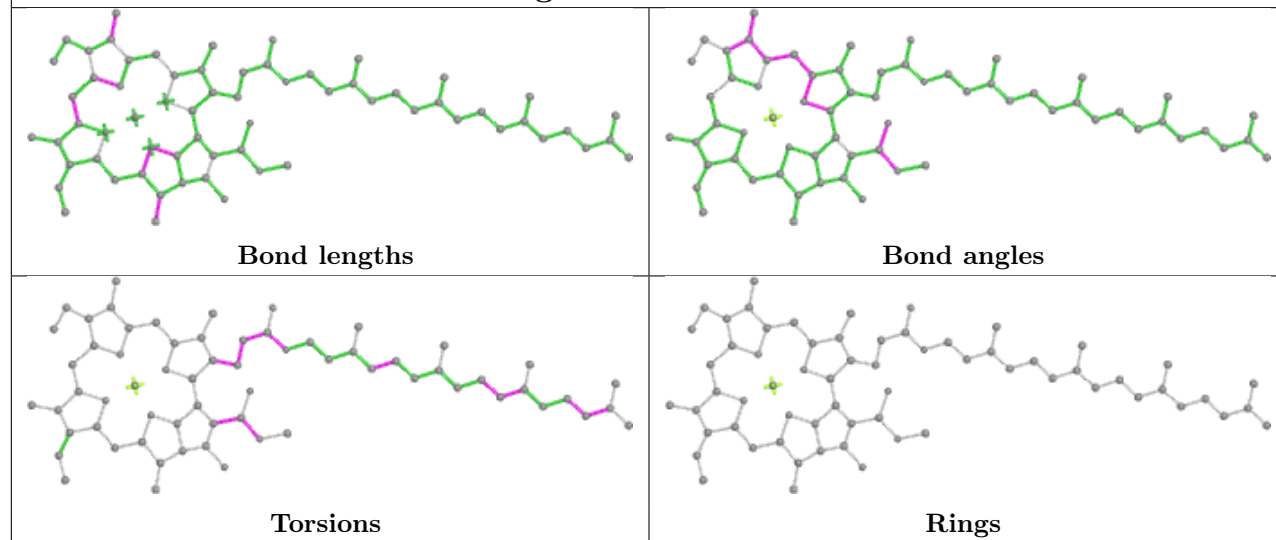
Ligand A86 B 305

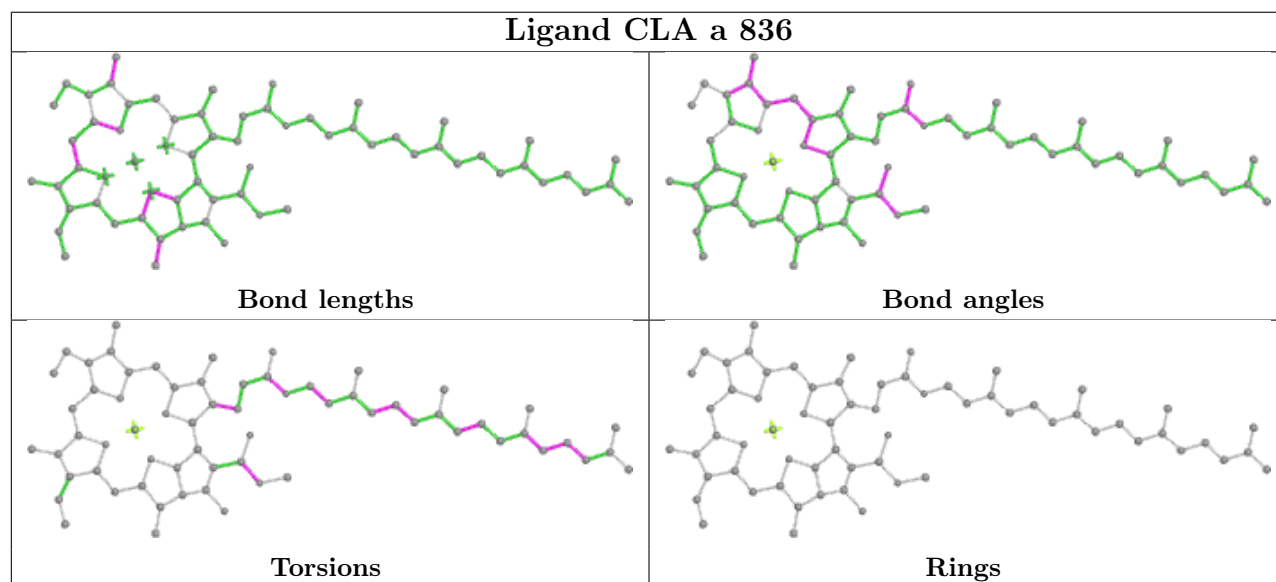
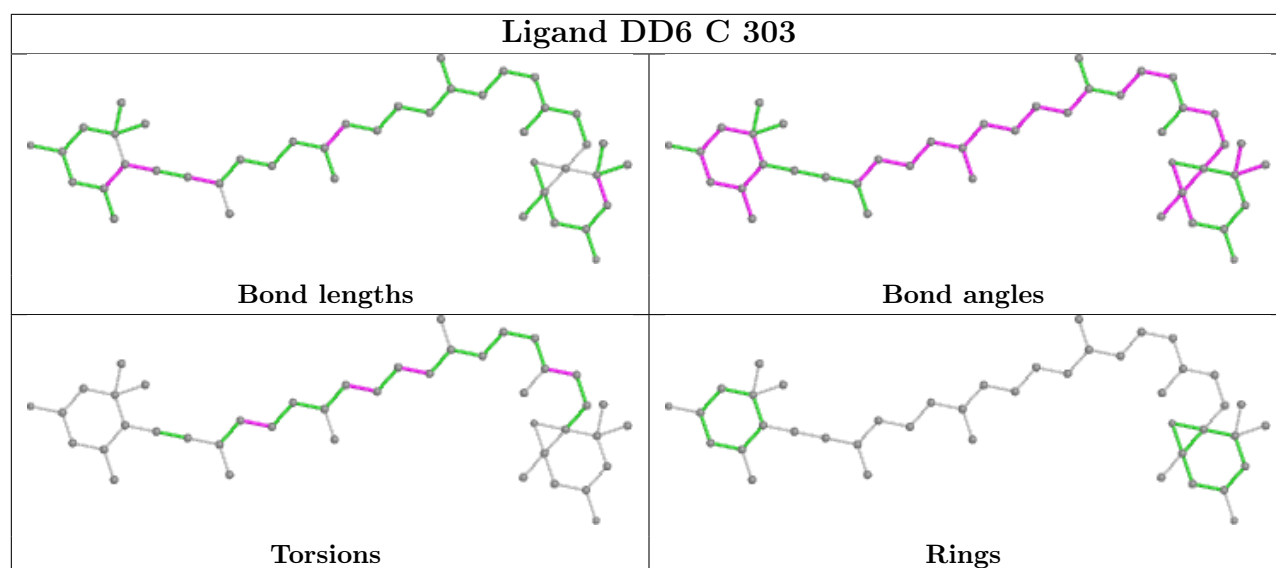


Ligand CLA b 827

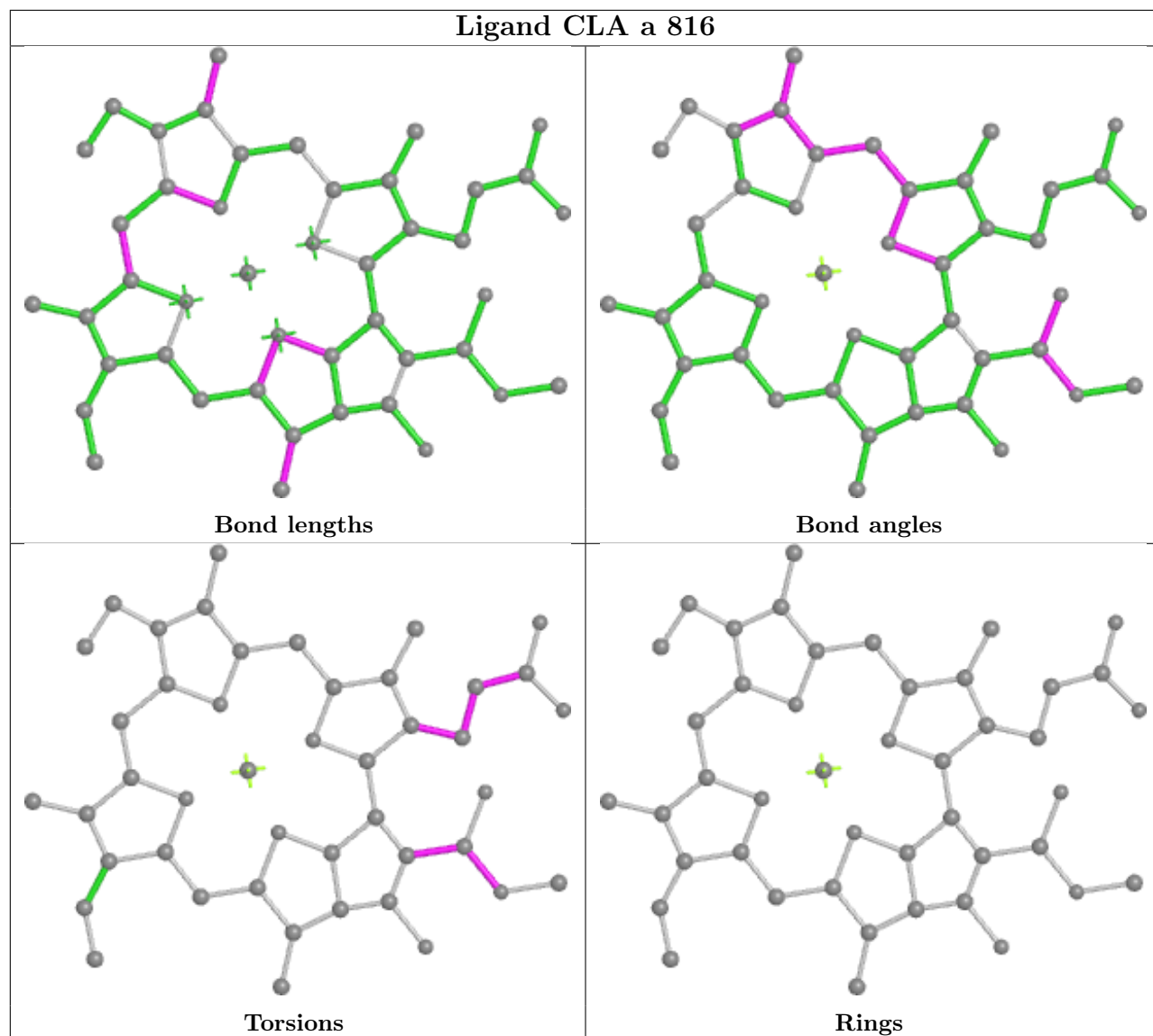


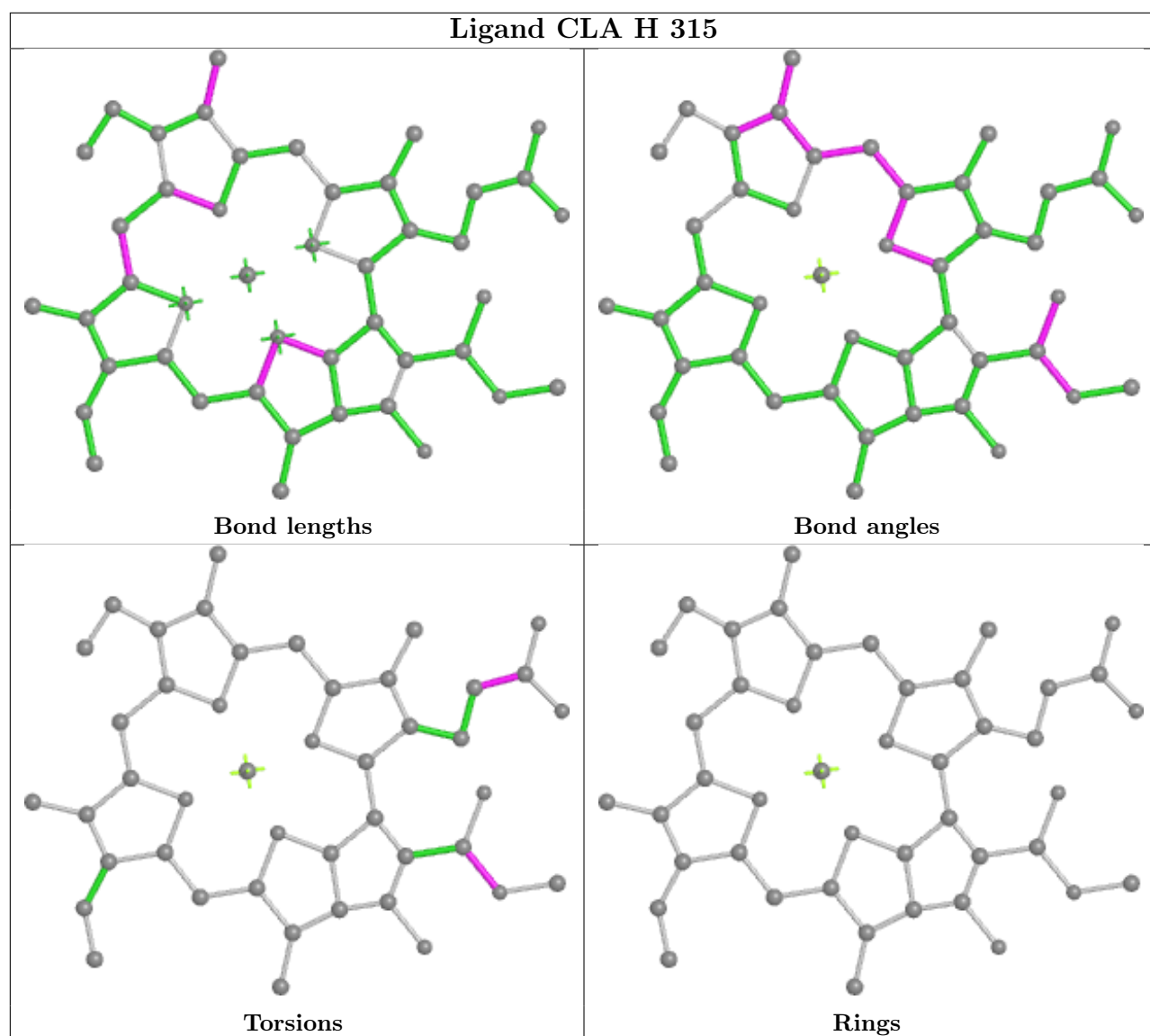
Ligand CLA b 822

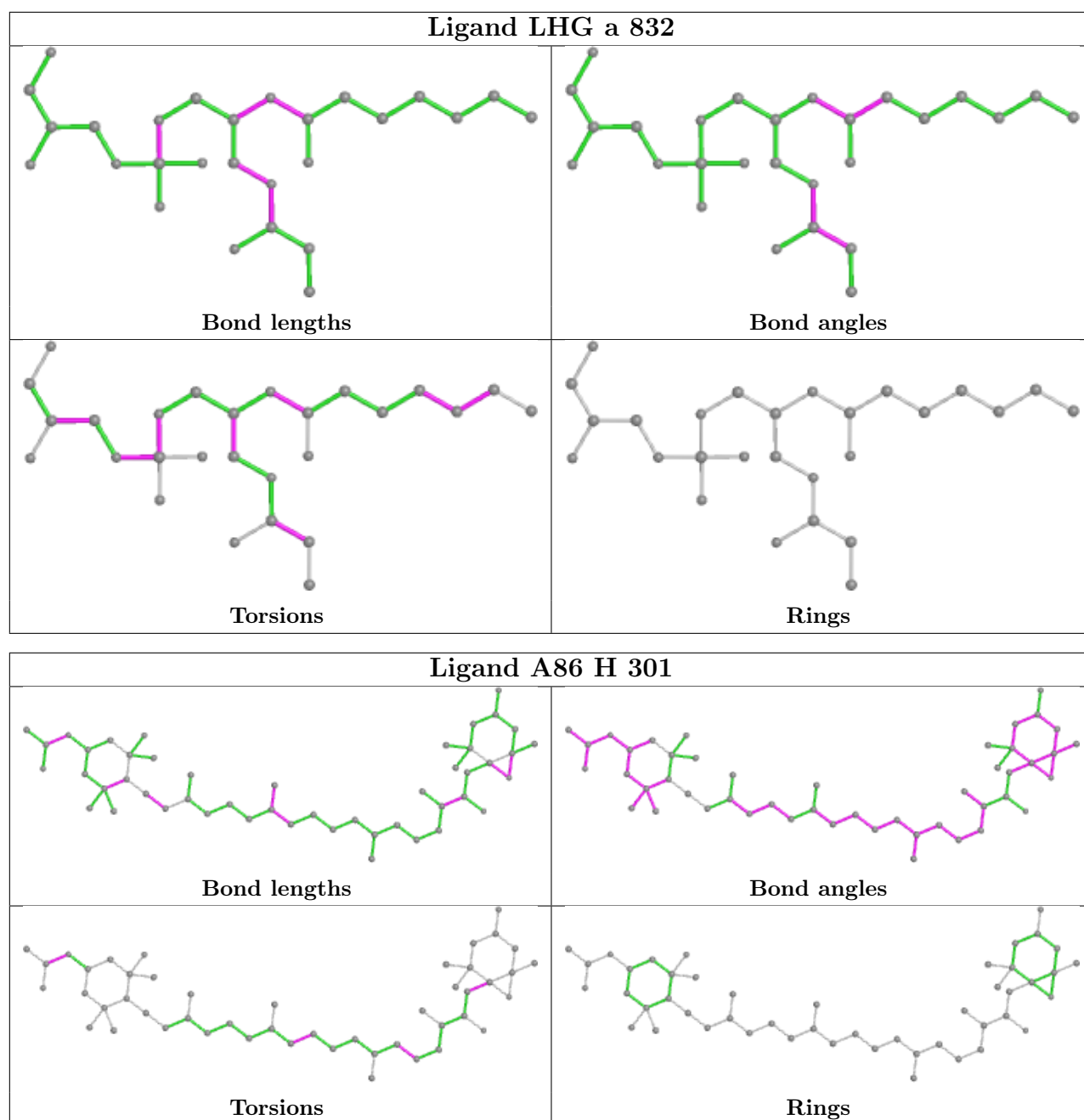


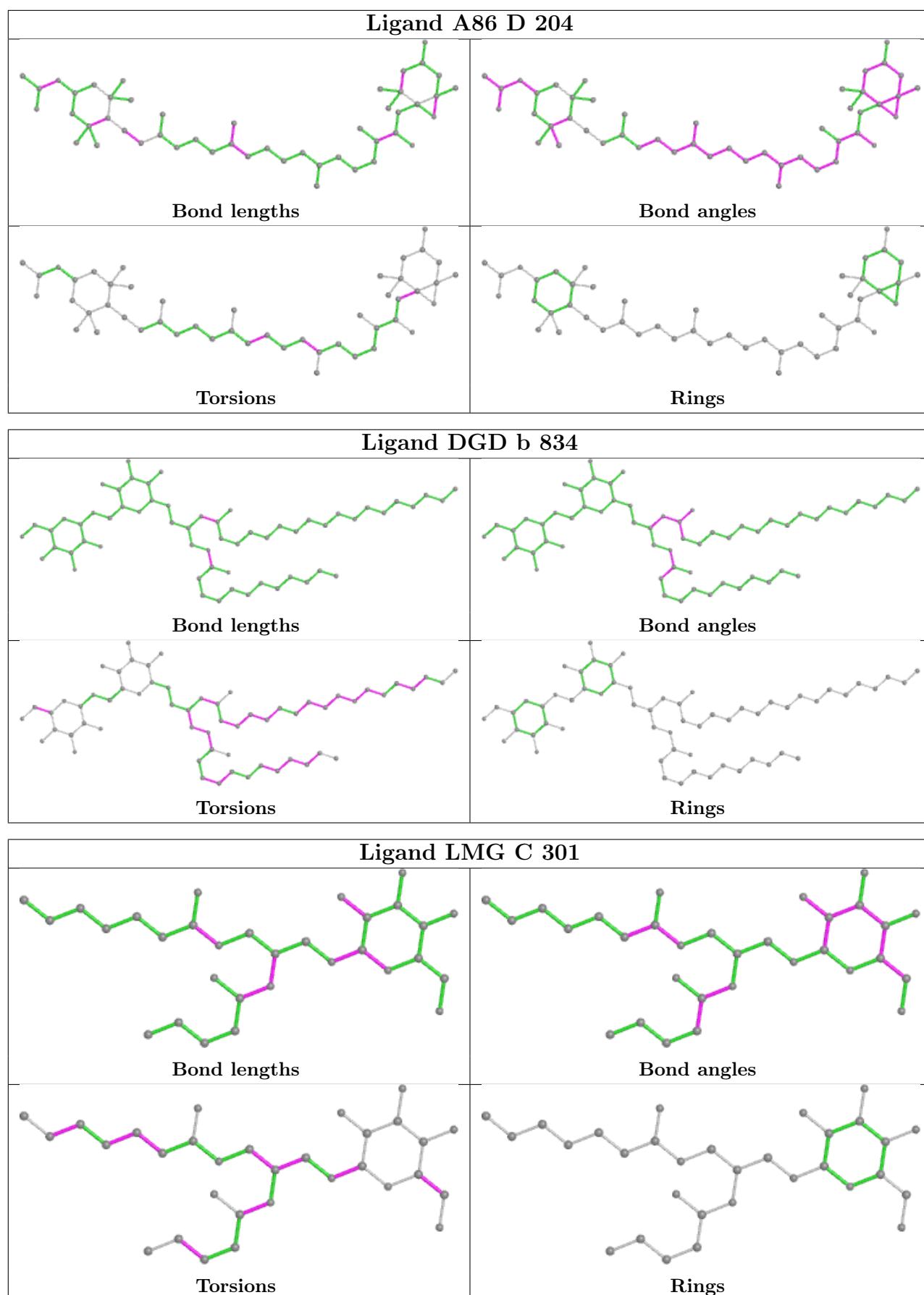


Ligand CLA a 816

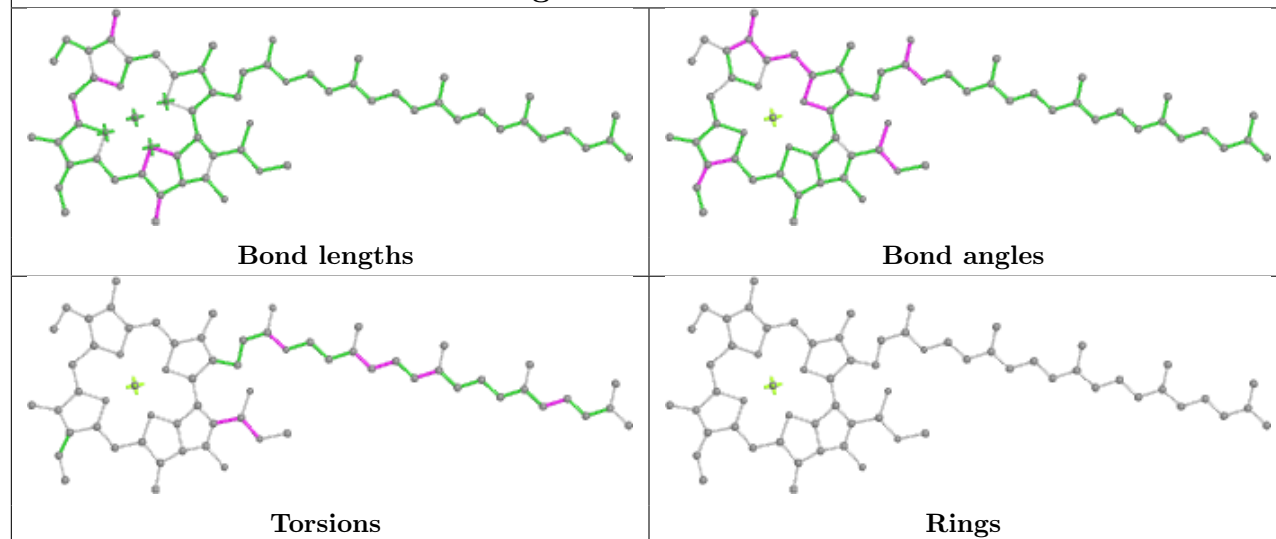




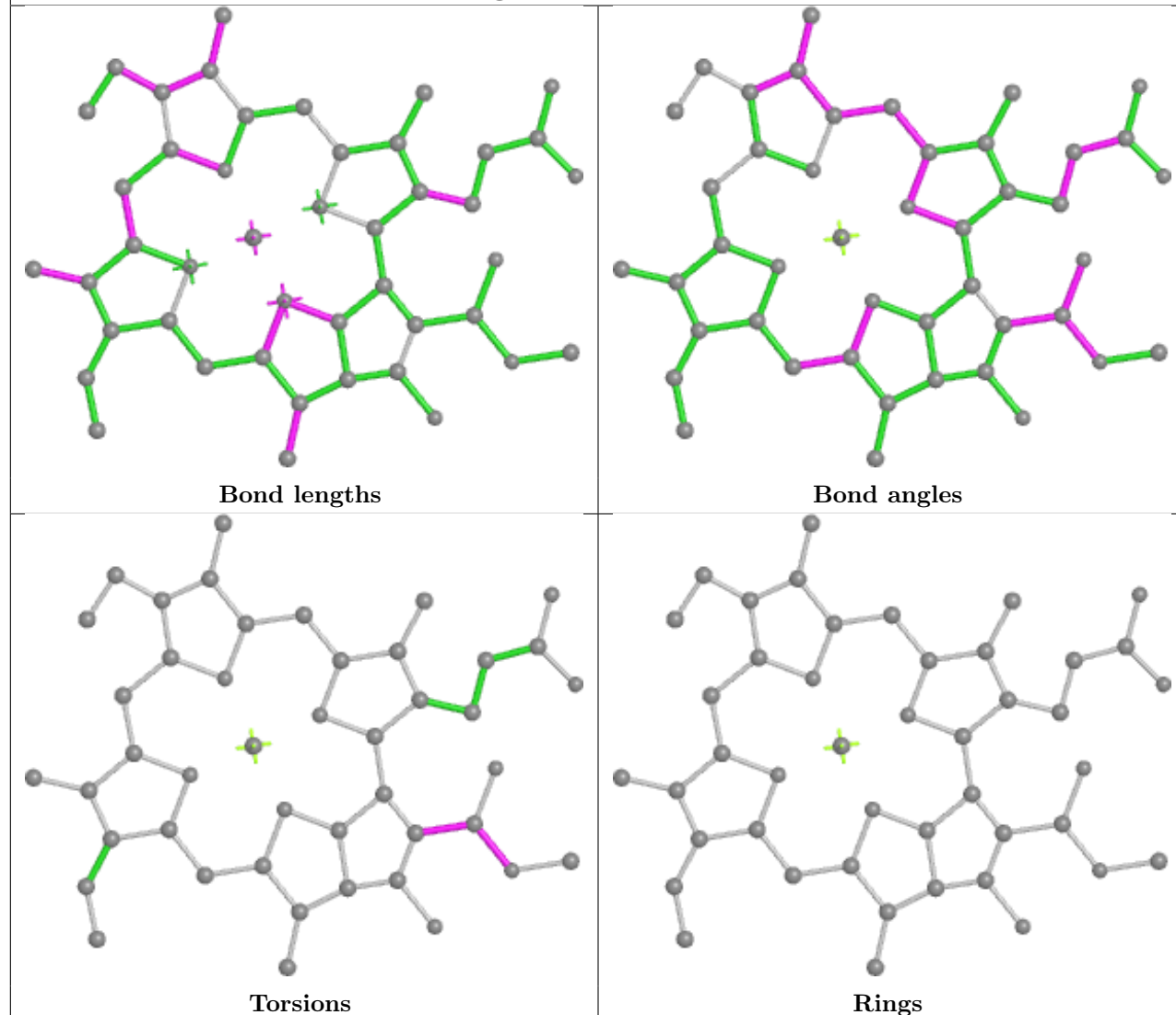


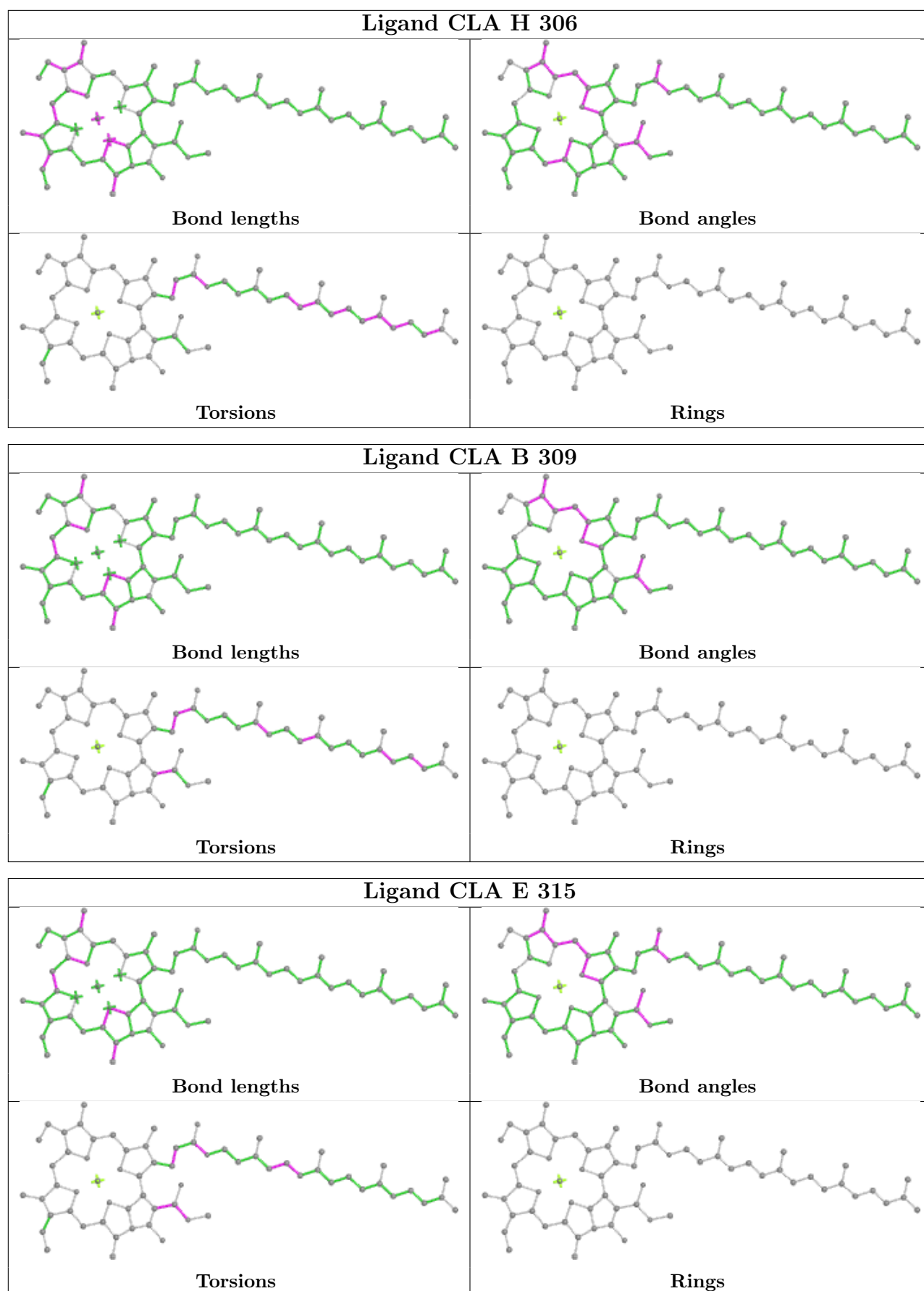


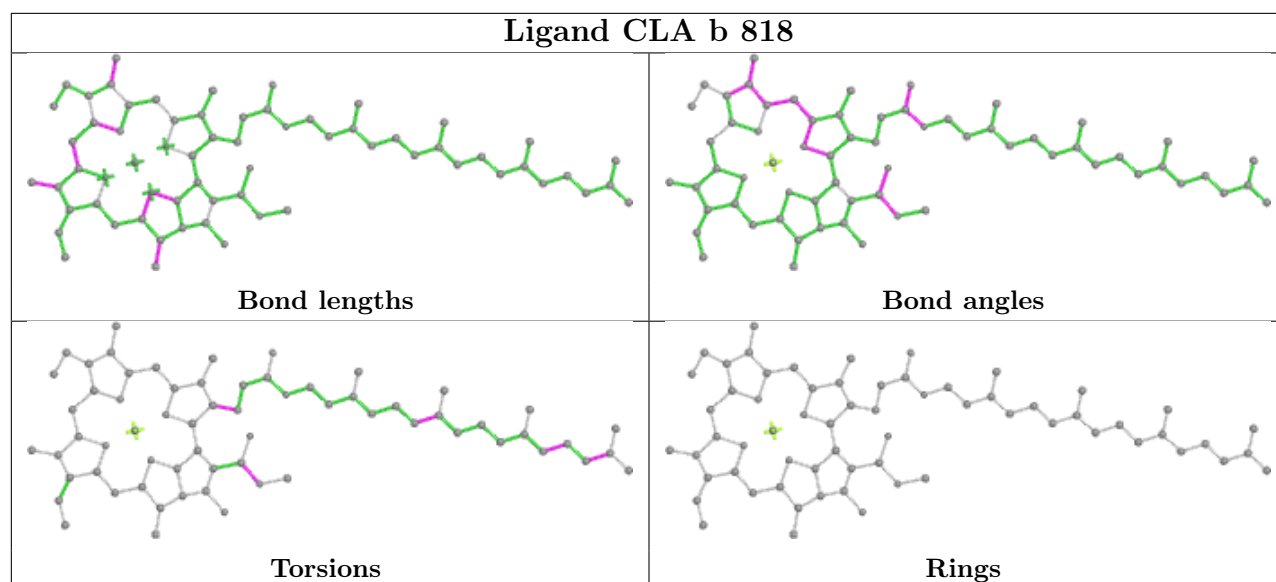
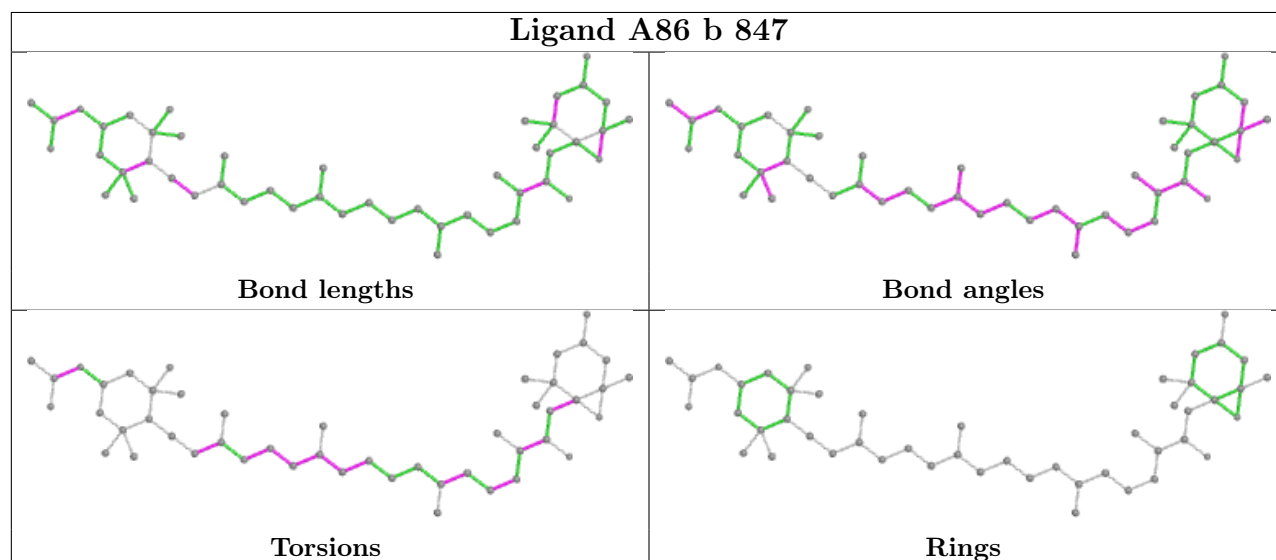
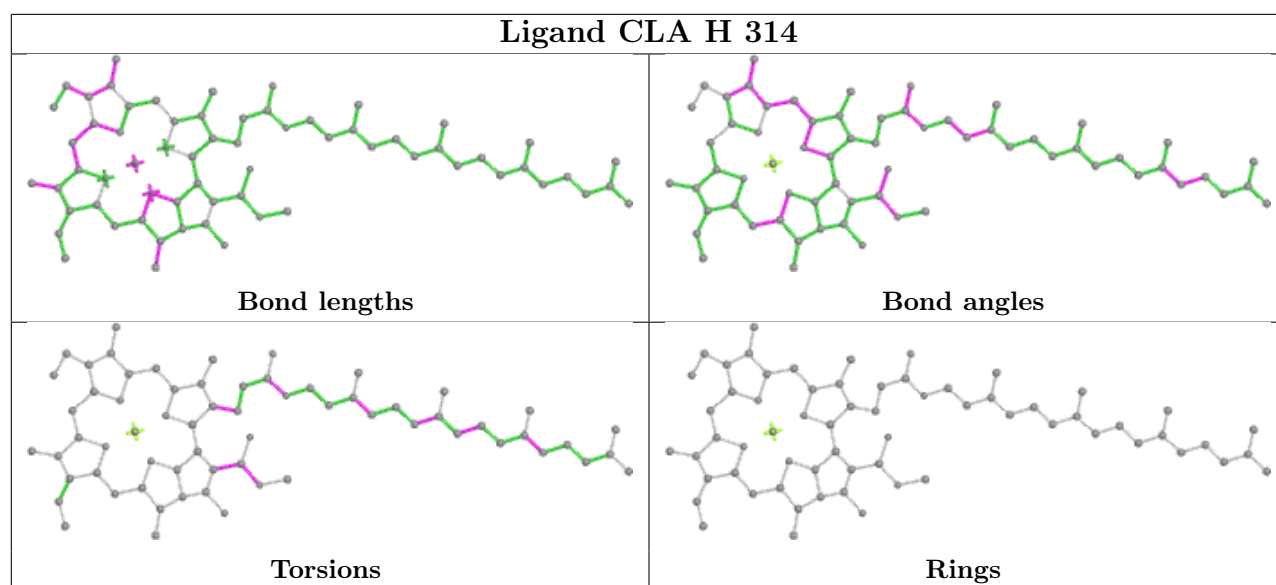
Ligand CLA B 311

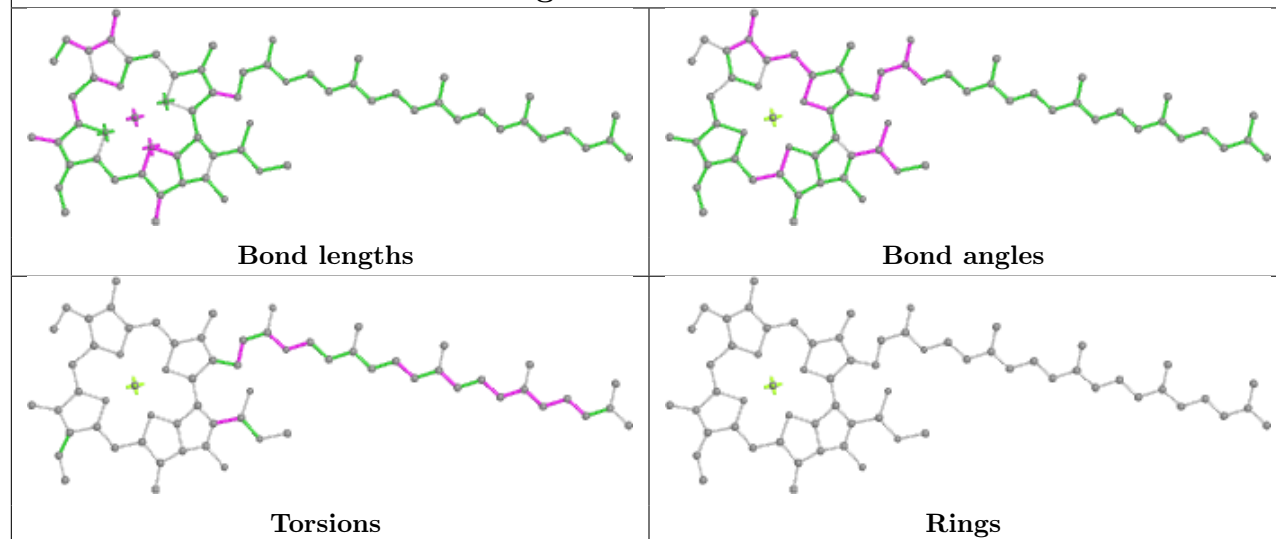
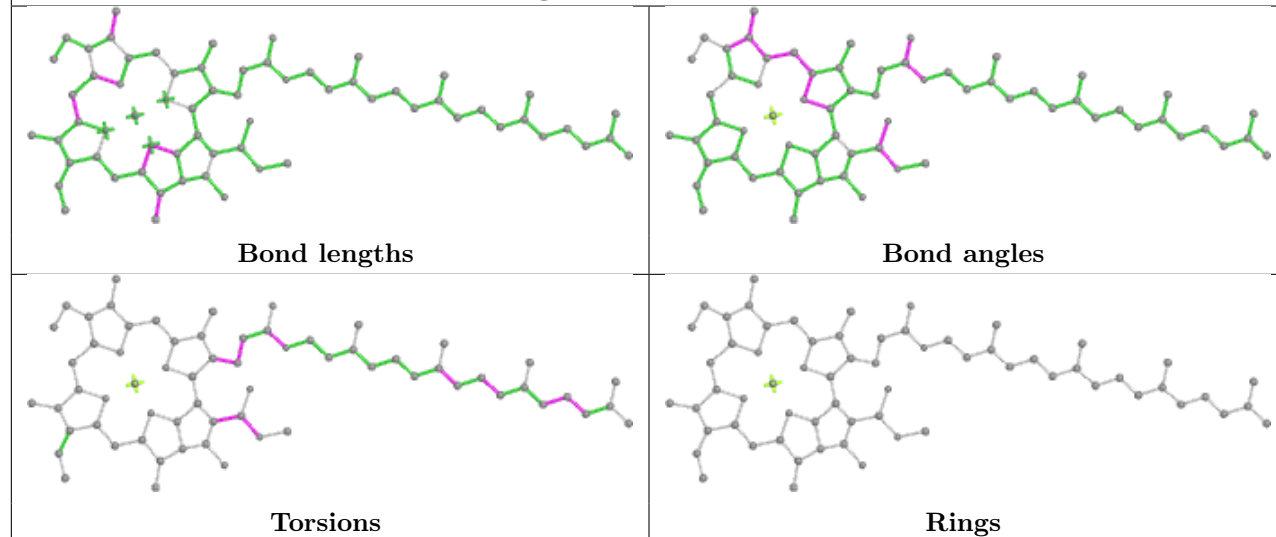


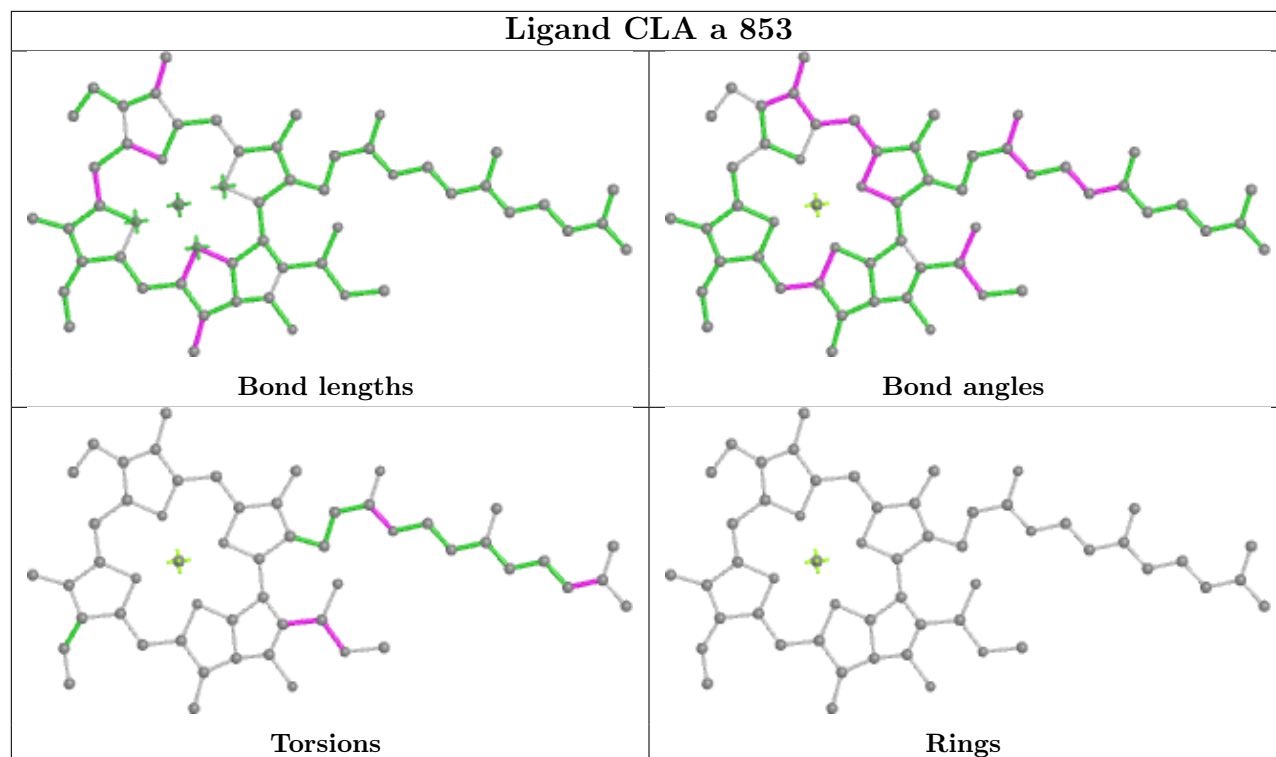
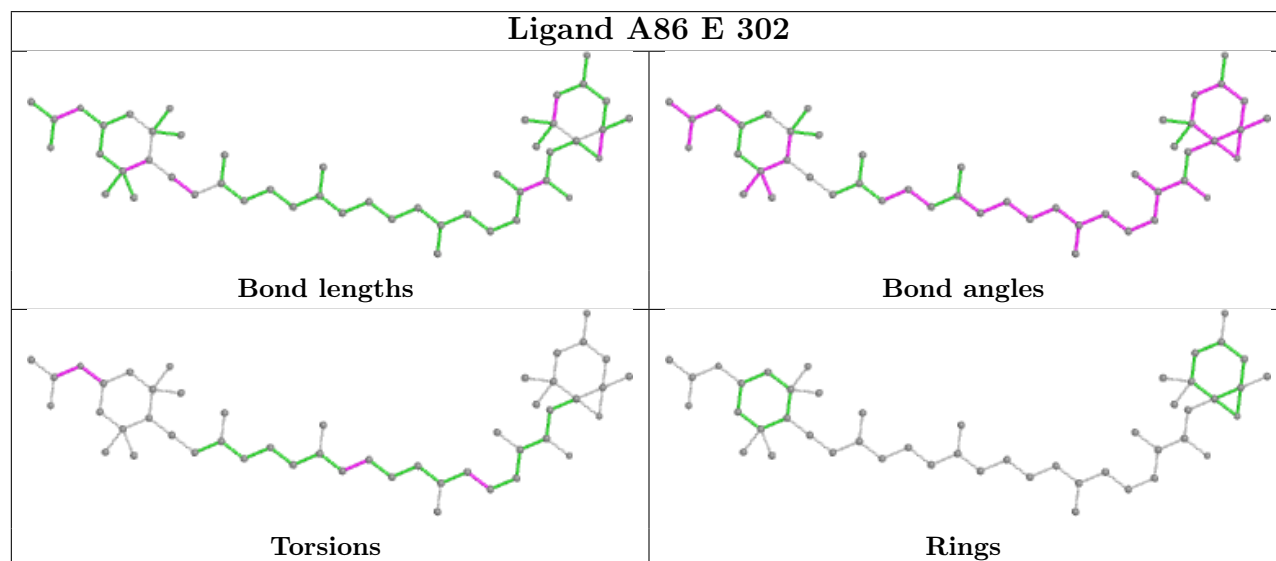
Ligand CLA E 314

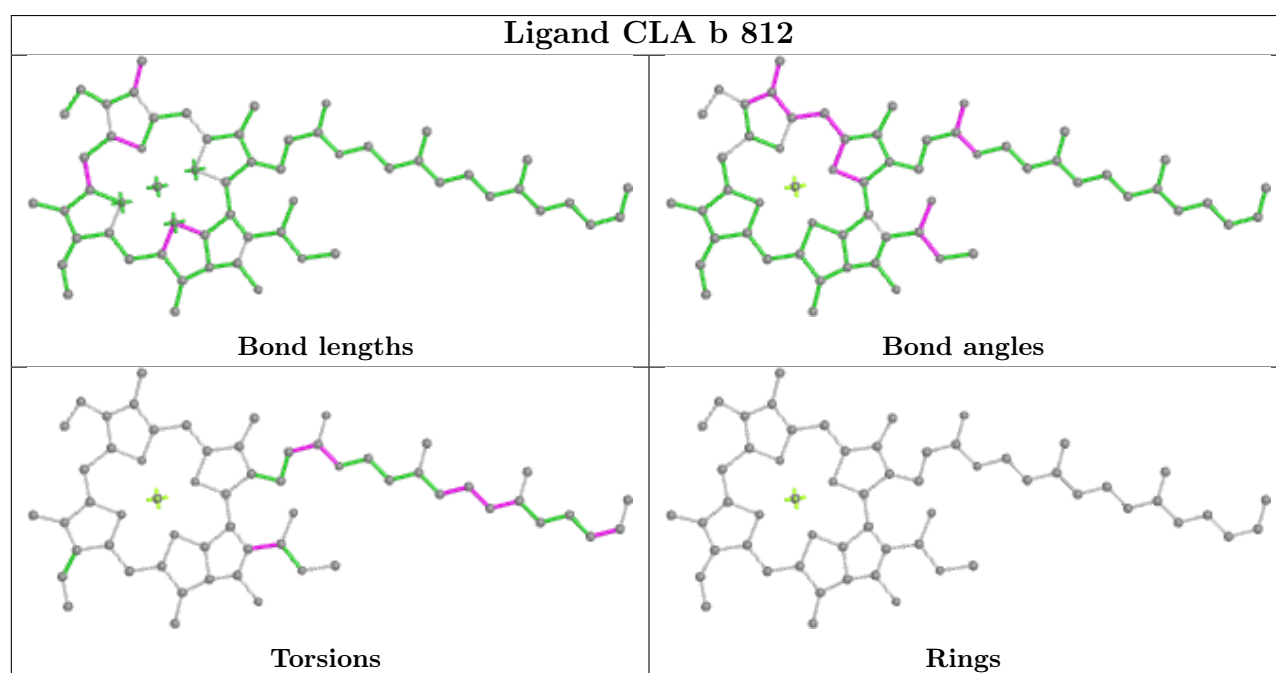
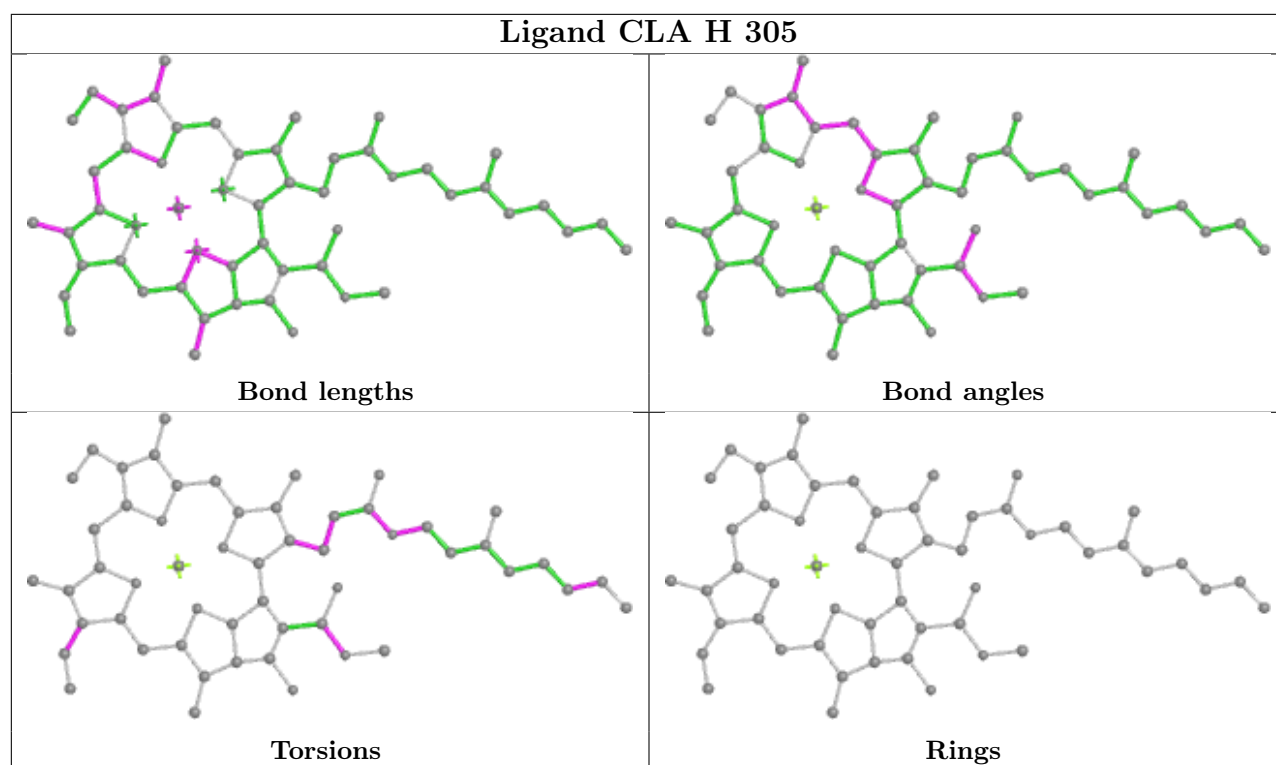


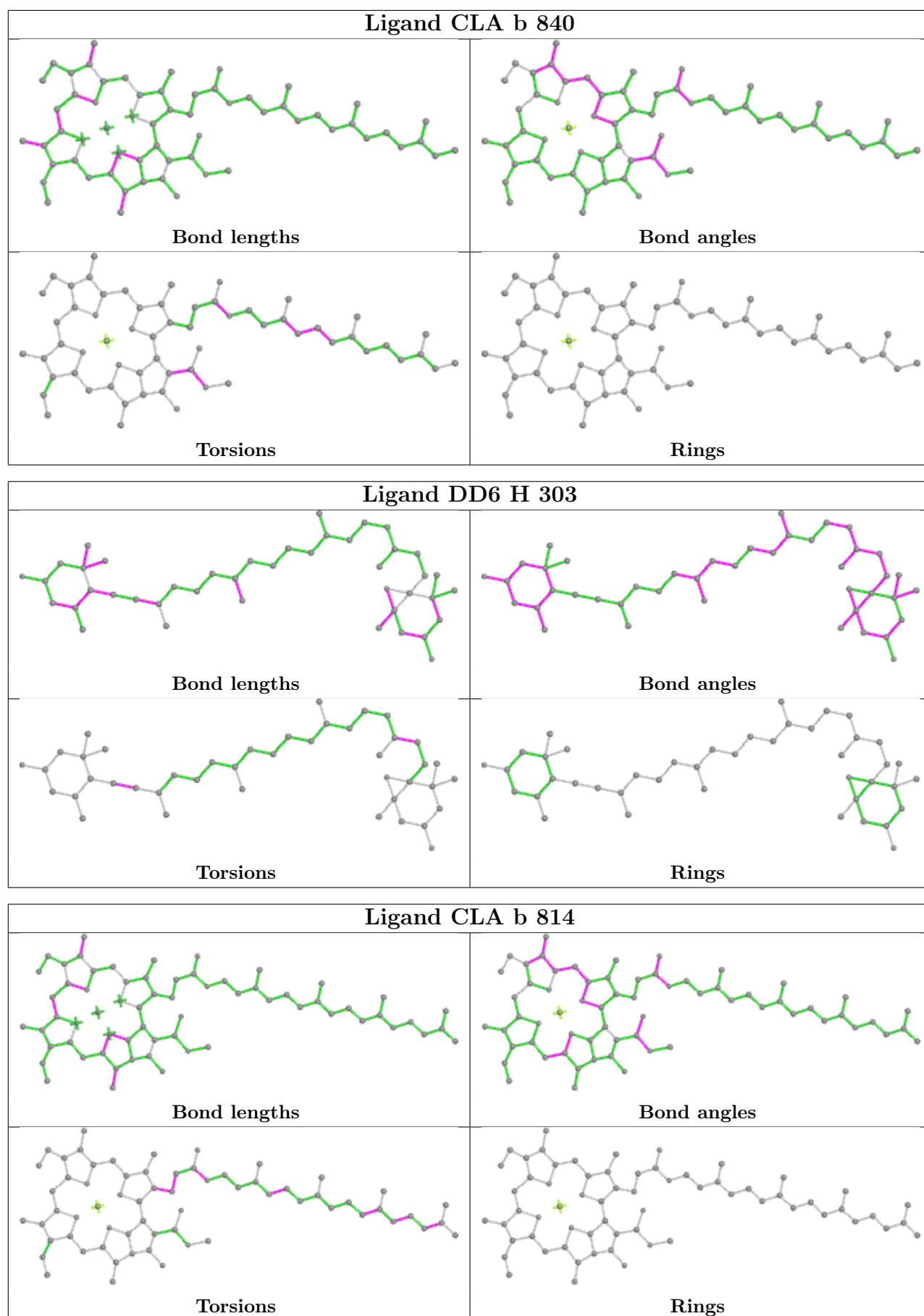




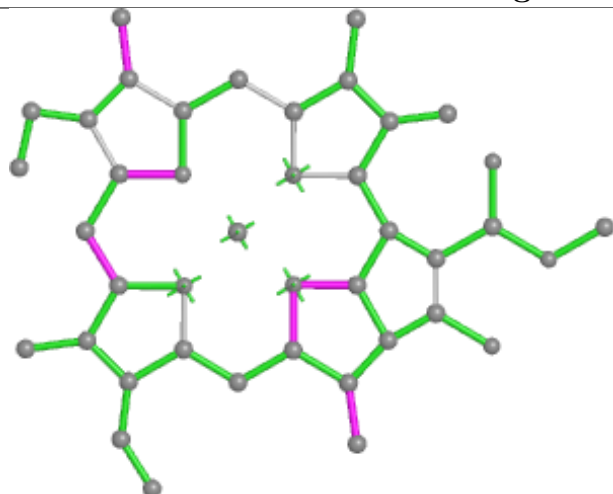
Ligand CLA a 803**Ligand CLA b 819**

Ligand CLA a 853**Ligand A86 E 302**

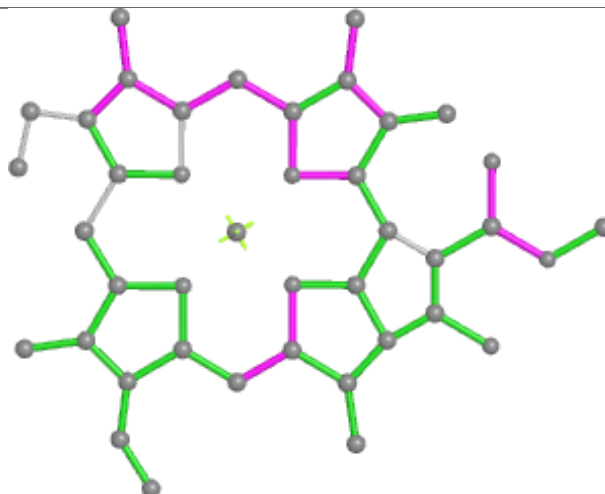




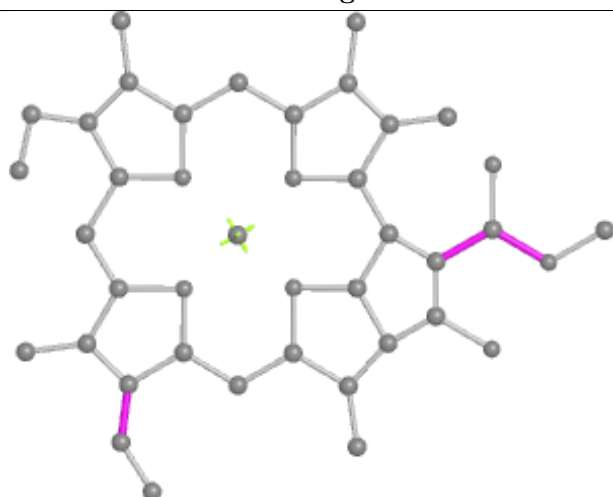
Ligand CLA D 217



Bond lengths



Bond angles

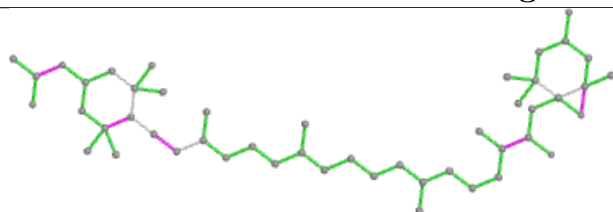


Torsions

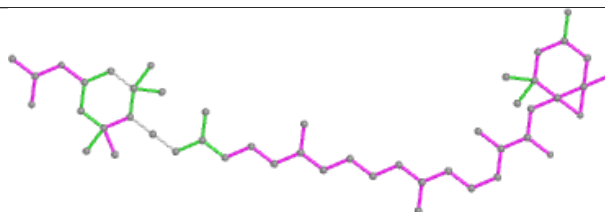


Rings

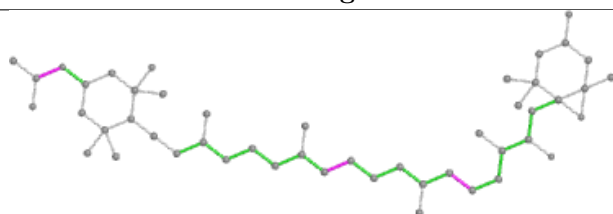
Ligand A86 H 304



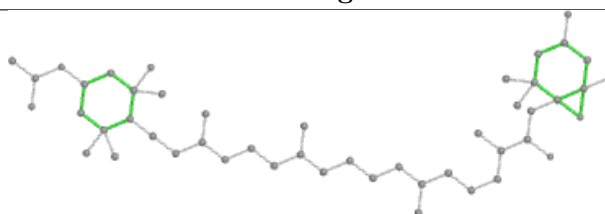
Bond lengths



Bond angles

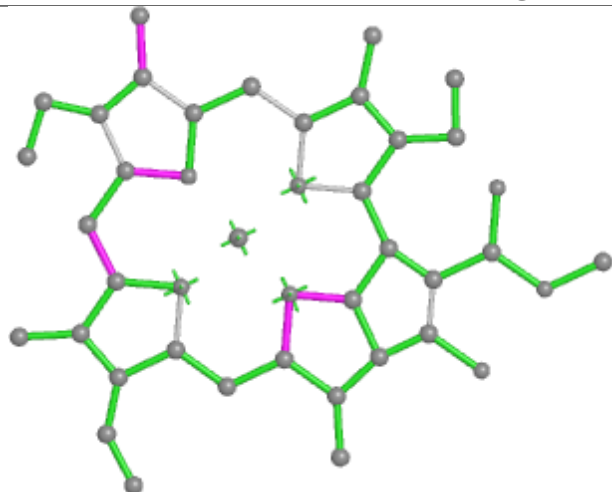


Torsions

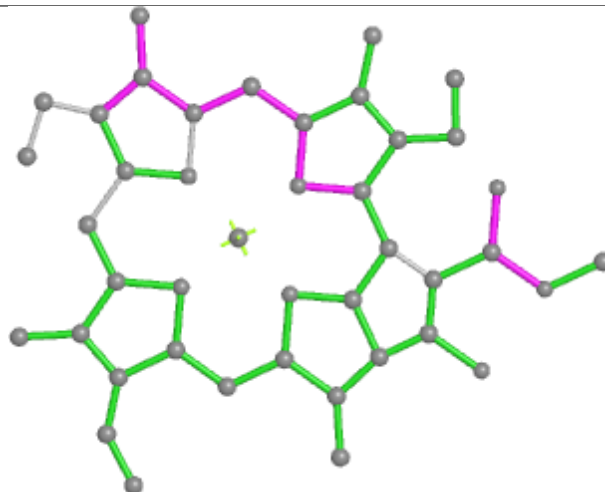


Rings

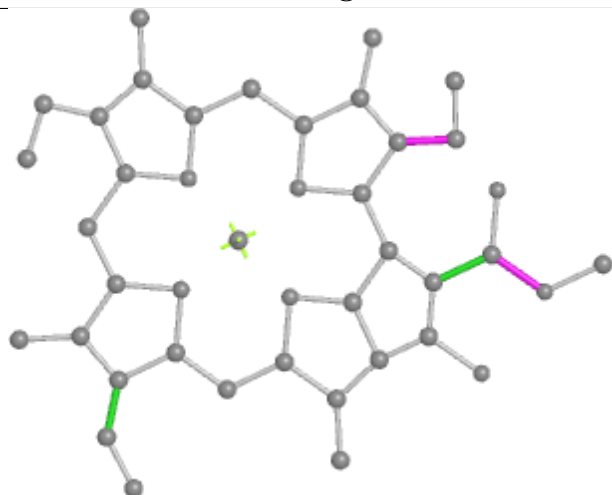
Ligand CLA C 315



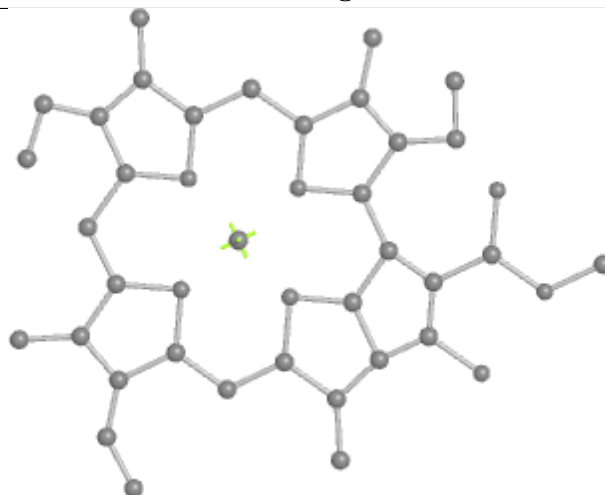
Bond lengths



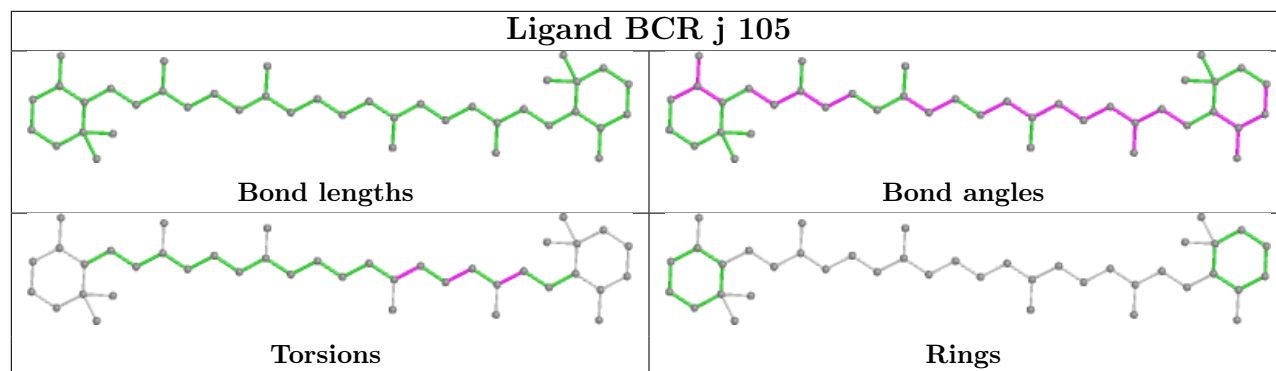
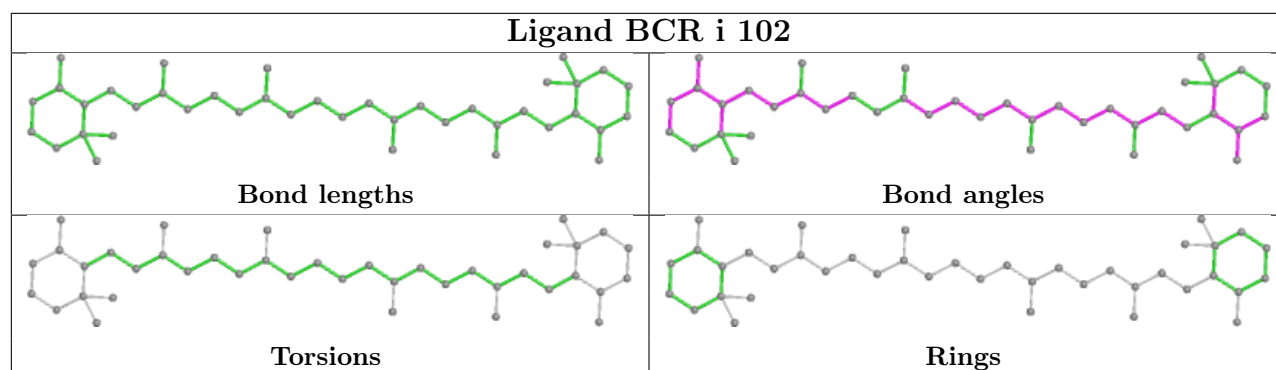
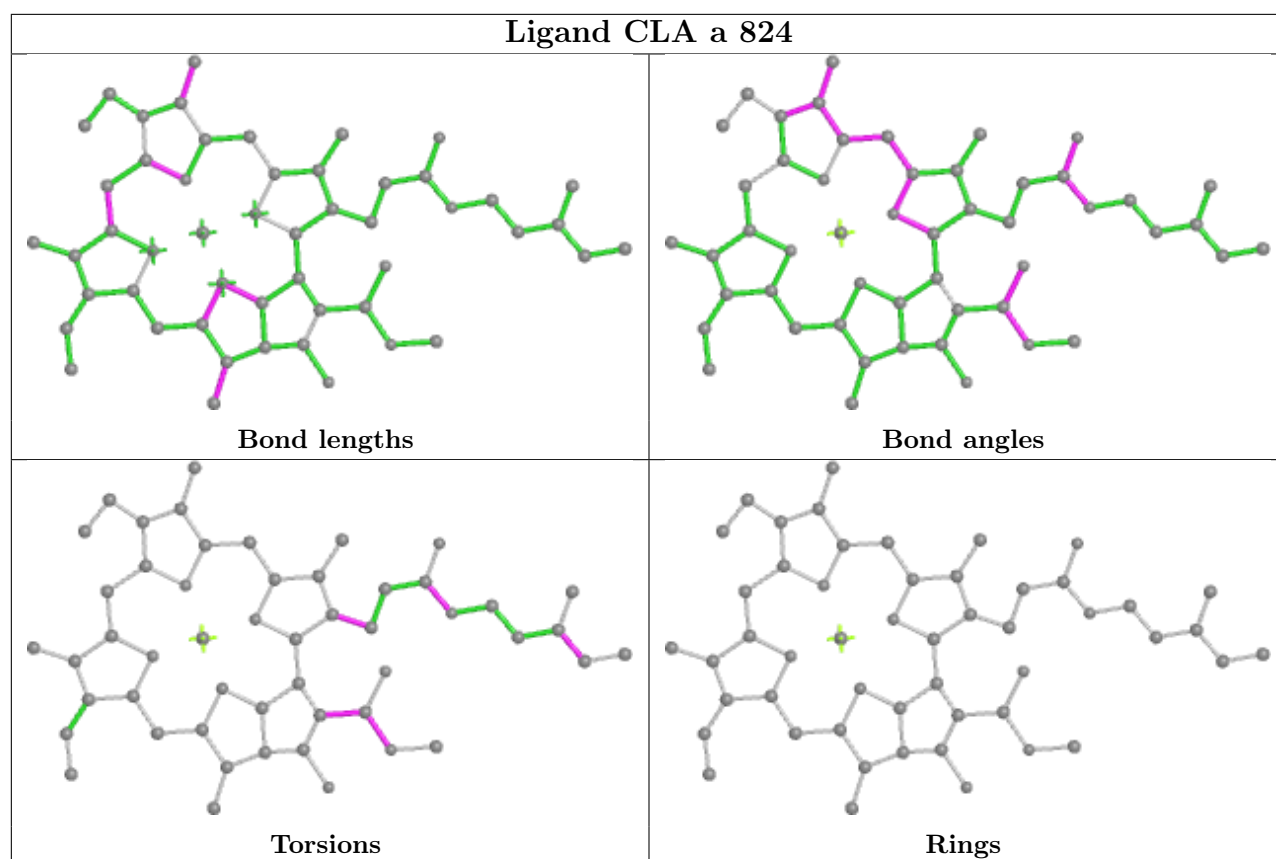
Bond angles

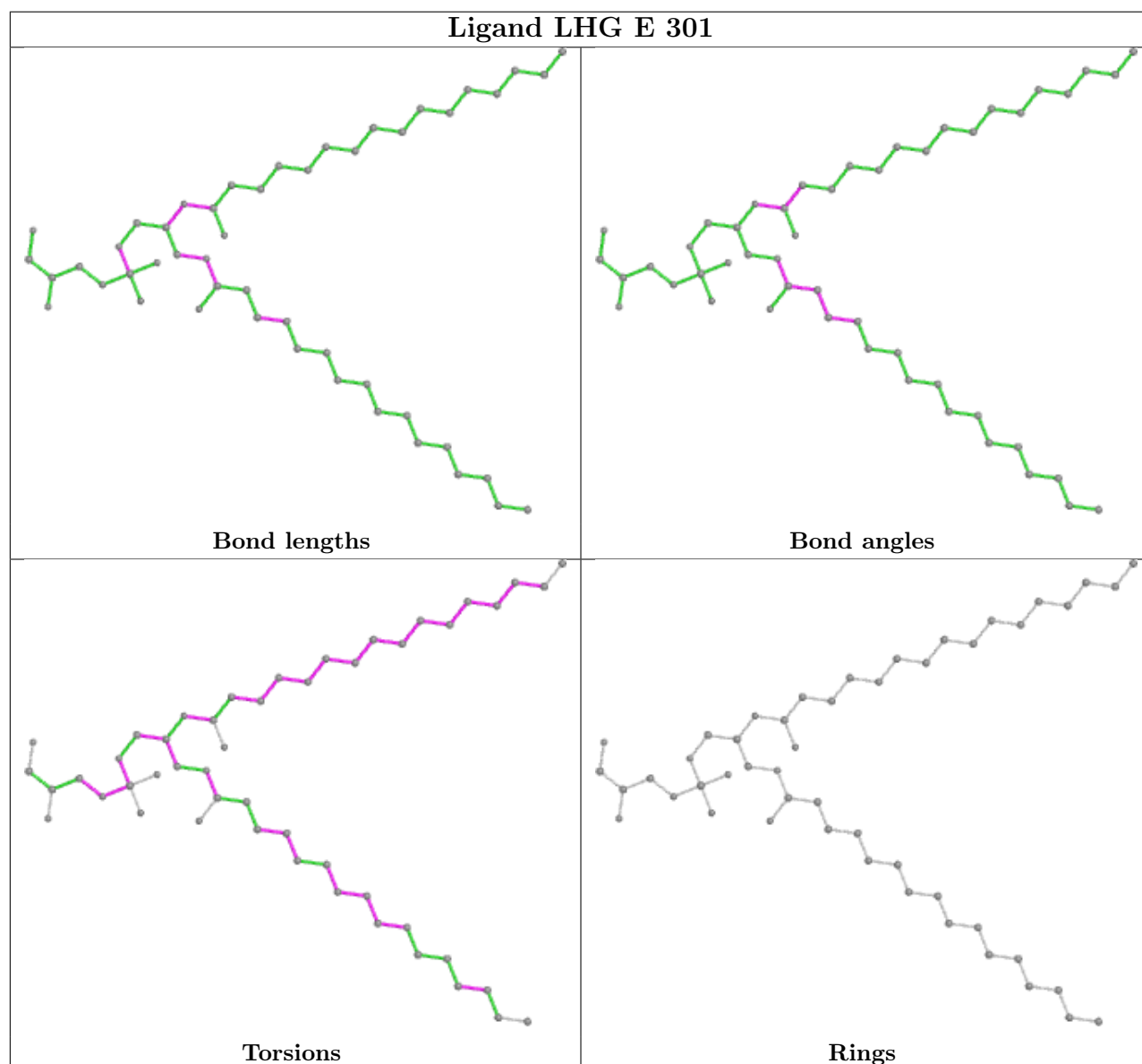
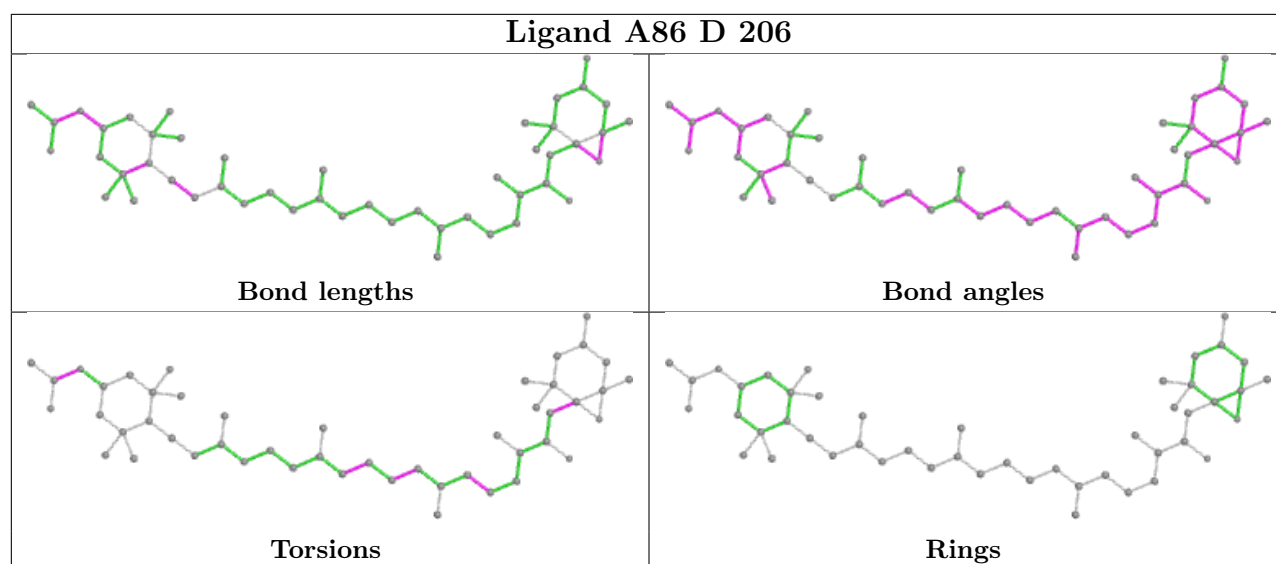


Torsions

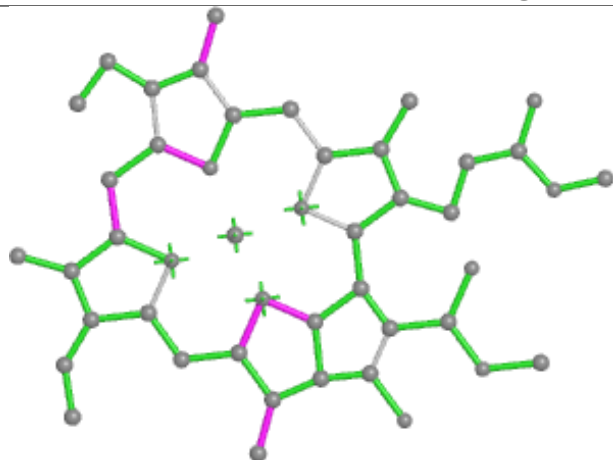


Rings

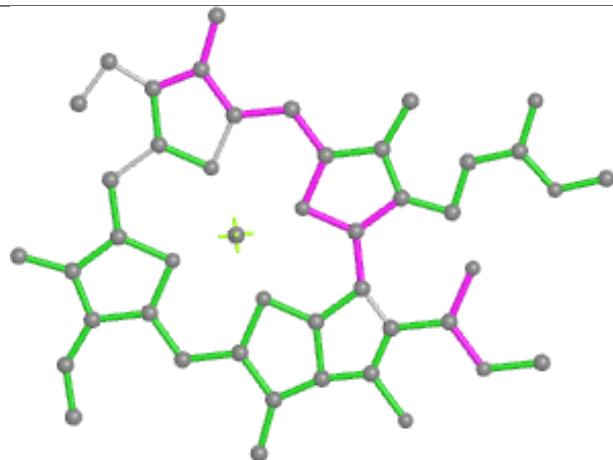




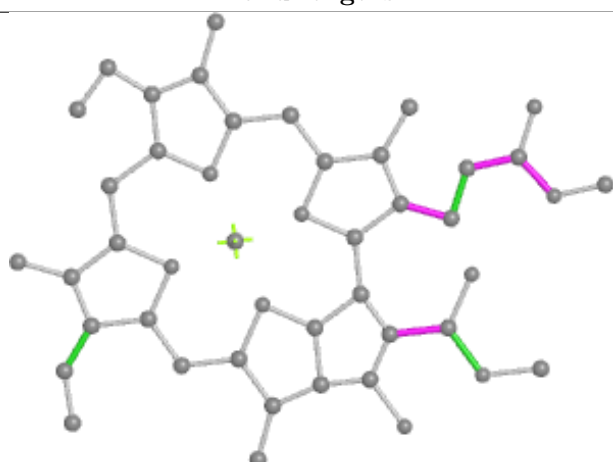
Ligand CLA E 311



Bond lengths



Bond angles

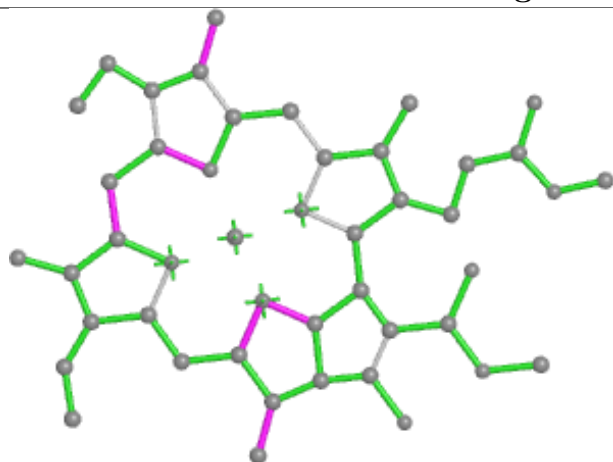


Torsions

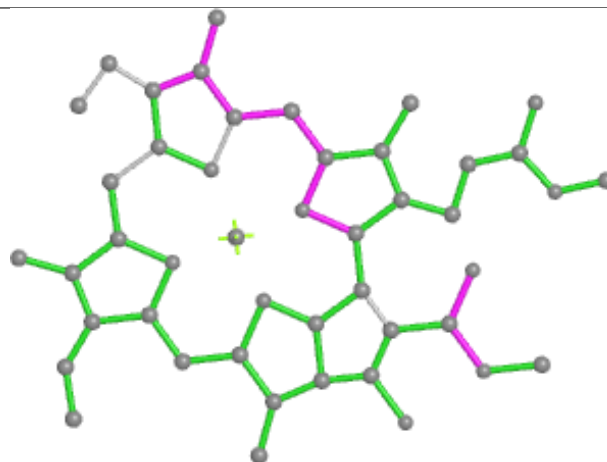


Rings

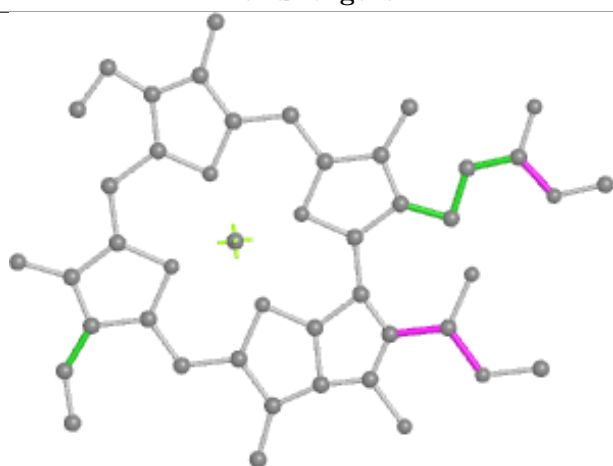
Ligand CLA B 310



Bond lengths



Bond angles

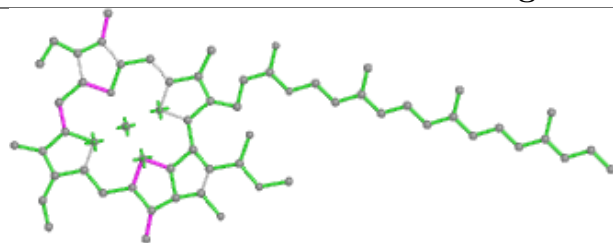


Torsions

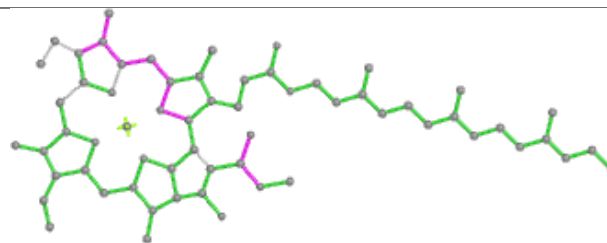


Rings

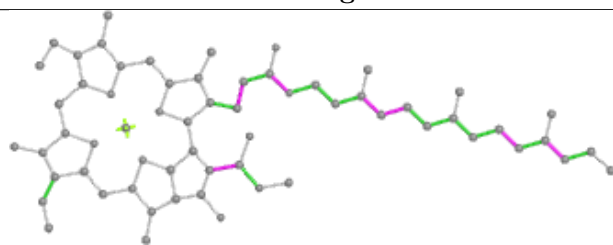
Ligand CLA a 809



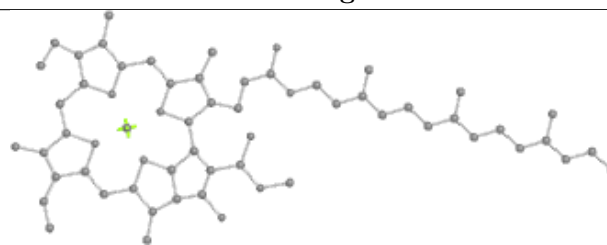
Bond lengths



Bond angles

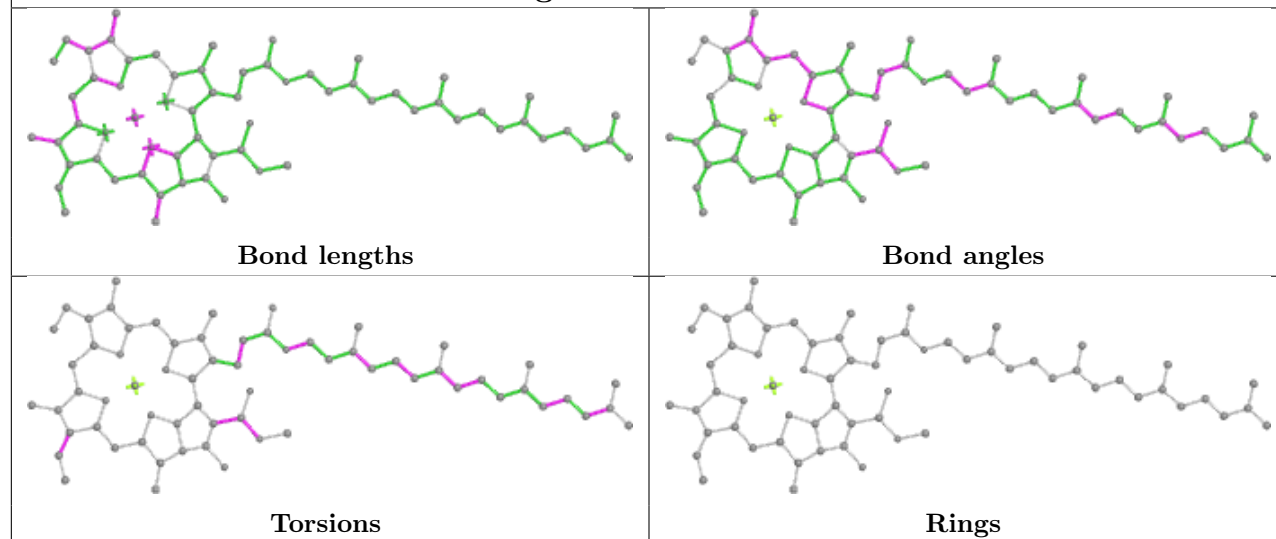


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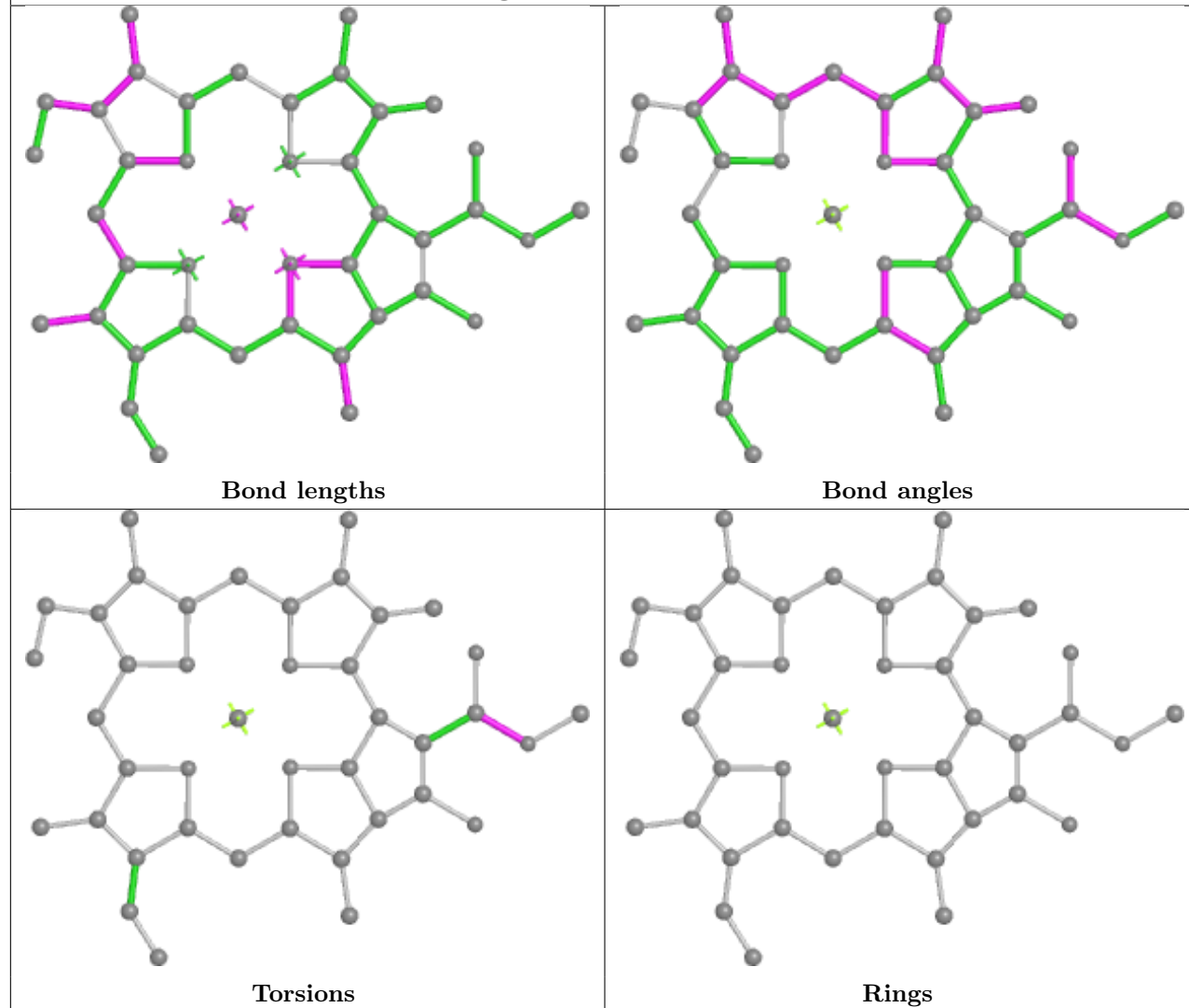


Rings

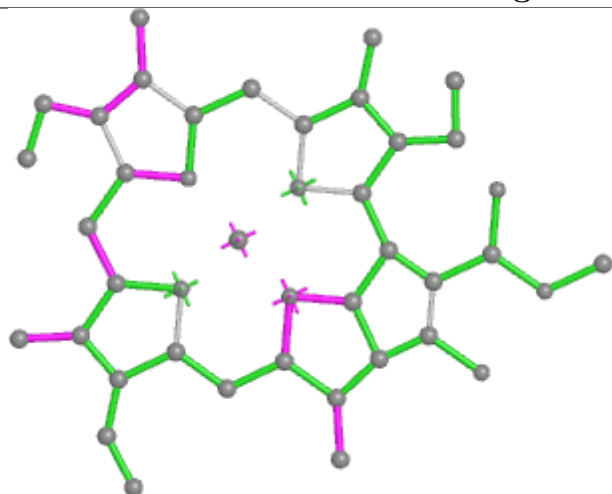
Ligand CLA b 829



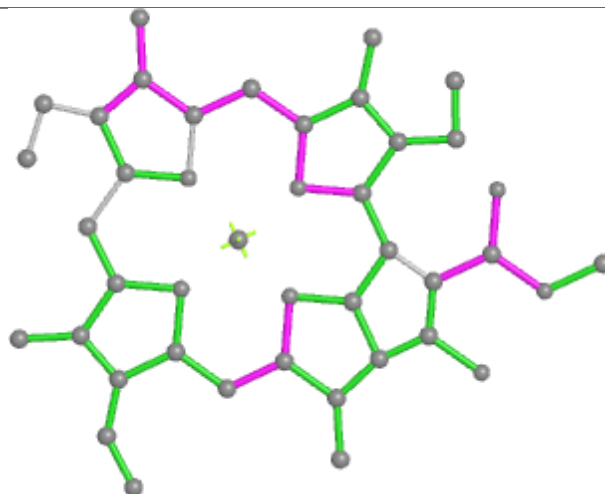
Ligand CLA B 314



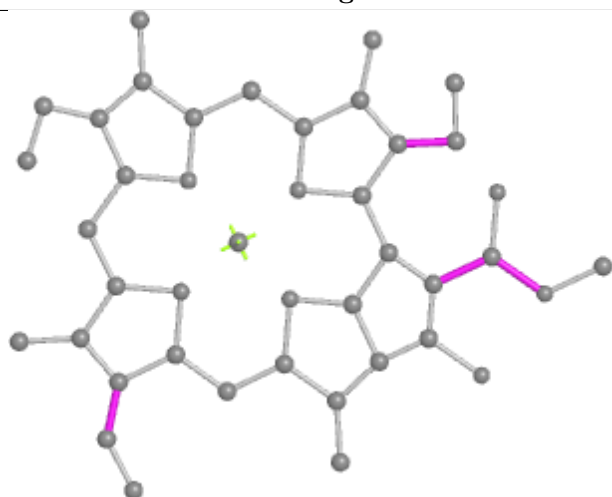
Ligand CLA C 317



Bond lengths



Bond angles

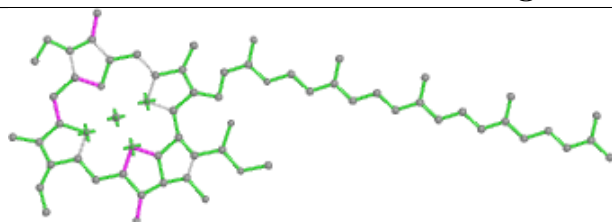


Torsions

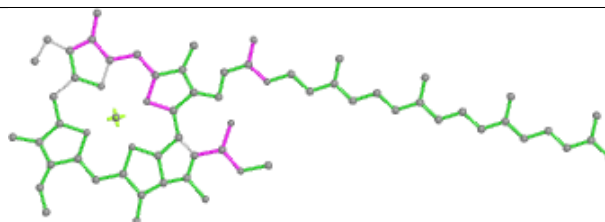


Rings

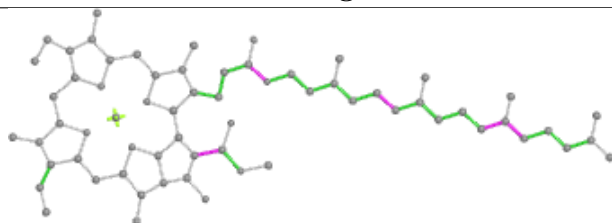
Ligand CLA a 820



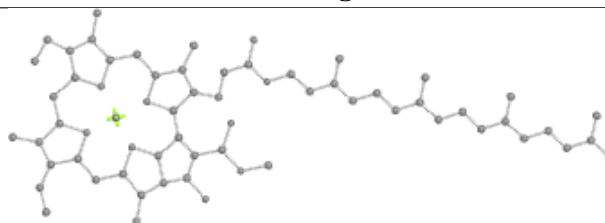
Bond lengths



Bond angles

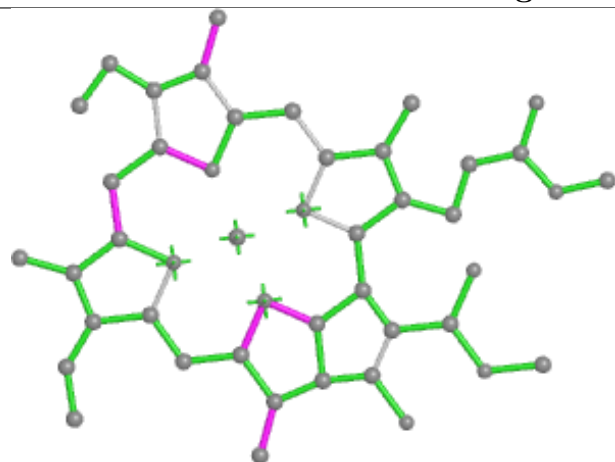


Torsions

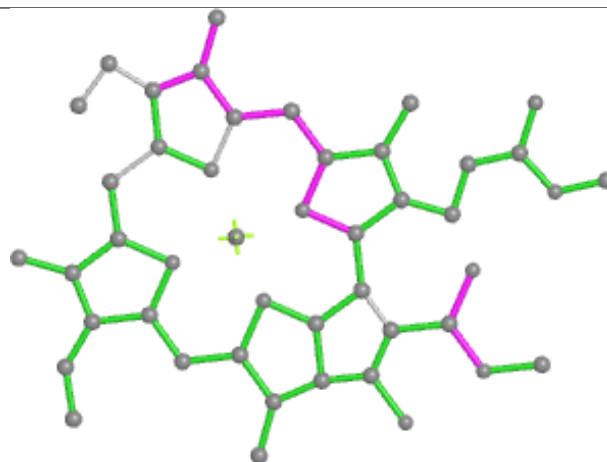


Rings

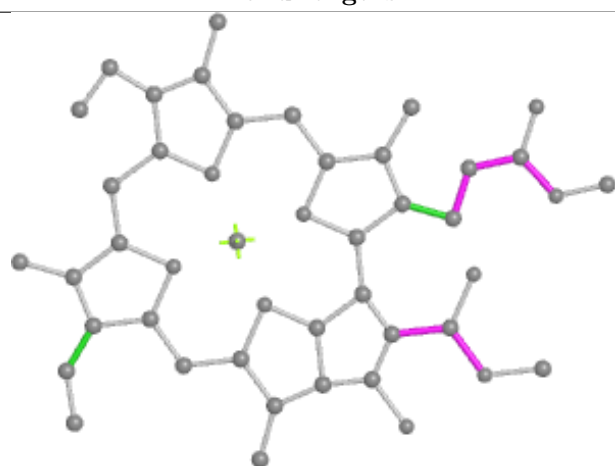
Ligand CLA H 309



Bond lengths



Bond angles

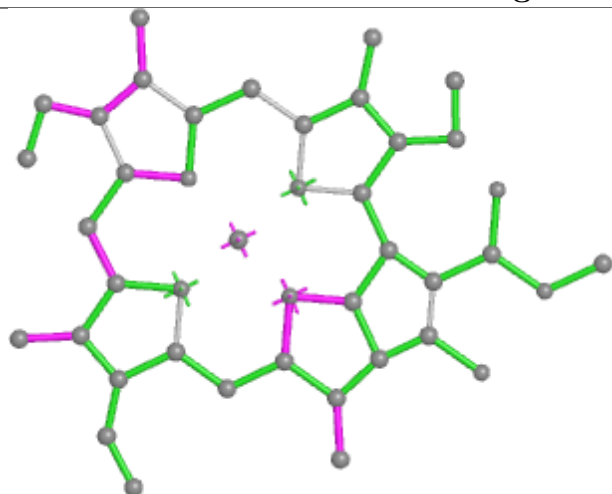


Torsions

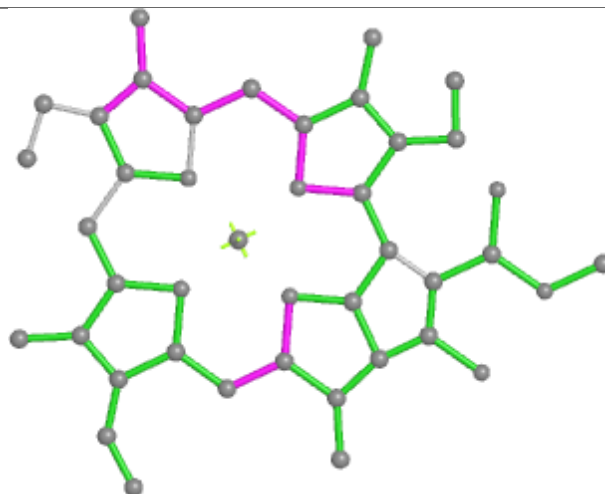


Rings

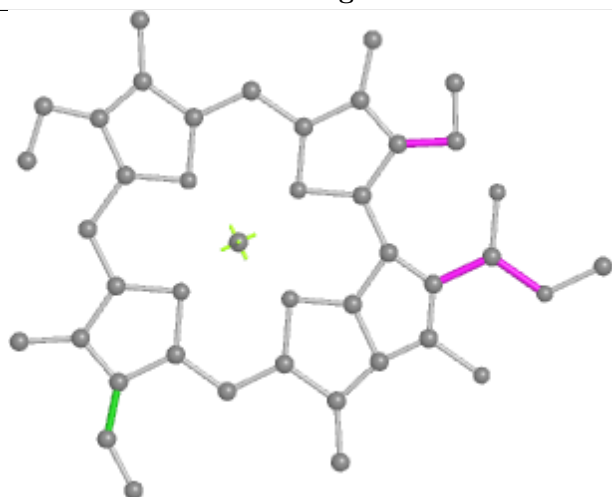
Ligand CLA C 318



Bond lengths



Bond angles

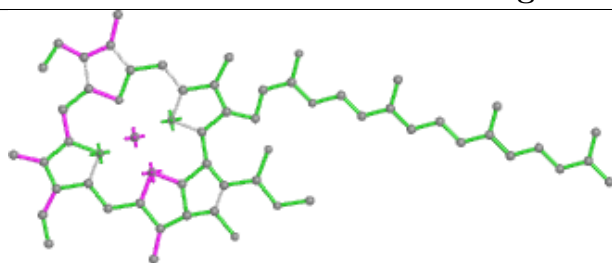


Torsions

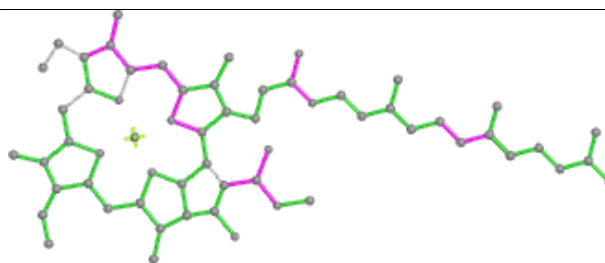


Rings

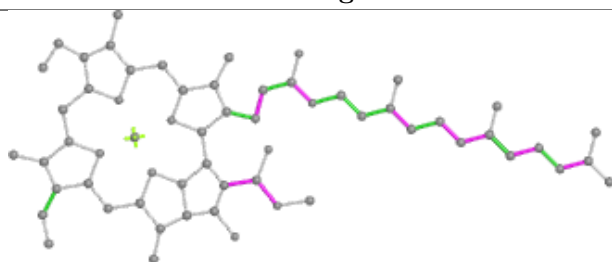
Ligand CLA a 825



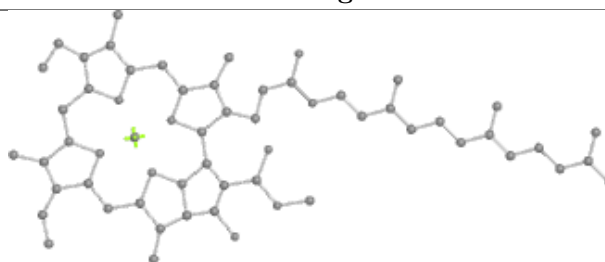
Bond lengths



Bond angles

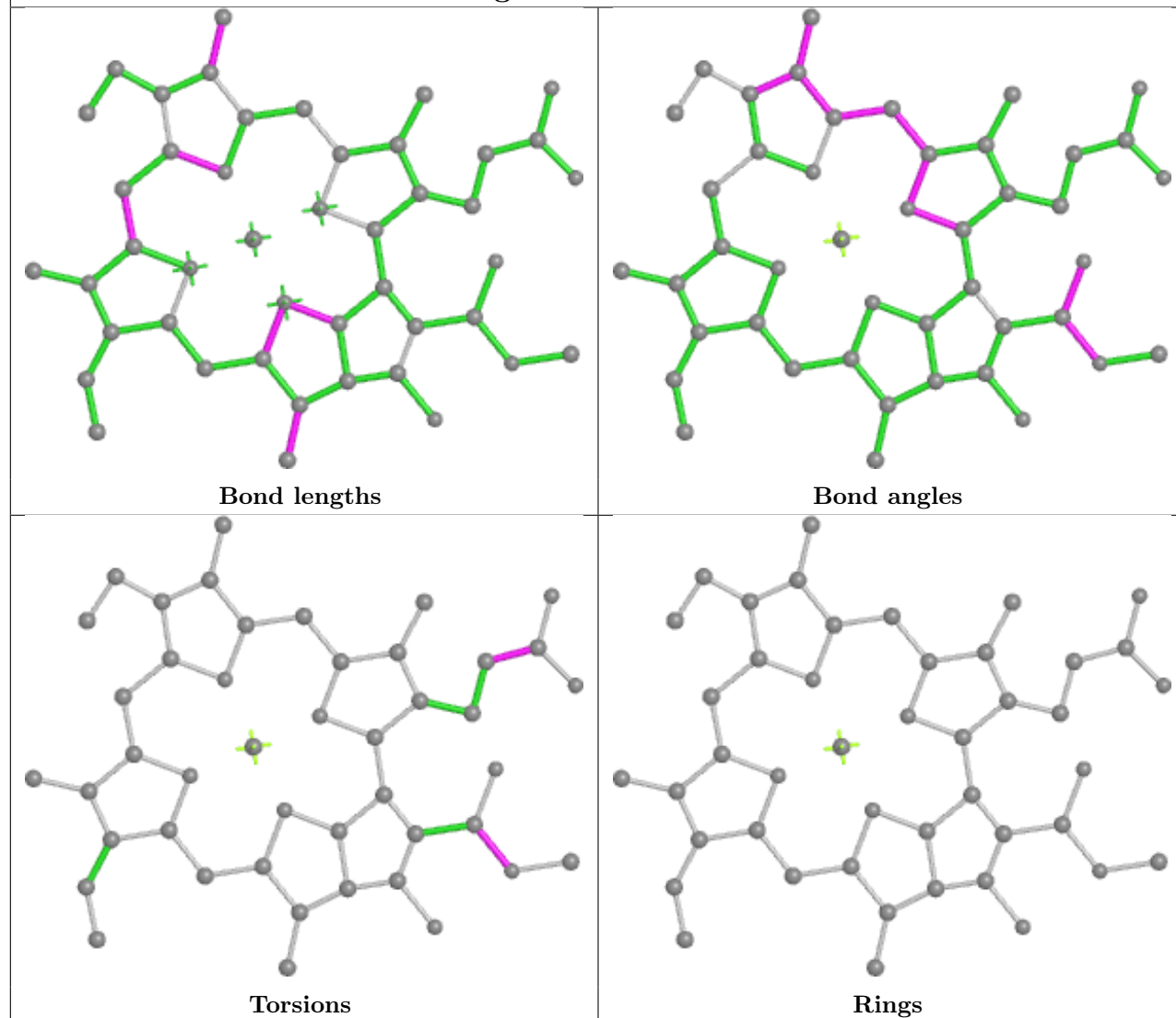


Torsions

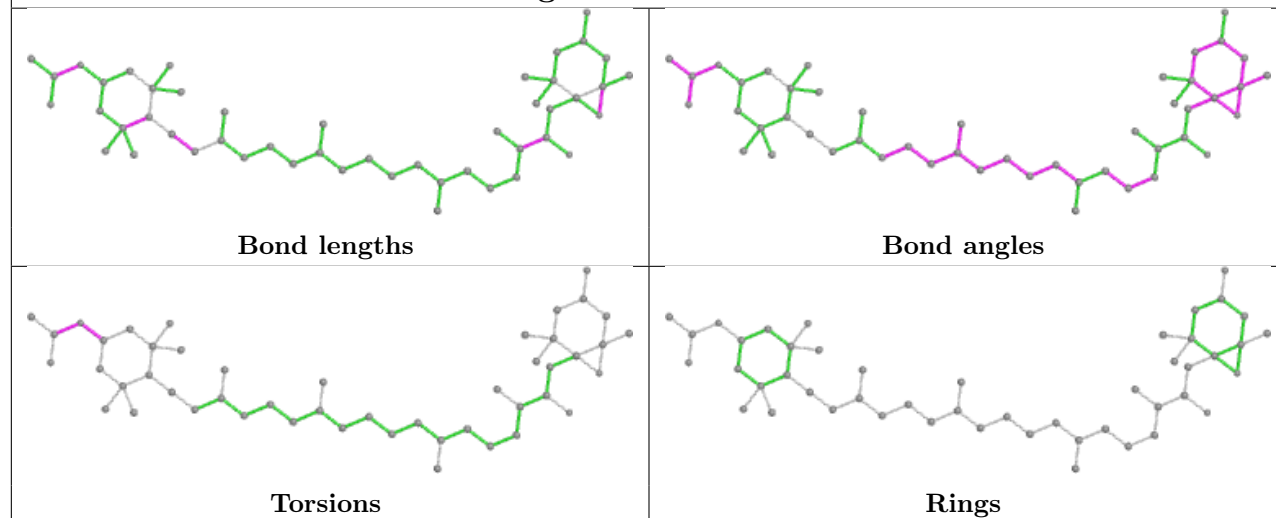


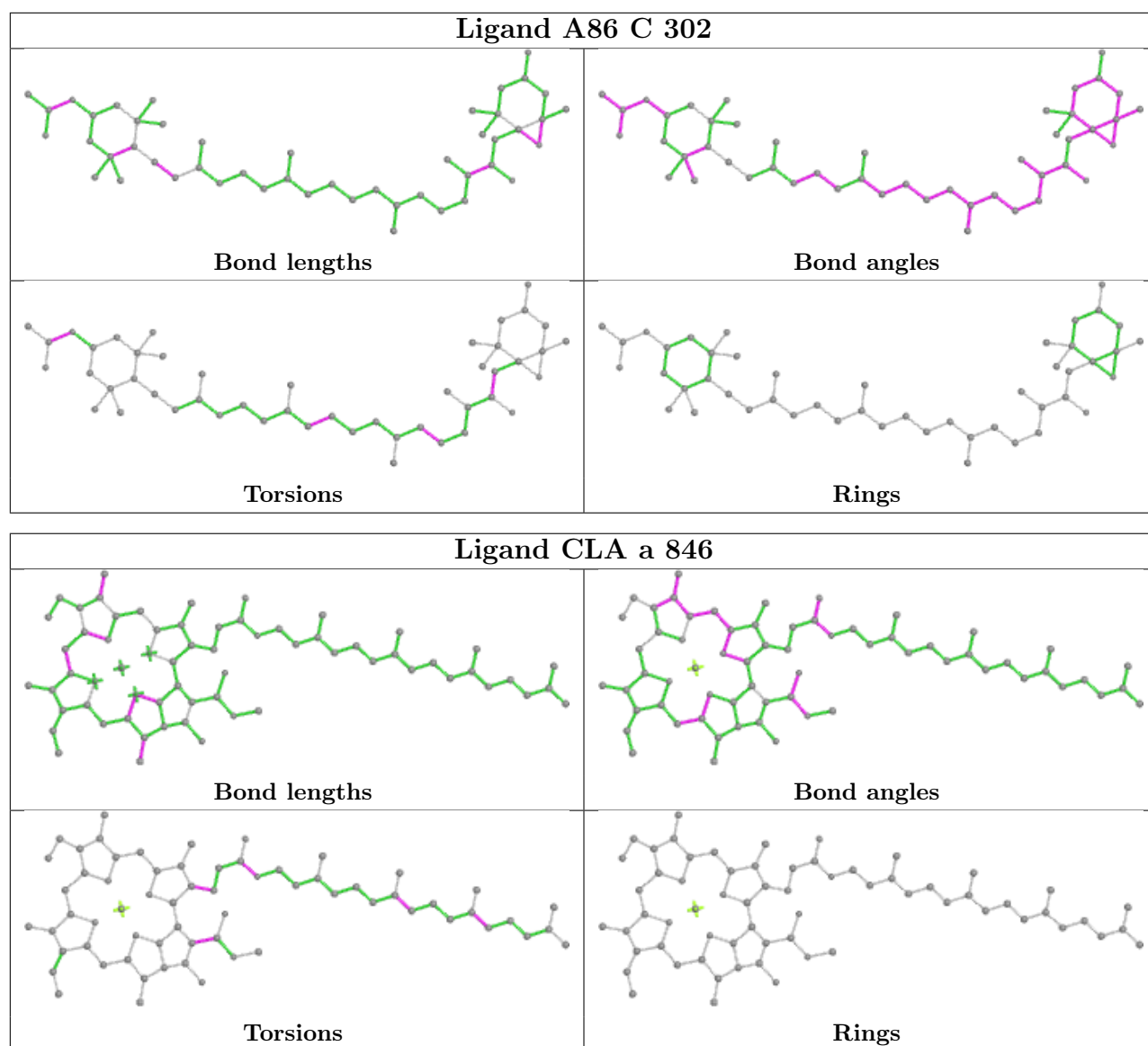
Rings

Ligand CLA a 812

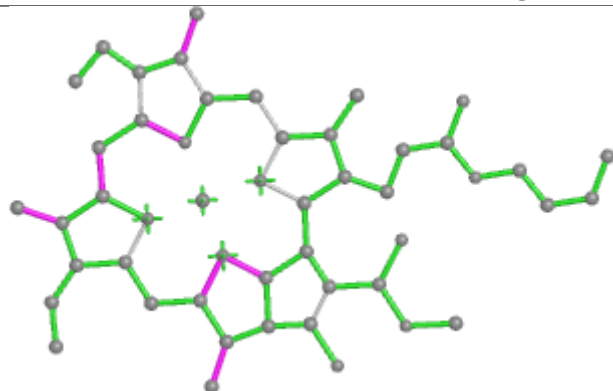


Ligand A86 C 304

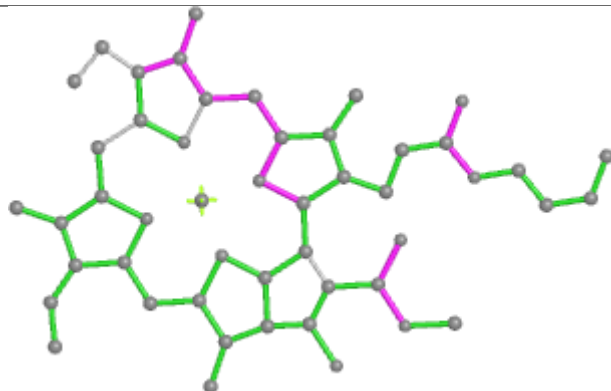




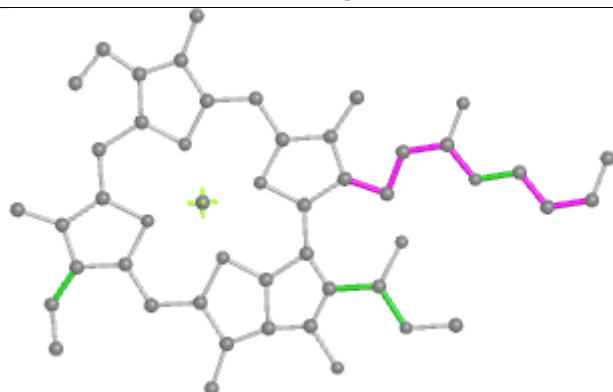
Ligand CLA D 209



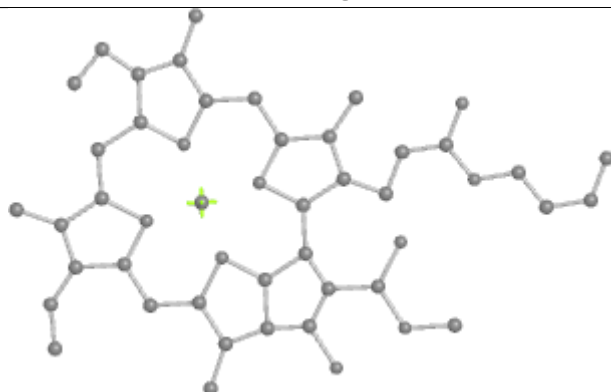
Bond lengths



Bond angles

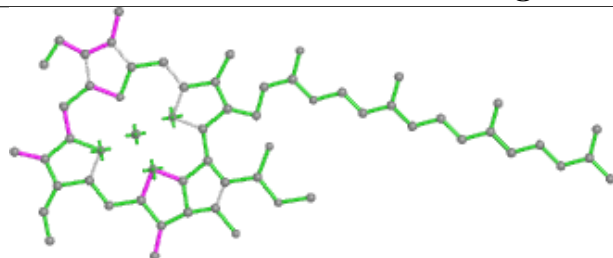


Torsions

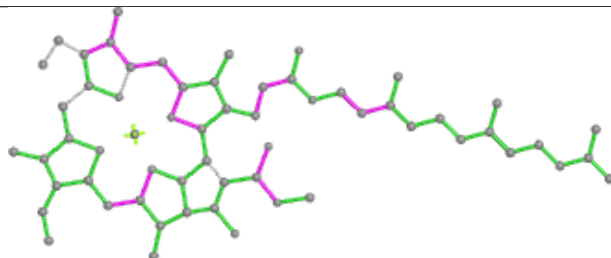


Rings

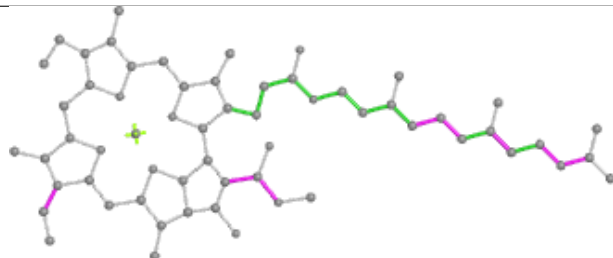
Ligand CLA C 311



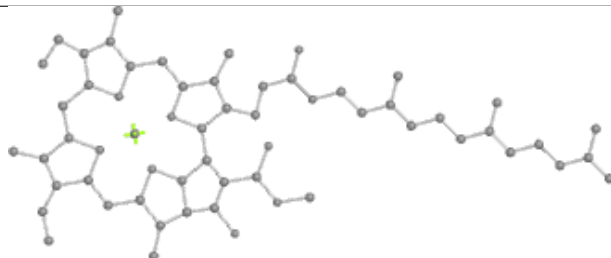
Bond lengths



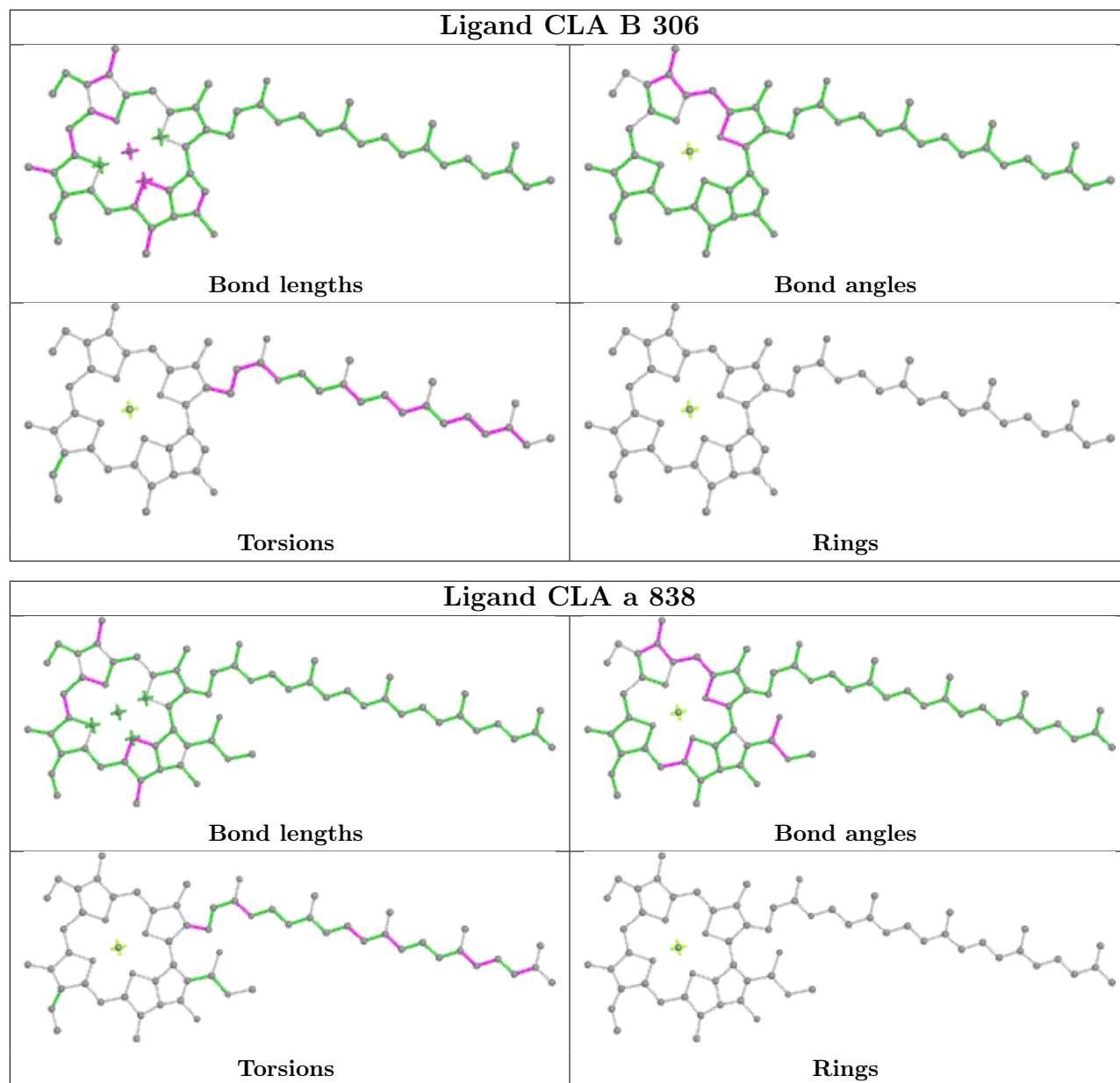
Bond angles



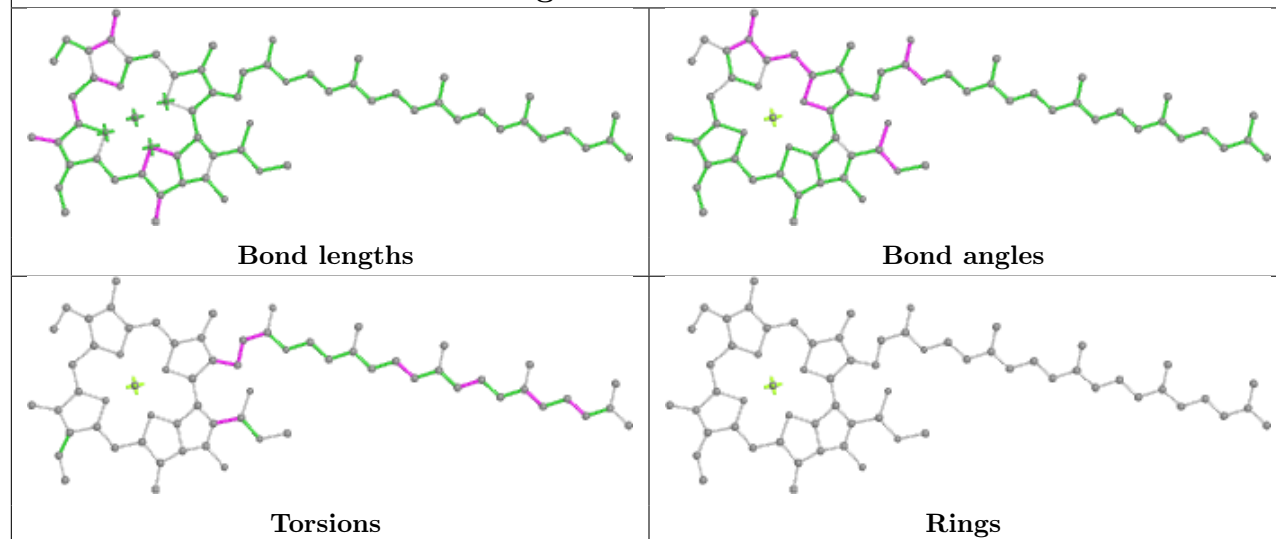
Torsions



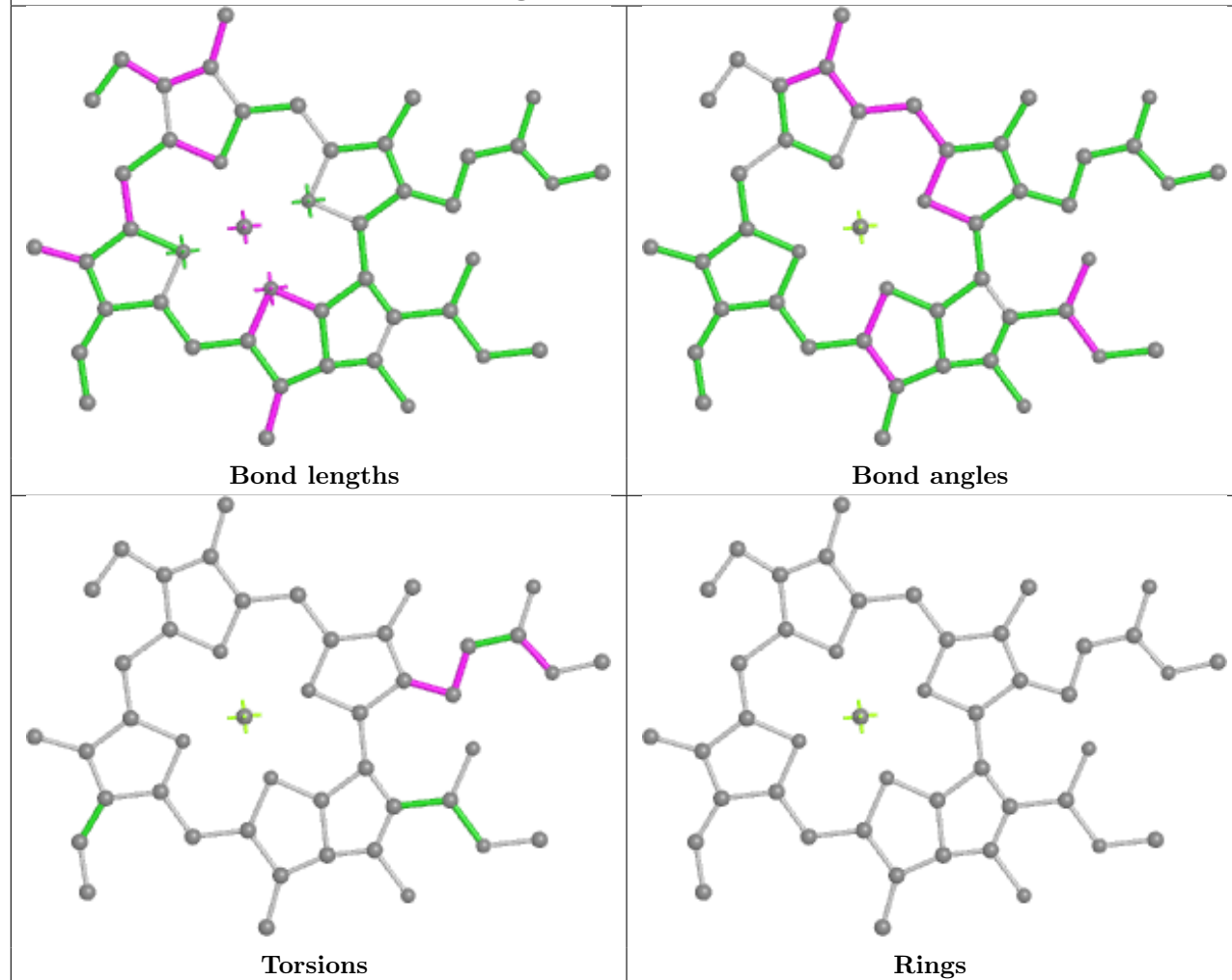
Rings



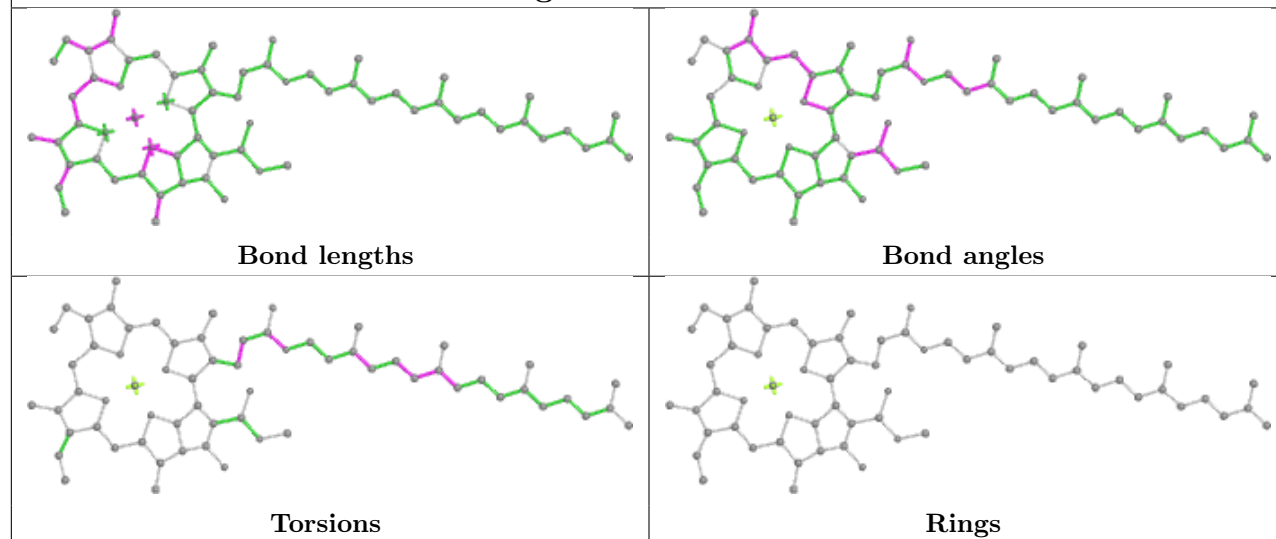
Ligand CLA a 808



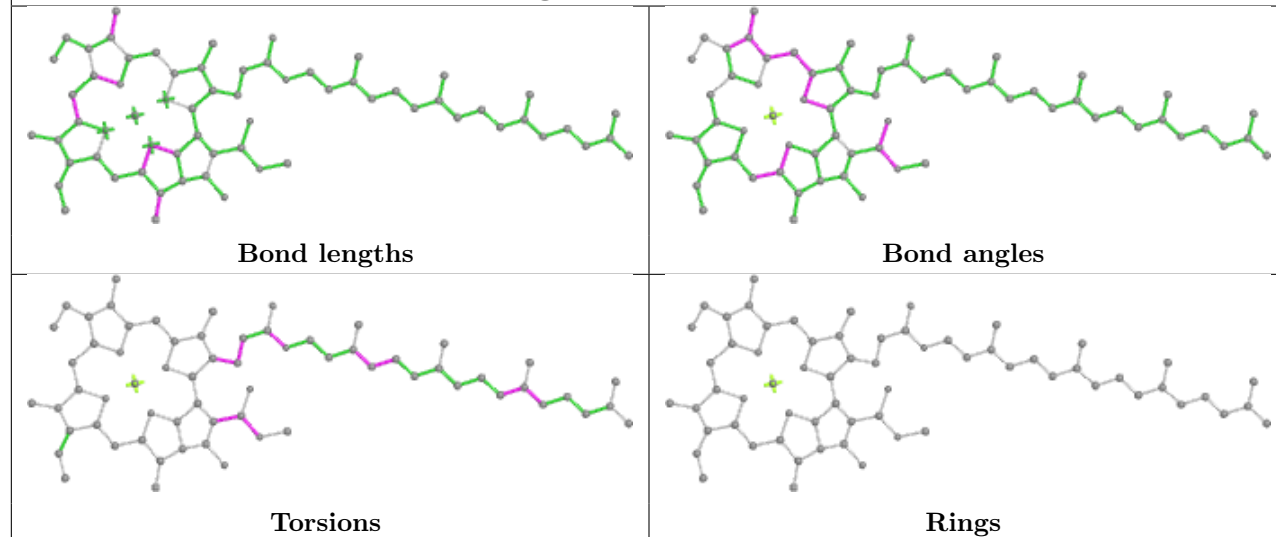
Ligand CLA D 216



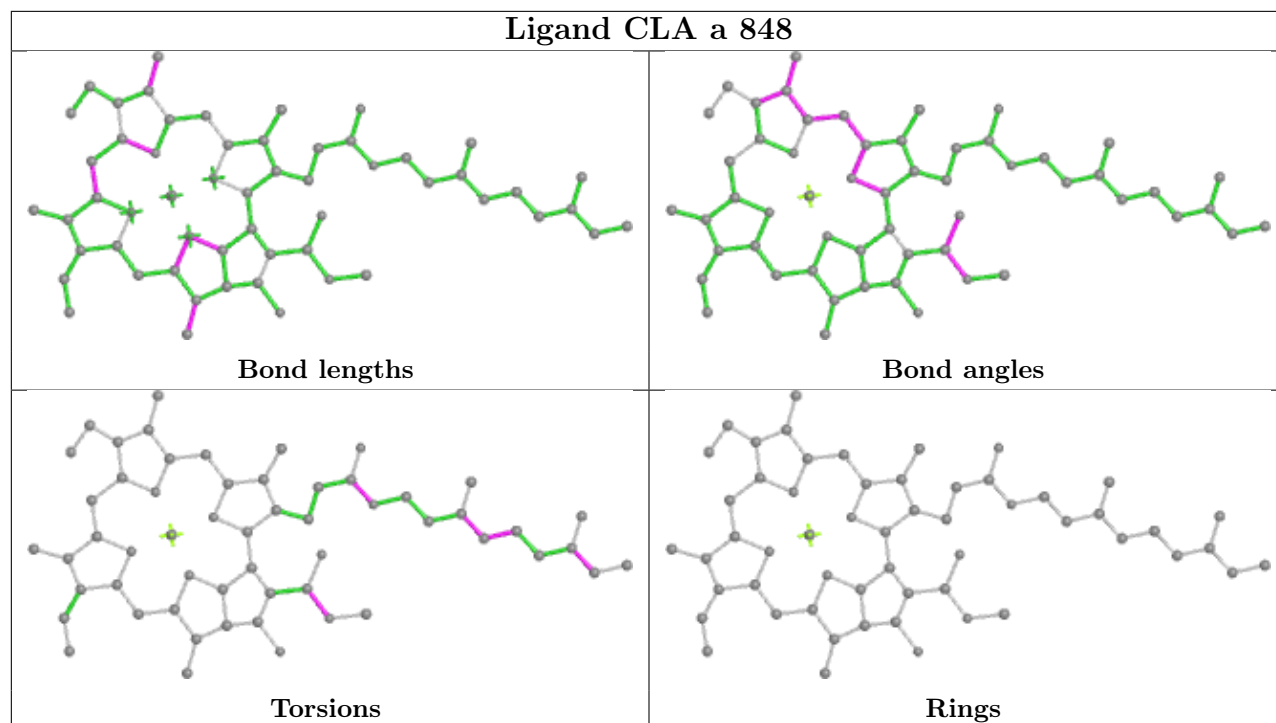
Ligand CLA b 801



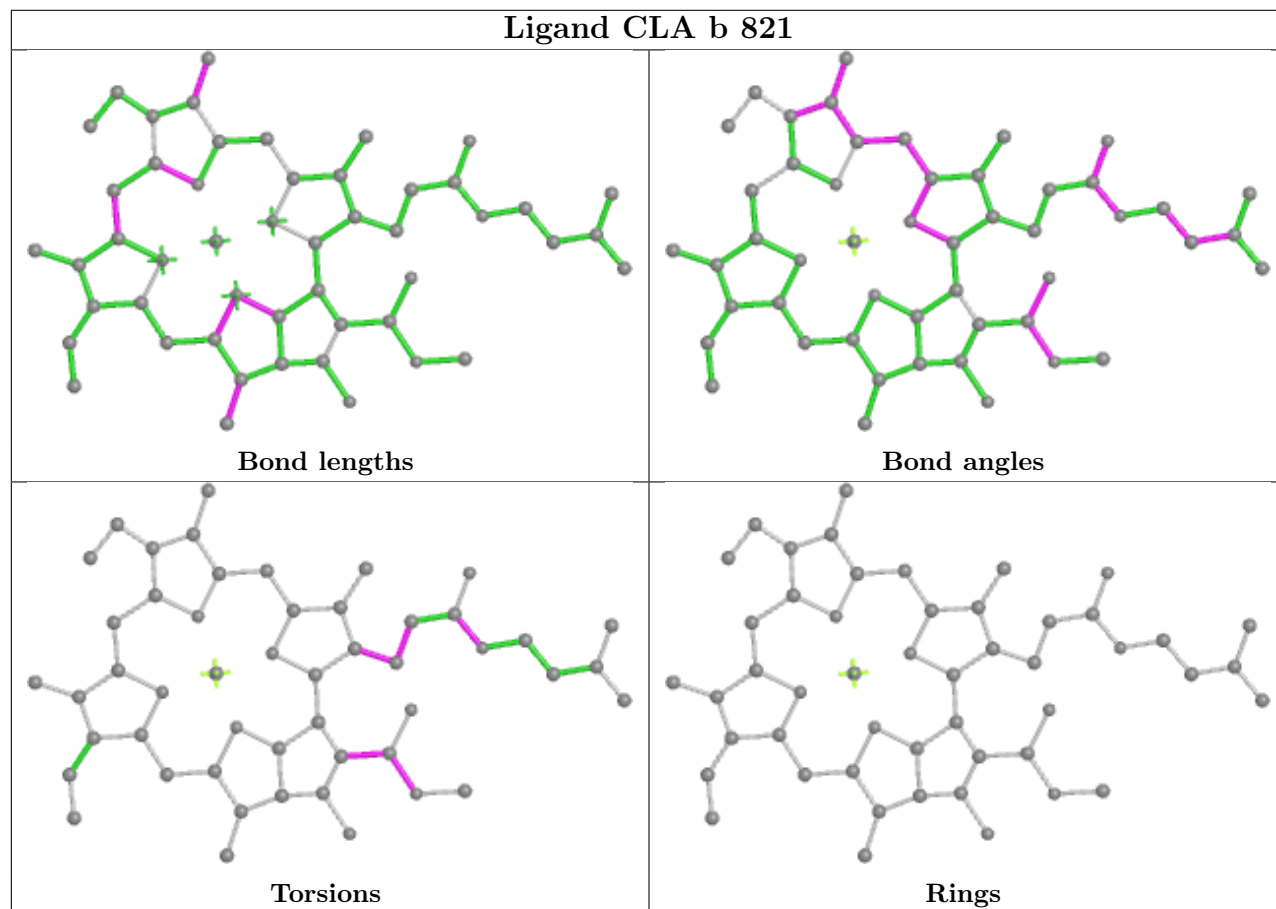
Ligand CLA a 844

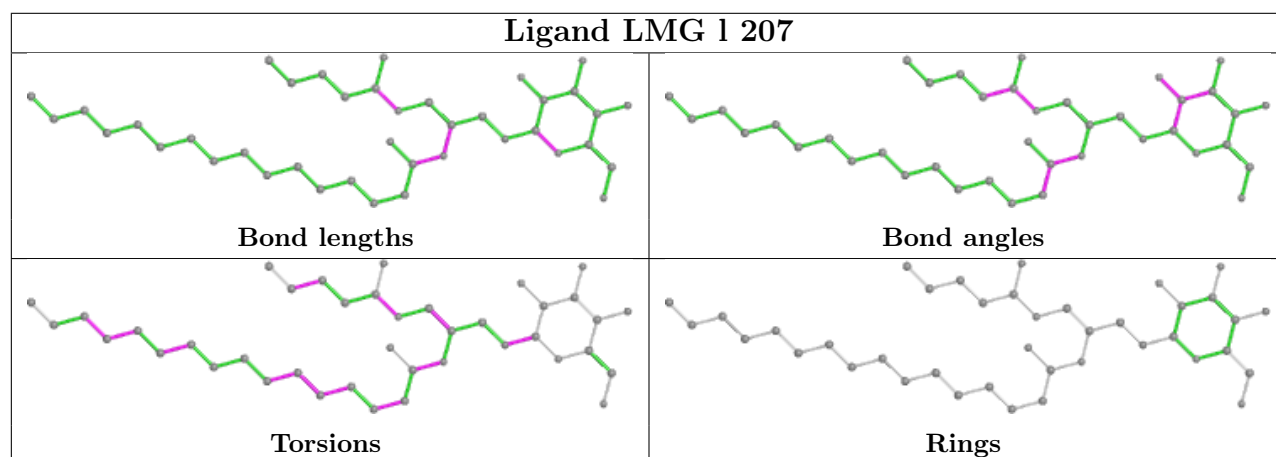
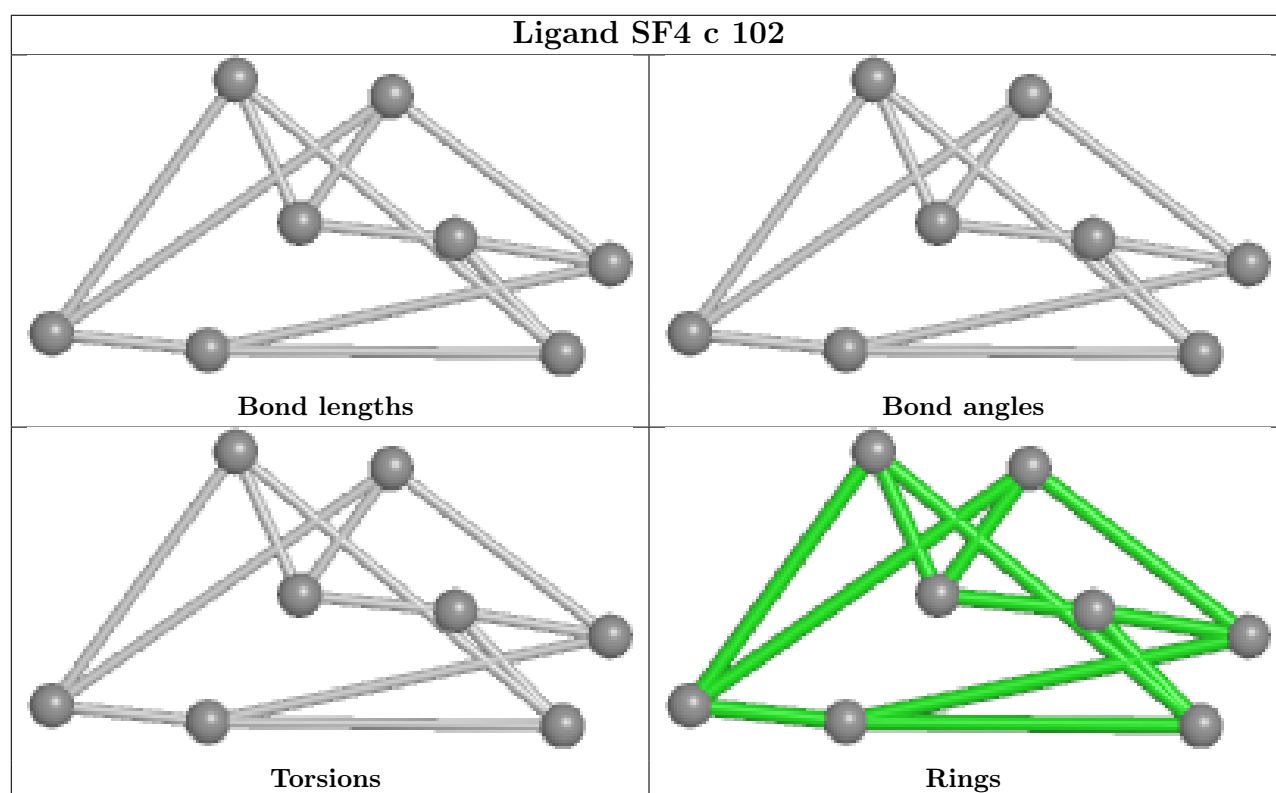
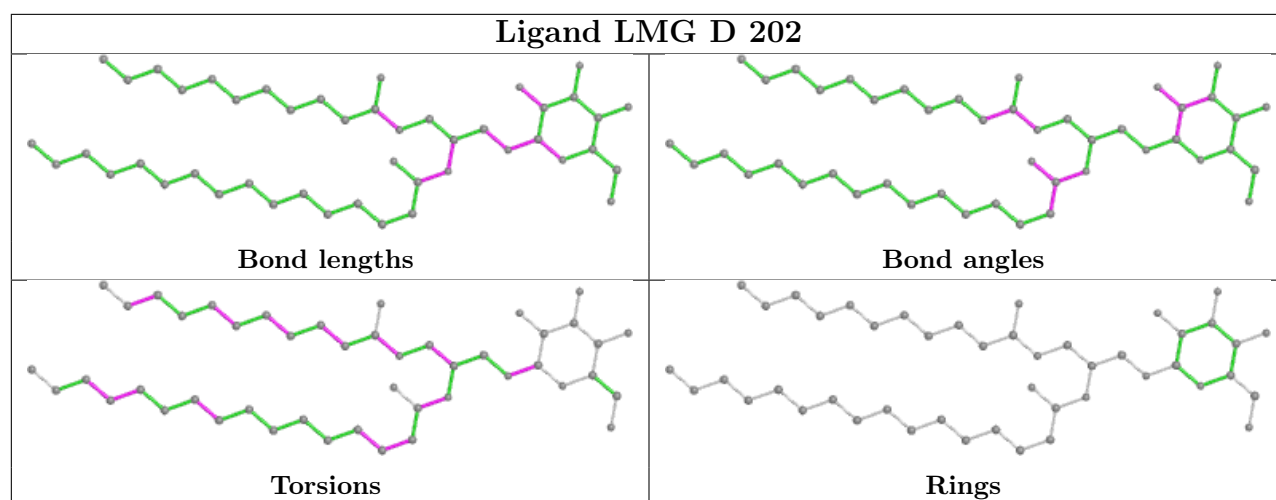


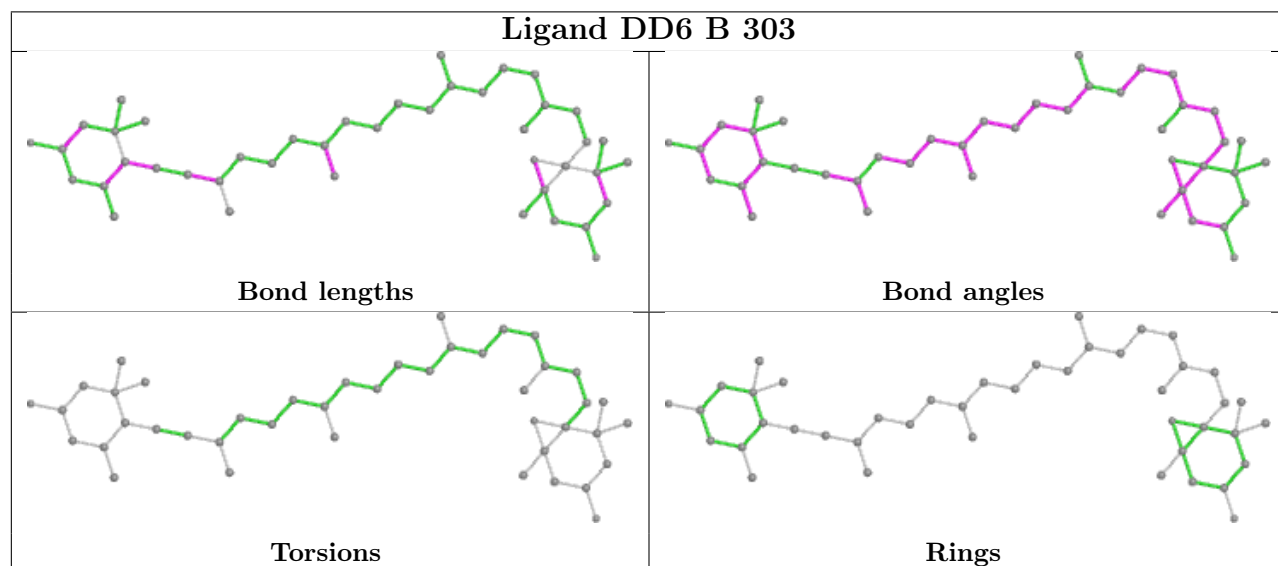
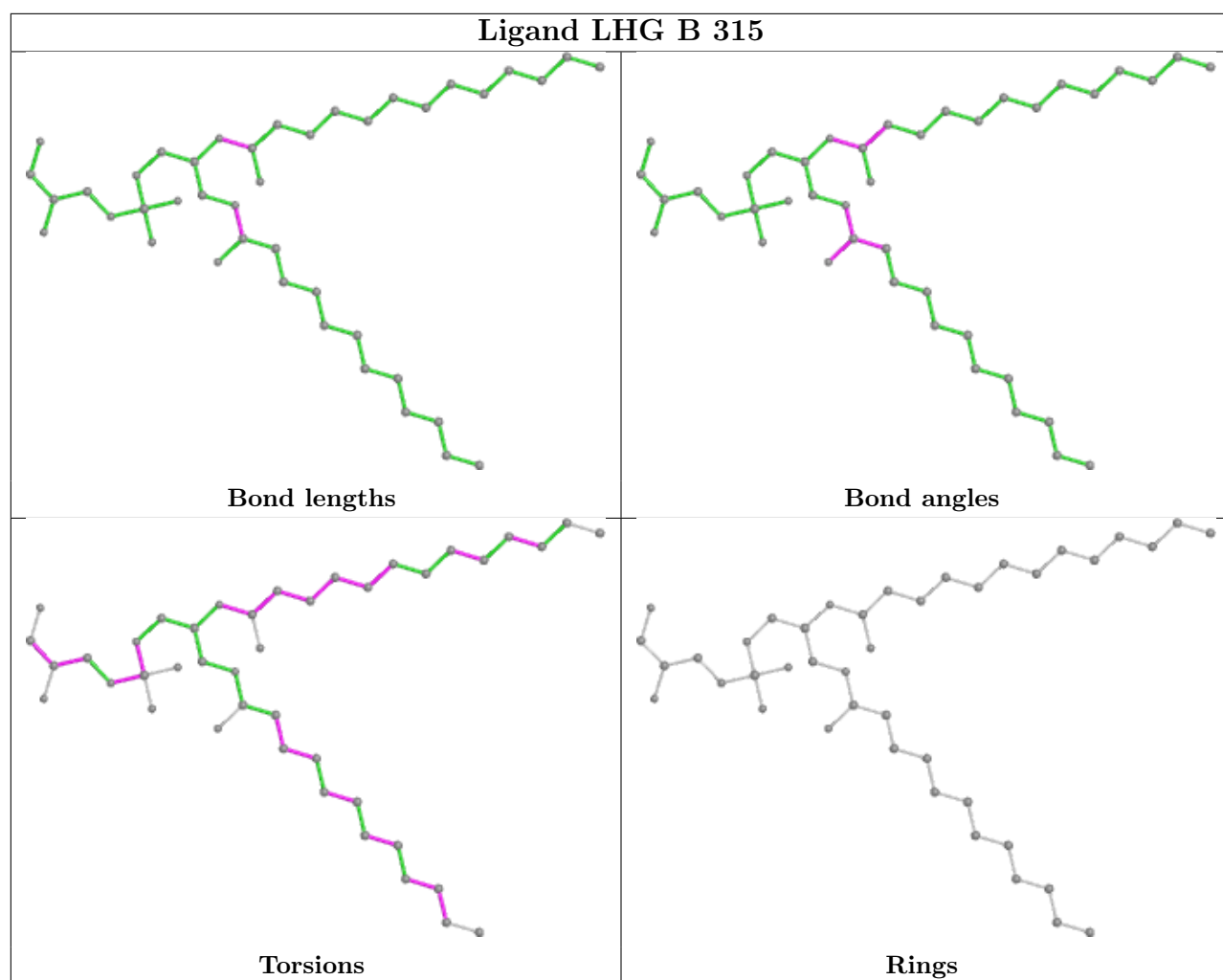
Ligand CLA a 848



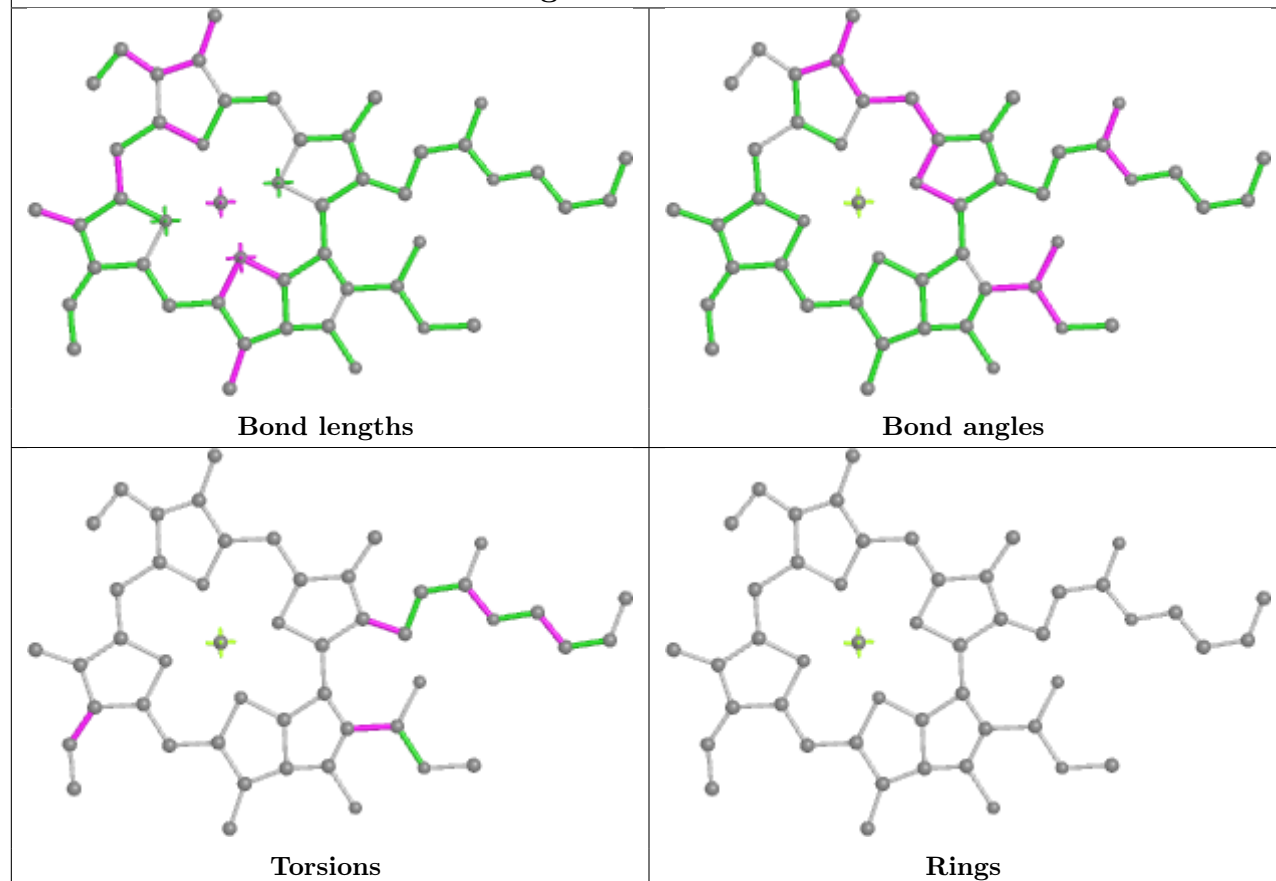
Ligand CLA b 821



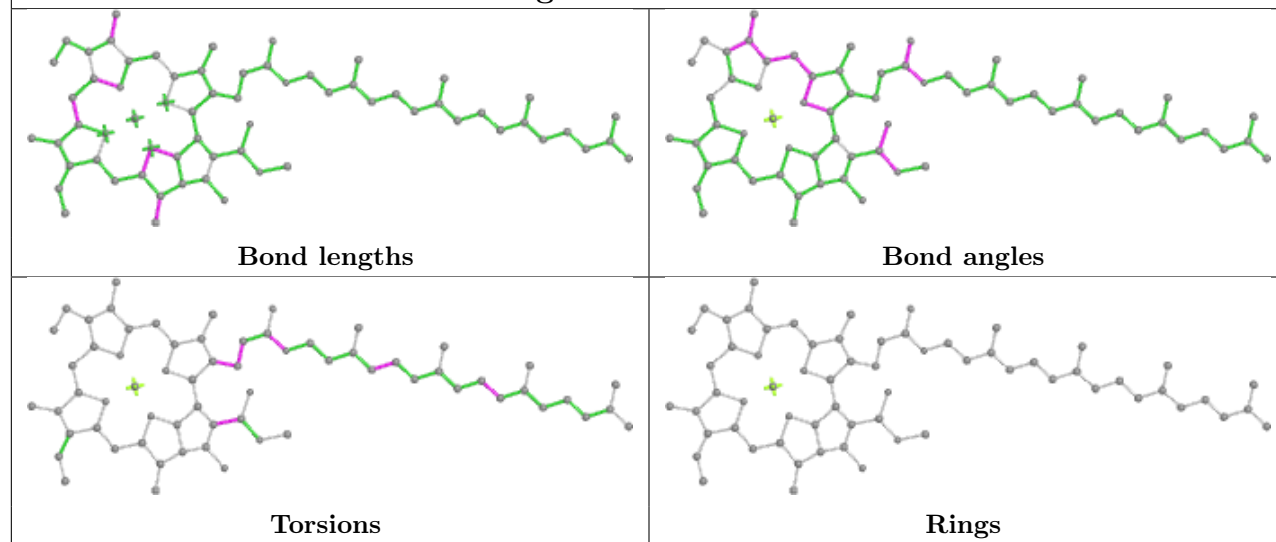


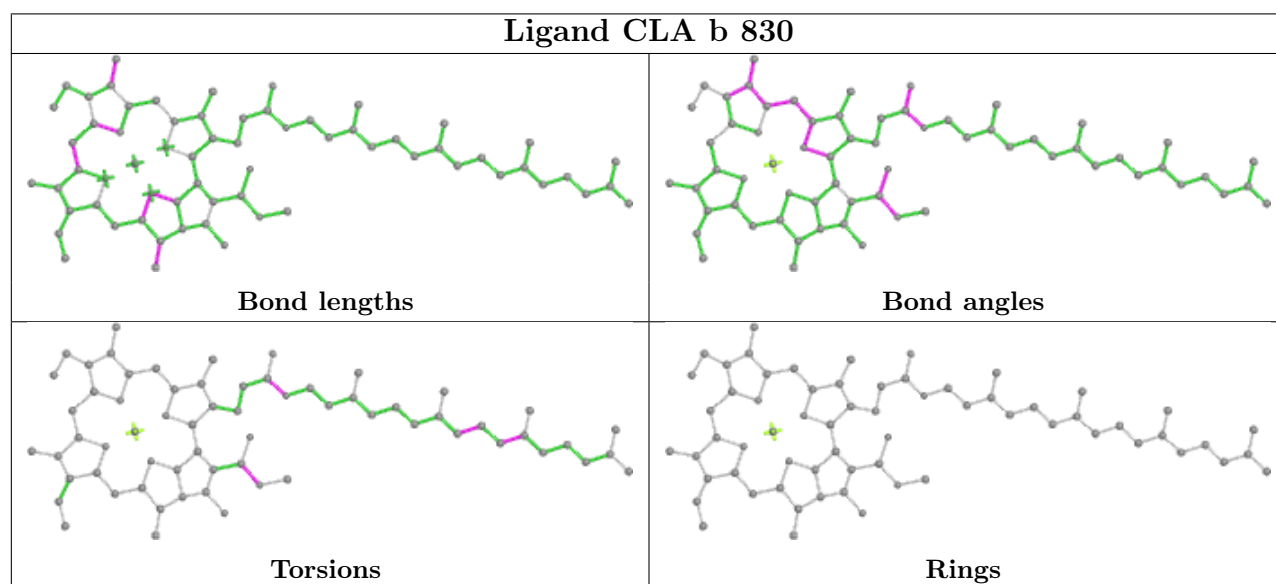
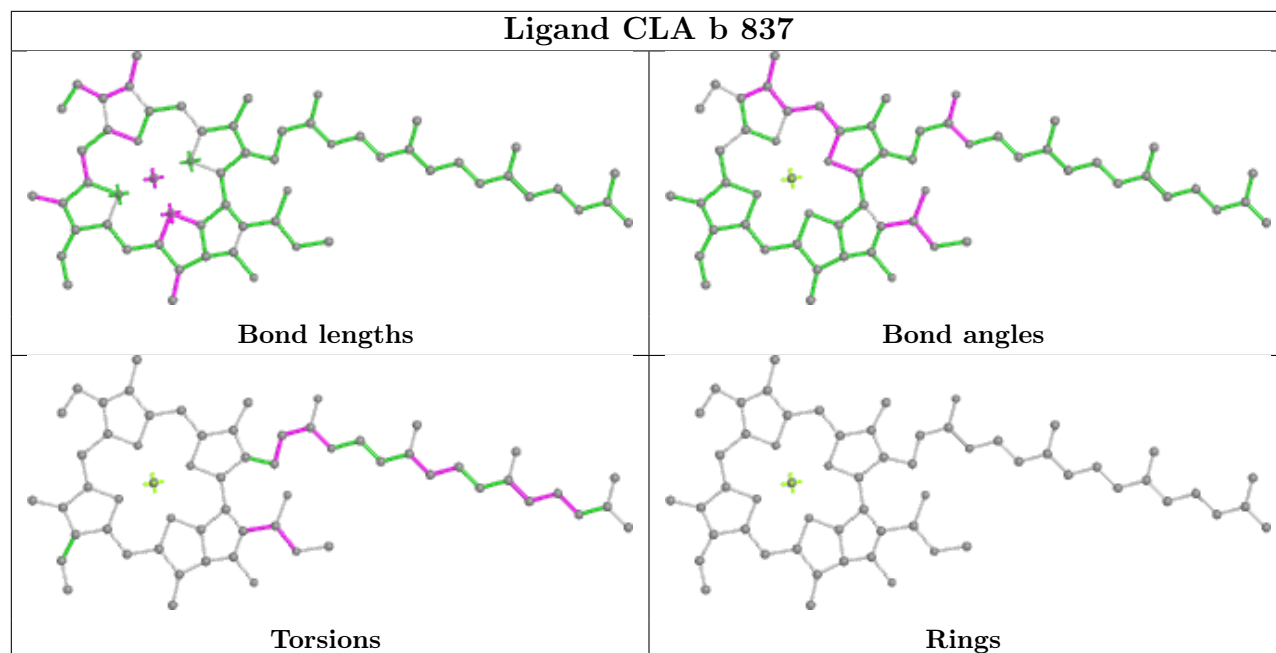
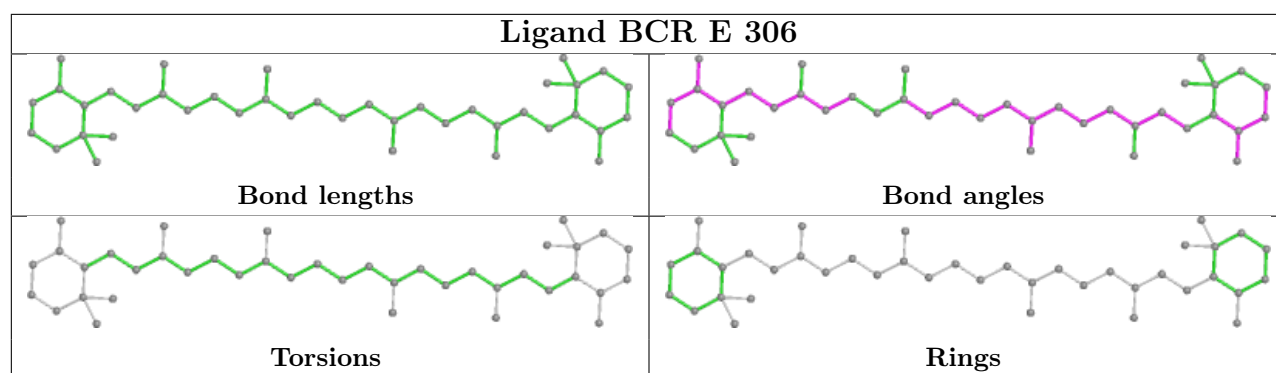


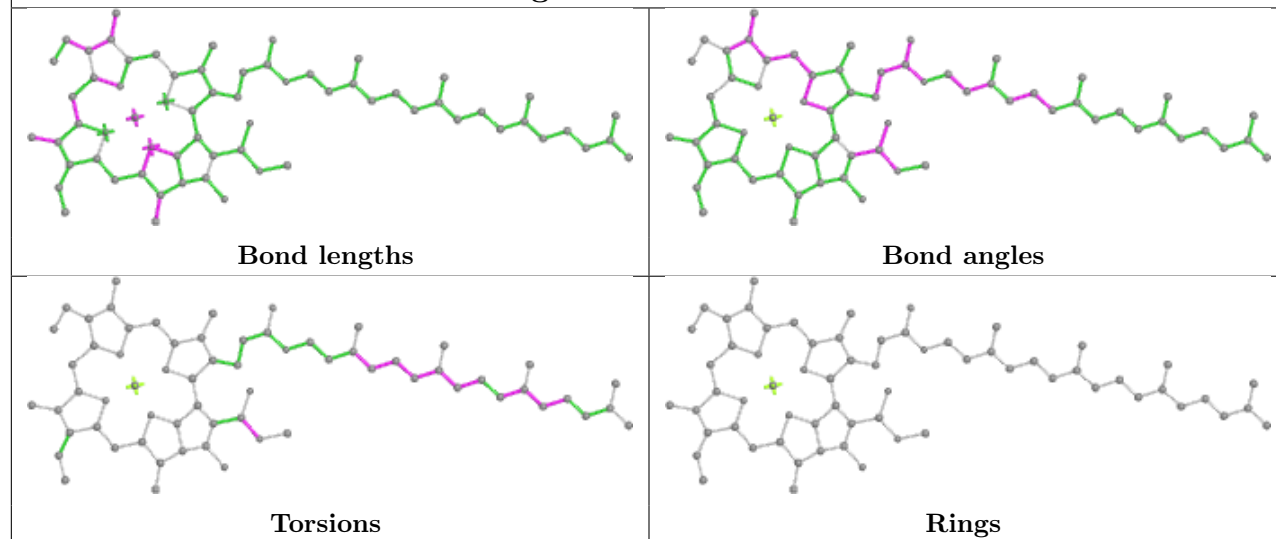
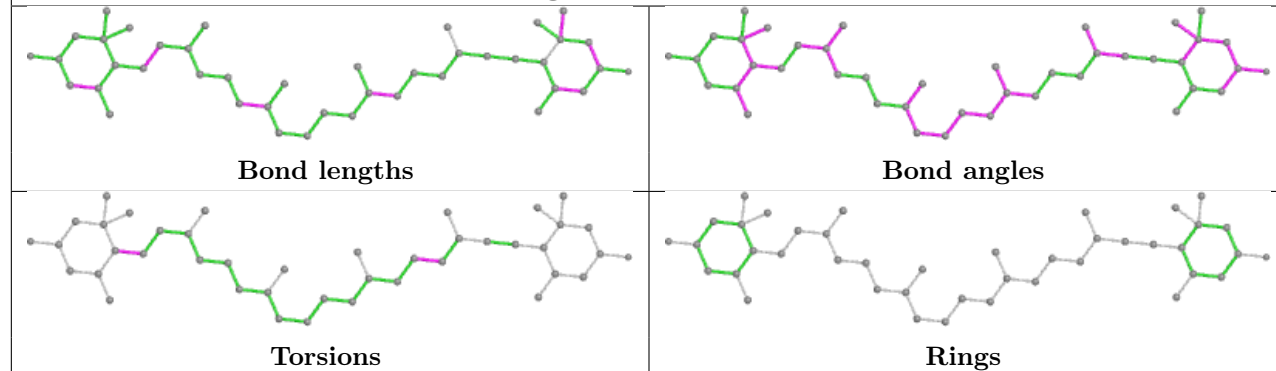
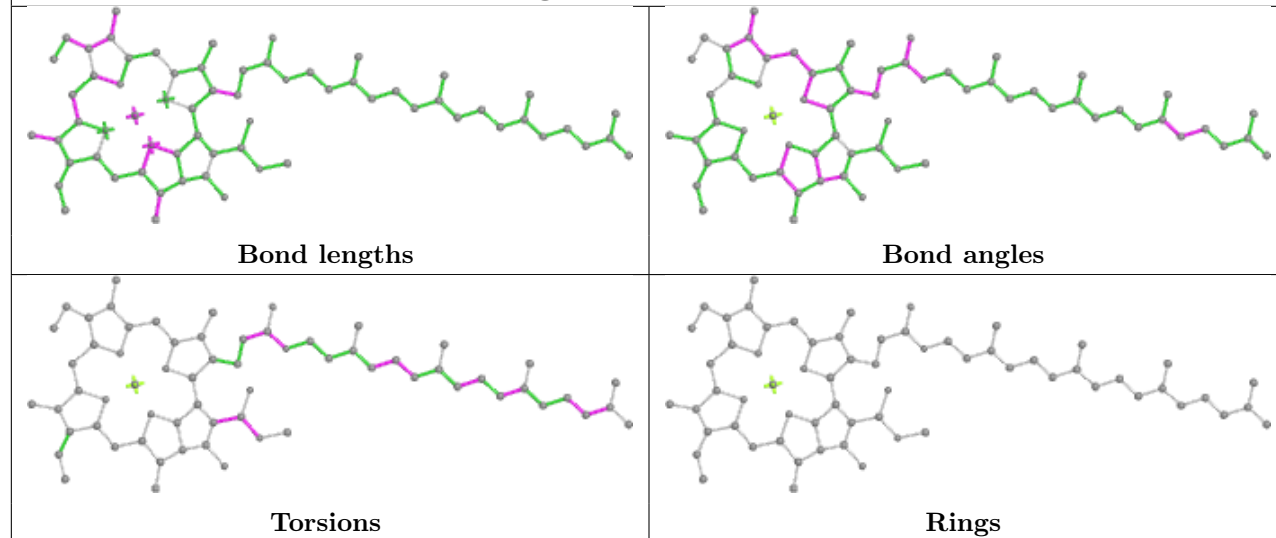
Ligand CLA 1 202

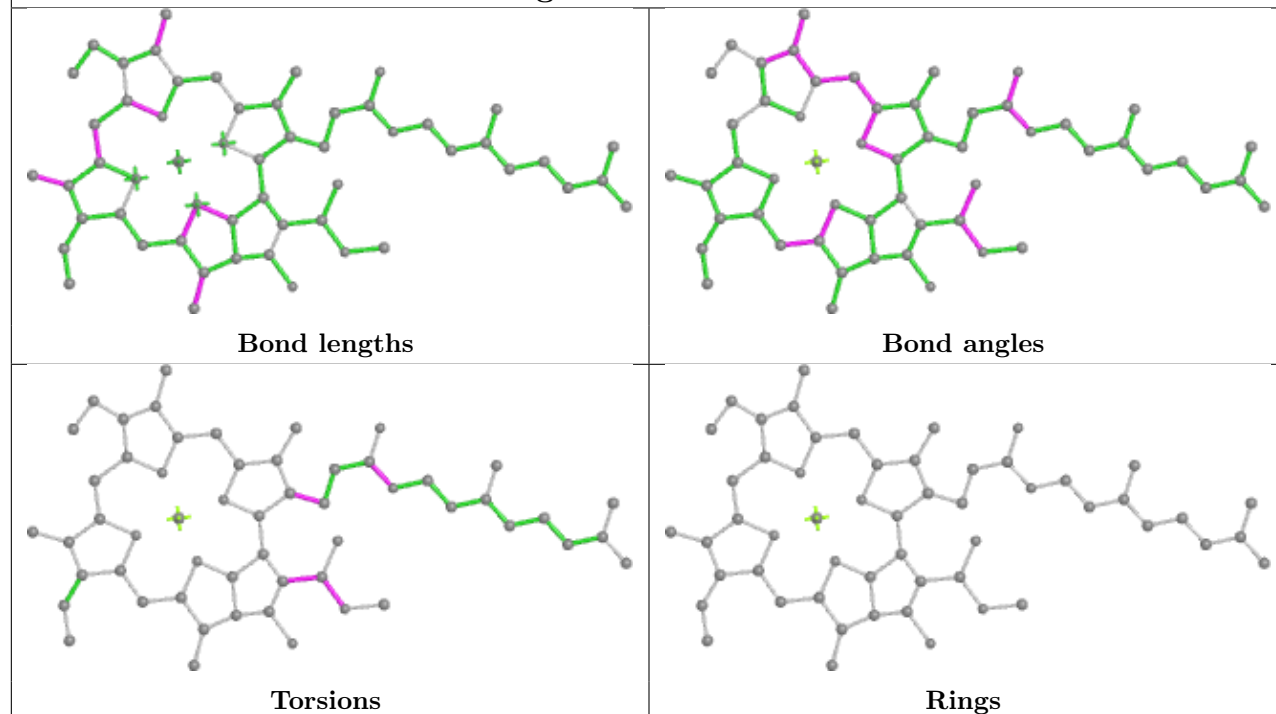
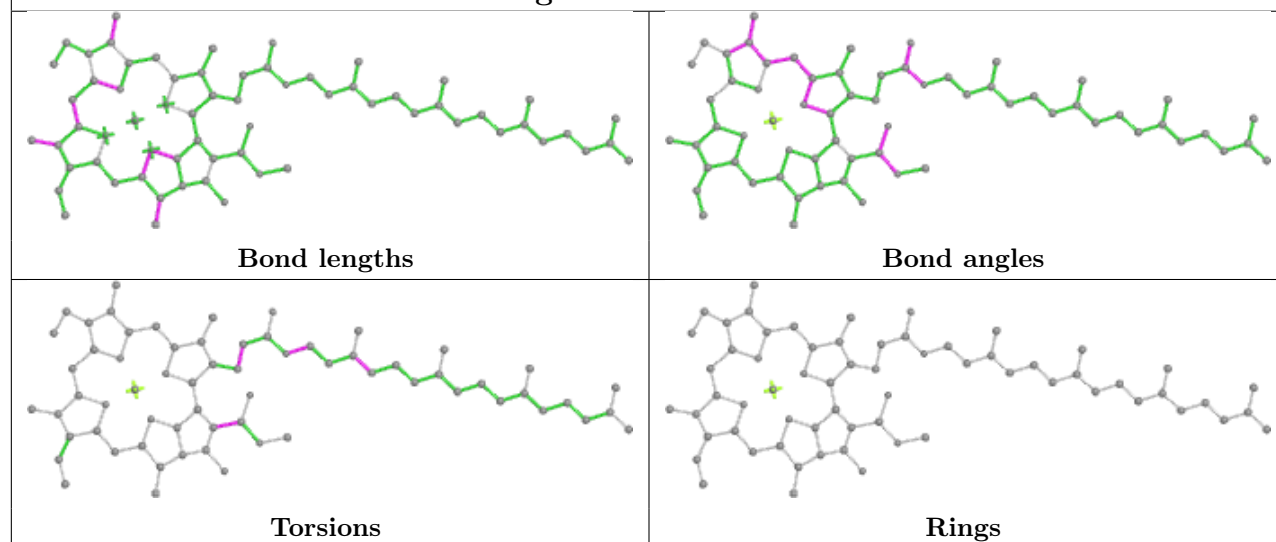


Ligand CLA a 839

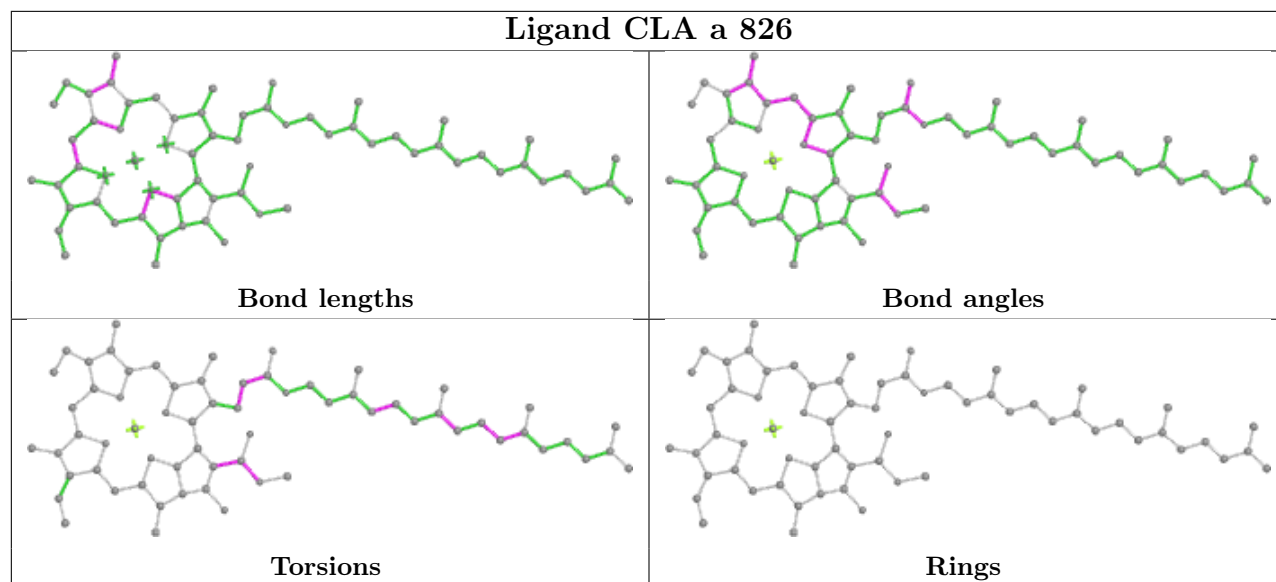




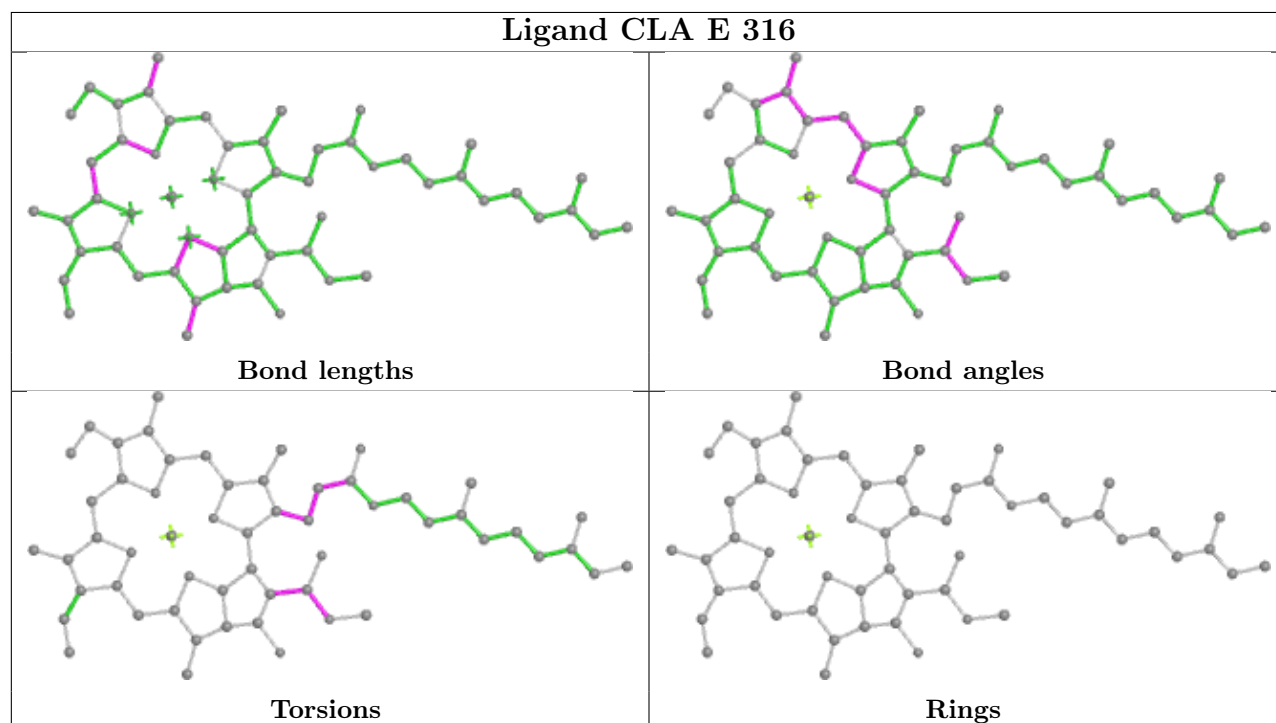
Ligand CLA D 208**Ligand ET4 l 206****Ligand CLA a 801**

Ligand CLA a 804**Ligand CLA b 838**

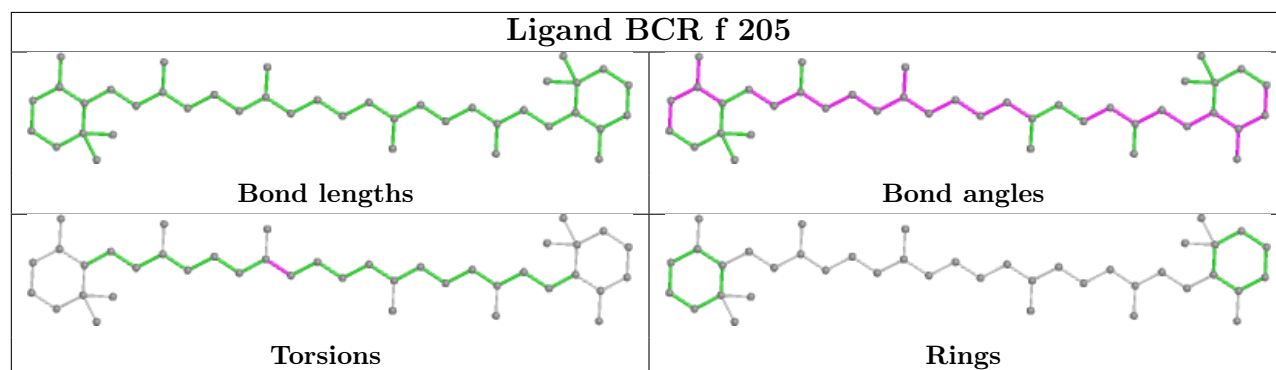
Ligand CLA a 826



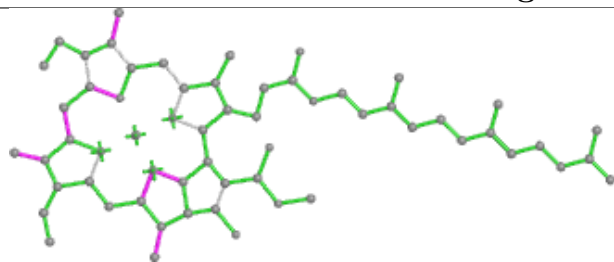
Ligand CLA E 316



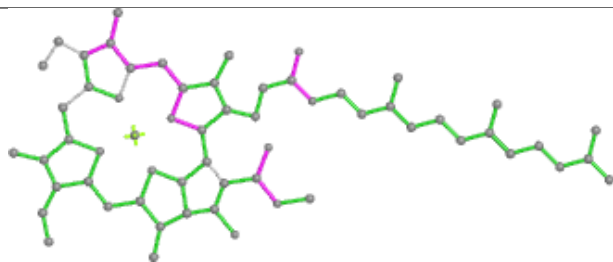
Ligand BCR f 205



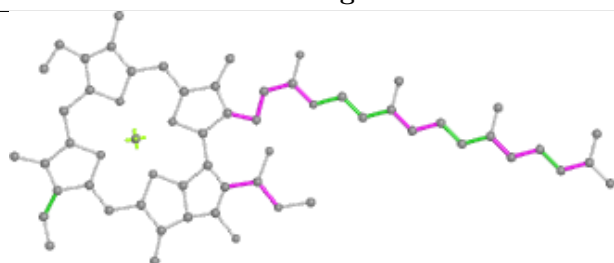
Ligand CLA b 817



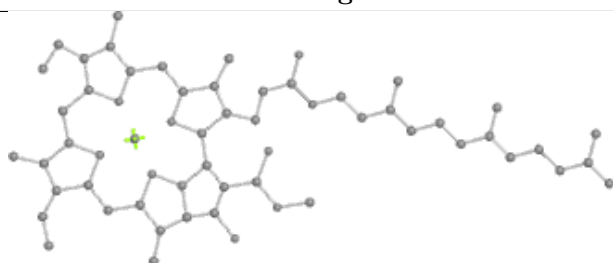
Bond lengths



Bond angles

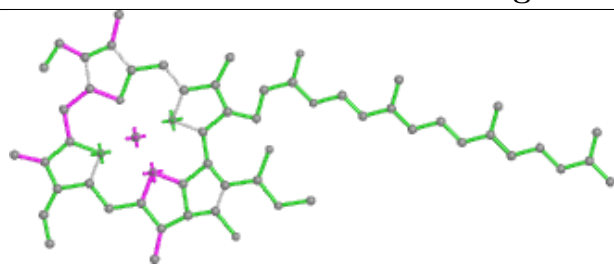


Torsions

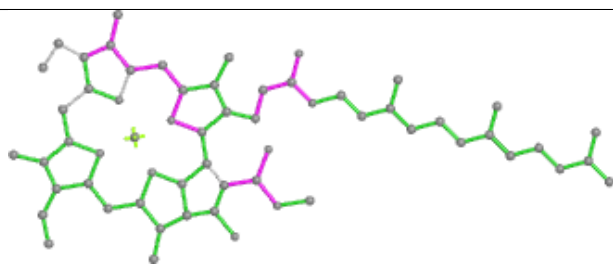


Rings

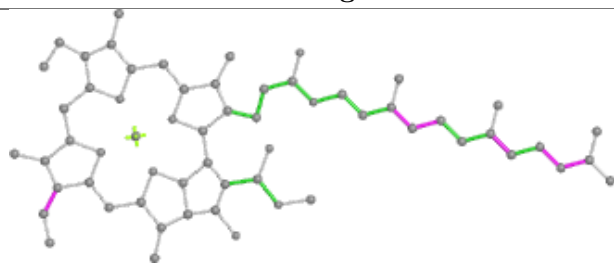
Ligand CLA H 310



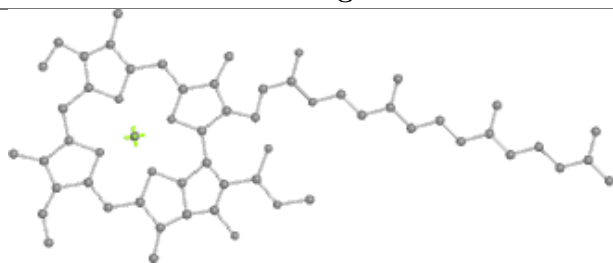
Bond lengths



Bond angles

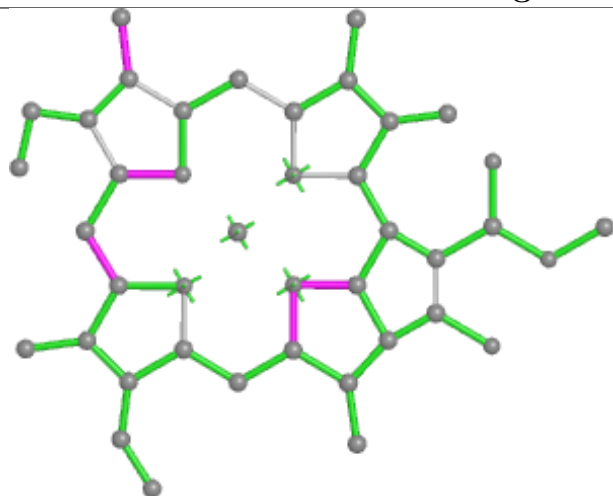


Torsions

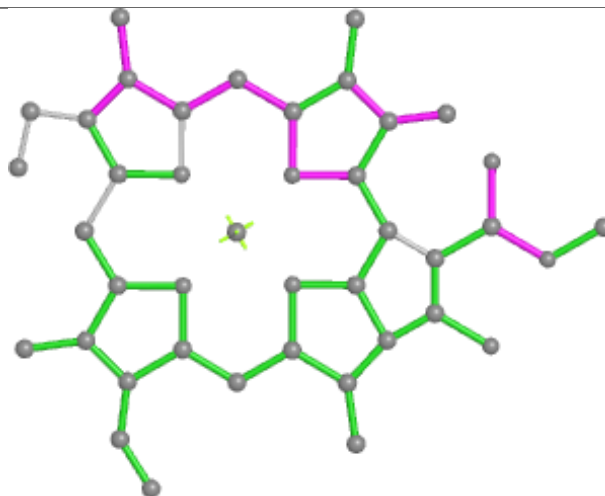


Rings

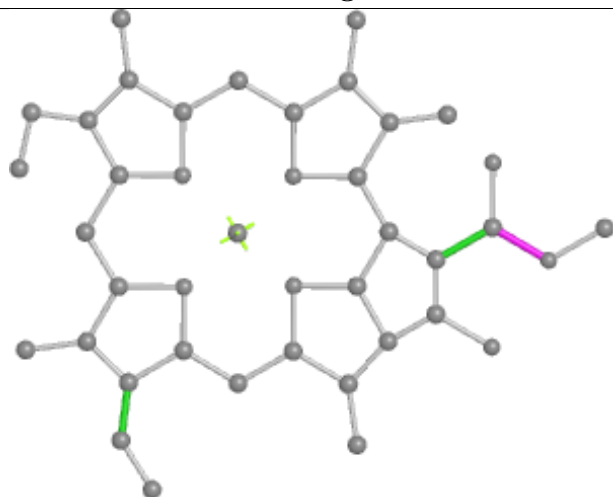
Ligand CLA D 215



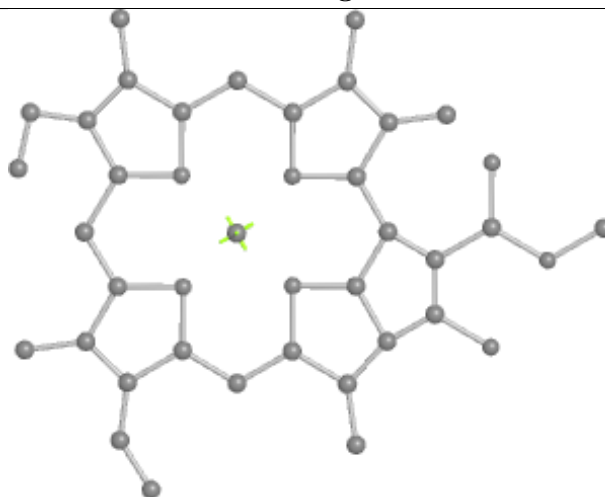
Bond lengths



Bond angles

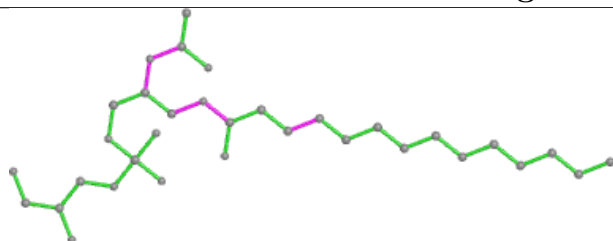


Torsions

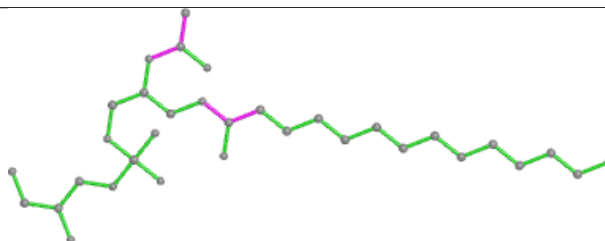


Rings

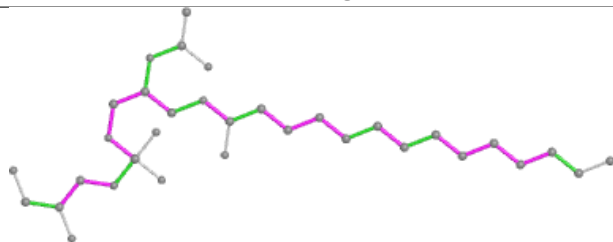
Ligand LHG a 835



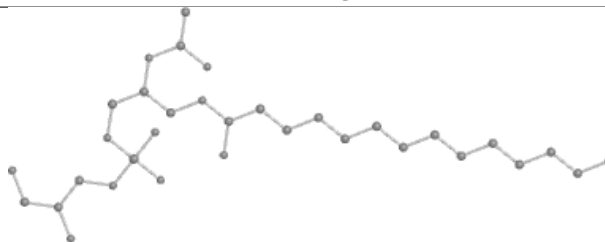
Bond lengths



Bond angles

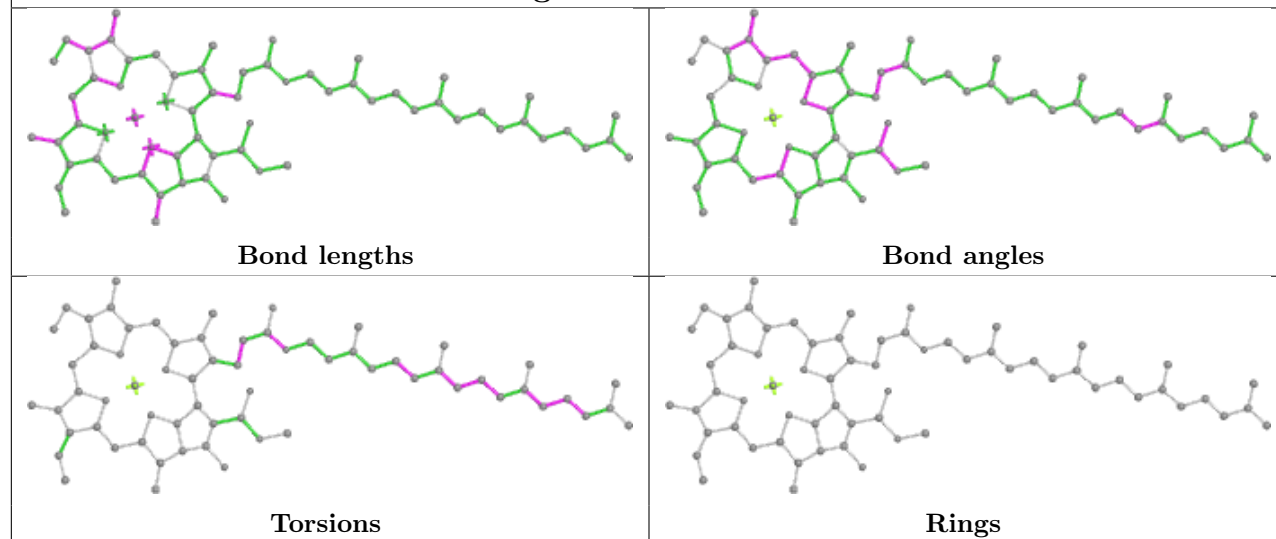


Torsions

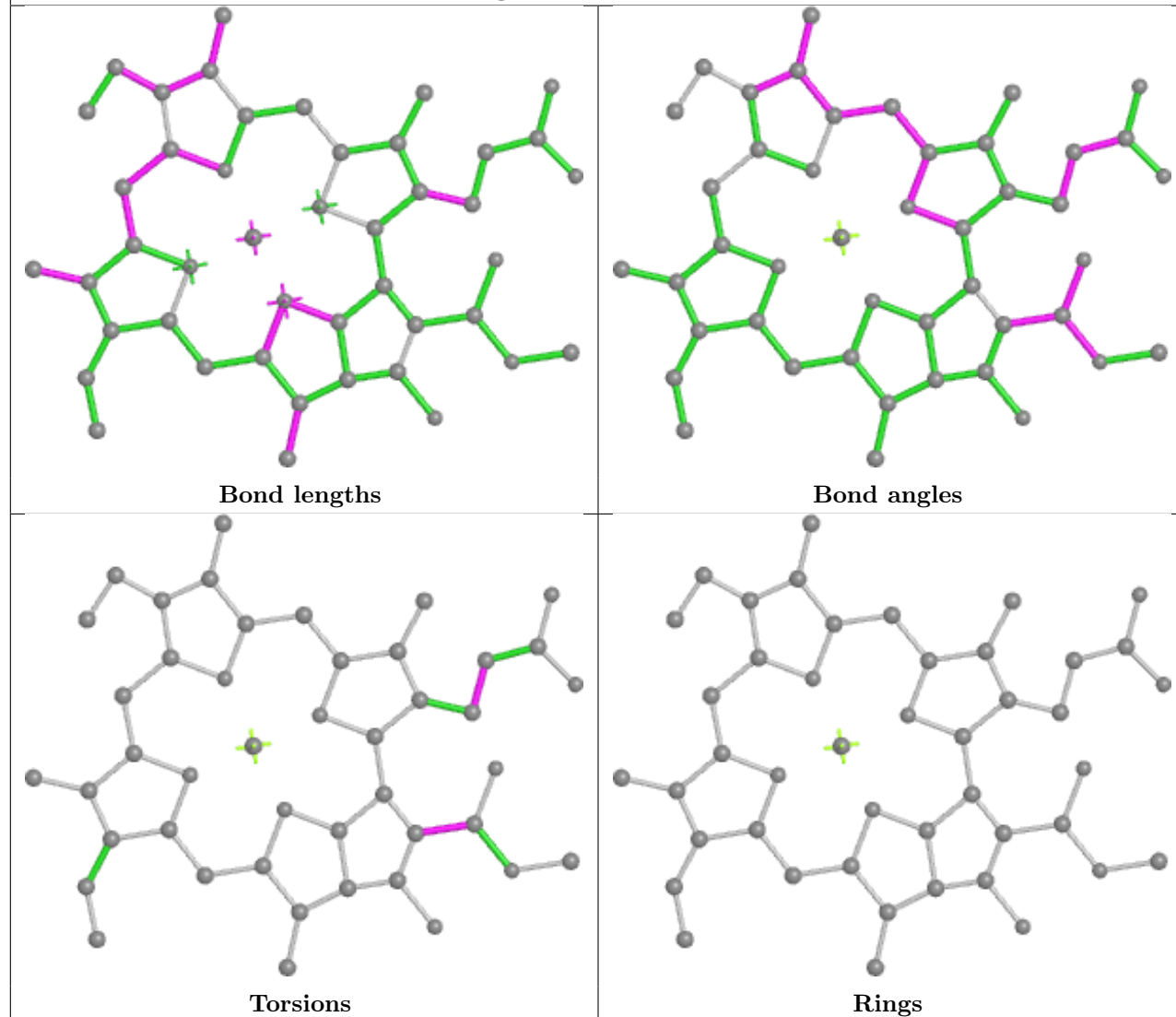


Rings

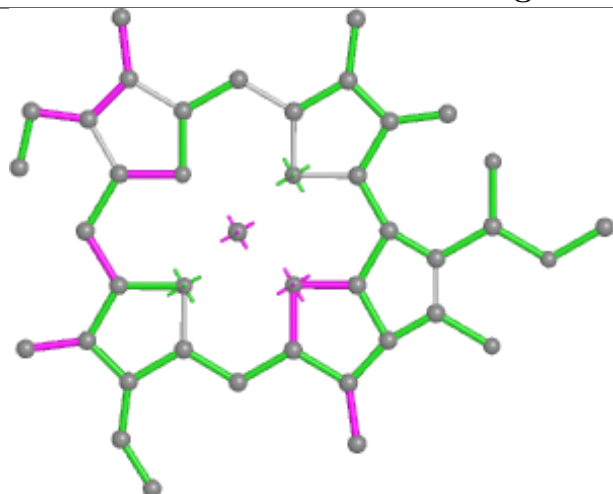
Ligand CLA E 312



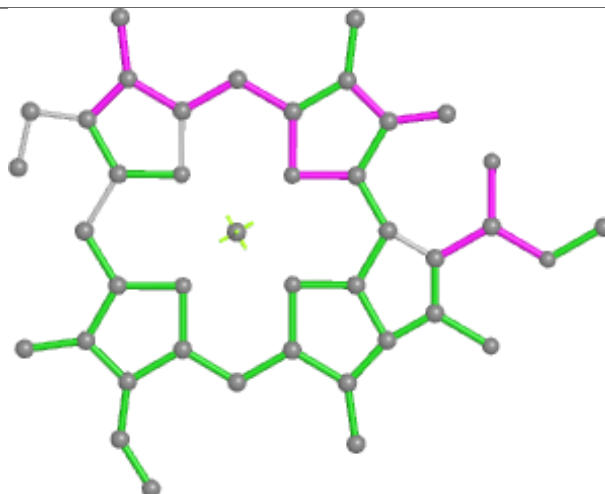
Ligand CLA b 804



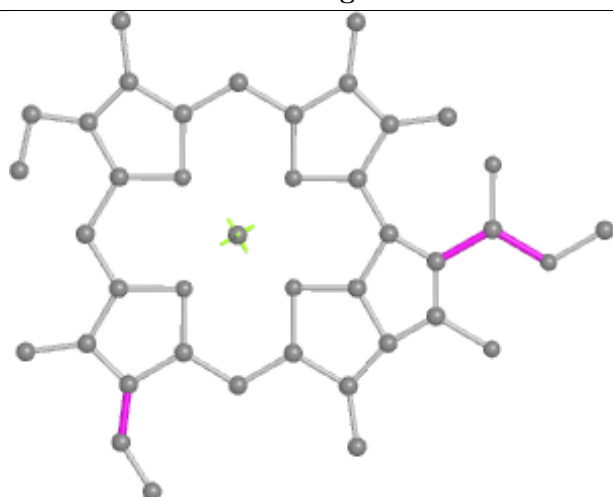
Ligand CLA C 314



Bond lengths



Bond angles

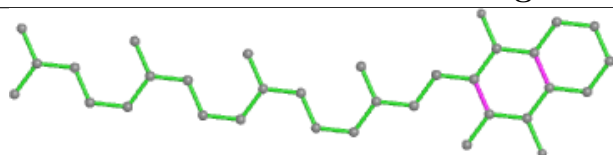


Torsions

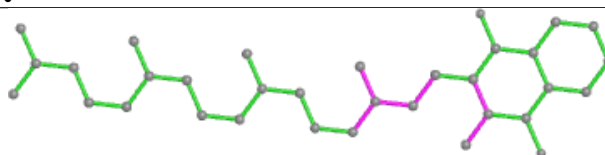


Rings

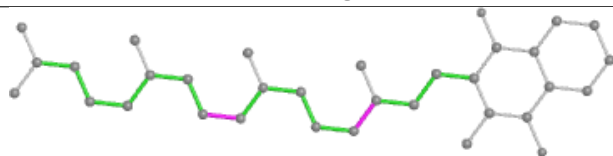
Ligand PQN b 831



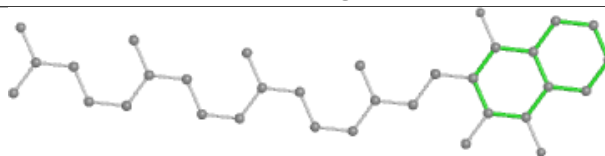
Bond lengths



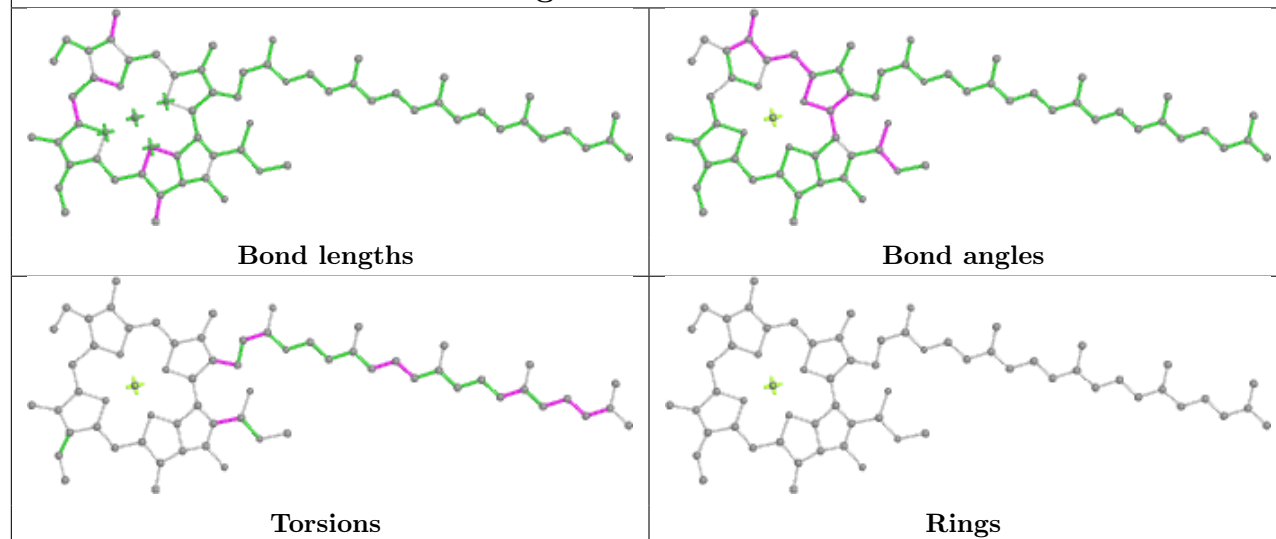
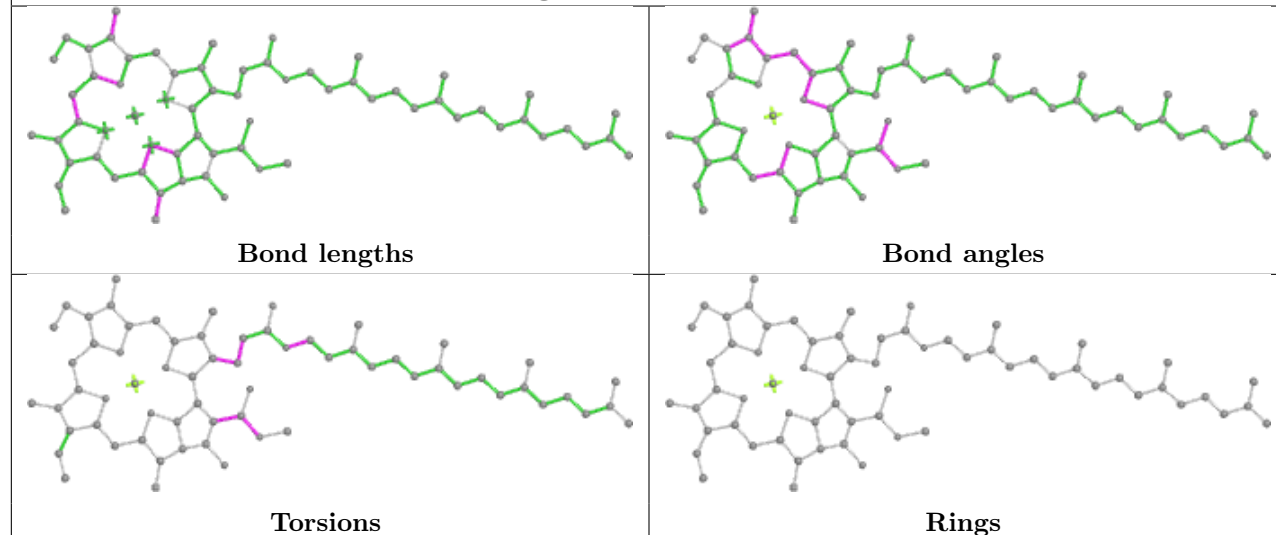
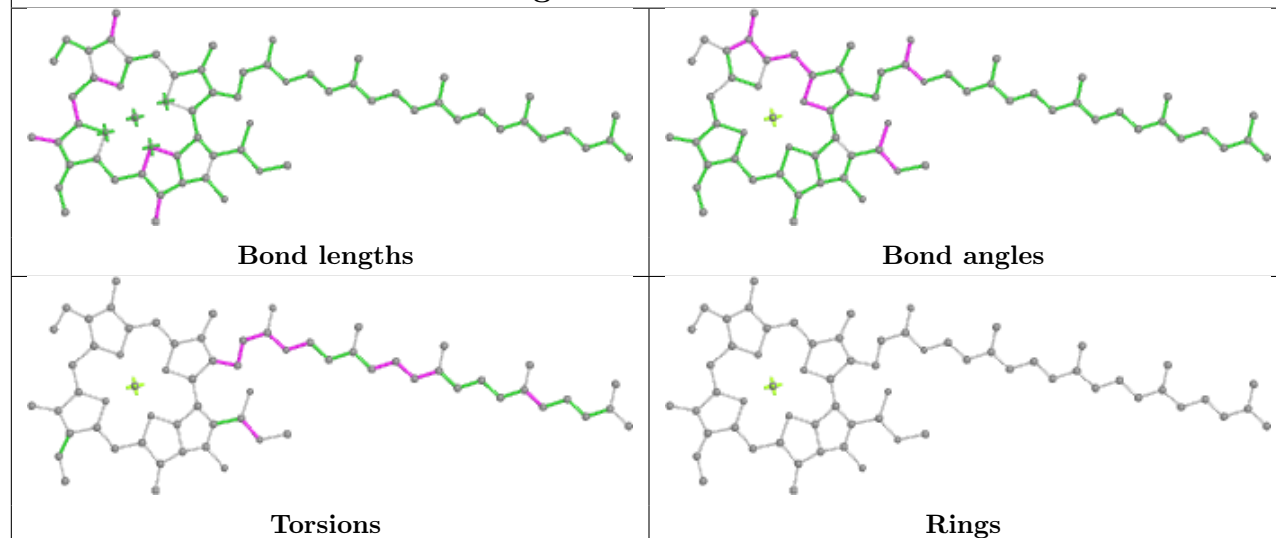
Bond angles



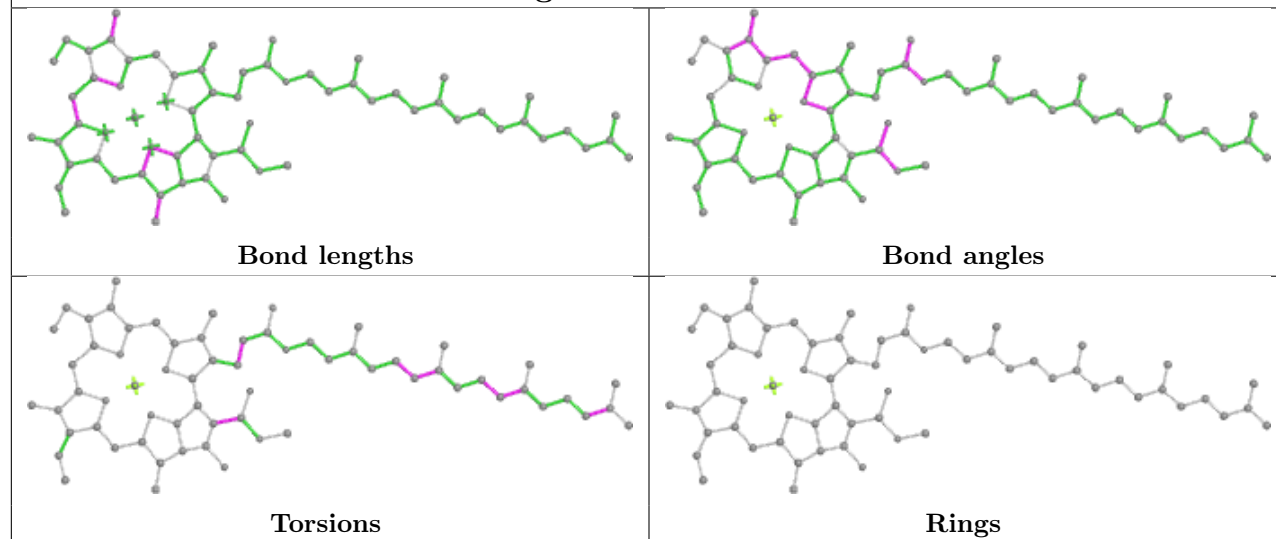
Torsions



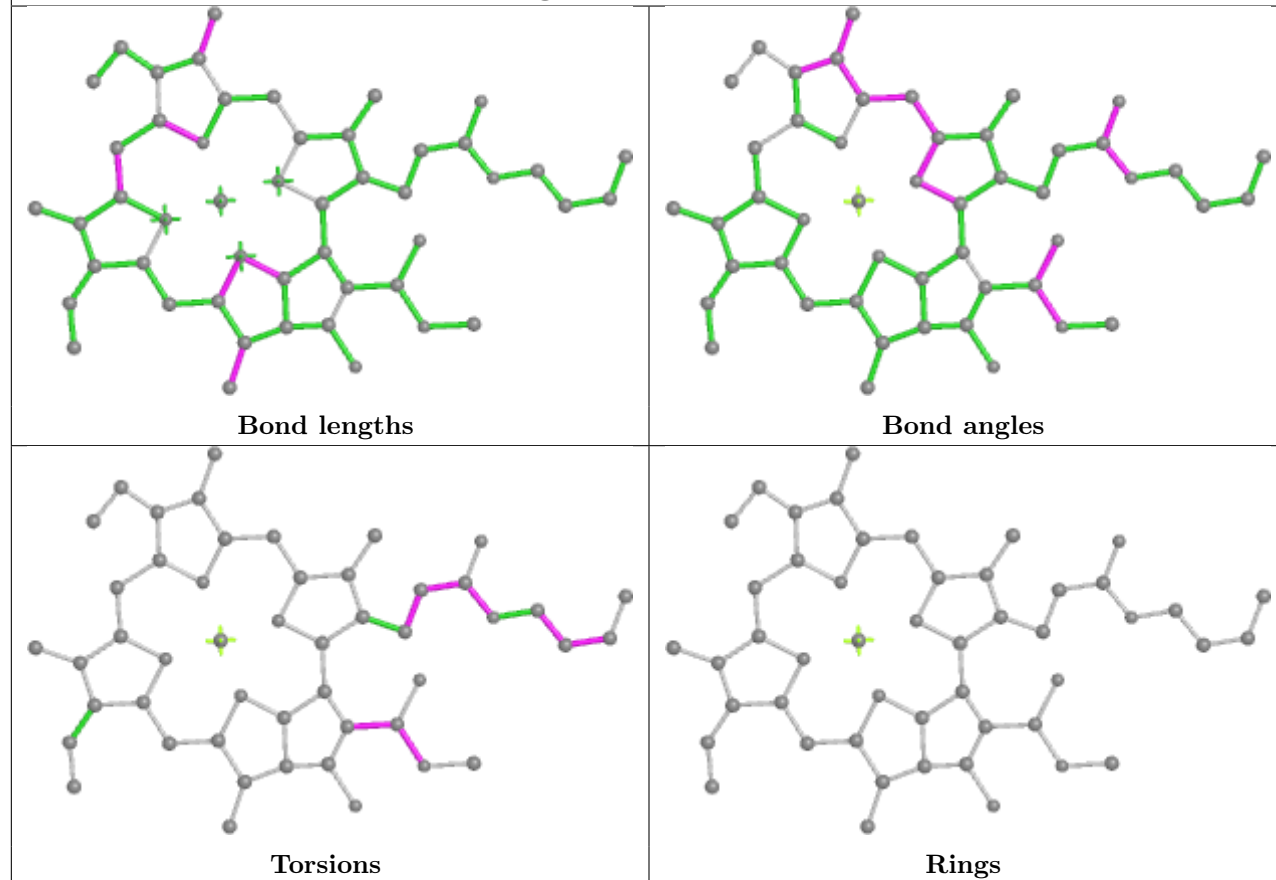
Rings

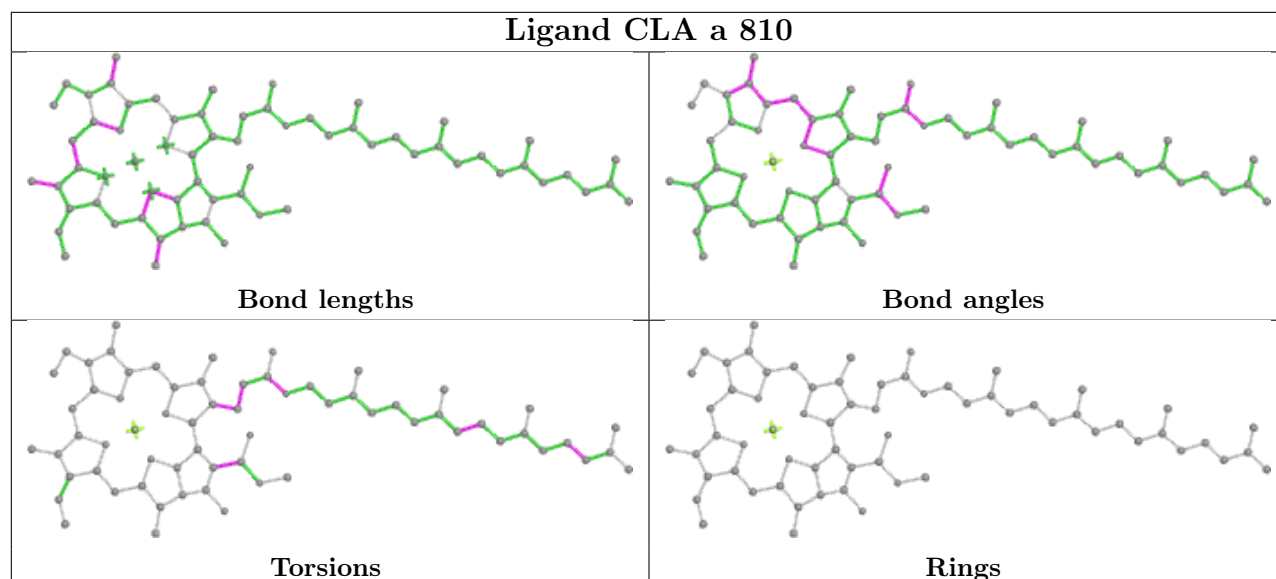
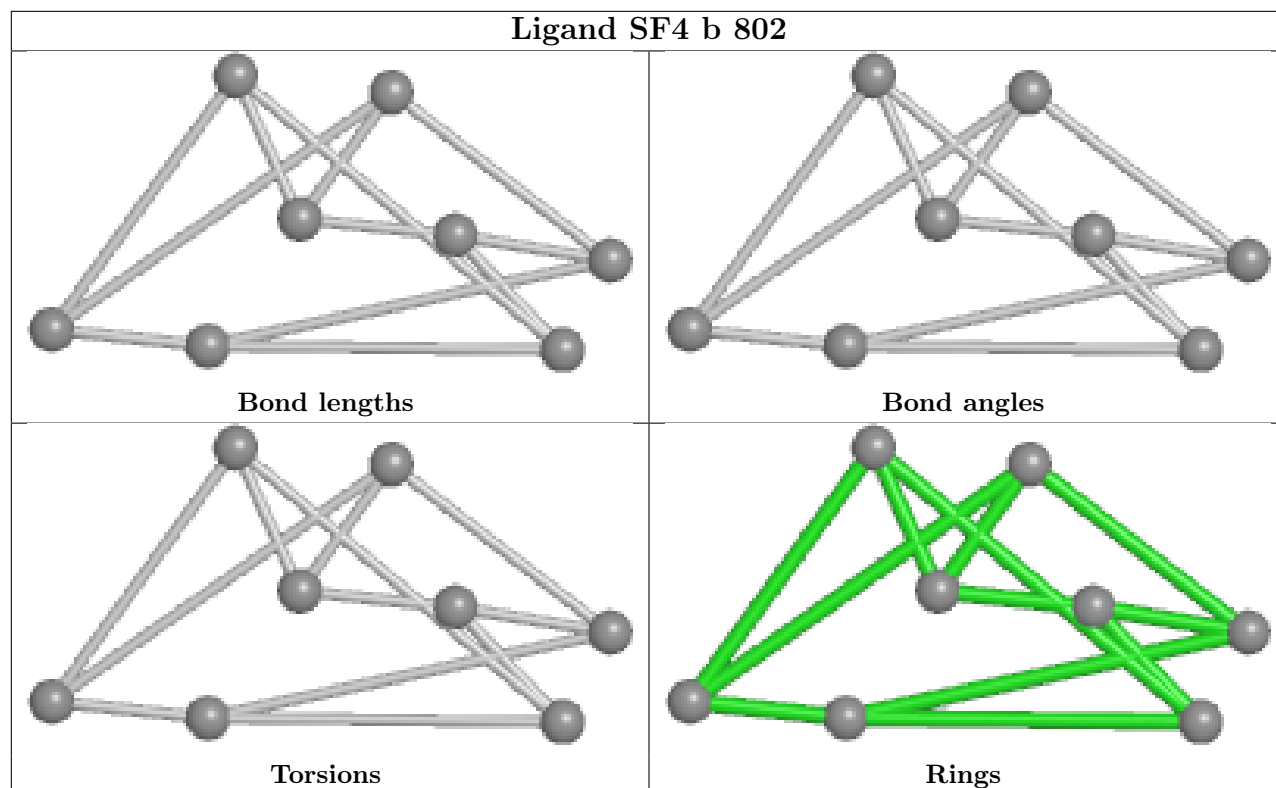
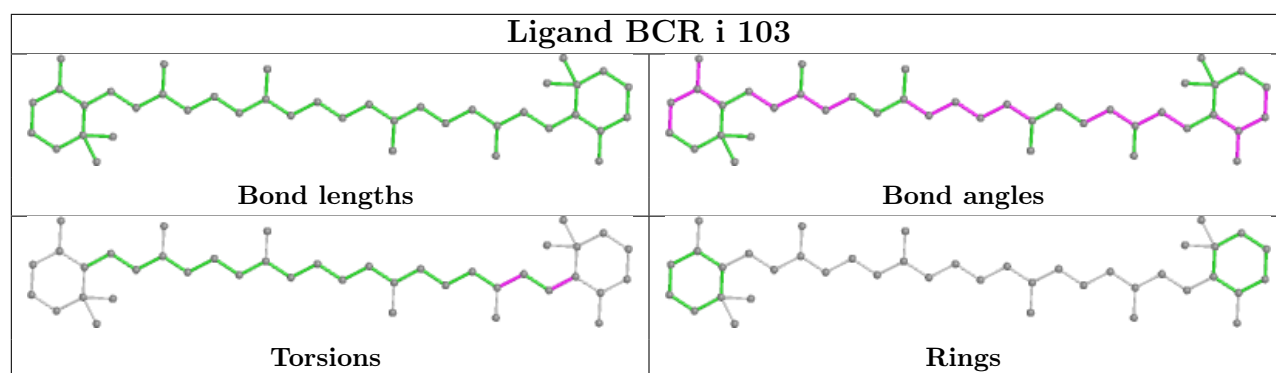
Ligand CLA a 843**Ligand CLA b 841****Ligand CLA E 309**

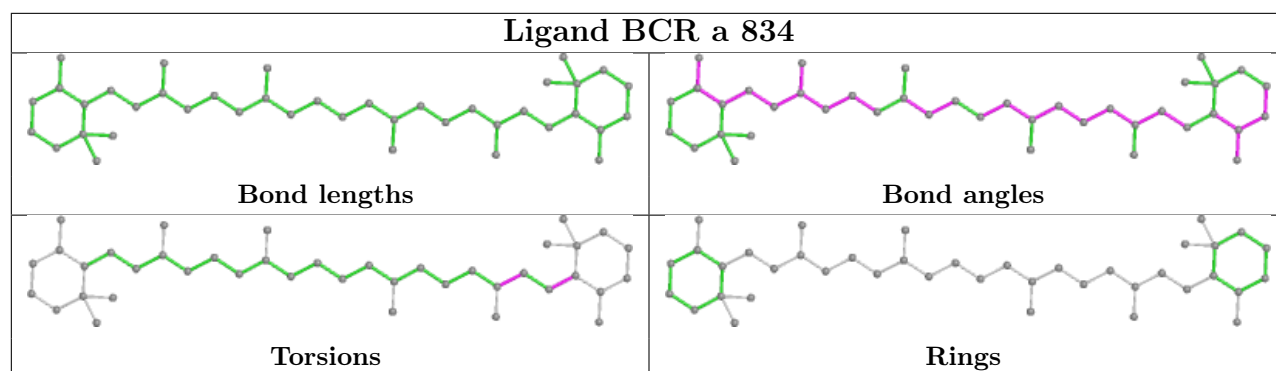
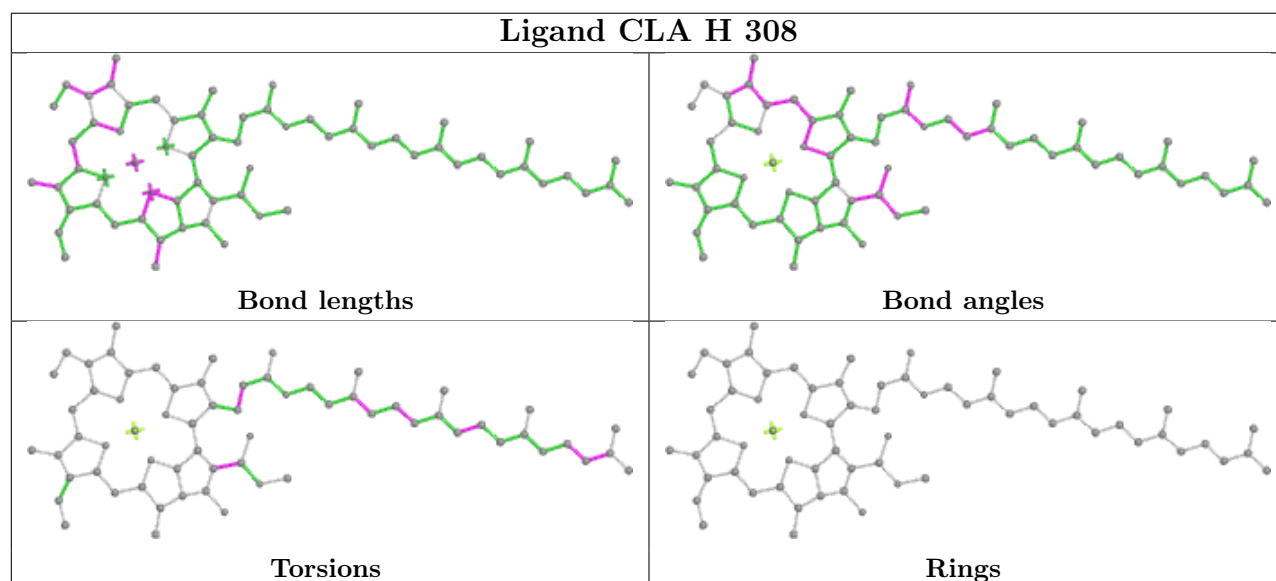
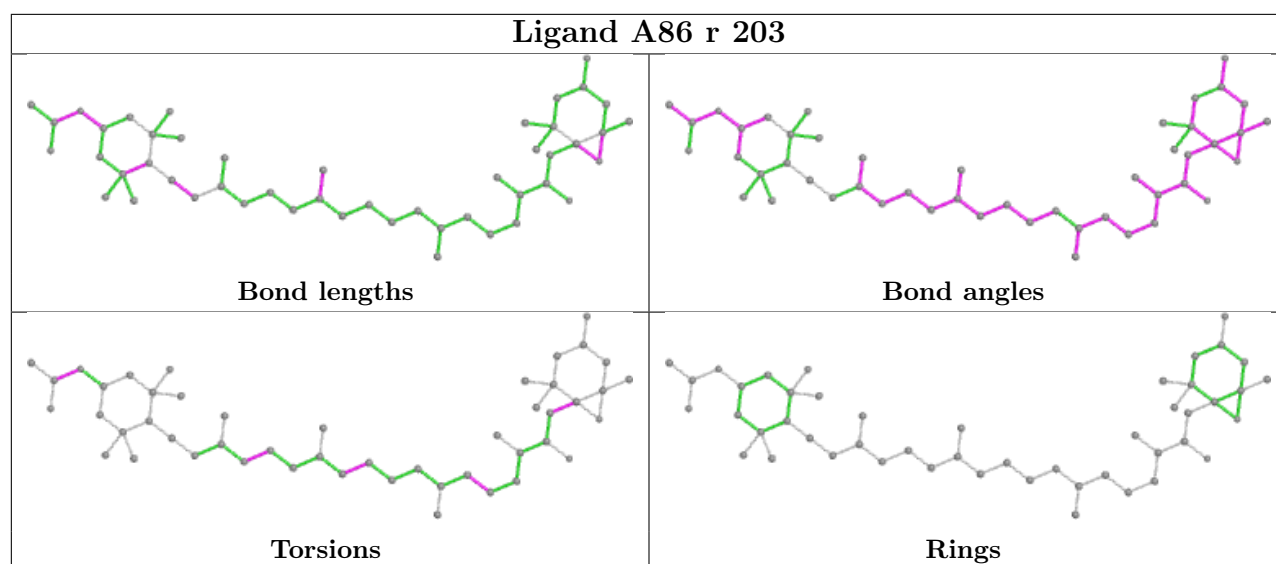
Ligand CLA b 807



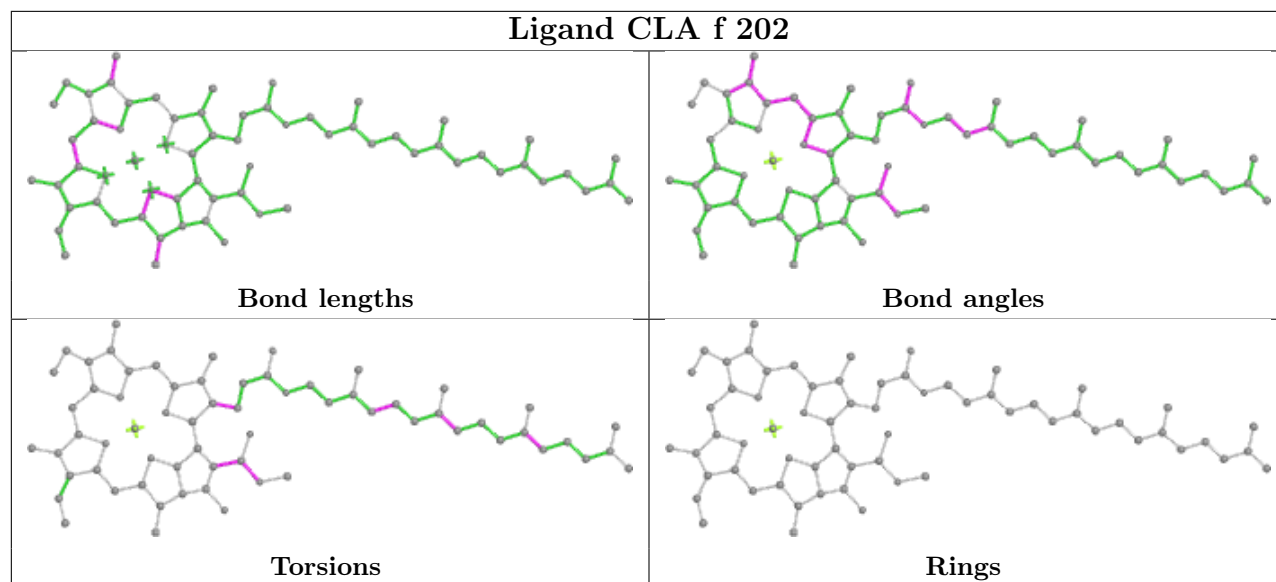
Ligand CLA a 817



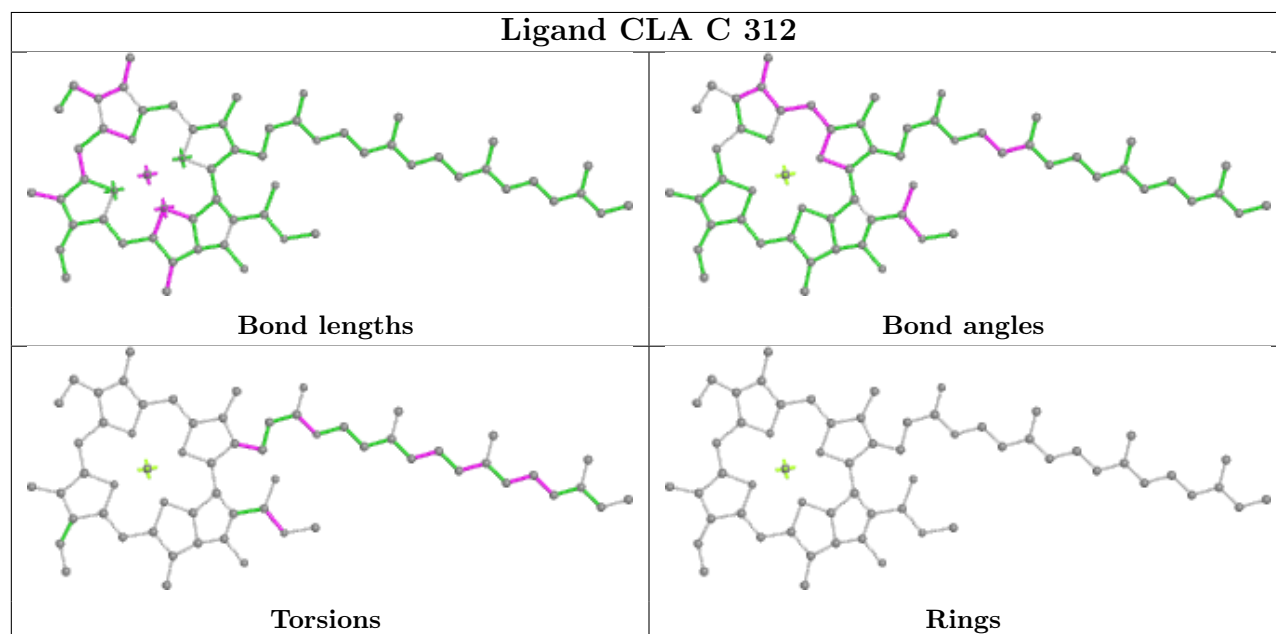


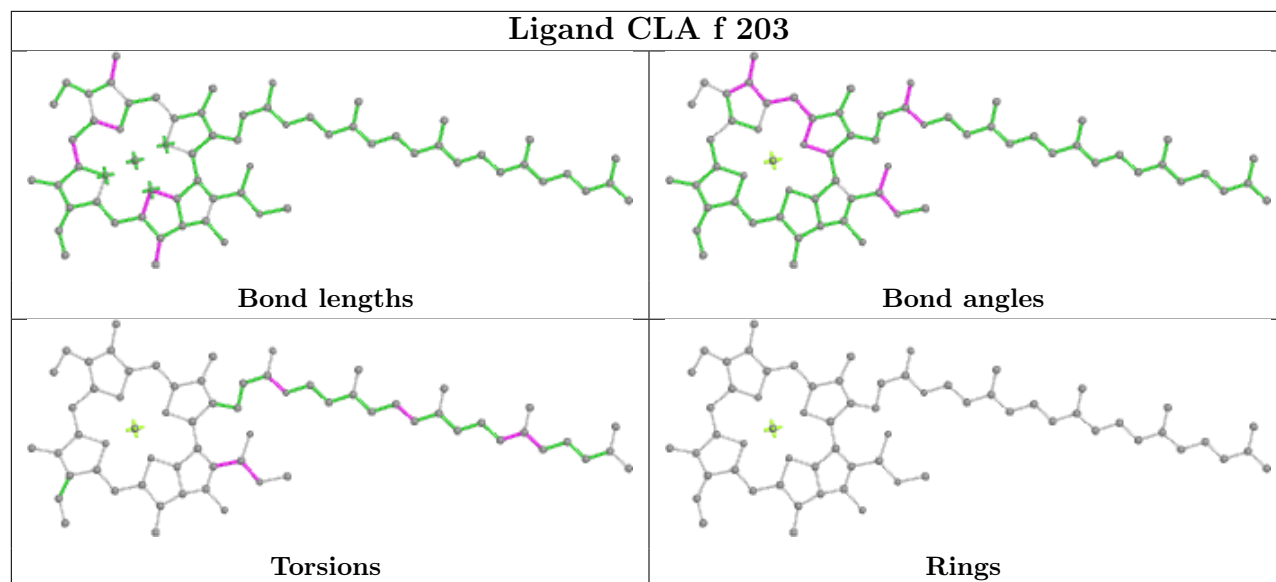
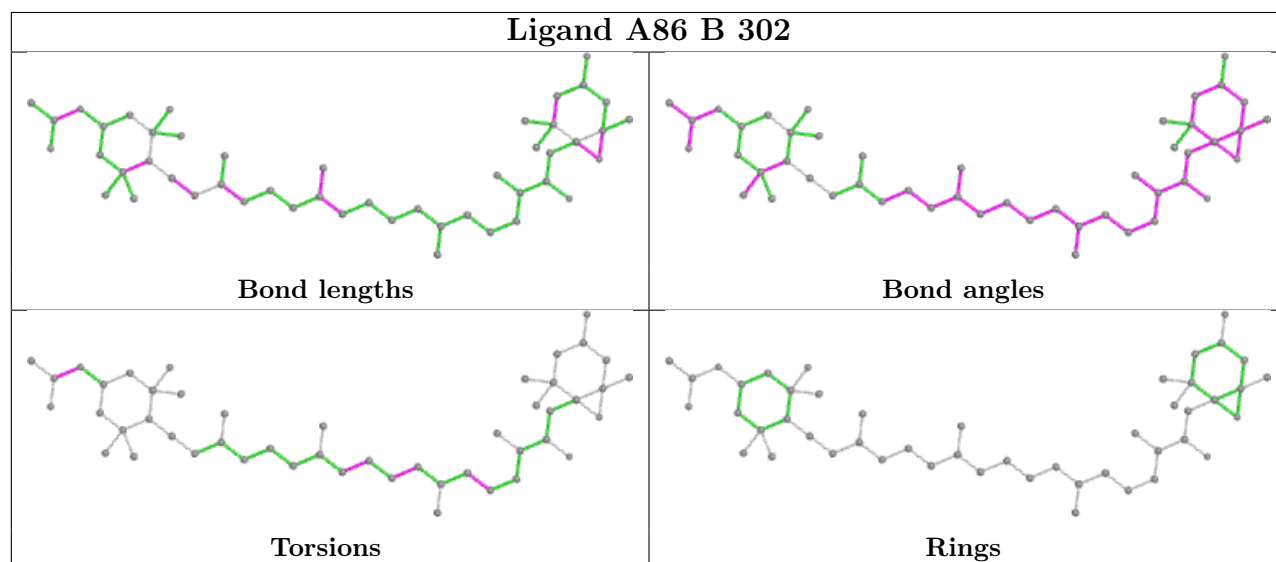


Ligand CLA f 202

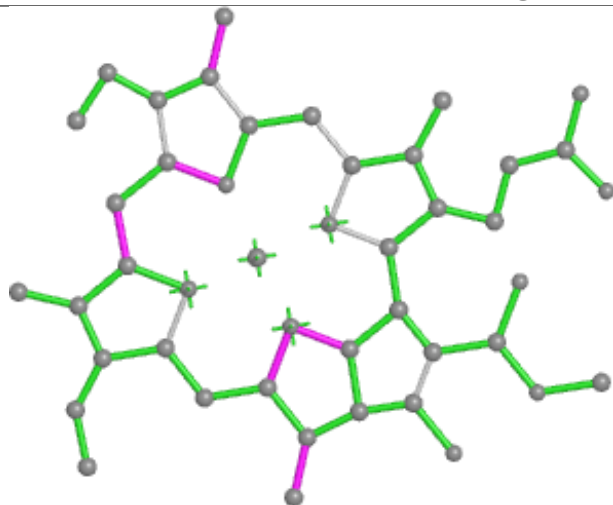


Ligand CLA C 312

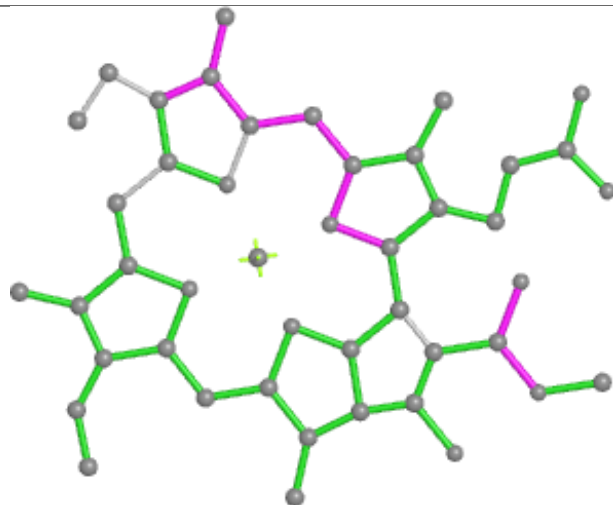


Ligand CLA f 203**Ligand A86 B 302**

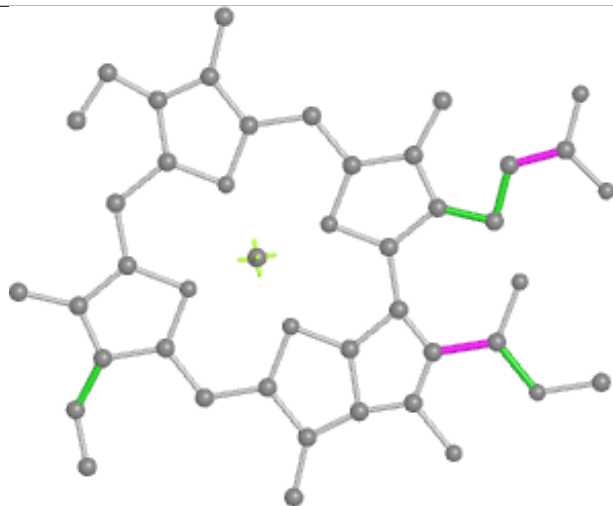
Ligand CLA C 306



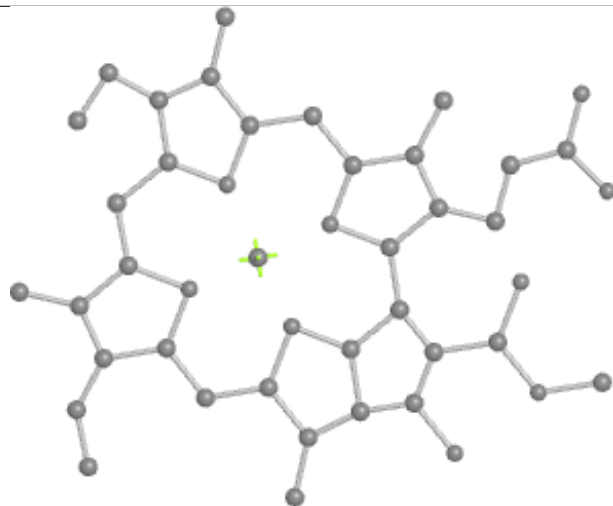
Bond lengths



Bond angles

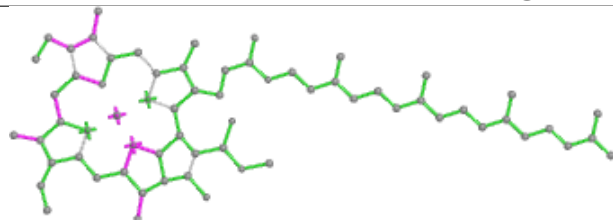


Torsions

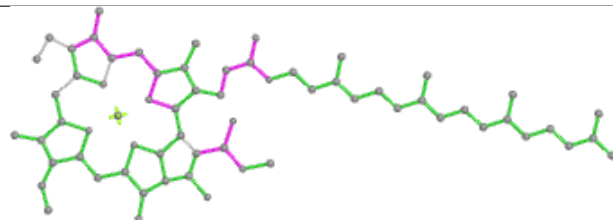


Rings

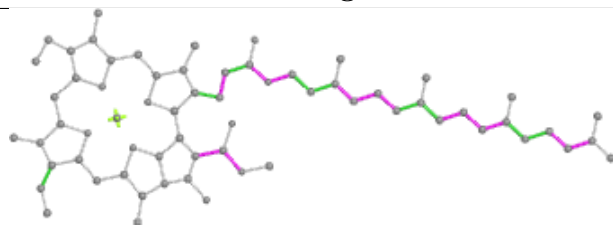
Ligand CLA a 841



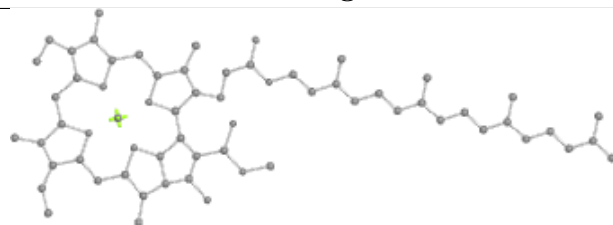
Bond lengths



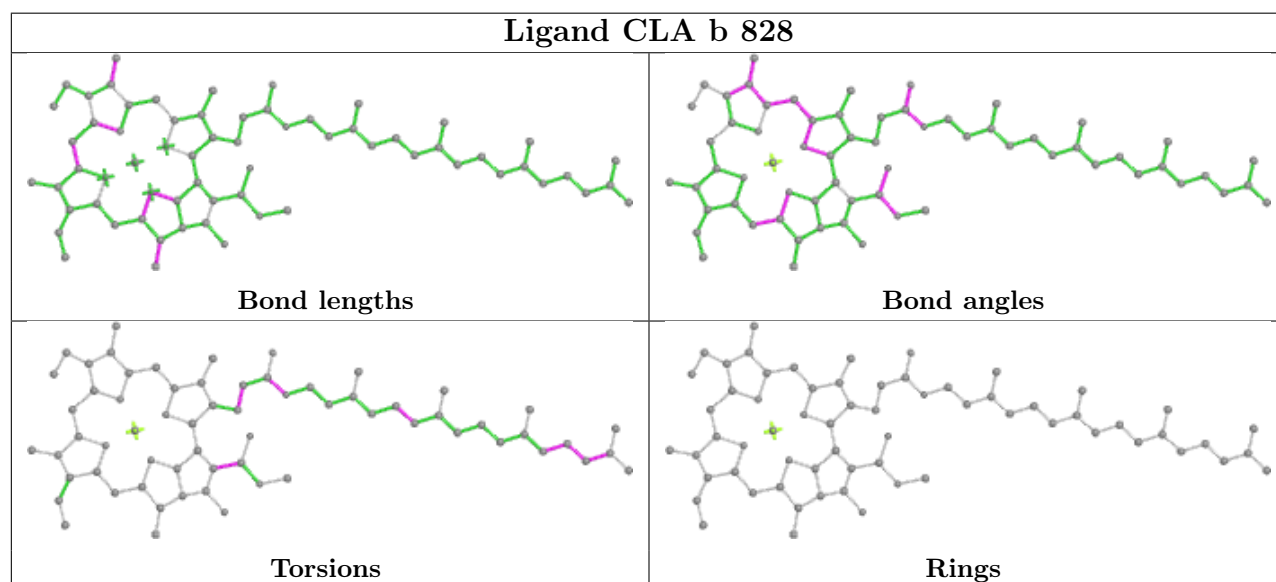
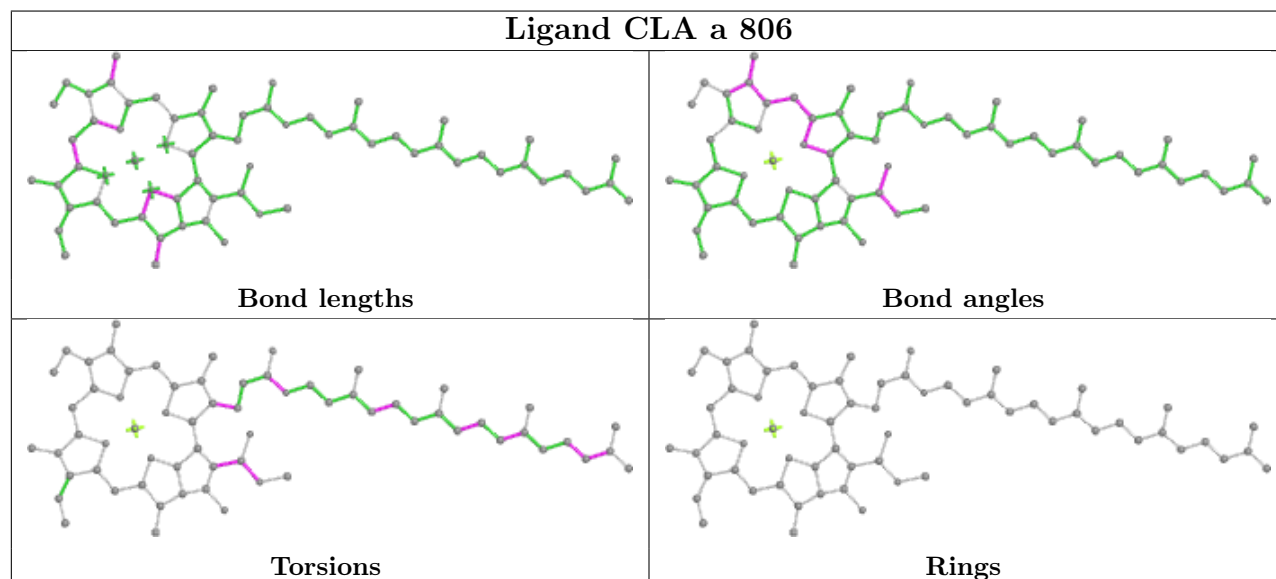
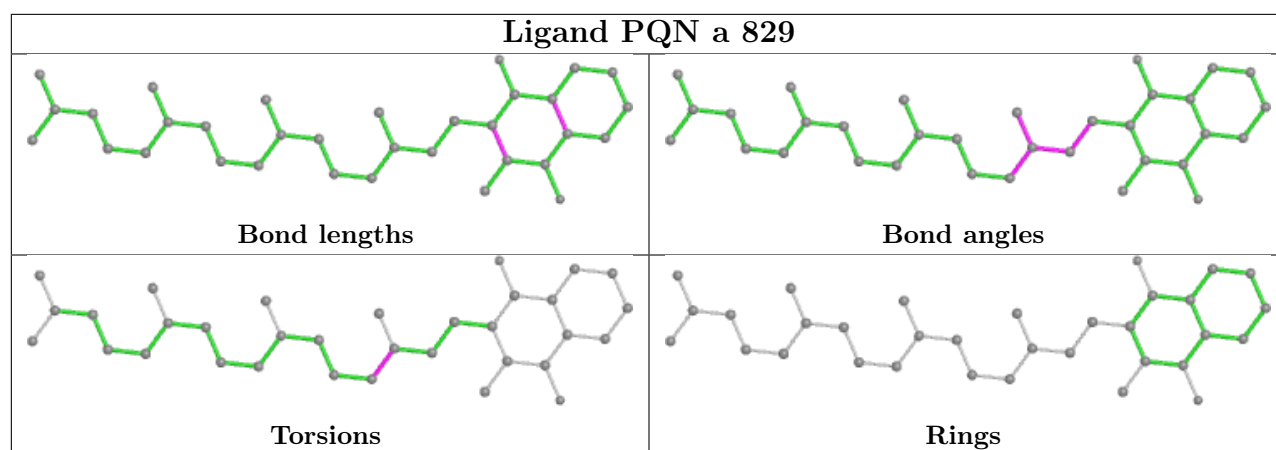
Bond angles

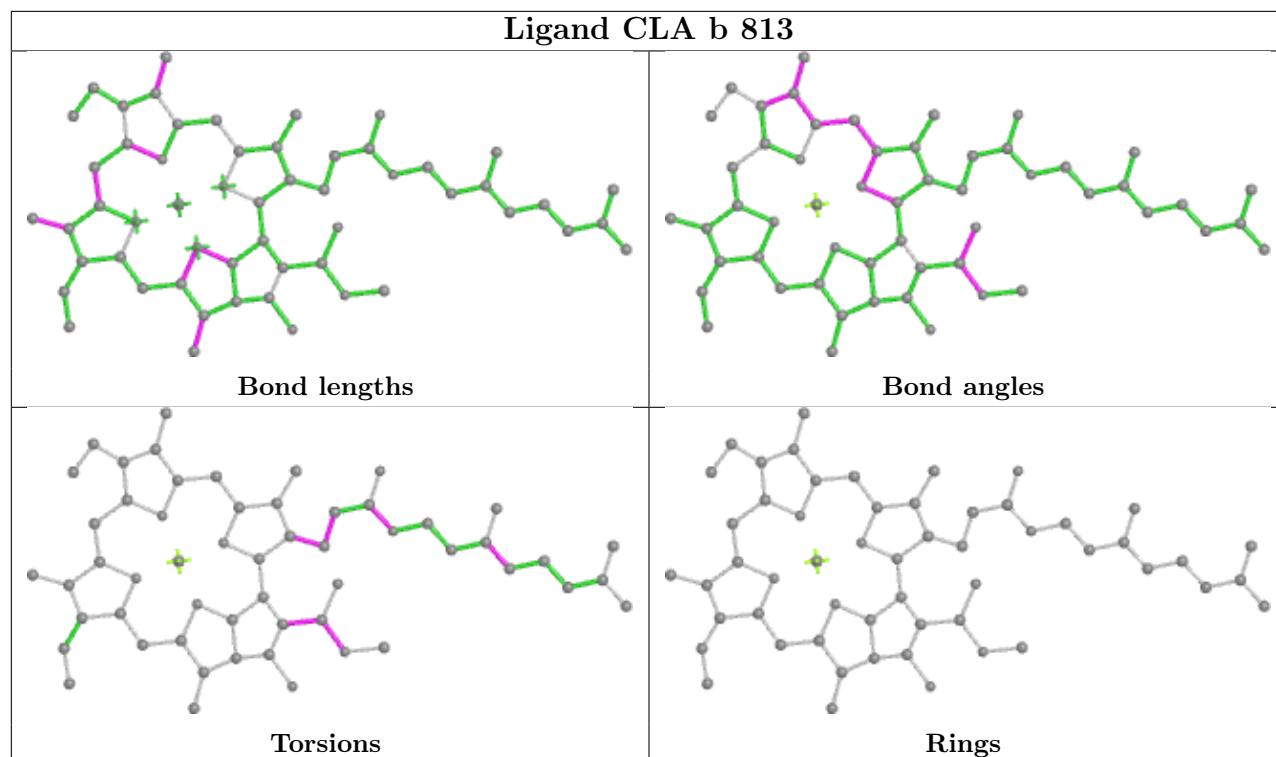
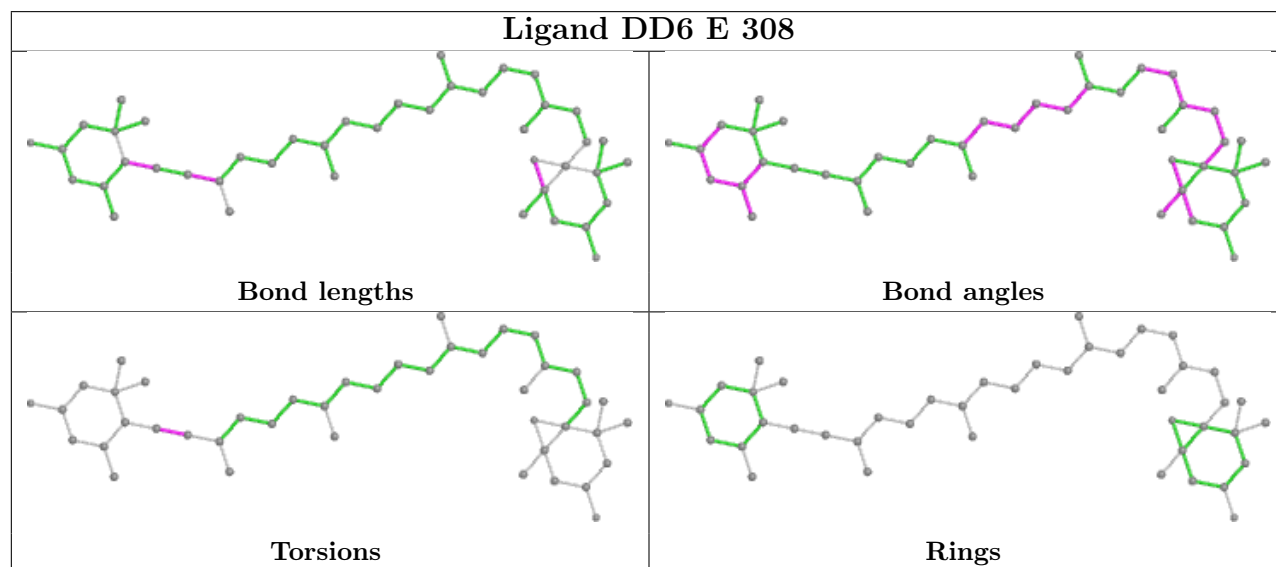


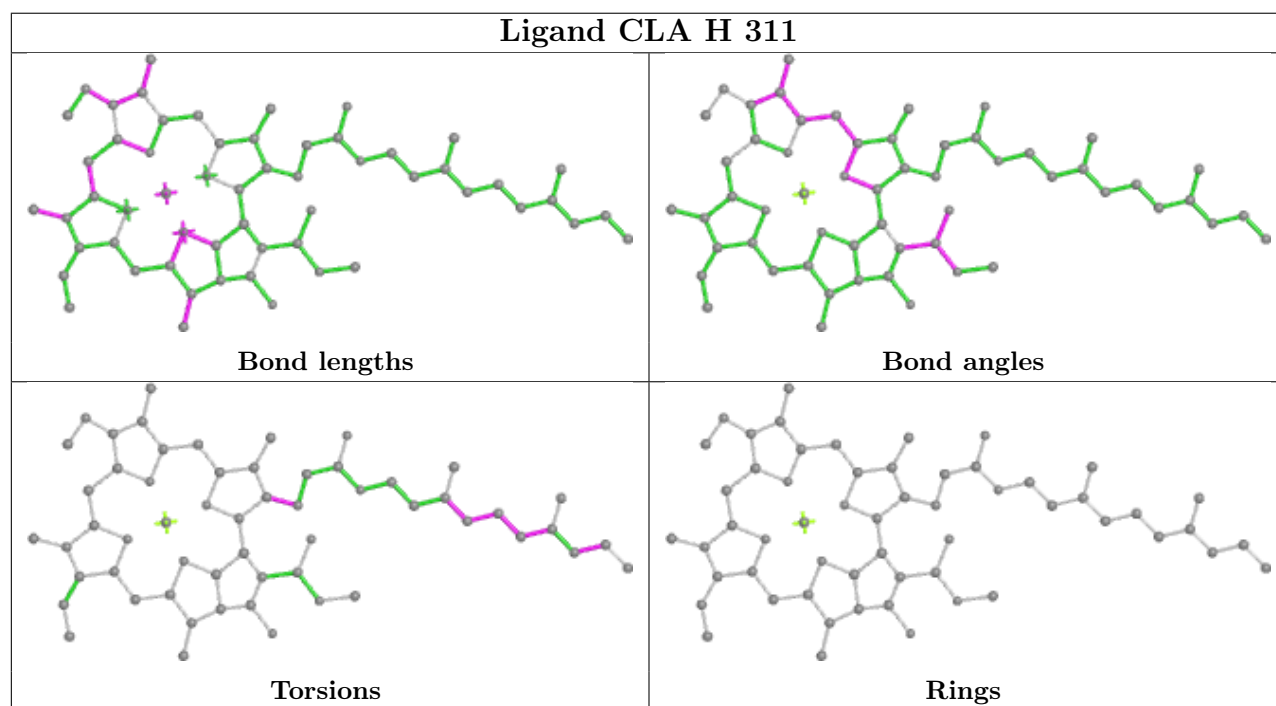
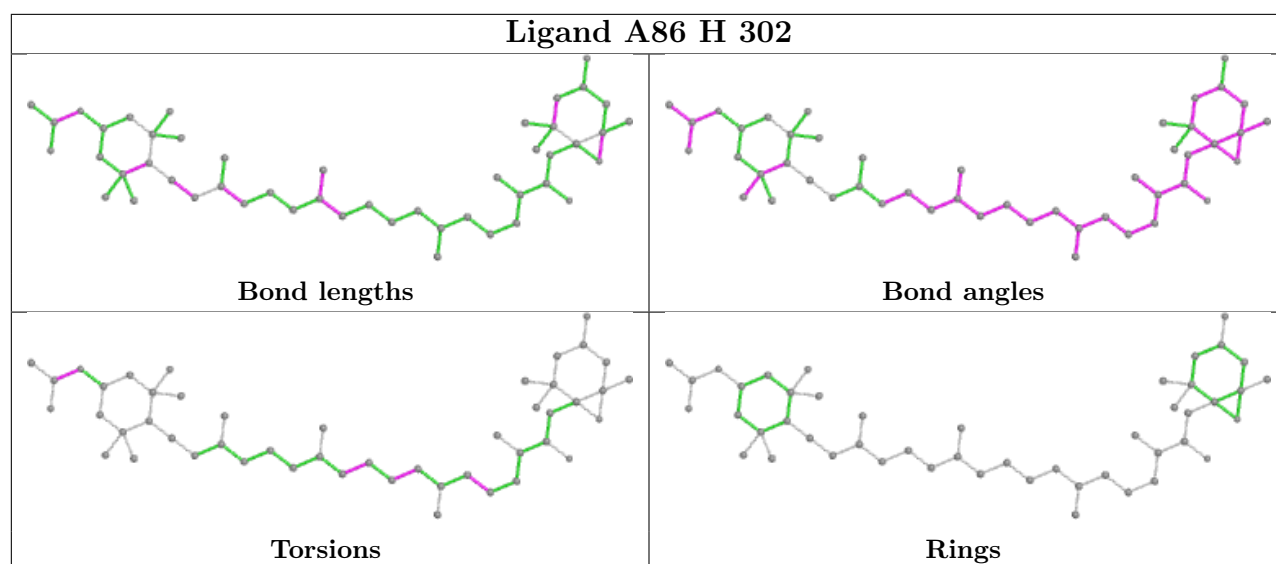
Torsions



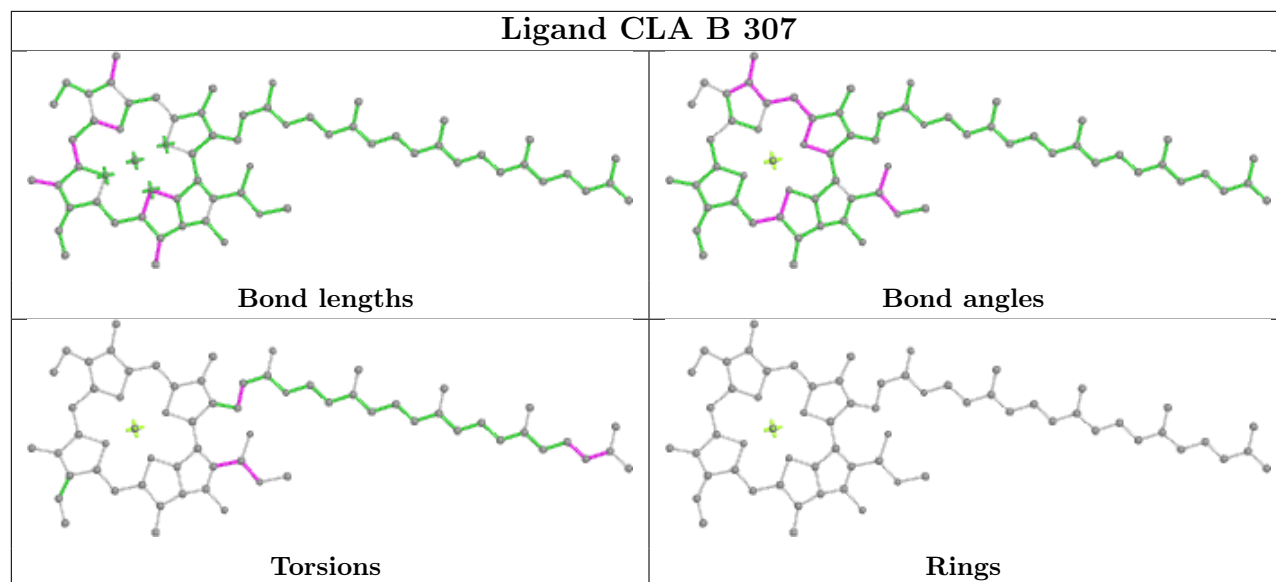
Rings



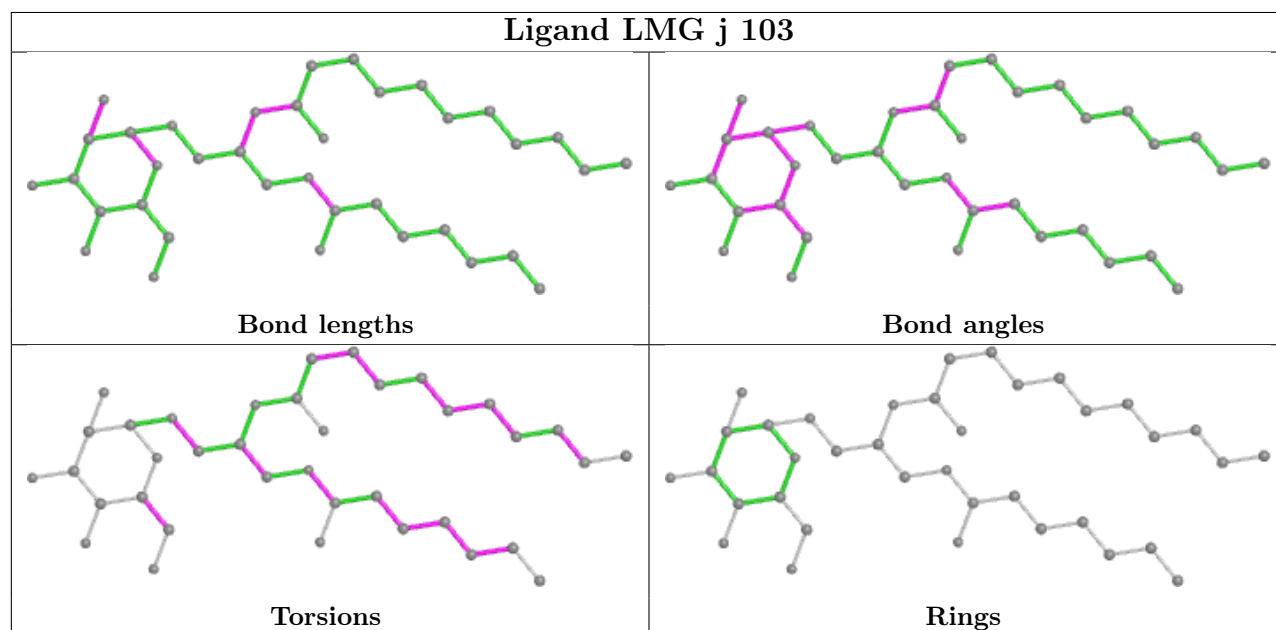
Ligand CLA b 813**Ligand DD6 E 308**



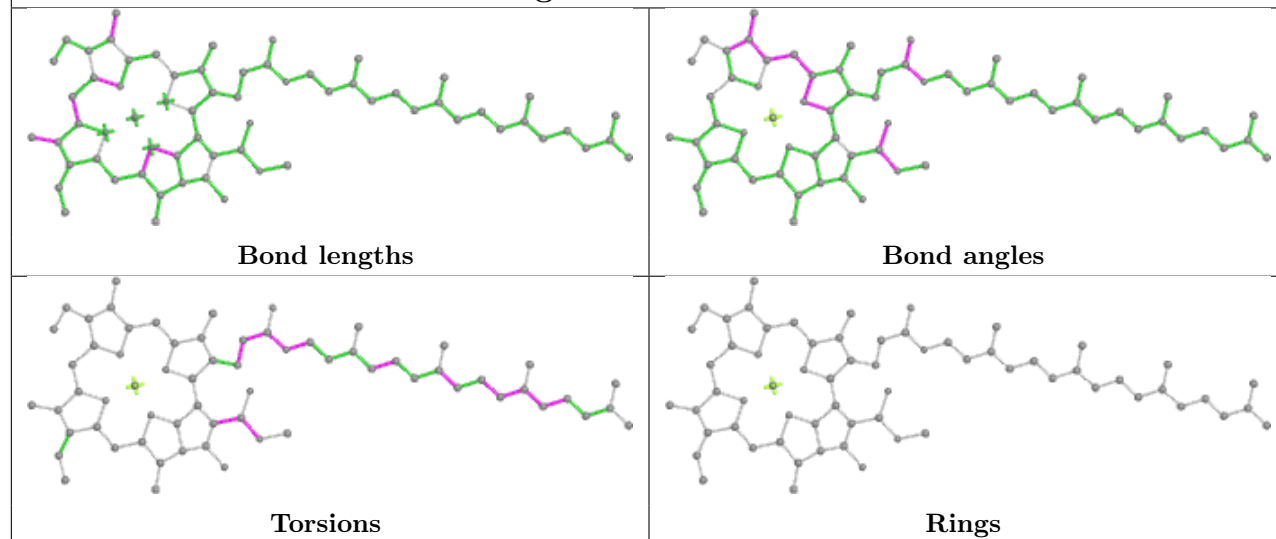
Ligand CLA B 307



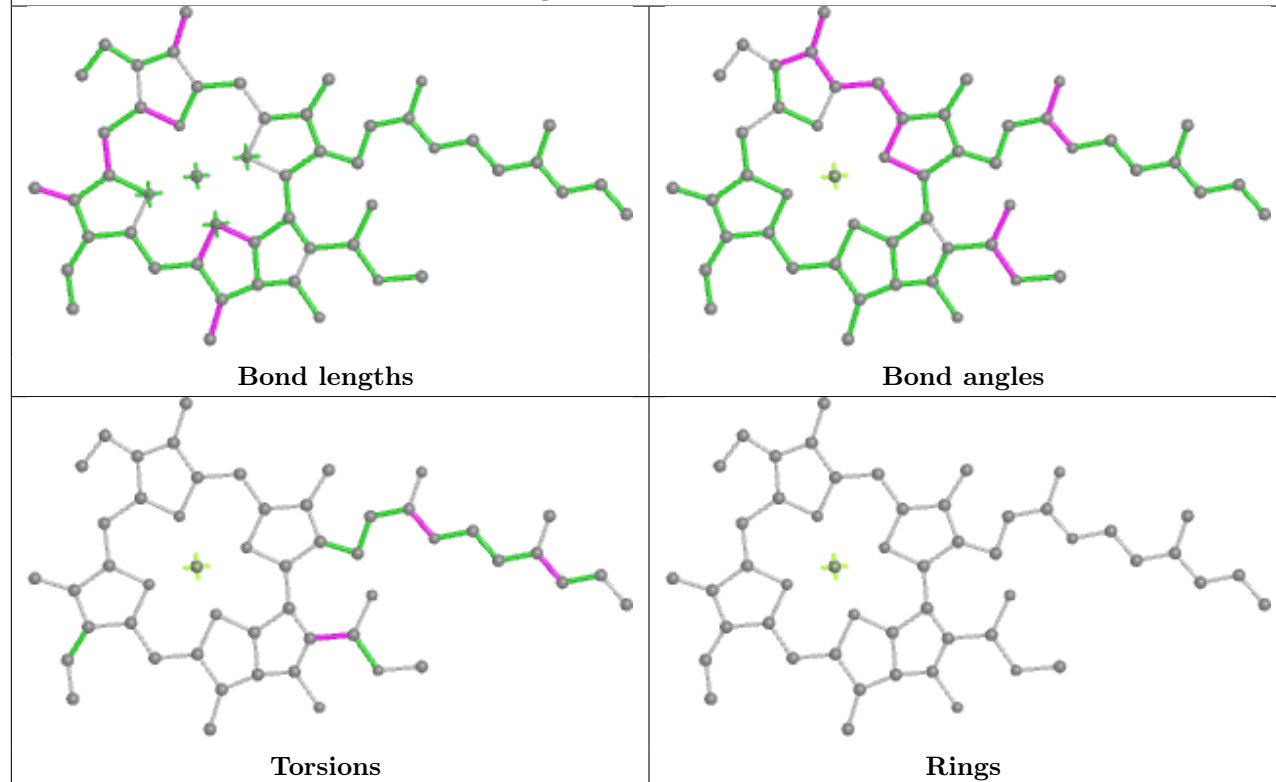
Ligand LMG j 103



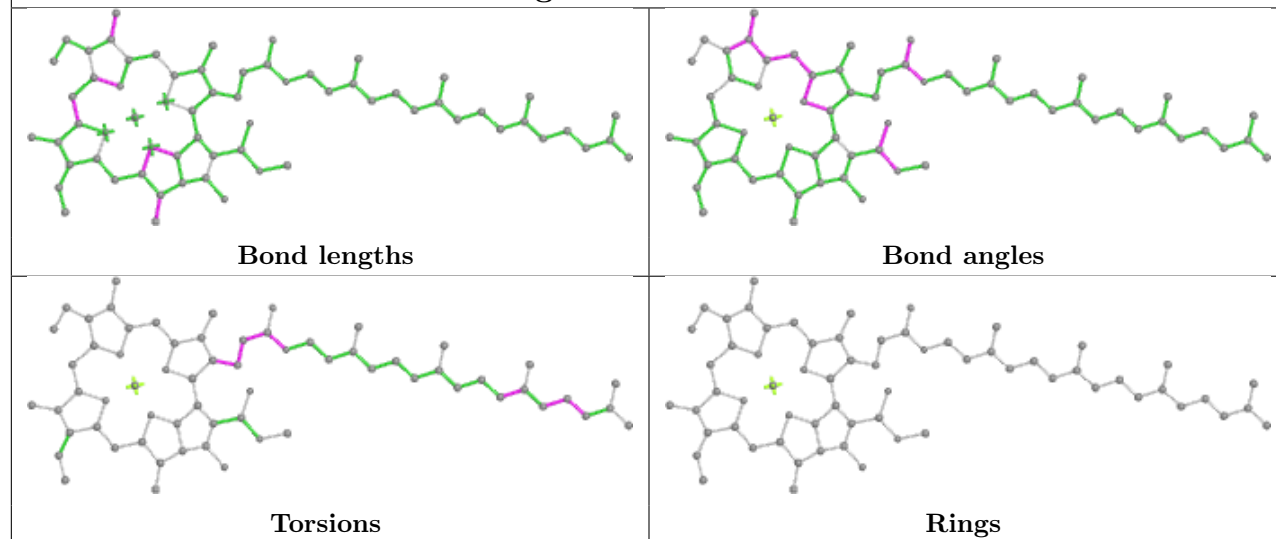
Ligand CLA b 806



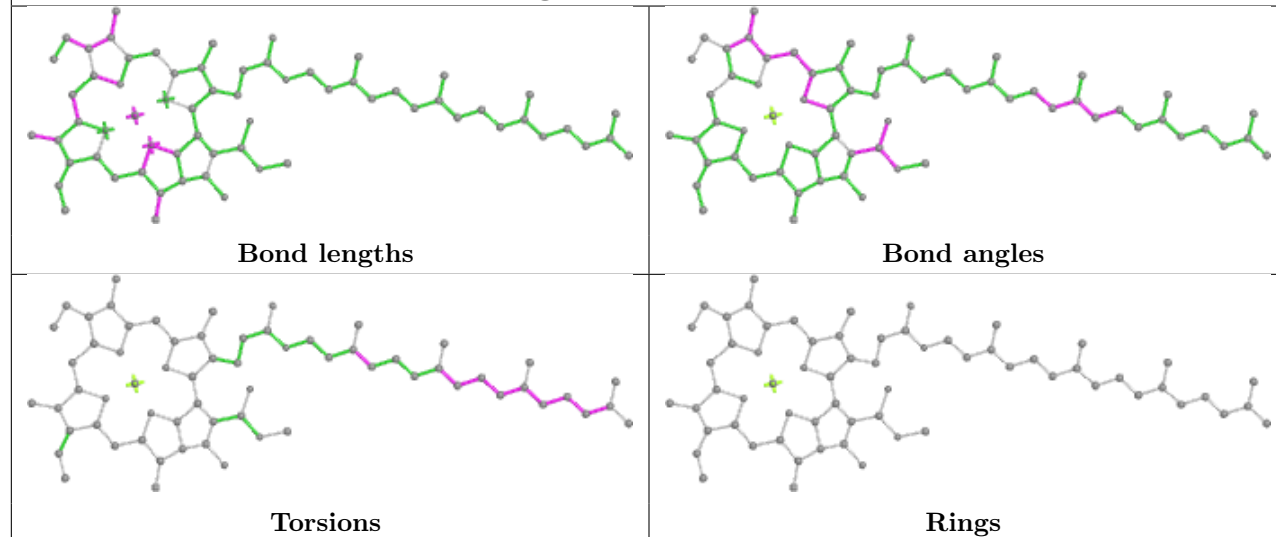
Ligand CLA a 830



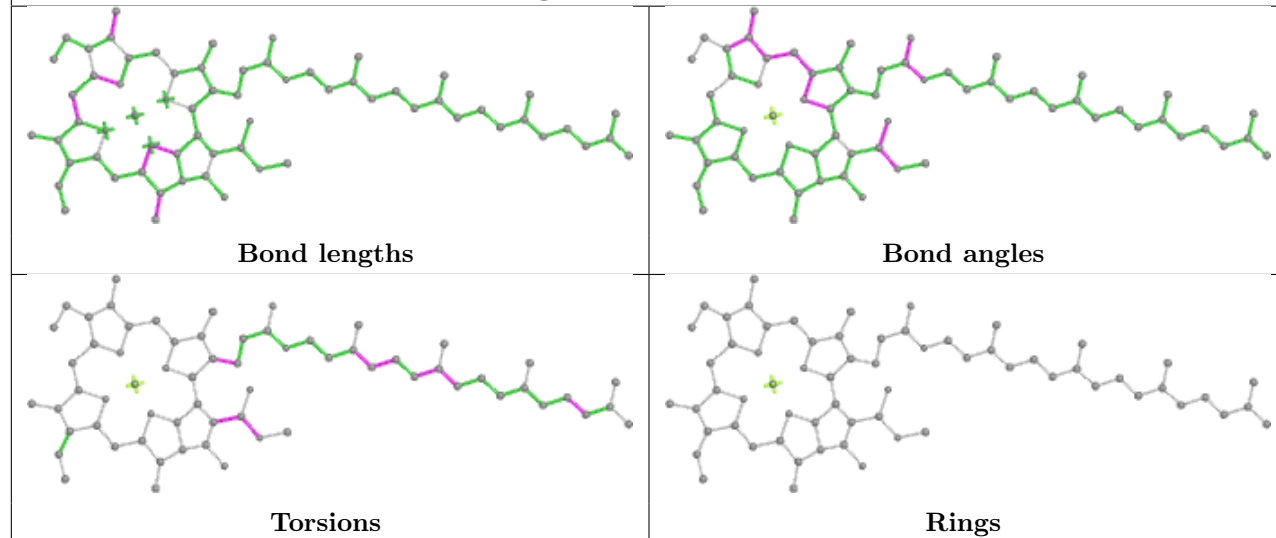
Ligand CLA b 808

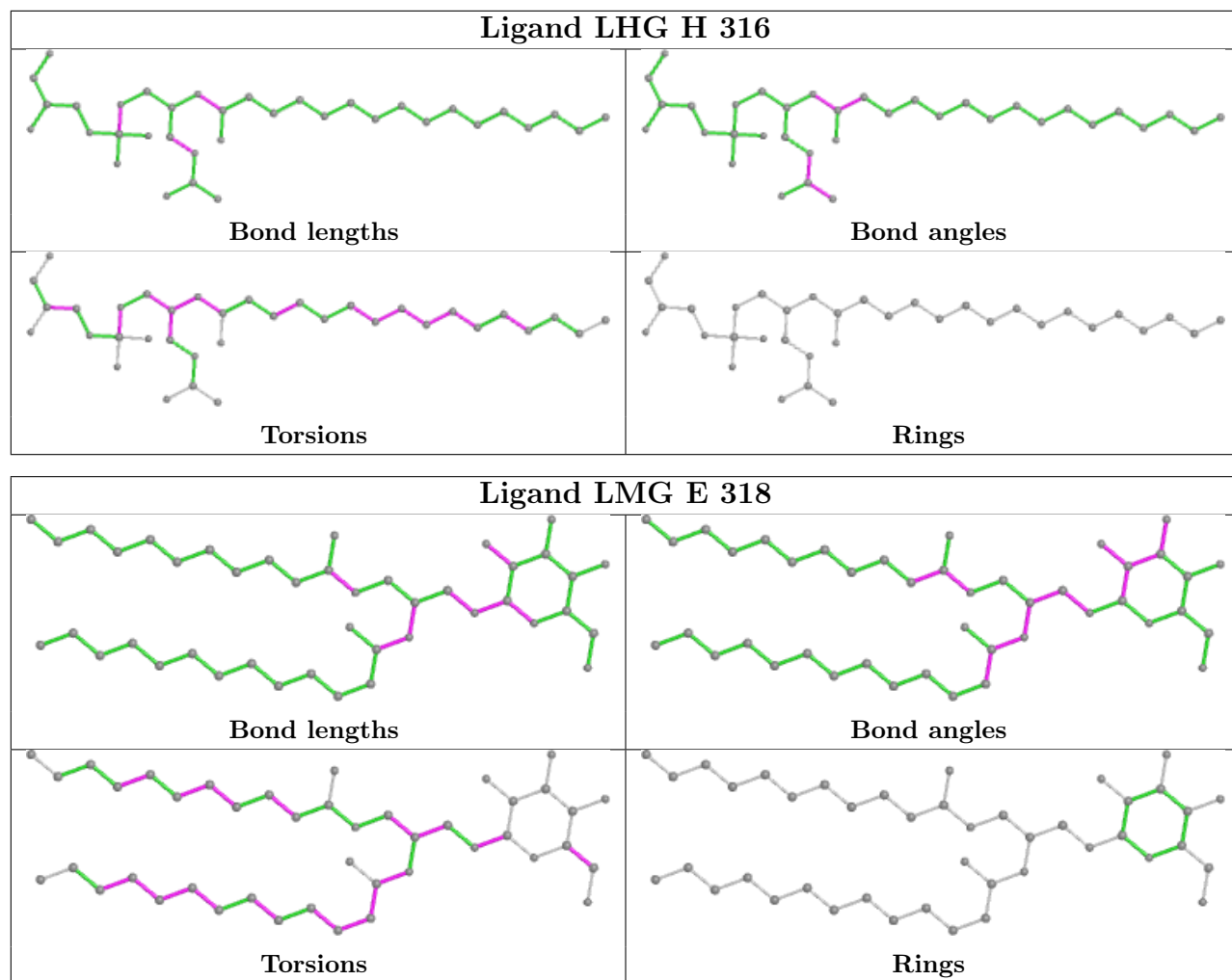


Ligand CLA a 840

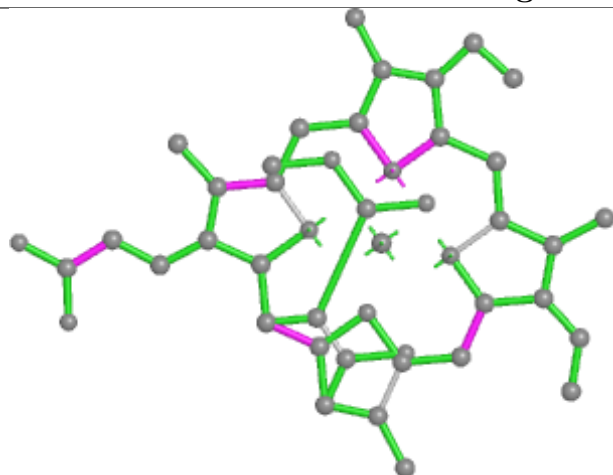


Ligand CLA b 805

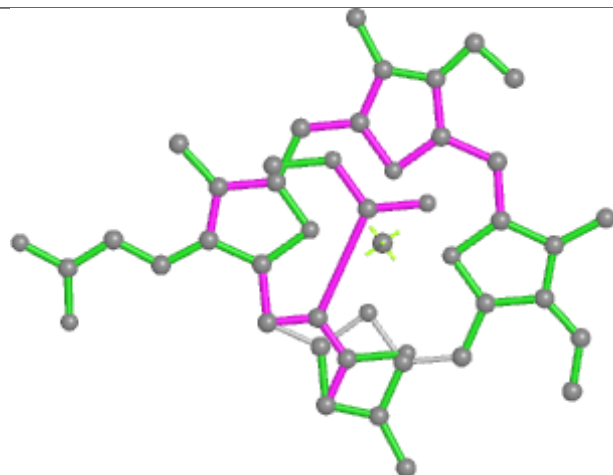




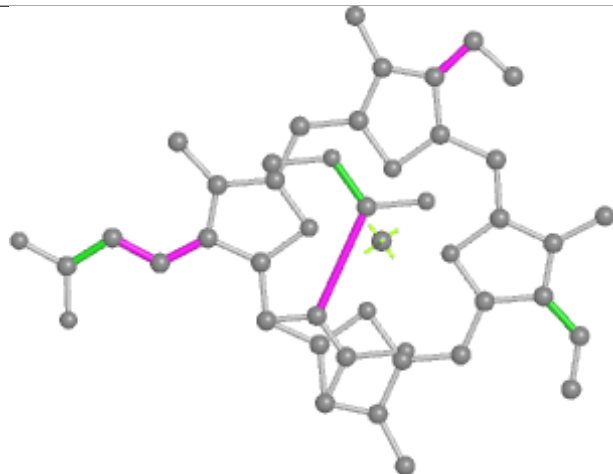
Ligand KC1 C 313



Bond lengths



Bond angles

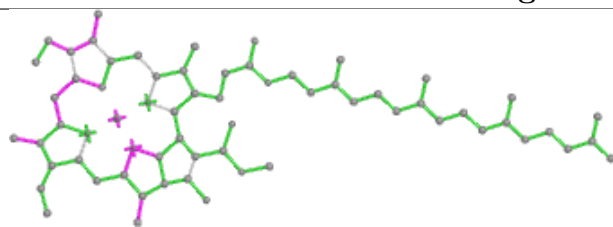


Torsions

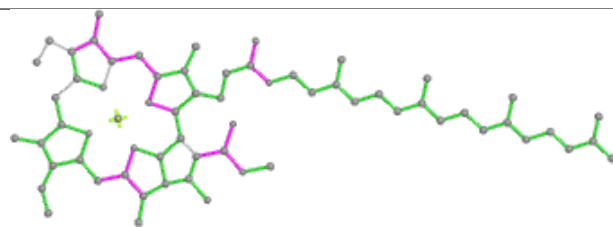


Rings

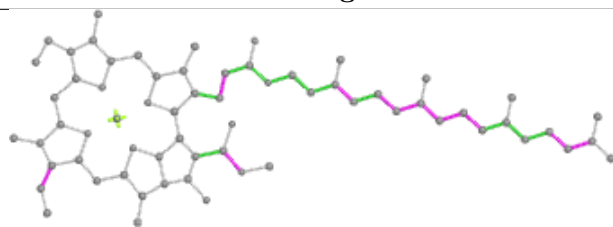
Ligand CLA a 854



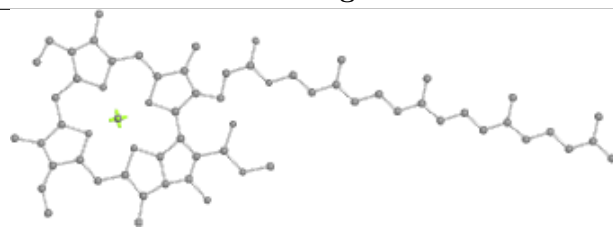
Bond lengths



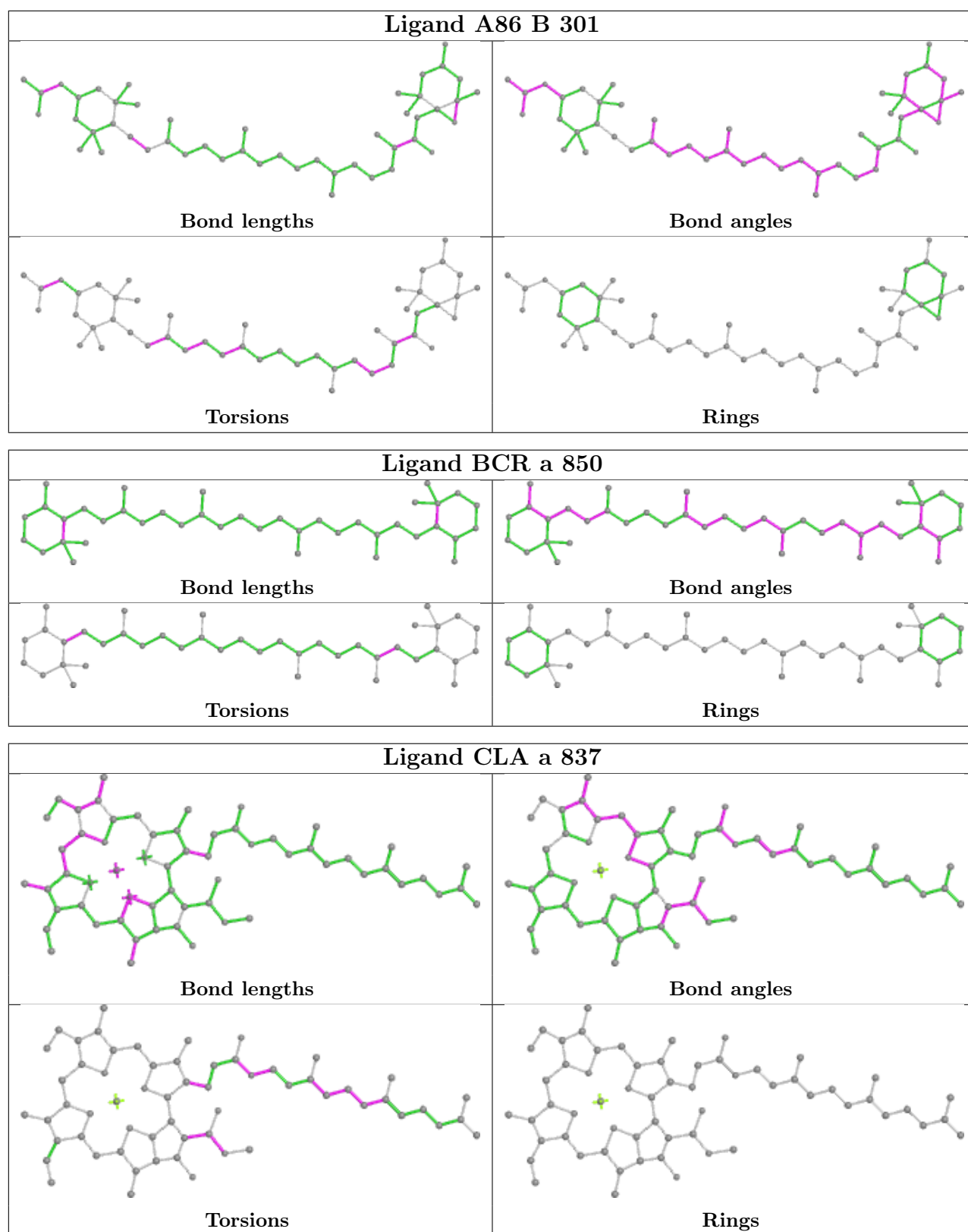
Bond angles

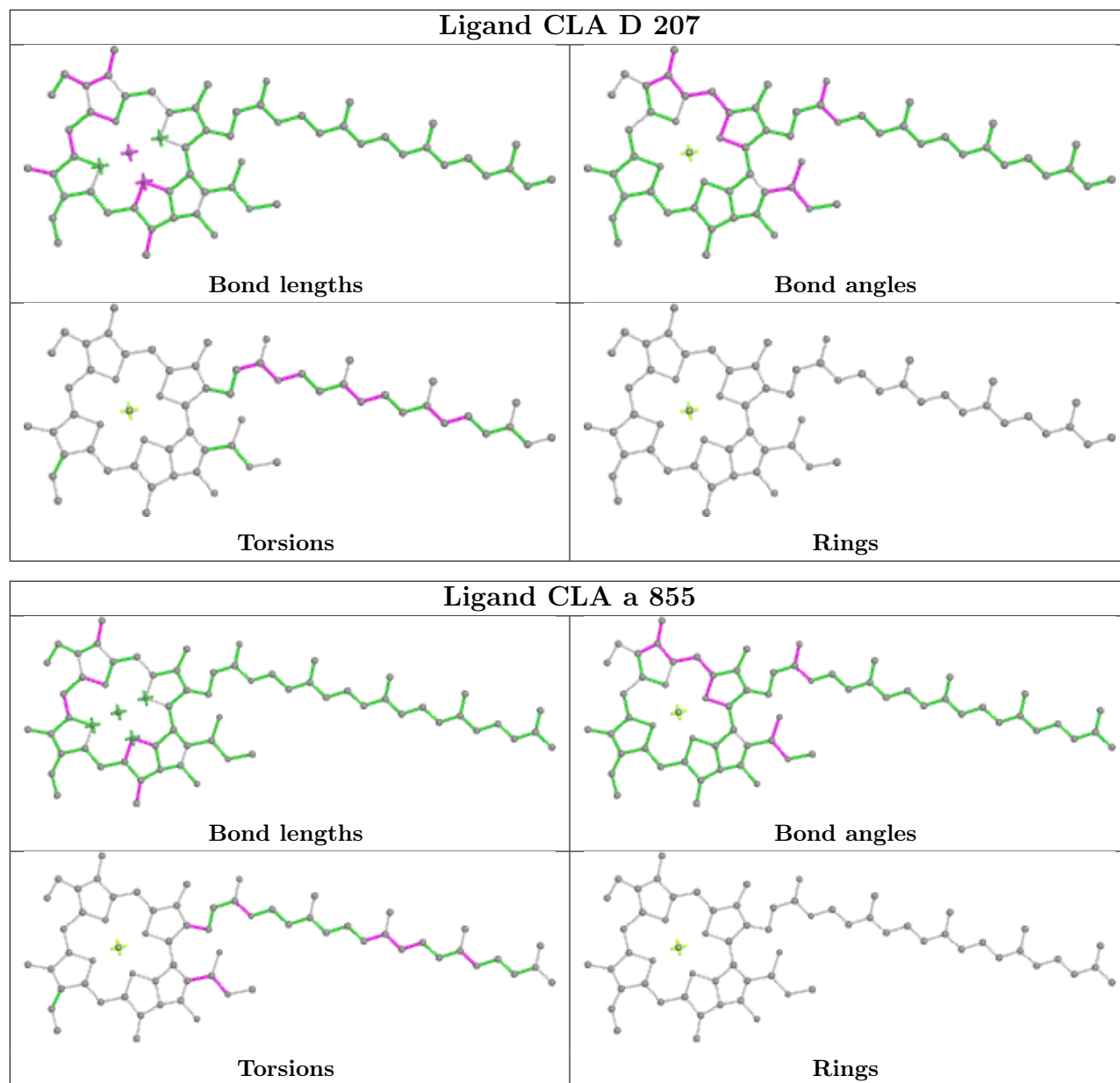


Torsions

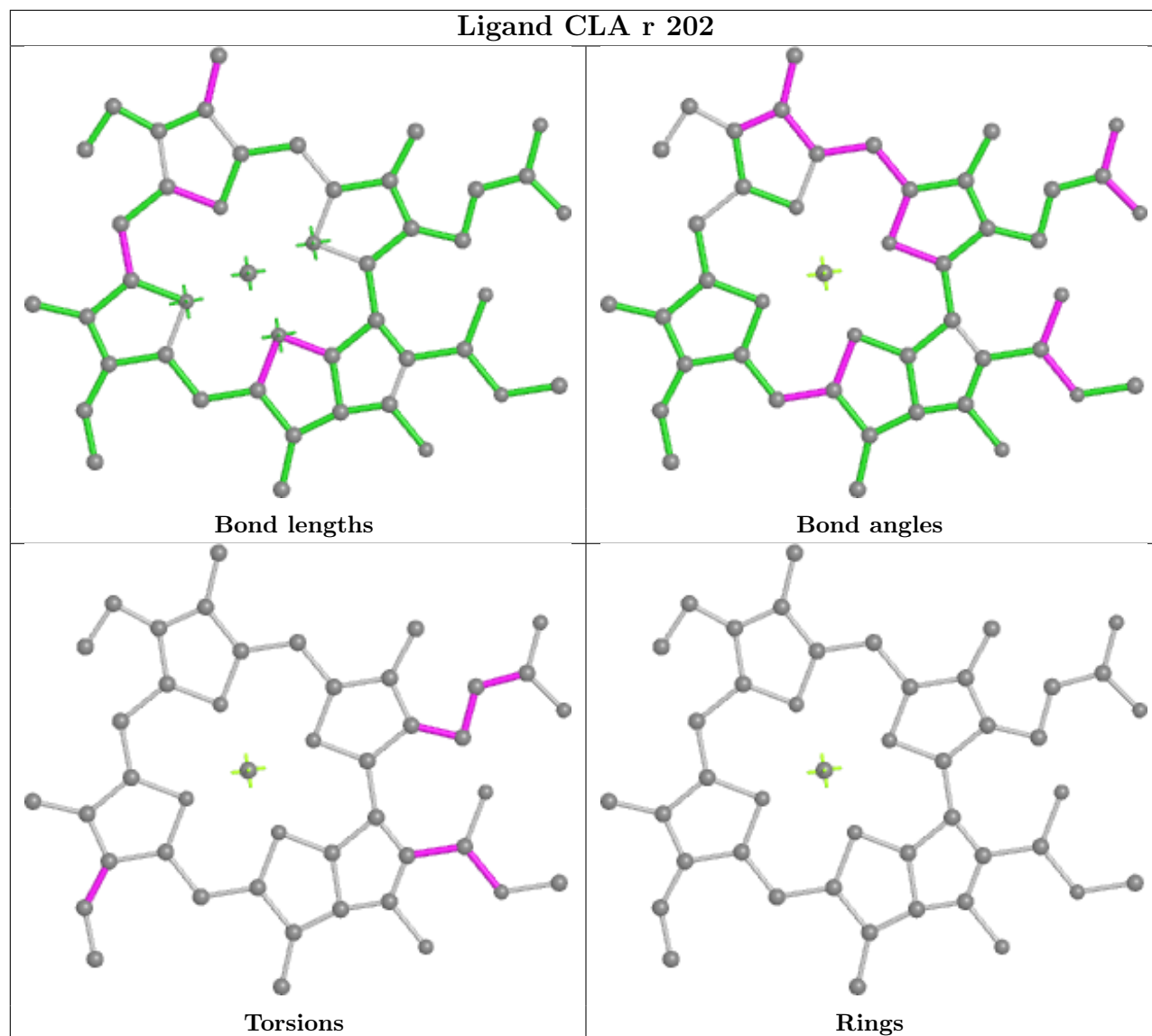


Rings

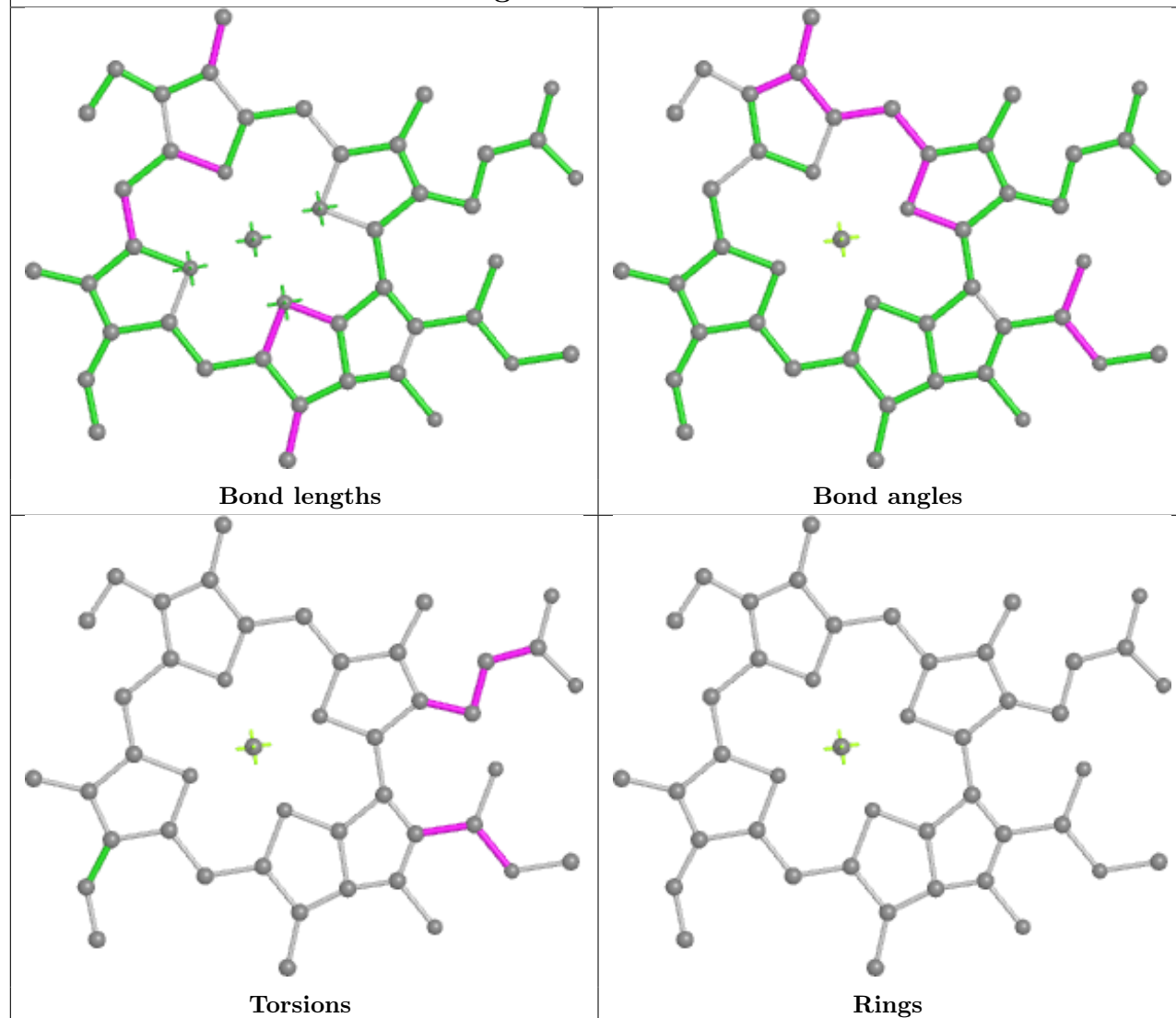




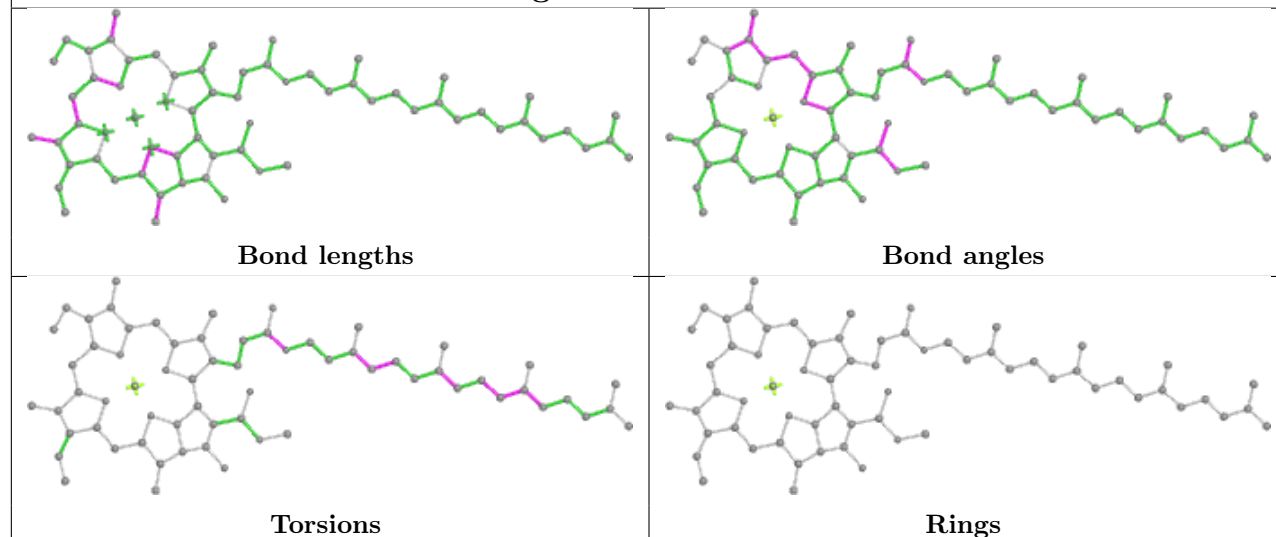
Ligand CLA r 202

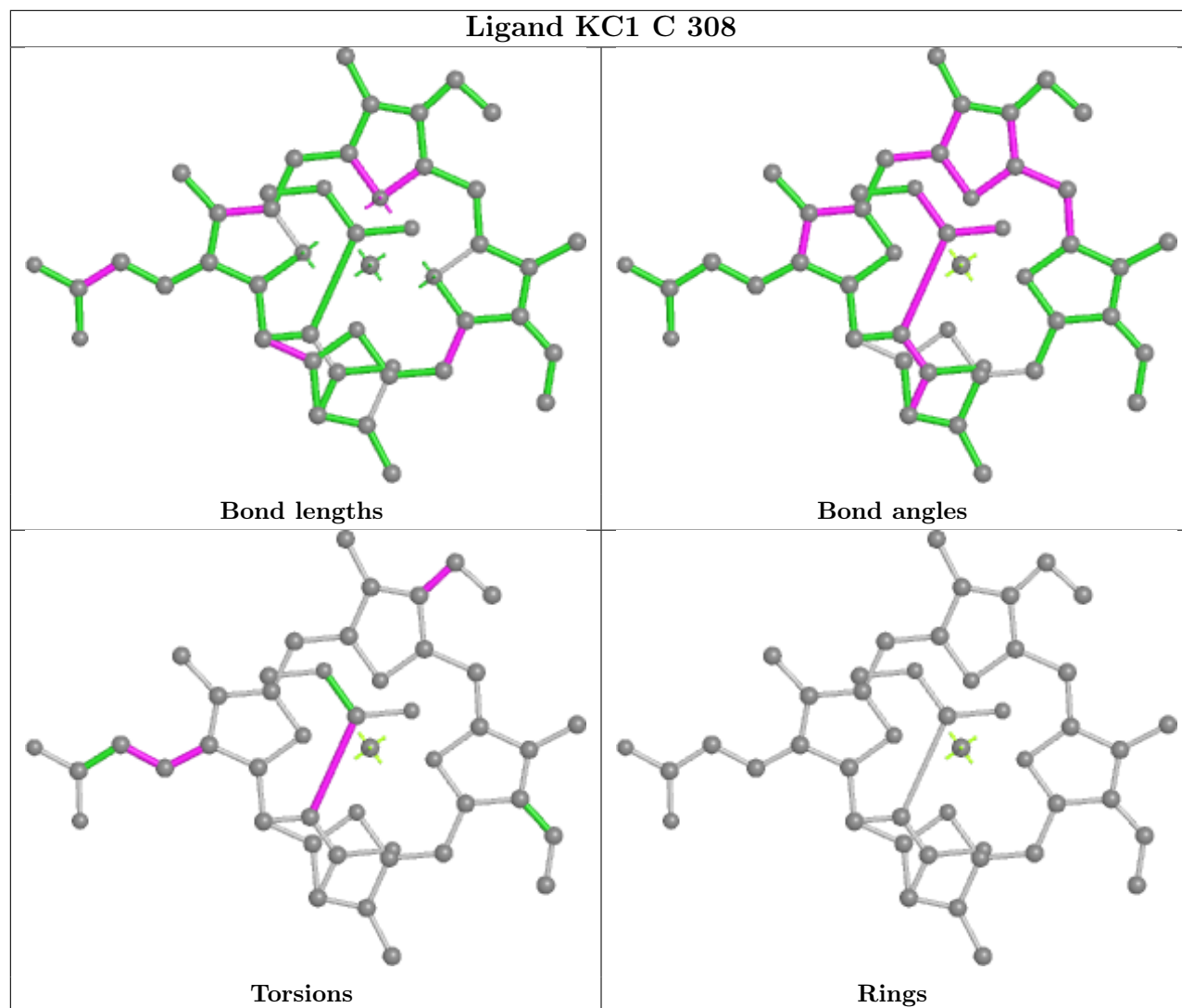
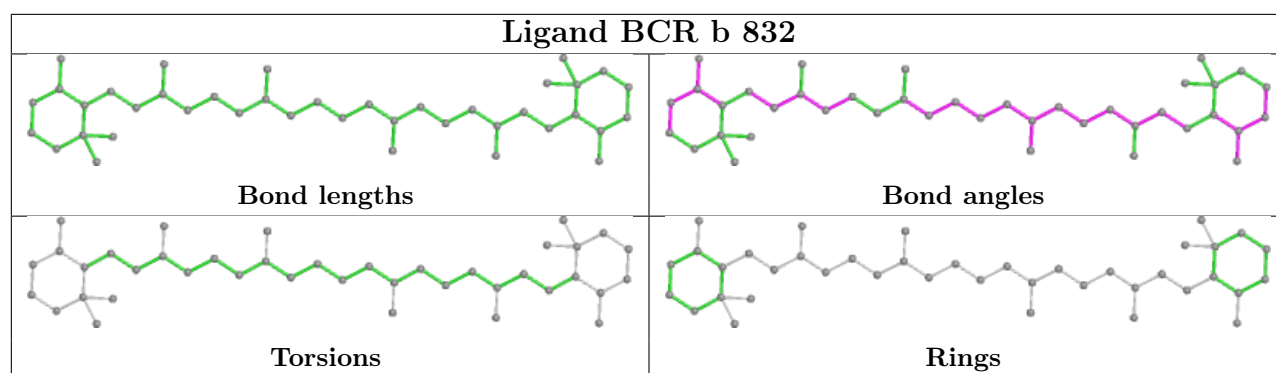


Ligand CLA a 823

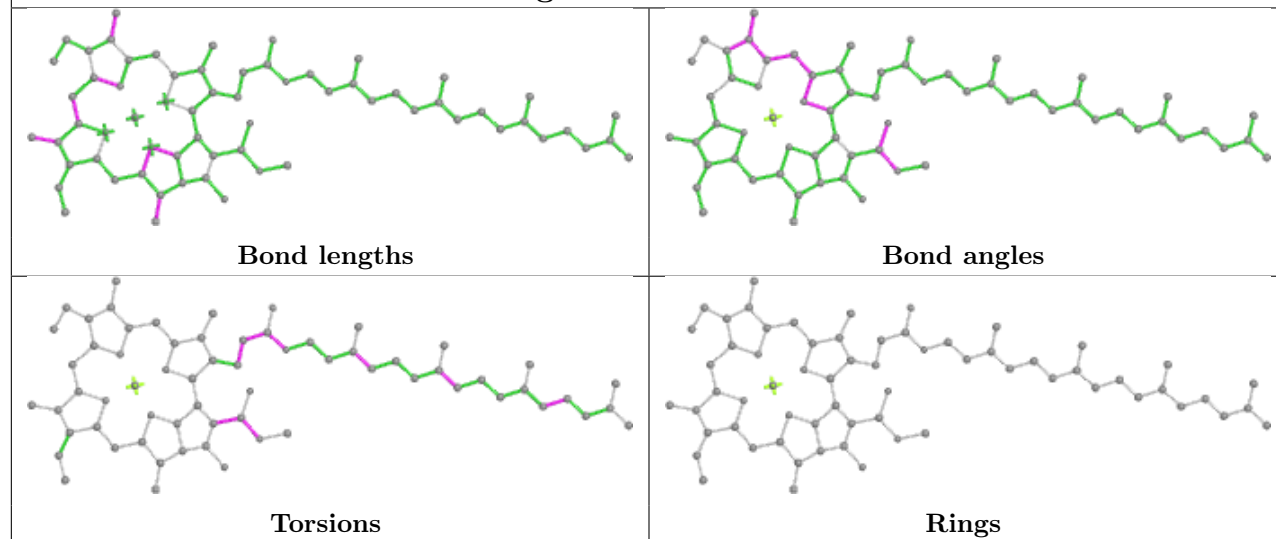


Ligand CLA B 308

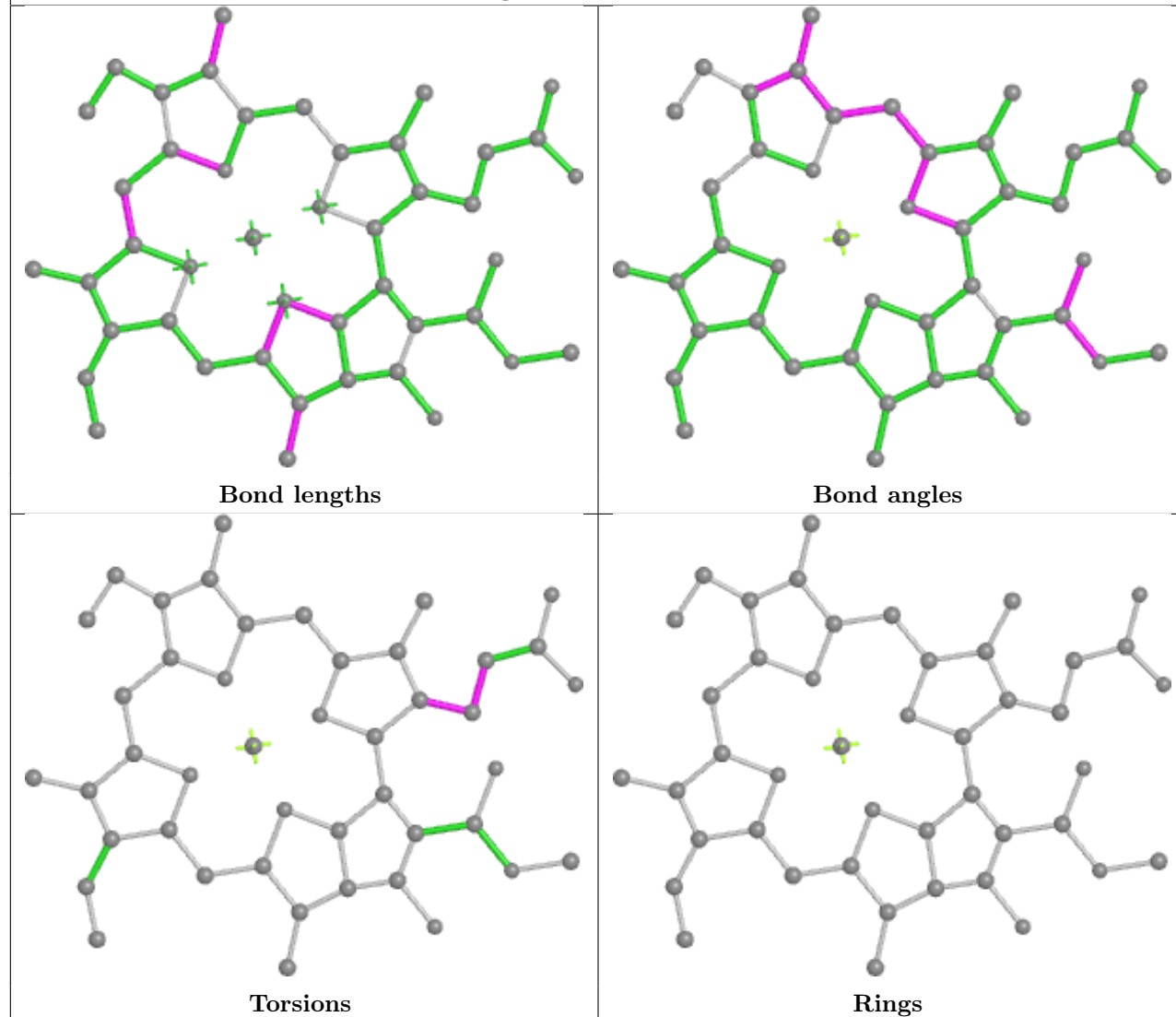


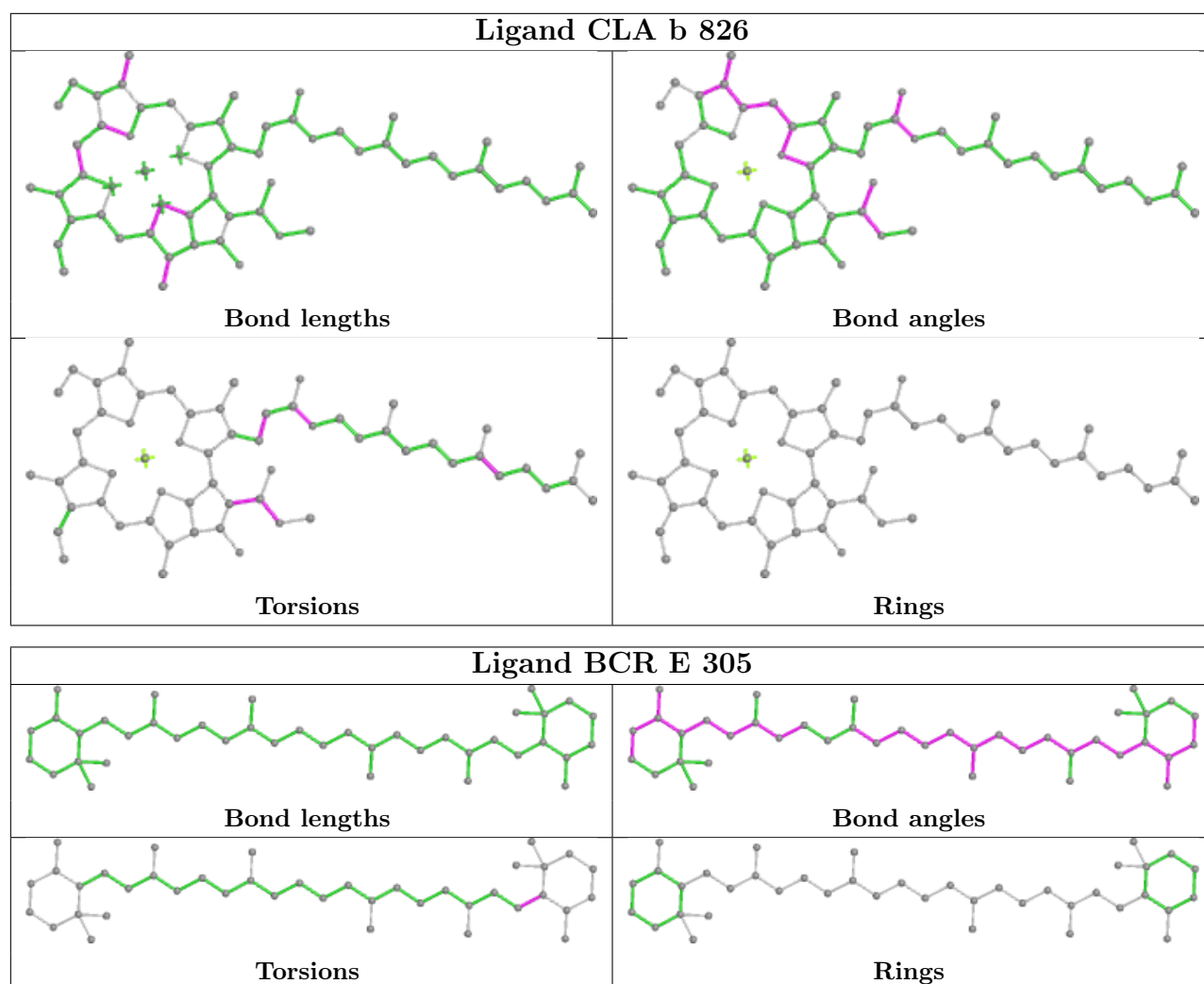


Ligand CLA a 847

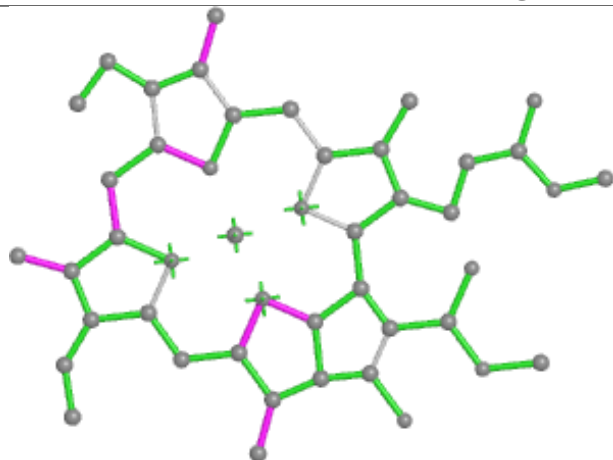


Ligand CLA f 204

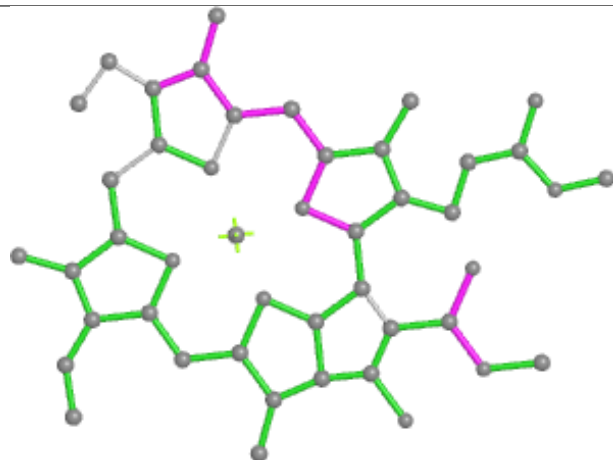




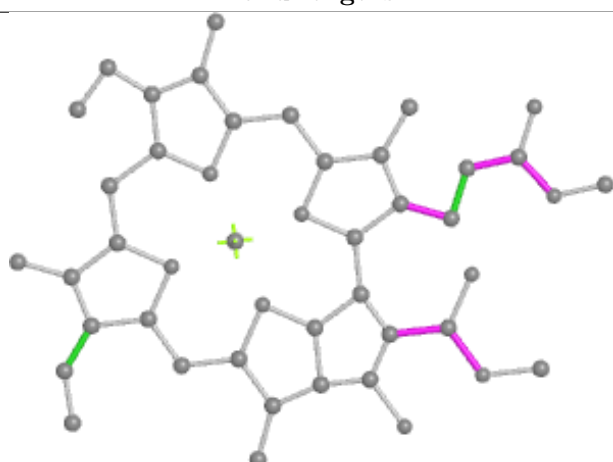
Ligand CLA D 211



Bond lengths



Bond angles

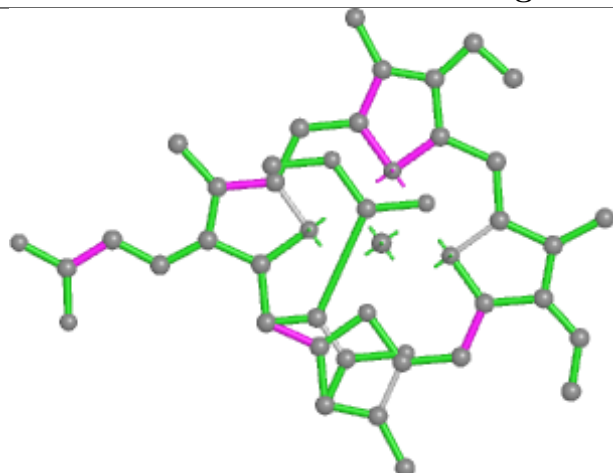


Torsions

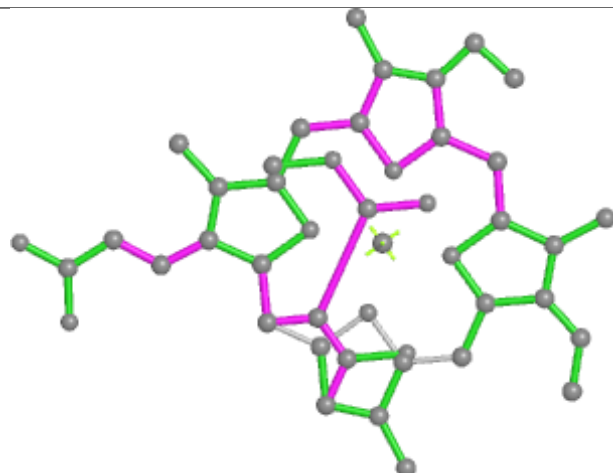


Rings

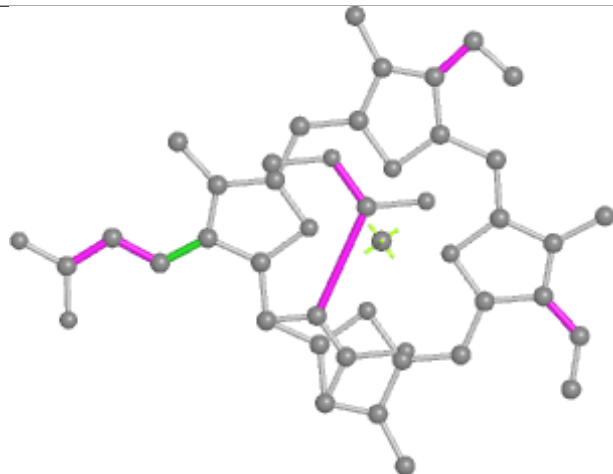
Ligand KC1 H 312



Bond lengths



Bond angles

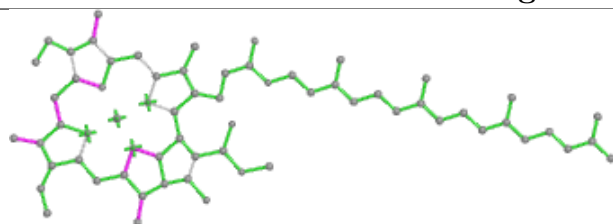


Torsions

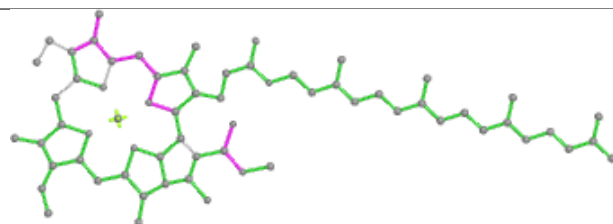


Rings

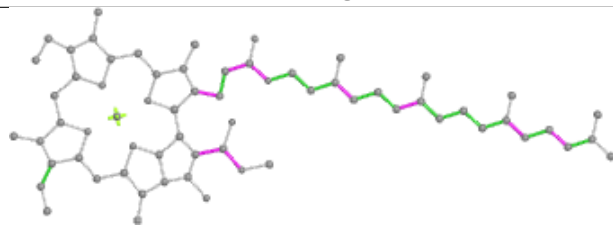
Ligand CLA a 805



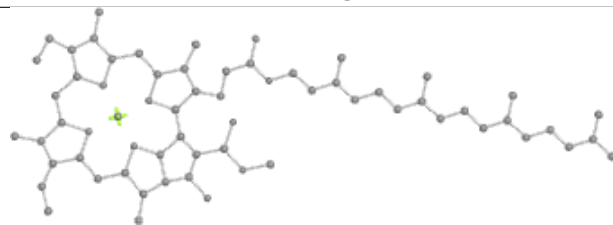
Bond lengths



Bond angles

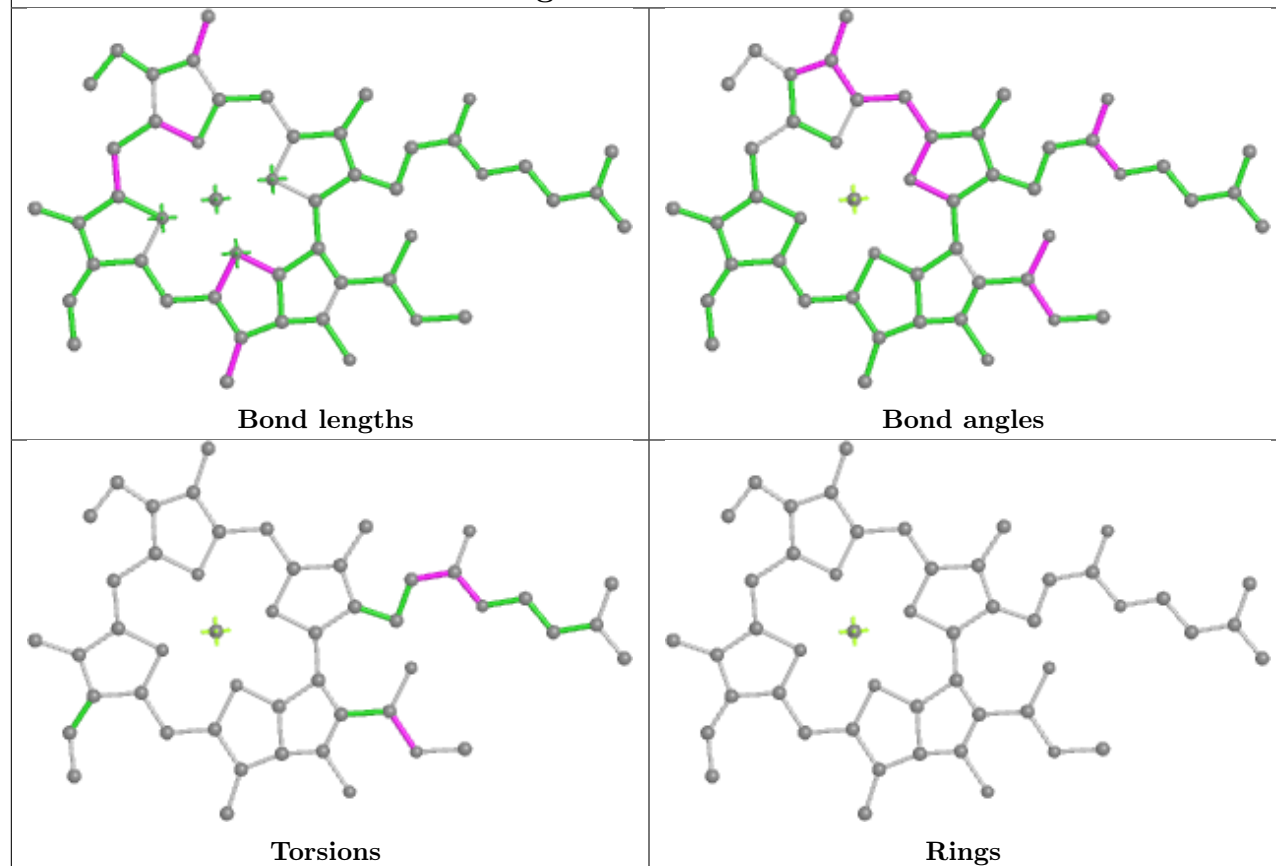


Torsions

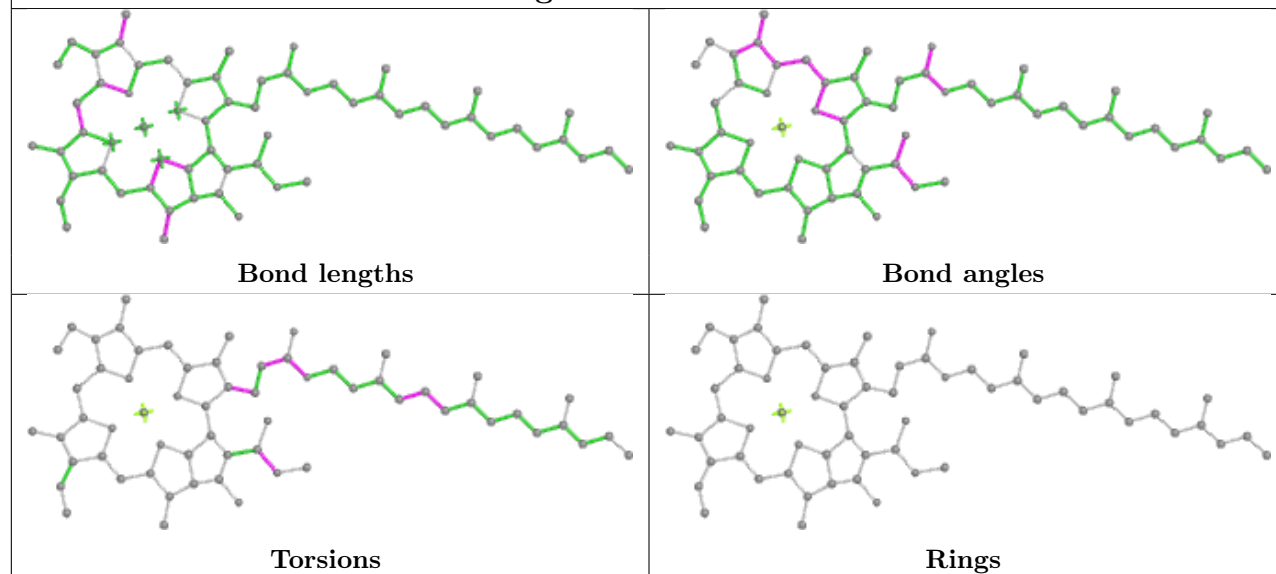


Rings

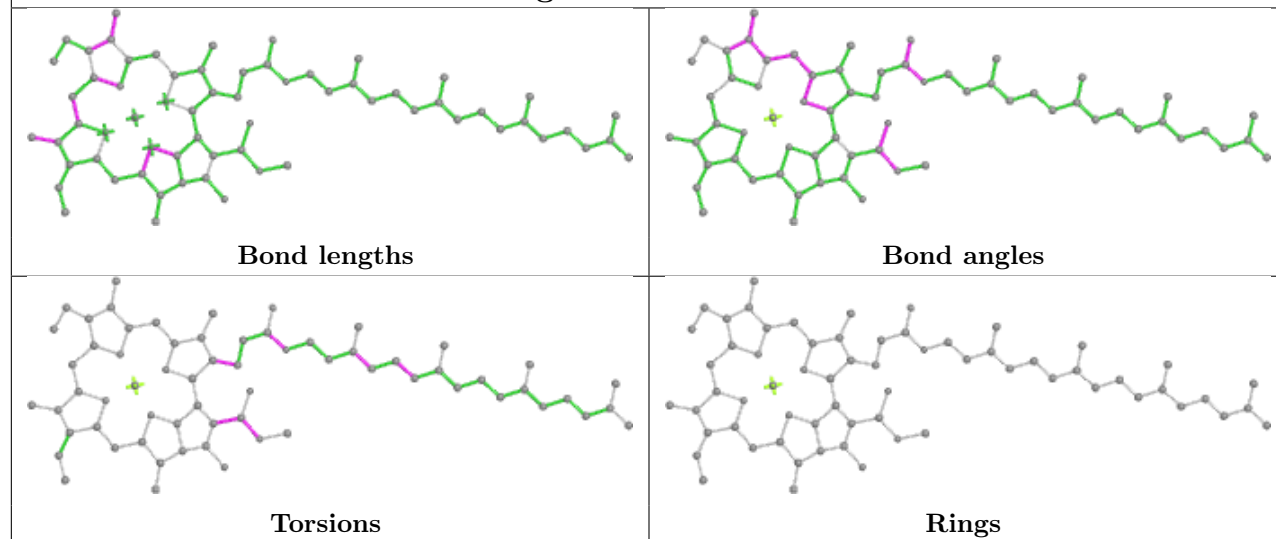
Ligand CLA a 822



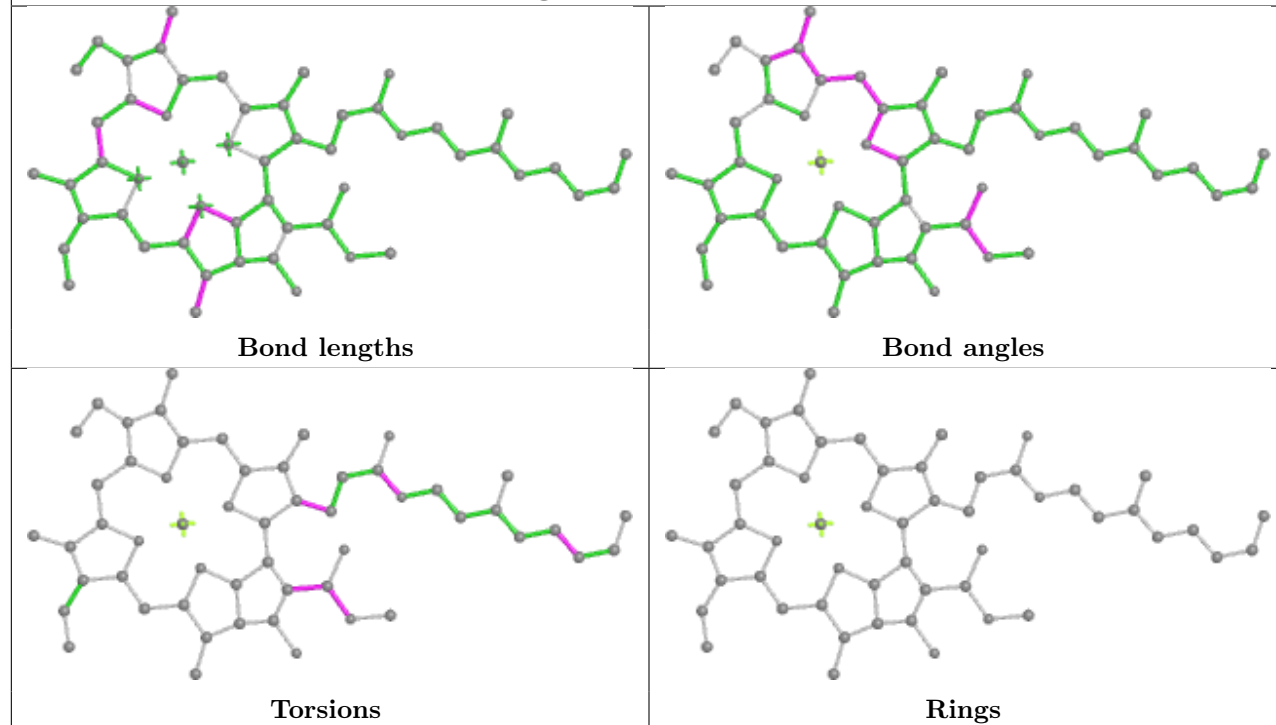
Ligand CLA b 844

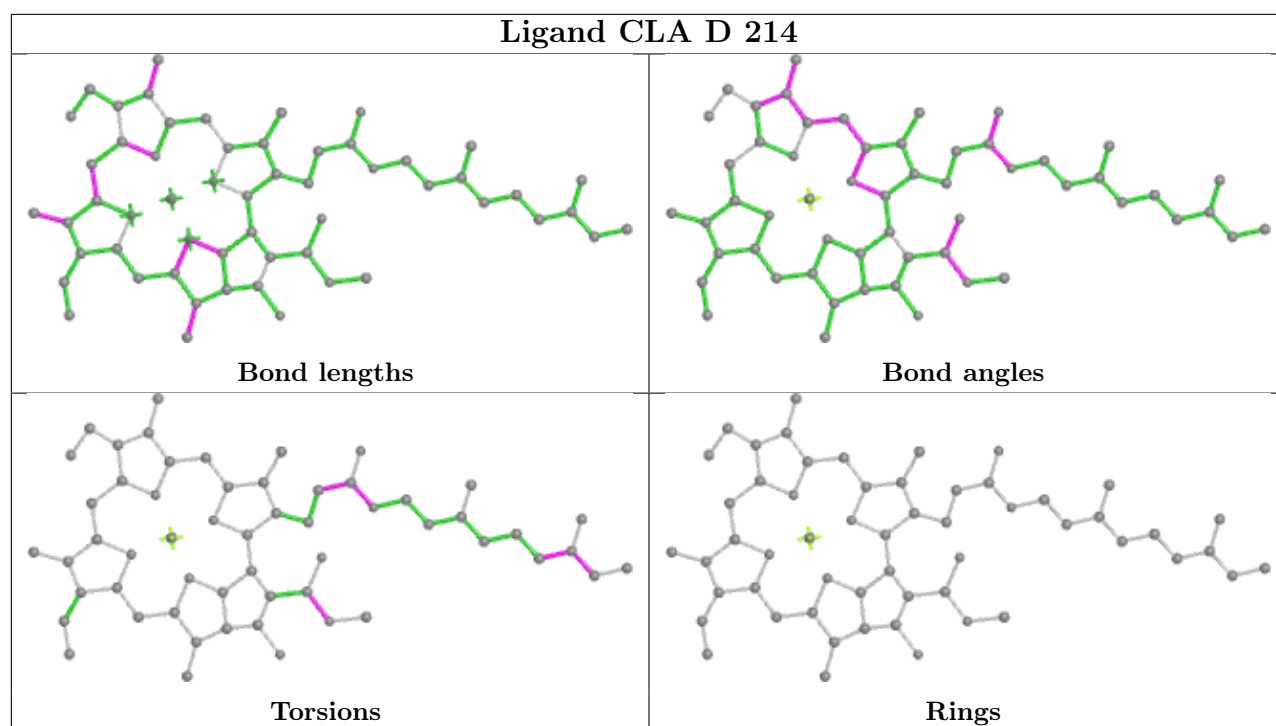


Ligand CLA a 821

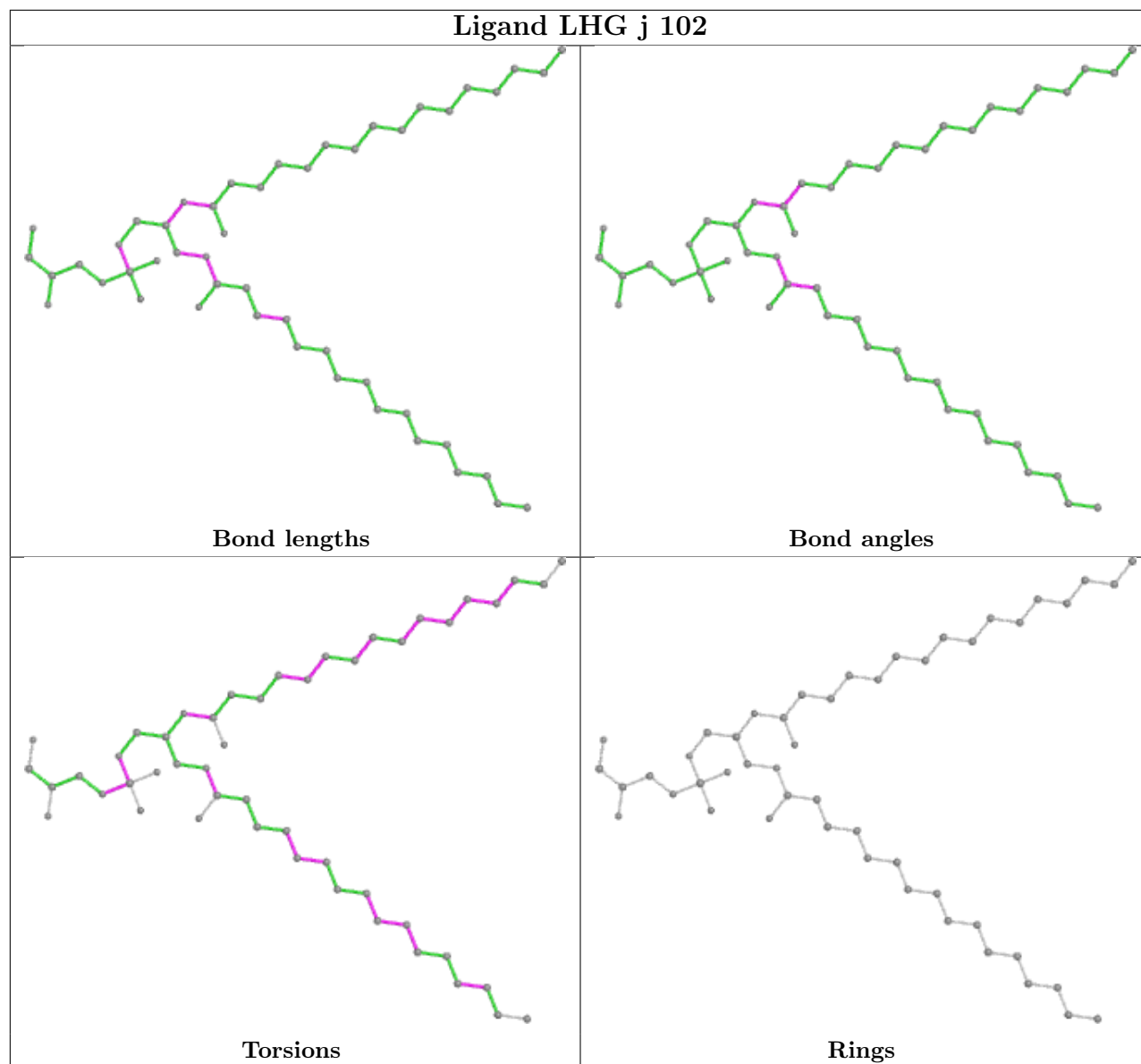


Ligand CLA b 848

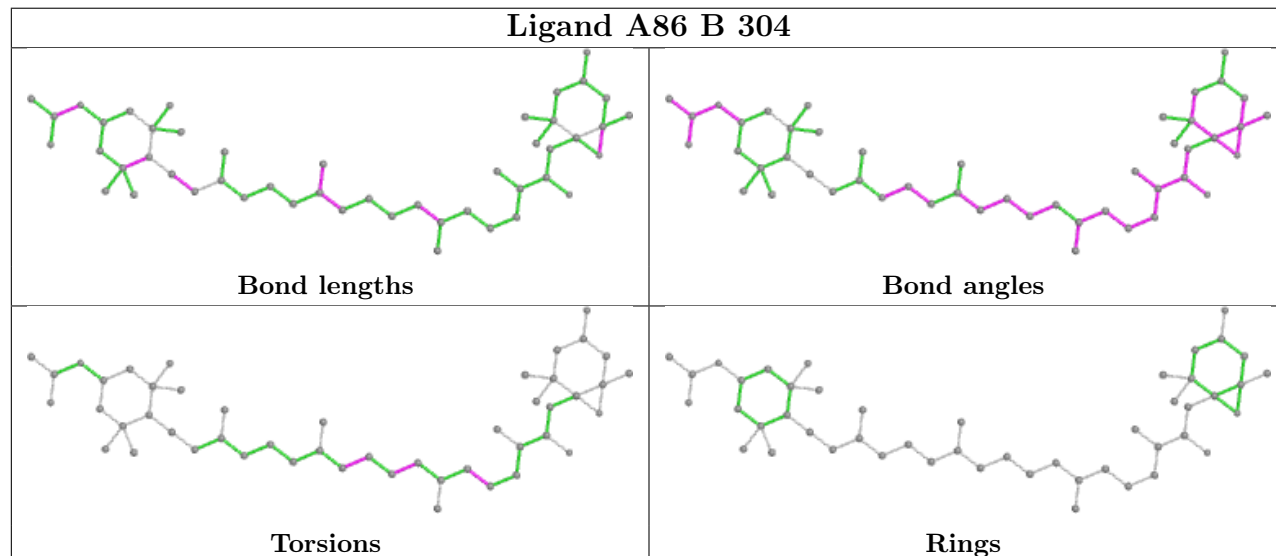




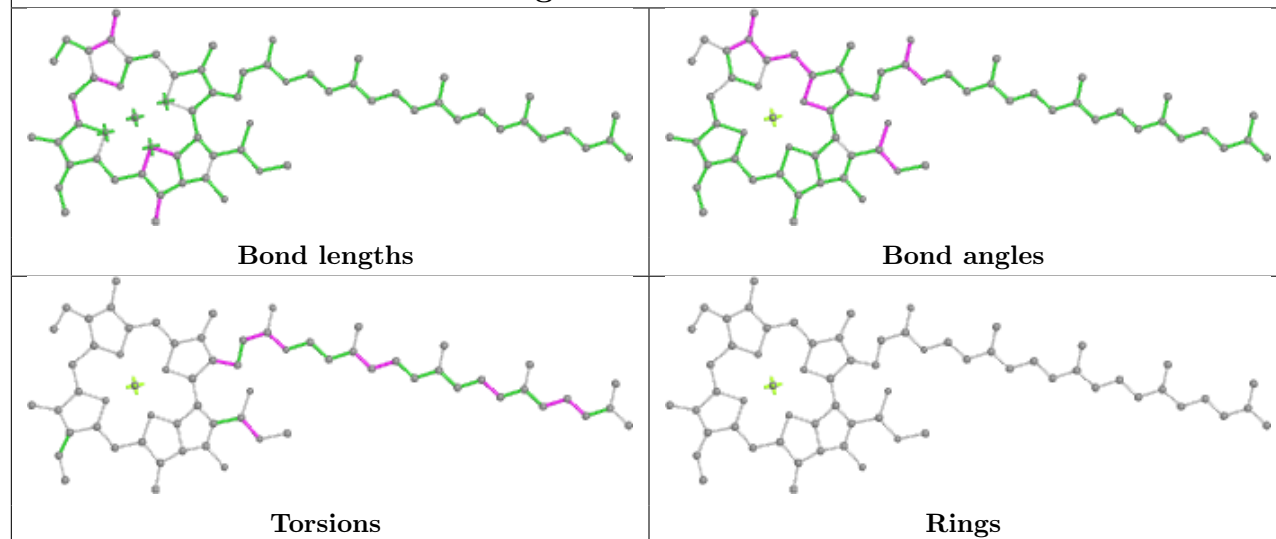
Ligand LHG j 102



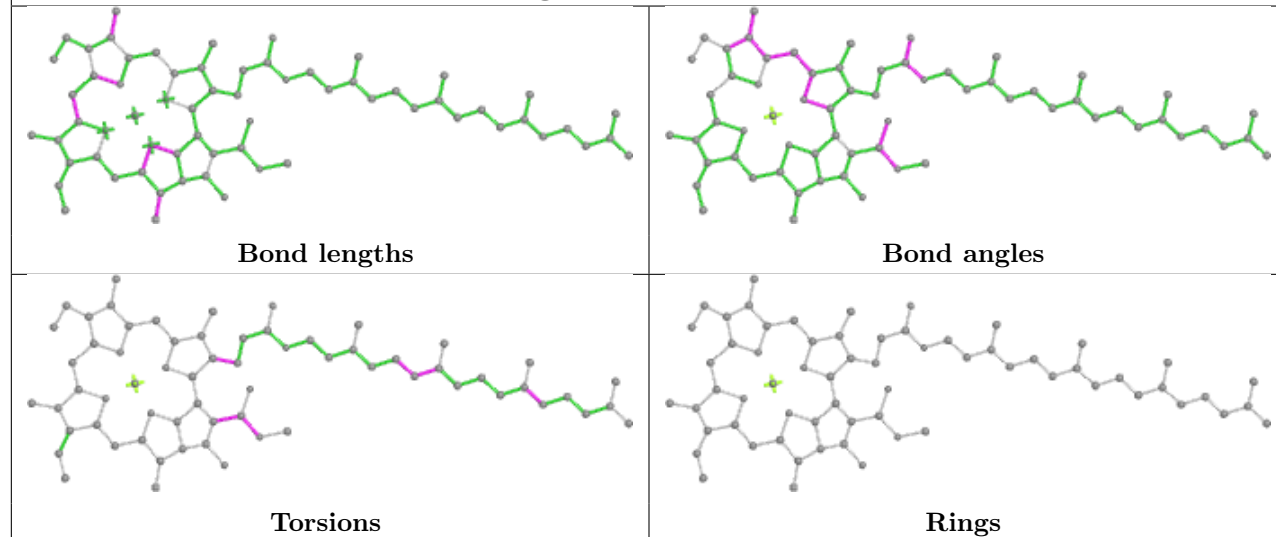
Ligand A86 B 304

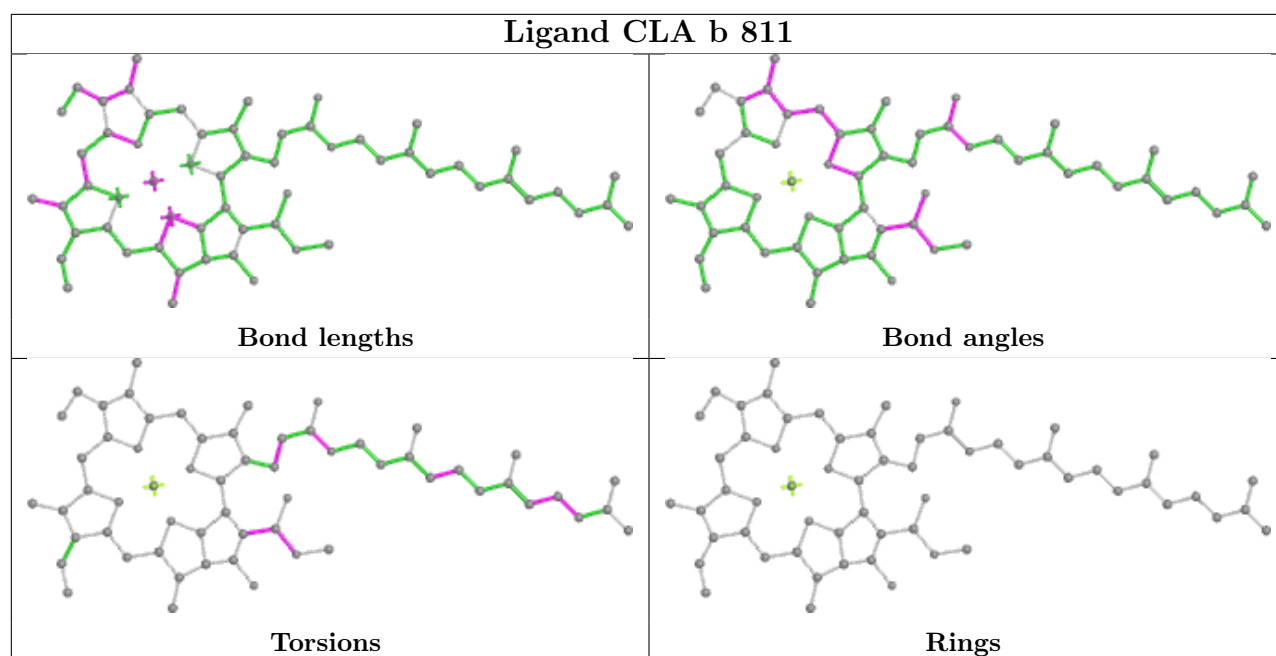


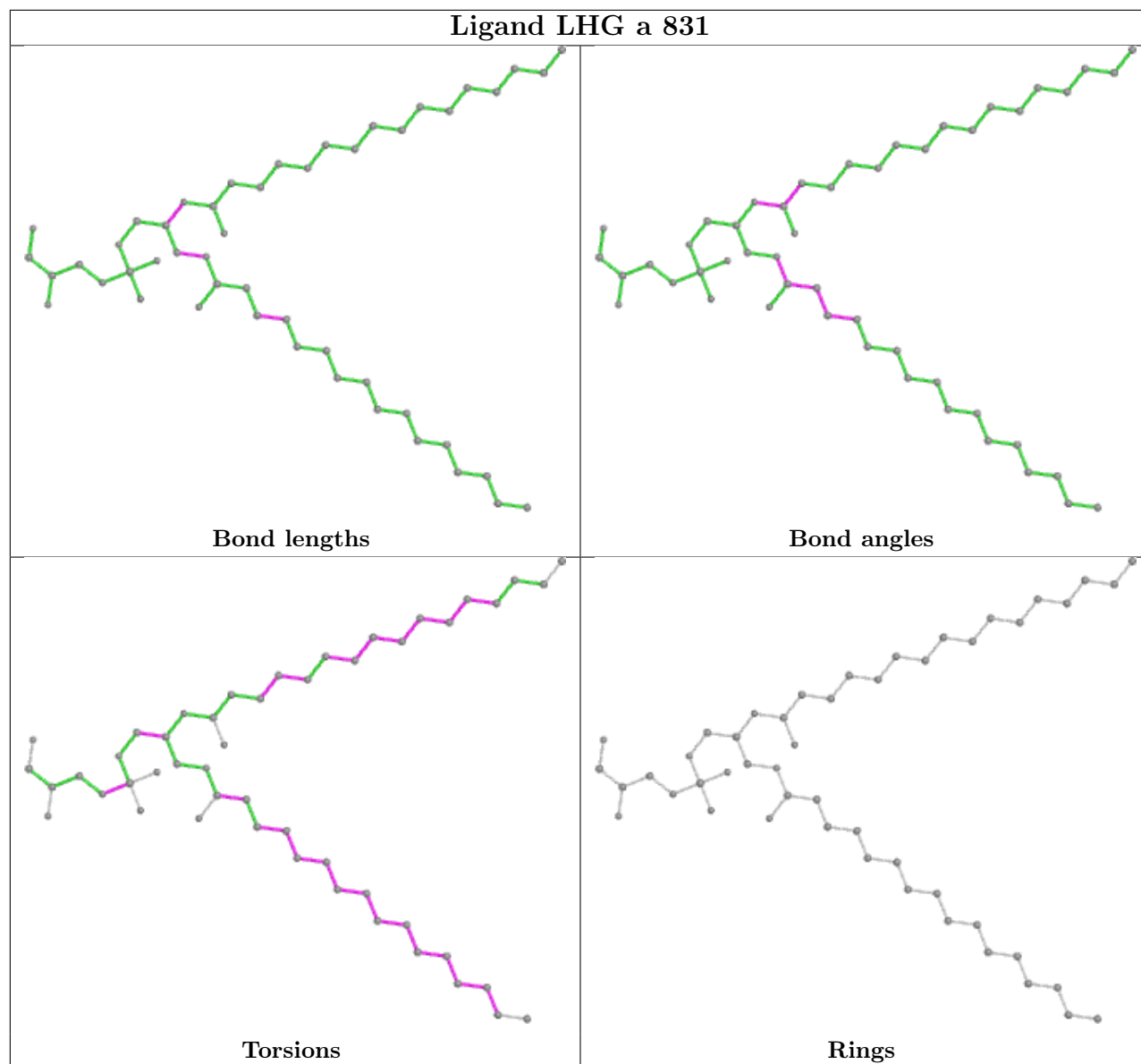
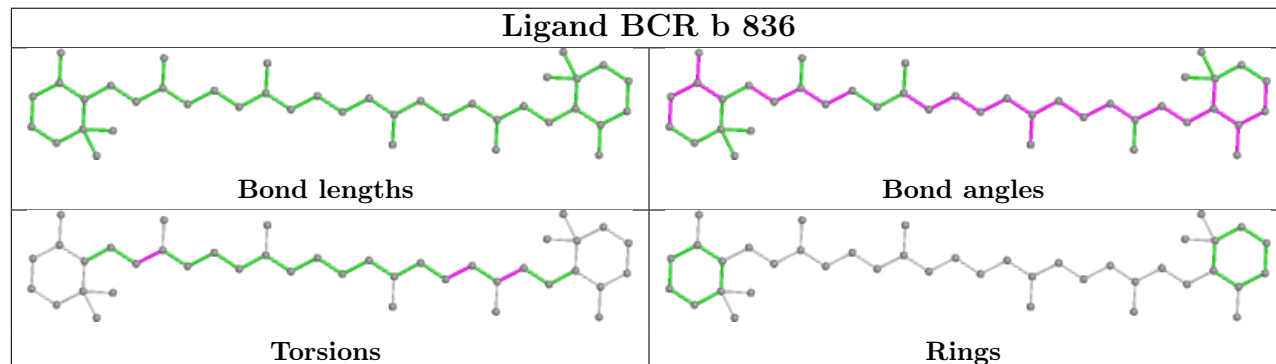
Ligand CLA b 849

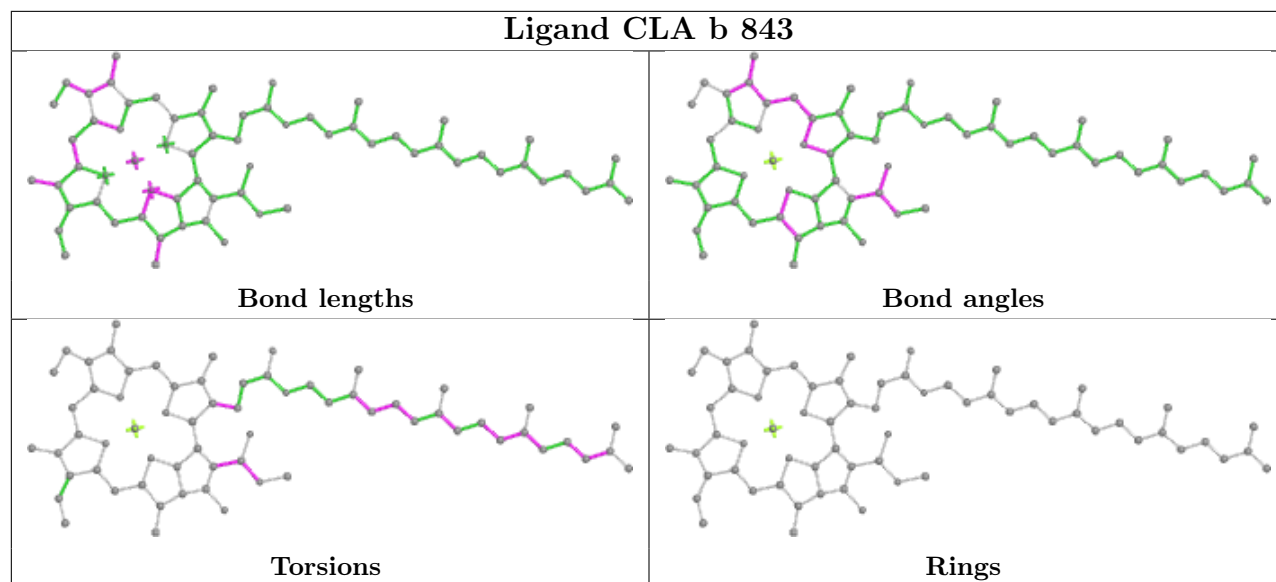
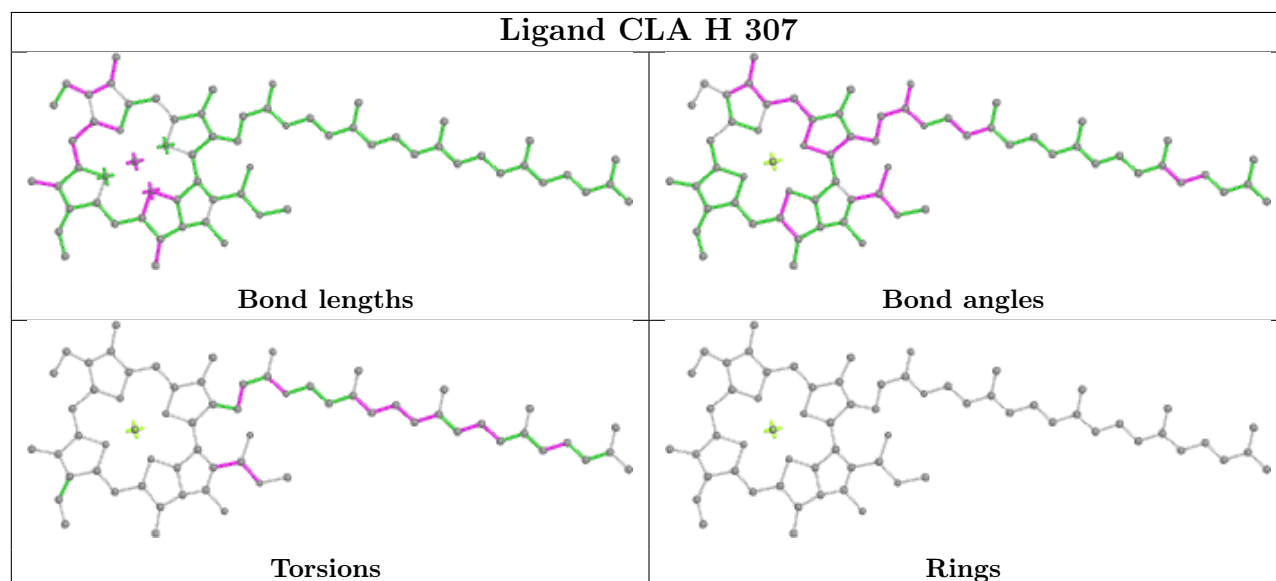
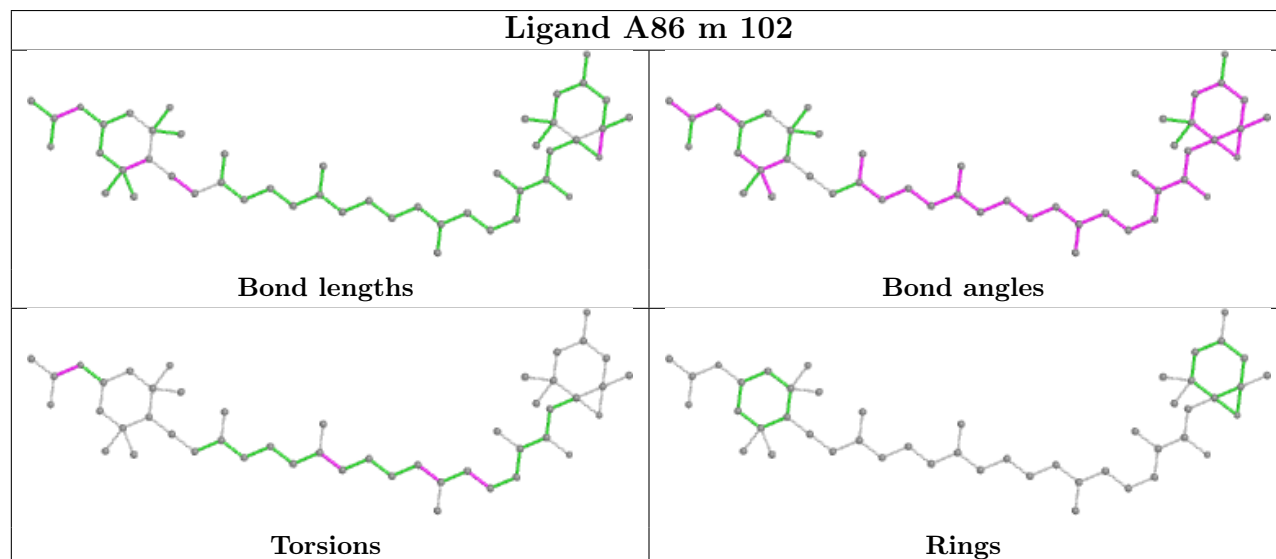


Ligand CLA a 828

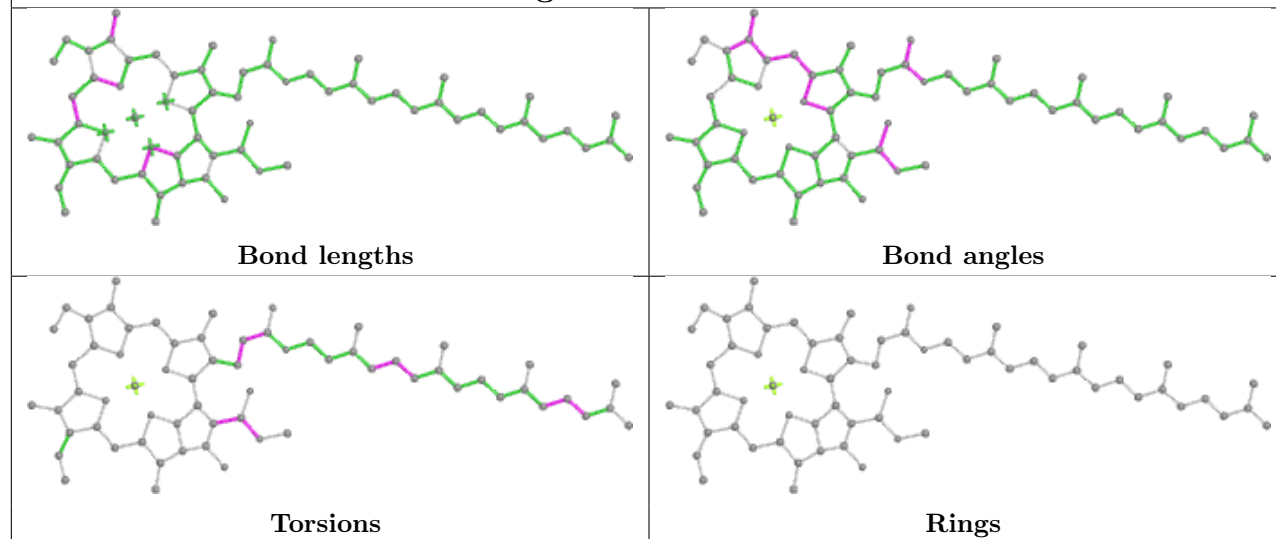




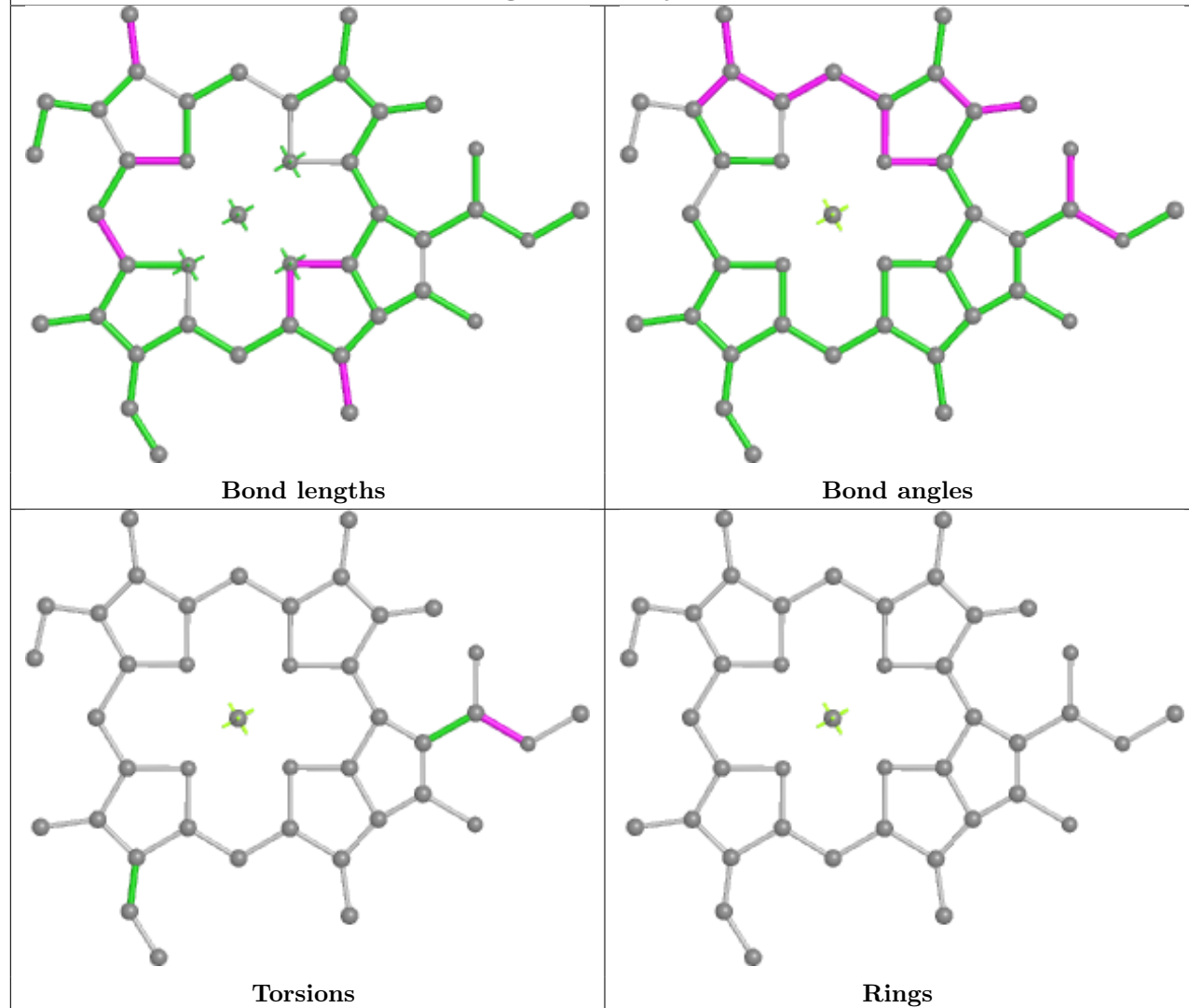
Ligand LHG a 831**Ligand BCR b 836**

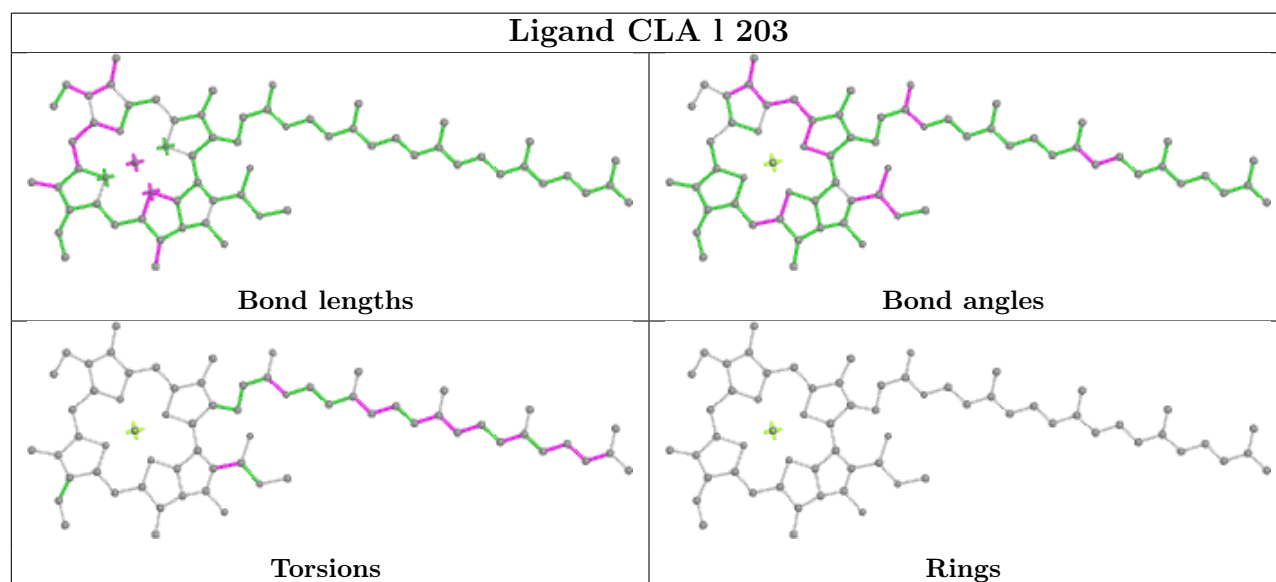
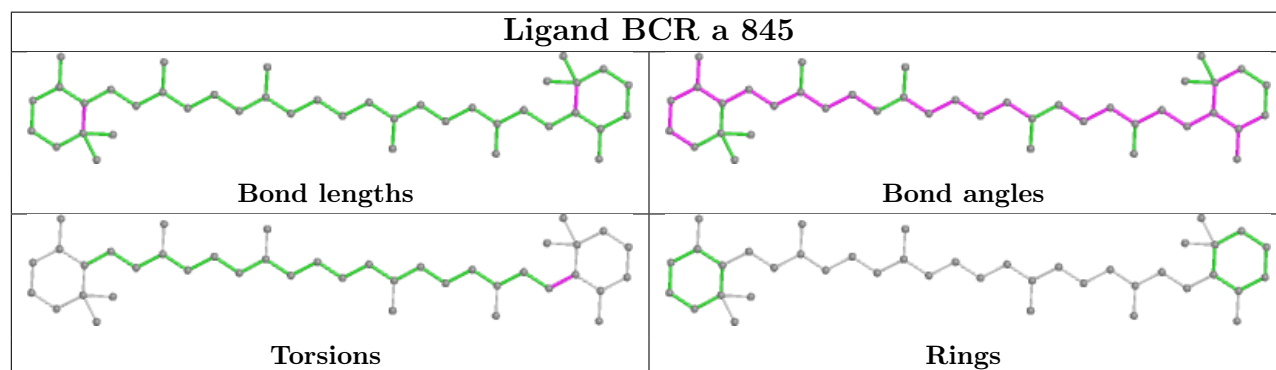
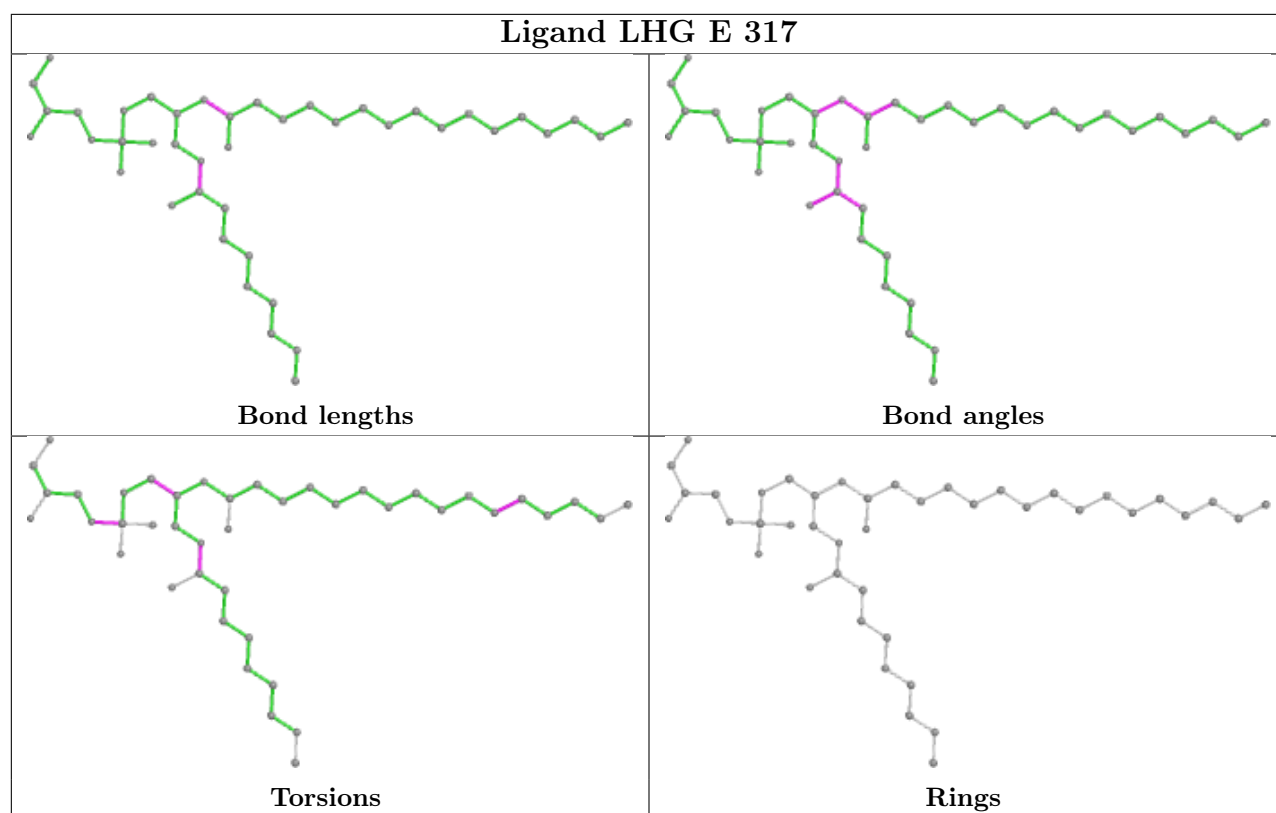
Ligand CLA b 843**Ligand CLA H 307****Ligand A86 m 102**

Ligand CLA a 827

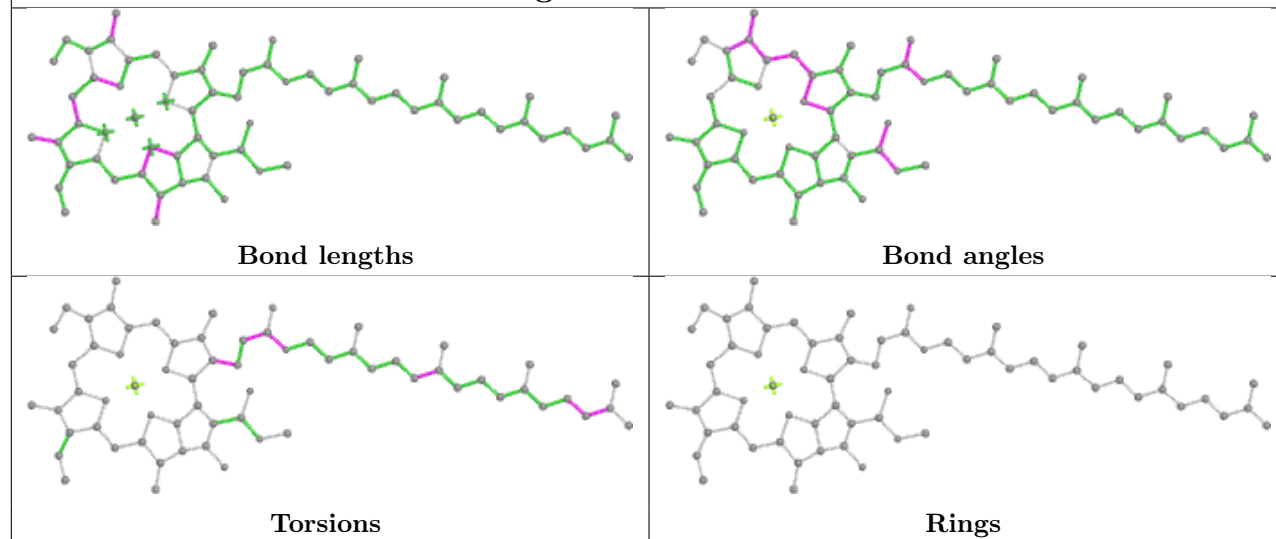


Ligand CLA j 104

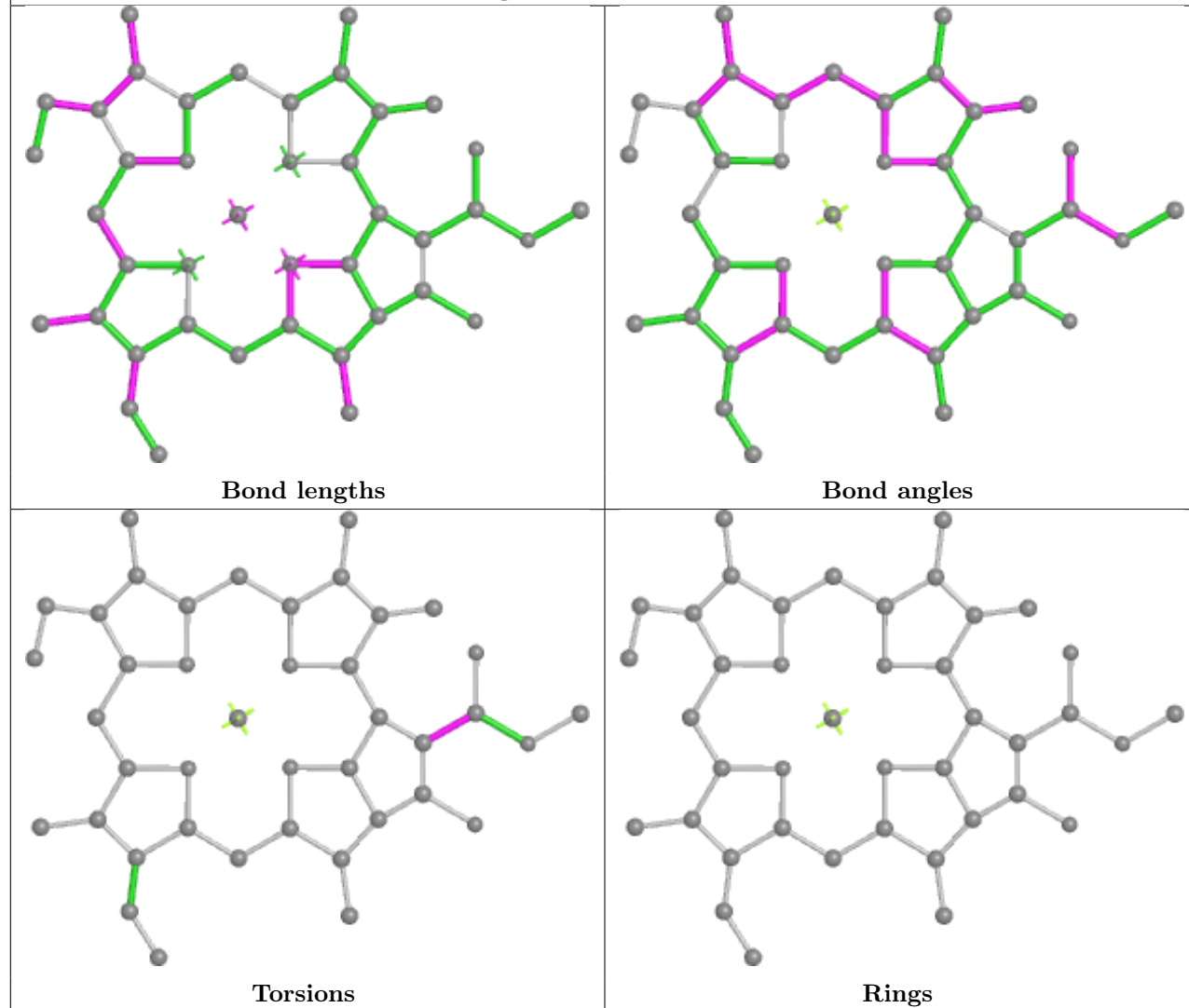




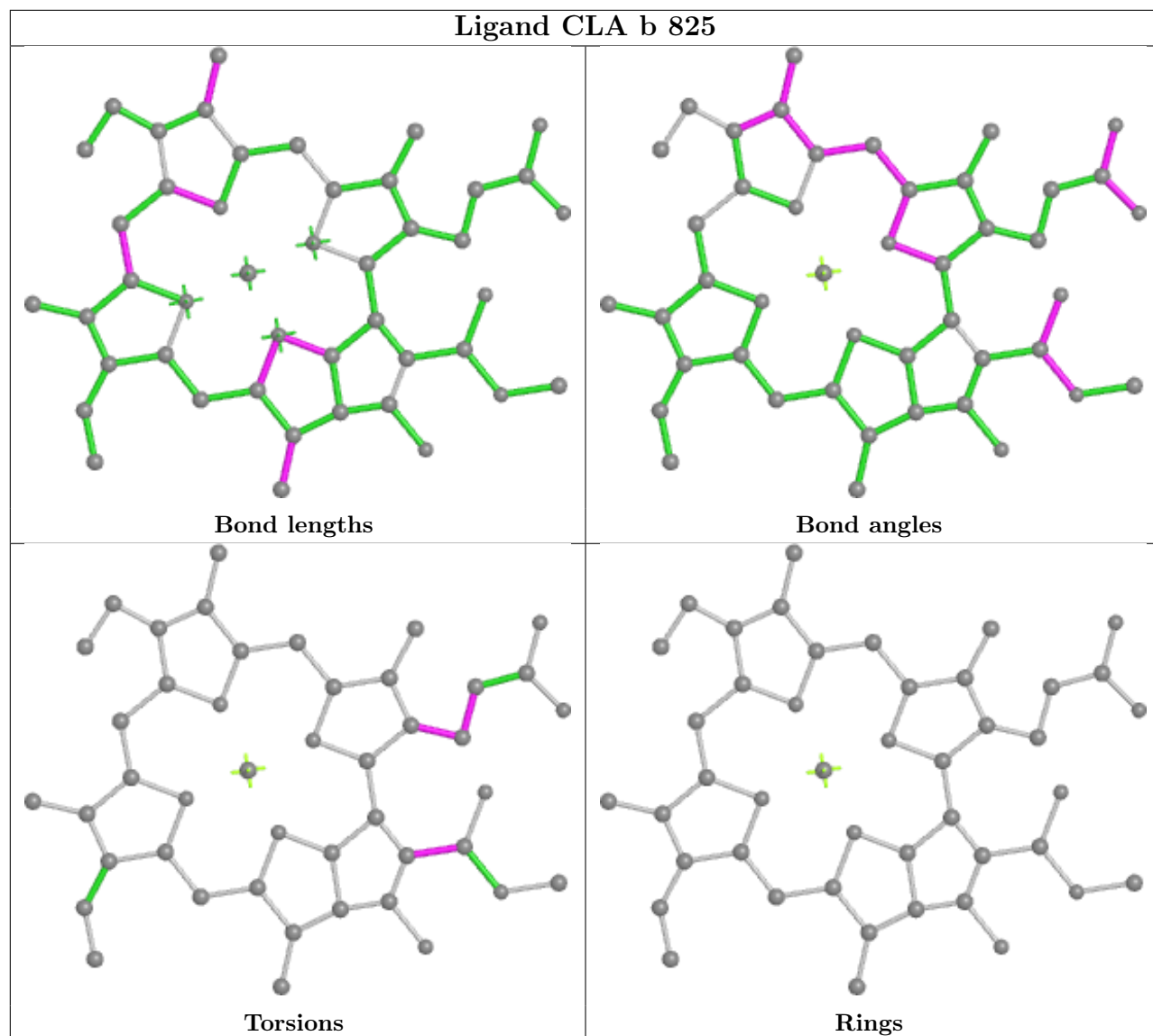
Ligand CLA b 810

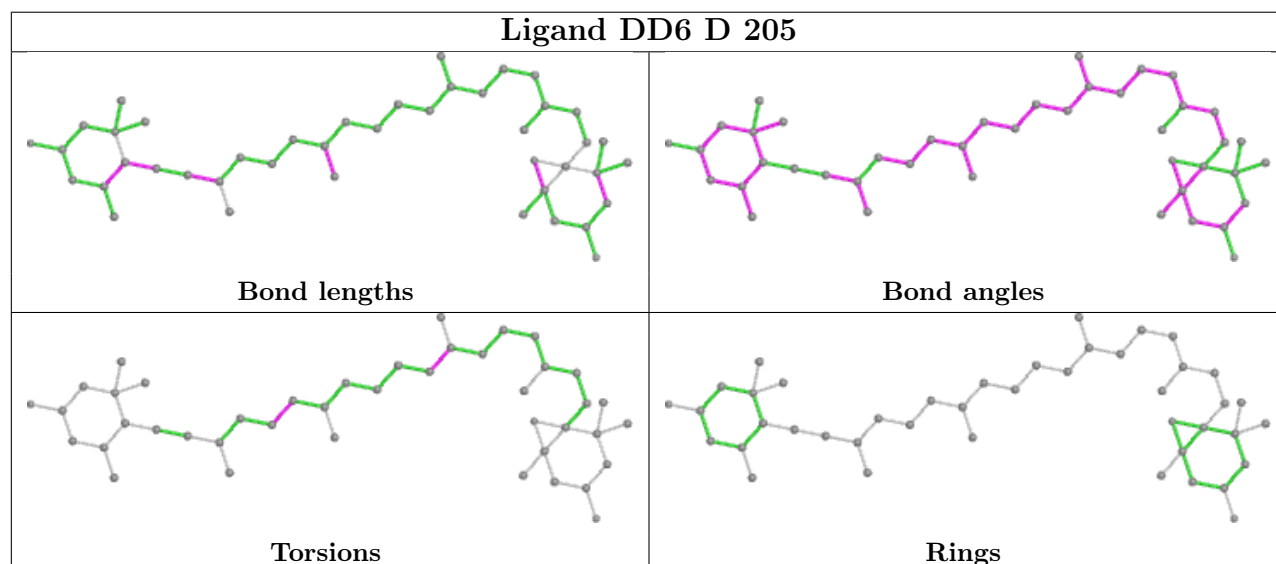
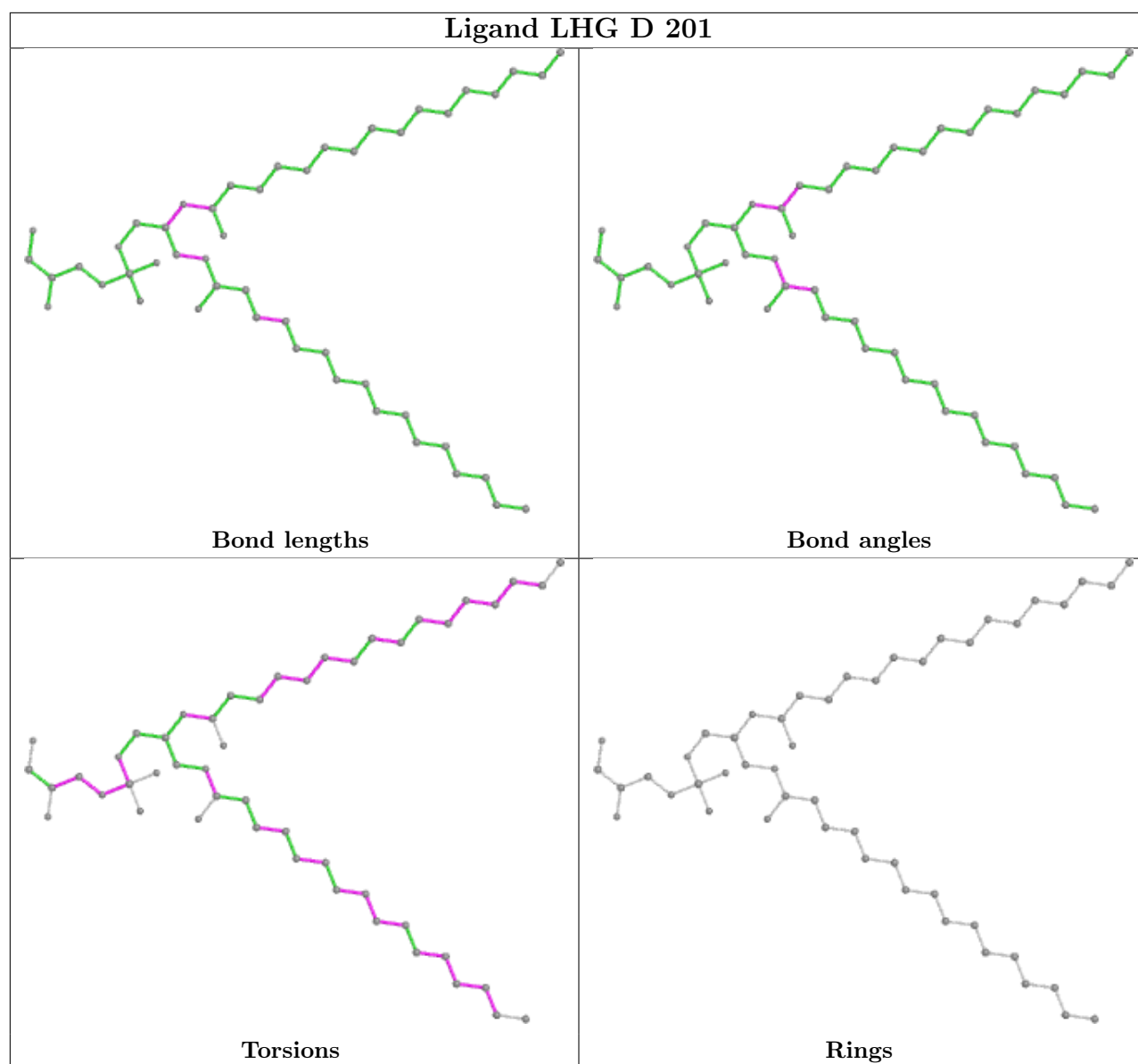


Ligand CLA C 316

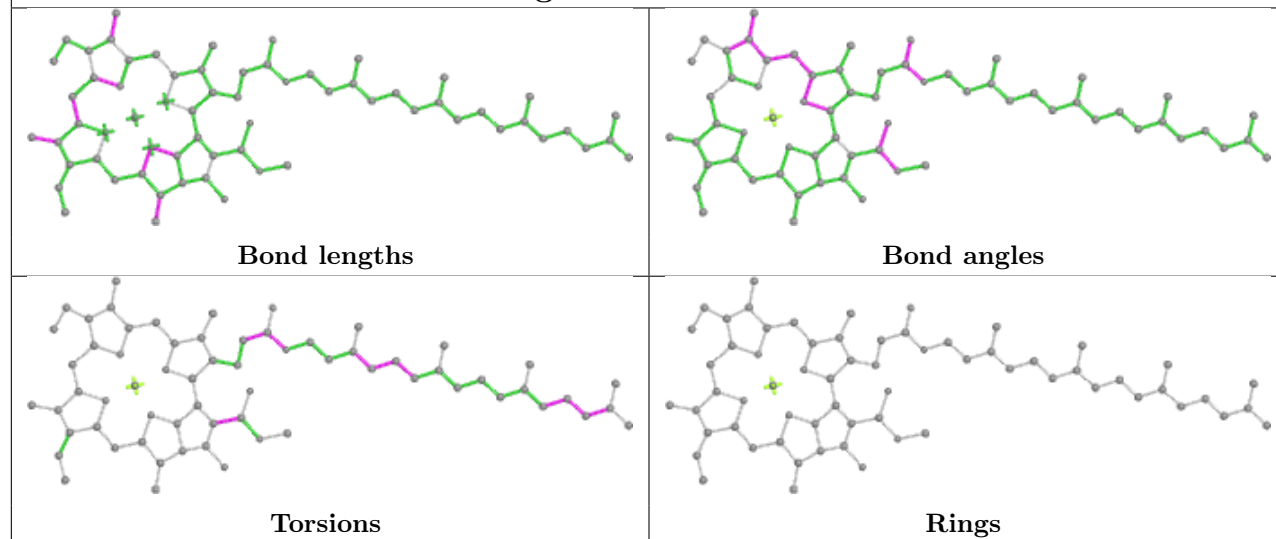


Ligand CLA b 825

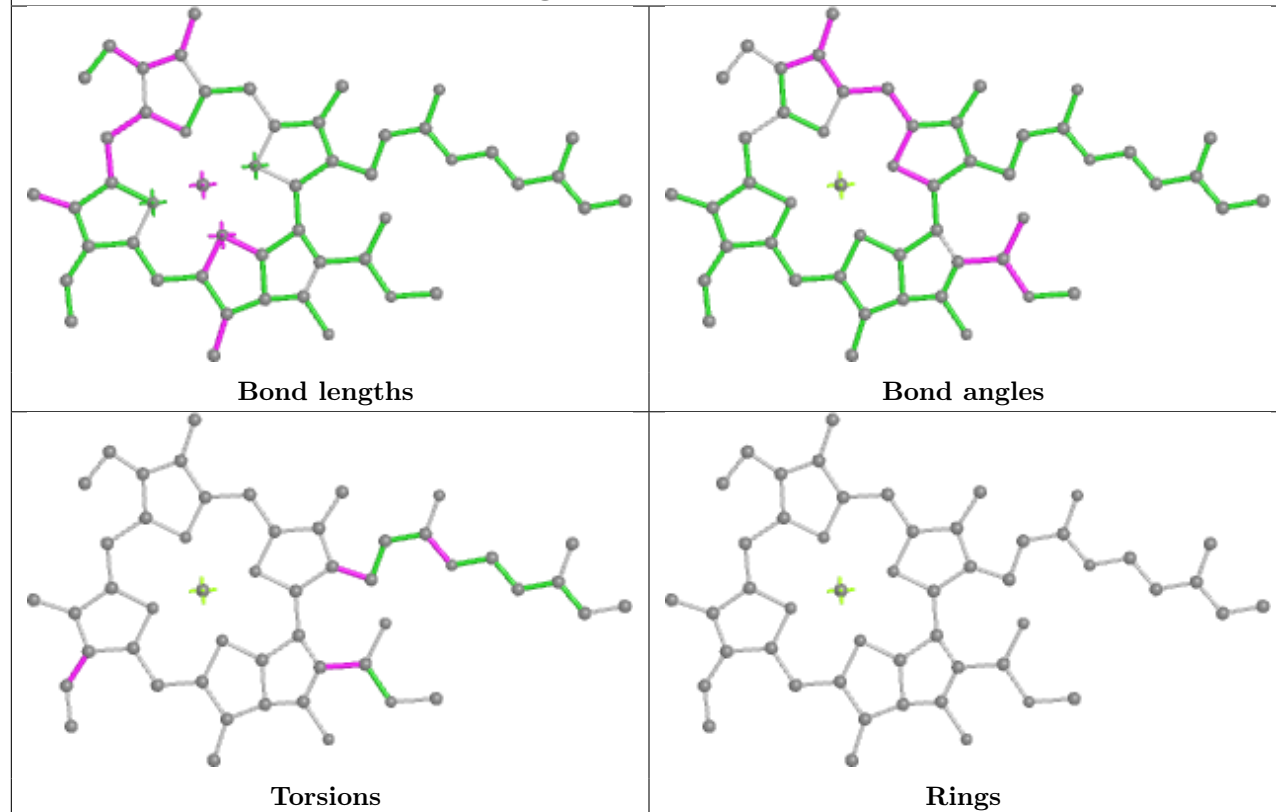


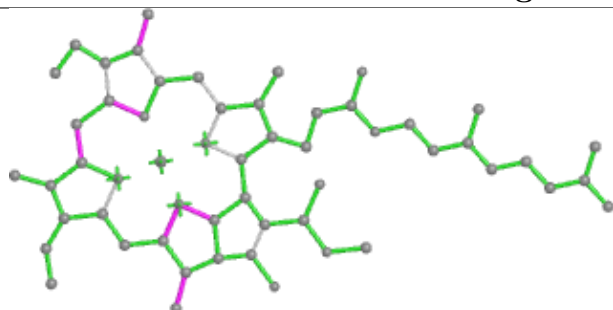


Ligand CLA b 846

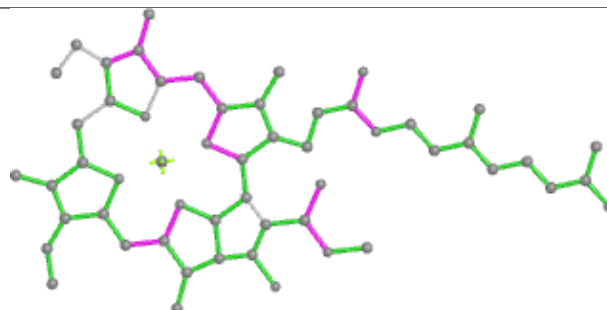


Ligand CLA a 818

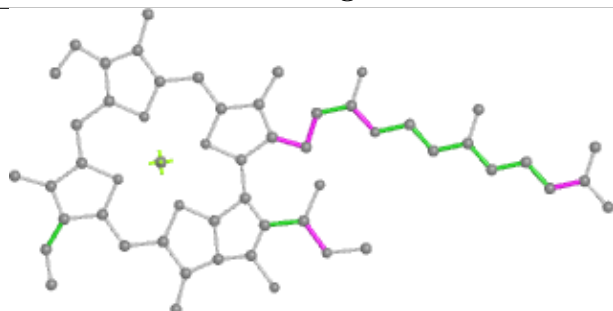


Ligand CLA E 313

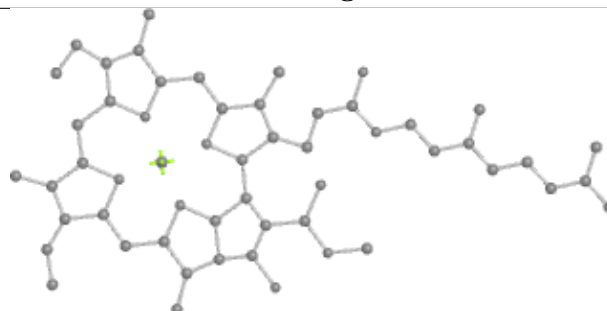
Bond lengths



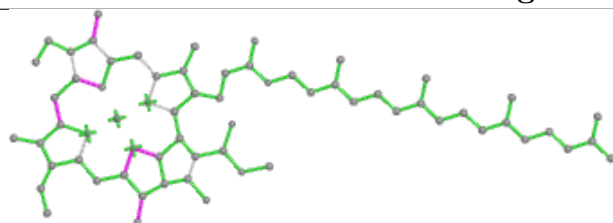
Bond angles



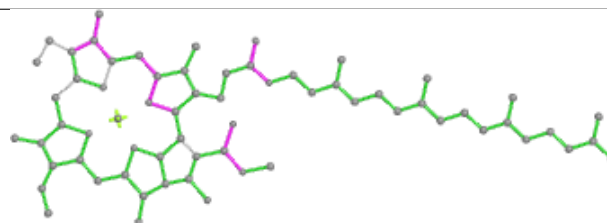
Torsions



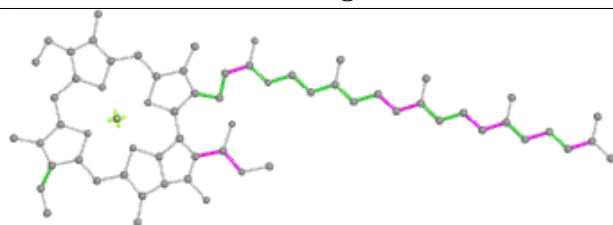
Rings

Ligand CLA b 850

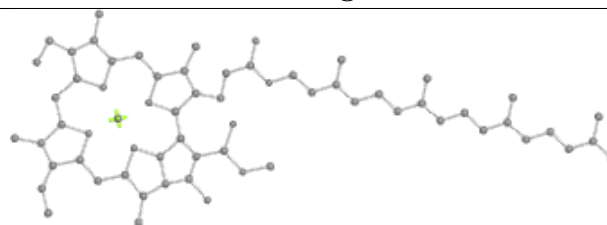
Bond lengths



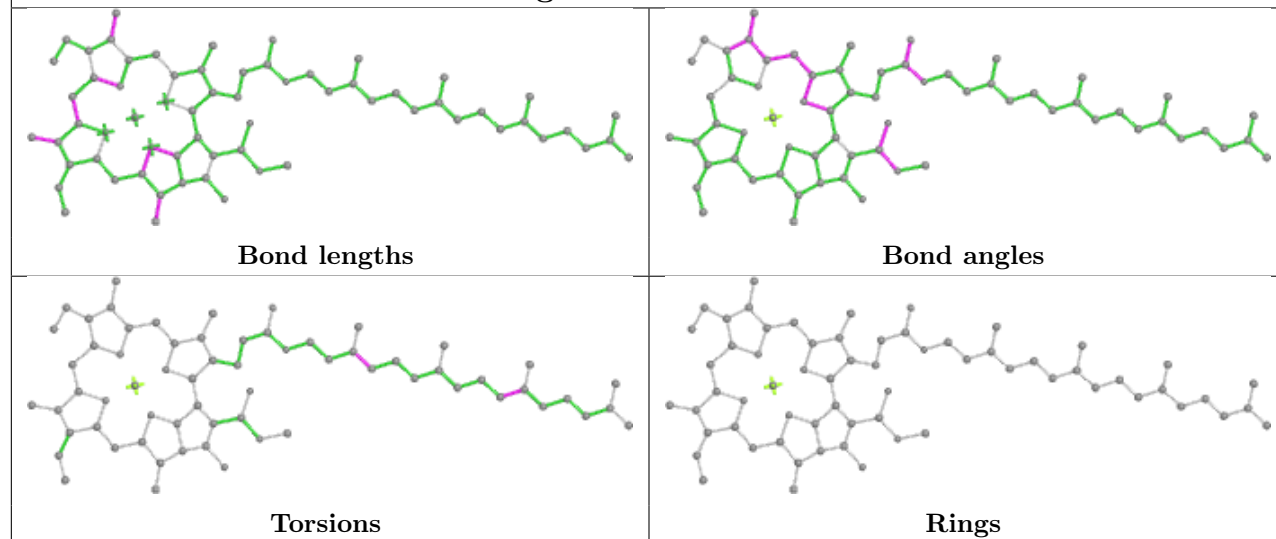
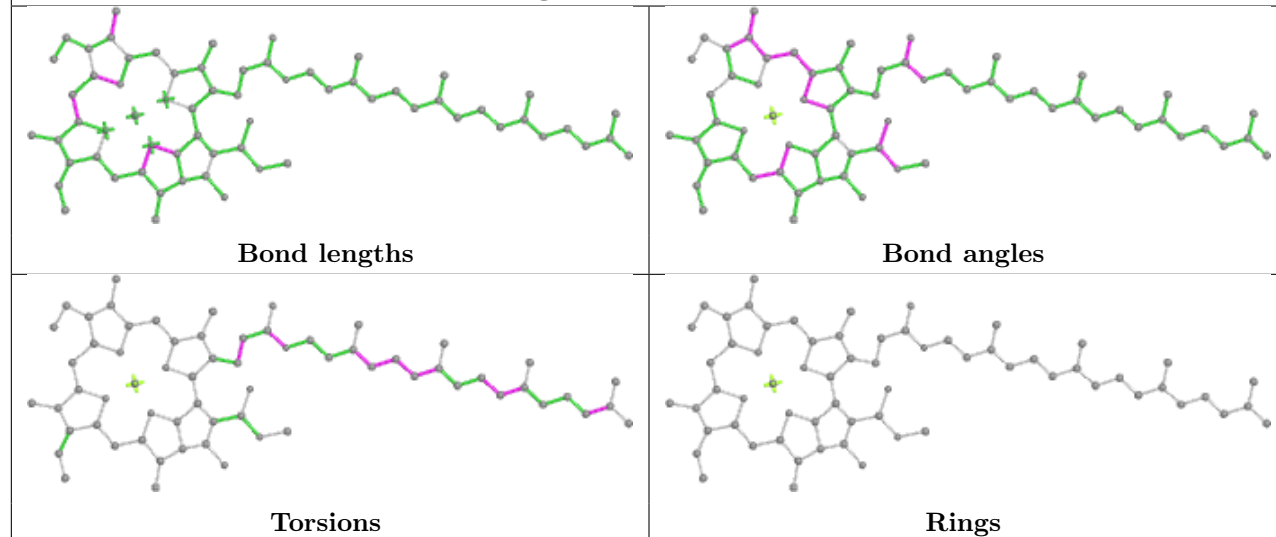
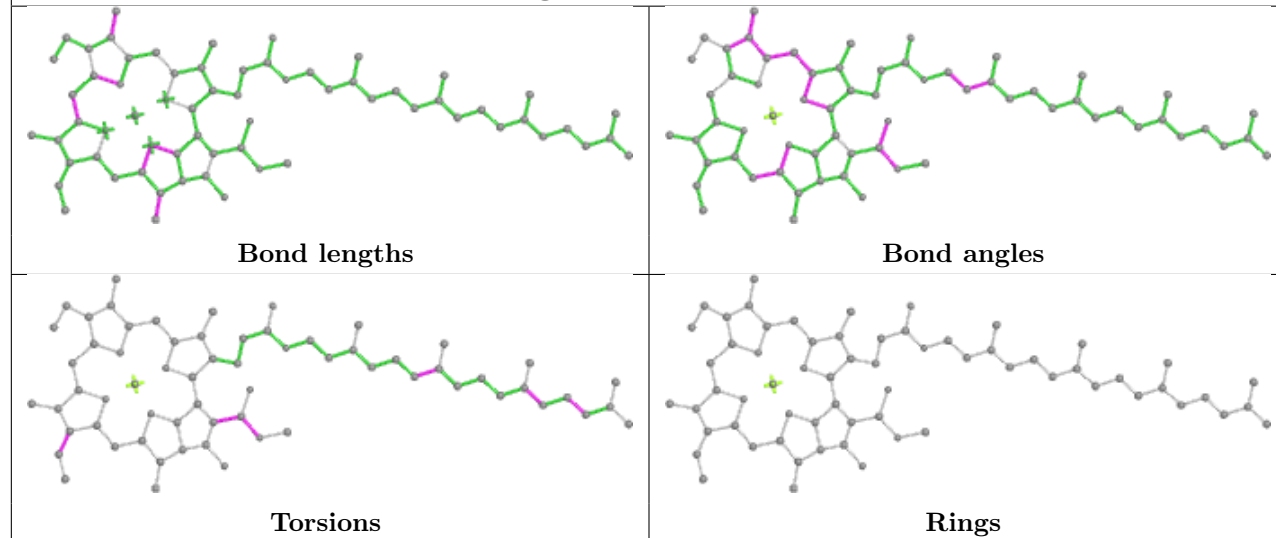
Bond angles

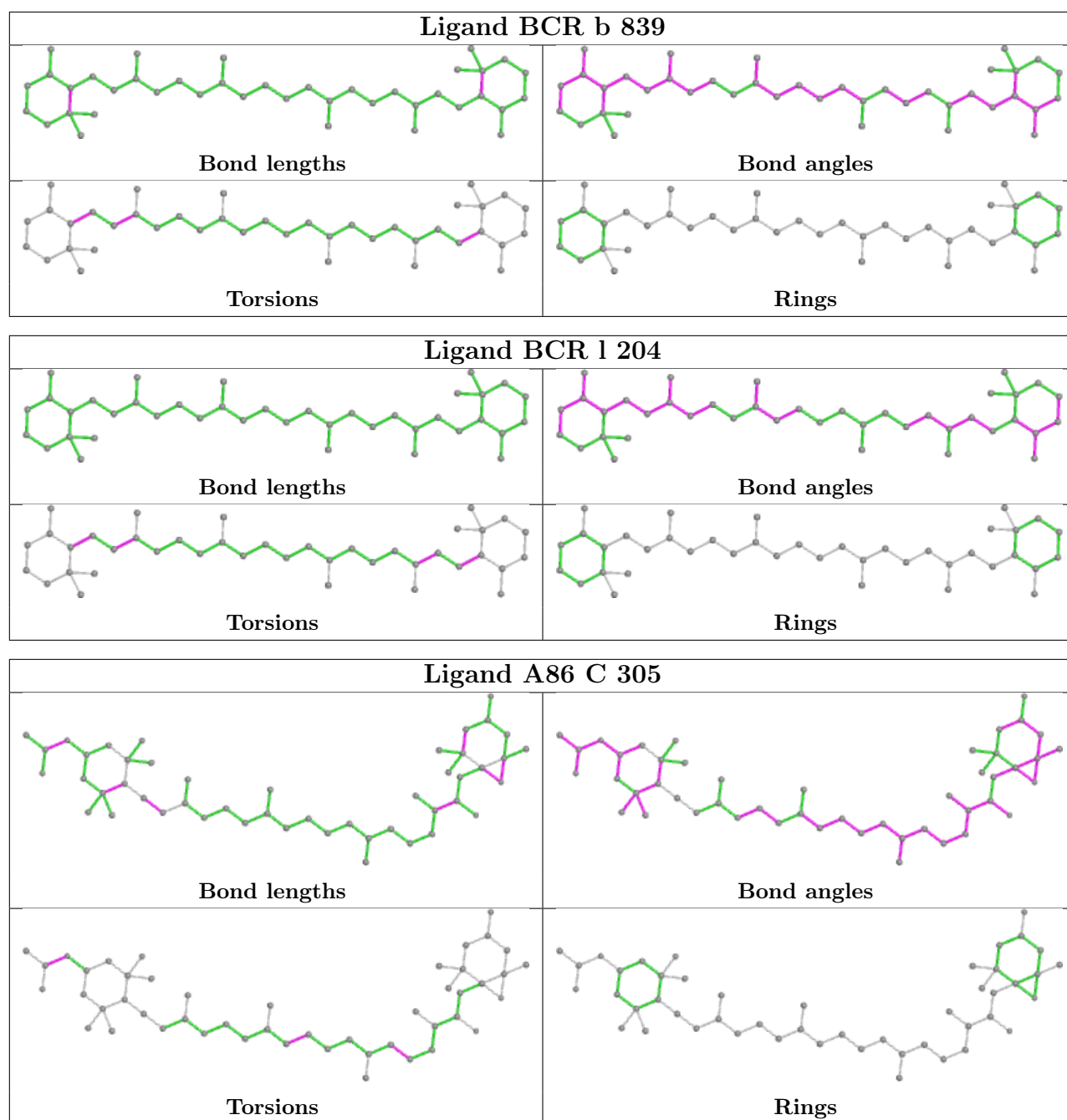


Torsions

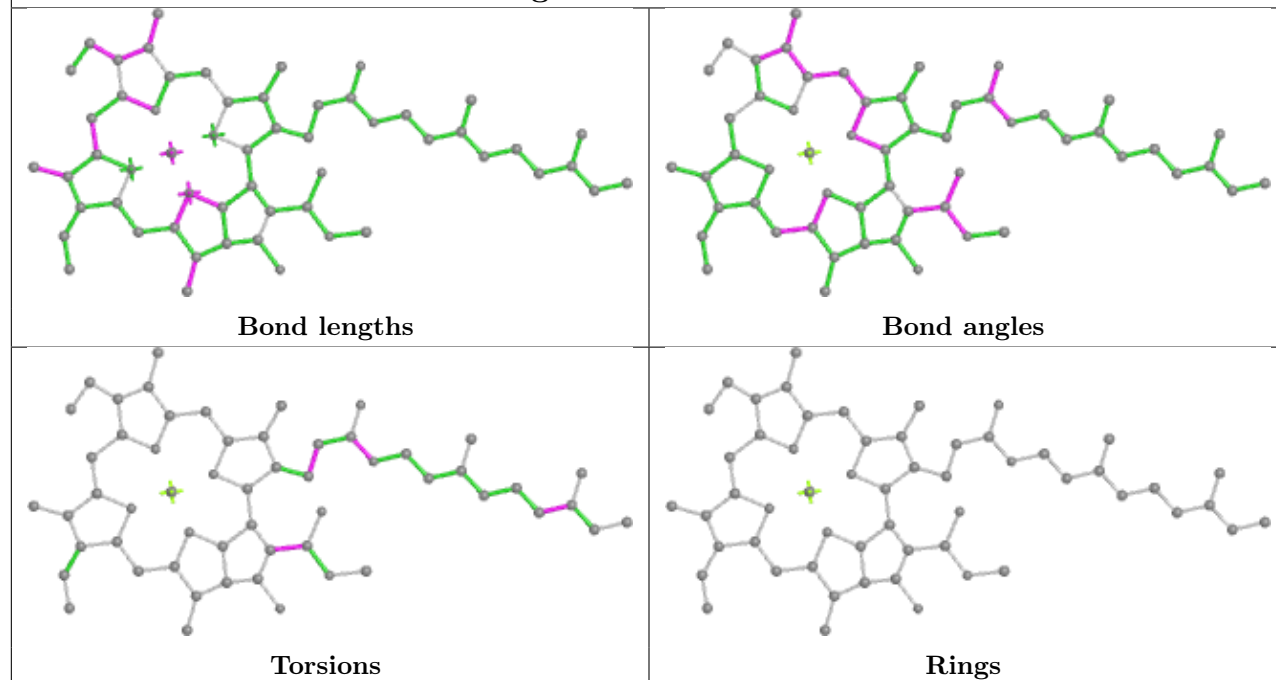


Rings

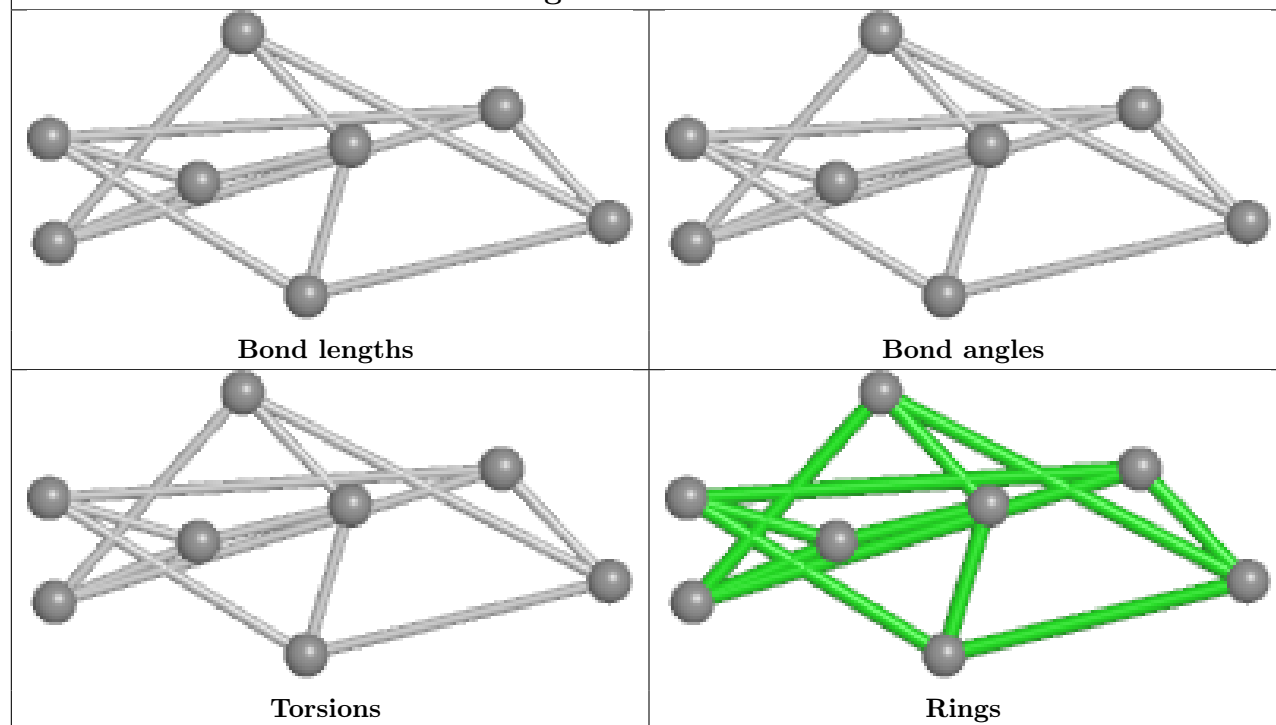
Ligand CLA a 819**Ligand CLA b 842****Ligand CLA a 802**



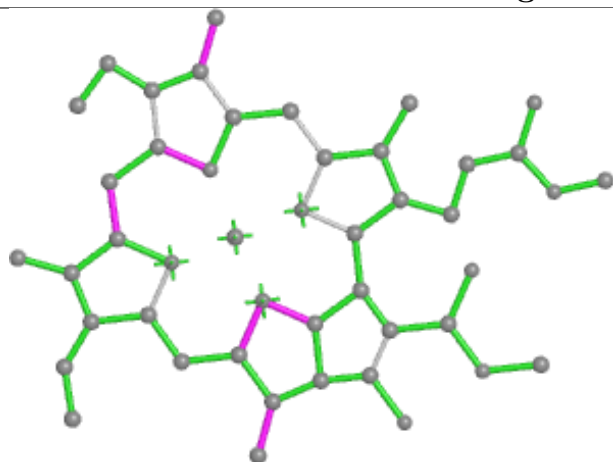
Ligand CLA D 210



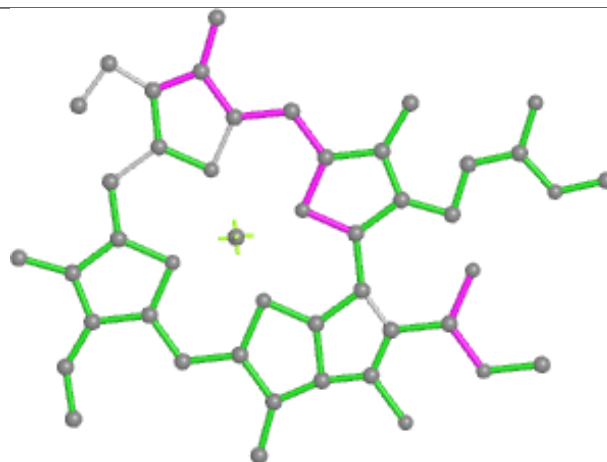
Ligand SF4 c 101



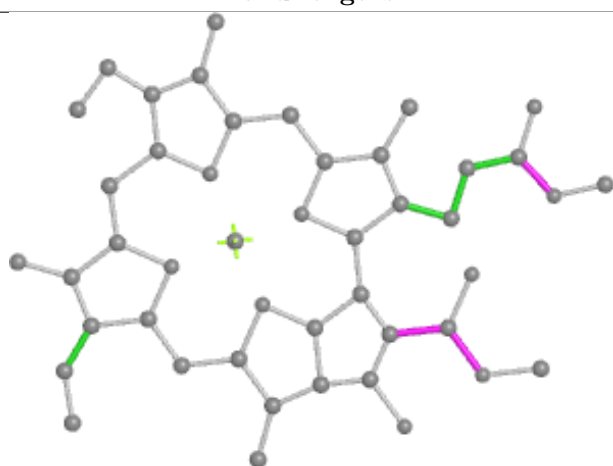
Ligand CLA b 815



Bond lengths



Bond angles

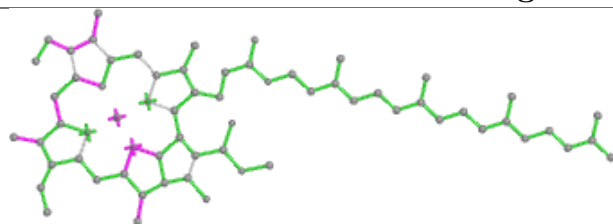


Torsions

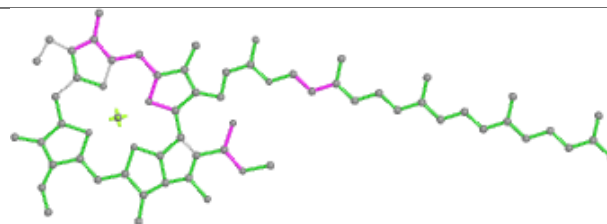


Rings

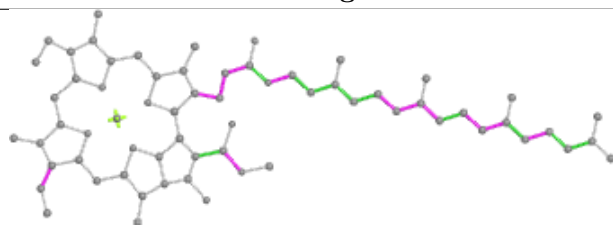
Ligand CLA b 824



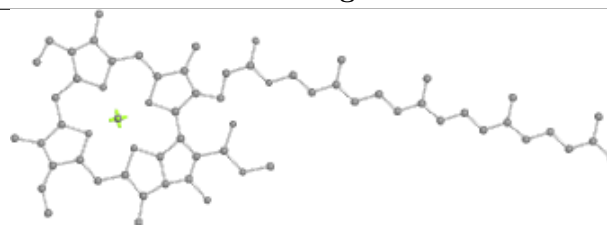
Bond lengths



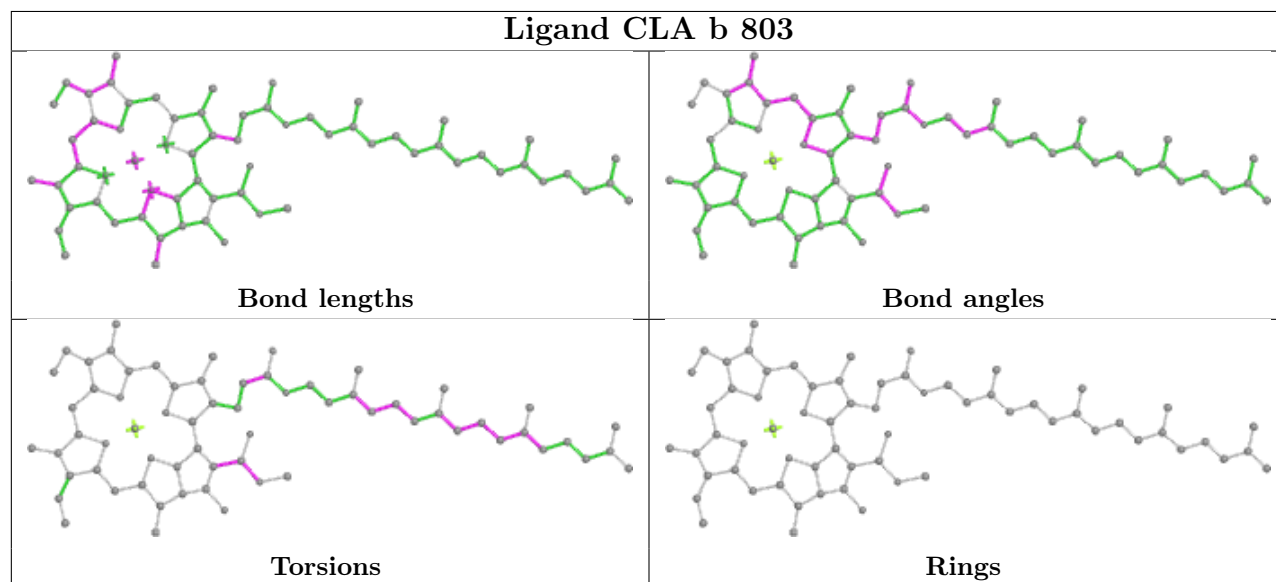
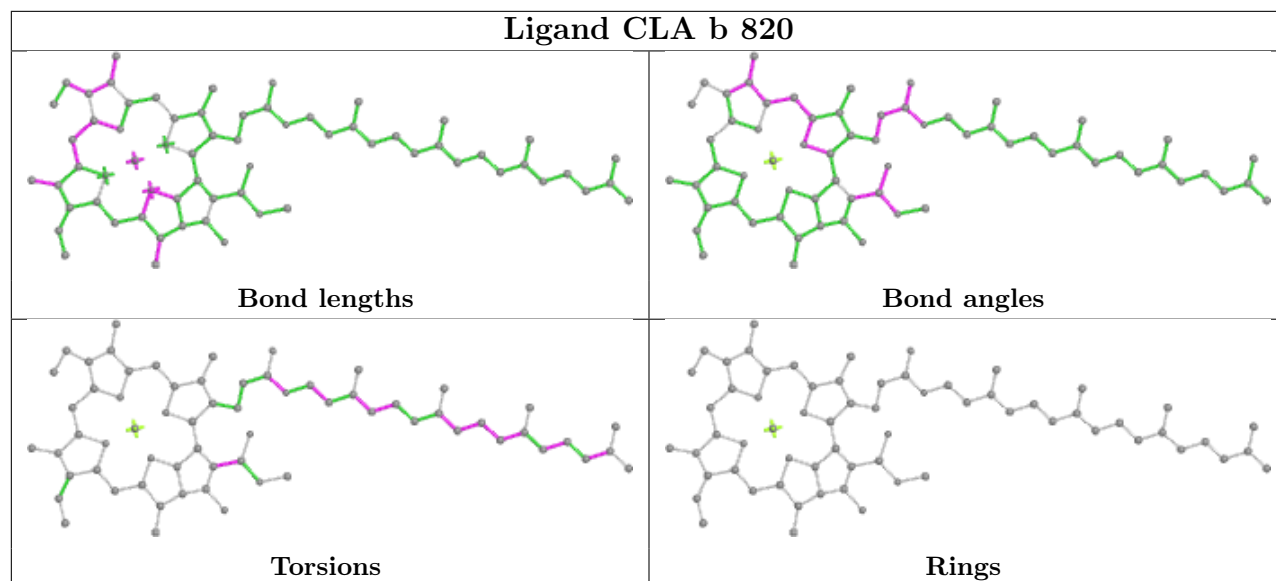
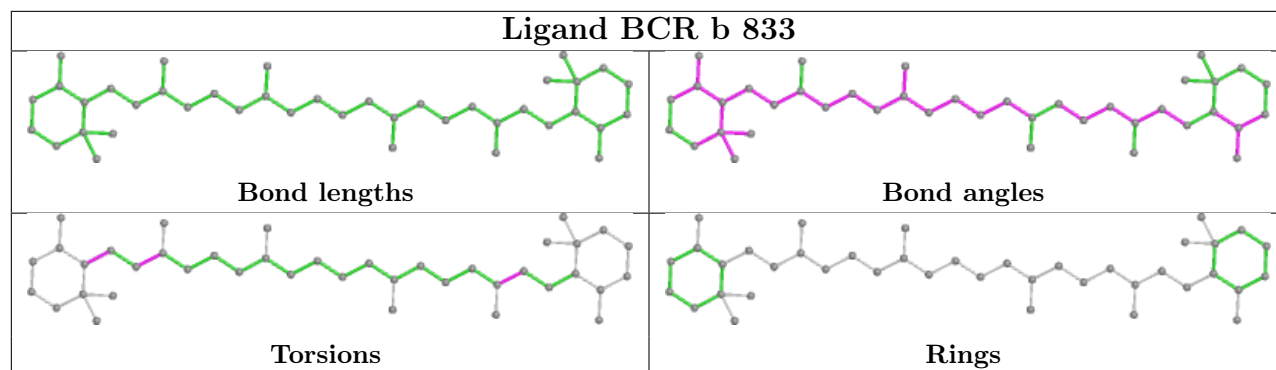
Bond angles

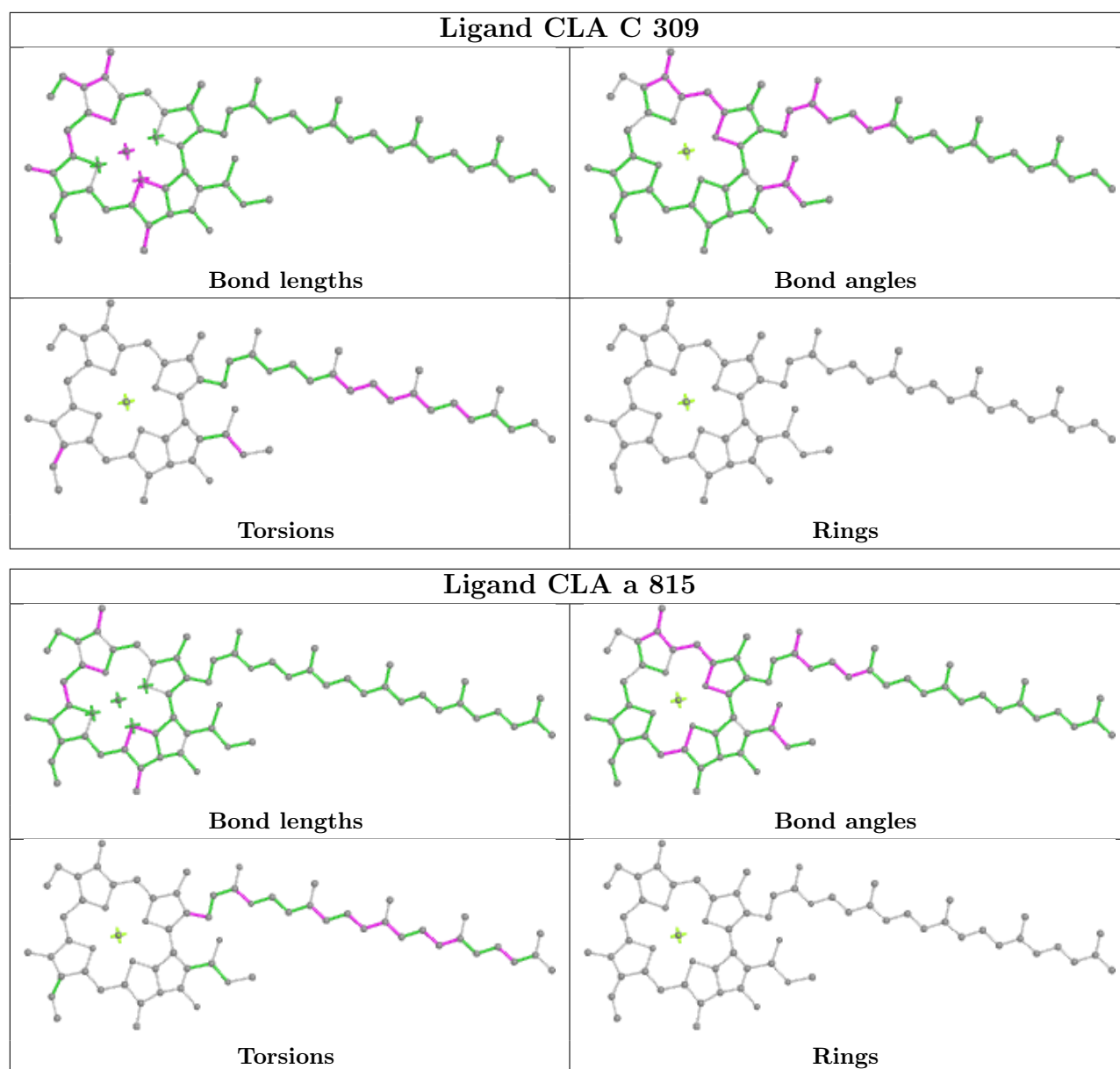


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

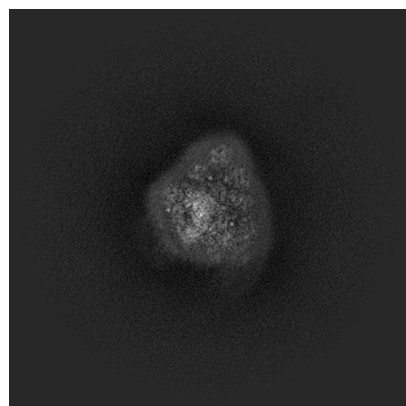
6 Map visualisation [i](#)

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

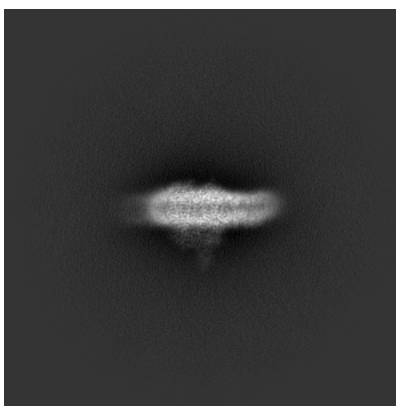
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

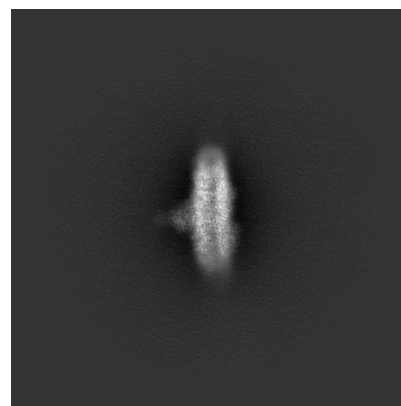
6.1.1 Primary map



X

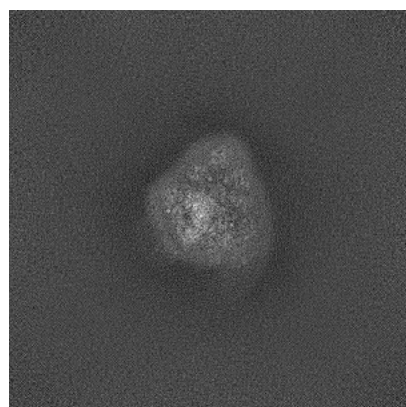


Y

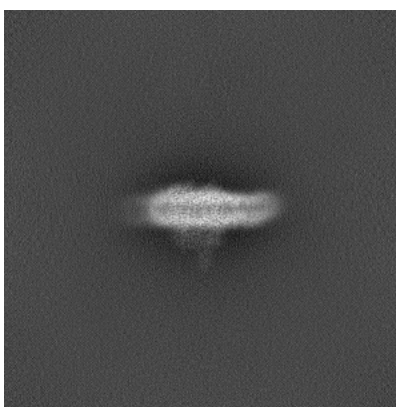


Z

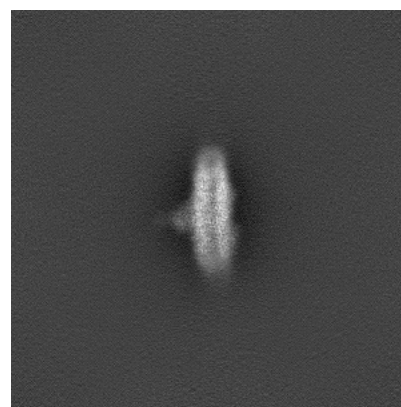
6.1.2 Raw map



X



Y

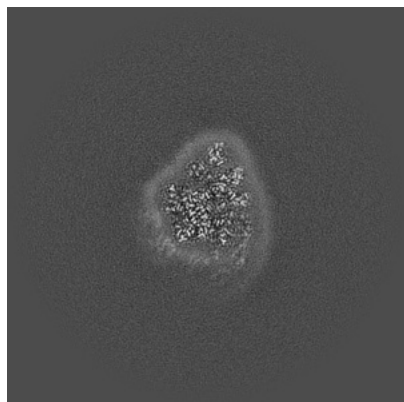


Z

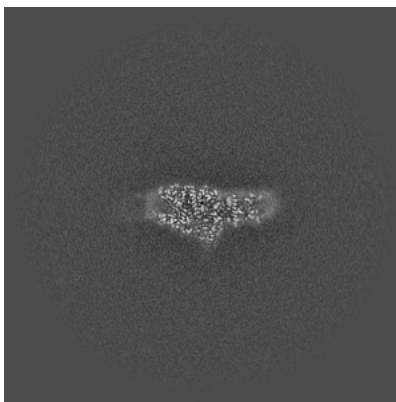
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

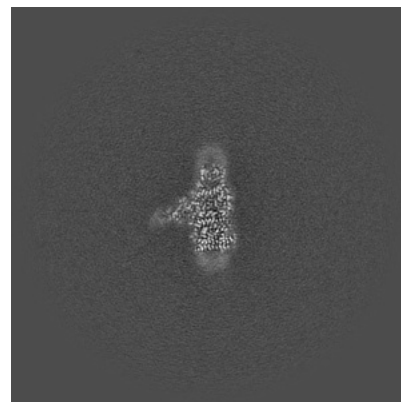
6.2.1 Primary map



X Index: 256

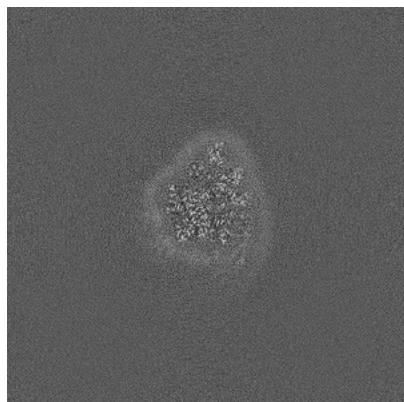


Y Index: 256

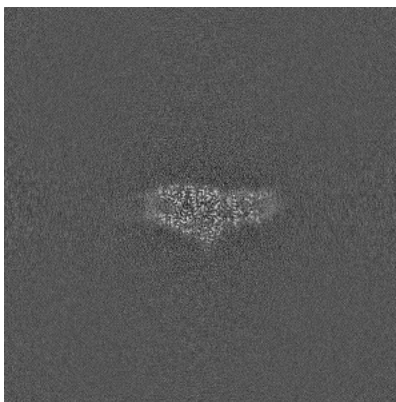


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

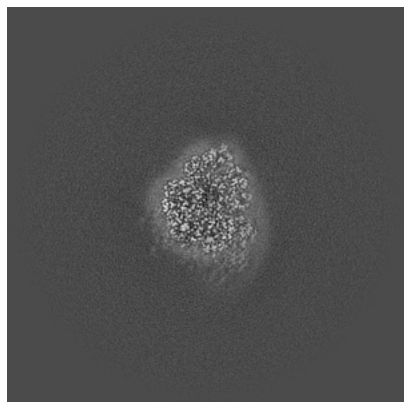


Z Index: 256

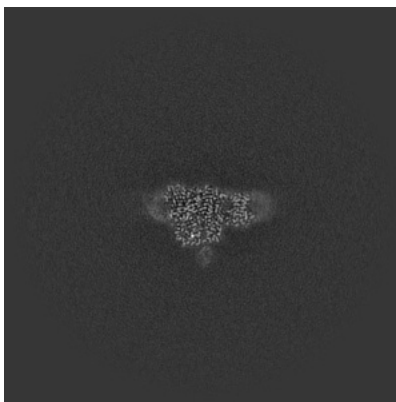
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

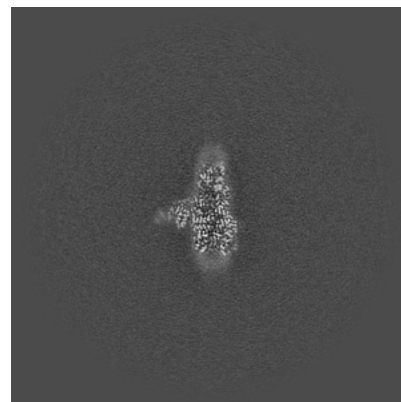
6.3.1 Primary map



X Index: 244

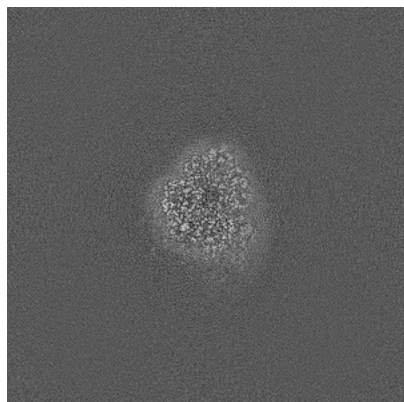


Y Index: 240

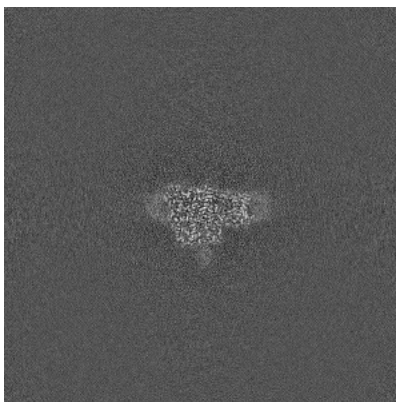


Z Index: 262

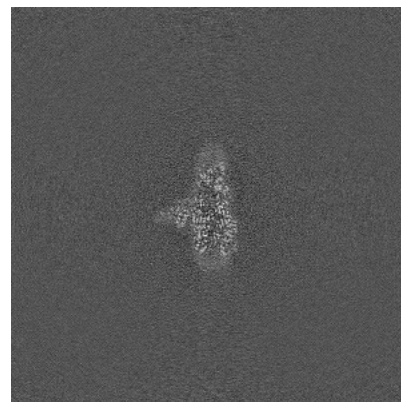
6.3.2 Raw map



X Index: 244



Y Index: 239

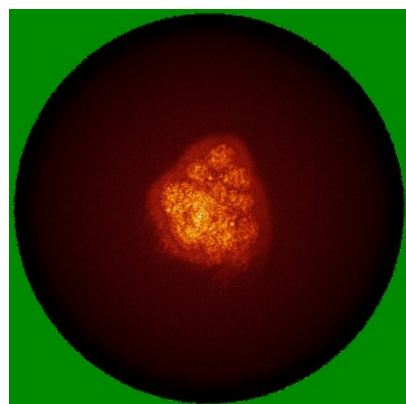


Z Index: 262

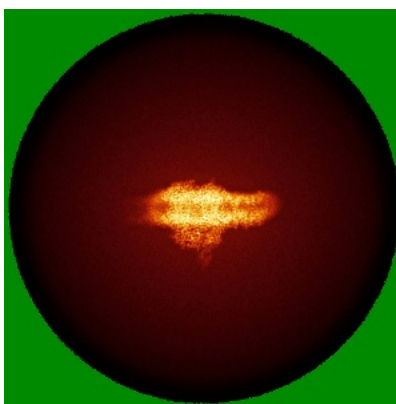
The images above show the largest variance slices of the map in three orthogonal directions.

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

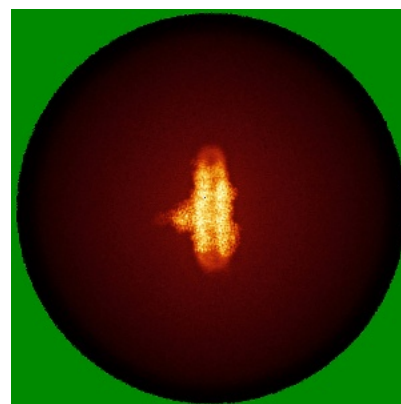
6.4.1 Primary map



X

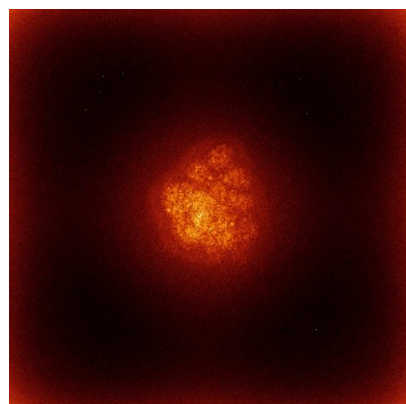


Y

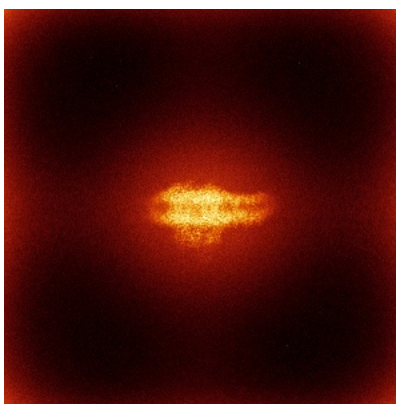


Z

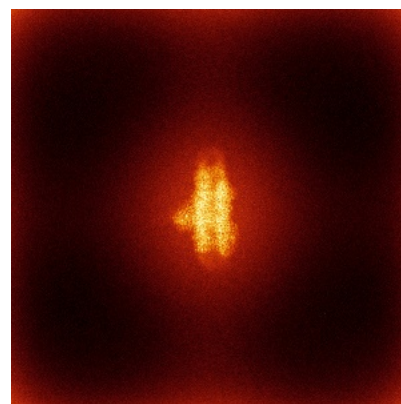
6.4.2 Raw map



X



Y

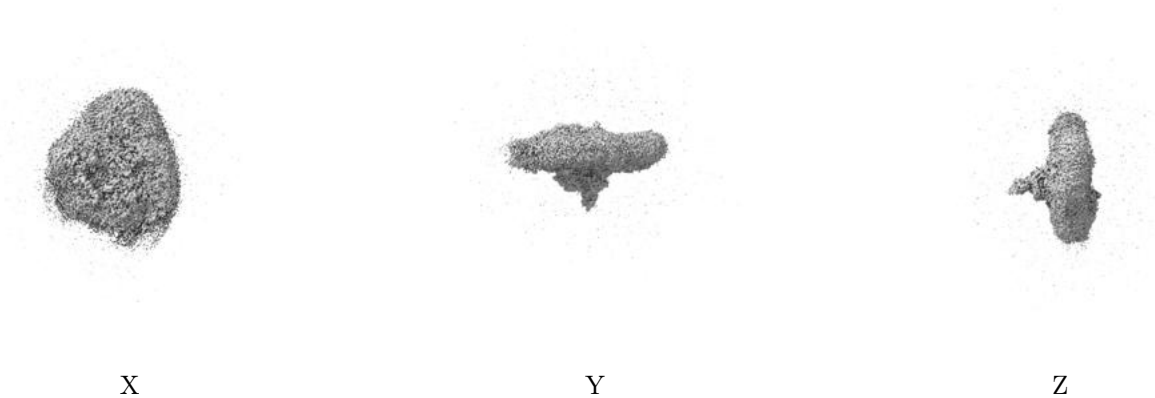


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

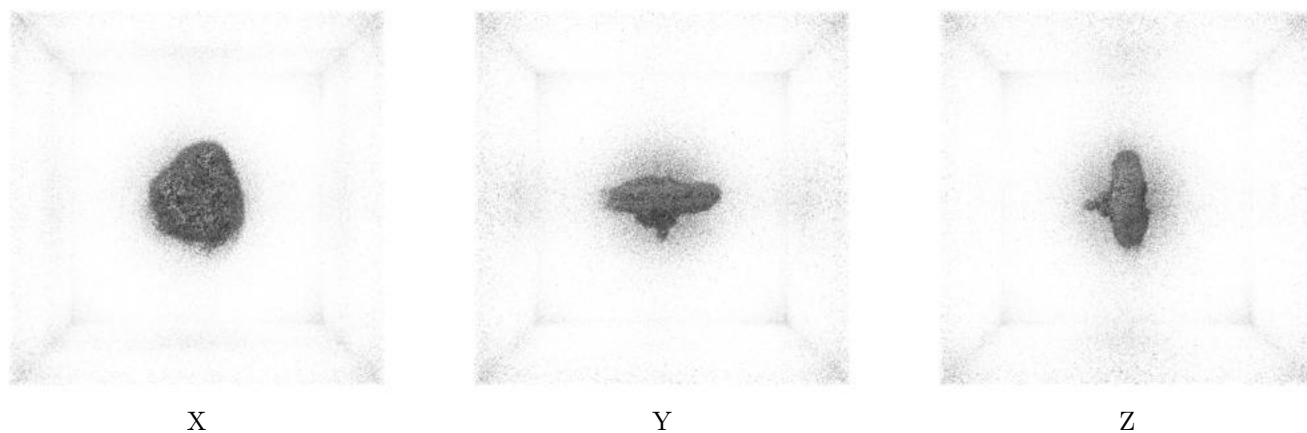
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

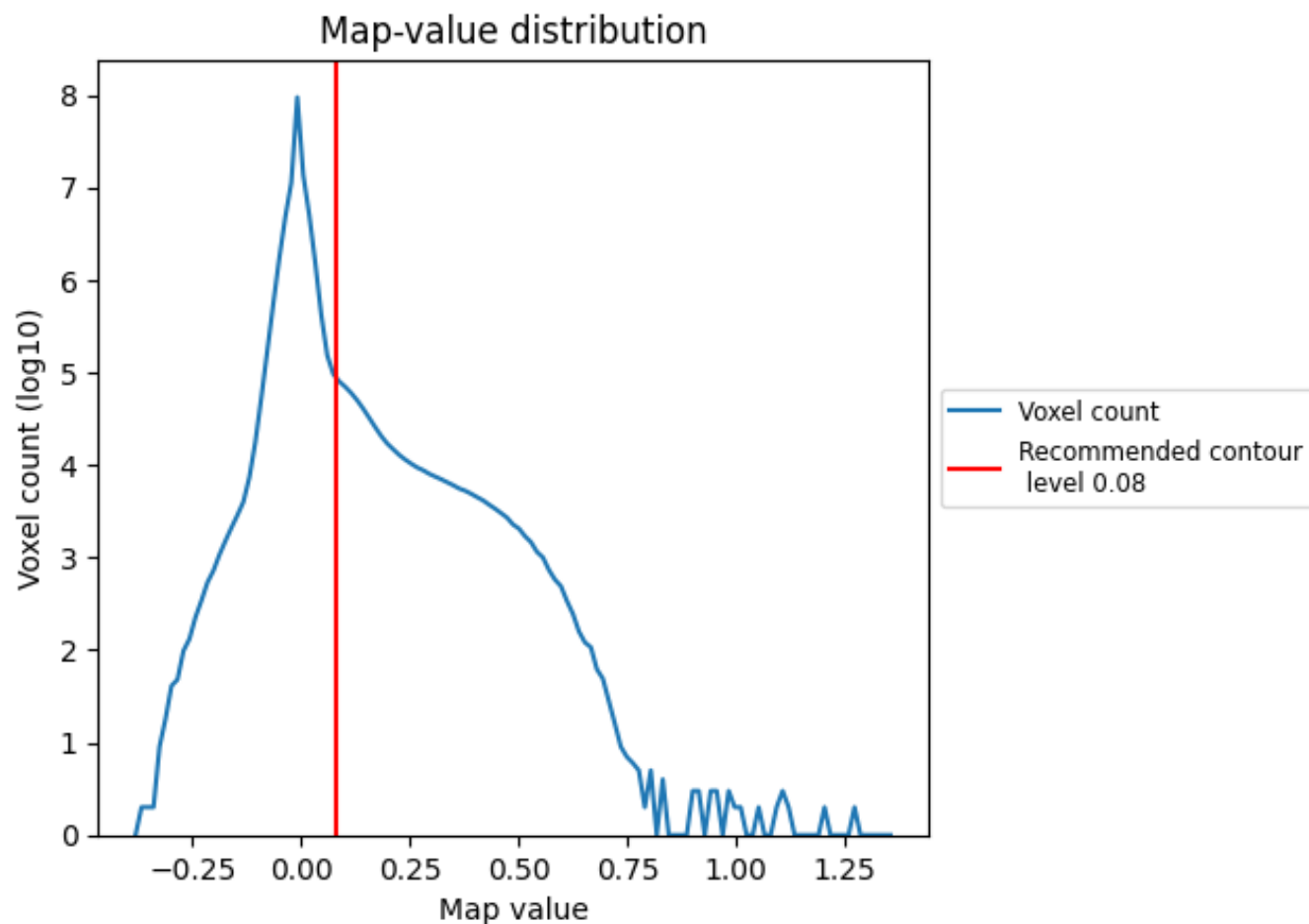
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

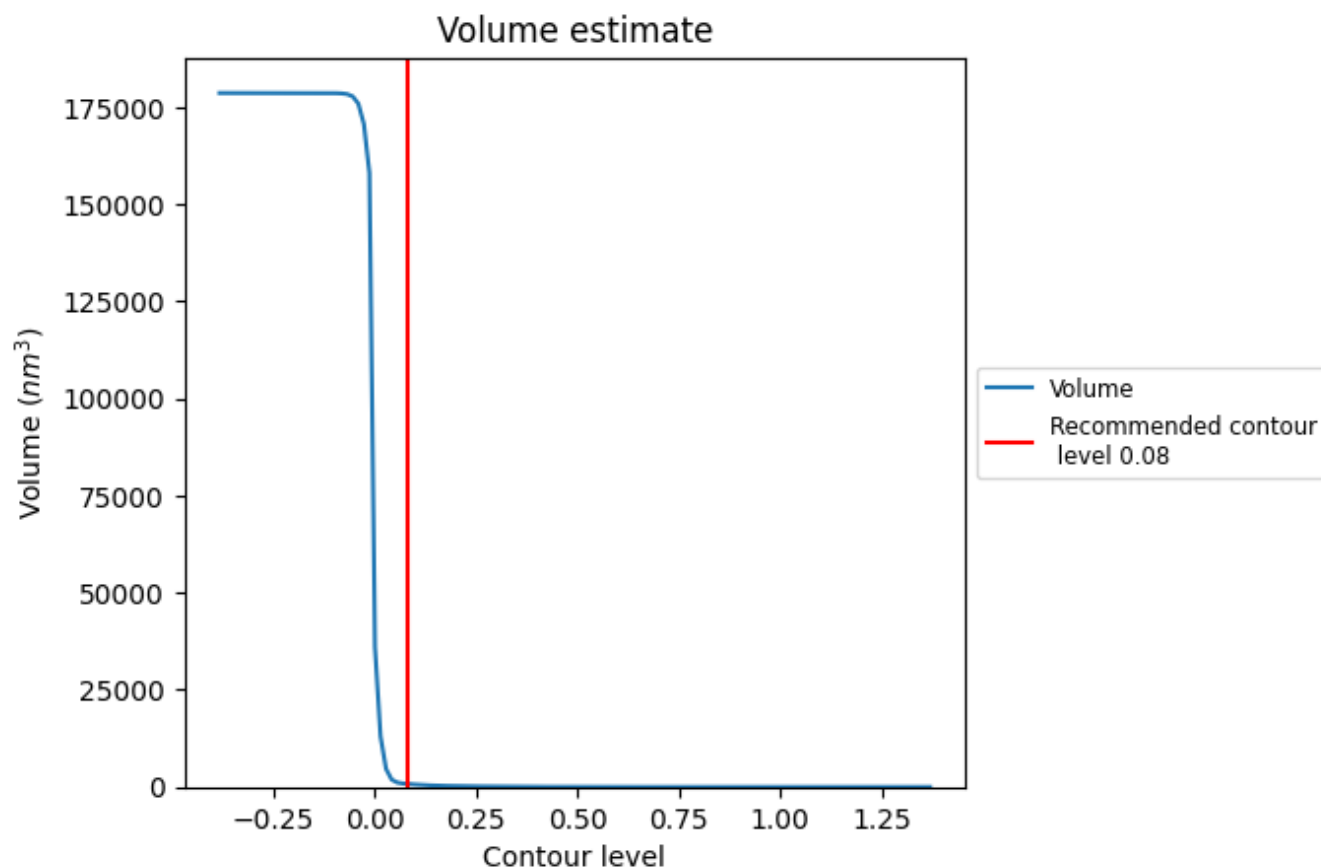
This section contains the results of statistical analysis of the map.

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.

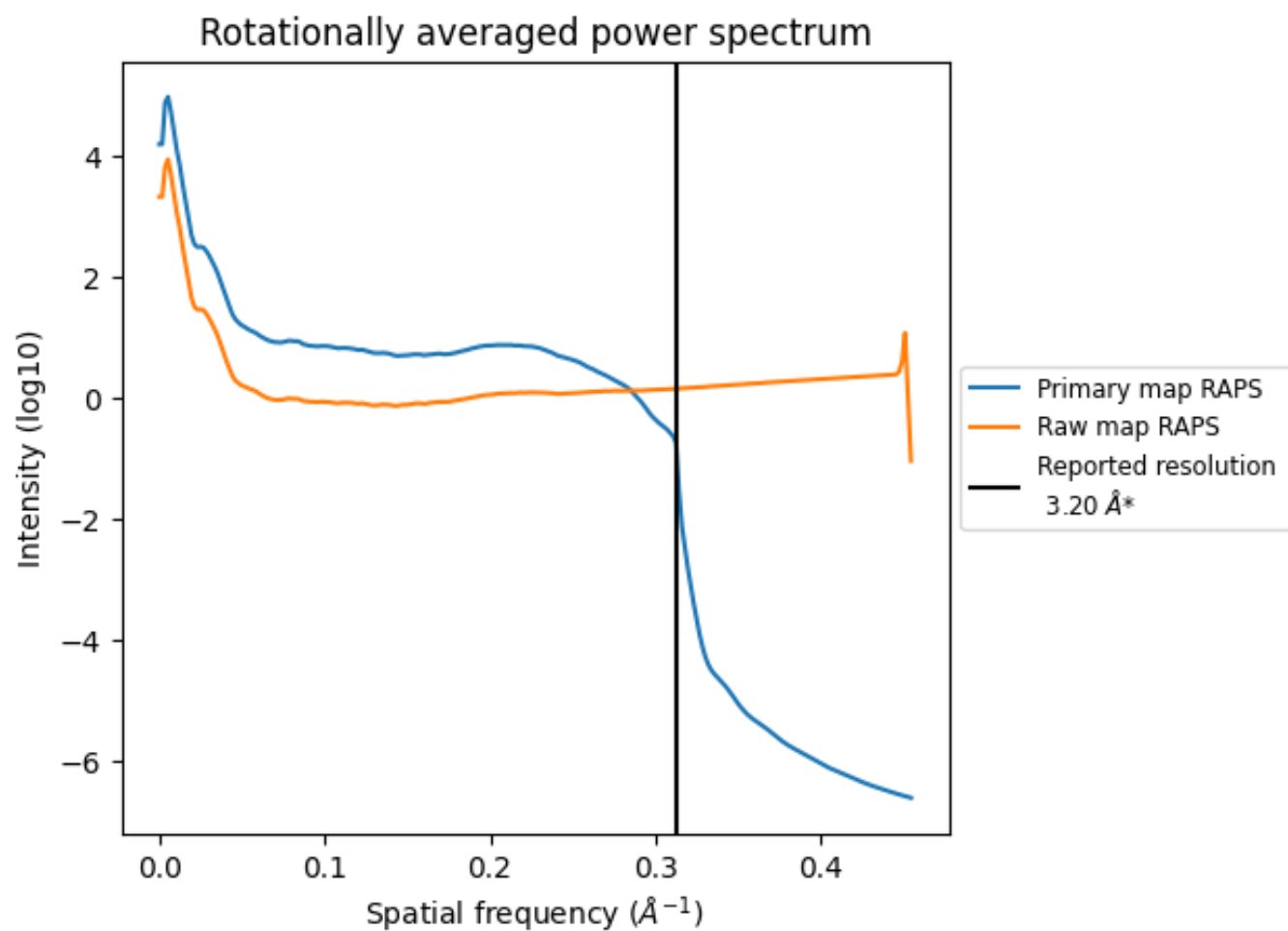
7.2 Volume estimate [i](#)



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 ⓘ

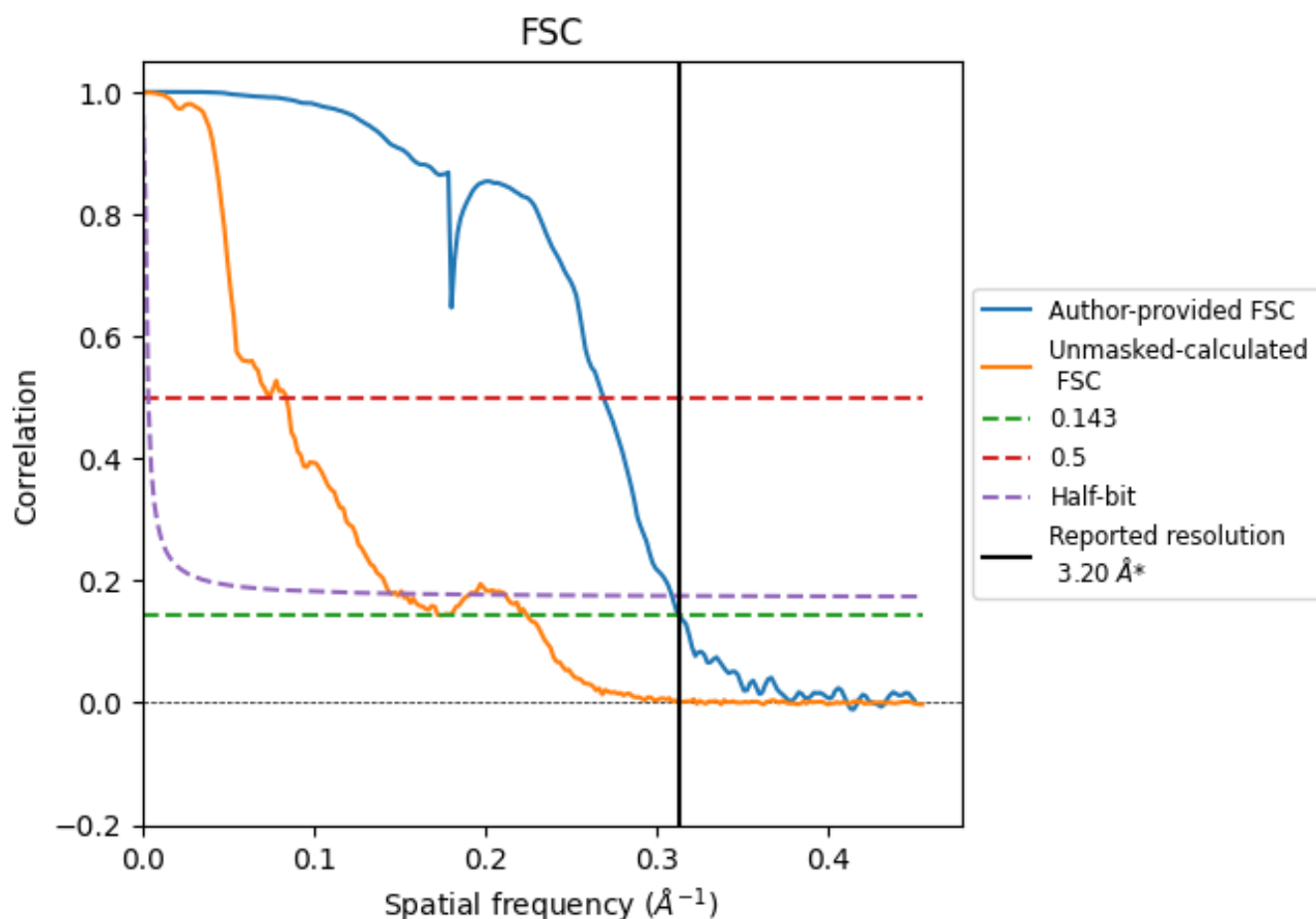


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

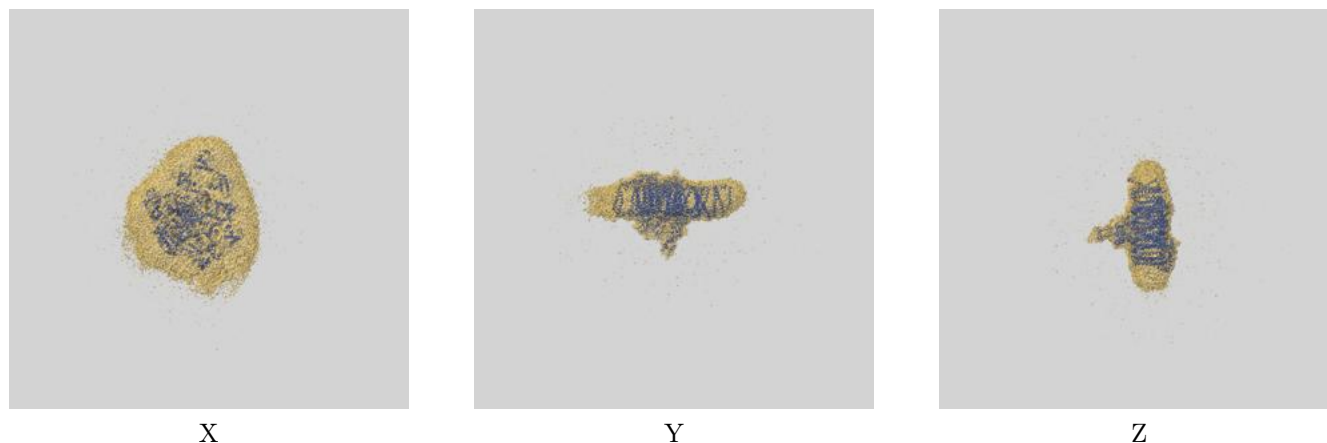
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.72	3.24
Unmasked-calculated*	5.75	11.93	6.88

*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](#)

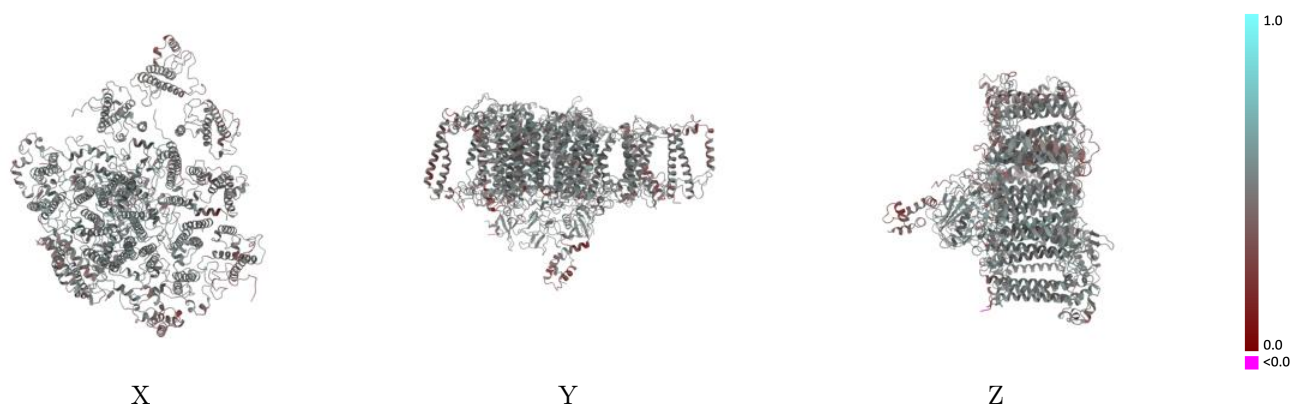
This section contains information regarding the fit between EMDB map EMD-60044 and PDB model 8ZET. Per-residue inclusion information can be found in [section 3](#) on [page 26](#).

9.1 Map-model overlay [i](#)



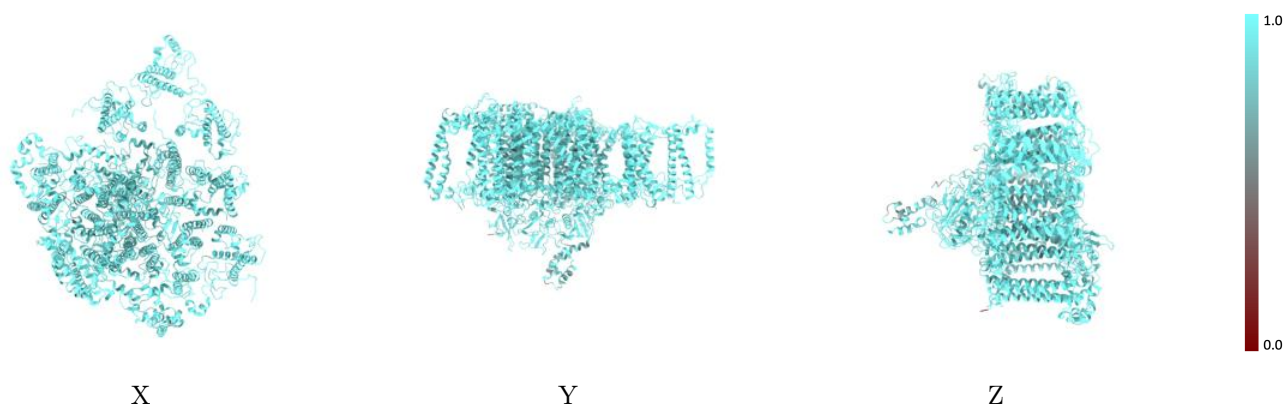
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



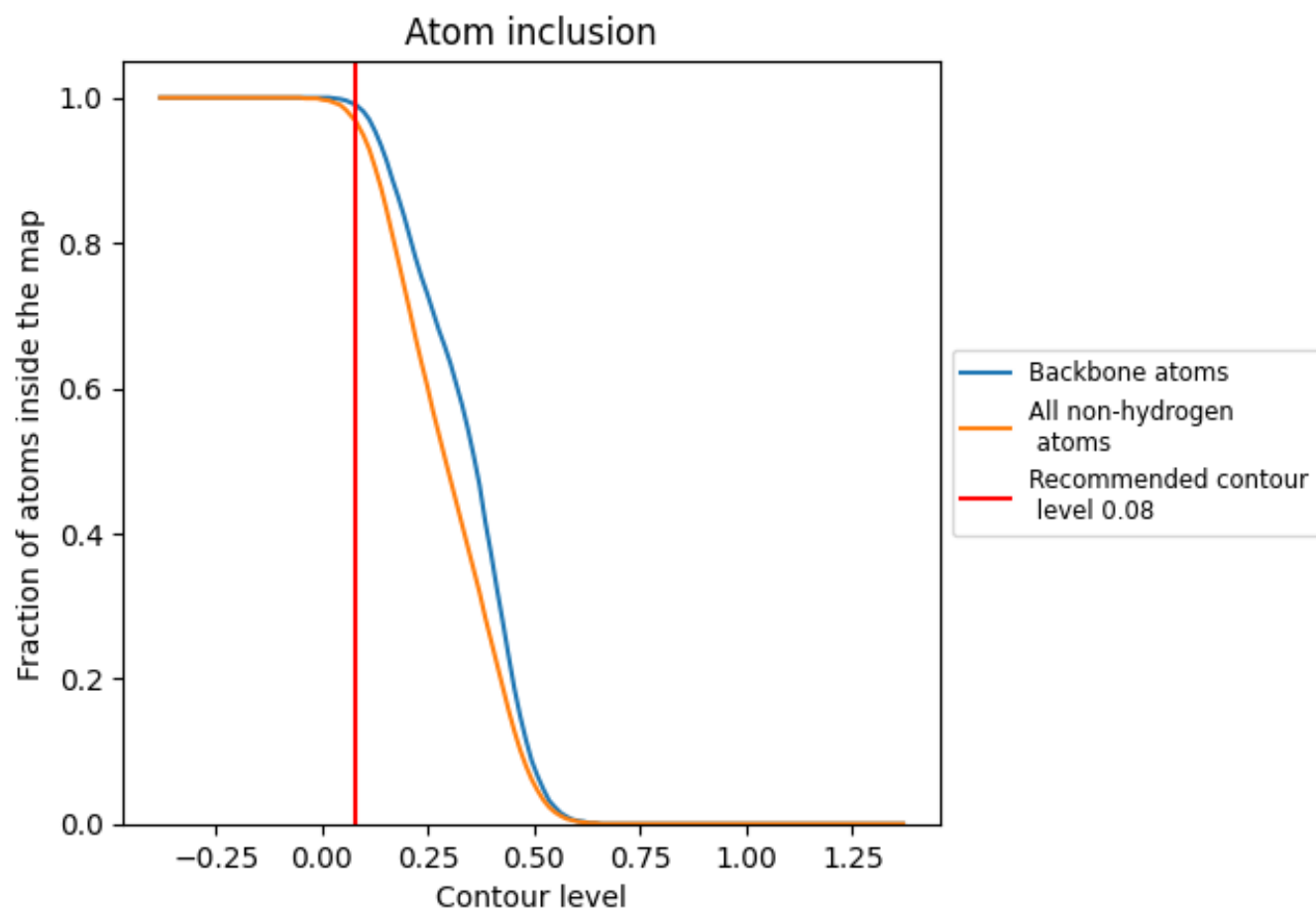
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div><div></div></div> 0.9670	<div><div></div></div> 0.4850
B	<div><div></div></div> 0.9740	<div><div></div></div> 0.4570
C	<div><div></div></div> 0.9780	<div><div></div></div> 0.4520
D	<div><div></div></div> 0.9670	<div><div></div></div> 0.4720
E	<div><div></div></div> 0.9700	<div><div></div></div> 0.4710
H	<div><div></div></div> 0.9600	<div><div></div></div> 0.4360
a	<div><div></div></div> 0.9740	<div><div></div></div> 0.5120
b	<div><div></div></div> 0.9690	<div><div></div></div> 0.5060
c	<div><div></div></div> 0.9880	<div><div></div></div> 0.5100
d	<div><div></div></div> 0.9790	<div><div></div></div> 0.5070
e	<div><div></div></div> 0.9510	<div><div></div></div> 0.4720
f	<div><div></div></div> 0.9650	<div><div></div></div> 0.4760
g	<div><div></div></div> 0.8680	<div><div></div></div> 0.4000
i	<div><div></div></div> 0.9640	<div><div></div></div> 0.5130
j	<div><div></div></div> 0.9490	<div><div></div></div> 0.4710
l	<div><div></div></div> 0.9770	<div><div></div></div> 0.5060
m	<div><div></div></div> 0.9440	<div><div></div></div> 0.4770
r	<div><div></div></div> 0.9330	<div><div></div></div> 0.3970

